Supplementary Information

for

Calculation-Assisted Regioselective Functionalization of the Imidazo[1,2-*a*]pyrazine Scaffold *via* Zinc and Magnesium Organometallic Intermediates

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General information

All reactions were carried out under an argon atmosphere in flame-dried glassware. Syringes which were used to transfer anhydrous solvents or reagents were purged with argon prior to use. Yields refer to isolated yields of compounds estimated to be >95% pure as determined by ^{1}H-NMR (25 °C) and capillary GC. All reagents were obtained from commercial sources and used without further purification unless otherwise stated. Reaction mixtures were cooled using an acetone / dry ice bath. The suspension formed during the work-up of reactions containing CuCN·2LiCl was dissolved by adding appropriate amounts of concentrated aqueous ammonia solution.

Solvents

CH_2Cl_2 was predried over P_2O_5 and distilled under nitrogen atmosphere.

THF was continuously refluxed and freshly distilled from sodium benzophenone ketyl under nitrogen and stored over molecular sieves.

All other solvents were purchased from chemical suppliers (*Merck*, *Acros Organics*) and used without further purification. Solvents for reaction workups and column chromatography were distilled prior to use.

Reagents

***n*BuLi** solutions in hexane were purchased from Albemarle or Sigma Aldrich and the concentration was determined by titration against *N*-benzylbenzamide in THF at –40 °C.[1]

TMPH was purchased from Albemarle (Frankfurt, Germany), freshly distilled over CaH_2 and stored under argon.

CuCN·2LiCl solution (1.00 M in THF) was prepared by drying CuCN (8.96 g, 100 mmol, 1.00 equiv) and LiCl (8.48 g, 200 mmol, 2.00 equiv) in a *Schlenk*-flask under vacuum for 5 h at 150 °C. After cooling to 25 °C, dry THF (100 mL) was added and the resulting mixture was stirred until the salts were dissolved.

[1] A. F. Burchat, J. M. Chong, N. Nielsen, *J. Organomet. Chem.* **1997**, *542*, 281-283.

$ZnCl_2$ solution (1.00 M in THF) was prepared by drying $ZnCl_2$ (27.3 g, 200 mmol) in a *Schlenk*-flask under vacuum for 5 h at 150 °C. After cooling to 25 °C, dry THF (200 mL) was added and the resulting mixture was stirred until the salts were dissolved.

***i*PrMgCl·LiCl**[2] in THF was purchased from Albemarle and used after titration against iodine (0.5 M solution in THF at 25 °C).[3] The reagent can also be prepared by flame drying magnesium turnings (24 g, 1.0 mol, 2.0 equiv) and anhydrous LiCl (25 g, 0.60 mol, 1.2 equiv) in a *Schlenk*-flask under vacuum at 450 °C. After the addition of anhydrous THF (500 mL), *i*PrCl (39 g, 0.50 mol, 1.0 equiv) was added dropwise at 25 °C using a dropping funnel until the reaction started. Then the reaction mixture was cooled to 0 °C and the addition was continued overnight while allowing the flask to warm up to 25 °C. The remaining solids were filtered off and the *i*PrMgCl·LiCl solution was titrated with iodine.

Chromatography

Flash column chromatographical purifications were performed using SiO_2 60 (0.040–0.063 mm, 230–400 mesh ASTM) or Florisil® PR grade (149-250 µm, 60-100 mesh) from Merck. Thin layer chromatography (TLC) was performed using aluminium plates covered with SiO_2 (Merck 60, F–254). Spots were visualized by UV light irradiation and/or by staining of the TLC plate with one of the reagents below, followed by heating with a heat gun if necessary.

- $KMnO_4$ (0.3 g), K_2CO_3 (20 g) and KOH (0.3 g) in water (300 mL).
- Neat iodine absorbed on silica gel (no heating required).

Preparative HPLC

For purification, an *Agilent Technologies* 1260 Infinity HPLC-System was used, consisting of two prep-pumps (acetonitrile/water, no additives), a MWD-detector (210 nm wavelength, 40 nm bandwidth, ref-wavelength 400 nm, ref-bandwidth 100 nm) and a fraction collector. Three different columns were used: 1) *Kinetix* EVO C18 5 µm column (length: 150 mm, diameter: 10 mm), 2) *Kinetix* EVO C18 5 µm column (length: 150 mm, diameter: 21.2 mm) and 3) *Waters* XBridge Prep C8 5 µm column (length: 150 mm, diameter: 30 mm).

Analytical data

NMR spectra were recorded on *Bruker* ARX 200, AC 300, WH 400 or AMX 600 instruments. Chemical shifts are reported as δ-values in ppm relative to the deuterated solvent peak: $CDCl_3$ (δ_H: 7.26; δ_C: 77.16). For the observation of the observed signal multiplicities, the following

[2] A. Krasovskiy, P. Knochel, *Angew. Chem. Int. Ed.* **2004**, *43*, 3333-3336.
[3] A. Krasovskiy, P. Knochel, *Synthesis* **2006**, 890-891.

abbreviations and combinations thereof were used: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), sext (sextet), sept (septet), m (multiplet) and br (broad). If not otherwise noted, the coupling constants given are either H-H or H-F coupling constants for proton signals and C-F coupling constants for carbon signals.

Melting points are uncorrected and were measured on a *Büchi* B.540 apparatus.

Infrared spectra were recorded from 4000-400 cm^{-1} on a *Perkin Elmer* Spectrum BX-59343 instrument. For detection a Smiths Detection DuraSampl IR II Diamond ATR sensor was used. The main absorption peaks are reported in cm^{-1}.

Gas chromatographical analysis (GC) was performed with instruments of the type Hewlett-Packard 6890 or 5890 Series II, using a column of the type HP 5 (Hewlett-Packard, 5% phenylmethylpolysiloxane; length: 10 m, diameter: 0.25 mm, film thickness 0.25 µm). The detection was accomplished using a flame ionization detector. Mass spectra (MS) and high resolution mass spectra (HRMS) were recorded on a *Finnigan* MAT 95Q or *Finnigan* MAT 90 instrument for electron impact ionization (EI). For the combination of gas chromatography with mass spectroscopic detection, a GC–MS of the type *Hewlett-Packard* 6890/MSD 5793 networking was used (column: HP 5–MS, Hewlett–Packard; 5% phenylmethylpolysiloxane; length: 15 m, diameter: 0.25 mm, film thickness: 0.25 µm).

TMPMgCl·LiCl (11)[4]

TMPH (14.8 g, 105 mmol, 1.05 equiv) was slowly added to a solution of *i*PrMgCl·LiCl in dry THF (1.05 M, 95 mL, 1.0 equiv). The resulting mixture was stirred under argon at 25 °C for 24 h before titrating the base against benzoic acid using 4-(phenylazo)-diphenylamine as an indicator.

$TMP_2Zn·2MgCl_2·2LiCl$ (12)[5]

$ZnCl_2$ (1.0 M, 2.5 mL, 0.5 equiv) was slowly added to a solution of TMPMgCl·LiCl in dry THF (0.91 M, 5.49 mL, 1.0 equiv). The resulting mixture was stirred under argon at 25 °C for 30 min before titrating the base against benzoic acid using 4-(phenylazo)-diphenylamine as an indicator.

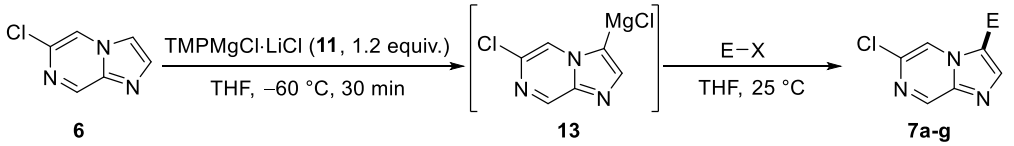
[4] A. Krasovskiy,V. Krasovskaya, P. Knochel, *Angew. Chem. Int. Ed*. **2006**, *45*, 2958-2961
[5] S. H. Wunderlich, P. Knochel, *Angew. Chem. Int. Ed*. **2007**, *46*, 7685-7688.

TMPLi (19)

A dry and argon flushed Schenk-flask, equipped with a magnetic stirring bar, was charged with TMPH (1.3 mL, 10.0 mmol, 1.0 equiv) and dry THF (10 mL). The reaction mixture was cooled to −40 °C and *n*-BuLi (1.6 M, 6.3 mL, 10 mmol, 1.0 equiv) was added dropwise. The reaction mixture was stirred at −40 °C for 30 min until a milky white solution was formed. The concentration was determined by titration of an aliquot with benzoic acid.

Typical procedures

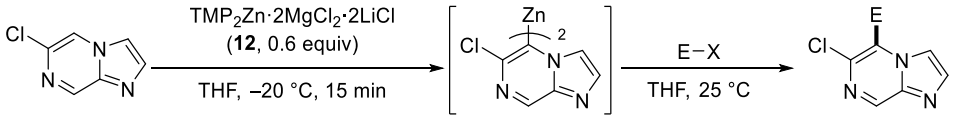
TP1: Typical procedure for the metalation of 6-chloroimidazo[1,2-*a*]pyrazine in position 3 using TMPMgCl·LiCl



6 **13** **7a-g**

Freshly prepared TMPMgCl·LiCl (**11**, 1.2 equiv.) was added dropwise to a cooled (−60 °C) solution of 6-chloroimidazo[1,2-*a*]pyrazine (**6**, 30.7 mg, 0.2 mmol,1.0 equiv) in dry THF (1 mL) and stirred for 30 min. Subsequently, the electrophile (1.5 equiv) was added, the cooling bath removed, and the temperature was allowed to rise to room temperature. The reaction mixture was continued stirring at room temperature, was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 20 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel (stationary phase) and the appropriate solvent mixture *i*-hexane/EtOAc.

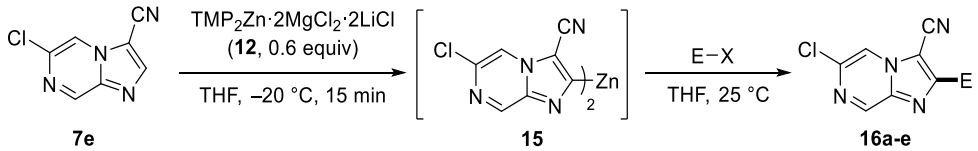
TP2: Typical procedure for the metalation of 6-chloroimidazo[1,2-*a*]pyrazine in position 5 using $(TMP)_2Zn·2MgCl_2·2LiCl$



6 **14** **8a-f**

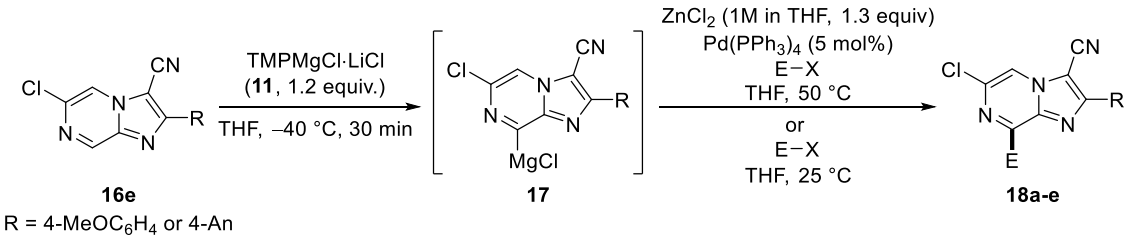
Freshly prepared $TMP_2Zn·2MgCl_2·2LiCl$ (**12**, 0.6 equiv, 0.12 mmol) was added dropwise to a cooled (−20 °C) solution of 6-chloroimidazo[1,2-*a*]pyrazine (**6**, 1.0 equiv, 0.2 mmol) in dry THF (1 mL) and stirred for 15 min. Subsequently, the electrophile (1.5 equiv) was added, the cooling bath was removed, and the temperature was allowed to rise to room temperature. The reaction mixture was continued stirring at room temperature, was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 20 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel (stationary phase) and the appropriate solvent mixture *i*-hexane/EtOAc.

TP3: Typical procedure for the second metalation in position 2 using $TMP_2Zn{\cdot}2MgCl_2{\cdot}2LiCl$



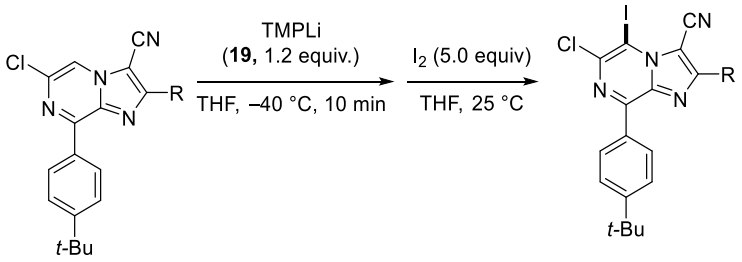
Freshly prepared $TMP_2Zn{\cdot}2MgCl_2{\cdot}2LiCl$ (**12**, 0.6 equiv, 0.12 mmol) was added dropwise to a cooled (−20 °C) solution of 6-chloroimidazo[1,2-*a*]pyrazine-3-carbonitrile (**7e**, 35.7 mg, 0.2 mmol, 1.0 equiv) in dry THF (1 mL) and stirred for 15 min. Subsequently, the electrophile (1.5 equiv) was added, the cooling bath was removed, and the temperature was allowed to rise to room temperature. The reaction mixture was continued stirring at room temperature, was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 20 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel (stationary phase) and the appropriate solvent mixture *i*-hexane/EtOAc.

TP4: Typical procedure for the third metalation in position 8 using TMPMgCl·LiCl



Freshly prepared TMPMgCl·LiCl (**11**, 0.24 mmol, 1.2 equiv) was added dropwise to a cooled (−40 °C) solution of 6-chloro-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (**16e**, 56.9 mg, 0.2 mmol, 1.0 equiv) in dry THF (2 mL) and stirred for 30 min. Subsequently the electrophile (1.5 equiv) was added, the cooling bath was removed, and the temperature was allowed to rise to room temperature. The reaction mixture was continued stirring at room temperature. In case, $ZnCl_2$ solution (1 M, 1.3 equiv) was added and the reaction mixture was stirred for additional 15 min at the same temperature (−40 °C) for transmetalation. The obtained zinc reagent was subsequently added dropwise into a separate reaction flask containing the catalyst (5 mol%) and electrophile (0.8 equiv) and stirred for 2 h at 50 °C. The reaction mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 20 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel (stationary phase) and the appropriate solvent mixture *i*-hexane/EtOAc.

TP5: Typical procedure for the fourth metalation in position 5 using TMPLi

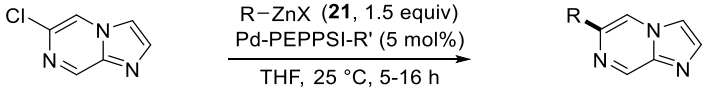


18e
R = 4-MeOC$_6$H$_4$ or 4-An

20

Freshly prepared TMPLi (**19**, 1.2 equiv, 0.12 mmol) was added dropwise to a cooled (−40 °C) solution of 8-(4-(*tert*-butyl)phenyl)-6-chloro-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile **18e** (41.6 mg, 0.1 mmol, 1 equiv) in dry THF (1 mL) and stirred for 10 min. Subsequently, iodine (127 mg, 0.5 mmol, 5.0 equiv) was added, and stirring continued for 5 min at the same temperature followed by additional 10 min at room temperature. Then, the mixture was quenched with saturated aqueous $Na_2S_2O_3$ solution and extracted with EtOAc (3 x 20 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel (stationary phase) and the appropriate solvent mixture *i*-hexane/EtOAc.

TP6: Typical procedure for the Pd-catalyzed cross-coupling of 6 with organozinc reagents



6 **22a-e**

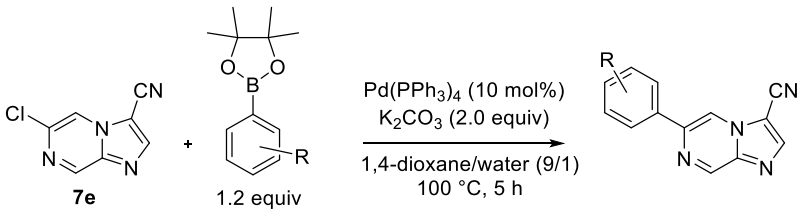
X = Cl·MgICl·LiCl, Cl·MgBrCl·LiCl or Cl·MgCl$_2$·LiCl; R = Alk, Ar, Bz; R' = *i*Pr or *i*Pent

A solution of a zinc reagent of type **21**[6] (in THF, 0.75 mmol, 1.5 equiv) was added dropwise to a solution of 6-chloroimidazo[1,2-*a*]pyrazine (**6**, 76.8 mg, 0.5 mmol,1.0 equiv) and Pd-PEPPSI-iPr (5 mol%, 17.0 mg) or Pd-PEPPSI-iPent (5 mol%, 19.8 mg) in THF (1.0 mL). The resulting reaction mixture was stirred at 25 °C for 5 h (in the case of Pd-PEPPSI-iPr) or at 25 °C for 16 h (in the case of Pd-PEPPSI-iPent) under argon. Then, the mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 15 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude

[6] a) A. Krasovskiy, P. Knochel, *Angew. Chem. Int. Ed.* **2004**, *43*, 3333-3336; *Angew. Chem.* **2004**, *116*, 3396-3399; b) A. Metzger, F. M. Piller, P. Knochel, *Chem. Commun.* **2008**, 5824-5826; c) V. Dhayalan, P. Knochel, *Synthesis* **2015**, 3246-3256; d) F. H. Lutter, L. Grokenberger, P. Spieß, J. M. Hammann, K. Karaghiosoff, P. Knochel, *Angew. Chem. Int. Ed.* **2020**, *59*, 5546-5550; *Angew. Chem.* **2020**, *132*, 5591-5595.

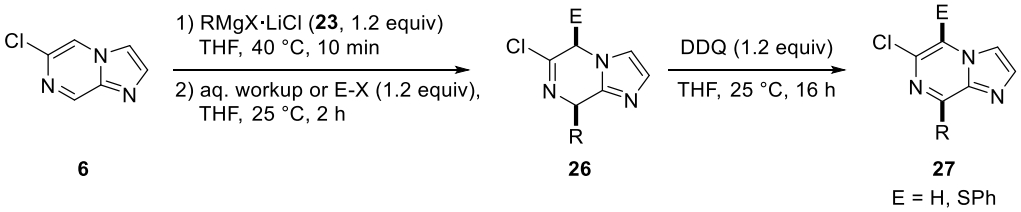
product was purified by flash chromatography using silica gel (stationary phase) and the appropriate solvent mixture *i*-hexane/EtOAc.

TP7: Typical procedure for the Suzuki–Miyaura cross coupling



A solution of 6-chloroimidazo[1,2-*a*]pyrazine-3-carbonitrile (**7e**, 71.4 mg, 0.4 mmol, 1.0 equiv), arylboronic acid pinacol ester (0.48 mmol, 1.2 equiv), $Pd(PPh_3)_4$ (46 mg, 0.04 mmol, 10 mol%) and K_2CO_3 (110 mg, 0.8 mmol, 2.0 equiv) in (1,4-dioxane/water (9/1), 1.3 mL) was purged with argon for 5 min. The resulting reaction mixture was stirred at 100 °C for 5 h in a closed system. Then, the mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 30 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel (stationary phase) and the appropriate solvent mixture *i*-hexane/EtOAc.

TP8: Typical procedure for the nucleophilic addition of Grignard reagents to 6

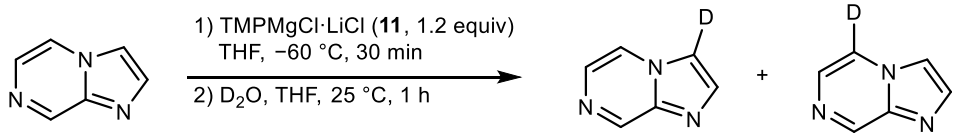


To a solution of 6-chloroimidazo[1,2-*a*]pyrazine (**6**, 76.8 mg, 0.5 mmol, 1.0 equiv) in THF (0.5 M) the corresponding organomagnesium reagent RMgX·LiCl (**23**, 1.2 equiv) was added at 40 °C. The mixture was stirred at 40 °C for 10 min. Then, the mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 20 mL; or the mixture was added to the solution of corresponding electrophile in THF and stirred at 25 °C for 2 h, then worked-up as usual, see **27f**). The collected organic layers were washed with brine, dried over $MgSO_4$ and concentrated *in vacuo.*

The resulting reaction mixture was dissolved in THF (1 mL, 0.5 M). Then, DDQ (36.0 mg, 0.6 mmol, 1.2 equiv) was added, and the reaction mixture was stirred at 25 °C for 16 h. The reaction mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 30 mL), dried over $MgSO_4$, concentrated *in vacuo* and purified *via* silica gel column chromatography to yield the desired 8-substituted 6-chloroimidazo[1,2-*a*]pyrazine of type **27**.

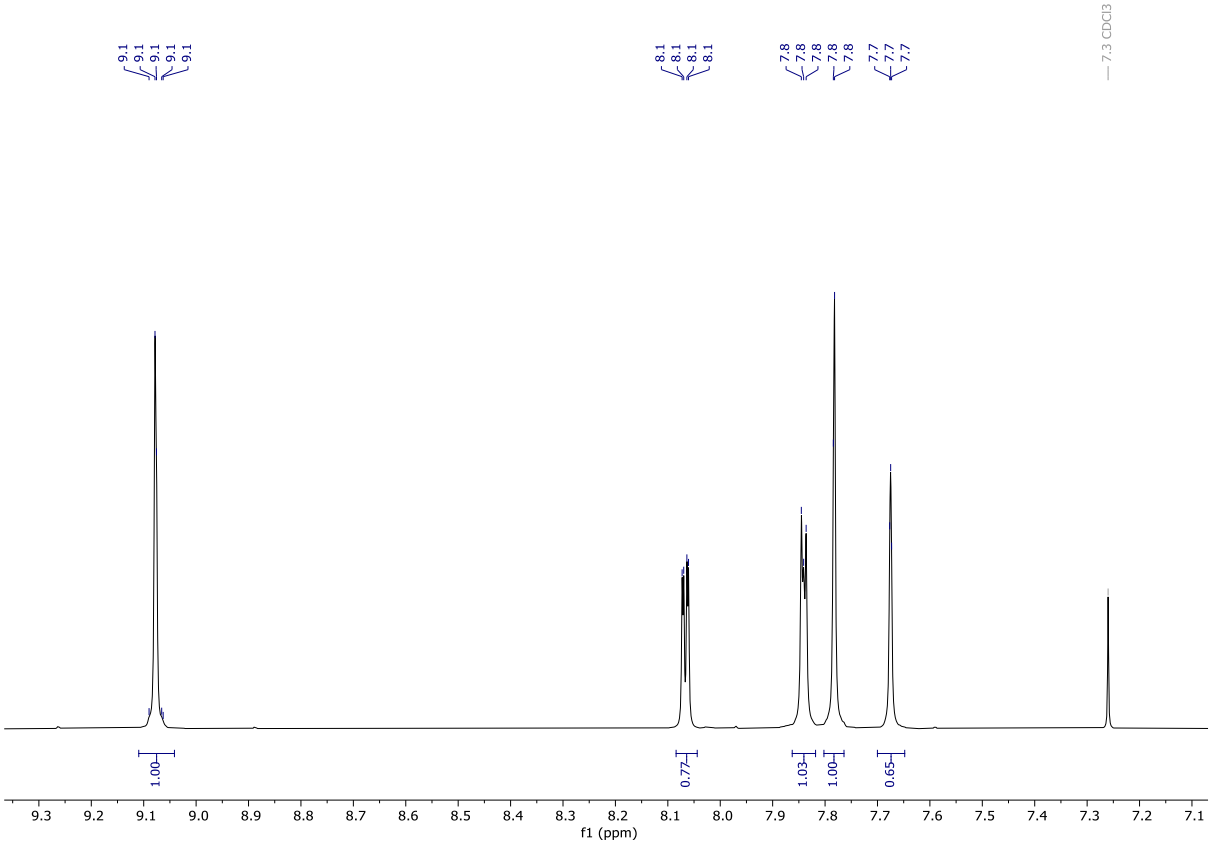
Mechanistic Investigations

Metalation of Imidazo[1,2-*a*]pyrazine (3)

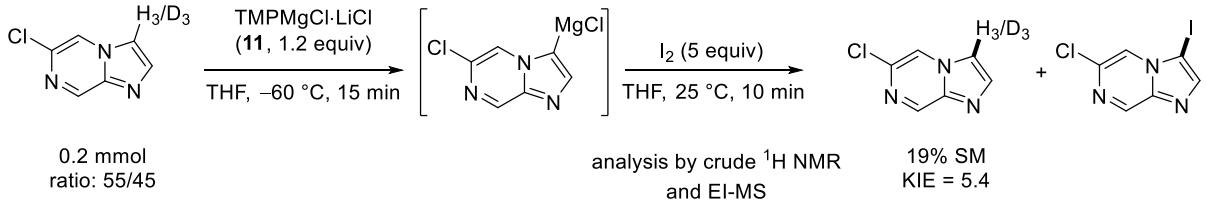


3 35% 23%

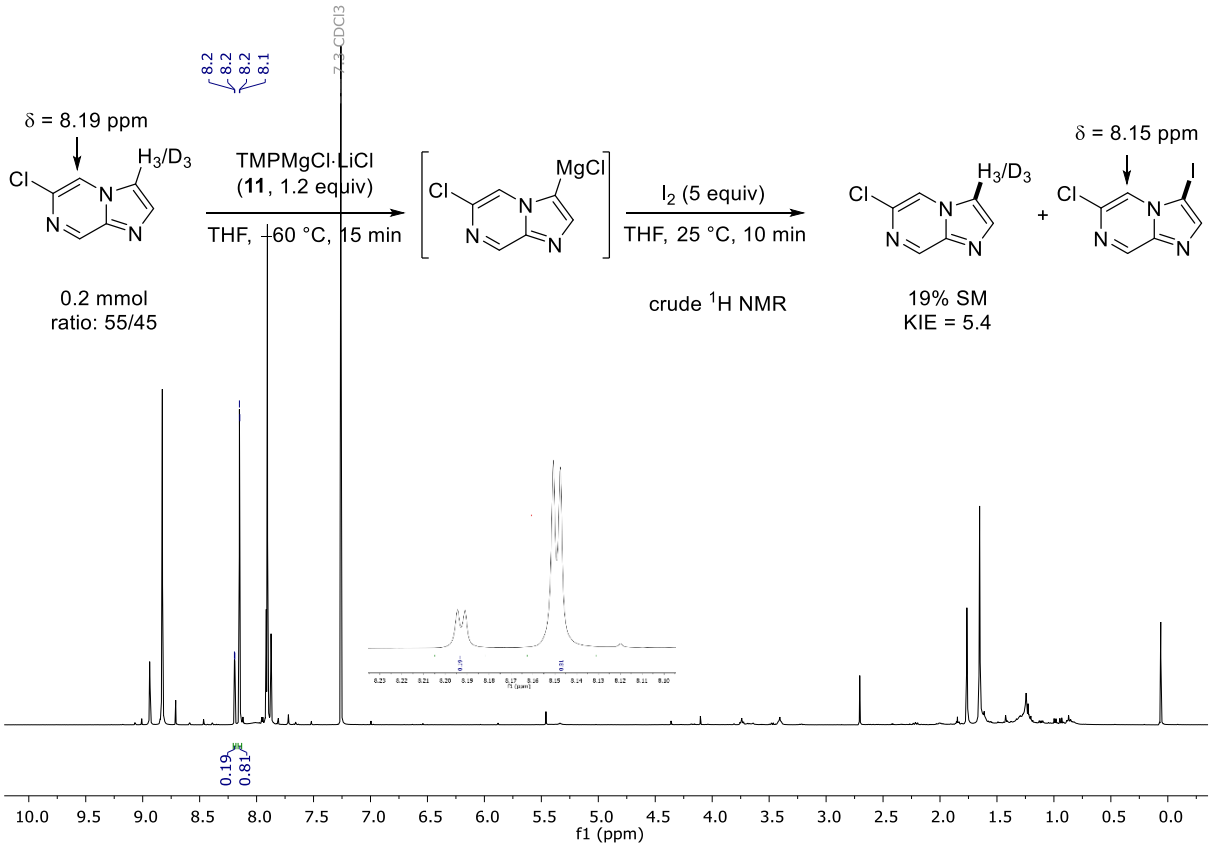
Freshly prepared TMPMgCl·LiCl (**11**, 1.2 equiv.) was added dropwise to a cooled (−60 °C) solution of imidazo[1,2-*a*]pyrazine (59.5 mg, 0.5 mmol,1.0 equiv) in dry THF (2.5 mL) and stirred for 30 min. Subsequently, D_2O (100 µL, 100 mg, 10 equiv) was added, the cooling bath was removed, and the temperature was allowed to rise to room temperature in 1 h. The reaction mixture then was diluted with Et_2O (10 mL), dried over $MgSO_4$, concentrated under reduced pressure and submitted for ^1H NMR to determine the regioselectivity of metalation.

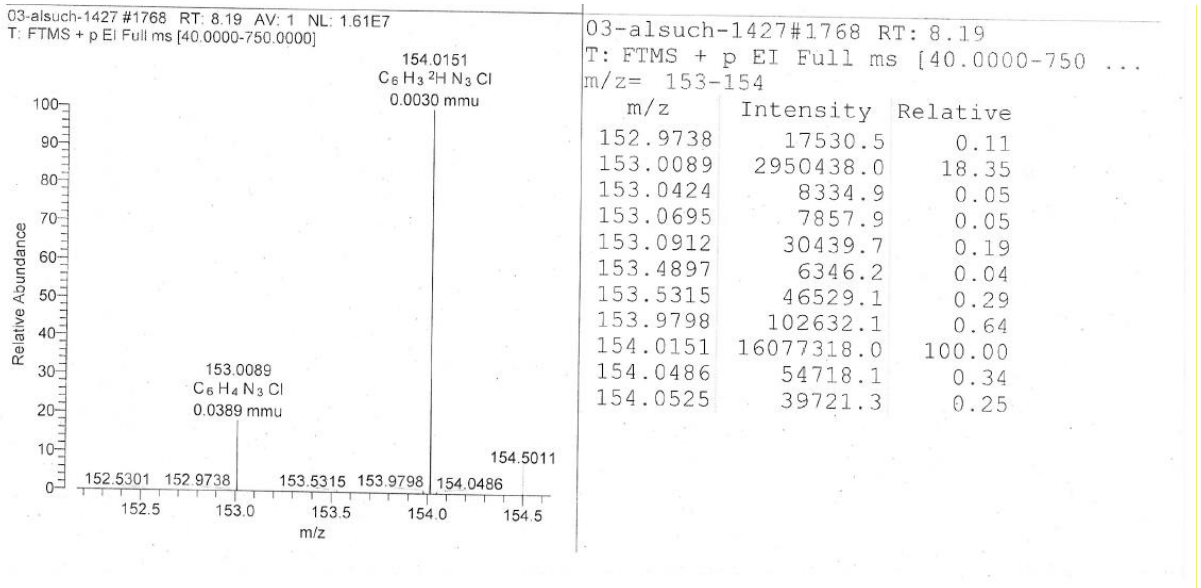


Kinetic Isotope Effect Study (Intermolecular Competition Experiment)



Freshly prepared TMPMgCl·LiCl (**11**, 1.2 equiv.) was added dropwise to a cooled (−60 °C) solution of *h*$_3$/*d*$_3$-6-chloroimidazo[1,2-*a*]pyrazine (ratio *h*$_3$/*d*$_3$ 55:45; 31.2 mg, 0.2 mmol,1.0 equiv) in dry THF (1 mL) and stirred for 15 min. Subsequently, I_2 (254 mg, 5 equiv) was added, the cooling bath removed, and the temperature was allowed to rise to room temperature in 10 min. The reaction mixture then was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 4 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The conversion was determined by ^{1}H NMR and a sample was submitted to EI-MS analysis to determine the isotopic distribution.



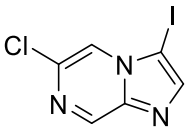


03-alsuch-1427#1768 RT: 8.19
T: FTMS + p EI Full ms [40.0000-750 ...
m/z= 153-154

m/z	Intensity	Relative
152.9738	17530.5	0.11
153.0089	2950438.0	18.35
153.0424	8334.9	0.05
153.0695	7857.9	0.05
153.0912	30439.7	0.19
153.4897	6346.2	0.04
153.5315	46529.1	0.29
153.9798	102632.1	0.64
154.0151	16077318.0	100.00
154.0486	54718.1	0.34
154.0525	39721.3	0.25

Products

6-Chloro-3-iodoimidazo[1,2-*a*]pyrazine (7a)



6-Chloro-3-iodoimidazo[1,2-*a*]pyrazine (**7a**) was prepared according to **TP1** on a 0.2 mmol scale using iodine (5 equiv, 1.0 mmol, 253 mg) as electrophile (10 min, 25 °C). Purified by flash chromatography using *i*-hexane/EtOAc (3/2, v/v) to afford desired compound **7a** as a white solid (0.15 mmol, 43.4 mg, 78%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.83 (d, *J* = 1.2, 1H), 8.15 (d, *J* = 1.2, 1H), 7.91 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 143.6, 142.9, 142.3, 136.3, 117.0, 65.2.

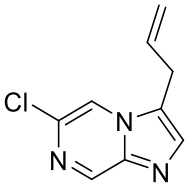
HRMS (EI): calculated for $C_6H_3ClIN_3^{\bullet+}$: 278.9055, found 278.9055 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 281 (32), 279 (100), 253 (10), 127 (96), 42 (17).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3109, 3014, 1602, 1483, 1433, 1399, 1316, 1284, 1260, 1219, 1144, 1074, 971, 954, 910, 880, 868, 824, 812, 805, 738.

Mp: 174.6–175.7 °C.

3-Allyl-6-chloroimidazo[1,2-*a*]pyrazine (7b)



3-Allyl-6-chloroimidazo[1,2-*a*]pyrazine (**7b**) was prepared according to **TP1** on a 0.2 mmol scale using allyl bromide (1.2 equiv, 0.24 mmol, 0.02 mL) as electrophile and CuCN·2LiCl (50 mol%, 0.1 mmol, 0.1 mL) as catalyst (25 °C, 1.5 h). Purified by flash chromatography using *i*-hexane/EtOAc (1/1 then 1/4 v/v) to afford desired compound **7b** as a white solid (0.11 mmol, 22 mg, 56%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.88 (d, *J* = .4, 1H), 7.94 (d, *J* = 1.3, 1H), 7.68 (s, 1H), 5.99–5.85 (m, 1H), 5.26 (dq, *J* = 10.0, 1.4, 1H), 5.13 (dq, *J* = 17.0, 1.6, 1H), 3.66 (dt, *J* = 6.1, 1.7, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 142.4, 140.3, 136.2, 134.7, 131.3, 124.4, 118.8, 114.4, 28.1.

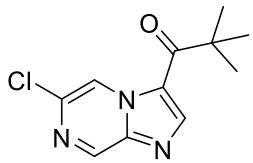
HRMS (EI): calculated for $C_9H_8ClN_3^{\bullet+}$: 193.0401, found 193.0401 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 194 (16), 193 (20), 192 (51), 168 (19), 166 (62), 158 (100), 157 (24), 156 (24), 113 (12), 86 (11), 44 (11), 42 (16).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3036, 1644, 1608, 1516, 1485, 1466, 1432, 1349, 1329, 1306, 1233, 1148, 1110, 1099, 1024, 995, 934, 912, 901, 871, 858, 828, 760, 718.

Mp: 69.9–70.8 °C.

1-(6-Chloroimidazo[1,2-*a*]pyrazin-3-yl)-2,2-dimethylpropan-1-one (7c)



1-(6-Chloroimidazo[1,2-*a*]pyrazin-3-yl)-2,2-dimethylpropan-1-on (**7c**) was prepared according to **TP1** on a 0.2 mmol scale using PivCl (1.5 equiv, 0.3 mmol, 0.037 mL) as electrophile and CuCN·2LiCl (50 mol%, 0.1 mmol, 0.1 mL) as catalyst (25 °C, 2 h). Purified by flash chromatography using *i-h*exane/EtOAc (3/2 v/v) to afford desired compound **7c** as a white solid (0.08 mmol, 19 mg, 40%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.73–9.69 (m, 1H), 9.09–9.04 (m, 1H), 8.55 (s, 1H), 1.45 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 197.8, 143.2, 142.3, 140.9, 138.0, 122.6, 119.7, 44.6, 28.3.

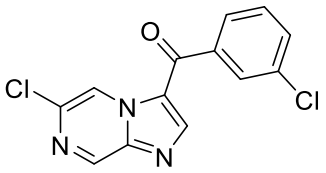
HRMS (EI): calculated for $C_{11}H_{12}ClN_3O^{\bullet+}$: 237.0663, found 237.0662 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 237 (9), 182 (33), 181 (25), 180 (100), 153 (28), 44 (12), 42 (15).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3141, 3123, 2977, 2360, 1858, 1702, 1632, 1598, 1495, 1475, 1448, 1396, 1367, 1314, 1278, 1241, 1182, 1144, 1119, 1050, 1020, 932, 918, 908, 853, 810, 735.

Mp: 149.8–151.8 °C.

(6-Chloroimidazo[1,2-*a*]pyrazin-3-yl)(3-chlorophenyl)methanone (7d)



Compound **7d** was prepared according to **TP1** on a 0.4 mmol scale using *m*-chlorobenzoyl chloride (1.5 equiv, 0.6 mmol, 0.076 mL) as electrophile (25 °C, 2 h) and CuCN·2LiCl (20 mol%, 0.08 mmol, 0.08 mL) as catalyst. Purified by flash chromatography using *i*-hexane/EtOAc (7/3 v/v) to afford desired compound **7d** as a light-yellow solid (0.29 mmol, 64 mg, 56%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.62 (d, *J* = 1.4, 1H), 9.14 (d, *J* = 1.4, 1H), 8.34 (s, 1H), 7.86 (t, *J* = 1.9, 1H), 7.76 (dt, *J* = 7.6, 1.4, 1H), 7.63 (ddd, *J* = 8.1, 2.1, 1.1, 1H), 7.52 (t, *J* = 7.9, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 183.7, 145.7, 142.7, 139.6, 138.3, 135.4, 133.2, 130.4, 129.0, 127.1, 119.3.

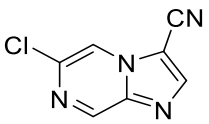
HRMS (EI): calculated for $C_{13}H_7Cl_2N_3O^{\bullet+}$: 290.9961, found 290.9961 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 293 (29), 291 (47), 290 (18), 256 (34), 207 (23), 182 (30), 180 (100), 139 (33), 111 (20), 73 (16).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 1619, 1603, 1563, 1494, 1448, 1416, 1341, 1315, 1215, 1180, 1126, 1047, 913, 898, 857, 809, 768, 743, 722, 691, 660.

Mp: 191.3–192.2 °C.

6-Chloroimidazo[1,2-*a*]pyrazine-3-carbonitrile (7e)



Compound **7e** was prepared according to **TP1** on a 0.2 mmol scale using TsCN (1.5 equiv, 0.3 mmol, 54.36 mg) as electrophile (25 °C, 2 h). Purified by flash chromatography using *i*-

hexane/EtOAc (3/2, v/v) to afford desired compound **7e** as a white solid (0.14 mmol, 25 mg, 70%).

Note: The reaction was also performed on gram scale. According to TP1 compound **6** (5 g, 32.6 mmol, 1.0 equiv) was treated with TMPMgCl·LiCl (39.1 mmol, 1.2 equiv) and TsCN (8.8 g, 48.9 mmol, 1.5 equiv). Compound **7e** was isolated in 52% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.09 (d, *J*=1.4, 1H), 8.42 (d, *J*=1.3, 1H), 8.30 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 143.8, 143.2, 140.7, 137.8, 116.8, 109.2, 100.2.

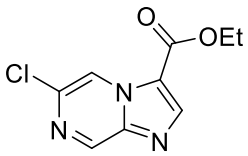
HRMS (EI): calculated for $C_7H_3ClN_4^{\bullet+}$: 178.0041, found 178.0041 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 180 (32), 178 (100), 143 (11), 42 (12).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3124, 3102, 3078, 3038, 2228, 1794, 1694, 1604, 1490, 1460, 1413, 1327, 1315, 1304, 1282, 1234, 1168, 1137, 1115, 1032, 914, 900, 849, 816, 753.

Mp: 169.9–171.6 °C.

Ethyl 6-chloroimidazo[1,2-*a*]pyrazine-3-carboxylate (7f)



Compound **7f** was prepared according to **TP1** on a 0.2 mmol scale using ethyl cyanoformate (1.5 equiv, 0.3 mmol, 0.03 mL) as electrophile (25 °C, 2 h). Purified by flash chromatography using *i*-hexane/EtOAc (3/2, v/v) to afford desired compound **7f** as a white solid (0.097 mmol, 22 mg, 48%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.25 (d, *J* = 1.4, 1H), 9.03 (d, *J* = 1.4 Hz, 1H), 8.38 (s, 1H), 4.46 (q, *J* = 7.1, 2H), 1.44 (t, *J* = 7.1, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.9, 142.7, 142.5, 141.8, 137.2, 118.5, 117.7, 61.6, 14.5.

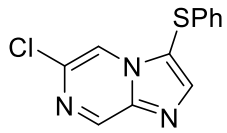
HRMS (EI): calculated for $C_9H_8ClN_3O_2^{\bullet+}$: 225.0300, found 225.0299 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 253 (16), 251 (10), 225 (30), 199 (19), 197 (59), 190 (17), 182 (32), 180 (100), 155 (12), 153 (39), 42 (29).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3093, 3039, 3012, 2979, 2360, 1882, 1700, 1602, 1504, 1454, 1419, 1388, 1368, 1341, 1302, 1286, 1248, 1206, 1150, 1126, 1095, 1031, 944, 914, 894, 876, 859, 767, 752, 737.

Mp: 124.6–126.5 °C.

6-Chloro-3-(phenylthio)imidazo[1,2-*a*]pyrazine (7g)



Compound **7g** was prepared according to **TP1** on a 0.4 mmol scale using $PhSO_2SPh$ (1.2 equiv, 0.48 mmol, 120 mg) as electrophile (25 °C, 2 h). Purified by flash chromatography using *i*-hexane/EtOAc (7/3, v/v) to afford desired compound **7g** as a white solid (0.26 mmol, 68 mg, 65%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.03 (d, *J* = 1.4 Hz, 1H), 8.26 (d, *J* = 1.4 Hz, 1H), 8.18 (s, 1H), 7.37–7.22 (m, 4H), 7.15–7.06 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 144.7, 142.6, 142.1, 136.1, 133.1, 129.8, 127.3, 127.3, 115.4, 115.1.

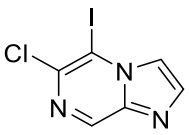
HRMS (EI): calculated for $C_{12}H_{18}ClN_3S^{\bullet+}$: 261.0122, found 261.0121 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 261 (8), 226 (99, 140 (13), 122 (9), 121 (100), 112 (20), 85 (11).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3057, 3103, 3015, 1597, 1577, 1479, 1461, 1438, 1402, 1313, 1285, 1221, 1150, 1128, 1088, 1079, 1021, 998, 948, 908, 889, 821, 806, 742, 730, 684.

Mp: 78.1–78.9 °C.

6-Chloro-5-iodoimidazo[1,2-*a*]pyrazine (8a)



Compound **8a** was prepared according to **TP2** on a 0.2 mmol scale using iodine (5 equiv, 1.0 mmol, 253 mg) as electrophile. Purified by flash chromatography using *i*-hexane/EtOAc (3/2, v/v) to afford desired compound **8a** as a white solid (0.11 mmol, 30.6 mg, 55%).

^{1}H NMR (400 MHz, DMSO-d_6) δ = 8.91 (s, 1H), 8.26 (s, 1H), 7.98 (d, *J* = 1.2, 1H).

^{13}C NMR (101 MHz, DMSO-d_{6z}) δ = 140.1, 139.8, 138.4, 136.5, 121.0, 89.5.

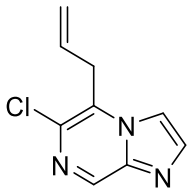
HRMS (EI): calculated for $C_6H_3ClIN_3^{\bullet+}$: 278.9055, found 278.9049 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 278 (100), 281 (30), 152 (28), 125 (11).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3147, 3110, 1741, 1578, 1469, 1437, 1313, 1294, 1217, 1148, 1134, 1110, 1076, 940, 919, 899, 872, 850.

Mp: 228.5–230.2 °C.

5-Allyl-6-chloroimidazo[1,2-*a*]pyrazine (8b)



Compound **8b** was prepared according to **TP2** on a 0.2 mmol scale using allyl bromide (1.2 equiv, 0.24 mmol, 0.02 mL) as electrophile and CuCN·2LiCl (20 mol%, 0.1 mmol, 0.04 mL) as catalyst. Purified by flash chromatography using *i*-hexane/EtOAc (7/3) to afford desired compound **8b** as an off-white solid (0.17 mmol, 33 mg, 85%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.86 (s, 1H), 7.86 (s, 1H), 7.70 (s, 1H), 5.88 (ddt, *J* = 16.4, 10.2, 6.0, 1H), 5.33–5.11 (m, 2H), 3.90 (dt, *J* = 6.0, 1.8, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 140.6, 140.4, 137.3, 133.7, 128.8, 126.5, 119.3, 112.8, 33.8.

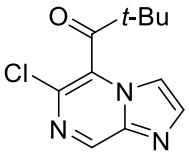
HRMS (EI): calculated for $C_9H_8ClN_3^{\bullet+}$: 193.0328, found 192.0327 $[M\text{-}H]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 192 (12), 61 (14), 44 (14), 43 (100).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3146, 3090, 3044, 3017, 2917, 1863, 1809, 1642, 1605, 1502, 1473, 1446, 1428, 1310, 1244, 1204, 1131, 1032, 994, 963, 937, 909, 851, 764, 750, 723.

Mp: 124.1–125.4 °C.

1-(6-Chloroimidazo[1,2-*a*]pyrazin-5-yl)-2,2-dimethylpropan-1-one (8c)



Compound **8c** was prepared according to **TP2** on a 0.3 mmol scale using pivaloyl chloride (1.5 equiv, 0.45 mmol, 54 mg) as electrophile and CuCN·2LiCl (20 mol%, 0.06 mmol, 0.06 mL) as catalyst (25 °C, 2 h). Purified by flash chromatography using *i*-hexane/EtOAc (7/3) to afford desired compound **8c** as an off-white solid (0.18 mmol, 43 mg, 60%).

^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.92 (d, *J* = 1.0 Hz, 1H), 7.88 (d, *J* = 1.3 Hz, 1H), 7.44–7.39 (m, 1H), 1.38 (d, *J* = 1.8 Hz, 9H).

^{13}C NMR (151 MHz, $CDCl_3$) δ = 205.3, 142.3, 140.0, 137.8, 129.7, 126.4, 113.6, 46.1, 27.5.

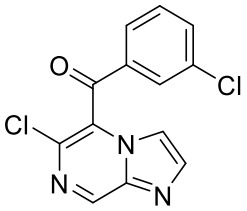
HRMS (EI): calculated for $C_{11}H_{12}ClN_3O^{\bullet+}$: 237.0663, found 237.0660 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 237 (10), 152 (33), 61 (13), 57 (51), 44 (13), 42 (100), 40 (19).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3110, 2970, 2908, 1690, 1598, 1471, 1444, 1310, 1126, 1108, 1069, 937, 929, 912, 870, 757, 745, 706.

Mp: 103.7–104.5 °C.

(6-Chloroimidazo[1,2-*a*]pyrazin-5-yl)(3-chlorophenyl)methanone (8d)



Compound **8d** was prepared according to **TP2** on a 0.4 mmol scale using *m*-chlorobenzoyl chloride (1.5 equiv, 0.6 mmol, 0.076 mL) as electrophile and CuCN·2LiCl (20 mol%, 0.08 mmol, 0.08 mL) as catalyst (25 °C, 2 h). Purified by flash chromatography using DCM/EtOAc (4/1 v/v) to afford desired compound **8d** as a yellow solid (0.20 mmol, 61 mg, 52%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.04 (s, 1H), 7.90 (t, *J* = 1.9, 2H), 7.78–7.70 (m, 2H), 7.67 (ddd, *J* = 8.0, 2.2, 1.1, 1H), 7.48 (t, *J* = 7.9, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 187.1, 143.8, 140.2, 138.2, 136.5, 136.0, 135.4, 133.6, 130.8, 129.5, 128.0, 123.4, 114.8.

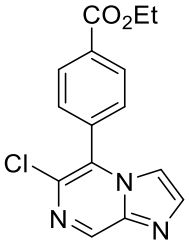
HRMS (EI): calculated for $C_{13}H_7Cl_2N_3O^{\bullet+}$: 290.9961, found 290.9957 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 291 (17), 264 (17), 262 (26), 141 (32), 139 (17), 139 (100), 111 (30).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3181, 3066, 1649, 1589, 1567, 1464, 1442, 1419, 1351, 1317, 1277, 1262, 1207, 1160, 1120, 1049, 946, 905, 886, 851, 799, 772, 758, 714, 678.

Mp: 156.2–157.8 °C.

Ethyl 4-(6-chloroimidazo[1,2-*a*]pyrazin-5-yl)benzoate (8e)



Compound **8e** was prepared according to **TP2** on a 0.3 mmol scale using 4-iodobenzoate (66 mg, 0.24 mmol, 0.8 equiv) as electrophile and $Pd(PPh_3)_4$ (5 mol%, 0.12 mmol, 14 mg) as catalyst (40 °C, 2 h). Purified by flash chromatography using *i*-hexane/EtOAc (3/2) to afford desired compound **8e** as an off-white solid (0.16 mmol, 48 mg, 53%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.95 (d, *J* = 0.8 Hz, 1H), 8.31–8.26 (m, 2H), 7.80 (d, *J* = 1.1 Hz, 1H), 7.68–7.62 (m, 2H), 7.38 (t, *J* = 0.9 Hz, 1H), 4.44 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 165.7, 141.7, 140.6, 137.3, 134.2, 133.3, 132.7, 130.9, 127.4, 113.6, 61.7, 14.5.

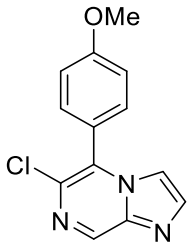
HRMS (EI): calculated for $C_{15}H_{12}ClN_3O_2^{\bullet+}$: 301.0613, found 301.0615 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 303 (31), 302 (18), 301 (100), 273 (27), 258 (17), 257 (10), 256 (50), 228 (11), 193 (15), 165 (10).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3148, 3095, 2992, 1707, 1610, 1468, 1443, 1365, 1296, 1281, 1254, 1178, 1129, 1113, 1021, 950, 920, 864, 849, 774, 740, 701.

Mp: 127.8–128.6 °C.

6-Chloro-5-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine (8f)



Compound **8f** was prepared according to **TP2** on a 0.3 mmol scale using 4-iodoanisole (56 mg, 0.24 mmol, 0.8 equiv) as electrophile and $Pd(PPh_3)_4$ (5 mol%, 0.12 mmol, 14 mg) as catalyst (40 °C, 2 h). Purified by flash chromatography using *i*-hexane/EtOAc (1/1 v/v) to afford desired compound **8f** as an off-white solid (0.19 mmol, 50 mg, 64%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.90 (s, 1H), 7.77 (d, *J* = 1.2 Hz, 1H), 7.53–7.40 (m, 3H), 7.17–7.07 (m, 2H), 3.91 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.2, 140.9, 140.8, 137.0, 133.3, 130.9, 128.3, 122.1, 115.0, 113.8, 55.6.

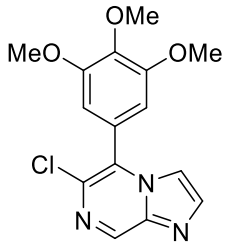
HRMS (EI): calculated for $C_{13}H_{10}ClN_3O^{\bullet+}$: 259.0507, found 259.0544$[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 259 (45), 216 (8), 61 (15), 43 (100).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3043, 2969, 2937, 1610, 1483, 1463, 1441, 1305, 1296, 1251, 1176, 1145, 1117, 1108, 1027, 952, 926, 874, 830, 812, 761, 749, 719, 673.

Mp: 199.4–200.2 °C.

6-Chloro-5-(3,4,5-trimethoxyphenyl)imidazo[1,2-a]pyrazine (8g)



Compound **8g** was prepared according to **TP2** on a 0.3 mmol scale using 5-iodo-1,2,3-trimethoxybenzene (71 mg, 0.24 mmol, 0.8 equiv) as electrophile and $Pd(PPh_3)_4$ (5 mol%, 0.12 mmol, 14 mg) as catalyst (40 °C, 2 h). Purified by flash chromatography using *i*-hexane/EtOAc (1/4 v/v) to afford desired compound **8g** as an off-white solid (0.13 mmol, 42 mg, 54%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.91 (s, 1H), 7.79 (d, *J* = 1.1 Hz, 1H), 7.49 (s, 1H), 6.73 (s, 2H), 3.96 (s, 3H), 3.88 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 154.3, 141.2, 140.7, 139.7, 137.1, 133.1, 128.3, 125.2, 114.0, 106.3, 61.2, 56.5.

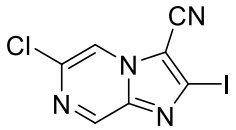
HRMS (EI): calculated for $C_{15}H_{14}ClN_3O_3^{\bullet+}$: 319.0718, found 319.0717 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 321(32), 320 (17), 319 (100), 306 (10), 304 (28), 261 (13), 218 (22), 190 (11), 144 (12).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3146, 3128, 2940, 2840, 1548, 1489, 1467, 1449, 1415, 1374, 1325, 1314, 1301, 1234, 1123, 1094, 1012, 993, 930, 910, 891, 850, 837, 812, 771, 746, 727, 691.

Mp: 194.4–195.2 °C.

6-Chloro-2-iodoimidazo[1,2-*a*]pyrazine-3-carbonitrile (16a)



Compound **16a** was prepared according to **TP3** on a 0.2 mmol scale using iodine (3 equiv, 0.6 mmol, 152.26 mg) as electrophile (25 °C, 10 min). Purified by flash chromatography using *i*-hexane/EtOAc (7/3 v/v) to afford desired compound **16a** as a white solid (0.10 mmol, 32 mg, 52%).

^{1}H NMR (400 MHz, DMSO-d_6) δ = 9.15 (d, *J*=1.3, 1H), 9.12 (d, *J*=1.3, 1H).

^{13}C NMR (101 MHz, DMSO-d_6) δ = 142.2, 141.2, 135.9, 118.9, 110.4, 107.6, 106.4.

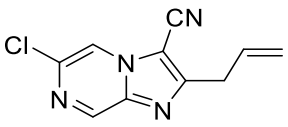
HRMS (EI): calculated for $C_7H_2ClIN_4^{\bullet+}$: 303,9007, found 303.9008 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 306 (29), 303 (100), 113 (28), 86 (12), 43 (10).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3087, 3025, 2227, 1703, 1604, 1454, 1410, 1318, 1308, 1278, 1217, 1184, 1135, 1046, 940, 855, 758.

Mp: 244.6–246.3 °C.

2-Allyl-6-chloroimidazo[1,2-*a*]pyrazine-3-carbonitrile (16b)



Compound **16b** was prepared according to **TP3** on a 0.2 mmol scale using allyl bromide (1.5 equiv, 0.3 mmol, 0.026 mL) as electrophile and CuCN·2LiCl (20 mol%, 0.04 mmol, 0.04 mL) as catalyst (25 °C, 1 h). Purified by flash chromatography using *i*-hexane/EtOAc (7/3 v/v) to afford desired compound **16b** as an off-white solid (0.1 mmol, 22 mg, 50%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.97 (s, 1H), 8.34–8.29 (m, 1H), 6.12–5.97 (m, 1H), 5.35–5.23 (m, 2H), 3.74 (d, *J* = 6.7 Hz, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 157.5, 142.1, 140.1, 137.3, 132.1, 119.2, 116.6, 109.6, 98.2, 33.5.

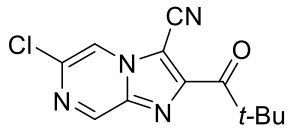
HRMS (EI): calculated for $C_{10}H_7ClN_4^{\bullet+}$: 218.0354, found 218.0349 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 219 (32), 218 (26), 217 (100), 194 (11), 192 (33).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3093, 3035, 3007, 2223, 1642, 1603, 1491, 1482, 1466, 1425, 1414, 1389, 1293, 1271, 1248, 1195, 1161, 1063, 995, 979, 956, 931, 857, 759, 964.

Mp: 117.5–118.7 °C.

6-Chloro-2-pivaloylimidazo[1,2-*a*]pyrazine-3-carbonitrile (16c)



Compound **16c** was prepared according to **TP3** on a 1.7 mmol scale using PivCl (1.5 equiv, 2.65 mmol, 0.324 mL) as electrophile and CuCN·2LiCl (50 mol%, 0.88 mmol, 0.88 mL) as catalyst (25 °C, 1 h). Purified by flash chromatography using *i*-hexane/EtOAc (4/1 v/v) to afford desired compound **16c** as an off-white solid (0.28 mmol, 74 mg, 33%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.14 (s, 1H), 8.43 (s, 1H), 1.47 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 199.9, 150.3, 144.7, 138.9, 138.6, 116.7, 109.2, 102.0, 44.6, 26.6.

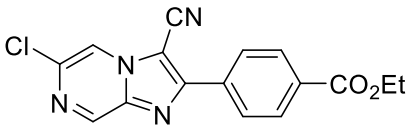
HRMS (EI): calculated for $C_{12}H_{11}ClN_4O^{\bullet+}$: 262.0616, found 262.0616 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 262 (8), 205 (15), 177 (26), 57 (100), 42 (18), 40 (35).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3112, 2957, 2932, 2872, 2226, 1680, 1600, 1494, 1472, 1458, 1420, 1390, 1377, 1299, 1278, 1246, 1173, 1077, 999, 937, 922, 828, 760, 701.

Mp: 169.3–171.7 °C.

Ethyl 4-(6-chloro-3-cyanoimidazo[1,2-*a*]pyrazin-2-yl)benzoate (16d)



Compound **16d** was prepared according to **TP3** on a 0.2 mmol scale using ethyl-4-iodobenzoate (1.5 equiv, 0.3 mmol, 82.8 mg) as electrophile and $Pd(PPh_3)_4$ (5 mol%, 11.5 mg) as catalyst (50 °C, 2 h). Purified by flash chromatography using *i*-hexane/EtOAc (4/1 v/v) to afford desired compound **16d** as a white solid (0.11 mmol, 36 mg, 55%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.08 (d, *J* = 1.4, 1H), 8.41 (d, *J* = 1.4, 1H), 8.28 (d, *J* = 8.7 Hz, 2H), 8.22 (d, *J* = 8.7 Hz, 2H), 4.43 (q, *J* = 7.1, 2H), 1.43 (t, *J* = 7.1, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 165.9, 153.6, 142.8, 140.4, 137.8, 134.0, 132.8, 130.6, 127.6, 116.7, 110.6, 61.6, 14.5.

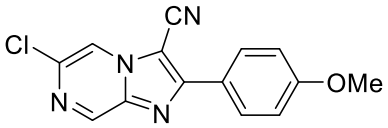
HRMS (EI): calculated for $C_{16}H_{11}ClN_4O_2^{\bullet+}$: 326.0565, found 326.0562 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 326 (27), 300 (22), 298 (73), 283 (32), 281 (100), 255 (16), 253 (52), 207 (52), 191 (16), 114 (22).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3049, 2218, 1701, 1598, 1569, 1467, 1409, 1372, 1306, 1277, 1247, 1225, 1178, 1132, 1110, 1035, 1015, 942, 926, 866, 850, 782, 758, 714.

Mp: 280.9–282.3 °C.

6-Chloro-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (16e)



Compound **16e** was prepared according to **TP3** on a 0.2 mmol scale using 4-iodoanisole (1.5 equiv, 0.3 mmol, 70.2 mg) as electrophile and $Pd(PPh_3)_4$ (5 mol%, 11.5 mg) as catalyst (50 °C, 2 h). Purified by flash chromatography using *i*-hexane/EtOAc (4/1 to 1/1, v/v) to afford desired compound **16e** as a white solid (0.14 mmol, 40.9 mg, 72%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.99 (d, *J* = 1.4, 1H), 8.35 (d, *J* = 1.3, 1H), 8.15 (d, *J* = 8.9, 2H), 7.05 (d, *J* = 8.9, 2H), 3.90 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.1, 154.9, 142.0, 140.4, 137.1, 129.3, 122.7, 116.6, 114.8, 111.3, 94.8, 55.6.

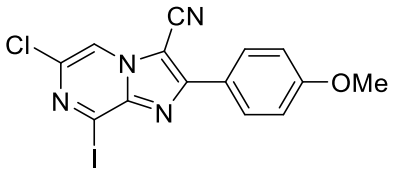
HRMS (EI): calculated for $C_{14}H_9ClN_4O^{\bullet+}$: 284.0459, found 284.0457 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 286 (32), 284 (100), 269 (37), 243 (15), 241 (51), 207 (15).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3114, 3011, 2848, 2216, 1611, 1576, 1537, 1474, 1460, 1449, 142, 1389, 1315, 1295, 1259, 1222, 1184, 1123, 1104, 1095, 1040, 1022, 946, 850, 826, 818, 798, 758, 740, 698, 686, 664.

Mp: 228.0–229.3 °C.

6-Chloro-8-iodo-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (18a)



Compound **18a** was prepared according to **TP4** on a 0.2 mmol scale using iodine (5 equiv, 1.0 mmol, 253 mg) as electrophile (25 °C, 10 min). Purified by flash chromatography using *i*-hexane/EtOAc (4/1, v/v) to afford desired compound **18a** as a white solid (0.13 mmol, 55.7 mg, 68%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.24 (s, 1H), 8.17 (d, *J* = 8.9, 2H), 7.03 (d, *J* = 8.9, 2H), 3.89 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.2, 154.4, 141.0, 135.4, 129.5, 122.3, 116.0, 114.7, 111.2, 110.9, 96.7, 55.6.

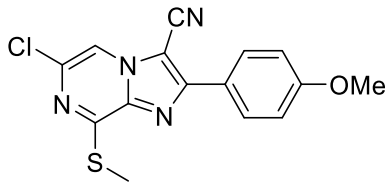
HRMS (EI): calculated for $C_{14}H_8ClIN_4O^{\bullet+}$: 409.9426, found 409.9420 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 412 (36), 411 (17), 409 (100), 284 (16), 57 (11).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3085, 2229, 1608, 1573, 1536, 1476, 1452, 1423, 1383, 1312, 1292, 1259, 1181, 1120, 1107, 1066, 1023, 958, 843, 812, 784, 739, 697, 686.

Mp: 228.3–229.7 °C.

6-Chloro-2-(4-methoxyphenyl)-8-(methylthio)imidazo[1,2-*a*]pyrazine-3-carbonitrile (18b)



Compound **18b** was prepared according to **TP4** on a 0.2 mmol scale using $PhSO_2SCH_3$ (1.5 equiv, 0.3 mmol, 56.5 mg) as electrophile (25 °C, 3 h). Purified by flash chromatography using *i*-hexane/EtOAc (7/3, v/v) to afford desired compound **18b** as a white solid (0.078 mmol, 25.8 mg, 39%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.18–8.10 (m, 2H), 7.99 (s, 1H), 7.05–6.97 (m, 2H), 3.88 (s, 3H), 2.71 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.8, 154.9, 153.3, 138.1, 136.2, 129.2, 122.9, 114.6, 111.5, 95.2, 55.6, 21.0, 12.8.

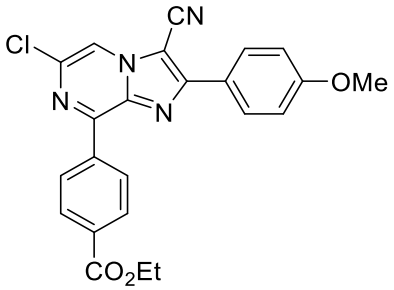
HRMS (EI): calculated for $C_{15}H_{11}ClN_4OS^{\bullet+}$: 330.0337, found 303.0334 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 332 (34), 331 (15), 330 (100), 329 (19), 297 (38), 284 (28), 269 (19), 224 (29), 209 (15).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2213, 1604, 1574, 1535, 1475, 1451, 1422, 1382, 1329, 1306, 1290, 1257, 1242, 1178, 1118, 1082, 1023, 964, 889, 844, 805, 785.

Mp: 230.1–231.9 °C.

Ethyl 4-(6-chloro-3-cyano-2-(4-methoxyphenyl)imidazo[1,2-a]pyrazin-8-yl)benzoate (18c)



Compound **18c** was prepared according to **TP4** on a 0.1 mmol scale using 4-iodobenzoate (1.5 equiv, 0.15 mmol, 41.4 mg) as electrophile and $Pd(PPh_3)_4$ (5 mol%, 5.7 mg) as catalyst (50 °C, 2 h). Purified by flash chromatography using *i*-hexane/CH_2Cl_2 (1/4, v/v) to afford desired compound **18c** as a yellow solid (0.045 mmol, 19.9 mg, 46%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.96–8.89 (m, 2H), 8.28 (s, 1H), 8.25–8.15 (m, 4H), 7.09–7.00 (m, 2H), 4.44 (q, *J* = 7.1, 2H), 3.90 (s, 3H), 1.45 (t, *J* = 7.1, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 166.2, 162.0, 154.1, 147.1, 139.0, 137.7, 136.3, 133.0, 130.1, 129.8, 129.3, 122.7, 115.4, 114.7, 111.5, 94.8, 61.5, 55.6, 14.5.

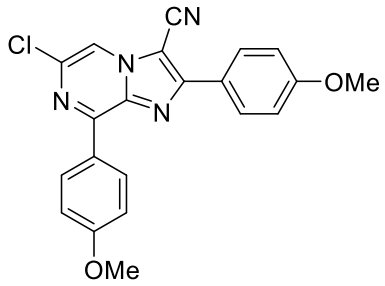
HRMS (EI): calculated for $C_{23}H_{17}ClN_4O_3^{\bullet+}$: 432.0984, found 432.0984 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 434 (32), 433 (25), 432 (100), 404 (24), 387 (37), 316 (29), 315 (19), 247 (15), 114 (27).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2956, 2902, 2220, 1714, 1611, 1576, 1483, 1446, 1418, 1391, 1341, 1309, 1274, 1253, 1184, 1125, 1109, 1097, 1018, 964, 888, 868, 841, 802, 795, 784, 754, 740, 695.

Mp: 211.0–212.5 °C.

6-Chloro-2,8-bis(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (18d)



Compound **18d** was prepared according to **TP4** on a 0.1 mmol scale using 4-iodoanisole (1.5 equiv, 0.15 mmol, 35.1 mg) as electrophile and $Pd(PPh_3)_4$ (5 mol%, 5.7 mg) as catalyst

(50 °C, 2 h). Purified by flash chromatography using *i*-hexane/EtOAc (4/1, v/v) to afford desired compound **18d** as a white solid (0.06 mmol, 24.2 mg, 62%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.94–8.87 (m, 2H), 8.26–8.18 (m, 3H), 7.12–7.02 (m, 4H), 3.93 (s, 3H), 3.91 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.8, 161.8, 153.6, 148.1, 138.8, 136.4, 132.2, 129.3, 126.7, 123.1, 114.7, 114.2, 113.8, 111.8, 94.6, 55.6.

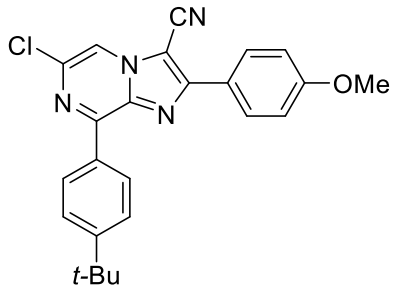
HRMS (EI): calculated for $C_{21}H_{15}ClN_4O_2^{\bullet+}$: 390.0878, found 390.0876 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 392 (37), 391 (23), 390 (100), 233 (16), 221 (24).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3088, 2960, 2835, 2213, 1601, 1575, 1515, 1477, 1460, 1420, 1388, 1346, 1307, 1256, 1174, 1163, 1098, 1021, 964, 848, 842, 796, 738, 694.

Mp: 192.7–194.2 °C.

8-(4-(*tert*-Butyl)phenyl)-6-chloro-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (18e)



Compound **18e** was prepared according to **TP4** on a 0.1 mmol scale using 4-*tert*-butyliodobenzene (1.5 equiv, 0.15 mmol, 0.026 mL) as electrophile and $Pd(PPh_3)_4$ (5 mol%, 5.7 mg) as catalyst (50 °C, 1 h). Purified by flash chromatography using *i*-hexane/EtOAc (9/1, v/v) to afford desired compound **18e** as a white solid (0.069 mmol, 28.8 mg, 69%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.80–8.72 (m, 2H), 8.26–8.17 (m, 3H), 7.64–7.56 (m, 2H), 7.04 (d, *J* = 8.9, 2H), 3.90 (s, 3H), 1.40 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.8, 155.5, 153.7, 148.6, 138.9, 136.4, 131.2, 130.0, 129.2, 125.8, 123.1, 114.6, 114.3, 111.8, 94.6, 55.6, 35.2, 31.3.

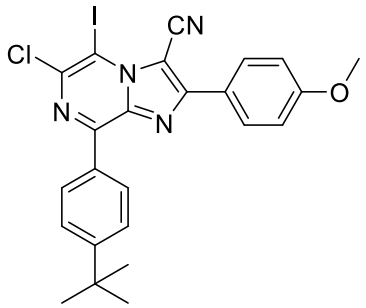
HRMS (EI): calculated for $C_{24}H_{21}ClN_4O^{\bullet+}$: 416.1398, found 416.1403 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 416 (46), 403 (30), 402 (23), 401 (100), 186 (27), 114 (17).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2952, 2904, 2835, 2213, 1614, 1576, 1478, 1462, 1419, 13891341, 1306, 1248, 1177, 1123, 1093, 1035, 1014, 966, 890, 849, 831, 790, 738, 708, 690.

Mp: 197.1–198.4 °C.

8-(4-(*tert*-Butyl)phenyl)-6-chloro-5-iodo-2-(4-methoxyphenyl)imidazo[1,2-a]pyrazine-3-carbonitrile (20)



Compound **20** was prepared according to **TP5** on a 0.1 mmol scale using iodine (5 equiv, 0.5 mmol, 127 mg) as electrophile (25 °C, 10 min). Purified by flash chromatography using *i*Hexane/EtOAc (10/0 to 9/1, v/v) to afford desired compound **20** as a yellow solid (0.04 mmol, 21.7 mg, 40%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.68 (d, *J*=8.6, 2H), 8.23 (d, *J*=8.9, 2H), 7.59 (d, *J*=8.6, 2H), 7.06 (d, *J*=8.9, 2H), 3.90 (s, 3H), 1.39 (s, 9H).

^{13}C NMR (201 MHz, $CDCl_3$) δ = 161.8, 156.0, 155.5, 147.4, 144.3, 139.4, 130.7, 130.2, 130.1, 129.9, 129.9, 125.8, 123.0, 114.5, 113.2, 82.0, 55.6, 35.2, 31.3.

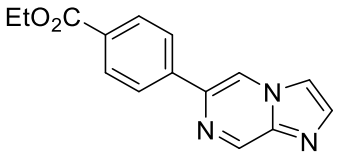
HRMS (EI): calculated for $C_{24}H_{20}ClIN_4O^{\bullet+}$: 542.0365, found 542.0370 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 544 (29), 543 (22), 542 (87), 529 (32), 528 (23), 527 (100), 403 (20), 402 (16), 401 (57).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2963, 2361, 2208, 1739, 1608, 1471, 1410, 1348, 1310, 1257, 1175, 1111, 1031, 954, 846, 836, 798, 740, 710, 696.

Mp: 270.3–272.0 °C.

Ethyl 4-(imidazo[1,2-*a*]pyrazin-6-yl)benzoate (22a)



Ethyl 4-iodobenzoate (0.8 mL, 5 mmol, 1.0 equiv) was dissolved in THF (5 mL) and cooled to −20 °C. Then, a solution of *i*PrMgCl·LiCl (1.2M in THF, 5.25 mmol, 1.05 equiv) was added dropwise at this temperature and the mixture was stirred at −20 °C for 30 min. The organometallic species was then let warm to room temperature and titrated against iodine.

Next, according to **TP6**, **6** (76.8 mg, 0.5 mmol, 1 equiv) and Pd-PEPPSI-iPr (5 mol%, 17.0 mg) were dissolved in THF (1.0 mL). Then, the freshly prepared zinc reagent (1.5 equiv, 0.75 mmol) was added dropwise. The resulting reaction mixture was stirred at 25 °C for 5 h. The reaction mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 15 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel and *i*-hexane/EtOAc (4/1, v/v) affording compound **22a** as an off-white solid (124.3 mg, 0.465 mmol, 93%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.30 – 9.24 (m, 1H), 8.57 (d, *J* = 1.5 Hz, 1H), 8.19 – 8.15 (m, 2H), 8.06 – 8.01 (m, 2H), 7.88 (d, *J* = 1.2 Hz, 1H), 7.81 – 7.79 (m, 1H), 4.42 (q, *J* = 7.1 Hz, 2H), 1.43 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 166.4, 143.5, 140.5, 140.2, 138.8, 136.4, 130.8, 130.4, 126.2, 116.0, 114.3, 61.3, 14.5.

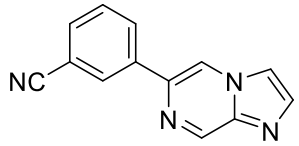
HRMS (EI): calculated for $C_{15}H_{13}N_3O_2^{\bullet+}$: 267.1008, found: 267.1003 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 267 (74), 239 (30), 222 (100), 194 (44), 140 (22).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3137 (w), 3105 (w), 3082 (w), 2992 (w), 2957 (w), 2924 (m), 2854 (m), 1694 (s), 1609 (m), 1574 (w), 1528 (w), 1491 (w), 1476 (m), 1450 (m), 1438 (m), 1409 (w), 1369 (m), 1347 (m), 1335 (m), 1315 (m), 1303 (m), 1274 (s), 1264 (s), 1180 (m), 1160 (w), 1145 (m), 1125 (m), 1107 (s), 1028 (w), 1016 (m), 934 (w), 913 (s), 876 (w), 864 (w), 853 (w), 839 (s), 806 (w), 774 (vs), 760 (vs), 733 (w), 697 (s), 675 (w), 653 (m).

Mp: 182 °C.

3-(Imidazo[1,2-*a*]pyrazin-6-yl)benzonitrile (22b)



3-Iodobenzonitrile (1.15 g, 5 mmol, 1.0 equiv) was dissolved in THF (5 mL) and cooled to −20 °C. Then, a solution of *i*PrMgCl·LiCl (1.2M in THF, 5.25 mmol, 1.05 equiv) was added dropwise at this temperature and the mixture was stirred at −20 °C for 30 min. The organometallic species was then let warm to room temperature and titrated against iodine.

Next, according to **TP6**, **6** (76.8 mg, 0.5 mmol, 1 equiv) and Pd-PEPPSI-iPr (5 mol%, 17.0 mg) were dissolved in THF (1.0 mL). Then, the freshly prepared zinc reagent (1.5 equiv, 0.75 mmol) was added dropwise. The resulting reaction mixture was stirred at 25 °C for 5 h. The reaction mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 15 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel and *i*-hexane/EtOAc (4/1, v/v) affording compound **22b** as an off-white solid (99.1 mg, 0.45 mmol, 90%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.24–9.18 (m, 1H), 8.54 (d, *J* = 1.6 Hz, 1H), 8.27 (t, *J* = 1.8 Hz, 1H), 8.23–8.17 (m, 1H), 7.88 (d, *J* = 1.1 Hz, 1H), 7.80 (t, *J* = 0.9 Hz, 1H), 7.70 (dt, *J* = 7.7, 1.4 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 143.7, 140.2, 137.8, 137.7, 136.6, 132.2, 130.5, 130.0, 130.0, 118.7, 115.8, 114.5, 113.4.

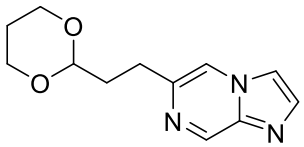
HRMS (EI): calculated for $C_{13}H_8N_4^{\bullet+}$: 220.0749, found: 220.0744 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z: 220 (100), 139 (10), 71 (13), 57 (20).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3156 (w), 3076 (w), 3035 (w), 2956 (m), 2922 (m), 2853 (m), 2227 (m), 2176 (w), 2140 (w), 1968 (w), 1906 (w), 1712 (w), 1682 (w), 1646 (w), 1613 (w), 1596 (w), 1580 (w), 1513 (m), 1479 (m), 1468 (m), 1448 (m), 1410 (m), 1347 (m), 1330 (m), 1323 (m), 1310 (m), 1300 (s), 1280 (m), 1261 (m), 1206 (m), 1173 (w), 1154 (w), 1135 (s), 1064 (m), 1044 (m), 928 (s), 914 (m), 885 (w), 858 (m), 848 (m), 806 (s), 794 (m), 760 (vs), 715 (m), 686 (s), 666 (w).

Mp: 248 °C.

6-(2-(1,3-Dioxan-2-yl)ethyl)imidazo[1,2-*a*]pyrazine (22c)



LiCl (318 mg, 7.5 mmol, 1.5 equiv) was dried in a sealed flask under high vacuum at 430 °C for 5 min with a heat gun. After cooling to room temperature and flushing the flask with Ar, Mg turnings (300 mg, 12.5 mmol, 2.5 equiv) were added as well as a solution of $ZnCl_2$ (1.0M in THF, 5 mL, 5 mmol, 1.0 equiv). Then, 2-(2-Bromoethyl)-1,3-dioxane (0.7 mL, 5 mmol, 1.0 equiv) was added dropwise and the solution was stirred at 25 °C for 2 h before titration against iodine to determine the concentration.

Next, according to **TP6**, **6** (76.8 mg, 0.5 mmol, 1 equiv) and Pd-PEPPSI-iPent (5 mol%, 19.8 mg) were dissolved in THF (1.0 mL). Then, the freshly prepared zinc reagent (1.5 equiv, 0.75 mmol) was added dropwise. The resulting reaction mixture was stirred at 25 °C for 16 h. The reaction mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 15 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel and *i*-hexane/EtOAc (4/1, v/v) affording compound **22c** as a yellow oil (79.3 mg, 0.34 mmol, 68%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.04 (d, *J* = 1.4 Hz, 1H), 7.90 (d, *J* = 1.5 Hz, 1H), 7.75 (d, *J* = 1.1 Hz, 1H), 7.61 (d, *J* = 0.9 Hz, 1H), 4.57 (t, *J* = 5.1 Hz, 1H), 4.15–4.06 (m, 2H), 3.82–3.69 (m, 2H), 2.85 (dd, *J* = 8.7, 6.8 Hz, 2H), 2.17–1.98 (m, 3H), 1.39–1.29 (m, 1H).

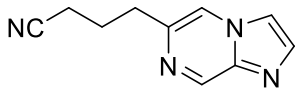
^{13}C NMR (101 MHz, $CDCl_3$) δ = 143.3, 141.8, 135.5, 116.0, 113.3, 101.4, 67.1, 53.6, 34.5, 29.1, 25.9.

HRMS (EI): calculated for $C_{12}H_{15}N_3O_2^{\bullet+}$: 233.1164, found: 233.1158 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z: 233 (16), 174 (26), 146 (100), 133 (41), 87 (45), 59 (17).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 2960 (m), 2928 (m), 2853 (m), 1622 (w), 1512 (m), 1491 (w), 1447 (m), 1431 (m), 1406 (m), 1379 (m), 1341 (m), 1303 (m), 1265 (w), 1243 (w), 1144 (s), 1130 (vs), 1082 (m), 1044 (m), 1000 (m), 972 (w), 932 (m), 885 (m), 851 (m), 832 (w), 784 (w), 748 (m), 739 (w).

4-(Imidazo[1,2-*a*]pyrazin-6-yl)butanenitrile (22d)



LiCl (318 mg, 7.5 mmol, 1.5 equiv) was dried in a sealed flask under high vacuum at 430 °C for 5 min with a heat gun. After cooling to room temperature and flushing the flask with Ar, Mg turnings (300 mg, 12.5 mmol, 2.5 equiv) were added as well as a solution of $ZnCl_2$ (1.0M in THF, 5 mL, 5 mmol, 1.0 equiv). Then, 4-bromobutanenitrile (0.5 mL, 5 mmol, 1.0 equiv) was added dropwise and the solution was stirred at 25 °C for 2 h before titration against iodine to determine the concentration.

Next, according to **TP6**, **6** (76.8 mg, 0.5 mmol, 1 equiv) and Pd-PEPPSI-iPent (5 mol%, 19.8 mg) were dissolved in THF (1.0 mL). Then, the freshly prepared zinc reagent (1.5 equiv, 0.75 mmol) was added dropwise. The resulting reaction mixture was stirred at 25 °C for 16 h. The reaction mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 15 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel and *i*-hexane/EtOAc (4/1, v/v) affording compound **22d** as a yellow oil (91.3 mg, 0.49 mmol, 98%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.11–9.08 (m, 1H), 8.01 (dt, *J* = 1.5, 0.8 Hz, 1H), 7.81 (d, *J* = 1.1 Hz, 1H), 7.67 (t, *J* = 0.9 Hz, 1H), 2.96–2.91 (m, 2H), 2.42 (t, *J* = 6.9 Hz, 2H), 2.18 (p, *J* = 7.2 Hz, 2H).

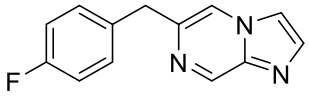
^{13}C NMR (101 MHz, $CDCl_3$) δ = 143.5, 139.9, 139.8, 135.6, 119.4, 116.8, 113.6, 32.9, 24.5, 16.6.

HRMS (EI): calculated for $C_{10}H_{10}N_4^{\bullet+}$: 186.0905, found: 186.0900 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z: 186 (15), 146 (21), 133 (100), 79 (12), 52 (13).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3150 (w), 3049 (w), 3019 (w), 2949 (m), 2921 (m), 2868 (w), 2239 (w), 1713 (w), 1627 (w), 1516 (m), 1489 (m), 1454 (m), 1449 (m), 1430 (m), 1368 (m), 1345 (m), 1321 (m), 1304 (m), 1260 (m), 1160 (m), 1140 (s), 1085 (w), 1074 (w), 1055 (w), 1024 (w), 941 (m), 928 (m), 920 (m), 886 (m), 873 (m), 838 (w), 782 (w), 760 (w), 738 (vs), 670 (m).

6-(4-Fluorobenzyl)imidazo[1,2-*a*]pyrazine (22e)



LiCl (318 mg, 7.5 mmol, 1.5 equiv) was dried in a sealed flask under high vacuum at 430 °C for 5 min with a heat gun. After cooling to room temperature and flushing the flask with Ar, Mg turnings (300 mg, 12.5 mmol, 2.5 equiv) were added as well as a solution of $ZnCl_2$ (1.0 M in THF, 5 mL, 5 mmol, 1.0 equiv). Then, 1-(chloromethyl)-4-fluorobenzene (0.6 mL, 5 mmol, 1.0 equiv) was added dropwise and the solution was stirred at 25 °C for 2 h before titration against iodine to determine the concentration.

Next, according to **TP6**, **6** (76.8 mg, 0.5 mmol, 1 equiv) and Pd-PEPPSI-iPent (5 mol%, 19.8 mg) were dissolved in THF (1.0 mL). Then, the freshly prepared zinc reagent (1.5 equiv, 0.75 mmol) was added dropwise. The resulting reaction mixture was stirred at 25 °C for 16 h. The reaction mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 15 mL). The collected organic layers were dried over $MgSO_4$ and concentrated under reduced pressure. The crude product was purified by flash chromatography using silica gel and *i*-hexane/EtOAc (4/1, v/v) affording compound **22e** as a white solid (107.8 mg, 0.475 mmol, 95%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.09–9.04 (m, 1H), 7.80–7.74 (m, 2H), 7.60 (d, *J* = 0.9 Hz, 1H), 7.29–7.23 (m, 2H), 7.07–6.98 (m, 2H), 4.10 (s, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.9 (d, *J* = 245.1 Hz), 143.5, 141.6, 139.9, 135.8, 134.1 (d, *J* = 3.4 Hz), 130.7 (d, *J* = 8.0 Hz), 116.7, 115.7 (d, *J* = 21.4 Hz), 113.6, 40.3.

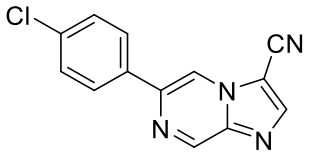
HRMS (EI): calculated for $C_{10}H_{10}N_4^{\bullet+}$: 226.0781, found: 226.0774 $[M-H]^{\bullet+}$.

MS (70 eV, EI) m/z: 226 (100), 133 (11), 109 (9), 57 (13).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3144 (w), 3114 (w), 3079 (w), 3054 (w), 3036 (w), 3002 (w), 2955 (w), 2922 (m), 2853 (m), 2578 (w), 1713 (w), 1619 (m), 1601 (m), 1508 (vs), 1486 (m), 1460 (m), 1438 (m), 1417 (w), 1381 (w), 1353 (m), 1337 (m), 1313 (s), 1302 (m), 1287 (m), 1260 (w), 1248 (m), 1238 (m), 1222 (vs), 1158 (m), 1148 (m), 1140 (s), 1093 (m), 1073 (w), 1016 (m), 980 (w), 959 (w), 952 (m), 939 (w), 916 (m), 886 (m), 864 (m), 849 (m), 836 (m), 826 (m), 813 (s), 782 (m), 775 (s), 751 (m), 730 (vs), 710 (m), 662 (w).

Mp: 110 °C.

6-(4-Chlorophenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (S1)



6-(4-Chlorophenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile was prepared according to **TP7** on a 0.4 mmol scale using 6-chloroimidazo[1,2-*a*]pyrazine-3-carbonitrile (**7e**, 71.4 mg, 0.4 mmol, 1.0 equiv), 4-chlorophenylboronic acid, pinacol ester (1.2 equiv, 0.48 mmol), $Pd(PPh_3)_4$ (46 mg, 0.04 mmol, 10 mol%) and K_2CO_3 (110 mg, 0.8 mmol, 2.0 equiv) in 1.3 mL 1,4-dioxane/water 9/1 (100 °C, 5 h). Purified by flash chromatography using *i*-hexane/EtOAc (7/3, v/v) to afford desired 6-(4-chlorophenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile as a white solid (0.19 mmol, 50 mg, 49%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.32 (d, *J*=1.6, 1H), 8.62 (d, *J*=1.6, 1H), 8.28 (s, 1H), 7.98–7.90 (m, 2H), 7.51 (d, *J*=8.6, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 143.7, 143.3, 143.2, 141.8, 140.9, 136.2, 133.5, 129.6, 127.9, 114.4, 109.9, 100.2.

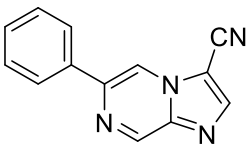
HRMS (EI): calculated for $C_{13}H_7ClN_4^{\bullet+}$: 254.0354, found 254.0355 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 256 (30), 254 (100), 219 (20), 123 (25), 114 (27).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3052, 2222, 1725, 1612, 1599, 1492, 1483, 1465, 1428, 1346, 1318, 1291, 1270, 1238, 1169, 1108, 1087, 1011, 910, 886, 861, 823, 808, 775, 654.

Mp: 220.5–222.6 °C.

6-Phenylimidazo[1,2-*a*]pyrazine-3-carbonitrile (S2)



6-Phenylimidazo[1,2-a]pyrazine-3-carbonitrile was prepared according to **TP7** on a 0.4 mmol scale using 6-chloroimidazo[1,2-*a*]pyrazine-3-carbonitrile (**7e**, 71.4 mg, 0.4 mmol, 1.0 equiv), phenylboronic acid, pinacol ester (1.2 equiv, 0.48 mmol), $Pd(PPh_3)_4$ (46 mg, 0.04 mmol, 10 mol%) and K_2CO_3 (110 mg, 0.8 mmol, 2.0 equiv) in 1.3 mL 1,4-dioxane/water 9/1 (100 °C,

5 h). Purified by flash chromatography using *i*-hexane/EtOAc (7/3, v/v) to afford desired 6-phenylimidazo[1,2-*a*]pyrazine-3-carbonitrile as a white solid (0.20 mmol, 42 mg, 48%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.32 (d, *J*=1.6, 1H), 8.61 (d, *J*=1.6, 1H), 8.27 (s, 1H), 8.01–7.93 (m, 2H), 7.57–7.43 (m, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 143.6, 143.1, 142.9, 140.9, 135.0, 130.0, 129.4, 126.7, 114.4, 110.0, 100.0.

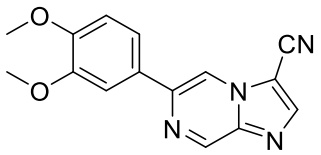
HRMS (EI): calculated for $C_{13}H_8N_4^{\bullet+}$: 220.0743, found 220.0744 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 219 (17), 165 (38), 116 (27), 114 (33), 103 (29), 89 (68), 77 (100), 76 (32), 74 (33), 66 (28), 63 (53).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3062, 2218, 1728, 1615, 1579, 1518, 1485, 1467, 1418, 1348, 1316, 1304, 1266, 1237, 1164, 1117, 1070, 1019, 913, 872, 820, 768, 749, 689, 665.

Mp: 157.0–159.5 °C

6-(3,4-Dimethoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (S3)



6-(3,4-Dimethoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile was prepared according to **TP7** on a 0.4 mmol scale using 6-chloroimidazo[1,2-*a*]pyrazine-3-carbonitrile (**7e**, 71.4 mg, 0.4 mmol, 1.0 equiv), 3,4-dimethoxyphenyboronic acid pinacol ester (1.2 equiv, 0.48 mmol), $Pd(PPh_3)_4$ (46 mg, 0.04 mmol, 10 mol%) and K_2CO_3 (110 mg, 0.8 mmol, 2.0 equiv) in 1.3 mL 1,4-dioxane/water 9/1 (100 °C, 5 h). Purified by flash chromatography using *i*hexane/EtOAc (3/7, v/v) to afford desired compound 6-(3,4-dimethoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile as a yellow solid (0.21 mmol, 59.5 mg, 53%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.31 (d, *J*=1.5, 1H), 8.56 (d, *J*=1.6, 1H), 8.27 (s, 1H), 7.59 (d, *J*=2.2, 1H), 7.52 (dd, *J*=8.4, 2.2, 1H), 7.01 (d, *J*=8.4, 1H), 4.02 (s, 3H), 3.97 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 150.8, 149.8, 143.4, 143.1, 142.8, 140.9, 127.8, 119.2, 113.6, 111.6, 110.2, 109.8, 99.8, 56.3, 56.2.

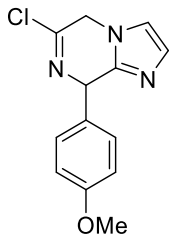
HRMS (EI): calculated for $C_{15}H_{12}N_4O_2^{\bullet+}$: 280.0955, found 280.0960 $[M]^{\bullet+}$.

MS (70 eV, EI) m/z (%): 281 (19), 280 (100), 237 (28), 97 (17), 83 (21), 73 (18), 69 (21), 57 (22), 55 (20).

IR (ATR) $\tilde{\nu}$ (cm^{-1}): 3412, 2979, 2941, 2220, 1613, 1598, 1585, 1522, 1499, 1469, 1432, 1370, 1333, 1318, 1293, 1261, 1236, 1214, 165, 1142, 1072, 1016, 950, 930, 882, 874, 862, 801, 769, 732, 666.

Mp: 245.7–248.1 °C

6-Chloro-8-(4-methoxyphenyl)-5,8-dihydroimidazo[1,2-*a*]pyrazine (26a)



LiCl (129 mg, 3.0 mmol, 1.2 equiv) was flame-dried in a sealed flask under high vacuum at 550 °C for 5 min with a heat gun. After cooling to room temperature and flushing the flask with Ar, Mg turnings (72 mg, 3.0 mmol, 1.2 equiv) were added. Then, 1-bromo-4-methoxybenzene (467.5 mg, 2.5 mmol, 1.0 equiv) was added dropwise and the solution was stirred at 25 °C for 16 h before titration against iodine to determine the concentration.[3]

To a solution of 6-chloroimidazo[1,2-*a*]pyrazine (**6**, 76.8 mg, 0.5 mmol, 1.0 equiv) in THF (0.5 M) (4-methoxyphenyl)magnesium bromide-lithium chloride (1.2 equiv, 0.6 mmol) was added at 40 °C. The reaction mixture was stirred at 40 °C for 10 min. Then, the mixture was quenched with saturated aqueous NH_4Cl solution and extracted with EtOAc (3 x 20 mL). The collected organic layers were dried over $MgSO_4$ and concentrated *in vacuo.* The product was purified by flash chromatography using *i*Hexane/EtOAc (1/9, v/v) to afford desired compound **26a** as a colorless oil (0.31 mmol, 82 mg, 63%).

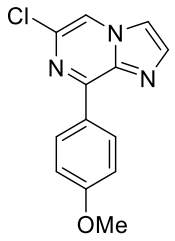
^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.23 – 7.17 (m, 2H), 7.13 (d, *J* = 1.4 Hz, 1H), 6.91 – 6.83 (m, 3H), 6.13 (t, *J* = 3.9 Hz, 1H), 4.93 (dd, *J* = 4.0, 0.9 Hz, 2H), 3.77 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 159.6, 148.5, 141.7, 130.8, 130.0, 130.0, 128.7, 116.4, 114.4, 62.2, 55.4, 50.2.

HRMS (EI): calculated for $C_{13}H_{10}ClON_3$: 259.0512, found: 259.0508 $[M\text{-}2H]^+$.

MS (70 eV, EI) m/z: 261 (32), 260 (14), 259 (100), 246 (16), 244 (50), 216 (30), 181 (16).

6-Chloro-8-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine (27a)



LiCl (129 mg, 3.0 mmol, 1.2 equiv) was flame-dried in a sealed flask under high vacuum at 550 °C for 5 min with a heat gun. After cooling to room temperature and flushing the flask with Ar, Mg turnings (72 mg, 3.0 mmol, 1.2 equiv) were added. Then, 1-bromo-4-methoxybenzene (467.5 mg, 2.5 mmol, 1.0 equiv) was added dropwise and the solution was stirred at 25 °C for 16 h before titration against iodine to determine the concentration.[3]

Compound **27a** was prepared according to **TP8** on a 0.5 mmol scale using (4-methoxyphenyl)magnesium bromide-lithium chloride (1.2 equiv, 0.6 mmol) as a nucleophile. Purified by flash chromatography using *i*Hexane/EtOAc (6/4, v/v) to afford desired compound **27a** as a colorless solid (0.34 mmol, 88 mg, 68%).

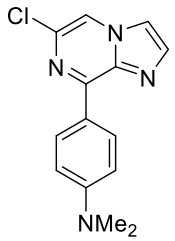
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.82 – 8.71 (m, 2H), 8.04 (s, 1H), 7.83 (d, *J* = 1.1 Hz, 1H), 7.67 (d, *J* = 1.1 Hz, 1H), 7.10 – 6.98 (m, 2H), 3.88 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.1, 148.5, 138.4, 136.0, 134.2, 131.8, 127.5, 114.6, 114.2, 113.9, 55.5.

HRMS (EI): calculated for $C_{13}H_9ClON_3$: 259.0512, found: 259.0506 $[M]^+$.

MS (70 eV, EI) m/z: 259 (99), 244 (65), 218 (32), 216 (100), 209 (25), 181 (40).

4-(6-Chloroimidazo[1,2-*a*]pyrazin-8-yl)-*N*,*N*-dimethylaniline (27b)



LiCl (129 mg, 3.0 mmol, 1.2 equiv) was flame-dried in a sealed flask under high vacuum at 550 °C for 5 min with a heat gun. After cooling to room temperature and flushing the flask with Ar, Mg turnings (72 mg, 3.0 mmol, 1.2 equiv) were added. Then, 4-bromo-*N*,*N*-dimethylaniline (500.2 mg, 2.5 mmol, 1.0 equiv) was added dropwise and the solution was stirred at 25 °C for 16 h before titration against iodine to determine the concentration.[3]

Compound **27b** was prepared according to **TP8** on a 0.5 mmol scale using (4-(dimethylamino)phenyl)magnesium bromide-lithium chloride (1.2 equiv, 0.6 mmol) as a nucleophile. Purified by recrystallization with acetone to afford desired compound **27b** as a colorless solid (0.39 mmol, 106 mg, 78%).

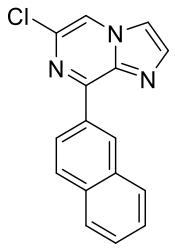
^{1}H NMR (400 MHz, DMSO) δ = 8.79 – 8.72 (m, 2H), 8.68 (s, 1H), 8.11 (d, *J* = 1.1 Hz, 1H), 7.87 (d, *J* = 1.1 Hz, 1H), 6.87 – 6.82 (m, 2H), 3.04 (s, 6H).

^{13}C NMR (101 MHz, DMSO) δ = 152.0, 150.9, 130.9, 129.2, 115.5, 114.7, 113.8, 111.2, 101.7, 53.5, 18.1, 16.7.

HRMS (EI): calculated for $C_{14}H_{13}ClN_4$: 272.0829, found: 272.0824 $[M]^+$.

MS (70 eV, EI) m/z: 274 (32), 273 (14), 273 (22), 272 (100), 271 (69), 256 (14).

6-Chloro-8-(naphthalen-2-yl)imidazo[1,2-*a*]pyrazine (27c)



LiCl (129 mg, 3.0 mmol, 1.2 equiv) was flame-dried in a sealed flask under high vacuum at 550 °C for 5 min with a heat gun. After cooling to room temperature and flushing the flask with Ar, Mg turnings (72 mg, 3.0 mmol, 1.2 equiv) were added. Then, 2-bromonaphthalene (517.5 mg, 2.5 mmol, 1.0 equiv) was added dropwise and the solution was stirred at 25 °C for 16 h before titration against iodine to determine the concentration.[3]

Compound **27c** was prepared according to **TP8** on a 0.5 mmol scale using naphthalen-2-ylmagnesium bromide-lithium chloride (1.2 equiv, 0.6 mmol) as a nucleophile. Purified by flash chromatography using *i*Hexane/EtOAc (6/4, v/v) to afford desired compound **27c** as a yellowish solid (0.18 mmol, 51 mg, 37%).

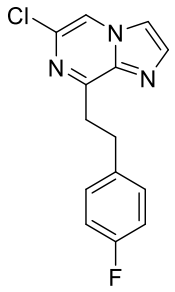
^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.52 – 9.45 (m, 1H), 8.73 (dd, *J* = 8.7, 1.8 Hz, 1H), 8.10 (s, 1H), 8.09 – 8.01 (m, 1H), 7.97 (d, *J* = 8.7 Hz, 1H), 7.91 (d, *J* = 1.1 Hz, 1H), 7.88 (dt, *J* = 7.7, 1.2 Hz, 1H), 7.70 (d, *J* = 1.1 Hz, 1H), 7.61 – 7.48 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 148.7, 138.7, 136.3, 134.7, 134.3, 133.1, 132.2, 131.3, 129.7, 128.2, 127.7, 127.7, 126.4, 126.0, 115.3, 114.4.

HRMS (EI): calculated for $C_{16}H_{10}ClN_3$: 279.0563, found: 279.0555 $[M]^+$.

MS (70 eV, EI) m/z: 279 (100), 278 (65), 242 (15).

6-Chloro-8-(4-fluorophenethyl)imidazo[1,2-*a*]pyrazine (27d)



LiCl (129 mg, 3.0 mmol, 1.2 equiv) was flame-dried in a sealed flask under high vacuum at 550 °C for 5 min with a heat gun. After cooling to room temperature and flushing the flask with Ar, Mg turnings (72 mg, 3.0 mmol, 1.2 equiv) were added. Then, 1-(2-bromoethyl)-4-fluorobenzene (507.5 mg, 2.5 mmol, 1.0 equiv) was added dropwise and the solution was stirred at 25 °C for 16 h before titration against iodine to determine the concentration.[3]

Compound **27d** was prepared according to **TP8** on a 0.5 mmol scale using (4-fluorophenethyl)magnesium bromide-lithium chloride (1.2 equiv, 0.6 mmol) as a nucleophile. Purified by preparative HPLC to afford desired compound **27d** as a colorless liquid (0.34 mmol, 92.1 mg, 67%).

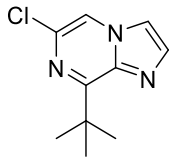
^{1}H NMR (400 MHz, DMSO) δ = 8.76 (s, 1H), 8.10 (s, 1H), 7.83 (s, 1H), 7.33 – 7.25 (m, 2H), 7.14 – 7.03 (m, 2H), 3.42 (dd, *J* = 9.3, 6.6 Hz, 2H), 3.14 (dd, *J* = 9.3, 6.6 Hz, 2H).

^{13}C NMR (101 MHz, DMSO) δ = 160.7 (d, *J* = 241.4 Hz), 153.3, 138.6, 137.1 (d, *J* = 3.1 Hz), 135.7, 132.1, 130.1 (d, *J* = 7.9 Hz), 116.5, 116.0, 115.0 (d, *J* = 21.0 Hz), 34.5, 31.6.

HRMS (EI): calculated for $C_{14}H_{11}ClFN_3$: 275.0626, found: 275.0620 $[M]^+$.

MS (70 eV, EI) m/z: 275 (100), 274 (51), 260 (16), 180 (17), 153 (42), 109 (61).

8-(*tert*-Butyl)-6-chloroimidazo[1,2-*a*]pyrazine (27e)



Compound **27e** was prepared according to **TP8** on a 0.5 mmol scale using *tert*-butylmagnesium bromide (1.2 equiv, 0.6 mmol) as a nucleophile. Purified by flash chromatography using EtOAc to afford desired compound **27e** as a yellowish solid (0.48 mmol, 100.0 mg, 95%).

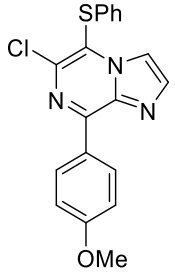
^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.05 (s, 1H), 7.76 (d, *J* = 1.1 Hz, 1H), 7.60 (d, *J* = 1.1 Hz, 1H), 1.61 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ = 161.9, 138.4, 134.7, 133.4, 115.2, 113.5, 39.4, 29.8, 28.8.

HRMS (EI): calculated for $C_{10}H_{12}ClN_3$: 209.0720, found: 209.0712 $[M]^+$.

MS (70 eV, EI) m/z: 209 (30), 196 (32), 194 (100), 167 (22), 153 (13).

6-Chloro-8-(4-methoxyphenyl)-5-(phenylthio)imidazo[1,2-*a*]pyrazine (27f)



LiCl (129 mg, 3.0 mmol, 1.2 equiv) was flame-dried in a sealed flask under high vacuum at 550 °C for 5 min with a heat gun. After cooling to room temperature and flushing the flask with Ar, Mg turnings (72 mg, 3.0 mmol, 1.2 equiv) were added. Then, 1-bromo-4-methoxybenzene (467.5 mg, 2.5 mmol, 1.0 equiv) was added dropwise and the solution was stirred at 25 °C for 16 h before titration against iodine to determine the concentration.[3]

To a solution of 6-chloroimidazo[1,2-*a*]pyrazine (**6**, 76.8 mg, 0.5 mmol, 1.0 equiv) in THF (0.5 M) (4-methoxyphenyl)magnesium bromide-lithium chloride (1.2 equiv, 0.6 mmol) was added at 40 °C. The reaction mixture was stirred at 40 °C for 10 min. Then, the resulting mixture was added dropwise to *S*-phenyl benzenethiosulfonate (150.2 mg, 0.6 mmol, 1.2 equiv) and stirred at 25 °C for 2 h. Then, the mixture was quenched with saturated aqueous

NH_4Cl solution and extracted with EtOAc (3 x 20 mL). The collected organic layers were dried over $MgSO_4$ and concentrated *in vacuo.* The product was purified by flash chromatography using *i*Hexane/EtOAc (9/1, v/v) to afford desired compound **27f** as a colorless oil (0.16 mmol, 60 mg, 33%).

^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.85 – 8.78 (m, 2H), 7.88 (d, *J* = 1.1 Hz, 1H), 7.78 (d, *J* = 1.1 Hz, 1H), 7.31 – 7.18 (m, 5H), 7.08 – 6.98 (m, 2H), 3.88 (s, 3H).

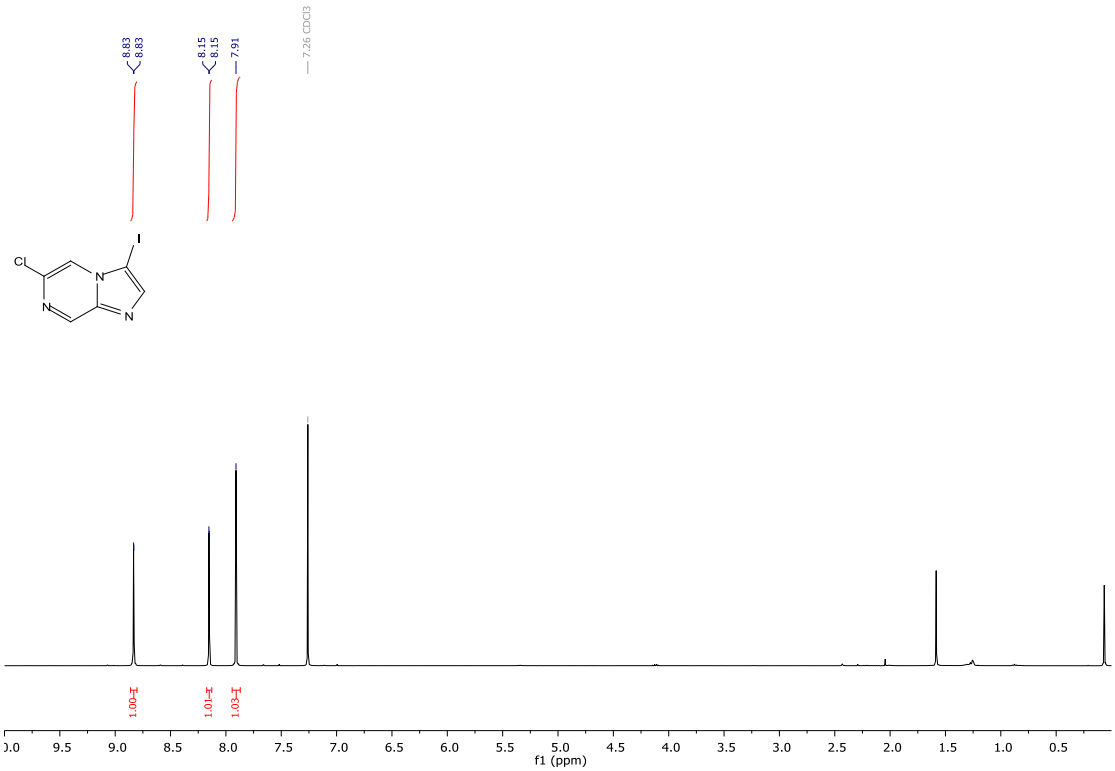
^{13}C NMR (101 MHz, $CDCl_3$) δ = 162.5, 148.3, 141.4, 138.7, 136.3, 132.2, 131.1, 129.9, 128.6, 127.9, 127.2, 118.6, 115.9, 114.1, 55.6.

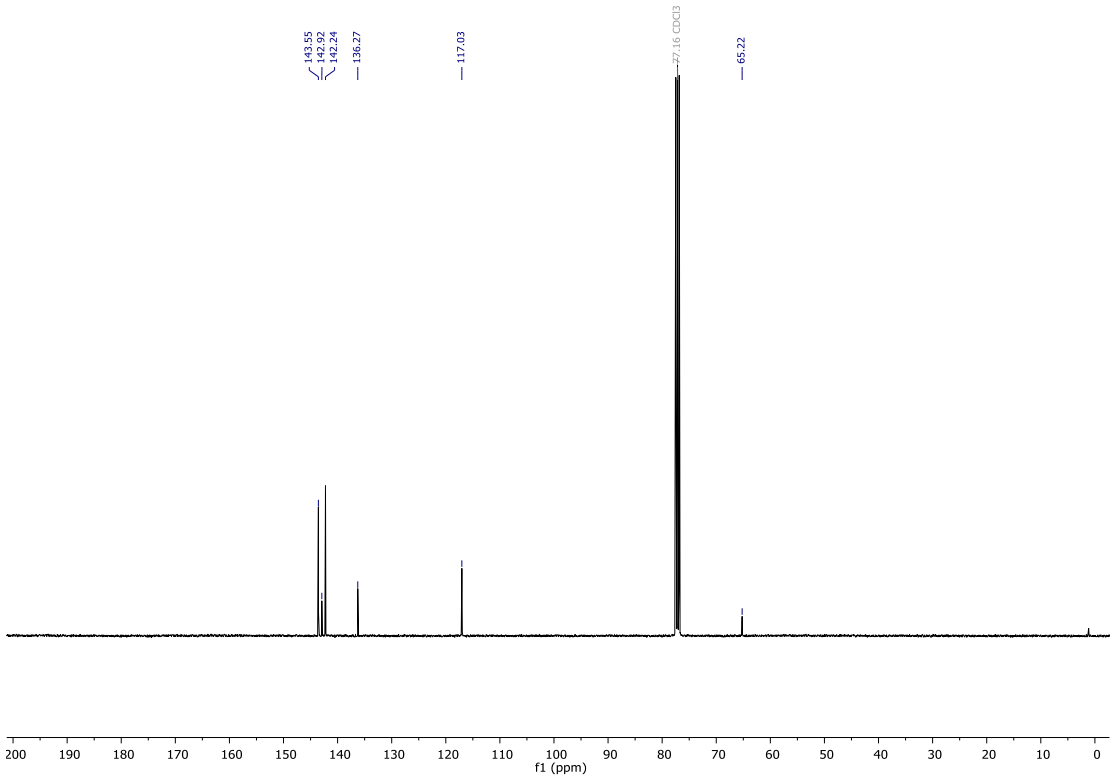
HRMS (EI): calculated for $C_{19}H_{14}ClOSN_3$: 367.0546, found: 367.0543 $[M]^+$.

MS (70 eV, EI) m/z: 367 (100), 366 (19), 332 (26), 290 (15), 185 (24).

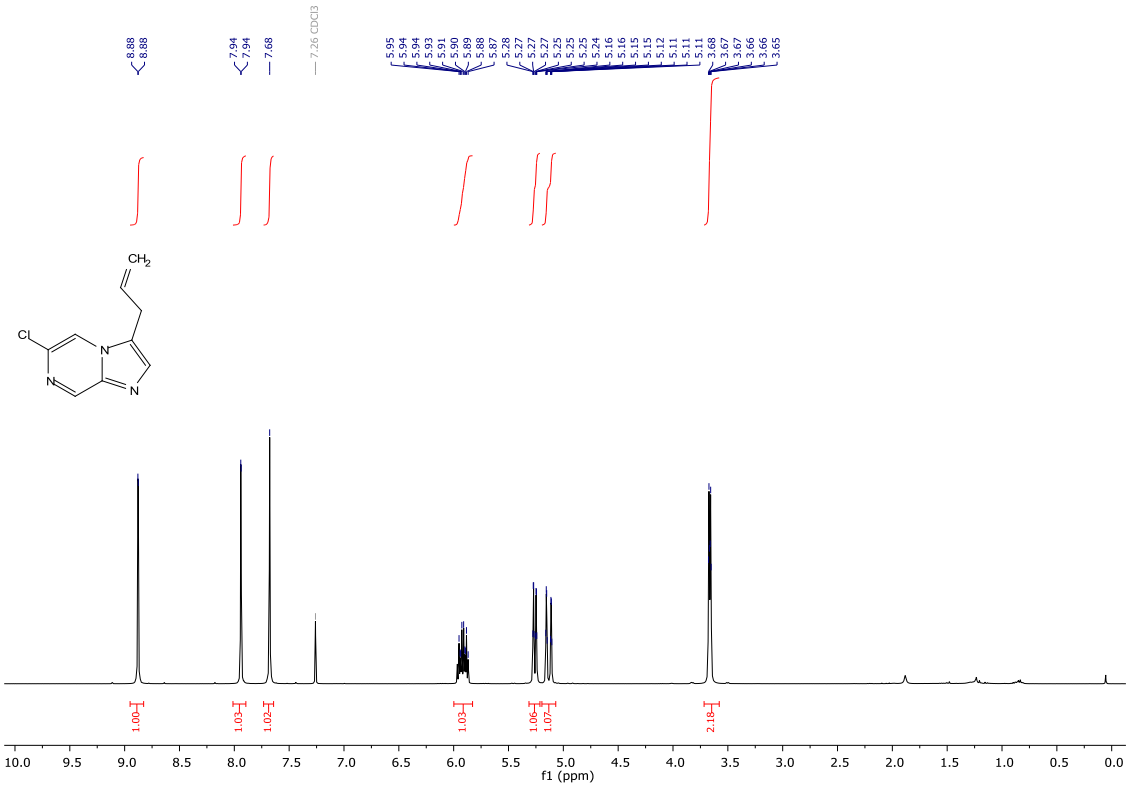
NMR Spectra

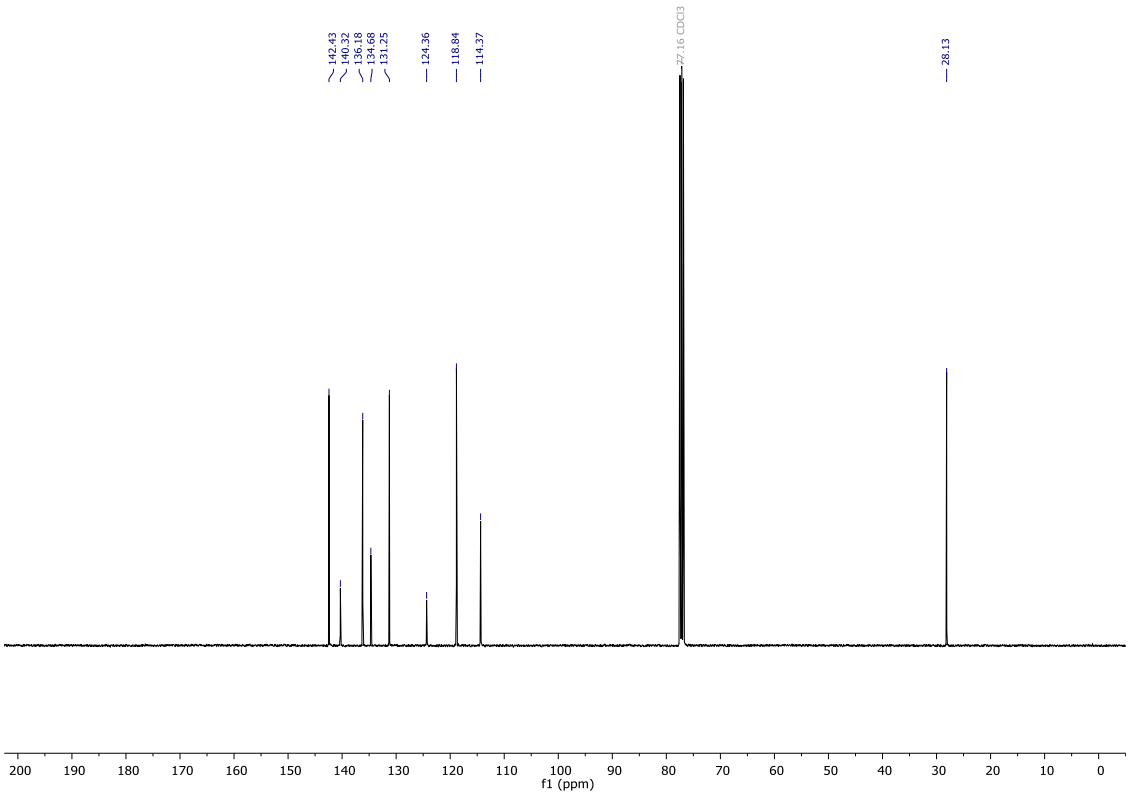
6-Chloro-8-iodoimidazo[1,2-*a*]pyrazine (7a)



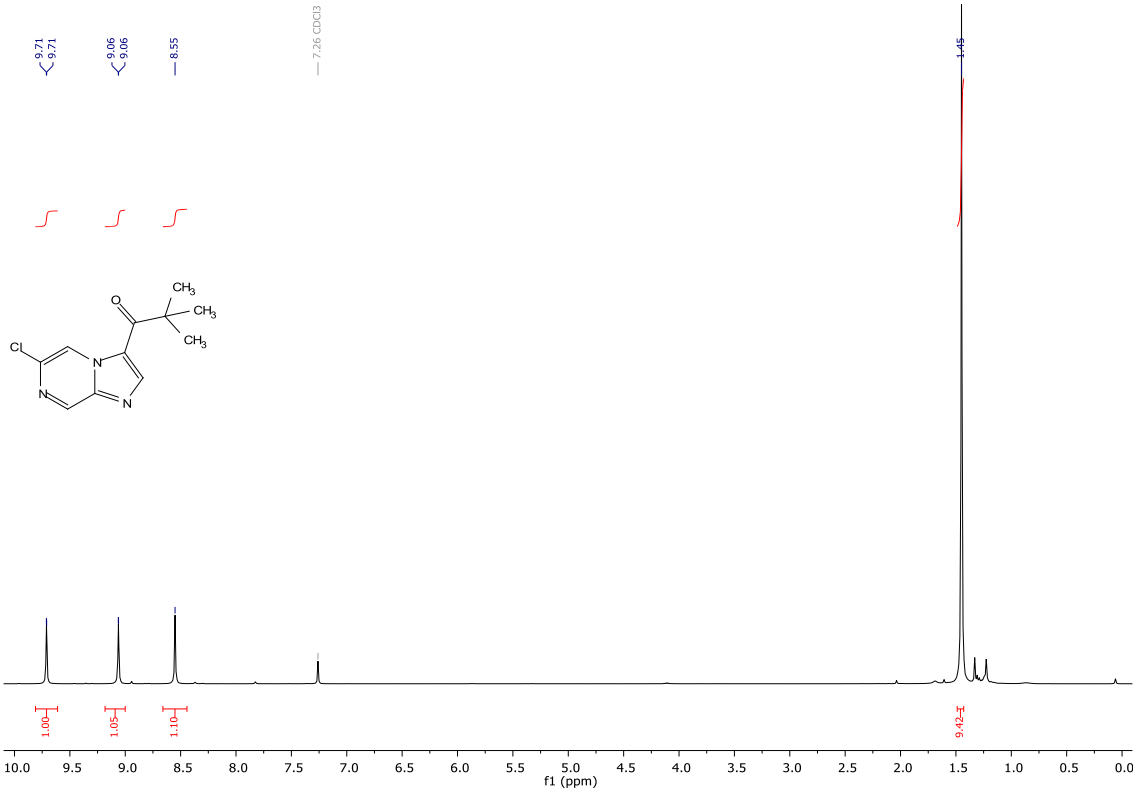


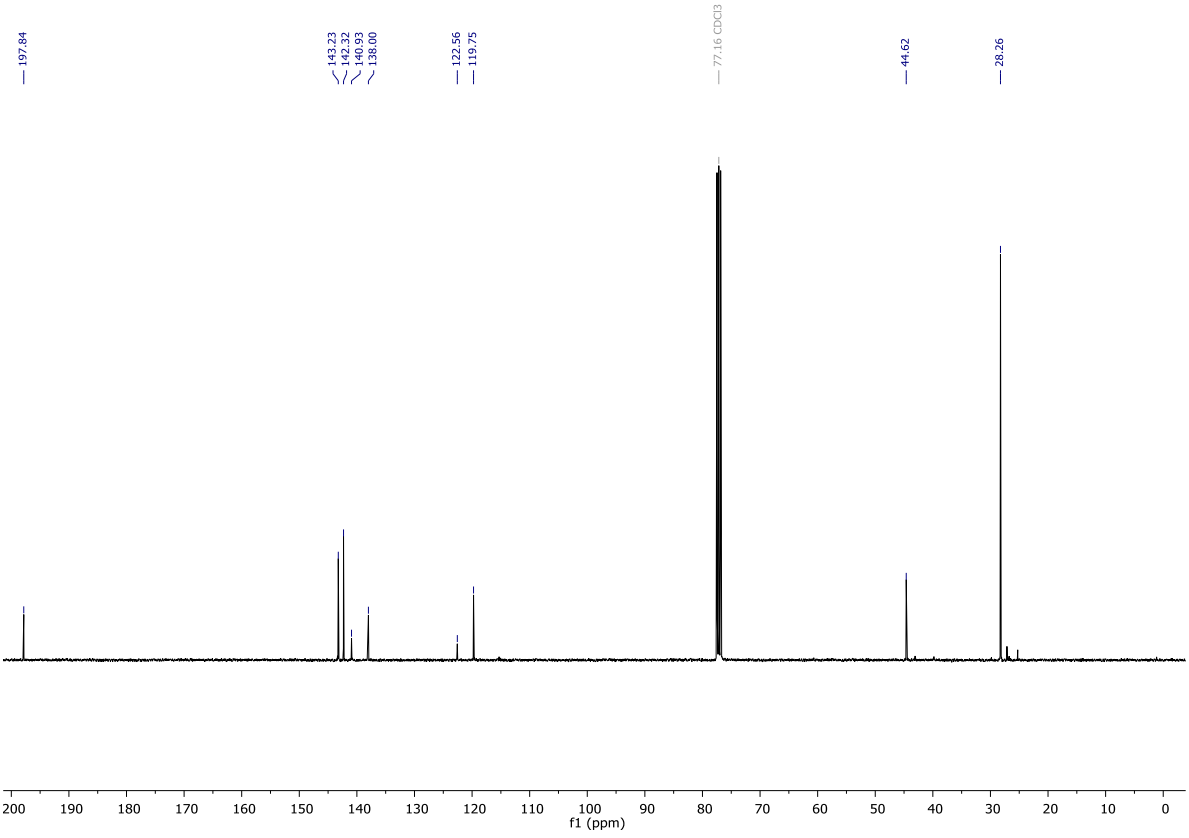
3-Allyl-6-chloroimidazo[1,2-*a*]pyrazine (7b)



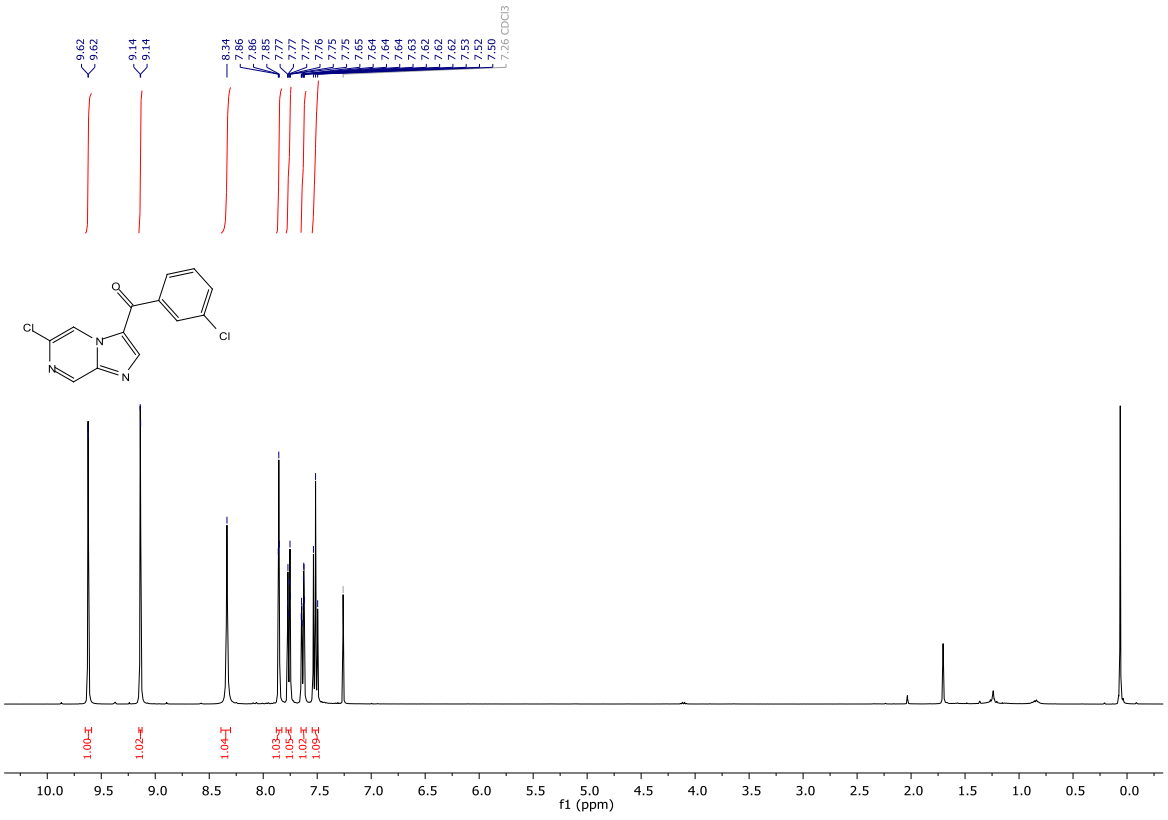


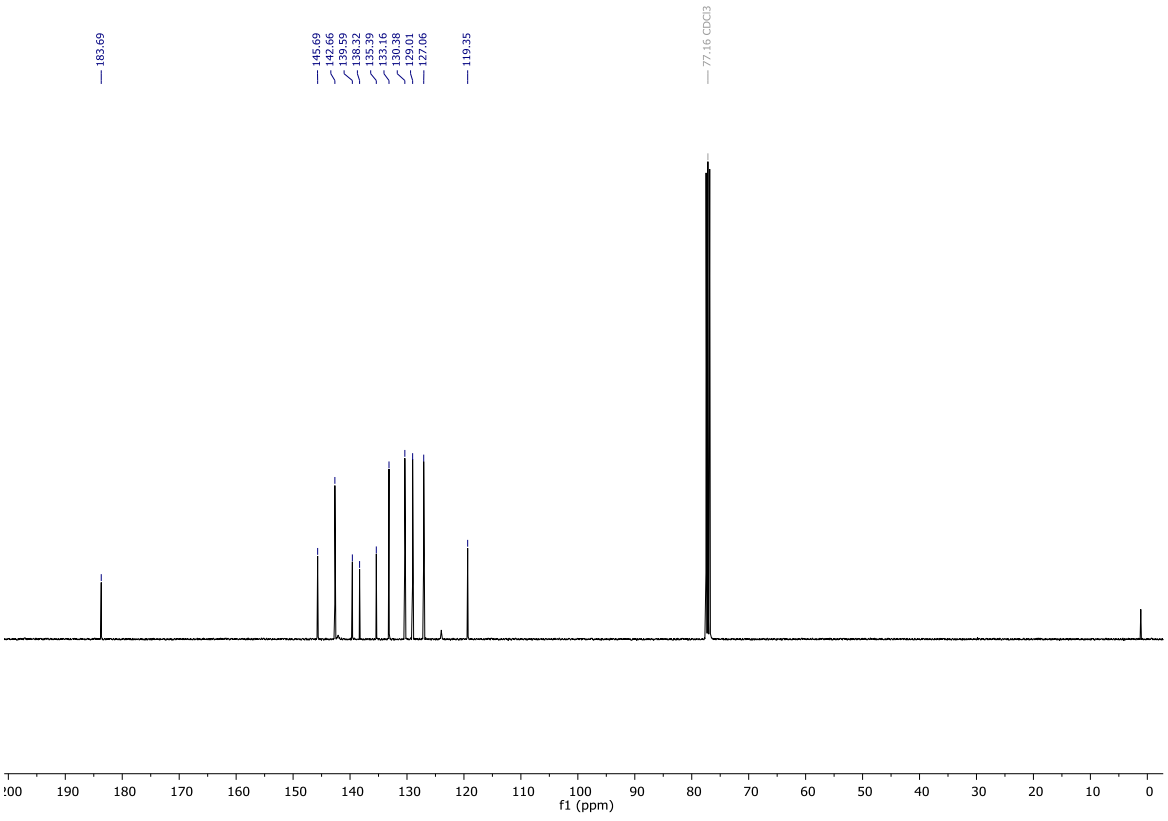
1-(6-Chloroimidazo[1,2-a]pyrazin-8-yl)-2,2-dimethylpropan-1-one (7c)



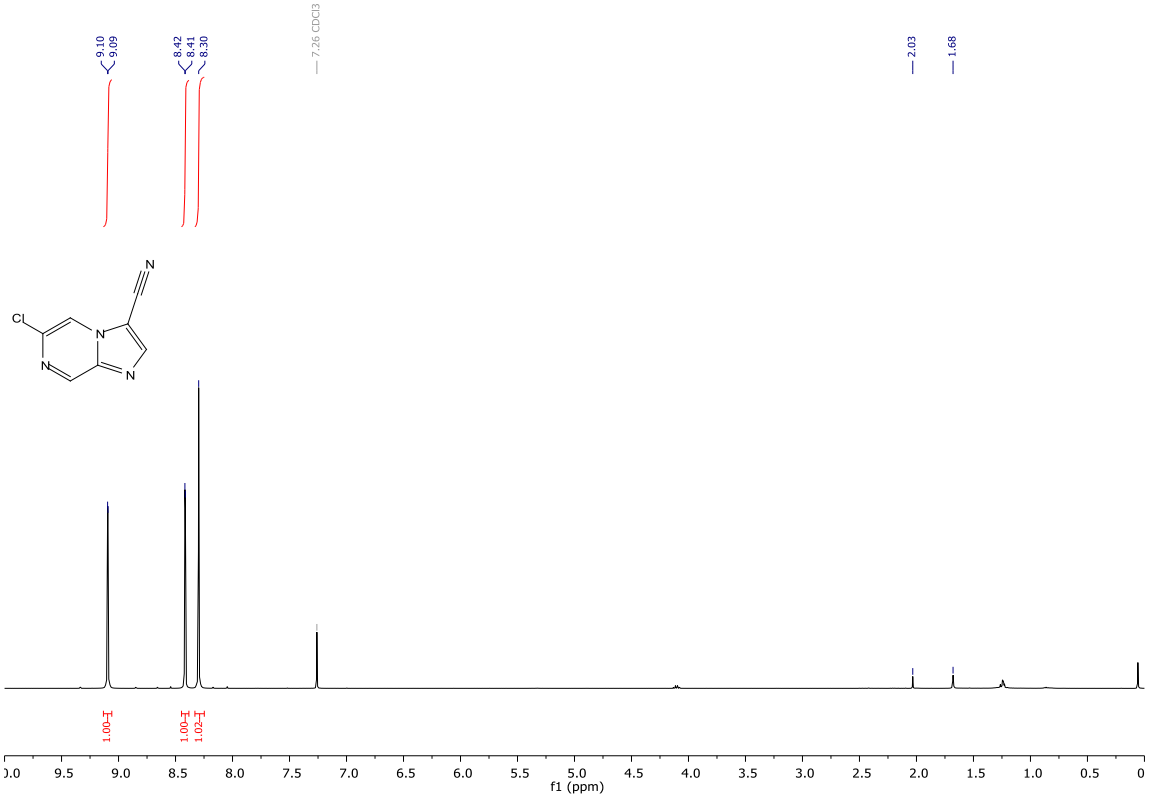


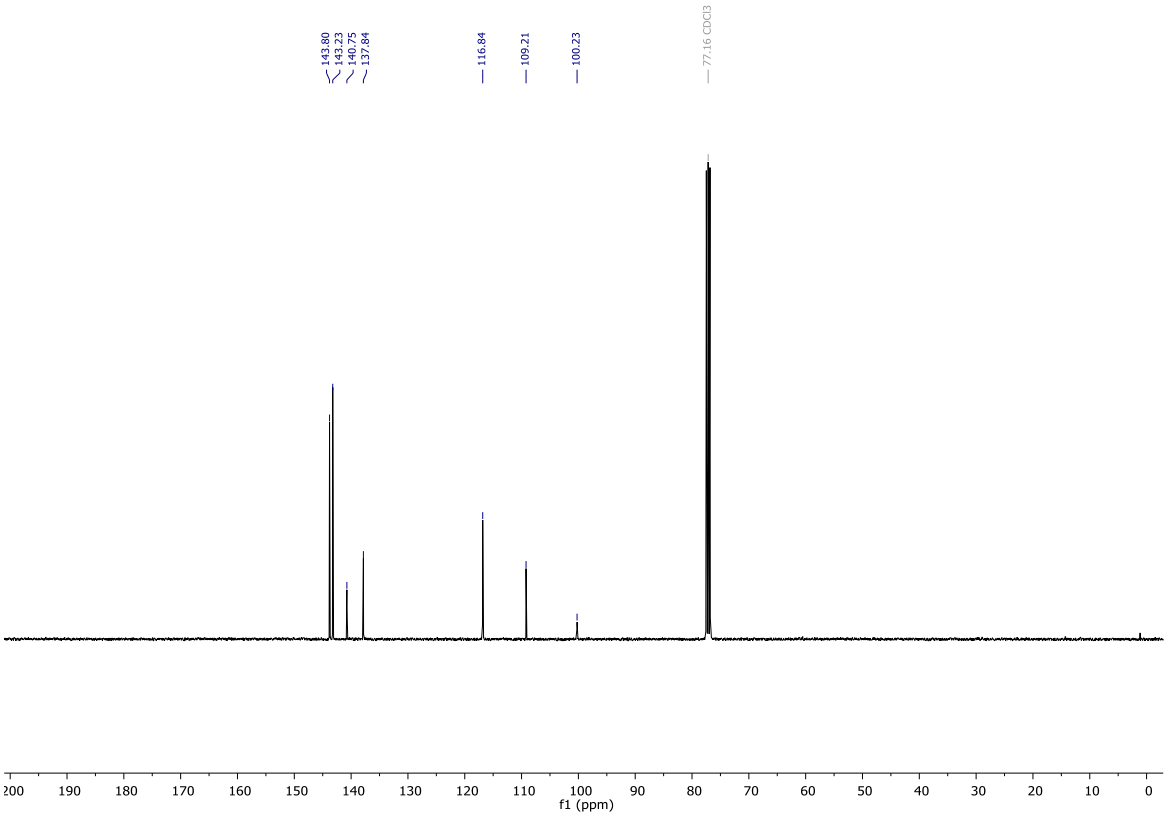
(6-Chloroimidazo[1,2-a]pyrazin-3-yl)(3-chlorophenyl)methanone (7d)



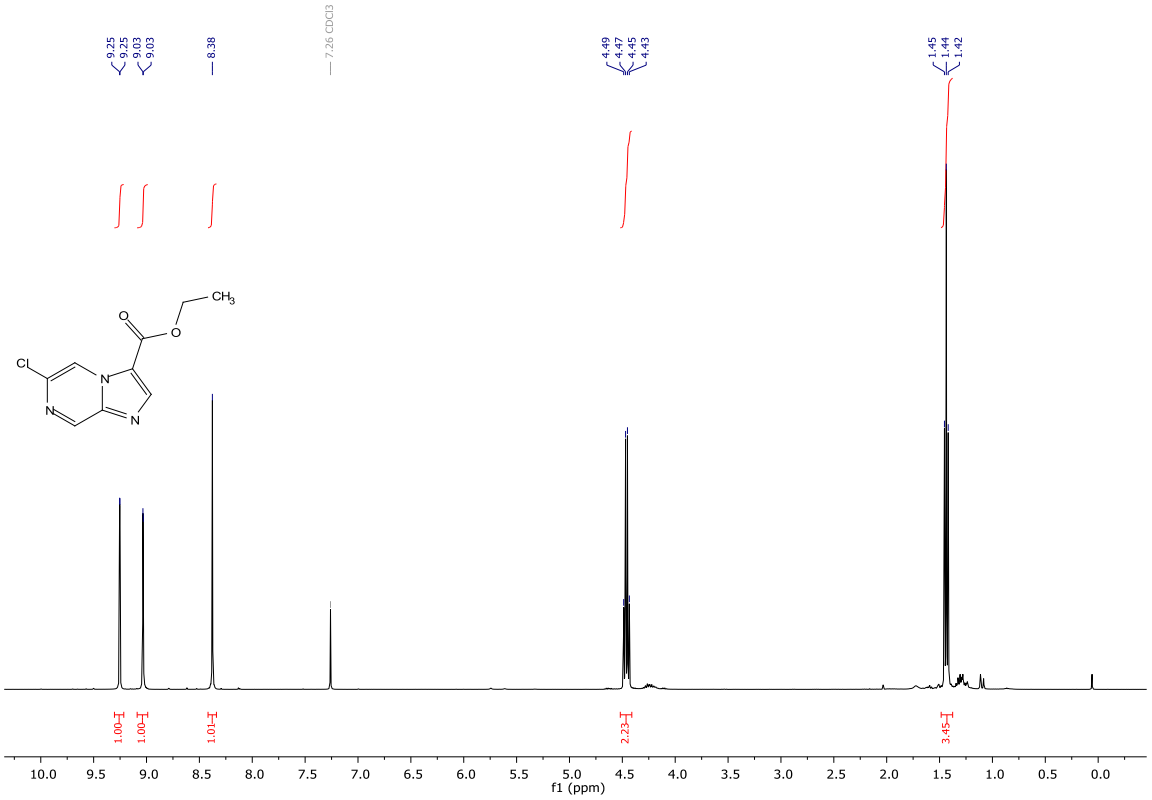


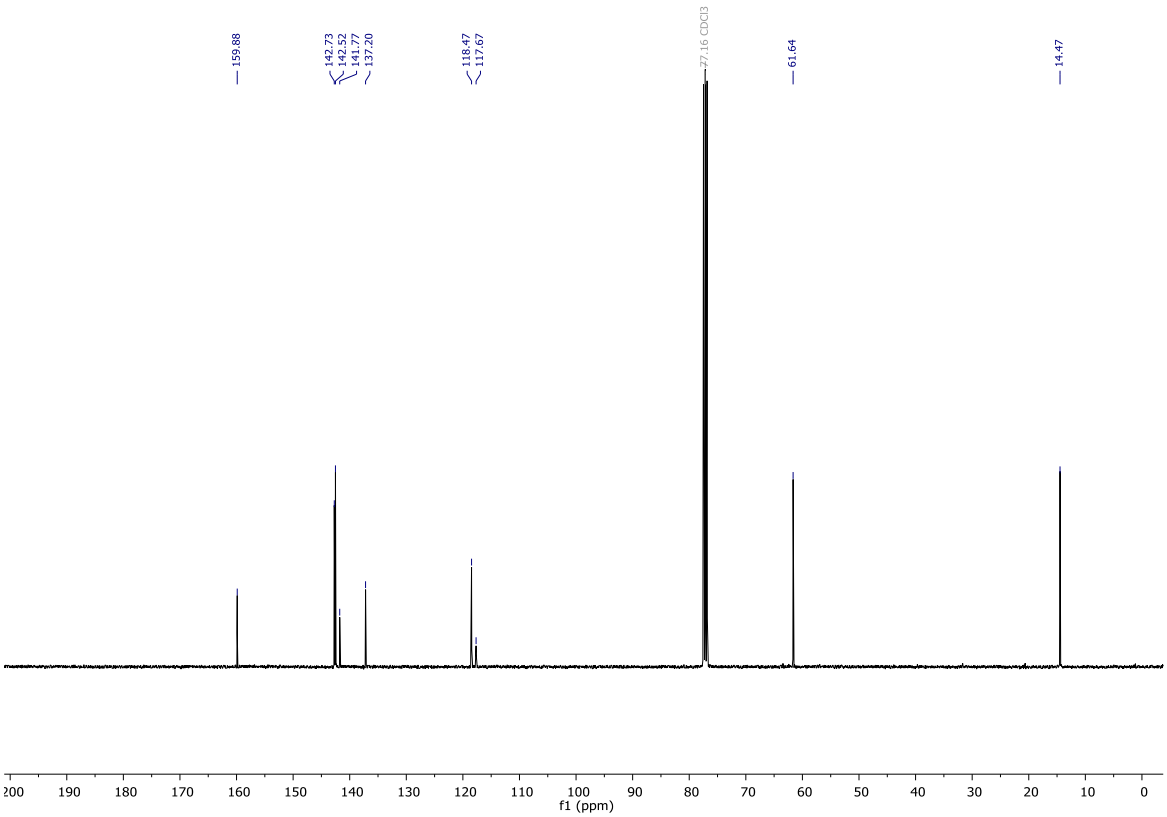
6-Chloroimidazo[1,2-a]pyrazine-8-carbonitrile (7e)



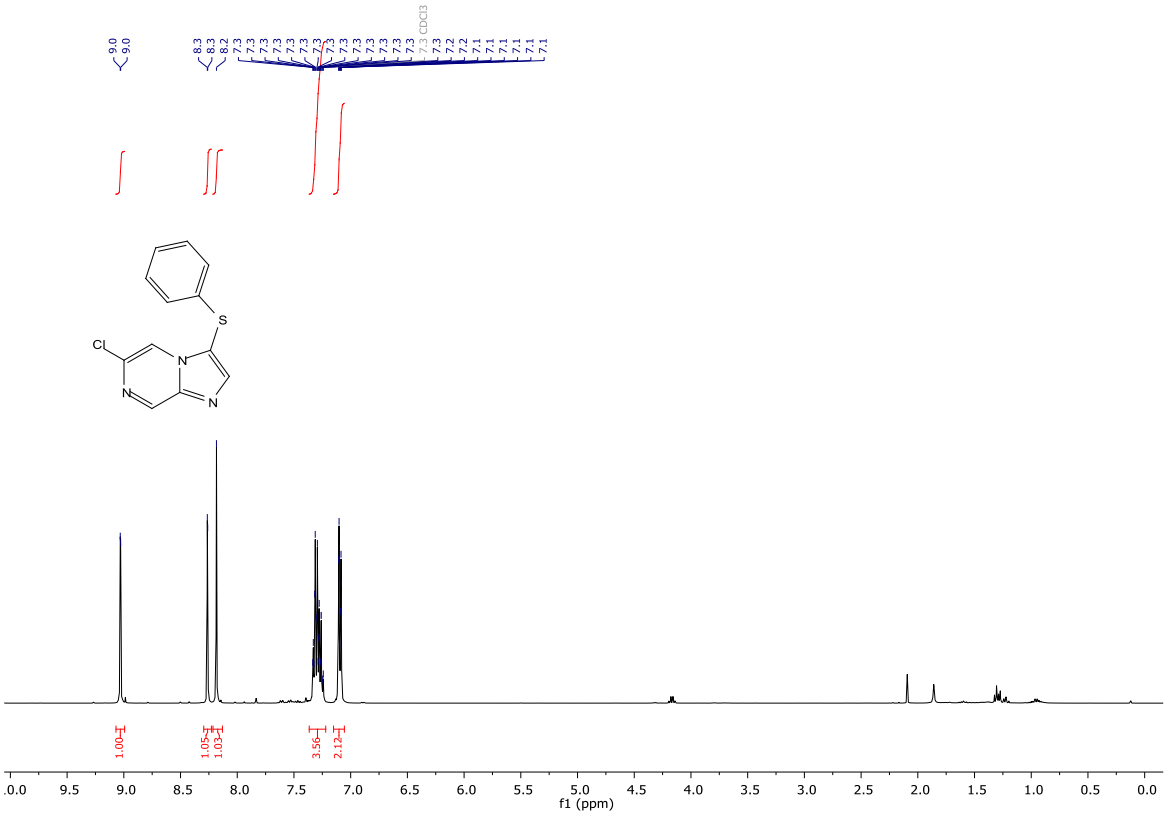


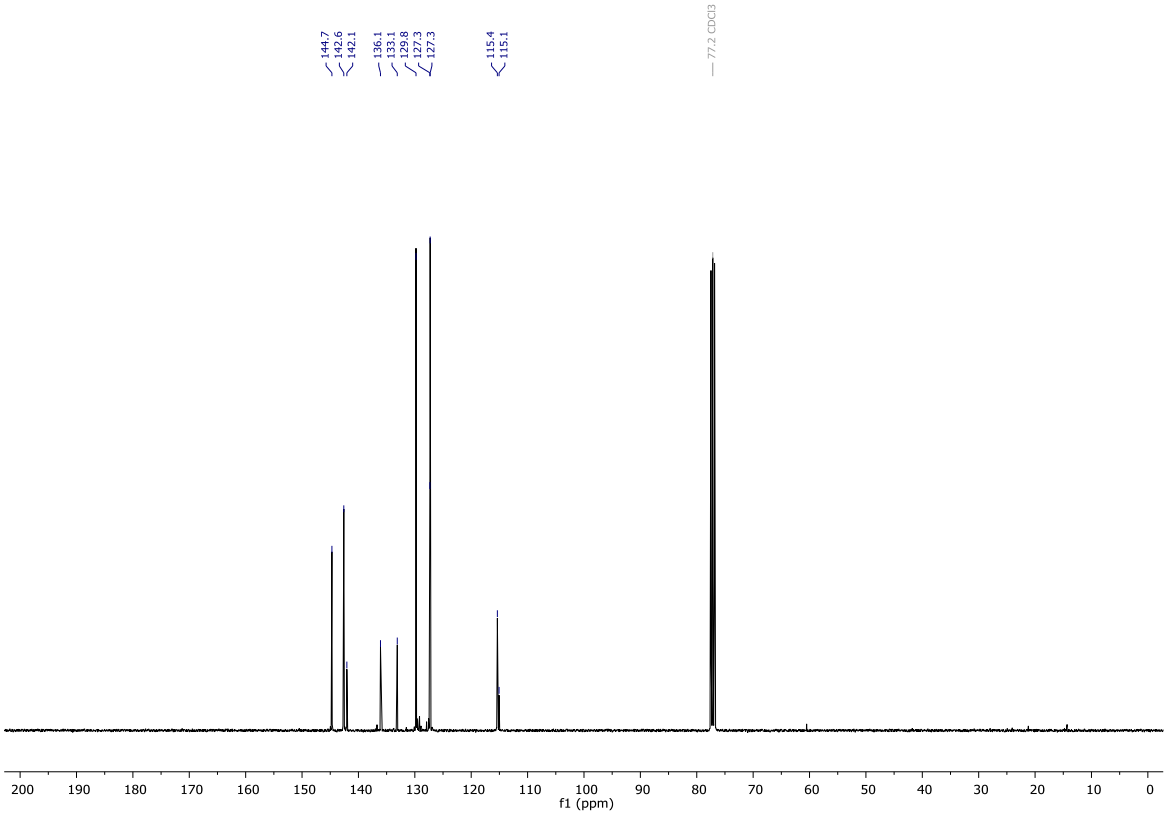
Ethyl 6-chloroimidazo[1,2-a]pyrazine-8-carboxylate (7f)



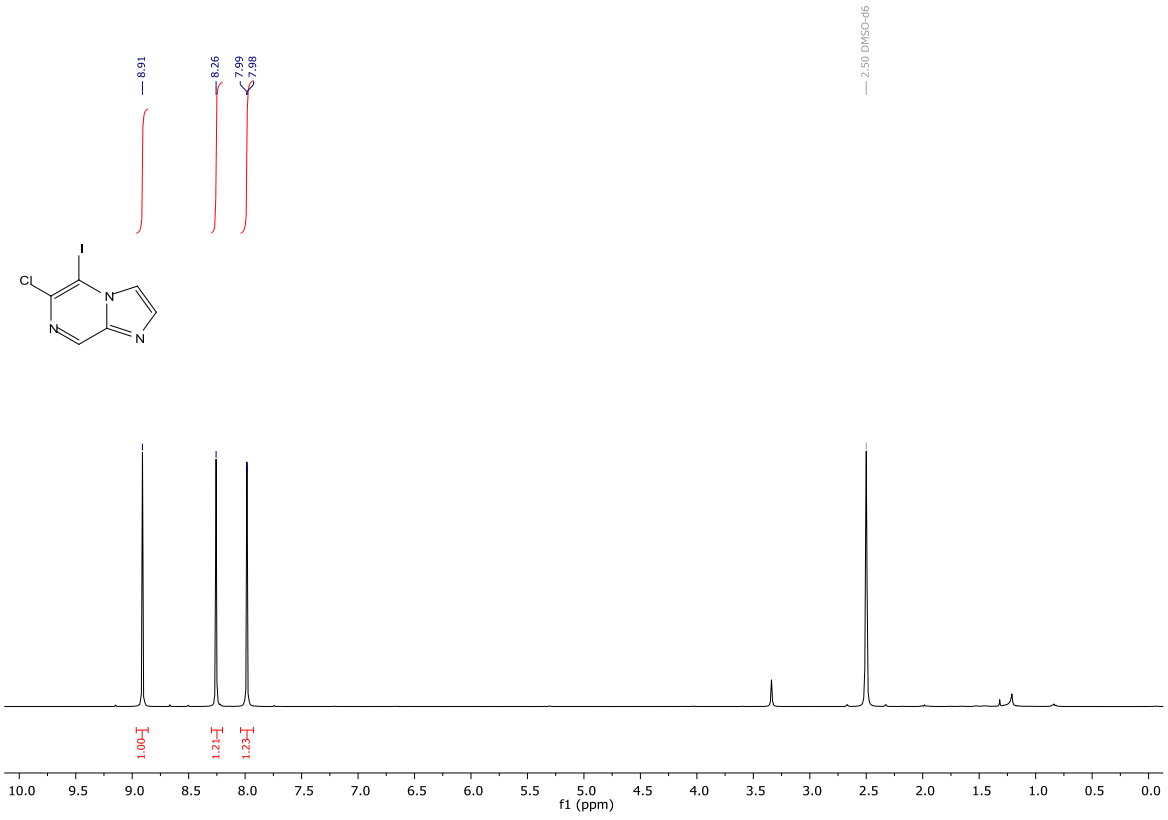


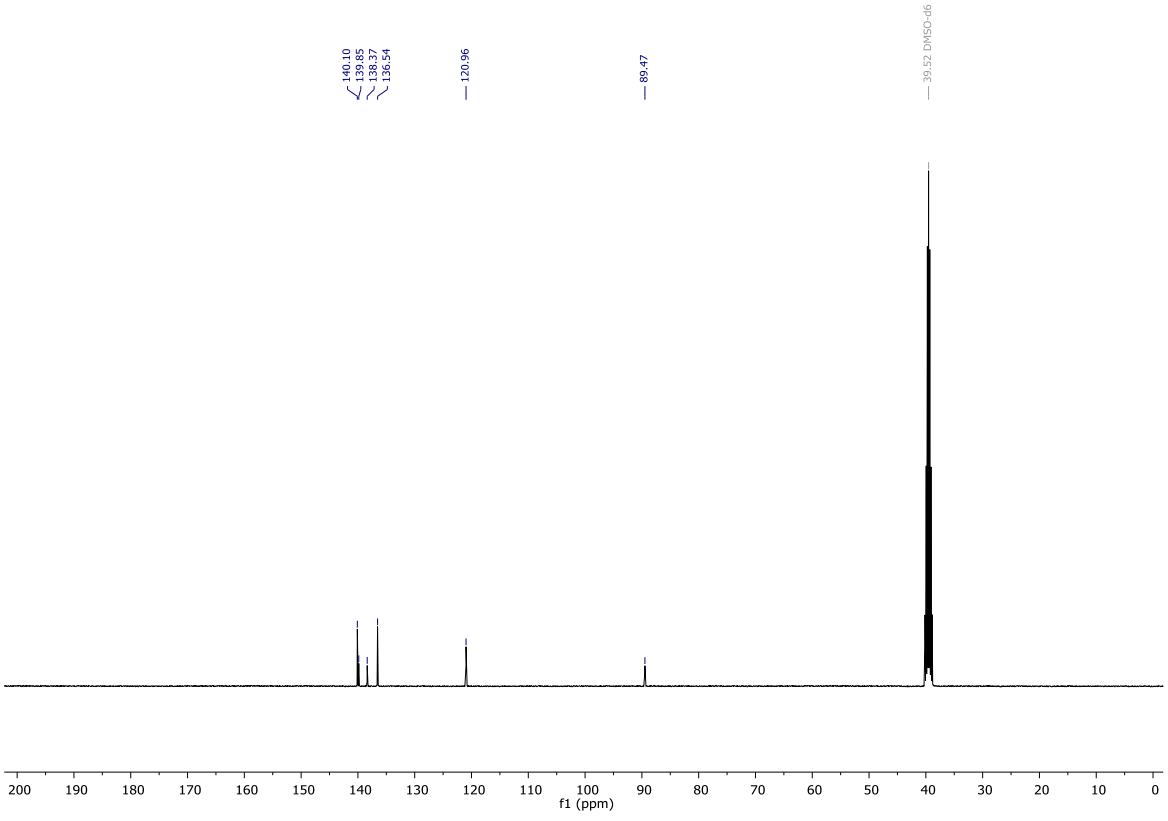
6-chloro-3-(phenylthio)imidazo[1,2-*a*]pyrazine (7g)



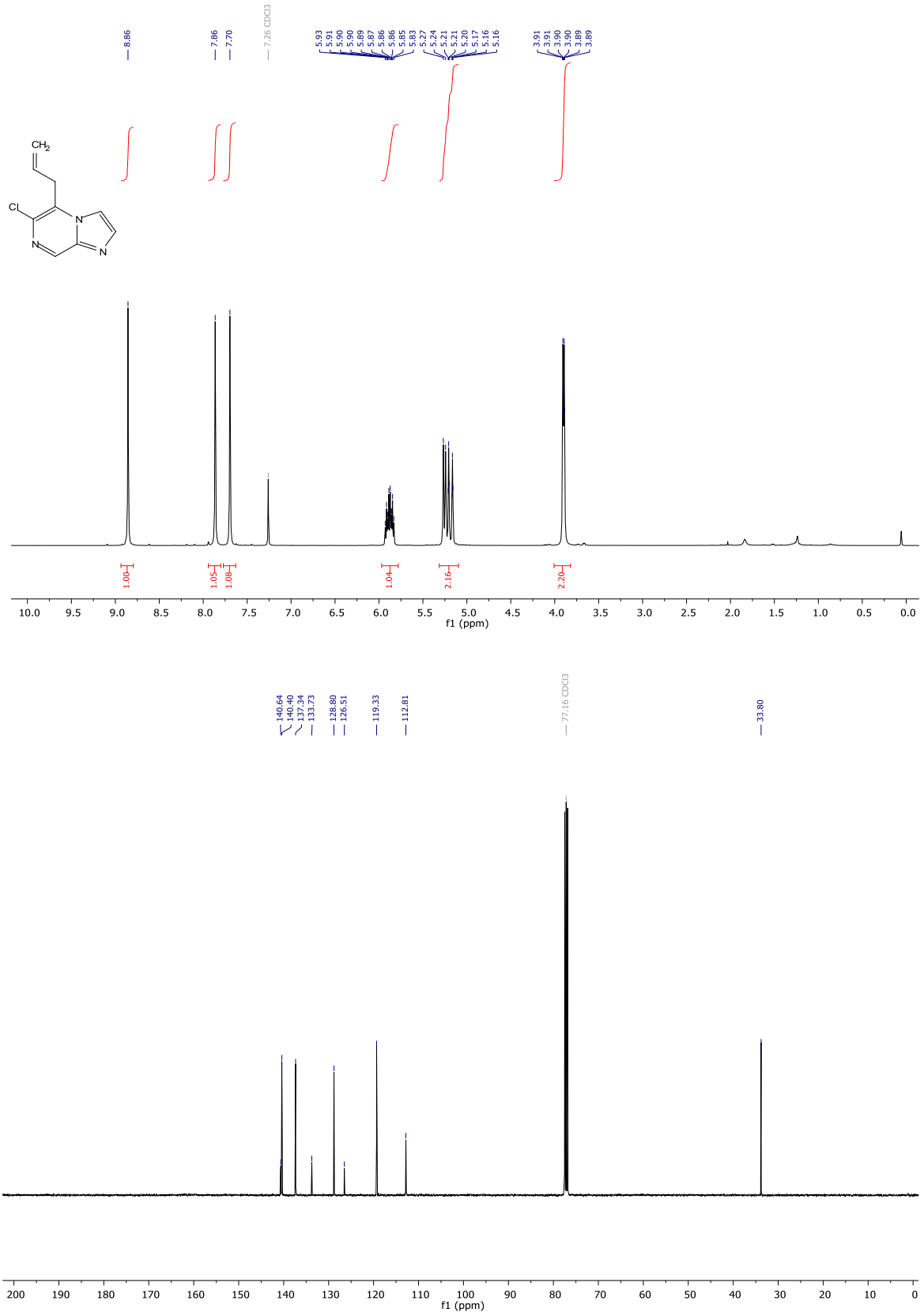


6-Chloro-5-iodoimidazo[1,2-*a*]pyrazine (8a)

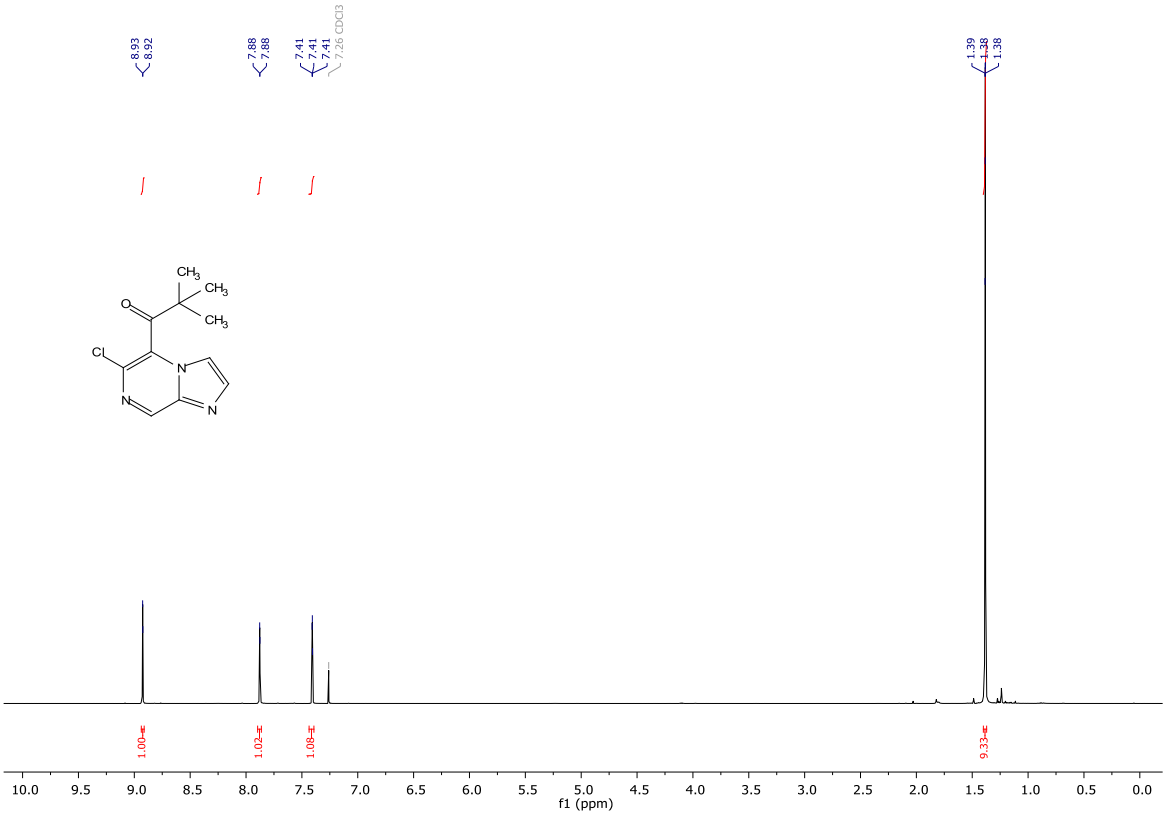


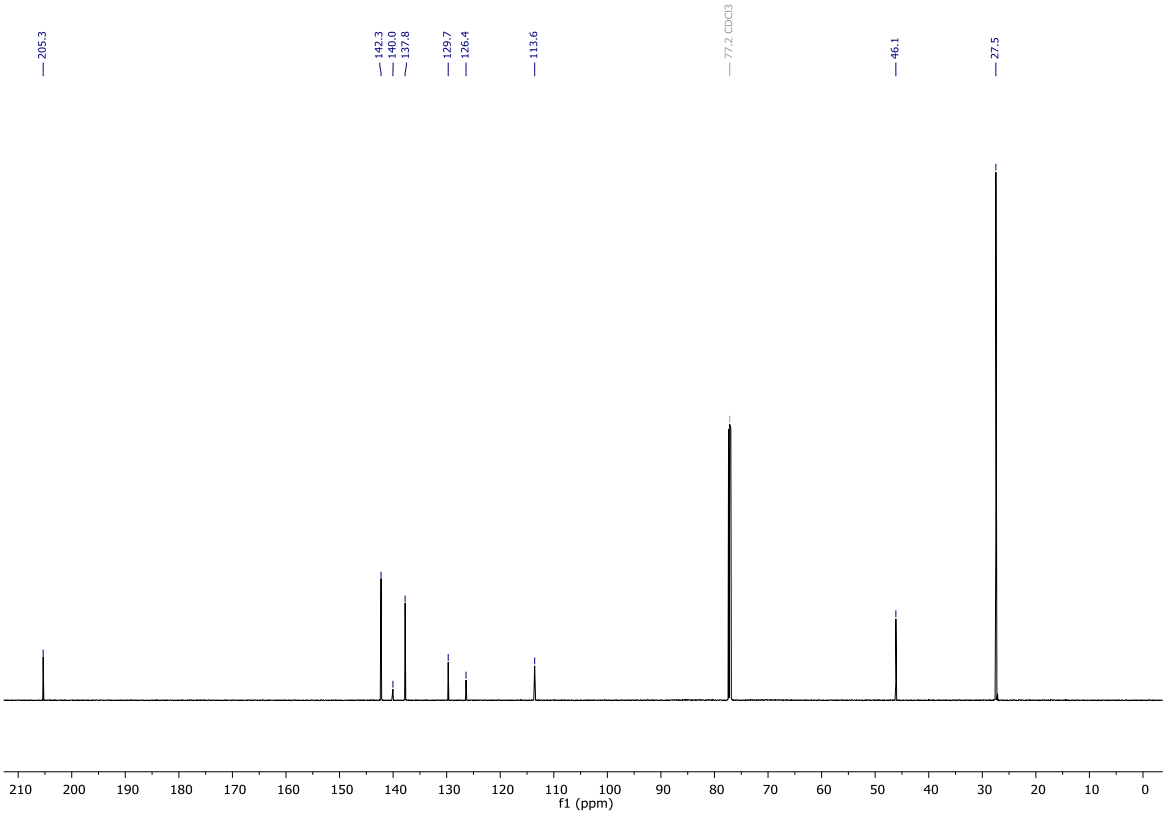


5-Allyl-6-chloroimidazo[1,2-*a*]pyrazine (8b)

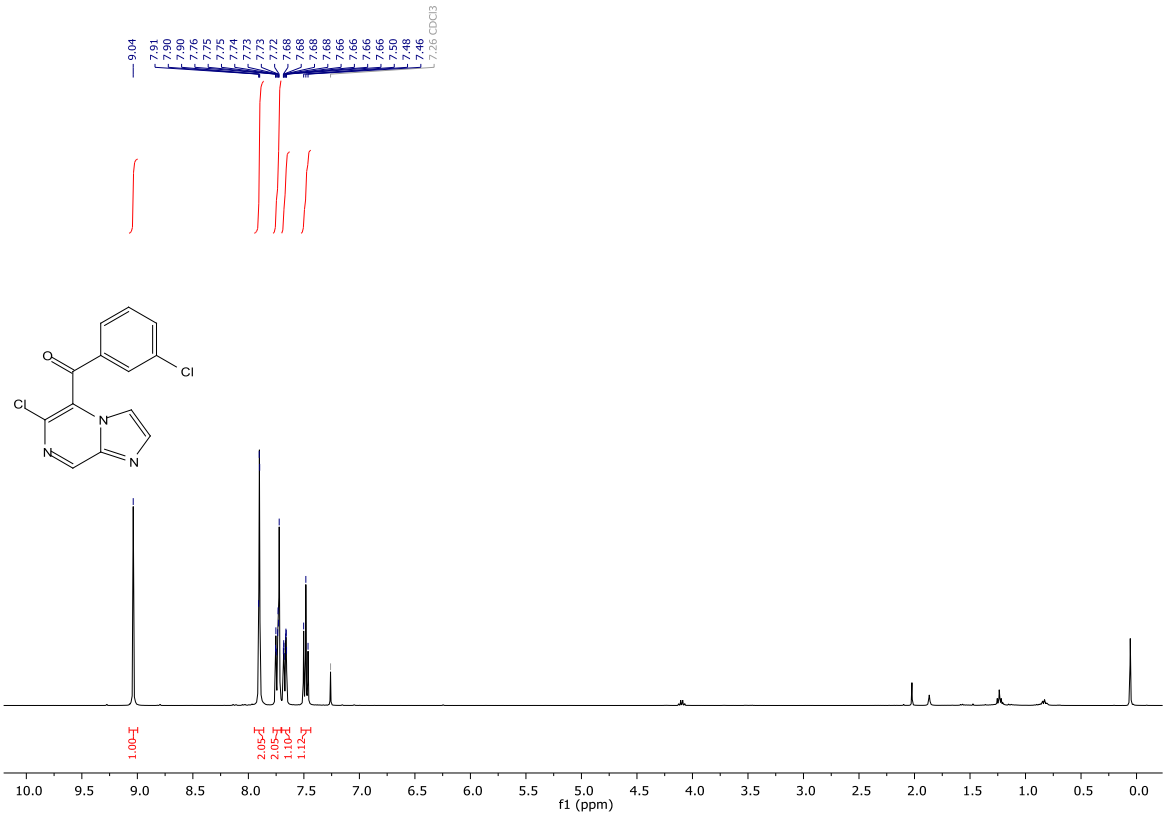


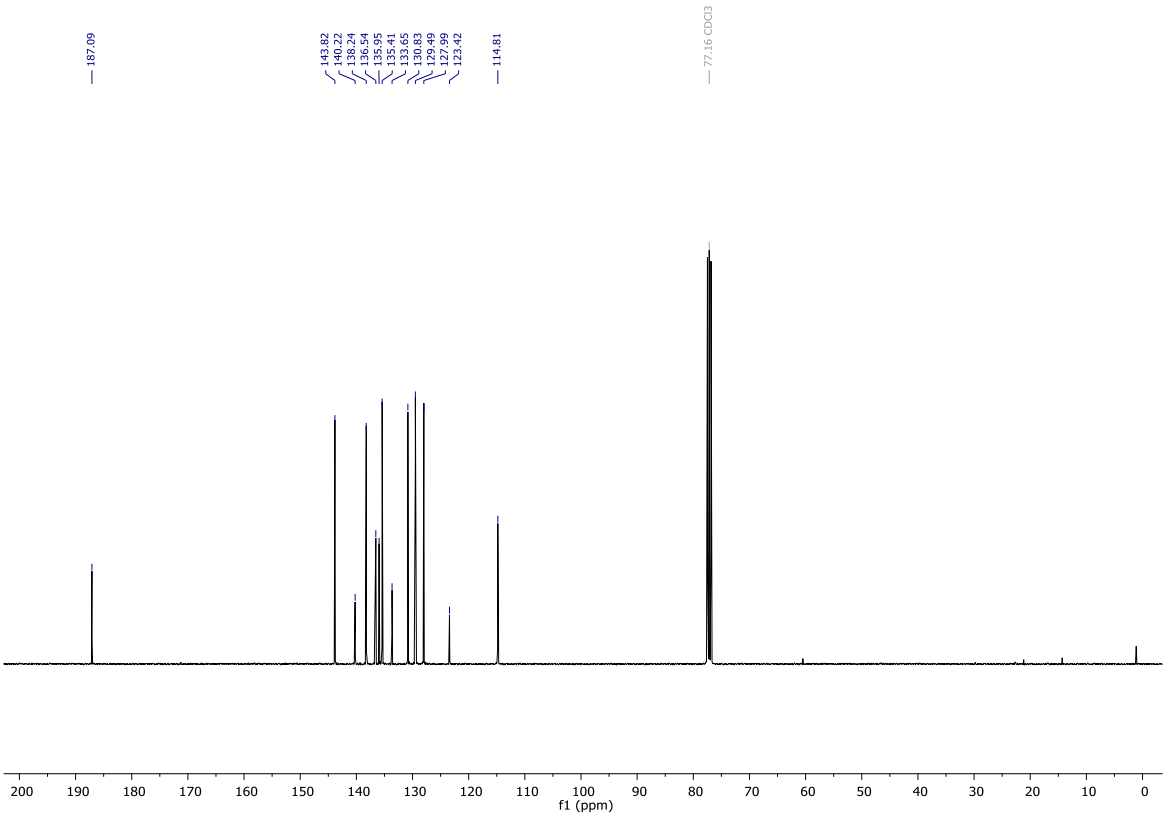
1-(6-Chloroimidazo[1,2-*a*]pyrazin-5-yl)-2,2-dimethylpropan-1-one (8c)



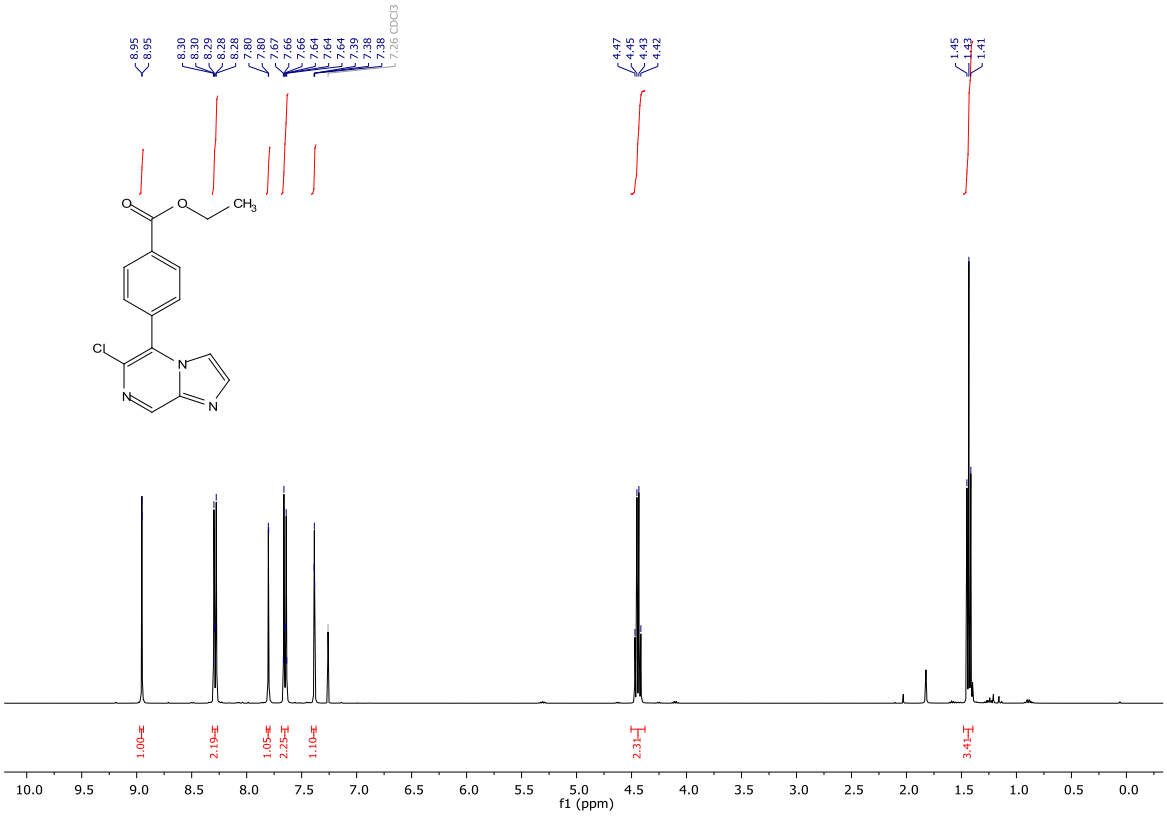


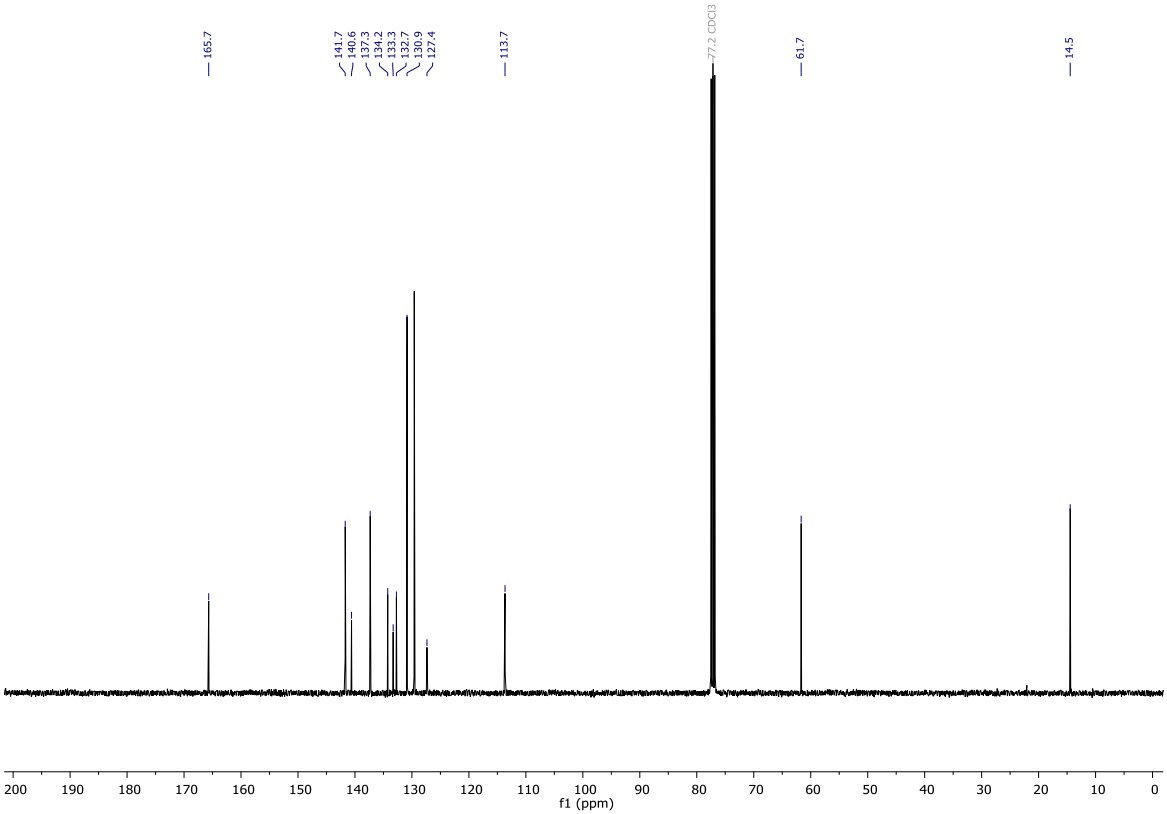
(6-Chloroimidazo[1,2-a]pyrazin-5-yl)(3-chlorophenyl)methanone (8d)



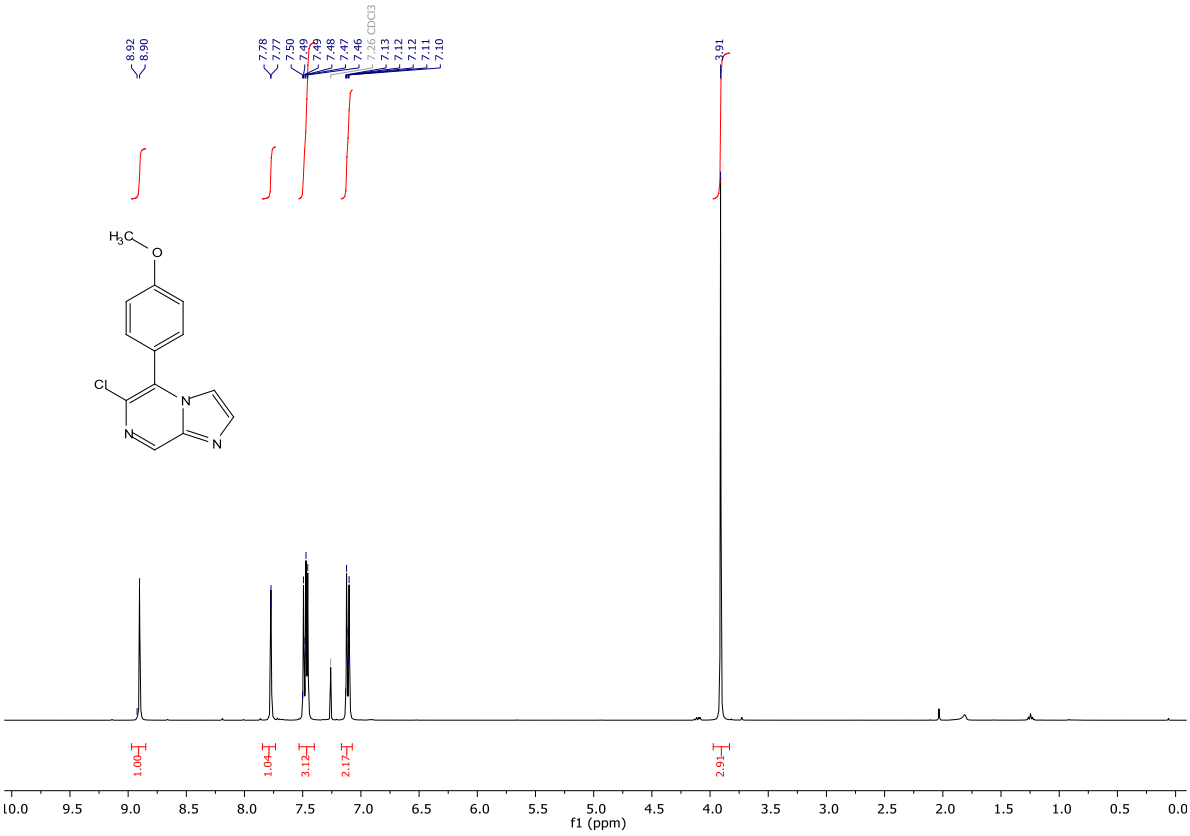


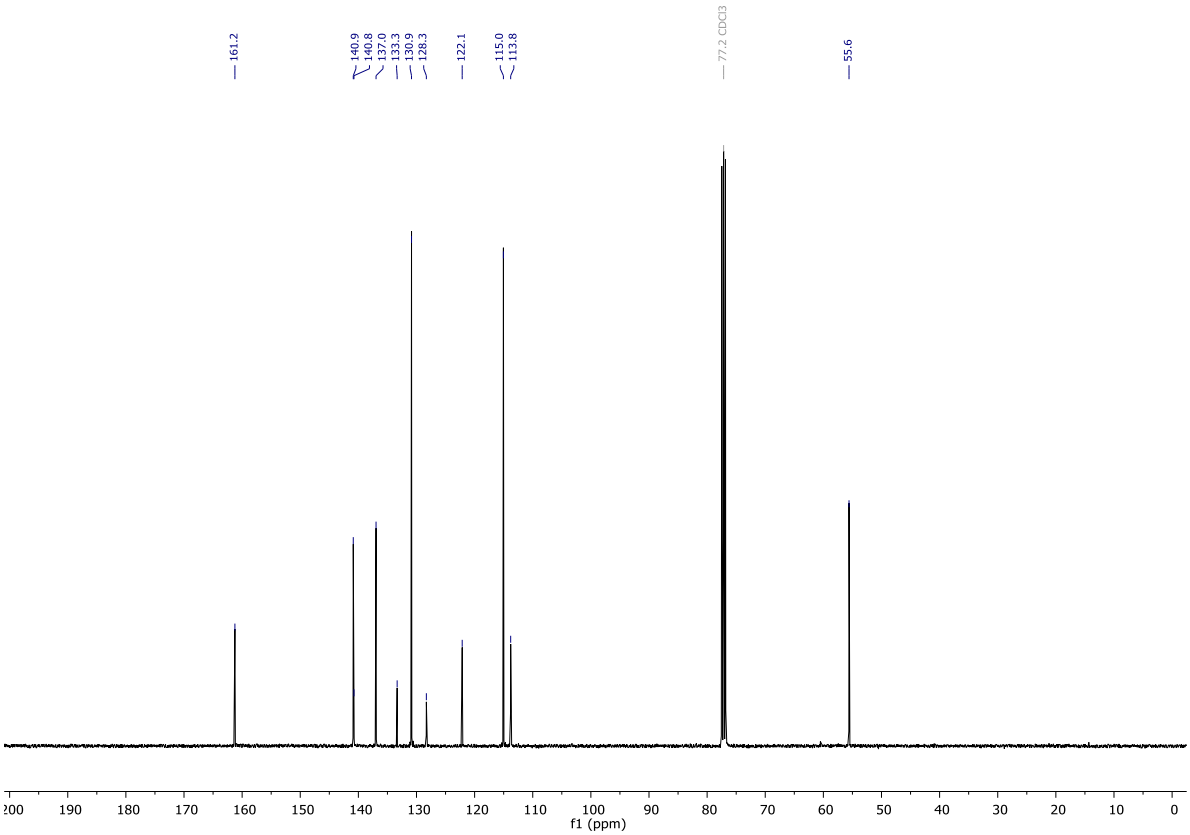
Ethyl 4-(6-chloroimidazo[1,2-*a*]pyrazin-5-yl)benzoate (8e)



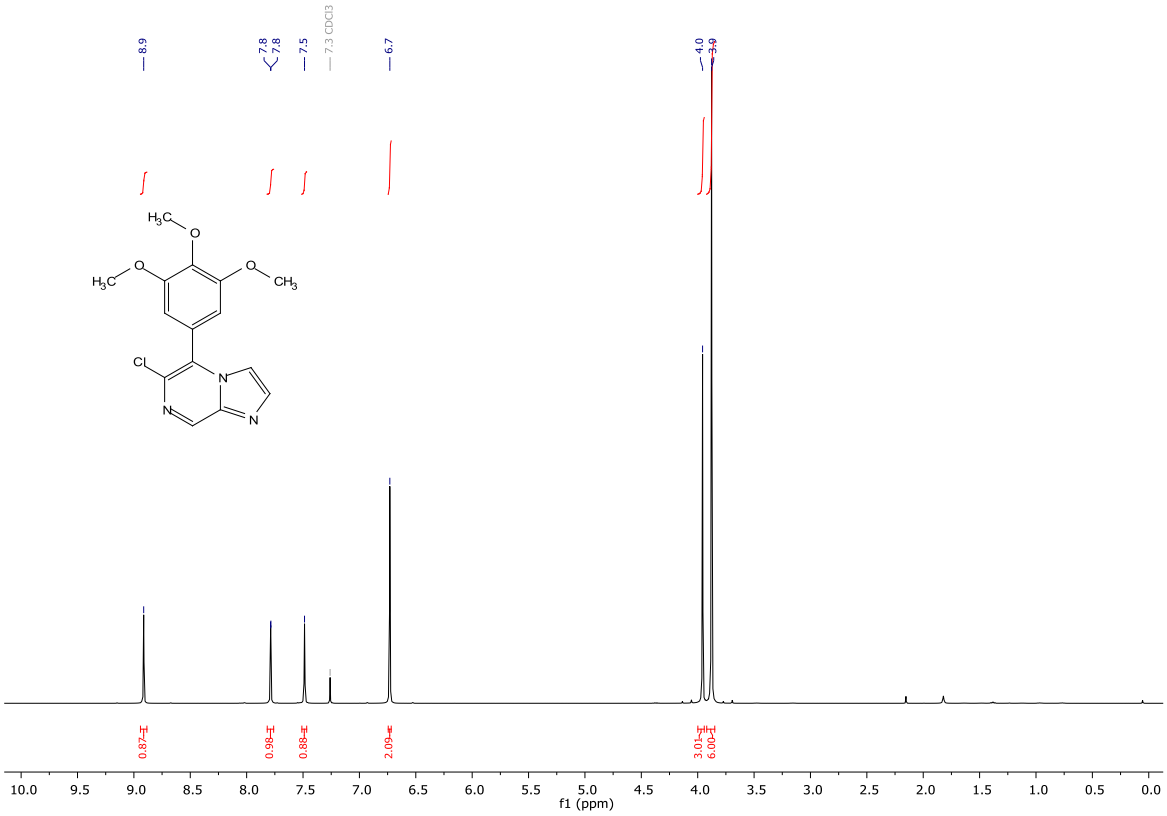


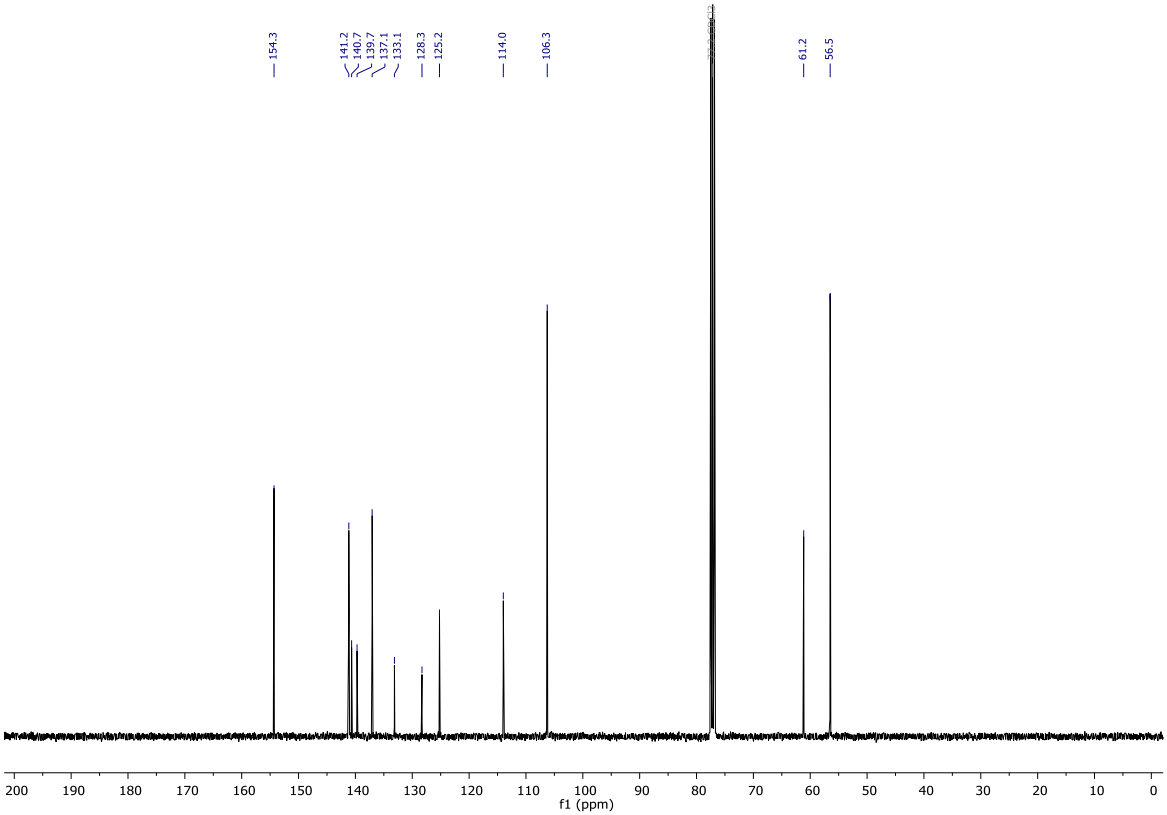
6-Chloro-5-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine (8f)



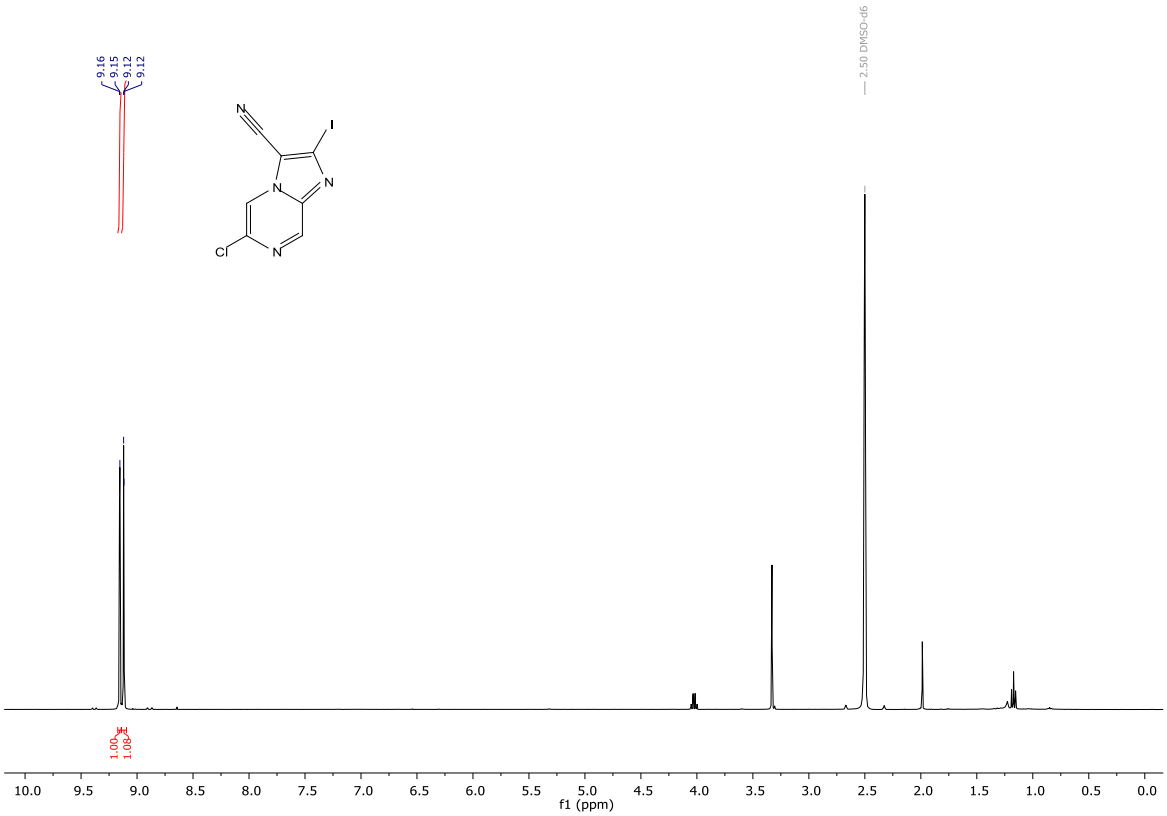


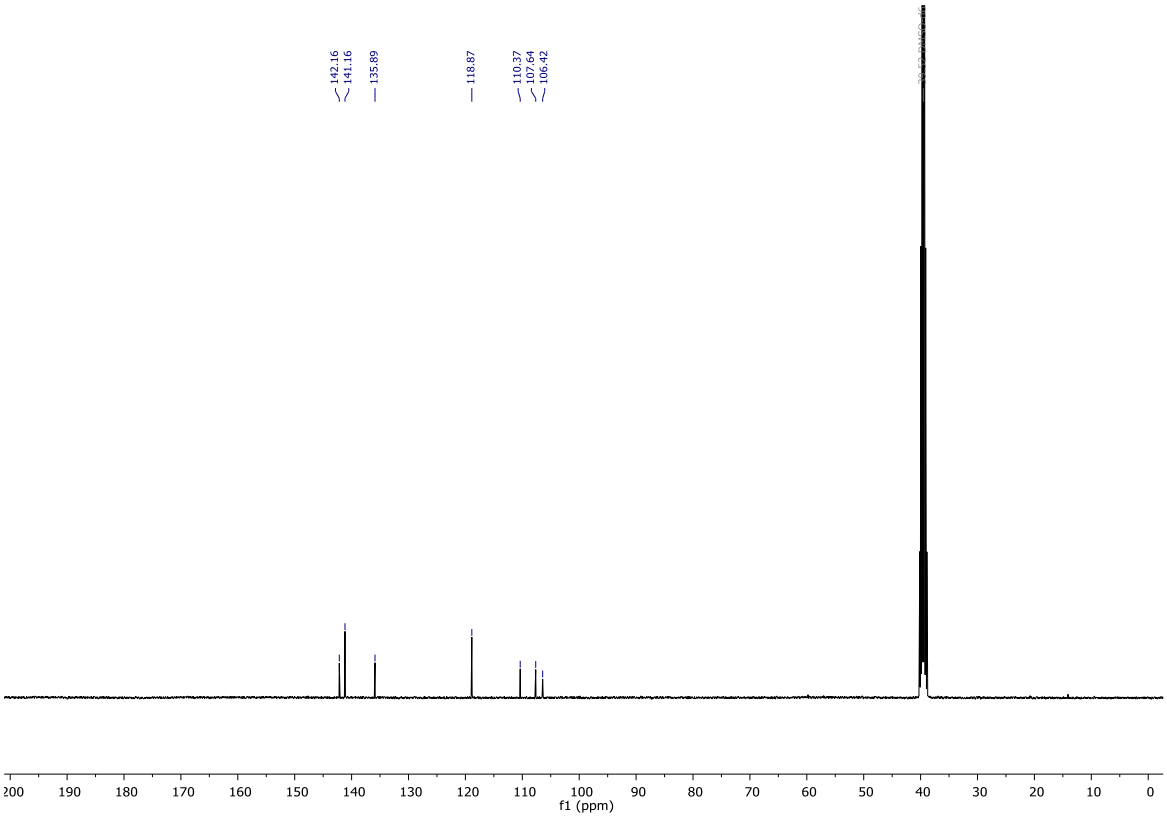
6-Chloro-5-(3,4,5-trimethoxyphenyl)imidazo[1,2-*a*]pyrazine (8g)



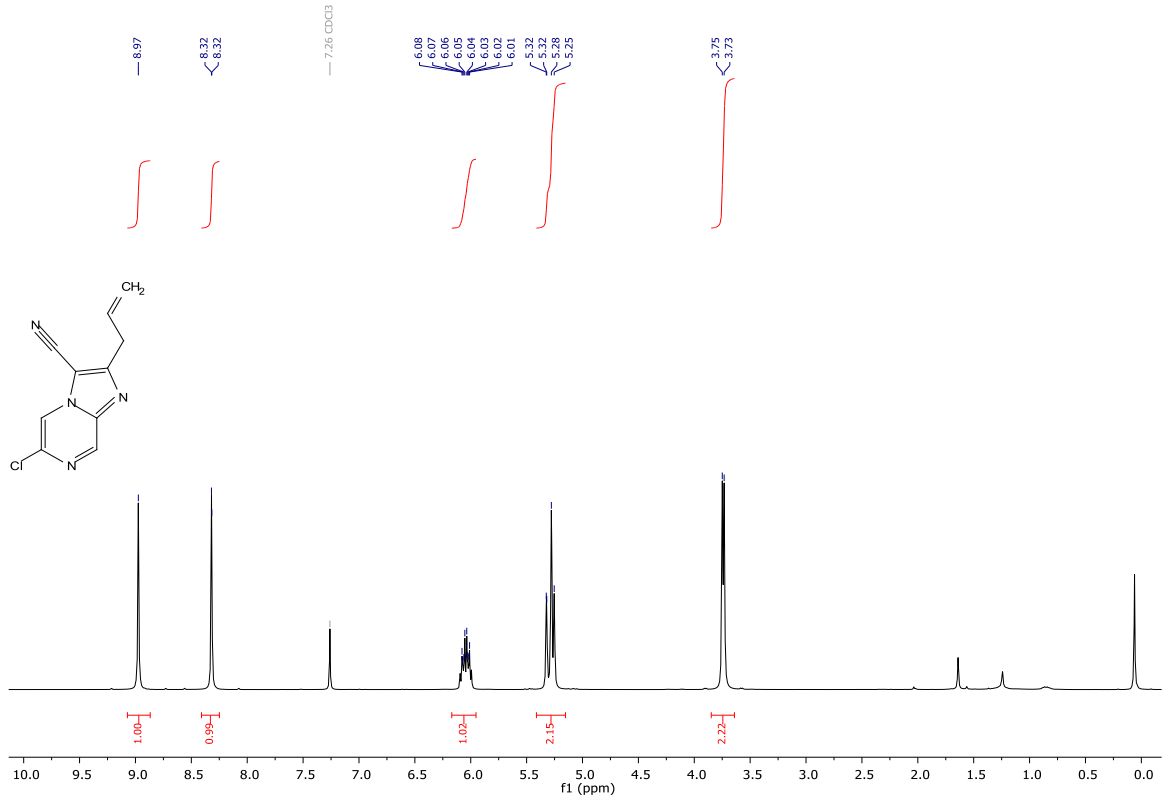


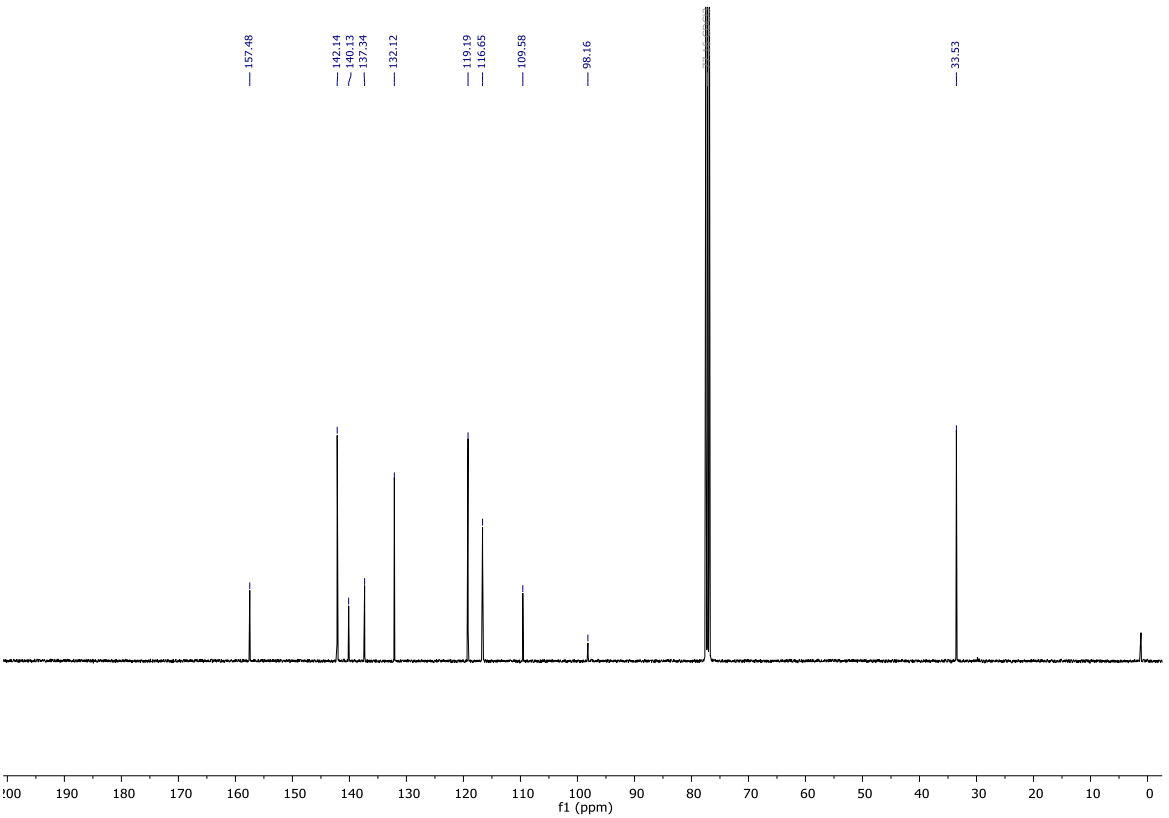
6-Chloro-2-iodoimidazo[1,2-*a*]pyrazine-3-carbonitrile (16a)



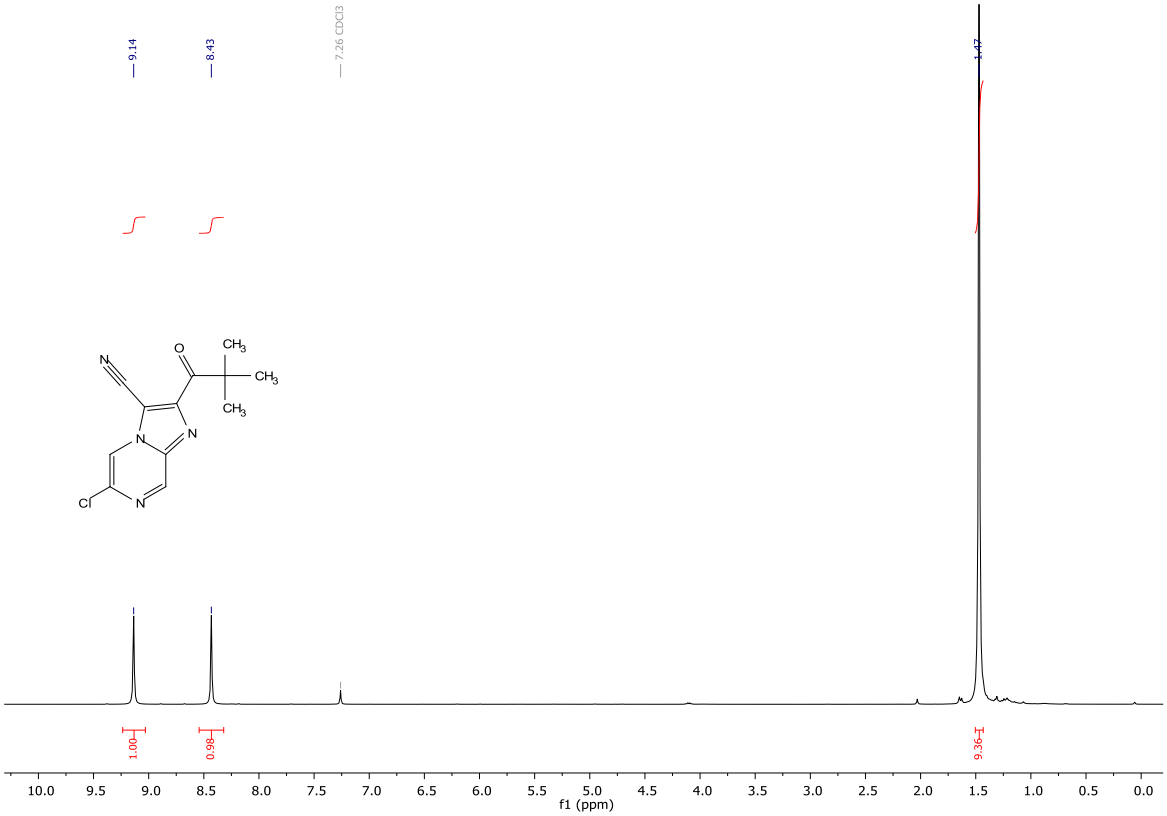


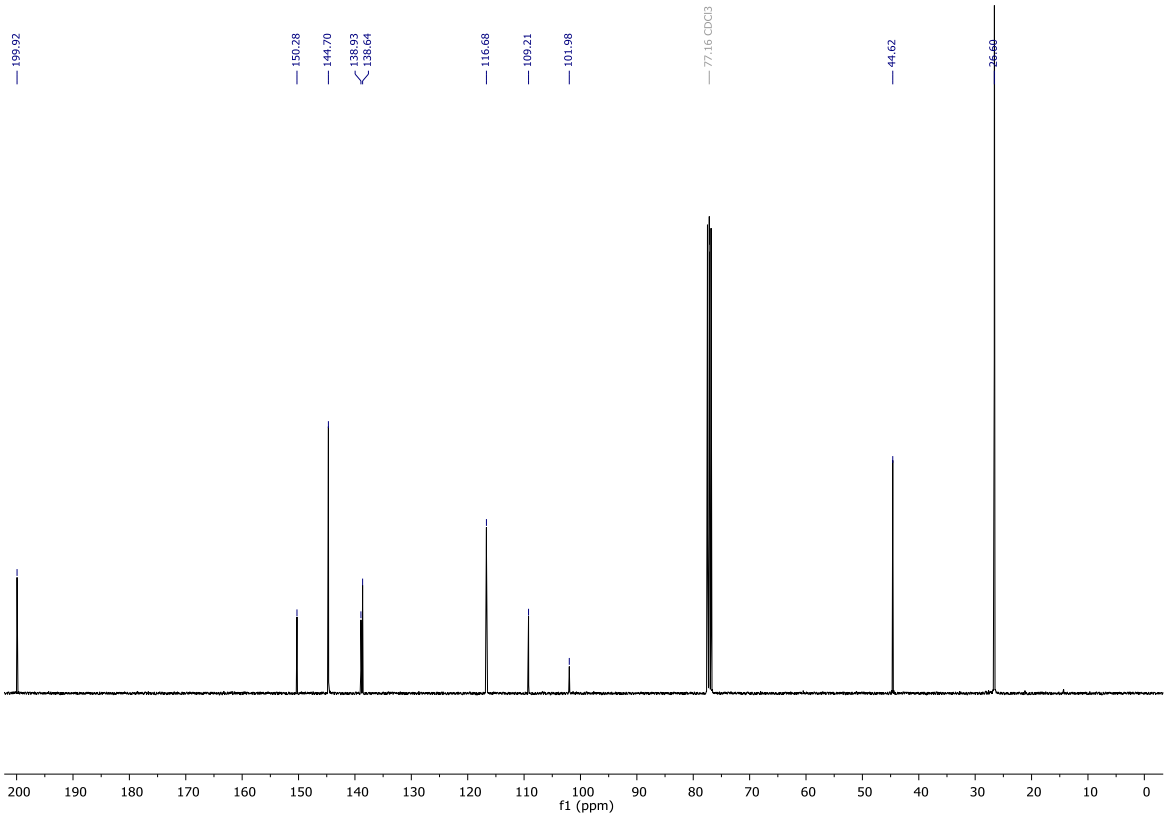
2-Allyl-6-chloroimidazo[1,2-*a*]pyrazine-3-carbonitrile (16b)



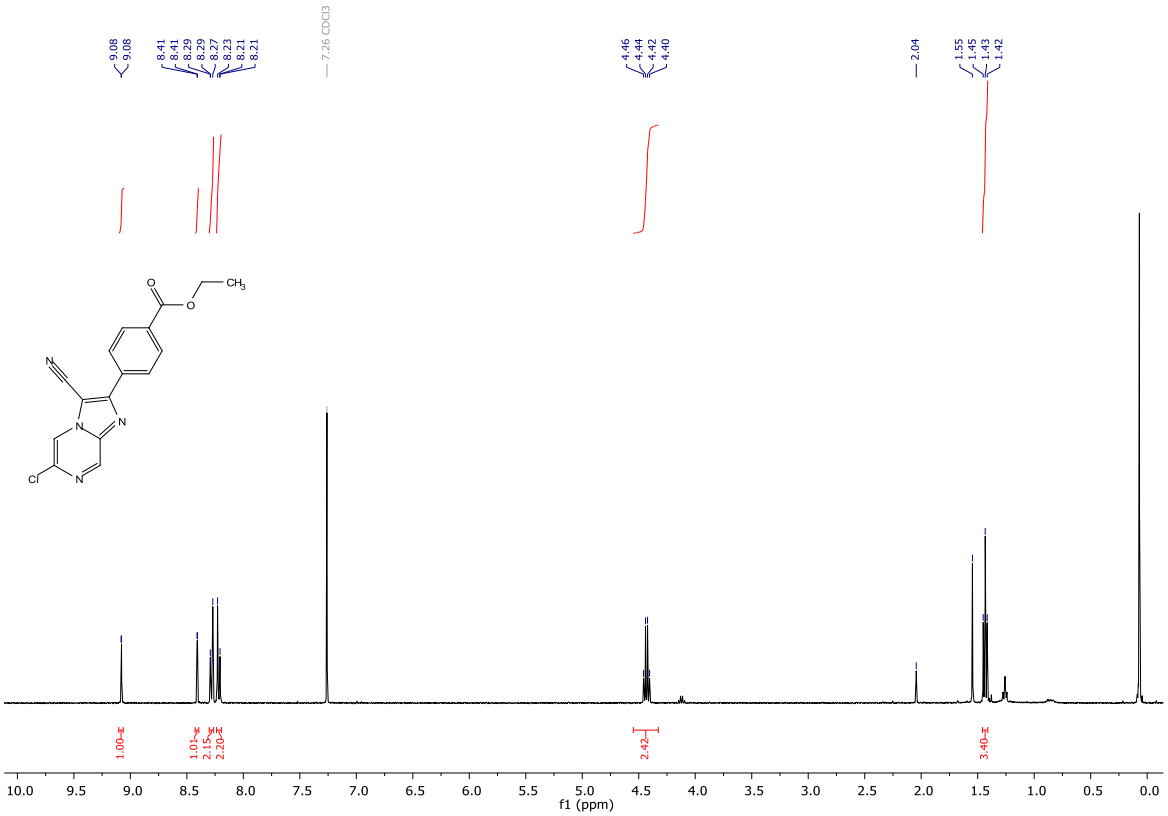


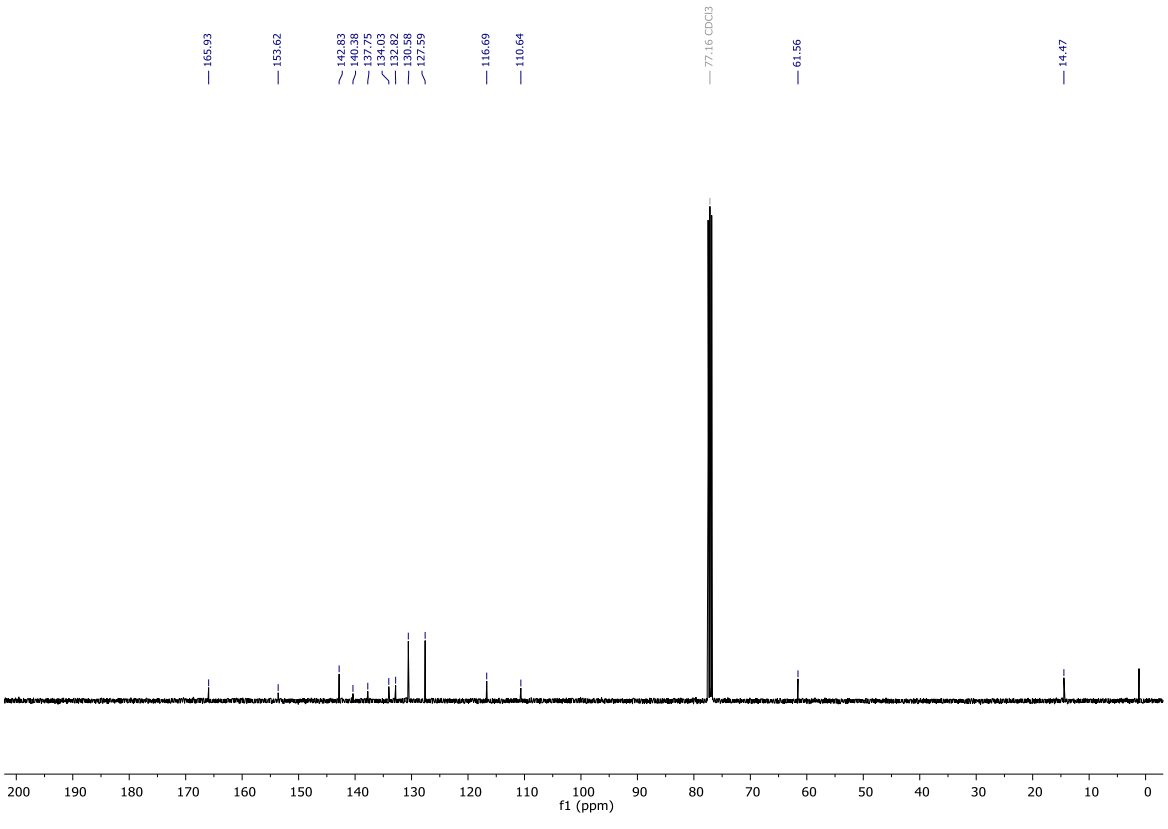
6-Chloro-2-pivaloylimidazo[1,2-*a*]pyrazine-3-carbonitrile (16c)



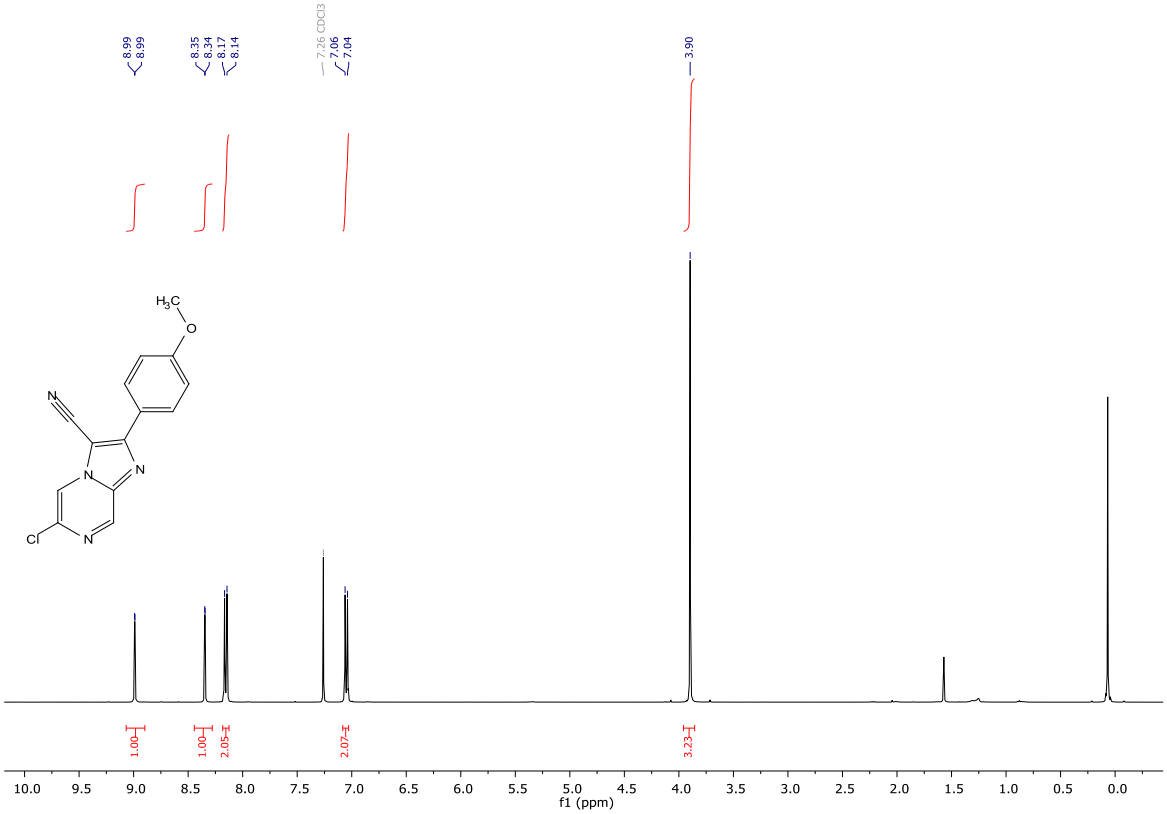


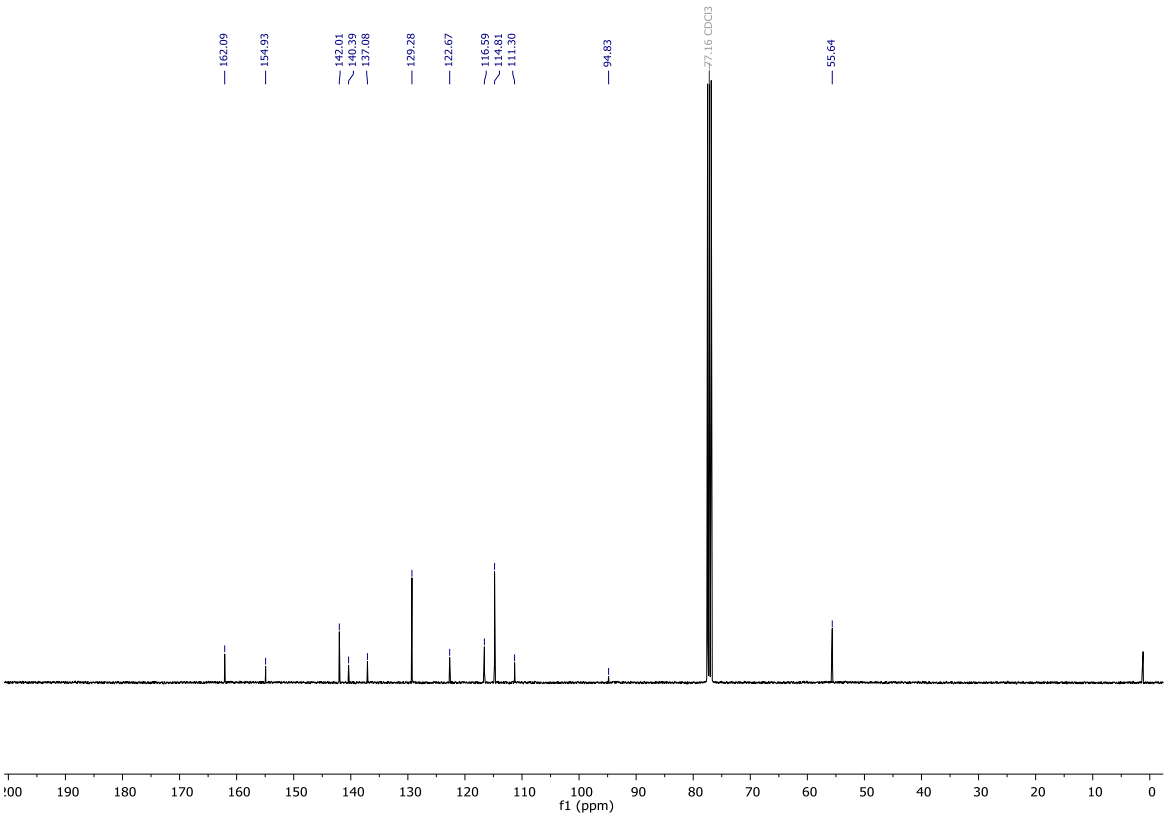
Ethyl 4-(6-chloro-3-cyanoimidazo[1,2-*a*]pyrazin-2-yl)benzoate (16d)



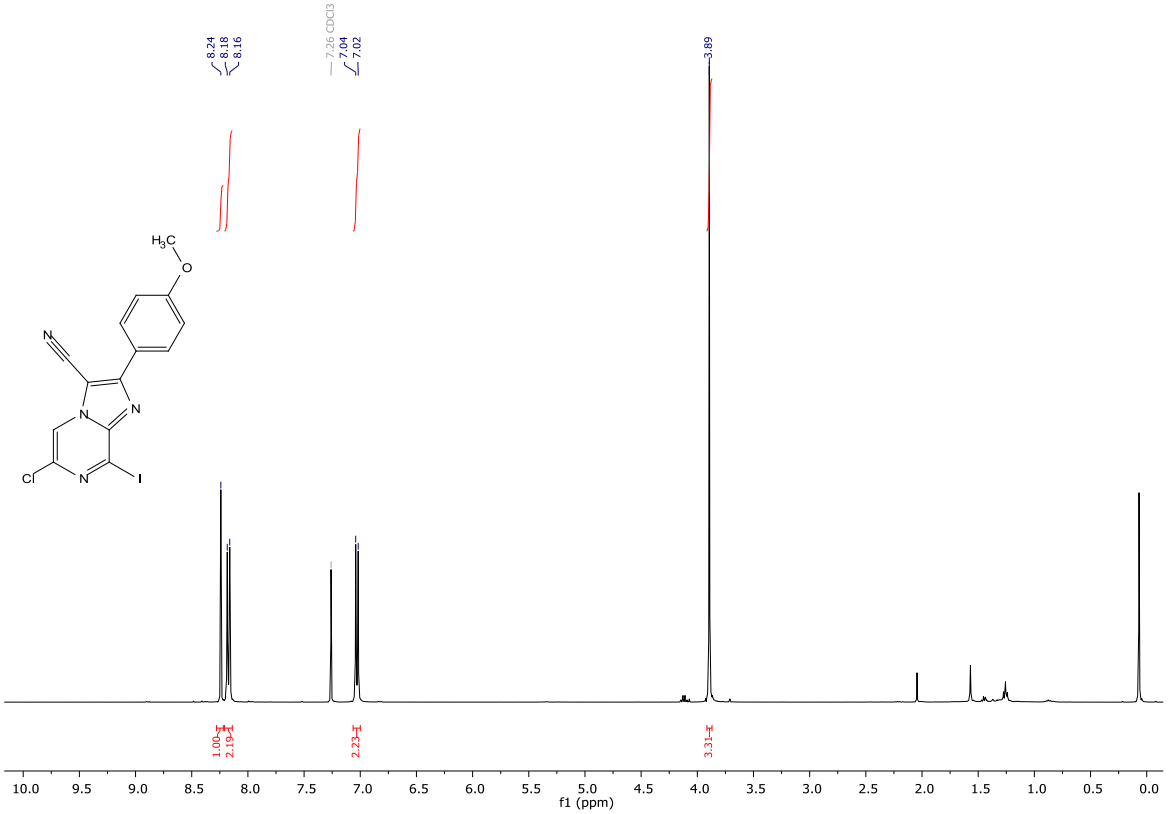


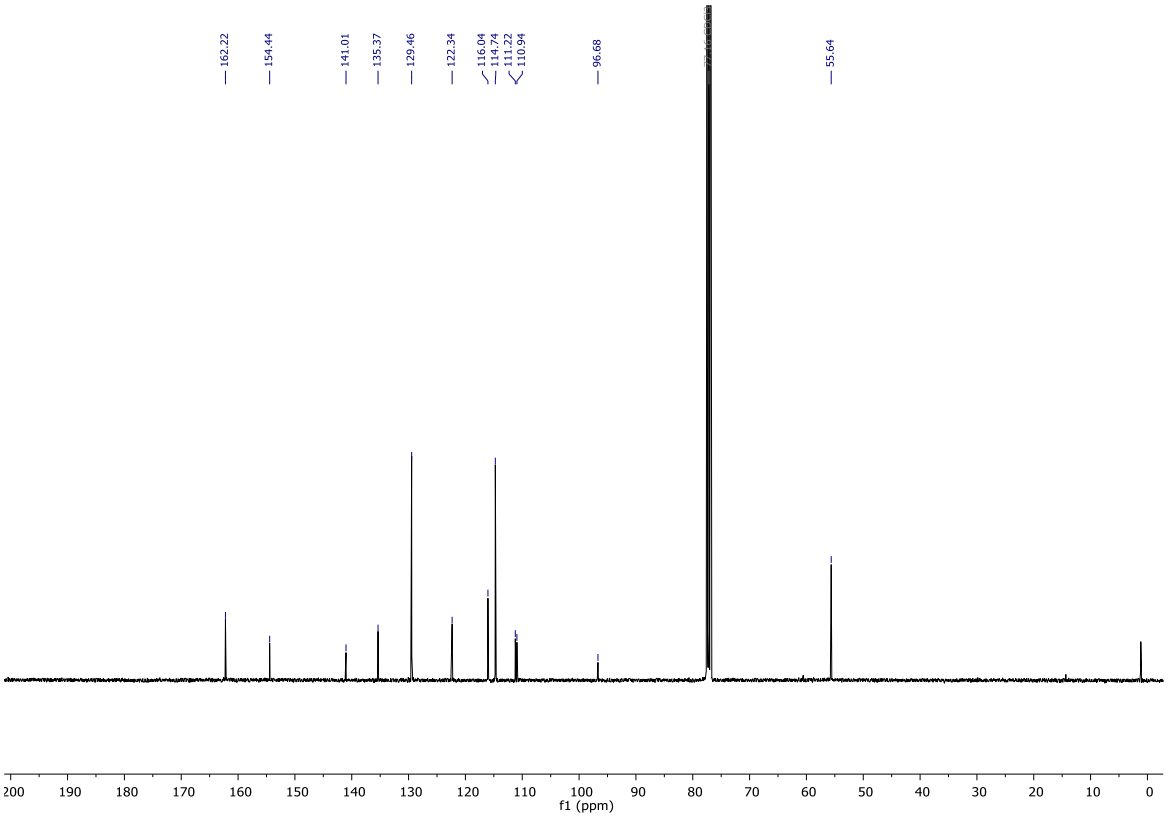
6-Chloro-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (16e)



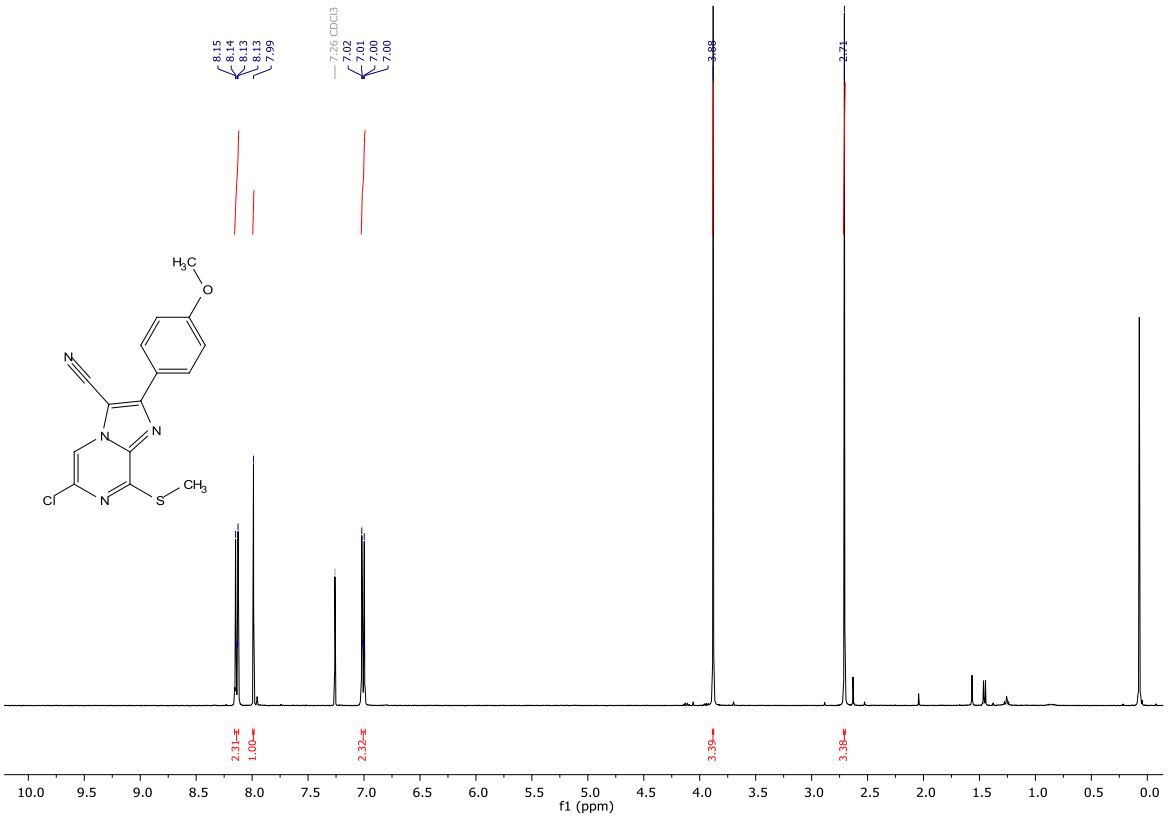


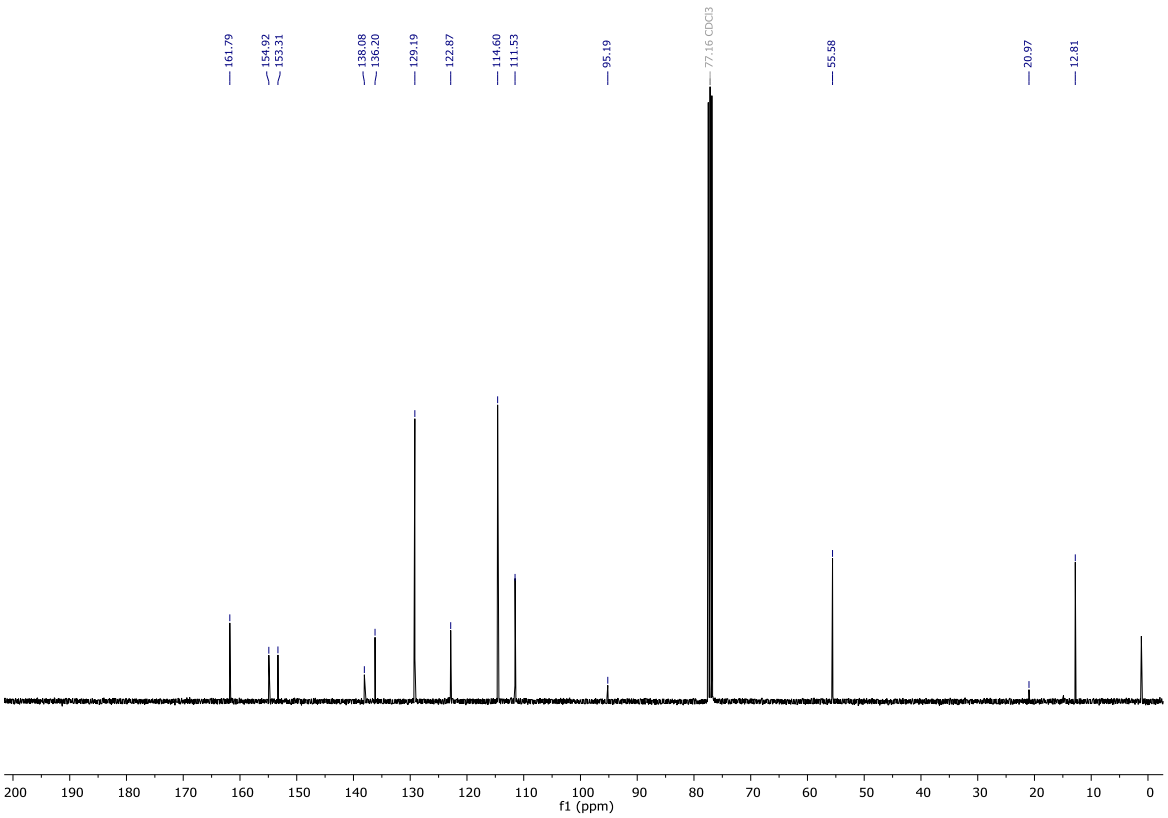
6-Chloro-8-iodo-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (18a)



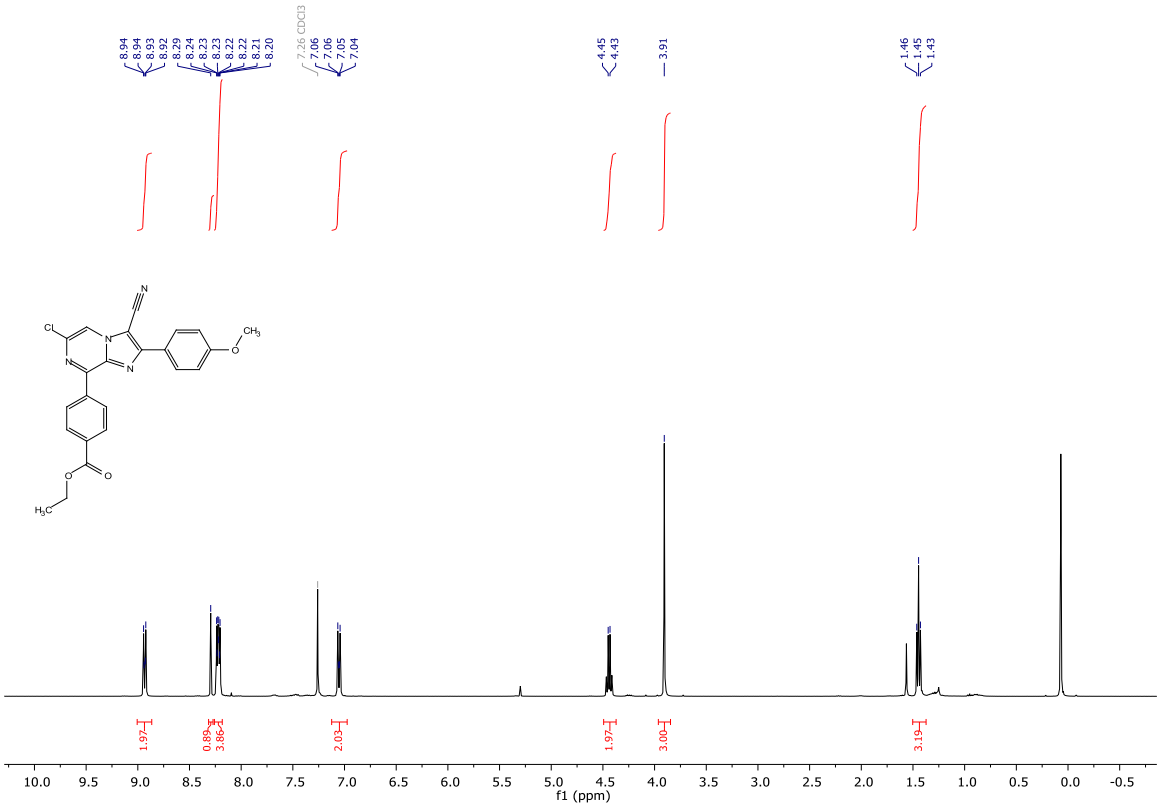


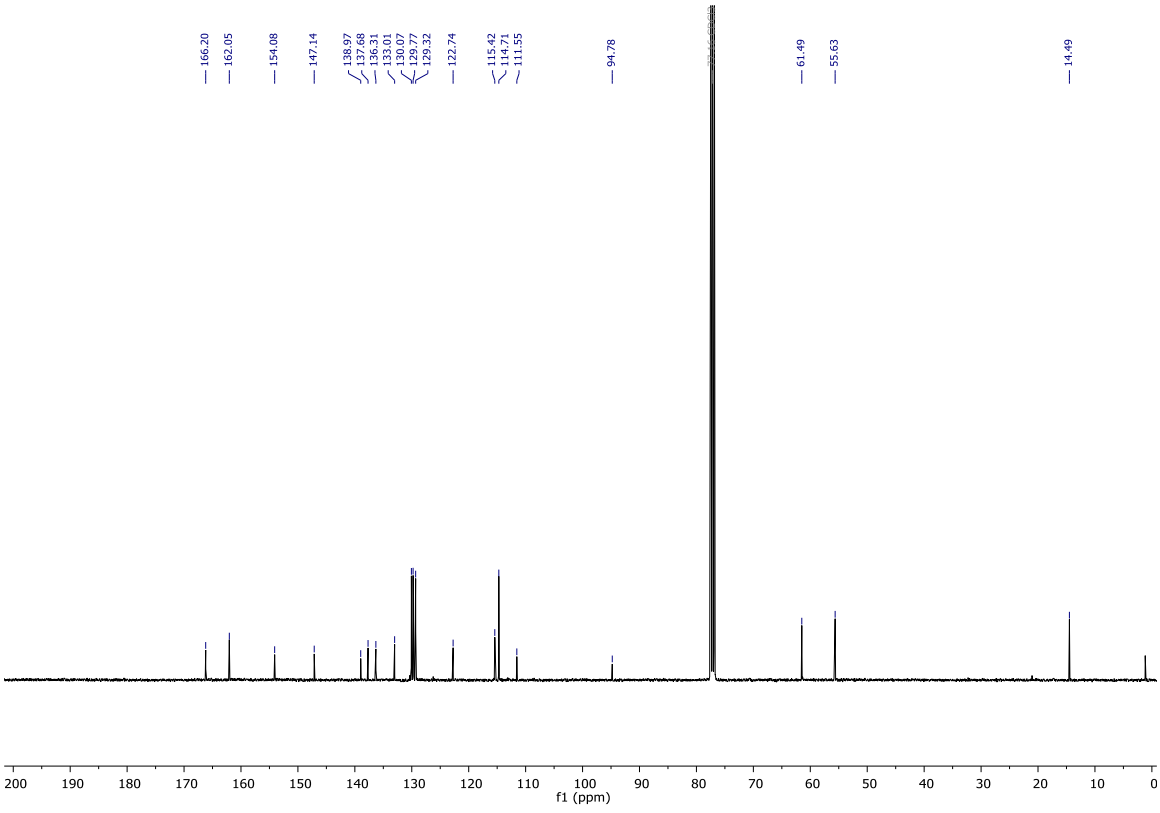
6-Chloro-2-(4-methoxyphenyl)-8-(methylthio)imidazo[1,2-*a*]pyrazine-3-carbonitrile (18b)



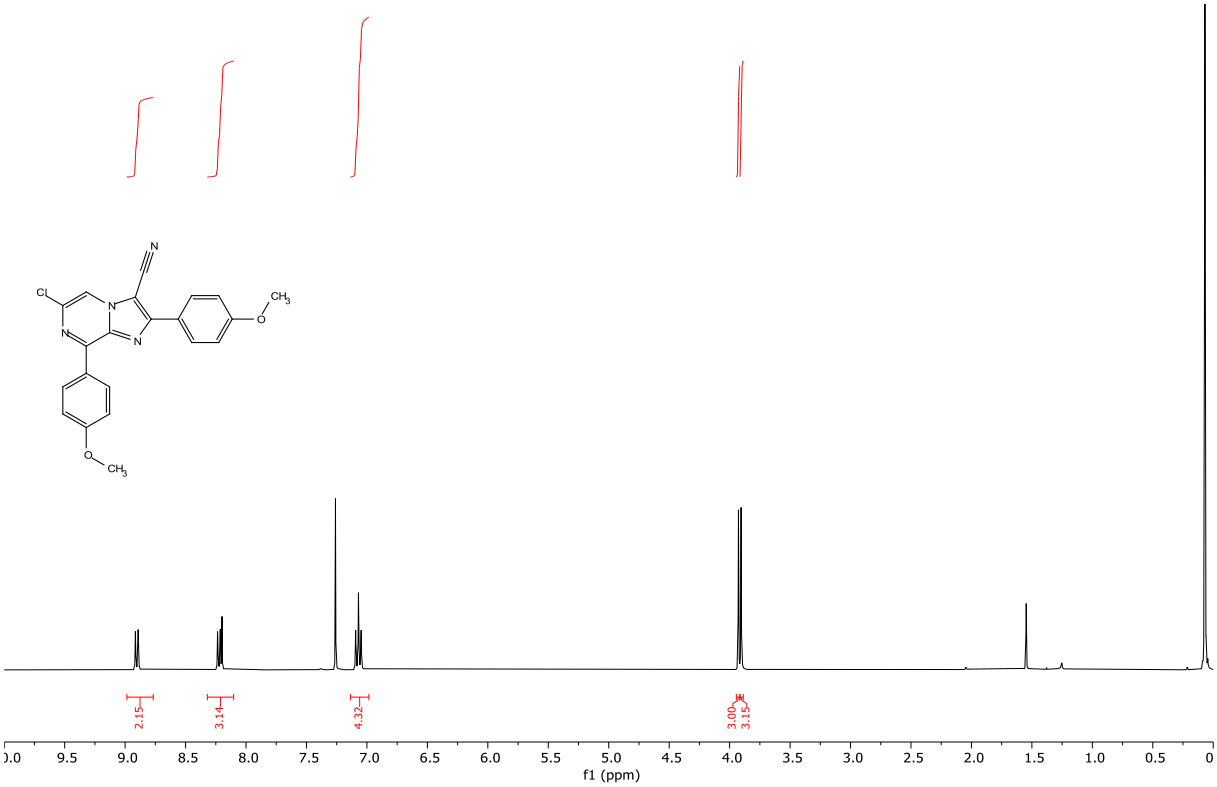


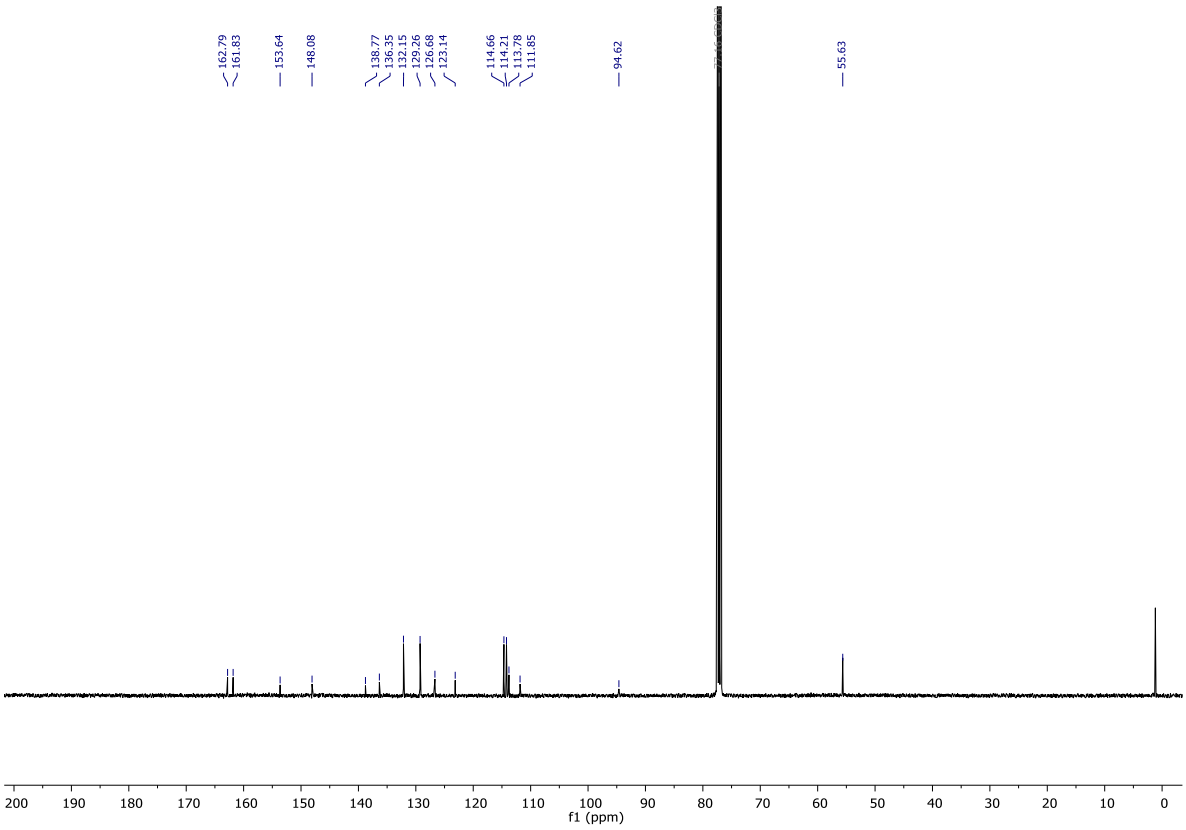
Ethyl 4-(6-chloro-3-cyano-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazin-8-yl)benzoate (18c)



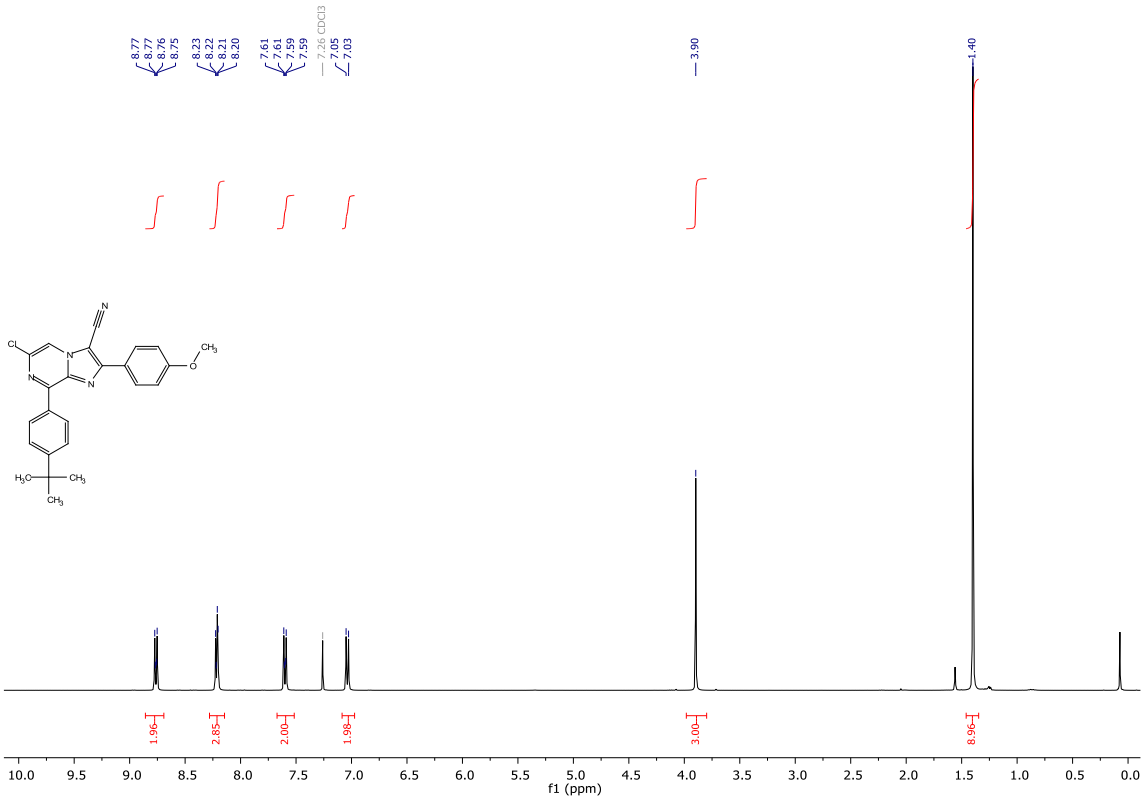


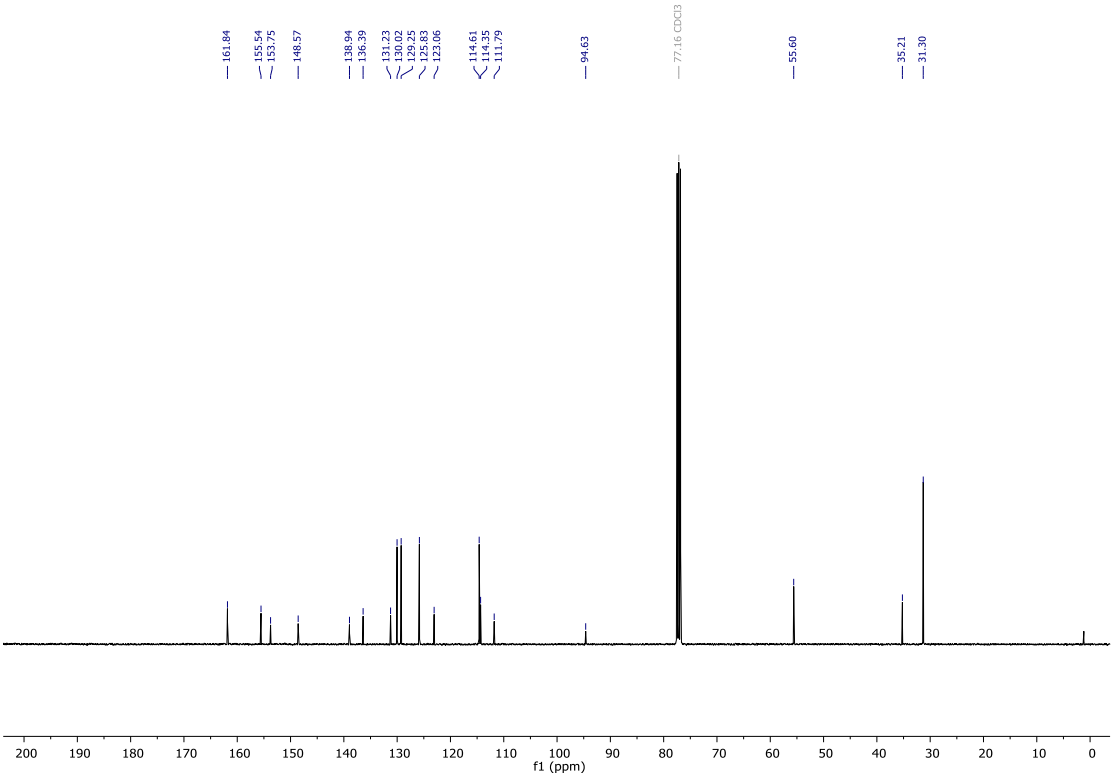
6-Chloro-2,8-bis(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (18d)



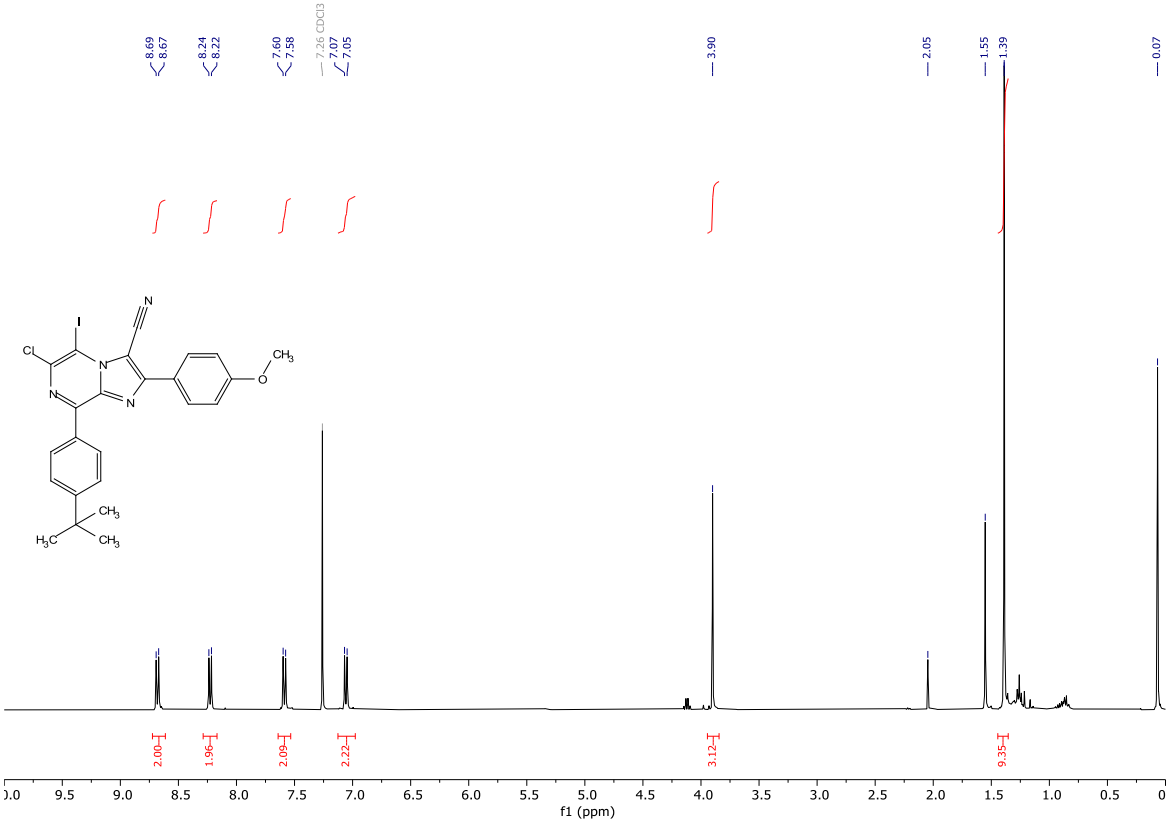


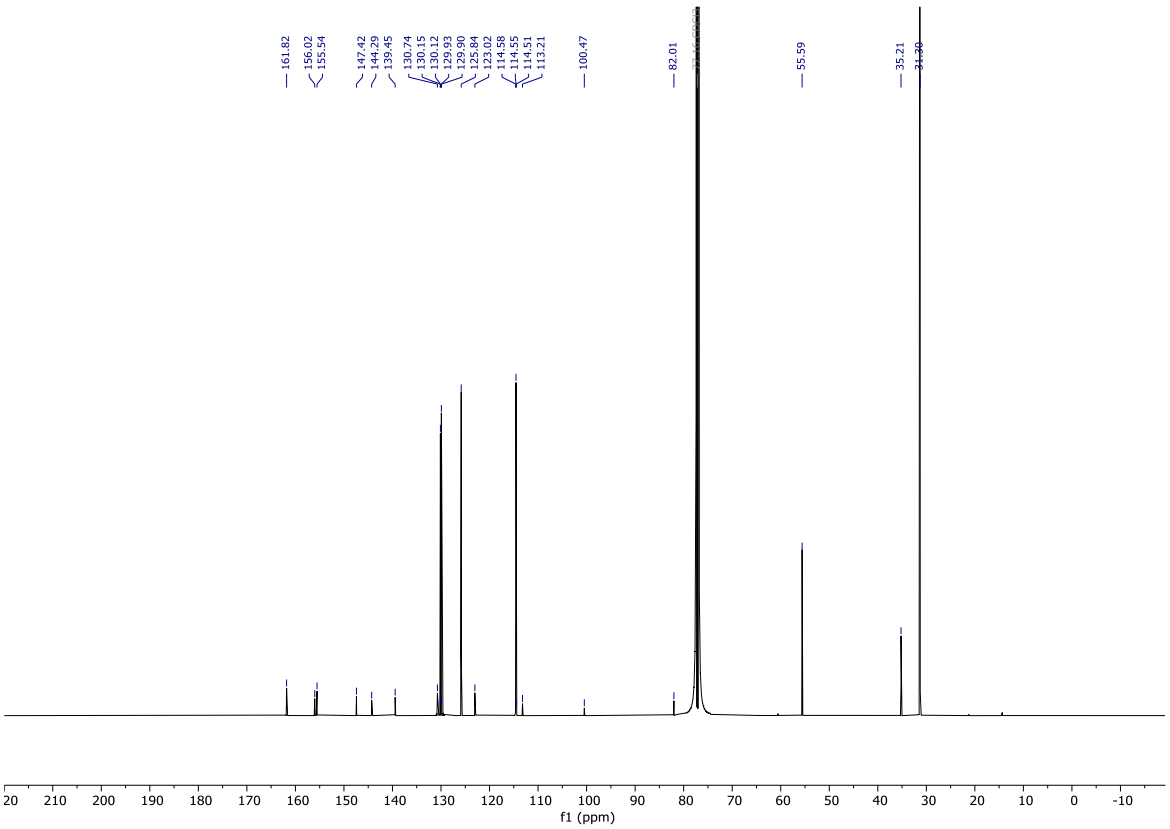
8-(4-(tert-Butyl)phenyl)-6-chloro-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (18e)



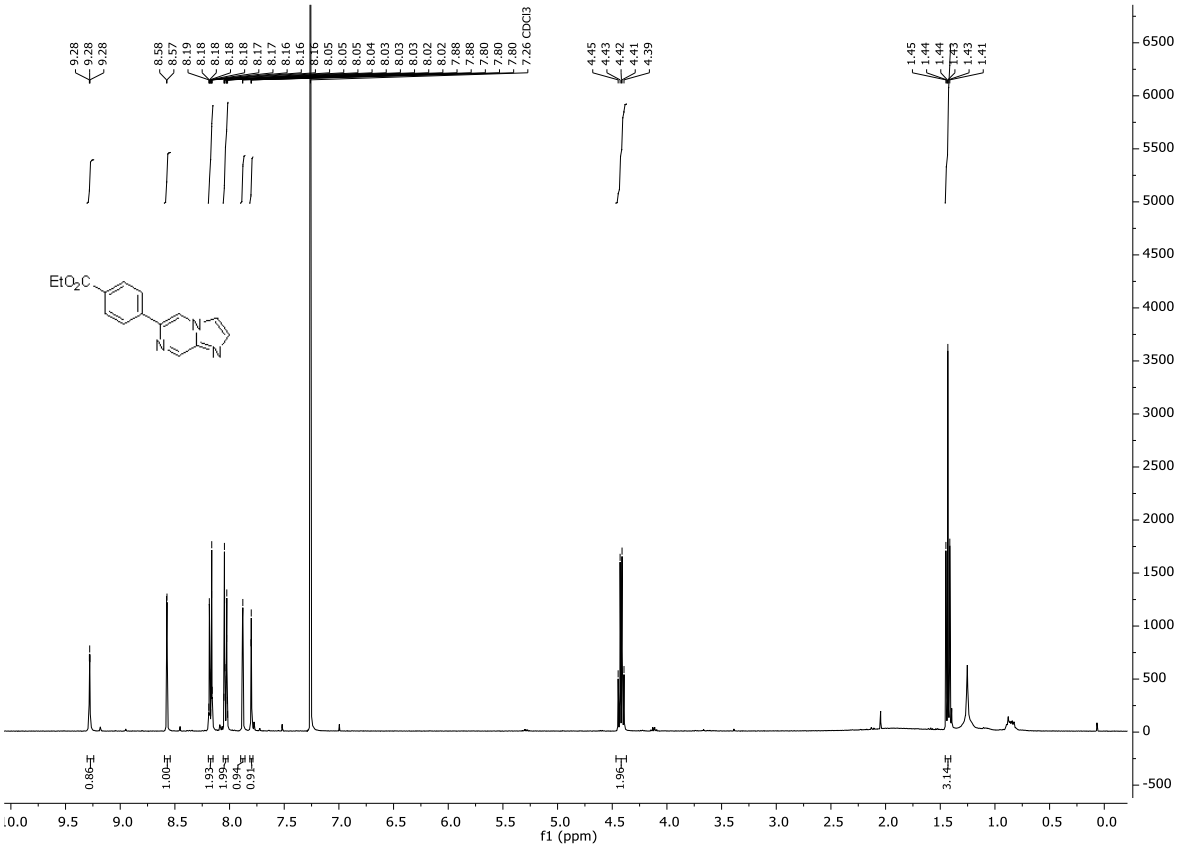


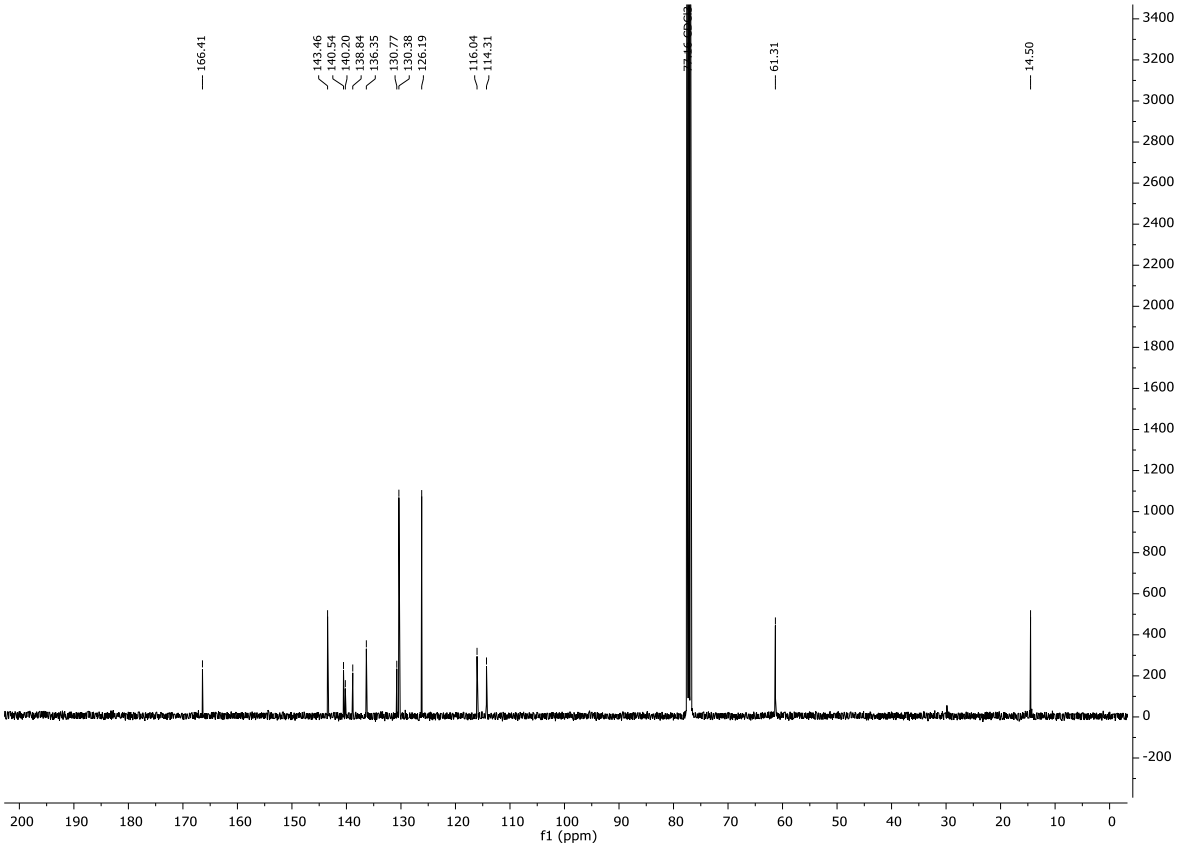
8-(4-(*tert*-Butyl)phenyl)-6-chloro-5-iodo-2-(4-methoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (20)



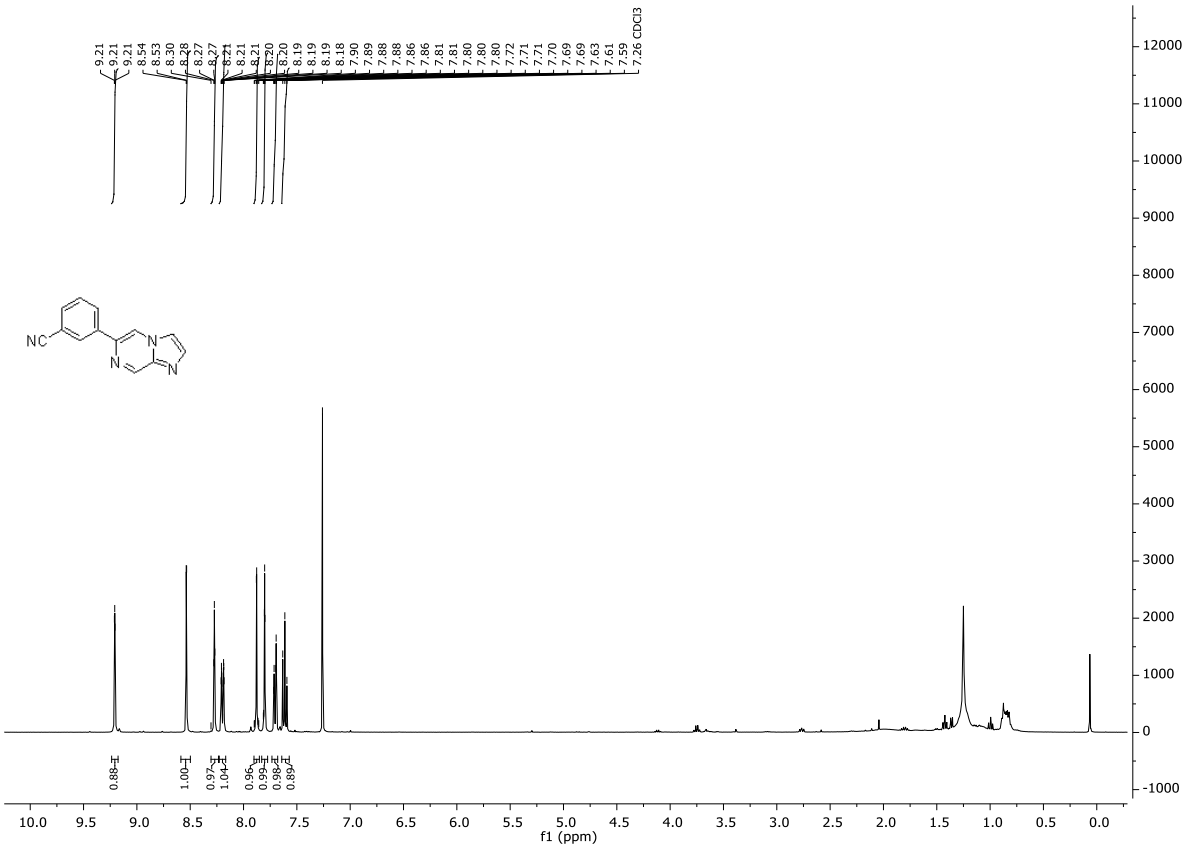


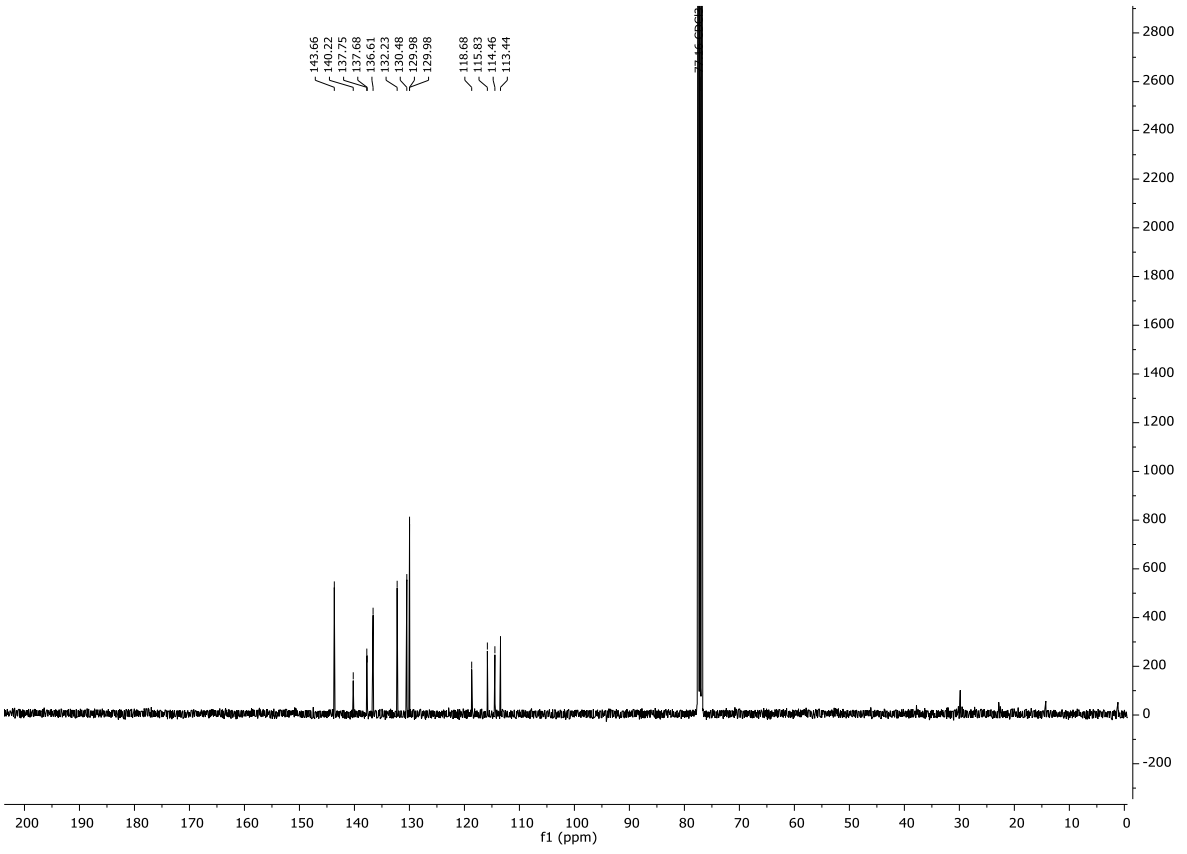
Ethyl 4-(imidazo[1,2-*a*]pyrazin-6-yl)benzoate (22a)



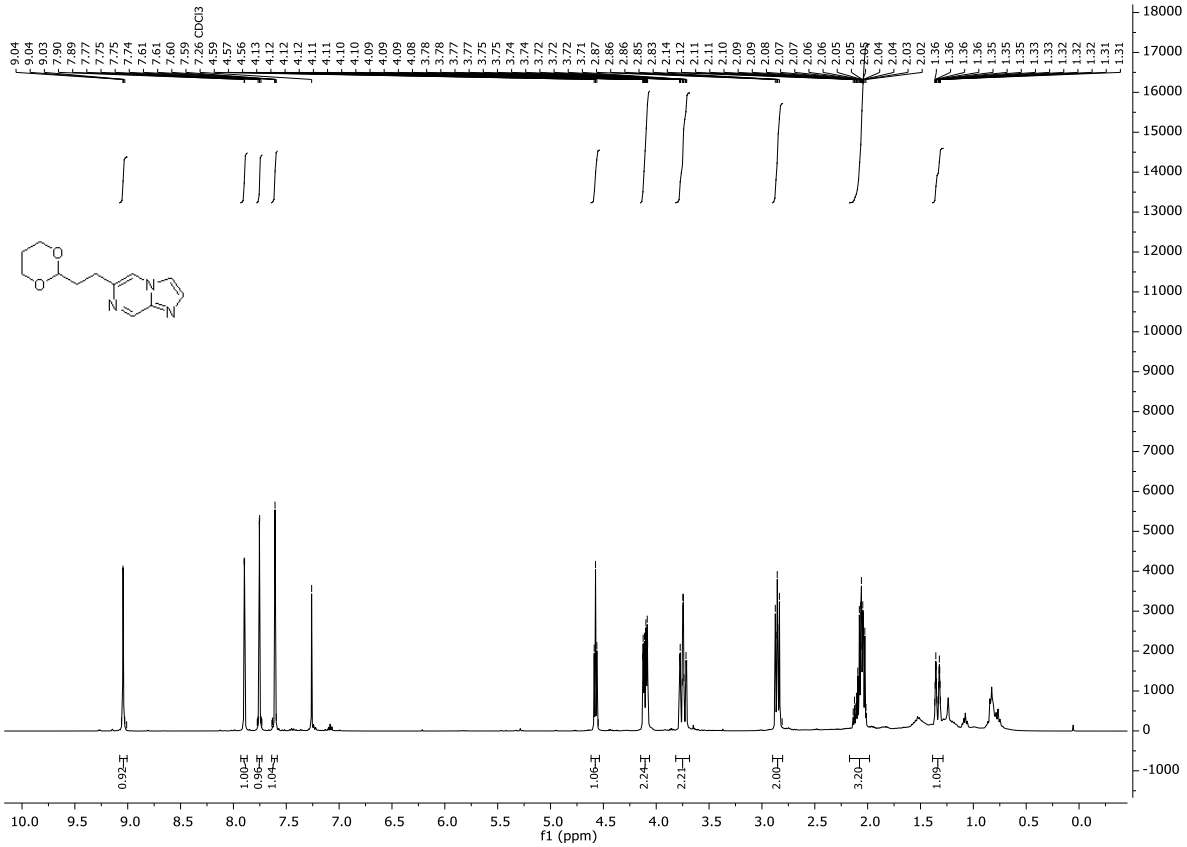


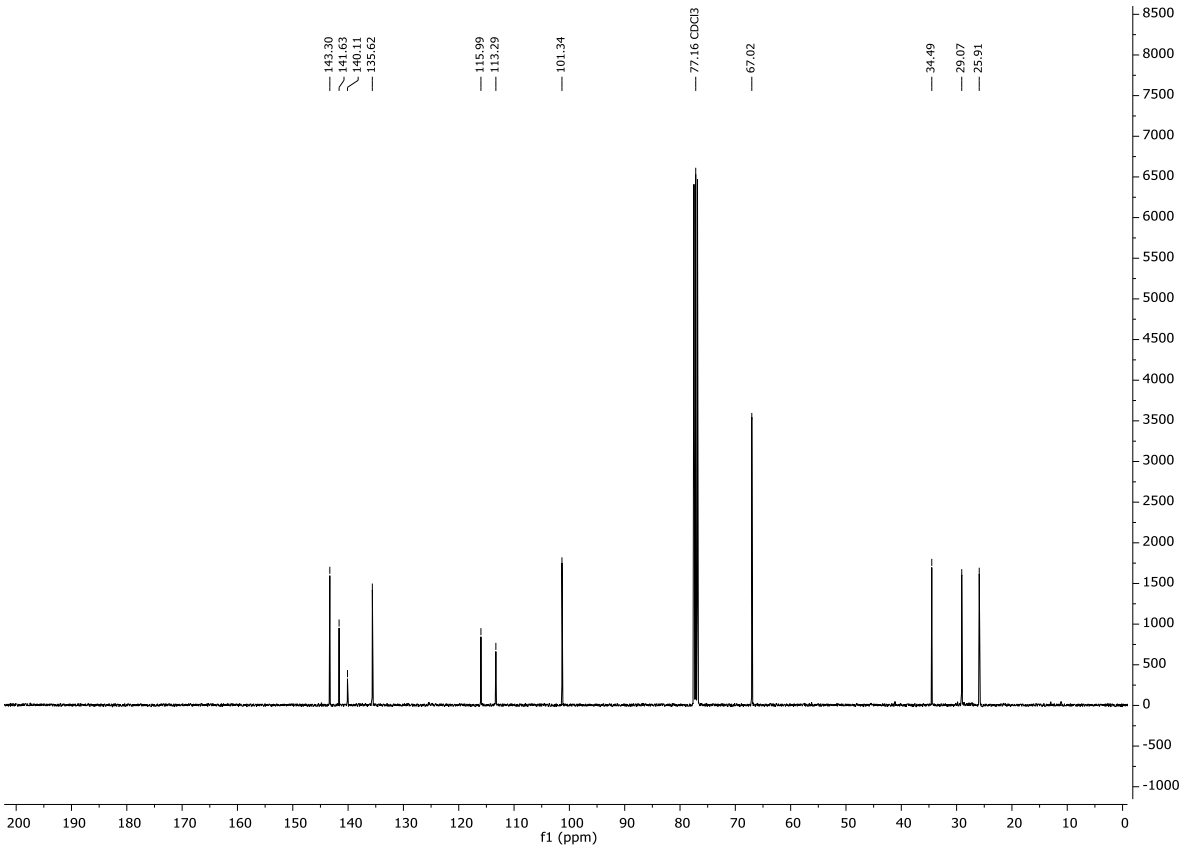
3-(Imidazo[1,2-*a*]pyrazin-6-yl)benzonitrile (22b)



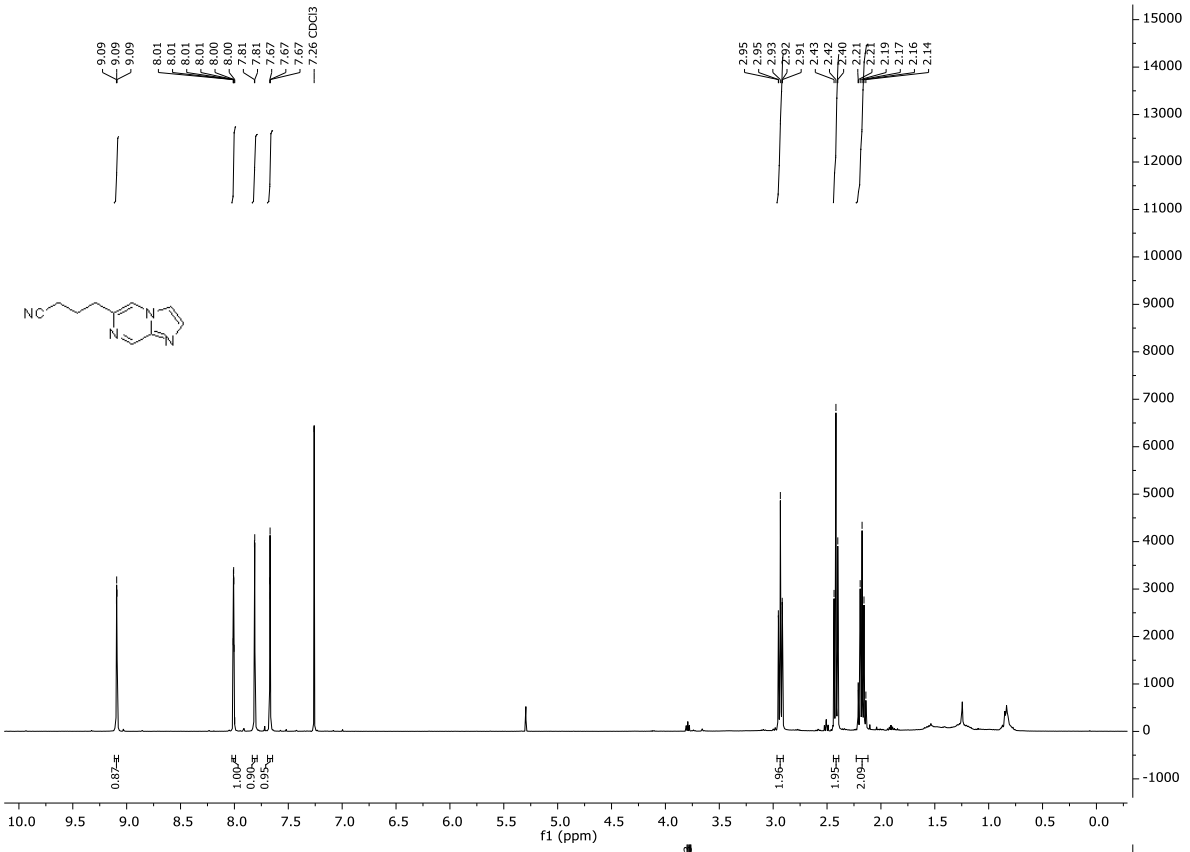


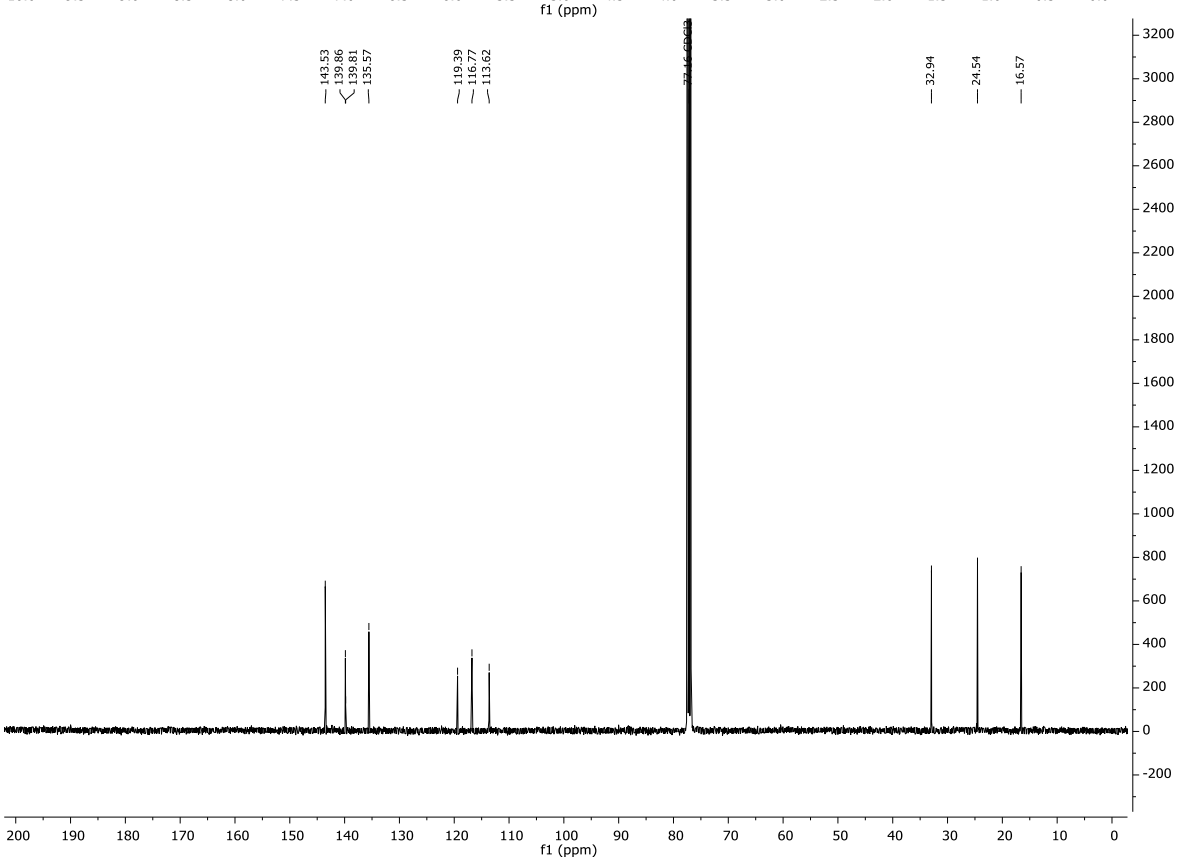
6-(2-(1,3-Dioxan-2-yl)ethyl)imidazo[1,2-*a*]pyrazine (22c)



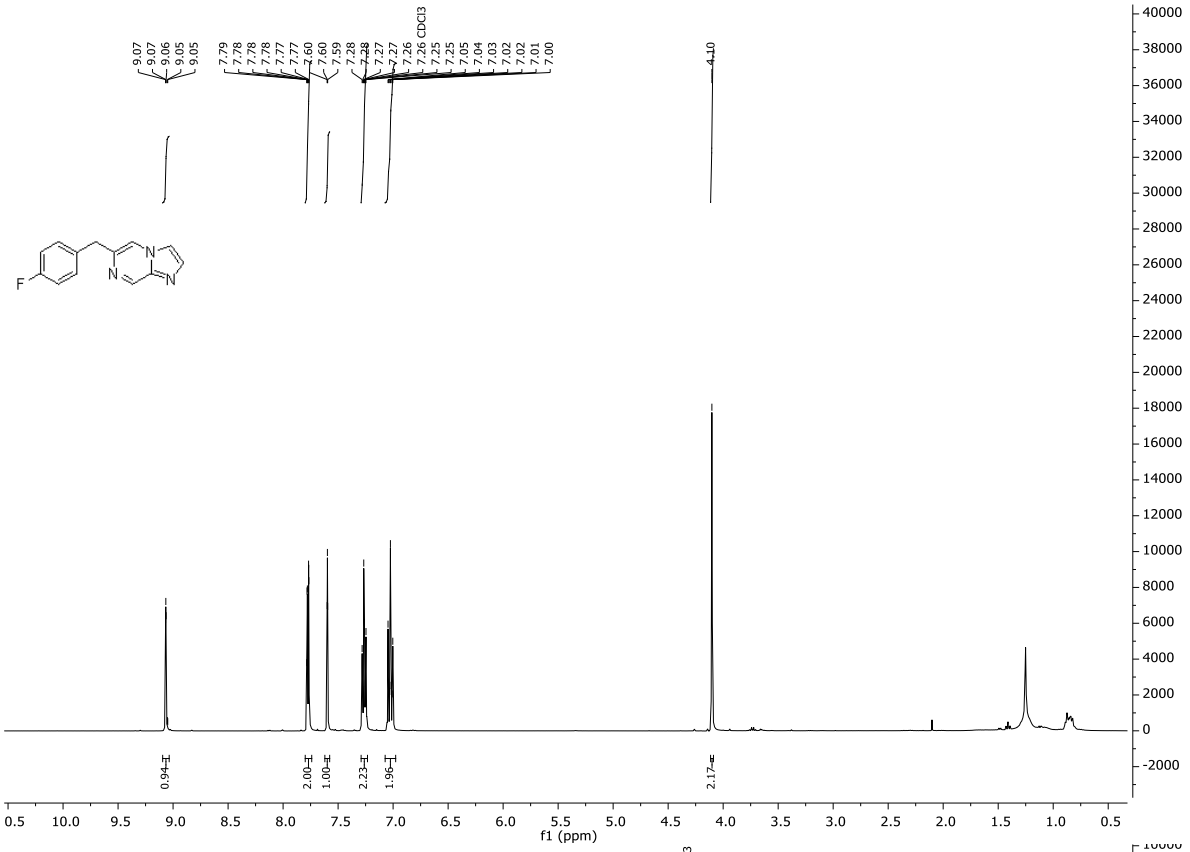


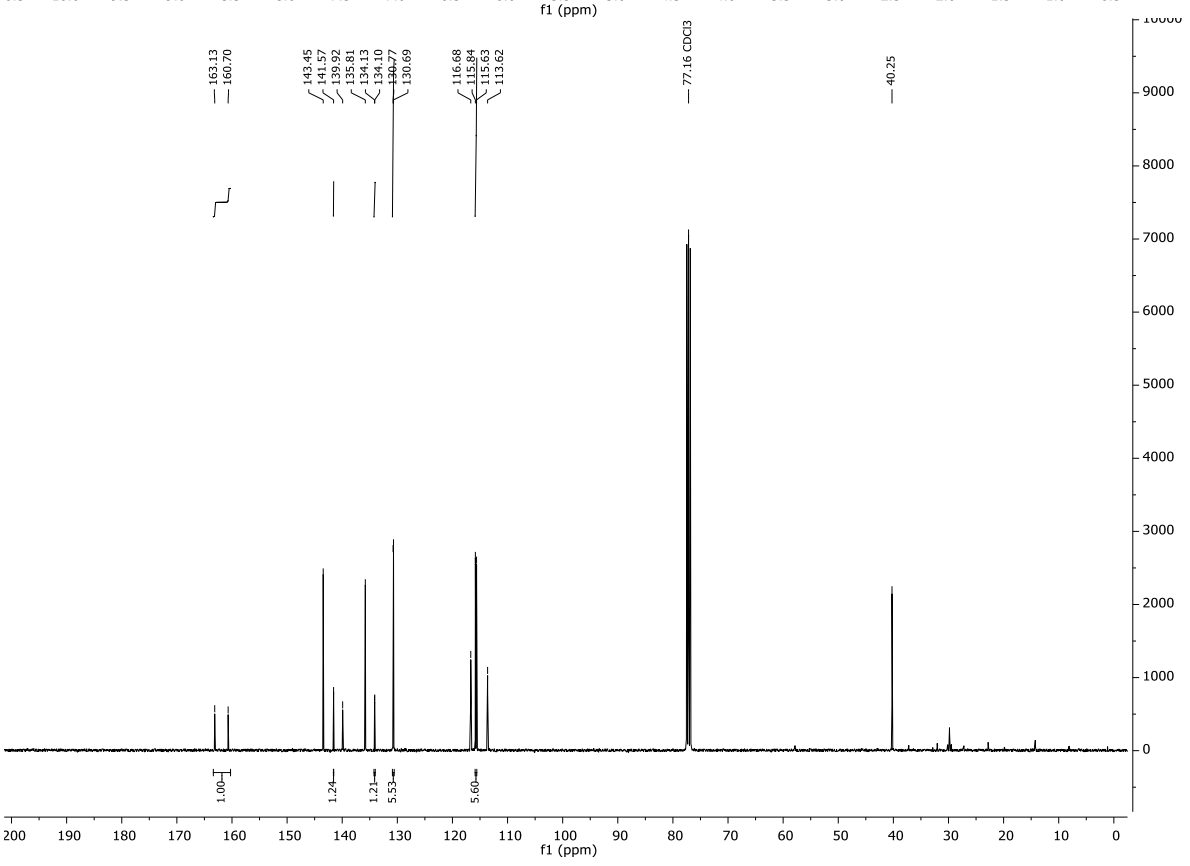
4-(Imidazo[1,2-*a*]pyrazin-6-yl)butanenitrile (22d)



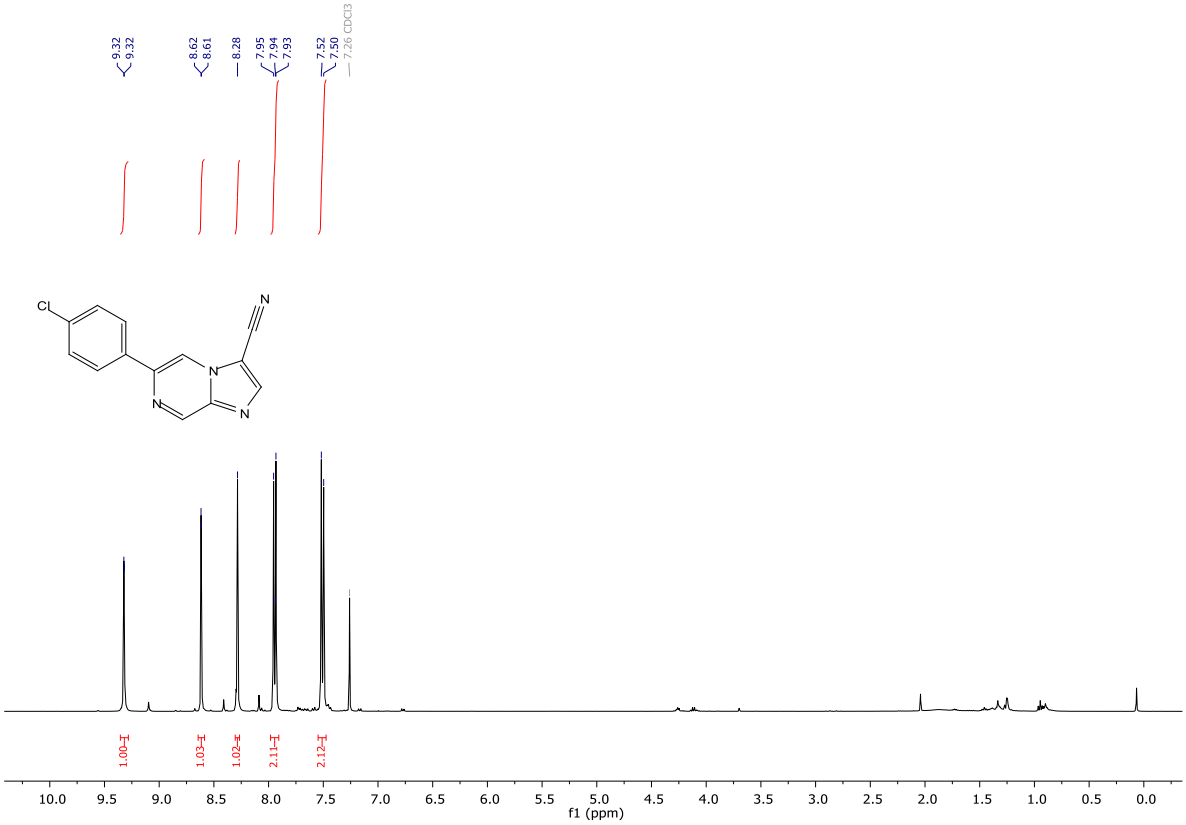


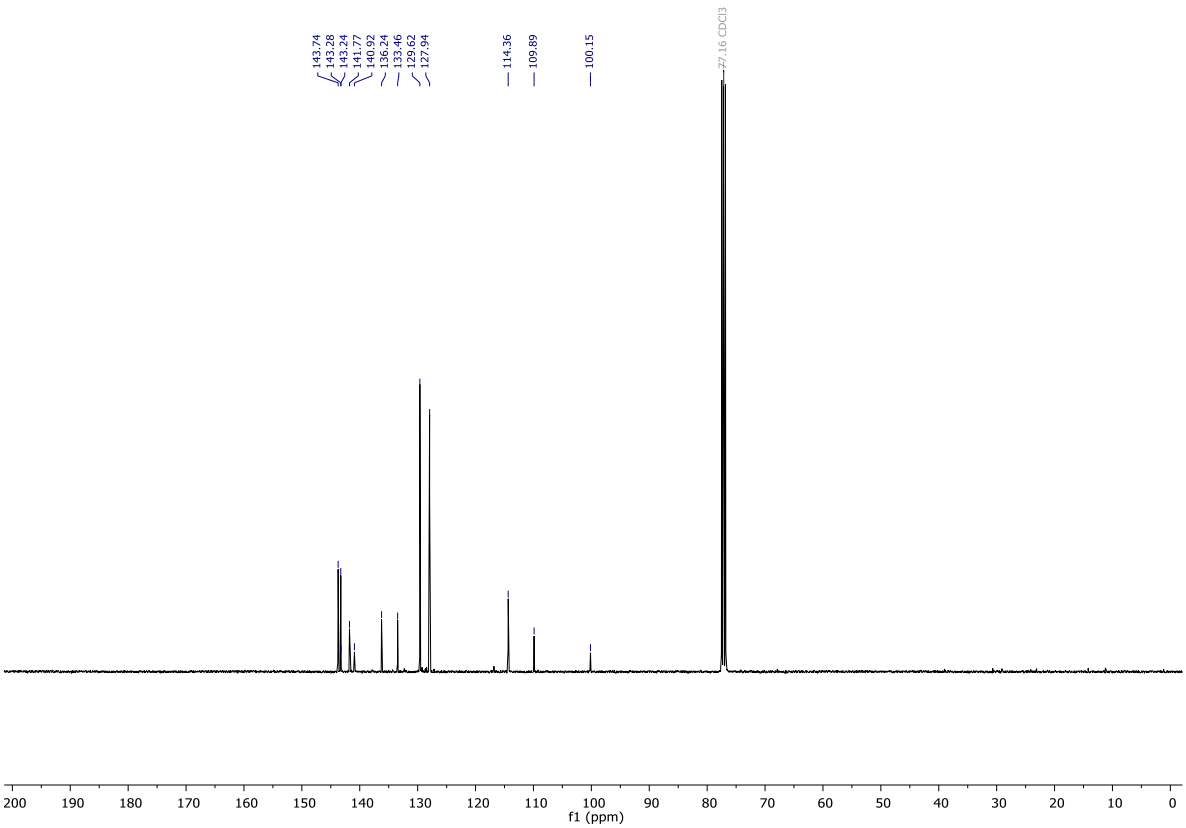
6-(4-Fluorobenzyl)imidazo[1,2-a]pyrazine (22e)



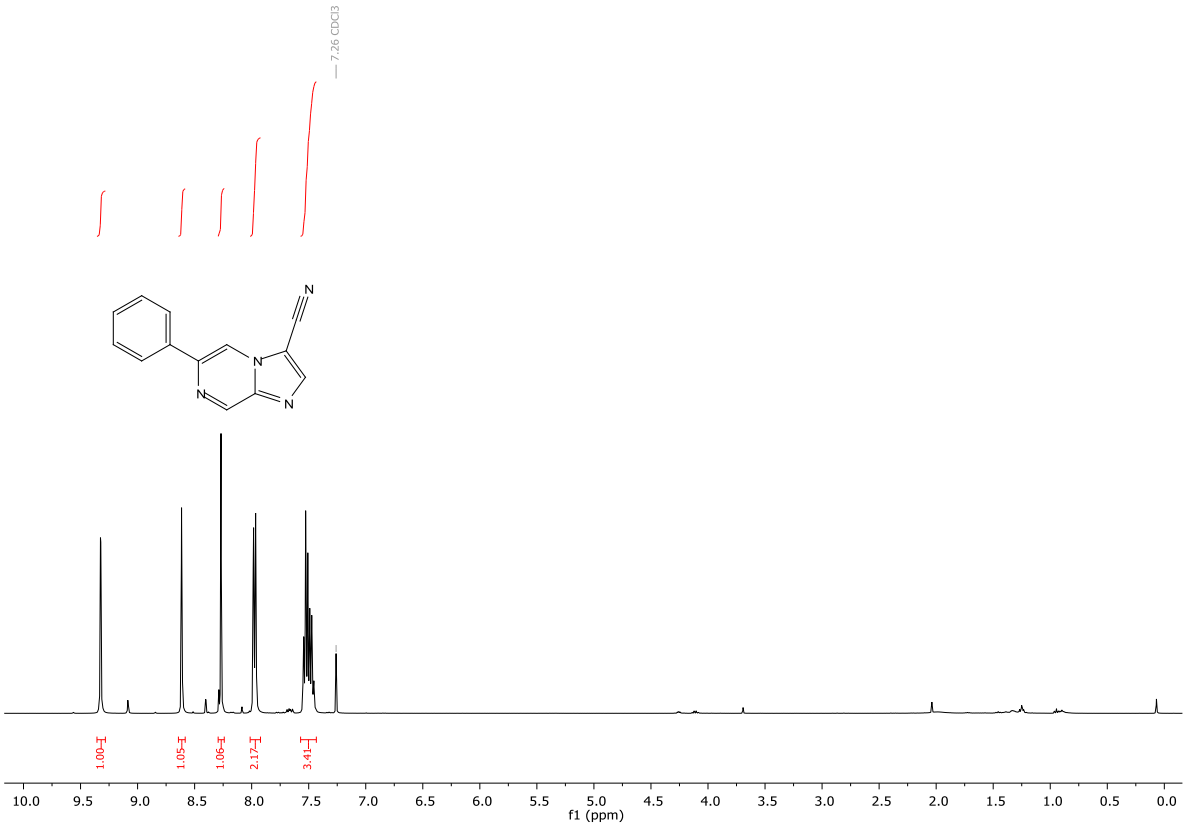


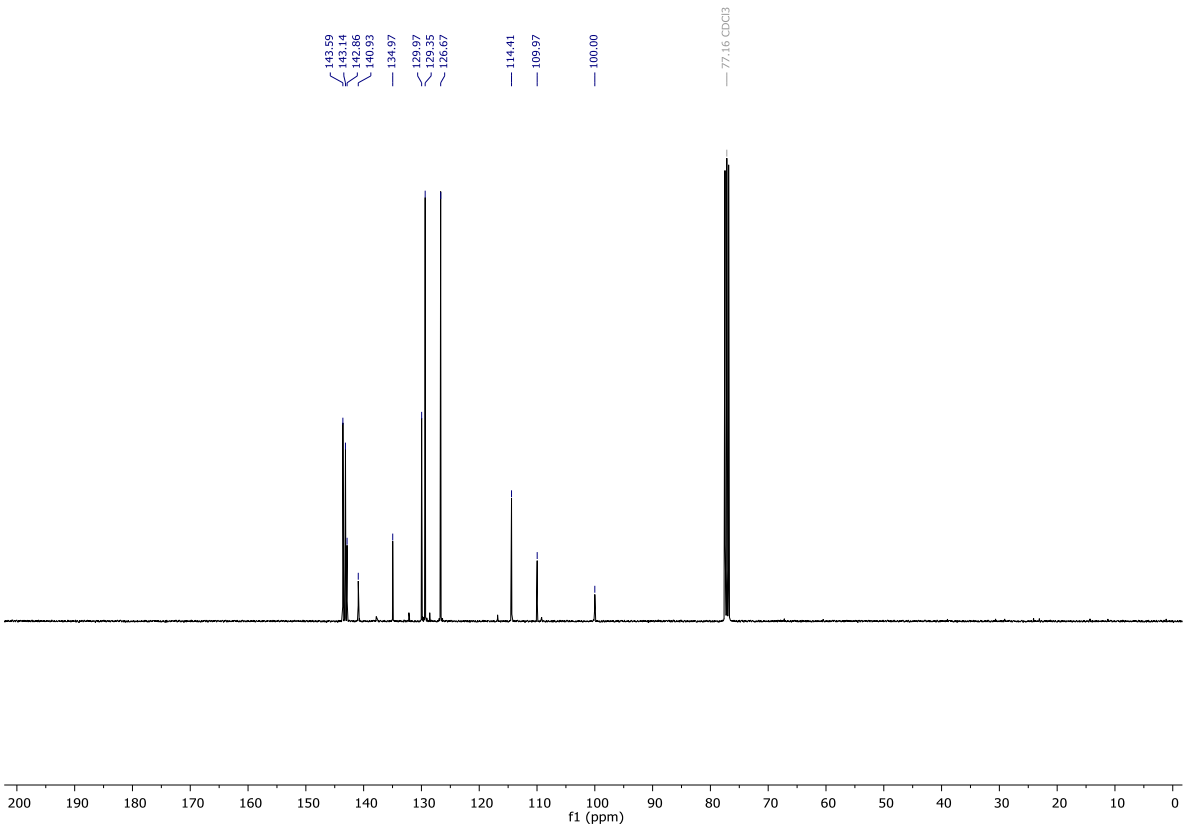
6-(4-Chlorophenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (S1)



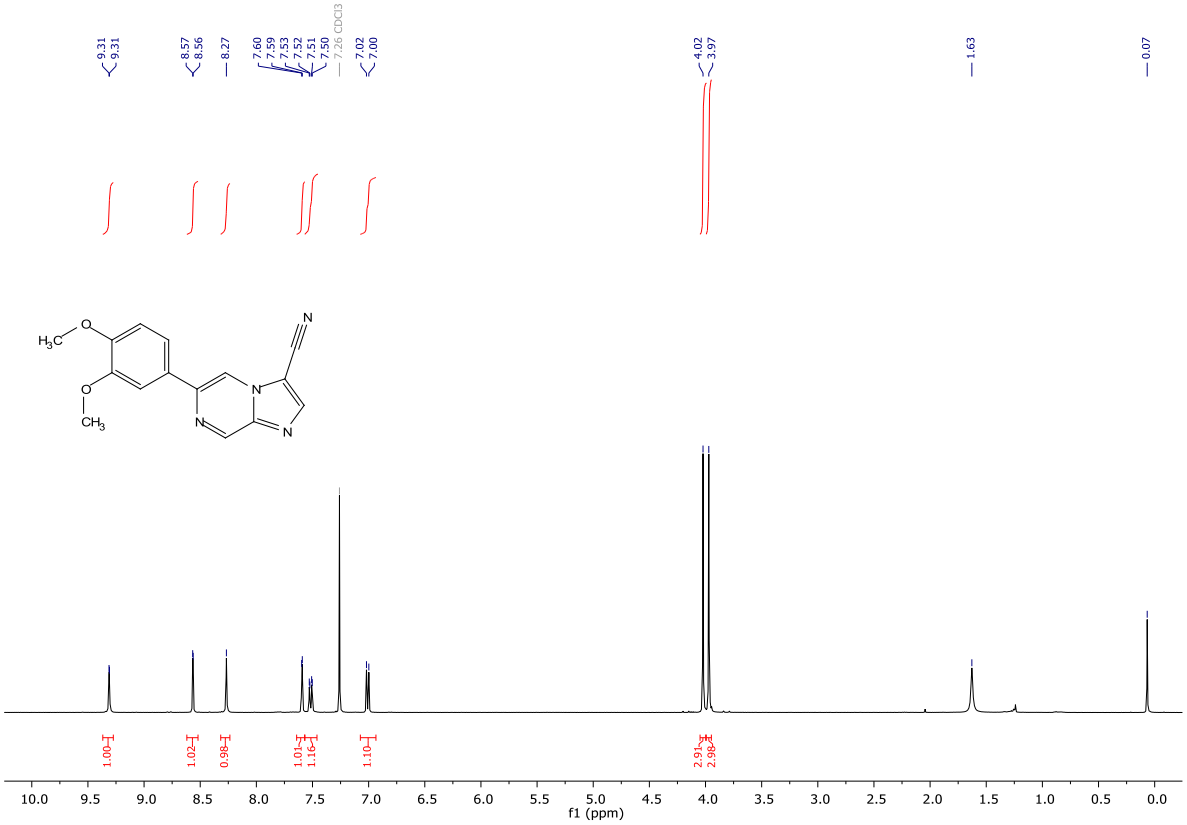


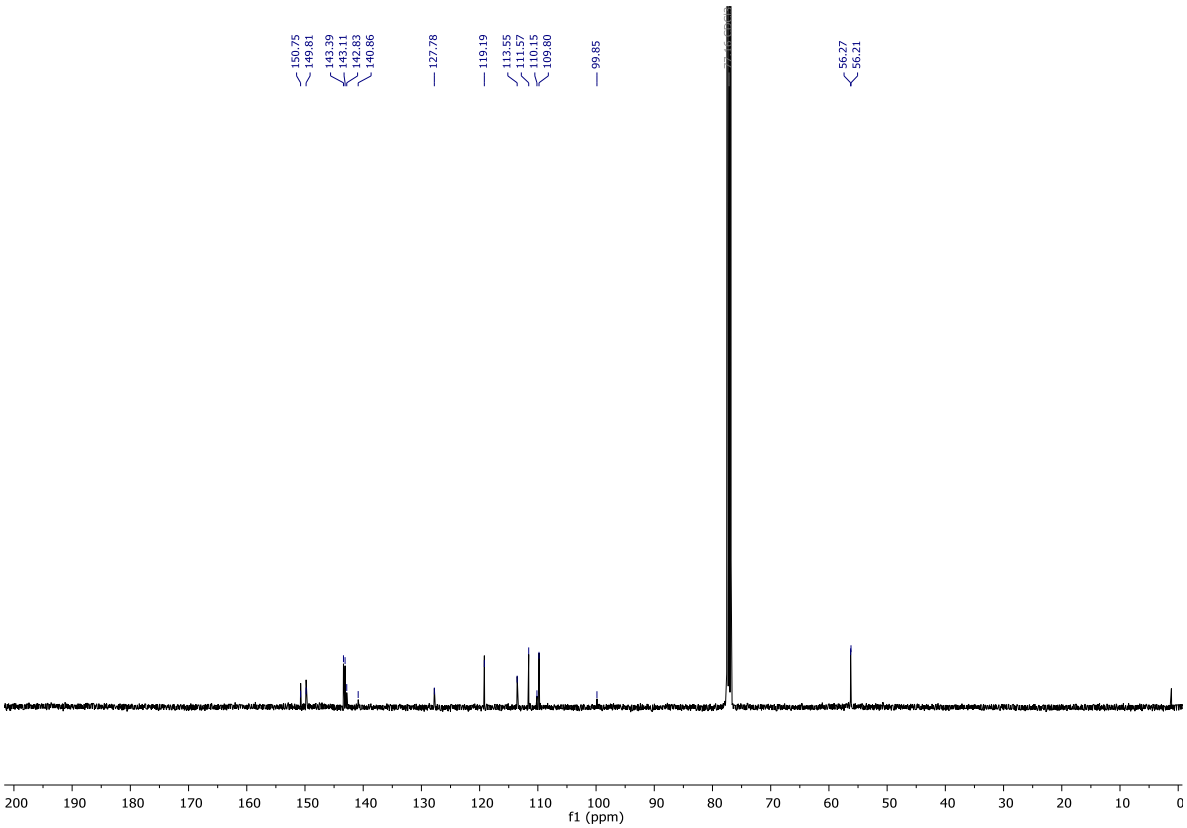
6-Phenylimidazo[1,2-*a*]pyrazine-3-carbonitrile (S2)



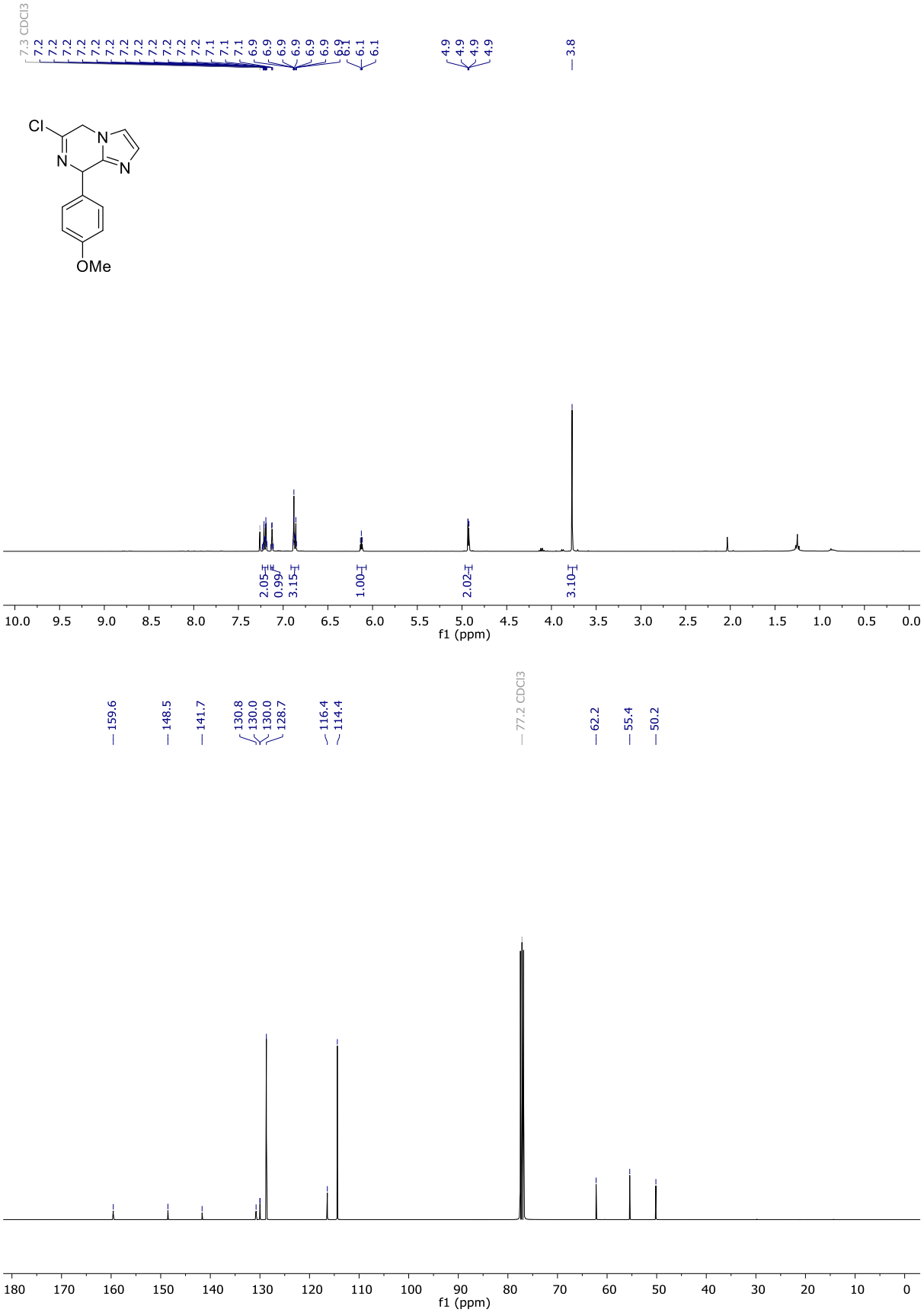


6-(3,4-Dimethoxyphenyl)imidazo[1,2-*a*]pyrazine-3-carbonitrile (S3)

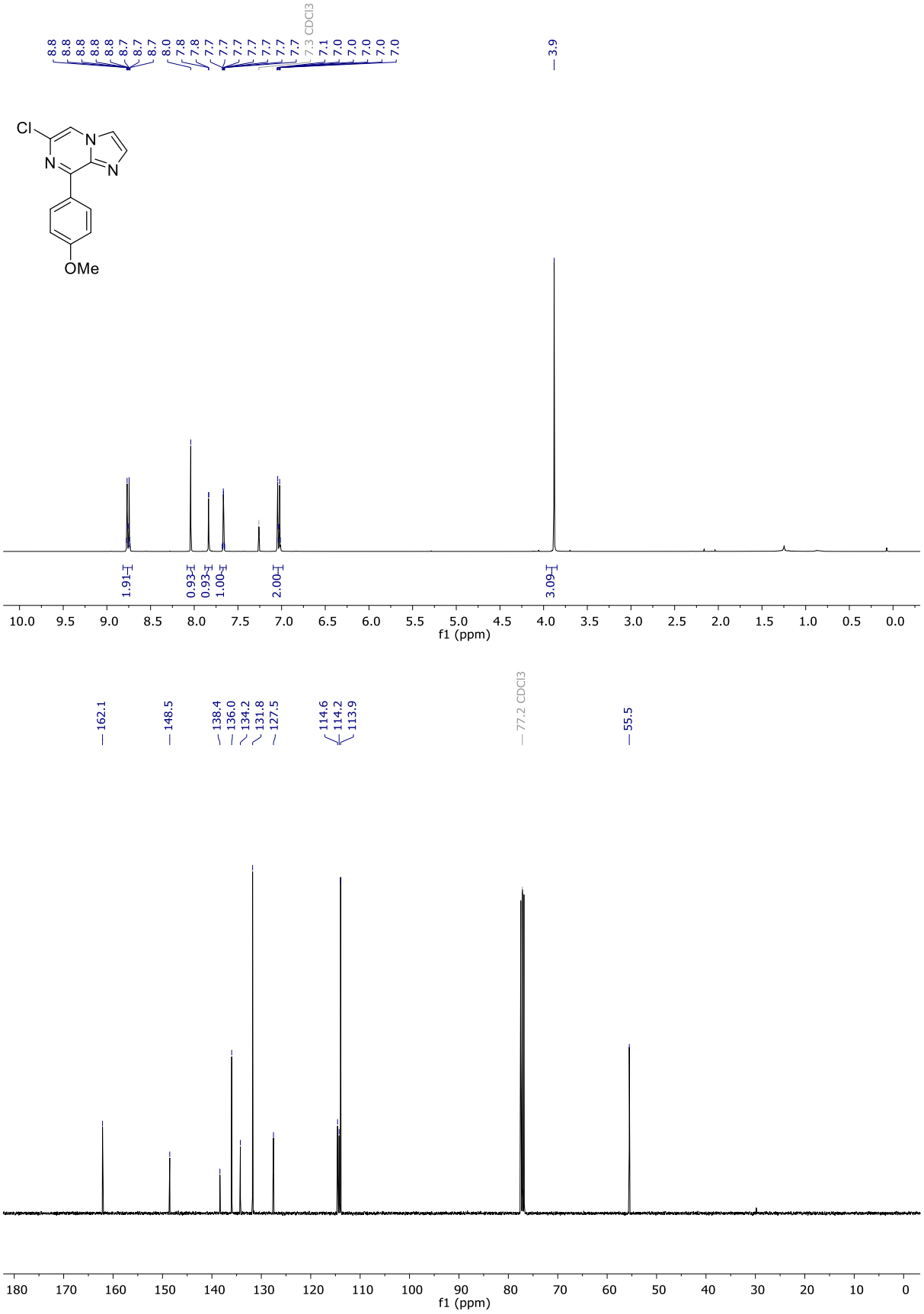




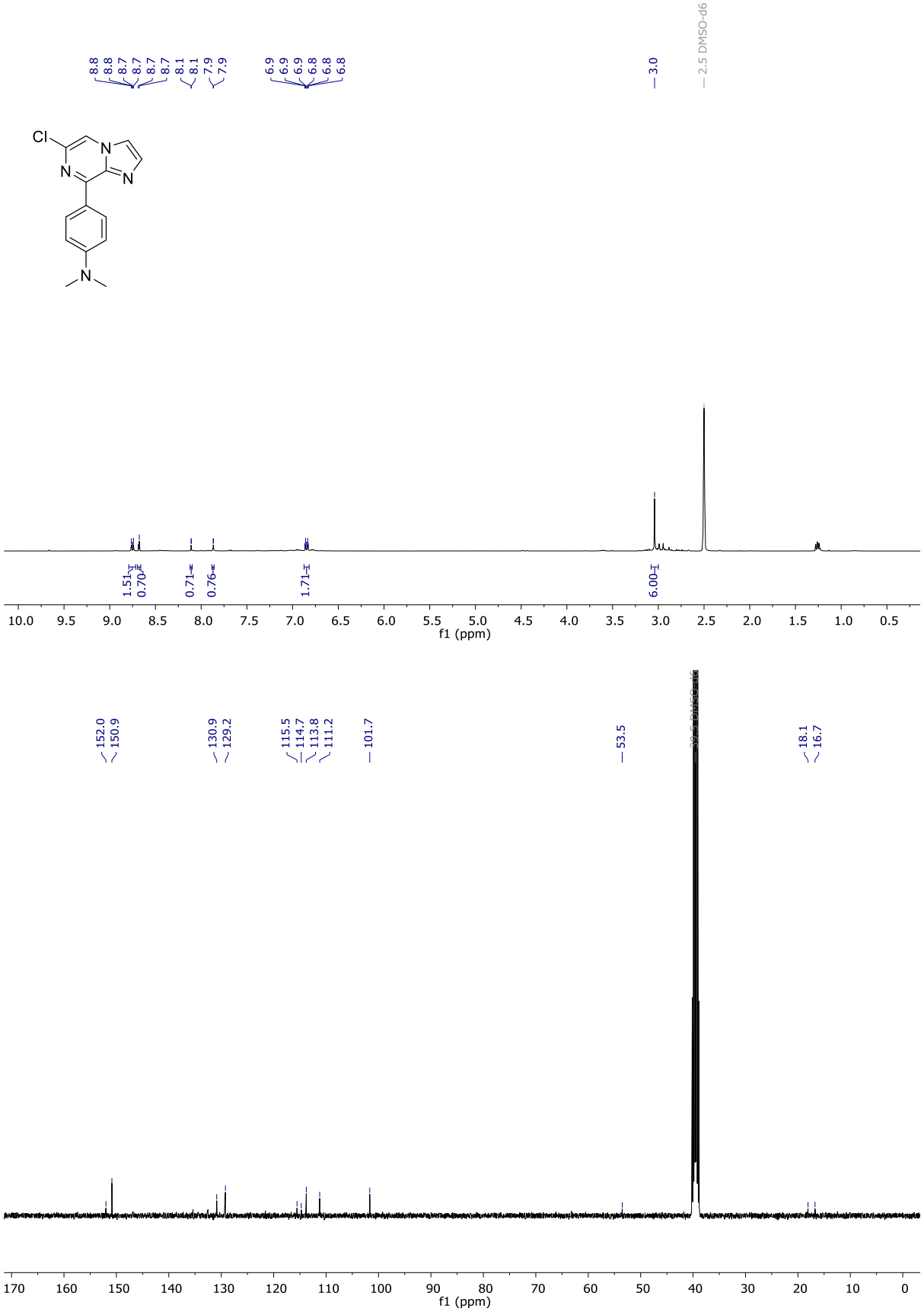
6-Chloro-8-(4-methoxyphenyl)-5,8-dihydroimidazo[1,2-*a*]pyrazine (26a)



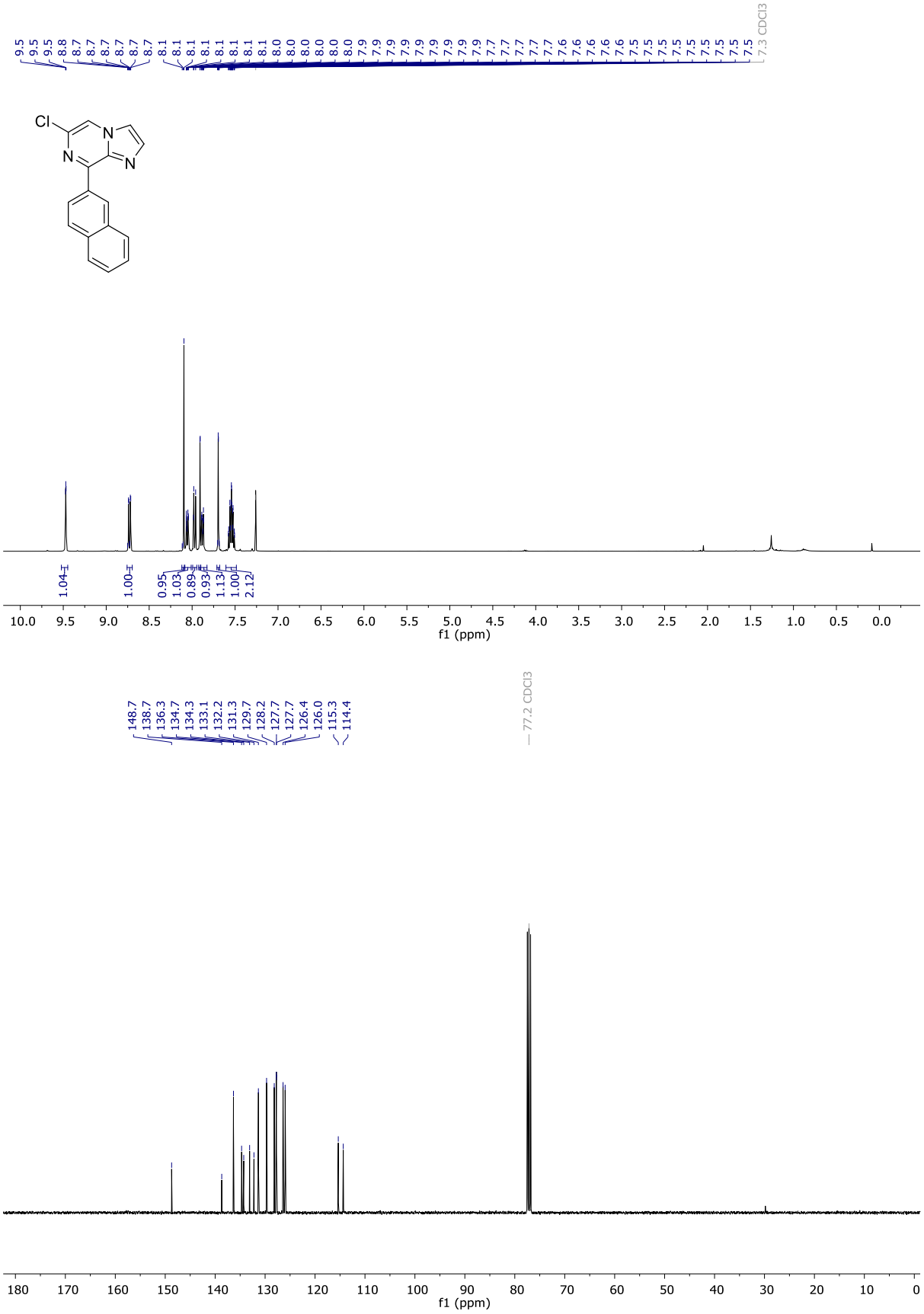
6-Chloro-8-(4-methoxyphenyl)imidazo[1,2-a]pyrazine (27a)



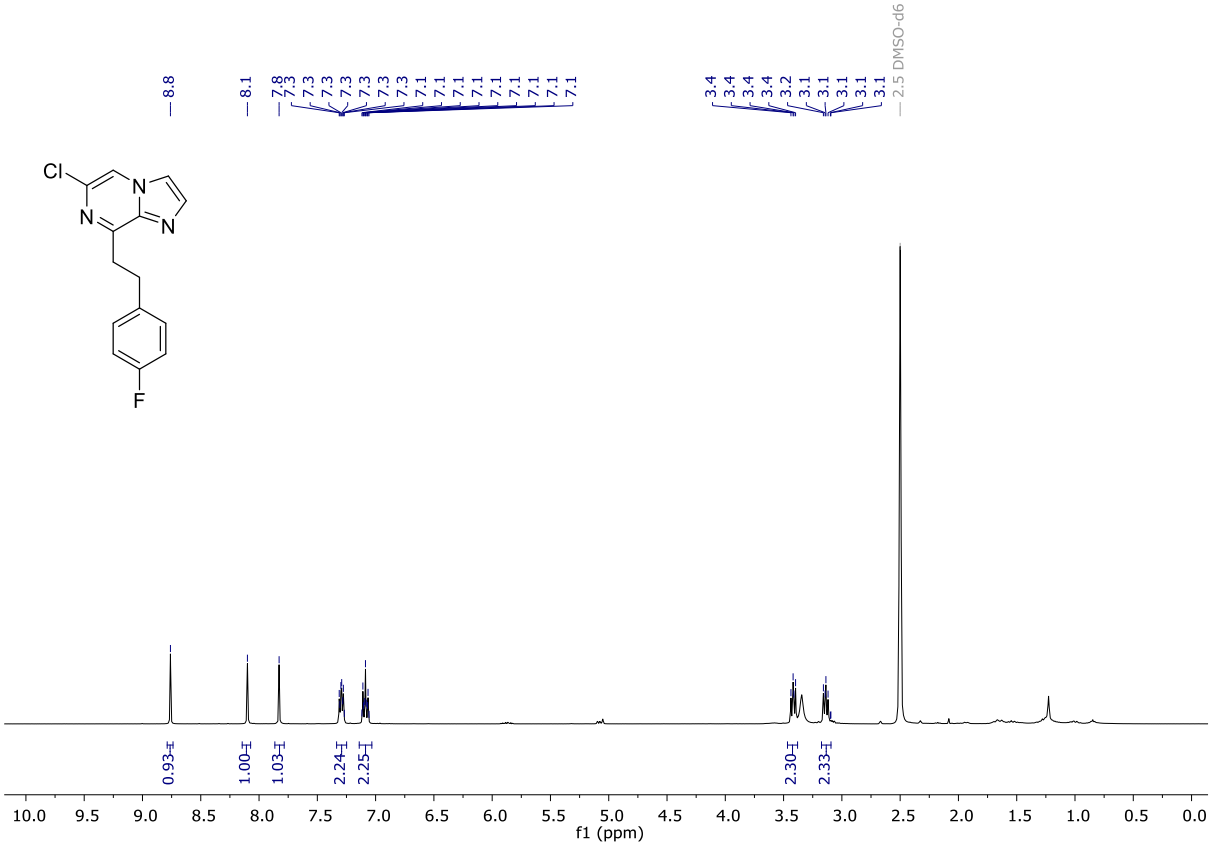
4-(6-Chloroimidazo[1,2-*a*]pyrazin-8-yl)-*N*,*N*-dimethylaniline (27b)

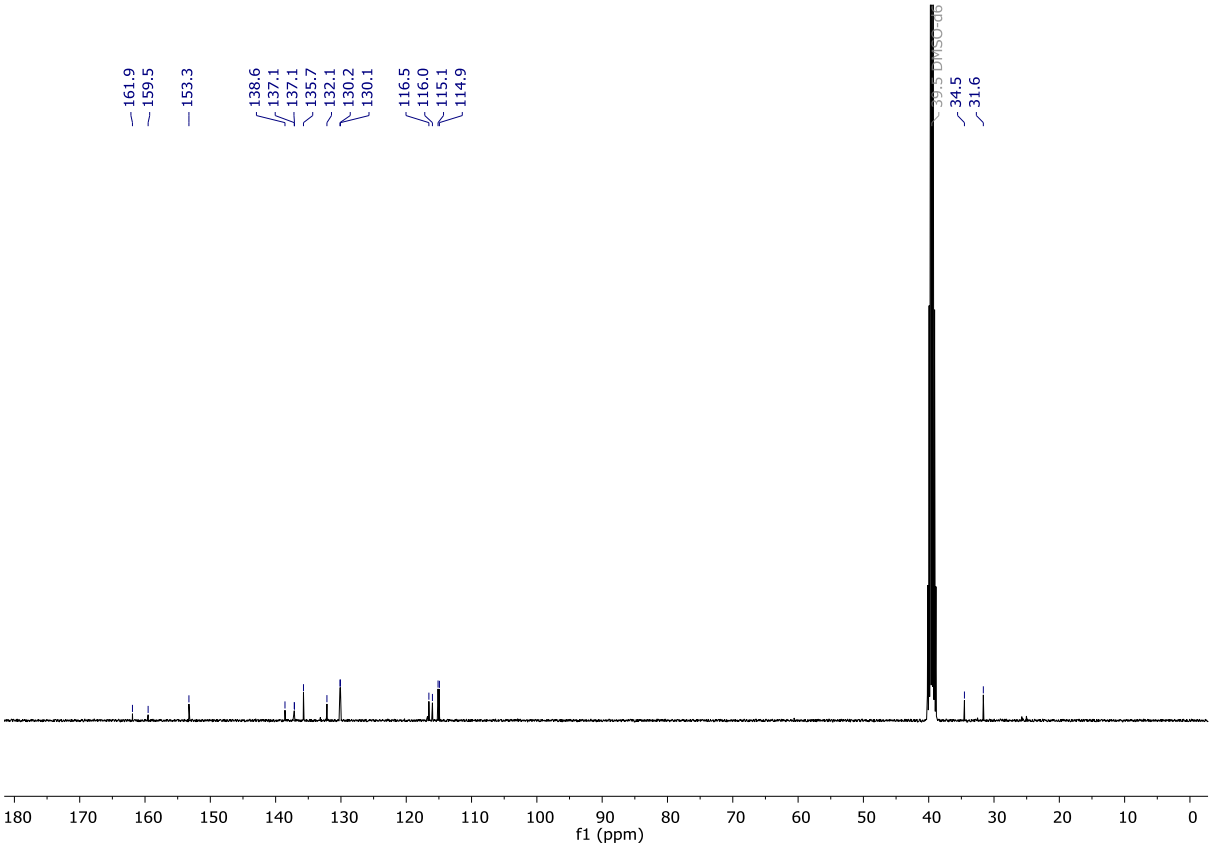


6-Chloro-8-(naphthalen-2-yl)imidazo[1,2-*a*]pyrazine (27c)

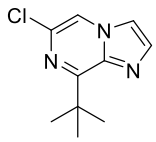


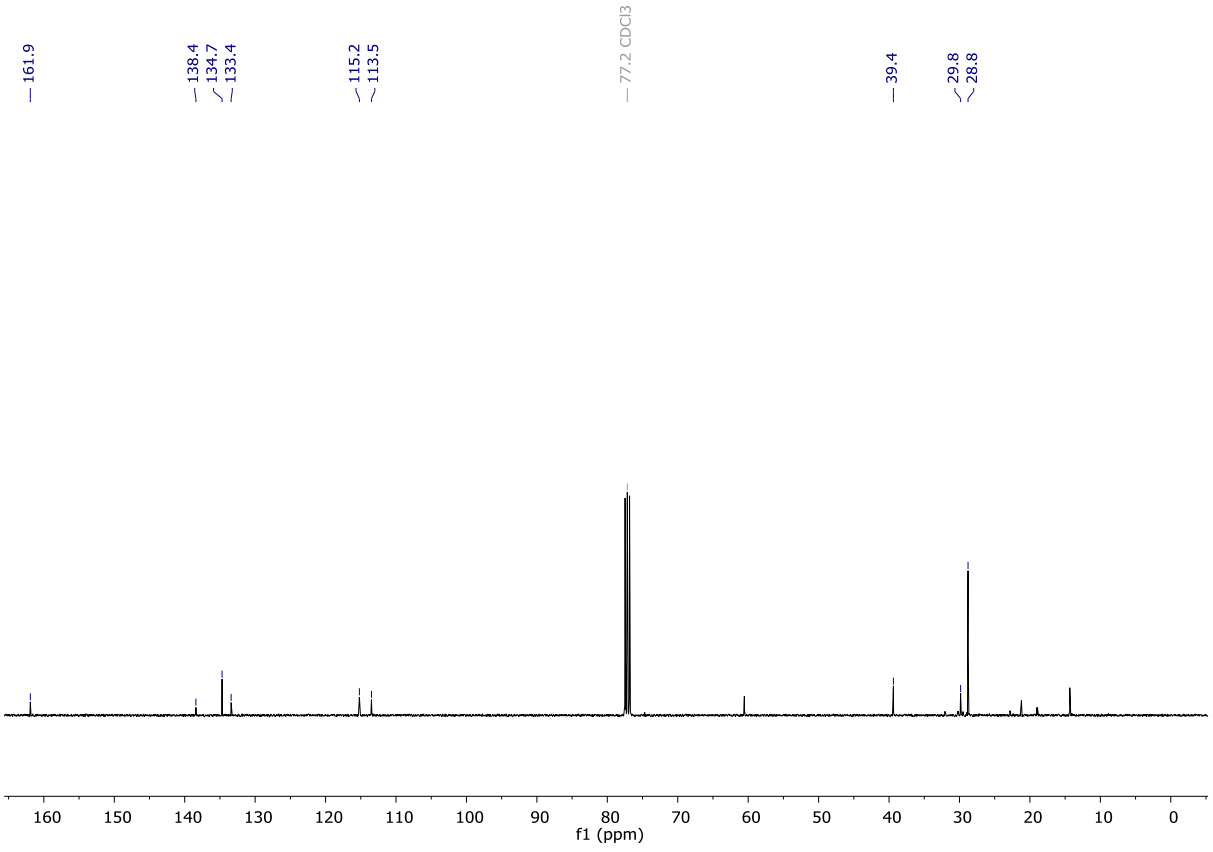
6-Chloro-8-(4-fluorophenethyl)imidazo[1,2-a]pyrazine (27d)



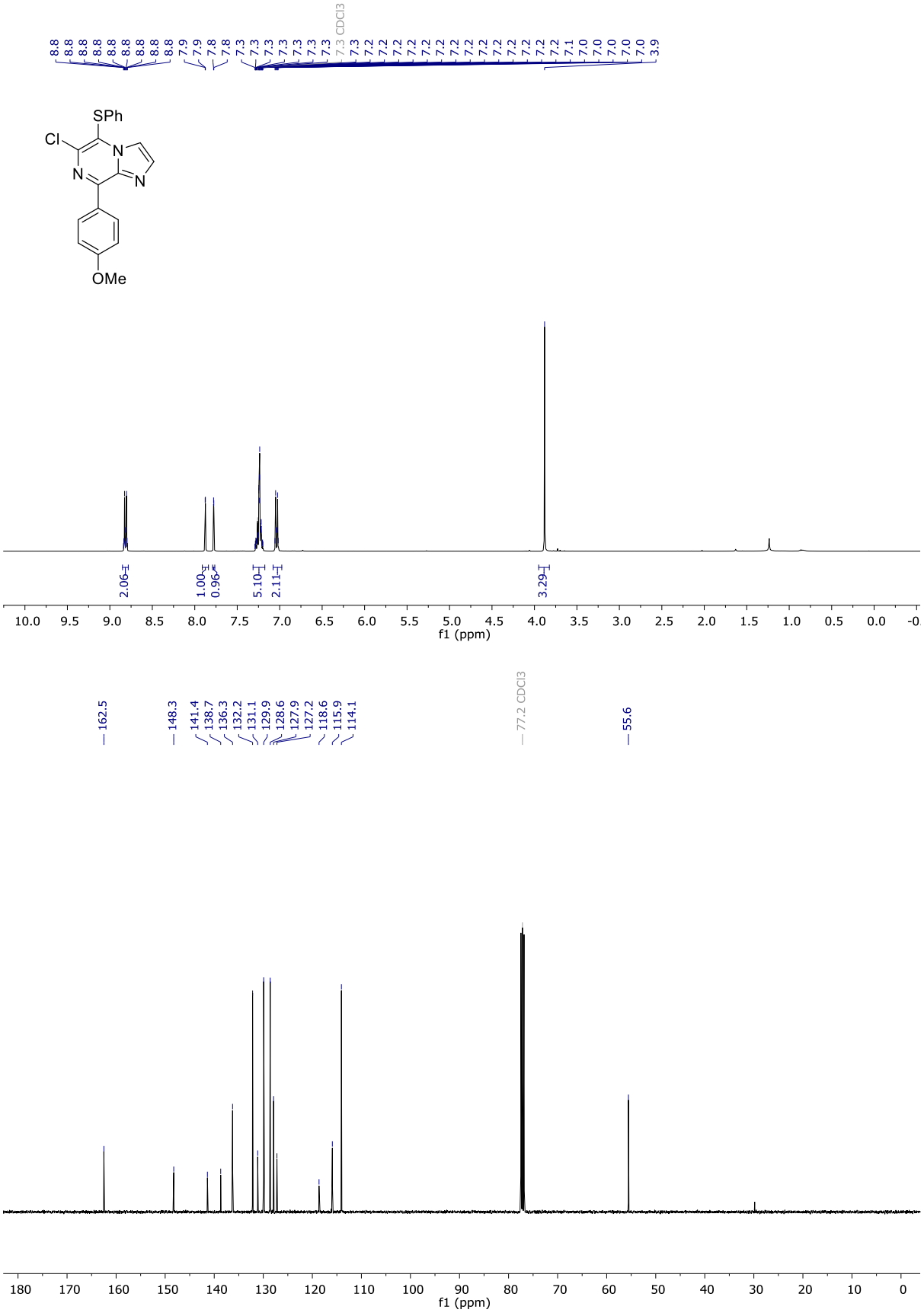


8-(*tert*-Butyl)-6-chloroimidazo[1,2-a]pyrazine (27e)





6-Chloro-8-(4-methoxyphenyl)-5-(phenylthio)imidazo[1,2-*a*]pyrazine (27f)



Details for X-ray data collection and structure refinement

Single Crystal X-Ray Diffraction Studies

Single crystals of compound **7a**, suitable for X-ray diffraction, were obtained by slow evaporation of $CDCl_3$ solution. The crystals were introduced into perfluorinated oil and a suitable single crystal was carefully mounted on the top of a thin glass wire. Data collection was performed with an Oxford Xcalibur 3 diffractometer equipped with a Spellman generator (50 kV, 40 mA) and a Kappa CCD detector, operating with Mo-K_α radiation (λ = 0.71071 Å).

Data collection and data reduction were performed with the CrysAlisPro software.[7] Absorption correction using the multiscan method[7] was applied. The structures were solved with SHELXS-97,[8] refined with SHELXL-97[9] and finally checked using PLATON.[10] Details for data collection and structure refinement are summarized in Table 1.

CCDC-2258909 contains supplementary crystallographic data for this compound. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Table 1. Details for X-ray data collection and structure refinement for compound **1**.

	7a
Empirical formula	$C_6H_3ClIN_3$
Formula mass	279.46
T[K]	123(2)
Crystal size [mm]	0.20 × 0.20 × 0.10
Crystal description	pale yellow block
Crystal system	triclinic
Space group	*P*-1
a [Å]	6.0804(3)

[7] CrysAlis CCD, Oxford Diffraction Ltd., Version 1.171.27p5 beta (release 01-04-2005 CrysAlis171.NET) (compiled Apr 1 2005, 17:53:34); CrysAlis RED, Oxford Diffraction Ltd., Version 1.171.27p5 beta (release 01-04-2005 CrysAlis171.NET) (compiled Apr 1 2005, 17:53:34).
[8] G. M. Sheldrick (1997) SHELXS-97: *Program for Crystal Structure Solution*, University of Göttingen, Germany.
[9] G. M. Sheldrick (1997) SHELXS-97: *Program for the Refinement of Crystal Structures*, University of Göttingen, Germany.
[10] A. L. Spek (1999) PLATON: *A Multipurpose Crystallographic Tool*, Utrecht University, Utrecht, the Netherlands.

b [Å]	9.9981(5)
c [Å]	13.2176(7)
α [°]	78.932(4)
β [°]	86.169(4)
γ [°]	79.771(4)
V [Å^3]	775.61(7)
Z	4
$\rho_{calcd.}$ [g cm^{-3}]	2.393
μ [mm^{-1}]	4.403
F(000)	520
Θ range [°]	2.11 – 25.24
Index ranges	-8 ≤ *h* ≤ 8
	-13 ≤ *k* ≤ 13
	-17 ≤ *l* ≤ 17
Reflns. collected	13809
Reflns. obsd.	2961
Reflns. unique	3820 (R_{int} = 0.0464)
R_1, wR_2 (2σ data)	0.0357, 0.0784
R_1, wR_2 (all data)	0.0550, 0.0880
GOOF on F^2	1.040
Peak/hole [e Å^{-3}]	2.044 / -0.858

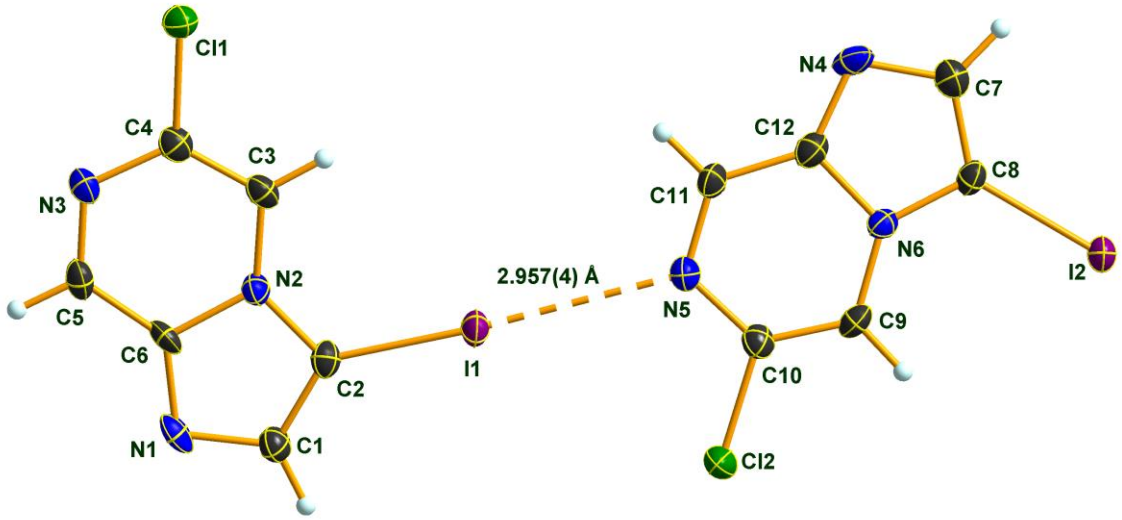


Figure 1. Molecular structure of compound **7a** in the crystal. DIAMOND[e)] representation; thermal ellipsoids are drawn at 50 % probability level.

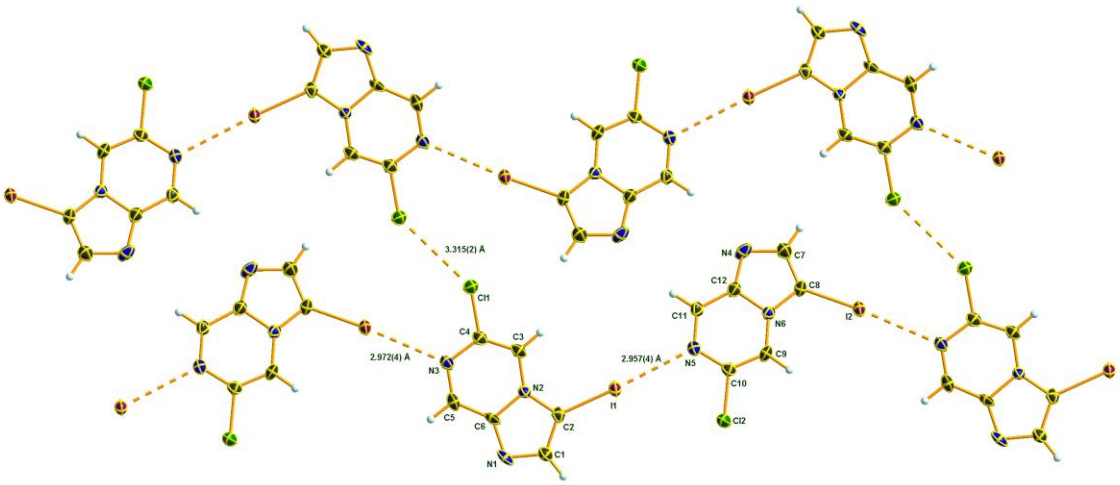


Figure 2. Halogen bonding in the crystal structure of compound **7a**. DIAMOND[e)] representation; thermal ellipsoids are drawn at 50 % probability level.

Table 2. Selected bond lengths (Å) of compound **7a**.

I1 – C2	2.076(5)	N5 – C10	1.360(7)
I2 – C8	2.074(5)	N4 – C12	1.335(7)
Cl1 – C4	1.732(5)	N4 – C7	1.367(7)
Cl2 – C10	1.728(5)	C3 – C4	1.360(7)
N2 – C2	1.364(6)	C6 – C5	1.427(7)
N2 – C3	1.372(7)	C2 – C1	1.370(7)

N2 – C6	1.392(6)	C9 – C10	1.349(7)
N6 – C8	1.354(7)	C11 – C12	1.410(8)
N6 – C9	1.373(7)	C8 – C7	1.375(7)
N6 – C12	1.397(6)	N1 – C1	1.342(7)
N3 – C5	1.311(7)	N1 – C6	1.356(7)
N3 – C4	1.364(7)	N5 – C11	1.316(7)

Table 3. Selected bond angles (°) of compound **7a**.

C2 – N2 – C3	132.3(5)	C9 – C10 – N5	124.9(5)
C2 – N2 – C6	105.8(4)	C9 – C10 – Cl2	118.7(4)
C3 – N2 – C6	121.8(4)	N5 – C10 – Cl2	116.3(4)
C8 – N6 – C9	132.5(4)	N1 – C1 – C2	113.4(5)
C8 – N6 – C12	106.8(4)	N5 – C11 – C12	122.8(5)
C9 – N6 – C12	120.6(5)	N6 – C8 – C7	105.9(4)
C5 – N3 – C4	117.5(5)	N6 – C8 – I2	122.3(4)
C1 – N1 – C6	103.3(4)	C7 – C8 – I2	131.7(4)
C11 – N5 – C10	117.3(5)	N3 – C5 – C6	122.5(5)
C12 – N4 – C7	104.4(4)	N4 – C12 – N6	111.1(5)
C4 – C3 – N2	116.3(5)	N4 – C12 – C11	131.9(5)
N1 – C6 – N2	111.7(5)	N6 – C12 – C11	117.0(5)
N1 – C6 – C5	131.7(5)	N4 – C7 – C8	111.8(5)
N2 – C6 – C5	116.5(5)	C3 – C4 – N3	125.3(5)
N2 – C2 – C1	105.7(4)	C3 – C4 – Cl1	118.0(4)
N2 – C2 – I1	121.6(4)	N3 – C4 – Cl1	116.7(4)
C1 – C2 – I1	132.5(4)	C10 – C9 – N6	117.4(5)

Table 4. Selected torsion angles (°) of compound **7a**.

C2 – N2 – C3 – C4	-177.5(5)	C6 – N1 – C1 – C2	-1.0(6)
C6 – N2 – C3 – C4	0.5(7)	N2 – C2 – C1 – N1	0.5(6)
C1 – N1 – C6 – N2	1.1(6)	I1 – C2 – C1 – N1	176.0(4)
C1 – N1 – C6 – C5	-177.8(6)	C10 – N5 – C11 – C12	2.2(8)
C2 – N2 – C6 – N1	-0.9(6)	C9 – N6 – C8 – C7	176.8(5)
C3 – N2 – C6 – N1	-179.3(4)	C12 – N6 – C8 – C7	-0.9(6)
C2 – N2 – C6 – C5	178.2(5)	C9 – N6 – C8 – I2	0.7(8)
C3 – N2 – C6 – C5	-0.2(7)	C12 – N6 – C8 – I2	-177.0(4)
C3 – N2 – C2 – C1	178.4(5)	C4 – N3 – C5 – C6	0.7(8)
C6 – N2 – C2 – C1	0.2(6)	N1 – C6 – C5 – N3	178.4(5)
C3 – N2 – C2 – I1	2.3(8)	N2 – C6 – C5 – N3	-0.4(8)
C6 – N2 – C2 – I1	-175.9(3)	C7 – N4 – C12 – N6	1.7(6)
N2 – C3 – C4 – N3	-0.2(8)	C7 – N4 – C12 – C11	-178.8(6)
N2 – C3 – C4 – Cl1	178.3(4)	C8 – N6 – C12 – N4	-0.5(6)

C5 – N3 – C4 – C3	-0.4(8)	C9 – N6 – C12 – N4	-178.6(5)
C5 – N3 – C4 – Cl1	-178.9(4)	C8 – N6 – C12 – C11	179.9(5)
C8 – N6 – C9 – C10	-177.9(5)	C9 – N6 – C12 – C11	1.8(7)
C12 – N6 – C9 – C10	-0.4(7)	N5 – C11 – C12 – N4	177.7(6)
N6 – C9 – C10 – N5	-0.3(8)	N5 – C11 – C12 – N6	-2.8(8)
N6 – C9 – C10 – Cl2	177.5(4)	C12 – N4 – C7 – C8	-2.3(6)
C11 – N5 – C10 – C9	-0.6(8)	N6 – C8 – C7 – N4	2.1(6)
C11 – N5 – C10 – Cl2	-178.4(4)	I2 – C8 – C7 – N4	177.6(4)

Single crystals of compound **8b**, suitable for X-ray diffraction, were obtained by slow evaporation of $CHCl_3$ solution. The crystals were introduced into perfluorinated oil and a suitable single crystal was carefully mounted on the top of a thin glass wire. Data collection was performed with an Oxford Xcalibur 3 diffractometer equipped with a Spellman generator (50 kV, 40 mA) and a Kappa CCD detector, operating with Mo-K_α radiation (λ = 0.71071 Å).

CCDC-2258910 contains supplementary crystallographic data for this compound. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Table 1. Details for X-ray data collection and structure refinement for compound **8b**.

	8b
Empirical formula	$C_9H_8ClN_3$
Formula mass	193.63
T[K]	123(2)
Crystal size [mm]	0.40 × 0.20 × 0.05
Crystal description	colorless block
Crystal system	monoclinic
Space group	*P*21/*c*
a [Å]	13.2253(10)
b [Å]	7.3421(4)
c [Å]	9.4392(6)
α [°]	90.0
β [°]	106.538(7)
γ [°]	90.0

V [Å^3]	878.64(10)
Z	4
$\rho_{calcd.}$ [g cm^{-3}]	1.464
μ [mm^{-1}]	0.385
F(000)	400
Θ range [°]	3.21 – 25.24
Index ranges	-17 ≤ *h* ≤ 17
	-9 ≤ *k* ≤ 9
	-12 ≤ *l* ≤ 12
Reflns. collected	14527
Reflns. obsd.	1735
Reflns. unique	2173 (R_{int} = 0.0629)
R_1, wR_2 (2σ data)	0.0432, 0.1053
R_1, wR_2 (all data)	0.0573, 0.1163
GOOF on F^2	1.060
Peak/hole [e Å^{-3}]	0.416 / -0.222

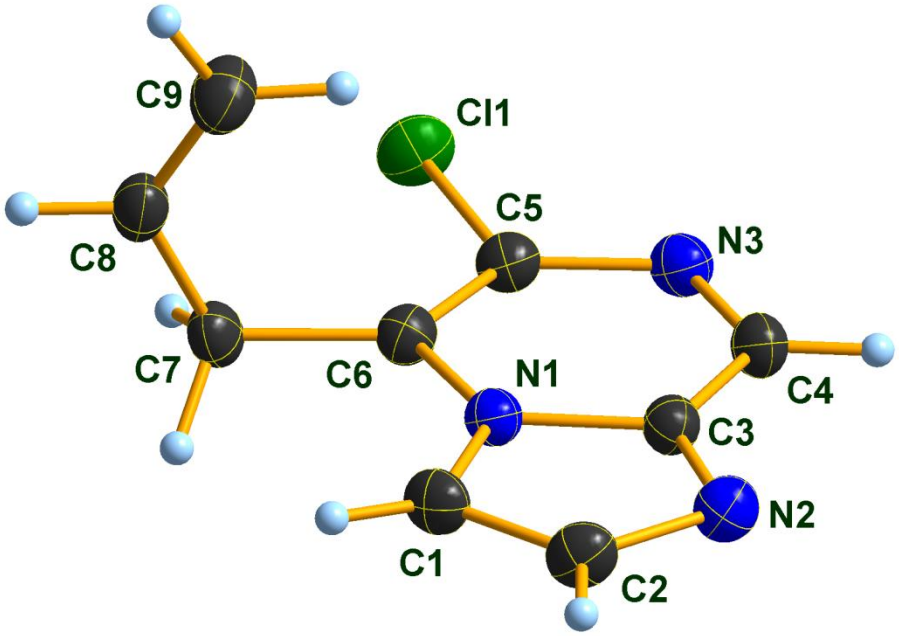


Figure 1. Molecular structure of compound **8b** in the crystal. DIAMOND[11] representation; thermal ellipsoids are drawn at 50 % probability level.

Table 2. Selected bond lengths (Å) of compound **8b**.

[11] DIAMOND, Crystal Impact GbR., Version 3.2i.

Cl1 – C5	1.746(2)	N3 – C5	1.363(2)
N1 – C1	1.372(2)	C6 – C5	1.360(3)
N1 – C6	1.386(2)	C6 – C7	1.502(2)
N1 – C3	1.400(2)	C7 – C8	1.500(3)
C1 – C2	1.373(3)	C8 – C9	1.309(3)
C2 – N2	1.362(2)	C3 – C4	1.410(3)
N2 – C3	1.329(2)	N3 – C4	1.314(2)

Table 3. Selected bond angles (°) of compound **8b**.

C1 – N1 – C6	131.6(2)	C6 – C5 – N3	127.0(2)
C1 – N1 – C3	106.6(1)	C6 – C5 – Cl1	119.5(1)
C6 – N1 – C3	121.8(2)	N3 – C5 – Cl1	113.4(1)
N1 – C1 – C2	105.1(2)	C8 – C7 – C6	114.8(2)
N2 – C2 – C1	112.4(2)	C9 – C8 – C7	126.7(2)
C3 – N2 – C2	104.7(2)	C5 – C6 – N1	114.6(2)
N2 – C3 – N1	111.2(2)	C5 – C6 – C7	127.6(2)
N2 – C3 – C4	131.7(2)	N1 – C6 – C7	117.7(2)
N1 – C3 – C4	117.1(2)	N3 – C4 – C3	122.8(2)
C4 – N3 – C5	116.6(2)		

Table 4. Selected torsion angles (°) of compound **8b**.

C6 – N1 – C1 – C2	-179.3(2)	C3 – N1 – C6 – C7	179.7(1)
C3 – N1 – C1 – C2	0.3(2)	C5 – N3 – C4 – C3	-0.3(3)
N1 – C1 – C2 – N2	-0.4(2)	N2 – C3 – C4 – N3	-179.0(2)
C1 – C2 – N2 – C3	0.3(2)	N1 – C3 – C4 – N3	0.7(3)
C2 – N2 – C3 – N1	-0.1(2)	N1 – C6 – C5 – N3	1.1(3)
C2 – N2 – C3 – C4	179.6(2)	C7 – C6 – C5 – N3	-179.2(2)
C1 – N1 – C3 – N2	-0.1(2)	N1 – C6 – C5 – Cl1	-178.8(1)
C6 – N1 – C3 – N2	179.5(1)	C7 – C6 – C5 – Cl1	1.0(3)
C1 – N1 – C3 – C4	-179.9(1)	C4 – N3 – C5 – C6	-0.6(3)
C6 – N1 – C3 – C4	-0.2(2)	C4 – N3 – C5 – Cl1	179.2(1)
C1 – N1 – C6 – C5	179.0(2)	C5 – C6 – C7 – C8	-101.0(2)
C3 – N1 – C6 – C5	-0.6(2)	N1 – C6 – C7 – C8	78.7(2)
C1 – N1 – C6 – C7	-0.8(3)	C6 – C7 – C8 – C9	3.7(3)

Single crystals of compound **16a**, suitable for X-ray diffraction, were obtained by slow evaporation of $CHCl_3$ solution. The crystals were introduced into perfluorinated oil and a suitable single crystal was carefully mounted on the top of a thin glass wire. Data collection was performed with an D8 Venture diffractometer equipped with a Bruker D8 Venture TXS rotating anode X-ray tube operating with Mo-K_α radiation (λ = 0.71073 Å) and a multilayer mirror optics monochromator.

CCDC-2258912 contains supplementary crystallographic data for this compound. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Table 5. Details for X-ray data collection and structure refinement for compound **16a**.

	16a
Empirical formula	$C_7H_2ClIN_4$
Formula mass	304.48
T[K]	173(2)
Crystal size [mm]	0.10 × 0.08 × 0.02
Crystal description	colorless platelet
Crystal system	monoclinic
Space group	*P*21/*n*
a [Å]	8.2171(2)
b [Å]	5.69960(10)
c [Å]	18.6448(5)
α [°]	90.0
β [°]	99.8020(10)
γ [°]	90.0
V [Å^3]	860.47(3)
Z	4
$\rho_{calcd.}$ [g cm^{-3}]	2.350
μ [mm^{-1}]	3.983
F(000)	568
Θ range [°]	3.74 – 25.24
Index ranges	-11 ≤ *h* ≤ 11
	-8 ≤ *k* ≤ 8
	-26 ≤ *l* ≤ 26
Reflns. collected	18326
Reflns. obsd.	2296
Reflns. unique	2609 (R_{int} = 0.0344)
R_1, wR_2 (2σ data)	0.0184, 0.0369
R_1, wR_2 (all data)	0.0230, 0.0386

GOOF on F^2	1.053
Peak/hole [e Å^{-3}]	0.457 / -0.397

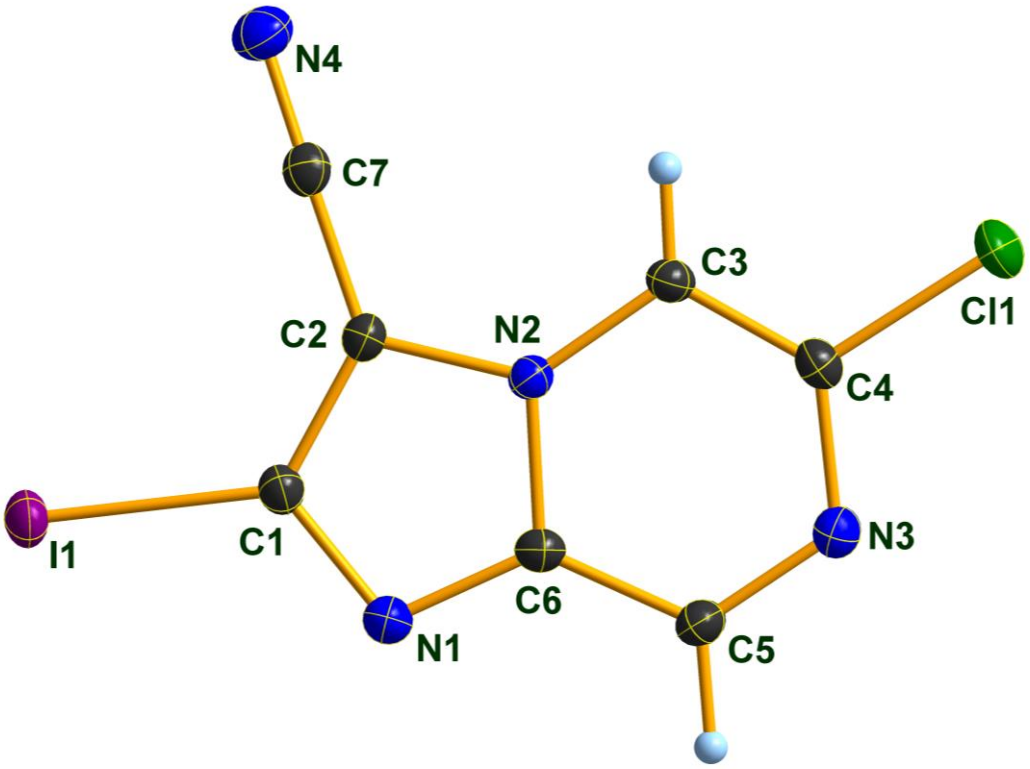


Figure 2. Molecular structure of compound **16a** in the crystal. DIAMOND[13] representation; thermal ellipsoids are drawn at 50 % probability level.

Table 6. Selected bond lengths (Å) of compound **16a**.

I1 – C1	2.070(2)	N2 – C6	1.385(2)
N1 – C6	1.347(2)	C4 – N3	1.355(2)
N1 – C1	1.348(2)	C4 – C3	1.361(2)
C1 – C2	1.392(2)	N4 – C7	1.149(2)
Cl1 – C4	1.719(2)	C6 – C5	1.411(2)
C2 – N2	1.377(2)	N3 – C5	1.316(2)
C2 – C7	1.418(2)	N2 – C3	1.366(2)

Table 7. Selected bond angles (°) of compound **16a**.

C6 – N1 – C1	104.9(1)	C3 – C4 – Cl1	118.3(1)
N1 – C1 – C2	111.7(2)	N1 – C6 – N2	111.7(2)
N1 – C1 – I1	122.7(1)	N1 – C6 – C5	131.0(2)
C2 – C1 – I1	125.6(1)	N2 – C6 – C5	117.3(2)
N2 – C2 – C1	105.6(1)	C4 – C3 – N2	116.2(2)
N2 – C2 – C7	122.4(2)	C5 – N3 – C4	117.6(2)

C1 – C2 – C7	131.8(2)	N3 – C5 – C6	122.1(2)
C3 – N2 – C2	132.1(2)	N4 – C7 – C2	177.4(2)
C3 – N2 – C6	121.7(2)	N3 – C4 – C3	125.2(2)
C2 – N2 – C6	106.2(1)	N3 – C4 – Cl1	116.5(1)

Table 8. Selected torsion angles (°) of compound **16a**.

C6 – N1 – C1 – C2	-0.5(2)	C2 – N2 – C6 – N1	-0.6(2)
C6 – N1 – C1 – I1	178.3(1)	C3 – N2 – C6 – C5	-0.5(2)
N1 – C1 – C2 – N2	0.2(2)	C2 – N2 – C6 – C5	177.3(2)
I1 – C1 – C2 – N2	-178.6(1)	N3 – C4 – C3 – N2	0.3(3)
N1 – C1 – C2 – C7	175.3(2)	Cl1 – C4 – C3 – N2	-179.4(1)
I1 – C1 – C2 – C7	-3.5(3)	C2 – N2 – C3 – C4	-176.8(2)
C1 – C2 – N2 – C3	177.7(2)	C6 – N2 – C3 – C4	0.4(2)
C7 – C2 – N2 – C3	2.1(3)	C3 – C4 – N3 – C5	-0.8(3)
C1 – C2 – N2 – C6	0.2(2)	Cl1 – C4 – N3 – C5	178.9(1)
C7 – C2 – N2 – C6	-175.5(2)	C4 – N3 – C5 – C6	0.7(3)
C1 – N1 – C6 – N2	0.6(2)	N1 – C6 – C5 – N3	177.3(2)
C1 – N1 – C6 – C5	-176.9(2)	N2 – C6 – C5 – N3	0.0(3)
C3 – N2 – C6 – N1	-178.4(2)		

Single crystals of compound **18a**, suitable for X-ray diffraction, were obtained by slow evaporation of $CHCl_3$ solution. The crystals were introduced into perfluorinated oil and a suitable single crystal was carefully mounted on the top of a thin glass wire. Data collection was performed with an D8 Venture diffractometer equipped with a Bruker D8 Venture TXS rotating anode X-ray tube operating with Mo-K_α radiation (λ = 0.71073 Å) and a multilayer mirror optics monochromator.

CCDC-2258911 contains supplementary crystallographic data for this compound. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Table 1. Details for X-ray data collection and structure refinement for compound **18a**.

	18a
Empirical formula	$C_{14}H_8ClIN_4O$
Formula mass	410.59
T[K]	173(2)
Crystal size [mm]	0.40 × 0.20 × 0.15
Crystal description	colorless block

Crystal system	triclinic
Space group	*P*-1
a [Å]	8.9084(3)
b [Å]	8.9556(3)
c [Å]	9.5787(3)
α [°]	75.6990(10)
β [°]	74.5870(10)
γ [°]	80.1380(10)
V [Å^3]	709.30(4)
Z	2
$\rho_{calcd.}$ [g cm^{-3}]	1.922
μ [mm^{-1}]	2.449
F(000)	396
Θ range [°]	3.16 – 25.24
Index ranges	-11 ≤ *h* ≤ 11
	-11 ≤ *k* ≤ 11
	-11 ≤ *l* ≤ 11
Reflns. collected	10790
Reflns. obsd.	2610
Reflns. unique	2820 (R_{int} = 0.0320)
R_1, wR_2 (2σ data)	0.0220, 0.0535
R_1, wR_2 (all data)	0.0246, 0.0551
GOOF on F^2	1.048
Peak/hole [e Å^{-3}]	1.195 / -0.377

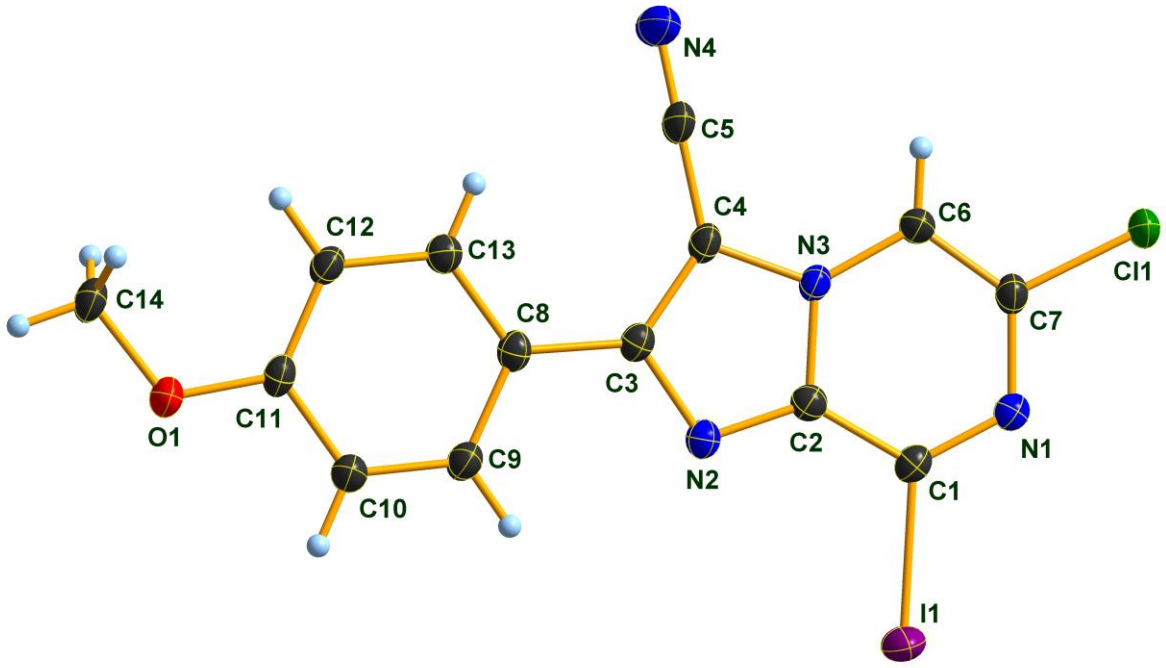


Figure 1. Molecular structure of compound **18a** in the crystal. DIAMOND[13] representation; thermal ellipsoids are drawn at 50 % probability level.

Table 2. Selected bond lengths (Å) of compound **18a**.

I1 – C1	2.079(2)	C5 – N4	1.140(3)
Cl1 – C7	1.727(2)	C5 – C4	1.424(3)
O1 – C11	1.356(3)	C6 – C7	1.360(3)
O1 – C14	1.430(3)	C8 – C13	1.396(3)
N1 – C1	1.304(3)	C10 – C11	1.398(3)
N1 – C7	1.357(3)	C11 – C12	1.391(3)
C1 – C2	1.418(3)	C13 – C12	1.390(3)
N2 – C2	1.323(3)	N3 – C6	1.371(3)
N2 – C3	1.356(3)	N3 – C4	1.379(3)
C2 – N3	1.384(3)	C9 – C10	1.376(3)
C3 – C4	1.402(3)	C9 – C8	1.401(3)
C3 – C8	1.464(3)		

Table 3. Selected bond angles (°) of compound **18a**.

C11 – O1 – C14	118.2(2)	N1 – C7 – C6	125.1(2)
C1 – N1 – C7	117.4(2)	N1 – C7 – Cl1	116.0(2)
N1 – C1 – C2	123.1(2)	C6 – C7 – Cl1	118.9(2)
N1 – C1 – I1	120.4(2)	C13 – C8 – C9	118.4(2)
C2 – C1 – I1	116.5(2)	C13 – C8 – C3	122.8(2)
C2 – N2 – C3	106.4(2)	C9 – C8 – C3	118.8(2)
N2 – C2 – N3	111.7(2)	C9 – C10 – C11	120.3(2)
N2 – C2 – C1	132.0(2)	O1 – C11 – C12	124.5(2)

N3 – C2 – C1	116.3(2)	O1 – C11 – C10	115.7(2)
N2 – C3 – C4	109.9(2)	C12 – C11 – C10	119.8(2)
N2 – C3 – C8	120.9(2)	C12 – C13 – C8	121.3(2)
C4 – C3 – C8	129.2(2)	C13 – C12 – C11	119.5(2)
C6 – N3 – C4	131.9(2)	N3 – C4 – C3	105.8(2)
C6 – N3 – C2	121.9(2)	N3 – C4 – C5	120.9(2)
C4 – N3 – C2	106.2(2)	C3 – C4 – C5	133.2(2)
C10 – C9 – C8	120.8(2)	C7 – C6 – N3	116.2(2)
N4 – C5 – C4	178.7(3)		

Table 4. Selected torsion angles (°) of compound **18a**.

C7 – N1 – C1 – C2	-1.2(3)	C4 – N3 – C6 – C7	178.5(2)
C7 – N1 – C1 – I1	179.2(2)	C2 – N3 – C6 – C7	0.3(3)
C3 – N2 – C2 – N3	-0.3(3)	C1 – N1 – C7 – C6	-0.8(4)
C3 – N2 – C2 – C1	179.9(2)	C1 – N1 – C7 – Cl1	179.3(2)
N1 – C1 – C2 – N2	-177.6(2)	N3 – C6 – C7 – N1	1.2(4)
I1 – C1 – C2 – N2	2.0(3)	N3 – C6 – C7 – Cl1	-178.9(2)
N1 – C1 – C2 – N3	2.5(3)	C10 – C9 – C8 – C13	0.8(4)
I1 – C1 – C2 – N3	-177.8(2)	C10 – C9 – C8 – C3	-179.8(2)
C2 – N2 – C3 – C4	0.9(3)	N2 – C3 – C8 – C13	178.6(2)
C2 – N2 – C3 – C8	-179.8(2)	C4 – C3 – C8 – C13	-2.2(4)
N2 – C2 – N3 – C6	178.1(2)	N2 – C3 – C8 – C9	-0.7(3)
C1 – C2 – N3 – C6	-2.1(3)	C4 – C3 – C8 – C9	178.4(2)
N2 – C2 – N3 – C4	-0.5(3)	C8 – C9 – C10 – C11	-0.1(4)
C1 – C2 – N3 – C4	179.4(2)	C14 – O1 – C11 – C12	-0.9(3)
C6 – N3 – C4 – C3	-177.4(2)	C14 – O1 – C11 – C10	-179.9(2)
C2 – N3 – C4 – C3	1.0(2)	C9 – C10 – C11 – O1	178.4(2)
C6 – N3 – C4 – C5	5.6(4)	C9 – C10 – C11 – C12	-0.6(4)
C2 – N3 – C4 – C5	-176.0(2)	C9 – C8 – C13 – C12	-0.9(4)
N2 – C3 – C4 – N3	-1.2(3)	C3 – C8 – C13 – C12	179.7(2)
C8 – C3 – C4 – N3	179.6(2)	C8 – C13 – C12 – C11	0.3(4)
N2 – C3 – C4 – C5	175.3(3)	O1 – C11 – C12 – C13	-178.4(2)
C8 – C3 – C4 – C5	-3.9(4)	C10 – C11 – C12 – C13	0.5(4)

Theoretical Studies

Computational details

As in earlier related studies,[12] we employ calculations at the CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory for the prediction of pK_a values of heterocyclic systems. Frequency calculations have been carried out to verify that the optimized structures are true minima. Thermochemical corrections to $\mathrm{H}^{\mathrm{gas}}$ and $\mathrm{G}^{\mathrm{gas}}$ at 298.15 K were calculated with GoodVibes using the quasi-harmonic approximation.[13] The furan/furan-2-ide reference system was used, whose pK_a value amounts to +35.0 in DMSO.[14] Pyrimidine was chosen as the protonated reference compound (positively charged) with a pK_a value of +0.55±0.15 in DMSO.[15]

Relative pK_a calculations

The thermodynamic cycles, illustrated in **Figure TF0.1** and in **Figure TF0.2**, utilize an isodesmic (proton exchange) reaction that involves the transfer of a proton between an acid and a reference compound. In line with this strategy, we use equations 1 and 2 to calculatethe relative pK_a values. This method offers several advantages, including the anticipated elimination of errors arising from differences in solvation free energies of the charged species on the reactant and product sides. Additionally, this approach assumes that the investigated structure and its reference are structurally similar and have comparable pK_a values. [16]

[12] M. Balkenhohl, H. Jangra, I. S. Makarov, S. M. Yang, H. Zipse, P. Knochel, *Angew. Chem. Int. Ed.* **2020**, *59*, 14992-14999.
[13] *GoodVibes*, rev. 3.0.1., as described in: G. Luchini, J. V. Alegre-Requena, I. Funes-Ardoiz, R. S. Paton, *F1000Research* **2020**, *9*, 291.
[14] A. Frischmuth, M. Fernandez, N. M. Barl, F. Achrainer, H. Zipse, G. Berionni, H. Mayr, K. Karaghiosoff, P. Knochel, *Angew. Chem. Int. Ed.* **2014**, *53*, 7928-7932.
[15] R. L. Benoit, M. Frechette, *Thermochim. Acta* **1988**, *127*, 125-127.
[16] R. Casasnovas, J. Ortega-Castro, J. Frau, J. Donoso, F. Muñoz, Int. J. Quantum Chem. **2014**, 114, 1350-1363.

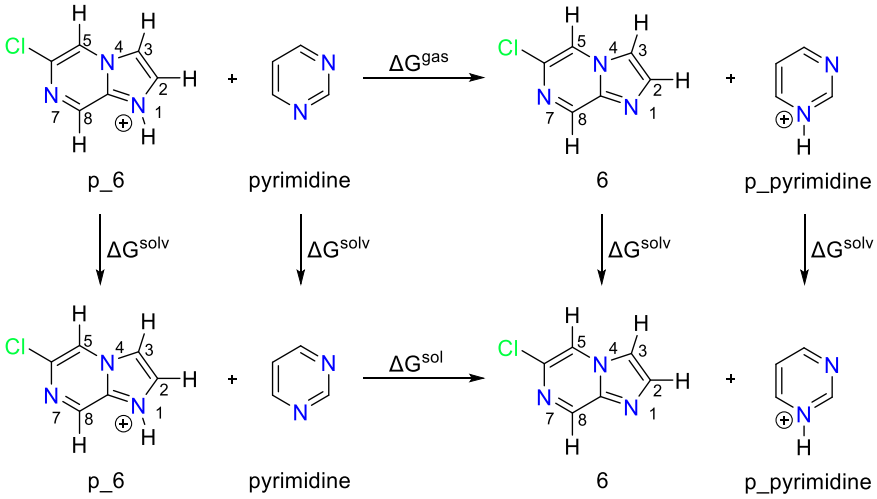


Figure TF0.1. Thermodynamic cycle used in the relative calculation of pK_a values for protonated (p_) molecules. Reference compound: protonated pyrimidine (p_pyrimidine) with a pKa value of 0.55±0.15 in DMSO.

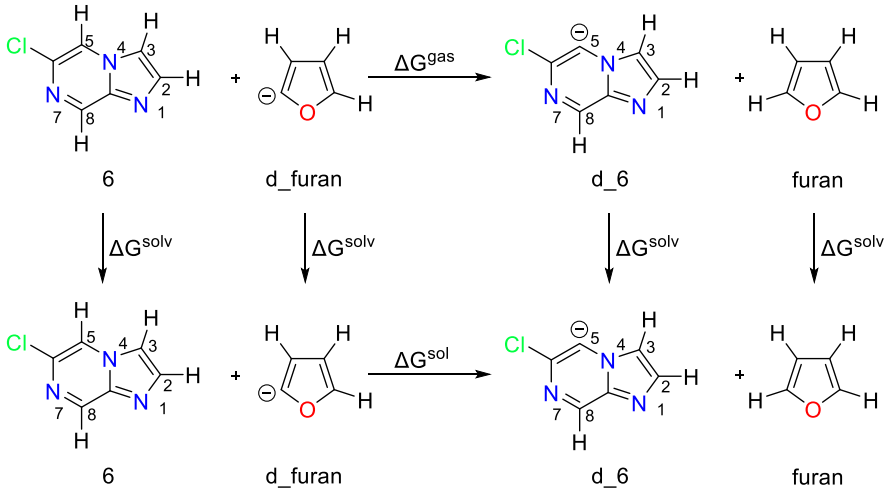


Figure TF0.2. Thermodynamic cycle used in the relative calculation of pK_a values for neutral molecules. Reference compound: furan with a pKa value of 35.0 in DMSO. ("d_" - deprotonated)

$$\Delta pK_a = \frac{\Delta G^{sol}}{2.303RT} \qquad \text{(eq. 1)}$$

$$pK_a(studied\ molcule) = pK_a(Ref) + \Delta pK_a \qquad \text{(eq. 2)}$$

Computational methods

Geometry optimizations have been performed using the B3LYP hybrid functional, complemented by the D3 dispersion correction. Geometry optimizations have been performed with the 6-31++G(2d,p) basis set. Thermal corrections at 298.15 K have been calculated at the same level as the geometry optimizations with quasi-harmonic treatment in GoodVibes v3.0.1 using Grimme's entropy treatment together with Head-Gordon's enthalpy treatment (**Table TT0.1**). Single-point calculations were then performed at the CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)//(U)B3LYP-D3/6-31++G(2d,p) level of theory. The solution phase free energies G^{sol} are computed by combining the solution phase single-point energy with thermal corrections calculated in the gas phase:

$$G^{sol} = E_{tot}^{\text{single-point in solution}} + ZPE^{gas} + \Delta G_{0K\rightarrow 298K}^{gas} + \Delta G_{0K\rightarrow 298K}^{1atm\rightarrow 1M}$$

$\Delta G_{0K\rightarrow 298K}^{1atm\rightarrow 1M}$ = +7.91 kJ mol^{-1} is the free energy difference for converting from the standard state concentration of 1 atm to the standard state concentration of 1 mol l^{-l}.

The initial structures of molecular complexes were generated randomly using the «kick» algorithm. [17] The individuality of the found conformers was confirmed using an energy criterion $\Delta E_{tot} > 10^{-7}$ Hartree [18] and comparing geometries by distances between each atom and the centroid point. [19] All calculations have been performed with *Gaussian 09, rev. D.01.*

Table TT0.1. GoodVibes usage example

```
Input
python3 -m goodvibes –qh mol3.log
Output
  GoodVibes v3.0.1 2023/06/29 00:08:23
  REF: Luchini, G.; Alegre-Requena J. V.; Guan, Y.; Funes-Ardoiz, I.; Paton, R. S. (2019).
     GoodVibes: GoodVibes 3.0.1 http://doi.org/10.5281/zenodo.595246
  Requested: --qh

  Temperature = 298.15 Kelvin   Pressure = 1 atm
  All energetic values below shown in Hartree unless otherwise specified.
  Using vibrational scale factor 1.0 for B3LYP/6-31++G(2d,p) level of theory

  Entropic quasi-harmonic treatment: frequency cut-off value of 100.0 wavenumbers will be applied.
  QS = Grimme: Using a mixture of RRHO and Free-rotor vibrational entropies.
  REF: Grimme, S. Chem. Eur. J. 2012, 18, 9955-9964

  Enthalpy quasi-harmonic treatment: frequency cut-off value of 100.0 wavenumbers will be applied.
  QH = Head-Gordon: Using an RRHO treatement with an approximation term for vibrational energy.
  REF: Li, Y.; Gomes, J.; Sharada, S. M.; Bell, A. T.; Head-Gordon, M. J. Phys. Chem. C 2015, 119, 1840-1850

  Structure                    E      ZPE          H        qh-H       T.S    T.qh-S      G(T)      qh-G(T)
  ********************************************************************************************************************
o mol3                      -395.9217110  0.1059700  -395.8089849  -395.8090418  0.0368243  0.0368315  -395.8458092  -395.8458733
  ********************************************************************************************************************
```

[17] a) D. Šakić, M. Hanževački, D. M. Smith, V. Vrček, Org. Biomol. Chem. 2015, 13, 11740-11752; b) D. Šakić, https://kick.science/KICK.html.
[18] V. Korotenko, https://github.com/vnkorotenko/ess.
[19] V. Korotenko, https://github.com/vnkorotenko/ccs.

Computational Results

Calculated pK_a values

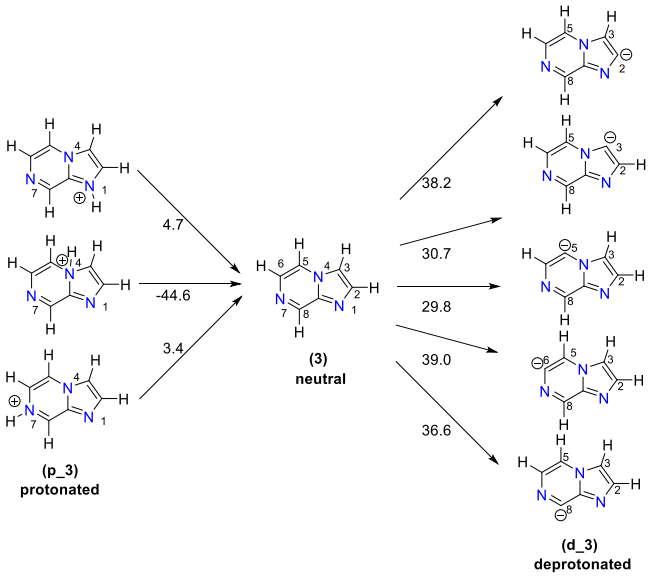


Figure TF1. Calculated pK_a values for system **3** (CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory).

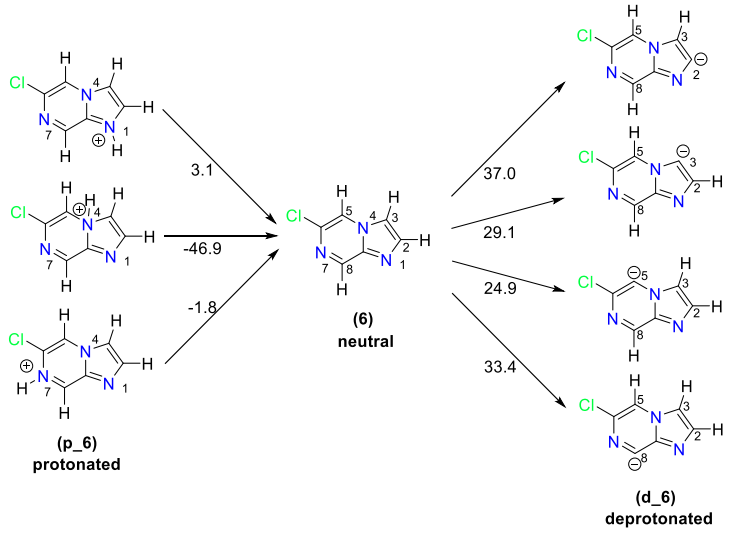


Figure TF2. Calculated pK_a values for system **6** (CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory).

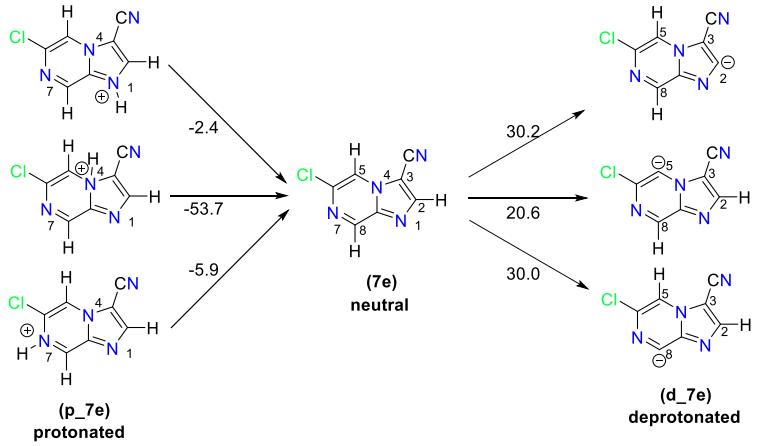


Figure TF3. Calculated pK_a values for system **7e** (CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory).

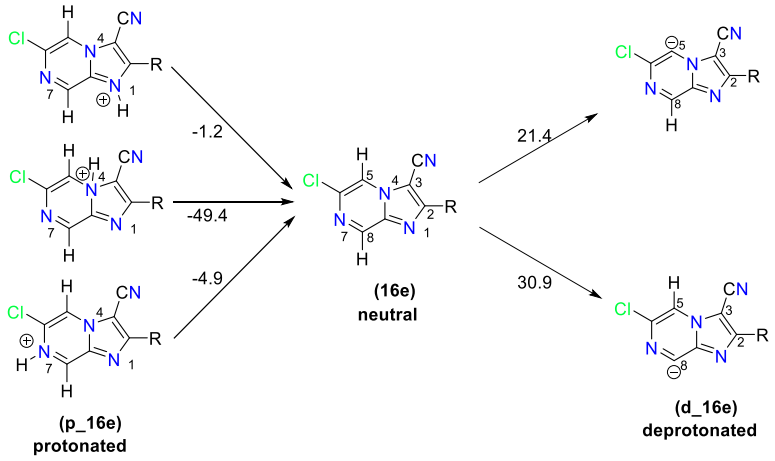


Figure TF4. Calculated pK_a values for system **16e** (CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory).

As shown in Figure TF1, the C-H bond acidity of compound **3** is largest at C5 position with pK_a(C5) = +29.8, closely followed by pK_a(C3) = +30.7. The basicity of the three nitrogen atoms is largest at N1 with pK_a(N1) = +4.7, closely followed by pK_a(N7) = +3.4. Introduction of an electron-withdrawing chlorine substituent at C6 as in compound **6** causes a general increase in C-H bond acidity and a decrease in basicity (Figure TF2). The most acidic position in compound **6** is C5 with pK_a(C5) = +24.9, all other positions being significantly less acidic. The most basic position is N1 with pK_a(N1) = +3.1, followed by pK_a(N7) = -1.8. The calculated pKa values for molecules **7e** and **16e** are presented in Figures **TF3** and **TF4**, respectively.

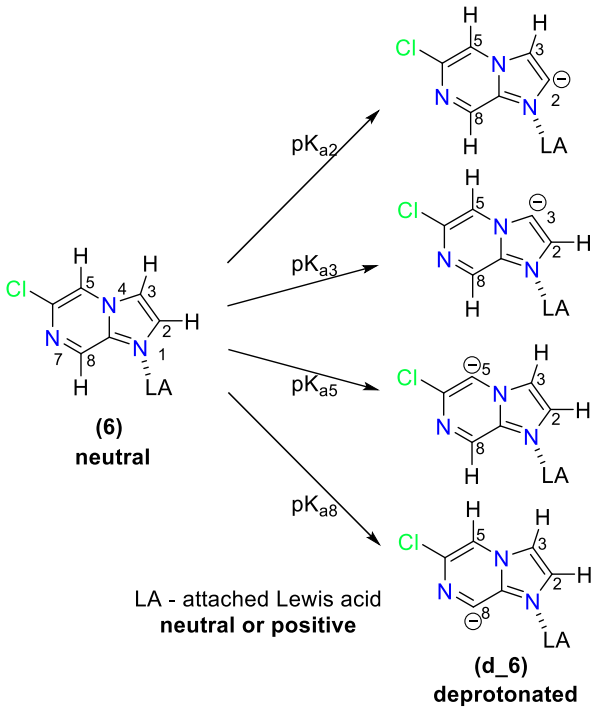


Figure TF5. Definitions of C-H bond pK_a values of Lewis acid complexes of **6**.

Table TT1. pK_a values of Lewis acid complexes of **6** calculated at the CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)// B3LYP-D3/6-31++G(2d,p) level of theory.

Lewis acid	C-H bond pK_a values of **6**			
	pK_{a2}	pK_{a3}	pK_{a5}	pK_{a8}
charge = 0				
-	37.0	29.1	**24.9**	33.4
LiCl	31.0	26.4	**22.7**	27.5
$MgCl_2$	26.0	24.4	**21.3**	23.0
Me_2NMgCl	30.8	25.1	**21.8**	30.6
TMPMgCl	30.9	25.0	**21.8**	31.5
$ZnCl_2$	28.8	24.1	**21.0**	Zn-C
Me_2NZnCl	29.8	24.4	**21.2**	30.0
TMPZnCl	31.5	24.9	**21.0**	35.0
charge = +1				
$MgCl^+$	21.6	22.7	**20.2**	Mg-C
$ZnCl^+$	Zn-C	21.0	**18.7**	Zn-C
charge = +2				
Mg^{+2}	24.3	21.3	**18.8**	Mg-C
Zn^{+2}	Zn-C	25.4	**21.2**	Zn-C
„Mg-C“ – Mg atom translation and formation of a Mg-C bond occurs during the geometry optimization; „Zn-C“ – Zn atom translation and formation of a Zn-C bond occurs during the geometry optimization.				

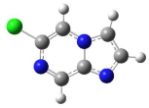
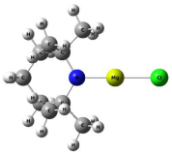
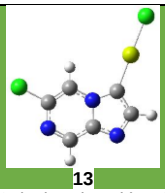
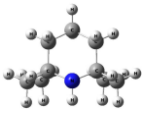
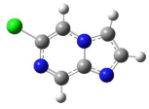
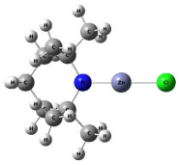
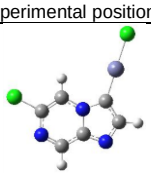
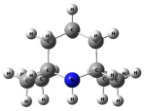
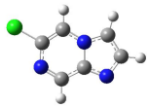
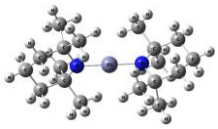
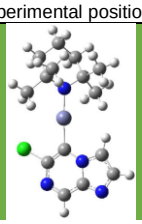
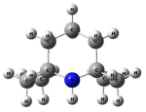
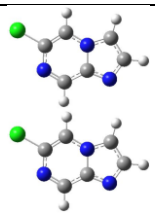
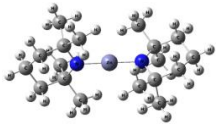
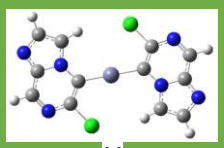
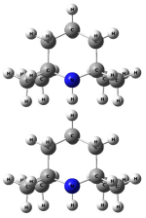
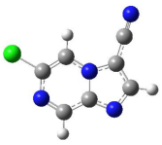
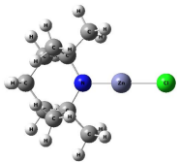
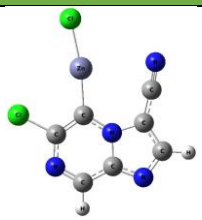
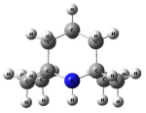
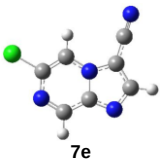
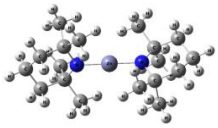
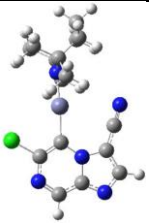
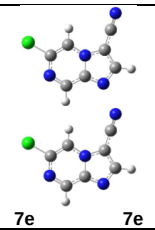
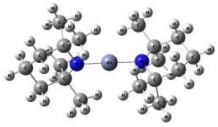
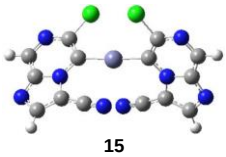
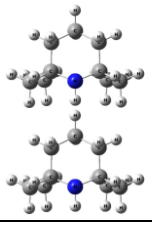
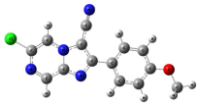
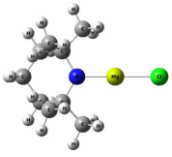
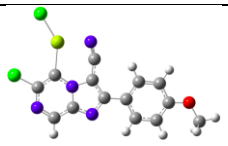
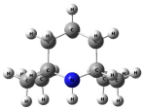
The C-H bond acidity profile of compound **6** was subsequently explored in the absence and the presence of Lewis acids coordinated to N1 (Figure TF5). Lewis acid coordination to N1 in compound **6** leads to an increase in acidity of all C-H bonds (**Table TT1**). The C5-H is the most acidic position in **6** irrespective of the choice of Lewis acid. In the class of neutral Lewis acids, the lowest pK_a values (+21.0) have been calculated for the zinc salts $ZnCl_2$ and TMPZnCl, closely followed by those for the magnesiums(II) salts (+21.2 - +21.8). The C-H bond pK_a values are lower for cationic and dicationic Lewis acids, but this may not reflect the true bonding situation in solution experiments.

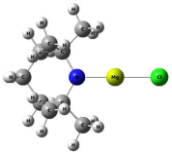
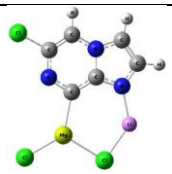
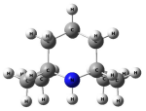
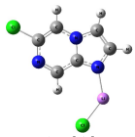
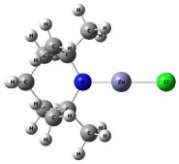
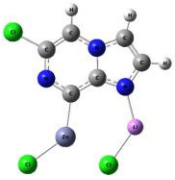
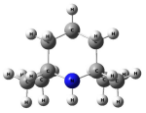
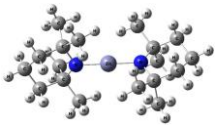
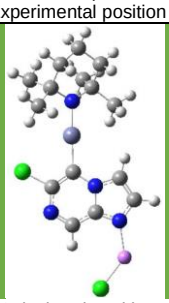
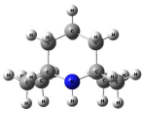
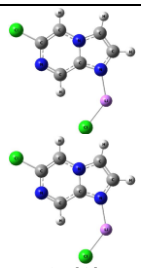
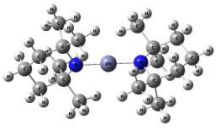
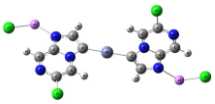
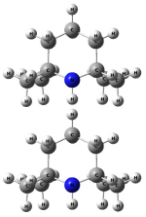
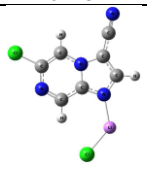
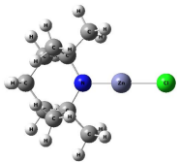
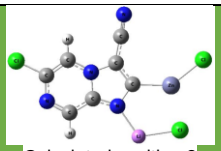
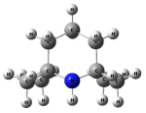
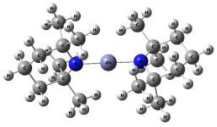
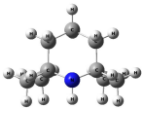
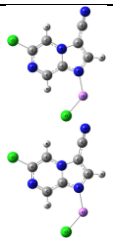
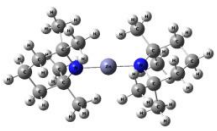
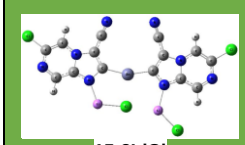
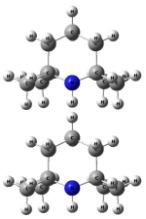
Thermodynamic stability of the intermediate

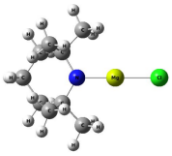
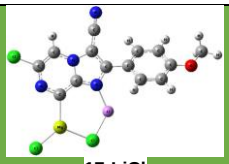
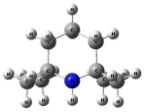
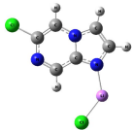
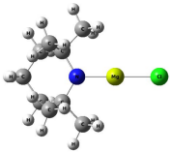
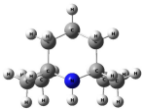
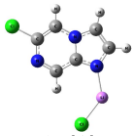
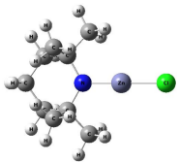
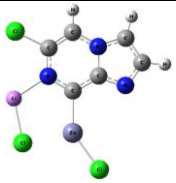
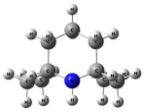
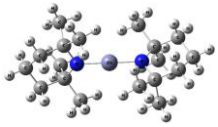
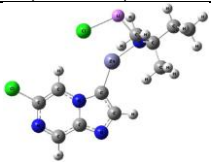
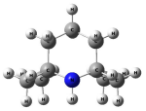
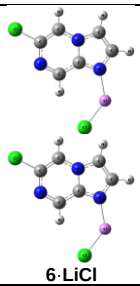
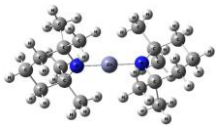
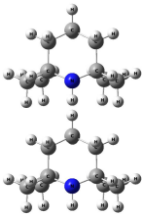
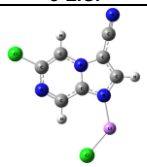
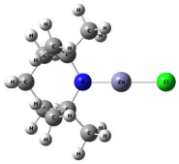
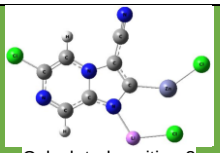
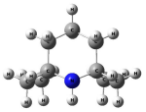
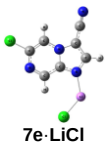
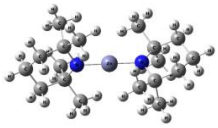
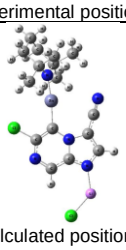
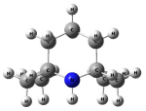
The stability of the organometallic intermediate with a carbon-metal bond in either position 3 or 5 depends on the charge of the Lewis acid (LA) attached to the deprotonated molecule 1: position 5 is favourable at charge = 0, while position 3 at charge > 0 (**Table TT2**). If the LA has a neutral charge, the stability of the resulting deprotonated anion plays a greater role in determining the stability of the intermediate. The pKa values suggest that the 5-carboanion of molecule 1 is the most stable in this case. However, if the LA has a positive charge, electrostatic interactions become more important and it is more favourable to form a carbon-metal bond with the most negatively charged carbon. Analysis of NBO charges reveals that the C3 atom is the most negatively charged among all carbon atoms in molecule **6** and in the corresponding organometallic intermediate. Therefore, when a positively charged LA is used, position 3 becomes more stable.

Table TT2. The calculated relative ΔG^{sol} values in kJ mol^{-1} for possible CH-deprotonation products with the attached Lewis acid (forming metal-carbon bond) at the CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory for compound **6**, **7e** and **16e**.

Attached Lewis acid	CH-deprotonation product of compound **6** + attached Lewis acid			
	Position 2	Position 3	Position 5	Position 8
charge=0	**charge=-1**			
nothing	68.7	23.9	**0.0**	48.3
$MgCl_2$	42.9	7.3	**0.0**	32.1
Me_2NMgCl	46.7	8.2	**0.0**	33.5
TMPMgCl	48.9	3.6	**0.0**	37.3
$ZnCl_2$	31.6	1.0	**0.0**	23.2
Me_2NZnCl	34.7	2.6	**0.0**	27.2
TMPZnCl	40.9	9.4	**0.0**	32.9
charge=+1	**charge=0**			
$MgCl^+$	51.0	**0.0**	18.3	30.8
$TMPMg^+$	31.8	**0.0**	10.5	34.8
$ZnCl^+$	20.2	**0.0**	2.6	16.2
$TMPZn^+$	28.0	3.8	**0.0**	22.5
charge=+2	**charge=+1**			
Mg^{+2}	61.7	**0.0**	42.6	38.8
Zn^{+2}	20.1	**0.0**	44.1	63.8
Attached Lewis acid	CH-deprotonation product of compound **7e** + attached Lewis acid			
	Position 2	Position 3	Position 5	Position 8
charge=0	**charge=-1**			
nothing	54.6	NO	**0.0**	53.9
charge=+1	**charge=0**			
$TMPZn^+$	11.4	NO	**0.0**	13.7
Attached Lewis acid	CH-deprotonation product of compound **16e** + attached Lewis acid			
	Position 2	Position 3	Position 5	Position 8
charge=0	**charge=-1**			
nothing	NO	NO	**0.0**	54.0
charge=+1	**charge=0**			
$MgCl^+$	NO	NO	**0.0**	28.0

 6		**Reaction1**	 **13** Calculated position 3 Experimental position 3	
 6		**Reaction2**	 Calculated position 3 Experimental position 5	
 6		**Reaction3**	 Calculated position 5 Experimental position 5	
 6 6		**Reaction4**	 **14** Calculated position 5 Experimental position 5	
 7e		**Reaction5**	 Calculated position 5 Experimental position 2	
 7e		**Reaction6**	 Calculated position 5 Experimental position 2	
 7e 7e		**Reaction7**	 **15** Calculated position 5 Experimental position 2	
 16e		**Reaction8**	 **17** Calculated position 5 Experiment position 8	

 **6·LiCl**		**Reaction11**	 **13·LiCl** Calculated position 8 Experimental position 3	
 **6·LiCl**		**Reaction12**	 Calculated position 8 Experimental position 5	
 **6·LiCl**		**Reaction13**	 Calculated position 5 Experimental position 5	
 **6·LiCl**		**Reaction14**	 **14·2LiCl** Calculated position 3 Experimental position 5	
 **7e·LiCl**		**Reaction15**	 Calculated position 2 Experimental position 2	
 **7e·LiCl**		**Reaction16**	 Calculated position 5 Experimental position 2	
 **7e·LiCl**		**Reaction17**	 **15·2LiCl** Calculated position 2 Experimental position 2	

 **16e·LiCl**		**Reaction18**	 **17·LiCl** Calculated position 8 Experimental position 8	
 **6·LiCl**		**Reaction21**	 **13·LiCl** Calculated position 5 Experimental position 3	
 **6·LiCl**		**Reaction22**	 Calculated position 8 Experimental position 5	
 **6·LiCl**		**Reaction23**	 Calculated position 3 Experimental position 5	
 **6·LiCl**		**Reaction24**	 **14·2LiCl** Calculated position 8 Experimental position 5	
 **7e·LiCl**		**Reaction25**	 Calculated position 2 Experimental position 2	
 **7e·LiCl**		**Reaction26**	 Calculated position 5 Experimental position 2	

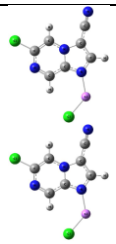
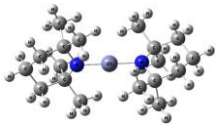
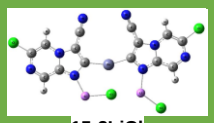
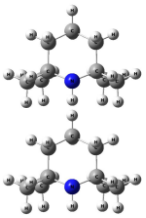
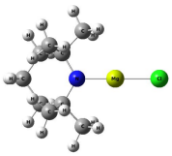
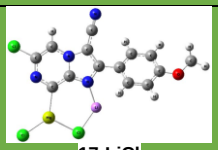
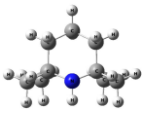
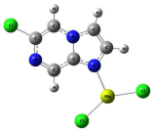
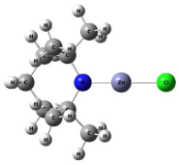
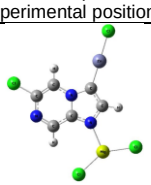
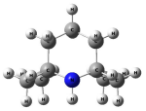
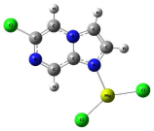
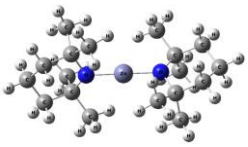
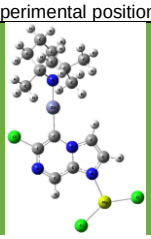
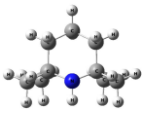
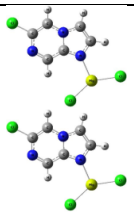
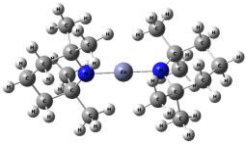
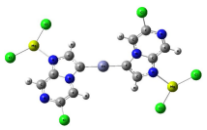
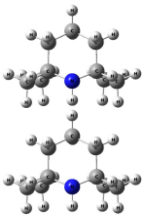
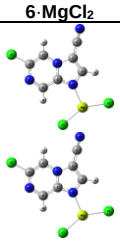
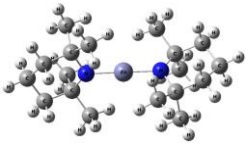
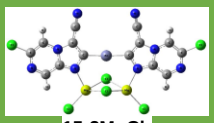
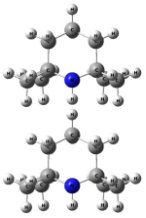
 **7e·LiCl**		**Reaction27**	 **15·2LiCl** Calculated position 2 Experimental position 2	
 **16e·LiCl**		**Reaction28**	 **17·LiCl** Calculated position 8 Experimental position 8	
 **6·$MgCl_2$**		**Reaction32**	 Calculated position 3 Experimental position 5	
 **6·$MgCl_2$**		**Reaction33**	 Calculated position 5 Experimental position 5	
 **6·$MgCl_2$**		**Reaction34**	 **14·2$MgCl_2$** Calculated position 3 Experimental position 5	
 **7e·$MgCl_2$**		**Reaction37**	 **15·2$MgCl_2$** Calculated position 2 Experimental position 2	

Figure TF6. The calculated reactions of proton/Mg^{+2} and proton/Zn^{+2} transfer. The most stable conformers/ intermediates by ΔG^{sol} (**DMSO**) are shown at the CPCM(**DMSO**)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory. Green color indicates the most thermodynamically stable (calculated) intermediate coinciding with the experimental intermediate.

Table TT3. The calculated ΔG^{sol} values for reactions 1-8, 11-18, 21-28, 32-34 and 37 with different intermediate (in positions 2,3,5,8). Thermal corrections for **scheme 2, scheme 3, scheme 5** and **scheme 6 in manuscript** at 298.15 K.

Scheme in manuscript	Reaction	CPCM(**DMSO**)/B3LYP-D3/6-311++G(2df,2p)// B3LYP-D3/6-31++G(2d,p) ΔG^{sol}					CPCM(**THF**)/B3LYP-D3/6-311++G(2df,2p)// B3LYP-D3/6-31++G(2d,p) ΔG^{sol}			
		Intermediate (298.15 K, **DMSO**)					Intermediate (298.15 K, **THF**)			
		2	3	5	8		2	3	5	8
Scheme 2	1	39.6	**-11.4***	6.9	19.4		39.4	**-2.0***	9.8	19.7
Scheme 3	2	-2.2	**-22.4**	-19.8*	-6.2		1.8	**-16.2**	-14.0*	-2.9
	3	10.7	-13.5	**-17.4***	5.2		12.2	-10.3	**-14.1***	6.0
	4	8.8	-33.7	**-35.7***	0.2		14.0	-23.8	**-27.3***	4.6
Scheme 5	5	-13.0*	-	**-17.9**	-10.9		-7.7*	-	**-14.1**	-6.2
	6	-3.6*	-	**-15.0**	-1.3		-1.4*	-	**-13.7**	0.3
	7	-16.7*	-	**-31.6**	-11.5		-8.6*	-	**-29.2**	-5.1
Scheme 6	8	-	-	**-9.3**	18.7*		-	-	**-9.1**	19.8*
Scheme in manuscript	Reaction	Intermediate + LiCl in position 1 (298.15 K, **DMSO**)					Intermediate + LiCl in position 1 (298.15 K, **THF**)			
		2	3	5	8		2	3	5	8
Scheme 2	11	7.9	-17.6*	4.9	**-40.8**		16.7	-7.5*	7.7	**-45.2**
Scheme 3	12	-27.7	-25.3	-1.9*	**-28.3**		**-31.2**	-18.4	1.3*	-30.4
	13	-2.2	-14.3	**-17.3***	6.4		-6.7	-11.5	**-14.4***	2.2
	14	-33.7	**-39.3**	-34.6*	-30.1		**-47.2**	-27.1	-26.2*	-45.6
Scheme 5	15	**-43.7***	-	-19.4	-33.7		**-44.8***	-	-15.2	-35.1
	16	-12.3*	-	**-17.1**	6.1		-15.6*	-	**-15.9**	2.5
	17	**-64.9***	-	-33.7	-62.9		-68.1*	-	-31.0	**-76.7**
Scheme 6	18	-	-	-14.2	**-54.4***		-	-	-12.9	**-57.3***
Scheme in manuscript	Reaction	Intermediate + LiCl in the best position (298.15 K, **DMSO**)					Intermediate + LiCl in the best position (298.15 K, **THF**)			
		2	3	5	8		2	3	5	8
Scheme 2	21	7.3	-40.6*	**-45.1**	-41.4		4.3	-42.0*	**-46.9**	-45.7
Scheme 3	22	-28.3	-28.2	-29.3*	**-30.5**		-31.8	-29.8	-30.2*	**-32.6**
	23	-2.8	**-20.9**	-20.7*	3.4		-7.2	**-24.3**	-23.6*	-1.1
	24	-34.9	-40.5	-35.8*	**-51.6**		-48.3	-28.1	-27.2*	**-62.8**
Scheme 5	25	**-43.7***	-	-22.4	-33.7		**-44.8***	-	-31.8	-35.1
	26	-12.3*	-	**-17.1**	6.1		-15.6*	-	**-15.9**	2.5
	27	**-64.9***	-	-33.7	-62.9		-68.1*	-	-31.0	**-76.7**
Scheme 6	28	-	-	-51.5	**-54.4***		-	-	**-61.5**	-57.3*
Scheme in manuscript	Reaction	Intermediate + $MgCl_2$ in the best position (298.15 K, **DMSO**)					Intermediate + $MgCl_2$ in the best position (298.15 K, **THF**)			
		2	3	5	8		2	3	5	8
Scheme 3	32	-14.6	**-26.5**	-20.9*	-10.7		-15.5	**-19.6**	-14.7*	-10.4
	33	-0.2	-18.2	**-19.6***	13.3		-2.1	-15.2	**-16.6***	11.2
	34	-42.1	**-45.0**	-38.9*	11.0		**-49.9**	-32.3	-28.9*	-2.7
Scheme 5	37	**-69.3***	-	-34.6	4.5		**-76.5***	-	-32.0	-8.8

***** - the asterisk indicates the position observed in the experiment. **Bold** indicates the most thermodynamically stable (calculated) intermediate. Green color marks the most thermodynamically stable (calculated) intermediate coinciding with the experimental intermediate.

Table TT4. The calculated ΔG^{sol} values for reactions 1-8, 11-18, 21-28, 32-34 and 37 with different intermediate (in positions 2,3,5,8). Thermal corrections for scheme 2 are at 213.15 K, for scheme 3 and scheme 5 at 253.15 K, scheme 6 at 233.15 K.

Scheme in manuscript	Reaction	CPCM(**DMSO**)/B3LYP-D3/6-311++G(2df,2p)// B3LYP-D3/6-31++G(2d,p) ΔG^{sol}				CPCM(**THF**)/B3LYP-D3/6-311++G(2df,2p)// B3LYP-D3/6-31++G(2d,p) ΔG^{sol}			
		Intermediate ($T_{exp.}$, **DMSO**)				Intermediate ($T_{exp.}$, **THF**)			
		2	3	5	8	2	3	5	8
Scheme 2	1	39.6	**-10.9***	7.1	19.3	39.4	**-1.5***	10.0	19.6
Scheme 3	2	-2.2	**-22.4**	-19.7*	-6.1	1.8	**-16.2**	-14.0*	-2.8
	3	11.0	-13.4	**-17.0***	5.5	12.5	-10.2	**-13.3***	6.3
	4	9.7	-33.0	**-35.0***	1.0	14.9	-23.1	**-26.7***	5.5
Scheme 5	5	-13.1*	-	**-18.0**	-10.9	-7.7*	-	**-14.3**	-6.2
	6	-3.5*	-	**-15.1**	-1.1	-1.3*	-	**-13.8**	0.5
	7	-16.2*	-	**-31.7**	-10.9	-8.1*	-	**-29.2**	-4.4
Scheme 6	8	-	-	**-10.3**	18.2*	-	-	**-10.0**	19.3*
Scheme in manuscript	Reaction	Intermediate + LiCl in position 1 ($T_{exp.}$, **DMSO**)				Intermediate + LiCl in position 1 ($T_{exp.}$, **THF**)			
		2	3	5	8	2	3	5	8
Scheme 2	11	8.4	-17.3*	4.8	**-41.5**	17.2	-7.2*	7.6	**-45.8**
Scheme 3	12	-28.1	-25.4	-2.0*	**-28.6**	**-31.7**	-18.4	1.2*	-30.8
	13	-2.5	-14.3	**-17.4***	5.9	-7.0	-11.5	**-14.5***	1.7
	14	-34.7	**-39.1**	-34.4*	-31.2	**-48.2**	-26.8	-26.0*	-46.7
Scheme 5	15	**-44.2***	-	-19.6	-34.2	**-45.3***	-	-15.4	-35.6
	16	-12.5*	-	**-17.4**	5.8	-15.8*	-	**-16.2**	2.3
	17	**-65.5***	-	-34.0	-64.1	-69.3*	-	-31.3	**-77.9**
Scheme 6	18	-	-	-14.8	**-55.1***	-	-	-13.5	**-58.1***
Scheme in manuscript	Reaction	Intermediate + LiCl in the best position ($T_{exp.}$, **DMSO**)				Intermediate + LiCl in the best position ($T_{exp.}$, **THF**)			
		2	3	5	8	2	3	5	8
Scheme 2	21	7.8	-41.0*	**-45.2**	-42.1	3.7	-42.4*	**-47.0**	-46.3
Scheme 3	22	-28.8	-28.5	-29.2*	**-30.9**	-32.2	-30.1	-30.1*	**-33.0**
	23	-3.1	**-21.4**	-21.3*	3.1	-7.5	**-24.8**	-24.2*	-1.4
	24	-35.9	-40.3	-35.6*	**-52.9**	-49.3	-27.9	-27.1*	**-64.6**
Scheme 5	25	**-44.2***	-	-23.5	-34.2	**-45.3***	-	-32.9	-35.6
	26	-12.5*	-	**-17.4**	5.8	-15.8*	-	**-16.2**	2.3
	27	**-65.5***	-	-34.0	-64.1	-69.3*	-	-31.3	**-77.9**
Scheme 6	28	-	-	-52.9	**-62.3***	-	-	-63.0	**-65.1***
Scheme in manuscript	Reaction	Intermediate + $MgCl_2$ in the best position ($T_{exp.}$, **DMSO**)				Intermediate + $MgCl_2$ in the best position ($T_{exp.}$, **THF**)			
		2	3	5	8	2	3	5	8
Scheme 3	32	-15.0	**-26.7**	-21.0*	-11.0	-15.9	**-19.7**	-14.8*	-10.7
	33	-0.6	-18.4	**-19.5***	13.1	-2.5	-15.4	**-16.5***	11.0
	34	-43.3	**-45.0**	-39.0*	9.6	**-51.1**	-32.3	-28.9*	-4.2
Scheme 5	37	**-70.7***	-	-35.1	2.9	**-77.8***	-	-32.4	-10.4

***** - the asterisk indicates the position observed in the experiment. **Bold** indicates the most thermodynamically stable (calculated) intermediate. Green color marks the most thermodynamically stable (calculated) intermediate coinciding with the experimental intermediate.

Table TT5. The estimated error values for the calculated ΔG^{sol} values in **Table TT3** and **Table TT4**. The expected free energy difference between the experimental observed intermediate relative to the second by stability intermediate based on concentration relation 95/5: -5.2 kJ/mol at 213.15 K, -5.7 kJ/mol at 233.15 K, -6.2 kJ/mol at 253.15 K, -7.3 kJ/mol at 298.15 K, 8.31446 $J \cdot K^{-1} \cdot mol^{-1}$.

Scheme in manuscript	Reaction	CPCM/B3LYP-D3/6-311++G(2df,2p)// B3LYP-D3/6-31++G(2d,p) ΔG^{sol}			
		Intermediate			
		(298.15 K, **DMSO**)	(298.15 K, **THF**)	($T_{exp.}$, **DMSO**)	($T_{exp.}$, **THF**)
Scheme 2	1				
Scheme 3	2	8.8	8.4	8.9	8.4
	3				
	4				
Scheme 5	5	11.1	12.6	11.1	12.8
	6	17.6	18.5	17.8	18.7
	7	21.1	26.8	21.7	27.3
Scheme 6	8	33.7	34.6	34.2	35.0
	AVERAGE	**18.5**	**20.2**	**18.7**	**20.4**
Scheme in manuscript	Reaction	Intermediate + LiCl in position 1			
		(298.15 K, **DMSO**)	(298.15 K, **THF**)	($T_{exp.}$, **DMSO**)	($T_{exp.}$, **THF**)
Scheme 2	11	28.4	42.9	29.4	43.8
Scheme 3	12	32.6	38.7	32.8	39.1
	13				
	14	10.9	27.2	10.9	28.4
Scheme 5	15				
	16	11.0	6.5	11.1	6.6
	17		14.8		14.8
Scheme 6	18				
	AVERAGE	**20.7**	**26.0**	**21.1**	**26.5**
Scheme in manuscript	Reaction	Intermediate + LiCl in the best position			
		(298.15 K, **DMSO**)	(298.15 K, **THF**)	($T_{exp.}$, **DMSO**)	($T_{exp.}$, **THF**)
Scheme 2	21	9.7	10.1	9.4	9.8
Scheme 3	22	7.4	8.6	7.9	9.1
	23	6.4	6.9	6.3	6.8
	24	22.0	41.8	23.5	43.7
Scheme 5	25				
	26	11.0	6.5	11.1	6.6
	27		14.8		14.8
Scheme 6	28		9.9		5.7
	AVERAGE	**11.3**	**14.1**	**11.6**	**13.8**
Scheme in manuscript	Reaction	Intermediate + $MgCl_2$ in the best position			
		(298.15 K, **DMSO**)	(298.15 K, **THF**)	($T_{exp.}$, **DMSO**)	($T_{exp.}$, **THF**)
Scheme 3	32	11.8	11.1	11.9	11.1
	33				
	34	12.3	27.2	12.2	28.4
Scheme 5	37				
	AVERAGE	**12.0**	**19.1**	**12.0**	**19.7**

In order to describe the thermodynamics of the processes depicted in the manuscript in schemes 2, 3, 5 and 6, the ΔG^{sol} values were computed for reactions 1-8 (as well as 11-18, 21-28, 32-34, and 37), in both **DMSO** and **THF**. Individual (unique) reactions in this list are reactions 1-8, the rest of the reactions are just modifications of reactions 1-8. For example, reactions 11-18 are reactions 1-8, but with the addition of LiCl fixed on the N1 atom. In a series of reactions 21-28 LiCl is no longer fixed, i.e. LiCl has isomeric freedom and can occupy another most favorable by free energy position (if any) in the substrate molecule. Reactions 32-34 and 37 are modifications of reactions 4 and 7, but with the addition of $MgCl_2$.

Reaction 1 (**Figure TF6, Table TT 3**) shows well that the product of the reaction between the TMPMgCl molecule and compound **6** is most thermodynamically stable in position 3 (only here the free energy is negative), which agrees with the experiment with the reagent TMPMgCl·LiCl (**11**). In reactions 2 and 5, we simulate a zincation reaction by mixture **12** ($TMP_2Zn{\cdot}2MgCl_2{\cdot}2LiCl$) in scheme 3 and 5 in manuscript, but as a reactant we consider a TMPZnCl particle that can be formed by this process: 2 TMP_2Zn + LiCl → $TMPZn^+Cl^-$ + $Li^+TMP_3Zn^-$. Comparing reactions 1 and 2, we see the effect of the metal change: position 3 is still the most favourable in terms of free energy, although other positions also began to show negative free energies, especially position 5. Compared to reaction 3, the TMP_2Zn substrate in reactions 3 and 4 more reflects the experimental mixture **12** ($TMP_2Zn{\cdot}2MgCl_2{\cdot}2LiCl$). We can see that position 5 is preferred in reactions 3 and 4, although it is slightly more pronounced in reaction 3.

Reactions 6 and 7 describe the thermodynamics of the reaction between **7e** and TMP_2Zn, while the most negative free energy is observed for the 5-intermediate, however, in the experiment, only the 2-intermediate is observed. We assume that the transition state for abstract hydrogen in position 5 (TS5, **Figure TF7** for compound **6**) is sterically hindered by the presence cyano group in position 3 and chlorine in position 6, which does not allow the N atoms from a wide TMP2Zn molecule to reach the CH5 bond (to form the proton transfer in position 5 - **TS5**), so the reaction is kinetically more favourable in position 2.

The free energy of reaction 7 indicates that when molecules **16e** and TMPMgCl react, the 5-intermediate is thermodynamically preferable. We remember that the CH bond in position 5 is more acidic than in position 8. However, only the product in position 8 is observed in the experiment. Here, we note that the free energy for **TS8** is indeed more negative than for TS5 (**Figure TF7** for compound **16e**).

Effect of LiCl in position 1

Comparing reaction 1 with 11, and 2 with 12, it can be seen that the addition of LiCl in position 1 greatly reduces the free energy of intermediate in positions 2 and 8, due to the additional stabilizing Li-Cl...M^{+2} interaction (where the metal M^{+2} is it Mg^{+2} or Zn^{+2}). It is because of this stabilizing interaction, comparing reaction 4 with 14 by the values of ΔG^{sol} (**THF**), it can be seen that when LiCl is added at position 1 instead of 5-intermediate (experiment), 2-intermediate will be the most stable. Also, comparing reaction 7 with 17, it can be seen that when LiCl is added in position 1 instead of 5-intermediate, 8-intermediate will be the most stable, although 2-intermediate (experiment) is very close in stability to 8-intermediate. Comparing reaction 8 with reaction 18, it can be seen that when LiCl is added in position 1 instead of 5-intermediate, 8-intermediate (experiment) will be the most stable.

Effect of the isomeric freedom of LiCl

A sufficient difference can be seen only in reactions 21-24 comparing to reaction 11-14 (**Table TT 3)**.

Effect of $MgCl_2$ in position 1

To describe regioselective zincation in **Scheme 3** and **Scheme 5**, given the composition of the reacting mixture **12** ($TMP_2Zn{\cdot}2MgCl_2{\cdot}2LiCl$), we think that instead of LiCl in position 1 (in reactions 14, 17), it would be more correct to consider $MgCl_2$ in position 1 (reactions 34, 37), because the Mg atom is more electronegative on the Pauling scale (1.31) than the Li atom (0.98). However, adding $MgCl_2$ in position 1 in reaction 34 does not change the order of product stability compared to reaction 14. Reaction 37 agrees well with the result of reaction 27, making the 2-intermediate molecule **15**$\cdot 2MgCl_2$ almost by -10 kJ/mol more stable in **THF** than the 2-intermediate molecule **15**$\cdot$2LiCl.

Effect of temperature on reaction thermodynamics

The results in **Table TT3** are presented for room temperature (298.15 K), however, when recalculating thermal corrections taking into account experimental temperatures in **Table TT4** (**in manuscript scheme 2** at 213.15 K, **scheme 3** and **scheme 5** at 253.15 K, **scheme 6** at 233.15 K), the described trends do not change.

Error estimation

We conclude that the model describing "product + LiCl in the best position" shows the smallest error independent of the applied temperature (**Table TT5**).

Simulation of the transition state for the magnesiation reaction

For the molecule **6,** After a detailed conformational analysis (**Figure TF7**), we were able to find only one structure of four-center cyclic [20] transition states at position 3. TS3 is very compact (four-center cyclic) involves both proton transfer and a short C...Mg^{+2} distance, both required for the formation of the intermediate. On the other hand, five-center cyclic proton transfer TS were observed in positions 2, 8, and six-center cyclic proton transfer TS in position 5. It is logical that after the proton transfer TS2, TS5 and TS8, the next Mg^{+2}-transfer TS should occur to form the expected intermediate in positions 2, 5 and 8 (not observed in the experiment), but we did not do further calculations in this direction.

For the molecule **16e, TS8** for proton transfer is more favourable comparing to **TS5**. At the same time, the possibility of LiCl coordination on the N1 atom (the N1 atom is free in **TS8**) is retained to stabilize the resulting 8-intermediate. A similar picture is observed for molecule **6** (**Figure TF7**).

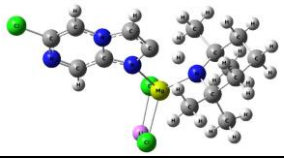
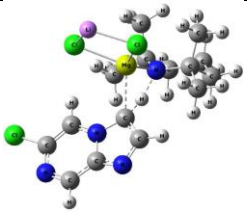
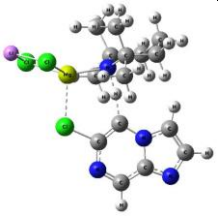
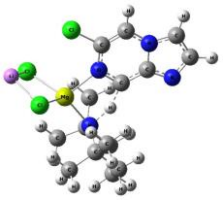
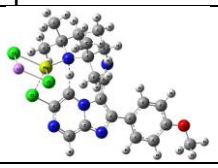
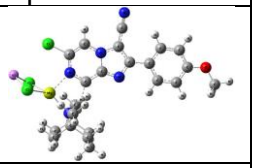
3D				
	TS2	TS3	TS5	TS8
$\Delta\Delta G^{sol}$	+9.7	+57.9	+22.5	0.0
Type	five-center cyclic proton transfer	four-center cyclic proton transfer	six-center cyclic proton transfer	five-center cyclic proton transfer
3D	-	-		
	-	-	TS5	TS8
$\Delta\Delta G^{sol}$	-	-	+36.0	0.0
Type	-	-	six-center cyclic proton transfer	five-center cyclic proton transfer

Figure TF7. The optimized structures of transitional states of proton/Mg^{+2} transfer between the molecule **6** and TMPMgCl·LiCl. The relative TS free energies ΔG^{sol} are in kJ mol^{-1} at the CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory for molecule **6** and at the CPCM(DMSO)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31G(d) level of theory for molecule **16e**.

[20] A. A. Vitale, J. San Filippo, J. Am. Chem. Soc. 1982, 104, 7341-7343.

Conclusions

The presence of a chlorine atom at position 6 makes molecule **6** more acidic and less basic than molecule **3**. Compound **6** is the most N-basic in position 1. Compound **6** is the most CH-acidic in position 5. Coordination of a cationic particles on the N1 atom makes molecule **6** more acidic.

Scheme 2 in manuscript shows that the product of the regioselective magnesiation of molecule **6** at position 3 is observed in the experiment. According to our calculations, the most stable product is indeed obtained at position 3 in Reaction 1. Analysis of NBO charges reveals that the C3 atom is the most negatively charged among all carbon atoms in molecule 6 and in the corresponding organometallic product. Therefore, position 3 becomes more stable.

In **Scheme 3 in manuscript**, regioselective zincation of molecule **6** gives the 5-intermediate. The most stable calculated product is indeed the 5-intermediate in reaction 3 and reaction 4. In reaction 3, the 5-intermediate is stabilized by the TMP group, while in reaction 4 the 5-intermediate (molecule **14**) is stabilized due to a more favourable conformation with two intramolecular non-covalent CH...Cl interactions.

In **Scheme 5 in manuscript**, regioselective zincation of molecule **7e** gives the 2-intermediate. To explain this result, we consider the reaction 25 with the most stable 2-intermediate in both **DMSO** and **THF**. Here, the 2-intermediate is stabilized by the neighbouring LiCl molecule (in the best position: at the N1 atom), which causes the additional stabilizing intramolecular non-covalent Li-Cl...Zn^{+2} interaction. The same type of stabilization is observed for the 8-intermediate in reaction 25, despite this, the 2-intermediate is about -10 kJ/mol more stable than the 8-intermediate.

In **Scheme 6 in manuscript**, regioselective magnesiation of molecule **16e** gives the 8-intermediate. Here we propose to consider reaction 18 to explain the result, in which the 8-intermediate is stabilized by intramolecular non-covalent Li-Cl...Mg^{+2} interaction. Although we do not know the exact reaction mechanism, we carefully assume that the Li-Cl...Mg^{+2} interaction provides the most favourable transition state for the reaction to Scheme 6.

Thermodynamic analysis of pKa

Table TT6. The calculated for pK_a values at the CPCM(**DMSO**)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory(T = 298.15 K).
"E1 and E2" – educt 1 and educt 2, "P1 and P2" – product 1 and product 2.

charge				filename				pK_a	ΔpK_a	ΔG^{sol} kJ/mol	G^{sol}				ΔG^{sol}			
E1	E2	P1	P2	E1	E2	P1	P2				E1	E2	P1	P2	E1	E2	P1	P2
1	0	0	1	p4_mol6	pyrimidine	mol6	p_pyrimidine	-46.9	-47.5	-271.2	-855.9115716	-264.3717510	-855.5920739	-264.7945278	286.0	0.0	0.0	0.0
1	0	0	1	p1_mol7e	pyrimidine	mol7e	p_pyrimidine	-2.4	-3.0	-17.0	-948.2858086	-264.3717510	-947.8694988	-264.7945278	0.0	0.0	0.0	0.0
1	0	0	1	p7_mol7e	pyrimidine	mol7e	p_pyrimidine	-5.9	-6.4	-36.6	-948.2783236	-264.3717510	-947.8694988	-264.7945278	19.7	0.0	0.0	0.0
1	0	0	1	p4_mol7e	pyrimidine	mol7e	p_pyrimidine	-53.7	-54.2	-309.7	-948.1743124	-264.3717510	-947.8694988	-264.7945278	292.7	0.0	0.0	0.0
1	0	0	1	p1_mol16e_2	pyrimidine	mol16e_2	p_pyrimidine	-1.2	-1.8	-10.2	-1293.9000730	-264.3717510	-1293.4811947	-264.7945278	0.0	0.0	0.0	0.0
1	0	0	1	p7_mol16e_1	pyrimidine	mol16e_2	p_pyrimidine	-4.9	-5.5	-31.4	-1293.8920181	-264.3717510	-1293.4811947	-264.7945278	21.1	0.0	0.0	0.0
1	0	0	1	p7_mol16e_2	pyrimidine	mol16e_2	p_pyrimidine	-4.9	-5.5	-31.3	-1293.8920541	-264.3717510	-1293.4811947	-264.7945278	21.1	0.0	0.0	0.0
1	0	0	1	p4_mol16e_2	pyrimidine	mol16e_2	p_pyrimidine	-49.5	-50.0	-285.6	-1293.7951849	-264.3717510	-1293.4811947	-264.7945278	275.4	0.0	0.0	0.0
0	-1	-1	0	mol3	d2_furan	d5_mol3	furan	29.8	-5.2	-29.8	-395.9537295	-229.5392932	-395.4383573	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	mol3	d2_furan	d3_mol3	furan	30.7	-4.3	-24.7	-395.9537295	-229.5392932	-395.4364176	-230.0660281	0.0	0.0	5.1	0.0
0	-1	-1	0	mol3	d2_furan	d8_mol3	furan	36.6	1.6	9.0	-395.9537295	-229.5392932	-395.4235533	-230.0660281	0.0	0.0	38.9	0.0
0	-1	-1	0	mol3	d2_furan	d2_mol3	furan	38.2	3.2	18.5	-395.9537295	-229.5392932	-395.4199480	-230.0660281	0.0	0.0	48.3	0.0
0	-1	-1	0	mol3	d2_furan	d6_mol3	furan	39.0	4.0	23.1	-395.9537295	-229.5392932	-395.4182068	-230.0660281	0.0	0.0	52.9	0.0
0	-1	-1	0	mol6	d2_furan	d5_mol6	furan	24.9	-10.1	-57.5	-855.5920739	-229.5392932	-855.0872382	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	mol6	d2_furan	d3_mol6	furan	29.1	-5.9	-33.6	-855.5920739	-229.5392932	-855.0781373	-230.0660281	0.0	0.0	23.9	0.0
0	-1	-1	0	mol6	d2_furan	d8_mol6	furan	33.4	-1.6	-9.2	-855.5920739	-229.5392932	-855.0688453	-230.0660281	0.0	0.0	48.3	0.0
0	-1	-1	0	mol6	d2_furan	d2_mol6	furan	37.0	2.0	11.2	-855.5920739	-229.5392932	-855.0610782	-230.0660281	0.0	0.0	68.7	0.0
0	-1	-1	0	mol7e	d2_furan	d5_mol7e	furan	20.6	-14.4	-82.3	-947.8694988	-229.5392932	-947.3741029	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	mol7e	d2_furan	d2_mol7e	furan	30.2	-4.8	-27.7	-947.8694988	-229.5392932	-947.3533042	-230.0660281	0.0	0.0	54.6	0.0
0	-1	-1	0	mol7e	d2_furan	d8_mol7e	furan	30.0	-5.0	-28.4	-947.8694988	-229.5392932	-947.3535848	-230.0660281	0.0	0.0	53.9	0.0
0	-1	-1	0	mol16e_2	d2_furan	d5_mol16e_2	furan	21.4	-13.6	-77.7	-1293.4811947	-229.5392932	-1292.9840515	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	mol16e_2	d2_furan	d5_mol16e_1	furan	21.5	-13.5	-77.3	-1293.4811947	-229.5392932	-1292.9839067	-230.0660281	0.0	0.0	0.4	0.0
0	-1	-1	0	mol16e_2	d2_furan	d8_mol16e_2	furan	30.8	-4.2	-23.7	-1293.4811947	-229.5392932	-1292.9634841	-230.0660281	0.0	0.0	54.0	0.0
0	-1	-1	0	mol16e_2	d2_furan	d8_mol16e_1	furan	30.8	-4.2	-23.7	-1293.4811947	-229.5392932	-1292.9634841	-230.0660281	0.0	0.0	54.0	0.0

Table TT7. The calculated for pK_a values at the CPCM(**DMSO**)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory (T = 298.15 K).
"E1 and E2" – educt 1 and educt 2, "P1 and P2" – product 1 and product 2. Lewis acid locally applied to nitrogen atom 1.

charge				filename				pK_a	ΔpK_a	ΔG^{sol} kJ/mol	G^{sol}				ΔG^{sol}			
E1	E2	P1	P2	E1	E2	P1	P2				E1	E2	P1	P2	E1	E2	P1	P2
0	-1	-1	0	mol3	d2_furan	d5_mol3	furan	29.8	-5.2	-29.8	-395.9537295	-229.5392932	-395.4383573	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	mol6	d2_furan	d5_mol6	furan	24.9	-10.1	-57.5	-855.5920739	-229.5392932	-855.0872382	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_LiCl_mol6_1	d2_furan	1_LiCl_d5_mol6_1	furan	22.7	-12.3	-70.1	-1323.5065405	-229.5392932	-1323.0065105	-230.0660281	0.0	0.0	0.0	0.0
2	-1	1	0	1_Mg_mol6	d2_furan	1_Mg_d8_mol6	furan	15.5	-19.5	-111.2	-1055.4895181	-229.5392932	-1055.0051525	-230.0660281	0.0	0.0	0.0	0.0
1	-1	0	0	1_MgCl_mol6_1	d2_furan	1_MgCl_d8_mol6	furan	17.9	-17.1	-97.4	-1515.9510196	-229.5392932	-1515.4613857	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_MgCl2_mol6	d2_furan	1_MgCl2_d5_mol6	furan	21.3	-13.7	-78.3	-1976.4042333	-229.5392932	-1975.9073272	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_C2H6NMgCl_mol6_aab	d2_furan	1_C2H6NMgCl_d5_mol6_aab	furan	21.9	-13.1	-74.8	-1650.6399503	-229.5392932	-1650.1416971	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d5_mol6_2	furan	22.0	-13.0	-73.9	-1924.5750199	-229.5392932	-1924.0764462	-230.0660281	0.0	0.0	0.0	0.0
2	-1	1	0	1_Zn_mol6	d2_furan	1_Zn_d8_mol6	furan	6.4	-28.6	-163.2	-2634.6553014	-229.5392932	-2634.1907114	-230.0660281	0.0	0.0	0.0	0.0
1	-1	0	0	1_ZnCl_mol6_2	d2_furan	1_ZnCl_d8_mol6	furan	4.8	-30.2	-172.2	-3095.1365133	-229.5392932	-3094.6753687	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_ZnCl2_mol6	d2_furan	1_ZnCl2_d8_mol6	furan	12.6	-22.4	-128.1	-3555.5867828	-229.5392932	-3555.1088479	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_C2H6NZnCl_mol6_aab	d2_furan	1_C2H6NZnCl_d5_mol6_aab	furan	21.3	-13.7	-78.3	-3229.8319033	-229.5392932	-3229.3350082	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_TMPZnCl_mol6_2	d2_furan	1_TMPZnCl_d5_mol6_2	furan	21.1	-13.9	-79.1	-3503.7704027	-229.5392932	-3503.2738089	-230.0660281	0.0	0.0	0.0	0.0
2	-1	1	0	1_Mg_mol6	d2_furan	1_Mg_d8_mol6	furan	15.5	-19.5	-111.2	-1055.4895181	-229.5392914	-1055.0051525	-230.0660281	0.0	0.0	0.0	0.0
2	-1	1	0	1_Mg_mol6	d2_furan	1_Mg_d5_mol6	furan	18.8	-16.2	-92.7	-1055.4895181	-229.5392914	-1054.9980792	-230.0660281	0.0	0.0	18.6	0.0
2	-1	1	0	1_Mg_mol6	d2_furan	1_Mg_d3_mol6	furan	21.3	-13.7	-78.5	-1055.4895181	-229.5392914	-1054.9926645	-230.0660281	0.0	0.0	32.8	0.0

2	-1	1	0	1_Mg_mol6	d2_furan	1_Mg_d2_mol6	furan	24.3	-10.7	-61.1	-1055.4895181	-229.5392914	-1054.9860424	-230.0660281	0.0	0.0	50.2	0.0
1	-1	0	0	1_MgCl_mol6_1	d2_furan	1_MgCl_d8_mol6	furan	17.9	-17.1	-97.4	-1515.9510196	-229.5392914	-1515.4613857	-230.0660281	0.0	0.0	0.0	0.0
1	-1	0	0	1_MgCl_mol6_1	d2_furan	1_MgCl_d5_mol6	furan	20.2	-14.8	-84.7	-1515.9510196	-229.5392914	-1515.4565346	-230.0660281	0.0	0.0	12.7	0.0
1	-1	0	0	1_MgCl_mol6_1	d2_furan	1_MgCl_d2_mol6	furan	21.6	-13.4	-76.8	-1515.9510196	-229.5392914	-1515.4535203	-230.0660281	0.0	0.0	20.7	0.0
1	-1	0	0	1_MgCl_mol6_1	d2_furan	1_MgCl_d3_mol6	furan	22.7	-12.3	-70.2	-1515.9510196	-229.5392914	-1515.4510069	-230.0660281	0.0	0.0	27.2	0.0
0	-1	-1	0	1_MgCl2_mol6	d2_furan	1_MgCl2_d5_mol6	furan	21.3	-13.7	-78.3	-1976.4042333	-229.5392914	-1975.9073272	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_MgCl2_mol6	d2_furan	1_MgCl2_d8_mol6	furan	23.0	-12.0	-68.6	-1976.4042333	-229.5392914	-1975.9036264	-230.0660281	0.0	0.0	9.7	0.0
0	-1	-1	0	1_MgCl2_mol6	d2_furan	1_MgCl2_d3_mol6	furan	24.4	-10.6	-60.4	-1976.4042333	-229.5392914	-1975.9004856	-230.0660281	0.0	0.0	18.0	0.0
0	-1	-1	0	1_MgCl2_mol6	d2_furan	1_MgCl2_d2_mol6	furan	26.0	-9.0	-51.3	-1976.4042333	-229.5392914	-1975.8970287	-230.0660281	0.0	0.0	27.0	0.0
0	-1	-1	0	1_C2H6NMgCl_mol6_aab	d2_furan	1_C2H6NMgCl_d5_mol6_aab	furan	21.8	-13.2	-75.4	-1650.6397130	-229.5392914	-1650.1416971	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_C2H6NMgCl_mol6_aab	d2_furan	1_C2H6NMgCl_d5_mol6_aap	furan	22.0	-13.0	-74.1	-1650.6397130	-229.5392914	-1650.1412151	-230.0660281	0.0	0.0	1.3	0.0
0	-1	-1	0	1_C2H6NMgCl_mol6_aab	d2_furan	1_C2H6NMgCl_d3_mol6_aab	furan	25.1	-9.9	-56.7	-1650.6397130	-229.5392914	-1650.1345547	-230.0660281	0.0	0.0	18.8	0.0
0	-1	-1	0	1_C2H6NMgCl_mol6_aab	d2_furan	1_C2H6NMgCl_d3_mol6_aap	furan	25.2	-9.8	-56.1	-1650.6397130	-229.5392914	-1650.1343510	-230.0660281	0.0	0.0	19.3	0.0
1	0	0	1	1_C2H6NMgCl_mol6_aab	d2_furan	1_C2H6NMgCl_d8_mol6_aab	furan	30.6	-4.4	-24.9	-1650.6397130	-229.5392914	-1650.1224516	-230.0660281	0.0	0.0	50.5	0.0
2	1	1	2	1_C2H6NMgCl_mol6_aab	d2_furan	1_C2H6NMgCl_d2_mol6_aap	furan	30.8	-4.2	-24.1	-1650.6397130	-229.5392914	-1650.1221568	-230.0660281	0.0	0.0	51.3	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d5_mol6_2	furan	21.8	-13.2	-75.2	-1924.5745358	-229.5392914	-1924.0764462	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d5_mol6_3	furan	22.4	-12.6	-71.8	-1924.5745358	-229.5392914	-1924.0751352	-230.0660281	0.0	0.0	3.4	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d5_mol6_1	furan	22.7	-12.3	-70.5	-1924.5745358	-229.5392914	-1924.0746413	-230.0660281	0.0	0.0	4.7	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d3_mol6_2	furan	25.0	-10.0	-57.0	-1924.5745358	-229.5392914	-1924.0695126	-230.0660281	0.0	0.0	18.2	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d3_mol6_3	furan	25.7	-9.3	-53.0	-1924.5745358	-229.5392914	-1924.0680006	-230.0660281	0.0	0.0	22.2	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d3_mol6_1	furan	25.9	-9.1	-51.9	-1924.5745358	-229.5392914	-1924.0675492	-230.0660281	0.0	0.0	23.4	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d2_mol6_2	furan	30.9	-4.1	-23.6	-1924.5745358	-229.5392914	-1924.0568046	-230.0660281	0.0	0.0	51.6	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d8_mol6_1	furan	31.5	-3.5	-19.7	-1924.5745358	-229.5392914	-1924.0553035	-230.0660281	0.0	0.0	55.5	0.0
0	-1	-1	0	1_TMPMgCl_mol6_2	d2_furan	1_TMPMgCl_d2_mol6_3	furan	31.7	-3.3	-18.6	-1924.5745358	-229.5392914	-1924.0549000	-230.0660281	0.0	0.0	56.6	0.0
0	-1	-1	0	1_LiCl_mol6_1	d2_furan	1_LiCl_d5_mol6_1	furan	22.6	-12.4	-70.8	-1323.5062793	-229.5392914	-1323.0065105	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_LiCl_mol6_1	d2_furan	1_LiCl_d3_mol6_2	furan	26.3	-8.7	-49.8	-1323.5062793	-229.5392914	-1322.9985279	-230.0660281	0.0	0.0	21.0	0.0
0	-1	-1	0	1_LiCl_mol6_1	d2_furan	1_LiCl_d8_mol6_2	furan	27.4	-7.6	-43.3	-1323.5062793	-229.5392914	-1322.9960403	-230.0660281	0.0	0.0	27.5	0.0
0	-1	-1	0	1_LiCl_mol6_1	d2_furan	1_LiCl_d8_mol6_1	furan	27.4	-7.6	-43.2	-1323.5062793	-229.5392914	-1322.9960086	-230.0660281	0.0	0.0	27.6	0.0
2	-1	1	0	1_Zn_mol6	d2_furan	1_Zn_d8_mol6	furan	6.4	-28.6	-163.2	-2634.6553014	-229.5392914	-2634.1907114	-230.0660281	0.0	0.0	0.0	0.0
2	-1	1	0	1_Zn_mol6	d2_furan	1_Zn_d3_mol6	furan	21.6	-13.4	-76.4	-2634.6553014	-229.5392914	-2634.1576630	-230.0660281	0.0	0.0	86.8	0.0
2	-1	1	0	1_Zn_mol6	d2_furan	1_Zn_d5_mol6	furan	21.2	-13.8	-78.9	-2634.6553014	-229.5392914	-2634.1586308	-230.0660281	0.0	0.0	84.2	0.0
2	-1	1	0	1_Zn_mol6	d2_furan	1_Zn_d2_mol6	furan	25.4	-9.6	-54.6	-2634.6553014	-229.5392914	-2634.1493792	-230.0660281	0.0	0.0	108.5	0.0
1	-1	0	0	1_ZnCl_mol6_2	d2_furan	1_ZnCl_d8_mol6	furan	4.8	-30.2	-172.2	-3095.1365133	-229.5392914	-3094.6753687	-230.0660281	0.0	0.0	0.0	0.0
1	-1	0	0	1_ZnCl_mol6_2	d2_furan	1_ZnCl_d2_mol6	furan	5.6	-29.4	-167.6	-3095.1365133	-229.5392914	-3094.6736158	-230.0660281	0.0	0.0	4.6	0.0
1	-1	0	0	1_ZnCl_mol6_2	d2_furan	1_ZnCl_d5_mol6	furan	18.7	-16.3	-93.2	-3095.1365133	-229.5392914	-3094.6452846	-230.0660281	0.0	0.0	79.0	0.0
1	-1	0	0	1_ZnCl_mol6_2	d2_furan	1_ZnCl_d3_mol6	furan	21.0	-14.0	-80.1	-3095.1365133	-229.5392914	-3094.6402771	-230.0660281	0.0	0.0	92.1	0.0
0	-1	-1	0	1_ZnCl2_mol6	d2_furan	1_ZnCl2_d8_mol6	furan	12.6	-22.4	-128.1	-3555.5867828	-229.5392914	-3555.1088479	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_ZnCl2_mol6	d2_furan	1_ZnCl2_d5_mol6	furan	21.0	-14.0	-79.8	-3555.5867828	-229.5392914	-3555.0904382	-230.0660281	0.0	0.0	48.3	0.0
0	-1	-1	0	1_ZnCl2_mol6	d2_furan	1_ZnCl2_d3_mol6	furan	24.1	-10.9	-62.3	-3555.5867828	-229.5392914	-3555.0837715	-230.0660281	0.0	0.0	65.8	0.0
0	-1	-1	0	1_ZnCl2_mol6	d2_furan	1_ZnCl2_d2_mol6	furan	28.8	-6.2	-35.2	-3555.5867828	-229.5392914	-3555.0734512	-230.0660281	0.0	0.0	92.9	0.0
0	-1	-1	0	1_C2H6NZnCl_mol6_aab	d2_furan	1_C2H6NZnCl_d5_mol6_aab	furan	21.2	-13.8	-78.7	-3229.8317585	-229.5392914	-3229.3350082	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_C2H6NZnCl_mol6_aab	d2_furan	1_C2H6NZnCl_d5_mol6_aap	furan	21.3	-13.7	-78.4	-3229.8317585	-229.5392914	-3229.3348997	-230.0660281	0.0	0.0	0.3	0.0
0	-1	-1	0	1_C2H6NZnCl_mol6_aab	d2_furan	1_C2H6NZnCl_d3_mol6_aap	furan	24.4	-10.6	-60.8	-3229.8317585	-229.5392914	-3229.3281790	-230.0660281	0.0	0.0	17.9	0.0
0	-1	-1	0	1_C2H6NZnCl_mol6_aab	d2_furan	1_C2H6NZnCl_d3_mol6_aab	furan	24.4	-10.6	-60.5	-3229.8317585	-229.5392914	-3229.3280625	-230.0660281	0.0	0.0	18.2	0.0
1	0	0	1	1_C2H6NZnCl_mol6_aab	d2_furan	1_C2H6NZnCl_d2_mol6_aab	furan	29.8	-5.2	-29.7	-3229.8317585	-229.5392914	-3229.3163249	-230.0660281	0.0	0.0	49.1	0.0
2	1	1	2	1_C2H6NZnCl_mol6_aab	d2_furan	1_C2H6NZnCl_d8_mol6_aab	furan	30.0	-5.0	-28.6	-3229.8317585	-229.5392914	-3229.3159086	-230.0660281	0.0	0.0	50.1	0.0
3	2	2	3	1_C2H6NZnCl_mol6_aab	d2_furan	1_C2H6NZnCl_d2_mol6_aap	furan	30.0	-5.0	-28.7	-3229.8317585	-229.5392914	-3229.3159466	-230.0660281	0.0	0.0	50.0	0.0
0	-1	-1	0	1_TMPZnCl_mol6_2	d2_furan	1_TMPZnCl_d5_mol6_2	furan	21.0	-14.0	-79.8	-3503.7701417	-229.5392914	-3503.2738089	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_TMPZnCl_mol6_2	d2_furan	1_TMPZnCl_d5_mol6_1	furan	22.8	-12.2	-69.9	-3503.7701417	-229.5392914	-3503.2700383	-230.0660281	0.0	0.0	9.9	0.0
0	-1	-1	0	1_TMPZnCl_mol6_2	d2_furan	1_TMPZnCl_d3_mol6_2	furan	24.9	-10.1	-57.4	-3503.7701417	-229.5392914	-3503.2652695	-230.0660281	0.0	0.0	22.4	0.0
0	-1	-1	0	1_TMPZnCl_mol6_2	d2_furan	1_TMPZnCl_d2_mol6_2	furan	31.5	-3.5	-19.8	-3503.7701417	-229.5392914	-3503.2509606	-230.0660281	0.0	0.0	60.0	0.0
0	-1	-1	0	1_TMPZnCl_mol6_2	d2_furan	1_TMPZnCl_d8_mol6_4	furan	35.0	0.0	-0.2	-3503.7701417	-229.5392914	-3503.2434872	-230.0660281	0.0	0.0	79.6	0.0
0	-1	-1	0	1_LiCl_mol6_1	d2_furan	1_LiCl_d5_mol6_1	furan	22.6	-12.4	-70.8	-1323.5062793	-229.5392914	-1323.0065105	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	1_LiCl_mol6_1	d2_furan	1_LiCl_d3_mol6_2	furan	26.3	-8.7	-49.8	-1323.5062793	-229.5392914	-1322.9985279	-230.0660281	0.0	0.0	21.0	0.0
0	-1	-1	0	1_LiCl_mol6_1	d2_furan	1_LiCl_d8_mol6_2	furan	27.4	-7.6	-43.3	-1323.5062793	-229.5392914	-1322.9960403	-230.0660281	0.0	0.0	27.5	0.0
0	-1	-1	0	1_LiCl_mol6_1	d2_furan	1_LiCl_d8_mol6_1	furan	27.4	-7.6	-43.2	-1323.5062793	-229.5392914	-1322.9960086	-230.0660281	0.0	0.0	27.6	0.0

Table TT8. The calculated for pK_a values at the CPCM(**DMSO**)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory (T = 298.15 K).
"E1 and E2" – educt 1 and educt 2, "P1 and P2" – product 1 and product 2. Structures in which the Lewis acid occupies the best by G^{sol} position.

charge				filename				pK_a	ΔpK_a	ΔG^{sol}	G^{sol}				ΔG^{sol}			
E1	E2	P1	P2	E1	E2	P1	P2			kJ/mol	E1	E2	P1	P2	E1	E2	P1	P2
2	-1	1	0	1_Mg_mol6	d2_furan	3_Mg_d3_mol6	furan	8.7	-26.3	-150.1	-1055.4895181	-229.5392932	-1055.0199463	-230.0660281	0.0	0.0	0.0	0.0
1	-1	0	0	MgCl_mol6_aal	d2_furan	Cl_Mg3_d3_mol6_aad	furan	13.0	-22.0	-125.8	-1515.9516214	-229.5392932	-1515.4727936	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	MgCl2_mol6_aac	d2_furan	MgCl2_d5_mol6_aaa	furan	15.1	-19.9	-113.4	-1976.4042295	-229.5392932	-1975.9207015	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	C2H6NMgCl_mol6_aab	d2_furan	C2H6NMgCl_d5_mol6_aaa	furan	16.0	-19.0	-108.5	-1650.6399503	-229.5392932	-1650.1545379	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	TMPMgCl_mol6_aal	d2_furan	TMPMgCl_d5_mol6_aac	furan	16.9	-18.1	-103.5	-1924.5750194	-229.5392932	-1924.0876957	-230.0660281	0.0	0.0	0.0	0.0
2	-1	1	0	1_Zn_mol6	d2_furan	Zn3_d3_mol6	furan	-4.8	-39.8	-227.0	-2634.6553014	-229.5392932	-2634.2150263	-230.0660281	0.0	0.0	0.0	0.0
1	-1	0	0	ZnCl_mol6_aag	d2_furan	Cl_Zn3_d3_mol6_aap	furan	2.1	-32.9	-187.9	-3095.1365131	-229.5392932	-3094.6813378	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	ZnCl2_mol6_aai	d2_furan	ZnCl2_d5_mol6_aaa	furan	8.5	-26.5	-151.3	-3555.5867828	-229.5392932	-3555.1176838	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	C2H6NZnCl_mol6_aak	d2_furan	C2H6NZnCl_d5_mol6_aad	furan	9.5	-25.5	-145.6	-3229.8319034	-229.5392932	-3229.3606175	-230.0660281	0.0	0.0	0.0	0.0
0	-1	-1	0	TMPZnCl_mol6_aax	d2_furan	TMPZnCl_d5_mol6_aao	furan	10.8	-24.2	-138.0	-3503.7695942	-229.5392932	-3503.2954256	-230.0660281	0.0	0.0	0.0	0.0

Thermodynamic analysis of the intermediate

Table TT9. The calculated for reaction free energy values at the CPCM(**DMSO**)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory (T = 298.15 K).
"E1 and E2" – educt 1 and educt 2, "P1 and P2" – product 1 and product 2.

charge				filename						ΔG^{sol}	G^{sol}				ΔG^{sol}			
E1	E2	P1	P2	E1	E2	P1	P2			kJ/mol	E1	E2	P1	P2	E1	E2	P1	P2
0	0	0	0	mol6	TMPMgCl	Cl_Mg3_d3_mol6_aad	TMPH_1		reaction1	-11.4	-855.5920739	-1068.9731777	-1515.4727936	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMPZnCl	Cl_Zn3_d3_mol6_aap	TMPH_1		reaction2	-22.4	-855.5920739	-2648.1775221	-3094.6813378	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMP2Zn_1	5_TMPZn_d5_mol6_b	TMPH_1		reaction3	-17.4	-855.5920739	-2596.3659178	-3042.8678070	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMP2Zn_1	mol14_pos5	TMPH_1		reaction4	-35.7	-855.5920739	-2596.3659178	-3489.3700527	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMPZnCl	5_ZnCl_d5_mol7e	TMPH_1		reaction5	-17.9	-947.8694988	-2648.1775221	-3186.9570329	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e	TMPH_1		reaction6	-15.0	-947.8694988	-2596.3659178	-3135.1443211	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	mol15_pos5	TMPH_1		reaction7	-31.6	-947.8694988	-2596.3659178	-3673.9233642	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol16e_2	TMPMgCl	mol17_pos5_2	TMPH_1		reaction8	-9.3	-1293.4811947	-1068.9731777	-1953.3611227	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMPMgCl	Cl_Mg3_d3_mol6_aad	TMPH_1			-11.4	-855.5920739	-1068.9731777	-1515.4727936	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMPMgCl	Cl_Mg3_d3_mol6_aaq	TMPH_1			-11.4	-855.5920739	-1068.9731777	-1515.4727883	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMPMgCl	Cl_Mg5_d5_mol6_aaa	TMPH_1			6.9	-855.5920739	-1068.9731777	-1515.4658247	-409.0967962	0.0	0.0	18.3	0.0
0	0	0	0	mol6	TMPMgCl	Cl_Mg8_d8_mol6_aar	TMPH_1			19.4	-855.5920739	-1068.9731777	-1515.4610636	-409.0967962	0.0	0.0	30.8	0.0
0	0	0	0	mol6	TMPMgCl	Cl_Mg2_d2_mol6_aaa	TMPH_1			39.6	-855.5920739	-1068.9731777	-1515.4533543	-409.0967962	0.0	0.0	51.0	0.0
0	0	0	0	mol6	TMPZnCl	Cl_Zn3_d3_mol6_aap	TMPH_1			-22.4	-855.5920739	-2648.1775221	-3094.6813378	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMPZnCl	Cl_Zn5_d5_mol6_aae	TMPH_1			-19.8	-855.5920739	-2648.1775221	-3094.6803399	-409.0967962	0.0	0.0	2.6	0.0
0	0	0	0	mol6	TMPZnCl	Cl_Zn8_d8_mol6_aac	TMPH_1			-6.2	-855.5920739	-2648.1775221	-3094.6751758	-409.0967962	0.0	0.0	16.2	0.0
0	0	0	0	mol6	TMPZnCl	Cl_Zn2_d2_mol6_aaq	TMPH_1			-2.2	-855.5920739	-2648.1775221	-3094.6736351	-409.0967962	0.0	0.0	20.2	0.0
0	0	0	0	mol6	TMP2Zn_1	5_TMPZn_d5_mol6_b	TMPH_1			-17.4	-855.5920739	-2596.3659178	-3042.8678070	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMP2Zn_1	5_TMPZn_d5_mol6_a	TMPH_1			-16.5	-855.5920739	-2596.3659178	-3042.8674641	-409.0967962	0.0	0.0	0.9	0.0
0	0	0	0	mol6	TMP2Zn_1	3_TMPZn_d3_mol6_a	TMPH_1			-13.5	-855.5920739	-2596.3659178	-3042.8663447	-409.0967962	0.0	0.0	3.8	0.0
0	0	0	0	mol6	TMP2Zn_1	3_TMPZn_d3_mol6_b	TMPH_1			-13.5	-855.5920739	-2596.3659178	-3042.8663443	-409.0967962	0.0	0.0	3.8	0.0
0	0	0	0	mol6	TMP2Zn_1	8_TMPZn_d8_mol6_a	TMPH_1			5.2	-855.5920739	-2596.3659178	-3042.8592231	-409.0967962	0.0	0.0	22.5	0.0
0	0	0	0	mol6	TMP2Zn_1	2_TMPZn_d2_mol6_a	TMPH_1			10.7	-855.5920739	-2596.3659178	-3042.8571388	-409.0967962	0.0	0.0	28.0	0.0
0	0	0	0	mol6	TMP2Zn_1	mol14_pos5	TMPH_1			-35.7	-855.5920739	-2596.3659178	-3489.3700527	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMP2Zn_1	mol14_pos3	TMPH_1			-33.7	-855.5920739	-2596.3659178	-3489.3692920	-409.0967962	0.0	0.0	2.0	0.0
0	0	0	0	mol6	TMP2Zn_1	mol14_pos8	TMPH_1			0.2	-855.5920739	-2596.3659178	-3489.3564080	-409.0967962	0.0	0.0	35.8	0.0
0	0	0	0	mol6	TMP2Zn_1	mol14_pos2	TMPH_1			8.8	-855.5920739	-2596.3659178	-3489.3531155	-409.0967962	0.0	0.0	44.5	0.0
0	0	0	0	mol7e	TMPZnCl	5_ZnCl_d5_mol7e	TMPH_1			-17.9	-947.8694988	-2648.1775221	-3186.9570329	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMPZnCl	2_ZnCl_d2_mol7e	TMPH_1			-13.0	-947.8694988	-2648.1775221	-3186.9551800	-409.0967962	0.0	0.0	4.9	0.0

0	0	0	0	mol7e	TMPZnCl	8_ZnCl_d8_mol7e	TMPH_1			-10.9	-947.8694988	-2648.1775221	-3186.9543791	-409.0967962	0.0	0.0	7.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e	TMPH_1			-15.0	-947.8694988	-2596.3659178	-3135.1443211	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_36	TMPH_1			-14.8	-947.8694988	-2596.3659178	-3135.1442698	-409.0967962	0.0	0.0	0.1	0.0
0	0	0	0	mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_40	TMPH_1			-4.2	-947.8694988	-2596.3659178	-3135.1402071	-409.0967962	0.0	0.0	10.8	0.0
0	0	0	0	mol7e	TMP2Zn_1	2_TMPZn_d2_mol7e	TMPH_1			-3.6	-947.8694988	-2596.3659178	-3135.1399886	-409.0967962	0.0	0.0	11.4	0.0
0	0	0	0	mol7e	TMP2Zn_1	8_TMPZn_d8_mol7e	TMPH_1			-1.3	-947.8694988	-2596.3659178	-3135.1391033	-409.0967962	0.0	0.0	13.7	0.0
0	0	0	0	mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_38	TMPH_1			0.9	-947.8694988	-2596.3659178	-3135.1382799	-409.0967962	0.0	0.0	15.9	0.0
0	0	0	0	mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_1	TMPH_1			3.4	-947.8694988	-2596.3659178	-3135.1373441	-409.0967962	0.0	0.0	18.3	0.0
0	0	0	0	mol7e	TMP2Zn_1	mol15_pos5	TMPH_1			-31.6	-947.8694988	-2596.3659178	-3673.9233642	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	mol15_pos2	TMPH_1			-16.7	-947.8694988	-2596.3659178	-3673.9176694	-409.0967962	0.0	0.0	15.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	mol15_pos8	TMPH_1			-11.5	-947.8694988	-2596.3659178	-3673.9157181	-409.0967962	0.0	0.0	20.1	0.0
0	0	0	0	mol16e_2	TMPMgCl	mol17_pos5_2	TMPH_1			-9.3	-1293.4811947	-1068.9731777	-1953.3611227	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol16e_2	TMPMgCl	mol17_pos5_1	TMPH_1			-9.3	-1293.4811947	-1068.9731777	-1953.3611142	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	mol16e_2	TMPMgCl	mol17_pos8_2	TMPH_1			18.7	-1293.4811947	-1068.9731777	-1953.3504641	-409.0967962	0.0	0.0	28.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1		reaction11	-40.8	-1323.5065405	-1068.9731777	-1983.3984783	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1		reaction12	-28.3	-1323.5065405	-2648.1775221	-3562.5980593	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1		reaction13	-17.3	-1323.5065405	-2596.3659178	-3510.7822417	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1		reaction14	-39.3	-1323.5065405	-2596.3659178	-4425.2003870	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1		reaction15	-43.7	-1415.7817642	-2648.1775221	-3654.8791290	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1		reaction16	-17.1	-1415.7817642	-2596.3659178	-3603.0573859	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1		reaction17	-64.9	-1415.7817642	-2596.3659178	-4609.7605802	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1		reaction18	-54.4	-1761.3908362	-1068.9731777	-2421.2879207	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1			-40.8	-1323.5065405	-1068.9731777	-1983.3984783	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_3MgCl_d3_mol6	TMPH_1			-17.6	-1323.5065405	-1068.9731777	-1983.3896387	-409.0967962	0.0	0.0	23.2	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_5MgCl_d5_mol6	TMPH_1			4.9	-1323.5065405	-1068.9731777	-1983.3810596	-409.0967962	0.0	0.0	45.7	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_2MgCl_d2_mol6	TMPH_1			7.9	-1323.5065405	-1068.9731777	-1983.3799045	-409.0967962	0.0	0.0	48.8	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1			-28.3	-1323.5065405	-2648.1775221	-3562.5980593	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1			-27.7	-1323.5065405	-2648.1775221	-3562.5978134	-409.0967962	0.0	0.0	0.6	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-25.3	-1323.5065405	-2648.1775221	-3562.5969118	-409.0967962	0.0	0.0	3.0	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_5ZnCl_d5_mol6_aae	TMPH_1			-1.9	-1323.5065405	-2648.1775221	-3562.5879810	-409.0967962	0.0	0.0	26.5	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1			-17.3	-1323.5065405	-2596.3659178	-3510.7822417	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_b	TMPH_1			-15.6	-1323.5065405	-2596.3659178	-3510.7816221	-409.0967962	0.0	0.0	1.6	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_a	TMPH_1			-14.3	-1323.5065405	-2596.3659178	-3510.7811169	-409.0967962	0.0	0.0	3.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_b	TMPH_1			-13.7	-1323.5065405	-2596.3659178	-3510.7808722	-409.0967962	0.0	0.0	3.6	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol6_c	TMPH_1			-2.2	-1323.5065405	-2596.3659178	-3510.7764818	-409.0967962	0.0	0.0	15.1	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol6_c	TMPH_1			6.4	-1323.5065405	-2596.3659178	-3510.7732410	-409.0967962	0.0	0.0	23.6	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1			-39.3	-1323.5065405	-2596.3659178	-4425.2003870	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos5	TMPH_1			-34.6	-1323.5065405	-2596.3659178	-4425.1985875	-409.0967962	0.0	0.0	4.7	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1			-33.7	-1323.5065405	-2596.3659178	-4425.1982362	-409.0967962	0.0	0.0	5.6	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos8	TMPH_1			-30.1	-1323.5065405	-2596.3659178	-4425.1968634	-409.0967962	0.0	0.0	9.3	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1			-43.7	-1415.7817642	-2648.1775221	-3654.8791290	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_8_ZnCl_d8_mol7e	TMPH_1			-33.7	-1415.7817642	-2648.1775221	-3654.8753417	-409.0967962	0.0	0.0	9.9	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_5_ZnCl_d5_mol7e	TMPH_1			-19.4	-1415.7817642	-2648.1775221	-3654.8698787	-409.0967962	0.0	0.0	24.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-17.1	-1415.7817642	-2596.3659178	-3603.0573859	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e	TMPH_1			-16.8	-1415.7817642	-2596.3659178	-3603.0572809	-409.0967962	0.0	0.0	0.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e	TMPH_1			-12.3	-1415.7817642	-2596.3659178	-3603.0555597	-409.0967962	0.0	0.0	4.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-4.9	-1415.7817642	-2596.3659178	-3603.0527634	-409.0967962	0.0	0.0	12.1	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_26	TMPH_1			-4.6	-1415.7817642	-2596.3659178	-3603.0526470	-409.0967962	0.0	0.0	12.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_31	TMPH_1			-4.6	-1415.7817642	-2596.3659178	-3603.0526439	-409.0967962	0.0	0.0	12.5	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-1.1	-1415.7817642	-2596.3659178	-3603.0513227	-409.0967962	0.0	0.0	15.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_38	TMPH_1			-0.1	-1415.7817642	-2596.3659178	-3603.0509327	-409.0967962	0.0	0.0	16.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_1	TMPH_1			0.4	-1415.7817642	-2596.3659178	-3603.0507159	-409.0967962	0.0	0.0	17.5	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol7e_20	TMPH_1			6.1	-1415.7817642	-2596.3659178	-3603.0485780	-409.0967962	0.0	0.0	23.1	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1			-64.9	-1415.7817642	-2596.3659178	-4609.7605802	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1			-62.9	-1415.7817642	-2596.3659178	-4609.7598132	-409.0967962	0.0	0.0	2.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_17	TMPH_1			-54.7	-1415.7817642	-2596.3659178	-4609.7566797	-409.0967962	0.0	0.0	10.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_13	TMPH_1			-45.8	-1415.7817642	-2596.3659178	-4609.7532802	-409.0967962	0.0	0.0	19.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8	TMPH_1			-45.0	-1415.7817642	-2596.3659178	-4609.7529765	-409.0967962	0.0	0.0	20.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_12	TMPH_1			-41.0	-1415.7817642	-2596.3659178	-4609.7514862	-409.0967962	0.0	0.0	23.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_1	TMPH_1			-41.0	-1415.7817642	-2596.3659178	-4609.7514846	-409.0967962	0.0	0.0	23.9	0.0

				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2	TMPH_1			-41.0	-1415.7817642	-2596.3659178	-4609.7514845	-409.0967962	0.0	0.0	23.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos5	TMPH_1			-33.7	-1415.7817642	-2596.3659178	-4609.7486857	-409.0967962	0.0	0.0	31.2	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1			-54.4	-1761.3908362	-1068.9731777	-2421.2879207	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_1	TMPH_1			-54.0	-1761.3908362	-1068.9731777	-2421.2877997	-409.0967962	0.0	0.0	0.3	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos5_1	TMPH_1			-14.2	-1761.3908362	-1068.9731777	-2421.2726326	-409.0967962	0.0	0.0	40.1	0.0
0	0	0	0	LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6	TMPH_1		reaction21	-45.1	-1323.5063098	-1068.9731777	-1983.3998594	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	LiCl_mol6_aan	TMPZnCl	LiCl_8ZnCl_d8_mol6_aac2	TMPH_1		reaction22	-30.5	-1323.5063098	-2648.1775221	-3562.5986478	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_a	TMPH_1		reaction23	-20.9	-1323.5063098	-2596.3659178	-3510.7833962	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8_38	TMPH_1		reaction24	-51.6	-1323.5063098	-2596.3659178	-4425.2045904	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1		reaction25	-43.7	-1415.7817642	-2648.1775221	-3654.8791290	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1		reaction26	-17.1	-1415.7817642	-2596.3659178	-3603.0573859	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1		reaction27	-64.9	-1415.7817642	-2596.3659178	-4609.7605802	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1		reaction28	-54.4	-1761.3908362	-1068.9731777	-2421.2879207	-409.0967962	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6	TMPH_1			-45.1	-1323.5063098	-1068.9731777	-1983.3998594	-409.0967962	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1			-41.4	-1323.5063098	-1068.9731777	-1983.3984783	-409.0967962	0.0	0.0	3.6	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d3_mol6	TMPH_1			-40.6	-1323.5063098	-1068.9731777	-1983.3981676	-409.0967962	0.0	0.0	4.4	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6_1	TMPH_1			-26.0	-1323.5063098	-1068.9731777	-1983.3925752	-409.0967962	0.0	0.0	19.1	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_3MgCl_d3_mol6	TMPH_1			-18.2	-1323.5063098	-1068.9731777	-1983.3896387	-409.0967962	0.0	0.0	26.8	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d8_mol6_1	TMPH_1			-16.6	-1323.5063098	-1068.9731777	-1983.3890274	-409.0967962	0.0	0.0	28.4	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d8_mol6	TMPH_1			-4.6	-1323.5063098	-1068.9731777	-1983.3844474	-409.0967962	0.0	0.0	40.5	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_5MgCl_d5_mol6	TMPH_1			4.3	-1323.5063098	-1068.9731777	-1983.3810596	-409.0967962	0.0	0.0	49.4	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_2MgCl_d2_mol6	TMPH_1			7.3	-1323.5063098	-1068.9731777	-1983.3799045	-409.0967962	0.0	0.0	52.4	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_8ZnCl_d8_mol6_aac2	TMPH_1			-30.5	-1323.5063098	-2648.1775221	-3562.5986478	-409.0967962	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_5ZnCl_d5_mol6_aae	TMPH_1			-29.3	-1323.5063098	-2648.1775221	-3562.5981844	-409.0967962	0.0	0.0	1.2	0.0
				LiCl_mol6_aan	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1			-28.9	-1323.5063098	-2648.1775221	-3562.5980593	-409.0967962	0.0	0.0	1.5	0.0
				LiCl_mol6_aan	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1			-28.3	-1323.5063098	-2648.1775221	-3562.5978134	-409.0967962	0.0	0.0	2.2	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-28.2	-1323.5063098	-2648.1775221	-3562.5977624	-409.0967962	0.0	0.0	2.3	0.0
				LiCl_mol6_aan	TMPZnCl	1_LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-25.9	-1323.5063098	-2648.1775221	-3562.5969118	-409.0967962	0.0	0.0	4.6	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_a	TMPH_1			-20.9	-1323.5063098	-2596.3659178	-3510.7833962	-409.0967962	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_b	TMPH_1			-16.2	-1323.5063098	-2596.3659178	-3510.7816201	-409.0967962	0.0	0.0	4.7	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_5TMPZn_d5_mol6_aa	TMPH_1			-20.7	-1323.5063098	-2596.3659178	-3510.7833030	-409.0967962	0.0	0.0	0.2	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1			-17.9	-1323.5063098	-2596.3659178	-3510.7822417	-409.0967962	0.0	0.0	3.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_b	TMPH_1			-16.3	-1323.5063098	-2596.3659178	-3510.7816221	-409.0967962	0.0	0.0	4.7	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_a	TMPH_1			-14.9	-1323.5063098	-2596.3659178	-3510.7811169	-409.0967962	0.0	0.0	6.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_b	TMPH_1			-14.3	-1323.5063098	-2596.3659178	-3510.7808722	-409.0967962	0.0	0.0	6.6	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol6_c	TMPH_1			-2.8	-1323.5063098	-2596.3659178	-3510.7764818	-409.0967962	0.0	0.0	18.2	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_8TMPZn_d8_mol6_a	TMPH_1			3.4	-1323.5063098	-2596.3659178	-3510.7741347	-409.0967962	0.0	0.0	24.3	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8_38	TMPH_1			-51.6	-1323.5063098	-2596.3659178	-4425.2045904	-409.0967962	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1			-34.9	-1323.5063098	-2596.3659178	-4425.1982362	-409.0967962	0.0	0.0	16.7	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1			-40.5	-1323.5063098	-2596.3659178	-4425.2003870	-409.0967962	0.0	0.0	11.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos8	TMPH_1			-31.3	-1323.5063098	-2596.3659178	-4425.1968634	-409.0967962	0.0	0.0	20.3	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos5	TMPH_1			-35.8	-1323.5063098	-2596.3659178	-4425.1985875	-409.0967962	0.0	0.0	15.8	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2	TMPH_1			-28.4	-1323.5063098	-2596.3659178	-4425.1957500	-409.0967962	0.0	0.0	23.2	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2_8	TMPH_1			-22.3	-1323.5063098	-2596.3659178	-4425.1934524	-409.0967962	0.0	0.0	29.2	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos2_15	TMPH_1			-22.3	-1323.5063098	-2596.3659178	-4425.1934528	-409.0967962	0.0	0.0	29.2	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1			-43.7	-1415.7817642	-2648.1775221	-3654.8791290	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_8_ZnCl_d8_mol7e	TMPH_1			-33.7	-1415.7817642	-2648.1775221	-3654.8753417	-409.0967962	0.0	0.0	9.9	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_5_ZnCl_d5_mol7e	TMPH_1			-22.4	-1415.7817642	-2648.1775221	-3654.8710311	-409.0967962	0.0	0.0	21.3	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_2_ZnCl_d2_mol7e	TMPH_1			-23.6	-1415.7817642	-2648.1775221	-3654.8714765	-409.0967962	0.0	0.0	20.1	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_5_ZnCl_d5_mol7e	TMPH_1			-19.4	-1415.7817642	-2648.1775221	-3654.8698787	-409.0967962	0.0	0.0	24.3	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_8_ZnCl_d8_mol7e	TMPH_1			-20.7	-1415.7817642	-2648.1775221	-3654.8703628	-409.0967962	0.0	0.0	23.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-17.1	-1415.7817642	-2596.3659178	-3603.0573859	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e	TMPH_1			-16.8	-1415.7817642	-2596.3659178	-3603.0572809	-409.0967962	0.0	0.0	0.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e	TMPH_1			-12.3	-1415.7817642	-2596.3659178	-3603.0555597	-409.0967962	0.0	0.0	4.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_2TMPZn_d2_mol7e	TMPH_1			-10.2	-1415.7817642	-2596.3659178	-3603.0547612	-409.0967962	0.0	0.0	6.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-4.9	-1415.7817642	-2596.3659178	-3603.0527634	-409.0967962	0.0	0.0	12.1	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_26	TMPH_1			-4.6	-1415.7817642	-2596.3659178	-3603.0526470	-409.0967962	0.0	0.0	12.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_31	TMPH_1			-4.6	-1415.7817642	-2596.3659178	-3603.0526439	-409.0967962	0.0	0.0	12.5	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-3.1	-1415.7817642	-2596.3659178	-3603.0520753	-409.0967962	0.0	0.0	13.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-1.1	-1415.7817642	-2596.3659178	-3603.0513227	-409.0967962	0.0	0.0	15.9	0.0

				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_38	TMPH_1			-0.1	-1415.7817642	-2596.3659178	-3603.0509327	-409.0967962	0.0	0.0	16.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_1	TMPH_1			0.4	-1415.7817642	-2596.3659178	-3603.0507159	-409.0967962	0.0	0.0	17.5	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_2TMPZn_d2_mol7e_28	TMPH_1			2.9	-1415.7817642	-2596.3659178	-3603.0497945	-409.0967962	0.0	0.0	19.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_38	TMPH_1			4.3	-1415.7817642	-2596.3659178	-3603.0492570	-409.0967962	0.0	0.0	21.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol7e_20	TMPH_1			6.1	-1415.7817642	-2596.3659178	-3603.0485780	-409.0967962	0.0	0.0	23.1	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_36	TMPH_1			6.5	-1415.7817642	-2596.3659178	-3603.0483997	-409.0967962	0.0	0.0	23.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1			-64.9	-1415.7817642	-2596.3659178	-4609.7605802	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1			-62.9	-1415.7817642	-2596.3659178	-4609.7598132	-409.0967962	0.0	0.0	2.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_mol15_pos8	TMPH_1			-56.8	-1415.7817642	-2596.3659178	-4609.7575029	-409.0967962	0.0	0.0	8.1	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_17	TMPH_1			-54.7	-1415.7817642	-2596.3659178	-4609.7566797	-409.0967962	0.0	0.0	10.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_13	TMPH_1			-45.8	-1415.7817642	-2596.3659178	-4609.7532802	-409.0967962	0.0	0.0	19.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8	TMPH_1			-45.0	-1415.7817642	-2596.3659178	-4609.7529765	-409.0967962	0.0	0.0	20.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_12	TMPH_1			-41.0	-1415.7817642	-2596.3659178	-4609.7514862	-409.0967962	0.0	0.0	23.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos5	TMPH_1			-33.7	-1415.7817642	-2596.3659178	-4609.7486857	-409.0967962	0.0	0.0	31.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_mol15_pos2_15	TMPH_1			-22.6	-1415.7817642	-2596.3659178	-4609.7444432	-409.0967962	0.0	0.0	42.4	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1			-54.4	-1761.3908362	-1068.9731777	-2421.2879207	-409.0967962	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_1	TMPH_1			-54.0	-1761.3908362	-1068.9731777	-2421.2877997	-409.0967962	0.0	0.0	0.3	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos5_22	TMPH_1			-51.5	-1761.3908362	-1068.9731777	-2421.2868189	-409.0967962	0.0	0.0	2.9	0.0
0	0	0	0	MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap	TMPH_1		reaction32	-26.5	-1976.4042295	-2648.1775221	-4215.4950591	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_b	TMPH_1		reaction33	-19.6	-1976.4042295	-2596.3659178	-4163.6808048	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos3	TMPH_1		reaction34	-45.0	-1976.4042295	-2596.3659178	-5730.9979115	-409.0967962	0.0	0.0	0.0	0.0
0	0	0	0	1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_7	TMPH_1		reaction37	-69.3	-2068.6769938	-2596.3659178	-5915.5527261	-409.0967962	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap	TMPH_1			-26.5	-1976.4042295	-2648.1775221	-4215.4950591	-409.0967962	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_5ZnCl_d5_mol6_aae	TMPH_1			-20.9	-1976.4042295	-2648.1775221	-4215.4929096	-409.0967962	0.0	0.0	5.6	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_2ZnCl_d2_mol6_aaq	TMPH_1			-14.6	-1976.4042295	-2648.1775221	-4215.4905129	-409.0967962	0.0	0.0	11.9	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_8ZnCl_d8_mol6_aac2	TMPH_1			-10.7	-1976.4042295	-2648.1775221	-4215.4890386	-409.0967962	0.0	0.0	15.8	0.0
				MgCl2_mol6_aac	TMPZnCl	MgCl2_8ZnCl_d8_mol6_aac23	TMPH_1			4.4	-1976.4042295	-2648.1775221	-4215.4832755	-409.0967962	0.0	0.0	30.9	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap2	TMPH_1			13.2	-1976.4042295	-2648.1775221	-4215.4799259	-409.0967962	0.0	0.0	39.7	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_b	TMPH_1			-19.6	-1976.4042295	-2596.3659178	-4163.6808048	-409.0967962	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_a	TMPH_1			-18.6	-1976.4042295	-2596.3659178	-4163.6804378	-409.0967962	0.0	0.0	1.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_3TMPZn_d3_mol6_a	TMPH_1			-18.2	-1976.4042295	-2596.3659178	-4163.6803011	-409.0967962	0.0	0.0	1.3	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_3TMPZn_d3_mol6_b	TMPH_1			-17.7	-1976.4042295	-2596.3659178	-4163.6800971	-409.0967962	0.0	0.0	1.9	0.0
				MgCl2_mol6_aac	TMP2Zn_1	MgCl2_3TMPZn_d3_mol6_a	TMPH_1			-4.6	-1976.4042295	-2596.3659178	-4163.6751080	-409.0967962	0.0	0.0	15.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_2TMPZn_d2_mol6_c	TMPH_1			-0.2	-1976.4042295	-2596.3659178	-4163.6734198	-409.0967962	0.0	0.0	19.4	0.0
				MgCl2_mol6_aac	TMP2Zn_1	MgCl2_5TMPZn_d5_mol6_aa	TMPH_1			0.3	-1976.4042295	-2596.3659178	-4163.6732525	-409.0967962	0.0	0.0	19.8	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_2TMPZn_d2_mol6_b	TMPH_1			9.0	-1976.4042295	-2596.3659178	-4163.6699406	-409.0967962	0.0	0.0	28.5	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_8TMPZn_d8_mol6_a2	TMPH_1			13.3	-1976.4042295	-2596.3659178	-4163.6682776	-409.0967962	0.0	0.0	32.9	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos3	TMPH_1			-45.0	-1976.4042295	-2596.3659178	-5730.9979115	-409.0967962	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2_27	TMPH_1			-42.1	-1976.4042295	-2596.3659178	-5730.9968147	-409.0967962	0.0	0.0	2.9	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5	TMPH_1			-38.9	-1976.4042295	-2596.3659178	-5730.9956150	-409.0967962	0.0	0.0	6.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2	TMPH_1			-16.3	-1976.4042295	-2596.3659178	-5730.9869901	-409.0967962	0.0	0.0	28.7	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5_29	TMPH_1			-6.4	-1976.4042295	-2596.3659178	-5730.9832072	-409.0967962	0.0	0.0	38.6	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5_31	TMPH_1			8.7	-1976.4042295	-2596.3659178	-5730.9774583	-409.0967962	0.0	0.0	53.7	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos8	TMPH_1			11.0	-1976.4042295	-2596.3659178	-5730.9765892	-409.0967962	0.0	0.0	56.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos8_1	TMPH_1			17.6	-1976.4042295	-2596.3659178	-5730.9740868	-409.0967962	0.0	0.0	62.6	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_7	TMPH_1			-69.3	-2068.6769938	-2596.3659178	-5915.5527261	-409.0967962	0.0	0.0	0.0	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2	TMPH_1			-55.2	-2068.6769938	-2596.3659178	-5915.5473257	-409.0967962	0.0	0.0	14.2	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos5	TMPH_1			-34.6	-2068.6769938	-2596.3659178	-5915.5395008	-409.0967962	0.0	0.0	34.7	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_9	TMPH_1			-4.9	-2068.6769938	-2596.3659178	-5915.5281738	-409.0967962	0.0	0.0	64.5	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos8	TMPH_1			4.5	-2068.6769938	-2596.3659178	-5915.5245813	-409.0967962	0.0	0.0	73.9	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_5	TMPH_1			19.2	-2068.6769938	-2596.3659178	-5915.5189952	-409.0967962	0.0	0.0	88.6	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_8	TMPH_1			50.3	-2068.6769938	-2596.3659178	-5915.5071680	-409.0967962	0.0	0.0	119.6	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos5_10	TMPH_1			84.6	-2068.6769938	-2596.3659178	-5915.4941073	-409.0967962	0.0	0.0	153.9	0.0

Table TT10. The calculated for reaction free energy values at the CPCM(**THF**)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory (T = 298.15 K).
"E1 and E2" – educt 1 and educt 2, "P1 and P2" – product 1 and product 2.

charge				filename						ΔG^{sol}	G^{sol}				ΔG^{sol}			
E1	E2	P1	P2	E1	E2	P1	P2			kJ/mol	E1	E2	P1	P2	E1	E2	P1	P2
0	0	0	0	mol6	TMPMgCl	3MgCl_d3_mol6_aad	TMPH_1		reaction1	-2.0	-855.5906667	-1068.9684886	-1515.4634893	-409.0964418	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMPZnCl	3ZnCl_d3_mol6_aap	TMPH_1		reaction2	-16.2	-855.5906667	-2648.1741618	-3094.6745648	-409.0964418	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMP2Zn_1	5_TMPZn_d5_mol6_b	TMPH_1		reaction3	-14.1	-855.5906667	-2596.3642905	-3042.8638942	-409.0964418	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMP2Zn_1	mol14_pos5	TMPH_1		reaction4	-27.3	-855.5906667	-2596.3642905	-3489.3631361	-409.0964418	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMPZnCl	5_ZnCl_d5_mol7e	TMPH_1		reaction5	-14.1	-947.8679064	-2648.1741618	-3186.9510014	-409.0964418	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	5TMPZn_d5_mol7e	TMPH_1		reaction6	-13.7	-947.8679064	-2596.3642905	-3135.1409695	-409.0964418	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	mol15_pos5	TMPH_1		reaction7	-29.2	-947.8679064	-2596.3642905	-3673.9183275	-409.0964418	0.0	0.0	0.0	0.0
0	0	0	0	mol16e_1	TMPMgCl	mol17_pos5_2	TMPH_1		reaction8	-9.1	-1293.4795050	-1068.9684886	-1953.3550029	-409.0964418	0.6	0.0	0.0	0.0
				mol6	TMPMgCl	3MgCl_d3_mol6_aad	TMPH_1			-2.0	-855.5906667	-1068.9684886	-1515.4634893	-409.0964418	0.0	0.0	0.0	0.0
				mol6	TMPMgCl	5MgCl_d5_mol6_aaa	TMPH_1			9.8	-855.5906667	-1068.9684886	-1515.4589754	-409.0964418	0.0	0.0	11.9	0.0
				mol6	TMPMgCl	8MgCl_d8_mol6_aar	TMPH_1			19.7	-855.5906667	-1068.9684886	-1515.4552258	-409.0964418	0.0	0.0	21.7	0.0
				mol6	TMPMgCl	2MgCl_d2_mol6_aaa	TMPH_1			39.4	-855.5906667	-1068.9684886	-1515.4477007	-409.0964418	0.0	0.0	41.5	0.0
				mol6	TMPZnCl	3ZnCl_d3_mol6_aap	TMPH_1			-16.2	-855.5906667	-2648.1741618	-3094.6745648	-409.0964418	0.0	0.0	0.0	0.0
				mol6	TMPZnCl	5ZnCl_d5_mol6_aae	TMPH_1			-14.0	-855.5906667	-2648.1741618	-3094.6737292	-409.0964418	0.0	0.0	2.2	0.0
				mol6	TMPZnCl	8ZnCl_d8_mol6_aac	TMPH_1			-2.9	-855.5906667	-2648.1741618	-3094.6694819	-409.0964418	0.0	0.0	13.3	0.0
				mol6	TMPZnCl	2ZnCl_d2_mol6_aaq	TMPH_1			1.8	-855.5906667	-2648.1741618	-3094.6676967	-409.0964418	0.0	0.0	18.0	0.0
				mol6	TMP2Zn_1	5_TMPZn_d5_mol6_b	TMPH_1			-14.1	-855.5906667	-2596.3642905	-3042.8638942	-409.0964418	0.0	0.0	0.0	0.0
				mol6	TMP2Zn_1	5_TMPZn_d5_mol6_a	TMPH_1			-13.4	-855.5906667	-2596.3642905	-3042.8636103	-409.0964418	0.0	0.0	0.7	0.0
				mol6	TMP2Zn_1	3_TMPZn_d3_mol6_b	TMPH_1			-10.3	-855.5906667	-2596.3642905	-3042.8624404	-409.0964418	0.0	0.0	3.8	0.0
				mol6	TMP2Zn_1	8_TMPZn_d8_mol6_a	TMPH_1			6.0	-855.5906667	-2596.3642905	-3042.8562211	-409.0964418	0.0	0.0	20.1	0.0
				mol6	TMP2Zn_1	2_TMPZn_d2_mol6_a	TMPH_1			12.2	-855.5906667	-2596.3642905	-3042.8538611	-409.0964418	0.0	0.0	26.3	0.0
				mol6	TMP2Zn_1	mol14_pos5	TMPH_1			-27.3	-855.5906667	-2596.3642905	-3489.3631361	-409.0964418	0.0	0.0	0.0	0.0
				mol6	TMP2Zn_1	mol14_pos3	TMPH_1			-23.8	-855.5906667	-2596.3642905	-3489.3618075	-409.0964418	0.0	0.0	3.5	0.0
				mol6	TMP2Zn_1	mol14_pos8	TMPH_1			4.6	-855.5906667	-2596.3642905	-3489.3509768	-409.0964418	0.0	0.0	31.9	0.0
				mol6	TMP2Zn_1	mol14_pos2	TMPH_1			14.0	-855.5906667	-2596.3642905	-3489.3474106	-409.0964418	0.0	0.0	41.3	0.0
				mol7e	TMPZnCl	5_ZnCl_d5_mol7e	TMPH_1			-14.1	-947.8679064	-2648.1741618	-3186.9510014	-409.0964418	0.0	0.0	0.0	0.0
				mol7e	TMPZnCl	2_ZnCl_d2_mol7e	TMPH_1			-7.7	-947.8679064	-2648.1741618	-3186.9485502	-409.0964418	0.0	0.0	6.4	0.0
				mol7e	TMPZnCl	8_ZnCl_d8_mol7e	TMPH_1			-6.2	-947.8679064	-2648.1741618	-3186.9479997	-409.0964418	0.0	0.0	7.9	0.0
				mol7e	TMP2Zn_1	5TMPZn_d5_mol7e	TMPH_1			-13.7	-947.8679064	-2596.3642905	-3135.1409695	-409.0964418	0.0	0.0	0.0	0.0
				mol7e	TMP2Zn_1	2TMPZn_d2_mol7e	TMPH_1			-1.4	-947.8679064	-2596.3642905	-3135.1362946	-409.0964418	0.0	0.0	12.3	0.0
				mol7e	TMP2Zn_1	8TMPZn_d8_mol7e	TMPH_1			0.3	-947.8679064	-2596.3642905	-3135.1356305	-409.0964418	0.0	0.0	14.0	0.0
				mol7e	TMP2Zn_1	mol15_pos5	TMPH_1			-29.2	-947.8679064	-2596.3642905	-3673.9183275	-409.0964418	0.0	0.0	0.0	0.0
				mol7e	TMP2Zn_1	mol15_pos2	TMPH_1			-8.6	-947.8679064	-2596.3642905	-3673.9104896	-409.0964418	0.0	0.0	20.6	0.0
				mol7e	TMP2Zn_1	mol15_pos8	TMPH_1			-5.1	-947.8679064	-2596.3642905	-3673.9091470	-409.0964418	0.0	0.0	24.1	0.0
				mol16e_1	TMPMgCl	mol17_pos5_2	TMPH_1			-9.1	-1293.4795050	-1068.9684886	-1953.3550029	-409.0964418	0.6	0.0	0.0	0.0
				mol16e_1	TMPMgCl	mol17_pos5_1	TMPH_1			-9.0	-1293.4795050	-1068.9684886	-1953.3549885	-409.0964418	0.6	0.0	0.0	0.0
				mol16e_1	TMPMgCl	mol17_pos8_2	TMPH_1			19.8	-1293.4795050	-1068.9684886	-1953.3439967	-409.0964418	0.6	0.0	28.9	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1		reaction11	-45.2	-1323.5004968	-1068.9684886	-1983.3897488	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1		reaction12	-31.2	-1323.5004968	-2648.1741618	-3562.5901175	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1		reaction13	-14.4	-1323.5004968	-2596.3642905	-3510.7738375	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1		reaction14	-47.2	-1323.5004968	-2596.3642905	-4425.1903919	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1		reaction15	-44.8	-1415.7751950	-2648.1741618	-3654.8699943	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1		reaction16	-15.9	-1415.7751950	-2596.3642905	-3603.0490896	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1		reaction17	-76.7	-1415.7751950	-2596.3642905	-4609.7510243	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1		reaction18	-57.3	-1761.3845877	-1068.9684886	-2421.2784609	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1			-45.2	-1323.5004968	-1068.9684886	-1983.3897488	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_3MgCl_d3_mol6	TMPH_1			-7.5	-1323.5004968	-1068.9684886	-1983.3754055	-409.0964418	0.0	0.0	37.7	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_5MgCl_d5_mol6	TMPH_1			7.7	-1323.5004968	-1068.9684886	-1983.3696212	-409.0964418	0.0	0.0	52.8	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_2MgCl_d2_mol6	TMPH_1			16.7	-1323.5004968	-1068.9684886	-1983.3661794	-409.0964418	0.0	0.0	61.9	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1			-31.2	-1323.5004968	-2648.1741618	-3562.5901175	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1			-30.4	-1323.5004968	-2648.1741618	-3562.5898125	-409.0964418	0.0	0.0	0.8	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-18.4	-1323.5004968	-2648.1741618	-3562.5852067	-409.0964418	0.0	0.0	12.9	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_5ZnCl_d5_mol6_aae	TMPH_1			1.3	-1323.5004968	-2648.1741618	-3562.5777405	-409.0964418	0.0	0.0	32.5	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1			-14.4	-1323.5004968	-2596.3642905	-3510.7738375	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_b	TMPH_1			-12.8	-1323.5004968	-2596.3642905	-3510.7732099	-409.0964418	0.0	0.0	1.6	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_a	TMPH_1			-11.5	-1323.5004968	-2596.3642905	-3510.7727102	-409.0964418	0.0	0.0	3.0	0.0

				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_b	TMPH_1			-10.7	-1323.5004968	-2596.3642905	-3510.7724379	-409.0964418	0.0	0.0	3.7	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol6_c	TMPH_1			-6.7	-1323.5004968	-2596.3642905	-3510.7708810	-409.0964418	0.0	0.0	7.8	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol6_c	TMPH_1			2.2	-1323.5004968	-2596.3642905	-3510.7675073	-409.0964418	0.0	0.0	16.6	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1			-47.2	-1323.5004968	-2596.3642905	-4425.1903919	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos8	TMPH_1			-45.6	-1323.5004968	-2596.3642905	-4425.1897700	-409.0964418	0.0	0.0	1.6	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2_8	TMPH_1			-35.8	-1323.5004968	-2596.3642905	-4425.1860302	-409.0964418	0.0	0.0	11.5	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2	TMPH_1			-34.0	-1323.5004968	-2596.3642905	-4425.1853692	-409.0964418	0.0	0.0	13.2	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1			-27.1	-1323.5004968	-2596.3642905	-4425.1827081	-409.0964418	0.0	0.0	20.2	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos5	TMPH_1			-26.2	-1323.5004968	-2596.3642905	-4425.1823754	-409.0964418	0.0	0.0	21.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1			-44.8	-1415.7751950	-2648.1741618	-3654.8699943	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_8_ZnCl_d8_mol7e	TMPH_1			-35.1	-1415.7751950	-2648.1741618	-3654.8662951	-409.0964418	0.0	0.0	9.7	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_5_ZnCl_d5_mol7e	TMPH_1			-15.2	-1415.7751950	-2648.1741618	-3654.8587040	-409.0964418	0.0	0.0	29.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-15.9	-1415.7751950	-2596.3642905	-3603.0490896	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e	TMPH_1			-15.6	-1415.7751950	-2596.3642905	-3603.0490022	-409.0964418	0.0	0.0	0.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e	TMPH_1			-15.6	-1415.7751950	-2596.3642905	-3603.0489825	-409.0964418	0.0	0.0	0.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_31	TMPH_1			-7.7	-1415.7751950	-2596.3642905	-3603.0459792	-409.0964418	0.0	0.0	8.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_26	TMPH_1			-7.5	-1415.7751950	-2596.3642905	-3603.0459107	-409.0964418	0.0	0.0	8.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-4.5	-1415.7751950	-2596.3642905	-3603.0447451	-409.0964418	0.0	0.0	11.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-3.3	-1415.7751950	-2596.3642905	-3603.0442951	-409.0964418	0.0	0.0	12.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_38	TMPH_1			1.0	-1415.7751950	-2596.3642905	-3603.0426579	-409.0964418	0.0	0.0	16.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_1	TMPH_1			1.5	-1415.7751950	-2596.3642905	-3603.0424747	-409.0964418	0.0	0.0	17.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol7e_20	TMPH_1			2.5	-1415.7751950	-2596.3642905	-3603.0420812	-409.0964418	0.0	0.0	18.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1			-76.7	-1415.7751950	-2596.3642905	-4609.7510243	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_17	TMPH_1			-68.1	-1415.7751950	-2596.3642905	-4609.7477204	-409.0964418	0.0	0.0	8.7	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1			-66.5	-1415.7751950	-2596.3642905	-4609.7471363	-409.0964418	0.0	0.0	10.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8	TMPH_1			-60.8	-1415.7751950	-2596.3642905	-4609.7449611	-409.0964418	0.0	0.0	15.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_12	TMPH_1			-54.4	-1415.7751950	-2596.3642905	-4609.7425105	-409.0964418	0.0	0.0	22.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_13	TMPH_1			-49.5	-1415.7751950	-2596.3642905	-4609.7406484	-409.0964418	0.0	0.0	27.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos5	TMPH_1			-31.0	-1415.7751950	-2596.3642905	-4609.7336094	-409.0964418	0.0	0.0	45.7	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1			-57.3	-1761.3845877	-1068.9684886	-2421.2784609	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_1	TMPH_1			-56.8	-1761.3845877	-1068.9684886	-2421.2782597	-409.0964418	0.0	0.0	0.5	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos5_2	TMPH_1			-12.7	-1761.3845877	-1068.9684886	-2421.2614859	-409.0964418	0.0	0.0	44.6	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6	TMPH_1		reaction21	-46.9	-1323.5002978	-1068.9684886	-1983.3901949	-409.0964418	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_8ZnCl_d8_mol6_aac2	TMPH_1		reaction22	-32.6	-1323.5002978	-2648.1741618	-3562.5904335	-409.0964418	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_a	TMPH_1		reaction23	-24.3	-1323.5002978	-2596.3642905	-3510.7773983	-409.0964418	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8_38	TMPH_1		reaction24	-62.8	-1323.5002978	-2596.3642905	-4425.1959111	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1		reaction25	-44.8	-1415.7751950	-2648.1741618	-3654.8699943	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1		reaction26	-15.9	-1415.7751950	-2596.3642905	-3603.0490896	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1		reaction27	-76.7	-1415.7751950	-2596.3642905	-4609.7510243	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos5_1	TMPH_1		reaction28	-61.5	-1761.3845877	-1068.9684886	-2421.2800516	-409.0964418	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6	TMPH_1			-46.9	-1323.5002978	-1068.9684886	-1983.3901949	-409.0964418	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1			-45.7	-1323.5002978	-1068.9684886	-1983.3897488	-409.0964418	0.0	0.0	1.2	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d3_mol6	TMPH_1			-42.0	-1323.5002978	-1068.9684886	-1983.3883337	-409.0964418	0.0	0.0	4.9	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6_1	TMPH_1			-31.6	-1323.5002978	-1068.9684886	-1983.3843941	-409.0964418	0.0	0.0	15.2	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d8_mol6_1	TMPH_1			-22.3	-1323.5002978	-1068.9684886	-1983.3808215	-409.0964418	0.0	0.0	24.6	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d8_mol6	TMPH_1			-12.3	-1323.5002978	-1068.9684886	-1983.3770464	-409.0964418	0.0	0.0	34.5	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_3MgCl_d3_mol6	TMPH_1			-8.0	-1323.5002978	-1068.9684886	-1983.3754055	-409.0964418	0.0	0.0	38.8	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d2_mol6	TMPH_1			4.3	-1323.5002978	-1068.9684886	-1983.3706922	-409.0964418	0.0	0.0	51.2	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_8ZnCl_d8_mol6_aac2	TMPH_1			-32.6	-1323.5002978	-2648.1741618	-3562.5904335	-409.0964418	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1			-31.8	-1323.5002978	-2648.1741618	-3562.5901175	-409.0964418	0.0	0.0	0.8	0.0
				LiCl_mol6_aan	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1			-31.0	-1323.5002978	-2648.1741618	-3562.5898125	-409.0964418	0.0	0.0	1.6	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_5ZnCl_d5_mol6_aae	TMPH_1			-30.2	-1323.5002978	-2648.1741618	-3562.5895098	-409.0964418	0.0	0.0	2.4	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-29.8	-1323.5002978	-2648.1741618	-3562.5893509	-409.0964418	0.0	0.0	2.8	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_a	TMPH_1			-24.3	-1323.5002978	-2596.3642905	-3510.7773983	-409.0964418	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_b	TMPH_1			-19.1	-1323.5002978	-2596.3642905	-3510.7754181	-409.0964418	0.0	0.0	5.2	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_5TMPZn_d5_mol6_aa	TMPH_1			-23.6	-1323.5002978	-2596.3642905	-3510.7771199	-409.0964418	0.0	0.0	0.7	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1			-14.9	-1323.5002978	-2596.3642905	-3510.7738375	-409.0964418	0.0	0.0	9.3	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_b	TMPH_1			-13.3	-1323.5002978	-2596.3642905	-3510.7732099	-409.0964418	0.0	0.0	11.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_a	TMPH_1			-12.0	-1323.5002978	-2596.3642905	-3510.7727102	-409.0964418	0.0	0.0	12.3	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_b	TMPH_1			-11.3	-1323.5002978	-2596.3642905	-3510.7724379	-409.0964418	0.0	0.0	13.0	0.0

				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol6_c	TMPH_1			-7.2	-1323.5002978	-2596.3642905	-3510.7708810	-409.0964418	0.0	0.0	17.1	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_8TMPZn_d8_mol6_a	TMPH_1			-1.1	-1323.5002978	-2596.3642905	-3510.7685526	-409.0964418	0.0	0.0	23.2	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8_38	TMPH_1			-62.8	-1323.5002978	-2596.3642905	-4425.1959111	-409.0964418	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1			-48.3	-1323.5002978	-2596.3642905	-4425.1903919	-409.0964418	0.0	0.0	14.5	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos8	TMPH_1			-46.6	-1323.5002978	-2596.3642905	-4425.1897700	-409.0964418	0.0	0.0	16.1	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2_8	TMPH_1			-36.8	-1323.5002978	-2596.3642905	-4425.1860302	-409.0964418	0.0	0.0	25.9	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos2_15	TMPH_1			-36.8	-1323.5002978	-2596.3642905	-4425.1860306	-409.0964418	0.0	0.0	25.9	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2	TMPH_1			-35.1	-1323.5002978	-2596.3642905	-4425.1853692	-409.0964418	0.0	0.0	27.7	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1			-28.1	-1323.5002978	-2596.3642905	-4425.1827081	-409.0964418	0.0	0.0	34.7	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos5	TMPH_1			-27.2	-1323.5002978	-2596.3642905	-4425.1823754	-409.0964418	0.0	0.0	35.5	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1			-44.8	-1415.7751950	-2648.1741618	-3654.8699943	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_5_ZnCl_d5_mol7e	TMPH_1			-31.8	-1415.7751950	-2648.1741618	-3654.8650194	-409.0964418	0.0	0.0	13.1	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_8_ZnCl_d8_mol7e	TMPH_1			-35.1	-1415.7751950	-2648.1741618	-3654.8662951	-409.0964418	0.0	0.0	9.7	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_2_ZnCl_d2_mol7e	TMPH_1			-25.5	-1415.7751950	-2648.1741618	-3654.8626347	-409.0964418	0.0	0.0	19.3	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_8_ZnCl_d8_mol7e	TMPH_1			-23.7	-1415.7751950	-2648.1741618	-3654.8619538	-409.0964418	0.0	0.0	21.1	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_5_ZnCl_d5_mol7e	TMPH_1			-15.2	-1415.7751950	-2648.1741618	-3654.8587040	-409.0964418	0.0	0.0	29.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-15.9	-1415.7751950	-2596.3642905	-3603.0490896	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e	TMPH_1			-15.6	-1415.7751950	-2596.3642905	-3603.0490022	-409.0964418	0.0	0.0	0.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e	TMPH_1			-15.6	-1415.7751950	-2596.3642905	-3603.0489825	-409.0964418	0.0	0.0	0.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_2TMPZn_d2_mol7e	TMPH_1			-14.0	-1415.7751950	-2596.3642905	-3603.0483883	-409.0964418	0.0	0.0	1.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-11.8	-1415.7751950	-2596.3642905	-3603.0475310	-409.0964418	0.0	0.0	4.1	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_31	TMPH_1			-7.7	-1415.7751950	-2596.3642905	-3603.0459792	-409.0964418	0.0	0.0	8.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_26	TMPH_1			-7.5	-1415.7751950	-2596.3642905	-3603.0459107	-409.0964418	0.0	0.0	8.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-4.5	-1415.7751950	-2596.3642905	-3603.0447451	-409.0964418	0.0	0.0	11.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-3.3	-1415.7751950	-2596.3642905	-3603.0442951	-409.0964418	0.0	0.0	12.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-3.0	-1415.7751950	-2596.3642905	-3603.0442050	-409.0964418	0.0	0.0	12.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_1	TMPH_1			-2.0	-1415.7751950	-2596.3642905	-3603.0438011	-409.0964418	0.0	0.0	13.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_38	TMPH_1			-0.3	-1415.7751950	-2596.3642905	-3603.0431519	-409.0964418	0.0	0.0	15.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-0.1	-1415.7751950	-2596.3642905	-3603.0430779	-409.0964418	0.0	0.0	15.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_38	TMPH_1			1.0	-1415.7751950	-2596.3642905	-3603.0426579	-409.0964418	0.0	0.0	16.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_1	TMPH_1			1.5	-1415.7751950	-2596.3642905	-3603.0424747	-409.0964418	0.0	0.0	17.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol7e_20	TMPH_1			2.5	-1415.7751950	-2596.3642905	-3603.0420812	-409.0964418	0.0	0.0	18.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1			-76.7	-1415.7751950	-2596.3642905	-4609.7510243	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_mol15_pos8	TMPH_1			-71.1	-1415.7751950	-2596.3642905	-4609.7488851	-409.0964418	0.0	0.0	5.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_17	TMPH_1			-68.1	-1415.7751950	-2596.3642905	-4609.7477204	-409.0964418	0.0	0.0	8.7	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1			-66.5	-1415.7751950	-2596.3642905	-4609.7471363	-409.0964418	0.0	0.0	10.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8	TMPH_1			-60.8	-1415.7751950	-2596.3642905	-4609.7449611	-409.0964418	0.0	0.0	15.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_12	TMPH_1			-54.4	-1415.7751950	-2596.3642905	-4609.7425105	-409.0964418	0.0	0.0	22.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_13	TMPH_1			-49.5	-1415.7751950	-2596.3642905	-4609.7406484	-409.0964418	0.0	0.0	27.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_mol15_pos2_15	TMPH_1			-35.7	-1415.7751950	-2596.3642905	-4609.7354119	-409.0964418	0.0	0.0	41.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_mol15_pos2_17	TMPH_1			-36.8	-1415.7751950	-2596.3642905	-4609.7358001	-409.0964418	0.0	0.0	40.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos5	TMPH_1			-31.0	-1415.7751950	-2596.3642905	-4609.7336094	-409.0964418	0.0	0.0	45.7	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos5_1	TMPH_1			-61.5	-1761.3845877	-1068.9684886	-2421.2800516	-409.0964418	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos5_22	TMPH_1			-60.1	-1761.3845877	-1068.9684886	-2421.2795323	-409.0964418	0.0	0.0	1.4	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1			-57.3	-1761.3845877	-1068.9684886	-2421.2784609	-409.0964418	0.0	0.0	4.2	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap	TMPH_1		reaction31	-19.6	-1976.3982356	-2648.1741618	-4215.4834023	-409.0964418	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_b	TMPH_1		reaction32	-16.6	-1976.3982356	-2596.3642905	-4163.6724235	-409.0964418	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2_27	TMPH_1		reaction33	-49.9	-1976.3982356	-2596.3642905	-5730.9868896	-409.0964418	0.0	0.0	0.0	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_7	TMPH_1		reaction36	-76.5	-2068.6704954	-2596.3642905	-5915.5415206	-409.0964418	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap	TMPH_1			-19.6	-1976.3982356	-2648.1741618	-4215.4834023	-409.0964418	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_2ZnCl_d2_mol6_aaq	TMPH_1			-15.5	-1976.3982356	-2648.1741618	-4215.4818431	-409.0964418	0.0	0.0	4.1	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_5ZnCl_d5_mol6_aae	TMPH_1			-14.7	-1976.3982356	-2648.1741618	-4215.4815550	-409.0964418	0.0	0.0	4.9	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_8ZnCl_d8_mol6_aac2	TMPH_1			-10.4	-1976.3982356	-2648.1741618	-4215.4799206	-409.0964418	0.0	0.0	9.1	0.0
				MgCl2_mol6_aac	TMPZnCl	MgCl2_8ZnCl_d8_mol6_aac23	TMPH_1			5.2	-1976.3982356	-2648.1741618	-4215.4739591	-409.0964418	0.0	0.0	24.8	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_b	TMPH_1			-16.6	-1976.3982356	-2596.3642905	-4163.6724235	-409.0964418	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_a	TMPH_1			-15.9	-1976.3982356	-2596.3642905	-4163.6721373	-409.0964418	0.0	0.0	0.8	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_3TMPZn_d3_mol6_a	TMPH_1			-15.2	-1976.3982356	-2596.3642905	-4163.6718866	-409.0964418	0.0	0.0	1.4	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_3TMPZn_d3_mol6_b	TMPH_1			-14.7	-1976.3982356	-2596.3642905	-4163.6716942	-409.0964418	0.0	0.0	1.9	0.0
				MgCl2_mol6_aac	TMP2Zn_1	MgCl2_3TMPZn_d3_mol6_a	TMPH_1			-9.0	-1976.3982356	-2596.3642905	-4163.6695112	-409.0964418	0.0	0.0	7.6	0.0
				MgCl2_mol6_aac	TMP2Zn_1	MgCl2_5TMPZn_d5_mol6_aa	TMPH_1			-4.5	-1976.3982356	-2596.3642905	-4163.6677856	-409.0964418	0.0	0.0	12.2	0.0

				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_2TMPZn_d2_mol6_c	TMPH_1			-2.1	-1976.3982356	-2596.3642905	-4163.6668922	-409.0964418	0.0	0.0	14.5	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_2TMPZn_d2_mol6_b	TMPH_1			6.4	-1976.3982356	-2596.3642905	-4163.6636290	-409.0964418	0.0	0.0	23.1	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_8TMPZn_d8_mol6_a2	TMPH_1			11.2	-1976.3982356	-2596.3642905	-4163.6618276	-409.0964418	0.0	0.0	27.8	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2_27	TMPH_1			-49.9	-1976.3982356	-2596.3642905	-5730.9868896	-409.0964418	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos3	TMPH_1			-32.3	-1976.3982356	-2596.3642905	-5730.9801944	-409.0964418	0.0	0.0	17.6	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5	TMPH_1			-28.9	-1976.3982356	-2596.3642905	-5730.9788903	-409.0964418	0.0	0.0	21.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2	TMPH_1			-21.7	-1976.3982356	-2596.3642905	-5730.9761433	-409.0964418	0.0	0.0	28.2	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos8	TMPH_1			-2.7	-1976.3982356	-2596.3642905	-5730.9689178	-409.0964418	0.0	0.0	47.2	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5_29	TMPH_1			-0.1	-1976.3982356	-2596.3642905	-5730.9678990	-409.0964418	0.0	0.0	49.9	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos8_1	TMPH_1			10.4	-1976.3982356	-2596.3642905	-5730.9639295	-409.0964418	0.0	0.0	60.3	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5_31	TMPH_1			20.3	-1976.3982356	-2596.3642905	-5730.9601513	-409.0964418	0.0	0.0	70.2	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_7	TMPH_1			-76.5	-2068.6704954	-2596.3642905	-5915.5415206	-409.0964418	0.0	0.0	0.0	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2	TMPH_1			-59.3	-2068.6704954	-2596.3642905	-5915.5349671	-409.0964418	0.0	0.0	17.2	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos5	TMPH_1			-32.0	-2068.6704954	-2596.3642905	-5915.5245678	-409.0964418	0.0	0.0	44.5	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_9	TMPH_1			-19.2	-2068.6704954	-2596.3642905	-5915.5197118	-409.0964418	0.0	0.0	57.3	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos8	TMPH_1			-8.8	-2068.6704954	-2596.3642905	-5915.5157604	-409.0964418	0.0	0.0	67.6	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_5	TMPH_1			7.3	-2068.6704954	-2596.3642905	-5915.5096277	-409.0964418	0.0	0.0	83.7	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_8	TMPH_1			41.1	-2068.6704954	-2596.3642905	-5915.4967287	-409.0964418	0.0	0.0	117.6	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos5_10	TMPH_1			85.6	-2068.6704954	-2596.3642905	-5915.4797824	-409.0964418	0.0	0.0	162.1	0.0

Table TT11. The calculated for reaction free energy values at the CPCM(**DMSO**)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory (T = $T_{experimental}$).
"E1 and E2" – educt 1 and educt 2, "P1 and P2" – product 1 and product 2.

charge				filename						ΔG^{sol}	G^{sol}				ΔG^{sol}			
E1	E2	P1	P2	E1	E2	P1	P2			kJ/mol	E1	E2	P1	P2	E1	E2	P1	P2
0	0	0	0	mol6	TMPMgCl	3_MgCl_d3_mol6_aad	TMPH_1		reaction1	-10.9	-855.5811928	-1068.9586982	-1515.4595266	-409.0844975	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMPZnCl	3_ZnCl_d3_mol6_aac	TMPH_1		reaction2	-22.4	-855.5861724	-2648.1694763	-3094.6741201	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMP2Zn_1	5_TMPZn_d5_mol6_b	TMPH_1		reaction3	-17.0	-855.5861724	-2596.3552027	-3042.8577834	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMP2Zn_1	mol14_pos5	TMPH_1		reaction4	-35.0	-855.5861724	-2596.3552027	-3489.3607760	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMPZnCl	5_ZnCl_d5_mol7e	TMPH_1		reaction5	-18.0	-947.8629812	-2648.1694763	-3186.9492594	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_36	TMPH_1		reaction6	-15.1	-947.8629812	-2596.3552027	-3135.1338599	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	mol15_pos5	TMPH_1		reaction7	-31.7	-947.8629812	-2596.3552027	-3673.9131114	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	mol16e_2	TMPMgCl	mol17_pos5_2	TMPH_1		reaction8	-10.3	-1293.4686930	-1068.9619145	-1953.3472864	-409.0872280	0.0	0.0	0.0	0.0
				mol6	TMPMgCl	3_MgCl_d3_mol6_aad	TMPH_1			-10.9	-855.5811928	-1068.9586982	-1515.4595266	-409.0844975	0.0	0.0	0.0	0.0
				mol6	TMPMgCl	3_MgCl_d3_mol6_aaq	TMPH_1			-10.8	-855.5811928	-1068.9586982	-1515.4595194	-409.0844975	0.0	0.0	0.0	0.0
				mol6	TMPMgCl	5_MgCl_d5_mol6_aaa	TMPH_1			7.1	-855.5811928	-1068.9586982	-1515.4526963	-409.0844975	0.0	0.0	17.9	0.0
				mol6	TMPMgCl	8_MgCl_d8_mol6_aar	TMPH_1			19.3	-855.5811928	-1068.9586982	-1515.4480387	-409.0844975	0.0	0.0	30.2	0.0
				mol6	TMPMgCl	2_MgCl_d2_mol6_aaa	TMPH_1			39.6	-855.5811928	-1068.9586982	-1515.4402968	-409.0844975	0.0	0.0	50.5	0.0
				mol6	TMPZnCl	3_ZnCl_d3_mol6_aac	TMPH_1			-22.4	-855.5861724	-2648.1694763	-3094.6741201	-409.0900593	0.0	0.0	0.0	0.0
				mol6	TMPZnCl	3_ZnCl_d3_mol6_aax	TMPH_1			-22.4	-855.5861724	-2648.1694763	-3094.6741150	-409.0900593	0.0	0.0	0.0	0.0
				mol6	TMPZnCl	3_ZnCl_d3_mol6_aap	TMPH_1			-22.4	-855.5861724	-2648.1694763	-3094.6741137	-409.0900593	0.0	0.0	0.0	0.0
				mol6	TMPZnCl	5_ZnCl_d5_mol6_aae	TMPH_1			-19.7	-855.5861724	-2648.1694763	-3094.6731069	-409.0900593	0.0	0.0	2.7	0.0
				mol6	TMPZnCl	8_ZnCl_d8_mol6_aac	TMPH_1			-6.1	-855.5861724	-2648.1694763	-3094.6679257	-409.0900593	0.0	0.0	16.3	0.0
				mol6	TMPZnCl	2_ZnCl_d2_mol6_aaq	TMPH_1			-2.2	-855.5861724	-2648.1694763	-3094.6664208	-409.0900593	0.0	0.0	20.2	0.0
				mol6	TMP2Zn_1	5_TMPZn_d5_mol6_b	TMPH_1			-17.0	-855.5861724	-2596.3552027	-3042.8577834	-409.0900593	0.0	0.0	0.0	0.0
				mol6	TMP2Zn_1	5_TMPZn_d5_mol6_a	TMPH_1			-16.4	-855.5861724	-2596.3552027	-3042.8575458	-409.0900593	0.0	0.0	0.6	0.0
				mol6	TMP2Zn_1	3_TMPZn_d3_mol6_b	TMPH_1			-13.4	-855.5861724	-2596.3552027	-3042.8564139	-409.0900593	0.0	0.0	3.6	0.0
				mol6	TMP2Zn_1	8_TMPZn_d8_mol6_a	TMPH_1			5.5	-855.5861724	-2596.3552027	-3042.8492399	-409.0900593	0.0	0.0	22.4	0.0
				mol6	TMP2Zn_1	2_TMPZn_d2_mol6_a	TMPH_1			11.0	-855.5861724	-2596.3552027	-3042.8471394	-409.0900593	0.0	0.0	27.9	0.0
				mol6	TMP2Zn_1	mol14_pos5	TMPH_1			-35.0	-855.5861724	-2596.3552027	-3489.3607760	-409.0900593	0.0	0.0	0.0	0.0
				mol6	TMP2Zn_1	mol14_pos3	TMPH_1			-33.0	-855.5861724	-2596.3552027	-3489.3599842	-409.0900593	0.0	0.0	2.1	0.0
				mol6	TMP2Zn_1	mol14_pos8	TMPH_1			1.0	-855.5861724	-2596.3552027	-3489.3470408	-409.0900593	0.0	0.0	36.1	0.0
				mol6	TMP2Zn_1	mol14_pos2	TMPH_1			9.7	-855.5861724	-2596.3552027	-3489.3437163	-409.0900593	0.0	0.0	44.8	0.0
				mol7e	TMPZnCl	5_ZnCl_d5_mol7e	TMPH_1			-18.0	-947.8629812	-2648.1694763	-3186.9492594	-409.0900593	0.0	0.0	0.0	0.0
				mol7e	TMPZnCl	2_ZnCl_d2_mol7e	TMPH_1			-13.1	-947.8629812	-2648.1694763	-3186.9473775	-409.0900593	0.0	0.0	4.9	0.0
				mol7e	TMPZnCl	8_ZnCl_d8_mol7e	TMPH_1			-10.9	-947.8629812	-2648.1694763	-3186.9465540	-409.0900593	0.0	0.0	7.1	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_36	TMPH_1			-15.1	-947.8629812	-2596.3552027	-3135.1338599	-409.0900593	0.0	0.0	0.0	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e	TMPH_1			-15.1	-947.8629812	-2596.3552027	-3135.1338594	-409.0900593	0.0	0.0	0.0	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_40	TMPH_1			-4.1	-947.8629812	-2596.3552027	-3135.1296812	-409.0900593	0.0	0.0	11.0	0.0
				mol7e	TMP2Zn_1	2_TMPZn_d2_mol7e	TMPH_1			-3.5	-947.8629812	-2596.3552027	-3135.1294474	-409.0900593	0.0	0.0	11.6	0.0
				mol7e	TMP2Zn_1	8_TMPZn_d8_mol7e	TMPH_1			-1.1	-947.8629812	-2596.3552027	-3135.1285383	-409.0900593	0.0	0.0	14.0	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_38	TMPH_1			0.8	-947.8629812	-2596.3552027	-3135.1278052	-409.0900593	0.0	0.0	15.9	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_1	TMPH_1			3.3	-947.8629812	-2596.3552027	-3135.1268724	-409.0900593	0.0	0.0	18.3	0.0
				mol7e	TMP2Zn_1	mol15_pos5	TMPH_1			-31.7	-947.8629812	-2596.3552027	-3673.9131114	-409.0900593	0.0	0.0	0.0	0.0
				mol7e	TMP2Zn_1	mol15_pos2	TMPH_1			-16.2	-947.8629812	-2596.3552027	-3673.9072223	-409.0900593	0.0	0.0	15.5	0.0
				mol7e	TMP2Zn_1	mol15_pos8	TMPH_1			-10.9	-947.8629812	-2596.3552027	-3673.9051836	-409.0900593	0.0	0.0	20.8	0.0
				mol16e_2	TMPMgCl	mol17_pos5_2	TMPH_1			-10.3	-1293.4686930	-1068.9619145	-1953.3472864	-409.0872280	0.0	0.0	0.0	0.0
				mol16e_2	TMPMgCl	mol17_pos5_1	TMPH_1			-10.2	-1293.4686930	-1068.9619145	-1953.3472537	-409.0872280	0.0	0.0	0.1	0.0
				mol16e_2	TMPMgCl	mol17_pos8_2	TMPH_1			18.2	-1293.4686930	-1068.9619145	-1953.3364555	-409.0872280	0.0	0.0	28.4	0.0
0	0	0	0	1_LiCl_mol6_1	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1		reaction11	-41.5	-1323.4935028	-1068.9586982	-1983.3835061	-409.0844975	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1		reaction12	-28.6	-1323.4994551	-2648.1694763	-3562.5897820	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1		reaction13	-17.4	-1323.4994551	-2596.3552027	-3510.7712236	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1		reaction14	-39.1	-1323.4994551	-2596.3552027	-4425.1888853	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1		reaction15	-44.2	-1415.7740903	-2648.1694763	-3654.8703328	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1		reaction16	-17.4	-1415.7740903	-2596.3552027	-3603.0458426	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1		reaction17	-65.5	-1415.7740903	-2596.3552027	-4609.7481992	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1		reaction18	-55.1	-1761.3767786	-1068.9619145	-2421.2724629	-409.0872280	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1			-41.5	-1323.4935028	-1068.9586982	-1983.3835061	-409.0844975	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_3MgCl_d3_mol6	TMPH_1			-17.3	-1323.4935028	-1068.9586982	-1983.3742927	-409.0844975	0.0	0.0	24.2	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_5MgCl_d5_mol6	TMPH_1			4.8	-1323.4935028	-1068.9586982	-1983.3658756	-409.0844975	0.0	0.0	46.3	0.0

				1_LiCl_mol6_1	TMPMgCl	1_LiCl_2MgCl_d2_mol6	TMPH_1			8.4	-1323.4935028	-1068.9586982	-1983.3645050	-409.0844975	0.0	0.0	49.9	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1			-28.6	-1323.4994551	-2648.1694763	-3562.5897820	-409.0900593	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1			-28.1	-1323.4994551	-2648.1694763	-3562.5895922	-409.0900593	0.0	0.0	0.5	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-25.4	-1323.4994551	-2648.1694763	-3562.5885429	-409.0900593	0.0	0.0	3.3	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_5ZnCl_d5_mol6_aae	TMPH_1			-2.0	-1323.4994551	-2648.1694763	-3562.5796205	-409.0900593	0.0	0.0	26.7	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1			-17.4	-1323.4994551	-2596.3552027	-3510.7712236	-409.0900593	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_b	TMPH_1			-15.6	-1323.4994551	-2596.3552027	-3510.7705445	-409.0900593	0.0	0.0	1.8	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_a	TMPH_1			-14.3	-1323.4994551	-2596.3552027	-3510.7700601	-409.0900593	0.0	0.0	3.1	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_b	TMPH_1			-13.8	-1323.4994551	-2596.3552027	-3510.7698440	-409.0900593	0.0	0.0	3.6	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol6_c	TMPH_1			-2.5	-1323.4994551	-2596.3552027	-3510.7655469	-409.0900593	0.0	0.0	14.9	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol6_c	TMPH_1			5.9	-1323.4994551	-2596.3552027	-3510.7623611	-409.0900593	0.0	0.0	23.3	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1			-39.1	-1323.4994551	-2596.3552027	-4425.1888853	-409.0900593	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1			-34.7	-1323.4994551	-2596.3552027	-4425.1872003	-409.0900593	0.0	0.0	4.4	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos5	TMPH_1			-34.4	-1323.4994551	-2596.3552027	-4425.1871093	-409.0900593	0.0	0.0	4.7	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos8	TMPH_1			-31.2	-1323.4994551	-2596.3552027	-4425.1858786	-409.0900593	0.0	0.0	7.9	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1			-44.2	-1415.7740903	-2648.1694763	-3654.8703328	-409.0900593	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_8_ZnCl_d8_mol7e	TMPH_1			-34.2	-1415.7740903	-2648.1694763	-3654.8665198	-409.0900593	0.0	0.0	10.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_5_ZnCl_d5_mol7e	TMPH_1			-19.6	-1415.7740903	-2648.1694763	-3654.8609807	-409.0900593	0.0	0.0	24.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-17.4	-1415.7740903	-2596.3552027	-3603.0458426	-409.0900593	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e	TMPH_1			-16.9	-1415.7740903	-2596.3552027	-3603.0456760	-409.0900593	0.0	0.0	0.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e	TMPH_1			-12.5	-1415.7740903	-2596.3552027	-3603.0439831	-409.0900593	0.0	0.0	4.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-5.0	-1415.7740903	-2596.3552027	-3603.0411553	-409.0900593	0.0	0.0	12.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_31	TMPH_1			-5.0	-1415.7740903	-2596.3552027	-3603.0411461	-409.0900593	0.0	0.0	12.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_26	TMPH_1			-4.9	-1415.7740903	-2596.3552027	-3603.0410879	-409.0900593	0.0	0.0	12.5	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-1.5	-1415.7740903	-2596.3552027	-3603.0398050	-409.0900593	0.0	0.0	15.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_38	TMPH_1			-0.3	-1415.7740903	-2596.3552027	-3603.0393374	-409.0900593	0.0	0.0	17.1	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_1	TMPH_1			0.4	-1415.7740903	-2596.3552027	-3603.0390970	-409.0900593	0.0	0.0	17.7	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol7e_20	TMPH_1			5.8	-1415.7740903	-2596.3552027	-3603.0370168	-409.0900593	0.0	0.0	23.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1			-65.5	-1415.7740903	-2596.3552027	-4609.7481992	-409.0900593	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1			-64.1	-1415.7740903	-2596.3552027	-4609.7476731	-409.0900593	0.0	0.0	1.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_17	TMPH_1			-55.9	-1415.7740903	-2596.3552027	-4609.7445580	-409.0900593	0.0	0.0	9.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_13	TMPH_1			-46.5	-1415.7740903	-2596.3552027	-4609.7409713	-409.0900593	0.0	0.0	19.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8	TMPH_1			-46.3	-1415.7740903	-2596.3552027	-4609.7408805	-409.0900593	0.0	0.0	19.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_12	TMPH_1			-42.3	-1415.7740903	-2596.3552027	-4609.7393718	-409.0900593	0.0	0.0	23.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos5	TMPH_1			-34.0	-1415.7740903	-2596.3552027	-4609.7361996	-409.0900593	0.0	0.0	31.5	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1			-55.1	-1761.3767786	-1068.9619145	-2421.2724629	-409.0872280	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_1	TMPH_1			-54.8	-1761.3767786	-1068.9619145	-2421.2723452	-409.0872280	0.0	0.0	0.3	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos5_1	TMPH_1			-14.8	-1761.3767786	-1068.9619145	-2421.2570899	-409.0872280	0.0	0.0	40.4	0.0
0	0	0	0	LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6	TMPH_1		reaction21	-45.2	-1323.4932725	-1068.9586982	-1983.3846802	-409.0844975	0.0	0.0	0.0	0.0
0	0	0	0	LiCl_mol6_aan	TMPZnCl	LiCl_8ZnCl_d8_mol6_aac2	TMPH_1		reaction22	-30.9	-1323.4992246	-2648.1694763	-3562.5904045	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_a	TMPH_1		reaction23	-21.4	-1323.4992246	-2596.3552027	-3510.7725271	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8_38	TMPH_1		reaction24	-52.9	-1323.4992246	-2596.3552027	-4425.1936667	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1		reaction25	-44.2	-1415.7740903	-2648.1694763	-3654.8703328	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1		reaction26	-17.4	-1415.7740903	-2596.3552027	-3603.0458426	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1		reaction27	-65.5	-1415.7740903	-2596.3552027	-4609.7481992	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos8_2	TMPH_1		reaction28	-62.3	-1761.3767786	-1068.9619145	-2421.2751881	-409.0872280	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6	TMPH_1			-45.2	-1323.4932725	-1068.9586982	-1983.3846802	-409.0844975	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1			-42.1	-1323.4932725	-1068.9586982	-1983.3835061	-409.0844975	0.0	0.0	3.1	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d3_mol6	TMPH_1			-41.0	-1323.4932725	-1068.9586982	-1983.3830947	-409.0844975	0.0	0.0	4.2	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6_1	TMPH_1			-26.4	-1323.4932725	-1068.9586982	-1983.3775462	-409.0844975	0.0	0.0	18.7	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d8_mol6_1	TMPH_1			-18.3	-1323.4932725	-1068.9586982	-1983.3744618	-409.0844975	0.0	0.0	26.8	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_3MgCl_d3_mol6	TMPH_1			-17.9	-1323.4932725	-1068.9586982	-1983.3742927	-409.0844975	0.0	0.0	27.3	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d8_mol6	TMPH_1			-5.3	-1323.4932725	-1068.9586982	-1983.3695024	-409.0844975	0.0	0.0	39.8	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_5MgCl_d5_mol6	TMPH_1			4.2	-1323.4932725	-1068.9586982	-1983.3658756	-409.0844975	0.0	0.0	49.4	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_2MgCl_d2_mol6	TMPH_1			7.8	-1323.4932725	-1068.9586982	-1983.3645050	-409.0844975	0.0	0.0	53.0	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_8ZnCl_d8_mol6_aac2	TMPH_1			-30.9	-1323.4992246	-2648.1694763	-3562.5904045	-409.0900593	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1			-29.2	-1323.4992246	-2648.1694763	-3562.5897820	-409.0900593	0.0	0.0	1.6	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_5ZnCl_d5_mol6_aae	TMPH_1			-29.2	-1323.4992246	-2648.1694763	-3562.5897455	-409.0900593	0.0	0.0	1.7	0.0
				LiCl_mol6_aan	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1			-28.8	-1323.4992246	-2648.1694763	-3562.5895922	-409.0900593	0.0	0.0	2.1	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-28.5	-1323.4992246	-2648.1694763	-3562.5894870	-409.0900593	0.0	0.0	2.4	0.0

				LiCl_mol6_aan	TMPZnCl	1_LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-26.0	-1323.4992246	-2648.1694763	-3562.5885429	-409.0900593	0.0	0.0	4.9	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_a	TMPH_1			-21.4	-1323.4992246	-2596.3552027	-3510.7725271	-409.0900593	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_5TMPZn_d5_mol6_aa	TMPH_1			-21.3	-1323.4992246	-2596.3552027	-3510.7724655	-409.0900593	0.0	0.0	0.2	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1			-18.0	-1323.4992246	-2596.3552027	-3510.7712236	-409.0900593	0.0	0.0	3.4	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_b	TMPH_1			-17.2	-1323.4992246	-2596.3552027	-3510.7709194	-409.0900593	0.0	0.0	4.2	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_b	TMPH_1			-16.2	-1323.4992246	-2596.3552027	-3510.7705445	-409.0900593	0.0	0.0	5.2	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_a	TMPH_1			-14.9	-1323.4992246	-2596.3552027	-3510.7700601	-409.0900593	0.0	0.0	6.5	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_b	TMPH_1			-14.4	-1323.4992246	-2596.3552027	-3510.7698440	-409.0900593	0.0	0.0	7.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol6_c	TMPH_1			-3.1	-1323.4992246	-2596.3552027	-3510.7655469	-409.0900593	0.0	0.0	18.3	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_8TMPZn_d8_mol6_a	TMPH_1			3.1	-1323.4992246	-2596.3552027	-3510.7632015	-409.0900593	0.0	0.0	24.5	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8_38	TMPH_1			-52.9	-1323.4992246	-2596.3552027	-4425.1936667	-409.0900593	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8	TMPH_1			-51.9	-1323.4992246	-2596.3552027	-4425.1932889	-409.0900593	0.0	0.0	1.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1			-40.3	-1323.4992246	-2596.3552027	-4425.1888853	-409.0900593	0.0	0.0	12.6	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1			-35.9	-1323.4992246	-2596.3552027	-4425.1872003	-409.0900593	0.0	0.0	17.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos5	TMPH_1			-35.6	-1323.4992246	-2596.3552027	-4425.1871093	-409.0900593	0.0	0.0	17.2	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1			-44.2	-1415.7740903	-2648.1694763	-3654.8703328	-409.0900593	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_8_ZnCl_d8_mol7e	TMPH_1			-34.2	-1415.7740903	-2648.1694763	-3654.8665198	-409.0900593	0.0	0.0	10.0	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_2_ZnCl_d2_mol7e	TMPH_1			-23.7	-1415.7740903	-2648.1694763	-3654.8625463	-409.0900593	0.0	0.0	20.4	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_5_ZnCl_d5_mol7e	TMPH_1			-23.5	-1415.7740903	-2648.1694763	-3654.8624606	-409.0900593	0.0	0.0	20.7	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_8_ZnCl_d8_mol7e	TMPH_1			-20.7	-1415.7740903	-2648.1694763	-3654.8613802	-409.0900593	0.0	0.0	23.5	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_5_ZnCl_d5_mol7e	TMPH_1			-19.6	-1415.7740903	-2648.1694763	-3654.8609807	-409.0900593	0.0	0.0	24.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-17.4	-1415.7740903	-2596.3552027	-3603.0458426	-409.0900593	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e	TMPH_1			-16.9	-1415.7740903	-2596.3552027	-3603.0456760	-409.0900593	0.0	0.0	0.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e	TMPH_1			-12.5	-1415.7740903	-2596.3552027	-3603.0439831	-409.0900593	0.0	0.0	4.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_2TMPZn_d2_mol7e	TMPH_1			-11.0	-1415.7740903	-2596.3552027	-3603.0434058	-409.0900593	0.0	0.0	6.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-5.0	-1415.7740903	-2596.3552027	-3603.0411553	-409.0900593	0.0	0.0	12.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_31	TMPH_1			-5.0	-1415.7740903	-2596.3552027	-3603.0411461	-409.0900593	0.0	0.0	12.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_26	TMPH_1			-4.9	-1415.7740903	-2596.3552027	-3603.0410879	-409.0900593	0.0	0.0	12.5	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-4.7	-1415.7740903	-2596.3552027	-3603.0410337	-409.0900593	0.0	0.0	12.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-1.5	-1415.7740903	-2596.3552027	-3603.0398050	-409.0900593	0.0	0.0	15.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_38	TMPH_1			-0.3	-1415.7740903	-2596.3552027	-3603.0393374	-409.0900593	0.0	0.0	17.1	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_1	TMPH_1			0.4	-1415.7740903	-2596.3552027	-3603.0390970	-409.0900593	0.0	0.0	17.7	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_2TMPZn_d2_mol7e_28	TMPH_1			2.4	-1415.7740903	-2596.3552027	-3603.0383193	-409.0900593	0.0	0.0	19.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_38	TMPH_1			3.3	-1415.7740903	-2596.3552027	-3603.0379899	-409.0900593	0.0	0.0	20.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_36	TMPH_1			4.9	-1415.7740903	-2596.3552027	-3603.0373659	-409.0900593	0.0	0.0	22.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol7e_20	TMPH_1			5.8	-1415.7740903	-2596.3552027	-3603.0370168	-409.0900593	0.0	0.0	23.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1			-65.5	-1415.7740903	-2596.3552027	-4609.7481992	-409.0900593	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1			-64.1	-1415.7740903	-2596.3552027	-4609.7476731	-409.0900593	0.0	0.0	1.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_mol15_pos8	TMPH_1			-58.1	-1415.7740903	-2596.3552027	-4609.7453761	-409.0900593	0.0	0.0	7.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_17	TMPH_1			-55.9	-1415.7740903	-2596.3552027	-4609.7445580	-409.0900593	0.0	0.0	9.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_13	TMPH_1			-46.5	-1415.7740903	-2596.3552027	-4609.7409713	-409.0900593	0.0	0.0	19.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8	TMPH_1			-46.3	-1415.7740903	-2596.3552027	-4609.7408805	-409.0900593	0.0	0.0	19.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_12	TMPH_1			-42.3	-1415.7740903	-2596.3552027	-4609.7393718	-409.0900593	0.0	0.0	23.2	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos5	TMPH_1			-34.0	-1415.7740903	-2596.3552027	-4609.7361996	-409.0900593	0.0	0.0	31.5	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos8_2	TMPH_1			-62.3	-1761.3767786	-1068.9619145	-2421.2751881	-409.0872280	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos8_1	TMPH_1			-61.2	-1761.3767786	-1068.9619145	-2421.2747739	-409.0872280	0.0	0.0	1.1	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1			-55.1	-1761.3767786	-1068.9619145	-2421.2724629	-409.0872280	0.0	0.0	7.2	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_1	TMPH_1			-54.8	-1761.3767786	-1068.9619145	-2421.2723452	-409.0872280	0.0	0.0	7.5	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos5_1	TMPH_1			-52.9	-1761.3767786	-1068.9619145	-2421.2716234	-409.0872280	0.0	0.0	9.4	0.0
0	0	0	0	MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap	TMPH_1		reaction32	-26.7	-1976.3964261	-2648.1694763	-4215.4859972	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_b	TMPH_1		reaction33	-19.5	-1976.3964261	-2596.3552027	-4163.6689845	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos3	TMPH_1		reaction34	-45.0	-1976.3964261	-2596.3552027	-5730.9850649	-409.0900593	0.0	0.0	0.0	0.0
0	0	0	0	1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_7	TMPH_1		reaction37	-70.7	-2068.6686058	-2596.3552027	-5915.5392259	-409.0900593	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap	TMPH_1			-26.7	-1976.3964261	-2648.1694763	-4215.4859972	-409.0900593	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_5ZnCl_d5_mol6_aae	TMPH_1			-21.0	-1976.3964261	-2648.1694763	-4215.4838282	-409.0900593	0.0	0.0	5.7	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_2ZnCl_d2_mol6_aaq	TMPH_1			-15.0	-1976.3964261	-2648.1694763	-4215.4815715	-409.0900593	0.0	0.0	11.6	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_8ZnCl_d8_mol6_aac2	TMPH_1			-11.0	-1976.3964261	-2648.1694763	-4215.4800477	-409.0900593	0.0	0.0	15.6	0.0
				MgCl2_mol6_aac	TMPZnCl	MgCl2_8ZnCl_d8_mol6_aac23	TMPH_1			4.3	-1976.3964261	-2648.1694763	-4215.4742085	-409.0900593	0.0	0.0	31.0	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap2	TMPH_1			13.5	-1976.3964261	-2648.1694763	-4215.4707095	-409.0900593	0.0	0.0	40.1	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_b	TMPH_1			-19.5	-1976.3964261	-2596.3552027	-4163.6689845	-409.0900593	0.0	0.0	0.0	0.0

				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_a	TMPH_1			-18.8	-1976.3964261	-2596.3552027	-4163.6687193	-409.0900593	0.0	0.0	0.7	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_3TMPZn_d3_mol6_a	TMPH_1			-18.4	-1976.3964261	-2596.3552027	-4163.6685758	-409.0900593	0.0	0.0	1.1	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_3TMPZn_d3_mol6_b	TMPH_1			-17.9	-1976.3964261	-2596.3552027	-4163.6683746	-409.0900593	0.0	0.0	1.6	0.0
				MgCl2_mol6_aac	TMP2Zn_1	MgCl2_3TMPZn_d3_mol6_a	TMPH_1			-5.1	-1976.3964261	-2596.3552027	-4163.6634983	-409.0900593	0.0	0.0	14.4	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_2TMPZn_d2_mol6_c	TMPH_1			-0.6	-1976.3964261	-2596.3552027	-4163.6617870	-409.0900593	0.0	0.0	18.9	0.0
				MgCl2_mol6_aac	TMP2Zn_1	MgCl2_5TMPZn_d5_mol6_aa	TMPH_1			-0.4	-1976.3964261	-2596.3552027	-4163.6617381	-409.0900593	0.0	0.0	19.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_2TMPZn_d2_mol6_b	TMPH_1			8.5	-1976.3964261	-2596.3552027	-4163.6583396	-409.0900593	0.0	0.0	27.9	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_8TMPZn_d8_mol6_a2	TMPH_1			13.1	-1976.3964261	-2596.3552027	-4163.6565679	-409.0900593	0.0	0.0	32.6	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos3	TMPH_1			-45.0	-1976.3964261	-2596.3552027	-5730.9850649	-409.0900593	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2_27	TMPH_1			-43.3	-1976.3964261	-2596.3552027	-5730.9844212	-409.0900593	0.0	0.0	1.7	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5	TMPH_1			-39.0	-1976.3964261	-2596.3552027	-5730.9827748	-409.0900593	0.0	0.0	6.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2	TMPH_1			-16.7	-1976.3964261	-2596.3552027	-5730.9743038	-409.0900593	0.0	0.0	28.3	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5_29	TMPH_1			-7.7	-1976.3964261	-2596.3552027	-5730.9708620	-409.0900593	0.0	0.0	37.3	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5_31	TMPH_1			7.6	-1976.3964261	-2596.3552027	-5730.9650305	-409.0900593	0.0	0.0	52.6	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos8	TMPH_1			9.6	-1976.3964261	-2596.3552027	-5730.9642970	-409.0900593	0.0	0.0	54.5	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos8_1	TMPH_1			15.9	-1976.3964261	-2596.3552027	-5730.9618713	-409.0900593	0.0	0.0	60.9	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_7	TMPH_1			-70.7	-2068.6686058	-2596.3552027	-5915.5392259	-409.0900593	0.0	0.0	0.0	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2	TMPH_1			-55.9	-2068.6686058	-2596.3552027	-5915.5335796	-409.0900593	0.0	0.0	14.8	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos5	TMPH_1			-35.1	-2068.6686058	-2596.3552027	-5915.5256702	-409.0900593	0.0	0.0	35.6	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_9	TMPH_1			-7.2	-2068.6686058	-2596.3552027	-5915.5150536	-409.0900593	0.0	0.0	63.5	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos8	TMPH_1			2.9	-2068.6686058	-2596.3552027	-5915.5111726	-409.0900593	0.0	0.0	73.7	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_5	TMPH_1			17.4	-2068.6686058	-2596.3552027	-5915.5056715	-409.0900593	0.0	0.0	88.1	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_8	TMPH_1			48.1	-2068.6686058	-2596.3552027	-5915.4939915	-409.0900593	0.0	0.0	118.8	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos5_10	TMPH_1			82.6	-2068.6686058	-2596.3552027	-5915.4808502	-409.0900593	0.0	0.0	153.3	0.0

Table TT12. The calculated for reaction free energy values at the CPCM(**THF**)/B3LYP-D3/6-311++G(2df,2p)//B3LYP-D3/6-31++G(2d,p) level of theory (T = $T_{experimental}$).
"E1 and E2" – educt 1 and educt 2, "P1 and P2" – product 1 and product 2.

charge				filename						ΔG^{sol}	G^{sol}				ΔG^{sol}			
E1	E2	P1	P2	E1	E2	P1	P2			kJ/mol	E1	E2	P1	P2	E1	E2	P1	P2
0	0	0	0	mol6	TMPMgCl	3_MgCl_d3_mol6_aad	TMPH_1		reaction1	-1.5	-855.5797856	-1068.9540091	-1515.4502223	-409.0841431	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMPZnCl	3_ZnCl_d3_mol6_aac	TMPH_1		reaction2	-16.2	-855.5847652	-2648.1661160	-3094.6673461	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	mol6	TMP2Zn_1	5_TMPZn_d5_mol6_a	TMPH_1		reaction3	-13.7	-855.5847652	-2596.3535754	-3042.8538706	-409.0897049	0.0	0.0	0.5	0.0
0	0	0	0	mol6	TMP2Zn_1	mol14_pos5	TMPH_1		reaction4	-26.7	-855.5847652	-2596.3535754	-3489.3538594	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMPZnCl	5_ZnCl_d5_mol7e	TMPH_1		reaction5	-14.3	-947.8613888	-2648.1661160	-3186.9432279	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_36	TMPH_1		reaction6	-13.8	-947.8613888	-2596.3535754	-3135.1305286	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	mol7e	TMP2Zn_1	mol15_pos5	TMPH_1		reaction7	-29.2	-947.8613888	-2596.3535754	-3673.9080747	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	mol16e_1	TMPMgCl	mol17_pos5_2	TMPH_1		reaction8	-10.0	-1293.4670033	-1068.9572254	-1953.3411666	-409.0868736	0.5	0.0	0.0	0.0
				mol6	TMPMgCl	3_MgCl_d3_mol6_aad	TMPH_1			-1.5	-855.5797856	-1068.9540091	-1515.4502223	-409.0841431	0.0	0.0	0.0	0.0
				mol6	TMPMgCl	3_MgCl_d3_mol6_aaq	TMPH_1			-1.5	-855.5797856	-1068.9540091	-1515.4502170	-409.0841431	0.0	0.0	0.0	0.0
				mol6	TMPMgCl	5_MgCl_d5_mol6_aaa	TMPH_1			10.0	-855.5797856	-1068.9540091	-1515.4458470	-409.0841431	0.0	0.0	11.5	0.0
				mol6	TMPMgCl	8_MgCl_d8_mol6_aar	TMPH_1			19.6	-855.5797856	-1068.9540091	-1515.4422009	-409.0841431	0.0	0.0	21.1	0.0
				mol6	TMPMgCl	2_MgCl_d2_mol6_aaa	TMPH_1			39.4	-855.5797856	-1068.9540091	-1515.4346432	-409.0841431	0.0	0.0	40.9	0.0
				mol6	TMPZnCl	3_ZnCl_d3_mol6_aac	TMPH_1			-16.2	-855.5847652	-2648.1661160	-3094.6673461	-409.0897049	0.0	0.0	0.0	0.0
				mol6	TMPZnCl	3_ZnCl_d3_mol6_aax	TMPH_1			-16.2	-855.5847652	-2648.1661160	-3094.6673417	-409.0897049	0.0	0.0	0.0	0.0
				mol6	TMPZnCl	3_ZnCl_d3_mol6_aap	TMPH_1			-16.2	-855.5847652	-2648.1661160	-3094.6673407	-409.0897049	0.0	0.0	0.0	0.0
				mol6	TMPZnCl	5_ZnCl_d5_mol6_aae	TMPH_1			-14.0	-855.5847652	-2648.1661160	-3094.6664962	-409.0897049	0.0	0.0	2.2	0.0
				mol6	TMPZnCl	8_ZnCl_d8_mol6_aac	TMPH_1			-2.8	-855.5847652	-2648.1661160	-3094.6622318	-409.0897049	0.0	0.0	13.4	0.0
				mol6	TMPZnCl	2_ZnCl_d2_mol6_aaq	TMPH_1			1.8	-855.5847652	-2648.1661160	-3094.6604824	-409.0897049	0.0	0.0	18.0	0.0
				mol6	TMP2Zn_1	5_TMPZn_d5_mol6_a	TMPH_1			-13.3	-855.5847652	-2596.3535754	-3042.8536920	-409.0897049	0.0	0.0	0.5	0.0
				mol6	TMP2Zn_1	5_TMPZn_d5_mol6_b	TMPH_1			-13.7	-855.5847652	-2596.3535754	-3042.8538706	-409.0897049	0.0	0.0	0.0	0.0
				mol6	TMP2Zn_1	3_TMPZn_d3_mol6_b	TMPH_1			-10.2	-855.5847652	-2596.3535754	-3042.8525100	-409.0897049	0.0	0.0	3.6	0.0
				mol6	TMP2Zn_1	8_TMPZn_d8_mol6_a	TMPH_1			6.3	-855.5847652	-2596.3535754	-3042.8462379	-409.0897049	0.0	0.0	20.0	0.0
				mol6	TMP2Zn_1	2_TMPZn_d2_mol6_a	TMPH_1			12.5	-855.5847652	-2596.3535754	-3042.8438617	-409.0897049	0.0	0.0	26.3	0.0
				mol6	TMP2Zn_1	mol14_pos5	TMPH_1			-26.7	-855.5847652	-2596.3535754	-3489.3538594	-409.0897049	0.0	0.0	0.0	0.0
				mol6	TMP2Zn_1	mol14_pos3	TMPH_1			-23.1	-855.5847652	-2596.3535754	-3489.3524997	-409.0897049	0.0	0.0	3.6	0.0
				mol6	TMP2Zn_1	mol14_pos8	TMPH_1			5.5	-855.5847652	-2596.3535754	-3489.3416096	-409.0897049	0.0	0.0	32.2	0.0
				mol6	TMP2Zn_1	mol14_pos2	TMPH_1			14.9	-855.5847652	-2596.3535754	-3489.3380114	-409.0897049	0.0	0.0	41.6	0.0
				mol7e	TMPZnCl	5_ZnCl_d5_mol7e	TMPH_1			-14.3	-947.8613888	-2648.1661160	-3186.9432279	-409.0897049	0.0	0.0	0.0	0.0
				mol7e	TMPZnCl	2_ZnCl_d2_mol7e	TMPH_1			-7.7	-947.8613888	-2648.1661160	-3186.9407477	-409.0897049	0.0	0.0	6.5	0.0
				mol7e	TMPZnCl	8_ZnCl_d8_mol7e	TMPH_1			-6.2	-947.8613888	-2648.1661160	-3186.9401746	-409.0897049	0.0	0.0	8.0	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_36	TMPH_1			-13.8	-947.8613888	-2596.3535754	-3135.1305286	-409.0897049	0.0	0.0	0.0	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e	TMPH_1			-13.8	-947.8613888	-2596.3535754	-3135.1305078	-409.0897049	0.0	0.0	0.1	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_40	TMPH_1			-2.4	-947.8613888	-2596.3535754	-3135.1261629	-409.0897049	0.0	0.0	11.5	0.0
				mol7e	TMP2Zn_1	2_TMPZn_d2_mol7e	TMPH_1			-1.3	-947.8613888	-2596.3535754	-3135.125753	-409.0897049	0.0	0.0	12.5	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_38	TMPH_1			2.1	-947.8613888	-2596.3535754	-3135.124442	-409.0897049	0.0	0.0	16.0	0.0
				mol7e	TMP2Zn_1	8_TMPZn_d8_mol7e	TMPH_1			0.5	-947.8613888	-2596.3535754	-3135.125066	-409.0897049	0.0	0.0	14.3	0.0
				mol7e	TMP2Zn_1	5_TMPZn_d5_mol7e_1	TMPH_1			4.3	-947.8613888	-2596.3535754	-3135.123615	-409.0897049	0.0	0.0	18.2	0.0
				mol7e	TMP2Zn_1	mol15_pos5	TMPH_1			-29.2	-947.8613888	-2596.3535754	-3673.9080747	-409.0897049	0.0	0.0	0.0	0.0
				mol7e	TMP2Zn_1	mol15_pos2	TMPH_1			-8.1	-947.8613888	-2596.3535754	-3673.9000425	-409.0897049	0.0	0.0	21.1	0.0
				mol7e	TMP2Zn_1	mol15_pos8	TMPH_1			-4.4	-947.8613888	-2596.3535754	-3673.8986125	-409.0897049	0.0	0.0	24.8	0.0
				mol16e_1	TMPMgCl	mol17_pos5_2	TMPH_1			-10.0	-1293.4670033	-1068.9572254	-1953.3411666	-409.0868736	0.5	0.0	0.0	0.0
				mol16e_1	TMPMgCl	mol17_pos5_1	TMPH_1			-9.9	-1293.4670033	-1068.9572254	-1953.3411280	-409.0868736	0.5	0.0	0.1	0.0
				mol16e_1	TMPMgCl	mol17_pos8_2	TMPH_1			19.3	-1293.4670033	-1068.9572254	-1953.3299881	-409.0868736	0.5	0.0	29.3	0.0
0	0	0	0	1_LiCl_mol6_1	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1		reaction11	-45.8	-1323.4874591	-1068.9540091	-1983.3747766	-409.0841431	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1		reaction12	-31.7	-1323.4934114	-2648.1661160	-3562.5818963	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1		reaction13	-14.5	-1323.4934114	-2596.3535754	-3510.7628194	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1		reaction14	-48.2	-1323.4934114	-2596.3535754	-4425.1793560	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1		reaction15	-45.3	-1415.7675211	-2648.1661160	-3654.8611981	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1		reaction16	-16.2	-1415.7675211	-2596.3535754	-3603.0375463	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1		reaction17	-77.9	-1415.7675211	-2596.3535754	-4609.7388842	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1		reaction18	-58.1	-1761.3705301	-1068.9572254	-2421.2630031	-409.0868736	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1			-45.8	-1323.4874591	-1068.9540091	-1983.3747766	-409.0841431	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_3MgCl_d3_mol6	TMPH_1			-7.2	-1323.4874591	-1068.9540091	-1983.3600595	-409.0841431	0.0	0.0	38.6	0.0
				1_LiCl_mol6_1	TMPMgCl	1_LiCl_5MgCl_d5_mol6	TMPH_1			7.6	-1323.4874591	-1068.9540091	-1983.3544372	-409.0841431	0.0	0.0	53.4	0.0

				1_LiCl_mol6_1	TMPMgCl	1_LiCl_2MgCl_d2_mol6	TMPH_1			17.2	-1323.4874591	-1068.9540091	-1983.3507799	-409.0841431	0.0	0.0	63.0	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1			-31.7	-1323.4934114	-2648.1661160	-3562.5818963	-409.0897049	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1			-30.8	-1323.4934114	-2648.1661160	-3562.5815352	-409.0897049	0.0	0.0	0.9	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-18.4	-1323.4934114	-2648.1661160	-3562.5768378	-409.0897049	0.0	0.0	13.3	0.0
				1_LiCl_mol6_1	TMPZnCl	1_LiCl_5ZnCl_d5_mol6_aae	TMPH_1			1.2	-1323.4934114	-2648.1661160	-3562.5693800	-409.0897049	0.0	0.0	32.9	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1			-14.5	-1323.4934114	-2596.3535754	-3510.7628194	-409.0897049	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_b	TMPH_1			-12.7	-1323.4934114	-2596.3535754	-3510.7621323	-409.0897049	0.0	0.0	1.8	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_a	TMPH_1			-11.5	-1323.4934114	-2596.3535754	-3510.7616534	-409.0897049	0.0	0.0	3.1	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_b	TMPH_1			-10.8	-1323.4934114	-2596.3535754	-3510.7614097	-409.0897049	0.0	0.0	3.7	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol6_c	TMPH_1			-7.0	-1323.4934114	-2596.3535754	-3510.7599461	-409.0897049	0.0	0.0	7.5	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol6_c	TMPH_1			1.7	-1323.4934114	-2596.3535754	-3510.7566274	-409.0897049	0.0	0.0	16.3	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1			-48.2	-1323.4934114	-2596.3535754	-4425.1793560	-409.0897049	0.0	0.0	0.0	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos8	TMPH_1			-46.7	-1323.4934114	-2596.3535754	-4425.1787852	-409.0897049	0.0	0.0	1.5	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2_8	TMPH_1			-36.8	-1323.4934114	-2596.3535754	-4425.1750000	-409.0897049	0.0	0.0	11.4	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos2	TMPH_1			-34.5	-1323.4934114	-2596.3535754	-4425.1741428	-409.0897049	0.0	0.0	13.7	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1			-26.8	-1323.4934114	-2596.3535754	-4425.1712064	-409.0897049	0.0	0.0	21.4	0.0
				1_LiCl_mol6_1	TMP2Zn_1	1_LiCl_mol14_pos5	TMPH_1			-26.0	-1323.4934114	-2596.3535754	-4425.1708972	-409.0897049	0.0	0.0	22.2	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1			-45.3	-1415.7675211	-2648.1661160	-3654.8611981	-409.0897049	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_8_ZnCl_d8_mol7e	TMPH_1			-35.6	-1415.7675211	-2648.1661160	-3654.8574732	-409.0897049	0.0	0.0	9.8	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_5_ZnCl_d5_mol7e	TMPH_1			-15.4	-1415.7675211	-2648.1661160	-3654.8498060	-409.0897049	0.0	0.0	29.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-16.2	-1415.7675211	-2596.3535754	-3603.0375463	-409.0897049	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e	TMPH_1			-15.8	-1415.7675211	-2596.3535754	-3603.0374059	-409.0897049	0.0	0.0	0.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e	TMPH_1			-15.8	-1415.7675211	-2596.3535754	-3603.0373973	-409.0897049	0.0	0.0	0.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_31	TMPH_1			-8.1	-1415.7675211	-2596.3535754	-3603.0344814	-409.0897049	0.0	0.0	8.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_26	TMPH_1			-7.8	-1415.7675211	-2596.3535754	-3603.0343516	-409.0897049	0.0	0.0	8.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-4.8	-1415.7675211	-2596.3535754	-3603.0332274	-409.0897049	0.0	0.0	11.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-3.4	-1415.7675211	-2596.3535754	-3603.0326870	-409.0897049	0.0	0.0	12.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_38	TMPH_1			0.9	-1415.7675211	-2596.3535754	-3603.0310626	-409.0897049	0.0	0.0	17.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_1	TMPH_1			1.4	-1415.7675211	-2596.3535754	-3603.0308558	-409.0897049	0.0	0.0	17.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol7e_20	TMPH_1			2.3	-1415.7675211	-2596.3535754	-3603.0305200	-409.0897049	0.0	0.0	18.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1			-77.9	-1415.7675211	-2596.3535754	-4609.7388842	-409.0897049	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_17	TMPH_1			-69.3	-1415.7675211	-2596.3535754	-4609.7355987	-409.0897049	0.0	0.0	8.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1			-67.1	-1415.7675211	-2596.3535754	-4609.7347553	-409.0897049	0.0	0.0	10.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8	TMPH_1			-62.1	-1415.7675211	-2596.3535754	-4609.7328651	-409.0897049	0.0	0.0	15.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_12	TMPH_1			-55.6	-1415.7675211	-2596.3535754	-4609.7303961	-409.0897049	0.0	0.0	22.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_13	TMPH_1			-50.2	-1415.7675211	-2596.3535754	-4609.7283395	-409.0897049	0.0	0.0	27.7	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos5	TMPH_1			-31.3	-1415.7675211	-2596.3535754	-4609.7211233	-409.0897049	0.0	0.0	46.6	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_2	TMPH_1			-58.1	-1761.3705301	-1068.9572254	-2421.2630031	-409.0868736	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos8_1	TMPH_1			-57.6	-1761.3705301	-1068.9572254	-2421.2628052	-409.0868736	0.0	0.0	0.5	0.0
				1_LiCl_mol16e_2	TMPMgCl	1_LiCl_mol17_pos5_1	TMPH_1			-13.5	-1761.3705301	-1068.9572254	-2421.2460049	-409.0868736	0.0	0.0	44.6	0.0
0	0	0	0	LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6	TMPH_1		reaction21	-47.0	-1323.4872605	-1068.9540091	-1983.3750157	-409.0841431	0.0	0.0	0.0	0.0
0	0	0	0	LiCl_mol6_aan	TMPZnCl	LiCl_8ZnCl_d8_mol6_aac2	TMPH_1		reaction22	-33.0	-1323.4932126	-2648.1661160	-3562.5821902	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_a	TMPH_1		reaction23	-24.8	-1323.4932126	-2596.3535754	-3510.7665292	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8	TMPH_1		reaction24	-64.6	-1323.4932126	-2596.3535754	-4425.1851790	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1		reaction25	-45.3	-1415.7675211	-2648.1661160	-3654.8611981	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1		reaction26	-16.2	-1415.7675211	-2596.3535754	-3603.0375463	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1		reaction27	-77.9	-1415.7675211	-2596.3535754	-4609.7388842	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos8_2	TMPH_1		reaction28	-65.1	-1761.3705301	-1068.9572254	-2421.2656716	-409.0868736	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6	TMPH_1			-47.0	-1323.4872605	-1068.9540091	-1983.3750157	-409.0841431	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_8MgCl_d8_mol6	TMPH_1			-46.3	-1323.4872605	-1068.9540091	-1983.3747766	-409.0841431	0.0	0.0	0.6	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d3_mol6	TMPH_1			-42.4	-1323.4872605	-1068.9540091	-1983.3732608	-409.0841431	0.0	0.0	4.6	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d5_mol6_1	TMPH_1			-32.1	-1323.4872605	-1068.9540091	-1983.3693651	-409.0841431	0.0	0.0	14.8	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d8_mol6_1	TMPH_1			-24.0	-1323.4872605	-1068.9540091	-1983.3662559	-409.0841431	0.0	0.0	23.0	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d8_mol6	TMPH_1			-13.1	-1323.4872605	-1068.9540091	-1983.3621014	-409.0841431	0.0	0.0	33.9	0.0
				LiCl_mol6_aan	TMPMgCl	1_LiCl_3MgCl_d3_mol6	TMPH_1			-7.7	-1323.4872605	-1068.9540091	-1983.3600595	-409.0841431	0.0	0.0	39.3	0.0
				LiCl_mol6_aan	TMPMgCl	MgClLiCl_d2_mol6	TMPH_1			3.7	-1323.4872605	-1068.9540091	-1983.3557106	-409.0841431	0.0	0.0	50.7	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_8ZnCl_d8_mol6_aac2	TMPH_1			-33.0	-1323.4932126	-2648.1661160	-3562.5821902	-409.0897049	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMPZnCl	1_LiCl_2ZnCl_d2_mol6_aaq	TMPH_1			-32.2	-1323.4932126	-2648.1661160	-3562.5818963	-409.0897049	0.0	0.0	0.8	0.0
				LiCl_mol6_aan	TMPZnCl	1_LiCl_8ZnCl_d8_mol6_aac	TMPH_1			-31.3	-1323.4932126	-2648.1661160	-3562.5815352	-409.0897049	0.0	0.0	1.7	0.0
				LiCl_mol6_aan	TMPZnCl	LiCl_3ZnCl_d3_mol6_aap	TMPH_1			-30.1	-1323.4932126	-2648.1661160	-3562.5810755	-409.0897049	0.0	0.0	2.9	0.0

				LiCl_mol6_aan	TMPZnCl	LiCl_5ZnCl_d5_mol6_aae	TMPH_1			-30.1	-1323.4932126	-2648.1661160	-3562.5810709	-409.0897049	0.0	0.0	2.9	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_a	TMPH_1			-24.8	-1323.4932126	-2596.3535754	-3510.7665292	-409.0897049	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_5TMPZn_d5_mol6_aa	TMPH_1			-24.2	-1323.4932126	-2596.3535754	-3510.7662824	-409.0897049	0.0	0.0	0.6	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_3TMPZn_d3_mol6_b	TMPH_1			-20.0	-1323.4932126	-2596.3535754	-3510.7647174	-409.0897049	0.0	0.0	4.8	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_a	TMPH_1			-15.1	-1323.4932126	-2596.3535754	-3510.7628194	-409.0897049	0.0	0.0	9.7	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol6_b	TMPH_1			-13.3	-1323.4932126	-2596.3535754	-3510.7621323	-409.0897049	0.0	0.0	11.5	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_a	TMPH_1			-12.0	-1323.4932126	-2596.3535754	-3510.7616534	-409.0897049	0.0	0.0	12.8	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_3TMPZn_d3_mol6_b	TMPH_1			-11.4	-1323.4932126	-2596.3535754	-3510.7614097	-409.0897049	0.0	0.0	13.4	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol6_c	TMPH_1			-7.5	-1323.4932126	-2596.3535754	-3510.7599461	-409.0897049	0.0	0.0	17.3	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_8TMPZn_d8_mol6_a	TMPH_1			-1.4	-1323.4932126	-2596.3535754	-3510.7576194	-409.0897049	0.0	0.0	23.4	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8	TMPH_1			-64.6	-1323.4932126	-2596.3535754	-4425.1851790	-409.0897049	0.0	0.0	0.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	LiCl_mol14_pos8_38	TMPH_1			-64.1	-1323.4932126	-2596.3535754	-4425.1849874	-409.0897049	0.0	0.0	0.5	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2_5	TMPH_1			-49.3	-1323.4932126	-2596.3535754	-4425.1793560	-409.0897049	0.0	0.0	15.3	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos8	TMPH_1			-47.8	-1323.4932126	-2596.3535754	-4425.1787852	-409.0897049	0.0	0.0	16.8	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2_8	TMPH_1			-37.8	-1323.4932126	-2596.3535754	-4425.1750000	-409.0897049	0.0	0.0	26.7	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos2	TMPH_1			-35.6	-1323.4932126	-2596.3535754	-4425.1741428	-409.0897049	0.0	0.0	29.0	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos3	TMPH_1			-27.9	-1323.4932126	-2596.3535754	-4425.1712064	-409.0897049	0.0	0.0	36.7	0.0
				LiCl_mol6_aan	TMP2Zn_1	1_LiCl_mol14_pos5	TMPH_1			-27.1	-1323.4932126	-2596.3535754	-4425.1708972	-409.0897049	0.0	0.0	37.5	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_2_ZnCl_d2_mol7e	TMPH_1			-45.3	-1415.7675211	-2648.1661160	-3654.8611981	-409.0897049	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_8_ZnCl_d8_mol7e	TMPH_1			-35.6	-1415.7675211	-2648.1661160	-3654.8574732	-409.0897049	0.0	0.0	9.8	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_5_ZnCl_d5_mol7e	TMPH_1			-32.9	-1415.7675211	-2648.1661160	-3654.8564489	-409.0897049	0.0	0.0	12.5	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_2_ZnCl_d2_mol7e	TMPH_1			-25.7	-1415.7675211	-2648.1661160	-3654.8537045	-409.0897049	0.0	0.0	19.7	0.0
				1_LiCl_mol7e	TMPZnCl	LiCl_8_ZnCl_d8_mol7e	TMPH_1			-23.7	-1415.7675211	-2648.1661160	-3654.8529712	-409.0897049	0.0	0.0	21.6	0.0
				1_LiCl_mol7e	TMPZnCl	1_LiCl_5_ZnCl_d5_mol7e	TMPH_1			-15.4	-1415.7675211	-2648.1661160	-3654.8498060	-409.0897049	0.0	0.0	29.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-16.2	-1415.7675211	-2596.3535754	-3603.0375463	-409.0897049	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e	TMPH_1			-15.8	-1415.7675211	-2596.3535754	-3603.0374059	-409.0897049	0.0	0.0	0.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e	TMPH_1			-15.8	-1415.7675211	-2596.3535754	-3603.0373973	-409.0897049	0.0	0.0	0.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_2TMPZn_d2_mol7e	TMPH_1			-14.8	-1415.7675211	-2596.3535754	-3603.0370329	-409.0897049	0.0	0.0	1.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-13.4	-1415.7675211	-2596.3535754	-3603.0364894	-409.0897049	0.0	0.0	2.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_31	TMPH_1			-8.1	-1415.7675211	-2596.3535754	-3603.0344814	-409.0897049	0.0	0.0	8.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_26	TMPH_1			-7.8	-1415.7675211	-2596.3535754	-3603.0343516	-409.0897049	0.0	0.0	8.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-4.8	-1415.7675211	-2596.3535754	-3603.0332274	-409.0897049	0.0	0.0	11.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_36	TMPH_1			-4.7	-1415.7675211	-2596.3535754	-3603.0331712	-409.0897049	0.0	0.0	11.5	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_40	TMPH_1			-3.4	-1415.7675211	-2596.3535754	-3603.0326870	-409.0897049	0.0	0.0	12.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_1	TMPH_1			-3.3	-1415.7675211	-2596.3535754	-3603.0326468	-409.0897049	0.0	0.0	12.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_5TMPZn_d5_mol7e_38	TMPH_1			-1.3	-1415.7675211	-2596.3535754	-3603.0318848	-409.0897049	0.0	0.0	14.9	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_2TMPZn_d2_mol7e_28	TMPH_1			-0.6	-1415.7675211	-2596.3535754	-3603.0316027	-409.0897049	0.0	0.0	15.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_38	TMPH_1			0.9	-1415.7675211	-2596.3535754	-3603.0310626	-409.0897049	0.0	0.0	17.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_5TMPZn_d5_mol7e_1	TMPH_1			1.4	-1415.7675211	-2596.3535754	-3603.0308558	-409.0897049	0.0	0.0	17.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_8TMPZn_d8_mol7e_20	TMPH_1			2.3	-1415.7675211	-2596.3535754	-3603.0305200	-409.0897049	0.0	0.0	18.4	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8_19	TMPH_1			-77.9	-1415.7675211	-2596.3535754	-4609.7388842	-409.0897049	0.0	0.0	0.0	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_mol15_pos8	TMPH_1			-72.3	-1415.7675211	-2596.3535754	-4609.7367583	-409.0897049	0.0	0.0	5.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_17	TMPH_1			-69.3	-1415.7675211	-2596.3535754	-4609.7355987	-409.0897049	0.0	0.0	8.6	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_15	TMPH_1			-67.1	-1415.7675211	-2596.3535754	-4609.7347553	-409.0897049	0.0	0.0	10.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos8	TMPH_1			-62.1	-1415.7675211	-2596.3535754	-4609.7328651	-409.0897049	0.0	0.0	15.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_12	TMPH_1			-55.6	-1415.7675211	-2596.3535754	-4609.7303961	-409.0897049	0.0	0.0	22.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos2_13	TMPH_1			-50.2	-1415.7675211	-2596.3535754	-4609.7283395	-409.0897049	0.0	0.0	27.7	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_mol15_pos2_17	TMPH_1			-37.6	-1415.7675211	-2596.3535754	-4609.7235174	-409.0897049	0.0	0.0	40.3	0.0
				1_LiCl_mol7e	TMP2Zn_1	LiCl_mol15_pos2_15	TMPH_1			-37.1	-1415.7675211	-2596.3535754	-4609.7233302	-409.0897049	0.0	0.0	40.8	0.0
				1_LiCl_mol7e	TMP2Zn_1	1_LiCl_mol15_pos5	TMPH_1			-31.3	-1415.7675211	-2596.3535754	-4609.7211233	-409.0897049	0.0	0.0	46.6	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos8_2	TMPH_1			-65.1	-1761.3705301	-1068.9572254	-2421.2656716	-409.0868736	0.0	0.0	0.0	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos8_1	TMPH_1			-64.4	-1761.3705301	-1068.9572254	-2421.2653928	-409.0868736	0.0	0.0	0.7	0.0
				1_LiCl_mol16e_2	TMPMgCl	LiCl_mol17_pos5_1	TMPH_1			-63.0	-1761.3705301	-1068.9572254	-2421.2648661	-409.0868736	0.0	0.0	2.1	0.0
0	0	0	0	MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap	TMPH_1		reaction32	-19.7	-1976.3904322	-2648.1661160	-4215.4743404	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_b	TMPH_1		reaction33	-16.5	-1976.3904322	-2596.3535754	-4163.6606032	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2_27	TMPH_1		reaction34	-51.1	-1976.3904322	-2596.3535754	-5730.9744961	-409.0897049	0.0	0.0	0.0	0.0
0	0	0	0	1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_7	TMPH_1		reaction37	-77.8	-2068.6621074	-2596.3535754	-5915.5280204	-409.0897049	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_3ZnCl_d3_mol6_aap	TMPH_1			-19.7	-1976.3904322	-2648.1661160	-4215.4743404	-409.0897049	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_2ZnCl_d2_mol6_aaq	TMPH_1			-15.9	-1976.3904322	-2648.1661160	-4215.4729017	-409.0897049	0.0	0.0	3.8	0.0
				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_5ZnCl_d5_mol6_aae	TMPH_1			-14.8	-1976.3904322	-2648.1661160	-4215.4724736	-409.0897049	0.0	0.0	4.9	0.0

				MgCl2_mol6_aac	TMPZnCl	1_MgCl2_8ZnCl_d8_mol6_aac2	TMPH_1			-10.7	-1976.3904322	-2648.1661160	-4215.4709297	-409.0897049	0.0	0.0	9.0	0.0
				MgCl2_mol6_aac	TMPZnCl	MgCl2_8ZnCl_d8_mol6_aac23	TMPH_1			5.1	-1976.3904322	-2648.1661160	-4215.4648921	-409.0897049	0.0	0.0	24.8	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_b	TMPH_1			-16.5	-1976.3904322	-2596.3535754	-4163.6606032	-409.0897049	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_5TMPZn_d5_mol6_a	TMPH_1			-16.1	-1976.3904322	-2596.3535754	-4163.6604188	-409.0897049	0.0	0.0	0.5	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_3TMPZn_d3_mol6_a	TMPH_1			-15.4	-1976.3904322	-2596.3535754	-4163.6601613	-409.0897049	0.0	0.0	1.2	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_3TMPZn_d3_mol6_b	TMPH_1			-14.9	-1976.3904322	-2596.3535754	-4163.6599717	-409.0897049	0.0	0.0	1.7	0.0
				MgCl2_mol6_aac	TMP2Zn_1	MgCl2_3TMPZn_d3_mol6_a	TMPH_1			-9.4	-1976.3904322	-2596.3535754	-4163.6579015	-409.0897049	0.0	0.0	7.1	0.0
				MgCl2_mol6_aac	TMP2Zn_1	MgCl2_5TMPZn_d5_mol6_aa	TMPH_1			-5.2	-1976.3904322	-2596.3535754	-4163.6562712	-409.0897049	0.0	0.0	11.4	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_2TMPZn_d2_mol6_c	TMPH_1			-2.5	-1976.3904322	-2596.3535754	-4163.6552594	-409.0897049	0.0	0.0	14.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_2TMPZn_d2_mol6_b	TMPH_1			6.0	-1976.3904322	-2596.3535754	-4163.6520280	-409.0897049	0.0	0.0	22.5	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_8TMPZn_d8_mol6_a2	TMPH_1			11.0	-1976.3904322	-2596.3535754	-4163.6501179	-409.0897049	0.0	0.0	27.5	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2_27	TMPH_1			-51.1	-1976.3904322	-2596.3535754	-5730.9744961	-409.0897049	0.0	0.0	0.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos3	TMPH_1			-32.3	-1976.3904322	-2596.3535754	-5730.9673478	-409.0897049	0.0	0.0	18.8	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5	TMPH_1			-28.9	-1976.3904322	-2596.3535754	-5730.9660501	-409.0897049	0.0	0.0	22.2	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos2	TMPH_1			-22.1	-1976.3904322	-2596.3535754	-5730.9634570	-409.0897049	0.0	0.0	29.0	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos8	TMPH_1			-4.2	-1976.3904322	-2596.3535754	-5730.9566256	-409.0897049	0.0	0.0	46.9	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5_29	TMPH_1			-1.4	-1976.3904322	-2596.3535754	-5730.9555538	-409.0897049	0.0	0.0	49.7	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos8_1	TMPH_1			8.7	-1976.3904322	-2596.3535754	-5730.9517140	-409.0897049	0.0	0.0	59.8	0.0
				MgCl2_mol6_aac	TMP2Zn_1	1_MgCl2_mol14_pos5_31	TMPH_1			19.2	-1976.3904322	-2596.3535754	-5730.9477235	-409.0897049	0.0	0.0	70.3	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_7	TMPH_1			-77.8	-2068.6621074	-2596.3535754	-5915.5280204	-409.0897049	0.0	0.0	0.0	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2	TMPH_1			-60.0	-2068.6621074	-2596.3535754	-5915.5212210	-409.0897049	0.0	0.0	17.9	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos5	TMPH_1			-32.4	-2068.6621074	-2596.3535754	-5915.5107372	-409.0897049	0.0	0.0	45.4	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_9	TMPH_1			-21.6	-2068.6621074	-2596.3535754	-5915.5065916	-409.0897049	0.0	0.0	56.3	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos8	TMPH_1			-10.4	-2068.6621074	-2596.3535754	-5915.5023517	-409.0897049	0.0	0.0	67.4	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_5	TMPH_1			5.5	-2068.6621074	-2596.3535754	-5915.4963040	-409.0897049	0.0	0.0	83.3	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos2_8	TMPH_1			38.9	-2068.6621074	-2596.3535754	-5915.4835522	-409.0897049	0.0	0.0	116.8	0.0
				1_MgCl2_mol7e	TMP2Zn_1	1_MgCl2_mol15_pos5_10	TMPH_1			83.6	-2068.6621074	-2596.3535754	-5915.4665253	-409.0897049	0.0	0.0	161.5	0.0

Raw data

Table TT13. The calculated DFT energies.
qh-δH.1 and qh-δG.1 values are obtained with GoodVibes using the quasi-harmonic approximation
"p" – protonated, "d" – deprotonated (Standard for 1 atm and 298 K)

Charge	№ conf.	Filename	(U)B3LYP-D3/6-31++G(2d,p)						CPCM(DMSO)/(U)B3LYP-D3/6-311++G(2df,2p)// (U)B3LYP-D3/6-31++G(2d,p)			
				298.15 K	253.15 K	233.15 K	213.15 K	298.15K			298.15K	298.15K
			$E_{tot\ gas}$	qh-δG.1	qh-δG.1	qh-δG.1	qh-δG.1	1st freq.	$E_{tot\ sol}$ **DMSO**	$E_{tot\ sol}$ **THF**	G_{sol} **DMSO**	G_{sol} **THF**
-1	1	1_C2H6NMgCl_d5_mol6_aab	-1649.9738583	0.1198525	0.1286464	0.1323693	0.1359744	20.76	-1650.2615496	-1650.2516948	-1650.1416971	-1650.1318423
-1	2	1_C2H6NMgCl_d5_mol6_aap	-1649.9730991	0.1200605	0.1288183	0.1325252	0.1361143	22.77	-1650.2612757	-1650.2513078	-1650.1412151	-1650.1312473
-1	3	1_C2H6NMgCl_d3_mol6_aap	-1649.9686966	0.1203637	0.1291279	0.1328378	0.1364299	19.80	-1650.2547147	-1650.2451466	-1650.1343510	-1650.1247828
-1	4	1_C2H6NMgCl_d3_mol6_aab	-1649.9678647	0.1203800	0.1291437	0.1328532	0.1364449	22.28	-1650.2549347	-1650.2452149	-1650.1345547	-1650.1248348
-1	5	1_C2H6NMgCl_d2_mol6_aap	-1649.9524908	0.1192001	0.1280182	0.1317506	0.1353645	9.58	-1650.2413569	-1650.2313920	-1650.1221568	-1650.1121918
-1	6	1_C2H6NMgCl_d8_mol6_aab	-1649.9473411	0.1191127	0.1279117	0.1316340	0.1352366	13.57	-1650.2415644	-1650.2306976	-1650.1224516	-1650.1115848
-1	1	1_C2H6NZnCl_d5_mol6_aab	-3229.0160320	0.1191643	0.1280690	0.1318401	0.1354925	21.28	-3229.4541726	-3229.4449414	-3229.3350082	-3229.3257770
-1	2	1_C2H6NZnCl_d5_mol6_aap	-3229.0145430	0.1190353	0.1279324	0.1317001	0.1353490	19.56	-3229.4539351	-3229.4444670	-3229.3348997	-3229.3254316
-1	3	1_C2H6NZnCl_d3_mol6_aap	-3229.0107397	0.1196205	0.1284991	0.1322584	0.1358989	19.39	-3229.4477995	-3229.4387462	-3229.3281790	-3229.3191256
-1	4	1_C2H6NZnCl_d3_mol6_aab	-3229.0096139	0.1195232	0.1284069	0.1321691	0.1358126	23.64	-3229.4475858	-3229.4383937	-3229.3280625	-3229.3188705
-1	5	1_C2H6NZnCl_d2_mol6_aap	-3228.9941234	0.1188123	0.1277210	0.1314917	0.1351422	10.02	-3229.4347590	-3229.4251467	-3229.3159466	-3229.3063343
-1	6	1_C2H6NZnCl_d2_mol6_aab	-3228.9894499	0.1185285	0.1274235	0.1311887	0.1348342	23.48	-3229.4348534	-3229.4245607	-3229.3163249	-3229.3060321
-1	7	1_C2H6NZnCl_d8_mol6_aab	-3228.9895496	0.1189227	0.1277845	0.1315328	0.1351598	22.57	-3229.4348313	-3229.4244579	-3229.3159086	-3229.3055352
-1	1	1_LiCl_d5_mol6_1	-1322.8029352	0.0472225	0.0543765	0.0574249	0.0603903	30.61	-1323.0537331	-1323.0423523	-1323.0065105	-1322.9951297
-1	2	1_LiCl_d3_mol6_2	-1322.7972624	0.0475656	0.0547193	0.0577677	0.0607331	29.27	-1323.0460935	-1323.0351103	-1322.9985279	-1322.9875446
-1	3	1_LiCl_d8_mol6_2	-1322.7905946	0.0461553	0.0533715	0.0564454	0.0594350	27.77	-1323.0421957	-1323.0309942	-1322.9960403	-1322.9848388
-1	4	1_LiCl_d2_mol6_1	-1322.7882927	0.0472418	0.0543628	0.0573947	0.0603426	30.84	-1323.0357907	-1323.0252317	-1322.9885489	-1322.9779899
-1	1	1_MgCl2_d5_mol6	-1975.6596992	0.0450763	0.0529073	0.0562410	0.0594814	24.94	-1975.9524036	-1975.9414053	-1975.9073272	-1975.8963290
-1	2	1_MgCl2_d8_mol6	-1975.6536951	0.0444269	0.0522958	0.0556438	0.0588968	30.63	-1975.9480534	-1975.9370190	-1975.9036264	-1975.8925920
-1	3	1_MgCl2_d3_mol6	-1975.6541230	0.0453609	0.0531948	0.0565299	0.0597718	21.96	-1975.9458466	-1975.9350687	-1975.9004856	-1975.8897078
-1	4	1_MgCl2_d2_mol6	-1975.6509939	0.0445533	0.0524280	0.0557802	0.0590385	24.65	-1975.9415821	-1975.9312007	-1975.8970287	-1975.8866473
-1	1	1_TMPMgCl_d5_mol6_2	-1924.0252424	0.2912098	0.3017122	0.3060941	0.3102982	22.93	-1924.3676560	-1924.3585624	-1924.0764462	-1924.0673526
-1	2	1_TMPMgCl_d5_mol6_3	-1924.0238530	0.2902117	0.3008220	0.3052514	0.3095028	10.92	-1924.3653469	-1924.3563873	-1924.0751352	-1924.0661755
-1	3	1_TMPMgCl_d5_mol6_1	-1924.0225920	0.2913817	0.3018525	0.3062209	0.3104119	21.52	-1924.3660231	-1924.3567214	-1924.0746413	-1924.0653397
-1	4	1_TMPMgCl_d3_mol6_3	-1924.0173461	0.2902481	0.3008760	0.3053138	0.3095739	8.79	-1924.3582487	-1924.3493669	-1924.0680006	-1924.0591187
-1	5	1_TMPMgCl_d3_mol6_2	-1924.0185853	0.2916434	0.3021300	0.3065050	0.3107019	20.63	-1924.3611561	-1924.3520459	-1924.0695126	-1924.0604025
-1	6	1_TMPMgCl_d3_mol6_1	-1924.0177938	0.2915303	0.3020230	0.3064014	0.3106023	19.94	-1924.3590795	-1924.3501788	-1924.0675492	-1924.0586484
-1	7	1_TMPMgCl_d2_mol6_2	-1923.9967890	0.2899977	0.3006060	0.3050326	0.3092796	4.04	-1924.3468023	-1924.3365822	-1924.0568046	-1924.0465844
-1	8	1_TMPMgCl_d2_mol6_3	-1923.9957535	0.2892568	0.2998933	0.3043329	0.3085932	8.95	-1924.3441568	-1924.3341319	-1924.0549000	-1924.0448750
-1	9	1_TMPMgCl_d8_mol6_2	-1923.9953113	0.2891463	0.2997562	0.3041836	0.3084317	16.07	-1924.3425013	-1924.3326081	-1924.0533550	-1924.0434617
-1	10	1_TMPMgCl_d8_mol6_1	-1923.9876490	0.2894329	0.3000257	0.3044454	0.3086857	8.57	-1924.3447364	-1924.3332484	-1924.0553035	-1924.0438154
-1	1	1_TMPZnCl_d5_mol6_2	-3503.0659774	0.2886229	0.2994989	0.3040442	0.3084095	0.82	-3503.5624319	-3503.5534829	-3503.2738089	-3503.2648600
-1	2	1_TMPZnCl_d5_mol6_1	-3503.0630924	0.2897933	0.3004592	0.3049112	0.3091834	13.37	-3503.5598317	-3503.5507932	-3503.2700383	-3503.2609999
-1	3	1_TMPZnCl_d5_mol6_3	-3503.0630178	0.2899490	0.3006382	0.3051014	0.3093853	9.38	-3503.5576783	-3503.5489626	-3503.2677293	-3503.2590136
-1	4	1_TMPZnCl_d5_mol6_4	-3503.0606902	0.2901124	0.3007626	0.3052092	0.3094770	18.75	-3503.5558704	-3503.5470159	-3503.2657579	-3503.2569035
-1	5	1_TMPZnCl_d3_mol6_2	-3503.0595245	0.2898375	0.3005896	0.3050801	0.3093907	2.73	-3503.5551070	-3503.5462535	-3503.2652695	-3503.2564160
-1	6	1_TMPZnCl_d3_mol6_4	-3503.0559162	0.2904298	0.3010888	0.3055388	0.3098095	10.31	-3503.5500637	-3503.5414345	-3503.2596338	-3503.2510047
-1	7	1_TMPZnCl_d2_mol6_2	-3503.0364887	0.2898167	0.3004599	0.3048987	0.3091555	9.19	-3503.5407773	-3503.5305460	-3503.2509606	-3503.2407293
-1	8	1_TMPZnCl_d8_mol6_4	-3503.0234617	0.2880486	0.2987948	0.3032803	0.3075843	11.74	-3503.5315358	-3503.5204778	-3503.2434872	-3503.2324291
-1	1	1_ZnCl2_d8_mol6	-3554.7003065	0.0430979	0.0511465	0.0545740	0.0579061	19.42	-3555.1519458	-3555.1406332	-3555.1088479	-3555.0975353
-1	2	1_ZnCl2_d5_mol6	-3554.6936369	0.0439290	0.0518823	0.0552687	0.0585604	25.38	-3555.1343673	-3555.1243453	-3555.0904382	-3555.0804163
-1	3	1_ZnCl2_d3_mol6	-3554.6881611	0.0442709	0.0522248	0.0556116	0.0589036	22.08	-3555.1280425	-3555.1181907	-3555.0837715	-3555.0739198
-1	4	1_ZnCl2_d2_mol6	-3554.6671766	0.0432127	0.0512166	0.0546235	0.0579344	16.63	-3555.1166640	-3555.1054523	-3555.0734512	-3555.0622395
-1	1	C2H6NMgCl_d3_mol6_aal	-1649.9916236	0.1202396	0.1290498	0.1327809	0.1363948	9.81	-1650.2716570	-1650.2630465	-1650.1514174	-1650.1428068
-1	2	C2H6NMgCl_d5_mol6_aad	-1649.9914136	0.1205710	0.1292959	0.1329886	0.1365638	21.98	-1650.2747821	-1650.2657916	-1650.1542110	-1650.1452205
-1	3	C2H6NMgCl_d5_mol6_aaa	-1649.9911433	0.1206152	0.1293209	0.1330055	0.1365728	25.93	-1650.2751531	-1650.2660126	-1650.1545379	-1650.1453973
-1	4	C2H6NMgCl_d3_mol6_aan	-1649.9899601	0.1211946	0.1298923	0.1335732	0.1371368	21.29	-1650.2715437	-1650.2627221	-1650.1503491	-1650.1415274
-1	5	C2H6NMgCl_d5_mol6_aar	-1649.9738583	0.1198524	0.1286463	0.1323692	0.1359743	20.75	-1650.2615493	-1650.2516945	-1650.1416969	-1650.1318421
-1	6	C2H6NMgCl_d5_mol6_aag	-1649.9730991	0.1200564	0.1288147	0.1325218	0.1361112	22.71	-1650.2612757	-1650.2513078	-1650.1412193	-1650.1312514
-1	7	C2H6NMgCl_d2_mol6_aai	-1649.9712548	0.1193205	0.1281443	0.1318807	0.1354994	22.23	-1650.2560886	-1650.2468156	-1650.1367681	-1650.1274951

-1	8	C2H6NMgCl_d8_mol6_aaa	-1649.9682831	0.1181472	0.1270447	0.1308130	0.1344631	15.15	-1650.2599320	-1650.2496869	-1650.1417848	-1650.1315396
-1	9	C2H6NMgCl_d5_mol6_aac	-1649.9689269	0.1189702	0.1277969	0.1315352	0.1351563	19.59	-1650.2526128	-1650.2434494	-1650.1336425	-1650.1244792
-1	10	C2H6NMgCl_d2_mol6_aae	-1649.9688145	0.1192025	0.1280258	0.1317610	0.1353781	18.01	-1650.2557487	-1650.2461508	-1650.1365461	-1650.1269482
-1	11	C2H6NMgCl_d3_mol6_aad	-1649.9686966	0.1203635	0.1291277	0.1328376	0.1364298	19.79	-1650.2547147	-1650.2451466	-1650.1343512	-1650.1247830
-1	12	C2H6NMgCl_d3_mol6_abs	-1649.9678647	0.1203796	0.1291433	0.1328528	0.1364445	22.27	-1650.2549346	-1650.2452147	-1650.1345549	-1650.1248351
-1	13	C2H6NMgCl_d3_mol6_aab	-1649.9556276	0.1189486	0.1278393	0.1316066	0.1352569	10.24	-1650.2435526	-1650.2337038	-1650.1246039	-1650.1147552
-1	14	C2H6NMgCl_d2_mol6_aap	-1649.9524908	0.1192005	0.1280186	0.1317510	0.1353649	9.58	-1650.2413570	-1650.2313921	-1650.1221565	-1650.1121915
-1	15	C2H6NMgCl_d2_mol6_aaa	-1649.9247808	0.1177517	0.1266810	0.1304631	0.1341269	9.84	-1650.2243438	-1650.2125892	-1650.1065920	-1650.0948374
-1	16	C2H6NMgCl_d8_mol6_aaf	-1649.9084229	0.1174165	0.1262996	0.1300597	0.1337006	21.10	-1650.2100419	-1650.1977496	-1650.0926254	-1650.0803331
-1	17	C2H6NMgCl_d8_mol6_aay	-1649.9041615	0.1166755	0.1256014	0.1293790	0.1330361	26.85	-1650.1998500	-1650.1885563	-1650.0831744	-1650.0718808
-1	18	C2H6NMgCl_d8_mol6_abm	-1649.9042808	0.1168966	0.1258058	0.1295776	0.1332301	18.78	-1650.2080977	-1650.1953851	-1650.0912010	-1650.0784884
-1	19	C2H6NMgCl_d8_mol6_abc	-1649.8987805	0.1162813	0.1252229	0.1290088	0.1326753	21.50	-1650.2020775	-1650.1895539	-1650.0857962	-1650.0732726
-1	20	C2H6NMgCl_d2_mol6_abu	-1649.8927152	0.1170689	0.1260096	0.1297954	0.1334618	23.32	-1650.1907938	-1650.1792213	-1650.0737248	-1650.0621523
-1	21	C2H6NMgCl_d8_mol6_aaj	-1649.8709630	0.1154428	0.1246492	0.1285549	0.1323423	15.35	-1650.2093126	-1650.1918667	-1650.0938697	-1650.0764239
-1	1	C2H6NZnCl_d3_mol6_aao	-3229.0470494	0.1199614	0.1288495	0.1326136	0.1362591	9.25	-3229.4795759	-3229.4712678	-3229.3596144	-3229.3513063
-1	2	C2H6NZnCl_d5_mol6_aad	-3229.0457124	0.1206364	0.1294154	0.1331300	0.1367254	26.21	-3229.4812539	-3229.4725963	-3229.3606175	-3229.3519598
-1	3	C2H6NZnCl_d3_mol6_abq	-3229.0440168	0.1202193	0.1290687	0.1328158	0.1364446	18.83	-3229.4780834	-3229.4695571	-3229.3578640	-3229.3493378
-1	4	C2H6NZnCl_d5_mol6_aau	-3229.0435647	0.1202116	0.1290058	0.1327283	0.1363324	26.65	-3229.4800719	-3229.4712407	-3229.3598602	-3229.3510290
-1	5	C2H6NZnCl_d2_mol6_aai	-3229.0281080	0.1189898	0.1279052	0.1316803	0.1353363	23.98	-3229.4664077	-3229.4572502	-3229.3474179	-3229.3382603
-1	6	C2H6NZnCl_d8_mol6_aaa	-3229.0211722	0.1179210	0.1268997	0.1307024	0.1343856	13.76	-3229.4681689	-3229.4577130	-3229.3502479	-3229.3397920
-1	7	C2H6NZnCl_d5_mol6_aab	-3229.0160320	0.1191643	0.1280691	0.1318402	0.1354926	21.28	-3229.4541725	-3229.4449413	-3229.3350081	-3229.3257769
-1	8	C2H6NZnCl_d5_mol6_aal	-3229.0145430	0.1190351	0.1279323	0.1317000	0.1353489	19.56	-3229.4539351	-3229.4444670	-3229.3349000	-3229.3254319
-1	9	C2H6NZnCl_d3_mol6_aad	-3229.0107397	0.1196206	0.1284992	0.1322585	0.1358990	19.39	-3229.4477995	-3229.4387462	-3229.3281789	-3229.3191256
-1	10	C2H6NZnCl_d3_mol6_aav	-3229.0096139	0.1195235	0.1284073	0.1321694	0.1358130	23.64	-3229.4475857	-3229.4383937	-3229.3280622	-3229.3188701
-1	11	C2H6NZnCl_d5_mol6_aac	-3229.0078980	0.1181918	0.1271712	0.1309766	0.1346642	11.65	-3229.4471552	-3229.4378729	-3229.3289633	-3229.3196811
-1	12	C2H6NZnCl_d3_mol6_aah	-3228.9970571	0.1191129	0.1280312	0.1318086	0.1354673	16.59	-3229.4372840	-3229.4277767	-3229.3181710	-3229.3086638
-1	13	C2H6NZnCl_d2_mol6_aaq	-3228.9941234	0.1188122	0.1277210	0.1314917	0.1351421	10.02	-3229.4347591	-3229.4251467	-3229.3159468	-3229.3063345
-1	14	C2H6NZnCl_d5_mol6_aba	-3228.9893824	0.1180160	0.1269541	0.1307418	0.1344119	28.57	-3229.4282999	-3229.4189480	-3229.3102839	-3229.3009320
-1	15	C2H6NZnCl_d5_mol6_aax	-3228.9849854	0.1174407	0.1264210	0.1302275	0.1339166	19.50	-3229.4276382	-3229.4176707	-3229.3101975	-3229.3002300
-1	16	C2H6NZnCl_d2_mol6_abk	-3228.9659402	0.1166616	0.1257669	0.1296261	0.1333657	4.07	-3229.4171050	-3229.4058146	-3229.3004433	-3229.2891529
-1	17	C2H6NZnCl_d2_mol6_aag	-3228.9661718	0.1171972	0.1262170	0.1300378	0.1337390	12.97	-3229.4178178	-3229.4064261	-3229.3006206	-3229.2892289
-1	18	C2H6NZnCl_d8_mol6_aaf	-3228.9570073	0.1166447	0.1256412	0.1294521	0.1331439	24.65	-3229.4069156	-3229.3955426	-3229.2902709	-3229.2788978
-1	19	C2H6NZnCl_d8_mol6_aat	-3228.9549545	0.1160713	0.1251535	0.1290025	0.1327322	7.28	-3229.4047641	-3229.3933876	-3229.2886927	-3229.2773162
-1	20	C2H6NZnCl_d8_mol6_aai	-3228.9518399	0.1162834	0.1252975	0.1291160	0.1328148	21.70	-3229.4011601	-3229.3899970	-3229.2848766	-3229.2737135
-1	21	C2H6NZnCl_d2_mol6_aan	-3228.9398386	0.1164031	0.1254819	0.1293297	0.1330583	17.74	-3229.3931267	-3229.3814639	-3229.2767236	-3229.2650608
-1	22	C2H6NZnCl_d8_mol6_abl	-3228.9338819	0.1162338	0.1253929	0.1292761	0.1330400	13.88	-3229.4093295	-3229.3941275	-3229.2930956	-3229.2778936
-1	23	C2H6NZnCl_d8_mol6_abm	-3228.9333158	0.1157355	0.1249484	0.1288561	0.1326450	14.89	-3229.4105990	-3229.3951569	-3229.2948634	-3229.2794213
-1	1	d2_furan	-229.4113591	0.0285971	0.0331904	0.0351779	0.0371319	596.23	-229.5678904	-229.5559555	-229.5392932	-229.5273584
-1	2	d3_furan	-229.4041312	0.0289875	0.0335748	0.0355602	0.0375127	604.61	-229.5603396	-229.5485201	-229.5313520	-229.5195326
-1	1	d5_mol16e_1	-1292.8198803	0.1487949	0.1575413	0.1612222	0.1647746	18.57	-1293.1327016	-1293.1231519	-1292.9839067	-1292.9743570
-1	2	d5_mol16e_2	-1292.8194434	0.1485446	0.1573193	0.1610128	0.1645777	13.66	-1293.1325962	-1293.1229805	-1292.9840515	-1292.9744359
-1	3	d8_mol16e_2	-1292.7918306	0.1472018	0.1560313	0.1597472	0.1633334	17.43	-1293.1106860	-1293.1001149	-1292.9634841	-1292.9529131
-1	4	d8_mol16e_1	-1292.7919128	0.1473855	0.1561926	0.1598985	0.1634746	21.51	-1293.1107477	-1293.1001471	-1292.9633622	-1292.9527615
-1	1	d5_mol3	-395.3197842	0.0620118	0.0674140	0.0697288	0.0719910	218.96	-395.5003691	-395.4903087	-395.4383573	-395.4282968
-1	2	d3_mol3	-395.3164491	0.0622630	0.0676626	0.0699768	0.0722386	214.46	-395.4986806	-395.4883470	-395.4364176	-395.4260839
-1	3	d6_mol3	-395.2893070	0.0604974	0.0659749	0.0683206	0.0706117	172.11	-395.4787043	-395.4671605	-395.4182068	-395.4066631
-1	4	d2_mol3	-395.2886744	0.0609953	0.0664366	0.0687670	0.0710433	199.08	-395.4809433	-395.4688921	-395.4199480	-395.4078967
-1	5	d8_mol3	-395.2866041	0.0601239	0.0655949	0.0679369	0.0702241	192.29	-395.4836772	-395.4707570	-395.4235533	-395.4106330
-1	1	d5_mol6	-854.9290523	0.0498208	0.0557166	0.0582362	0.0606932	112.23	-855.1370591	-855.1274071	-855.0872382	-855.0775862
-1	2	d3_mol6	-854.9210037	0.0501914	0.0560859	0.0586053	0.0610622	119.51	-855.1283288	-855.1187605	-855.0781373	-855.0685690
-1	3	d8_mol6	-854.8965647	0.0480828	0.0540483	0.0565955	0.0590779	103.76	-855.1169281	-855.1050583	-855.0688453	-855.0569754
-1	4	d2_mol6	-854.8930351	0.0489122	0.0548490	0.0573848	0.0598566	114.59	-855.1099904	-855.0988011	-855.0610782	-855.0498889
-1	1	d5_mol7e	-947.1926829	0.0458465	0.0523502	0.0551208	0.0578162	97.49	-947.4199494	-947.4108663	-947.3741029	-947.3650197
-1	2	d2_mol7e	-947.1653648	0.0450445	0.0515803	0.0543638	0.0570712	98.40	-947.3983487	-947.3883000	-947.3533042	-947.3432554
-1	3	d8_mol7e	-947.1642990	0.0443948	0.0509630	0.0537604	0.0564813	87.37	-947.3979797	-947.3877586	-947.3535848	-947.3433637
-1	1	MgCl2_d3_mol6_aaa	-1975.6780389	0.0459807	0.0537956	0.0571229	0.0603571	23.64	-1975.9639001	-1975.9541169	-1975.9179193	-1975.9081362
-1	2	MgCl2_d5_mol6_aaa	-1975.6751653	0.0441722	0.0521527	0.0555545	0.0588639	5.43	-1975.9648737	-1975.9546023	-1975.9207015	-1975.9104300
-1	3	MgCl2_d5_mol6_aab	-1975.6755912	0.0453626	0.0531959	0.0565315	0.0597740	20.73	-1975.9655396	-1975.9552617	-1975.9201769	-1975.9098990
-1	4	MgCl2_d5_mol6_abb	-1975.6596992	0.0450764	0.0529074	0.0562411	0.0594814	24.94	-1975.9524032	-1975.9414050	-1975.9073267	-1975.8963286
-1	5	MgCl2_d2_mol6_aaa	-1975.6569272	0.0445354	0.0524421	0.0558088	0.0590817	22.50	-1975.9489036	-1975.9383189	-1975.9043682	-1975.8937835

-1	6	MgCl2_d8_mol6_aar	-1975.6548981	0.0439106	0.0518462	0.0552253	0.0585102	23.68	-1975.9523973	-1975.9410508	-1975.9084866	-1975.8971401
-1	7	MgCl2_d5_mol6_aam	-1975.6540108	0.0447315	0.0525627	0.0558958	0.0591351	28.85	-1975.9415345	-1975.9314819	-1975.8968029	-1975.8867504
-1	8	MgCl2_d8_mol6_aai	-1975.6536951	0.0444269	0.0522958	0.0556438	0.0588968	30.63	-1975.9480535	-1975.9370191	-1975.9036265	-1975.8925921
-1	9	MgCl2_d3_mol6_aag	-1975.6541230	0.0453609	0.0531947	0.0565299	0.0597717	21.96	-1975.9458465	-1975.9350687	-1975.9004855	-1975.8897077
-1	10	MgCl2_d8_mol6_aao	-1975.6515034	0.0443553	0.0522213	0.0555691	0.0588227	33.83	-1975.9474087	-1975.9362145	-1975.9030533	-1975.8918591
-1	11	MgCl2_d2_mol6_aap	-1975.6509939	0.0445533	0.0524280	0.0557803	0.0590385	24.65	-1975.9415821	-1975.9312007	-1975.8970288	-1975.8866474
-1	12	MgCl2_d3_mol6_aac	-1975.6391033	0.0442778	0.0521904	0.0555609	0.0588385	21.84	-1975.9306146	-1975.9198716	-1975.8863368	-1975.8755937
-1	13	MgCl2_d3_mol6_aan	-1975.6383295	0.0444511	0.0523708	0.0557444	0.0590248	11.00	-1975.9333839	-1975.9221434	-1975.8889328	-1975.8776922
-1	14	MgCl2_d5_mol6_abj	-1975.6226196	0.0431486	0.0510983	0.0544856	0.0577801	21.65	-1975.9178234	-1975.9064690	-1975.8746748	-1975.8633204
-1	15	MgCl2_d2_mol6_aak	-1975.6080190	0.0429131	0.0508735	0.0542632	0.0575585	22.21	-1975.9112037	-1975.8985340	-1975.8682906	-1975.8556208
-1	16	MgCl2_d3_mol6_aae	-1975.6027169	0.0420007	0.0500783	0.0535224	0.0568736	5.75	-1975.8961839	-1975.8852031	-1975.8541832	-1975.8432024
-1	17	MgCl2_d8_mol6_aae	-1975.5884628	0.0416449	0.0496558	0.0530674	0.0563844	17.19	-1975.8963714	-1975.8826813	-1975.8547265	-1975.8410363
-1	18	MgCl2_d8_mol6_aag	-1975.5850928	0.0414426	0.0494315	0.0528300	0.0561316	31.44	-1975.8844112	-1975.8721479	-1975.8429685	-1975.8307052
-1	19	MgCl2_d8_mol6_aas	-1975.5829890	0.0408232	0.0488852	0.0523194	0.0556586	17.63	-1975.8899607	-1975.8765383	-1975.8491374	-1975.8357151
-1	20	MgCl2_d8_mol6_aah	-1975.5817278	0.0403489	0.0485034	0.0519752	0.0553498	9.57	-1975.8931485	-1975.8792261	-1975.8527995	-1975.8388772
-1	21	MgCl2_d2_mol6_aas	-1975.5734555	0.0419340	0.0499131	0.0533096	0.0566106	30.33	-1975.8756025	-1975.8630253	-1975.8336684	-1975.8210913
-1	1	TMPMgCl_d3_mol6_aba	-1924.0413017	0.2925927	0.3030112	0.3073566	0.3115246	18.11	-1924.3789061	-1924.3705943	-1924.0863133	-1924.0780015
-1	2	TMPMgCl_d5_mol6_abo	-1924.0388158	0.2909162	0.3014573	0.3058573	0.3100800	11.33	-1924.3783138	-1924.3698343	-1924.0873976	-1924.0789181
-1	3	TMPMgCl_d5_mol6_aaj	-1924.0390628	0.2915272	0.3020109	0.3063843	0.3105798	14.69	-1924.3784538	-1924.3699971	-1924.0869266	-1924.0784698
-1	4	TMPMgCl_d3_mol6_abh	-1924.0383002	0.2914113	0.3019303	0.3063208	0.3105342	18.40	-1924.3738235	-1924.3657980	-1924.0824122	-1924.0743866
-1	5	TMPMgCl_d5_mol6_aas	-1924.0379509	0.2920233	0.3024556	0.3068060	0.3109782	16.22	-1924.3795395	-1924.3706692	-1924.0875162	-1924.0786458
-1	6	TMPMgCl_d5_mol6_aac	-1924.0365165	0.2912192	0.3017333	0.3061209	0.3103309	13.87	-1924.3789149	-1924.3700117	-1924.0876957	-1924.0787925
-1	7	TMPMgCl_d5_mol6_aag	-1924.0252424	0.2912074	0.3017104	0.3060925	0.3102967	22.84	-1924.3676557	-1924.3585622	-1924.0764483	-1924.0673547
-1	8	TMPMgCl_d5_mol6_aav	-1924.0225920	0.2913800	0.3018509	0.3062194	0.3104105	21.55	-1924.3660229	-1924.3567213	-1924.0746429	-1924.0653412
-1	9	TMPMgCl_d2_mol6_aah	-1924.0178307	0.2901663	0.3007781	0.3052078	0.3094590	13.58	-1924.3592214	-1924.3503584	-1924.0690550	-1924.0601920
-1	10	TMPMgCl_d8_mol6_aae	-1924.0163693	0.2891162	0.2997731	0.3042224	0.3084931	14.72	-1924.3624820	-1924.3529328	-1924.0733658	-1924.0638165
-1	11	TMPMgCl_d8_mol6_aaf	-1924.0155223	0.2891466	0.2998188	0.3042749	0.3085522	9.55	-1924.3626410	-1924.3529313	-1924.0734943	-1924.0637847
-1	12	TMPMgCl_d3_mol6_aak	-1924.0177938	0.2915302	0.3020229	0.3064013	0.3106022	19.95	-1924.3590794	-1924.3501787	-1924.0675491	-1924.0586484
-1	13	TMPMgCl_d8_mol6_aao	-1924.0154662	0.2892421	0.2999001	0.3043498	0.3086209	7.46	-1924.3623905	-1924.3527097	-1924.0731484	-1924.0634676
-1	14	TMPMgCl_d2_mol6_aar	-1924.0153328	0.2895393	0.3001820	0.3046254	0.3088903	13.59	-1924.3570134	-1924.3480322	-1924.0674740	-1924.0584928
-1	15	TMPMgCl_d2_mol6_aab	-1924.0153121	0.2901270	0.3007046	0.3051189	0.3093549	21.35	-1924.3573880	-1924.3483460	-1924.0672610	-1924.0582189
-1	16	TMPMgCl_d5_mol6_aaw	-1924.0142400	0.2892289	0.2999673	0.3044542	0.3087634	1.72	-1924.3592169	-1924.3499442	-1924.0699879	-1924.0607152
-1	17	TMPMgCl_d5_mol6_aaa	-1924.0143972	0.2903516	0.3009109	0.3053171	0.3095448	17.12	-1924.3579698	-1924.3488483	-1924.0676181	-1924.0584966
-1	18	TMPMgCl_d5_mol6_aay	-1924.0146734	0.2907560	0.3012896	0.3056847	0.3099015	15.71	-1924.3568136	-1924.3478810	-1924.0660575	-1924.0571249
-1	19	TMPMgCl_d3_mol6_aam	-1924.0038935	0.2911900	0.3017038	0.3060904	0.3102987	14.39	-1924.3493586	-1924.3398838	-1924.0581686	-1924.0486938
-1	20	TMPMgCl_d3_mol6_abw	-1924.0025889	0.2910830	0.3016124	0.3060069	0.3102238	19.31	-1924.3482746	-1924.3388202	-1924.0571915	-1924.0477372
-1	21	TMPMgCl_d2_mol6_abq	-1923.9992093	0.2896546	0.3002722	0.3047042	0.3089575	13.27	-1924.3439075	-1924.3344277	-1924.0542528	-1924.0447730
-1	22	TMPMgCl_d5_mol6_aau	-1923.9958457	0.2908469	0.3013328	0.3057062	0.3099009	14.61	-1924.3380913	-1924.3290396	-1924.0472444	-1924.0381926
-1	23	TMPMgCl_d3_mol6_abv	-1923.9764367	0.2901038	0.3007064	0.3051311	0.3093767	14.53	-1924.3275433	-1924.3173053	-1924.0374395	-1924.0272014
-1	24	TMPMgCl_d2_mol6_aav	-1923.9726318	0.2896555	0.3002349	0.3046483	0.3088820	12.59	-1924.3300101	-1924.3185511	-1924.0403546	-1924.0288956
-1	25	TMPMgCl_d2_mol6_aac	-1923.9720536	0.2898631	0.3004541	0.3048727	0.3091117	11.91	-1924.3300284	-1924.3185319	-1924.0401652	-1924.0286687
-1	26	TMPMgCl_d5_mol6_abp	-1923.9684713	0.2882939	0.2990306	0.3035189	0.3078307	12.33	-1924.3309015	-1924.3190953	-1924.0426075	-1924.0308014
-1	27	TMPMgCl_d5_mol6_abj	-1923.9685358	0.2884125	0.2991407	0.3036256	0.3079344	12.97	-1924.3318573	-1924.3198266	-1924.0434448	-1924.0314140
-1	28	TMPMgCl_d5_mol6_aah	-1923.9663716	0.2878154	0.2986525	0.3031851	0.3075411	7.79	-1924.3332013	-1924.3207013	-1924.0453858	-1924.0328858
-1	29	TMPMgCl_d5_mol6_abu	-1923.9652601	0.2875141	0.2983788	0.3029240	0.3072926	8.16	-1924.3340696	-1924.3212362	-1924.0465554	-1924.0337221
-1	30	TMPMgCl_d5_mol6_abm	-1923.9624591	0.2870536	0.2979843	0.3025597	0.3069592	10.10	-1924.3283436	-1924.3160057	-1924.0412899	-1924.0289520
-1	31	TMPMgCl_d8_mol6_abm	-1923.9617982	0.2887896	0.2993728	0.3037874	0.3080221	14.03	-1924.3158373	-1924.3046376	-1924.0270477	-1924.0158480
-1	32	TMPMgCl_d3_mol6_aau	-1923.9598903	0.2885021	0.2992644	0.3037645	0.3080883	11.86	-1924.3240627	-1924.3119409	-1924.0355605	-1924.0234387
-1	33	TMPMgCl_d3_mol6_aar	-1923.9581495	0.2883548	0.2991691	0.3036922	0.3080388	11.41	-1924.3250511	-1924.3125612	-1924.0366963	-1924.0242064
-1	34	TMPMgCl_d2_mol6_abe	-1923.9470953	0.2892267	0.2998151	0.3042314	0.3084670	19.62	-1924.3091563	-1924.2970447	-1924.0199295	-1924.0078179
-1	35	TMPMgCl_d8_mol6_aas	-1923.9388883	0.2859016	0.2967700	0.3013155	0.3056837	10.62	-1924.3004568	-1924.2884199	-1924.0145551	-1924.0025182
-1	36	TMPMgCl_d8_mol6_abi	-1923.9371256	0.2851521	0.2961589	0.3007656	0.3051947	6.24	-1924.3028788	-1924.2901942	-1924.0177267	-1924.0050421
-1	37	TMPMgCl_d2_mol6_aaa	-1923.9382888	0.2872476	0.2980824	0.3026091	0.3069559	10.09	-1924.3035993	-1924.2911391	-1924.0163516	-1924.0038914
-1	38	TMPMgCl_d2_mol6_abb	-1923.9351481	0.2859014	0.2968268	0.3013981	0.3057925	10.44	-1924.2937654	-1924.2822415	-1924.0078639	-1923.9963401
-1	39	TMPMgCl_d8_mol6_abr	-1923.9343788	0.2855443	0.2964982	0.3010809	0.3054857	12.13	-1924.3035753	-1924.2902700	-1924.0180309	-1924.0047256
-1	40	TMPMgCl_d8_mol6_abx	-1923.9338495	0.2862705	0.2971835	0.3017492	0.3061378	10.88	-1924.3060856	-1924.2923377	-1924.0198150	-1924.0060672
-1	41	TMPMgCl_d2_mol6_abi	-1923.9332251	0.2865251	0.2974186	0.3019758	0.3063559	13.88	-1924.2943393	-1924.2824347	-1924.0078142	-1923.9959095
-1	1	TMPZnCl_d3_mol6_aba	-3503.0920403	0.2913447	0.3019562	0.3063842	0.3106324	14.40	-3503.5831744	-3503.5750664	-3503.2918297	-3503.2837217
-1	2	TMPZnCl_d5_mol6_aaj	-3503.0910889	0.2913101	0.3018823	0.3062924	0.3105223	13.73	-3503.5861807	-3503.5776001	-3503.2948706	-3503.2862899
-1	3	TMPZnCl_d5_mol6_aao	-3503.0895417	0.2907434	0.3013495	0.3057743	0.3100186	16.22	-3503.5861691	-3503.5774012	-3503.2954256	-3503.2866577

-1	4	TMPZnCl_d3_mol6_aav	-3503.0894657	0.2911316	0.3017548	0.3061889	0.3104437	17.22	-3503.5779241	-3503.5701115	-3503.2867925	-3503.2789798
-1	5	TMPZnCl_d5_mol6_abn	-3503.0895888	0.2916979	0.3022371	0.3066325	0.3108479	18.34	-3503.5864433	-3503.5775871	-3503.2947454	-3503.2858891
-1	6	TMPZnCl_d5_mol6_abx	-3503.0897523	0.2922107	0.3026925	0.3070626	0.3112529	14.65	-3503.5856049	-3503.5768378	-3503.2933941	-3503.2846271
-1	7	TMPZnCl_d2_mol6_aah	-3503.0740975	0.2905152	0.3011634	0.3056058	0.3098670	19.09	-3503.5703510	-3503.5614588	-3503.2798358	-3503.2709435
-1	8	TMPZnCl_d8_mol6_abe	-3503.0680926	0.2898545	0.3005155	0.3049636	0.3092307	17.00	-3503.5727391	-3503.5626079	-3503.2828846	-3503.2727533
-1	9	TMPZnCl_d8_mol6_aax	-3503.0682245	0.2903363	0.3009627	0.3053944	0.3096444	16.81	-3503.5730422	-3503.5628764	-3503.2827058	-3503.2725400
-1	10	TMPZnCl_d8_mol6_abn	-3503.0663253	0.2885451	0.2993126	0.3038085	0.3081236	10.26	-3503.5706585	-3503.5605891	-3503.2821134	-3503.2720439
-1	11	TMPZnCl_d8_mol6_aaf	-3503.0671139	0.2895391	0.3002926	0.3047800	0.3090850	4.50	-3503.5723097	-3503.5620990	-3503.2827705	-3503.2725598
-1	12	TMPZnCl_d5_mol6_aav	-3503.0659774	0.2886421	0.2995152	0.3040592	0.3084232	0.86	-3503.5624319	-3503.5534830	-3503.2737897	-3503.2648408
-1	13	TMPZnCl_d8_mol6_aag	-3503.0638139	0.2891985	0.2999086	0.3043789	0.3086685	11.77	-3503.5668012	-3503.5568388	-3503.2776027	-3503.2676402
-1	14	TMPZnCl_d5_mol6_abv	-3503.0630924	0.2897932	0.3004591	0.3049112	0.3091833	13.37	-3503.5598317	-3503.5507932	-3503.2700384	-3503.2609999
-1	15	TMPZnCl_d5_mol6_aas	-3503.0547994	0.2900337	0.3007051	0.3051593	0.3094333	12.71	-3503.5548741	-3503.5455109	-3503.2648403	-3503.2554772
-1	16	TMPZnCl_d5_mol6_aab	-3503.0546943	0.2905199	0.3011359	0.3055650	0.3098138	12.62	-3503.5543000	-3503.5449697	-3503.2637800	-3503.2544497
-1	17	TMPZnCl_d5_mol6_aam	-3503.0519973	0.2905573	0.3011729	0.3056017	0.3098501	16.77	-3503.5539576	-3503.5443300	-3503.2634002	-3503.2537727
-1	18	TMPZnCl_d3_mol6_aag	-3503.0435550	0.2904917	0.3011309	0.3055712	0.3098317	16.16	-3503.5451974	-3503.5355594	-3503.2547057	-3503.2450676
-1	19	TMPZnCl_d5_mol6_aaq	-3503.0413784	0.2901049	0.3007150	0.3051431	0.3093921	15.93	-3503.5371208	-3503.5282722	-3503.2470159	-3503.2381673
-1	20	TMPZnCl_d2_mol6_aam	-3503.0385526	0.2898263	0.3004827	0.3049283	0.3091926	9.37	-3503.5402330	-3503.5304484	-3503.2504066	-3503.2406221
-1	21	TMPZnCl_d5_mol6_aac	-3503.0251972	0.2878726	0.2987816	0.3033469	0.3077359	8.48	-3503.5410445	-3503.5292128	-3503.2531719	-3503.2413402
-1	22	TMPZnCl_d5_mol6_aaz	-3503.0239591	0.2873452	0.2983253	0.3029227	0.3073443	8.75	-3503.5343621	-3503.5233315	-3503.2470169	-3503.2359863
-1	23	TMPZnCl_d3_mol6_abx	-3503.0178059	0.2892198	0.3000261	0.3045454	0.3088880	12.73	-3503.5337716	-3503.5218969	-3503.2445518	-3503.2326770
-1	24	TMPZnCl_d3_mol6_aar	-3503.0178586	0.2894334	0.3002249	0.3047379	0.3090744	11.50	-3503.5338995	-3503.5220187	-3503.2444660	-3503.2325852
-1	25	TMPZnCl_d2_mol6_abf	-3503.0132004	0.2890711	0.2997669	0.3042302	0.3085124	15.67	-3503.5260208	-3503.5145575	-3503.2369496	-3503.2254864
-1	26	TMPZnCl_d8_mol6_aah	-3502.9935673	0.2843810	0.2955595	0.3002426	0.3047479	7.60	-3503.5086383	-3503.4965939	-3503.2242573	-3503.2122129
-1	27	TMPZnCl_d8_mol6_abi	-3502.9941044	0.2854545	0.2965186	0.3011508	0.3056054	10.14	-3503.5126608	-3503.5000824	-3503.2272063	-3503.2146279
-1	28	TMPZnCl_d8_mol6_aaq	-3502.9933802	0.2848754	0.2959849	0.3006375	0.3051125	7.52	-3503.5096781	-3503.4974618	-3503.2248026	-3503.2125864
-1	29	TMPZnCl_d8_mol6_aad	-3502.9934862	0.2849963	0.2961006	0.3007508	0.3052233	7.24	-3503.5087410	-3503.4966824	-3503.2237446	-3503.2116860
-1	30	TMPZnCl_d8_mol6_aam	-3502.9938142	0.2861166	0.2971385	0.3017514	0.3061863	8.62	-3503.5138821	-3503.5010732	-3503.2277654	-3503.2149565
-1	31	TMPZnCl_d2_mol6_abm	-3502.9908379	0.2860081	0.2970674	0.3016991	0.3061541	8.82	-3503.5024898	-3503.4910473	-3503.2164816	-3503.2050392
-1	32	TMPZnCl_d2_mol6_abe	-3502.9932218	0.2887079	0.2994251	0.3039006	0.3081968	17.74	-3503.5111007	-3503.4988024	-3503.2223928	-3503.2100945
-1	33	TMPZnCl_d2_mol6_aaf	-3502.9900802	0.2855905	0.2967005	0.3013542	0.3058308	9.59	-3503.5034340	-3503.4917334	-3503.2178435	-3503.2061428
-1	34	TMPZnCl_d2_mol6_aaw	-3502.9872800	0.2872250	0.2981603	0.3027346	0.3071307	13.30	-3503.5132283	-3503.4997034	-3503.2260033	-3503.2124784
-1	1	ZnCl2_d3_mol6_aaa	-3554.7257535	0.0451535	0.0530758	0.0564492	0.0597281	24.90	-3555.1624410	-3555.1532315	-3555.1172874	-3555.1080780
-1	2	ZnCl2_d5_mol6_aaa	-3554.7212165	0.0447369	0.0526624	0.0560370	0.0593172	21.33	-3555.1624207	-3555.1526419	-3555.1176838	-3555.1079050
-1	3	ZnCl2_d2_mol6_aaa	-3554.7055633	0.0437891	0.0517974	0.0552077	0.0585227	23.45	-3555.1494277	-3555.1392308	-3555.1056386	-3555.0954417
-1	4	ZnCl2_d8_mol6_aad	-3554.7003065	0.0430965	0.0511452	0.0545728	0.0579049	19.42	-3555.1519458	-3555.1406332	-3555.1088492	-3555.0975366
-1	5	ZnCl2_d5_mol6_aaf	-3554.6936369	0.0439289	0.0518823	0.0552687	0.0585604	25.38	-3555.1343672	-3555.1243452	-3555.0904382	-3555.0804163
-1	6	ZnCl2_d3_mol6_aag	-3554.6881611	0.0442709	0.0522248	0.0556116	0.0589036	22.07	-3555.1280423	-3555.1181906	-3555.0837713	-3555.0739196
-1	7	ZnCl2_d5_mol6_aam	-3554.6829590	0.0431076	0.0511197	0.0545334	0.0578532	22.75	-3555.1231857	-3555.1133857	-3555.0800780	-3555.0702780
-1	8	ZnCl2_d3_mol6_aan	-3554.6712828	0.0438582	0.0518473	0.0552492	0.0585560	15.93	-3555.1151083	-3555.1046857	-3555.0712501	-3555.0608274
-1	9	ZnCl2_d2_mol6_aaj	-3554.6671766	0.0432127	0.0512166	0.0546235	0.0579344	16.63	-3555.1166641	-3555.1054524	-3555.0734514	-3555.0622397
-1	10	ZnCl2_d5_mol6_aae	-3554.6618883	0.0421825	0.0502287	0.0536582	0.0569942	21.31	-3555.1054643	-3555.0950116	-3555.0632818	-3555.0528291
-1	11	ZnCl2_d3_mol6_aae	-3554.6413194	0.0419520	0.0500001	0.0534304	0.0567671	27.43	-3555.0882926	-3555.0775169	-3555.0463405	-3555.0355648
-1	12	ZnCl2_d2_mol6_aao	-3554.6398723	0.0411298	0.0493166	0.0528056	0.0561991	4.37	-3555.0948314	-3555.0826035	-3555.0537015	-3555.0414736
-1	13	ZnCl2_d2_mol6_aal	-3554.6401024	0.0423553	0.0503998	0.0538244	0.0571528	15.60	-3555.0956514	-3555.0832892	-3555.0532961	-3555.0409338
-1	14	ZnCl2_d8_mol6_aaj	-3554.6294497	0.0407632	0.0488682	0.0523214	0.0556795	13.02	-3555.0822882	-3555.0700271	-3555.0415249	-3555.0292639
-1	15	ZnCl2_d8_mol6_aal	-3554.6226324	0.0402942	0.0484199	0.0518813	0.0552470	18.90	-3555.0755863	-3555.0634368	-3555.0352921	-3555.0231426
-1	16	ZnCl2_d8_mol6_aah	-3554.6147159	0.0390261	0.0473196	0.0508527	0.0542879	11.64	-3555.0735461	-3555.0605803	-3555.0345199	-3555.0215541
-1	17	ZnCl2_d8_mol6_abj	-3554.6145066	0.0391394	0.0474240	0.0509538	0.0543863	5.25	-3555.0725078	-3555.0596468	-3555.0333683	-3555.0205073
-1	18	ZnCl2_d2_mol6_aag	-3554.6112621	0.0405923	0.0487087	0.0521671	0.0555303	17.50	-3555.0673082	-3555.0548301	-3555.0267158	-3555.0142377
-1	19	ZnCl2_d2_mol6_aax	-3554.6038303	0.0400238	0.0482566	0.0517652	0.0551776	14.00	-3555.0677089	-3555.0540440	-3555.0276851	-3555.0140201
0	1	1_C2H6NMgCl_mol6_aab	-1650.5308139	0.1343963	0.1431438	0.1468438	0.1504248	22.36	-1650.7743467	-1650.7696146	-1650.6399503	-1650.6352183
0	2	1_C2H6NMgCl_mol6_aap	-1650.5301588	0.1340425	0.1428305	0.1465489	0.1501484	17.73	-1650.7732140	-1650.7685447	-1650.6391714	-1650.6345022
0	1	1_C2H6NZnCl_mol6_aab	-3229.5740728	0.1337500	0.1425970	0.1463398	0.1499623	26.24	-3229.9656533	-3229.9618343	-3229.8319033	-3229.8280842
0	2	1_C2H6NZnCl_mol6_aap	-3229.5729056	0.1330528	0.1419920	0.1457766	0.1494416	18.71	-3229.9646002	-3229.9607620	-3229.8315473	-3229.8277092
0	1	1_LiCl_8MgCl_d8_mol6	-1983.1747973	0.0469032	0.0550588	0.0585194	0.0618754	15.88	-1983.4453815	-1983.4366521	-1983.3984783	-1983.3897488
0	2	1_LiCl_5MgCl_d5_mol6	-1983.1393957	0.0462923	0.0545561	0.0580677	0.0614763	23.62	-1983.4273520	-1983.4159135	-1983.3810596	-1983.3696212
0	3	1_LiCl_3MgCl_d3_mol6	-1983.1299715	0.0459350	0.0542819	0.0578323	0.0612810	25.92	-1983.4355738	-1983.4213405	-1983.3896387	-1983.3754055
0	4	1_LiCl_2MgCl_d2_mol6	-1983.1229750	0.0453217	0.0536974	0.0572603	0.0607212	26.63	-1983.4252263	-1983.4115011	-1983.3799045	-1983.3661794
0	1	1_LiCl_mol14_pos8	-4424.7774922	0.1222825	0.1332673	0.1378687	0.1422926	14.44	-4425.3191459	-4425.3120525	-4425.1968634	-4425.1897700

0	2	1_LiCl_mol14_pos2_5	-4424.7720533	0.1221629	0.1331988	0.1378235	0.1422710	12.31	-4425.3203992	-4425.3125548	-4425.1982362	-4425.1903919
0	3	1_LiCl_mol14_pos2_8	-4424.7707914	0.1221084	0.1331386	0.1377614	0.1422073	12.98	-4425.3155608	-4425.3081386	-4425.1934524	-4425.1860302
0	4	1_LiCl_mol14_pos2	-4424.7505128	0.1212545	0.1324809	0.1371944	0.1417330	12.12	-4425.3170046	-4425.3066238	-4425.1957500	-4425.1853692
0	5	1_LiCl_mol14_pos8_38	-4424.7412481	0.1226101	0.1335639	0.1381521	0.1425634	15.77	-4425.3116322	-4425.3003109	-4425.1890220	-4425.1777007
0	6	1_LiCl_mol14_pos5	-4424.7144152	0.1192201	0.1306983	0.1355298	0.1401905	6.46	-4425.3178077	-4425.3015956	-4425.1985875	-4425.1823754
0	7	1_LiCl_mol14_pos3	-4424.7090211	0.1196662	0.1311679	0.1360107	0.1406833	7.06	-4425.3200532	-4425.3023744	-4425.2003870	-4425.1827081
0	8	1_LiCl_mol14_pos2_15	-4424.6986273	0.1185304	0.1300884	0.1349555	0.1396521	6.98	-4425.3055439	-4425.2885819	-4425.1870135	-4425.1700515
0	1	1_LiCl_mol15_pos8_19	-4609.2711139	0.1143985	0.1265386	0.1316167	0.1364932	11.40	-4609.8742118	-4609.8654228	-4609.7598132	-4609.7510243
0	2	1_LiCl_mol15_pos8	-4609.2704970	0.1145509	0.1266469	0.1317048	0.1365608	13.99	-4609.8675274	-4609.8595120	-4609.7529765	-4609.7449611
0	3	1_LiCl_mol15_pos2_17	-4609.2671624	0.1144862	0.1266079	0.1316787	0.1365482	12.98	-4609.8711659	-4609.8622066	-4609.7566797	-4609.7477204
0	4	1_LiCl_mol15_pos2_12	-4609.2596282	0.1142115	0.1263259	0.1313903	0.1362514	9.78	-4609.8656978	-4609.8567221	-4609.7514862	-4609.7425105
0	5	1_LiCl_mol15_pos2_15	-4609.2370913	0.1128543	0.1252353	0.1304244	0.1354141	7.65	-4609.8734345	-4609.8599906	-4609.7605802	-4609.7471363
0	6	1_LiCl_mol15_pos2_13	-4609.2357797	0.1132283	0.1255372	0.1306922	0.1356465	7.84	-4609.8665085	-4609.8538768	-4609.7532802	-4609.7406484
0	7	1_LiCl_mol15_pos5	-4609.2143152	0.1118888	0.1243749	0.1296166	0.1346625	11.04	-4609.8605745	-4609.8454982	-4609.7486857	-4609.7336094
0	1	1_LiCl_mol16e_2	-1761.2355286	0.1605612	0.1704578	0.1746188	0.1786309	24.40	-1761.5513975	-1761.5451490	-1761.3908362	-1761.3845877
0	1	1_LiCl_mol17_pos8_2	-2421.0509760	0.1463525	0.1572402	0.1618103	0.1662104	13.64	-2421.4342733	-2421.4248135	-2421.2879207	-2421.2784609
0	2	1_LiCl_mol17_pos8_1	-2421.0505803	0.1463566	0.1572420	0.1618111	0.1662102	14.21	-2421.4341564	-2421.4246163	-2421.2877997	-2421.2782597
0	3	1_LiCl_mol17_pos5_2	-2421.0256279	0.1461224	0.1570538	0.1616454	0.1660684	17.88	-2421.4184011	-2421.4076084	-2421.2722786	-2421.2614859
0	4	1_LiCl_mol17_pos5_1	-2421.0240263	0.1459517	0.1568965	0.1614944	0.1659239	17.08	-2421.4185844	-2421.4074994	-2421.2726326	-2421.2615476
0	1	1_LiCl_mol6_1	-1323.3623715	0.0615453	0.0686307	0.0716483	0.0745830	45.98	-1323.5680858	-1323.5620421	-1323.5065405	-1323.5004968
0	2	1_LiCl_mol6_2	-1323.3595388	0.0612710	0.0683815	0.0714114	0.0743593	30.62	-1323.5667180	-1323.5606639	-1323.5054469	-1323.4993928
0	1	1_LiCl_mol7e	-1415.6054956	0.0574424	0.0651163	0.0683761	0.0715404	36.54	-1415.8392067	-1415.8326374	-1415.7817642	-1415.7751950
0	1	1_LiCl_2TMPZn_d2_mol6_c	-3510.6027920	0.2932979	0.3042328	0.3087880	0.3131525	18.34	-3511.0697797	-3511.0641790	-3510.7764818	-3510.7708810
0	2	1_LiCl_2TMPZn_d2_mol6_b	-3510.6001549	0.2932321	0.3041652	0.3087216	0.3130890	19.72	-3511.0652480	-3511.0598406	-3510.7720158	-3510.7666084
0	3	1_LiCl_8TMPZn_d8_mol6_c	-3510.5995859	0.2936837	0.3045636	0.3090945	0.3134349	13.81	-3511.0669248	-3511.0611911	-3510.7732410	-3510.7675073
0	4	1_LiCl_8TMPZn_d8_mol6_d	-3510.5970011	0.2929190	0.3038809	0.3084494	0.3128282	12.44	-3511.0638835	-3511.0581553	-3510.7709645	-3510.7652362
0	5	1_LiCl_5TMPZn_d5_mol6_a	-3510.5911352	0.2932323	0.3042504	0.3088488	0.3132606	19.46	-3511.0754740	-3511.0670699	-3510.7822417	-3510.7738375
0	6	1_LiCl_5TMPZn_d5_mol6_b	-3510.5904705	0.2928478	0.3039254	0.3085507	0.3129899	11.04	-3511.0744699	-3511.0660578	-3510.7816221	-3510.7732099
0	7	1_LiCl_3TMPZn_d3_mol6_a	-3510.5908277	0.2932983	0.3043551	0.3089707	0.3133999	14.82	-3511.0744153	-3511.0660086	-3510.7811169	-3510.7727102
0	8	1_LiCl_3TMPZn_d3_mol6_b	-3510.5906084	0.2935093	0.3045375	0.3091406	0.3135573	18.64	-3511.0743815	-3511.0659473	-3510.7808722	-3510.7724379
0	9	1_LiCl_8TMPZn_d8_mol6_a	-3510.5868861	0.2935432	0.3045064	0.3090793	0.3134652	23.25	-3511.0623863	-3511.0554408	-3510.7688430	-3510.7618976
0	1	1_LiCl_2TMPZn_d2_mol7e	-3602.8470458	0.2886215	0.3001981	0.3050214	0.3096428	12.87	-3603.3441813	-3603.3376041	-3603.0555597	-3603.0489825
0	2	1_LiCl_2TMPZn_d2_mol7e_31	-3602.8440673	0.2897008	0.3011986	0.3059832	0.3105634	14.65	-3603.3423447	-3603.3356801	-3603.0526439	-3603.0459792
0	3	1_LiCl_2TMPZn_d2_mol7e_26	-3602.8428318	0.2885540	0.3001131	0.3049288	0.3095428	9.19	-3603.3412011	-3603.3344647	-3603.0526470	-3603.0459107
0	4	1_LiCl_2TMPZn_d2_mol7e_28	-3602.8430678	0.2891321	0.3006498	0.3054462	0.3100402	12.22	-3603.3404548	-3603.3338772	-3603.0513227	-3603.0447451
0	5	1_LiCl_8TMPZn_d8_mol7e_20	-3602.8404568	0.2888508	0.3004120	0.3052251	0.3098338	9.97	-3603.3374288	-3603.3309321	-3603.0485780	-3603.0420812
0	6	1_LiCl_5TMPZn_d5_mol7e	-3602.8382089	0.2889394	0.3005443	0.3053842	0.3100249	10.84	-3603.3462203	-3603.3379416	-3603.0572809	-3603.0490022
0	7	1_LiCl_5TMPZn_d5_mol7e_36	-3602.8385804	0.2894290	0.3009723	0.3057842	0.3103965	13.49	-3603.3468150	-3603.3385186	-3603.0573859	-3603.0490896
0	8	1_LiCl_5TMPZn_d5_mol7e_40	-3602.8320578	0.2886510	0.3002591	0.3051006	0.3097430	13.84	-3603.3414144	-3603.3329461	-3603.0527634	-3603.0442951
0	9	1_LiCl_5TMPZn_d5_mol7e_38	-3602.8321042	0.2890331	0.3006284	0.3054653	0.3101040	8.08	-3603.3399659	-3603.3316910	-3603.0509327	-3603.0426579
0	10	1_LiCl_5TMPZn_d5_mol7e_1	-3602.8316640	0.2886736	0.3002925	0.3051393	0.3097873	13.12	-3603.3393895	-3603.3311483	-3603.0507159	-3603.0424747
0	11	1_LiCl_8TMPZn_d8_mol7e	-3602.8311192	0.2898419	0.3013427	0.3061359	0.3107297	21.75	-3603.3354380	-3603.3276701	-3603.0455961	-3603.0378281
0	12	1_LiCl_8TMPZn_d8_mol7e_16	-3602.8240856	0.2886057	0.3002062	0.3050425	0.3096783	18.08	-3603.3263063	-3603.3188683	-3603.0377005	-3603.0302626
0	13	1_LiCl_8TMPZn_d8_mol7e_11	-3602.8238016	0.2888180	0.3003711	0.3051880	0.3098057	22.28	-3603.3262088	-3603.3187298	-3603.0373907	-3603.0299117
0	14	1_LiCl_8TMPZn_d8_mol7e_14	-3602.8244446	0.2895573	0.3010757	0.3058776	0.3104808	22.49	-3603.3294144	-3603.3215513	-3603.0398570	-3603.0319939
0	1	1_LiCl_2ZnCl_d2_mol6_aaq	-3562.2257812	0.0465520	0.0547732	0.0582627	0.0616471	39.70	-3562.6443655	-3562.6366695	-3562.5978134	-3562.5901175
0	2	1_LiCl_8ZnCl_d8_mol6_aac	-3562.2227686	0.0460934	0.0543707	0.0578843	0.0612923	11.67	-3562.6441527	-3562.6359059	-3562.5980593	-3562.5898125
0	3	1_LiCl_5ZnCl_d5_mol6_aae	-3562.2000810	-0.0054872	0.0028733	0.0064293	0.0098830	24.82	-3562.5824938	-3562.5722534	-3562.5879810	-3562.5777405
0	4	1_LiCl_3ZnCl_d3_mol6_aap	-3562.1998995	0.0459186	0.0542875	0.0578473	0.0613051	27.63	-3562.6428305	-3562.6311254	-3562.5969118	-3562.5852067
0	1	1_LiCl_2_ZnCl_d2_mol7e	-3654.4697471	0.0424624	0.0512586	0.0549848	0.0585937	26.62	-3654.9215914	-3654.9124567	-3654.8791290	-3654.8699943
0	2	1_LiCl_8_ZnCl_d8_mol7e	-3654.4667983	0.0422594	0.0510813	0.0548183	0.0584376	16.09	-3654.9176011	-3654.9085546	-3654.8753417	-3654.8662951
0	3	1_LiCl_5_ZnCl_d5_mol7e	-3654.4468649	0.0417390	0.0506370	0.0544129	0.0580740	23.90	-3654.9116178	-3654.9004430	-3654.8698787	-3654.8587040
0	1	1_MgCl2_mol14_pos2_27	-5730.4681535	0.1179634	0.1303569	0.1355536	0.1405514	10.54	-5731.1147782	-5731.1048531	-5730.9968147	-5730.9868896
0	2	1_MgCl2_mol14_pos8	-5730.4585676	0.1180407	0.1303329	0.1354816	0.1404296	18.59	-5731.0946299	-5731.0869586	-5730.9765892	-5730.9689178
0	3	1_MgCl2_mol14_pos2	-5730.4457247	0.1157329	0.1284192	0.1337477	0.1388786	5.02	-5731.1027230	-5731.0918762	-5730.9869901	-5730.9761433
0	4	1_MgCl2_mol14_pos8_1	-5730.4427227	0.1189078	0.1311233	0.1362379	0.1411518	14.01	-5731.0929946	-5731.0828374	-5730.9740868	-5730.9639295
0	5	1_MgCl2_mol14_pos5	-5730.4156114	0.1149028	0.1277430	0.1331458	0.1383548	4.19	-5731.1105179	-5731.0937931	-5730.9956150	-5730.9788903
0	6	1_MgCl2_mol14_pos5_29	-5730.4177152	0.1176530	0.1299982	0.1351751	0.1401546	17.88	-5731.1008603	-5731.0855520	-5730.9832072	-5730.9678990
0	7	1_MgCl2_mol14_pos3	-5730.4126850	0.1155548	0.1284014	0.1338075	0.1390200	4.87	-5731.1134664	-5731.0957492	-5730.9979115	-5730.9801944
0	8	1_MgCl2_mol14_pos5_31	-5730.3970797	0.1170921	0.1295199	0.1347353	0.1397545	13.54	-5731.0945504	-5731.0772434	-5730.9774583	-5730.9601513

0	1	1_MgCl2_mol15_pos2_7	-5914.9584400	0.1101110	0.1236112	0.1292630	0.1346919	9.34	-5915.6628371	-5915.6516317	-5915.5527261	-5915.5415206
0	2	1_MgCl2_mol15_pos8_s1	-5914.9505290	0.1095588	0.1230943	0.1287606	0.1342032	12.37	-5915.6480092	-5915.6381560	-5915.5384503	-5915.5285972
0	3	1_MgCl2_mol15_pos2_9	-5914.9517796	0.1125547	0.1256749	0.1311491	0.1363948	13.91	-5915.6407285	-5915.6322666	-5915.5281738	-5915.5197118
0	4	1_MgCl2_mol15_pos8	-5914.9429935	0.1101366	0.1235453	0.1291529	0.1345354	16.63	-5915.6347179	-5915.6258970	-5915.5245813	-5915.5157604
0	5	1_MgCl2_mol15_pos2	-5914.9391962	0.1080734	0.1218195	0.1275818	0.1331219	7.37	-5915.6553992	-5915.6430406	-5915.5473257	-5915.5349671
0	6	1_MgCl2_mol15_pos2_5	-5914.9353069	0.1109174	0.1242411	0.1298101	0.1351533	14.74	-5915.6299127	-5915.6205451	-5915.5189952	-5915.5096277
0	7	1_MgCl2_mol15_pos5	-5914.9140825	0.1076305	0.1214611	0.1272658	0.1328514	9.54	-5915.6471313	-5915.6321983	-5915.5395008	-5915.5245678
0	8	1_MgCl2_mol15_pos2_8	-5914.9172144	0.1122226	0.1253991	0.1309003	0.1361743	14.85	-5915.6193906	-5915.6089514	-5915.5071680	-5915.4967287
0	9	1_MgCl2_mol15_pos5_10	-5914.8806003	0.1114155	0.1246726	0.1302135	0.1355298	16.23	-5915.6055228	-5915.5911979	-5915.4941073	-5915.4797824
0	1	1_MgCl2_mol6	-1976.2137842	0.0591785	0.0669821	0.0703016	0.0735264	27.39	-1976.4634119	-1976.4574179	-1976.4042333	-1976.3982394
0	1	1_MgCl2_mol7e	-2068.4547913	0.0550332	0.0634212	0.0669812	0.0704339	24.83	-2068.7320271	-2068.7255286	-2068.6769938	-2068.6704954
0	1	1_MgCl2_2TMPZn_d2_mol6_c	-4163.4486505	0.2911934	0.3028262	0.3076772	0.3123279	13.57	-4163.9646133	-4163.9580857	-4163.6734198	-4163.6668922
0	2	1_MgCl2_2TMPZn_d2_mol6_b	-4163.4473741	0.2914352	0.3030362	0.3078745	0.3125136	19.67	-4163.9613758	-4163.9550642	-4163.6699406	-4163.6636290
0	3	1_MgCl2_5TMPZn_d5_mol6_b	-4163.4428568	0.2900926	0.3019129	0.3068506	0.3115901	7.51	-4163.9708974	-4163.9625162	-4163.6808048	-4163.6724235
0	4	1_MgCl2_5TMPZn_d5_mol6_a	-4163.4435833	0.2909140	0.3026325	0.3075251	0.3122195	16.24	-4163.9713519	-4163.9630514	-4163.6804378	-4163.6721373
0	5	1_MgCl2_3TMPZn_d3_mol6_a	-4163.4435198	0.2912756	0.3030009	0.3078966	0.3125941	15.48	-4163.9715768	-4163.9631623	-4163.6803011	-4163.6718866
0	6	1_MgCl2_3TMPZn_d3_mol6_b	-4163.4434840	0.2913128	0.3030353	0.3079298	0.3126263	12.74	-4163.9714100	-4163.9630071	-4163.6800971	-4163.6716942
0	7	1_MgCl2_8TMPZn_d8_mol6_a2	-4163.4422437	0.2903950	0.3021047	0.3069891	0.3116725	8.26	-4163.9586726	-4163.9522227	-4163.6682776	-4163.6618276
0	8	1_MgCl2_8TMPZn_d8_mol6_a	-4163.4417638	0.2901382	0.3018307	0.3067083	0.3113855	17.00	-4163.9575308	-4163.9511367	-4163.6673926	-4163.6609984
0	1	1_MgCl2_2ZnCl_d2_mol6_aaq	-4215.0671446	0.0441579	0.0530993	0.0568932	0.0605714	31.55	-4215.5346709	-4215.5260011	-4215.4905129	-4215.4818431
0	2	1_MgCl2_8ZnCl_d8_mol6_aac2	-4215.0614704	0.0436533	0.0526442	0.0564592	0.0601579	17.81	-4215.5326920	-4215.5235740	-4215.4890386	-4215.4799206
0	3	1_MgCl2_5ZnCl_d5_mol6_aae	-4215.0511562	0.0431647	0.0522461	0.0561055	0.0598511	23.38	-4215.5360744	-4215.5247198	-4215.4929096	-4215.4815550
0	4	1_MgCl2_3ZnCl_d3_mol6_aap	-4215.0515669	0.0437319	0.0527938	0.0566446	0.0603817	22.99	-4215.5387910	-4215.5271343	-4215.4950591	-4215.4834023
0	5	1_MgCl2_3ZnCl_d3_mol6_aap2	-4215.0053003	0.0416414	0.0508578	0.0547774	0.0585834	22.95	-4215.5215674	-4215.5057765	-4215.4799259	-4215.4641350
0	6	1_MgCl2_5ZnCl_d5_mol6_aae2	-4214.9963445	0.0412604	0.0504779	0.0543973	0.0582026	17.99	-4215.5205855	-4215.5034697	-4215.4793251	-4215.4622092
0	1	1_MgCl_d8_mol6	-1515.2931991	0.0485445	0.0556263	0.0586417	0.0615737	49.54	-1515.5099302	-1515.5040435	-1515.4613857	-1515.4554990
0	2	1_MgCl_d2_mol6	-1515.2865180	0.0484745	0.0555674	0.0585889	0.0615277	38.22	-1515.5019948	-1515.4963128	-1515.4535203	-1515.4478383
0	3	1_MgCl_d3_mol6	-1515.2419576	0.0468104	0.0540380	0.0571201	0.0601198	32.56	-1515.4978174	-1515.4856631	-1515.4510069	-1515.4388526
0	4	1_MgCl_d5_mol6	-1515.2405572	0.0463612	0.0535975	0.0566831	0.0596863	32.70	-1515.5028959	-1515.4894888	-1515.4565346	-1515.4431276
0	1	1_TMPZnCl_mol6_2	-3503.6265224	0.3041260	0.3147845	0.3192311	0.3234965	20.84	-3504.0745287	-3504.0713617	-3503.7704027	-3503.7672357
0	2	1_TMPZnCl_mol6_1	-3503.6239367	0.3027034	0.3135511	0.3180831	0.3224347	2.22	-3504.0722978	-3504.0690305	-3503.7695943	-3503.7663270
0	3	1_TMPZnCl_mol6_3	-3503.6239530	0.3037178	0.3144136	0.3188780	0.3231620	10.11	-3504.0693436	-3504.0665218	-3503.7656258	-3503.7628040
0	4	1_TMPZnCl_mol6_4	-3503.6222189	0.3044409	0.3150535	0.3194817	0.3237300	23.28	-3504.0667328	-3504.0639554	-3503.7622919	-3503.7595144
0	1	1_ZnCl2_mol6	-3555.2471047	0.0576751	0.0656348	0.0690223	0.0723141	24.18	-3555.6444579	-3555.6394311	-3555.5867828	-3555.5817559
0	1	1_ZnCl_d8_mol6	-3094.3520404	0.0473786	0.0546256	0.0577149	0.0607209	45.59	-3094.7227473	-3094.7170244	-3094.6753687	-3094.6696457
0	2	1_ZnCl_d2_mol6	-3094.3503609	0.0476410	0.0548553	0.0579304	0.0609225	40.83	-3094.7212569	-3094.7153213	-3094.6736158	-3094.6676803
0	3	1_ZnCl_d3_mol6	-3094.2949200	0.0468392	0.0540762	0.0571616	0.0601640	43.22	-3094.6871164	-3094.6774275	-3094.6402771	-3094.6305882
0	4	1_ZnCl_d5_mol6	-3094.2928339	0.0463772	0.0536265	0.0567170	0.0597244	42.38	-3094.6916619	-3094.6807529	-3094.6452846	-3094.6343757
0	1	C2H6NH	-135.1862246	0.0667220	0.0712777	0.0732451	0.0751754	234.27	-135.2245893	-135.2241579	-135.1578673	-135.1574359
0	1	C2H6NMgCl	-794.9622406	0.0491602	0.0551346	0.0577024	0.0602129	63.39	-795.0881111	-795.0818215	-795.0389509	-795.0326612
0	1	C2H6NMgClLiCl	-1262.8400630	0.0472496	0.0542997	0.0573115	0.0602433	45.15	-1263.0113035	-1263.0037579	-1262.9640538	-1262.9565083
0	1	C2H6NMgCl_mol6_aab	-1650.5308139	0.1343963	0.1431438	0.1468438	0.1504248	22.36	-1650.7743467	-1650.7696146	-1650.6399503	-1650.6352183
0	2	C2H6NMgCl_mol6_aap	-1650.5301588	0.1340425	0.1428305	0.1465489	0.1501484	17.73	-1650.7732140	-1650.7685447	-1650.6391714	-1650.6345022
0	3	C2H6NMgCl_mol6_aag	-1650.5193603	0.1340556	0.1428230	0.1465331	0.1501250	22.58	-1650.7655538	-1650.7605626	-1650.6314982	-1650.6265070
0	4	C2H6NMgCl_mol6_aaq	-1650.5191397	0.1338548	0.1426518	0.1463743	0.1499780	19.82	-1650.7653370	-1650.7603822	-1650.6314821	-1650.6265274
0	5	C2H6NMgCl_mol6_aaa	-1650.4994221	0.1314294	0.1405234	0.1443780	0.1481138	4.86	-1650.7447632	-1650.7399048	-1650.6133338	-1650.6084754
0	6	C2H6NMgCl_mol6_aai	-1650.5002758	0.1324452	0.1413618	0.1451382	0.1487961	12.67	-1650.7487119	-1650.7432725	-1650.6162667	-1650.6108272
0	7	C2H6NMgCl_mol6_aam	-1650.4994169	0.1316742	0.1407296	0.1445672	0.1482859	8.46	-1650.7447960	-1650.7399241	-1650.6131217	-1650.6082499
0	8	C2H6NMgCl_mol6_acr	-1650.5006709	0.1333181	0.1421316	0.1458613	0.1494721	22.22	-1650.7443137	-1650.7394442	-1650.6109956	-1650.6061260
0	9	C2H6NMgCl_mol6_adt	-1650.4971156	0.1320394	0.1410463	0.1448625	0.1485600	5.03	-1650.7431293	-1650.7378871	-1650.6110898	-1650.6058476
0	10	C2H6NMgCl_mol6_abp	-1650.4963537	0.1320284	0.1409651	0.1447520	0.1484215	20.97	-1650.7475801	-1650.7417234	-1650.6155517	-1650.6096949
0	11	C2H6NMgCl_mol6_aba	-1650.4942206	0.1317566	0.1407181	0.1445166	0.1481981	16.23	-1650.7440081	-1650.7382947	-1650.6122515	-1650.6065380
0	12	C2H6NMgCl_mol6_ach	-1650.4887206	0.1318029	0.1408349	0.1446651	0.1483784	13.87	-1650.7541584	-1650.7460856	-1650.6223555	-1650.6142826
0	13	C2H6NMgCl_mol6_aae	-1650.4865079	0.1307942	0.1399320	0.1438107	0.1475737	10.51	-1650.7536553	-1650.7453429	-1650.6228610	-1650.6145486
0	14	C2H6NMgCl_mol6_aac	-1650.4863455	0.1307470	0.1398810	0.1437577	0.1475185	17.69	-1650.7504989	-1650.7429449	-1650.6197519	-1650.6121979
0	15	C2H6NMgCl_mol6_acs	-1650.4863213	0.1308569	0.1399987	0.1438788	0.1476430	11.82	-1650.7503947	-1650.7428545	-1650.6195377	-1650.6119976
0	16	C2H6NMgCl_mol6_aak	-1650.4858584	0.1306761	0.1398347	0.1437225	0.1474945	13.15	-1650.7497420	-1650.7421974	-1650.6190659	-1650.6115212
0	17	C2H6NMgCl_mol6_adm	-1650.4822462	0.1280880	0.1375972	0.1416417	0.1455711	1.11	-1650.7467375	-1650.7391020	-1650.6186495	-1650.6110140
0	18	C2H6NMgCl_mol6_adn	-1650.4823915	0.1289947	0.1383920	0.1423864	0.1462654	2.55	-1650.7453591	-1650.7379380	-1650.6163643	-1650.6089433
0	1	C2H6NZnCl_1	-2374.0216873	0.0479619	0.0541238	0.0567766	0.0593731	21.91	-2374.2880001	-2374.2836837	-2374.2400382	-2374.2357217

0	1	C2H6NZnCl_mol6_aak	-3229.5740728	0.1337499	0.1425969	0.1463397	0.1499622	26.24	-3229.9656533	-3229.9618343	-3229.8319034	-3229.8280844
0	2	C2H6NZnCl_mol6_aap	-3229.5729056	0.1330527	0.1419919	0.1457766	0.1494415	18.70	-3229.9646002	-3229.9607621	-3229.8315474	-3229.8277093
0	3	C2H6NZnCl_mol6_aaq	-3229.5648439	0.1327253	0.1416712	0.1454598	0.1491293	23.46	-3229.9583555	-3229.9543648	-3229.8256301	-3229.8216394
0	4	C2H6NZnCl_mol6_abk	-3229.5643916	0.1329558	0.1418808	0.1456600	0.1493202	20.24	-3229.9578765	-3229.9538638	-3229.8249206	-3229.8209079
0	5	C2H6NZnCl_mol6_acl	-3229.5593601	0.1324002	0.1413771	0.1451790	0.1488615	11.48	-3229.9547438	-3229.9504525	-3229.8223435	-3229.8180523
0	6	C2H6NZnCl_mol6_abo	-3229.5557611	0.1316802	0.1407046	0.1445307	0.1482394	25.29	-3229.9536557	-3229.9488337	-3229.8219755	-3229.8171534
0	7	C2H6NZnCl_mol6_aab	-3229.5552478	0.1317900	0.1408215	0.1446498	0.1483602	8.29	-3229.9514057	-3229.9468042	-3229.8196157	-3229.8150142
0	8	C2H6NZnCl_mol6_acn	-3229.5552473	0.1322050	0.1411948	0.1450038	0.1486946	11.38	-3229.9523219	-3229.9476152	-3229.8201168	-3229.8154102
0	9	C2H6NZnCl_mol6_aad	-3229.5541093	0.1321447	0.1411535	0.1449721	0.1486731	19.58	-3229.9520876	-3229.9472010	-3229.8199429	-3229.8150563
0	10	C2H6NZnCl_mol6_aai	-3229.5525055	0.1310377	0.1401361	0.1439963	0.1477399	14.92	-3229.9520175	-3229.9468481	-3229.8209797	-3229.8158104
0	11	C2H6NZnCl_mol6_aat	-3229.5528945	0.1318024	0.1408536	0.1446920	0.1484133	16.24	-3229.9521672	-3229.9472052	-3229.8203647	-3229.8154027
0	12	C2H6NZnCl_mol6_abl	-3229.5518762	0.1318377	0.1408742	0.1447059	0.1484206	14.71	-3229.9504378	-3229.9454794	-3229.8186000	-3229.8136417
0	13	C2H6NZnCl_mol6_abd	-3229.5496797	0.1297042	0.1390076	0.1429598	0.1467960	9.46	-3229.9470223	-3229.9424525	-3229.8173181	-3229.8127483
0	14	C2H6NZnCl_mol6_abf	-3229.5510259	0.1313690	0.1404476	0.1442977	0.1480305	17.49	-3229.9499527	-3229.9449899	-3229.8185837	-3229.8136209
0	15	C2H6NZnCl_mol6_ach	-3229.5498454	0.1315405	0.1406459	0.1445093	0.1482562	15.02	-3229.9561785	-3229.9499799	-3229.8246379	-3229.8184393
0	16	C2H6NZnCl_mol6_aae	-3229.5469512	0.1298023	0.1391160	0.1430737	0.1469161	6.56	-3229.9543781	-3229.9480409	-3229.8245757	-3229.8182386
0	17	C2H6NZnCl_mol6_aav	-3229.5454789	0.1292385	0.1386121	0.1425963	0.1464651	7.51	-3229.9503828	-3229.9447295	-3229.8211443	-3229.8154909
0	18	C2H6NZnCl_mol6_abu	-3229.5473235	0.1312634	0.1404259	0.1443137	0.1480844	15.23	-3229.9507979	-3229.9451916	-3229.8195345	-3229.8139281
0	19	C2H6NZnCl_mol6_ace	-3229.5454240	0.1296962	0.1390097	0.1429665	0.1468074	10.87	-3229.9505458	-3229.9448535	-3229.8208495	-3229.8151572
0	20	C2H6NZnCl_mol6_acv	-3229.5456436	0.1301196	0.1393990	0.1433404	0.1471659	8.01	-3229.9508888	-3229.9451839	-3229.8207691	-3229.8150643
0	21	C2H6NZnCl_mol6_aac	-3229.5457762	0.1303974	0.1396296	0.1435495	0.1473531	14.29	-3229.9511461	-3229.9454225	-3229.8207487	-3229.8150250
0	22	C2H6NZnCl_mol6_aaf	-3229.5455687	0.1306597	0.1398640	0.1437716	0.1475628	13.69	-3229.9504495	-3229.9447634	-3229.8197897	-3229.8141036
0	23	C2H6NZnCl_mol6_adn	-3229.5421588	0.1285718	0.1380580	0.1420920	0.1460105	3.52	-3229.9459769	-3229.9404333	-3229.8174051	-3229.8118614
0	1	C2H6NZn_d3_mol6	-2768.6903500	0.1237589	0.1319807	0.1354664	0.1388454	20.93	-2769.0541512	-2769.0493586	-2768.9303922	-2768.9255996
0	2	C2H6NZn_d5_mol6	-2768.6891562	0.1226197	0.1309273	0.1344514	0.1378692	7.44	-2769.0539838	-2769.0490691	-2768.9313640	-2768.9264494
0	3	C2H6NZn_d8_mol6	-2768.6857421	0.1228162	0.1310694	0.1345679	0.1379591	27.88	-2769.0465740	-2769.0426991	-2768.9237577	-2768.9198829
0	4	C2H6NZn_d2_mol6	-2768.6827127	0.1221939	0.1305391	0.1340788	0.1375115	6.39	-2769.0448312	-2769.0406147	-2768.9226373	-2768.9184208
0	1	C4H12N2Zn_7	-2048.3555050	0.1246238	0.1316548	0.1346548	0.1375740	53.91	-2048.6125180	-2048.6099609	-2048.4878942	-2048.4853370
0	1	furan	-230.0467664	0.0434762	0.0480625	0.0500480	0.0520011	614.68	-230.1095043	-230.1091082	-230.0660281	-230.0656320
0	1	1_LiCl_8MgCl_d8_mol6	-1983.1747973	0.0469032	0.0550588	0.0585194	0.0618754	15.88	-1983.4453815	-1983.4366521	-1983.3984783	-1983.3897488
0	2	MgClLiCl_d5_mol6_1	-1983.1711911	0.0462170	0.0544034	0.0578772	0.0612460	26.05	-1983.4387922	-1983.4306112	-1983.3925752	-1983.3843941
0	3	MgClLiCl_d5_mol6	-1983.1674954	0.0458170	0.0540808	0.0575905	0.0609962	6.63	-1983.4456765	-1983.4360120	-1983.3998594	-1983.3901949
0	4	MgClLiCl_d8_mol6	-1983.1680338	0.0465299	0.0546737	0.0581272	0.0614749	31.03	-1983.4309774	-1983.4235764	-1983.3844474	-1983.3770464
0	5	MgClLiCl_d8_mol6_1	-1983.1687664	0.0483840	0.0563297	0.0596932	0.0629496	43.44	-1983.4374114	-1983.4292056	-1983.3890274	-1983.3808215
0	6	MgClLiCl_d3_mol6	-1983.1656061	0.0466117	0.0548198	0.0583044	0.0616846	21.93	-1983.4447794	-1983.4349455	-1983.3981676	-1983.3883337
0	7	MgClLiCl_d2_mol6	-1983.1613397	0.0464337	0.0545947	0.0580574	0.0614153	27.20	-1983.4244557	-1983.4171260	-1983.3780219	-1983.3706922
0	8	1_LiCl_5MgCl_d5_mol6	-1983.1393957	0.0462923	0.0545561	0.0580677	0.0614763	23.62	-1983.4273520	-1983.4159135	-1983.3810596	-1983.3696212
0	9	1_LiCl_3MgCl_d3_mol6	-1983.1299715	0.0459350	0.0542819	0.0578323	0.0612810	25.92	-1983.4355738	-1983.4213405	-1983.3896387	-1983.3754055
0	10	1_LiCl_2MgCl_d2_mol6	-1983.1229750	0.0453217	0.0536974	0.0572603	0.0607212	26.63	-1983.4252263	-1983.4115011	-1983.3799045	-1983.3661794
0	1	1_LiCl_mol14_pos8	-4424.7774922	0.1222825	0.1332673	0.1378687	0.1422926	14.44	-4425.3191459	-4425.3120525	-4425.1968634	-4425.1897700
0	2	LiCl_mol14_pos8	-4424.7739594	0.1218777	0.1329058	0.1375267	0.1419704	15.27	-4425.3261948	-4425.3180848	-4425.2043170	-4425.1962071
0	3	1_LiCl_mol14_pos2_5	-4424.7720533	0.1221629	0.1331988	0.1378235	0.1422710	12.31	-4425.3203992	-4425.3125548	-4425.1982362	-4425.1903919
0	4	1_LiCl_mol14_pos2_8	-4424.7707914	0.1221084	0.1331386	0.1377614	0.1422073	12.98	-4425.3155608	-4425.3081386	-4425.1934524	-4425.1860302
0	5	1_LiCl_mol14_pos2	-4424.7505128	0.1212545	0.1324809	0.1371944	0.1417330	12.12	-4425.3170046	-4425.3066238	-4425.1957500	-4425.1853692
0	6	1_LiCl_mol14_pos8_38	-4424.7412481	0.1226101	0.1335639	0.1381521	0.1425634	15.77	-4425.3116322	-4425.3003109	-4425.1890220	-4425.1777007
0	7	1_LiCl_mol14_pos5	-4424.7144152	0.1192201	0.1306983	0.1355298	0.1401905	6.46	-4425.3178077	-4425.3015956	-4425.1985875	-4425.1823754
0	8	1_LiCl_mol14_pos3	-4424.7090211	0.1196662	0.1311679	0.1360107	0.1406833	7.06	-4425.3200532	-4425.3023744	-4425.2003870	-4425.1827081
0	9	1_LiCl_mol14_pos2_15	-4424.6986273	0.1185304	0.1300884	0.1349555	0.1396521	6.98	-4425.3055439	-4425.2885819	-4425.1870135	-4425.1700515
0	1	1_LiCl_mol15_pos8_19	-4609.2711139	0.1143985	0.1265386	0.1316167	0.1364932	11.40	-4609.8742118	-4609.8654228	-4609.7598132	-4609.7510243
0	2	1_LiCl_mol15_pos8	-4609.2704970	0.1145509	0.1266469	0.1317048	0.1365608	13.99	-4609.8675274	-4609.8595120	-4609.7529765	-4609.7449611
0	3	1_LiCl_mol15_pos2_15_s1	-4609.2679758	0.1143257	0.1264736	0.1315561	0.1364374	12.04	-4609.8760087	-4609.8665538	-4609.7616830	-4609.7522281
0	4	1_LiCl_mol15_pos2_17	-4609.2671624	0.1144862	0.1266079	0.1316787	0.1365482	12.98	-4609.8711659	-4609.8622066	-4609.7566797	-4609.7477204
0	5	1_LiCl_mol15_pos2_12	-4609.2596282	0.1142115	0.1263259	0.1313903	0.1362514	9.78	-4609.8656978	-4609.8567221	-4609.7514862	-4609.7425105
0	6	1_LiCl_mol15_pos2_15	-4609.2370913	0.1128543	0.1252353	0.1304244	0.1354141	7.65	-4609.8734345	-4609.8599906	-4609.7605802	-4609.7471363
0	7	1_LiCl_mol15_pos2_13	-4609.2357797	0.1132283	0.1255372	0.1306922	0.1356465	7.84	-4609.8665085	-4609.8538768	-4609.7532802	-4609.7406484
0	8	1_LiCl_mol15_pos5	-4609.2143152	0.1118888	0.1243749	0.1296166	0.1346625	11.04	-4609.8605745	-4609.8454982	-4609.7486857	-4609.7336094
0	1	LiCl_mol16e_6	-1761.2370222	0.1600723	0.1700172	0.1742004	0.1782350	6.28	-1761.5498154	-1761.5440809	-1761.3897430	-1761.3840085
0	2	1_LiCl_mol16e_2	-1761.2355286	0.1605612	0.1704578	0.1746188	0.1786309	24.40	-1761.5513975	-1761.5451490	-1761.3908362	-1761.3845877
0	3	LiCl_mol16e_7	-1761.2340810	0.1601603	0.1700737	0.1742431	0.1782642	9.20	-1761.5496110	-1761.5434436	-1761.3896107	-1761.3832832
0	4	LiCl_mol16e_3	-1761.2334526	0.1606038	0.1705001	0.1746616	0.1786745	18.82	-1761.5531069	-1761.5464179	-1761.3925031	-1761.3858141

0	5	LiCl_mol16e_4	-1761.2334492	0.1607576	0.1706354	0.1747887	0.1787936	20.98	-1761.5529037	-1761.5462325	-1761.3921460	-1761.3854748
0	1	LiCl_mol17_pos5_1	-2421.0688513	0.1478440	0.1585448	0.1630295	0.1673428	14.92	-2421.4346530	-2421.4278957	-2421.2868089	-2421.2800516
0	2	LiCl_mol17_pos5_22	-2421.0626489	0.1465135	0.1573334	0.1618727	0.1662416	20.23	-2421.4333324	-2421.4260459	-2421.2868189	-2421.2795323
0	3	1_LiCl_mol17_pos8_2	-2421.0509760	0.1463525	0.1572402	0.1618103	0.1662104	13.64	-2421.4342733	-2421.4248135	-2421.2879207	-2421.2784609
0	4	1_LiCl_mol17_pos8_1	-2421.0505803	0.1463566	0.1572420	0.1618111	0.1662102	14.21	-2421.4341564	-2421.4246163	-2421.2877997	-2421.2782597
0	5	1_LiCl_mol17_pos5_2	-2421.0256279	0.1461224	0.1570538	0.1616454	0.1660684	17.88	-2421.4184011	-2421.4076084	-2421.2722786	-2421.2614859
0	6	1_LiCl_mol17_pos5_1	-2421.0240263	0.1459517	0.1568965	0.1614944	0.1659239	17.08	-2421.4185844	-2421.4074994	-2421.2726326	-2421.2615476
0	1	LiCl_mol6_aan	-1323.3623761	0.0615389	0.0686241	0.0716416	0.0745762	46.30	-1323.5678487	-1323.5618367	-1323.5063098	-1323.5002978
0	2	LiCl_mol6_aas	-1323.3595278	0.0612460	0.0683588	0.0713896	0.0743384	29.67	-1323.5664308	-1323.5604145	-1323.5051847	-1323.4991685
0	3	LiCl_mol6_aac	-1323.3576953	0.0611839	0.0682951	0.0713250	0.0742727	44.00	-1323.5661313	-1323.5598135	-1323.5049473	-1323.4986295
0	4	LiCl_mol6_aab	-1323.3440488	0.0598091	0.0670276	0.0701044	0.0730984	27.36	-1323.5544895	-1323.5479643	-1323.4946803	-1323.4881552
0	5	LiCl_mol6_aal	-1323.3259205	0.0560918	0.0637414	0.0670162	0.0702121	13.67	-1323.5576296	-1323.5487751	-1323.5015377	-1323.4926833
0	1	LiCl_mol7e_2	-1415.6056357	0.0572453	0.0648965	0.0681477	0.0713045	29.77	-1415.8346627	-1415.8288855	-1415.7774174	-1415.7716402
0	2	1_LiCl_mol7e	-1415.6054956	0.0574424	0.0651163	0.0683761	0.0715404	36.54	-1415.8392067	-1415.8326374	-1415.7817642	-1415.7751950
0	3	LiCl_mol7e_1	-1415.6020549	0.0573253	0.0650042	0.0682669	0.0714345	31.59	-1415.8379698	-1415.8312254	-1415.7806445	-1415.7739001
0	4	LiCl_mol7e_4	-1415.5989282	0.0567713	0.0644751	0.0677490	0.0709281	23.67	-1415.8301264	-1415.8240961	-1415.7733550	-1415.7673247
0	1	LiCl_3TMPZn_d3_mol6_a	-3510.6093795	0.2940297	0.3048988	0.3094255	0.3137620	13.22	-3511.0774260	-3511.0714280	-3510.7833962	-3510.7773983
0	2	LiCl_5TMPZn_d5_mol6_aa	-3510.6078231	0.2937387	0.3045762	0.3090883	0.3134100	21.33	-3511.0770417	-3511.0708586	-3510.7833030	-3510.7771199
0	3	1_LiCl_2TMPZn_d2_mol6_c	-3510.6027920	0.2932979	0.3042328	0.3087880	0.3131525	18.34	-3511.0697797	-3511.0641790	-3510.7764818	-3510.7708810
0	4	1_LiCl_2TMPZn_d2_mol6_b	-3510.6001549	0.2932321	0.3041652	0.3087216	0.3130890	19.72	-3511.0652480	-3511.0598406	-3510.7720158	-3510.7666084
0	5	1_LiCl_8TMPZn_d8_mol6_c	-3510.5995859	0.2936837	0.3045636	0.3090945	0.3134349	13.81	-3511.0669248	-3511.0611911	-3510.7732410	-3510.7675073
0	6	1_LiCl_8TMPZn_d8_mol6_d	-3510.5970011	0.2929190	0.3038809	0.3084494	0.3128282	12.44	-3511.0638835	-3511.0581553	-3510.7709645	-3510.7652362
0	7	1_LiCl_5TMPZn_d5_mol6_a	-3510.5911352	0.2932323	0.3042504	0.3088488	0.3132606	19.46	-3511.0754740	-3511.0670699	-3510.7822417	-3510.7738375
0	8	1_LiCl_5TMPZn_d5_mol6_b	-3510.5904705	0.2928478	0.3039254	0.3085507	0.3129899	11.04	-3511.0744699	-3511.0660578	-3510.7816221	-3510.7732099
0	9	1_LiCl_3TMPZn_d3_mol6_a	-3510.5908277	0.2932983	0.3043551	0.3089707	0.3133999	14.82	-3511.0744153	-3511.0660086	-3510.7811169	-3510.7727102
0	10	1_LiCl_3TMPZn_d3_mol6_b	-3510.5906084	0.2935093	0.3045375	0.3091406	0.3135573	18.64	-3511.0743815	-3511.0659473	-3510.7808722	-3510.7724379
0	11	1_LiCl_8TMPZn_d8_mol6_a	-3510.5868861	0.2935432	0.3045064	0.3090793	0.3134652	23.25	-3511.0623863	-3511.0554408	-3510.7688430	-3510.7618976
0	1	LiCl_5TMPZn_d5_mol7e_40	-3602.8630218	0.2934035	0.3044451	0.3090250	0.3133996	27.72	-3603.3454789	-3603.3409345	-3603.0520753	-3603.0475310
0	2	1_LiCl_2TMPZn_d2_mol7e	-3602.8470458	0.2886215	0.3001981	0.3050214	0.3096428	12.87	-3603.3441813	-3603.3376041	-3603.0555597	-3603.0489825
0	3	1_LiCl_2TMPZn_d2_mol7e_31	-3602.8440673	0.2897008	0.3011986	0.3059832	0.3105634	14.65	-3603.3423447	-3603.3356801	-3603.0526439	-3603.0459792
0	4	1_LiCl_2TMPZn_d2_mol7e_26	-3602.8428318	0.2885540	0.3001131	0.3049288	0.3095428	9.19	-3603.3412011	-3603.3344647	-3603.0526470	-3603.0459107
0	5	1_LiCl_2TMPZn_d2_mol7e_28	-3602.8430678	0.2891321	0.3006498	0.3054462	0.3100402	12.22	-3603.3404548	-3603.3338772	-3603.0513227	-3603.0447451
0	6	1_LiCl_8TMPZn_d8_mol7e_20	-3602.8404568	0.2888508	0.3004120	0.3052251	0.3098338	9.97	-3603.3374288	-3603.3309321	-3603.0485780	-3603.0420812
0	7	1_LiCl_5TMPZn_d5_mol7e	-3602.8382089	0.2889394	0.3005443	0.3053842	0.3100249	10.84	-3603.3462203	-3603.3379416	-3603.0572809	-3603.0490022
0	8	1_LiCl_5TMPZn_d5_mol7e_36	-3602.8385804	0.2894290	0.3009723	0.3057842	0.3103965	13.49	-3603.3468150	-3603.3385186	-3603.0573859	-3603.0490896
0	9	1_LiCl_5TMPZn_d5_mol7e_40	-3602.8320578	0.2886510	0.3002591	0.3051006	0.3097430	13.84	-3603.3414144	-3603.3329461	-3603.0527634	-3603.0442951
0	10	1_LiCl_5TMPZn_d5_mol7e_38	-3602.8321042	0.2890331	0.3006284	0.3054653	0.3101040	8.08	-3603.3399659	-3603.3316910	-3603.0509327	-3603.0426579
0	11	1_LiCl_5TMPZn_d5_mol7e_1	-3602.8316640	0.2886736	0.3002925	0.3051393	0.3097873	13.12	-3603.3393895	-3603.3311483	-3603.0507159	-3603.0424747
0	12	1_LiCl_8TMPZn_d8_mol7e	-3602.8311192	0.2898419	0.3013427	0.3061359	0.3107297	21.75	-3603.3354380	-3603.3276701	-3603.0455961	-3603.0378281
0	13	1_LiCl_8TMPZn_d8_mol7e_16	-3602.8240856	0.2886057	0.3002062	0.3050425	0.3096783	18.08	-3603.3263063	-3603.3188683	-3603.0377005	-3603.0302626
0	14	1_LiCl_8TMPZn_d8_mol7e_11	-3602.8238016	0.2888180	0.3003711	0.3051880	0.3098057	22.28	-3603.3262088	-3603.3187298	-3603.0373907	-3603.0299117
0	15	1_LiCl_8TMPZn_d8_mol7e_14	-3602.8244446	0.2895573	0.3010757	0.3058776	0.3104808	22.49	-3603.3294144	-3603.3215513	-3603.0398570	-3603.0319939
0	1	1_LiCl_2ZnCl_d2_mol6_aaq	-3562.2257812	0.0465520	0.0547732	0.0582627	0.0616471	39.70	-3562.6443655	-3562.6366695	-3562.5978134	-3562.5901175
0	2	1_LiCl_8ZnCl_d8_mol6_aac	-3562.2227686	0.0460934	0.0543707	0.0578843	0.0612923	11.67	-3562.6441527	-3562.6359059	-3562.5980593	-3562.5898125
0	3	LiCl_8ZnCl_d8_mol6_aac2	-3562.2228587	0.0462228	0.0544661	0.0579646	0.0613574	22.24	-3562.6448707	-3562.6366563	-3562.5986478	-3562.5904335
0	4	LiCl_2ZnCl_d2_mol6_aaq	-3562.2106358	0.0451878	0.0535375	0.0570828	0.0605221	21.36	-3562.6340519	-3562.6258361	-3562.5888641	-3562.5806482
0	5	1_LiCl_5ZnCl_d5_mol6_aae	-3562.2000810	-0.0054872	0.0028733	0.0064293	0.0098830	24.82	-3562.5824938	-3562.5722534	-3562.5879810	-3562.5777405
0	6	1_LiCl_3ZnCl_d3_mol6_aap	-3562.1998995	0.0459186	0.0542875	0.0578473	0.0613051	27.63	-3562.6428305	-3562.6311254	-3562.5969118	-3562.5852067
0	1	LiCl_5_ZnCl_d5_mol7e	-3654.4840198	0.0441576	0.0527281	0.0563500	0.0598520	32.37	-3654.9151888	-3654.9091771	-3654.8710311	-3654.8650194
0	2	1_LiCl_2_ZnCl_d2_mol7e	-3654.4697471	0.0424624	0.0512586	0.0549848	0.0585937	26.62	-3654.9215914	-3654.9124567	-3654.8791290	-3654.8699943
0	3	1_LiCl_8_ZnCl_d8_mol7e	-3654.4667983	0.0422594	0.0510813	0.0548183	0.0584376	16.09	-3654.9176011	-3654.9085546	-3654.8753417	-3654.8662951
0	4	1_LiCl_5_ZnCl_d5_mol7e	-3654.4468649	0.0417390	0.0506370	0.0544129	0.0580740	23.90	-3654.9116178	-3654.9004430	-3654.8698787	-3654.8587040
0	1	MgCl2_mol14_pos8_4	-5730.4814899	0.1214304	0.1333826	0.1383755	0.1431648	25.57	-5731.1132695	-5731.1060845	-5730.9918390	-5730.9846540
0	2	1_MgCl2_mol14_pos2_27	-5730.4681535	0.1179634	0.1303569	0.1355536	0.1405514	10.54	-5731.1147782	-5731.1048531	-5730.9968147	-5730.9868896
0	3	MgCl2_mol14_pos8_1_2	-5730.4686872	0.1189920	0.1312558	0.1363908	0.1413245	13.40	-5731.1171712	-5731.1076063	-5730.9981792	-5730.9886143
0	4	MgCl2_mol14_pos8_5	-5730.4633065	0.1189339	0.1311972	0.1363320	0.1412656	11.87	-5731.1118934	-5731.1023195	-5730.9929594	-5730.9833856
0	5	1_MgCl2_mol14_pos8	-5730.4585676	0.1180407	0.1303329	0.1354816	0.1404296	18.59	-5731.0946299	-5731.0869586	-5730.9765892	-5730.9689178
0	6	MgCl2_mol14_pos8_2	-5730.4577621	0.1173787	0.1298024	0.1350106	0.1400187	13.75	-5731.1039451	-5731.0947550	-5730.9865664	-5730.9773762
0	7	1_MgCl2_mol14_pos2	-5730.4457247	0.1157329	0.1284192	0.1337477	0.1388786	5.02	-5731.1027230	-5731.0918762	-5730.9869901	-5730.9761433
0	8	1_MgCl2_mol14_pos8_1	-5730.4427227	0.1189078	0.1311233	0.1362379	0.1411518	14.01	-5731.0929946	-5731.0828374	-5730.9740868	-5730.9639295

0	9	1_MgCl2_mol14_pos5	-5730.4156114	0.1149028	0.1277430	0.1331458	0.1383548	4.19	-5731.1105179	-5731.0937931	-5730.9956150	-5730.9788903
0	10	1_MgCl2_mol14_pos5_29	-5730.4177152	0.1176530	0.1299982	0.1351751	0.1401546	17.88	-5731.1008603	-5731.0855520	-5730.9832072	-5730.9678990
0	11	1_MgCl2_mol14_pos3	-5730.4126850	0.1155548	0.1284014	0.1338075	0.1390200	4.87	-5731.1134664	-5731.0957492	-5730.9979115	-5730.9801944
0	12	MgCl2_mol14_pos5_29_2	-5730.4088280	0.1156243	0.1281047	0.1333395	0.1383752	19.79	-5731.0677712	-5731.0558765	-5730.9521469	-5730.9402522
0	13	1_MgCl2_mol14_pos5_31	-5730.3970797	0.1170921	0.1295199	0.1347353	0.1397545	13.54	-5731.0945504	-5731.0772434	-5730.9774583	-5730.9601513
0	14	MgCl2_mol14_pos5_2	-5730.3863418	0.1131408	0.1261521	0.1316308	0.1369157	7.96	-5731.0890948	-5731.0714552	-5730.9759539	-5730.9583144
0	15	MgCl2_mol14_pos3_2	-5730.3818028	0.1142757	0.1272452	0.1327060	0.1379734	6.43	-5731.0907272	-5731.0721379	-5730.9764515	-5730.9578622
0	16	MgCl2_mol14_pos5_s1	-5730.3797431	0.1158547	0.1281750	0.1333354	0.1382947	28.15	-5731.0177186	-5731.0092652	-5730.9018639	-5730.8934104
0	17	MgCl2_mol14_pos5_3	-5730.3725625	0.1137164	0.1264065	0.1317368	0.1368695	15.30	-5731.0398556	-5731.0269379	-5730.9261392	-5730.9132215
0	18	MgCl2_mol14_pos5_s2	-5730.3263058	0.1134302	0.1262555	0.1316460	0.1368388	6.09	-5731.0413128	-5731.0215250	-5730.9278825	-5730.9080948
0	1	1_MgCl2_mol15_pos2_7	-5914.9584400	0.1101110	0.1236112	0.1292630	0.1346919	9.34	-5915.6628371	-5915.6516317	-5915.5527261	-5915.5415206
0	2	1_MgCl2_mol15_pos2_9	-5914.9517796	0.1125547	0.1256749	0.1311491	0.1363948	13.91	-5915.6407285	-5915.6322666	-5915.5281738	-5915.5197118
0	3	1_MgCl2_mol15_pos8	-5914.9429935	0.1101366	0.1235453	0.1291529	0.1345354	16.63	-5915.6347179	-5915.6258970	-5915.5245813	-5915.5157604
0	4	1_MgCl2_mol15_pos2	-5914.9391962	0.1080734	0.1218195	0.1275818	0.1331219	7.37	-5915.6553992	-5915.6430406	-5915.5473257	-5915.5349671
0	5	1_MgCl2_mol15_pos2_5	-5914.9353069	0.1109174	0.1242411	0.1298101	0.1351533	14.74	-5915.6299127	-5915.6205451	-5915.5189952	-5915.5096277
0	6	1_MgCl2_mol15_pos5	-5914.9140825	0.1076305	0.1214611	0.1272658	0.1328514	9.54	-5915.6471313	-5915.6321983	-5915.5395008	-5915.5245678
0	7	1_MgCl2_mol15_pos2_8	-5914.9172144	0.1122226	0.1253991	0.1309003	0.1361743	14.85	-5915.6193906	-5915.6089514	-5915.5071680	-5915.4967287
0	8	1_MgCl2_mol15_pos5_10	-5914.8806003	0.1114155	0.1246726	0.1302135	0.1355298	16.23	-5915.6055228	-5915.5911979	-5915.4941073	-5915.4797824
0	1	MgCl2_mol6_aac	-1976.2137842	0.0591820	0.0669854	0.0703047	0.0735294	27.35	-1976.4634116	-1976.4574177	-1976.4042295	-1976.3982356
0	2	MgCl2_mol6_aah	-1976.1982921	0.0572948	0.0652865	0.0686920	0.0720047	11.72	-1976.4504254	-1976.4442743	-1976.3931306	-1976.3869794
0	3	MgCl2_mol6_aak	-1976.1993370	0.0584705	0.0663368	0.0696847	0.0729385	18.22	-1976.4532891	-1976.4468133	-1976.3948185	-1976.3883428
0	4	MgCl2_mol6_aao	-1976.1795183	0.0574048	0.0653194	0.0686894	0.0719656	22.22	-1976.4305248	-1976.4241992	-1976.3731200	-1976.3667944
0	5	MgCl2_mol6_abq	-1976.1768208	0.0564817	0.0645270	0.0679547	0.0712882	16.91	-1976.4307275	-1976.4241915	-1976.3742458	-1976.3677098
0	6	MgCl2_mol6_aaa	-1976.1767339	0.0566080	0.0646372	0.0680573	0.0713830	15.66	-1976.4309602	-1976.4244161	-1976.3743522	-1976.3678080
0	7	MgCl2_mol6_aab	-1976.1714203	0.0559096	0.0639765	0.0674158	0.0707623	13.61	-1976.4252294	-1976.4185726	-1976.3693197	-1976.3626629
0	8	MgCl2_mol6_aaf	-1976.1598527	0.0538347	0.0621955	0.0657679	0.0692492	9.94	-1976.4331990	-1976.4239487	-1976.3793643	-1976.3701140
0	9	MgCl2_mol6_abm	-1976.1349485	0.0565733	0.0644705	0.0678280	0.0710886	33.77	-1976.3840696	-1976.3781708	-1976.3274962	-1976.3215975
0	10	MgCl2_mol6_aad	-1976.0872777	0.0514284	0.0596243	0.0631004	0.0664699	33.14	-1976.3243722	-1976.3208576	-1976.2729437	-1976.2694292
0	11	MgCl2_mol6_aax	-1976.0616462	0.0545192	0.0626624	0.0661319	0.0695060	17.82	-1976.2981390	-1976.2941684	-1976.2436198	-1976.2396492
0	1	1_MgCl2_mol7e	-2068.4547913	0.0550332	0.0634212	0.0669812	0.0704339	24.83	-2068.7320271	-2068.7255286	-2068.6769938	-2068.6704954
0	1	MgCl2_3TMPZn_d3_mol6_a	-4163.4582307	0.2917048	0.3033145	0.3081550	0.3127950	11.28	-4163.9668128	-4163.9612160	-4163.6751080	-4163.6695112
0	2	MgCl2_5TMPZn_d5_mol6_aa	-4163.4575785	0.2922140	0.3037284	0.3085264	0.3131238	20.66	-4163.9654665	-4163.9599996	-4163.6732525	-4163.6677856
0	3	MgCl2_8TMPZn_d8_mol6_d	-4163.4508675	0.2904757	0.3021660	0.3070410	0.3117146	11.20	-4163.9570476	-4163.9520700	-4163.6665719	-4163.6615942
0	4	1_MgCl2_2TMPZn_d2_mol6_c	-4163.4486505	0.2911934	0.3028262	0.3076772	0.3123279	13.57	-4163.9646133	-4163.9580857	-4163.6734198	-4163.6668922
0	5	1_MgCl2_2TMPZn_d2_mol6_b	-4163.4473741	0.2914352	0.3030362	0.3078745	0.3125136	19.67	-4163.9613758	-4163.9550642	-4163.6699406	-4163.6636290
0	6	1_MgCl2_5TMPZn_d5_mol6_b	-4163.4428568	0.2900926	0.3019129	0.3068506	0.3115901	7.51	-4163.9708974	-4163.9625162	-4163.6808048	-4163.6724235
0	7	1_MgCl2_5TMPZn_d5_mol6_a	-4163.4435833	0.2909140	0.3026325	0.3075251	0.3122195	16.24	-4163.9713519	-4163.9630514	-4163.6804378	-4163.6721373
0	8	1_MgCl2_3TMPZn_d3_mol6_a	-4163.4435198	0.2912756	0.3030009	0.3078966	0.3125941	15.48	-4163.9715768	-4163.9631623	-4163.6803011	-4163.6718866
0	9	1_MgCl2_3TMPZn_d3_mol6_b	-4163.4434840	0.2913128	0.3030353	0.3079298	0.3126263	12.74	-4163.9714100	-4163.9630071	-4163.6800971	-4163.6716942
0	10	1_MgCl2_8TMPZn_d8_mol6_a2	-4163.4422437	0.2903950	0.3021047	0.3069891	0.3116725	8.26	-4163.9586726	-4163.9522227	-4163.6682776	-4163.6618276
0	11	1_MgCl2_8TMPZn_d8_mol6_a	-4163.4417638	0.2901382	0.3018307	0.3067083	0.3113855	17.00	-4163.9575308	-4163.9511367	-4163.6673926	-4163.6609984
0	1	1_MgCl2_2ZnCl_d2_mol6_aaq	-4215.0671446	0.0441579	0.0530993	0.0568932	0.0605714	31.55	-4215.5346709	-4215.5260011	-4215.4905129	-4215.4818431
0	2	1_MgCl2_8ZnCl_d8_mol6_aac2	-4215.0614704	0.0436533	0.0526442	0.0564592	0.0601579	17.81	-4215.5326920	-4215.5235740	-4215.4890386	-4215.4799206
0	3	1_MgCl2_5ZnCl_d5_mol6_aae	-4215.0511562	0.0431647	0.0522461	0.0561055	0.0598511	23.38	-4215.5360744	-4215.5247198	-4215.4929096	-4215.4815550
0	4	1_MgCl2_3ZnCl_d3_mol6_aap	-4215.0515669	0.0437319	0.0527938	0.0566446	0.0603817	22.99	-4215.5387910	-4215.5271343	-4215.4950591	-4215.4834023
0	5	MgCl2_8ZnCl_d8_mol6_aac	-4215.0389566	0.0411081	0.0503503	0.0542773	0.0580880	12.62	-4215.5094899	-4215.5007294	-4215.4683817	-4215.4596213
0	6	MgCl2_2ZnCl_d2_mol6_aaq	-4215.0368442	0.0416097	0.0507945	0.0546959	0.0584811	16.00	-4215.5088328	-4215.4996557	-4215.4672230	-4215.4580459
0	7	1_MgCl2_3ZnCl_d3_mol6_aap2	-4215.0053003	0.0416414	0.0508578	0.0547774	0.0585834	22.95	-4215.5215674	-4215.5057765	-4215.4799259	-4215.4641350
0	8	1_MgCl2_5ZnCl_d5_mol6_aae2	-4214.9963445	0.0412604	0.0504779	0.0543973	0.0582026	17.99	-4215.5205855	-4215.5034697	-4215.4793251	-4215.4622092
0	1	8_MgCl_d8_mol6_aar	-1515.2932341	0.0485845	0.0556640	0.0586784	0.0616094	49.82	-1515.5096481	-1515.5038104	-1515.4610636	-1515.4552258
0	2	5_MgCl_d5_mol6_aaa	-1515.2927636	0.0481508	0.0552842	0.0583233	0.0612792	47.68	-1515.5139755	-1515.5071263	-1515.4658247	-1515.4589754
0	3	2_MgCl_d2_mol6_aaa	-1515.2864909	0.0484553	0.0555505	0.0585730	0.0615128	37.53	-1515.5018097	-1515.4961561	-1515.4533543	-1515.4477007
0	4	3_MgCl_d3_mol6_aaq	-1515.2836619	0.0479350	0.0551406	0.0582133	0.0612039	31.56	-1515.5207234	-1515.5114210	-1515.4727883	-1515.4634859
0	5	8_MgCl_d8_mol6_aae	-1515.1607835	0.0472040	0.0543519	0.0573973	0.0603594	34.02	-1515.4722209	-1515.4509385	-1515.4250169	-1515.4037344
0	6	3_MgCl_d3_mol6_aaf	-1515.1365723	0.0459630	0.0533362	0.0564835	0.0595484	24.60	-1515.4325941	-1515.3955865	-1515.3866310	-1515.3496234
0	1	5_MgCl_d5_mol7e	-1607.5522145	0.0452670	0.0528339	0.0560467	0.0591640	32.34	-1607.7945163	-1607.7883188	-1607.7492493	-1607.7430517
0	2	8_MgCl_d8_mol7e	-1607.5371639	0.0443066	0.0519965	0.0552634	0.0584344	40.39	-1607.7829219	-1607.7762968	-1607.7386153	-1607.7319901
0	3	2_MgCl_d2_mol7e	-1607.5292707	0.0434010	0.0511998	0.0545165	0.0577382	28.90	-1607.7901338	-1607.7813378	-1607.7467328	-1607.7379368
0	1	mol14_pos5	-3489.0228264	0.1225781	0.1318548	0.1357675	0.1395493	8.55	-3489.4926308	-3489.4857142	-3489.3700527	-3489.3631361
0	2	mol14_pos3	-3489.0196860	0.1232317	0.1325395	0.1364659	0.1402610	6.16	-3489.4925237	-3489.4850392	-3489.3692920	-3489.3618075

0	3	mol14_pos8	-3489.0114145	0.1216163	0.1309835	0.1349337	0.1387510	8.80	-3489.4780244	-3489.4725932	-3489.3564080	-3489.3509768
0	4	mol14_pos2	-3489.0085425	0.1216432	0.1310424	0.1350074	0.1388400	6.65	-3489.4747587	-3489.4690538	-3489.3531155	-3489.3474106
0	1	mol15_pos5	-3673.5308560	0.1157600	0.1260128	0.1303217	0.1344747	17.21	-3674.0391242	-3674.0340876	-3673.9233642	-3673.9183275
0	2	mol15_pos8	-3673.5068160	0.1136028	0.1241373	0.1285698	0.1328453	4.09	-3674.0293210	-3674.0227498	-3673.9157181	-3673.9091470
0	3	mol15_pos2	-3673.5069817	0.1145064	0.1249535	0.1293475	0.1335846	8.25	-3674.0321758	-3674.0249961	-3673.9176694	-3673.9104896
0	1	mol16e_2	-1293.3933941	0.1624039	0.1712026	0.1749056	0.1784794	12.20	-1293.6435987	-1293.6419090	-1293.4811947	-1293.4795050
0	2	mol16e_1	-1293.3935825	0.1627296	0.1714881	0.1751731	0.1787291	19.11	-1293.6436615	-1293.6419901	-1293.4809319	-1293.4792605
0	1	mol17_pos5_1	-1953.1836866	0.1485676	0.1583270	0.1624281	0.1663808	26.06	-1953.5096819	-1953.5035562	-1953.3611142	-1953.3549885
0	2	mol17_pos5_2	-1953.1837255	0.1487202	0.1584630	0.1625565	0.1665015	26.07	-1953.5098429	-1953.5037232	-1953.3611227	-1953.3550029
0	3	mol17_pos8_1	-1953.1697210	0.1480646	0.1579131	0.1620527	0.1660430	26.64	-1953.4982884	-1953.4918785	-1953.3502237	-1953.3438139
0	4	mol17_pos8_2	-1953.1694608	0.1479241	0.1577867	0.1619327	0.1659295	25.17	-1953.4983883	-1953.4919209	-1953.3504641	-1953.3439967
0	1	mol3	-395.9217110	0.0758377	0.0812596	0.0835820	0.0858509	211.39	-396.0295672	-396.0281484	-395.9537295	-395.9523107
0	1	mol6	-855.5167140	0.0637447	0.0696462	0.0721675	0.0746258	115.72	-855.6558186	-855.6544115	-855.5920739	-855.5906667
0	1	mol7e	-947.7638999	0.0596118	0.0661294	0.0689054	0.0716059	101.68	-947.9291106	-947.9275182	-947.8694988	-947.8679064
0	1	pyrimidine	-264.3494742	0.0495596	0.0543706	0.0564492	0.0584907	353.36	-264.4213106	-264.4204172	-264.3717510	-264.3708575
0	1	TMP2Zn_1	-2596.4596189	0.4653300	0.4760451	0.4804784	0.4847080	16.47	-2596.8312478	-2596.8296205	-2596.3659178	-2596.3642905
0	1	TMPH_1	-409.2326871	0.2350136	0.2417505	0.2445818	0.2473123	132.21	-409.3318099	-409.3314555	-409.0967962	-409.0964418
0	2	TMPH_2	-409.2321069	0.2353812	0.2421055	0.2449321	0.2476586	130.20	-409.3314995	-409.3311067	-409.0961183	-409.0957254
0	1	TMPMgCl	-1069.0161812	0.2186717	0.2266002	0.2299349	0.2331512	44.86	-1069.1918494	-1069.1871603	-1068.9731777	-1068.9684886
0	1	TMPMgClLiCl_2	-1536.8991700	0.2183857	0.2272016	0.2308985	0.2344558	32.32	-1537.1205478	-1537.1140542	-1536.9021621	-1536.8956685
0	2	TMPMgClLiCl	-1536.8902310	0.2166631	0.2256558	0.2294302	0.2330644	12.74	-1537.1137783	-1537.1073776	-1536.8971152	-1536.8907144
0	1	TMPMgCl_mol6_abc	-1924.5829318	0.3042729	0.3148560	0.3192721	0.3235093	13.85	-1924.8772803	-1924.8739499	-1924.5730073	-1924.5696769
0	2	TMPMgCl_mol6_aak	-1924.5817680	0.3035969	0.3142869	0.3187514	0.3230377	2.33	-1924.8760113	-1924.8726501	-1924.5724144	-1924.5690532
0	3	TMPMgCl_mol6_aal	-1924.5836406	0.3058822	0.3163290	0.3206837	0.3248590	27.30	-1924.8809017	-1924.8771638	-1924.5750194	-1924.5712816
0	4	TMPMgCl_mol6_aaa	-1924.5816859	0.3054298	0.3159009	0.3202675	0.3244554	24.42	-1924.8782733	-1924.8745612	-1924.5728435	-1924.5691313
0	5	TMPMgCl_mol6_aba	-1924.5692330	0.3037784	0.3144048	0.3188401	0.3230965	7.74	-1924.8678909	-1924.8640389	-1924.5641124	-1924.5602604
0	6	TMPMgCl_mol6_aao	-1924.5696071	0.3047870	0.3153111	0.3197007	0.3239111	16.36	-1924.8692960	-1924.8653642	-1924.5645089	-1924.5605772
0	7	TMPMgCl_mol6_aaj	-1924.5698855	0.3052574	0.3157425	0.3201145	0.3243072	15.31	-1924.8700418	-1924.8660235	-1924.5647843	-1924.5607661
0	8	TMPMgCl_mol6_aab	-1924.5552660	0.3036013	0.3142244	0.3186584	0.3229133	17.48	-1924.8509695	-1924.8474473	-1924.5473681	-1924.5438460
0	9	TMPMgCl_mol6_aae	-1924.5530442	0.3034696	0.3141359	0.3185897	0.3228648	15.18	-1924.8574847	-1924.8527406	-1924.5540150	-1924.5492709
0	10	TMPMgCl_mol6_aaz	-1924.5532130	0.3037753	0.3143906	0.3188226	0.3230768	21.61	-1924.8545726	-1924.8502781	-1924.5507972	-1924.5465028
0	11	TMPMgCl_mol6_aas	-1924.5532401	0.3041218	0.3146923	0.3191024	0.3233331	23.57	-1924.8547302	-1924.8505161	-1924.5506084	-1924.5463942
0	12	TMPMgCl_mol6_aai	-1924.5461929	0.3022907	0.3130421	0.3175350	0.3218500	19.86	-1924.8540065	-1924.8487600	-1924.5517157	-1924.5464693
0	13	TMPMgCl_mol6_abi	-1924.5435991	0.3016157	0.3125019	0.3170564	0.3214346	10.64	-1924.8572349	-1924.8512721	-1924.5556191	-1924.5496564
0	14	TMPMgCl_mol6_abh	-1924.5437163	0.3020251	0.3128773	0.3174169	0.3217801	15.86	-1924.8566490	-1924.8507838	-1924.5546239	-1924.5487586
0	15	TMPMgCl_mol6_aad	-1924.5441325	0.3028022	0.3135657	0.3180658	0.3223896	16.67	-1924.8578915	-1924.8519165	-1924.5550893	-1924.5491142
0	16	TMPMgCl_mol6_aan	-1924.5416592	0.3009007	0.3118694	0.3164607	0.3208756	8.10	-1924.8552450	-1924.8493205	-1924.5543443	-1924.5484197
0	17	TMPMgCl_mol6_abe	-1924.5408757	0.3012302	0.3121717	0.3167518	0.3211560	10.20	-1924.8529729	-1924.8472966	-1924.5517427	-1924.5460664
0	1	5_TMPMg_d5_mol6	-1463.6667741	0.2935363	0.3034817	0.3076320	0.3116148	19.04	-1463.9320138	-1463.9280599	-1463.6384775	-1463.6345235
0	2	8_TMPMg_d8_mol6	-1463.6623647	0.2940871	0.3039573	0.3080726	0.3120196	17.01	-1463.9233373	-1463.9202198	-1463.6292502	-1463.6261327
0	3	3_TMPMg_d3_mol6	-1463.6603139	0.2935946	0.3035831	0.3077532	0.3117565	15.84	-1463.9360832	-1463.9304723	-1463.6424886	-1463.6368777
0	4	2_TMPMg_d2_mol6	-1463.6526211	0.2921261	0.3022456	0.3064735	0.3105341	9.29	-1463.9224840	-1463.9180136	-1463.6303579	-1463.6258874
0	1	TMPZnCl	-2648.0754991	0.2182859	0.2263317	0.2297180	0.2329857	12.86	-2648.3958080	-2648.3924478	-2648.1775221	-2648.1741618
0	1	TMPZnCl_mol6_aax	-3503.6239367	0.3027035	0.3135512	0.3180832	0.3224348	2.23	-3504.0722978	-3504.0690305	-3503.7695942	-3503.7663269
0	2	TMPZnCl_mol6_abf	-3503.6222189	0.3044408	0.3150535	0.3194816	0.3237300	23.28	-3504.0667329	-3504.0639554	-3503.7622920	-3503.7595146
0	3	TMPZnCl_mol6_aaj	-3503.6136509	0.3044776	0.3150953	0.3195253	0.3237754	20.89	-3504.0647036	-3504.0612189	-3503.7602260	-3503.7567413
0	4	TMPZnCl_mol6_abq	-3503.6123396	0.3039779	0.3146633	0.3191250	0.3234078	12.78	-3504.0629750	-3504.0594916	-3503.7589971	-3503.7555136
0	5	TMPZnCl_mol6_abr	-3503.6126310	0.3044981	0.3151225	0.3195564	0.3238110	19.46	-3504.0626149	-3504.0592526	-3503.7581168	-3503.7547544
0	6	TMPZnCl_mol6_abs	-3503.6117676	0.3041295	0.3147854	0.3192348	0.3235057	16.94	-3504.0627023	-3504.0590737	-3503.7585728	-3503.7549441
0	7	TMPZnCl_mol6_abb	-3503.6116650	0.3042001	0.3148641	0.3193174	0.3235925	16.03	-3504.0658373	-3504.0617308	-3503.7616372	-3503.7575307
0	8	TMPZnCl_mol6_abl	-3503.6102046	0.3038480	0.3145412	0.3190086	0.3232986	17.51	-3504.0628835	-3504.0590332	-3503.7590355	-3503.7551852
0	9	TMPZnCl_mol6_aab	-3503.6088558	0.3030851	0.3138281	0.3183175	0.3226293	19.70	-3504.0579885	-3504.0545970	-3503.7549033	-3503.7515118
0	10	TMPZnCl_mol6_aas	-3503.6068879	0.3030707	0.3138248	0.3183195	0.3226368	15.26	-3504.0629078	-3504.0586358	-3503.7598371	-3503.7555650
0	11	TMPZnCl_mol6_aag	-3503.6069039	0.3039183	0.3145559	0.3189981	0.3232624	25.59	-3504.0620387	-3504.0577205	-3503.7581204	-3503.7538021
0	12	TMPZnCl_mol6_aai	-3503.6049887	0.3030126	0.3137712	0.3182675	0.3225860	14.55	-3504.0623625	-3504.0577501	-3503.7593498	-3503.7547375
0	13	TMPZnCl_mol6_aav	-3503.6043195	0.3028548	0.3136375	0.3181456	0.3224770	16.33	-3504.0596021	-3504.0553946	-3503.7567472	-3503.7525398
0	14	TMPZnCl_mol6_abj	-3503.6028698	0.3015915	0.3125443	0.3171283	0.3215356	10.58	-3504.0614098	-3504.0567380	-3503.7598182	-3503.7551464
0	15	TMPZnCl_mol6_abu	-3503.6023609	0.3016269	0.3125795	0.3171631	0.3215697	11.26	-3504.0615100	-3504.0567693	-3503.7598830	-3503.7551423
0	16	TMPZnCl_mol6_aan	-3503.6035182	0.3030058	0.3138150	0.3183351	0.3226785	13.20	-3504.0620943	-3504.0574171	-3503.7590884	-3503.7544113
0	17	TMPZnCl_mol6_aaf	-3503.6024695	0.3024039	0.3133015	0.3178615	0.3222453	7.99	-3504.0609825	-3504.0563399	-3503.7585786	-3503.7539360

0	18	TMPZnCl_mol6_abg	-3503.6006013	0.3016200	0.3125980	0.3171937	0.3216131	8.58	-3504.0584013	-3504.0539029	-3503.7567812	-3503.7522828
0	1	5_TMPZn_d5_mol6_b	-3042.7431415	0.2939589	0.3039825	0.3081682	0.3121869	8.36	-3043.1617660	-3043.1578531	-3042.8678070	-3042.8638942
0	2	5_TMPZn_d5_mol6_a	-3042.7438310	0.2948056	0.3047239	0.3088629	0.3128348	23.12	-3043.1622698	-3043.1584160	-3042.8674641	-3042.8636103
0	3	3_TMPZn_d3_mol6_b	-3042.7427847	0.2951707	0.3051011	0.3092456	0.3132232	14.00	-3043.1615150	-3043.1576112	-3042.8663443	-3042.8624404
0	4	8_TMPZn_d8_mol6_a	-3042.7383975	0.2941769	0.3041601	0.3083266	0.3123252	12.85	-3043.1534001	-3043.1503980	-3042.8592231	-3042.8562211
0	5	2_TMPZn_d2_mol6_a	-3042.7354910	0.2941601	0.3041595	0.3083333	0.3123394	12.66	-3043.1512989	-3043.1480212	-3042.8571388	-3042.8538611
0	1	5_TMPZn_d5_mol7e	-3134.9955674	0.2910549	0.3015166	0.3058782	0.3100604	14.90	-3135.4353760	-3135.4320245	-3135.1443211	-3135.1409695
0	2	5_TMPZn_d5_mol7e_36	-3134.9959083	0.2915053	0.3019152	0.3062533	0.3104116	21.12	-3135.4357751	-3135.4324439	-3135.1442698	-3135.1409385
0	3	5_TMPZn_d5_mol7e_40	-3134.9894049	0.2902522	0.3007781	0.3051684	0.3093792	17.62	-3135.4304593	-3135.4269410	-3135.1402071	-3135.1366888
0	4	5_TMPZn_d5_mol7e_38	-3134.9895252	0.2910083	0.3014830	0.3058518	0.3100421	9.68	-3135.4292882	-3135.4259247	-3135.1382799	-3135.1349164
0	5	5_TMPZn_d5_mol7e_1	-3134.9888787	0.2908902	0.3013619	0.3057285	0.3099162	13.03	-3135.4282344	-3135.4249765	-3135.1373441	-3135.1340862
0	6	8_TMPZn_d8_mol7e	-3134.9868222	0.2900944	0.3006594	0.3050662	0.3092931	12.56	-3135.4291978	-3135.4257250	-3135.1391033	-3135.1356305
0	7	2_TMPZn_d2_mol7e	-3134.9870950	0.2904551	0.3009963	0.3053927	0.3096093	11.84	-3135.4304438	-3135.4267497	-3135.1399886	-3135.1362946
0	8	8_TMPZn_d8_mol7e_20	-3134.9806229	0.2890643	0.2997685	0.3042363	0.3085233	7.11	-3135.4246599	-3135.4209748	-3135.1355955	-3135.1319104
0	9	8_TMPZn_d8_mol7e_16	-3134.9806979	0.2894850	0.3001247	0.3045638	0.3088222	18.25	-3135.4248471	-3135.4211490	-3135.1353620	-3135.1316640
0	10	2_TMPZn_d2_mol7e_31	-3134.9805606	0.2894338	0.3000915	0.3045385	0.3088048	14.08	-3135.4260180	-3135.4220501	-3135.1365842	-3135.1326162
0	11	2_TMPZn_d2_mol7e_29	-3134.9805183	0.2895803	0.3002142	0.3046528	0.3089123	6.94	-3135.4247405	-3135.4209127	-3135.1351602	-3135.1313324
0	12	2_TMPZn_d2_mol7e_28	-3134.9805054	0.2897680	0.3003920	0.3048264	0.3090818	8.33	-3135.4245520	-3135.4207468	-3135.1347839	-3135.1309788
0	13	8_TMPZn_d8_mol7e_11	-3134.9806321	0.2899643	0.3005466	0.3049623	0.3091990	12.40	-3135.4240053	-3135.4203794	-3135.1340410	-3135.1304151
0	14	2_TMPZn_d2_mol7e_26	-3134.9804805	0.2899134	0.3005084	0.3049295	0.3091712	11.74	-3135.4244141	-3135.4206353	-3135.1345007	-3135.1307218
0	15	8_TMPZn_d8_mol7e_14	-3134.9802080	0.2898861	0.3004626	0.3048758	0.3091101	15.69	-3135.4231639	-3135.4196051	-3135.1332778	-3135.1297189
0	1	ZnCl2_mol6_aai	-3555.2471047	0.0576751	0.0656348	0.0690223	0.0723142	24.19	-3555.6444580	-3555.6394311	-3555.5867828	-3555.5817560
0	2	ZnCl2_mol6_aaz	-3555.2339545	0.0571338	0.0651337	0.0685397	0.0718507	21.20	-3555.6344334	-3555.6290400	-3555.5772995	-3555.5719061
0	3	ZnCl2_mol6_aab	-3555.2205595	0.0562011	0.0642356	0.0676586	0.0709876	24.78	-3555.6182990	-3555.6130878	-3555.5620978	-3555.5568866
0	4	ZnCl2_mol6_aar	-3555.2153630	0.0550829	0.0632219	0.0666940	0.0700738	20.26	-3555.6189382	-3555.6129339	-3555.5638552	-3555.5578509
0	5	ZnCl2_mol6_abq	-3555.2144758	0.0542271	0.0625184	0.0660575	0.0695036	6.80	-3555.6146618	-3555.6091921	-3555.5604347	-3555.5549650
0	6	ZnCl2_mol6_aan	-3555.2151405	0.0549956	0.0631857	0.0666784	0.0700774	16.36	-3555.6155049	-3555.6100491	-3555.5605092	-3555.5550535
0	7	ZnCl2_mol6_abm	-3555.1649962	0.0558629	0.0638000	0.0671744	0.0704512	39.87	-3555.5535053	-3555.5495176	-3555.4976423	-3555.4936546
0	8	ZnCl2_mol6_aam	-3555.0921596	0.0533090	0.0614851	0.0649655	0.0683481	20.65	-3555.4948247	-3555.4892454	-3555.4415156	-3555.4359363
0	9	ZnCl2_mol6_aad	-3554.9943142	0.0510202	0.0593491	0.0628912	0.0663313	17.06	-3555.4282325	-3555.4158553	-3555.3772122	-3555.3648350
0	1	5_ZnCl_d5_mol6_aae	-3094.3545958	0.0474654	0.0546984	0.0577830	0.0607851	46.20	-3094.7278054	-3094.7211946	-3094.6803399	-3094.6737292
0	2	3_ZnCl_d3_mol6_aap	-3094.3549353	0.0479897	0.0552138	0.0582944	0.0612924	43.01	-3094.7293275	-3094.7225545	-3094.6813378	-3094.6745648
0	3	8_ZnCl_d8_mol6_aac	-3094.3520173	0.0473381	0.0545882	0.0576789	0.0606863	44.28	-3094.7225139	-3094.7168200	-3094.6751758	-3094.6694819
0	4	2_ZnCl_d2_mol6_aaq	-3094.3503611	0.0476409	0.0548552	0.0579303	0.0609224	40.85	-3094.7212760	-3094.7153377	-3094.6736351	-3094.6676967
0	5	5_ZnCl_d5_mol6_aab	-3094.2134952	0.0443687	0.0519060	0.0551258	0.0582630	16.12	-3094.6230770	-3094.5885613	-3094.5787083	-3094.5441926
0	6	5_ZnCl_d5_mol6_aah	-3094.1841339	0.0444339	0.0519439	0.0551493	0.0582705	11.65	-3094.6401257	-3094.6140880	-3094.5956917	-3094.5696541
0	7	5_ZnCl_d5_mol6_aaf	-3094.1814474	0.0435256	0.0510833	0.0543116	0.0574567	25.22	-3094.6310920	-3094.5982832	-3094.5875663	-3094.5547576
0	1	5_ZnCl_d5_mol7e	-3186.6055598	0.0436718	0.0514453	0.0547514	0.0579628	37.96	-3187.0007047	-3186.9946733	-3186.9570329	-3186.9510014
0	2	8_ZnCl_d8_mol7e	-3186.5986837	0.0433674	0.0511925	0.0545205	0.0577531	41.32	-3186.9977466	-3186.9913672	-3186.9543791	-3186.9479997
0	3	2_ZnCl_d2_mol7e	-3186.5984027	0.0435609	0.0513634	0.0546813	0.0579040	37.47	-3186.9987410	-3186.9921111	-3186.9551800	-3186.9485502
+1	1	1_MgCl_mol6_1	-1515.6827823	0.0602252	0.0674813	0.0705753	0.0735867	23.67	-1516.0112448	-1515.9907238	-1515.9510196	-1515.9304986
+1	1	1_Mg_d8_mol6	-1054.7533989	0.0518928	0.0582008	0.0608878	0.0635019	110.14	-1055.0570453	-1055.0354431	-1055.0051525	-1054.9835503
+1	2	1_Mg_d5_mol6	-1054.6635855	0.0480987	0.0546429	0.0574343	0.0601521	58.81	-1055.0461779	-1055.0060738	-1054.9980792	-1054.9579750
+1	3	1_Mg_d2_mol6	-1054.6628957	0.0490781	0.0555930	0.0583719	0.0610774	69.93	-1055.0351206	-1055.0014959	-1054.9860424	-1054.9524178
+1	4	1_Mg_d3_mol6	-1054.6621544	0.0487993	0.0553399	0.0581303	0.0608474	44.76	-1055.0414638	-1055.0042864	-1054.9926645	-1054.9554871
+1	1	1_ZnCl_mol6_2	-3094.7315316	0.0603980	0.0676416	0.0707291	0.0737335	40.31	-3095.1969113	-3095.1787139	-3095.1365133	-3095.1183159
+1	1	1_Zn_d8_mol6	-2633.7935173	0.0495349	0.0561342	0.0589503	0.0616927	100.50	-2634.2402464	-2634.2192903	-2634.1907114	-2634.1697554
+1	2	1_Zn_d5_mol6	-2633.7155870	0.0453896	0.0522595	0.0551941	0.0580538	18.30	-2634.2040204	-2634.1643047	-2634.1586308	-2634.1189151
+1	3	1_Zn_d2_mol6	-2633.7151190	0.0477817	0.0544941	0.0573592	0.0601498	64.81	-2634.1971609	-2634.1639435	-2634.1493792	-2634.1161617
+1	4	1_Zn_d3_mol6	-2633.7121215	0.0472270	0.0539255	0.0567852	0.0595709	51.62	-2634.2048901	-2634.1689103	-2634.1576630	-2634.1216832
+1	1	MgCl_mol6_aal	-1515.6696042	0.0602414	0.0674949	0.0705871	0.0735961	25.81	-1516.0118628	-1515.9911904	-1515.9516214	-1515.9309489
+1	2	MgCl_mol6_aac	-1515.6697712	0.0604852	0.0676973	0.0707698	0.0737584	39.21	-1515.9955455	-1515.9774566	-1515.9350603	-1515.9169713
+1	3	MgCl_mol6_aah	-1515.6188128	0.0580942	0.0654584	0.0686013	0.0716624	19.88	-1515.9689112	-1515.9465161	-1515.9108169	-1515.8884218
+1	4	MgCl_mol6_abm	-1515.5660987	0.0556239	0.0632549	0.0665189	0.0697026	13.86	-1515.9749622	-1515.9445927	-1515.9193382	-1515.8889687
+1	5	MgCl_mol6_abg	-1515.5150954	0.0595221	0.0667544	0.0698330	0.0728257	32.47	-1515.9461444	-1515.9091564	-1515.8866222	-1515.8496343
+1	1	1_Mg_d8_mol6	-1054.7533989	0.0518928	0.0582008	0.0608878	0.0635019	110.14	-1055.0570453	-1055.0354431	-1055.0051525	-1054.9835503
+1	2	2_Mg_d2_mol6	-1054.7297190	0.0513515	0.0577023	0.0604096	0.0630447	70.73	-1055.0478069	-1055.0247203	-1054.9964553	-1054.9733687
+1	3	5_Mg_d5_mol6	-1054.7270991	0.0505045	0.0568978	0.0596214	0.0622708	91.91	-1055.0542140	-1055.0290586	-1055.0037094	-1054.9785541
+1	4	8_Mg_d8_mol6	-1054.7272549	0.0510584	0.0574475	0.0601708	0.0628211	107.91	-1055.0513118	-1055.0276262	-1055.0002533	-1054.9765678

+1	5	3_Mg_d3_mol6	-1054.7045964	0.0487902	0.0553787	0.0581919	0.0609327	45.60	-1055.0687366	-1055.0376882	-1055.0199463	-1054.9888979
+1	6	3_Mg_d5_mol6	-1054.7019671	0.0501753	0.0565188	0.0592215	0.0618510	95.26	-1055.0192603	-1054.9949896	-1054.9690849	-1054.9448143
+1	7	7_Mg_d5_mol6	-1054.6850970	0.0491170	0.0555846	0.0583402	0.0610212	63.62	-1055.0329055	-1055.0043464	-1054.9837884	-1054.9552294
+1	8	7_Mg_d8_mol6	-1054.6839808	0.0494255	0.0558804	0.0586297	0.0613038	92.45	-1055.0250674	-1054.9948300	-1054.9756418	-1054.9454044
+1	9	1_Mg_d5_mol6	-1054.6635855	0.0480987	0.0546429	0.0574343	0.0601521	58.81	-1055.0461779	-1055.0060738	-1054.9980792	-1054.9579750
+1	10	1_Mg_d2_mol6	-1054.6628957	0.0490781	0.0555930	0.0583719	0.0610774	69.93	-1055.0351206	-1055.0014959	-1054.9860424	-1054.9524178
+1	11	1_Mg_d3_mol6	-1054.6621544	0.0487993	0.0553399	0.0581303	0.0608474	44.76	-1055.0414638	-1055.0042864	-1054.9926645	-1054.9554871
+1	12	7_Mg_d3_mol6	-1054.6524619	0.0488049	0.0552862	0.0580477	0.0607343	56.76	-1055.0209877	-1054.9871649	-1054.9721828	-1054.9383599
+1	13	7_Mg_d2_mol6	-1054.6420307	0.0485488	0.0550961	0.0578875	0.0606043	68.67	-1055.0013049	-1054.9611158	-1054.9527560	-1054.9125670
+1	14	3_Mg_d8_mol6	-1054.6292516	0.0456627	0.0524728	0.0553825	0.0582185	31.83	-1054.9577248	-1054.9122997	-1054.9120620	-1054.8666369
+1	1	p1_mol16e_1	-1293.7572809	0.1756350	0.1844238	0.1881171	0.1916779	30.13	-1294.0756250	-1294.0655675	-1293.8999900	-1293.8899324
+1	2	p1_mol16e_2	-1293.7566491	0.1756591	0.1844395	0.1881289	0.1916859	31.60	-1294.0757321	-1294.0655362	-1293.9000730	-1293.8898770
+1	3	p7_mol16e_1	-1293.7508718	0.1759682	0.1847433	0.1884308	0.1919864	28.98	-1294.0679864	-1294.0579988	-1293.8920181	-1293.8820306
+1	4	p7_mol16e_2	-1293.7506037	0.1757444	0.1845434	0.1882416	0.1918078	24.04	-1294.0677985	-1294.0577970	-1293.8920541	-1293.8820525
+1	5	p4_mol16e_2	-1293.6513137	0.1732368	0.1821085	0.1858378	0.1894342	28.04	-1293.9684217	-1293.9583701	-1293.7951849	-1293.7851332
+1	6	p4_mol16e_1	-1293.6510958	0.1732315	0.1821012	0.1858297	0.1894254	26.27	-1293.9681600	-1293.9581286	-1293.7949284	-1293.7848970
+1	1	p1_mol3	-396.2925964	0.0890962	0.0945580	0.0968943	0.0991750	207.97	-396.4746477	-396.4646557	-396.3855514	-396.3755594
+1	2	p7_mol3	-396.2893922	0.0894735	0.0949189	0.0972489	0.0995239	213.62	-396.4721953	-396.4620514	-396.3827217	-396.3725779
+1	3	p4_mol3	-396.1781061	0.0858091	0.0913932	0.0937806	0.0961103	152.05	-396.3641625	-396.3534188	-396.2783533	-396.2676097
+1	1	p1_mol6	-855.8818445	0.0769130	0.0828496	0.0853831	0.0878517	111.31	-856.0974070	-856.0870027	-856.0204939	-856.0100897
+1	2	p7_mol6	-855.8742530	0.0772614	0.0831874	0.0857168	0.0881818	121.26	-856.0869495	-856.0770090	-856.0096881	-855.9997475
+1	3	p4_mol6	-855.7668907	0.0737468	0.0797931	0.0823733	0.0848873	84.99	-855.9853184	-855.9743255	-855.9115716	-855.9005787
+1	1	p1_mol7e	-948.1090638	0.0723387	0.0789038	0.0816967	0.0844116	98.46	-948.3581474	-948.3463387	-948.2858086	-948.2740000
+1	2	p7_mol7e	-948.1049697	0.0727389	0.0792926	0.0820814	0.0847927	101.69	-948.3510626	-948.3397348	-948.2783236	-948.2669958
+1	3	p4_mol7e	-947.9945228	0.0691396	0.0758129	0.0786524	0.0814127	74.17	-948.2434521	-948.2315865	-948.1743124	-948.1624469
+1	1	p_pyrimidine	-264.7016864	0.0630341	0.0678800	0.0699713	0.0720242	330.03	-264.8575619	-264.8468884	-264.7945278	-264.7838543
+1	1	ZnCl_mol6_aag	-3094.7315316	0.0603980	0.0676416	0.0707292	0.0737335	40.31	-3095.1969111	-3095.1787138	-3095.1365131	-3095.1183157
+1	2	ZnCl_mol6_aac	-3094.7255307	0.0601793	0.0674379	0.0705320	0.0735430	48.59	-3095.1821335	-3095.1652636	-3095.1219542	-3095.1050843
+1	3	ZnCl_mol6_aah	-3094.6910806	0.0588496	0.0661529	0.0692683	0.0723015	33.12	-3095.1582792	-3095.1393114	-3095.0994295	-3095.0804617
+1	4	ZnCl_mol6_aan	-3094.6745718	0.0579851	0.0653429	0.0684828	0.0715407	33.97	-3095.1412461	-3095.1223674	-3095.0832610	-3095.0643823
+1	5	ZnCl_mol6_aaj	-3094.6500796	0.0576050	0.0650325	0.0682021	0.0712884	29.36	-3095.1023980	-3095.0861413	-3095.0447930	-3095.0285362
+1	6	ZnCl_mol6_aas	-3094.6291752	0.0551355	0.0627874	0.0660571	0.0692437	19.60	-3095.1432331	-3095.1115110	-3095.0880976	-3095.0563754
+1	7	ZnCl_mol6_aax	-3094.6236248	0.0565633	0.0641021	0.0673201	0.0704540	28.04	-3095.1414967	-3095.1098014	-3095.0849333	-3095.0532381
+1	8	ZnCl_mol6_abm	-3094.6217852	0.0567669	0.0643050	0.0675223	0.0706554	25.83	-3095.1315474	-3095.1036640	-3095.0747805	-3095.0468971
+1	9	ZnCl_mol6_abd	-3094.6161410	0.0545121	0.0622853	0.0656113	0.0688561	9.61	-3095.1458361	-3095.1146753	-3095.0913240	-3095.0601632
+1	10	ZnCl_mol6_aar	-3094.6108065	0.0585812	0.0660253	0.0692032	0.0722986	17.82	-3095.0367178	-3095.0252925	-3094.9781365	-3094.9667113
+1	11	ZnCl_mol6_aak	-3094.5990487	0.0588517	0.0662386	0.0693912	0.0724616	21.53	-3095.0230799	-3095.0118856	-3094.9642282	-3094.9530338
+1	12	ZnCl_mol6_abg	-3094.5687594	0.0585181	0.0658907	0.0690307	0.0720838	38.65	-3095.0996852	-3095.0642776	-3095.0411670	-3095.0057594
+1	1	3_Zn_d3_mol6	-2634.0141878	0.0499214	0.0565064	0.0593172	0.0620551	94.07	-2634.2649477	-2634.2339665	-2634.2150263	-2634.1840451
+1	2	7_Zn_d8_mol6	-2633.7935173	0.0495349	0.0561343	0.0589504	0.0616928	100.51	-2634.2402469	-2634.2192908	-2634.1907119	-2634.1697559
+1	3	2_Zn_d2_mol6	-2633.7743925	0.0484628	0.0551031	0.0579363	0.0606951	63.43	-2634.2558488	-2634.2296343	-2634.2073860	-2634.1811714
+1	4	5_Zn_d5_mol6	-2633.7713295	0.0483478	0.0549735	0.0578005	0.0605533	82.86	-2634.2465835	-2634.2205904	-2634.1982356	-2634.1722426
+2	1	7_Mg_mol6	-1054.9846738	0.0635404	0.0699232	0.0726412	0.0752847	88.36	-1055.5293799	-1055.4795463	-1055.4658394	-1055.4160059
+2	2	1_Mg_mol6	-1054.9648527	0.0646044	0.0710072	0.0737388	0.0763991	75.70	-1055.5541226	-1055.4984450	-1055.4895181	-1055.4338406
+2	3	3_Mg_mol6	-1054.9216045	0.0608936	0.0674293	0.0702165	0.0729302	71.48	-1055.5100389	-1055.4519604	-1055.4491452	-1055.3910667
+2	1	7_Zn_mol6	-2634.4731333	0.0622816	0.0689180	0.0717496	0.0745071	70.19	-2634.7094357	-2634.6500698	-2634.6471541	-2634.5877881
+2	2	1_Zn_mol6	-2633.9861162	0.0606289	0.0672910	0.0701340	0.0729029	60.36	-2634.7159304	-2634.6582727	-2634.6553014	-2634.5976437
+2	3	3_Zn_mol6	-2633.9608995	0.0590412	0.0657826	0.0686606	0.0714643	66.24	-2634.6862522	-2634.6285499	-2634.6272109	-2634.5695086
0	1	TS8_TMPMgClLiCl_mol6_aav	-2392.425333	0.3015303	0.3127971	0.3174829	0.3219673	-1284.51	-2392.772833		-2392.471303	
0	2	TS2_TMPMgClLiCl_mol6_aaj	-2392.423484	0.3021875	0.3134105	0.3180764	0.3225404	-1297.66	-2392.769259		-2392.467071	
0	3	TS2_TMPMgClLiCl_mol6_aaj_s1	-2392.426315					-41.56				
0	4	TS2_TMPMgClLiCl_mol6_aaf	-2392.417331	0.3009962	0.3123564	0.3170837	0.3216094	-1274.67	-2392.763812		-2392.462815	
0	5	TS5_TMPMgClLiCl_mol6_acn	-2392.412515	0.3014941	0.3127845	0.317478	0.321968	-1328.2	-2392.763545		-2392.462051	
0	6	TS8_TMPMgClLiCl_mol6_abz	-2392.410701	0.3015296	0.3128032	0.3174915	0.3219781	-1335.57	-2392.756601		-2392.455071	
0	7	TS3_TMPMgClLiCl_mol6_1	-2392.406686	0.3041344	0.3151636	0.3197402	0.3241129	-1310.11	-2392.747846		-2392.443712	
0	8	TS3_TMPMgClLiCl_mol6_acb	-2392.40085	0.3026649	0.313837	0.3184821	0.3229266	-1431.22	-2392.751157		-2392.448492	
0	9	TS2_TMPMgClLiCl_mol6_aaj_s2	-2392.387505					-1293.48				
0	10	TS5_TMPMgClLiCl_mol6_acn_s1	-2392.383473					-1339.27				

0	11	TS5_TMPMgClLiCl_mol6_acn_s2	-2392.374327					-1330.33				
0	12	TS3_TMPMgClLiCl_mol6_1_s1	-2392.368185					-1349.24				
0	13	TS3_TMPMgClLiCl_mol6_acb_s1	-2392.364667					-1372.01				
0	14	TS3_TMPMgClLiCl_mol6_1_s2	-2392.362846					-1283.75				
0	15	TS2_TMPMgClLiCl_mol6_aaj_s3	-2392.360684					-1199.87				
Charge	№ conf.	Filename	(U)B3LYP-D3/6-31G(d)						CPCM(DMSO)/(U)B3LYP-D3/6-311++G(2df,2p)// (U)B3LYP-D3/6-31G(d)			
				298.15 K	253.15 K	233.15 K	213.15 K	298.15K			298.15K	298.15K
			$E_{tot\ gas}$	qh-δG.1	qh-δG.1	qh-δG.1	qh-δG.1	1st freq.	$E_{tot\ sol}$ **DMSO**	$E_{tot\ sol}$ **THF**	G_{sol} **DMSO**	G_{sol} **THF**
0	1	TS8_TMPMgClLiCl_mol16e_aav1	-2830.198445	0.3927433	0.4069398	0.4128151	0.4184183	-1310.78	-2830.76219		-2830.369447	
0	2	TS8_TMPMgClLiCl_mol16e_aav2	-2830.198327	0.3928343	0.4070194	0.4128895	0.4184877	-1311.39	-2830.762445		-2830.369611	
0	3	TS8_TMPMgClLiCl_mol16e_abz2	-2830.190355	0.3928005	0.4069829	0.4128506	0.4184454	-1218.26	-2830.74575		-2830.35295	
0	4	TS8_TMPMgClLiCl_mol16e_abz1	-2830.190205	0.3932347	0.4073633	0.4132077	0.4187796	-1213.13	-2830.746394		-2830.353159	
0	5	TS5_TMPMgClLiCl_mol16e_acn1	-2830.180722	0.3939525	0.4079845	0.4137828	0.4193065	-1439.74	-2830.749381		-2830.355429	
0	6	TS5_TMPMgClLiCl_mol16e_acn2	-2830.180518	0.3939695	0.4080053	0.4138055	0.4193314	-1432.71	-2830.749858		-2830.355888	