Supporting Information

An expedient metal-free cascade route to chromonyl diene scaffolds: thermodynamic vs kinetic control

Abdolali Alizadeh,*[,a] Akram Bagherinejad,[a] Jasmine Kayanian,[a] and Robert Vianello[b]

[a]*Department of Chemistry, Tarbiat Modares University, P.O. Box 14115-175, Tehran, Iran*

[b]*Laboratory for the Computational Design and Synthesis of Functional Materials, Department of Organic Chemistry and Biochemistry, Rud-er Bos˘kovic´ Institute, Bijenic˘ka 54, 10000 Zagreb, Croatia*

aalizadeh@modares.ac.ir

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Experimental

The chromonyl barbituric's acid, and ylidenemalononitrile were prepared according to the reported procedure. All other chemicals and solvents were purchased from Merck or Aldrich and were used without further purification. Elemental analyses for C, H, and N were performed using a Heraeus CHN–O–Rapid analyzer. Mass spectra were recorded on a FINNIGAN-MATT 8430 mass spectrometer operating at an ionization potential of 70 eV. ^{1}H NMR (300 MHz), and ^{13}C NMR (75 MHz) spectra were obtained using Bruker DRX-300 AVANCE and Bruker DRX-400 AVANCE spectrometers. IR spectra were recorded as KBr pellets on a NICOLET FT-IR 100 spectrometer; absorbencies are reported in cm^{-1}.

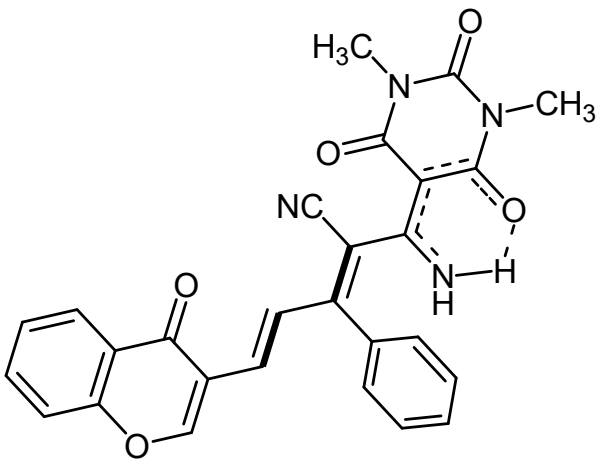
General procedure for preparation of compounds 3a, 3b, 3c,3e, and 3g.

A mixture of 3-formylchromone **1** (1.0 mmol) and 1,3-dimethylbarbituric acid (1.0 mmol) in HOAc/H_2O was magnetically stirred for 0.5 h. The resulting yellow precipitation (0.75 mmol) was reacted with the carbanion obtained from alkylidene malononitrile **2** (1.0 mmol) with piperidine (10 mol%) in MeCN. After completion of the reaction at ambient temperature, the precipitate was washed with acetone to afford the pure products in high yield.

General procedure for preparation of compounds 3d, 3f, 3h, and 3i.

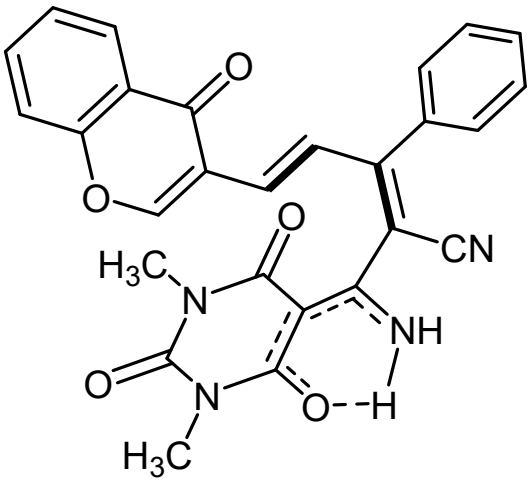
A mixture of 3-formylchromone **1** (1.0 mmol) and 1,3-dimethylbarbituric acid in HOAc/H_2O was magnetically stirred for 0.5 h. The resulting yellow precipitation (0.75 mmol) was reacted with the carbanion obtained from alkylidene malononitrile **2** (1.0 mmol) with piperidine (10 mol%) in MeCN. After completion of the reaction at refluxing temperature (80 °C), the precipitate was washed with acetone to afford the pure products in high yield.

(2*E*,4*E*)-2-[Amino(1,3-dimethyl-2,4,6-trioxotetrahydro-5(2*H*)-pyrimidinylidene)methyl]-5-(4-oxo-4*H*-chromen-3-yl)-3-phenyl-2,4-pentadienenitrile (3a).



Cream powder, mp = 189-190 °C, 0.301 g, yield: 72%. IR (KBr) (ν_{max}, cm^{-1}): 3331 (NH), 2213 (CN), 1717, 1638 and 1614 (C=O), 1556 and 1463 (Ar). Anal. Calcd. for $C_{27}H_{20}N_4O_5$ (480.47): C, 67.49; H, 4.20; N, 11.66%. Found: C, 67.44; H, 4.17; N, 11.61%. MS (EI, 70 eV): *m/z* (%) = 480 (100), 453 (55), 365 (91), 337 (98), 190 (36), 171 (34), 129 (35), 121 (80), 92 (95), 77 (49). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 3.13 (3H, s, CH_3), 3.23 (3H, s, CH_3), 6.26 (1H, d, $^3J_{HH}$ = 15.7 Hz, CH^4), 7.17 (1H, t, $^3J_{HH}$ = 7.3 Hz, CH_{para} of Ph), 7.38-7.61 (5H, m, 4 CH of Ph and CH^8 of chromone), 7.65 (1H, t, $^3J_{HH}$ = 8.4 Hz, CH^6 of chromone), 7.82 (1H, td, $^3J_{HH}$ = 8.6 Hz, $^4J_{HH}$ = 1.7 Hz, CH^7 of chromone), 7.97 (1H, d, $^3J_{HH}$ = 15.8 Hz, CH^5), 8.07 (1H, dd, $^3J_{HH}$ = 7.9 Hz, $^4J_{HH}$ = 1.6 Hz, CH^5 of chromone), 8.67 (1H, s, CH^2 of chromone), 9.99 (1H, d, $^2J_{HH}$ = 3.9 Hz, NH), 10.93 (1H, d, $^2J_{HH}$ = 4.0 Hz, NH). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 27.39 (CH_3), 27.61 (CH_3), 90.22 (C^5), 109.11 (*C*-CN), 116.47 (CN), 118.79 (CH^8 of chromone), 118.91 (C^{4a} of chromone), 123.39 (CH^6 of chromone), 125.46 (CH^4 of chromone), 125.99 (CH^4 of chromone), 126.93 (C^3 of chromone), 128.65 (2 CH_{ortho} of Ph), 129.09 (2 CH_{meta} of Ph), 129.33 (CH_{para} of Ph), 133.55 (CH^7 of chromone), 134.48 (CH^5), 135.25 (C_{ipso} of Ph), 150.89 (C^3), 153.77 (CH^2 of chromone), 154.94 (C=O), 159.74 (C^{8a} of chromone), 161.10 (C=O), 163.09 (C=O), 164.75 (*C*-NH_2), 175.25 (C=O).

(2*E*,4*E*)-2-[Amino(1,3-dimethyl-2,4,6-trioxotetrahydro-5(2*H*)-pyrimidinylidene)methyl]-5-(4-oxo-4*H*-chromen-3-yl)-3-phenyl-2,4-pentadienenitrile (3'a).



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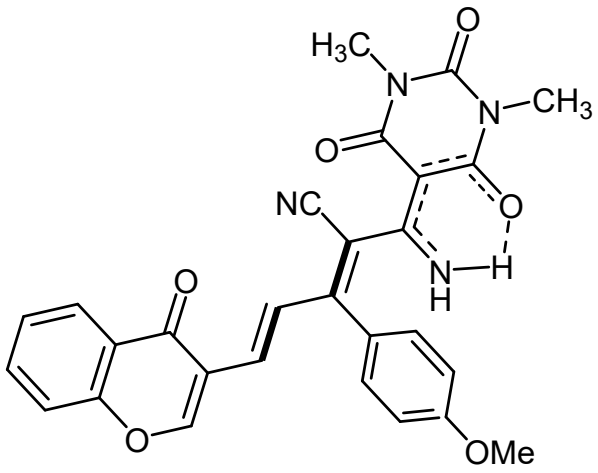
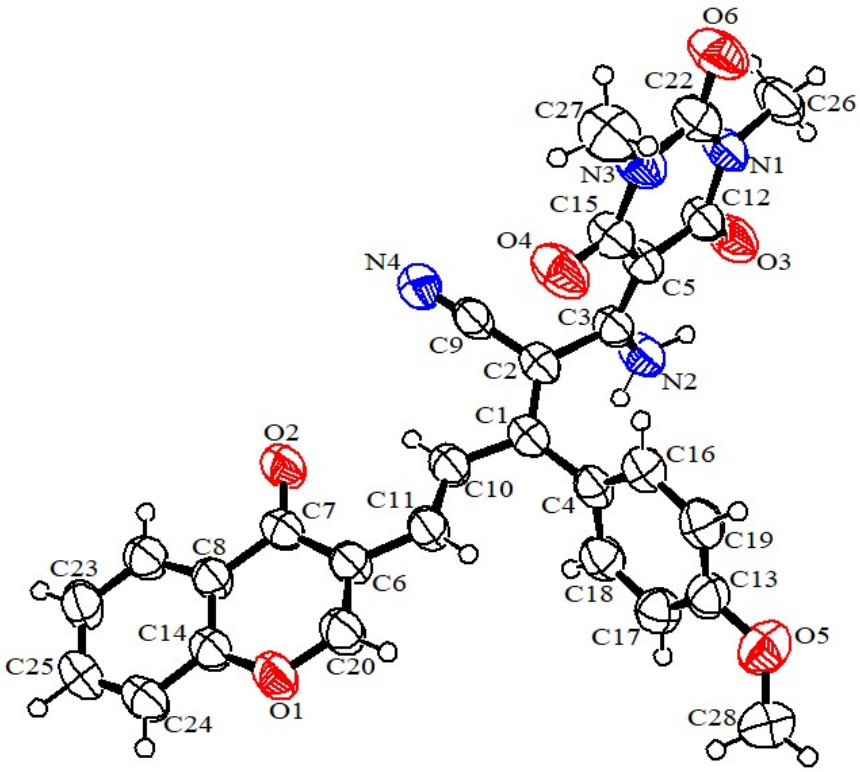
(2*E*,4*E*)-2-[Amino(1,3-dimethyl-2,4,6-trioxotetrahydro-5(2*H*)-pyrimidinylidene)methyl]-3-(4-methoxyphenyl)-5-(4-oxo-4*H*-chromen-3-yl)-2,4-pentadienenitrile (3b).



Cream powder, mp = 195-196 °C, 0.428 g, yield: 84%. IR (KBr) (ν_{max}, cm^{-1}): 3420 (NH), 2213 (CN), 1716, 1643 and 1615 (C=O), 1557 and 1463 (Ar). Anal. Calcd. for $C_{28}H_{22}N_4O_6$ (510.50): C, 65.88; H, 4.34; N, 10.97%. Found: C, 65.84; H, 4.29; N, 10.93%. MS (EI, 70 eV): *m/z* (%) = 510 (100), 453 (55), 365 (91), 337 (98), 190 (36), 171 (34), 129 (35), 121 (80), 92 (95), 77 (49). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 3.13 (3H, s, CH_3), 3.23 (3H, s, CH_3), 3.85 (3H, s, OCH_3), 6.32 (1H, d, $^3J_{HH}$ = 15.6 Hz, CH^4), 6.97 (1H, d, $^3J_{HH}$ = 8.3 Hz, CH^8 of chromone), 7.14 (2H, d, $^3J_{HH}$ = 8.2 Hz, 2 CH of Ar), 7.44 (2H, d, $^3J_{HH}$ = 8.2 Hz, 2 CH of Ar), 7.65 (1H, t, $^3J_{HH}$ = 7.8 Hz, CH^6 of chromone), 7.79 (1H, t, $^3J_{HH}$ = 8.0 Hz, CH^7 of chromone), 7.94 (1H, d, $^3J_{HH}$ = 15.6 Hz, CH^5), 8.07 (1H, d, $^3J_{HH}$ = 7.9 Hz, CH^5 of chromone), 8.69 (1H, s, CH^2 of chromone), 9.94 (1H, d, $^2J_{HH}$ = 4.0 Hz, NH), 10.92 (1H, d, $^2J_{HH}$ = 4.0 Hz, NH). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 27.38 (CH_3), 27.61 (CH_3), 55.17 (OCH_3), 90.21 (C^5), 108.60 (C-CN), 114.02 (2 CH of Ar), 116.74 (CN), 118.64 (C^{4a} of chromone), 119.03 (CH^8 of chromone), 123.42 (CH^6 of chromone), 125.56 (C^3 of chromone), 125.68 (CH^5 of chromone), 127.25 (CH^4), 129.65 (C_{ipso} of Ar), 130.34 (CH^5), 130.75 (2 CH of Ar), 134.57 (CH^7 of chromone), 150.89 (C^3), 153.65 (CH^2 of chromone), 154.96 (C=O), 159.36 (C_{ipso}-OCH_3), 159.99 (C^{8a} of chromone), 161.07 (C=O), 163.39 (C=O), 164.79 (*C*-NH_2), 175.26 (C=O). Crystal data for **3b** $C_{28}H_{22}N_4O_6$ (CCDC 1970238): M_W = 575.55, orthorhombic, P 21 21 21, a = 9.7052(19) Å, b = 13.015(3) Å, c = 19.712(4) Å, α = 90.00, β = 90.00, γ = 90.00, V = 2489.9(9) Å^3, Z = 4, Dc = 1.395 mg/m^3, F (000) = 1096, crystal dimension 0.25 × 0.20 × 0.15 mm, radiation, Mo Kα (λ = 0.71073 Å), $2.1 \leq 2\theta \leq 25.0$, intensity data were collected at 293.15 K with a

Bruker APEX area-detector diffractometer, and employing $\omega/2\theta$ scanning technique, in the range of $-11 \leq h \leq 11$, $-15 \leq k \leq 15$, $-23 \leq l \leq 21$; the structure was solved by a direct method, all non-hydrogen atoms were positioned and anisotropic thermal parameters refined from 4325 observed reflections with R (into) = 0.0750 by a full-matrix least-squares technique converged to R1 = 0.0490, and wR2 = 0.1234 [I>2sigma(I)].



Ortep diagram of **3b**

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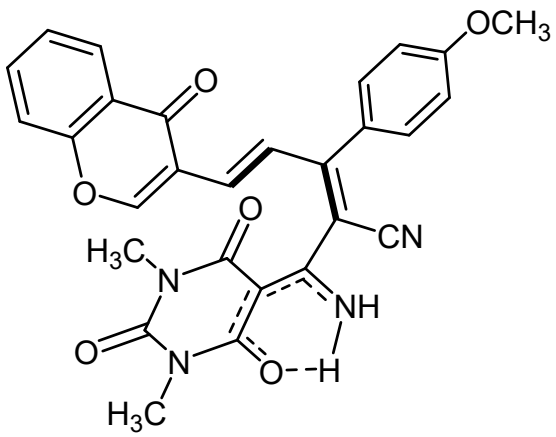

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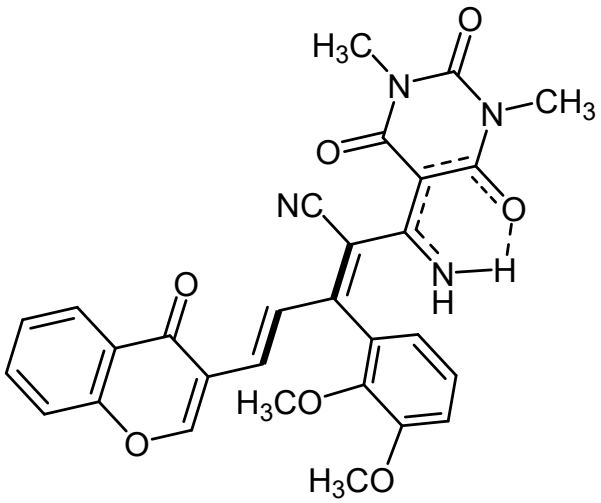

Cream powder, mp = 197-198 °C, 0.421 g, yield: 78%. IR (KBr) (ν_{max}, cm^{-1}): 3332 (NH), 2215 (CN), 1712, 1648 and 1615 (C=O), 1547 and 1467 (Ar). Anal. Calcd. for $C_{29}H_{24}N_4O_7$ (540.52): C, 64.44; H, 4.48; N, 10.37%. Found: C, 64.41; H, 4.45; N, 10.34%. MS (EI, 70 eV): *m/z* (%) = 540 (9), 431 (7), 384 (11), 319 (17), 121 (11), 92 (10), 43 (100). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 3.13 (3H, s, CH_3), 3.23 (3H, s, CH_3), 3.80 (3H, s, OCH_3), 3.85 (3H, s, OCH_3), 6.39 (1H, d, $^3J_{HH}$ = 15.6 Hz, CH^4), 6.73 (1H, d, $^3J_{HH}$ = 7.5 Hz, CH of Ar), 7.05 (1H, t, $^3J_{HH}$ = 7.9 Hz, CH of Ar), 7.17 (1H, d, $^3J_{HH}$ = 8.0 Hz, CH of Ar), 7.49 (1H, t, $^3J_{HH}$ = 8.1 Hz, CH^6 of chromone), 7.68 (1H, d, $^3J_{HH}$ = 8.4 Hz, CH^8 of chromone), 7.80 (1H, t, $^3J_{HH}$ = 8.7 Hz, CH^7 of chromone), 7.94 (1H, d, $^3J_{HH}$ = 15.6 Hz, CH^5), 8.17 (1H, d, $^3J_{HH}$ = 7.9 Hz, CH^5 of chromone), 8.69 (1H, s, CH^2 of chromone), 9.93 (1H, d, $^2J_{HH}$ = 4.1 Hz, NH), 10.92 (1H, d, $^2J_{HH}$ = 4.0 Hz, NH). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 27.38 (CH_3), 27.58 (CH_3), 55.15 (OCH_3), 55.73 (OCH_3), 90.78 (C^5), 108.25 (C-CN), 111.53 (CN), 112.73 (CH of Ar), 115.72 (CH of Ar), 116.77 (CH of Ar), 118.67 (C^3 of chromone), 118.91 (CH^8 of chromone), 121.58 (C^{4a} of chromone), 122.17 (C_{ipso} of Ar), 123.54 (CH^6 of chromone), 125.69 (CH^5 of chromone), 127.26 (CH^4), 129.38 (CH^5), 134.28 (CH^7 of chromone), 148.04 (C_{ipso}-OCH_3), 149.60 (C_{ipso}-OCH_3), 150.89 (C^3), 153.73 (CH^2 of chromone), 154.94 (C=O), 159.47 (C^{8a} of chromone), 161.04 (C=O), 163.40 (C=O), 164.76 (*C*-NH_2), 175.30 (C=O).

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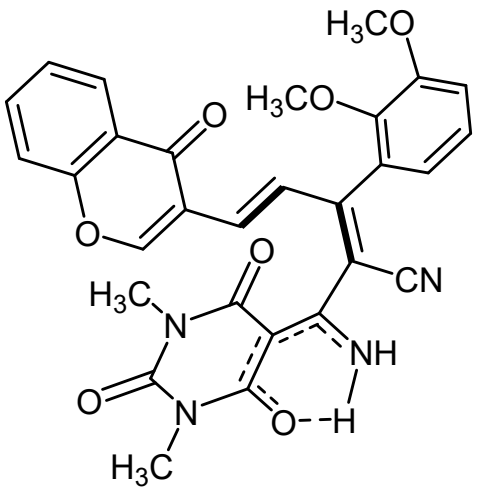

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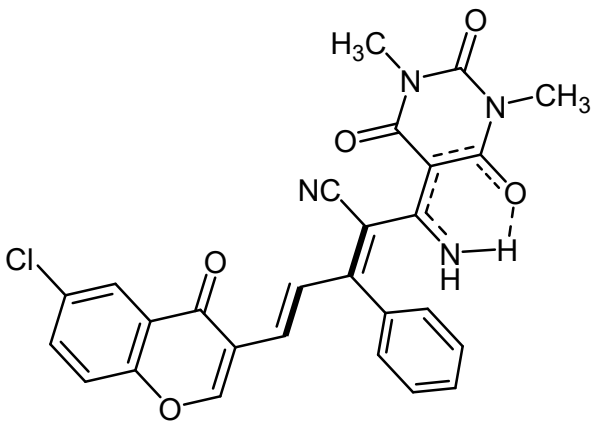
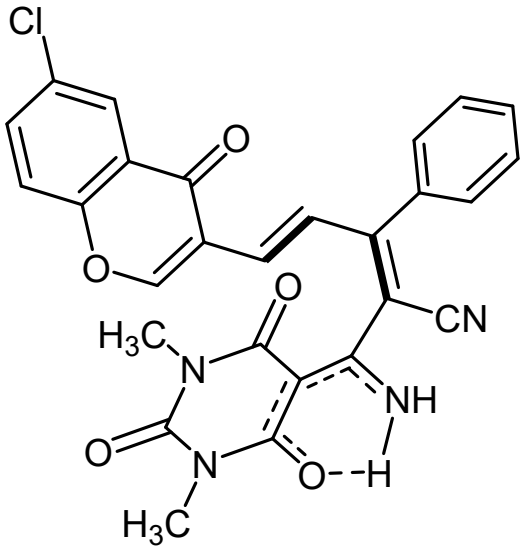
(2*E*,4*E*)-2-[Amino(1,3-dimethyl-2,4,6-trioxotetrahydro-5(2*H*)-pyrimidinylidene)methyl]-5-(6-chloro-4-oxo-4*H*-chromen-3-yl)-3-phenyl-2,4-pentadienenitrile (3d).



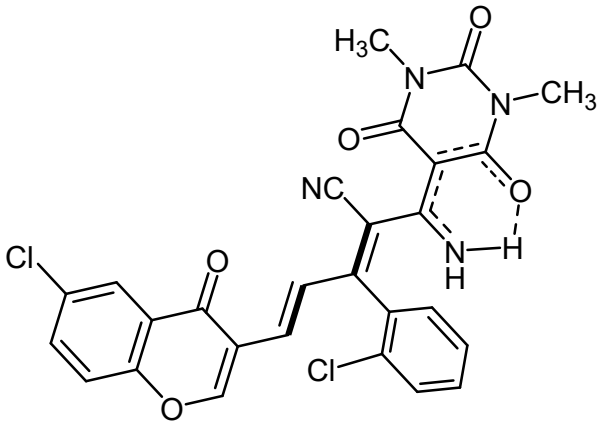
Cream powder, mp = 189-190 °C, 0.344 g, yield: 67%. IR (KBr) (ν_{max}, cm^{-1}): 3429 (NH), 2229 (CN), 1647 and 1607 (C=O), 1559 and 1467 (Ar). Anal. Calcd. for $C_{27}H_{19}ClN_4O_5$ (514.92): C, 62.98; H, 3.72; N, 10.88%. Found: C, 62.95; H, 3.69; N, 10.84%. MS (EI, 70 eV): *m/z* (%) = 514 (50), 487 (100), 399 (48), 371 (52), 190 (55), 155 (61), 126 (96), 98 (29), 58 (71). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 3.14 (3H, s, CH_3), 3.24 (3H, s, CH_3), 6.24 (1H, d, $^3J_{HH}$ = 15.6 Hz, CH^4), 7.16 (1H, td, $^3J_{HH}$ = 7.0 Hz, $^4J_{HH}$ = 2.0 Hz, CH_{para} of Ph), 7.48 (2H, dd, $^3J_{HH}$ = 7.8 Hz, $^4J_{HH}$ = 1.7 Hz, 2 CH_{ortho} of Ph), 7.58 (2H, t, $^3J_{HH}$ = 7.1 Hz, 2 CH_{meta} of Ph), 7.73 (1H, d, $^3J_{HH}$ = 8.9 Hz, CH^8 of chromone), 7.89 (1H, dd, $^3J_{HH}$ = 9.0 Hz, $^4J_{HH}$ = 2.5 Hz, CH^7 of chromone), 7.94 (1H, d, $^3J_{HH}$ = 15.7 Hz, CH^5), 8.01 (1H, d, $^4J_{HH}$ = 2.5 Hz, CH^5 of chromone), 8.69 (1H, s, CH^2 of chromone), 9.98 (1H, bs, NH), 10.91 (1H, bs, NH). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 27.36 (CH_3), 27.59 (CH_3), 90.24 (C^5), 109.32 (C-CN), 116.40 (CN), 118.95 (CH^8 of chromone), 120.95 (C^3 of chromone), 124.51 (CH^5 of chromone), 124.51 (C^{4a} of chromone), 128.63 (2 CH_{meta} of Ph), 129.07 (2 CH_{ortho} of Ph), 129.14 (CH^4), 129.33 (CH_{para} of Ph), 130.42 (CH^5), 132.26 (C_{ipso}-Cl), 134.26 (C_{ipso} of Ph), 135.18 (CH^7 of chromone), 150.87 (C^3), 153.52 (C=O), 153.59 (CH^2 of chromone), 159.49 (C^{8a} of chromone), 161.09 (C=O), 163.03 (C=O), 174.17 (*C*-NH_2), 174.72 (C=O).

(2*E*,4*E*)-2-[Amino(1,3-dimethyl-2,4,6-trioxotetrahydro-5(2*H*)-pyrimidinylidene)methyl]-5-(6-chloro-4-oxo-4*H*-chromen-3-yl)-3-phenyl-2,4-pentadienenitrile (3'd).



Cream powder, mp = 189-190 °C, 0.344 g, yield: 67%. IR (KBr) (ν_{max}, cm^{-1}): 3429 (NH), 2229 (CN), 1647 and 1607 (C=O), 1559 and 1467 (Ar). Anal. Calcd. for $C_{27}H_{19}ClN_4O_5$ (514.92): C, 62.98; H, 3.72; N, 10.88%. Found: C, 62.95; H, 3.69; N, 10.84%. MS (EI, 70 eV): *m/z* (%) = 514 (50), 487 (100), 399 (48), 371 (52), 190 (55), 155 (61), 126 (96), 98 (29), 58 (71). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 3.09 (3H, s, CH_3), 3.16 (3H, s, CH_3), 6.28 (1H, d, $^3J_{HH}$ = 15.6 Hz, CH^4), 7.15 (1H, t, $^3J_{HH}$ = 7.0 Hz, CH_{para} of Ph), 7.38-7.59 (4H, m, 4 CH of Ph), 7.77 (1H, d, $^3J_{HH}$ = 9.1 Hz, CH^8 of chromone), 7.85 (1H, dd, $^3J_{HH}$ = 8.7 Hz, $^4J_{HH}$ = 2.5 Hz, CH^7 of chromone), 8.11 (1H, d, $^4J_{HH}$ = 2.6 Hz, CH^5 of chromone), 8.54 (1H, d, $^3J_{HH}$ = 15.5 Hz, CH^5), 8.72 (1H, s, CH^2 of chromone), 9.44 (1H, bs, NH), 10.36 (1H, bs, NH). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 27.19 (CH_3), 27.59 (CH_3), 90.78 (C^5), 108.96 (C-CN), 115.49 (CN), 118.83 (CH^8 of chromone), 120.99 (C^3 of chromone), 124.44 (CH^5 of chromone), 124.63 (C^{4a} of chromone), 127.26 (CH^4), 128.41 (2 CH_{meta} of Ph), 128.68 (2 CH_{ortho} of Ph), 129.62 (CH_{para} of Ph), 130.48 (CH^5), 132.74 (C_{ipso}-Cl), 133.48 (CH^7 of chromone), 134.26 (C_{ipso} of Ph), 150.81 (C^3), 153.52 (C=O), 154.40 (CH^2 of chromone), 159.84 (C^{8a} of chromone), 161.36 (C=O), 163.46 (C=O), 174.23 (*C*-NH_2), 174.28 (C=O).

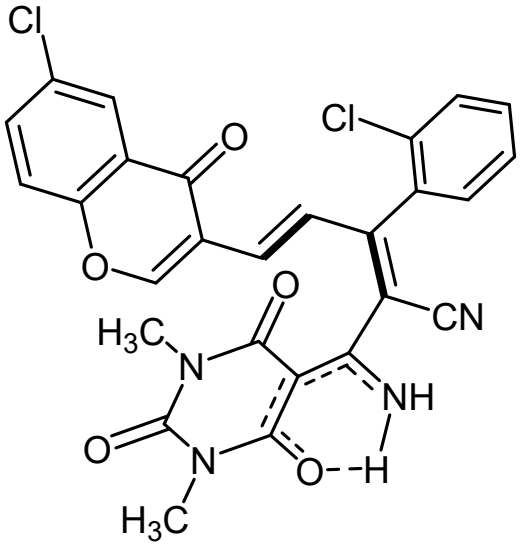
(2*E*,4*E*)-2-[Amino(1,3-dimethyl-2,4,6-trioxotetrahydro-5(2*H*)-pyrimidinylidene)methyl]-5-(6-chloro-4-oxo-4*H*-chromen-3-yl)-3-(2-chlorophenyl)-2,4-pentadienenitrile (3e).



Cream powder, mp = 196-197 °C, 0.345 g, yield: 63%. IR (KBr) (ν_{max}, cm^{-1}): 3323 (NH), 2223 (CN), 1712, 1650 and 1610 (C=O), 1553 and 1467 (Ar). Anal. Calcd. for $C_{27}H_{18}Cl_2N_4O_5$ (549.36): C, 59.03; H, 3.30; N, 10.20%. Found: C, 58.98; H, 3.27; N, 10.16%. MS (EI, 70 eV): *m/z* (%) = 548

(1), 535 (9), 411 (58), 409 (100), 357 (55), 205 (95), 126 (40), 98 (18), 75 (20), 63 (26). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 3.06 (3H, s, CH_3), 3.13 (3H, s, CH_3), 6.10 (1H, d, $^{3}J_{HH}$ = 16.4 Hz, CH^4), 6.98 (1H, d, $^{3}J_{HH}$ = 7.5 Hz, CH of Ar), 7.34-7.65 (3H, m, 3 CH of Ar), 7.74 (1H, d, $^{3}J_{HH}$ = 16.2 Hz, CH^5), 7.76 (1H, d, $^{3}J_{HH}$ = 9.2 Hz, CH^8 of chromone), 7.88 (1H, dd, $^{3}J_{HH}$ = 9.0 Hz, $^{4}J_{HH}$ = 2.6 Hz, CH^7 of chromone), 8.11 (1H, d, $^{4}J_{HH}$ = 2.6 Hz, CH^5 of chromone), 8.71 (1H, s, CH^2 of chromone), 9.23 (1H, bs, NH), 10.40 (1H, bs, NH). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 27.61 (CH_3), 27.44 (CH_3), 82.02 (C^5), 106.24 (C-CN), 115.70 (CN), 118.67 (CH^8 of chromone), 119.71 (C^3 of chromone), 121.23 (C^{4a} of chromone), 124.58 (CH^5 of chromone), 126.60 (CH of Ar), 127.19 (CH^4), 129.38 (CH of Ar), 129.85 (CH of Ar), 130.47 (CH of Ar), 130.89 (C_{ipso} of Ar), 131.09 (C_{ipso}-Cl), 132.03 (C_{ipso}-Cl), 132.15 (CH^5), 134.13 (CH^7 of chromone), 150.80 (C^3), 153.55 (C=O), 153.55 (CH^2 of chromone), 158.13 (C^{8a} of chromone), 160.78 (C=O), 164.66 (C=O), 168.24 (*C*-NH_2), 174.39 (C=O).

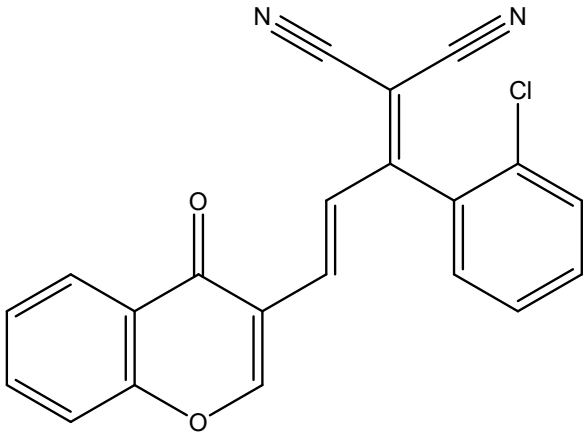
(2*E*,4*E*)-2-[Amino(1,3-dimethyl-2,4,6-trioxotetrahydro-5(2*H*)-pyrimidinylidene)methyl]-5-(6-chloro-4-oxo-4*H*-chromen-3-yl)-3-(2-chlorophenyl)-2,4-pentadienenitrile (3'e).



Cream powder, mp = 196-197 °C, 0.345 g, yield: 63%. IR (KBr) (ν_{max}, cm^{-1}): 3323 (NH), 2223 (CN), 1712, 1650 and 1610 (C=O), 1553 and 1467 (Ar). Anal. Calcd. for $C_{27}H_{18}Cl_2N_4O_5$ (549.36): C, 59.03; H, 3.30; N, 10.20%. Found: C, 58.98; H, 3.27; N, 10.16%. MS (EI, 70 eV): *m/z* (%) = 548

(1), 535 (9), 411 (58), 409 (100), 357 (55), 205 (95), 126 (40), 98 (18), 75 (20), 63 (26). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 3.09 (3H, s, CH_3), 3.16 (3H, s, CH_3), 6.04 (1H, d, $^{3}J_{HH}$ = 15.5 Hz, CH^4), 7.34-7.65 (4H, m, 4 CH of Ar), 7.76 (1H, d, $^{3}J_{HH}$ = 9.2 Hz, CH^8 of chromone), 7.85 (1H, dd, $^{3}J_{HH}$ = 9.7 Hz, $^{4}J_{HH}$ = 2.6 Hz, CH^7 of chromone), 7.99 (1H, d, $^{4}J_{HH}$ = 2.5 Hz, CH^5 of chromone), 8.54 (1H, d, $^{3}J_{HH}$ = 15.6 Hz, CH^5), 8.71 (1H, s, CH^2 of chromone), 9.52 (1H, bs, NH), 9.93 (1H, bs, NH). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 27.23 (CH_3), 28.01 (CH_3), 82.02 (C^5), 106.24 (C-CN), 115.09 (CN), 118.78 (CH^8 of chromone), 119.71 (C^3 of chromone), 120.86 (C^{4a} of chromone), 124.58 (CH^5 of chromone), 126.49 (CH of Ar), 127.72 (CH^4), 129.72 (CH of Ar), 130.08 (CH of Ar), 130.47 (CH of Ar), 130.84 (CH^5), 131.17 (C_{ipso}-Cl), 131.94 (C_{ipso}-Cl), 132.10 (C_{ipso} of Ar), 134.56 (CH^7 of chromone), 150.80 (C^3), 153.55 (C=O), 153.55 (CH^2 of chromone), 158.13 (C^{8a} of chromone), 160.78 (C=O), 164.66 (C=O), 168.24 (*C*-NH_2), 174.25 (C=O).

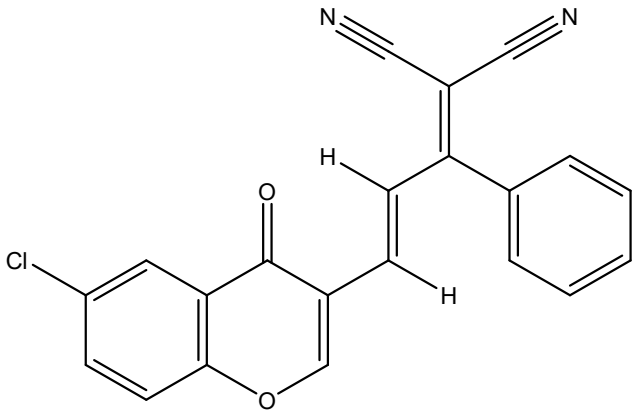
[(2*E*)-1-(2-Chlorophenyl)-3-(4-oxo-4*H*-chromen-3-yl)-2-propen-1-ylidene]malononitrile (3f).



Yellow powder, mp = 234-235 °C, 0.268 g, yield: 75%. IR (KBr) (ν_{max}, cm^{-1}): 2225 (CN), 1653 and 1618 (C=O), 1563 and 1466 (Ar). Anal. Calcd. for $C_{21}H_{11}ClN_2O_2$ (358.78): C, 70.30; H, 3.09; N, 7.81%. Found: C, 70.26; H, 2.97; N, 7.78%. MS (EI, 70 eV): *m/z* (%) = 358 (28), 323 (60), 295 (15), 171 (100), 120 (13), 92 (45), 64 (18). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 6.60 (1H, d, $^{3}J_{HH}$ = 15.2 Hz, CH^3), 7.51 (1H, t, $^{3}J_{HH}$ = 7.9 Hz, CH^8 of chromone), 7.57 (1H, t, $^{3}J_{HH}$ = 7.8 Hz, CH^6 of chromone), 7.60 (1H, d, $^{3}J_{HH}$ = 7.7 Hz, CH of Ar), 7.65 (1H, t, $^{3}J_{HH}$ = 7.7 Hz, CH of Ar), 7.70 (1H, d, $^{3}J_{HH}$ = 7.9 Hz, CH of Ar), 7.73 (1H, d, $^{3}J_{HH}$ = 7.8 Hz, CH of Ar), 7.85 (1H, t, $^{3}J_{HH}$ = 7.9 Hz, CH^7

of chromone), 8.17 (1H, d, $^{3}J_{HH}$ = 8.0 Hz, CH^{5} of chromone), 8.66 (1H, d, $^{3}J_{HH}$ = 15.3 Hz, CH^{2}), 8.87 (1H, s, CH^{2} of chromone). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 83.35 (*C*-CN), 112.38 (CN), 112.99 (CN), 118.16 (C^{3} of chromone), 118.62 (CH^{8} of chromone), 123.50 (C^{4a} of chromone), 125.53 (CH^{6} of chromone), 125.61 (CH^{5} of chromone), 126.50 (CH of Ar), 127.93 (CH of Ar), 130.16 (CH of Ar), 130.57 (CH of Ar), 131.08 (C$_{ipso}$ of Ar), 131.51 (C$_{ipso}$-Cl), 132.29 (CH^{2}), 134.88 (CH^{7} of chromone), 141.47 (CH^{3}), 154.83 (CH^{2} of chromone), 163.60 (C^{8a} of chromone), 169.82 (C^{1}), 175.32 (C=O).

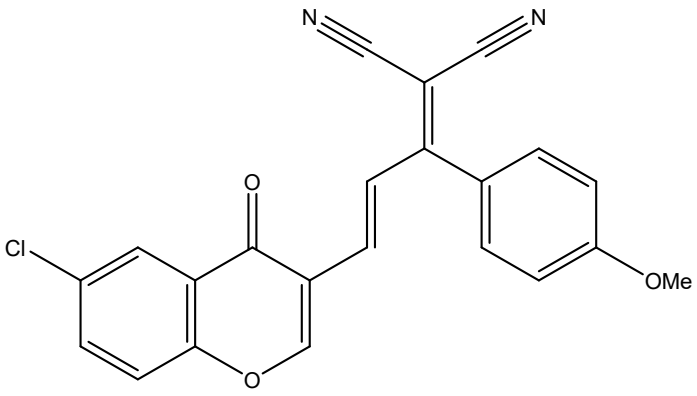
[(2*E*)-3-(6-Chloro-4-oxo-4*H*-chromen-3-yl)-1-phenyl-2-propen-1-ylidene]malononitrile (3g).



Yellow powder, mp = 233-234 °C, 0.279 g, yield: 78%. IR (KBr) (ν_{max}, cm^{-1}): 2229 (CN), 1647 and 1607 (C=O), 1559 and 1467 (Ar). Anal. Calcd. for $C_{21}H_{11}ClN_2O_2$ (358.78): C, 70.30; H, 3.09; N, 7.81%. Found: C, 70.27; H, 2.98; N, 7.77%. MS (EI, 70 eV): *m/z* (%) = 358 (28), 323 (60), 295 (15), 171 (100), 120 (13), 92 (45), 64 (18). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 6.68 (1H, d, $^{3}J_{HH}$ = 15.3 Hz, CH^{3}), 7.49 (2H, t, $^{3}J_{HH}$ = 7.0 Hz, 2 CH$_{meta}$ of Ph), 7.61 (2H, d, $^{3}J_{HH}$ = 7.1 Hz, 2 CH$_{ortho}$ of Ph), 7.62 (1H, t, $^{3}J_{HH}$ = 7.0 Hz, CH$_{para}$ of Ph), 7.78 (1H, d, $^{3}J_{HH}$ = 9.0 Hz, CH^{8} of chromone), 7.89 (1H, dd, $^{3}J_{HH}$ = 8.9 Hz, $^{4}J_{HH}$ = 2.6 Hz, CH^{7} of chromone), 8.09 (1H, d, $^{3}J_{HH}$ = 2.6 Hz, CH^{5} of chromone), 8.60 (1H, d, $^{3}J_{HH}$ = 15.4 Hz, CH^{2}), 8.87 (1H, s, CH^{2} of chromone). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 81.92 (*C*-CN), 113.06 (CN), 113.86 (CN), 118.35 (CH^{8} of chromone), 121.31 (C^{3} of chromone), 124.51 (C^{4a} of chromone), 124.69 (CH^{5} of chromone), 126.90 (2 CH$_{meta}$ of Ph), 129.07 (2CH$_{ortho}$ of Ph), 129.39 (CH$_{para}$ of Ph), 130.89 (CH^{2}), 131.19 (C$_{ipso}$-Cl), 132.51 (CH^{7} of

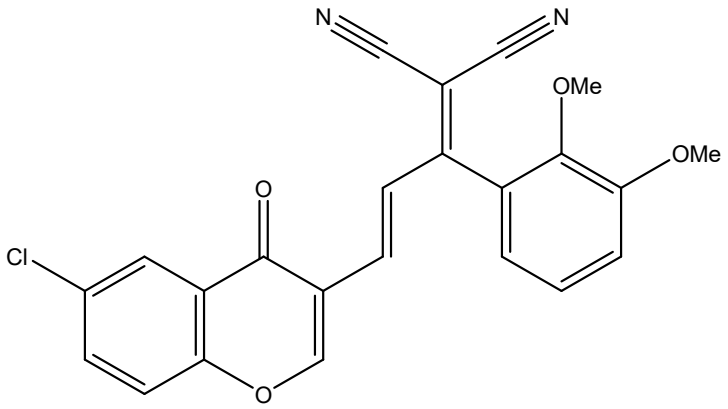
chromone), 134.66 (C_{ipso} of Ar), 141.11 (CH^3), 153.47 (CH^2 of chromone), 163.09 (C^{8a} of chromone), 171.88 (C^1), 174.22 (C=O).

[(2*E*)-3-(6-Chloro-4-oxo-4*H*-chromen-3-yl)-1-(4-methoxyphenyl)-2-propen-1-ylidene]malononitrile (3h)

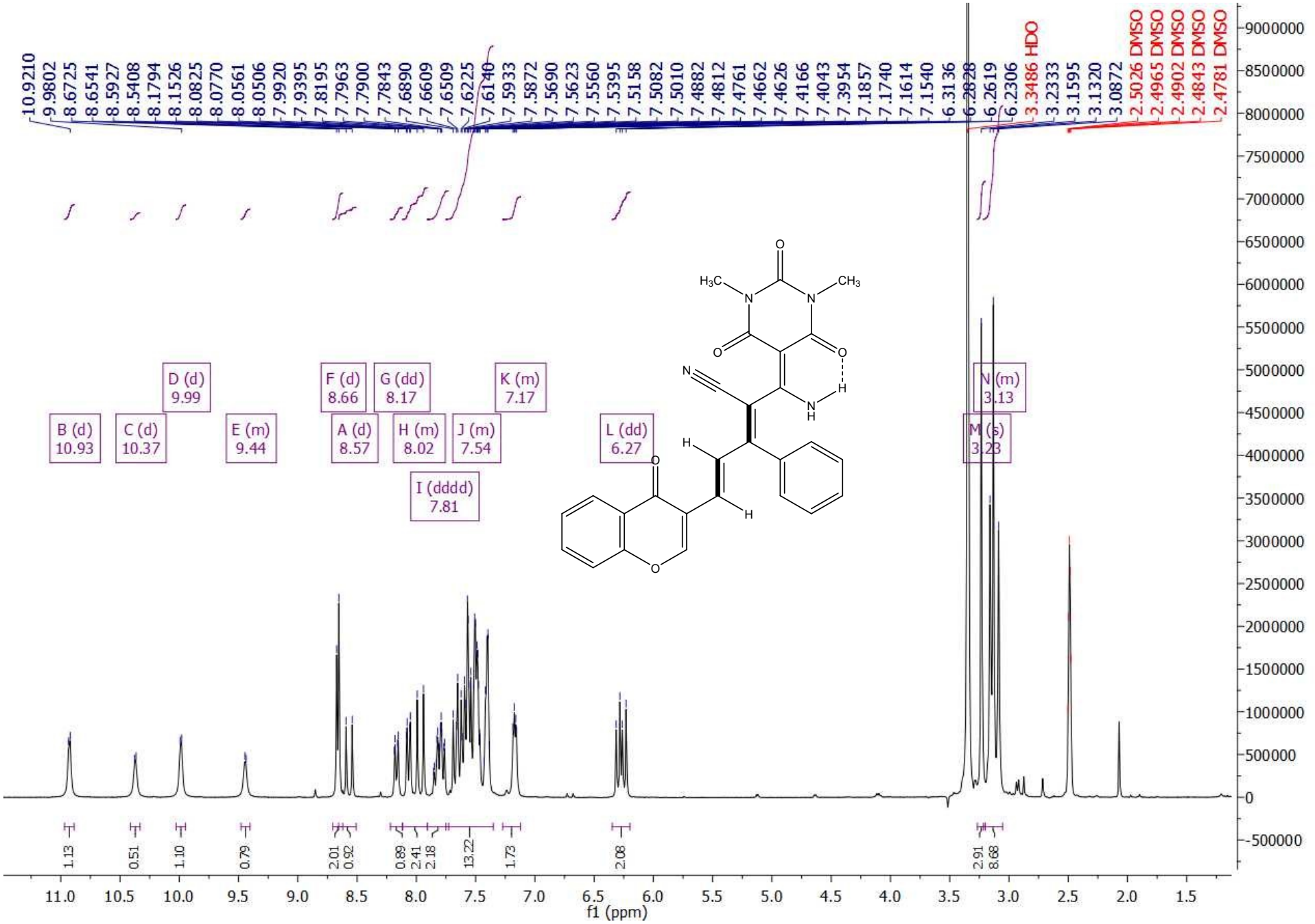


Yellow powder, mp = 238-234 °C, 0.314 g, yield: 81%. IR (KBr) (ν_{max}, cm^{-1}): 2225 (CN), 1647 and 1600 (C=O), 1560 and 1467 (Ar). Anal. Calcd. for $C_{22}H_{13}ClN_2O_3$ (388.80): C, 67.96; H, 3.37; N, 7.21%. Found: C, 67.94; H, 3.35; N, 7.19%. MS (EI, 70 eV): *m/z* (%) = 388 (79), 361 (19), 323 (100), 205 (35), 164 (18), 126 (23), 63 (16). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 3.86 (3H, s, CH_3), 6.76 (1H, d, $^3J_{HH}$ = 15.4 Hz, CH^3), 7.16 (2H, d, $^3J_{HH}$ = 8.8 Hz, 2 CH of Ar), 7.47 (2H, d, $^3J_{HH}$ = 8.8 Hz, 2 CH of Ar), 7.79 (1H, d, $^3J_{HH}$ = 9.0 Hz, CH^8 of chromone), 7.90 (1H, dd, $^3J_{HH}$ = 9.0 Hz, $^4J_{HH}$ = 2.5 Hz, CH^7 of chromone), 8.11 (1H, d, $^3J_{HH}$ = 2.5 Hz, CH^5 of chromone), 8.57 (1H, dd, $^3J_{HH}$ = 15.3 Hz, $^4J_{HH}$ = 2.0 Hz, CH^2), 8.89 (1H, d, $^4J_{HH}$ = 2.1 Hz, CH^2 of chromone). ^{13}C NMR (75.00 MHz, DMSO-d_6): δ_C 55.48 (CH_3), 80.43 (*C*-CN), 113.44 (CN), 114.33 (CN), 114.40 (2 CH of Ar), 118.46 (CH^8 of chromone), 121.14 (C^3 of chromone), 124.48 (CH^5 of chromone), 124.61 (C^{4a} of chromone), 124.71 (CH^2), 127.13 (C_{ipso} of Ar), 130.84 (C_{ipso}-Cl), 131.29 (2 CH of Ar), 134.63 (CH^7 of chromone), 140.95 (CH^2), 153.49 (CH^2 of chromone), 161.65 (C_{ipso}-OCH_3), 162.92 (C^{8a} of chromone), 171.60 (C^1), 174.26 (C=O).

[(2*E*)-3-(6-Chloro-4-oxo-4*H*-chromen-3-yl)-1-(2,3-dimethoxyphenyl)-2-propen-1-ylidene]malononitrile (3i)



Yellow powder, mp = 237-239 °C, 0.259 g, yield: 62%. IR (KBr) (ν_{max}, cm^{-1}): 2215 (CN), 1664 and 1619 (C=O), 1580 and 1469 (Ar). Anal. Calcd. for $C_{23}H_{15}ClN_2O_4$ (418.83): C, 65.96; H, 3.61; N, 6.69%. Found: C, 65.93; H, 3.58; N, 6.66%. MS (EI, 70 eV): *m/z* (%) = 418 (18), 370 (12), 260 (24), 217 (26), 190 (24), 154 (44), 126 (100), 98 (35), 63 (56). ^{1}H NMR (300.13 MHz, DMSO-d_6): δ_H 3.80 (3H, s, CH_3), 3.81 (3H, s, CH_3), 6.86 (1H, d, $^3J_{HH}$ = 15.2 Hz, CH^3), 6.87 (1H, d, $^3J_{HH}$ = 8.3 Hz, CH of Ar), 7.12 (1H, t, $^3J_{HH}$ = 8.0 Hz, CH of Ar), 7.15 (1H, d, $^3J_{HH}$ = 15.2 Hz, CH^2), 7.19 (1H, d, $^3J_{HH}$ = 8.4 Hz, CH of Ar), 7.90 (1H, d, $^3J_{HH}$ = 9.0 Hz, CH^8 of chromone), 7.94 (1H, dd, $^3J_{HH}$ = 9.0 Hz, $^4J_{HH}$ = 2.8 Hz, CH^7 of chromone), 8.08 (1H, d, $^3J_{HH}$ = 2.7 Hz, CH^5 of chromone), 8.75 (1H, d, $^4J_{HH}$ = 2.8 Hz, CH^2 of chromone). Due to the low solubility, the carbon spectrum could not be analyzed.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E (m) 9.44
F (d) 8.66
A (d) 8.57
G (dd) 8.17
H (m) 8.02
I (dddd) 7.81
J (m) 7.54
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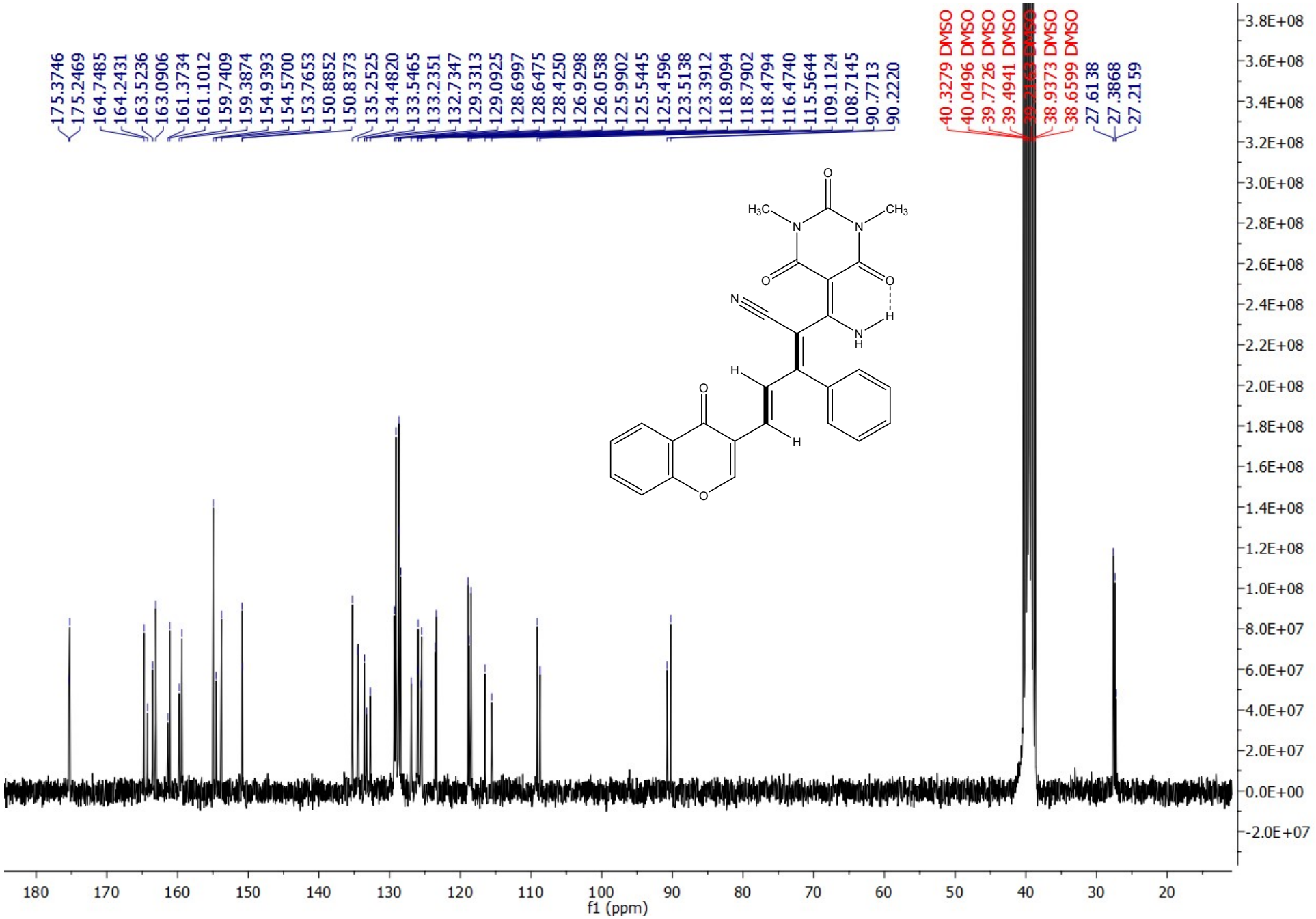
M (s) 3.23
f1 (ppm)

^{1}H NMR of **3a**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160
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110
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70
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50
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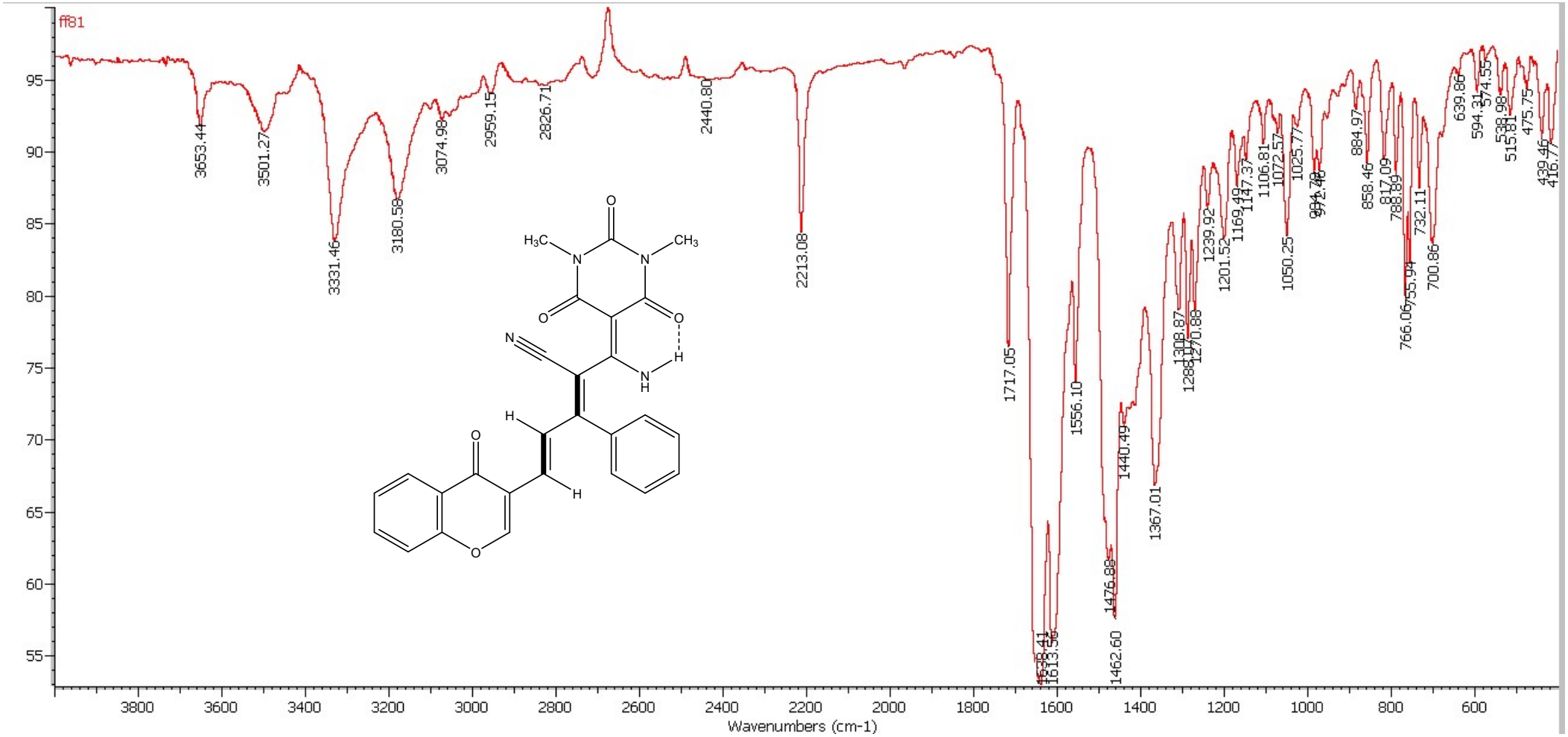
30
20
f1 (ppm)

^{13}C NMR of **3a**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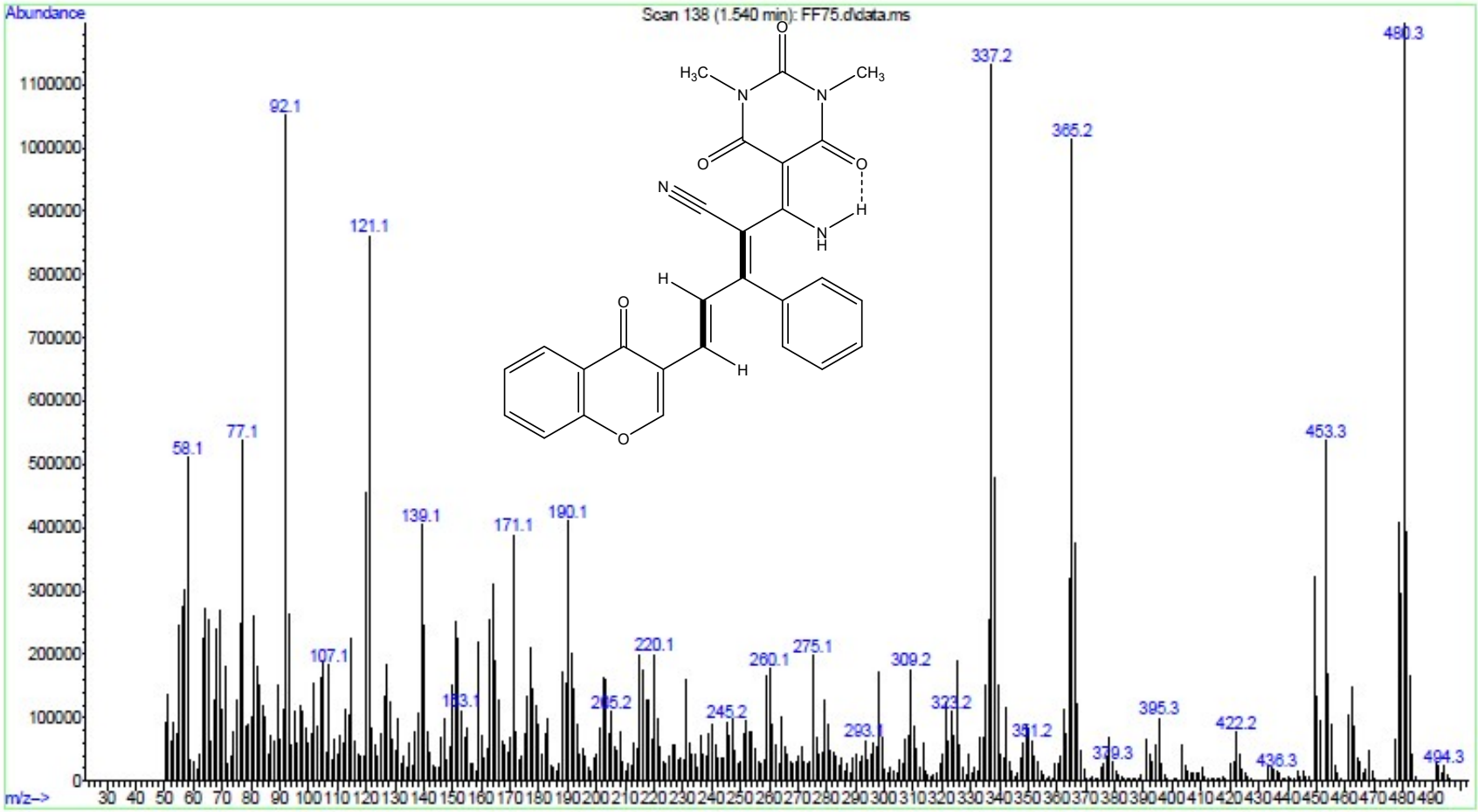
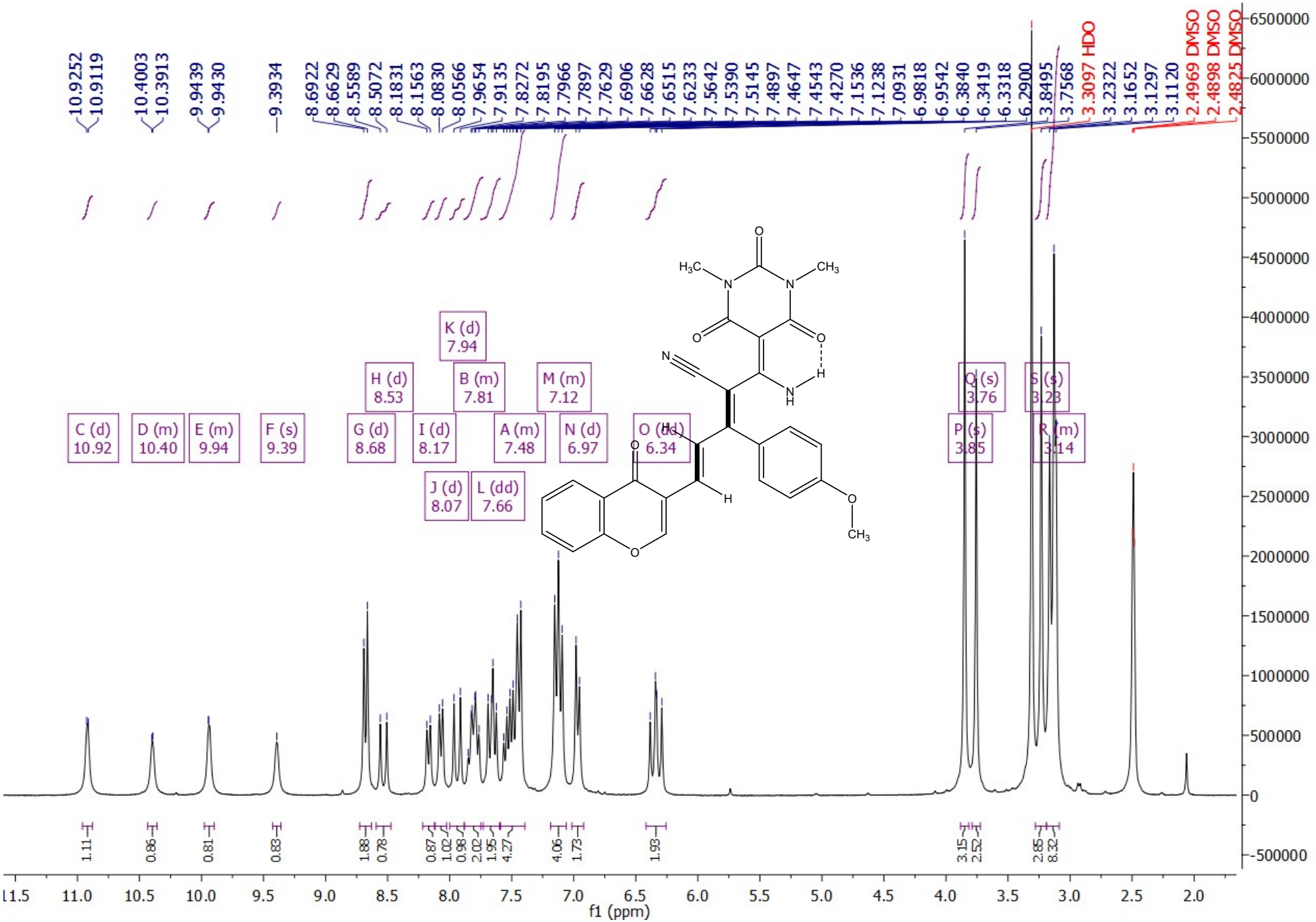
3180.58
3074.98
2959.15
2826.71
2440.80
2213.08
1717.05
1556.10
1476.88
1462.60
1440.49
1367.01
1308.87
1270.88
1239.92
1201.52
1169.49
1147.37
1106.81
1072.57
1050.25
1025.77
884.97
858.46
817.09
788.89
766.06
755.94
732.11
700.86
639.86
594.31
574.55
538.98
515.81
475.75
439.46
Wavenumbers (cm-1)

IR of **3a**

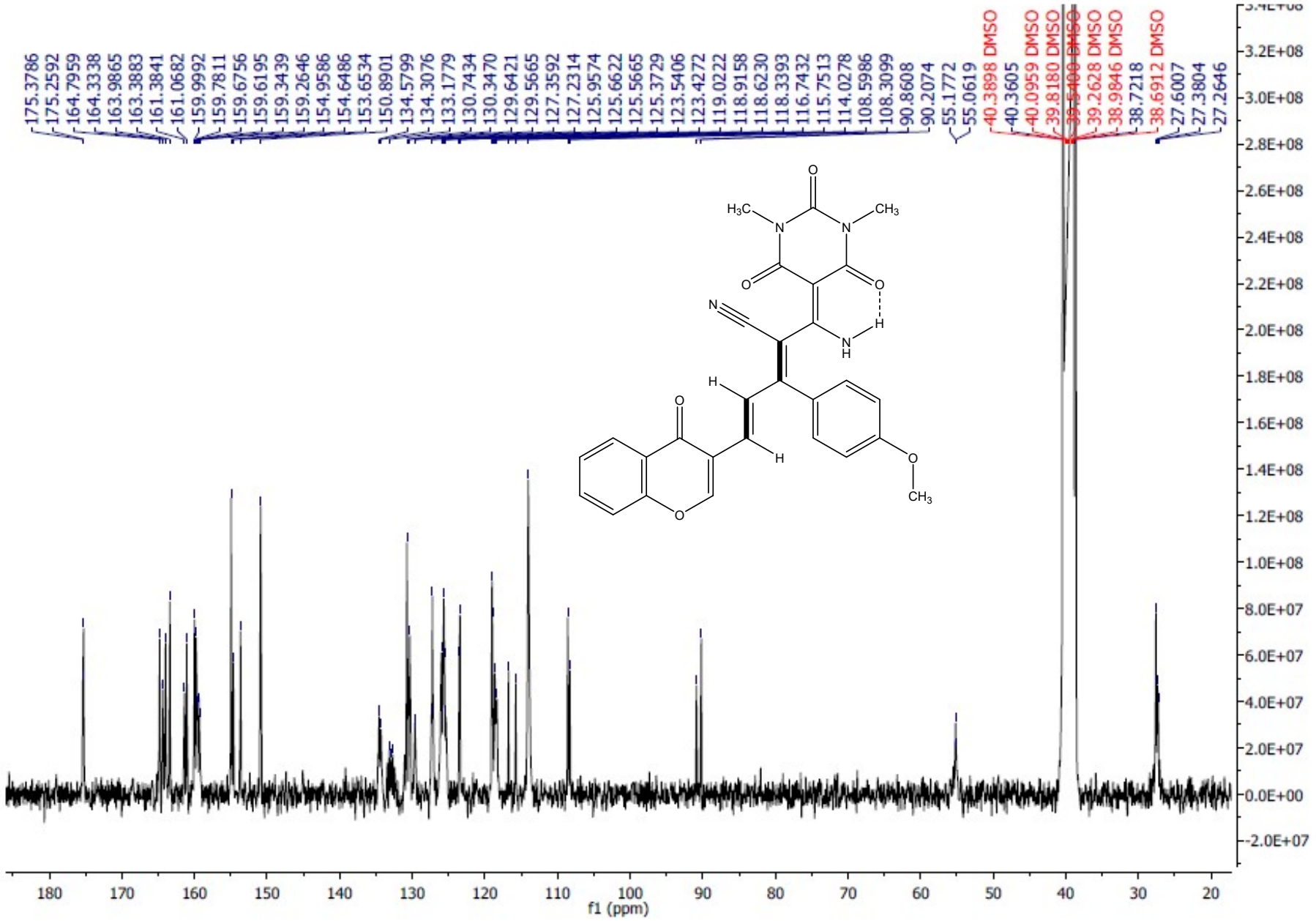
File C:\MSDCHEM\3\DATA\Snapshot\FF75.d
Operator :
Acquired : 1 Feb 2021 11:14 using AcqMethod default.m
Instrument : DIRECT PROBE
Sample Name:
Misc Info :
Vial Number: 1



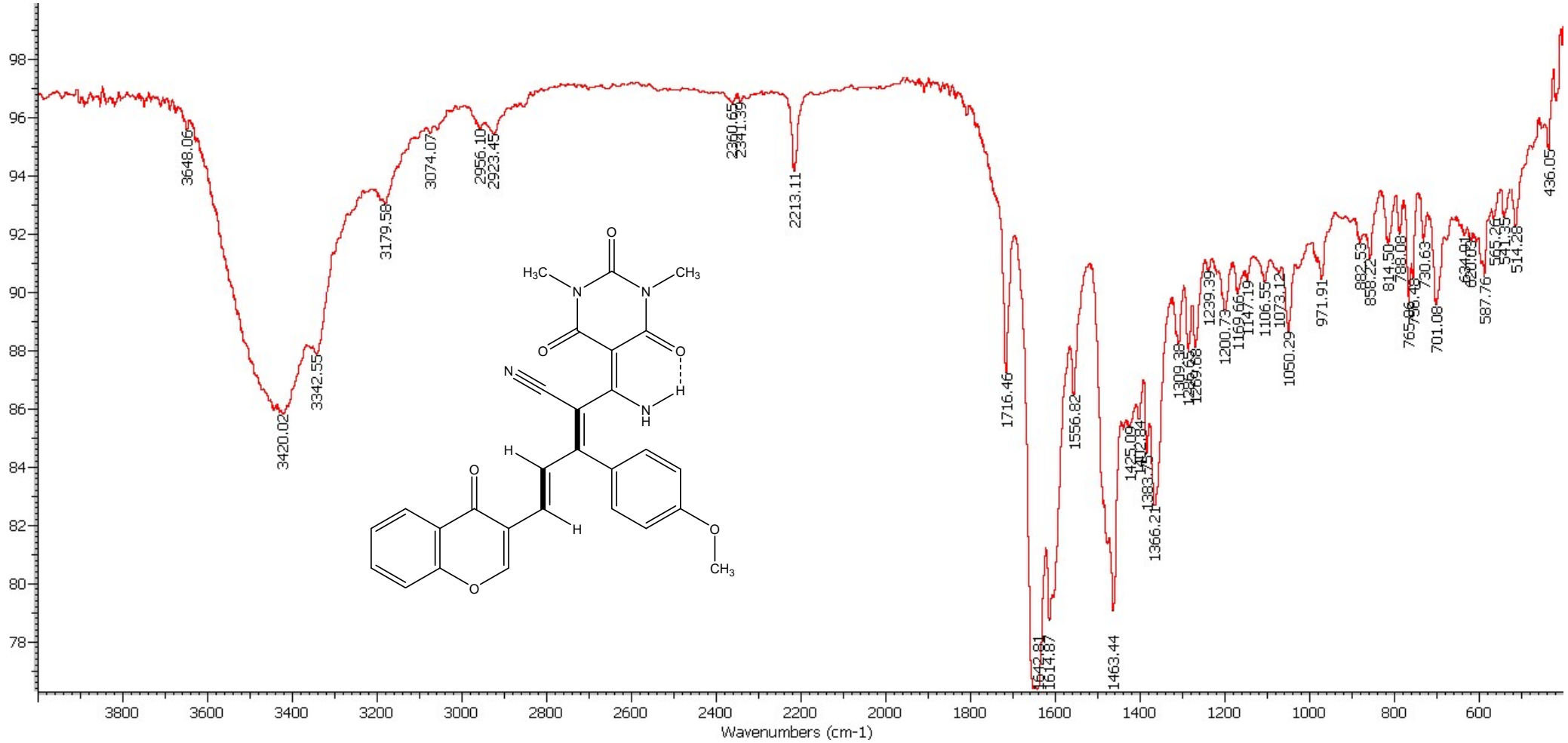
Mass of compound **3a**


10.9252
10.9119
10.4003
10.3913
9.9439
9.9430
9.3934
8.6922
8.6629
8.5589
8.5072
8.1831
8.1563
8.0830
8.0566
7.9654
7.9135
7.8272
7.8195
7.7966
7.7897
7.7629
7.6906
7.6628
7.6515
7.6233
7.5642
7.5390
7.5145
7.4897
7.4647
7.4543
7.4270
7.1536
7.1238
7.0931
6.9818
6.9542
6.3840
6.3419
6.3318
6.2900
3.8495
3.7568
3.3097 HDO
3.2322
3.1652
3.1297
3.1120
2.4969 DMSO
2.4898 DMSO
2.4825 DMSO
C (d) 10.92
D (m) 10.40
E (m) 9.94
F (s) 9.39
G (d) 8.68
H (d) 8.53
I (d) 8.17
J (d) 8.07
K (d) 7.94
L (dd) 7.66
B (m) 7.81
A (m) 7.48
M (m) 7.12
N (d) 6.97
O (dd) 6.34
P (s) 3.85
Q (s) 3.76
S (s) 3.23
R (m) 3.14
1.11
0.86
0.81
0.83
1.88
0.78
0.87
1.02
0.98
2.02
1.95
4.27
4.06
1.73
1.93
3.15
2.52
2.85
8.32
f1 (ppm)

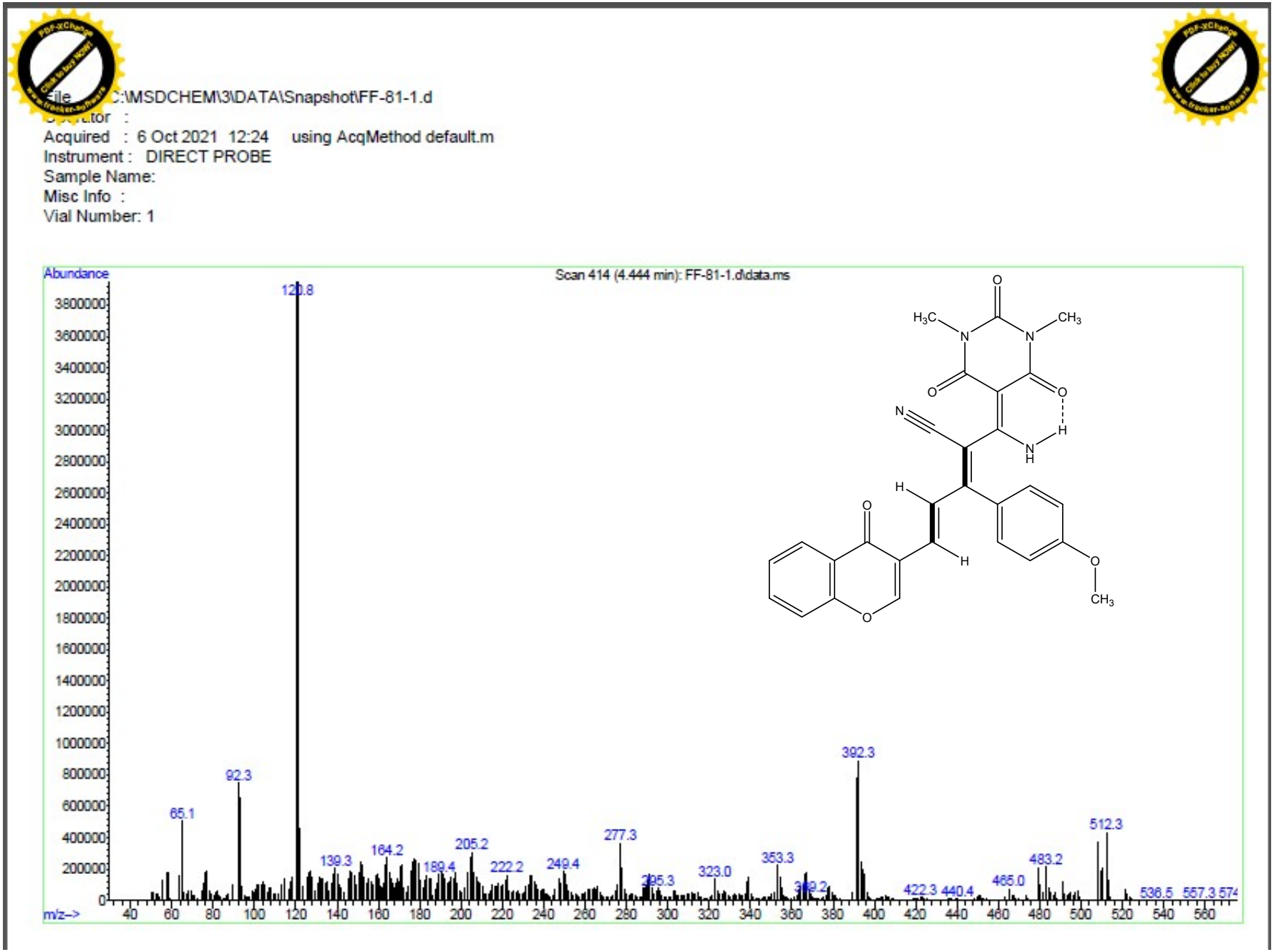
^{1}H NMR of **3b**


175.3786
175.2592
164.7959
164.3338
163.9865
163.3883
161.3841
161.0682
159.9992
159.7811
159.6756
159.6195
159.3439
159.2646
154.9586
154.6486
153.6534
150.8901
134.5799
134.3076
133.1779
130.7434
130.3470
129.6421
129.5665
127.3592
127.2314
125.9574
125.6622
125.5665
125.3729
123.5406
123.4272
119.0222
118.9158
118.6230
118.3393
116.7432
115.7513
114.0278
108.5986
108.3099
90.8608
90.2074
55.1772
55.0619
40.3898 DMSO
40.3605
40.0959 DMSO
39.8180 DMSO
39.5400 DMSO
39.2628 DMSO
38.9846 DMSO
38.7218
38.6912 DMSO
27.6007
27.3804
27.2646
f1 (ppm)

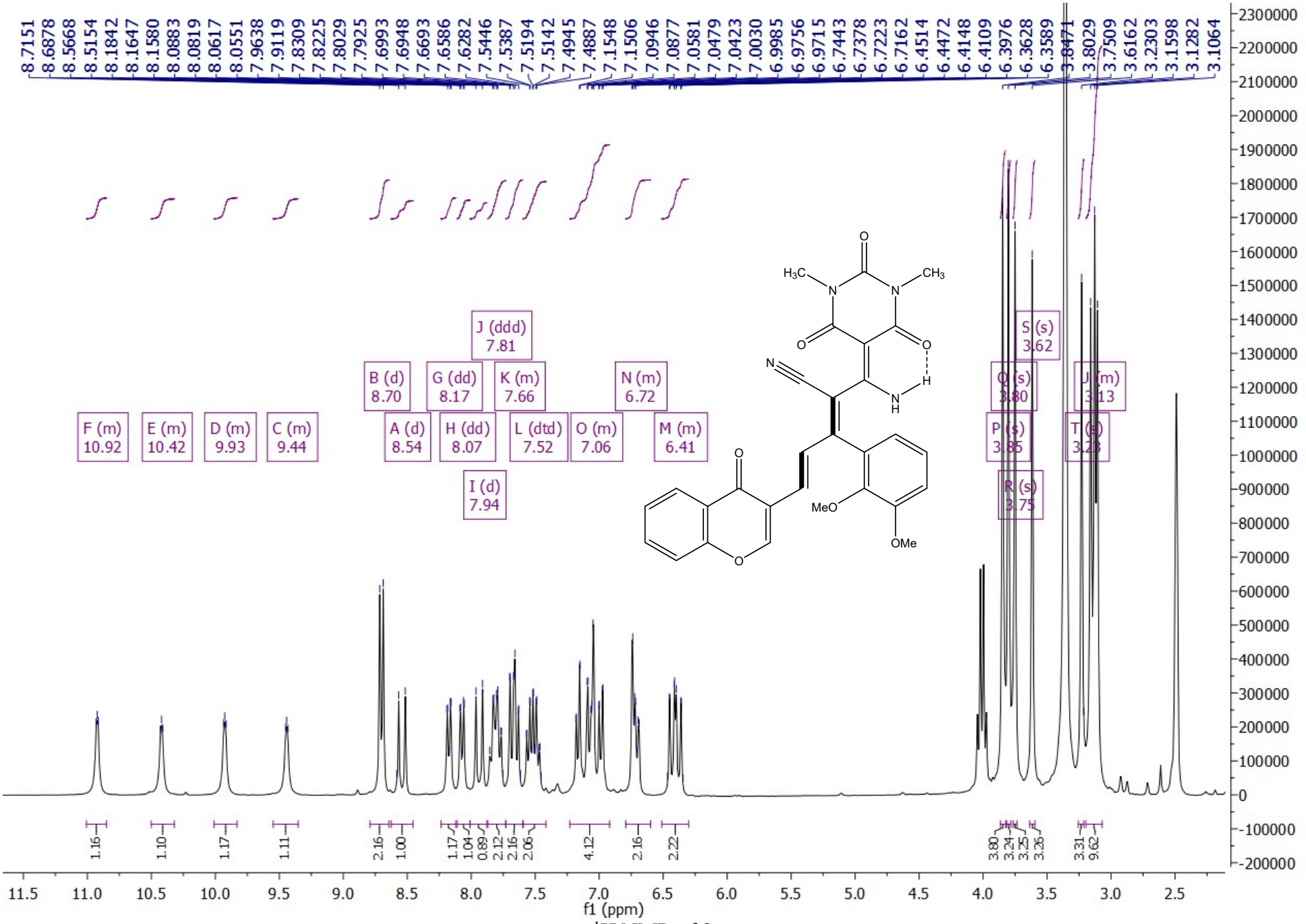
^{13}C NMR of **3b**


3648.06
3420.02
3342.55
3179.58
3074.07
2956.10
2923.45
2360.65
2341.39
2213.11
1716.46
1642.81
1614.87
1556.82
1463.44
1425.05
1412.84
1383.75
1366.21
1309.38
1286.63
1269.68
1239.39
1200.73
1169.66
1147.19
1106.55
1073.12
1050.29
971.91
882.53
858.22
814.50
788.08
765.96
730.63
701.08
634.01
620.01
587.76
565.26
541.95
514.28
436.05
Wavenumbers (cm-1)

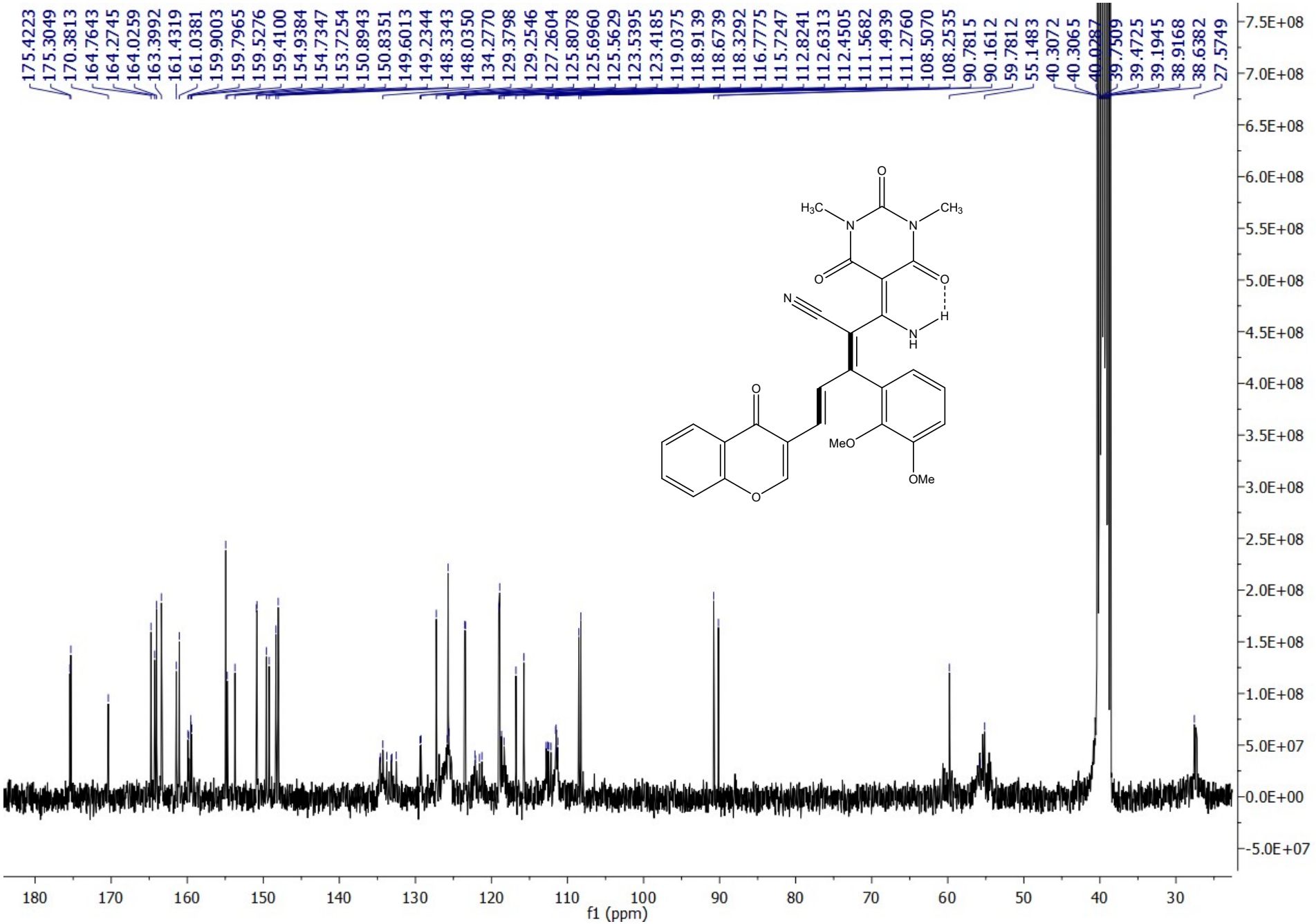
IR of **3b**



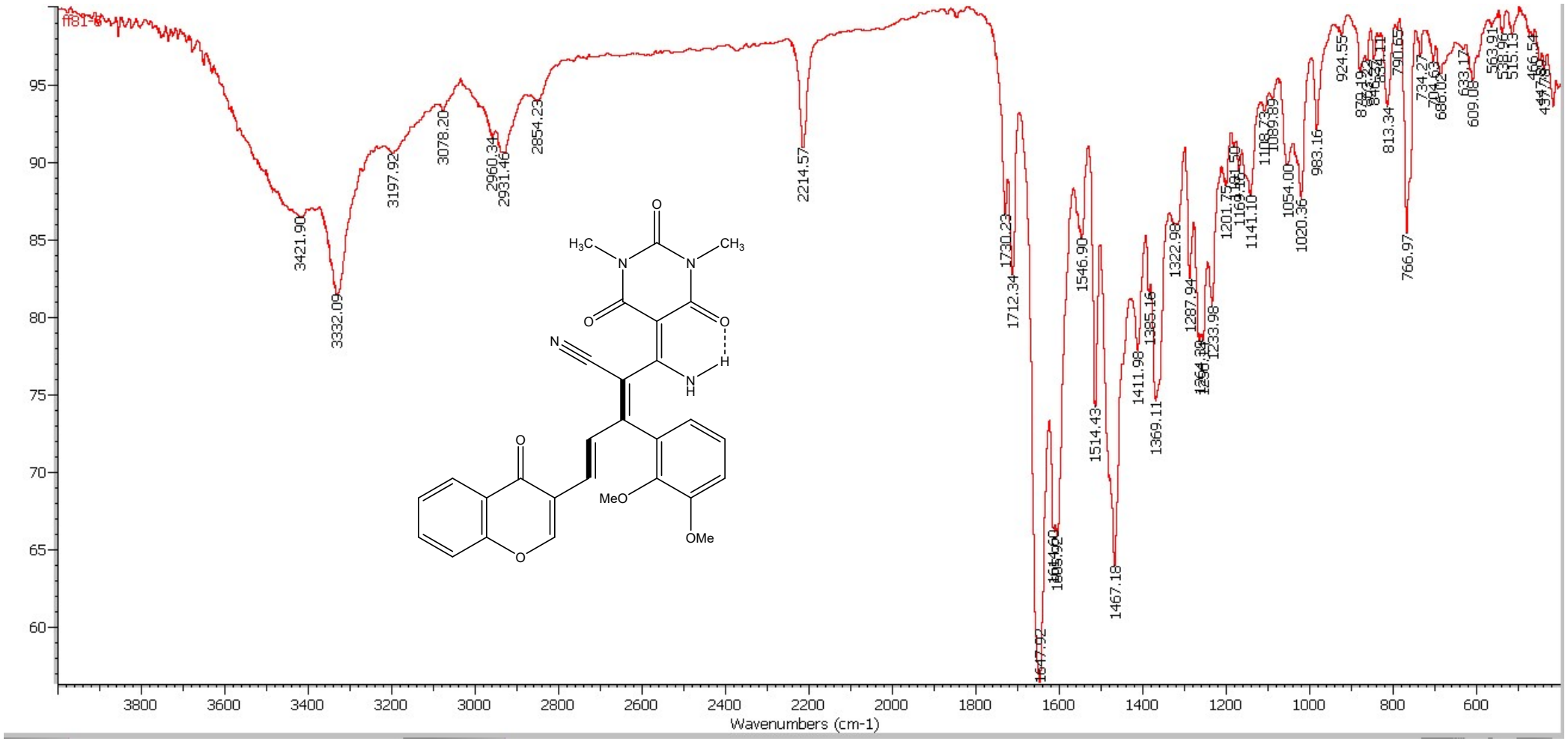
Mass of compound **3b**


F (m) 10.92
E (m) 10.42
D (m) 9.93
C (m) 9.44
B (d) 8.70
A (d) 8.54
J (ddd) 7.81
G (dd) 8.17
H (dd) 8.07
I (d) 7.94
K (m) 7.66
L (dtd) 7.52
N (m) 6.72
O (m) 7.06
M (m) 6.41
S (s) 3.62
Q (s) 3.80
P (s) 3.85
R (s) 3.75
U (m) 3.13
T (s) 3.23
MeO
OMe
f1 (ppm)

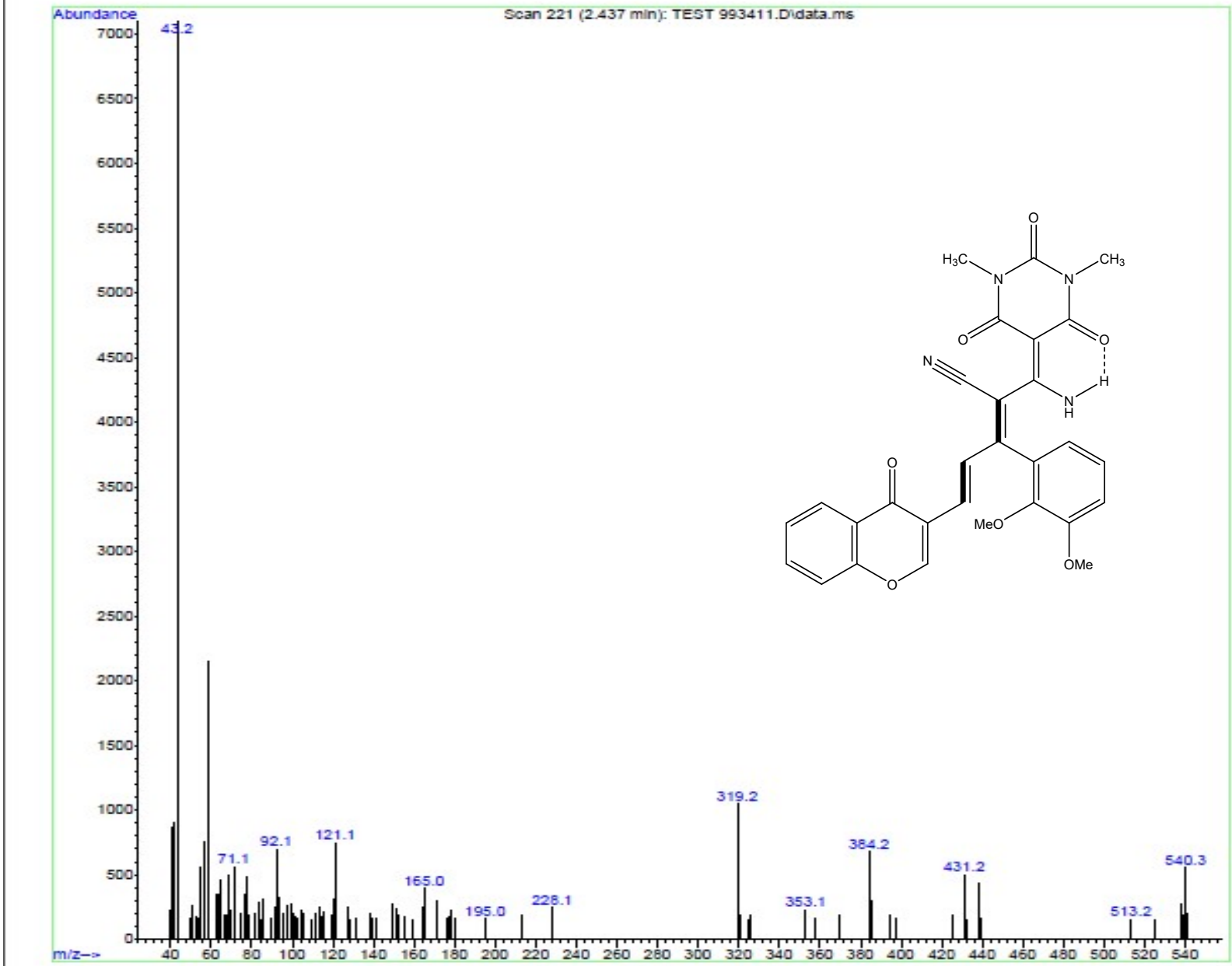
^{1}H NMR of **3c**


175.4223
175.3049
170.3813
164.7643
164.2745
164.0259
163.3992
161.4319
161.0381
159.9003
159.7965
159.5276
159.4100
154.9384
154.7347
153.7254
150.8943
150.8351
149.6013
149.2344
148.3343
148.0350
134.2770
129.3798
129.2546
127.2604
125.8078
125.6960
125.5629
123.5395
123.4185
119.0375
118.9139
118.6739
118.3292
116.7775
115.7247
112.8241
112.6313
112.4505
111.5682
111.4939
111.2760
108.5070
108.2535
90.7815
90.1612
59.7812
55.1483
40.3072
40.3065
40.0287
39.7509
39.4725
39.1945
38.9168
38.6382
27.5749
7.5E+08
7.0E+08
6.5E+08
6.0E+08
5.5E+08
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)
H3C
CH3
N
O
H
MeO
OMe

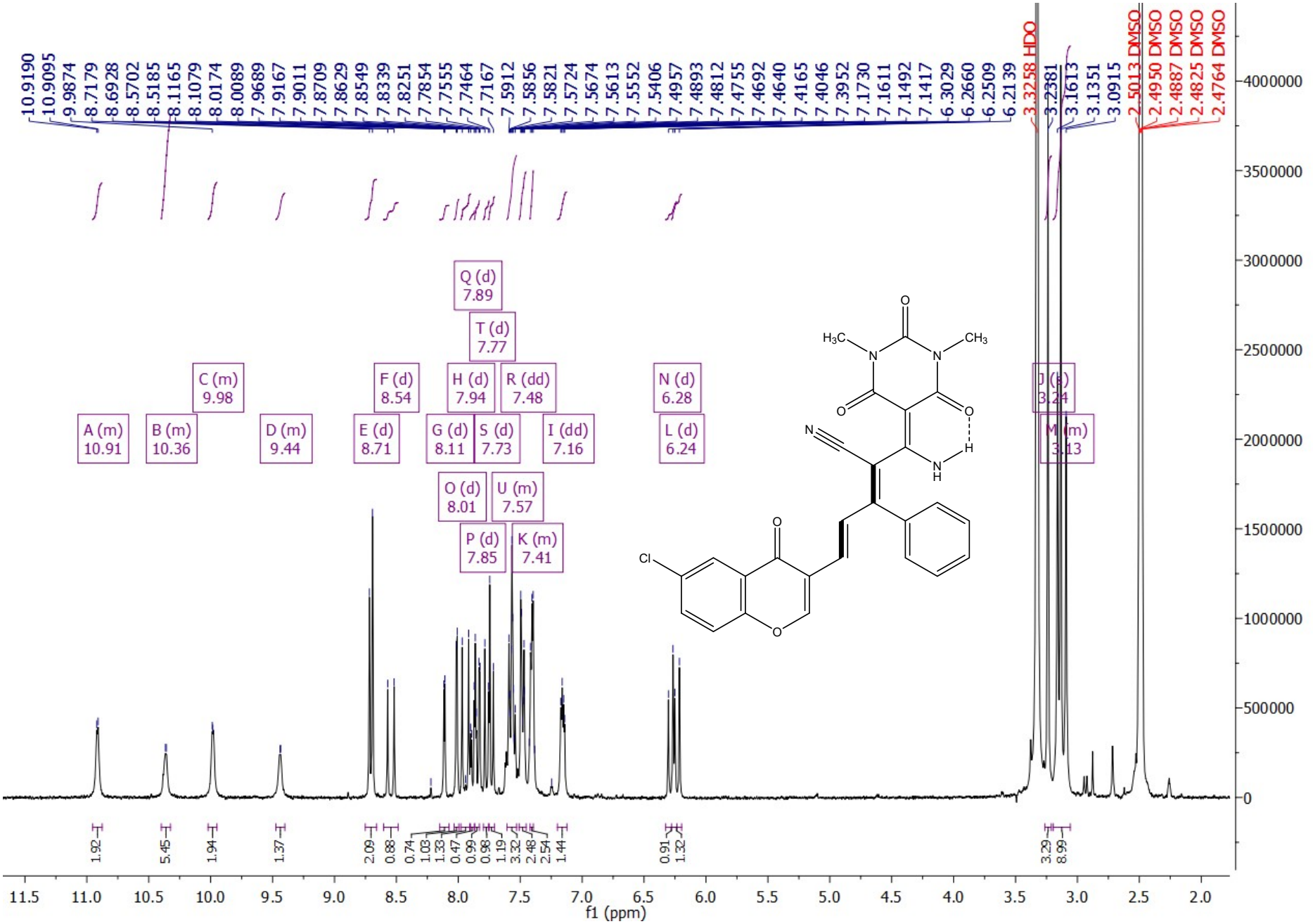
^{13}C NMR of **3c**


ff81-a
3421.90
3332.09
3197.92
3078.20
2960.34
2931.46
2854.23
2214.57
1730.23
1712.34
1647.92
1546.90
1514.43
1467.18
1411.98
1385.16
1369.11
1322.98
1287.94
1233.98
1201.75
1164.50
1141.10
1108.73
1089.89
1054.00
1020.36
983.16
924.55
813.34
790.65
766.97
734.27
680.02
633.17
609.08
563.91
538.96
515.18
466.54
H3C
CH3
N
O
H
MeO
OMe
95
90
85
80
75
70
65
60
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumbers (cm-1)

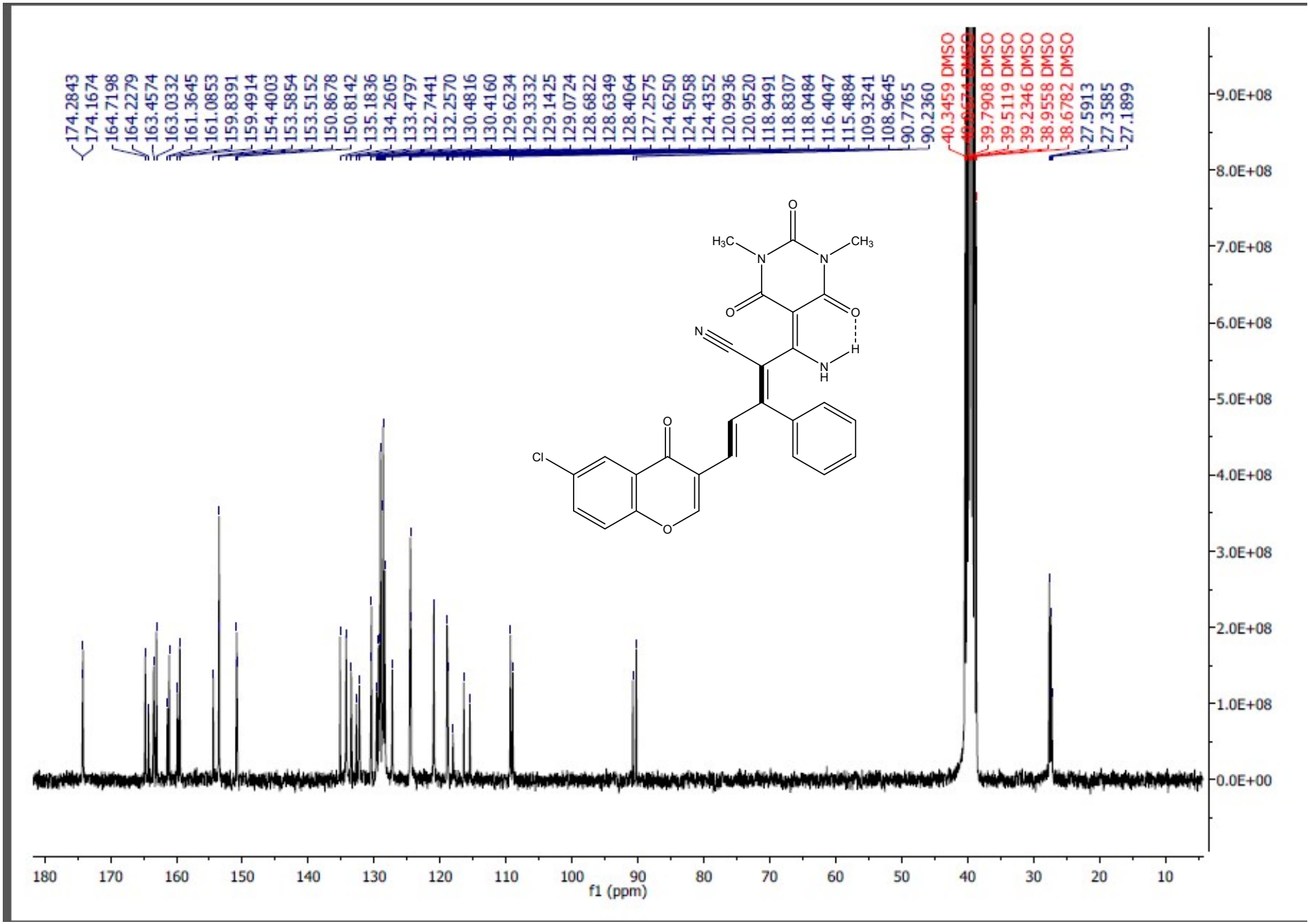
IR of **3c**



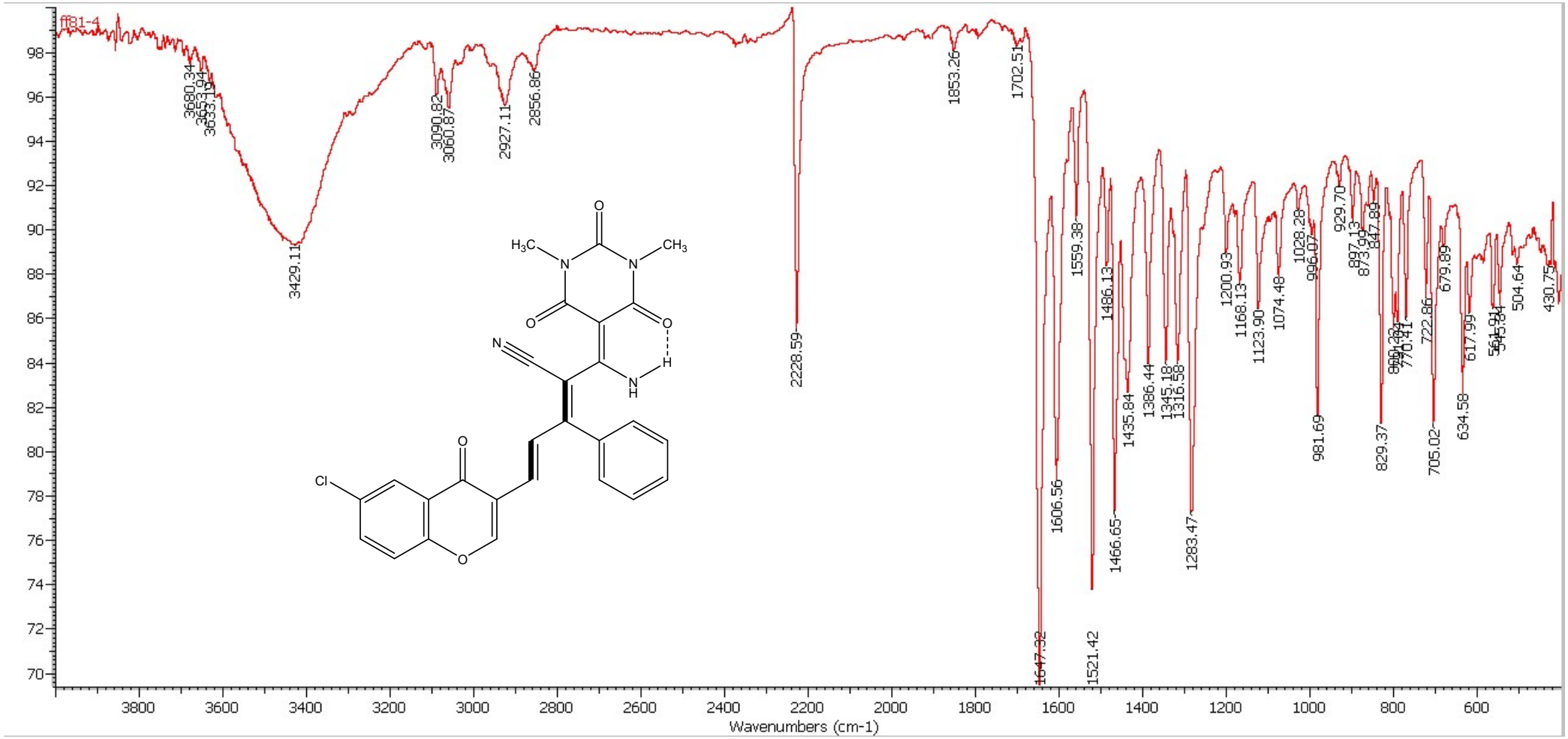
Mass of compound **3c**


A (m) 10.91
B (m) 10.36
C (m) 9.98
D (m) 9.44
E (d) 8.71
F (d) 8.54
G (d) 8.11
H (d) 7.94
I (dd) 7.16
J (s) 3.24
K (m) 7.41
L (d) 6.24
M (m) 3.13
N (d) 6.28
O (d) 8.01
P (d) 7.85
Q (d) 7.89
R (dd) 7.48
S (d) 7.73
T (d) 7.77
U (m) 7.57
f1 (ppm)

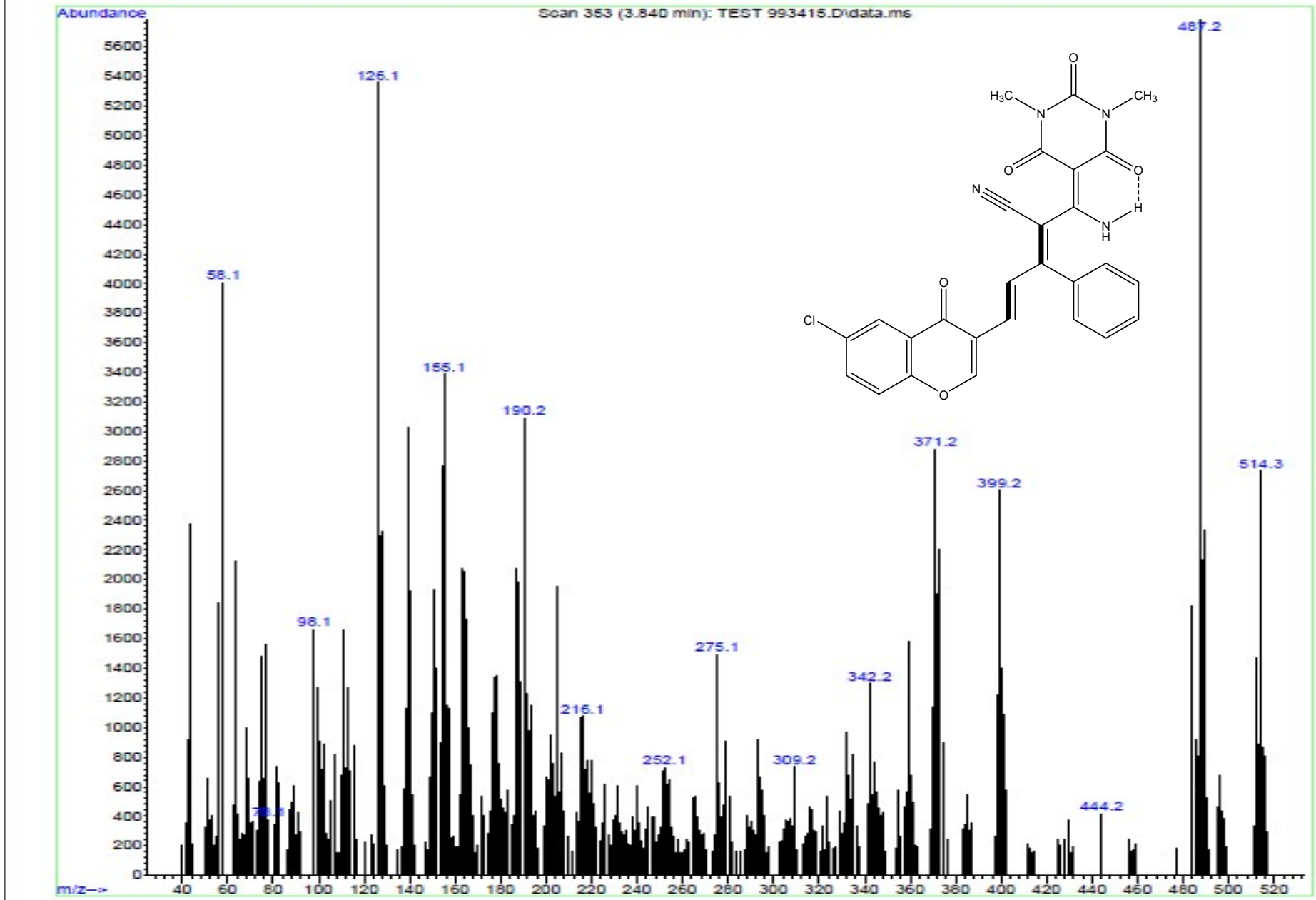
^{1}H NMR of **3d**


174.2843
174.1674
164.7198
164.2279
163.4574
163.0332
161.3645
161.0853
159.8391
159.4914
154.4003
153.5854
153.5152
150.8678
150.8142
135.1836
134.2605
133.4797
132.7441
132.2570
130.4816
130.4160
129.6234
129.3332
129.1425
129.0724
128.6822
128.6349
128.4064
127.2575
124.6250
124.5058
124.4352
120.9936
120.9520
118.9491
118.8307
118.0484
116.4047
115.4884
109.3241
108.9645
90.7765
90.2360
40.3459 DMSO
39.7908 DMSO
39.5119 DMSO
39.2346 DMSO
38.9558 DMSO
38.6782 DMSO
27.5913
27.3585
27.1899
9.0E+08
8.0E+08
7.0E+08
6.0E+08
5.0E+08
4.0E+08
3.0E+08
2.0E+08
1.0E+08
0.0E+00
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

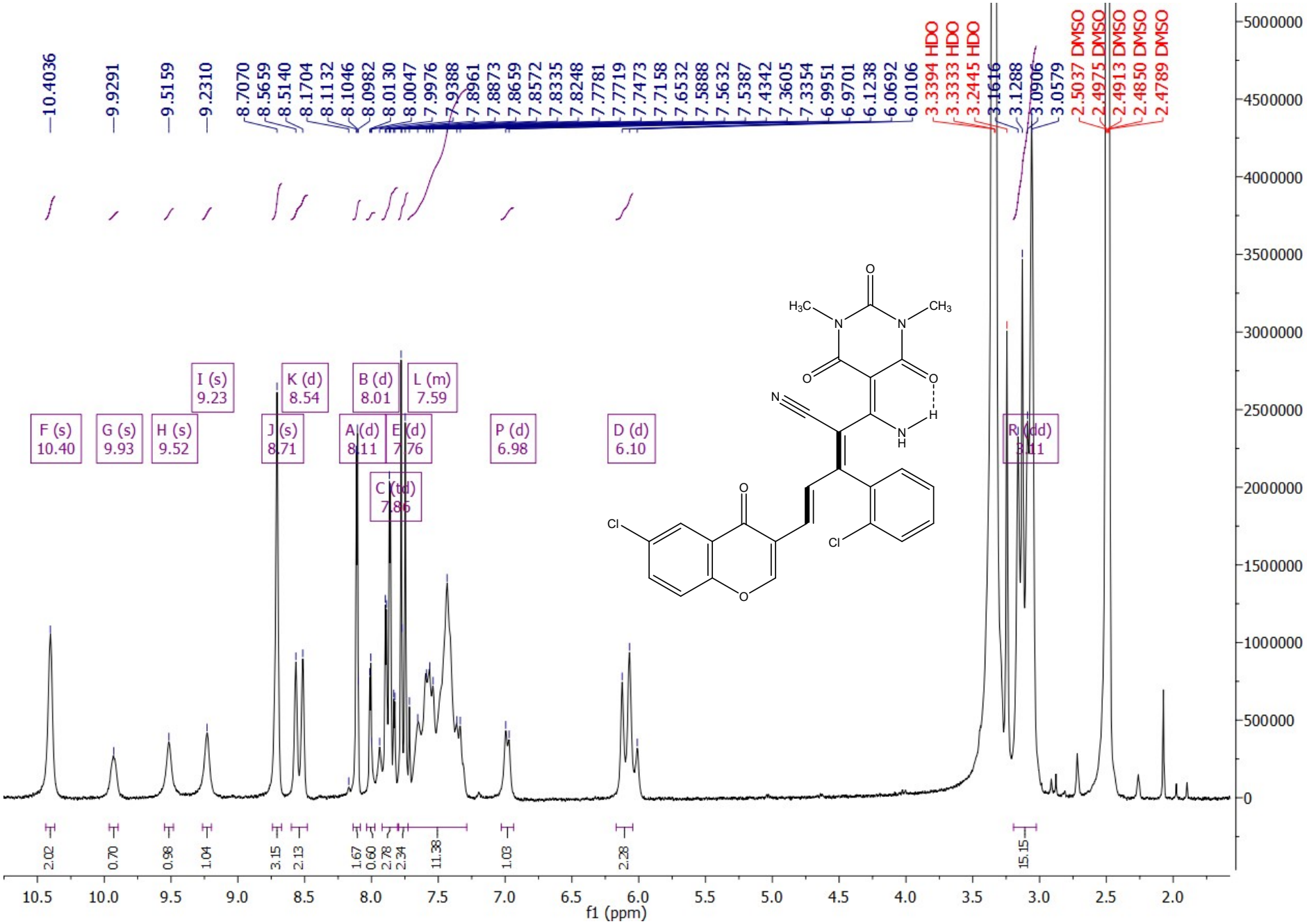
^{13}C NMR of **3d**


ff81-4
3680.34
3653.94
3633.10
3429.11
3090.82
3060.87
2927.11
2856.86
2228.59
1853.26
1702.51
1647.32
1606.56
1559.38
1521.42
1486.13
1466.65
1435.84
1386.44
1345.18
1316.58
1283.47
1200.93
1168.13
1123.90
1074.48
1028.28
996.07
981.69
929.70
897.13
873.99
847.89
829.37
770.41
722.86
705.02
679.89
634.58
617.99
561.91
545.84
504.64
430.75
Wavenumbers (cm-1)

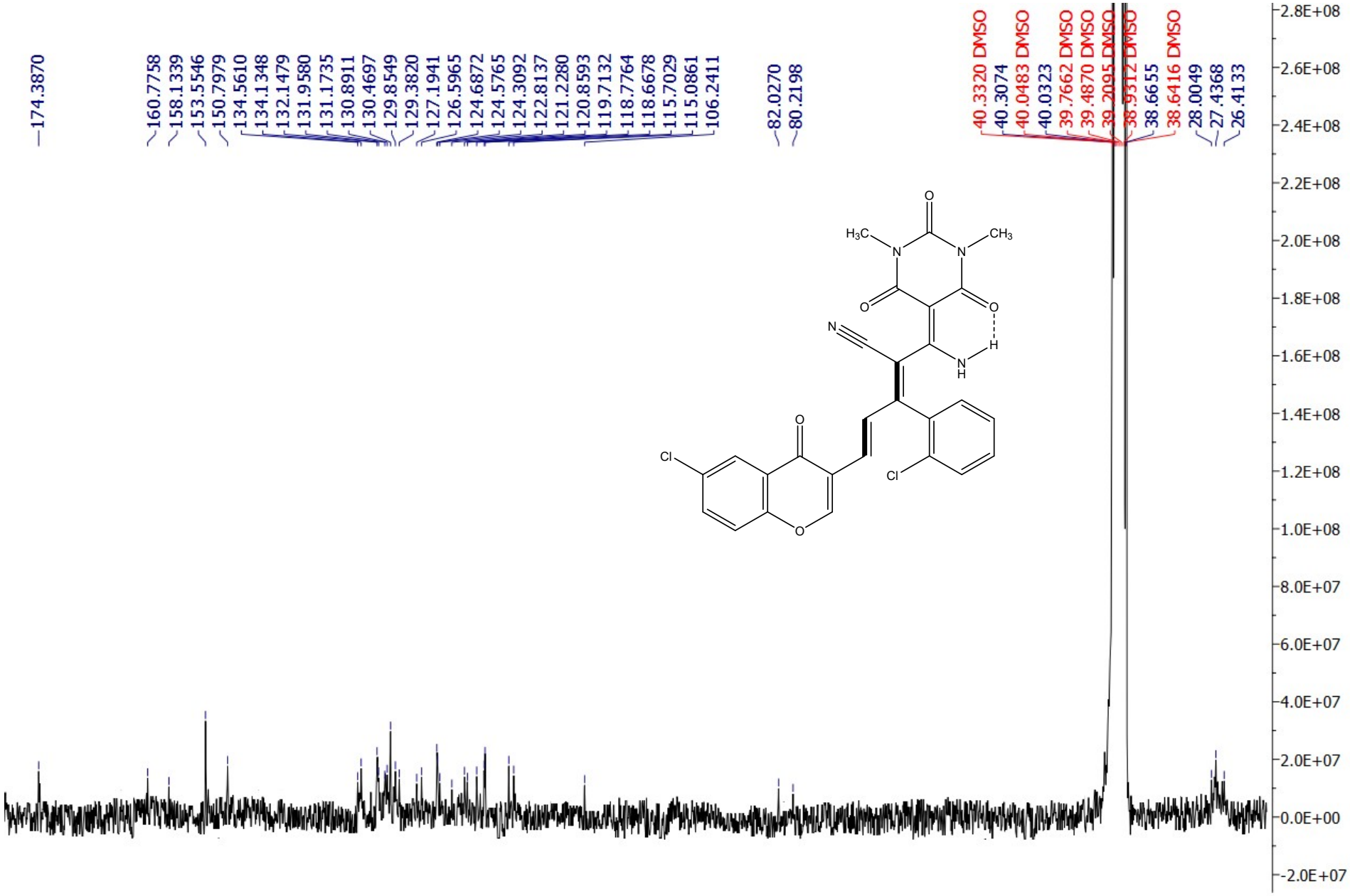
IR of **3d**



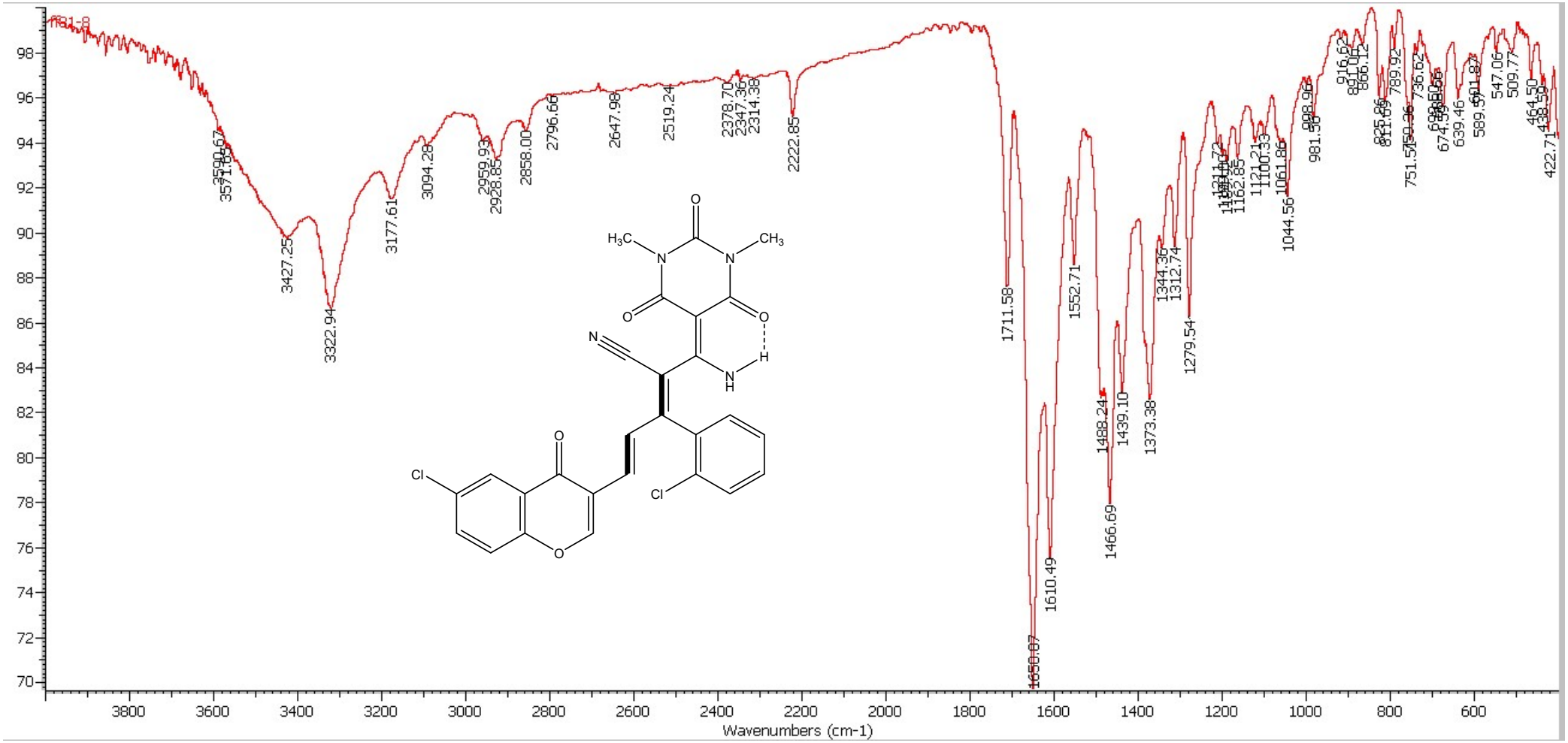
Mass of compound **3d**


F (s) 10.40
G (s) 9.93
H (s) 9.52
I (s) 9.23
J (s) 8.71
K (d) 8.54
A (d) 8.11
B (d) 8.01
C (td) 7.86
E (d) 7.76
L (m) 7.59
P (d) 6.98
D (d) 6.10
R (dd) 3.11
f1 (ppm)

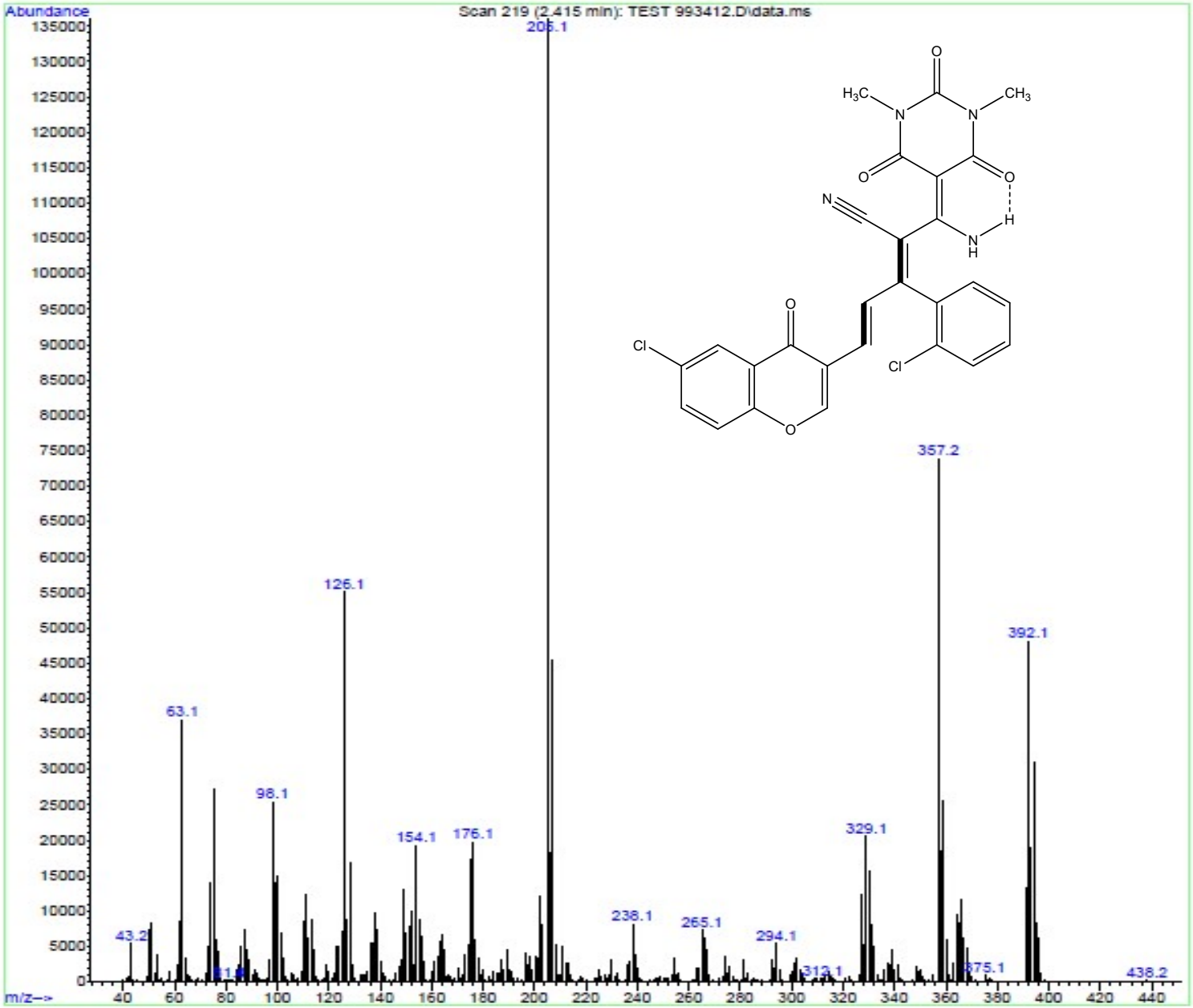
^{1}H NMR of **3e**


174.3870
160.7758
158.1339
153.5546
150.7979
134.5610
134.1348
132.1479
131.9580
131.1735
130.8911
130.4697
129.8549
129.3820
127.1941
126.5965
124.6872
124.5765
124.3092
122.8137
121.2280
120.8593
119.7132
118.7764
118.6678
115.7029
115.0861
106.2411
82.0270
80.2198
40.3320 DMSO
40.3074
40.0483 DMSO
40.0323
39.7662 DMSO
39.4870 DMSO
39.2095 DMSO
38.9312 DMSO
38.6655
38.6416 DMSO
28.0049
27.4368
26.4133
2.8E+08
2.6E+08
2.4E+08
2.2E+08
2.0E+08
1.8E+08
1.6E+08
1.4E+08
1.2E+08
1.0E+08
8.0E+07
6.0E+07
4.0E+07
2.0E+07
0.0E+00
-2.0E+07
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

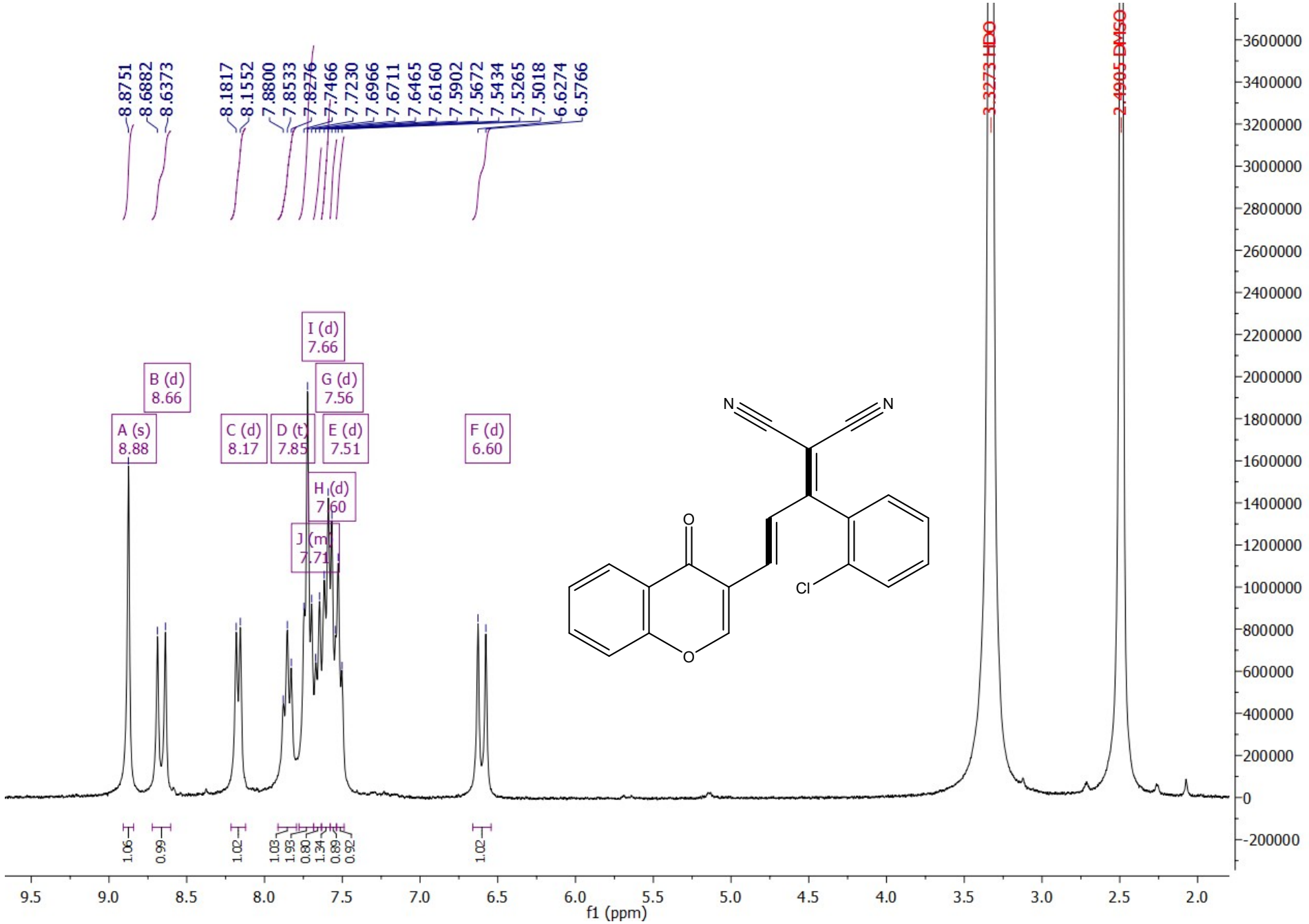
^{13}C NMR of **3e**


3427.25
3322.94
3177.61
3094.28
2959.93
2928.85
2858.00
2796.66
2647.98
2519.24
2378.70
2347.36
2314.38
2222.85
1711.58
1656.87
1610.49
1552.71
1466.69
1488.24
1439.10
1373.38
1344.36
1312.74
1279.54
1162.85
1121.21
1100.33
1061.86
1044.56
981.56
916.62
866.12
789.92
751.51
736.62
674.39
639.46
589.56
547.06
509.77
464.50
422.71
Wavenumbers (cm-1)

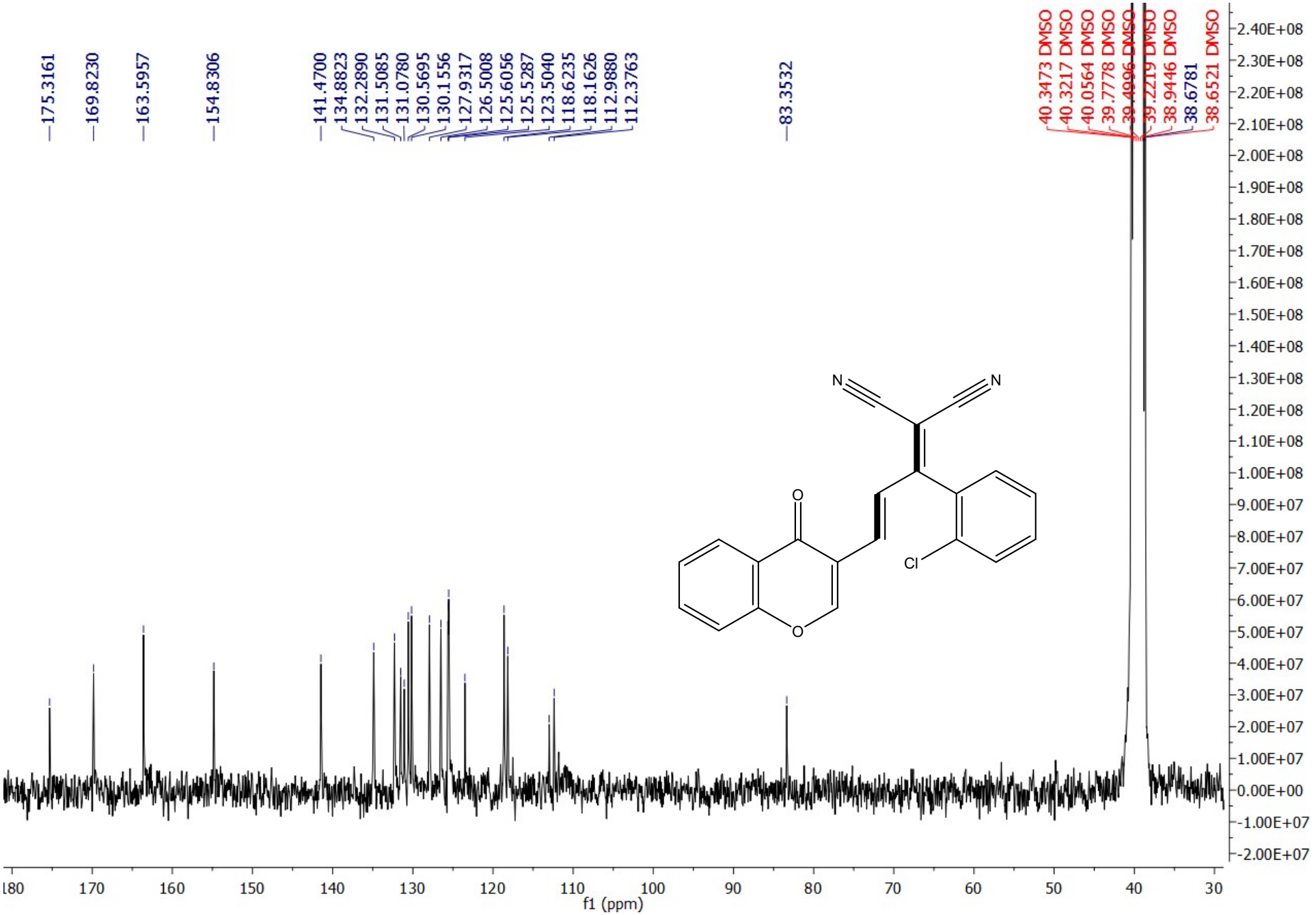
IR of **3e**



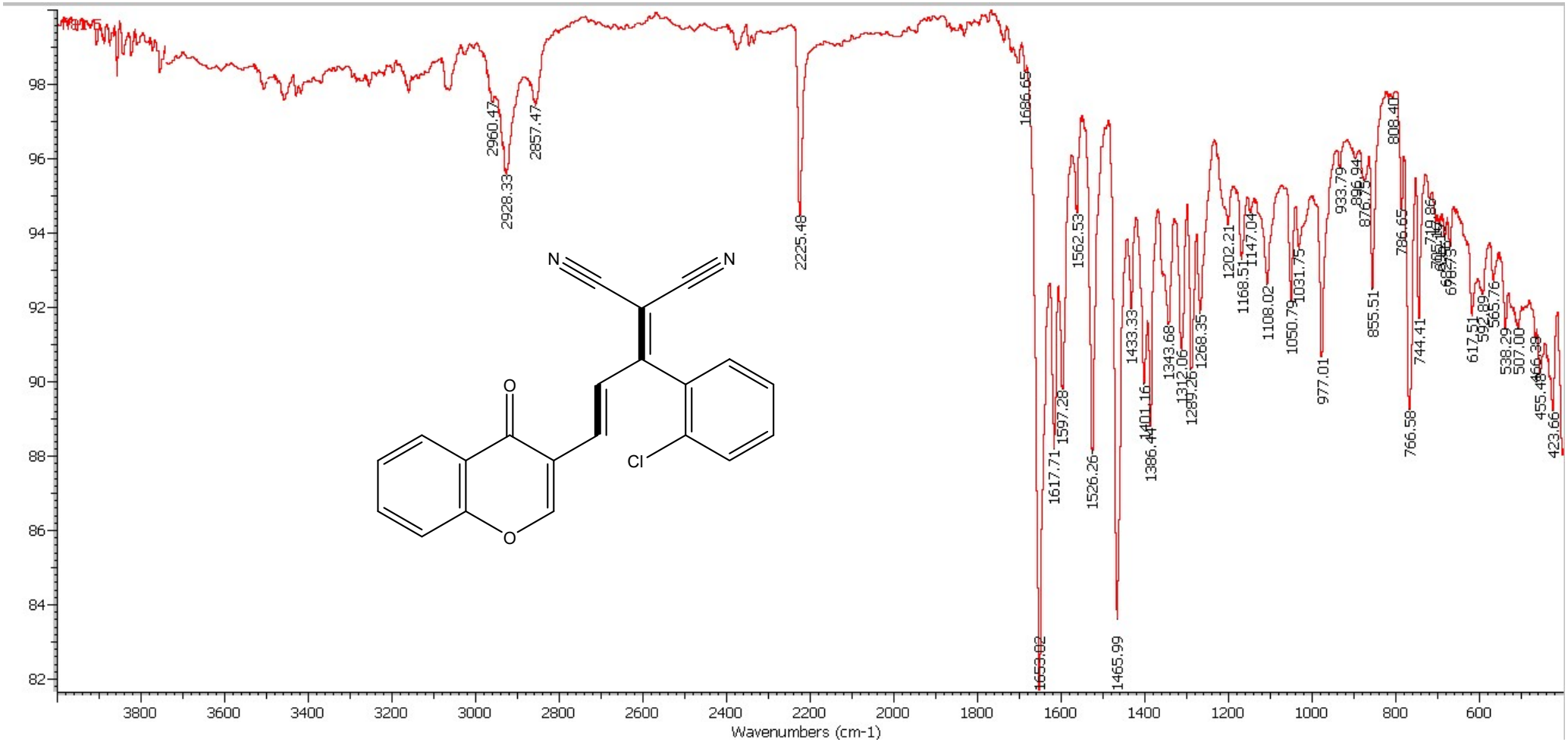
Mass of compound **3e**


8.8751
8.6882
8.6373
8.1817
8.1552
7.8800
7.8533
7.8276
7.7466
7.7230
7.6966
7.6711
7.6465
7.6160
7.5902
7.5672
7.5434
7.5265
7.5018
6.6274
6.5766
3.3273 HDO
2.4995 DMSO
A (s) 8.88
B (d) 8.66
C (d) 8.17
D (t) 7.85
E (d) 7.51
F (d) 6.60
G (d) 7.56
H (d) 7.60
I (d) 7.66
J (m) 7.71
N
N
O
O
Cl
1.06
0.99
1.02
1.03
1.93
0.80
1.34
0.89
0.92
1.02
f1 (ppm)

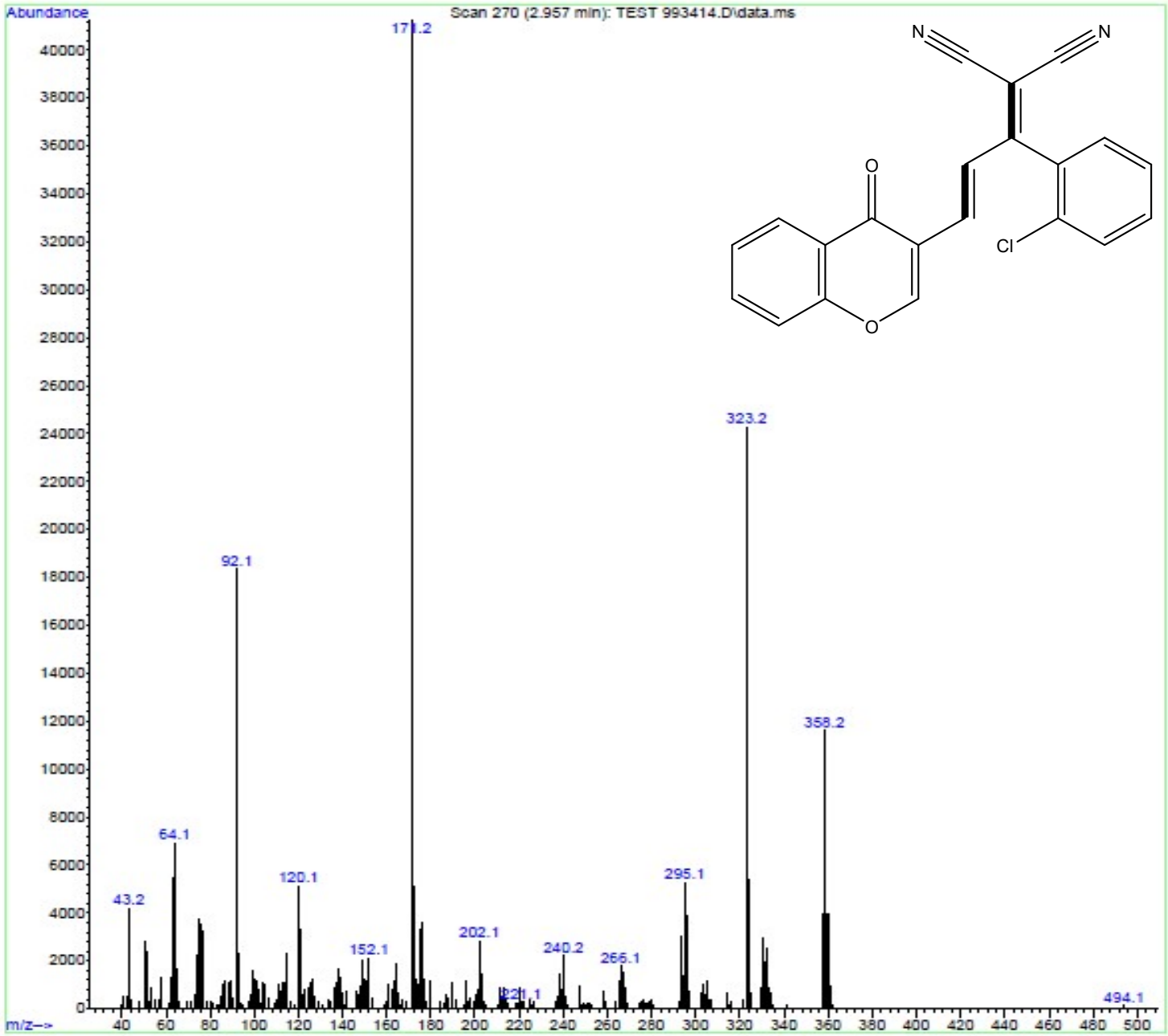
^{1}H NMR of **3f**


175.3161
169.8230
163.5957
154.8306
141.4700
134.8823
132.2890
131.5085
131.0780
130.5695
130.1556
127.9317
126.5008
125.6056
125.5287
123.5040
118.6235
118.1626
112.9880
112.3763
83.3532
40.3473 DMSO
40.3217 DMSO
40.0564 DMSO
39.7778 DMSO
39.4996 DMSO
39.2219 DMSO
38.9446 DMSO
38.6781
38.6521 DMSO
N
N
O
O
Cl
f1 (ppm)

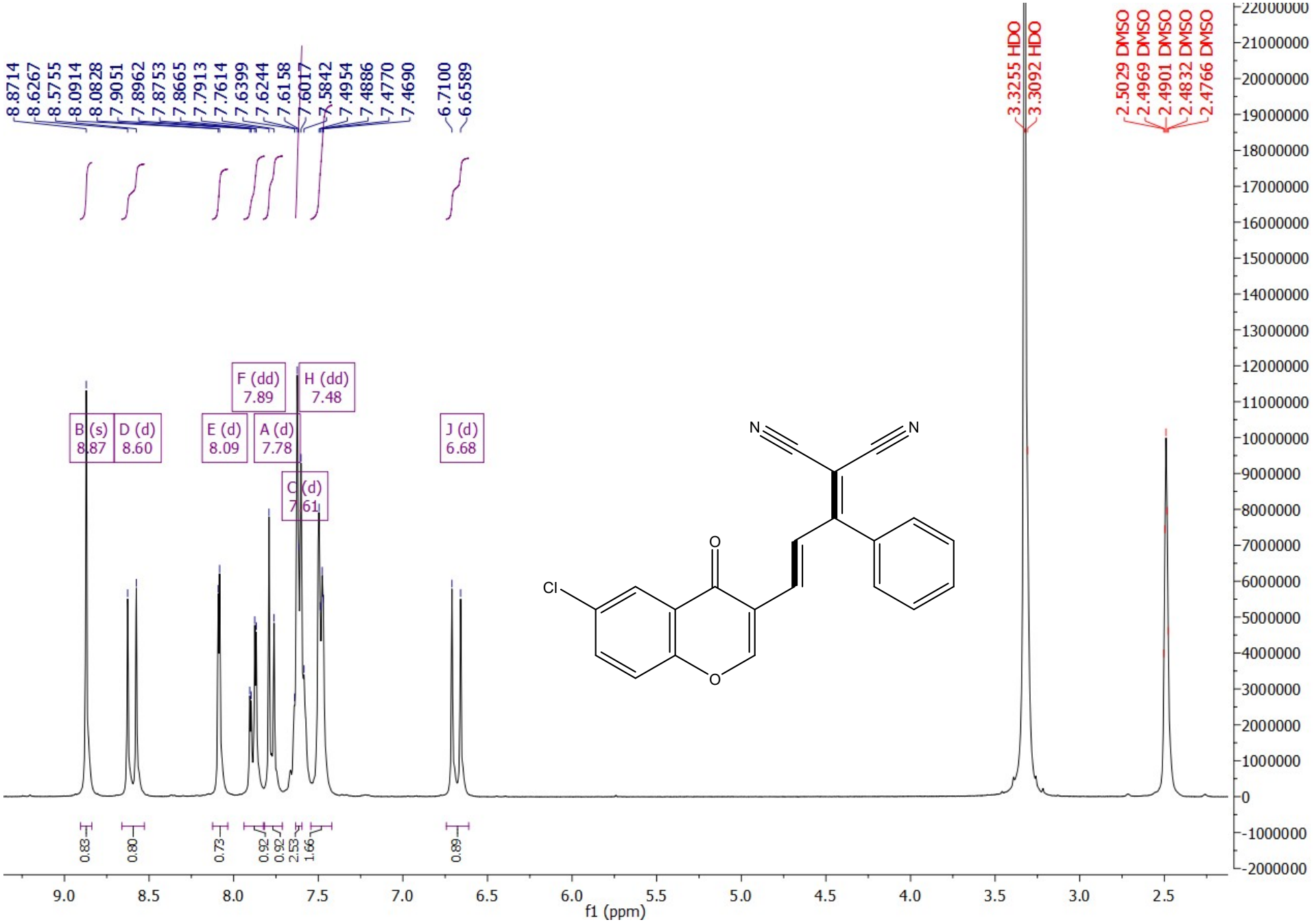
^{13}C NMR of **3f**


N
N
O
O
Cl
2960.47
2928.33
2857.47
2225.48
1686.65
1653.02
1617.71
1597.28
1562.53
1526.26
1465.99
1433.33
1401.16
1386.44
1343.68
1312.06
1289.26
1268.35
1202.21
1168.51
1147.04
1108.02
1050.79
1031.75
977.01
933.79
896.94
876.73
855.51
808.40
786.65
766.58
744.41
719.86
617.51
565.89
538.29
507.00
455.48
423.66
98
96
94
92
90
88
86
84
82
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
Wavenumbers (cm-1)

IR of **3f**



Mass of compound **3f**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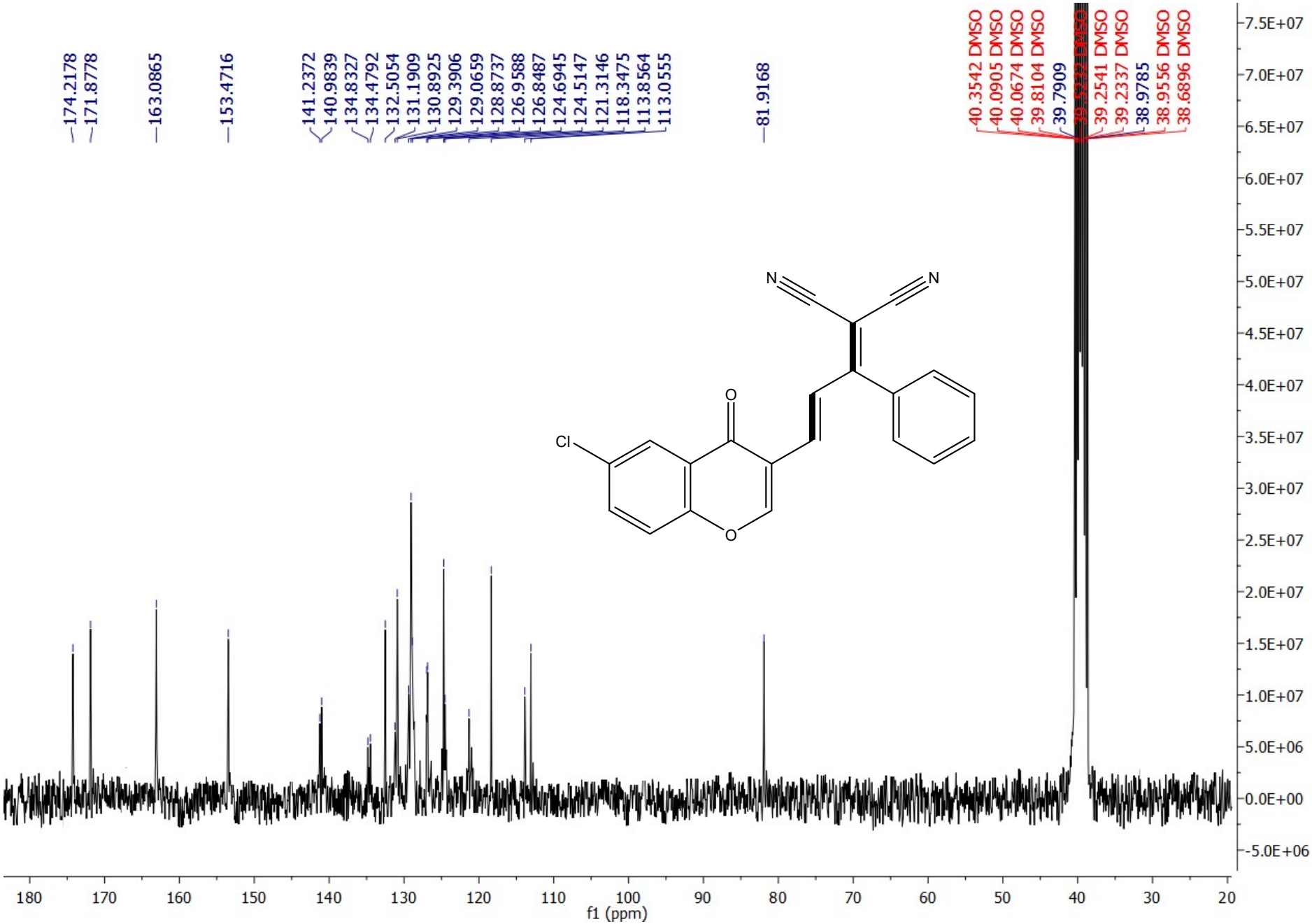
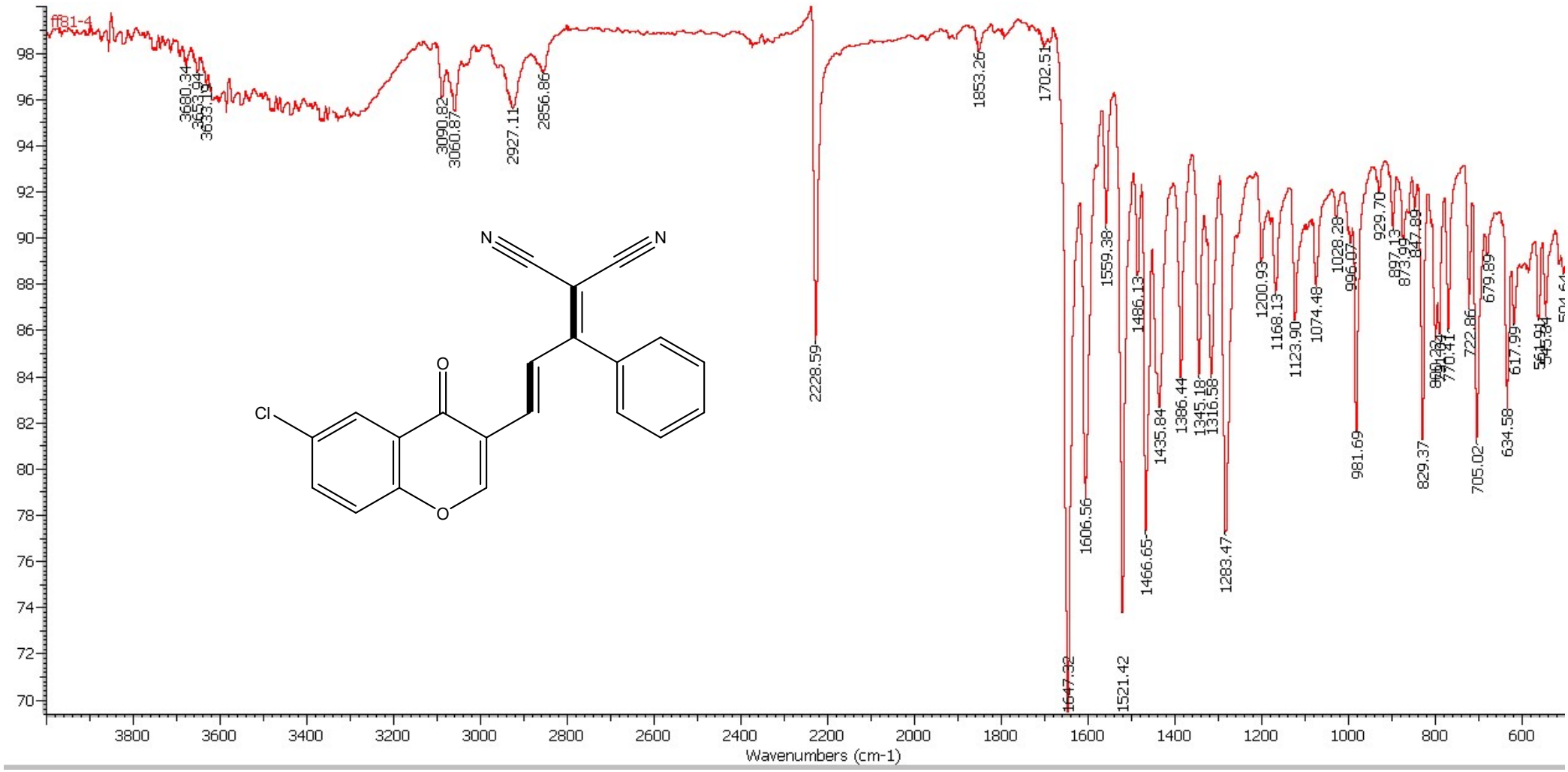
8.6267
8.5755
8.0914
8.0828
7.9051
7.8962
7.8753
7.8665
7.7913
7.7614
7.6399
7.6244
7.6158
7.6017
7.5842
7.4954
7.4886
7.4770
7.4690
6.7100
6.6589
3.3255 HDO
3.3092 HDO
2.5029 DMSO
2.4969 DMSO
2.4901 DMSO
2.4832 DMSO
2.4766 DMSO
B (s) 8.87
D (d) 8.60
E (d) 8.09
F (dd) 7.89
A (d) 7.78
H (dd) 7.48
C (d) 7.61
J (d) 6.68
0.83
0.80
0.73
0.92
0.92
2.53
1.66
0.89
N
N
O
Cl
O
f1 (ppm)

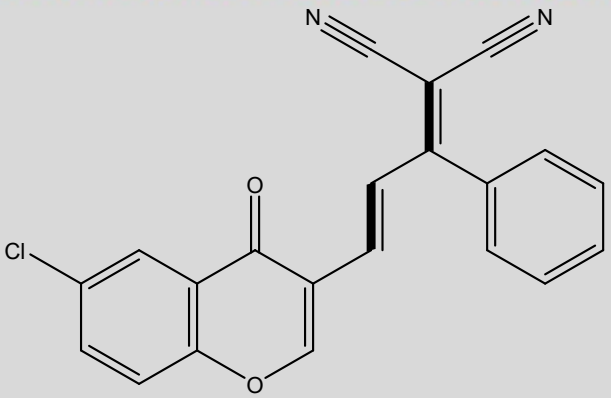
^{1}H NMR of **3g**


174.2178
171.8778
163.0865
153.4716
141.2372
140.9839
134.8327
134.4792
132.5054
131.1909
130.8925
129.3906
129.0659
128.8737
126.9588
126.8487
124.6945
124.5147
121.3146
118.3475
113.8564
113.0555
81.9168
40.3542 DMSO
40.0905 DMSO
40.0674 DMSO
39.8104 DMSO
39.7909
39.2541 DMSO
39.2337 DMSO
38.9785
38.9556 DMSO
38.6896 DMSO
N
N
O
Cl
O
7.5E+07
7.0E+07
6.5E+07
6.0E+07
5.5E+07
5.0E+07
4.5E+07
4.0E+07
3.5E+07
3.0E+07
2.5E+07
2.0E+07
1.5E+07
1.0E+07
5.0E+06
0.0E+00
-5.0E+06
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

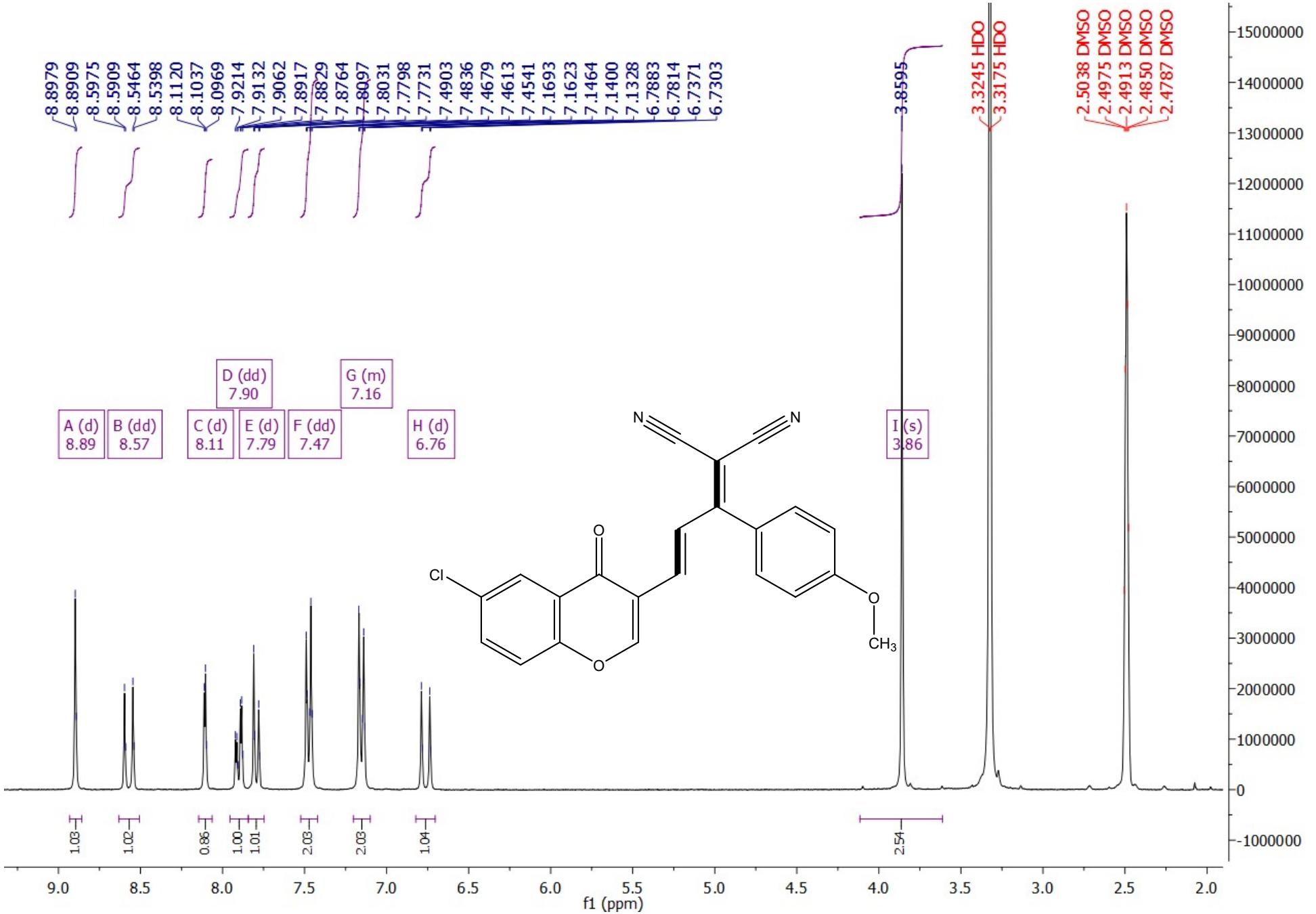
^{13}C NMR of **3g**


ff81-4
3680.34
3653.94
3633.15
3090.82
3060.87
2927.11
2856.86
2228.59
1853.26
1702.51
1647.32
1606.56
1559.38
1521.42
1486.13
1466.65
1435.84
1386.44
1345.18
1316.58
1283.47
1200.93
1168.13
1123.90
1074.48
1028.28
996.07
981.69
929.70
897.13
873.99
847.89
829.37
770.41
722.86
705.02
679.89
634.58
617.99
561.91
545.84
Cl
O
O
N
N
Wavenumbers (cm-1)

IR of **3g**



Mass of compound **3g**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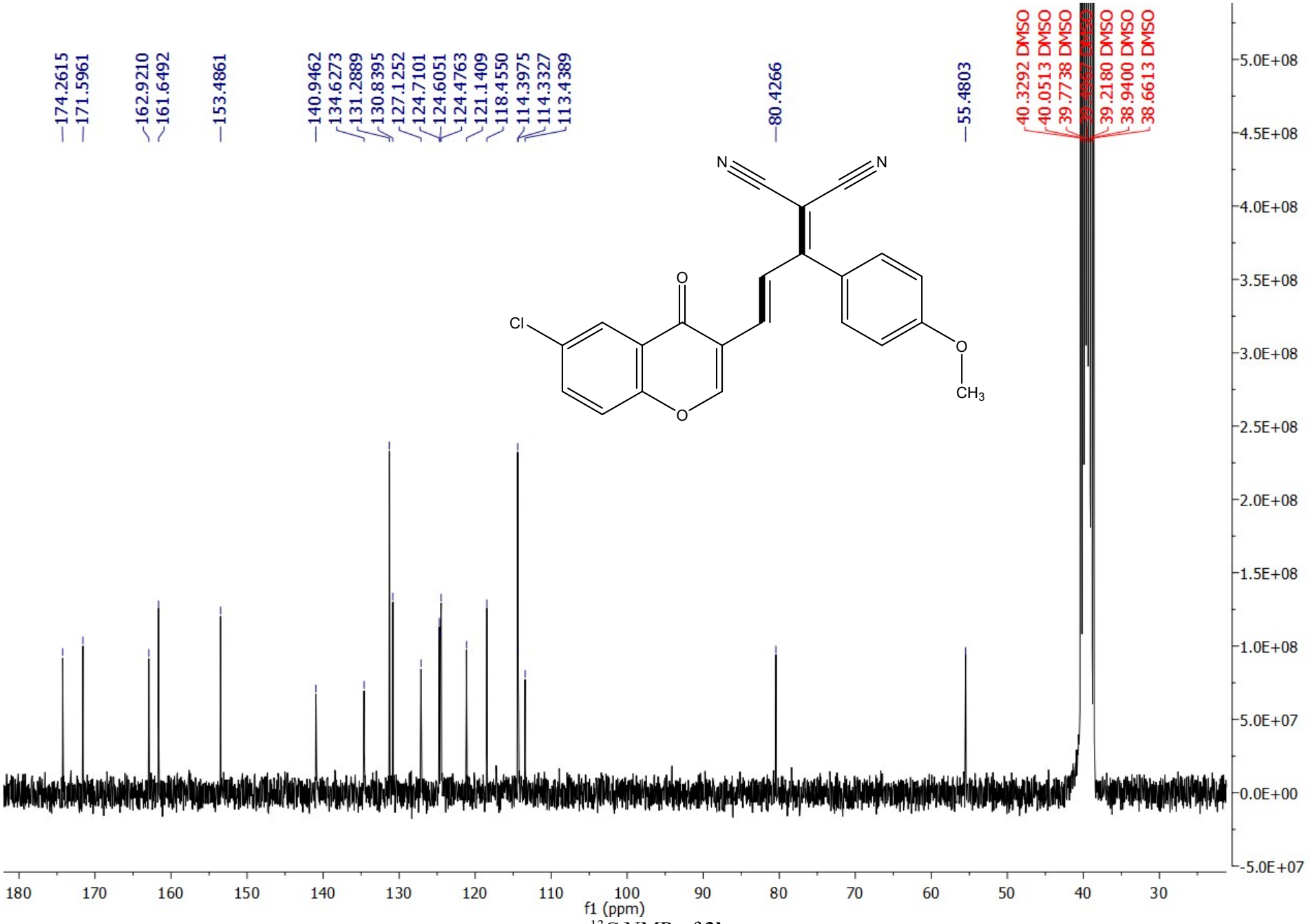
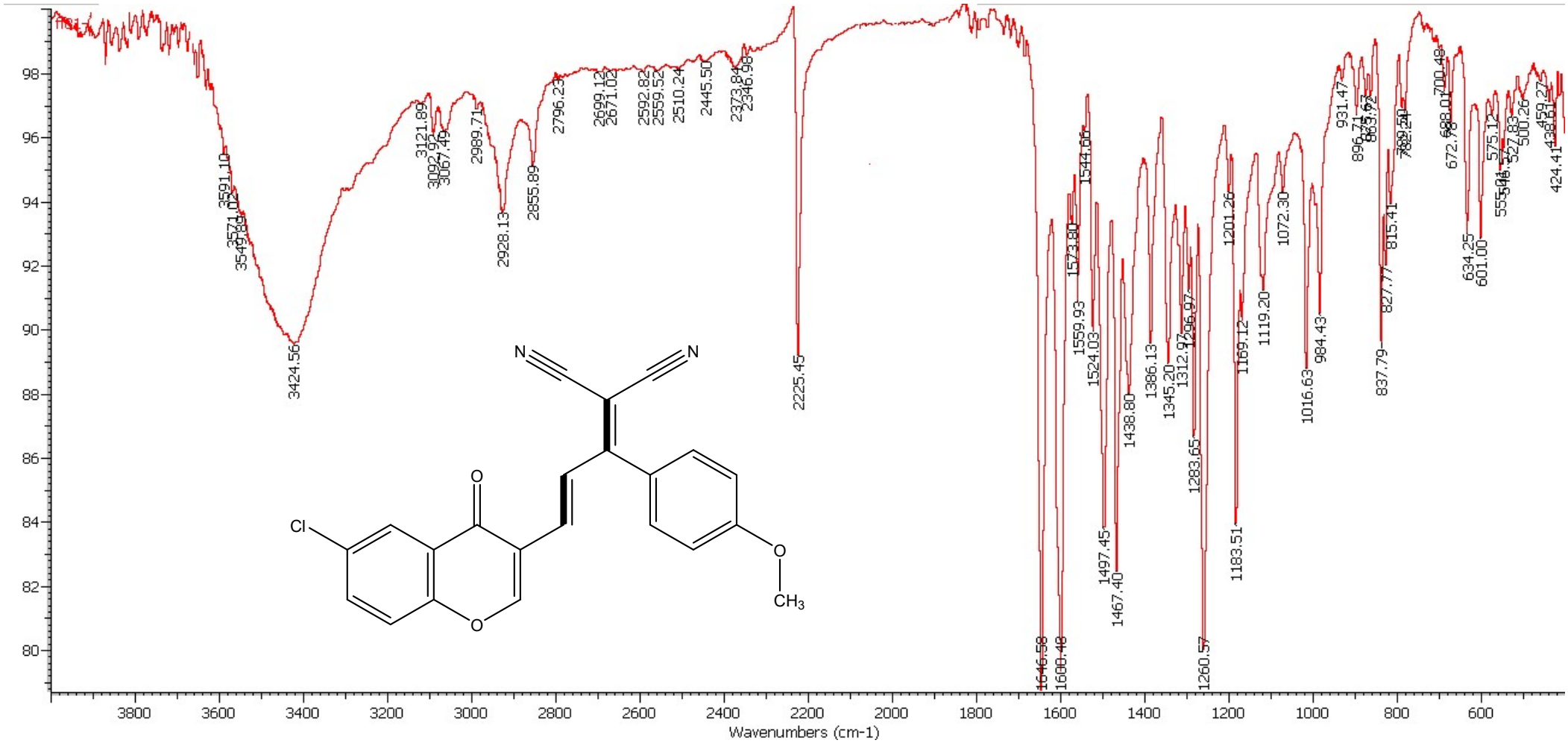
8.5975
8.5909
8.5464
8.5398
8.1120
8.1037
8.0969
7.9214
7.9132
7.9062
7.8917
7.8829
7.8764
7.8097
7.8031
7.7798
7.7731
7.4903
7.4836
7.4679
7.4613
7.4541
7.1693
7.1623
7.1464
7.1400
7.1328
6.7883
6.7814
6.7371
6.7303
3.8595
3.3245 HDO
3.3175 HDO
2.5038 DMSO
2.4975 DMSO
2.4913 DMSO
2.4850 DMSO
2.4787 DMSO
A (d) 8.89
B (dd) 8.57
C (d) 8.11
D (dd) 7.90
E (d) 7.79
F (dd) 7.47
G (m) 7.16
H (d) 6.76
I (s) 3.86
N
N
O
Cl
O
O
CH3
1.03
1.02
0.86
1.00
1.01
2.03
2.03
1.04
2.54
f1 (ppm)

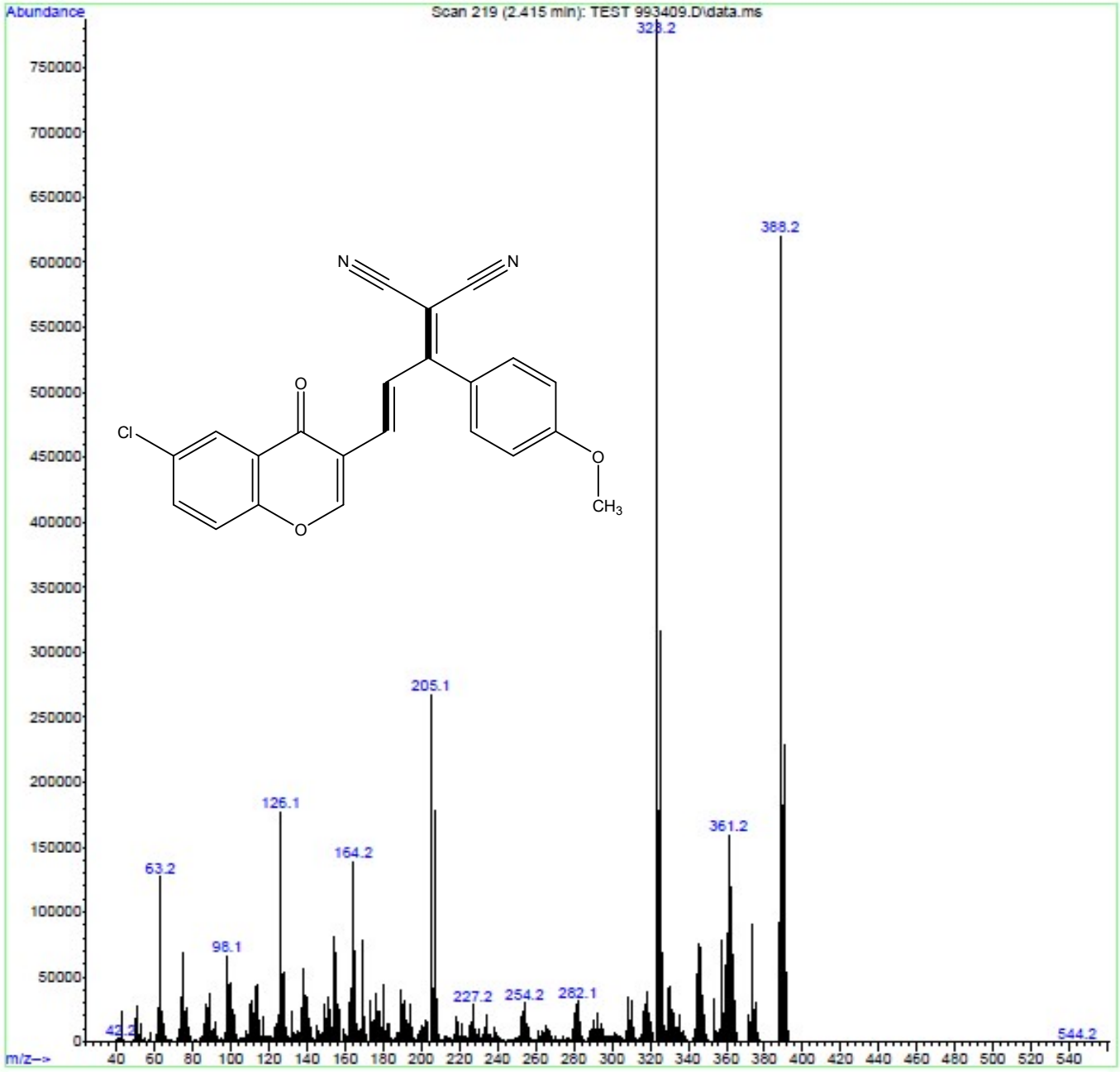
^{1}H NMR of **3h**


174.2615
171.5961
162.9210
161.6492
153.4861
140.9462
134.6273
131.2889
130.8395
127.1252
124.7101
124.6051
124.4763
121.1409
118.4550
114.3975
114.3327
113.4389
80.4266
55.4803
40.3292 DMSO
40.0513 DMSO
39.7738 DMSO
39.2180 DMSO
38.9400 DMSO
38.6613 DMSO
N
N
O
Cl
O
O
CH3
5.0E+08
4.5E+08
4.0E+08
3.5E+08
3.0E+08
2.5E+08
2.0E+08
1.5E+08
1.0E+08
5.0E+07
0.0E+00
-5.0E+07
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
f1 (ppm)

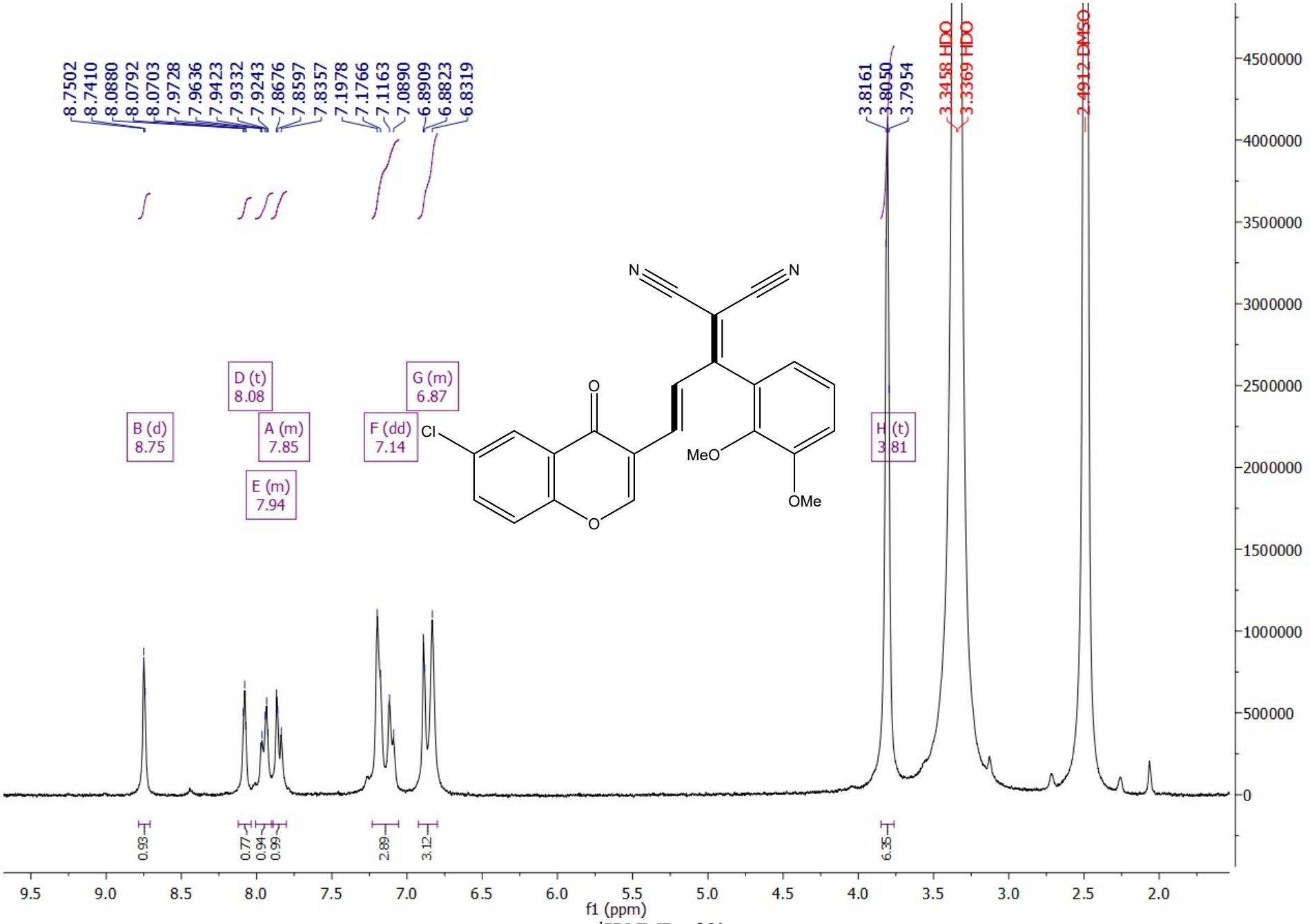
^{13}C NMR of **3h**


Cl
O
O
O
N
N
CH3
Wavenumbers (cm-1)
3800
3600
3400
3200
3000
2800
2600
2400
2200
2000
1800
1600
1400
1200
1000
800
600
100
98
96
94
92
90
88
86
84
82
80
3424.56
3121.89
3092.92
3067.46
2989.71
2928.13
2855.89
2796.23
2699.12
2671.02
2592.82
2559.52
2510.24
2445.50
2373.84
2346.98
2225.45
1646.58
1600.48
1573.80
1559.93
1544.66
1524.03
1497.45
1467.40
1438.80
1386.13
1345.20
1312.97
1296.97
1283.65
1260.57
1201.26
1183.51
1169.12
1119.20
1072.30
1016.63
984.43
931.47
896.75
863.67
837.79
827.77
815.41
782.24
700.48
672.68
634.25
601.00
575.12
555.84
527.83
500.26
459.27
438.61
424.41

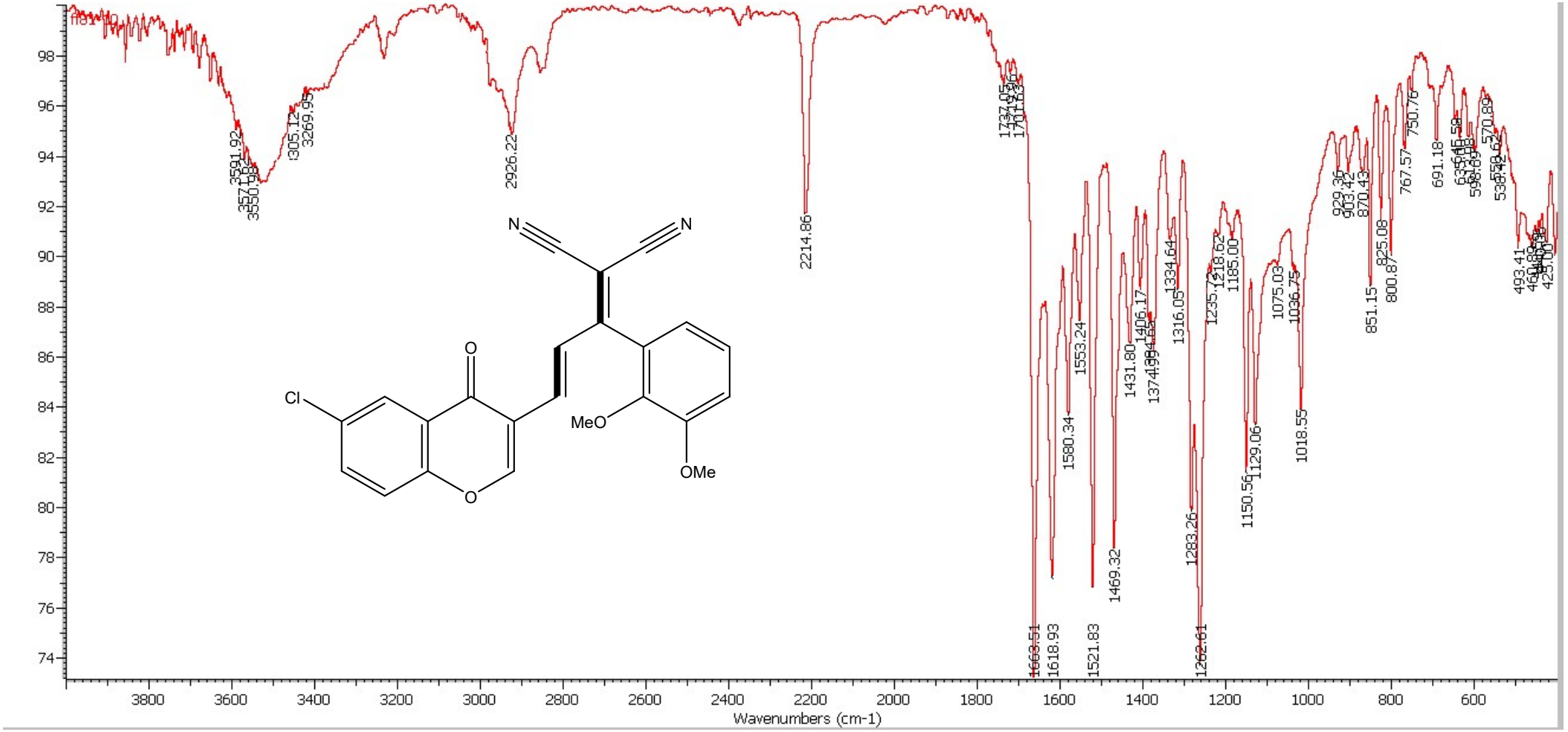
IR of **3h**



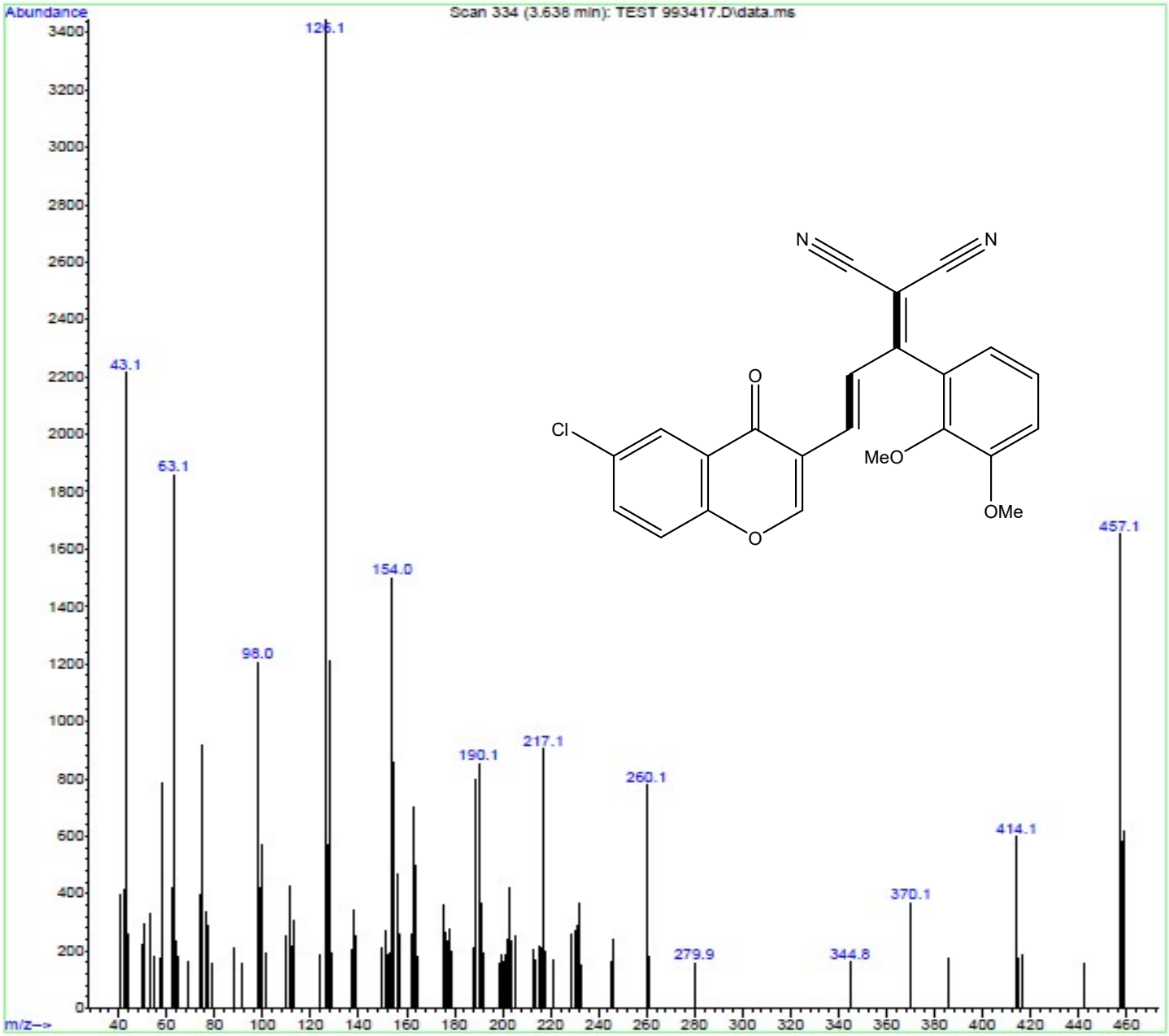
Mass of compound **3h**


8.7502
8.7410
8.0880
8.0792
8.0703
7.9728
7.9636
7.9423
7.9332
7.9243
7.8676
7.8597
7.8357
7.1978
7.1766
7.1163
7.0890
6.8909
6.8823
6.8319
3.8161
3.8050
3.7954
3.3458 HDO
3.3369 HDO
2.4912 DMSO
B (d) 8.75
D (t) 8.08
A (m) 7.85
E (m) 7.94
F (dd) 7.14
G (m) 6.87
H (t) 3.81
N
N
O
Cl
MeO
OMe
O
0.93
0.77
0.94
0.99
2.89
3.12
6.35
f1 (ppm)

^{1}H NMR of **3i**



IR of **3i**



Mass of compound **3i**

Computational Section

Considering the importance of accurately selecting functions in the isomerization calculations, calculated single-point energies of stereoisomers of substituted chromonyl triene barbiturate were carried out using ORCA[1] with a domain-based local pair natural orbital coupled-cluster method, DLPNO-CCSD(T),[2-3] with DEF2-QZVPP and DEF2-QZVPP/C basis sets.[4] Moreover, several DFT functionals (with Def2-TZVP and, 6-311++G (d,p) basis sets),[5] were gauged with CCSD results and find a reliable method for predicting isomerization energies including the explicit account of the dispersion interactions.[6] The results elucidated the M06-2X /def2-TZVP approach as an optimal compromise between the accuracy and feasibility relative to CCSD results (Table 1). Therefore, all computational values reported here are obtained by, the M06-2X /def2-TZVP//B3LYP/6-31G(d) model. The B3LYP/6-31G(d) method[7] was applied to optimize geometries of reagents, intermediates, transition states, and to obtain vibrational frequencies for all molecules. It is important to refer that the AIM[8] and NMR calculations were carried out by the M06-2X /def2-TZVP level of theory via the integral equation formalism polarizable continuum model (IEF-PCM)[9] in acetonitrile solvent.

All quantum chemical calculations were performed using the Gaussian 09 program.[10] Considering the formation of different products from similar reactants motivated us to computationally evaluate the plausible reaction pathways. It seems that the chromonyl triene barbiturates $\mathbf{P_{3a\text{-}3e}}$ were obtained through the C-C bond dissociation of the formed spirocyclic intermediate $\mathbf{In_{1a\text{-}I}}$, unlike dienes $\mathbf{P_{3f\text{-}3i}}$ which likely do not involve a simple C-C cleavage. Accordingly, two possible pathways were investigated to rationalize the variety of the synthesized products $\mathbf{P_{3a\text{-}3i}}$. Considering a neutral diene **A** obtained from the [1,5]-sigmatropic H-shift of akylidenemalononitrile **2b** and deprotonated akylidenemalononitrile **2b** as a carbanion **B** (nucleophilicity parameters N = 2.88, 4.42 eV, respectively; Table 3), initial analysis considered the nucleophilic attack of the latter to the chromonyl barbituric's acid **1b** or the annulation of the neutral diene **A** with dienophile **1b**. Such a

strategy is based on the demonstrated stability of the keteneimine $R_2C=C=NH$ moiety that typically surpasses its alkylnitrile tautomeric analogoue[11-13]. The calculated reaction free energy with the annulation intermediate (ΔG_R = 10.15 kcal/mol) show that the formed spirobarbiturate species **C** has a lower relative stability than the anionic $\mathbf{In_{1b}}$ (ΔG_R = -12.40 kcal/mol) resulting from the carbanionic attack. Moreover, the kinetic aspects of both reactions promote the carbanionic pathway as a much more feasible, seen in 17.73 kcal/mol lower activation barrier (Fig. 3). The latter is particularly valid, given a typically high acidity of the C–H bond directly attached to the malononitrile moiety, as in **A**, which allows an efficient carbanion formation in solution. As an illustration, the pK_a value of system **A**, with two additional cyano substituents at the deprotonating C–H moiety, is 3.2 in acetonitrile, while that of an analogous derivative without the *p*-methoxyphenyl moiety is 3.3,[14] thereby verifying an earlier conclusion.

Table 1. Relative energies of *s*-trans,*s*-trans compared to s-trans,s-cis-conformers calculated using various DFT functionals and basis sets

Basis set	M062X	M062X-D3	B3LYP	B3LYP-BJD3	Wb97XD	Cam-B3LYP
Def2-TZVP	0.45	-0.46	9.22	-0.81	-0.31	0.04
6-311++g(d,p)	-0.34	-1.25	3.16	-0.93	-0.87	-0.14
DLPNO-CCSD DEF2-QZVPP DEF2-QZVPP/C					0.41	

Table 2. B3LYP/6-3G(d) global electronic chemical potential, μ, chemical hardness, η, electrophilicity, ω, and nucleophilicity, N, in eV, of chromonyl barbituric's acid **1b**, neutral diene **A**, and carbanion **B** in CH_3CN

Compound	$\boldsymbol{\mu}$	$\boldsymbol{\eta}$	$\boldsymbol{\omega}$	$\boldsymbol{N}$
chromonyl barbituric's acid **1b**	-4.62	4.08	1.59	2.10
neutral diene **A**	-3.53	4.69	1.08	2.88
carbanion **B**	-2.21	4.25	0.38	4.42

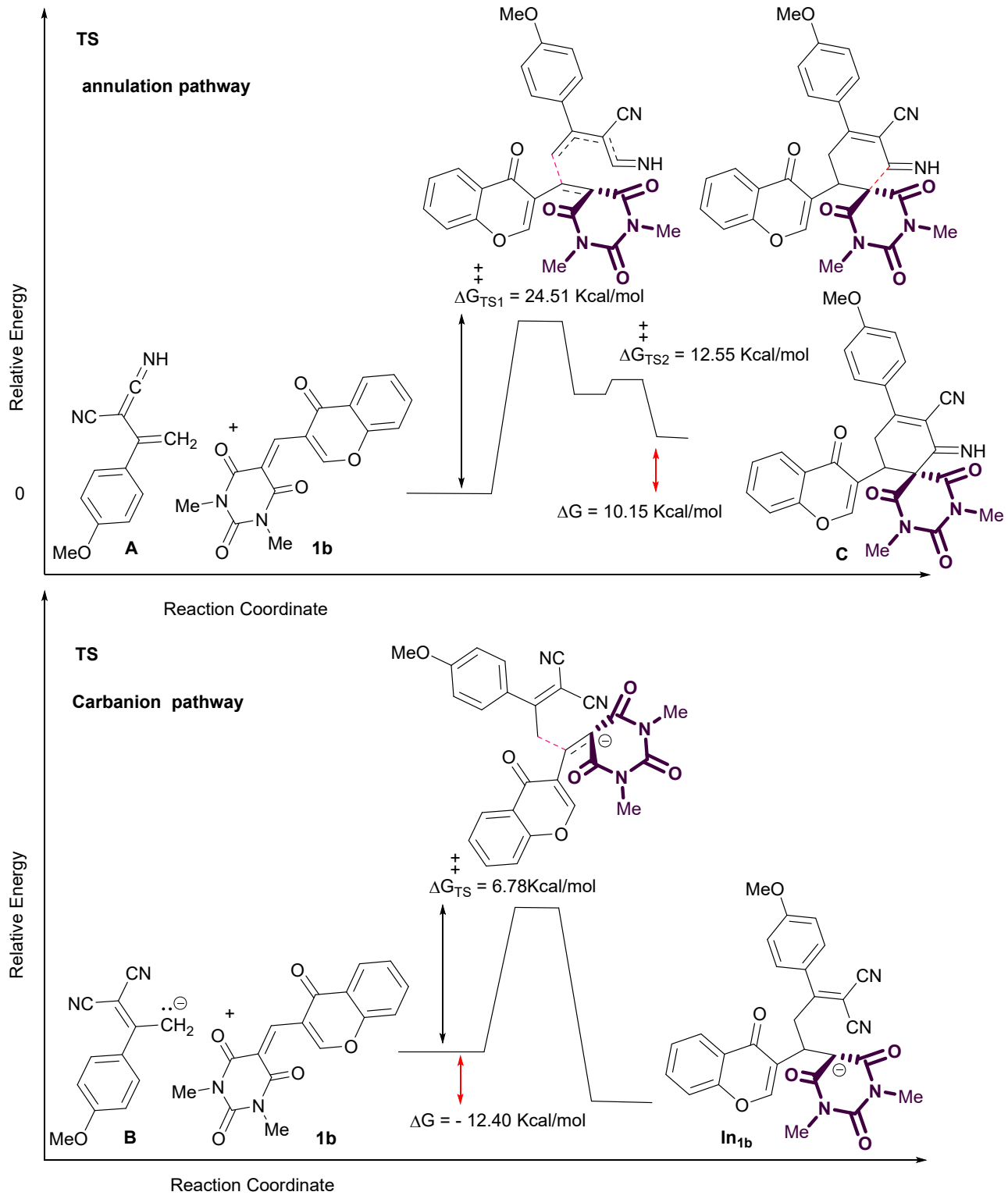


Fig 1. Reaction profiles for the kinetic studies of the proposed $\mathbf{In_{1b}}$ and spirobarbiturate species **C** calculated at the B3LYP/6-31G(d) level of theory.

Table 3: Single point energy $\mathbf{P_{3b}}$ and $\mathbf{P_{3'b}}$ compounds with different methods				
Compound	$\mathbf{P_{3b}}$		$\mathbf{P_{3'b}}$	
Methods	6-311++g(d,p)	DEF2-TZVP	6-311++g(d,p)	DEF2-TZVP
M06-2X-D3	-1750.39048	-1750.58393	-1750.39247	-1750.58466
CAM-B3LYP	-1750.27033	-1750.47144	-1750.27055	-1750.47139
WRB97XD	-1750.46776	-1750.66399	-1750.46914	-1750.66449
B3LYP-D3BJ	-1751.20919	-1751.40764	-1751.21067	-1751.40894
B3LYP	-1751.06294	-1751.26139	-1751.05789	-1751.24669
M062x	-1750.38556	-1750.57901	-1750.3861	-1750.57829
Reference Method	DEF2-QZVPP DEF2-QZVPP/C		DEF2-QZVPP DEF2-QZVPP/C	
DLPNO-CCSD	-1747.807091330795		-1747.806438573041	

Single point input for $\mathbf{P_{3b}}$ compound

0 1

O 5.91673900 0.87490500 1.15664600

O 3.87068200 -1.82523000 -1.13468200

O -5.07217900 0.03974800 -1.90863900

O -2.07412300 -1.67509000 1.32710300

O -1.51881700 5.38678500 0.85149900

O -6.54020300 -2.50761100 1.56329800

N -5.80107000 -1.22852900 -0.18546400

N -2.51696700 0.35002100 -2.30838600

N -4.30091000 -2.14881700 1.40357500

N -0.38014400 -3.23993400 -1.43311100

C 0.06014900 0.15149000 -0.61221200

C -0.90404100 -0.75810900 -0.94920600

C -2.33684300 -0.39825600 -1.21948100

C -0.32768800 1.54368100 -0.25092400

C -3.41424400 -0.87438000 -0.46265300

C 3.82962400 0.16425000 0.18210900

C 4.46876500 -1.01803500 -0.43667300

C 5.91551100 -1.15298200 -0.15105800

C -0.59659000 -2.12961900 -1.19065900

C 1.45794300 -0.25351500 -0.54332400

H 1.72440700 -1.21287800 -0.96803000

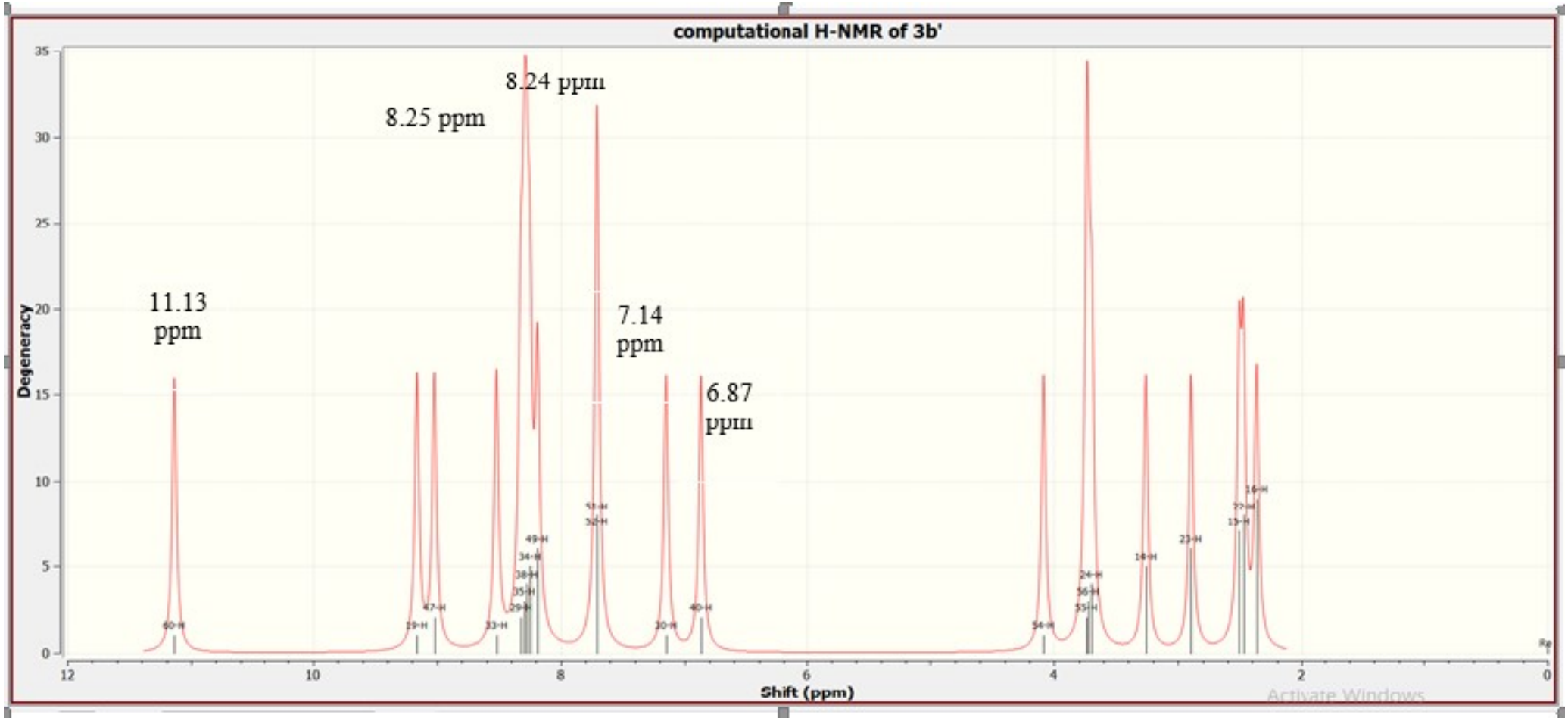
C 2.41746000 0.49116100 0.05008800
H 2.12772300 1.43416100 0.50629300
C -4.77454900 -0.63888500 -0.91743500
C -1.08809600 4.16249200 0.44168800
C 6.58165600 -0.20659900 0.63185600
C -3.17095500 -1.57588400 0.79372400
C -1.20379500 1.77875300 0.82166800
H -1.57404900 0.93643300 1.39454000
C -0.21024900 3.94661300 -0.62566700
H 0.18080700 4.77270900 -1.20408800
C 0.16895100 2.64494300 -0.95308800
H 0.85317100 2.48977600 -1.78028400
C -1.57530500 3.06820600 1.16767000
H -2.24304400 3.25391400 2.00027900
C 4.60374100 1.00993100 0.91712500
H 4.21342600 1.89958500 1.39626400
C 6.65539700 -2.23454100 -0.65762400
H 6.13078400 -2.96440600 -1.26201400
C -5.61111600 -2.00134600 0.96395200
C 8.00656800 -2.35110300 -0.38354800
H 8.57051300 -3.18866100 -0.77629900
C 7.94344800 -0.30796400 0.91750200
H 8.41652000 0.45000300 1.52933400
C 8.64975800 -1.38474300 0.40562600
H 9.70811700 -1.47825700 0.61965600
C -7.17430600 -1.01758800 -0.66331500
H -7.40221400 0.04845900 -0.67333400
H -7.84364900 -1.54339700 0.00983700
H -7.27493400 -1.40242600 -1.67826200
C -4.11987500 -2.92624500 2.63773800
H -3.05289200 -3.05441600 2.78994400
H -4.61488400 -3.89041700 2.53386200
H -4.55853500 -2.39884300 3.48648600
C -1.07080600 6.54113800 0.15097300
H 0.01766300 6.64692200 0.21071500

H -1.54278200 7.38873400 0.64450000
H -1.37979200 6.51503200 -0.89930100
H -3.47775500 0.57561200 -2.57344700
H -1.72481400 0.60792100 -2.87386600

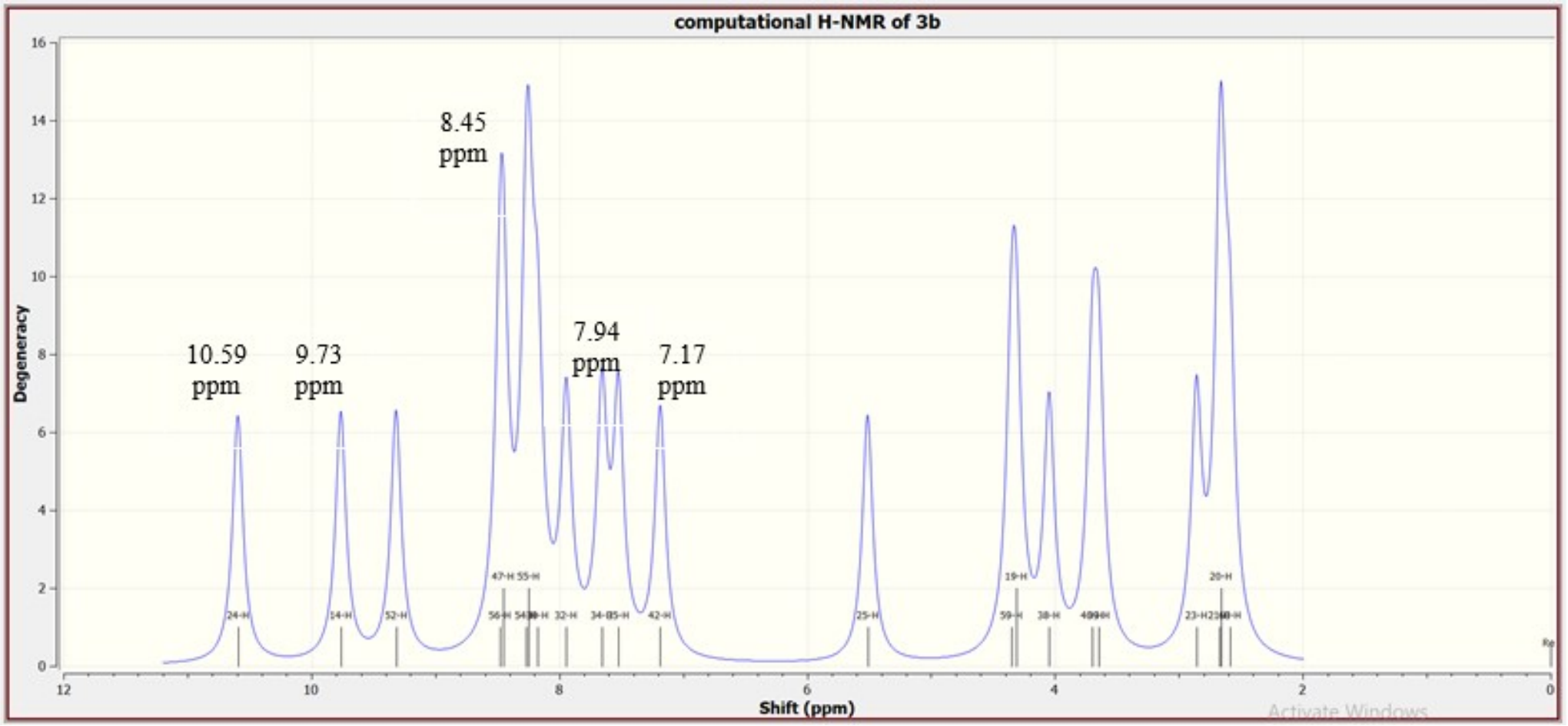
Single point input for **$P_{3'b}$** compound

0 1
O 0.98956100 -2.43639600 0.28322200
C 1.44312200 -0.74902500 -1.33355300
O -0.91875400 1.01276100 2.05182200
C 1.80398800 -1.84153600 -0.41025100
O 1.87223800 3.59761300 -0.74751200
O 3.57748300 0.37835000 1.93469300
O 3.72946900 -0.46007900 -2.00765300
N 2.71350000 2.09937600 0.71918600
C 1.63556800 2.71993100 0.09232600
N 1.32322700 0.71443400 2.02627200
C 0.11955000 -0.15960200 -1.40858500
C 0.31528300 2.23483300 0.42878800
C 1.16648100 -0.34974400 3.02357500
H 2.13521900 -0.54745700 3.46781000
H 0.79139000 -1.25294900 2.54228900
H 0.45261900 -0.02329200 3.77436300
C 2.43086200 -0.15162600 -2.05173300
C 3.74321600 -3.13517100 0.50018900
H 3.03487200 -3.66854900 1.11919600
C 2.59979300 1.00943900 1.58112100
C 4.05979000 2.50691400 0.31251500
H 4.31415400 2.07757700 -0.65810500
H 4.76437000 2.15230600 1.05599800
H 4.08932400 3.58927400 0.23103100
C 4.14989600 -1.44947800 -1.15520000
C 3.24360500 -2.15095100 -0.36209000
C 0.14839600 1.31176700 1.54381000
C 5.51674000 -1.70160600 -1.11542800

H 6.18063900 -1.12713500 -1.74672700
H 0.04640000 0.69278100 -2.07787400
C 5.98333900 -2.67866700 -0.25664500
C 5.09622700 -3.39779200 0.55367200
H 7.04498500 -2.88357400 -0.20944300
H 5.47582400 -4.15604900 1.22552600
H 2.24924100 0.67729800 -2.72377400
C -0.75547500 2.52385500 -0.42964400
C -0.95321900 -0.46527100 -0.66009800
H -0.94082500 -1.35057500 -0.04130200
N -0.66471300 3.49915300 -1.33269500
H -1.41083600 3.65749700 -1.98891100
C -2.13458800 0.38633000 -0.54323200
C -2.03520400 1.75295700 -0.47538000
C -3.42108400 -0.31043500 -0.41221400
C -4.38305600 0.08500700 0.52015300
C -3.68590700 -1.44834300 -1.19196100
C -5.57945200 -0.60255400 0.65947700
H -4.18065800 0.92069100 1.17493300
C -4.87837000 -2.13026500 -1.07671800
H -2.94686600 -1.78609600 -1.90739600
C -5.83973300 -1.71017900 -0.14995900
H -6.29073700 -0.27413400 1.40222900
H -5.09256800 -2.99645600 -1.68814300
C -7.99916600 -2.07393200 0.80960300
H -8.80534400 -2.78802200 0.66001400
H -7.64933700 -2.13361400 1.84434600
H -8.36611500 -1.06363200 0.60707900
O -6.97597800 -2.44564300 -0.10491000
C -3.19035200 2.58352200 -0.54624000
N -4.07242200 3.32258800 -0.64627400
H 0.21343700 4.01214100 -1.38365400



The computational ^{1}H NMR data for **3′b** at M06-2X-D3/def2-TZVP level of theory



The computational ^{1}H NMR data for **3b** at M06-2X-D3/def2-TZVP level of theory

Table 4: Thermodynamic parameters for reactants at b3lyp/6-31g (d) level of theory

Compounds	G		H	S	E
1	-1102.374169		-1102.304271	147.112	-1102.586084
1′	-1561.979676		-1561.906335	154.359	-1562.179620
2	anion	-647.274438	-647.218425	117.889	-647.412226
3		-761.756975	-761.693871	132.814	-761.922542
4		-992.387009	-992.333181	113.292	-992.482974
5		-532.781723	-532.731830	105.010	-532.890226
2′	net	-647.779987	-647.723403	119.093	-647.929757
3′		-762.262492	-762.199154	133.306	-762.440538
4′		-992.889571	-992.835214	114.404	-992.997594
5′		-533.286040	-533.235476	106.421	-533.406459

1,3-Dimethyl-5-[(4-oxo-4*H*-chromen-3-yl) methylene]-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione (**1**)
Charge= 0 multiplicity= 1

O 0.89395700 0.83488400 -1.29435500
C 1.03872300 -1.14178100 0.04804400
O -0.45565500 1.15358500 1.15859100
C 1.56966000 0.08391200 -0.60293000
O -2.91196100 -2.57037400 -0.40165100
O -4.81722300 1.56573400 -0.08655200
O 3.23460600 -1.83336000 0.74667900
N -3.87089500 -0.51838000 -0.23984800
C -2.77534200 -1.37418800 -0.18218500
N -2.60495700 1.39363500 0.42203400
C -0.36843800 -1.51957500 -0.01290200
C -1.46539300 -0.73534600 0.11373700
C -2.61478500 2.81573200 0.78661200
H -3.04358500 3.39484700 -0.03210000

H	-1.58456400	3.10936000	0.97433100
H	-3.21887000	2.97634200	1.68400200
C	1.91210900	-2.02048900	0.60973000
C	3.66043600	1.44864100	-0.86704100
H	3.05189800	2.18140700	-1.38674700
C	-3.82791600	0.86060800	0.01388800
C	-5.16074500	-1.11633800	-0.60493000
H	-5.89607900	-0.31736000	-0.65593800
H	-5.44963900	-1.85687000	0.14494800
H	-5.06965400	-1.61967100	-1.57002100
C	3.79427600	-0.66659000	0.27393100
C	3.02142400	0.29025600	-0.39422800
C	-1.42366400	0.66174200	0.60181600
C	5.16493200	-0.49942100	0.48126300
H	5.72276000	-1.27004500	1.00297800
H	-0.58682300	-2.56644900	-0.22154100
C	5.77123300	0.65751500	0.00801400
C	5.02036100	1.63404700	-0.66711400
H	6.83634000	0.80340600	0.16323700
H	5.50718700	2.53325200	-1.03254100
H	1.61098100	-2.97109700	1.03816900

5-[(6-Chloro-4-oxo-4*H*-chromen-3-yl)methylene]-1,3-dimethyl-2,4,6(1*H*,3*H*,5*H*)-pyrimidinetrione (**1′**)
Charge= 0 multiplicity= 1

O	0.50751100	0.61382800	-1.11455200
C	0.30520300	-1.49065300	0.01016600
O	-0.89967300	0.85279300	1.32090200
C	1.03157300	-0.29327800	-0.48297900
O	-3.77714200	-2.27492500	-0.74953500
O	-5.10409700	2.02486500	0.01785800
O	2.34458400	-2.55150300	0.72195600
N	-4.44989200	-0.14014900	-0.36503200
C	-3.48829400	-1.14480700	-0.38008000

N	-2.96302400	1.47975500	0.56605000
C	-1.13644400	-1.65414800	-0.15004200
C	-2.11770300	-0.74014200	0.03403100
C	-2.79293000	2.83690900	1.10063300
H	-3.09604400	3.56264300	0.34503500
H	-1.74246500	2.95575500	1.35585400
H	-3.41264100	2.97702800	1.99062400
C	1.01694300	-2.53508000	0.51188900
C	3.29293100	0.78348100	-0.51985200
H	2.82605800	1.64518000	-0.98318000
C	-4.22817900	1.17865400	0.05918300
C	-5.79167300	-0.49936300	-0.84042100
H	-6.40625700	0.39682600	-0.81278200
H	-6.21492400	-1.27537100	-0.19798600
H	-5.72552200	-0.89104900	-1.85786700
C	3.08131900	-1.43682700	0.39807300
C	2.48614600	-0.31812800	-0.19443000
C	-1.90391900	0.57209000	0.68671000
C	4.44982100	-1.48210200	0.67421500
H	4.87469700	-2.36856100	1.13303300
H	-1.48563000	-2.62685800	-0.49486000
C	5.23640000	-0.38521600	0.35295700
C	4.64939000	0.74245400	-0.24350300
H	6.30105600	-0.39419600	0.55918900
H	0.56641900	-3.47102600	0.82553300
Cl	5.66427500	2.11699200	-0.64365000

[1-(4-Methoxyphenyl)ethylidene]malononitrile (carbanion) (**2**)
Charge= -1 multiplicity= 1

O	-4.03029600	-0.16459000	0.16244300
N	1.76295400	2.62430100	0.96785300
N	5.02789500	0.05434600	-0.50328800
C	0.15320800	-0.59405700	-0.01523700
C	1.62877400	-0.82129900	-0.08968200

C -0.67908400 -1.48815700 0.68378600
C -0.46832900 0.48406900 -0.65939700
C -2.65676400 -0.24642100 0.06364100
C -2.05942400 -1.32674200 0.72288100
C -1.85404900 0.66287900 -0.63038400
C 2.06560200 -2.09041100 -0.31159100
C 2.51585100 0.33144500 0.04182700
C -4.66347200 0.94051800 -0.44622100
C 2.09821700 1.57620400 0.55563700
C 3.88999700 0.19251100 -0.24895000
H -0.21929600 -2.31688900 1.21433100
H 0.14272000 1.19889200 -1.19957400
H -2.69350500 -2.01790600 1.27175000
H -2.28672600 1.51301400 -1.14710200
H 1.36652100 -2.89460800 -0.51838900
H 3.12501300 -2.32155600 -0.36546600
H -5.73132100 0.83385400 -0.23641700
H -4.51190900 0.95290800 -1.53555100
H -4.30823900 1.89524500 -0.03294500

[2-(1-(2,3-Dimethoxyphenyl)ethylidene)]malononitrile (carbanion) (**3**)
Charge= -1 multiplicity= 1

N -2.08972800 1.86375800 2.08815800
N -4.98201500 -0.52717000 -0.24840200
C -0.11575300 0.28117100 -0.56898800
C -1.48800400 -0.30716800 -0.72335900
C 0.99934500 -0.49495100 -0.21494500
C 0.07907800 1.65249000 -0.81642900
C 2.45492400 1.44885300 -0.40445500
C 2.28188000 0.09244300 -0.12662900
C 1.34121400 2.22450900 -0.74399700
C -1.67335600 -1.25925700 -1.67093700
C -2.54227000 0.23771700 0.13070100
C -2.28526000 1.12410300 1.19648200
C -3.87901500 -0.17041800 -0.06220000

H	-0.78548700	2.25623800	-1.07206100
H	1.47170300	3.28443700	-0.94904600
H	-0.84723600	-1.60485400	-2.28245600
H	-2.65240900	-1.69511700	-1.84805300
H	3.43551100	1.90861000	-0.34450100
O	0.92240800	-1.84824100	0.02953900
O	3.29900100	-0.75690800	0.24337000
C	4.59112400	-0.20864500	0.36879200
H	5.24039200	-1.03152400	0.67988800
H	4.96156100	0.19876000	-0.58398800
H	4.63066000	0.58712000	1.12751600
C	0.24366100	-2.20105500	1.23403800
H	0.78003200	-1.81340700	2.11167800
H	-0.78565300	-1.82948000	1.24218600
H	0.23644800	-3.29446000	1.26884300

[1-(2-Chlorophenyl) ethylidene] malononitrile (carbanion) (**4**)
Charge= -1 multiplicity = 1

N	1.56746600	2.15701900	-1.81532500
N	4.41703400	-0.43734100	0.36723200
C	-0.48291700	0.12198400	0.42218800
C	0.89492200	-0.44855700	0.56981900
C	-1.58145800	-0.55794800	-0.12801400
C	-0.72913300	1.42790500	0.88635400
C	-3.06305200	1.30174300	0.29364200
C	-2.85524800	0.01388100	-0.19244400
C	-1.99009200	2.01312300	0.83337600
C	1.05465500	-1.52323500	1.38126500
C	1.97485100	0.26604800	-0.10178000
C	1.74525000	1.29198300	-1.04067500
C	3.31338500	-0.10790200	0.14017900
H	0.11150000	1.97903900	1.29561800
H	-3.66975200	-0.55346800	-0.63150400
H	-2.13325200	3.02369800	1.20786500

H 0.20825300 -1.97405200 1.88830100

H 2.03534600 -1.95555900 1.55535000

H -4.05449900 1.74541200 0.24057400

Cl -1.41623900 -2.18217500 -0.81194200

1,1-Dicyano-2-phenylpropene (carbanion) (**5**)
Charge= -1 multiplicity = 1
N -1.27674800 2.61765000 -0.82728300

N -4.20727400 -0.46141900 0.34401900

C 0.72559200 -0.40519100 0.05542200

C -0.70707200 -0.83380200 0.04820400

C 1.68944100 -1.12461800 -0.67198400

C 1.16484500 0.69547900 0.81122300

C 3.46012600 0.31434500 0.13362000

C 3.03923900 -0.77469500 -0.63190100

C 2.51347600 1.04743400 0.85294400

C -0.96899900 -2.16194800 0.18443700

C -1.73908400 0.19271300 -0.06095500

C -1.47810800 1.51139100 -0.48670800

C -3.09091800 -0.15141700 0.15388000

H 1.35877700 -1.96054000 -1.28179700

H 0.43699200 1.27205800 1.37189200

H 3.76236100 -1.34812400 -1.20923100

H 2.82578700 1.90173000 1.45010600

H -0.17108300 -2.87254200 0.37499500

H -1.98714000 -2.53897800 0.18590700

H 4.51122500 0.59463400 0.16188500

[1-(4-Methoxyphenyl) ethylidene]malononitrile (neutral diene) (**2′**)
Charge= 0 multiplicity= 1
O -4.03068200 -0.13189300 0.21543200

N 1.74795600 2.60046200 0.79189700

N 5.02397600 0.02156300 -0.48515000

C 0.11572000 -0.63247100 -0.03692200

C 1.58019100 -0.88120200 -0.12272300

C -0.70380200 -1.47257900 0.74027000

C -0.50068400 0.40942600 -0.74242500
C -2.67810300 -0.23751600 0.08616400
C -2.07650500 -1.28327800 0.80295300
C -1.88099200 0.61171100 -0.69044800
C 2.08089600 -2.11319400 -0.32016600
C 2.49423700 0.28429300 0.03021400
C -4.69592100 0.90599800 -0.48874600
C 2.10428400 1.47109600 0.50856100
C 3.89030400 0.15311400 -0.25383700
H -0.24748800 -2.27475000 1.31308200
H 0.09760000 1.06616700 -1.36726100
H -2.70669700 -1.92708900 1.40850200
H -2.31825100 1.42310700 -1.26071600
H 1.41909000 -2.95844600 -0.47553200
H 3.14873400 -2.30425000 -0.35313900
H -5.75425900 0.80256000 -0.24323100
H -4.56383400 0.80581200 -1.57397600
H -4.34523500 1.89715500 -0.17238800
H 1.73452000 2.87832400 1.77660100

[2-(1-(2,3-Dimethoxyphenyl) ethylidene)]malononitrile (neutral diene) (**3′**)
Charge=0 multiplicity= 1
N -2.40172100 2.10634700 -1.69359600
N -5.00319000 -0.78997900 0.24685600
C -0.14317000 0.21277200 0.56233000
C -1.46315300 -0.47823500 0.65269700
C 1.02455800 -0.48634600 0.21362000
C -0.05047000 1.58884800 0.84767600
C 2.33231300 1.55628900 0.42683000
C 2.26495000 0.19064400 0.14526600
C 1.16970500 2.24701300 0.78012700
C -1.64717400 -1.59638600 1.37203700
C -2.60263500 0.13951300 -0.08261800
C -2.46867000 1.11753400 -0.98498000
C -3.93107700 -0.36217900 0.09297200

H	-0.94331200	2.13223600	1.14011600
H	1.22789000	3.30680500	1.01093000
H	-0.82300500	-2.04877800	1.90952800
H	-2.61581600	-2.08248200	1.43700300
H	-2.23886600	1.97957600	-2.69595800
H	3.27872300	2.08289500	0.38324500
O	0.98830100	-1.84137600	-0.00510000
O	3.33529400	-0.58354200	-0.19979400
C	1.09049100	-2.24845700	-1.37108000
H	0.25465300	-1.84965400	-1.96124500
H	2.04032700	-1.92891200	-1.81193700
H	1.03859500	-3.33942700	-1.36647000
C	4.61639600	0.02569100	-0.24020300
H	5.31475100	-0.76800000	-0.51130000
H	4.66273800	0.82319200	-0.99376000
H	4.89655600	0.43710000	0.73813700

[1-(2-Chlorophenyl)ethylidene]malononitrile (neutral diene) (**4′**)
Charge= 0 multiplicity= 1

N	1.16446200	-0.98819600	-2.48631700
N	4.33120500	0.32942800	0.25525500
C	-0.63644700	0.61370300	0.25151800
C	0.80584900	0.76887900	0.61429600
C	-1.33233000	-0.60098700	0.36886700
C	-1.34993300	1.72713200	-0.22018600
C	-3.36170100	0.41638700	-0.44522200
C	-2.68040000	-0.70515100	0.02574700
C	-2.69721000	1.63697400	-0.56558500
C	1.17503800	1.44584800	1.71142900
C	1.80587200	0.19083700	-0.31900000
C	1.46888800	-0.35913800	-1.49076000
C	3.20107700	0.25357600	-0.01488400
H	-0.82397800	2.67301000	-0.31207700
H	-3.18636200	-1.65821200	0.13689200

H	-3.22376200	2.51581800	-0.92610600
H	0.42875000	1.85386000	2.38460100
H	2.21868100	1.59139400	1.97308600
H	1.07937000	-0.49498300	-3.37867600
H	-4.41154700	0.33227300	-0.71130100
Cl	-0.52606100	-2.03118500	0.99727700

1,1-Dicyano-2-phenylpropene (neutral diene) (**5′**)
Charge= 0 multiplicity= 1

N	-1.25165700	2.59209000	-0.62316500
N	-4.20866100	-0.48320500	0.28562400
C	0.76093900	-0.44986400	0.08212900
C	-0.66234300	-0.89144400	0.08602900
C	1.70045700	-1.11485400	-0.72212700
C	1.20116800	0.60935000	0.89299500
C	3.46923900	0.31367200	0.10249000
C	3.04285500	-0.73802400	-0.71056800
C	2.54410400	0.98479500	0.90417800
C	-0.99712400	-2.18746900	0.20597300
C	-1.71540900	0.15069300	-0.05369400
C	-1.46581100	1.40916800	-0.43313400
C	-3.09342500	-0.18457600	0.13395000
H	1.36636300	-1.92146400	-1.36840600
H	0.49451900	1.12620400	1.53578800
H	3.75439000	-1.26202200	-1.34315200
H	2.86801300	1.79977400	1.54578100
H	-0.23198300	-2.94295700	0.34834900
H	-2.02983800	-2.52095400	0.18956600
H	-1.22188900	2.94096300	-1.58449400
H	4.51475500	0.60958500	0.11003400

Table 5: Thermodynamic parameters for TS_1 at b3lyp/6-31g (d) level of theory

Compound TS_1	G	H	S	E
TS_{1a}	-1635.144298	-1635.046189	206.487	-1635.487433
TS_{1b}	-1749.637807	-1749.533802	218.898	-1750.010414
TS_{1c}	-1864.120309	-1864.008539	235.239	-1864.520068
TS_{1d}	-2094.752884	-2094.651395	213.600	-2095.084163
TS_{1e}	-2554.362292	-2554.257272	221.034	-2554.681712
TS_{1f}	-2094.753532	-2094.651853	214.002	-2095.084771
TS_{1h}	-2209.246547	-2209.139048	226.252	-2209.607148
TS_{1i}	-2323.729317	-2323.613815	243.094	-2324.116839

TS_{1a}

Imaginary Freq = -201.84

Charge= -1 multiplicity= 1

C 3.02790600 -2.74804300 -2.30635400

C 1.70860000 -3.37964600 -0.38232700

O -0.67916700 -1.59479000 1.57438400

C 0.02733500 -1.83832700 0.59315700

O 1.64317200 -0.38982800 -2.36234200

O 2.32297500 -4.44399000 -0.35976500

H 3.98890600 -2.84435000 -1.79194700

N 1.97105100 -2.42182100 -1.35243400

C 1.31089000 -1.17185300 -1.46757200

N 0.73344700 -3.05985900 0.55507800

H 3.06651700 -1.93329800 -3.02672300

C 0.23888000 -0.93952300 -0.51935300

C 0.48454700 -3.99998300 1.64429000

H 0.97684100 -4.93763800 1.39439100

H -0.59239300 -4.13900200 1.75805900

H	0.87902100	-3.60861800	2.58808000
H	2.80718400	-3.69684200	-2.80228800
C	-5.25232300	-1.33154500	0.11012900
H	-4.93200000	-2.36745700	0.06413000
C	-1.91571700	0.42851900	-0.37392400
O	-2.56208600	-1.88923800	-0.57764500
C	-2.44823900	1.68309600	-0.37753700
C	-0.46338100	0.27104400	-0.62760300
O	-3.75734000	1.99851200	-0.23118300
C	-4.66311800	0.99573800	-0.03538100
C	-4.27018000	-0.34479900	-0.07877700
C	-2.85648000	-0.72059900	-0.34903400
C	-5.99205700	1.37055800	0.19303100
H	-6.24703300	2.42531500	0.21547400
H	-0.06853000	0.92685300	-1.39830600
C	-6.94168500	0.37631600	0.38459700
C	-6.57333500	-0.97958500	0.34446700
H	-7.97706900	0.65310000	0.56606300
H	-7.32511200	-1.74950200	0.49580000
H	-1.86166500	2.58832100	-0.49676100
C	0.46826000	4.12796100	-0.27895200
C	0.37642700	1.61736500	1.09644200
H	0.36717100	0.73373700	1.72210400
N	-0.55513600	4.65584800	-0.49424000
C	1.58349800	2.15215200	0.64954500
C	1.66278900	3.41982200	-0.00313000
H	-0.48154100	2.27145900	1.19153500
C	2.82351600	1.34404300	0.82660100
C	3.71221800	1.11526300	-0.23677400
C	3.11181600	0.76707000	2.07476300
C	4.85395800	0.33674900	-0.05221400
H	3.48373900	1.51629300	-1.21734200
C	4.25843400	-0.00414700	2.26062400
H	2.43427500	0.94125300	2.90549700
C	5.13479200	-0.22193500	1.19621500

H 5.52254400 0.16166300 -0.89125700

H 4.46556600 -0.43588000 3.23696300

C 2.87517800 4.05875200 -0.36505400

N 3.85512100 4.62164600 -0.66798400

H 6.02658800 -0.82821100 1.33674700

$TS_{\mathbf{1b}}$

Charge = -1 multip1icity = 1

Imaginary Freq = -187.83

C -2.70334500 -2.46554800 2.48987000

C -1.49060800 -3.20550700 0.53495300

O 0.94577100 -1.60644000 -1.51936700

C 0.25470400 -1.78908500 -0.51484200

O -1.18024000 -0.19524700 2.46033800

O -2.17007700 -4.22960700 0.55108300

H -3.68591400 -2.51351700 2.00990700

N -1.66302000 -2.21784400 1.49577700

C -0.92324800 -1.00987000 1.57011800

N -0.52846600 -2.96102800 -0.43727700

H -2.66919500 -1.63874400 3.19665800

C 0.13517000 -0.86212700 0.58938800

C -0.37493900 -3.92917900 -1.51982700

H -0.92607100 -4.82631800 -1.24534200

H 0.68607800 -4.14651400 -1.65846000

H -0.76464800 -3.52064000 -2.45810400

H -2.52263200 -3.41810700 2.99476600

C 5.57155200 -1.60541500 -0.21899100

H 5.18981100 -2.61921300 -0.15310800

C 2.36851600 0.36110600 0.36045900

O 2.87688300 -1.99008800 0.56698100

C 2.97703300 1.58080600 0.33650000

C 0.92013000 0.29750700 0.66266500

O 4.29724900 1.81315200 0.14387800

C 5.13216500 0.75483400 -0.07399000

C 4.65908500 -0.55859000 -0.00571300

C	3.23510400	-0.84405200	0.31573900
C	6.47306100	1.04514100	-0.35038100
H	6.79164600	2.08192400	-0.39054500
H	0.58835800	0.99340500	1.42777700
C	7.35251700	-0.00719100	-0.56527400
C	6.90293600	-1.33741700	-0.50092200
H	8.39615900	0.20381500	-0.78402000
H	7.60022900	-2.15334600	-0.67089700
H	2.45106300	2.52094900	0.46873200
C	0.19940900	4.18294600	0.33150300
C	0.11281200	1.69104100	-1.07540900
H	0.06131700	0.80033100	-1.68897500
N	1.25777000	4.64425400	0.53162900
C	-1.05019100	2.28619400	-0.59381200
C	-1.04045100	3.55218300	0.07113700
H	1.00530900	2.29406000	-1.18864500
C	-2.33531400	1.55099000	-0.74292000
C	-3.21669400	1.37134300	0.33139900
C	-2.69003900	0.98528900	-1.98204700
C	-4.40914700	0.66067100	0.18515400
H	-2.95093200	1.75658100	1.30888600
C	-3.87852900	0.28675200	-2.14578500
H	-2.02516800	1.11364200	-2.83104000
C	-4.74824300	0.12071100	-1.05987900
H	-5.05454300	0.53351500	1.04683700
H	-4.15483700	-0.14052000	-3.10508900
C	-6.78516100	-0.81624500	-0.24166200
H	-7.61376100	-1.39598700	-0.65529500
H	-6.30733700	-1.39280500	0.56221600
H	-7.17395200	0.12257900	0.17644600
O	-5.89596800	-0.58341600	-1.31763400
C	-2.20586800	4.25696500	0.46203800
N	-3.14691800	4.87069700	0.78962300

$TS_{\mathbf{1c}}$

Imaginary Freq = -171.68

Charge= -1 multiplicity= 1

C	1.34345400	3.88699400	2.54342400
C	0.37950800	3.92792000	0.32583300
O	-1.23923700	1.41895800	-1.64062800
C	-0.77823500	1.95167600	-0.62999900
O	0.42136800	1.32103300	2.78470600
O	0.78425400	5.08168400	0.20374000
H	2.36059000	4.11049600	2.20623300
N	0.59633600	3.20404600	1.49128200
C	0.15441100	1.87753600	1.71350000
N	-0.29623100	3.28206800	-0.69712600
H	1.36885100	3.21724500	3.40085300
C	-0.63263500	1.29002400	0.64906500
C	-0.45545600	4.02963700	-1.94097800
H	-0.99850800	4.95956100	-1.75220300
H	-1.00982600	3.39023900	-2.62527400
H	0.52133700	4.28270500	-2.36475100
H	0.85420300	4.83020100	2.80037500
C	-5.90088800	0.60570200	-0.86118900
H	-5.75411000	1.67838800	-0.93602000
C	-2.47586000	-0.45702700	0.40950500
O	-3.49287200	1.71625100	0.12860700
C	-2.80571100	-1.77347400	0.53484500
C	-1.13747400	-0.00376500	0.85965300
O	-4.00485500	-2.33089900	0.24212300
C	-5.00213700	-1.54002900	-0.25076700
C	-4.83053700	-0.15798300	-0.36599700
C	-3.56084500	0.49375900	0.05227000
C	-6.19685100	-2.17074800	-0.61640200
H	-6.28094100	-3.24722600	-0.50634500
H	-0.80036800	-0.45116100	1.79001200
C	-7.23630800	-1.39451500	-1.11020700
C	-7.09036200	-0.00201400	-1.23484200
H	-8.16879300	-1.87139400	-1.40112800
H	-7.91073300	0.59572600	-1.62284900

H -2.12289600 -2.53883600 0.88781700
C 0.28153800 -3.79973900 1.24256000
C 0.22474500 -1.43594500 -0.44274800
H 0.29873600 -0.66230900 -1.19631600
N -0.70424900 -4.42105500 1.36070800
C 1.36372200 -1.82535000 0.25528200
C 1.43066900 -2.99061000 1.07217700
H -0.56144800 -2.16488500 -0.59572000
C 2.59140400 -0.96843000 0.17921100
C 3.41175300 -1.02198200 -0.95450100
C 2.93136000 -0.10364200 1.23286000
C 4.56170000 -0.20803400 -1.04003400
C 4.06184100 0.69940700 1.14009300
H 2.28662700 -0.04594200 2.10259700
C 4.88251800 0.65482600 0.00889200
H 4.31296600 1.37364000 1.95453900
C 2.61979000 -3.41800600 1.71580800
N 3.59279500 -3.80719400 2.23614200
H 5.76038000 1.28940000 -0.04478900
O 3.08451800 -1.84545500 -2.00807700
O 5.29565600 -0.33988700 -2.19316400
C 6.44081000 0.47484700 -2.33889700
H 6.86397300 0.22778800 -3.31552700
H 6.18570300 1.54362400 -2.31648300
H 7.18970000 0.27302200 -1.55961900
C 3.83324900 -3.06051900 -2.06451200
H 4.89347000 -2.86385500 -2.26519300
H 3.73610700 -3.62745200 -1.13073800
H 3.40873000 -3.64061400 -2.88839400

$TS_{\mathbf{1d}}$

Imaginary Freq = -194.06

Charge = -1 multip1icity = 1

C 3.23255100 -2.98885500 -2.28290800
C 1.79792400 -3.47736200 -0.39957700

O	-0.43026100	-1.44635800	1.50578300
C	0.27466800	-1.76270100	0.54430300
O	2.12434600	-0.48818300	-2.35459700
O	2.28746100	-4.60390000	-0.36943700
H	4.16219000	-3.19533300	-1.74407300
N	2.19378800	-2.54985200	-1.35421800
C	1.68360400	-1.23310200	-1.47566200
N	0.83814500	-3.05533600	0.51372000
H	3.38223800	-2.18031500	-2.99565500
C	0.62050200	-0.88484300	-0.55177600
C	0.45270200	-3.96919100	1.58589900
H	0.84268100	-4.95480700	1.34022500
H	-0.63586200	-3.98612500	1.66775000
H	0.86141200	-3.63176400	2.54425900
H	2.91931900	-3.90414100	-2.79167200
C	-4.88235300	-0.63020300	-0.04456600
H	-4.69513300	-1.69633900	-0.10460400
C	-1.35731100	0.72919700	-0.43298600
O	-2.27650000	-1.48991600	-0.69319300
C	-1.73452900	2.03890100	-0.42346000
C	0.06997800	0.40012700	-0.66207500
O	-3.00032200	2.50747000	-0.29469600
C	-4.02104100	1.61934500	-0.13413300
C	-3.79240300	0.24250300	-0.19423600
C	-2.42796900	-0.29877000	-0.44735000
C	-5.30168200	2.14352500	0.07650600
H	-5.43577000	3.21962900	0.11494900
H	0.55773100	1.01315900	-1.41450500
C	-6.36991600	1.27295600	0.23186100
C	-6.14690000	-0.11169100	0.16995300
H	-7.37175900	1.65357500	0.39940900
H	-1.04216800	2.86930800	-0.51586500
C	1.42440100	4.12293700	-0.23255400
C	1.02860600	1.62505700	1.10610700
H	0.90725300	0.73774800	1.71439600

N 0.46756700 4.76036300 -0.45764200
C 2.29556300 2.02441800 0.68518200
C 2.52814700 3.28401400 0.05334300
H 0.24854600 2.37071100 1.19883900
C 3.43251100 1.07780800 0.86739100
C 4.31038900 0.76971500 -0.18488400
C 3.62884300 0.44810400 2.10797600
C 5.35215200 -0.13755200 0.00277600
H 4.14923200 1.21348100 -1.16040000
C 4.67603400 -0.45281900 2.29706700
H 2.95994700 0.68303100 2.93071900
C 5.54252600 -0.74895800 1.24355000
H 6.01303400 -0.37142800 -0.82796400
H 4.81351800 -0.92391600 3.26743800
C 3.81049100 3.78861900 -0.27832200
N 4.85234400 4.24251700 -0.55626600
H 6.35643400 -1.45581400 1.38658200
Cl -7.52108700 -1.20144000 0.36797600

TS_{1e}

Imaginary Freq = -143.93

Charge = -1 multip1icity = 1

C 5.79075900 0.12175200 -2.16031100
C 5.31409200 -1.51494600 -0.44638900
O 2.40814400 -2.22111200 1.49915400
C 3.06023900 -1.67474500 0.60571200
O 3.18923100 0.93303000 -1.96495700
O 6.48184900 -1.88634200 -0.53177600
H 6.62786100 0.54858200 -1.60059700
N 4.82887200 -0.48957400 -1.24493000
C 3.49797600 -0.00712500 -1.22906800
N 4.41045600 -2.07299500 0.44945200
H 5.26008900 0.89889100 -2.70643400
C 2.57335800 -0.67504800 -0.32263600
C 4.88981000 -3.11869100 1.35236800

H 5.93052100 -3.31696300 1.10552300
H 4.28541600 -4.02128400 1.22984800
H 4.79592700 -2.78883700 2.39059700
H 6.18806400 -0.63012000 -2.84774700
C -3.23907700 -2.33317400 -1.29235600
H -3.14911800 -2.08470800 -2.34385000
C 0.03007400 -0.96250500 0.05962100
O -0.88524000 -0.98173600 -2.14985700
C -0.19746600 -1.30395300 1.35678700
C 1.23010300 -0.26842000 -0.42794700
O -1.30622700 -1.93606600 1.80591700
C -2.29219000 -2.27302500 0.92740000
C -2.19275600 -1.96277900 -0.43251600
C -0.99611800 -1.25846800 -0.95568200
C -3.40861400 -2.93989800 1.44487300
H -3.45172600 -3.15684600 2.50703800
H 1.03134900 0.29235800 -1.33395200
C -4.43680100 -3.30248100 0.58777400
C -4.33977200 -2.99483200 -0.77853300
H -5.31301000 -3.81821900 0.96574600
H 0.47603400 -1.09252600 2.17226900
C -0.08014900 1.47920600 3.28618800
C 1.29201600 1.77939600 0.73619800
H 1.88036000 2.10896500 -0.11133700
N 0.38578000 0.82677500 4.13863900
C 0.07669400 2.40096800 1.00384900
C -0.62207300 2.26508200 2.23666600
H 1.82430400 1.29796400 1.54903500
C -0.47507400 3.32528200 -0.03976200
C -1.69239400 3.15611300 -0.72005600
C 0.29003500 4.45497500 -0.38071200
C -2.12677300 4.06887900 -1.68338000
C -0.13218100 5.37543800 -1.33572600
C -1.34878700 5.18226400 -1.98965300
H -3.07030900 3.89301400 -2.18902800

H 0.48705300 6.23801400 -1.56680200

C -1.80414200 2.98647100 2.54406100

N -2.76746500 3.58446800 2.83017700

H -1.69365100 5.88968700 -2.73936100

Cl -5.65884900 -3.47016400 -1.85120500

H 1.23435400 4.60082500 0.13471300

Cl -2.71843400 1.75862700 -0.42982500

TS_{1f}

Imaginary Freq = -153.31

Charge = -1 multip1icity = 1

C -5.27617000 -2.10599600 -1.56452600

C -5.28383800 -0.12463800 -0.18047900

O -2.68010300 1.82469400 1.28444400

C -3.15881300 0.94767800 0.56076000

O -2.54846900 -1.97121900 -1.56657500

O -6.51148900 -0.17780800 -0.17949200

H -5.88026700 -2.67510500 -0.85212000

N -4.52746500 -1.05958300 -0.87139300

C -3.11274400 -1.06749900 -0.94495900

N -4.57187300 0.84843200 0.50899500

H -4.54594400 -2.75151900 -2.04820700

C -2.41866900 0.01710200 -0.26526100

C -5.32228200 1.82192300 1.30077200

H -6.38140400 1.62514200 1.14922800

H -5.06818900 2.83588300 0.98094300

H -5.06023300 1.72716200 2.35817100

H -5.94887800 -1.66268300 -2.30403300

C 2.40282300 3.27932100 -2.19247100

H 2.33237000 2.81531100 -3.17117800

C -0.11083800 1.19227700 -0.25218900

O 0.59174600 1.09330800 -2.53497200

C 0.06908500 1.82824400 0.93693000

C -1.02566600 0.06385100 -0.47338000

O 0.91757600 2.86078400 1.13967200

C	1.67140300	3.33008000	0.10201600
C	1.59678800	2.75207300	-1.16995000
C	0.68287800	1.61318300	-1.42193100
C	2.52087100	4.40920200	0.37073400
H	2.54884500	4.82101500	1.37437500
H	-0.70775400	-0.55137800	-1.30729400
C	3.30693300	4.91252600	-0.65675700
C	3.25011300	4.34857900	-1.94313200
H	3.97322300	5.74839500	-0.45950900
H	-0.43621800	1.56479400	1.85272400
C	1.08133800	-0.45943800	3.24714400
C	-0.30716400	-1.63543000	0.97226400
H	-0.81352500	-2.28857600	0.27216900
N	0.49376300	0.15008100	4.05490600
C	1.06391300	-1.77890600	1.16303300
C	1.77099800	-1.20677700	2.25756900
H	-0.90442500	-1.21049300	1.77139700
C	1.81051700	-2.65444400	0.20167600
C	2.84177800	-2.23420500	-0.65476600
C	1.44684100	-4.01145300	0.13829300
C	3.48088700	-3.12248800	-1.52231900
C	2.07793200	-4.90892000	-0.71836400
C	3.10254800	-4.46211000	-1.55239200
H	4.26681000	-2.75150000	-2.17165600
H	1.76956300	-5.95085900	-0.73332900
C	3.14740900	-1.44586500	2.50383300
N	4.27516600	-1.64455800	2.74106600
H	3.60554000	-5.14819500	-2.22903300
H	0.65060800	-4.35285600	0.79262100
Cl	3.35488300	-0.55474200	-0.71585000
H	3.87242100	4.75017000	-2.73833400

$TS_{\mathbf{h1}}$

Imaginary Freq = -179.59

Charge = -1 multip1icity = 1

C	-2.96275700	-2.61675800	2.47955100
C	-1.61074300	-3.24949600	0.57863400
O	0.70827600	-1.42671500	-1.42550200
C	0.00479000	-1.66858600	-0.44228600
O	-1.69244000	-0.19465200	2.45654400
O	-2.17507100	-4.34077900	0.59236800
H	-3.91565800	-2.78399300	1.96789300
N	-1.92192400	-2.27185800	1.51498100
C	-1.32116400	-0.99019800	1.59022500
N	-0.64782400	-2.91694300	-0.36709400
H	-3.04652400	-1.77843000	3.16833600
C	-0.25389000	-0.74155700	0.63854600
C	-0.35277900	-3.88045000	-1.42464600
H	-0.81447000	-4.82699800	-1.15133100
H	0.72962400	-3.98508600	-1.52266100
H	-0.74997600	-3.53096300	-2.38331100
H	-2.69446000	-3.53317900	3.01160000
C	5.24048300	-0.88349500	-0.02162900
H	4.98263600	-1.93286600	0.06577200
C	1.83019300	0.72343600	0.43691200
O	2.60198300	-1.54780800	0.72179200
C	2.29568200	2.00402400	0.39168100
C	0.39212500	0.49926700	0.71024900
O	3.58631800	2.38099300	0.21826400
C	4.53836700	1.42151700	0.04620600
C	4.21784100	0.06504900	0.14109700
C	2.82776300	-0.37543400	0.44430900
C	5.84498600	1.85192400	-0.21192600
H	6.05128900	2.91529400	-0.27630900
H	-0.03657400	1.16722200	1.45162500
C	6.84593000	0.90690400	-0.37997100
C	6.53054000	-0.45763100	-0.28304600
H	7.86599200	1.21420900	-0.58409800
H	1.66440900	2.88145700	0.48839600
C	-0.73048900	4.27838800	0.27695300

C -0.52825300 1.76989000 -1.08286000
H -0.47237900 0.86539400 -1.67536400
N 0.27205500 4.84759900 0.48683000
C -1.75648500 2.24590900 -0.63252000
C -1.89286000 3.51813100 0.00656700
H 0.29733800 2.46197300 -1.19469000
C -2.95340300 1.37574000 -0.78853900
C -3.83452800 1.12797200 0.27239100
C -3.21905900 0.74796900 -2.02013600
C -4.94166600 0.29173900 0.12041800
H -3.63331700 1.56176000 1.24492800
C -4.32290800 -0.07658800 -2.18968900
H -2.55349600 0.92774900 -2.85919600
C -5.19401700 -0.30952000 -1.11718800
H -5.58915300 0.11663900 0.97203100
H -4.53149500 -0.55195400 -3.14343900
C -7.14087300 -1.43472800 -0.31708900
H -7.89463500 -2.10757000 -0.73275900
H -6.62547200 -1.93849900 0.51207600
H -7.63461300 -0.53142800 0.06699000
O -6.25469900 -1.13698000 -1.37966600
C -3.13298900 4.10431800 0.36172200
N -4.13924000 4.62200800 0.65977000
Cl 7.82032400 -1.64325000 -0.49775800

$TS_{\mathbf{1i}}$

Imaginary Freq = -162.86

Charge= -1 multiplicity= 1

C -1.90333500 3.76360600 -2.63607200
C -0.78664600 3.85066700 -0.49219700
O 0.93554100 1.37432300 1.42819100
C 0.40869700 1.88549500 0.43878100
O -1.03464600 1.17704100 -2.86550400
O -1.16711600 5.01269900 -0.37490200
H -2.89503300 4.00183100 -2.23864900

N	-1.09327000	3.09853500	-1.61929000
C	-0.68860200	1.75964500	-1.83231800
N	-0.04789300	3.22401000	0.49948800
H	-1.98911400	3.07522500	-3.47458000
C	0.16102000	1.18819000	-0.80592500
C	0.20799100	4.00467000	1.70681800
H	0.74943400	4.91986200	1.45306000
H	0.79974200	3.37692300	2.37019800
H	-0.73349700	4.28513100	2.18894700
H	-1.42555800	4.69682600	-2.94503700
C	5.48360000	0.39716200	0.40840900
H	5.38239400	1.47574500	0.44944900
C	1.96629200	-0.60429700	-0.62046900
O	3.06965300	1.54195200	-0.48964900
C	2.24644400	-1.93487400	-0.71447900
C	0.61876100	-0.12235000	-1.00723600
O	3.44405900	-2.52114100	-0.46874800
C	4.48946000	-1.74730500	-0.06426500
C	4.36925700	-0.35751900	0.00739900
C	3.09827600	0.32283700	-0.36600200
C	5.68515400	-2.39957600	0.25844900
H	5.73614700	-3.48118900	0.18814600
H	0.21037800	-0.59139000	-1.89744700
C	6.77711600	-1.64590700	0.66177000
C	6.66323700	-0.24847600	0.73317700
H	7.71416100	-2.12717300	0.92055500
H	1.52168100	-2.68984200	-0.99959600
C	-0.93443700	-3.86799300	-1.19338500
C	-0.70794300	-1.48081500	0.43270700
H	-0.70864500	-0.68308800	1.16423600
N	0.02752200	-4.51807300	-1.34871700
C	-1.89635000	-1.84113500	-0.19300600
C	-2.04788300	-3.02088100	-0.97894600
H	0.06118200	-2.23285600	0.55845100
C	-3.08369900	-0.93511800	-0.07383600

C	-3.79888000	-0.87011200	1.12880800
C	-3.49098900	-0.13898300	-1.15771600
C	-4.91178300	-0.01048100	1.25029600
C	-4.58182200	0.71211300	-1.02904000
H	-2.92404700	-0.16923000	-2.08115300
C	-5.29851500	0.78328000	0.16952200
H	-4.88320600	1.33358000	-1.86798300
C	-3.28249100	-3.42229300	-1.54940500
N	-4.29201000	-3.79023600	-2.01222200
H	-6.14777700	1.45291900	0.25004700
O	-3.40652700	-1.62120800	2.21386500
O	-5.54402000	-0.03063100	2.46865700
C	-6.64499900	0.83630800	2.65113000
H	-6.98660300	0.67737300	3.67672900
H	-6.35864100	1.88986700	2.52565000
H	-7.46667300	0.60728900	1.95744100
C	-4.16437900	-2.81523700	2.40983100
H	-5.20970700	-2.58643300	2.65114800
H	-4.12557200	-3.45734400	1.52131200
H	-3.70185400	-3.33415600	3.25377500
Cl	8.06644200	0.69132100	1.24637700

Table 6: Thermodynamic parameters for intermediates **1a-1i** at b3lyp/6-31g (d) level of theory

Intermediate **1**	G	H	S	E
In_{1a}	-1635.174085	-1635.076669	205.030	-1635.521132
In_{1b}	-1749.668383	-1749.564904	217.789	-1750.044839
In_{1c}	-1864.147823	-1864.037856	231.445	-1864.552469
In_{1d}	-2094.783251	-2094.682270	212.530	-2095.118264
In_{1e}	-2554.385223	-2554.280502	220.404	-2554.707462
In_{1f}	-2094.776113	-2094.674960	212.895	-2095.110388
In_{1h}	-2209.277611	-2209.170549	225.332	-2209.642032
In_{1i}	-2323.757254	-2323.643574	239.261	-2324.149724

In_{1a}

Charge= -1 multiplicity= 1

C 0.75886300 4.11846300 2.24227400
C 1.01170400 3.89365300 -0.14611800
O 0.77637900 1.09251600 -2.35408200
C 0.68585500 1.67632200 -1.25161300
O 0.14749800 1.46227900 2.34287700
O 1.28177300 5.09727500 -0.19929700
H 1.75412700 4.55552200 2.37293300
N 0.72377800 3.27441400 1.05481800
C 0.39389500 1.89181800 1.19686400
N 0.97913200 3.07648500 -1.26341400
H 0.50640300 3.48096600 3.08783500
C 0.37351600 1.10839600 0.00917300
C 1.29212000 3.66992500 -2.55856700
H 1.37013100 4.74649700 -2.41757000
H 0.50658200 3.42328500 -3.27652400
H 2.23545500 3.27263300 -2.94934300
H 0.04108300 4.93997200 2.15026200
C -4.92384000 -0.45959400 -1.36835300

H	-4.59576100	-0.45426100	-2.40320600
C	-1.56509500	-0.43205700	0.39489600
O	-2.13038100	-0.44368800	-1.92833400
C	-2.07632000	-0.44150300	1.64863100
C	-0.04761500	-0.33726300	0.22752000
O	-3.40197800	-0.45645200	1.97220900
C	-4.31982300	-0.46029500	0.96414200
C	-3.92587200	-0.45199000	-0.37974800
C	-2.48498900	-0.43734800	-0.74952500
C	-5.67179200	-0.47434300	1.33107100
H	-5.93171200	-0.47961300	2.38505100
H	0.35899400	-0.61063200	1.20870100
C	-6.63787800	-0.48020800	0.33462700
C	-6.26640600	-0.47286000	-1.02111400
H	-7.68969100	-0.49055400	0.60961400
H	-1.46342800	-0.38629500	2.53820600
C	0.46841800	-4.27403900	-0.45472600
C	0.47323400	-1.39252400	-0.81180700
H	0.68703300	-0.85390900	-1.74395500
N	-0.47072900	-4.94214400	-0.62415200
C	1.68841200	-2.13308400	-0.33969900
C	1.65961100	-3.50847100	-0.22295100
H	-0.31823600	-2.10652500	-1.04241600
C	2.91733700	-1.37238800	-0.02174100
C	3.71376700	-1.69555800	1.09313900
C	3.29908800	-0.28579300	-0.83129100
C	4.86971400	-0.97295300	1.37529600
H	3.41232200	-2.49731400	1.75814200
C	4.46966100	0.41885700	-0.55573300
H	2.68022000	0.01067400	-1.67232100
C	5.25811000	0.07985700	0.54443400
H	5.46281000	-1.22968900	2.24903600
H	4.75347700	1.24966700	-1.19612100
C	2.79937900	-4.32480300	0.08105000
N	3.68711100	-5.04474100	0.30747100

H 6.16208100 0.64298000 0.76363100

H -7.03158500 -0.47824600 -1.79279800

In_{1b}

Charge= -1 multiplicity= 1

C 0.63202900 -4.03178100 -2.18296000

C 0.74360900 -3.82652500 0.21775200

O 0.27430700 -1.06388500 2.43670200

C 0.26775400 -1.63763100 1.32551900

O -0.08552700 -1.40300000 -2.29104200

O 1.05743000 -5.01939200 0.27328000

H 1.64924400 -4.42901900 -2.26139200

N 0.49790200 -3.20420600 -0.99112700

C 0.11755800 -1.83502400 -1.13719500

N 0.61753800 -3.02492900 1.33940900

H 0.40248300 -3.39413600 -3.03493900

C 0.00030700 -1.06759800 0.05522100

C 0.88566700 -3.62031100 2.64369900

H 1.01746700 -4.69078900 2.49647200

H 0.05277100 -3.41613500 3.32047400

H 1.78868100 -3.18802100 3.08866200

H -0.05728900 -4.88129200 -2.14005200

C -5.42223600 0.25785900 1.19984600

H -5.14225400 0.26277100 2.24873600

C -1.98770200 0.38708300 -0.40604200

O -2.66015700 0.36551000 1.88867500

C -2.44078200 0.37990700 -1.68198000

C -0.47648300 0.35968000 -0.17053900

O -3.74958100 0.33711900 -2.06665400

C -4.71204800 0.29564900 -1.10216700

C -4.38041400 0.29911200 0.25846600

C -2.95881600 0.34739500 0.69463600

C -6.04498200 0.25095900 -1.53112000

H -6.25601300 0.24936400 -2.59599000

H -0.03952800 0.65929900 -1.13057600

C -7.05528500 0.20933000 -0.58043400
C -6.74665000 0.21263500 0.79099100
H -8.09273000 0.17397000 -0.90371600
H -1.78561200 0.35638000 -2.54239400
C -0.20089200 4.28665000 0.42499800
C -0.04926400 1.43016100 0.89609600
H 0.14271300 0.89909100 1.83593200
N -1.18847800 4.89976100 0.50535400
C 1.15323200 2.22309000 0.47417200
C 1.04782600 3.59179100 0.30396200
H -0.88045600 2.10920400 1.08900200
C 2.43363000 1.52534300 0.25865700
C 3.30830700 1.88357100 -0.78117500
C 2.80750800 0.44726200 1.09156400
C 4.52024100 1.22634600 -0.97745200
H 3.03142400 2.66972500 -1.47429000
C 4.02389300 -0.19462800 0.92006500
H 2.14095600 0.10961300 1.87896000
C 4.89041500 0.18905400 -0.11292400
H 5.15512300 1.52448700 -1.80372500
H 4.31598800 -1.01632600 1.56633100
C 6.95406500 -0.19001100 -1.25190700
H 7.80410600 -0.86637100 -1.13909400
H 6.49511900 -0.34702100 -2.23715000
H 7.30546800 0.84838300 -1.18183500
O 6.05904000 -0.51166600 -0.20188200
C 2.15233300 4.46915700 0.04740100
N 3.00980100 5.23476100 -0.14527800
H -7.54603600 0.18050300 1.52653900

In_{1c}

Charge= -1 multiplicity= 1

C 0.10903100 4.21437300 2.03042100
C 0.06344400 4.05117800 -0.37522000
O -0.27416800 1.28327800 -2.61087400

C	-0.24440700	1.83419000	-1.48839600
O	-0.26963400	1.51694100	2.13872600
O	0.23672800	5.27307700	-0.43063500
H	1.07836300	4.72368200	2.04523700
N	-0.01861700	3.39160800	0.83510600
C	-0.21573900	1.98257600	0.98150900
N	-0.05955900	3.25373400	-1.49983500
H	0.01571700	3.54395200	2.88317300
C	-0.33459000	1.22141100	-0.21308400
C	0.02960500	3.89209700	-2.80785400
H	0.04333200	4.96898700	-2.64902300
H	-0.82412200	3.59554600	-3.42151000
H	0.93948700	3.57798700	-3.33144400
H	-0.67224900	4.98105000	2.05408000
C	-5.61329900	-0.82456800	-0.82336600
H	-5.45204700	-0.76117400	-1.89510400
C	-2.03822600	-0.51077500	0.40561900
O	-2.95631900	-0.51953800	-1.80281600
C	-2.34479200	-0.60183400	1.72137800
C	-0.58005900	-0.26388800	0.01555600
O	-3.59718700	-0.75476000	2.24307800
C	-4.65609500	-0.82337900	1.38772700
C	-4.47868100	-0.74295600	0.00080700
C	-3.12031900	-0.57719100	-0.58403900
C	-5.92737700	-0.97972200	1.95557000
H	-6.01838500	-1.03640700	3.03587100
H	-0.00242300	-0.52445000	0.91049500
C	-7.03204600	-1.05624200	1.11881400
C	-6.87837500	-0.97884300	-0.27635600
H	-8.02263500	-1.17690600	1.55043300
H	-1.60816700	-0.51006300	2.50797300
C	0.42368700	-4.09554500	-1.31909200
C	-0.13346900	-1.22724400	-1.13502700
H	-0.16767900	-0.64566300	-2.06895600
N	-0.39180400	-4.90684000	-1.50240200

C	1.23806300	-1.79571300	-0.95032100
C	1.47094600	-3.14338100	-1.08856900
H	-0.85028700	-2.04310000	-1.24730900
C	2.37181900	-0.86576900	-0.69291800
C	3.17573700	-0.98933800	0.45594000
C	2.61580800	0.16957000	-1.61179600
C	4.22437800	-0.06485100	0.66810000
C	3.68449800	1.03291100	-1.42079200
H	1.94737600	0.30321100	-2.45540800
C	4.49089400	0.91765100	-0.28590800
H	3.87963300	1.82363800	-2.13921300
C	2.78421000	-3.71586000	-1.05302700
N	3.83574600	-4.21725900	-1.04895200
H	5.30021100	1.62229900	-0.13130700
O	2.81995600	-1.93381300	1.37832900
O	4.91457100	-0.19227800	1.84821600
C	3.82347800	-2.74905300	1.99294300
H	4.60987500	-3.01392400	1.28029800
H	4.25819700	-2.25095800	2.86271600
H	3.30630400	-3.66069300	2.30361100
C	5.91051800	0.76748200	2.14269700
H	5.49638800	1.78425600	2.17010200
H	6.29357700	0.50723700	3.13206000
H	6.73617400	0.73630300	1.41769900
H	-7.75042900	-1.04048500	-0.92199200

$In_{\mathbf{1d}}$

Charge = -1 multiplicity= 1

C	-1.55224700	-4.11158800	2.22862600
C	-1.57656200	-3.86852700	-0.17158700
O	-1.04363700	-1.06833700	-2.32885200
C	-1.07862200	-1.65946600	-1.22748400
O	-0.86411600	-1.47693900	2.40300900
O	-1.87961700	-5.06198000	-0.25756500
H	-2.56802900	-4.51840800	2.26177000

N	-1.38036000	-3.26397500	1.05549400
C	-1.02108900	-1.89425400	1.23654100
N	-1.41375200	-3.04873900	-1.27579600
H	-1.36140600	-3.48591900	3.09877500
C	-0.86939400	-1.10662100	0.06144500
C	-1.62250900	-3.62739100	-2.59861300
H	-1.74928800	-4.70111200	-2.47243400
H	-0.76479300	-3.40528000	-3.23759300
H	-2.51093000	-3.19716000	-3.07387300
H	-0.85400500	-4.95424000	2.19864700
C	4.56698400	0.29746100	-0.81734700
H	4.34317700	0.31225600	-1.87835600
C	1.06857100	0.36970100	0.63423300
O	1.85059000	0.38168700	-1.62719500
C	1.46126100	0.35139600	1.93023800
C	-0.42927700	0.32471300	0.32771400
O	2.75224700	0.31751900	2.37507000
C	3.75649500	0.29849700	1.45736600
C	3.48987600	0.31548100	0.08330500
C	2.08837500	0.35336100	-0.42092200
C	5.06995100	0.26263200	1.94358200
H	5.23834200	0.24953900	3.01561700
H	-0.91481900	0.60555100	1.27005400
C	6.12628500	0.24359000	1.04562900
C	5.86189000	0.26127800	-0.33290700
H	7.15110200	0.21513800	1.40033500
H	0.76764000	0.30874500	2.75884000
C	-0.76178700	4.27188300	-0.33212900
C	-0.82108300	1.40064600	-0.74591600
H	-0.96194300	0.87479000	-1.69869700
N	0.21215700	4.90799800	-0.39361100
C	-2.05410400	2.17209500	-0.37995000
C	-1.99412600	3.54346600	-0.23428700
H	0.00757200	2.09398900	-0.89460500
C	-3.32992700	1.44547900	-0.19593400

C	-4.22099700	1.77733100	0.84217900
C	-3.66318900	0.38276800	-1.05702200
C	-5.41963200	1.08694100	0.99887900
H	-3.96213100	2.55981100	1.54687200
C	-4.87506800	-0.28924800	-0.90788100
H	-2.97429500	0.07806900	-1.83847800
C	-5.75634700	0.05853500	0.11653800
H	-6.08695400	1.34956100	1.81542700
H	-5.11974500	-1.10168700	-1.58679900
C	-3.13206600	4.39182400	-0.02618600
N	-4.01482400	5.13655900	0.12740700
Cl	7.22340100	0.23678000	-1.45776400
H	-6.69354500	-0.47930200	0.23762600

$In_{\mathbf{1e}}$

Charge= -1 multiplicity= 1

C	1.07191400	4.30685200	2.07229800
C	1.10328900	4.01685600	-0.32249800
O	0.71081600	1.15152400	-2.42368300
C	0.72376300	1.76293200	-1.33164400
O	0.54151400	1.64009900	2.30210200
O	1.34050700	5.22302200	-0.43470500
H	2.06411100	4.76901900	2.09435900
N	0.94369500	3.42793600	0.91682500
C	0.66550500	2.04286600	1.12691900
N	0.98191300	3.16679400	-1.40947000
H	0.91749500	3.68899100	2.95520200
C	0.55284100	1.22521100	-0.03107700
C	1.14995100	3.73066200	-2.74433400
H	1.21034900	4.81248000	-2.63992800
H	0.30569100	3.44260500	-3.37469400
H	2.06218200	3.34780000	-3.21532800
H	0.32875000	5.10946300	2.02784000
C	-4.80779200	-0.50139700	-0.74137800
H	-4.61286400	-0.50767000	-1.80816700

C	-1.27295200	-0.36099500	0.61288400
O	-2.11449700	-0.42830700	-1.62611400
C	-1.62977300	-0.35954800	1.91944500
C	0.21055900	-0.22862600	0.26444700
O	-2.90777800	-0.39997600	2.39956000
C	-3.93629200	-0.44389500	1.51001300
C	-3.70708700	-0.45145500	0.12908500
C	-2.32008100	-0.40873100	-0.41347700
C	-5.23570700	-0.48336800	2.03238900
H	-5.37499700	-0.47482300	3.10864200
H	0.73930400	-0.47694400	1.19254200
C	-6.31563700	-0.53107400	1.16404000
C	-6.08877000	-0.53967900	-0.22128600
H	-7.33019100	-0.56134300	1.54697300
H	-0.91717700	-0.27377900	2.72820900
C	1.11587600	-4.15360900	-1.01755500
C	0.62694400	-1.27355000	-0.82002500
H	0.61769100	-0.74768500	-1.78806100
N	0.27628400	-4.93651800	-1.21223000
C	1.97814300	-1.88278500	-0.61412000
C	2.18614300	-3.23049700	-0.76915500
H	-0.11659500	-2.07064100	-0.88841700
C	3.14086400	-0.99300300	-0.33540000
C	3.92120400	-1.06352400	0.83134400
C	3.48331300	-0.02090000	-1.29184700
C	5.01970700	-0.22600900	1.02282300
C	4.58715200	0.80766700	-1.11455600
H	2.84750300	0.10101300	-2.16317200
C	5.36069500	0.70127900	0.04123100
H	5.59098800	-0.30241000	1.94158700
H	4.82838300	1.54792900	-1.87172900
C	3.48875400	-3.83157500	-0.74698400
N	4.52769200	-4.35658100	-0.76305800
H	6.21830200	1.35120100	0.19320000
Cl	3.50993900	-2.16465400	2.14495200

Cl -7.47968300 -0.60111900 -1.30791000

In_{1f}

Charge = -1 multiplicity= 1

C 0.12689500 4.27162800 2.10672200
C 0.37539300 4.04151700 -0.28145700
O 0.38972500 1.20430400 -2.45555800
C 0.25893600 1.78844300 -1.35588300
O -0.20806400 1.56824200 2.24705300
O 0.52494700 5.26506000 -0.35340300
H 1.07444400 4.80851600 2.21893800
N 0.16248500 3.41317800 0.92972500
C -0.02350900 2.00556100 1.09274400
N 0.41148700 3.21005300 -1.38848400
H -0.04939900 3.62268000 2.96286100
C 0.02021100 1.20905900 -0.08469800
C 0.64504500 3.81558400 -2.69471000
H 0.61084000 4.89618500 -2.56779900
H -0.11832400 3.47758600 -3.39914300
H 1.62065400 3.51543100 -3.09317900
H -0.67124400 5.01537400 2.01505600
C -5.12560900 -0.91222000 -1.26097300
H -4.83848700 -0.87028800 -2.30710600
C -1.72671400 -0.52802300 0.37880400
O -2.37253800 -0.59409400 -1.92236700
C -2.18718600 -0.59290500 1.65052100
C -0.23491600 -0.27318800 0.15616300
O -3.49085100 -0.74963900 2.02187500
C -4.43951800 -0.85043500 1.04795800
C -4.09846700 -0.79839200 -0.30939200
C -2.68195900 -0.62846700 -0.73109900
C -5.76773900 -1.01003500 1.46395100
H -5.98660000 -1.04390400 2.52669200
H 0.23557800 -0.50316200 1.11974800
C -6.76365400 -1.11878100 0.50341500

C	-6.44526200	-1.07023900	-0.86494500
H	-7.79744400	-1.24222900	0.81653400
H	-1.55107900	-0.47531800	2.51730800
C	1.06629600	-4.08330300	-1.17259700
C	0.34672600	-1.25683900	-0.90953400
H	0.38209000	-0.70656400	-1.86369100
N	0.31058000	-4.91595400	-1.47501600
C	1.71561800	-1.77693900	-0.60319400
C	2.03733500	-3.09828100	-0.79068000
H	-0.32963500	-2.10092200	-1.06088200
C	2.77942900	-0.82037000	-0.18550100
C	3.45993700	-0.88943900	1.04223300
C	3.12704800	0.21884800	-1.06664100
C	4.47133100	0.01497300	1.36480900
C	4.14592300	1.11513400	-0.75826600
H	2.56089400	0.33508900	-1.98573500
C	4.82378700	1.00985500	0.45618300
H	4.96573900	-0.06348400	2.32696400
H	4.39382000	1.90632100	-1.45976900
C	3.37441300	-3.60537600	-0.67448800
N	4.44715600	-4.05419700	-0.61763900
H	5.61343000	1.71198200	0.71022000
H	-7.23335900	-1.15692200	-1.60818700
Cl	3.02186100	-2.07724400	2.26903600

$In_{\mathbf{1h}}$

Charge= -1 multiplicity= 1

C	-1.26515000	-4.02221600	2.23028700
C	-1.22118100	-3.81801600	-0.17307400
O	-0.57603800	-1.06397300	-2.35881200
C	-0.65219400	-1.63639000	-1.24990400
O	-0.52649900	-1.40028900	2.38214700
O	-1.54372700	-5.00713300	-0.24767600
H	-2.28876000	-4.41023300	2.24226300
N	-1.04658000	-3.19692100	1.04917900

C -0.66330400 -1.83215600 1.21814600
N -1.01367900 -3.01964500 -1.28518000
H -1.08583300 -3.38614400 3.09535800
C -0.46604800 -1.06659800 0.03530800
C -1.20134500 -3.61494100 -2.60375100
H -1.35312000 -4.68376700 -2.46430700
H -0.32372100 -3.42018000 -3.22436200
H -2.06890700 -3.17462800 -3.10739500
H -0.58209400 -4.87779800 2.23246800
C 5.01693300 0.21628500 -0.77372600
H 4.81067900 0.22967900 -1.83830600
C 1.49745500 0.37145400 0.61951100
O 2.31724400 0.35491700 -1.62881000
C 1.86876200 0.35338400 1.92183500
C 0.00369900 0.35754500 0.29018700
O 3.15142600 0.29412500 2.38819400
C 4.16973400 0.24809400 1.48731400
C 3.92594100 0.26270200 0.10900400
C 2.53394500 0.32778300 -0.41860600
C 5.47408900 0.18692800 1.99513400
H 5.62469200 0.17672900 3.06985000
H -0.48910300 0.66006200 1.22176800
C 6.54426600 0.13991200 1.11477300
C 6.30269300 0.15515000 -0.26794900
H 7.56234000 0.09163800 1.48636600
H 1.16082300 0.33122100 2.73911400
C -0.21117900 4.27670200 -0.27687600
C -0.34871500 1.43140200 -0.79938400
H -0.47916000 0.90397200 -1.75139400
N 0.78633200 4.87886600 -0.27428300
C -1.57435700 2.22708400 -0.45399400
C -1.47140400 3.59239100 -0.25797000
H 0.49501400 2.10913500 -0.93386900
C -2.87054400 1.53535800 -0.33876000
C -3.81668700 1.88992300 0.63808700

C -3.18934000 0.46687700 -1.20639600
C -5.04333800 1.23880600 0.73969300
H -3.58667200 2.66796000 1.35696300
C -4.41838800 -0.16888200 -1.12954900
H -2.46939900 0.13061800 -1.94581700
C -5.35577800 0.21139500 -0.15889900
H -5.73488700 1.53379800 1.52033800
H -4.66733400 -0.98300900 -1.80286900
C -7.49935100 -0.16361500 0.82302600
H -8.34255900 -0.83366100 0.64222800
H -7.11470100 -0.33172000 1.83775300
H -7.83858600 0.87748700 0.73614800
O -6.53137700 -0.48239000 -0.16145300
C -2.58461200 4.47595300 -0.06937800
N -3.44777600 5.24629900 0.07168900
Cl 7.68161000 0.09486500 -1.37031600

In_{1i}

Charge= -1 multiplicity= 1

C 0.89021300 4.23982700 2.01740300
C 0.72688300 4.05143100 -0.38166600
O 0.12039200 1.28354900 -2.56023900
C 0.23869000 1.84485700 -1.44931300
O 0.35688600 1.57021900 2.18002800
O 0.96963700 5.25970000 -0.46173500
H 1.88636900 4.69290300 1.98001400
N 0.66054600 3.41193600 0.84079800
C 0.38898300 2.01949600 1.01519300
N 0.50514800 3.25023300 -1.48863100
H 0.79910600 3.58599700 2.88313900
C 0.17549700 1.25261300 -0.16222200
C 0.57052500 3.86785700 -2.80820000
H 0.65719900 4.94349500 -2.66502900
H -0.32793500 3.61776900 -3.37701300
H 1.43373900 3.49260700 -3.36906800

H	0.15552500	5.05010900	2.06611100
C	-5.22332200	-0.48246900	-0.51156400
H	-5.11493700	-0.44630200	-1.59001400
C	-1.59056600	-0.36964700	0.55627700
O	-2.61226200	-0.35743300	-1.60819100
C	-1.84074700	-0.42198900	1.88634900
C	-0.13995000	-0.21350600	0.09776400
O	-3.07599600	-0.48949600	2.46695900
C	-4.17264900	-0.50594800	1.66256100
C	-4.05594500	-0.45858000	0.26836900
C	-2.71739900	-0.38544300	-0.38309500
C	-5.42559900	-0.57436500	2.28600100
H	-5.47736200	-0.60839200	3.36952300
H	0.46157500	-0.49590500	0.97004800
C	-6.57217300	-0.59588800	1.50656800
C	-6.45787500	-0.54951800	0.10826800
H	-7.55232500	-0.64787200	1.96864700
H	-1.06508800	-0.36254400	2.63739300
C	0.59692000	-4.11216600	-1.17950300
C	0.19895400	-1.21485900	-1.05684400
H	0.14965100	-0.64601100	-1.99752600
N	-0.26977900	-4.88174600	-1.29482300
C	1.54746700	-1.85012400	-0.92501800
C	1.70299100	-3.21128200	-1.03225600
H	-0.56281300	-1.99461200	-1.11932100
C	2.73862200	-0.97407100	-0.75185800
C	3.58802800	-1.10472500	0.36287200
C	2.99270400	0.01719100	-1.71544800
C	4.69167500	-0.23092000	0.49668800
C	4.11202200	0.82836100	-1.60159600
H	2.29355300	0.15995500	-2.53209400
C	4.96331800	0.70608400	-0.50070900
H	4.31424900	1.58454600	-2.35439700
C	2.98531800	-3.85119100	-1.04166600
N	4.00880200	-4.40664700	-1.07168500

Cl	-7.93233300	-0.57864800	-0.86442800
H	5.81419100	1.37127700	-0.40640700
O	3.22772100	-2.00052700	1.33089100
O	5.42871500	-0.35832700	1.64776000
C	4.21583600	-2.84979700	1.92450000
H	4.95154200	-3.17825300	1.18472500
H	4.71781600	-2.34950800	2.75588300
H	3.66717500	-3.72220000	2.28904500
C	6.48666800	0.55498800	1.86446500
H	6.12815200	1.59292300	1.87687500
H	6.90177200	0.30502500	2.84344500
H	7.27420300	0.45678600	1.10398600

Table 7: Thermodynamic parameters for TS_2 [1,5]-H shift at b3lyp/6-31g (d) level of theory

TS_2	G	H	S	E
$TS_{2a(1,5)}$	-1635.152019	-1635.054957	204.284	-1635.493811
$TS_{2b(1,5)}$	-1749.645178	-1749.542279	216.570	-1750.016578
$TS_{2c(1,5)}$	-1864.128564	-1864.018703	231.222	-1864.528009
$TS_{2d(1,5)}$	-2094.760840	-2094.660330	211.540	-2095.090730
$TS_{2e(1,5)}$	-2554.367352	-2554.262217	221.277	-2554.684007
$TS_{2f(1,5)}$	-2094.758652	-2094.656770	214.429	-2095.087003
$TS_{2h(1,5)}$	-2209.254082	-2209.147675	223.953	-2209.613510
$TS_{2i(1,5)}$	-2323.737995	-2323.624645	238.564	-2324.125507

$TS_{2a(1,5)}$

Imaginary Freq = -1198.29

Charge = -1 multiplicity= 1

C 3.93647200 -3.45751500 0.99989200

C 2.42056000 -3.67788100 -0.86059900

O -0.55637300 -1.91803200 -1.76869600

C 0.51023300 -2.16009300 -1.06811000

O 2.41689100 -1.35514700 1.87293500

O 3.09031300 -4.62683200 -1.26899100

H 3.80080500 -4.49918800 1.30570500

N 2.75875000 -2.98180100 0.28173200

C 2.03028200 -1.87094700 0.81621000

N 1.27158200 -3.23908100 -1.51594600

H 4.05235200 -2.81575100 1.87151900

C 0.90074800 -1.44491800 0.05348600

C 0.83014300 -3.95985500 -2.70780900

H 1.56452100 -4.73936800 -2.90126400

H 0.76266800 -3.27523100 -3.55749200

H -0.15784400 -4.39825500 -2.54088100

H	4.82103900	-3.40342000	0.35789400
C	2.63741200	3.66902000	-1.49204800
H	2.35033200	3.34414300	-2.48734800
C	0.93017900	1.00531700	0.60019800
O	1.03701200	1.32835500	-1.76811600
C	1.36749400	1.47752100	1.78921600
C	0.08612100	-0.26800200	0.57639800
O	2.13872800	2.58428300	1.97922200
C	2.54240600	3.29172400	0.88566500
C	2.18441200	2.89627200	-0.40941200
C	1.34424300	1.68945600	-0.62988600
C	3.33057900	4.42692600	1.11455900
H	3.58555000	4.69454900	2.13519100
H	-0.15279300	-0.48984000	1.62265500
C	3.76387600	5.17298100	0.02752200
C	3.41804100	4.79561500	-1.28192900
H	4.37679000	6.05516900	0.19455700
H	1.16257800	0.99176000	2.73438500
C	-2.05775100	-2.02248800	1.97551900
C	-1.23389500	-0.01706500	-0.19437200
H	-1.09876700	-1.02132400	-1.13358000
N	-1.41297100	-2.87723200	2.44269100
C	-2.52529400	-0.15016000	0.38406500
C	-2.91136200	-1.02577600	1.42015800
H	-1.16579400	0.81565800	-0.89069700
C	-3.60039700	0.67733100	-0.25164100
C	-4.77534300	0.09481600	-0.75176700
C	-3.43166500	2.06410100	-0.39108500
C	-5.74915400	0.87486800	-1.37384800
H	-4.91655000	-0.97723900	-0.66072000
C	-4.41170200	2.84731000	-0.99961200
H	-2.52717100	2.52629600	-0.00660100
C	-5.57348100	2.25430100	-1.49686800
H	-6.64770600	0.40220200	-1.76273100
H	-4.26561400	3.92132400	-1.08701500

C	-4.21168600	-0.99247600	2.00383100
N	-5.25929800	-0.99111000	2.52186200
H	-6.33600400	2.86254500	-1.97781000
H	3.76377000	5.38725100	-2.12537700

$TS_{\mathbf{2b}(1,5)}$

Imaginary Freq = -1195.73

Charge = -1 multiplicity= 1

C	5.26450100	-2.36591600	0.54493000
C	3.67577000	-2.94357400	-1.17250600
O	0.26418400	-2.02013000	-1.71236400
C	1.42410300	-1.98323700	-1.12788000
O	3.34546800	-0.76072200	1.65462600
O	4.52475800	-3.67281900	-1.68577900
H	5.43806800	-3.41205700	0.81419800
N	3.93596300	-2.20505200	-0.03650500
C	3.00091400	-1.33835200	0.61552300
N	2.39068000	-2.81249000	-1.69533500
H	5.29770200	-1.73334600	1.43024700
C	1.72719500	-1.21113200	-0.01746300
C	2.03210300	-3.60257000	-2.87088600
H	2.92073900	-4.15607700	-3.16809800
H	1.70023800	-2.94498300	-3.67879500
H	1.21607000	-4.28990900	-2.63040500
H	6.03319200	-2.06729300	-0.17444100
C	1.90745300	4.21102400	-1.46656200
H	1.62052900	3.84274400	-2.44667800
C	1.16977800	1.14597200	0.64280600
O	0.95735900	1.53608400	-1.70830400
C	1.58103400	1.69218500	1.80914000
C	0.69002800	-0.30451000	0.63432300
O	2.04921000	2.95989200	1.98153500
C	2.14528300	3.77197400	0.89045200
C	1.77986700	3.32308100	-0.38500900
C	1.26824700	1.94148100	-0.58608800

C	2.62652400	5.07055200	1.10116900
H	2.89983100	5.37467800	2.10672500
H	0.62375900	-0.60587500	1.68604600
C	2.74180800	5.92757900	0.01572700
C	2.38199000	5.49965600	-1.27426800
H	3.11508800	6.93708300	0.16868400
H	2.47709900	6.17949300	-2.11673700
H	1.60329800	1.14966300	2.74536300
C	-0.76038200	-2.61984000	2.09854900
C	-0.72083600	-0.39420900	0.00159300
H	-0.42298700	-1.31383100	-0.99216400
N	0.12908200	-3.30113600	2.42967400
C	-1.86718600	-0.87191400	0.69262600
C	-1.89492200	-1.85047100	1.71071600
H	-0.94070100	0.43838800	-0.66273300
C	-3.17927900	-0.33413600	0.21871500
C	-4.23770400	-1.17738900	-0.14081600
C	-3.37748600	1.05268000	0.08733200
C	-5.45015900	-0.67220400	-0.61340700
H	-4.11123700	-2.25209900	-0.06316200
C	-4.58219500	1.57235900	-0.36641100
H	-2.57399800	1.72940700	0.36216700
C	-5.62805500	0.71056000	-0.72216600
H	-6.23880300	-1.36330400	-0.88890600
H	-4.73707300	2.64362100	-0.45340300
C	-7.86888600	0.48734200	-1.51367000
H	-8.67283000	1.16082600	-1.82002800
H	-7.62194700	-0.18240500	-2.34916500
H	-8.20862500	-0.11797400	-0.66212000
O	-6.77634000	1.31607800	-1.16471700
C	-3.07872700	-2.16327500	2.44009900
N	-4.02132600	-2.44219500	3.07274000

$TS_{\mathbf{2c}(1,5)}$

Imaginary Freq = -1187.86

Charge = -1 multiplicity= 1

C	5.41078000	-2.21240100	1.08542700
C	4.06197100	-2.83085200	-0.81387800
O	0.74007100	-1.94951000	-1.80582400
C	1.80832000	-1.90545900	-1.06775100
O	3.34720000	-0.61812700	1.91806000
O	4.98119400	-3.54853300	-1.20893900
H	5.57384200	-3.25430400	1.37635200
N	4.16205000	-2.08350200	0.34158800
C	3.13949800	-1.22462300	0.86010300
N	2.85388500	-2.72134700	-1.50034100
H	5.31745600	-1.57929300	1.96605900
C	1.94641100	-1.13959000	0.07925600
C	2.66942900	-3.50852600	-2.71721900
H	3.60019200	-4.04293600	-2.89745300
H	2.43375300	-2.85057100	-3.55786700
H	1.84284700	-4.21381100	-2.59132100
H	6.25678100	-1.89462200	0.46810900
C	2.07453500	4.20606100	-1.62949800
H	1.87875800	3.78279000	-2.60986400
C	1.25507700	1.22264000	0.56377900
O	1.23274800	1.48875100	-1.81267100
C	1.55192800	1.83570200	1.73133800
C	0.82296600	-0.24123800	0.58754500
O	1.97136100	3.12389900	1.87677600
C	2.13195200	3.88629000	0.75788100
C	1.88481300	3.36644900	-0.51905000
C	1.43321000	1.96040700	-0.69135300
C	2.55745800	5.20824700	0.94158000
H	2.73882400	5.56820600	1.94949500
H	0.67621500	-0.49320500	1.64293400
C	2.73619200	6.01659000	-0.17225900
C	2.49483600	5.51709900	-1.46407500
H	3.06661500	7.04384900	-0.04006100
H	1.50849900	1.33985700	2.69233300

C	-0.66626300	-2.47186900	2.20312900
C	-0.51352600	-0.42503600	-0.17027200
H	-0.05320100	-1.26950200	-1.16366400
N	0.17307000	-2.88849700	2.90044700
C	-1.65448600	-1.08239600	0.35425500
C	-1.74908300	-2.03036800	1.38836600
H	-0.77298700	0.42039000	-0.80391000
C	-2.91857500	-0.81465600	-0.41740000
C	-3.14243100	-1.47765500	-1.63407400
C	-3.85039700	0.12482000	0.03894000
C	-4.28759700	-1.21602800	-2.37587400
H	-2.41034700	-2.20012500	-1.98143000
C	-5.00368200	0.40055700	-0.72922300
C	-5.22296000	-0.27785700	-1.92946700
H	-4.46037000	-1.73777400	-3.31344600
C	-2.99356600	-2.65365100	1.69500200
N	-4.00519300	-3.16455000	1.98265300
H	-6.10784100	-0.07678800	-2.52317000
H	2.63840400	6.15939600	-2.32888400
O	-3.58768000	0.82528500	1.19011400
O	-5.84068700	1.36344100	-0.22107300
C	-7.00068400	1.68696300	-0.96023600
H	-7.51180700	2.46752400	-0.39180700
H	-6.75238300	2.07229200	-1.95919100
H	-7.67085300	0.82256700	-1.06967800
C	-4.45342400	0.56689300	2.30250700
H	-5.45240800	0.98144000	2.13055600
H	-4.52507800	-0.50742000	2.50113800
H	-3.99145100	1.06660200	3.15794900

$TS_{\mathbf{2d}(1,5)}$

Imaginary Freq = -1196.57

Charge= -1 multiplicity= 1

C	-0.28928300	5.34188000	0.91643700
C	0.79216700	4.44421800	-1.04165800

O 1.85353100 1.14266000 -1.91227900
C 1.27219900 2.04770900 -1.18425700
O -0.35091000 2.80144400 1.93536700
O 0.83119000 5.57912500 -1.51633600
H 0.50947500 6.06842000 1.09249500
N 0.22725600 4.18585500 0.19077900
C 0.14690800 2.89629100 0.80569100
N 1.31750800 3.33841100 -1.70820800
H -0.68158100 4.96961300 1.86112800
C 0.65329600 1.80735000 0.03305000
C 1.97104000 3.54746400 -2.99854500
H 1.87813000 4.60514600 -3.23720300
H 1.49007200 2.93600700 -3.76658800
H 3.02455600 3.25980800 -2.94006200
H -1.07598100 5.83406400 0.33657500
C -4.08842100 -1.08062200 -0.77873400
H -3.79287300 -1.07787200 -1.82212300
C -0.84786200 -0.01996500 0.87028300
O -1.43140300 -0.33538100 -1.43044400
C -1.33416800 -0.02880100 2.13207200
C 0.59988900 0.41165000 0.64192000
O -2.60170600 -0.36775300 2.50236700
C -3.49070000 -0.71313900 1.53159600
C -3.12781600 -0.71800000 0.17955200
C -1.74786400 -0.34730000 -0.23997900
C -4.78456300 -1.06133600 1.94041400
H -5.02974600 -1.04328900 2.99741300
H 1.05128500 0.48417300 1.63778100
C -5.72460300 -1.41879200 0.98601600
C -5.36426300 -1.42483300 -0.37097900
H -6.73256100 -1.69152200 1.27998900
H -0.75413500 0.26724500 2.99613200
C 3.51219700 0.45049800 1.70107500
C 1.35691400 -0.66703100 -0.17145200
H 1.77779700 0.14286600 -1.21254800

N	3.61218400	1.54263300	2.10332700
C	2.49793900	-1.36419100	0.31090700
C	3.46988700	-0.88835500	1.21506300
H	0.69487200	-1.29607700	-0.76209800
C	2.72165300	-2.71914700	-0.28783300
C	3.93030600	-3.05106800	-0.91945900
C	1.69883400	-3.68035000	-0.25737900
C	4.10857100	-4.30406500	-1.50419200
H	4.72731800	-2.31580100	-0.96030900
C	1.88143900	-4.93905600	-0.82872400
H	0.75970600	-3.43581400	0.23029700
C	3.08695100	-5.25430700	-1.45796800
H	5.04924000	-4.53746800	-1.99675500
H	1.07994700	-5.67253900	-0.78395200
C	4.51308700	-1.71761100	1.72193300
N	5.37506000	-2.36362400	2.17504400
Cl	-6.57743800	-1.88483200	-1.56853700
H	3.22885800	-6.23308000	-1.91015100

$TS_{\mathbf{2e}(1,5)}$

Imaginary Freq = -1184.45

Charge= -1 multiplicity= 1

C	1.08289800	5.40119300	-1.07229000
C	-0.04886600	4.68270300	0.93121200
O	-1.45239700	1.54412200	1.91873200
C	-0.79895900	2.36154500	1.14898300
O	0.83471200	2.84360300	-2.01953300
O	0.05605500	5.82503300	1.37704100
H	0.37331600	6.21542600	-1.24603900
N	0.44948000	4.33187100	-0.30706500
C	0.36690500	3.02691500	-0.88866000
N	-0.67957300	3.66088600	1.63986700
H	1.40214200	4.96431700	-2.01682100
C	-0.25684200	2.02634400	-0.08223400
C	-1.25846100	3.97220200	2.94502300

H -1.02838600 5.01444300 3.15734600
H -0.83068000 3.31947000 3.71044600
H -2.34104500 3.81688000 2.92676900
H 1.93883200 5.80602700 -0.52370700
C 4.04619500 -1.43012300 0.90300300
H 3.72979800 -1.36908700 1.93844200
C 1.00654700 -0.00051300 -0.84531000
O 1.49069300 -0.33755300 1.47386700
C 1.51402300 -0.09822600 -2.09473300
C -0.37580300 0.61942600 -0.65751000
O 2.73673200 -0.60127500 -2.42633300
C 3.55200400 -1.03725000 -1.42764700
C 3.16126600 -0.96883100 -0.08513500
C 1.83127700 -0.41693200 0.29261400
C 4.80020700 -1.55429100 -1.79784300
H 5.06923600 -1.58949300 -2.84857800
H -0.79546200 0.72621400 -1.66348100
C 5.66569500 -2.00786900 -0.81421600
C 5.27711000 -1.94056000 0.53323500
H 6.63723500 -2.41185100 -1.07821600
H 0.99421600 0.24795900 -2.97823900
C -3.23877800 1.01988800 -1.87026600
C -1.28310900 -0.32154300 0.17123600
H -1.52526200 0.53116200 1.23096000
N -3.11722600 2.00890800 -2.47901400
C -2.56184900 -0.76940800 -0.25041800
C -3.47221100 -0.18435200 -1.14406000
H -0.73056100 -1.08425100 0.71608700
C -3.05707500 -1.98232000 0.48660100
C -3.84094000 -1.81956800 1.63846700
C -2.73631900 -3.29111500 0.10388100
C -4.28407800 -2.91391300 2.37797100
H -4.09569300 -0.80999800 1.94689800
C -3.17669900 -4.39810700 0.82961700
C -3.95214500 -4.20653400 1.97166700

H	-4.88831500	-2.75604700	3.26706600
H	-2.91087800	-5.39561300	0.49554400
C	-4.75440200	-0.76715300	-1.37393500
N	-5.80947300	-1.22108400	-1.58608400
H	-4.29468700	-5.06840600	2.53842200
Cl	6.39543200	-2.52458700	1.76868400
Cl	-1.75885300	-3.58260800	-1.33412900

$TS_{\mathbf{2f}(1,5)}$

Imaginary Freq = -1185.87

Charge = -1 multiplicity= 1

C	4.33699600	-3.23146400	1.16643600
C	2.88699700	-3.57413600	-0.72824400
O	-0.14866700	-1.99028000	-1.76347800
C	0.90274000	-2.16808700	-1.02155600
O	2.68586200	-1.19150700	1.94601600
O	3.61940900	-4.49171700	-1.09880000
H	4.25641200	-4.27499300	1.48472800
N	3.15262400	-2.83971700	0.40924000
C	2.35080500	-1.75905500	0.89904000
N	1.73612100	-3.21091300	-1.42590200
H	4.38920800	-2.57106000	2.03022900
C	1.21233300	-1.42187600	0.10491500
C	1.37816800	-3.96876300	-2.62262000
H	2.16509400	-4.70288300	-2.78442700
H	1.29500100	-3.29721000	-3.48119500
H	0.41472900	-4.46740300	-2.48220700
H	5.23447300	-3.13202900	0.54812700
C	2.57963800	3.71396300	-1.70352800
H	2.29466700	3.32901600	-2.67778400
C	1.08110500	1.04605200	0.53668400
O	1.12461400	1.26635000	-1.84397900
C	1.50708900	1.59634600	1.69566900
C	0.32343700	-0.27844600	0.58240100
O	2.21269000	2.75458400	1.82094000

C	2.55128300	3.43653100	0.68969000
C	2.19497600	2.96357000	-0.57963100
C	1.42859500	1.69877600	-0.72989500
C	3.27231600	4.62629100	0.85320700
H	3.52840500	4.95379600	1.85593600
H	0.11135900	-0.46724000	1.64023800
C	3.63910000	5.34868000	-0.27355600
C	3.29331200	4.89390400	-1.55815600
H	4.19931800	6.27305000	-0.15719900
H	1.34645100	1.14275500	2.66502600
C	-1.66362100	-2.10924500	2.17921100
C	-1.01396200	-0.16401200	-0.18864100
H	-0.76575000	-1.12408300	-1.14606300
N	-0.94487000	-2.74376300	2.84576600
C	-2.28002000	-0.50271700	0.35500800
C	-2.60909800	-1.38599900	1.39492400
H	-1.05882300	0.69978000	-0.84878200
C	-3.44242800	0.07495500	-0.40339200
C	-4.01863900	-0.66038800	-1.44981000
C	-3.96389400	1.34943600	-0.14670300
C	-5.06877900	-0.14727500	-2.20800100
H	-3.62178200	-1.64897700	-1.66075100
C	-5.01866400	1.87598200	-0.89266200
C	-5.57107800	1.12365000	-1.92761100
H	-5.49361100	-0.74014500	-3.01336900
H	-5.39707700	2.86532000	-0.65738600
C	-3.97064900	-1.64850400	1.73215600
N	-5.07467500	-1.88196300	2.03386900
H	-6.39234900	1.53353100	-2.50982600
Cl	-3.29623600	2.33804900	1.15114500
H	3.58627400	5.46798100	-2.43314300

$TS_{\mathbf{2h}(1,5)}$

Imaginary Freq = -1194.44

Charge= -1 multiplicity= 1

C	3.90462900	-4.32946500	0.43826500
C	2.32660000	-4.15040200	-1.37464300
O	-0.56298500	-2.10253000	-1.86501800
C	0.50746700	-2.51675300	-1.25597800
O	2.54001700	-2.32180900	1.70402500
O	2.92491200	-5.05362700	-1.95878200
H	3.71246200	-5.39790100	0.57402300
N	2.73901500	-3.67454000	-0.14661400
C	2.09446500	-2.63138400	0.59111200
N	1.18881700	-3.54458000	-1.90510100
H	4.08534900	-3.84932400	1.39834100
C	0.97249600	-2.02114700	-0.04771200
C	0.67007900	-4.03179700	-3.18146400
H	1.35108600	-4.80600700	-3.52949900
H	0.61801000	-3.21227000	-3.90309900
H	-0.33649400	-4.43885400	-3.05023200
H	4.77200200	-4.22008100	-0.21981900
C	2.98268800	3.16853900	-0.74453800
H	2.65667800	3.04739600	-1.77169500
C	1.16391200	0.28858500	0.91202500
O	1.24211700	1.01865300	-1.36712800
C	1.65800700	0.51679100	2.14990600
C	0.24146600	-0.91003300	0.69586400
O	2.50287800	1.52640600	2.50460000
C	2.92426500	2.38865100	1.53982800
C	2.51294100	2.25041800	0.20887100
C	1.59227800	1.15125100	-0.19354600
C	3.78851200	3.41887400	1.93252200
H	4.08757600	3.49260000	2.97310600
H	0.01281700	-1.29649400	1.69562000
C	4.24523800	4.32029300	0.98323300
C	3.83491600	4.18471400	-0.35264100
H	4.91546800	5.12542000	1.26493000
H	1.44531900	-0.11510500	3.00206000
C	-1.96731600	-2.76830200	1.81461300

C	-1.07762400	-0.45457300	0.02510600
H	-1.02946400	-1.30071800	-1.07577600
N	-1.36600300	-3.73545900	2.07533400
C	-2.35917200	-0.60564700	0.62116800
C	-2.76641900	-1.63087800	1.50280400
H	-0.97332000	0.47489100	-0.52990100
C	-3.39425500	0.38282100	0.18925800
C	-4.64165700	-0.02074600	-0.30247600
C	-3.12693700	1.76352300	0.23364500
C	-5.59335900	0.90388500	-0.73570100
H	-4.87287900	-1.07908100	-0.36157400
C	-4.06790900	2.69710500	-0.17875200
H	-2.16855200	2.10422000	0.61384600
C	-5.30962200	2.27164500	-0.66911100
H	-6.54239700	0.54525700	-1.11794400
H	-3.86400400	3.76254900	-0.13035300
C	-7.44487100	2.88605900	-1.54148600
H	-7.96675700	3.81611200	-1.77869900
H	-7.36988200	2.27297500	-2.45032100
H	-8.01804400	2.33199900	-0.78558700
O	-6.17011400	3.26566900	-1.05806100
C	-4.03254000	-1.61988600	2.15723700
N	-5.05331200	-1.64508800	2.72618800
Cl	4.42830300	5.34500800	-1.54397700

$TS_{\mathbf{2i}(1,5)}$

Imaginary Freq = -1185.07

Charge= -1 multiplicity= 1

C	-3.55277700	4.65050000	1.09059700
C	-2.06556400	4.62464000	-0.80632700
O	0.53670600	2.38191200	-1.80449900
C	-0.44411300	2.80776500	-1.06632100
O	-2.39597400	2.30905500	1.91394300
O	-2.57672200	5.67397500	-1.19725900
H	-3.24251800	5.65639400	1.38823200

N	-2.48525700	3.99087200	0.34542800
C	-1.94236700	2.76975100	0.85909300
N	-1.02605500	4.00031200	-1.49440300
H	-3.74925600	4.03575500	1.96720200
C	-0.90534400	2.17472400	0.07731500
C	-0.51258200	4.63416400	-2.70671000
H	-1.11419600	5.52377500	-2.88268200
H	-0.58802800	3.94468300	-3.55170400
H	0.53929900	4.90449300	-2.57689600
H	-4.45055400	4.73989500	0.47124300
C	-3.36418400	-2.56785600	-1.63710000
H	-3.00262800	-2.27680900	-2.61841200
C	-1.31819800	-0.24994300	0.55646600
O	-1.41495500	-0.49999400	-1.82174800
C	-1.85780000	-0.66884700	1.72247400
C	-0.28709300	0.87517800	0.58254700
O	-2.80397500	-1.64276700	1.86559700
C	-3.27884400	-2.25411500	0.74772500
C	-2.82547100	-1.89662300	-0.52805900
C	-1.80092700	-0.83304400	-0.70002200
C	-4.24325900	-3.25338500	0.93556800
H	-4.57441400	-3.50523000	1.93607700
H	-0.04461100	1.03476800	1.63825400
C	-4.74551800	-3.88950400	-0.18776500
C	-4.31885200	-3.56097400	-1.48367800
H	-1.60534000	-0.24346700	2.68471200
C	2.02609400	2.22877100	2.19430900
C	0.99413900	0.45527300	-0.17622700
H	0.95066600	1.42335400	-1.16809600
N	1.45138700	2.97510000	2.88493700
C	2.30696400	0.54218100	0.35113300
C	2.80653900	1.35196500	1.38600300
H	0.85657400	-0.41621700	-0.81259200
C	3.32490000	-0.25715500	-0.41679300
C	3.82691800	0.23958000	-1.62967900

C	3.73905600	-1.51388200	0.03948900
C	4.74009600	-0.50289400	-2.36791100
H	3.49498000	1.21314700	-1.97689400
C	4.65391400	-2.27230700	-0.72475200
C	5.15822100	-1.75994700	-1.92149300
H	5.13205400	-0.11075600	-3.30261200
C	4.19695000	1.36066400	1.69919700
N	5.32876900	1.37137000	1.99211800
H	5.86468500	-2.33231700	-2.51242600
H	-4.73515600	-4.08069400	-2.33965000
O	3.18612200	-2.02672300	1.18680400
O	4.97306900	-3.50723600	-0.21664000
C	5.87288700	-4.31161100	-0.95186600
H	5.98054400	-5.23872800	-0.38406600
H	5.48485800	-4.54500100	-1.95331800
H	6.85787000	-3.83475700	-1.05481100
C	4.07039300	-2.17716600	2.30462800
H	4.78808100	-2.98665300	2.13452800
H	4.60384200	-1.24326500	2.50951300
H	3.43082900	-2.42705000	3.15514300
Cl	-5.95992600	-5.15177000	0.01718000

Table 8: Thermodynamic parameters for TS_2 [1,3]-H shift at b3lyp/6-31g (d) level of theory

TS_2	G	H	S	E
$TS_2\mathbf{a}_{(1,3)}$	-1635.123209	-1635.025868	204.872	-1635.464297
$TS_2\mathbf{b}_{(1,3)}$	-1749.616354	-1749.512902	217.733	-1749.986732
$TS_2\mathbf{c}_{(1,3)}$	-1864.1001	-1863.990439	135.744	-1864.499223
$TS_2\mathbf{d}_{(1,3)}$	-2094.731953	-2094.631114	212.234	-2095.061080
$TS_2\mathbf{e}_{(1,3)}$	-2554.337112	-2554.232564	220.040	-2554.653795
$TS_2\mathbf{f}_{(1,3)}$	-2094.726194	-2094.624718	213.574	-2095.054321
$TS_2\mathbf{h}_{(1,3)}$	-2209.225070	-2209.118171	224.988	-2209.583545
$TS_2\mathbf{i}_{(1,3)}$	-2323.709051	-2323.595966	238.009	-2324.096278

$TS_{\mathbf{2a}(1,3)}$

Imaginary Freq = -1582.98

Charge= -1 multiplicity= 1

C 0.63096200 4.65119000 -1.99490300

C 1.59206600 4.04373000 0.13966300

O 1.58349000 0.99250000 2.00777900

C 1.26525700 1.78910700 1.12456800

O -0.41276300 2.11989000 -2.11560700

O 2.09855200 5.16114200 0.19620800

H 0.21540300 5.57611300 -1.58626500

N 0.79374800 3.66303600 -0.93122000

C 0.20644900 2.38520400 -1.08353900

N 1.79150100 3.10390800 1.14015500

H -0.04045600 4.21650200 -2.73280400

C 0.30072300 1.50196500 0.07239400

C 2.66804500 3.50339200 2.23845200

H 3.67668900 3.71193000 1.86857600

H 2.68957000 2.67553400 2.94472600

H 2.28341000 4.40979100 2.71323300

H 1.59690300 4.88345700 -2.45358500
C 4.30816600 -2.14983500 -1.15911800
H 4.57069900 -1.31059100 -1.79569600
C 0.87616500 -1.05212000 0.03223700
O 2.43106300 -0.01085600 -1.44483700
C 0.64766800 -2.13948100 0.79984500
C -0.16331200 0.03567900 -0.11296200
O 1.49658200 -3.19344000 0.96058200
C 2.69486900 -3.17401500 0.31024600
C 3.05918100 -2.10380700 -0.51700900
C 2.13939600 -0.95650200 -0.71023000
C 3.54312200 -4.27186800 0.50382100
H 3.22105000 -5.07859900 1.15469300
H -0.55965800 -0.00958600 -1.13104200
C 4.77161800 -4.29188800 -0.14120300
C 5.15899700 -3.22911700 -0.97634600
H 5.43769300 -5.13863900 0.00399900
H -0.25094200 -2.28463900 1.38619000
C -3.06708000 -0.47626600 3.15666100
C -1.31138600 0.05387800 0.91042200
N -2.69122200 -0.41083600 4.26141600
C -2.63990200 -0.40716900 0.71970500
C -3.52555800 -0.57302000 1.81327700
H -0.94947000 0.02050000 1.93991600
C -3.16329000 -0.70664400 -0.64542500
C -3.77598700 -1.94585800 -0.90197900
C -3.05304000 0.21417700 -1.70023200
C -4.25718300 -2.25760800 -2.17184700
H -3.86693300 -2.66872500 -0.09721700
C -3.53901300 -0.09904700 -2.97000600
H -2.57291100 1.17240100 -1.53852700
C -4.14257500 -1.33339300 -3.21212900
H -4.72396300 -3.22400000 -2.34668900
H -3.43694100 0.62860300 -3.77088400
C -4.92544300 -0.77603900 1.66544400

N	-6.07881200	-0.95115500	1.58890700
H	-0.96988300	1.45456600	0.73331700
H	6.12396500	-3.25623700	-1.47527900
H	-4.51960400	-1.57480800	-4.20331600

$TS_{\mathbf{2b}(1,3)}$

Imaginary Freq = -1586.33

Charge= -1 multiplicity= 1

C	-1.47473100	-4.24037400	-2.57252100
C	-2.75133600	-3.65319800	-0.60403500
O	-2.54961900	-0.89667000	1.66742200
C	-2.20654700	-1.64929800	0.75546100
O	0.06011900	-2.02030000	-2.09886100
O	-3.47314000	-4.62339600	-0.81883000
H	-1.35792500	-5.27340100	-2.23431200
N	-1.67098400	-3.35742600	-1.42517300
C	-0.81801500	-2.24088600	-1.26254100
N	-2.97748000	-2.80213500	0.46760700
H	-0.58023600	-3.89725500	-3.08865000
C	-0.99039100	-1.48455100	-0.02821800
C	-4.14286500	-3.10029800	1.29651200
H	-5.06199300	-3.03020800	0.70660300
H	-4.15554200	-2.36809300	2.10171900
H	-4.06855800	-4.11549300	1.69498500
H	-2.33839800	-4.19541800	-3.24290100
C	-3.79611400	3.09867000	-1.45962800
H	-4.07015800	2.41449100	-2.25668600
C	-1.01635700	1.12335700	0.20591200
O	-2.37209300	0.62918100	-1.69188400
C	-0.75470500	2.04127600	1.16130500
C	-0.21100100	-0.15200000	0.10480300
O	-1.38858900	3.23868900	1.31005200
C	-2.38674700	3.56356400	0.43992600
C	-2.76087500	2.69963400	-0.59741000
C	-2.07083000	1.39920000	-0.77794700

C	-3.01892100	4.79949300	0.62759700
H	-2.69807100	5.43685800	1.44553200
H	0.40366800	-0.09128200	-0.79735400
C	-4.03923000	5.16897300	-0.23734000
C	-4.43196100	4.31838300	-1.28579500
H	-4.53721500	6.12530200	-0.09876400
H	-0.00288300	1.91293000	1.92982400
C	1.90272300	-0.60356400	3.93153300
C	0.64996300	-0.53813400	1.31935000
N	1.27614800	-0.66742000	4.91624400
C	2.05117900	-0.37031000	1.47001600
C	2.67146800	-0.50813600	2.73820800
H	0.07814300	-0.53136600	2.24929300
C	2.92662800	-0.07261200	0.30144100
C	3.85225500	0.97851400	0.36696600
C	2.86031600	-0.80993200	-0.89645100
C	4.68222700	1.29727200	-0.70854300
H	3.92270400	1.56826700	1.27535100
C	3.68501000	-0.50674200	-1.97199400
H	2.15079600	-1.62292600	-0.99937100
C	4.60332600	0.54686700	-1.88587800
H	5.37978000	2.12168200	-0.61147300
H	3.62791200	-1.07832200	-2.89307000
C	6.32881300	1.80543500	-2.95117200
H	6.83278500	1.79944200	-3.92067100
H	5.85704900	2.78618600	-2.79705700
H	7.07043800	1.64055900	-2.15725700
O	5.37289900	0.76456300	-3.00068500
C	4.07726400	-0.62864200	2.91635500
N	5.22681700	-0.72298000	3.10839700
H	0.07919000	-1.79927900	0.86752500
H	-5.23289100	4.61875900	-1.95596900

$TS_{\mathbf{2d}(1,3)}$

Imaginary Freq = -1584.29

Charge= -1 multiplicity= 1

C	-0.95294300	4.65889900	-2.13731600
C	-0.04852600	4.41240200	0.09254600
O	0.63501100	1.53935900	2.11255900
C	0.18077800	2.18912400	1.17017000
O	-1.24062300	1.93256100	-2.19610200
O	0.12082600	5.62797200	0.12640200
H	-1.64384800	5.44106200	-1.81180900
N	-0.61534500	3.78974600	-1.01230200
C	-0.81161300	2.39498200	-1.13742900
N	0.31989200	3.59752100	1.15350300
H	-1.40936200	4.03021500	-2.89932100
C	-0.57901700	1.61188000	0.07034400
C	0.95821700	4.26086900	2.28815200
H	1.89589400	4.73276400	1.97902500
H	1.15101900	3.49481900	3.03686400
H	0.29936800	5.03677700	2.68649700
H	-0.05341000	5.13979800	-2.53325000
C	4.35501600	-0.83259600	-0.64432800
H	4.44186200	0.01777800	-1.31155600
C	0.66818200	-0.68455300	0.22126800
O	2.01021000	0.68372800	-1.19933500
C	0.67600400	-1.76194500	1.03578000
C	-0.61045300	0.06928500	-0.06495000
O	1.76235600	-2.53420200	1.32517800
C	2.96068200	-2.21035600	0.76751500
C	3.09367100	-1.11592400	-0.09548600
C	1.91734800	-0.27320600	-0.43026700
C	4.05736200	-3.02011300	1.09031600
H	3.91723400	-3.85894400	1.76432000
H	-0.88845800	-0.11984800	-1.10548000
C	5.29821700	-2.73080500	0.54397500
C	5.43476200	-1.63437600	-0.32262600
H	6.16117700	-3.34370900	0.78147200
H	-0.19722900	-2.12599400	1.56191900

C	-3.52093200	-1.13057700	3.00742400
C	-1.80383200	-0.19477000	0.86820300
N	-3.26596700	-0.93283000	4.13072200
C	-2.93307500	-1.01416200	0.60686100
C	-3.82509300	-1.38840600	1.64156500
H	-1.53643100	-0.09196100	1.92170800
C	-3.23780000	-1.48753900	-0.77515600
C	-3.46259000	-2.85522100	-1.01136900
C	-3.29660000	-0.60364600	-1.86507300
C	-3.73122100	-3.32543700	-2.29512000
H	-3.41882800	-3.55104600	-0.17927100
C	-3.56937700	-1.07656900	-3.14899000
H	-3.11408800	0.45462400	-1.71830100
C	-3.78796200	-2.43660400	-3.37042800
H	-3.89823300	-4.38812400	-2.45353900
H	-3.60438900	-0.37304300	-3.97666100
C	-5.09790100	-1.97777900	1.40554500
N	-6.14785700	-2.46957800	1.25639400
Cl	7.02425100	-1.28705600	-1.00720300
H	-1.84009900	1.24048500	0.63783600
H	-3.99954800	-2.80220100	-4.37260100

$TS_{\mathbf{2e}(1,3)}$

Imaginary Freq = -1567.49

Charge= -1 multiplicity= 1

C	0.58139500	4.82056100	2.17479300
C	-0.40512500	4.57237500	-0.01982400
O	-0.98151100	1.71514100	-2.09764300
C	-0.53666500	2.36823600	-1.15259200
O	1.05610100	2.11696200	2.13795800
O	-0.65442700	5.77463600	-0.01119300
H	1.21509800	5.64836700	1.84519000
N	0.24968400	3.96039700	1.04146200
C	0.54316600	2.57866400	1.11740300
N	-0.76531200	3.76360400	-1.08866100

H	1.10114900	4.20053300	2.90267300
C	0.29771800	1.81382300	-0.09855400
C	-1.49052600	4.41430300	-2.17733900
H	-2.44229300	4.81702400	-1.81762800
H	-1.66572200	3.65718000	-2.93938200
H	-0.89901000	5.24091200	-2.57948300
H	-0.32773400	5.24034900	2.61555200
C	-4.44448800	-0.95666900	0.63249000
H	-4.57763200	-0.12079300	1.31031200
C	-0.78780900	-0.55989000	-0.27858800
O	-2.19283400	0.69633000	1.18396000
C	-0.73421400	-1.62955500	-1.10174700
C	0.44012000	0.27616900	-0.00253400
O	-1.77184400	-2.46762100	-1.38485600
C	-2.98166500	-2.22705200	-0.81052400
C	-3.17438600	-1.15239600	0.06592700
C	-2.05047900	-0.23998000	0.39695900
C	-4.02776700	-3.10267000	-1.12933100
H	-3.84177100	-3.92438600	-1.81323100
H	0.75973700	0.08746500	1.02707100
C	-5.27794600	-2.89951900	-0.56570800
C	-5.47424300	-1.82293600	0.31420400
H	-6.10239600	-3.56459600	-0.79963200
H	0.15687200	-1.93870900	-1.63265900
C	3.65959600	-0.43730600	-2.99353200
C	1.63502400	0.11904500	-0.95755500
N	3.48715400	-0.16195300	-4.11585700
C	2.84023200	-0.56662600	-0.67058100
C	3.85704200	-0.77188400	-1.62565800
H	1.36424700	0.19826200	-2.01221700
C	3.11781400	-1.02277000	0.72909400
C	3.04912700	-2.37038300	1.11553100
C	3.46027500	-0.08811000	1.71904100
C	3.32573800	-2.77824200	2.41963800
C	3.73594500	-0.47992500	3.02710700

H	3.48556000	0.96255900	1.45379700
C	3.67570900	-1.82786900	3.37720500
H	3.26159800	-3.83096100	2.67402300
H	3.98874400	0.27132700	3.76944000
C	5.13522200	-1.28943600	-1.28067500
N	6.19348600	-1.71195100	-1.02133400
Cl	-7.07453500	-1.58552100	1.02052300
H	1.56793700	1.53817700	-0.71772300
H	3.89058600	-2.14492100	4.39438300
Cl	2.57178200	-3.61517300	-0.04190200

$TS_{\mathbf{2f}(1,3)}$

Imaginary Freq = -1578.81

Charge= -1 multiplicity= 1

C	-0.54515900	4.52267300	-1.81685300
C	0.66118900	4.20797400	0.25631100
O	1.64779100	1.26926900	2.04977000
C	1.06261900	1.94793200	1.20374100
O	-0.77679300	1.79072300	-1.95486500
O	0.82112800	5.42454000	0.31753500
H	-1.18301000	5.28838000	-1.36769900
N	-0.04530800	3.62000800	-0.78334700
C	-0.23537700	2.22502800	-0.93969700
N	1.18496600	3.35902000	1.22224000
H	-1.10656900	3.91487800	-2.52394000
C	0.16387600	1.40679700	0.19918900
C	1.96627700	3.98900500	2.28300100
H	2.84218500	4.49575000	1.86618800
H	2.27674700	3.19645000	2.96149900
H	1.35847900	4.73217800	2.80608000
H	0.28471100	5.02325900	-2.32560400
C	4.93238600	-1.01433300	-1.32726300
H	4.92289200	-0.12828100	-1.95440100
C	1.40304500	-0.89673800	0.06625800
O	2.53640900	0.53919800	-1.46349600

C	1.52090800	-2.01348200	0.81674200
C	0.10481400	-0.12541400	0.00577200
O	2.62970200	-2.80174500	0.90635100
C	3.74013000	-2.45233600	0.19598200
C	3.75550800	-1.31453900	-0.62078500
C	2.55135100	-0.45596000	-0.73794700
C	4.86190500	-3.28246300	0.31717600
H	4.80630800	-4.15321700	0.96286400
H	-0.32955500	-0.26032600	-0.99007900
C	6.01202900	-2.96273100	-0.39051500
C	6.05123000	-1.82565300	-1.21657300
H	6.88854800	-3.59954200	-0.30161400
H	0.73158900	-2.40113800	1.44860700
C	-2.57807700	-1.53424200	3.26435100
C	-0.94766300	-0.44039900	1.08052900
N	-2.24071100	-1.46259300	4.38071200
C	-2.14669600	-1.15825200	0.86375300
C	-2.97397700	-1.63335800	1.90177400
H	-0.54881000	-0.45777200	2.09625700
C	-2.60536100	-1.41273500	-0.54104700
C	-3.41644500	-0.52202500	-1.25843200
C	-2.20860000	-2.59223200	-1.18905700
C	-3.80832300	-0.78668400	-2.57083000
C	-2.59343800	-2.87069500	-2.49852700
H	-1.58562400	-3.29485800	-0.64297500
C	-3.39424000	-1.96282100	-3.19152200
H	-4.43053300	-0.06881600	-3.09430800
H	-2.26867900	-3.79228700	-2.97382200
C	-4.23582300	-2.24000200	1.65429300
N	-5.26781500	-2.75860600	1.47575500
H	-1.00845700	0.98646400	0.94415900
H	-3.69892400	-2.16535500	-4.21494200
Cl	-3.98716200	0.96324100	-0.51177400
H	6.95810600	-1.58543400	-1.76490700

$TS_{\mathbf{2h}(1,3)}$

Imaginary Freq = -1588.81

Charge= -1 multiplicity= 1

C	-0.06631500	4.35717600	-2.94345900
C	1.12053300	4.42262800	-0.83664800
O	1.56664100	1.99642800	1.75468800
C	1.09663100	2.50271400	0.73525800
O	-0.86826500	1.82095700	-2.27977900
O	1.51923500	5.54632300	-1.12968500
H	-0.53518200	5.32598100	-2.75206100
N	0.27746700	3.70957800	-1.67948600
C	-0.19557100	2.40153300	-1.42578100
N	1.49301000	3.80553400	0.34896300
H	-0.75003900	3.69149300	-3.46651200
C	0.07499200	1.87680400	-0.09247400
C	2.41776200	4.54784800	1.20257100
H	3.36792100	4.71458800	0.68584200
H	2.57601100	3.94804100	2.09687000
H	1.99111900	5.52136400	1.45743700
H	0.83224500	4.52449000	-3.54495000
C	4.28588600	-1.69248100	-0.70371500
H	4.42161800	-1.05591500	-1.57103300
C	0.87901600	-0.54395800	0.49550800
O	2.20754600	0.13716000	-1.36529000
C	0.81628200	-1.38308100	1.55202000
C	-0.26557300	0.38820000	0.16893200
O	1.77162100	-2.28962500	1.90733000
C	2.90393300	-2.37263300	1.15728500
C	3.09858000	-1.55915300	0.03451600
C	2.06202100	-0.57625100	-0.37247000
C	3.86763000	-3.30923500	1.55323000
H	3.68353200	-3.92131400	2.43017900
H	-0.73364300	0.03610600	-0.75440400
C	5.03661700	-3.43183100	0.81813300
C	5.23441400	-2.61804600	-0.30898400

H	5.79684900	-4.14943600	1.10770800
H	-0.01316600	-1.41627100	2.24683900
C	-2.78303200	0.52501700	3.76309300
C	-1.32382200	0.60723700	1.26287400
N	-2.30369600	0.87962600	4.76844000
C	-2.61141600	0.01510800	1.34600600
C	-3.36514800	0.07387500	2.54572200
H	-0.87640400	0.88241300	2.21991200
C	-3.23054500	-0.66213100	0.17215500
C	-3.79131200	-1.93962600	0.31244800
C	-3.27265800	-0.06759600	-1.10372600
C	-4.37067400	-2.61194000	-0.76428900
H	-3.76915600	-2.42593500	1.28246700
C	-3.85170300	-0.72351900	-2.18215200
H	-2.84035100	0.91331500	-1.26423500
C	-4.40709100	-1.99887100	-2.02069500
H	-4.78827700	-3.60016000	-0.60733900
H	-3.87986800	-0.25993500	-3.16326500
C	-5.54861200	-3.83904900	-3.02432100
H	-5.92965700	-4.09048200	-4.01699600
H	-4.81787800	-4.60003000	-2.71607200
H	-6.38129200	-3.83634500	-2.30736700
O	-4.95623100	-2.56047200	-3.14507300
C	-4.74998700	-0.24161700	2.62032500
N	-5.88545700	-0.49889300	2.72764600
Cl	6.73007200	-2.79361700	-1.23001800
H	-1.12429700	1.92971300	0.68265300

$TS_{\mathbf{2i}(1,3)}$

Imaginary Freq = -1572.31

Charge= -1 multiplicity= 1

C	0.87830200	-4.73580900	2.75009000
C	1.89390600	-4.49592700	0.56820800
O	1.78102500	-1.87772100	-1.87008400
C	1.47722300	-2.50701200	-0.85529800

O -0.31814300 -2.30074700 2.33100600
O 2.46805100 -5.56638100 0.75006400
H 0.52767300 -5.74624400 2.52294100
N 1.02812600 -3.96767700 1.51691600
C 0.35982100 -2.72576200 1.39466200
N 2.08165600 -3.75974100 -0.59314700
H 0.15727000 -4.20483900 3.36876100
C 0.45694200 -2.08533900 0.08985900
C 3.03005800 -4.30623200 -1.56035900
H 2.72023900 -5.30999200 -1.86296100
H 4.03011200 -4.37396500 -1.12122200
H 3.03805500 -3.63024900 -2.41342000
H 1.83723700 -4.81592100 3.27107200
C 4.24535000 1.92405600 0.42966600
H 4.61697300 1.19358200 1.13970600
C 0.83853600 0.47037300 -0.36557700
O 2.54734000 -0.24123700 1.14455400
C 0.46831800 1.44775000 -1.22291800
C -0.11447600 -0.65607200 -0.03558800
O 1.22235800 2.53218000 -1.56561000
C 2.46170700 2.66422300 -1.02157800
C 2.96157800 1.73045600 -0.10593500
C 2.14186300 0.56041900 0.30225300
C 3.21722300 3.77846200 -1.41007500
H 2.79738600 4.48117300 -2.12250300
H -0.56811400 -0.45072500 0.93907600
C 4.48438000 3.95863400 -0.87743700
C 4.98768400 3.02435600 0.04199800
H 5.08698200 4.81345400 -1.16551300
H -0.49207300 1.48107500 -1.72142200
C -3.16264900 -1.37678600 -3.20794900
C -1.21800500 -0.96706700 -1.06024300
N -2.85327800 -1.82292700 -4.24267000
C -2.57468600 -0.59006900 -0.93988500
C -3.53344500 -0.83221800 -1.94779700

H	-0.84021100	-1.11624000	-2.07378700
C	-3.05400300	0.04203100	0.33200600
C	-3.25136200	1.42878900	0.38542000
C	-3.28075800	-0.73235100	1.48048400
C	-3.67937900	2.03495400	1.58638000
C	-3.71967300	-0.13224900	2.65400400
H	-3.09062000	-1.79913800	1.44778700
C	-3.92597500	1.24844600	2.71319400
H	-3.89202000	-0.73686500	3.53979900
C	-4.91402000	-0.55688300	-1.76471800
N	-6.05248400	-0.31625600	-1.64288900
H	-4.25756700	1.70241400	3.64040500
O	-2.93314800	2.19252700	-0.71404000
O	-3.80598200	3.40174200	1.55338000
C	-4.02288300	2.86029200	-1.36523100
H	-4.83495400	2.15980100	-1.58433400
H	-4.39741400	3.68768800	-0.75429200
H	-3.61399100	3.24972900	-2.30111700
C	-4.20142500	4.05717100	2.74200000
H	-3.48595200	3.88512200	3.55800600
H	-4.22494000	5.12309500	2.50380700
H	-5.20044800	3.73885100	3.07165200
H	-0.79626900	-2.26388200	-0.60446700
Cl	6.60362300	3.27597500	0.70838700

Table 9: Thermodynamic parameters for Intermediates **2a-2i** [1,5]-H shift at b3lyp/6-31g (d) level of theory

Intermediate 2	G	H	S	E
$In_{\mathbf{2a(1,5)}}$	-1635.152843	-1635.055477	204.925	-1635.499014
$In_{\mathbf{2b(1,5)}}$	-1749.645945	-1749.542549	217.615	-1750.021444
$In_{\mathbf{2c(1,5)}}$	-1864.128884	-1864.018688	231.927	-1864.532504
$In_{\mathbf{2d(1,5)}}$	-2094.761620	-2094.660705	212.393	-2095.095734
$In_{\mathbf{2e(1,5)}}$	-2554.367744	-2554.262190	222.157	-2554.688497
$In_{\mathbf{2f(1,5)}}$	-2094.759179	-2094.656926	215.210	-2095.091712
$In_{\mathbf{2h(1,5)}}$	-2209.254564	-2209.147783	224.739	-2209.618201
$In_{\mathbf{2i(1,5)}}$	-2323.737784	-2323.624043	239.388	-2324.129359

$In_{\mathbf{2a}(1,5)}$

Charge= -1 multiplicity= 1

C -3.26333000 4.00897100 1.05982700

C -1.83395800 3.89698900 -0.87731600

O 0.73549100 1.63039700 -1.88281500

C -0.24468500 2.06855000 -1.09717500

O -2.10526900 1.68405600 1.92684700

O -2.34610200 4.93323400 -1.29504800

H -2.92470900 5.01675800 1.31562600

N -2.22766900 3.30658800 0.30609600

C -1.68150400 2.10609500 0.84864600

N -0.81679000 3.23789300 -1.56882900

H -3.44652600 3.42716900 1.96106600

C -0.66350000 1.46381400 0.05846100

C -0.31948800 3.83627300 -2.80817100

H -0.91418600 4.72951000 -2.98758400

H -0.42716200 3.13217500 -3.63735100

H 0.73736700 4.09636100 -2.70518200

H -4.17461700 4.09416400 0.46069400

C -3.18618100 -3.26830600 -1.49981600
H -2.84045400 -2.98382700 -2.48879700
C -1.10907800 -0.92681300 0.64151400
O -1.23787700 -1.19498400 -1.72938400
C -1.62835000 -1.33233000 1.82160800
C -0.05516100 0.17909200 0.62321000
O -2.56606900 -2.30616000 1.98939200
C -3.06055200 -2.93253400 0.88352200
C -2.63063200 -2.58595100 -0.40413200
C -1.61087300 -1.52392300 -0.60023500
C -4.01867900 -3.93294400 1.09187300
H -4.32358300 -4.16759600 2.10686600
H 0.17969200 0.40460000 1.66984000
C -4.55037800 -4.59191100 -0.00759100
C -4.13519000 -4.26103600 -1.30953300
H -5.29477700 -5.36952200 0.14371000
H -1.35694900 -0.89702500 2.77464800
C 2.24835100 1.87441500 1.79961900
C 1.21339500 -0.35499000 -0.03826600
N 1.67602500 2.85081000 2.10300400
C 2.50670400 -0.21307000 0.42961900
C 2.98189400 0.72595700 1.41260300
H 1.05522500 -1.10101500 -0.81089500
C 3.52818100 -1.11462300 -0.20012900
C 4.73658100 -0.60876800 -0.70584500
C 3.28225400 -2.49086200 -0.32729400
C 5.65876300 -1.44769100 -1.32935700
H 4.94434600 0.45213100 -0.61089700
C 4.20661100 -3.33364700 -0.94511800
H 2.35881600 -2.89621500 0.07585500
C 5.39876800 -2.81447200 -1.45187900
H 6.58476700 -1.03183100 -1.71964500
H 3.99649100 -4.39799500 -1.02508500
C 4.23565400 0.56675300 2.05624000
N 5.26219600 0.45707000 2.61005800

H 6.12167100 -3.46924800 -1.93346900

H 1.15211700 0.84839500 -1.40037500

H -4.55895800 -4.78409100 -2.16256900

$In_{\mathbf{2b}(1,5)}$

Charge= -1 multiplicity= 1

C 4.92172900 -2.88105300 0.60914400

C 3.33497100 -3.17626400 -1.18047100

O 0.09667400 -1.81235000 -1.81556800

C 1.24158700 -1.93764800 -1.15008300

O 3.19307700 -1.06609500 1.71109900

O 4.09776700 -3.98729700 -1.70122000

H 4.94161500 -3.95004900 0.83864300

N 3.64644900 -2.52204800 -0.00621100

C 2.81284500 -1.56997500 0.65186300

N 2.09694500 -2.85436300 -1.73776700

H 5.00833600 -2.29300500 1.52074400

C 1.57013000 -1.26012600 -0.00557200

C 1.68325900 -3.54870300 -2.95753300

H 2.50532300 -4.20192900 -3.24260900

H 1.47560800 -2.82642400 -3.75128700

H 0.77857400 -4.13372900 -2.77158800

H 5.74650400 -2.66094700 -0.07492400

C 2.33113000 4.06962800 -1.49255700

H 1.99519900 3.71912600 -2.46355300

C 1.30876000 1.13170900 0.67673300

O 1.11419900 1.49463000 -1.67720400

C 1.78999000 1.64630600 1.83012100

C 0.65314200 -0.24831000 0.68371100

O 2.38996900 2.86093600 1.97439300

C 2.55277200 3.64291100 0.86910900

C 2.12736500 3.21540400 -0.39550400

C 1.47512800 1.89183900 -0.56624100

C 3.16675400 4.88842700 1.05354700

H 3.48189100 5.17815600 2.05104000

H	0.60446500	-0.56620600	1.73164300
C	3.35485600	5.71305600	-0.04660800
C	2.93697800	5.30553300	-1.32575300
H	3.83051700	6.68146400	0.08624900
H	1.76279600	1.12064700	2.77583600
C	-0.88688100	-2.61691700	1.93837700
C	-0.77760800	-0.12033400	0.16487900
N	-0.01927400	-3.38482700	2.11346000
C	-1.91169300	-0.66311400	0.74127600
C	-1.96784100	-1.73107600	1.70712900
H	-0.93357800	0.65585100	-0.57805400
C	-3.21907000	-0.10183600	0.26996300
C	-4.28126400	-0.93100200	-0.11131700
C	-3.41294600	1.28727100	0.16696700
C	-5.48618600	-0.41096700	-0.58775900
H	-4.16272100	-2.00721000	-0.04032900
C	-4.60740000	1.82284200	-0.29918600
H	-2.61104000	1.95234500	0.47344400
C	-5.65349100	0.97426200	-0.68120000
H	-6.27854900	-1.09277800	-0.87638300
H	-4.75601300	2.89667700	-0.36688500
C	-3.12733700	-1.97948200	2.48494700
N	-4.06830300	-2.20438100	3.14595200
H	-0.48948000	-1.21344000	-1.25182300
O	-6.79556400	1.59441300	-1.12850100
C	-7.89161300	0.77646900	-1.48686700
H	-8.69116200	1.45708500	-1.79008000
H	-7.64801100	0.11114900	-2.32734800
H	-8.23804500	0.16542900	-0.64184000
H	3.08968700	5.96012000	-2.17959400

$In_{\mathbf{2c}(1,5)}$

Charge= -1 multiplicity= 1

C	5.14428600	-2.61100400	1.18605400
C	3.83441700	-3.00985400	-0.79765300

O 0.67506400 -1.77608500 -1.92088000
C 1.70843400 -1.86152600 -1.08939700
O 3.21706700 -0.83639500 1.98324600
O 4.69559100 -3.79462200 -1.18948500
H 5.18881400 -3.67608300 1.42917300
N 3.94942300 -2.32614600 0.39527500
C 2.99642900 -1.39466700 0.90724000
N 2.67664500 -2.74826000 -1.53192100
H 5.07148100 -2.01367000 2.09282300
C 1.83355200 -1.17066300 0.08783600
C 2.47956800 -3.45951800 -2.79527500
H 3.36080400 -4.07873000 -2.94955700
H 2.36395700 -2.74648500 -3.61568600
H 1.58175200 -4.08148900 -2.74433700
H 6.04408100 -2.34937400 0.62130900
C 2.40271900 4.11782300 -1.61253200
H 2.18921400 3.69915200 -2.59114200
C 1.34656100 1.22763800 0.60364500
O 1.37755600 1.45788900 -1.77380500
C 1.67341300 1.82857100 1.76908500
C 0.78561600 -0.19118000 0.62185600
O 2.18294300 3.08478900 1.90446600
C 2.40868100 3.82141900 0.77928900
C 2.14105700 3.30614600 -0.49576500
C 1.59380100 1.93476400 -0.65670500
C 2.92369200 5.11227800 0.95461800
H 3.11722700 5.47025900 1.96092200
H 0.65711000 -0.45889500 1.67596300
C 3.17189900 5.89343700 -0.16518000
C 2.91181800 5.39782000 -1.45494800
H 3.57142300 6.89659600 -0.03937300
H 1.57808000 1.34980000 2.73513000
C -0.71680600 -2.53958100 2.02542100
C -0.58509600 -0.21336200 -0.05696900
N 0.14865100 -3.00519200 2.66269100

C -1.68750600 -0.95379700 0.31856800
C -1.79763800 -2.02584600 1.26539300
H -0.77615100 0.60389400 -0.74535400
C -2.94836300 -0.62287200 -0.43796200
C -3.17545600 -1.19297200 -1.70060500
C -3.88645200 0.27578500 0.08398500
C -4.31581200 -0.87495700 -2.42783400
H -2.45009500 -1.89877700 -2.09452100
C -5.03747600 0.60868600 -0.66516700
C -5.25236400 0.02824600 -1.91636200
H -4.48575500 -1.32615500 -3.40210100
C -3.04223300 -2.66306400 1.49616500
N -4.06690500 -3.18839600 1.71661000
H -0.00685900 -1.19082200 -1.44970300
H -6.13527000 0.27423200 -2.49616300
O -3.64571200 0.88499700 1.29075000
O -5.87945600 1.52634900 -0.08390700
C -4.49236300 0.48049400 2.37408700
H -5.50951100 0.86772500 2.24520300
H -4.51761400 -0.61006000 2.46542000
H -4.04819000 0.91361300 3.27436600
C -7.04584300 1.89071600 -0.79130100
H -7.56503000 2.61825600 -0.16265900
H -6.80818300 2.35585300 -1.75878600
H -7.70572500 1.02890100 -0.96592600
H 3.11009900 6.01909900 -2.32419600

$In_{\mathbf{2d}(1,5)}$

Charge= -1 multiplicity= 1

C 0.23034300 5.29295400 -0.94851600
C -0.72112000 4.35890900 1.05942600
O -1.67163900 1.04608600 1.99397800
C -1.13920200 1.96653400 1.19499200
O 0.31020500 2.75411700 -1.97305500
O -0.75713900 5.48615100 1.54697500

H -0.59569200 5.99854300 -1.07270500
N -0.21889400 4.11910100 -0.20356700
C -0.14406900 2.84084400 -0.82975500
N -1.18381800 3.23536200 1.74621700
H 0.57846000 4.93805500 -1.91654600
C -0.60413600 1.72595600 -0.04339000
C -1.77273200 3.42631200 3.07245100
H -1.69151900 4.48629900 3.30375300
H -1.23410900 2.83072900 3.81402000
H -2.82103400 3.11622400 3.06887500
H 1.03577700 5.79809400 -0.40754000
C 4.12093900 -1.12433600 0.78012900
H 3.81113800 -1.11824800 1.81934800
C 0.90904400 -0.06076200 -0.92079900
O 1.45236800 -0.36346900 1.38823600
C 1.41129900 -0.07109400 -2.17578300
C -0.54695000 0.34509000 -0.69822700
O 2.68360600 -0.41474200 -2.52498800
C 3.55648300 -0.76210700 -1.54012500
C 3.17496200 -0.76199400 -0.19279300
C 1.79104200 -0.38665000 0.20332400
C 4.85487500 -1.11591500 -1.92945900
H 5.11484800 -1.10274400 -2.98294500
H -0.98892500 0.47593400 -1.69257700
C 5.78008500 -1.47306500 -0.96074700
C 5.40129800 -1.47340400 0.39136200
H 6.79102000 -1.75035900 -1.23986700
H 0.84300700 0.21977600 -3.04946000
C -3.50320400 0.66646500 -1.52624100
C -1.28100100 -0.80037800 -0.00487900
N -3.54191000 1.81254500 -1.76663700
C -2.51008900 -1.32344800 -0.36429200
C -3.50410200 -0.71414800 -1.20831400
H -0.67805000 -1.39734800 0.67232900
C -2.85106700 -2.65508700 0.23816600

C	-4.08083300	-2.87303100	0.87995400
C	-1.92719600	-3.71130200	0.20133100
C	-4.36956600	-4.09960200	1.47585800
H	-4.80797400	-2.06814000	0.91312600
C	-2.21659700	-4.94205200	0.79112600
H	-0.97967800	-3.55969400	-0.30743200
C	-3.43921600	-5.14043900	1.43408300
H	-5.32583800	-4.24289400	1.97350900
H	-1.48739100	-5.74778800	0.74310800
C	-4.56862200	-1.46226700	-1.77328200
N	-5.45332200	-2.05533300	-2.26088200
H	-3.66779300	-6.09902700	1.89450800
H	-1.68947000	0.18903300	1.46070100
Cl	6.59621200	-1.93207100	1.60688800

$In_{\mathbf{2e}(1,5)}$

Charge= -1 multiplicity= 1

C	0.90391900	5.39073400	-1.12030400
C	-0.10327000	4.61482600	0.92788600
O	-1.33165700	1.43143100	1.98727000
C	-0.74147200	2.27693900	1.14820500
O	0.74174800	2.82122600	-2.05661000
O	-0.02503100	5.75482400	1.37947700
H	0.15260600	6.17459800	-1.24846600
N	0.35156400	4.28994200	-0.33399900
C	0.30029500	2.98995600	-0.91824300
N	-0.65609400	3.56129200	1.65848100
H	1.19287400	4.97597000	-2.08399900
C	-0.26596200	1.95225500	-0.09579400
C	-1.18550800	3.84444700	2.99312300
H	-0.99540100	4.89725200	3.19104000
H	-0.68642800	3.21869500	3.73746600
H	-2.25885500	3.63898300	3.02669700
H	1.76920300	5.82370900	-0.60981400
C	4.10106400	-1.36862100	0.90555600

H	3.77706000	-1.29601900	1.93786500
C	1.05268900	-0.01892600	-0.88969300
O	1.52082500	-0.30183600	1.43716100
C	1.56944800	-0.12578800	-2.13405200
C	-0.35054900	0.55219200	-0.70646200
O	2.80270100	-0.61436800	-2.44713000
C	3.61647400	-1.02251700	-1.43520700
C	3.21574100	-0.93804500	-0.09616200
C	1.87521700	-0.40195200	0.26074200
C	4.87497200	-1.52644500	-1.78824800
H	5.15152400	-1.57580300	-2.83641700
H	-0.75754700	0.70112200	-1.71243700
C	5.74048500	-1.94968800	-0.79135600
C	5.34228500	-1.86561300	0.55251100
H	6.71970100	-2.34331100	-1.04223900
H	1.04841800	0.19299400	-3.02729500
C	-3.24219100	1.14369400	-1.72144300
C	-1.22513100	-0.46992700	0.02016500
N	-3.07955100	2.18209900	-2.23770000
C	-2.53828700	-0.78555100	-0.27051500
C	-3.49220500	-0.10068600	-1.08957200
H	-0.68988000	-1.18221400	0.64036900
C	-3.06546200	-1.99513300	0.45325800
C	-3.85369400	-1.82145400	1.60170000
C	-2.78932700	-3.31242100	0.06308400
C	-4.33263700	-2.90406600	2.33509100
H	-4.08862700	-0.80638100	1.90854600
C	-3.26496600	-4.41034400	0.78259200
C	-4.03640500	-4.20417100	1.92408800
H	-4.93783500	-2.73260200	3.22128000
H	-3.03038700	-5.41339900	0.44153100
C	-4.79261800	-0.63092700	-1.29705800
N	-5.87121800	-1.04650300	-1.48363300
H	-1.43326900	0.56201200	1.47490900
H	-4.40632200	-5.05912300	2.48443300

Cl	-1.83093400	-3.64234100	-1.38153300
Cl	6.46117700	-2.41007800	1.80446100

$In_{\mathbf{2f}(1,5)}$

Charge= -1 multiplicity= 1

C	3.91525300	-3.64657200	1.22760600
C	2.52114000	-3.75278600	-0.73593400
O	-0.25218100	-1.80383600	-1.86501500
C	0.74392600	-2.11880600	-1.04239300
O	2.49915700	-1.43046300	1.99232800
O	3.15412500	-4.73650700	-1.11295700
H	3.69555500	-4.68329500	1.49649800
N	2.81972600	-3.09031100	0.43707000
C	2.13581500	-1.93930700	0.93053200
N	1.45386800	-3.22948900	-1.46778500
H	4.00467900	-3.02994000	2.11982900
C	1.05766100	-1.44887900	0.11118400
C	1.06606000	-3.90245900	-2.70780600
H	1.76462000	-4.72394100	-2.85260300
H	1.11620800	-3.20450600	-3.54753900
H	0.04366000	-4.28208800	-2.62971900
H	4.84495700	-3.63036300	0.65110000
C	2.94006900	3.48413000	-1.70337000
H	2.61858900	3.11481000	-2.67227200
C	1.20045600	1.00415900	0.57738600
O	1.26411800	1.17409700	-1.80416700
C	1.67903600	1.52478200	1.72902600
C	0.29722100	-0.22486500	0.62592000
O	2.49237200	2.61188000	1.83572800
C	2.88982700	3.24373900	0.69428900
C	2.48889400	2.78874200	-0.56872000
C	1.60757800	1.60064500	-0.69838800
C	3.71900000	4.36317700	0.84068200
H	4.00576900	4.67981000	1.83853600
H	0.10821300	-0.42966300	1.68532700

C	4.14941600	5.03235000	-0.29628200
C	3.76076300	4.59414500	-1.57447200
H	4.79305100	5.90229200	-0.19308200
H	1.47312000	1.10527700	2.70530600
C	-1.75832800	-2.11672100	2.03023500
C	-1.03701300	0.09395200	-0.04926100
N	-1.03434500	-2.83483300	2.60605800
C	-2.29139900	-0.30393100	0.36879600
C	-2.67559700	-1.28780900	1.33636000
H	-1.01020700	0.90393400	-0.77152300
C	-3.43042800	0.34606100	-0.36974500
C	-4.05511500	-0.34640100	-1.41887300
C	-3.89807100	1.63726000	-0.09113500
C	-5.08574600	0.22144500	-2.16371300
H	-3.71294600	-1.35372800	-1.63797500
C	-4.93327800	2.22140300	-0.82370500
C	-5.52642700	1.51126000	-1.86511000
H	-5.54498900	-0.34280400	-2.97106100
H	-5.26642600	3.22261500	-0.57048600
C	-4.04246500	-1.51428900	1.64491900
N	-5.16261700	-1.72096800	1.91657400
H	-0.75816900	-1.05398300	-1.40829300
H	4.10416800	5.12666100	-2.45729500
H	-6.33240600	1.96625100	-2.43542600
Cl	-3.19847600	2.58434900	1.22304400

$In_{\mathbf{2h}(1,5)}$

Charge= -1 multiplicity= 1

C	3.38709900	4.67448900	-0.47220600
C	1.91901800	4.23647600	1.38841900
O	-0.66480800	1.83439300	1.94086100
C	0.33156500	2.39770100	1.26379000
O	2.25281300	2.53066800	-1.74430500
O	2.41835800	5.18761500	1.98501200
H	3.04840000	5.71016300	-0.56384400

N	2.33935300	3.85401400	0.13073400
C	1.80800400	2.76325000	-0.61767000
N	0.89033300	3.46981800	1.93781300
H	3.59311800	4.25188400	-1.45364000
C	0.77841400	1.99531400	0.03236400
C	0.36459500	3.85151700	3.24921300
H	0.95463200	4.69939200	3.59075900
H	0.45378200	3.01669500	3.94911100
H	-0.68972000	4.12900400	3.16790900
H	4.28448600	4.66024400	0.15309000
C	3.31664200	-2.91826400	0.75517600
H	2.96641100	-2.82125100	1.77687900
C	1.24333200	-0.25244400	-0.95837200
O	1.36088700	-0.93979300	1.32916900
C	1.77457700	-0.43809600	-2.18744500
C	0.18182700	0.82732900	-0.75433800
O	2.72096100	-1.36215000	-2.51846200
C	3.21102200	-2.16989900	-1.53880000
C	2.77031600	-2.06105600	-0.21411700
C	1.73964000	-1.05635900	0.16204400
C	4.17862200	-3.11279400	-1.90929700
H	4.49695200	-3.16703300	-2.94532000
H	-0.04676600	1.23073000	-1.74753900
C	4.71018900	-3.95464100	-0.94453700
C	4.27126200	-3.84778200	0.38499100
H	5.46062200	-4.69186000	-1.20932200
H	1.50827000	0.15845300	-3.05004500
C	-2.12134100	2.67781900	-1.64277600
C	-1.08803200	0.17840800	-0.20788800
N	-1.56009700	3.70151300	-1.74278400
C	-2.37505000	0.37626900	-0.67617400
C	-2.84038100	1.46616800	-1.49488300
H	-0.93078400	-0.68317800	0.43375400
C	-3.39369300	-0.63342600	-0.24189800
C	-4.63785100	-0.24859000	0.27300900

C	-3.11947900	-2.01105700	-0.31098800
C	-5.57319900	-1.18637900	0.71428800
H	-4.87940900	0.80729800	0.33661000
C	-4.04065200	-2.95879700	0.11769300
H	-2.16887700	-2.33630600	-0.72317400
C	-5.27605100	-2.55063500	0.63523100
H	-6.52149000	-0.84061000	1.11065300
H	-3.82843700	-4.02201300	0.05249400
C	-4.06989500	1.40487600	-2.19928200
N	-5.07668400	1.38036900	-2.79790700
H	-1.06841100	1.14506900	1.32179100
Cl	4.96220800	-4.93029000	1.59592600
O	-6.12137100	-3.55800400	1.03289700
C	-7.39509300	-3.19299700	1.52661600
H	-7.90711500	-4.12871400	1.76446900
H	-7.32085400	-2.58221500	2.43751000
H	-7.97986200	-2.64106100	0.77776300

$In_{\mathbf{2i}\,(1,\,5)}$

Charge= -1 multiplicity= 1

C	-3.70072300	-4.52301400	-1.06790400
C	-2.47756800	-4.25300200	0.99180200
O	0.06437400	-1.96917700	2.03542900
C	-0.83210100	-2.47115500	1.19280900
O	-2.35670900	-2.34166900	-2.03672400
O	-3.08224900	-5.21568200	1.45843300
H	-3.39915700	-5.56941900	-1.16524900
N	-2.71072000	-3.78614800	-0.28581800
C	-2.05498600	-2.67122100	-0.88809300
N	-1.51121600	-3.55693000	1.72017200
H	-3.74930600	-4.04576600	-2.04471200
C	-1.07976100	-1.99803000	-0.06998300
C	-1.19660200	-4.01635800	3.07350400
H	-1.85391300	-4.85795600	3.28180000
H	-1.36489900	-3.21155400	3.79373500

H	-0.15001300	-4.32666700	3.13473600
H	-4.67554500	-4.49076100	-0.57233700
C	-3.38646600	3.00068400	0.82249800
H	-3.14062000	2.80419800	1.86023600
C	-1.31507300	0.34558800	-0.90918100
O	-1.61566200	0.85637500	1.40676900
C	-1.71421600	0.65828600	-2.16203600
C	-0.34439400	-0.81275400	-0.69926000
O	-2.57374600	1.66127100	-2.50002600
C	-3.10692800	2.42268800	-1.50591100
C	-2.80078500	2.18591300	-0.16017800
C	-1.87107800	1.09003600	0.22389300
C	-3.97969300	3.45123500	-1.88396500
H	-4.19453300	3.60432500	-2.93659300
H	-0.05359100	-1.15497400	-1.69797000
C	-4.55118800	4.25032400	-0.90573300
C	-4.24693200	4.01514900	0.44468000
H	-5.22956400	5.05247600	-1.17615800
H	-1.39755400	0.11568300	-3.04312700
C	1.92408900	-2.68970900	-1.72287700
C	0.90541200	-0.31228600	0.02681800
N	1.29831400	-3.48545600	-2.31192000
C	2.21191400	-0.68702000	-0.21609700
C	2.72715500	-1.76260800	-1.01181300
H	0.77399400	0.59453000	0.60886700
C	3.24174100	0.12253100	0.52920100
C	3.55506400	-0.19912300	1.85923200
C	3.86908600	1.21873400	-0.07459200
C	4.47710600	0.55646300	2.57289300
H	3.07394200	-1.05797900	2.31788400
C	4.79520500	1.99389900	0.65911800
C	5.10108300	1.65752100	1.97893600
H	4.71758600	0.29653800	3.60060000
C	4.12397000	-1.97372300	-1.12724500
N	5.27579800	-2.15152700	-1.25284600

H	0.56732100	-1.26057000	1.50977800
H	5.81375800	2.24407900	2.54831000
Cl	-4.98672500	5.04536100	1.67270500
O	3.52575400	1.57750500	-1.35484000
O	5.33022900	3.06910400	-0.00846200
C	4.53033300	1.36131700	-2.35405200
H	5.35535100	2.07426600	-2.24416500
H	4.91421000	0.33717500	-2.30833100
H	4.03280500	1.52390700	-3.31398300
C	6.26295600	3.87505700	0.68067700
H	6.55854000	4.66009700	-0.01955600
H	5.82072500	4.33791900	1.57448500
H	7.15388600	3.30540200	0.98117900

Table 10: Thermodynamic parameters for intermediates **2a-2i** [1,3]-H shift at b3lyp/6-31g (d) level of theory

Intermediate **2**	G	H	S	E
$In_{2a(1,3)}$	-1635.156778	-1635.056407	211.249	-1635.500389
$In_{2b(1,3)}$	-1749.649167	-1749.542906	223.643	-1750.022272
$In_{2c(1,3)}$	-1864.135459	-1864.023456	235.730	-1864.538006
$In_{2d(1,3)}$	-2094.752645	-2094.648799	218.564	-2095.083950
$In_{2e(1,3)}$	-2554.370697	-2554.264306	223.919	-2554.691286
$In_{2f(1,3)}$	-2094.763138	-2094.659956	217.165	-2095.095410
$In_{2h(1,3)}$	-2209.256884	-2209.147304	230.630	-2209.618170
$In_{2i(1,3)}$	-2323.743651	-2323.628063	243.276	-2324.134102

In_{2a} (1,3)

Charge= -1 multiplicity= 1

C 3.12239700 -2.73948900 1.95769900

C 2.79883000 -2.52180900 -0.44122100

O -0.12864300 -2.27921100 -2.44318400

C 0.55945800 -2.21587300 -1.44284500

O 0.39104600 -2.49105600 2.21571600

O 4.00819100 -2.66720800 -0.55426100

H 3.57516300 -3.73234000 1.88464800

N 2.21140800 -2.50751900 0.83462900

C 0.84525500 -2.36355300 1.08695700

N 1.94569600 -2.41355000 -1.52798900

H 2.53313000 -2.66180000 2.86920600

C -0.01645700 -1.94751900 -0.07650600

C 2.51820800 -2.44217300 -2.87601800

H 3.58986700 -2.60171800 -2.78186000

H 2.31098800 -1.48780700 -3.36506900

H 2.05644200 -3.24577600 -3.45405900

H 3.92129900 -1.99520600 1.94469200

C	3.53730200	2.55835600	-0.83258800
H	3.56867800	2.19582800	-1.85504600
C	0.63019900	0.52703300	0.52049400
O	1.70637000	0.51039400	-1.60862500
C	0.69848300	1.02781900	1.77743100
C	-0.50624500	-0.42311700	0.17108400
O	1.58409800	1.96131000	2.22172500
C	2.50247700	2.46014200	1.34270700
C	2.56390200	2.00739900	0.01832500
C	1.62527000	0.96743400	-0.46704300
C	3.38201900	3.43659600	1.82564200
H	3.29864200	3.75819200	2.85893300
H	-1.09664200	-0.53903600	1.08357300
C	4.33240100	3.96586600	0.96390300
C	4.41282700	3.52833900	-0.36981400
H	5.01817800	4.72676800	1.32743100
H	0.02389100	0.73835100	2.57491900
C	-2.85416400	1.77638500	-2.85197600
C	-1.37505800	0.15218100	-0.90351400
N	-2.33015700	2.25342400	-3.78551100
C	-2.70127300	0.46361500	-0.74476800
C	-3.47249600	1.21042600	-1.71267700
H	-0.88436400	0.42861800	-1.83038400
C	-3.43119400	0.05249100	0.49961600
C	-3.84582800	1.00816200	1.43973400
C	-3.71500900	-1.29730200	0.75449900
C	-4.50403700	0.62416700	2.60790900
H	-3.65036300	2.05804500	1.24109500
C	-4.37730700	-1.68448300	1.92117500
H	-3.42393700	-2.04168400	0.01797000
C	-4.77071300	-0.72465100	2.85435800
H	-4.81523000	1.38070700	3.32491500
H	-4.58876500	-2.73664100	2.09791500
C	-4.86878400	1.39337200	-1.59073700
N	-6.02624500	1.56353000	-1.50603300

H -5.28683300 -1.02386300 3.76384900

H 5.15966600 3.95255100 -1.03497000

H -0.94601200 -2.51709000 -0.01537800

$In_{\mathbf{2b}}$ (1,3)

Charge= -1 multiplicity= 1

C 2.96553200 -3.29999600 1.61547600

C 3.15836200 -2.50050600 -0.67146600

O 0.72501000 -1.55651200 -3.08495600

C 1.18930700 -1.78754100 -1.98530100

O 0.24945100 -2.90010600 1.38688100

O 4.35967500 -2.71130600 -0.57729800

H 3.40494600 -4.27505100 1.38741500

N 2.31721400 -2.73992800 0.42764300

C 0.93362900 -2.54906500 0.43549700

N 2.55562800 -2.07219400 -1.84358900

H 2.19823200 -3.40282500 2.38018900

C 0.34751600 -1.80408600 -0.73546500

C 3.39708600 -1.82827100 -3.01754200

H 4.41980600 -2.09131500 -2.75749800

H 3.32612800 -0.77203000 -3.28632700

H 3.04284100 -2.43312500 -3.85529200

H 3.76276200 -2.63300300 1.95042100

C 4.11074700 2.45164300 0.36502400

H 4.34773500 2.33756100 -0.68790000

C 0.92464800 0.39867900 0.57120900

O 2.42893800 0.79330600 -1.23796100

C 0.73984100 0.58302900 1.90056200

C -0.13987000 -0.34784800 -0.22034000

O 1.53774700 1.31284000 2.72780800

C 2.63552600 1.92924700 2.19894300

C 2.96345900 1.79593400 0.84340700

C 2.11963400 0.97652600 -0.05925000

C 3.42058800 2.69214900 3.07188600

H 3.12933100 2.76818800 4.11470900

H -0.91368200 -0.62712700 0.49936800
C 4.54708800 3.33118300 2.57332800
C 4.89589100 3.21336900 1.21644000
H 5.16190800 3.92860900 3.24154300
H -0.09603900 0.16847700 2.45214400
C -1.68991600 2.74131200 -2.95228400
C -0.74315600 0.53605400 -1.26701600
N -0.95451800 3.39294400 -3.59132400
C -2.05925700 0.92308900 -1.29337000
C -2.56729400 1.96100100 -2.16353700
H -0.05747100 0.98284800 -1.97870900
C -3.05947400 0.28832800 -0.37502800
C -3.69375300 1.02798700 0.62915000
C -3.40314800 -1.06870700 -0.49775100
C -4.62052600 0.44576600 1.49779200
H -3.46216300 2.08427700 0.72956000
C -4.32634800 -1.66477200 0.35481900
H -2.94880800 -1.65542900 -1.29164200
C -4.93998400 -0.90868300 1.36016600
H -5.08818800 1.05746300 2.26165400
H -4.59377900 -2.71251900 0.25386300
C -6.52333000 -0.84593500 3.14512800
H -7.19637000 -1.55229500 3.63775200
H -5.83483000 -0.42588200 3.89256400
H -7.11385600 -0.02740600 2.71033900
O -5.83842600 -1.58339900 2.15346800
C -3.94789800 2.23500700 -2.29328800
N -5.08784600 2.48633300 -2.40956400
H 5.77873300 3.72087100 0.83803000
H -0.58913400 -2.29832100 -1.00103800

$In_{\mathbf{2c}\ (1,3)}$

Charge= -1 multiplicity= 1

C -3.24784400 1.06895600 3.34179600
C -3.33351700 2.24922100 1.21774100

O	-0.78908700	3.36993300	-1.01188100
C	-1.30819600	2.73577500	-0.11406100
O	-0.50782100	1.00720700	3.03209600
O	-4.54581300	2.32125000	1.36421700
H	-3.68738700	1.88995700	3.91597000
N	-2.54265500	1.58231400	2.16630600
C	-1.15287900	1.46303700	2.09818300
N	-2.68218500	2.85895700	0.15987900
H	-2.51611700	0.53873400	3.94830000
C	-0.51077200	1.82319900	0.78404700
C	-3.52857100	3.54795400	-0.81567200
H	-4.21119500	4.22541000	-0.29983900
H	-4.10484700	2.81294000	-1.38384000
H	-2.86556800	4.09433400	-1.48333700
H	-4.05173000	0.40115300	3.02561900
C	-4.24486900	-1.84194100	-1.56212000
H	-4.51946300	-0.95808600	-2.12892500
C	-1.01088000	-0.65415500	0.02775100
O	-2.54584200	0.44826300	-1.42517500
C	-0.76183100	-1.80673500	0.69602600
C	0.02597700	0.45742500	0.09255100
O	-1.54101600	-2.92203500	0.67719200
C	-2.68139300	-2.91353800	-0.07247800
C	-3.05844400	-1.78449600	-0.81088100
C	-2.22121800	-0.56129800	-0.79432300
C	-3.45601600	-4.08005800	-0.06909700
H	-3.12509700	-4.93179500	0.51669300
H	0.76316500	0.13769600	0.83090300
C	-4.62286500	-4.11066100	-0.81967300
C	-5.02149600	-2.99014300	-1.56969800
H	-5.23063700	-5.01181900	-0.82603000
H	0.12719000	-1.97329000	1.29142500
C	1.94626500	0.79352400	-3.88844300
C	0.70293700	0.64002600	-1.22776600
N	1.30630300	0.87820700	-4.86677200

C	2.05704800	0.59507300	-1.40808600
C	2.70686000	0.67732000	-2.70211700
H	0.06462400	0.78280800	-2.09361600
C	2.98384300	0.50421400	-0.22721800
C	3.17690800	-0.68788000	0.48115600
C	3.69191300	1.64839500	0.18172000
C	4.06609000	-0.74083800	1.57625800
C	4.55840500	1.59973600	1.26586400
H	3.55298600	2.56964700	-0.37509500
C	4.75270700	0.40793400	1.97167800
H	5.09757100	2.49283700	1.57145200
C	4.10949400	0.59955800	-2.85039300
N	5.27219100	0.52839700	-2.99344600
H	5.43589900	0.38486200	2.81350900
O	2.46183000	-1.82852100	0.17609600
O	4.18242700	-1.96599600	2.18376600
C	3.02753000	-2.62004700	-0.87329400
H	3.12189700	-2.03991000	-1.79686700
H	4.01069800	-3.00937000	-0.57849600
H	2.33809400	-3.45400200	-1.03110400
C	5.06353800	-2.06968800	3.28247600
H	4.76218700	-1.41378500	4.11181000
H	5.01243100	-3.11016000	3.61279300
H	6.09942600	-1.83103300	3.00151200
H	-5.93646400	-3.02729900	-2.15431600
H	0.41700700	2.35501800	1.00767600

$In_{\mathbf{2d}\ (1,3)}$

Charge= -1 multiplicity= 1

C	-1.97073200	-4.56792900	2.15702400
C	-1.16899000	-4.47753900	-0.13807000
O	0.49014700	-1.88164100	-1.90218500
C	-0.28919800	-2.38104200	-1.12138800
O	-1.43614600	-1.87254100	2.28053800
O	-1.34193000	-5.68460100	-0.20617000

H	-2.77817300	-5.22623900	1.83365800
N	-1.51448300	-3.76504700	1.01787200
C	-1.32970500	-2.38899600	1.18075700
N	-0.56847600	-3.76281800	-1.16868100
H	-2.31231400	-3.87795700	2.92592400
C	-1.11845600	-1.60579500	-0.11136900
C	-0.04361400	-4.55058800	-2.28907500
H	-0.82215100	-5.22437500	-2.64863200
H	0.81967800	-5.14600200	-1.97563700
H	0.25781400	-3.85103500	-3.06627800
H	-1.15470700	-5.18329600	2.54799200
C	4.20627600	1.10661600	-0.71247200
H	4.01463500	1.28665400	-1.76460300
C	0.73344000	0.11729500	0.45857900
O	1.57522400	0.85046600	-1.67877500
C	1.09041100	-0.04113000	1.75611900
C	-0.74876000	-0.10011100	0.10732000
O	2.33441700	0.12964400	2.28959300
C	3.35057100	0.49540900	1.45711000
C	3.12436300	0.72531500	0.09695300
C	1.76066400	0.57995600	-0.50038100
C	4.62386000	0.63567600	2.02227100
H	4.75812600	0.45088200	3.08327300
H	-1.30114100	0.15424200	1.01473100
C	5.68633500	1.00941300	1.21286000
C	5.46485100	1.24141800	-0.15343700
H	6.68217800	1.12367400	1.62761900
H	0.39018600	-0.33657600	2.52814900
C	-2.93332800	1.64483300	-3.27042700
C	-1.30925100	0.74453600	-1.01216900
N	-2.85537400	1.13186000	-4.32243900
C	-2.30655500	1.67182600	-0.86403300
C	-3.03791600	2.23025200	-1.98860400
H	-0.97618700	0.50020600	-2.01452600
C	-2.71810700	2.14604000	0.49639000

C	-1.78503500	2.72627700	1.37034800
C	-4.04768000	2.02917500	0.93300000
C	-2.16109400	3.15841400	2.64346500
H	-0.75929900	2.84552100	1.03307200
C	-4.42548600	2.45585000	2.20523000
H	-4.78389000	1.60310500	0.25813300
C	-3.48339900	3.02159600	3.06771900
H	-1.42091400	3.61062000	3.30035700
H	-5.46079300	2.35194800	2.52241000
C	-3.84473700	3.38420300	-1.87697700
N	-4.52807700	4.33532600	-1.80135600
Cl	6.83120000	1.71558200	-1.16459000
H	-3.77998700	3.36019500	4.05807700
H	-2.12463000	-1.57813500	-0.56792700

$In_{\mathbf{2e}\ (1,3)}$

Charge= -1 multiplicity= 1

C	-2.02806600	3.62053100	2.06747900
C	-1.91496700	3.30115600	-0.33926500
O	0.72782200	2.28587500	-2.49029200
C	0.10743000	2.41706100	-1.45270100
O	0.55508000	2.66893600	2.18409800
O	-3.05043200	3.75348100	-0.38967900
H	-2.21217700	4.69606200	1.99441800
N	-1.27604500	3.14894900	0.90248700
C	0.01986800	2.65949200	1.08335100
N	-1.18629200	2.95954000	-1.46782500
H	-1.42609100	3.40153900	2.94714500
C	0.67490600	2.02803200	-0.11438100
C	-1.81033600	3.12232900	-2.78322100
H	-2.80232100	3.54239100	-2.63404300
H	-1.87315200	2.14442600	-3.26544000
H	-1.19911400	3.78412100	-3.40112100
H	-2.99187000	3.10955000	2.11662300
C	-3.96195600	-1.38961700	-0.53228000

H	-3.97089700	-1.04656900	-1.56074600
C	-0.54123300	-0.19990800	0.58716500
O	-1.70783100	0.05926300	-1.47942100
C	-0.65411600	-0.65308600	1.85902500
C	0.77377300	0.42278400	0.14693800
O	-1.72443100	-1.31135100	2.38222300
C	-2.79778300	-1.55397900	1.57797300
C	-2.82554100	-1.11882000	0.24768100
C	-1.67573800	-0.37595900	-0.32795400
C	-3.87465900	-2.25041100	2.13997600
H	-3.81697500	-2.57361600	3.17420200
H	1.42689600	0.40649900	1.02327800
C	-4.99041600	-2.51392600	1.36064800
C	-5.02351200	-2.07851000	0.02576600
H	-5.83558300	-3.05374700	1.77407400
H	0.12619400	-0.55145300	2.60327700
C	2.52630100	-2.09731300	-3.05598100
C	1.40310000	-0.36385400	-0.95539800
N	1.87194400	-2.49280100	-3.94374400
C	2.70242000	-0.79587500	-0.94930000
C	3.29914400	-1.61869400	-1.97267400
H	0.77496000	-0.61962700	-1.80156000
C	3.63349200	-0.35619900	0.14394400
C	3.77756100	-1.01294800	1.37359400
C	4.43254200	0.78089000	-0.06460100
C	4.66388300	-0.56572200	2.35521000
C	5.32296300	1.24274900	0.90200700
H	4.34378700	1.29152600	-1.01909200
C	5.43949500	0.56659500	2.11691700
H	4.74138800	-1.10784100	3.29204600
H	5.92697600	2.12440800	0.70469100
C	4.65944700	-1.99902100	-1.93211000
N	5.78787500	-2.31768300	-1.91226500
H	6.13161200	0.91426700	2.87960600
Cl	2.81458700	-2.44841500	1.73932600

Cl	-6.45454700	-2.42435100	-0.94298600
H	1.72365200	2.33272200	-0.11797400

$In_{\mathbf{2f}\,(1,3)}$

Charge= -1 multiplicity= 1

C	-3.13897000	2.58201400	2.31381100
C	-2.82031300	2.71658800	-0.09166000
O	0.09166500	2.56107300	-2.12596500
C	-0.60460300	2.40120300	-1.14178600
O	-0.43482700	2.09466700	2.51342700
O	-4.01495800	2.96827000	-0.17331000
H	-3.51578000	3.60508000	2.40056000
N	-2.24211900	2.46155100	1.16245400
C	-0.89068000	2.18107500	1.38075700
N	-1.97236300	2.71093900	-1.18785500
H	-2.56182600	2.31832900	3.19785800
C	-0.05840200	1.88842700	0.16300000
C	-2.53422300	2.98653200	-2.51207500
H	-3.59107000	3.21109600	-2.38772500
H	-2.39808100	2.10432200	-3.14151900
H	-2.00966400	3.83071600	-2.96525100
H	-3.99143900	1.91096600	2.18964200
C	-3.96472900	-2.14460400	-1.20969800
H	-3.96542400	-1.63264600	-2.16663500
C	-0.88727100	-0.60051000	0.38710900
O	-1.95112600	-0.18309300	-1.70673800
C	-0.99373200	-1.27943400	1.55438100
C	0.31688500	0.30152300	0.17193500
O	-1.95861200	-2.18502800	1.86798400
C	-2.92112400	-2.46338200	0.93981500
C	-2.94370000	-1.81555800	-0.30182700
C	-1.91519100	-0.80342700	-0.64214300
C	-3.88436800	-3.41805400	1.28717500
H	-3.82790100	-3.89590400	2.26004300
H	0.90862600	0.24561800	1.08933700

C	-4.88084100	-3.72611200	0.37163300
C	-4.92401700	-3.08990300	-0.88133700
H	-5.63222400	-4.46796900	0.62941800
H	-0.28990300	-1.17937000	2.37190300
C	2.69333800	-1.27410300	-3.22963400
C	1.14504100	-0.15945600	-0.98248500
N	2.17773200	-1.62541500	-4.22150300
C	2.50088100	-0.34048900	-0.93621600
C	3.29959400	-0.85426000	-2.02314100
H	0.62330200	-0.37878600	-1.90749900
C	3.27061300	0.07013800	0.28615900
C	3.47408200	-0.74718200	1.40632800
C	3.84481400	1.35228500	0.32475500
C	4.20395300	-0.31781400	2.51636700
C	4.57677800	1.79901800	1.42257000
H	3.70921300	1.99164800	-0.54271600
C	4.75736200	0.96052300	2.52307500
H	4.33503600	-0.98674700	3.36072200
H	5.00840000	2.79642600	1.41607100
C	4.70342500	-0.98238700	-1.92831900
N	5.86966500	-1.08947300	-1.86436400
H	5.32765200	1.29488000	3.38600600
H	-5.70820000	-3.34152700	-1.58980000
Cl	2.78996600	-2.37505300	1.46233900
H	0.91472300	2.36353100	0.30423000

$In_{\mathbf{2h}}$ (1,3)

Charge= -1 multiplicity= 1

C	1.99095000	-3.77907400	1.90791800
C	2.28607300	-3.23659700	-0.44298100
O	0.01359400	-2.12543400	-2.94056000
C	0.44811000	-2.32585500	-1.82301300
O	-0.61682100	-2.93266700	1.64088900
O	3.43439200	-3.64113900	-0.32706000
H	2.24215700	-4.83490000	1.77373900

N	1.43205800	-3.22462100	0.67261500
C	0.10234600	-2.79879300	0.66045300
N	1.74983900	-2.81914600	-1.65106900
H	1.23247400	-3.66866500	2.68031500
C	-0.36702600	-2.08140900	-0.57894700
C	2.60301900	-2.83729600	-2.84208900
H	3.57422100	-3.23199000	-2.55283000
H	2.69747400	-1.81749500	-3.22124500
H	2.14572200	-3.46206700	-3.61271400
H	2.90217600	-3.24019600	2.17561000
C	4.05854800	1.58063500	0.08553300
H	4.26340600	1.32771900	-0.94867200
C	0.58813300	0.11216000	0.50348500
O	2.10833800	0.08131800	-1.33734100
C	0.45811800	0.45378800	1.80845700
C	-0.59788400	-0.52358600	-0.20855300
O	1.37680000	1.12617000	2.55748100
C	2.54861300	1.49827500	1.96979600
C	2.82960900	1.17992000	0.63542000
C	1.84854700	0.42363100	-0.18372400
C	3.46463100	2.20503900	2.75873500
H	3.21247500	2.43493200	3.78881300
H	-1.39330100	-0.59911200	0.53720000
C	4.67341300	2.59737000	2.20516900
C	4.96017300	2.27954200	0.86743300
H	5.39707400	3.14763500	2.79693600
H	-0.42300400	0.23587200	2.40037300
C	-1.65882000	2.50820000	-3.22033200
C	-1.06572200	0.34576800	-1.33344600
N	-0.83751000	2.95253800	-3.92845400
C	-2.29444300	0.95584900	-1.38332800
C	-2.63721300	1.97668600	-2.34767200
H	-0.33357600	0.59196000	-2.09475800
C	-3.36307300	0.60029000	-0.39428000
C	-3.83156300	1.53570900	0.53485400

C	-3.93895400	-0.68142800	-0.37293100
C	-4.82001500	1.21362300	1.46845900
H	-3.41873500	2.54015500	0.52331600
C	-4.92670300	-1.01919600	0.54601800
H	-3.61508000	-1.41475400	-1.10662600
C	-5.37215900	-0.07118900	1.47449900
H	-5.15368200	1.97062600	2.16983500
H	-5.37363600	-2.00892800	0.55636900
C	-6.86931100	0.44403700	3.26063800
H	-7.63933500	-0.08194700	3.83062600
H	-6.09743900	0.80973400	3.95312600
H	-7.32245000	1.30550000	2.75054300
O	-6.35028700	-0.49634700	2.34240500
C	-3.95211500	2.47596200	-2.49020500
N	-5.03350400	2.91157200	-2.61905700
Cl	6.50492100	2.78830400	0.18829200
H	-1.37659200	-2.43523400	-0.79787900

$In_{\mathbf{2i}\,(1,3)}$

Charge= -1 multiplicity= 1

C	-2.32422300	2.72023800	3.05814800
C	-2.48383000	3.17736000	0.67527800
O	-0.07197700	3.12665000	-1.94839600
C	-0.56944000	2.89552800	-0.86367200
O	0.33163000	2.11824900	2.61812700
O	-3.65207300	3.48549900	0.86453100
H	-2.58571800	3.73906000	3.35871500
N	-1.68965400	2.71985100	1.73879000
C	-0.34432700	2.36322600	1.62863300
N	-1.87783000	3.31286600	-0.56163900
H	-1.60760900	2.29616100	3.75886500
C	0.19484500	2.19410200	0.23189600
C	-2.72681500	3.79509100	-1.65269500
H	-3.24258400	4.70643700	-1.34523100
H	-3.46369700	3.02955000	-1.90942900

H	-2.07577900	3.98289100	-2.50398900
H	-3.23945300	2.12567000	3.02623300
C	-4.19655000	-1.39100300	-0.58784600
H	-4.42444700	-0.69381400	-1.38626400
C	-0.69233600	-0.28844600	0.34308700
O	-2.22641300	0.53423600	-1.28811100
C	-0.51874600	-1.20689600	1.32508600
C	0.47761000	0.61732700	-0.01304800
O	-1.42806300	-2.14585500	1.70701400
C	-2.62948000	-2.19201900	1.06719900
C	-2.94098100	-1.29833700	0.03548400
C	-1.96065600	-0.26805800	-0.39073100
C	-3.54157500	-3.16903300	1.48532800
H	-3.26456500	-3.84570000	2.28713600
H	1.24075500	0.43191200	0.74475800
C	-4.77763800	-3.25171600	0.86331600
C	-5.09452700	-2.35700200	-0.17203000
H	-5.49925000	-4.00151800	1.16950500
H	0.40055300	-1.31836500	1.88588000
C	1.99775000	-0.63270500	-3.98348600
C	1.03029100	0.26972500	-1.35761500
N	1.27671800	-0.75123000	-4.89977500
C	2.33760000	-0.06014700	-1.58469600
C	2.85373600	-0.49818600	-2.86593400
H	0.33176700	0.24225300	-2.18756100
C	3.35954100	0.06674600	-0.48867500
C	3.46305200	-0.87001100	0.54614400
C	4.25144400	1.15389800	-0.50013200
C	4.44424500	-0.73017200	1.55124500
C	5.21070300	1.29750300	0.49379200
H	4.18063800	1.87365200	-1.30946800
C	5.31558800	0.35954900	1.52612700
H	5.89310300	2.14339300	0.47257700
C	4.20748300	-0.85640400	-3.05238100
N	5.32639200	-1.16698500	-3.22189000

Cl	-6.67381400	-2.48202300	-0.94584600
H	6.07236700	0.48376300	2.29280800
O	2.57307600	-1.92037700	0.65045800
O	4.45603700	-1.71610500	2.50585400
C	2.95185700	-3.09029500	-0.08189700
H	3.07167400	-2.86504900	-1.14654600
H	3.88423500	-3.51181100	0.31520300
H	2.14019000	-3.81049400	0.05305700
C	5.42466500	-1.62333900	3.52976200
H	5.30222400	-0.70812600	4.12645300
H	5.26806600	-2.49307600	4.17258100
H	6.44819500	-1.65033700	3.12928100
H	1.20133600	2.61892100	0.21647800

Table 11: Thermodynamic parameters for TS_3 at b3lyp/6-31g (d) level of theory in cycloaddition step

TS	G	H	S	E
TS_{3a}	-1635.121379	-1635.026324	200.060	-1635.467885
TS_{3b}	-1749.613782	-1749.512587	212.982	-1749.989503
TS_{3c}	-1864.094396	-1863.986460	227.171	-1864.498455
TS_{3d}	-2094.730007	-2094.631462	207.406	-2095.064553
TS_{3e}	-2554.334544	-2554.232647	214.460	-2554.657262

TS_{3a}

Imaginary Freq = -147.35

Charge = -1 multiplicity= 1

C -0.30053100 3.16938200 2.96850500

C 0.28736700 3.81162800 0.71777600

O 0.95705900 1.87604500 -2.22427100

C 0.54251100 2.11069800 -1.08289800

O -0.29160700 0.56979600 2.10190800

O 0.40284500 4.97605300 1.09658600

H -1.06887600 3.94437500 3.03395000

N -0.08790500 2.79528200 1.57483800

C -0.13013200 1.41597500 1.21871300

N 0.52743200 3.45574400 -0.60901300

H 0.62137500 3.56183600 3.41051300

C -0.01987800 1.13802300 -0.18870700

C 1.05563000 4.50928300 -1.47250400

H 0.38368200 5.37070300 -1.46404700

H 1.14174100 4.08596000 -2.47189800

H 2.03949800 4.84206000 -1.12394200

H -0.61104500 2.26726700 3.49282400

C 5.05510800 -0.83875400 0.71408400

H 5.06293800 0.15081000 1.15990100

C 1.45732600 -0.98410400 -0.49505300

O	2.71081700	0.73234600	0.63946300
C	1.57310400	-2.22200400	-1.02816500
C	0.08385800	-0.30322600	-0.63627700
O	2.67904400	-3.01744900	-1.03537300
C	3.81684600	-2.54116600	-0.45063500
C	3.85143100	-1.26939200	0.13110700
C	2.64896300	-0.38778600	0.13778300
C	4.93938400	-3.37810600	-0.46233900
H	4.86389400	-4.35647800	-0.92657700
H	-0.10363000	-0.25241700	-1.71874200
C	6.11568500	-2.92802000	0.12093400
C	6.17676400	-1.65442000	0.71210900
H	6.99379300	-3.56885200	0.11795600
H	0.75253000	-2.72640100	-1.52721700
C	-2.28006500	1.50501800	-0.87209900
C	-1.01357500	-1.16126900	-0.03324100
N	-2.53139100	2.71688600	-0.87017500
C	-2.31893500	-0.95544600	-0.29238900
C	-2.75247900	0.23344300	-1.07207900
H	-0.71844600	-1.93795300	0.66462300
C	-3.36587500	-1.85995000	0.25202600
C	-4.62422900	-1.36627300	0.63897500
C	-3.12907900	-3.23826000	0.40269100
C	-5.59369000	-2.21071800	1.17744600
H	-4.83152200	-0.30699600	0.52414100
C	-4.09507700	-4.08253500	0.94640900
C	-5.33508000	-3.57333100	1.33843500
H	-6.55619200	-1.80007700	1.47412000
H	-3.88404000	-5.14485400	1.04994600
C	-3.72714100	0.09019200	-2.10056400
N	-4.52485500	-0.04789700	-2.94406100
H	-6.09390400	-4.23246400	1.75387200
H	-1.77277100	3.35556900	-1.11409100
H	-2.17922400	-3.64810600	0.07076500
H	7.10269200	-1.31172300	1.16602100

TS_{3b}

Imaginary Freq = -147.90

Charge = -1 multiplicity= 1

C	-1.10377800	-3.04971200	3.12589300
C	-2.04899900	-3.56502600	0.96623300
O	-2.20325600	-1.69156300	-2.08599100
C	-1.81482900	-1.99364800	-0.95130500
O	-0.25189100	-0.67619700	2.05423700
O	-2.54370000	-4.58515600	1.44317100
H	-0.65880000	-4.04426400	3.21613900
N	-1.27258800	-2.70532000	1.71869400
C	-0.76839600	-1.45689900	1.25068300
N	-2.24530600	-3.22352500	-0.37143700
H	-2.06930400	-3.05755800	3.64264200
C	-0.87638400	-1.24002900	-0.16778800
C	-3.17787400	-4.06298400	-1.11982200
H	-2.85841000	-5.10686200	-1.07584900
H	-3.18272900	-3.69481100	-2.14443400
H	-4.18638800	-3.99798400	-0.69682800
H	-0.45451200	-2.29126400	3.55989600
C	-4.82616000	2.48463200	0.83122500
H	-5.15577900	1.58923600	1.34860300
C	-1.51583900	1.25207100	-0.56560100
O	-3.21621600	0.16756000	0.75284300
C	-1.21849900	2.41909700	-1.18174600
C	-0.49228700	0.11299800	-0.72506300
O	-1.96271700	3.56046800	-1.19239000
C	-3.14901700	3.56003800	-0.51731500
C	-3.59486600	2.41871500	0.15764100
C	-2.79249900	1.16187800	0.16803000
C	-3.89376000	4.74574100	-0.53371500
H	-3.50660100	5.60516400	-1.07219400
H	-0.42331300	-0.06343300	-1.80832900
C	-5.10654900	4.78364600	0.14021400
C	-5.57692100	3.65073500	0.82616700

H -5.69357800 5.69859900 0.13454000
H -0.31019900 2.56542300 -1.75644400
C 1.04293100 -2.44016500 -0.92969200
C 0.88366500 0.54861200 -0.25321000
N 0.84441600 -3.65863000 -0.83969600
C 2.00454600 -0.13089800 -0.56154200
C 1.92320800 -1.44122700 -1.25806900
H 0.94193900 1.41839700 0.39304000
C 3.34598600 0.36641200 -0.15910500
C 4.37395400 -0.51790700 0.22219900
C 3.63967500 1.73661300 -0.13465400
C 5.61617400 -0.05312200 0.63208700
H 4.18292500 -1.58628600 0.20552900
C 4.88202800 2.22190600 0.28040900
C 5.87901400 1.32215000 0.66844000
H 6.40159200 -0.74082200 0.93177000
H 5.06104200 3.29182200 0.27845500
C 2.80528400 -1.72457900 -2.33972100
N 3.53449500 -1.93651700 -3.22872200
H -0.10846200 -3.99287900 -0.99190900
H 2.88250600 2.44330400 -0.46265000
O 7.13887800 1.68261500 1.08639600
C 7.44543300 3.06038800 1.13802100
H 6.78519700 3.60098900 1.83134800
H 8.47528500 3.12936600 1.49734400
H 7.37801400 3.53236400 0.14729800
H -6.52777200 3.69101000 1.35066000

TS_{3c}

Imaginary Freq = -182.42

Charge = -1 multiplicity= 1

C 0.50289000 2.86813300 3.10391700
C 1.74198200 3.64523200 1.18864500
O 2.52370200 2.11978000 -1.94239300
C 1.94807400 2.24163300 -0.85274100

O	0.05753200	0.54756100	1.75374700
O	2.03726000	4.66167300	1.81541200
H	-0.05412800	3.80609500	3.17694400
N	0.94865700	2.65746700	1.72933200
C	0.62793000	1.40494100	1.09297200
N	2.19057800	3.42346200	-0.11652100
H	1.35822300	2.92492700	3.78537200
C	0.97630000	1.31799500	-0.31303200
C	3.11370800	4.39532800	-0.69958300
H	3.05637000	5.30593600	-0.10639900
H	2.83031900	4.57879200	-1.73719100
H	4.14016800	4.01158400	-0.69091000
H	-0.12705400	2.01933300	3.36364200
C	3.67143400	-3.60784700	1.40824000
H	2.84366200	-3.80874700	2.08124700
C	2.09983000	-0.93108600	-0.78248100
O	1.21612400	-2.25226600	1.02282400
C	3.18560500	-0.78159600	-1.58031100
C	0.89445500	-0.01955900	-1.05508300
O	4.36809700	-1.45355900	-1.47666600
C	4.51146800	-2.37060100	-0.47760300
C	3.46238100	-2.64621900	0.40577300
C	2.14933600	-1.94853500	0.28458400
C	5.74626200	-3.02466600	-0.38064300
H	6.53123300	-2.77767500	-1.08872400
H	0.99833500	0.27371800	-2.10918300
C	5.92790800	-3.96830900	0.62109900
C	4.88893900	-4.26302900	1.52062300
H	6.88310100	-4.48037600	0.70709300
H	3.23039300	-0.05186800	-2.37818700
C	-0.84263600	2.30102400	-1.25377200
C	-0.43757900	-0.71865500	-0.92743200
N	-0.59179300	3.42779400	-1.72545900
C	-1.63679900	-0.10852700	-1.00463000
C	-1.82330200	1.33656000	-1.20118300

H -0.42162200 -1.78013600 -0.71649600
C -2.86051100 -0.97019400 -0.92720000
C -3.76008200 -0.88738600 0.15075700
C -3.09773800 -1.91344800 -1.94029600
C -4.87026000 -1.76190500 0.20297600
C -4.20601200 -2.75057200 -1.89880900
C -5.09905900 -2.67620600 -0.82765000
H -4.38436800 -3.46628500 -2.69754500
C -3.13644900 1.86326600 -1.36672800
N -4.21254300 2.29817200 -1.51043200
H -0.00492000 4.04423500 -1.16143600
H -2.40024700 -1.96156700 -2.77085000
H -5.95564600 -3.34048500 -0.79337200
O -3.46118200 -0.02975400 1.17016700
O -5.66008000 -1.66708300 1.32640700
C -4.45125400 0.90079000 1.61776900
H -4.97160900 1.35680100 0.77011300
H -5.16907600 0.42805500 2.29458700
H -3.89444000 1.67578500 2.15099900
C -6.77616100 -2.52414400 1.42626100
H -6.48008300 -3.58312600 1.42569900
H -7.25415000 -2.28720400 2.38007800
H -7.49627800 -2.35818700 0.61194100
H 5.04193300 -5.00318900 2.30153100

TS_{3d}

Imaginary Freq = -151.32

Charge = -1 multiplicity= 1

C -0.84409600 3.14907000 2.95995300
C -0.42291000 3.85039300 0.68911800
O 0.24128900 1.99027100 -2.30260700
C -0.13494800 2.18778800 -1.14106200
O -0.68751200 0.56328300 2.06230300
O -0.37573700 5.01700800 1.07445700
H -1.66375100 3.86352200 3.07323800

N	-0.67703800	2.80219800	1.55279400
C	-0.63763400	1.42713200	1.18315800
N	-0.22219400	3.52339600	-0.65204800
H	0.06775100	3.60644500	3.35798600
C	-0.58471900	1.17016800	-0.23232600
C	0.18449100	4.61982300	-1.52824100
H	-0.54692000	5.42963200	-1.47617800
H	0.25080900	4.21244100	-2.53571400
H	1.15784300	5.02047100	-1.22469600
H	-1.05866500	2.22253000	3.48962700
C	4.65269700	-0.44620900	0.36953800
H	4.62084600	0.53117200	0.83796700
C	1.02054000	-0.83645600	-0.65125400
O	2.21059200	0.94226400	0.45799900
C	1.19455700	-2.05242000	-1.21815100
C	-0.40386800	-0.25545900	-0.70372000
O	2.35322200	-2.76607600	-1.30214800
C	3.48190500	-2.21991900	-0.76925200
C	3.45869600	-0.96109600	-0.16101400
C	2.19734700	-0.16708900	-0.06777000
C	4.66129500	-2.96952200	-0.85834100
H	4.63774700	-3.94227700	-1.33892300
H	-0.65546100	-0.20854400	-1.77331900
C	5.83419000	-2.45130400	-0.33071000
C	5.81685000	-1.18810100	0.28103600
H	6.76025100	-3.01335700	-0.38767200
H	0.38631800	-2.60540300	-1.68420000
C	-2.89015800	1.38034400	-0.78736200
C	-1.39944100	-1.19760500	-0.05178200
N	-3.22840900	2.57077700	-0.76172900
C	-2.72848700	-1.08215100	-0.23563100
C	-3.28697500	0.08033400	-0.97330100
H	-1.01089000	-1.95718100	0.61855500
C	-3.67658300	-2.06513800	0.35229000
C	-4.94015000	-1.66554900	0.82172700

C	-3.33671900	-3.42538400	0.46330000
C	-5.81504200	-2.58308800	1.40097100
H	-5.22617700	-0.62174600	0.73879500
C	-4.20800400	-4.34268200	1.04733700
C	-5.45408700	-3.92652300	1.52117400
H	-6.78383200	-2.24489800	1.76156400
H	-3.91880700	-5.38909300	1.11868400
C	-4.31096000	-0.12100500	-1.94247200
N	-5.14700300	-0.30676900	-2.73827300
H	-6.13945100	-4.64272100	1.96852500
H	-2.53425800	3.26541600	-1.04135200
Cl	7.32118300	-0.54792600	0.94589300
H	-2.38251200	-3.76300900	0.06842100

TS_{3e}

Imaginary Freq = -135.94

Charge = -1 multiplicity= 1

C	-0.34805700	3.49113000	2.88690800
C	0.10902800	4.08762200	0.59275600
O	0.54439600	2.09729700	-2.35752000
C	0.21479300	2.35661100	-1.19421000
O	-0.45297100	0.87719300	2.05962900
O	0.26922900	5.25456200	0.94549200
H	-1.10314300	4.27521300	2.98948800
N	-0.23039900	3.09152500	1.48895300
C	-0.32474500	1.71031300	1.15676700
N	0.25799800	3.70770600	-0.74066000
H	0.60440000	3.88144100	3.26026600
C	-0.30232200	1.40905400	-0.24796300
C	0.75243600	4.73779700	-1.65168900
H	0.09928900	5.61287700	-1.61577400
H	0.76854800	4.29831600	-2.64765800
H	1.76207000	5.05500500	-1.36894600
H	-0.63229500	2.60125200	3.44594900
C	4.79167300	-0.59612000	0.32976400

H	4.86524500	0.42869300	0.67619300
C	1.10863700	-0.75633600	-0.56259500
O	2.49173200	1.01631300	0.30944800
C	1.14899200	-2.04500800	-0.97482000
C	-0.25161300	-0.04159600	-0.67025200
O	2.23433500	-2.86959300	-0.99324400
C	3.42549500	-2.37373500	-0.55763500
C	3.53838500	-1.05495400	-0.10736900
C	2.35926100	-0.13919300	-0.08485000
C	4.52757000	-3.23748400	-0.58064000
H	4.39832000	-4.25421700	-0.93740200
H	-0.47759200	-0.00879400	-1.74606800
C	5.76007900	-2.77376200	-0.14667600
C	5.87918500	-1.45052900	0.30636700
H	6.62827900	-3.42408300	-0.15503900
H	0.27782100	-2.57431000	-1.34490400
C	-2.60723400	1.83139800	-0.80871300
C	-1.34429600	-0.86164300	-0.00883300
N	-2.82049100	3.04940000	-0.80150100
C	-2.65137700	-0.62379500	-0.20516600
C	-3.11465600	0.56885200	-0.96164000
H	-1.04006900	-1.65650300	0.66287900
C	-3.70350300	-1.46263300	0.43583000
C	-4.73889500	-0.82154000	1.14515300
C	-3.76342100	-2.86759800	0.39130200
C	-5.74796300	-1.52542300	1.79229800
H	-4.72403500	0.26330100	1.18090300
C	-4.77072000	-3.59058800	1.03354300
C	-5.76479000	-2.92016700	1.74109400
H	-6.51940500	-0.98558900	2.33506600
H	-4.77288500	-4.67338600	0.96277400
C	-4.18185300	0.43738500	-1.89621700
N	-5.05874100	0.30862500	-2.65813300
H	-6.54872900	-3.48617300	2.23764400
Cl	-2.58994900	-3.82773200	-0.52836700

H	-2.07020900	3.66455000	-1.12008500
Cl	7.45768500	-0.88126200	0.85416600

Table 12: Thermodynamic parameters for intermediates **3a-3e** at b3lyp/6-31g (d) level of theory

Intermediate **3**	G	H	S	E
In_{3a}	-1635.687039	-1635.593535	196.795	-1636.052440
In_{3b}	-1750.180599	-1750.081044	209.530	-1750.575299
In_{3c}	-1864.663769	-1864.557955	222.704	-1865.087490
In_{3d}	-2095.292299	-2095.195305	204.141	-2095.645659
In_{3e}	-2554.896952	-2554.796012	212.446	-2555.237872

In_{3a}

Charge= 0 multiplicity= 1

C 1.13734800 1.12301900 3.30629200
C 2.02818900 2.16750000 1.26914600
O 0.50267200 2.87892800 -1.89949800
C 0.65441900 2.40117400 -0.77947700
O -1.22004100 0.96348300 2.02515300
O 3.10287400 2.36978400 1.80420000
H 2.17023700 1.31245100 3.58803500
N 0.97150800 1.52895700 1.90249800
C -0.28287900 1.30121900 1.33524900
N 1.80020700 2.62669600 -0.04389600
H 0.89993000 0.06120000 3.38679700
C -0.38779200 1.45779400 -0.19159600
C 2.89559500 3.40606600 -0.64046300
H 3.10363100 4.28306500 -0.02442400
H 2.57849900 3.70584400 -1.63646500
H 3.79829600 2.79401500 -0.68972700
H 0.45653700 1.69625700 3.93944200
C 3.62257200 -2.63481200 1.07209700
H 3.05574800 -2.78701800 1.98477000
C 1.18483700 -0.53413100 -0.94068100
O 1.01896400 -1.44289100 1.25280300

C	1.97815200	-0.41853000	-2.03376300
C	-0.20291200	0.07054900	-0.97545000
O	3.21554900	-0.93641400	-2.16830500
C	3.74427500	-1.66775600	-1.13255500
C	3.02549200	-1.87315300	0.05220100
C	1.67509000	-1.29476800	0.22038900
C	5.02510400	-2.19405000	-1.32024600
H	5.54482200	-2.00934300	-2.25456600
H	-0.38279700	0.39677500	-2.01214600
C	5.59165400	-2.94215300	-0.29694400
C	4.89166500	-3.16511300	0.90153900
H	6.58652300	-3.35783400	-0.42822200
H	1.68846500	0.11854900	-2.93115600
C	-1.80880100	1.92479600	-0.52704100
C	-1.30021300	-0.88886600	-0.59338100
N	-2.01104300	3.27906800	-0.56121900
C	-2.56709100	-0.44742600	-0.46692000
C	-2.81629000	0.99752300	-0.63694500
H	-1.04510600	-1.92051400	-0.38668900
C	-3.68527100	-1.36674500	-0.13939200
C	-4.64024300	-1.02524600	0.83227600
C	-3.79087500	-2.61370800	-0.77623200
C	-5.66469000	-1.91094200	1.16166600
H	-4.56321000	-0.07252700	1.34706200
C	-4.81575200	-3.49885000	-0.44560600
C	-5.75694900	-3.14995900	0.52458300
H	-6.39065500	-1.63281800	1.92090800
H	-4.88518100	-4.45702500	-0.95402700
C	-4.12176900	1.49576900	-0.92667700
N	-5.14796700	1.98988000	-1.17801400
H	-6.55982800	-3.83677500	0.77898400
H	-1.30023100	3.81388500	-1.04808200
H	-2.95709700	3.57025100	-0.78754200
H	-3.07299000	-2.87653900	-1.54833400
H	5.34812400	-3.75242800	1.69254700

In_{3b}

Charge= 0 multiplicity= 1

C	-1.78186500	-0.92088300	3.33568900
C	-2.93902500	-1.76125700	1.33848600
O	-1.69317100	-2.88936100	-1.83147300
C	-1.70263100	-2.36429400	-0.72233000
O	0.51807500	-1.36336200	2.01780000
O	-4.02014600	-1.68606300	1.89346200
H	-2.82387500	-0.85463700	3.63893000
N	-1.74716200	-1.38417900	1.94041200
C	-0.48616200	-1.47908300	1.34971800
N	-2.85460200	-2.28944800	0.03443900
H	-1.29876100	0.05613800	3.38531700
C	-0.45255400	-1.68848900	-0.17357700
C	-4.11710000	-2.79369200	-0.52656600
H	-4.51620700	-3.58426800	0.11198800
H	-3.90213400	-3.17851100	-1.52062500
H	-4.84779600	-1.98398000	-0.57453500
H	-1.24173600	-1.62535400	3.97200400
C	-3.33816100	3.27916500	1.03348900
H	-2.73450700	3.31108500	1.93461900
C	-1.51393000	0.60764400	-0.95218500
O	-1.09522200	1.50096900	1.21450400
C	-2.33257000	0.66105200	-2.03130600
C	-0.31282100	-0.31383000	-0.98998800
O	-3.41194900	1.45820100	-2.16448800
C	-3.72985800	2.31922000	-1.14255100
C	-2.96091700	2.37268600	0.02713400
C	-1.78586200	1.49039100	0.19421500
C	-4.84963500	3.13436800	-1.32835800
H	-5.41583900	3.05875000	-2.25079200
H	-0.23792100	-0.69702400	-2.02007400
C	-5.20038900	4.02052100	-0.31866200
C	-4.44520600	4.09576000	0.86458300
H	-6.06825800	4.66060400	-0.44872200

H -2.19732000 0.04931900 -2.91738500
C 0.80731800 -2.49062200 -0.51847500
C 0.98966400 0.36045100 -0.64555400
N 0.67691300 -3.85449100 -0.52119700
C 2.11693200 -0.36991200 -0.52928600
C 2.00530200 -1.83578500 -0.66872400
H 0.99279800 1.42596800 -0.45421300
C 3.43146800 0.25473600 -0.25025000
C 4.31177600 -0.28744900 0.70580800
C 3.82241100 1.42711300 -0.90841700
C 5.52199800 0.32483200 0.99387500
H 4.02993700 -1.18611100 1.24562300
C 5.03794900 2.05435700 -0.62980000
C 5.89607500 1.50161500 0.32768500
H 6.19721600 -0.08770700 1.73683800
H 5.30666900 2.95549200 -1.16918300
C 3.14502800 -2.64002500 -0.97022000
N 4.01555400 -3.37191400 -1.22910200
H -0.15082500 -4.21172500 -0.98555800
H 1.52053700 -4.36920700 -0.75447900
H 3.17199700 1.84997800 -1.66914200
O 7.10768900 2.02252800 0.67921800
C 7.53940500 3.21058000 0.03673800
H 6.85101000 4.04534600 0.22502000
H 8.51559400 3.44516400 0.46529100
H 7.64460800 3.06880600 -1.04718000
H -4.73216000 4.79381400 1.64517500

In_{3c}

Charge= 0 multiplicity= 1

C -2.48776000 -1.09749200 3.22804900
C -3.27522500 -1.94085100 1.05960100
O -1.50196500 -2.84813600 -1.92328000
C -1.71214700 -2.36767000 -0.81441200
O 0.00470000 -1.30314200 2.25059100

O	-4.42685800	-1.96871600	1.45411600
H	-3.56461700	-1.12024900	3.37628900
N	-2.21518300	-1.50071100	1.84039400
C	-0.87879500	-1.47667600	1.43908700
N	-2.96425100	-2.40588200	-0.23319700
H	-2.09501300	-0.09043300	3.37646900
C	-0.60798600	-1.62918300	-0.06801900
C	-4.08957200	-2.97753400	-0.98785900
H	-4.51262100	-3.82158200	-0.43945900
H	-3.70452200	-3.30330900	-1.95124100
H	-4.86733800	-2.22241300	-1.11717700
H	-1.99172000	-1.78528400	3.91645200
C	-3.93906100	3.10322600	0.91447400
H	-3.46176000	3.13251800	1.88852200
C	-1.70612700	0.62738900	-0.89955300
O	-1.63111800	1.45173500	1.33244400
C	-2.37632500	0.68048400	-2.07654900
C	-0.45288700	-0.21765800	-0.80771400
O	-3.47737600	1.41822000	-2.32512600
C	-3.98043400	2.21475300	-1.32581400
C	-3.37649900	2.26337600	-0.06273900
C	-2.18042600	1.44422600	0.22932100
C	-5.11564200	2.97039900	-1.63131500
H	-5.54982000	2.90112900	-2.62322000
H	-0.21276800	-0.54479000	-1.83163900
C	-5.65120800	3.79114300	-0.64787500
C	-5.06388600	3.86032400	0.62740800
H	-6.53323900	4.38460100	-0.87072600
H	-2.08545500	0.11836700	-2.95805100
C	0.73823700	-2.34091400	-0.23949100
C	0.74756600	0.51981200	-0.27081300
N	0.69462500	-3.71377700	-0.24433400
C	1.88939500	-0.14525700	-0.03231200
C	1.89867400	-1.60976700	-0.21130400
H	0.67686500	1.58691100	-0.10078400

C	3.09725800	0.55483500	0.49402300
C	3.09530300	1.02410200	1.81612400
C	4.21430600	0.76731900	-0.32788000
C	4.20481200	1.69160100	2.32033900
H	2.22409500	0.83393300	2.43467700
C	5.32490700	1.48007800	0.18083900
C	5.31751700	1.92006900	1.50715300
H	4.21206900	2.04349000	3.34797900
C	3.12440700	-2.33531600	-0.27542000
N	4.08074400	-2.99975200	-0.34243900
H	6.16994000	2.45758300	1.90659200
O	4.11815200	0.34398300	-1.62688100
O	6.34707900	1.71929600	-0.69955400
C	5.21494300	-0.36460200	-2.22078800
H	5.98926700	0.32211000	-2.56863300
H	5.64121500	-1.08776700	-1.51912600
H	4.78460500	-0.90410800	-3.06805100
C	7.48936400	2.41310300	-0.22804200
H	8.16908900	2.48213700	-1.07959400
H	7.23463400	3.42497700	0.11438200
H	7.98485100	1.87101600	0.58837500
H	-5.49415000	4.50716200	1.38599300
H	-0.01815500	-4.11919500	-0.84129000
H	1.59584400	-4.17177700	-0.33929500

$In_{\mathbf{3d}}$

Charge= 0 multiplicity= 1

C	-0.75532400	-1.13251000	3.28104800
C	-1.25957000	-2.56689500	1.35125600
O	0.61594700	-3.30577400	-1.61740300
C	0.28709800	-2.74579000	-0.57630800
O	1.61503200	-0.63642200	2.11392100
O	-2.31133600	-2.92292000	1.84999900
H	-1.75211100	-1.49045100	3.52681100
N	-0.40477600	-1.65224100	1.95028800

C	0.82035800	-1.23874400	1.42563400
N	-0.84231100	-3.11953600	0.12322200
H	-0.73141200	-0.04253500	3.24170300
C	1.07253200	-1.54590300	-0.06084200
C	-1.70844800	-4.17640800	-0.42133200
H	-1.78665300	-4.99574800	0.29582500
H	-1.25832500	-4.52228600	-1.34879500
H	-2.70825400	-3.77681700	-0.60222400
H	-0.03003200	-1.48444400	4.01802700
C	-3.74518100	1.75711100	0.44731300
H	-3.29862600	2.13324300	1.36073000
C	-0.79984600	-0.02187000	-1.14251500
O	-0.99307000	1.15669900	0.91828200
C	-1.46729200	-0.42878600	-2.25022500
C	0.67904000	-0.32703800	-1.02569900
O	-2.76944000	-0.19731100	-2.51649800
C	-3.50912900	0.52733000	-1.61743300
C	-2.94138000	1.01689600	-0.43536900
C	-1.51874600	0.75346400	-0.11919000
C	-4.85098300	0.75574500	-1.93572000
H	-5.25646000	0.36052900	-2.86102900
H	0.99918800	-0.72721000	-2.00080000
C	-5.63450300	1.48772700	-1.05638300
C	-5.07348900	1.98532200	0.13217200
H	-6.67818000	1.67889900	-1.28078200
H	-1.00877800	-0.99814900	-3.05199600
C	2.57964900	-1.74560100	-0.25780400
C	1.53095400	0.87614800	-0.71406300
N	3.04795700	-3.02339500	-0.10478500
C	2.84633600	0.72260900	-0.46475300
C	3.38897500	-0.64964200	-0.43337200
H	1.06181800	1.85016800	-0.65642800
C	3.73155300	1.88409100	-0.20003000
C	4.65470700	1.86163800	0.85825600
C	3.63895100	3.04317400	-0.98704500

C 5.45450700 2.97142900 1.12482000
H 4.72648600 0.98004600 1.48773000
C 4.43940100 4.15255400 -0.71925400
H 2.94707500 3.06105300 -1.82460500
C 5.35062200 4.12009000 0.33783200
H 6.15825200 2.93911600 1.95214300
H 4.35854000 5.03872200 -1.34335400
C 4.78591600 -0.89831100 -0.58615400
N 5.90584300 -1.19666000 -0.71664900
H 5.97914700 4.98230800 0.54405100
Cl -6.08540100 2.90944500 1.22680000
H 2.49792200 -3.74744000 -0.55356900
H 4.04791000 -3.13790000 -0.23901500

In_{3e}

Charge= 0 multiplicity= 1

C 1.21302800 1.57893200 3.19706400
C 1.73442500 2.74557800 1.09826400
O -0.21560700 3.30134800 -1.86124500
C 0.11931200 2.83355400 -0.77795200
O -1.23667300 1.14178400 2.18354700
O 2.83102700 3.06926100 1.51531100
H 2.24209800 1.88714700 3.36454700
N 0.84061300 1.97440200 1.82985900
C -0.43286900 1.60234300 1.40125800
N 1.30542500 3.18940300 -0.16852000
H 1.11220700 0.49587000 3.28108700
C -0.73083800 1.76521300 -0.10052300
C 2.22298200 4.10681500 -0.86178000
H 2.39147000 4.99419200 -0.24860000
H 1.76040400 4.37867700 -1.80758500
H 3.18197900 3.61234000 -1.02816300
H 0.54721700 2.06213400 3.91551000
C 3.82036800 -1.85441300 0.62043500
H 3.38439000 -2.08592900 1.58557300

C	0.96535900	-0.01930700	-1.06630900
O	1.14678400	-0.97146000	1.10821500
C	1.61423000	0.20015200	-2.23628700
C	-0.47760200	0.41985800	-0.93349100
O	2.88036300	-0.17072500	-2.51634700
C	3.59654800	-0.84981000	-1.56419900
C	3.04228400	-1.15230000	-0.31486800
C	1.66095900	-0.73394200	0.01491100
C	4.90037500	-1.22702600	-1.89847500
H	5.29626100	-0.97557100	-2.87664400
H	-0.81188700	0.72942700	-1.93631500
C	5.65884800	-1.91939000	-0.96669200
C	5.11095900	-2.22957700	0.28976400
H	6.67279000	-2.22370200	-1.20220000
H	1.16860800	0.71027600	-3.08386900
C	-2.22480100	2.07023700	-0.25590900
C	-1.40619200	-0.66819400	-0.45793200
N	-2.58296300	3.39216400	-0.21452400
C	-2.68667300	-0.37305800	-0.17991700
C	-3.12307600	1.03251300	-0.27056500
H	-1.02383000	-1.67464200	-0.34603800
C	-3.65640400	-1.39754000	0.29712100
C	-4.18242900	-1.26911000	1.59456200
C	-4.07811800	-2.49768300	-0.46556200
C	-5.07893500	-2.19888300	2.11240800
H	-3.85336900	-0.42794200	2.19769200
C	-4.97920900	-3.43544700	0.04075100
C	-5.47838500	-3.28533200	1.33269100
H	-5.46277700	-2.07606100	3.12090100
H	-5.28660400	-4.26905100	-0.58149400
C	-4.50845000	1.36499100	-0.34885500
N	-5.61654200	1.72011000	-0.42470400
H	-6.18060000	-4.01624500	1.72367900
Cl	-3.50948600	-2.73174600	-2.11990500
Cl	6.09059400	-3.10715200	1.45000700

H -2.00704600 4.01689500 -0.76812600

H -3.57719500 3.57420400 -0.31178200

Table 13: Thermodynamic parameters for TS_3 at b3lyp/6-31g (d) level of theory in the liberalization step of 1,3-dimethyl barbituric acid.

TS_3	G	H	S	E
TS_{3f}	-2094.757380	-2094.655921	213.538	-2095.089546
TS_{3g}	-2094.758942	-2094.656978	214.601	-2095.090609
TS_{3h}	-2209.251357	-2209.143587	226.821	-2209.612659
TS_{3i}	-2323.736054	-2323.622916	238.120	-2324.127100

TS_{3f}

Imaginary Freq = -277.96

Charge = -1 multiplicity= 1

C 3.51899400 2.23321900 -1.83809000

C 2.47883900 2.69333800 0.30304300

O -0.92500300 2.61277200 1.36308700

C 0.04549100 2.41499800 0.63555600

O 1.01927200 1.55162400 -2.77820300

O 3.58721300 3.02553300 0.71115000

H 3.93076500 3.24294400 -1.92667200

N 2.31537800 2.24113700 -1.00985800

C 1.08270300 1.86130500 -1.58549100

N 1.33458700 2.76165200 1.08489600

H 3.22712000 1.85636700 -2.81678200

C -0.03615700 1.76597300 -0.66430300

C 1.46009700 3.18625300 2.47829000

H 2.49969000 3.45494000 2.65268500

H 1.16289200 2.36296300 3.13294000

H 0.80270800 4.03856200 2.66607600

H 4.28190200 1.59322300 -1.38693700

C 4.23701400 -1.67387800 1.41328200

H 4.02976600 -1.22669900 2.38016400

C 1.02382700 -0.83426300 -0.42593600

O 1.77275800 -0.29060500 1.77993300

C 1.40219800 -1.39408900 -1.60291100

C	-0.32693000	-0.21695800	-0.33957600
O	2.57999800	-2.02241200	-1.84710200
C	3.49644500	-2.11390700	-0.83705500
C	3.24886500	-1.55246500	0.42149700
C	1.97713800	-0.83864100	0.69702800
C	4.69050200	-2.78705800	-1.11995300
H	4.83957400	-3.20560200	-2.11023100
H	-0.85664200	-0.30680200	-1.28568200
C	5.64834400	-2.89678800	-0.12128100
C	5.42421900	-2.33965700	1.14964200
H	6.57936000	-3.41785300	-0.32893900
H	0.78300200	-1.39008000	-2.49127300
C	-2.65595900	-1.29320700	3.18201100
C	-1.11547500	-0.48722100	0.82148200
N	-2.14812300	-1.66029100	4.16905300
C	-2.50587600	-0.48999300	0.84448500
C	-3.27388100	-0.85886600	1.97954700
H	-0.59515300	-0.69605300	1.74890000
C	-3.27810900	-0.03958300	-0.36003300
C	-3.73916000	-0.90269000	-1.36251600
C	-3.57839800	1.32678500	-0.49307600
C	-4.47497600	-0.43757300	-2.45373700
C	-4.31318100	1.80529700	-1.57619800
H	-3.19926900	2.00338100	0.26741000
C	-4.76491300	0.92120000	-2.55703200
H	-4.81495200	-1.14033900	-3.20733900
H	-4.53178900	2.86700900	-1.65261700
C	-4.69248400	-0.83686200	1.97273300
N	-5.86223900	-0.82444800	1.98956800
H	-5.34020500	1.28382800	-3.40510700
H	6.18254200	-2.43047100	1.92223000
Cl	-3.38885300	-2.63072700	-1.28518800
H	-0.99702000	1.90337100	-1.14561200

TS_{3g}

Imaginary Freq = -277.05

Charge = -1 multiplicity= 1

C	2.38343900	3.46017300	-0.54054300
C	1.41394300	2.60414100	1.51035700
O	-1.86593400	1.44352800	2.28801200
C	-0.92014700	1.79490100	1.58725900
O	-0.02302900	2.91990000	-1.77052200
O	2.47609800	2.87257000	2.06207700
H	2.61419100	4.43444300	-0.09961600
N	1.24795000	2.84412200	0.14234200
C	0.06041500	2.60021400	-0.58162700
N	0.32289100	2.07747100	2.18644000
H	2.10009400	3.57555700	-1.58526200
C	-0.97335600	1.87095200	0.13409100
C	0.45765900	1.77456600	3.61058500
H	1.46369000	2.05279700	3.91677400
H	0.29083100	0.70605600	3.76711000
H	-0.28798800	2.33271500	4.18254200
H	3.26898000	2.82627900	-0.44505900
C	3.90815700	-1.36558500	0.25343100
H	3.71592300	-1.51143500	1.31050000
C	0.48216000	-0.26826900	-0.94620800
O	1.31184300	-0.78562200	1.23907900
C	0.85218600	-0.08272500	-2.23868600
C	-0.93825600	-0.01893300	-0.57485500
O	2.09146400	-0.29225000	-2.75533700
C	3.08158200	-0.72522000	-1.92317800
C	2.84883100	-0.92678100	-0.55802900
C	1.50736100	-0.67301500	0.03051200
C	4.34036400	-0.95402600	-2.49125000
H	4.48309500	-0.78489700	-3.55356700
H	-1.52109500	0.27409900	-1.44590100
C	5.37769600	-1.39164800	-1.68204200
C	5.15001200	-1.59431600	-0.31126800

H	6.36146200	-1.57681900	-2.09985100
H	0.17656900	0.26907500	-3.00802600
C	-2.71143100	-3.22590900	1.75198500
C	-1.57937500	-0.97496300	0.27493200
N	-2.05163100	-3.94793300	2.39261400
C	-2.93816600	-1.27923100	0.23568900
C	-3.51033000	-2.35912700	0.95909900
H	-0.96048200	-1.51581700	0.98146700
C	-3.87277700	-0.46215700	-0.60500100
C	-4.32723200	-0.92941500	-1.84562500
C	-4.31809700	0.78602600	-0.14369500
C	-5.19886900	-0.16017800	-2.61816300
C	-5.19541500	1.55029400	-0.91512100
H	-3.96330200	1.14411600	0.81892600
C	-5.63577100	1.08174900	-2.15462200
H	-5.54173300	-0.53550600	-3.57961500
H	-5.53640500	2.51422000	-0.54471500
C	-4.89903100	-2.65075400	0.92281000
N	-6.03712400	-2.92136100	0.90822800
H	-6.31804300	1.67961300	-2.75452900
H	-1.96912200	2.07258400	-0.24182600
Cl	6.48528400	-2.15117200	0.69534300
H	-3.99794700	-1.90283600	-2.19906400

$TS_{\mathbf{3h}}$

Imaginary Freq = -277.19

Charge = -1 multiplicity= 1

C	-2.53979500	-3.55767600	0.27260800
C	-1.85950300	-2.14331800	2.12091400
O	1.24206600	-0.56362000	2.89243000
C	0.40423700	-1.15613600	2.21692800
O	-0.03438000	-3.16098200	-0.80477000
O	-2.96350600	-2.34780300	2.61473600
H	-2.77376200	-4.40477400	0.92411700
N	-1.52341900	-2.70483200	0.88470400

C	-0.27330000	-2.55815900	0.24490300
N	-0.88252100	-1.37992400	2.74369700
H	-2.13029700	-3.90935100	-0.67273500
C	0.63049000	-1.59034400	0.84535200
C	-1.19736000	-0.74161300	4.02097900
H	-2.21490600	-1.01700400	4.28933700
H	-1.10968900	0.34211100	3.91159900
H	-0.49253600	-1.07422800	4.78725600
H	-3.45960700	-2.98938000	0.11088000
C	-4.39950500	1.13391500	-0.37260200
H	-4.34574700	1.55135700	0.62663100
C	-0.79521600	0.07613100	-0.89438500
O	-1.91228300	1.04413600	0.98892000
C	-0.99418700	-0.45250600	-2.12822200
C	0.58142600	0.04894800	-0.32612400
O	-2.17154000	-0.48387600	-2.80651100
C	-3.27880800	0.05262400	-2.21814200
C	-3.22560900	0.60331900	-0.93268300
C	-1.95294400	0.61996500	-0.16435500
C	-4.47068900	0.02397200	-2.95181000
H	-4.47338300	-0.41309500	-3.94502100
H	1.28207300	-0.40059300	-1.02716200
C	-5.62242200	0.55479700	-2.39135800
C	-5.57499000	1.10730900	-1.10123300
H	-6.55744800	0.54481600	-2.94116000
H	-0.21113000	-0.92329700	-2.70899300
C	1.84219200	3.91748300	1.16486800
C	1.05813500	1.24289200	0.30283400
N	1.06003000	4.72032300	1.49793300
C	2.38870300	1.65676900	0.30645000
C	2.79104900	2.94791200	0.74311400
H	0.32639500	1.88909500	0.77373900
C	3.47168000	0.73988900	-0.17352800
C	4.09715400	0.93166000	-1.40803000
C	3.90300500	-0.32828000	0.63305700

C 5.11543700 0.08148200 -1.85047500
H 3.79012900 1.76307100 -2.03660600
C 4.91988200 -1.17566400 0.20857400
H 3.42804900 -0.47993300 1.59855900
C 5.53069600 -0.97636600 -1.03664800
H 5.57602700 0.26224900 -2.81542900
H 5.26226000 -1.99824800 0.82951800
C 7.19031900 -1.68925900 -2.59721400
H 7.93815200 -2.48396300 -2.65452600
H 6.50398600 -1.77941600 -3.45128900
H 7.69470700 -0.71429400 -2.64990800
O 6.52214200 -1.86844400 -1.36461000
C 4.15021100 3.35646700 0.76847800
N 5.25947100 3.72778300 0.79345000
Cl -7.05305100 1.77540200 -0.41169300
H 1.67195100 -1.80294800 0.63643500

TS_{3i}

Imaginary Freq = -278.75

Charge = -1 multiplicity= 1

C 2.98465200 2.76505100 -2.16787700
C 2.38017900 2.98435800 0.17107700
O -0.75578700 2.69790300 1.85961900
C 0.06702500 2.59766700 0.95328200
O 0.36125500 2.05866900 -2.65278600
O 3.54013700 3.31200600 0.39814400
H 3.35483900 3.79257800 -2.23212300
N 1.97046500 2.65040400 -1.12324100
C 0.65658300 2.27198200 -1.47358400
N 1.41904700 2.94852400 1.16714300
H 2.50981000 2.47411700 -3.10337200
C -0.25101000 2.05566400 -0.35994500
C 1.87033000 3.25789800 2.52213600
H 2.33871000 4.24520100 2.55059800
H 2.59786200 2.50937200 2.84651800

H 0.99067200 3.23076800 3.16248800
H 3.83299200 2.11258100 -1.94361600
C 4.43448700 -1.36991500 0.51388500
H 4.42229300 -1.02436200 1.54150800
C 0.90459200 -0.50493000 -0.56725100
O 2.07415200 -0.13401700 1.48846300
C 1.05114100 -0.93958900 -1.84490800
C -0.41780100 0.04156700 -0.15974700
O 2.17144500 -1.49259800 -2.37871900
C 3.27135700 -1.63614100 -1.58534100
C 3.27035400 -1.20375200 -0.25438500
C 2.06315500 -0.57009100 0.33880300
C 4.40167400 -2.22947900 -2.15983700
H 4.36495100 -2.55088700 -3.19561900
H -1.12442900 0.00237400 -0.98572500
C 5.54389500 -2.39295700 -1.39107100
C 5.54867000 -1.95965500 -0.05538600
H 6.43149500 -2.85111800 -1.81405800
H 0.26605900 -0.88203500 -2.58803400
C -1.97264400 -1.47655500 3.60954600
C -0.95377600 -0.36026300 1.10218500
N -1.27131500 -1.88733000 4.45002400
C -2.31404400 -0.46209000 1.37122600
C -2.82857000 -0.99029800 2.58579000
H -0.25747600 -0.60991900 1.89441800
C -3.31997500 0.03427400 0.37294800
C -3.91155700 -0.82682500 -0.55811300
C -3.67666000 1.39401800 0.38402400
C -4.85604800 -0.32439400 -1.48205800
C -4.61930700 1.87710100 -0.51548900
H -3.19230100 2.05094700 1.09989000
C -5.21349000 1.02413500 -1.45134700
H -4.89781200 2.92754300 -0.49993000
C -4.22032100 -1.11002400 2.82531100
N -5.36622400 -1.23723400 3.03059800

Cl	7.01336400	-2.17914700	0.90055700
H	-5.94039400	1.41874200	-2.15273700
O	-3.51268400	-2.14064300	-0.61586000
O	-5.35488000	-1.23839100	-2.37766100
C	-4.47988300	-3.10627300	-0.18476500
H	-4.87607900	-2.84963800	0.80312500
H	-5.30164400	-3.18955800	-0.90465900
H	-3.94437300	-4.05766500	-0.12841600
C	-6.29904000	-0.78404900	-3.32584000
H	-5.87990200	-0.00301600	-3.97572300
H	-6.55873500	-1.65445300	-3.93307200
H	-7.20770100	-0.39540700	-2.84467200
H	-1.29276100	2.18675000	-0.62710800

Table 14: Thermodynamic parameters for Products **f-i** at b3lyp/6-31g (d) level of theory

Product	G	H	S	E
P_f	-1526.729636	-1526.653288	160.688	-1526.939590
P_g	-1526.732196	-1526.656280	159.778	-1526.942710
P_h	-1641.227897	-1641.146116	172.124	-1641.468026
P_i	-1755.709158	-1755.619530	188.638	-1755.976381
1,3-Dimethylbarbituric Acid	-568.034635	-567.988045	98.056	-568.133785

P_f

Charge= 0 multiplicity= 1

C 4.49130300 -1.76654400 -0.71421100
H 3.88371900 -2.58384600 -1.08863000
C 1.80757000 0.79504500 0.11152200
O 1.66097900 -1.41474300 -0.80091100
C 2.67970900 1.74824000 0.55747500
C 0.39422700 1.12976200 0.13734600
O 4.01302700 1.63364200 0.61019300
C 4.60071200 0.46294300 0.18719000
C 3.82829000 -0.59916000 -0.29744700
C 2.35339100 -0.49404700 -0.37057100
C 5.99304100 0.39373600 0.26626300
H 6.54810000 1.24387000 0.64869000
H 0.17868300 2.12345900 0.51874800
C 6.62281200 -0.77154000 -0.15180300
C 5.87324000 -1.85407300 -0.64279400
H 7.70524600 -0.84202700 -0.09703700
H 2.35981500 2.72066400 0.91814900
C -1.82110600 3.12675800 -0.31794500
C -0.63042200 0.32289600 -0.23991100
N -1.21876400 4.12124500 -0.38696900
C -2.04576700 0.65513100 -0.22386000
C -2.59145700 1.92359800 -0.23203400

H -0.39235800 -0.68496500 -0.55855800
C -2.97885200 -0.51034500 -0.29931100
C -3.77307600 -0.68653900 -1.44420700
C -3.06560400 -1.48037300 0.71283900
C -4.61162500 -1.78955800 -1.58065500
H -3.71513000 0.05252600 -2.23731800
C -3.90940200 -2.58312600 0.59081800
C -4.67868800 -2.73901300 -0.56126000
H -5.21088700 -1.90335600 -2.47873200
H -3.96173800 -3.30552100 1.39812900
C -4.00575700 2.14191800 -0.15212200
N -5.14585700 2.36777500 -0.08492100
H 6.37908000 -2.75880300 -0.96612500
H -5.33253400 -3.60120100 -0.65496900
Cl -2.14570200 -1.30525900 2.20086500

P_g

Charge= 0 multiplicity= 1
C -3.92473700 0.99945900 -0.32388600
H -3.48117600 1.92883000 -0.66255900
C -0.83380400 -1.10465900 0.32345800
O -1.08990400 1.14837400 -0.44928600
C -1.51784600 -2.21300600 0.73491400
C 0.61861700 -1.19062600 0.29987600
O -2.85129500 -2.33193400 0.81564200
C -3.63772400 -1.26320800 0.46144500
C -3.07182300 -0.06079700 0.02425800
C -1.60110500 0.09584500 -0.07246400
C -5.02077100 -1.43409600 0.55916800
H -5.42059100 -2.38256700 0.90162500
H 1.01537200 -2.13340300 0.66720800
C -5.85260600 -0.37968900 0.21252800
C -5.29588400 0.83306900 -0.22751600
H -6.92979800 -0.48609000 0.27880200
H -1.02891200 -3.13354600 1.03648900

C	2.95917300	-2.76170600	-0.65872100
C	1.47848500	-0.22851900	-0.11312600
N	2.46761900	-3.78050100	-0.93677900
C	2.93602600	-0.33933000	-0.12638800
C	3.61048500	-1.53261900	-0.31668700
H	1.07200300	0.72820200	-0.41895100
C	3.67213100	0.93618700	0.05370800
C	4.80687800	1.25691400	-0.71220600
C	3.20108400	1.87678400	0.98865600
C	5.45871800	2.47488000	-0.53410600
H	5.16587100	0.56460900	-1.46565400
C	3.86385600	3.08689700	1.17449300
C	4.99463800	3.38963900	0.41283200
H	6.32825600	2.71020800	-1.14087500
C	5.02964800	-1.66670900	-0.17014900
N	6.17487500	-1.83930600	-0.04914900
H	3.49533700	3.79484100	1.91138100
H	5.50757800	4.33728200	0.55187000
Cl	-6.36790500	2.15207100	-0.65951500
H	2.32194100	1.64530500	1.58255700

P_h

Charge= 0 multiplicity= 1

C	4.28100700	-1.30719300	-0.34880200
H	3.70011200	-2.14352500	-0.72067600
C	1.55293600	1.23591200	0.35076500
O	1.45993400	-1.00376600	-0.49462000
C	2.39813100	2.20836800	0.80296200
C	0.13148700	1.54938400	0.32235100
O	3.73350800	2.11317300	0.89535000
C	4.34530900	0.94617800	0.51001900
C	3.60194600	-0.13734500	0.02975900
C	2.12597800	-0.05698400	-0.08043000
C	5.73705000	0.89326200	0.62091100
H	6.27751100	1.75534700	0.99702500

H -0.11830800 2.52635700 0.72819400
C 6.39615000 -0.26740500 0.24391900
C 5.66001500 -1.36235200 -0.23936000
H 7.47589400 -0.33446400 0.31959900
H 2.05703100 3.18434500 1.13217900
C -1.87886400 3.49294100 -0.67382400
C -0.86237100 0.75430900 -0.13895700
N -1.21736200 4.41082500 -0.95213900
C -2.28506600 1.10003500 -0.15519800
C -2.73747900 2.39939200 -0.33118700
H -0.60778400 -0.23972600 -0.48685900
C -3.21760100 -0.03241300 0.00195900
C -4.43513900 -0.11477300 -0.69480100
C -2.87464000 -1.10804200 0.85158100
C -5.28861600 -1.20380000 -0.54445600
H -4.71614100 0.66758300 -1.39035600
C -3.72113800 -2.18884300 1.02207300
C -4.94060100 -2.24636100 0.32574200
H -6.21142500 -1.23275800 -1.11148000
C -4.10653100 2.78742400 -0.16969200
N -5.20181800 3.16061100 -0.03551900
H -3.46464800 -3.00596600 1.68840700
Cl 6.51575700 -2.81969300 -0.70927400
H -1.93816600 -1.07781300 1.40002800
O -5.69833400 -3.34735000 0.55493000
C -6.95164300 -3.46264300 -0.10900000
H -6.82572600 -3.49561100 -1.19845200
H -7.38284900 -4.40413000 0.23424200
H -7.62187800 -2.63567200 0.15614100

P_i

Charge= 0 multiplicity= 1

C 4.61492100 -1.24704600 -0.18354500
H 4.06541200 -2.12553700 -0.50207500
C 1.82207300 1.30743200 0.10170500

O	1.80815100	-1.00369100	-0.53414100
C	2.63182100	2.33485900	0.49711700
C	0.40260300	1.59952700	-0.03008100
O	3.96072100	2.27170700	0.67251700
C	4.60589000	1.08163500	0.44509100
C	3.90289900	-0.05604900	0.03463700
C	2.43510000	-0.01106600	-0.16948300
C	5.98900400	1.06217700	0.64180700
H	6.49752000	1.96606600	0.95986700
H	0.13792100	2.62304000	0.21439100
C	6.68080000	-0.11994900	0.42340600
C	5.98542800	-1.26924400	0.01116100
H	7.75466900	-0.16216600	0.56865700
H	2.26140100	3.33255800	0.70895000
C	-1.93385300	3.45478900	-0.50632200
C	-0.56482300	0.72307200	-0.40288900
N	-1.39267200	4.48401300	-0.43313900
C	-1.99533400	0.97275500	-0.53130600
C	-2.61817200	2.20246300	-0.59545100
H	-0.26641400	-0.30133400	-0.59055700
C	-2.82316800	-0.26409000	-0.65866700
C	-2.59264800	-1.13837100	-1.73681300
C	-3.79842500	-0.58293200	0.29805800
C	-3.34382300	-2.29738600	-1.86736000
H	-1.83521700	-0.88983800	-2.47376200
C	-4.56067600	-1.76657300	0.15591300
C	-4.32770300	-2.61669000	-0.92638200
H	-3.17346500	-2.96300200	-2.70827600
C	-4.02718700	2.33088700	-0.81834800
N	-5.16064800	2.48939500	-1.02972000
H	-4.90811500	-3.52416800	-1.04599700
Cl	6.88183200	-2.75281800	-0.25842300
O	-4.03650000	0.27989400	1.33386200
O	-5.49630500	-1.98102300	1.12367400
C	-3.65435600	-0.17657200	2.63618200

H	-4.22014800	-1.06563600	2.92803500
H	-2.57834500	-0.39221500	2.67168100
H	-3.88277700	0.64523700	3.31787100
C	-6.34957500	-3.10905700	0.99460500
H	-7.03362800	-3.06177800	1.84342100
H	-6.92496500	-3.06967400	0.06110700
H	-5.78508300	-4.05000900	1.03437900

Table 15: Thermodynamic parameters for TS_4 at b3lyp/6-31g (d) level of theory

TS_4	G	H	S	E
TS_{4a}	-1635.666274	-1635.572421	197.531	-1636.029157
TS_{4b}	-1750.161198	-1750.061460	209.917	-1750.553669
TS_{4c}	-1864.641600	-1864.534297	225.838	-1865.061515
TS_{4d}	-2095.271219	-2095.173914	204.795	-2095.622121
TS_{4e}	-2554.873752	-2554.772871	212.322	-2555.212439

TS_{4a}

Imaginary Freq = -305.65

Charge = 0 multiplicity= 1

C -0.62636300 -0.42001500 3.44827900

C -1.82024000 -1.74347700 1.76047800

O -0.73131600 -3.06085600 -1.40403800

C -0.67228500 -2.44435500 -0.32398600

O 1.58408500 -0.68514500 1.94226500

O -2.84882800 -1.72015300 2.42096700

H -1.59489500 -0.56643100 3.92079100

N -0.63885400 -1.13990300 2.17018200

C 0.56875300 -1.16820800 1.44923500

N -1.78223300 -2.40483400 0.52723400

H -0.44816100 0.64245400 3.26236400

C 0.48620500 -1.69259000 0.09240700

C -3.01265900 -3.09881300 0.13510000

H -3.30798700 -3.79924500 0.91901700

H -2.80648100 -3.62509900 -0.79429100

H -3.82457600 -2.37998400 -0.00477900

H 0.17570300 -0.80784600 4.07879200

C -3.83624100 2.71607700 0.59206300

H -3.24429700 3.21663800 1.35114600

C -1.18655300 0.57610100 -1.09055300

O -1.05214700 2.08849700 0.75945000

C	-2.03923700	-0.00596300	-1.98721300
C	0.21419200	0.17630500	-1.14012700
O	-3.34976400	0.23968700	-2.08981100
C	-3.93286700	1.14943300	-1.23272000
C	-3.17883700	1.80628000	-0.25325900
C	-1.72907100	1.54283300	-0.10975500
C	-5.30110300	1.37321200	-1.39203100
H	-5.84290900	0.83898400	-2.16536900
H	0.44897800	-0.49405700	-1.96550200
C	-5.92606500	2.27936200	-0.54424200
C	-5.19527700	2.95216600	0.44909100
H	-6.99065200	2.46458900	-0.65316000
H	-1.72358200	-0.75601400	-2.70471100
C	1.78608700	-1.97261300	-0.60097300
C	1.28453700	0.95341600	-0.63338700
N	2.01483700	-3.26048100	-0.90099700
C	2.56151000	0.42177000	-0.57094300
C	2.75965900	-0.99002000	-0.84864700
H	1.06781100	1.89652800	-0.15013300
C	3.70313200	1.27297800	-0.18990500
C	4.73274300	0.77689900	0.62991600
C	3.76597900	2.61051500	-0.62125400
C	5.79135600	1.59830600	1.00787700
H	4.67547700	-0.24176100	0.99807100
C	4.83071900	3.42656400	-0.24932700
H	2.98605500	2.99612500	-1.27143800
C	5.84641900	2.92253300	0.56683400
H	6.57293600	1.20517900	1.65183300
H	4.87193200	4.45390000	-0.60069100
C	3.99916600	-1.45759900	-1.37411500
N	4.96267800	-1.93141800	-1.83216400
H	6.67771300	3.55929800	0.85731200
H	1.20283400	-3.85970800	-1.00353100
H	2.84851700	-3.50567500	-1.42512600
H	-5.69760100	3.65575700	1.10589300

TS_{4b}

Imaginary Freq = -319.62

Charge = 0 multiplicity= 1

C	-1.09804100	-0.30452800	3.45033400
C	-2.57443100	-1.42633900	1.84171500
O	-1.84624400	-3.08634800	-1.26417300
C	-1.63961300	-2.44337800	-0.21877000
O	0.97753500	-1.09138200	1.93414100
O	-3.56217400	-1.16186300	2.51204300
H	-2.06617300	-0.22363200	3.93918400
N	-1.28606900	-1.06103300	2.20776900
C	-0.12563900	-1.37089900	1.47543700
N	-2.69905200	-2.13770100	0.64245300
H	-0.70526200	0.68752600	3.21231700
C	-0.34272900	-1.92018100	0.14167600
C	-4.05373600	-2.58074900	0.29926900
H	-4.46857700	-3.17138800	1.11869700
H	-3.98015900	-3.17769600	-0.60709200
H	-4.70425900	-1.71716900	0.13655600
H	-0.38240900	-0.82391500	4.09023600
C	-3.63691200	3.29922500	0.50688500
H	-2.93481100	3.69327900	1.23417800
C	-1.54070300	0.57422300	-1.10898100
O	-1.04656600	2.10343400	0.66531800
C	-2.51691600	0.15134300	-1.96661100
C	-0.25554400	-0.11836200	-1.15902100
O	-3.74860600	0.66641700	-2.06446500
C	-4.10548000	1.71383200	-1.24267200
C	-3.20714000	2.23535400	-0.30441300
C	-1.84311600	1.67560200	-0.16821100
C	-5.39834900	2.21781800	-1.39362600
H	-6.05872300	1.77945200	-2.13442800
H	-0.18938700	-0.85129900	-1.96186100
C	-5.79710100	3.27100000	-0.58011600
C	-4.91753800	3.81357900	0.37157100

H -6.80027800 3.67423800 -0.68315900
H -2.38397300 -0.67752900 -2.65379300
C 0.85787800 -2.50617600 -0.54404100
C 0.96683700 0.45002000 -0.72063300
N 0.80689900 -3.83113000 -0.76425700
C 2.11270000 -0.32591600 -0.65648200
C 2.00359900 -1.76299800 -0.86370600
H 0.95716700 1.43632500 -0.27725200
C 3.41152000 0.28414200 -0.34759100
C 4.37918600 -0.39195000 0.42622100
C 3.71702500 1.58053100 -0.79413200
C 5.58752500 0.20518400 0.73915700
H 4.15674200 -1.37983500 0.81430000
C 4.93295700 2.18896800 -0.49589700
C 5.87822700 1.49995500 0.27755200
H 6.32670700 -0.30600000 1.34730400
H 5.13713500 3.18429200 -0.87300300
C 3.09775600 -2.50197600 -1.39988900
N 3.92620100 -3.18443700 -1.85906900
H -0.11553100 -4.24630500 -0.83980800
H 1.55937700 -4.27160200 -1.28340600
H 2.99825900 2.11238900 -1.41060300
O 7.09423200 1.99283900 0.63138500
C 7.44784300 3.30085600 0.20415000
H 6.75458700 4.05396100 0.60018300
H 8.44702300 3.48390100 0.60269900
H 7.47475000 3.37230200 -0.89076100
H -5.24384600 4.63496100 1.00219200

TS_{4c}

Imaginary Freq = -294.77

Charge = 0 multiplicity= 1

C 1.94611400 0.84400300 3.40502200
C 3.08817200 1.73306900 1.42278200
O 1.78478000 2.88262900 -1.72610100

C	1.78103300	2.41127700	-0.57365800
O	-0.38365300	1.35369000	2.17002700
O	4.18306500	1.58494400	1.94735400
H	2.98386800	0.85865900	3.73011100
N	1.89308900	1.41159600	2.05367700
C	0.61481400	1.59102700	1.49288600
N	2.98342100	2.25214600	0.12837600
H	1.56737800	-0.18144800	3.38216400
C	0.58656600	1.95592100	0.08721800
C	4.24287400	2.65010200	-0.50677000
H	4.77051800	3.36232600	0.13109500
H	3.99411900	3.10124100	-1.46492100
H	4.88688600	1.77822200	-0.65088400
H	1.32127700	1.43671900	4.07553800
C	4.05390000	-3.18367600	0.69271600
H	3.48008200	-3.47961100	1.56469700
C	1.64983000	-0.74968300	-0.95876300
O	1.47851900	-1.99873300	1.07484000
C	2.47603000	-0.43840900	-2.00380500
C	0.35204200	-0.09582600	-0.91372500
O	3.69738300	-0.94161500	-2.20745900
C	4.20646900	-1.85791500	-1.31011800
C	3.47381800	-2.25192300	-0.18440700
C	2.12708200	-1.69447700	0.07629700
C	5.47929400	-2.36070500	-1.58240700
H	6.00846600	-2.02351700	-2.46743500
H	0.13904100	0.52641200	-1.78139300
C	6.02877600	-3.28262600	-0.69989500
C	5.31752300	-3.69575800	0.43876500
H	7.01894500	-3.68354100	-0.89572000
H	2.21425000	0.28166900	-2.77208600
C	-0.73085900	2.39407500	-0.47853500
C	-0.76744800	-0.57154800	-0.19299000
N	-0.78633000	3.67643700	-0.86490700
C	-1.90579300	0.20203500	-0.09942400

C	-1.88482000	1.58676000	-0.50873200
H	-0.70012200	-1.50362500	0.35262700
C	-3.14115500	-0.37329300	0.51172800
C	-3.23933100	-0.46873200	1.90818400
C	-4.17470200	-0.83915100	-0.31135100
C	-4.38005000	-1.02076500	2.47802300
H	-2.42730800	-0.08747900	2.51771200
C	-5.31524500	-1.43131300	0.27894900
C	-5.41453000	-1.50118000	1.67072700
H	-4.47168600	-1.08630900	3.55833700
C	-3.10214700	2.24911300	-0.84067500
N	-4.04436600	2.86155000	-1.15573400
H	-6.28949000	-1.94472500	2.13193900
O	-3.97251100	-0.77097300	-1.66508100
O	-6.25336200	-1.92842600	-0.58478500
C	-5.00917700	-0.22711600	-2.49623200
H	-5.79970900	-0.95874000	-2.67388400
H	-5.42863600	0.68132300	-2.05311000
H	-4.51823000	0.02921300	-3.43813800
C	-7.42053800	-2.52045900	-0.03849200
H	-8.02183200	-2.83682200	-0.89286800
H	-7.17762000	-3.39622700	0.57759400
H	-7.99418600	-1.80358500	0.56365500
H	5.76033100	-4.41538300	1.12055800
H	0.08919800	4.13066800	-1.09706900
H	-1.63126500	4.03338400	-1.29867500

$TS_{\mathbf{4d}}$

Imaginary Freq = -307.53

Charge = 0 multiplicity= 1

C	-0.32652400	-0.38335900	3.39889900
C	-1.17013500	-2.05756000	1.81364300
O	0.31059400	-3.45040400	-1.15365900
C	0.19866900	-2.73371400	-0.14177000
O	1.97438900	-0.37874200	2.00829500

O	-2.22224800	-2.15857600	2.42786900
H	-1.27979600	-0.65609100	3.84569900
N	-0.14037300	-1.21058700	2.20149700
C	1.09105500	-1.08644000	1.53282500
N	-0.94546800	-2.81746300	0.65933300
H	-0.32604000	0.67178400	3.11294500
C	1.17890000	-1.74565300	0.23659200
C	-2.00666900	-3.76272000	0.29885100
H	-2.21331300	-4.42551200	1.14162900
H	-1.65791600	-4.33006500	-0.56123400
H	-2.92642700	-3.22450700	0.05411300
H	0.49376200	-0.56015700	4.09687400
C	-3.87063300	1.84043200	0.11165600
H	-3.42443400	2.52052800	0.82820800
C	-0.80576200	0.05501800	-1.23380800
O	-1.04513100	1.75196000	0.43901500
C	-1.49230300	-0.76391200	-2.08681400
C	0.64572000	-0.08361000	-1.19244300
O	-2.81997100	-0.77652100	-2.25756900
C	-3.59802300	0.09418900	-1.52894500
C	-3.02774300	0.97770400	-0.60665300
C	-1.56174400	1.00207200	-0.38550700
C	-4.97533700	0.04959300	-1.75308100
H	-5.37902900	-0.65111800	-2.47607300
H	1.03963400	-0.77684200	-1.93393500
C	-5.79794900	0.90861500	-1.03861300
C	-5.23738000	1.80043200	-0.10935600
H	-6.87129100	0.89447200	-1.19268700
H	-1.01119300	-1.51405000	-2.70524100
C	2.54412000	-1.84677200	-0.37610700
C	1.53018500	0.92116700	-0.73282500
N	3.01663900	-3.09272700	-0.52949000
C	2.87751500	0.64077300	-0.57130200
C	3.33847600	-0.73054900	-0.69129700
H	1.12399000	1.85062100	-0.35739000

C	3.82649100	1.72010000	-0.24505800
C	4.88663300	1.50387700	0.65381700
C	3.66818800	2.99852000	-0.81076600
C	5.75941800	2.53908300	0.97732300
H	4.99610400	0.53266500	1.12414100
C	4.54839200	4.02888700	-0.49262000
H	2.86500200	3.16923100	-1.52170300
C	5.59645000	3.80187800	0.40291800
H	6.56593900	2.36100000	1.68289200
H	4.42106200	5.00743600	-0.94727200
C	4.66869500	-1.01280200	-1.11829600
N	5.72448900	-1.34619200	-1.48799100
H	6.28360000	4.60611500	0.65163000
Cl	-6.29671700	2.87714400	0.77990100
H	2.33426400	-3.84044600	-0.59272500
H	3.90995200	-3.23095900	-0.99083700

$TS_{\mathbf{4e}}$

Imaginary Freq = -305.23

Charge = 0 multiplicity= 1

C	0.66598800	1.03559500	3.39191900
C	1.57268000	2.38727800	1.55354300
O	0.09523600	3.42670200	-1.55682000
C	0.19100000	2.86333300	-0.45068100
O	-1.67207500	0.98978400	2.06990200
O	2.64807800	2.50037700	2.12361100
H	1.65306600	1.29505000	3.76748200
N	0.49838600	1.68676300	2.08780700
C	-0.75850900	1.55478500	1.47199800
N	1.36506300	2.97955200	0.30259700
H	0.57535000	-0.04689300	3.26973500
C	-0.84374200	2.02398300	0.09753900
C	2.47736800	3.77901600	-0.22006400
H	2.75464100	4.54625300	0.50579000
H	2.14240200	4.23209600	-1.15057100

H	3.35009800	3.14438600	-0.39619000
H	-0.11159300	1.38011400	4.07611900
C	3.93164500	-1.91445900	0.38299700
H	3.46208000	-2.44372200	1.20426500
C	0.96072100	-0.12439300	-1.15313900
O	1.13164800	-1.55027200	0.76146200
C	1.67557700	0.50569900	-2.13453800
C	-0.47299000	0.12043500	-1.10326800
O	2.99383800	0.39280000	-2.33153100
C	3.73086900	-0.41754800	-1.49693900
C	3.12968400	-1.10690800	-0.43861600
C	1.67456000	-0.98348500	-0.18306900
C	5.09916800	-0.51261500	-1.75649000
H	5.52778600	0.03895500	-2.58637800
H	-0.84508100	0.73498900	-1.92140100
C	5.88117200	-1.31591000	-0.93883500
C	5.28950900	-2.01304900	0.12739600
H	6.94679600	-1.40758100	-1.11780600
H	1.22892100	1.18814900	-2.84965800
C	-2.21611800	2.12942500	-0.49496700
C	-1.41072800	-0.73731500	-0.48191200
N	-2.61326600	3.36821600	-0.81407400
C	-2.72245200	-0.33168400	-0.33476900
C	-3.09548800	1.03744300	-0.62149000
H	-1.06959900	-1.65249300	-0.01726300
C	-3.75260300	-1.25144800	0.20453900
C	-4.48582500	-0.84035000	1.33389800
C	-4.03208100	-2.52400700	-0.32569900
C	-5.44311400	-1.66363400	1.91625700
H	-4.25191700	0.12671200	1.76625300
C	-5.00121100	-3.34983200	0.24288200
C	-5.70335100	-2.92017700	1.36752700
H	-5.98267300	-1.32558700	2.79577300
H	-5.20227100	-4.31826200	-0.20211500
C	-4.43450900	1.35001700	-0.99830400

N	-5.49446500	1.69879300	-1.33987100
H	-6.45433900	-3.56934300	1.80875200
Cl	6.29752800	-3.02258700	1.14531400
H	-1.89033600	4.05843000	-0.98490600
H	-3.51268700	3.50421700	-1.26418800
Cl	-3.21681000	-3.11712000	-1.77109000

Table 16: Thermodynamic parameters for TS annulation at b3lyp/6-31g (d) level of theory

Annulation	G	H	S	E
TS_1 annulation	-1750.115092	-1750.013966	212.837	-1750.502763
TS_2 annulation	-1750.130478	-1750.031584	208.140	-1750.521607

TS1annulation

Charge=0 multiplicity=1

Imaginary Freq = -330.85

O	2.48264600	-0.96963800	1.68351800
C	2.12250300	-0.88356000	-0.68800400
O	2.36948200	1.76650500	0.74660200
C	2.90905600	-1.12584300	0.53935900
O	-1.53590500	0.84352100	-1.75183900
O	-0.23672800	5.13760500	-0.87756400
O	3.85553500	-1.84486700	-2.06898300
N	-0.92222400	2.98635800	-1.29850000
C	-0.70230300	1.60776800	-1.26450600
N	1.10649100	3.44094900	-0.16039500
C	0.77679100	-0.24488100	-0.77401300
C	0.53210200	1.13928300	-0.62941700
C	1.99962800	4.45406500	0.41371500
H	2.24419200	5.19372600	-0.35001900
H	2.89397300	3.94398700	0.76350100
H	1.50941400	4.96751900	1.24597800
C	2.63857300	-1.30282300	-1.87379500
C	5.17164300	-1.83459200	1.36327500
H	4.83277500	-1.57282200	2.36009500
C	-0.03739100	3.93621700	-0.79424200
C	-2.18531100	3.45145800	-1.88435400
H	-2.31858100	2.99285100	-2.86554900
H	-2.13488600	4.53471200	-1.96445400
H	-3.01872300	3.15764700	-1.24052700

C	4.69388300	-1.98925500	-0.99137100
C	4.27245900	-1.64772200	0.29843300
C	1.40265900	2.08344500	0.02670000
C	5.96882400	-2.50207000	-1.24443300
H	6.24886700	-2.75463000	-2.26178100
H	0.15743100	-0.65865300	-1.56457800
C	6.83931800	-2.67023100	-0.17603200
C	6.44275900	-2.33595100	1.13043000
H	7.83525100	-3.06470100	-0.35600200
H	7.13387400	-2.47342300	1.95658100
H	2.10734100	-1.21637300	-2.81594300
C	-0.33474300	0.84571600	2.27757100
C	-0.37306700	-1.40655100	0.65987000
H	0.47679400	-1.26546700	1.32128200
N	0.69886700	1.04456300	2.84591900
H	1.55321900	1.35981800	2.32762500
C	-1.57430600	-0.75979700	0.94869900
C	-1.52201900	0.47362000	1.71561700
H	-0.42419400	-2.37731700	0.17618300
C	-2.87021700	-1.27560300	0.47392800
C	-4.02015600	-1.19662000	1.27439700
C	-2.98176500	-1.92800300	-0.77219900
C	-5.23524600	-1.74443700	0.86562300
H	-3.97028900	-0.72424000	2.24983400
C	-4.18356500	-2.46667800	-1.19404600
H	-2.12338800	-1.96655900	-1.43336100
C	-5.32443700	-2.38196500	-0.37714600
H	-6.09507900	-1.66954200	1.52077800
H	-4.27494800	-2.94794500	-2.16251200
C	-7.64994800	-2.86331700	-0.11781000
H	-8.41855900	-3.35745200	-0.71429700
H	-7.54786600	-3.38153300	0.84440600
H	-7.94137800	-1.82057300	0.06086800
O	-6.45447500	-2.94463600	-0.88192900

C	-2.57912100	1.43514800	1.75857100
N	-3.41874600	2.24128900	1.80076700

TS_2 annulation

Charge=0 multiplicity=1

Imaginary Freq = -207.30

O	2.19976400	-1.41415800	1.75162600
C	1.87876700	-1.00146800	-0.58576700
O	2.54076300	1.51014000	0.77400900
C	2.63381300	-1.44850700	0.59711600
O	-1.59555300	1.14627300	-1.45264200
O	0.53708400	5.17612400	-1.07417900
O	3.65073800	-1.69617900	-2.07151400
N	-0.58329500	3.17287200	-1.20989100
C	-0.61805000	1.78612000	-1.04300500
N	1.56174500	3.31966400	-0.23255800
C	0.49917400	-0.35853400	-0.53149100
C	0.49302500	1.15323100	-0.35696600
C	2.67301600	4.17864300	0.19109600
H	3.05116400	4.73621500	-0.66795200
H	3.44537300	3.53615300	0.60677700
H	2.33196400	4.89618300	0.94266400
C	2.43225900	-1.17524900	-1.80905900
C	4.82705600	-2.42359500	1.33462500
H	4.46115800	-2.34008400	2.35267700
C	0.50419700	3.97262700	-0.86286000
C	-1.74511200	3.80526800	-1.84175100
H	-1.89594400	3.39231100	-2.84235600
H	-1.55089000	4.87399500	-1.89517400
H	-2.63895500	3.60523700	-1.24622000
C	4.43449500	-2.09296400	-1.01880100
C	3.97776500	-1.99192100	0.30050900

C	1.59703900	1.94523500	0.06428800
C	5.69770600	-2.60672500	-1.32694300
H	6.00848300	-2.66648800	-2.36483600
H	0.04792000	-0.50068700	-1.51918700
C	6.51703700	-3.02381700	-0.28690800
C	6.08361800	-2.93296900	1.04730900
H	7.50219700	-3.42317300	-0.51075800
H	6.73546500	-3.26254200	1.85089900
H	1.93823700	-0.89140800	-2.73279800
C	-0.21157900	0.98808900	2.00197300
C	-0.46805400	-1.17756100	0.43305300
H	0.12752200	-1.41608300	1.32146900
N	0.78056300	1.08412800	2.66320600
H	1.71683100	1.28467200	2.18679200
C	-1.72011700	-0.48719700	0.88432200
C	-1.54353000	0.63890000	1.68511300
H	-0.70991400	-2.12422200	-0.05400400
C	-3.03497100	-1.02788700	0.55189100
C	-4.12205600	-0.96233400	1.45241400
C	-3.24908800	-1.65708400	-0.68867900
C	-5.35518500	-1.49686500	1.12527700
H	-3.98937900	-0.51646200	2.43176600
C	-4.48962000	-2.17736100	-1.03732500
H	-2.44614600	-1.68933900	-1.41670500
C	-5.55450800	-2.10411300	-0.12600300
H	-6.18484000	-1.46209000	1.82357200
H	-4.62027800	-2.62826000	-2.01392300
C	-2.55768500	1.57182500	2.06217700
N	-3.35019000	2.36173900	2.38387800
O	-6.79909600	-2.59029500	-0.35299200
C	-7.07365500	-3.21126300	-1.60332700
H	-6.44415600	-4.09667200	-1.75712800
H	-8.12068700	-3.51428200	-1.55949100
H	-6.93103100	-2.51218200	-2.43665600

Table 16: Thermodynamic parameters for Products ($\mathbf{P_{a-e}}$ and $\mathbf{P_{a'-e'}}$) at M062x-def2tzvp// b3lyp/6-31g (d) level of theory

Product	G	H	S	E
$\mathbf{P_{3a}}$	-1635.707272	-1635.609097	206.627	-1636.077900
$\mathbf{P_{3a'}}$	-1635.701824	-1635.602329	209.406	-1636.069952
$\mathbf{P_{3b}}$	-1750.201217	-1750.097093	219.147	-1750.606164
$\mathbf{P_{3b'}}$	-1750.196799	-1750.090997	222.678	-1750.598729
$\mathbf{P_{3c}}$	-1864.685816	-1864.574187	234.942	-1865.123491
$\mathbf{P_{3c'}}$	-1864.679438	-1864.567173	236.282	-1865.118589
$\mathbf{P_{3d}}$	-2095.312650	-2095.211014	213.911	-2095.679336
$\mathbf{P_{3d'}}$	-2095.307128	-2095.204174	216.684	-2095.671310
$\mathbf{P_{3e}}$	-2554.918498	-2554.813652	220.666	-2555.282148
$\mathbf{P_{3e'}}$	-2554.911549	-2554.805399	223.411	-2555.272778

P_{3a}

Charge= 0 multiplicity= 1

O 5.92802500 1.06333400 1.15774500

O 3.71972800 -1.52938100 -1.12535800

O -5.12388500 0.70963900 -1.87574500

O -2.22113000 -1.31909900 1.28865100

O -6.72827600 -2.00053400 1.42046700

N -5.91585800 -0.64157500 -0.24197400

N -2.54688400 0.97212600 -2.19976100

N -4.47320500 -1.69612600 1.31820100

N -0.53326400 -2.75614900 -1.53646600

C 0.00380000 0.57322500 -0.50465000

C -0.99082000 -0.28380000 -0.90010200

C -2.40706500 0.14230100 -1.16300500

C -0.34828500 1.95169100 -0.05306400

C -3.51479400 -0.34694400 -0.45703800

C	3.78637500	0.44371600	0.22851600
C	4.36610800	-0.74972700	-0.42926600
C	5.81490500	-0.93977400	-0.18867900
C	-0.72370000	-1.65016700	-1.22527400
C	1.38948400	0.12598200	-0.46530200
H	1.62303600	-0.82666200	-0.92733500
C	2.38334800	0.82149100	0.13929700
H	2.13415200	1.75961900	0.63256100
C	-4.85926900	-0.03848100	-0.92012600
C	-1.03433600	4.52896500	0.82128800
C	6.53885300	-0.03128700	0.59240400
C	-3.31321200	-1.13738900	0.75307400
C	-1.21850600	2.12484000	1.03467800
H	-1.60904800	1.24682100	1.54091800
C	-0.16361500	4.36501800	-0.25870300
H	0.24471500	5.23433100	-0.76719900
C	0.18504400	3.08489300	-0.68825900
H	0.86630700	2.95877200	-1.52571300
C	-1.55509200	3.40736100	1.46893300
H	-2.22505100	3.52934100	2.31570000
C	4.61228600	1.24819500	0.95798900
H	4.26948900	2.14394200	1.46599600
C	6.49963000	-2.03754700	-0.73863000
H	5.92790900	-2.73558600	-1.34144400
C	-5.77117000	-1.48536100	0.86455700
C	7.85612000	-2.20791700	-0.50805700
H	8.37865400	-3.05865700	-0.93496100
C	7.90575700	-0.18631500	0.83506700
H	8.42424100	0.54409500	1.44739100
C	8.55788600	-1.27970100	0.28006800
H	9.62050000	-1.41498400	0.46007400
C	-7.27141300	-0.36192100	-0.72777000
H	-7.47205400	0.71061900	-0.67054100
H	-7.96584600	-0.91533000	-0.10037900
H	-7.36235100	-0.67476800	-1.77048500

C	-4.34322600	-2.54701900	2.50674200
H	-3.28105700	-2.65233500	2.71446500
H	-4.79821800	-3.52031600	2.31276800
H	-4.85493100	-2.08791600	3.35657100
H	-3.49978600	1.24149600	-2.45987200
H	-1.73995800	1.24513100	-2.74035800
H	-1.30246800	5.52681900	1.15765100

$P_{3a'}$

Charge= 0 multiplicity= 1

O	2.07458100	-2.06488900	1.25063600
C	2.00605400	-0.87315200	-0.82565300
O	-2.52295700	0.85493100	1.41125200
C	2.67273300	-1.48420400	0.34621000
O	-0.60266900	3.39567400	-2.13263000
O	-0.22809200	4.71048200	2.20869100
O	4.11865100	-0.14831400	-1.74347400
N	-0.42961200	4.04072900	0.04292700
C	-0.84054000	3.13908800	-0.93987800
N	-1.34581300	2.74558300	1.80293100
C	0.56390900	-0.87931100	-1.04024600
C	-1.51764400	1.93088700	-0.48448700
C	-1.64295700	2.57264300	3.22957500
H	-1.15663400	3.38112000	3.76987400
H	-1.26973400	1.60299800	3.56551300
H	-2.72355600	2.59977800	3.39010700
C	2.78052700	-0.26148500	-1.76752800
C	4.91571800	-1.87590800	1.40542400
H	4.38945300	-2.38476200	2.20636500
C	-0.64033100	3.87956500	1.41457800
C	0.27685600	5.26534200	-0.35076800
H	1.27129100	5.28200800	0.10127000
H	-0.27566400	6.14003900	-0.00076300
H	0.34937100	5.26732700	-1.43539700

C	4.81247800	-0.68740300	-0.68622900
C	4.14682900	-1.34748400	0.35353000
C	-1.84855400	1.76161000	0.93472800
C	6.20184300	-0.54320100	-0.70421900
H	6.67255800	-0.02274000	-1.53171100
H	0.24912200	-0.41454400	-1.97277500
C	6.93717300	-1.07468900	0.34706000
C	6.29554800	-1.74238400	1.40444400
H	8.01833500	-0.97050900	0.34827800
H	6.88325400	-2.15248200	2.22018800
H	2.37156100	0.21382600	-2.65336700
C	-1.88659500	0.95849600	-1.42322200
C	-0.37526400	-1.40739500	-0.22238200
H	-0.04909500	-1.93010100	0.66968500
N	-1.74143400	1.14962600	-2.74160300
H	-2.07392100	0.45112700	-3.39089500
C	-1.81966900	-1.40570100	-0.47524200
C	-2.49434400	-0.36626400	-1.05763600
C	-2.54737000	-2.60992900	0.00356000
C	-3.71319400	-2.48430900	0.77695200
C	-2.04080200	-3.89260100	-0.26494400
C	-4.36864000	-3.62073600	1.24775700
H	-4.07672800	-1.49510700	1.03385900
C	-2.70605200	-5.02597200	0.19684100
H	-1.13020000	-3.99648000	-0.84859500
C	-3.87281600	-4.89209000	0.95329600
H	-5.26487400	-3.51105200	1.85189200
H	-2.31224300	-6.01296300	-0.02984400
C	-3.86784100	-0.46198800	-1.44282000
N	-4.96695100	-0.46978300	-1.83169300
H	-1.37593600	2.05386700	-3.04904100
H	-4.38813200	-5.77604400	1.31941400

P_{3b}

Charge= 0 multiplicity= 1

O	5.97120000	0.88202700	1.11608900
O	3.85784800	-1.85700600	-1.08475000
O	-5.04179400	-0.00285000	-1.98921100
O	-2.13562200	-1.63570900	1.39269700
O	-6.61580500	-2.48003400	1.49941900
N	-5.81813800	-1.23815900	-0.25908000
N	-2.46917300	0.32241600	-2.29191100
N	-4.37184800	-2.09832700	1.41252600
N	-0.36396600	-3.27722900	-1.26046300
C	0.07271600	0.15036300	-0.55488400
C	-0.89628900	-0.76900700	-0.87078700
C	-2.32022700	-0.41077700	-1.18578400
C	-0.31683700	1.54853300	-0.22215800
C	-3.42512700	-0.87496700	-0.45780500
C	3.85522800	0.16516400	0.19678500
C	4.47500400	-1.03387000	-0.41262700
C	5.92681300	-1.17224200	-0.15484500
C	-0.58885700	-2.15213800	-1.05976000
C	1.47145700	-0.25522200	-0.48798500
H	1.73412800	-1.22371600	-0.89849000
C	2.44213000	0.49770100	0.08391900
H	2.16238800	1.45028500	0.53098600
C	-4.76973800	-0.65642900	-0.96836400
C	-1.08789900	4.18105200	0.42258100
C	6.61780600	-0.21458300	0.59679500
C	-3.22115900	-1.54620100	0.82170800
C	-1.24212500	1.79632500	0.80994100
H	-1.64193100	0.95688500	1.37114100
C	-0.16093400	3.95274900	-0.60313200
H	0.26455000	4.77568500	-1.16589600
C	0.22171500	2.64523000	-0.90763600
H	0.94322000	2.47833800	-1.70310200
C	-1.61903000	3.09210300	1.13138500
H	-2.32428800	3.29015300	1.93239200
C	4.65175400	1.02019900	0.90066200

H	4.27896400	1.92352500	1.37281400
C	6.64740000	-2.26931000	-0.65843800
H	6.10082800	-3.00568800	-1.23854200
C	-5.66639700	-1.97795400	0.91859200
C	8.00629500	-2.39151100	-0.41210300
H	8.55655200	-3.24207200	-0.80303900
C	7.98665800	-0.32078700	0.85475000
H	8.47883900	0.44658200	1.44313200
C	8.67455200	-1.41460000	0.34573800
H	9.73909500	-1.51219400	0.53836300
C	-7.17241400	-1.05149700	-0.79049900
H	-7.41141800	0.01393000	-0.83086100
H	-7.85960300	-1.57328400	-0.12893800
H	-7.23157100	-1.45691800	-1.80322900
C	-4.23630500	-2.83544700	2.67407100
H	-3.17586200	-2.87864500	2.91085000
H	-4.64851600	-3.83981100	2.55849500
H	-4.78479000	-2.32465100	3.46974700
H	-3.42543900	0.53719400	-2.58759000
H	-1.66145600	0.57542200	-2.84092700
O	-1.52844300	5.40984000	0.80933000
C	-1.03288700	6.55254800	0.12748600
H	-1.28794900	6.52676800	-0.93993900
H	-1.51817700	7.41157600	0.59364700
H	0.05541700	6.64705700	0.23726300

$P_{3b'}$

Charge= 0 multiplicity= 1

O	0.97359900	-2.65039500	1.11131200
C	1.62997200	-1.56560400	-0.92045800
O	-1.19063600	2.10188500	1.41684100
C	1.81900700	-2.46937200	0.23630700
O	1.91990800	3.49118800	-1.91897200
O	2.84558800	3.90639100	2.51627200

O	3.81878000	-2.09845700	-1.78992000
N	2.36252400	3.69240500	0.30253000
C	1.54240200	3.28530000	-0.75209000
N	0.82915500	2.96273900	1.95118700
C	0.42702300	-0.77419400	-1.14949000
C	0.29120900	2.62522500	-0.40064300
C	0.44674600	2.83685600	3.36212300
H	1.28597900	3.17611700	3.96438400
H	0.20656400	1.79505300	3.58439400
H	-0.43949300	3.44391500	3.56270800
C	2.63833500	-1.45877400	-1.83291400
C	3.45251500	-4.04626100	1.30954500
H	2.71117900	-4.20102800	2.08663500
C	2.05991500	3.53751200	1.65668900
C	3.64475100	4.34310800	0.00997300
H	4.46452900	3.75205500	0.42505000
H	3.66947600	5.33476900	0.46713000
H	3.73538300	4.41745700	-1.07068800
C	4.07492700	-2.95100400	-0.74261000
C	3.12746600	-3.16138100	0.26636200
C	-0.11466500	2.52255000	1.00553500
C	5.31729700	-3.58984200	-0.73851300
H	6.01929800	-3.39414500	-1.54231500
H	0.43882800	-0.19780500	-2.07321600
C	5.61263800	-4.45875200	0.30362700
C	4.68061800	-4.68895500	1.33024500
H	6.57471400	-4.96259600	0.32184400
H	4.92549200	-5.37044200	2.13935100
H	2.58111000	-0.81808100	-2.70701400
C	-0.53627500	2.13909300	-1.42626100
C	-0.66474200	-0.70527000	-0.35461800
H	-0.70625300	-1.32919300	0.53072800
N	-0.26551000	2.36760200	-2.71889000
H	-0.91485800	2.06225400	-3.42975900
C	-1.85620500	0.10084800	-0.64285200

C	-1.79567500	1.35635400	-1.19563100
C	-3.14700500	-0.51113500	-0.26309000
C	-4.15082700	0.23459400	0.38829600
C	-3.38100700	-1.87537200	-0.49231100
C	-5.34374200	-0.35807300	0.76705900
H	-3.96797800	1.27522100	0.63200400
C	-4.58251100	-2.47997700	-0.12923200
H	-2.61595400	-2.47385200	-0.97902200
C	-5.57459200	-1.71794600	0.50329400
H	-6.11328300	0.20822000	1.28158700
H	-4.73273400	-3.53291000	-0.33724400
C	-2.95719200	2.02886500	-1.68647600
N	-3.84435400	2.62134800	-2.15815100
H	0.55447100	2.93916700	-2.93494100
O	-6.77895500	-2.20150300	0.90942900
C	-7.07020600	-3.57331000	0.68415500
H	-8.07267500	-3.73428800	1.08413900
H	-7.06327100	-3.81539500	-0.38647600
H	-6.36056600	-4.22651500	1.20818000

P_{3c}

Charge= 0 multiplicity= 1

O	5.92302100	0.53157900	1.23507300
O	3.71217300	-2.06295400	-1.04412900
O	-5.10924000	0.45442100	-1.65936700
O	-2.21319700	-2.14644500	1.07042500
O	-6.74420500	-2.60856900	1.29422900
N	-5.91603200	-1.07191400	-0.19661100
N	-2.53246700	0.67613600	-2.01366600
N	-4.48083000	-2.39967400	1.14606500
N	-0.52813300	-3.07773900	-1.98625000
C	-0.00987600	0.02113100	-0.36884300
C	-0.98968900	-0.76101800	-0.91602900
C	-2.40308300	-0.29073900	-1.10104800
C	-0.39490600	1.28510400	0.33707700

C	-3.51017100	-0.84688700	-0.44775200
C	3.77304900	-0.10553500	0.33363000
C	4.35882600	-1.27980900	-0.35238100
C	5.81578600	-1.44855200	-0.14435100
C	-0.71763700	-2.04544800	-1.48156800
C	1.37601200	-0.41956200	-0.36154100
H	1.61534800	-1.33551700	-0.88989500
C	2.36363700	0.25255700	0.27588100
H	2.10469800	1.16268800	0.81469200
C	-4.85200300	-0.42661100	-0.82197300
C	-1.05620800	3.59936400	1.76267800
C	6.54019000	-0.54136200	0.63774100
C	-3.30983700	-1.82295900	0.61953700
C	-1.04021300	1.18940100	1.57976700
H	-1.27520500	0.20466600	1.97140300
C	-0.40095300	3.71128700	0.53292800
C	-0.09082400	2.54404700	-0.20309600
C	-1.37651600	2.34229800	2.27966600
H	-1.88331200	2.27154800	3.23756800
C	4.59980300	0.69821100	1.06247600
H	4.25270600	1.58016100	1.59099200
C	6.50753200	-2.52449100	-0.72763500
H	5.93495500	-3.22125300	-1.33116300
C	-5.77948500	-2.06611300	0.77831400
C	7.87120900	-2.67564800	-0.52822500
C	7.91452200	-0.67739900	0.84934600
H	8.43322000	0.05120800	1.46370200
C	8.57348100	-1.74935200	0.26177600
H	9.64184200	-1.86923100	0.41734600
C	-7.27010000	-0.67069300	-0.59220100
H	-7.41933400	0.39098700	-0.38107600
H	-7.97139700	-1.27615600	-0.02321000
H	-7.40501700	-0.83136300	-1.66431300
C	-4.35750600	-3.42158200	2.19184600
H	-3.29601700	-3.60303700	2.34265500

H -4.86491800 -4.33507300 1.87521300
H -4.82093000 -3.07057200 3.11747900
H -3.48006600 0.99909900 -2.22631300
H -1.71691100 0.99860900 -2.51354500
H -1.30861800 4.48965300 2.32700100
H 8.39903900 -3.50954600 -0.98116700
O 0.55205800 2.56263500 -1.41456300
O -0.00999300 4.89948700 -0.02246400
C 0.11287400 3.47071500 -2.43010600
H -0.98261700 3.53098800 -2.46132800
H 0.51888900 4.47252500 -2.27947600
H 0.48394000 3.05727700 -3.37162900
C -0.32416600 6.10026400 0.66683000
H 0.15597400 6.13502400 1.65327900
H 0.06659600 6.90949400 0.04744900
H -1.40805100 6.22522000 0.78749000

$P_{3c'}$

Charge= 0 multiplicity= 1
O 0.66038400 -2.70689600 1.39718100
C 1.44670600 -1.80019700 -0.67673300
O -0.43878900 2.70160300 1.48366700
C 1.48545700 -2.71683800 0.48544300
O 2.45538500 3.03680100 -2.28620900
O 3.92749300 3.92882800 1.92759100
O 3.45484400 -2.77397300 -1.60374100
N 3.17304000 3.48537300 -0.17333700
C 2.18724500 3.07794500 -1.07316200
N 1.73878800 3.27095100 1.70091300
C 0.42610700 -0.77941400 -0.88065700
C 0.89441200 2.70703000 -0.51098800
C 1.50419700 3.41281400 3.14254000
H 2.44815000 3.68813500 3.60644700
H 1.13515900 2.46820600 3.54752700

H	0.74967300	4.18264600	3.32189300
C	2.43031100	-1.90354600	-1.61622700
C	2.78041700	-4.60746000	1.51274200
H	2.04742200	-4.60296900	2.31281500
C	3.00309200	3.58010300	1.21015300
C	4.50197000	3.85299000	-0.67590100
H	5.25806800	3.19329000	-0.24386800
H	4.73522500	4.88027600	-0.38762100
H	4.48162100	3.75428800	-1.75828000
C	3.55623600	-3.66449800	-0.56240800
C	2.61782200	-3.67142700	0.47630500
C	0.63897000	2.87147300	0.92348300
C	4.63453000	-4.55246300	-0.59372800
H	5.33658000	-4.50823900	-1.41983000
H	0.55558300	-0.19778000	-1.79082700
C	4.77116000	-5.46695500	0.44220500
C	3.84394300	-5.49653400	1.49814900
H	5.60429800	-6.16385300	0.43247200
H	2.48183800	-1.26506100	-2.49229700
C	-0.10836900	2.22346200	-1.36091900
C	-0.63798600	-0.53143700	-0.08344600
H	-0.79632000	-1.17349900	0.77522000
N	0.03830500	2.19368600	-2.69186800
H	-0.72007000	1.86947700	-3.27441200
C	-1.65576300	0.49807600	-0.29704100
C	-1.43822400	1.71564300	-0.87891800
C	-2.99677900	0.21080700	0.29544900
C	-3.46719400	1.00780200	1.35350500
C	-3.75099200	-0.88395500	-0.14563400
C	-4.68421000	0.70892800	1.95262900
H	-2.85888600	1.83756800	1.69695700
C	-4.98572200	-1.18267000	0.47097200
C	-5.44627700	-0.37910500	1.51715900
H	-5.05021500	1.32126500	2.77157000
C	-2.50866600	2.62703000	-1.14026900

N	-3.33092800	3.40080400	-1.43011000
H	0.91140600	2.55921600	-3.07916700
H	-6.39269600	-0.59638800	1.99910200
H	3.96324600	-6.21685700	2.30190600
O	-3.25339000	-1.67927300	-1.14929900
O	-5.64567200	-2.27303800	-0.02145000
C	-3.94185000	-1.59999700	-2.40048000
H	-4.96932200	-1.96530200	-2.31352500
H	-3.94975400	-0.56855500	-2.77755300
H	-3.38388200	-2.23643400	-3.09147800
C	-6.87206900	-2.64352600	0.58910000
H	-7.20921800	-3.53732400	0.06113500
H	-6.73586100	-2.87991300	1.65234200
H	-7.62936300	-1.85479000	0.48843100

P_{3d}

Charge= 0 multiplicity= 1

O	5.23113700	1.84225100	1.25230500
O	3.32836800	-1.09320600	-0.88641800
O	-5.65768300	0.27147300	-1.98375300
O	-2.66586100	-1.24050200	1.38022200
O	-7.09887000	-2.30510500	1.49042200
N	-6.36860700	-1.01325000	-0.26120300
N	-3.10608700	0.73750900	-2.28159400
N	-4.87713300	-1.81071100	1.40291600
N	-0.78292500	-2.72583100	-1.29398400
C	-0.57767100	0.70465800	-0.50483400
C	-1.47962400	-0.26632900	-0.85492800
C	-2.92098700	0.00766100	-1.17884300
C	-1.06254400	2.07547200	-0.16791200
C	-3.99822600	-0.52303700	-0.45671100
C	3.17911300	0.96962300	0.32131100
C	3.87903700	-0.20965000	-0.23526900
C	5.33365400	-0.24916300	0.05064300
C	-1.08166500	-1.62258500	-1.07090800

C	0.84090800	0.38806100	-0.40082500
H	1.16983600	-0.57105700	-0.78474800
C	1.75106800	1.21250000	0.17183500
H	1.40617100	2.15795400	0.58705500
C	-5.35285900	-0.37309800	-0.96679100
C	-1.99755700	4.63843500	0.49061000
C	5.95009200	0.77285300	0.78032700
C	-3.75737900	-1.19753500	0.81483300
C	-1.97413500	2.25033500	0.88514900
H	-2.29915800	1.38112300	1.44951800
C	-1.08639300	4.47332400	-0.55528300
H	-0.74287600	5.33532500	-1.12089300
C	-0.61420100	3.20130300	-0.87753700
H	0.09793100	3.07487100	-1.68887100
C	-2.43465900	3.52616400	1.21203000
H	-3.13585500	3.65034000	2.03276000
C	3.90936000	1.89392600	1.00974800
H	3.47531100	2.78837600	1.44442300
C	6.11889400	-1.31897600	-0.40981900
H	5.63481400	-2.10810000	-0.97406100
C	-6.17747300	-1.75181000	0.91164600
C	7.47538400	-1.33885100	-0.13376300
C	7.31902600	0.75466800	1.06033200
H	7.76007400	1.56580700	1.62990200
C	8.08394400	-0.30697300	0.60048500
H	9.14837100	-0.34546800	0.80455300
C	-7.73134600	-0.89459200	-0.79125300
H	-8.02676700	0.15687200	-0.82277300
H	-8.38959400	-1.45759400	-0.13411200
H	-7.76884400	-1.29427000	-1.80722300
C	-4.70224100	-2.55239200	2.65719200
H	-3.64049100	-2.54527400	2.89183200
H	-5.06424200	-3.57481200	2.53250100
H	-5.27387100	-2.07710800	3.45848700
H	-4.07200200	0.89773100	-2.58108700

H	-2.31275600	1.04011900	-2.82653800
H	-2.36212300	5.63038000	0.74326100
Cl	8.46432300	-2.67073500	-0.70517300

$P_{3d'}$

Charge=0 multiplicity=1

O	2.07490800	-1.64695400	0.79156400
C	1.56545900	-0.38135400	-1.17830800
O	-2.95286700	0.39764700	1.58596700
C	2.45293100	-0.91967000	-0.12426700
O	-1.89059400	3.37371700	-1.97967200
O	-1.34053200	4.58713000	2.37272500
O	3.40296500	0.76993000	-2.24330800
N	-1.62640500	3.96588500	0.20203500
C	-1.95990700	3.03782900	-0.78499700
N	-2.11245600	2.46220900	1.96851400
C	0.13251700	-0.64388500	-1.25068100
C	-2.35695100	1.70950900	-0.33329800
C	-2.23147000	2.18820500	3.40545700
H	-1.85415900	3.05597200	3.94085400
H	-1.65289600	1.29684500	3.65666300
H	-3.27728200	2.00357000	3.66292200
C	2.11079300	0.41222200	-2.14484000
C	4.82513100	-0.95158700	0.68147100
H	4.49521600	-1.59081500	1.49250300
C	-1.66898200	3.72128800	1.57718700
C	-1.19857800	5.31417300	-0.18941000
H	-0.18600300	5.50262700	0.17472500
H	-1.86718300	6.05703400	0.25104100
H	-1.23114700	5.36597200	-1.27474000
C	4.29063600	0.31291700	-1.30236400
C	3.87264100	-0.51280000	-0.25326400
C	-2.50820200	1.43186700	1.09945800
C	5.62359200	0.70895900	-1.44131400

H 5.90810600 1.35084700 -2.26827200
H -0.35909000 -0.20123400 -2.11473900
C 6.55453900 0.26911100 -0.51223200
C 6.14619400 -0.56099200 0.54550600
H 7.59521000 0.56221700 -0.59704900
H 1.53022000 0.85034400 -2.95003300
C -2.63546600 0.71883300 -1.28308200
C -0.60196700 -1.37352900 -0.38047500
H -0.09273000 -1.86735500 0.43937900
N -2.65873500 0.97694500 -2.59803600
H -2.92776200 0.25241000 -3.24825400
C -2.04310200 -1.62750200 -0.48513200
C -2.95314000 -0.70741800 -0.93121900
C -2.48571100 -2.96294900 -0.00570800
C -3.55966200 -3.08383500 0.89154300
C -1.79281200 -4.11925600 -0.40171000
C -3.94453900 -4.33895600 1.35982900
H -4.06181900 -2.18907700 1.24361300
C -2.18881100 -5.37275000 0.05898400
H -0.95075600 -4.03159400 -1.08286600
C -3.26707900 -5.48510300 0.94002100
H -4.77135600 -4.41949100 2.05988700
H -1.65400400 -6.26099900 -0.26591200
C -4.32335800 -1.03662500 -1.17276600
N -5.44111500 -1.22860700 -1.44271300
H -2.49814500 1.94346300 -2.89096100
H -3.57172600 -6.46231500 1.30491000
Cl 7.34229800 -1.10502500 1.70783600

P_{3e}

Charge=0 multiplicity=1

O 5.22082400 1.61547200 1.44976300
O 3.33674400 -1.22211300 -0.83276300
O -5.67911600 0.42939700 -1.71745700
O -2.54191500 -1.74275900 1.11560000

O	-7.00176700	-2.66023900	1.36300100
N	-6.33239800	-1.10933600	-0.19143800
N	-3.13321400	0.89126200	-2.08793900
N	-4.77132900	-2.22705600	1.20313500
N	-0.75409600	-2.63085900	-1.91348200
C	-0.57420900	0.53618400	-0.36877800
C	-1.46332100	-0.34321200	-0.91900300
C	-2.91434800	-0.01800300	-1.13599400
C	-1.09309700	1.78573700	0.27261000
C	-3.96127100	-0.65340000	-0.45649100
C	3.17237500	0.76983100	0.48686500
C	3.88269100	-0.36588100	-0.14254500
C	5.34131600	-0.39806800	0.12320400
C	-1.05575300	-1.60924100	-1.44347000
C	0.84467900	0.22649000	-0.29529800
H	1.18650300	-0.67587200	-0.78955000
C	1.74048500	0.99982200	0.36348100
H	1.38098700	1.89521300	0.86881300
C	-5.33834200	-0.38603600	-0.84536300
C	-2.04619900	4.07908900	1.59903700
C	5.95075800	0.58873100	0.90529700
C	-3.66600600	-1.55624400	0.65202900
C	-1.69999300	1.68985700	1.53549900
H	-1.79906500	0.70460300	1.98193800
C	-1.45905500	4.19971500	0.33967700
H	-1.37000100	5.16618700	-0.14477700
C	-0.99006000	3.05759500	-0.30783600
C	-2.17059700	2.82381300	2.19559600
H	-2.63622900	2.72526900	3.17173600
C	3.89606400	1.66145700	1.22357100
H	3.45393700	2.52242300	1.71408800
C	6.13744300	-1.42535200	-0.40967700
H	5.65875000	-2.18715800	-1.01460700
C	-6.09743400	-2.04334500	0.82309700
C	7.49751500	-1.43908100	-0.15140400

C	7.32330000	0.57678900	1.16729400
H	7.75874700	1.36005300	1.77865700
C	8.09903300	-0.44269200	0.63572000
H	9.16654800	-0.47529000	0.82408600
C	-7.71970400	-0.86465400	-0.60119400
H	-7.97628800	0.18416800	-0.43394900
H	-8.35740600	-1.51415700	-0.00657600
H	-7.83435000	-1.08262600	-1.66544500
C	-4.54796700	-3.18684800	2.29079200
H	-3.47386000	-3.25750100	2.44465900
H	-4.96385900	-4.15780600	2.01477700
H	-5.04330500	-2.84406800	3.20287300
H	-4.10803300	1.11396100	-2.30690900
H	-2.35768600	1.29649100	-2.59369500
H	-2.41213000	4.96781100	2.10516900
Cl	8.50003500	-2.71815000	-0.81273800
Cl	-0.29673900	3.23896500	-1.92071200

$P_{3e'}$

Charge=0 multiplicity=1

O	2.26398400	-1.41815700	0.92944400
C	1.71250900	-0.11933000	-1.00809400
O	-2.87136000	0.73425700	1.66353700
C	2.62098400	-0.67105300	0.02123800
O	-1.99905400	3.38857300	-2.19571300
O	-1.69453400	5.12473700	2.00183600
O	3.52156600	1.08177100	-2.06806900
N	-1.85908800	4.24473700	-0.09051400
C	-2.08245300	3.18778800	-0.97247300
N	-2.25707600	2.90517100	1.82607600
C	0.28262600	-0.39727900	-1.06989100
C	-2.38971100	1.89070700	-0.38082200
C	-2.37765100	2.77880900	3.28351200
H	-2.11689400	3.73877800	3.72215800

H -1.70485400 1.99609400 3.64054400
H -3.40087100 2.50106200 3.54725800
C 2.23492500 0.70697400 -1.96007700
C 5.00642000 -0.70256400 0.78673500
H 4.69529400 -1.36558800 1.58599000
C -1.92049600 4.15051300 1.30248200
C -1.53444700 5.57368600 -0.62305300
H -0.54922900 5.88544400 -0.26862600
H -2.27203600 6.30050000 -0.27628400
H -1.54617400 5.50377100 -1.70780800
C 4.42864600 0.60774500 -1.15464100
C 4.03496200 -0.24845900 -0.12076400
C -2.53076700 1.75418200 1.07210400
C 5.75576200 1.01903300 -1.30496700
H 6.02117600 1.68427600 -2.11973200
H -0.22793700 0.08267200 -1.90137300
C 6.70563300 0.56366200 -0.40292500
C 6.32167300 -0.29684300 0.63950600
H 7.74232600 0.86775800 -0.49725200
H 1.63788900 1.15898900 -2.74533900
C -2.57787700 0.78475600 -1.21618200
C -0.41790600 -1.19498800 -0.23142900
H 0.12627300 -1.72319600 0.54345100
N -2.57348400 0.88197900 -2.55165100
H -2.75370500 0.06451300 -3.11705200
C -1.85469100 -1.47125900 -0.28283900
C -2.82259400 -0.60786000 -0.70541700
C -2.27622200 -2.76904500 0.33012300
C -2.95878400 -2.74684600 1.55721900
C -1.97423400 -4.01645000 -0.23447300
C -3.31955300 -3.93086900 2.19670400
H -3.18877400 -1.78209300 1.99899700
C -2.33822200 -5.20664400 0.39216100
C -3.00881800 -5.15975100 1.61413600
H -3.84446100 -3.89161200 3.14647700

H	-2.10042500	-6.15448600	-0.07854300
C	-4.20239700	-0.98143100	-0.74359600
N	-5.33828100	-1.22442300	-0.83469900
H	-2.45133300	1.81338800	-2.95605500
H	-3.29015800	-6.08750100	2.10422900
Cl	7.54135600	-0.85976400	1.76810200
Cl	-1.15602200	-4.11185800	-1.792777

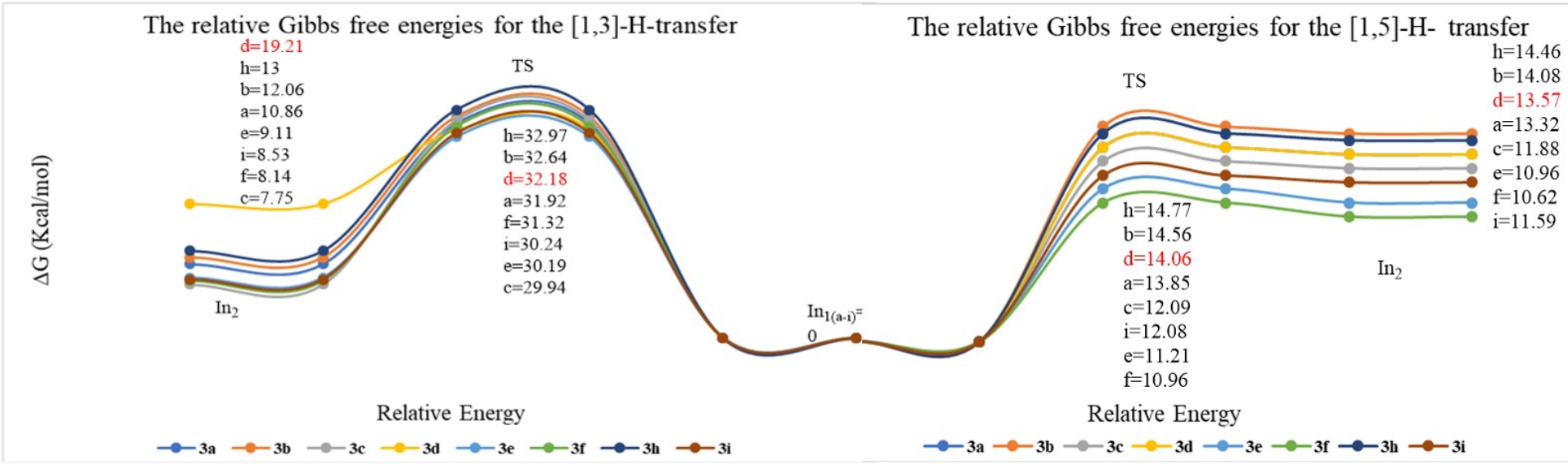


Fig. 2. Relative Gibbs free energies for the mechanism of [1,3] and [1,5]-H-transfer (all values in kcal mol^{-1}).

Table 17. Electron density (ρ BCP), Laplacian (∇2ρ BCP), potential energy (V BCP), kinetic energy (G BCP), total electron energy densities (HBCP= GBCP-VBCP,) and interaction energy (ΔEHB= ½ VBCP), calculated at the respective bond critical points, by M06-2X/def2-tzvp in acetonitrile solvent

Parameter	Distance	ρ_{BCP}^*	$\nabla^2\rho_{BCP}^*$	V_{BCP}^*	G_{BCP}^*	H_{BCP}^*	ΔE_{HB}
BCP (O_3-C_{42}) **3b'**	2.9	0.014	-0.22	-0.01	0.012	0.002	----
BCP (O_1-H_{15}) **3b'**	2.6	0.007	-0.11	-0.004	0.006	0.002	-1.26
BCP (O_1-H_{38}) **3b'**	2.2	0.017	-0.28	-0.013	0.015	0.003	-3.77
BCP (O_6-C_{26}) **3b'**	3.3	0.006	-0.08	-0.003	0.004	0.001	----
BCP (O_7-H_{22}) **3b'**	2.8	0.005	-0.07	-0.003	0.004	0.001	-0.94
BCP (N_8-C_{17}) **3b'**	3.4	0.006	-0.08	-0.003	0.004	0.001	-----
BCP (C_2-N_{10}) **3b'**	3.4	0.006	-0.08	-0.003	0.004	0.001	-----
BCP(C_{12}-C_{11}) **3b'**	3.0	0.014	-0.18	-0.009	0.010	0.001	------
CCP **3b'**	----	0.003	-0.05	-0.001	0.002	0.001	----
CCP **3b'**	----	0.005	-0.07	-0.002	0.003	0.001	----
CCP **3b'**	----	0.01	-0.19	-0.002	0.010	0.008	----
BCP (O_1-H_{24}) **3b**	1.8	0.036	-0.54	-0.035	0.034	-0.001	-10.98
BCP (O_2-C_9) **3b**	2. 7	0.018	-0.28	-0.014	0.016	0.002	-----
BCP (O_2-H_{32}) **3b**	2.6	0.006	-0.09	-0.004	0.005	0.001	-1.26
BCP(O_{57}-H_{14}) **3b**	2.2	0.017	-0.28	-0.013	0.015	0.002	-4.08
CCP **3b**	----	0.006	-0.09	+.006	0.006	0.012	----

Despite having three cage critical points, the stability of $\mathbf{P_{3b'}}$ originates in numerous intramolecular interactions. Thus, the linear product $\mathbf{P_{3b}}$ could arise from two rotations in the σ bonds of $\mathbf{P_{3b'}}$, as shown in Scheme 2. The driving force for these rotations could be a reduction in the instability resulting from the repulsion of cage critical points and forming the stronger non-bonding interactions, as in linear product $\mathbf{P_{3b}}$ (Fig 3).

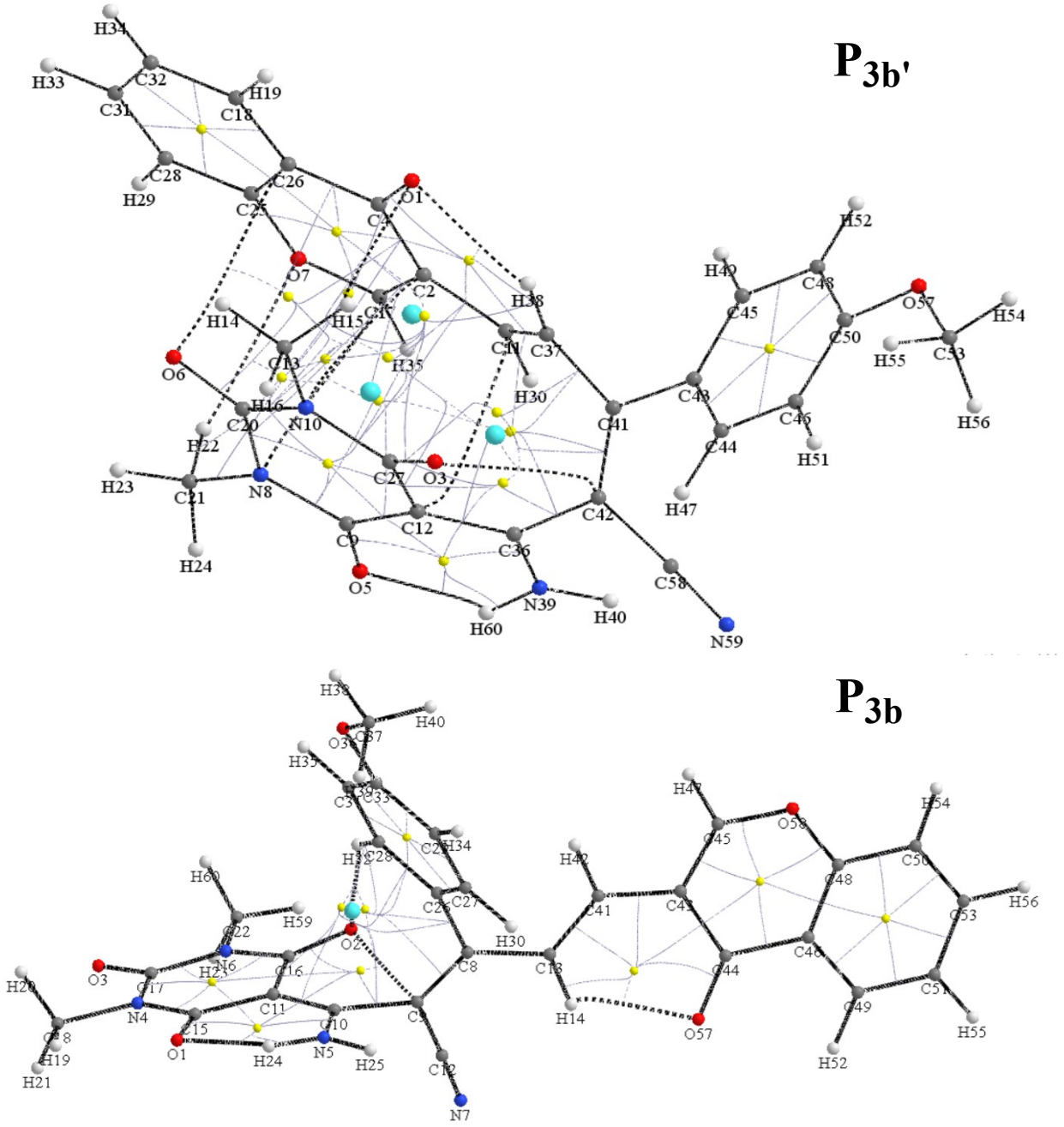


Fig. 3. The molecular graph of stereoisomers $\mathbf{P_{3b}}$, $\mathbf{P_{3b'}}$.

Reference

1 F. Neese, The ORCA program system, Wiley Interdiscip. *Rev. Comput. Mol. Sci*., 2012, **2**, 73.

2 C. Riplinger and F. Neese, *J. Chem. Phys*., 2013, **138**, 034106.

3 C. Riplinger, B. Sandhoefer, A. Hansen and F. Neese, *J. Chem. Phys*., 2013, **139**, 134101.

4 F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys*., 2005, **7**, 3297.

5 (a) Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215; (b) M. Walker, A. J. Harvey, A. Sen and C. E. Dessent, *J. Phys. Chem. A*, 2013, **117**, 12590.

6 (a) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104; (b) S. Ehrlich, J. Moellmann and S. *Grimme*, *Acc. Chem. Res*, 2013, **46**, 916; (c) S. Ehrlich, H. F. Bettinger and S. Grimme, *Angew. Chem. Int. Ed*., 2013, **52**, 10892.

7 (a) A. J. Becke, *Chem. Phys*, 1993, **98**, 5648; (b) L. R. Domingo, M. Ríos-Gutiérrez and P. Pérez, *Molecules*, 2016, **21**, 748.

8 (a) AIMAll (Version 17.01.25), T. A. Keith, TK Gristmill Software, Overland Park KS; R. W. F. Bader, *Chem. Rev*., 1991, **91**, 893; (b) R. F. W. Bader, *J. Phys. Chem. A*, 2010, **114**, 7431; (c) R. F. W. Bader, In Atoms in Molecules: A Quantum Theory; The International Series of Monographs of Chemistry; J. Halpen, M. L. H. Gren, Eds.; Clarendon Press: Oxford, U.K., 1990.

9 (a) B. Mennucci and J. Tomasi, *J. Chem. Phys*., 1997, **106**, 5151; (b) V. Barone and M. Cossi, *J. Phys. Chem. A*, 1998, **102**, 1995.

10 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski,

J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta,- F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian Development Version, Revision J.05, Gaussian, Inc., Wallingford, CT, 2019.

11 R. vianello, and Z. B. Maksić, *Tetrahedron*, 2005, **61**, 9381.

12 R. Vianello, and Z. B. Maksić, *Tetrahedron lett*, 2005, **46**, 3711.

13 Z. B. Maksić, and R. Vianello, *New J. Chem*., 2004, **28**, 843.

14 A. Kütt, T. Rodima, J. Saame, E. Raamat, V. Mäemets, I. Kaljurand, I. A. Koppel, R. Y. Garlyauskayte, Y. L. Yagupolskii, L. M. Yagupolskii and E. Bernhardt, *J. Org. Chem*., 2011, **76**, 391.