Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

HFIP-assisted, cobalt-catalyzed three-component electrophilic C–H amination/cyclization/directing group removal cascade to naphtho[1,2-*d*]imidazoles

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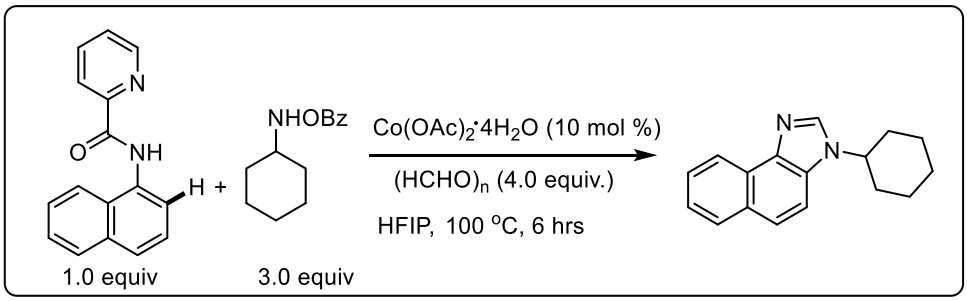
General Information: Air-sensitive reagents were handled under a dry nitrogen atmosphere. Unless otherwise stated, all commercial reagents were used without additional purification. Solvents were dried using standard methods and distilled before use. TLC was performed on silica gel plates (Merck silica gel 60, f_{254}), and the spots were visualized with UV light (254 and 365 nm) or by charring the plate dipped in $KMnO_4$ or vanillin charring solution. ^{1}H NMR spectra were recorded at 400 MHz (JEOL-JNM-ECZ400S/L1), ^{13}C NMR spectra were recorded at 100 MHz (JEOL-JNM-ECZ400S/L1) and ^{19}F NMR spectra were recorded at 376 MHz (JEOL-JNM-ECZ400S/L1) frequency in $CDCl_3$ or DMSO-d6 solvent using TMS as the internal standard. Chemical shifts were measured in parts per million (ppm) referenced to 0.0 ppm for tetramethylsilane. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br. = broad, dt = doublet of triplet, td = triplet of doublet, dd = doublet of doublet. Coupling constants, *J* were reported in Hertz unit (Hz). HRMS (m/z) were measured using ESI technique (Q-Tof Micro mass spectrometer). Crystals were grown in dichloromethane and crystal data was recorded in (Bruker Kappa Apex-2, CCD Area Detector) instrument.

Preparation of starting materials:

Starting materials are prepared according to our previous method.[1]

Representative Procedure for imidazole:



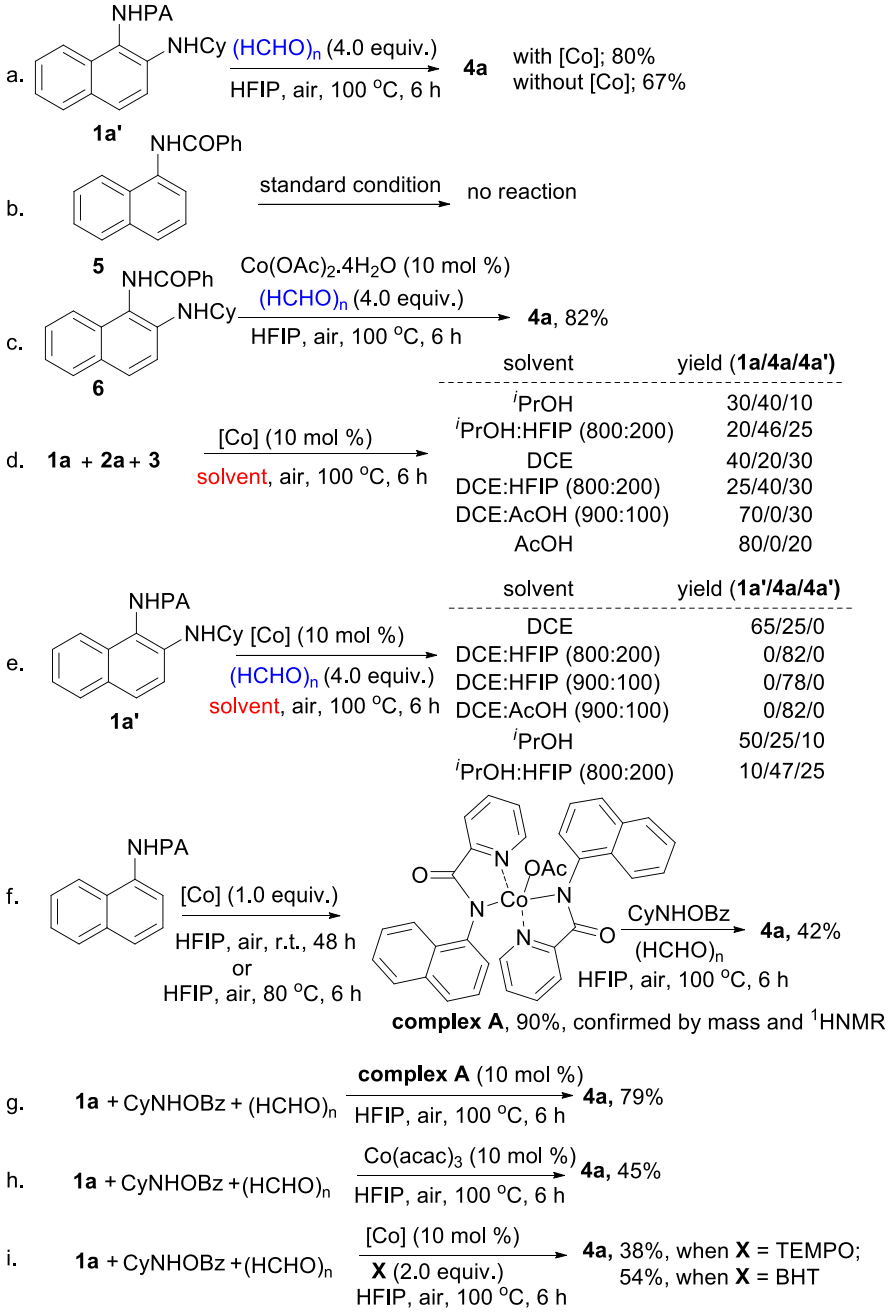
In an oven dried 15 mL sealed tube containing a stir bar was added corresponding picolinamide (0.3 mmol, 1.0 equiv.), *O*-benzoylhydroxylamine (0.9 mmol, 3.0 equiv.), $(HCHO)_n$ (36 mg, 1.2 mmol, 4.0 equiv.) and $Co(OAc)_2{\cdot}4H_2O$ (0.03 mmol). HFIP (3 mL) was then added. The mixture was stirred at 100 °C for 6 hrs. After allotted time the reaction mixture was cooled to room temperature. The mixture was diluted with DCM (50 mL) and washed with saturated aq. $NaHCO_3$ or NaOH solution (25mL), followed by brine solution (25 mL) and dried over anhydrous Na_2SO_4, and evaporated in *vacuo*. The crude mixture was loaded on a silica gel column chromatography and purified using (Hexane/Acetone) to give the desired imidazole product.

[**N.B.** During this whole process EtOAc can't be used because it is hydrolyzed by the imidazole product generating AcOH which can't be removed by simple rotary evaporation.]

Control experiments:

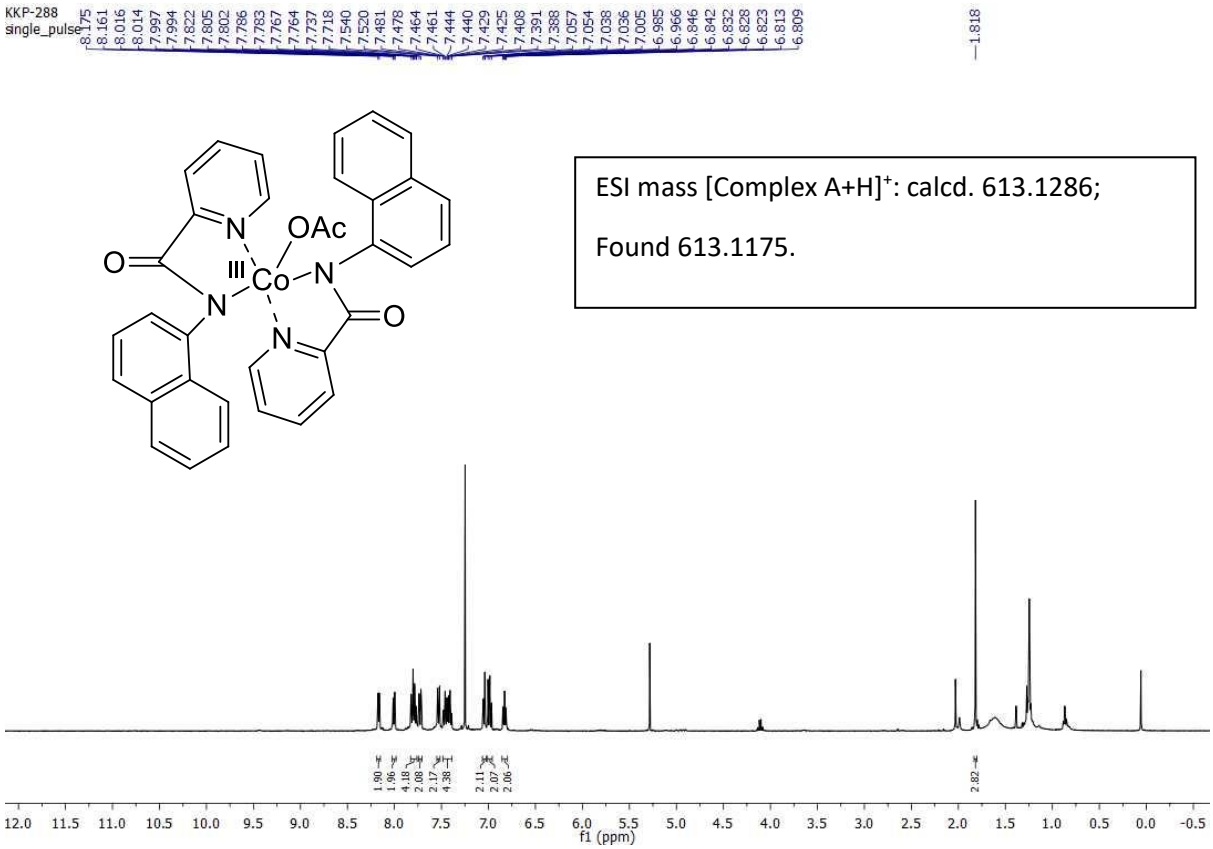
To gain insight into the mechanism some control experiments were performed. When the pre-formed *ortho* amino picolinamide was subjected to react with paraformaldehyde in presence or absence of Co-catalyst the product was obtained in 80% and 67% yield respectively in 6 hrs. This indicates that cobalt catalyst may have slight assistance in the subsequent reaction after amination. Though benzamide (**5**) didn't afford the desired product, the *ortho* amino benzamide of naphthylamine (**6**) successfully furnished the product in 82% yield. These experiments suggest that the pyridine N-atom is necessary for C-H amination step but for the subsequent reactions it is not required. Then to check the solvent effect in both C-H amination as well as next cyclization cascade, we performed the main reaction and also from intermediate **1a'** in various mixed solvents.

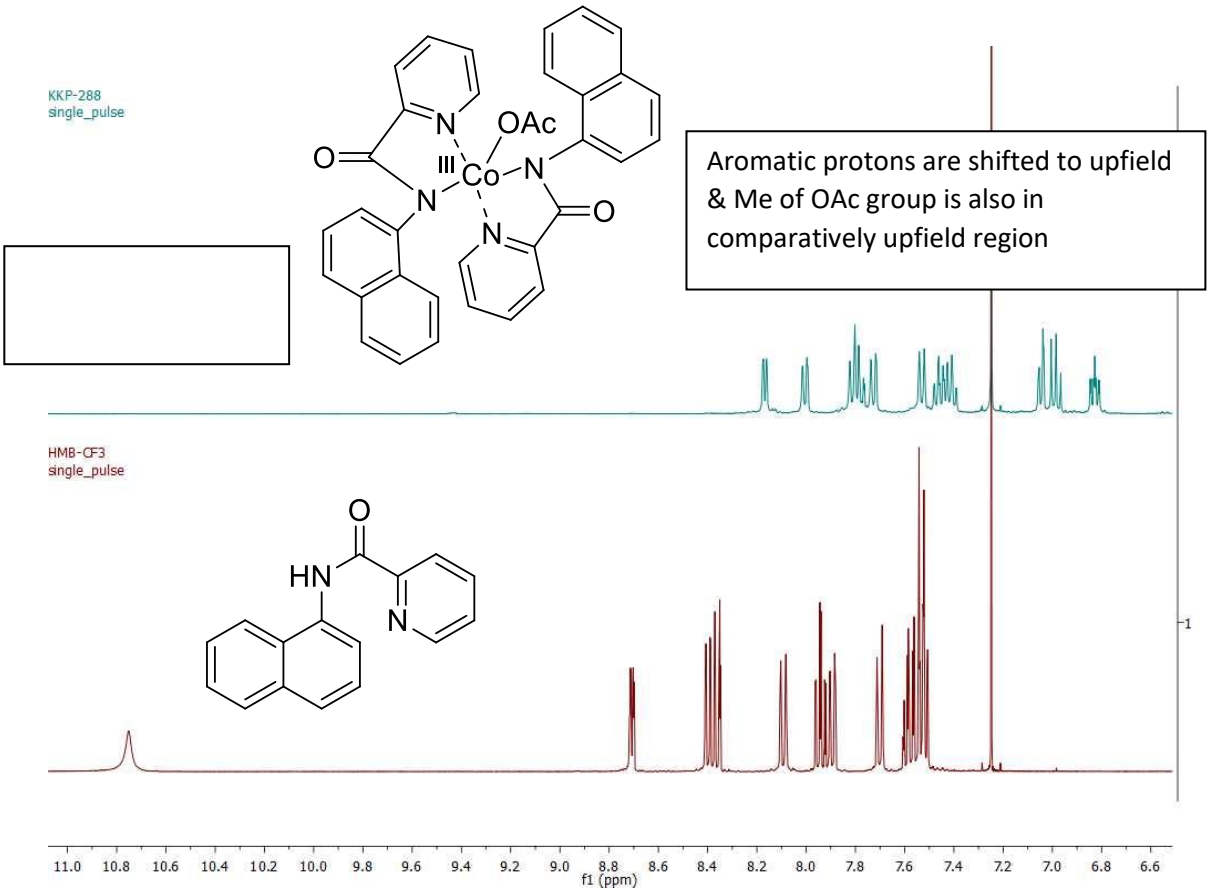
Enhanced yield of the desired product in presence of HFIP in both cases suggests that HFIP has role in the whole process. When the substrate was treated with 1.0 equiv. of $Co(OAc)_2.4H_2O$ in HFIF, substrate is found to be consumed with the formation of an orange-coloured complex which was isolated by column chromatography and electrospray ionization mass spectrometry (ESI-MS)



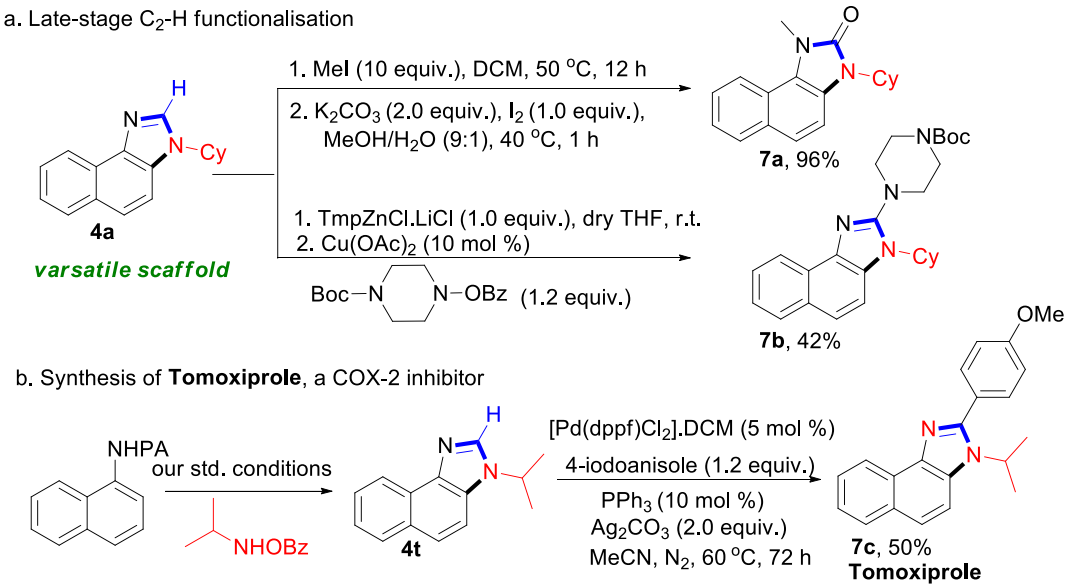
as well as ^{1}HNMR confirms the formation of complex **A**. This complex is formed only in HFIP and other solvent systems found ineffective for this complex formation. When this complex was

treated with amine source and $(HCHO)_n$, the product was obtained in 42% yield with the recovery of **1a**. Also, it evident from reaction **e** that after amination HFIP is acting as acid and probably facilitating the iminium formation. When 1a was treated under standard conditions with 2a and 3 using 10 mol % of this complex instead of $Co(OAc)_2.4H_2O$ 79% of the desired product was obtained. So, this indicates that this Co(III)-complex may be an intermediate in this reaction. $Co(acac)_3$ was also able to furnish the product in 45% yield. Since Co(III) salt is giving the product in good amount so we may assume that our reaction may be undergoing through initial oxidation of Co(II) to Co(III). When standard reactions were performed in presence of stoichiometric amounts of radical quenchers such as TEMPO or BHT product formation was inhibited slightly but not significantly. From this experiment we may think that probably the reaction is not going through any radical intermediate.





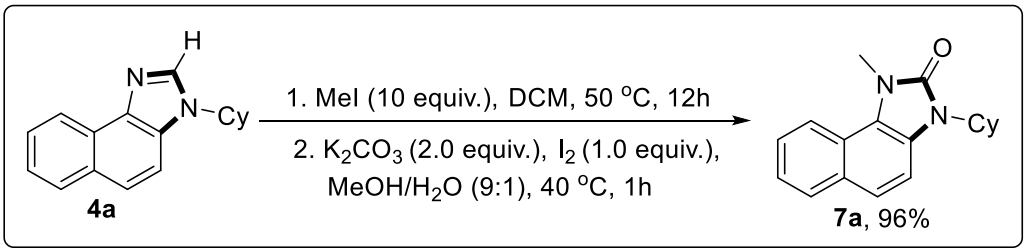
Product derivatization:



The imidazole product formed by our method is further utilized for the synthesis of naphthimidazolone (**7a**) and 2-amino naphthimidazole (**7b**). A COX-2 inhibitor

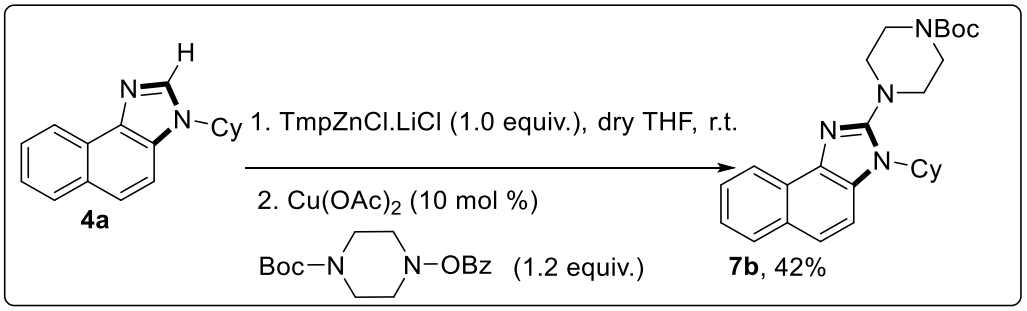
Tomoxiprole has also been synthesized by C_2-H arylation of compound **4t**, prepared by our method (**7c**).

Procedure for C2-H oxidation:



C2-H oxidation was performed following a previous method under slightly changed condition.[2] In an oven dried R.B. containing a stir bar charged with **4a** (0.5 mmol) in DCM was added MeI (10 equiv.). Then the mixture fitted with reflux condenser was heated at 50 ^oC for 12 hrs. After cooling to room temperature the solvent was evaporated under rotary evaporation. To this K_2CO_3 (2.0 equiv.), I_2 (1.0 equiv.) and MeOH/H_2O (9:1) 3 mL were added and heated to 40 ^oC for 1 h). After cooling to room temperature the solvent was evaporated. 50 mL EtOAc was added to it and washed with water and dried over anhydrous Na_2SO_4, and evaporated in *vacuo*. The crude mixture was loaded on a silica gel column chromatography and purified using (Hexane/EtOAc) to give the desired imidazolone product.

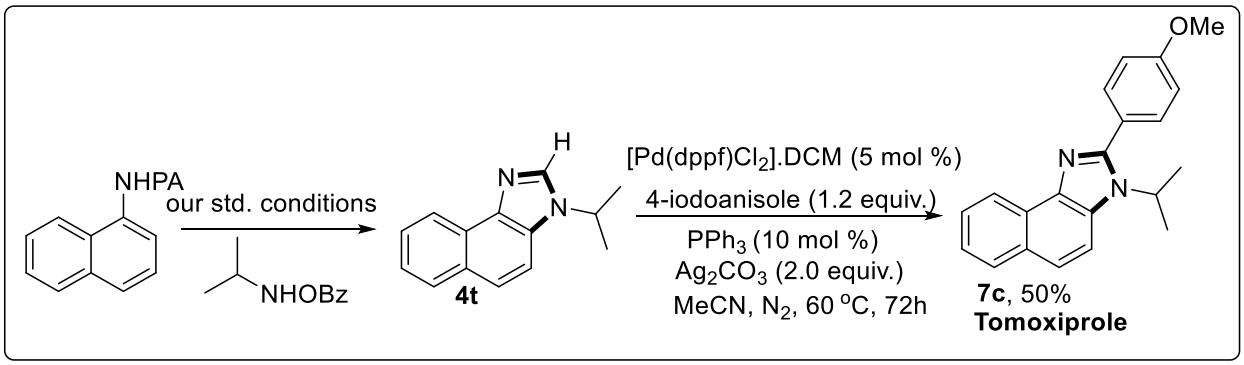
Procedure for C2-H amination:



C2-H amination was performed following a previous method under slightly changed condition.[3] In an oven dried R.B. containing a stir bar and charged with **4a** (0.5 mmol) in dry THF under Ar atmosphere was added TmpZnCl.LiCl in THF solution (1.0 equiv.) dropwise and strirred at room temperature for 30 minutes. After that a mixture of Cu(OAc)2 (10 mol%), the amine-OBz (1.2 equiv.) in dry THF under Ar atmosphere was added dropwise to the previous mixture at room

temperature and stirred at r.t. for 12 hrs. After this time the reaction was quenched with saturated NH_4Cl solution. Then after solvent evaporation EtOAc was added and washed with water dried over anhydrous Na_2SO_4, and evaporated in *vacuo*. The crude mixture was loaded on a silica gel column chromatography and purified using (Hexane/EtOAc) to give the desired product.

Procedure for the synthesis of Tomoxiprole:



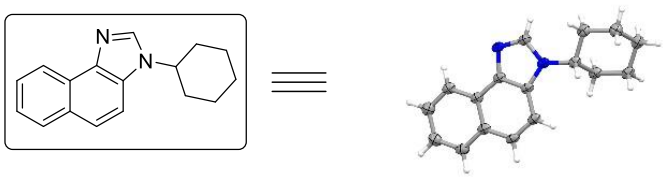
4t was prepared following our method. C2-H arylation was performed following a previous method.[4] An oven dried reaction vial containing a stir bar and charged with **4t** (0.5 mmol) was added [Pd(dppf)Cl_2].DCM (5 mol %), PPh_3 (10 mol %), 4-iododoanisole (1.2 equiv.), Ag_2CO_3 (2.0 equiv.) and then MeCN (4 mL) was added. Then the mixture was heated to 60 ^oC for 72 hrs. After the allotted time the mixture was cooled to room temperature and filtered through celite pad. Then crude obtained after the solvent evaporation was purified by silica gel column chromatography using (Hexane/EtOAc) to give the desired product.

Crystal structure:

The crystals were grown in dichloromethane solvent. The pure compound was dissolved in dichloromethane slow evaporation led to the crystal **4a**. The crystal data was collected in X-ray spectroscopy (Bruker Kappa Apex-2, CCD Area Detector), and the data was analyzed using OLEX2 software. The structure is given below. The corresponding cif file has been uploaded separately as supporting information.

Thermal ellipsoid plot of **4a**. Ellipsoids are represented with 50% probability.

X-ray determined molecular structure of **4a,** CCDC: 2220979



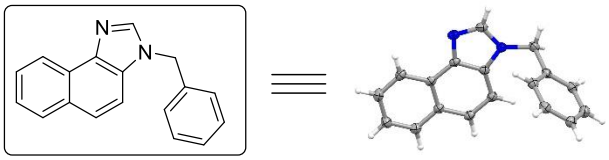
Identification code	HM1418
Empirical formula	$C_{17}H_{18}N_2$
Formula weight	250.33
Temperature/K	100.0
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	13.2417(9)
b/Å	12.7619(9)
c/Å	7.8090(5)
α/°	90
β/°	99.428(3)
γ/°	90
Volume/Å^3	1301.81(15)
Z	4
ρ_{calc}g/cm^3	1.277
μ/mm^{-1}	0.580
F(000)	536.0
Crystal size/mm^3	0.15 × 0.12 × 0.02
Radiation	Cu Kα (λ = 1.54178)
2Θ range for data collection/°	9.688 to 144.96
Index ranges	$-16 \leq h \leq 15$, $-15 \leq k \leq 15$, $-8 \leq l \leq 9$
Reflections collected	25331
Independent reflections	2532 [R_{int} = 0.0811, R_{sigma} = 0.0436]
Data/restraints/parameters	2532/0/173
Goodness-of-fit on F^2	1.071

Final R indexes [I>=2σ (I)]	R_1 = 0.0672, wR_2 = 0.1766
Final R indexes [all data]	R_1 = 0.0699, wR_2 = 0.1801
Largest diff. peak/hole / e Å^{-3}	0.46/-0.37

The crystals were grown in dichloromethane solvent. The pure compound was dissolved in dichloromethane slow evaporation led to the crystal **4ac**. The crystal data was collected in X-ray spectroscopy (Bruker Kappa Apex-2, CCD Area Detector), and the data was analyzed using OLEX2 software. The structure is given below. The corresponding cif file has been uploaded separately as supporting information.

Thermal ellipsoid plot of **4ac**. Ellipsoids are represented with 50% probability.

X-ray determined molecular structure of **4ac,** CCDC: 2220977

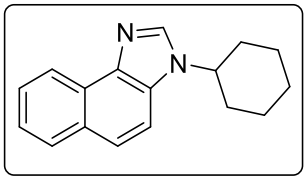


Identification code	HM1804_2_0m
Empirical formula	$C_{18}H_{14}N_2$
Formula weight	258.31
Temperature/K	100.00
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	6.5843(3)
b/Å	9.6121(4)
c/Å	20.5866(8)
α/°	90
β/°	93.7440(10)
γ/°	90
Volume/Å^3	1300.12(9)
Z	4

ρ_{calc}g/cm^3	1.320
μ/mm^{-1}	0.607
F(000)	544.0
Crystal size/mm^3	0.15 × 0.12 × 0.02
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	8.608 to 144.446
Index ranges	$-7 \leq h \leq 8$, $-11 \leq k \leq 11$, $-25 \leq l \leq 24$
Reflections collected	23131
Independent reflections	2472 [R_{int} = 0.0487, R_{sigma} = 0.0328]
Data/restraints/parameters	2472/0/181
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0422, wR_2 = 0.1115
Final R indexes [all data]	R_1 = 0.0432, wR_2 = 0.1125
Largest diff. peak/hole / e Å^{-3}	0.20/-0.17

Spectral data

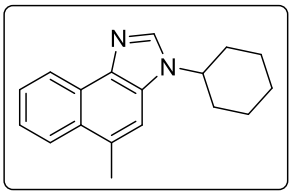
3-cyclohexyl-3*H*-naphtho[1,2-*d*]imidazole (4a)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a white solid (66 mg, 88% yield); mp: 148-150 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.65-8.63 (m, 1H), 8.03 (s, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.64-7.60 (m, 1H), 7.54 (d, *J* = 8.0 Hz, 1H), 7.49-7.45 (m, 1H), 4.31-4.23 (m, 1H), 2.27-2.23 (m, 2H), 2.01-1.96 (m, 2H), 1.89-1.78 (m, 3H), 1.58-1.46 (m, 2H), 1.39-1.27 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.3, 138.1, 130.2, 129.7, 128.4, 127.5, 126.6, 124.5,

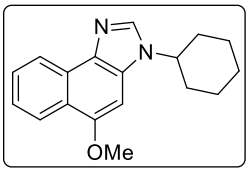
123.7, 121.8, 110.8, 55.7, 33.7, 25.8, 25.5; HRMS (ESI, m/z) calcd. For $C_{17}H_{19}N_2$ $[M+H]^+$: 251.1548; found: 251.1571.

3-cyclohexyl-5-methyl-3*H*-naphtho[1,2-*d*]imidazole (4b)



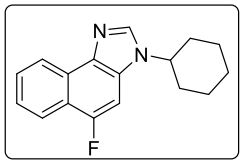
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy solid (71 mg, 90% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.47-8.44 (m, 1H), 8.23 (s, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 0.8 Hz, 1H), 7.59-7.55 (m, 1H), 7.49-7.45 (m, 1H), 4.43-4.35 (m, 1H), 2.69 (s, 3H), 2.06-2.02 (m, 2H), 1.89-1.88 (m, 4H), 1.69 (d, *J* = 12.8 Hz, 1H), 1.53-1.43 (m, 2H), 1.33 - 1.25 (m 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 139.2, 137.8, 129.6, 129.4, 129.3, 127.5, 126.4, 125.4, 124.6, 122.1, 112.5, 54.9, 33.5, 25.7, 25.4, 20.3; HRMS (ESI, m/z) calcd. For $C_{18}H_{21}N_2$ $[M+H]^+$: 265.1705; found: 265.1713.

3-cyclohexyl-5-methoxy-3*H*-naphtho[1,2-*d*]imidazole (4c)



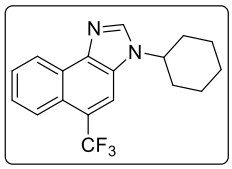
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light orange solid (66 mg, 78% yield); mp: 98-100 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.39-8.36 (m, 1H), 8.18-8.16 (m, 2H), 7.59-7.55 (m, 1H), 7.43-7.39 (m, 1H), 7.24 (s, 1H), 4.46-4.39 (m, 1H), 2.69 (s, 3H), 2.06-2.03 (m, 2H), 1.85-1.67 (m, 4H), 1.69 (d, *J* = 12.8 Hz, 1H), 1.55-1.44 (m, 2H), 1.31-1.21 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 152.4, 138.3, 132.8, 130.0, 127.6, 127.3, 124.1, 123.1, 122.9, 121.5, 91.3, 56.6, 54.5, 33.6, 25.8, 25.4; HRMS (ESI, m/z) calcd. For $C_{18}H_{21}N_2O$ $[M+H]^+$: 281.1654; found: 281.1643.

3-cyclohexyl-5-fluoro-3*H*-naphtho[1,2-*d*]imidazole (4d)



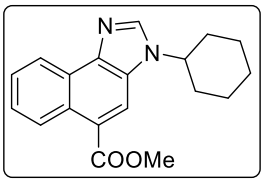
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a creamy white solid (58 mg, 72% yield); mp: 114-116 ^oC. ^1H NMR (400 MHz, DMSO-d6): δ 8.47-8.44 (m, 1H), 8.34 (s, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.82 (d, *J* = 11.2 Hz, 1H), 7.68-7.64 (m, 1H), 7.56-7.52 (m, 1H), 4.45-4.37 (m, 1H), 2.05-2.01 (m, 2H), 1.87-1.77 (m, 4H), 1.68 (d, *J* = 12.8 Hz, 1H), 1.52-1.41 (m, 2H), 1.32-1.21 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 155.2 (d, *J* = 242.0 Hz), 140.3, 135.2, 128.7 (d, *J* = 13.8 Hz), 127.9, 127.3 (d, *J* = 6.2 Hz), 125.2 (d, *J* = 1.3 Hz), 121.9 (d, *J* = 2.7 Hz), 121.4 (d, *J* = 5.6 Hz), 120.3 (d, *J* = 18.5, Hz), 97.2 (d, *J* = 26.7 Hz), 55.1, 33.4, 25.7, 25.3; ^{19}F NMR (376 MHz, DMSO-d6): δ -128.5; HRMS (ESI, m/z) calcd. For $C_{17}H_{18}FN_2$ $[M+H]^+$: 269.1454; found: 269.1442.

3-cyclohexyl-5-(trifluoromethyl)-3*H*-naphtho[1,2-*d*]imidazole (4e)



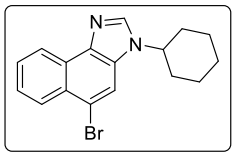
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light orange solid (43 mg, 45% yield); mp: 98-100 ^oC. ^1H NMR (600 MHz, DMSO-d6): δ 8.64-8.63 (m, 2H), 8.44 (s, 1H), 8.15 (d, *J* = 8.4 Hz, 1H), 7.75 (t, *J* = 7.2 Hz 1H), 7.69-7.66 (m, 1H), 4.71-4.66 (m, 1H), 2.10-2.08 (m, 2H), 1.90-1.87 (m, 4H), 1.74 (d, *J* = 12.6 Hz, 1H), 1.59-1.52 (m, 2H), 1.34-1.27 (m, 1H); ^{13}C NMR (150 MHz, DMSO-d6): δ 142.3, 141.1, 127.4, 127.1, 126.1, 126.0, 124.7, 124.3, 124.1, 112.1, 118.9 (q, *J* = 31.9 Hz), 112.2 (q, *J* = 8.9 Hz), 54.3, 33.2, 25.0, 24.8; ^{19}F NMR (376 MHz, DMSO-d6): δ -156.9; HRMS (ESI, m/z) calcd. For $C_{18}H_{18}F_3N_2$ $[M+H]^+$: 319.1422; found: 319.1412.

methyl 3-cyclohexyl-3*H*-naphtho[1,2-*d*]imidazole-5-carboxylate (4f)



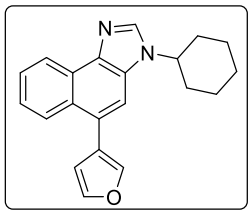
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy solid (46 mg, 50% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.82 (d, *J* = 8.8 Hz, 1H), 8.57-8.54 (m, 2H), 8.48 (s, 1H), 7.66-7.62 (m, 1H), 7.58-7.54 (m, 1H), 4.59-4.52 (m, 1H), 3.94 (s, 3H), 2.08-2.03 (m, 2H), 1.89-1.79 (m, 4H), 1.69 (d, *J* = 12.4 Hz, 1H), 1.56-1.46 (m, 2H), 1.30-1.20 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 168.1, 142.9, 142.2, 128.4, 127.9, 127.4, 127.0, 126.6, 126.2, 122.2, 121.9, 116.8, 54.9, 52.7, 33.7, 25.6, 25.4; HRMS (ESI, m/z) calcd. For $C_{19}H_{21}N_2O_2$ $[M+H]^+$: 309.1603; found: 309.1605.

5-bromo-3-cyclohexyl-3*H*-naphtho[1,2-*d*]imidazole (4g)



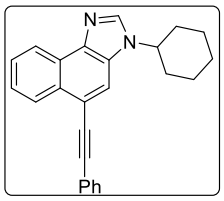
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a creamy white solid (82 mg, 83% yield); mp: 118-120 ºC. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.67-8.64 (m, 1H), 8.31-8.28 (m, 1H), 8.03 (s, 1H), 7.89 (s, 1H), 7.67-7.63 (m, 1H), 7.59-7.57 (m, 1H), 4.24-4.17 (m, 1H), 2.25-2.21 (m, 2H), 2.00-1.95 (m, 2H), 1.84-1.75 (m, 3H), 1.57-1.45 (m, 2H), 1.37-1.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.0, 138.5, 129.6, 128.3, 128.0, 127.9, 127.4, 125.8, 122.2, 117.7, 114.9, 55.9, 33.7, 25.7, 25.4; HRMS (ESI, m/z) calcd. For $C_{17}H_{18}BrN_2$ $[M+H]^+$: 329.0653; found: 329.0663.

3-cyclohexyl-5-(furan-3-yl)-3*H*-naphtho[1,2-*d*]imidazole (4h)



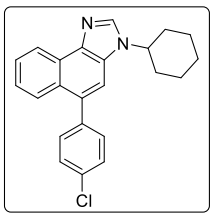
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light yellow solid (81 mg, 85% yield); mp: 156-158 ^oC. ^1H NMR (400 MHz, DMSO-d6): δ 8.72-8.69 (m, 1H), 8.12 (dt, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 8.05 (s, 1H), 7.67 (dd, J_1 = 1.6 Hz, J_2 = 0.8 Hz, 1H), 7.66-7.62 (m, 1H), 7.60 (t, J = 1.6 Hz, 1H), 7.52 (s, 1H), 7.49-7.45 (m, 1H), 6.72 (dd, J_1 = 1.6 Hz, J_2 = 0.8 Hz, 1H), 4.32-4.24 (m, 1H), 2.29-2.25 (m, 2H), 2.01-1.96 (m, 2H), 1.90-1.80 (m, 3H), 1.58-1.46 (m, 2H), 1.39-1.31 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 142.9, 140.5, 139.1, 138.3, 129.2, 129.0, 127.6, 126.6, 126.5, 125.5, 124.8, 122.1, 113.0, 111.7, 55.7, 33.8, 25.8, 25.5; HRMS (ESI, m/z) calcd. For $C_{21}H_{21}N_2O$ $[M+H]^+$: 317.1654; found: 317.1664.

3-cyclohexyl-5-(phenylethynyl)-3*H*-naphtho[1,2-*d*]imidazole (4i)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a yellow fluffy solid (60 mg, 57% yield); mp: 68-70 ^oC. ^1H NMR (400 MHz, DMSO-d6): δ 8.51-8.42 (m, 3H), 8.24 (s, 1H), 7.69-7.59 (m, 4H), 7.47-7.40 (m, 3H), 4.54 (t, J = 11.2 Hz, 1H), 2.07 (d, J = 9.2 Hz, 2H), 1.90-1.84 (m, 4H), 1.70 (d, J = 12.4 Hz, 1H), 1.56-1.47 (m, 2H), 1.33-1.23 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 141.6, 139.8, 131.9, 129.7, 129.43, 129.39, 129.3, 127.5, 127.2, 126.8, 125.9, 123.2, 122.2, 117.0, 114.6, 93.7, 88.9, 55.0, 33.6, 25.7, 25.4; HRMS (ESI, m/z) calcd. For $C_{25}H_{23}N_2$ $[M+H]^+$: 351.1861; found: 351.1846.

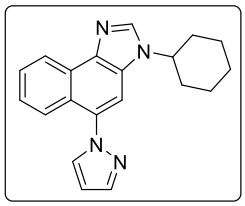
5-(4-chlorophenyl)-3-cyclohexyl-3*H*-naphtho[1,2-*d*]imidazole (4j)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a yellow powder (93 mg, 86% yield); mp:

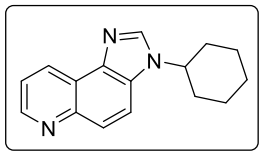
124-126 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.54 (d, *J* = 8.0 Hz, 1H), 8.38 (s, 1H), 7.76-7.72 (m, 2H), 7.61-7.39 (m, 6H), 4.49 (t, *J* = 10.4 Hz, 1H), 2.07-2.04 (m, 2H), 1.88-1.79 (m, 4H), 1.66 (d, *J* = 11.2 Hz, 1H), 1.51-1.41 (m, 2H), 1.29-1.23 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 140.4, 140.1, 138.7, 133.9, 132.6, 132.5, 129.5, 128.9, 128.2, 127.5, 126.7, 126.5, 125.0, 122.1, 113.2, 54.9, 33.6, 25.7, 25.4; HRMS (ESI, m/z) calcd. For $C_{23}H_{22}ClN_2$ $[M+H]^+$: 361.1472; found: 361.1471.

3-cyclohexyl-5-(1H-pyrazol-1-yl)-3*H*-naphtho[1,2-*d*]imidazole (4k)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy solid (38 mg, 40% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.55-8.54 (m, 1H), 8.49 (s, 1H), 8.15 (dd, J_1 = 2.4 Hz, J_2 = 0.8 Hz, 1H), 8.05 (s, 1H), 7.81 (dd, J_1 = 2.0 Hz, J_2 = 0.8 Hz, 1H), 7.66-7.62 (m, 1H), 7.53-7.52 (m, 1H), 7.48-7.43 (m, 1H), 6.58 (t, *J* = 2.0 Hz, 1H), 4.57-4.50 (m, 1H), 2.08-2.04 (m, 2H), 1.91-1.81 (m, 4H), 1.68 (d, *J* = 12.4 Hz, 1H), 1.54-1.43 (m, 2H), 1.33-1.25 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 141.4, 140.8, 138.8, 133.6, 133.1, 128.7, 127.5, 127.2, 126.5, 125.6, 124.3, 121.9, 110.9, 106.8, 55.0, 33.6, 25.6, 25.3; HRMS (ESI, m/z) calcd. For $C_{20}H_{21}N_4$ $[M+H]^+$: 317.1766; found: 317.1755.

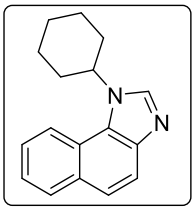
3-cyclohexyl-3*H*-imidazo[4,5-*f*]quinoline (4l)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a pale yellow solid (40 mg, 53% yield); mp: 144-146 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.82 (dd, J_1 = 4.4 Hz, J_2 = 2.0 Hz, 1H), 8.79-8.77 (m, 1H), 8.43 (s, 1H), 8.06 (d, *J* = 9.2 Hz, 1H), 7.81 (d, *J* = 9.2 Hz, 1H), 7.56 (dd, J_1 = 8.0 Hz, J_2 = 4.0 Hz, 1H), 4.50-4.42 (m, 1H), 2.05-2.02 (m, 2H), 1.89-1.79 (m, 4H), 1.67 (d, *J* = 13.2 Hz, 1H),

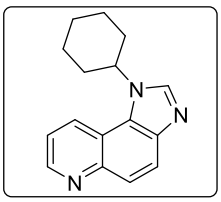
1.52-1.42 (m, 2H), 1.30-1.22 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 148.7, 145.9, 141.1, 138.4, 129.9, 129.8, 124.2, 122.3, 121.8, 115.5, 55.2, 33.2, 25.7, 25.3; HRMS (ESI, m/z) calcd. For $C_{16}H_{18}N_3$ $[M+H]^+$: 252.1501; found: 252.1502.

1-cyclohexyl-1*H*-naphtho[1,2-*d*]imidazole (4m)



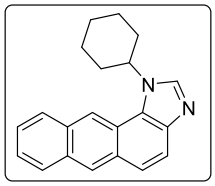
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a white powder (30 mg, 40% yield); mp: 140-142 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.36 (s, 1H), 8.28 (d, J = 8.4 Hz, 1H), 8.02 (dd, J_1 = 8.4 Hz, J_2 = 1.2 Hz, 1H), 7.75 (d, J = 8.4 Hz, 1H), 7.67 (d, J = 8.8 Hz, 1H), 7.65-7.60 (m, 1H), 7.50-7.46 (m, 1H), 4.91-4.84 (m, 1H), 2.26 (d, J = 12.0 Hz, 2H), 1.89-1.58 (m, 7H), 1.34-1.26 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 141.6, 140.4, 131.4, 129.9, 127.3, 126.8, 124.5, 123.8, 122.4, 120.9, 120.6, 56.9, 33.8, 25.8, 25.6; HRMS (ESI, m/z) calcd. For $C_{17}H_{19}N_2$ $[M+H]^+$: 251.1548; found: 251.1545.

1-cyclohexyl-1*H*-imidazo[4,5-*f*]quinoline (4n)



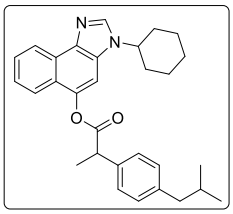
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown solid (32 mg, 42% yield); mp: 148-150 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.84 (dd, J_1 = 4.4 Hz, J_2 = 1.6 Hz, 1H), 8.68 (d, J = 8.4 Hz, 1H), 8.45 (s, 1H), 7.99 (d, J = 8.8 Hz, 1H), 7.80 (d, J = 8.8 Hz, 1H), 7.62 (dd, J_1 = 8.8 Hz, J_2 = 4.4 Hz, 1H), 4.91-4.84 (m, 1H), 2.34 (d, J = 11.2 Hz, 2H), 1.88-1.60 (m, 7H), 1.33-1.25 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 148.1, 146.5, 141.4, 141.3, 129.4, 126.6, 124.9, 123.9, 121.5, 117.5, 56.8, 33.6, 25.6, 25.5; HRMS (ESI, m/z) calcd. For $C_{16}H_{18}N_3$ $[M+H]^+$: 252.1501; found: 252.1497.

1-cyclohexyl-1*H*-anthra[1,2-*d*]imidazole (4o)



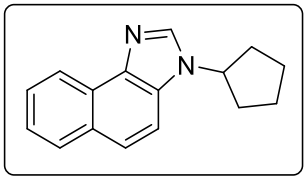
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a creamy white solid (61 mg, 68% yield); mp: 154-156 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.79 (s, 1H), 8.65 (s, 1H), 8.36 (s, 1H), 8.19 (d, *J* = 8.0 Hz, 1H), 8.07 (d, *J* = 8.8 Hz, 1H), 7.81 (d, *J* = 8.8 Hz, 1H), 7.73 (d, *J* = 9.2 Hz, 1H), 7.57-7.49 (m, 2H), 5.14-5.07 (m, 1H), 2.35 (d, *J* = 12.0 Hz, 2H), 1.93-1.77 (m, 7H), 1.37-1.28 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 141.0, 139.6, 131.6, 130.5, 130.1, 128.9, 128.3, 128.2, 126.4, 126.3, 125.8, 124.5, 121.8, 121.5, 118.9, 57.0, 33.8, 25.7, 25.5; HRMS (ESI, m/z) calcd. For $C_{21}H_{21}N_2$ $[M+H]^+$: 301.1705; found: 301.1703.

3-cyclohexyl-3*H*-naphtho[1,2-*d*]imidazol-5-yl 2-(4-isobutylphenyl)propanoate (4p)



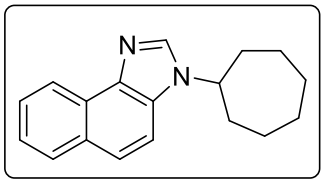
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy liquid (91 mg, 67% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.43 (dt, J_1 = 8.4 Hz, J_2 = 0.8 Hz, 1H), 8.35 (s, 1H), 7.68 (s, 1H), 7.57-7.53 (m, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.24-7.19 (m, 4H), 4.44 -4.36 (m, 1H), 4.24 (q, *J* = 6.8 Hz, 1H), 2.44 (d, *J* = 6.8 Hz, 2H), 2.04-1.99 (m, 2H), 1.86-1.79 (m, 5H), 1.67 (d, *J* = 12.0 Hz, 1H), 1.58 (d, *J* = 7.2 Hz, 3H), 1.51-1.41 (m, 2H), 1.28-1.18 (m, 1H), 0.85 (d, *J* = 6.4 Hz, 6H); ^{13}C NMR (100 MHz, DMSO-d6): δ 173.8, 160.5, 142.6, 140.9, 140.5, 137.9, 136.8, 129.9, 128.9, 128.1, 127.3, 124.8, 123.7, 118.2, 105.4, 55.0, 44.9, 44.8, 33.5, 33.4, 32.8, 30.2, 25.6, 25.3, 22.7, 22.6, 18.6; HRMS (ESI, m/z) calcd. For $C_{30}H_{35}N_2O_2$ $[M+H]^+$: 455.2699; found: 455.2697.

3-cyclopentyl-3*H*-naphtho[1,2-*d*]imidazole (4q)



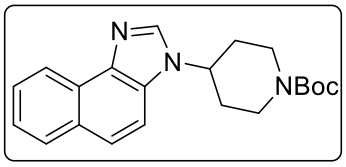
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a creamy white solid (61 mg, 86% yield); mp: 114-116 ^oC. ^1H NMR (400 MHz, DMSO-d6): δ 8.47-8.44 (m, 1H), 8.31 (s, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.74 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.59-7.55 (m, 1H), 7.46-7.41 (m, 1H), 4.93-4.86 (m, 1H), 2.23-2.14 (m, 2H), 1.97-1.89 (m, 2H), 1.86-1.77 (m, 2H), 1.72-1.67 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d6): δ 140.2, 139.2, 130.5, 130.2, 128.9, 127.4, 126.7, 124.7, 123.4, 121.7, 112.4, 56.9, 32.7, 24.1; HRMS (ESI, m/z) calcd. For $C_{16}H_{17}N_2$ $[M+H]^+$: 237.1392; found: 237.1394.

3-cycloheptyl-3*H*-naphtho[1,2-*d*]imidazole (4r)



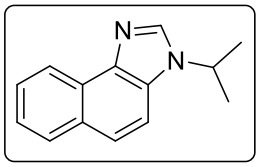
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a creamy white solid (54 mg, 68% yield); mp: 98-100 ^oC. ^1H NMR (400 MHz, DMSO-d6): δ 8.42 (d, *J* = 8.0 Hz, 1H), 8.33 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.78 (d, *J* = 9.2 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.58-7.54 (m, 1H), 7.45-7.41 (m, 1H), 4.66-4.59 (m, 1H), 2.08-2.03 (m, 4H), 1.79-1.58 (m, 8H); ^{13}C NMR (100 MHz, DMSO-d6): δ 140.2, 138.9, 130.1, 129.7, 128.9, 127.4, 126.7, 124.6, 123.3, 121.6, 112.4, 57.5, 35.5, 27.5, 24.7; HRMS (ESI, m/z) calcd. For $C_{18}H_{21}N_2$ $[M+H]^+$: 265.1705; found: 265.1714.

***tert*-butyl 4-(3H-naphtho[1,2-*d*]imidazol-3-yl)piperidine-1-carboxylate (4s)**



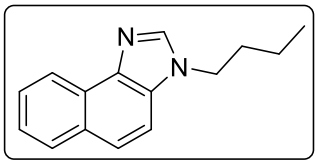
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a creamy white solid (84 mg, 80% yield); mp: 182-184 ^oC. ^1H NMR (400 MHz, DMSO-d6): δ 8.42 (d, *J* = 8.0 Hz, 1H), 8.39 (s, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.8 Hz, 1H), 7.59-7.54 (m, 1H), 7.46-7.40 (m, 1H), 4.72-4.64 (m, 1H), 4.13 (d, *J* = 11.6 Hz, 2H), 2.95 (br.s, 2H), 2.07-1.89 (m, 4H), 1.41 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d6): δ 154.3, 140.0, 138.8, 130.2, 130.0, 128.9, 127.3, 126.8, 124.7, 123.4, 121.6, 112.1, 79.5, 53.1, 32.6, 28.6; HRMS (ESI, m/z) calcd. For $C_{21}H_{26}N_3O2$ $[M+H]^+$: 352.2025; found: 352.2029.

3-isopropyl-3*H*-naphtho[1,2-*d*]imidazole (4t)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a creamy white solid (38 mg, 60% yield); mp: 108-110 ^oC. ^1H NMR (400 MHz, DMSO-d6): δ 8.44-8.43 (m, 1H), 8.35 (s, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.79 (d, *J* = 8.8 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.58-7.54 (m, 1H), 7.46-7.41 (m, 1H), 4.88-4.78 (m, 1H), 1.55 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, DMSO-d6): δ 139.9, 139.1, 130.1, 129.9, 128.9, 127.4, 126.7, 124.6, 123.3, 121.6, 112.3, 47.8, 23.1; HRMS (ESI, m/z) calcd. For $C_{14}H_{15}N_2$ $[M+H]^+$: 211.1235; found: 211.1240.

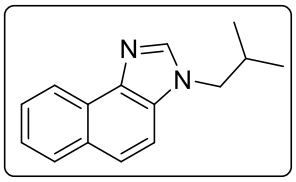
3-butyl-3*H*-naphtho[1,2-*d*]imidazole (4u)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy solid (33 mg, 48% yield). ^1H NMR (400 MHz, DMSO-d6): δ 8.44-8.41 (m, 1H), 8.24 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.75 (d, *J* = 8.8 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.58-7.54 (m, 1H), 7.45-7.41 (m, 1H), 4.30 (t, *J* = 7.2 Hz, 1H), 1.77 (qu, *J* = 7.2 Hz, 2H), 1.27-1.18 (m, 2H), 0.85 (t, *J* = 7.2 Hz, 3H); ^{13}C

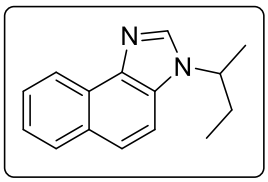
NMR (100 MHz, DMSO-d6): δ 142.4, 138.9, 130.6, 130.1, 128.9, 127.3, 126.7, 124.6, 123.5, 121.6, 112.0, 44.6, 32.5, 19.9, 13.9; HRMS (ESI, m/z) calcd. For $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1392; found: 225.1402.

3-isobutyl-3*H*-naphtho[1,2-*d*]imidazole (4v)



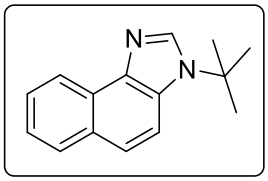
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown solid (50 mg, 74% yield); mp: 74-76 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.44-8.42 (m, 1H), 8.22 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.76 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.59-7.55 (m, 1H), 7.46-7.41 (m, 1H), 4.12 (d, *J* = 7.2 Hz, 2H), 2.16-2.08 (m, 1H), 0.83 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, DMSO-d6): δ 142.8, 138.8, 130.9, 130.1, 128.9, 127.3, 126.7, 124.6, 123.5, 121.5, 112.3, 51.9, 29.6, 20.2; HRMS (ESI, m/z) calcd. For $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1392; found: 225.1402.

3-(*sec*-butyl)-3*H*-naphtho[1,2-*d*]imidazole (4w)



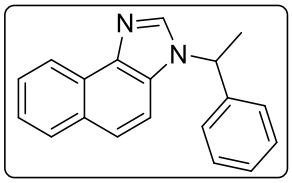
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy solid (54 mg, 81% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.45-8.43 (m, 1H), 8.33 (s, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 8.8 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.58-7.54 (m, 1H), 7.45-7.41 (m, 1H), 4.62-4.53 (m, 1H), 1.97-1.82 (m, 2H), 1.53 (d, *J* = 6.8 Hz, 3H), 0.71 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d6): δ 140.5, 139.0, 130.2, 130.1, 128.9, 127.4, 126.7, 124.6, 123.3, 121.6, 112.4, 53.6, 29.8, 21.2, 11.0; HRMS (ESI, m/z) calcd. For $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1392; found: 225.1401.

3-(*tert*-butyl)-3*H*-naphtho[1,2-*d*]imidazole (4x)



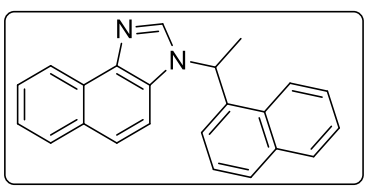
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy solid (29 mg, 43% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.46-8.44 (m, 1H), 8.23 (s, 1H), 7.98-7.94 (m, 2H), 7.67 (d, *J* = 9.2 Hz, 1H), 7.58-7.54 (m, 1H), 7.46-7.42 (m, 1H), 1.72 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d6): δ 140.5, 140.0, 129.6, 129.5, 128.6, 127.4, 126.6, 124.8, 122.9, 121.7, 114.7, 56.8, 29.8; HRMS (ESI, m/z) calcd. For $C_{15}H_{17}N_2$ $[M+H]^+$: 225.1392; found: 225.1388.

3-(1-phenylethyl)-3*H*-naphtho[1,2-*d*]imidazole (4y)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a yellow solid (69 mg, 85% yield); mp: 114-116 ^{o}C. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.58 (s, 1H), 8.46-8.43 (m, 1H), 7.91 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 8.8 Hz, 1H), 7.58-7.55 (m, 2H), 7.43-7.41 (m, 1H), 7.30-7.28 (m, 4H), 7.24-7.21 (m, 1H), 5.94 (q, *J* = 6.8 Hz, 1H), 1.97 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d6): δ 142.4, 140.5, 139.2, 130.3, 130.2, 129.3, 128.9, 128.2, 127.3, 126.8, 126.6, 124.8, 123.5, 121.6, 112.5, 55.0, 21.7; HRMS (ESI, m/z) calcd. For $C_{19}H_{17}N_2$ $[M+H]^+$: 273.1392; found: 273.1382.

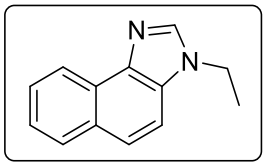
3-(1-(naphthalen-1-yl)ethyl)-3*H*-naphtho[1,2-*d*]imidazole (4z)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a creamy white solid (83 mg, 86% yield);

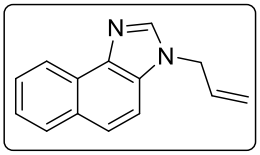
mp: 178-180 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.66 (dd, J_1 = 8.0 Hz, J_2 = 0.4 Hz, 1H), 8.11 (s, 1H), 7.97-7.87 (m, 3H), 7.82 (d, J = 8.4 Hz, 1H), 7.66-7.62 (m, 1H), 7.57 (d, J = 8.8 Hz, 1H), 7.53-7.46 (m, 3H), 7.37 (t, J = 8.0 Hz, 1H), 7.27 (dd, J_1 = 8.8 Hz, J_2 = 1.6 Hz, 1H), 7.15 (d, J = 7.2 Hz, 1H), 6.46 (q, J = 6.4 Hz, 1H), 2.15 (d, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d6): δ 139.3, 139.0, 136.0, 134.0, 130.4, 130.0, 129.4, 129.2, 128.4, 127.3, 127.2, 126.8, 126.2, 125.6, 124.8, 124.3, 123.3, 122.0, 121.9, 110.9, 51.9, 21.4; HRMS (ESI, m/z) calcd. For $C_{23}H_{19}N_2$ $[M+H]^+$: 323.1548; found: 323.1550.

3-ethyl-3*H*-naphtho[1,2-*d*]imidazole (4aa)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown solid (33 mg, 56% yield); mp: 120-122 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.45-8.42 (m, 1H), 8.27 (s, 1H), 7.97-7.95 (m, 1H), 7.76 (d, J = 8.8 Hz, 1H), 7.70 (d, J = 8.8 Hz, 1H), 7.59-7.55 (m, 1H), 7.46-7.42 (m, 1H), 4.34 (q, J = 7.2 Hz, 2H), 1.42 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, DMSO-d6): δ 141.9, 139.1, 130.3, 130.1, 128.9, 127.3, 126.7, 124.6, 123.4, 121.6, 111.9, 39.9, 16.3; HRMS (ESI, m/z) calcd. For $C_{13}H_{13}N_2$ $[M+H]^+$: 197.1079; found: 197.1080.

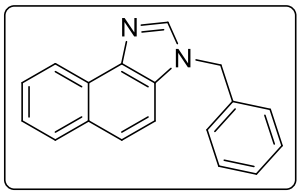
3-allyl-3*H*-naphtho[1,2-*d*]imidazole (4ab)



The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy liquid (29 mg, 46% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.46-8.43 (m, 1H), 8.24 (s, 1H), 7.96 (d, J = 8.0 Hz, 1H), 7.72-7.66 (m, 2H), 7.60-7.56 (m, 1H), 7.46-7.42 (m, 1H), 6.10-6.01 (m, 1H), 5.20-5.16 (m, 1H), 5.09-5.04 (m, 1H), 5.00-4.98 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d6): δ 142.4, 139.0,

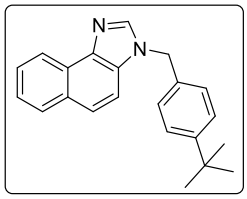
134.3, 130.6, 130.2, 129.0, 127.3, 126.8, 124.7, 123.6, 121.6, 117.9, 112.1, 47.3; HRMS (ESI, m/z) calcd. For $C_{14}H_{13}N_2$ $[M+H]^+$: 209.1079; found: 209.1087.

3-benzyl-3*H*-naphtho[1,2-*d*]imidazole (4ac)



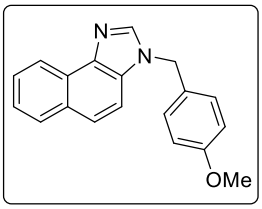
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown solid (46.4 mg, 60% yield); mp: 96-98 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.44 (s, 1H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.67 (s, 2H), 7.59-7.56 (m, 1H), 7.46-7.42 (m, 1H), 7.29-7.20 (m, 6H), 5.59 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d6): δ 142.7, 139.2, 137.7, 130.5, 130.2, 129.3, 128.9, 128.3, 127.8, 127.3, 126.8, 124.8, 123.7, 121.6, 112.2, 48.4; HRMS (ESI, m/z) calcd. For $C_{18}H_{15}N_2$ $[M+H]^+$: 259.1235; found: 259.1239.

3-(4-(*tert*-butyl)benzyl)-3*H*-naphtho[1,2-*d*]imidazole (4ad)



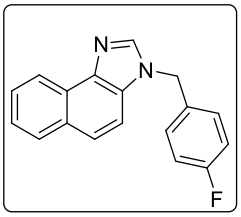
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a pale yellow solid (49 mg, 52% yield); mp: 88-90 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.45-8.42 (m, 2H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.66 (d, *J* = 9.2 Hz, 1H), 7.57-7.55 (m, 1H), 7.45-7.41 (m, 1H), 7.31-7.28 (m, 2H), 7.23-7.19 (m, 2H), 5.53 (s, 2H), 1.17 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d6): δ 150.7, 142.6, 139.2, 134.8, 130.5, 130.1, 128.9, 127.6, 127.3, 126.8, 125.9, 124.7, 123.7, 121.6, 112.2, 48.0, 34.7, 31.6; HRMS (ESI, m/z) calcd. For $C_{22}H_{23}N_2$ $[M+H]^+$: 315.1861; found: 315.1860.

3-(4-methoxybenzyl)-3*H*-naphtho[1,2-*d*]imidazole (4ae)



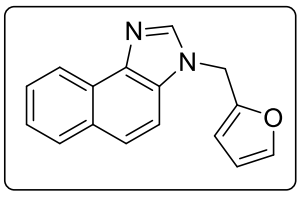
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown solid (48 mg, 55% yield); mp: 106-108 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.47-8.42 (m, 1H), 8.42 (s, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.70-7.65 (m, 2H), 7.59-7.55 (m, 1H), 7.45-7.41 (m, 1H), 7.29-7.25 (m, 2H), 6.87-6.83 (m, 2H), 5.49 (s, 2H), 3.65 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d6): δ 159.4, 142.5, 139.2, 130.4, 130.1, 129.5, 129.4, 128.9, 127.3, 126.8, 124.7, 123.6, 121,6, 114.6, 112.2, 55.6, 47.9; HRMS (ESI, m/z) calcd. For $C_{19}H_{17}N_2O$ $[M+H]^+$: 289.1341; found: 289.1340.

3-(4-fluorobenzyl)-3*H*-naphtho[1,2-*d*]imidazole (4af)



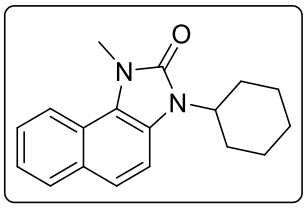
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy solid (29 mg, 35% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.43-8.41 (m, 2H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.71-7.66 (m, 2H), 7.59-7.55 (m, 1H), 7.46-7.42 (m, 1H), 7.38-7.34 (m, 2H), 7.16-7.11 (m, 2H), 5.58 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d6): δ 162.2 (d, *J* = 242.5 Hz), 142.6, 139.2, 133.9, 130.2, 131.1 (d, *J* = 56.3 Hz), 130.1 (d, *J* = 8.2 Hz), 129.1, 128.9, 127.3, 126.9, 124.8 (d, *J* = 104.0 Hz), 121.6, 116.1 (d, *J* = 21.3 Hz), 112.1, 47.6; HRMS (ESI, m/z) calcd. For $C_{18}H_{14}FN_2$ $[M+H]^+$: 277.1141; found: 277.1137.

3-(furan-2-ylmethyl)-3*H*-naphtho[1,2-*d*]imidazole (4ag)



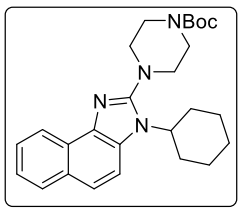
The general procedure for imidazole was followed. Column chromatography (SiO_2, eluting with 90:10 hexane/acetone) afforded the desired product as a light brown gummy liquid (28 mg, 38% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.44-8.42 (m, 1H), 8.34 (s, 1H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.8 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.59-7.55 (m, 2H), 7.46-7.43 (m, 1H), 6.55 (dd, J_1 = 3.2 Hz, J_2 = 0.8 Hz, 1H), 6.39 (dd, J_1 = 3.2 Hz, J_2 = 2.0 Hz, 1H), 5.62 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d6): δ 150.4, 143.8, 142.4, 139.0, 130.4, 130.2, 128.9, 127.2, 126.8, 124.8, 123.8, 121.6, 112.1, 111.2, 109.5, 41.5; HRMS (ESI, m/z) calcd. For $C_{16}H_{13}N_2O$ $[M+H]^+$: 249.1028; found: 249.1020.

3-cyclohexyl-1-methyl-1,3-dihydro-2*H*-naphtho[1,2-*d*]imidazol-2-one (7a)



Column chromatography (SiO_2, eluting with 80:20 hexane/EtOAc) afforded the desired product as a creamy white powder (134 mg, 96% yield); mp: 122-124 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.33 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.8 Hz, 1H), 7.50-7.46 (m, 2H), 7.38-7.34 (m, 1H), 4.42-4.35 (m, 1H), 3.94 (s, 3H), 2.29-2.18 (m, 2H), 1.95-1.89 (m, 4H), 1.77 (d, *J* = 12.4 Hz, 1H), 1.54-1.42 (m, 2H), 1.37-1.30 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d6): δ 154.2, 129.6, 129.4, 126.1, 124.7, 123.4, 122.9, 121.7, 120.9, 120.2, 110.5, 53.6, 31.0, 30.6, 26.2, 25.5; HRMS (ESI, m/z) calcd. For $C_{18}H_{21}N_2O$ $[M+H]^+$: 281.1654; found: 281.1649.

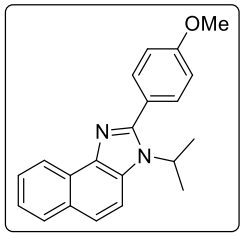
***tert*-butyl 4-(3-cyclohexyl-3*H*-naphtho[1,2-*d*]imidazol-2-yl)piperazine-1-carboxylate (7b)**



Column chromatography (SiO_2, eluting with 85:15 hexane/EtOAc) afforded the desired product as a white solid (91 mg, 42% yield); mp: 172-174 ºC. ^{1}H NMR (400 MHz, DMSO-d6): δ 8.54-8.52 (m, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.58-7.52 (m, 2H), 7.43-7.39 (m, 1H), 4.36-4.28 (m, 1H), 3.66 (t, *J* = 4.8 Hz, 4H), 3.23 (t, *J* = 5.2 Hz, 4H), 2.31-2.21 (m, 2H), 2.01-

1.91 (m, 4H), 1.49 (s, 9H), 1.48-1.37 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d6): δ 155.5, 154.9, 137.1, 129.6, 128.8, 128.2, 126.7, 125.9, 124.1, 121.8, 121.7, 112.5, 80.1, 55.8, 31.9, 28.5, 26.4, 25.6; HRMS (ESI, m/z) calcd. For $C_{26}H_{35}N_4O_2$ $[M+H]^+$: 435.2760; found: 435.2750.

3-isopropyl-2-(4-methoxyphenyl)-3*H*-naphtho[1,2-*d*]imidazole (7c)



Column chromatography (SiO_2, eluting with 80:20 hexane/EtOAc) afforded the desired product as a creamy white solid (79 mg, 50% yield). ^{1}H NMR (400 MHz, DMSO-d6): δ 8.72-8.69 (m, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.75 (d, *J* = 9.2 Hz, 1H), 7.67-7.57 (m, 4H), 7.49-7.45 (m, 1H), 7.07-7.03 (m, 2H), 4.90-4.83 (m, 1H), 3.88 (s, 3H), 1.68 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, DMSO-d6): δ 160.7, 151.6, 139.4, 131.2, 129.9, 129.8, 128.2, 127.3, 126.3, 124.6, 123.7, 122.9, 122.0, 114.3, 112.7, 55.5, 48.9, 22.0; HRMS (ESI, m/z) calcd. For $C_{21}H_{21}N_2O$ $[M+H]^+$: 317.1654; found: 317.1646.

References:

1. Begam, H. M.; Nandi, S.; Jana, R., A Directing Group Switch in Copper-Catalyzed Electrophilic C–H Amination/Migratory Annulation Cascade: Divergent Access to Benzimidazolone/Benzimidazole. *Chem. Sci*. **2022**, 13, 5726-5733.
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3. McDonald, S. L.; Hendrick, C. E.; Wang, Q., Copper-Catalyzed Electrophilic Amination of Heteroarenes and Arenes by C–H Zincation. *Angew. Chem. Int. Ed*., 2014, 53, 4667-4670.
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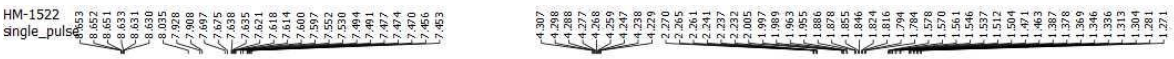
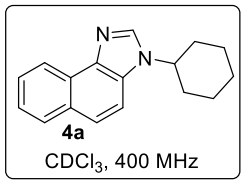
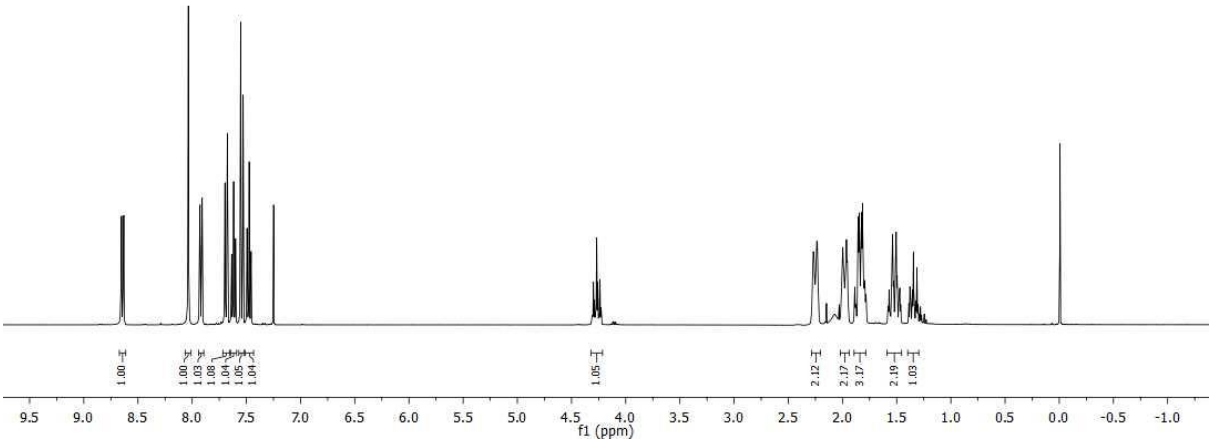
^{1}H and ^{13}C NMR spectra

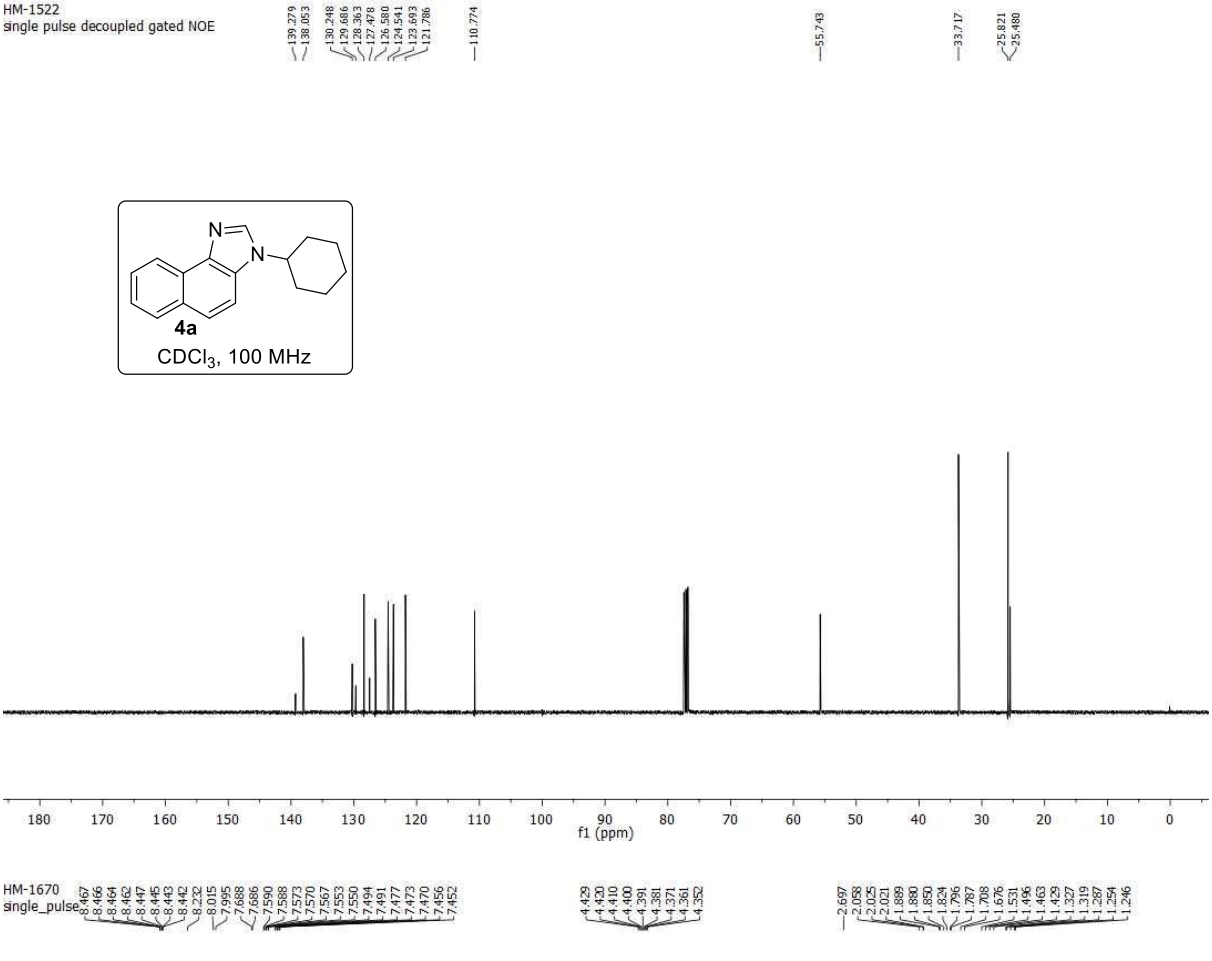


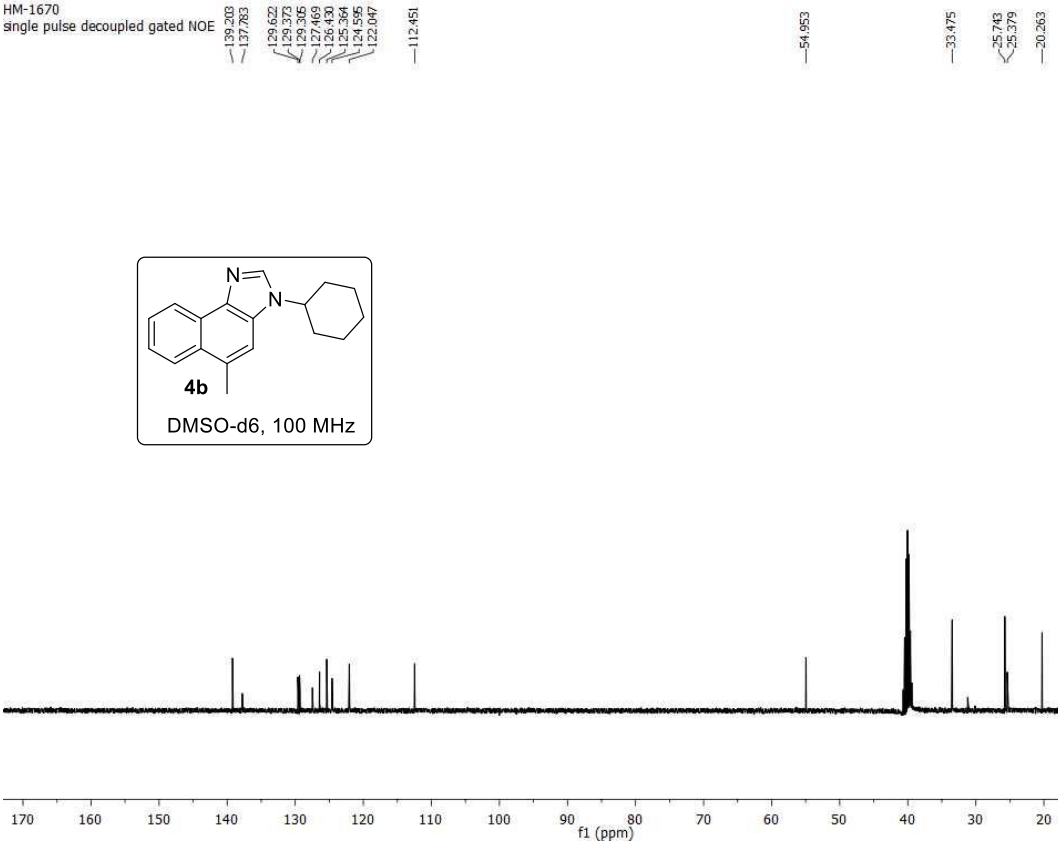


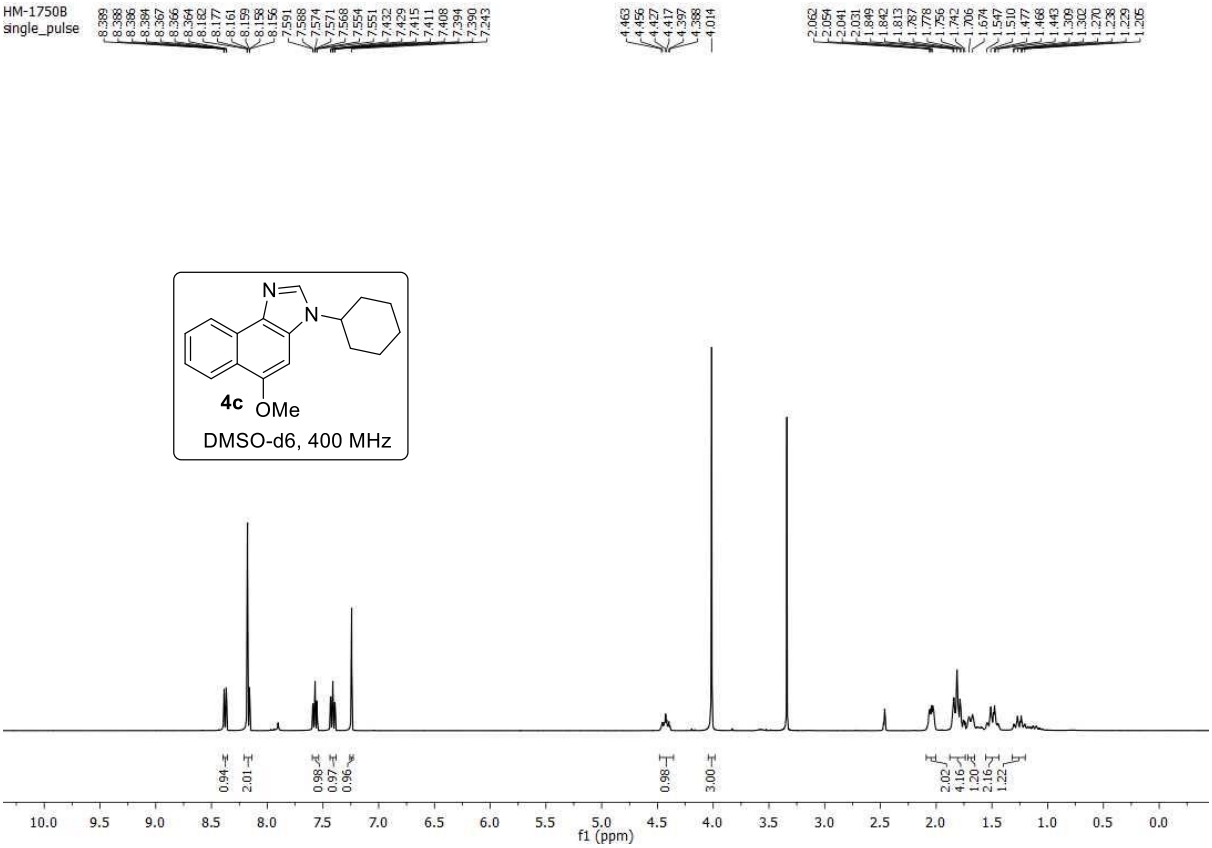
4a

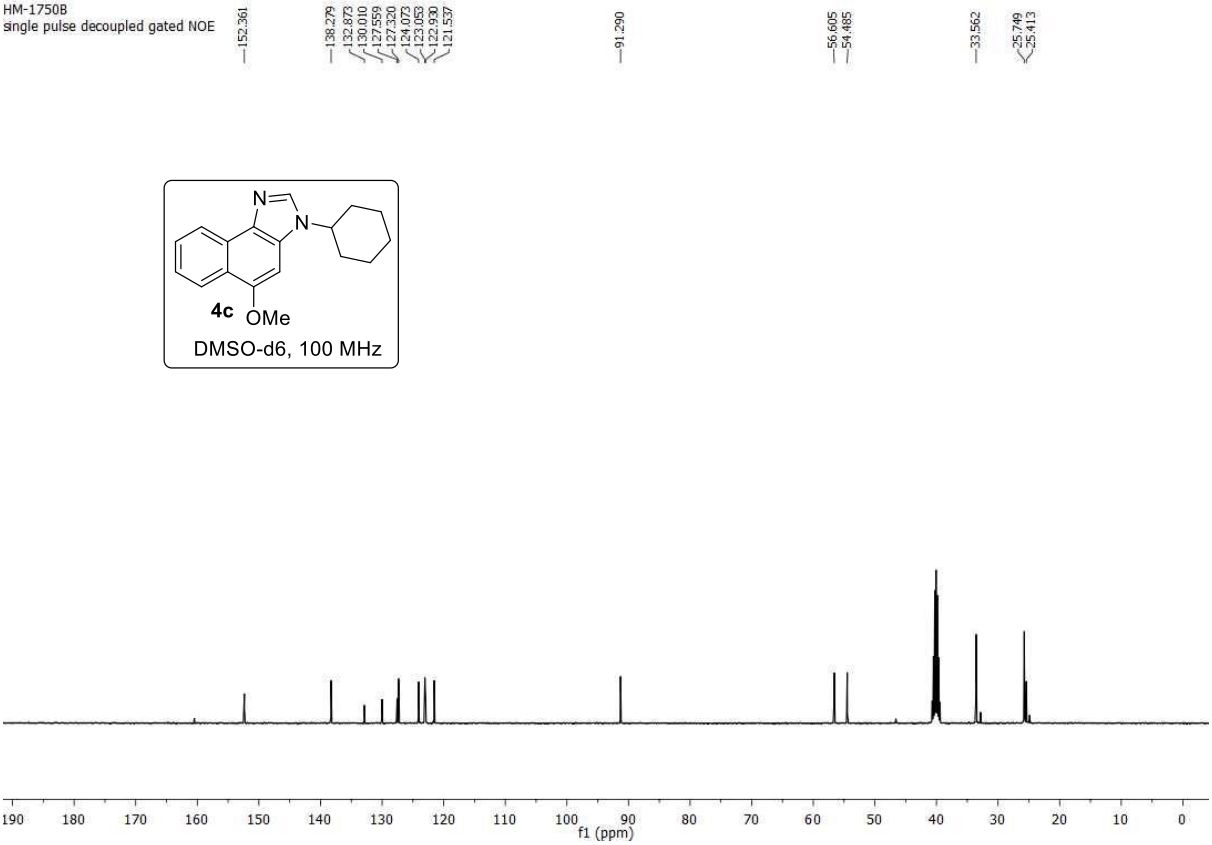
$CDCl_3$, 400 MHz

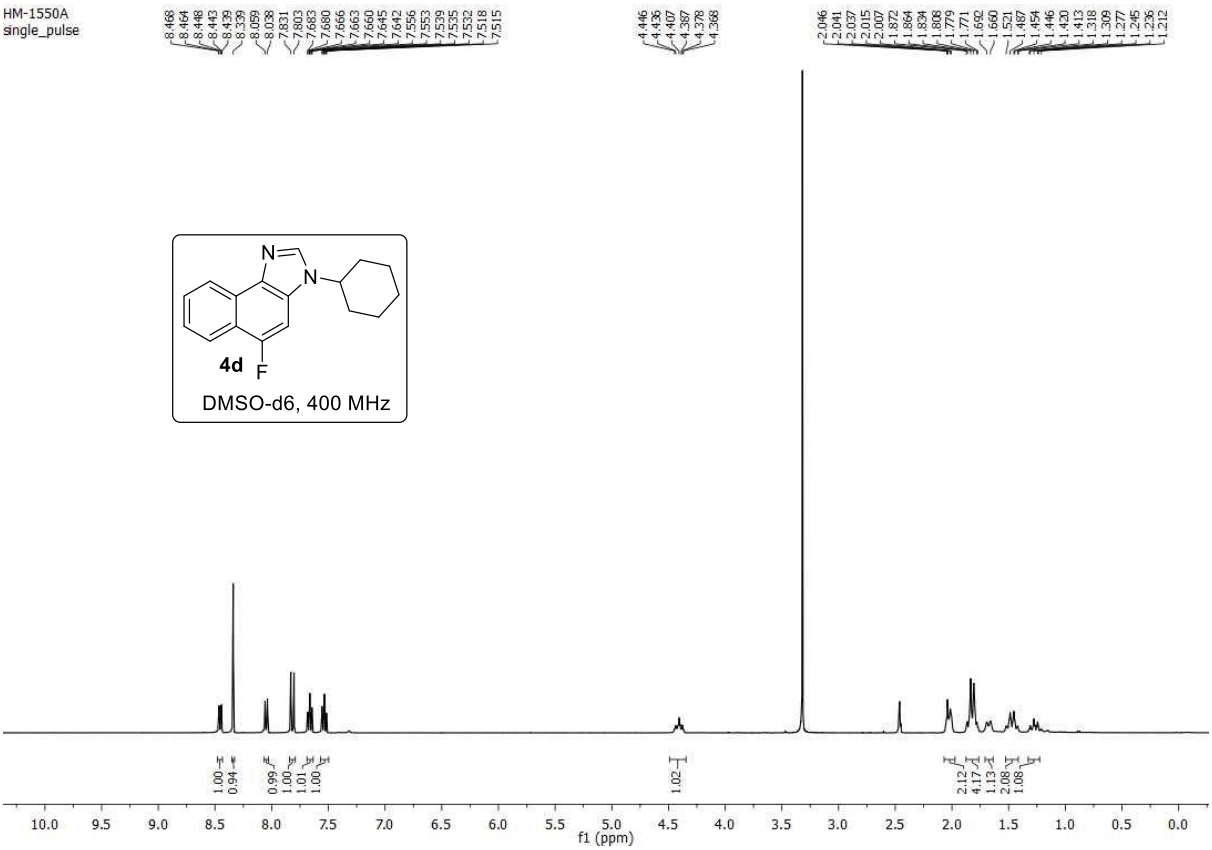


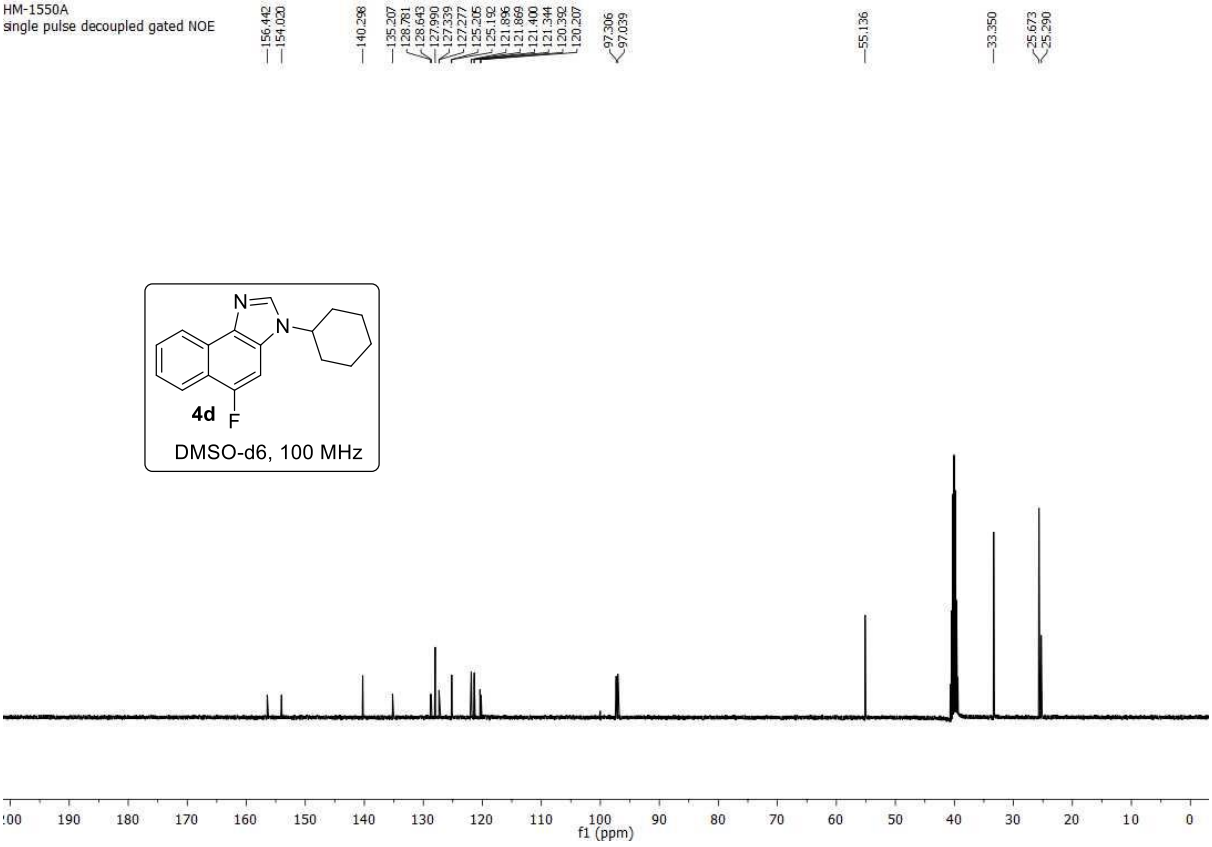

HM-1522
single pulse decoupled gated NOE
139.279
138.053
130.248
129.686
128.383
127.478
126.560
124.541
123.693
121.786
110.774
55.743
33.717
25.821
25.480
4a
CDCl3, 100 MHz
f1 (ppm)
HM-1670
single_pulse
4b
DMSO-d6, 400 MHz
f1 (ppm)

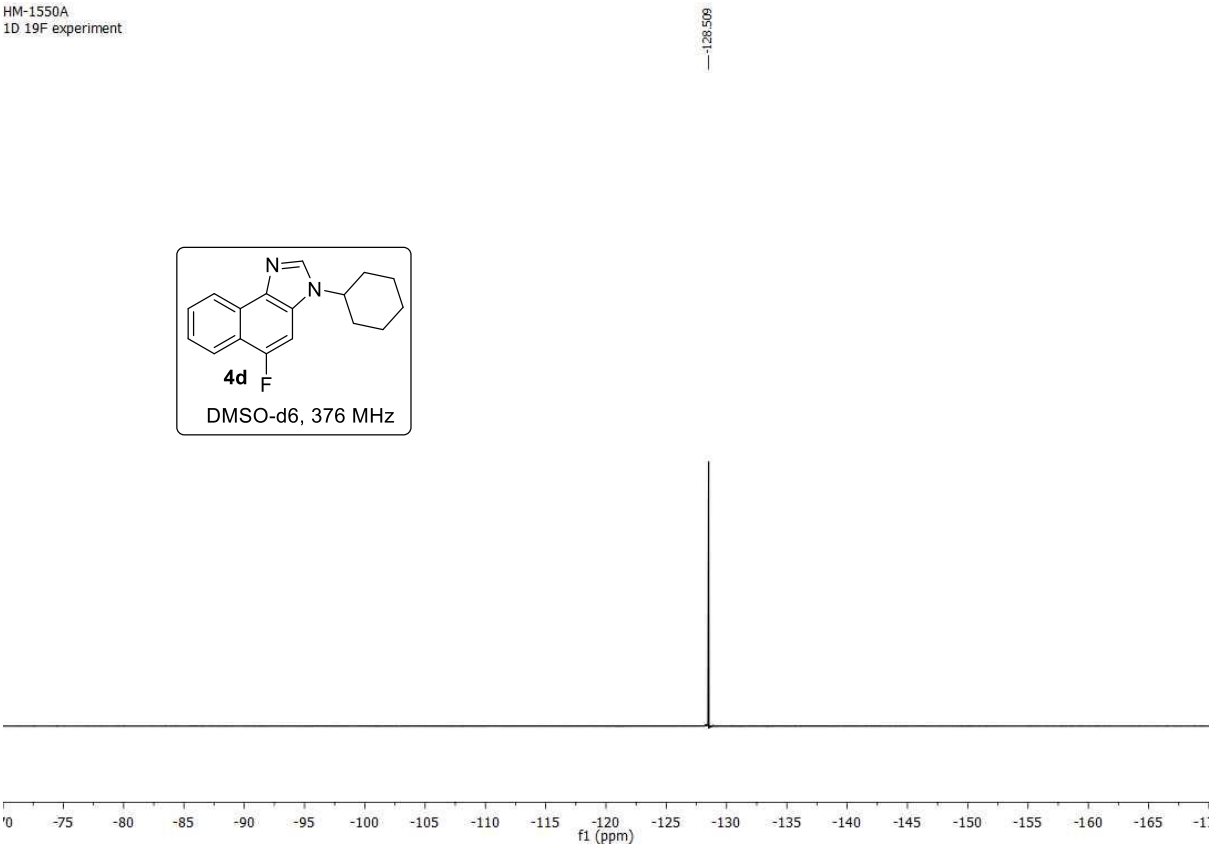

HM-1670
single pulse decoupled gated NOE
139.203
137.783
129.622
129.373
129.305
127.469
126.430
125.364
124.595
122.047
112.451
54.953
33.475
25.743
25.379
20.263
4b
DMSO-d6, 100 MHz
f1 (ppm)


HM-1750B
single_pulse
8.389
8.388
8.386
8.384
8.367
8.366
8.364
8.182
8.177
8.161
8.159
8.158
8.156
7.591
7.588
7.574
7.571
7.568
7.554
7.551
7.432
7.429
7.415
7.411
7.408
7.394
7.390
7.243
4.463
4.456
4.427
4.417
4.397
4.388
4.014
2.062
2.054
2.041
2.031
1.849
1.842
1.813
1.787
1.778
1.756
1.742
1.706
1.674
1.547
1.510
1.477
1.468
1.443
1.309
1.302
1.270
1.238
1.229
1.205
4c
OMe
DMSO-d6, 400 MHz
0.94
2.01
0.98
0.97
0.96
0.98
3.00
2.02
4.16
1.20
2.16
1.22
f1 (ppm)

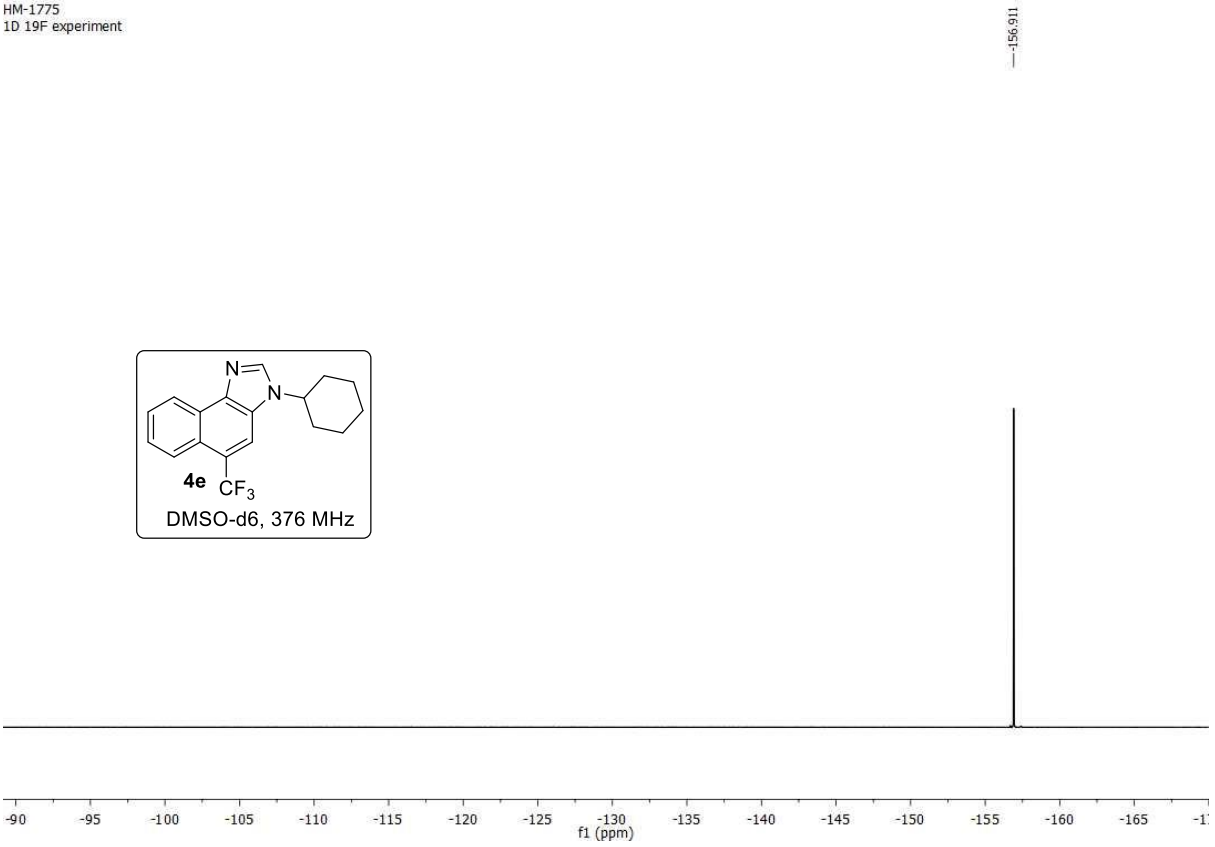

HM-1750B
single pulse decoupled gated NOE
152.361
138.279
132.873
130.010
127.559
127.320
124.073
123.053
122.930
121.537
91.290
56.605
54.485
33.562
25.749
25.413
4c
OMe
DMSO-d6, 100 MHz
f1 (ppm)


HM-1550A
single_pulse
4d
F
DMSO-d6, 400 MHz
f1 (ppm)

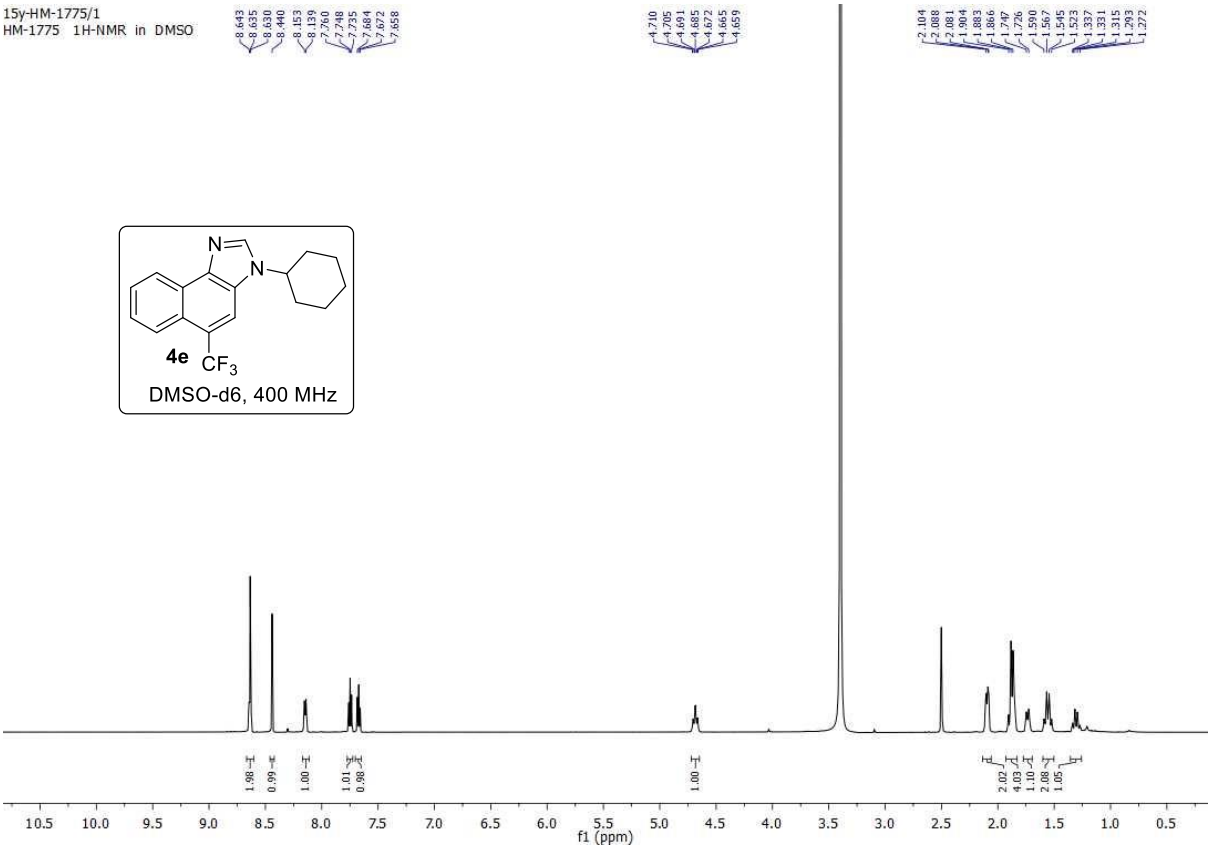

HM-1550A
single pulse decoupled gated NOE
156.442
154.030
140.258
135.207
128.781
128.643
127.990
127.339
127.277
125.205
125.192
121.896
121.869
121.400
121.344
120.392
120.207
97.306
97.039
55.136
33.350
25.673
25.290
4d
F
DMSO-d6, 100 MHz
f1 (ppm)

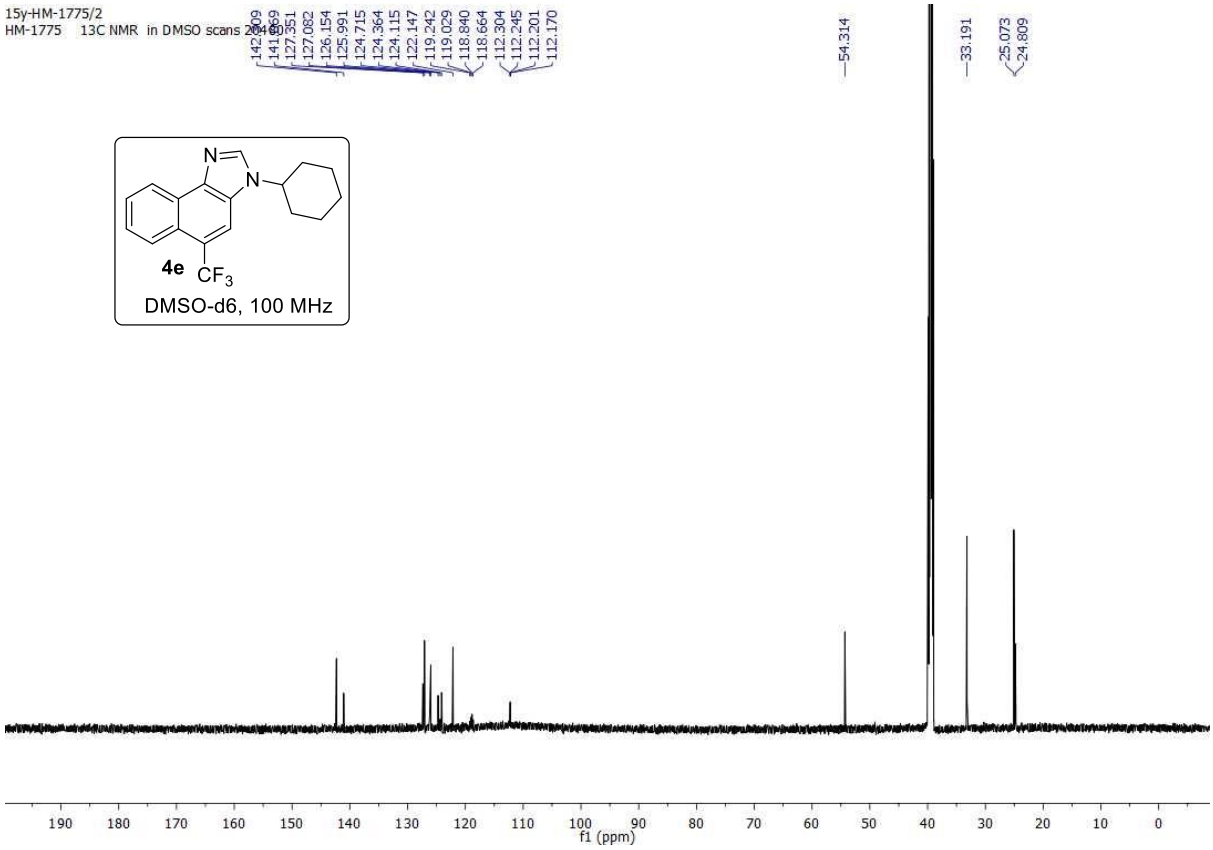

HM-1550A
1D 19F experiment
-128.509
4d
F
DMSO-d6, 376 MHz
f1 (ppm)

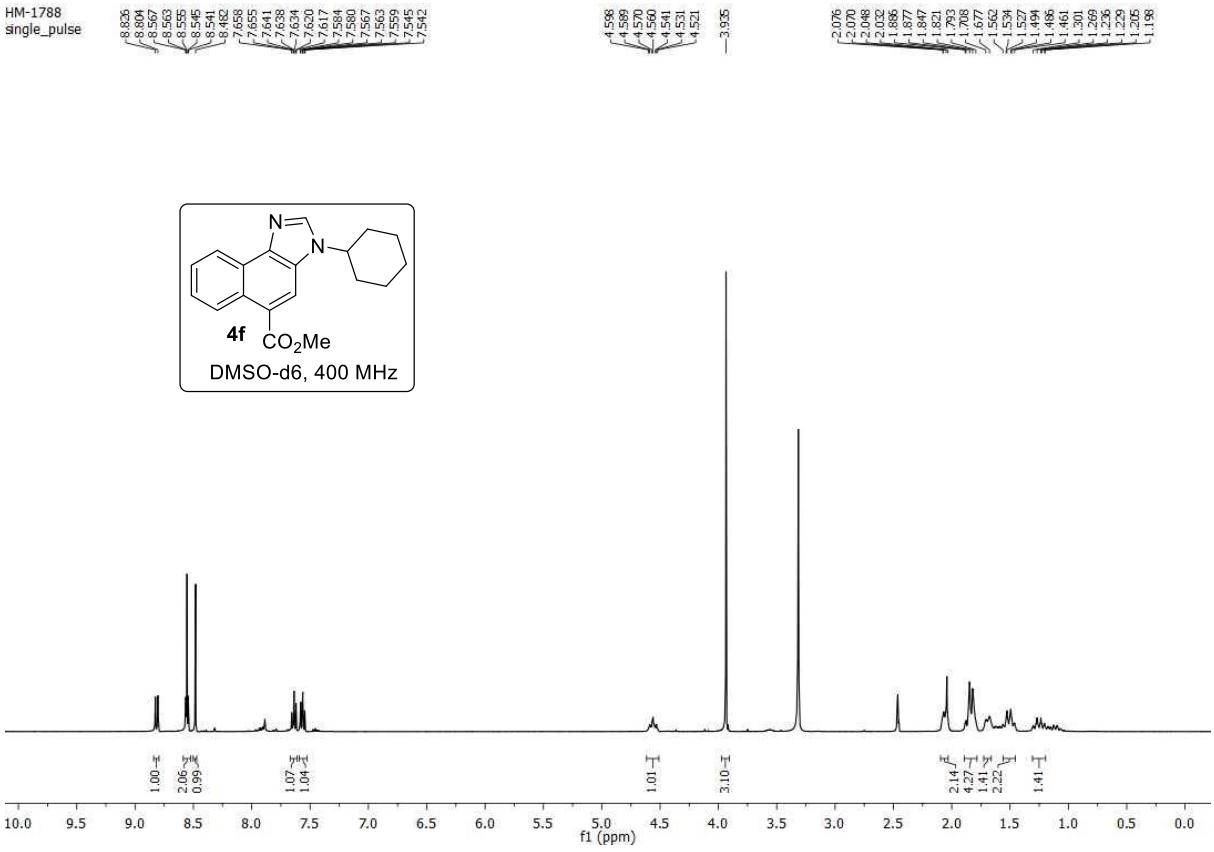
HM-1775
1D 19F experiment

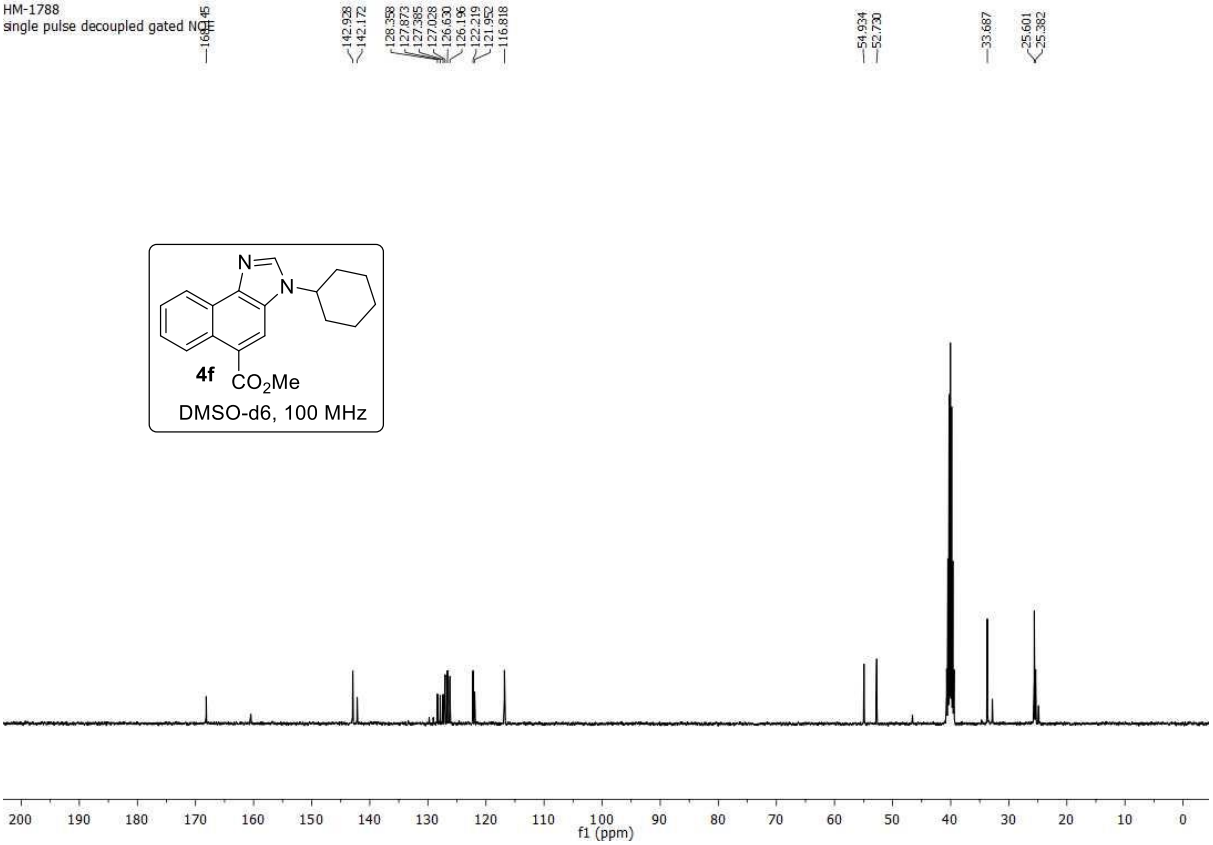


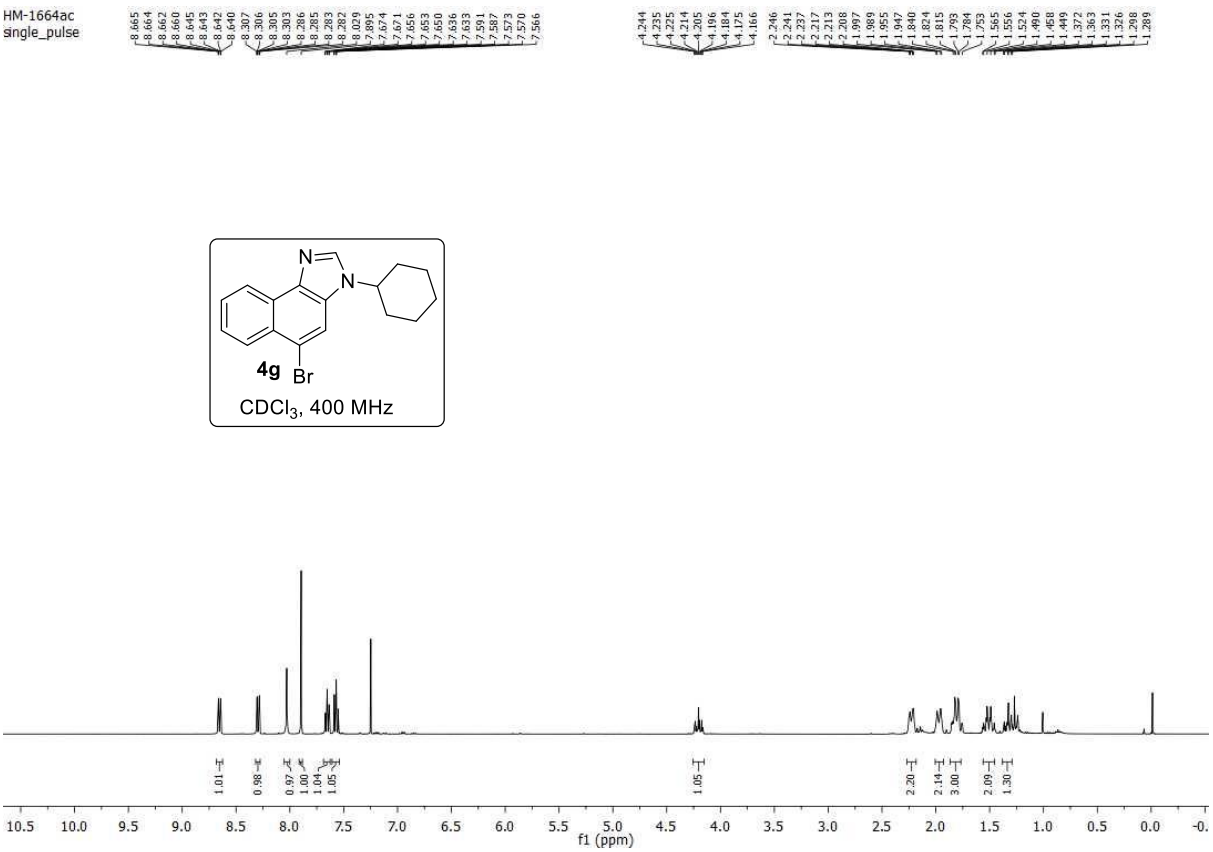
15y-HM-1775/1
HM-1775 1H-NMR in DMSO

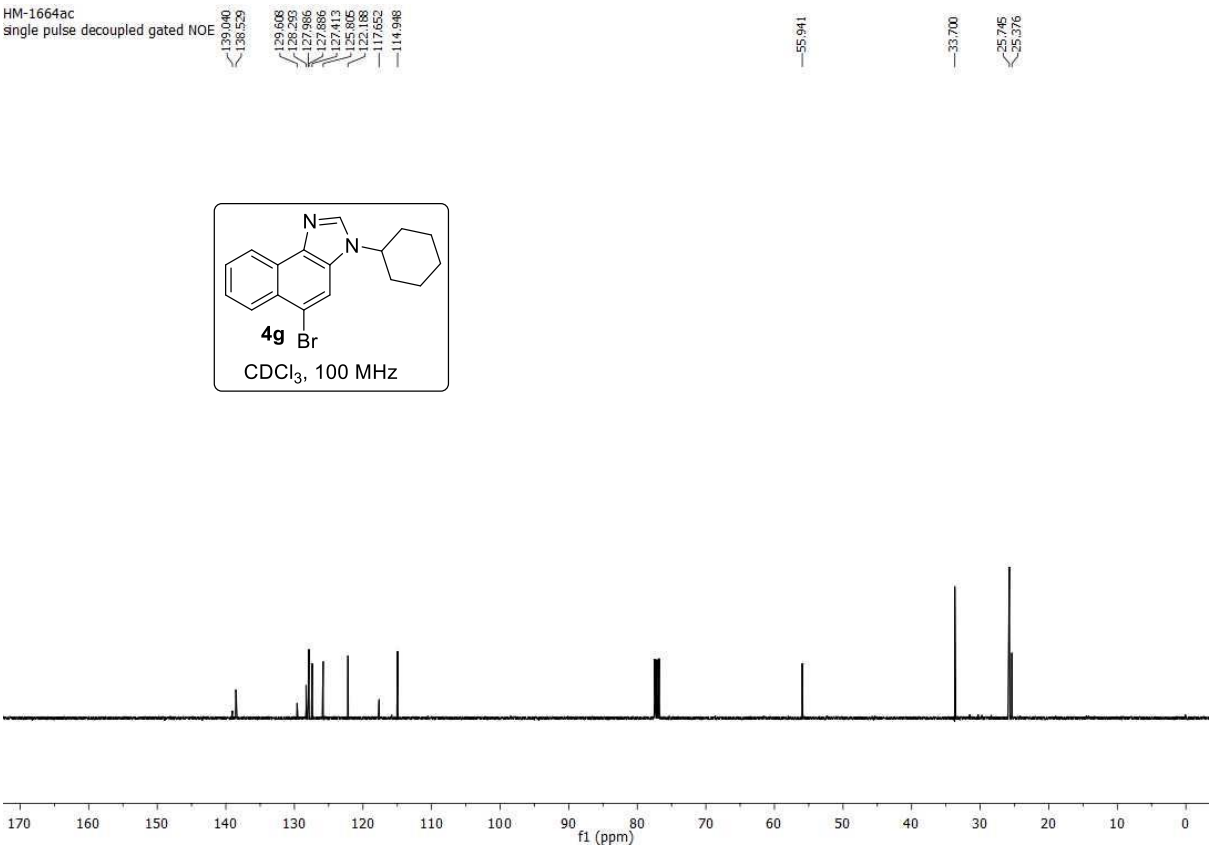


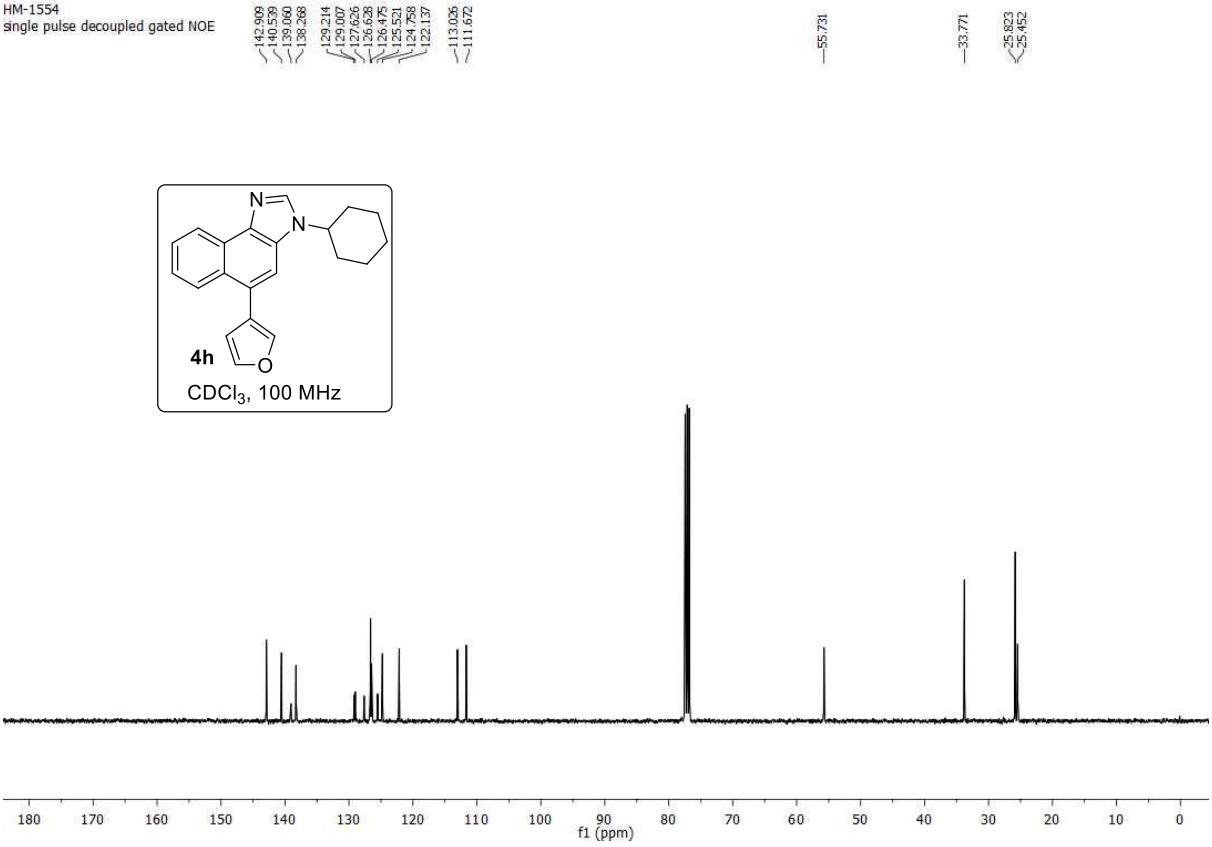

15y-HM-1775/2
HM-1775 13C NMR in DMSO scans 20480
142.209
141.469
127.351
127.082
126.154
125.991
124.715
124.364
124.115
122.147
119.242
119.029
118.840
118.664
112.304
112.245
112.201
112.170
54.314
33.191
25.073
24.809
4e
CF3
DMSO-d6, 100 MHz
f1 (ppm)

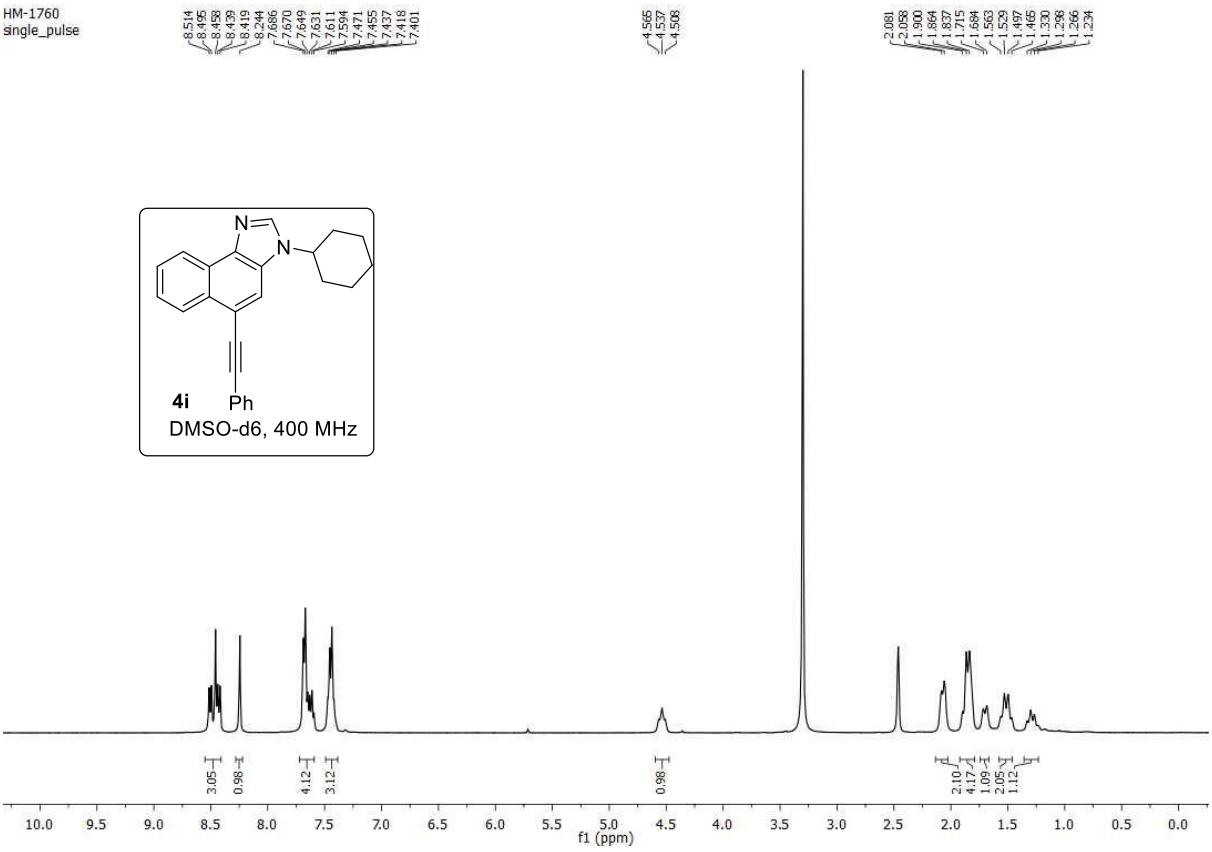

HM-1788
single_pulse
8.836
8.804
8.567
8.563
8.555
8.545
8.541
8.482
7.658
7.655
7.641
7.638
7.634
7.620
7.617
7.584
7.580
7.567
7.563
7.559
7.545
7.542
4.598
4.589
4.570
4.560
4.541
4.531
4.521
3.935
2.076
2.070
2.048
2.032
1.886
1.877
1.847
1.821
1.793
1.708
1.677
1.562
1.534
1.527
1.494
1.486
1.461
1.301
1.269
1.236
1.229
1.205
1.198
4f
CO2Me
DMSO-d6, 400 MHz
1.00
2.06
0.99
1.07
1.04
1.01
3.10
2.14
4.27
1.41
2.22
1.41
f1 (ppm)

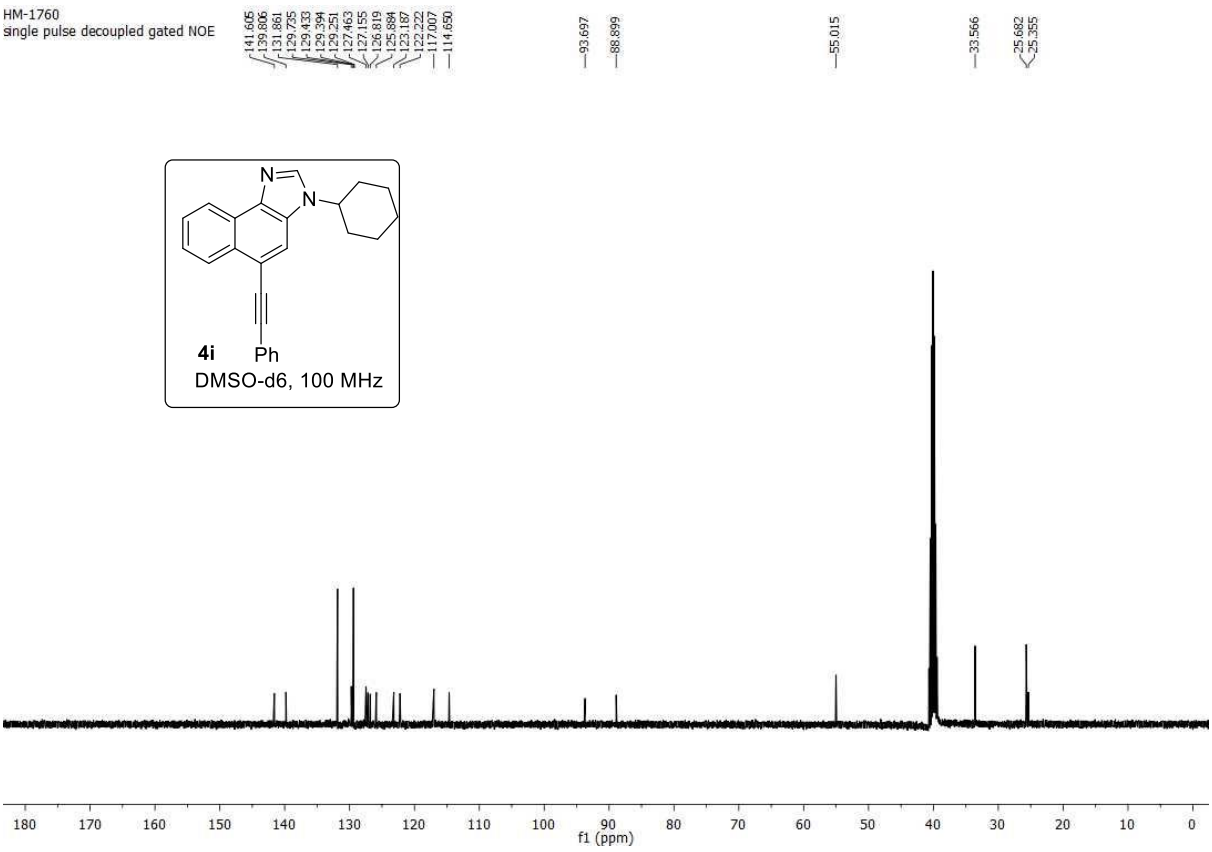

HM-1788
single pulse decoupled gated NOE
166.145
142.928
142.172
128.358
127.873
127.385
127.028
126.630
126.196
122.219
121.952
116.818
54.934
52.730
33.687
25.601
25.382
4f
CO2Me
DMSO-d6, 100 MHz
f1 (ppm)

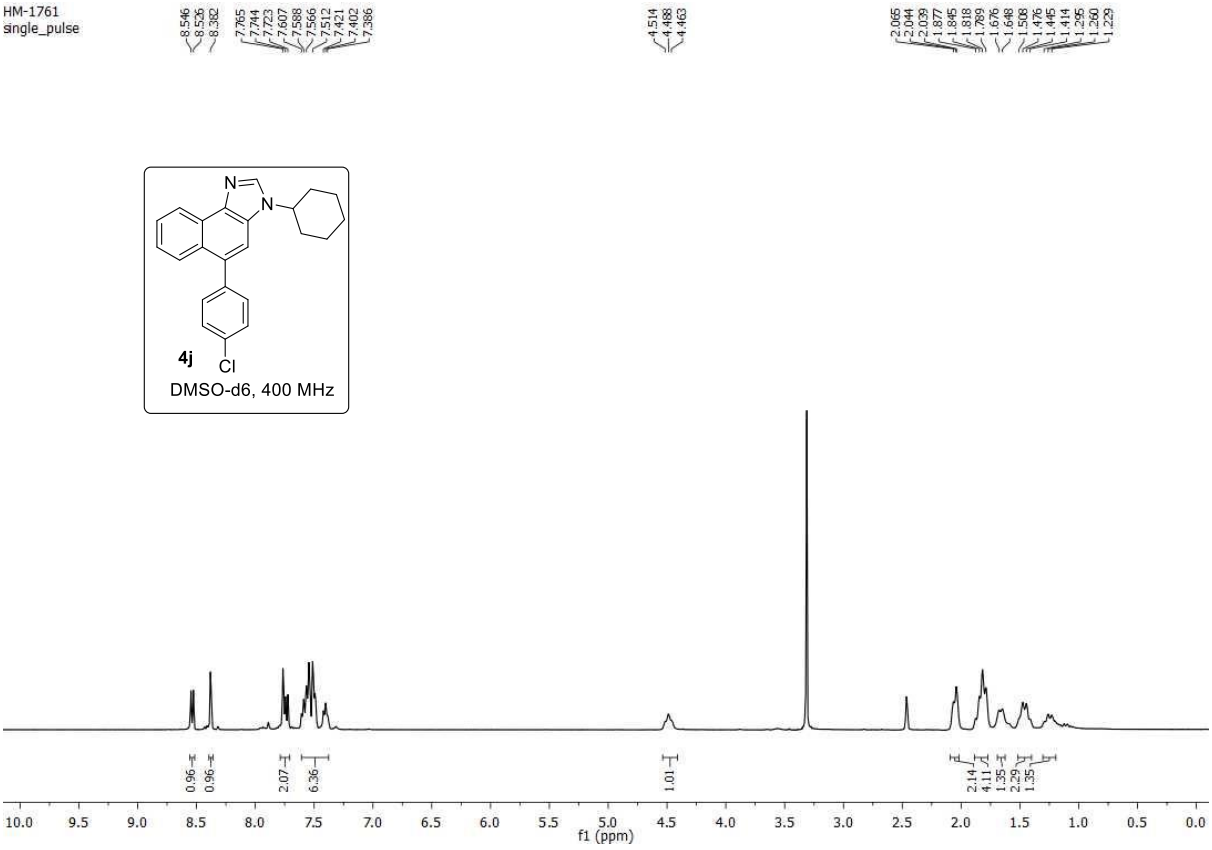

HM-1664ac
single_pulse
4g
Br
CDCl3, 400 MHz
f1 (ppm)

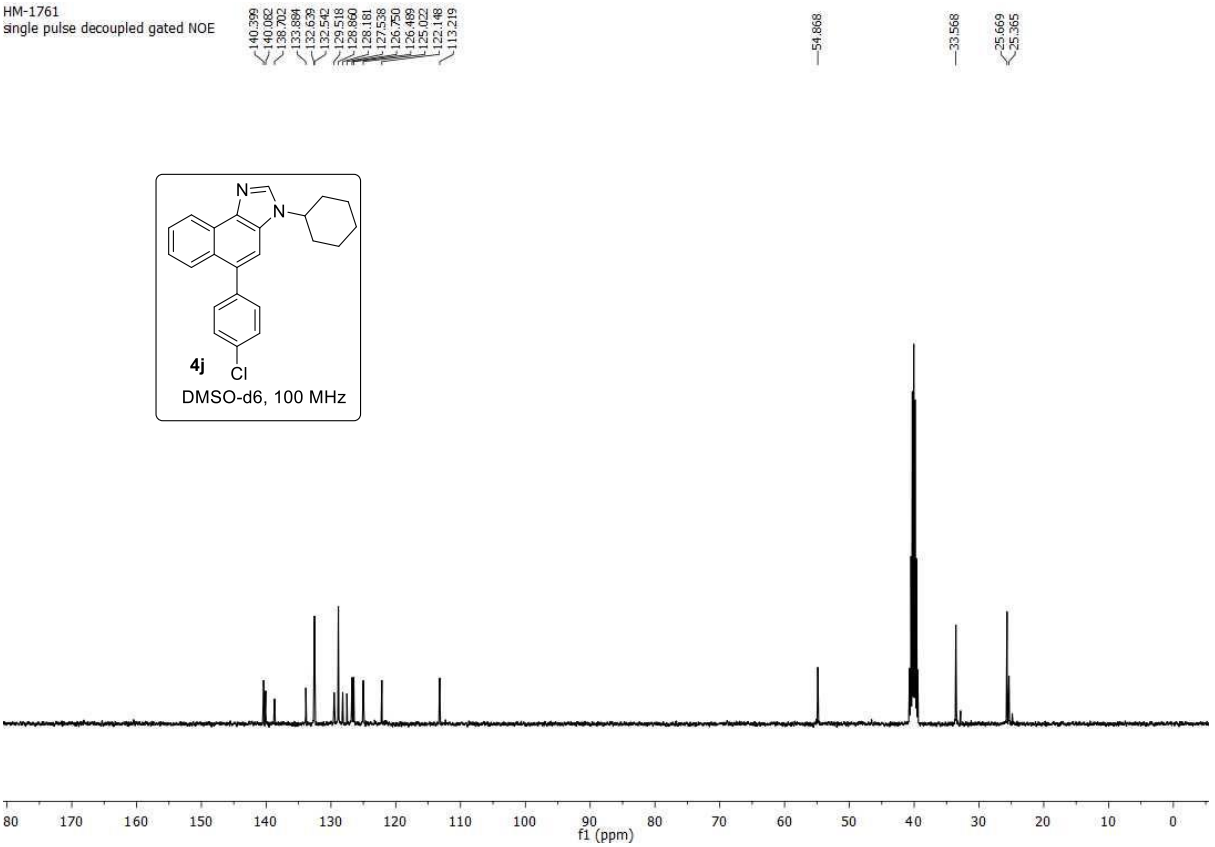

HM-1664ac
single pulse decoupled gated NOE
139.040
138.529
129.608
128.293
127.986
127.886
127.413
125.805
122.188
117.652
114.948
55.941
33.700
25.745
25.376
4g
Br
CDCl3, 100 MHz
f1 (ppm)
HM-1554
single_pulse
4h
CDCl3, 400 MHz
f1 (ppm)

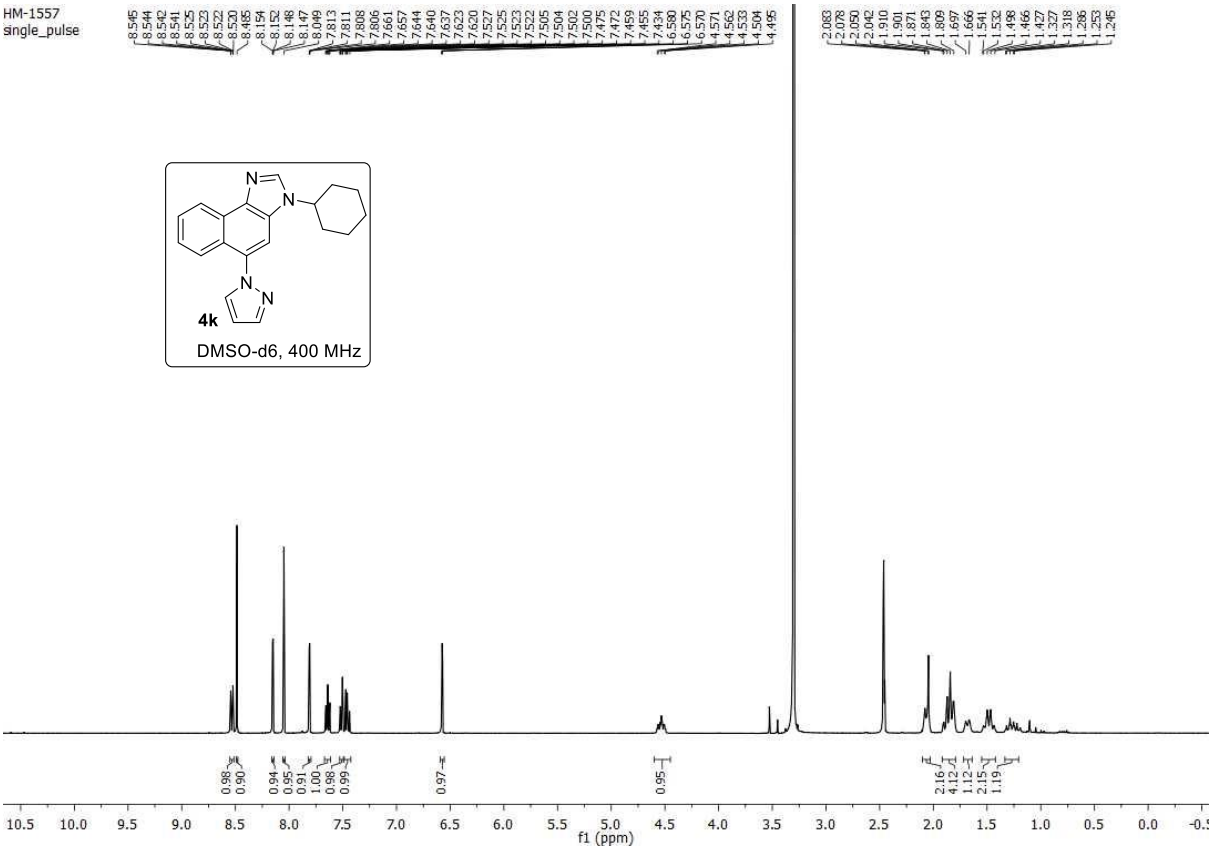

HM-1554
single pulse decoupled gated NOE
142.909
140.539
139.060
138.268
129.214
129.007
127.626
126.628
126.475
125.521
124.758
122.137
113.026
111.672
55.731
33.771
25.823
25.452
4h
CDCl3, 100 MHz
f1 (ppm)

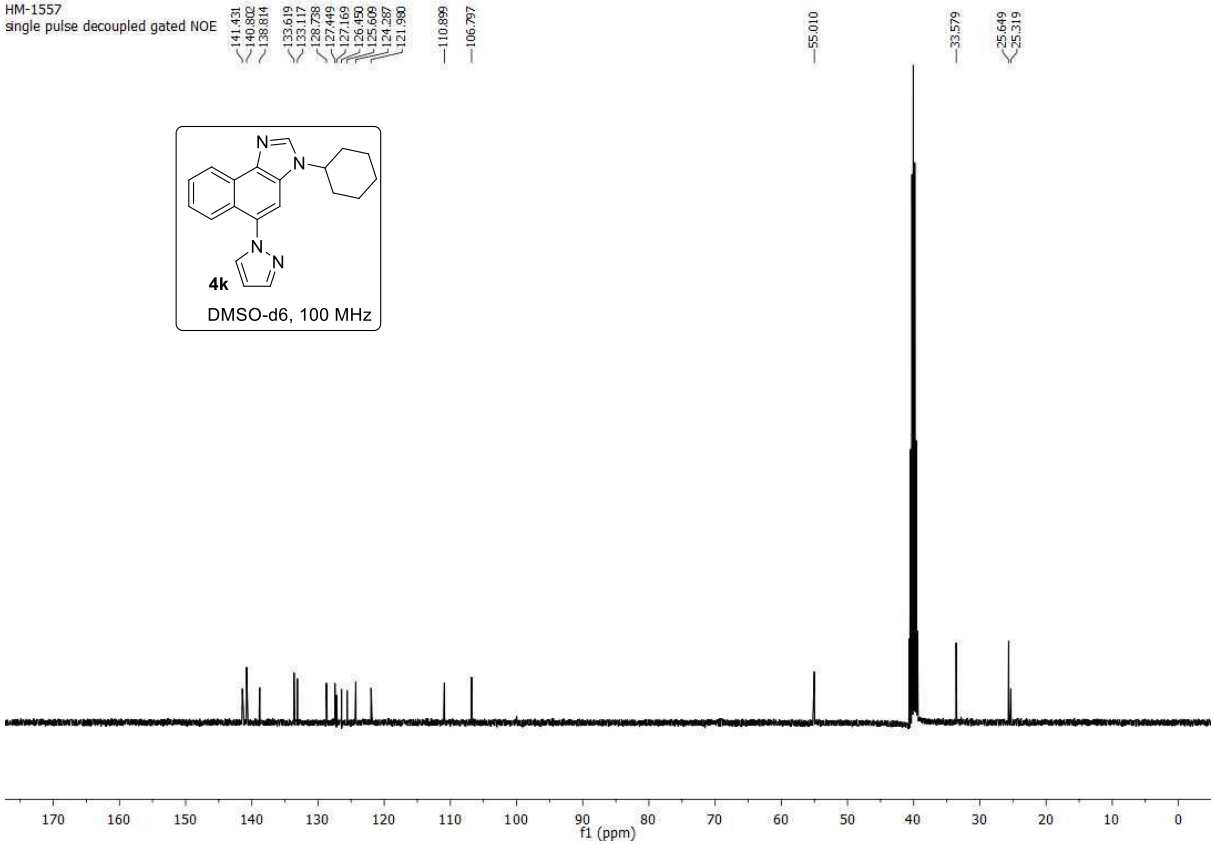

HM-1760
single_pulse
8.514
8.495
8.458
8.439
8.419
7.744
7.696
7.670
7.649
7.631
7.611
7.594
7.471
7.455
7.437
7.418
7.401
4.565
4.537
4.508
2.091
2.058
1.900
1.864
1.637
1.715
1.684
1.563
1.529
1.497
1.465
1.330
1.298
1.266
1.234
4i Ph
DMSO-d6, 400 MHz
3.05
0.98
4.12
3.12
0.98
2.10
4.17
1.09
2.05
1.12
f1 (ppm)

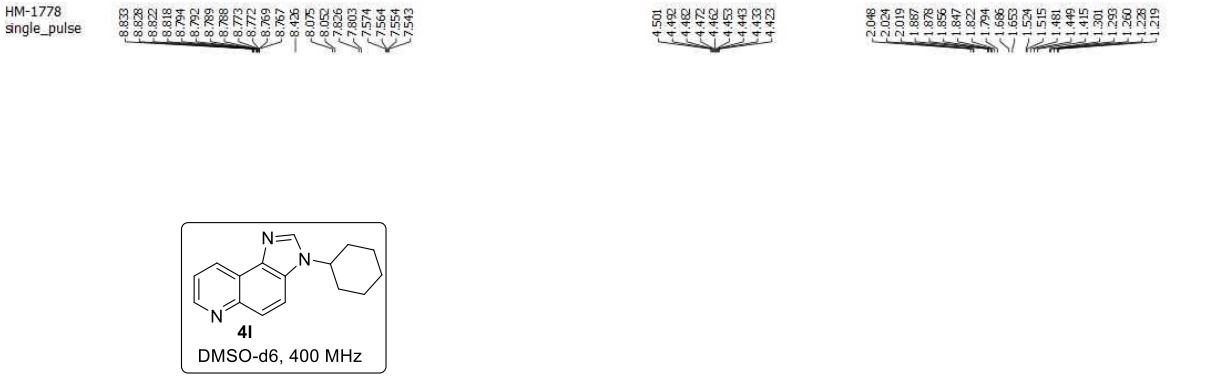

HM-1760
single pulse decoupled gated NOE
141.605
139.806
131.861
129.735
129.433
129.394
129.251
127.463
127.155
126.819
125.884
123.187
122.222
117.007
114.650
93.697
88.899
55.015
33.566
25.682
25.355
4i
Ph
DMSO-d6, 100 MHz
f1 (ppm)


HM-1761
single_pulse
8.546
8.536
8.382
7.765
7.744
7.723
7.607
7.588
7.566
7.512
7.421
7.402
7.386
4.514
4.488
4.463
2.065
2.044
2.039
1.877
1.845
1.818
1.789
1.676
1.648
1.508
1.476
1.445
1.414
1.295
1.260
1.229
4j
Cl
DMSO-d6, 400 MHz
0.96
0.96
2.07
6.36
1.01
2.14
4.11
1.35
2.29
1.35
f1 (ppm)

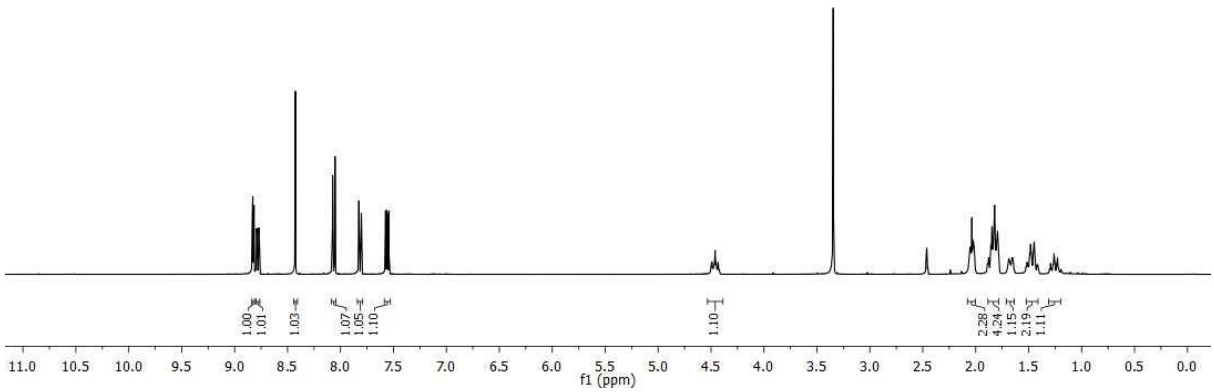

HM-1761
single pulse decoupled gated NOE
140.399
140.082
138.702
133.884
132.639
132.542
129.518
128.860
128.181
127.538
126.750
126.489
125.022
122.148
113.219
54.868
33.568
25.669
25.365
4j
Cl
DMSO-d6, 100 MHz
f1 (ppm)


HM-1557
single_pulse
4k
DMSO-d6, 400 MHz
0.98
0.90
0.94
0.95
0.91
1.00
0.98
0.99
0.97
0.95
2.16
4.12
1.12
2.15
1.19
f1 (ppm)


HM-1557
single pulse decoupled gated NOE
141.431
140.802
138.814
133.619
133.117
128.738
127.449
127.169
126.493
125.608
124.287
121.980
110.899
106.797
55.010
33.579
25.649
25.319
4k
DMSO-d6, 100 MHz
f1 (ppm)

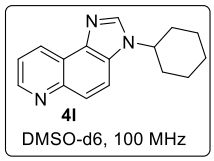

HM-1778
single_pulse
8.833
8.828
8.822
8.818
8.794
8.792
8.789
8.788
8.773
8.772
8.769
8.767
8.406
8.075
8.052
7.826
7.803
7.574
7.564
7.554
7.543
4.501
4.492
4.482
4.472
4.462
4.453
4.443
4.433
4.423
2.048
2.024
2.019
1.887
1.878
1.856
1.847
1.822
1.794
1.686
1.653
1.524
1.515
1.481
1.449
1.415
1.301
1.293
1.260
1.228
1.219

4l
DMSO-d6, 400 MHz

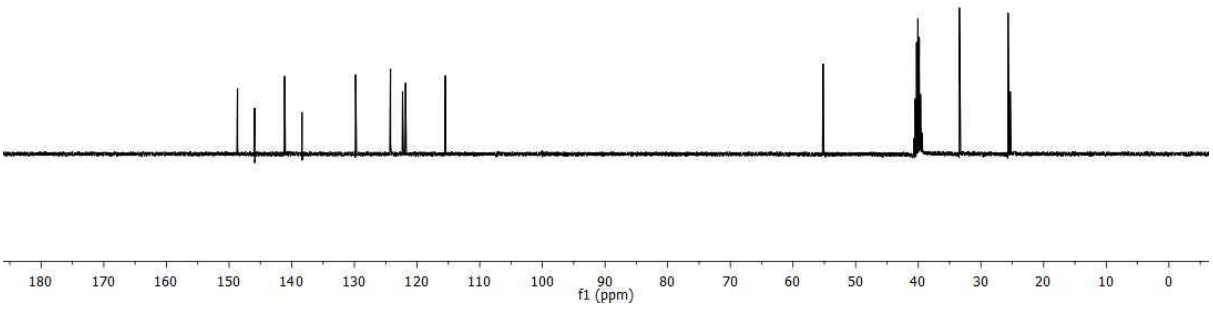

1.00
1.01
1.03
1.07
1.05
1.10
1.10
2.28
4.24
1.15
2.19
1.11
f1 (ppm)

HM-1778
single pulse decoupled gated NOE

148.656
145.917
141.134
138.362
129.871
129.807
124.238
122.313
121.843
115.482
55.192
33.443
25.671
25.324

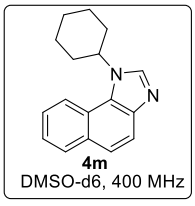


4l
DMSO-d6, 100 MHz



HM-1796-1
single_pulse

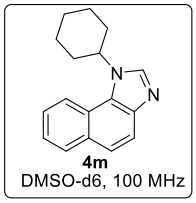
8.356
8.290
8.269
8.031
8.028
8.010
8.007
7.760
7.739
7.683
7.661
7.646
7.642
7.628
7.625
7.621
7.607
7.604
7.496
7.493
7.479
7.476
7.473
7.458
7.456
4.911
4.903
4.883
4.875
4.866
4.846
4.838
2.275
2.245
1.890
1.859
1.834
1.804
1.796
1.772
1.727
1.655
1.647
1.623
1.615
1.583
1.335
1.325
1.293
1.261



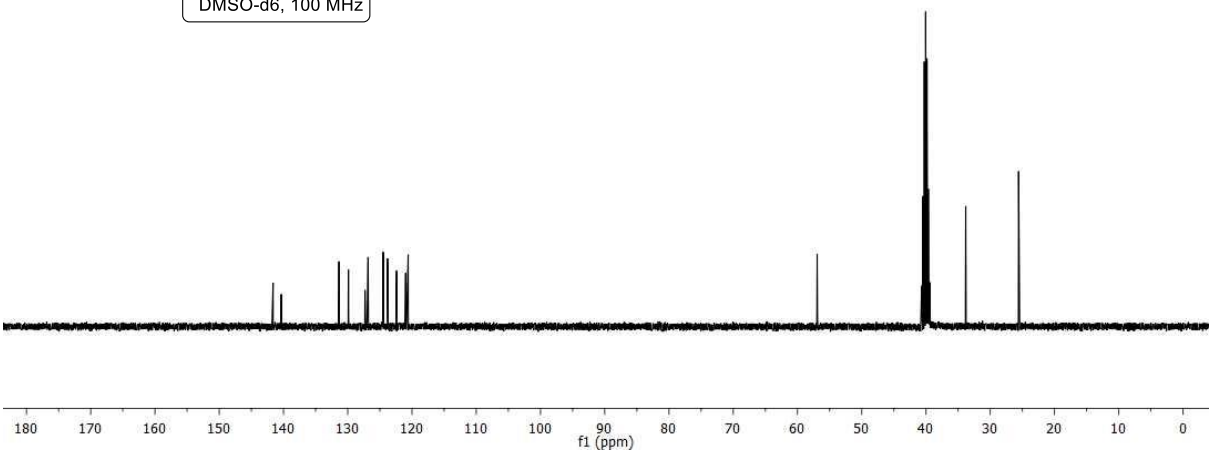
4m
DMSO-d6, 400 MHz

HM-1796-[1]
single pulse decoupled gated NOE

141.616
140.347
131.359
129.891
127.310
126.830
124.488
123.808
122.390
120.981
120.594
56.944
33.827
25.597
25.587

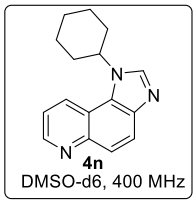


4m
DMSO-d6, 100 MHz

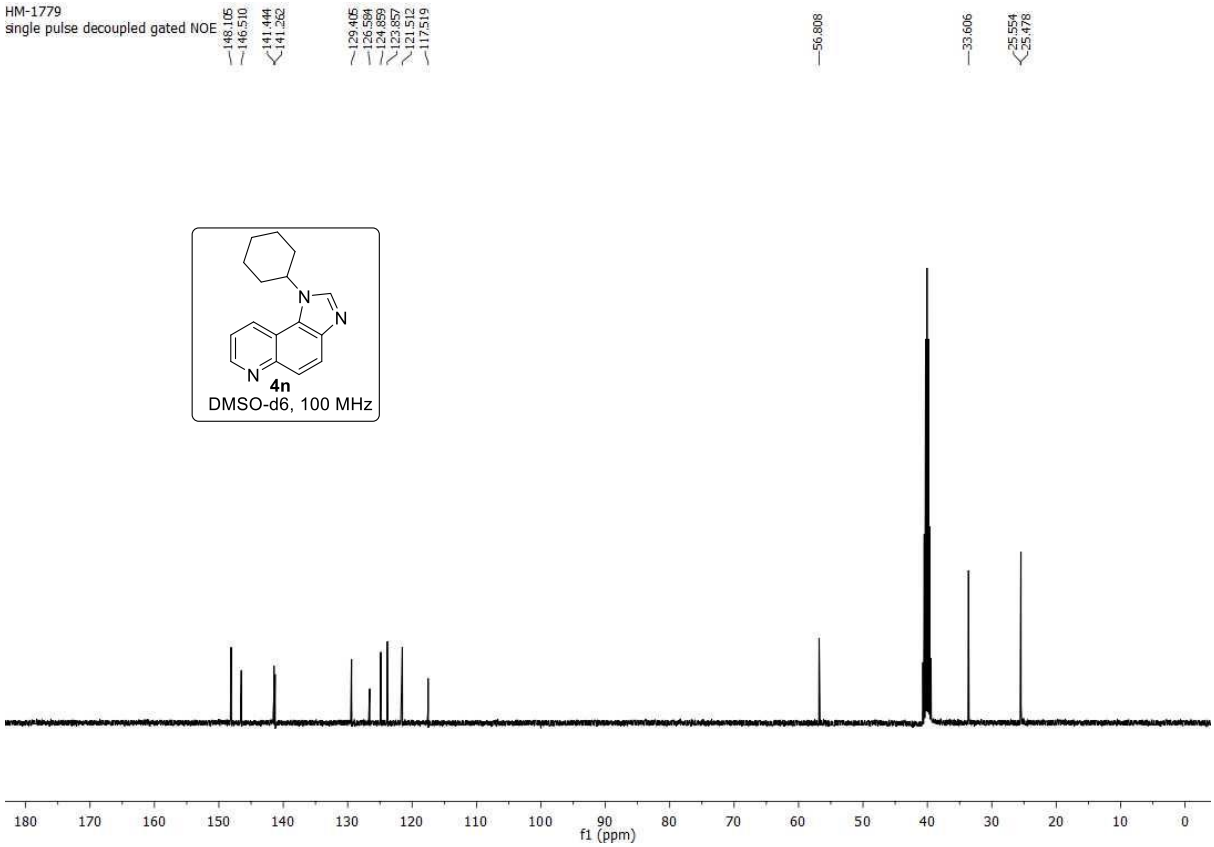


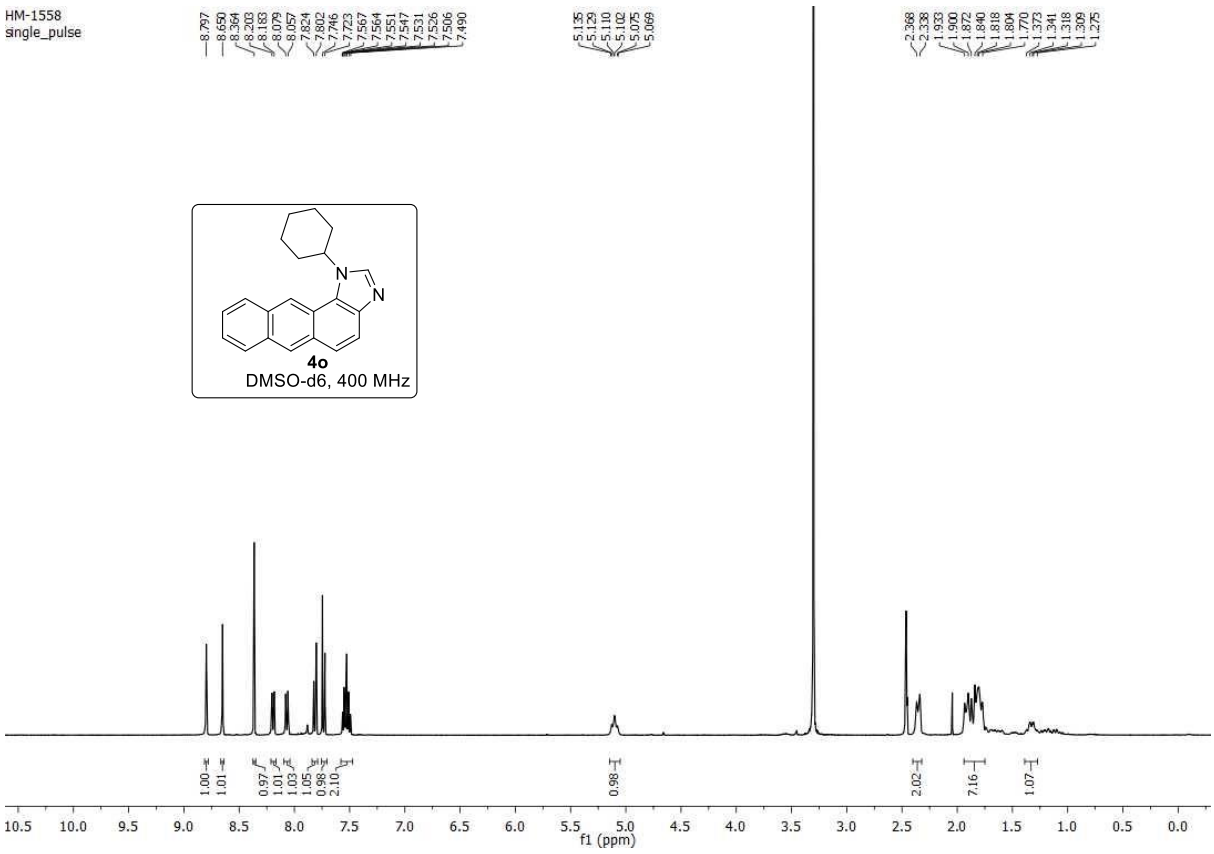
HM-1779
single_pulse

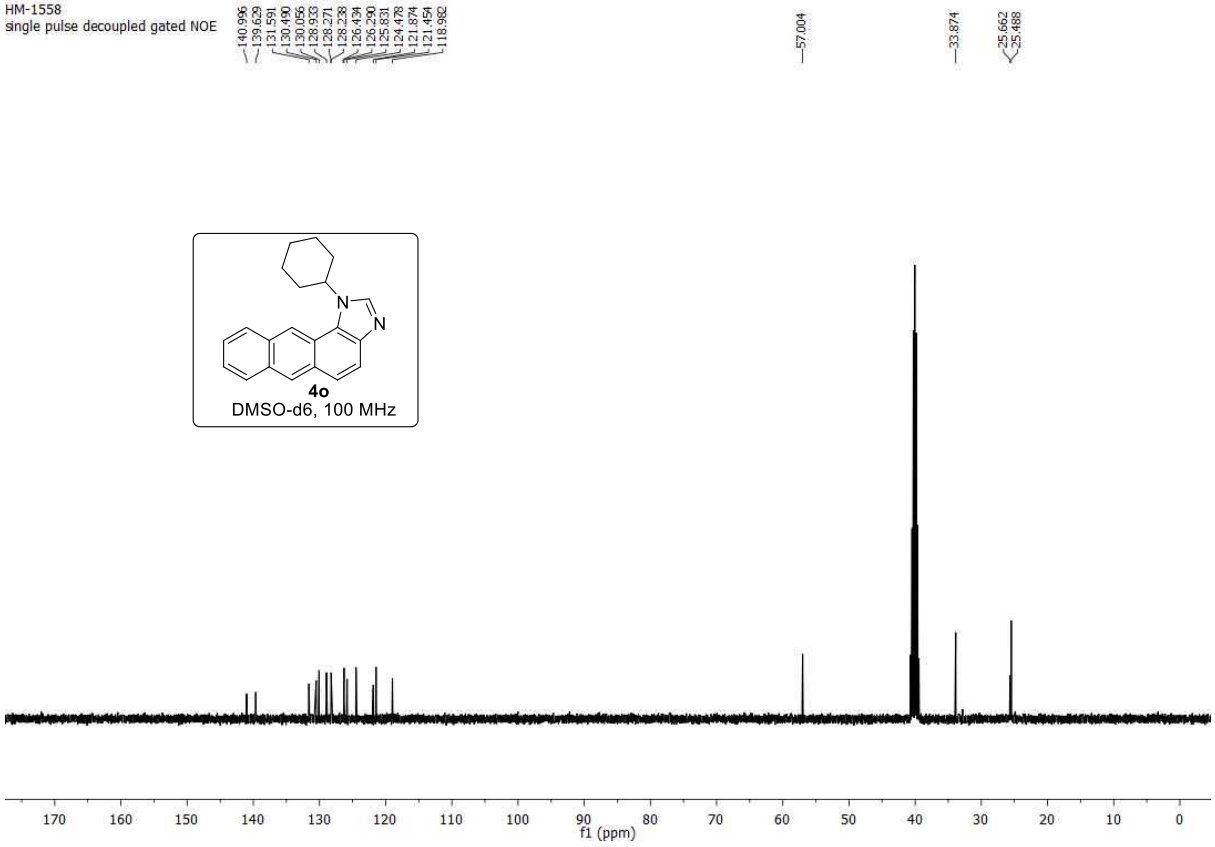
8.848
8.844
8.837
8.834
8.692
8.671
8.450
8.005
7.983
7.812
7.790
7.638
7.627
7.616
7.606
4.905
4.898
4.889
4.869
4.840
2.249
2.221
1.880
1.864
1.840
1.779
1.757
1.724
1.690
1.658
1.627
1.595
1.328
1.323
1.299
1.291
1.268
1.259
1.250

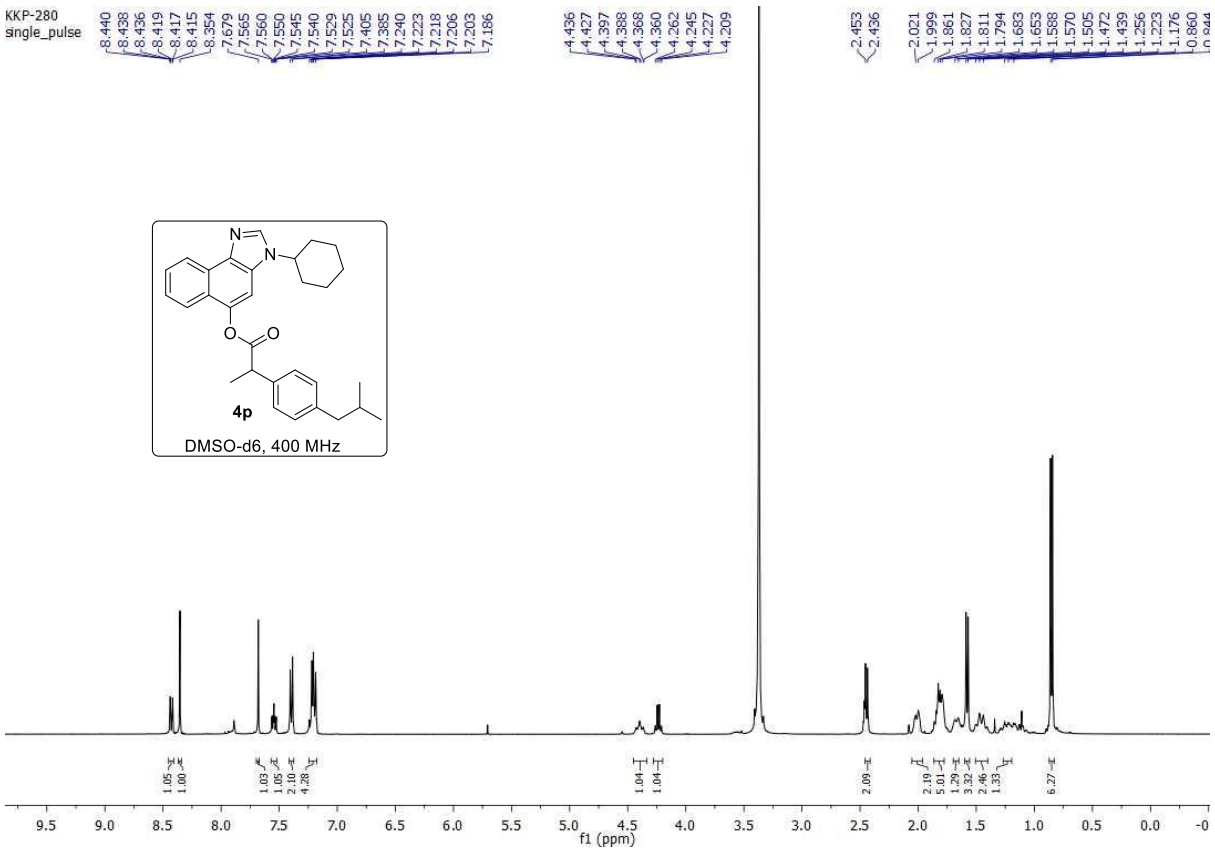


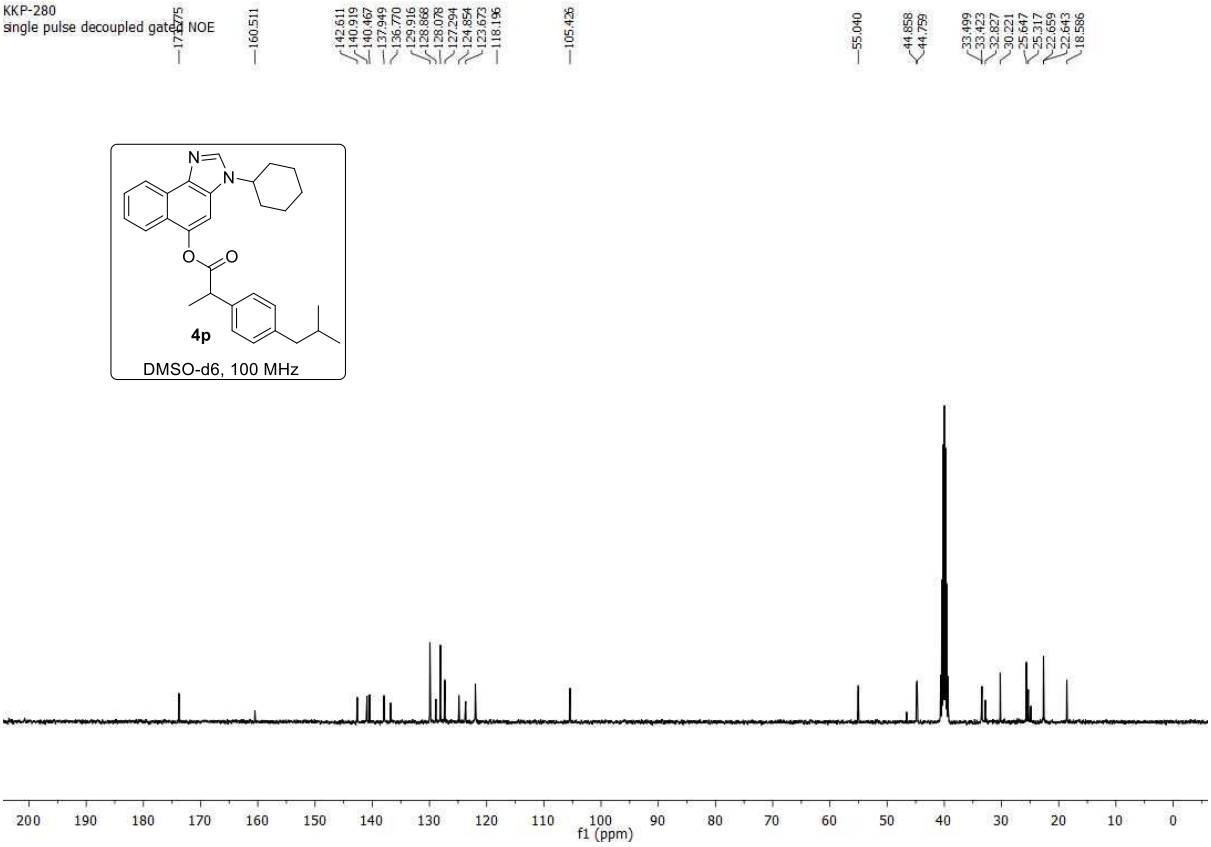
4n
DMSO-d6, 400 MHz

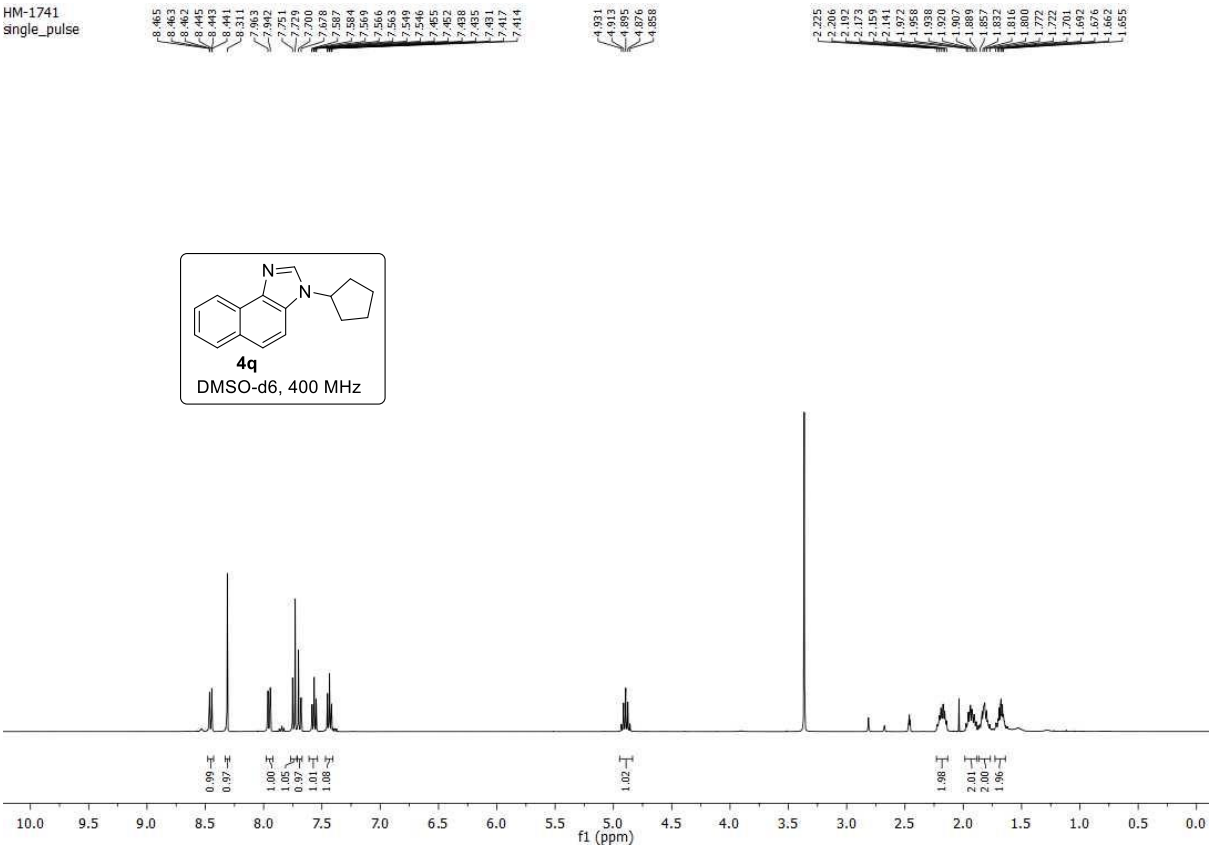

HM-1779
single pulse decoupled gated NOE
148.105
146.510
141.444
141.262
129.405
126.584
124.859
123.857
121.512
117.519
56.808
33.606
25.554
25.478
4n
DMSO-d6, 100 MHz
f1 (ppm)

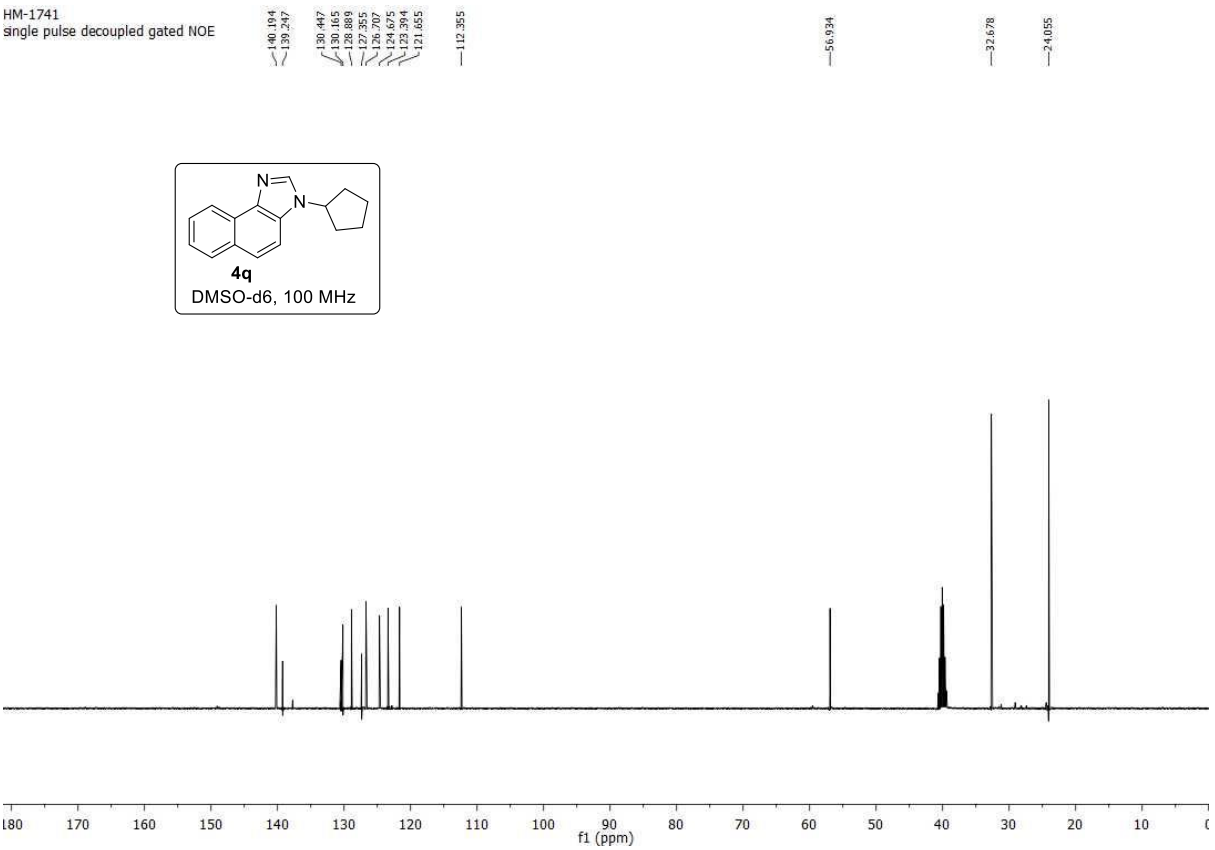

HM-1558
single_pulse
8.797
8.650
8.364
8.203
8.183
8.079
8.057
7.824
7.802
7.746
7.723
7.567
7.564
7.551
7.547
7.531
7.526
7.506
7.490
5.135
5.129
5.110
5.102
5.075
5.069
2.368
2.338
1.933
1.900
1.872
1.840
1.818
1.804
1.770
1.373
1.341
1.318
1.309
1.275
4o
DMSO-d6, 400 MHz
1.00
1.01
0.97
1.01
1.03
1.05
0.98
2.10
0.98
2.02
7.16
1.07
f1 (ppm)

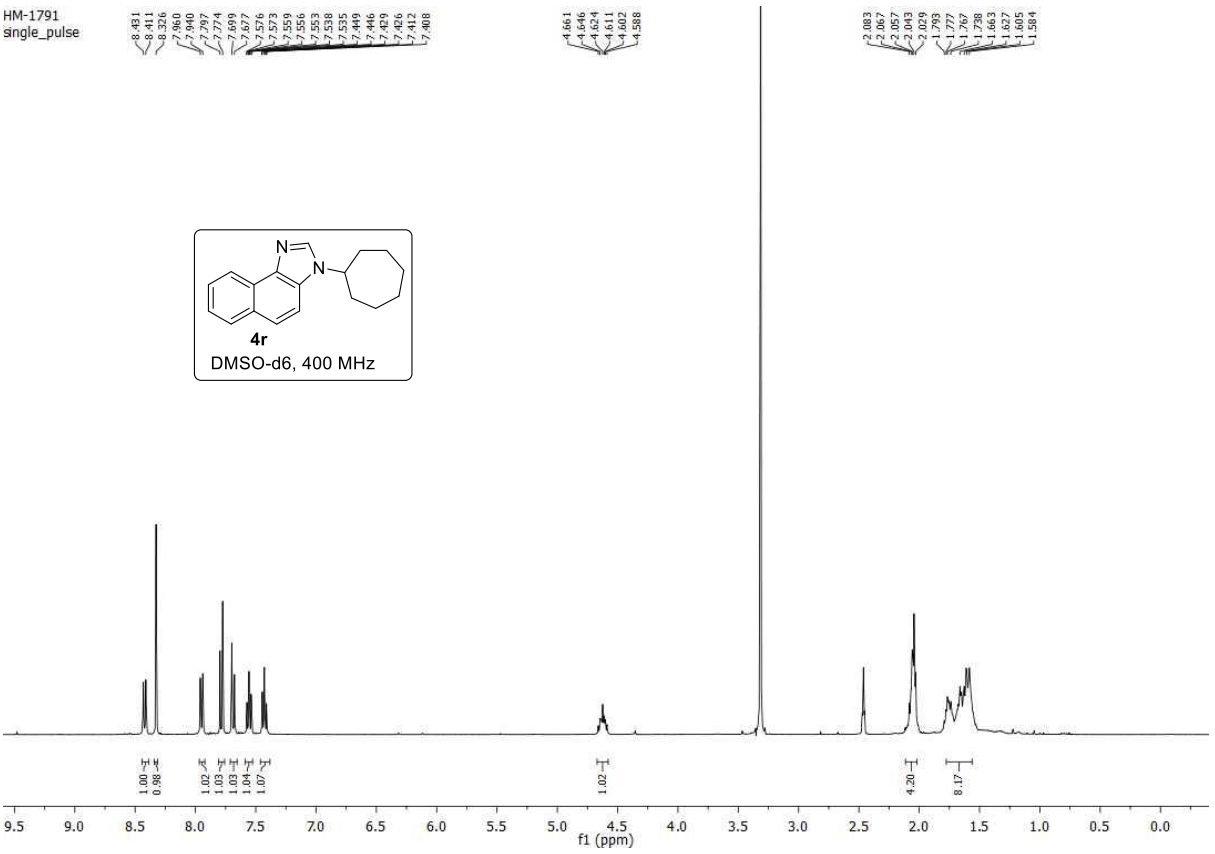

HM-1558
single pulse decoupled gated NOE
140.996
139.629
131.591
130.490
130.056
128.933
128.271
128.238
126.434
126.290
125.831
124.478
121.874
121.454
118.982
57.004
33.874
25.662
25.488
4o
DMSO-d6, 100 MHz
f1 (ppm)

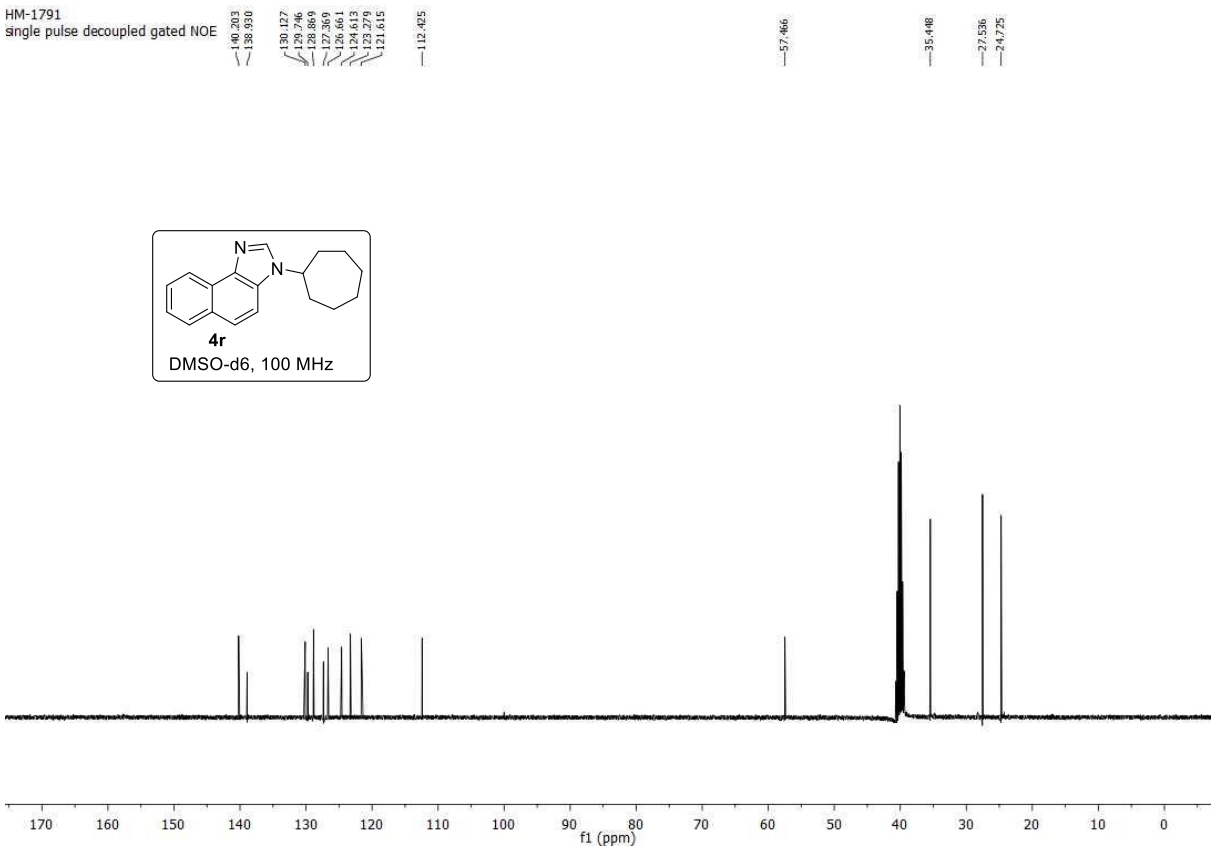

KKP-280
single_pulse
8.440
8.438
8.436
8.419
8.417
8.415
8.354
7.679
7.565
7.560
7.550
7.545
7.540
7.529
7.525
7.405
7.385
7.240
7.223
7.218
7.206
7.203
7.186
4.436
4.427
4.397
4.388
4.368
4.360
4.262
4.245
4.227
4.209
2.453
2.436
2.021
1.999
1.861
1.827
1.811
1.794
1.683
1.653
1.588
1.570
1.505
1.472
1.439
1.256
1.223
1.176
0.860
4p
DMSO-d6, 400 MHz
f1 (ppm)

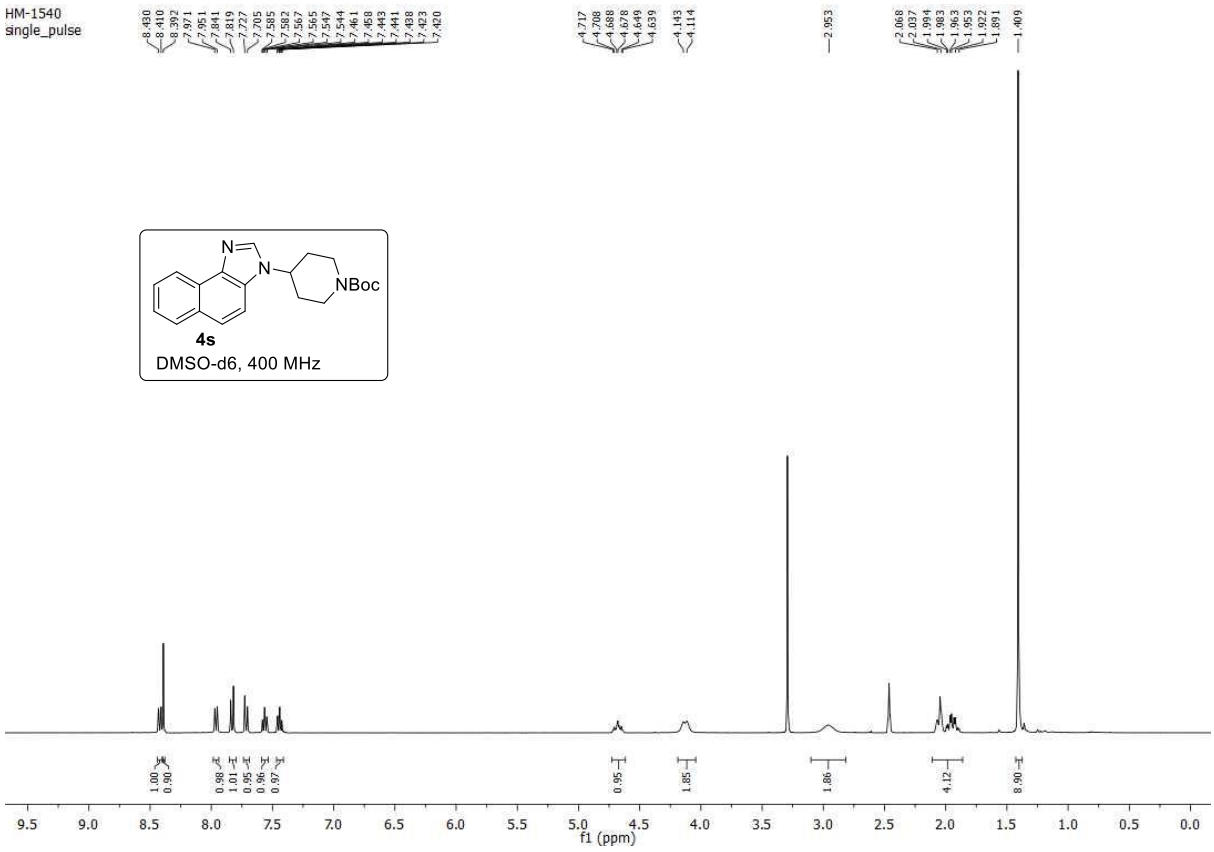

KKP-280
single pulse decoupled gated NOE
4p
DMSO-d6, 100 MHz
f1 (ppm)

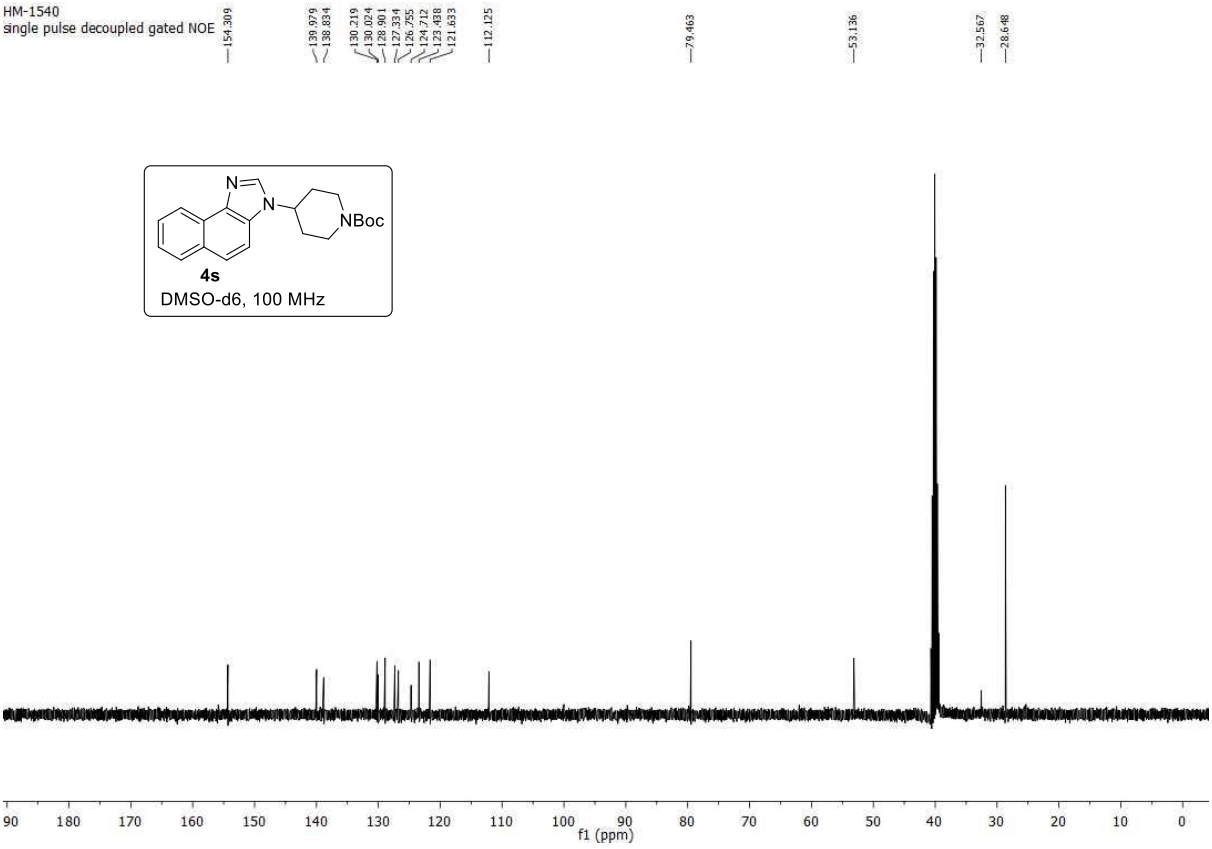

HM-1741
single_pulse
4q
DMSO-d6, 400 MHz
f1 (ppm)

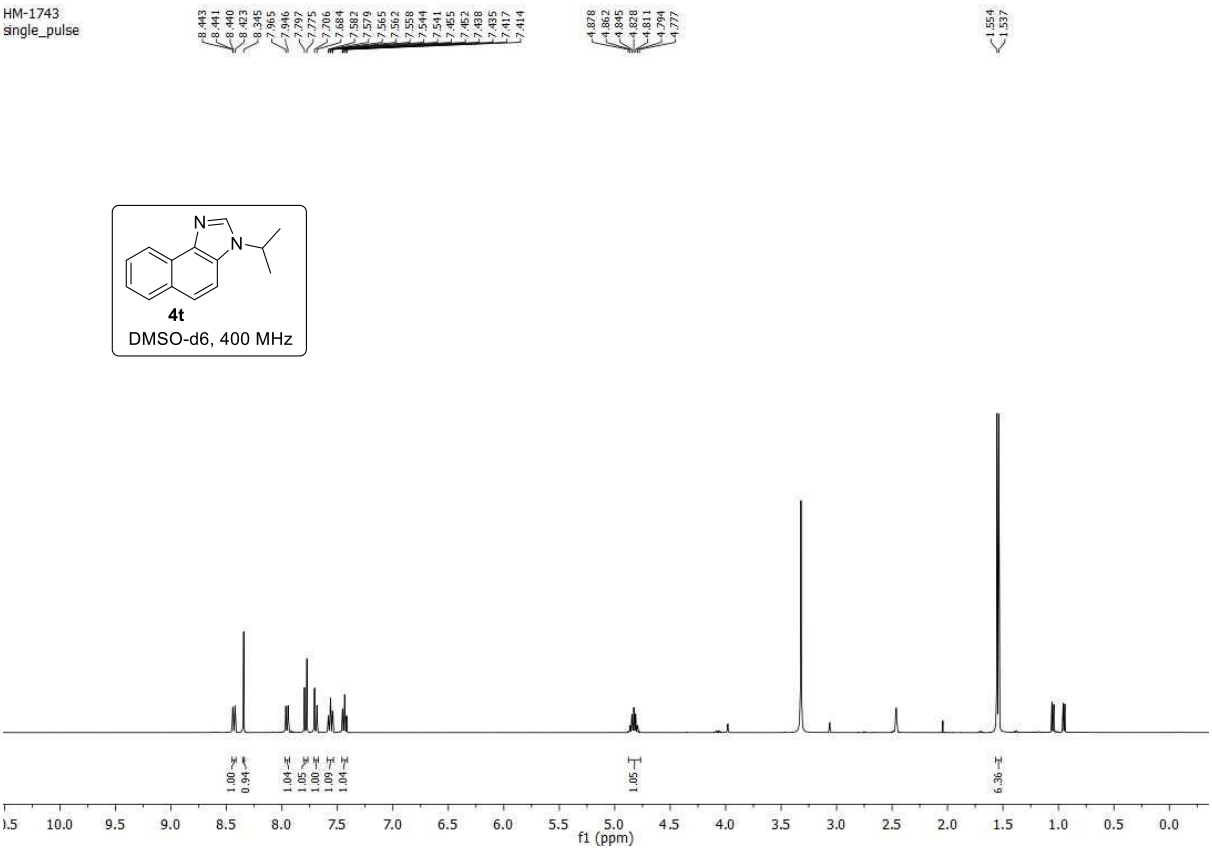

HM-1741
single pulse decoupled gated NOE
140.194
139.247
130.447
130.165
128.889
127.355
126.707
124.675
123.394
121.655
112.355
56.934
32.678
24.055
4q
DMSO-d6, 100 MHz
f1 (ppm)


HM-1791
single_pulse
8.481
8.411
8.326
7.960
7.940
7.797
7.774
7.699
7.677
7.576
7.573
7.559
7.556
7.553
7.538
7.535
7.449
7.446
7.429
7.426
7.412
7.408
4.661
4.656
4.624
4.611
4.602
4.588
2.083
2.067
2.057
2.043
2.029
1.793
1.777
1.767
1.738
1.663
1.627
1.605
1.584
1.00
0.98
1.02
1.03
1.03
1.04
1.07
1.02
4.20
8.17
4r
DMSO-d6, 400 MHz
f1 (ppm)

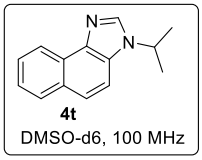

HM-1791
single pulse decoupled gated NOE
140.203
138.930
130.127
129.746
128.869
127.369
126.661
124.613
123.279
121.615
112.425
57.466
35.448
27.536
24.725
4r
DMSO-d6, 100 MHz
f1 (ppm)

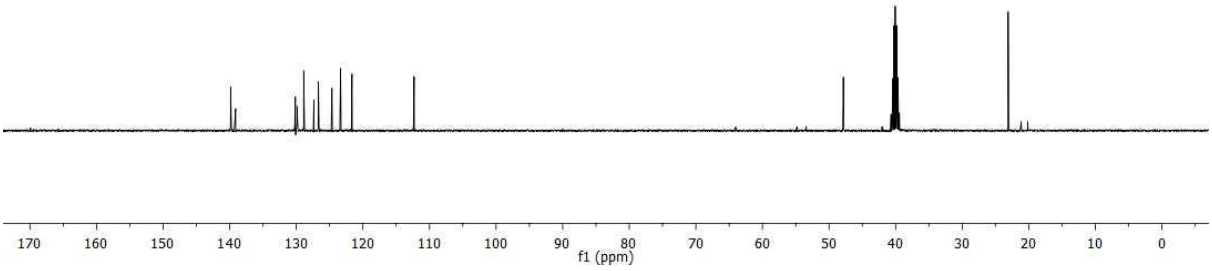

HM-1540
single_pulse
8.430
8.410
8.392
7.971
7.951
7.841
7.819
7.727
7.705
7.585
7.582
7.567
7.565
7.547
7.544
7.461
7.458
7.443
7.441
7.438
7.423
7.420
4.717
4.708
4.688
4.678
4.649
4.639
4.143
4.114
2.953
2.068
2.037
1.994
1.983
1.963
1.953
1.922
1.891
1.469
NBoc
4s
DMSO-d6, 400 MHz
1.00
0.90
0.98
1.01
0.95
0.96
0.97
0.95
1.85
1.86
4.12
8.90
f1 (ppm)


HM-1540
single pulse decoupled gated NOE
154.309
139.979
138.834
130.219
130.024
128.901
127.334
126.755
124.712
123.488
121.633
112.125
79.463
53.136
32.567
28.648
N
N
NBoc
4s
DMSO-d6, 100 MHz
f1 (ppm)

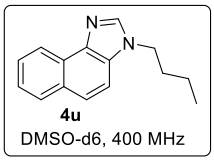

HM-1743
single_pulse
8.443
8.441
8.440
8.423
8.345
7.965
7.946
7.797
7.775
7.706
7.684
7.582
7.579
7.565
7.562
7.558
7.544
7.541
7.465
7.462
7.438
7.435
7.417
7.414
4.878
4.862
4.845
4.828
4.811
4.794
4.777
1.554
1.537
N
N
4t
DMSO-d6, 400 MHz
1.00
0.94
1.04
1.05
1.00
1.09
1.04
1.05
6.36
f1 (ppm)

HM-1743
single pulse decoupled gated NOE

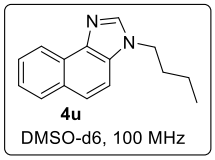


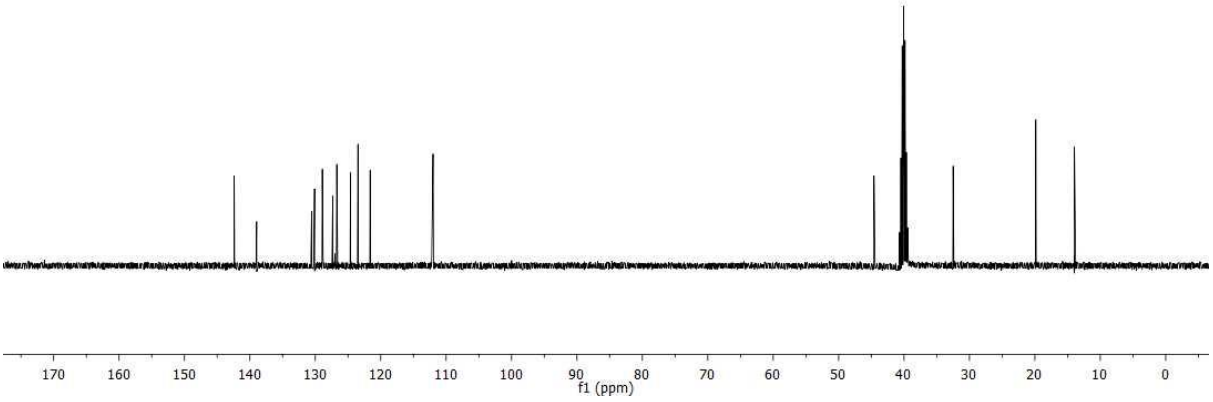


HM-1527
single_pulse

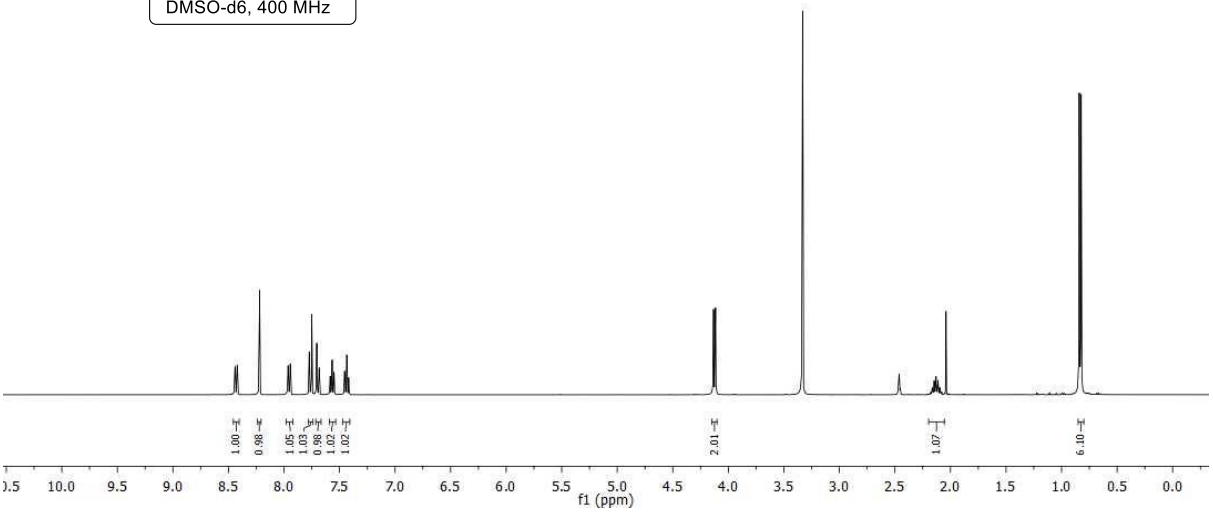


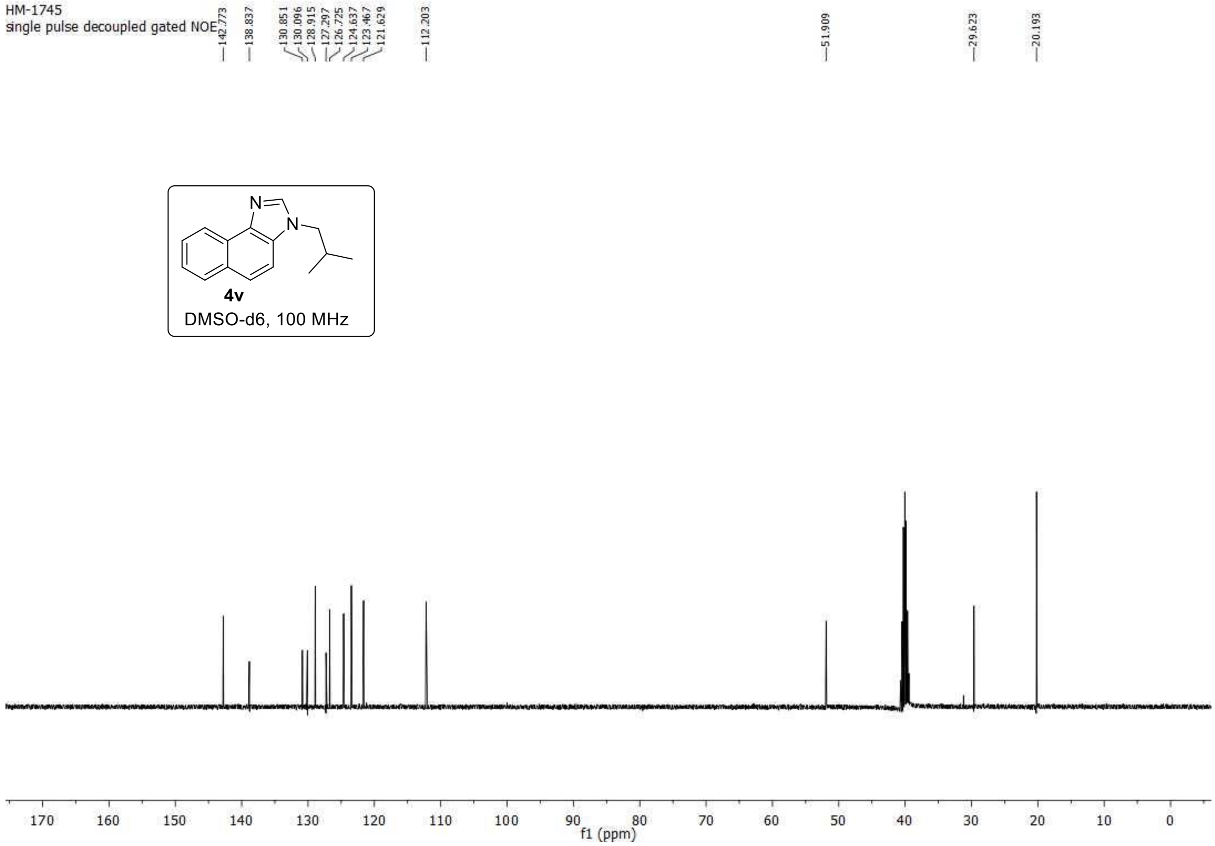
HM-1527
single pulse decoupled gated NOE

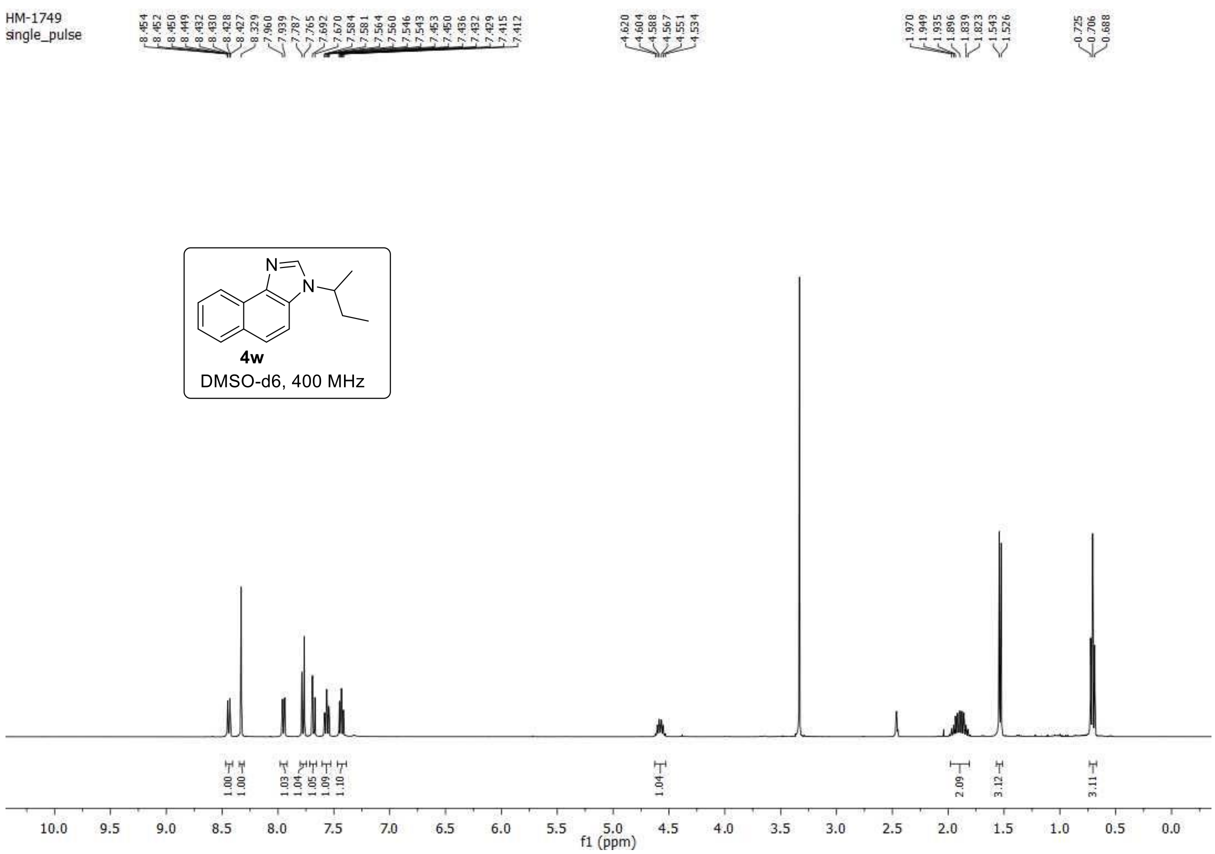




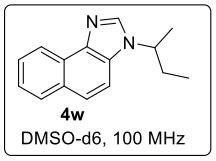
HM-1745
single_pulse



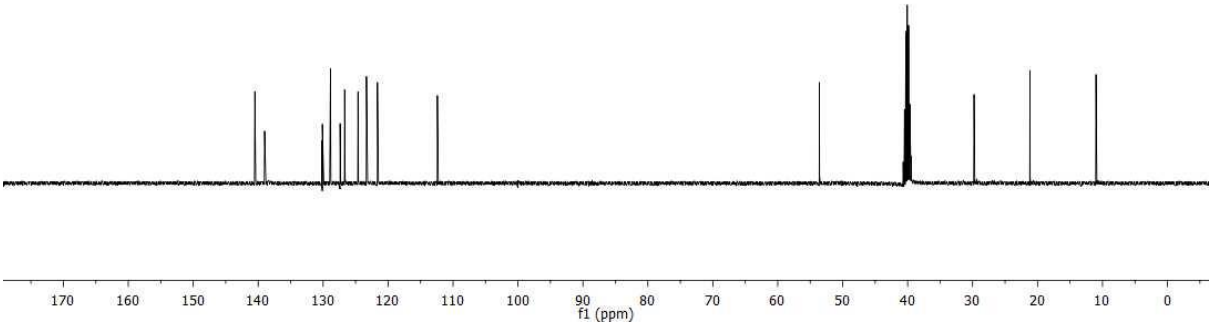

HM-1745
single pulse decoupled gated NOE
142.773
138.837
130.851
130.096
128.915
127.297
126.725
124.637
123.467
121.629
112.203
51.909
29.623
20.193
4v
DMSO-d6, 100 MHz
f1 (ppm)


HM-1749
single_pulse
8.454
8.452
8.450
8.449
8.432
8.430
8.428
8.427
8.329
7.960
7.939
7.787
7.765
7.692
7.670
7.584
7.581
7.564
7.560
7.546
7.543
7.453
7.450
7.436
7.432
7.429
7.415
7.412
4.620
4.604
4.588
4.567
4.551
4.534
1.970
1.949
1.935
1.896
1.839
1.823
1.543
1.526
0.725
0.706
0.688
4w
DMSO-d6, 400 MHz
1.00
1.00
1.03
1.04
1.05
1.09
1.10
1.04
2.09
3.12
3.11
f1 (ppm)

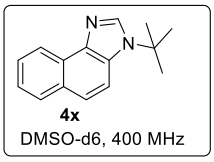
HM-1749
single pulse decoupled gated NOE



4w
DMSO-d6, 100 MHz

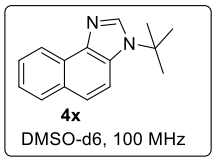


HM-1530
single_pulse

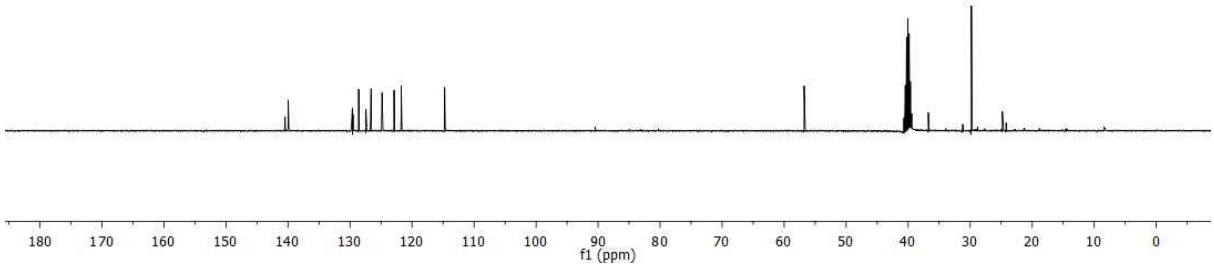


4x
DMSO-d6, 400 MHz

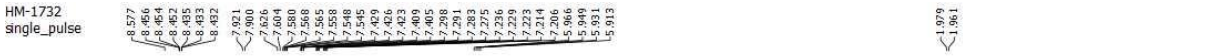
HM-1530
single pulse decoupled gated NOE

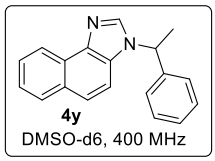


4x
DMSO-d6, 100 MHz

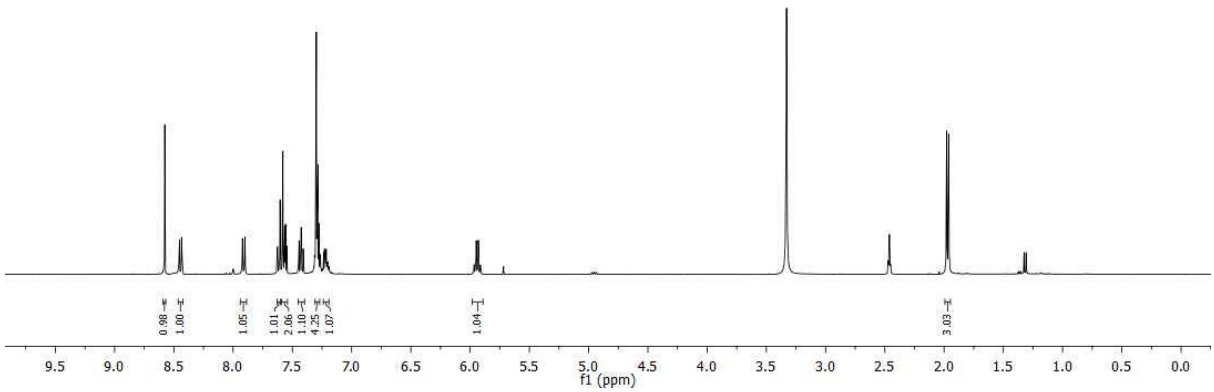


HM-1732
single_pulse

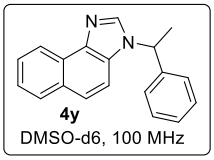


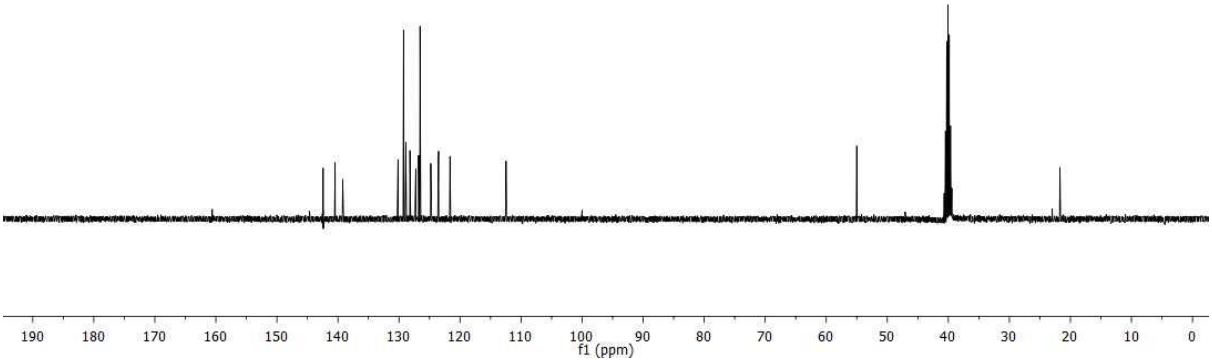


4y
DMSO-d6, 400 MHz

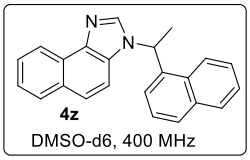


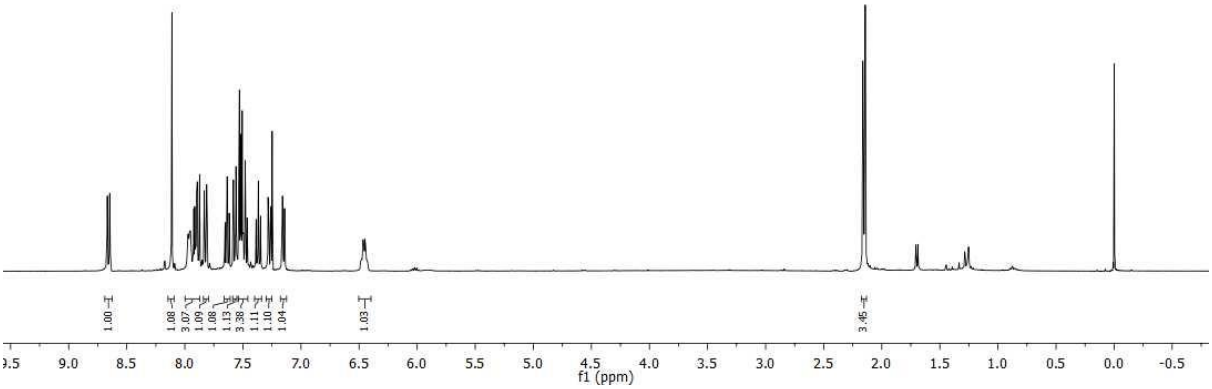
HM-1732
single pulse decoupled gated NOE

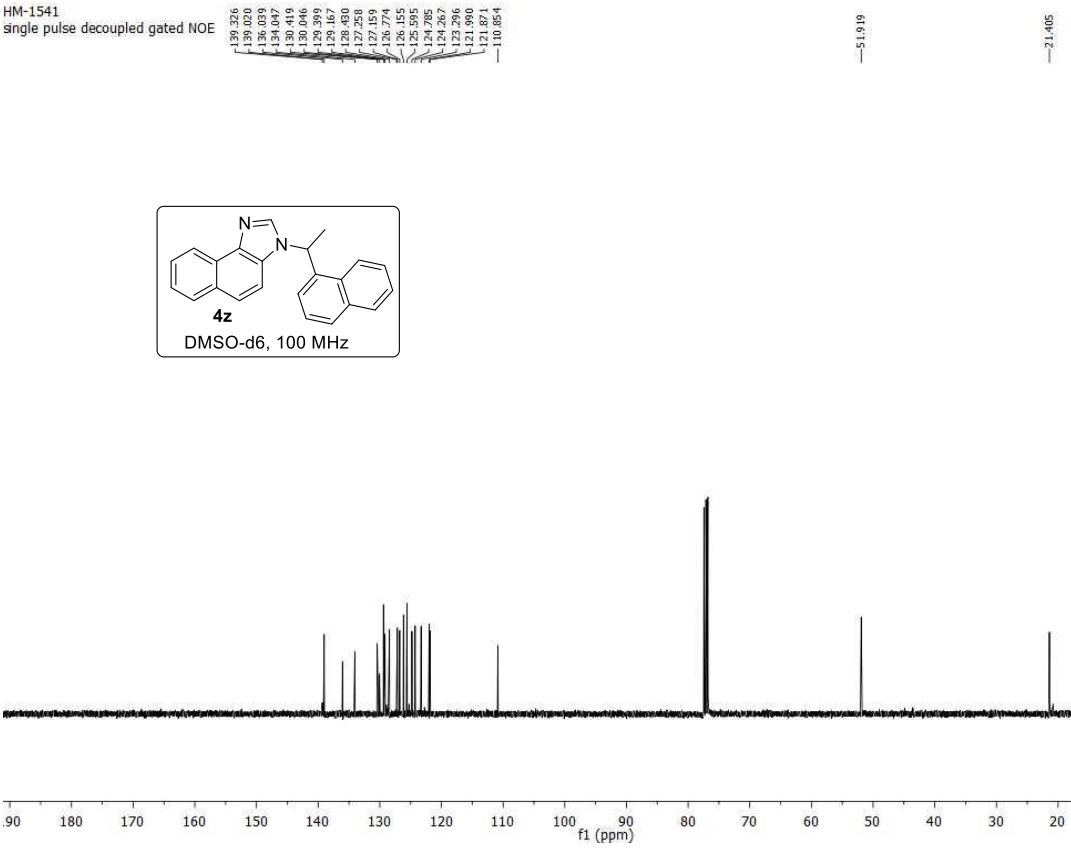


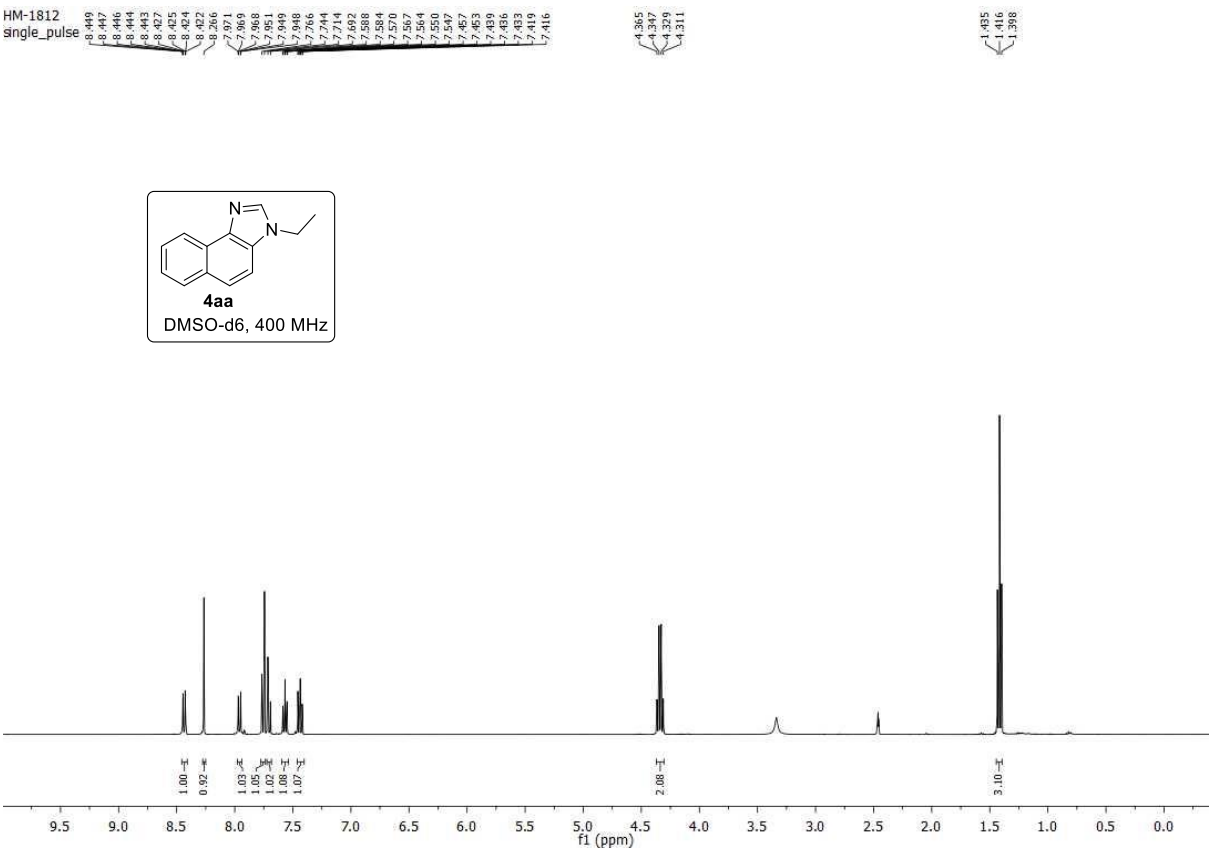


HM-1541
single_pulse

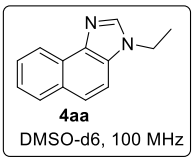




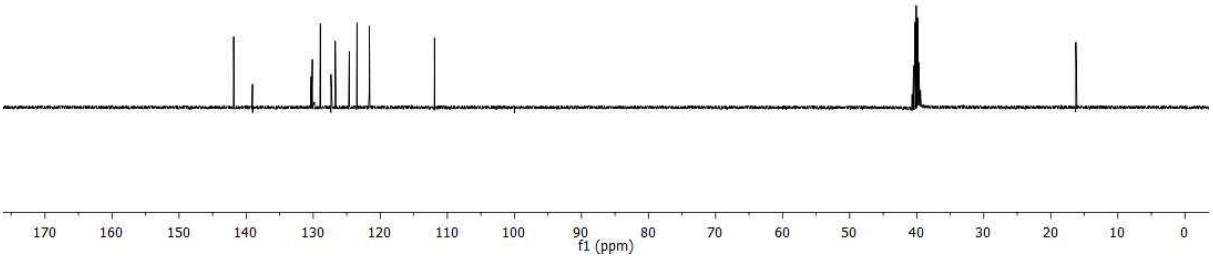

HM-1541
single pulse decoupled gated NOE
139.326
139.020
136.039
134.047
130.419
130.046
129.399
129.167
128.480
127.258
127.159
126.774
126.155
125.595
124.785
124.267
123.296
121.990
121.871
110.854
51.919
21.405
4z
DMSO-d6, 100 MHz
f1 (ppm)


HM-1812
single_pulse
8.449
8.447
8.446
8.444
8.443
8.427
8.425
8.424
8.422
8.266
7.971
7.969
7.968
7.951
7.949
7.948
7.766
7.744
7.714
7.692
7.588
7.584
7.570
7.567
7.564
7.550
7.547
7.467
7.463
7.439
7.436
7.433
7.419
7.416
4.365
4.347
4.329
4.311
1.435
1.416
1.398
4aa
DMSO-d6, 400 MHz
1.00
0.92
1.03
1.05
1.02
1.08
1.07
2.08
3.10
f1 (ppm)

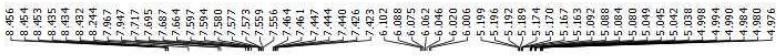
HM-1812
single pulse decoupled gated NOE

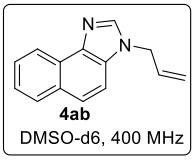


4aa
DMSO-d6, 100 MHz

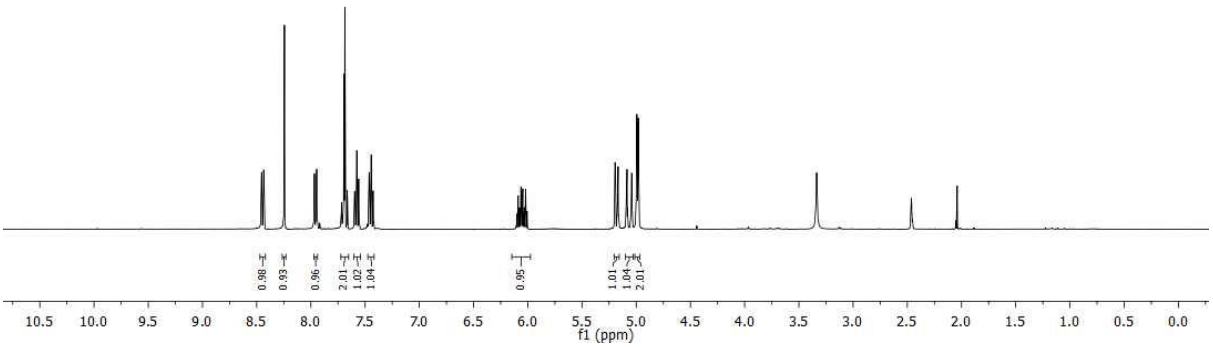


HM-1805
single_pulse



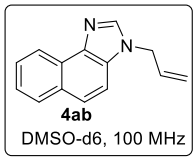


4ab
DMSO-d6, 400 MHz

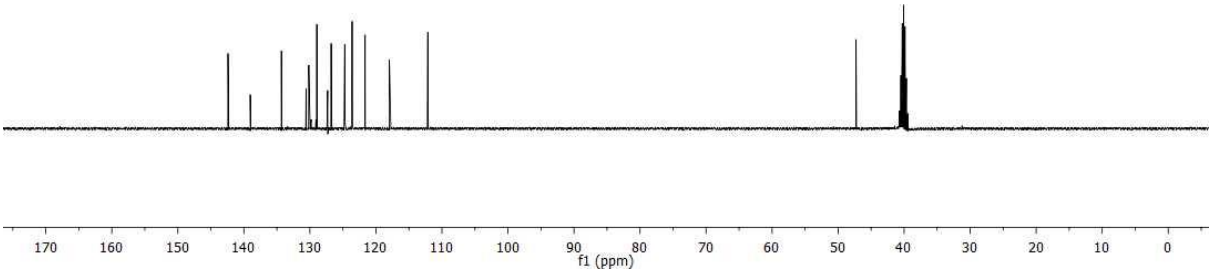


HM-1805
single pulse decoupled gated NOE

142.404
139.034
134.319
130.583
130.170
128.953
127.303
126.777
124.718
123.602
121.637
117.960
112.141
47.278

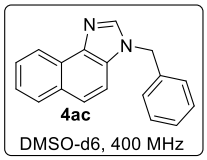


4ab
DMSO-d6, 100 MHz



KKP-299
single_pulse

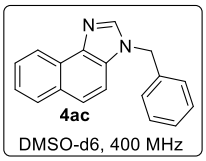
8.441
7.945
7.924
7.667
7.597
7.594
7.579
7.576
7.573
7.559
7.556
7.457
7.454
7.440
7.437
7.434
7.420
7.417
7.296
7.290
7.282
7.244
7.224
7.204
5.585

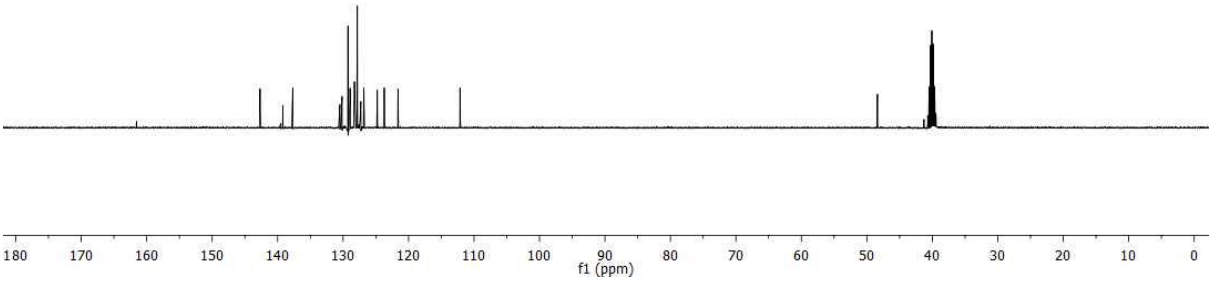


4ac
DMSO-d6, 400 MHz

HM-1804
single pulse decoupled gated NOE

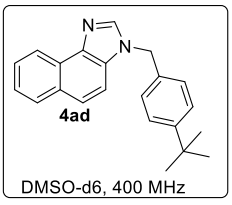
142.686
139.183
137.688
130.486
130.152
129.257
128.936
128.278
127.823
127.276
126.831
124.775
123.714
121.620
112.152
48.380

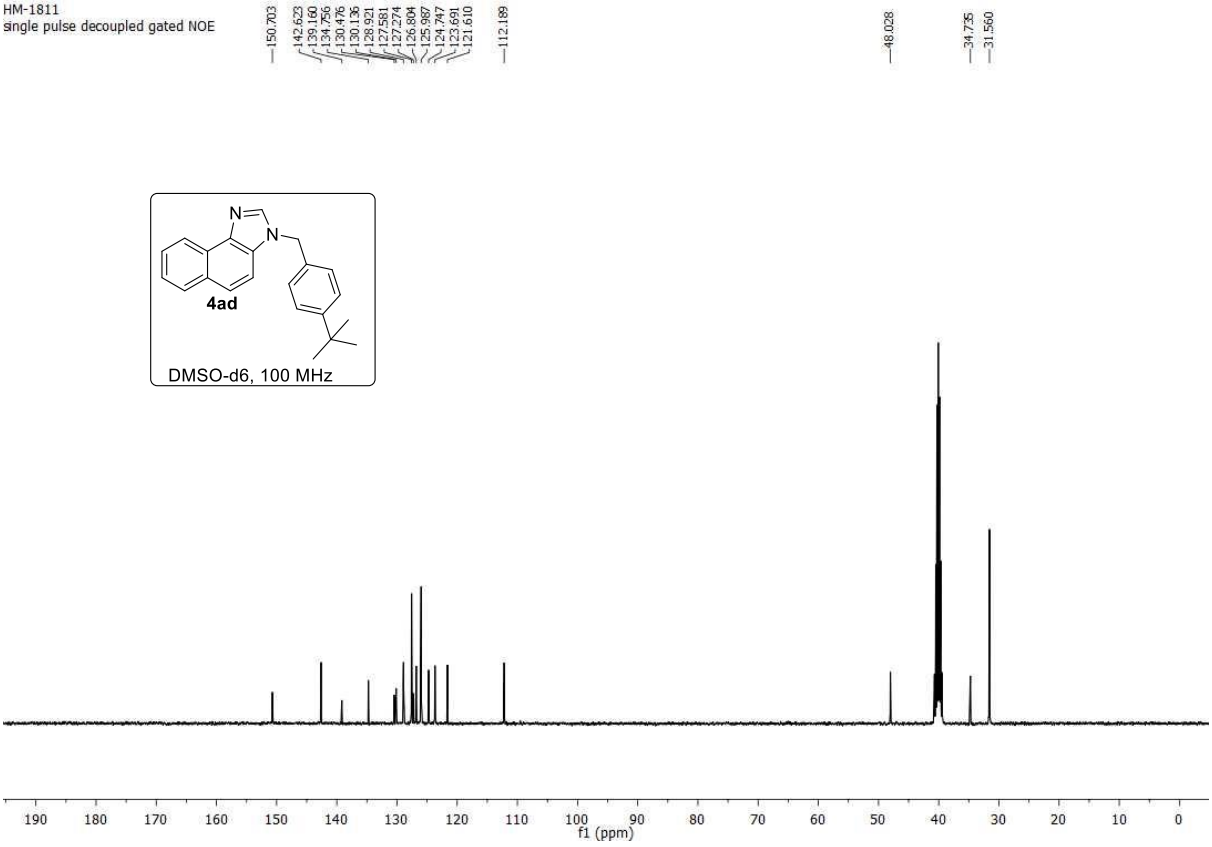


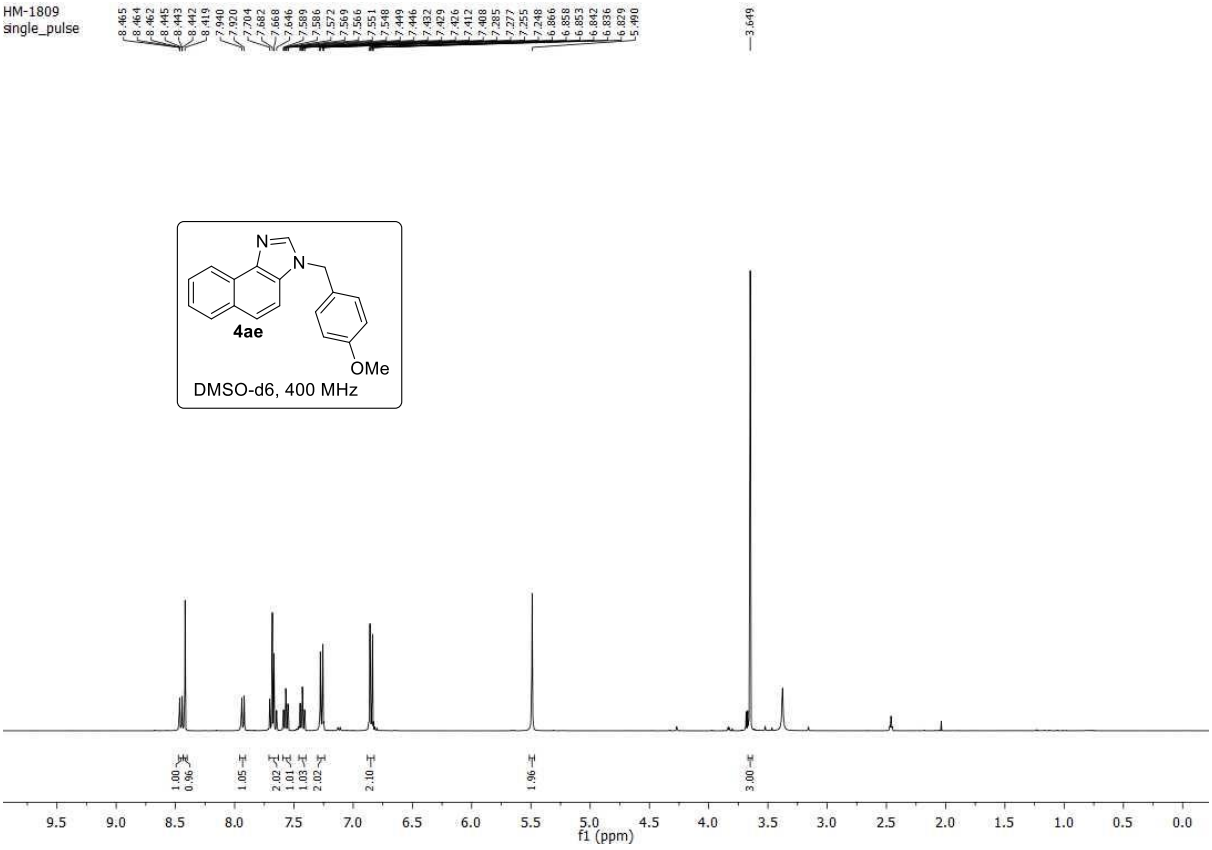


HM-1811
single_pulse

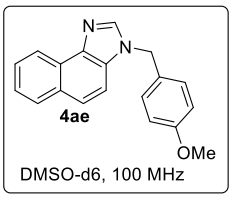
8.445
8.444
8.442
8.425
8.423
7.941
7.921
7.718
7.696
7.674
7.651
7.570
7.566
7.563
7.549
7.546
7.461
7.466
7.464
7.451
7.428
7.414
7.410
7.312
7.307
7.302
7.291
7.285
7.280
7.226
7.221
7.216
7.204
7.200
7.194
5.534
1.167

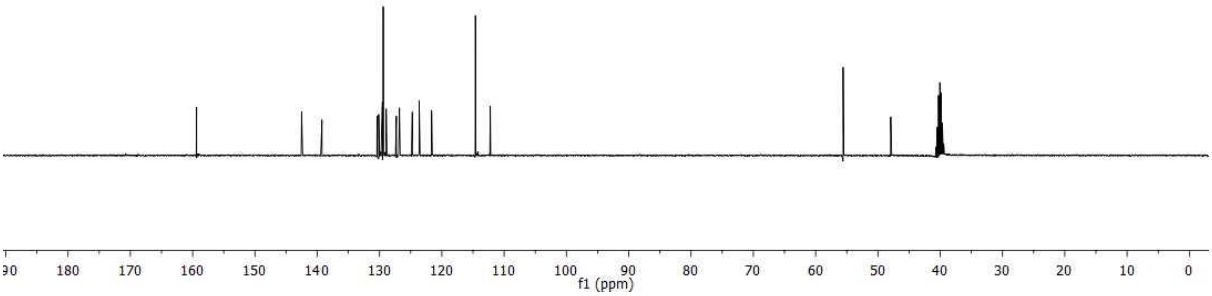



HM-1811
single pulse decoupled gated NOE
150.703
142.623
139.160
134.756
130.476
130.136
128.921
127.581
127.274
126.804
125.987
124.747
123.691
121.610
112.189
48.028
34.735
31.560
4ad
DMSO-d6, 100 MHz
f1 (ppm)

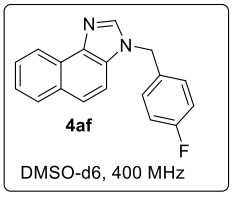

HM-1809
single_pulse
3.649
4ae
OMe
DMSO-d6, 400 MHz
f1 (ppm)

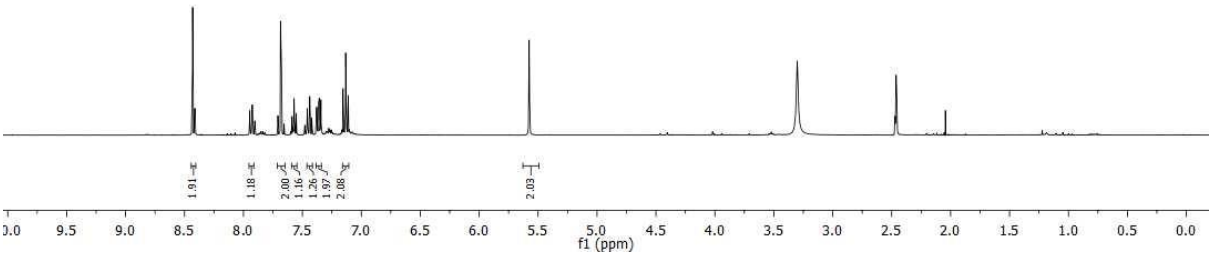
HM-1809
single pulse decoupled gated NOE

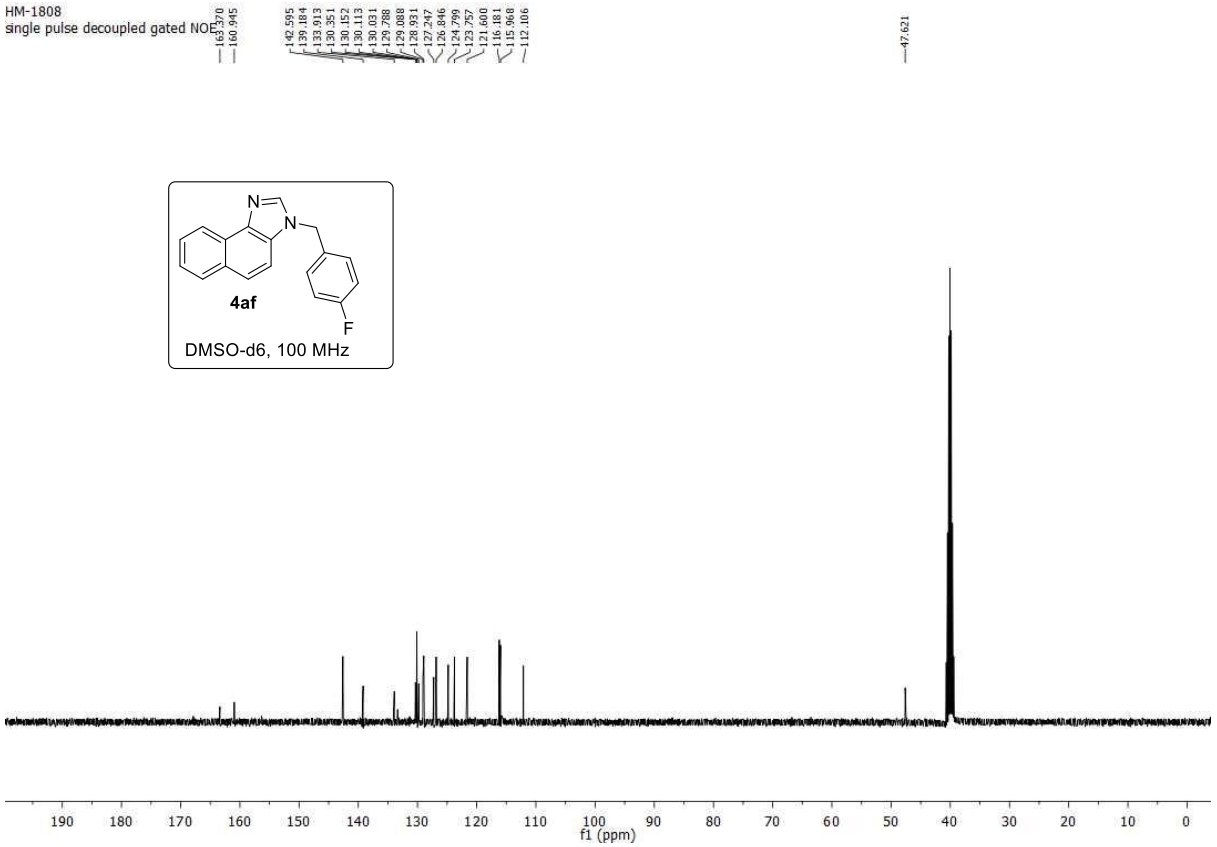


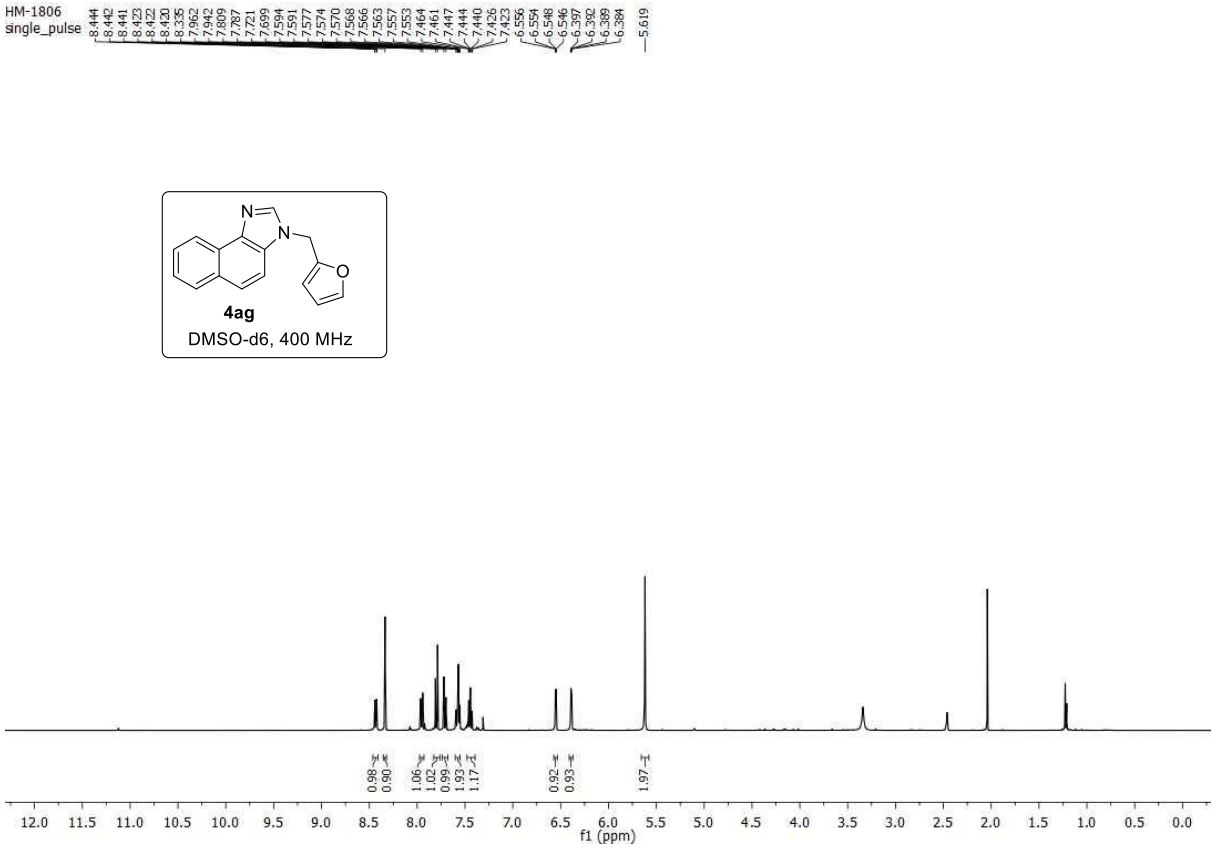


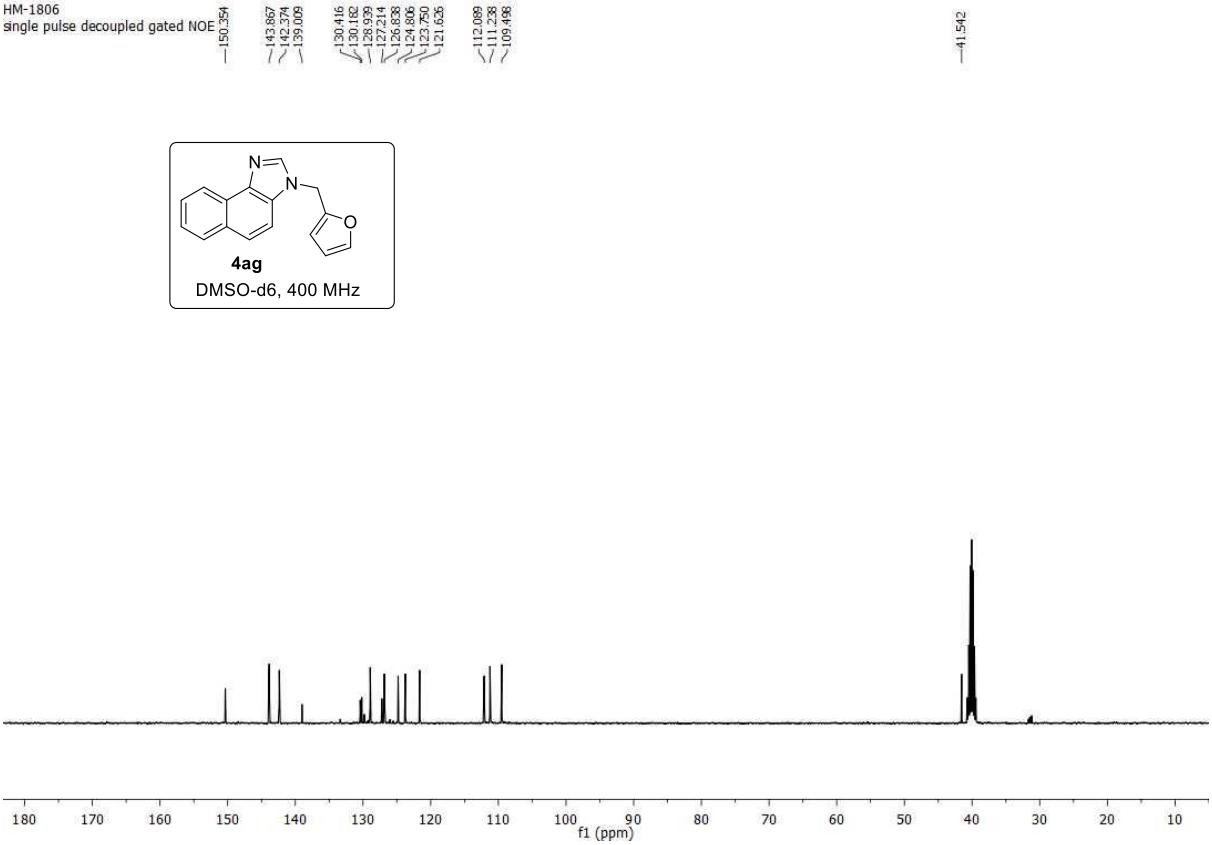
HM-1808
single_pulse

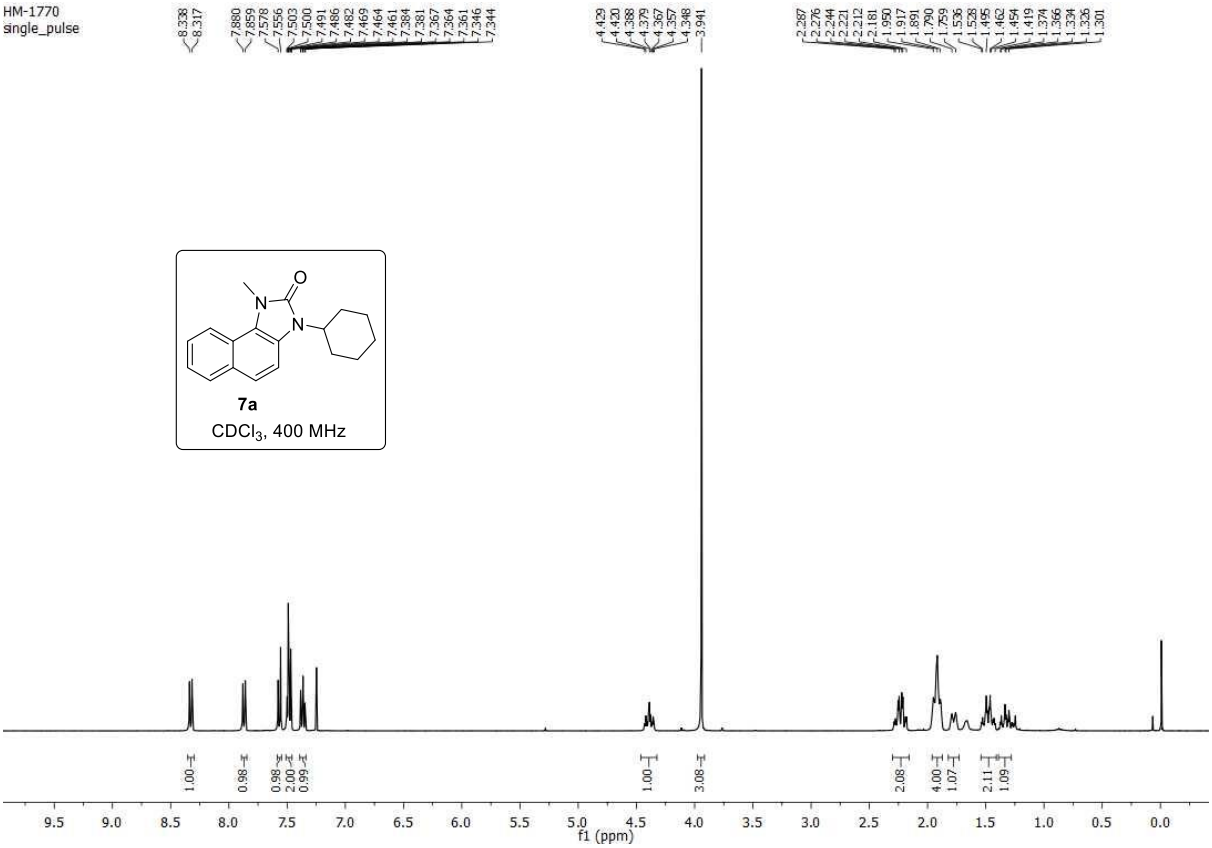


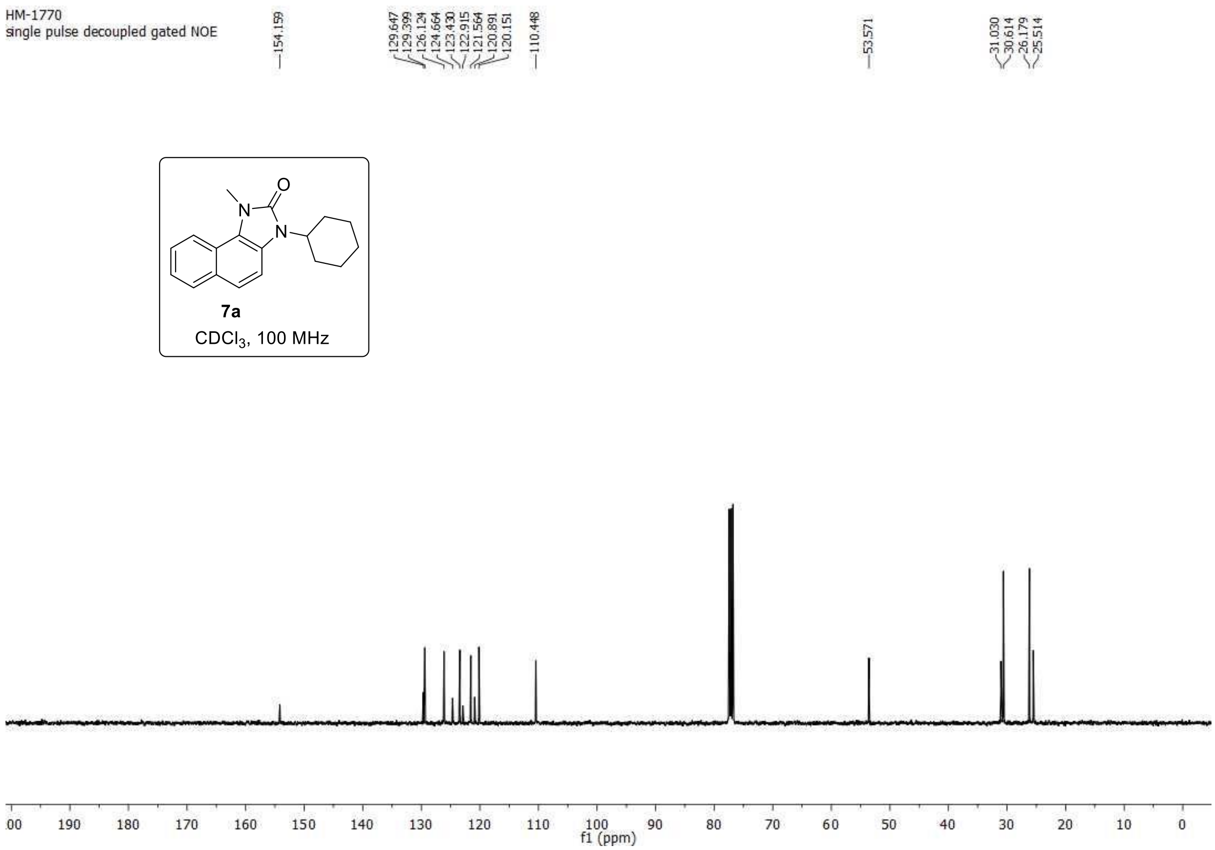


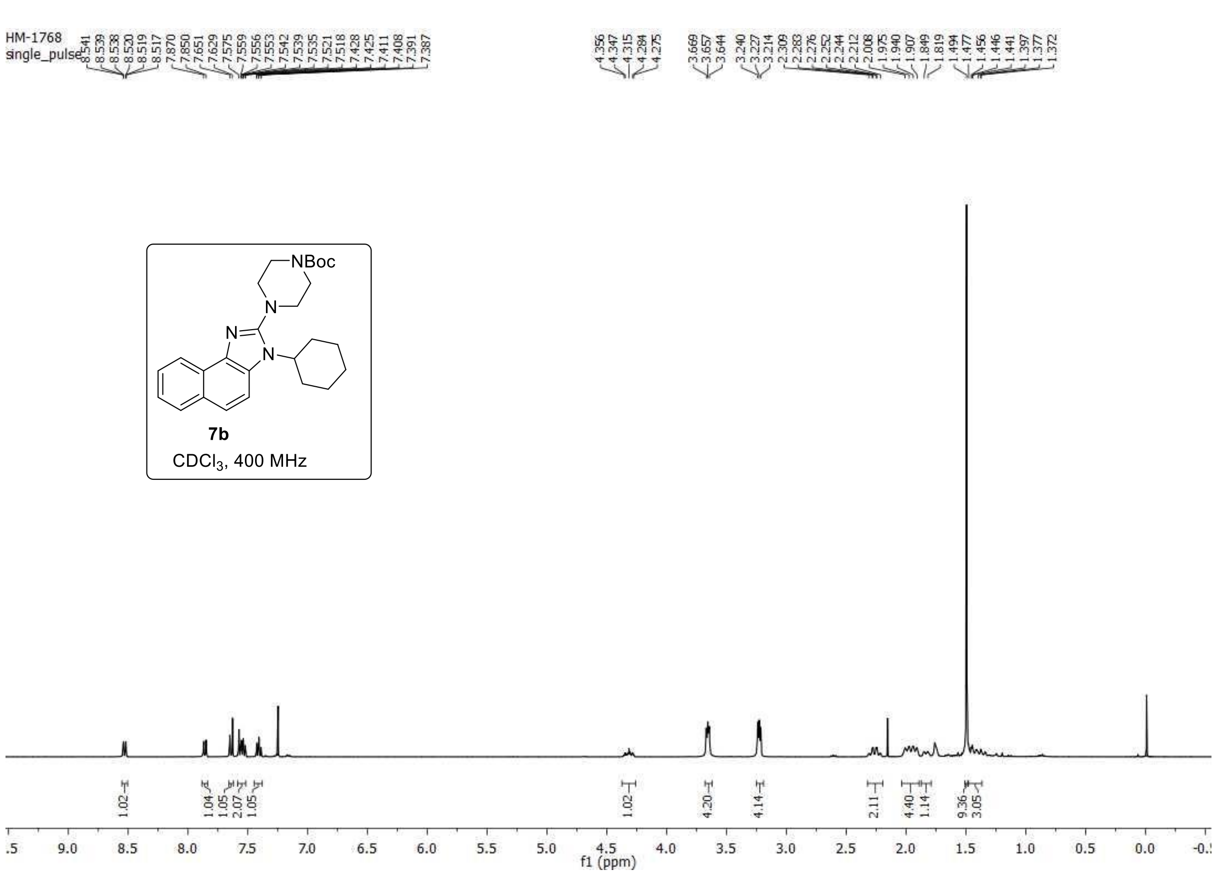

HM-1808
single pulse decoupled gated NOE
163.370
160.945
142.595
139.164
133.913
130.351
130.152
130.113
130.031
129.788
129.088
128.931
127.247
126.846
124.799
123.757
121.600
116.181
115.968
112.106
47.621
4af
DMSO-d6, 100 MHz
f1 (ppm)

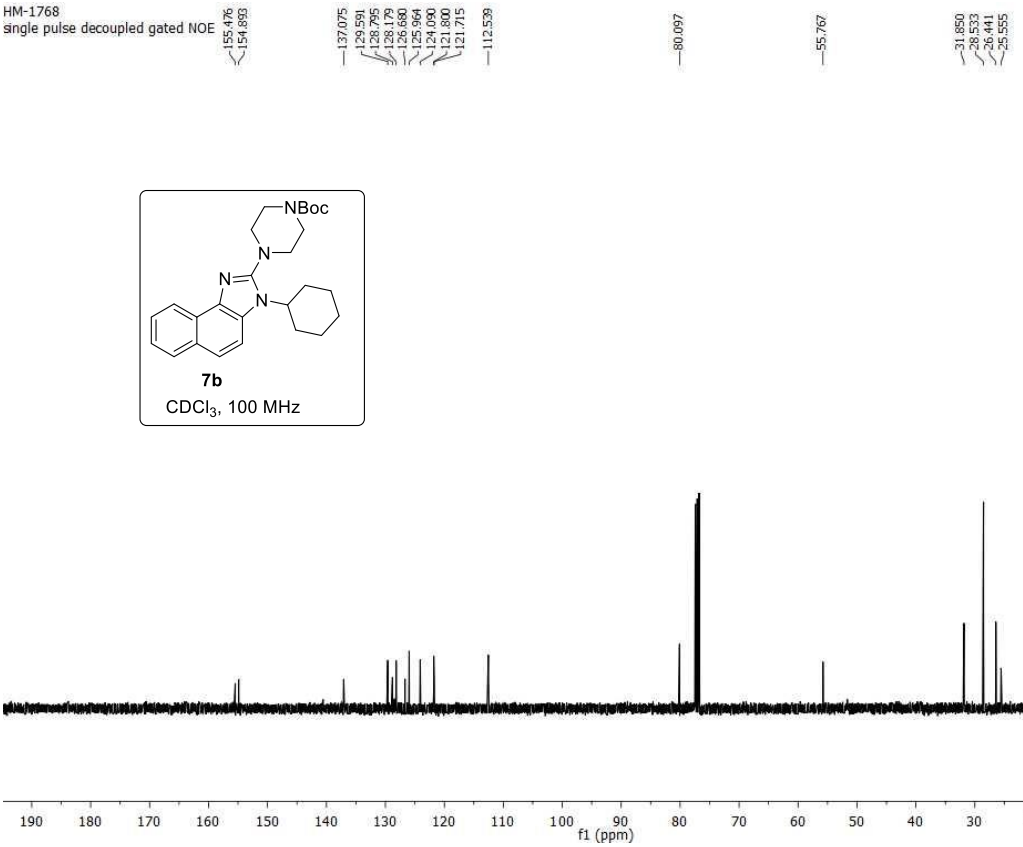

HM-1806
single_pulse
8.444
8.442
8.441
8.423
8.422
8.420
8.335
7.962
7.942
7.809
7.787
7.721
7.699
7.594
7.591
7.577
7.574
7.570
7.568
7.566
7.563
7.557
7.553
7.464
7.461
7.447
7.444
7.440
7.426
7.423
6.556
6.554
6.548
6.546
6.397
6.392
6.389
6.384
5.619
4ag
DMSO-d6, 400 MHz
0.98
0.90
1.06
1.02
0.99
1.93
1.17
0.92
0.93
1.97
f1 (ppm)

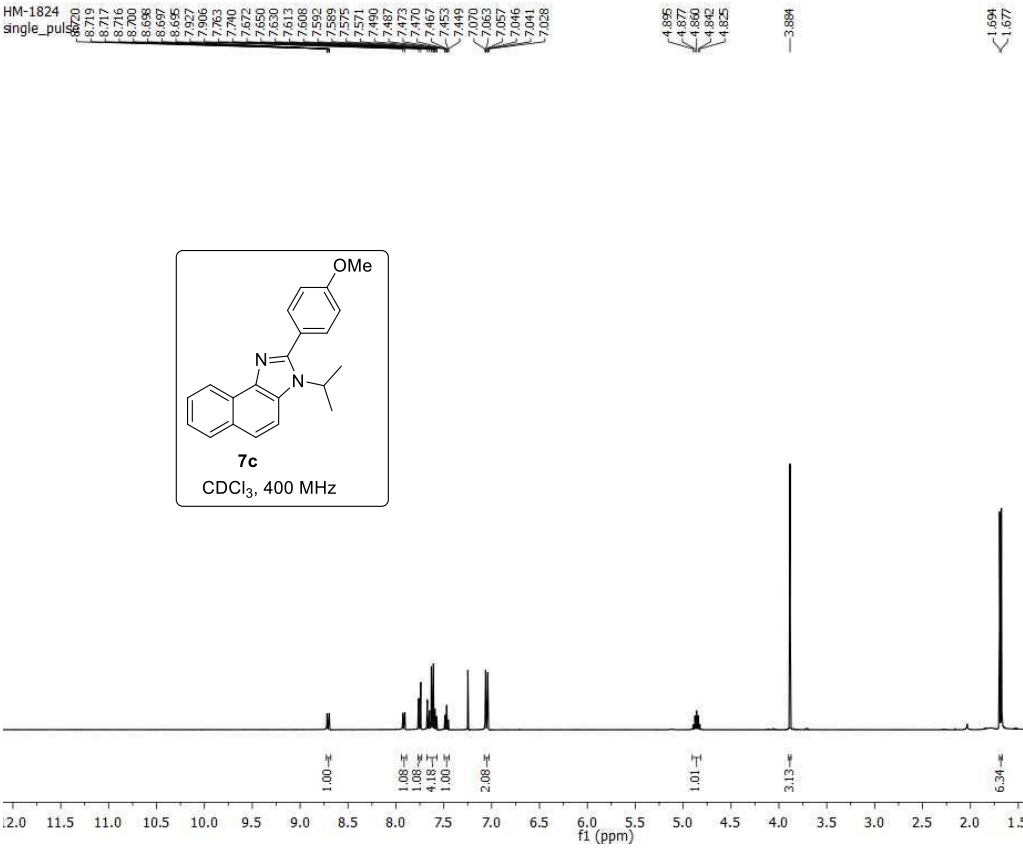

HM-1806
single pulse decoupled gated NOE
150.354
143.867
142.374
139.009
130.416
130.182
128.939
127.214
126.838
124.806
123.750
121.635
112.089
111.238
109.498
41.542
4ag
DMSO-d6, 400 MHz
f1 (ppm)

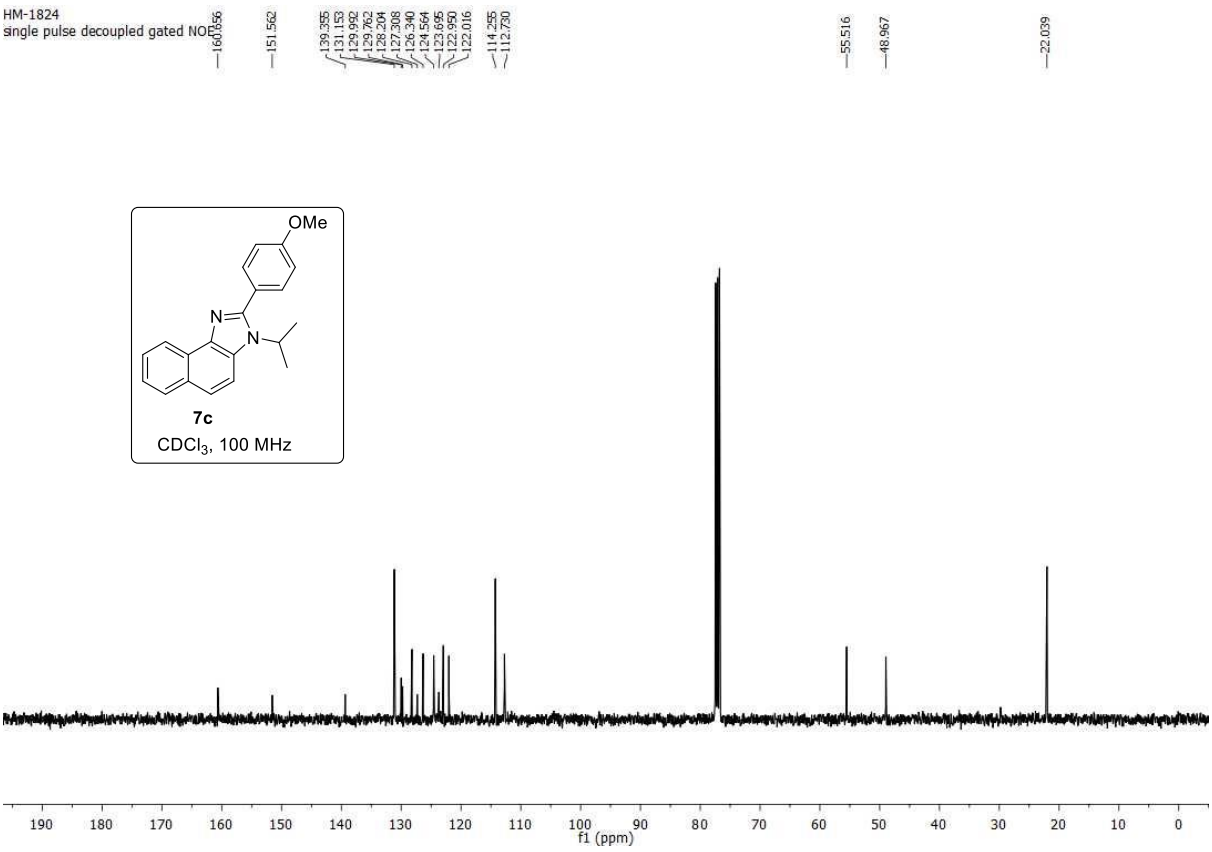

HM-1770
single_pulse
8.338
8.317
7.880
7.859
7.578
7.556
7.503
7.500
7.491
7.486
7.482
7.469
7.464
7.461
7.384
7.381
7.367
7.364
7.361
7.346
7.344
4.429
4.420
4.388
4.379
4.367
4.357
4.348
3.941
2.287
2.276
2.244
2.221
2.212
2.181
1.950
1.917
1.891
1.790
1.759
1.536
1.528
1.495
1.462
1.454
1.419
1.374
1.366
1.334
1.326
1.301
7a
CDCl3, 400 MHz
1.00
0.98
0.98
2.00
0.99
1.00
3.08
2.08
4.00
1.07
2.11
1.09
f1 (ppm)


HM-1770
single pulse decoupled gated NOE
154.159
129.647
129.399
126.124
124.664
123.430
122.915
121.564
120.891
120.151
110.448
53.571
31.030
30.614
26.179
25.514
7a
CDCl$_3$, 100 MHz
f1 (ppm)


HM-1768
single_pulse
8.541
8.539
8.538
8.520
8.519
8.517
7.870
7.850
7.651
7.629
7.575
7.559
7.556
7.553
7.542
7.539
7.535
7.521
7.518
7.428
7.425
7.411
7.408
7.391
7.387
4.356
4.347
4.315
4.284
4.275
3.669
3.657
3.644
3.240
3.227
3.214
2.309
2.283
2.276
2.252
2.244
2.212
2.008
1.975
1.940
1.907
1.849
1.819
1.494
1.477
1.456
1.446
1.441
1.397
1.377
1.372
NBoc
7b
CDCl$_3$, 400 MHz
1.02
1.04
1.05
2.07
1.05
1.02
4.20
4.14
2.11
4.40
1.14
9.36
3.05
f1 (ppm)


HM-1768
single pulse decoupled gated NOE
155.476
154.893
137.075
129.591
128.795
128.179
126.680
125.964
124.090
121.800
121.715
112.539
80.097
55.767
31.850
28.533
26.441
25.555
NBoc
N
N
N
7b
CDCl3, 100 MHz
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


HM-1824
single_pulse
8.720
8.719
8.717
8.716
8.700
8.698
8.697
8.695
7.927
7.906
7.763
7.740
7.672
7.650
7.630
7.613
7.608
7.592
7.589
7.575
7.571
7.490
7.487
7.473
7.470
7.467
7.453
7.449
7.070
7.063
7.057
7.046
7.041
7.028
4.895
4.877
4.860
4.842
4.825
3.894
1.694
1.677
OMe
N
N
7c
CDCl3, 400 MHz
1.00
1.08
1.08
4.18
1.00
2.08
1.01
3.13
6.34
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


HM-1824
single pulse decoupled gated NOE
160.656
151.562
139.355
131.153
129.992
129.762
128.204
127.308
126.340
124.564
123.695
122.950
122.016
114.255
112.730
55.516
48.967
22.039
OMe
N
N
7c
CDCl3, 100 MHz
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)