Supporting Information

Phosphine free Mn-complex catalysed dehydrogenative C-C and C-heteroatom bond formation: a sustainable approach to synthesize quinoxaline, pyrazine, benzothiazole and quinoline derivatives

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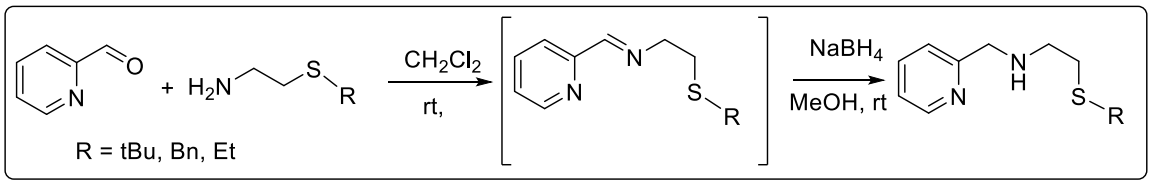
1. General Considerations:

Unless otherwise stated, all chemicals were purchased from common commercial sources and used as received. All solvents were dried by using standard protocol. The synthesis of catalyst was performed under argon atmosphere with freshly distilled dry THF. All catalytic reactions were carried out under argon atmosphere using dried glassware and standard syringe/septa techniques. DRX-400 Varian spectrometer and Bruker Avance III 600 and 400 spectrometers were used to record ^{1}H and ^{13}C NMR spectra using $CDCl_3$ and DMSO-d_6 as solvent and TMS as an internal standard. Chemical shifts (δ) are reported in ppm and spin-spin coupling constant (J) are expressed in Hz, and other data are reported as follows: s = singlet, d = doublet, dd = doublet of doublet, dt = doublet of triplet, t = triplet, m = multiplet, q = quartet, and br s = broad singlet. X-ray crystallographic data were collected using Agilent Super Nova (Single source at offset, Eos) diffractometer. FTIR were collected on PerkinElmer IR spectrometer. Q-Tof ESI-MS instrument (model HAB 273) was used for recording mass spectra. SRL silica gel (100-200 mesh) was used for column chromatography.

2. Synthesis and characterization of Ligands:



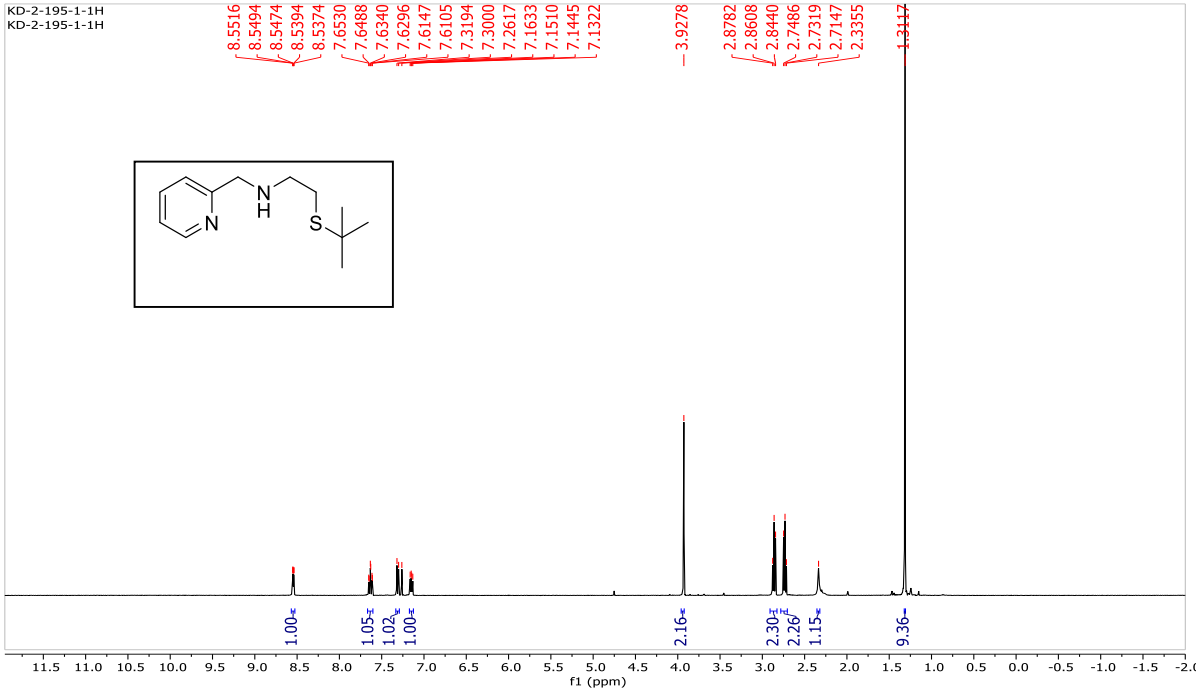
Pyridine-2-carboxaldehyde (15.76 mmol) and amino-thiol compound (15.0 mmol,) were dissolved in dry CH_2Cl_2 (35 mL) and then Na_2SO_4 (16.9 mmol) was added to it. The resulting suspension was stirred for 20 h at room temperature. Then, it was filtered and the filter residue was washed thoroughly with CH_2Cl_2 and the combined solvent was removed under reduced pressure. The residue obtained was directly used for the next step without further purification. The residue was dissolved in methanol (30 ml) and $NaBH_4$ (53.6 mmol) was added portion wise in stirring condition at 0 $^{\circ}$C and the stirring was continued for overnight at room temperature. Then the solvent was evaporated and 40 mL of water was added. After that, it was extracted by CH_2Cl_2 and the combined organic phase was dried over Na_2SO_4. Then the solvent was evaporated to get the crude product, which was purified further by silica gel column chromatography using 20-40 % ethyl acetate in hexane.

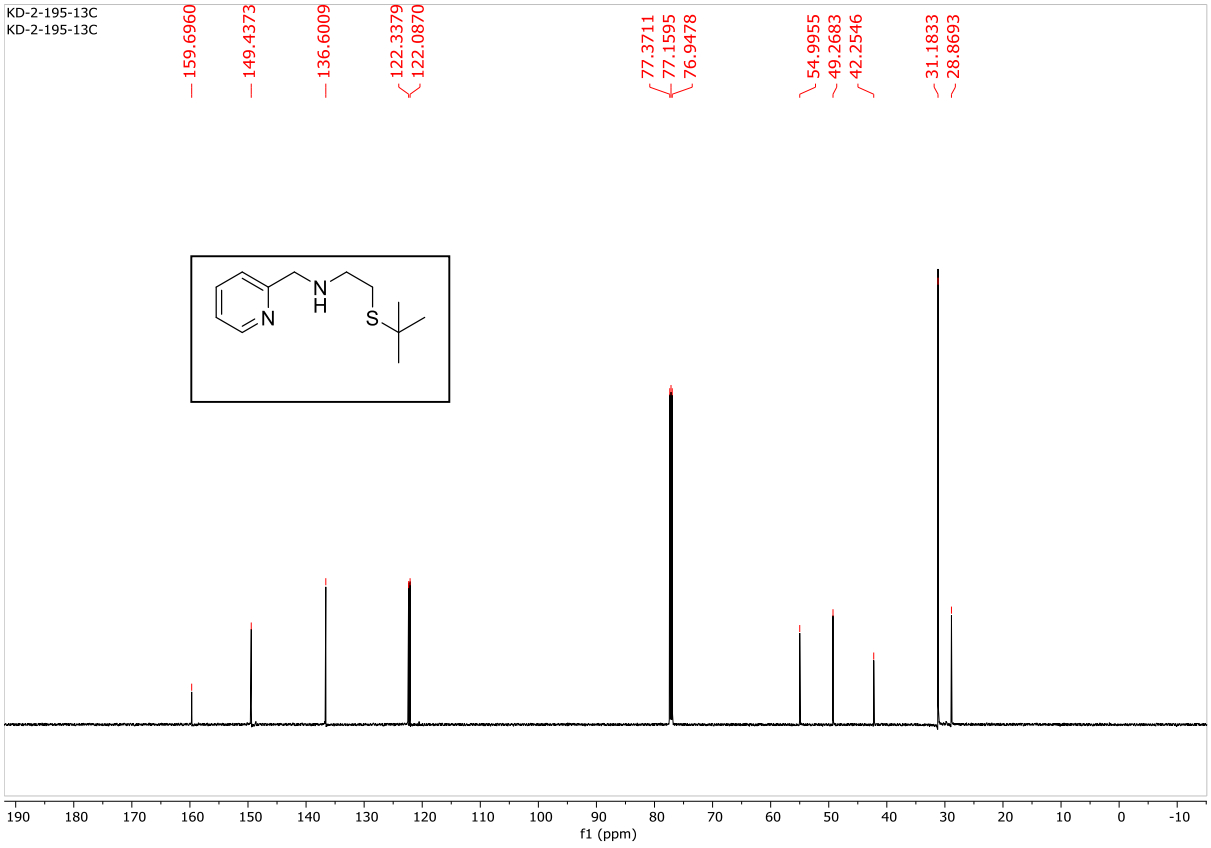
a) 2-(ethylthio)-N-(pyridin-2-ylmethyl)ethan-1-amine:[1] Brown oil (3.077 g, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (d, J = 2.76 Hz, 1H), 7.60 (dt, J = 5.1 Hz, J = 0.84 Hz, 1H), 7.28 (d, J = 5.2 Hz, 1H), 7.13 -7.11 (m, 1H), 3.90 (s, 2H), 2.83 (t, J = 4.4 Hz, 2H), 2.69 (t, J = 4.44 Hz, 2H), 2.49 (m, 2H), 2.35 (br s, 1H), 1.21 (t, J = 4.92 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.73, 149.37, 136.52, 122.25, 122.01, 54.96, 48.35, 31.96, 25.83, 14.90.

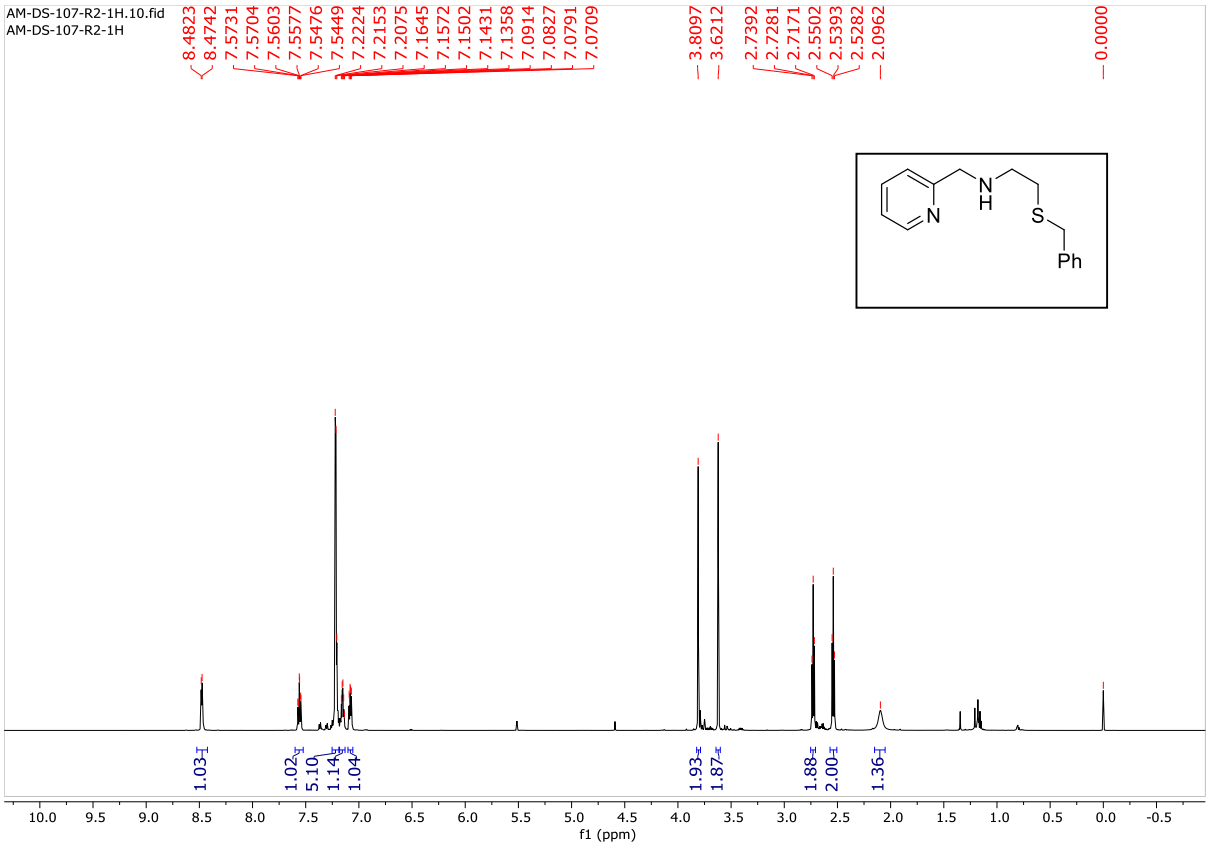
b) 2-(tert-butylthio)-N-(pyridin-2-ylmethyl)ethan-1-amine:[2] Brown oil (2.949 g, 88%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 - 8.53 (m, 1H), 7.63 (td, *J* = 7.6, 1.7 Hz, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.15 (dd, *J* = 7.5, 4.9 Hz, 1H), 3.93 (s, 2H), 2.86 (t, *J* = 6.8 Hz, 2H), 2.73 (t, *J* = 6.8 Hz, 2H), 2.34 (s, 1H), 1.31 (s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.70, 149.44, 136.60, 122.34, 122.09, 55.00, 49.27, 42.25, 31.18, 28.87.

c) 2-(benzylthio)-N-(pyridin-2-ylmethyl)ethan-1-amine:[3] Brown oil (1.388 g, 91%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (d, *J* = 4.8 Hz, 1H), 7.56 (td, *J* = 7.7, 1.6 Hz, 1H), 7.22 - 7.21

(m, 5H), 7.15 (dt, *J* = 8.6, 4.4 Hz, 1H), 7.08 (dd, *J* = 7.3, 5.1 Hz, 1H), 3.81 (s, 2H), 3.62 (s, 2H), 2.73 (t, *J* = 6.6 Hz, 2H), 2.54 (t, *J* = 6.6 Hz, 2H), 2.10 (s, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.70, 149.38, 138.39, 136.57, 128.91, 128.58, 127.07, 122.29, 122.05, 54.88, 47.86, 36.03, 31.58.



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7.2224
7.2153
7.2075
7.1645
7.1572
7.1502
7.1431
7.1358
7.0914
7.0827
7.0791
7.0709
3.8097
3.6212
2.7392
2.7281
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2.5502
2.5393
2.5282
2.0962
0.0000
N
H
N
S
Ph
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1.02
5.10
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1.04
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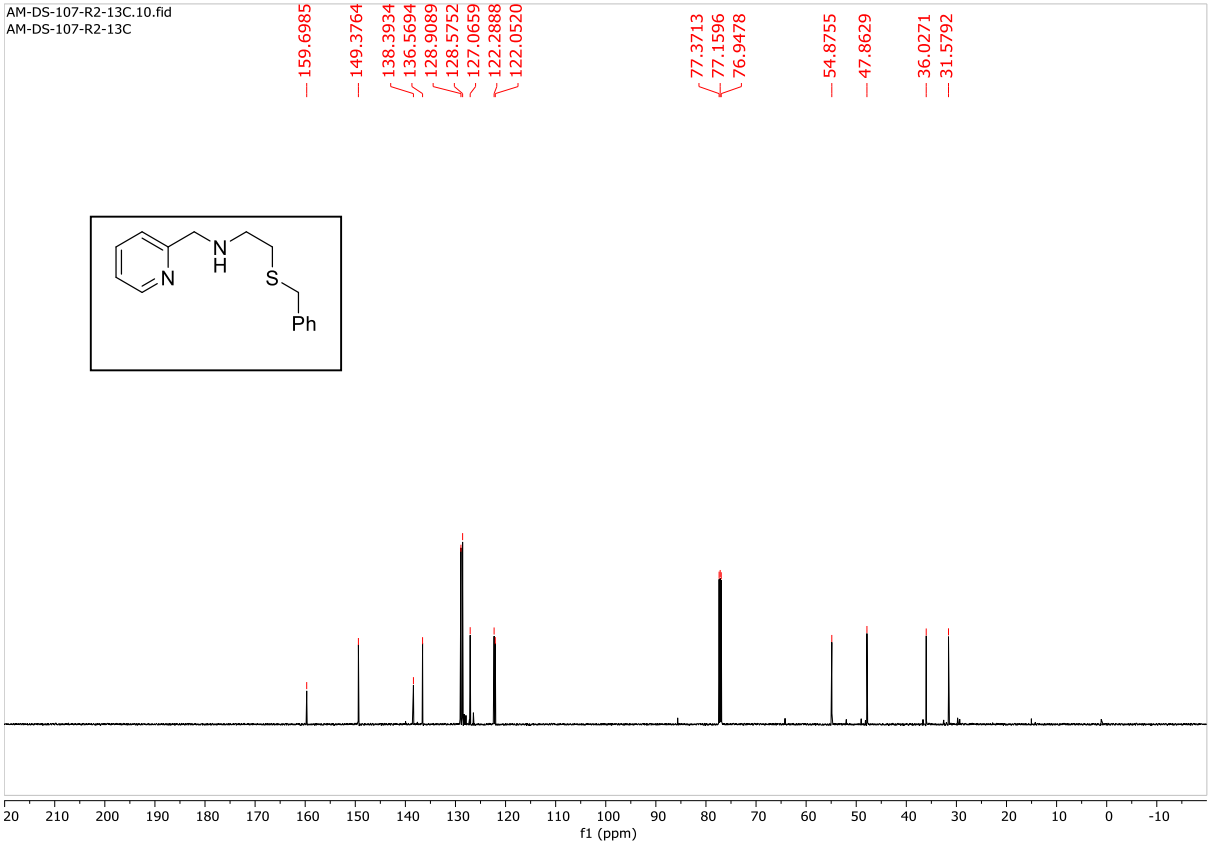
1.36
f1 (ppm)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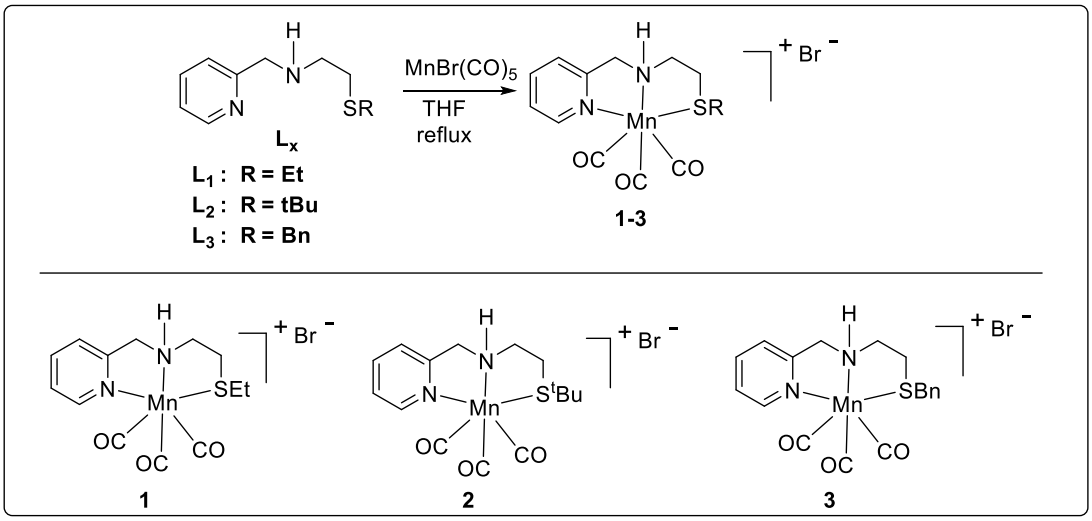
S
Ph
f1 (ppm)

3. Synthesis and characterization of NNS-Mn(I) complexes:



Ligand [($PyCH_2$)HN(CH_2CH_2SR), R= Et, *t*Bu, Bn] (5.0 mmol) was taken in 20 mL dry THF and was added dropwise to the orange-yellow suspension of [$MnBr(CO)_5$] (5.0 mmol) in 12 mL degassed dry THF. Then, the suspension was refluxed for overnight under argon atmosphere. After cooling it down to the room temperature, the solvent was evaporated to obtain the residue, which was further washed with hexane and dried under vacuum to get yellow solid of Mn-complex. The single crystal was grown by slow diffusion of toluene in the THF solution of the complex.

a) Complex-1:[4]

Yellow solid (1.980 g, 95%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.69 (br s, 1H), 8.26 (br s, 1H), 7.87 (br s, 1H), 7.71 (br s, 1H), 7.40 (br s, 1H), 4.81(br s, 1H), 4.58 (br s, 1H), 3.39-3.35 (m, 2H), 2.98-2.87 (m, 2H), 2.05 (br s, 2H), 1.45 (br s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 218.92, 216.57, 161.90, 152.64, 139.58, 125.25, 122.70, 60.41, 54.57, 33.07, 31.85, 13.42.

IR (cm^{-1}): 3059, 2920, 2875, 2030, 1946, 1920, 1609, 1462, 1286, 1196, 1083, 949, 910, 821, 769, 689, 637.

HRMS (ESI) calcd for $C_{13}H_{16}MnN_2O_3S$ $[M]^+$: 335.0262; found: 335.0263.

b) Complex-2:

Yellow solid (1.670 g, 92%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.65 (br s, 1H), 8.24 (br s, 1H), 7.81 (br s, 1H), 7.64 (br s, 1H), 7.20 (br s, 1H), 4.74-4.49 (m, 2H), 3.23 (br s, 2H), 2.81- 2.04 (m, 2H), 1.43 (br s, 9H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 219.85, 217.05, 161.94, 153.09, 139.44, 125.41, 122.59, 60.43, 55.94, 49.71, 30.73, 29.92.

IR (cm^{-1}): 3409, 3071, 2960, 2924, 2032, 1943, 1925, 1605, 1442, 1365, 1264, 1159, 1015, 766, 634, 533.

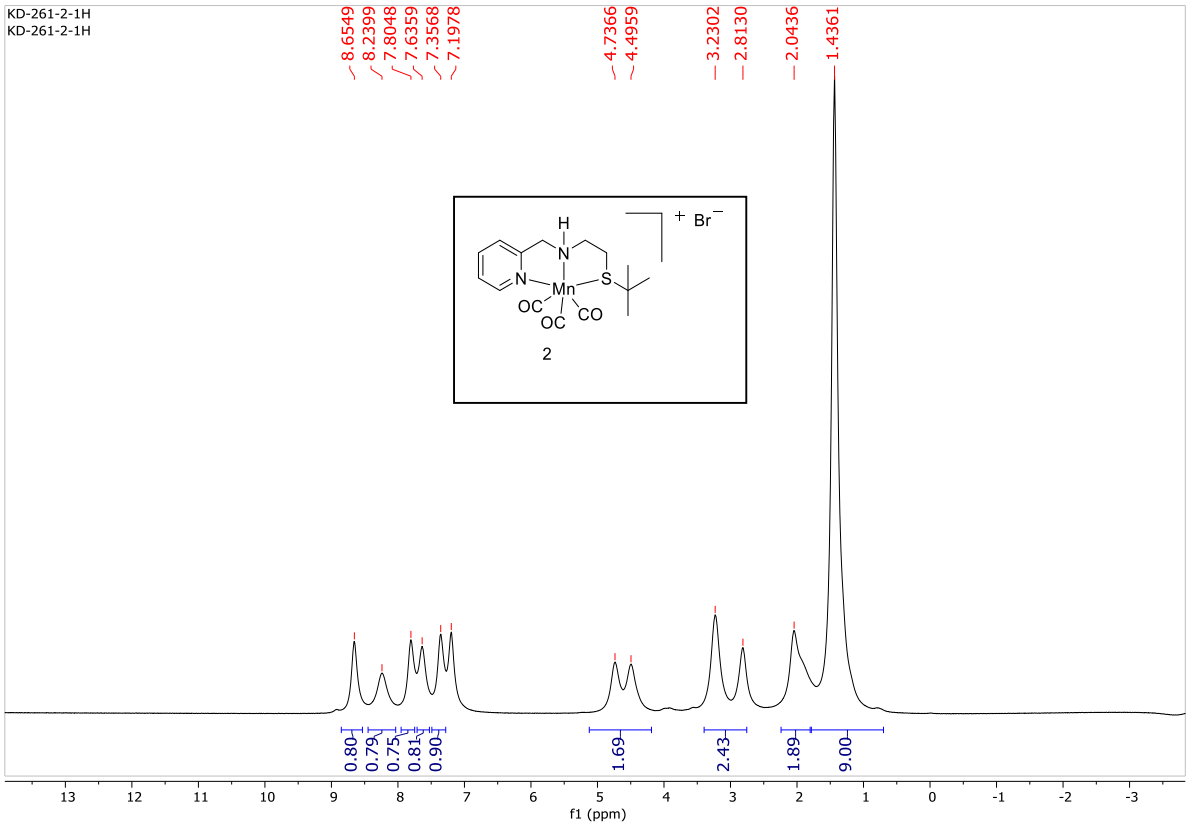
HRMS (ESI) calcd for $C_{15}H_{20}MnN_2O_3S$ $[M]^+$: 363.0575; found: 363.0579.

c) Complex-3:

Yellow solid 1.151 g, 89%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.29 (br s, 1H), 7.89 (br s, 1H), 7.51 (br s, 1H), 7.37 (br s, 1H), 6.98-6.92 (m, 6H), 4.42-4.26 (m, 2H), 3.72-3.67 (m, 2H), 3.06 (br s, 2H), 2.45 (br s, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 219.02, 218.62, 216.68, 162.06, 152.77, 139.52, 133.73, 129.40, 129.20, 128.78, 125.29, 122.69, 60.04, 53.89, 41.74, 32.12.

IR (cm^{-1}): 3420, 3072, 2914, 2033, 1926, 1631, 1422, 1291, 1073, 768, 704, 685, 633, 532.

HRMS (ESI) calcd for $C_{18}H_{18}MnN_2O_3S$ $[M]^+$: 397.0419; found: 397.0413.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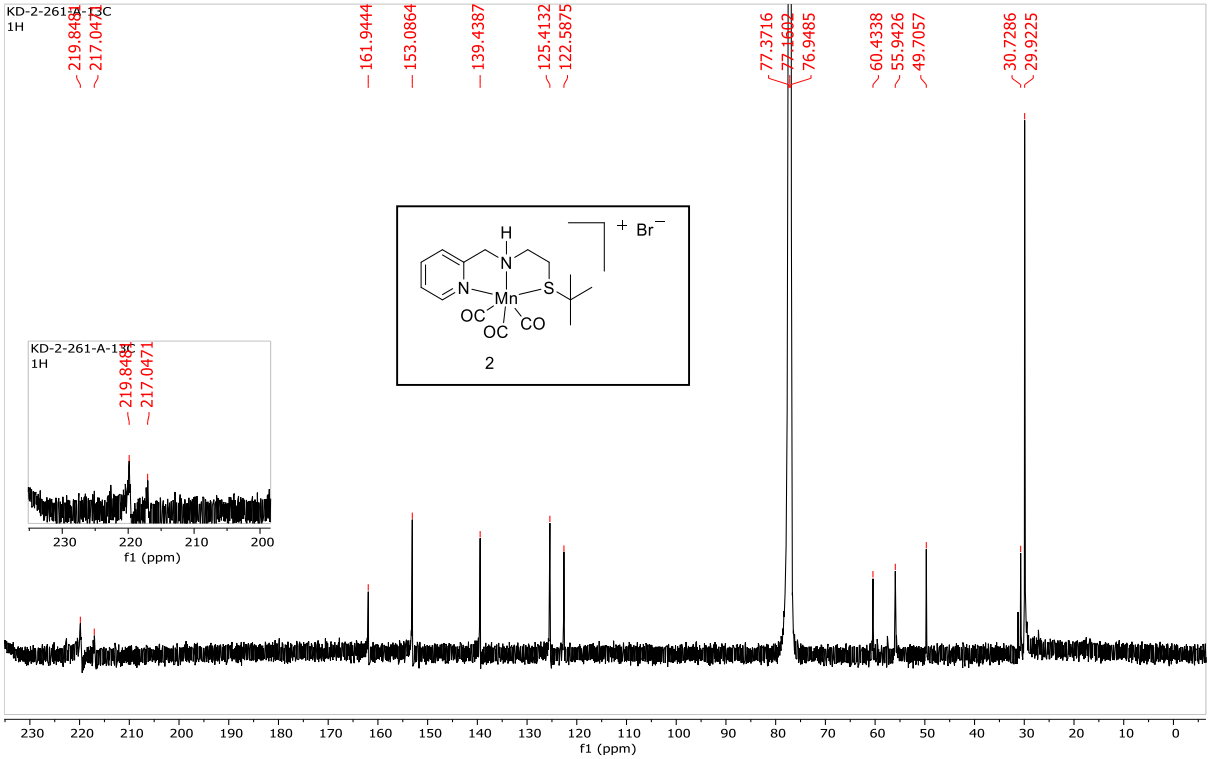
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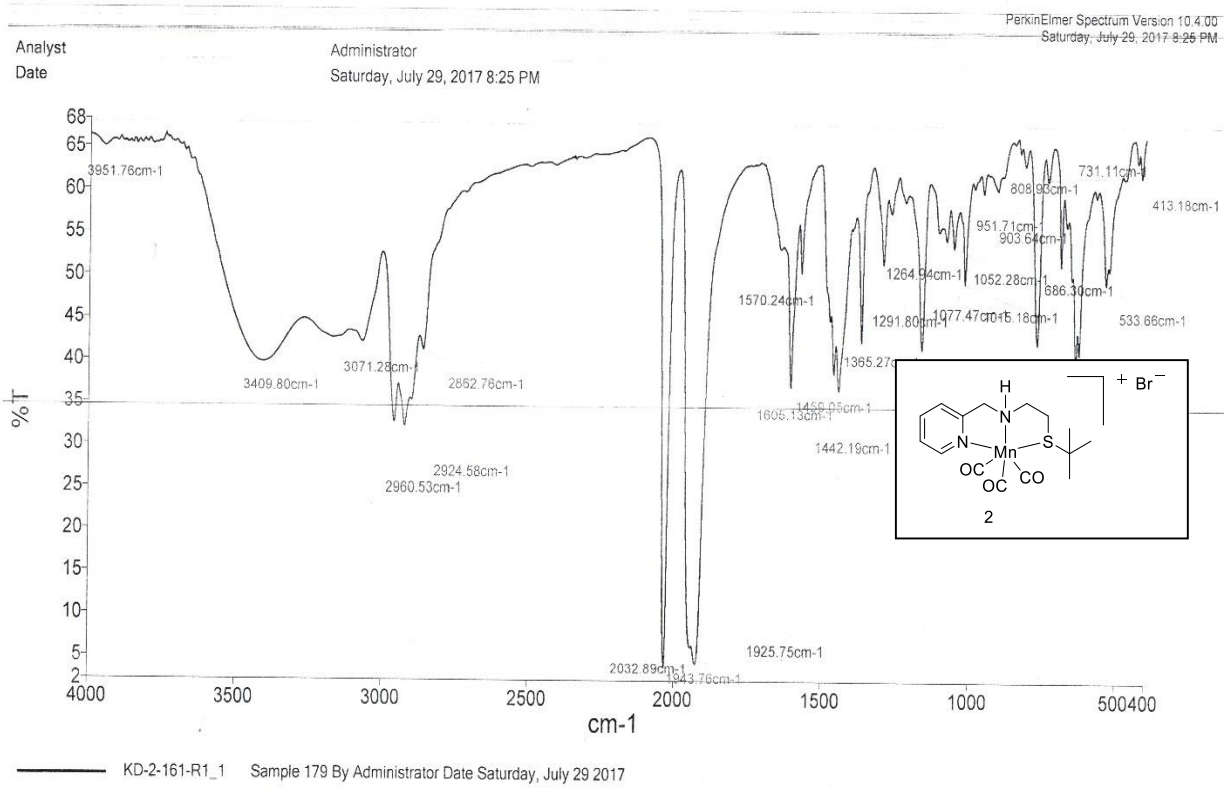
219.8486
217.0471
f1 (ppm)
f1 (ppm)
2


PerkinElmer Spectrum Version 10.4.00
Saturday, July 29, 2017 8:25 PM
Analyst
Date
Administrator
Saturday, July 29, 2017 8:25 PM
%T
cm-1
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3409.80cm-1
3071.28cm-1
2862.76cm-1
2924.58cm-1
2960.53cm-1
2032.89cm-1
1925.75cm-1
1570.24cm-1
1605.13cm-1
1459.05cm-1
1442.19cm-1
1365.27cm-1
1291.80cm-1
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808.93cm-1
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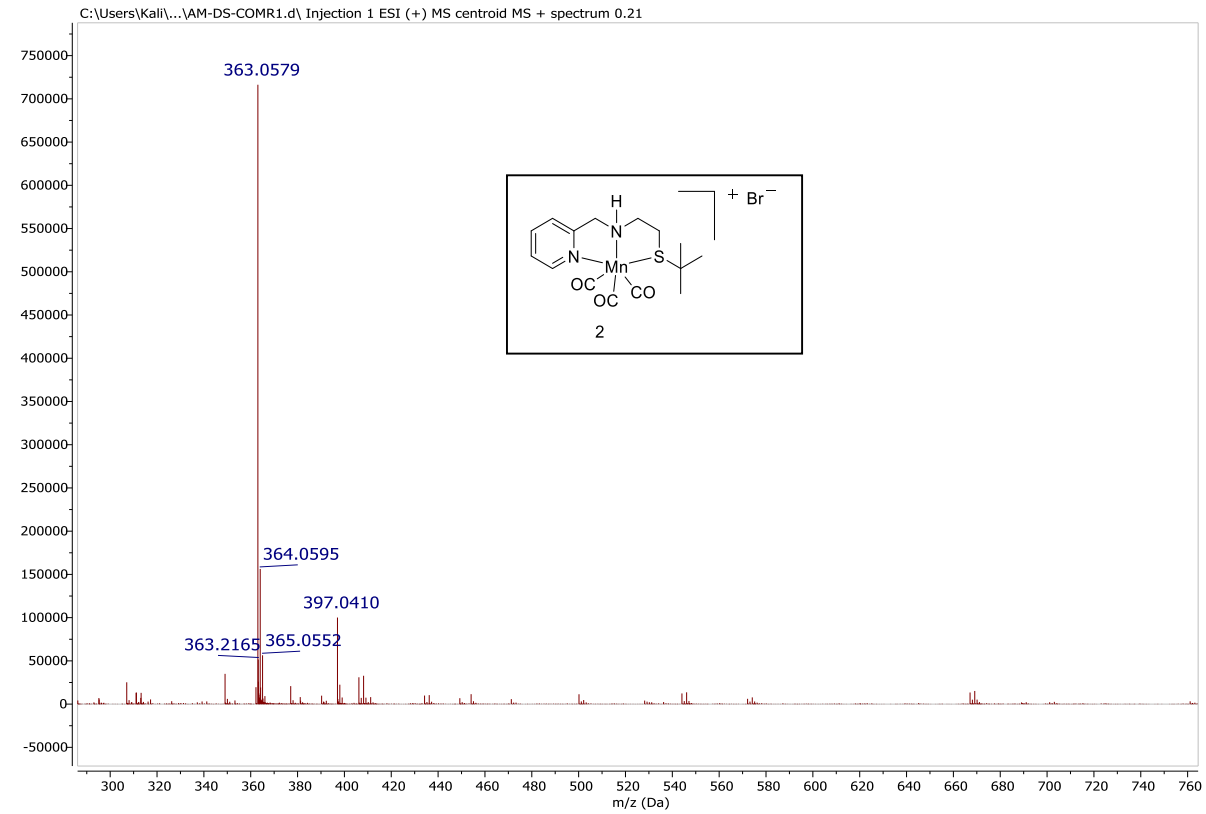
+ Br−
2
KD-2-161-R1_1 Sample 179 By Administrator Date Saturday, July 29 2017


C:\Users\Kali\...\AM-DS-COMR1.d\ Injection 1 ESI (+) MS centroid MS + spectrum 0.21
363.0579
364.0595
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363.2165
365.0552
m/z (Da)
+ Br−
2

Crystal Structure of Complex-3:

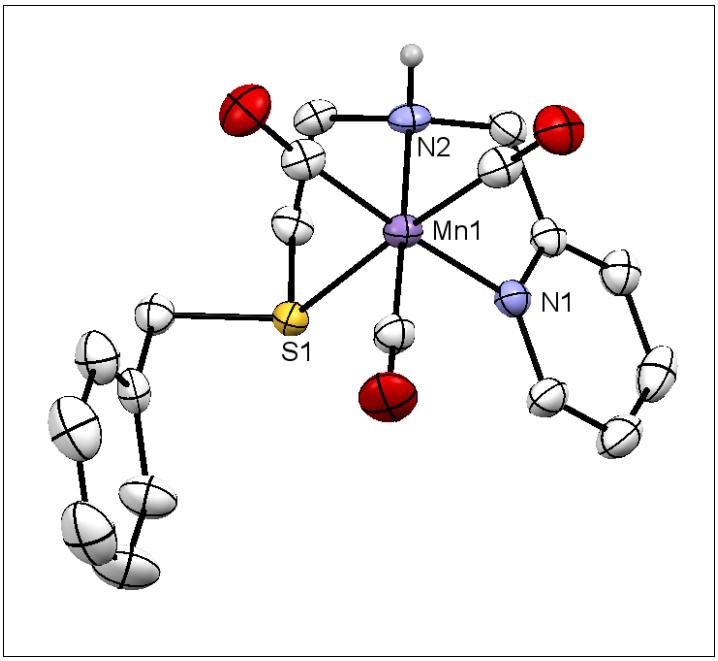


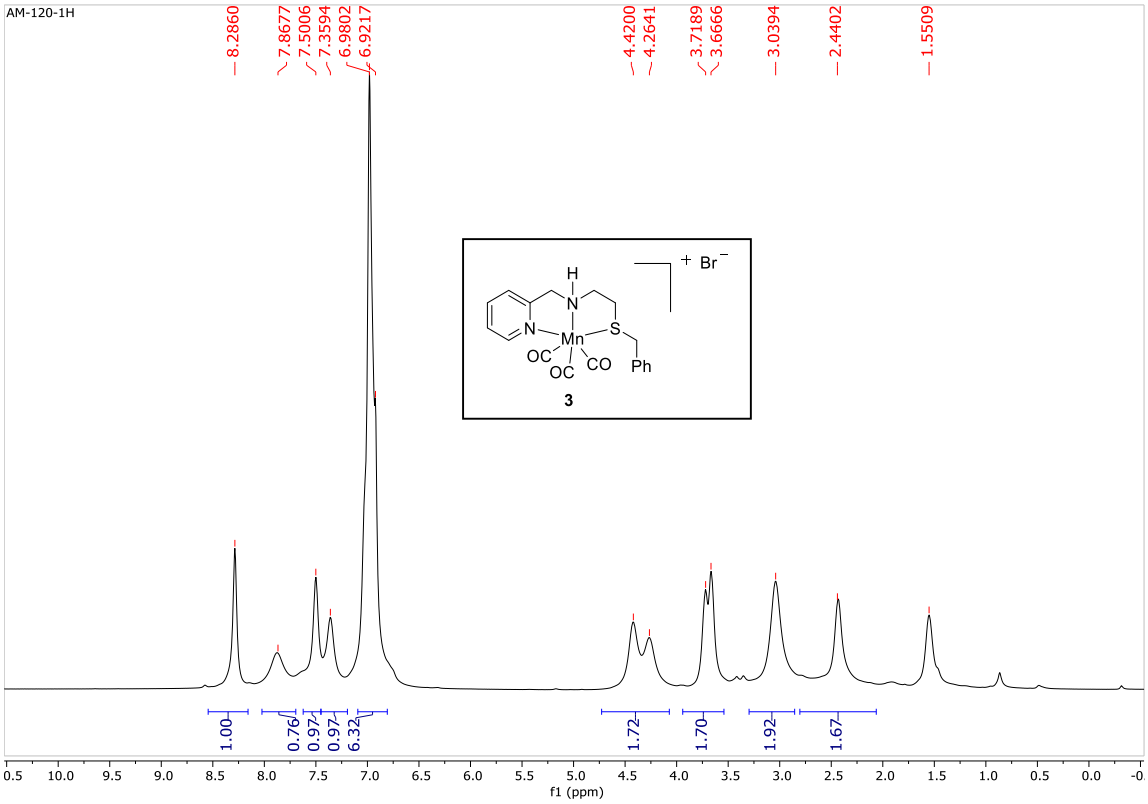
Table of Cat_3

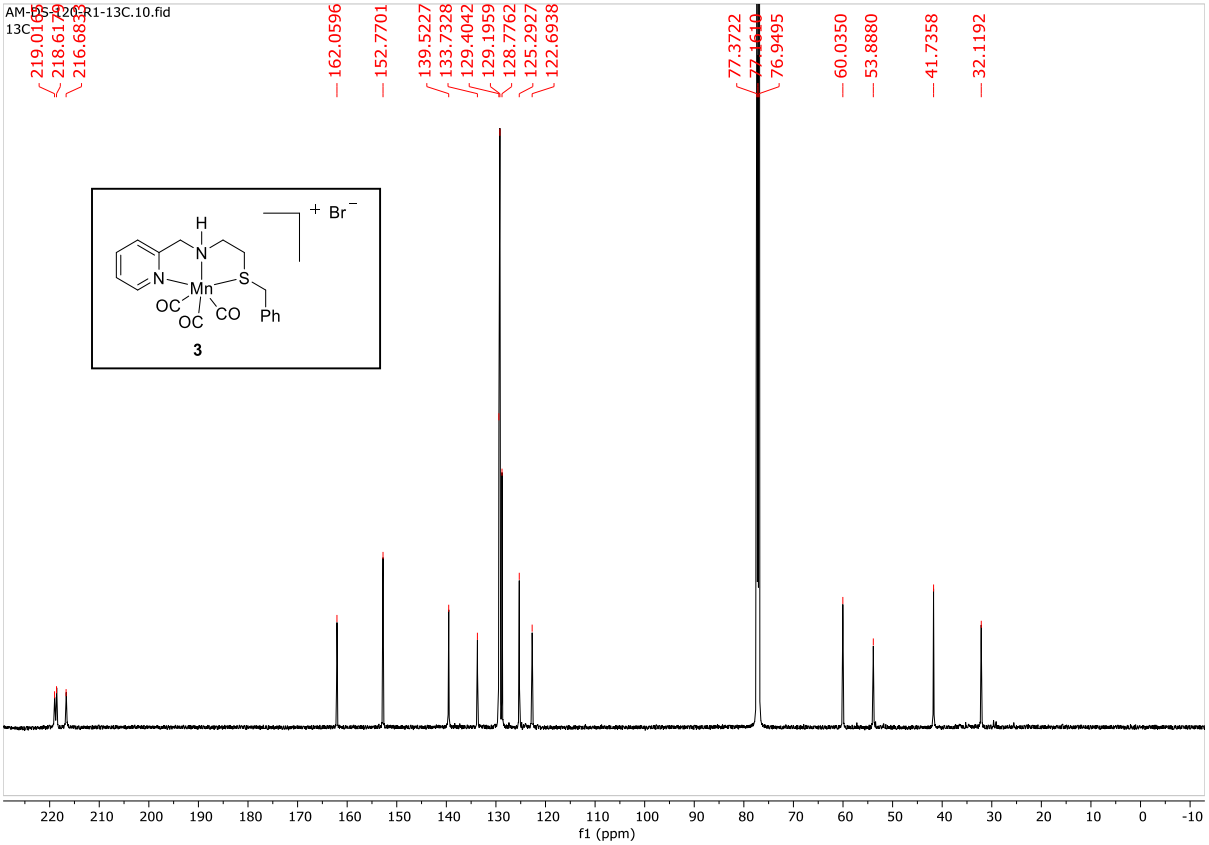
Empirical formula	C18 H18 Br Mn N2 O3 S
Formula weight	477.25
Temperature, T	293 K
Crystal system	orthorhombic
Space group	'P b c a'
Unit cell dimensions	a=16.5242(15) Å α=90° b=9.5030(8) Å β=90° c=26.035(3) Å γ=90°
Volume, V (Å^3)	4088.2(7)
Z	8
Density (calculated), Mg·m^{-3}	1.551
Absorption coefficient, μ (mm^{-1})	2.721
F(000)	1920.0
Crystal size, mm^3	0.34 × 0.31 × 0.29
Theta range for data collection	2.92to 25.00
Index ranges	-19 ≤ h ≤ 14, -11 ≤ k ≤ 10, -25 ≤ l ≤ 30
Reflections collected	2262
Independent reflections	3597
Completeness to theta	0.999
Absorption correction	Multi-scan
Max. and min. transmission	1.00000 and 0.57204
Refinement method	'SHELXL-97(Sheldrick, 1997)'
Data / restraints / parameters	3597 /0/235

Goodness-of-fit on F^2	0.956
Final R indices [I>2sigma(I)]	R1 = 0.0448(2444), wR=2 0.1531(3597)
R indices (all data)	R1 = 0.0816, wR=2 0.1273
Extinction coefficient	2.721
Largest diff. peak and hole	0.473 and -0.530 e·$Å^{-3}$

Selected Bond length and bond angles

Bond lengths [Å]	**Bond angles [°]**
Mn1-N1 2.058(4)	N1 Mn1 S1 81.01(12)
Mn1-N2 2.081(4)	N2 Mn1 S1 84.23(12)
Mn1- S1 2.3617(15)	N1 Mn1 N2 80.65(18)
Mn1- C16 1.811(6)	C16 Mn1 S1 173.8(2)
Mn1-C17 1.806(6)	C17 Mn1 S1 92.61(19)
Mn1-C18 1.807(6)	C18 Mn1 S1 96.81(18)

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76.9495
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N
Mn
S
OC
OC
CO
Ph
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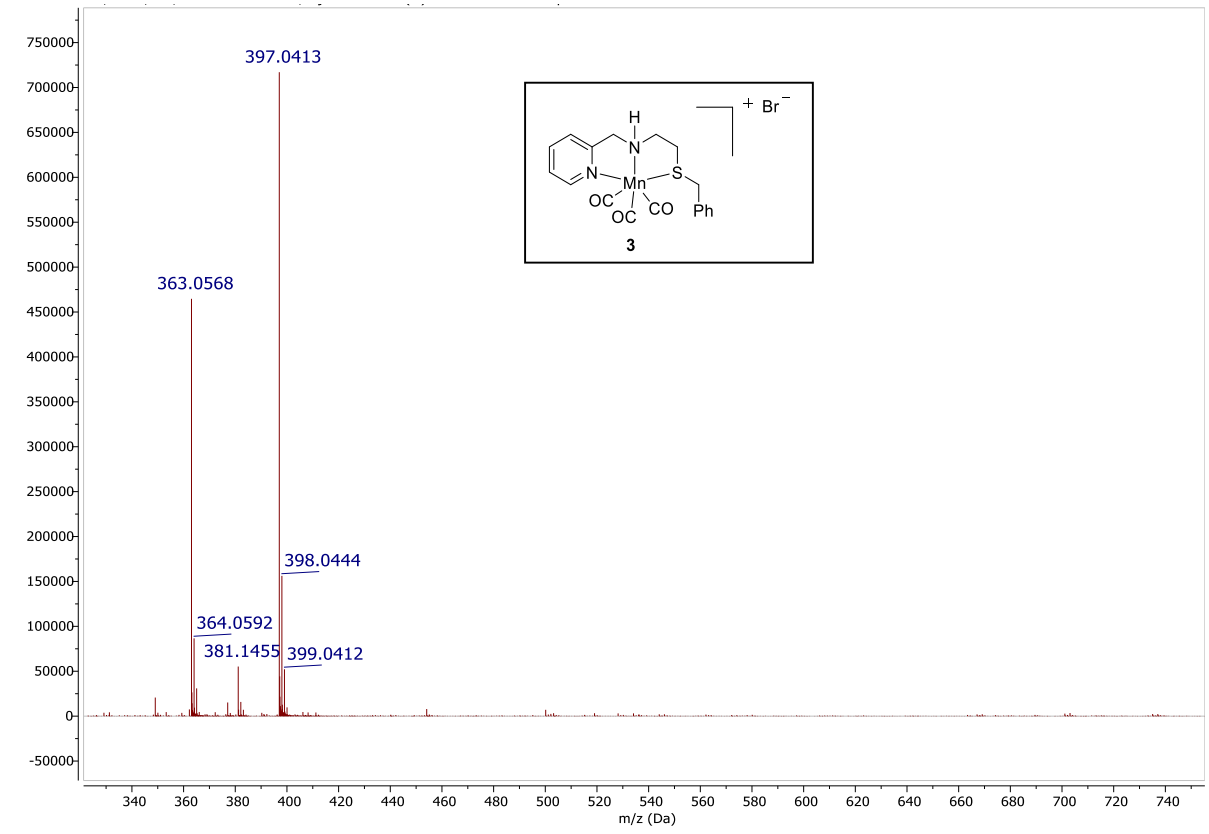
f1 (ppm)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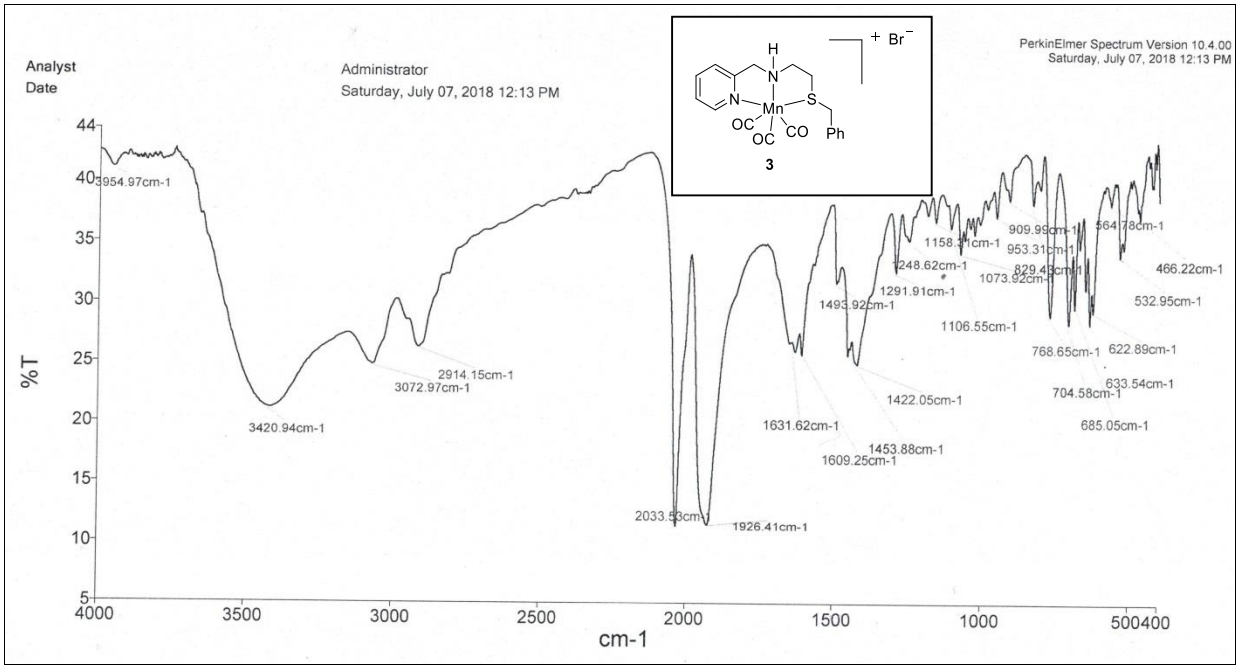
m/z (Da)



4. General experimental procedure for the synthesis of quinoxalines:

A mixture of 1,2-diaminobenzene (1.0 mmol), 1,2-diol (1.27 mmol) and KOH (0.27 mmol) was stirred under neat condition at 140 °C in an open system under argon in the presence of 4 mol % catalyst **2**. After the specified time, the reaction mixture was cooled to room temperature and chloroform was added to dilute the mixture. Then it was filtered through celite and filtrate was concentrated under reduced pressure. The crude residue was purified further by silica gel column chromatography using 2% -5 % ethyl acetate in hexane as an eluent.

5. General experimental procedure for the synthesis of benzothiazoles:

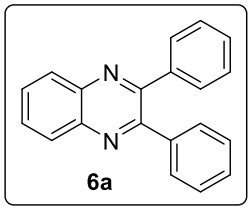
A mixture of 2-Aminothiophenol (1.0 mmol), primary alcohol (1.27 mmol), KOH (0.27 mmol) and complex **2** (0.04 mmol) was stirred at 140 °C for the specified time under neat condition in an open system under argon. Then the reaction mixture was cooled to room temperature and was diluted with chloroform. Then it was filtered through celite and the filtrate was concentrated under vacuum. Then silica gel column chromatography was performed to obtain the pure product.

6. General experimental procedure for the synthesis of quinolines:

A mixture of 2-amino benzyl alcohol (1.0 mmol), secondary alcohol (1.27 mmol), *t*BuOK (1.2 mmol) and catalyst **2** (0.05 mmol) was stirred under neat condition at 140 °C for 36 h in an open system under argon. After cooling to room temperature, chloroform was added and filtered through celite. The filtrate was concentrated to get the crude residue, which was purified further by column chromatography using silica gel as stationary phase and 2%-5% ethyl acetate in hexane as an eluent.

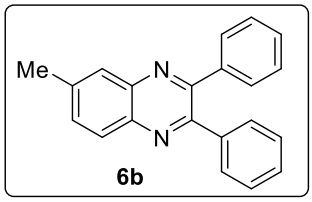
7. Spectroscopic characterization of the quinoxaline, benzothiazole and quinoline derivatives:

2,3-diphenylquinoxaline (6a)[5]



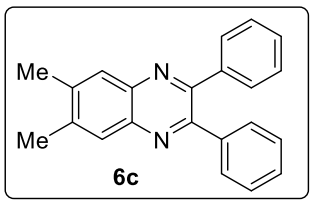
White solid (203 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21- 8.17 (m, 2H), 7.80 - 7.75 (m, 2H), 7.54-7.52 (m, 4H), 7.39 - 7.31 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.61, 141.37, 139.21, 130.09, 129.97, 129.34, 128.94, 128.41.

6-methyl-2,3-diphenylquinoxaline (6b)[5]



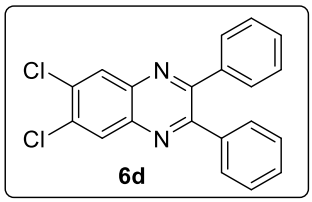
White solid (225 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.5 Hz, 1H), 7.96 (s, 1H), 7.60 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.55 - 7.48 (m, 4H), 7.39 - 7.29 (m, 6H), 2.62 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.45, 152.70, 141.42, 140.61, 139.83, 139.35, 132.42, 129.96, 129.95, 128.83, 128.81, 128.74, 128.35, 128.15, 22.04.

6,7-dimethyl-2,3-diphenylquinoxaline (6c)[5]



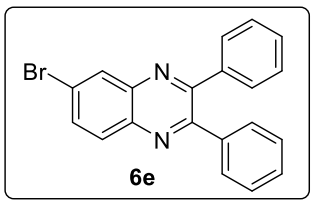
White solid (252 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 2H), 7.50 (dd, *J* = 7.5, 2.1 Hz, 4H), 7.35 - 7.29 (m, 6H), 2.52 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.61, 140.63, 140.34, 139.51, 129.96, 128.63, 128.33, 128.30, 20.55.

6,7-dichloro-2,3-diphenylquinoxaline (6d)[6]



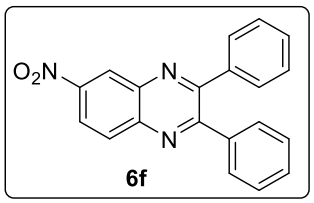
Brown solid (299 mg, 77%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.20 (s, 2H), 7.43 - 7.41 (m, 4H), 7.32 - 7.30 (m, 2H), 7.27-7.25 (m, *J* = 7.6 Hz, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.59, 140.04, 138.47, 134.54, 129.91, 129.89, 129.42, 128.48.

6-bromo-2,3-diphenylquinoxaline(6e)[7]



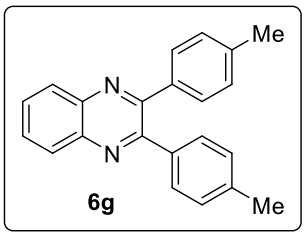
White solid (287 mg, 74%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.36 (d, *J* = 2.1 Hz, 1H), 8.03 (d, *J* = 8.9 Hz, 1H), 7.83 (dd, *J* = 8.9, 2.0 Hz, 1H), 7.51 (d, *J* = 7.2 Hz, 4H), 7.40-7.37 (m, 2H), 7.35-7.33 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.31, 153.82, 141.82, 140.01, 138.77, 138.67, 133.58, 131.53, 130.58, 129.93, 129.86, 129.22, 129.15, 128.43, 128.41, 123.93.

6-nitro-2,3-diphenylquinoxaline (6f)[5]



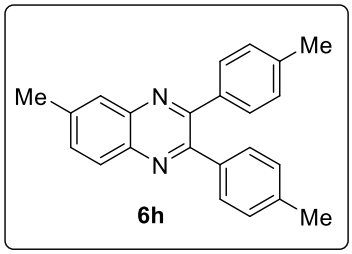
Yellow solid (191 mg, 58%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.07 (d, *J* = 2.4 Hz, 1H), 8.58-8.47(m, 1H), 8.29 (d, *J* = 9.1 Hz, 1H), 7.59 - 7.52 (m, 4H), 7.49-7.41 (m, 2H), 7.37 (t, *J* = 7.5 Hz, 4H). ^{13}C NMR (150, MHz, $CDCl_3$) δ 154.31, 153.82, 141.82, 140.01, 138.77, 138.67, 133.58, 131.53, 130.58, 129.93, 129.86, 129.22, 129.15, 128.43, 128.41, 123.92.

2,3-di-p-tolylquinoxaline (6g)[5]



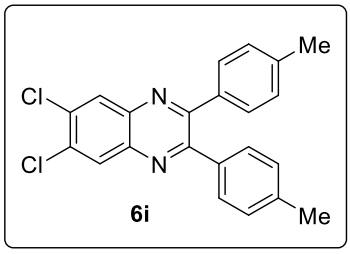
White solid (245 mg, 79%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 6.4, 3.4 Hz, 2H), 7.33 (dd, *J* = 6.4, 3.4 Hz, 2H) 7.45 (d, *J* = 8.0 Hz, 4H), 7.16 (d, *J* = 7.9 Hz, 4H), 2.37 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.51, 141.18, 138.78, 136.41, 129.78, 129.72, 129.15, 129.04, 21.43.

6-methyl-2,3-di-p-tolylquinoxaline (6h)[5]



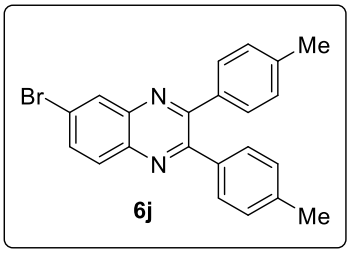
White solid (266 mg, 82%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (d, *J* = 8.5 Hz, 1H), 7.93 (s, 1H), 7.56 (d, *J* = 8.5 Hz, 1H), 7.47 - 7.41 (m, 4H), 7.14 (d, *J* = 8.1 Hz, 4H), 2.60 (s, 3H), 2.37 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 153.34, 152.61, 141.22, 140.15, 139.63, 138.62, 138.54, 136.53, 132.02, 129.77, 129.74, 128.98, 128.64, 127.98, 21.94, 21.40.

6,7-dichloro-2,3-di-p-tolylquinoxaline (6i):



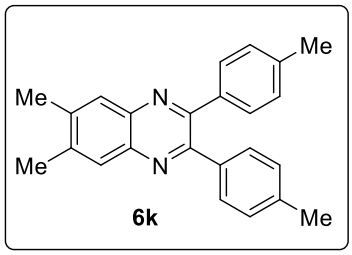
White solid (299 mg, 77%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 (s, 2H), 7.41 (d, *J* = 8.2 Hz, 4H), 7.15 (d, *J* = 8.0 Hz, 4H), 2.38 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.50, 139.87, 139.42, 135.70, 134.03, 129.76, 129.72, 129.12, 21.48. HRMS (ESI) calcd for $C_{22}H_{16}Cl_2N_2$ $[M+H]^+$:379.0769; found: 379.0770.

6-bromo-2,3-di-p-tolylquinoxaline (6j)[8]



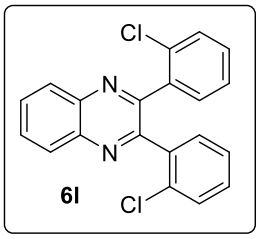
White solid (287 mg, 74%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.33 (d, *J* = 2.1 Hz, 1H), 8.00 (d, *J* = 8.9 Hz, 1H), 7.79 (dd, *J* = 8.9, 1.9 Hz, 1H), 7.43 (d, *J* = 8.1 Hz, 4H), 7.15 (d, *J* = 8.0 Hz, 4H), 2.37 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.28, 153.81, 141.73, 139.90, 139.22, 139.13, 136.07, 135.97, 133.22, 131.42, 130.48, 129.81, 129.74, 129.12, 129.10, 123.53, 21.48.

6,7-dimethyl-2,3-di-p-tolylquinoxaline (6k)[5]



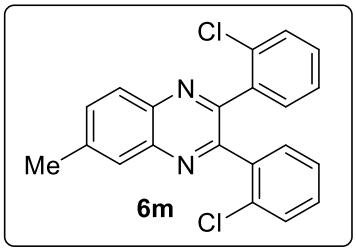
White solid (287 mg, 85%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.90 (s, 2H), 7.42 (d, *J* = 8.0 Hz, 4H), 7.13 (d, *J* = 8.0 Hz, 4H), 2.49 (s, 6H), 2.36 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 152.51, 140.17, 140.12, 138.40, 136.66, 129.75, 128.92, 128.14, 21.38, 20.44.

2,3-bis(2-chlorophenyl)quinoxaline (6l)[9]



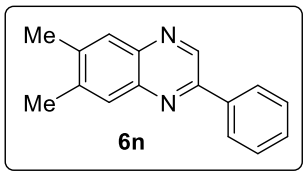
White solid (253 mg, 72%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.15 (dd, *J* = 6.4, 3.4 Hz, 2H), 7.76 (dd, *J* = 6.0, 3.2 Hz, 2H), 7.37 (s, 2H), 7.22 (d, *J* = 7.8 Hz, 2H), 7.18-7.13 (m, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 152.73, 141.29, 137.27, 131.30, 130.70, 130.23, 129.63, 129.47, 126.50. HRMS (ESI) calcd for $C_{20}H_{12}Cl_2N_2$ $[M+H]^+$: 351.0456; found: 351.0457.

2,3-bis(2-chlorophenyl)-6-methylquinoxaline (6m)



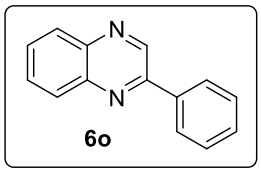
White solid (284 mg, 78%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.6 Hz, 1H), 8.00 (s, 1H), 7.67 (d, *J* = 8.5 Hz, 1H), 7.44 (s, 2H), 7.30 (d, *J* = 7.5 Hz, 2H), 7.24-7.19 (m, 4H), 2.62 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 152.53, 151.73, 141.34, 141.33, 139.76, 137.39, 137.37, 133.00, 131.29, 131.25, 130.09, 130.07, 129.57, 128.93, 128.22, 126.44, 126.42, 22.05.
HRMS (ESI) calcd for $C_{21}H_{14}Cl_2N_2$ $[M+H]^+$:: 365.0612; found: 365.0613

6,7-dimethyl-2-phenylquinoxaline (6n)[10]



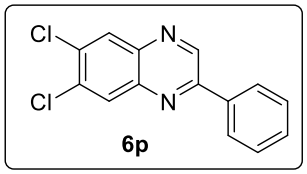
Yellow solid (182 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.15 (d, *J* = 7.0 Hz, 2H), 7.88 (s, 1H), 7.83 (s, 1H) 7.56 - 7.47 (m, 3H), 2.48 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.08, 142.46, 141.32, 140.89, 140.62, 140.21, 137.21, 129.92, 129.16, 128.74, 128.22, 127.47, 20.46, 20.43.

2-phenylquinoxaline (6o)[10]



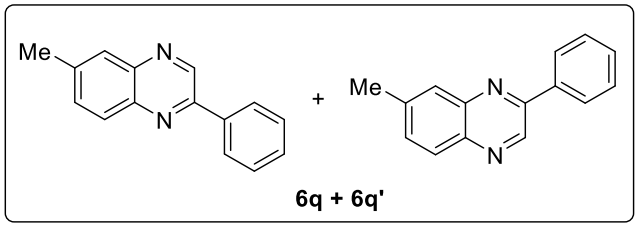
White solid (136 mg, 66%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.20 - 8.11 (m, 4H), 7.80 - 7.73 (m, 2H), 7.59 - 7.51 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.99, 143.50, 142.44, 141.72, 136.92, 130.42, 130.32, 129.76, 129.67, 129.29, 129.26, 127.69.

6,7-dichloro-2-phenylquinoxaline (6p)[10]



Pale yellow solid (176 mg, 64%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.27 (s, 1H), 8.23 (s, 1H), 8.18 (dd, *J* = 7.8, 1.7 Hz, 2H), 7.61 - 7.52 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.66, 144.29, 141.12, 140.28, 136.00, 134.95, 134.03, 130.79, 130.20, 129.79, 129.29, 127.59.

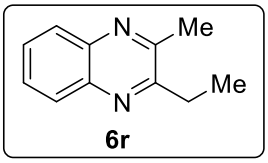
6-methyl-2-phenylquinoxaline & 7-methyl-2-phenylquinoxaline (6q : 6q′= 45: 55)[10]



6q + 6q'

Brown solid (161 mg, 74%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.28 (s, 1H), 9.26 (s, 1H), 8.18 (dd, *J* = 7.0, 4.1 Hz, 4H), 8.05 (d, *J* = 8.5 Hz, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.93 (s, 1H), 7.89 (s, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.57 (t, *J* = 7.0 Hz, 5H), 7.52 (dd, *J* = 6.9, 3.5 Hz, 2H), 2.61 (s, 6H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 151.79, 151.08, 143.28, 142.49, 142.40, 141.65, 140.87, 140.79, 140.17, 140.09, 136.97, 132.66, 131.93, 130.12, 130.02, 129.17, 128.65, 128.51, 128.01, 127.56, 127.47, 21.95, 21.92.

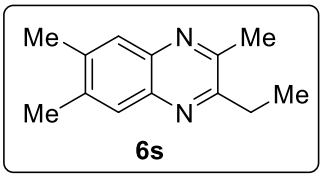
2-ethyl-3-methylquinoxaline (6r)[9]



6r

White solid (89 mg, 52%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 - 7.90 (m, 2H), 7.60 - 7.57 (m, 2H), 2.96 - 2.92 (m, 2H), 2.68 - 2.67 (m, 3H), 1.36 - 1.33 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.51, 153.05, 141.17, 140.85, 128.76, 128.70, 128.53, 128.25, 28.98, 22.71, 11.97.

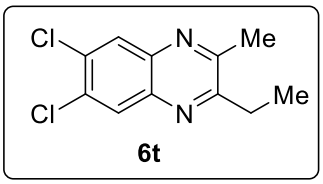
2-ethyl-3,6,7-trimethylquinoxaline (6s)[11]



6s

White solid (114 mg, 56%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (s, 1H), 7.70 (s, 1H), 2.97 (q, *J* = 7.5 Hz, 2H), 2.70 (s, 3H), 2.44 (s, 6H), 1.37 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.63, 152.03, 140.18, 139.88, 139.07, 139.02, 127.80, 127.53, 29.04, 22.73, 20.39, 20.34, 12.25.

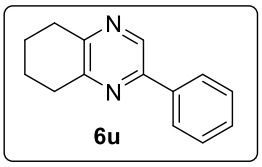
6,7-dichloro-2-ethyl-3-methylquinoxaline (6t)[12]



6t

Yellow solid (128 mg, 53%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (s, 1H), 8.04 (s, 1H), 2.99 (q, *J* = 7.4 Hz, 2H), 2.71 (s, 3H), 1.39 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.91, 154.66, 140.07, 139.72, 133.07, 133.05, 129.46, 129.15, 29.02, 22.86, 11.60.

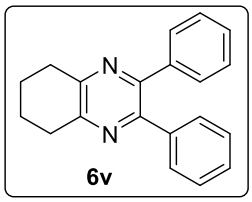
2-phenyl-5,6,7,8-tetrahydroquinoxaline (6u)[13]



6u

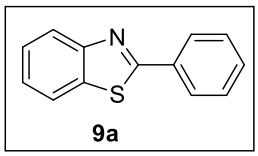
Colourless Oil (151mg, 72%) ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.74 (s, 1H), 7.97 (d, *J* = 8.2 Hz, 2H), 7.49 (dd, *J* = 10.8, 3.7 Hz, 2H), 7.45 - 7.41 (m, 1H), 3.03-2.99 (m, 4H), 1.95 (d, *J* = 2.0 Hz, 4H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 152.39, 151.21, 149.72, 138.85, 136.95, 129.28, 128.96, 126.80, 32.23, 31.74, 22.74.

2,3-diphenyl-5,6,7,8-tetrahydroquinoxaline (6v)[14]



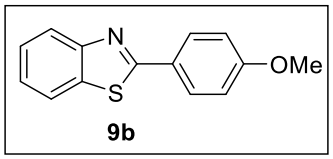
White solid (236 mg, 82%) ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.40 - 7.39 (m, 4H), 7.29 - 7.27 (m, 6H), 3.08 - 3.05 (m, 4H), 2.00 - 1.98 (m, 4 H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 150.65, 149.65, 139.06, 129.73, 128.29, 128.22, 31.91, 22.91.

2-Phenylbenzo[*d*]thiazole (9a)[15]



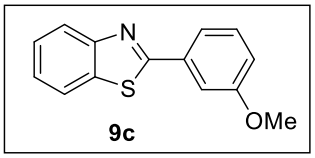
White solid (177 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11-8.08 (m, 3H), 7.90 (d, J = 7.96 Hz, 1H), 7.51-7.48 (m, 4H), 7.40 - 7.37 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.19, 154.28, 135.20, 133.76, 131.10, 129.15, 127.69, 126.44, 125.32, 123.37, 121.75.

2-(4-methoxyphenyl)benzo[d]thiazole (9b)[15]



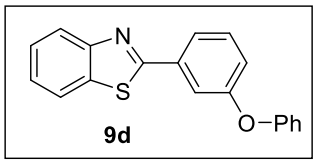
White solid (210 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05-8.03 (m, 3H), 7.87 (d, J = 7.92 Hz, 1H), 7.47 (td, J = 7.68, 1.04 Hz, 1H), 7.35 (td, J = 7.56, 0.88 Hz, 1H), 7.02-6.98 (m, 2H), 3.88 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.01, 162.06, 154.36, 134.99, 129.25, 126.57, 126.34, 124.93, 122.96, 121.64, 114.51, 55.60.

2-(3-methoxyphenyl)benzo[d]thiazole (9c)[15]



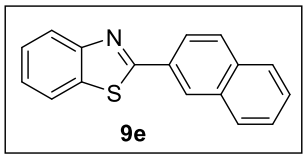
White solid (205 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, J = 8.16 Hz 1H), 7.89 (d, J = 7.96 Hz, 1H), 7.67 (t, J = 2.28 Hz, 1H), 7.64 (d, J = 7.72 Hz, 1H), 7.49 (td, J = 7.70, 1.0 Hz 1H), 7.41 - 7.37 (m, 2H), 7.03 (dd, J = 8.24, 2.48 Hz 1H) 3.91 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.06, 160.17, 154.18, 135.21, 135.01, 130.16, 126.43, 125.35, 123.36, 121.73, 120.35, 117.46, 112.15, 55.62.

2-(3-phenoxyphenyl)benzo[d]thiazole (9d)[16]



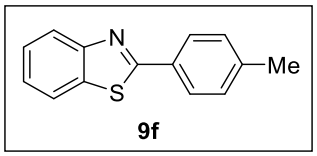
White solid (252 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 8.16 Hz, 1H), 7.89 (d, J = 7.96 Hz, 1H), 7.83 - 7.89 (m, 2H), 7.51 - 7.43 (m, 2H), 7.41 - 7.36 (m, 3H), 7.17 - 7.12 (m, 2H) ,7.10-7.08 (m, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.38, 158.03, 156.93, 154.18, 135.49, 135.23, 130.50, 130.05, 126.51, 125.47, 123.82, 123.48, 122.54, 121.75, 121.31, 119.23, 117.83.

2-(naphthalen-2-yl)benzo[d]thiazole (9e)[15]



White solid (222 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.22 (dd, J = 8.4, 1.6 Hz, 1H), 8.13 (d, J = 8.16 Hz, 1H), 7.98 - 7.87 (m, 4H), 7.56 - 7.50 (m, 3H), 7.42-7.38 (t, J = 8.04, Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.23, 154.36, 135.25, 134.73, 133.30, 131.10, 128.95, 128.00, 127.70, 127.58, 127.01, 126.52, 125.37, 124.56, 123.36, 121.77.

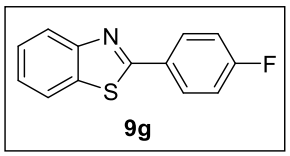
2-(p-tolyl)benzo[d]thiazole (9f)[17]



9f

White solid (192 mg, 85%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, J = 8.16 Hz, 1H), 7.99 (d, J = 8.12 Hz, 2H), 7.89 (d, J = 7.96 Hz, 1H), 7.48 (t, J = 8.16 Hz, 1H), 7.37(t, J = 7.40 Hz, 1H), 7.30 (d, J = 8.0 Hz, 2H), 2.43 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.39, 154.30, 141.57, 135.08, 131.10, 129.86, 127.62, 126.38, 125.14, 123.18, 121.71, 21.66.

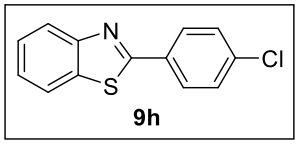
2-(4-fluorophenyl)benzo[d]thiazole (9g)[15]



9g

White solid (174 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 - 8.05 (m, 3H), 7.89 (d, J = 7.96 Hz, 1H), 7.49 (t, J = 8.2 Hz, 1H), 7.38 (t, J = 8.04 Hz, 1H), 7.18 (t, J = 8.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.86, 164.58 (d, J = 251.8Hz), 154.22, 135.17, 130.08 (d, J = 3.25 Hz), 129.64 (d, J = 8.62 Hz), 126.54, 125.37, 123.31, 121.74, 116.28 (d, J = 21.98 Hz).

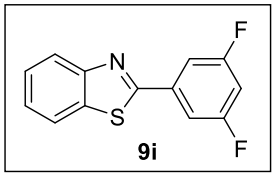
2-(4-chlorophenyl)benzo[d]thiazole (9h)[15]



9h

White solid (201 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.2 Hz, 1H), 8.03 - 8.01 (m, 2H), 7.90 (d, J = 8.0 Hz, 1H), 7.52 - 7.45 (m, 3H), 7.42 - 7.36 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.76, 154.20, 137.16, 135.19, 132.24, 129.41, 128.84, 126.62, 125.55, 123.43, 121.79.

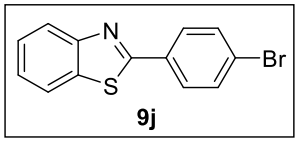
2-(3,5-difluorophenyl)benzo[d]thiazole (9i)[18]



9i

Yellow solid (173 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, J = 8.1 Hz, 1H), 7.91 (d, J = 7.9 Hz, 1H), 7.62 (d, J = 6.0 Hz, 2H), 7.52 (t, J = 7.5 Hz, 1H), 7.42 (t, J = 7.5 Hz, 1H), 6.93 (t, J = 8.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.21 (t, J = 3.4 Hz), 163.37(dd, J =246, 12.7 Hz), 153.97, 136.71 (t, J = 9.9 Hz), 135.26, 126.85, 126.03, 123.81, 121.87, 110.71-110.44 (m), 106.19 (t, J = 25.4 Hz).

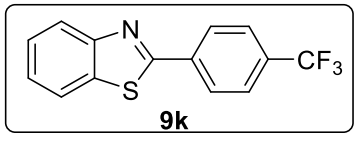
2-(4-bromophenyl)benzo[d]thiazole (9j)[17]



9j

White solid (229 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, J = 8.2 Hz, 1H), 7.93 - 7.86 (m, 3H), 7.60 - 7.59 (m, 2H), 7.50 (t, J = 7.6 Hz, 1H), 7. 40 (t, J = 7.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.72, 154.13, 135.10, 132.58, 132.27, 128.94, 126.57, 125.51, 125.49, 123.39, 121.73.

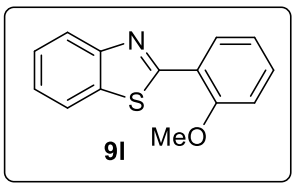
2-(4-(trifluoromethyl)phenyl)benzo[d]thiazole (9k)[15]



9k

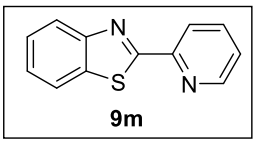
White solid (209 mg, 75%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.18 (d, J = 8.1 Hz, 2H), 8.10 (d, J = 8.2 Hz, 1H), 7.90 (d, J = 8.0 Hz, 1H), 7.73 (d, J = 8.2 Hz, 2H), 7.52 (t, J = 7.4 Hz, 1H), 7.42 (t, J = 7.4 Hz, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 166.15, 154.11, 136.81, 135.28, 132.51, (q, J = 32.7 Hz), 127.84, 126.10, (q, J = 32.7 Hz), 125.90, 124.83, 123.72, 123.03, 121.85.

2-(2-methoxyphenyl)benzo[d]thiazole (9l)[19]



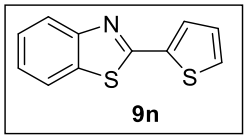
White solid (198 mg, 82%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.54 (dd, *J* = 7.8, 1.4 Hz, 1H), 8.10 (d, *J* = 8.1 Hz, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.51 - 7.41 (m, 2H), 7.39 - 7.36 (m, 1H), 7.15 - 7.13 (m, 1H), 7.07 (d, *J* = 8.3 Hz, 1H), 4.06 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.28, 157.33, 152.24, 136.21, 131.91, 129.63, 126.02, 124.71, 122.88, 122.35, 121.33, 121.28, 111.77, 55.82.

2-(pyridin-2-yl)benzo[d]thiazole (9m)[17]



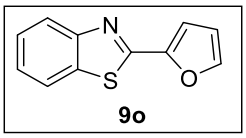
Yellow solid (163 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.8 Hz, 1H), 8.36 (d, *J* = 7.9 Hz, 1H), 8.09 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 7.9 Hz, 1H), 7.82 (td, *J* = 7.8, 1.6 Hz, 1H), 7.51 - 7.47 (m, 1H), 7.41 (d, *J* = 7.9 Hz, 1H), 7.40 - 7.34 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.47, 154.38, 151.49, 149.74, 137.09, 136.22, 126.37, 125.74, 125.35, 123.68, 122.11, 120.85.

2-(thiophen-2-yl)benzo[d]thiazole (9n)[15]



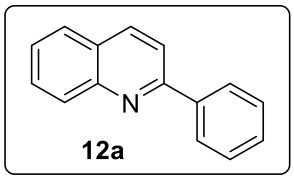
White solid (154 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.2 Hz, 1H), 7.85 (d, *J* = 8.0, Hz, 1H), 7.65 (dd, *J* = 3.7, 1.1 Hz, 1H), 7.51 - 7.45 (m, 2H), 7.38 - 7.34 (m, 1H), 7.13 (dd, *J* = 5.0, 3.8 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.51, 153.80, 137.45, 134.80, 129.42, 128.73, 128.16, 126.55, 125.35, 123.09, 121.57.

2-(furan-2-yl)benzo[d]thiazole (9o)[15]



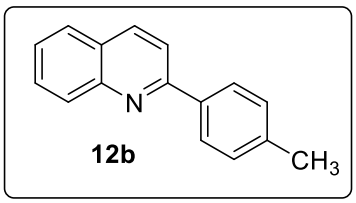
White solid (139 mg, 69%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.2 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.59 (d, *J* = 1.0 Hz, 1H), 7.50 - 7.46 (m, 1H), 7.39 - 7.35 (m, 1H), 7.19 (d, *J* = 3.5 Hz, 1H), 6.58 (dd, *J* = 3.4, 1.7 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.66, 153.85, 148.85, 144.80, 134.38, 126.58, 125.30, 123.22, 121.67, 112.64, 111.53.

2-phenylquinoline (12a)[20]



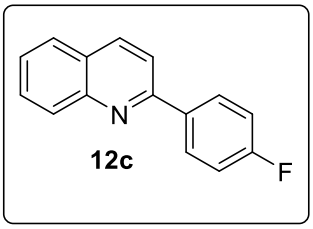
White solid (166 mg, 81%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 (d, J = 8.6 Hz, 1H), 8.20 - 8.16 (m, 3H), 7.88 (d, J = 8.6 Hz, 1H), 7.83 (d, J = 8.1 Hz, 1H), 7.74 (ddd, J = 8.4, 6.9, 1.4 Hz, 1H), 7.55 - 7.52 (m, 3H), 7.49 - 7.46 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.52, 148.42, 139.83, 136.91, 129.88, 129.79, 129.45, 128.98, 127.71, 127.60, 127.32, 126.42, 119.16.

2-(4-Tolyl)quinolone (12b)[20]



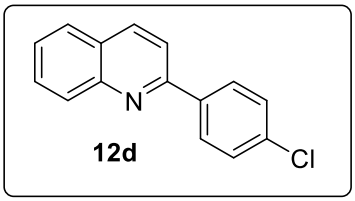
Pale yellow oil (180 mg, 83%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.4 Hz, 1H), 8.17 (d, *J* = 8.6 Hz, 1H), 8.10 (d, *J* = 8.1 Hz, 2H), 7.85 (d, *J* = 8.6 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.74 (t, *J* = 7.5 Hz, 1H), 7.52 (t, *J* = 7.3 Hz, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 2.45 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.37, 148.33, 139.46, 136.91, 136.74, 129.70, 129.65, 127.52, 127.51, 127.15, 126.15, 118.92, 21.44.

2-(4-fluorophenyl)quinolone (12c)[20]



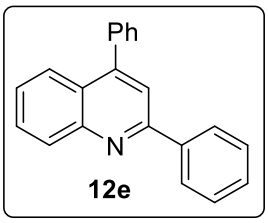
Pale yellow solid (173 mg, 78%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.19 - 8.14 (m, 4H), 7.82 - 7.79 (m, 2H), 7.73 (ddd, *J* = 8.4, 6.8, 1.4 Hz, 1H), 7.54-7.51 (m, 1H), 7.23-7.19 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.82 (d, *J* = 249.2 Hz), 156.24, 148.23, 136.95, 135.82 (d, *J* = 2.9 Hz), 129.84, 129.64, 129.50 (d, *J* = 8.6 Hz), 127.58, 127.15, 126.44, 118.71, 115.86 (d, J = 21.6 Hz).

2-(4-chlorophenyl)quinolone (12d)[20]



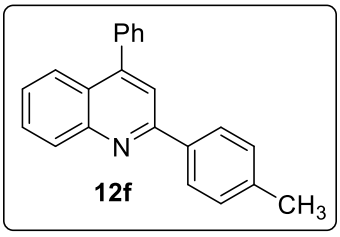
White solid (205 mg, 86%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.20 (d, *J* = 8.6 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 8.13 - 8.09 (m, 2H), 7.82 - 7.81 (m, 2H), 7.75 (ddd, *J* = 8.4, 6.8, 1.5 Hz, 1H), 7.55 - 7.52 (m, 1H), 7.51 - 7.48 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.08, 148.30, 138.12, 137.07, 135.62, 129.95, 129.77, 129.11, 128.91, 127.60, 127.30, 126.60, 118.66.

2,4-diphenylquinoline (12e)[21]



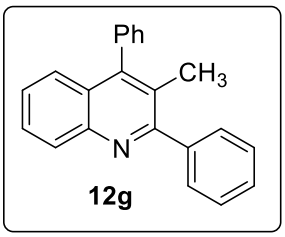
Brown solid (216 mg, 77%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (d, *J* = 8.4 Hz, 1H), 8.22 (d, *J* = 7.2 Hz, 2H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.84 (s, 1H), 7.75 (ddd, *J* = 8.3, 6.9, 1.3 Hz, 1H), 7.62 - 7.51 (m, 7H), 7.51 - 7.46 (m, 2H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.00, 149.26, 148.89, 139.74, 138.47, 130.20, 129.66, 129.64, 129.45, 128.95, 128.70, 128.51, 127.69, 126.44, 125.85, 125.74, 119.49.

4-phenyl-2-(p-tolyl)quinolone (12f)[21]



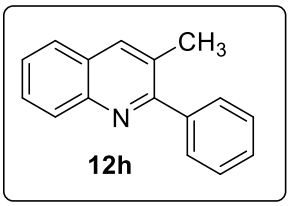
Slightly yellow solid (233 mg, 79%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.32 - 8.28 (m, 1H), 8.15 (t, *J* = 7.7 Hz, 2H), 7.95 - 7.92 (m, 1H), 7.84 (d, *J* = 4.2 Hz, 1H), 7.76 (t, *J* = 7.5 Hz, 1H), 7.60-7.52 (m, 5H), 7.48 (t, *J* = 7.6 Hz, 1H), 7.37 - 7.36 (m, 2H), 2.47 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.85, 149.03, 148.85, 139.45, 138.49, 136.83, 130.08, 129.61, 129.49, 128.61, 128.40, 127.49, 126.18, 125.70, 125.65, 119.22, 21.41.

3-methyl-4-phenyl-2-(p-tolyl)quinolone (12g)[21]



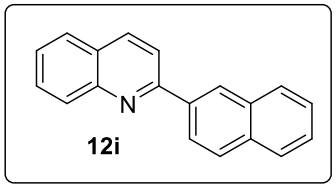
Yellow solid (251 mg, 85%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.4 Hz, 1H), 7.66-7.64 (m, 1H), 7.62 - 7.61 (m, 2H), 7.55 (t, *J* = 7.4 Hz, 2H), 7.51-7.48 (m, 3H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.40 - 7.39 (m, 2H), 7.32 - 7.31 (m, 2H), 2.15 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.96, 147.91, 146.33, 141.61, 137.84, 129.54, 129.45, 129.05, 128.78, 128.68, 128.46, 128.23, 127.97, 127.19, 126.87, 126.38, 126.12, 18.75.

3-methyl-2-(p-tolyl)quinolone (12h)[22]



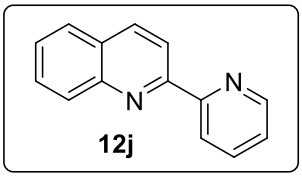
Yellow oil (165 mg, 75%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.4 Hz, 1H), 8.01 (s, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.68 - 7.65 (m, 1H), 7.60 (d, *J* = 7.9 Hz, 2H), 7.53 - 7.48 (m, 3H), 7.44 (t, *J* = 7.4 Hz, 1H), 2.49 (s, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 160.62, 146.68, 140.93, 136.84, 129.35, 129.31, 128.93, 128.85, 128.40, 128.28, 127.67, 126.80, 126.50, 20.73.

2-(naphthalen-2-yl)quinolone (12i)[22]



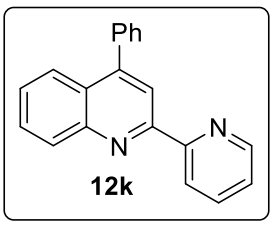
White solid (216 mg, 85%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.62 (s, 1H), 8.38 (dd, *J* = 8.6, 1.7 Hz, 1H), 8.25 (t, *J* = 7.6 Hz, 2H), 8.05 - 7.99 (m, 3H), 7.91 (dd, *J* = 5.9, 3.4 Hz, 1H), 7.85 (d, *J* = 7.8 Hz, 1H), 7.78 - 7.75 (m, 1H), 7.56 - 7.53 (m, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.29, 148.47, 137.06, 136.96, 133.96, 133.60, 129.87, 129.83, 128.95, 128.71, 127.85, 127.63, 127.34, 127.28, 126.84, 126.48, 126.47, 125.18, 119.30.

2-(pyridin-2-yl)quinolone (12j)[22]



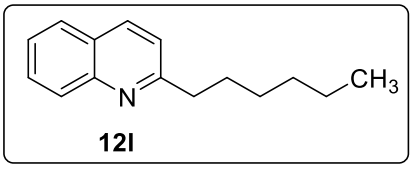
Yellow solid (152 mg, 75%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.7 Hz, 1H), 8.65 (d, *J* = 7.9 Hz, 1H), 8.56 (d, *J* = 8.6 Hz, 1H), 8.28 (d, *J* = 8.6 Hz, 1H), 8.18 (d, *J* = 8.5 Hz, 1H), 7.87 - 7.84 (m, 2H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.36 - 7.34 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.42, 156.25, 149.28, 148.01, 137.08, 136.94, 129.90, 129.68, 128.34, 127.73, 126.87, 124.15, 121.94, 119.06.

2-(4-phenylnaphthalen-2-yl)pyridine (12k)[23]



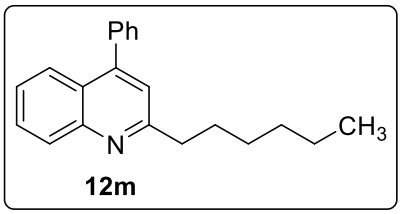
Yellow solid (186 mg, 66%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.73 (d, *J* = 4.0 Hz, 1H), 8.70 (d, *J* = 7.9 Hz, 1H), 8.53 (s, 1H), 8.26 (d, *J* = 8.4 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.89 (td, *J* = 7.8, 1.7 Hz, 1H), 7.77 - 7.72 (m, 1H), 7.62 - 7.58 (m, 2H), 7.56 - 7.46 (m, 4H), 7.40 - 7.34 (m, 1H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 156.47, 155.74, 149.41, 149.30, 148.59, 138.46, 137.10, 130.30, 129.79, 129.55, 128.59, 128.44, 126.93, 126.87, 125.94, 124.19, 122.00, 119.37.

2-hexylquinoline (12l)[24]



Pale yellow oil (130 mg, 61%) ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.97 - 7.94 (m, 2H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.59 - 7.56 (m, 1H), 7.39 - 7.36 (m, 1H), 7.19 (dd, *J* = 8.9, 3.3 Hz, 1H), 2.87 (t, *J* = 8.0, Hz, 2H), 1.74 - 1.68 (m, 2H), 1.35 - 1.30 (m, 2H), 1.26 - 1.20 (m, 4H), 0.79 (t, *J* = 7.0 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 163.20, 147.93, 136.26, 129.39, 128.84, 127.55, 126.76, 125.69, 121.44, 39.47, 31.82, 30.17, 29.33, 22.66, 14.18.

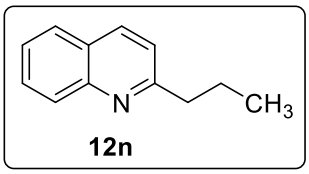
2-hexyl-4-phenylquinoline (12m)[25]



12m

Pale yellow oil (185 mg, 64%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.5 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.70 - 7.67 (m, 1H), 7.54 - 7.47 (m, 5H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.25 (s, 1H), 3.02 - 2.99 (m, 2H), 1.87-1.82 (m, 2H), 1.78 - 1.43 (m, 2H), 1.36 - 1.31 (m, 4H), 0.89 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.77, 148.61, 148.48, 138.40, 129.64, 129.31, 129.29, 128.62, 128.39, 125.80, 125.73, 125.36, 121.70, 39.54, 31.85, 30.24, 29.43, 22.69, 14.22.

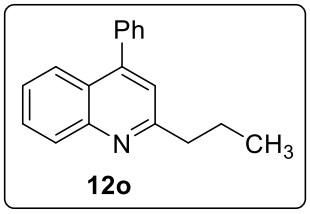
2-propylquinoline (12n)[20]



12n

Colorless oil (101 mg, 58%) ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 8.4, 3.2 Hz, 2H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.67 (t, *J* = 7.7 Hz, 1H), 7.46 (t, *J* = 7.5 Hz, 1H), 7.28 (d, *J* = 8.4 Hz, 1H), 3.08 - 2.83 (m, 2H), 1.87 - 1.81 (m, 2H), 1.01 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.98, 147.93, 136.29, 129.42, 128.84, 127.57, 126.79, 125.73, 121.49, 41.36, 23.42, 14.12.

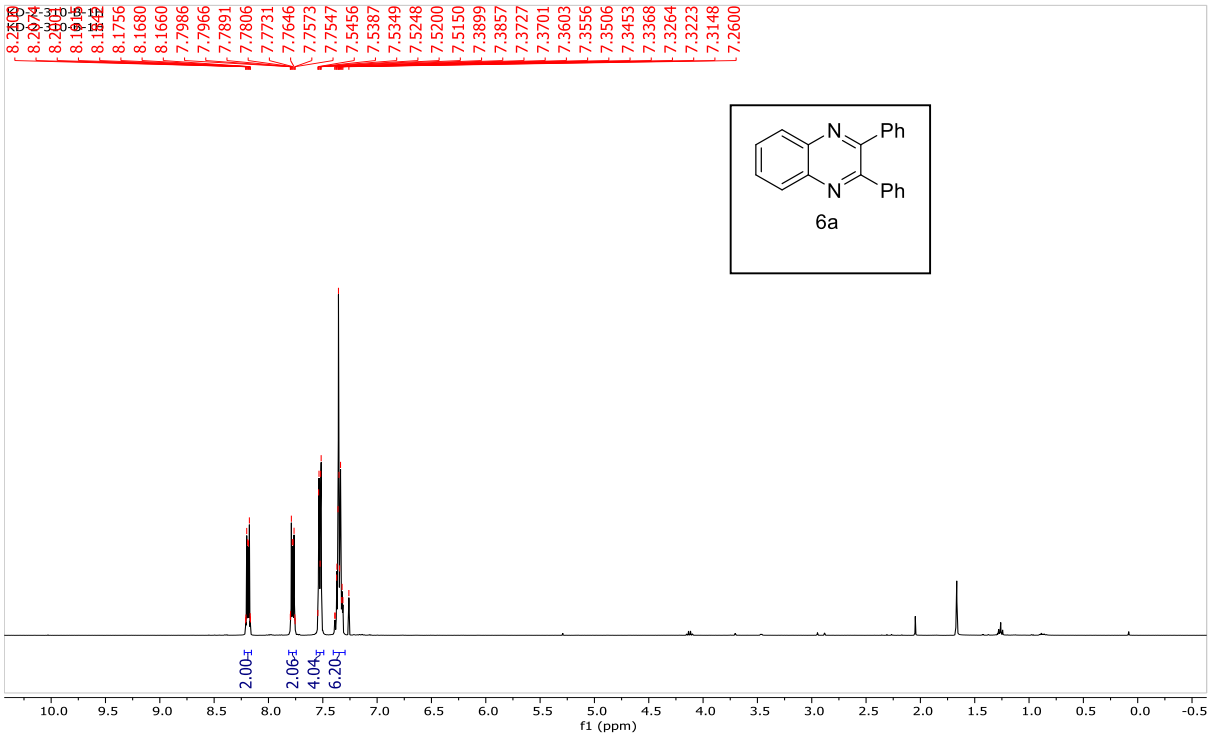
4-phenyl-2-propylquinoline (12o)[26]

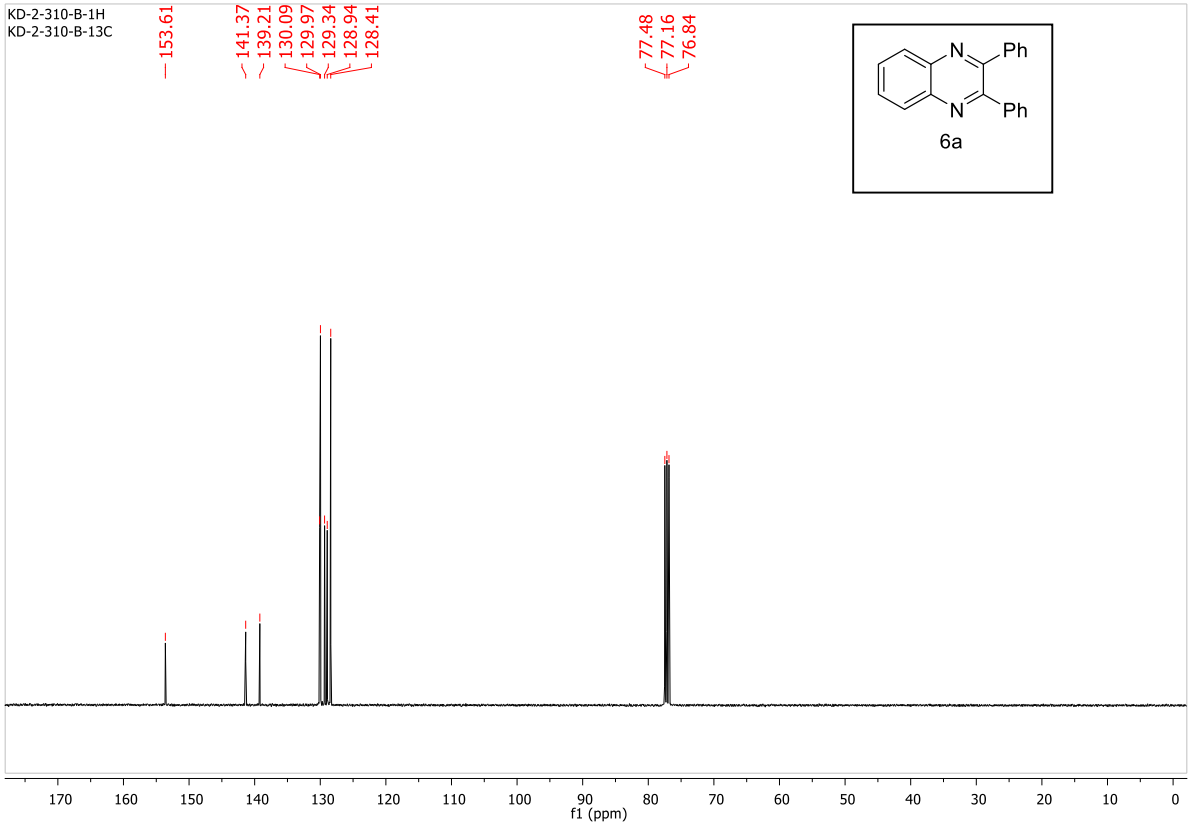


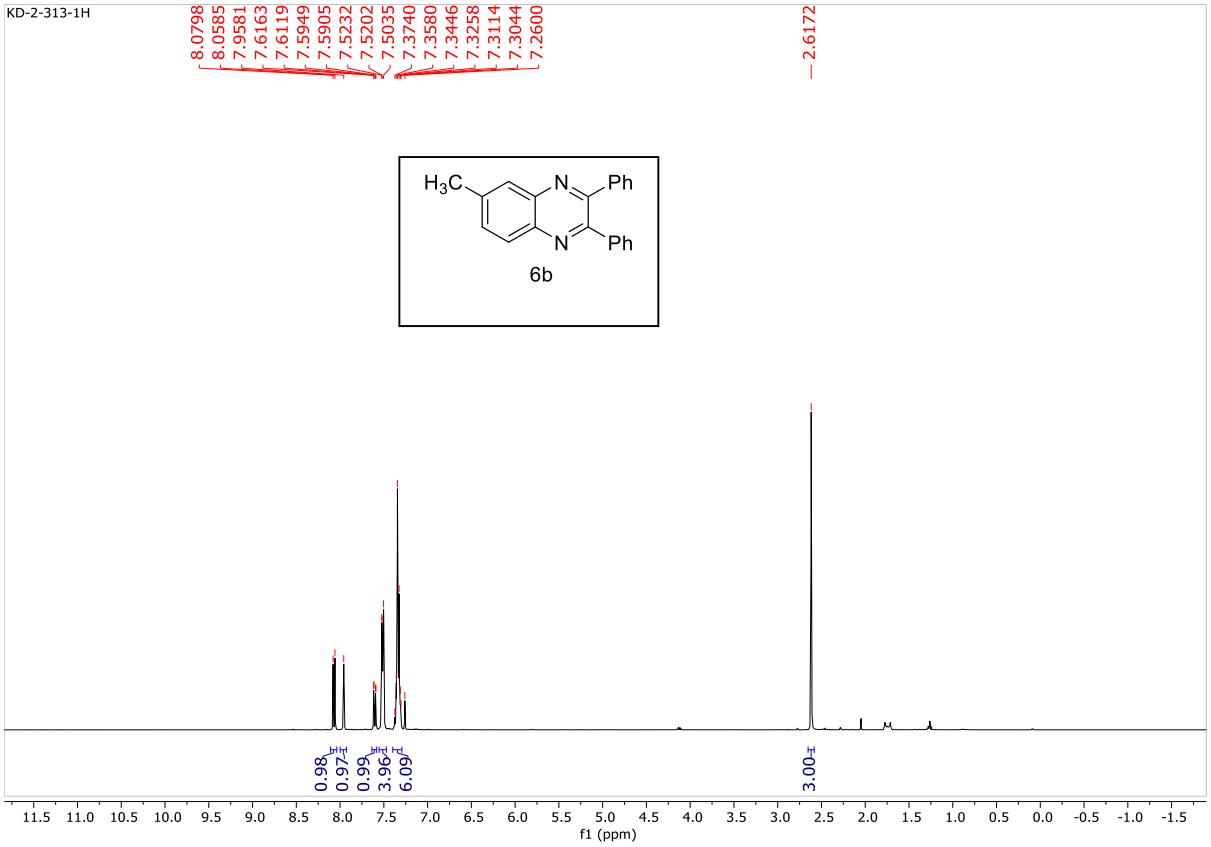
12o

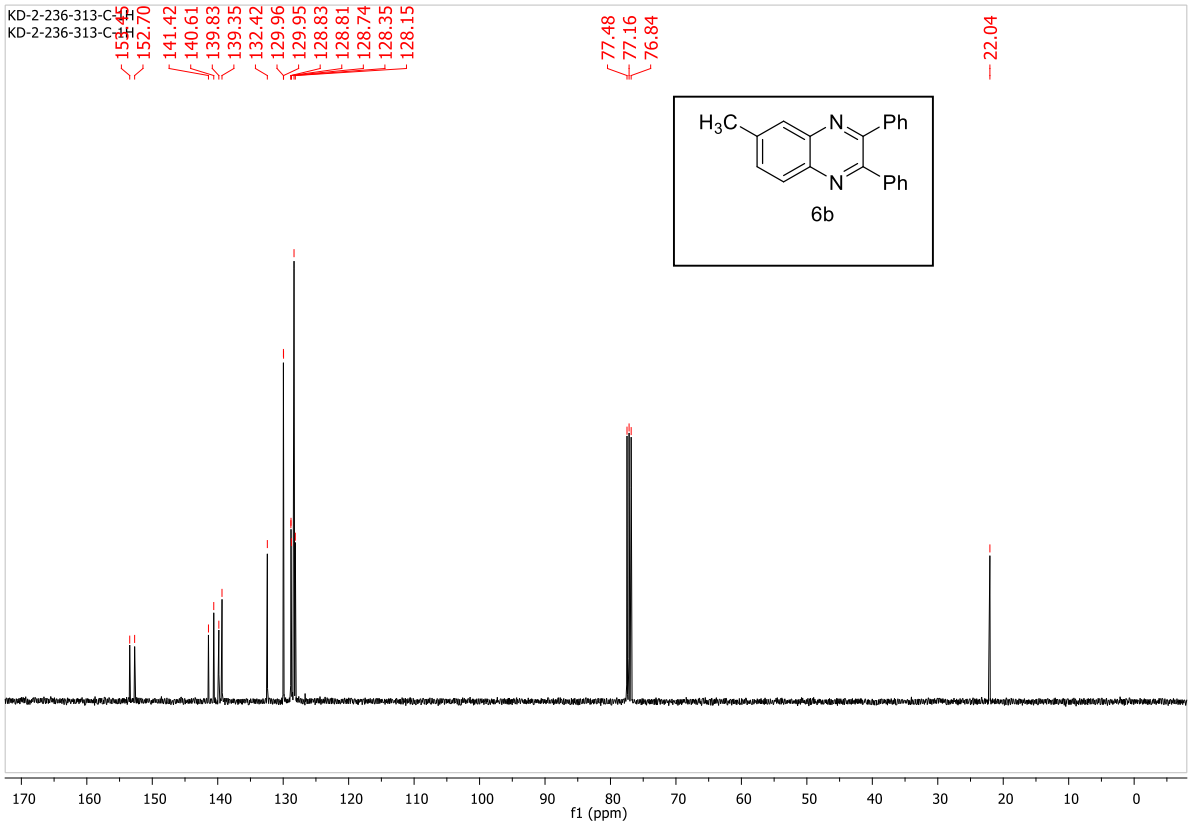
Colorless oil (153mg, 62%) ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.3 Hz, 1H), 7.69 (t, *J* = 7.3 Hz, 1H), 7.54 - 7.47 (m, 5H), 7.43 (t, *J* = 7.5 Hz, 1H), 7.25 (s, 1H), 3.05 - 2.92 (m, 2H), 1.92 - 1.85 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.55, 148.63, 148.49, 138.40, 129.60, 129.34, 129.29, 128.63, 128.41,125.84, 125.75, 125.39, 121.76, 41.43, 23.49, 14.23.

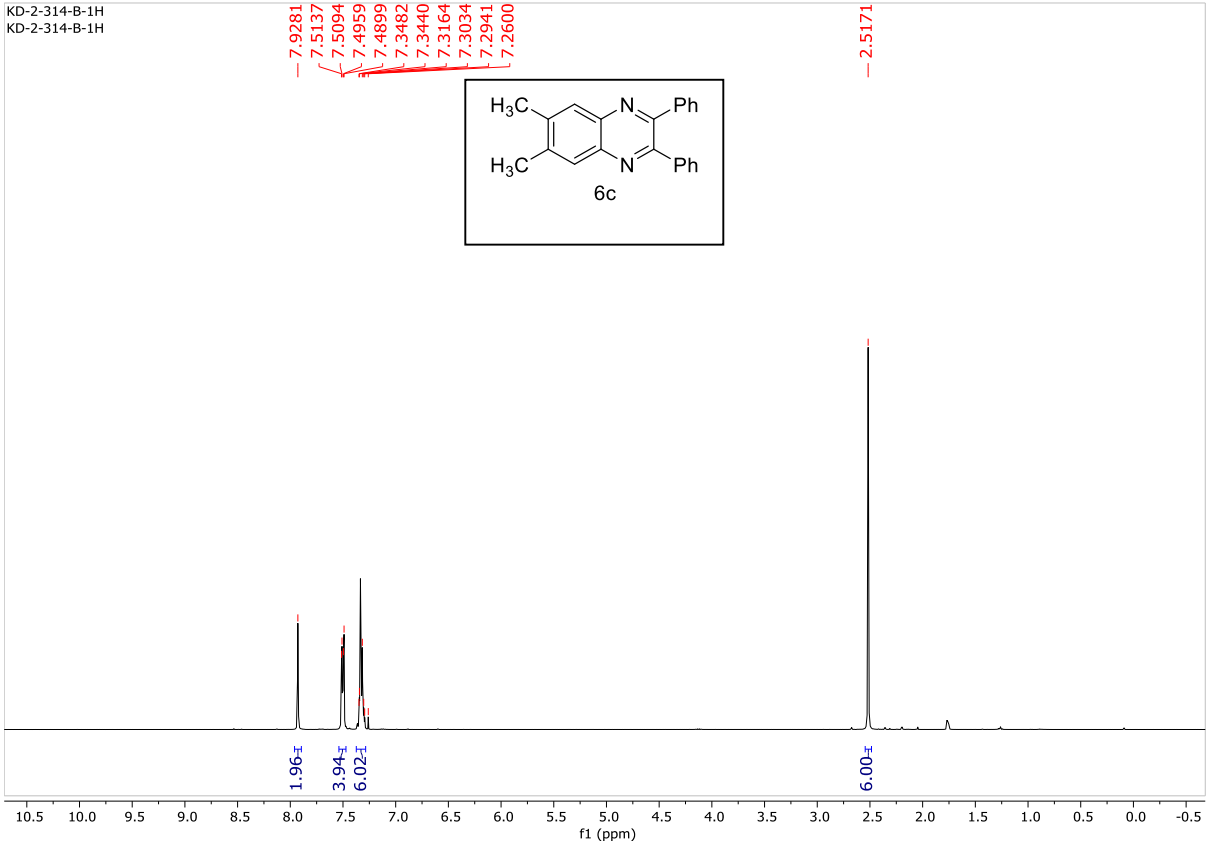
8. Figures reproducing ^{1}H and ^{13}C NMR spectra:

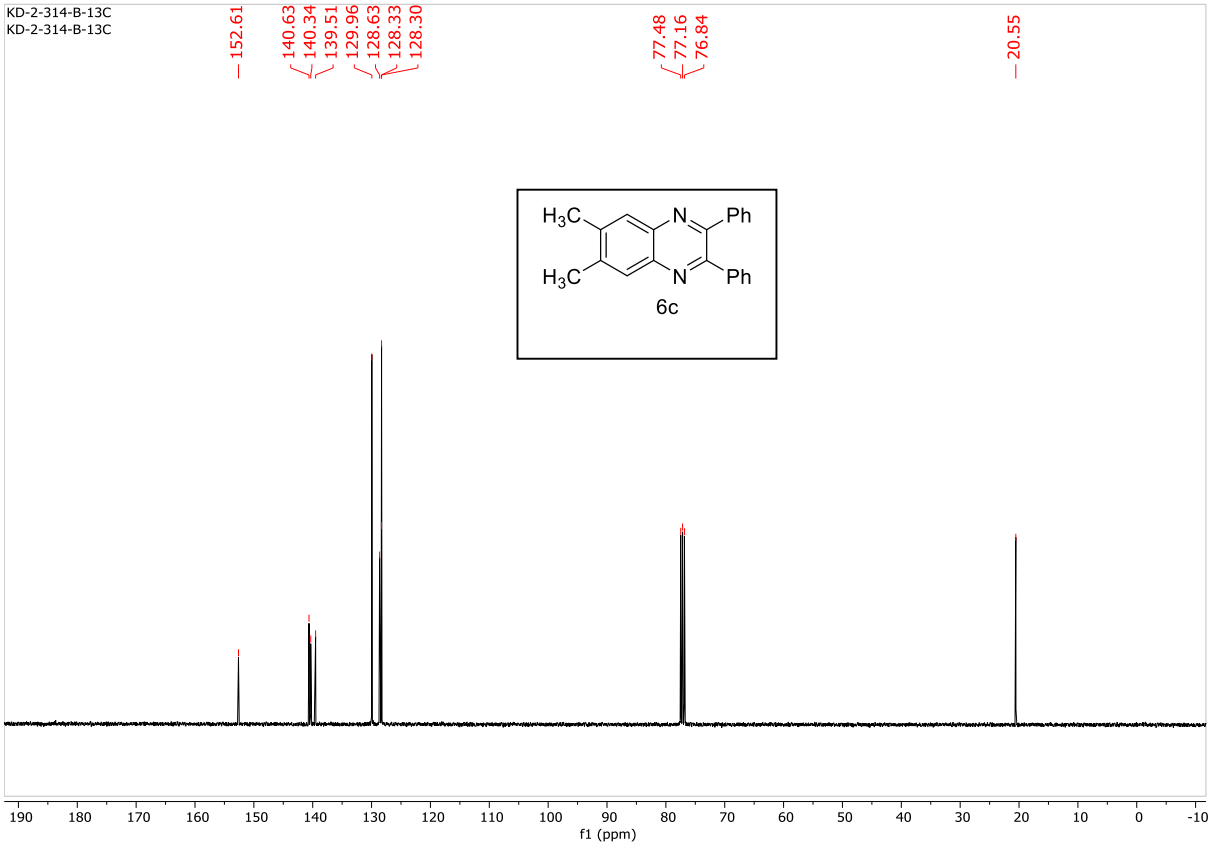


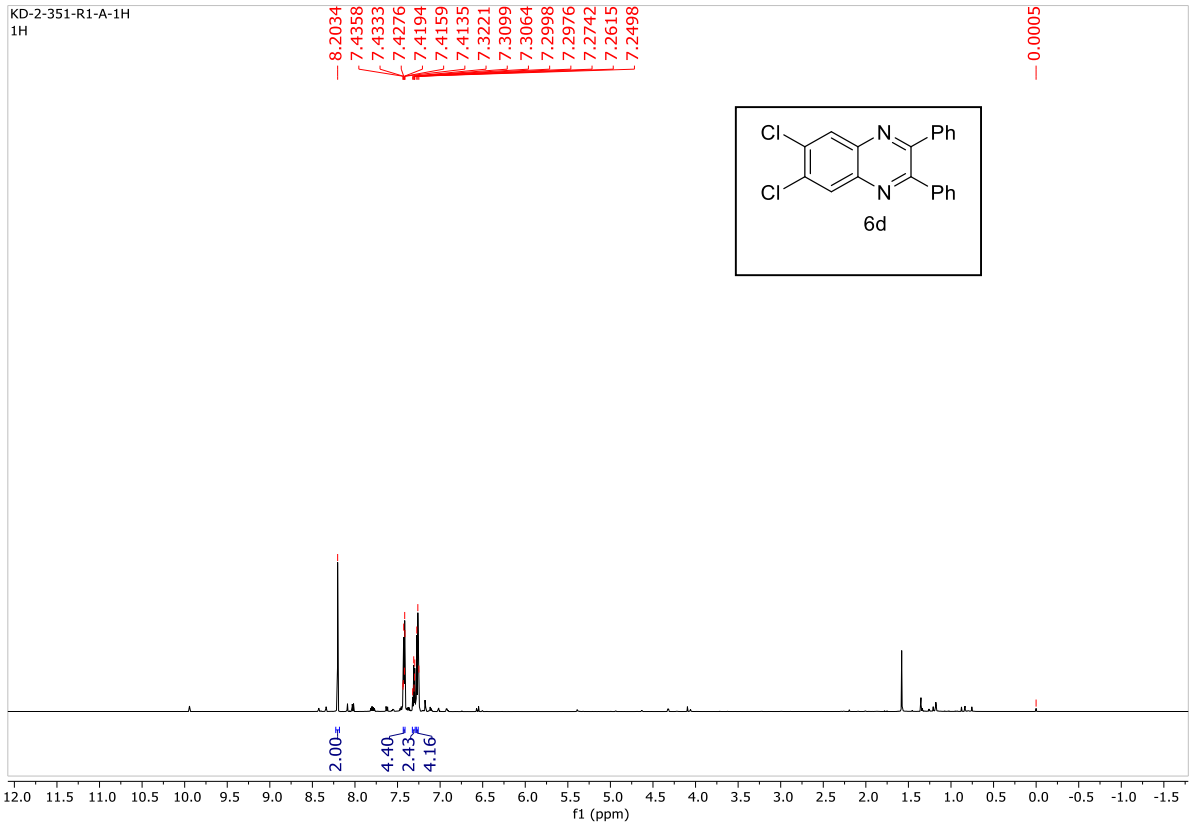


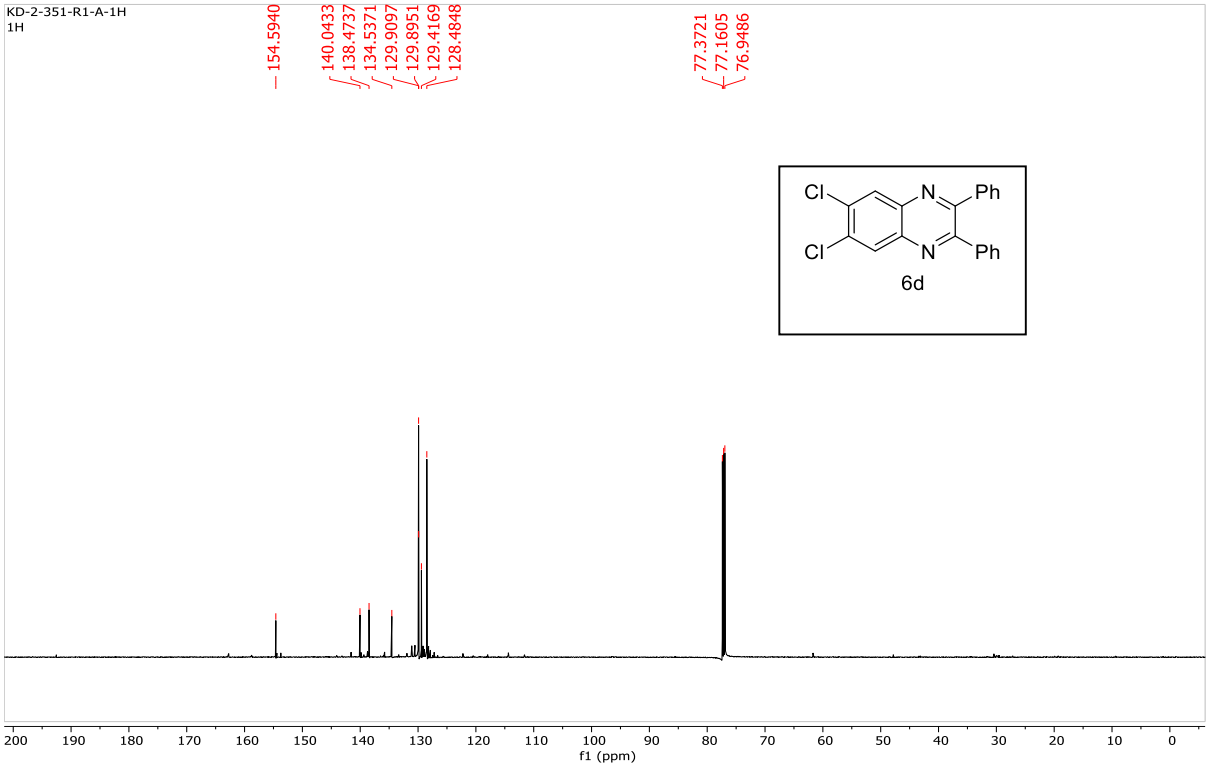

KD-2-313-1H
8.0798
8.0585
7.9581
7.6163
7.6119
7.5949
7.5905
7.5232
7.5202
7.5035
7.3740
7.3580
7.3446
7.3258
7.3114
7.3044
7.2600
2.6172
H3C
N
Ph
N
Ph
6b
0.98
0.97
0.99
3.96
6.09
3.00
f1 (ppm)

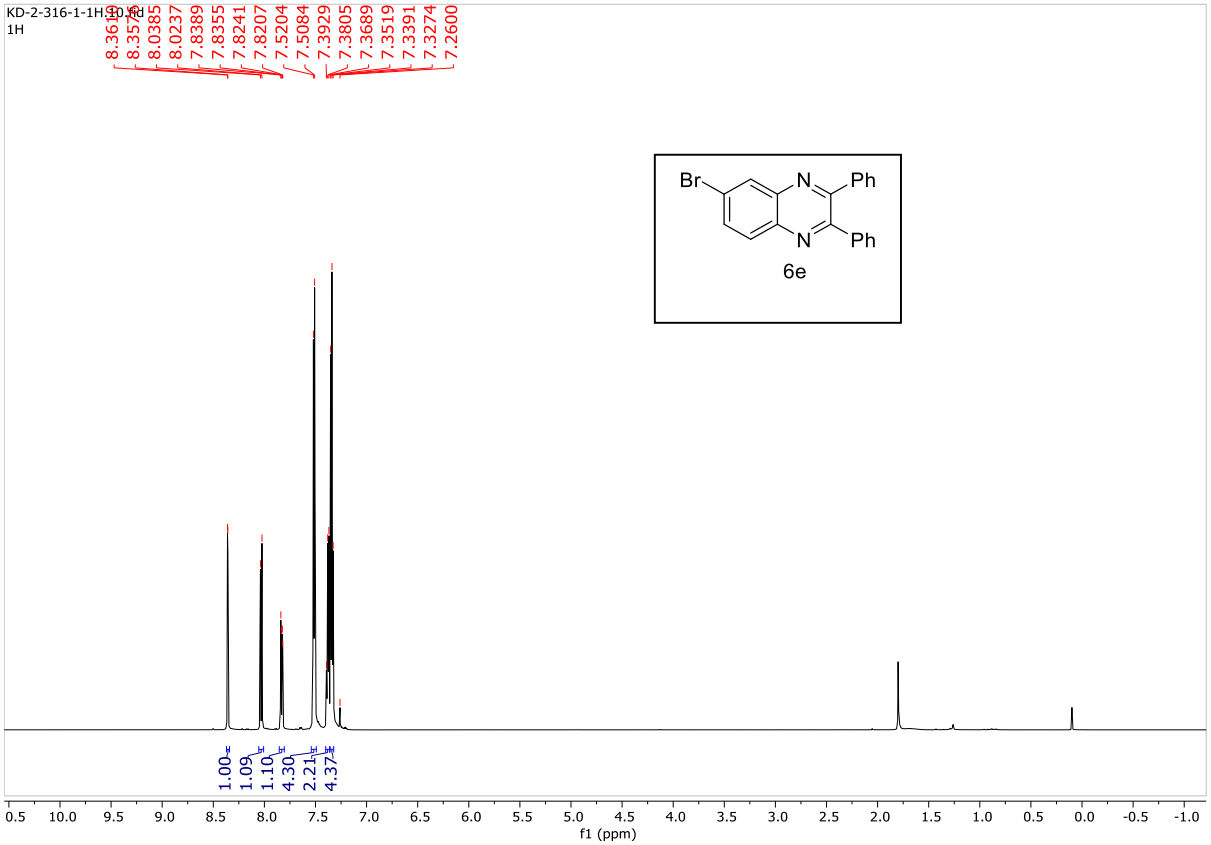

KD-2-236-313-C-1H
KD-2-236-313-C-1H
152.70
141.42
140.61
139.83
139.35
132.42
129.96
129.95
128.83
128.81
128.74
128.35
128.15
77.48
77.16
76.84
22.04
H3C
N
Ph
N
Ph
6b
f1 (ppm)

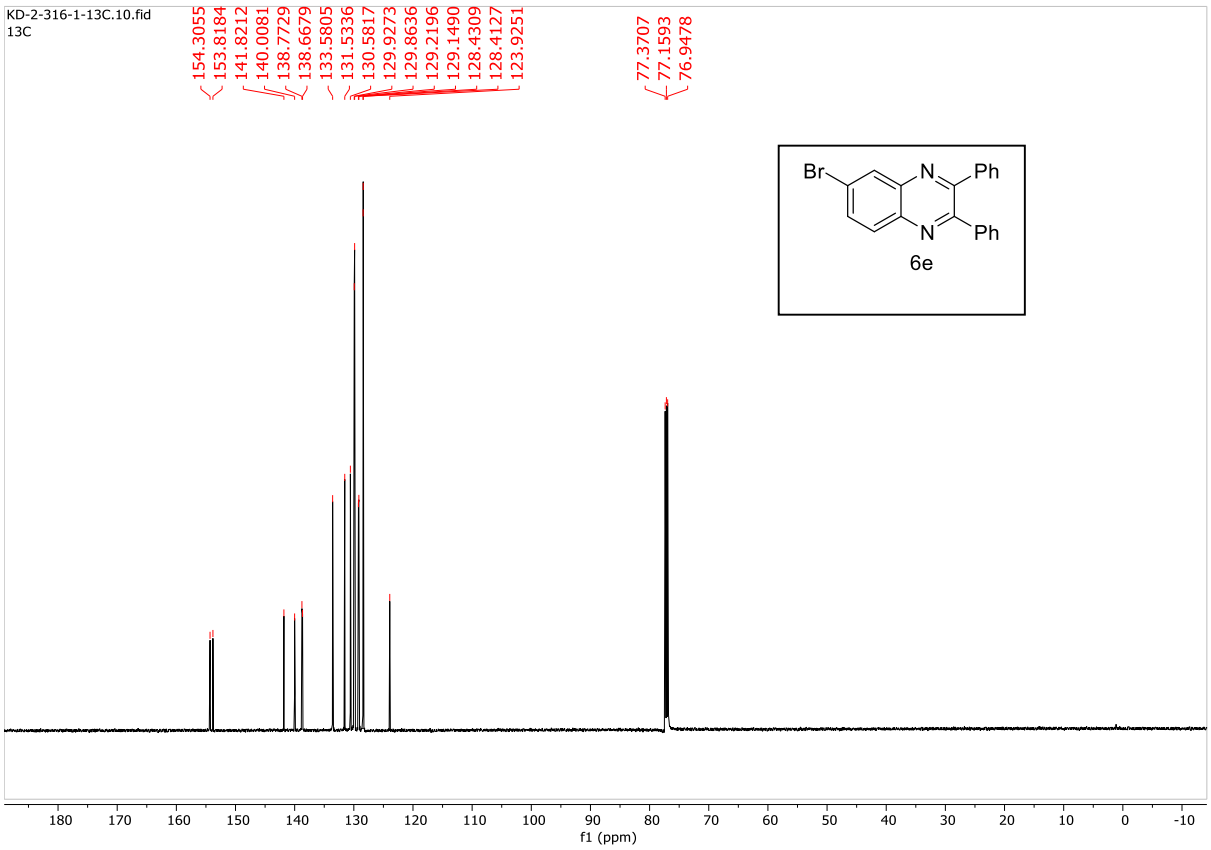

KD-2-314-B-1H
KD-2-314-B-1H
7.9281
7.5137
7.5094
7.4959
7.4899
7.3482
7.3440
7.3164
7.3034
7.2941
7.2600
2.5171
H3C
N
Ph
H3C
N
Ph
6c
1.96
3.94
6.02
6.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

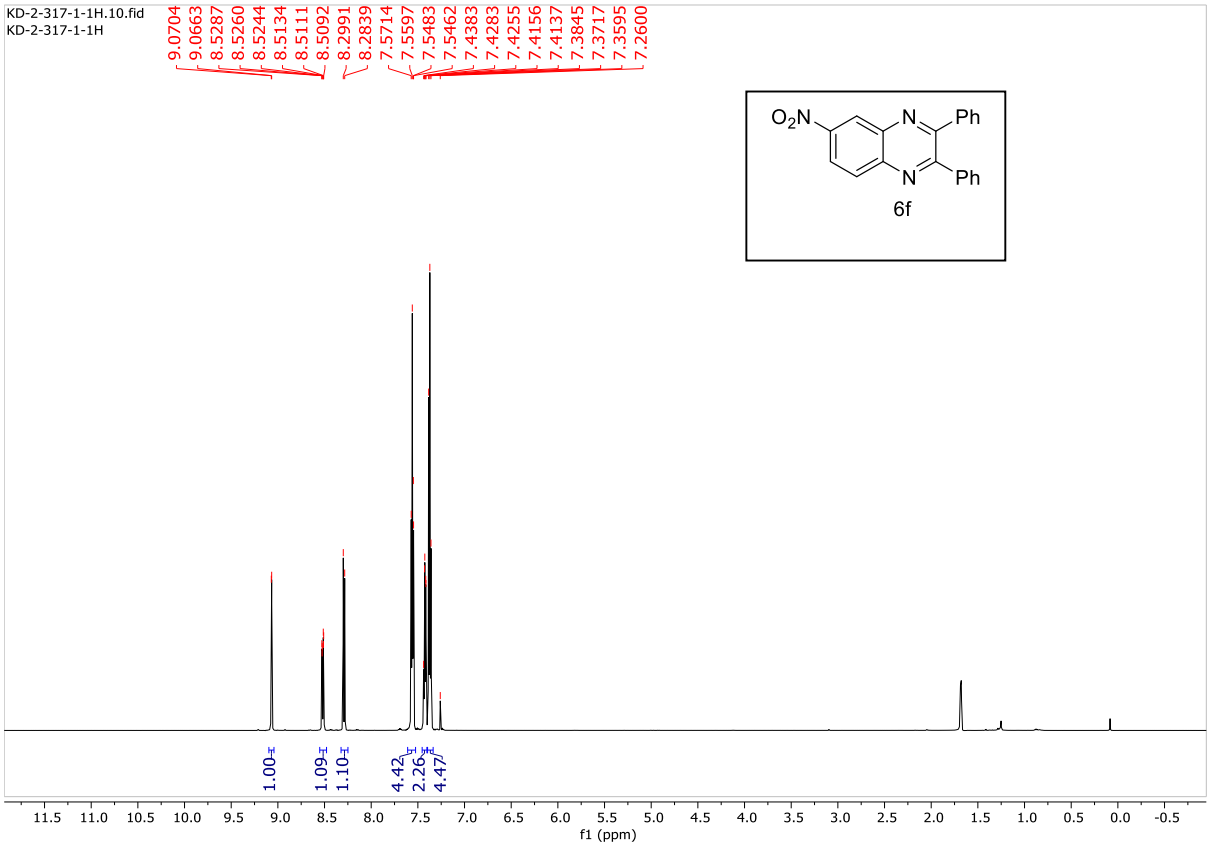

KD-2-314-B-13C
KD-2-314-B-13C
152.61
140.63
140.34
139.51
129.96
128.63
128.33
128.30
77.48
77.16
76.84
20.55
H3C
N
Ph
H3C
N
Ph
6c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

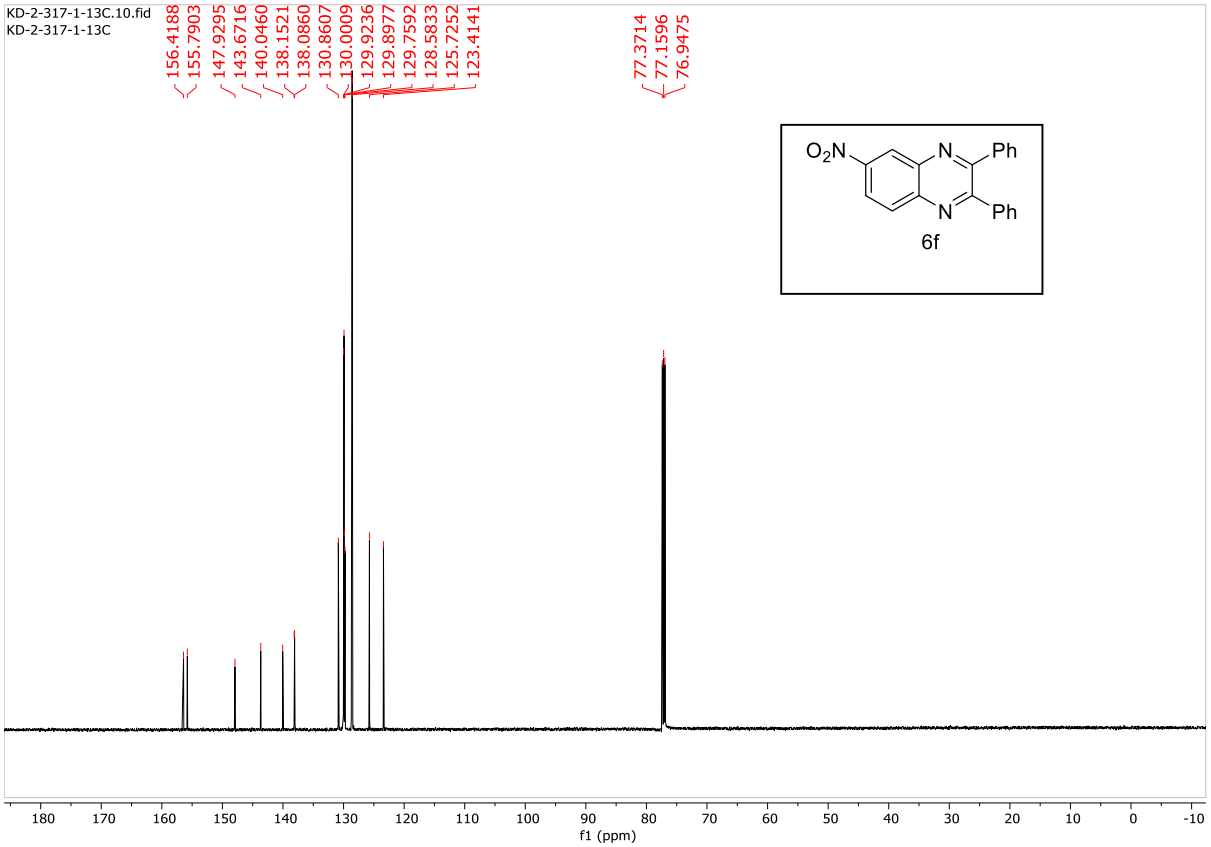

KD-2-351-R1-A-1H
1H
8.2034
7.4358
7.4333
7.4276
7.4194
7.4159
7.4135
7.3221
7.3099
7.3064
7.2998
7.2976
7.2742
7.2615
7.2498
0.0005
Cl
Cl
N
N
Ph
Ph
6d
2.00
4.40
2.43
4.16
f1 (ppm)

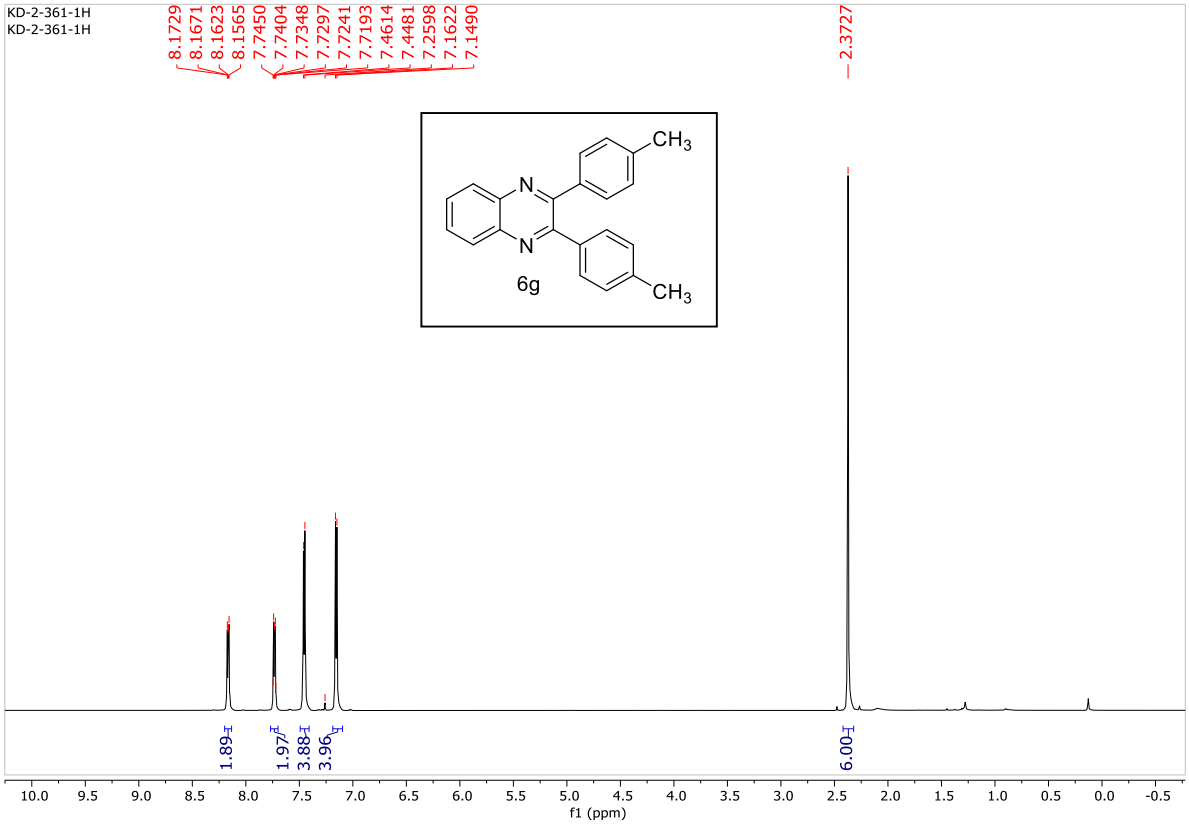

KD-2-351-R1-A-1H
1H
154.5940
140.0433
138.4737
134.5371
129.9097
129.8951
129.4169
128.4848
77.3721
77.1605
76.9486
Cl
Cl
N
N
Ph
Ph
6d
f1 (ppm)

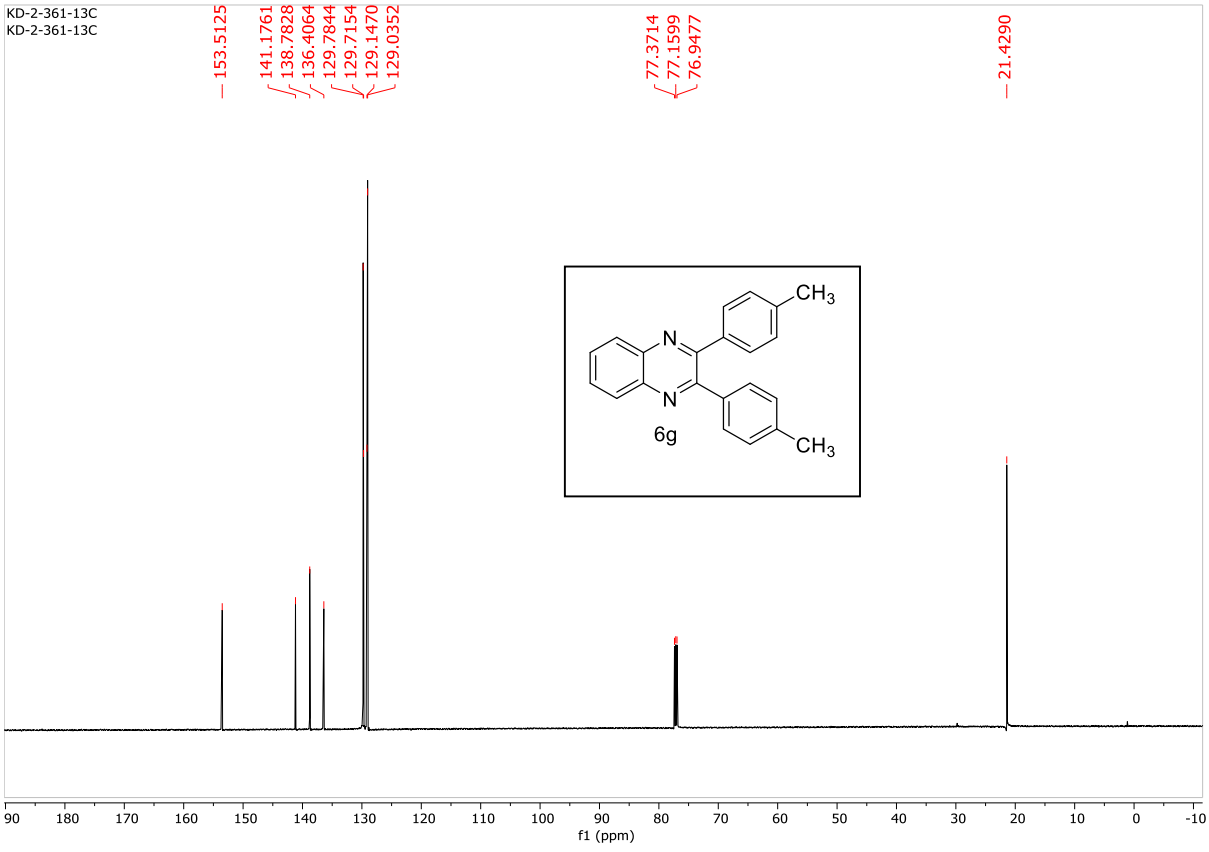

KD-2-316-1-1H.10.fid
1H
8.3619
8.3578
8.0385
8.0237
7.8389
7.8355
7.8241
7.8207
7.5204
7.5084
7.3929
7.3805
7.3689
7.3519
7.3391
7.3274
7.2600
Br
N
Ph
N
Ph
6e
1.00
1.09
1.10
4.30
2.21
4.37
f1 (ppm)

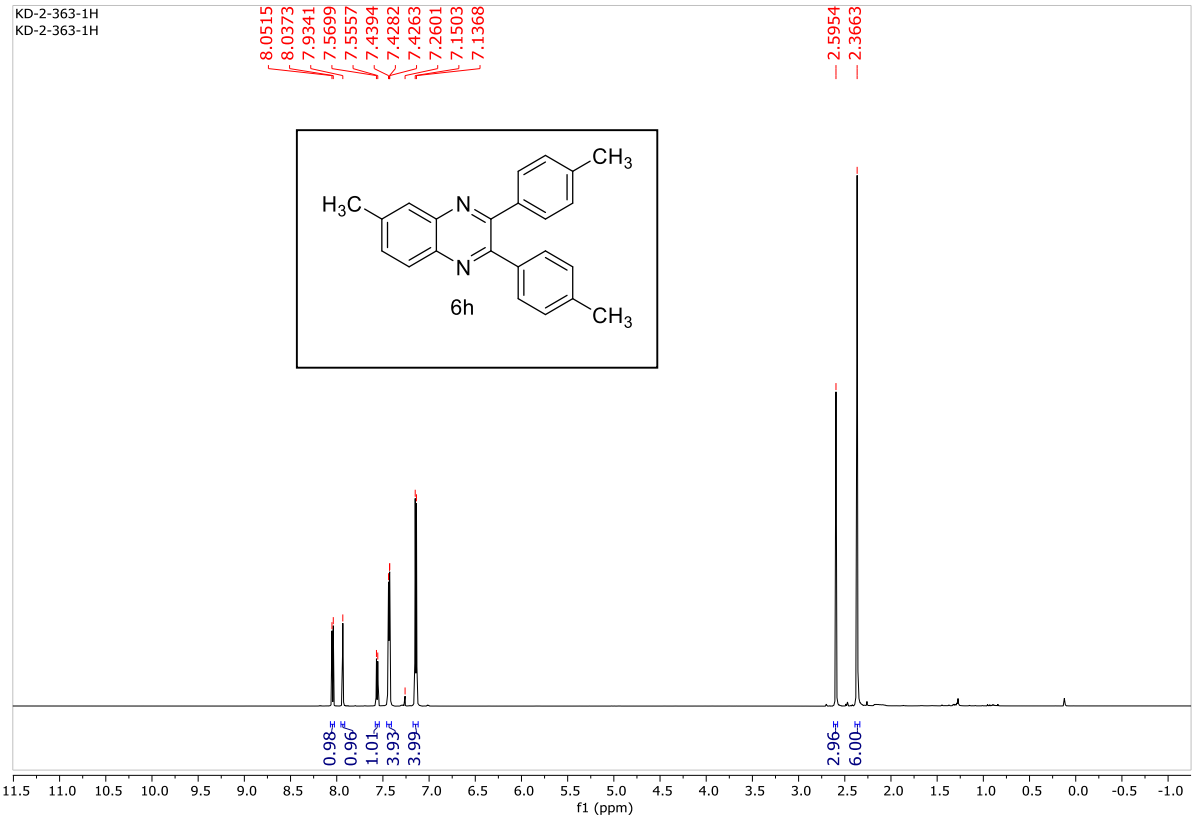

KD-2-316-1-13C.10.fid
13C
154.3055
153.8184
141.8212
140.0081
138.7729
138.6679
133.5805
131.5336
130.5817
129.9273
129.8636
129.2196
129.1490
128.4309
128.4127
123.9251
77.3707
77.1593
76.9478
Br
N
Ph
N
Ph
6e
f1 (ppm)

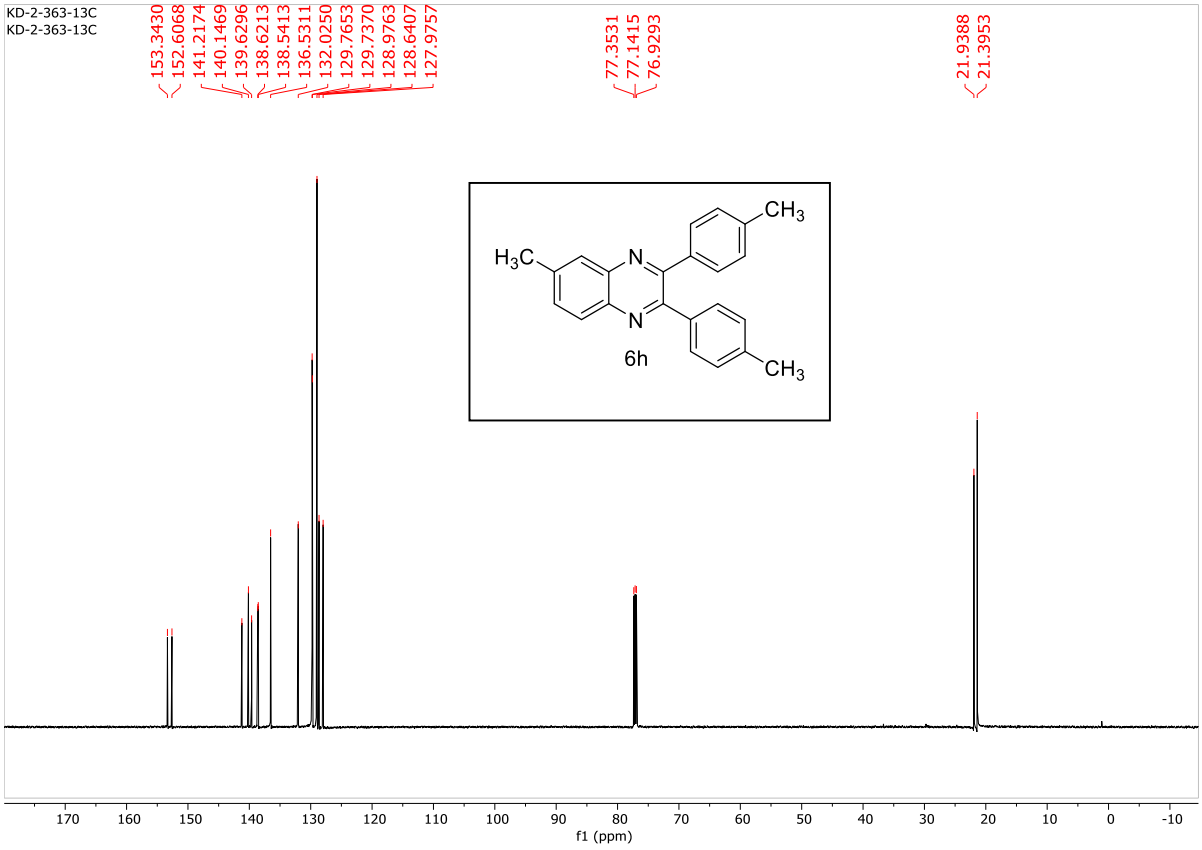

KD-2-317-1-1H.10.fid
KD-2-317-1-1H
9.0704
9.0663
8.5287
8.5260
8.5244
8.5134
8.5111
8.5092
8.2991
8.2839
7.5714
7.5597
7.5483
7.5462
7.4383
7.4283
7.4255
7.4156
7.4137
7.3845
7.3717
7.3595
7.2600
O2N
N
Ph
N
Ph
6f
1.00
1.09
1.10
4.42
2.26
4.47
f1 (ppm)

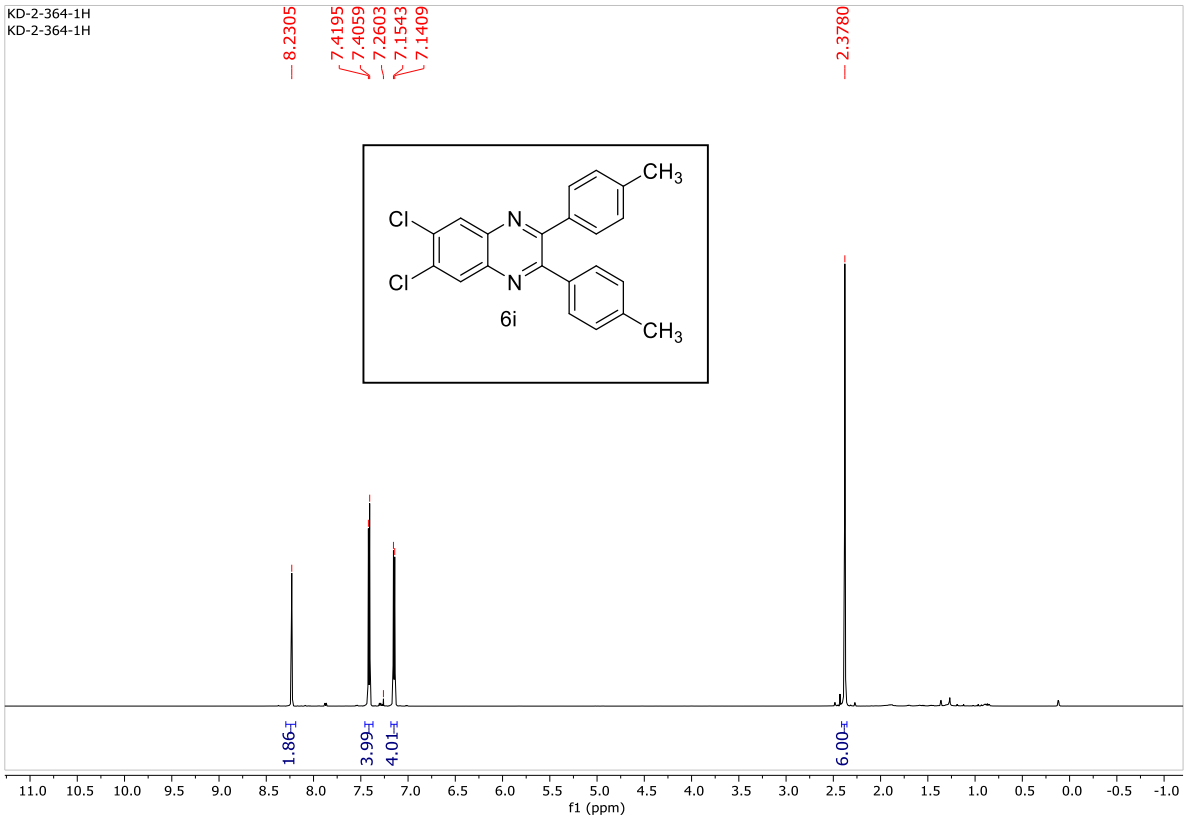

KD-2-317-1-13C.10.fid
KD-2-317-1-13C
156.4188
155.7903
147.9295
143.6716
140.0460
138.1521
138.0860
130.8607
130.0009
129.9236
129.8977
129.7592
128.5833
125.7252
123.4141
77.3714
77.1596
76.9475
O2N
N
Ph
N
Ph
6f
f1 (ppm)

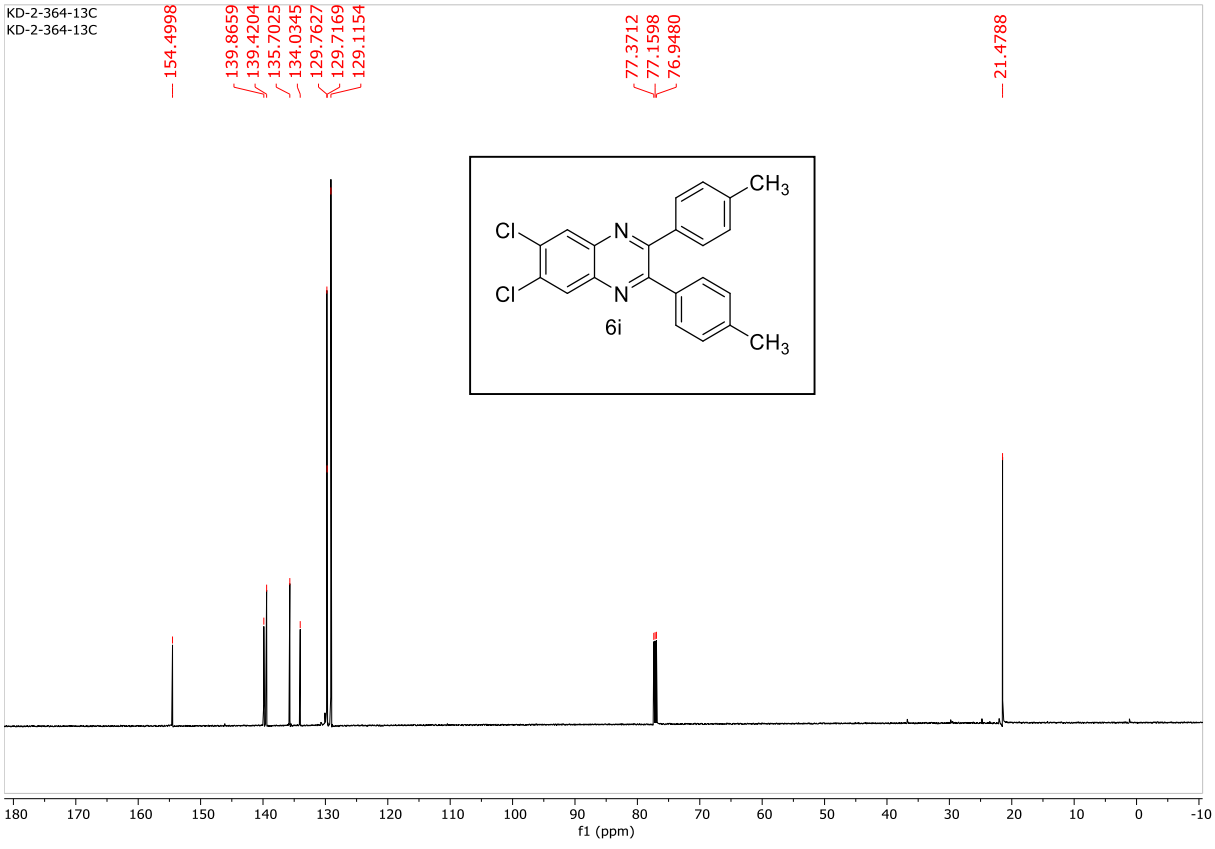

KD-2-361-1H
KD-2-361-1H
8.1729
8.1671
8.1623
8.1565
7.7450
7.7404
7.7348
7.7297
7.7241
7.7193
7.4614
7.4481
7.2598
7.1622
7.1490
2.3727
CH3
N
N
CH3
6g
1.89
1.97
3.88
3.96
6.00
f1 (ppm)

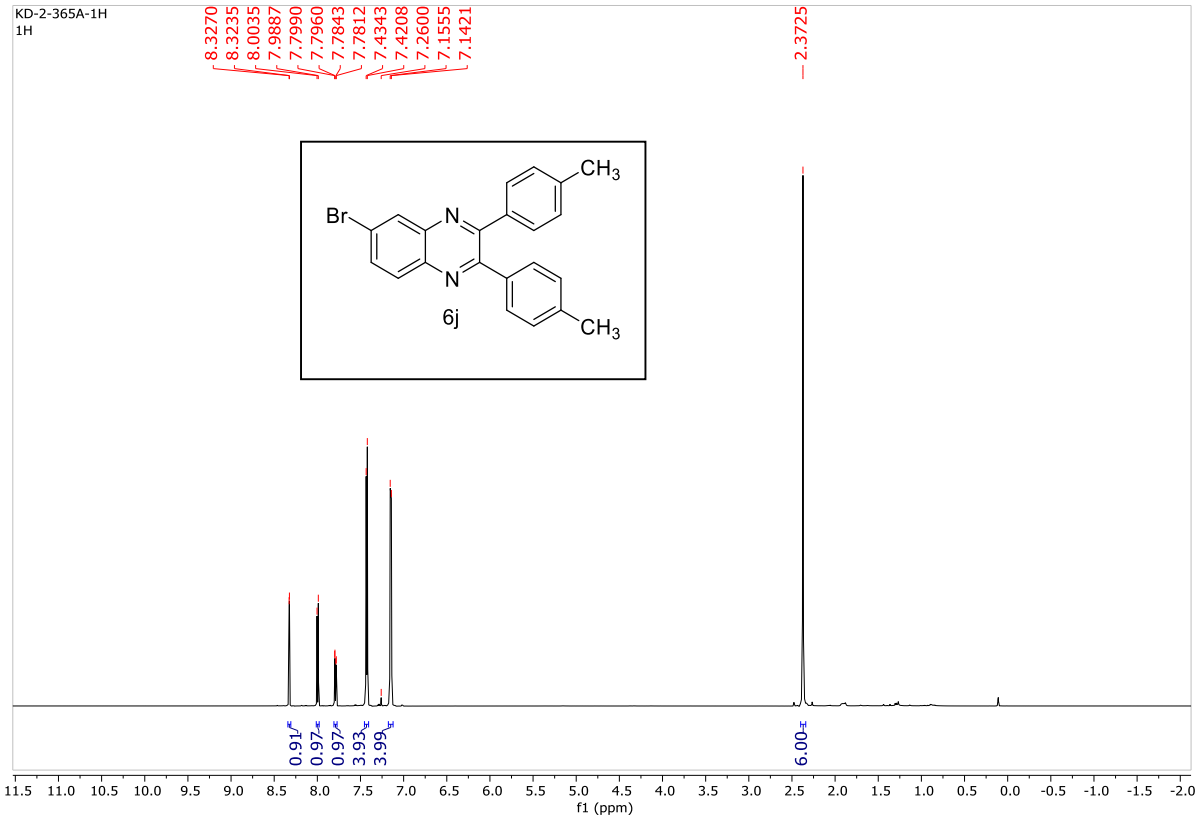

KD-2-361-13C
KD-2-361-13C
153.5125
141.1761
138.7828
136.4064
129.7844
129.7154
129.1470
129.0352
77.3714
77.1599
76.9477
21.4290
CH3
N
N
CH3
6g
f1 (ppm)

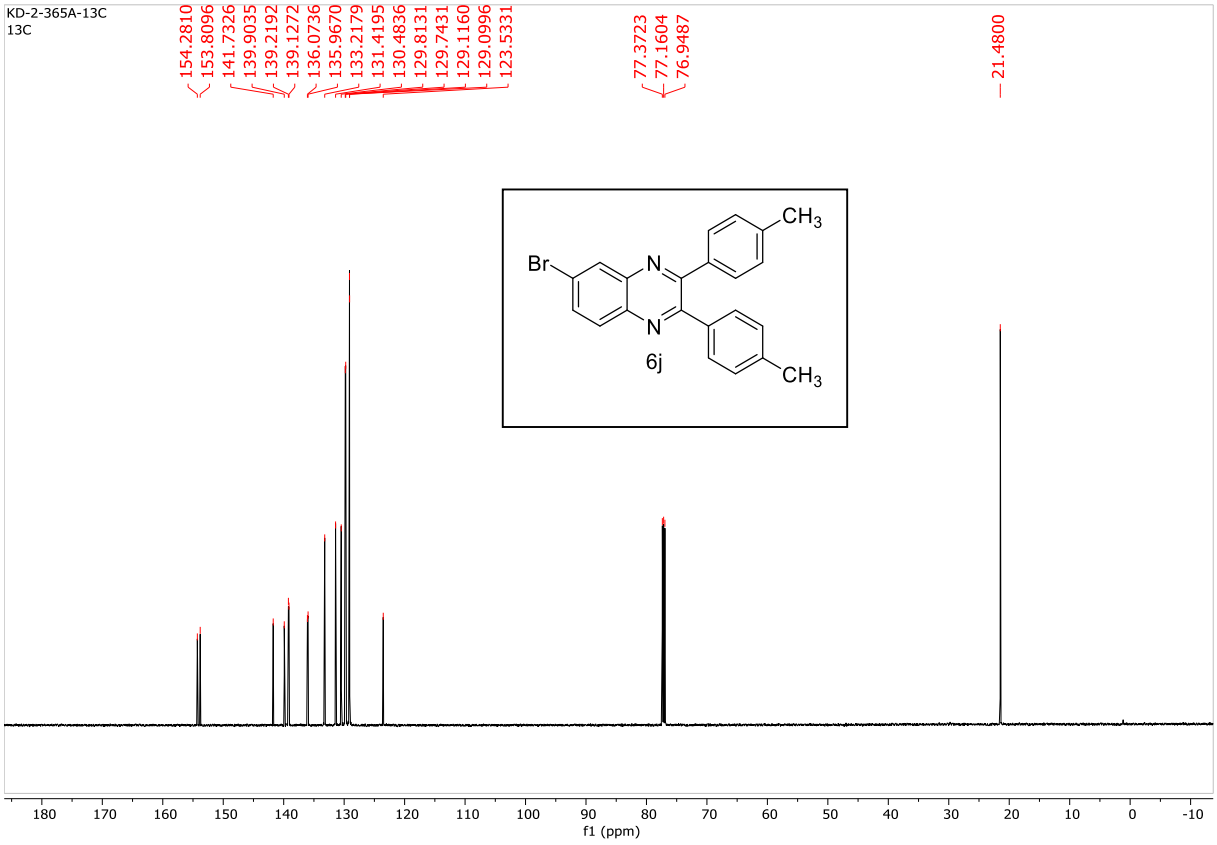

KD-2-363-1H
KD-2-363-1H
8.0515
8.0373
7.9341
7.5699
7.5557
7.4394
7.4282
7.4263
7.2601
7.1503
7.1368
2.5954
2.3663
CH3
H3C
N
N
6h
CH3
0.98
0.96
1.01
3.93
3.99
2.96
6.00
f1 (ppm)


KD-2-363-13C
KD-2-363-13C
153.3430
152.6068
141.2174
140.1469
139.6296
138.6213
138.5413
136.5311
132.0250
129.7653
129.7370
128.9763
128.6407
127.9757
77.3531
77.1415
76.9293
21.9388
21.3953
CH3
H3C
N
N
6h
CH3
f1 (ppm)


KD-2-364-1H
KD-2-364-1H
8.2305
7.4195
7.4059
7.2603
7.1543
7.1409
2.3780
Cl
Cl
N
N
CH3
CH3
6i
1.86
3.99
4.01
6.00
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 -0.5 -1.0
f1 (ppm)


KD-2-364-13C
KD-2-364-13C
154.4998
139.8659
139.4204
135.7025
134.0345
129.7627
129.7169
129.1154
77.3712
77.1598
76.9480
21.4788
Cl
Cl
N
N
CH3
CH3
6i
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


KD-2-365A-1H
1H
8.3270
8.3235
8.0035
7.9887
7.7990
7.7960
7.7843
7.7812
7.4343
7.4208
7.2600
7.1555
7.1421
2.3725
Br
N
N
CH3
CH3
6j
0.91
0.97
0.97
3.93
3.99
6.00
f1 (ppm)


KD-2-365A-13C
13C
154.2810
153.8096
141.7326
139.9035
139.2192
139.1272
136.0736
135.9670
133.2179
131.4195
130.4836
129.8131
129.7431
129.1160
129.0996
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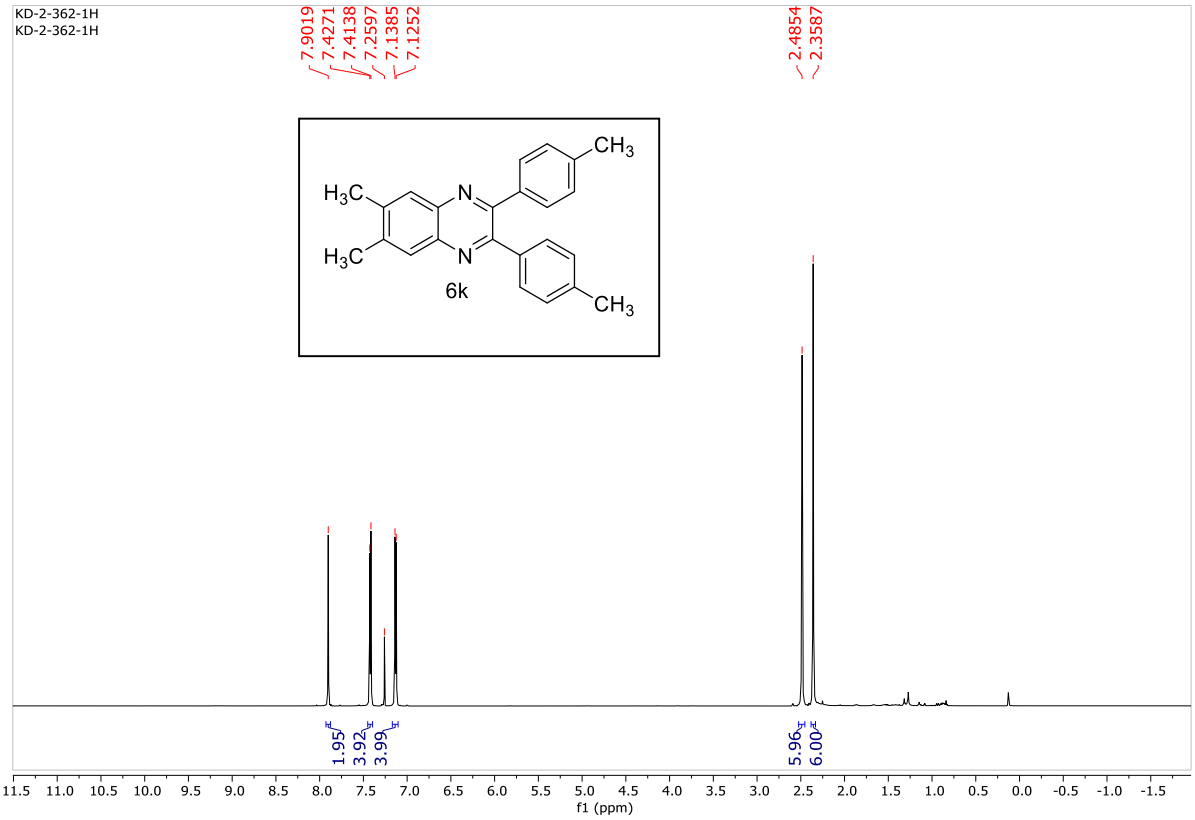
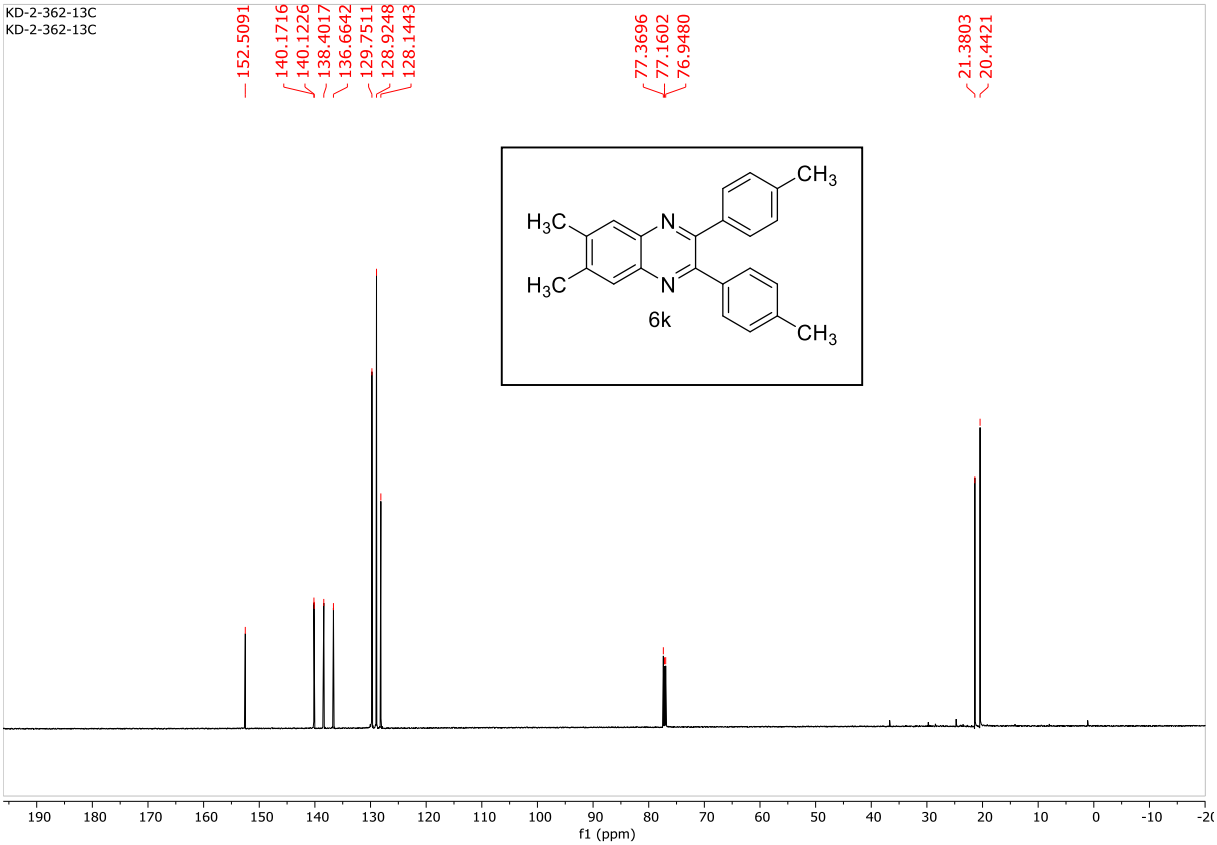
Br
N
N
CH3
CH3
6j
f1 (ppm)


KD-2-362-1H
KD-2-362-1H
7.9019
7.4271
7.4138
7.2597
7.1385
7.1252
2.4854
2.3587
6k
1.95
3.92
3.99
5.96
6.00
f1 (ppm)


KD-2-362-13C
KD-2-362-13C
152.5091
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140.1226
138.4017
136.6642
129.7511
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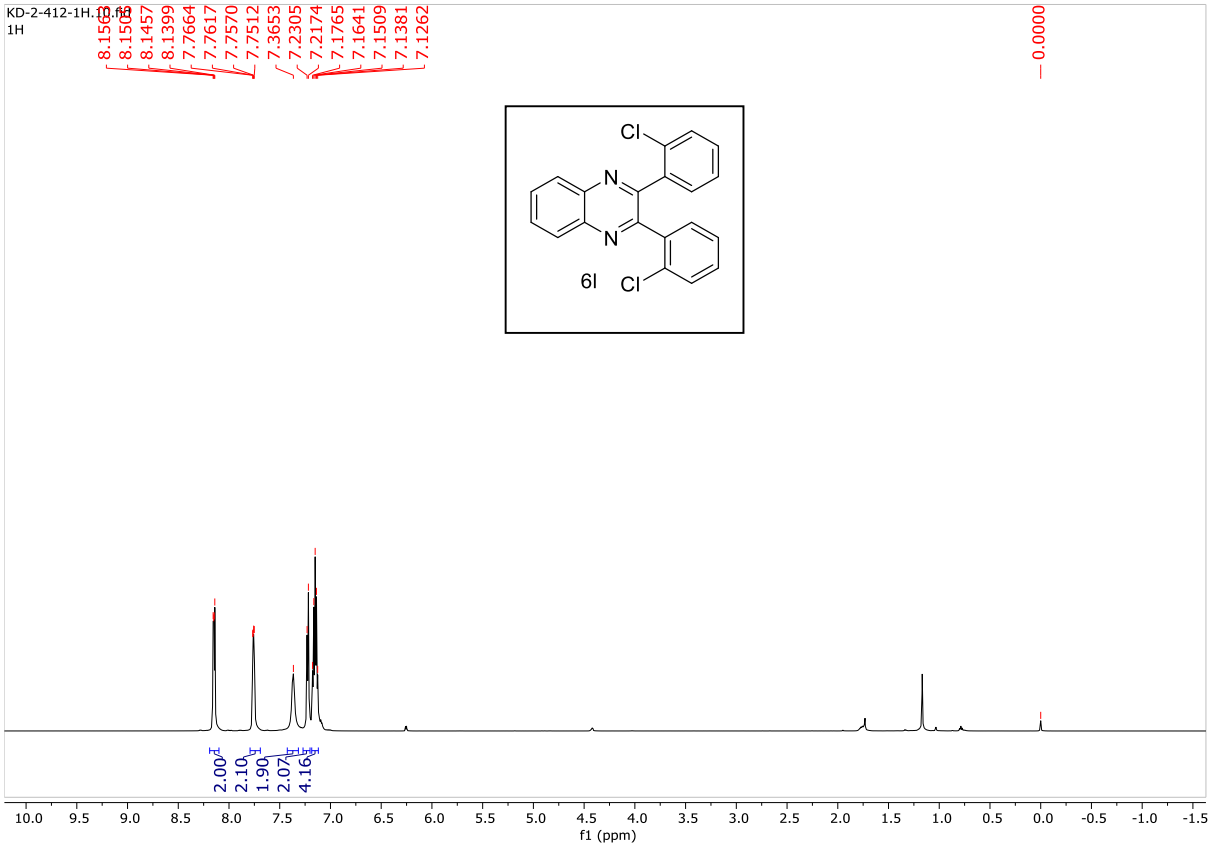
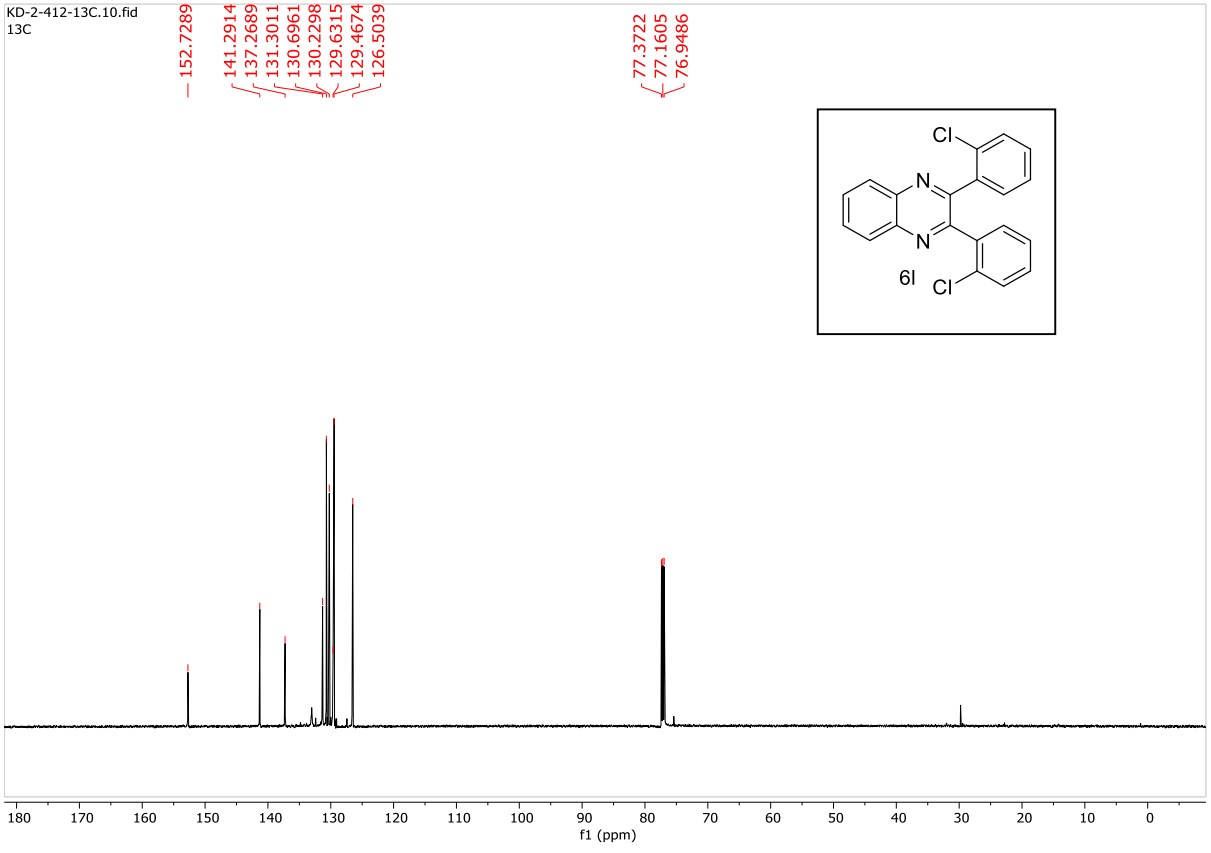
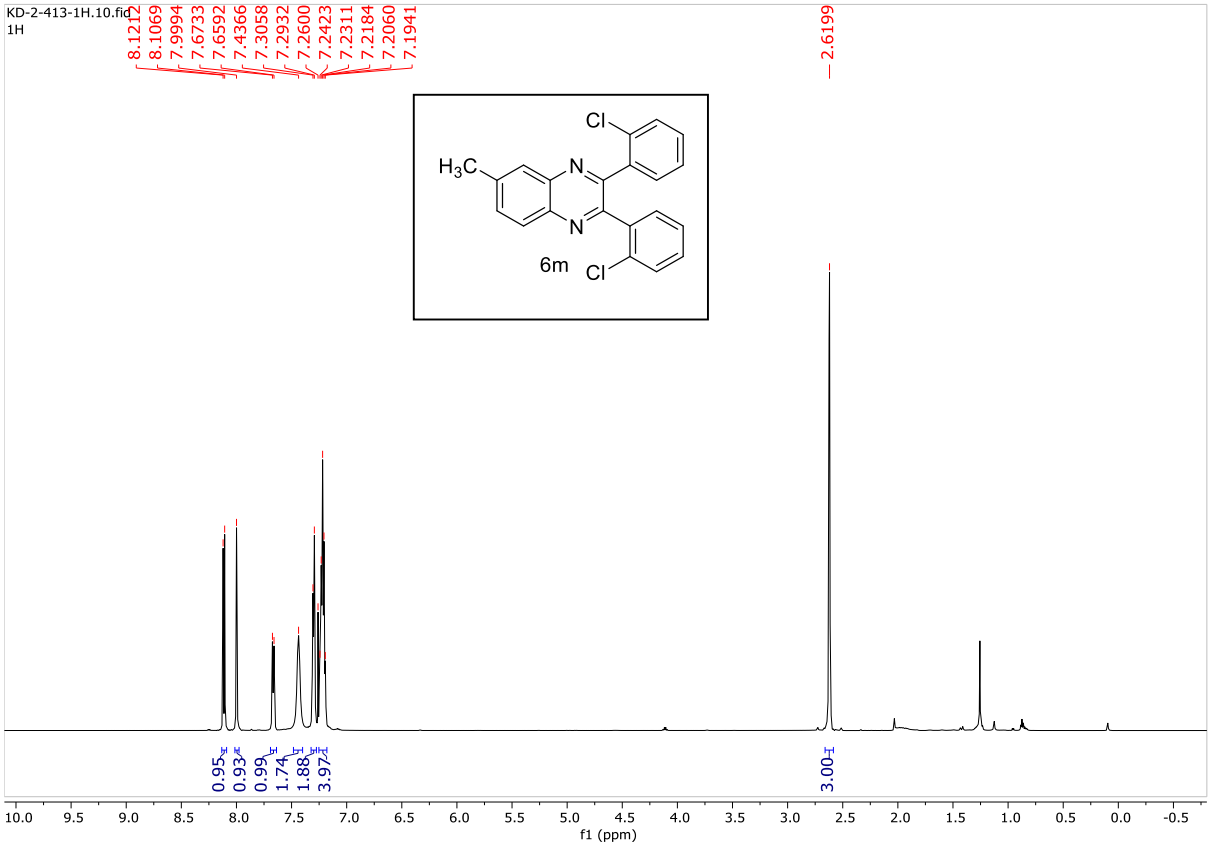
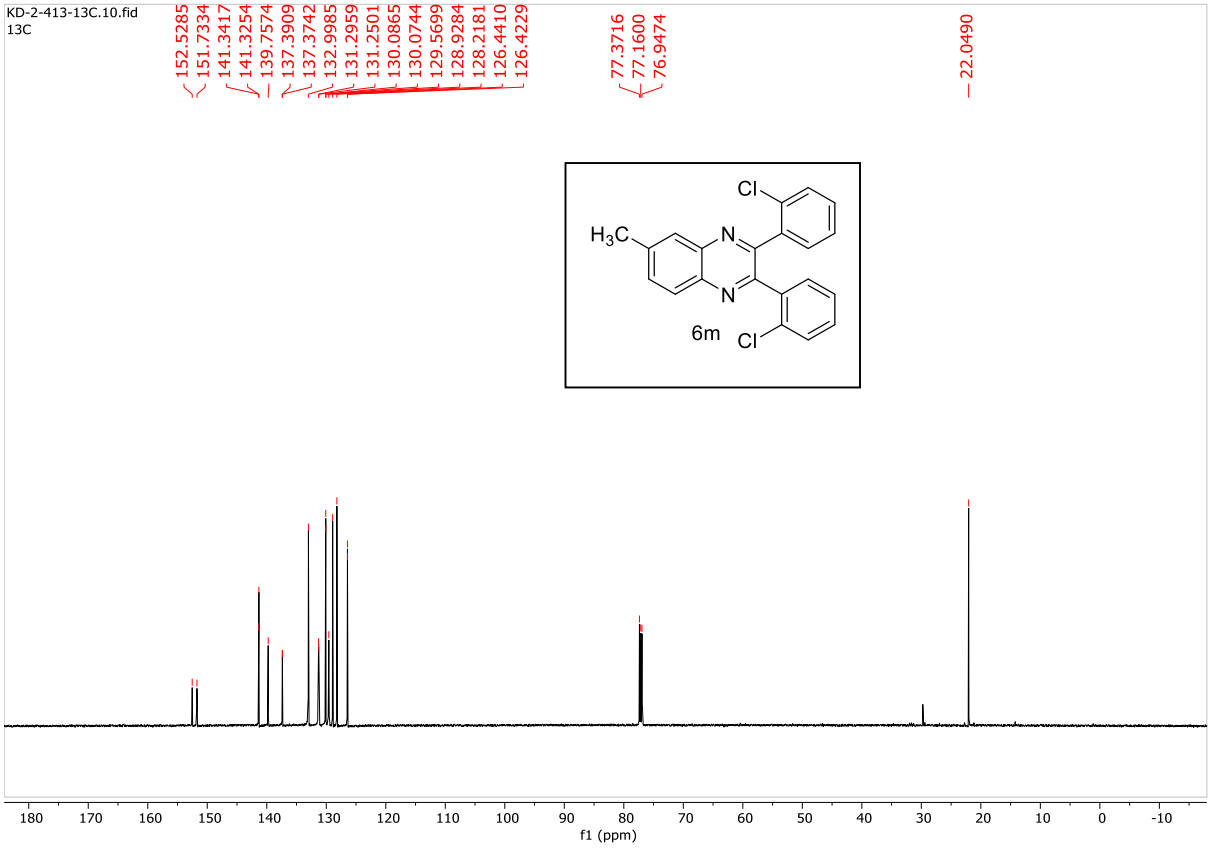
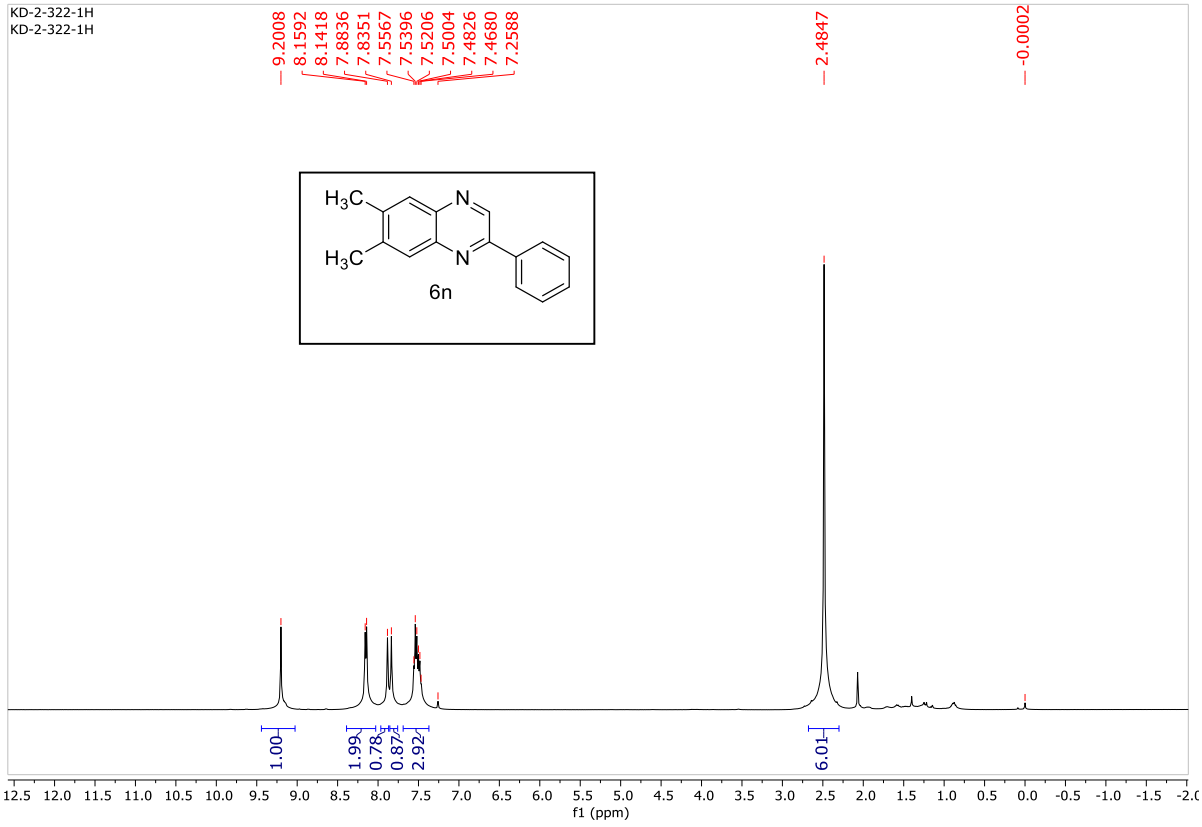
76.9480
21.3803
20.4421
6k
f1 (ppm)

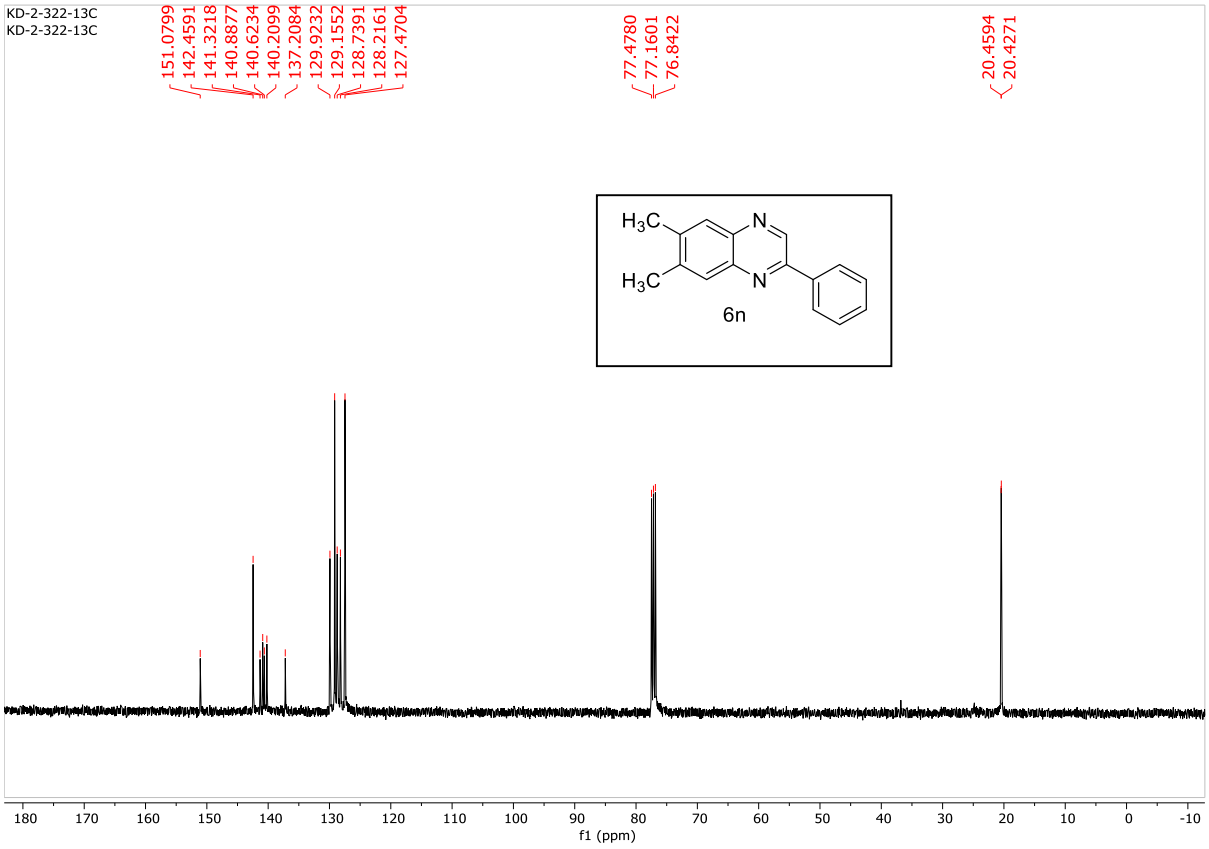

KD-2-412-1H.10.fid
1H
8.1506
8.1457
8.1399
7.7664
7.7617
7.7570
7.7512
7.3653
7.2305
7.2174
7.1765
7.1641
7.1509
7.1381
7.1262
0.0000
Cl
N
N
6l
Cl
2.00
2.10
1.90
2.07
4.16
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

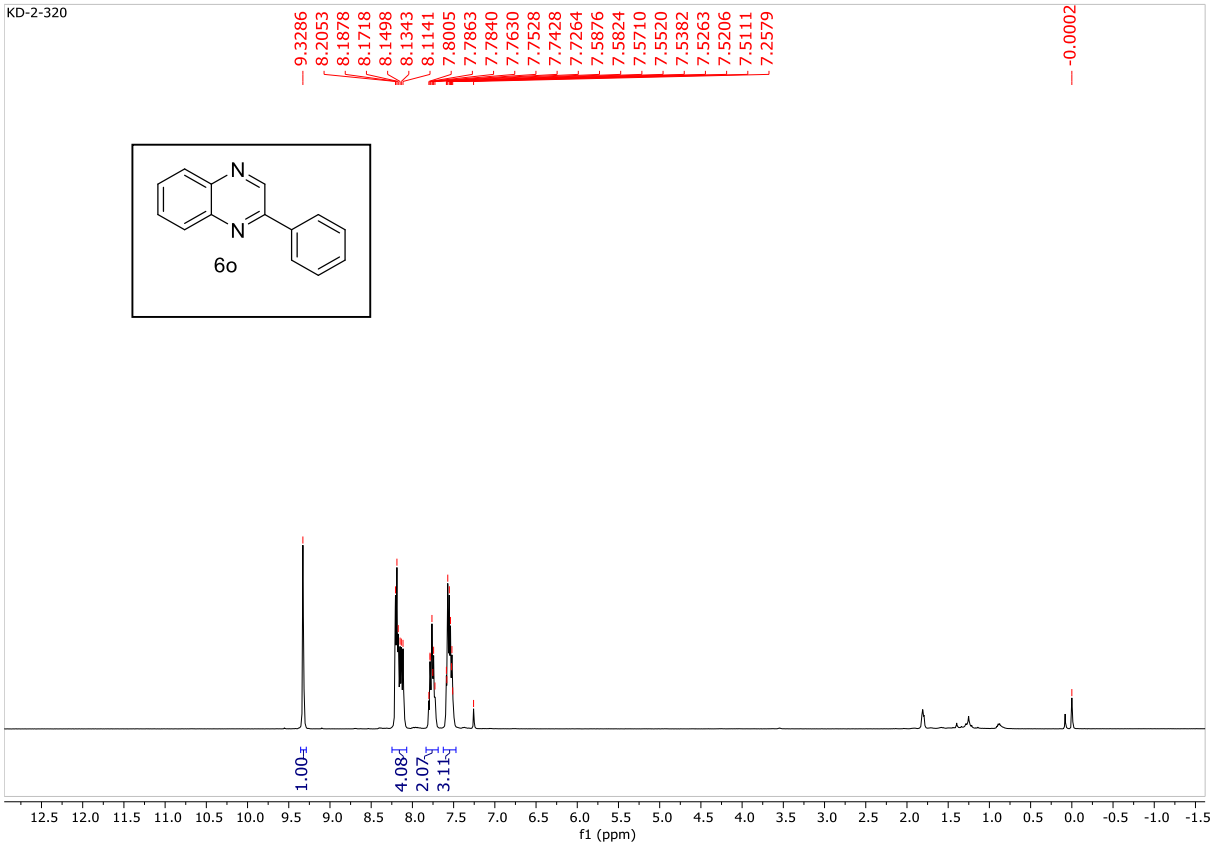

KD-2-412-13C.10.fid
13C
152.7289
141.2914
137.2689
131.3011
130.6961
130.2298
129.6315
129.4674
126.5039
77.3722
77.1605
76.9486
Cl
N
N
6l
Cl
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

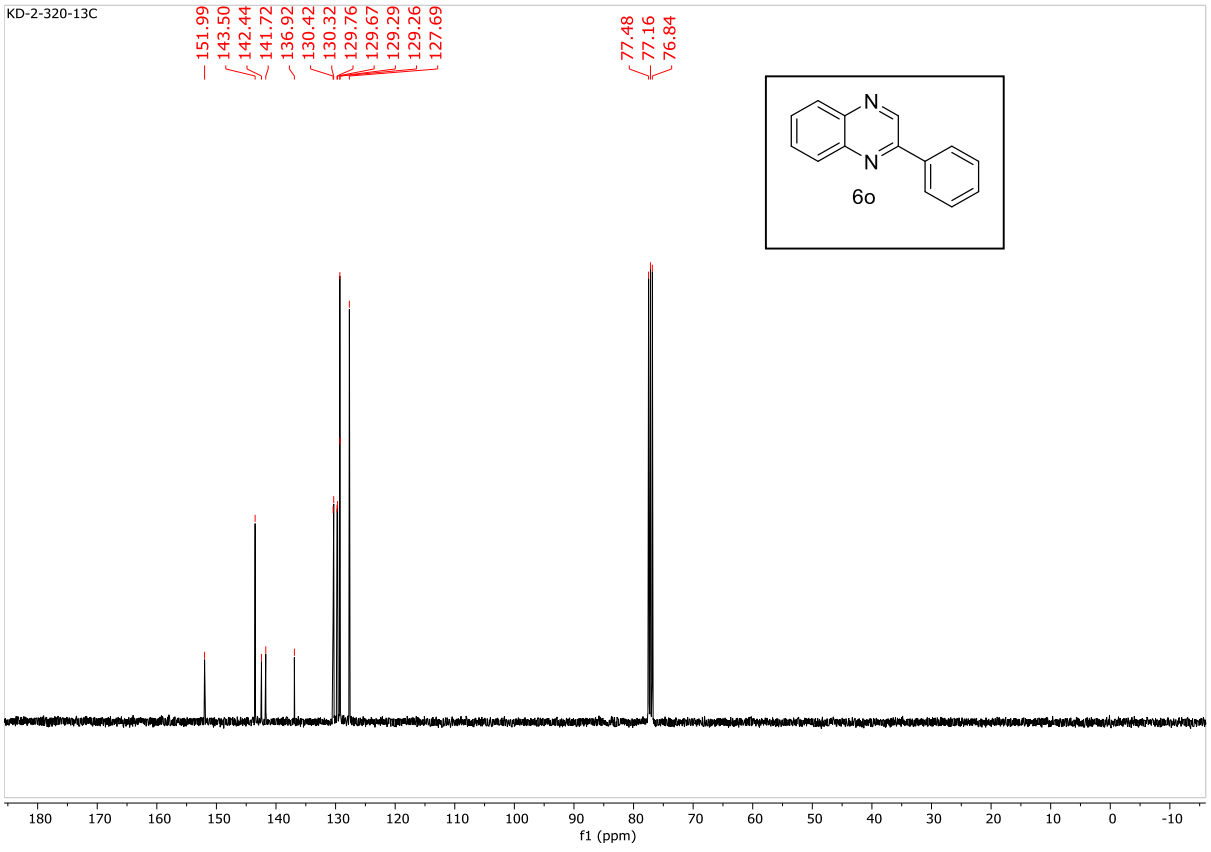

KD-2-413-1H.10.fid
1H
8.1212
8.1069
7.9994
7.6733
7.6592
7.4366
7.3058
7.2932
7.2600
7.2423
7.2311
7.2184
7.2060
7.1941
2.6199
Cl
H3C
N
N
6m
Cl
0.95
0.93
0.99
1.74
1.88
3.97
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

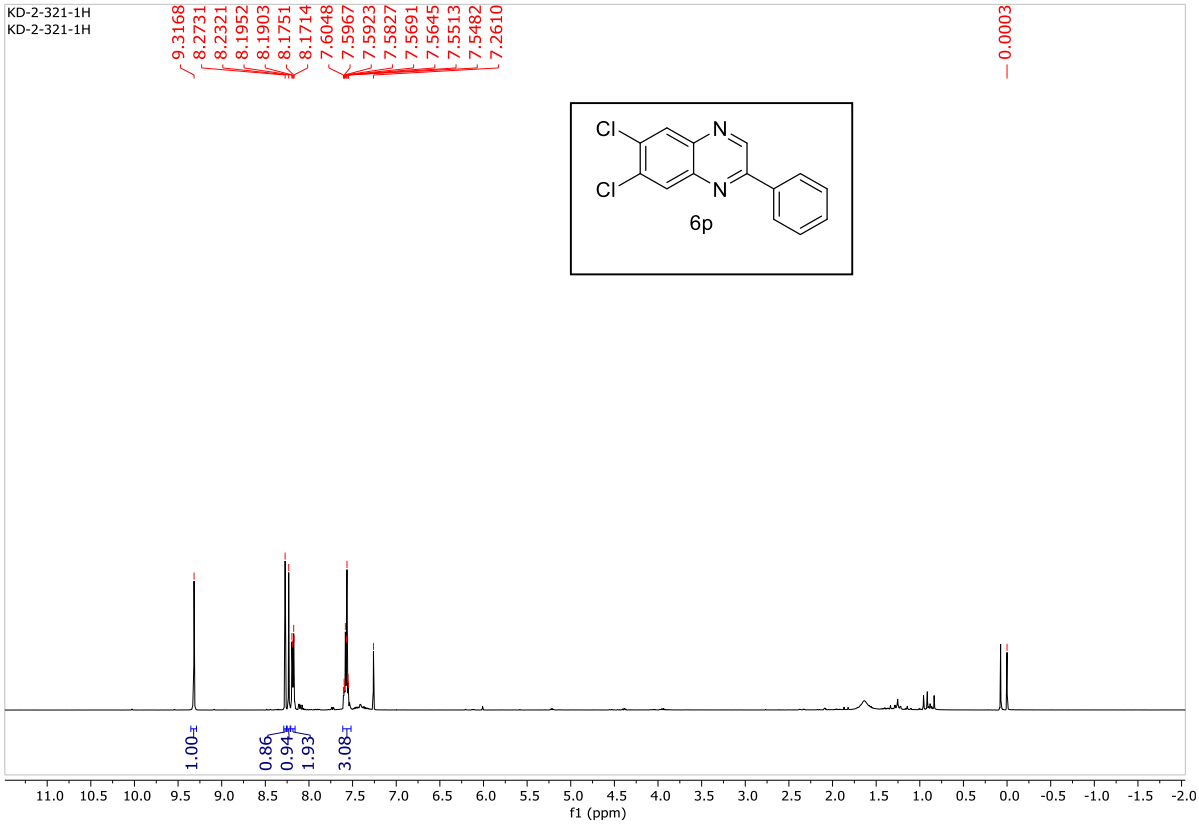

KD-2-413-13C.10.fid
13C
152.5285
151.7334
141.3417
141.3254
139.7574
137.3909
137.3742
132.9985
131.2959
131.2501
130.0865
130.0744
129.5699
128.9284
128.2181
126.4410
126.4229
77.3716
77.1600
76.9474
22.0490
Cl
H3C
N
N
6m
Cl
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

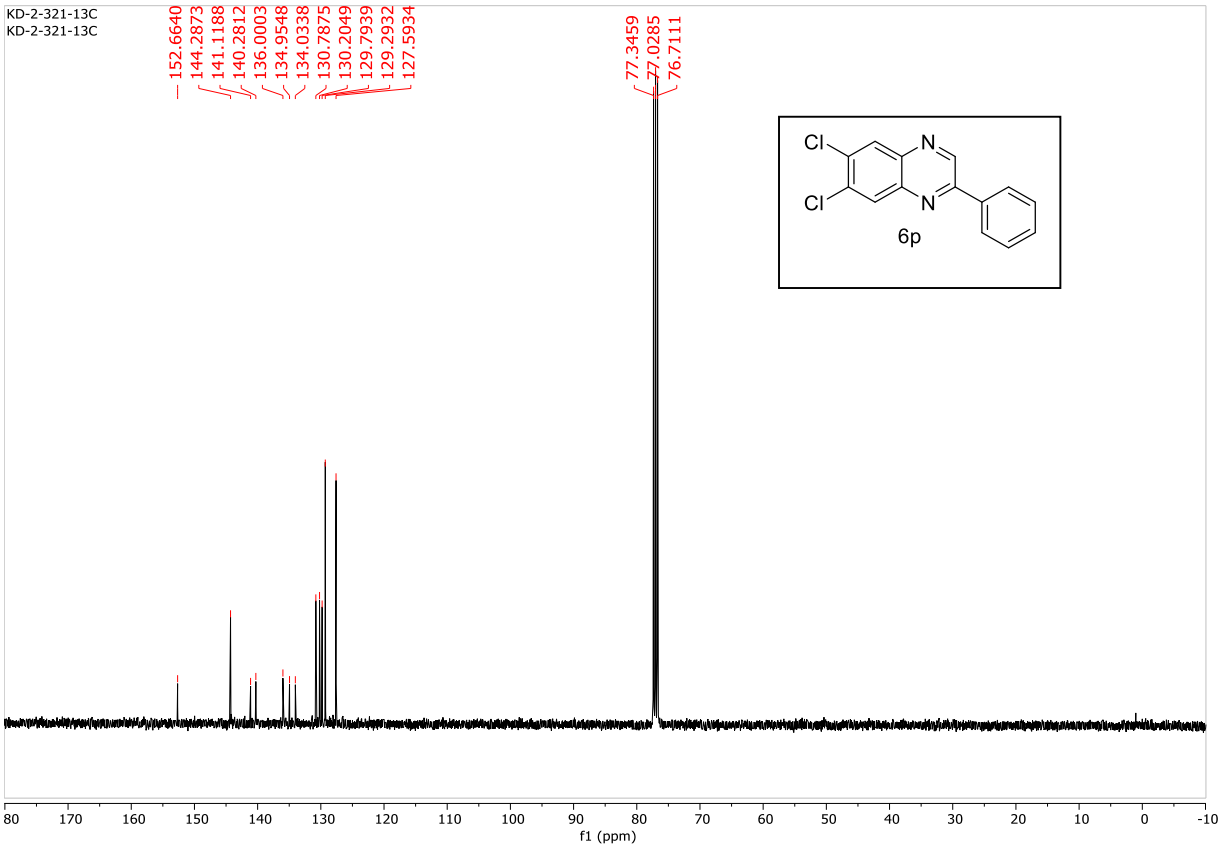

KD-2-322-1H
KD-2-322-1H
9.2008
8.1592
8.1418
7.8836
7.8351
7.5567
7.5396
7.5206
7.5004
7.4826
7.4680
7.2588
2.4847
-0.0002
H3C
H3C
N
N
6n
1.00
1.99
0.78
0.87
2.92
6.01
f1 (ppm)

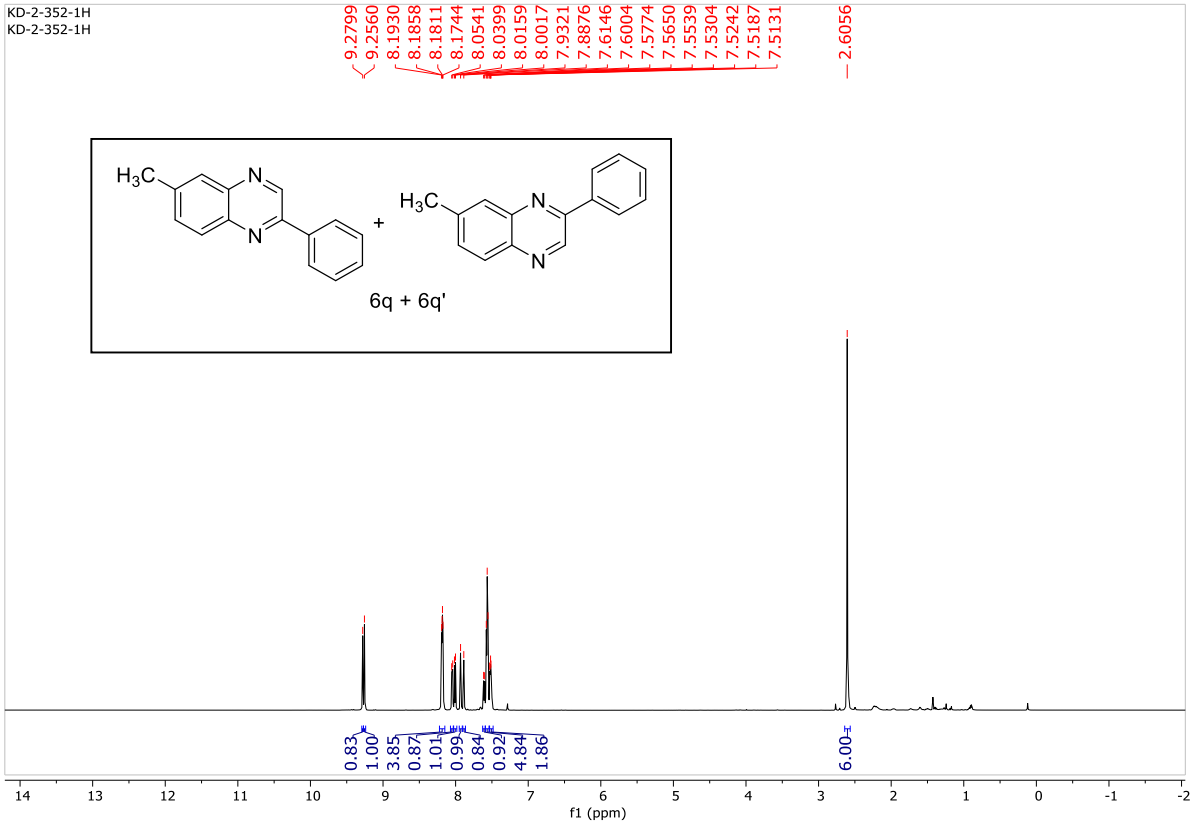

KD-2-322-13C
KD-2-322-13C
151.0799
142.4591
141.3218
140.8877
140.6234
140.2099
137.2084
129.9232
129.1552
128.7391
128.2161
127.4704
77.4780
77.1601
76.8422
20.4594
20.4271
H3C
H3C
N
N
6n
f1 (ppm)

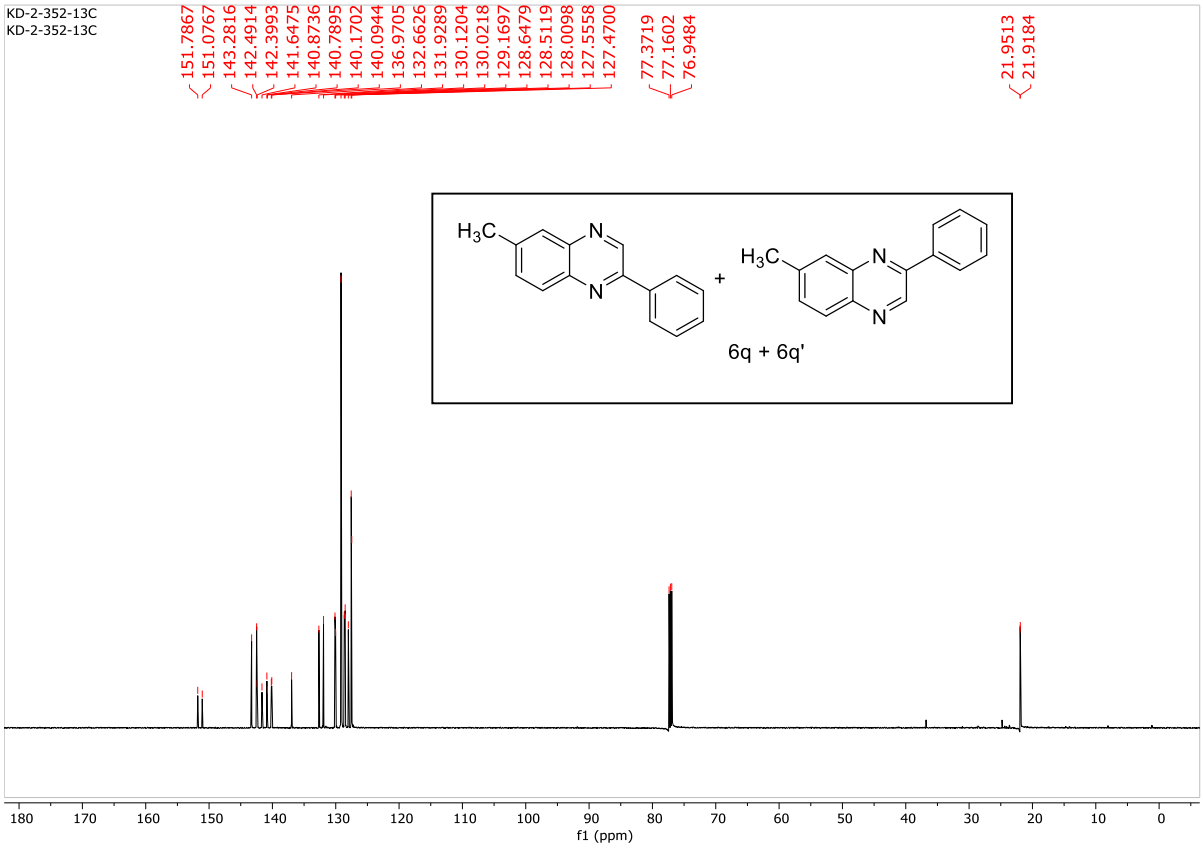

KD-2-320
9.3286
8.2053
8.1878
8.1718
8.1498
8.1343
8.1141
7.8005
7.7863
7.7840
7.7630
7.7528
7.7428
7.7264
7.5876
7.5824
7.5710
7.5520
7.5382
7.5263
7.5206
7.5111
7.2579
-0.0002
6o
1.00
4.08
2.07
3.11
f1 (ppm)

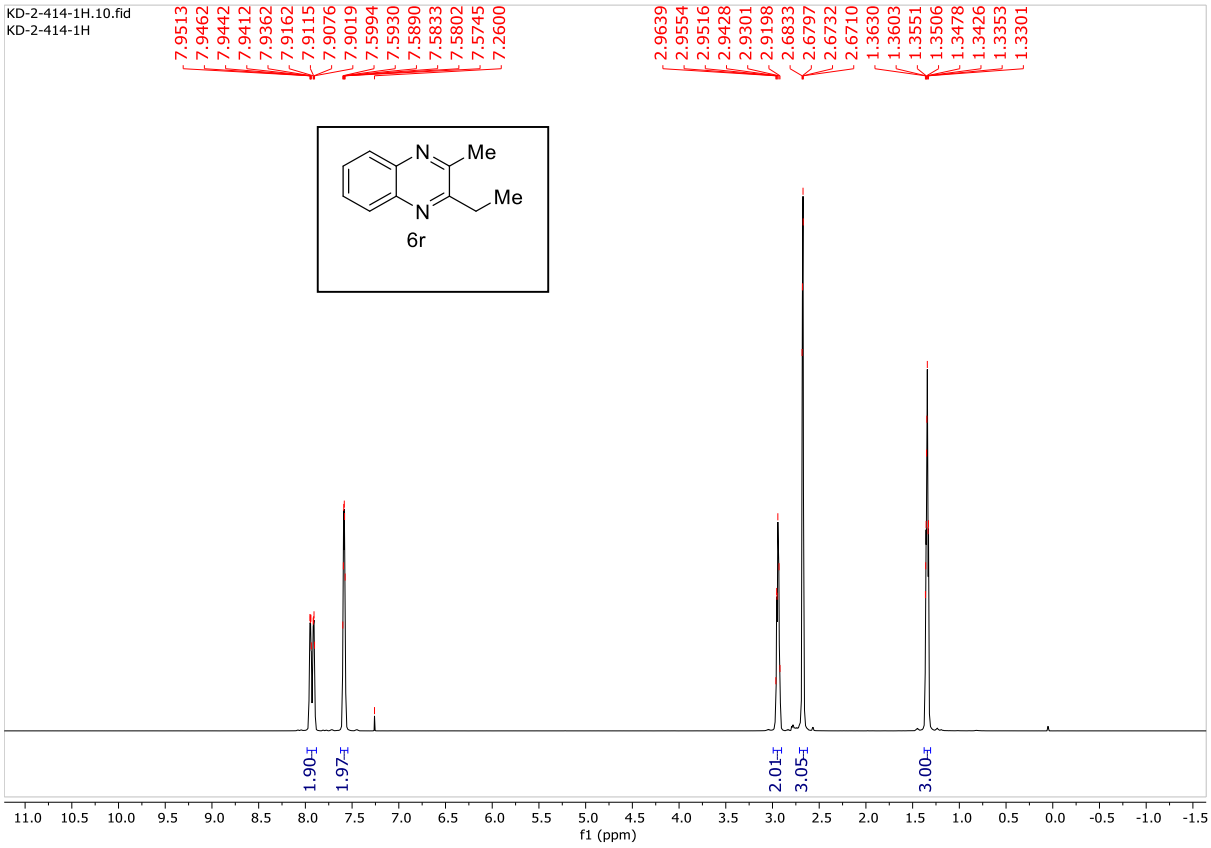

KD-2-320-13C
151.99
143.50
142.44
141.72
136.92
130.42
130.32
129.76
129.67
129.29
129.26
127.69
77.48
77.16
76.84
6o
f1 (ppm)

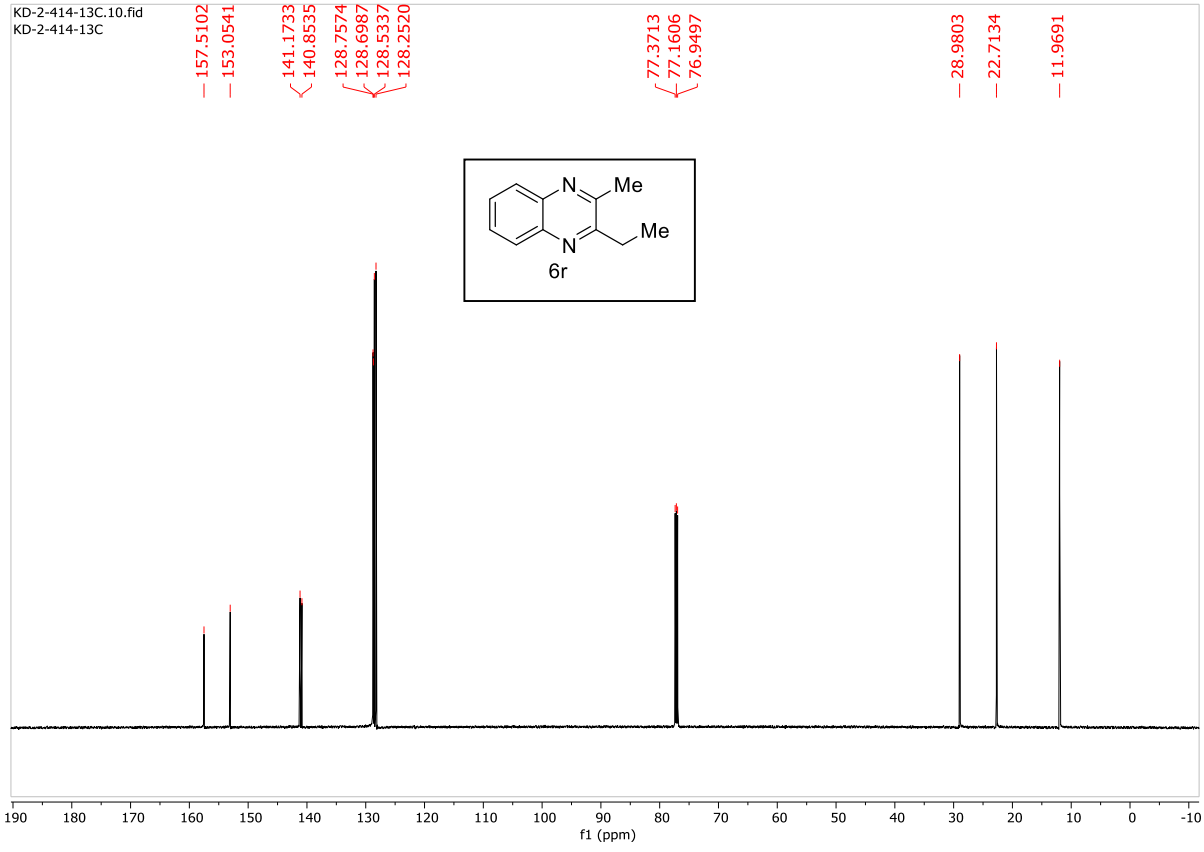

KD-2-321-1H
KD-2-321-1H
9.3168
8.2731
8.2321
8.1952
8.1903
8.1751
8.1714
7.6048
7.5967
7.5923
7.5827
7.5691
7.5645
7.5513
7.5482
7.2610
0.0003
Cl
Cl
N
N
6p
1.00
0.86
0.94
1.93
3.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
f1 (ppm)

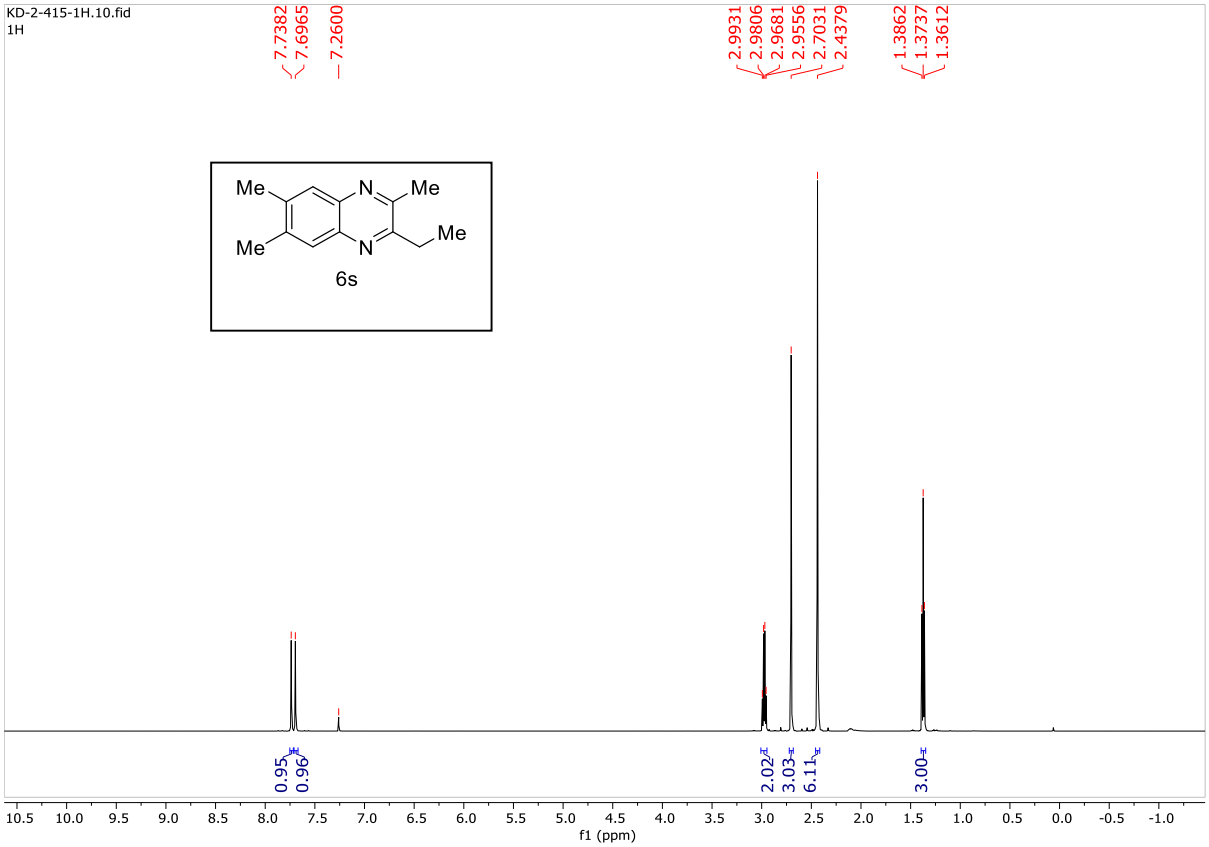

KD-2-321-13C
KD-2-321-13C
152.6640
144.2873
141.1188
140.2812
136.0003
134.9548
134.0338
130.7875
130.2049
129.7939
129.2932
127.5934
77.3459
77.0285
76.7111
Cl
Cl
N
N
6p
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

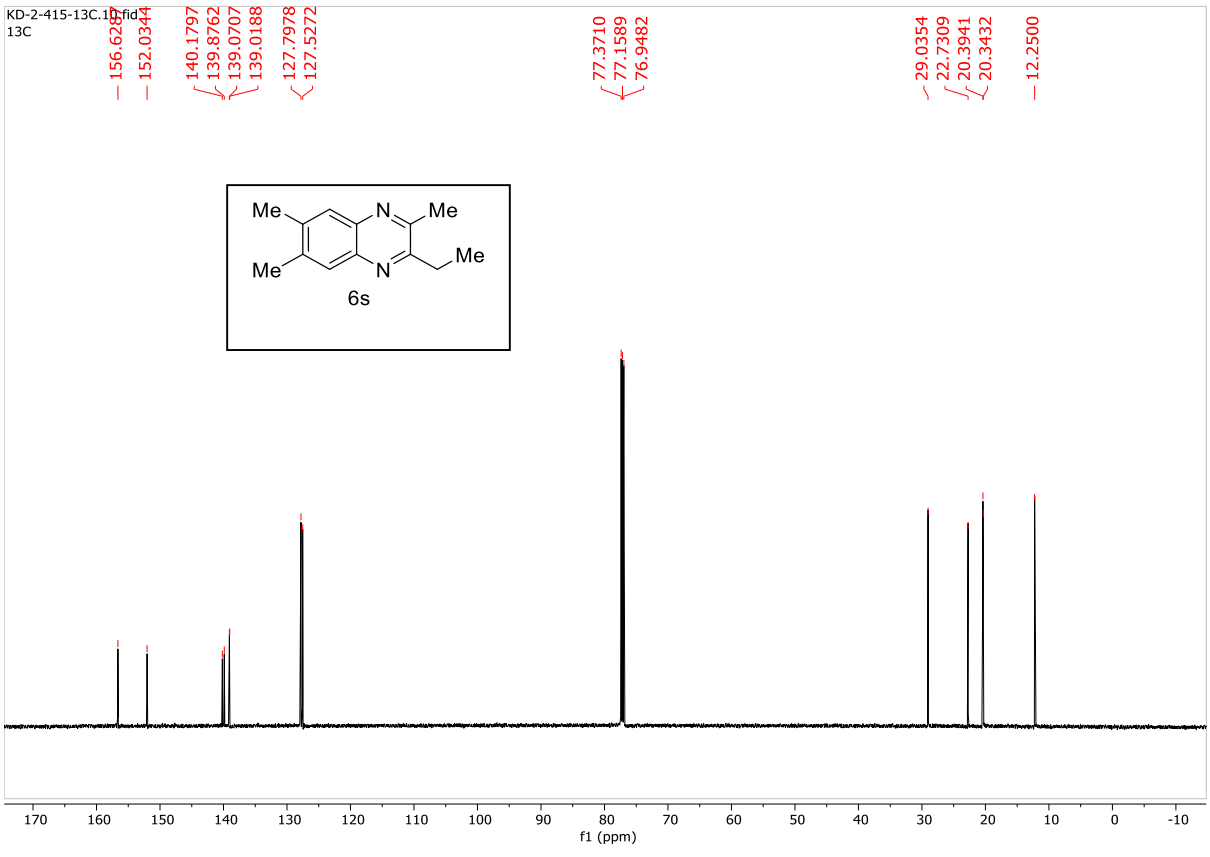

KD-2-352-1H
KD-2-352-1H
9.2799
9.2560
8.1930
8.1858
8.1811
8.1744
8.0541
8.0399
8.0159
8.0017
7.9321
7.8876
7.6146
7.6004
7.5774
7.5650
7.5539
7.5304
7.5242
7.5187
7.5131
2.6056
H3C
N
N
+
H3C
N
N
6q + 6q'
0.83
1.00
3.85
0.87
1.01
0.99
0.84
0.92
4.84
1.86
6.00
f1 (ppm)

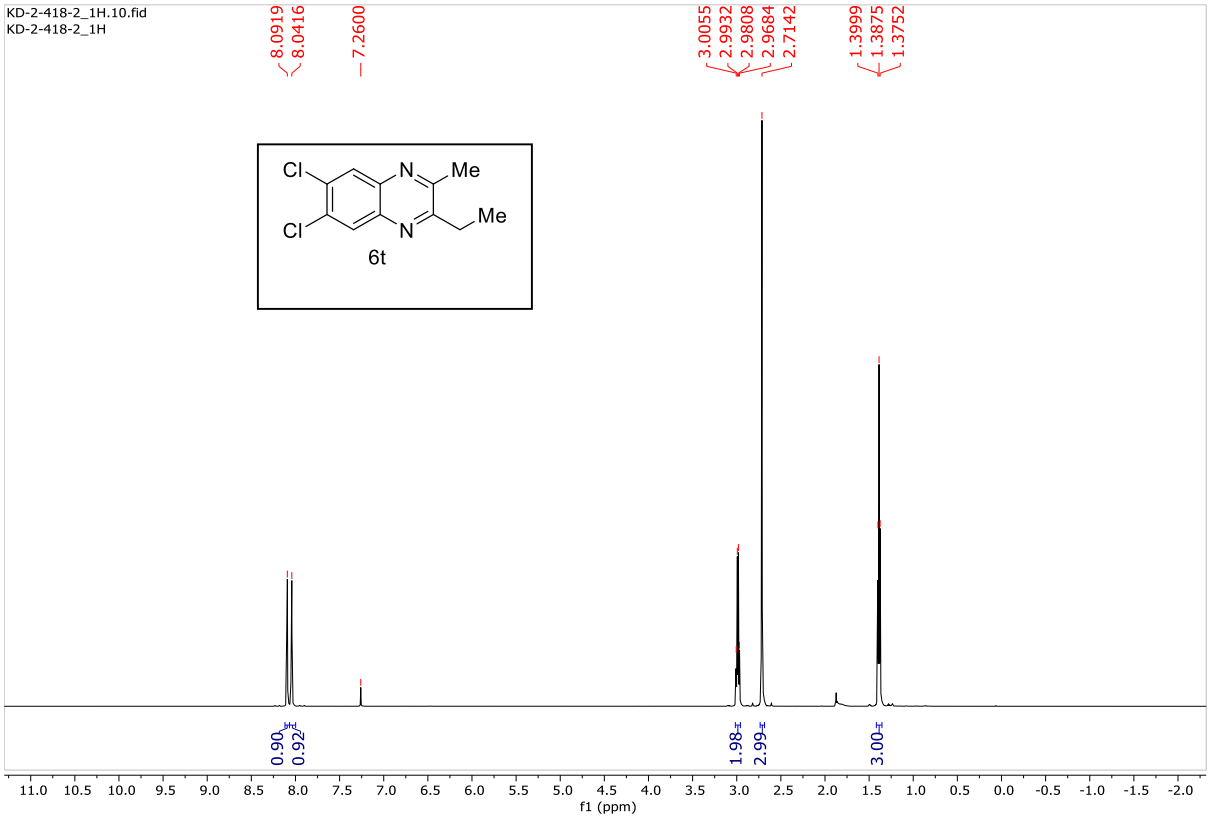

KD-2-352-13C
KD-2-352-13C
151.7867
151.0767
143.2816
142.4914
142.3993
141.6475
140.8736
140.7895
140.1702
140.0944
136.9705
132.6626
131.9289
130.1204
130.0218
129.1697
128.6479
128.5119
128.0098
127.5558
127.4700
77.3719
77.1602
76.9484
21.9513
21.9184
H3C
N
N
+
H3C
N
N
6q + 6q'
f1 (ppm)

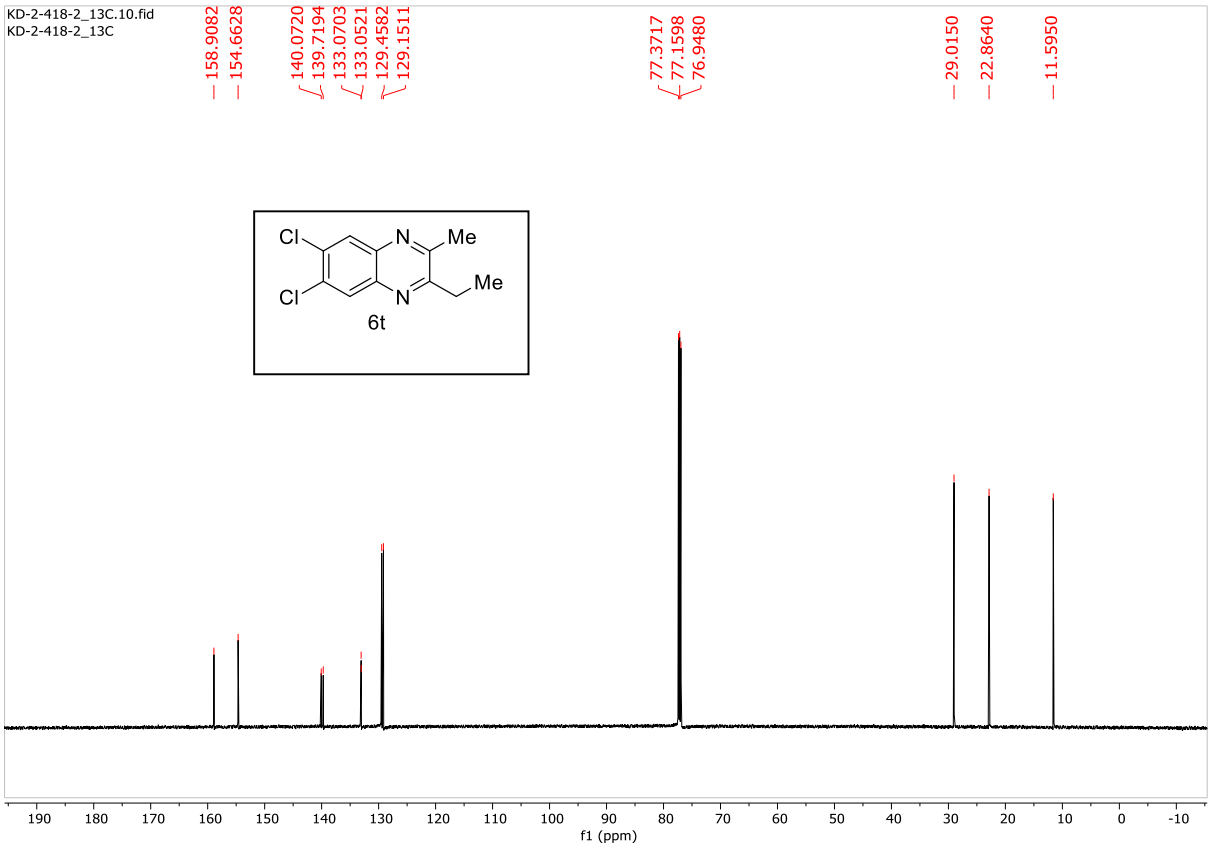

KD-2-414-1H.10.fid
KD-2-414-1H
7.9513
7.9462
7.9442
7.9412
7.9362
7.9162
7.9115
7.9076
7.9019
7.5994
7.5930
7.5890
7.5833
7.5802
7.5745
7.2600
2.9639
2.9554
2.9516
2.9428
2.9301
2.9198
2.6833
2.6797
2.6732
2.6710
1.3630
1.3603
1.3551
1.3506
1.3478
1.3426
1.3353
1.3301
N
Me
N
Me
6r
1.90
1.97
2.01
3.05
3.00
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 -0.5 -1.0 -1.5
f1 (ppm)

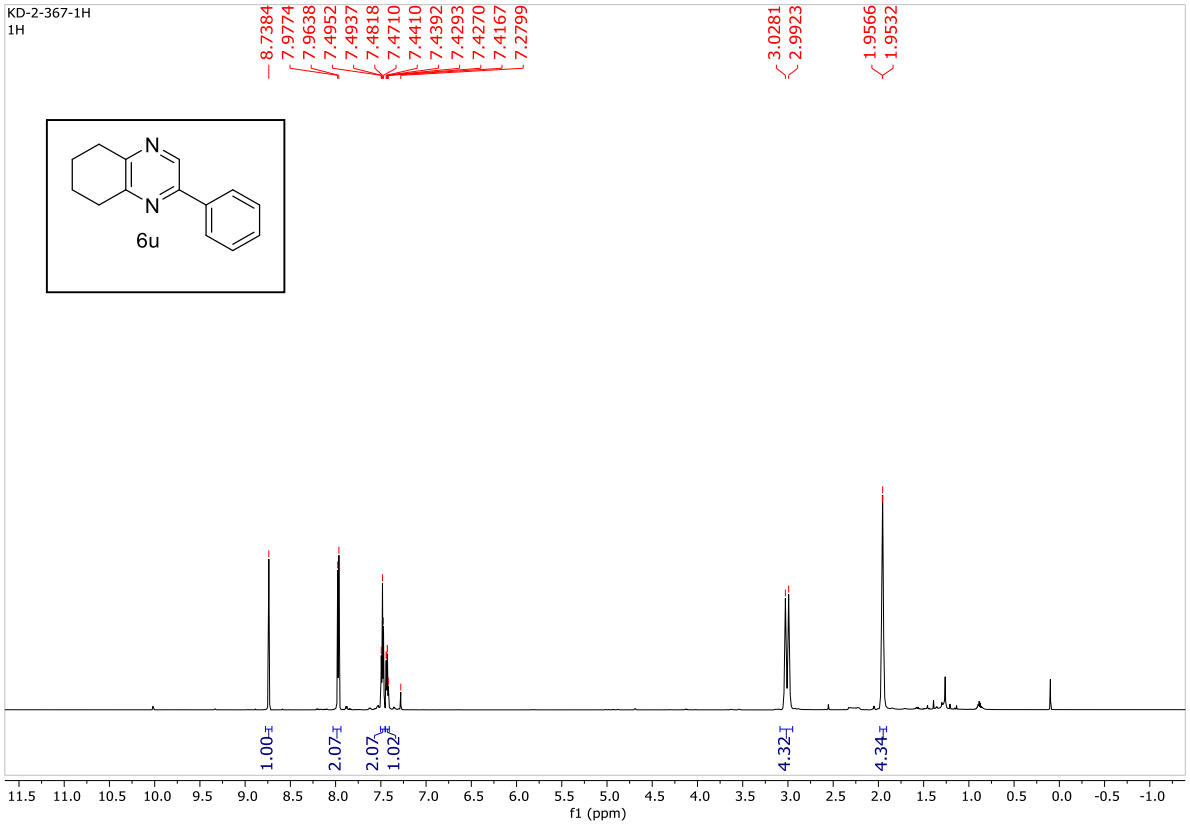

KD-2-414-13C.10.fid
KD-2-414-13C
157.5102
153.0541
141.1733
140.8535
128.7574
128.6987
128.5337
128.2520
77.3713
77.1606
76.9497
28.9803
22.7134
11.9691
N
Me
N
Me
6r
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

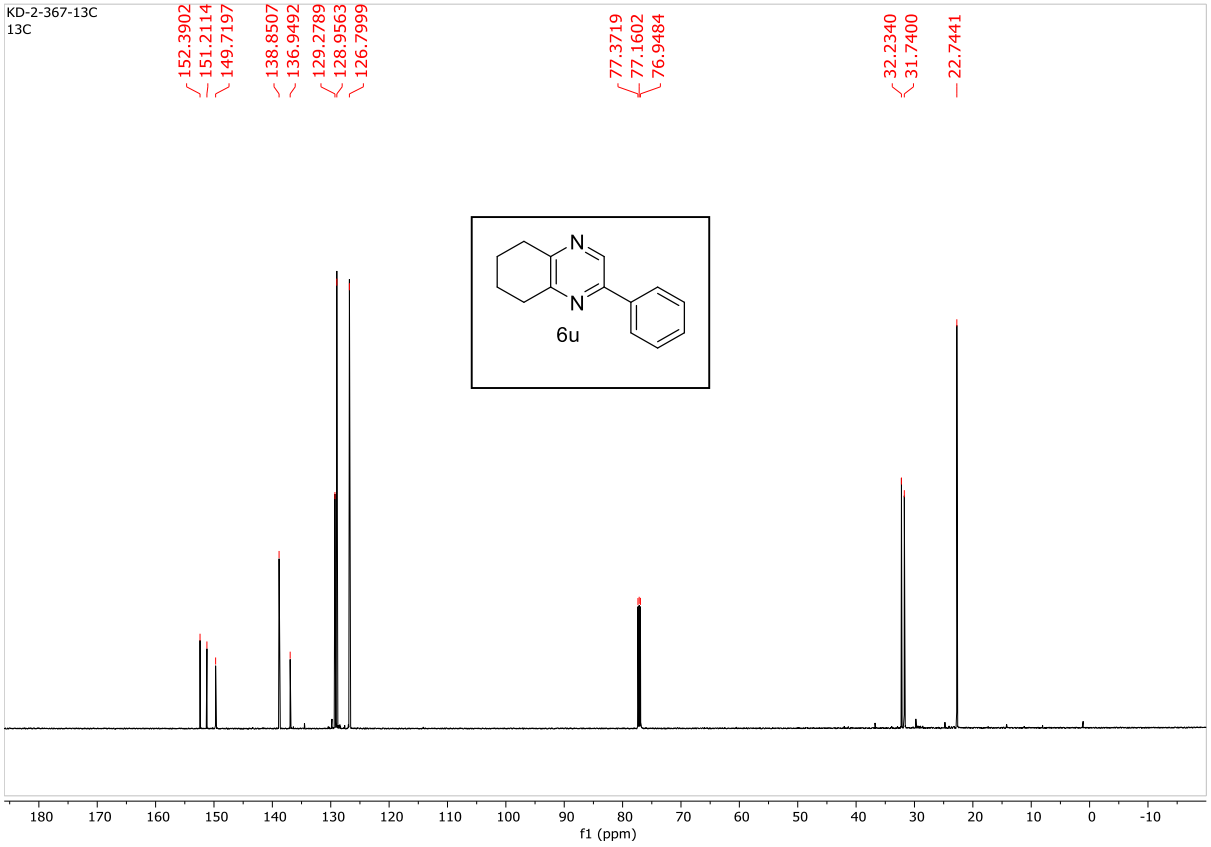

KD-2-415-1H.10.fid
1H
7.7382
7.6965
7.2600
2.9931
2.9806
2.9681
2.9556
2.7031
2.4379
1.3862
1.3737
1.3612
Me
N
Me
Me
Me
N
6s
0.95
0.96
2.02
3.03
6.11
3.00
f1 (ppm)

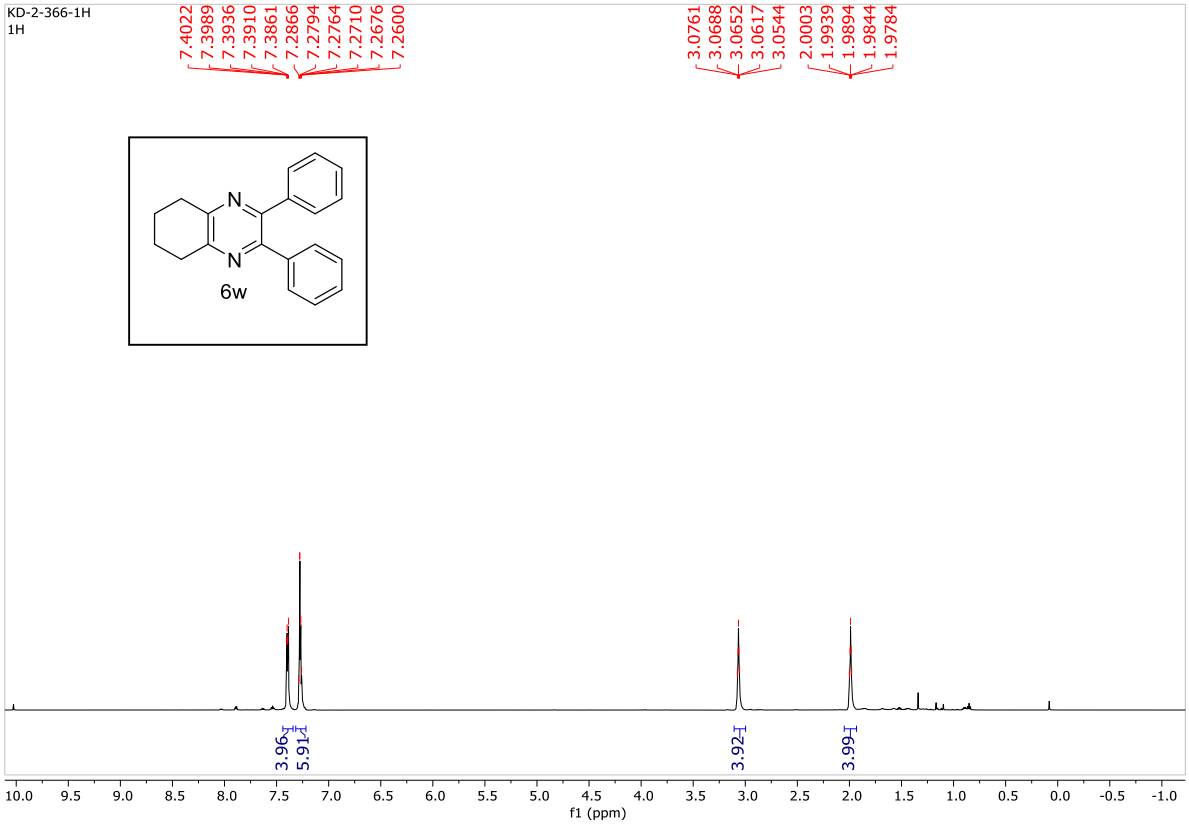

KD-2-415-13C.10.fid
13C
156.6284
152.0344
140.1797
139.8762
139.0707
139.0188
127.7978
127.5272
77.3710
77.1589
76.9482
29.0354
22.7309
20.3941
20.3432
12.2500
Me
N
Me
Me
Me
N
6s
f1 (ppm)

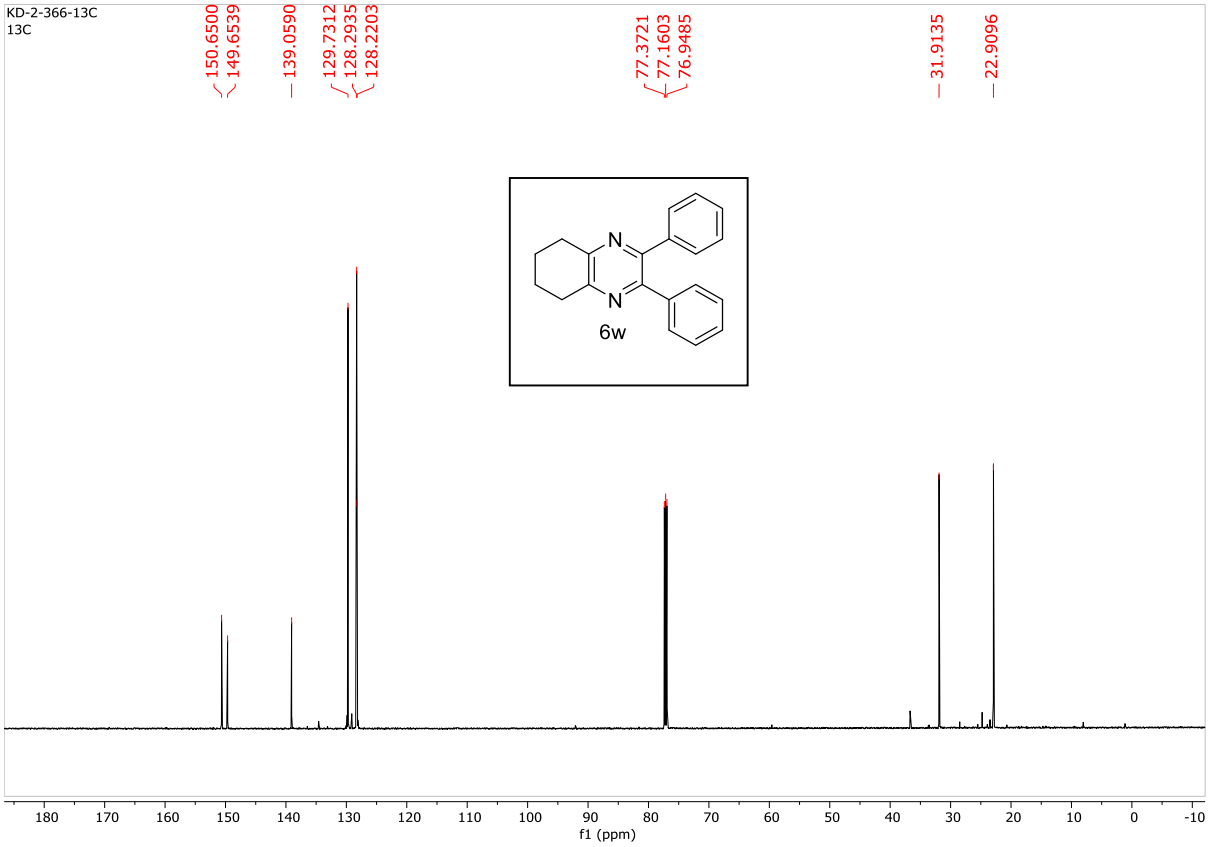

KD-2-418-2_1H.10.fid
KD-2-418-2_1H
8.0919
8.0416
7.2600
3.0055
2.9932
2.9808
2.9684
2.7142
1.3999
1.3875
1.3752
Cl
Cl
N
N
Me
Me
6t
0.90
0.92
1.98
2.99
3.00
f1 (ppm)

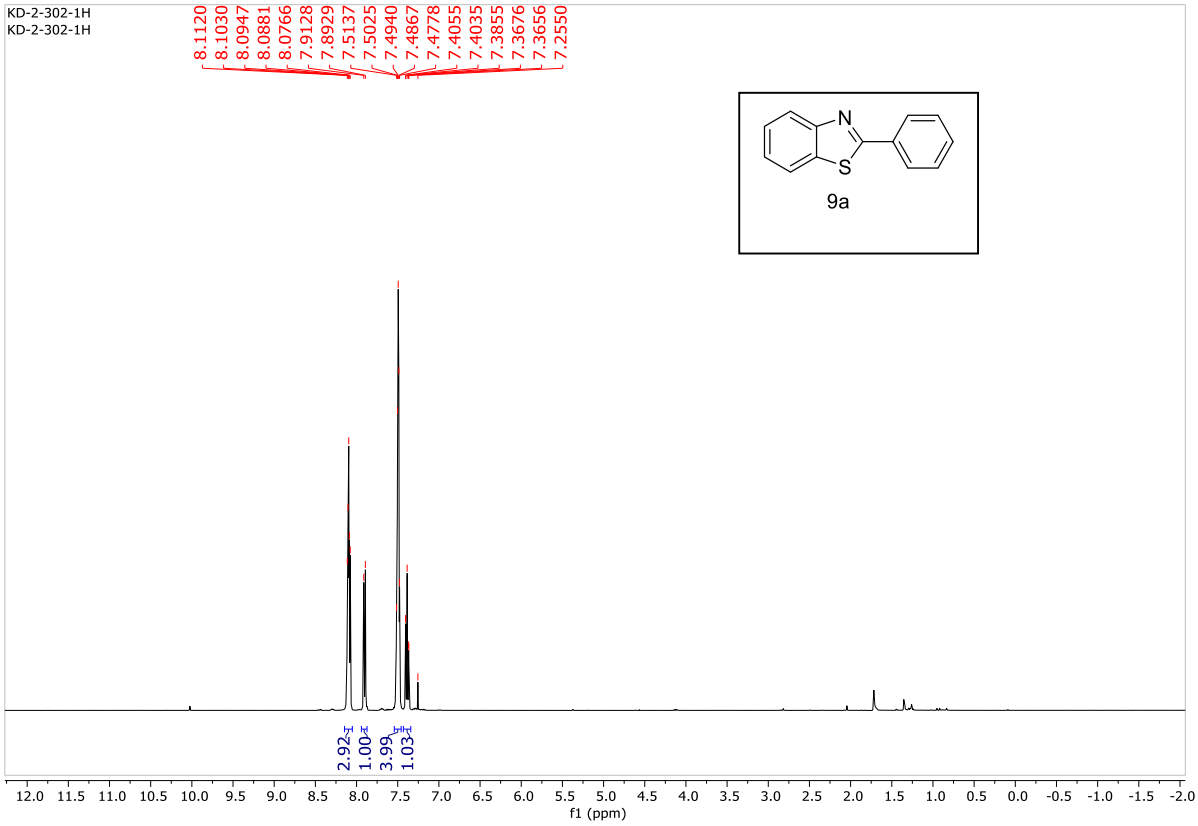

KD-2-418-2_13C.10.fid
KD-2-418-2_13C
158.9082
154.6628
140.0720
139.7194
133.0703
133.0521
129.4582
129.1511
77.3717
77.1598
76.9480
29.0150
22.8640
11.5950
Cl
Cl
N
N
Me
Me
6t
f1 (ppm)

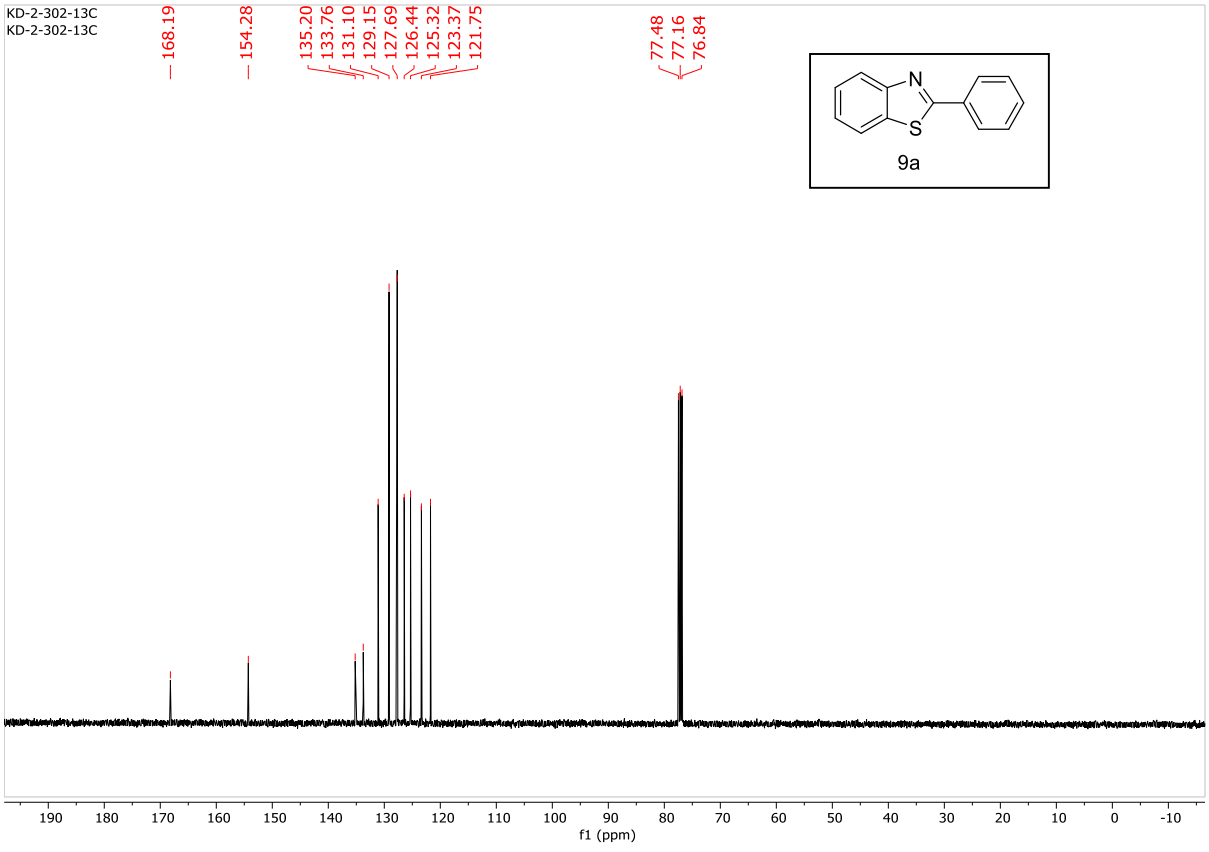

KD-2-367-1H
1H
8.7384
7.9774
7.9638
7.4952
7.4937
7.4818
7.4710
7.4410
7.4392
7.4293
7.4270
7.4167
7.2799
3.0281
2.9923
1.9566
1.9532
N
N
6u
1.00
2.07
2.07
1.02
4.32
4.34
f1 (ppm)

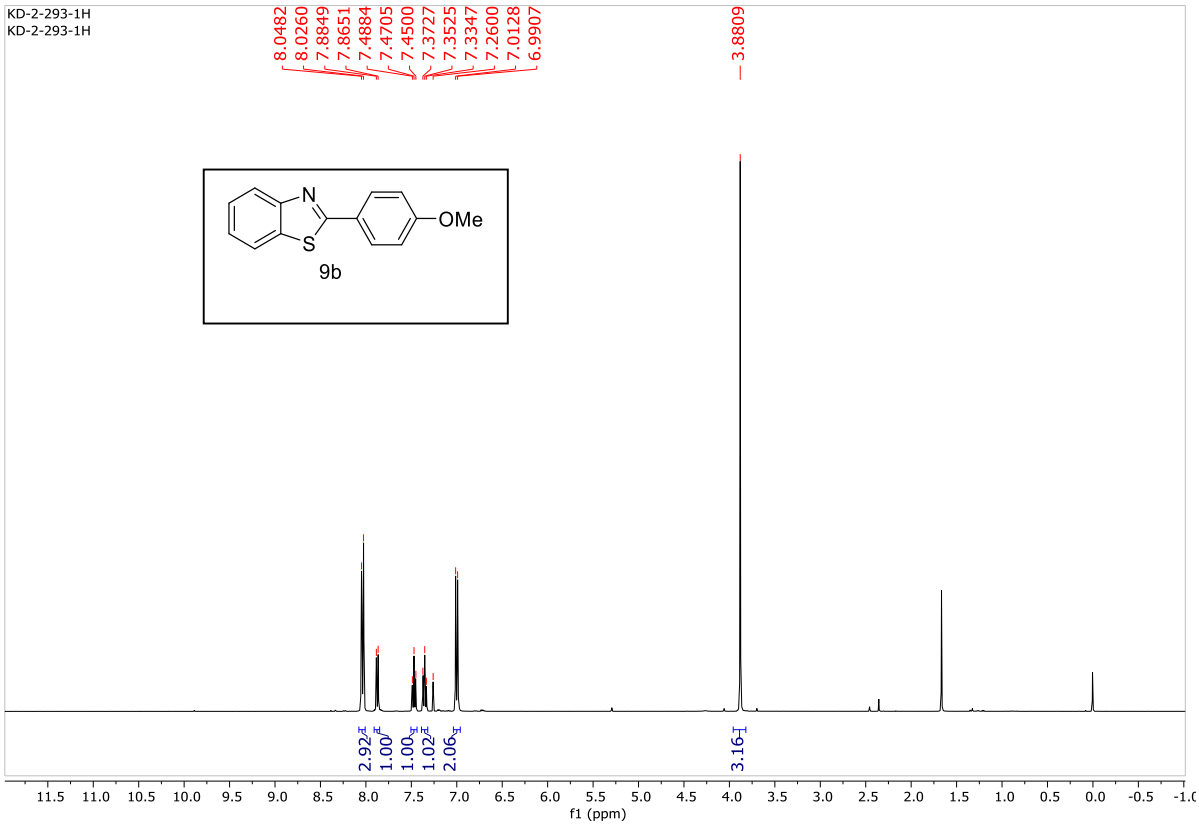

KD-2-367-13C
13C
152.3902
151.2114
149.7197
138.8507
136.9492
129.2789
128.9563
126.7999
77.3719
77.1602
76.9484
32.2340
31.7400
22.7441
N
N
6u
f1 (ppm)

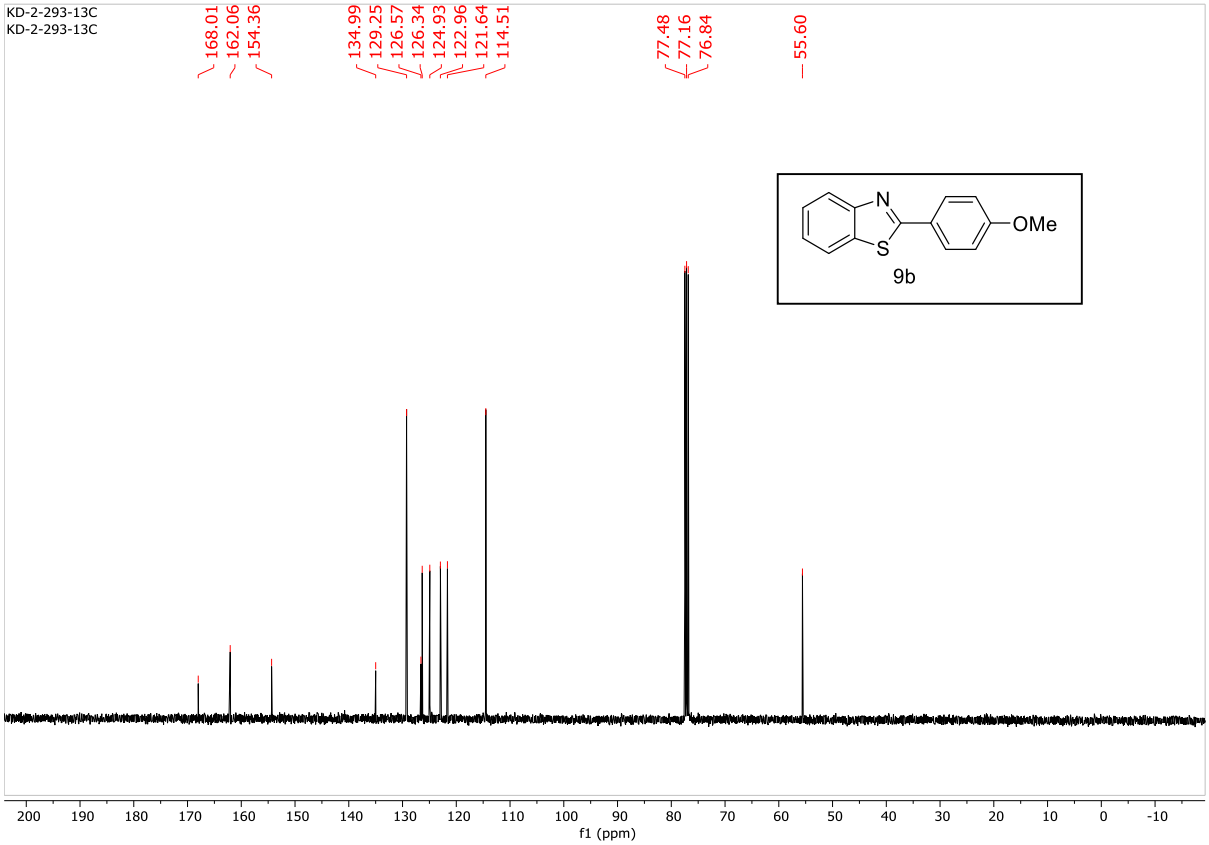

KD-2-366-1H
1H
7.4022
7.3989
7.3936
7.3910
7.3861
7.2866
7.2794
7.2764
7.2710
7.2676
7.2600
3.0761
3.0688
3.0652
3.0617
3.0544
2.0003
1.9939
1.9894
1.9844
1.9784
N
N
6w
3.96
5.91
3.92
3.99
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

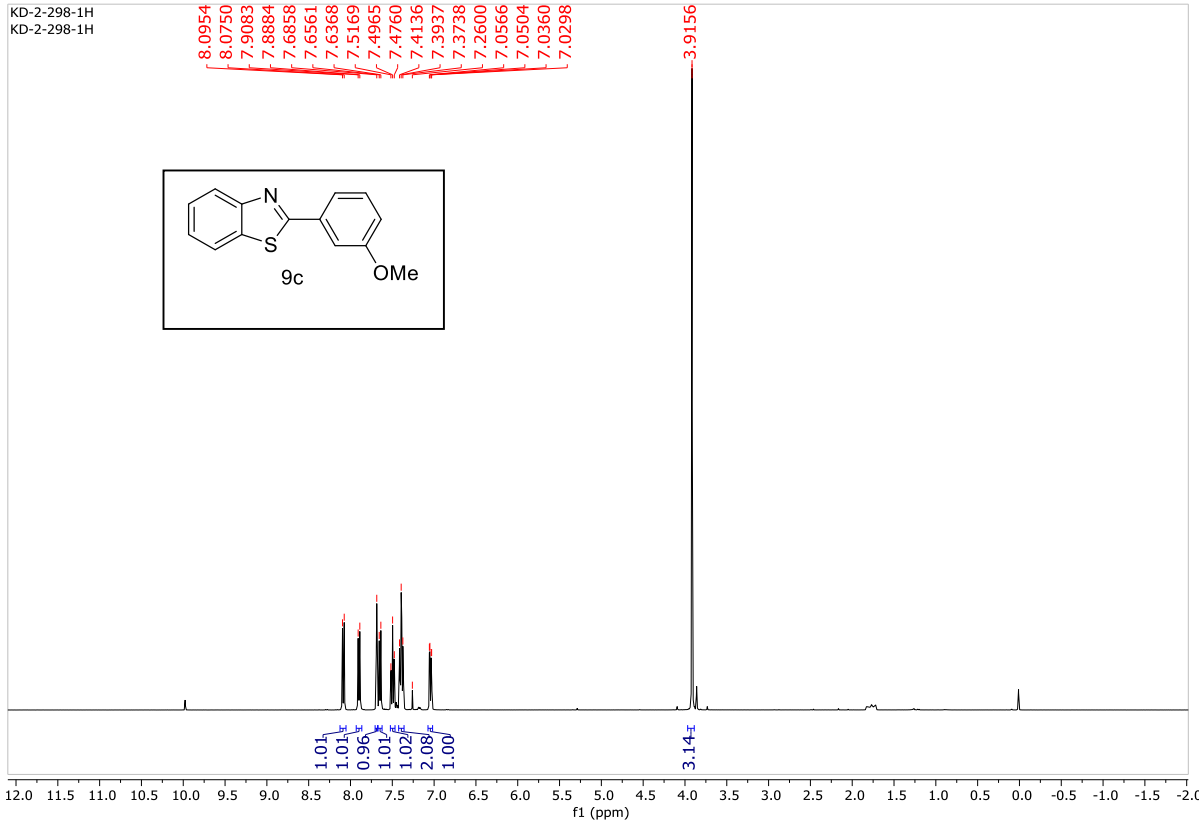

KD-2-366-13C
13C
150.6500
149.6539
139.0590
129.7312
128.2935
128.2203
77.3721
77.1603
76.9485
31.9135
22.9096
N
N
6w
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

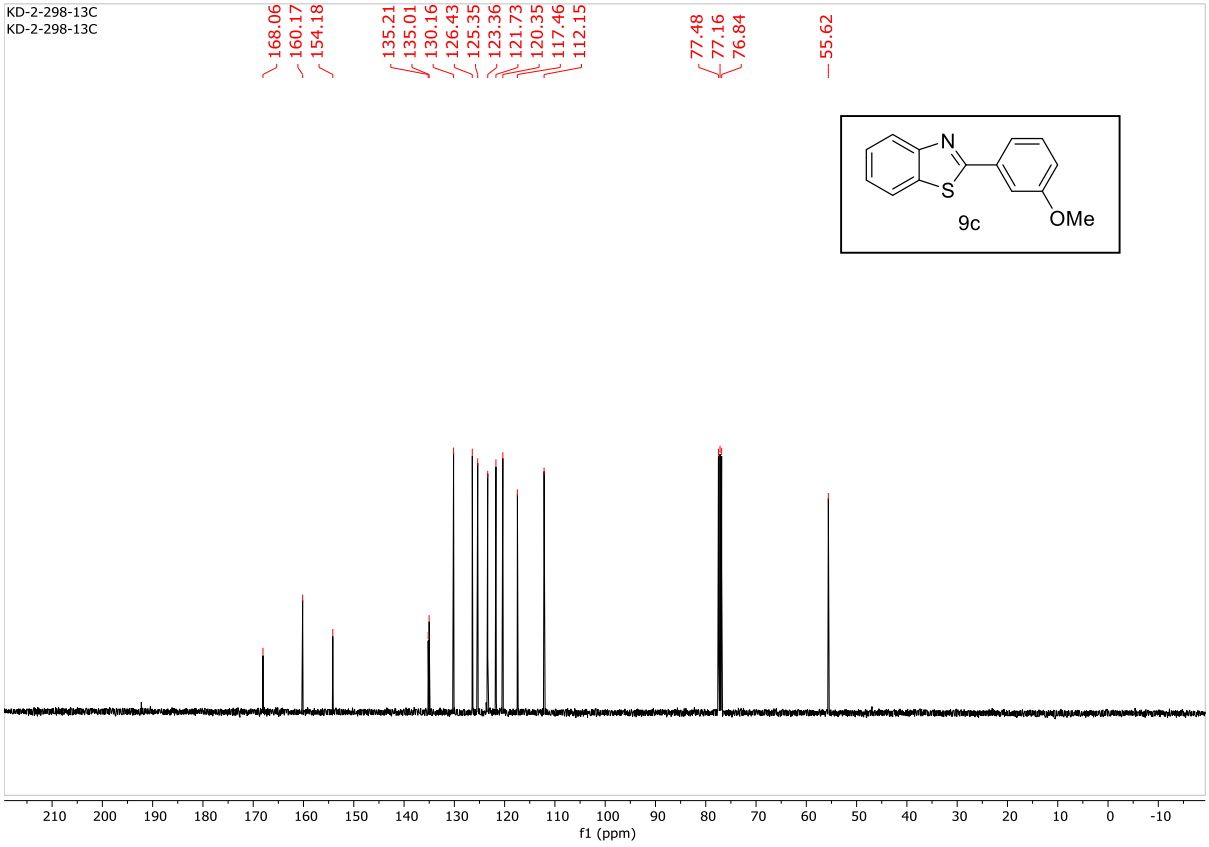

KD-2-302-1H
KD-2-302-1H
8.1120
8.1030
8.0947
8.0881
8.0766
7.9128
7.8929
7.5137
7.5025
7.4940
7.4867
7.4778
7.4055
7.4035
7.3855
7.3676
7.3656
7.2550
N
S
9a
2.92
1.00
3.99
1.03
f1 (ppm)

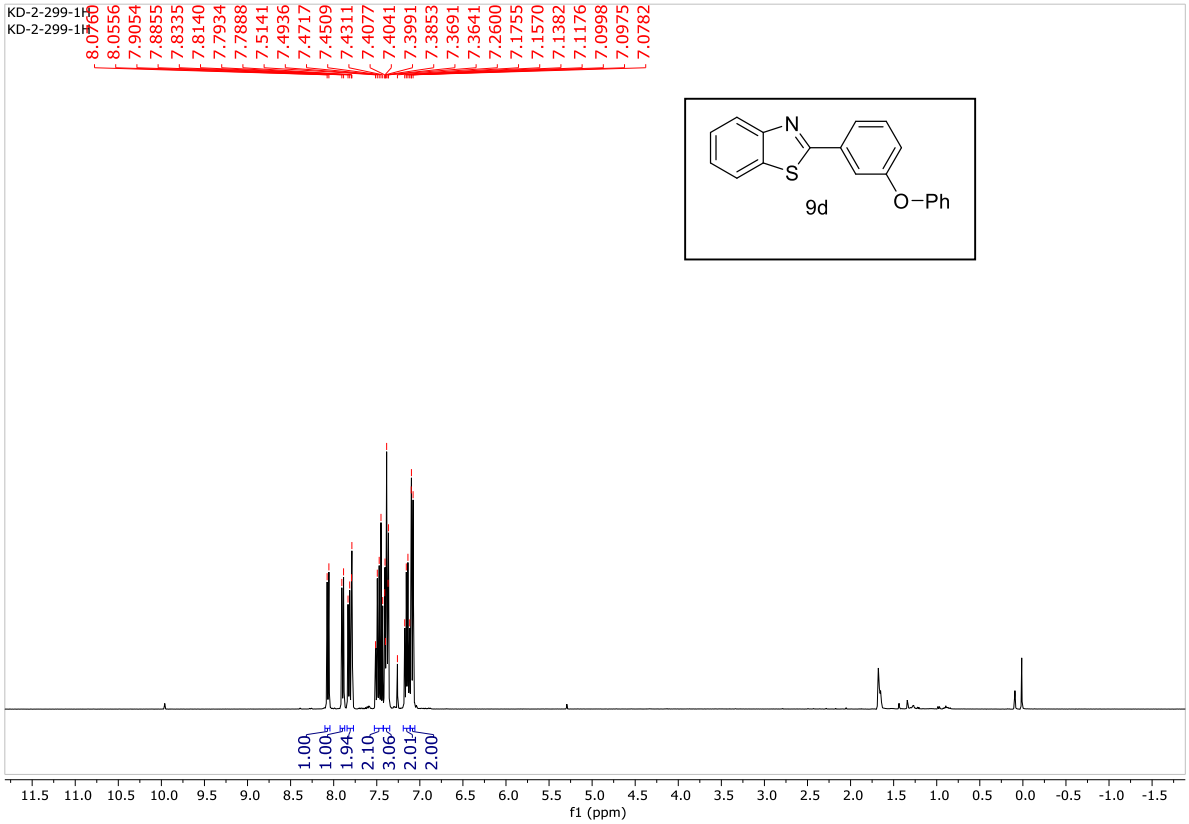

KD-2-302-13C
KD-2-302-13C
168.19
154.28
135.20
133.76
131.10
129.15
127.69
126.44
125.32
123.37
121.75
77.48
77.16
76.84
N
S
9a
f1 (ppm)

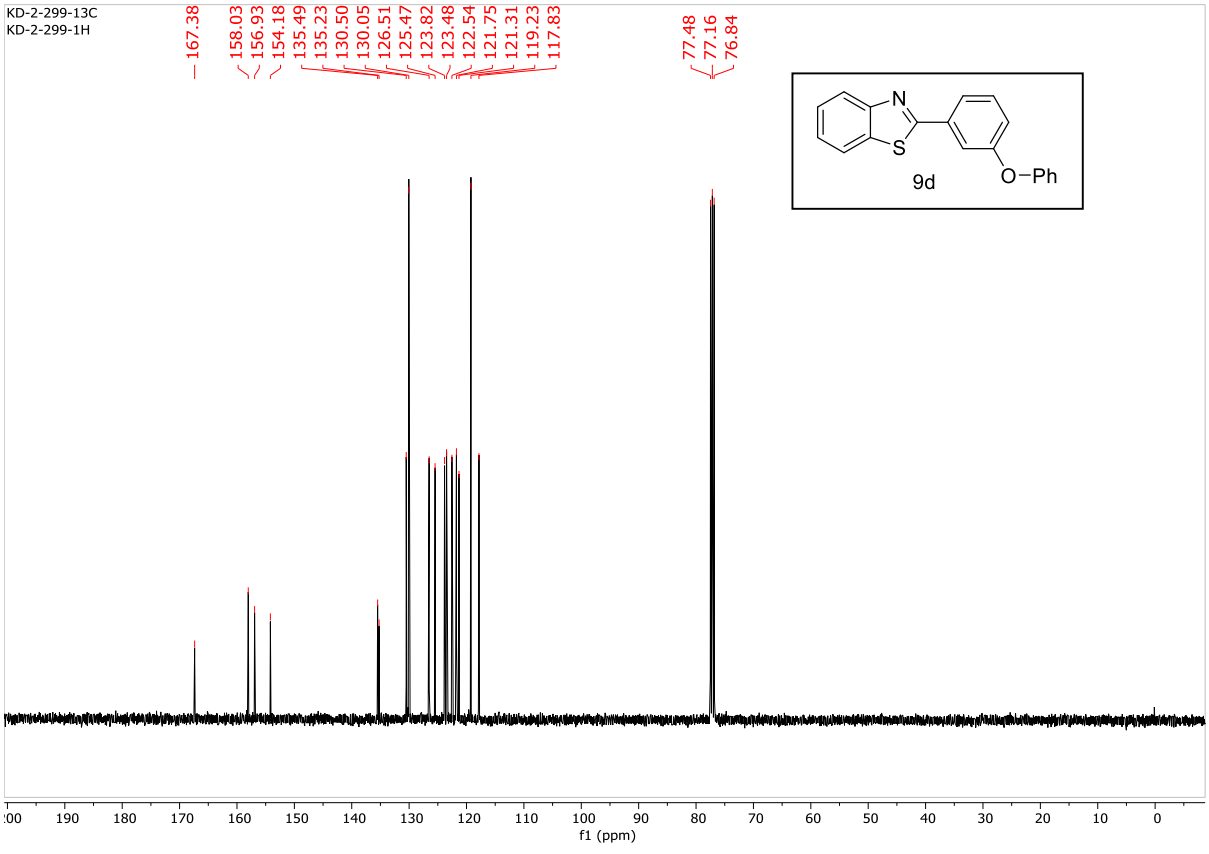

KD-2-293-1H
KD-2-293-1H
8.0482
8.0260
7.8849
7.8651
7.4884
7.4705
7.4500
7.3727
7.3525
7.3347
7.2600
7.0128
6.9907
3.8809
N
S
OMe
9b
2.92
1.00
1.00
1.02
2.06
3.16
f1 (ppm)

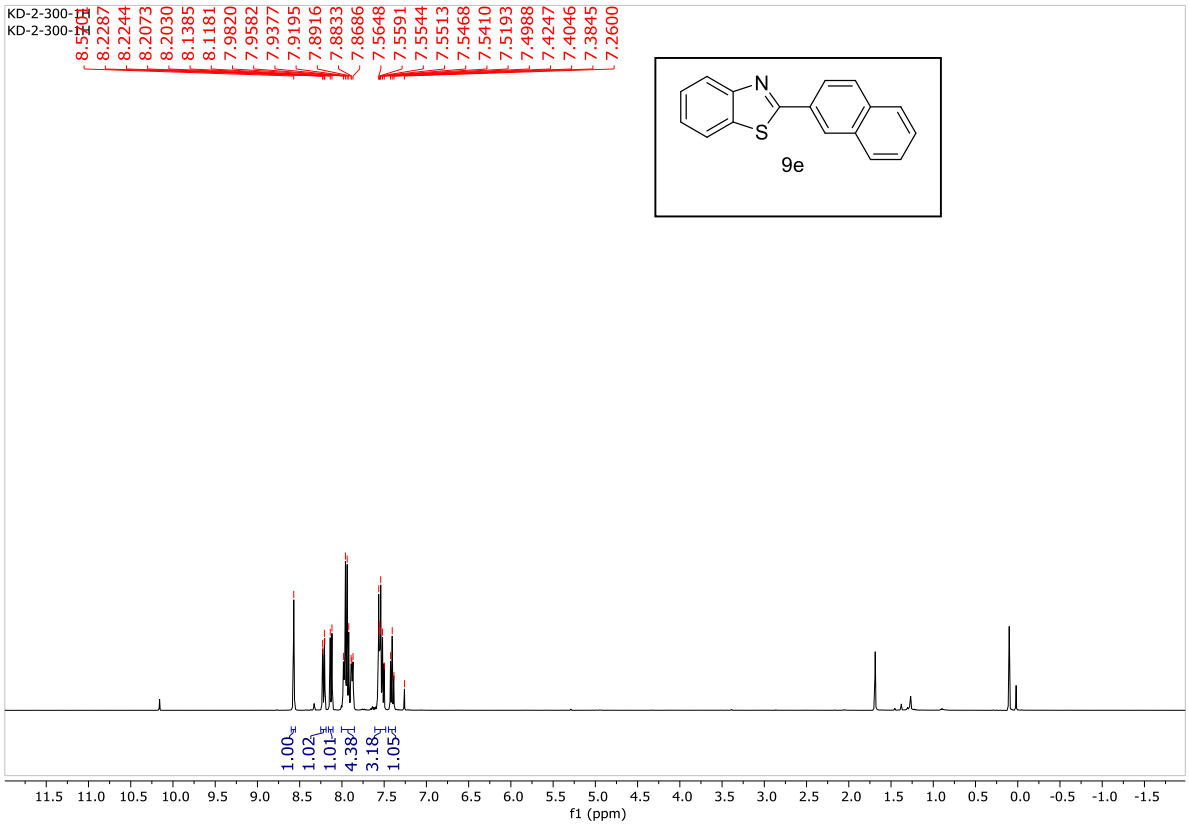

KD-2-293-13C
KD-2-293-13C
168.01
162.06
154.36
134.99
129.25
126.57
126.34
124.93
122.96
121.64
114.51
77.48
77.16
76.84
55.60
N
S
OMe
9b
f1 (ppm)

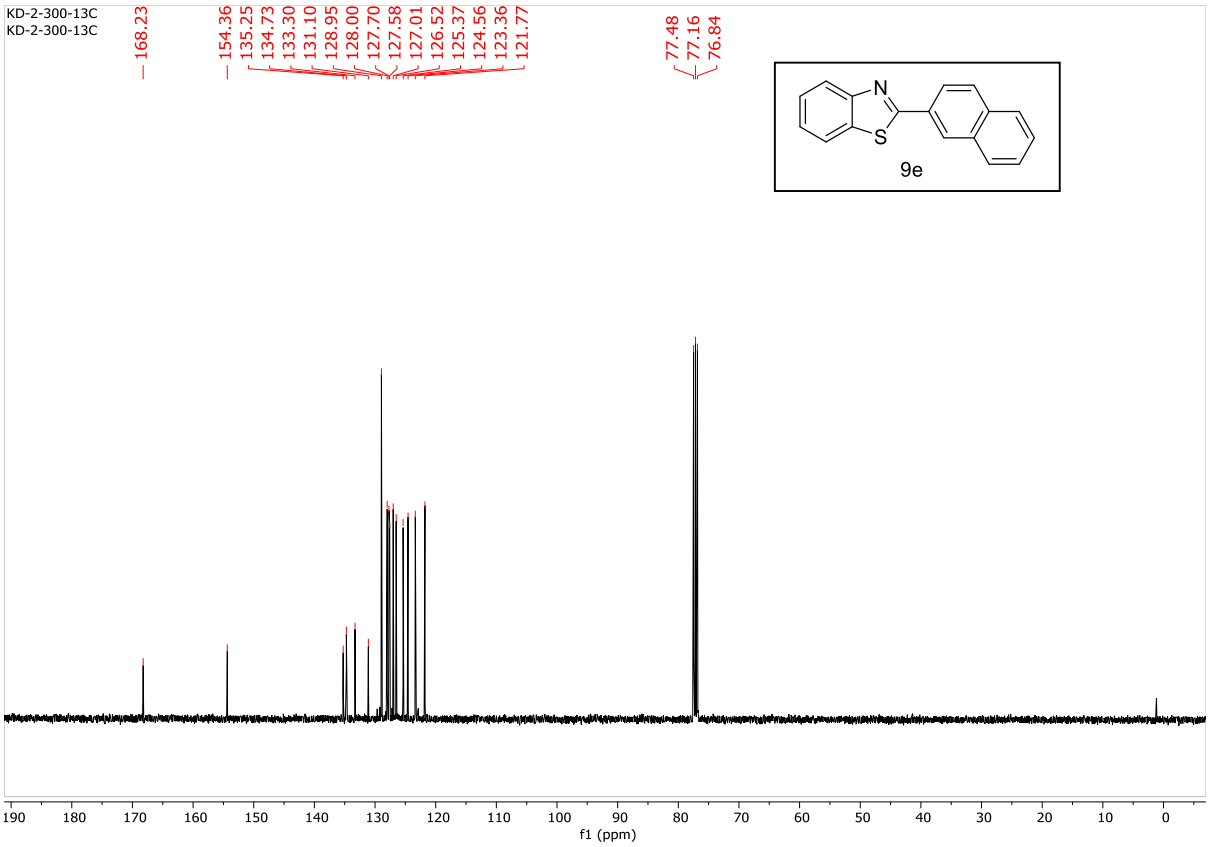

KD-2-298-1H
KD-2-298-1H
8.0954
8.0750
7.9083
7.8884
7.6858
7.6561
7.6368
7.5169
7.4965
7.4760
7.4136
7.3937
7.3738
7.2600
7.0566
7.0504
7.0360
7.0298
3.9156
N
S
9c
OMe
1.01
1.01
0.96
1.01
1.02
2.08
1.00
3.14
f1 (ppm)

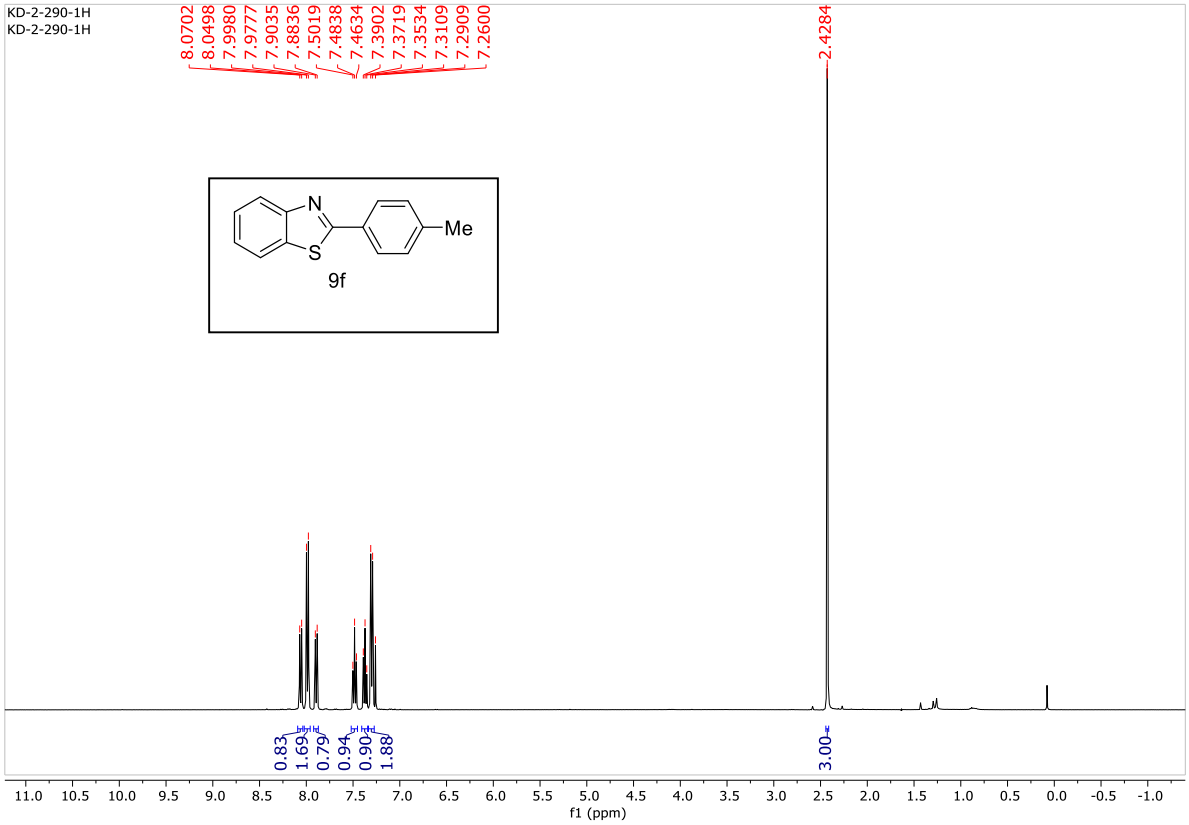

KD-2-298-13C
KD-2-298-13C
168.06
160.17
154.18
135.21
135.01
130.16
126.43
125.35
123.36
121.73
120.35
117.46
112.15
77.48
77.16
76.84
55.62
N
S
9c
OMe
f1 (ppm)

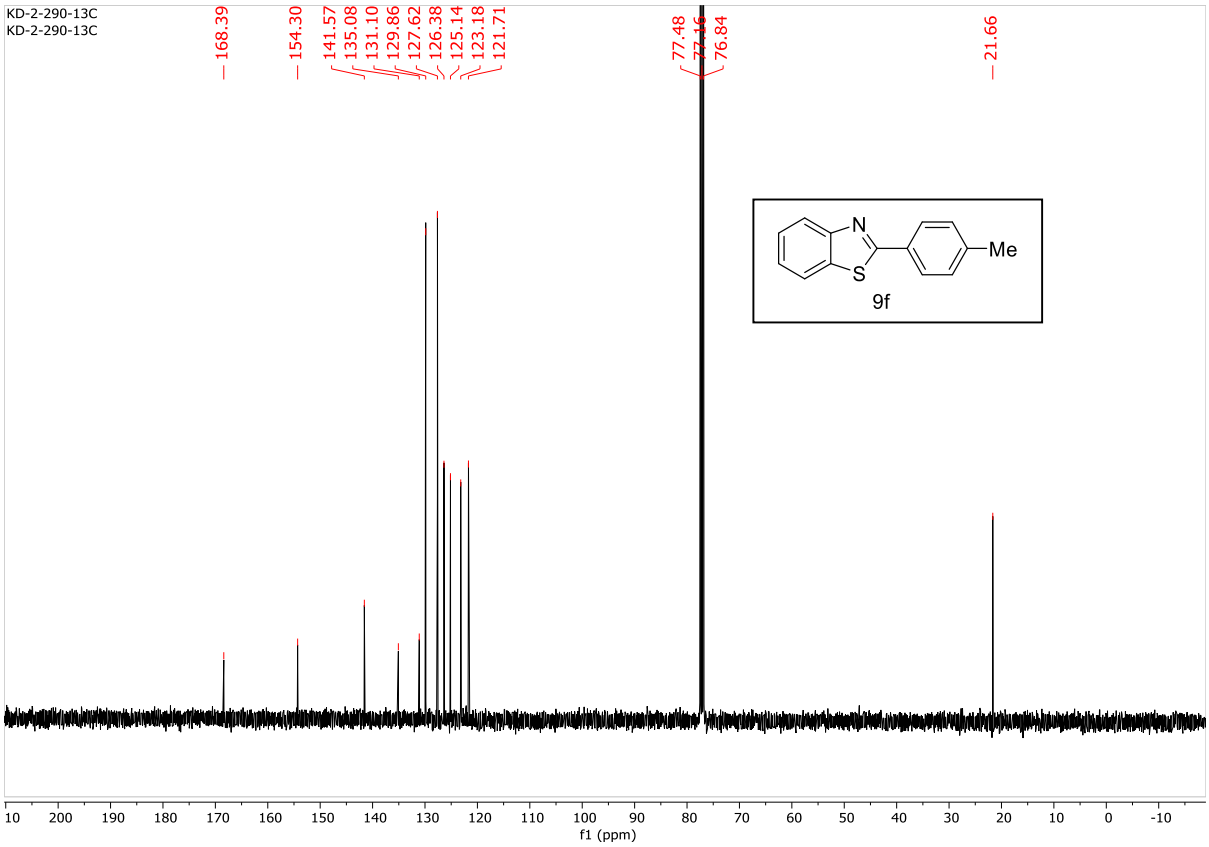

KD-2-299-1H
KD-2-299-1H
8.0760
8.0556
7.9054
7.8855
7.8335
7.8140
7.7934
7.7888
7.5141
7.4936
7.4717
7.4509
7.4311
7.4077
7.4041
7.3991
7.3853
7.3691
7.3641
7.2600
7.1755
7.1570
7.1382
7.1176
7.0998
7.0975
7.0782
N
S
9d
O−Ph
1.00
1.00
1.94
2.10
3.06
2.01
2.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 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 -0.5 -1.0 -1.5
f1 (ppm)

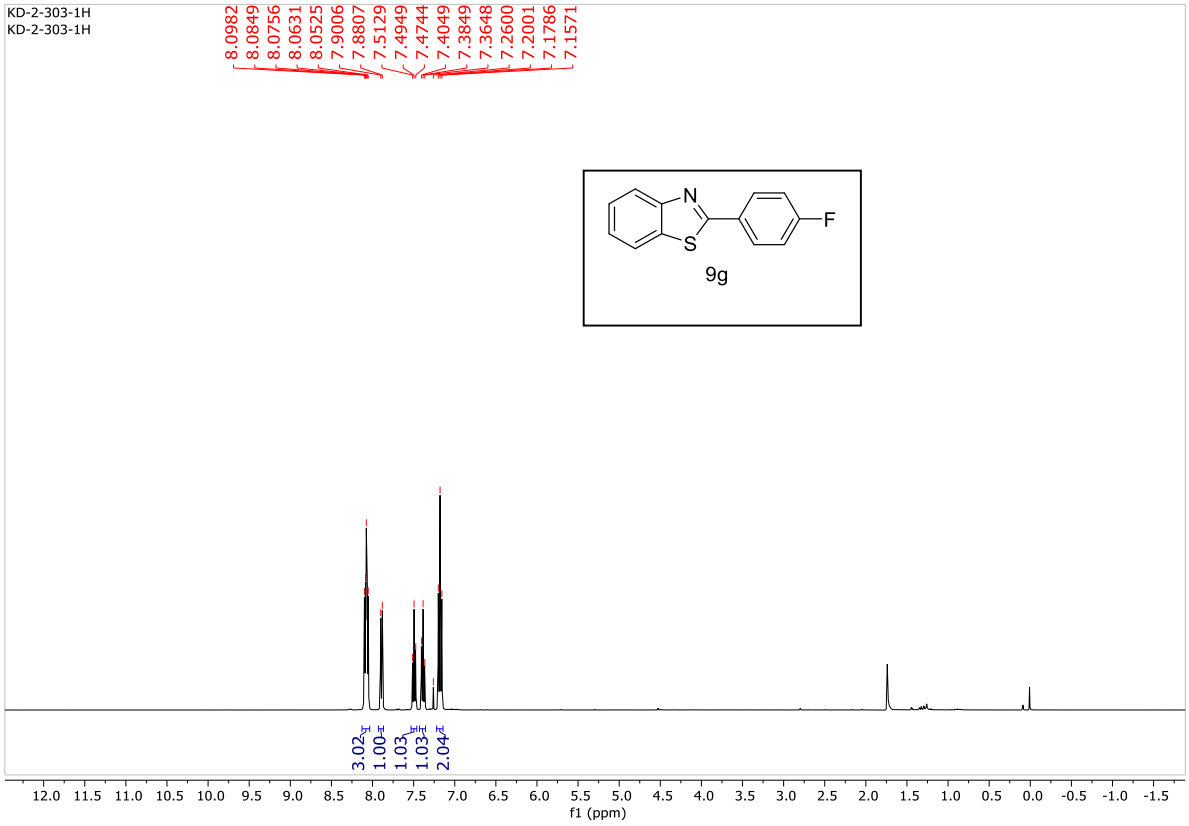

KD-2-299-13C
KD-2-299-1H
167.38
158.03
156.93
154.18
135.49
135.23
130.50
130.05
126.51
125.47
123.82
123.48
122.54
121.75
121.31
119.23
117.83
77.48
77.16
76.84
N
S
9d
O−Ph
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

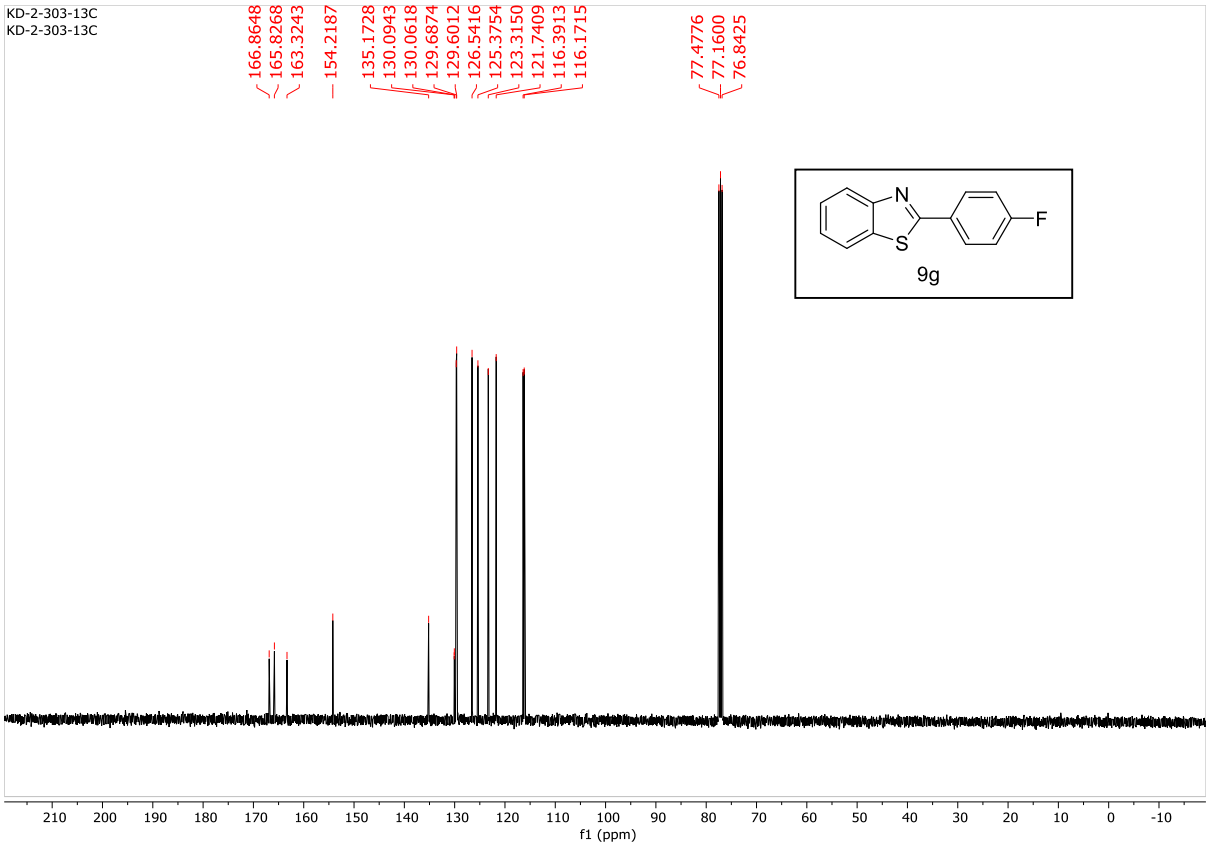

KD-2-300-1H
KD-2-300-1H
8.5200
8.2287
8.2244
8.2073
8.2030
8.1385
8.1181
7.9820
7.9582
7.9377
7.9195
7.8916
7.8833
7.8686
7.5648
7.5591
7.5544
7.5513
7.5468
7.5410
7.5193
7.4988
7.4247
7.4046
7.3845
7.2600
N
S
9e
1.00
1.02
1.01
4.38
3.18
1.05
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

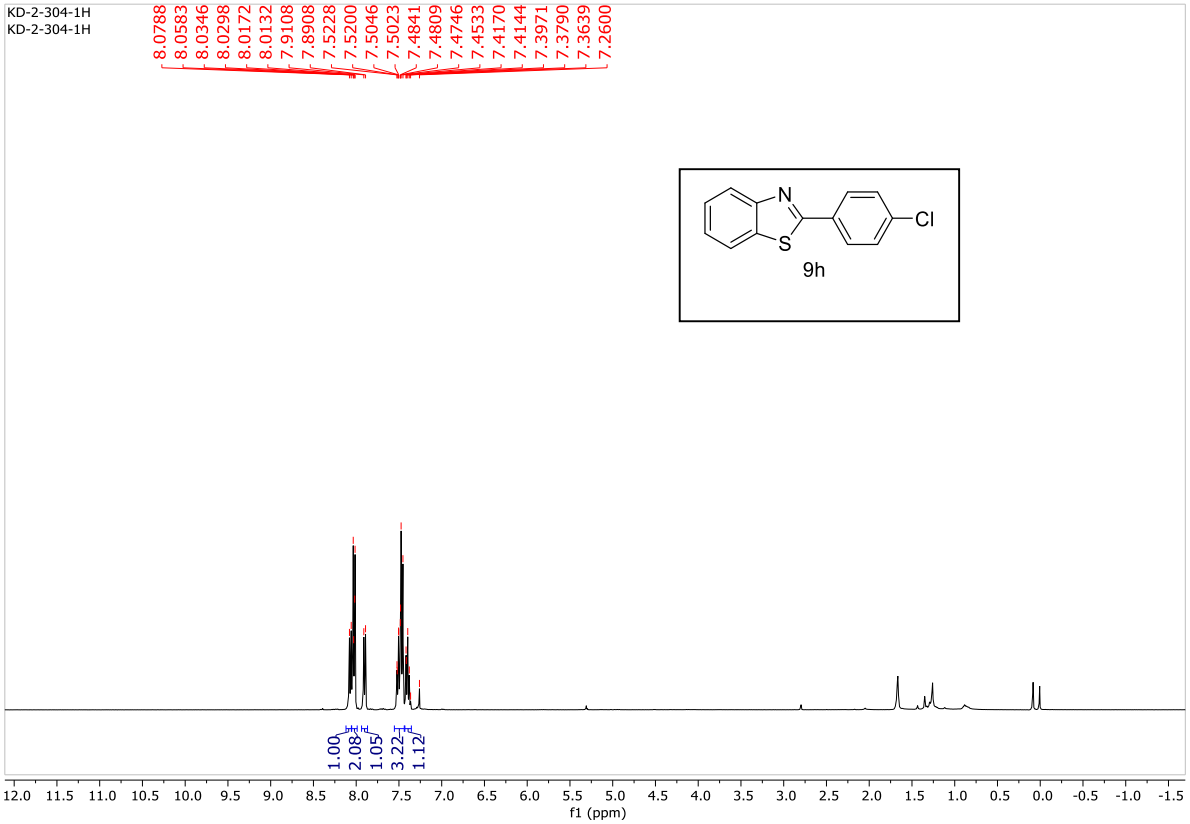

KD-2-300-13C
KD-2-300-13C
168.23
154.36
135.25
134.73
133.30
131.10
128.95
128.00
127.70
127.58
127.01
126.52
125.37
124.56
123.36
121.77
77.48
77.16
76.84
N
S
9e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

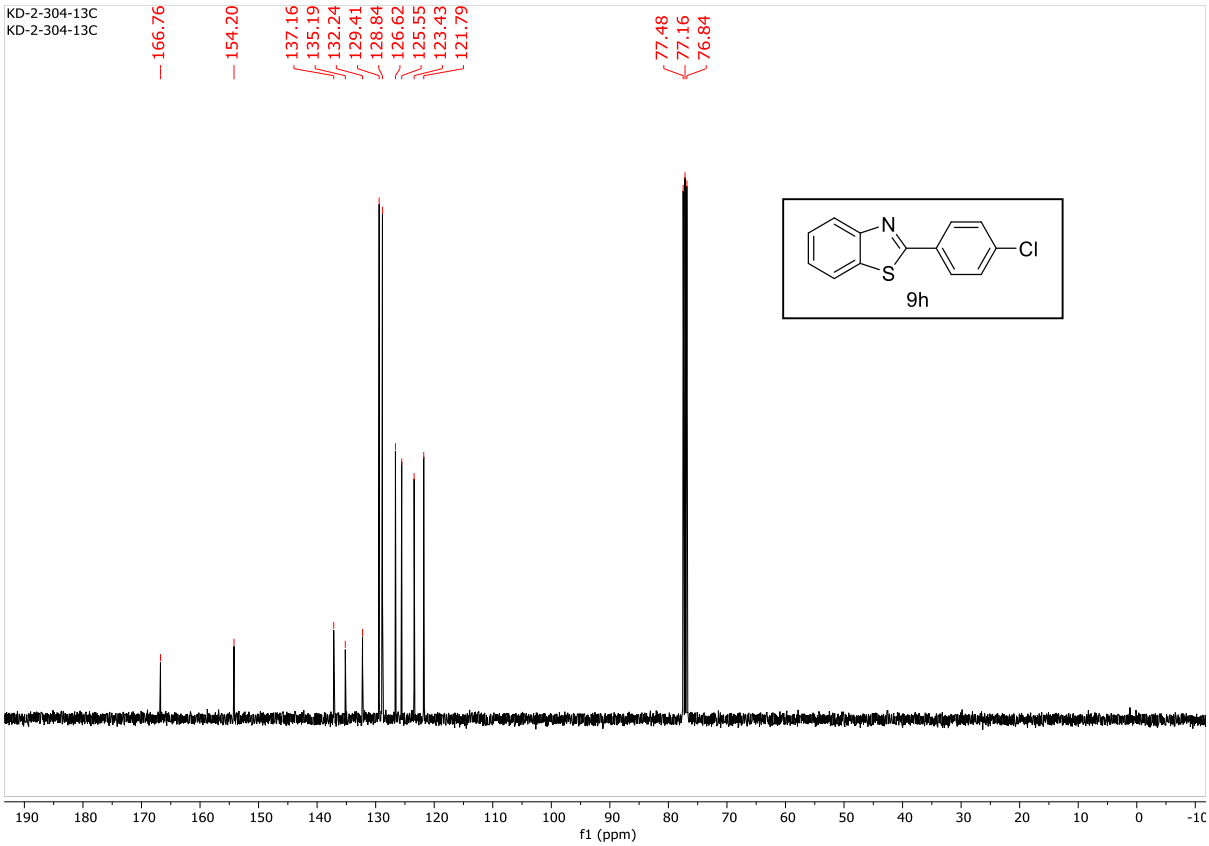

KD-2-290-1H
KD-2-290-1H
8.0702
8.0498
7.9980
7.9777
7.9035
7.8836
7.5019
7.4838
7.4634
7.3902
7.3719
7.3534
7.3109
7.2909
7.2600
2.4284
N
S
Me
9f
0.83
1.69
0.79
0.94
0.90
1.88
3.00
f1 (ppm)

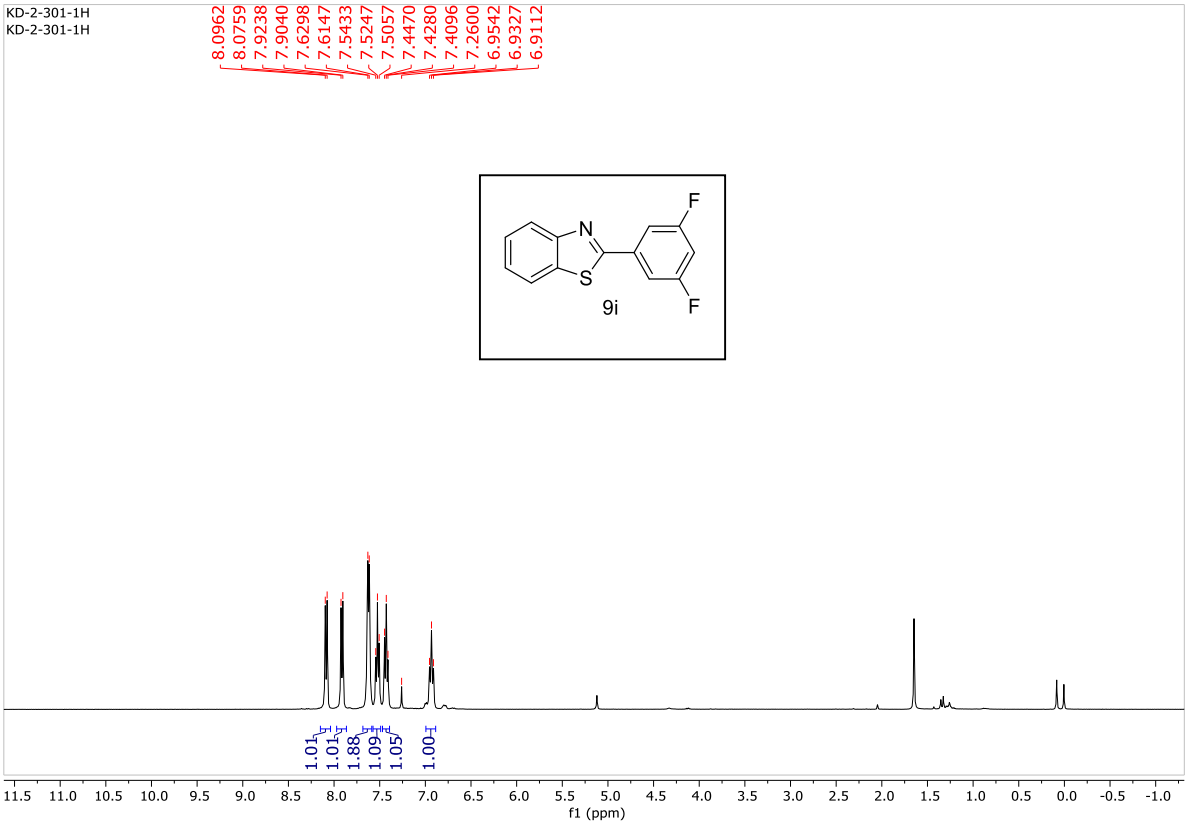

KD-2-290-13C
KD-2-290-13C
168.39
154.30
141.57
135.08
131.10
129.86
127.62
126.38
125.14
123.18
121.71
77.48
77.16
76.84
21.66
N
S
Me
9f
f1 (ppm)

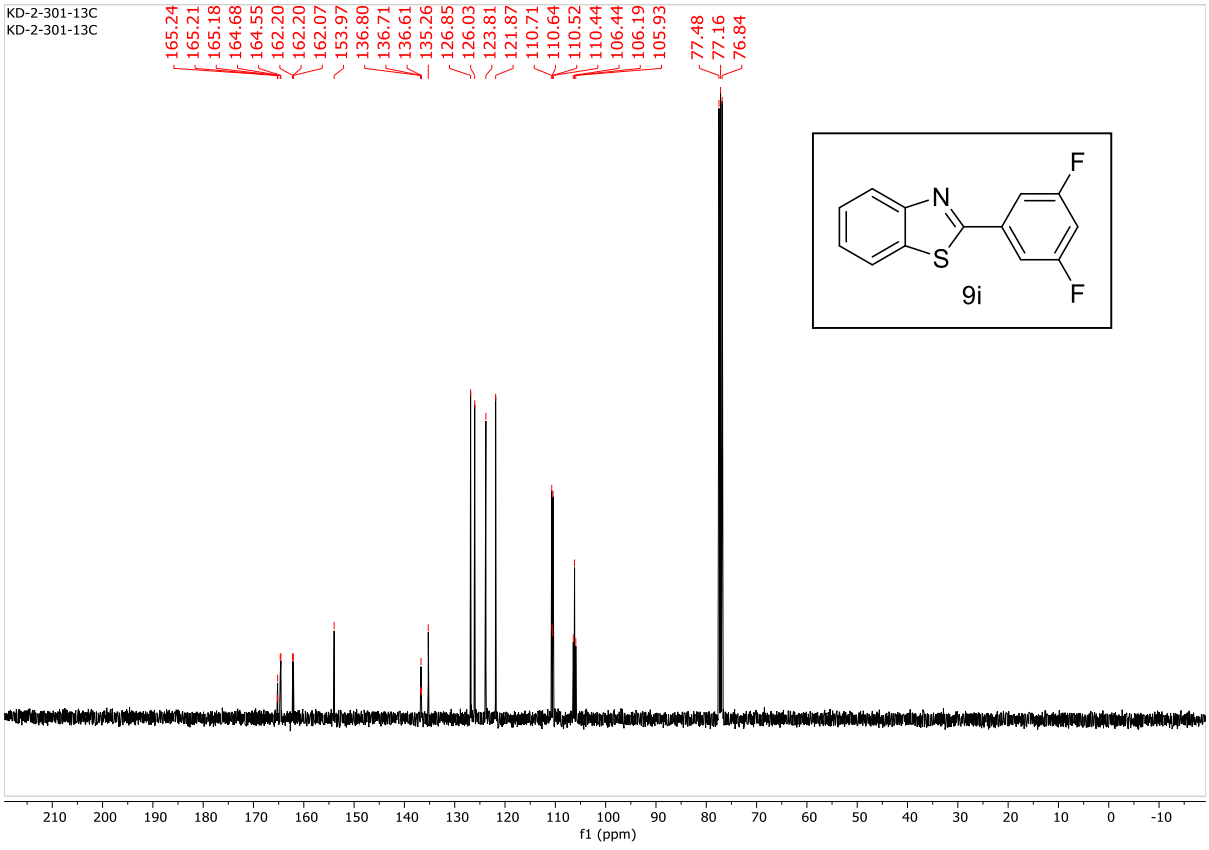

KD-2-303-1H
KD-2-303-1H
8.0982
8.0849
8.0756
8.0631
8.0525
7.9006
7.8807
7.5129
7.4949
7.4744
7.4049
7.3849
7.3648
7.2600
7.2001
7.1786
7.1571
N
S
F
9g
3.02
1.00
1.03
1.03
2.04
f1 (ppm)

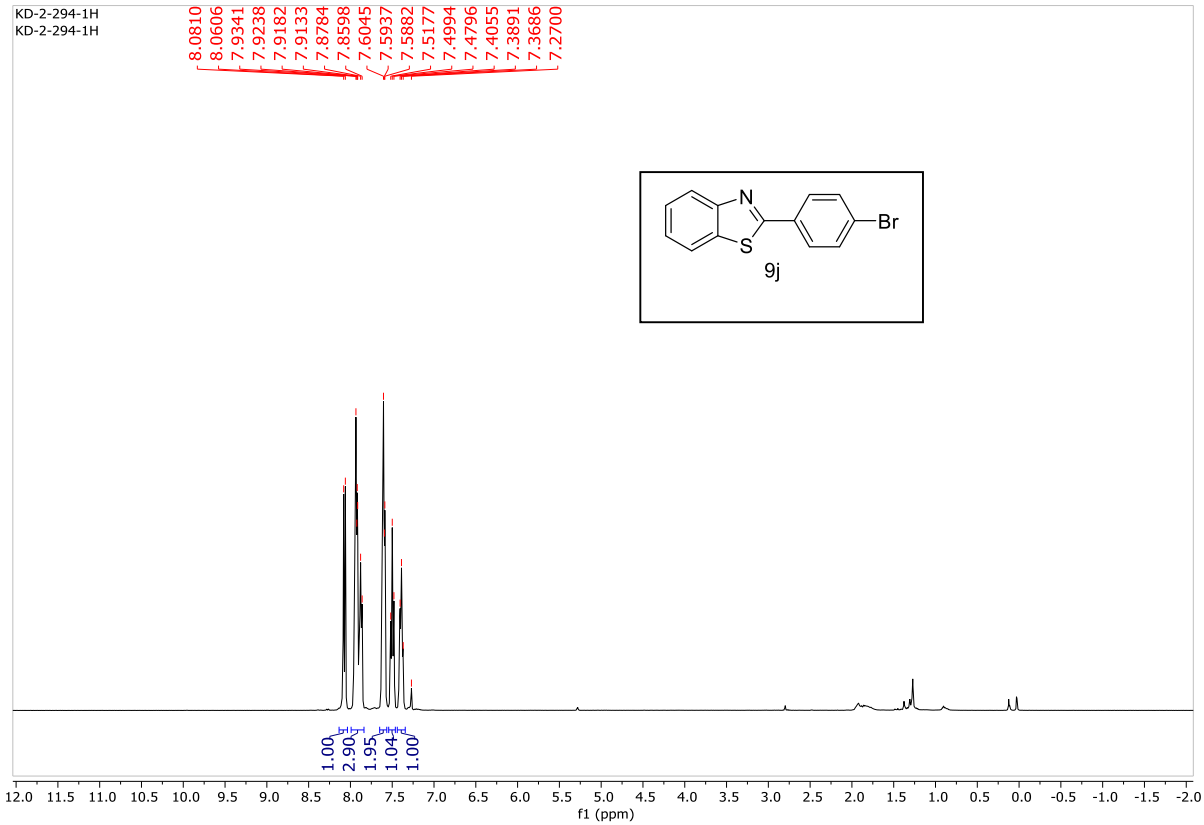

KD-2-303-13C
KD-2-303-13C
166.8648
165.8268
163.3243
154.2187
135.1728
130.0943
130.0618
129.6874
129.6012
126.5416
125.3754
123.3150
121.7409
116.3913
116.1715
77.4776
77.1600
76.8425
N
S
F
9g
f1 (ppm)

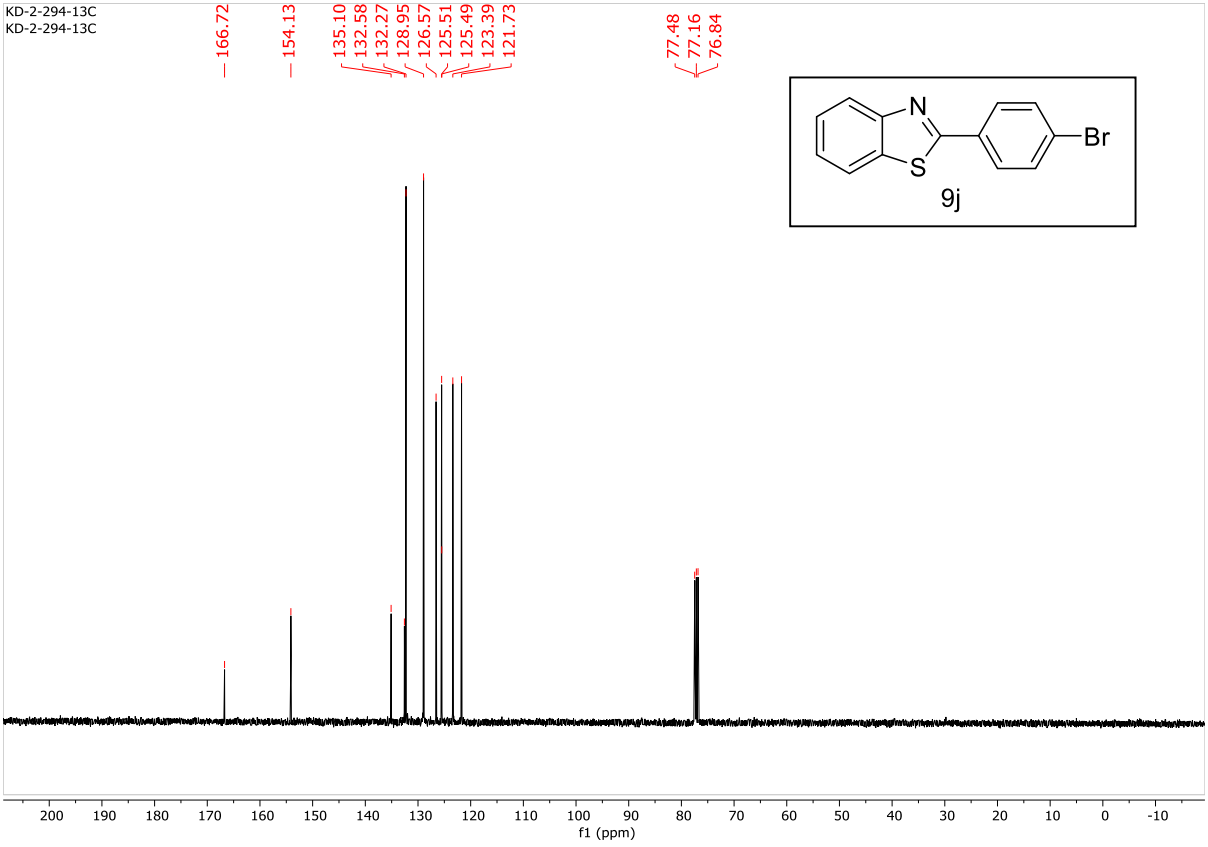

KD-2-304-1H
KD-2-304-1H
8.0788
8.0583
8.0346
8.0298
8.0172
8.0132
7.9108
7.8908
7.5228
7.5200
7.5046
7.5023
7.4841
7.4809
7.4746
7.4533
7.4170
7.4144
7.3971
7.3790
7.3639
7.2600
N
S
Cl
9h
1.00
2.08
1.05
3.22
1.12
f1 (ppm)

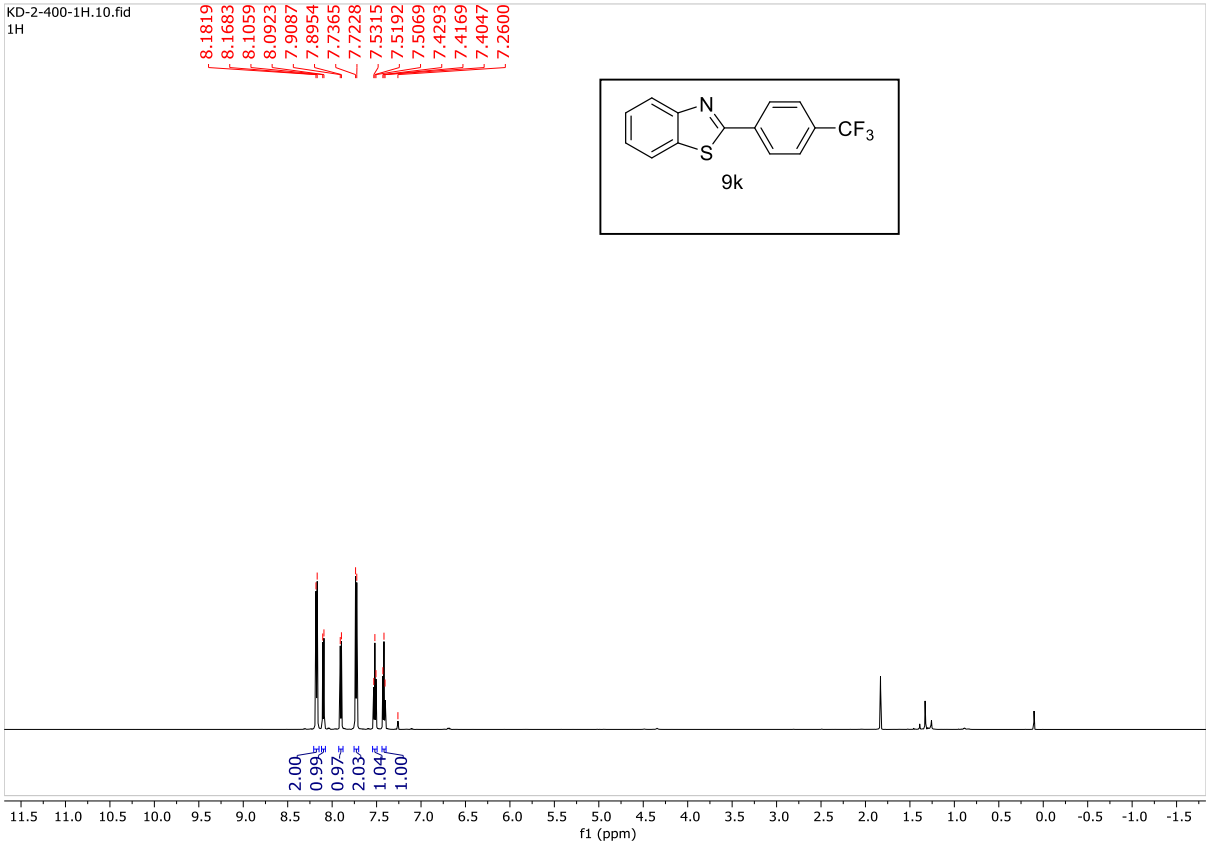

KD-2-304-13C
KD-2-304-13C
166.76
154.20
137.16
135.19
132.24
129.41
128.84
126.62
125.55
123.43
121.79
77.48
77.16
76.84
N
S
Cl
9h
f1 (ppm)

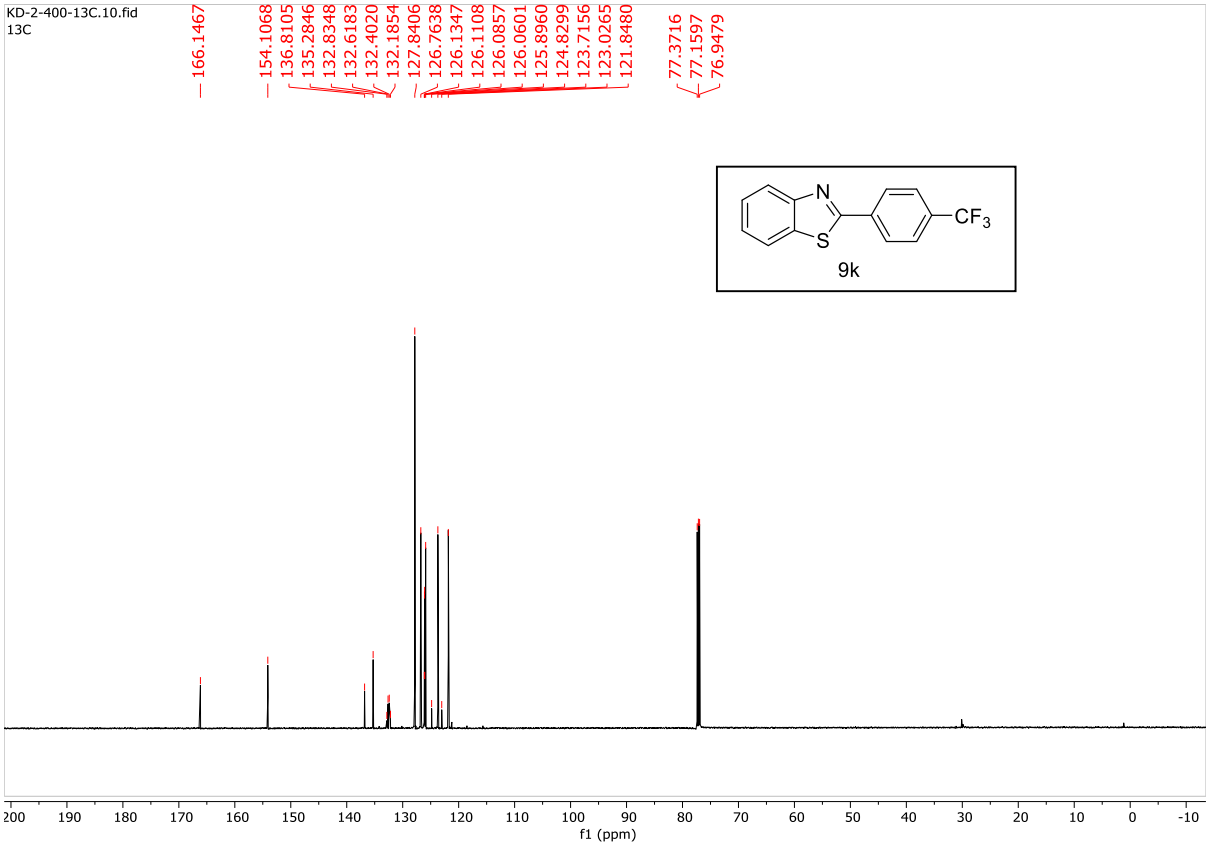

KD-2-301-1H
KD-2-301-1H
8.0962
8.0759
7.9238
7.9040
7.6298
7.6147
7.5433
7.5247
7.5057
7.4470
7.4280
7.4096
7.2600
6.9542
6.9327
6.9112
N
S
F
F
9i
1.01
1.01
1.88
1.09
1.05
1.00
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

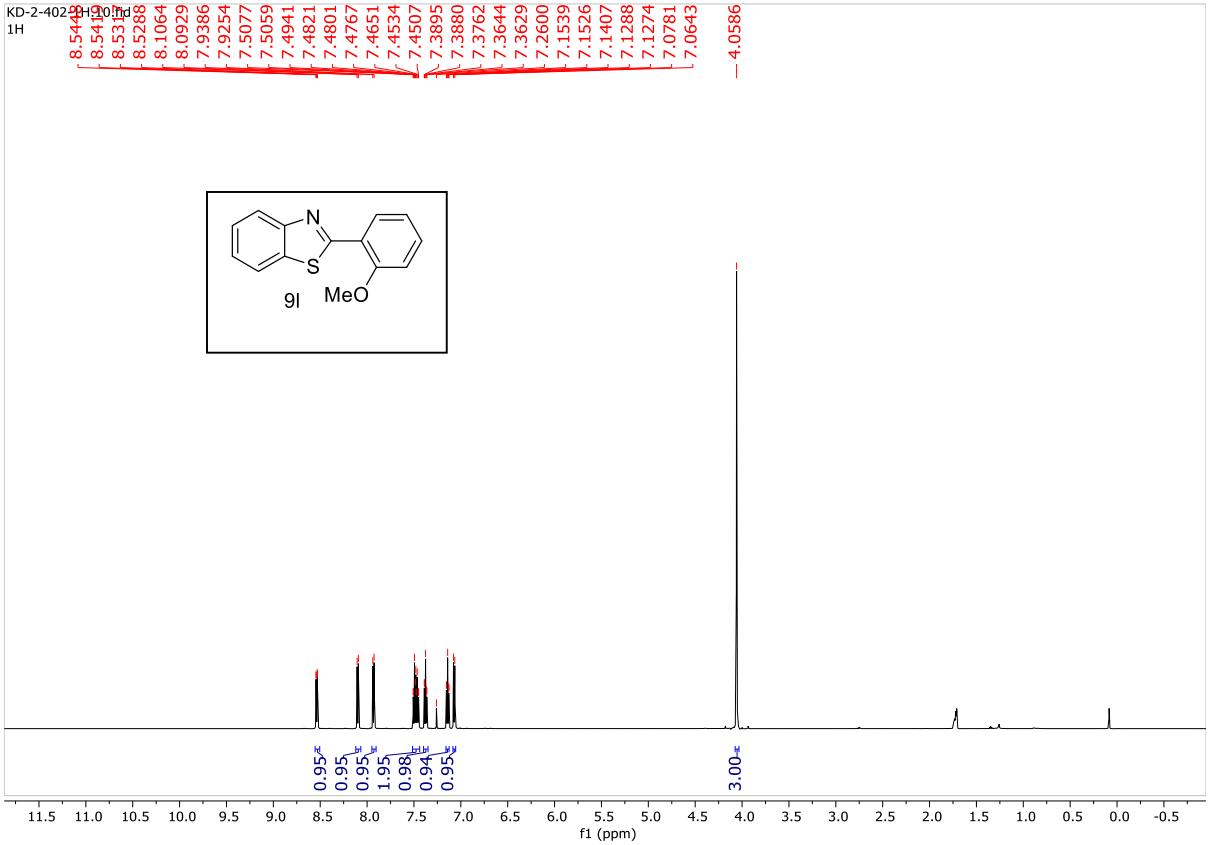

KD-2-301-13C
KD-2-301-13C
165.24
165.21
165.18
164.68
164.55
162.20
162.20
162.07
153.97
136.80
136.71
136.61
135.26
126.85
126.03
123.81
121.87
110.71
110.64
110.52
110.44
106.44
106.19
105.93
77.48
77.16
76.84
N
S
F
F
9i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

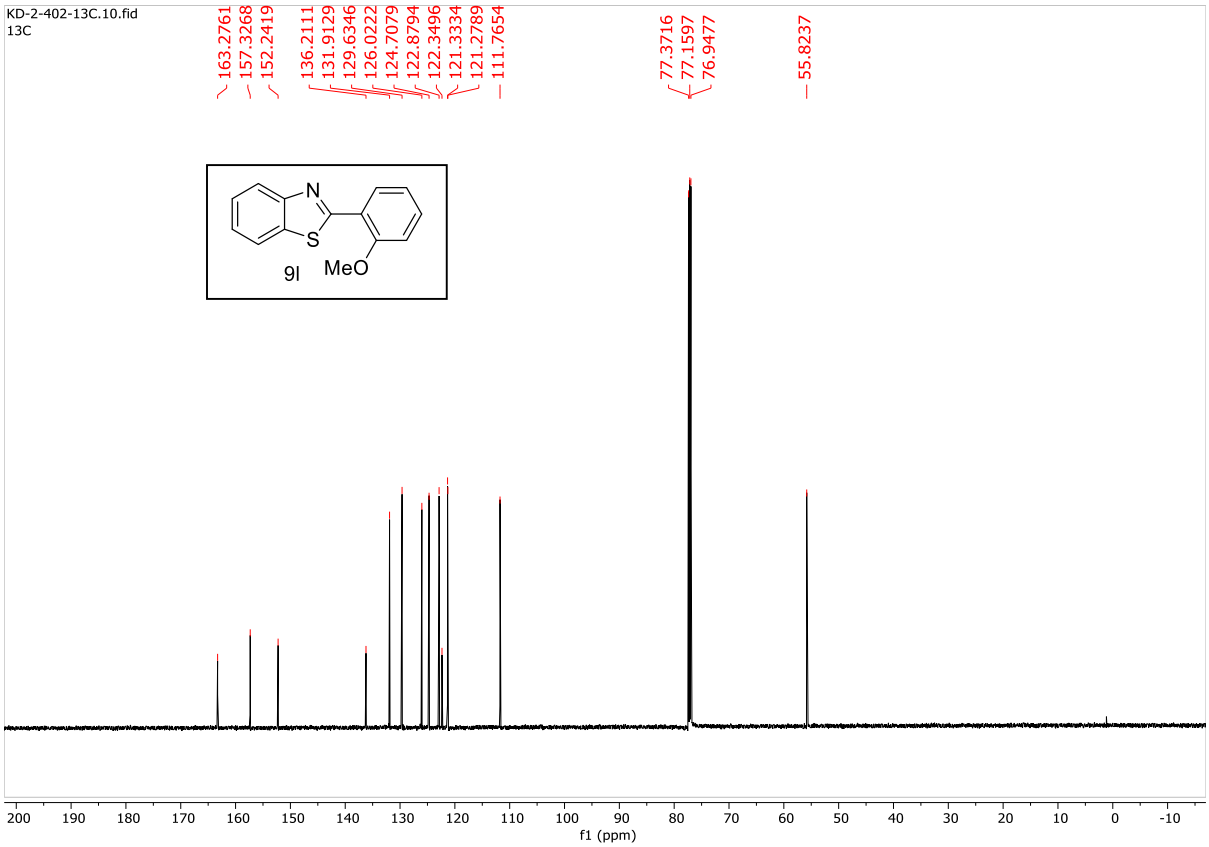

KD-2-294-1H
KD-2-294-1H
8.0810
8.0606
7.9341
7.9238
7.9182
7.9133
7.8784
7.8598
7.6045
7.5937
7.5882
7.5177
7.4994
7.4796
7.4055
7.3891
7.3686
7.2700
N
S
Br
9j
1.00
2.90
1.95
1.04
1.00
f1 (ppm)

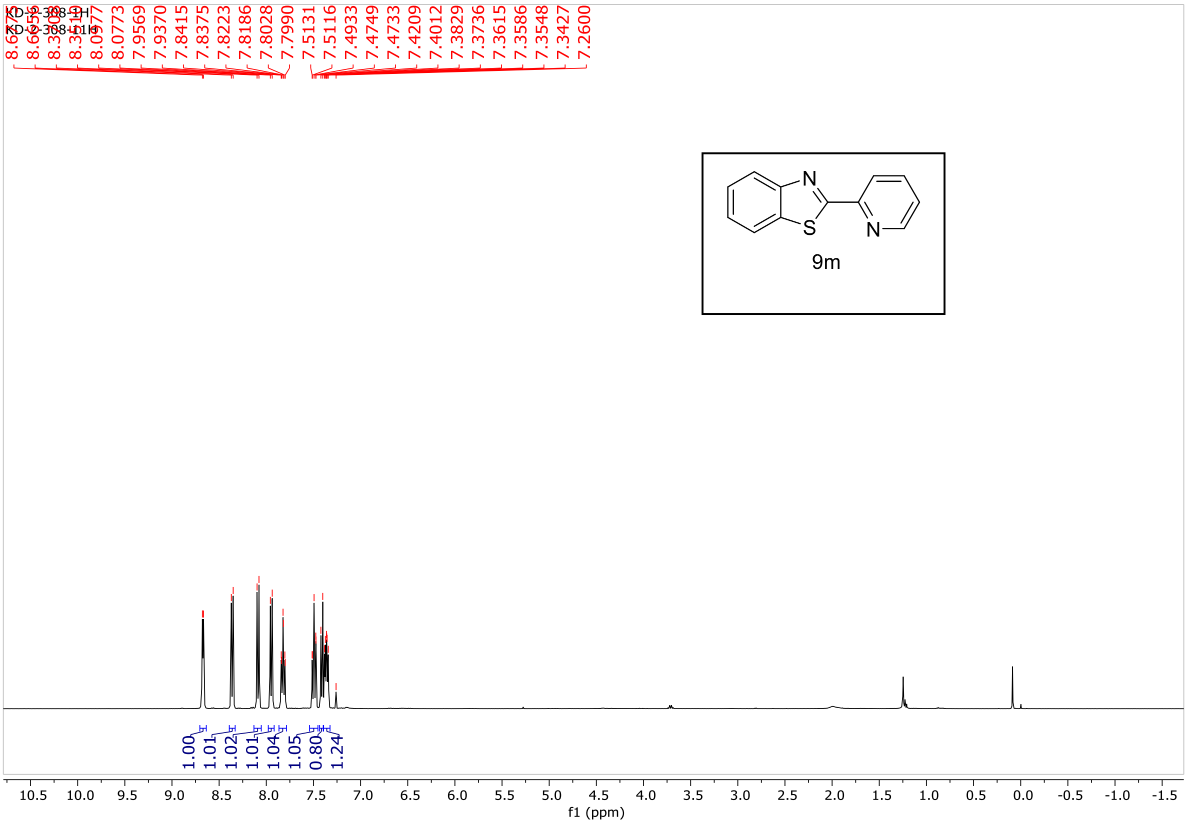

KD-2-294-13C
KD-2-294-13C
166.72
154.13
135.10
132.58
132.27
128.95
126.57
125.51
125.49
123.39
121.73
77.48
77.16
76.84
N
S
Br
9j
f1 (ppm)

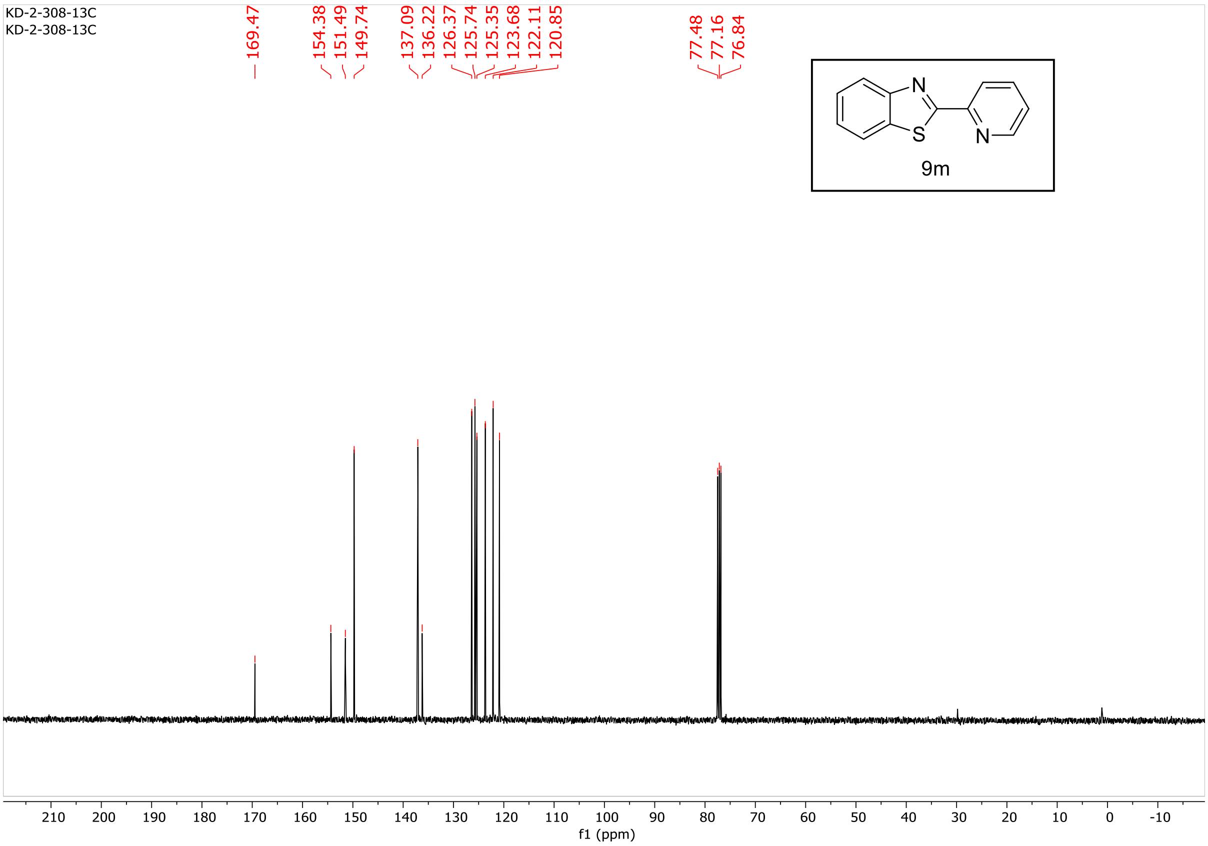

KD-2-400-1H.10.fid
1H
8.1819
8.1683
8.1059
8.0923
7.9087
7.8954
7.7365
7.7228
7.5315
7.5192
7.5069
7.4293
7.4169
7.4047
7.2600
N
S
CF3
9k
2.00
0.99
0.97
2.03
1.04
1.00
f1 (ppm)

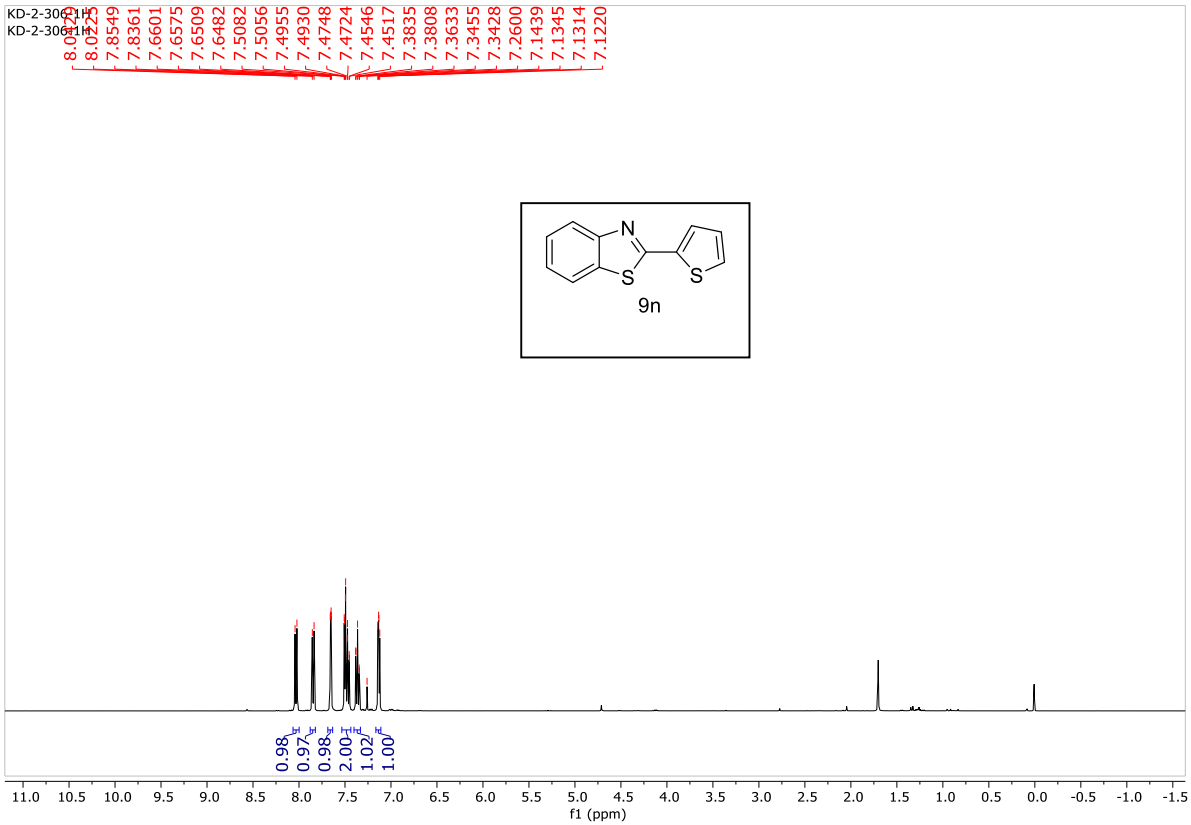

KD-2-400-13C.10.fid
13C
166.1467
154.1068
136.8105
135.2846
132.8348
132.6183
132.4020
132.1854
127.8406
126.7638
126.1347
126.1108
126.0857
126.0601
125.8960
124.8299
123.7156
123.0265
121.8480
77.3716
77.1597
76.9479
N
S
CF3
9k
f1 (ppm)

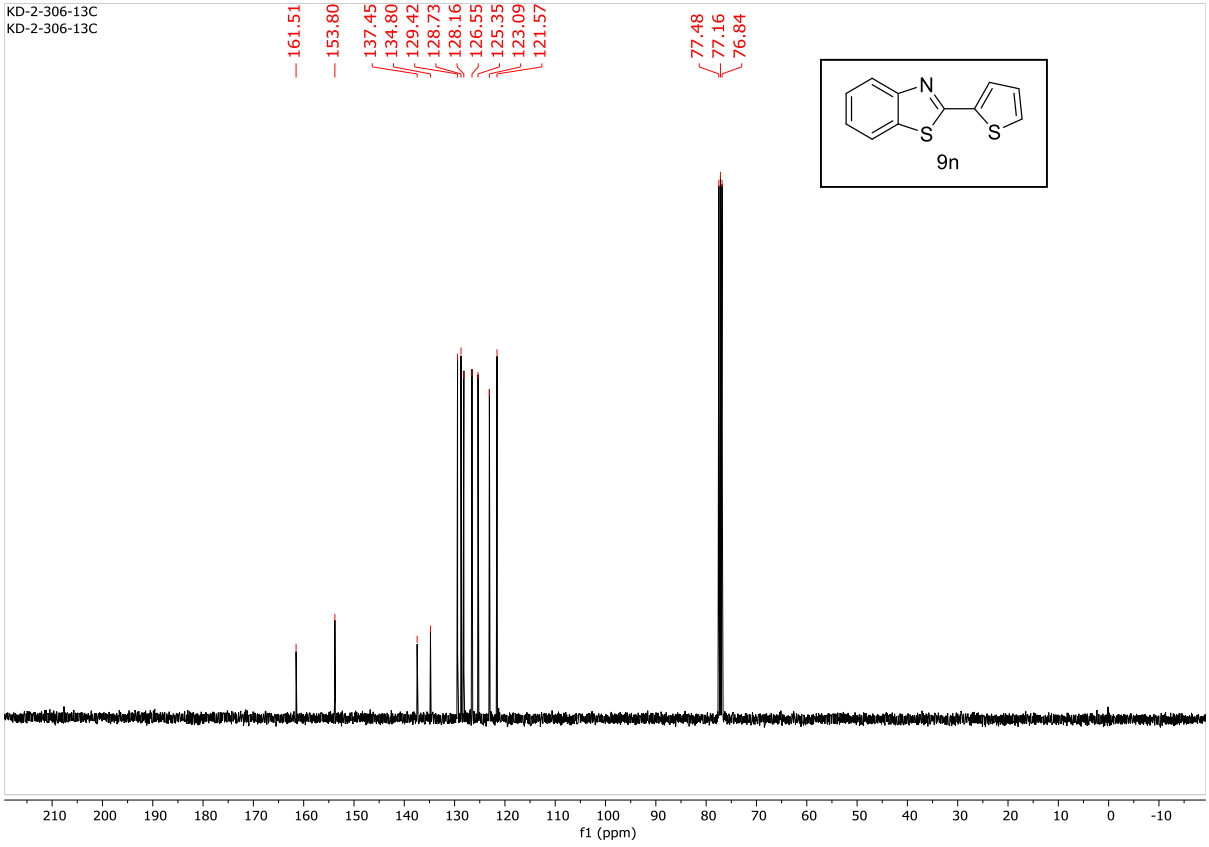

KD-2-402-1H.10.fid
1H
8.5441
8.5311
8.5288
8.1064
8.0929
7.9386
7.9254
7.5077
7.5059
7.4941
7.4821
7.4801
7.4767
7.4651
7.4534
7.4507
7.3895
7.3880
7.3762
7.3644
7.3629
7.2600
7.1539
7.1526
7.1407
7.1288
7.1274
7.0781
7.0643
4.0586
N
S
MeO
9l
0.95
0.95
0.95
1.95
0.98
0.94
0.95
3.00
f1 (ppm)

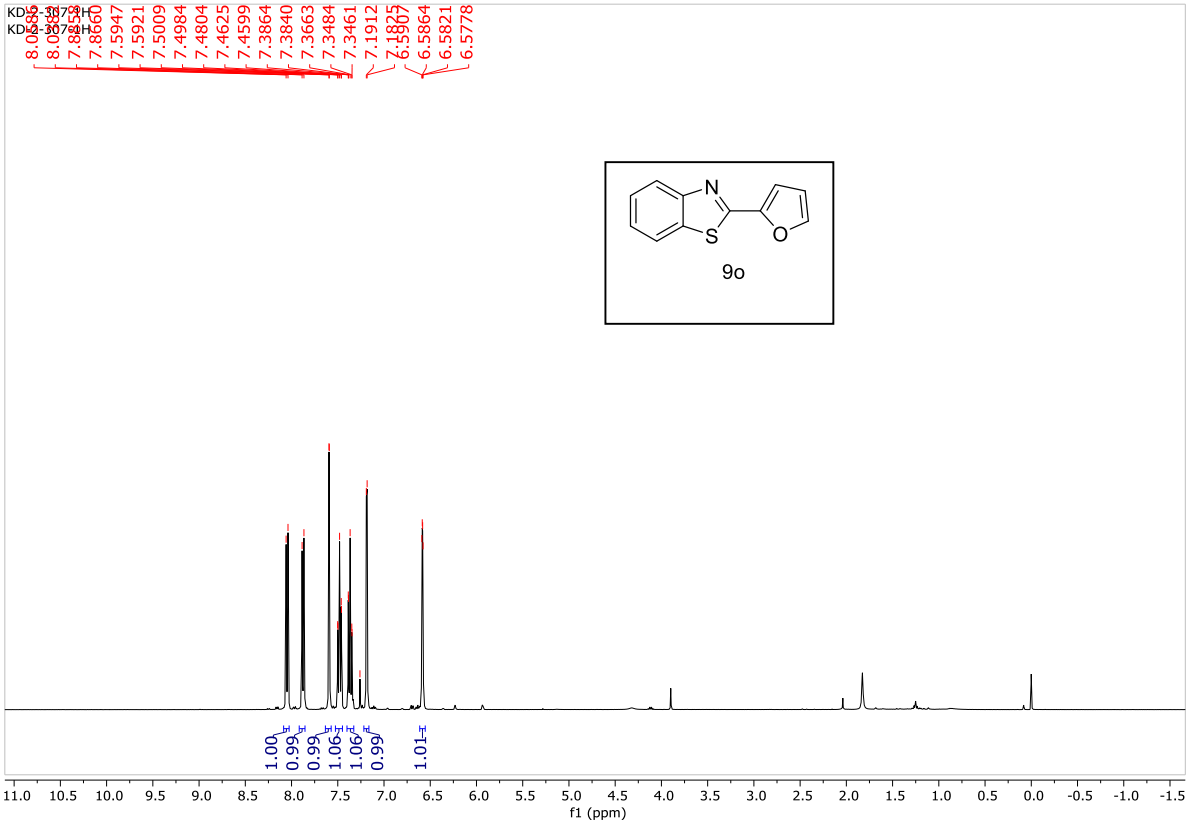

KD-2-402-13C.10.fid
13C
163.2761
157.3268
152.2419
136.2111
131.9129
129.6346
126.0222
124.7079
122.8794
122.3496
121.3334
121.2789
111.7654
77.3716
77.1597
76.9477
55.8237
N
S
MeO
9l
f1 (ppm)

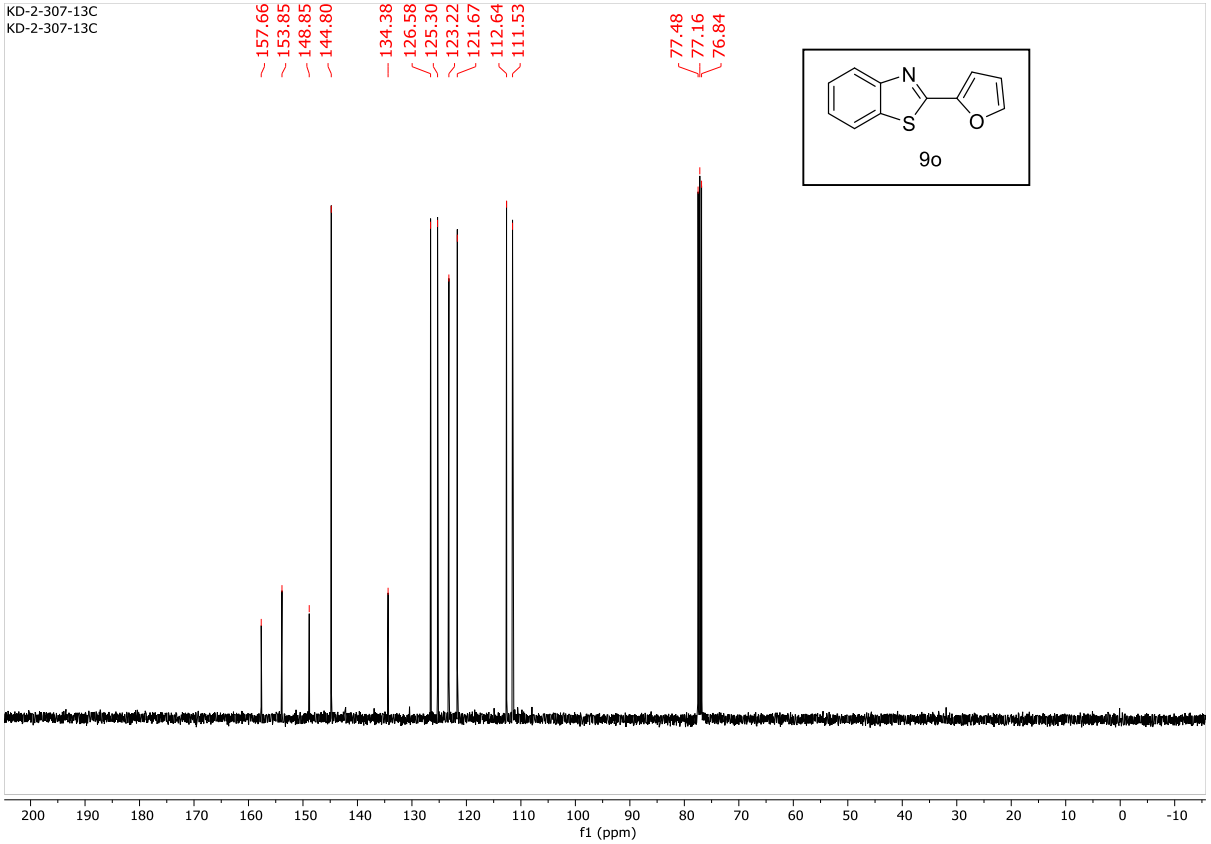

KD-2-308-1H
8.0773
7.9569
7.9370
7.8415
7.8375
7.8223
7.8186
7.8028
7.7990
7.5131
7.5116
7.4933
7.4749
7.4733
7.4209
7.4012
7.3829
7.3736
7.3615
7.3586
7.3548
7.3427
7.2600
N
S
N
9m
1.00
1.01
1.02
1.01
1.04
1.05
0.80
1.24
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

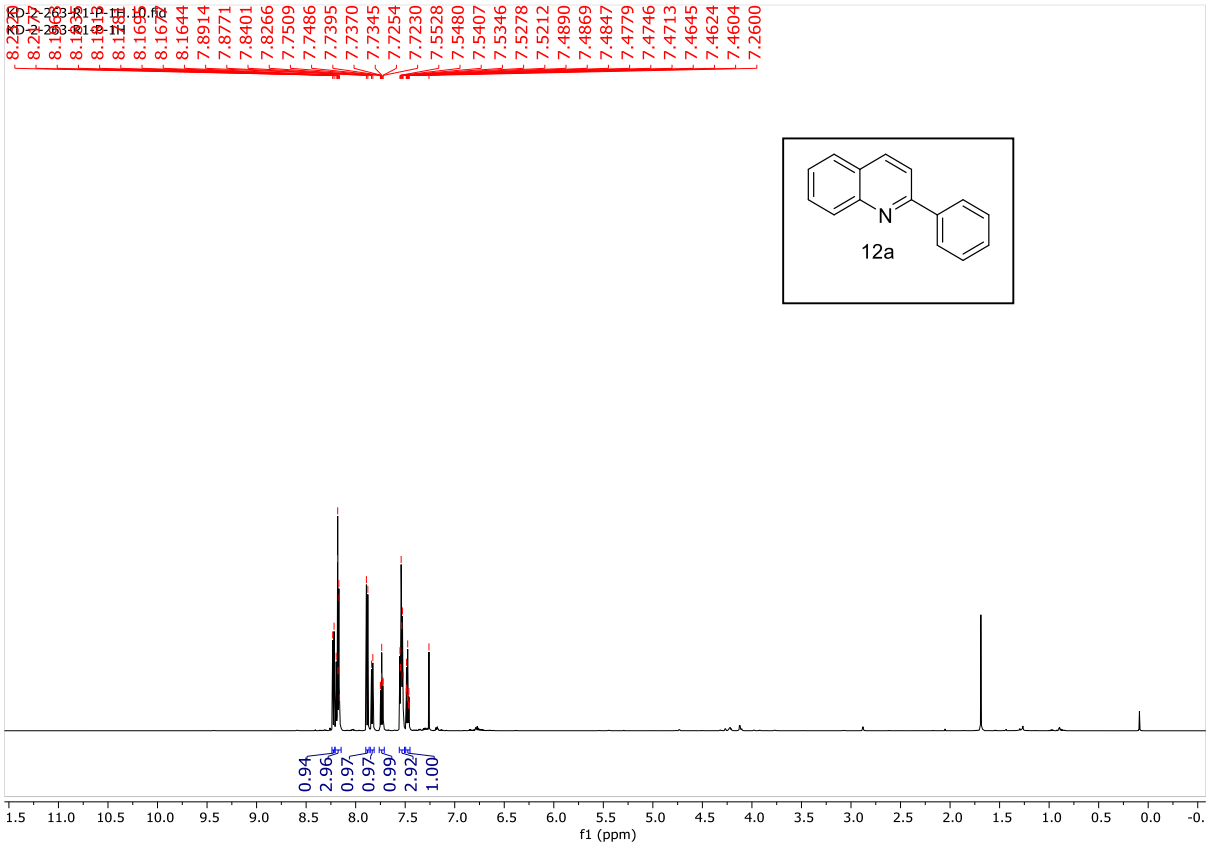

KD-2-308-13C
KD-2-308-13C
169.47
154.38
151.49
149.74
137.09
136.22
126.37
125.74
125.35
123.68
122.11
120.85
77.48
77.16
76.84
N
S
N
9m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

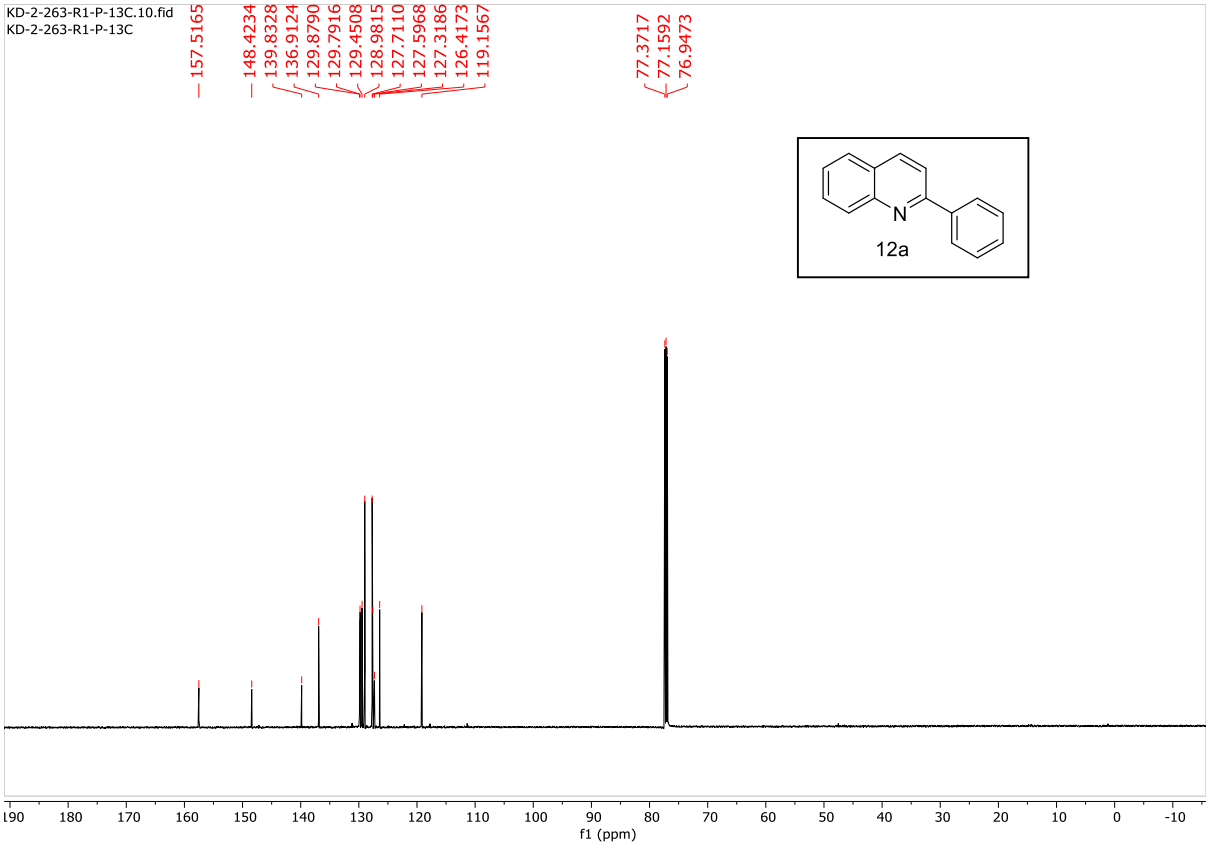

KD-2-306-1H
KD-2-306-1H
8.0225
8.0122
7.8549
7.8361
7.6601
7.6575
7.6509
7.6482
7.5082
7.5056
7.4955
7.4930
7.4748
7.4724
7.4546
7.4517
7.3835
7.3808
7.3633
7.3455
7.3428
7.2600
7.1439
7.1345
7.1314
7.1220
N
S
S
9n
0.98
0.97
0.98
2.00
1.02
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

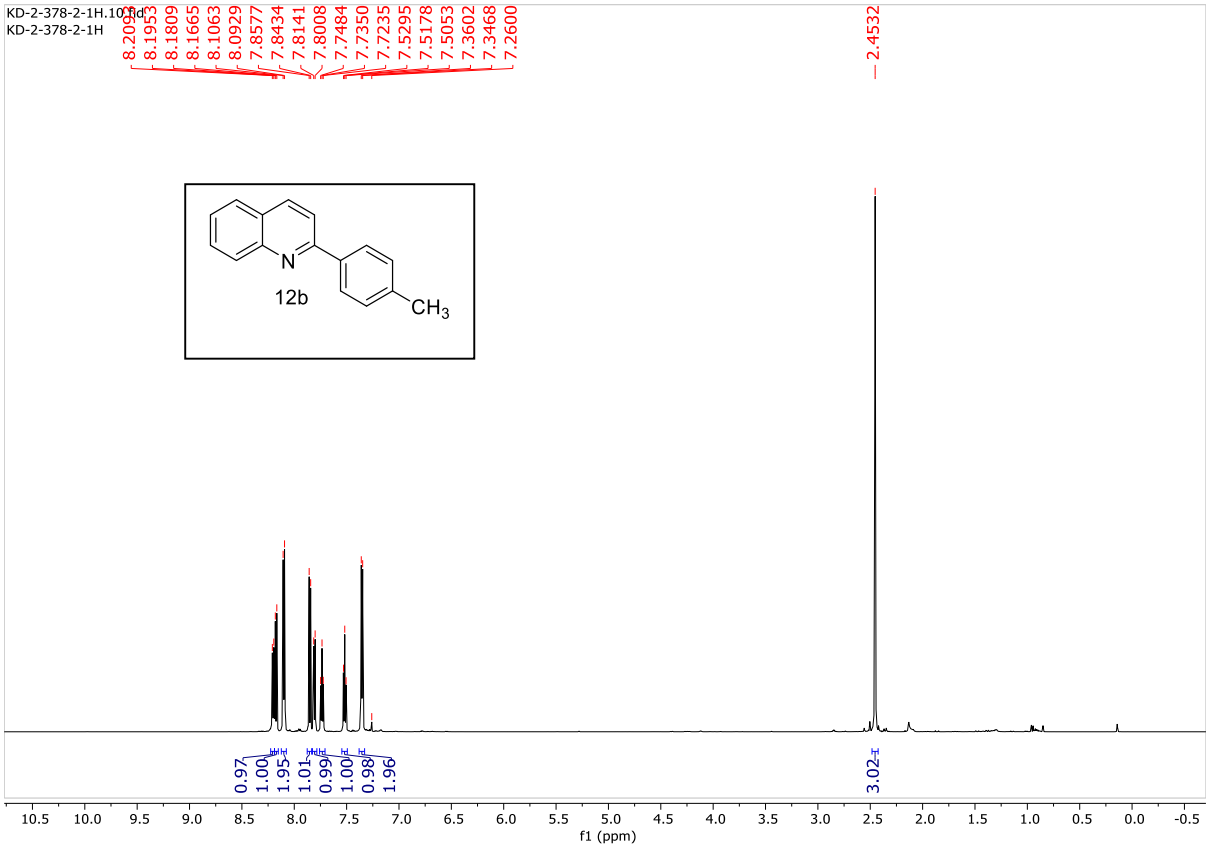

KD-2-306-13C
KD-2-306-13C
161.51
153.80
137.45
134.80
129.42
128.73
128.16
126.55
125.35
123.09
121.57
77.48
77.16
76.84
N
S
S
9n
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

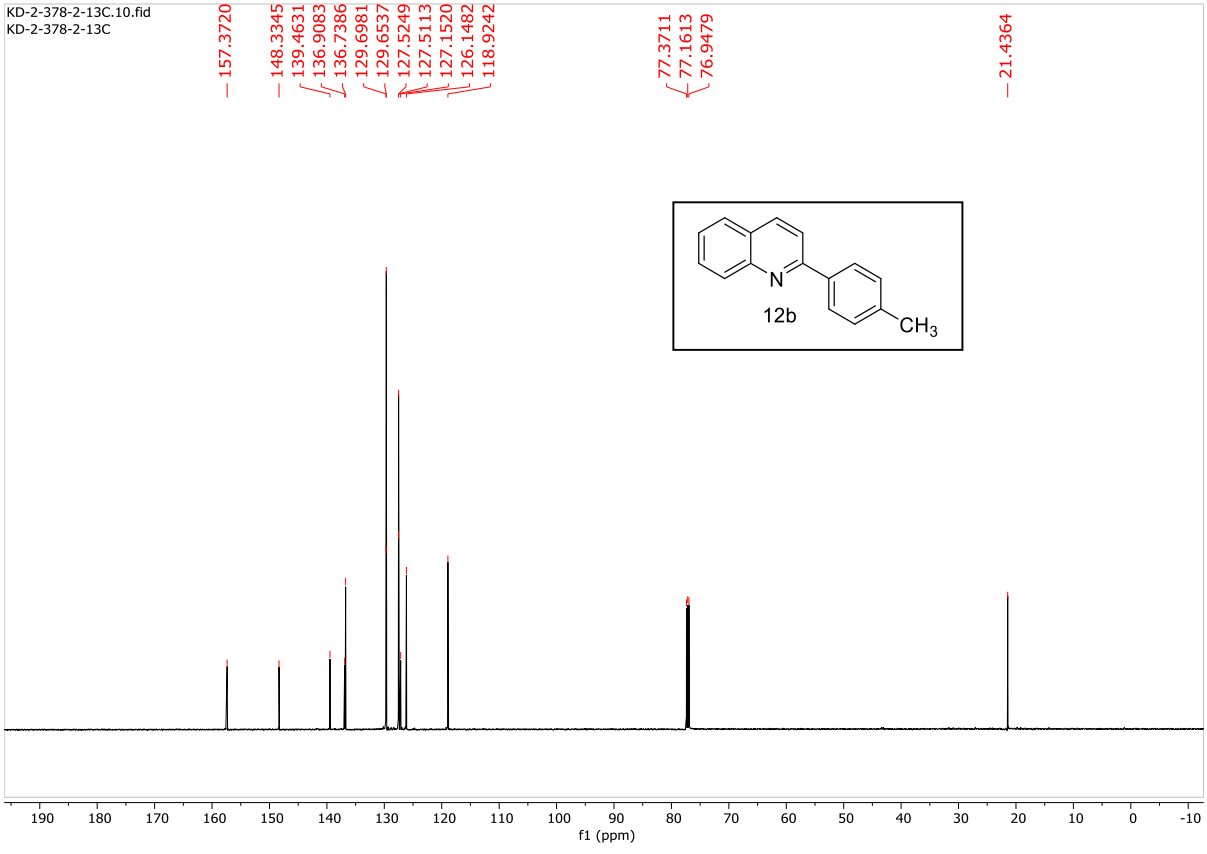

KD-2-307-1H
KD-2-307-1H
8.0686
8.0553
7.8553
7.8660
7.5947
7.5921
7.5009
7.4984
7.4804
7.4625
7.4599
7.3864
7.3840
7.3663
7.3484
7.3461
7.1912
7.1825
6.5907
6.5864
6.5821
6.5778
N
S
O
9o
1.00
0.99
0.99
1.06
1.06
0.99
1.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

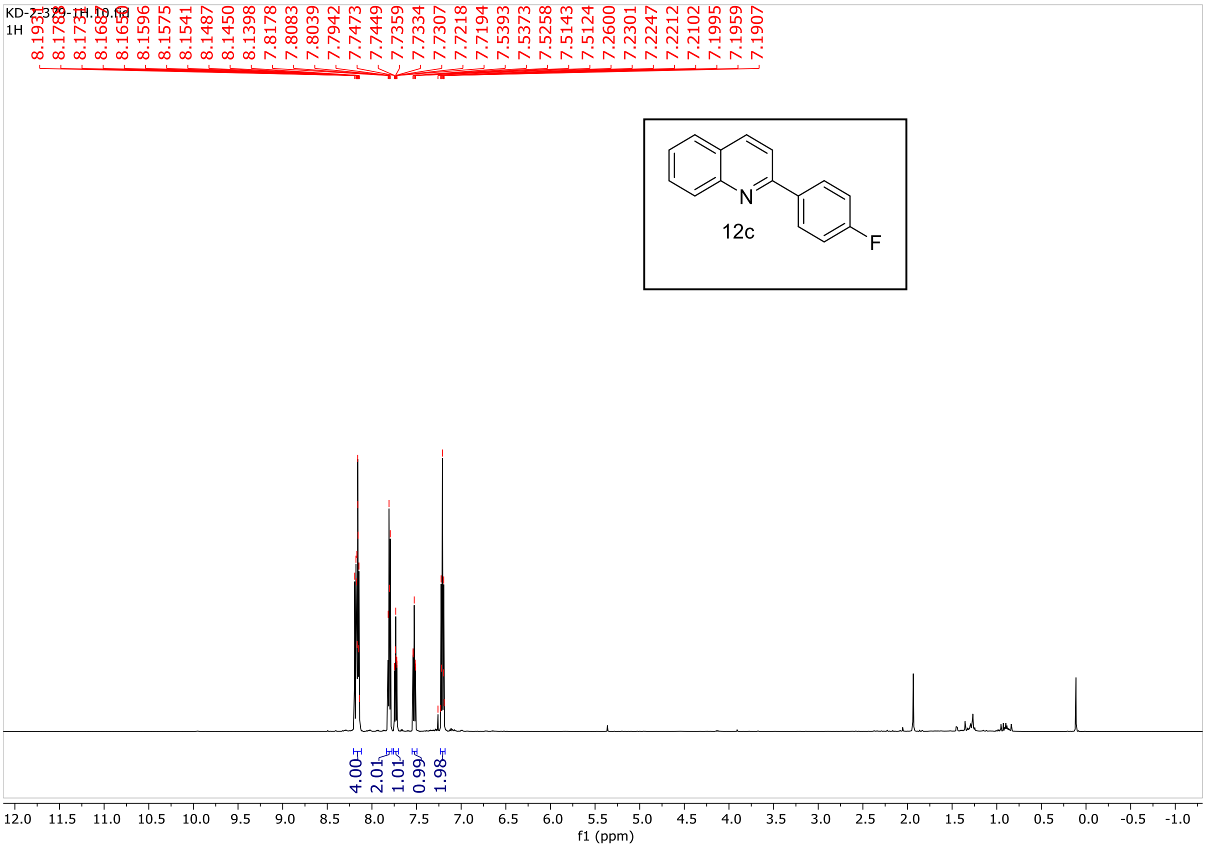

KD-2-307-13C
KD-2-307-13C
157.66
153.85
148.85
144.80
134.38
126.58
125.30
123.22
121.67
112.64
111.53
77.48
77.16
76.84
N
S
O
9o
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

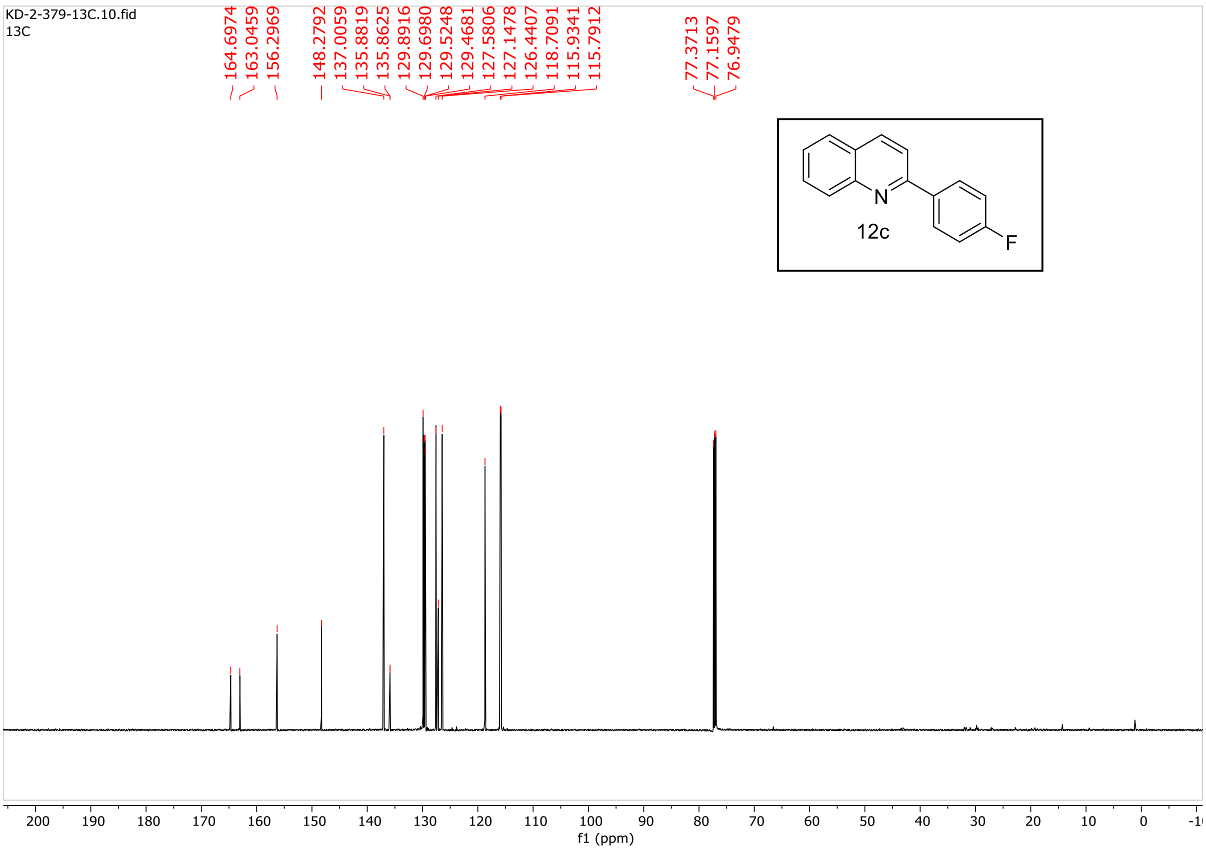

8.2600
8.1644
7.8914
7.8771
7.8401
7.8266
7.7509
7.7486
7.7395
7.7370
7.7345
7.7254
7.7230
7.5528
7.5480
7.5407
7.5346
7.5278
7.5212
7.4890
7.4869
7.4847
7.4779
7.4746
7.4713
7.4645
7.4624
7.4604
7.2600
N
12a
0.94
2.96
0.97
0.97
0.99
2.92
1.00
f1 (ppm)

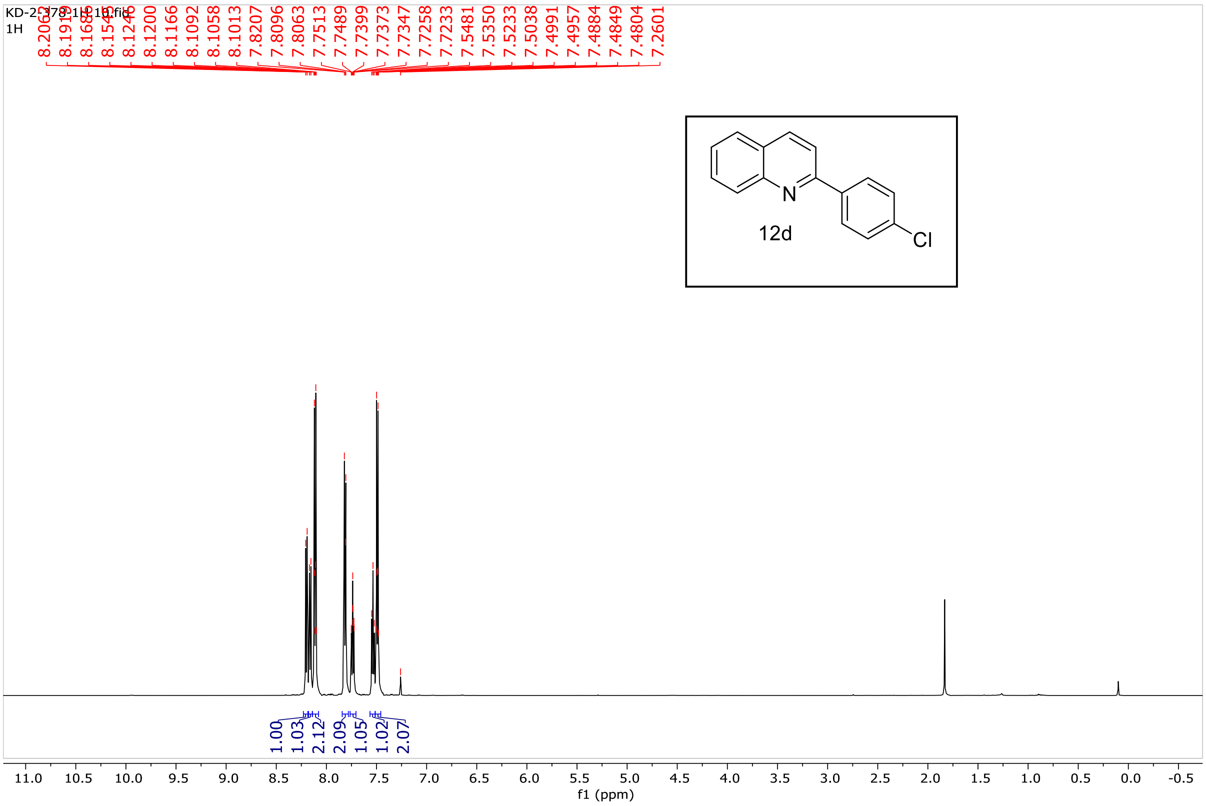

KD-2-263-R1-P-13C.10.fid
KD-2-263-R1-P-13C
157.5165
148.4234
139.8328
136.9124
129.8790
129.7916
129.4508
128.9815
127.7110
127.5968
127.3186
126.4173
119.1567
77.3717
77.1592
76.9473
N
12a
f1 (ppm)

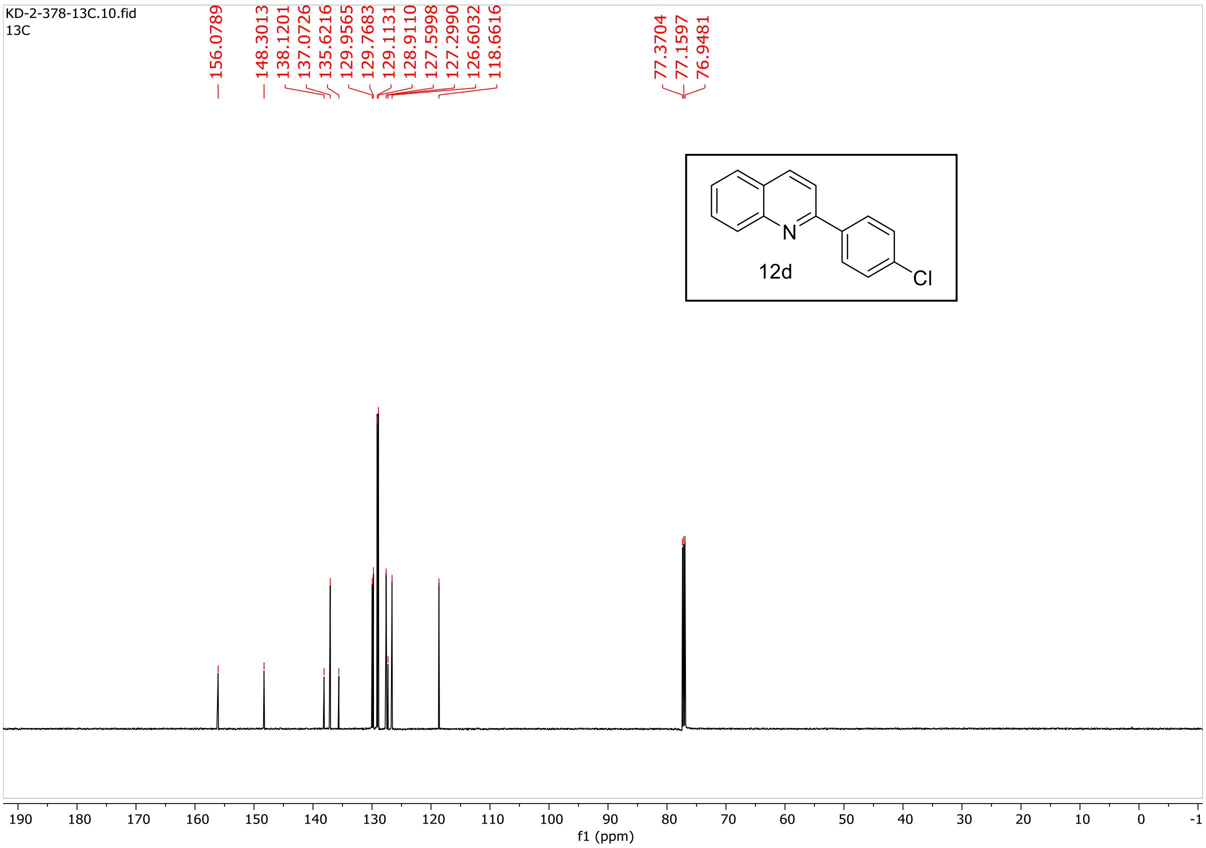

KD-2-378-2-1H.10.fid
KD-2-378-2-1H
8.2094
8.1953
8.1809
8.1665
8.1063
8.0929
7.8577
7.8434
7.8141
7.8008
7.7484
7.7350
7.7235
7.5295
7.5178
7.5053
7.3602
7.3468
7.2600
2.4532
N
12b
CH3
0.97
1.00
1.95
1.01
0.99
1.00
0.98
1.96
3.02
f1 (ppm)

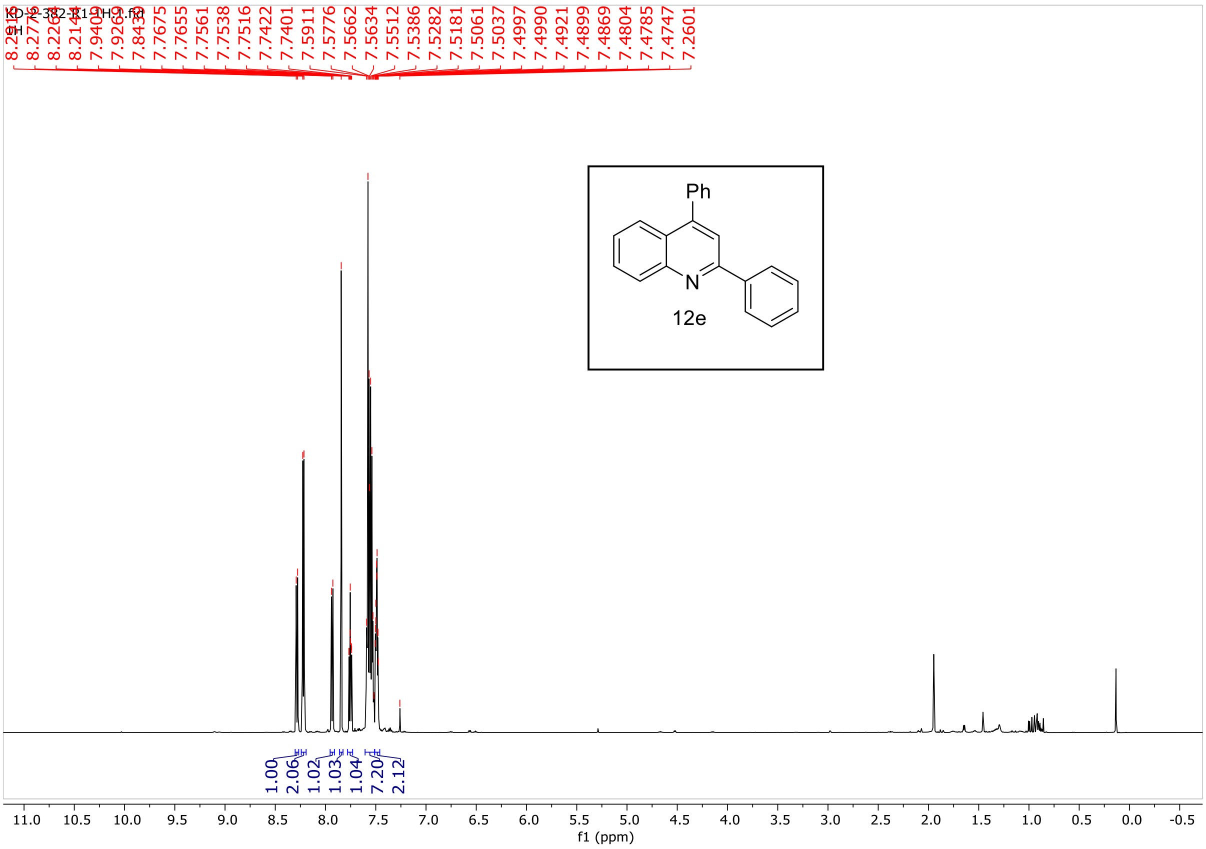

KD-2-378-2-13C.10.fid
KD-2-378-2-13C
157.3720
148.3345
139.4631
136.9083
136.7386
129.6981
129.6537
127.5249
127.5113
127.1520
126.1482
118.9242
77.3711
77.1613
76.9479
21.4364
N
12b
CH3
f1 (ppm)

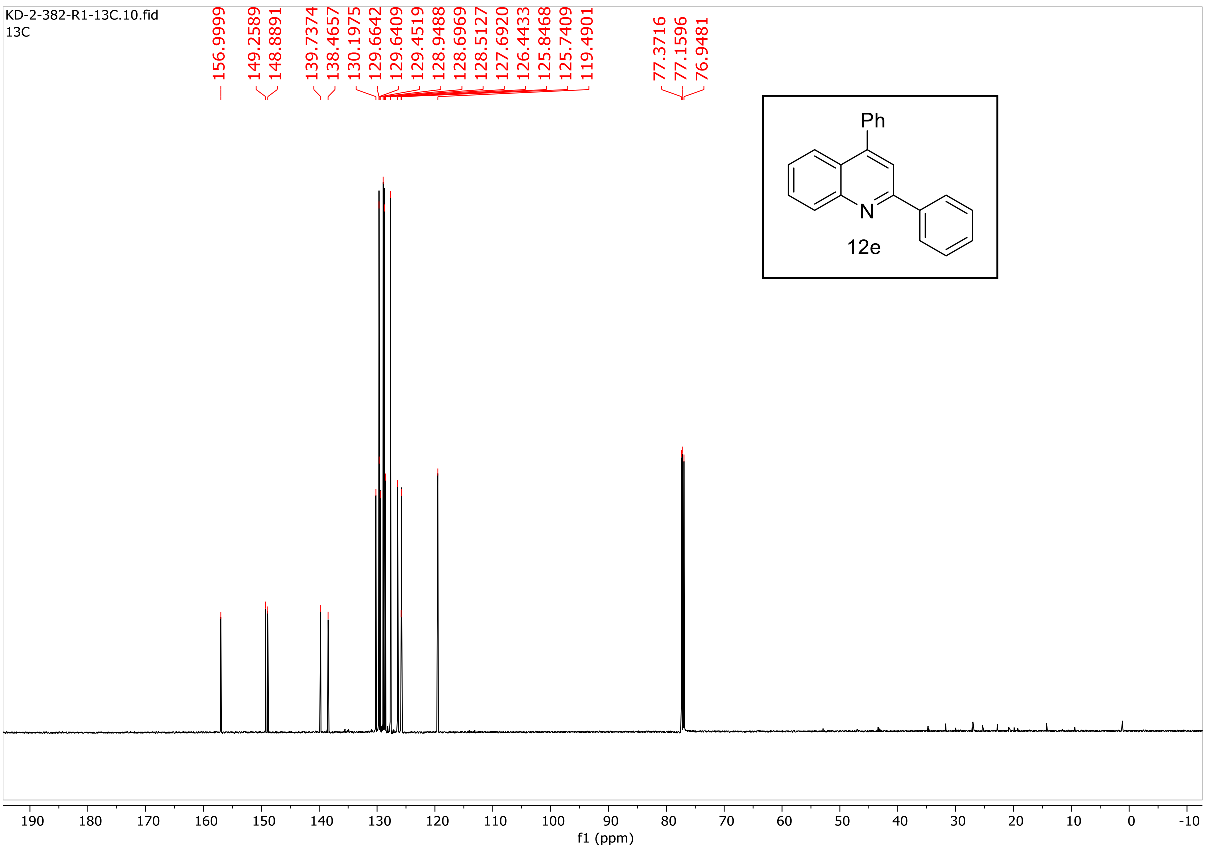

KD-2-379-1H.10.fid
1H
8.1596
8.1575
8.1541
8.1487
8.1450
8.1398
7.8178
7.8083
7.8039
7.7942
7.7473
7.7449
7.7359
7.7334
7.7307
7.7218
7.7194
7.5393
7.5373
7.5258
7.5143
7.5124
7.2600
7.2301
7.2247
7.2212
7.2102
7.1995
7.1959
7.1907
N
12c
F
4.00
2.01
1.01
0.99
1.98
f1 (ppm)

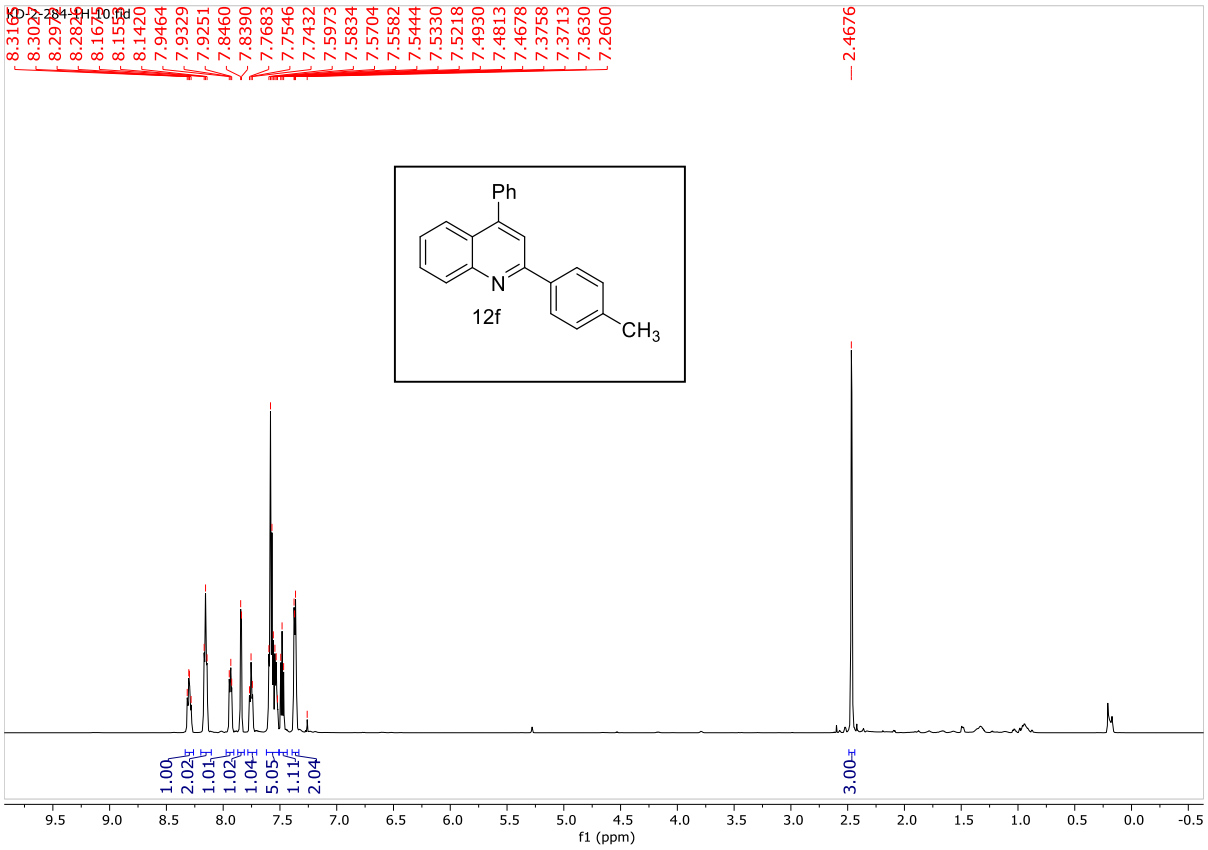

KD-2-379-13C.10.fid
13C
164.6974
163.0459
156.2969
148.2792
137.0059
135.8819
135.8625
129.8916
129.6980
129.5248
129.4681
127.5806
127.1478
126.4407
118.7091
115.9341
115.7912
77.3713
77.1597
76.9479
N
12c
F
f1 (ppm)

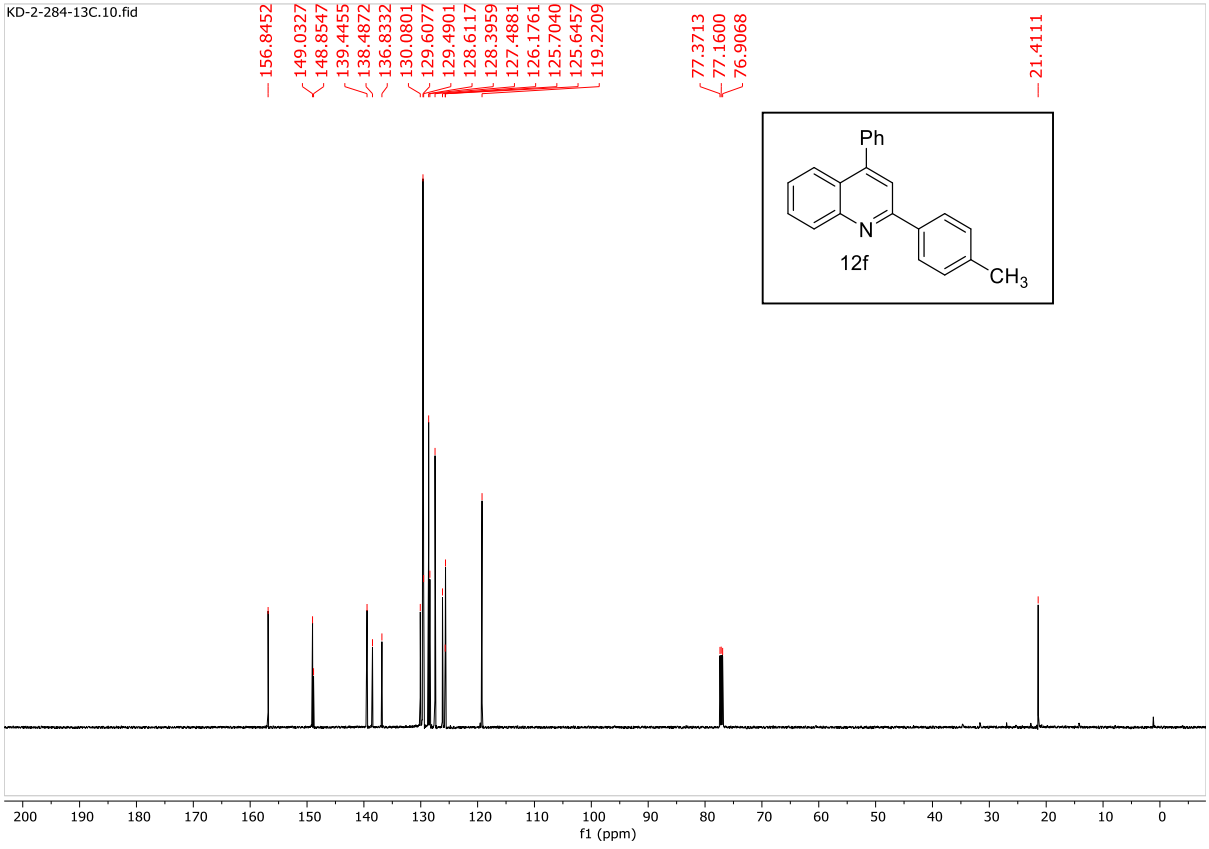

KD-2-378-1H.10.fid
1H
12d
N
Cl
f1 (ppm)

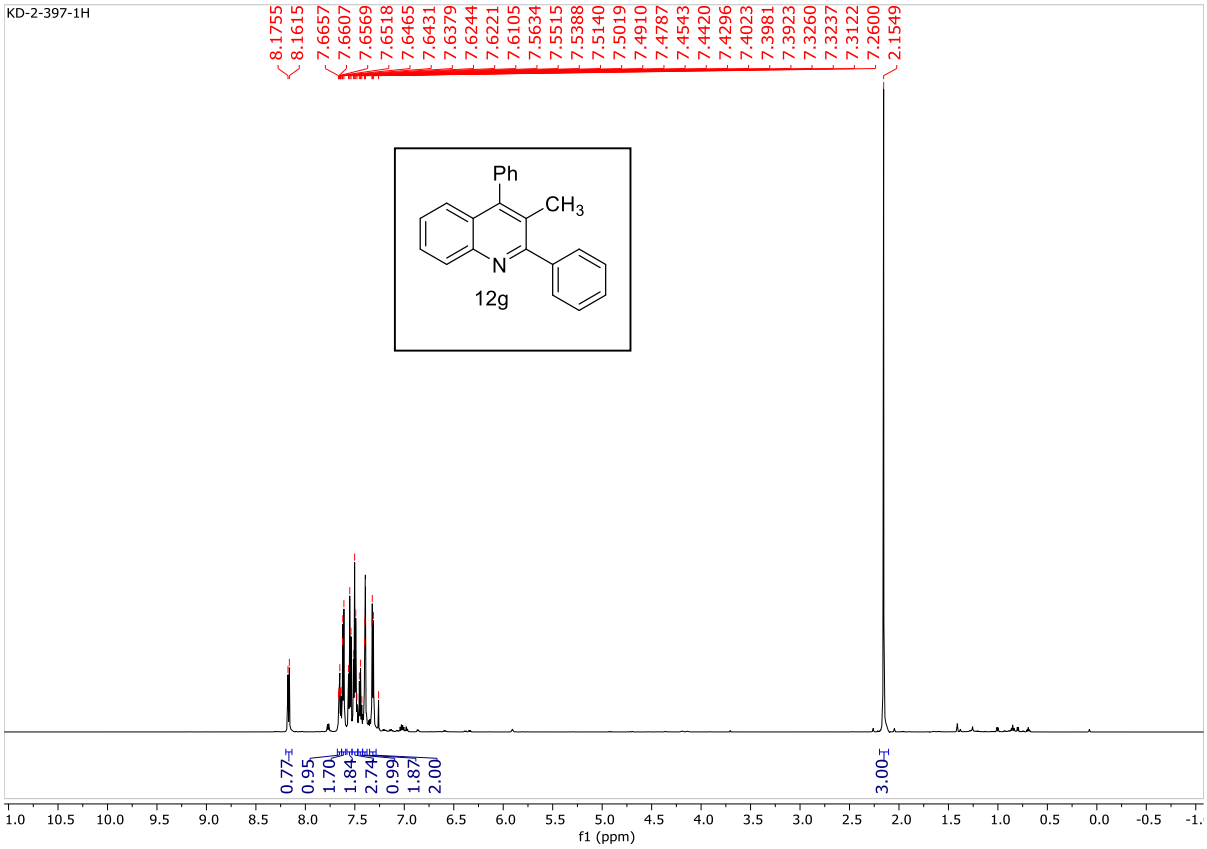

KD-2-378-13C.10.fid
13C
156.0789
148.3013
138.1201
137.0726
135.6216
129.9565
129.7683
129.1131
128.9110
127.5998
127.2990
126.6032
118.6616
77.3704
77.1597
76.9481
12d
N
Cl
f1 (ppm)

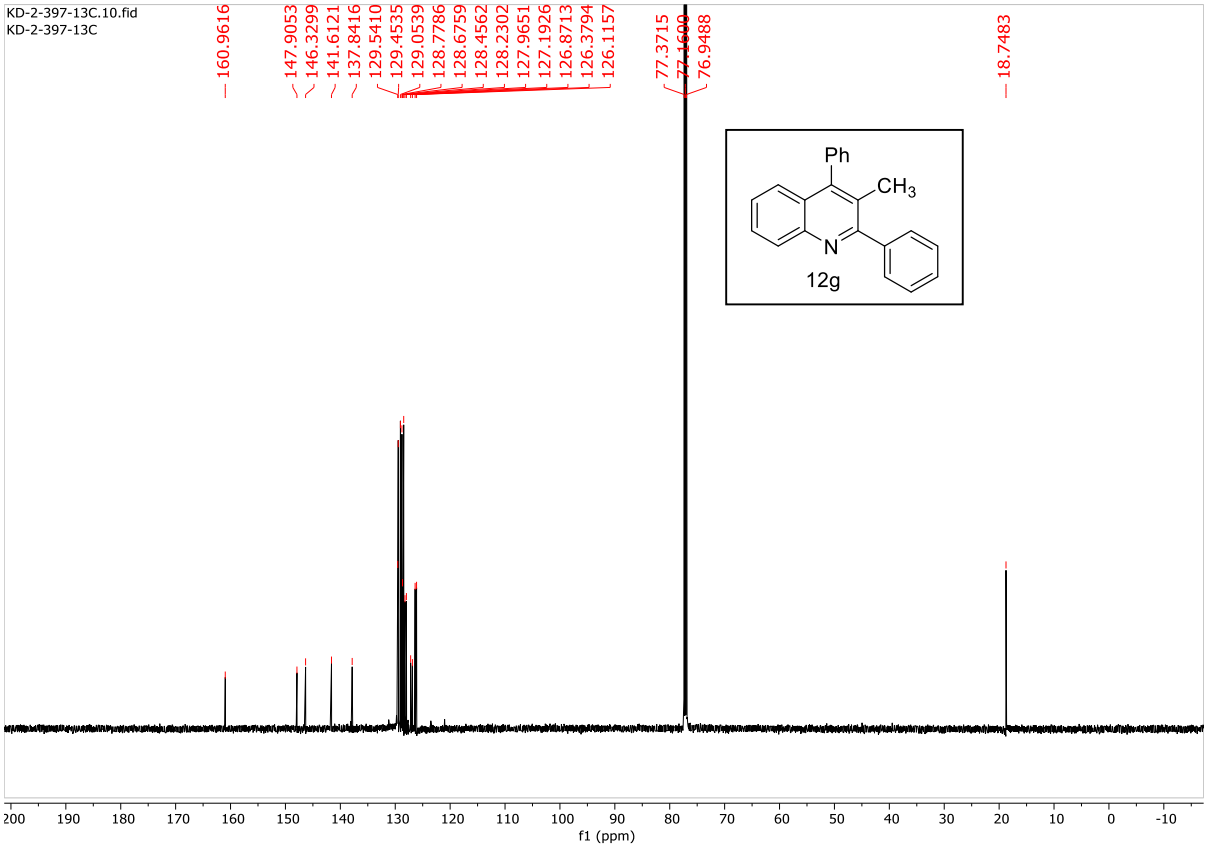

KD-2-382-R1-1H.1.fid
1H
8.2916
8.2776
8.2264
8.2144
7.9409
7.9269
7.8439
7.7675
7.7655
7.7561
7.7538
7.7516
7.7422
7.7401
7.5911
7.5776
7.5662
7.5634
7.5512
7.5386
7.5282
7.5181
7.5061
7.5037
7.4997
7.4990
7.4921
7.4899
7.4869
7.4804
7.4785
7.4747
7.2601
Ph
N
12e
1.00
2.06
1.02
1.03
1.04
7.20
2.12
f1 (ppm)

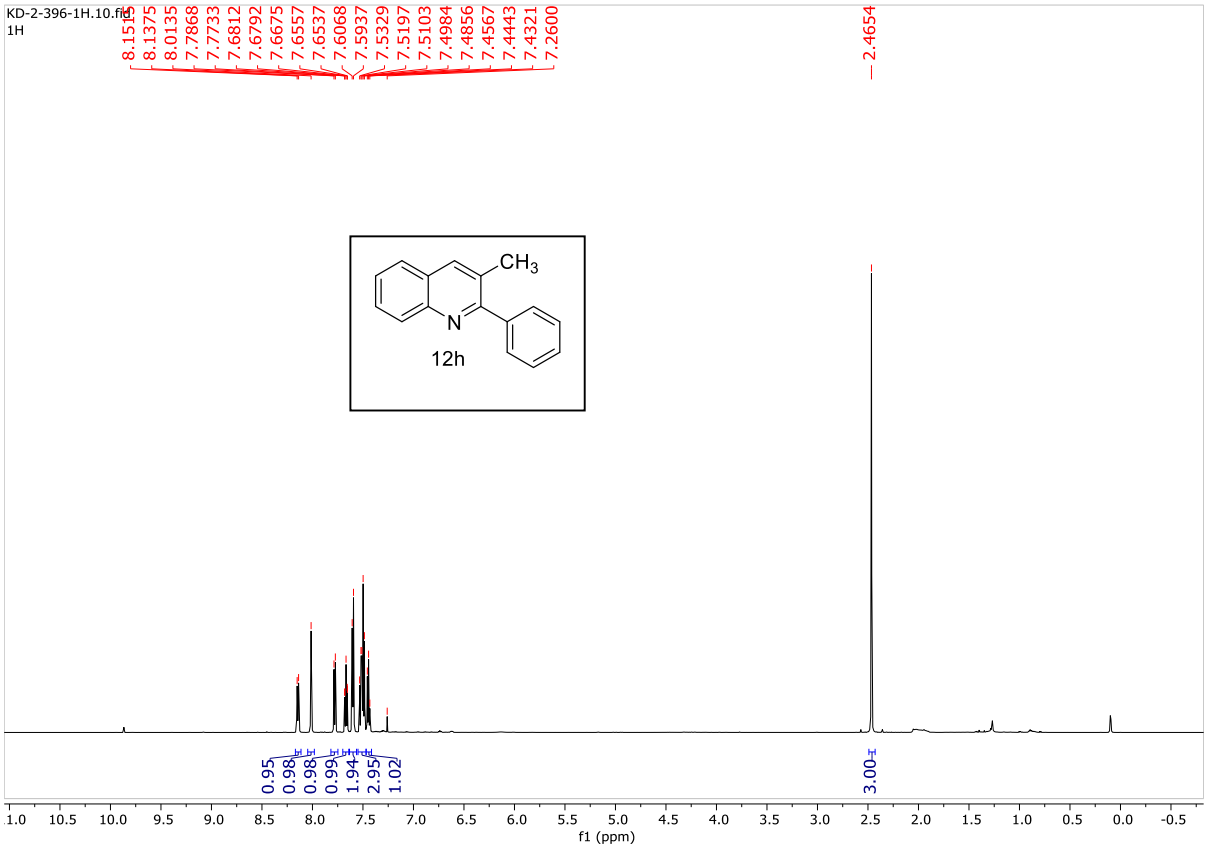

KD-2-382-R1-13C.10.fid
13C
156.9999
149.2589
148.8891
139.7374
138.4657
130.1975
129.6642
129.6409
129.4519
128.9488
128.6969
128.5127
127.6920
126.4433
125.8468
125.7409
119.4901
77.3716
77.1596
76.9481
Ph
N
12e
f1 (ppm)

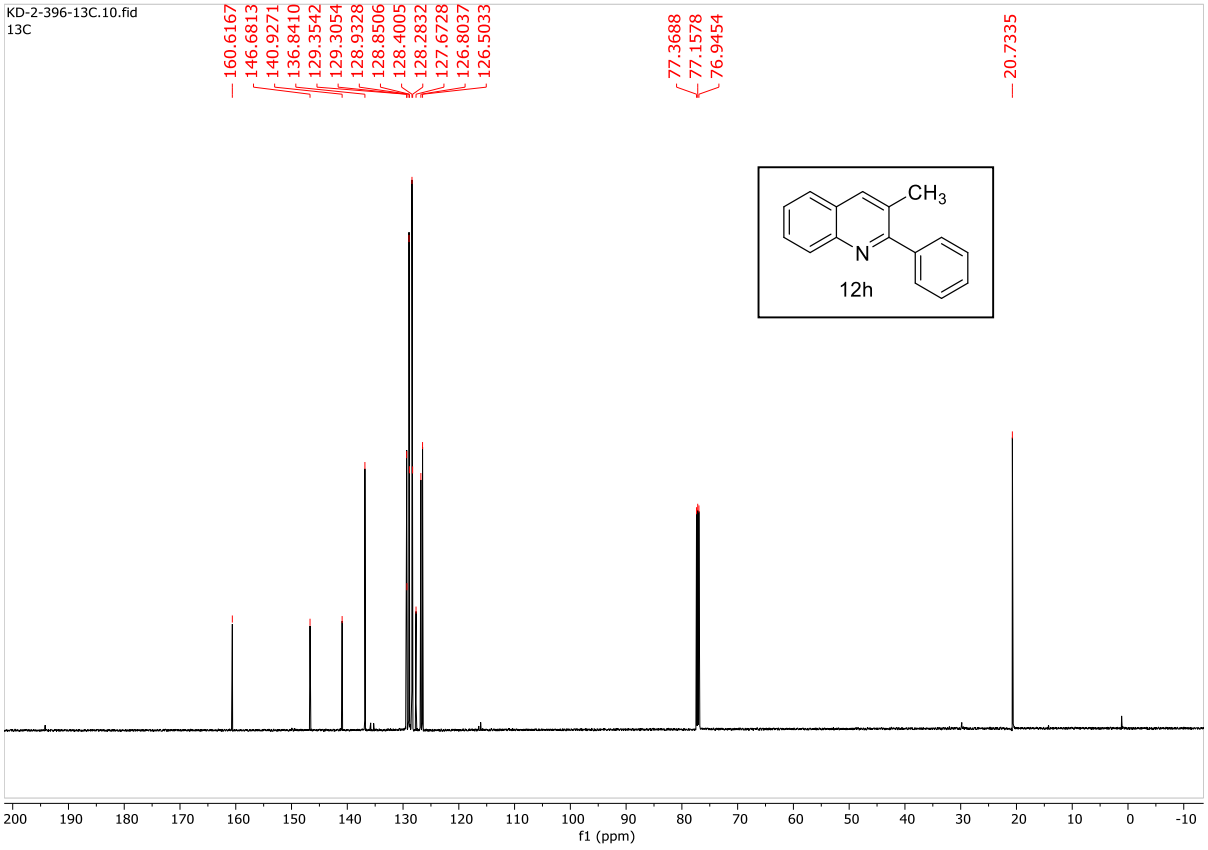

KD-2-284-1H-10.fid
8.3161
8.3024
8.2971
8.2824
8.1674
8.1554
8.1420
7.9464
7.9329
7.9251
7.8460
7.8390
7.7683
7.7546
7.7432
7.5973
7.5834
7.5704
7.5582
7.5444
7.5330
7.5218
7.4930
7.4813
7.4678
7.3758
7.3713
7.3630
7.2600
2.4676
Ph
N
12f
CH3
1.00
2.02
1.01
1.02
1.04
5.05
1.11
2.04
3.00
f1 (ppm)

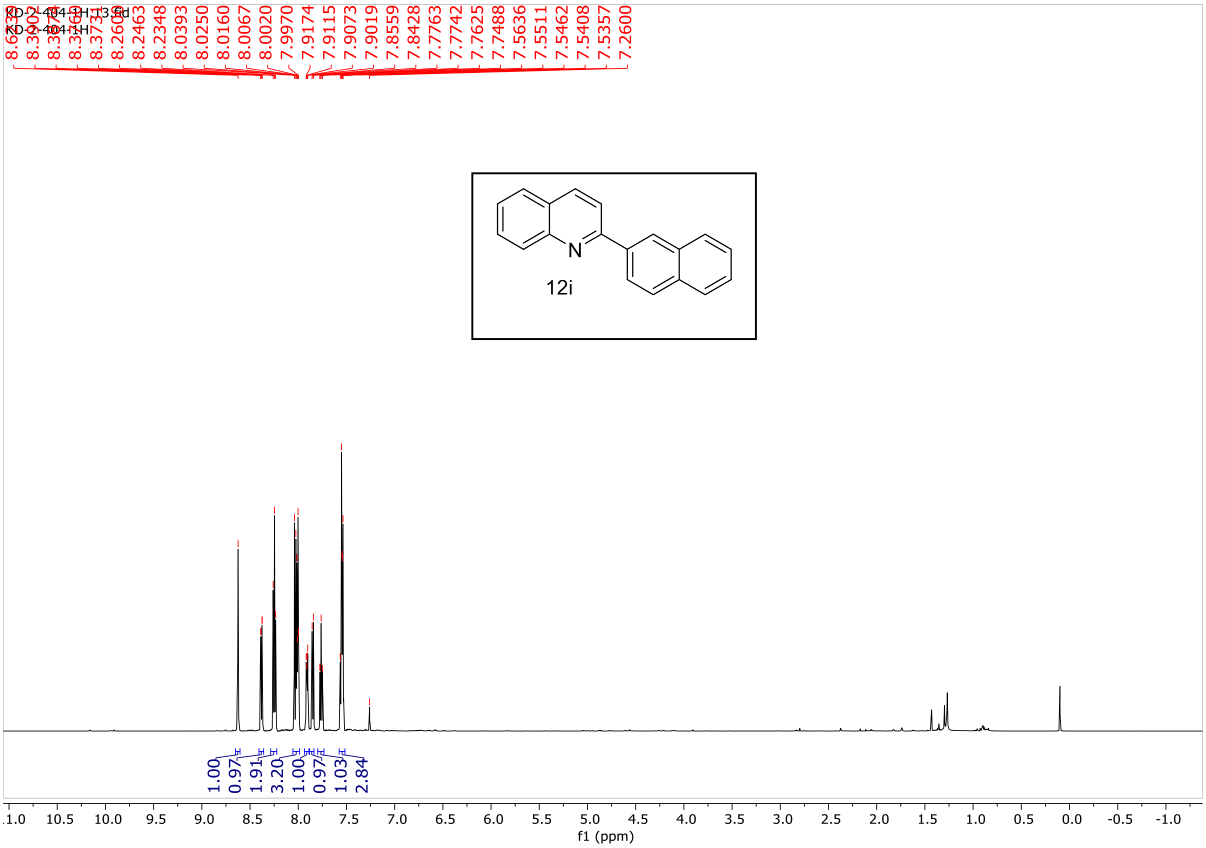

KD-2-284-13C.10.fid
156.8452
149.0327
148.8547
139.4455
138.4872
136.8332
130.0801
129.6077
129.4901
128.6117
128.3959
127.4881
126.1761
125.7040
125.6457
119.2209
77.3713
77.1600
76.9068
21.4111
Ph
N
12f
CH3
f1 (ppm)

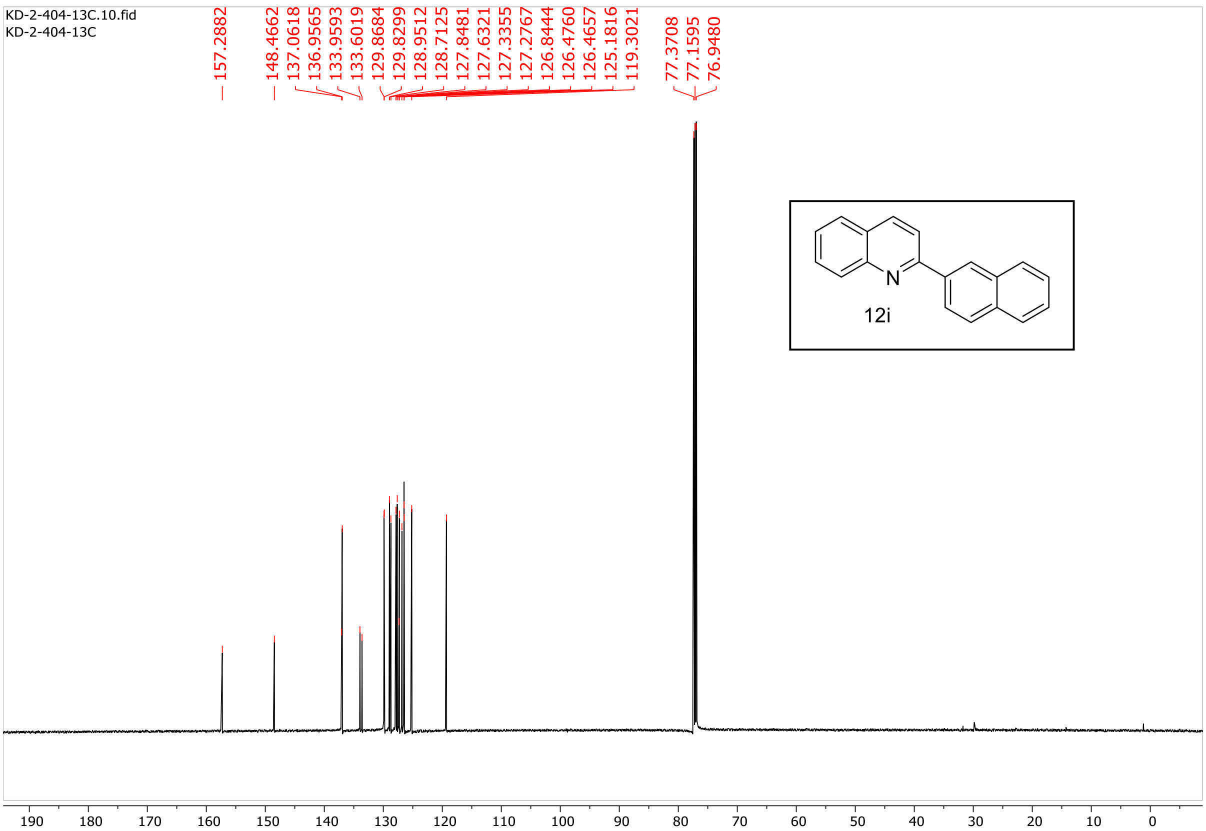

KD-2-397-1H
8.1755
8.1615
7.6657
7.6607
7.6569
7.6518
7.6465
7.6431
7.6379
7.6244
7.6221
7.6105
7.5634
7.5515
7.5388
7.5140
7.5019
7.4910
7.4787
7.4543
7.4420
7.4296
7.4023
7.3981
7.3923
7.3260
7.3237
7.3122
7.2600
2.1549
Ph
CH3
N
12g
0.77
0.95
1.70
1.84
2.74
0.99
1.87
2.00
3.00
f1 (ppm)

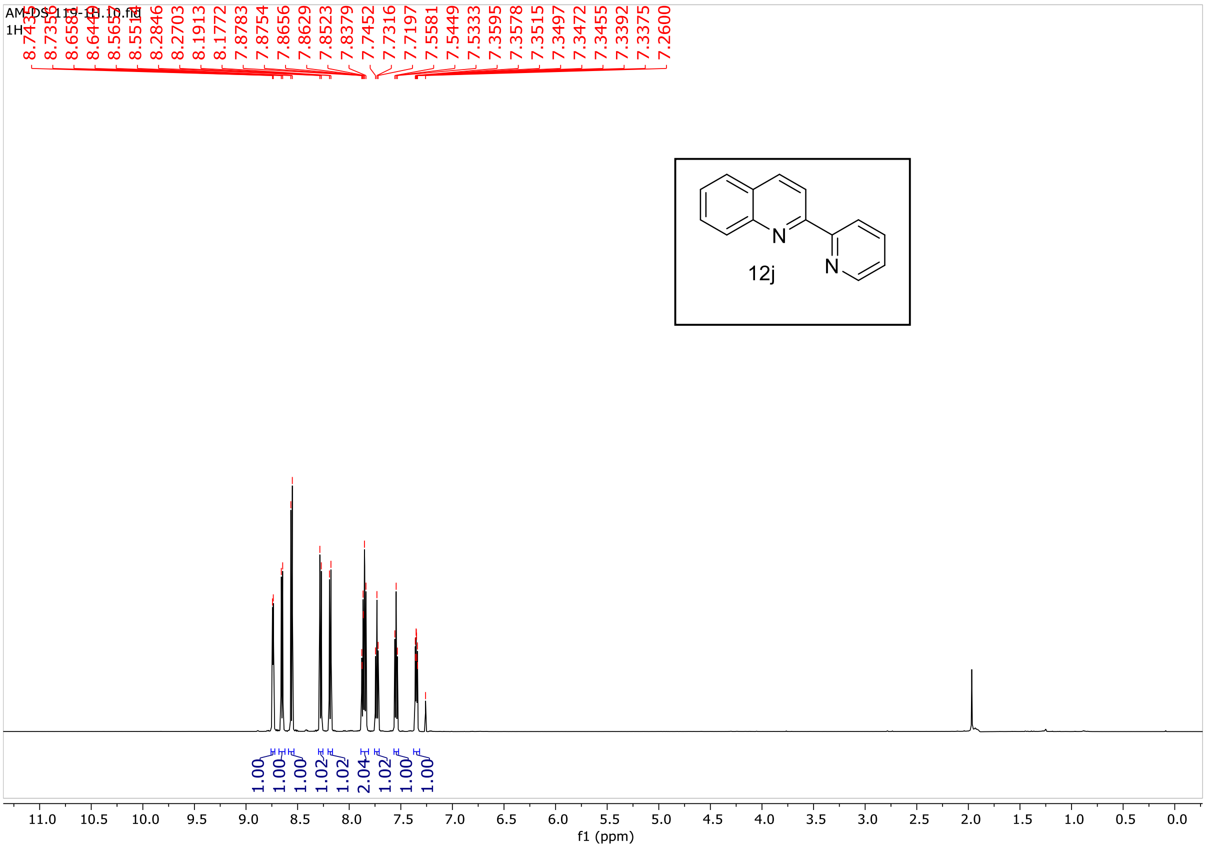

KD-2-397-13C.10.fid
KD-2-397-13C
160.9616
147.9053
146.3299
141.6121
137.8416
129.5410
129.4535
129.0539
128.7786
128.6759
128.4562
128.2302
127.9651
127.1926
126.8713
126.3794
126.1157
77.3715
77.1600
76.9488
18.7483
Ph
CH3
N
12g
f1 (ppm)

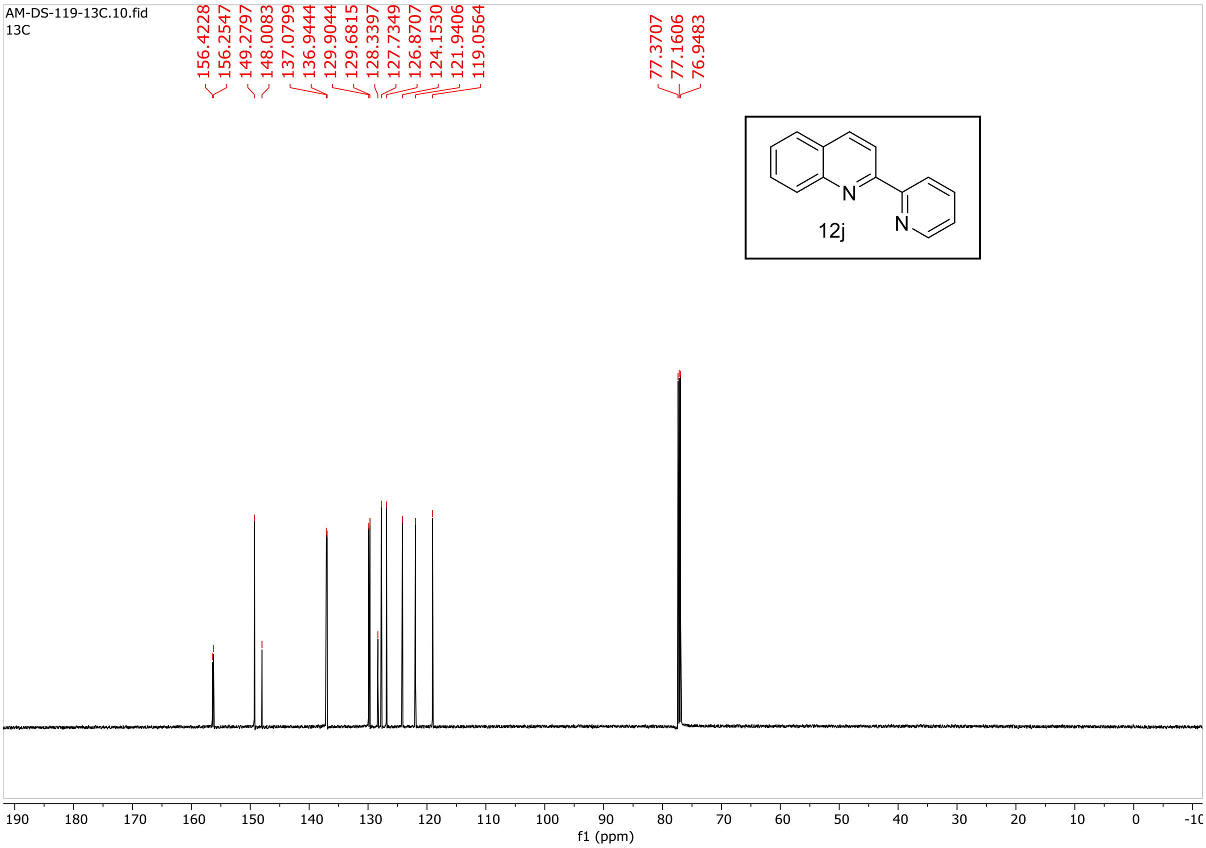

KD-2-396-1H.10.fid
1H
8.1512
8.1375
8.0135
7.7868
7.7733
7.6812
7.6792
7.6675
7.6557
7.6537
7.6068
7.5937
7.5329
7.5197
7.5103
7.4984
7.4856
7.4567
7.4443
7.4321
7.2600
2.4654
CH3
N
12h
0.95
0.98
0.98
0.99
1.94
2.95
1.02
3.00
f1 (ppm)

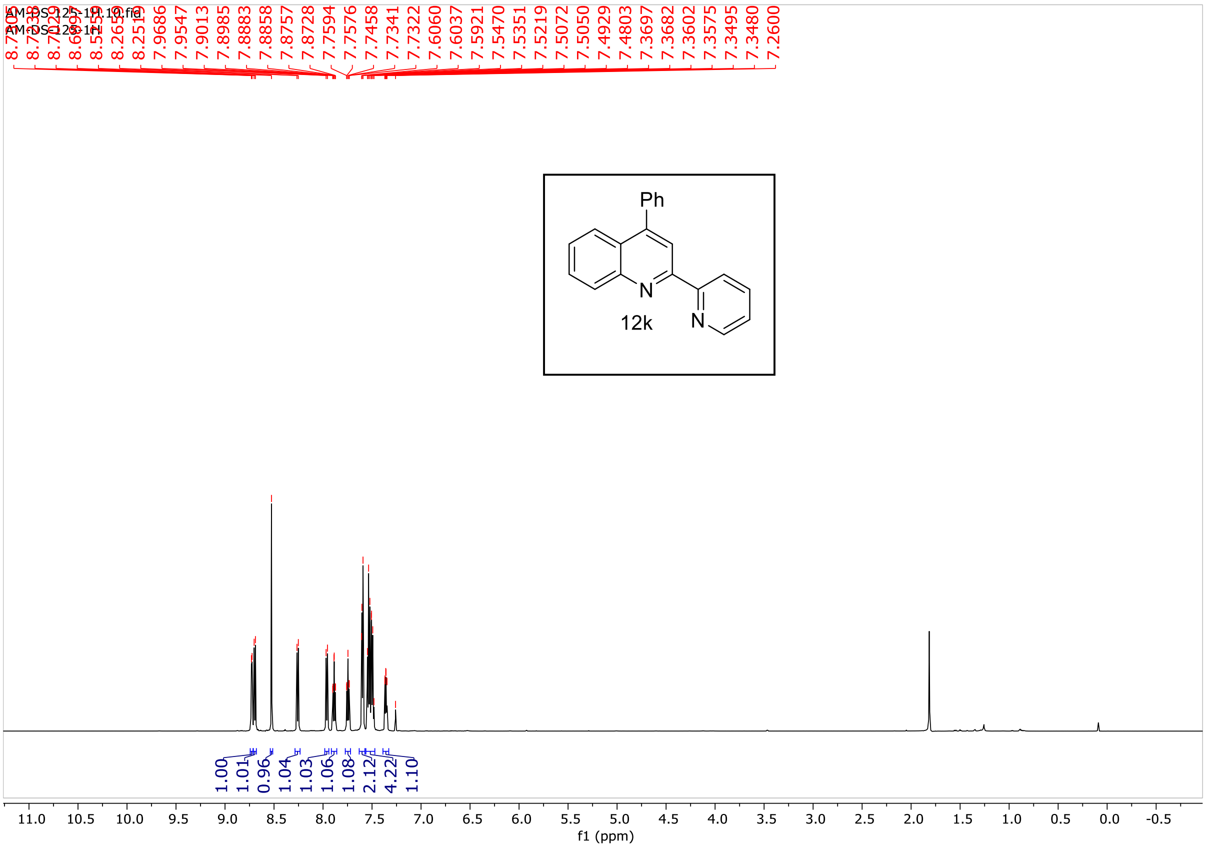

KD-2-396-13C.10.fid
13C
160.6167
146.6813
140.9271
136.8410
129.3542
129.3054
128.9328
128.8506
128.4005
128.2832
127.6728
126.8037
126.5033
77.3688
77.1578
76.9454
20.7335
CH3
N
12h
f1 (ppm)

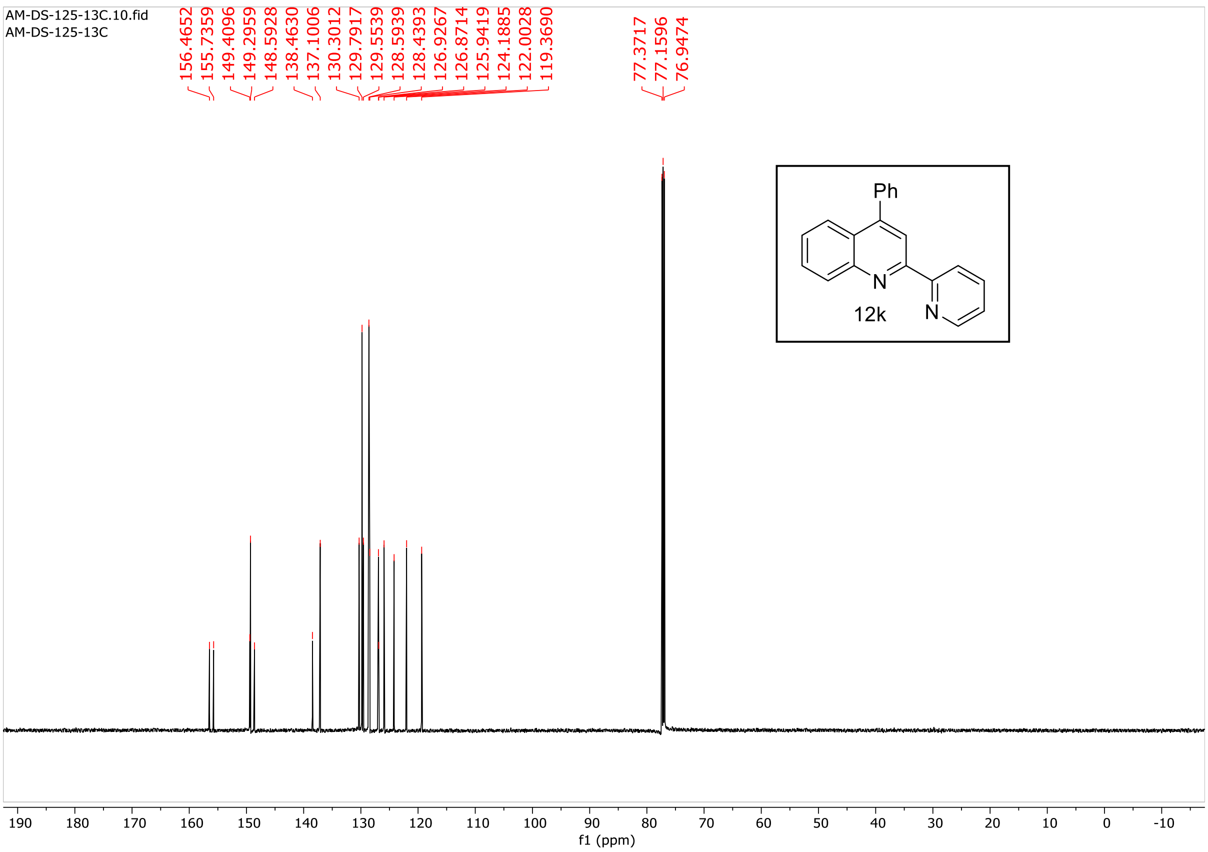

KD-2-404-1H.13.fid
KD-2-404-1H
12i
N
f1 (ppm)

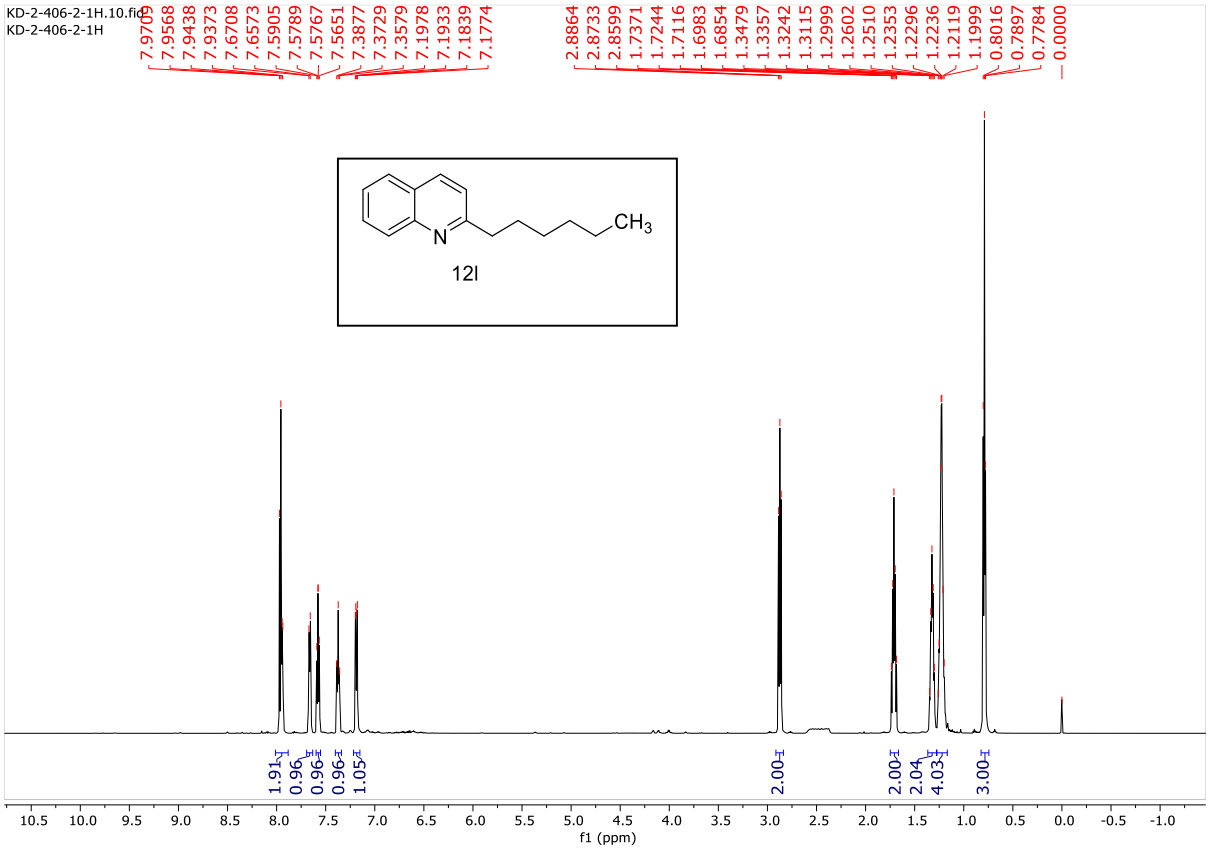

KD-2-404-13C.10.fid
KD-2-404-13C
157.2882
148.4662
137.0618
136.9565
133.9593
133.6019
129.8684
129.8299
128.9512
128.7125
127.8481
127.6321
127.3355
127.2767
126.8444
126.4760
126.4657
125.1816
119.3021
77.3708
77.1595
76.9480
12i
N
f1 (ppm)


AM-DS-119-1H.10.fid
1H
12j
f1 (ppm)


AM-DS-119-13C.10.fid
13C
156.4228
156.2547
149.2797
148.0083
137.0799
136.9444
129.9044
129.6815
128.3397
127.7349
126.8707
124.1530
121.9406
119.0564
77.3707
77.1606
76.9483
12j
f1 (ppm)


AM-DS-125-1H.10.fid
AM-DS-125-1H
12k
Ph
N
1.00
1.01
0.96
1.04
1.03
1.06
1.08
2.12
4.22
1.10
f1 (ppm)


AM-DS-125-13C.10.fid
AM-DS-125-13C
156.4652
155.7359
149.4096
149.2959
148.5928
138.4630
137.1006
130.3012
129.7917
129.5539
128.5939
128.4393
126.9267
126.8714
125.9419
124.1885
122.0028
119.3690
77.3717
77.1596
76.9474
Ph
N
12k
f1 (ppm)


KD-2-406-2-1H.10.fid
KD-2-406-2-1H
7.9709
7.9568
7.9438
7.9373
7.6708
7.6573
7.5905
7.5789
7.5767
7.5651
7.3877
7.3729
7.3579
7.1978
7.1933
7.1839
7.1774
2.8864
2.8733
2.8599
1.7371
1.7244
1.7116
1.6983
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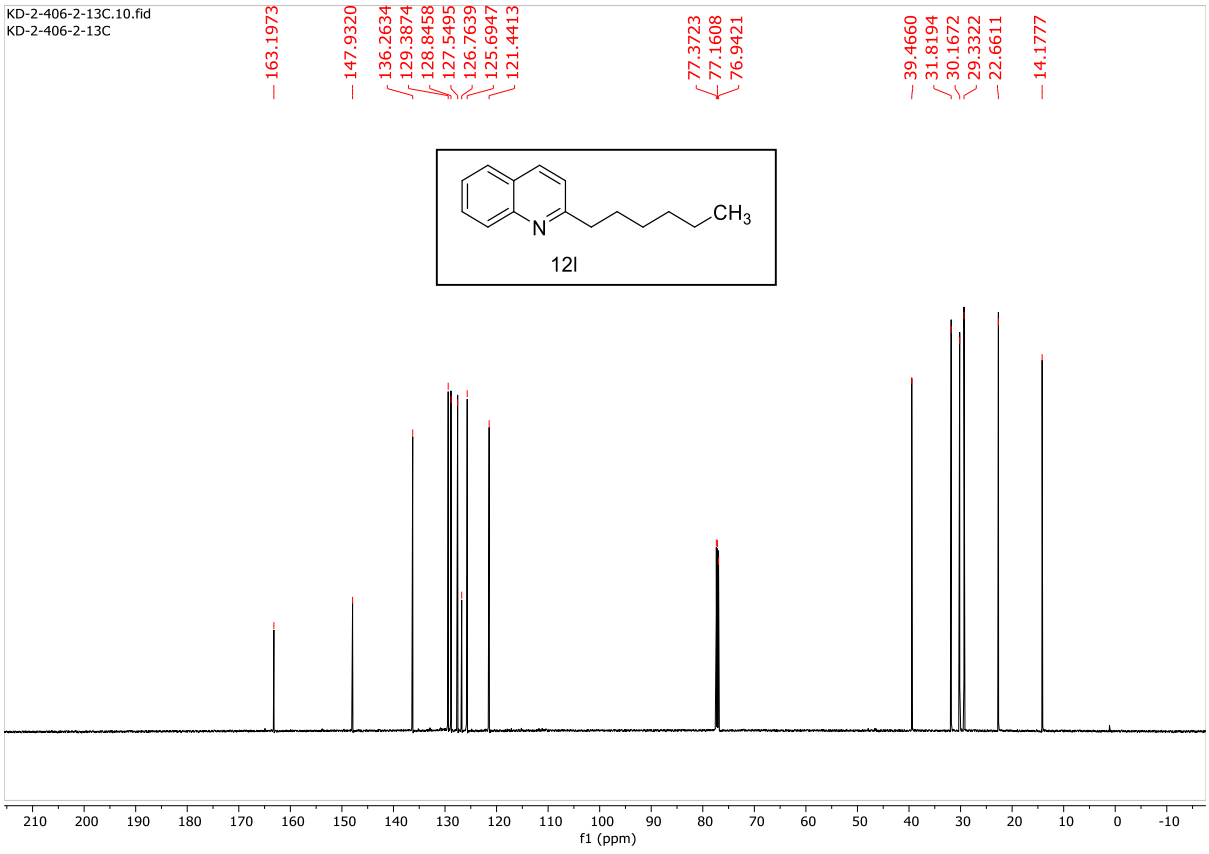
1.3479
1.3357
1.3242
1.3115
1.2999
1.2602
1.2510
1.2353
1.2296
1.2236
1.2119
1.1999
0.8016
0.7897
0.7784
0.0000
CH3
N
12l
1.91
0.96
0.96
0.96
1.05
2.00
2.00
2.04
4.03
3.00
f1 (ppm)


KD-2-406-2-13C.10.fid
KD-2-406-2-13C
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147.9320
136.2634
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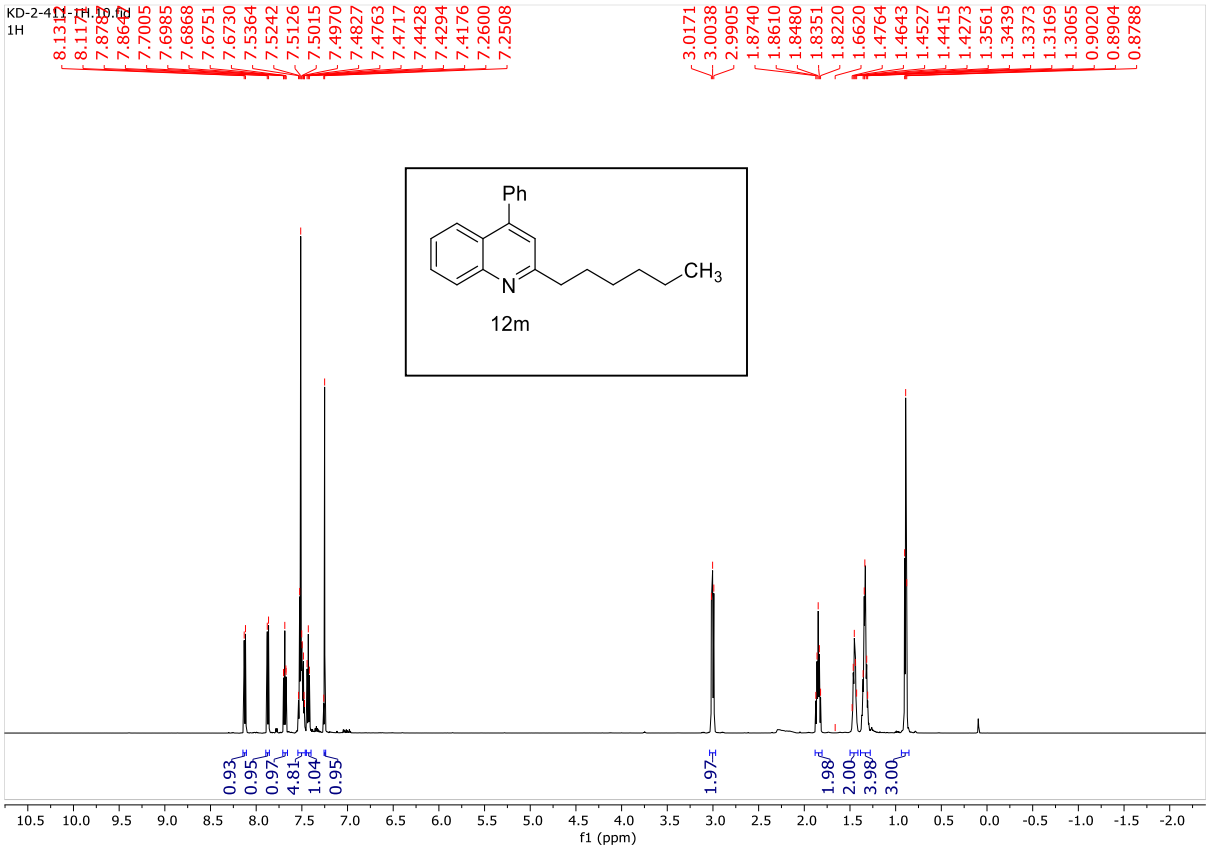
128.8458
127.5495
126.7639
125.6947
121.4413
77.3723
77.1608
76.9421
39.4660
31.8194
30.1672
29.3322
22.6611
14.1777
CH3
N
12l
f1 (ppm)


KD-2-411-1H.10.fid
1H
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8.1172
7.8787
7.8642
7.7005
7.6985
7.6868
7.6751
7.6730
7.5364
7.5242
7.5126
7.5015
7.4970
7.4827
7.4763
7.4717
7.4428
7.4294
7.4176
7.2600
7.2508
3.0171
3.0038
2.9905
1.8740
1.8610
1.8480
1.8351
1.8220
1.6620
1.4764
1.4643
1.4527
1.4415
1.4273
1.3561
1.3439
1.3373
1.3169
1.3065
0.9020
0.8904
0.8788
Ph
N
CH3
12m
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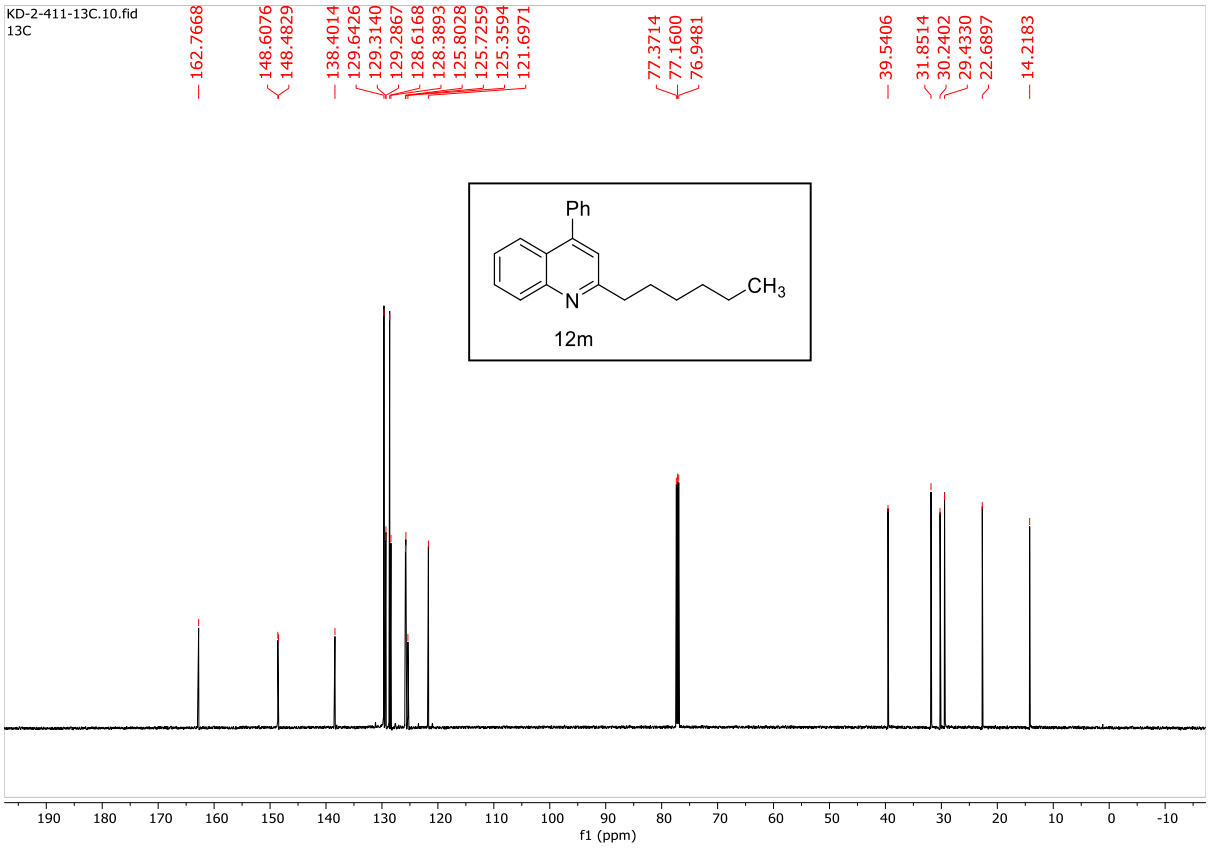
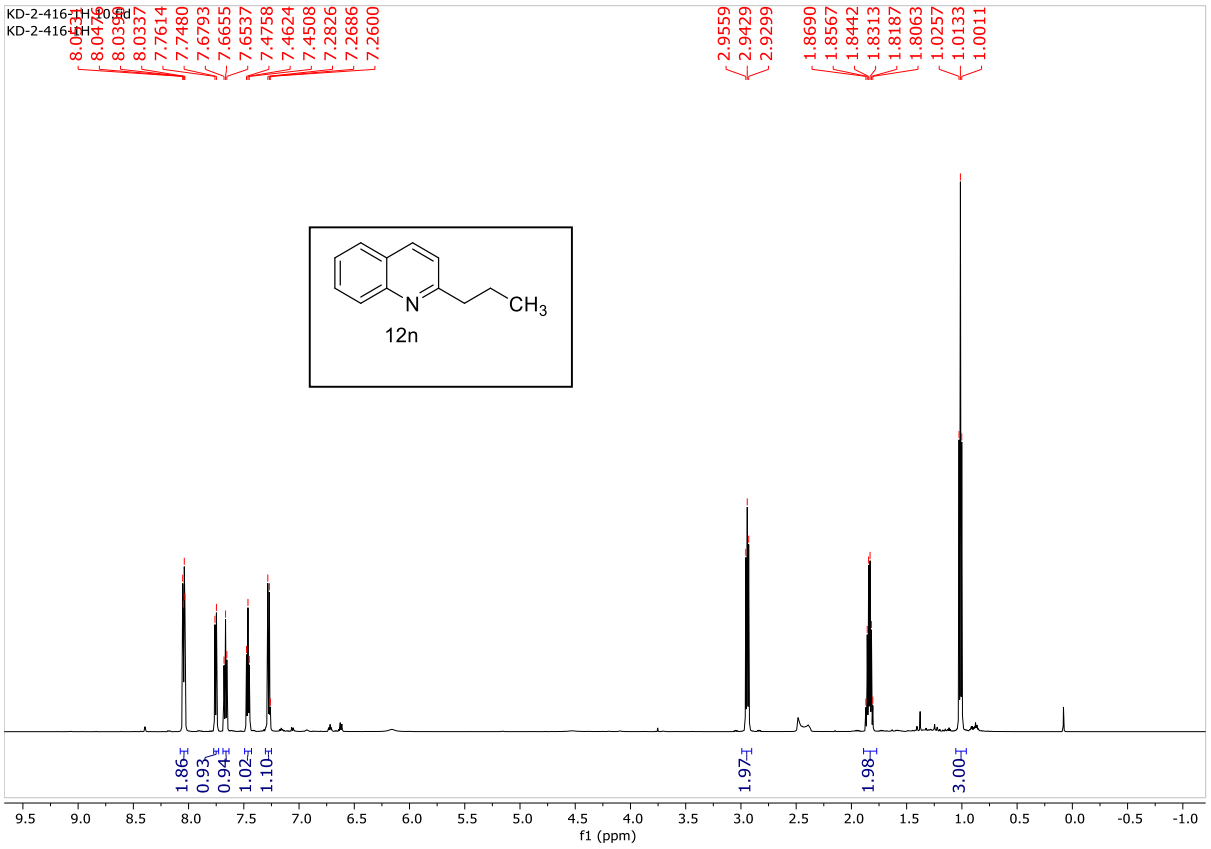
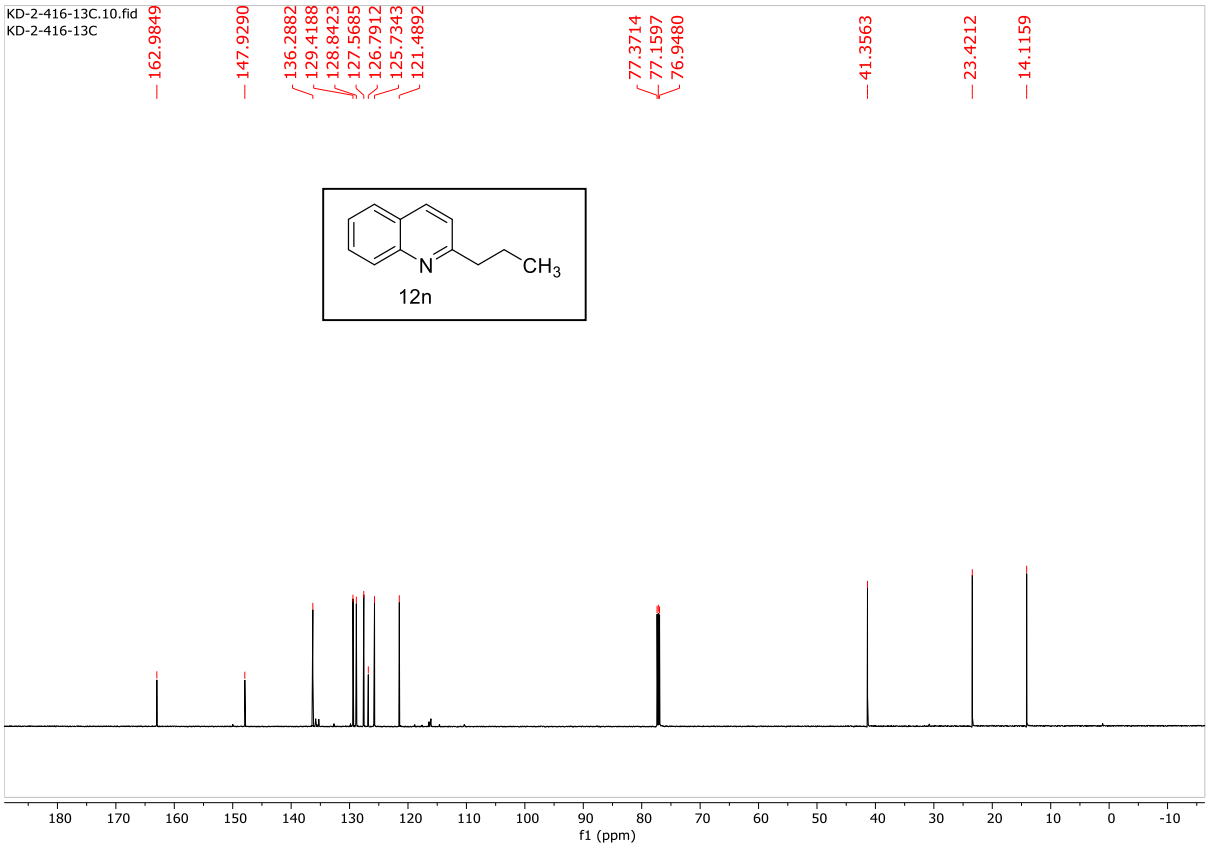
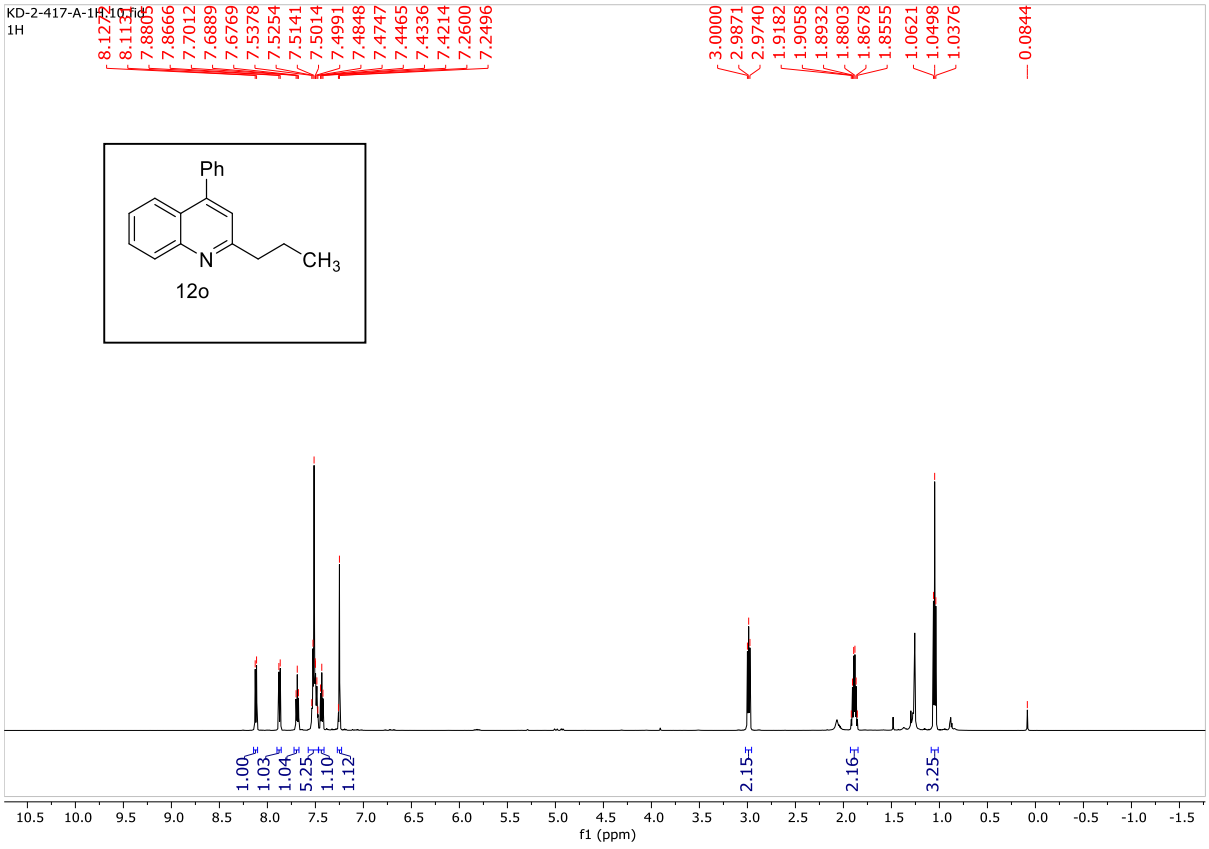
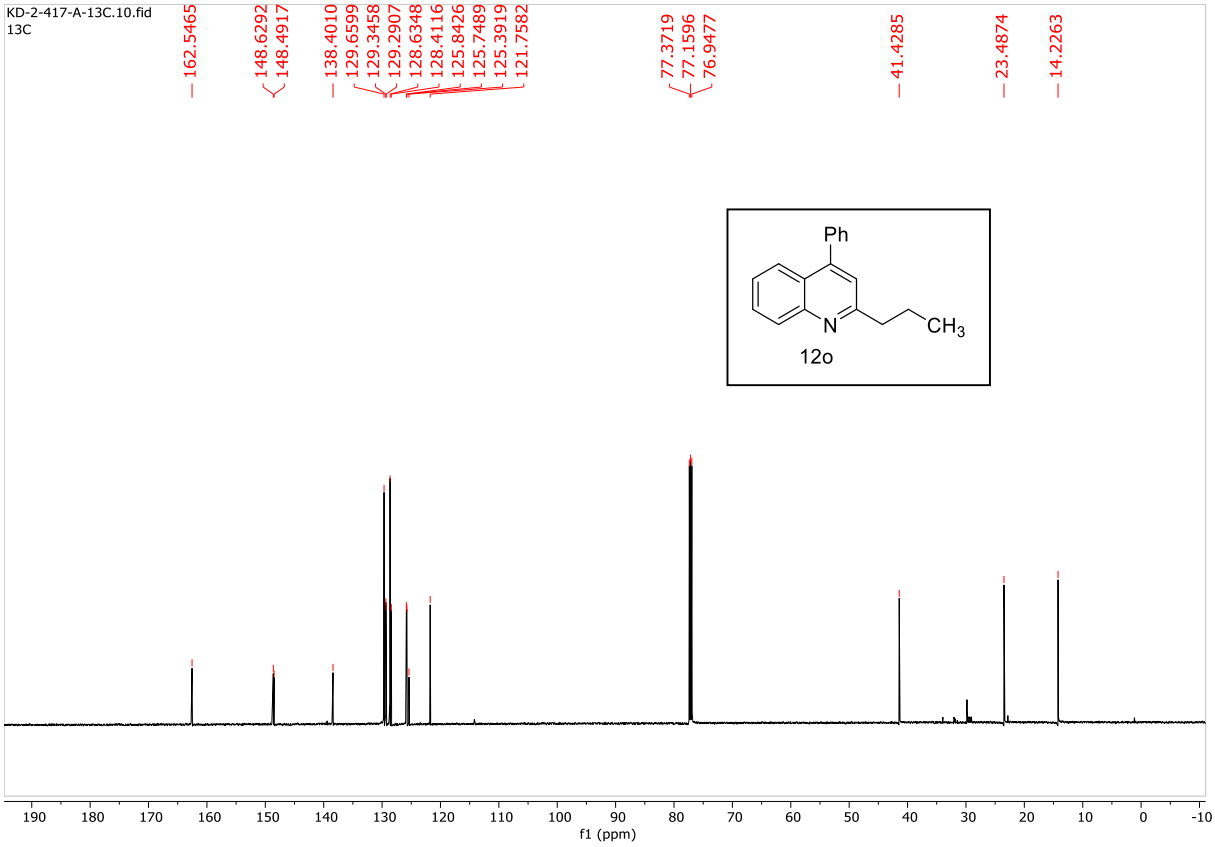
0.95
0.97
4.81
1.04
0.95
1.97
1.98
2.00
3.98
3.00
f1 (ppm)


KD-2-411-13C.10.fid
13C
162.7668
148.6076
148.4829
138.4014
129.6426
129.3140
129.2867
128.6168
128.3893
125.8028
125.7259
125.3594
121.6971
77.3714
77.1600
76.9481
39.5406
31.8514
30.2402
29.4330
22.6897
14.2183
Ph
N
CH3
12m
f1 (ppm)


KD-2-416-1H.10.fid
KD-2-416-1H
8.0337
7.7614
7.7480
7.6793
7.6655
7.6537
7.4758
7.4624
7.4508
7.2826
7.2686
7.2600
2.9559
2.9429
2.9299
1.8690
1.8567
1.8442
1.8313
1.8187
1.8063
1.0257
1.0133
1.0011
N
CH3
12n
1.86
0.93
0.94
1.02
1.10
1.97
1.98
3.00
f1 (ppm)


KD-2-416-13C.10.fid
KD-2-416-13C
162.9849
147.9290
136.2882
129.4188
128.8423
127.5685
126.7912
125.7343
121.4892
77.3714
77.1597
76.9480
41.3563
23.4212
14.1159
N
CH3
12n
f1 (ppm)


KD-2-417-A-1H.10.fid
1H
8.1272
8.1134
7.8805
7.8666
7.7012
7.6889
7.6769
7.5378
7.5254
7.5141
7.5014
7.4991
7.4848
7.4747
7.4465
7.4336
7.4214
7.2600
7.2496
3.0000
2.9871
2.9740
1.9182
1.9058
1.8932
1.8803
1.8678
1.8555
1.0621
1.0498
1.0376
0.0844
Ph
N
CH3
12o
1.00
1.03
1.04
5.25
1.10
1.12
2.15
2.16
3.25
f1 (ppm)


KD-2-417-A-13C.10.fid
13C
162.5465
148.6292
148.4917
138.4010
129.6599
129.3458
129.2907
128.6348
128.4116
125.8426
125.7489
125.3919
121.7582
77.3719
77.1596
76.9477
41.4285
23.4874
14.2263
Ph
N
CH3
12o
f1 (ppm)

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