Electronic Supplementary Material (ESI) for ChemComm.

Tandem one-pot CO_2 reduction-silyloxycarbonylation of aryl/vinyl halides to access carboxylic acids

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Supplementary information

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General: All the reagents and solvents were used as such received unless otherwise specified. ^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$/DMSO-d_6 on a Bruker Avance 400 NMR spectrometer. Chemical shifts are given in ppm with reference to TMS attributed to 0 ppm and spin-spin coupling constants, *J*, are given in Hz. HRMS data were recorded on a Finnigan MAT 95 system.

I. Experimental Procedures:

1. General procedure for preparation of mono carboxylic acids

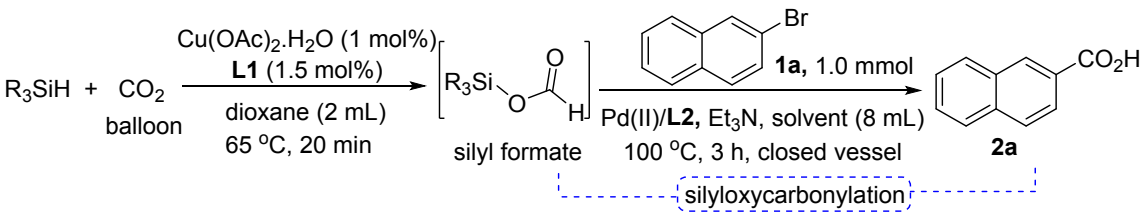
To a mixture of $Cu(OAc)_2.H_2O$ (0.01 mmol, 1.0 mol%) and 1,2-bis(diphenylphosphaneyl)benzene (0.015 mmol, 1.5 mol%) in an oven dried Schlenk tube connected to a CO_2 balloon, a solution of PMHS (2.5 mmol, 2.5 equiva.) in 1,4-dioxane (2.0 mL) was added, flushed the tube with CO_2 and heated the resulting blue solution to 65 ℃ while vigorously stirring for 20 minutes under balloon pressure CO_2 and the solution becomes light brown. This formate solution was removed from the heating bath and added toluene (8 ml), aryl/vinyl bromide (1.0 mmol, 1.0 equiv.), $Pd(OAc)_2$ (3 mol%, 0.03 equiva.), xantphos (6 mol%, 0.06 equiva.) and Et_3N (2.5 mmol, 2.5 equiva.) sequentially under CO_2 atmosphere. CO_2 was removed, the Schlenk tube was closed and heated to 100 ℃ for the time period until the disappearance of aryl bromide as shown by TLC. Then, the reaction mixture was cooled to ambient temperature and added 10 ml of 1N NaOH or $NaHCO_3$ and stirred for 10 min. The resulting emulsion was filtered and the filtrate was extracted with EtOAc (3*15 mL), organic fractions separated and discarded. Aqueous layer was acidified with 1.0 N HCl or citric acid and extracted with EtOAc (3*15 mL). The later organic fractions were dried over Na_2SO_4 and concentred to get the pure acid compound.

2. General procedure for preparation of di/tri-carboxylic acids from dihaloaryls

To a mixture of $Cu(OAc)_2.H_2O$ (0.02 mmol, 2 mol%) and 1,2-bis(diphenylphosphinyl)benzene **L1** (0.03 mmol, 3 mol%) in an oven dried Schlenk tube connected to a CO_2 balloon, a solution of PMHS (4.0 mmol, 4.0 equiva.) in 1,4-dioxane (3.0 mL) was added, flushed the tube with CO_2, heated the resulting blue solution to 65 ℃ while vigorously stirring for 25 minutes under CO_2 balloon pressure and the solution becomes light brown. This formate solution was removed from the heating bath and added toluene (12 ml), aryl dihalide (1.0 mmol, 1.0 equiv.), $Pd(OAc)_2$ (5 mol%, 0.05 mmol), xantphos **L2** (10 mol%, 0.1 mmol) and Et_3N (4.0 mmol, 4.0 equiva.) sequentially under CO_2 atmosphere. The

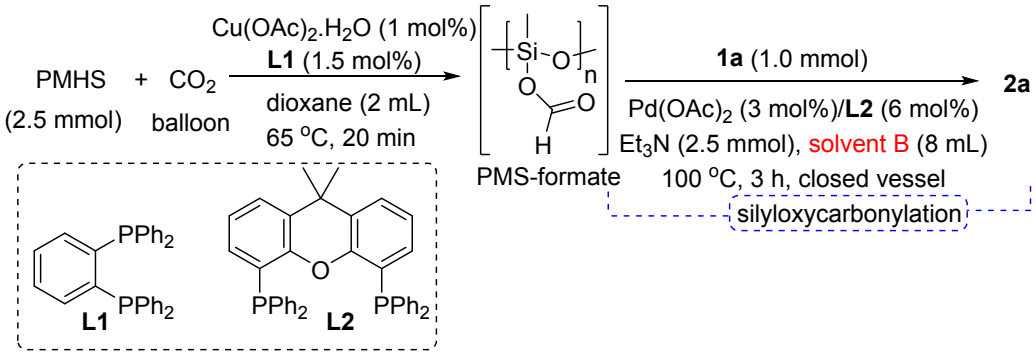
Schlenk tube was closed, CO_2 balloon was removed, and heated to 100 ℃ for the time 10 h – 20 h. Then, the reaction mixture was cooled to ambient temperature and added 20 ml of 1N NaOH and stirred for 10 min. The resulting emulsion was filtered and the filtrate was extracted with EtOAc (3*20 mL), aqueous portion separated was acidified with 1.0 N HCl or 1M citric acid, solid precipitated was filtered, suck dried to get the pure diacid. If no precipitation occurs, extracted with EtOAc (3*30 mL) and these organic fractions were dried over Na_2SO_4 and concentrated to get the pure diacid compound. (Note: For tricarboxylation: PMHS (5.0 equiva.), $Pd(OAc)_2$ (8 mol%), **L2** (16 mol%) and Et_3N (5.0 equiva.)

3. General procedure for optimization studies:



To a mixture of $Cu(OAc)_2.H_2O$ (0.01 mmol, 1.0 mol%) and 1,2-bis(diphenylphosphaneyl)benzene (0.015 mmol, 1.5 mol%) in an oven dried Schlenk tube connected to a CO_2 balloon, a solution of R_3SiH (2.5 equiva.) in 1,4-dioxane (2.0 mL) was added, flushed the tube with CO_2. Heated the resulting blue solution to 65 ℃ with vigorous stirring for 20 minutes under CO_2 balloon pressure and the solution becomes light brown. To silyloxycarbonylation take effect, this formate solution was lifted up the heating bath and added solvent B (8 mL), aryl bromide (1.0 mmol, 1.0 equiv.), Pd(II), **L2** and Et_3N (2.5 equiva.) sequentially under CO_2 atmosphere. CO_2 was removed, the Schlenk tube was closed and heated to 100 ℃ for 3 h. Then, the reaction mixture was cooled to ambient temperature, added 0.5 ml of H_2O, concentrated to dryness under reduced pressure and determined the constituents by ^1H NMR.

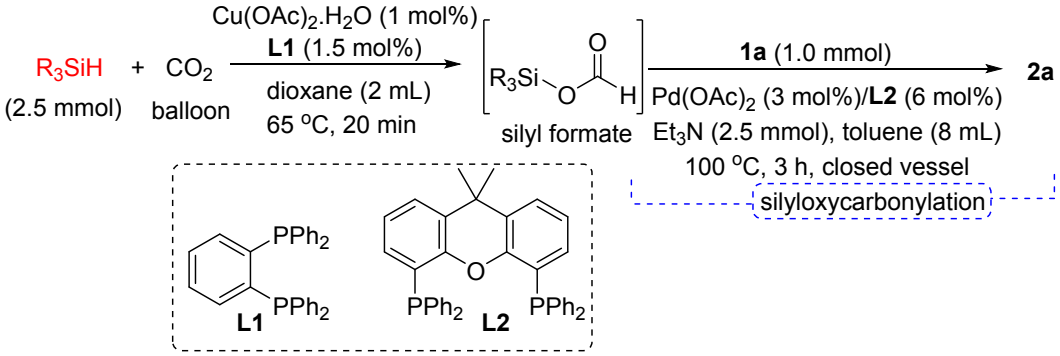
Table S1: Solvent screening for silyloxycarbonylation



entry	Solvent B	% conversion[a]	2a[a] %
1	Dioxane	100	60
2	THF	50	45
3	ACN	100	46

[a] determined by ^{1}H NMR

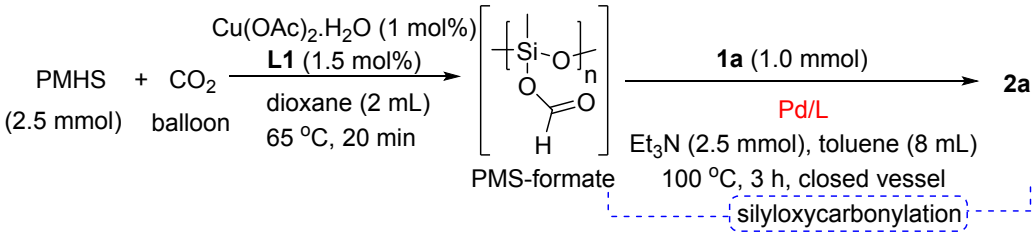
Table S2: Screening of hydrosilane[c]



entry	R_3SiH	% conversion[a]	2a[a] %	Debrominated 1a
1	PMHS[b]	90	60	nd
2	Et_3SiH	0	nd	trace

[a] see table S1; [b] 2.0 equiva.; nd = not determined

Table S3: Catalyst screening for silyloxycarbonylation

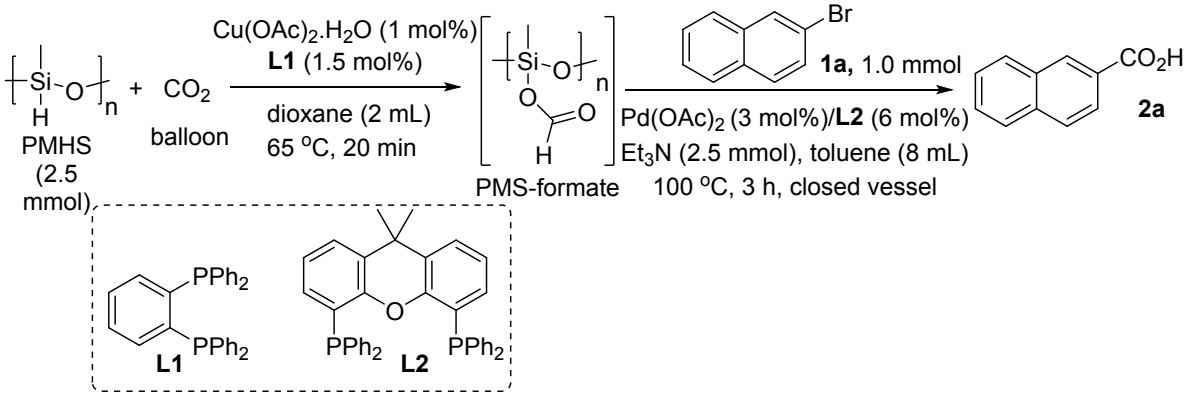


entry	Catalyst (Pd/L)	Conversion[a] %	2a[b] %
1	$Pd(OAc)_2$ (3 mol%)/PPh_3 (6 mol%)	60	0
2	$Pd(OAc)_2$ (3 mol%)/**L1** (6 mol%)	36	0
6	$PdCl_2$ (3 mol%)/**L2** (6 mol%)	100	69
3	$Pd_2(dba)_3$ (3 mol%)/**L2** (6 mol%)	100	81
4	$Pd(OAc)_2$ (3 mol%)/**L2** (3 mol%)	95	45
5[c]	$Pd(OAc)_2$ (1 mol%)/**L2** (2 mol%)	100	90
6[d]	$Pd(OAc)_2$ (3 mol%)/**L2** (3 mol%)	100	60

[a] see table S1; [b] isolated yield; [c] reaction time 6 h; [d] time 16 h.

Table S4: Control reactions

Standard reaction



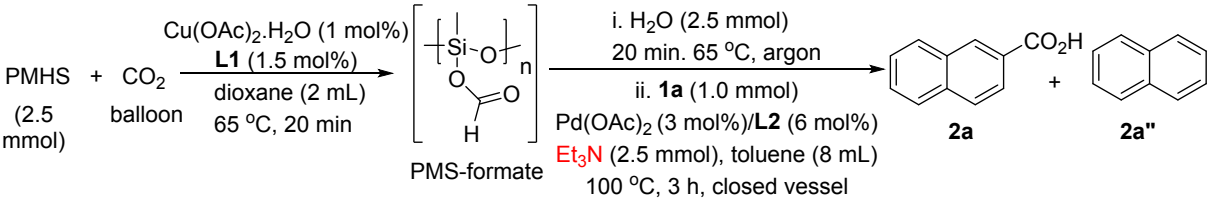
Deviations from standard reaction condition:

entry	condition	Conversion[a] %	2a[a] %
1	Standard	100	98
2	Without Et_3N	0	nd
3	Without $Pd(OAc)_2$/**L2**	0	nd
4	toluene instead of dioxane	100	62
5	$Pd(OAc)_2$/**L2** instead of $Cu(OAc)_2.H_2O$/**L1**	70	48
6	One-time addition	0	nd

[a] see table S1

Table S5: Hydrolysis role

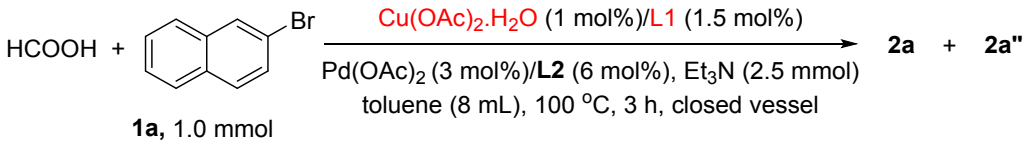
Standard condition:



S No	Conditions	Conversion (%)	Yield (%)	
			2a	2a”
1	standard	< 10	0	trace
2	without Et_3N	< 10	0	trace

To a mixture of $Cu(OAc)_2.H_2O$ (1.0 mol%) and 1,2-bis(diphenylphosphaneyl)benzene (1.5 mol%) in an oven dried Schlenk tube connected to a CO_2 balloon, a solution of PMHS (2.5 mmol) in 1,4-dioxane (2.0 mL) was added, flushed the tube with CO_2. Heated the resulting blue solution to 65 ℃ with vigorous stirring for 20 minutes under CO_2 balloon pressure and the solution becomes light brown. Removed CO_2, added H_2O (2.5 mmol) and stirred at 65 ℃ under Ar-atmosphere for 20 min. This solution was lifted up the heating bath and added toluene (8 mL), aryl bromide (1.0 mmol, 1.0 equiv.), Pd(II), **L2** and Et_3N (2.5 equiva.) sequentially under Ar-atmosphere. The Schlenk tube was closed and heated to 100 ℃ for 3 h. Then, the reaction mixture was cooled to ambient temperature, added 0.5 ml of H_2O, concentrated to dryness under reduced pressure and determined the constituents by ^1H NMR.

Table S6: Formic acid role

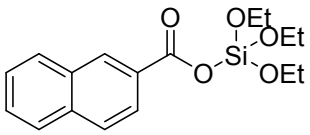


S No	Conditions	Conversion (%)	Yield (%)	
			2a	2a”
1	standard	> 95	0	85
2	without $Cu(OAc)_2.H_2O$/**L1**	> 95	0	90

To a mixture of $Cu(OAc)_2.H_2O$ (1.0 mol%) and 1,2-bis(diphenylphosphaneyl)benzene (1.5 mol%) in an oven dried Schlenk tube, added toluene (8 mL), aryl bromide (1.0 mmol, 1.0 equiv.), $Pd(OAc)_2$ (3 mol%), **L2** (6mol%) and Et_3N (2.5 equiva.) sequentially under Ar-atmosphere. The Schlenk tube was closed, a solution of HCOOH (2.5 mmol) in 1,4-dioxane (2.0 mL) was added and heated to 100 ℃ for 3 h. Then, the reaction mixture was cooled to ambient temperature, added 0.5 ml of H_2O, concentrated to dryness under reduced pressure and determined the constituents by ^1H NMR.

4. Procedure for silyl ester (2a'):

To a mixture of $Cu(OAc)_2.H_2O$ (0.01 mmol, 1.0 mol%) and 1,2-bis(diphenylphosphaneyl)benzene (0.015 mmol, 1.5 mol%) in an oven dried Schlenk tube connected to a CO_2 balloon, a solution of $(EtO)_3SiH$ (2.5 equiva.) in 1,4-dioxane (2.0 mL) was added, flushed the tube with CO_2. Heated the resulting blue solution to 65 ℃ with vigorous stirring for 20 minutes under CO_2 balloon pressure and the solution becomes light brown. To silyloxycarbonylation take effect, this formate solution lifted up the heating bath and added toluene (8 mL), aryl bromide (1.0 mmol, 1.0 equiv.), Pd(OAc) (3 mol%), **L2** (6 mol%) and dry Et_3N (2.5 equiva.) sequentially under CO_2 atmosphere. CO_2 was removed, the Schlenk tube was closed and heated to 100 ℃ for 3 h. The Schlenk tube was cooled to ambient temperature, 1 mL of the reaction mass was taken under argon environment and concentrated to dryness. The sample was dissolved in deuterated solvent, added di-*tert*-butyl oxalate as internal standard, and recorded the NMR spectra.



2-Naphthoic (triethyl silicic) anhydride (**2a'**): ^1H NMR (400 MHz, Chloroform-*d*) δ 8.65 (d, J = 1.8 Hz, 1H), 8.10 – 8.05 (m, 1H), 7.90 (dd, J = 8.1, 5.8 Hz, 3H), 7.64 – 7.51 (m, 2H), 4.07 (dq, J = 9.4, 7.0 Hz, 6H), 1.32 (t, J = 7.0 Hz, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3, 165.1, 135.7, 132.5, 132.2, 131.8, 129.5, 128.5, 128.2, 127.8, 126.7, 125.8, 60.1, 18.0; ^{29}Si NMR (139 MHz, DMSO-*d6*) δ -92.5.

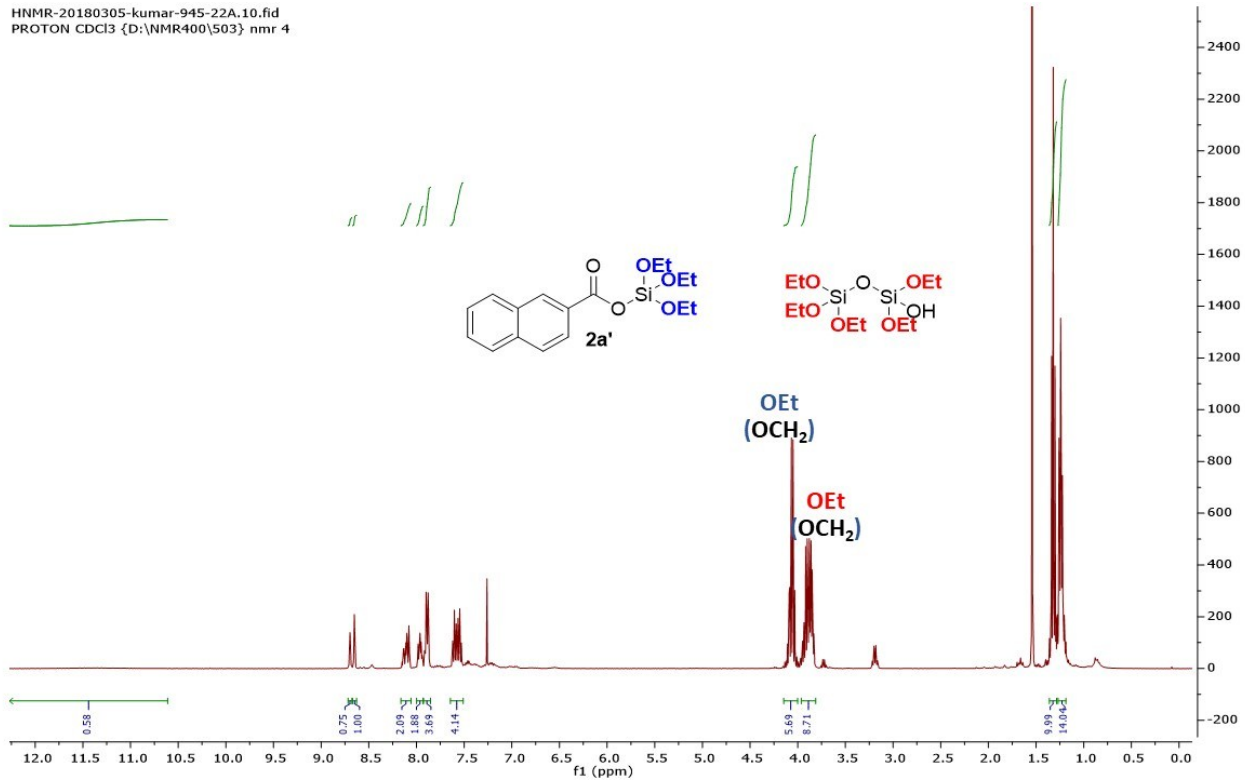


Figure S1: ^{1}H NMR of compound **2a`** and **2a** (*in situ*)

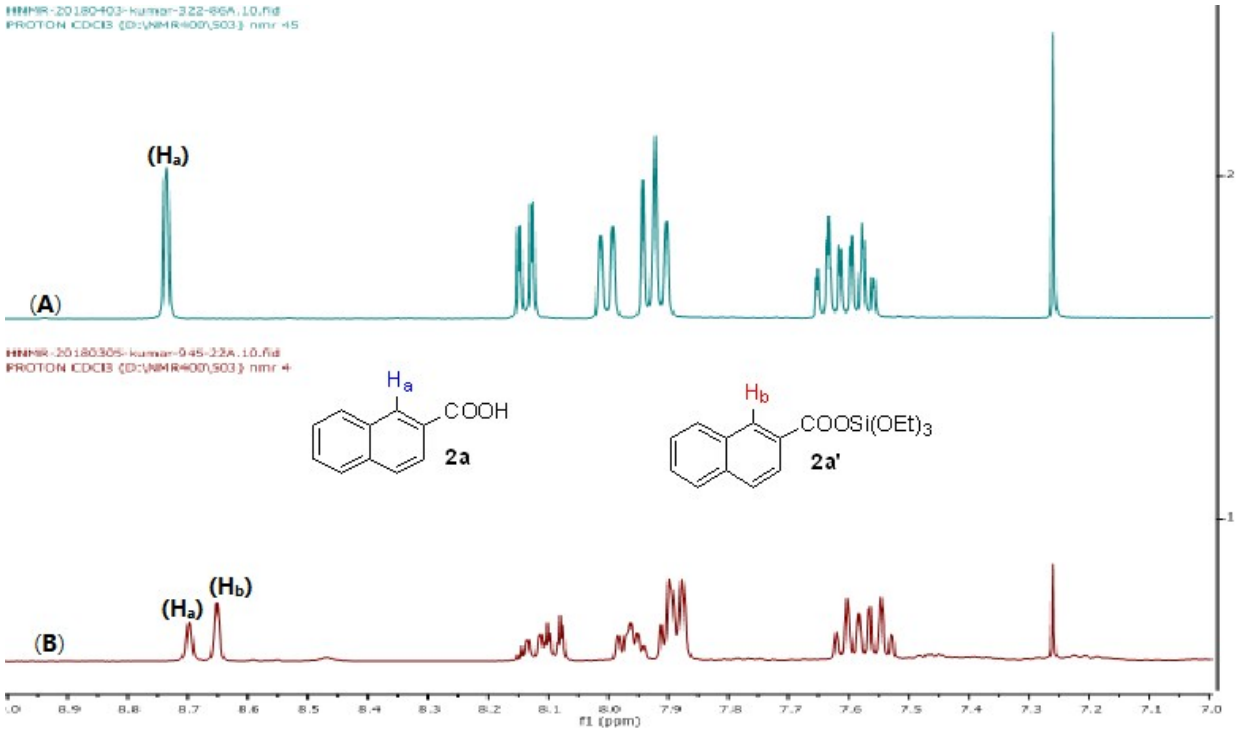


Figure S2: expansion region; (**A**) ^{1}H NMR of compound **2a**, (**B**) ^{1}H NMR of compound **2a**+**2a`** (*in situ*)

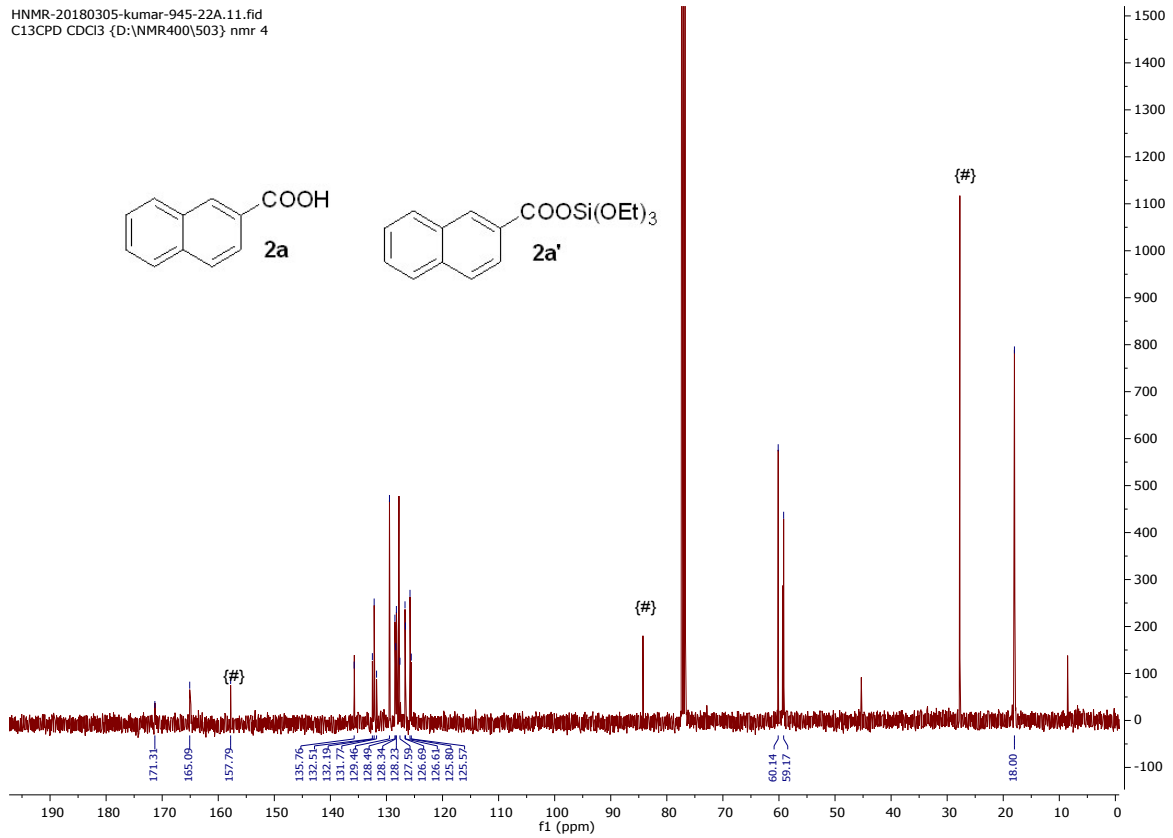


Figure S3: ^{13}C NMR of compound **2a** + **2a`** (*in situ*); {#} $(CO_2tBu)_2$

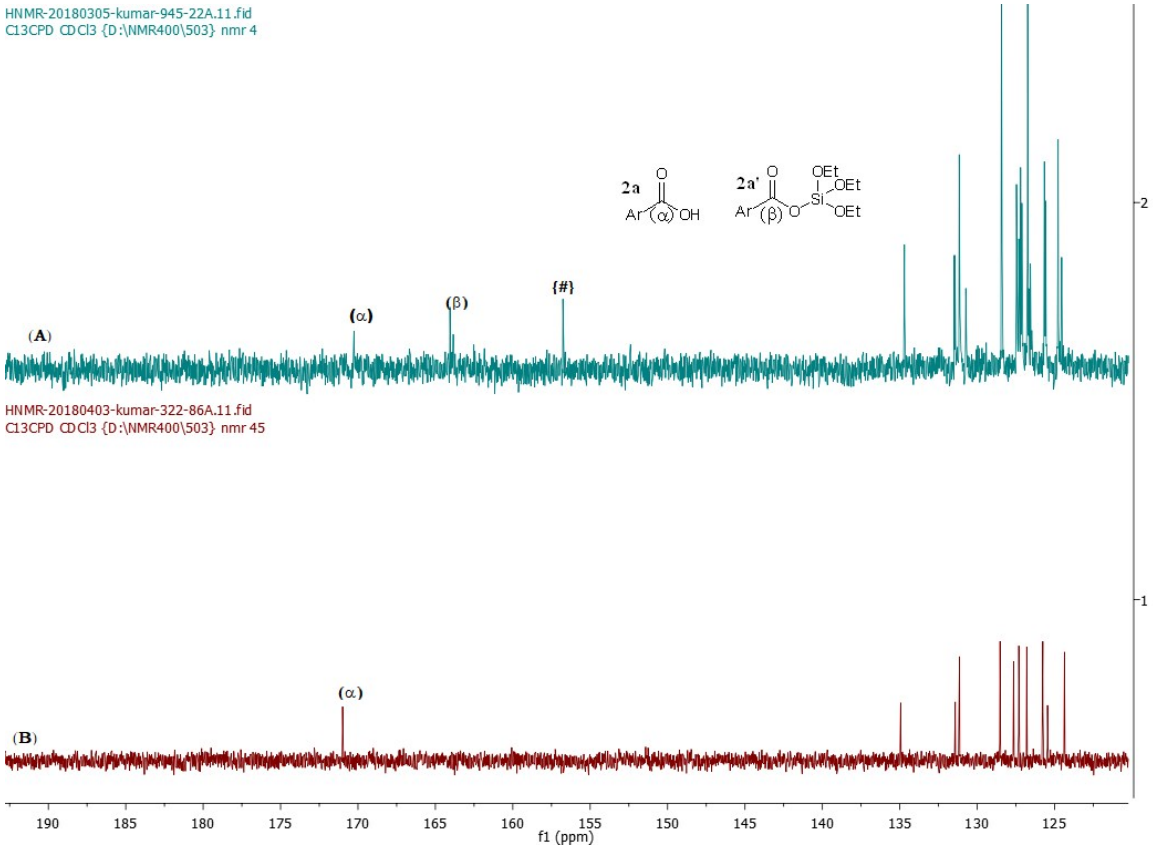


Figure S4: expansion region; (**A**) ^{13}C spectra of **2a**+**2a'** (*in situ*); (**B**) ^{13}C spectra of **2a**; {#} $(CO_2tBu)_2$

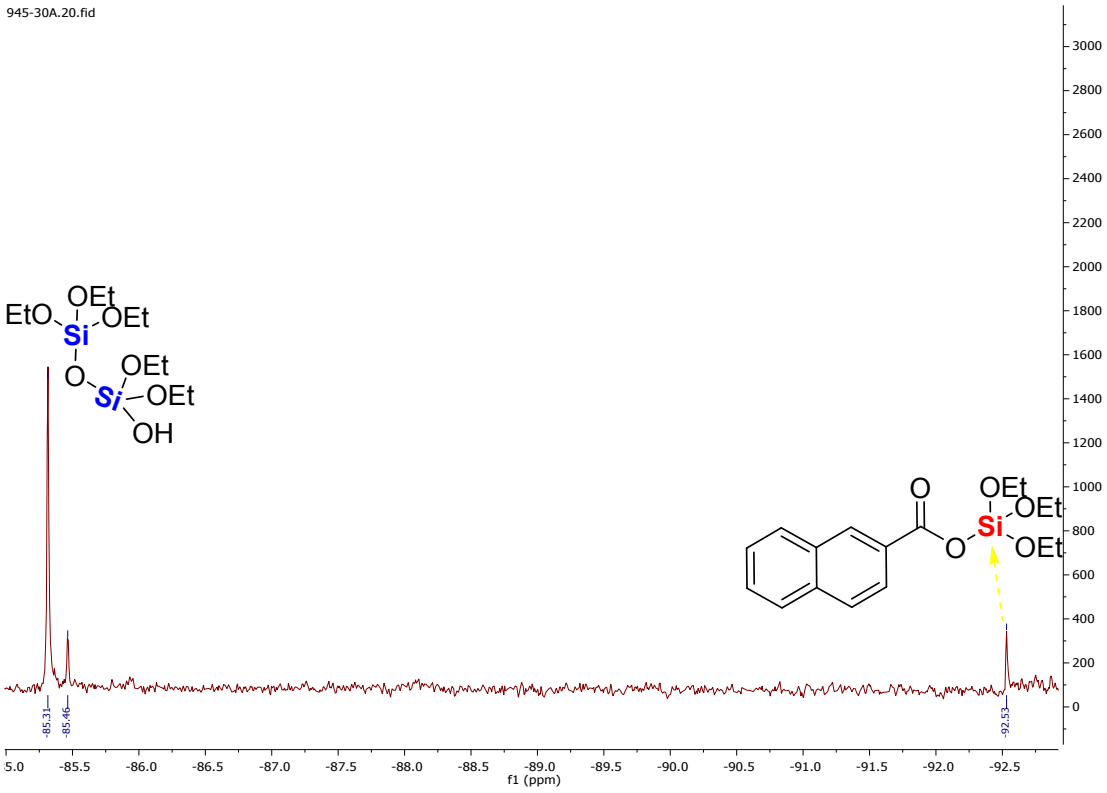
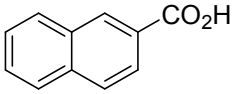
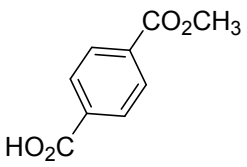


Figure S5: ^{29}Si NMR in DMSO-d6 of compound **2a`** (*in situ*)[25]

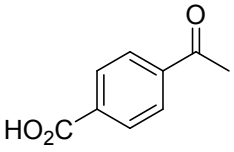
II. Spectral data:



2-Naphthoic acid (2a)[1]: white solid; yield 98%; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.77 – 8.70 (m, 1H), 8.14 (dd, J = 8.6, 1.7 Hz, 1H), 8.03 – 7.97 (m, 1H), 7.96 – 7.88 (m, 2H), 7.61 (dddd, J = 22.1, 8.1, 6.9, 1.4 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 136.0, 132.5, 132.2, 129.6, 128.7, 128.3, 127.8, 126.8, 126.5, 125.4.

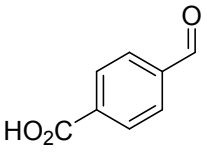


4-(Methoxycarbonyl)benzoic acid (2c)[1]: white solid; yield 94%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.34 (s, 1H), 8.05 (s, 4H), 3.88 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 167.1, 166.1, 135.3, 133.7, 130.1, 129.9, 53.0.

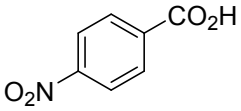


4-Acetylbenzoic acid (2d)[1]: half-white solid, yield 72%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.04 (d, J = 1.6 Hz, 4H), 2.62 (d, J = 1.6 Hz,

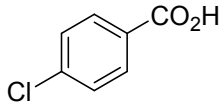
3H); ^{13}C NMR (101 MHz, DMSO) δ 198.2, 167.1, 140.3, 135.0, 130.0, 128.8, 27.5.



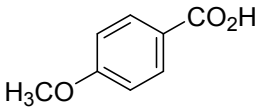
4-Formylbenzoic acid (**2e**)[1]: half-white solid, yield 97%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.31 (s, 1H), 10.10 (s, 1H), 8.17 – 8.07 (m, 2H), 8.05 – 7.97 (m, 2H); ^{13}C NMR (101 MHz, DMSO) δ 193.5, 167.0, 139.4, 136.1, 130.4, 130.0.



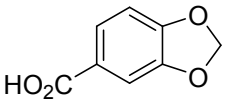
4-Nitrobenzoic acid (**2f**)[3]: pale yellow solid; yield 96%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.42 (s, 1H), 8.41 – 8.25 (m, 2H), 8.23 – 8.06 (m, 2H); ^{13}C NMR (101 MHz, DMSO) δ 166.3, 150.5, 136.9, 131.2, 124.2.



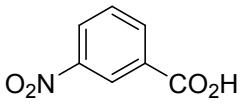
4-Chlorobenzoic acid (**2g**)[2]: white solid; yield 77%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.16 (s, 1H), 7.93 (d, J = 8.1 Hz, 2H), 7.56 (d, J = 8.1 Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 166.9, 138.2, 131.6, 130.1, 129.2.



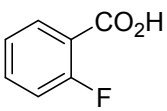
4-Methoxybenzoic acid (**2h**)[1]: white solid; yield 90%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.59 (s, 1H), 7.92 – 7.85 (m, 2H), 7.05 – 6.96 (m, 2H), 3.81 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 167.5, 163.4, 131.9, 123.5, 114.3, 56.0.



Benzo[*d*][1,3]dioxole-5-carboxylic acid (**2i**)[1]: white solid, yield 96%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.74 (s, 1H), 7.54 (dd, J = 8.1, 1.7 Hz, 1H), 7.35 (d, J = 1.7 Hz, 1H), 6.99 (d, J = 8.1 Hz, 1H), 6.11 (s, 2H); ^{13}C NMR (101 MHz, DMSO) δ 167.1, 151.6, 148.0, 125.4, 125.2, 109.3, 108.5, 102.4.

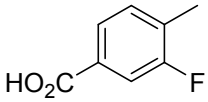


3-Nitrobenzoic acid (**2j**)[1]: pale yellow solid, yield 77%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.60 (t, J = 2.0 Hz, 1H), 8.45 (dd, J = 8.3, 2.4 Hz, 1H), 8.33 (d, J = 7.9 Hz, 1H), 7.80 (t, J = 8.0 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 166.0, 148.4, 135.89, 133.0, 131.0, 127.8, 124.2.

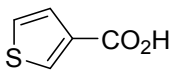


2-Fluorobenzoic acid (**2k**)[4]: White solid, yield 45%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.18 (s, 1H), 7.87 (td, J = 7.6, 1.7 Hz, 1H), 7.64 (dddd, J = 7.9, 6.9, 5.0, 1.9 Hz, 1H), 7.36 – 7.26 (m, 2H); ^{13}C NMR

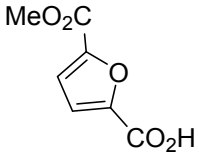
(101 MHz, DMSO) δ 165.5, 162.8, 160.2, 135.1, 132.3, 124.9, 119.7, 117.4, 117.2.



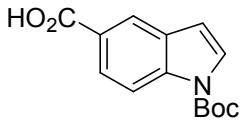
3-Fluoro-4-methylbenzoic acid (**2l**)[5]: white solid, yield 84%; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.81 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.74 (dd, *J* = 10.0, 1.6 Hz, 1H), 7.30 (t, *J* = 7.7 Hz, 1H), 2.37 (d, *J* = 2.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 162.2, 159.8, 131.6, 128.8, 125.8, 116.8, 116.5.



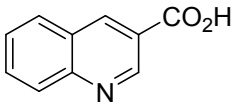
Thiophene-3-carboxylic acid (**2m**)[6]: half-white solid; yield 94%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.66 (s, 1H), 8.24 (dd, *J* = 3.0, 1.2 Hz, 1H), 7.59 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.42 (dd, *J* = 5.1, 1.1 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 164.0, 134.8, 133.7, 128.2, 127.7.



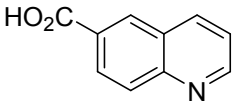
5-(Methoxycarbonyl)furan-2-carboxylic acid (**2n**)[7]: white solid; yield 75%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.45 (s, 1H), 7.40 (d, *J* = 3.6 Hz, 1H), 7.33 (d, *J* = 3.6 Hz, 1H), 3.86 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 159.2, 158.4, 147.8, 146.1, 119.4, 118.8, 52.7.



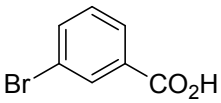
1-(*tert*-Butoxycarbonyl)-1*H*-indole-5-carboxylic acid (**2o**): half-white solid, yield 54%; ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.40 (s, 1H), 8.23 (d, *J* = 8.8 Hz, 1H), 8.10 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.68 (d, *J* = 3.7 Hz, 1H), 6.68 (d, *J* = 3.8 Hz, 1H), 1.70 (d, *J* = 1.4 Hz, 9H); ^{13}C NMR (101 MHz, DMSO) δ 167.8, 144.6, 125.7, 122.6, 121.4, 119.4, 119.0, 110.3, 103.1, 79.8, 23.4; HRMS: calcd for $C_{14}H_{16}NO_4$ ($M+H^+$): 262.1074, Found: 262.1072.



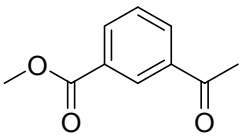
Quinoline-3-carboxylic acid (**2p**)[9]: half-white solid, yield 92%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.36 (s, 1H), 9.31 (d, *J* = 2.1 Hz, 1H), 8.96 (d, *J* = 2.1 Hz, 1H), 8.18 (d, *J* = 8.1 Hz, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.98 – 7.83 (m, 1H), 7.70 (t, *J* = 7.5 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 166.8, 150.3, 149.6, 139.0, 132.4, 130.0, 129.3, 127.9, 127.1, 124.1.



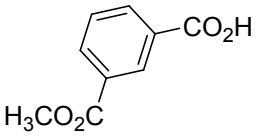
Quinoline-6-carboxylic acid (**2q**)[10]: white solid, yield 78%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.23 (s, 1H), 9.00 (dd, J = 4.2, 1.7 Hz, 1H), 8.66 (d, J = 1.9 Hz, 1H), 8.55 (dd, J = 8.5, 1.7 Hz, 1H), 8.21 (dd, J = 8.8, 1.9 Hz, 1H), 8.08 (d, J = 8.8 Hz, 1H), 7.61 (dd, J = 8.3, 4.2 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 167.5, 153.1, 149.8, 138.0, 131.4, 129.8, 129.3, 129.2, 127.7, 122.7.



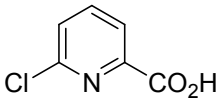
3-Bromobenzoic acid (**2r**)[11]: light grey solid; yield 52%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.05 (bs, 1H); 8.03 (t, J = 1.8 Hz, 1H), 7.92 (dt, J = 7.5, 1.3 Hz, 1H), 7.82 (dd, J = 8.1, 2.0 Hz, 1H), 7.47 (t, J = 7.9 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 166.4, 136.0, 133.5, 132.2, 131.4, 128.7, 122.2.



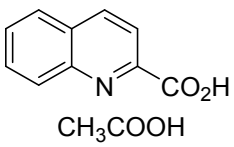
Methyl 3-acetylbenzoate (**2s**)[12]: white solid; yield 76%; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.57 (dt, J = 1.8, 1.1 Hz, 1H), 8.21 (dt, J = 7.7, 1.5 Hz, 1H), 8.14 (ddd, J = 7.8, 1.8, 1.3 Hz, 1H), 7.54 (td, J = 7.8, 0.6 Hz, 1H), 3.94 (s, 3H), 2.64 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.2, 166.3, 137.3, 133.9, 132.3, 130.7, 129.5, 128.8, 52.4, 26.7.



3-(Methoxycarbonyl)benzoic acid (**2t**)[13]: white solid, yield 20%; ^{1}H NMR (400 MHz, Chloroform-d) δ 8.77 (d, J = 1.7 Hz, 1H), 8.30 (dt, J = 7.8, 1.9 Hz, 2H), 7.59 (t, J = 7.8 Hz, 1H), 3.97 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 166.1, 134.7, 134.3, 131.4, 130.8, 129.6, 128.8, 52.5.

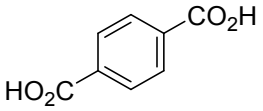


6-Chloropicolinic acid (**2u**)[14]: half-white solid; yield 45%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.40 (s, 1H), 8.07 – 8.00 (m, 2H), 7.74 (dd, J = 6.1, 2.8 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 165.3, 150.6, 149.3, 141.6, 128.4, 124.5.

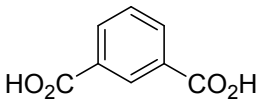


Quinoline-2-carboxylic acid (**2v**)[2]: made salt with AcOH after extraction with EtOAc and concentrated to obtaine half-white solid. yield 45%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.65 (s, 1H), 8.55 (d, J = 8.5 Hz, 1H), 8.22 – 8.02 (m, 3H), 7.87 (t, J = 7.7 Hz, 1H), 7.74 (t, J

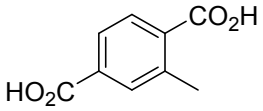
= 7.5 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 166.8, 149.2, 147.3, 138.1, 131.0, 130.2, 129.3, 129.0, 128.5, 121.2.



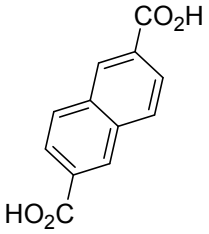
Terephthalic acid (**3a**)[15]: half-white solid; yield 93%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.19 (s, 2H), 8.03 (s, 4H); ^{13}C NMR (101 MHz, DMSO) δ 167.2, 135.0, 129.9.



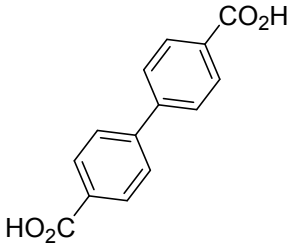
Isophthalic acid (**3b**)[16]: light grey solid, yield 62%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.15 (s, 2H), 8.47 (d, J = 1.8 Hz, 1H), 8.16 (dd, J = 7.8, 1.7 Hz, 2H), 7.63 (t, J = 7.8 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 167.1, 133.9, 131.7, 130.5, 129.6.



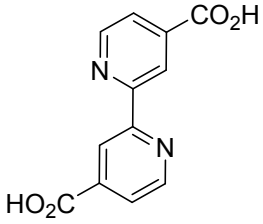
2-Methyl terephthalic acid (**3c**)[17]: pale yellow solid, yield 72%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.17 (bs, 2H), 7.93 – 7.77 (m, 3H), 2.54 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 168.7, 167.2, 139.4, 135.1, 133.6, 132.6, 130.6, 127.1, 21.4; HRMS: calcd for $C_9H_7O_4$ (M-H^+) 179.0350, Found 179.0358.



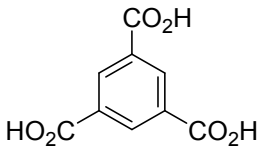
Naphthalene-2,6-dicarboxylic acid (**3d**)[18]: half white solid, yield 93%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.23 (s, 2H), 8.65 (s, 2H), 8.19 (d, J = 8.6 Hz, 2H), 8.04 (d, J = 8.6 Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 167.7, 134.7, 130.7, 130.2, 126.4.



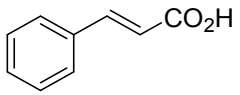
[1,1'-biphenyl]-4,4'-dicarboxylic acid (**3e**)[19]: white solid, yield 91%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.96 (s, 2H), 8.08 – 8.01 (m, 4H), 7.89 – 7.82 (m, 4H); ^{13}C NMR (101 MHz, DMSO) δ 167.5, 143.6, 130.9, 130.5, 127.6.



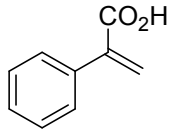
[2,2'-bipyridine]-4,4'-dicarboxylic acid (**3f**)[20]: milky white solid; yield 84%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.82 (s, 2H), 8.92 (d, J = 4.9 Hz, 2H), 8.87 – 8.84 (m, 2H), 7.92 (dd, J = 5.0, 1.6 Hz, 2H); ^{13}C NMR (101 MHz, DMSO) δ 166.5, 155.9, 151.1, 140.1, 123.9, 120.0.



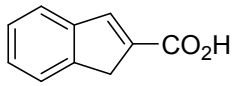
Benzene-1,3,5-tricarboxylic acid (**4**)[21]: white solid; yield 97%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.34 (s, 3H), 8.63 (s, 3H); ^{13}C NMR (101 MHz, DMSO) δ 166.4, 134.1, 132.4.



***trans*-Cinnamic acid** (**8a**)[22]: white solid; yield 91%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.41 (s, 1H), 7.71 – 7.64 (m, 2H), 7.59 (dd, J = 16.0, 1.7 Hz, 1H), 7.40 (q, J = 2.6 Hz, 3H), 6.53 (dd, J = 16.0, 1.8 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 168.1, 144.3, 134.6, 130.6, 129.3, 128.6, 119.6.



2-Phenylacrylic acid (**8b**)[23]: white solid, yield 89%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 (s, 1H), 7.46 – 7.40 (m, 2H), 7.40 – 7.32 (m, 3H), 6.23 (d, J = 1.2 Hz, 1H), 5.96 (d, J = 1.2 Hz, 1H); ^{13}C NMR (101 MHz, DMSO) δ 168.1, 141.9, 137.1, 128.5, 128.4, 128.3, 126.4.



1*H*-indene-2-carboxylic acid (**8c**)[24]: white solid, yield 93%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.51 (s, 1H), 7.68 (d, J = 2.1 Hz, 1H), 7.62 – 7.50 (m, 2H), 7.33 (dt, J = 5.2, 2.1 Hz, 2H), 3.62 (s, 2H); ^{13}C NMR (101 MHz, DMSO) δ 166.2, 145.2, 143.1, 140.7, 139.0, 127.8, 127.3, 124.9, 123.8, 38.6.

III. References

1. Compounds **2a**, **2b**, **2c**, **2d**, **2e**, **2h**, **2i**, **2j**, **2n**, **2s**, **8a**: X. Zhang, W.-Z. Zhang, L. -L Shi, C. -X. Guo, L. -L. Zhang and X.-B. Lu, *Chem. Commun.* 2012, **48**, 6292.
2. Compounds **2b, 2c, 2g, 2j, 2v**: M. Yoshida, Y. Katagiri, W.-B. Zhu, K. Shishido, *Org. Biomol. Chem.* 2009, **7**, 4062.
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6. Compound **2m**: W. Han, F. Jin and Q. Zhou, *Synthesis (Stuttg).* 2015, **47**, 1861.
7. Compound **2n**: C. Schmuck and U. Machon, *European J. Org. Chem.* 2006, **19**, 4385.

8. Compound **2o**: new compound
9. Compound **2p**: S. Korsager, R. H. Taaning and T. Skrydstrup, *J. Am. Chem. Soc.* 2013, **135**, 2891.
10. Compound **2q**: J. T. Joseph, A. M. Sajith, R. C. Ningegowda, and S. Shashikanth, *Adv. Synth. Catal.* 2017, **359**, 419.
11. Compound **2r**: Z. Yang, R. Luo, Z. Zhu, X. Yang and W. Tang, *Organometallics* 2017, **36**, 4095.
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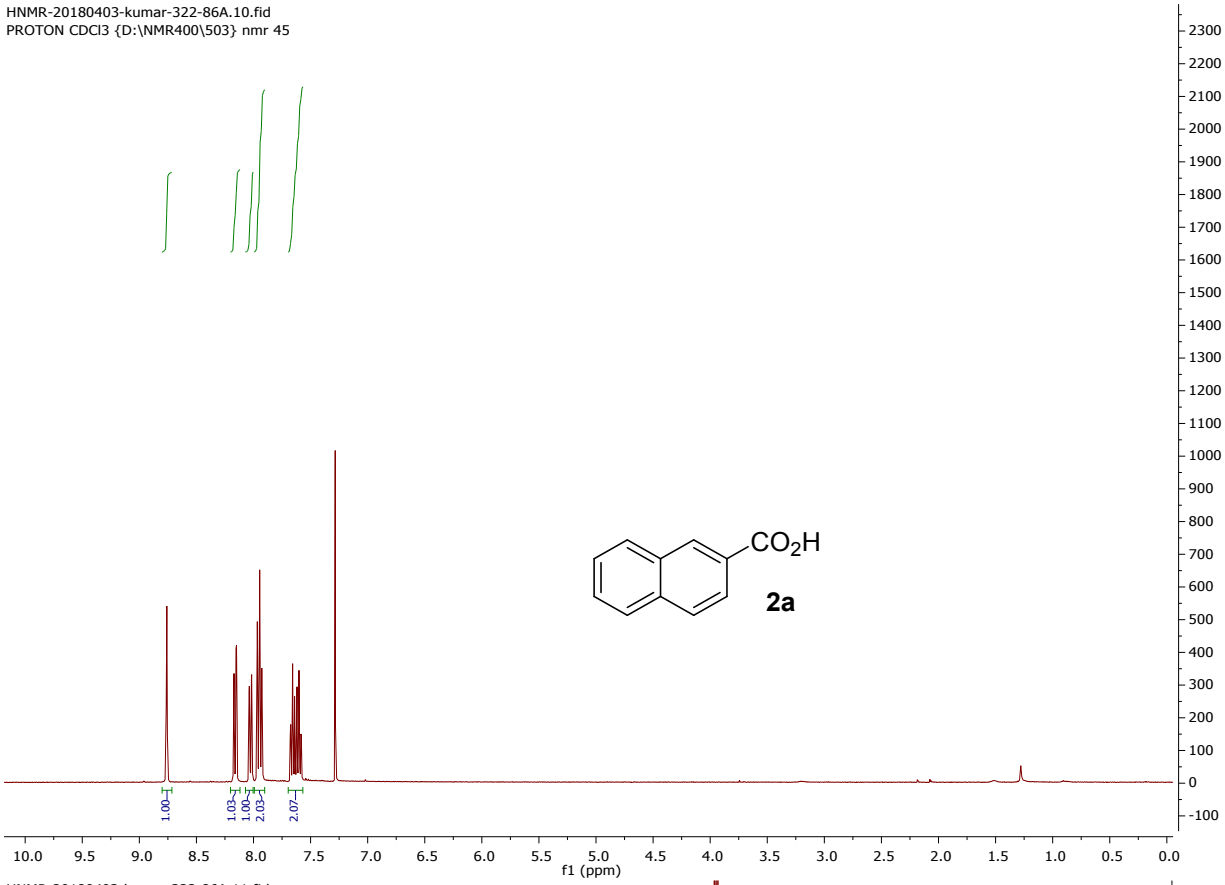
14. Compound **2u**: S. Rádl, P. Hezký, J. Proška, L. Hejnová and I. Krejcí, I. *Arch. Pharm. (Weinheim)*. 2000, **333**, 107.
15. Compound **3a**: S. Hazra, M. Deb and A. J. Elias, *Green Chem.* 2017, **19**, 5548.
16. Compound **3b**: S. D. Friis, T. L. Andersen and T. Skrydstrup, *Org. Lett.* 2013, **15**, 1378.
17. Compound **3c**: L. Anzalone and J. A. Hirsch, *J. Org. Chem.* 1985, **50**, 2128.
18. Compuond **3d**: T. C. Bruice, Y. C. Yip, A. Blaskó, F. C. Lightstone, K. A. Browne, M. E. Petyak, and J. Luo, *Tetrahedron* 1997, **53**, 8105.
19. Compound **3e**: V. Medabalmi and K. Ramanujam, *J. Electrochem. Soc.* 2017, **164**, A1720.
20. Compound **3f**: T. M. Postma, W. R. J. D. Galloway, F. B. L. Cougnon, G. D. Pantoş, J. E. Stokes and D. R. Spring, *Synlett* 2013, **24**, 765.
21. Compound **4**: BTC; (a) N. Leventis, C. Chidambareswarapattar, D. P. Mohite, Z. J. Larimore, H. Lu, and C. Sotiriou-Leventis, *J. Mater. Chem.* 2011, **21**, 11981; (b) Sigma-Aldrich Cat. No: 482749
22. Compound **8a**: F. P. Wu, J. B. Peng, X. Qi and X. F. Wu, *J. Org. Chem.* 2017, **82**, 9710.
23. Compound **8b**: J. Hou, J. -H. Xie, and Q. -L. Zhou, *Angew. Chemie Int. Ed.* 2015, **54**, 6302.
24. Compound **8c**: C. Song, P. Chen, and Y. Tang, *RSC Adv.* 2017, **7**, 11233.
25. ^{29}Si NMR of disiloxane: a) J. Brus and P. Karhan. Petr Kotlik. *Collect. Czech. Chem. Commun*. **1996**, *61*, 691; b) T. Kemmitt and Henderson. W. *Aust. J. Chem.*, 1998, **51**, 1031.

IV. Copies of ^{1}H NMR and ^{13}C NMR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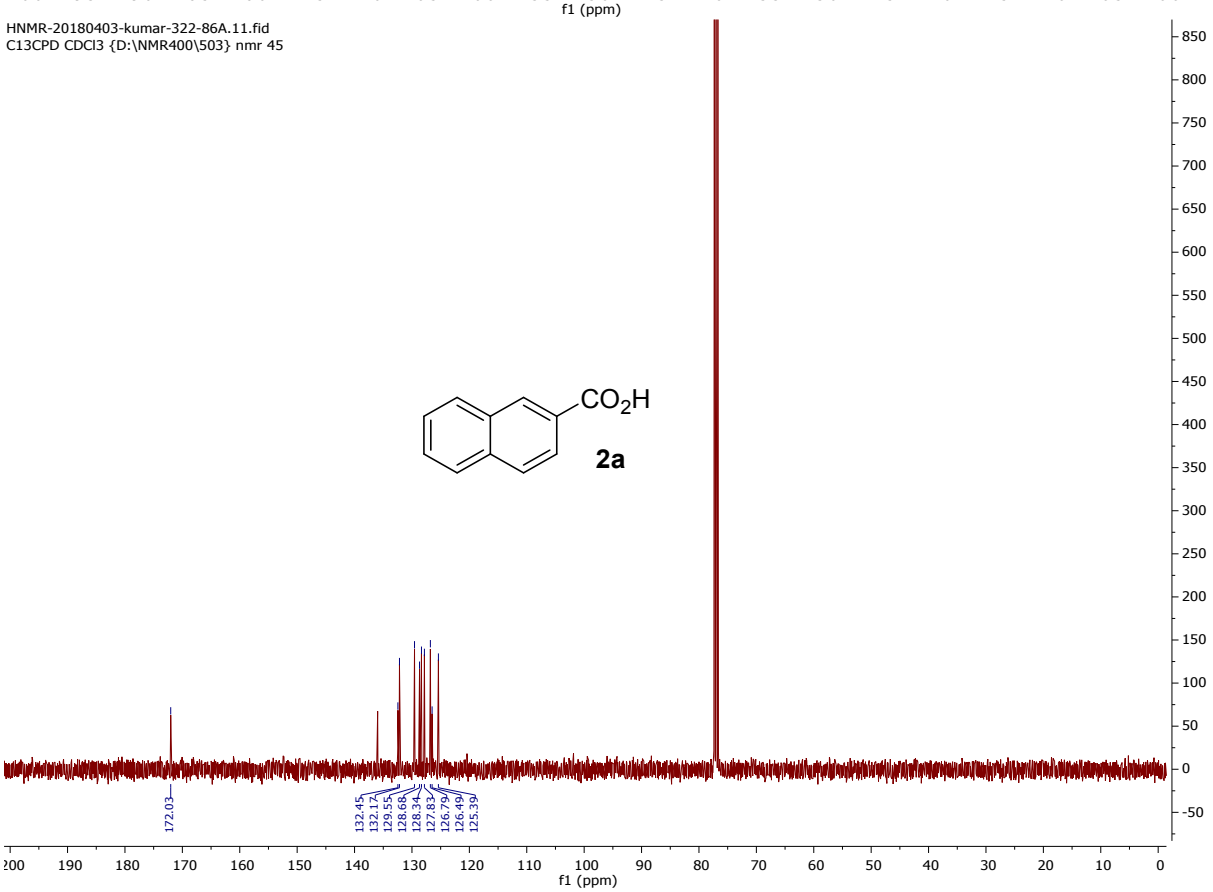
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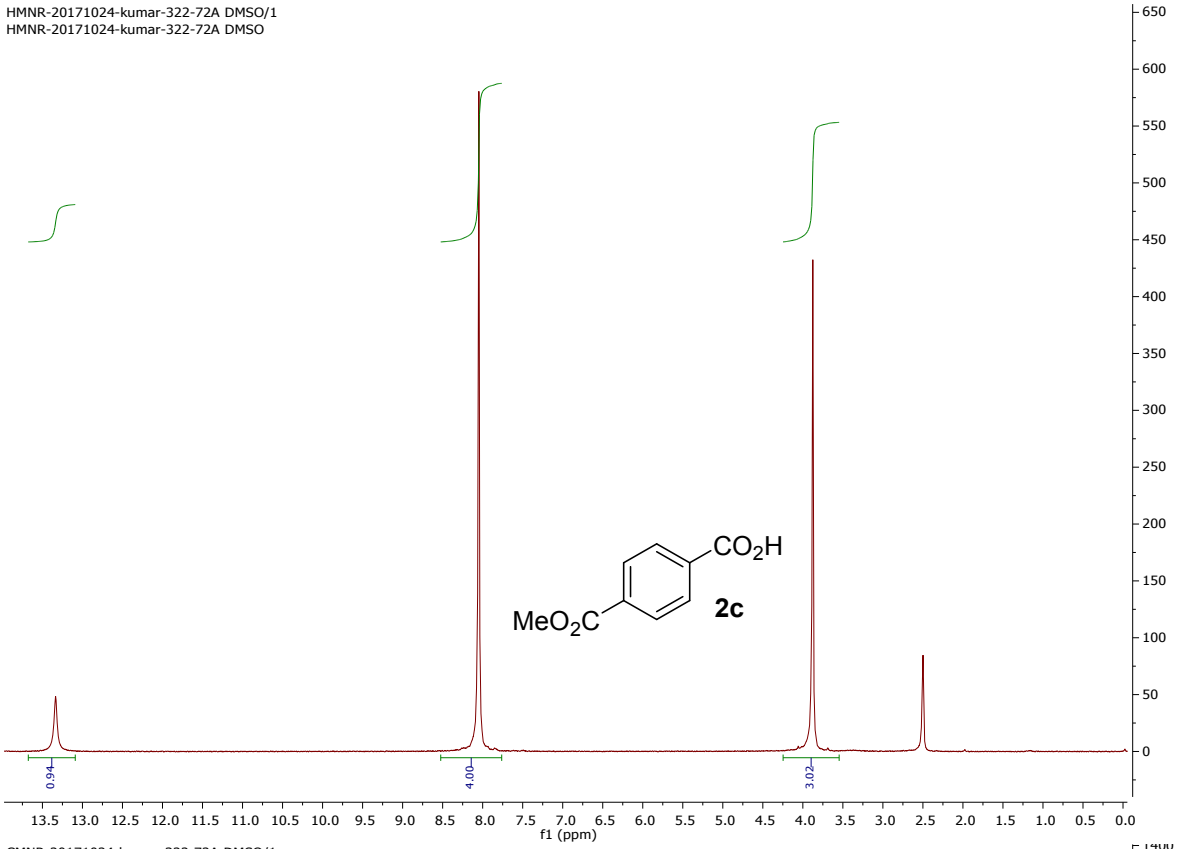
f1 (ppm)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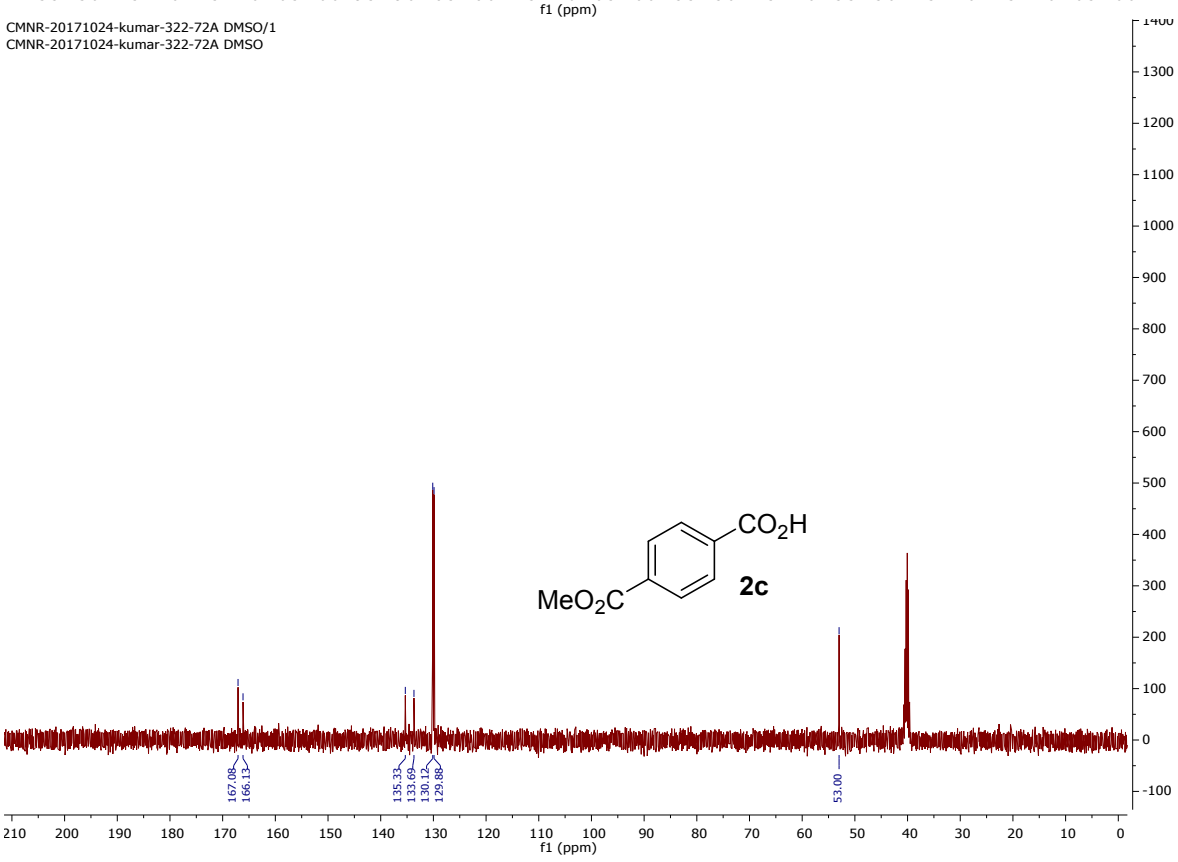
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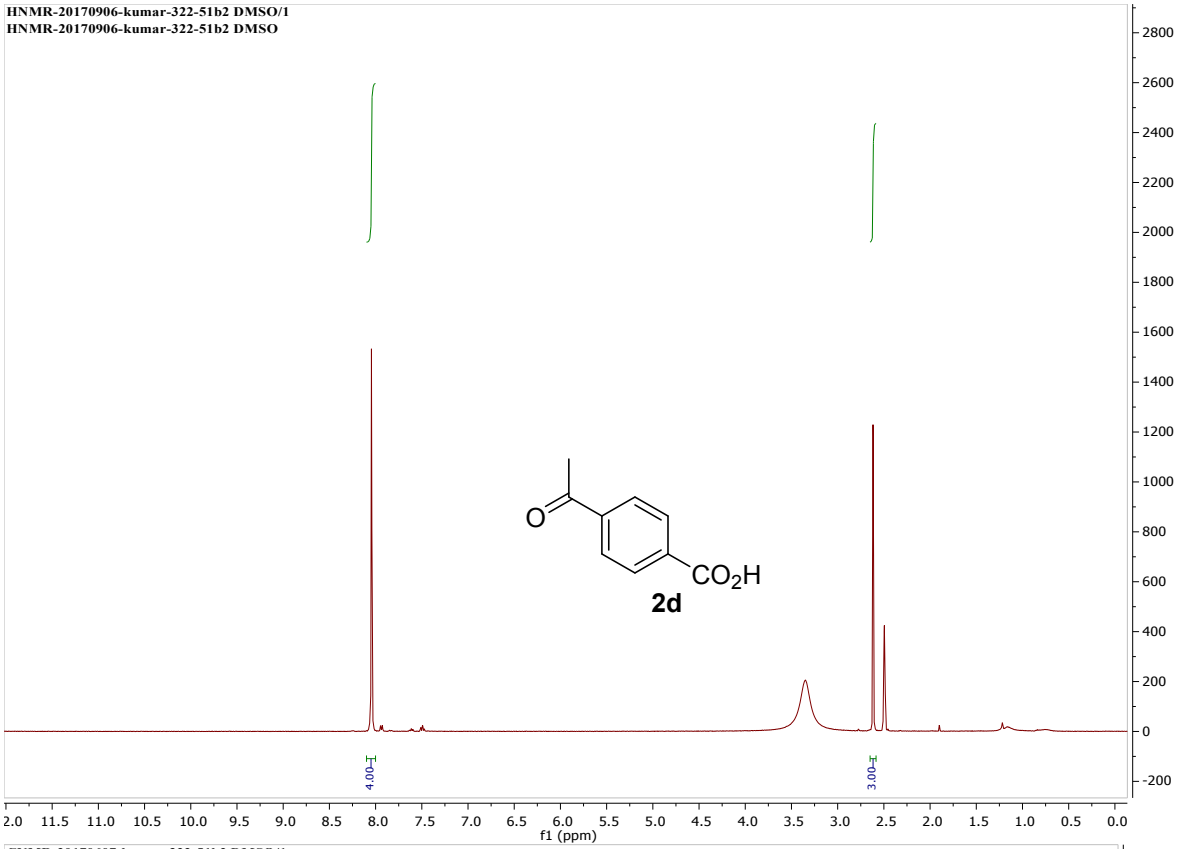
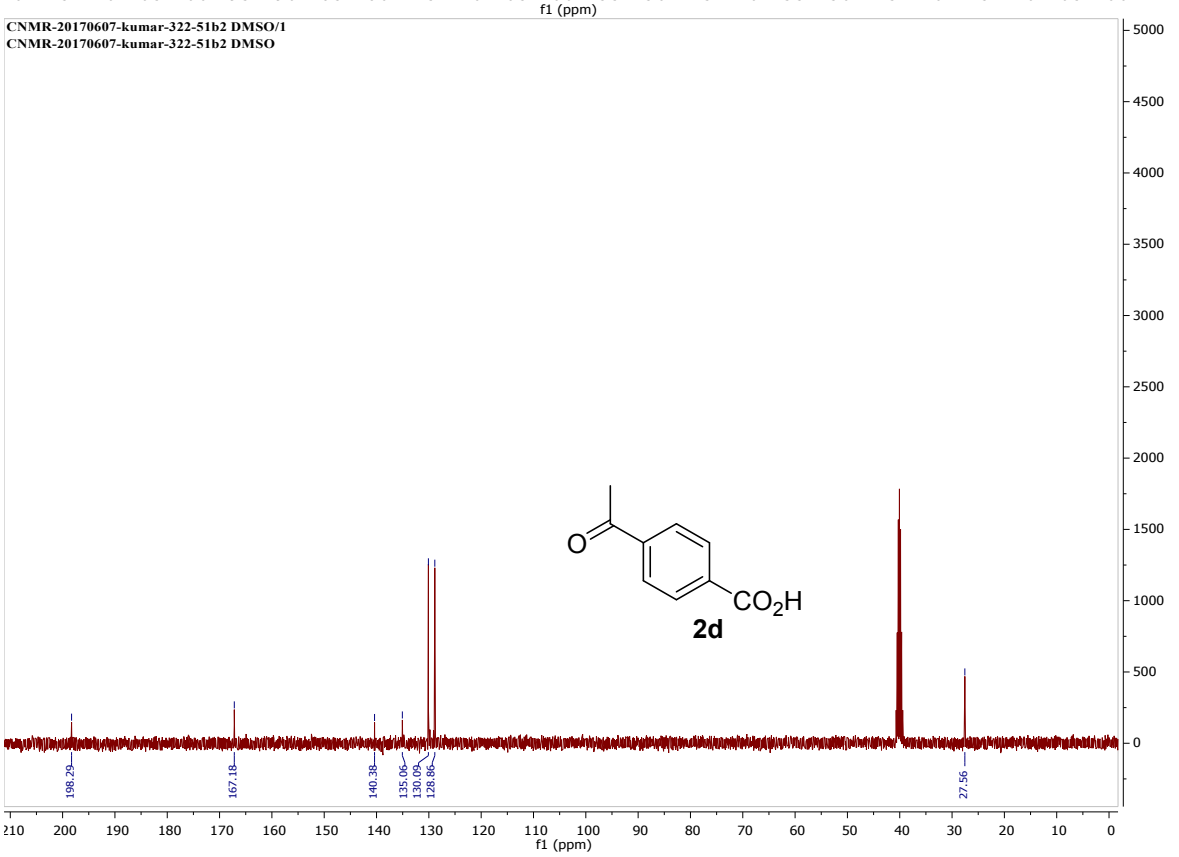
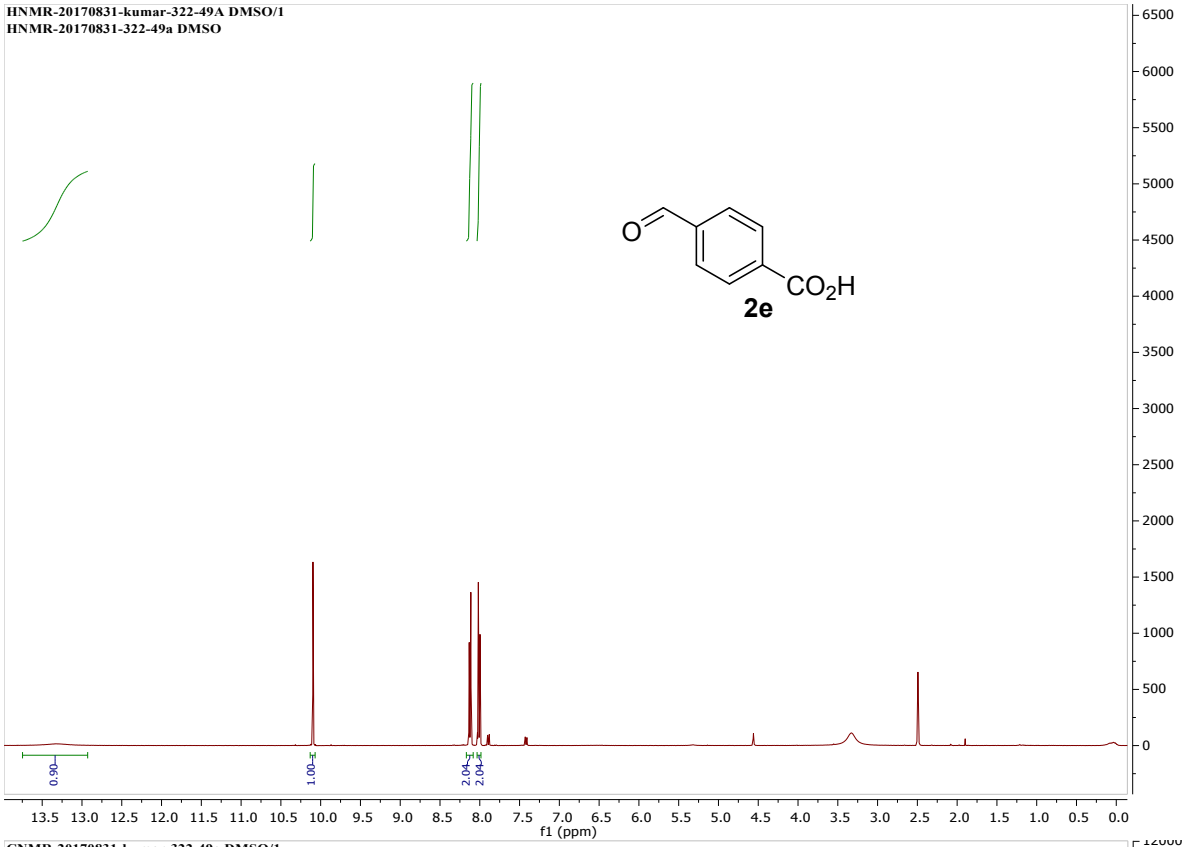
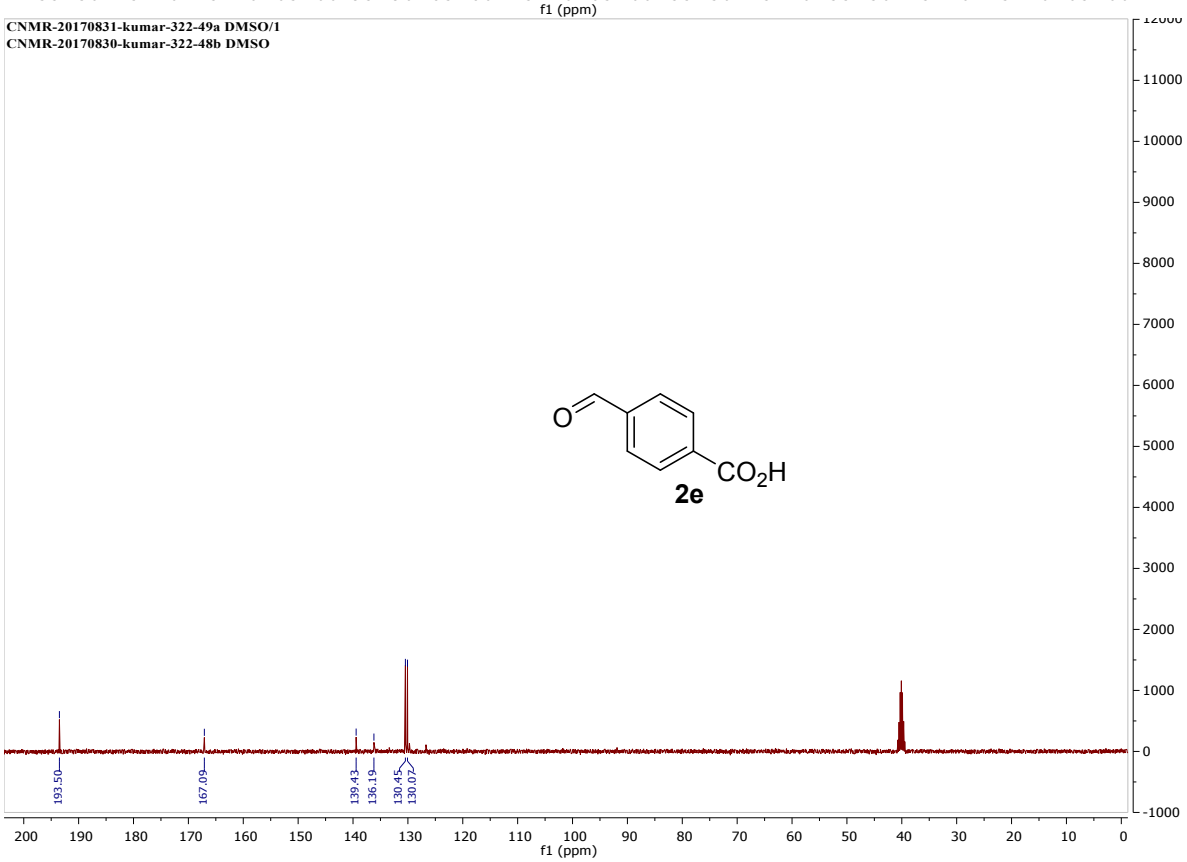
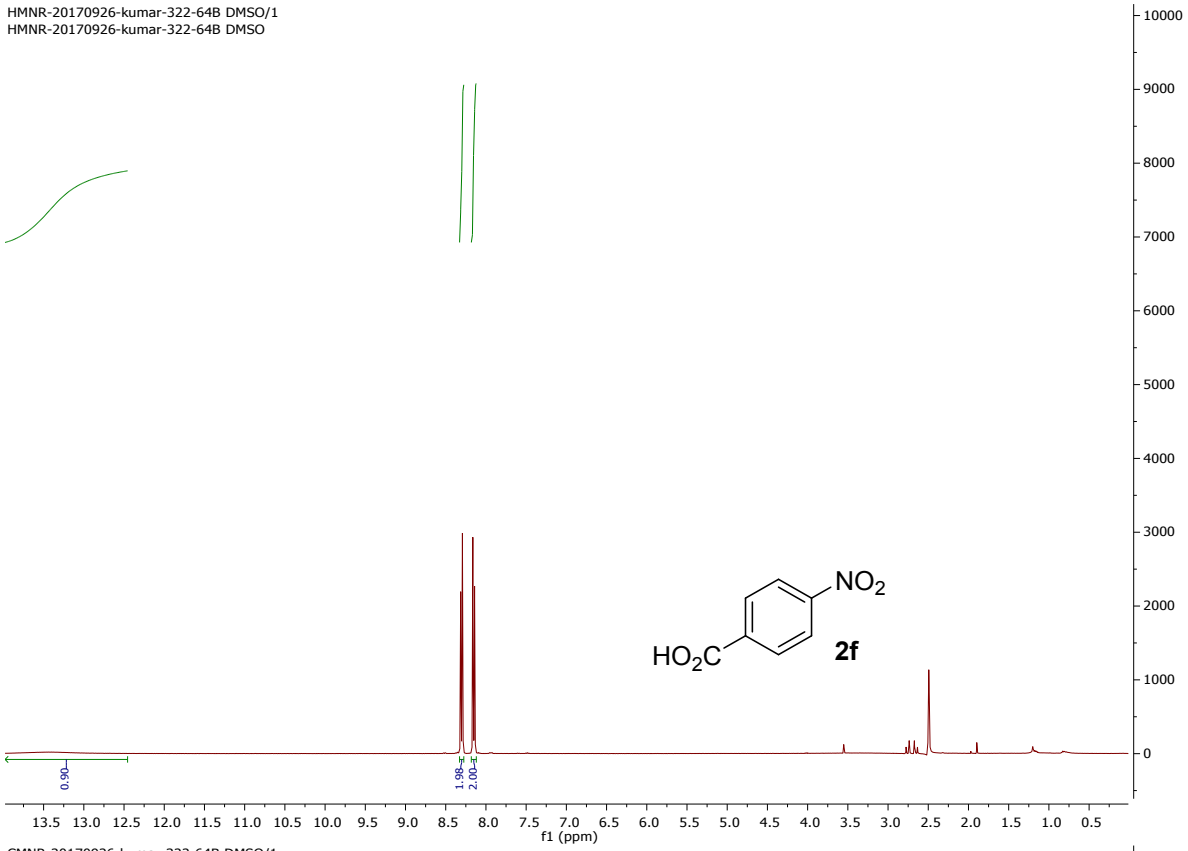
53.00
f1 (ppm)

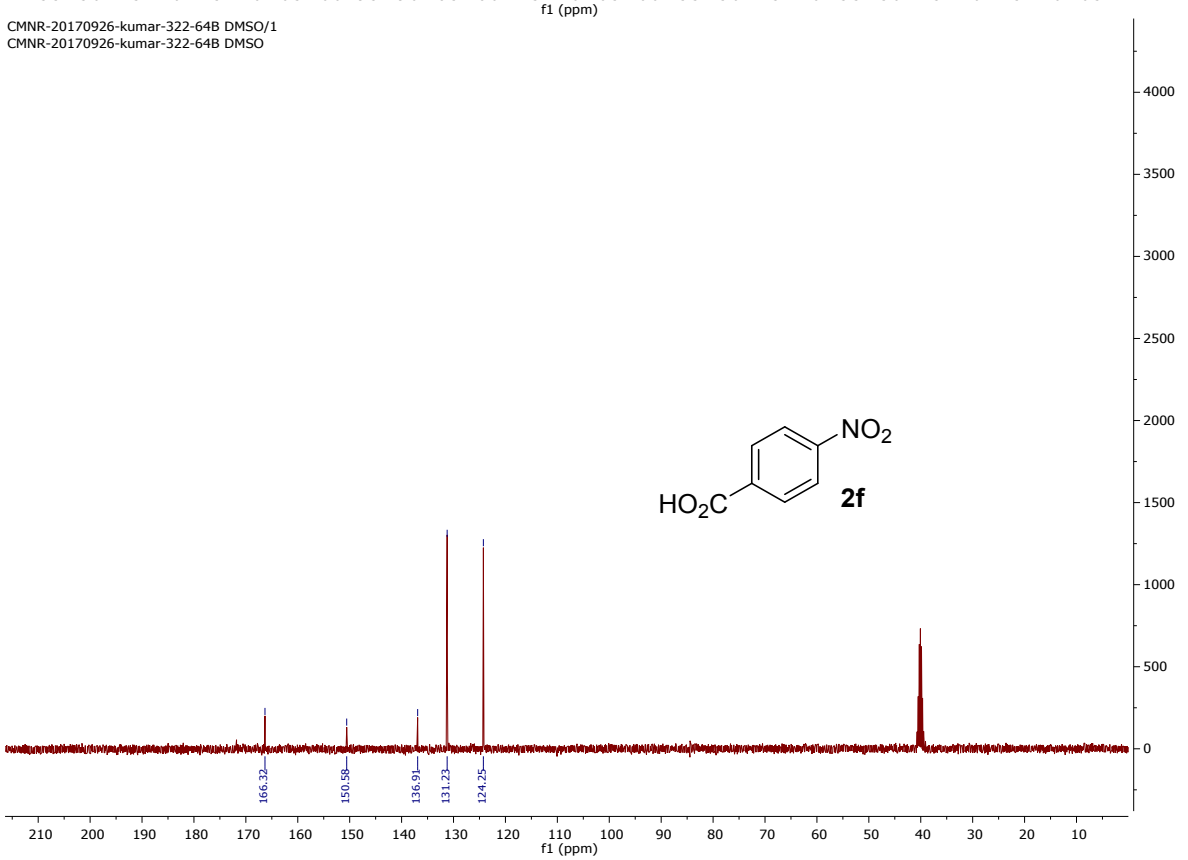

HNMR-20170906-kumar-322-51b2 DMSO/1
HNMR-20170906-kumar-322-51b2 DMSO
O
CO2H
2d
4.00
3.00
f1 (ppm)

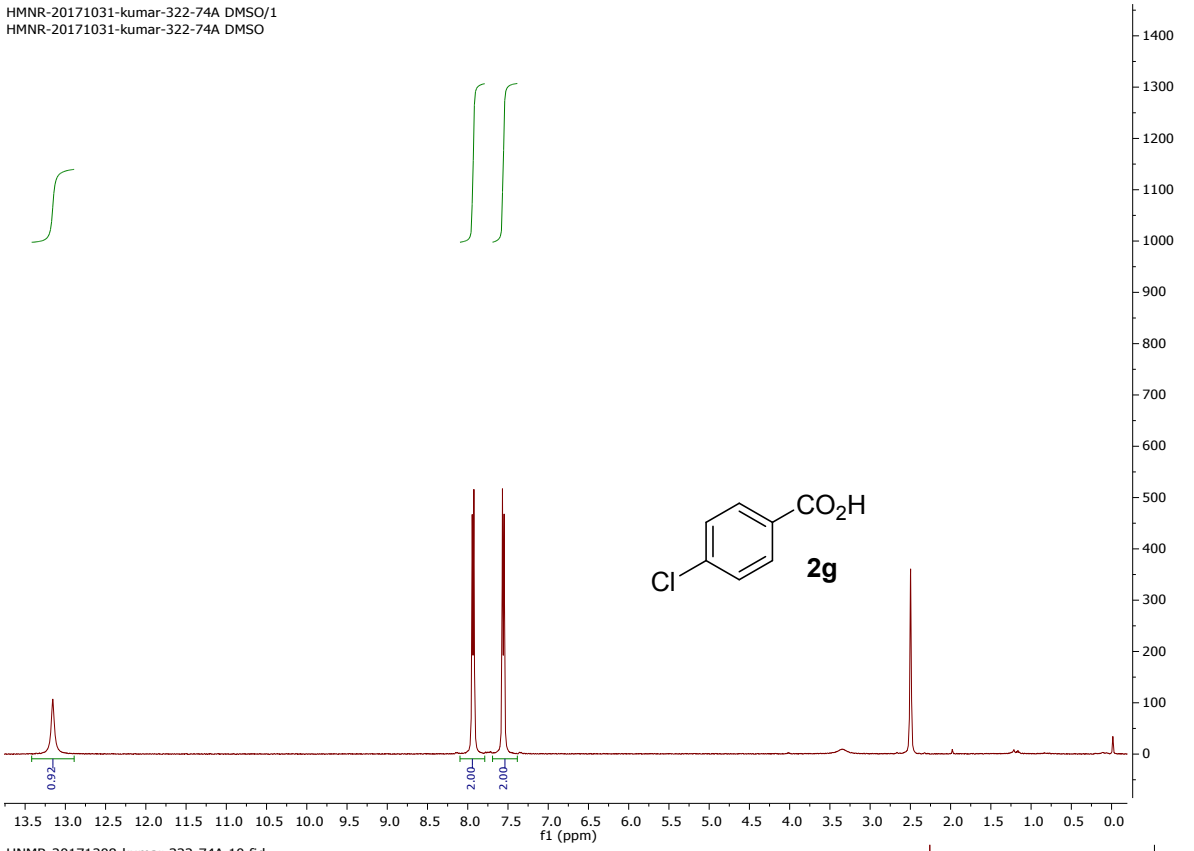

CNMR-20170607-kumar-322-51b2 DMSO/1
CNMR-20170607-kumar-322-51b2 DMSO
O
CO2H
2d
198.29
167.18
140.38
135.06
130.09
128.86
27.56
f1 (ppm)

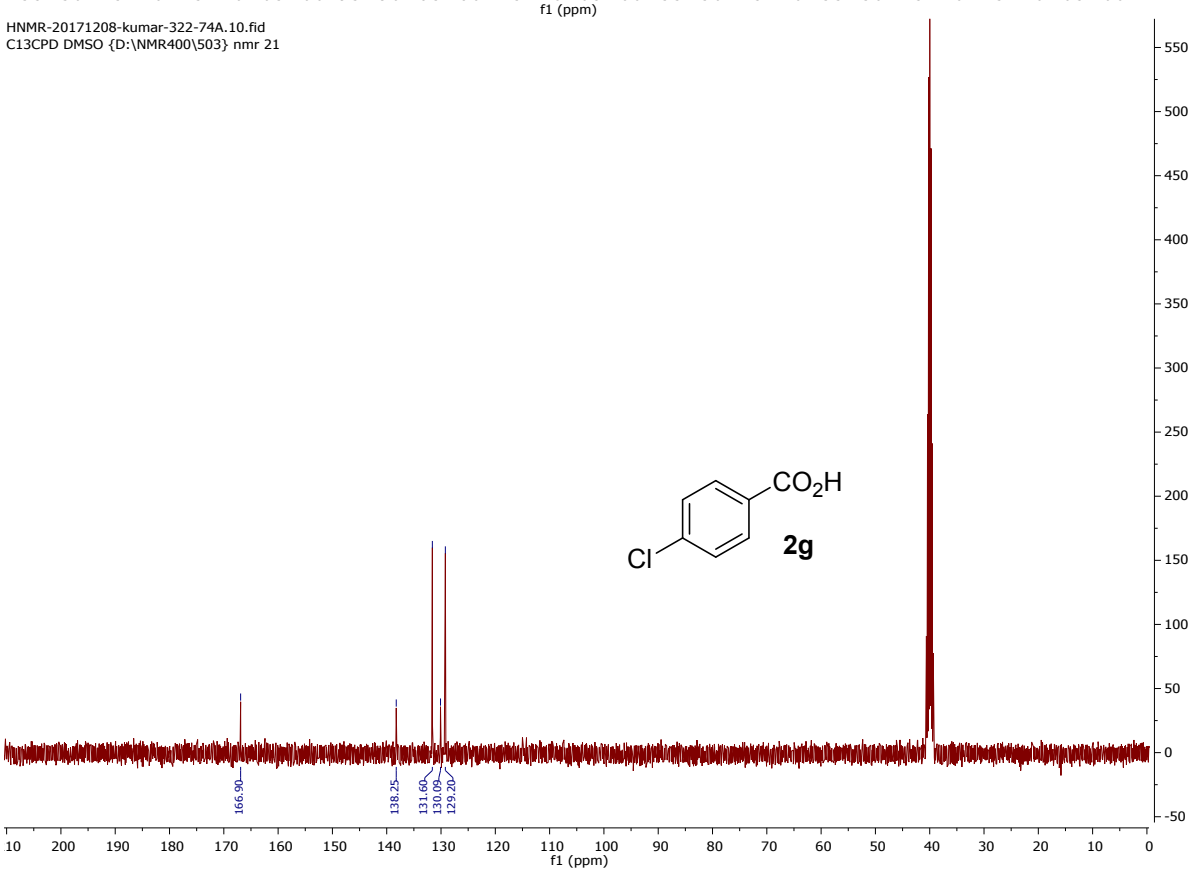

HNMR-20170831-kumar-322-49A DMSO/1
HNMR-20170831-322-49a DMSO
O
CO2H
2e
0.90
1.00
2.04
2.04
f1 (ppm)

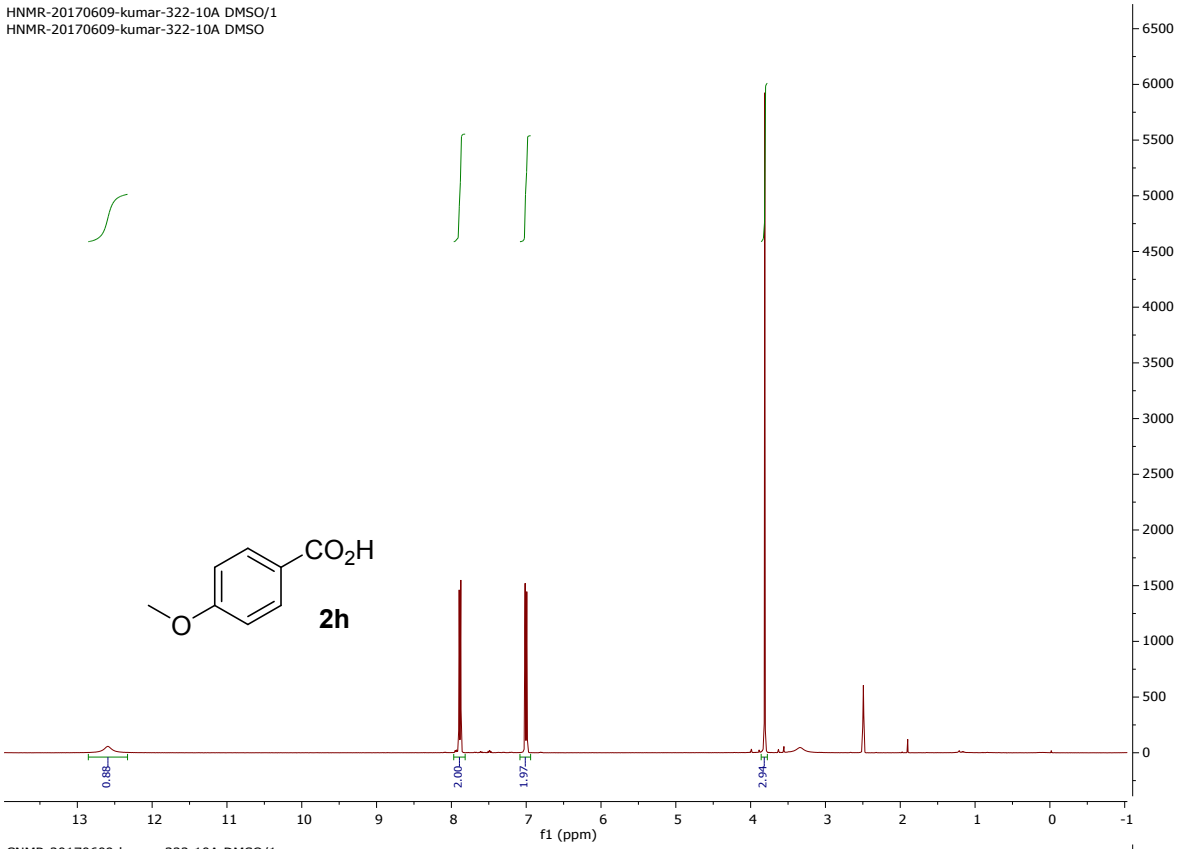

CNMR-20170831-kumar-322-49a DMSO/1
CNMR-20170830-kumar-322-48b DMSO
O
CO2H
2e
193.50
167.09
139.43
136.19
130.45
130.07
f1 (ppm)

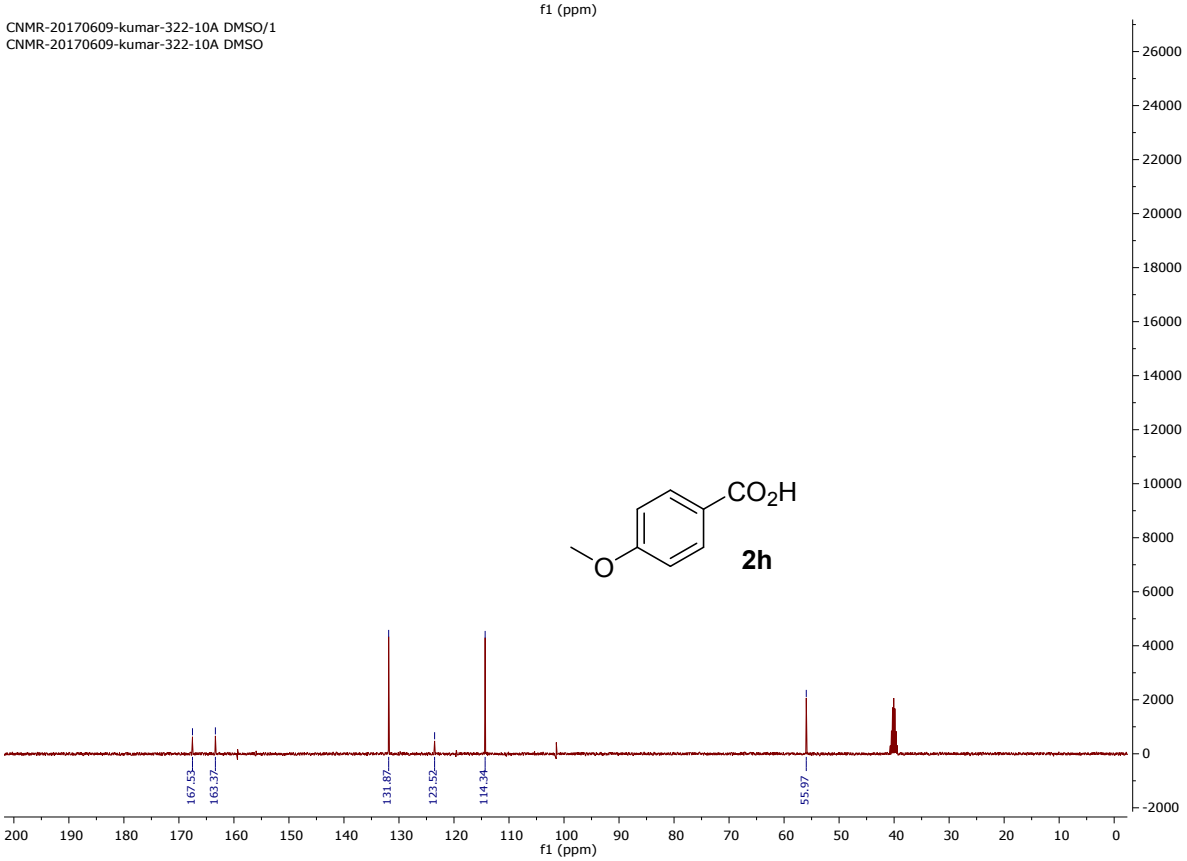

HMNR-20170926-kumar-322-64B DMSO/1
HMNR-20170926-kumar-322-64B DMSO
NO2
HO2C
2f
0.90
1.98
2.00
f1 (ppm)

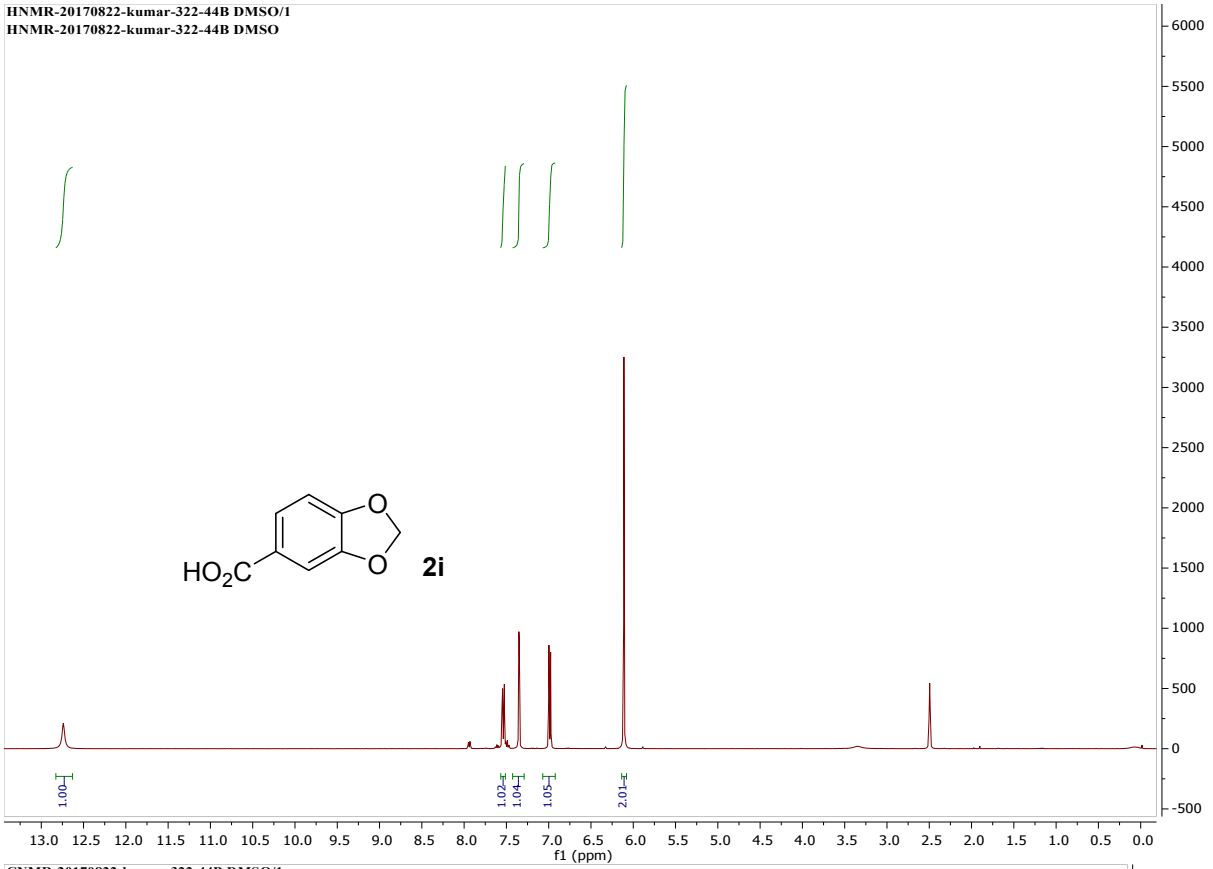

CMNR-20170926-kumar-322-64B DMSO/1
CMNR-20170926-kumar-322-64B DMSO
NO2
HO2C
2f
166.32
150.58
136.91
131.23
124.25
f1 (ppm)

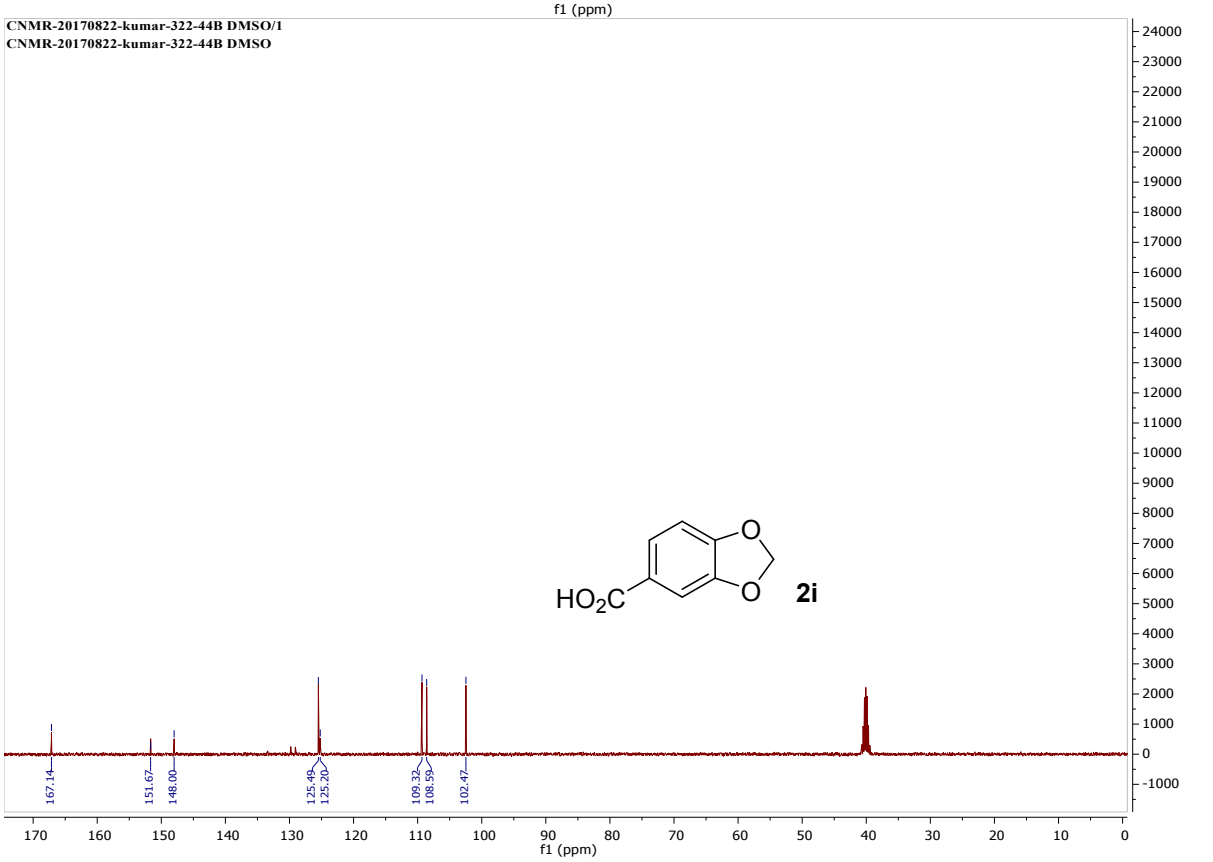

HMNR-20171031-kumar-322-74A DMSO/1
HMNR-20171031-kumar-322-74A DMSO
CO2H
Cl
2g
0.92
2.00
2.00
f1 (ppm)

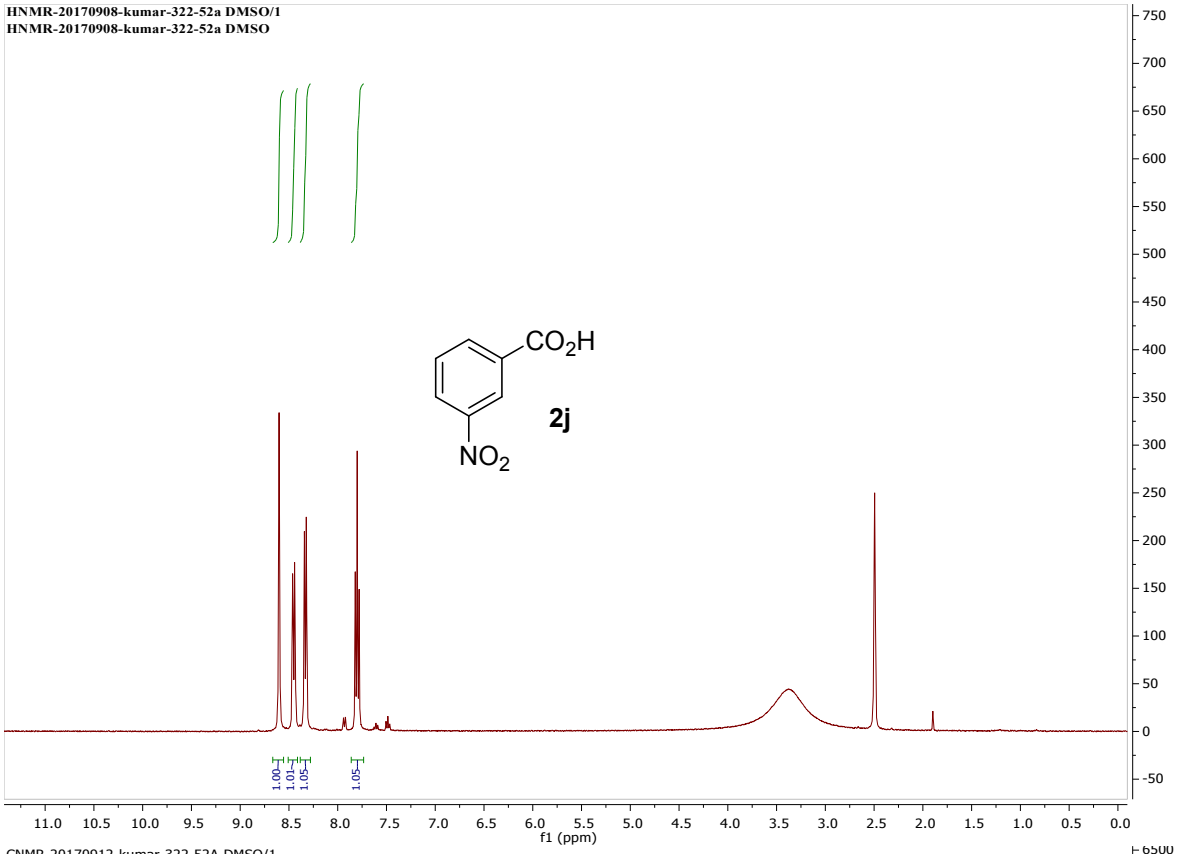

HNMR-20171208-kumar-322-74A.10.fid
C13CPD DMSO {D:\NMR400\503} nmr 21
CO2H
Cl
2g
166.90
138.25
131.60
130.09
129.20
f1 (ppm)

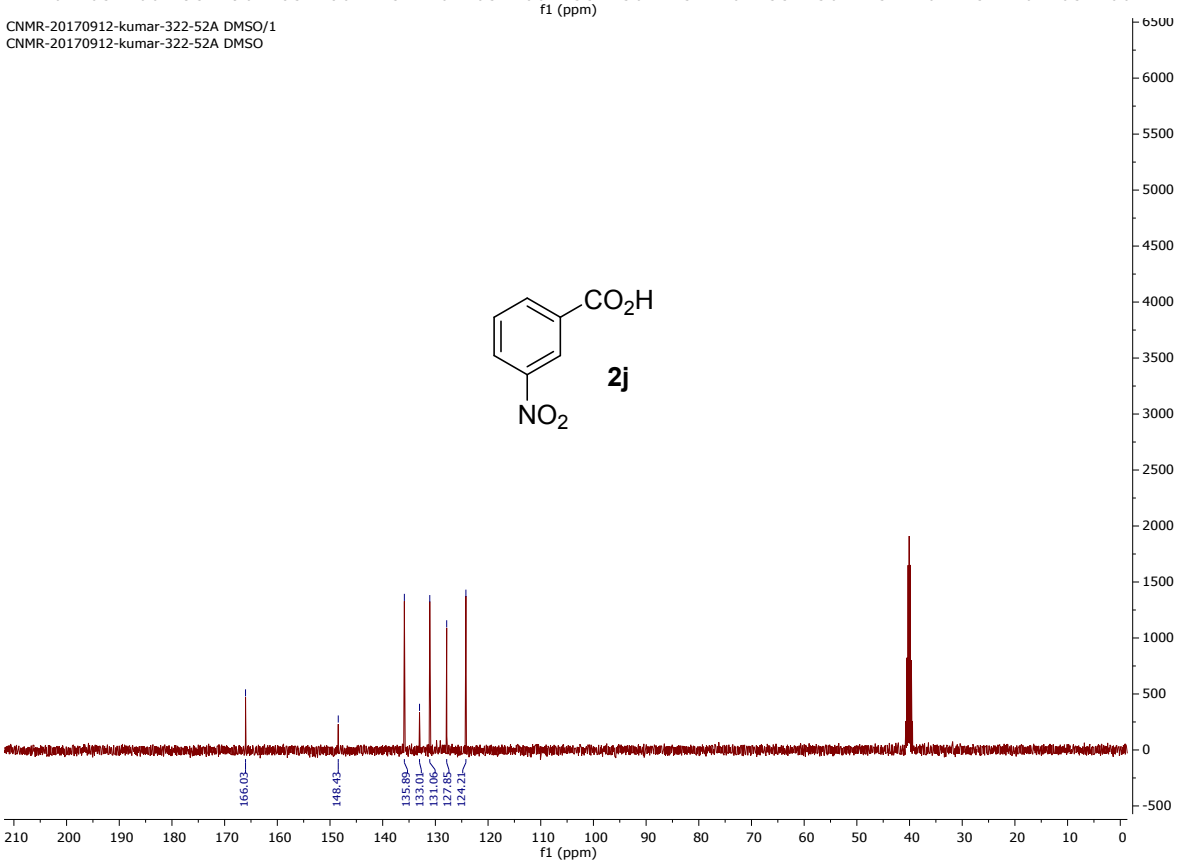

HNMR-20170609-kumar-322-10A DMSO/1
HNMR-20170609-kumar-322-10A DMSO
CO2H
O
2h
0.88
2.00
1.97
2.94
f1 (ppm)


CNMR-20170609-kumar-322-10A DMSO/1
CNMR-20170609-kumar-322-10A DMSO
CO2H
O
2h
167.53
163.37
131.87
123.52
114.34
55.97
f1 (ppm)

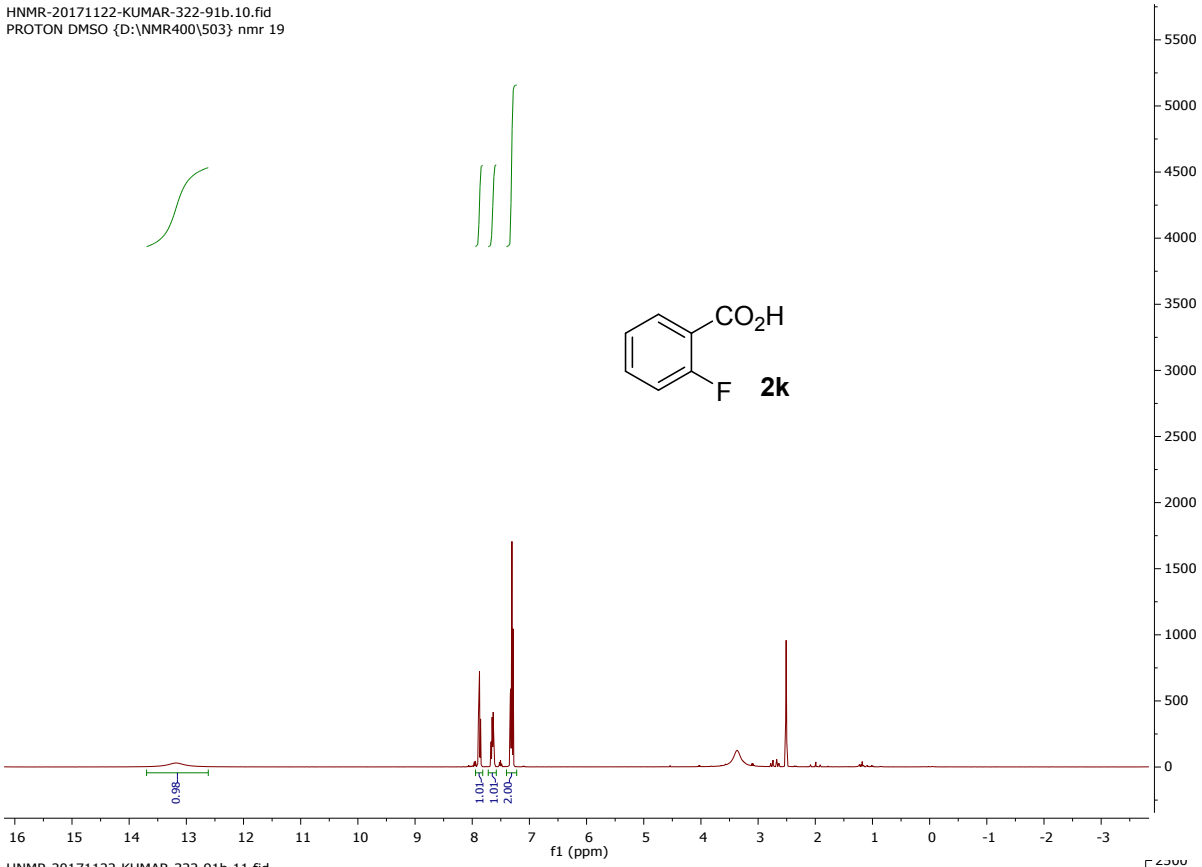

HNMR-20170822-kumar-322-44B DMSO/1
HNMR-20170822-kumar-322-44B DMSO
HO2C
O
O
2i
1.00
1.02
1.04
1.05
2.01
f1 (ppm)


CNMR-20170822-kumar-322-44B DMSO/1
CNMR-20170822-kumar-322-44B DMSO
HO2C
O
O
2i
167.14
151.67
148.00
125.49
125.20
109.32
108.59
102.47
f1 (ppm)

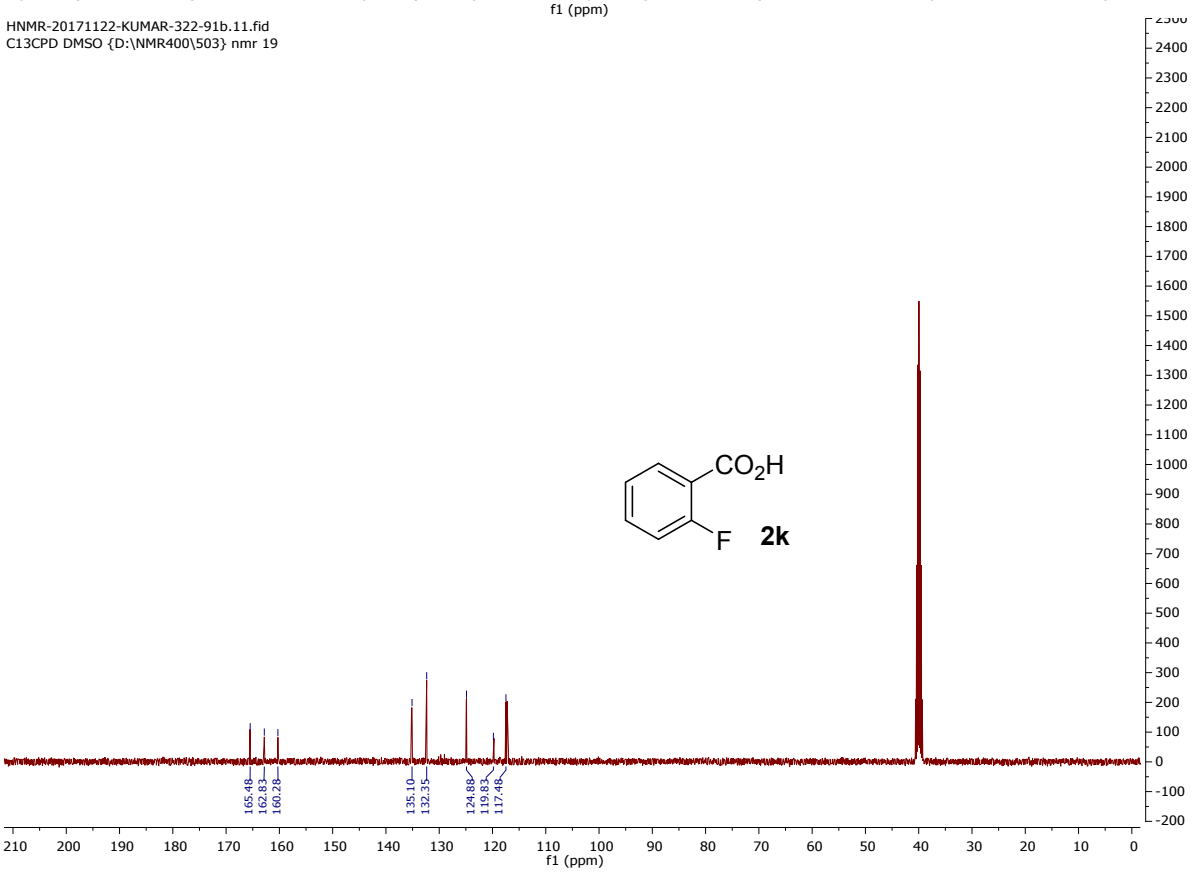

HNMR-20170908-kumar-322-52a DMSO/1
HNMR-20170908-kumar-322-52a DMSO
CO2H
2j
NO2
1.00
1.01
1.05
1.05
f1 (ppm)

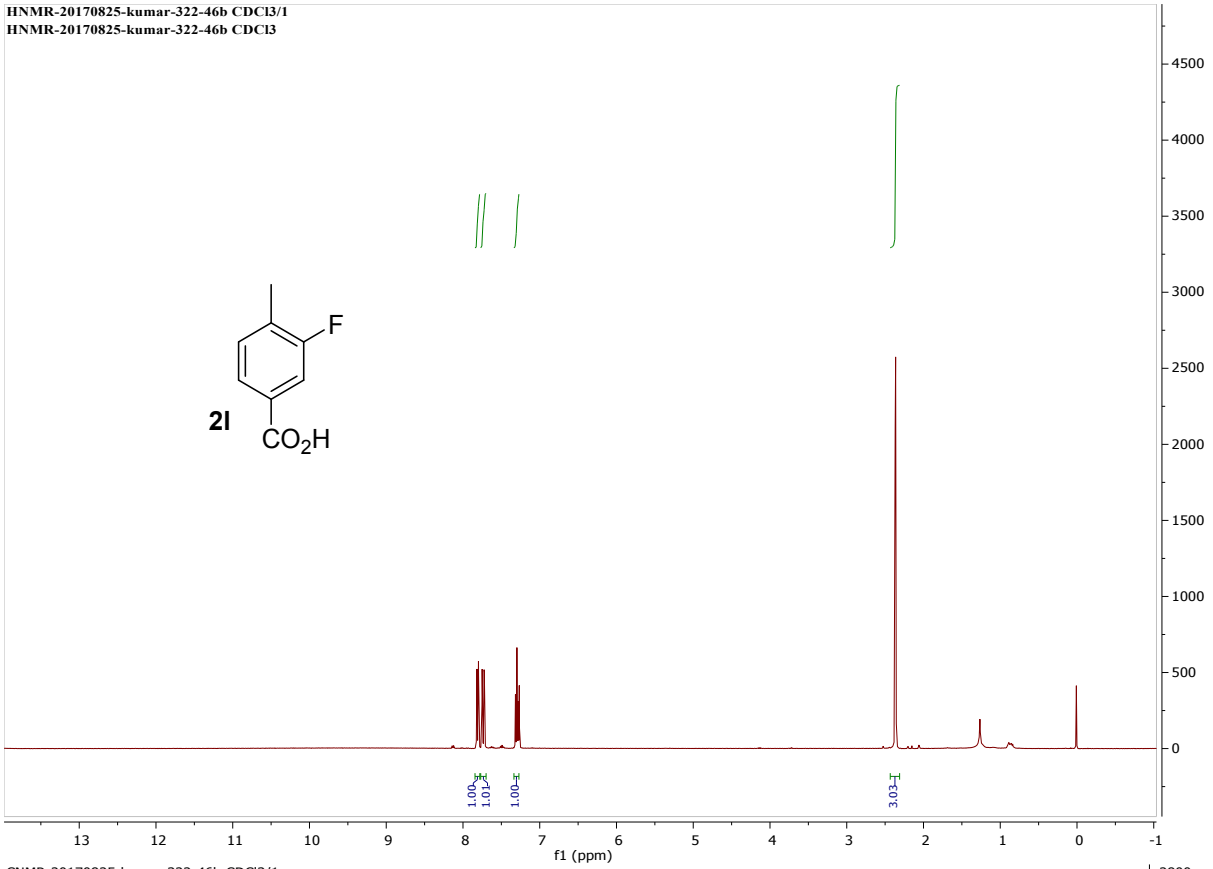

CNMR-20170912-kumar-322-52A DMSO/1
CNMR-20170912-kumar-322-52A DMSO
CO2H
2j
NO2
166.03
148.43
135.89
133.01
131.06
127.85
124.21
f1 (ppm)

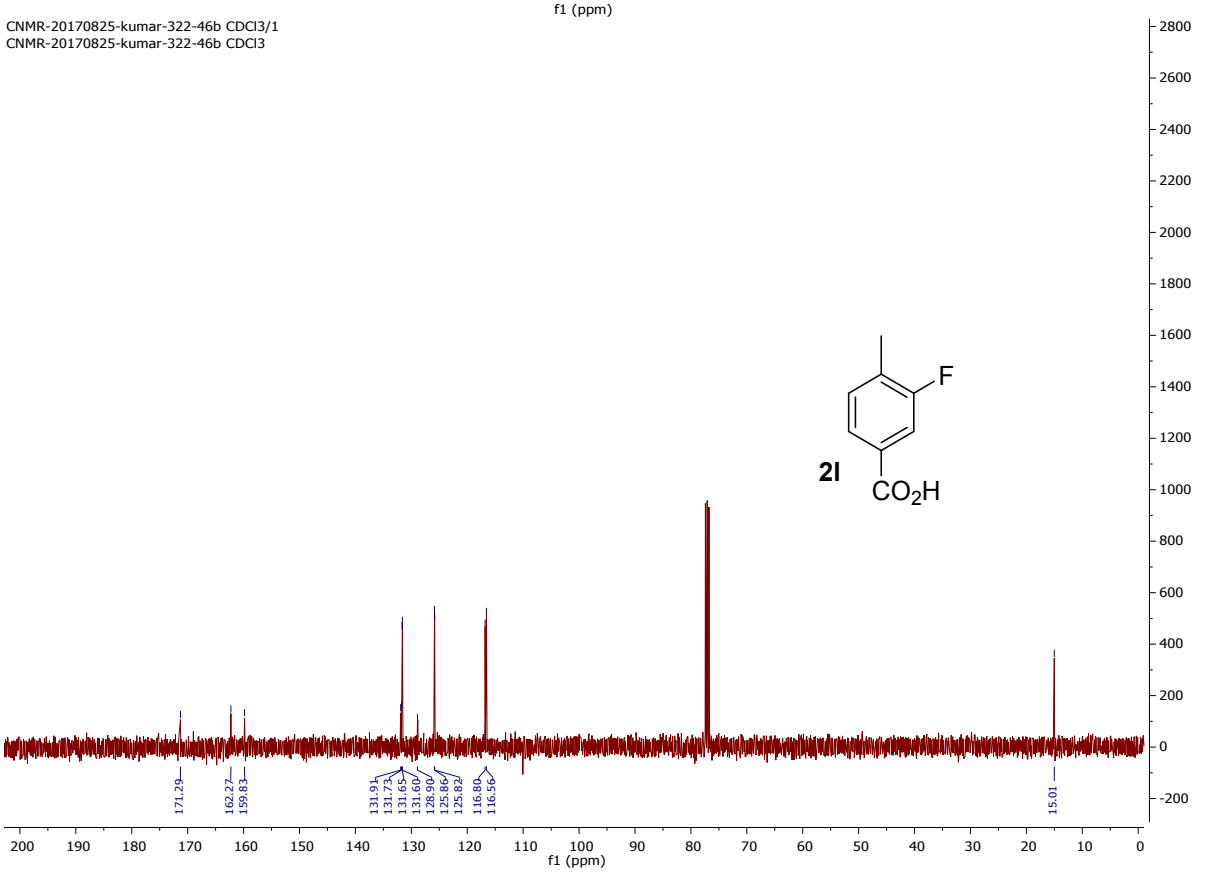
HNMR-20171122-KUMAR-322-91b.10.fid
PROTON DMSO {D:\NMR400\503} nmr 19

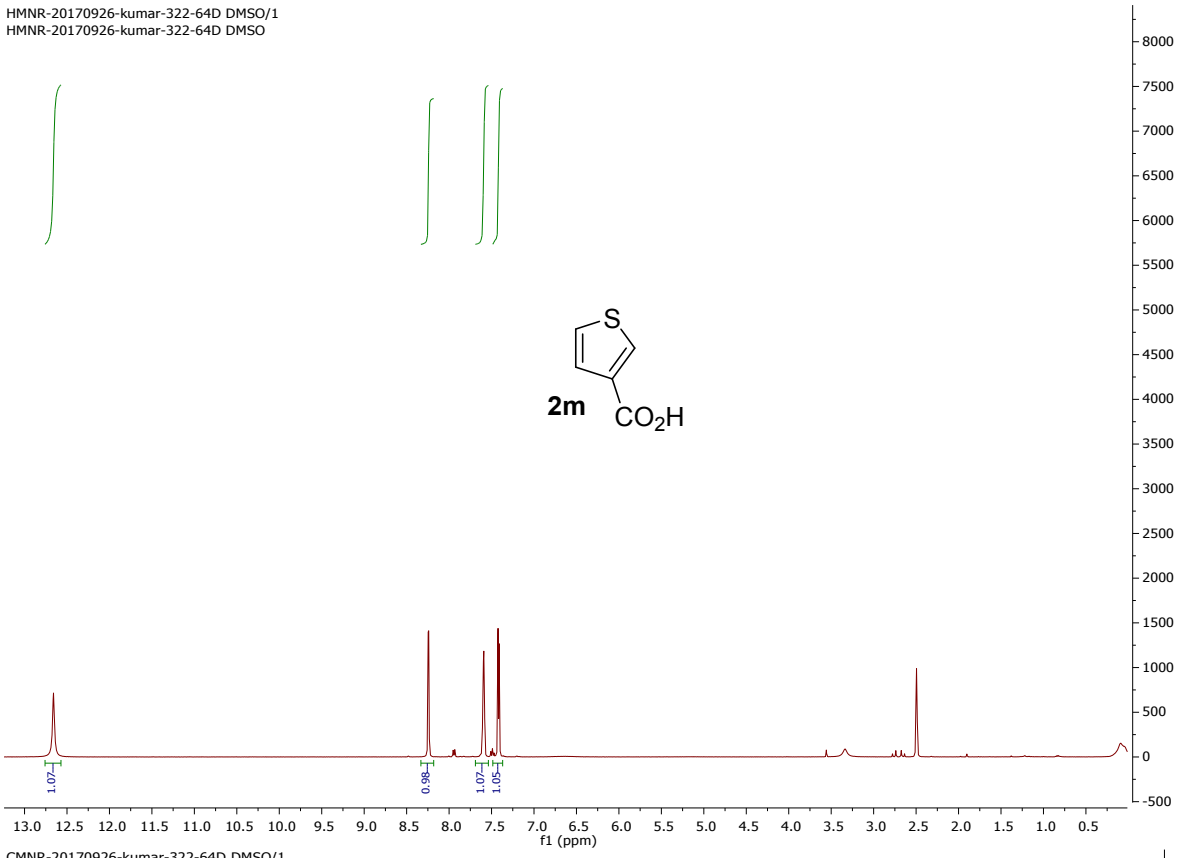


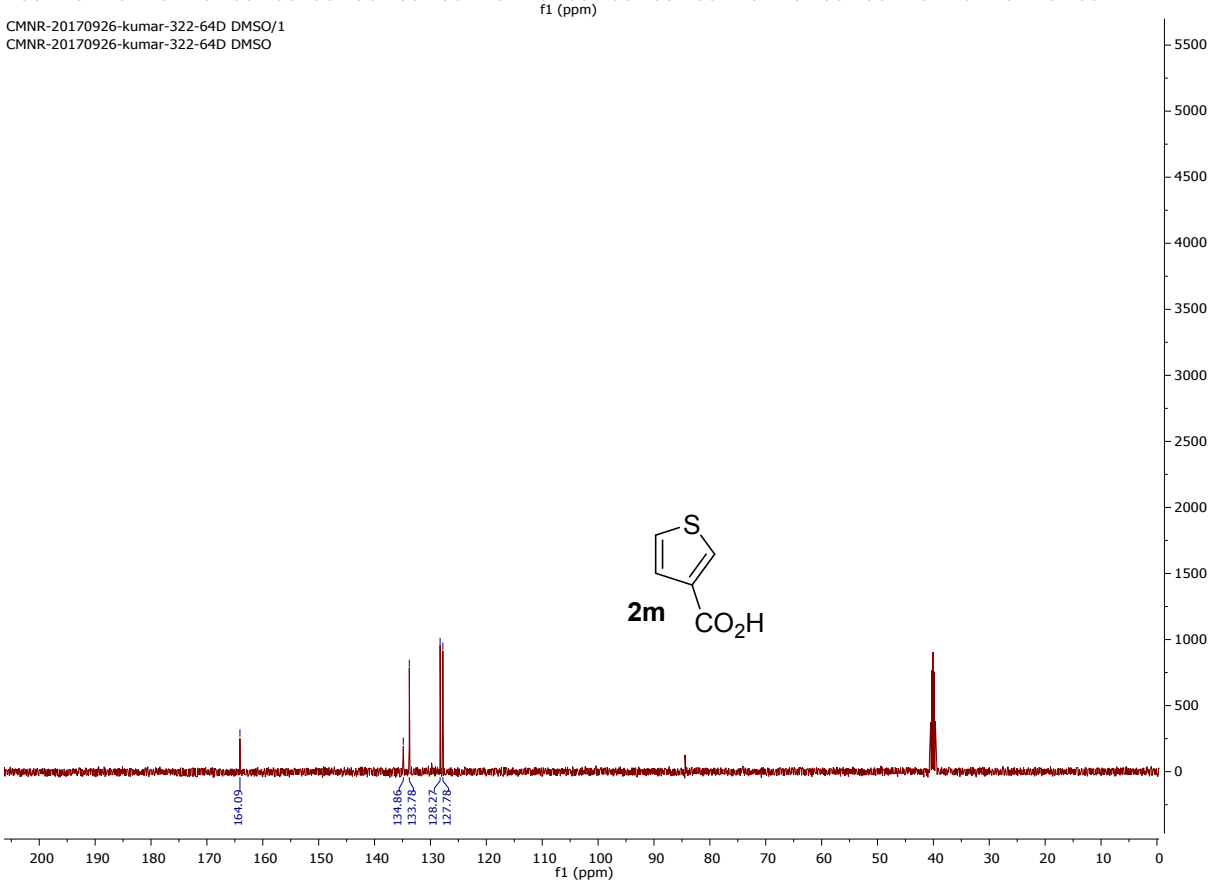
HNMR-20171122-KUMAR-322-91b.11.fid
C13CPD DMSO {D:\NMR400\503} nmr 19

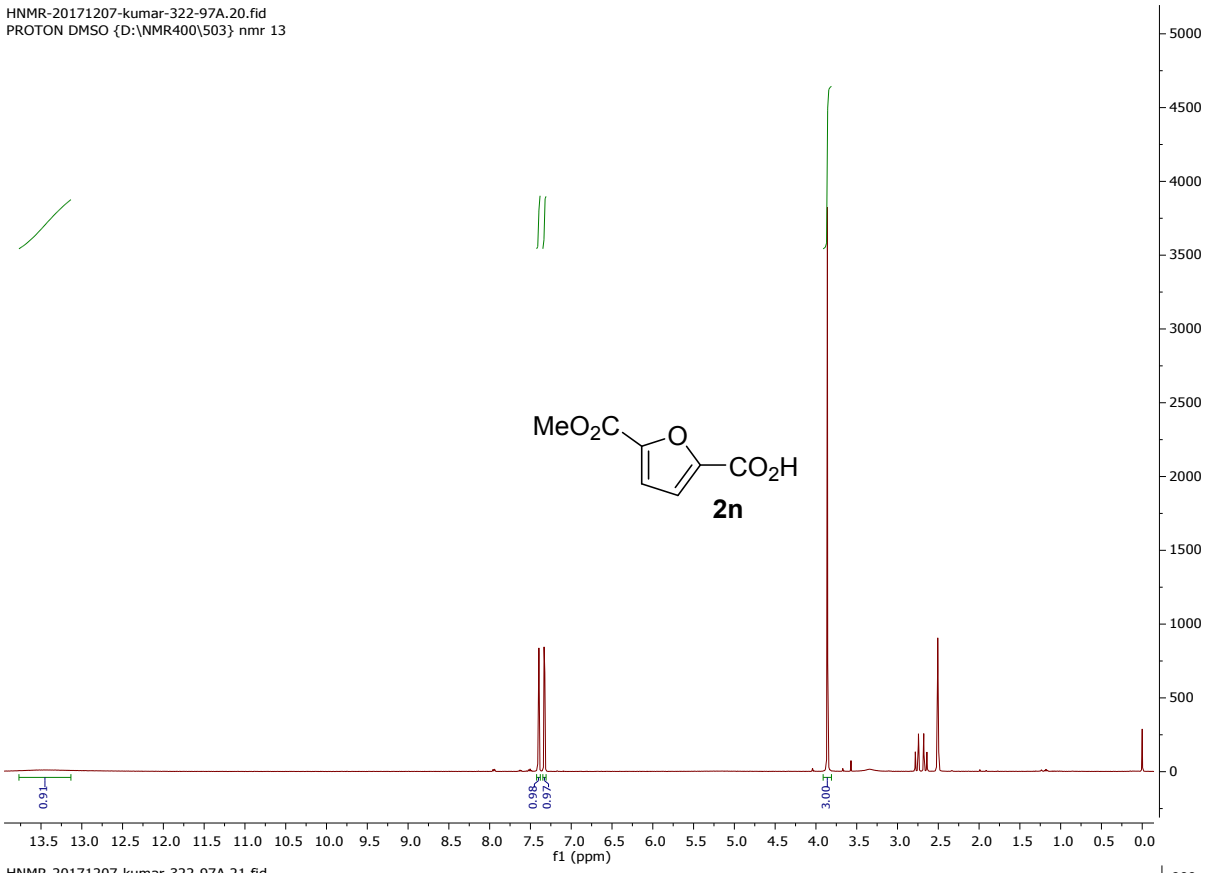


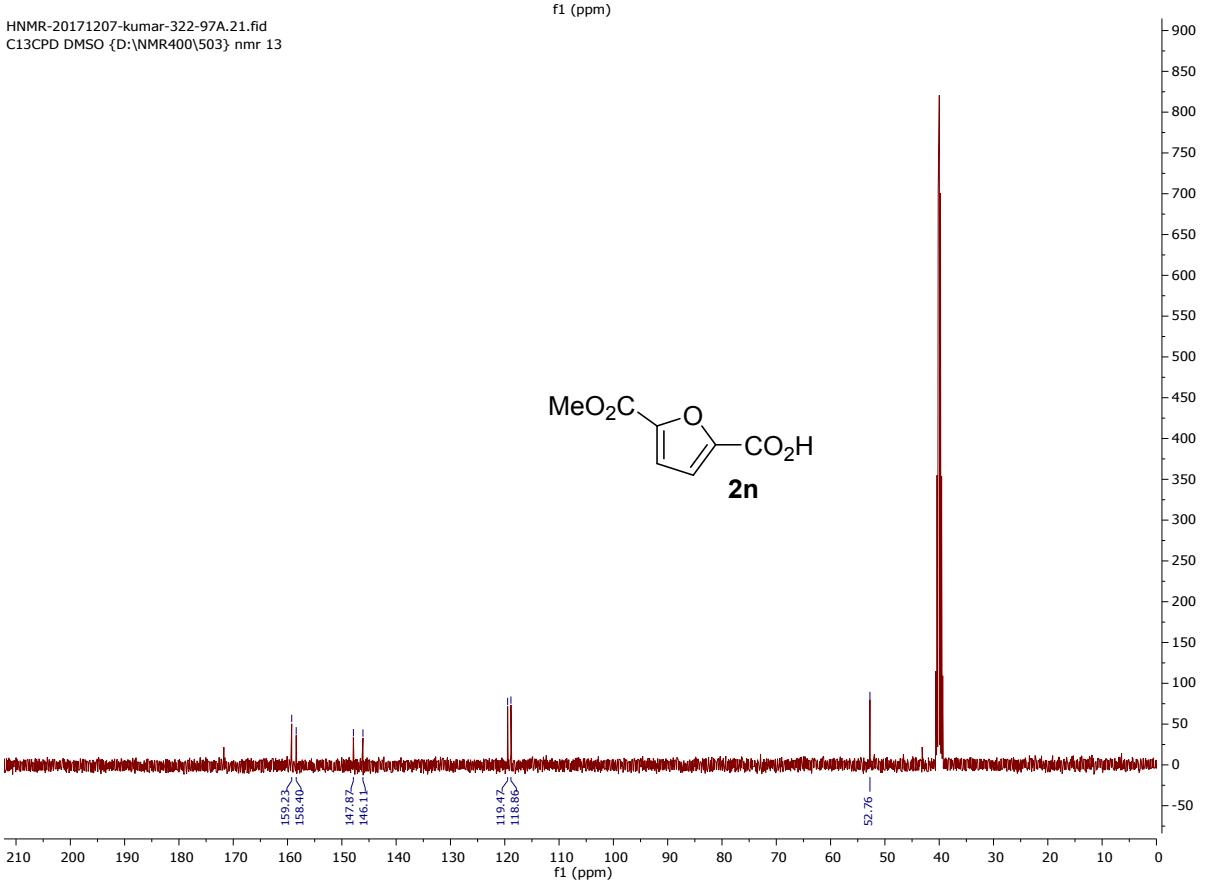

HNMR-20170825-kumar-322-46b CDCl3/1
HNMR-20170825-kumar-322-46b CDCl3
F
2l
CO2H
1.00
1.01
1.00
3.03
f1 (ppm)

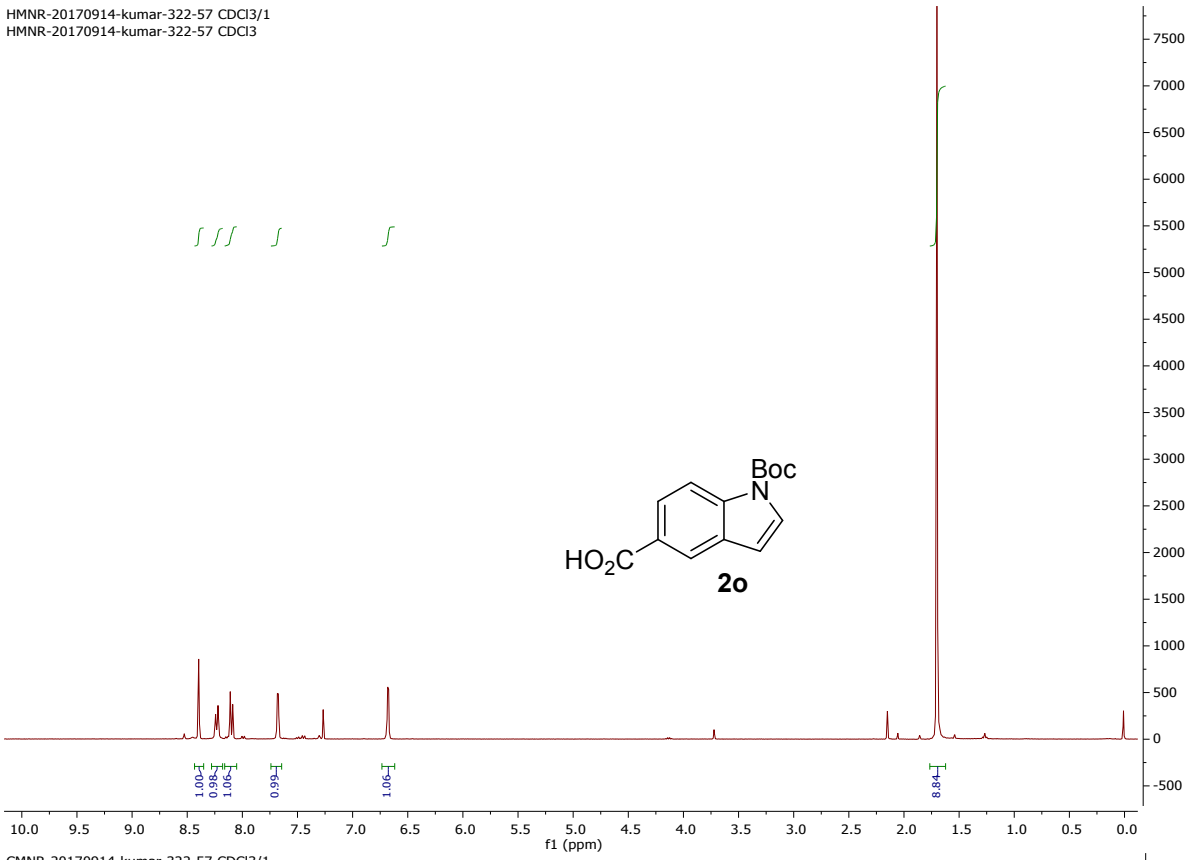

CNMR-20170825-kumar-322-46b CDCl3/1
CNMR-20170825-kumar-322-46b CDCl3
F
2l
CO2H
171.29
162.27
159.83
131.91
131.73
131.65
131.60
128.90
125.86
125.82
116.80
116.56
15.01
f1 (ppm)

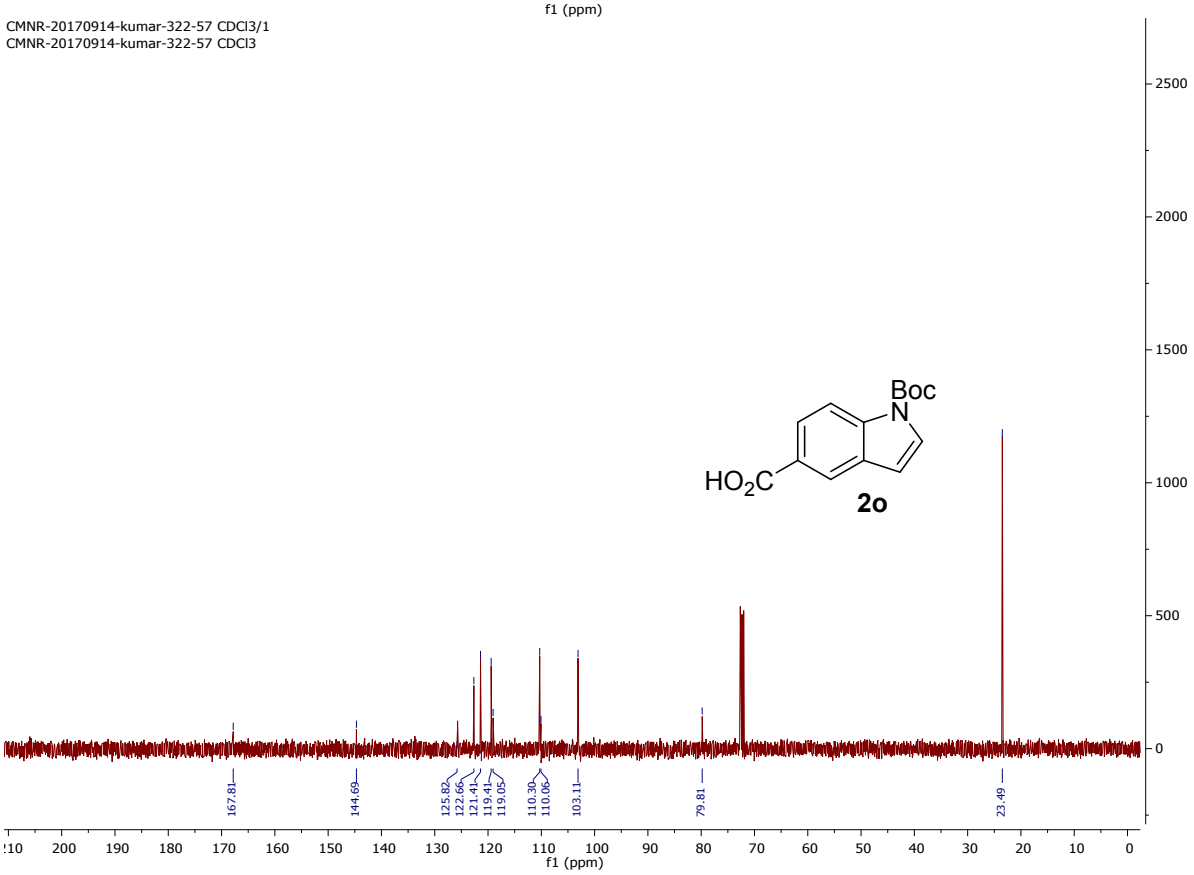

HMNR-20170926-kumar-322-64D DMSO/1
HMNR-20170926-kumar-322-64D DMSO
S
2m
CO2H
1.07
0.98
1.07
1.05
f1 (ppm)

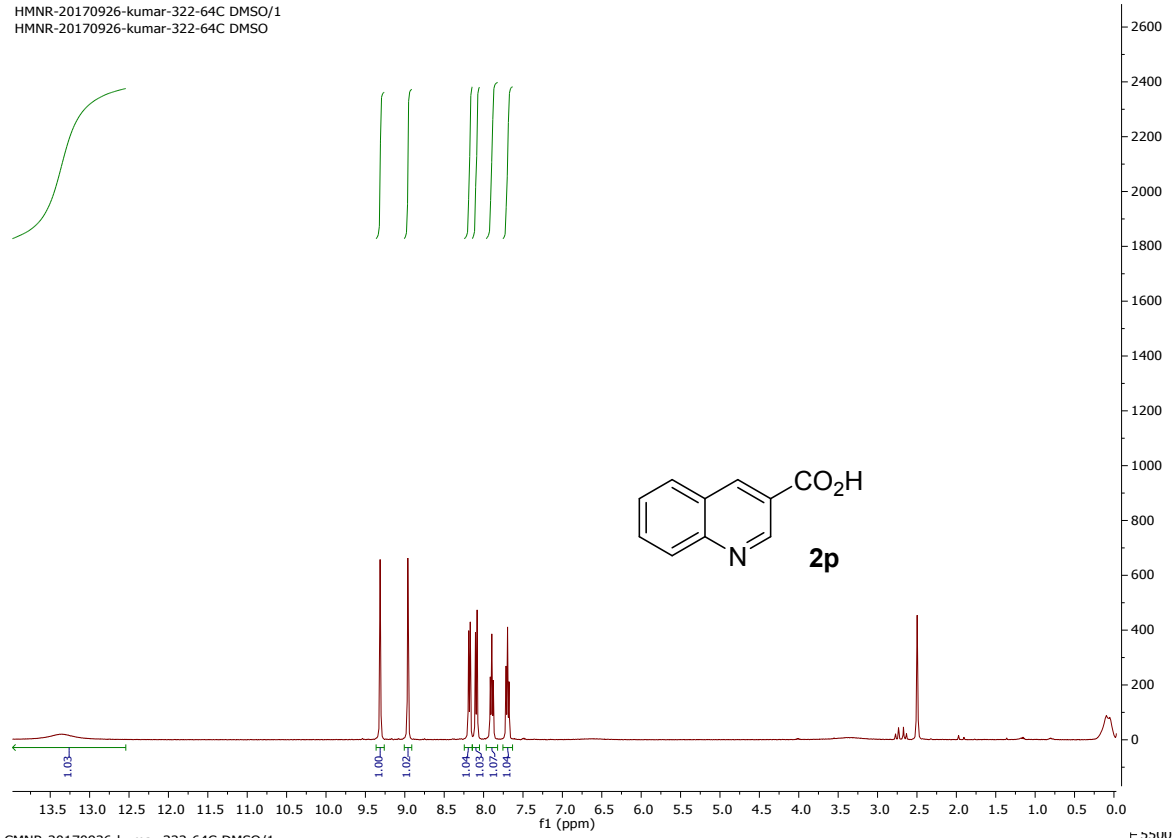

CMNR-20170926-kumar-322-64D DMSO/1
CMNR-20170926-kumar-322-64D DMSO
S
2m
CO2H
164.09
134.86
133.78
128.27
127.78
f1 (ppm)

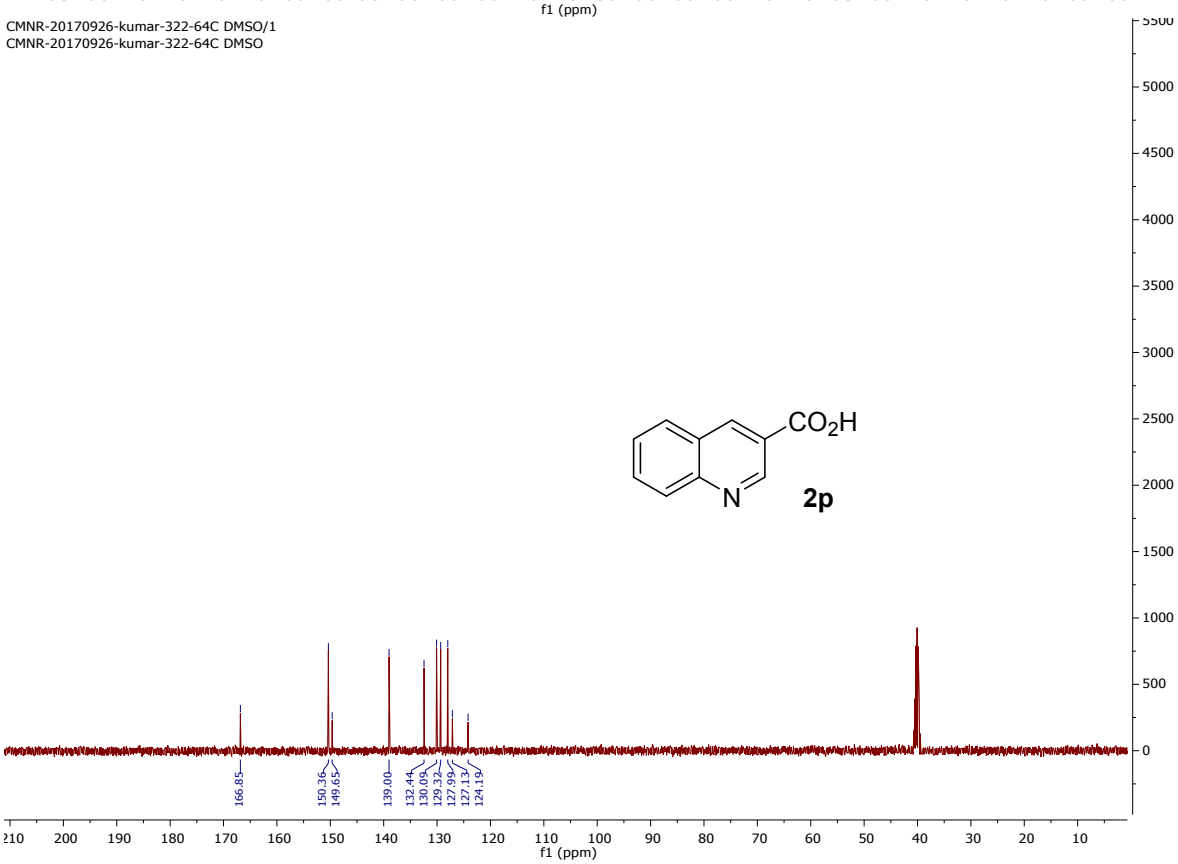

HNMR-20171207-kumar-322-97A.20.fid
PROTON DMSO {D:\NMR400\503} nmr 13
MeO2C
O
CO2H
2n
0.91
0.98
0.97
3.00
f1 (ppm)

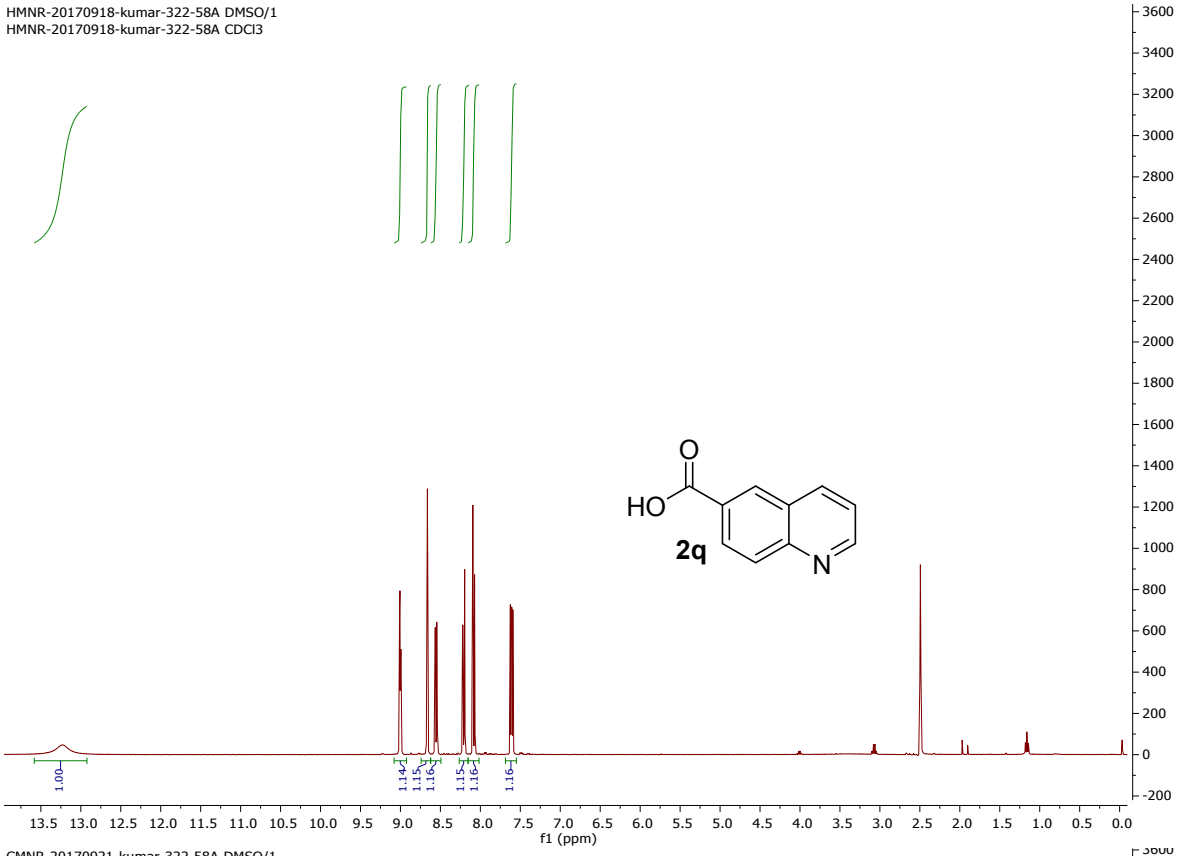

HNMR-20171207-kumar-322-97A.21.fid
C13CPD DMSO {D:\NMR400\503} nmr 13
MeO2C
O
CO2H
2n
159.23
158.40
147.87
146.11
119.47
118.86
52.76
f1 (ppm)

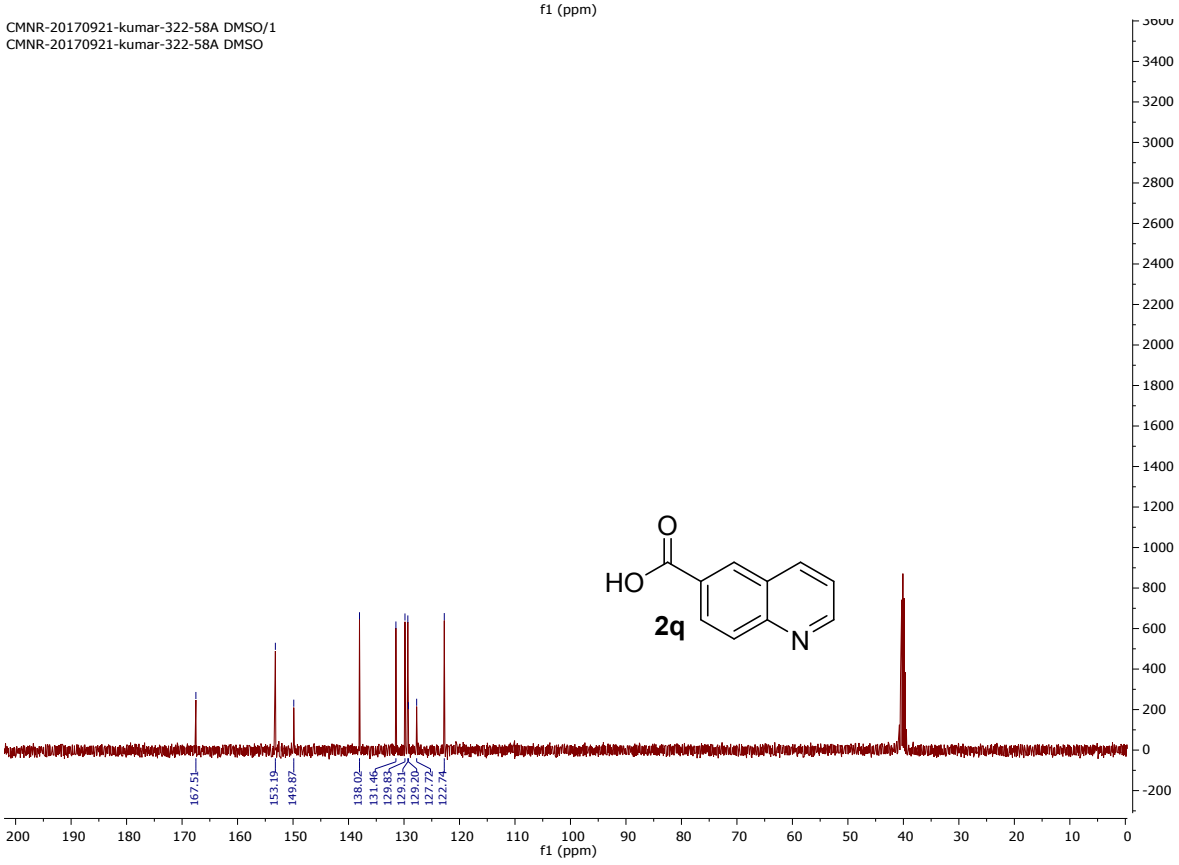

HMNR-20170914-kumar-322-57 CDCl3/1
HMNR-20170914-kumar-322-57 CDCl3
Boc
N
HO2C
2o
1.00
0.98
1.06
0.99
1.06
8.84
f1 (ppm)

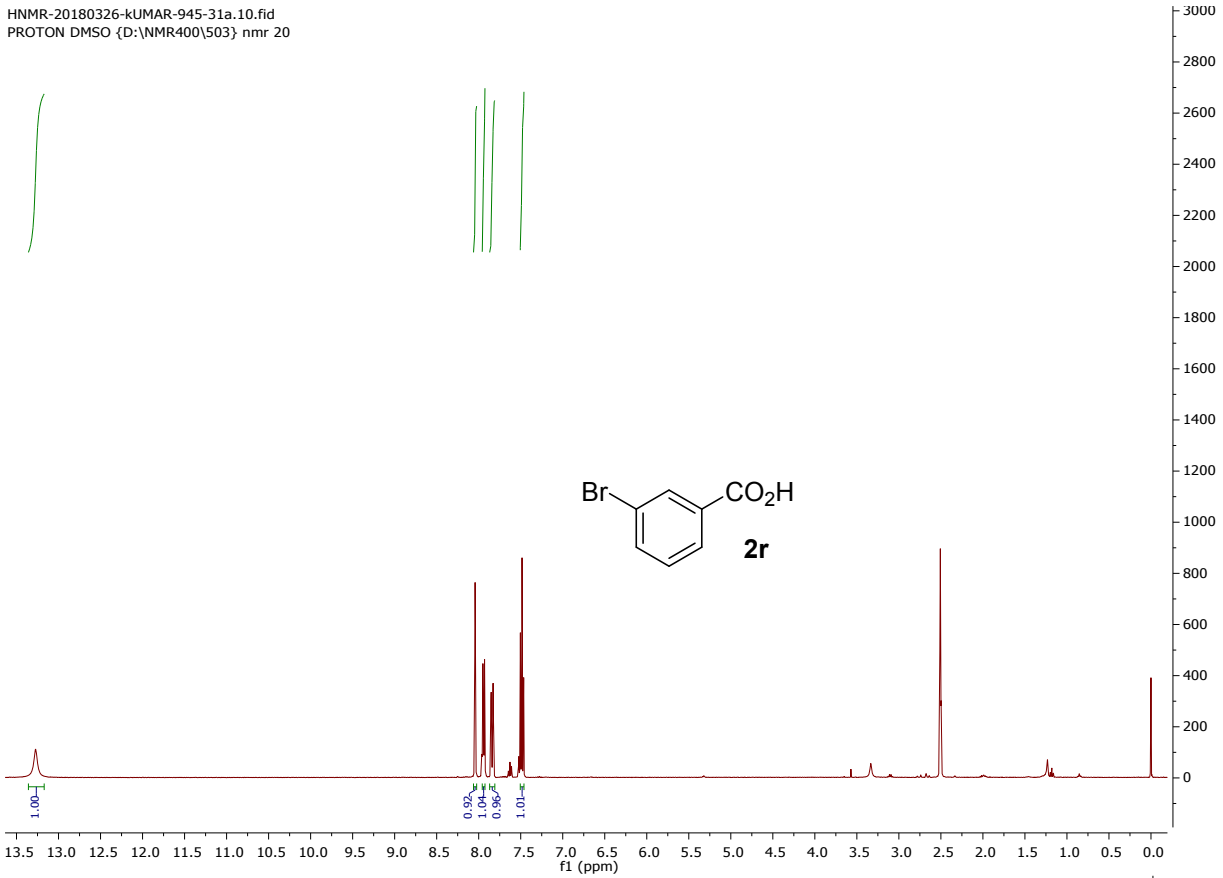

CMNR-20170914-kumar-322-57 CDCl3/1
CMNR-20170914-kumar-322-57 CDCl3
Boc
N
HO2C
2o
167.81
144.69
125.82
122.66
121.41
119.41
119.05
110.30
110.06
103.11
79.81
23.49
f1 (ppm)

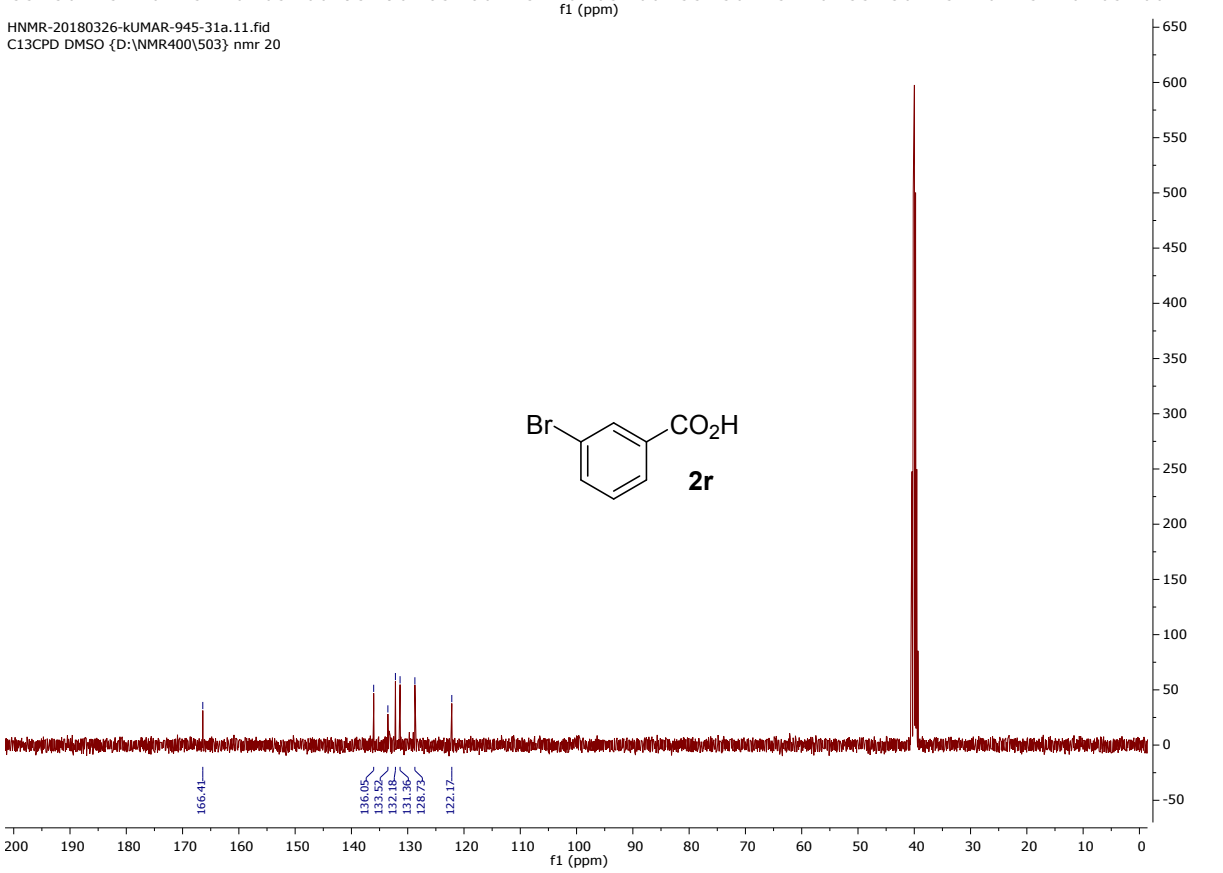

HMNR-20170926-kumar-322-64C DMSO/1
HMNR-20170926-kumar-322-64C DMSO
CO2H
N
2p
1.03
1.00
1.02
1.04
1.03
1.07
1.04
f1 (ppm)

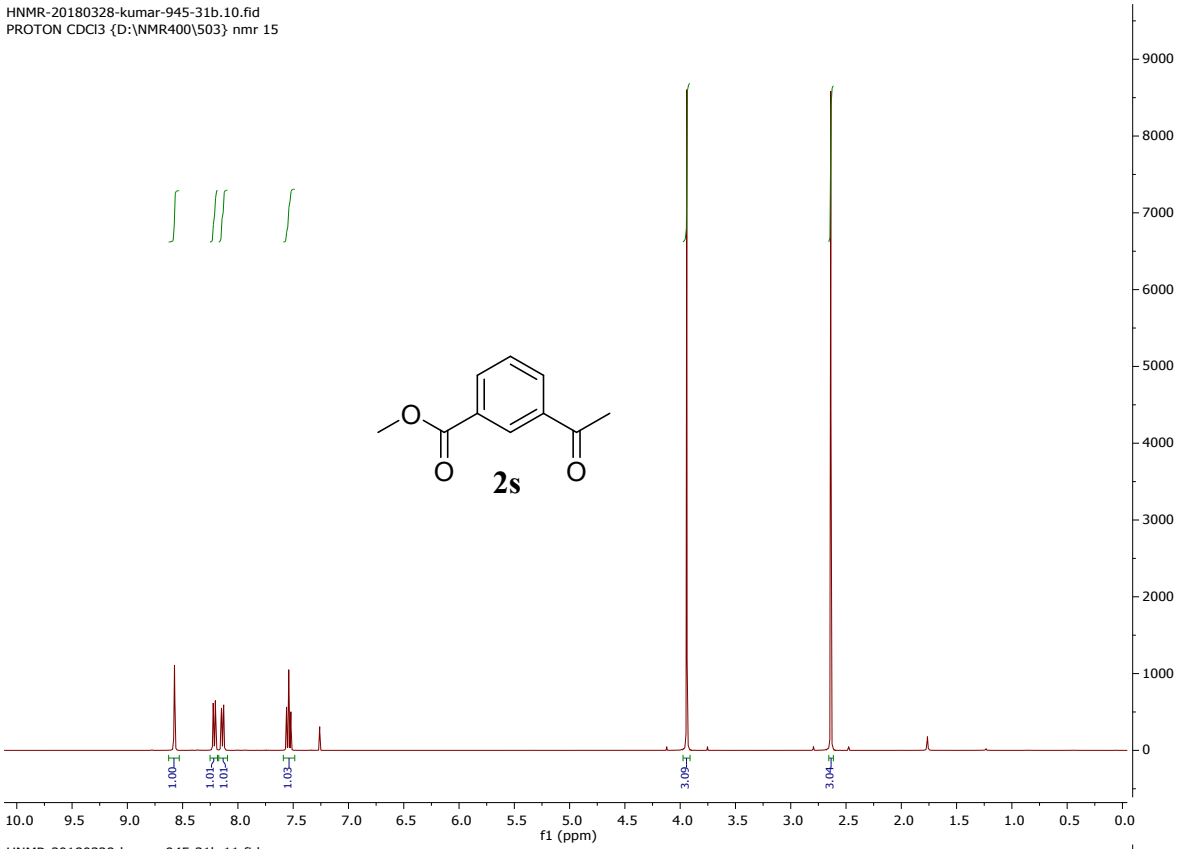

CMNR-20170926-kumar-322-64C DMSO/1
CMNR-20170926-kumar-322-64C DMSO
CO2H
N
2p
166.85
150.36
149.65
139.00
132.44
130.09
129.32
127.99
127.13
124.19
f1 (ppm)

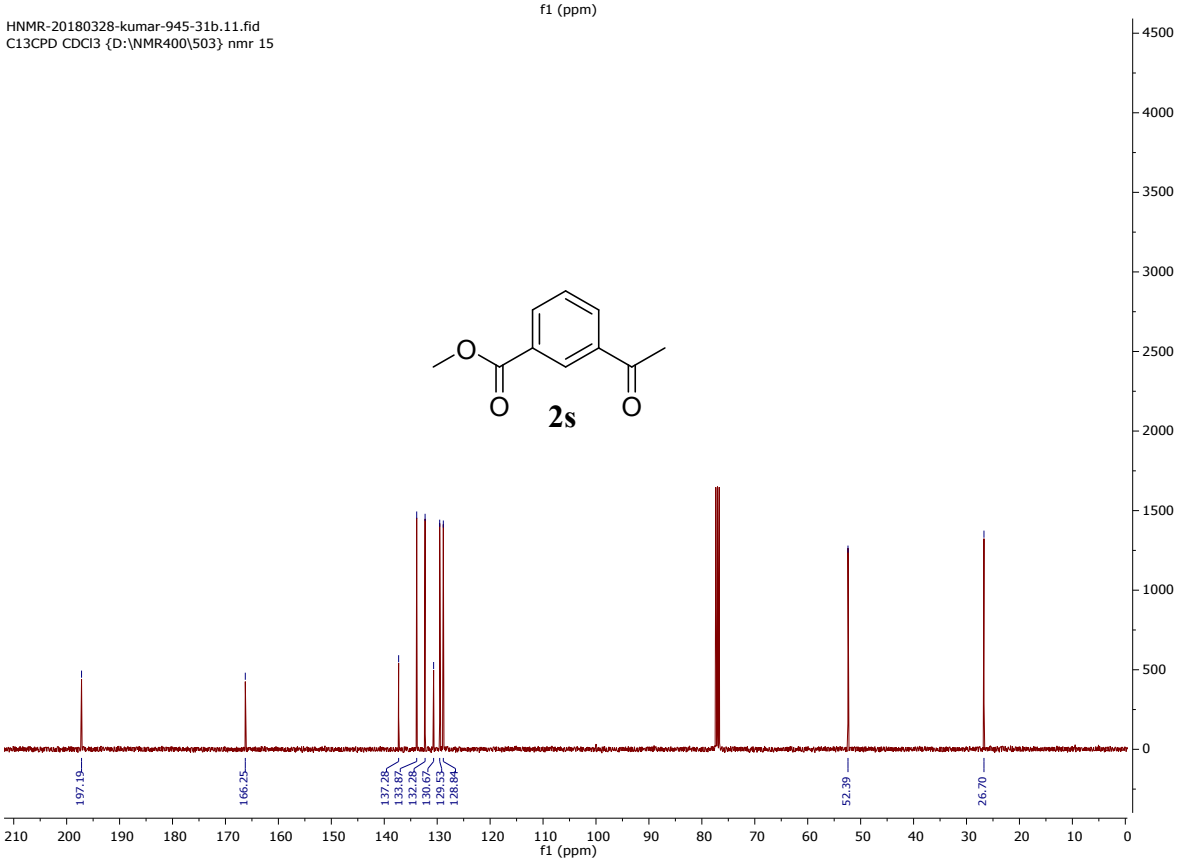

HMNR-20170918-kumar-322-58A DMSO/1
HMNR-20170918-kumar-322-58A CDCl3
HO
O
N
2q
1.00
1.14
1.15
1.16
1.15
1.16
1.16
f1 (ppm)

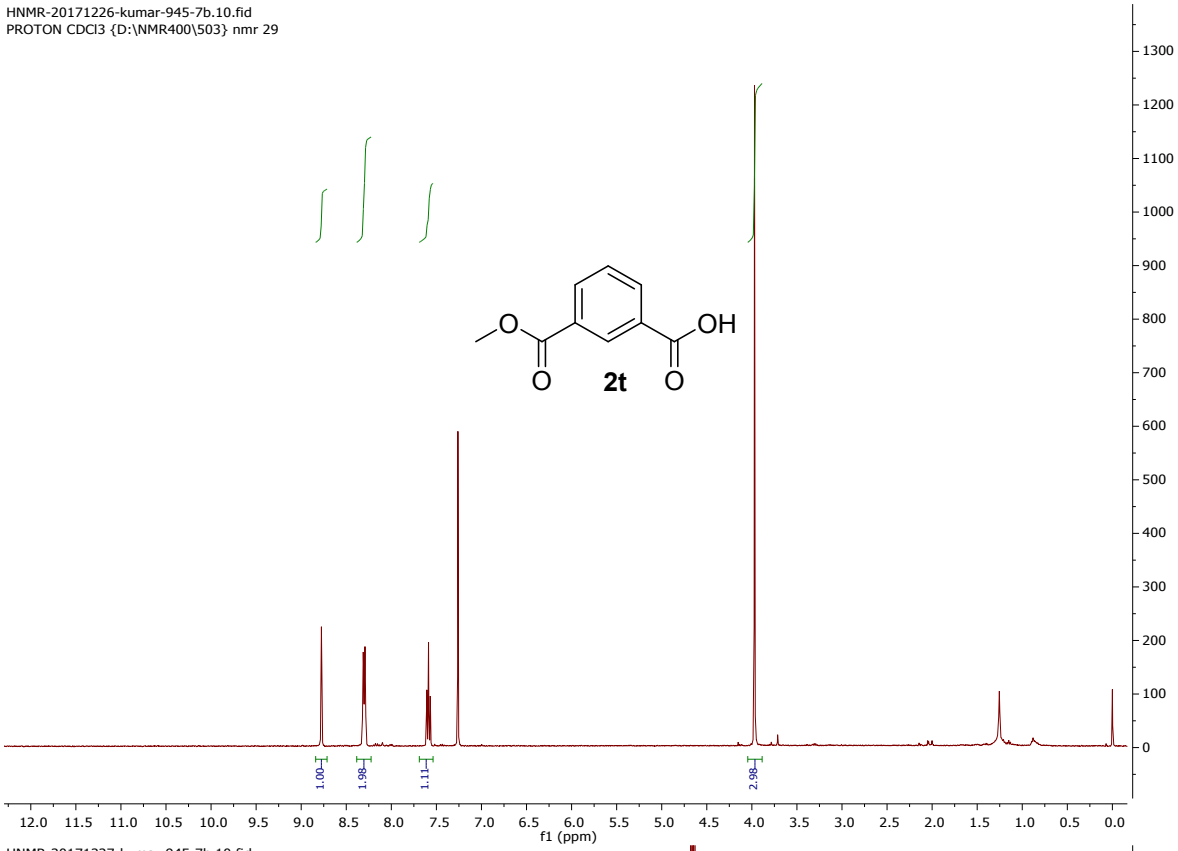

CMNR-20170921-kumar-322-58A DMSO/1
CMNR-20170921-kumar-322-58A DMSO
HO
O
N
2q
167.51
153.19
149.87
138.02
131.46
129.83
129.31
129.20
127.72
122.74
f1 (ppm)

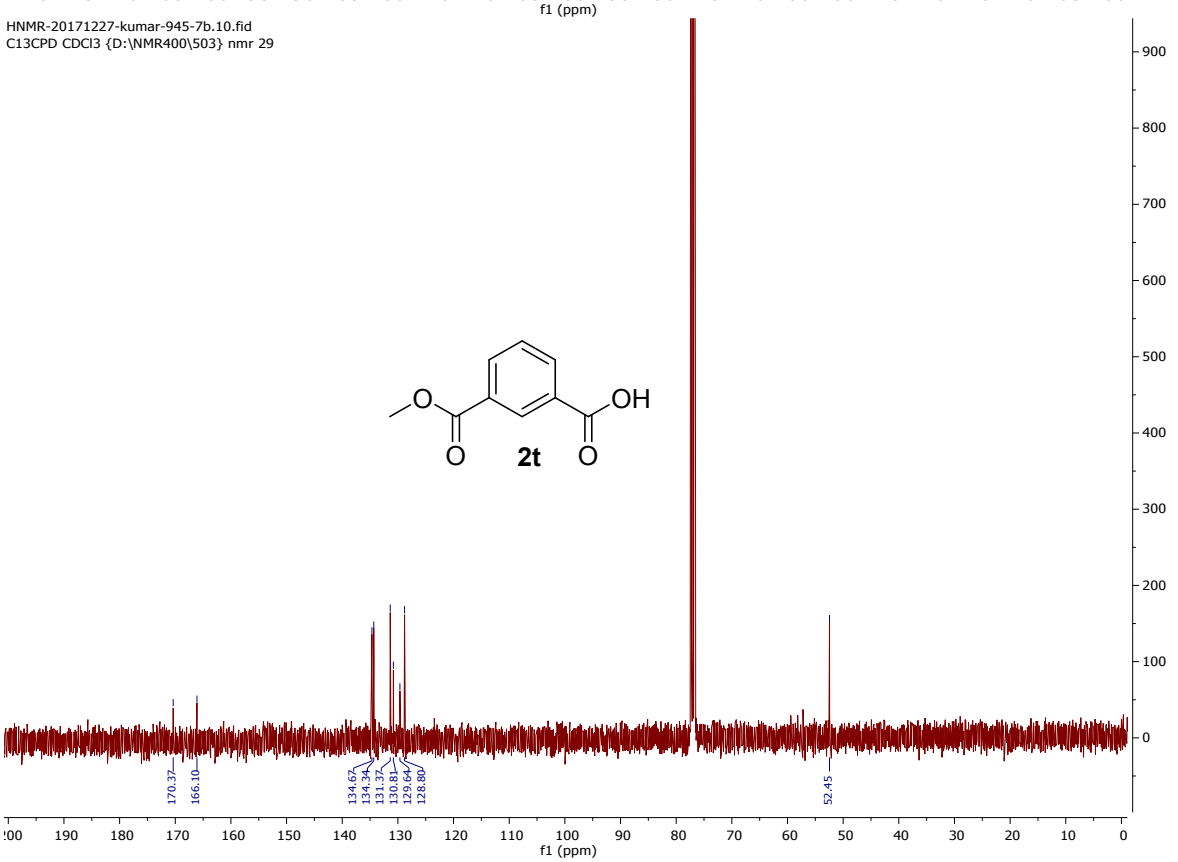

HNMR-20180326-kUMAR-945-31a.10.fid
PROTON DMSO {D:\NMR400\503} nmr 20
Br
CO2H
2r
1.00
0.92
1.04
0.96
1.01
f1 (ppm)

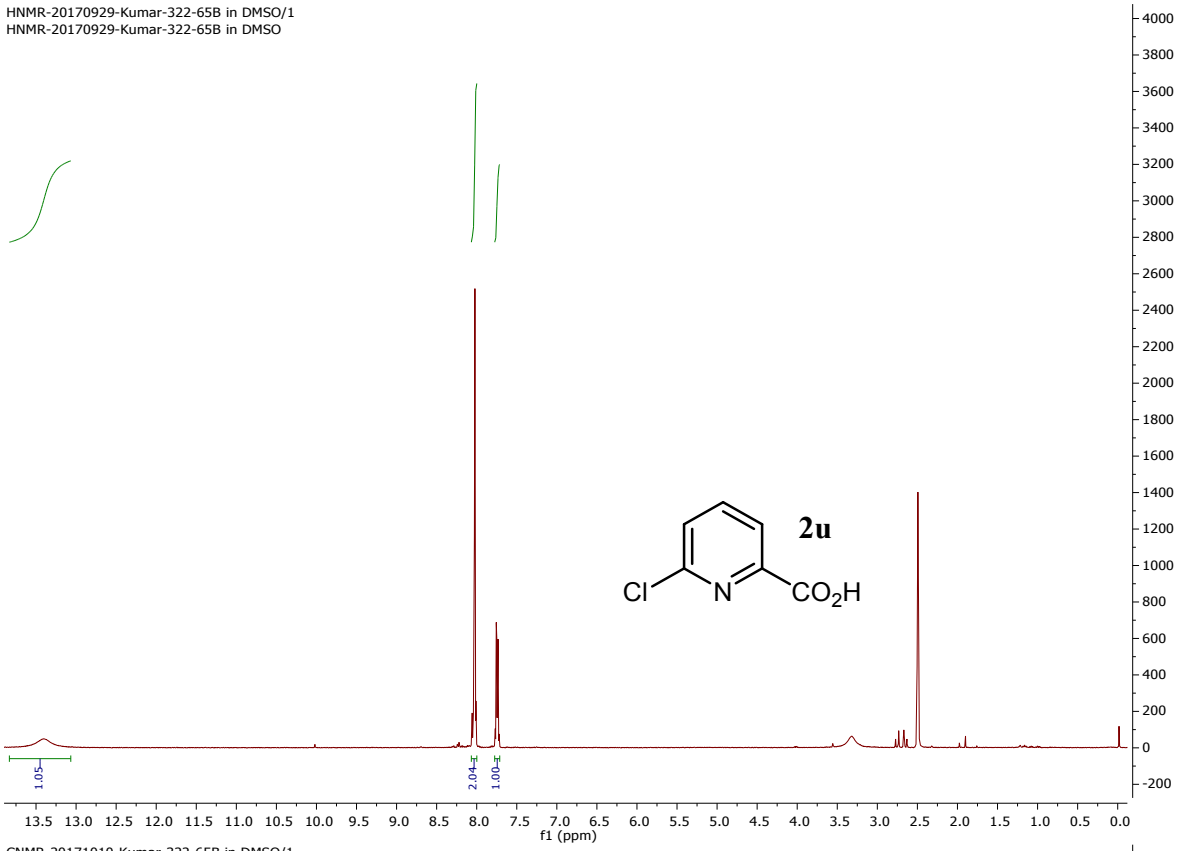

HNMR-20180326-kUMAR-945-31a.11.fid
C13CPD DMSO {D:\NMR400\503} nmr 20
Br
CO2H
2r
166.41
136.05
133.52
132.18
131.36
128.73
122.17
f1 (ppm)

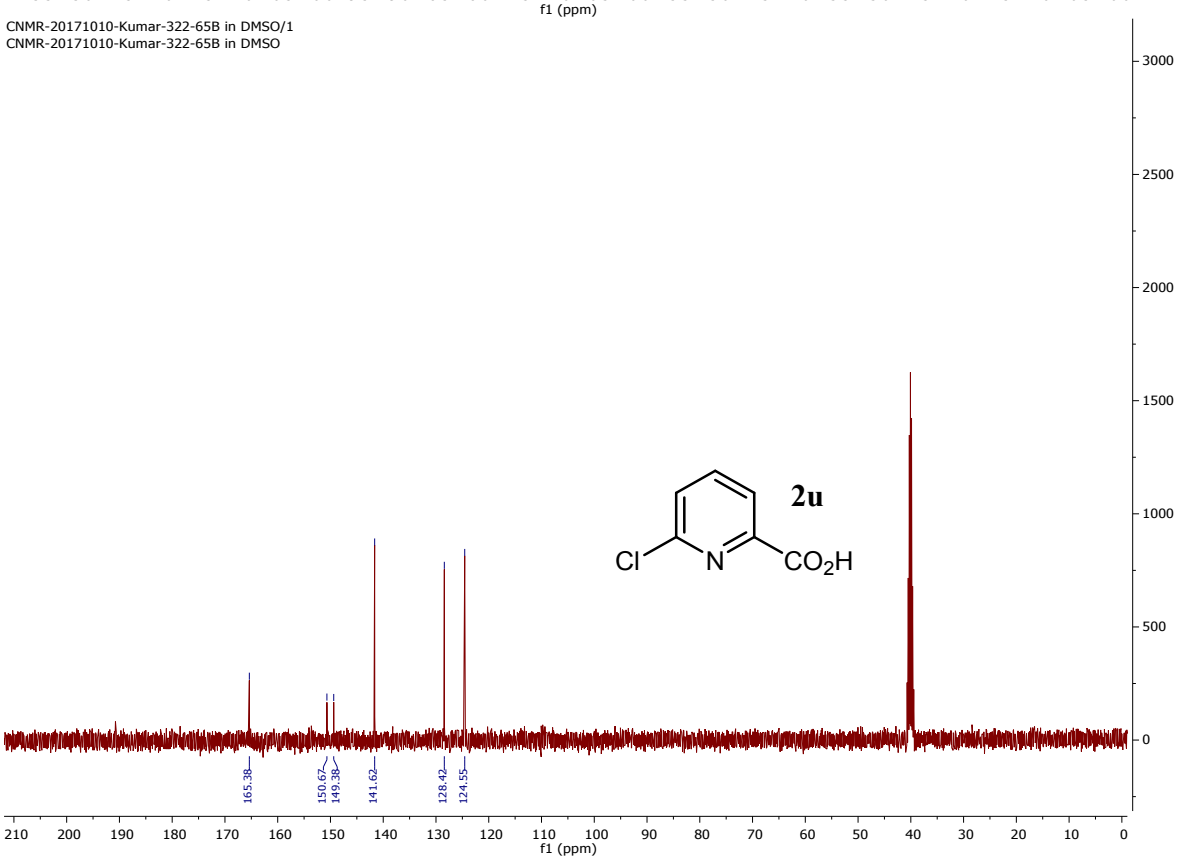

HNMR-20180328-kumar-945-31b.10.fid
PROTON CDCl3 {D:\NMR400\503} nmr 15
2s
1.00
1.01
1.01
1.03
3.09
3.04
f1 (ppm)

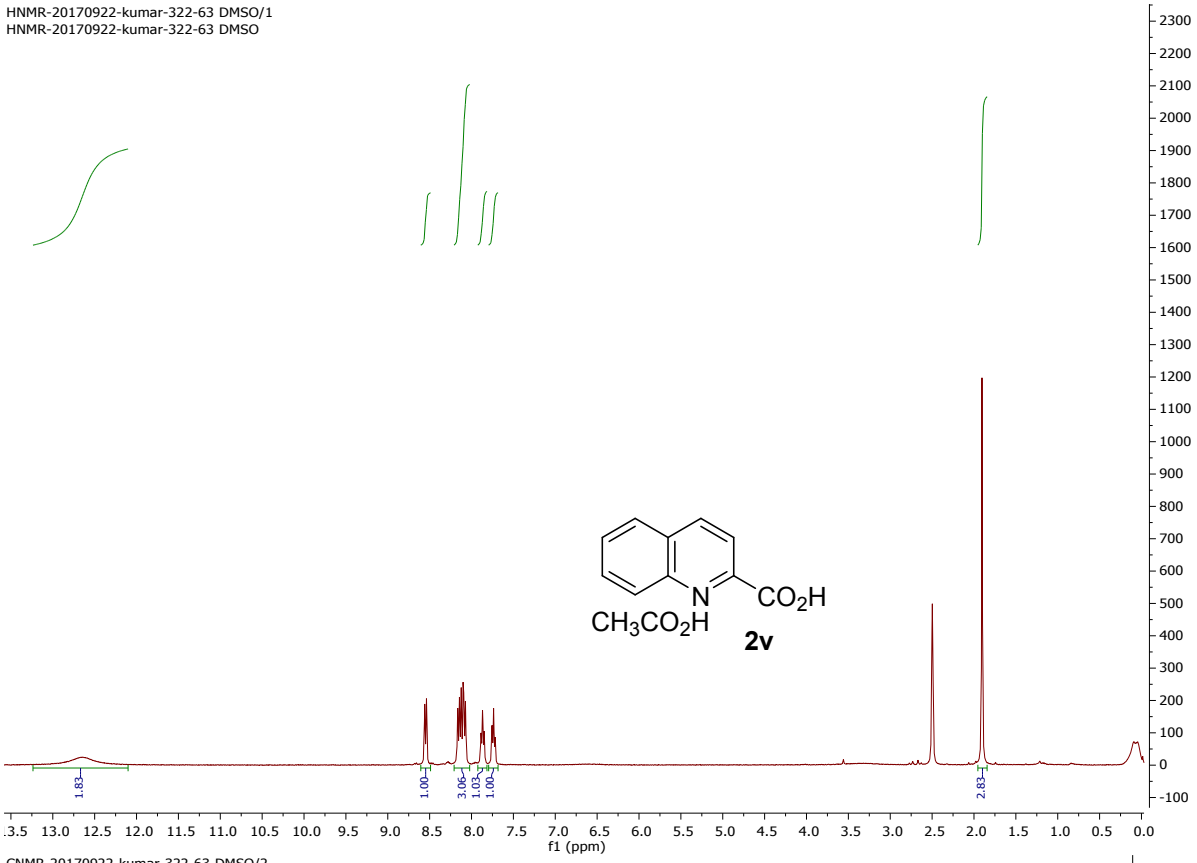

HNMR-20180328-kumar-945-31b.11.fid
C13CPD CDCl3 {D:\NMR400\503} nmr 15
2s
197.19
166.25
137.28
133.82
132.28
130.67
129.53
128.84
52.39
26.70
f1 (ppm)

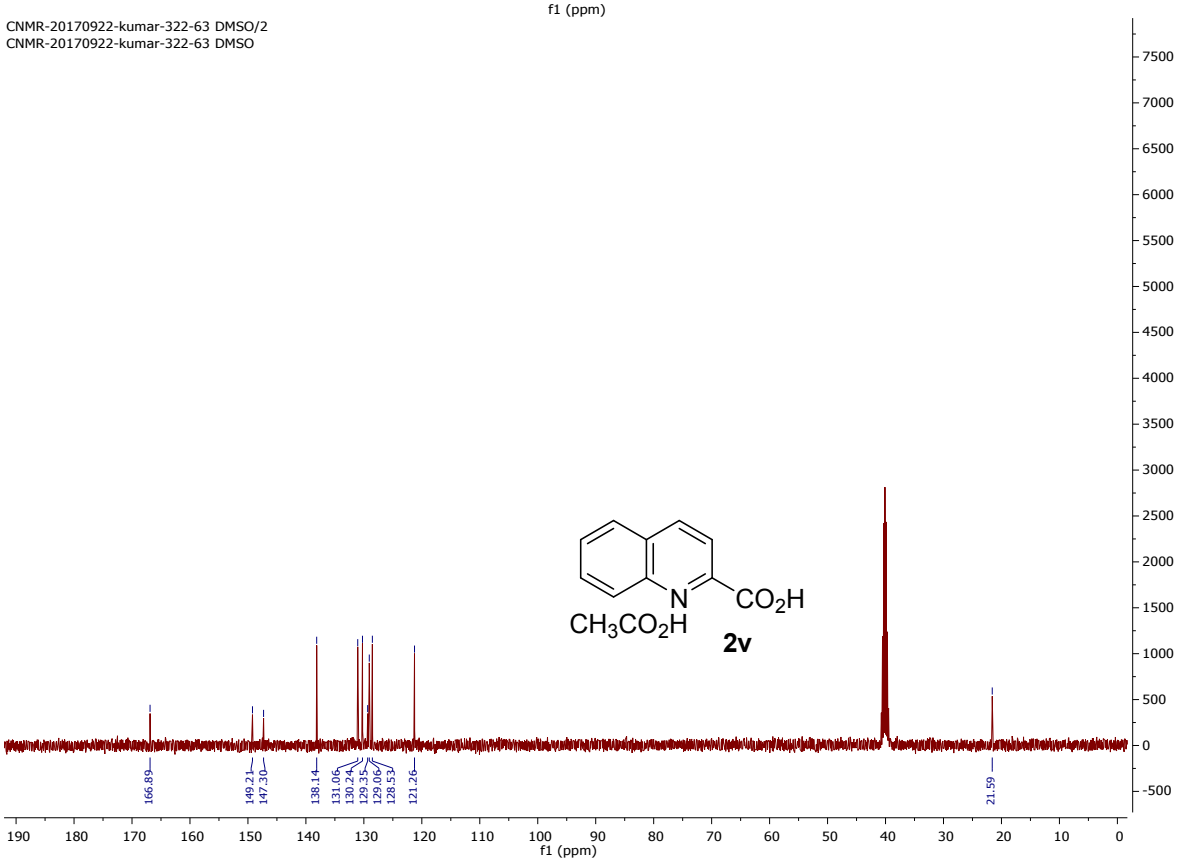

HNMR-20171226-kumar-945-7b.10.fid
PROTON CDCl3 {D:\NMR400\503} nmr 29
O
OH
O
2t
O
1.00
1.98
1.11
2.98
f1 (ppm)

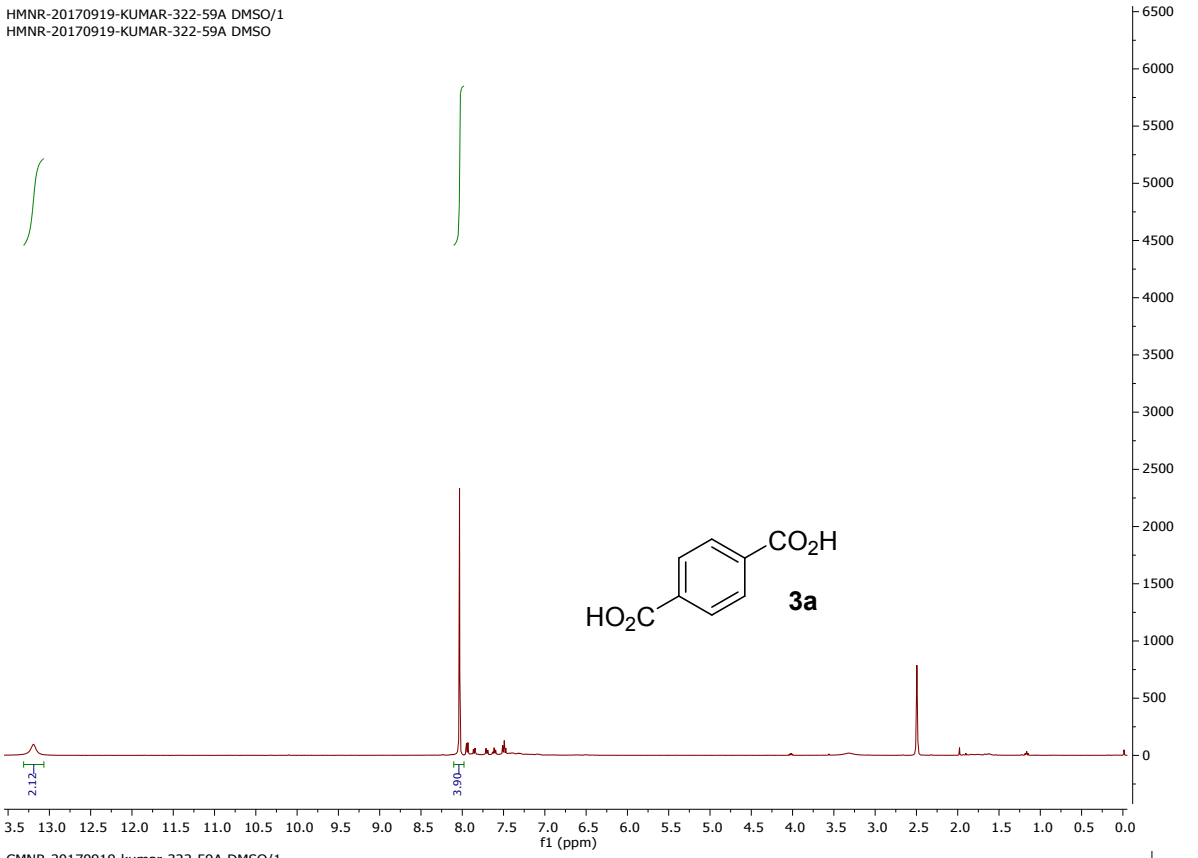

HNMR-20171227-kumar-945-7b.10.fid
C13CPD CDCl3 {D:\NMR400\503} nmr 29
O
OH
O
2t
O
170.37
166.10
134.67
134.34
131.37
130.81
129.64
128.80
52.45
f1 (ppm)

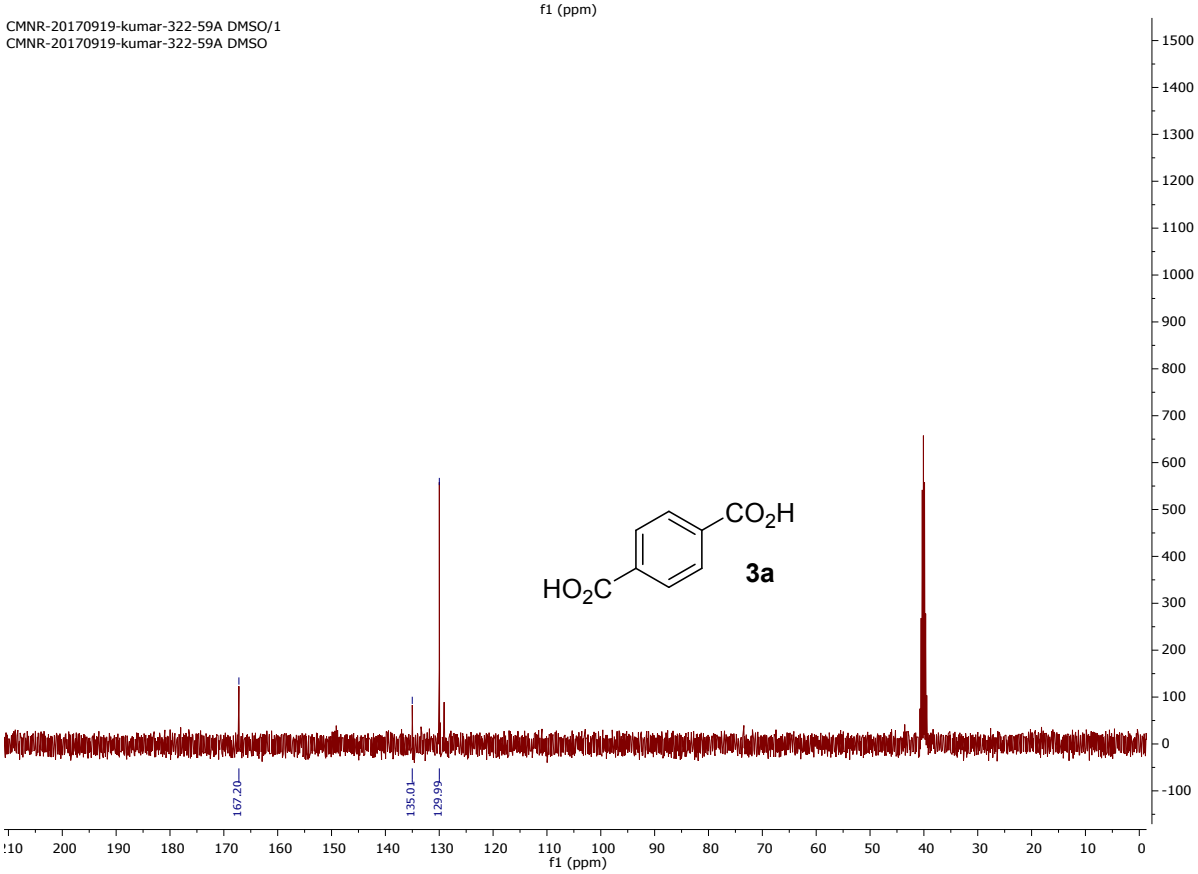

HNMR-20170929-Kumar-322-65B in DMSO/1
HNMR-20170929-Kumar-322-65B in DMSO
2u
Cl
N
CO2H
1.05
2.04
1.00
f1 (ppm)


CNMR-20171010-Kumar-322-65B in DMSO/1
CNMR-20171010-Kumar-322-65B in DMSO
2u
Cl
N
CO2H
165.38
150.67
149.38
141.62
128.42
124.55
f1 (ppm)

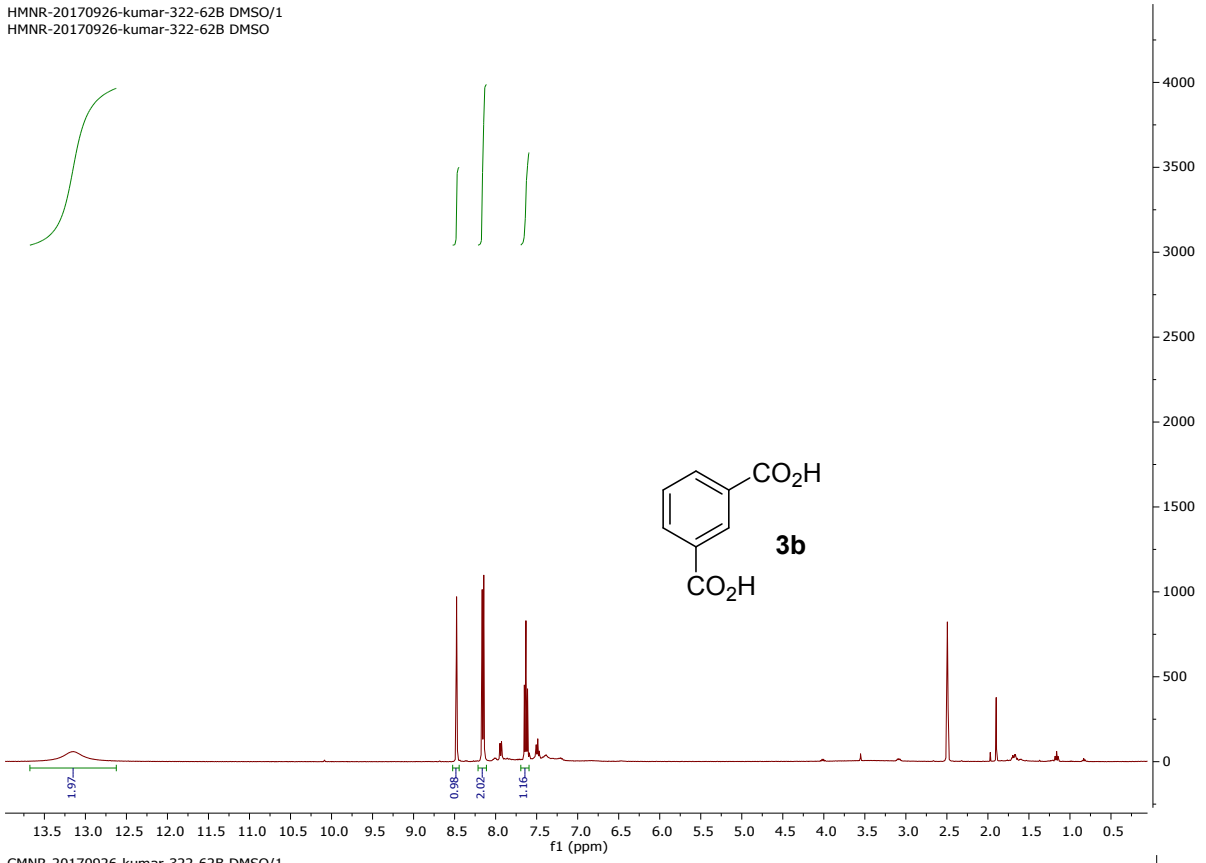

HNMR-20170922-kumar-322-63 DMSO/1
HNMR-20170922-kumar-322-63 DMSO
CO2H
N
CH3CO2H
2v
1.83
1.00
3.06
1.03
1.00
2.83
f1 (ppm)


CNMR-20170922-kumar-322-63 DMSO/2
CNMR-20170922-kumar-322-63 DMSO
CO2H
N
CH3CO2H
2v
166.89
149.21
147.30
138.14
131.06
130.24
129.35
129.06
128.53
121.26
21.59
f1 (ppm)

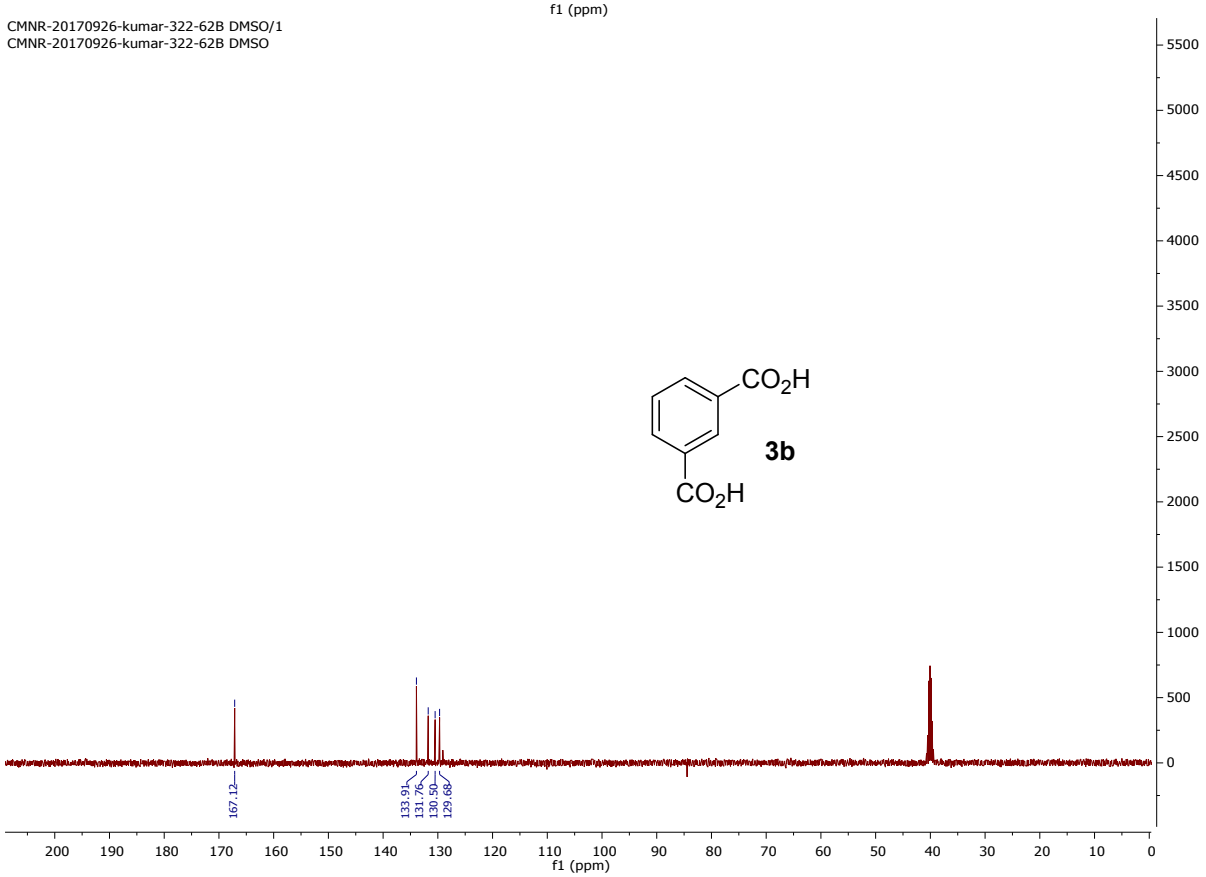

HMNR-20170919-KUMAR-322-59A DMSO/1
HMNR-20170919-KUMAR-322-59A DMSO
CO2H
HO2C
3a
2.12
3.90
f1 (ppm)

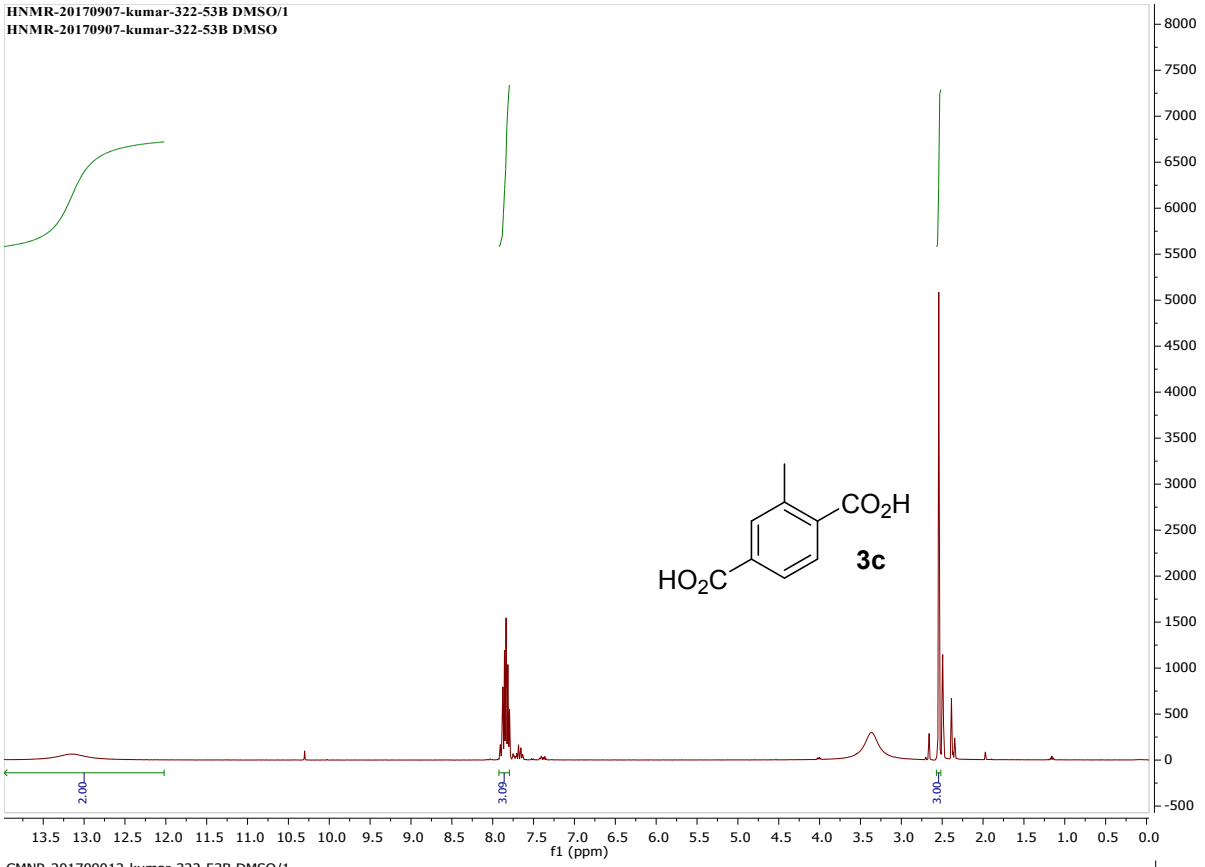

CMNR-20170919-kumar-322-59A DMSO/1
CMNR-20170919-kumar-322-59A DMSO
CO2H
HO2C
3a
167.20
135.01
129.99
f1 (ppm)

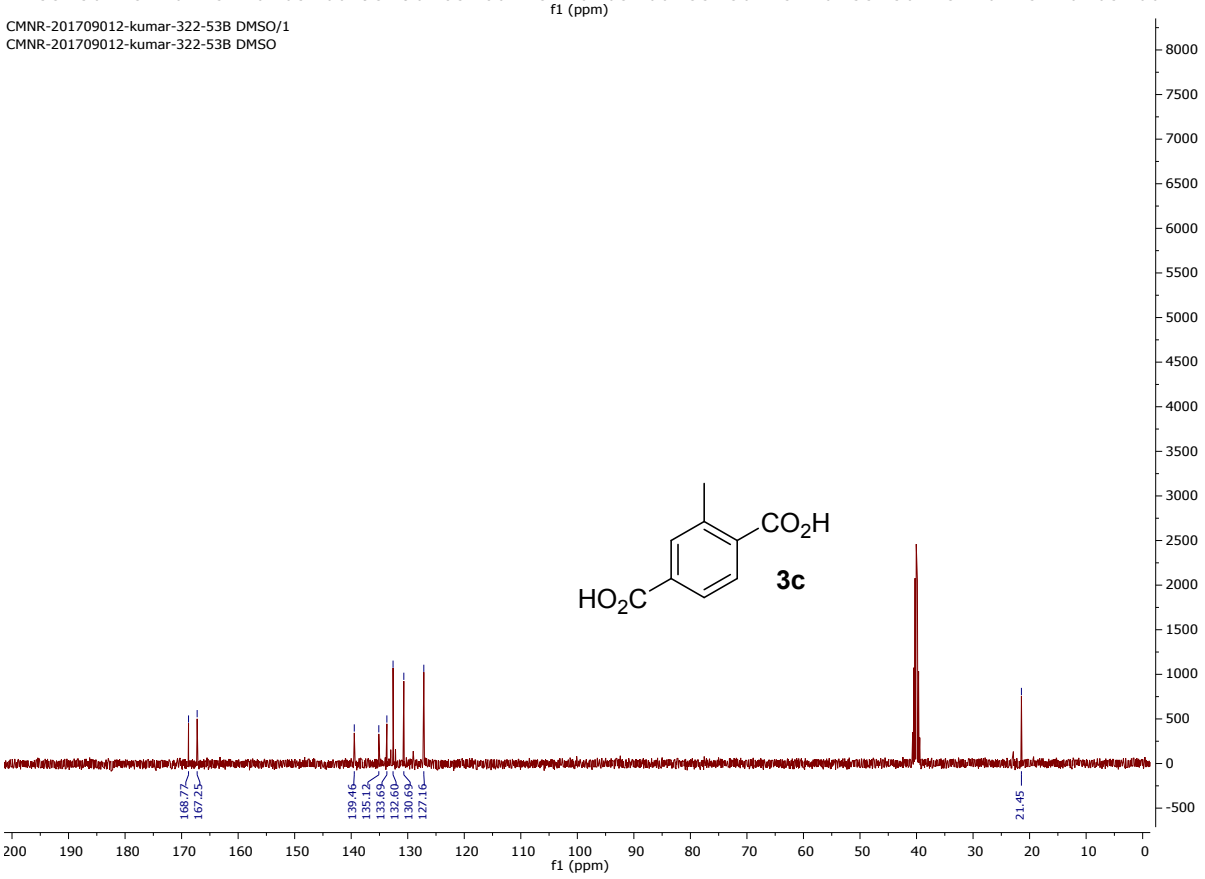
HMNR-20170926-kumar-322-62B DMSO/1
HMNR-20170926-kumar-322-62B DMSO

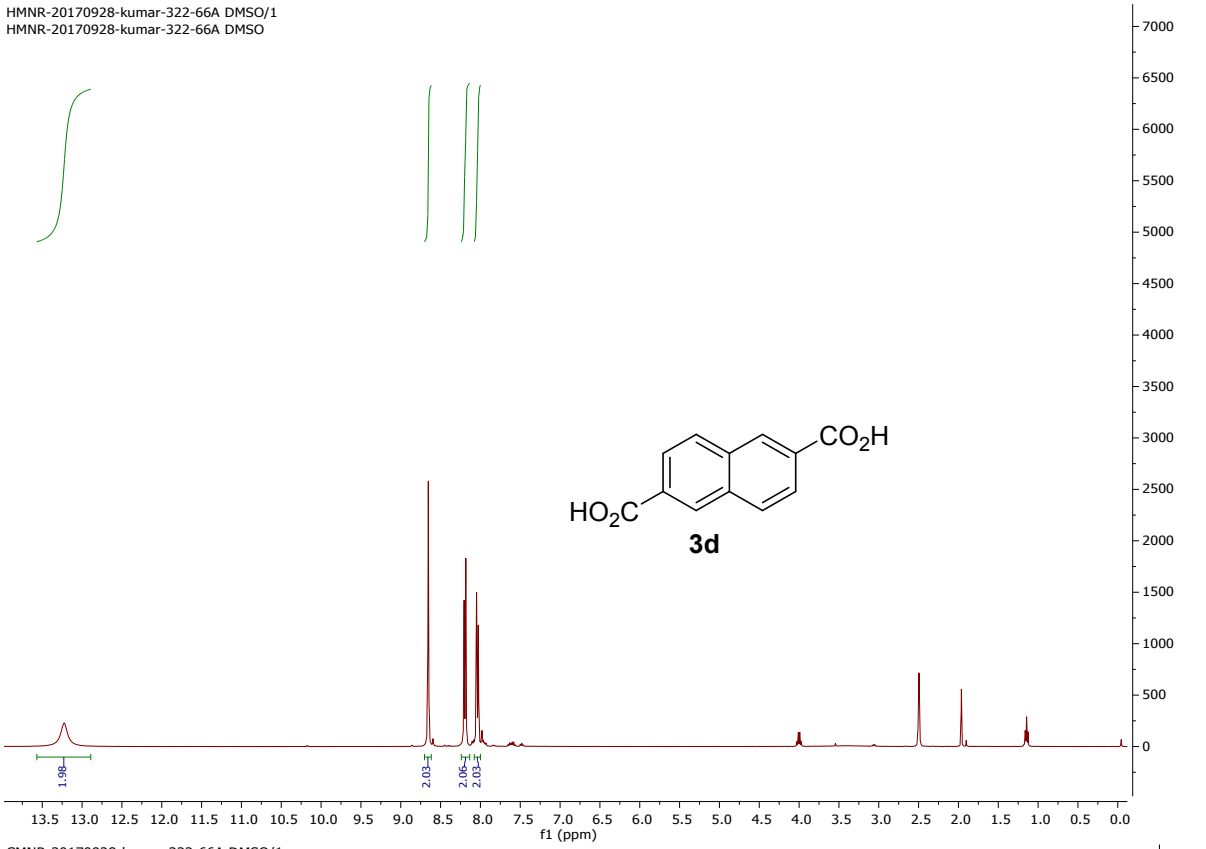


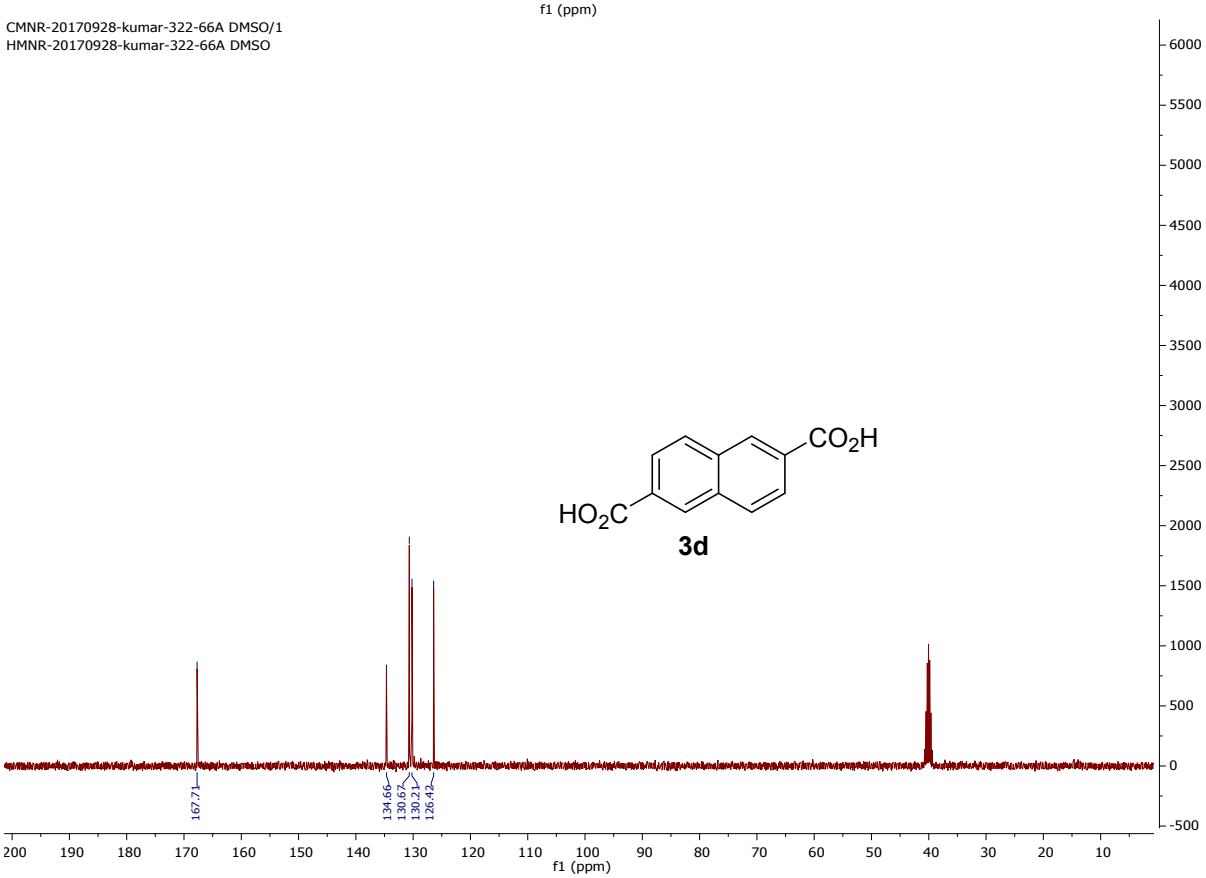
CMNR-20170926-kumar-322-62B DMSO/1
CMNR-20170926-kumar-322-62B DMSO

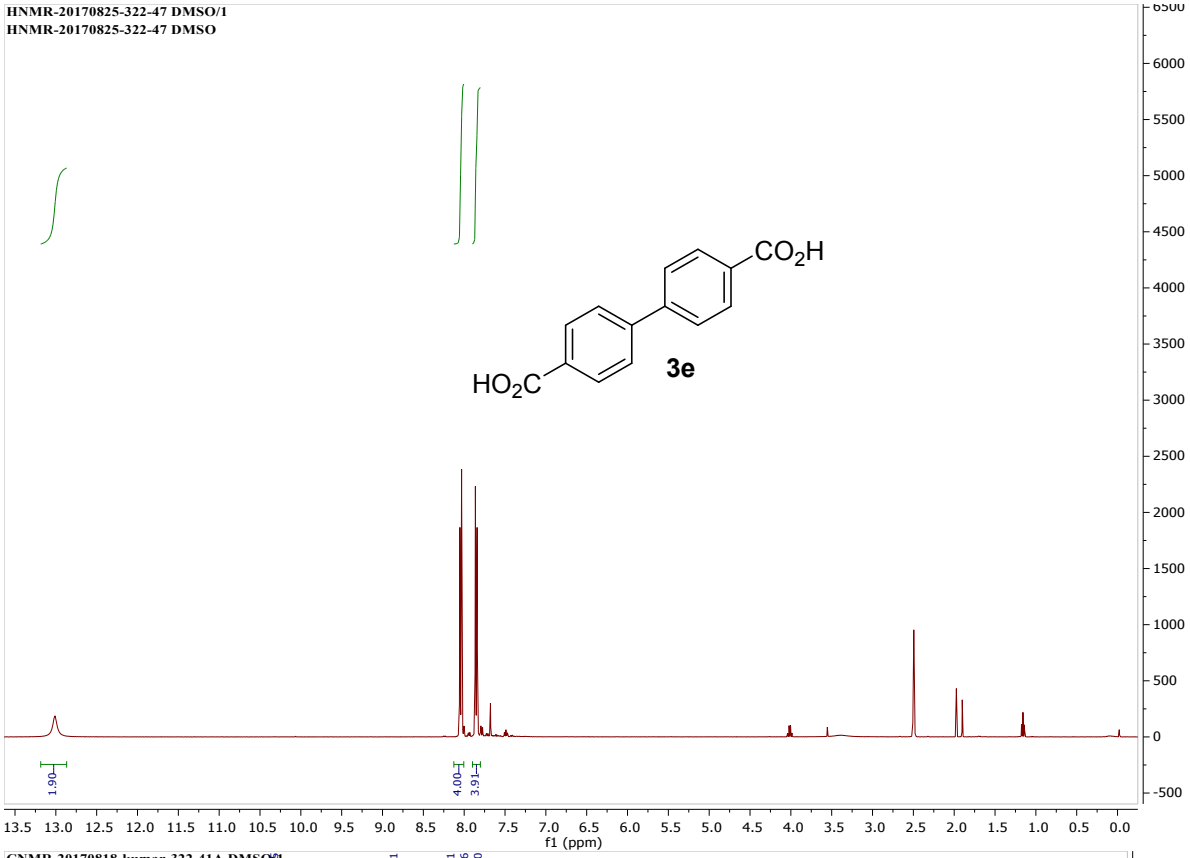


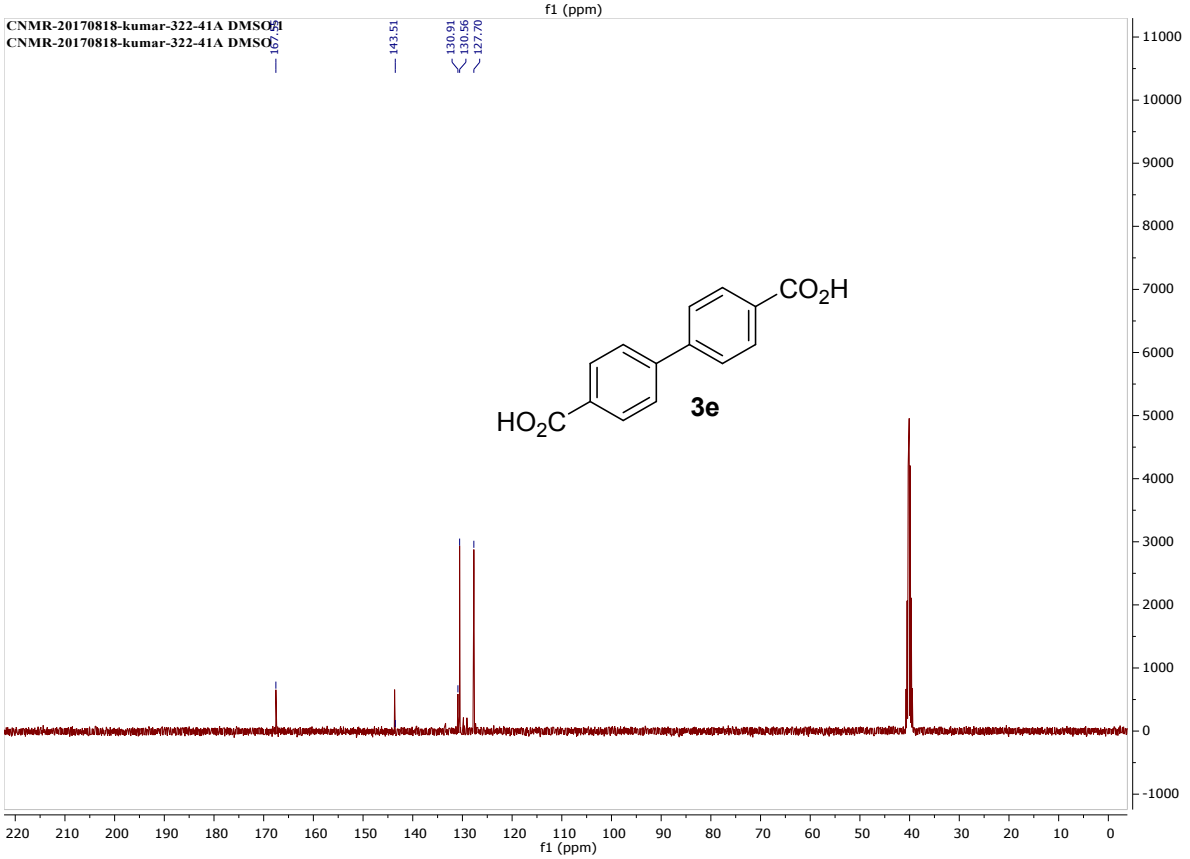

HNMR-20170907-kumar-322-53B DMSO/1
HNMR-20170907-kumar-322-53B DMSO
CO2H
HO2C
3c
2.00
3.09
3.00
f1 (ppm)

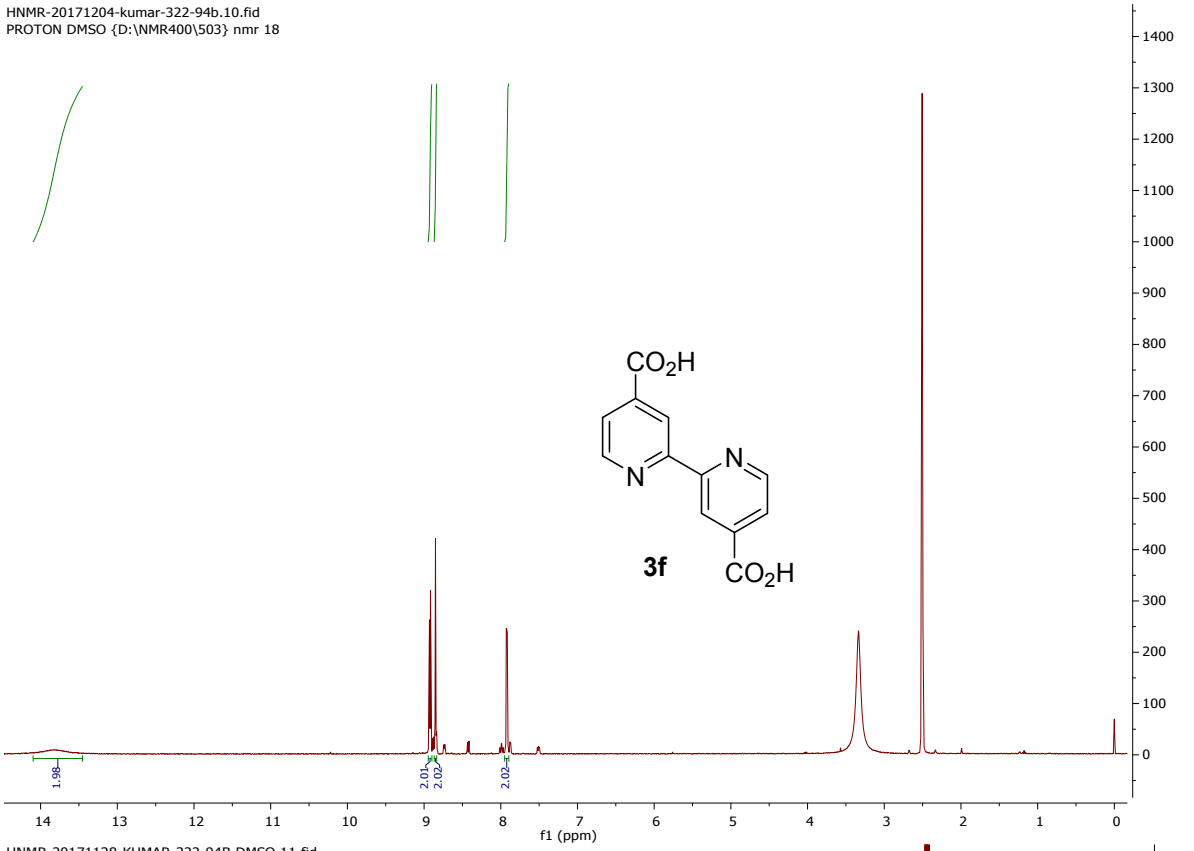

CMNR-201709012-kumar-322-53B DMSO/1
CMNR-201709012-kumar-322-53B DMSO
CO2H
HO2C
3c
168.77
167.25
139.46
135.12
133.69
132.60
130.69
127.16
21.45
f1 (ppm)

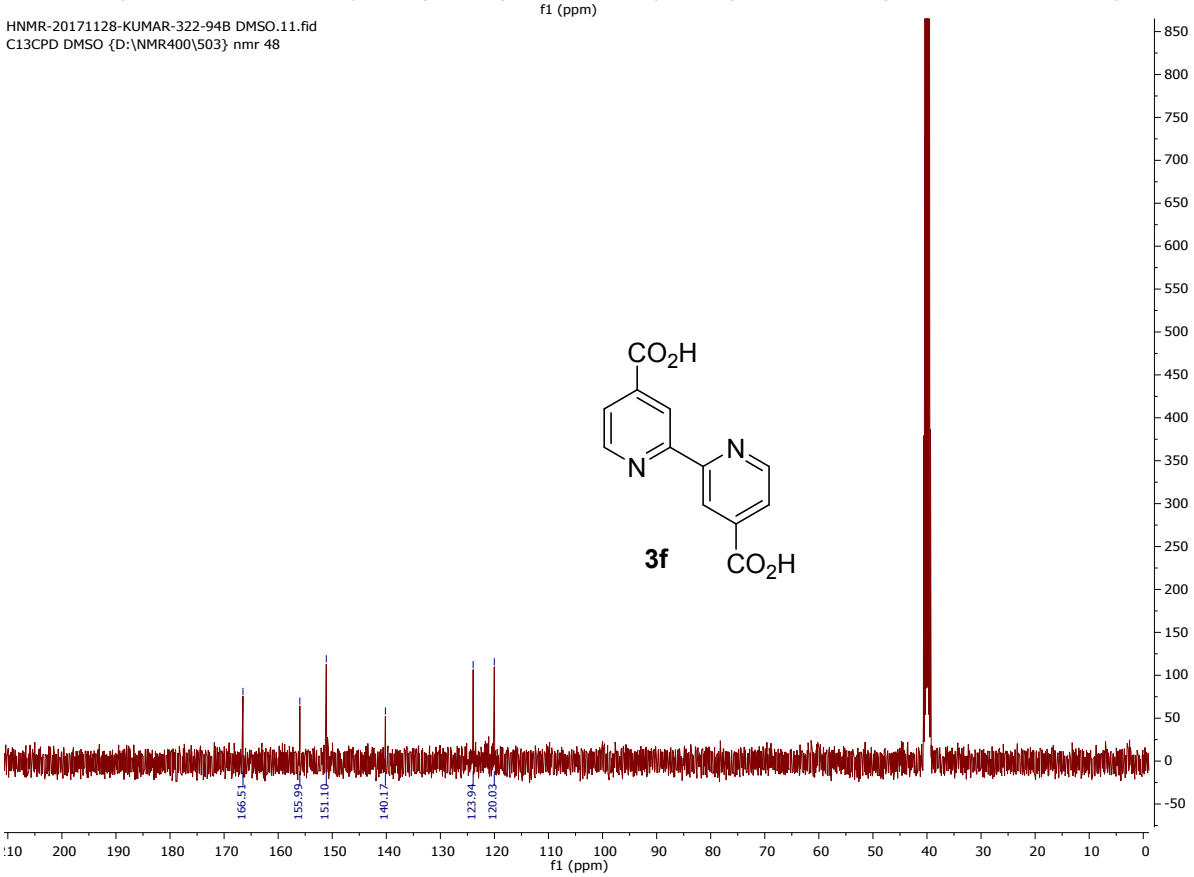

HMNR-20170928-kumar-322-66A DMSO/1
HMNR-20170928-kumar-322-66A DMSO
CO2H
HO2C
3d
1.98
2.03
2.06
2.03
f1 (ppm)

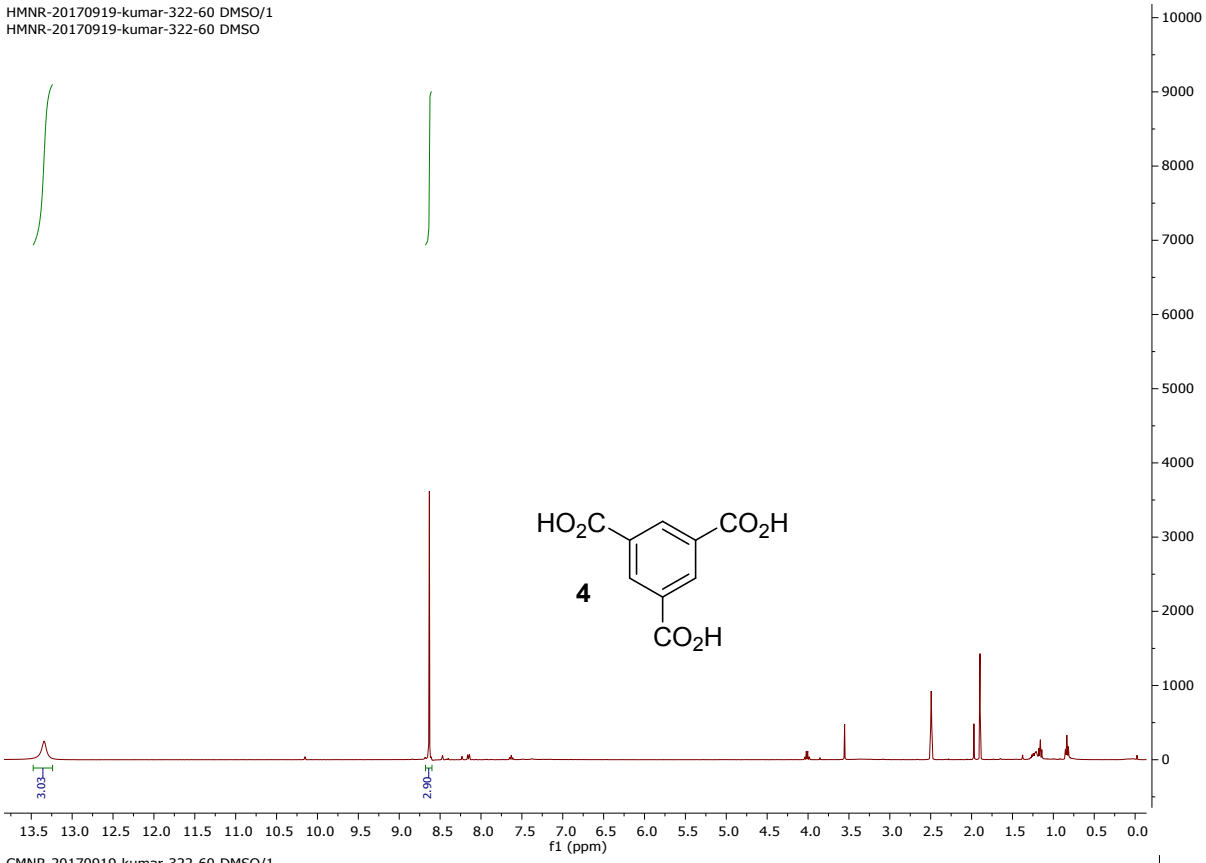

CMNR-20170928-kumar-322-66A DMSO/1
HMNR-20170928-kumar-322-66A DMSO
CO2H
HO2C
3d
167.71
134.66
130.67
130.21
126.42
f1 (ppm)

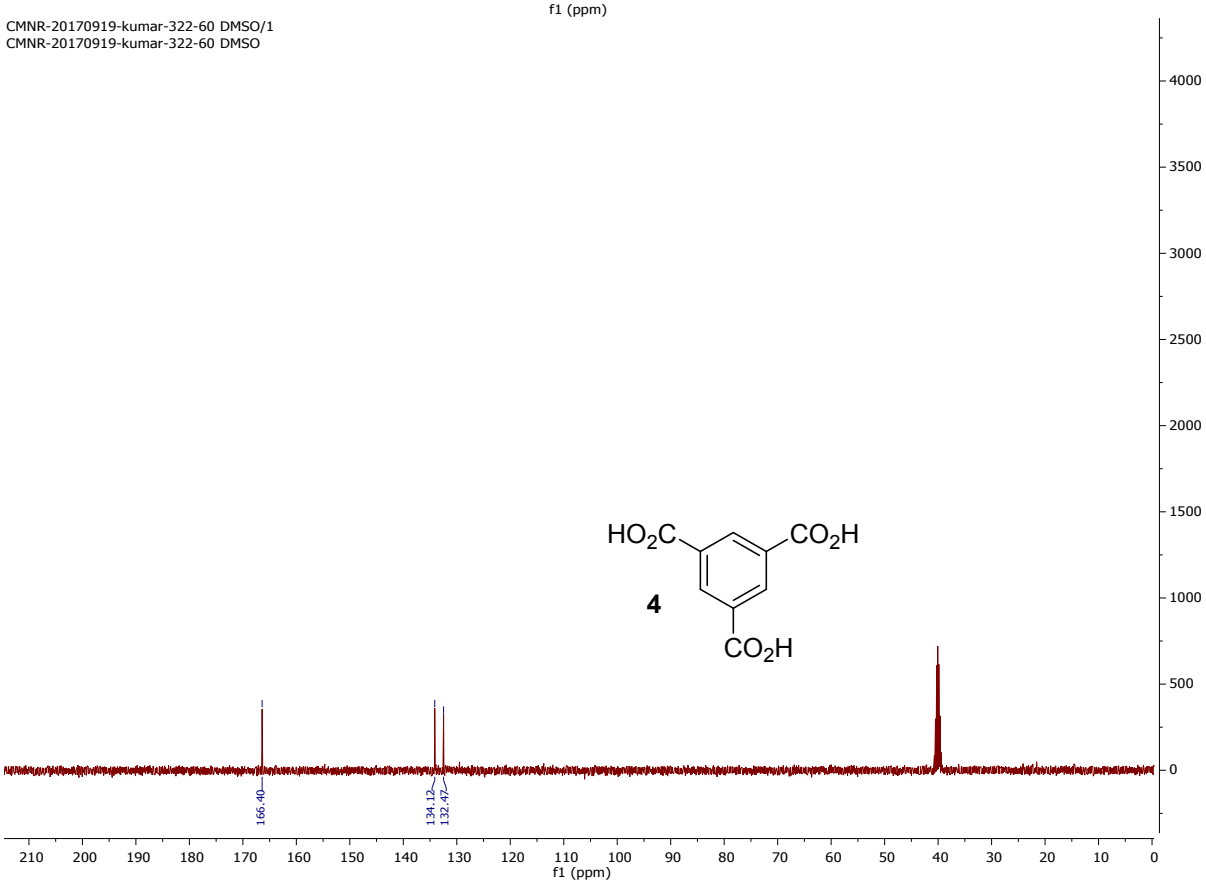

HNMR-20170825-322-47 DMSO/1
HNMR-20170825-322-47 DMSO
CO2H
HO2C
3e
1.90
4.00
3.91
f1 (ppm)

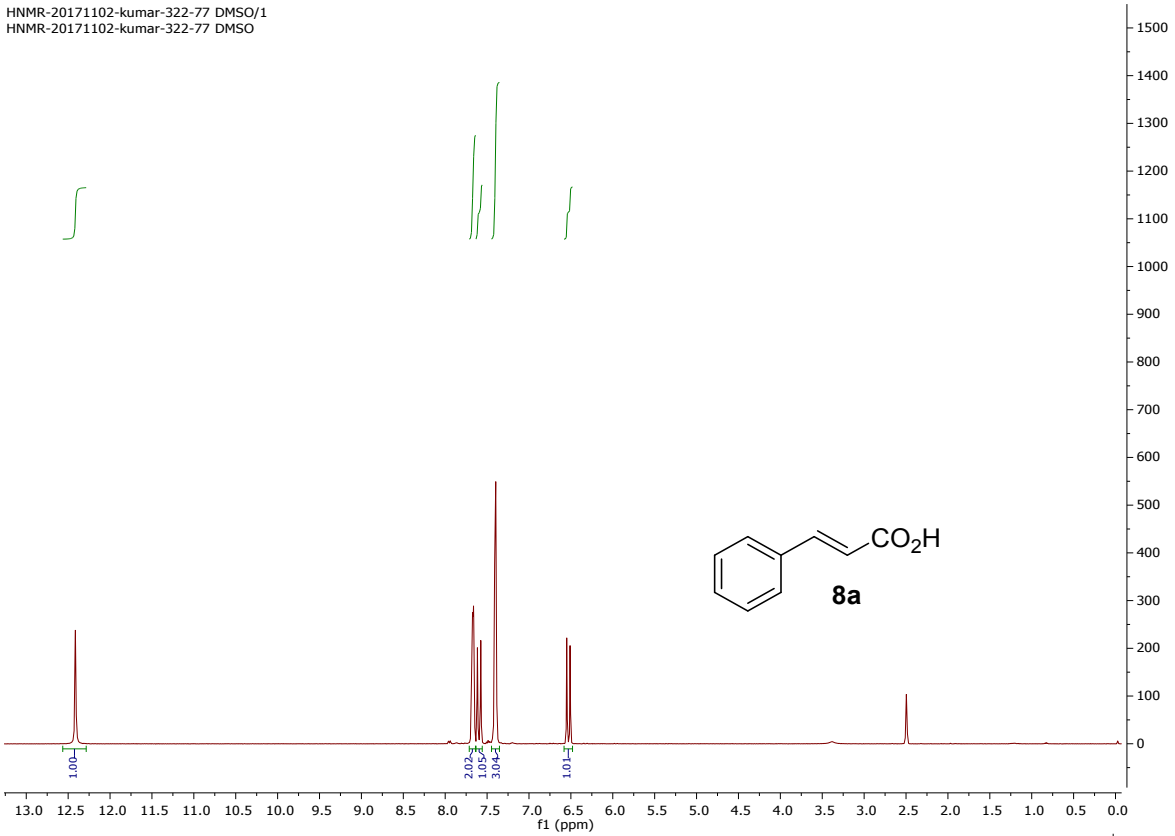

CNMR-20170818-kumar-322-41A DMSO/1
CNMR-20170818-kumar-322-41A DMSO
167.24
143.51
130.91
130.56
127.70
CO2H
HO2C
3e
f1 (ppm)

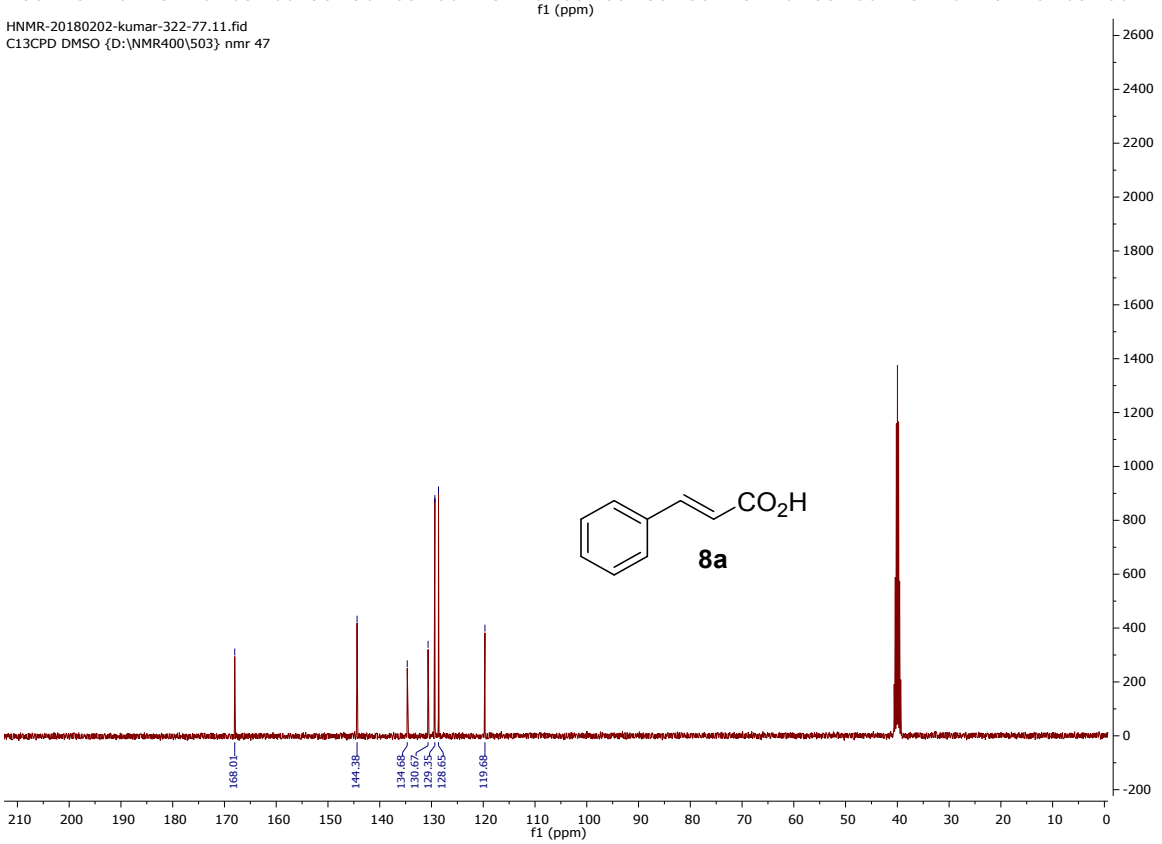

HNMR-20171204-kumar-322-94b.10.fid
PROTON DMSO {D:\NMR400\503} nmr 18
CO2H
N
N
CO2H
3f
1.98
2.01
2.02
2.02
f1 (ppm)

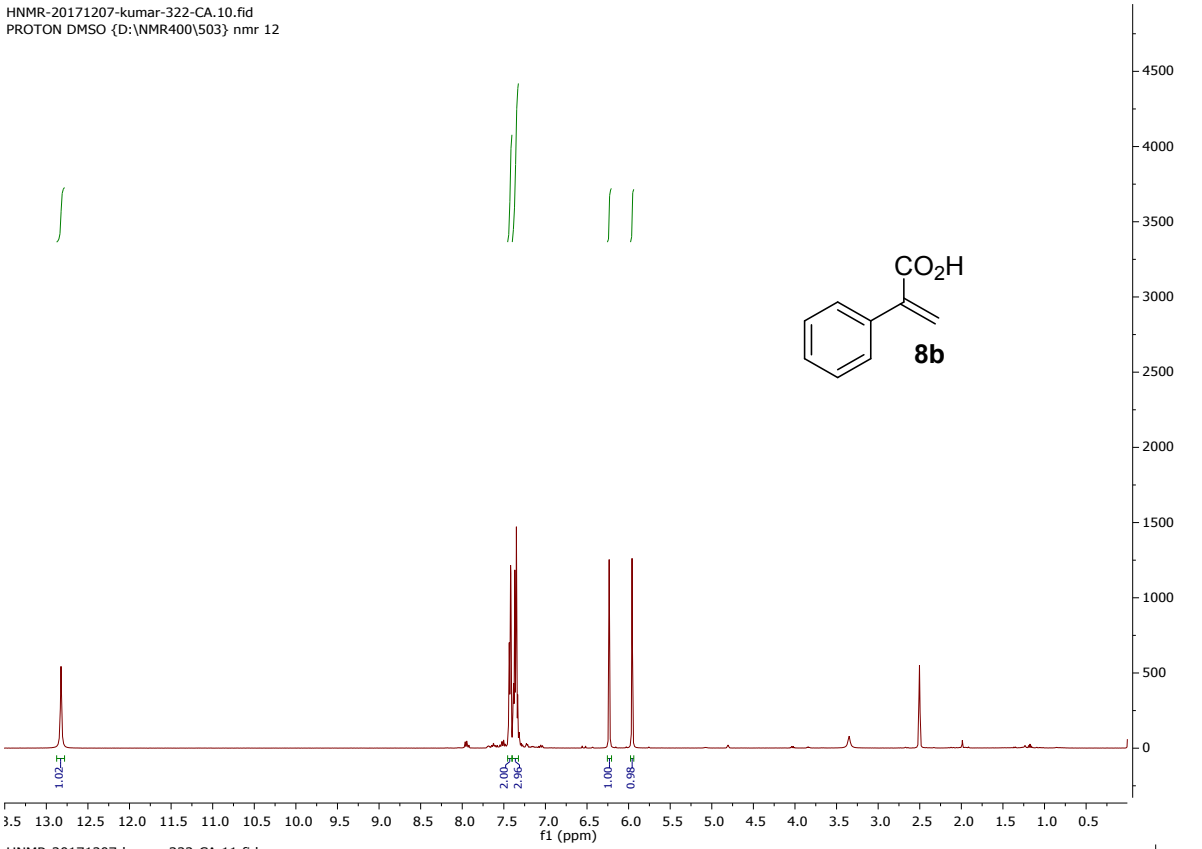

HNMR-20171128-KUMAR-322-94B DMSO.11.fid
C13CPD DMSO {D:\NMR400\503} nmr 48
CO2H
N
N
CO2H
3f
166.51
155.99
151.10
140.17
123.94
120.03
f1 (ppm)

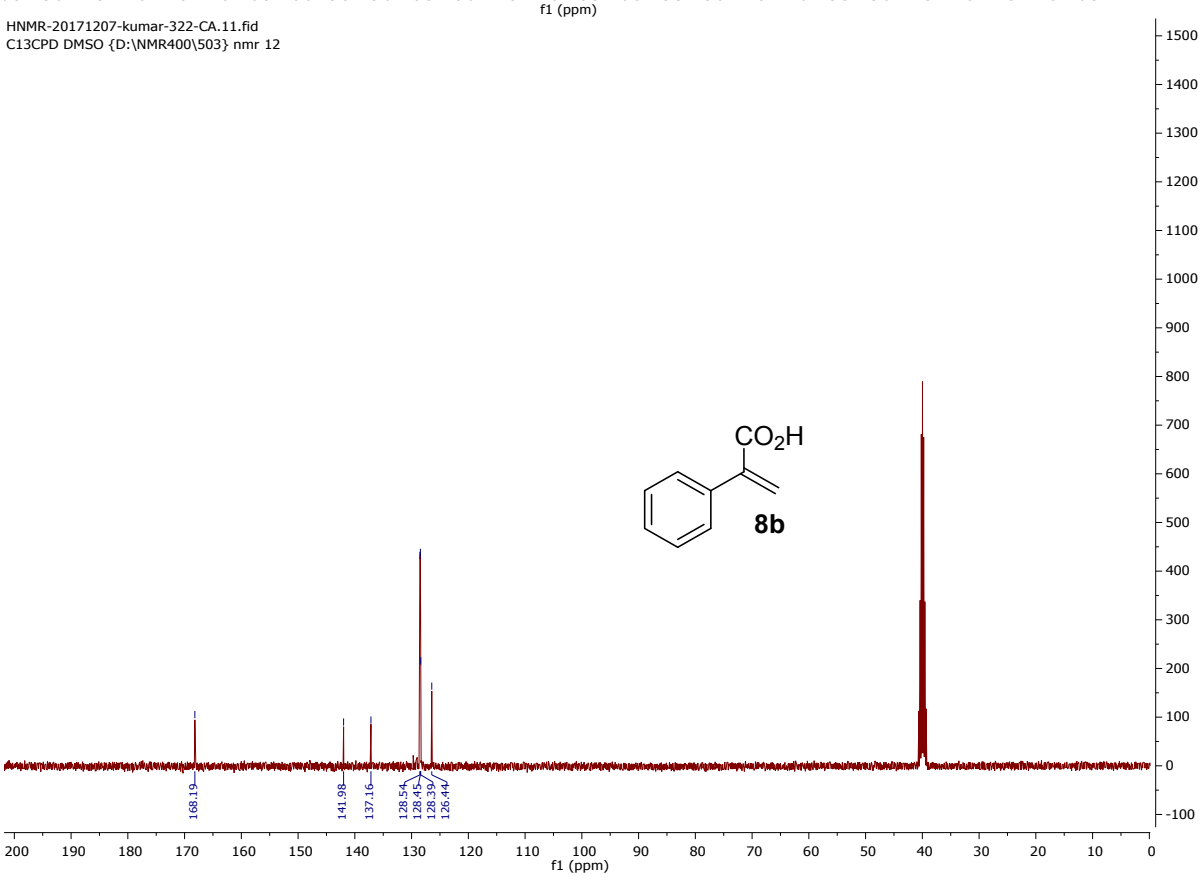

HMNR-20170919-kumar-322-60 DMSO/1
HMNR-20170919-kumar-322-60 DMSO
HO2C
CO2H
CO2H
4
3.03
2.90
f1 (ppm)

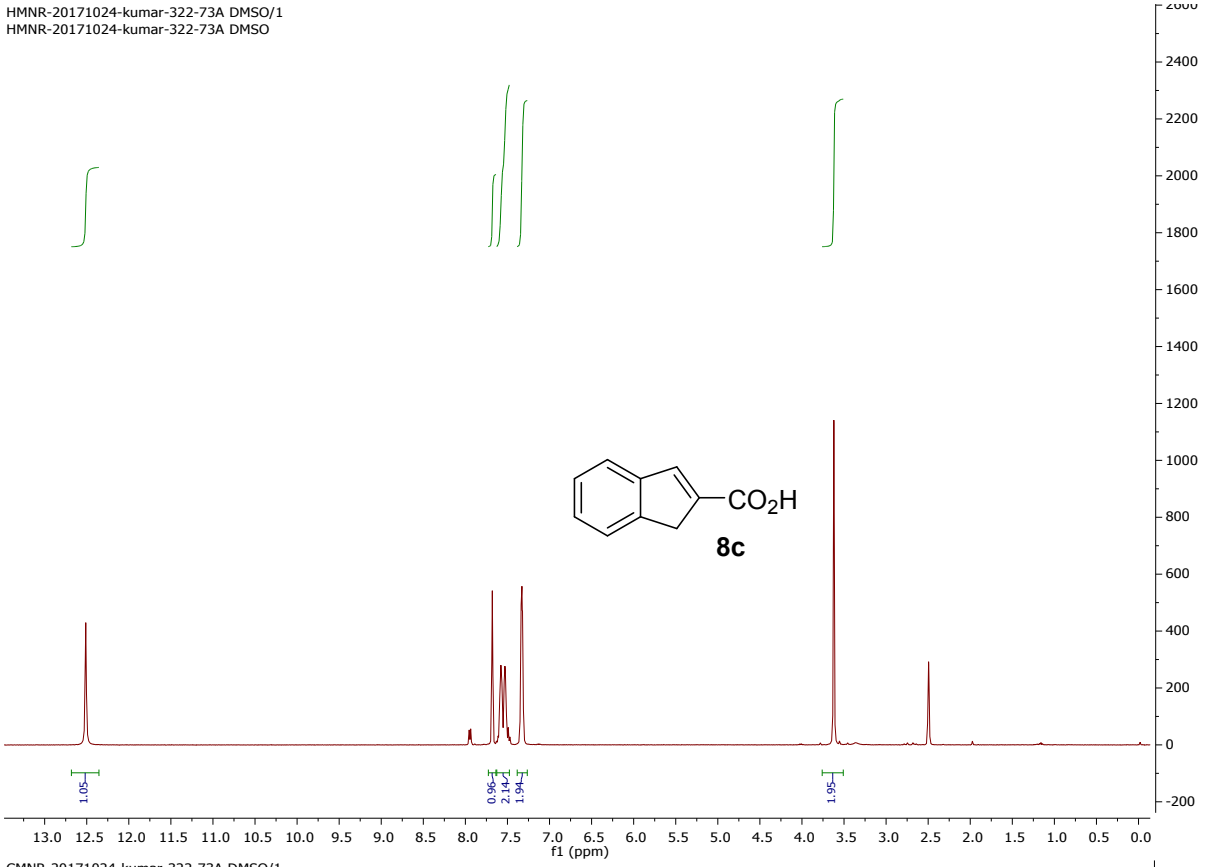

CMNR-20170919-kumar-322-60 DMSO/1
CMNR-20170919-kumar-322-60 DMSO
HO2C
CO2H
CO2H
4
166.40
134.12
132.47
f1 (ppm)

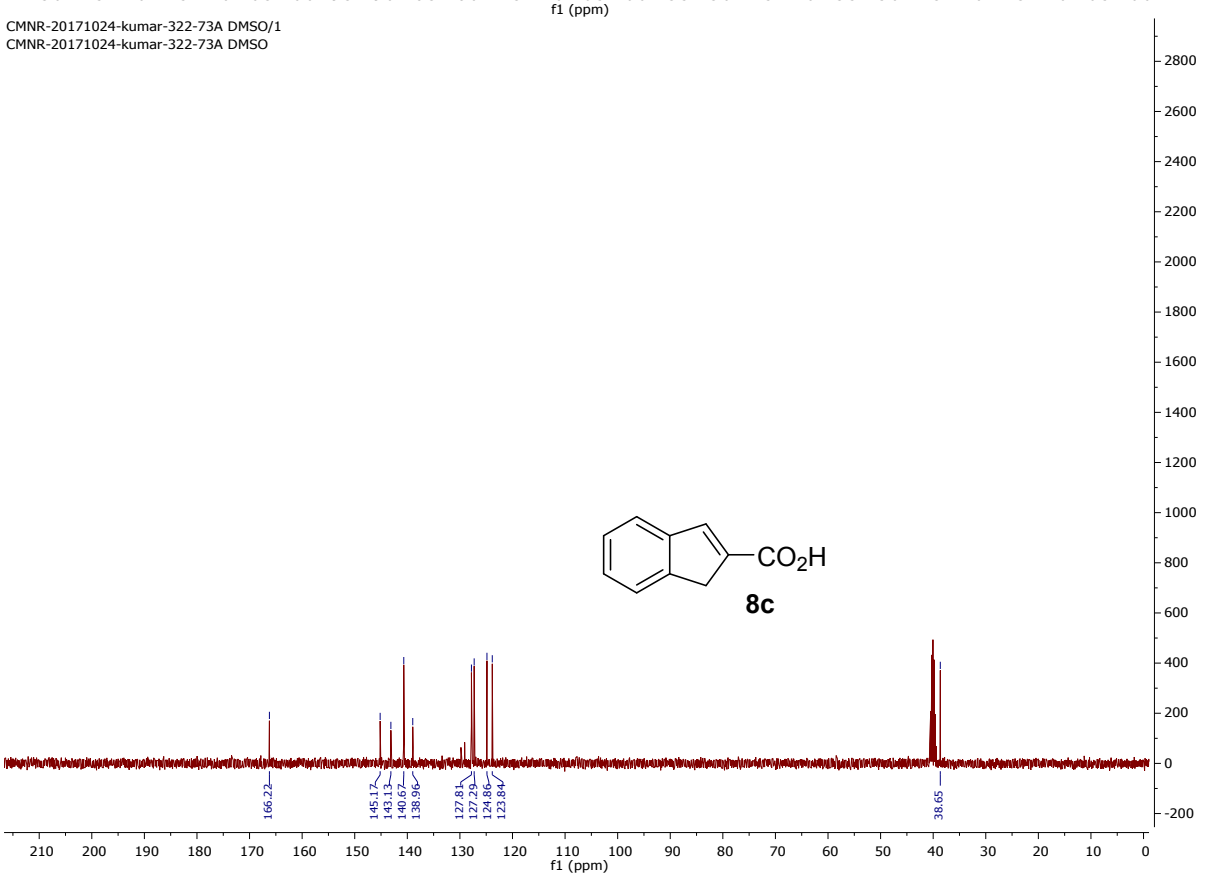

HNMR-20171102-kumar-322-77 DMSO/1
HNMR-20171102-kumar-322-77 DMSO
CO2H
8a
1.00
2.02
1.05
3.04
1.01
f1 (ppm)


HNMR-20180202-kumar-322-77.11.fid
C13CPD DMSO {D:\NMR400\503} nmr 47
CO2H
8a
168.01
144.38
134.68
130.67
129.32
128.65
119.68
f1 (ppm)


HNMR-20171207-kumar-322-CA.10.fid
PROTON DMSO {D:\NMR400\503} nmr 12
CO2H
8b
1.02
2.00
2.96
1.00
0.98
f1 (ppm)


HNMR-20171207-kumar-322-CA.11.fid
C13CPD DMSO {D:\NMR400\503} nmr 12
CO2H
8b
168.19
141.98
137.16
128.54
128.45
128.39
126.44
f1 (ppm)


HMNR-20171024-kumar-322-73A DMSO/1
HMNR-20171024-kumar-322-73A DMSO
CO2H
8c
1.05
0.96
2.14
1.94
1.95
f1 (ppm)


CMNR-20171024-kumar-322-73A DMSO/1
CMNR-20171024-kumar-322-73A DMSO
CO2H
8c
166.22
145.17
143.13
140.67
138.96
127.81
127.29
124.86
123.84
38.65
f1 (ppm)