Supporting Information

Cobalt-based nanoparticles prepared from MOF-carbon templates as efficient hydrogenation catalysts

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Supplementary figures

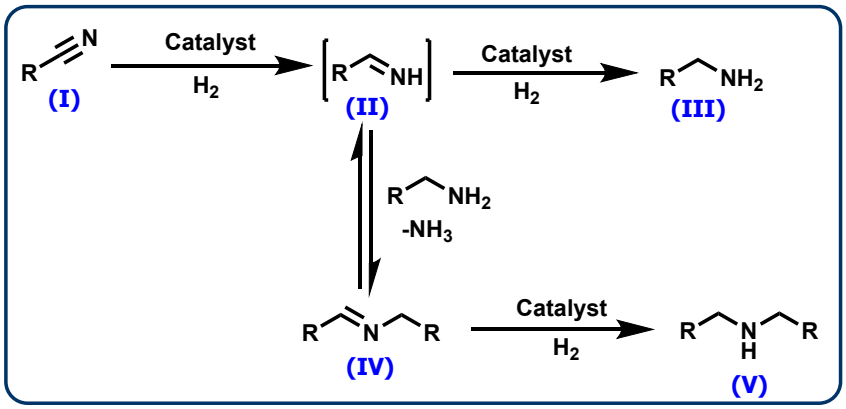


Fig. S1. Reaction pathway for the catalytic hydrogenation of nitriles: Formation of desired and un-desired products.

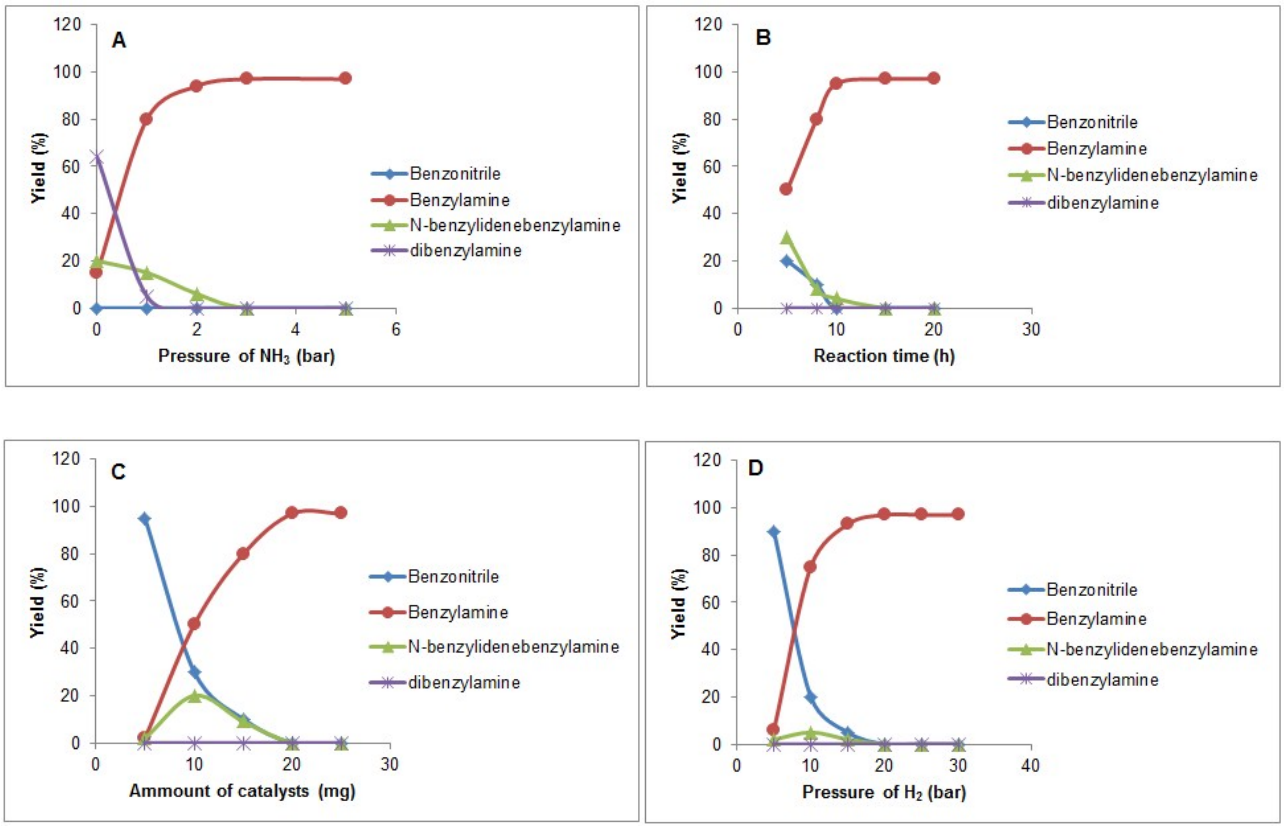


Fig. 2. Studies on the effect of ammonia (A), reaction time (B), amount of catalyst (C) and pressure of hydrogen (D) on the hydrogenation of benzonitrile. Reaction conditions: A: 0.5 mmol benzonitrile, 25 mg catalyst (3.8 mol% Co), 3 mL toluene, 25 bar H_2, 0-5 bar NH_3, 120 ^{0}C, 16 h. B: same as A with 5 bar NH_3, 120 ^{o}C, 0-20 h. C: Same as A with 5-25 mg catalyst and 5 bar NH_3. D: Same as A with 5-30 bar H_2 and 5 bar NH_3.

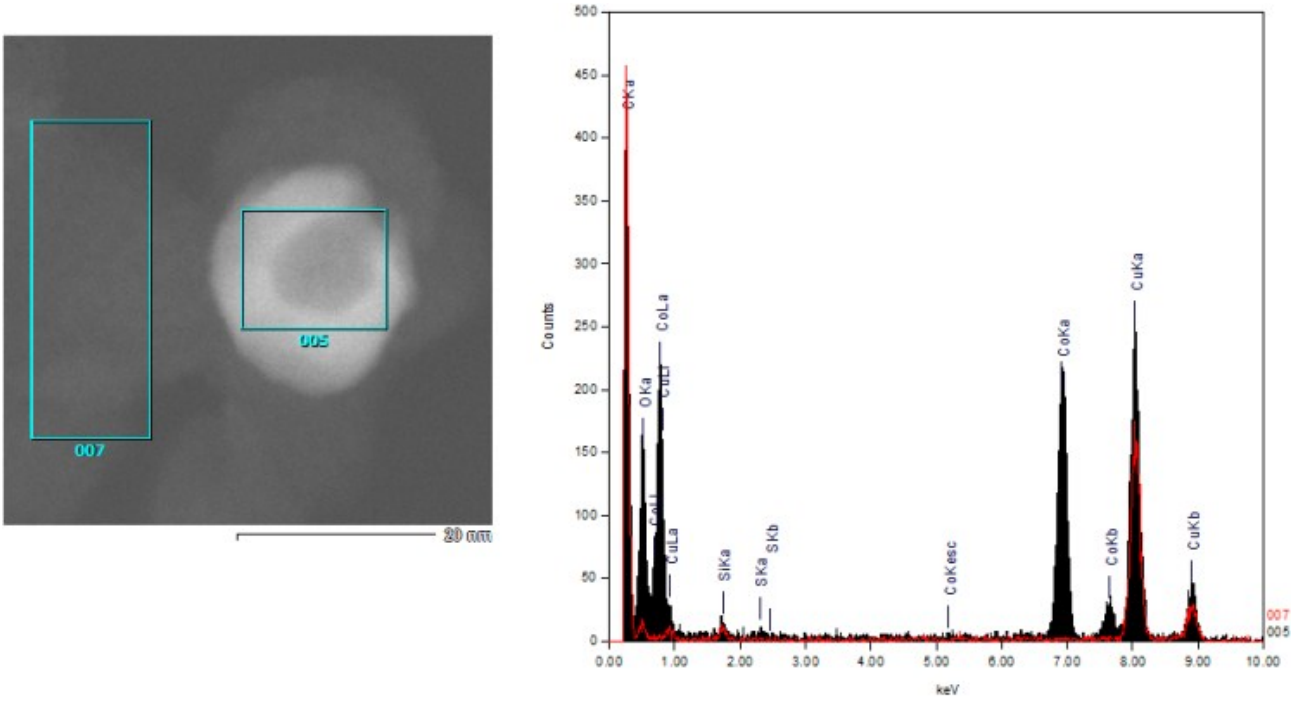


Fig. S3. HAADF-STEM/EDX images of cobalt-terephthalic acid MOF@C-800- catalyst.

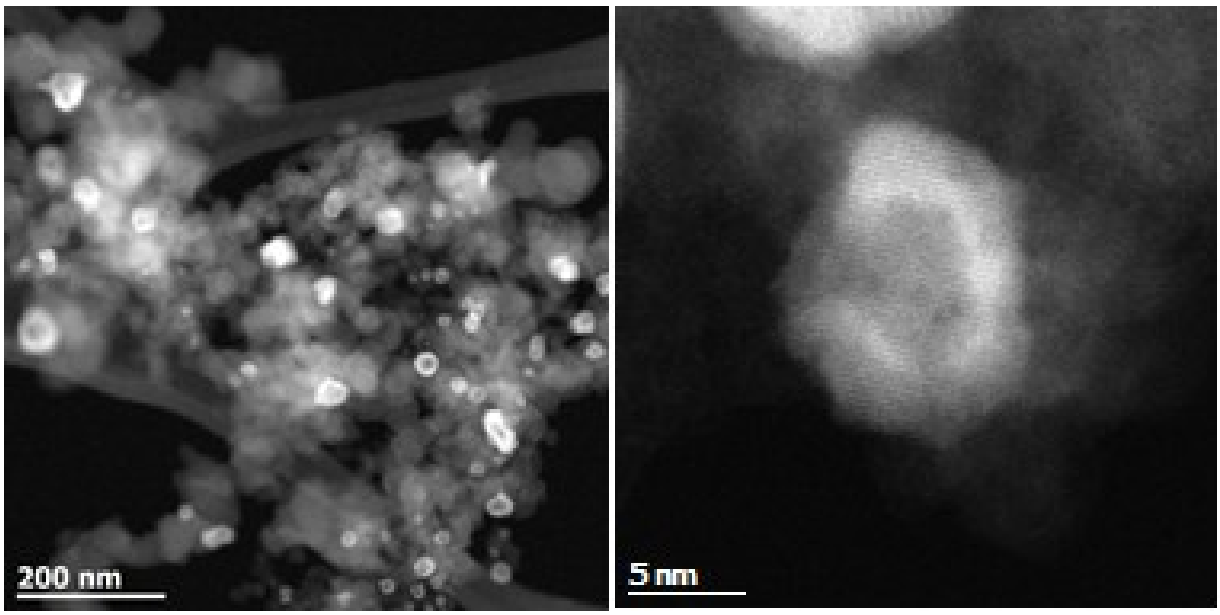


Fig. S4. TEM images cobalt nitrate@C-800.

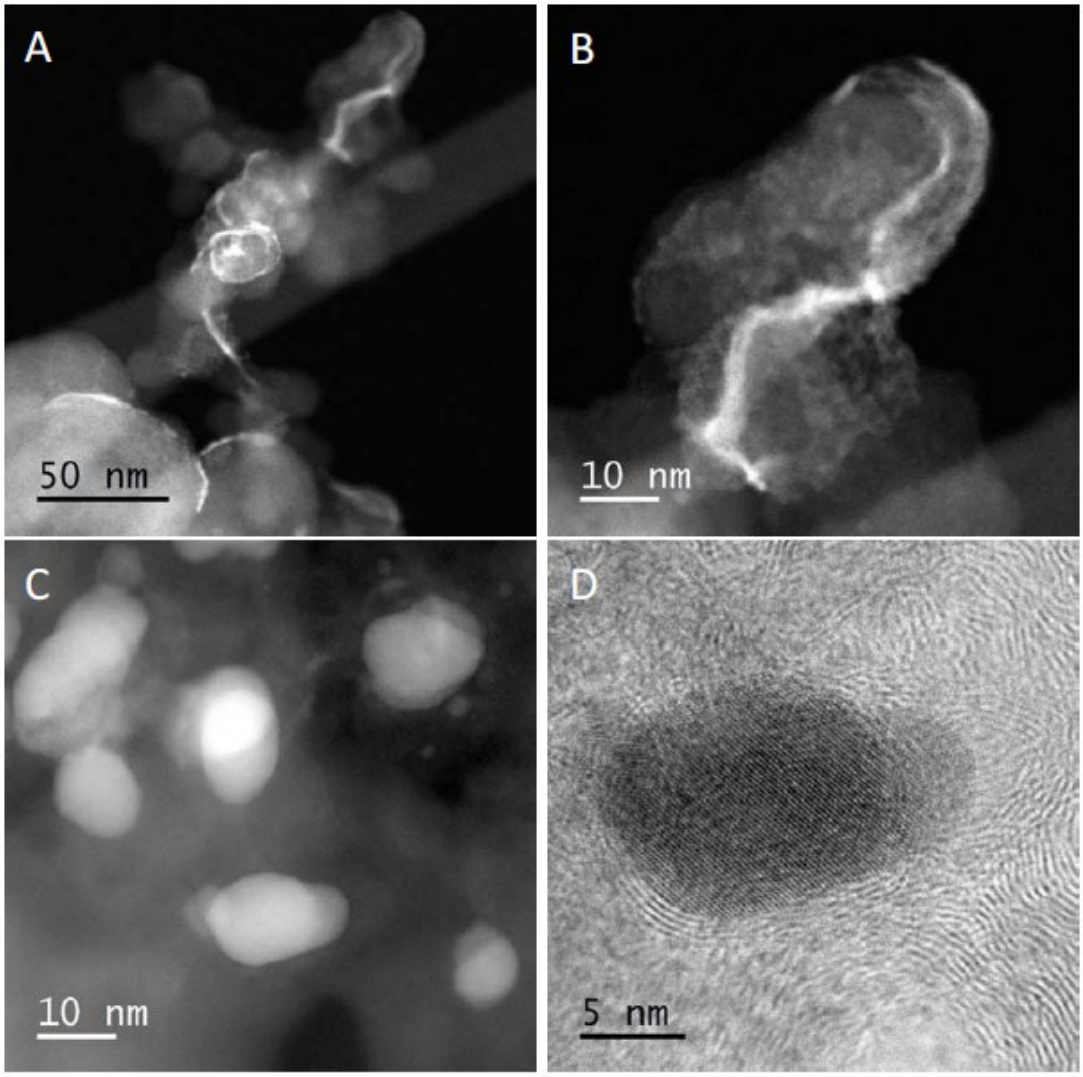


Fig. S5: HAADF-STEM images (A-C) and ABF-STEM image (D) of used catalyst. (A) and (B) show the new Co_3O_4 structures grown during reaction on the surface of the carbon support. (C) shows Co metal and Co_3O_4 particles. (D) shows a high resolution ABF image of a metal Co particle (see EDXS from S6) highlighting the encapsulation with several layers of graphenes.

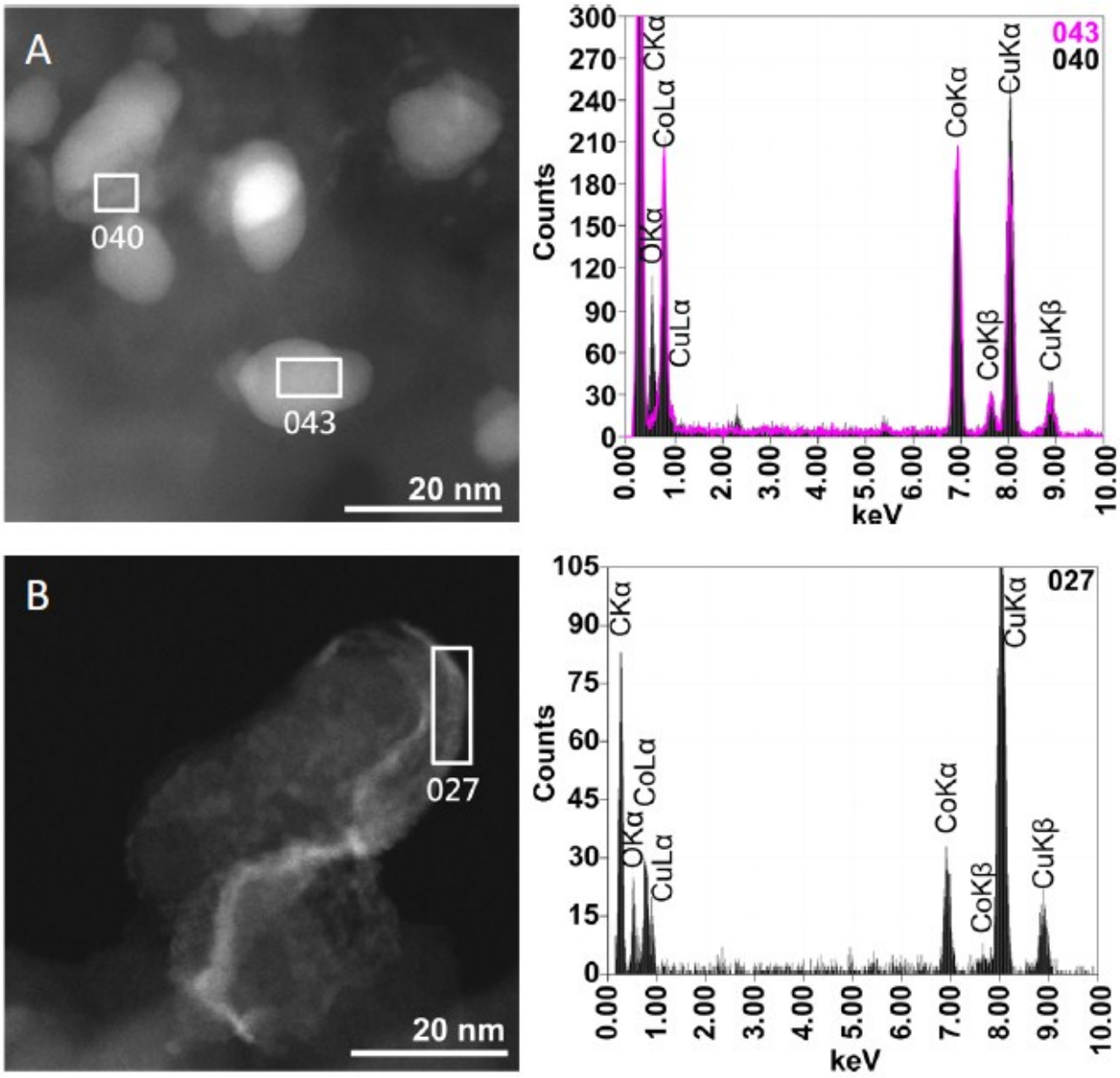


Fig. S6: HAADF-STEM images with EDX spectra from marked areas showing morphology comparable to the fresh specimen in the case of metallic Co particles (A, area 043) and changes in the case of cobalt oxide structures (A, area 040). Additionally a cobalt oxide phase has grown on the surface of carbon support (B, area 027).

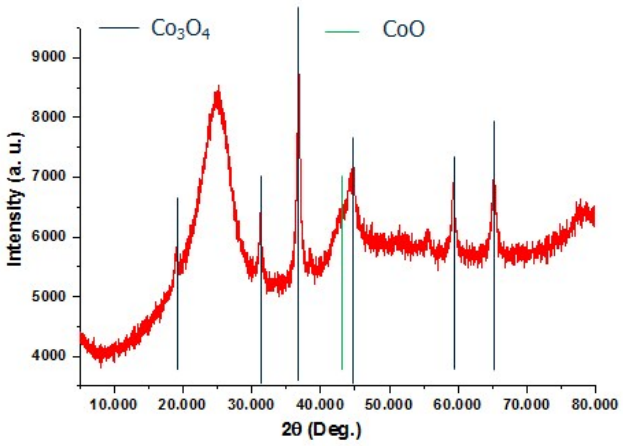


Fig. S7. XRD spectra of cobalt-terephthalic acid MOF@C-800 catalyst.

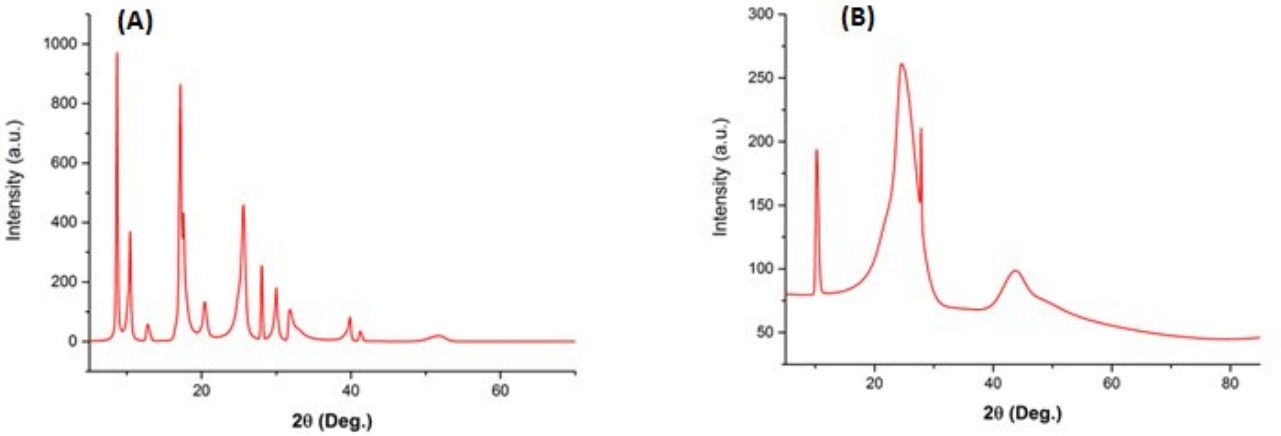


Fig. S8. XRD spectra of (A) Cobalt-terephthalic acid MOF and cobalt-terephthalic acid MOF-carbon template.

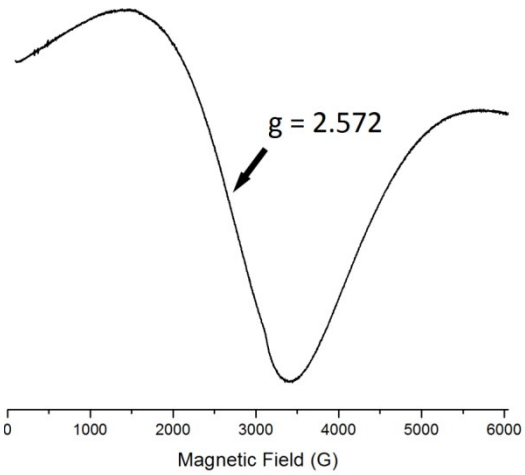


Fig. S9. EPR spectra of cobalt-terephthalic acid MOF@C-800 catalyst.

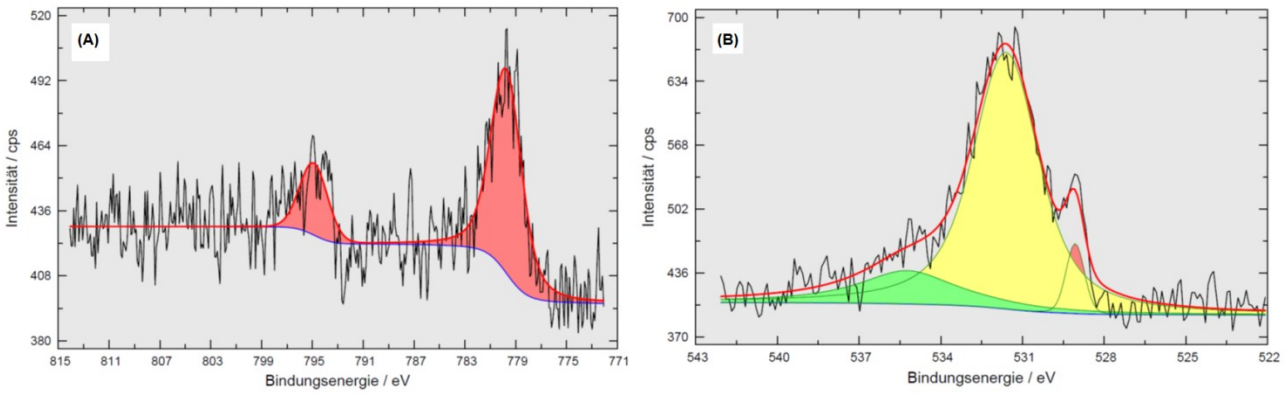
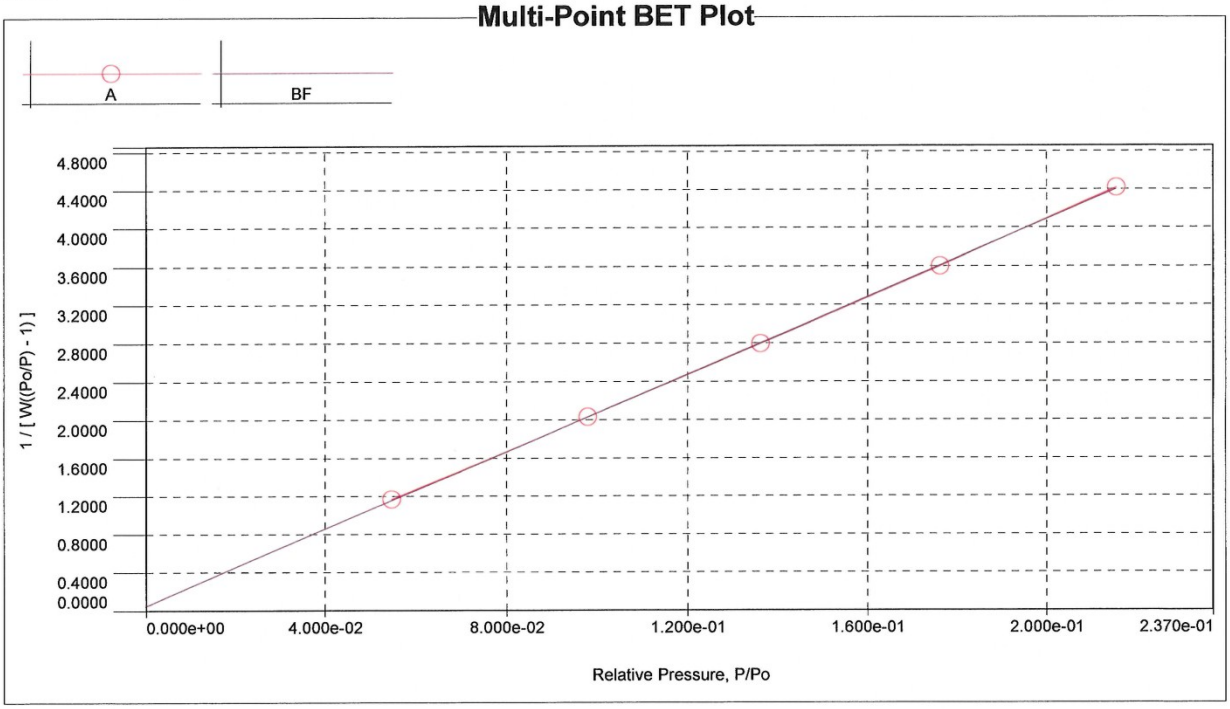


Fig. S10. XPS of Co2p (A) and O1s (B) electrons for cobalt-terephthalic acid MOF@C-800.

Analysis				Report			
Operator:	Struve	**Date:**	2017/11/14	**Operator:**	Struve	**Date:**	2017/11/16
Sample ID:	MK-34B	**Filename:**		MK-34B.qps			
Sample Desc:	Co3O4/Carbon, pressed, fresh, black	**Comment:**		120°C/0,5h, 220°C/2h, Thiru			
Sample weight:	0.0894 g	**Sample Volume:**		1 cc			
Outgas Time:	2.0 hrs	**OutgasTemp:**		220.0 C			
Analysis gas:	Nitrogen	**Bath Temp:**		273.0 K			
Press. Tolerance:	0.100/0.100 (ads/des)	**Equil time:**		20/20 sec (ads/des)	**Equil timeout:**		240/240 sec (ads/des)
Analysis Time:	240.7 min	**End of run:**		2017/11/14 22:34:19	**Instrument:**		Nova Station A
Cell ID:	0						

Multi-Point BET Plot



Multi-Point BET

Relative Pressure [P/Po]	Volume @ STP [cc/g]	1 / [W((Po/P) - 1)]	Relative Pressure [P/Po]	Volume @ STP [cc/g]	1 / [W((Po/P) - 1)]
5.46290e-02	39.7848	1.1621e+00	1.76050e-01	47.5872	3.5925e+00
9.79640e-02	42.9322	2.0240e+00	2.15359e-01	49.7683	4.4125e+00
1.36020e-01	45.1916	2.7874e+00			

MBET summary

Slope =	20.194
Intercept =	4.918e-02
Correlation coefficient, r =	0.999959
C constant=	411.620
Surface Area =	172.031 m²/g

Single Point Surface Area

Relative Pressure [P/Po]	Volume @ STP [cc/g]	1 / [W((P/Po) - 1)]	Slope	Surf. Area [m²/g]
2.98052e-01	54.6741	6.2138e+00	20.8480	167.0434

Fig. S9. Sorption isotherm of cobalt-terephthalic acid MOF@C-800 catalyst.

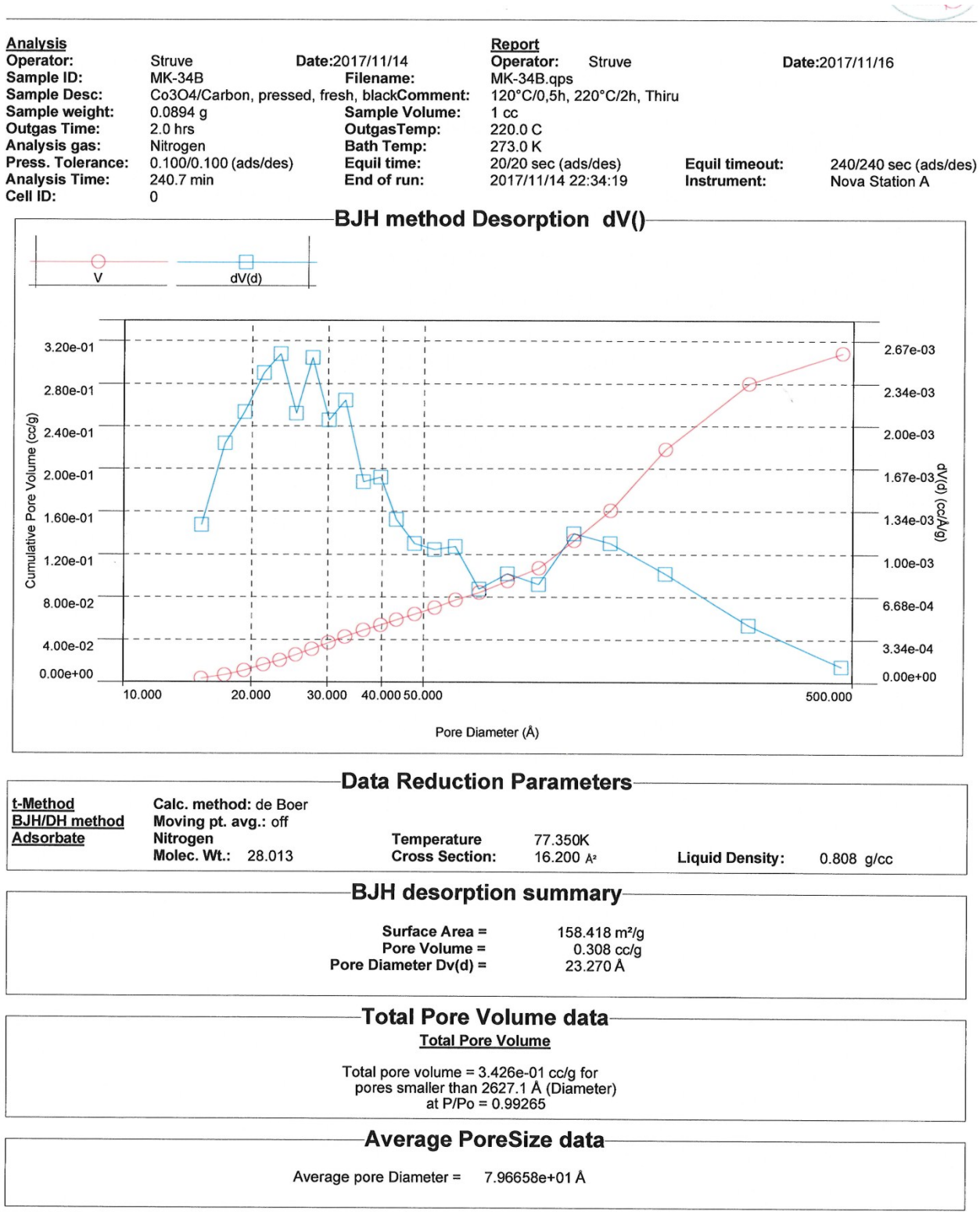
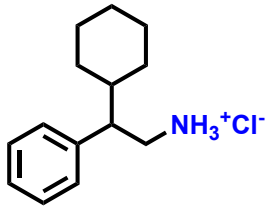


Fig. S10. Pore-size distribution calculated from the desorption isotherm for Cobalt-terephthalic acid MOF@C-800 catalyst.

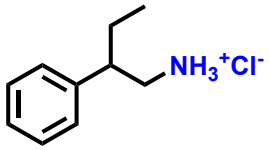
NMR Data

KM10-42



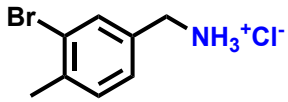
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.10 (br s, 3H), 7.44 – 7.07 (m, 5H), 3.24 (dd, J = 12.8, 5.6 Hz, 1H), 3.05 (dd, J = 12.7, 9.4 Hz, 1H), 2.89 – 2.72 (m, 1H), 1.87 – 1.47 (m, 5H), 1.44 – 1.30 (m, 1H), 1.26 – 0.58 (m, 5H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 139.96 , 129.21 , 128.76 , 127.30 , 49.24 , 41.35 , 40.29 , 31.26 , 29.72 , 26.35 , 26.26 , 26.04 .**Off white solid.**

KM10-47



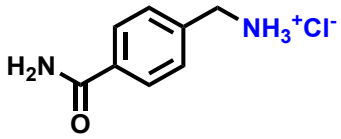
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.24 (br s, 3H), 7.51 – 7.08 (m, 5H), 3.14 – 2.96 (m, 1H), 2.98 – 2.80 (m, 2H), 1.91 – 1.71 (m, 1H), 1.62 – 1.41 (m, 1H), 0.67 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 141.49 , 129.06 , 128.36 , 127.37 , 45.26 , 44.17 , 26.28 , 11.88 . **Brown solid.**

KM10-48



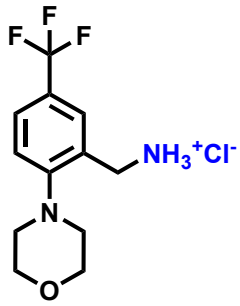
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.67 (br s, 3H), 7.79 (d, *J* = 1.9 Hz, 1H), 7.49 – 7.32 (m, 2H), 3.99 (s, 2H), 2.35 (s, 3H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 137.79 , 134.39 , 133.02 , 131.50 , 128.92 , 124.43 , 41.53 , 22.58 . **White solid.**

KM10-52



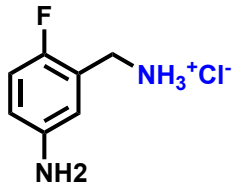
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.68 (br s, 3H), 8.08 (br s, 1H), 7.92 (d, *J* = 8.3 Hz, 2H), 7.59 (d, *J* = 8.3 Hz, 2H), 7.43 (br s, 1H), 4.07 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 167.85 , 137.65 , 134.57 , 129.17 , 128.10 , 42.20 . **White solid.**

KM10-72



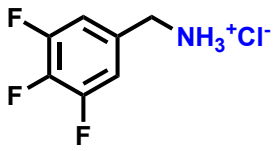
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.80 (br s, 3H), 8.05 (d, *J* = 1.8 Hz, 1H), 7.70 (dd, *J* = 8.5, 1.7 Hz, 1H), 7.39 (d, *J* = 8.3 Hz, 1H), 4.17 (s, 2H), 3.86 – 3.68 (m, 4H), 2.94 – 2.82 (m, 4H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 155.02 , 130.46 , 127.02 (q, J = 3.5 Hz), 126.67 (q, J = 3.6 Hz), 124.73 (q, *J* = 271.7 Hz), 124.62 (q, *J* = 32.1 Hz), 121.37 , 66.76 , 52.82 , 37.77 . **Off white solid.**

KM10-73



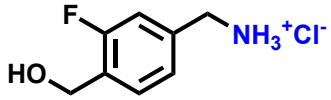
^{1}H NMR (300 MHz, DMSO-d_6) δ 10.50 (br s, 2H), 8.73 (br s, 3H), 7.61 (dd, *J* = 6.3, 2.5 Hz, 1H), 7.54 – 7.32 (m, 2H), 4.05 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 159.65 (d, *J* = 247.1 Hz), 129.36 , 126.28 (d, *J* = 3.6 Hz), 126.11 (d, *J* = 8.9 Hz), 122.89 (d, *J* = 16.5 Hz), 117.24 (d, *J* = 23.4 Hz), 35.90. **Off white solid.**

KM10-74



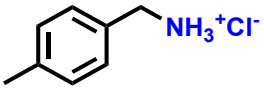
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.80 (br s, 3H), 7.76 – 7.41 (m, 2H), 4.05 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 150.32 (ddd, *J* = 247.1, 9.7, 3.9 Hz), 139.00 (dt, *J* = 249.7, 15.5 Hz), 131.91 (td, *J* = 8.4, 4.8 Hz), 114.77 – 114.38 (m), 41.36. **Off white solid.**

KM10-77



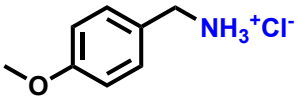
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.68 (br s, 3H), 7.55 – 7.43 (m, 1H), 7.42 – 7.28 (m, 2H), 5.35 (br s, 1H), 4.54 (s, 2H), 4.01 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 159.68 (d, *J* = 244.1 Hz), 135.37 (d, *J* = 8.0 Hz), 129.74 (d, *J* = 15.0 Hz), 129.54 (d, *J* = 5.4 Hz), 125.28 (d, *J* = 3.1 Hz), 115.89 (d, *J* = 22.5 Hz), 55.49, 41.86. **Off white solid.**

KM10-24



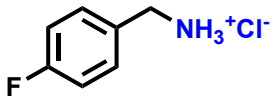
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.62 (br s, 3H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 3.94 (s, 2H), 2.30 (s, 3H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 138.11 , 131.55 , 129.47 , 129.44 , 42.31 , 21.23 . **White solid.**

KM10-45



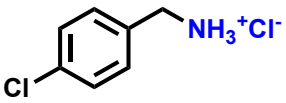
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.66 (br s, 3H), 7.47 (d, *J* = 9.0 Hz, 2H), 6.94 (d, *J* = 8.7 Hz, 2H), 3.92 (s, 2H), 3.74 (s, 3H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 159.73 , 131.07 , 126.46 , 114.30 , 55.67 , 42.05 . **White solid.**

KM10-56



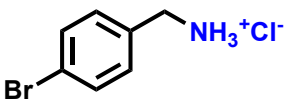
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.72 (br s, 3H), 7.65 – 7.56 (m, 2H), 7.30 – 7.17 (m, 2H), 4.00 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 162.49 (d, *J* = 244.5 Hz), 131.89 (d, *J* = 8.4 Hz), 130.87 (d, *J* = 3.1 Hz), 115.73 (d, *J* = 21.5 Hz), 41.79. **White solid.**

KM10-57



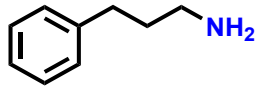
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.72 (br s, 3H), 7.57 (d, *J* = 8.5 Hz, 2H), 7.48 (d, *J* = 8.6 Hz, 2H), 4.01 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 133.61 , 133.54 , 131.48 , 128.92 , 41.83 . **White solid.**

KM10-58



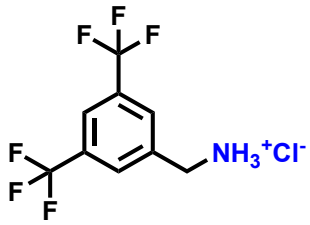
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.73 (br s, 3H), 7.60 (d, *J* = 8.6 Hz, 2H), 7.51 (d, *J* = 8.7 Hz, 2H), 4.00 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 133.99 , 131.82 , 131.82 , 122.12 , 41.88 . **White solid.**

KM10-60



^{1}H NMR (300 MHz, DMSO-d_6) δ 7.47 – 6.93 (m, 5H), 3.44 (br s, 2H), 2.78 – 2.39 (m, 4H), 1.70 (t, *J* = 7.5 Hz, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 142.49 , 128.72 , 128.68 , 126.07 , 41.05 , 34.34 , 32.97 . **Brown oil.**

KM10-61

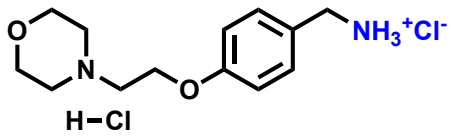


^{1}H NMR (300 MHz, DMSO-d_6) δ 8.92 (br s, 3H), 8.51 – 8.28 (m, 2H), 8.22 – 7.90 (m, 1H), 4.26 (s, 2H). **^{19}F NMR (282 MHz, DMSO-d_6)** δ -61.38 . **White solid.**

KM10-63

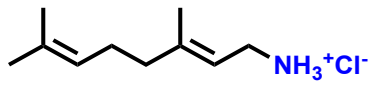
^{1}H NMR (300 MHz, DMSO-d_6) δ 5.66 (br s, 3H), 2.62 (t, *J* = 7.3 Hz, 2H), 1.45-1.42 (m, 2H), 1.25-1.22 (m, 14H), 0.86 (t, *J* = 6.6 Hz, 3H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 40.44, 31.80 , 30.25 , 29.48 , 29.47 , 29.28 , 29.22 , 26.67 , 22.58 , 14.36 . **Off white solid.**

KM10-83



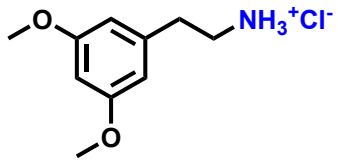
^{1}H NMR (300 MHz, DMSO-d_6) δ 11.99 (br s, 1H), 8.65 (br s, 3H), 7.49 (d, *J* = 8.7 Hz, 2H), 7.02 (d, *J* = 8.7 Hz, 2H), 4.37 (s, 2H), 4.01 – 3.78 (m, 6H), 3.62 – 3.36 (m, 4H), 3.34 – 3.14 (m, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 157.98 , 131.12 , 127.38 , 115.15 , 63.55 , 62.94 , 55.12 , 52.08 , 41.98 . **Yellow solid.**

KM10-89



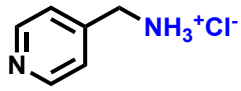
^{1}H NMR (300 MHz, DMSO-d_6) δ 5.40 (br s, 3H), 5.24 (t, *J* = 6.9 Hz, 1H), 5.06 (t, *J* = 6.0 Hz, 1H), 3.32 (d, *J* = 6.9 Hz, 2H), 2.14 – 1.83 (m, 4H), 1.66 – 1.57 (m, 6H), 1.54 (s, 3H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 138.69 , 131.21 , 124.21 , 122.15 , 48.84 , 39.55 , 26.43 , 25.76 , 17.79 , 16.36 . **Brown gum.**

KM10-95



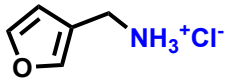
^{1}H NMR (300 MHz, DMSO-d_6) δ 7.96 (br s, 3H), 6.92 – 6.82 (m, 2H), 6.75 (dd, *J* = 8.2, 2.0 Hz, 1H), 3.74 (s, 3H), 3.71 (s, 3H), 3.11 – 2.94 (m, 2H), 2.93 – 2.78 (m, 2H). **13C NMR (75 MHz, DMSO-d6)** δ 149.22 , 148.03 , 130.41 , 120.97 , 112.97 , 112.44 , 56.00 , 55.93 , 40.62 , 33.19 .**Yellow solid.**

KM10-97



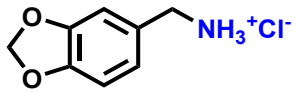
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.82 (m, 5H), 7.78 – 7.43 (m, 2H), 4.07 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 150.14 , 143.40 , 124.51 , 41.41 . **Brown solid.**

KM10-98



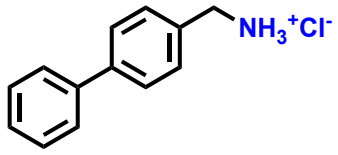
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.28 (br s, 3H), 7.79 - 7368 (m, 2H), 6.73 (s, 1H), 3.91 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 144.15 , 142.37 , 119.32 , 111.59 , 33.83 . **Brown solid.**

KM10-101



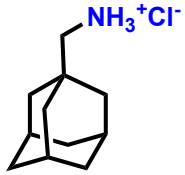
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.65 (br s, 3H), 7.18 (s, 1H), 6.99 (d, *J* = 7.9 Hz, 1H), 6.92 (d, *J* = 7.7 Hz, 1H), 6.03 (s, 2H), 3.90 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 147.67 , 147.66 , 128.15 , 123.37 , 110.03 , 108.62 , 101.64 , 42.38 . **White solid.**

KM10-103



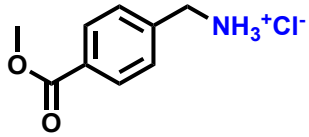
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.78 (br s, 3H), 7.87 – 7.58 (m, 6H), 7.58 – 7.28 (m, 3H), 4.06 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 140.59 , 140.02 , 133.78 , 130.13 , 129.45 , 128.12 , 127.18 , 127.15 , 42.25 .

KM10-120



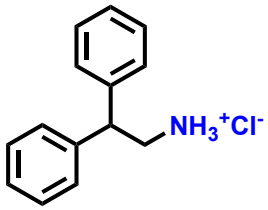
^{1}H NMR (300 MHz, DMSO-d_6) δ 5.33 (br s, 3H), 2.31 (s, 2H), 1.99 – 1.87 (m, 3H), 1.75 – 1.52 (m, 6H), 1.52 – 1.42 (m, 6H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 52.58 , 39.75 , 36.94 , 33.05 , 28.12 . **White solid.**

KM10-54



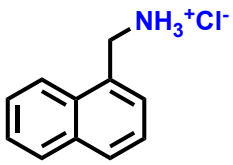
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.82 (br s, 3H), 7.96 (d, *J* = 8.5 Hz, 2H), 7.68 (d, *J* = 8.5 Hz, 2H), 4.11 (s, 2H), 3.85 (s, 3H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 166.35 , 139.92 , 129.85 , 129.70 , 129.65 , 52.71 , 42.12 . **White solid.**

KM10-109



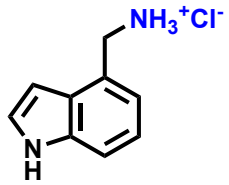
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.20 (br s, 3H), 7.59 – 7.05 (m, 10H), 4.46 (t, *J* = 7.8 Hz, 1H), 3.52 (d, *J* = 7.8 Hz, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 141.69 , 129.19 , 128.32 , 127.39 , 49.03 , 42.94 . **Off white solid.**

KM10-110



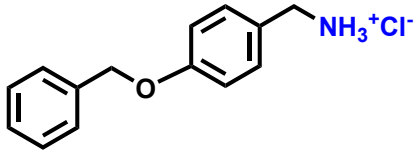
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.41 (br s, 3H), 8.23 – 8.10 (m, 1H), 8.05 – 7.91 (m, 2H), 7.70 (dd, *J* = 7.1, 1.2 Hz, 1H), 7.67 – 7.44 (m, 3H), 4.50 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 133.64 , 131.12 , 130.95 , 129.29 , 129.07 , 127.55 , 127.14 , 126.62 , 125.82 , 123.95 , 39.75 . **Off white solid.**

KM10-124



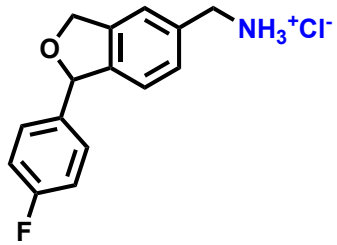
^{1}H NMR (300 MHz, DMSO-d_6) δ 11.50 (s, 1H), 8.66 (br s, 3H), 7.48 – 7.37 (m, 2H), 7.19 – 7.08 (m, 2H), 6.72 – 6.63 (m, 1H), 4.24 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 136.28 , 127.03 , 126.16 , 125.42 , 121.23 , 119.37 , 112.27 , 99.74 , 40.44 . **Off white solid.**

KM10-127



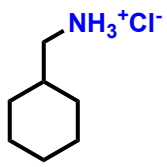
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.59 (br s, 3H), 7.65 – 7.23 (m, 7H), 7.03 (d, *J* = 8.7 Hz, 2H), 5.13 (s, 2H), 3.92 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 158.75 , 137.42 , 131.05 , 128.90 , 128.29 , 128.08 , 126.72 , 115.24 , 69.62 , 42.04 . **White solid.**

KM10-128



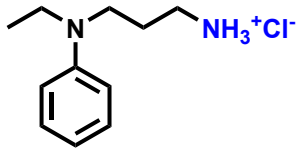
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.67 (br s, 3H), 7.53 (s, 1H), 7.44 – 7.34 (m, 3H), 7.23 – 7.14 (m, 2H), 7.08 (d, *J* = 7.8 Hz, 1H), 6.19 (s, 1H), 5.30 (dd, *J* = 12.8, 2.6 Hz, 1H), 5.12 (d, *J* = 12.2 Hz, 1H), 4.02 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 162.16 (d, *J* = 243.4 Hz), 142.54 , 139.49 , 139.25 (d, *J* = 2.8 Hz), 134.29 , 129.05 , 128.90 (d, *J* = 8.3 Hz), 122.60 , 122.46 , 115.72 (d, *J* = 21.4 Hz), 84.47 , 72.85 , 42.38 . **White solid.**

KM10-138



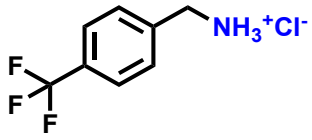
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.20 (br s, 3H), 2.72 – 2.49 (m, 2H), 1.93 – 1.46 (m, 6H), 1.23 – 0.67 (m, 5H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 44.80 , 35.76 , 30.30 , 26.13 , 25.54 . **White solid.**

KM10-144



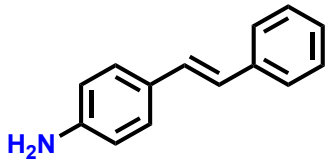
^{1}H NMR (300 MHz, DMSO-d_6) δ 7.67 (br s, 3H), 7.32 – 6.98 (m, 2H), 6.68 (d, *J* = 8.2 Hz, 2H), 6.66 – 6.41 (m, 1H), 3.45 – 3.14 (m, 4H), 2.94 – 2.67 (m, 2H), 1.99 – 1.68 (m, 2H), 1.04 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 147.87 , 129.56 , 115.68 , 112.26 , 47.17 , 44.56 , 37.30 , 26.00 , 12.49 . **Off white solid.**

KM10-121



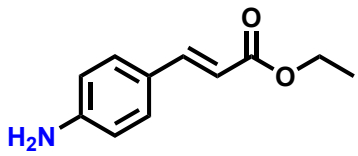
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.85 (br s, 3H), 7.93 – 7.56 (m, 4H), 4.12 (s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 139.30 , 130.27 , 129.26 (q, *J* = 31.8 Hz), 125.76 , 124.59 (d, *J* = 272.1 Hz), 41.99 . **White solid.**

KM10-182



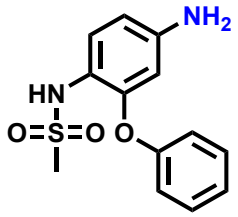
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.45 – 7.05 (m, 7H), 7.00 – 6.74 (m, 2H), 6.54 (d, *J* = 8.0 Hz, 2H), 3.42 (br s, 2H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 146.22 , 138.02 , 128.77 , 128.67 , 128.06 , 127.81 , 126.96 , 126.18 , 125.16 , 115.28 . **Yellow solid.**

KM10-186



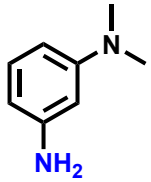
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.51 (d, *J* = 15.9 Hz, 1H), 7.24 (d, *J* = 8.2 Hz, 2H), 6.54 (d, *J* = 8.6 Hz, 2H), 6.14 (d, *J* = 15.9 Hz, 1H), 4.15 (q, *J* = 7.1 Hz, 2H), 3.82 (br s, 2H), 1.23 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 167.76 , 148.82 , 144.93 , 129.86 , 124.62 , 114.83 , 113.61 , 60.18 , 14.39 . **Yellow solid.**

KM10-200



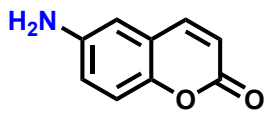
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.34 – 7.21 (m, 3H), 7.13 – 7.02 (m, 1H), 6.95 – 6.88 (m, 2H), 6.32 (dd, *J* = 8.6, 2.5 Hz, 1H), 6.08 (d, *J* = 2.5 Hz, 1H), 3.55 (br s, 2H), 2.82 (s, 3H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 155.81 , 150.57 , 146.26 , 130.12 , 127.28 , 124.28 , 118.87 , 117.76 , 110.61 , 104.53 , 39.00 . **Brown solid.**

KM10-252



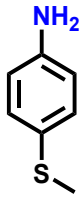
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.26 – 6.90 (m, 1H), 6.41 – 5.89 (m, 3H), 3.40 (br s, 2H), 2.96 (s, 6H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 151.88 , 147.35 , 129.88 , 104.38 , 103.86 , 99.71 , 40.64 . **Brown gum.**

KM10-244



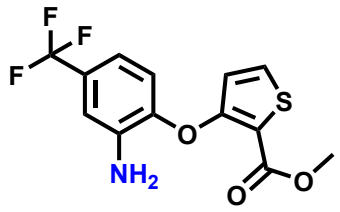
^{1}H NMR (300 MHz, DMSO-d_6) δ 7.85 (d, *J* = 9.5 Hz, 1H), 7.10 (d, *J* = 8.8 Hz, 1H), 6.86 (dd, *J* = 8.8, 2.7 Hz, 1H), 6.74 (d, *J* = 2.7 Hz, 1H), 6.35 (d, *J* = 9.5 Hz, 1H), 5.16 (br s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 160.98 , 145.91 , 145.74 , 144.77 , 119.51 , 119.30 , 116.98 , 116.29 , 110.81 . **Yellow solid.**

KM10-255



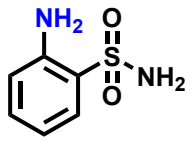
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.09 (d, *J* = 8.5 Hz, 2H), 6.53 (d, *J* = 8.5 Hz, 2H), 3.42 (br s, 2H), 2.32 (s, 3H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 145.16 , 131.07 , 125.73 , 115.78 , 18.81 . **Brown gum.**

KM10-256



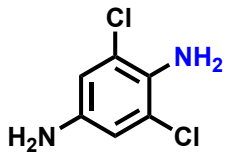
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.35 (d, *J* = 5.5 Hz, 1H), 6.99 – 6.92 (m, 1H), 6.87 – 6.79 (m, 2H), 6.66 (d, *J* = 5.5 Hz, 1H), 3.86 (br s, 2H), 3.77 (s, 3H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 161.50 , 156.96 , 146.67 , 138.27 , 130.48 , 127.03 (q, *J* = 32.4 Hz), 124.06 (q, *J* = 271.8 Hz) , 120.89 , 117.96 , 117.50 , 115.18 (q, *J* = 3.9 Hz), 112.94 (q, *J* = 3.7 Hz), 51.98 . **Yellow gum.**

KM10-269



^{1}H NMR (300 MHz, DMSO-d_6) δ 7.55 (d, *J* = 7.8 Hz, 1H), 7.33 – 7.14 (m, 3H), 6.80 (dd, *J* = 8.2, 1.4 Hz, 1H), 6.67 – 6.54 (m, 1H), 5.84 (br s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 146.00 , 133.32 , 128.33 , 124.68 , 117.15 , 115.43 . **Off white solid.**

KM10-267

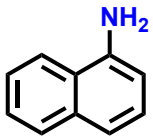


^{1}H NMR (300 MHz, Chloroform-*d*) δ 6.52 (s, 2H), 3.60 (br s, 4H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 138.37 , 132.53 , 120.81 , 115.43 . **Brown solid.**

KM10-242

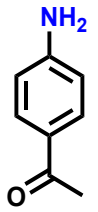
^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.67 (dd, *J* = 4.2, 1.7 Hz, 1H), 7.96 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.33 – 7.19 (m, 2H), 7.05 (dd, *J* = 8.2, 1.3 Hz, 1H), 6.83 (dd, *J* = 7.5, 1.3 Hz, 1H), 4.84 (br s, 2H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 147.42 , 143.98 , 138.43 , 136.01 , 128.87 , 127.40 , 121.34 , 116.03 , 110.05 . **Brown solid.**

KM10-251



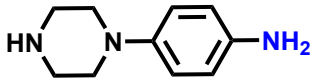
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.94 – 7.78 (m, 2H), 7.62 – 7.44 (m, 2H), 7.43 – 7.27 (m, 2H), 6.83 (dd, *J* = 6.6, 1.8 Hz, 1H), 4.16 (br s, 2H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 142.15 , 134.46 , 128.61 , 126.40 , 125.90 , 124.90 , 123.72 , 120.86 , 119.02 , 109.74 . **Brown solid.**

KM10-277



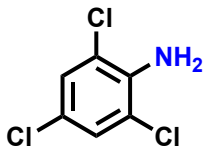
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 8.7 Hz, 2H), 6.56 (d, *J* = 8.7 Hz, 2H), 4.13 (br s, 2H), 2.42 (s, 3H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 196.52 , 151.28 , 130.80 , 113.71 , 26.08 . **Off white solid.**

KM10-265



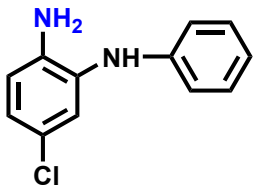
^{1}H NMR (300 MHz, Chloroform-*d*) δ 6.75 (d, *J* = 8.8 Hz, 2H), 6.57 (d, *J* = 8.7 Hz, 2H), 3.01 - 2.93 (m, 11H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 144.87 , 140.33 , 118.61 , 116.14 , 52.17 , 46.18 . **Brown gum.**

KM10-268



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.07 (s, 2H), 4.32 (br s, 2H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 139.04, 127.59 , 121.85, 119.70 . **Brown solid.**

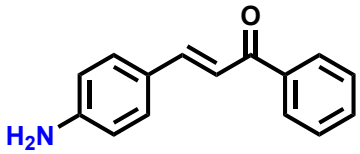
KM10-272



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.38 – 7.24 (m, 2H), 7.16 (d, *J* = 2.3 Hz, 1H), 7.06 – 6.90 (m, 2H), 6.83 (dt, *J* = 7.7, 1.1 Hz, 2H), 6.74 (d, *J* = 8.4 Hz, 1H), 5.34 (br s, 1H), 3.76 (br s, 2H). **^{13}C NMR (75 MHz,**

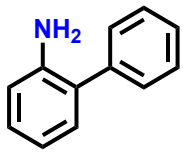
Chloroform-*d*) δ 144.33 , 139.69 , 130.42 , 129.53 , 124.77 , 123.45 , 123.23 , 120.27 , 117.15 , 116.15 . **Brown solid.**

KM10-270



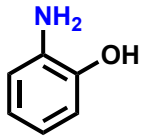
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.92 (d, *J* = 6.8 Hz, 2H), 7.67 (d, *J* = 15.6 Hz, 1H), 7.52 – 7.35 (m, 5H), 7.26 (d, *J* = 15.6 Hz, 1H), 6.59 (d, *J* = 8.5 Hz, 2H), 3.90 (br s, 2H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 190.80 , 149.23 , 145.57 , 138.84 , 132.34 , 130.53 , 128.51 , 128.36 , 125.07 , 117.94 , 114.87 . **Yellow solid.**

KM10-270



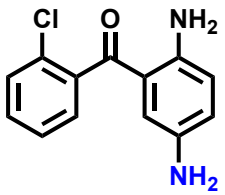
^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.66 – 7.42 (m, 5H), 7.31 – 7.23 (m, 2H), 7.02 – 6.92 (m, 1H), 6.86 (dt, *J* = 7.3, 1.1 Hz, 1H), 3.78 (br s, 2H). **^{13}C NMR (75 MHz, Chloroform-*d*)** δ 143.67 , 139.71 , 130.59 , 129.23 , 128.95 , 128.64 , 127.73 , 127.29 , 118.75 , 115.75 . **Colorless gum**.

KM10-273



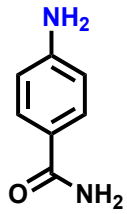
^{1}H NMR (300 MHz, DMSO-d_6) δ 8.97 (br s, 1H), 6.68 (ddd, *J* = 7.7, 1.4, 0.4 Hz, 1H), 6.65 – 6.54 (m, 2H), 6.43 (ddd, *J* = 7.7, 7.1, 2.0 Hz, 1H), 4.47 (br s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 144.47 , 136.94 , 120.02 , 117.00 , 114.97 , 114.88 . **Brown solid.**

KM10-281



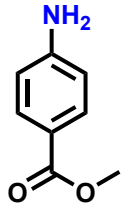
^{1}H NMR (300 MHz, DMSO-d_6) δ 7.60 – 7.31 (m, 5H), 6.83 (dd, *J* = 8.8, 2.6 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 1H), 6.32 (d, *J* = 2.6 Hz, 1H), 4.37 (br s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 196.22 , 145.44 , 140.72 , 137.77 , 130.83 , 129.99 , 129.73 , 128.68 , 127.60 , 126.05 , 118.46 , 116.61 , 116.25 . **Pale brown solid.**

KM10-284



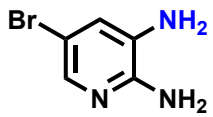
^{1}H NMR (300 MHz, DMSO-d_6) δ 7.63 (m, 3H), 6.95 (br s, 1H), 6.56 (d, *J* = 8.6 Hz, 2H), 5.63 (br s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 168.75 , 152.15 , 129.64 , 121.34 , 113.00 . **Off white solid.**

KM10-285



^{1}H NMR (300 MHz, DMSO-d_6) δ 7.67 (d, *J* = 8.7 Hz, 2H), 6.60 (d, *J* = 8.7 Hz, 2H), 5.97 (br s, 2H), 3.74 (s, 3H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 166.85 , 153.92 , 131.55 , 116.27 , 113.14 , 51.56 . **Off white solid.**

KM10-266



^{1}H NMR (300 MHz, DMSO-d_6) δ 7.29 (d, *J* = 2.2 Hz, 1H), 6.82 (d, *J* = 2.2 Hz, 1H), 5.61 (br s, 2H), 5.01 (br s, 2H). **^{13}C NMR (75 MHz, DMSO-d_6)** δ 147.85 , 134.47 , 132.34 , 119.55 , 106.88 . **Brown solid.**

NMR spectra

170428.f341.10.fid
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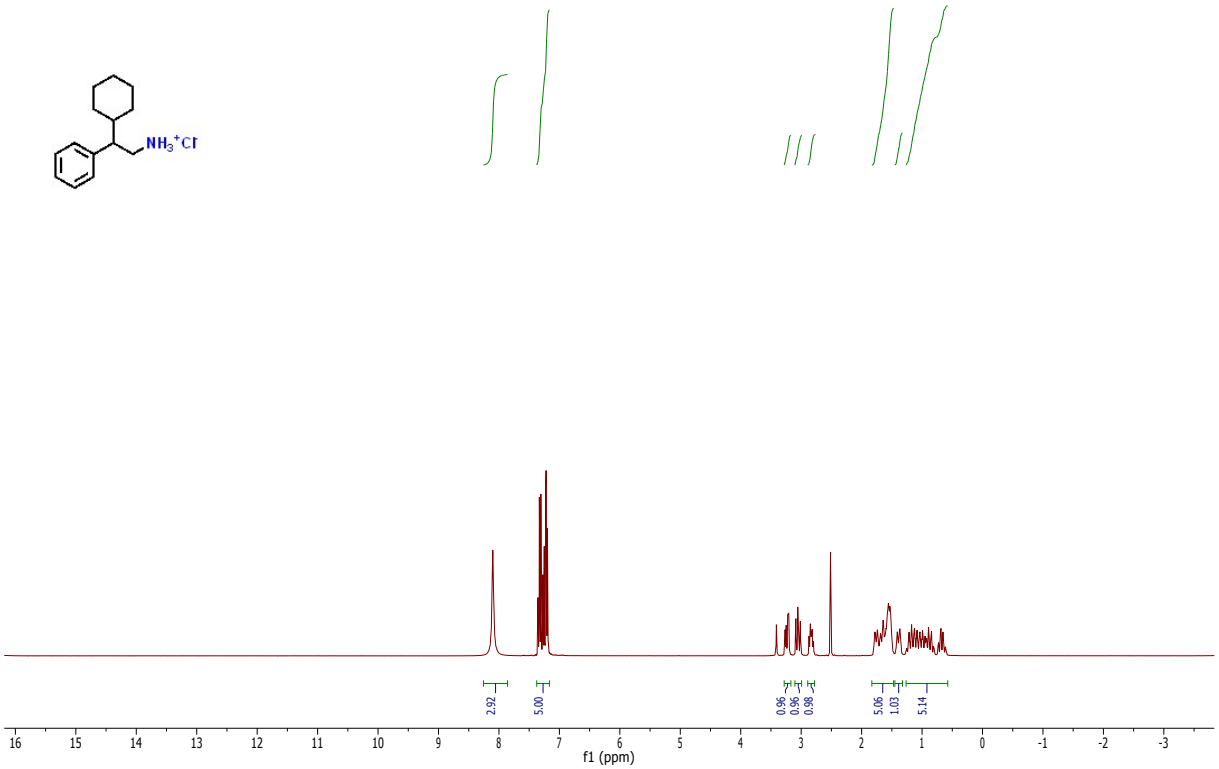
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1704 41



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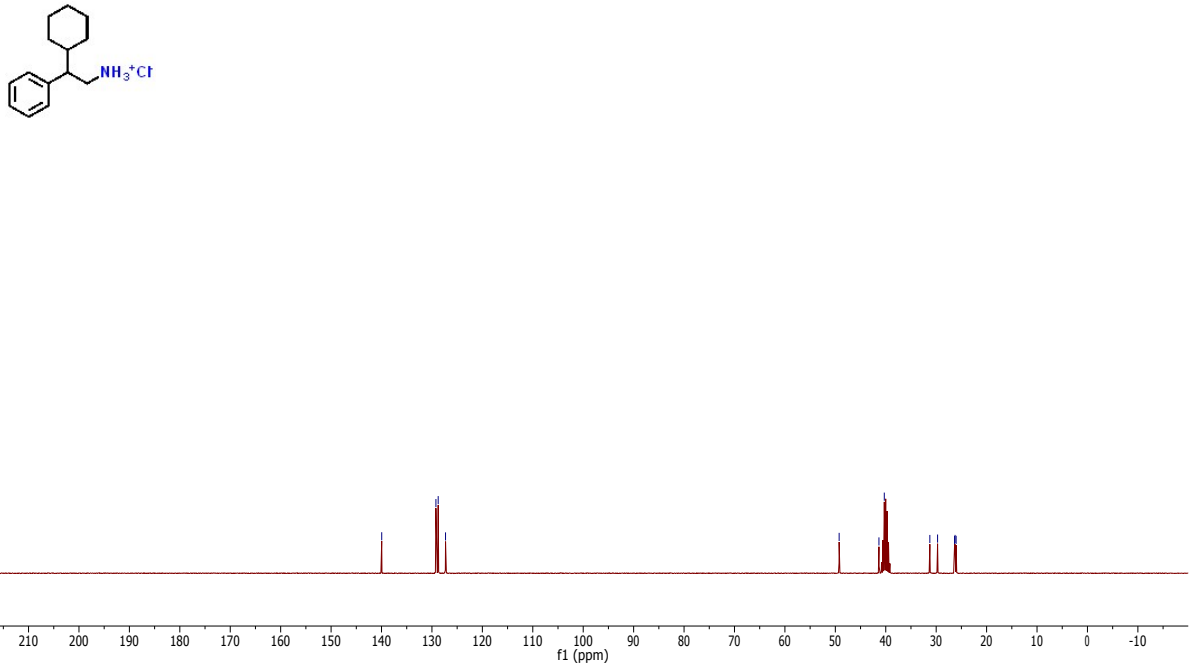
Kathir KMID-42
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1704 41



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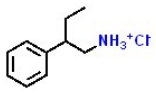
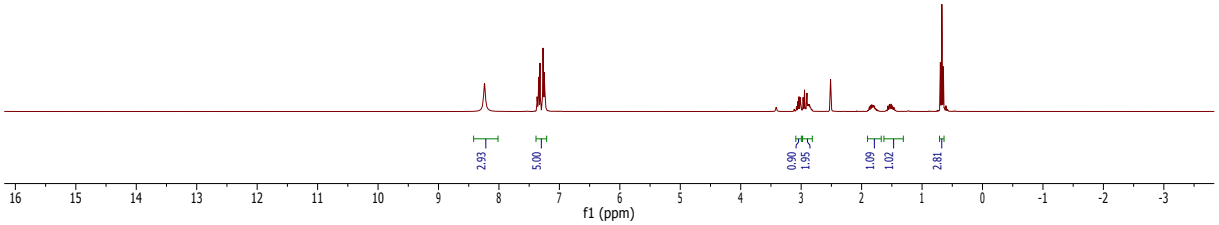
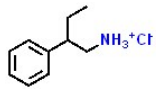
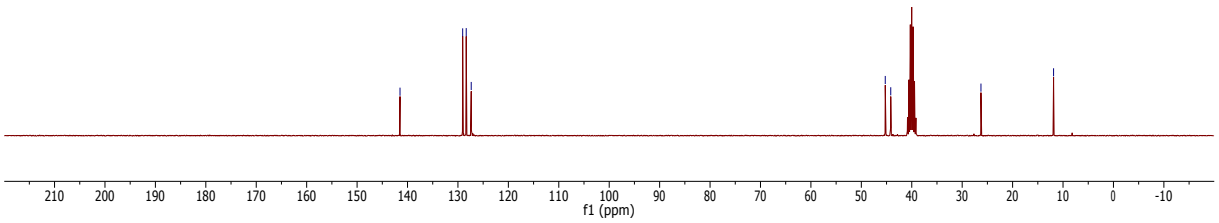




170428.f342.11.fid
Kathir KMID-47
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1704 42

141.49
129.06
128.36
127.37
45.26
44.17
26.28
11.88





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Kathir KMID-48
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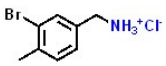

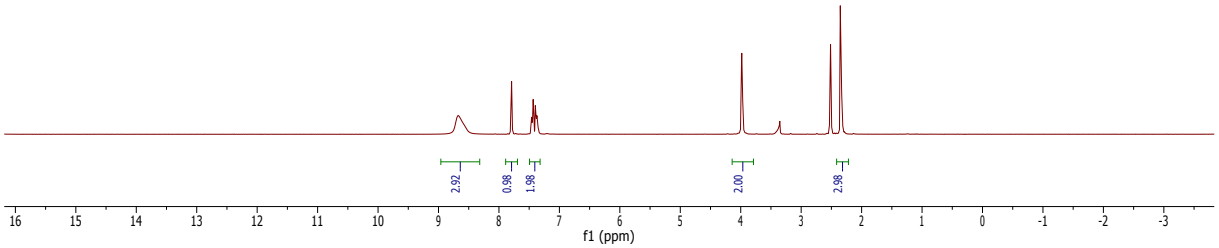

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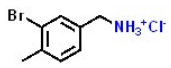
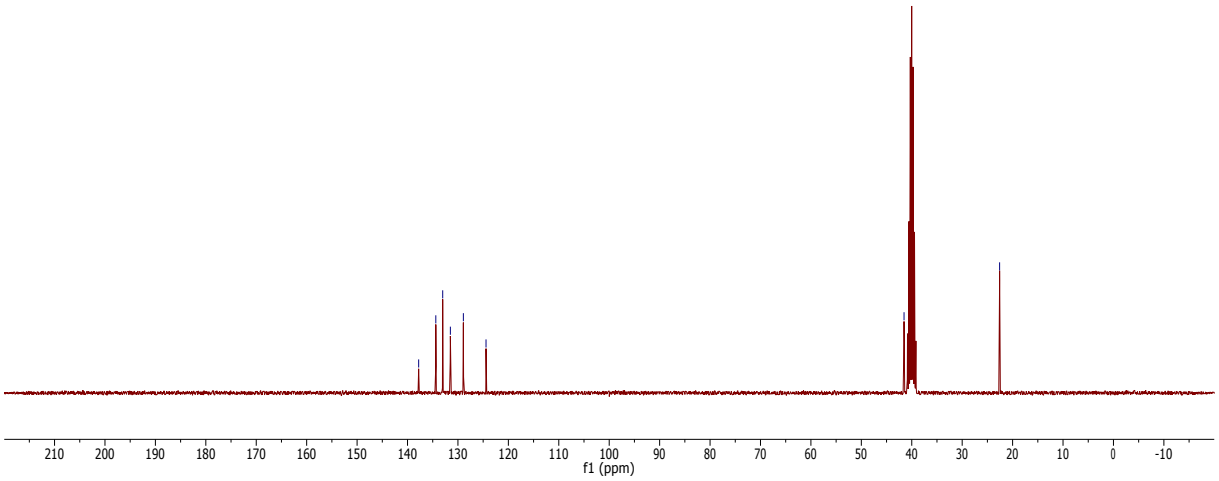
Kathir KMID-48
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1704 43





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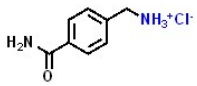

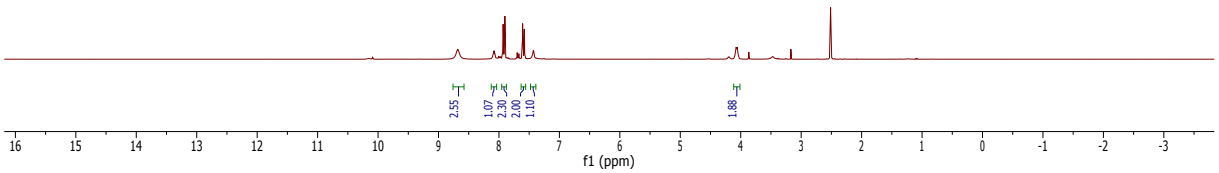

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Kathir KMID-52
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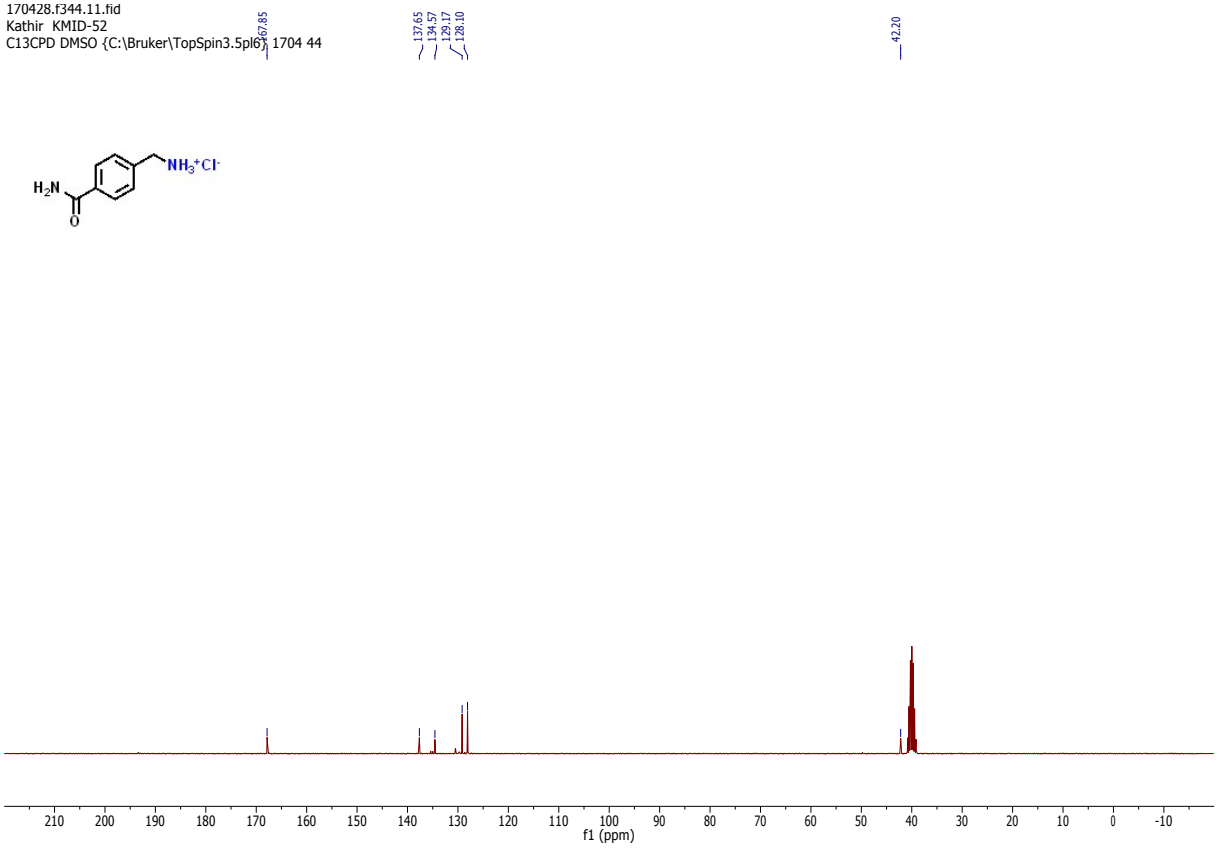

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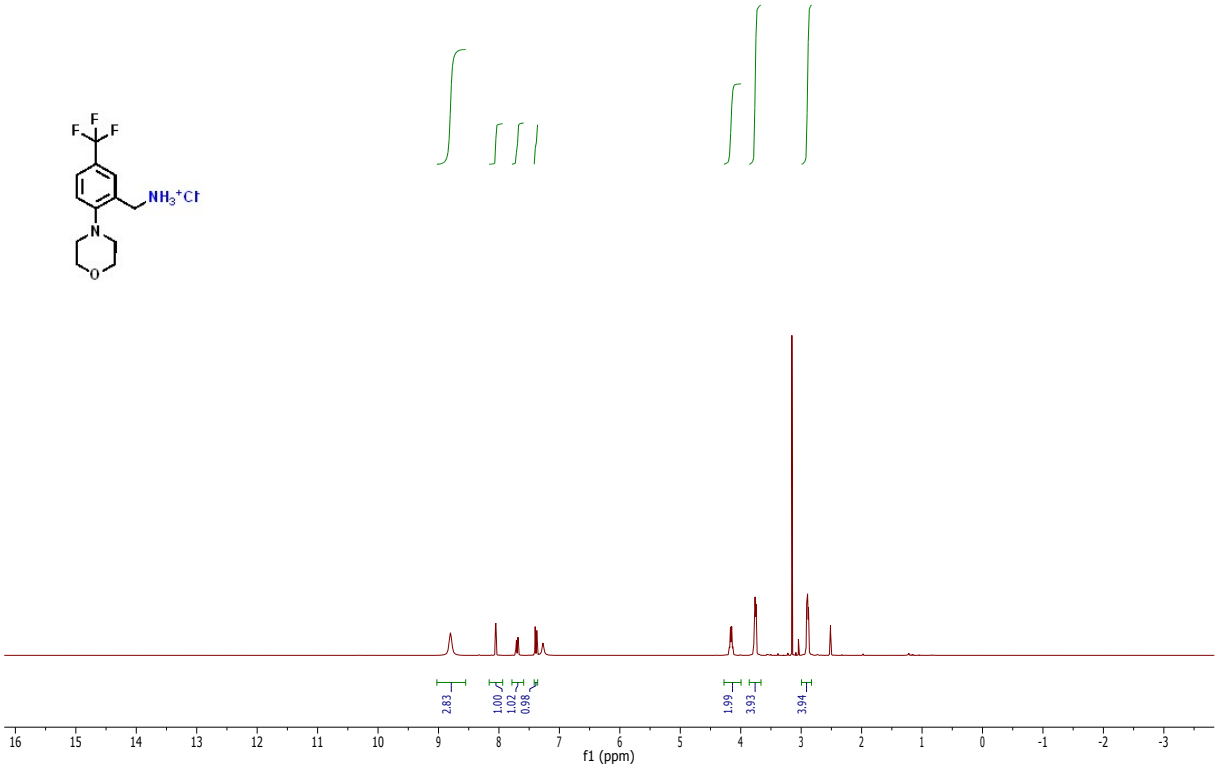

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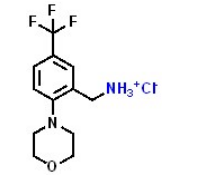
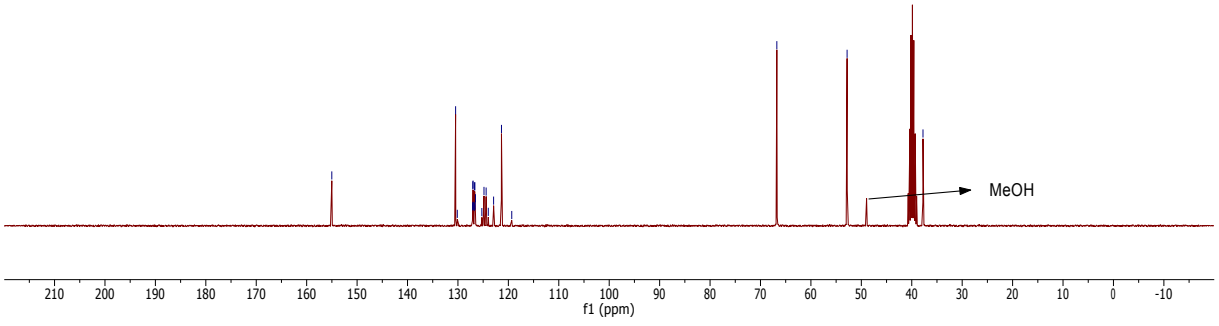
Kathir KMID-72
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1704 52





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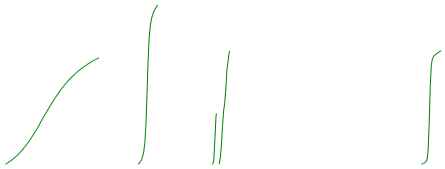

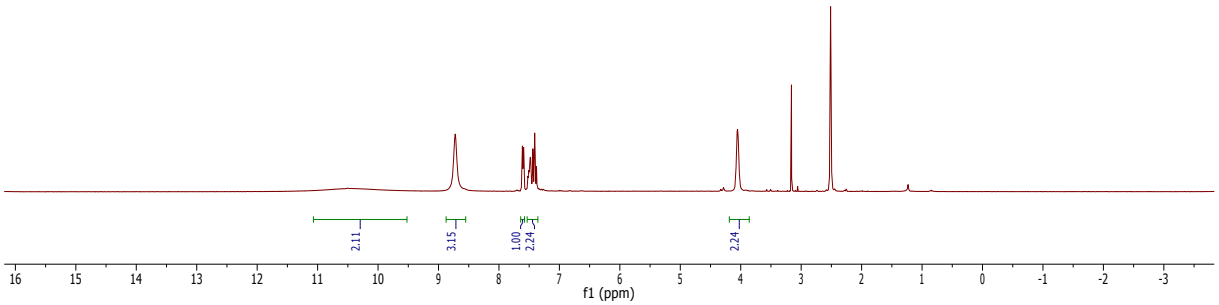

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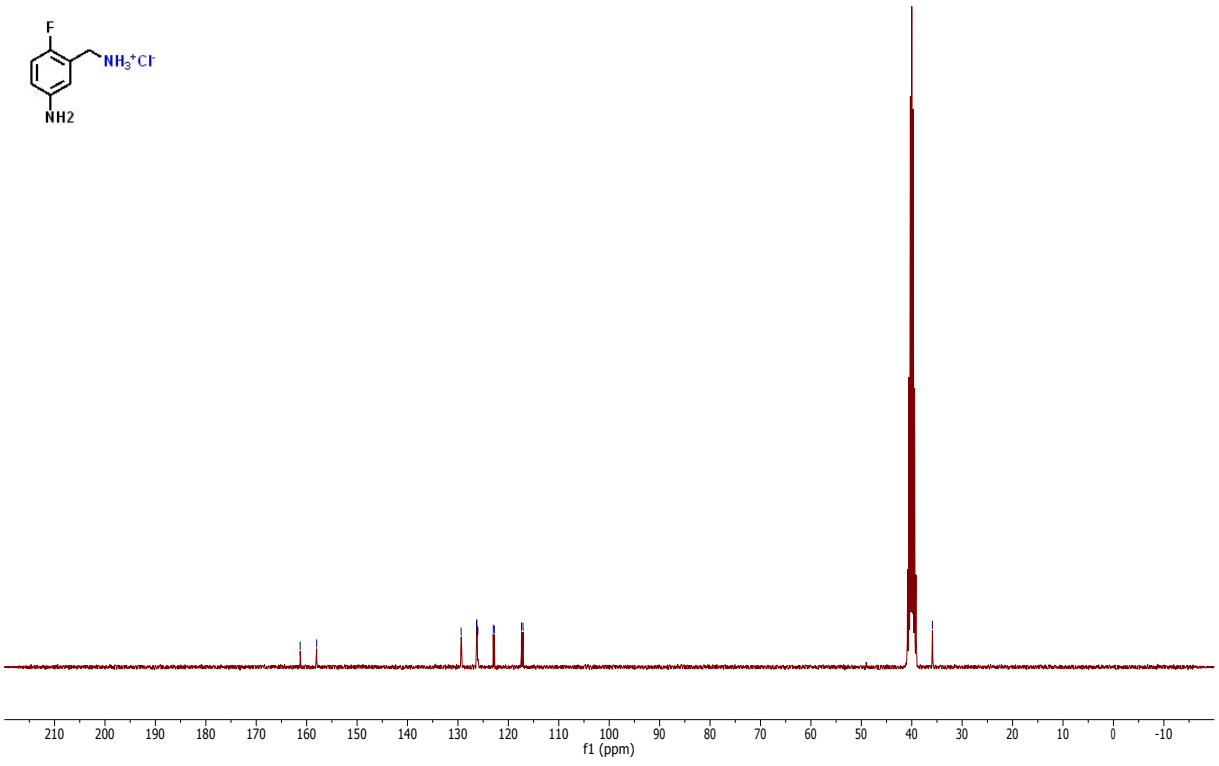

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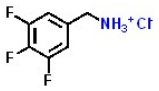

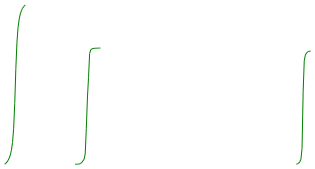

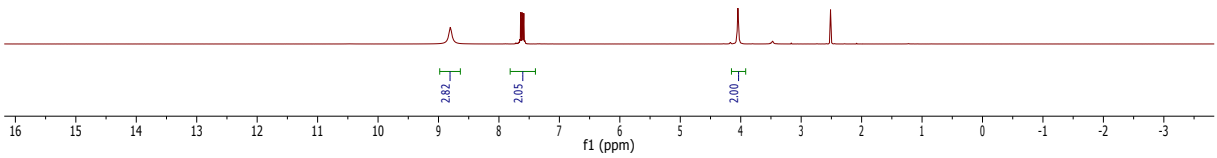

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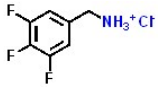

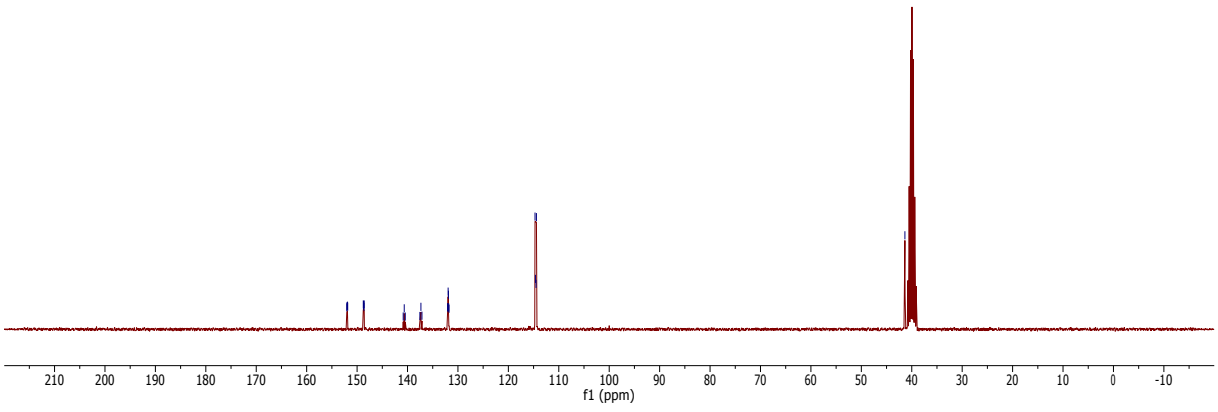

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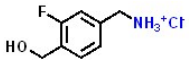

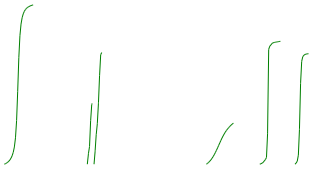

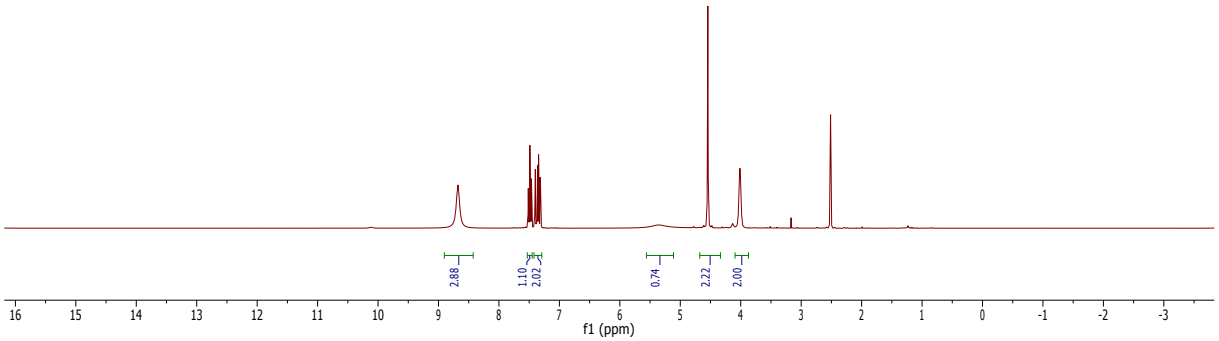

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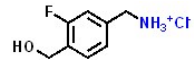
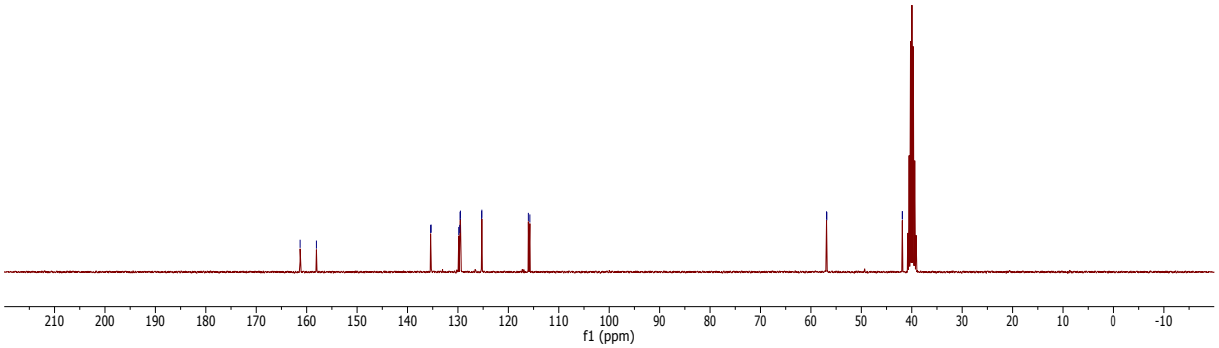
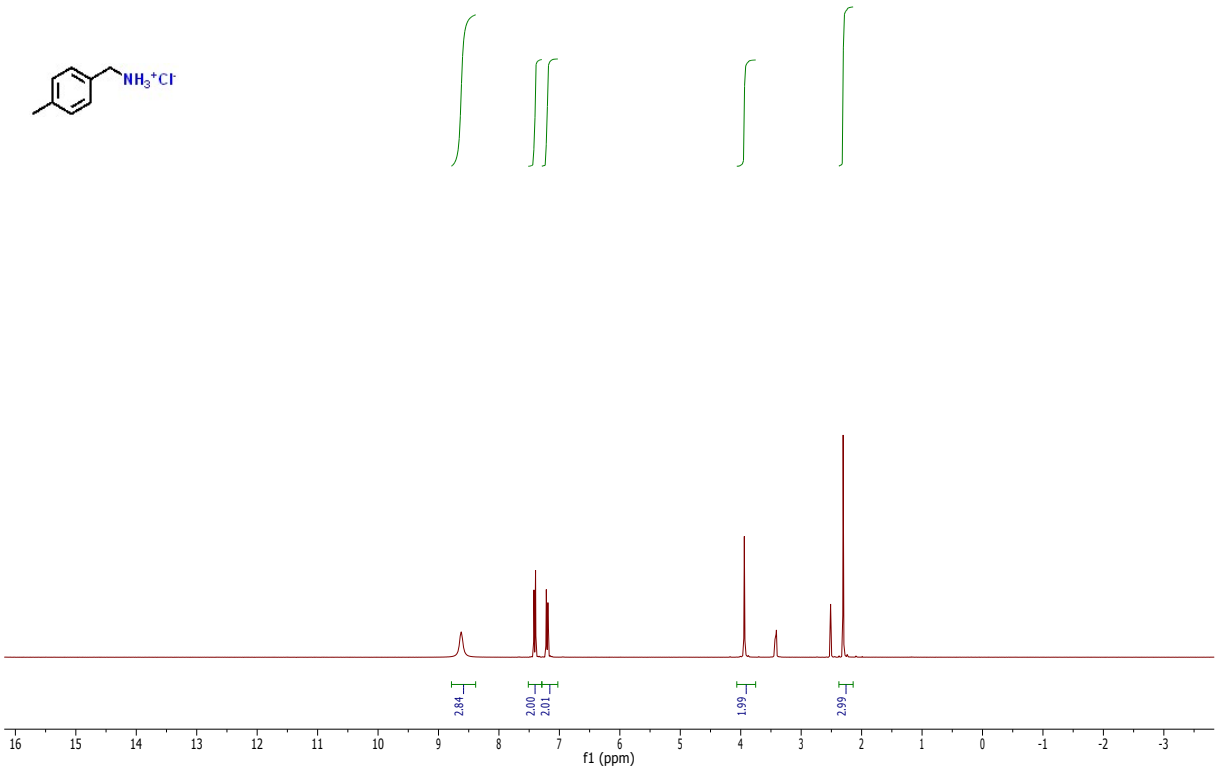




170503.f301.10.fid
Kathir/ KM10-24
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 1



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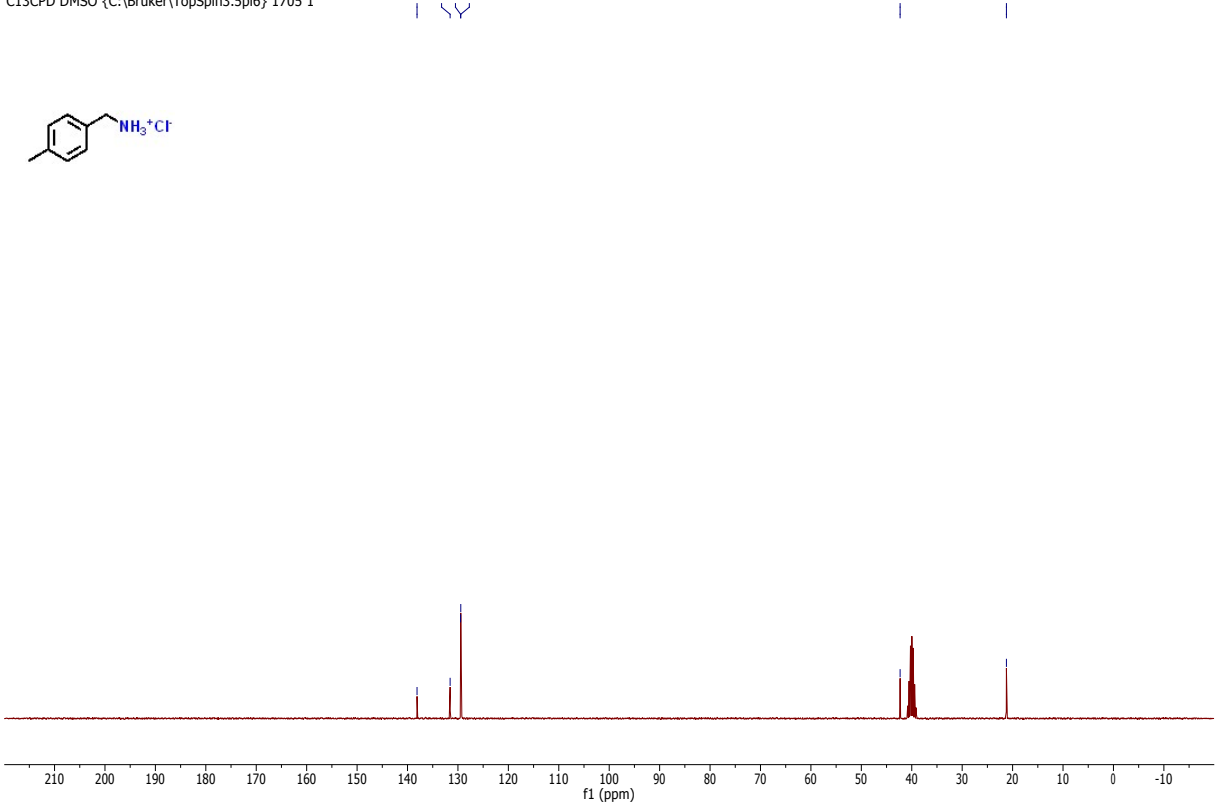

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Kathir/ KM10-45
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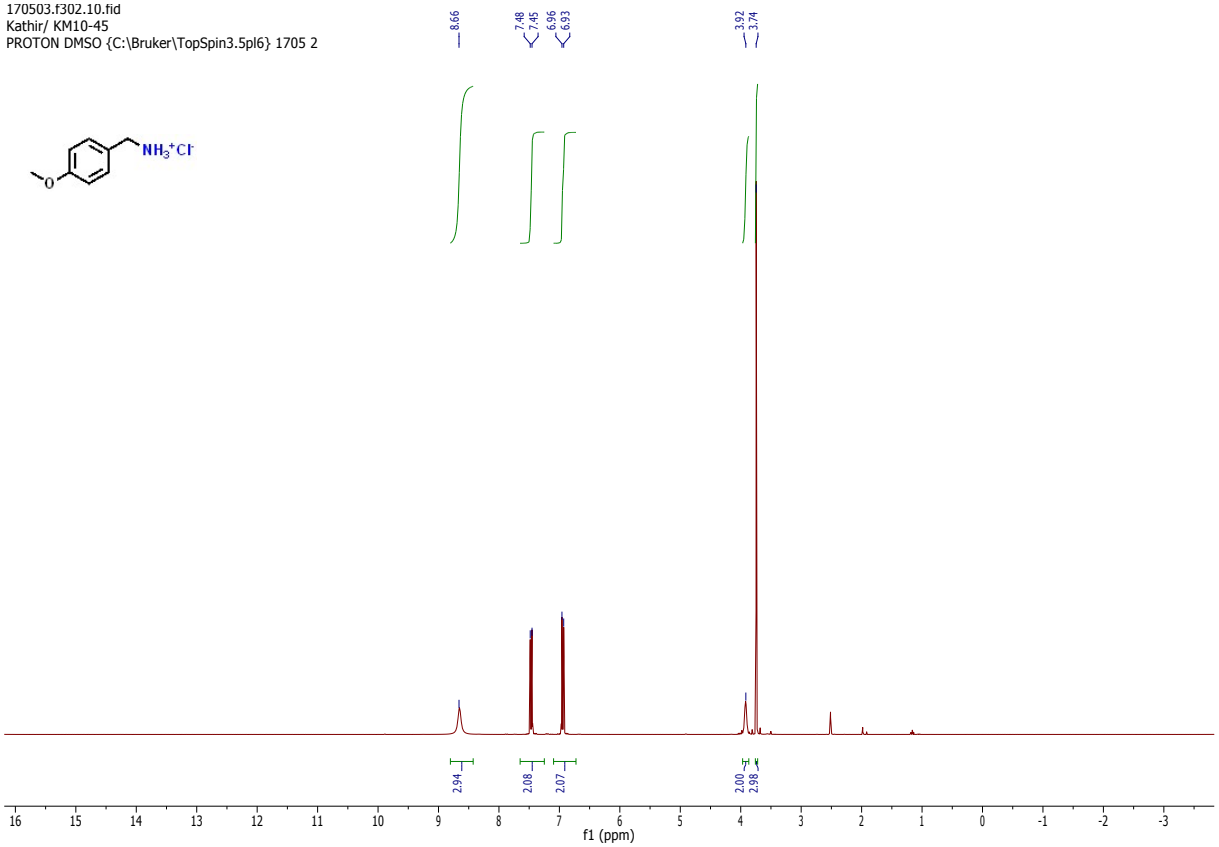

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Kathir/ KM10-45
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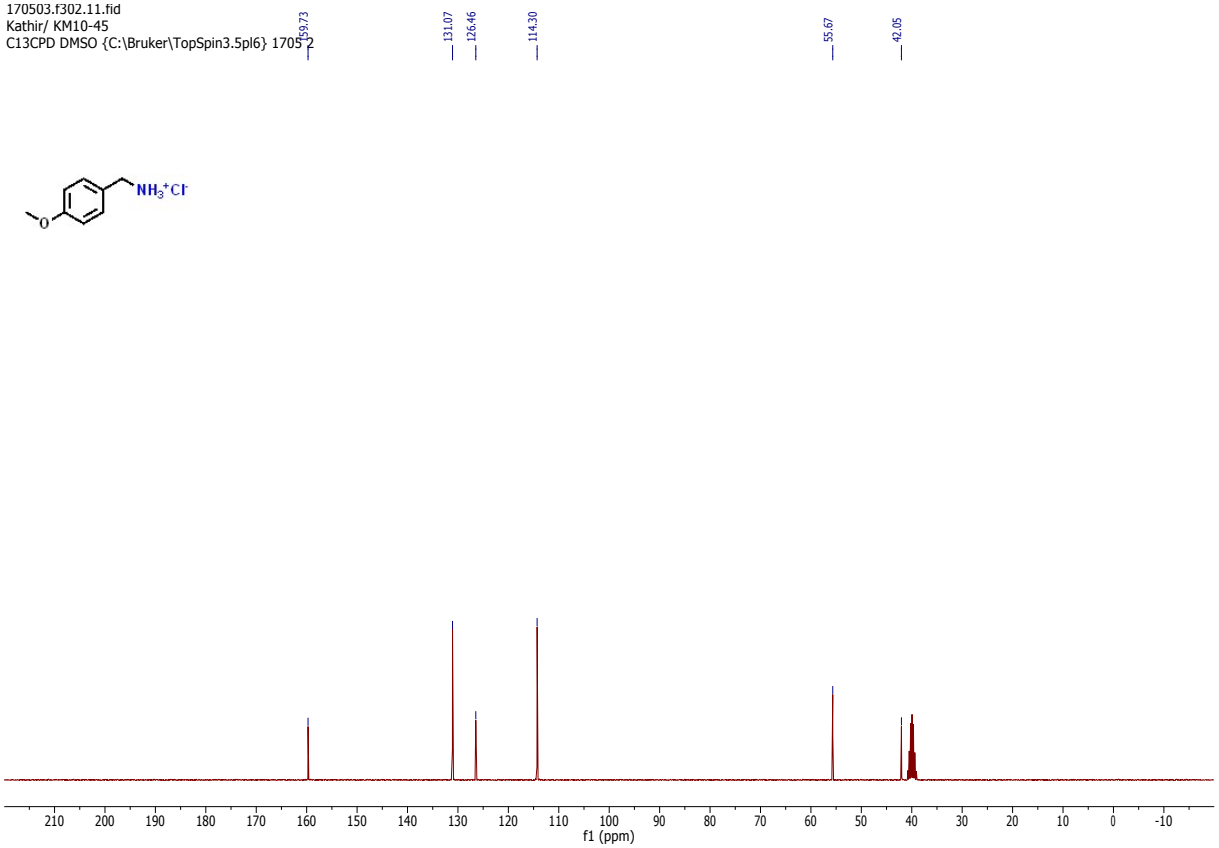

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Kathir/ KM10-56
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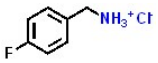

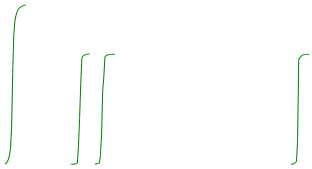

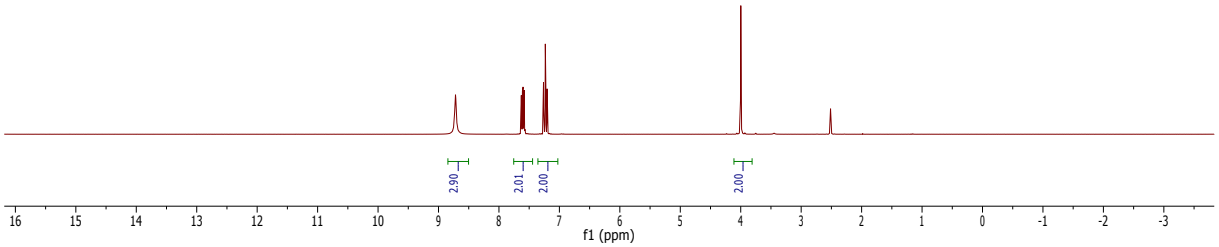

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Kathir/ KM10-56
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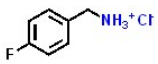

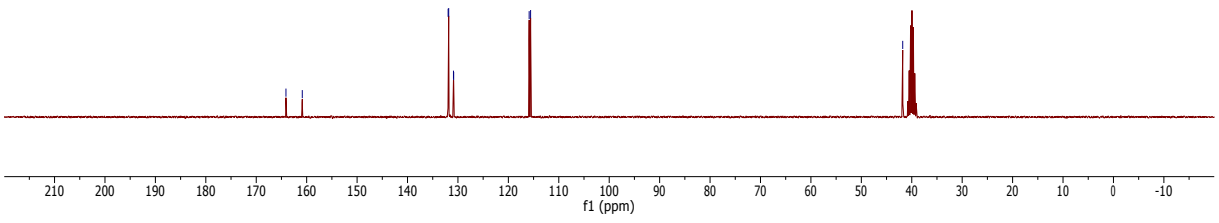

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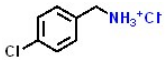
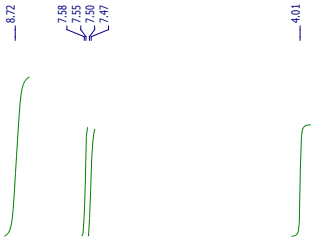
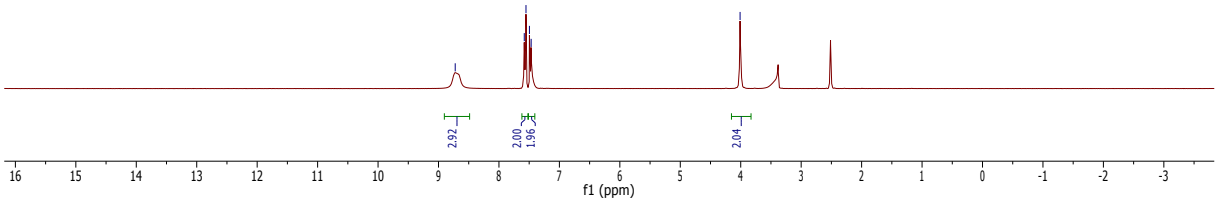
Kathir/ KM10-57
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 4







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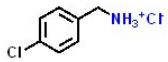
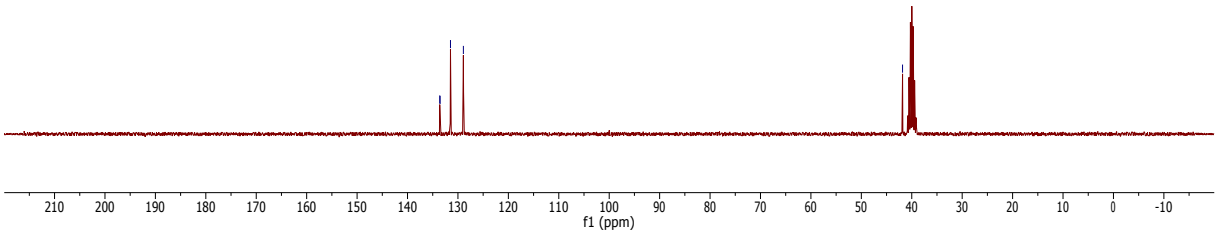
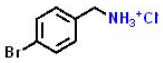
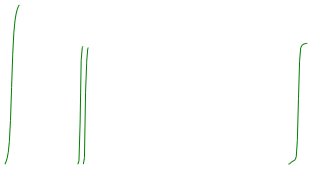
Kathir/ KM10-57
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 4

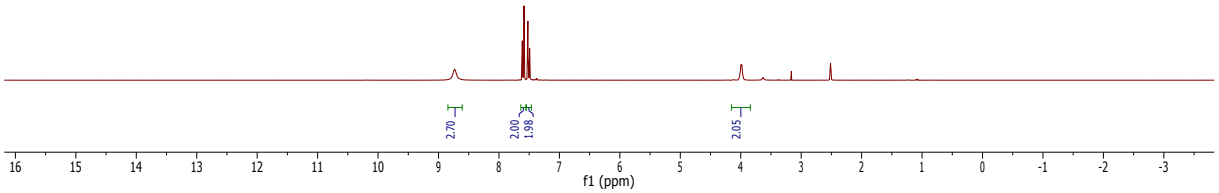




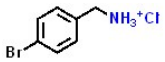
170503.f305.10.fid
Kathir/ KM10-58
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 5

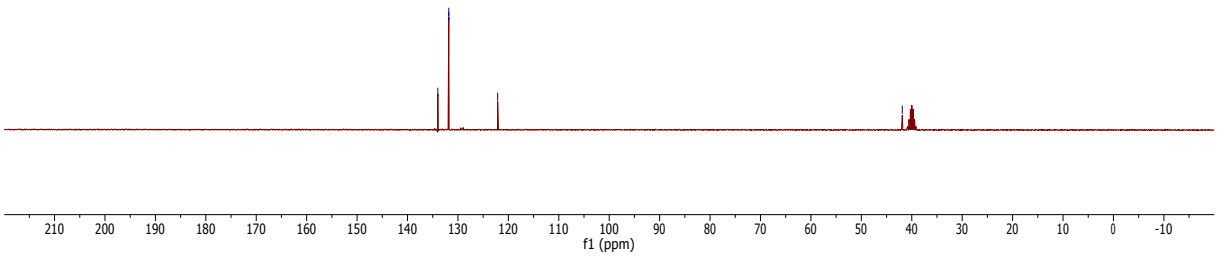






170503.f305.11.fid
Kathir/ KM10-58
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 5





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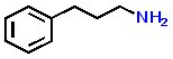
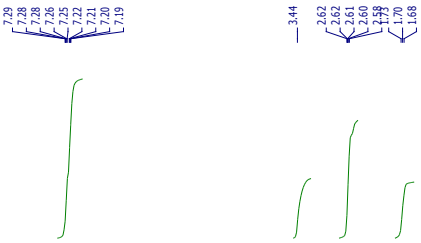
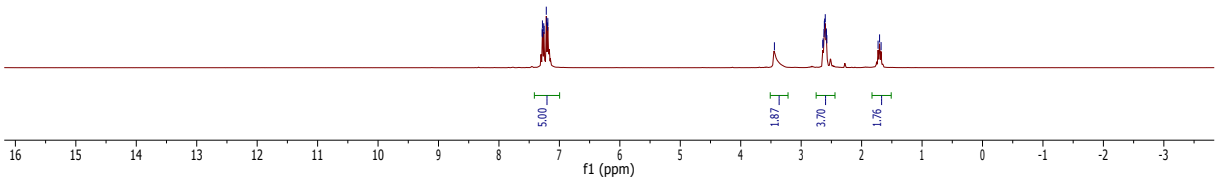
Kathir/ KM10-60
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 6







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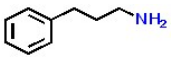
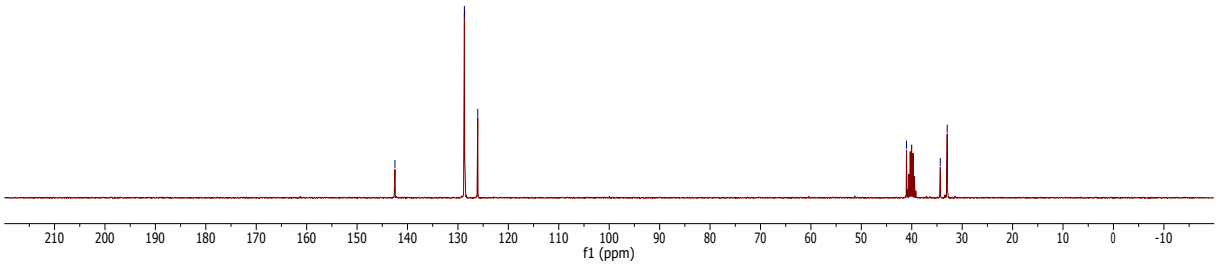
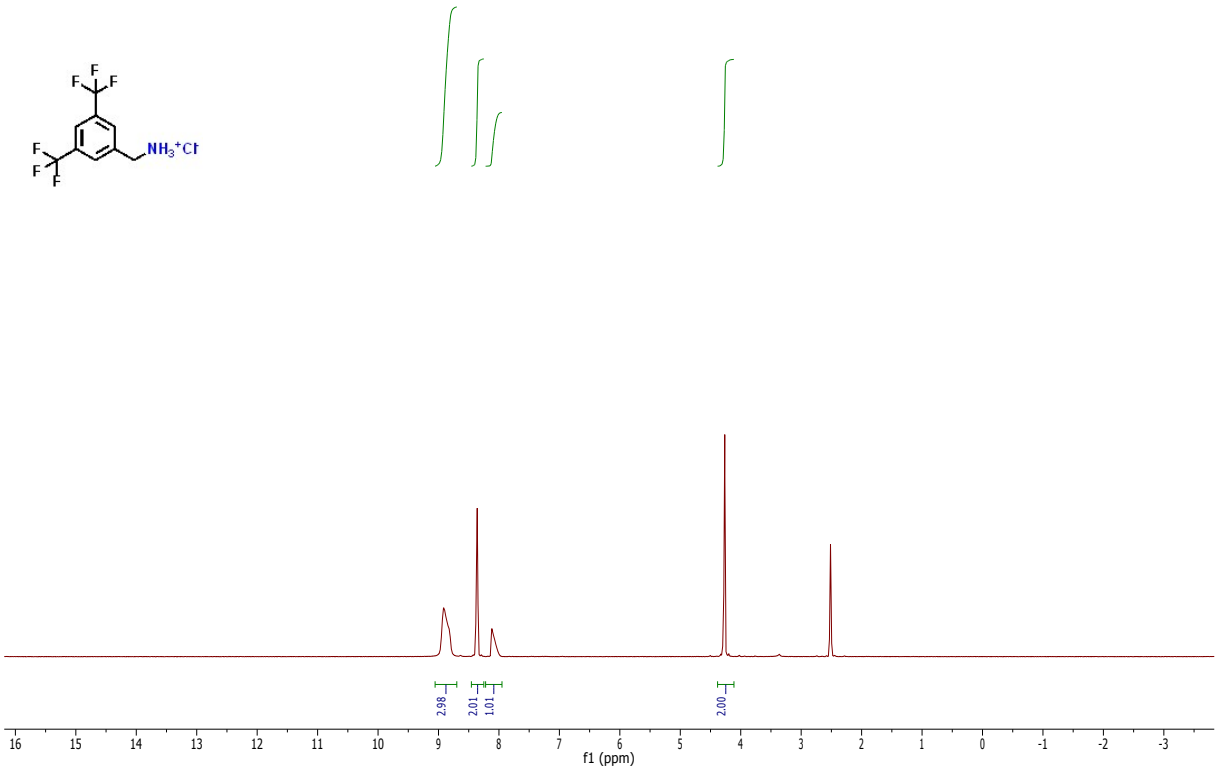
Kathir/ KM10-60
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 6





170503.f307.10.fid
Kathir/ KM10-61
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 7



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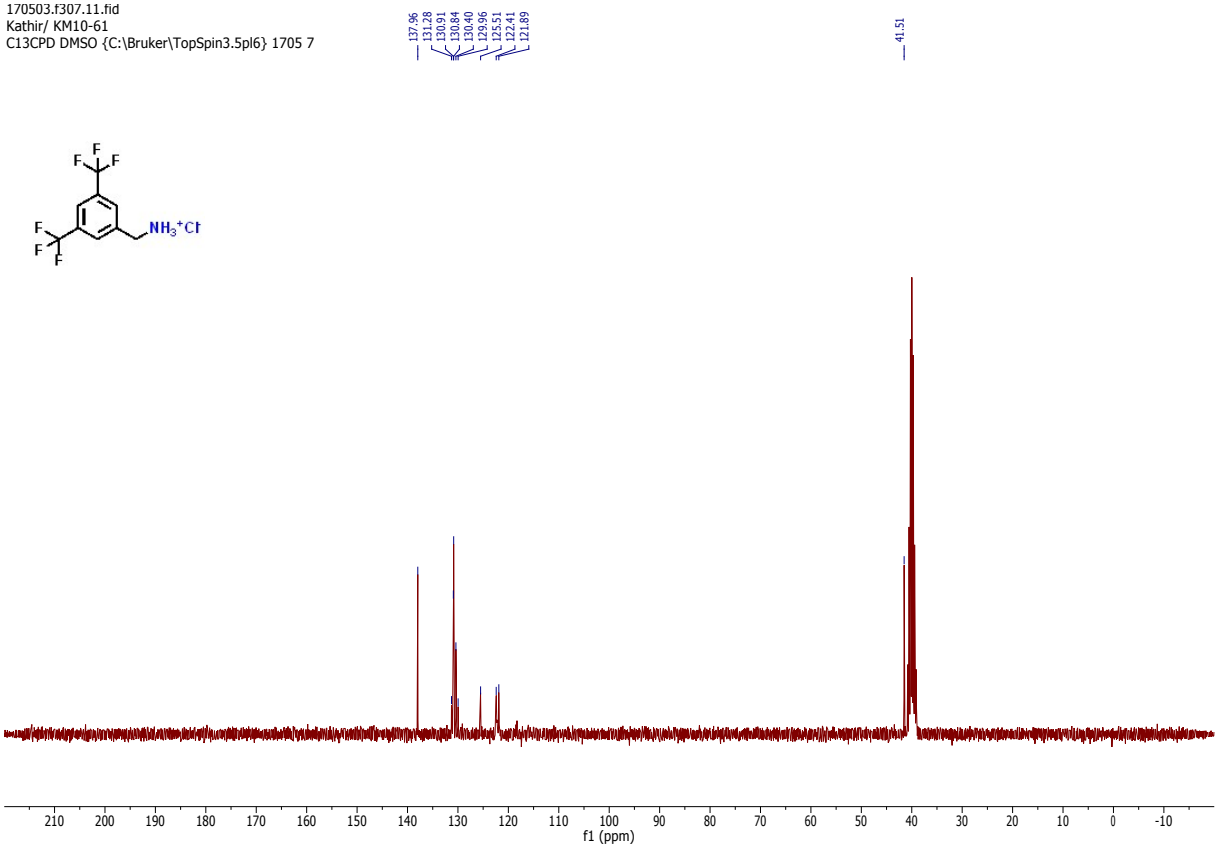
Kathir/ KM10-61
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 7



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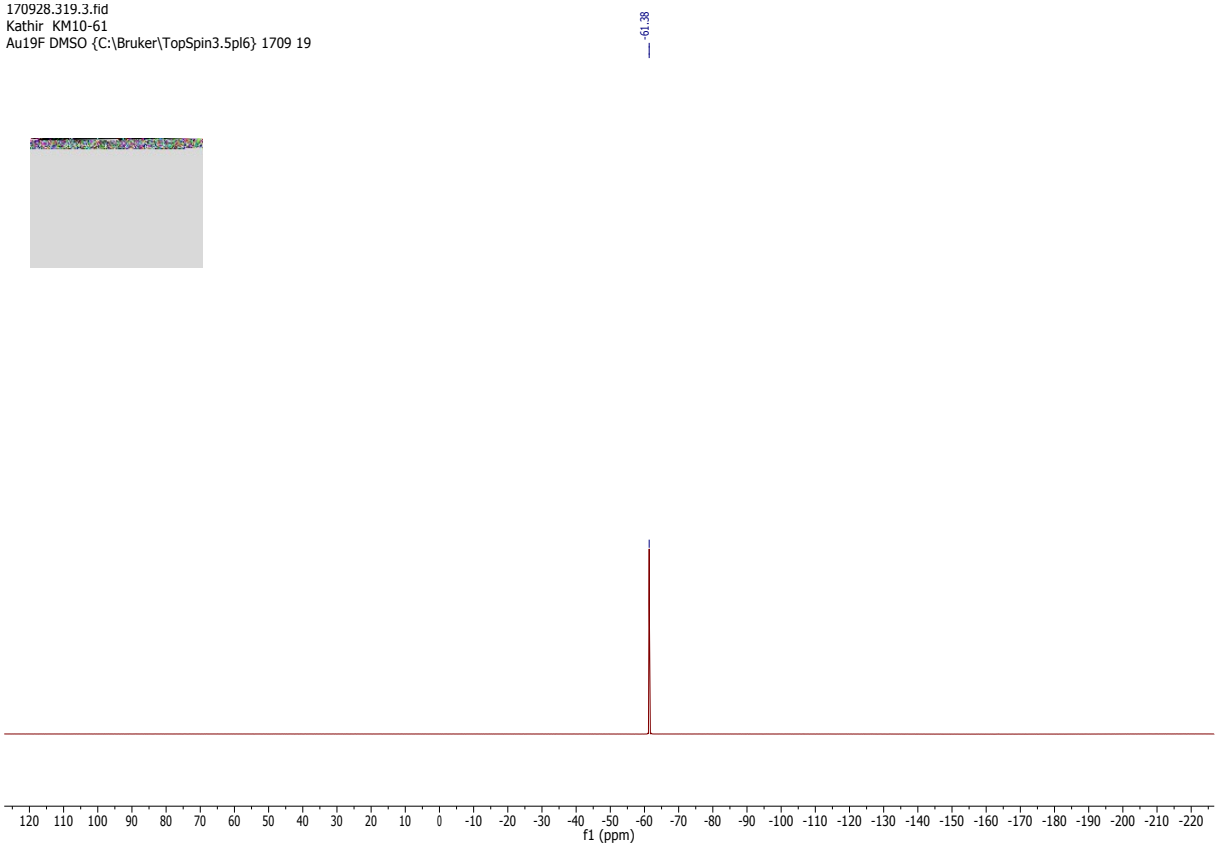
Kathir KM10-61
Au19F DMSO {C:\Bruker\TopSpin3.5pl6} 1709 19



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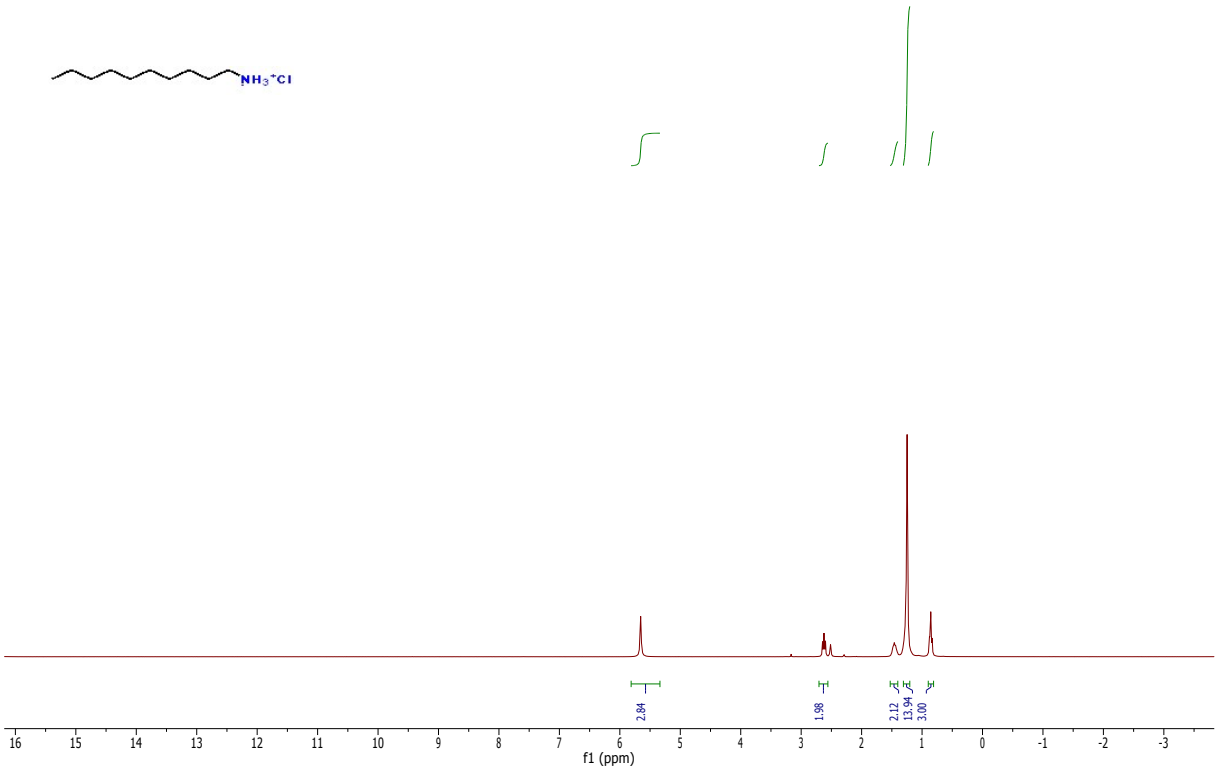
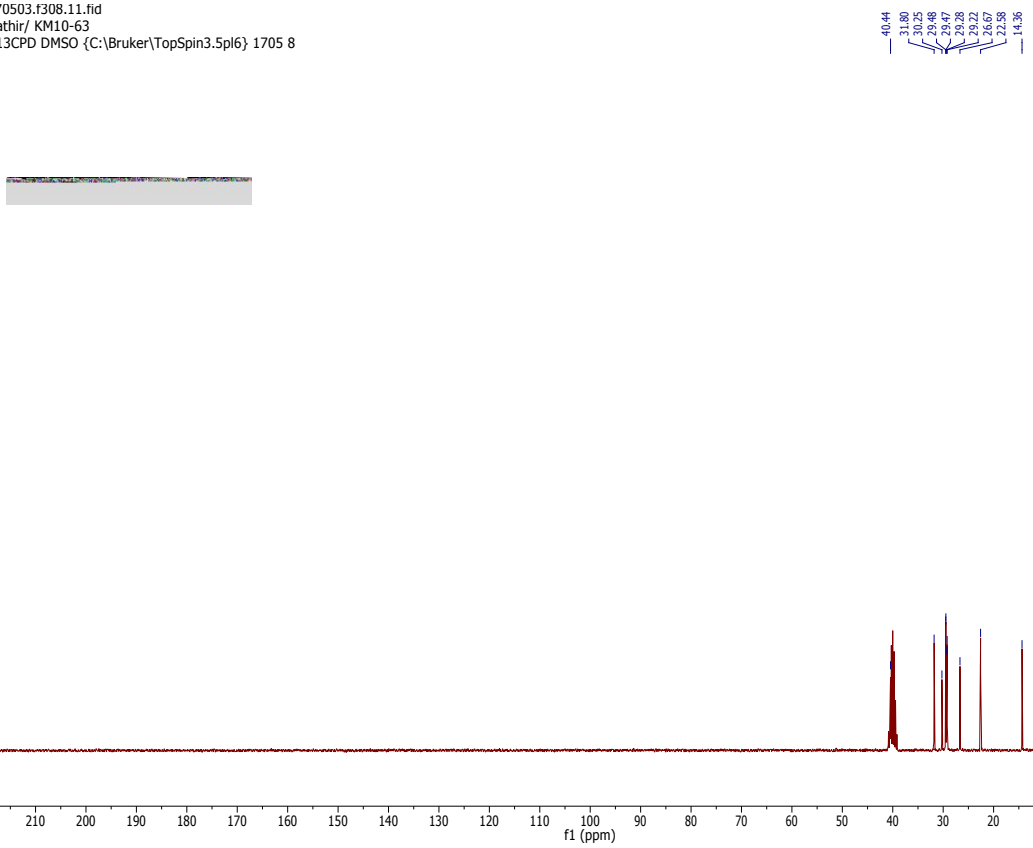
Kathir/ KM10-63
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 8



170503.f308.11.fid
Kathir/ KM10-63
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 8



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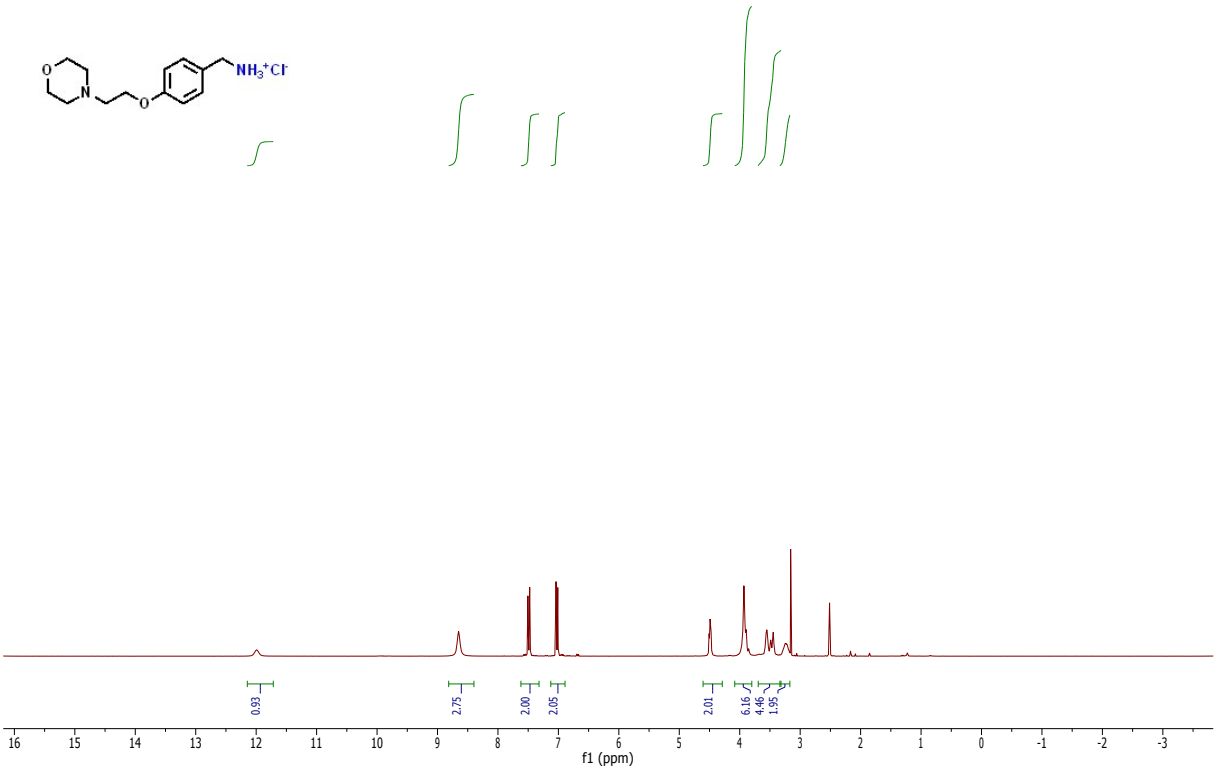
Kathir/ KM10-83
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 9



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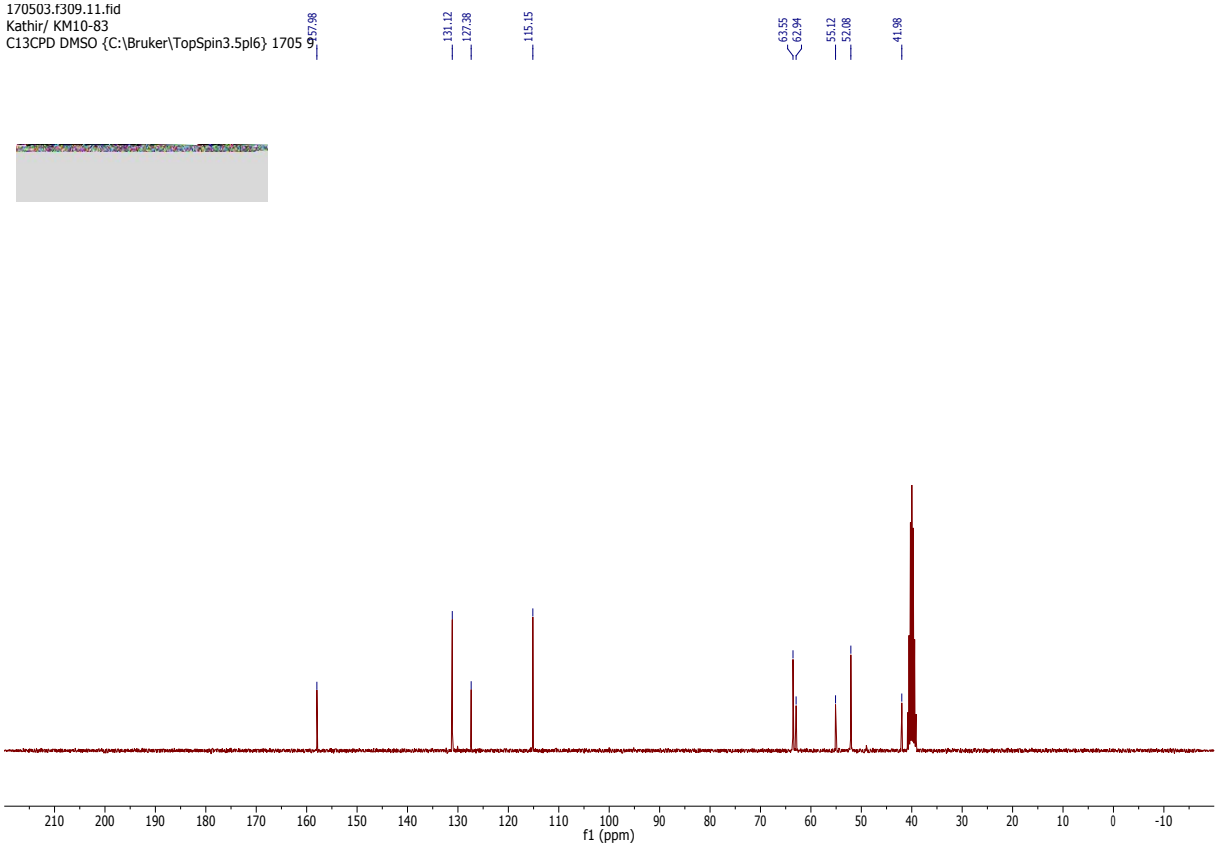
Kathir/ KM10-83
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 9



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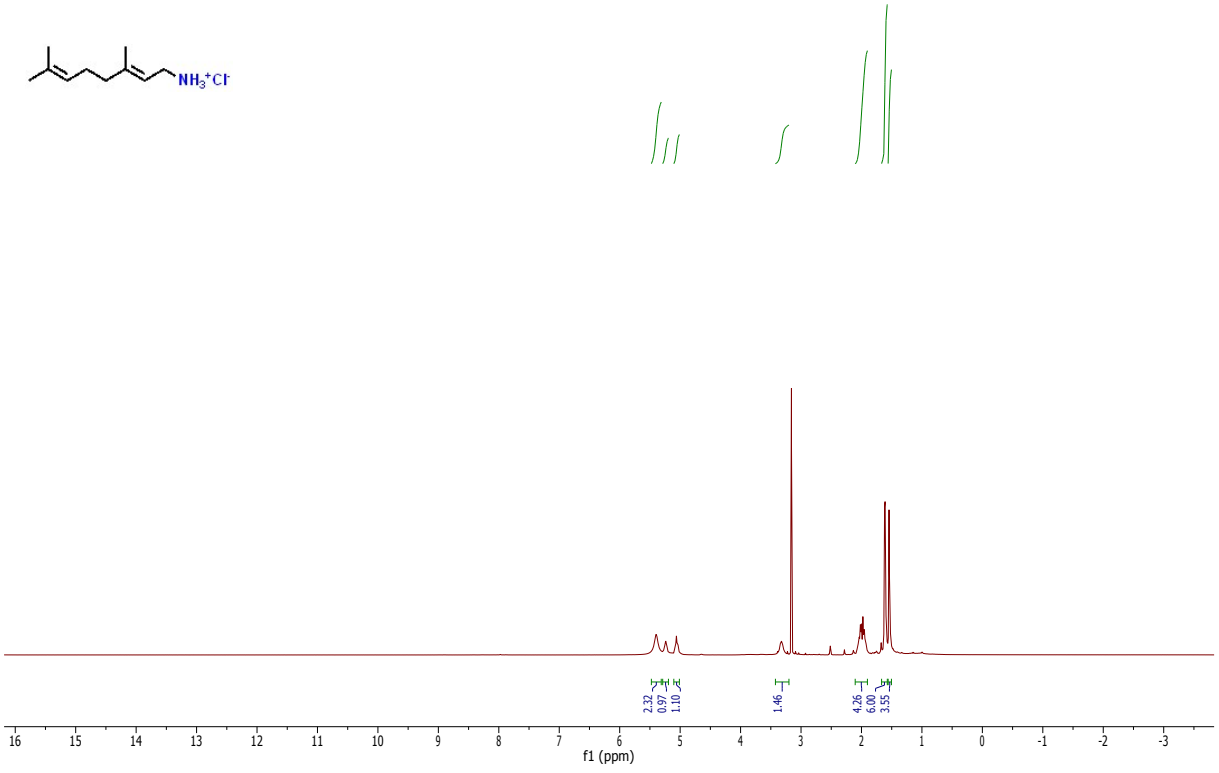
Kathir/ KM10-89
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 10



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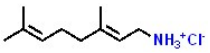
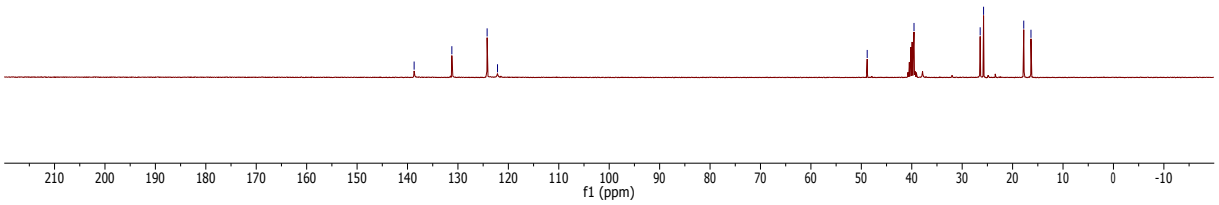
Kathir/ KM10-89
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 10





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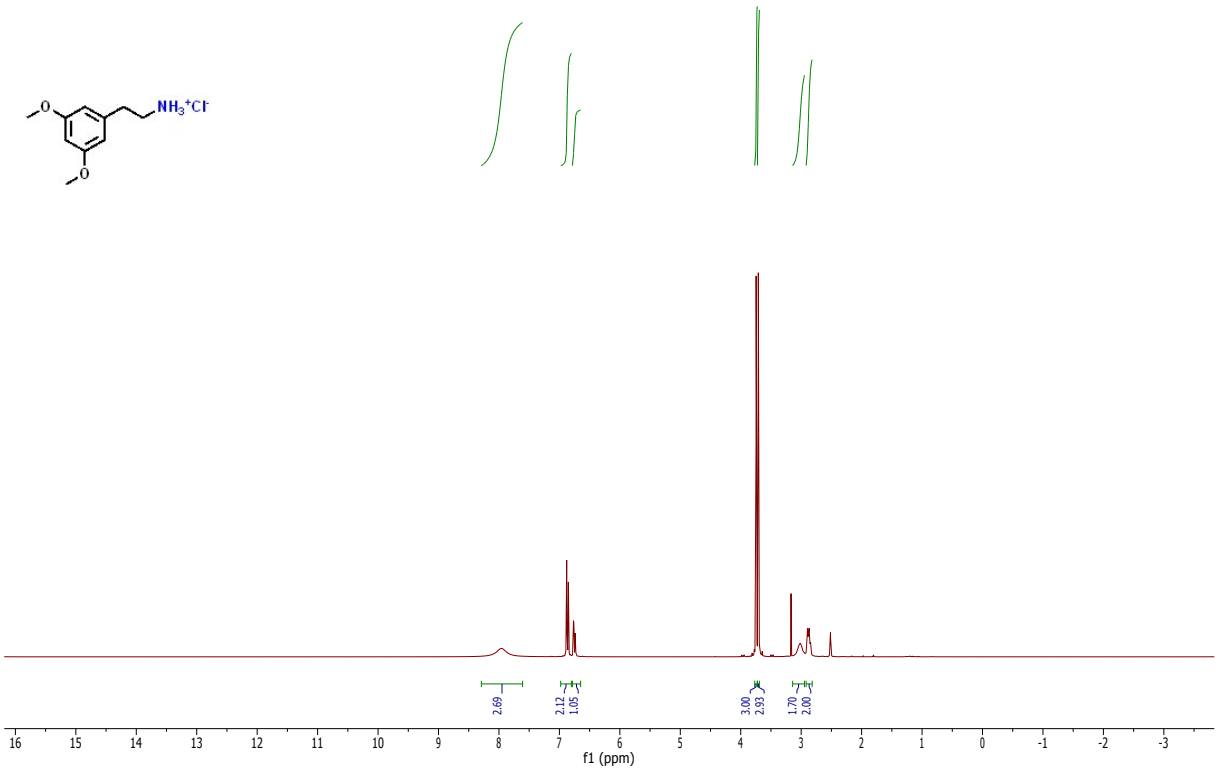
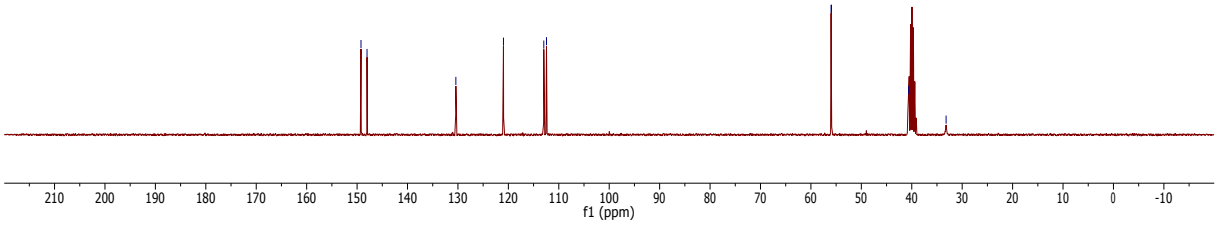
Kathir/ KM10-95
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 11



170503.f311.11.fid
Kathir/ KM10-95
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 11

149.22
148.03
130.41
120.97
112.97
112.44
56.00
55.93
40.62
33.19



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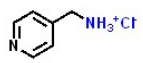
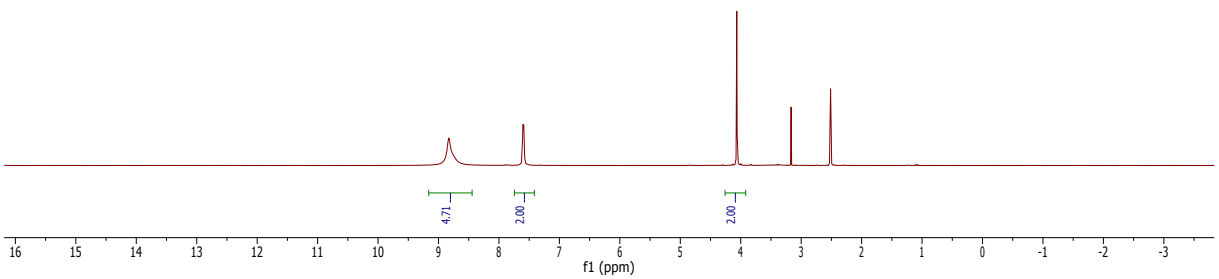
Kathir/ KM10-97
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 12





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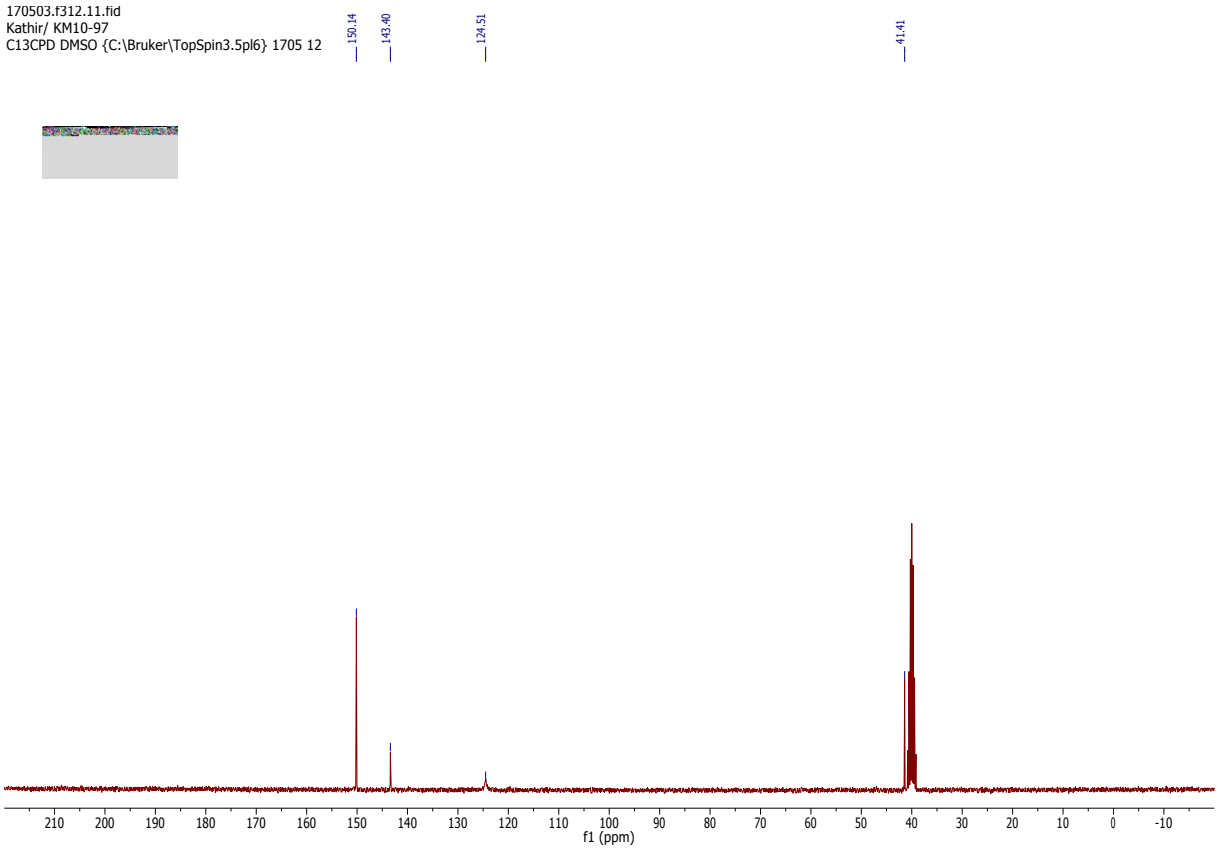
Kathir/ KM10-97
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 12



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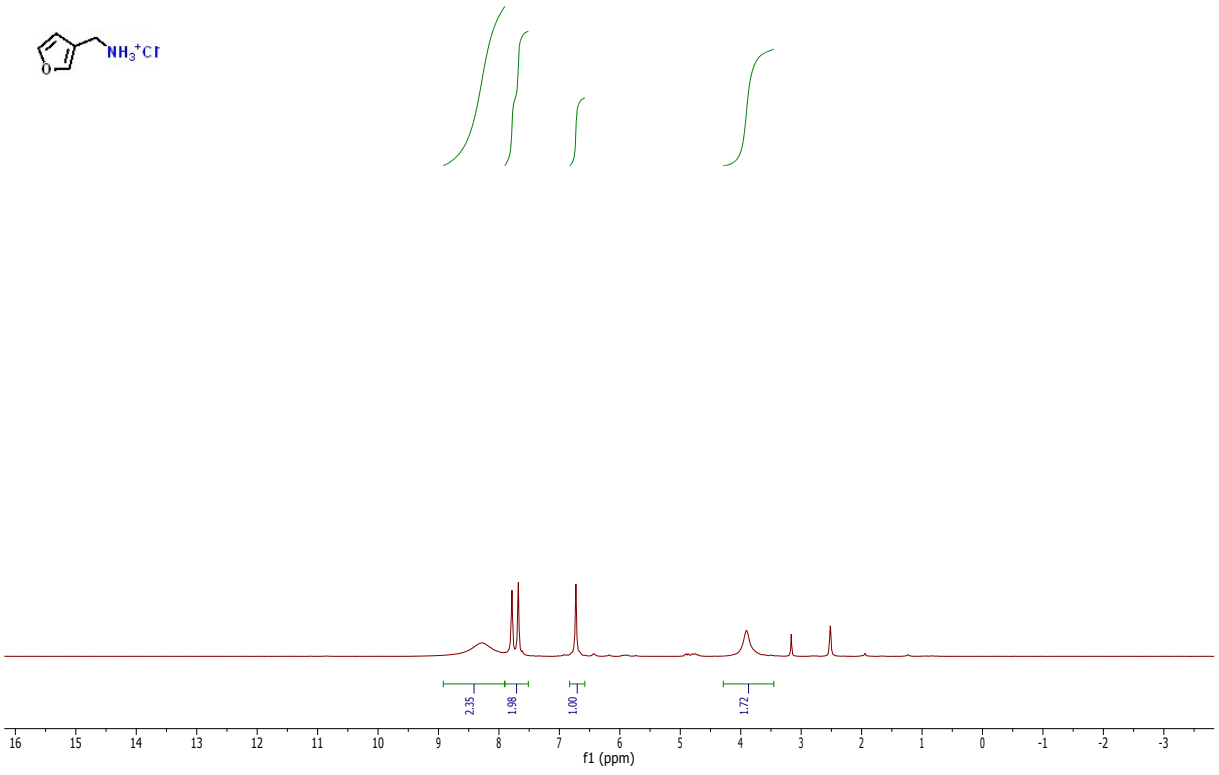
Kathir/ KM10-98
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 13



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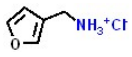
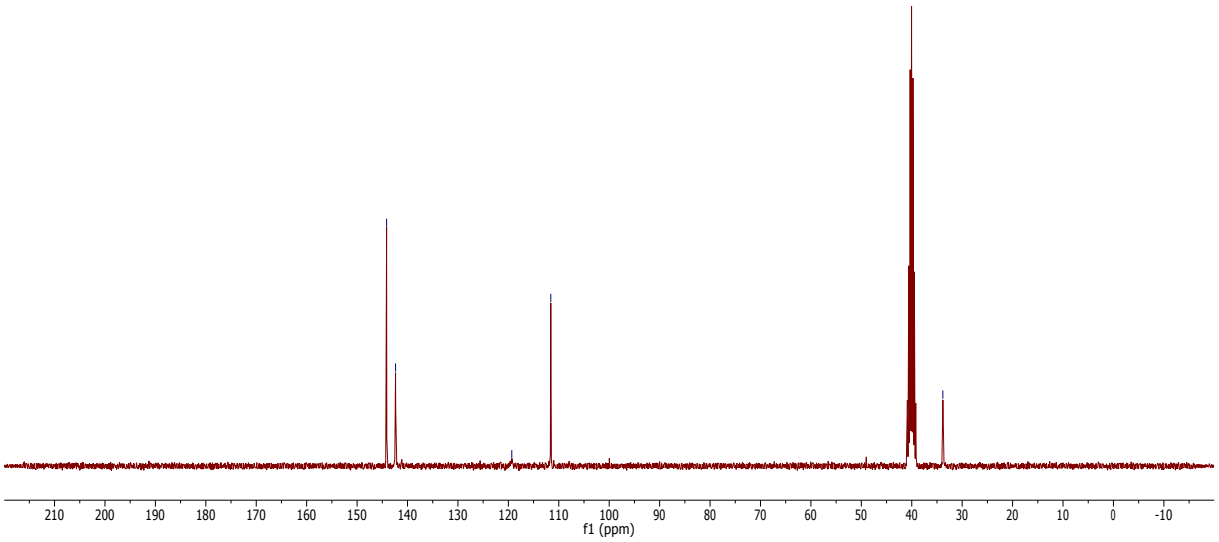
Kathir/ KM10-98
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 13





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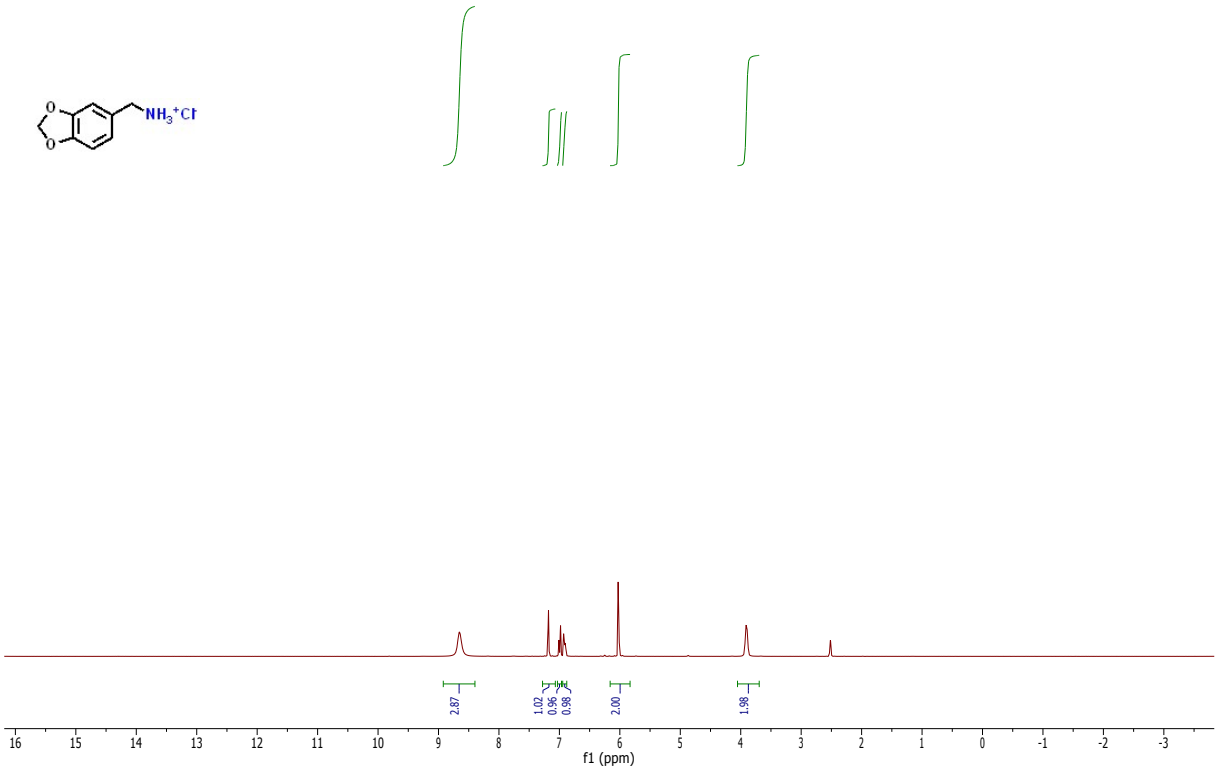
Kathir/ KM10-101
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 14



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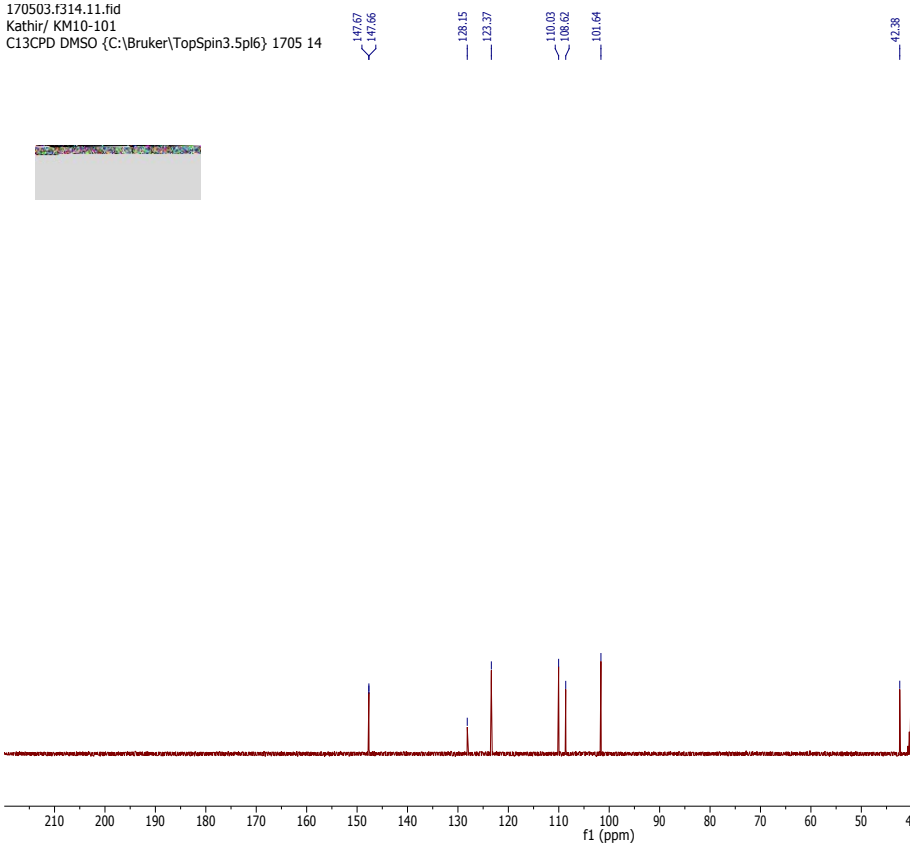
Kathir/ KM10-101
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 14



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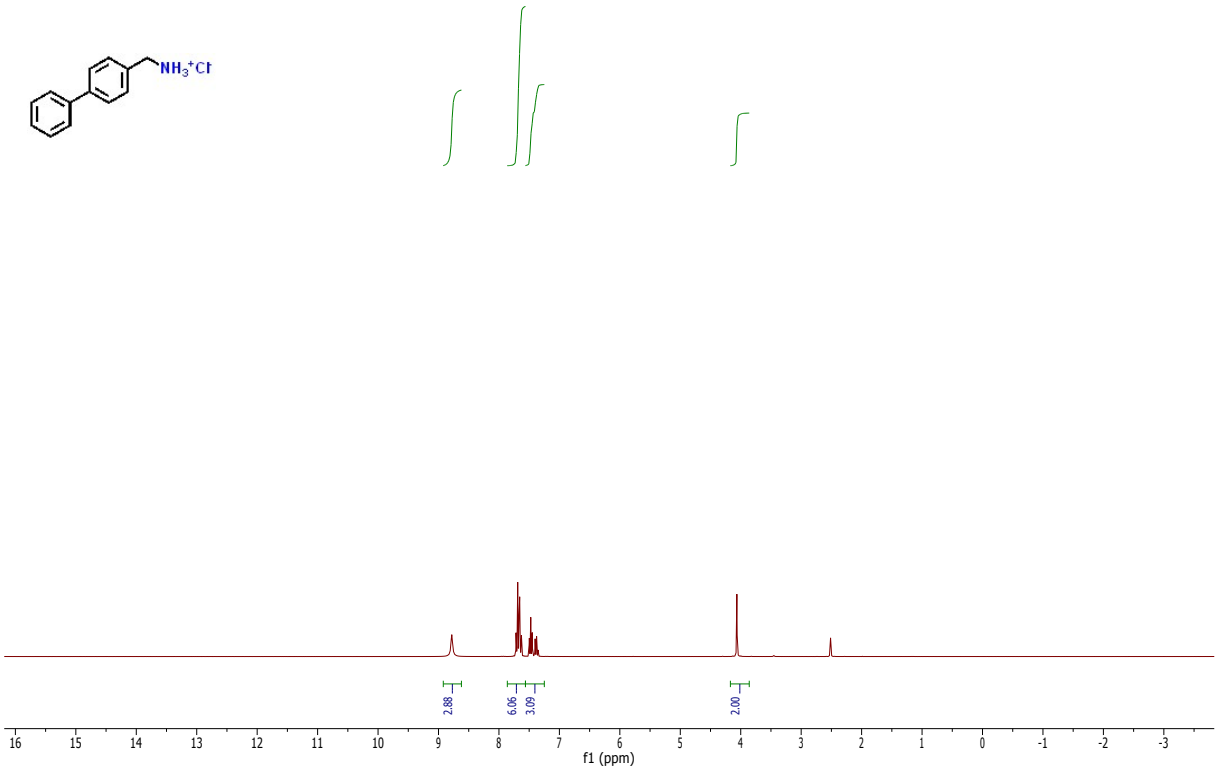
Kathir/ KM10-103
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 15



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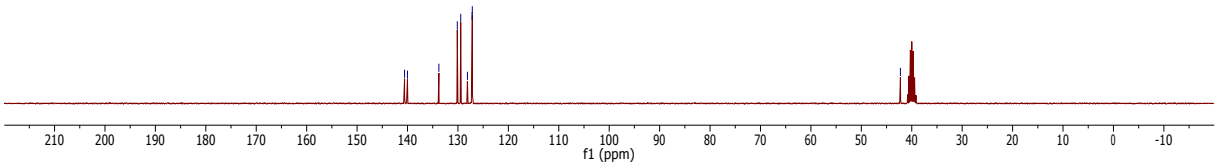
Kathir/ KM10-103
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 15



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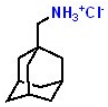
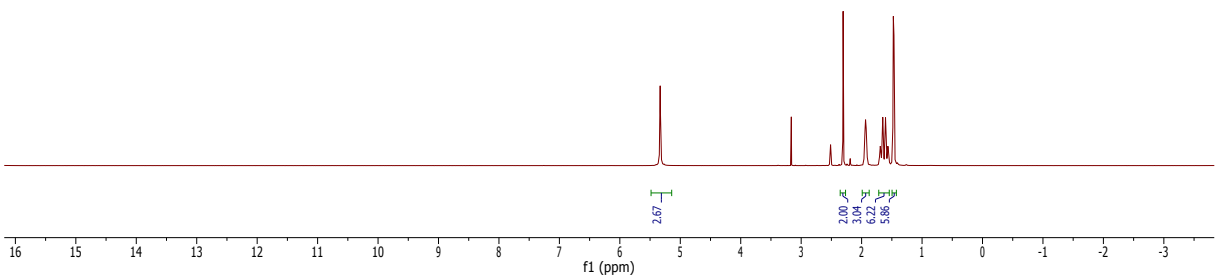
Kathir/ KM10-120
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1705 16





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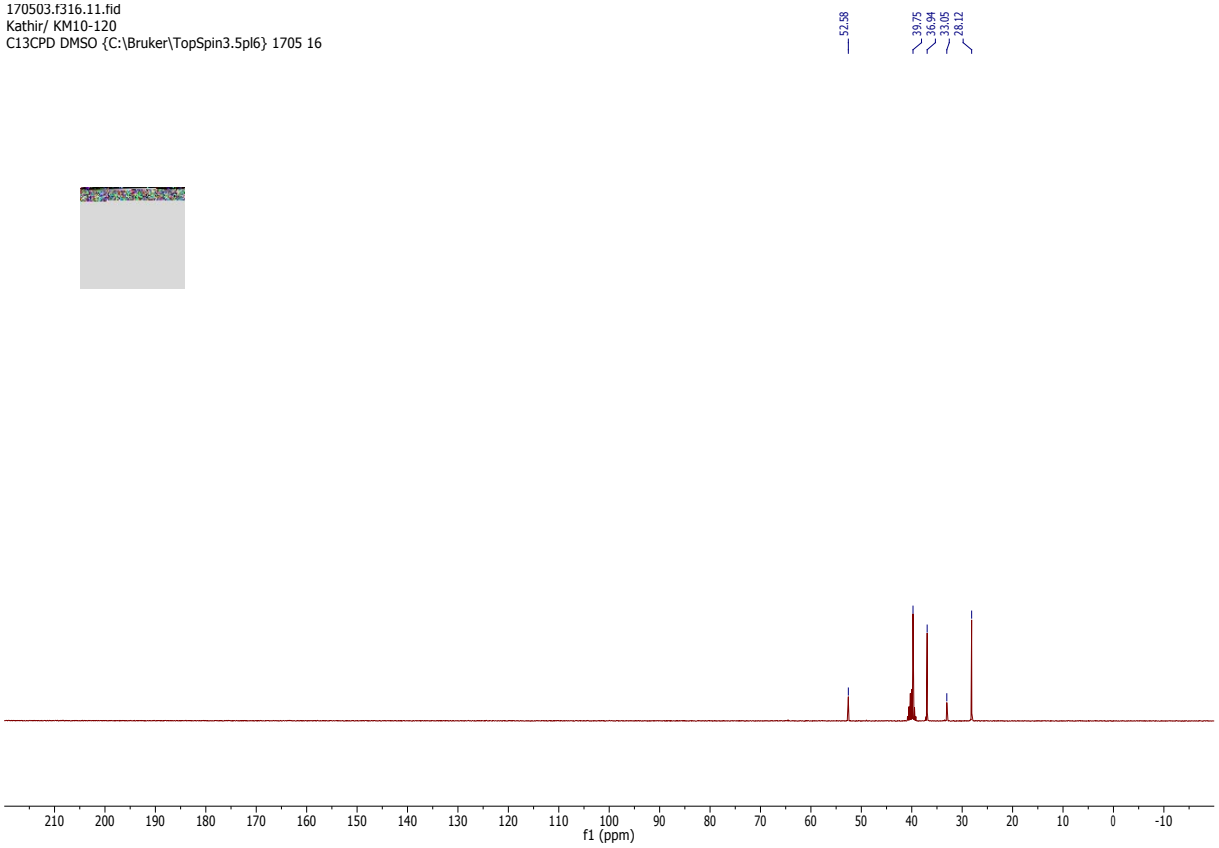
Kathir/ KM10-120
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1705 16



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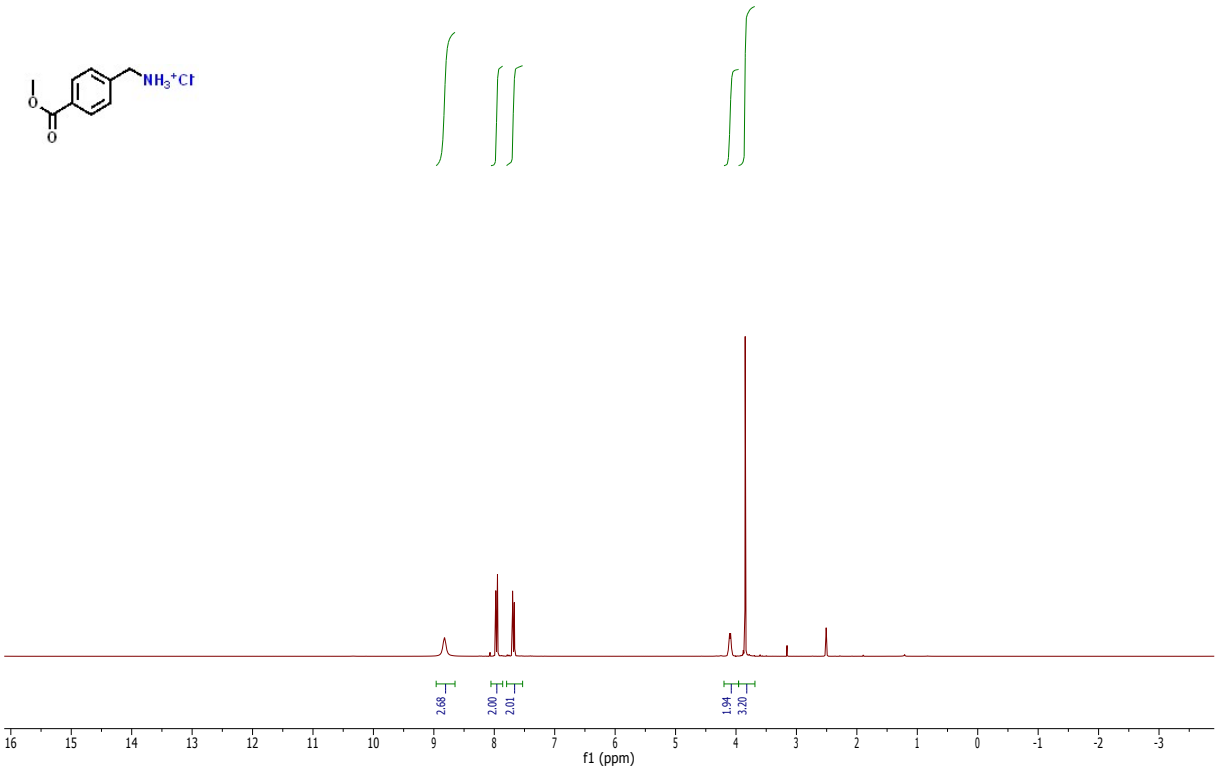
Kathir KMIO-54
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1705 5



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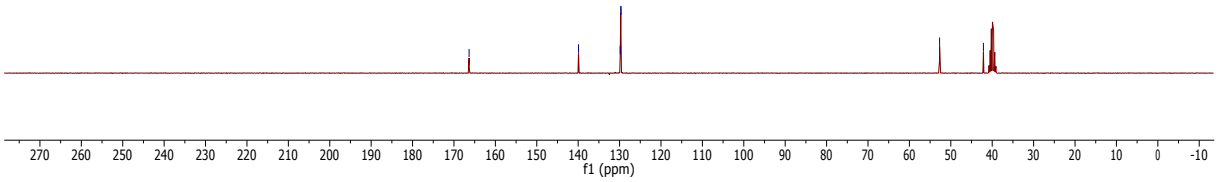
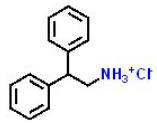
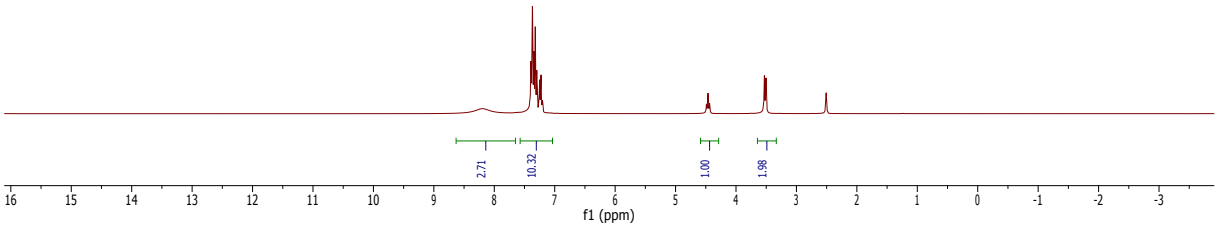
Kathir KMIO-54
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1705 5



170504.307.1.fid
Kathir KMIO-109
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1705 7





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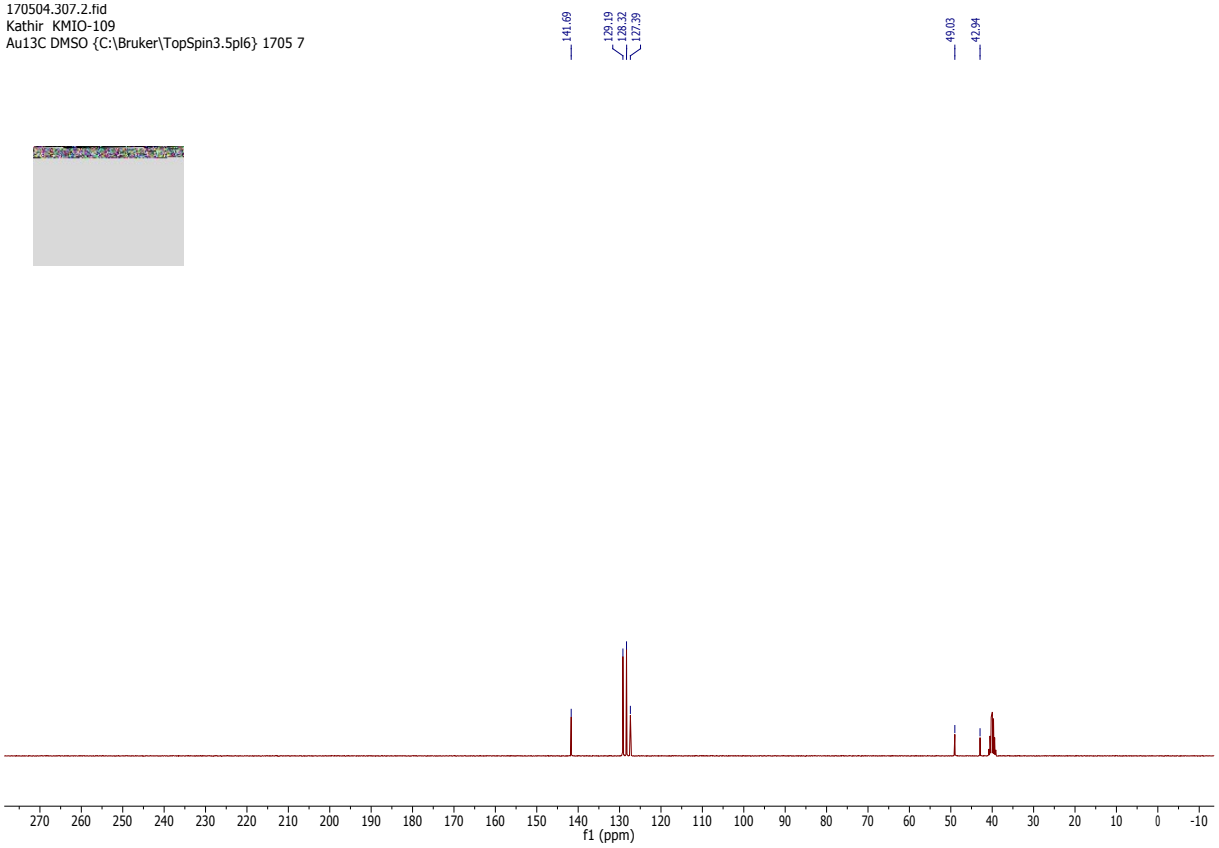
Kathir KMIO-109
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1705 7



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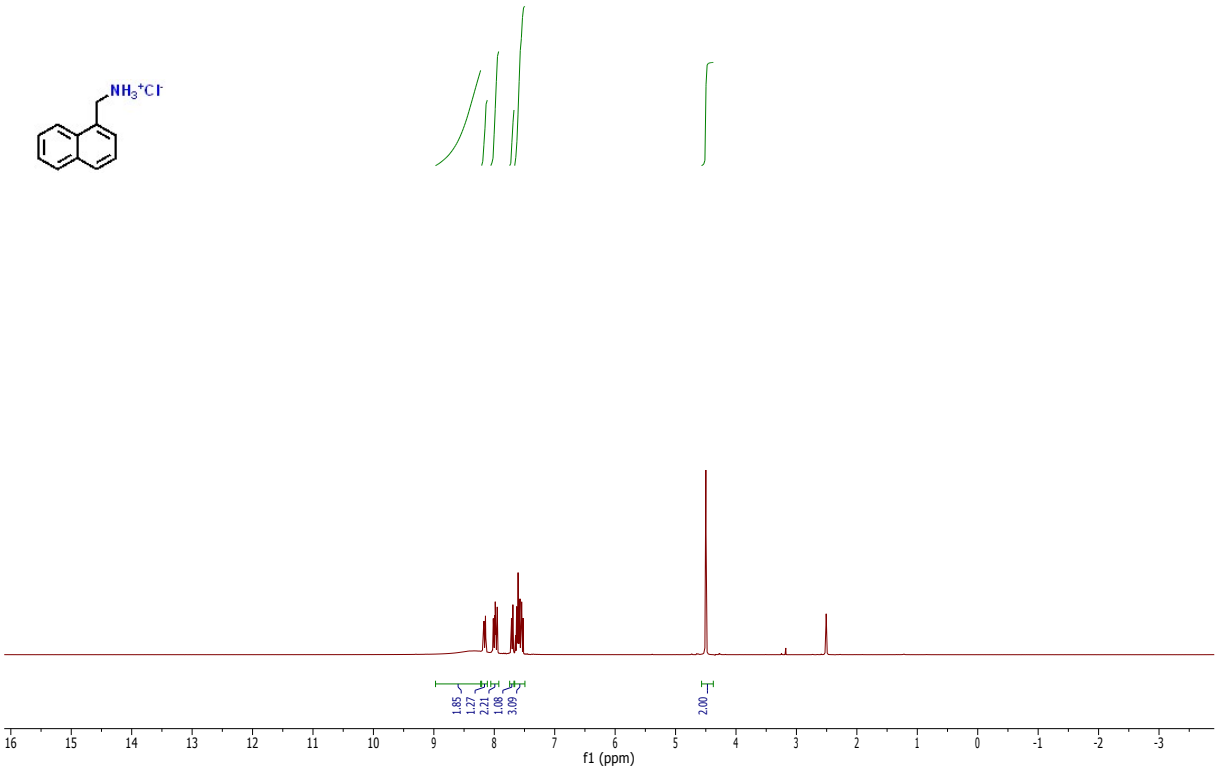
Kathir KMIO-110
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1705 8



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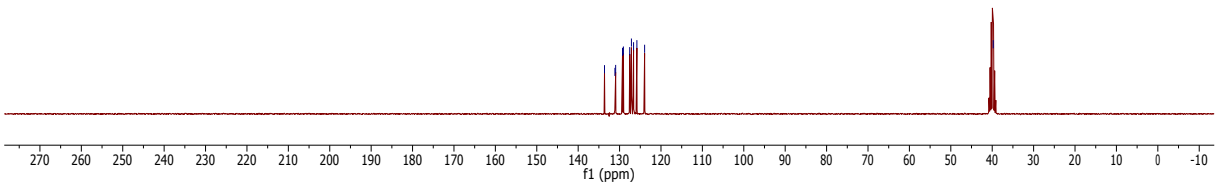
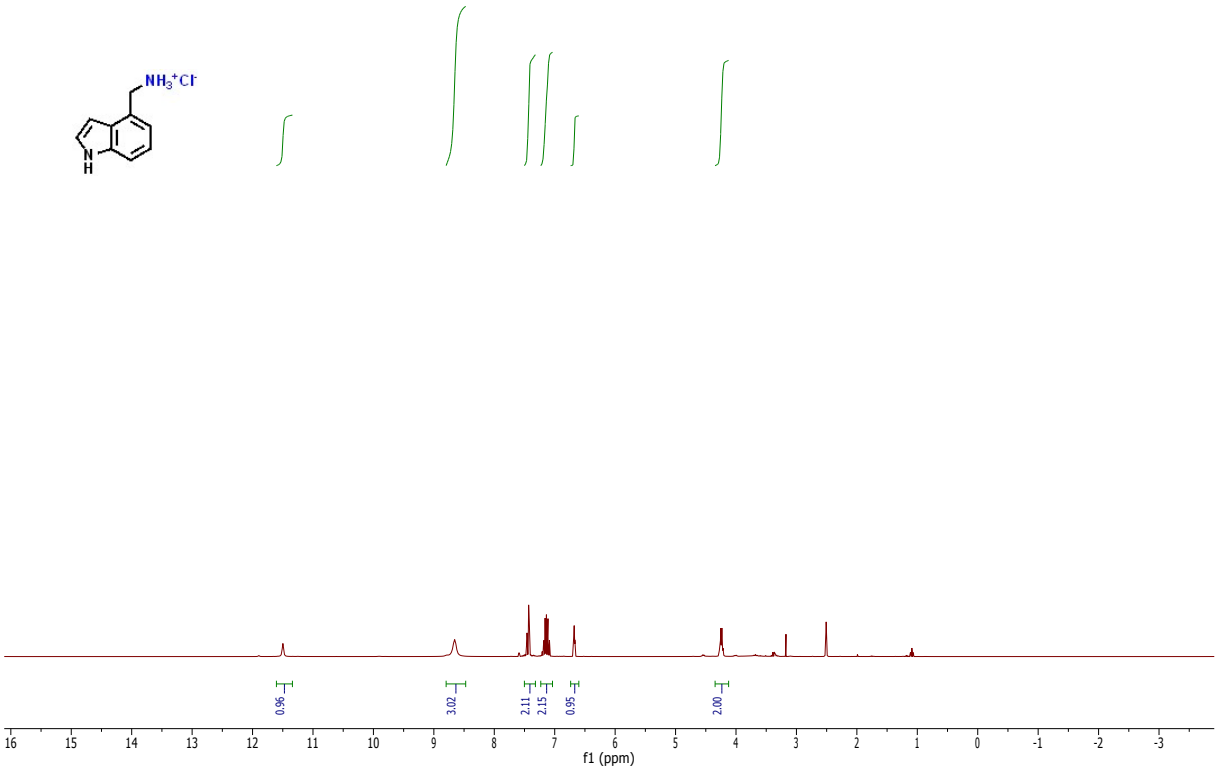
Kathir KMIO-110
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1705 8



170508.302.1.fid
Kathir KM10-124
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1705 2



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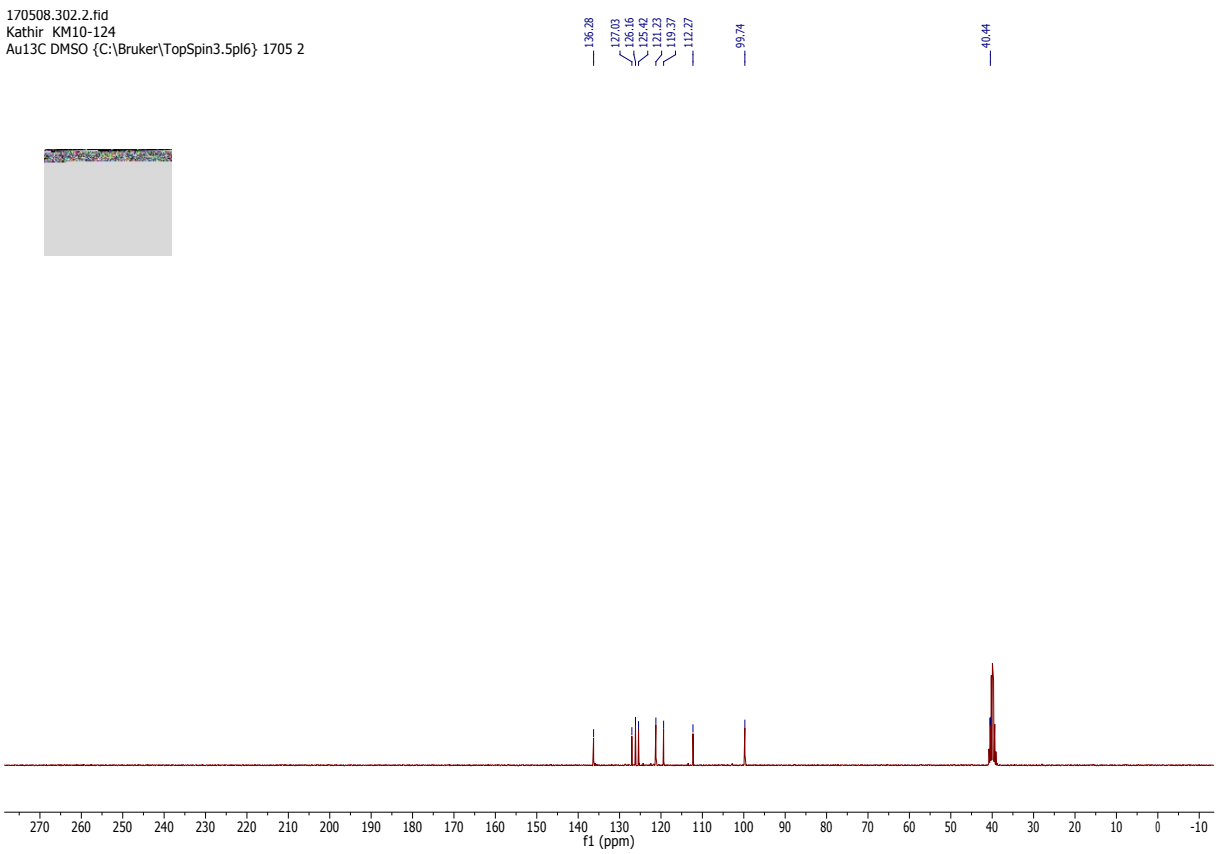
Kathir KM10-124
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1705 2



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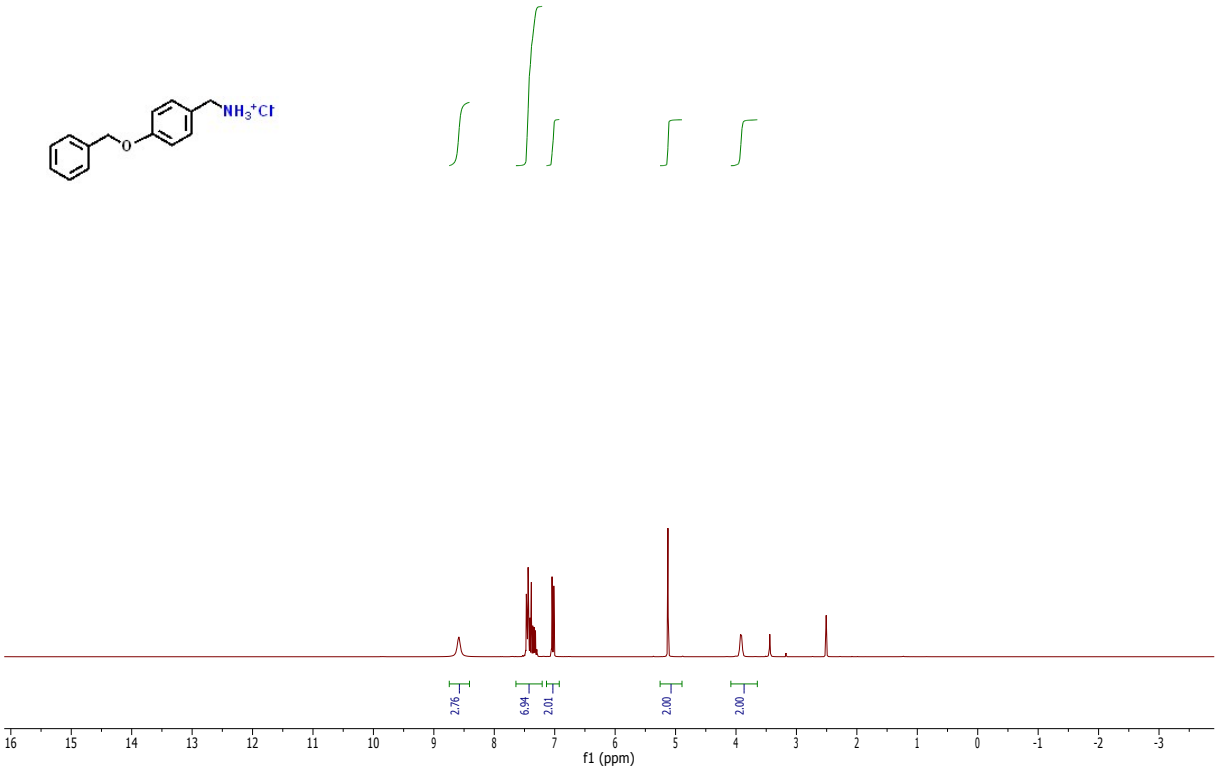
Kathir KM10-127
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1705 3



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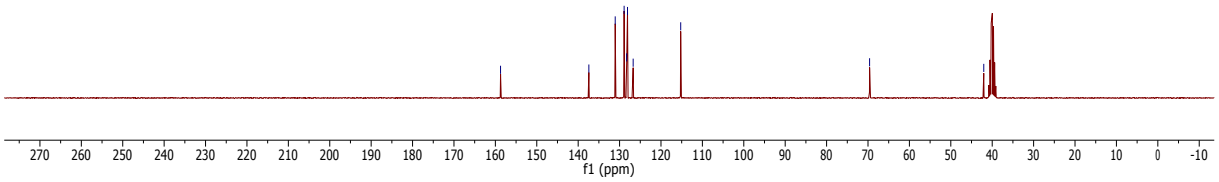
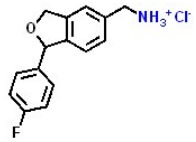
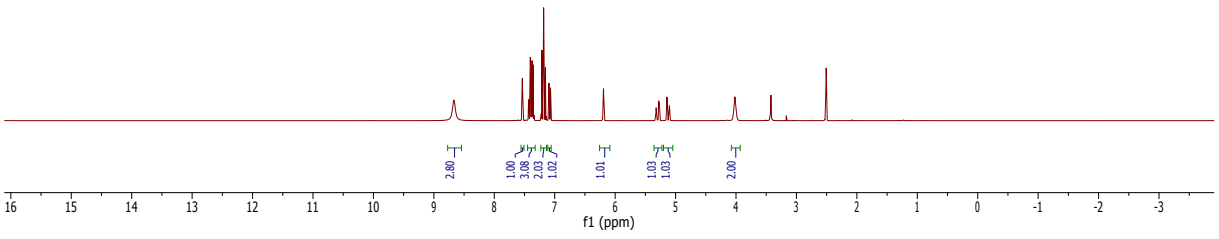
Kathir KM10-127
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1705 3

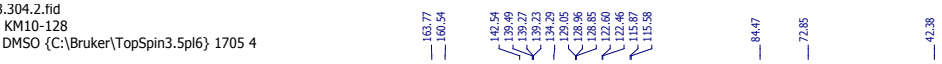


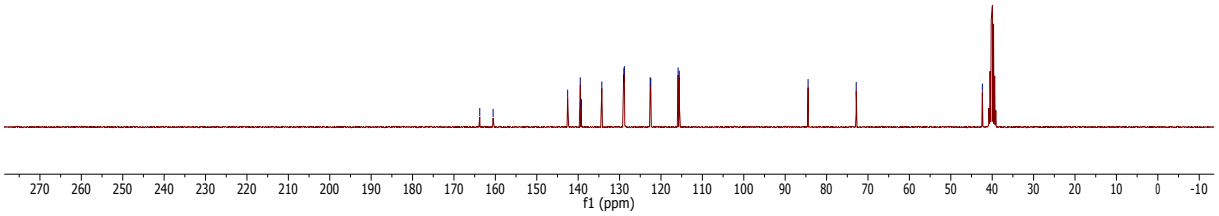
170508.304.1.fid
Kathir KM10-128
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1705 4



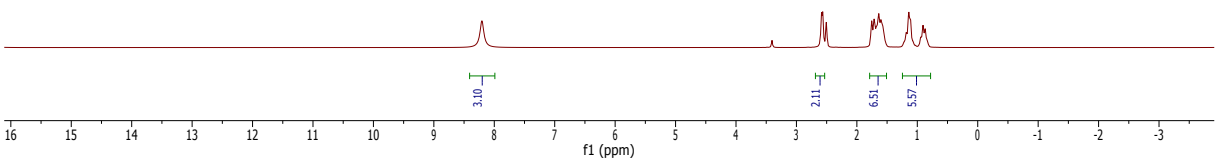


170508.304.2.fid
Kathir KM10-128
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1705 4





170509.302.1.fid
Kathir KM10-138
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1705 2



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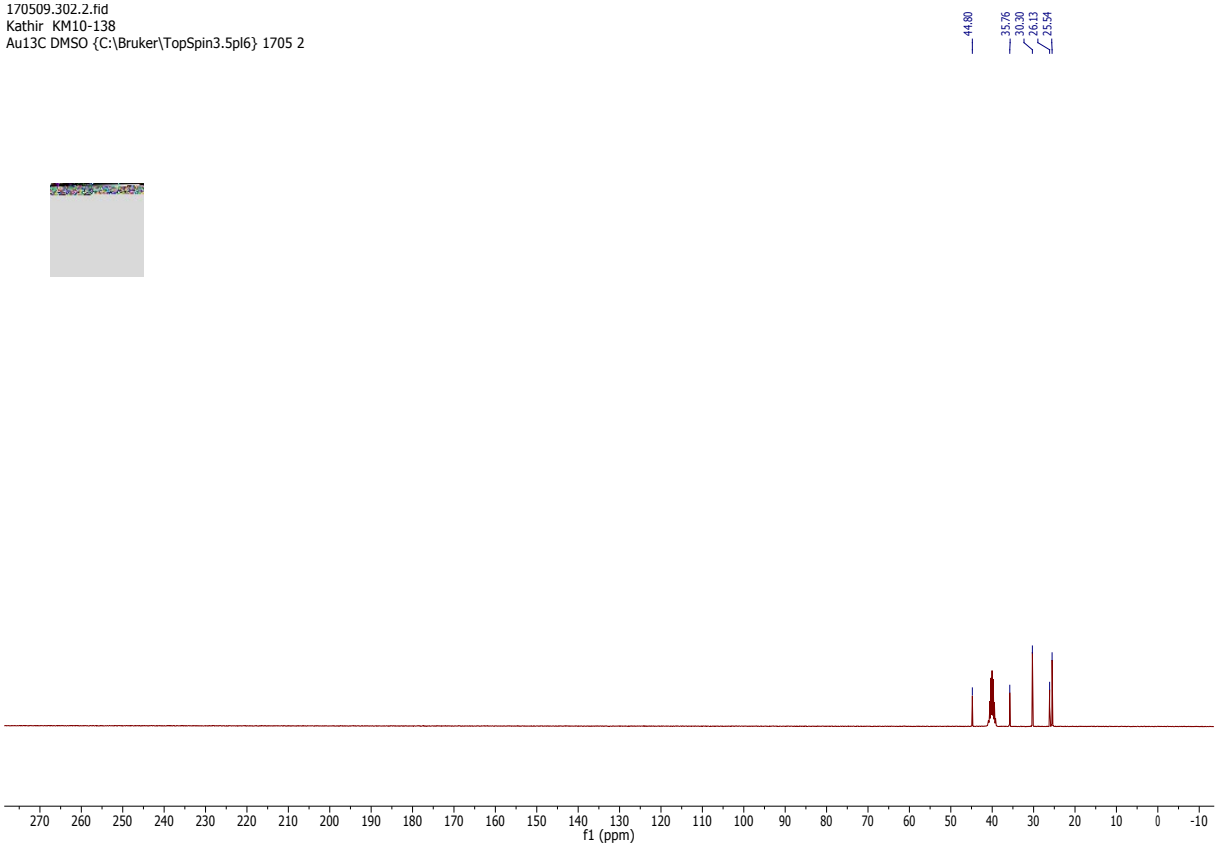
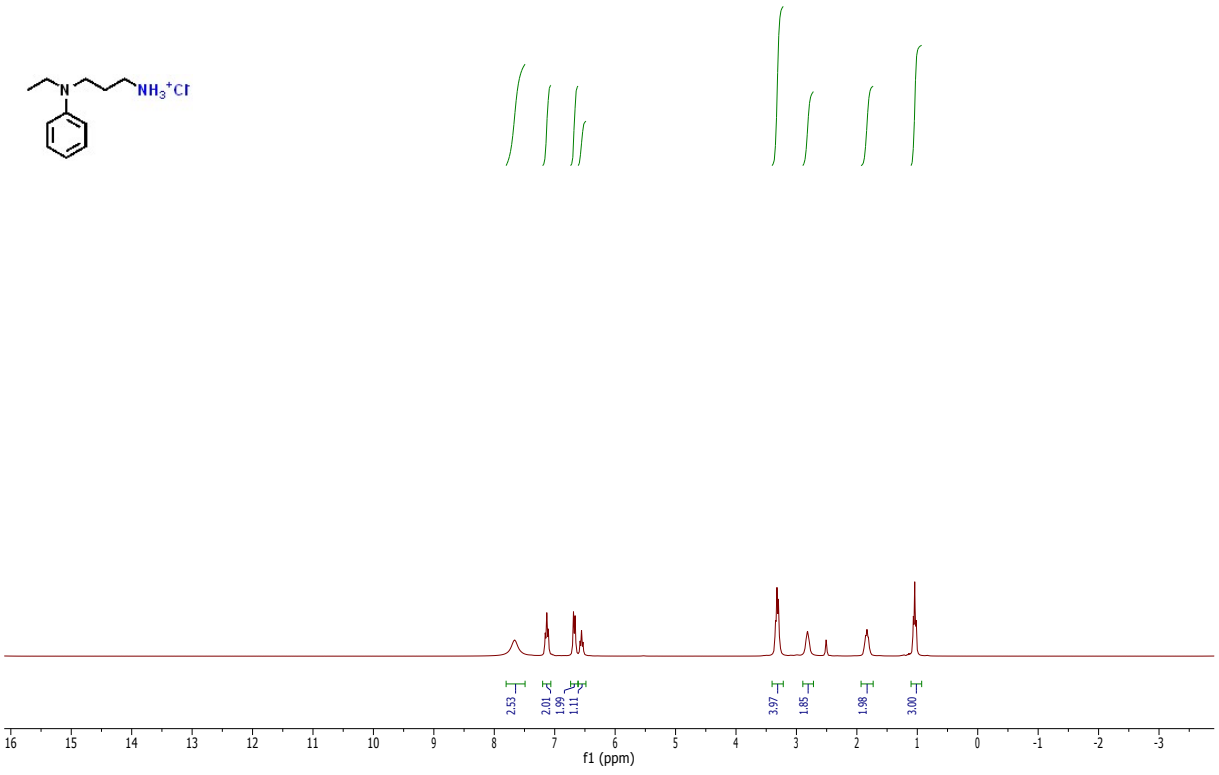
Kathir KM10-138
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1705 2



170509.304.1.fid
Kathir KM10-144
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1705 4



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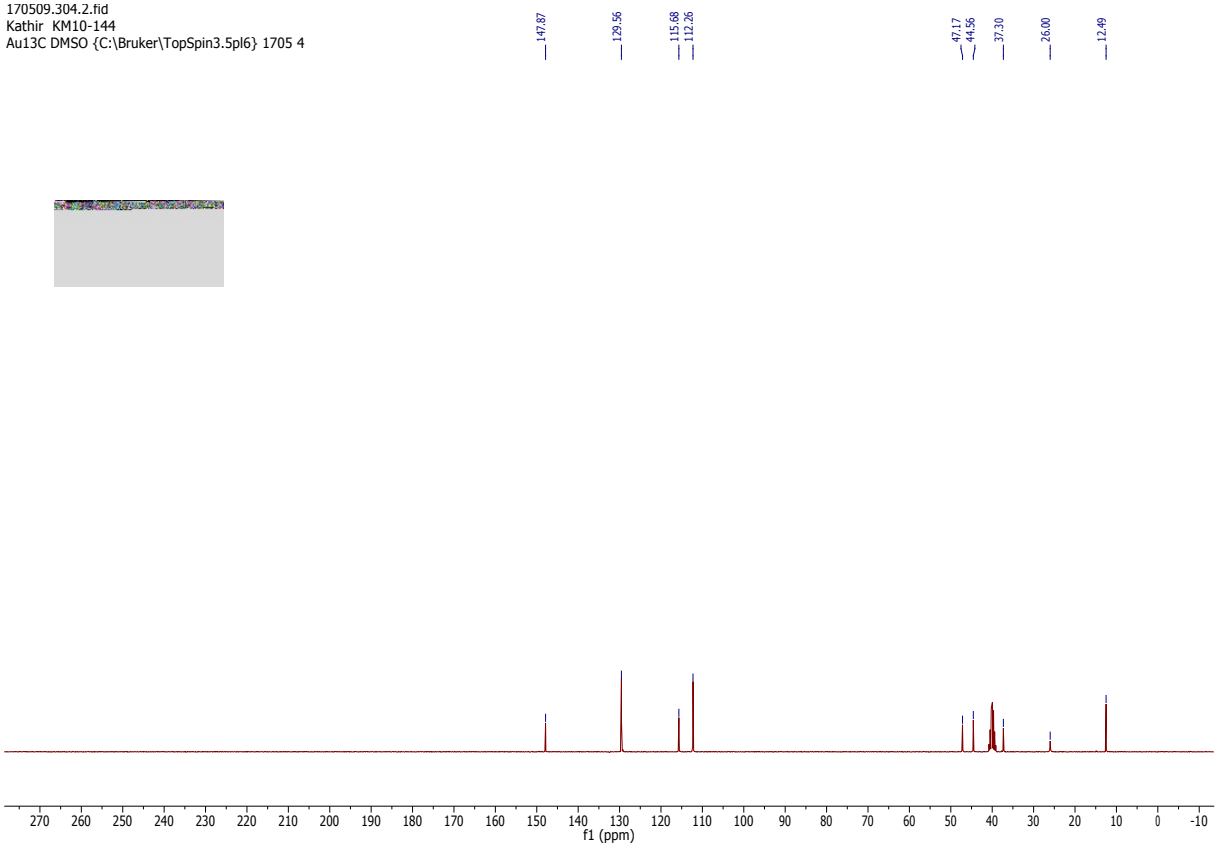
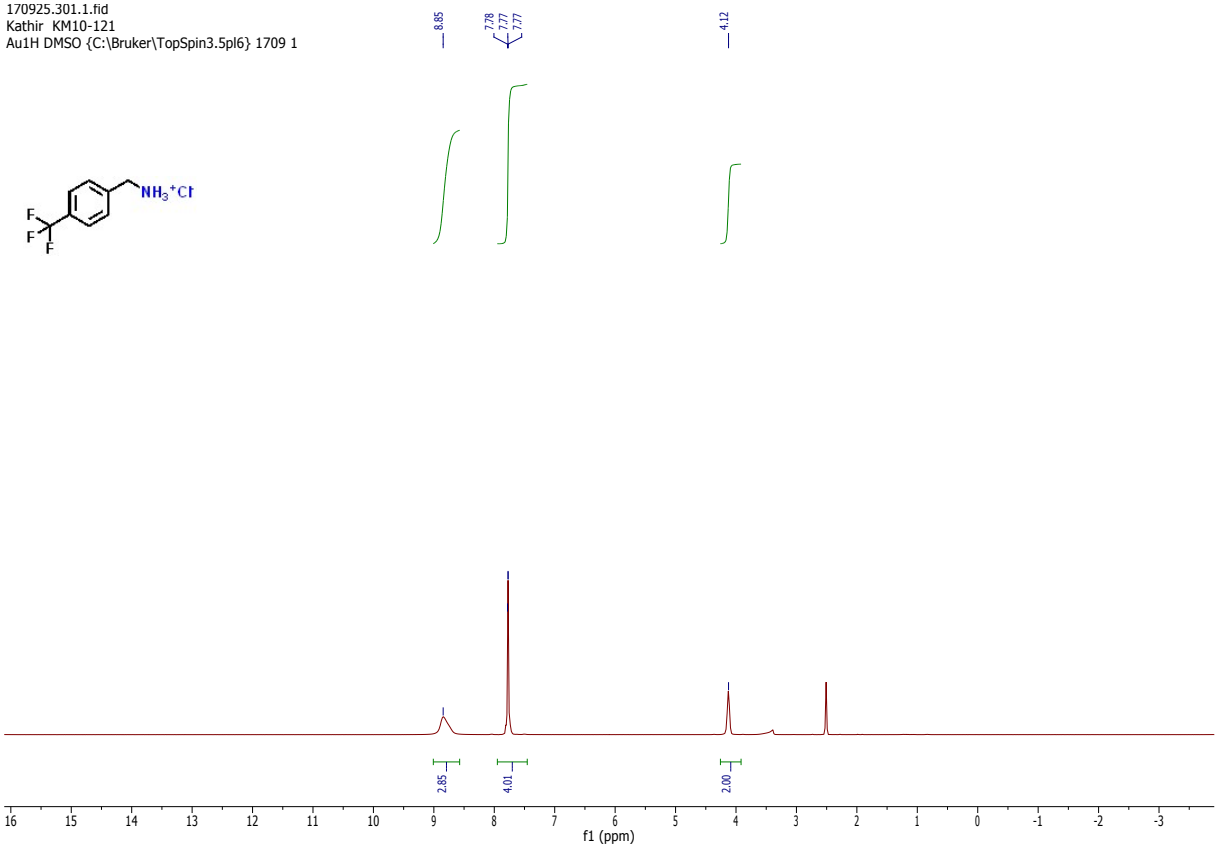
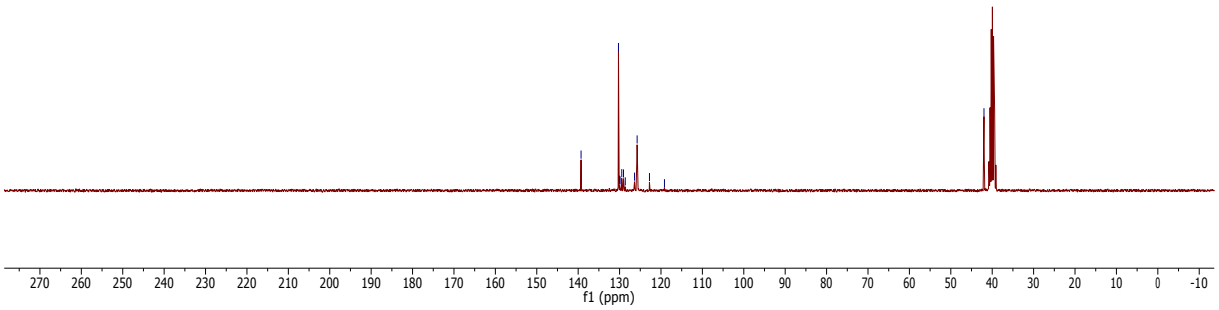
Kathir KM10-144
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1705 4



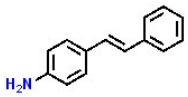
170925.301.1.fid
Kathir KM10-121
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1709 1

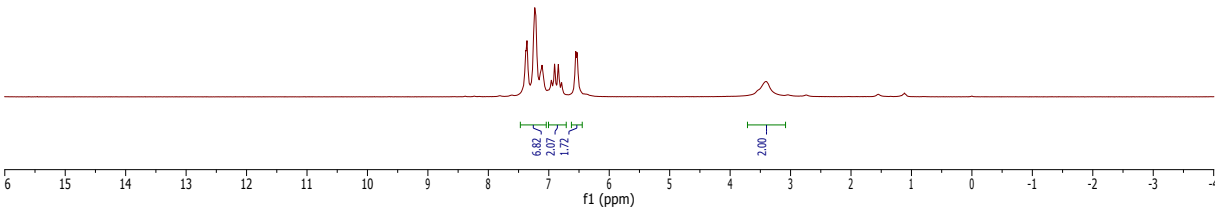


170925.301.2.fid
Kathir KM10-121
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1709 1

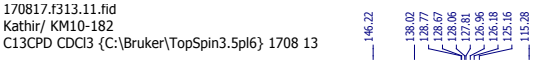


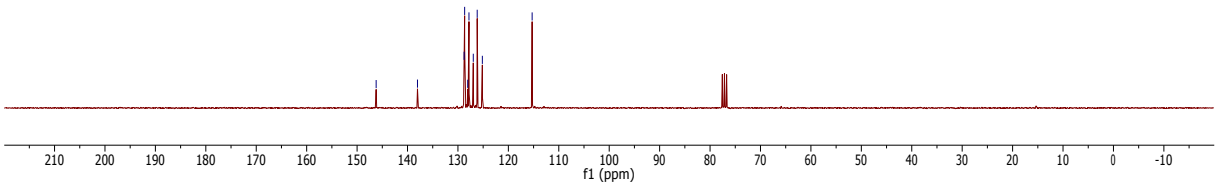
170817.f313.10.fid
Kathir/ KM10-182
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 13



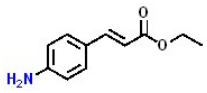


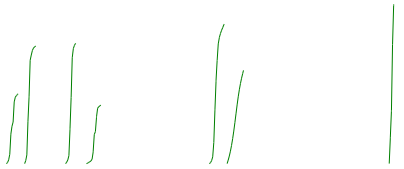
170817.f313.11.fid
Kathir/ KM10-182
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 13

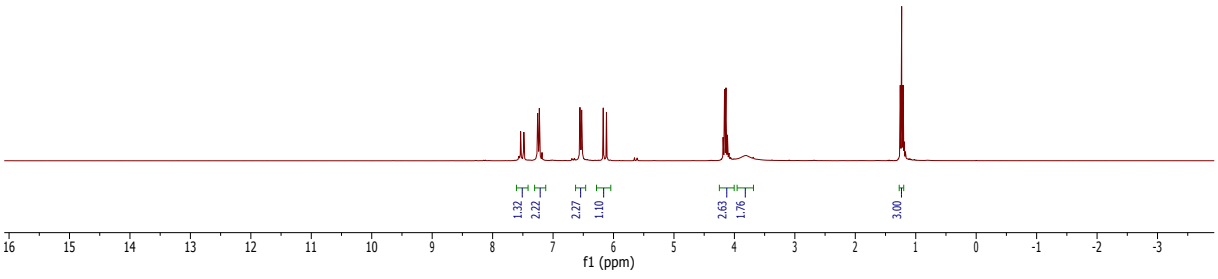




170817.f314.10.fid
Kathir/ KM10-186
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 14







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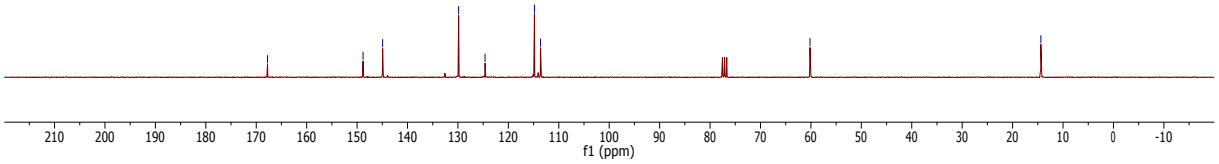
Kathir/ KM10-186
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 14



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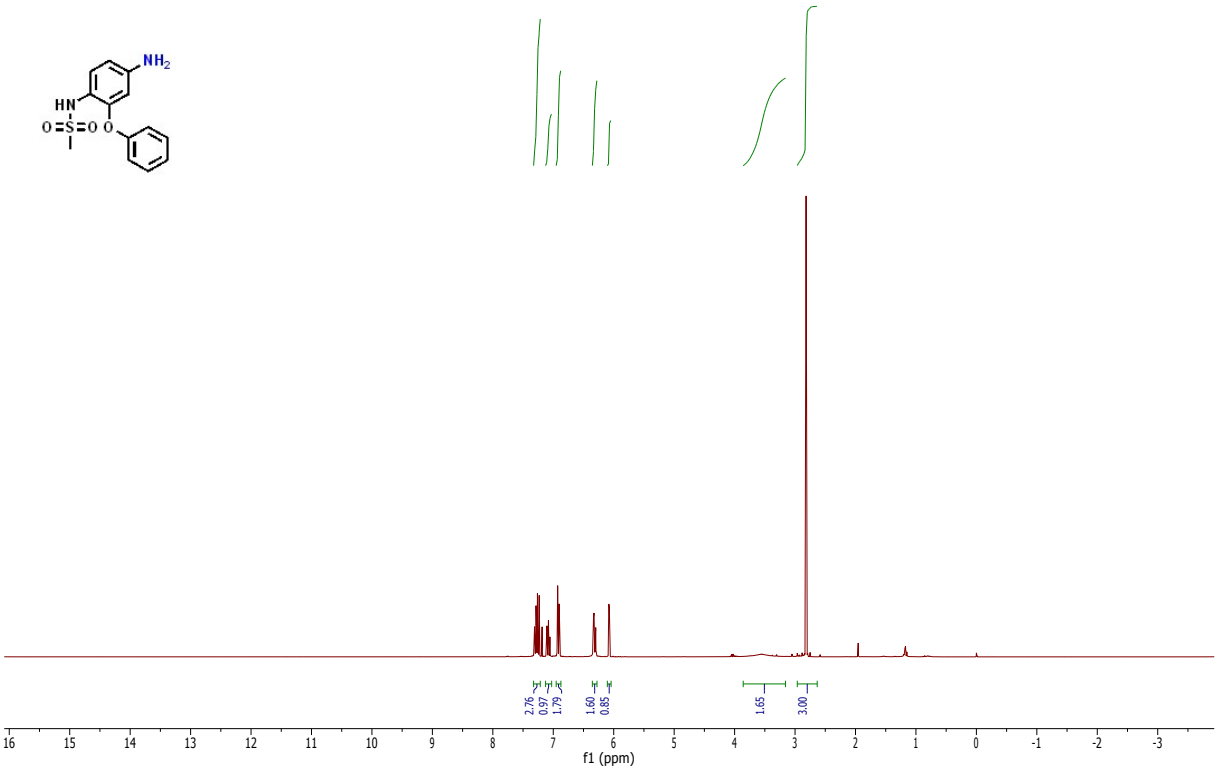
Kathir/ KM10-200
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 16



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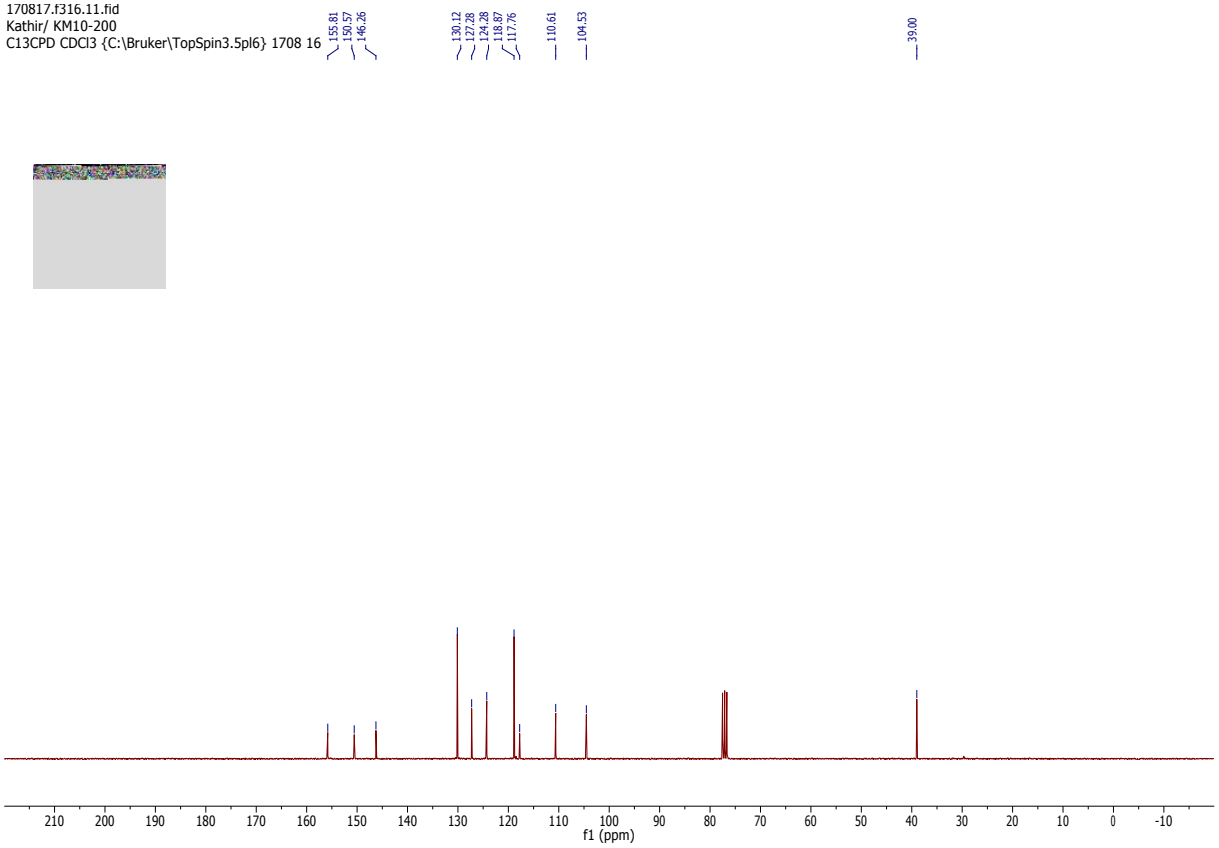
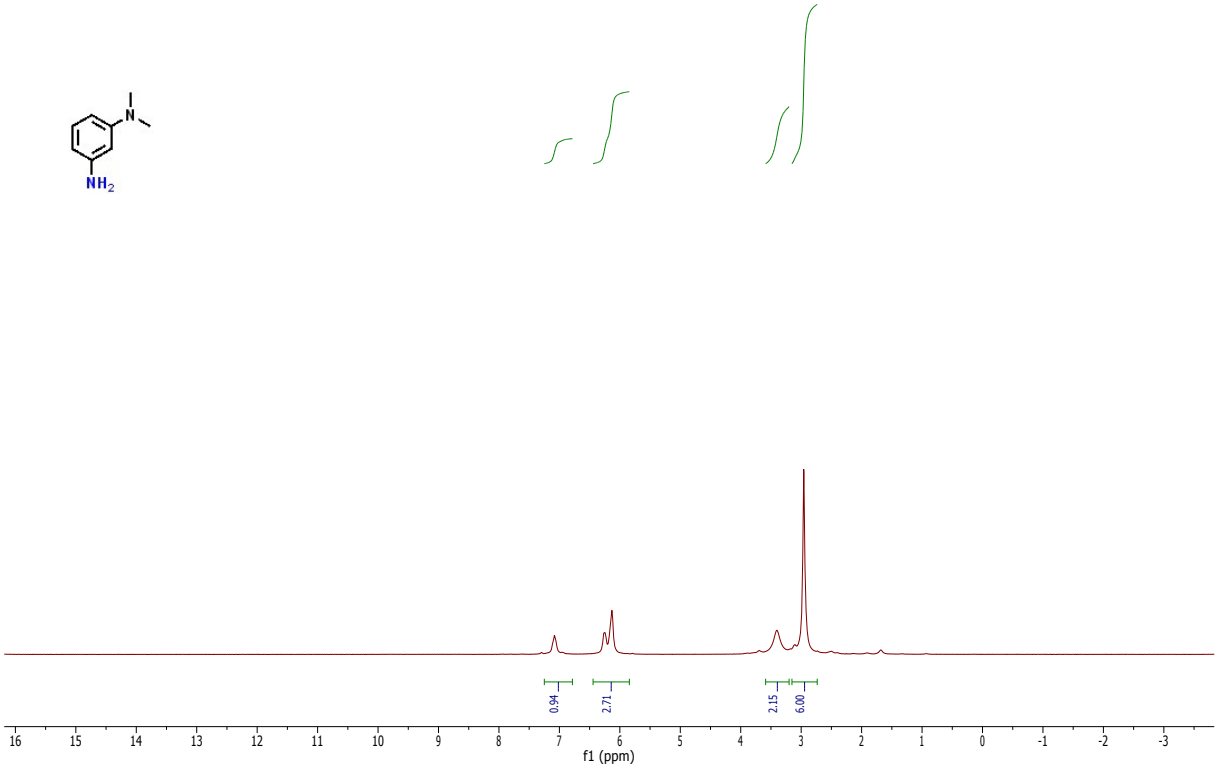
Kathir/ KM10-200
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 16



170818.f302.10.fid
Kathir/ KM10-252
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 2



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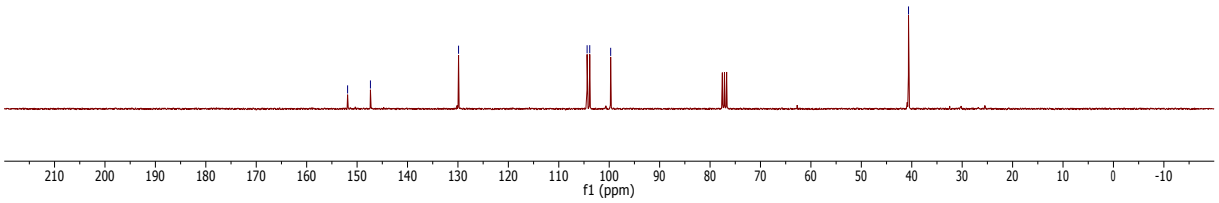
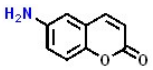
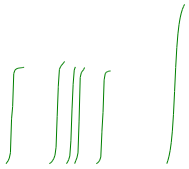
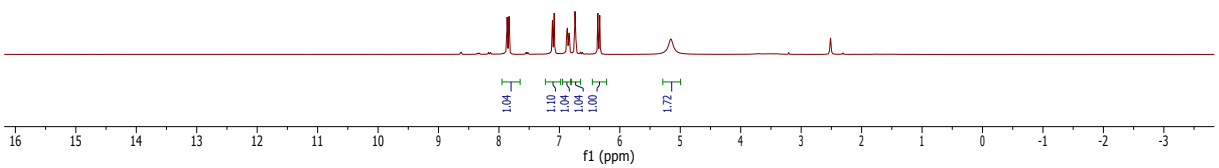
Kathir/ KM10-252
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 2



170818.f301.10.fid
Kathir/ KM10-244
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1708 1







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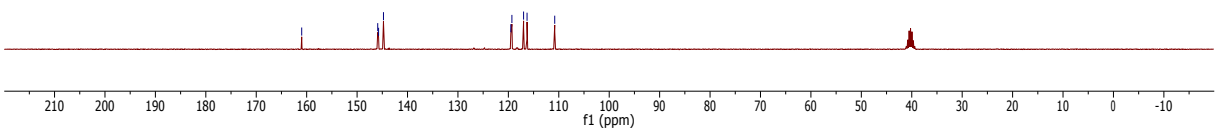
Kathir/ KM10-244
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1708 1



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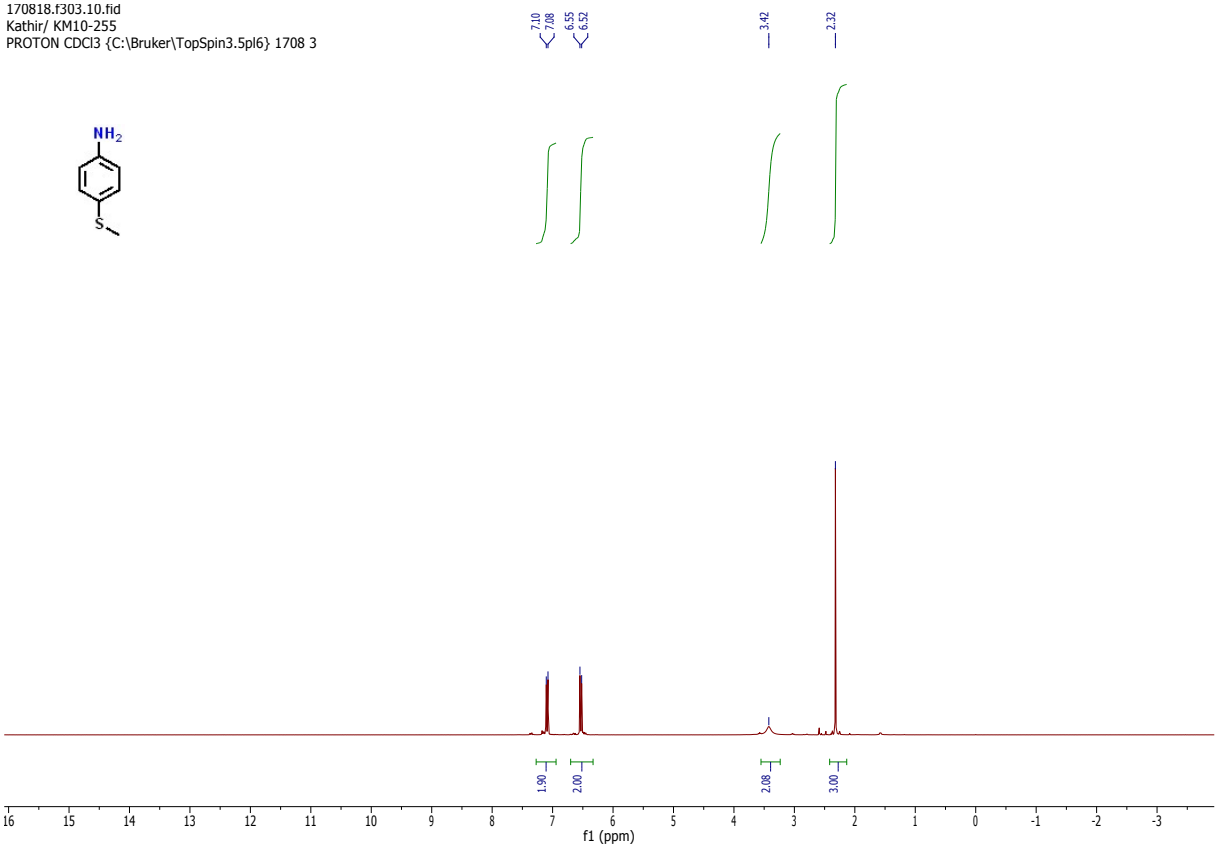
Kathir/ KM10-255
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 3



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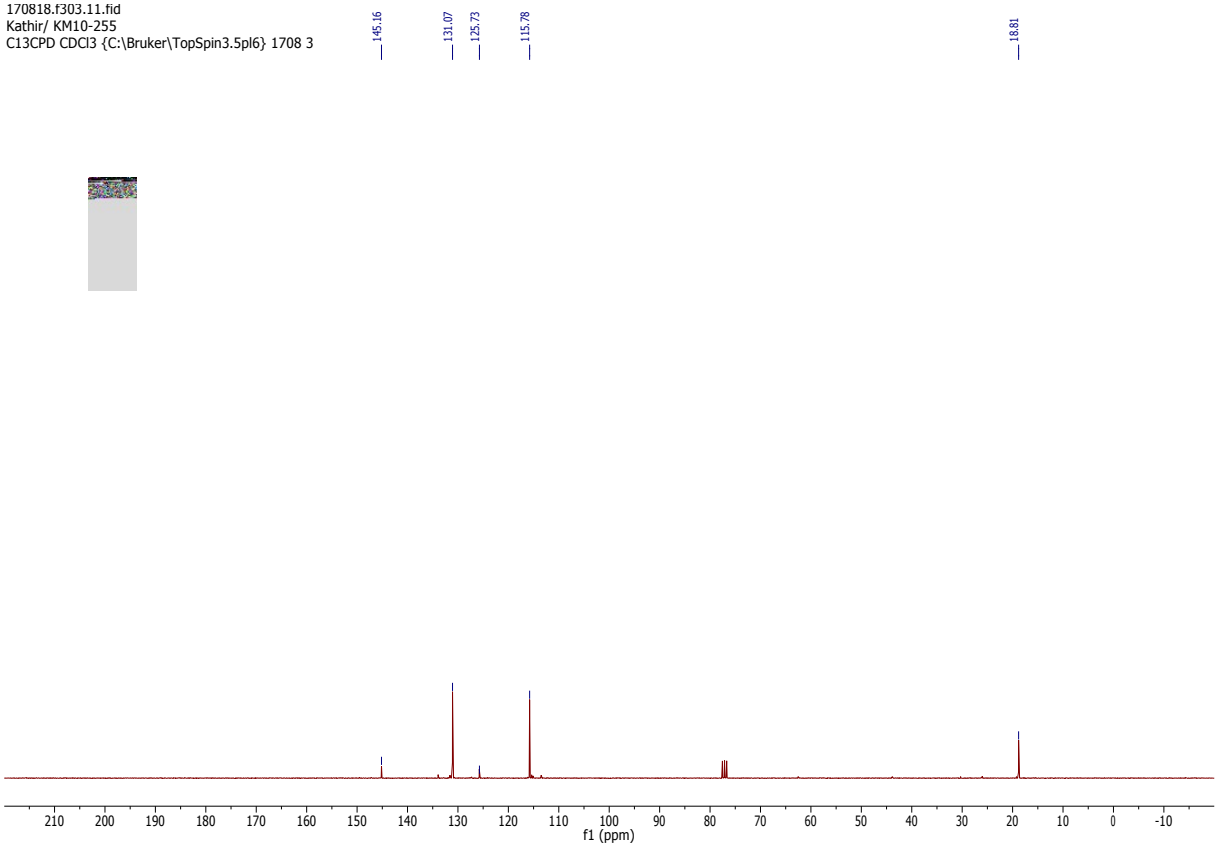
Kathir/ KM10-255
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 3



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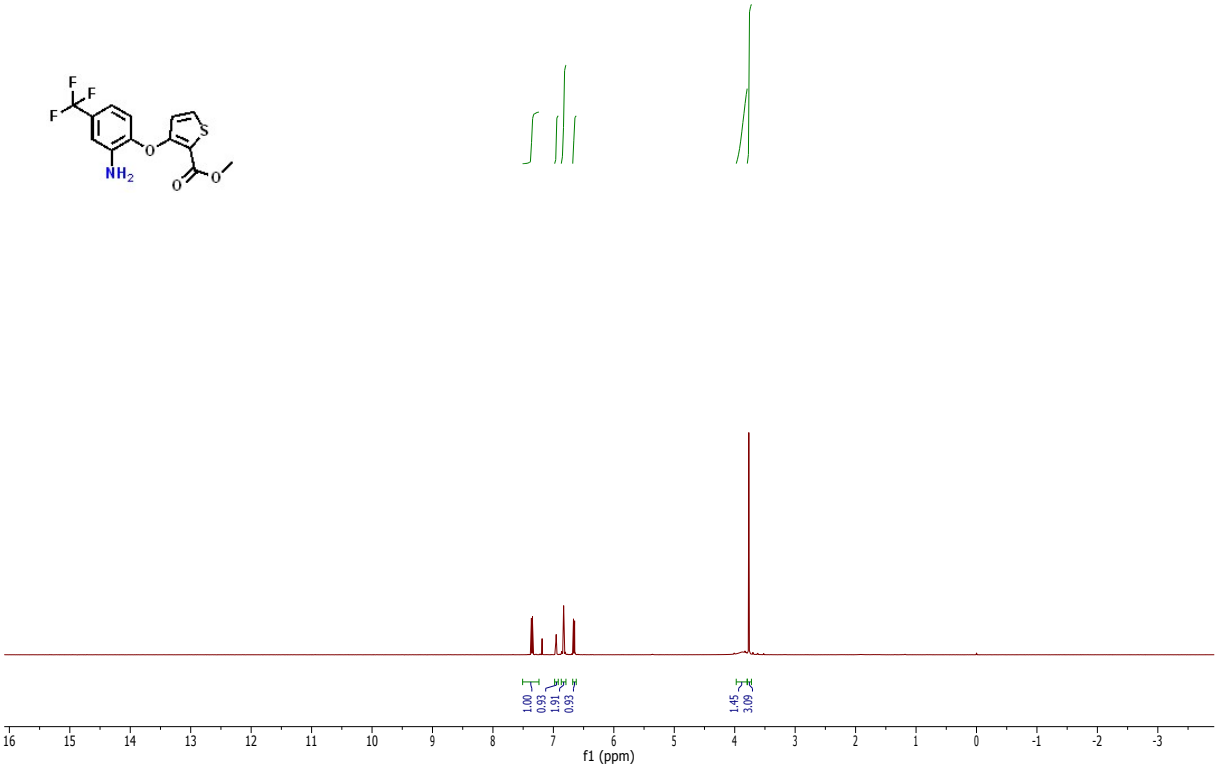
Kathir/ KM10-256
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 4



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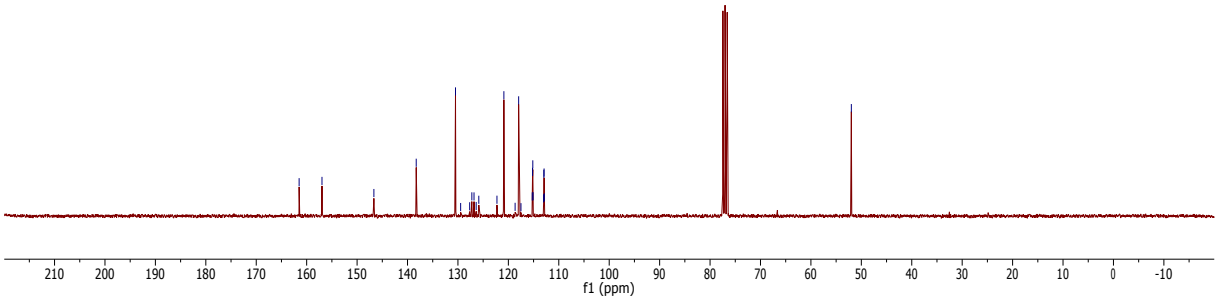
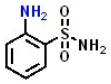
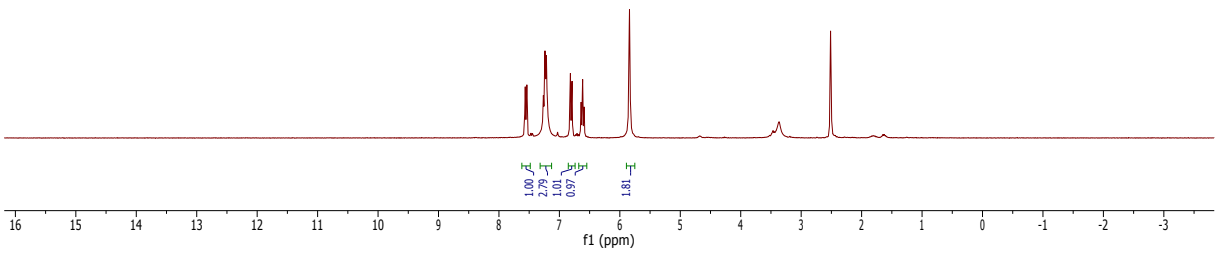
Kathir/ KM10-256
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 4



170822.f332.10.fid
Kathir KM10-269
PROTON DMSO {C:\Bruker\TopSpin3.5pl6} 1708 32





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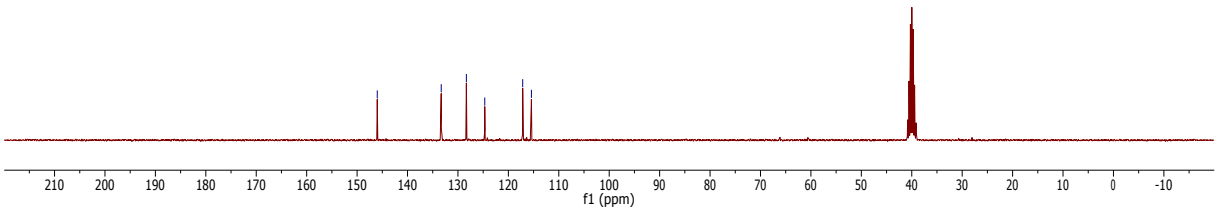
Kathir KM10-269
C13CPD DMSO {C:\Bruker\TopSpin3.5pl6} 1708 32



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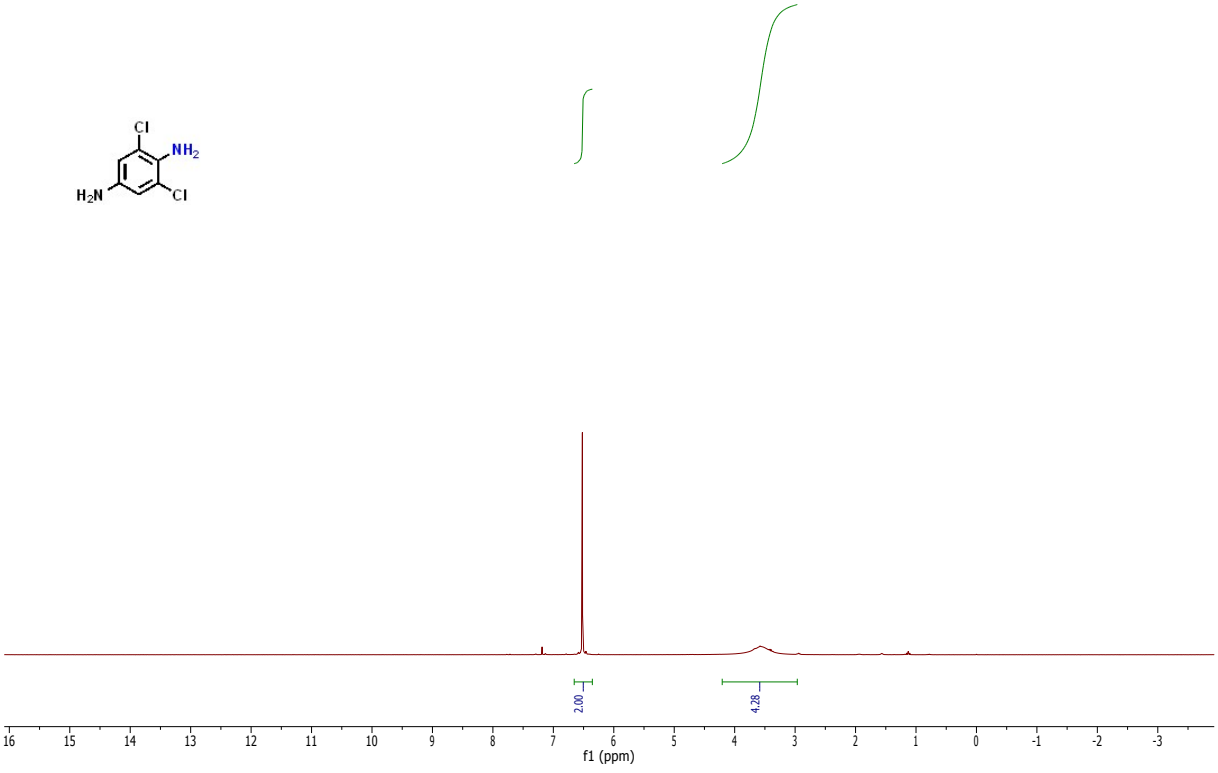
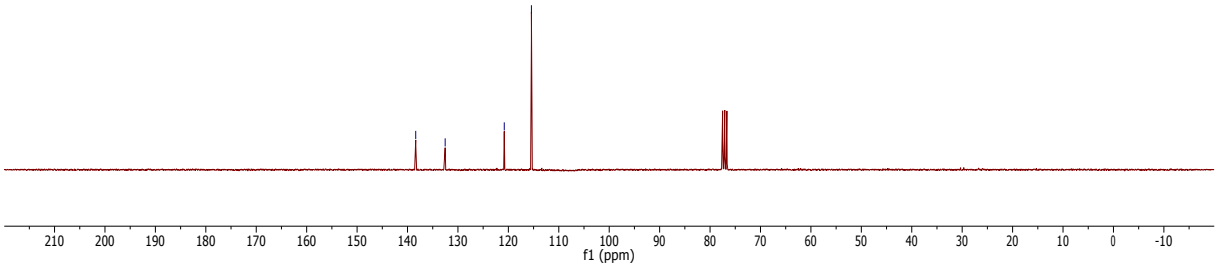
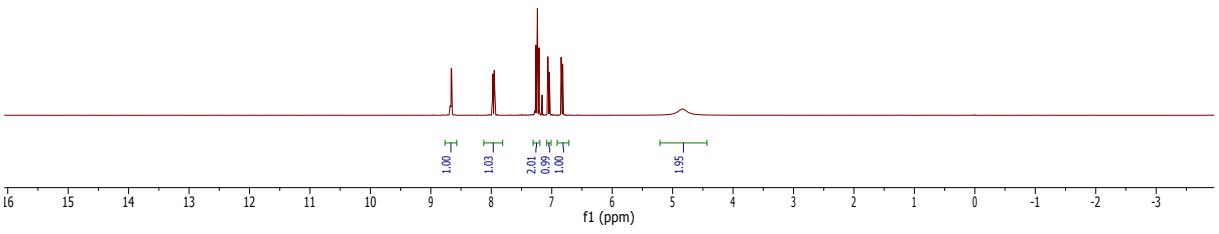
Kathir KM10-267
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 34



170822.f334.11.fid
Kathir KM10-267
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 34

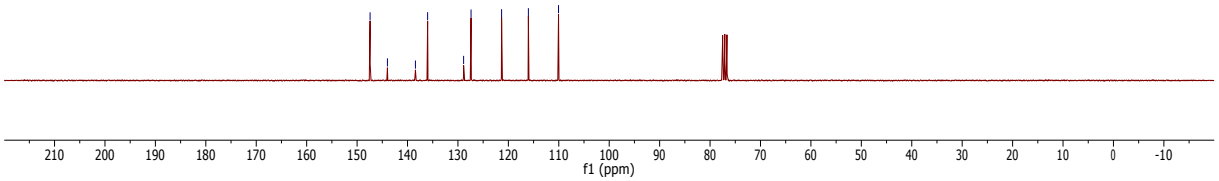


170822.f336.10.fid
Kathir KM10-242
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 36



170822.f336.11.fid
Kathir KM10-242
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 36

147.42
143.98
138.43
136.01
128.87
127.40
121.34
116.03
110.05



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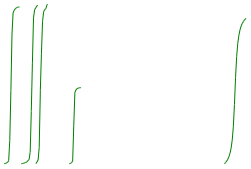
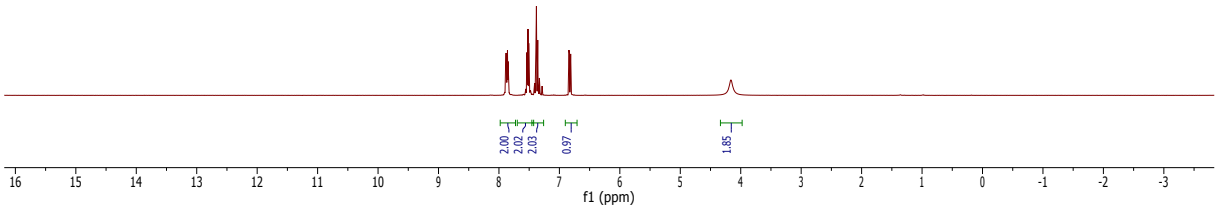
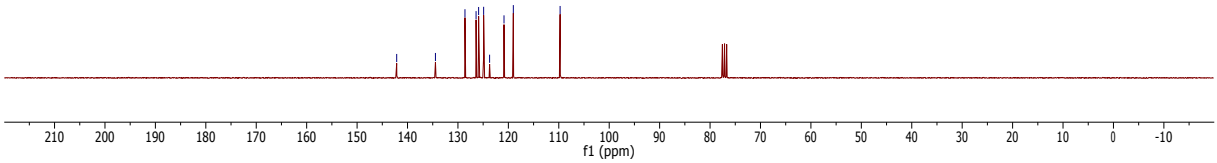
Kathir KM10-251
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 37



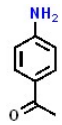


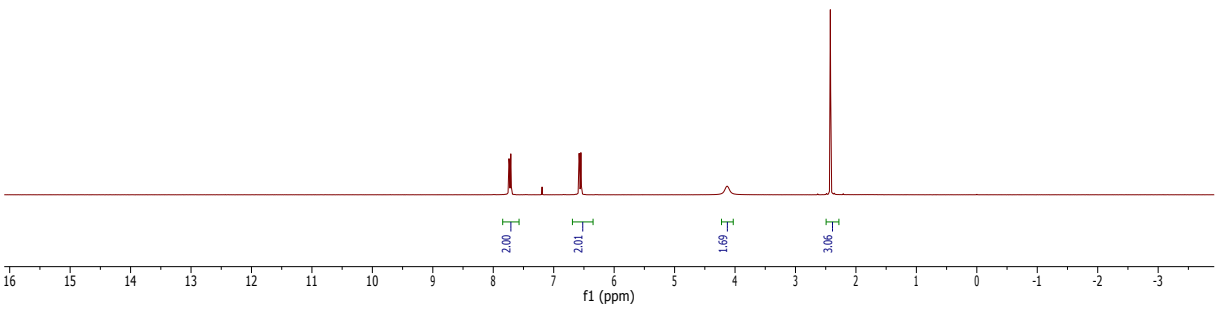
170822.f337.11.fid
Kathir KM10-251
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 37

142.15
134.46
128.61
126.40
125.90
124.90
123.72
120.86
119.02
109.74



170822.f338.10.fid
Kathir KM10-277
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 38





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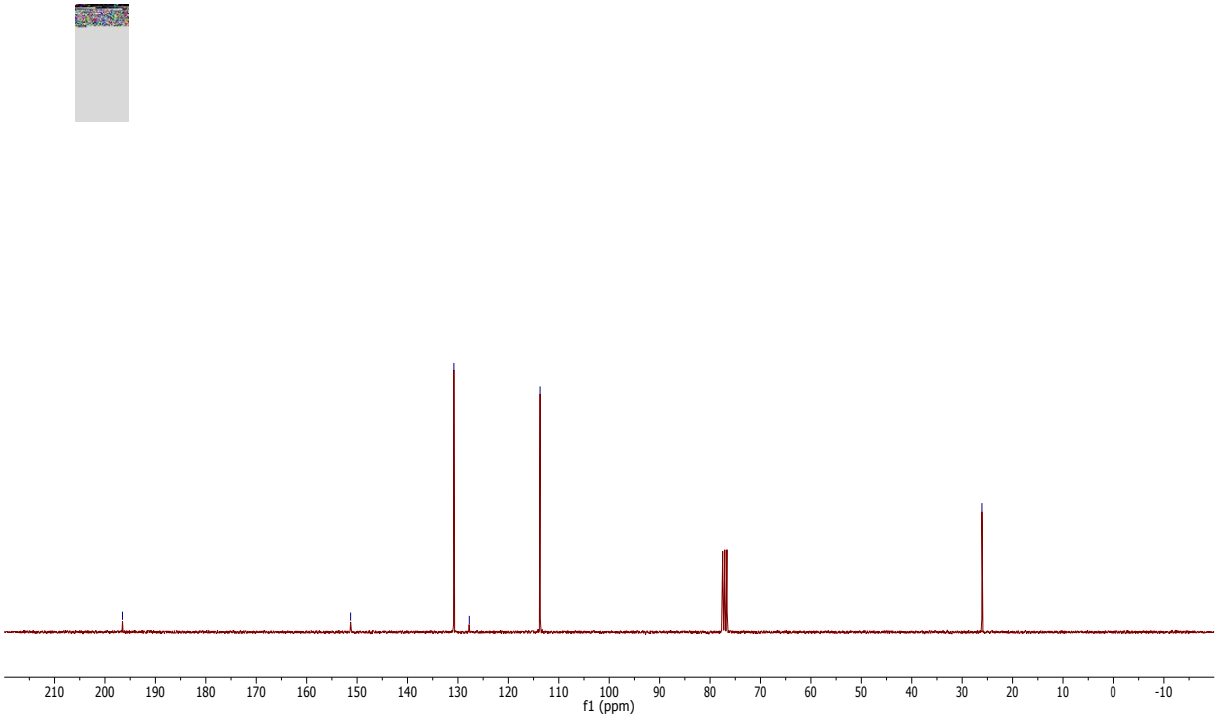
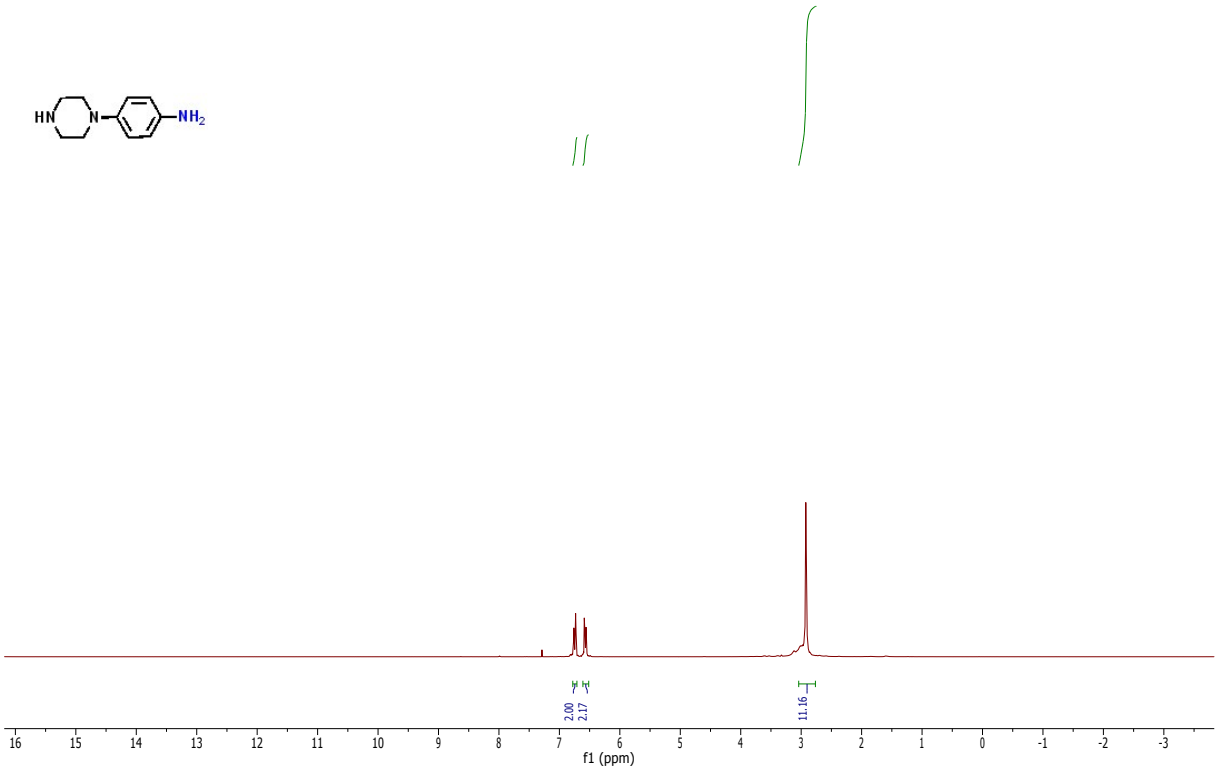
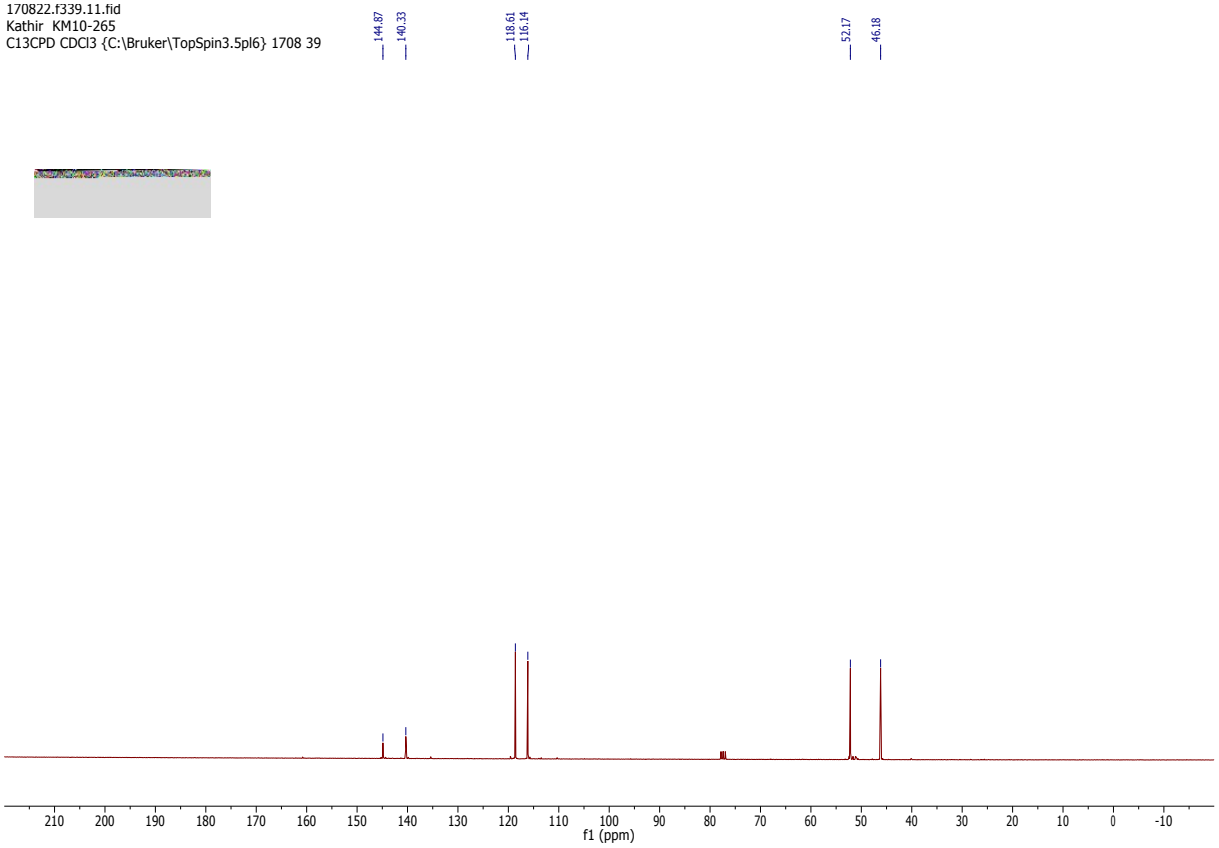
Kathir KM10-277
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 38



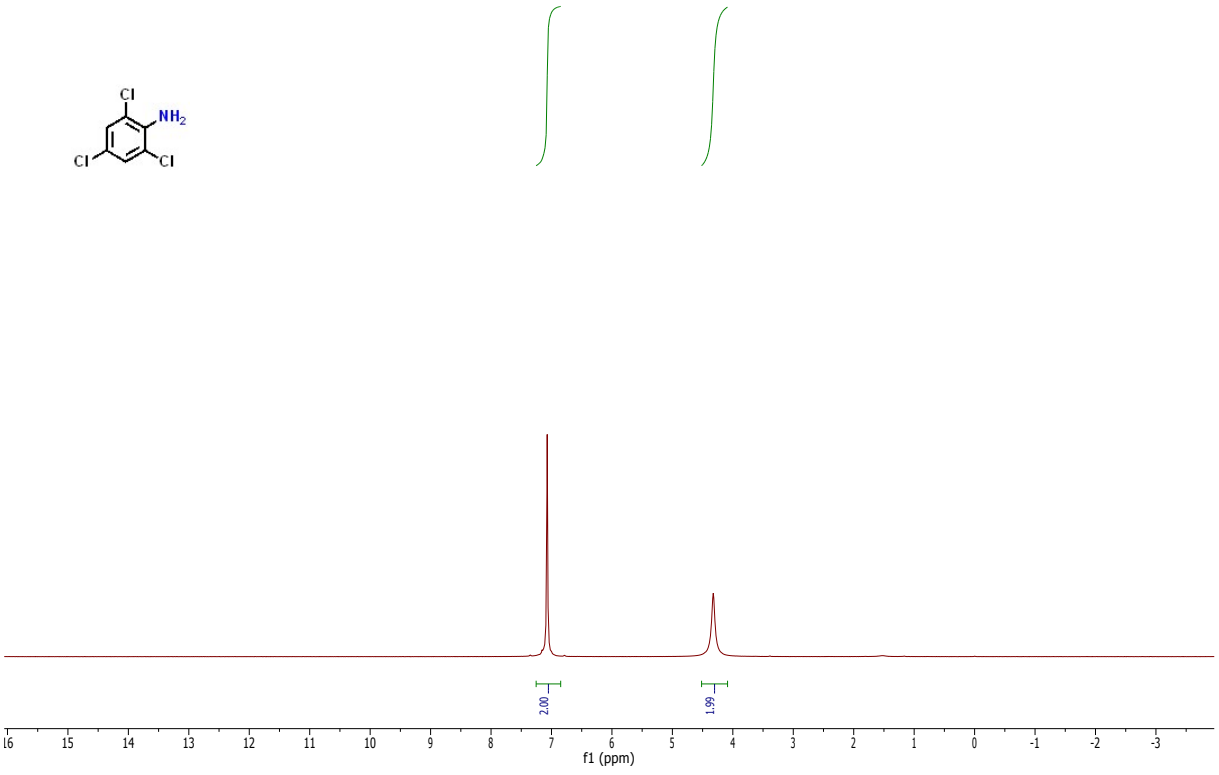
170822.f339.10.fid
Kathir KM10-265
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 39



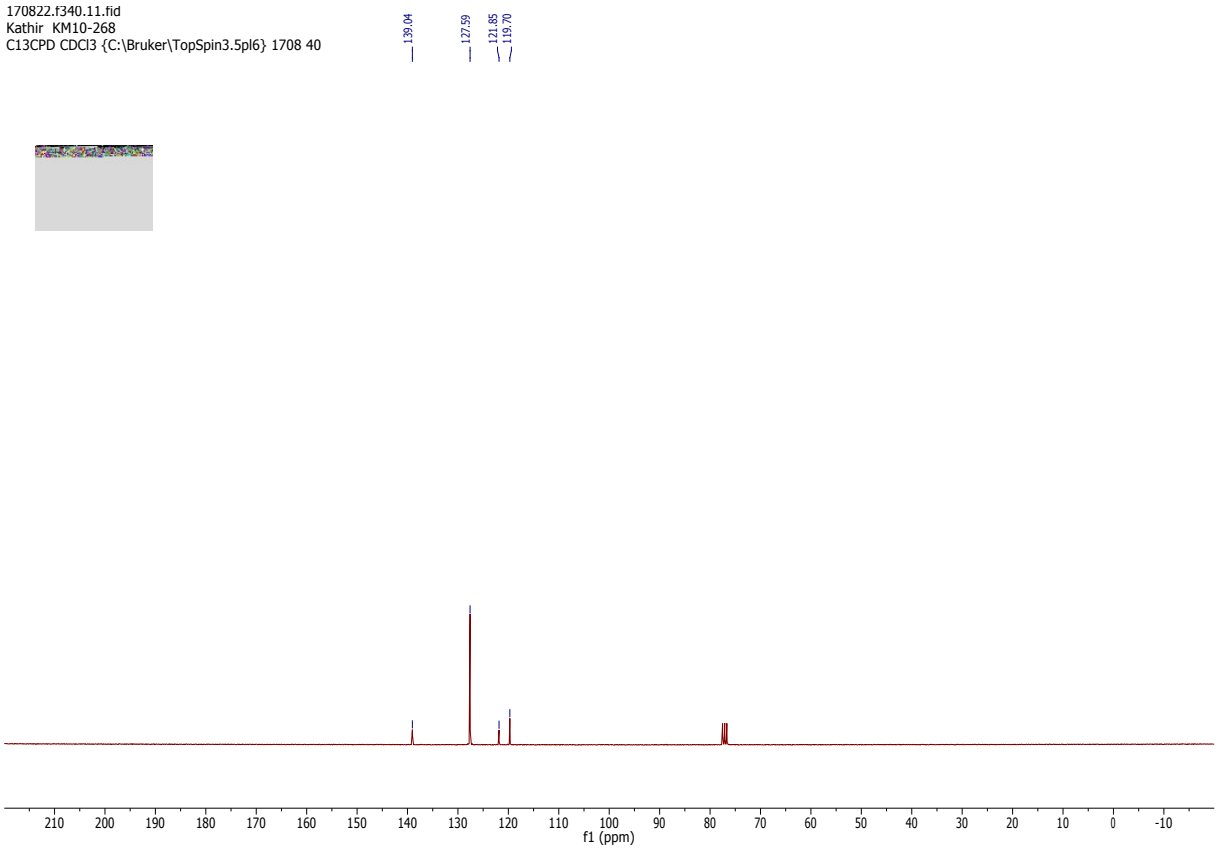
170822.f339.11.fid
Kathir KM10-265
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 39



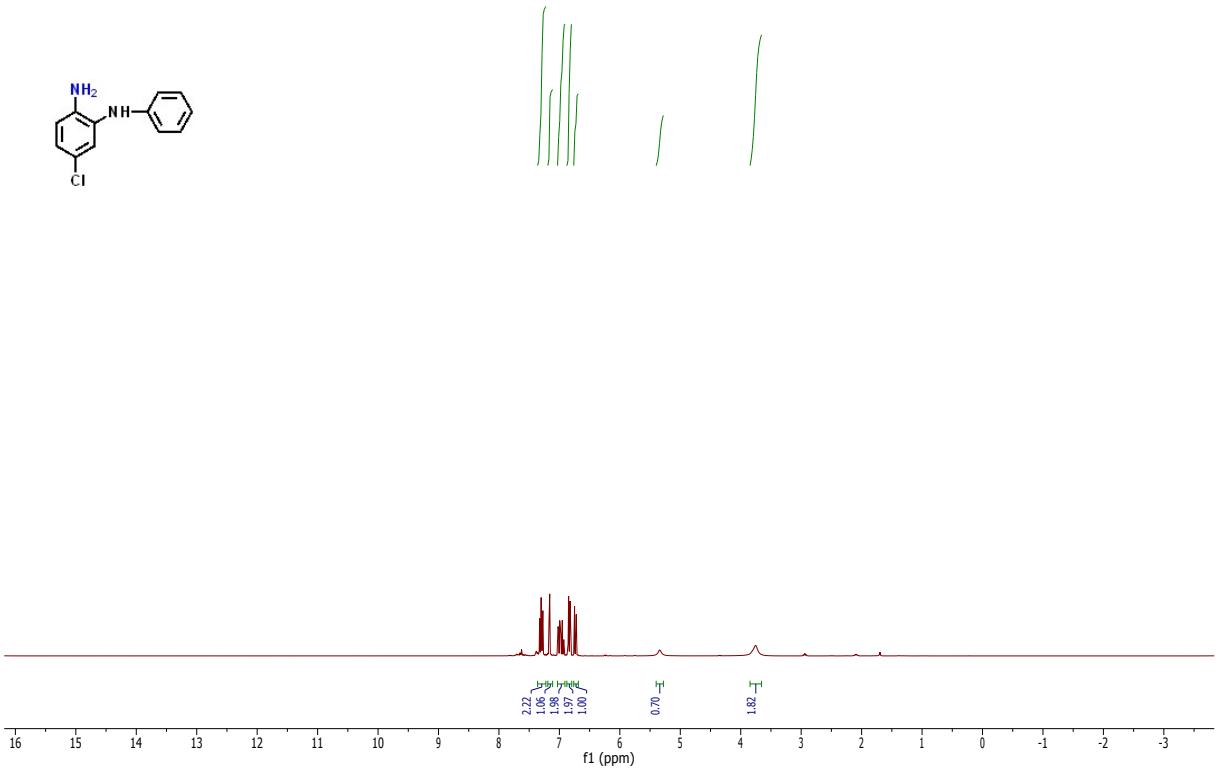
170822.f340.10.fid
Kathir KM10-268
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 40



170822.f340.11.fid
Kathir KM10-268
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 40

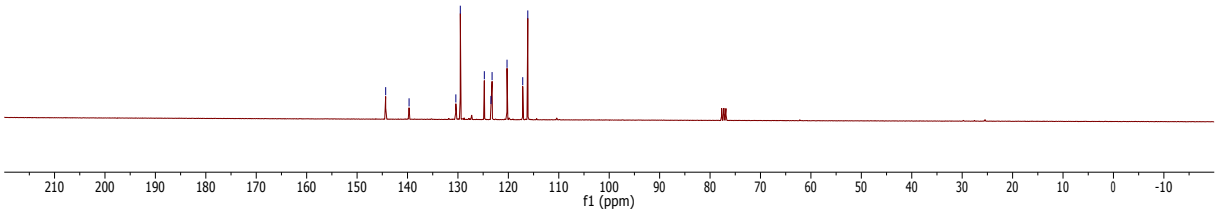


170823.f311.10.fid
Kathir KM10-272
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 11

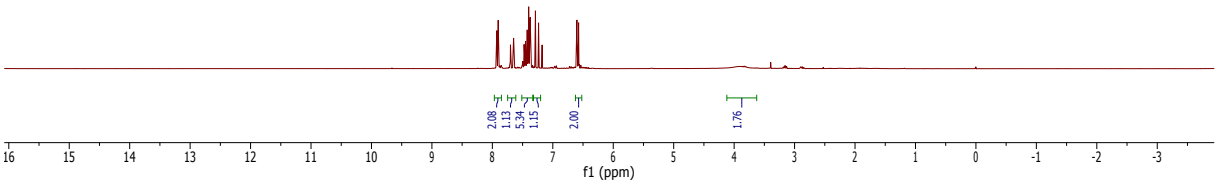


170823.f311.11.fid
Kathir KM10-272
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 11

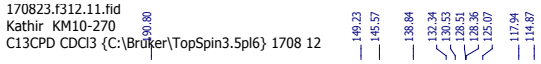
144.33
139.69
130.42
129.53
124.77
123.45
123.23
120.27
117.15
116.15

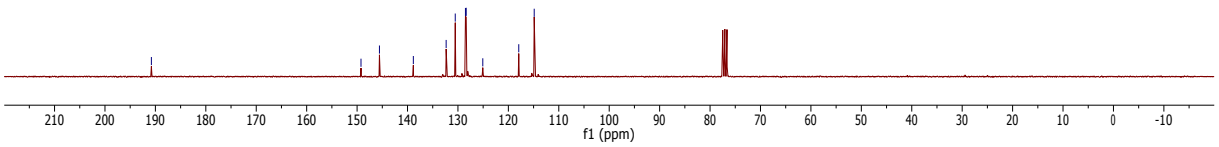


170823.f312.10.fid
Kathir KM10-270
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 12

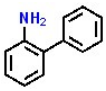


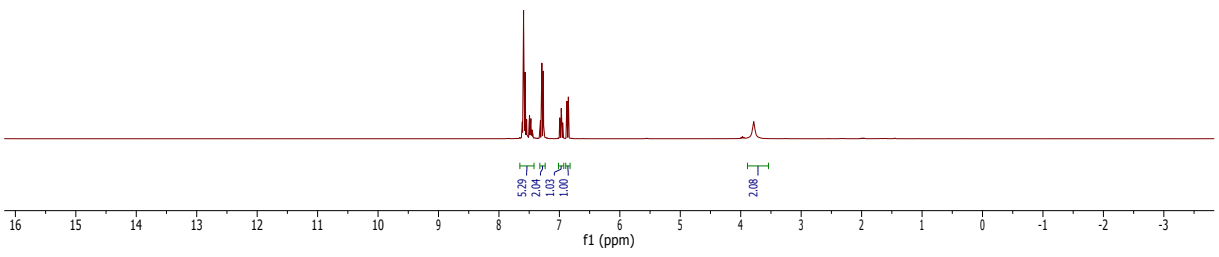
170823.f312.11.fid
Kathir KM10-270
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 12





170823.f313.10.fid
Kathir KM10-271
PROTON CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 13





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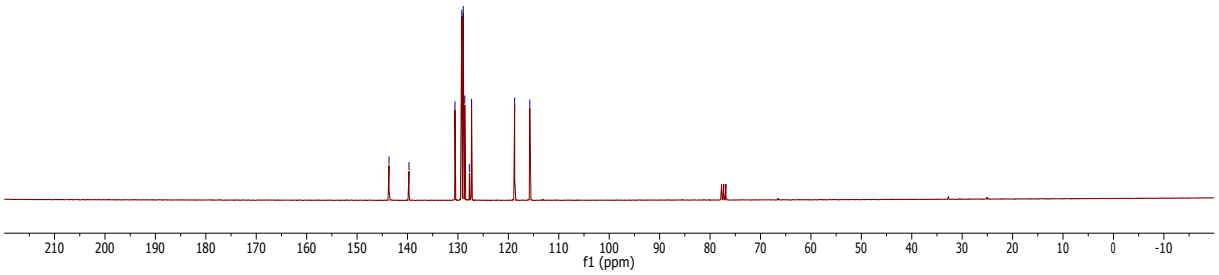
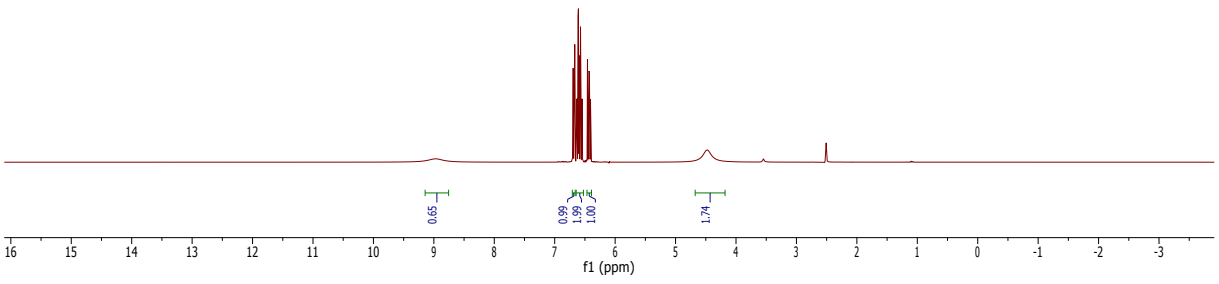
Kathir KM10-271
C13CPD CDCl3 {C:\Bruker\TopSpin3.5pl6} 1708 13



170828.311.1.fid
Kathir KM10-273
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1708 11



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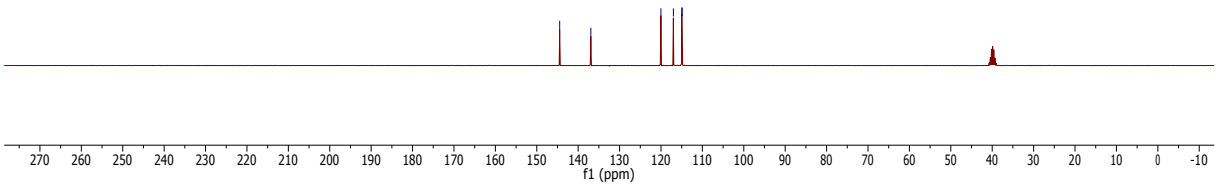
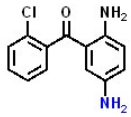
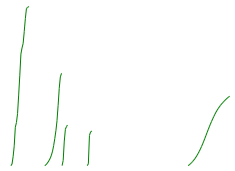
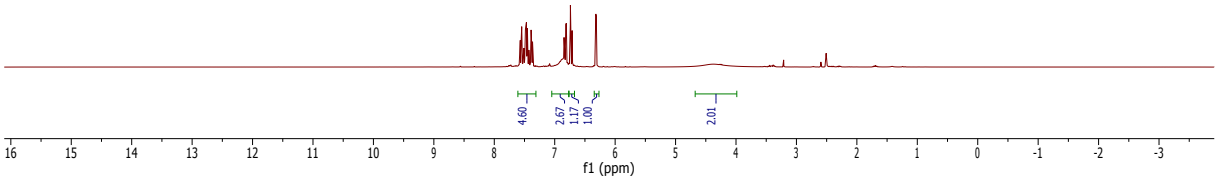
Kathir KM10-273
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1708 11



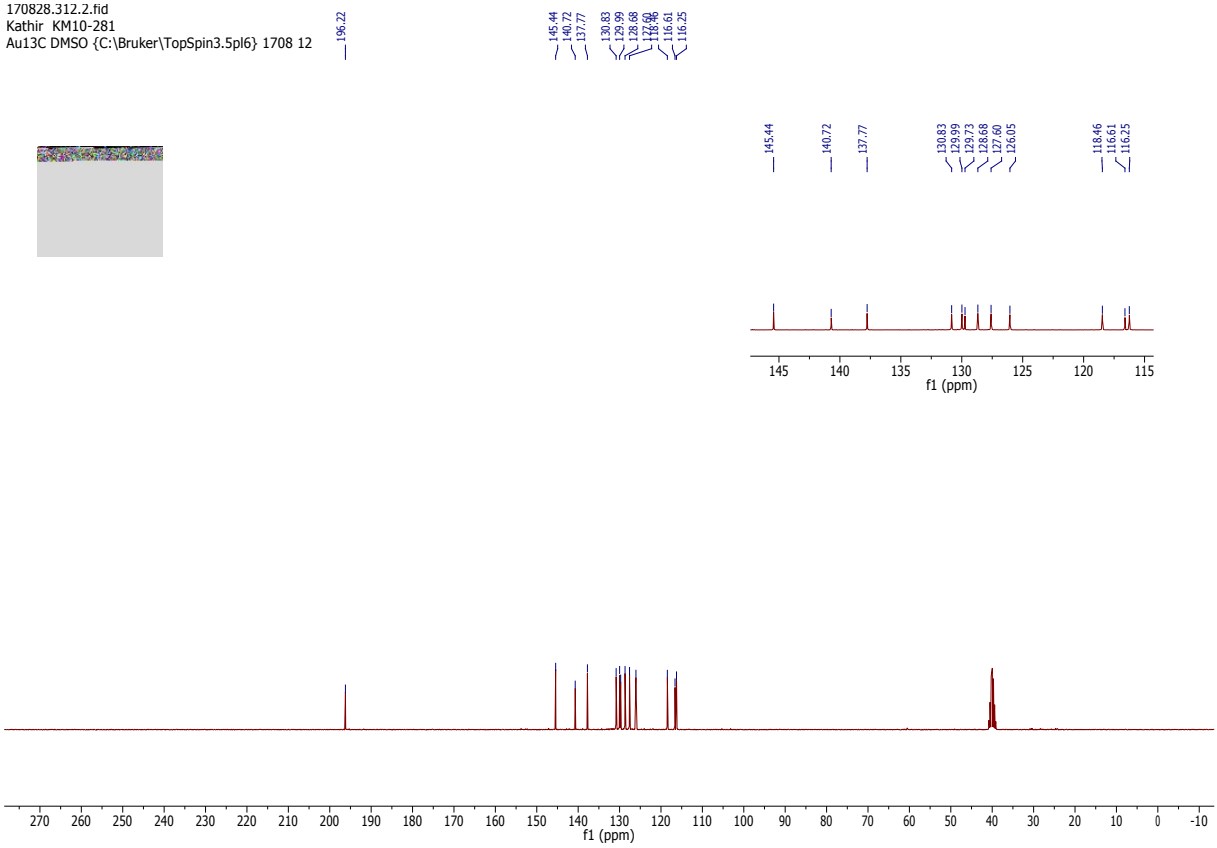
170828.312.1.fid
Kathir KM10-281
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1708 12



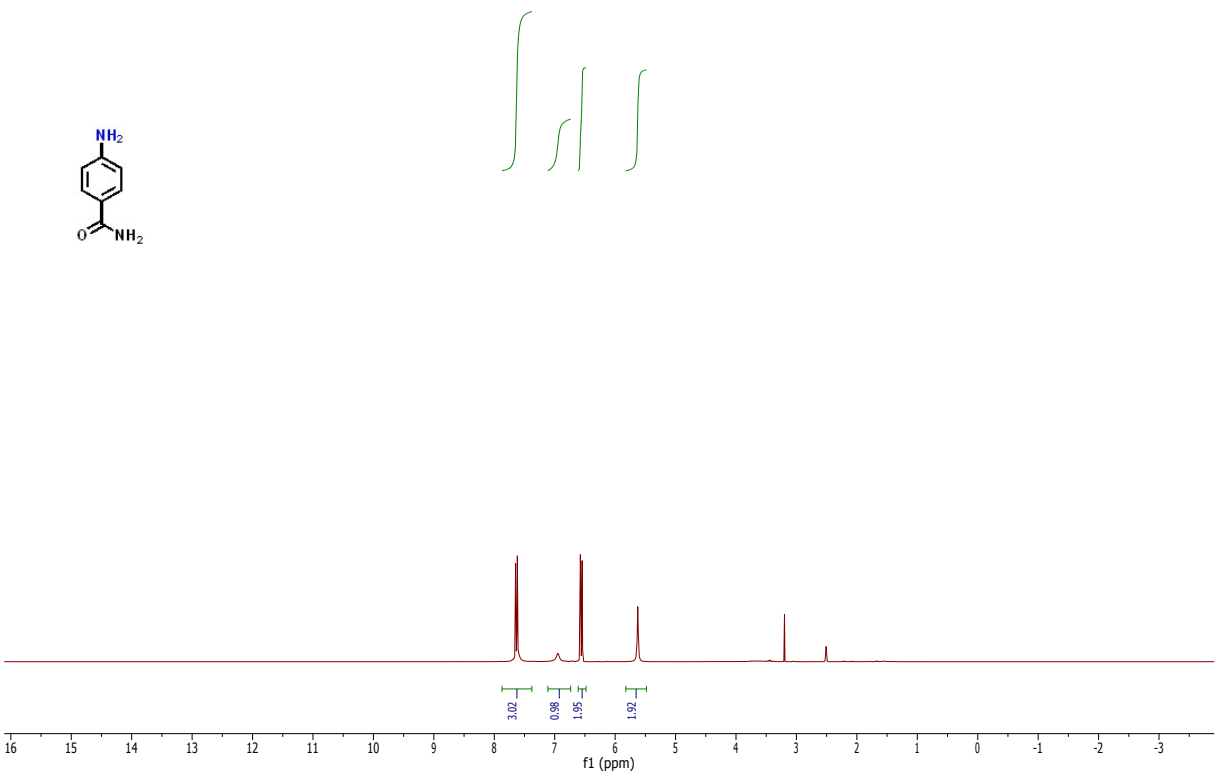




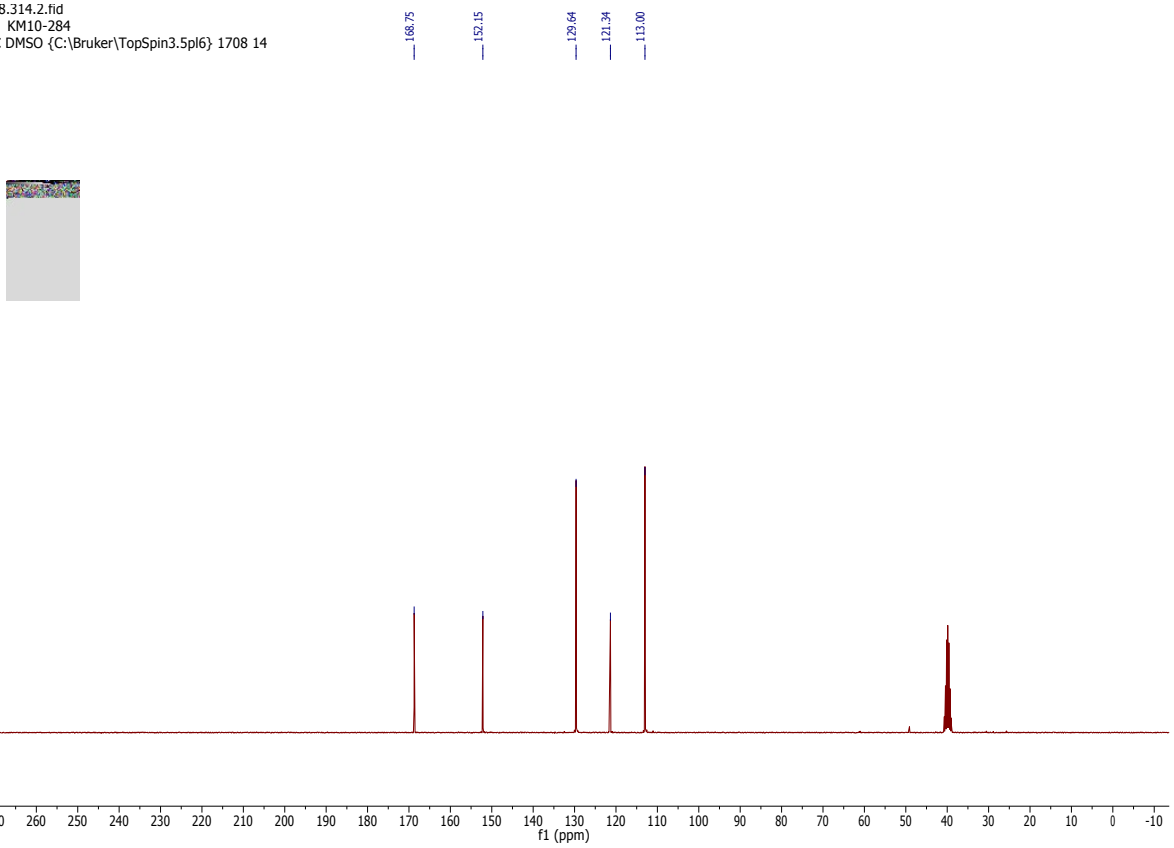
170828.312.2.fid
Kathir KM10-281
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1708 12



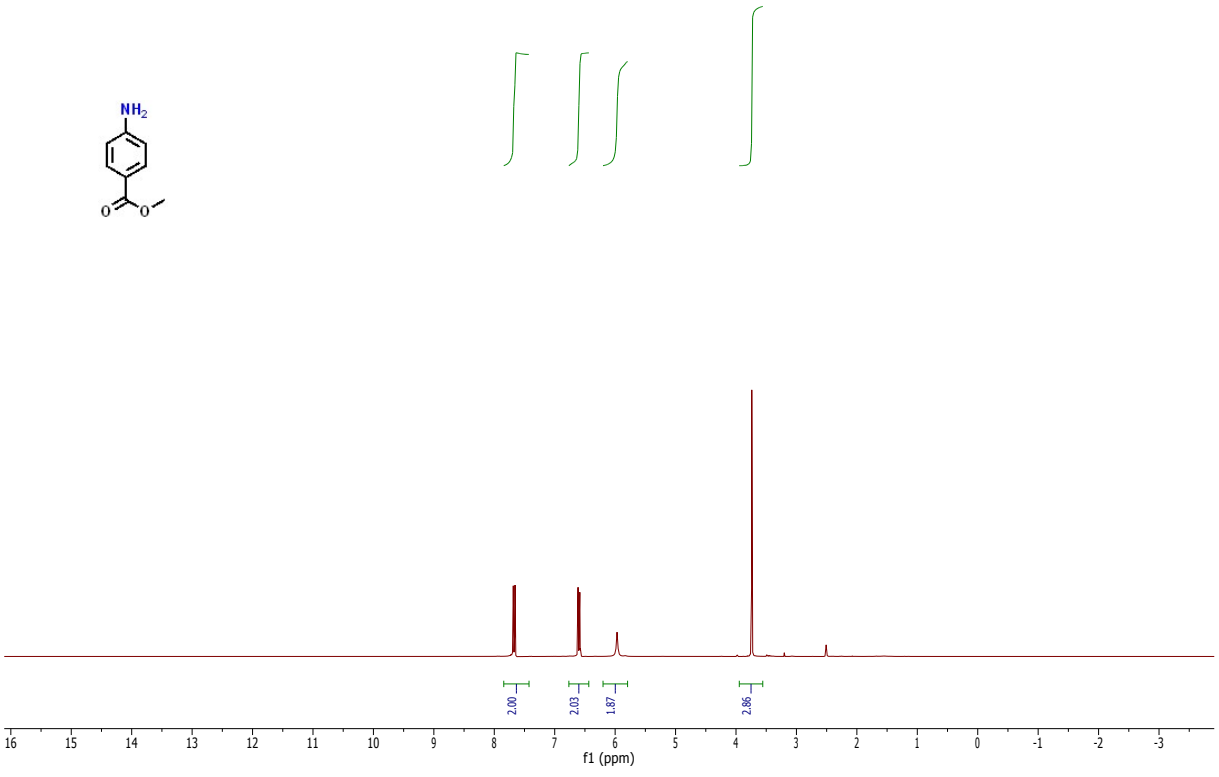
170828.314.1.fid
Kathir KM10-284
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1708 14



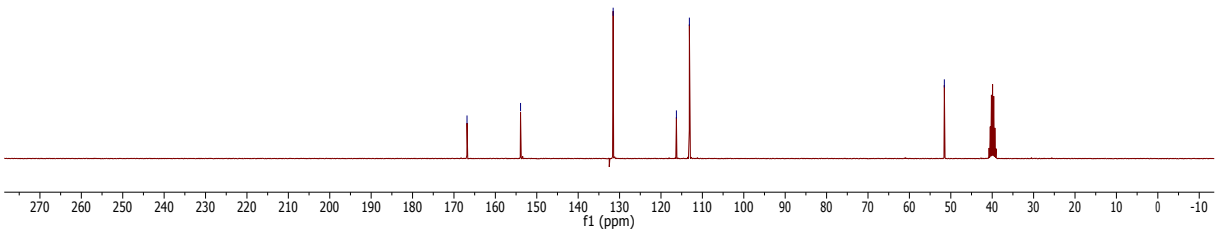
170828.314.2.fid
Kathir KM10-284
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1708 14



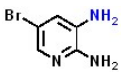
170828.315.1.fid
Kathir KM10-285
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1708 15

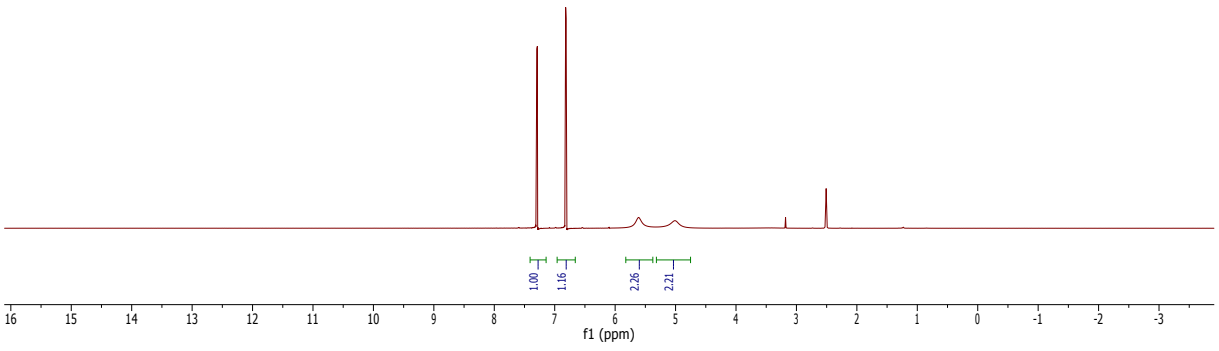


170828.315.2.fid
Kathir KM10-285
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1708 15



170828.310.1.fid
Kathir KM10-266
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1708 10





170828.310.2.fid
Kathir KM10-266
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1708 10