

Supporting Information

General and selective synthesis of primary amines using Ni-based homogeneous catalysts

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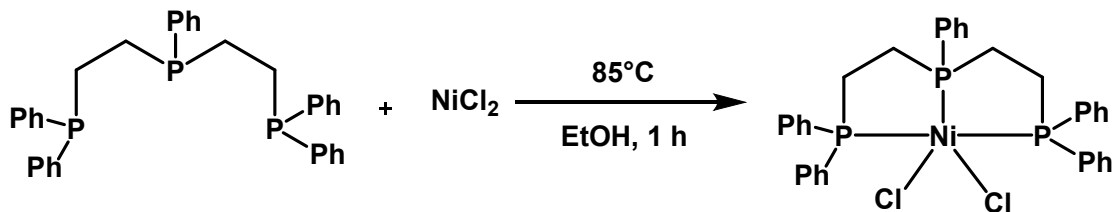
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S1. Materials and methods

Unless specified, all substrates were obtained commercially from various chemical companies and their purity has been checked before use. Unless otherwise stated, all commercial reagents were used as received without purification. All catalytic reactions were carried out in 300 mL and 100 mL autoclaves (PARR Instrument Company). In order to avoid unspecific reactions, catalytic reactions were carried out either in glass vials, which were placed inside the autoclave, or glass/Teflon vessel fitted autoclaves. GC conversion and yields were determined by GC-FID, HP6890 with FID detector, column HP530 m x 250 mm x 0.25 μ m. ^1H , ^{13}C NMR data were recorded on a Bruker ARX 300 and Bruker ARX 400 spectrometers using DMSO- d_6 , CD_3OD and CDCl_3 solvents. HRMS data were recorded on EI-HRMS: Mass Spectrometer MAT 95XP (Thermo Electron), 70eV.

X-ray crystal structure analysis of complex A: Data were collected on a Bruker Kappa APEX II Duo diffractometer. The structure was solved by direct methods (SHELXS-97: Sheldrick, G. M. Acta Cryst. **2008**, *A64*, 112.) and refined by full-matrix least-squares procedures on F^2 (SHELXL-2014: Sheldrick, G. M. Acta Cryst. **2015**, *C71*, 3.). XP (Bruker AXS) was used for graphical representations.

S2. Synthesis and characterization of [(Ph₂PCH₂CH₂)₂PPh]NiCl₂ complex ^{6a}



The anhydrous NiCl₂ (64.8 mg, 1.0 mmol) in ethanol (6 mL) was stirred at 85 °C under argon to obtain pale yellow solution. To this, triphos ((phenylphosphanediyl) bis(ethane-2,1-diyl)) bis(diphenylphosphane) (535.55 mg, 1. mmol) was added and stirring was continued at 85 °C for 1 h. Upon adding, the ligand pale yellow solution was turned into brown color. After the completion of reaction, the heating and stirring was switched off and allowed to cool for overnight. Dark brown crystals were observed along with a brown solid. The crystals were separated carefully and recrystallized again with ethanol for measuring X-ray diffraction analysis. The remaining reaction mixture was concentrated under reduced pressure to remove ethanol. The brown colored solid was washed with diethyl ether (3 x 10 mL) and dried under high vacuum for 2h to get the [(Ph₂PCH₂CH₂)₂PPh]NiCl₂ complex as pale brown color solid (600 mg , 90% yield).

¹H NMR (400 MHz, Chloroform-*d*) δ 8.85 – 8.50 (m, 2H), 8.03 – 7.76 (m, 4H), 7.68 – 7.26 (m, 19H), 4.41 – 3.98 (m, 2H), 3.44 – 2.87 (m, 4H), 2.34 – 2.02 (m, 2H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 134.75 (Vd, *J* = 10.2 Hz), 134.10 (Vt, *J* = 5.7 Hz), 133.62 , 132.88 (Vt, *J* = 5.7 Hz), 132.00 (Vd, *J* = 15.2 Hz), 130.16 (Vd, *J* = 10.6 Hz), 129.59 (Vt, *J* = 5.1 Hz), 129.17 (Vt, *J* = 5.4 Hz), 30.90 , 28.47 .

³¹P NMR (162 MHz, Chloroform-*d*) δ 111.06 (t, *J* = 48.3 Hz), 48.55 (d, *J* = 48.3 Hz).

ESI-HRMS (m/z pos): Calculated for [C₃₄H₃₃ClNiP₃]: 627.0842; found: 627.0852.

Elemental analysis: Calculated for [C₃₄H₃₃Cl₂NiP₃]: C, 61.49; H, 5.01; Cl, 10.68; Ni, 8.84. Found: C, 61.81; H, 4.58; Cl, 10.36; Ni, 7.83.

Crystal data for complex A: C₃₄H₃₃Cl₂NiP₃, *M* = 664.12, monoclinic, space group *P*2₁/*m*, *a* = 8.1732(6), *b* = 20.6167(15), *c* = 9.3736(7) Å, β = 103.6446(11)°, *V* = 1534.9(2) Å³, *T* = 150(2) K, *Z* = 2, 26537 reflections measured, 3812 independent reflections (*R*_{int} = 0.0219), final *R* values (*I* > 2σ(*I*)): *R*₁ = 0.0232, *wR*₂ = 0.0593, final *R* values (all data): *R*₁ = 0.0246, *wR*₂ = 0.0604, GOF on *F*²: 1.047, 196 parameters.

CCDC 1869414 contains the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

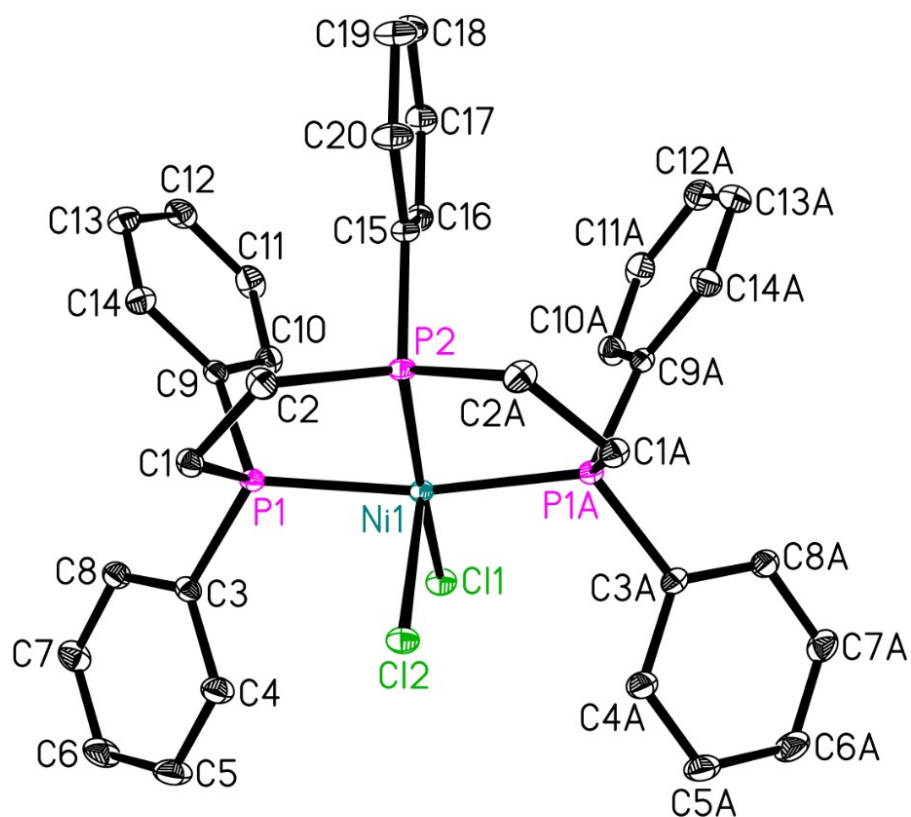


Figure S1. Molecular structure of complex **A** in the crystal. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen atoms are omitted for clarity. Symmetry transformation used to generate equivalent atoms: $x, -y+1/2, z$.

S3. General procedure for the synthesis of primary amines

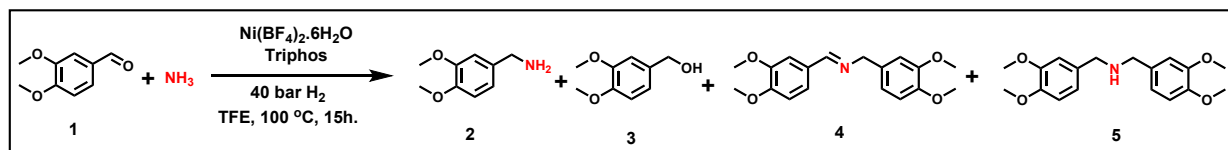
The magnetic stirring bar and $\text{Ni}(\text{BF}_4)_2 \cdot 6\text{H}_2\text{O}$ (4 mol%) and linear triphos ((**L1**; phenylphosphanediy)bis(ethane-2,1-diyl))bis(diphenylphosphane) (4 mol%) were transferred to 8 mL glass vial and then 2 mL degassed (degassed under argon for 15 minutes before adding) trifluoroethanol (TFE) solvent was added. The colorless solution turned in to brown color, which was stirred under argon for 15 minutes. Then, 0.5 mmol of corresponding carbonyl compound was added and the vial was fitted with septum, cap and needle. The reaction vials (8 vials with different substrates at a time) were placed into a 300 mL autoclave. The autoclave was flushed with hydrogen twice at 30 bar pressure and then it was pressurized with 5-7 bar ammonia gas and 40 bar hydrogen. The autoclave was placed into an aluminum block preheated at 120 °C-130 (placed 30 minutes before counting the reaction time in ordered to attain reaction temperature) and the reactions were stirred for required time. During the reaction, the inside temperature of the autoclave was measured to be 100-120 °C (10 °C less then temperature set at aluminum block) and this temperature was used as the reaction temperature. After the completion of the reactions, the autoclave was cooled to room temperature. The remaining ammonia and hydrogen were discharged and the vials containing reaction products were removed from the autoclave. The reaction mixture was filtered off and washed thoroughly with ethyl acetate. The reaction products were analyzed by GC-MS. The corresponding primary amines were converted to their respective hydrochloride salt and characterized by NMR and GC-MS analysis. For converting into hydrochloride salt of amine, 1-2 mL methanolic HCl (0.5M HCl in methanol) was added to the ether solution of respective amine and stirred at room temperature for 4-5 h. Then, solvent was removed, and the resulted hydrochloride salt of amine is dried under high vacuum. The yields were determined by GC for the selected amines: After completion of the reaction, n-hexadecane (100 μL) as standard was added to the reaction vials and the reaction products were diluted with ethyl acetate followed by filtration using plug of silica and then analyzed by GC.

S4. General procedure for the hydrogenation of nitroarenes to aromatic primary amines

The magnetic stirring bar and $\text{Ni}(\text{BF}_4)_2 \cdot 6\text{H}_2\text{O}$ (4 mol%) and linear triphos ((phenylphosphanediy1)bis(ethane-2,1-diyl))bis(diphenylphosphane) (4 mol%) were transferred to 8 mL glass vial and then 2 mL degassed (degassed under argon for 15 minutes before adding) trifluoroethanol (TFE) solvent was added. The colorless solution turned in to brown color, which was stirred under argon for 15 minutes. Then, 0.5 mmol corresponding nitro compounds was added and the vial was fitted with septum, cap and needle. The reaction vials (8 vials with different substrates at a time) were placed into a 300 mL autoclave. The autoclave was flushed with hydrogen twice at 30 bar pressure and then it was pressurized 40 bar hydrogen. The autoclave was placed into an aluminum block preheated at 130 °C (placed 30 minutes before counting the reaction time in ordered to attain reaction temperature) and the reactions were stirred for required time. During the reaction the inside temperature of the autoclave was measured to be 120 °C and this temperature was used as the reaction temperature. After the completion of the reactions, the autoclave was cooled to room temperature. The remaining hydrogen was discharged and the vials containing reaction products were removed from the autoclave. The reaction mixture was filtered off and washed thoroughly with ethyl acetate. The reaction products were analyzed by GC-MS. The corresponding anilines were isolated by column chromatography to their respective amines, which were characterized by NMR and GC-MS analysis. The yields were determined by GC for the selected amines: After completion of the reaction, n-hexadecane (100 μL) as standard was added to the reaction vials and the reaction products were diluted with ethyl acetate followed by filtration using plug of silica and then analyzed by GC.

S5. Solvent screening

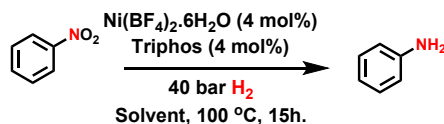
Table S1. Influence of solvents on Ni-triphos catalyzed reductive amination of veratraldehyde



Entry	Solvent	Conv. (%)	Yield of 2 (%)	Yield of 3 (%)	Yield of 4 (%)	Yield of 5 (%)
1	Toluene	4	-	-	2	-
2	THF	20	-	-	18	-
3	<i>t</i> -Amyl alcohol	22	-	-	20	-
4	<i>t</i> -buOH	25	-	-	23	-
5	EtOH	50	-	-	48	-
6	MeOH	70	-	-	68	-
7	Trifluoroethanol	>99	96	-	2	-

Reaction conditions: 0.5 mmol veratraldehyde, 4 mol% $\text{Ni}(\text{BF}_4)_2 \cdot 6\text{H}_2\text{O}$, 4 mol% triphos (L1), 5-7 bar NH_3 , 40 bar H_2 , 2 mL solvent, 100 °C, 15 h, GC yields using n-hexadecane as standard.

Table S2. Influence of solvents on Ni-triphos catalyzed hydrogenation of nitrobenzene

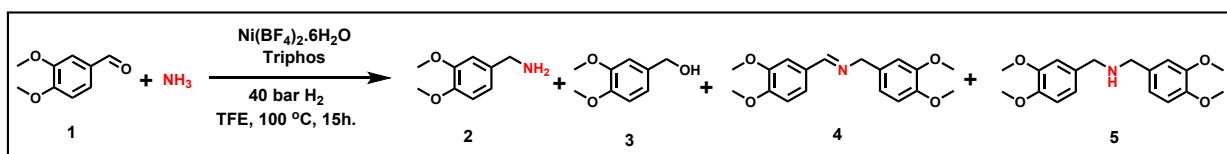


Entry	Solvent	Conv. (%)	Yield of aniline (%)
1 ^a	Toluene	4	2
2 ^a	THF	6	4
3 ^a	IPA	32	30
4 ^a	EtOH	23	21
5 ^a	MeOH	13	11
6 ^a	Trifluoroethanol	72	70
7 ^b	Trifluoroethanol	75	72
8 ^c	Trifluoroethanol	>99	97

Reaction conditions: 0.5 mmol nitrobenzene, 4 mol% $\text{Ni}(\text{BF}_4)_2 \cdot 6\text{H}_2\text{O}$, 4 mol% triphos (L1), 40 bar H_2 , 2 mL solvent, 100 °C, 15 h, GC yields using n-hexadecane as standard. ^bsame as for 24h. ^cSame as 'a' at 120 °C for 24h.

S6. Catalytic poison test

Table S3.



Entry	Catalytic poison	Conv. (%)	Yield of 2 (%)	Yield of 3 (%)	Yield of 4 (%)	Yield of 5 (%)
1a	Hg (2 eq)	>99	93	-	5	-
2a	PPh3 (50 mol%)	>99	92	-	6	-

Reaction conditions: 0.5 mmol veratraldehyde, 4 mol% Ni(BF₄)₂·6H₂O, 4 mol% triphos (**L1**), 5-7 bar NH₃, 40 bar H₂, 2 mL trifluoroethanol (TFE), 100 °C, 15 h, GC yields using n-hexadecane as standard.

S7. Computational details

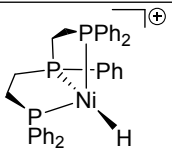
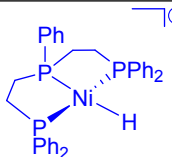
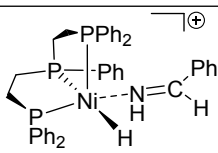
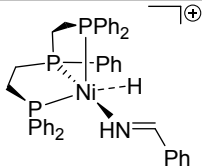
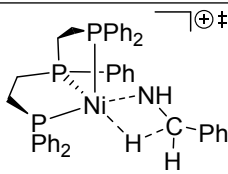
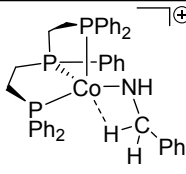
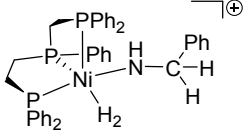
DFT calculation

All calculations were carried out with Gaussian 16 program.^{S1} Geometry optimization was carried out in gas phase at the B3PW91^{S2} level with the TZVP^{S3} basis set. All optimized structures were further characterized either as energy minimums without imaginary frequencies or transition states with only one imaginary frequency by frequency calculations, which provided zero-point vibrational energies and thermodynamic corrections to enthalpy and Gibbs free energy at 298.15 K under 1 atmosphere. On the basis of B3PW91/TZVP geometries in gas phase, single-point energies including solvation effect of 2,2,2-trifluoroethanol (TFE) as solvent (dielectric constant $\epsilon = 26.69$) based on solute electron density (SMD^{S4}) and van der Waals dispersion (D3^{S5}) with the gas phase optimized geometries were computed (B3PW91-SMD-D3). The Gibbs free energies at 298.15 K were further corrected to standard state in solution with a standard concentration of 1 mol/L ($p = 24.5$ atm) from standard state in gas phase ($p = 1$ atm).

- S1. Frisch, M. J. *et al.* Gaussian software, version 16 revision D01. *Gaussian Inc.: Wallingford, CT, USA* (2016)
- S2. Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* 1993, **98**, 5648-5652.
- S3. Schäfer, A., Huber, C. & Ahlrichs, R. Fully optimized contracted Gaussian basis sets of triple zeta valence quality for atoms Li to Kr. *J. Chem. Phys.* 1994, **100**, 5829-5835
- S4. Marenich, A. V., Cramer, C. J. & Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* 2009, **113**, 6378-6396

- S5. Grimme, S., Ehrlich, S. & Goerigk, L. Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* 2011, **32**, 1456-1465

Table S4. Energetic data from B3PW91 full optimization (B3PW91/FOpt) as well as from single-point calculations with the B3PW91 optimized geometries including solvation effect and van der Waals dispersion correction (B3PW91-SCRF-D3//SP)

	B3PW91		B3PW91-SCRF-D3//SP
H2	HF=-1,178636 ZPE= 0,010064 NImag=0 Htot= -1,165268 Gtot= -1,180066	DH= 0,013368 DG = -0,001430	HF=-1,1784042
Ph-CH=NH	HF=-325,6720957 ZPE= 0,122294 NImag=0 Htot= -325,542365 Gtot= -325,580510	DH = 0,129730 DG = 0,091586	HF=-325,7093359
PhCH2NH2	HF=-326,8931026 ZPE= 0,145783 NImag=0 Htot= -326,739071 Gtot= -326,779504	DH = 0,154032 DG = 0,113599	HF=-326,9349566
	HF=-3848,1898173 ZPE= 0,581578 NImag=0 Htot= -3847,571055 Gtot= -3847,681819	DH = 0,618763 DG = 0,507999	HF=-3848,496691
	HF=-3848,1958745 ZPE=0,581223 NImag=0 Htot= -3847,577519 Gtot= -3847,689688	DH = 0,618355 DG = 0,506187	HF=-3848,5022471
	HF=-4173,8847115 ZPE= 0,706071 NImag=0 Htot= -4173,133471 Gtot= -4173,263221	DH = 0,751241 DG = 0,621491	HF=-4174,2400989
	HF=-4173,8809159 ZPE= 0,705803 NImag=0 Htot= -4173,129924 Gtot= -4173,259768	DH = 0,750992 DG = 0,621148	HF=-4174,2359305
	HF=-4173,8560405 ZPE= 0,704914 NImag=1 (-515) Htot= -4173,106739 Gtot= -4173,233294	DH = 0,749301 DG = 0,622746	HF= -4174,2238259
	HF=-4173,8604368 ZPE=0,707619 NImag=0 Htot=-4173,108237 Gtot= -4173,235999	DH = 0,752200 DG = 0,624438	HF=-4174,2261163
	HF=-4175,0315883 ZPE=0,724763 NImag=0 Htot=-4174,260570 Gtot= -4174,392754	DH = 0,771018 DG = 0,638834	HF=-4175,4030651

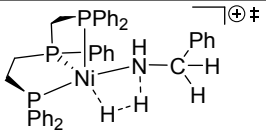
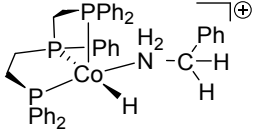
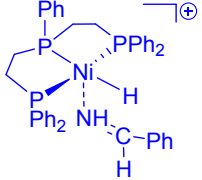
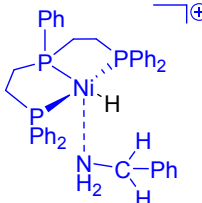
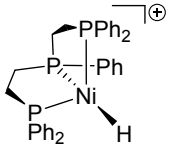
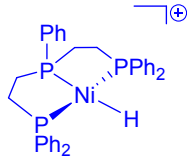
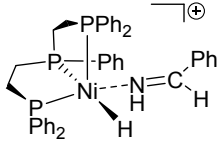
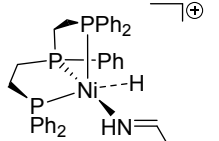
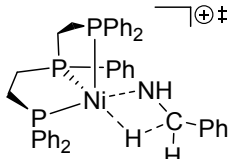
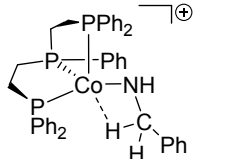
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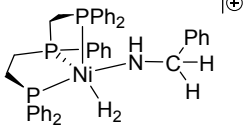
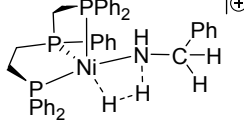
Table S5. B3PW91 optimized Cartesian Coordinates

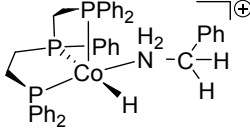
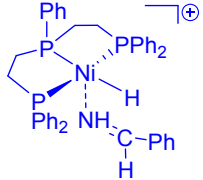
Ph-CH=NH H,0,-0.0474876739,-0.1281681285,-0.0555576751 C,0,-0.0291740412,-0.0465083908,1.024871828 C,0,0.0170699424,0.1037518339,3.8049483417 C,0,-0.0344085352,-1.2206416834,1.7831357401 C,0,-0.0011081343,1.1867085949,1.6531808906 C,0,0.0220773038,1.2654403182,3.0438849325 C,0,-0.0110733866,-1.133456896,3.1754529458 H,0,0.0028349699,2.0946595995,1.0602095654 H,0,0.0440300003,2.2335197941,3.5321138422 H,0,-0.0150617479,-2.0437409298,3.7677304751 H,0,0.0350663721,0.1615948253,4.8874368333 C,0,-0.063989135,-2.5427658915,1.1416429596 H,0,-0.0653337876,-3.3896145294,1.8419984143 H,0,-0.1046136035,-3.6784383921,-0.3699429567 N,0,-0.0861474737,-2.6913803885,-0.1194206798	Ph-CH₂NH₂ C,0,-0.0399531934,0.0791716512,1.0764204017 C,0,0.004558161,0.0047736352,3.8782686864 C,0,0.124608206,-1.1272910153,1.7571888373 C,0,-0.1930423763,1.2461695307,1.8252581236 C,0,-0.1689470691,1.2127644565,3.2136284597 C,0,0.1495410681,-1.1669542349,3.1453796938 H,0,0.2296015641,-2.0489136307,1.1917058955 H,0,-0.3381552174,2.1933210624,1.3133703945 H,0,-0.293253318,2.1303066407,3.7785975208 H,0,0.2749441556,-2.1152208696,3.6568385859 H,0,0.0201729907,-0.0242187706,4.9620525035 C,0,-0.0024413612,0.1275199553,-0.4343510864 H,0,-0.6475889996,0.9351711923,-0.791056968 H,0,-0.415383172,-0.7998527648,-0.8408163132 N,0,1.3219779275,0.3217715196,-1.0270687075 H,0,1.7312414314,1.1867942597,-0.6920225844 H,0,1.946656201,-0.4227682125,-0.7381837767
H₂ H,0,0.,0.,0.372594 H,0,0.,0.,-0.372594	
 C,0,2.1622727786,-1.6367521574,-2.4069399926 H,0,2.3876221995,-0.768749638,-3.0323055003 H,0,2.9558348418,-2.3646462377,-2.5932858061 C,0,0.7823865625,-2.2047906209,-2.7416070782 H,0,0.6861053884,-3.2305107231,-2.3814359645 H,0,0.6120745988,-2.2245470162,-3.8204651854 C,0,-1.5751144609,-0.2614164702,-3.106948833 H,0,-1.48177076,-0.6682213399,-4.1161992335 H,0,-2.6168167674,-0.3797721897,-2.8002702163 C,0,-1.1876686881,1.2173143021,-3.0718960765 H,0,-1.9536941653,1.8203163766,-3.5647835646 H,0,-0.2415582089,1.3858280747,-3.593528149 C,0,3.9168330039,-0.1865538784,-0.6093626438 C,0,5.065351611,-0.9643685731,-0.4512474681 H,0,4.9864734338,-2.0336897856,-0.2903674996 C,0,6.3175863787,-0.3667477764,-0.4784495558 H,0,7.2058252552,-0.9740433393,-0.3475281161 C,0,6.4319976086,1.0058229499,-0.6651080146 H,0,7.4113375151,1.4700878231,-0.6829676268 C,0,5.2913152946,1.7829333382,-0.8194722293 H,0,5.377052902,2.8549382629,-0.9549746253 C,0,4.0354302784,1.1910693611,-0.7857929806 H,0,3.1433468208,1.7999063574,-0.8812616074 C,0,2.3547852593,-2.4018714934,0.4694424771 C,0,2.1754576183,-2.1546950168,1.8336978565 H,0,1.9849238332,-1.1444150648,2.1813044501 C,0,2.2538796657,-3.1939690047,2.7489713541 H,0,2.1234197321,-2.9913817372,3.8058159347 C,0,2.4993088407,-4.4909789902,2.3118655218 H,0,2.5585406875,-5.3028792021,3.0274739728 C,0,2.6710350008,-4.7447158326,0.957788763 H,0,2.86445779,-5.7541649549,0.6134187103 C,0,2.6015783859,-3.7047877962,0.0381311115 H,0,2.7485083484,-3.9230033559,-1.0133423099 C,0,-1.7128050976,-2.5327752368,-1.247563266 C,0,-2.6626588869,-3.139610758,-2.0721709475 H,0,-2.7672791994,-2.8422547814,-3.1098268462 C,0,-3.4854173642,-4.1379674216,-1.5694445088	 C,0,-0.7407516334,-1.5300679364,2.6700067412 H,0,-0.3796305593,-1.9513180863,3.6100992758 H,0,-1.7543289223,-1.1652064028,2.8585772081 C,0,-0.7551130275,-2.5685803752,1.5436360842 H,0,-1.4549199418,-3.3789576034,1.7571998654 H,0,0.2361742561,-3.0036794676,1.3916039379 C,0,-0.7551130275,-2.5685803752,-1.5436360842 H,0,0.2361742561,-3.0036794676,-1.3916039379 H,0,-1.4549199418,-3.3789576034,-1.7571998654 C,0,-0.7407516334,-1.5300679364,-2.6700067412 H,0,-1.7543289223,-1.1652064028,-2.8585772081 H,0,-0.3796305593,-1.9513180863,-3.6100992758 C,0,1.9869647933,-0.3790407685,2.5661689991 C,0,2.3970704242,-1.5601530772,3.1832101373 H,0,1.6833752853,-2.3334362093,3.4404220129 C,0,3.7387831996,-1.7628407789,3.4859581408 H,0,4.0469985283,-2.6846640162,3.9657954452 C,0,4.6771776117,-0.7873190093,3.1813254865 H,0,5.7219357484,-0.9447437564,3.423106831 C,0,4.2739202776,0.3924969568,2.5654652289 H,0,5.0035904164,1.1573769107,2.3258270568 C,0,2.9395094217,0.5927388363,2.2491523912 H,0,2.6322226869,1.5090049916,1.7576403124 C,0,-3.0335159878,-1.5280770723,0. C,0,-3.8287003828,-2.677366918,0. H,0,-3.3753452207,-3.663503537,0. C,0,-5.211280246,-2.5675577807,0. H,0,-5.8231933697,-3.4621866608,0. C,0,-5.8106995362,-1.3122519675,0. H,0,-6.8914172287,-1.2297074534,0. C,0,-5.0269434476,-0.1666030818,0. H,0,-5.4930479502,0.8118409393,0. C,0,-3.6415486558,-0.2727891645,0. H,0,-3.0289806706,0.6222047556,0. C,0,1.9869647933,-0.3790407685,-2.5661689991 C,0,2.3970704242,-1.5601530772,-3.1832101373 H,0,1.6833752853,-2.3334362093,-3.4404220129 C,0,3.7387831996,-1.7628407789,-3.4859581408

H,0,-4.2210016591,-4.6040649738,-2.2148519822 C,0,-3.3663174184,-4.5390123833,-0.243891109 H,0,-4.0111652167,-5.3181858915,0.1457921841 C,0,-2.4211197426,-3.9418337975,0.5796998487 H,0,-2.3256768597,-4.2523196916,1.613742732 C,0,-1.5976041185,-2.9402356241,0.0818822989 H,0,-0.8595592134,-2.4795993896,0.7297472055 C,0,-2.5991019481,1.8886892633,-0.5803500418 C,0,-3.5016080168,2.8767520292,-0.9800503344 H,0,-3.2083930679,3.6257857739,-1.7074991548 C,0,-4.7738697016,2.9189297925,-0.4294785684 H,0,-5.4695749836,3.6897247018,-0.740637479 C,0,-5.1527735982,1.9824336991,0.5268067617 H,0,-6.1461283136,2.0220677935,0.9587843327 C,0,-4.2566666407,1.004022515,0.9347545744 H,0,-4.5462034899,0.2790701389,1.6866162231 C,0,-2.9812640212,0.9584557523,0.3853434856 H,0,-2.2784237793,0.2002298572,0.7132772857 C,0,-0.3407611605,3.516178458,-1.4455706355 C,0,-0.4566659203,4.2593582599,-2.6207831361 H,0,-0.8730032883,3.8208019395,-3.5196083519 C,0,-0.0312618854,5.5822428265,-2.6562188841 H,0,-0.1197623347,6.1495034049,-3.5756458493 C,0,0.5009069459,6.1745132638,-1.5194848048 H,0,0.8286773061,7.2072380787,-1.5484567981 C,0,0.6157425361,5.4397064996,-0.3447441358 H,0,1.0333472305,5.897199052,0.5447335604 C,0,0.2048788036,4.1158018071,-0.3088347535 H,0,0.3150133058,3.5422039898,0.6050060419 Ni,0,0.4484040915,0.2457481177,-0.5883114493 P,0,2.2587668369,-0.966189493,-0.6659225826 P,0,-0.5739427028,-1.2424760679,-1.872739028 P,0,-0.919270086,1.782855517,-1.310268812 H,0,1.2023830757,1.2952873275,0.0935750496	H,0,4.0469985283,-2.6846640162,-3.9657954452 C,0,4.6771776117,-0.7873190093,-3.1813254865 H,0,5.7219357484,-0.9447437564,-3.423106831 C,0,4.2739202776,0.3924969568,-2.5654652289 H,0,5.0035904164,1.1573769107,-2.3258270568 C,0,2.9395094217,0.5927388363,-2.2491523912 H,0,2.6322226869,1.5090049916,-1.7576403124 Ni,0,-0.0366951401,0.1975116267,0. P,0,0.2338881652,-0.0162765411,2.1560733375 P,0,-1.2079200897,-1.643310378,0. P,0,0.2338881652,-0.0162765411,-2.1560733375 H,0,0.8027604258,1.4166847455,0. C,0,-0.2876520606,1.2971451842,-3.315952235 C,0,-0.0843191825,1.168442452,-4.6914369121 C,0,-0.9150629128,2.4351812899,-2.8129087384 C,0,-0.5180245782,2.1662976558,-5.5515272675 H,0,0.4261857648,0.2998532151,-5.0932225786 C,0,-1.3466322442,3.4327704205,-3.6783075019 H,0,-1.0477354668,2.5448016491,-1.7421515344 C,0,-1.1509618739,3.2971479861,-5.046048786 H,0,-0.3564395341,2.0652891076,-6.6185514191 H,0,-1.8296288602,4.3189649893,-3.2829786362 H,0,-1.4849819275,4.0766225888,-5.7211629222 C,0,-0.2876520606,1.2971451842,3.315952235 C,0,-0.0843191825,1.168442452,4.6914369121 C,0,-0.9150629128,2.4351812899,2.8129087384 C,0,-0.5180245782,2.1662976558,5.5515272675 H,0,0.4261857648,0.2998532151,5.0932225786 C,0,-1.3466322442,3.4327704205,3.6783075019 H,0,-1.0477354668,2.5448016491,1.7421515344 C,0,-1.1509618739,3.2971479861,5.046048786 H,0,-0.3564395341,2.0652891076,6.6185514191 H,0,-1.8296288602,4.3189649893,3.2829786362 H,0,-1.4849819275,4.0766225888,5.7211629222
 C,0,2.1951866702,1.8651533487,1.6335440586 H,0,2.7562503808,1.0484698848,2.0946637004 H,0,2.7965681026,2.7731204234,1.717900469 C,0,0.8457229584,2.047052393,2.3164344122 H,0,0.375906496,2.9765062289,1.9857009542 H,0,0.9415067203,2.1015523519,3.4035187652 C,0,-0.2220613763,-0.6475623366,3.1338348767 H,0,0.0104290778,-0.2178727862,4.1113274775 H,0,-1.2180322901,-1.0913097359,3.1969882199 C,0,0.7927369592,-1.7108228763,2.7278969677 H,0,0.7053642483,-2.6065889853,3.3475318443 H,0,1.8159173286,-1.3467965108,2.8493988191 C,0,3.6143080322,1.0431498881,-0.7975007388 C,0,4.7676313787,1.1491910133,-0.0211695638 H,0,4.7120750569,1.4321029162,1.0228535499 C,0,6.0161220625,0.8948608233,-0.5792112311 H,0,6.9048933707,0.9802645614,0.0356539465 C,0,6.1249293472,0.5392595494,-1.9157608136 H,0,7.099278557,0.3469877037,-2.3500041797 C,0,4.9789787086,0.4322729672,-2.6967956862 H,0,5.0569631826,0.1558019758,-3.7421111269 C,0,3.7328536084,0.6770673471,-2.1405837441 H,0,2.8442881171,0.5855633326,-2.7564275984 C,0,1.5312062763,3.0008850005,-0.9666425993 C,0,2.3858859087,4.1006836728,-0.8620888118 H,0,3.3148434436,4.0238920774,-0.3070618513 C,0,2.0650470383,5.296663954,-1.4868736074 H,0,2.7329837818,6.146126381,-1.3999288342 C,0,0.8951547274,5.4036305043,-2.2324184203	 C,0,0.1344728033,2.4110748696,-2.3054003449 H,0,0.3009452502,1.7212902091,-3.136979159 H,0,-0.3017833955,3.3246049562,-2.7155572903 C,0,1.456460488,2.7154383444,-1.6089148342 H,0,1.3280251921,3.4901608366,-0.8485072114 H,0,2.2063271066,3.0758947968,-2.3179849381 C,0,2.7975917008,0.0866713533,-2.0351655394 H,0,3.1365399038,0.6649420385,-2.8981911663 H,0,3.6760426432,-0.3887815238,-1.5932345643 C,0,1.77635845,-0.9721491945,-2.4411144963 H,0,2.2534328776,-1.8001546064,-2.9692960752 H,0,1.0131923574,-0.5532328907,-3.0997386493 C,0,-2.4049636683,0.9739292852,-2.2281453435 C,0,-2.4351840725,1.159911066,-3.6109618069 H,0,-1.6522177213,1.7146103493,-4.1139326987 C,0,-3.4874832617,0.6557533681,-4.3687703933 H,0,-3.4992095592,0.8143231204,-5.4413852391 C,0,-4.5260688649,-0.0299293732,-3.7547318694 H,0,-5.3502282087,-0.4128615402,-4.3455913906 C,0,-4.5070743037,-0.2174132316,-2.3768927855 H,0,-5.3159266015,-0.7498701565,-1.8895271089 C,0,-3.4514487223,0.2714884863,-1.6229500563 H,0,-3.446057939,0.1171859293,-0.5486951793 C,0,-1.8677494318,3.0508945192,-0.3251651776 C,0,-2.8989014794,3.7536876016,-0.9535695632 H,0,-3.2783106559,3.4222131832,-1.9132627041 C,0,-3.4541456054,4.8739815289,-0.3513498032 H,0,-4.2552483966,5.4090369921,-0.8488345242

H,0,0.650367289,6.3380599904,-2.724346045 C,0,0.0487142867,4.310564334,-2.3530935964 H,0,-0.8570444751,4.3868099782,-2.944249913 C,0,0.3658428521,3.1127302574,-1.72134296 H,0,-0.2857190857,2.2514675363,-1.8170220478 C,0,-1.9863097769,1.4547042563,2.0638649561 C,0,-2.8279083137,1.1705507675,3.1400709452 H,0,-2.5320035168,0.4646052106,3.9063060056 C,0,-4.0589896528,1.8047303487,3.2553458155 H,0,-4.700765577,1.5784209448,4.0991095751 C,0,-4.46364258524,3.7277660891,2.3005227055 H,0,-5.4232580176,3.2225803713,2.395470171 C,0,-3.6311323368,3.0198762607,1.2267921584 H,0,-3.9376466613,3.7445633069,0.4811124312 C,0,-2.4029329774,2.384758078,1.1060448467 H,0,-1.7576218145,2.6260802533,0.2673164232 C,0,-0.7588416637,-3.296795157,0.7817596248 C,0,-1.0947578014,-3.7539473667,-0.4957948095 H,0,-0.5223692905,-3.4205051499,-1.3548296919 C,0,-2.1422770226,-4.6446415193,-0.6734428542 H,0,-2.3843017398,-4.9996928108,-1.6687327227 C,0,-2.8814295355,-5.0807061201,0.4208660582 H,0,-3.702218263,-5.7747709223,0.2817308873 C,0,-2.5601101781,-4.6280326653,1.6924927663 H,0,-3.1272974156,-4.969286582,2.5511723444 C,0,-1.5027482501,-3.7427974392,1.8734700114 H,0,-1.2622165727,-3.4190206228,2.8793422317 C,0,2.113511396,-3.1899312857,0.6260663391 C,0,2.1677342863,-4.47898048,1.1620254943 H,0,1.3192022728,-4.8824272536,1.7035016319 C,0,3.2998799935,-5.2608513925,0.9851348472 H,0,3.3327761729,-6.2618476535,1.4000852235 C,0,4.385589887,-4.76511193,0.2713704928 H,0,5.2676482343,-5.3795220294,0.1309838405 C,0,4.3347550502,-3.4869181219,-0.2674983302 H,0,5.1748629934,-3.0986221229,-0.8315381857 C,0,3.201300542,-2.7012757831,-0.0934007288 H,0,3.1592549064,-1.7086441446,-0.5259336293 Ni,0,0.3633429818,-0.161362424,-0.1039905323 P,0,1.9266230226,1.3914115864,-0.1516742741 P,0,-0.3352232463,0.6823406015,1.8331142918 P,0,0.6485968732,-2.1162562549,0.9111282839 N,0,-1.3199802234,-0.1221346065,-1.2069924866 H,0,1.1027029671,-0.7425483085,-1.2106926375 C,0,-1.5441632701,-0.4349295865,-2.4284605771 C,0,-2.8275999958,-0.4841064852,-3.1243920699 C,0,-4.0550976429,-0.2578358612,-2.4895141985 C,0,-2.817201584,-0.7675669336,-4.4943801338 C,0,-5.2345087097,-0.3103595313,-3.2107040672 H,0,-4.0989224028,-0.0481695175,-1.4257387952 C,0,-3.999972924,-0.8181173239,-5.2162508127 H,0,-1.8708026482,-0.9471872543,-4.9942526964 C,0,-5.210274565,-0.5887741618,-4.575277676 H,0,-6.1804634265,-0.1375362758,-2.7108604597 H,0,-3.9780413461,-1.0369783296,-6.2773030864 H,0,-6.1374046319,-0.6291690844,-5.1352930253 H,0,-2.1740520481,0.1109959027,-0.7025732805 H,0,-0.6719879269,-0.69059045,-3.0295701333	C,0,-2.9887700485,5.3079921235,0.8845785631 H,0,-3.4246770657,6.1830892354,1.3528719897 C,0,-1.9668015959,4.6141615844,1.517613462 H,0,-1.601604572,4.9455422717,2.4833234638 C,0,-1.4139282481,3.4881555416,0.9191312714 H,0,-0.621392395,2.9424798229,1.4184456699 C,0,3.5957533798,1.8457747884,0.1576141355 C,0,4.6989702038,2.3012376986,-0.569809325 H,0,4.6934249823,2.2827494924,-1.6544050585 C,0,5.8190079416,2.7865706001,0.0895967142 H,0,6.669510432,3.139498278,0.1088731659 C,0,5.8491882807,2.8214645728,1.4790333653 H,0,6.7252860792,3.200780152,1.9923129778 C,0,4.7571250788,2.3692808691,2.2070597874 H,0,4.7787826586,2.3933476144,3.2905981246 C,0,3.6347655377,1.8814618289,1.5494136509 H,0,2.7811644957,1.5245933732,2.1144405704 C,0,2.202042271,-2.6309966306,-0.1088731659 C,0,2.6726974908,-2.2983077361,1.1596686382 H,0,2.2596657617,-1.4335416198,1.6676255034 C,0,3.6636708775,-3.0642847009,1.7637265575 H,0,4.0234238257,-2.799569991,2.7514372233 C,0,4.1909899436,-4.1640123103,1.1019468841 H,0,4.9645896748,-4.760976538,1.5713213498 C,0,3.7253157394,-4.5028559843,-0.1649876114 H,0,4.1343009763,-5.3634320849,-0.6820466689 C,0,2.7342127325,-3.7432098241,-0.7678900308 H,0,2.3666163235,-4.0275470693,-1.7481539898 C,0,-0.3491577901,-2.7866898101,-1.4513703645 C,0,-0.6401852116,-3.8891758803,-0.6426577786 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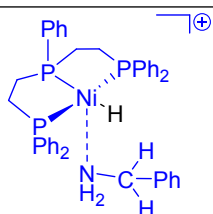
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 C,0,1.6330044057,-1.9386496723,-2.0981447989 H,0,2.2672785074,-1.0933767528,-2.3726745366 H,0,2.1236749698,-2.8506319563,-2.4443173409 C,0,0.2421257963,-1.7981759651,-2.7025417672 H,0,-0.3080376304,-2.7374889504,-2.6109231004 H,0,0.279596989,-1.5460004015,-3.7651705408 C,0,-0.4205427826,1.1051002908,-2.5870160697 H,0,-0.4146841437,0.9788771313,-3.6735325747 H,0,-1.2719216208,1.7409213546,-2.3330483143 C,0,0.8816632582,1.7471077605,-2.1124400964 H,0,0.9934437907,2.7345358272,-2.5663341276 H,0,1.7456372362,1.1629690859,-2.4370327538 C,0,3.1769615734,-2.0124068923,0.4138757291 C,0,4.3061875933,-1.8046213012,-0.3771568965 H,0,4.2148463729,-1.5902898665,-1.4347995994 C,0,5.5759770289,-1.8801620429,0.1831535674 H,0,6.4470895581,-1.7255500131,-0.442985381 C,0,5.7286904729,-2.1543820516,1.5348844508 H,0,6.702253172,-2.2169307746,1.96816643 C,0,4.6023462288,-2.3559578,2.3310887001 H,0,4.7194607932,-2.5764062219,3.3863240628 C,0,3.3380134787,-2.2860650515,1.7752538674 H,0,2.471560028,-2.4670618145,2.4028480053 C,0,0.8100959788,-3.618367548,0.1393611211 C,0,1.5367601088,-4.7624242898,-0.2014108097 H,0,2.5070816414,-4.6751757801,-0.6787515125 C,0,1.0318104525,-6.0204387395,0.0900667745 H,0,1.6000872886,-6.9039344066,-0.1773201757 C,0,-0.1953932353,-6.1483538956,0.7333353264 H,0,-0.5840283585,-7.1331545261,0.9659548062 C,0,-0.9163125681,-5.015671049,1.0840037343 H,0,-1.8677948079,-5.1119674352,1.5944991993 C,0,-0.4176348158,-3.7517887968,0.786725508 H,0,-0.98403197,-2.8657397621,1.0594545216 C,0,-2.4941062422,-0.941800864,-2.2359519468 C,0,-3.2379377402,-0.1893559342,-3.1475602319 H,0,-2.8189675517,0.6909022948,-3.6189132061 C,0,-4.533879762,-0.5688260932,-3.4705021768 H,0,-5.102662837,0.0197535544,-4.1809453635 C,0,-5.0984141748,-1.6961416951,-2.8885777761 H,0,-6.1112207402,-1.9873186567,-3.1414831253 C,0,-4.3646823715,-2.4476984229,-1.9792828064 H,0,-4.8035989673,-3.3244749369,-1.5177693998 C,0,-3.070400456,-2.0730001079,-1.6503200641 H,0,-2.5110466436,-2.657203311,-0.9283685392 C,0,0.170486583,3.4501987855,0.1544011833 C,0,0.3232944679,3.9425563742,1.4543779285 H,0,0.942039226,3.4077303117,2.1678186523	 C,0,-1.7283131268,-1.8706700583,2.002247623 H,0,-2.3480422732,-1.0092947573,2.2600590051 H,0,-2.2537072744,-2.7688411596,2.3328889747 C,0,-0.3532146185,-1.771679837,2.6510171541 H,0,0.1630836326,-2.7321457482,2.5916147917 H,0,-0.4171197407,-1.5043043141,3.7085412146 C,0,0.5261444528,1.0773038732,2.6170588895 H,0,0.5940100105,0.9265355271,3.6980935767 H,0,1.3763424138,1.6933247675,2.3138040814 C,0,-0.78208111,1.7632191458,2.2306108984 H,0,-0.8374861063,2.750869276,2.6927240315 H,0,-1.6429064784,1.2010172568,2.5998379255 C,0,-3.2147470867,-1.8847132795,-0.5435930673 C,0,-4.3613659691,-1.7455299553,0.2367873989 H,0,-4.2936832645,-1.6001313876,1.3078528198 C,0,-5.6187299268,-1.7993001884,-0.3534483291 H,0,-6.5041252087,-1.6961794712,0.2631959476 C,0,-5.7407934878,-1.9862744913,-1.7229033122 H,0,-6.7226794279,-2.0325112267,-2.1796000938 C,0,-4.6002074052,-2.1196492724,-2.5076447096 H,0,-4.6895610538,-2.2702432748,-3.5773693157 C,0,-3.344246526,-2.0681555098,-1.9229395146 H,0,-2.4620590927,-2.1879087298,-2.5434821997 C,0,-0.89435181,-3.5444799762,-0.2453197054 C,0,-1.5940113515,-4.682269453,0.1649884412 H,0,-2.522472568,-4.5879390106,0.7180634409 C,0,-1.1182888245,-5.9453630589,-0.1533057054 H,0,-1.6651860247,-6.8237529068,0.169728035 C,0,0.0503119073,-6.0851479488,-0.89550104 H,0,0.4150845065,-7.073863947,-1.1491299563 C,0,0.7416412508,-4.9589545998,-1.3193568961 H,0,1.6450436808,-5.0633277531,-1.9093704968 C,0,0.2728418953,-3.6908953212,-0.9931218674 H,0,0.8123888023,-2.8113192441,-1.3282101505 C,0,2.4352154029,-1.1077697364,2.1166364194 C,0,3.3384194762,-0.3449490299,2.8578108237 H,0,3.058117115,0.6222501084,3.2554838175 C,0,4.6172578832,-0.82665077,3.1085820114 H,0,5.3095409784,-0.228709645,3.6898815268 C,0,5.0068747737,-2.0659133695,2.6204102244 H,0,6.0059396786,-2.4370652768,2.8167042536 C,0,4.1136378638,-2.8295010629,1.8780696876 H,0,4.4135374273,-3.79665507,1.4918689894 C,0,2.8363041556,-2.3537907241,1.6238011451 H,0,2.1512607032,-2.9570843469,1.0365603192 C,0,-0.1734196068,3.4592108862,-0.0802328927 C,0,-0.3310248005,3.9014590091,-1.3966307419 H,0,-0.9297032514,3.3259721418,-2.0954835288

C,0,-0.2958041759,5.1202072292,1.8417892518 H,0,-0.1602782174,5.4919797224,2.8509714938 C,0,-1.090108152,5.8215736451,0.9406302887 H,0,-1.5772666007,6.7407111896,1.2445650807 C,0,-1.2510102279,5.3407688267,-0.3503767831 H,0,-1.8619848513,5.8852240313,-1.0616360981 C,0,-0.6234091799,4.1625669595,-0.7428977352 H,0,-0.7569633012,3.8214569022,-1.7625846779 C,0,2.7892820512,2.3703519543,-0.0520238204 C,0,3.3101538667,3.4819921118,-0.7208641186 H,0,2.6784496236,1.6592271915,0.8221158283 C,0,4.6303030575,3.8597888502,-0.530095639 H,0,5.024747659,4.7235099277,-1.0533332481 C,0,5.4421932353,3.1422800734,0.3430967978 H,0,6.4711601298,3.4458256378,0.4988985122 C,0,4.9299529653,2.0457872095,1.0207475769 H,0,5.5553194562,1.4885915575,1.7083871841 C,0,3.6084496236,1.6592271915,0.8221158283 H,0,3.2173737928,0.7992129012,1.3535266996 Ni,0,-0.0998356901,-0.4063448587,0.2809424628 P,0,1.4685315643,-1.9433383128,-0.2505367639 P,0,-0.7719076704,-0.5285729766,-1.7878254016 P,0,1.0252842439,1.8638601538,-0.252133937 N,0,-1.850839943,-0.0162670823,0.8245695498 H,0,-2.5767575565,-0.0225054253,0.1149047632 H,0,0.1005650305,-0.7637658905,1.9935199902 H,0,0.5135014801,-0.0994775852,1.9100332891 C,0,-2.114075087,1.1081611483,1.7160839628 H,0,-1.4752104483,1.0058766028,2.6027428126 H,0,-1.8714425309,2.0833125568,1.2762646654 C,0,-3.5647296576,1.1175977191,2.134656651 C,0,-4.0805995633,0.0812781589,2.9147316579 C,0,-4.4177905853,2.1439481067,1.7349819931 C,0,-5.4155020252,0.077039539,3.2925081865 H,0,-3.4249592265,-0.7242229905,3.2281818202 C,0,-5.7561863257,2.1423175841,2.1110339304 H,0,-4.0271473217,2.9587179029,1.1331724247 C,0,-6.2576264804,1.1085794085,2.8905091081 H,0,-5.8013212863,-0.7283969494,3.9077042549 H,0,-6.4064361162,2.9520122113,1.7988974143 H,0,-7.2998720814,1.1077712135,3.1889308567	C,0,0.25633551,5.0840666152,-1.8191162693 H,0,0.1174457056,5.4179610024,-2.8410227895 C,0,1.0227912108,5.8375917615,-0.9370677575 H,0,1.4855417842,6.7598713378,-1.2682372273 C,0,1.1898786708,5.4037465499,0.3698905353 H,0,1.7824431003,5.9874912454,1.0652774535 C,0,0.5954853353,4.2211409905,0.7971095856 H,0,0.7382539796,3.9139438124,1.8266419721 C,0,-2.7633331529,2.3160879427,0.1851746061 C,0,-3.3745965524,3.2703166893,1.003225104 H,0,-2.8161607941,3.7549198072,1.796306292 C,0,-4.6988064919,3.6256571674,0.7954508763 H,0,-5.164745994,4.3657534399,1.4361678743 C,0,-5.4219820032,3.0476797779,-0.2430838949 H,0,-6.4536548215,3.3355000286,-0.4102942319 C,0,-4.8186409244,2.1093944477,-1.067791569 H,0,-5.3758621627,1.6593802315,-1.8810443777 C,0,-3.4954697887,1.7406738182,-0.8513958851 H,0,-3.0330632434,0.999692127,-1.4933721999 Ni,0,0.0358084217,-0.2995913635,-0.2921055223 P,0,-1.520292285,-1.8596721087,0.1581341892 P,0,0.7339368294,-0.5486163351,1.7525534152 P,0,-0.9867493695,1.8647403359,0.3766292727 N,0,1.8327830826,-0.0132768458,-1.01334926 H,0,2.4639928491,-0.668811334,-0.5670185916 H,0,0.4789719269,-0.3111096269,-1.8473408646 H,0,-0.4014416169,-0.3293323231,-1.8866434239 C,0,2.4351493841,1.3076575568,-1.0841138462 H,0,1.7656122925,1.9629212264,-1.6485586891 H,0,2.5742345004,1.7872648725,-0.1029278653 C,0,3.779062775,1.2392844976,-1.7728554308 C,0,3.8686520531,0.8599046608,-3.1131813469 C,0,4.9506769466,1.5401782641,-1.0832925205 C,0,5.0994720042,0.7928754336,-3.7487398614 H,0,2.96311033,0.6163632632,-3.6586747596 C,0,6.1867727247,1.4749906547,-1.7171199353 H,0,4.8953754349,1.8375066442,-0.0405155698 C,0,6.2634577642,1.1011267672,-3.0514940605 H,0,5.1538825229,0.5053833203,-4.7929443324 H,0,7.089620647,1.7188450862,-1.1682205944 H,0,7.2252558187,1.0518574822,-3.5492644439
 C,0,2.2976617516,1.721769575,1.6536948567 H,0,2.8403012736,0.8317353044,1.9818181156 H,0,2.9658740595,2.5796570285,1.7589472452 C,0,1.0346243245,1.9269741,2.4809081147 H,0,0.6420370438,2.9335823341,2.3240784576 H,0,1.2306570743,1.8256613338,3.5510374667 C,0,-0.3525087873,-0.6358004685,3.2092223549 H,0,-0.1430200093,-0.2608783311,4.2141877735 H,0,-1.3736157713,-1.0222536402,3.2102743324 C,0,0.6133155902,-1.7411273444,2.8026102147 H,0,0.4417973186,-2.6554578521,3.3760472585 H,0,1.6493095028,-1.4462071597,2.9870993509 C,0,3.4453253964,1.0608432964,-0.9601198754 C,0,4.6777414371,1.1547569463,-0.3142078233 H,0,4.7381743164,1.4253015453,0.7328858728 C,0,5.8557680624,0.8983788812,-1.0078253003 H,0,6.807144341,0.9724083413,-0.4933283559 C,0,5.8149098363,0.554588397,-2.351448881 H,0,6.7344455683,0.3605517691,-2.8915369958 C,0,4.5897388544,0.4597844594,-3.0027460177 H,0,4.5507330214,0.1905752115,-4.0520887896	 C,0,1.0341357918,-2.6713372931,1.7599582358 H,0,0.6042154717,-3.6262660562,2.0669034702 H,0,2.1115114933,-2.8213494535,1.6583399471 C,0,0.7640180245,-1.5715214661,2.7969659792 H,0,1.3293370816,-1.7480377951,3.7142980005 H,0,-0.2969238053,-1.5144395724,3.0527072452 C,0,0.764787641,1.5820981882,2.7902530989 H,0,-0.2961355903,1.526578582,3.0464196695 H,0,1.330339249,1.7622859993,3.7067280967 C,0,1.0352277143,2.6773293194,1.7484957435 H,0,2.1126573356,2.8263460018,1.6459748342 H,0,0.6058873686,3.633792567,2.0514524067 C,0,-1.1058726249,-3.1581287375,-0.2176271876 C,0,-1.8977984292,-3.5826849385,0.8480697267 H,0,-1.6048206209,-3.3790976799,1.8718481654 C,0,-3.0746130104,-4.2841289309,0.6148373081 H,0,-3.6764986165,-4.617985168,1.4524322821 C,0,-3.4743297576,-4.5620666657,-0.6851228656 H,0,-4.3892260008,-5.1141675993,-0.866421011 C,0,-2.6943555221,-4.1332404863,-1.7527434516

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 H,0,-4.9798091388,3.9282403225,3.0403379
 C,0,-3.1419304569,3.7394203081,1.9411077307
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 C,0,-2.0243771074,2.9556196641,1.6961972119
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 C,0,-0.8492107699,-3.2519519203,0.7139948186
 C,0,-1.0150807411,-3.7826444822,-0.5701031292
 H,0,-0.3045470153,-3.53563738,-1.353388273
 C,0,-2.0574350808,-4.6561648682,-0.8440154662
 H,0,-2.164261689,-5.0708648955,-1.839951044
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 H,0,5.0635992528,-3.0247389519,-0.8000522588
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 Ni,0,0.2627233046,-0.0979513235,-0.0069834236
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 P,0,0.5376771023,-2.0655238734,0.9658075713
 N,0,-1.4559200518,-0.2181057926,-1.2514536587
 H,0,-1.1926683693,0.1402176589,-2.1646840419
 H,0,-1.5772598259,-1.2180724796,-1.3928796664
 H,0,0.9884716653,-0.71237284,-1.1043829978
 C,0,-2.7788251898,0.3498644542,-0.8899851482
 H,0,-3.0733581602,-0.0926891392,0.0625564101
 H,0,-2.6472871428,1.4182248737,-0.7151632233
 C,0,-3.836988768,0.1117717849,-1.9343176489
 C,0,-4.6144233657,-1.0460794358,-1.907738678
 C,0,-4.0307484967,1.0259642959,-2.9698588798
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 C,0,-4.9717427091,0.7856391276,-3.9624041706
 H,0,-3.4481206432,1.9423909643,-2.9953060843
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H,0,-2.9982435253,-4.3514119086,-2.7702894717
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 H,0,-0.9143093607,-3.1094689062,-2.3625457616
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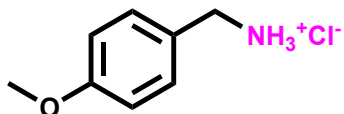


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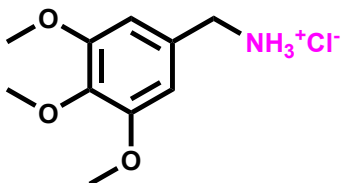
S8. NMR Data

(4-methoxyphenyl)methanamine hydrochloride



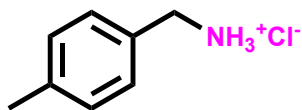
^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.56 (br s, 3H), 7.45 (d, $J = 9.0$ Hz, 2H), 6.95 (d, $J = 8.7$ Hz, 2H), 3.92 (s, 2H), 3.75 (s, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 159.74 , 131.03 , 126.47 , 114.31 , 55.65 , 42.04 . White solid.

(3,4,5-trimethoxyphenyl)methanamine hydrochloride



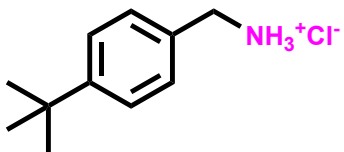
^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.67 (br s, 3H), 6.97 (s, 2H), 3.94 (s, 2H), 3.78 (s, 6H), 3.64 (s, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 153.22 , 137.70 , 130.08 , 107.03 , 60.46 , 56.47 , 42.83 . Off white solid.

p-tolylmethanamine hydrochloride



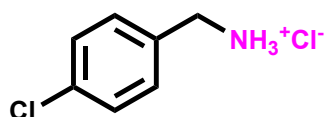
^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.63 (br s, 3H), 7.40 (d, $J = 8.0$ Hz, 2H), 7.20 (d, $J = 7.8$ Hz, 2H), 3.94 (s, 2H), 2.30 (s, 3H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 138.10 , 131.54 , 129.46 , 129.44 , 42.30 , 21.22 . White solid.

(4-(tert-butyl)phenyl)methanamine hydrochloride



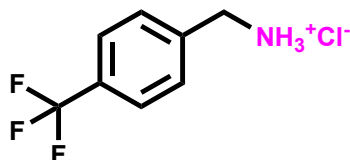
^1H NMR (400 MHz, $\text{DMSO-}d_6$) δ 8.60 (br s, 3H), 7.54 – 7.14 (m, 4H), 3.95 (s, 2H), 1.27 (s, 9H). ^{13}C NMR (101 MHz, $\text{DMSO-}d_6$) δ 151.33 , 131.63 , 129.25 , 125.72 , 42.23 , 34.79 , 31.54 . White solid.

(4-chlorophenyl)methanamine hydrochloride



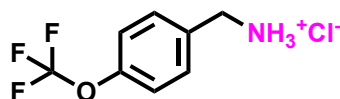
^1H NMR (400 MHz, DMSO- d_6) δ 8.70 (br s, 3H), 7.57 (d, J = 8.5 Hz, 2H), 7.47 (d, J = 8.4 Hz, 2H), 4.00 (s, 2H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 133.59 , 133.51 , 131.48 , 128.90 , 41.81 . **White solid.**

(4-(trifluoromethyl)phenyl)methanamine hydrochloride



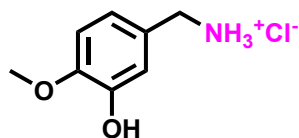
^1H NMR (400 MHz, DMSO- d_6) δ 8.81 (br s, 3H), 7.95 – 7.53 (m, 4H), 4.12 (s, 2H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 139.30 , 130.27 , 129.26 (q, J = 31.8 Hz), 125.74 (q, J = 3.7 Hz), 124.58 (q, J = 272.2 Hz), 41.99. **White solid.**

(4-(trifluoromethoxy)phenyl)methanamine hydrochloride



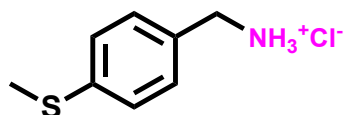
^1H NMR (400 MHz, DMSO- d_6) δ 8.70 (br s, 3H), 7.69 (d, J = 8.7 Hz, 2H), 7.41 (d, J = 7.8 Hz, 2H), 4.07 (s, 2H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 148.70 , 134.06 , 131.67 , 121.52 , 120.48 (q, J = 256.3 Hz), 41.77 . **Off white solid.**

(3-hydroxy-4-methoxyphenyl)methanamine hydrochloride



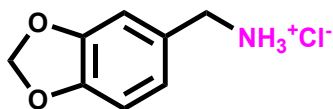
^1H NMR (400 MHz, DMSO- d_6) δ 8.49 (br s, 3H), 7.22 – 6.82 (m, 3H), 3.90 (s, 2H), 3.81 (s, 3H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 148.27 , 146.87 , 126.82 , 120.45 , 116.84 , 112.51 , 56.15 , 42.32 . **Brown solid.**

(4-(methylthio)phenyl)methanamine hydrochloride



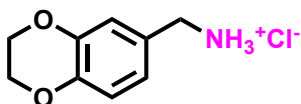
^1H NMR (400 MHz, DMSO- d_6) δ 7.99 (br s, 3H), 7.46 (d, J = 8.3 Hz, 2H), 7.26 (d, J = 8.3 Hz, 2H), 3.95 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 138.95 , 131.05 , 130.18 , 126.22 , 42.10 , 15.14 . **Brown solid.**

benzo[d][1,3]dioxol-5-ylmethanamine hydrochloride



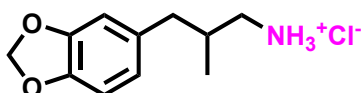
^1H NMR (400 MHz, DMSO- d_6) δ 8.58 (br s, 3H), 7.16 (d, J = 1.7 Hz, 1H), 6.98 (dd, J = 8.0, 1.7 Hz, 1H), 6.93 (dd, J = 7.9, 0.4 Hz, 1H), 6.03 (s, 2H), 3.90 (s, 2H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 147.69, 147.67, 128.17, 123.35, 109.99, 108.65, 101.63, 42.37. **Off white solid.**

(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)methanamine hydrochloride



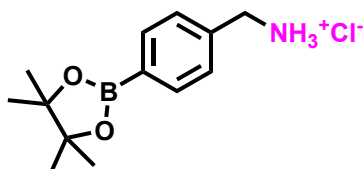
^1H NMR (400 MHz, DMSO- d_6) δ 8.29 (br s, 3H), 7.07 (d, J = 2.1 Hz, 1H), 6.96 (dd, J = 8.3, 2.1 Hz, 1H), 6.85 (d, J = 8.3 Hz, 1H), 4.23 (s, 4H), 3.86 (s, 2H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 143.91, 143.57, 127.44, 122.54, 118.40, 117.45, 64.56, 64.52, 42.05. **Off white solid.**

(benzo[d][1,3]dioxol-5-yl)-2-methylpropan-1-amine hydrochloride



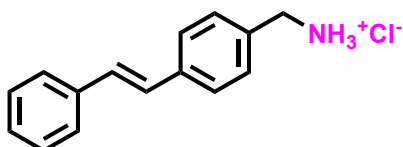
^1H NMR (400 MHz, DMSO- d_6) δ 8.30 (br s, 3H), 6.81 – 6.78 (m, 2H), 6.63 (dd, J = 8.0, 1.6 Hz, 1H), 5.95 (s, 2H), 2.73 – 2.63 (m, 2H), 2.63 – 2.54 (m, 1H), 2.28 (dd, J = 13.5, 8.3 Hz, 1H), 2.08 – 1.96 (m, 1H), 0.85 (d, J = 6.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 147.58, 145.86, 133.85, 122.38, 109.74, 108.43, 101.13, 44.25, 39.72, 33.72, 17.30. **Pale brown solid.**

(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanamine hydrochloride



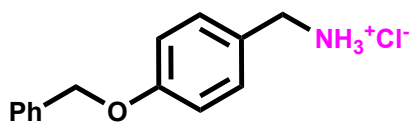
^1H NMR (400 MHz, DMSO- d_6) δ 8.61 (br s, 3H), 7.69 (d, J = 8.0 Hz, 2H), 7.52 (d, J = 8.1 Hz, 2H), 4.02 (s, 2H), 1.30 (s, 12H). ^{13}C NMR (101 MHz, DMSO- d_6) δ 137.85, 134.96, 129.42, 128.77, 84.22, 42.50, 25.13. **Off white solid.**

(E)-(4-styrylphenyl)methanamine hydrochloride



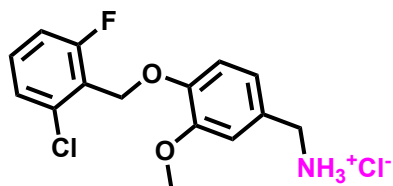
^1H NMR (300 MHz, DMSO- d_6) δ 8.61 (br s, 3H), 7.69 – 7.56 (m, 4H), 7.52 (d, J = 8.0 Hz, 2H), 7.45 – 7.32 (m, 3H), 7.32 – 7.20 (m, 2H), 4.02 (s, 2H). ^{13}C NMR (75 MHz, DMSO- d_6) δ 137.59, 137.32, 133.76, 129.86, 129.46, 129.40, 129.20, 128.26, 128.22, 127.00, 42.37. **Yellow solid.**

(4-(benzyloxy)phenyl)methanamine hydrochloride



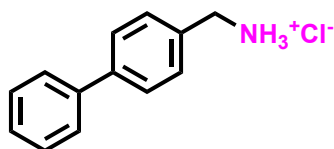
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.59 (br s, 3H), 7.49 – 7.25 (m, 7H), 7.02 (d, *J* = 8.7 Hz, 2H), 5.12 (s, 2H), 3.91 (s, 2H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ 158.74 , 137.41 , 131.06 , 128.90 , 128.28 , 128.08 , 126.70 , 115.23 , 69.61 , 42.03 . **Off white solid.**

(4-((2-chloro-6-fluorobenzyl)oxy)-3-methoxyphenyl)methanamine hydrochloride



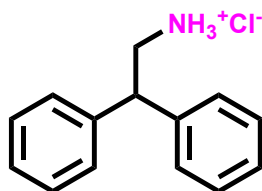
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.55 (br s, 3H), 7.56 – 7.46 (m, 1H), 7.45 – 7.38 (m, 1H), 7.36 – 7.26 (m, 2H), 7.13 (d, *J* = 8.2 Hz, 1H), 7.03 (dd, *J* = 8.2, 2.0 Hz, 1H), 5.12 (s, 2H), 3.95 (s, 2H), 3.75 (s, 3H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ 161.94 (d, *J* = 249.9 Hz), 149.52 , 148.10 , 136.00 (d, *J* = 5.1 Hz), 132.29 (d, *J* = 9.9 Hz), 127.91 , 126.18 (d, *J* = 3.2 Hz), 122.49 (d, *J* = 17.9 Hz), 121.85 , 115.23 (d, *J* = 22.4 Hz), 114.14 , 113.80 , 62.12 , 56.07 , 42.47 . **Off white solid.**

[1,1'-biphenyl]-4-ylmethanamine hydrochloride



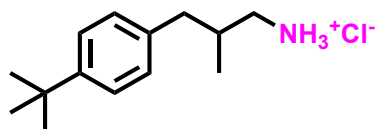
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.75 (br s, 3H), 7.77 – 7.58 (m, 6H), 7.50 – 7.44 (m, 2H), 7.41 – 7.34 (m, 1H), 4.06 (s, 2H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ 140.59 , 139.99 , 133.74 , 130.12 , 129.45 , 128.12 , 127.19 , 127.14 , 42.25 . **Off white solid.**

KM24-108 2,2-diphenylethan-1-amine hydrochloride



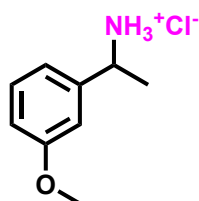
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.20 (br s, 3H), 7.41 – 7.30 (m, 8H), 7.27 – 7.20 (m, 2H), 4.41 (t, *J* = 7.9 Hz, 1H), 3.53 (d, *J* = 7.9 Hz, 2H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ 141.56 , 129.22 , 128.29 , 127.45 , 48.97 , 42.82 . **Pale brown solid.**

3-(4-(tert-butyl)phenyl)-2-methylpropan-1-amine hydrochloride



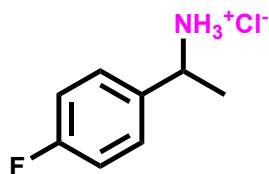
¹H NMR (400 MHz, DMSO-*d*₆) δ 8.36 (br s, 3H), 7.34 (d, *J* = 8.2 Hz, 2H), 7.17 (d, *J* = 8.3 Hz, 2H), 2.81 – 2.71 (m, 2H), 2.71 – 2.62 (m, 1H), 2.39 (dd, *J* = 13.5, 8.3 Hz, 1H), 2.19 – 2.06 (m, 1H), 1.29 (s, 9H), 0.92 (d, *J* = 6.6 Hz, 3H). **¹³C NMR (101 MHz, DMSO-*d*₆)** δ 148.65 , 136.95 , 129.15 , 125.39 , 44.37 , 39.67 , 34.50 , 33.54 , 31.65 , 17.46 . **Pale brown solid.**

1-(3-methoxyphenyl)ethan-1- amine hydrochloride



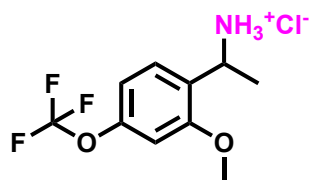
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.57 (br s, 3H), 7.31 (dd, *J* = 8.2, 7.6 Hz, 1H), 7.27 – 7.19 (m, 1H), 7.14 – 7.04 (m, 1H), 6.91 (ddd, *J* = 8.3, 2.6, 0.9 Hz, 1H), 4.33 (q, *J* = 6.8 Hz, 1H), 3.77 (s, 3H), 1.52 (d, *J* = 6.7 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 159.85, 141.54, 130.18 , 119.34 , 114.19 , 113.05 , 55.70 , 50.48 , 21.37 . **White solid.**

1-(4-fluorophenyl)ethan-1- amine hydrochloride



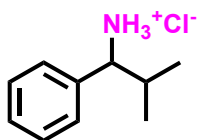
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.76 (br s, 3H), 7.78 – 7.48 (m, 2H), 7.35 – 7.10 (m, 2H), 4.50 – 4.24 (m, 1H), 1.52 (d, *J* = 6.8 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 162.34 (d, *J* = 244.4 Hz), 136.19 (d, *J* = 3.1 Hz), 129.71 (d, *J* = 8.4 Hz), 115.85 (d, *J* = 21.4 Hz), 49.80 , 21.25 . **Brown solid.**

1-(2-methoxy-4-(trifluoromethoxy)phenyl)ethan-1-amine hydrochloride



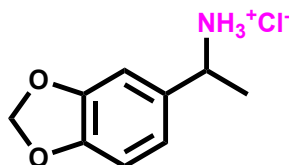
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.58 (br s, 3H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.26 – 6.84 (m, 2H), 4.79 – 4.40 (m, 1H), 3.94 (s, 3H), 1.55 (d, *J* = 6.7 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 157.82 , 149.65 , 128.81 , 126.76 , 120.49 (q, *J* = 256.5 Hz), 112.91 , 105.51 , 56.76 , 44.66 , 19.56 . **Off white solid.**

KM24-154 2-methyl-1-phenylpropan-1-amine hydrochloride



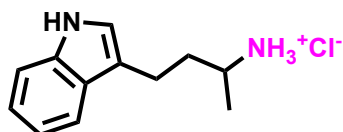
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.08 (br s, 3H), 7.53 – 7.44 (m, 2H), 7.42 – 7.28 (m, 3H), 4.06 – 3.70 (m, 1H), 2.30 – 2.06 (m, 1H), 0.99 (d, *J* = 6.2 Hz, 3H), 0.67 (d, *J* = 6.3 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 137.93 , 128.82 , 128.65 , 128.33 , 60.57 , 32.60 , 20.03 , 18.96 . **Off white solid.**

1-(benzo[d][1,3]dioxol-5-yl)ethan-1-amine hydrochloride



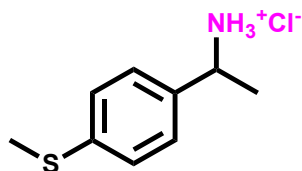
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.66 (br s, 3H), 7.21 (d, *J* = 1.7 Hz, 1H), 6.99 (dd, *J* = 8.1, 1.7 Hz, 1H), 6.91 (d, *J* = 8.0 Hz, 1H), 6.02 (s, 2H), 4.40 – 4.12 (m, 1H), 1.49 (d, *J* = 6.7 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 147.81 , 147.52 , 133.69 , 121.10 , 108.65 , 107.85 , 101.64 , 50.34 , 21.30 . **Off white solid.**

4-(1H-indol-3-yl)butan-2-amine hydrochloride



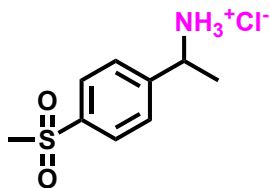
¹H NMR (300 MHz, DMSO-*d*₆) δ 11.01 (s, 1H), 8.32 (br s, 3H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 1H), 7.18 (d, *J* = 2.1 Hz, 1H), 7.14 – 7.02 (m, 1H), 7.03 – 6.94 (m, 1H), 3.31 – 3.02 (m, 1H), 2.88 – 2.65 (m, 2H), 2.20 – 1.98 (m, 1H), 1.91 – 1.68 (m, 1H), 1.30 (d, *J* = 6.5 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 136.81 , 127.40 , 122.81 , 121.40 , 118.85 , 118.64 , 113.59 , 111.95 , 47.13 , 35.17 , 21.26 , 18.54 . **Brown solid.**

1-(4-(methylthio)phenyl)ethan-1-amine hydrochloride



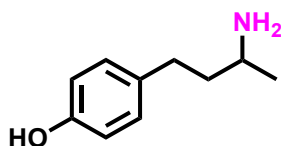
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.31 (br s, 3H), 7.48 (d, *J* = 7.9 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 4.53 – 4.08 (m, 1H), 2.47 (s, 3H), 1.51 (d, *J* = 6.4 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 138.88 , 136.38 , 128.07 , 126.44 , 50.09 , 21.27 , 15.29 . **Brown solid.**

1-(4-(methylsulfonyl)phenyl)ethan-1-amine hydrochloride



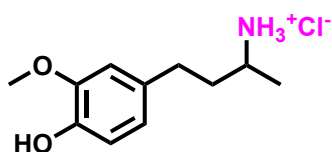
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.87 (br s, 3H), 7.98 (d, *J* = 8.4 Hz, 2H), 7.84 (d, *J* = 8.4 Hz, 2H), 4.66 – 4.42 (m, 1H), 3.24 (s, 3H), 1.55 (d, *J* = 6.8 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 145.49 , 141.06 , 128.44 , 127.74 , 50.03 , 43.85 , 21.12 . **Pale brown solid.**

4-(3-aminobutyl)phenol



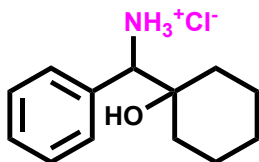
¹H NMR (300 MHz, DMSO-*d*₆) δ 6.98 (d, *J* = 8.4 Hz, 2H), 6.68 (d, *J* = 8.4 Hz, 2H), 6.28 (br s, 2H), 3.02 – 2.78 (m, 1H), 2.66 – 2.33 (m, 2H), 1.82 – 1.48 (m, 2H), 1.10 (d, *J* = 6.4 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 155.88 , 132.03 , 129.44 , 115.57 , 46.57 , 39.49 , 31.06 , 21.37 . **Brown solid.**

4-(4-hydroxy-3-methoxyphenyl)butan-2-amine hydrochloride



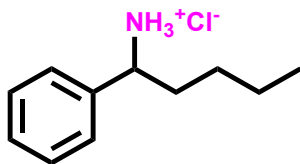
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.27 (br s, 3H), 6.84 (d, *J* = 1.9 Hz, 1H), 6.78 (d, *J* = 7.9 Hz, 1H), 6.64 (dd, *J* = 8.0, 1.9 Hz, 1H), 3.79 (s, 3H), 3.27 – 2.98 (m, 1H), 2.71 – 2.55 (m, 2H), 2.10 – 1.85 (m, 1H), 1.88 – 1.62 (m, 1H), 1.28 (d, *J* = 6.5 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 147.90 , 145.10 , 132.10 , 120.70 , 115.82 , 112.91 , 56.02 , 46.86 , 36.50 , 30.86 , 18.46 . **Pale yellow solid.**

(1-hydroxycyclohexyl)(phenyl)methanamine hydrochloride



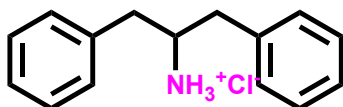
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.45 (br s, 3H), 7.57 – 7.42 (m, 2H), 7.45 – 7.24 (m, 3H), 5.04 (s, 1H), 4.11 (s, 1H), 1.89 – 0.90 (m, 10H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 135.87 , 129.40 , 128.62 , 128.38 , 71.20 , 63.23 , 34.87 , 33.02 , 25.48 , 21.47 , 21.12 . **Off white solid.**

1-phenylpentan-1-amine hydrochloride



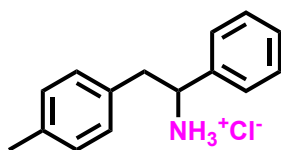
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.59 (br s, 3H), 7.56 – 7.46 (m, 2H), 7.46 – 7.34 (m, 3H), 4.15 (dd, *J* = 9.5, 5.4 Hz, 1H), 2.05 – 1.91 (m, 1H), 1.89 – 1.70 (m, 1H), 1.30 – 0.93 (m, 4H), 0.80 (t, *J* = 7.1 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 138.41 , 129.15 , 128.94 , 127.91 , 54.94 , 34.36 , 27.65 , 22.10 , 14.18 . **Pale brown solid.**

1,3-diphenylpropan-2-amine hydrochloride



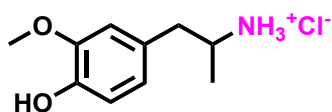
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.26 (br s, 3H), 7.44 – 7.08 (m, 10H), 3.76 – 3.56 (m, 1H), 3.03 (dd, *J* = 13.9, 6.2 Hz, 2H), 2.80 (dd, *J* = 13.9, 6.9 Hz, 2H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 136.96 , 129.84 , 129.07 , 127.25 , 53.61 , 38.17 . **Brown solid.**

1-phenyl-2-(p-tolyl)ethan-1-amine hydrochloride



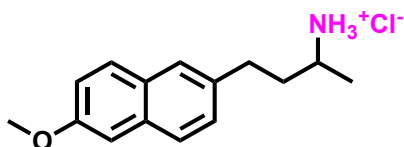
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.87 (br s, 3H), 7.50 – 7.37 (m, 2H), 7.36 – 7.25 (m, 3H), 7.06 – 6.84 (m, 4H), 4.53 – 4.29 (m, 1H), 3.42 (dd, *J* = 13.4, 5.0 Hz, 1H), 3.08 (dd, *J* = 13.3, 10.2 Hz, 1H), 2.18 (s, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 137.56 , 135.97 , 133.58 , 129.56 , 129.29 , 128.86 , 128.86 , 128.38 , 56.43 , 40.25 , 21.07 . **White solid.**

1-(4-hydroxy-3-methoxyphenyl)propan-2-amine hydrochloride



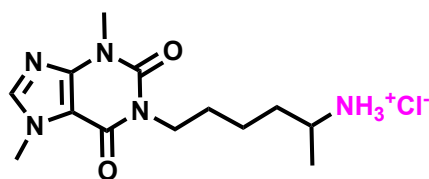
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.19 (br s, 3H), 6.80 (d, *J* = 1.9 Hz, 1H), 6.74 (d, *J* = 8.0 Hz, 1H), 6.60 (dd, *J* = 8.0, 1.9 Hz, 1H), 3.75 (s, 3H), 3.39 – 3.23 (m, 1H), 2.93 (dd, *J* = 13.4, 5.2 Hz, 1H), 2.58 (dd, *J* = 9.0, 4.4 Hz, 1H), 1.12 (d, *J* = 6.7 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 147.98 , 145.80 , 127.84 , 121.92 , 115.94 , 113.73 , 56.00 , 48.66 , 31.76 , 18.04 . **Brown solid.**

4-(6-methoxynaphthalen-2-yl)butan-2-amine hydrochloride



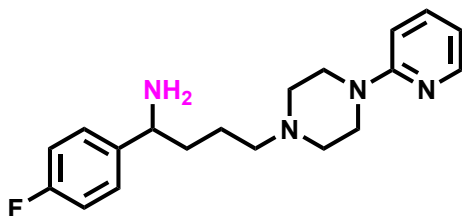
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.33 (br s, 3H), 7.74 (dd, *J* = 8.7, 2.7 Hz, 2H), 7.65 – 7.60 (m, 1H), 7.34 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.26 (d, *J* = 2.5 Hz, 1H), 7.12 (dd, *J* = 8.9, 2.5 Hz, 1H), 3.83 (s, 3H), 3.32 – 3.09 (m, 1H), 2.93 – 2.66 (m, 2H), 2.18 – 1.93 (m, 1H), 1.93 – 1.70 (m, 1H), 1.28 (d, *J* = 6.5 Hz, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 157.26 , 136.54 , 133.26 , 129.25 , 129.02 , 128.02 , 127.31 , 126.40 , 119.00 , 106.23 , 55.60 , 46.97 , 36.21 , 31.28 , 18.51 . **Off white solid.**

6-(3,7-dimethyl-2,6-dioxo-2,3,6,7-tetrahydro-1H-purin-1-yl)hexan-2-amine hydrochloride



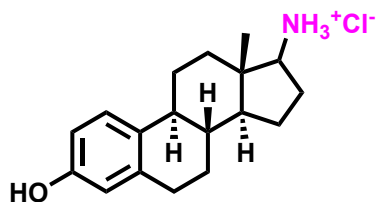
¹H NMR (300 MHz, Methanol-*d*₄) δ 7.91 (s, 1H), 4.83 (br s, 3H), 3.89 (s, 3H), 3.87 – 3.81 (m, 2H), 3.40 (s, 3H), 3.29 – 3.15 (m, 1H), 1.71 – 1.47 (m, 4H), 1.44 – 1.30 (m, 2H), 1.24 (d, *J* = 6.5 Hz, 3H). **¹³C NMR (75 MHz, Methanol-*d*₄)** δ 154.88 , 151.35 , 147.73 , 142.34 , 107.26 , 47.55 , 40.46 , 33.88 , 32.92 , 28.96 , 27.13 , 22.29 , 17.33 . **White solid.**

1-(4-fluorophenyl)-4-(4-(pyridin-2-yl)piperazin-1-yl)butan-1-amine



¹H NMR (300 MHz, Chloroform-*d*) δ 8.14 – 8.04 (m, 1H), 7.45 – 7.33 (m, 1H), 7.29 – 7.21 (m, 2H), 6.98 – 6.89 (m, 2H), 6.58 – 6.47 (m, 2H), 3.87 (t, *J* = 6.9 Hz, 1H), 3.65 (br s, 2H), 3.49 – 3.38 (m, 4H), 2.49 – 2.37 (m, 4H), 2.34 – 2.25 (m, 2H), 1.93 – 1.27 (m, 4H). **¹³C NMR (75 MHz, Chloroform-*d*)** δ 161.96 (d, *J* = 245.2 Hz), 159.46 , 147.91 , 140.36 , 137.44 , 128.11 (d, *J* = 7.9 Hz), 115.36 (d, *J* = 21.2 Hz), 113.31 , 107.07 , 58.33 , 55.45 , 52.96 , 45.09 , 36.85 , 23.69 . **Brown solid.**

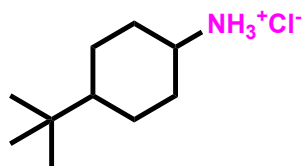
(8R,9S,13S,14S)-3-hydroxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-amine hydrochloride (diastereomeric mixture)



¹H NMR (300 MHz, DMSO-*d*₆) (diastereomeric mixture) δ 9.09 (br s, 1H), 8.24 (br s, 3H), 7.03 (d, J = 8.1 Hz, 1H), 6.53 (dd, J = 8.4, 2.5 Hz, 1H), 6.46 (d, J = 2.6 Hz, 1H), 3.22 – 2.91 (m, 1H), 2.86 – 2.61 (m, 2H), 2.30 – 2.00 (m, 4H), 1.85 – 1.51 (m, 4H), 1.35 – 1.20 (m, 5H), 0.75 (s, 3H). **¹³C NMR (75 MHz, DMSO-*d*₆)** (diastereomeric mixture) δ 155.52, 155.41, 137.44, 137.41, 130.82, 130.36, 126.53, 126.42, 115.43, 115.40, 113.26, 113.21, 59.95, 59.24, 51.27, 49.98, 47.93, 43.99, 43.86, 43.56, 43.27, 39.16, 38.66, 36.23, 29.64, 29.53, 28.38, 28.26, 27.50, 27.44, 26.71, 26.18, 26.09, 23.55, 18.33, 12.15. (traces of ethylacetate solvent peak was observed in the NMR spectra).

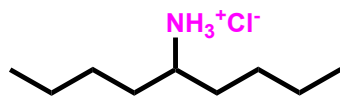
HRMS (EI): Calcd for C₁₈H₂₅NO [M]⁺ 271.1930; found 271.1929. **Off white solid.**

4-(tert-butyl)cyclohexan-1-amine hydrochloride (diastereomeric mixture)



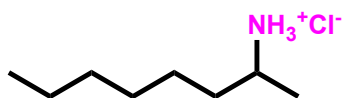
¹H NMR (300 MHz, DMSO-*d*₆) (diastereomeric mixture) δ 7.43 (br s, 3H), 3.32 – 2.56 (m, 1H), 2.19 – 1.23 (m, 7H), 1.06 – 0.87 (m, 2H), 0.78 (s, 9H). **¹³C NMR (75 MHz, DMSO-*d*₆)** (diastereomeric mixture) δ 49.94, 47.50, 46.72, 46.01, 32.72, 32.47, 30.89, 28.93, 27.94, 27.81, 25.37, 20.71. **Off white solid.**

Nonan-5-amine hydrochloride



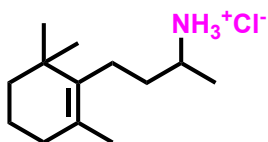
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.10 (br s, 3H), 3.11 – 2.84 (m, 1H), 1.57 – 1.47 (m, 4H), 1.33 – 1.20 (m, 8H), 0.90 – 0.81 (m, 6H). **¹³C NMR (75 MHz, DMSO-*d*₆)** δ 51.09, 31.92, 27.01, 22.44, 14.20. **White solid.**

Octan-2-amine hydrochloride



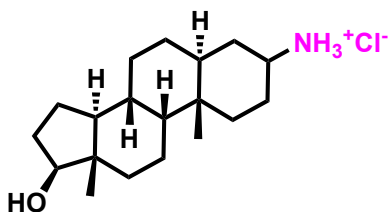
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.09 (br s, 3H), 3.29 – 3.04 (m, 1H), 1.73 – 1.59 (m, 1H), 1.58 – 1.42 (m, 1H), 1.40 – 1.27 (m, 8H), 1.23 (d, *J* = 6.5 Hz, 3H), 0.96 – 0.89 (m, 3H). ¹³C NMR (75 MHz, DMSO-*d*₆) δ 47.23 , 34.52 , 31.51 , 28.88 , 25.18 , 22.44 , 18.53 , 14.40 . **White solid.**

4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-amine hydrochloride



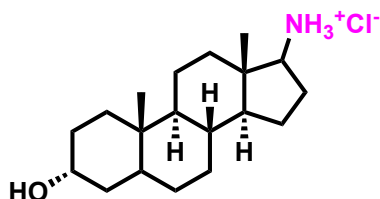
¹H NMR (300 MHz, DMSO-*d*₆) δ 8.14 (br s, 3H), 3.20 – 3.05 (m, 1H), 2.07 – 1.92 (m, 2H), 1.87 (t, *J* = 6.2 Hz, 2H), 1.75 – 1.59 (m, 1H), 1.56 (s, 3H), 1.54 – 1.44 (m, 3H), 1.42 – 1.33 (m, 2H), 1.22 (d, *J* = 6.5 Hz, 3H), 0.97 (s, 3H), 0.97 (s, 3H). ¹³C NMR (75 MHz, DMSO-*d*₆) δ 136.49 , 127.31 , 47.71 , 39.78 , 35.18 , 35.05 , 32.69 , 28.84 , 24.60 , 20.07 , 19.48 , 18.43 . **Brown solid.**

(5S,8R,9R,10S,13S,14S,17S)-17-hydroxy-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-3-amine hydrochloride (diastereomeric mixture)



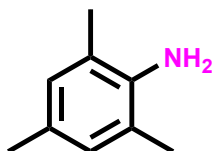
¹H NMR (300 MHz, DMSO-*d*₆) (diastereomeric mixture) δ 8.07 (br s, 3H), 4.44 (s, 1H), 3.57 – 3.33 (m, 1H), 1.99 – 0.81 (m, 23H), 0.75 (s, 3H), 0.63 (s, 3H). ¹³C NMR (75 MHz, DMSO-*d*₆) (diastereomeric mixture) δ 80.52, 80.48 , 54.07 , 53.68 , 52.92, 52.71, 51.21 , 51.01 , 49.90 , 46.68 , 44.57 , 44.02, 42.18, 43.02 , 38.42 , 37.11 , 37.05 , 36.49 , 36.00 , 35.56 , 35.48 , 32.76 , 31.61 , 31.26 , 30.98 , 30.30 , 28.44 , 28.21 , 26.32 , 26.27 , 24.29 , 23.51 , 20.79 , 20.72 , 20.41 , 12.28 , 11.80 , 11.55 . **HRMS (EI):** Calcd for C₁₉H₃₃NO [M]⁺ 291.2556; found 291.2549. **White solid.**

(3R,8R,9S,10S,13S,14S)-3-hydroxy-10,13-dimethylhexadecahydro-1H-cyclopenta[a]phenanthren-17-amine hydrochloride (diastereomeric mixture)



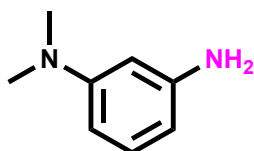
¹H NMR (300 MHz, DMSO-*d*₆) (diastereomeric mixture) δ 7.98 (br s, 3H), 3.90 – 3.71 (m, 1H), 3.14 – 2.96 (m, 1H), 2.29 – 1.89 (m, 1H), 1.79 – 0.86 (m, 21H), 0.83 – 0.56 (m, 6H). ¹³C NMR (75 MHz, DMSO-*d*₆) δ 64.62, 64.47, 59.92, 59.09, 54.22, 53.80, 53.69, 52.40, 49.01, 48.93, 43.57, 42.22, 38.97, 36.26, 36.15, 36.11, 35.70, 35.26, 32.58, 32.47, 32.41, 32.36, 31.91, 29.07, 28.64, 28.58, 28.23, 26.57, 24.96, 23.80, 20.24, 20.16, 18.26, 18.07, 12.12, 12.08, 11.57, 11.53. HRMS (EI): Calcd for C₁₉H₃₃NO [M]⁺ 291.2556; found 291.2549. **White solid.**

2,4,6-trimethylaniline



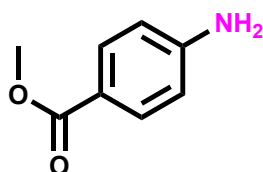
¹H NMR (300 MHz, Chloroform-*d*) δ 6.82 – 6.52 (m, 2H), 3.42 (br s, 2H), 2.12 (s, 3H), 2.07 (s, 6H). ¹³C NMR (75 MHz, Chloroform-*d*) δ 140.00, 128.91, 127.32, 122.03, 20.44, 17.66. **Brown oil.**

N1,N1-dimethylbenzene-1,3-diamine



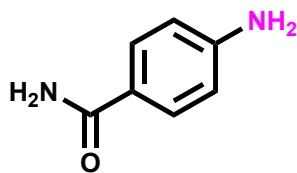
¹H NMR (300 MHz, Chloroform-*d*) δ 7.02 – 6.88 (m, 1H), 6.18 – 6.07 (m, 1H), 6.07 – 5.93 (m, 2H), 3.37 (br s, 2H), 2.83 (s, 6H). ¹³C NMR (75 MHz, Chloroform-*d*) δ 151.85, 147.30, 129.87, 104.30, 103.82, 99.63, 40.62. **Brown gum.**

methyl 4-aminobenzoate



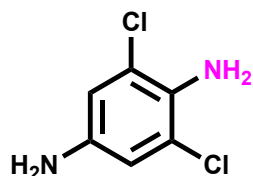
¹H NMR (300 MHz, DMSO-*d*₆) δ 7.67 (d, *J* = 8.7 Hz, 2H), 6.60 (d, *J* = 8.7 Hz, 2H), 5.95 (br s, 2H), 3.73 (s, 3H). ¹³C NMR (75 MHz, DMSO-*d*₆) δ 166.90, 153.89, 131.55, 116.31, 113.17, 51.58. **Brown solid.**

4-aminobenzamide



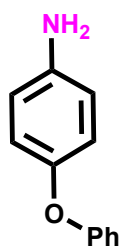
^1H NMR (300 MHz, DMSO- d_6) δ 7.63 (d, J = 8.6 Hz, 2H), 6.94 (s, 1H), 6.57 (d, J = 8.6 Hz, 2H), 5.62 (s, 1H), 3.63 (br s, 2H). ^{13}C NMR (75 MHz, DMSO- d_6) δ 168.85 , 152.17 , 129.65 , 121.29 , 113.04 . **Pale brown solid.**

2,6-dichlorobenzene-1,4-diamine



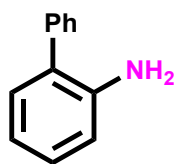
^1H NMR (300 MHz, Chloroform- d) δ 6.53 (s, 2H), 3.79 (br s, 2H), 3.41 (br s, 2H). ^{13}C NMR (75 MHz, Chloroform- d) δ 138.36 , 132.53 , 120.81 , 115.41 . **Brown solid.**

4-phenoxyaniline



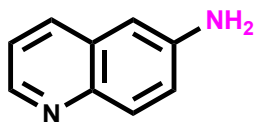
^1H NMR (300 MHz, DMSO- d_6) δ 7.34 – 7.24 (m, 2H), 7.04 – 6.95 (m, 1H), 6.89 – 6.83 (m, 2H), 6.77 (d, J = 8.8 Hz, 2H), 6.62 (d, J = 8.8 Hz, 2H), 5.02 (br s, 2H). ^{13}C NMR (75 MHz, DMSO- d_6) δ 159.44 , 145.98 , 145.88 , 130.11 , 122.17 , 121.39 , 116.87 , 115.39 . **Pale brown solid.**

[1,1'-biphenyl]-2-amine



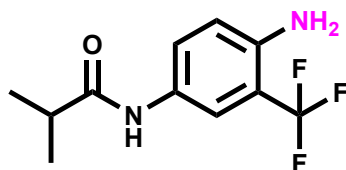
^1H NMR (300 MHz, Chloroform- d) δ 7.61 – 7.49 (m, 4H), 7.48 – 7.37 (m, 1H), 7.31 – 7.19 (m, 2H), 6.99 – 6.89 (m, 1H), 6.84 (dd, J = 8.1, 1.3 Hz, 1H), 3.85 (br s, 2H). ^{13}C NMR (75 MHz, Chloroform- d) δ 143.48 , 139.60 , 130.54 , 129.19 , 128.90 , 128.59 , 127.77 , 127.26 , 118.80 , 115.76 . **Off white Solid.**

Quinolin-6-amine



¹H NMR (300 MHz, DMSO-*d*₆) δ 8.47 (dd, *J* = 4.2, 1.7 Hz, 1H), 7.98 – 7.88 (m, 1H), 7.70 (d, *J* = 9.0 Hz, 1H), 7.27 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.17 (dd, *J* = 9.0, 2.5 Hz, 1H), 6.79 (d, *J* = 2.5 Hz, 1H), 5.66 (br s, 2H). ¹³C NMR (75 MHz, DMSO-*d*₆) δ 147.52 , 145.39 , 142.33 , 133.43 , 130.30 , 129.91 , 122.14 , 121.66 , 105.19 . **Brown solid.**

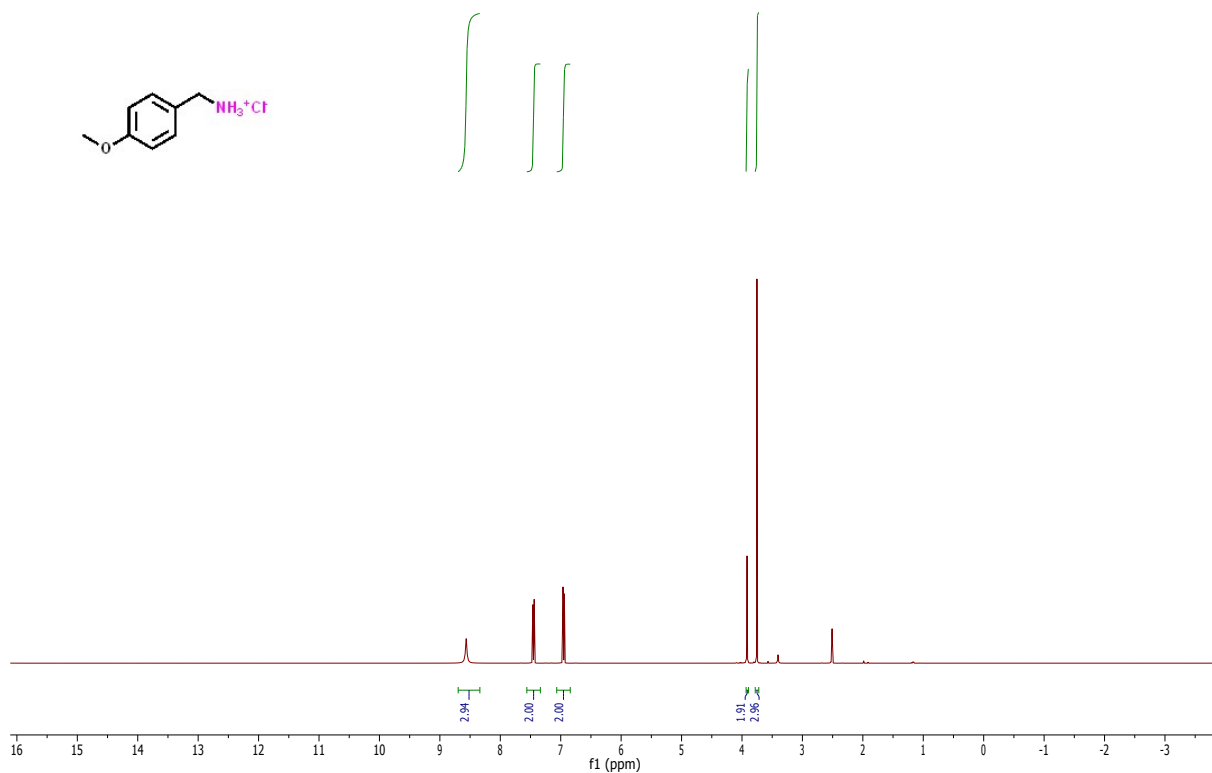
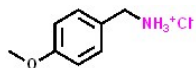
N-(4-amino-3-(trifluoromethyl)phenyl)isobutyramide



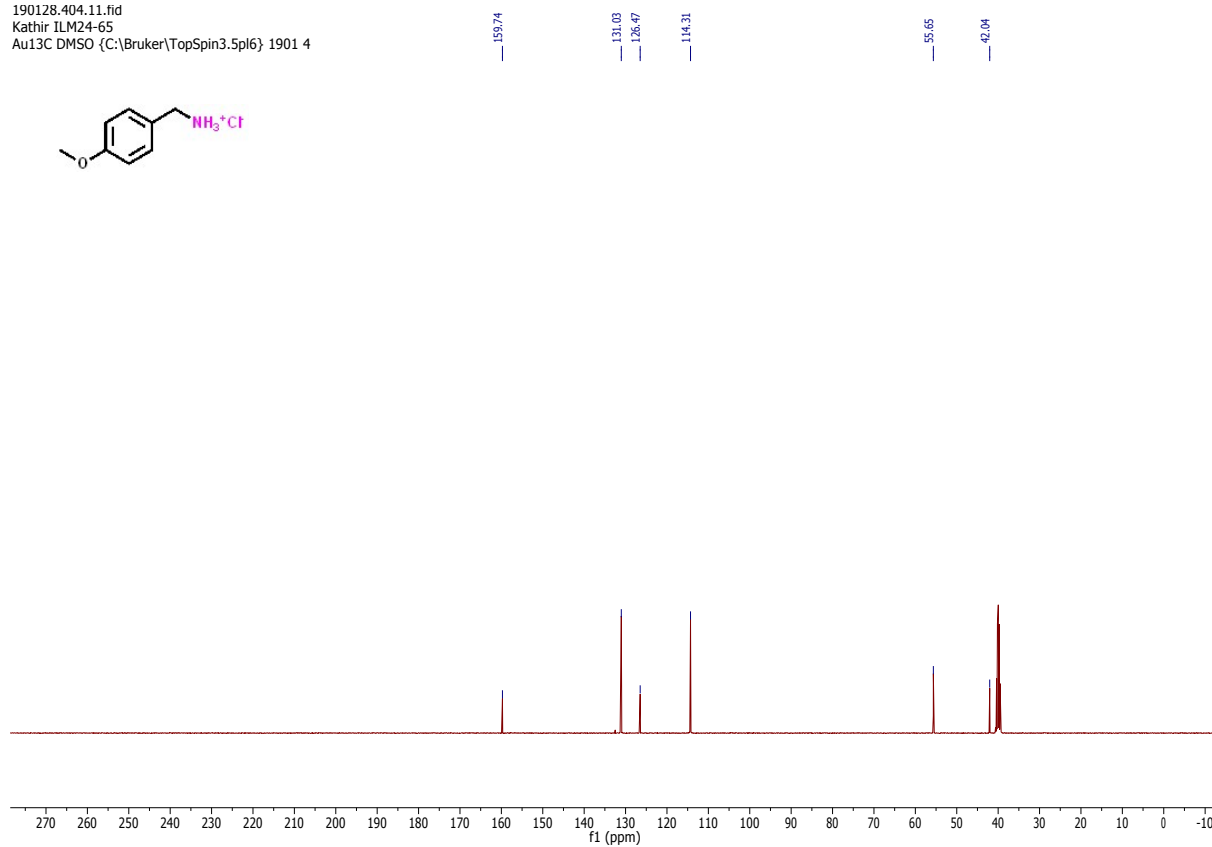
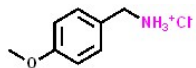
¹H NMR (300 MHz, DMSO-*d*₆) δ 9.63 (s, 1H), 7.73 (d, *J* = 2.4 Hz, 1H), 7.48 – 7.37 (m, 1H), 6.79 (dd, *J* = 8.8, 0.9 Hz, 1H), 5.32 (br s, 2H), 2.57 – 2.48 (m, 1H), 1.08 (d, *J* = 6.8 Hz, 6H). ¹³C NMR (75 MHz, DMSO-*d*₆) δ 175.11 , 142.48 , 128.79 , 126.44 (q, *J* = 272.0 Hz), 125.44, 117.61 , 117.39 (q, *J* = 5.6 Hz), 110.72 (q, *J* = 29.5 Hz), 35.21 , 19.97 . **Yellow Solid.**

S9. NMR and HRMS spectra

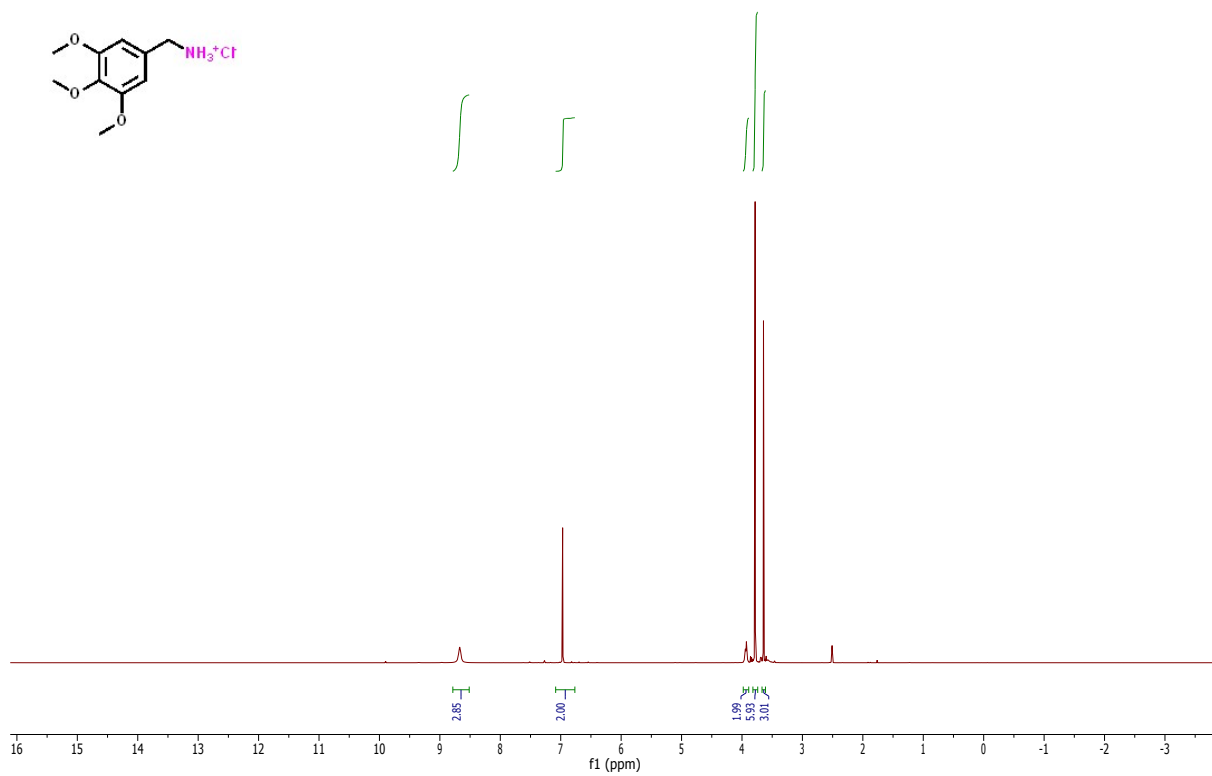
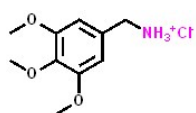
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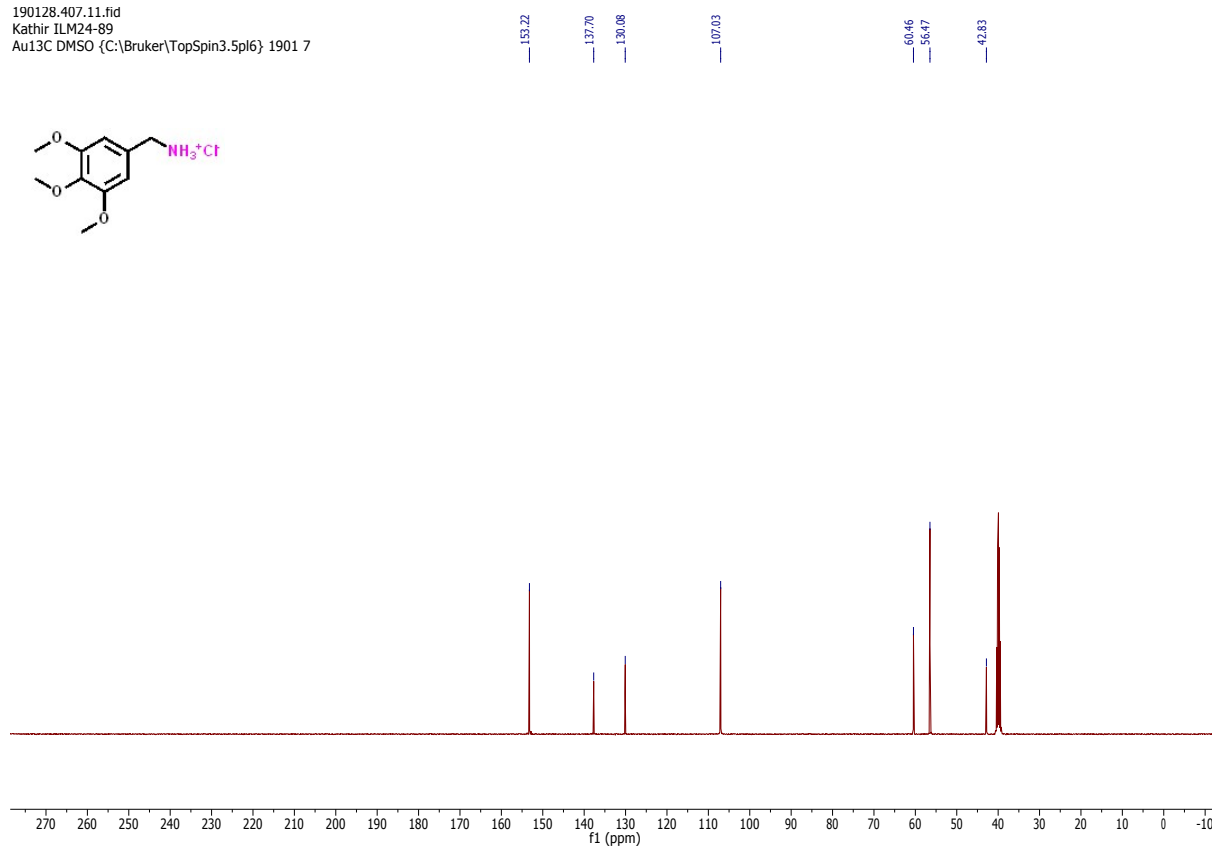
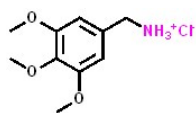
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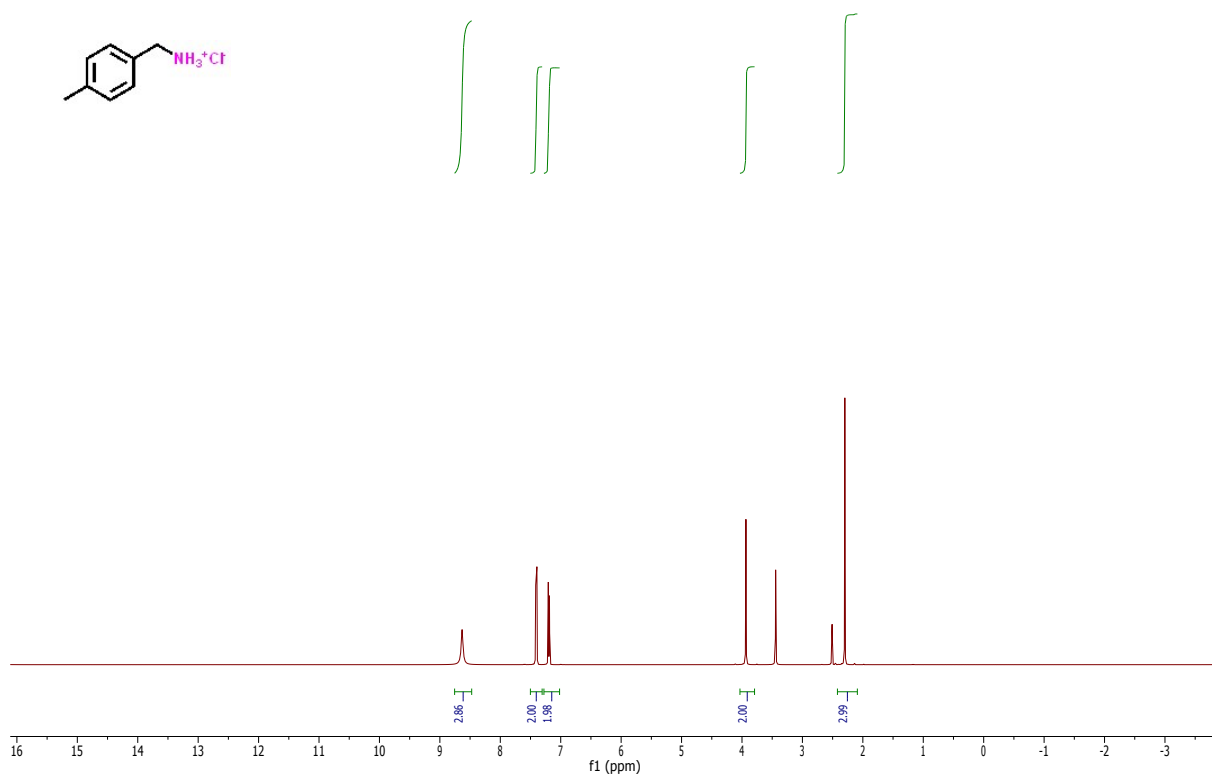
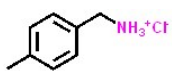
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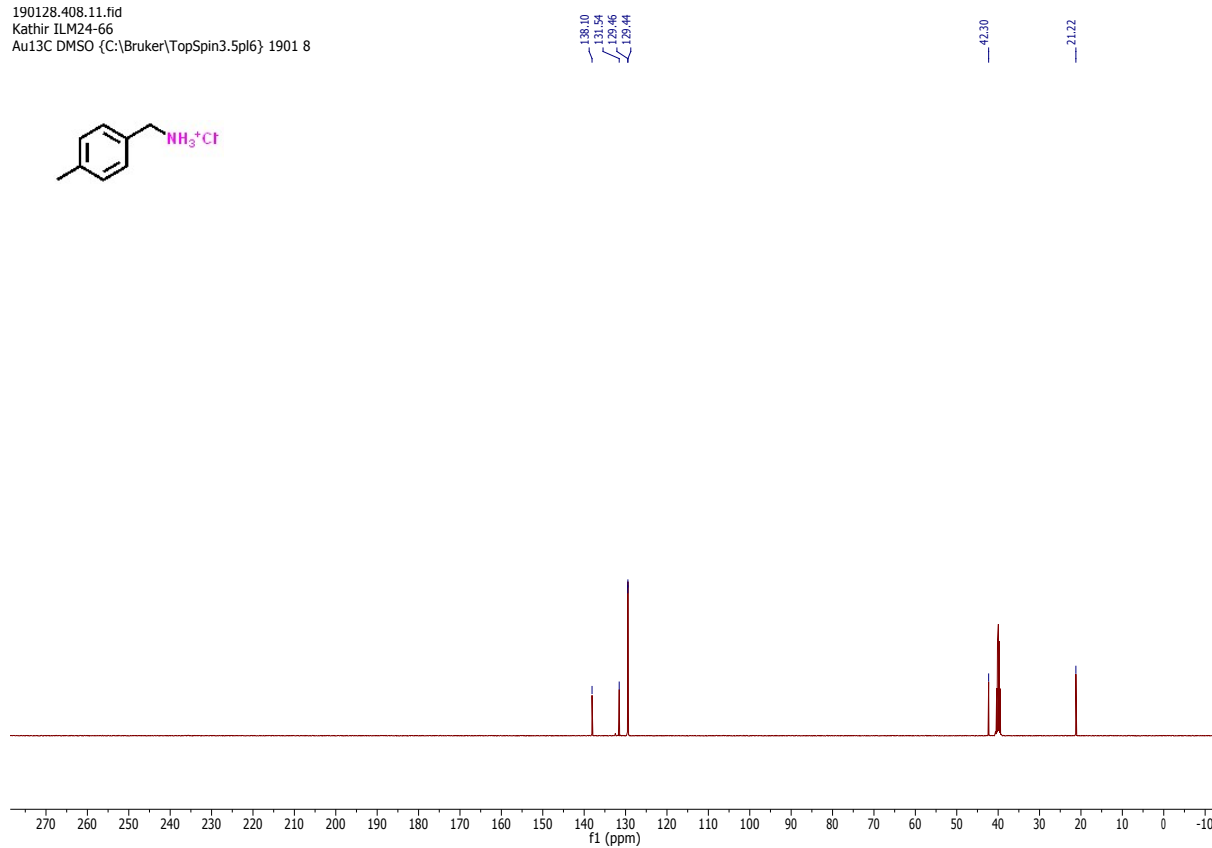
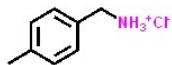
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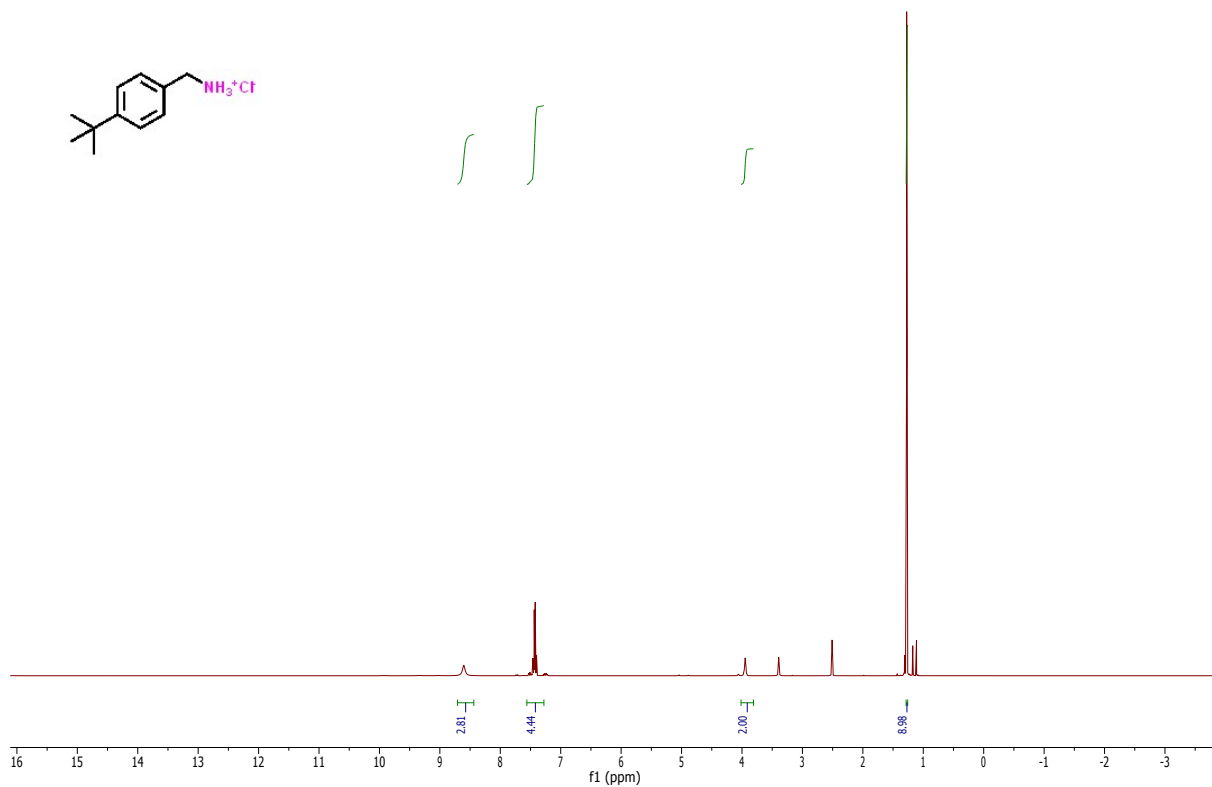
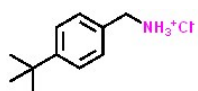
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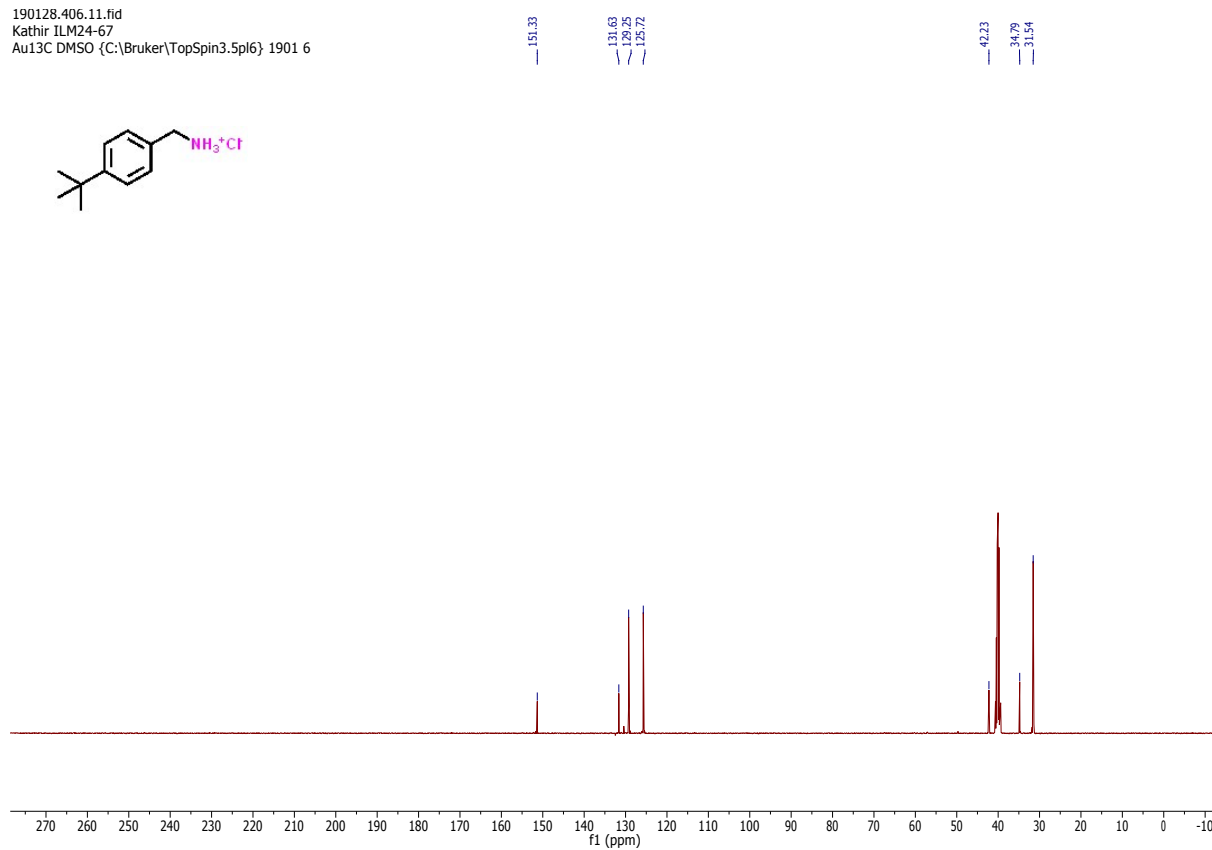
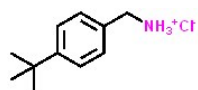
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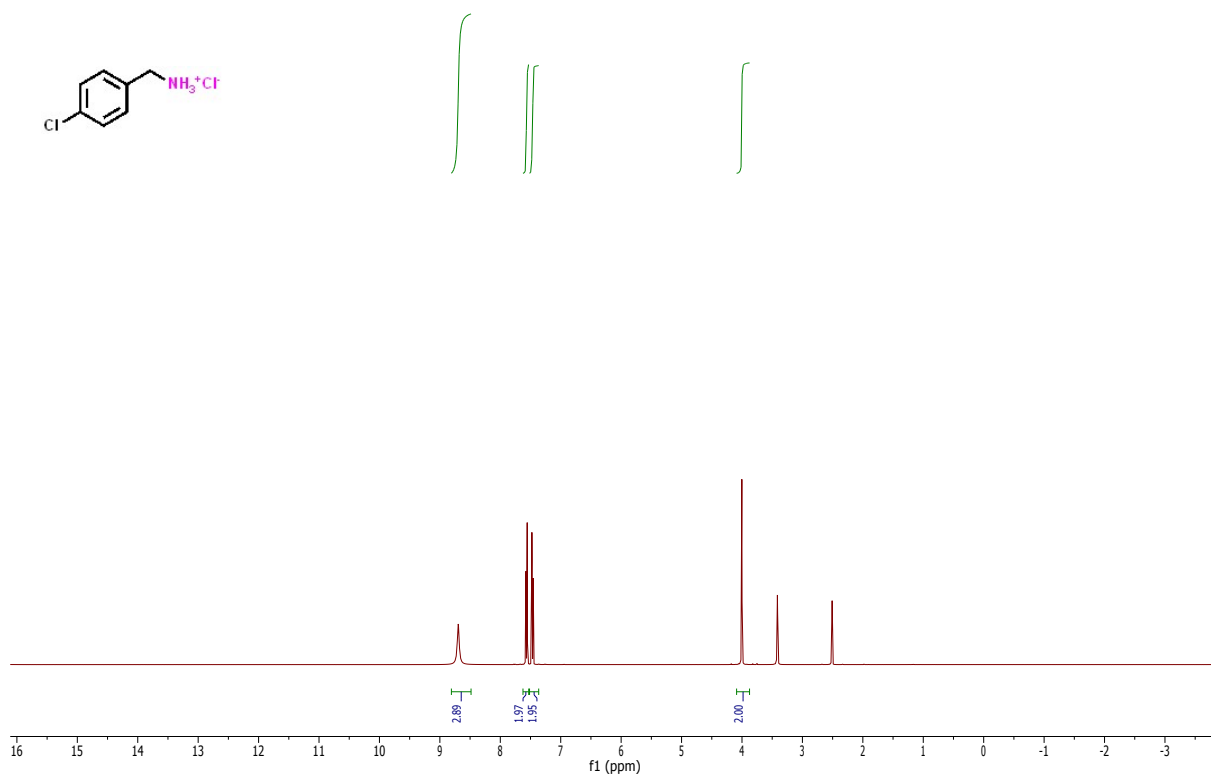
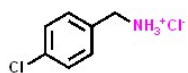
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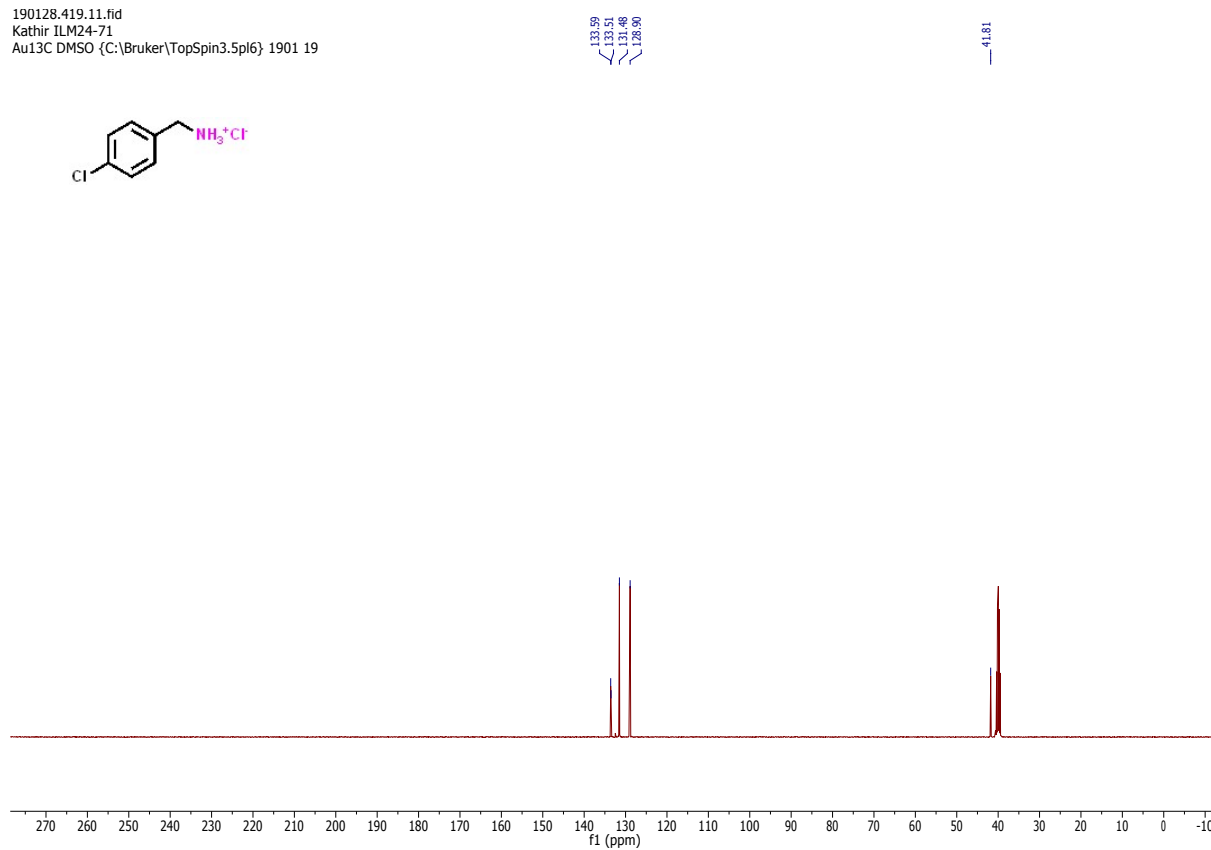
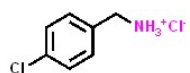
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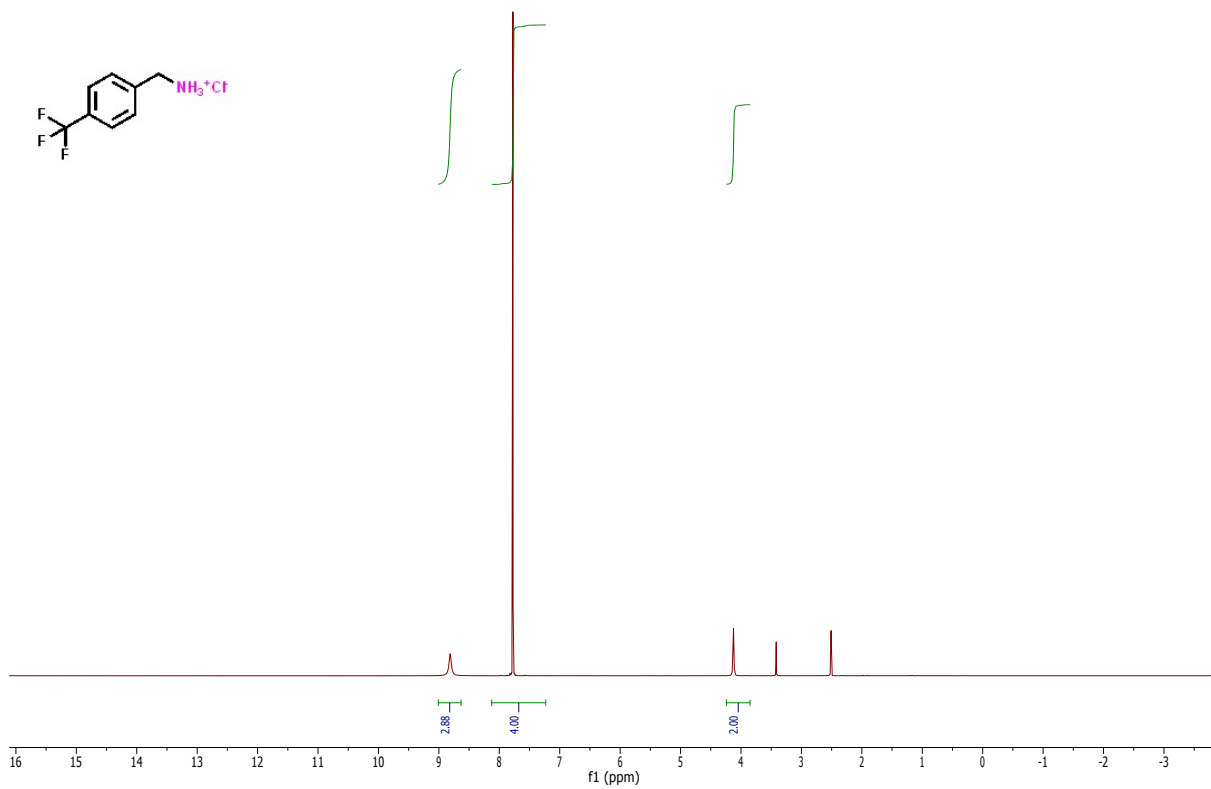
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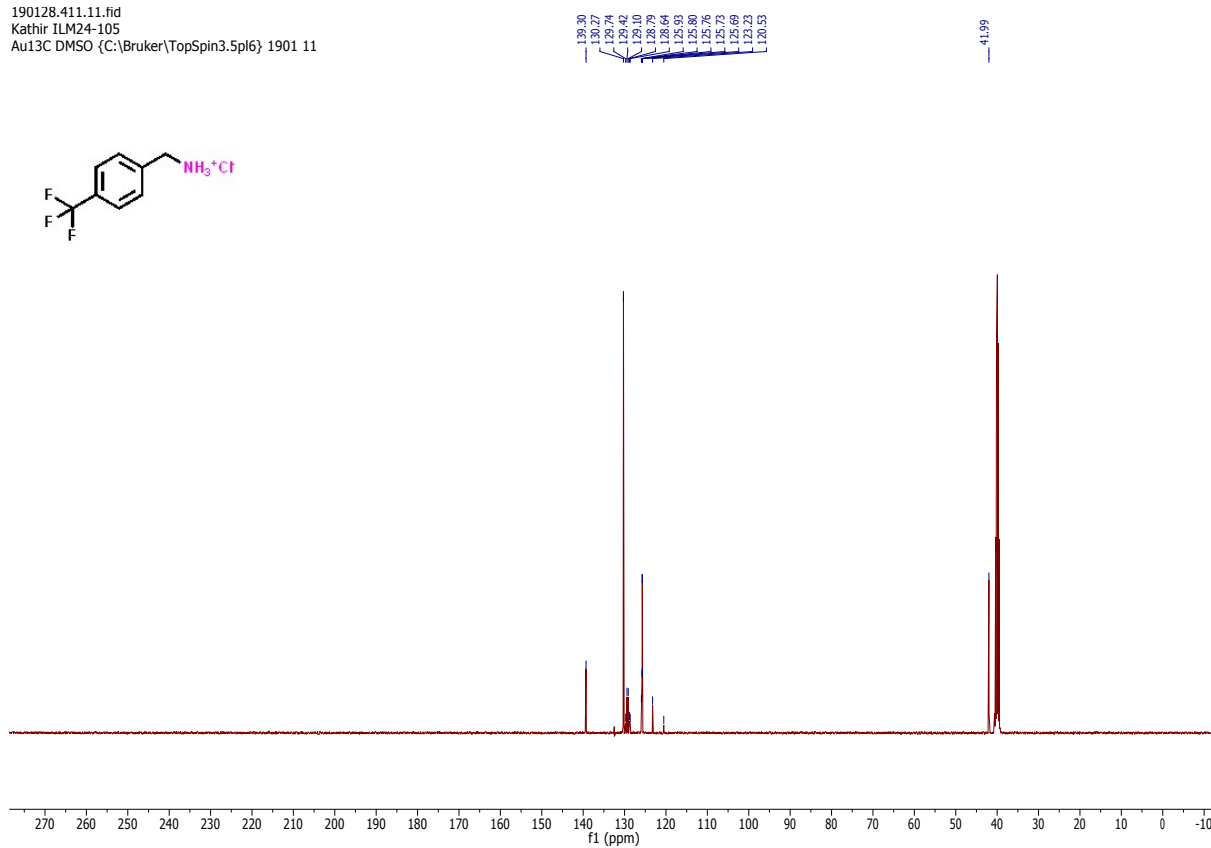
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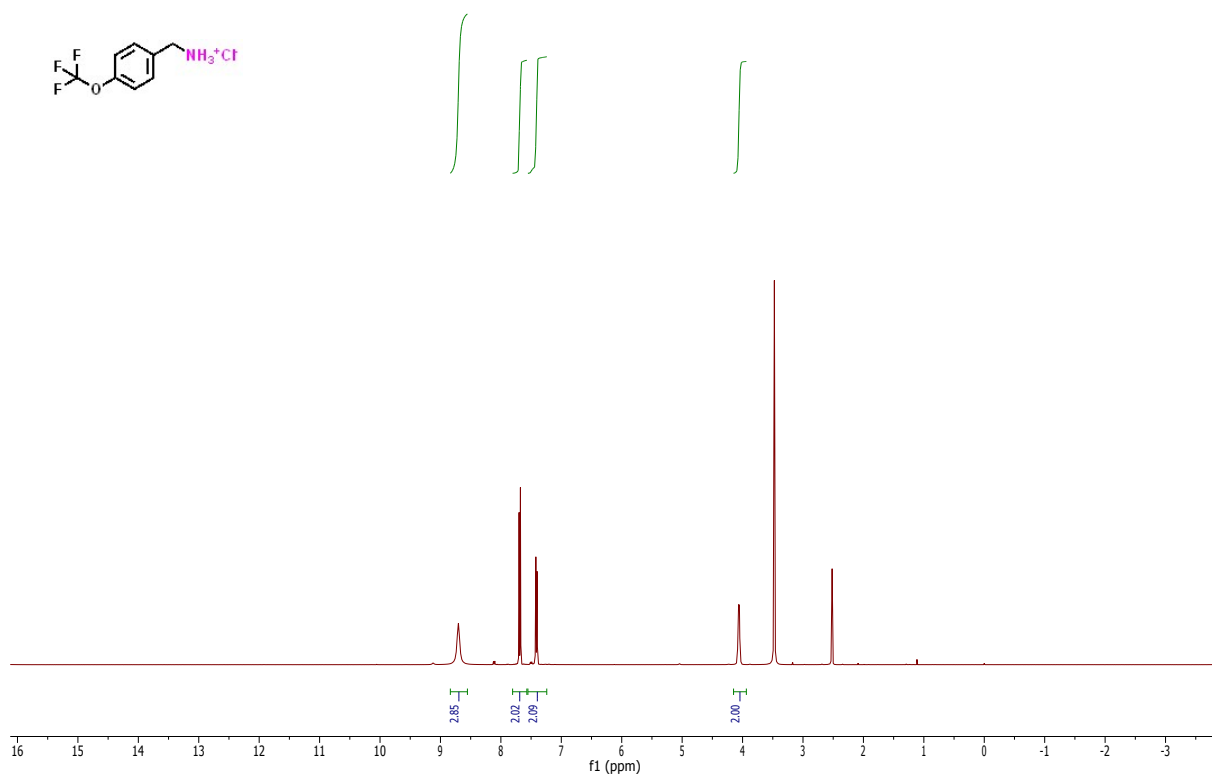
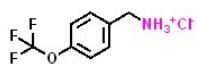
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Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1901 11



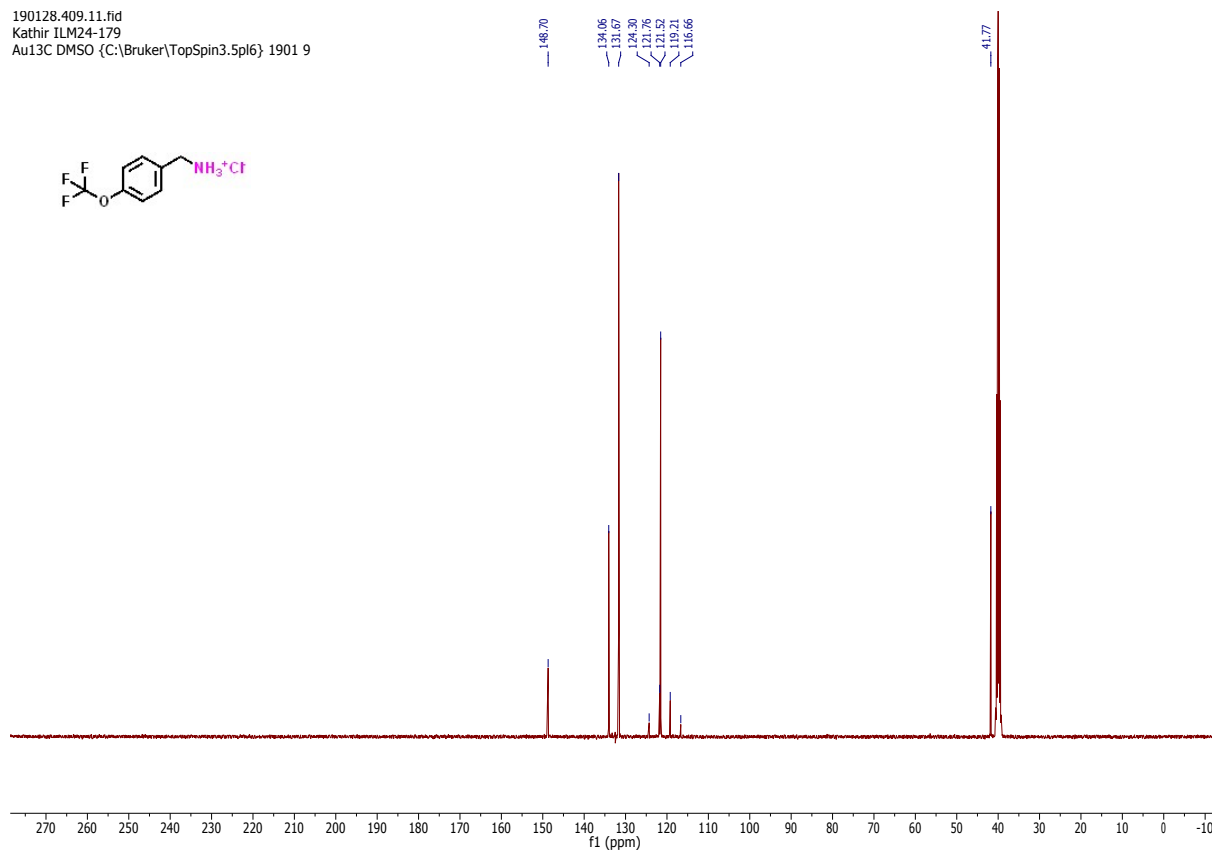
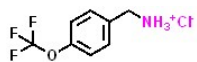
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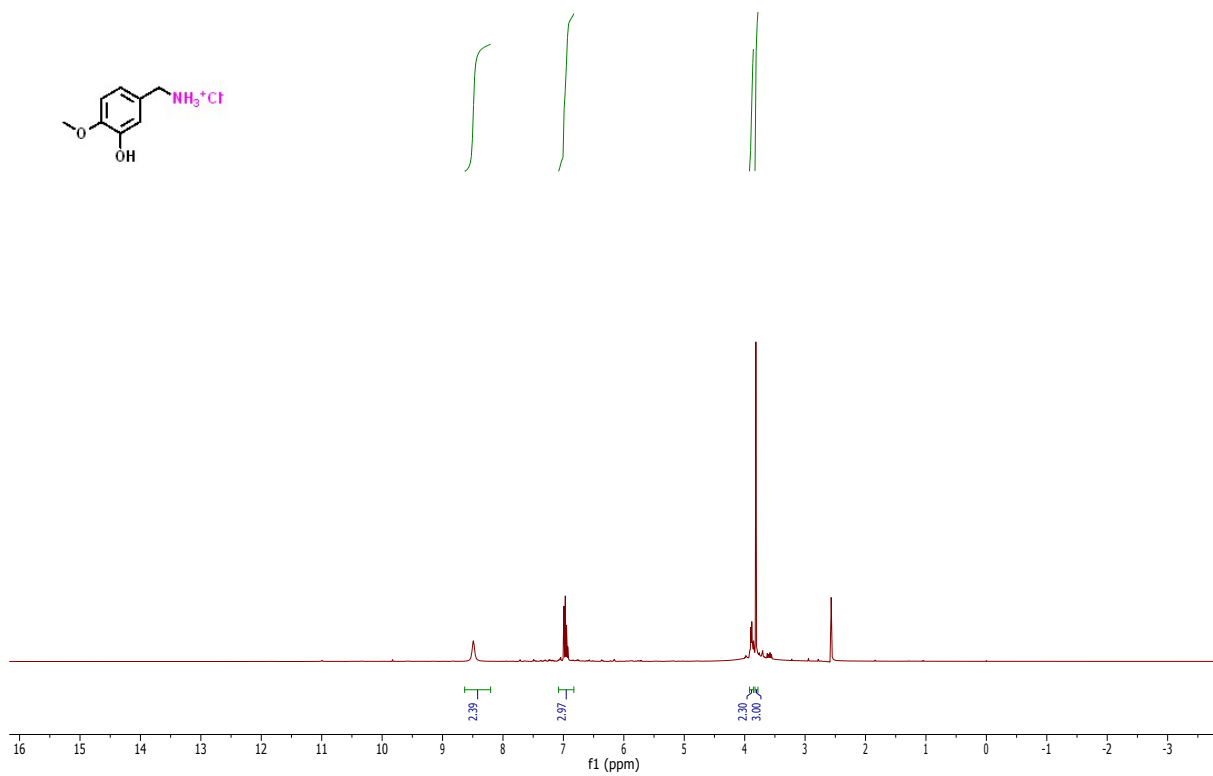
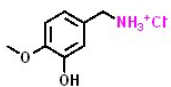
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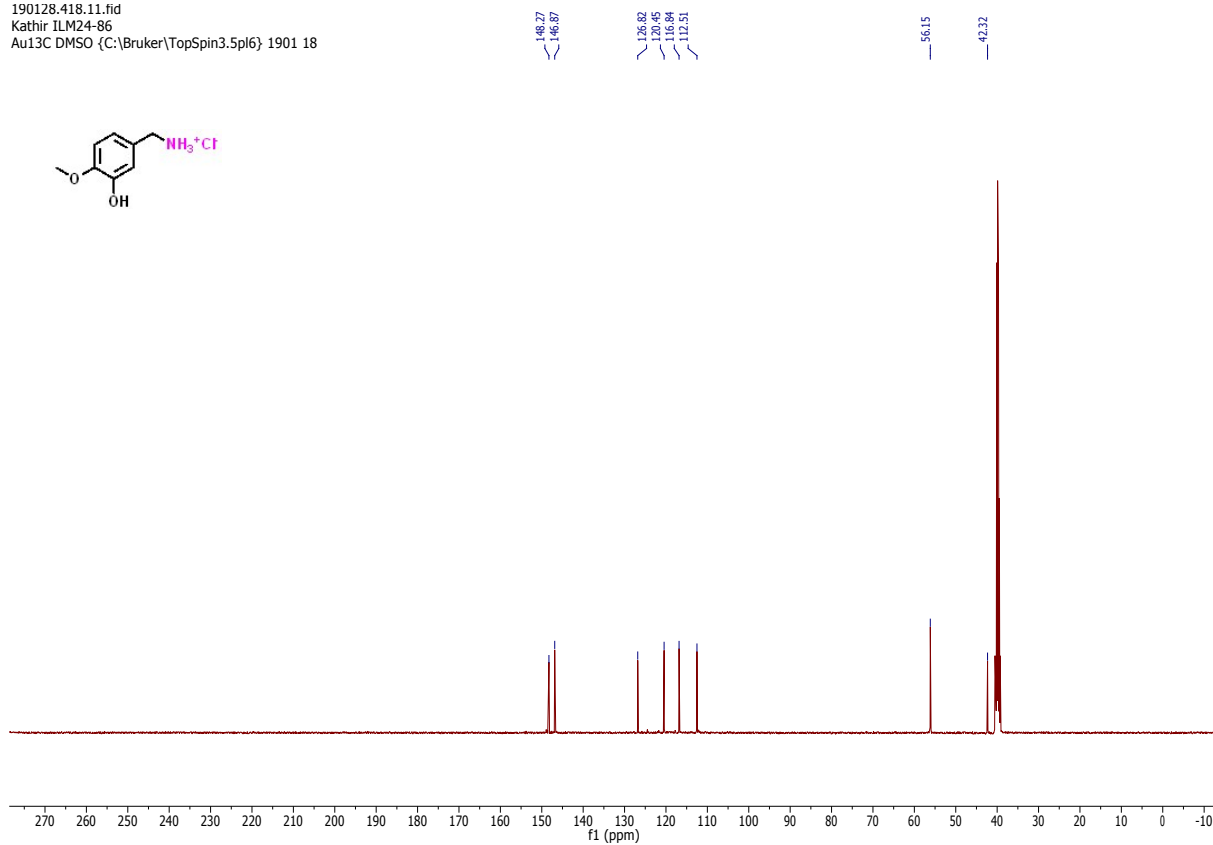
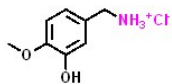
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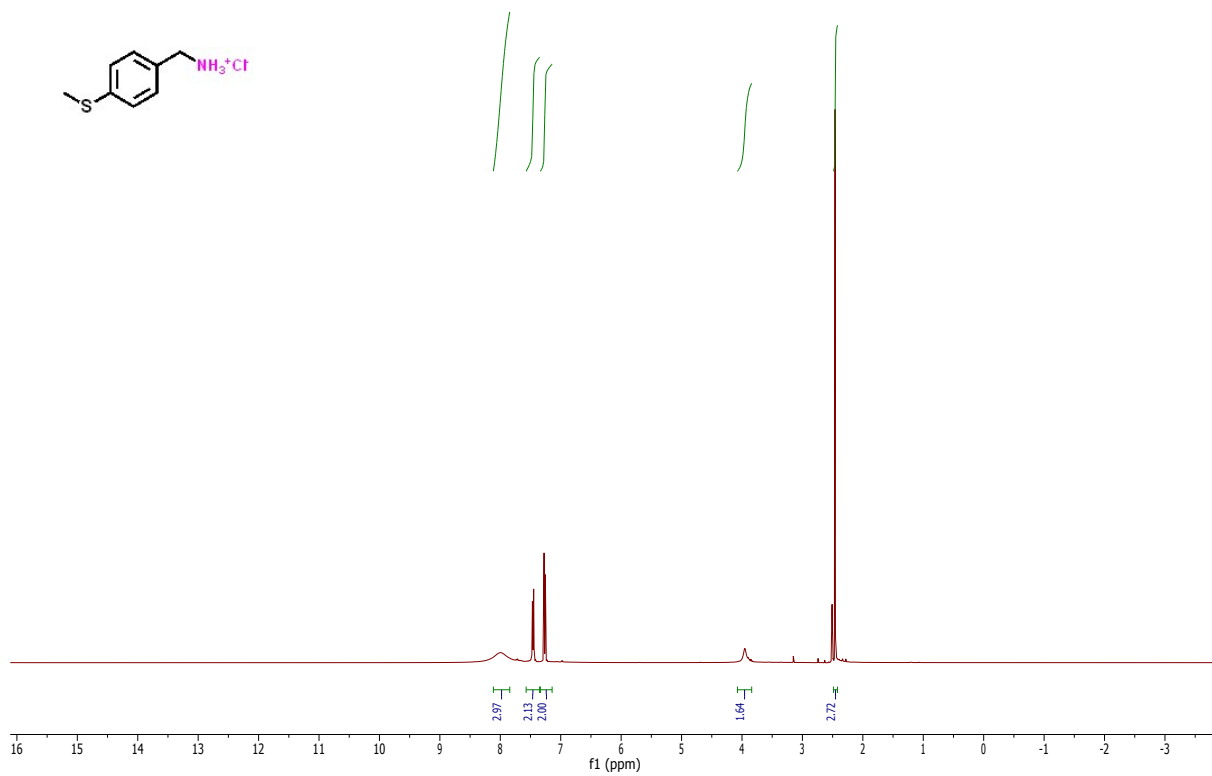
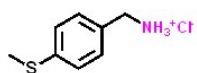
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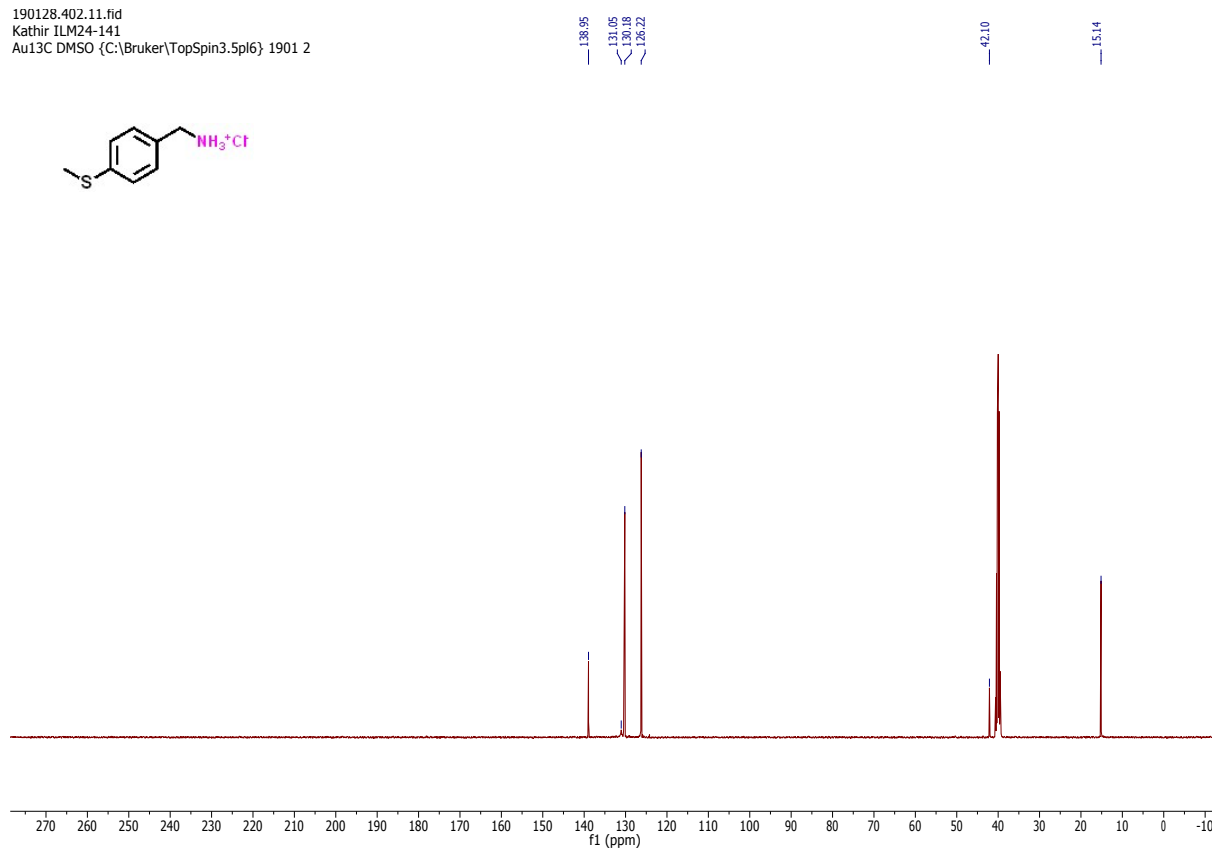
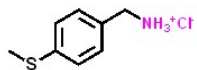
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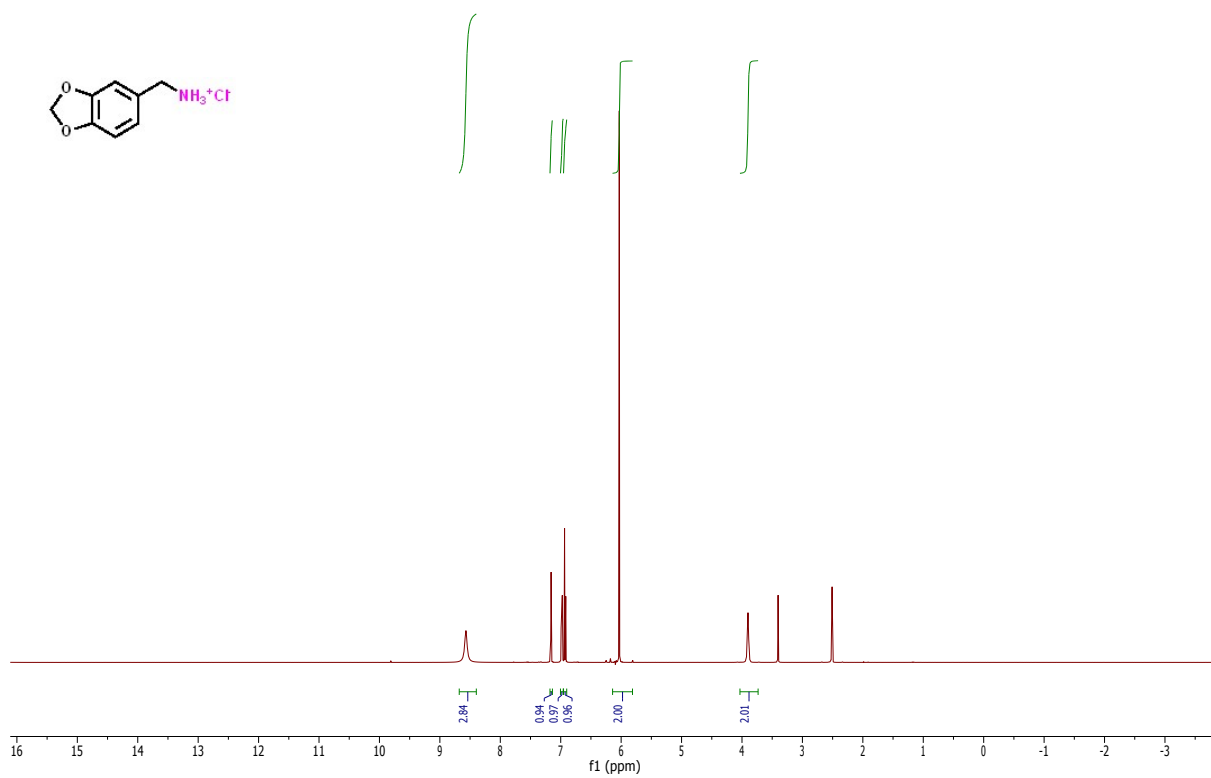
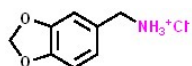
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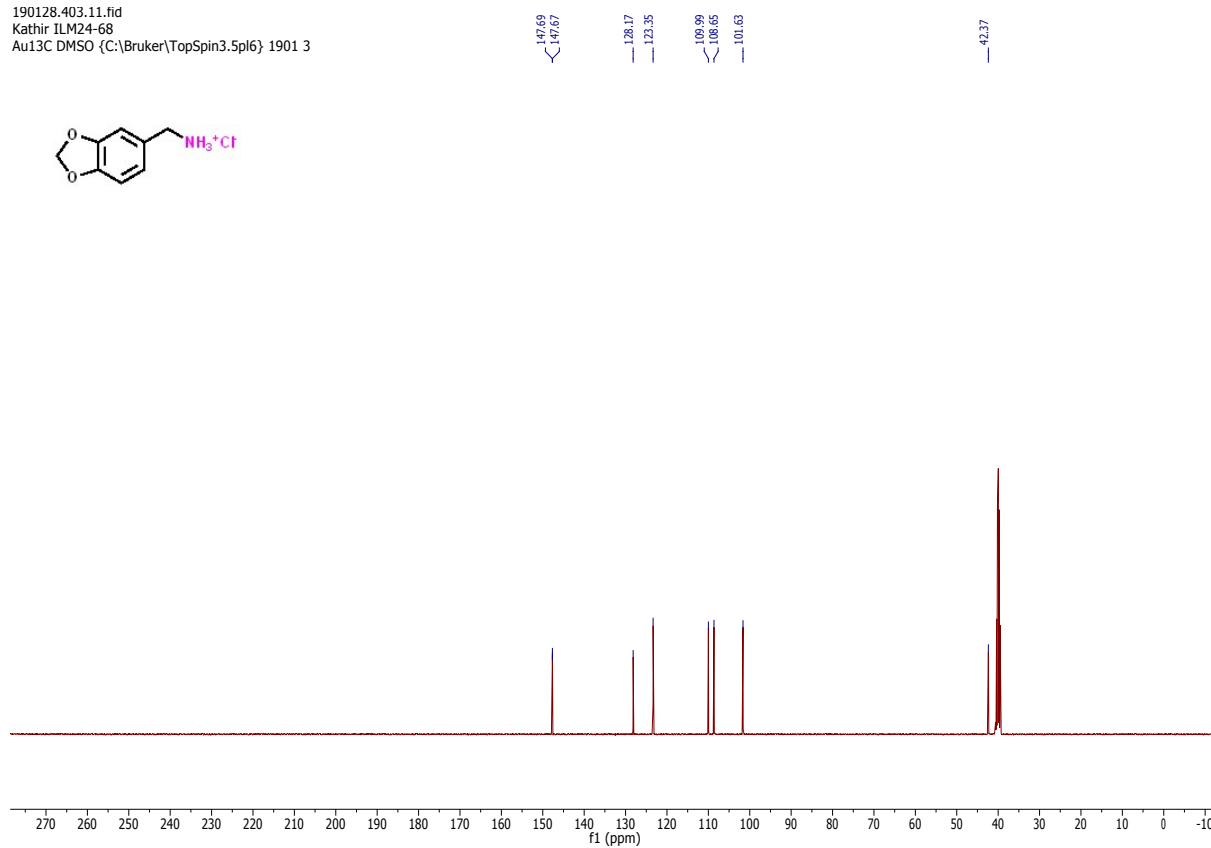
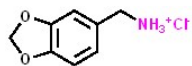
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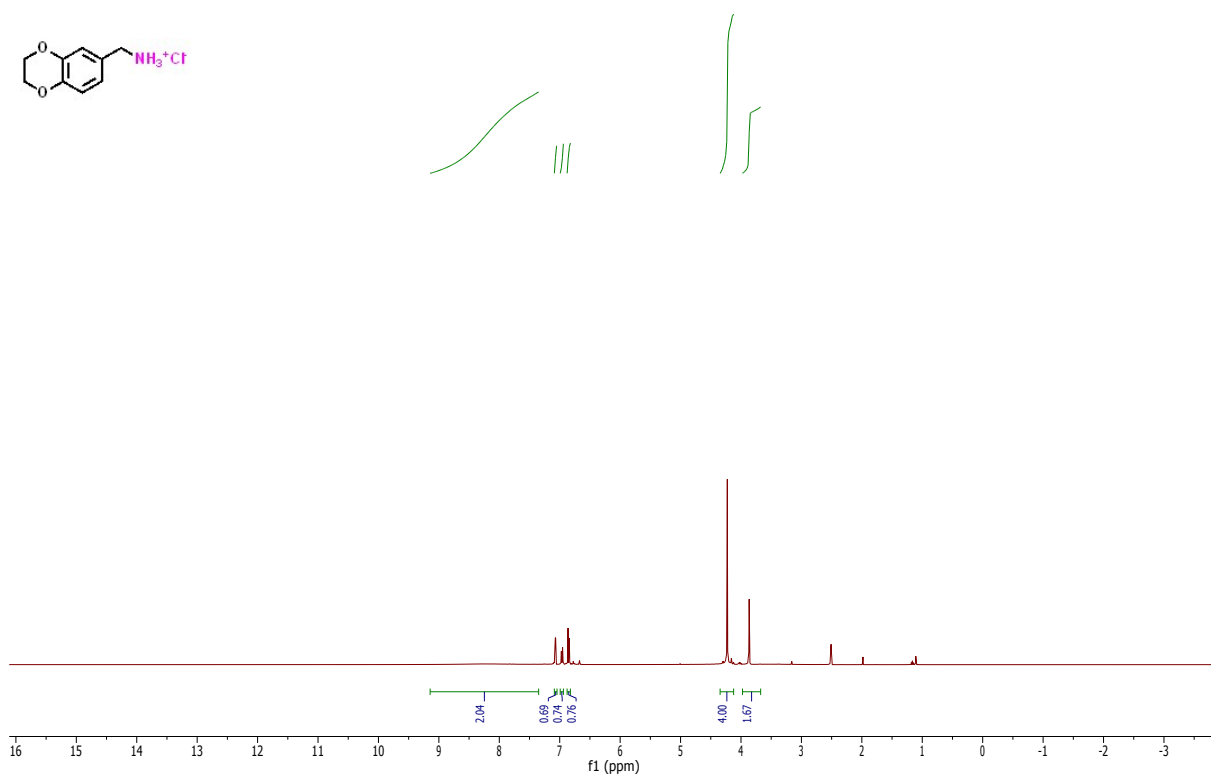
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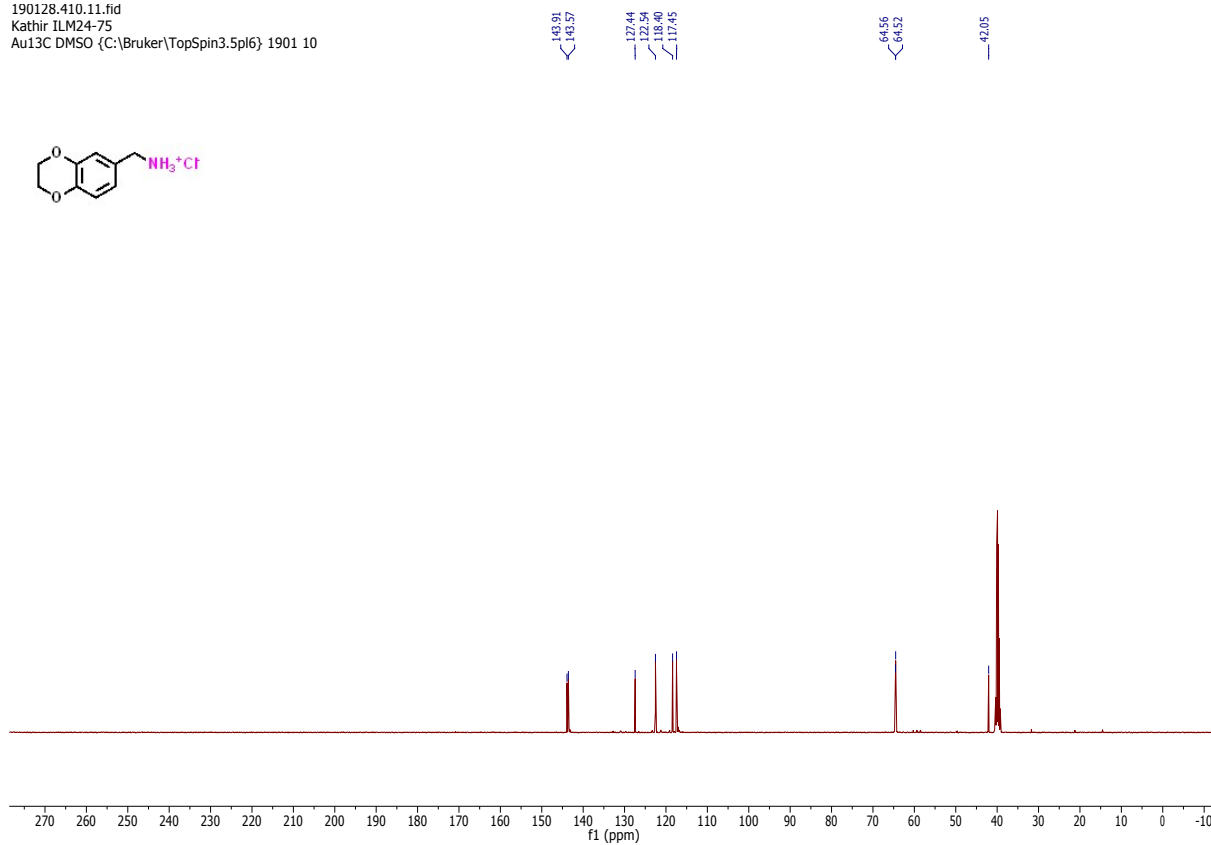
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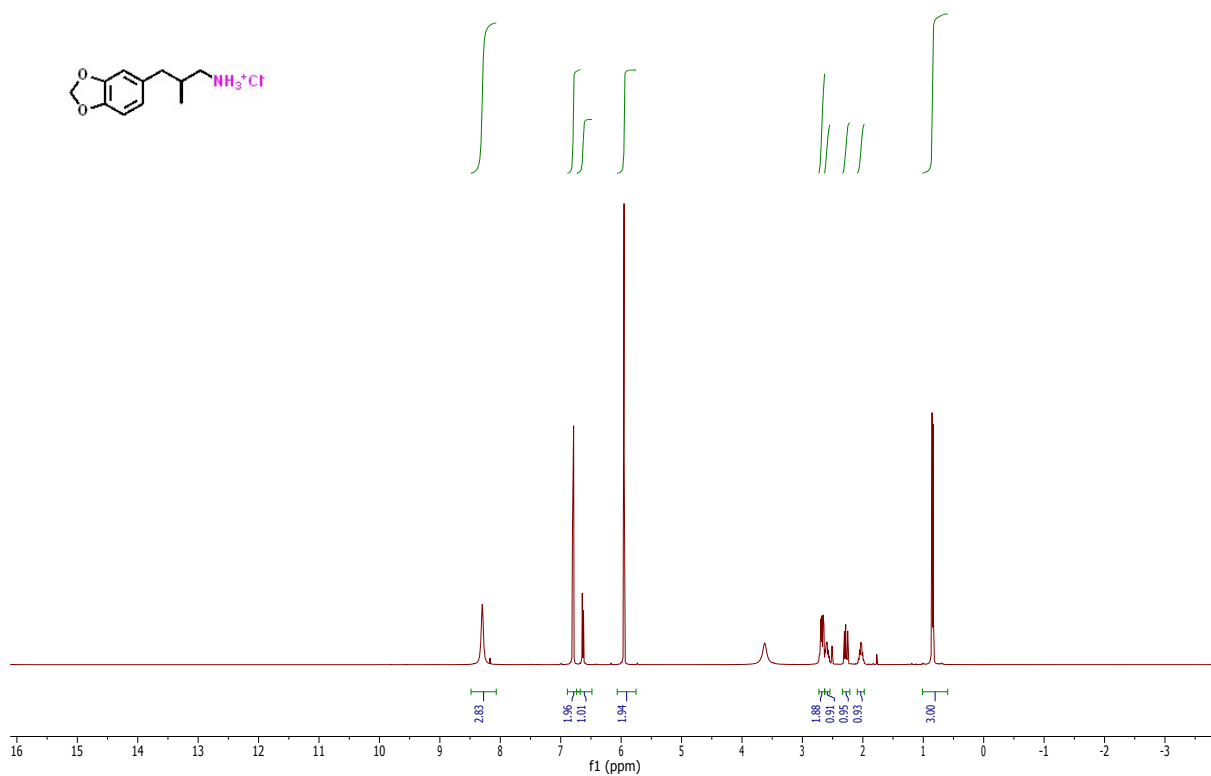
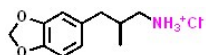
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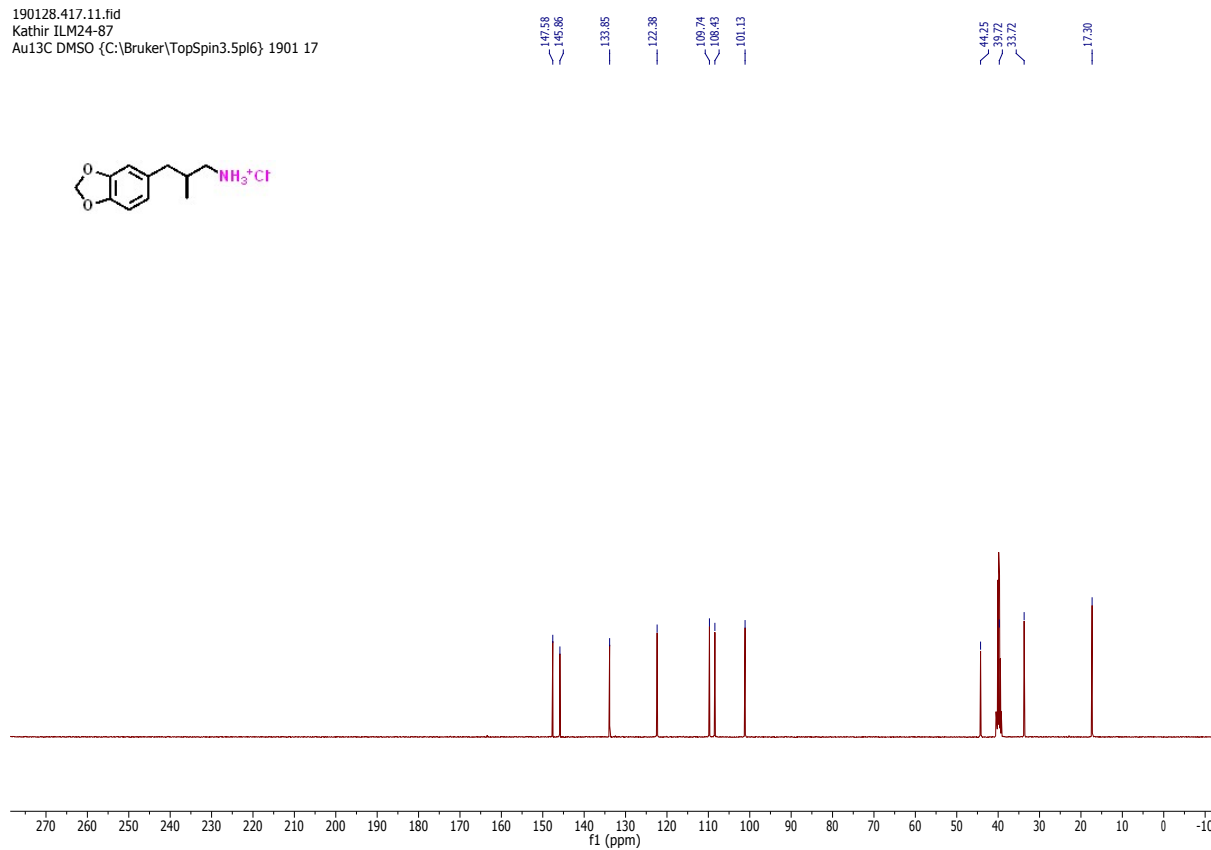
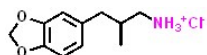
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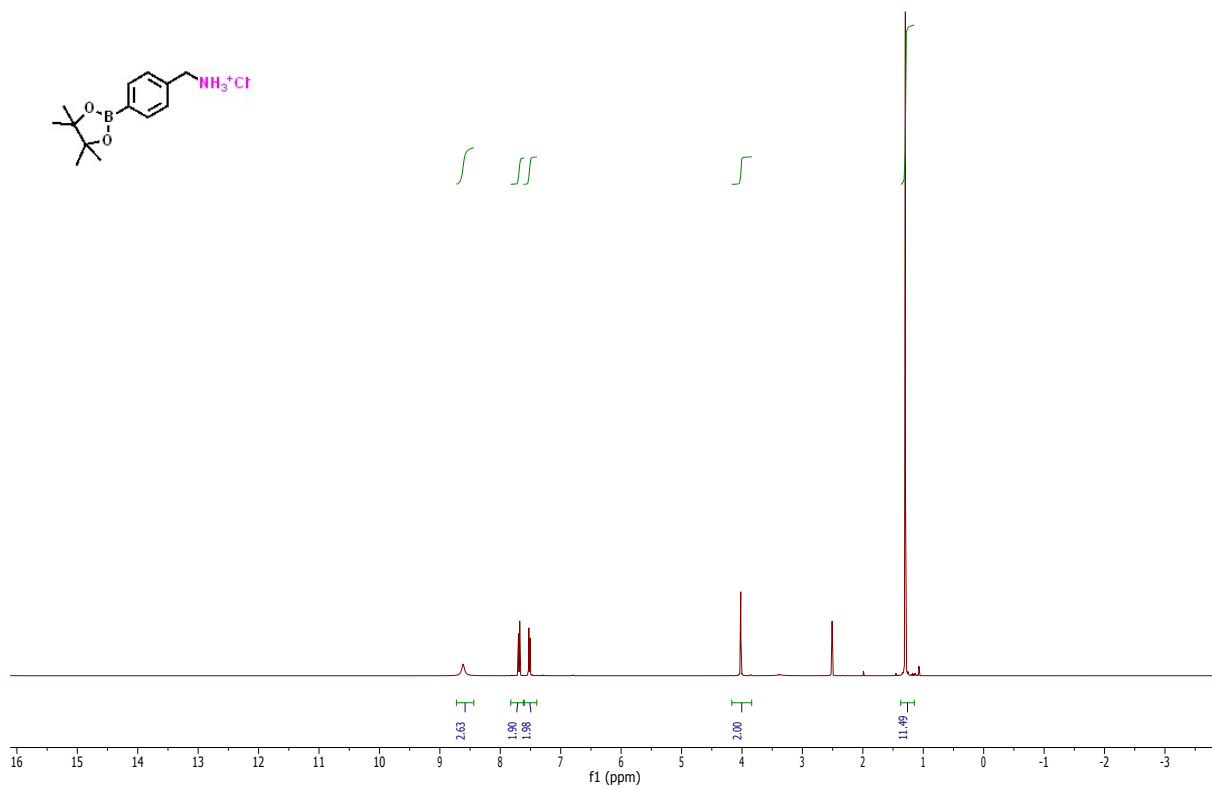
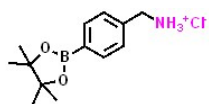
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 Kathir ILM24-87
 Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1901 17



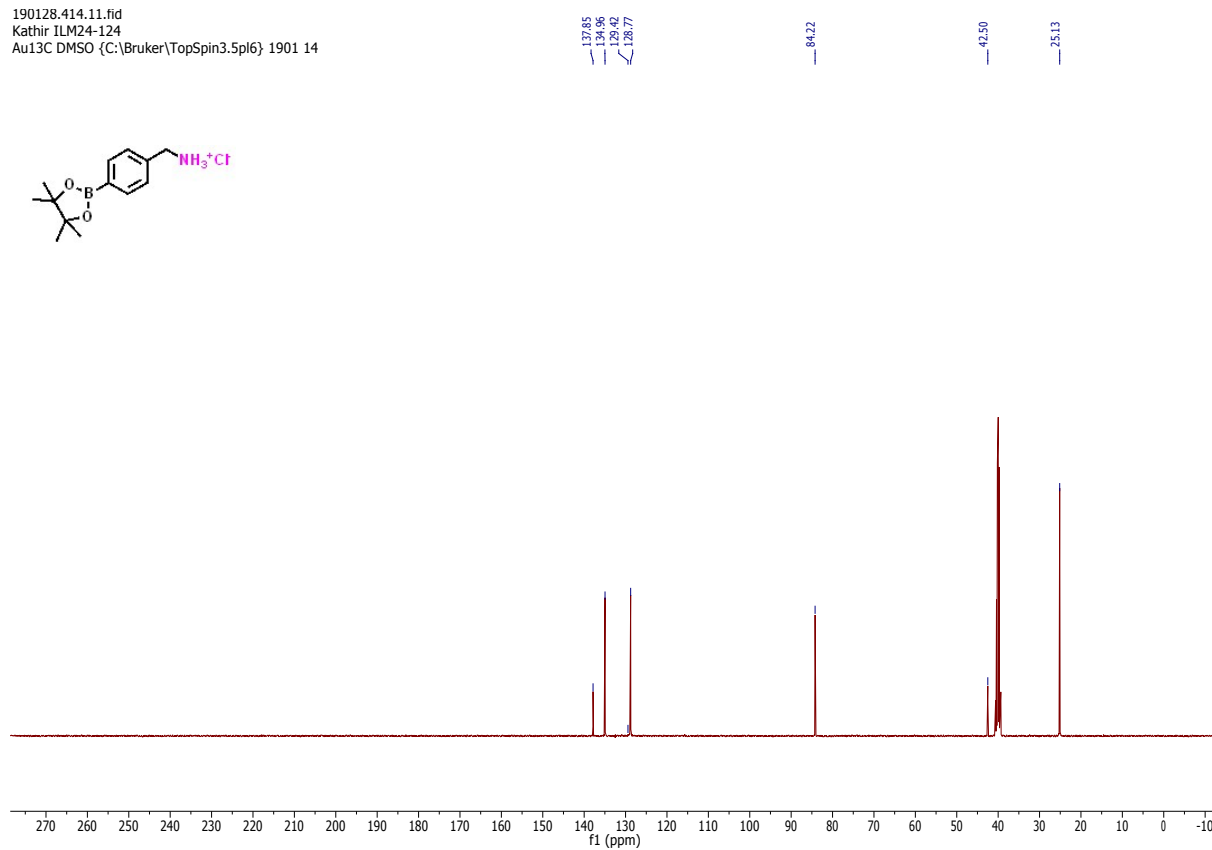
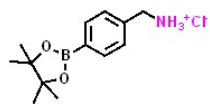
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 Kathir ILM24-87
 Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1901 17



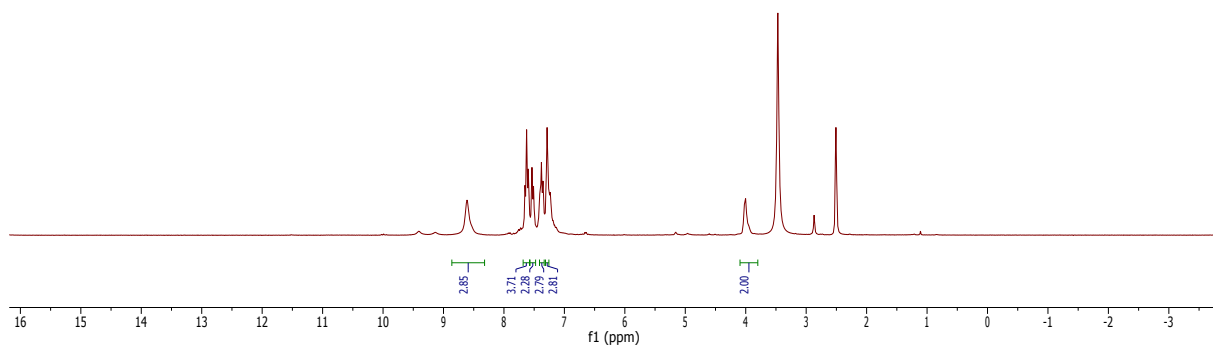
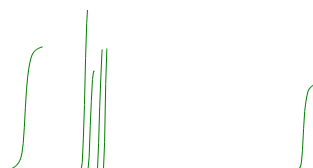
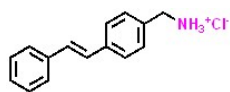
190128.414.10.fid
Kathir ILM24-124
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1901 14



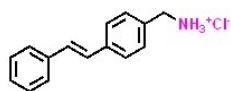
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Kathir ILM24-124
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1901 14



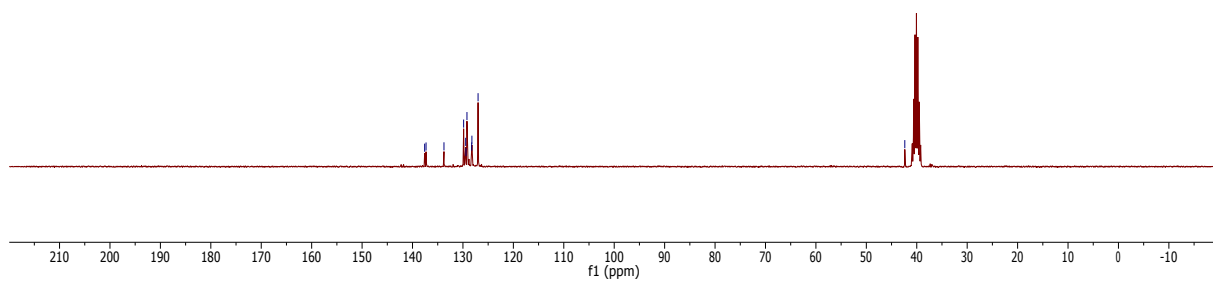
190128.f350.10.fid
 Kathir KM24-98
 PROTON DMSO {C:\Bruker\TopSpin3.6.0} 1901 50



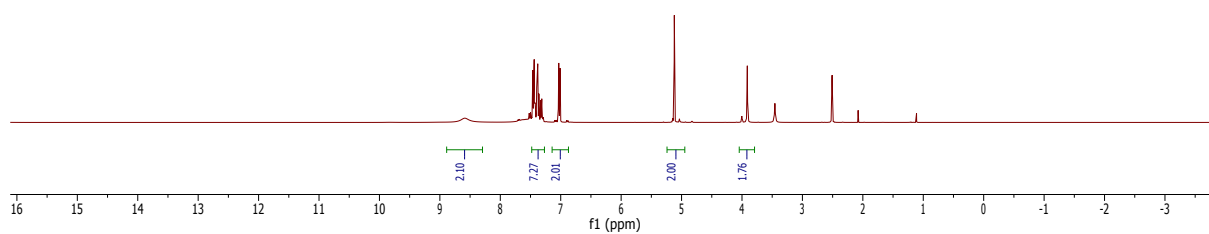
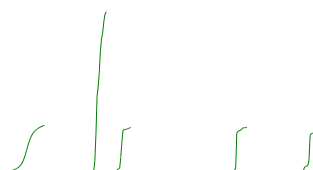
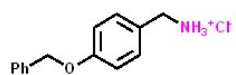
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 Kathir KM24-98
 C13CPD DMSO {C:\Bruker\TopSpin3.6.0} 1901 50



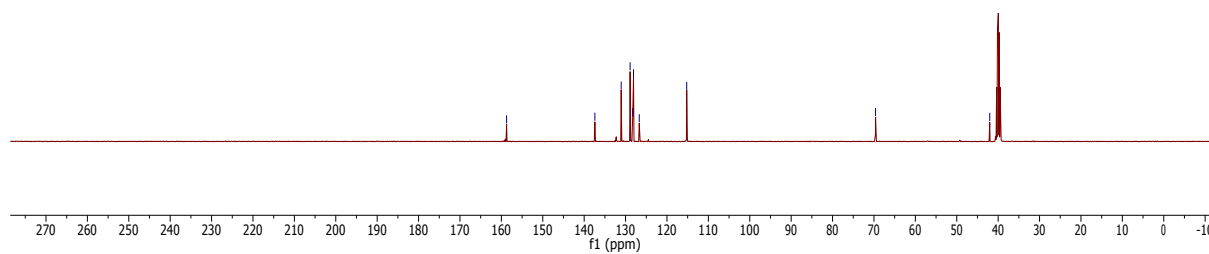
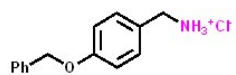
40.37



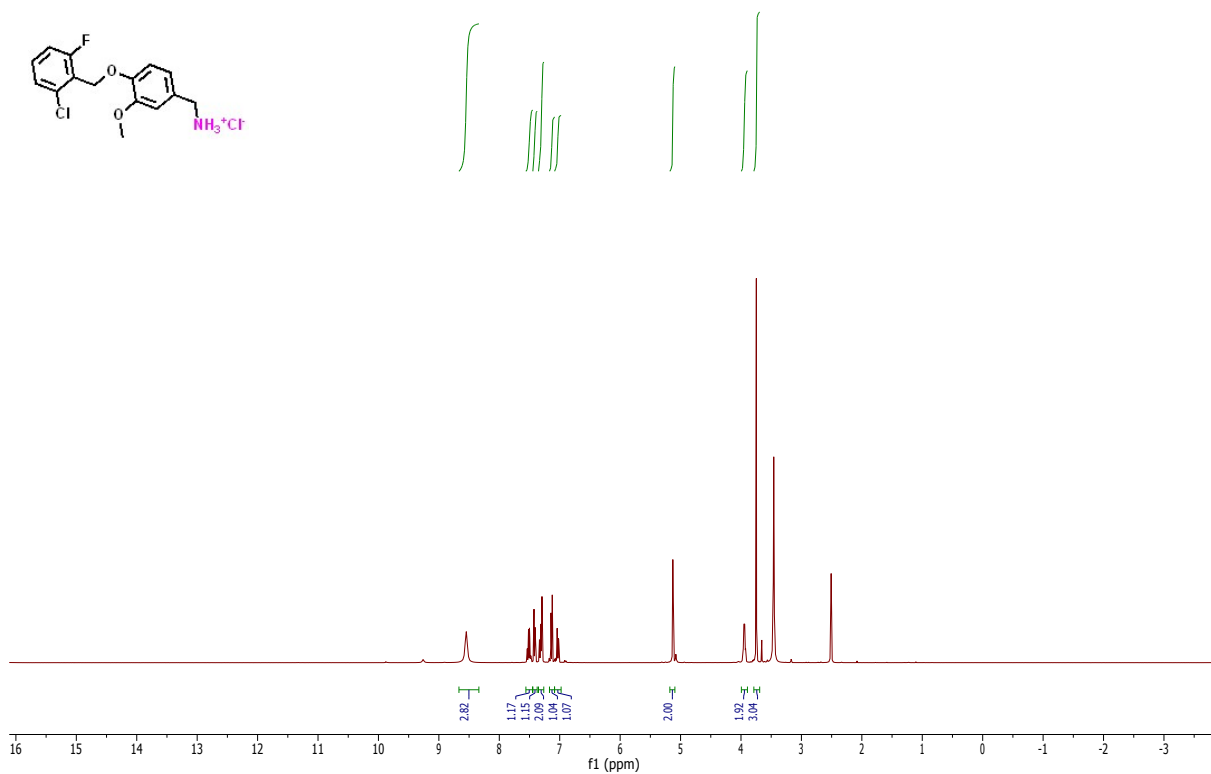
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 Kathir ILM24-126
 Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1901 15



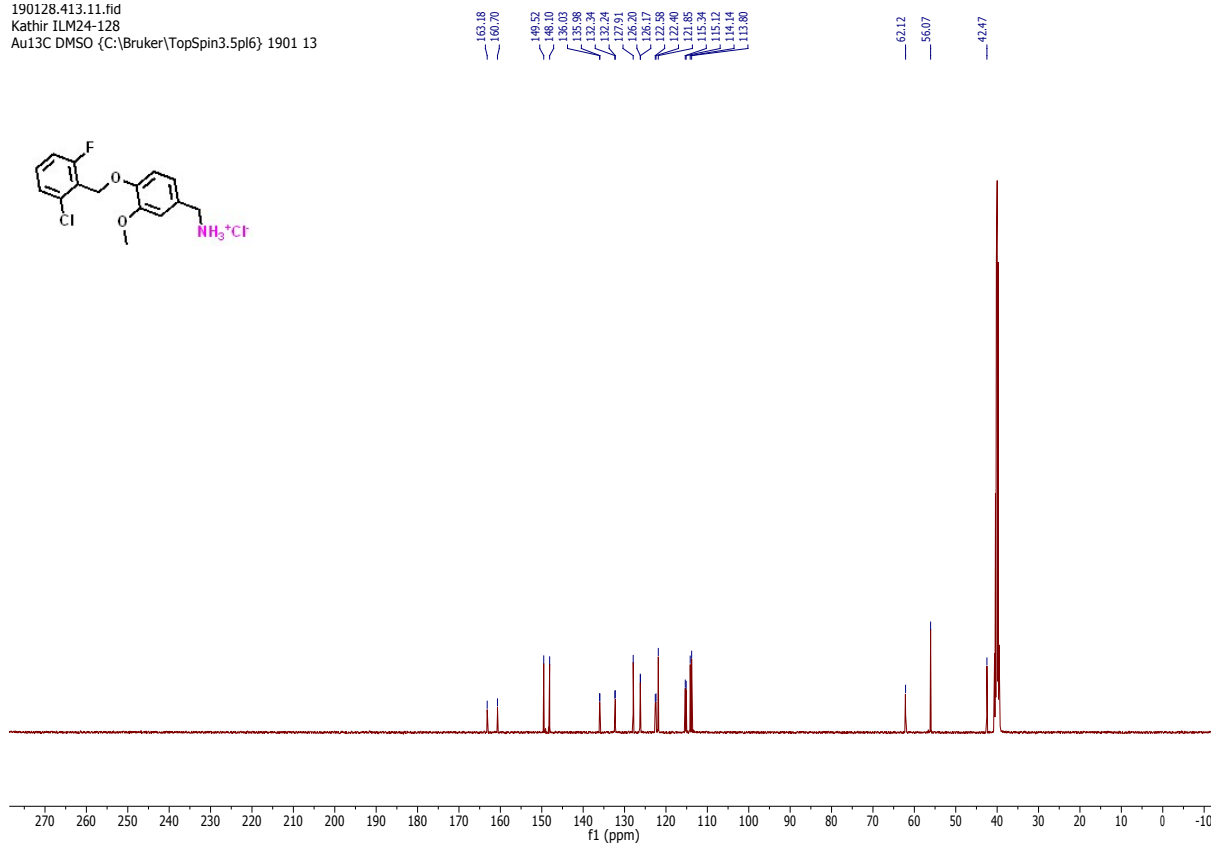
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 Kathir ILM24-126
 Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1901 15



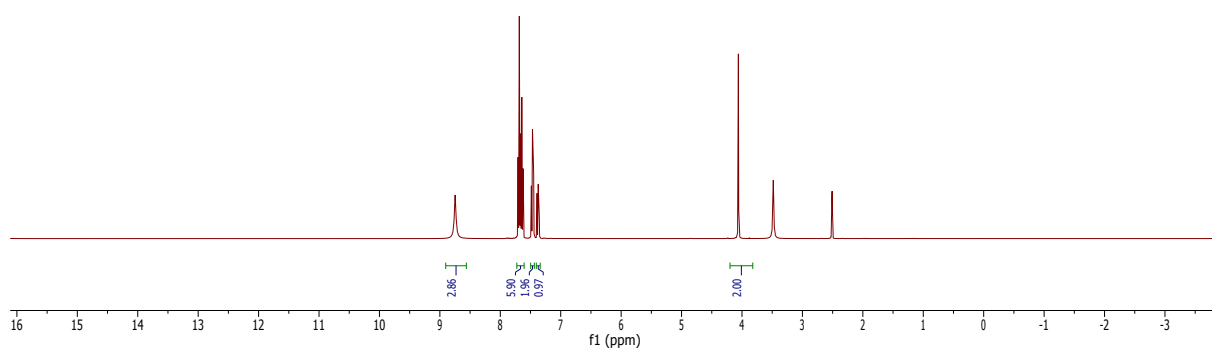
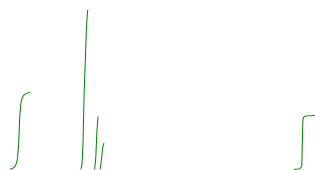
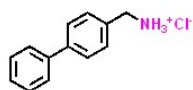
190128.413.10.fid
Kathir ILM24-128
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1901 13



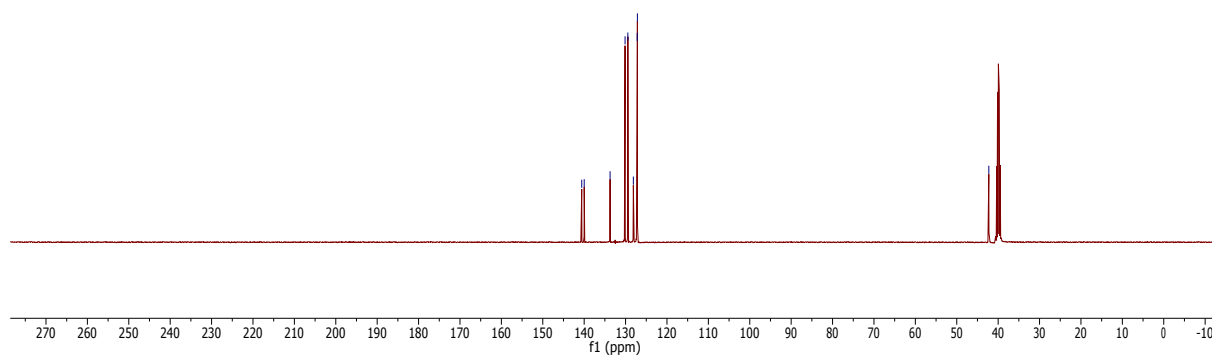
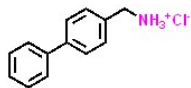
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Kathir ILM24-128
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1901 13



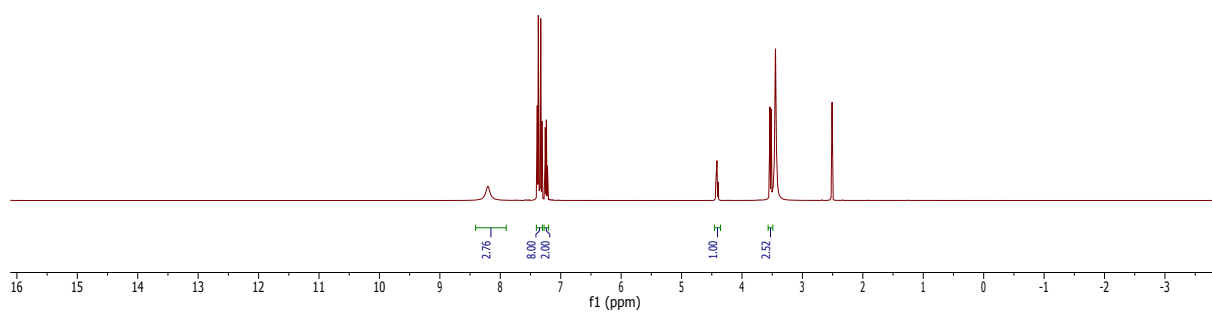
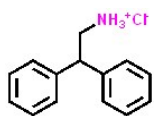
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Kathir ILM24-108
Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1901 5



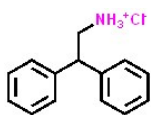
190128.405.11.fid
Kathir ILM24-108
Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1901 5



190128.416.10.fid
 Kathir ILM24-180
 Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1901 16

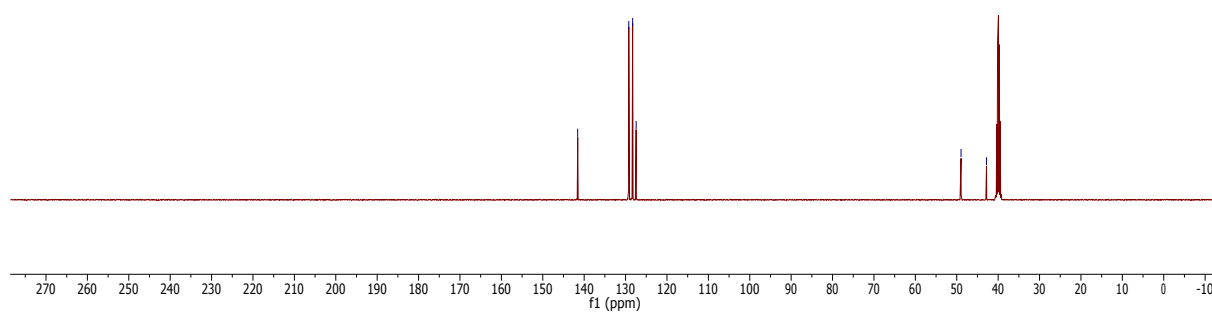


190128.416.11.fid
 Kathir ILM24-180
 Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1901 16

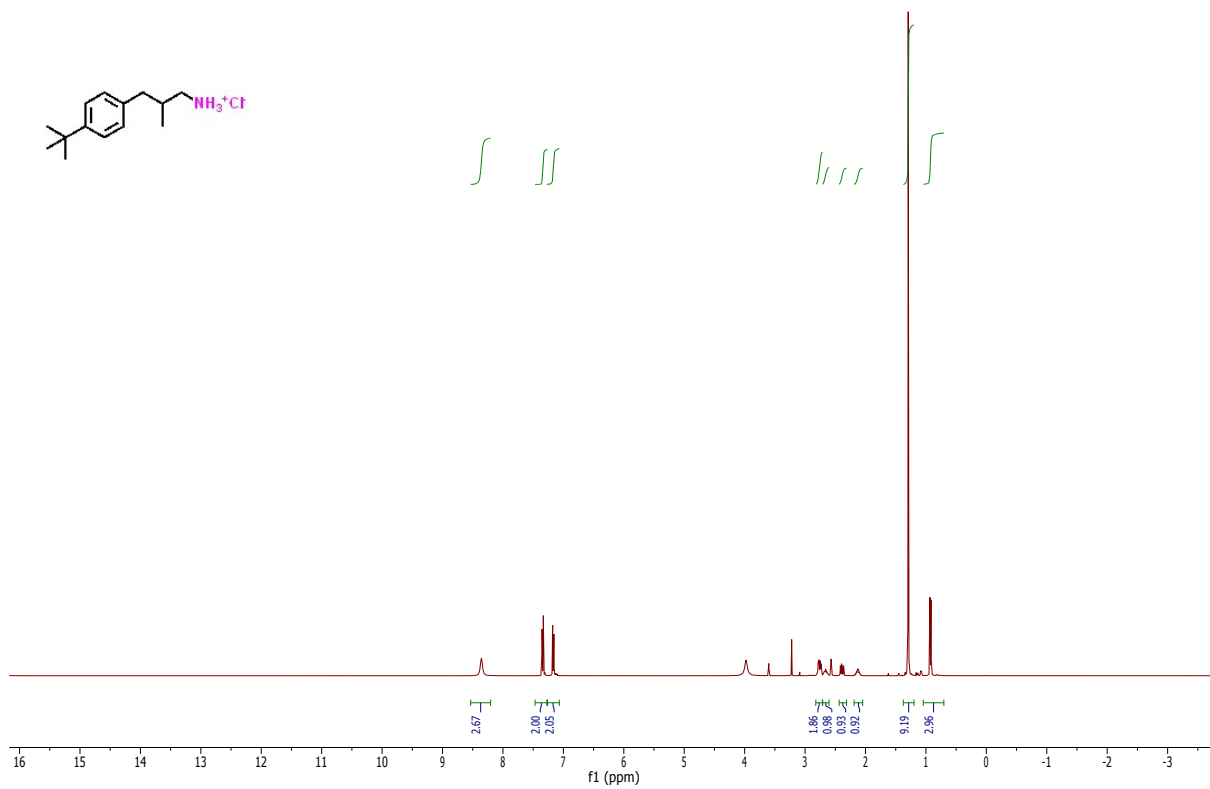


141.56
 129.22
 128.29
 127.45

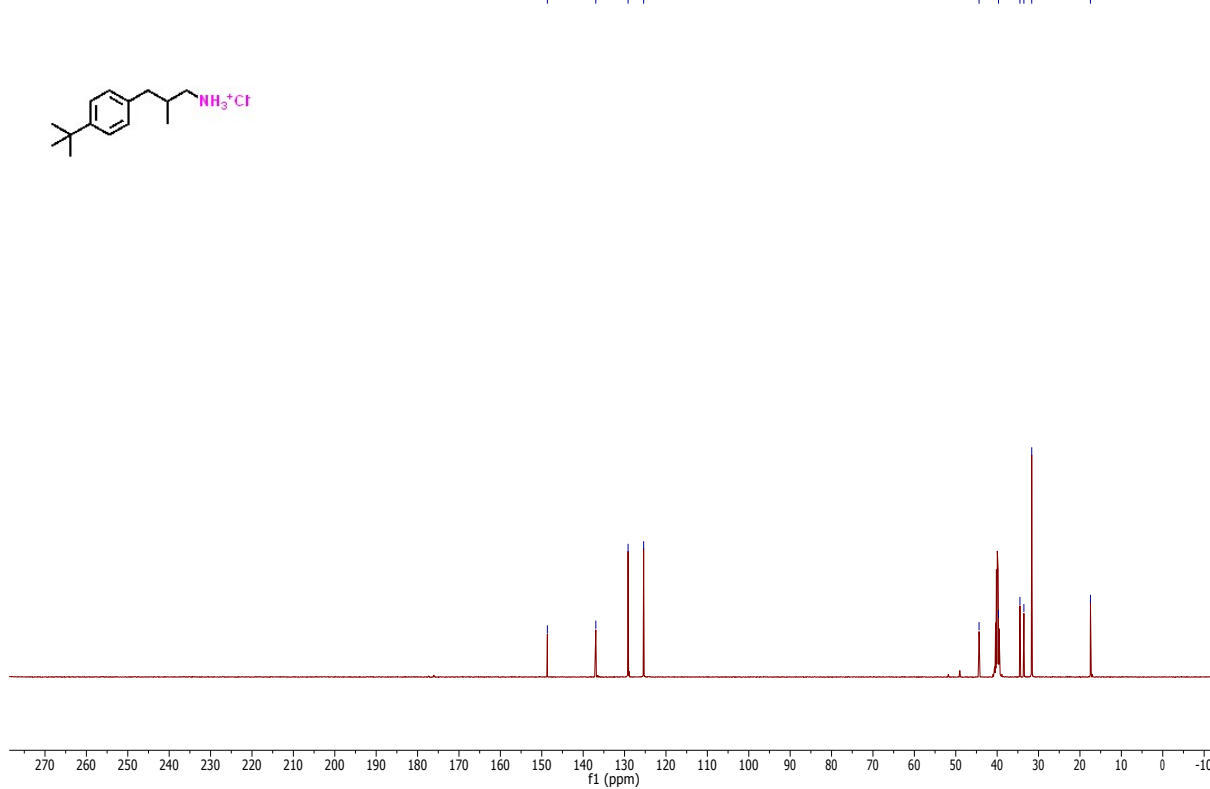
48.97
 42.82



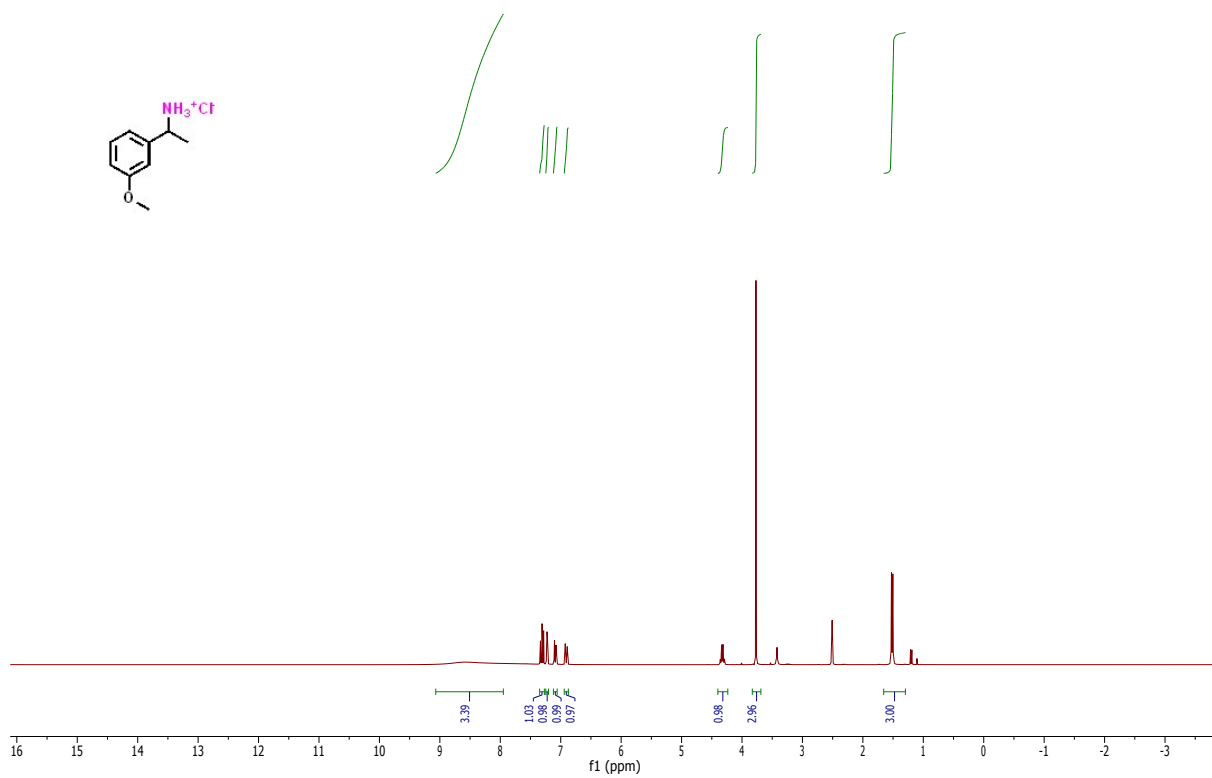
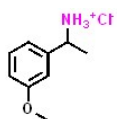
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 Kathir ILM24-100
 Au1H DMSO {C:\Bruker\TopSpin3.5pl6} 1901 12



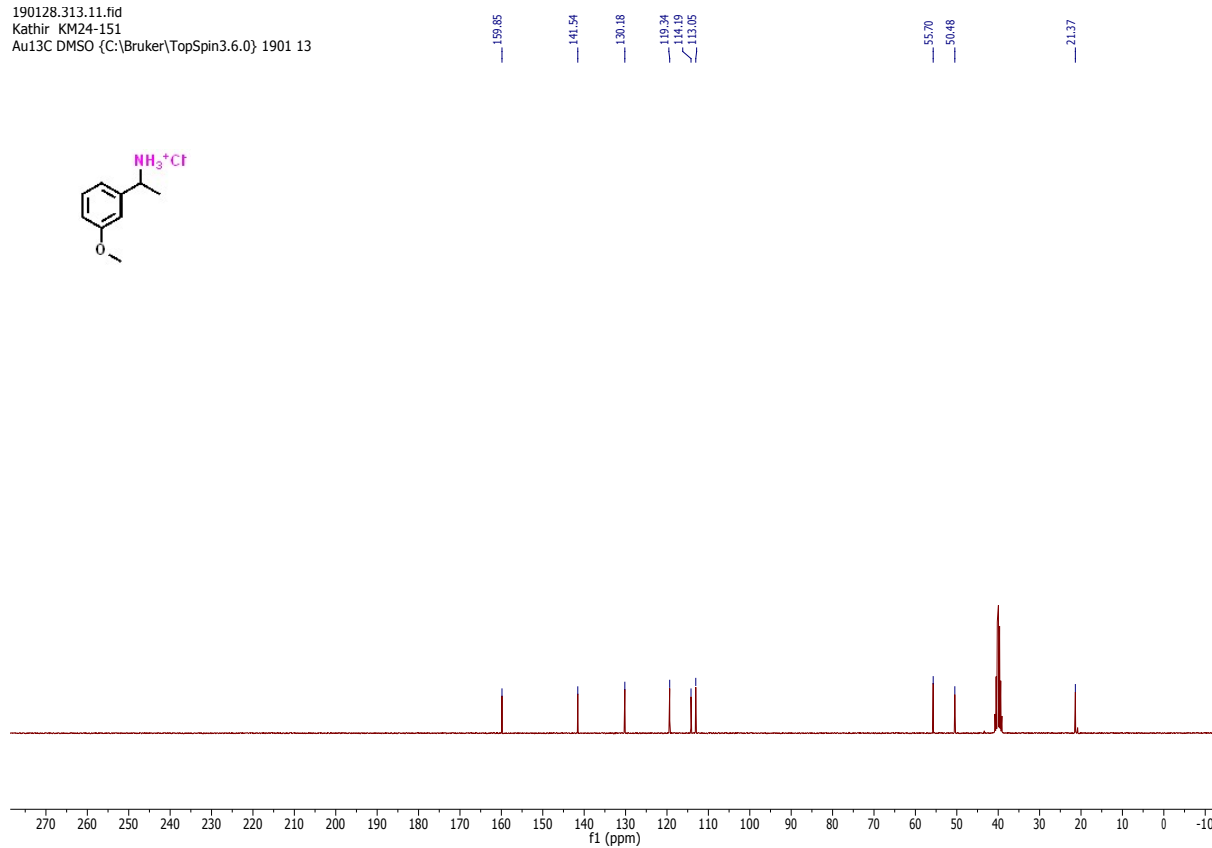
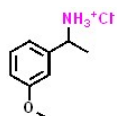
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 Kathir ILM24-100
 Au13C DMSO {C:\Bruker\TopSpin3.5pl6} 1901 12



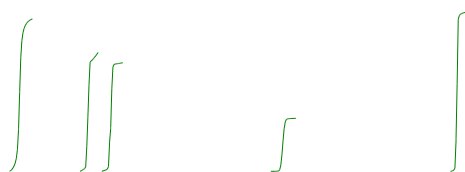
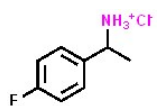
190128.313.10.fid
 Kathir KM24-151
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 13



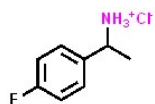
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 Kathir KM24-151
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 13



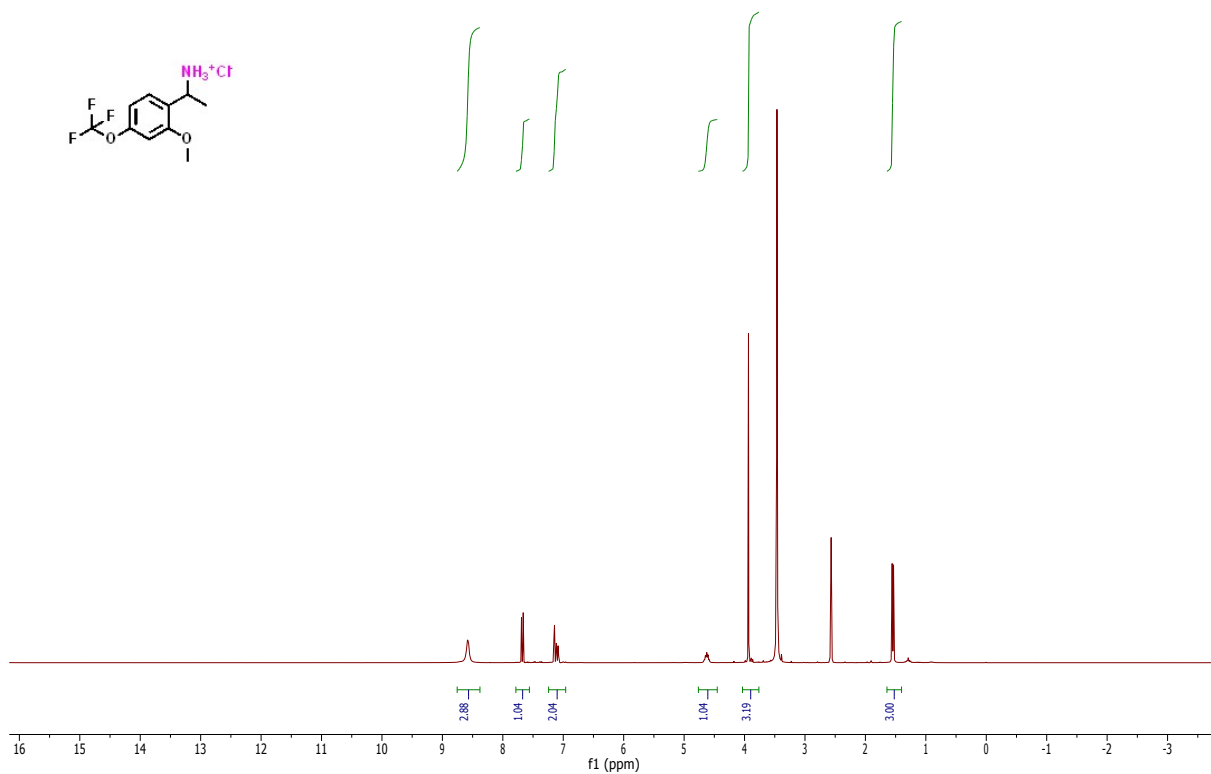
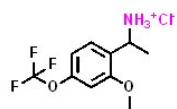
190128.312.10.fid
 Kathir KM24-150
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 12



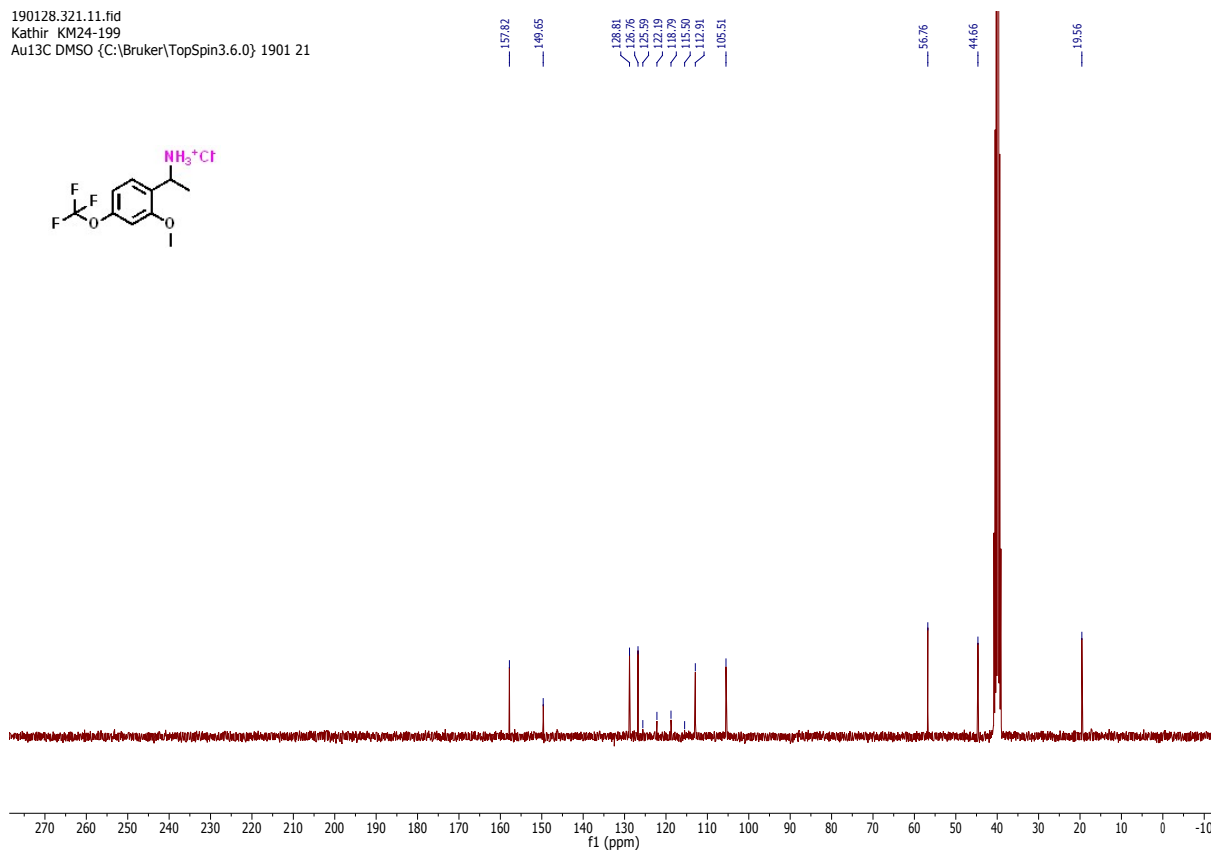
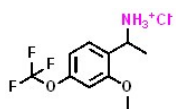
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 Kathir KM24-150
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 12



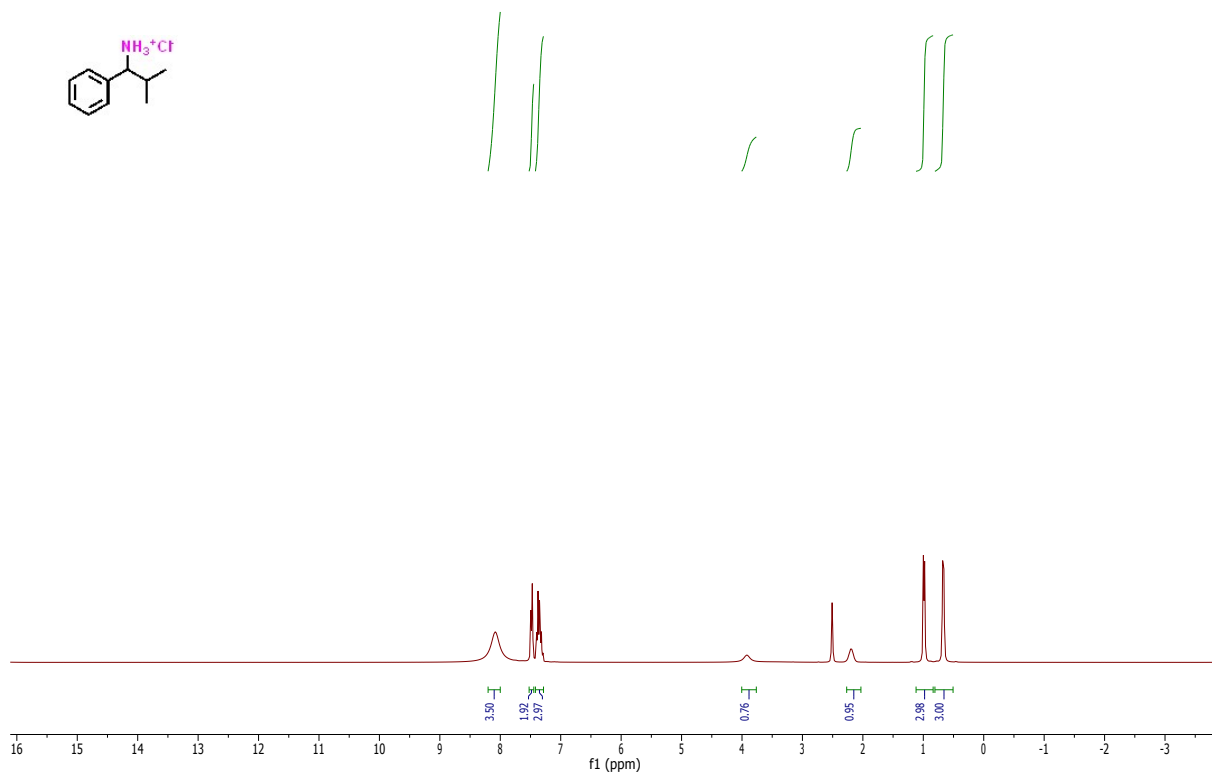
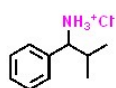
190128.321.10.fid
 Kathir KM24-199
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 21



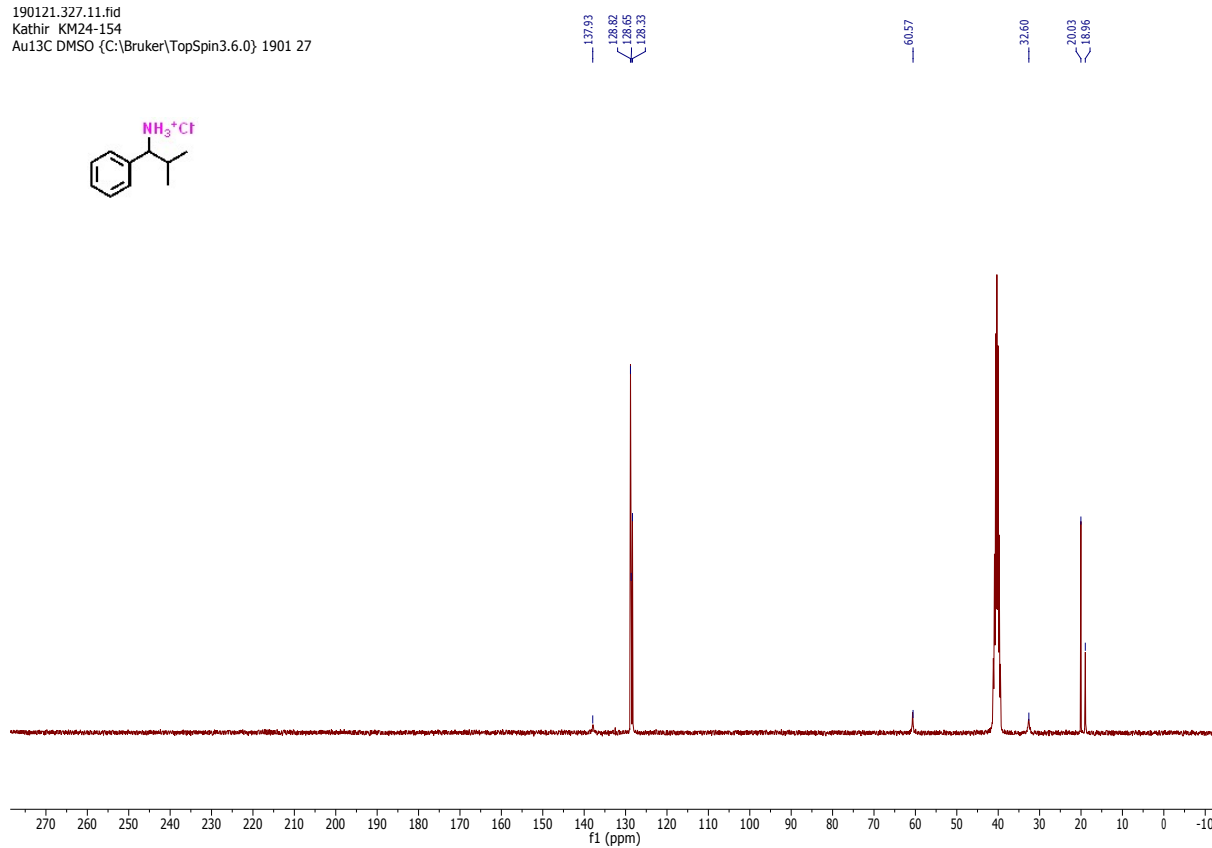
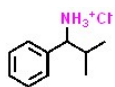
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 Kathir KM24-199
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 21



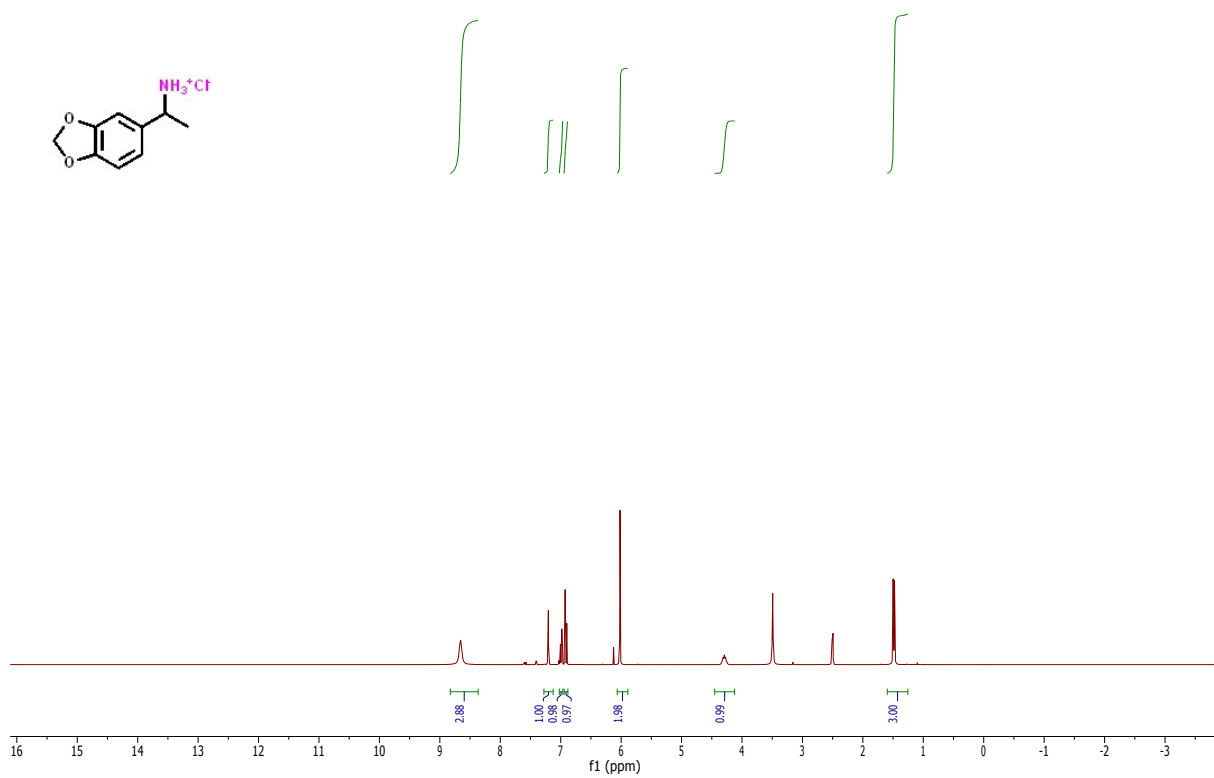
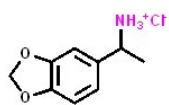
190121.327.10.fid
 Kathir KM24-154
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 27



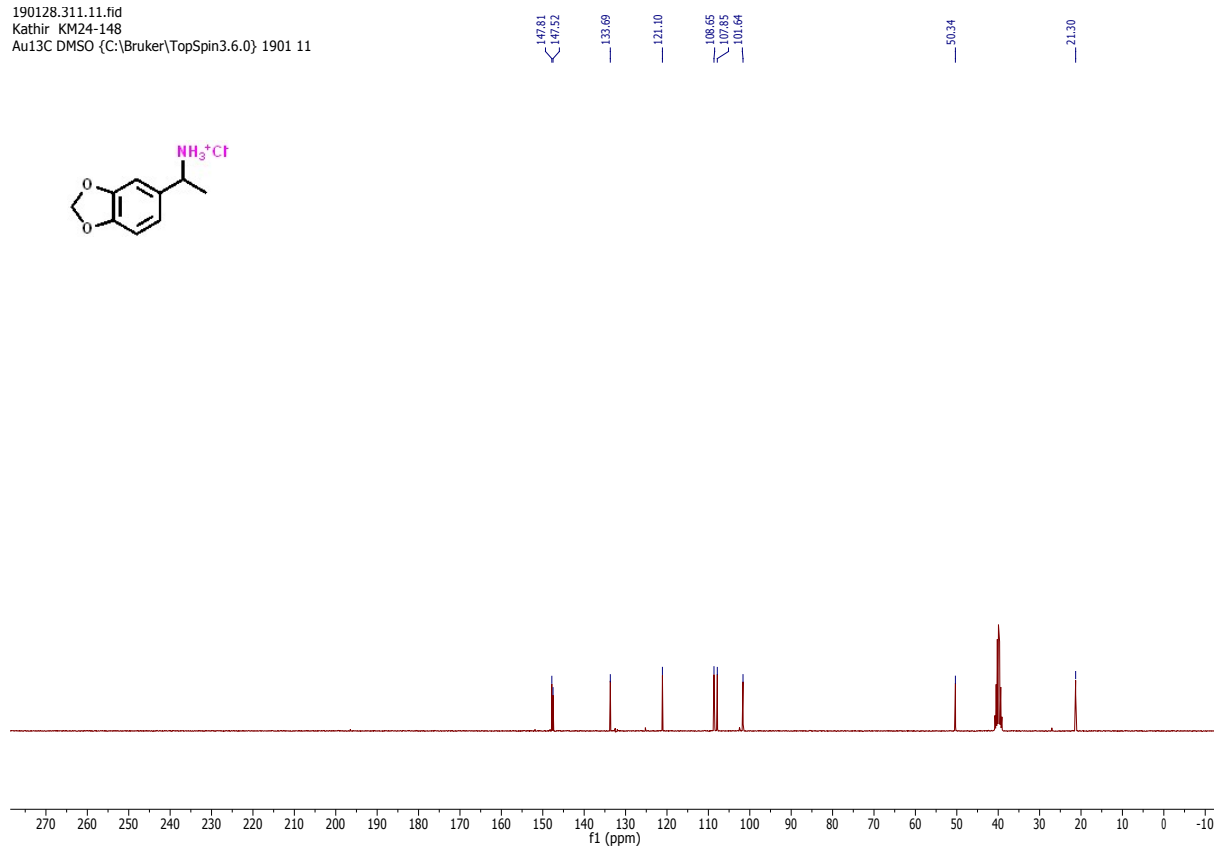
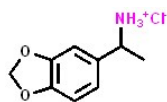
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 Kathir KM24-154
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 27



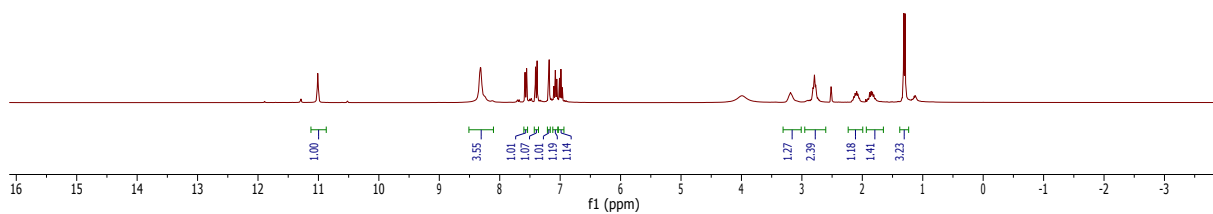
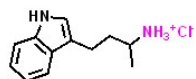
190128.311.10.fid
 Kathir KM24-148
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 11



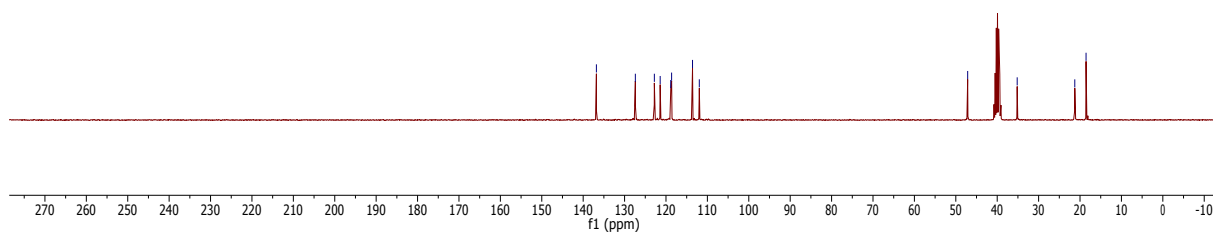
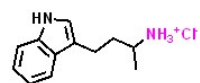
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 Kathir KM24-148
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 11



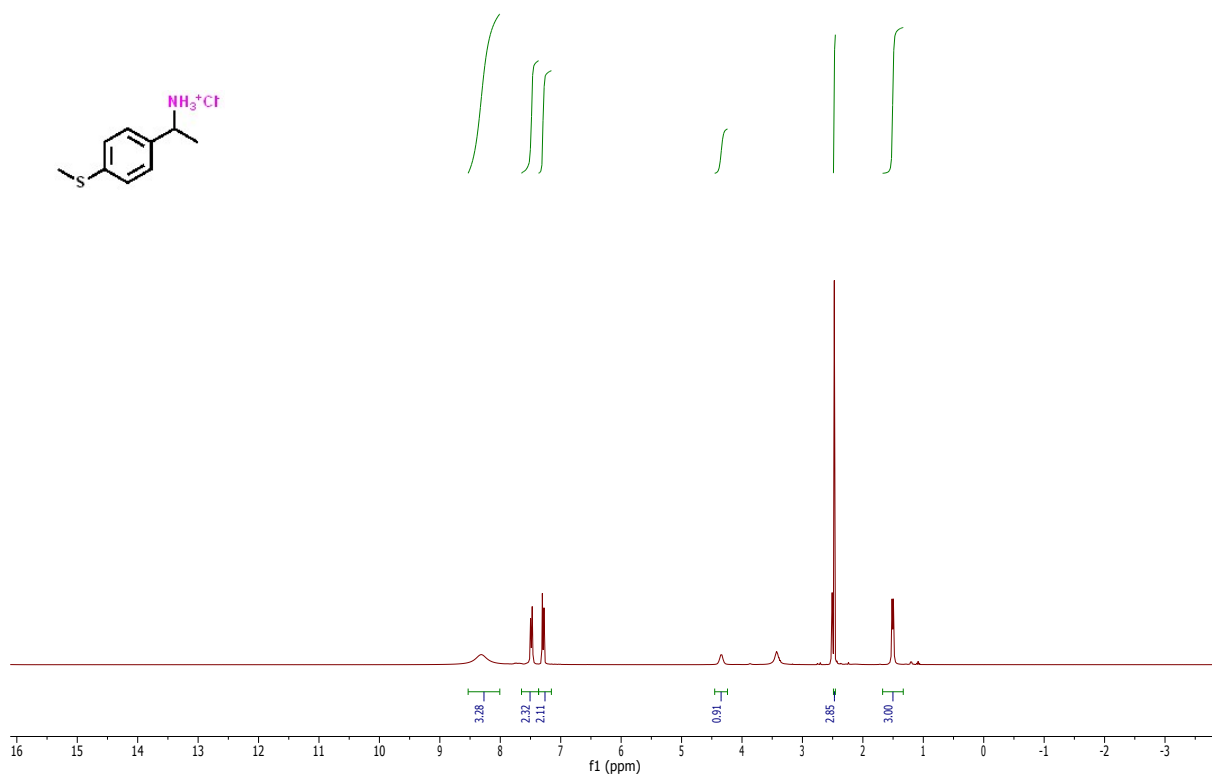
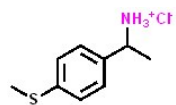
190128.324.10.fid
 Kathir KM24-206
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 24



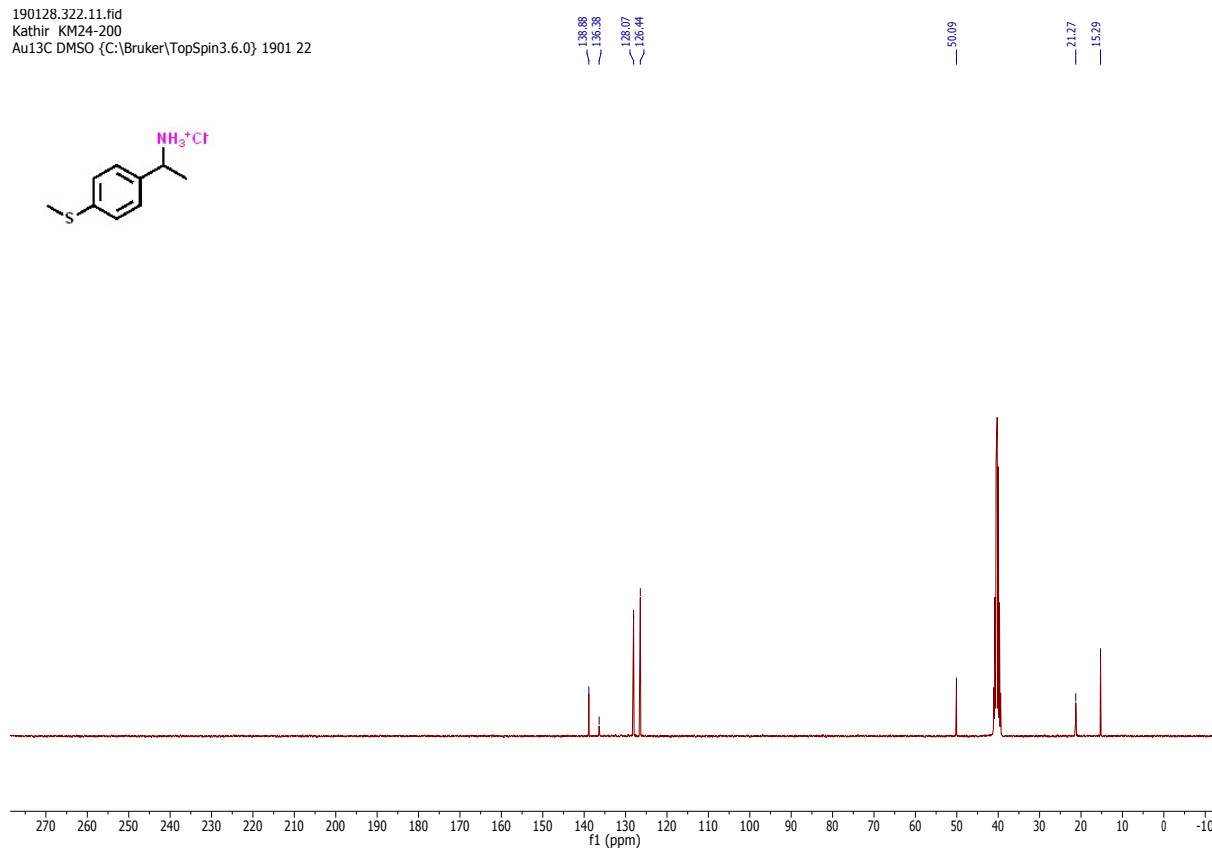
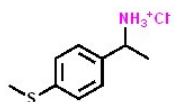
190128.324.11.fid
 Kathir KM24-206
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 24



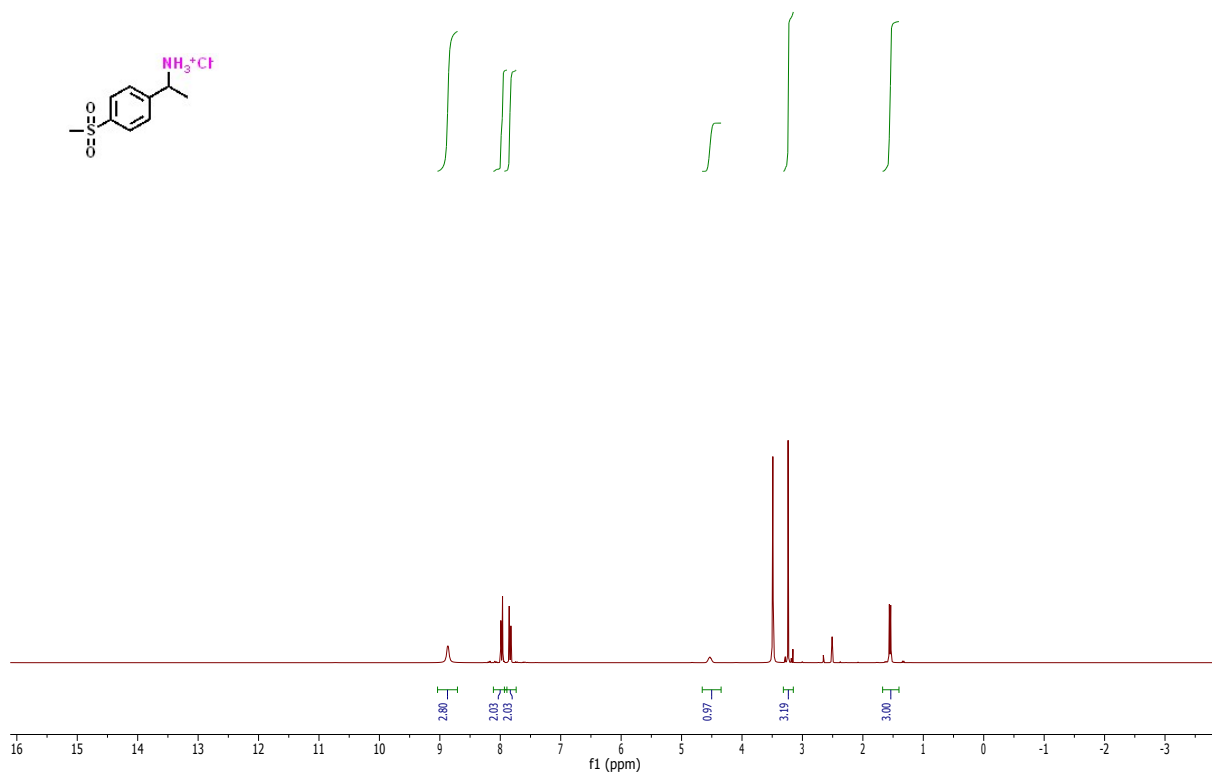
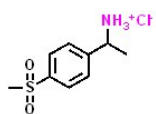
190128.322.10.fid
 Kathir KM24-200
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 22



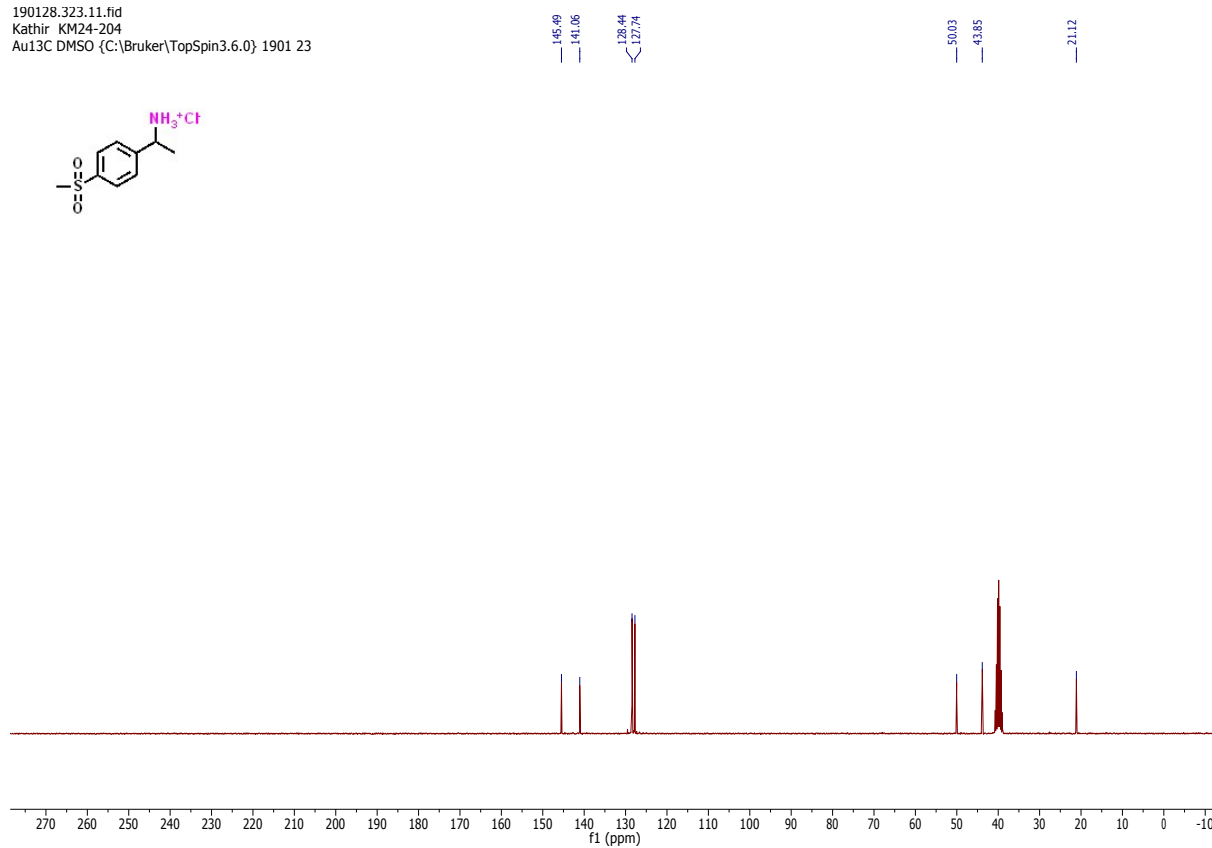
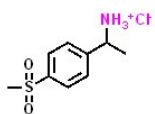
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 Kathir KM24-200
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 22



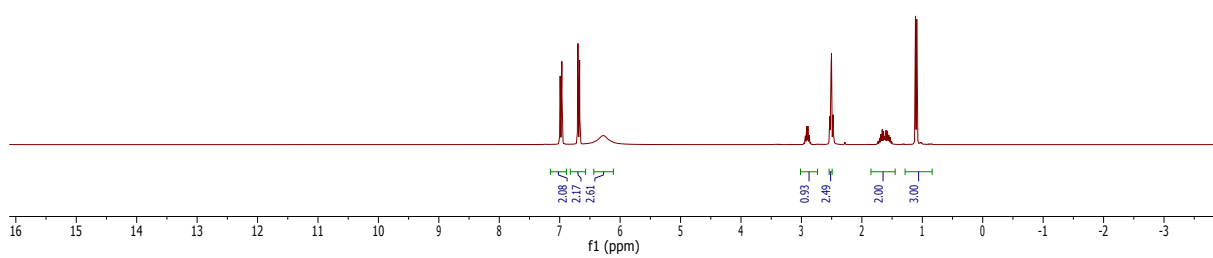
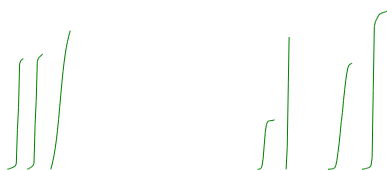
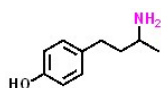
190128.323.10.fid
 Kathir KM24-204
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 23



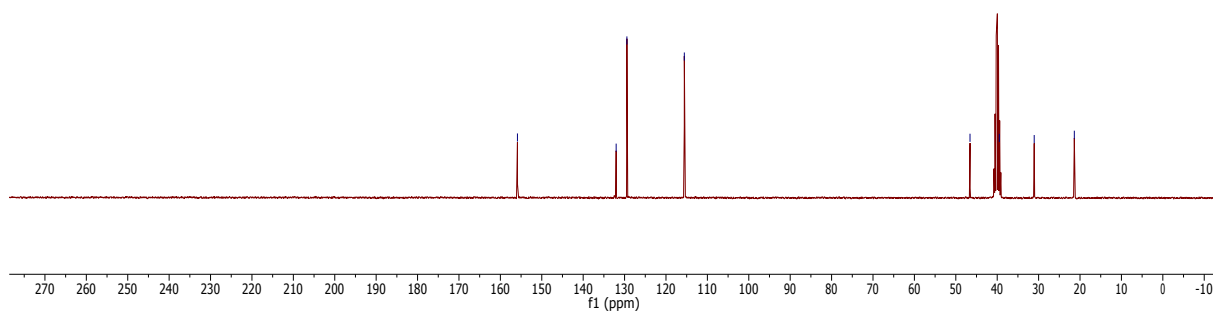
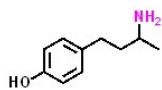
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 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 23



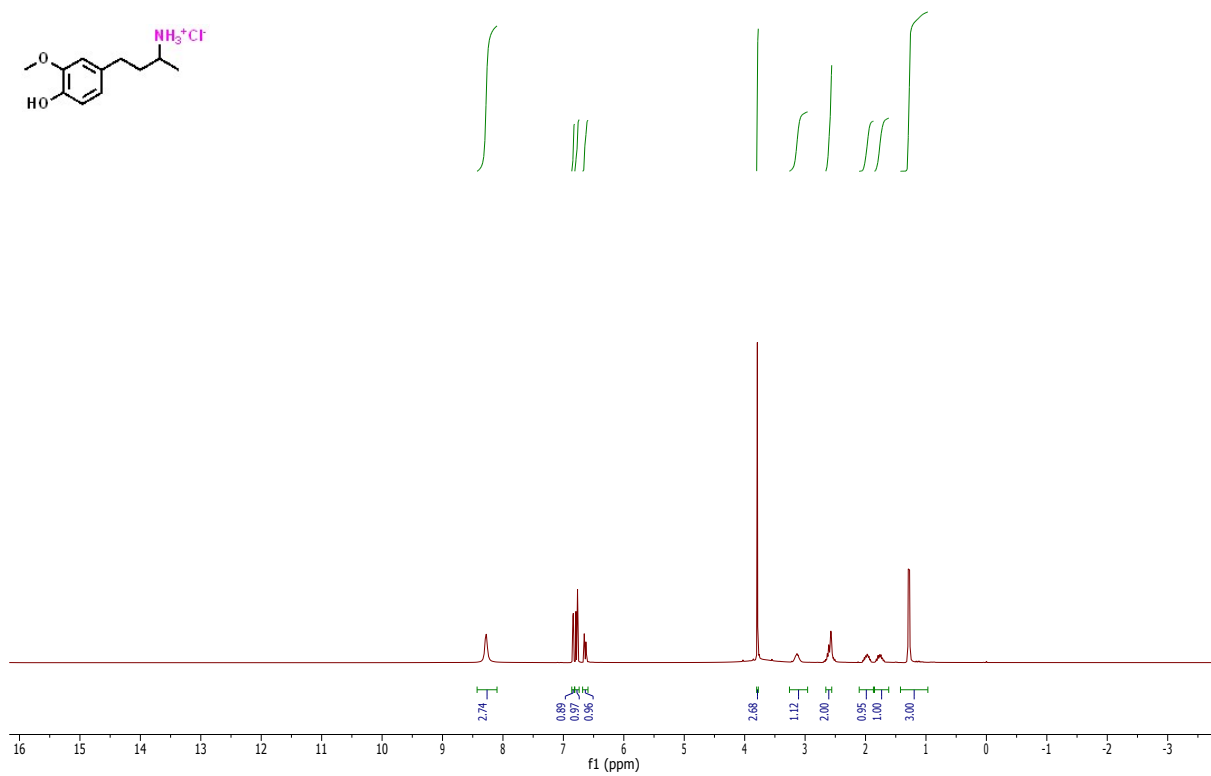
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 Kathir KM24-50
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 29



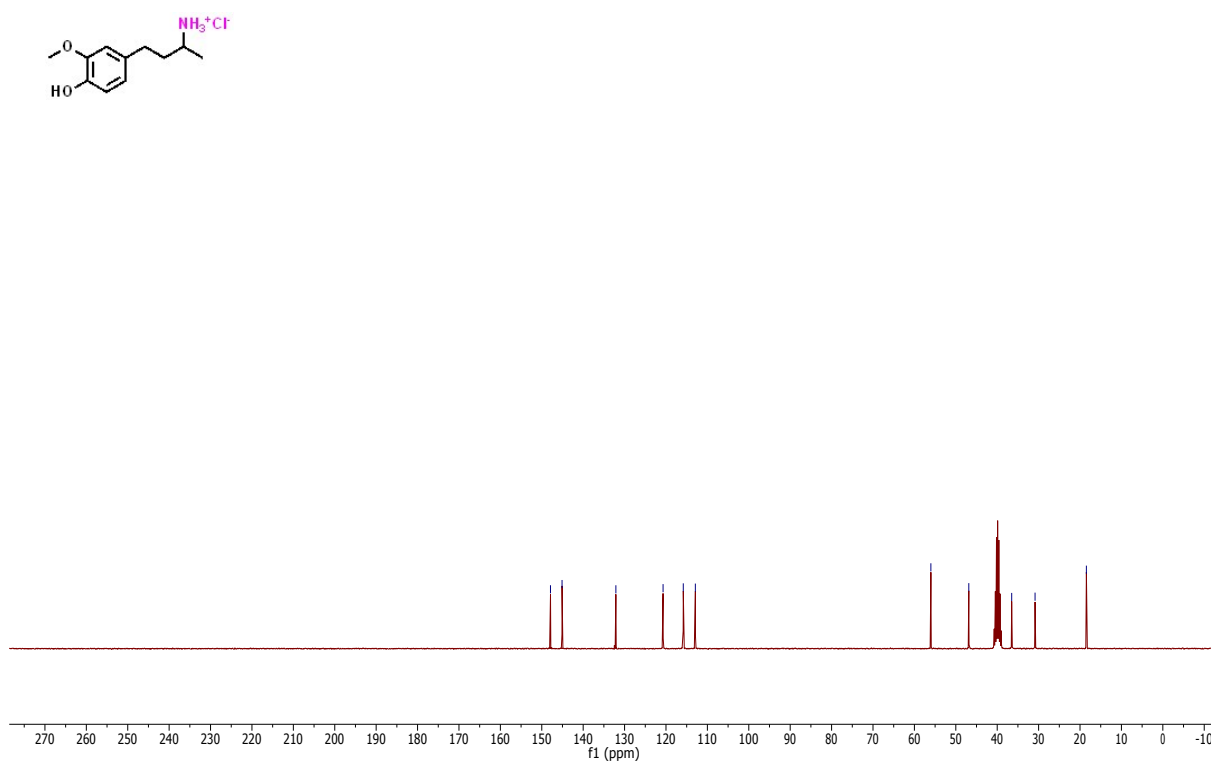
190128.329.11.fid
 Kathir KM24-50
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 29



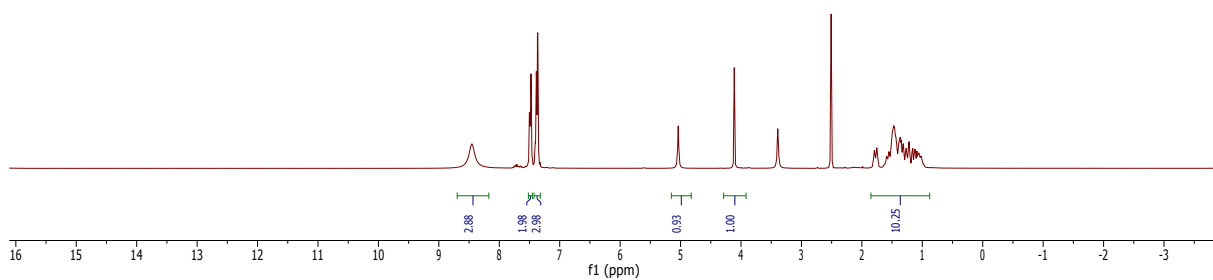
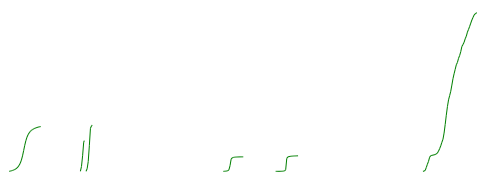
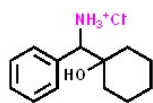
190128.326.10.fid
 Kathir KM24-209
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 26



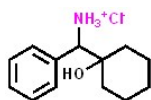
190128.326.11.fid
 Kathir KM24-209
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 26



190128.318.10.fid
 Kathir KM24-193
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 18



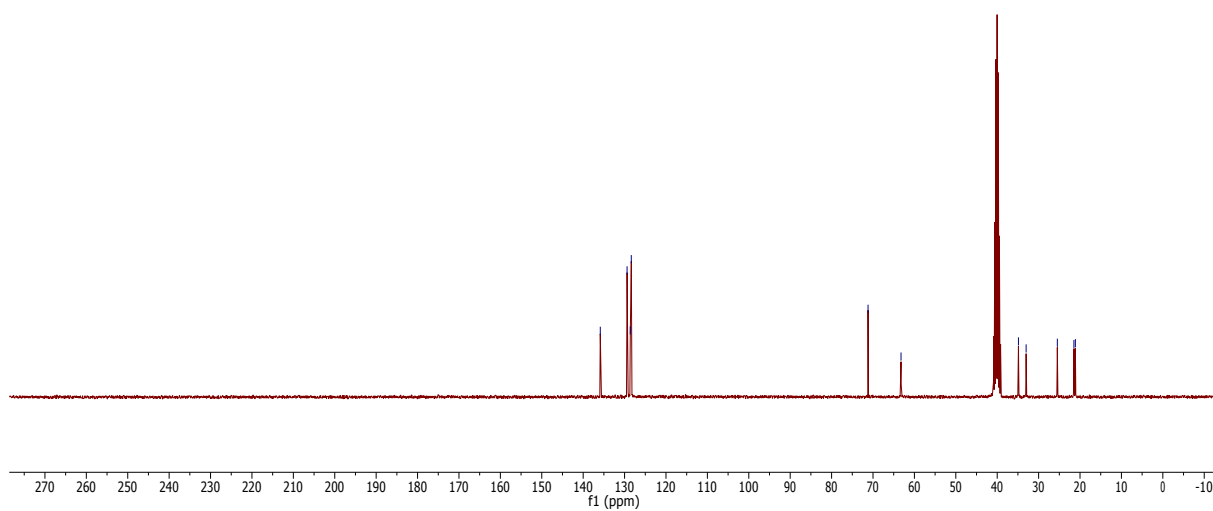
190128.318.11.fid
 Kathir KM24-193
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 18



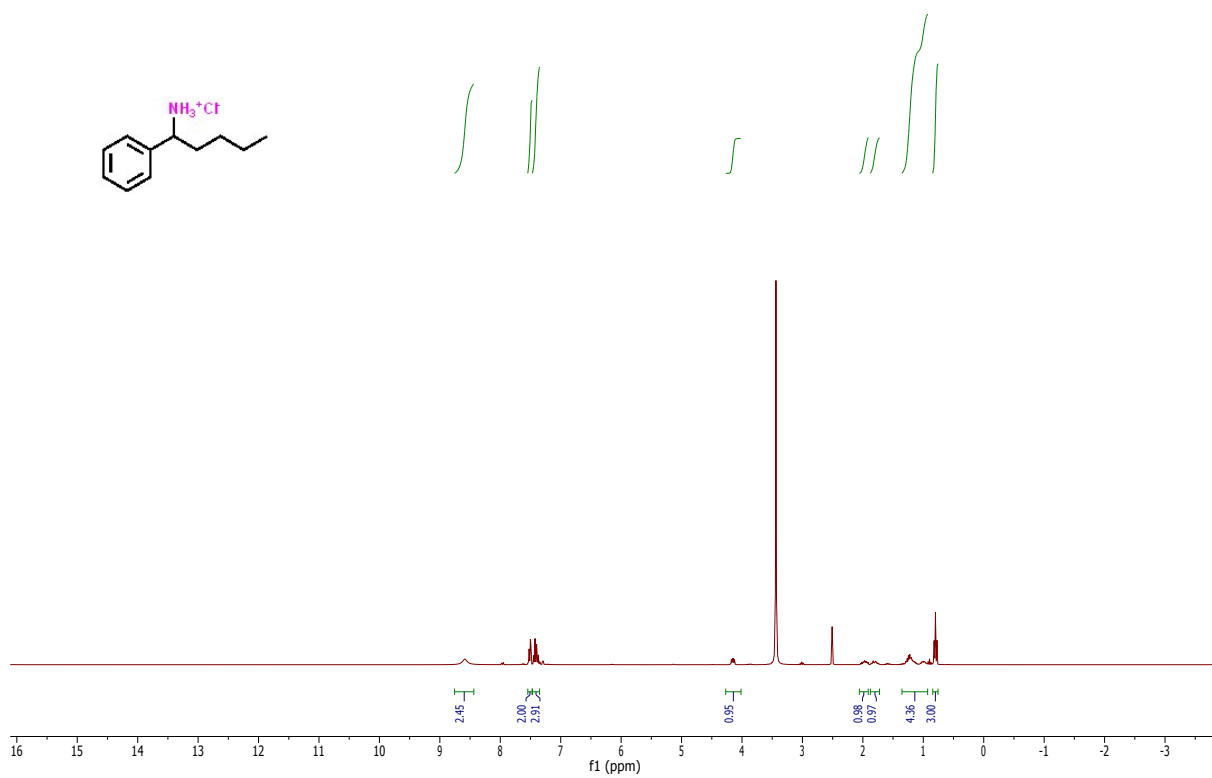
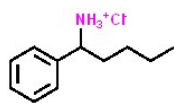
135.67
 135.60
 128.62
 128.38

71.20
 63.23

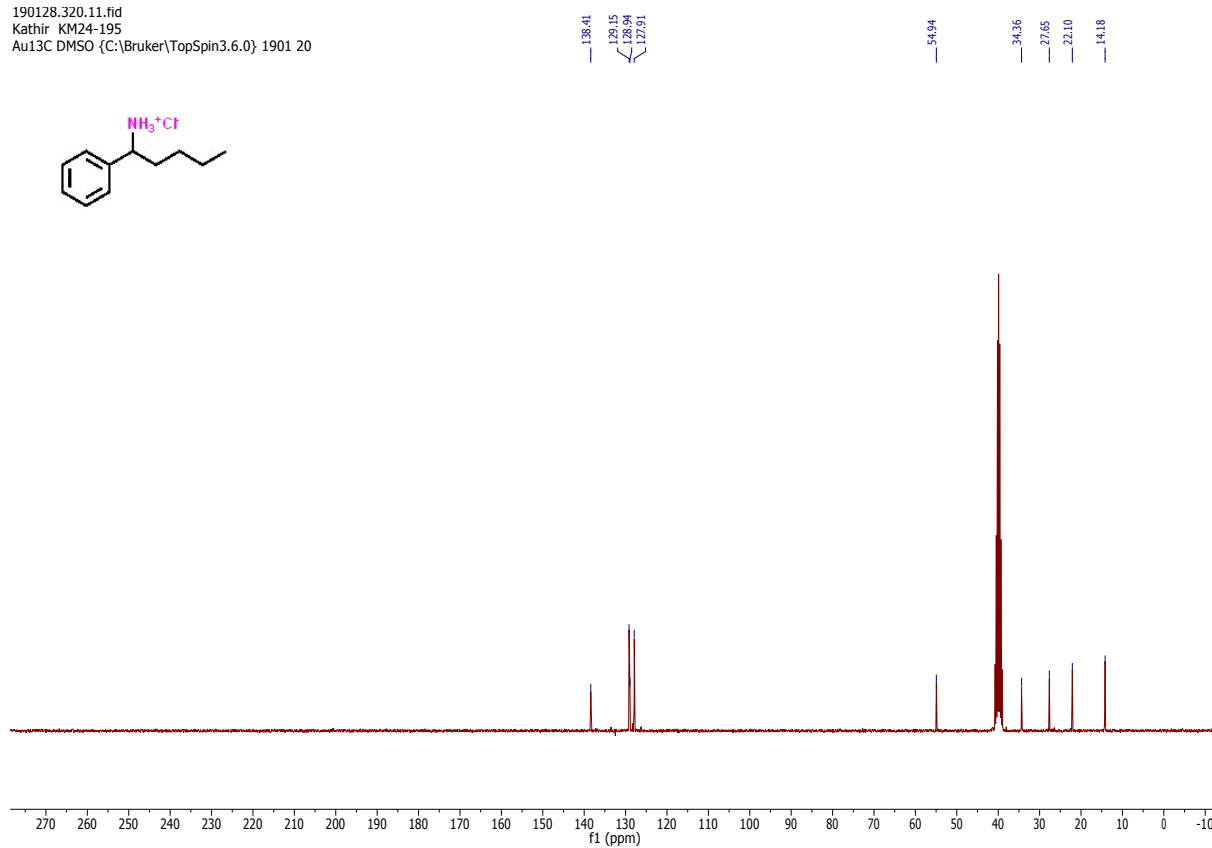
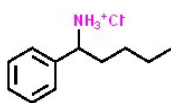
34.87
 33.02
 25.48
 21.47
 21.12



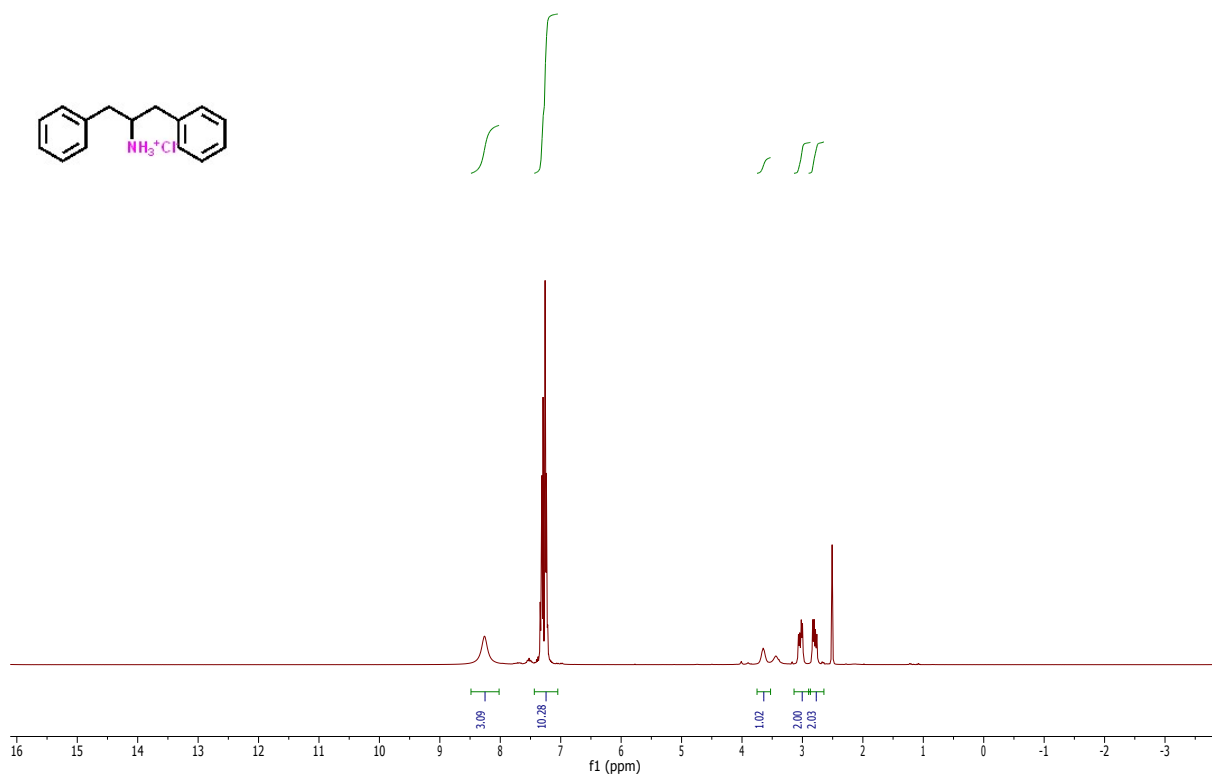
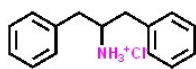
190128.320.10.fid
 Kathir KM24-195
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 20



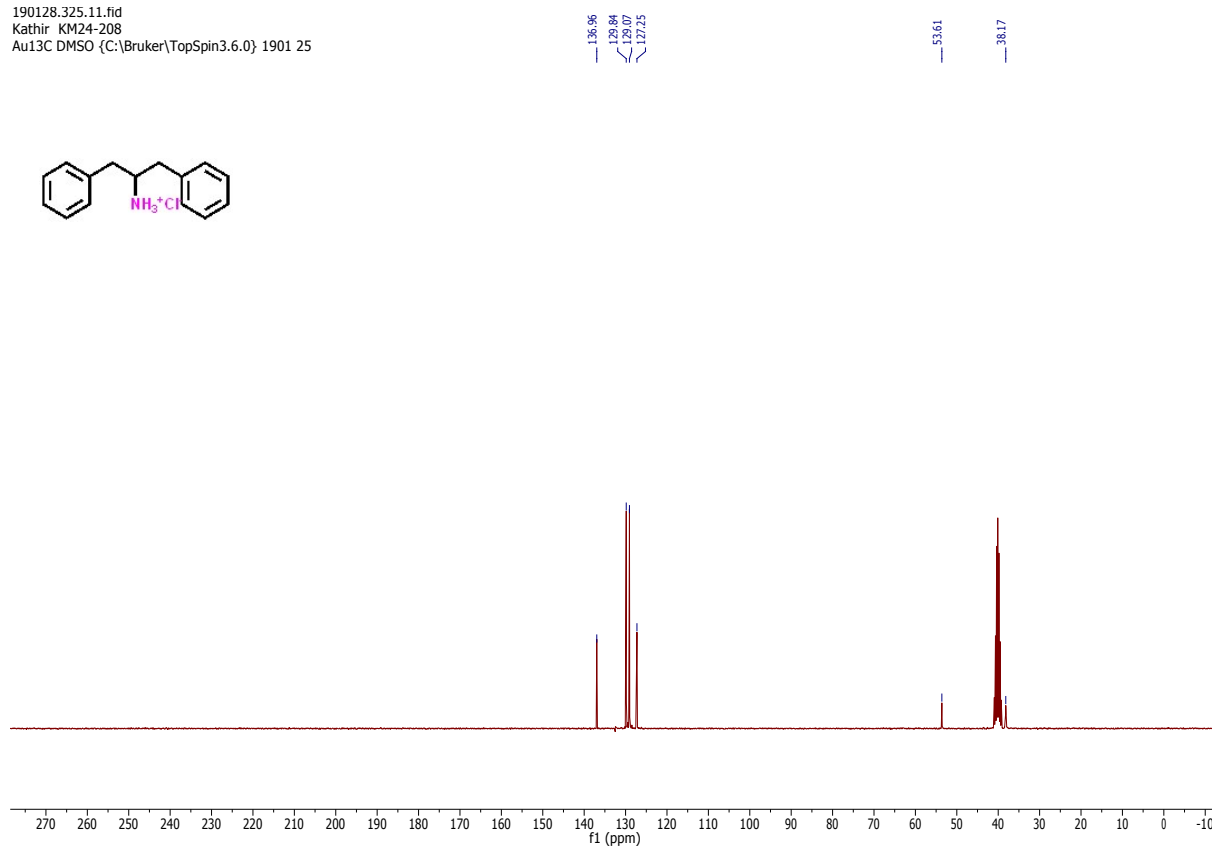
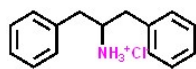
190128.320.11.fid
 Kathir KM24-195
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 20



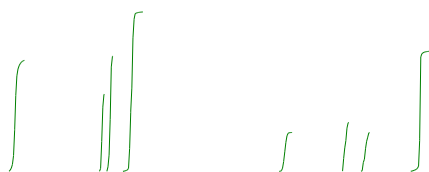
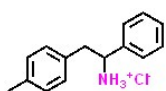
190128.325.10.fid
 Kathir KM24-208
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 25



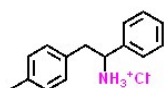
190128.325.11.fid
 Kathir KM24-208
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 25



190128.327.10.fid
 Kathir KM24-212
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 27



190128.327.11.fid
 Kathir KM24-212
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 27

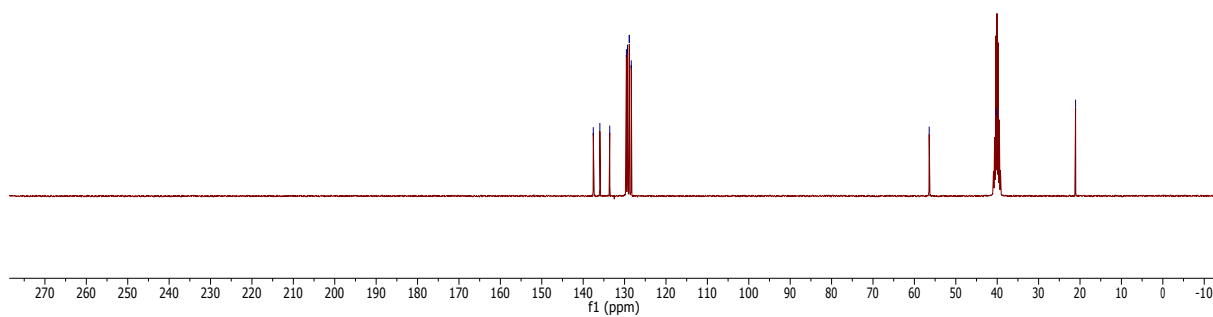


137.56
 135.86
 133.38
 129.95
 129.29
 128.86
 128.38

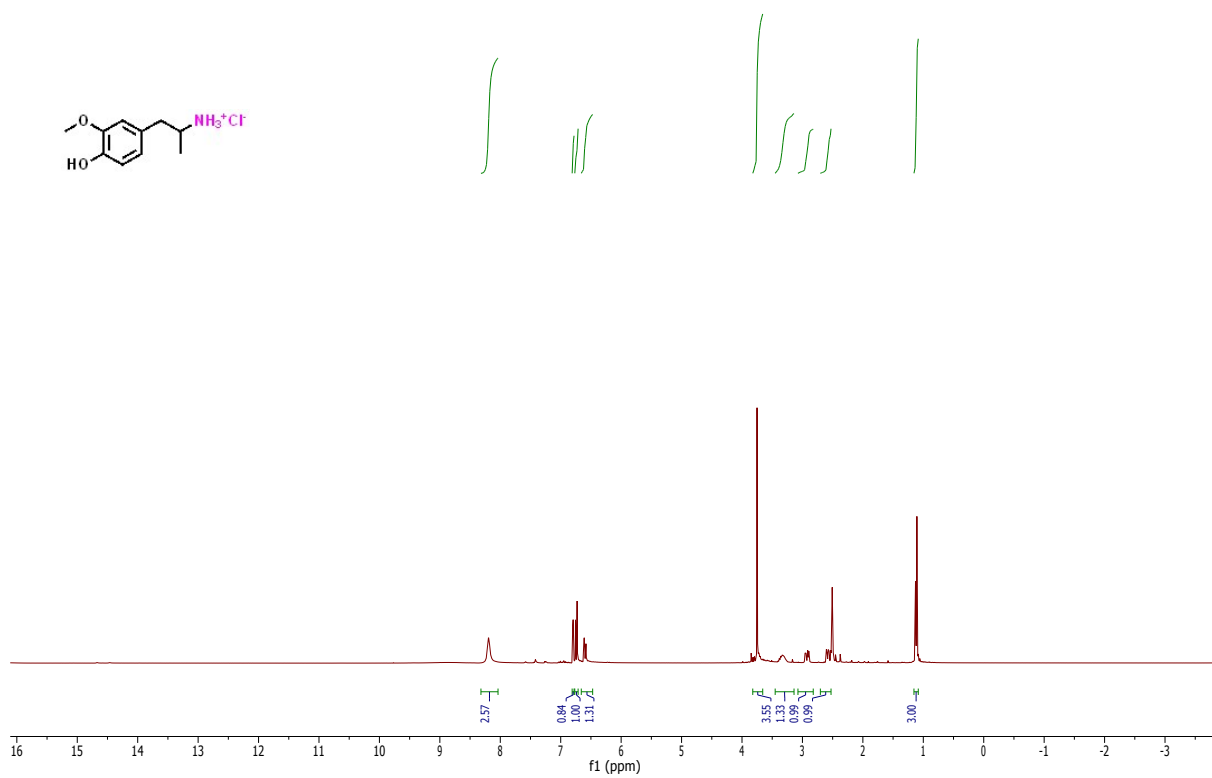
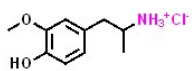
56.43

40.25

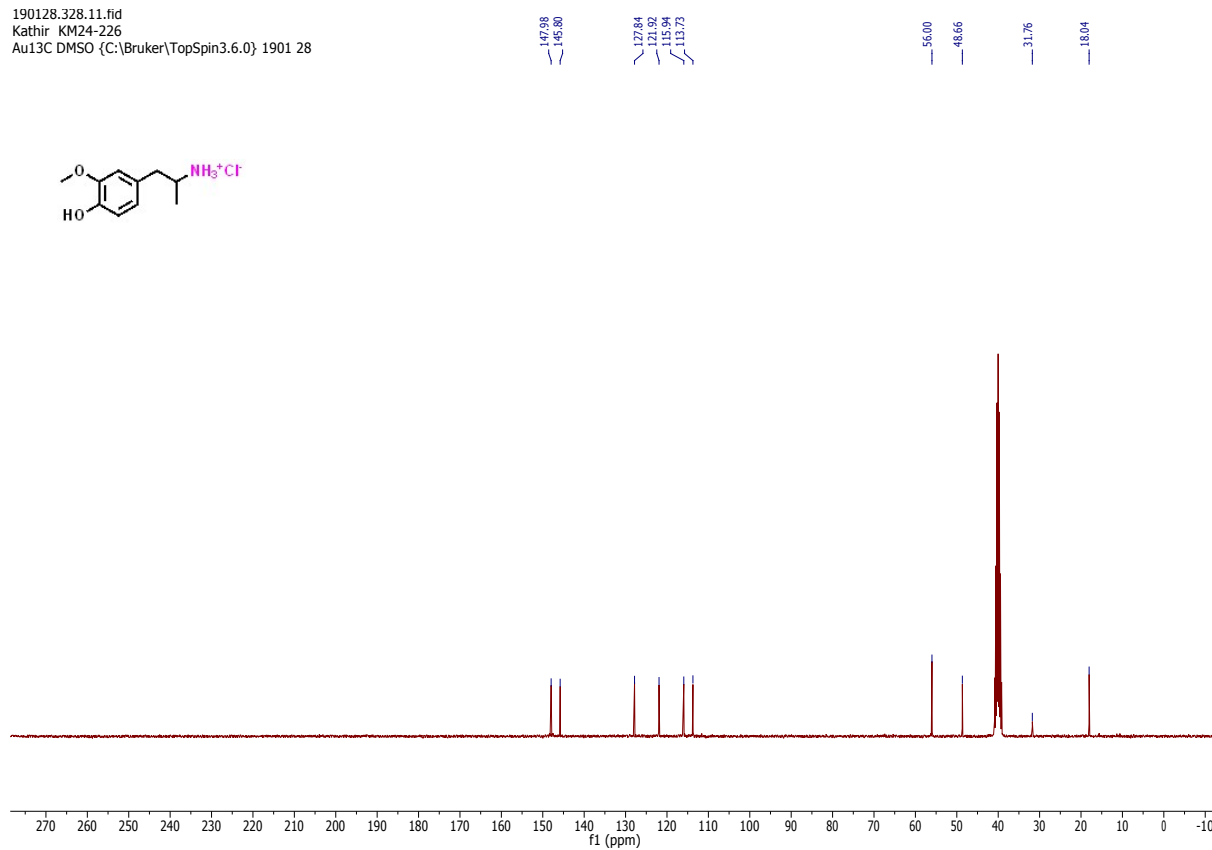
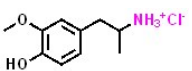
21.07



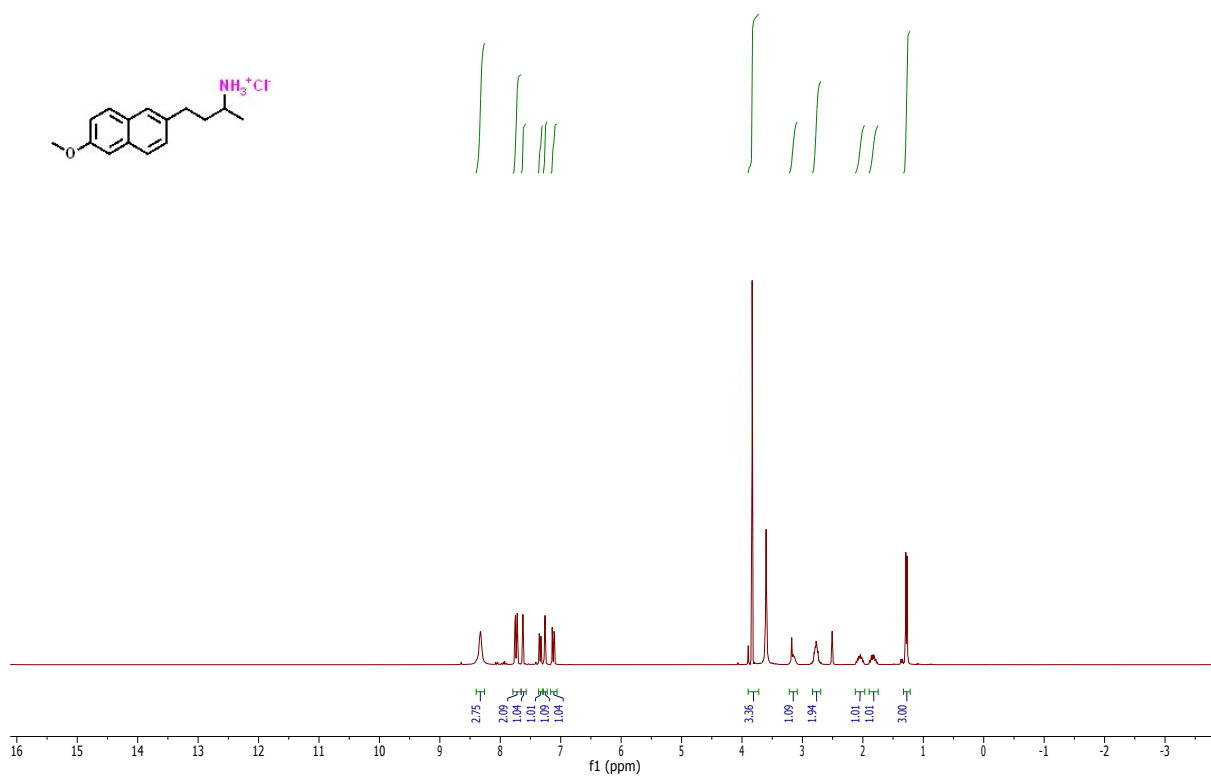
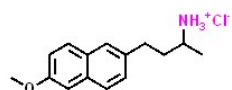
190128.328.10.fid
 Kathir KM24-226
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 28



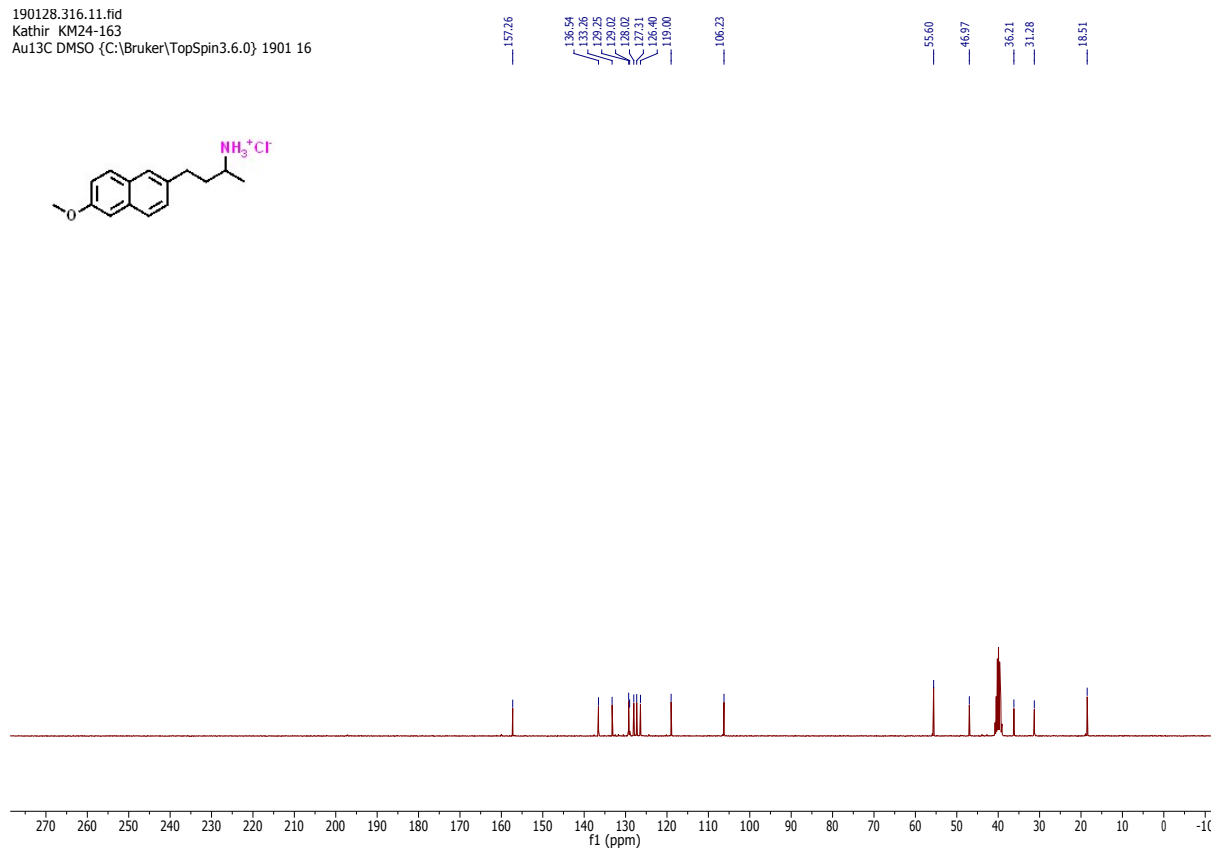
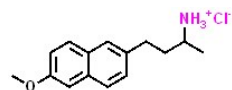
190128.328.11.fid
 Kathir KM24-226
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 28



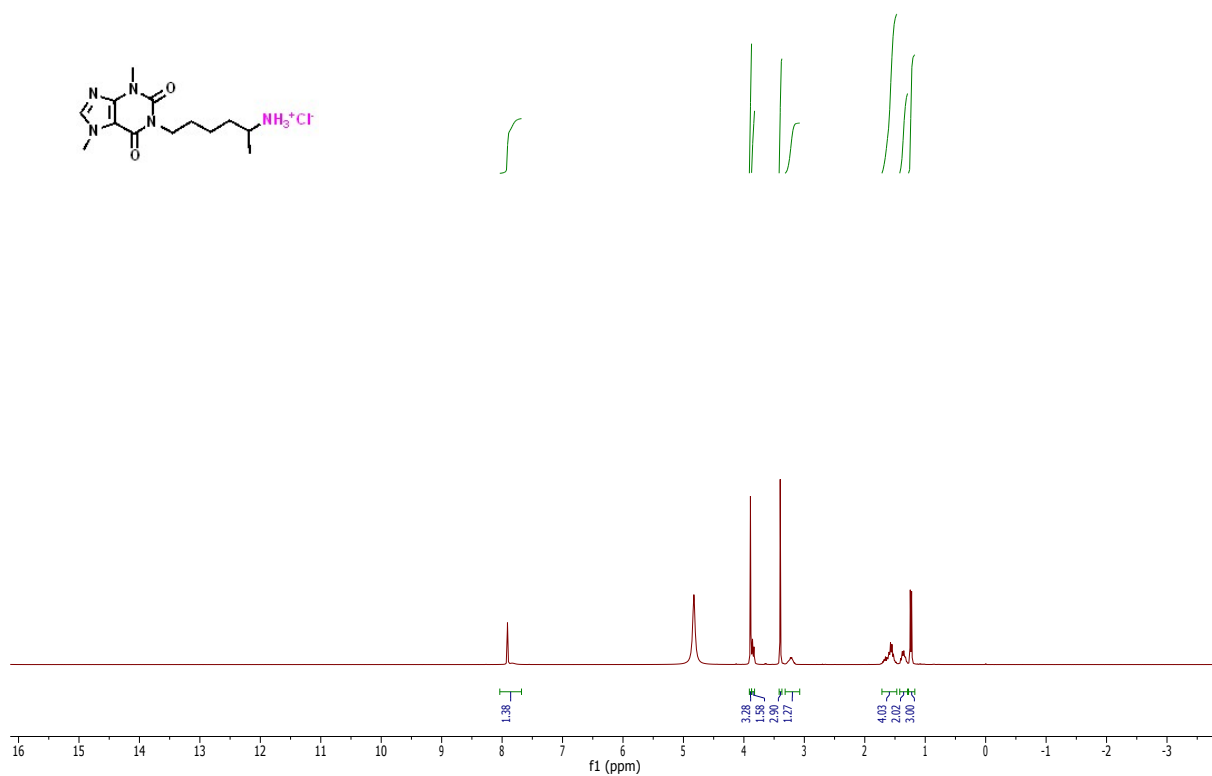
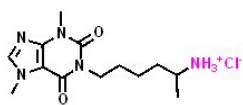
190128.316.10.fid
 Kathir KM24-163
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 16



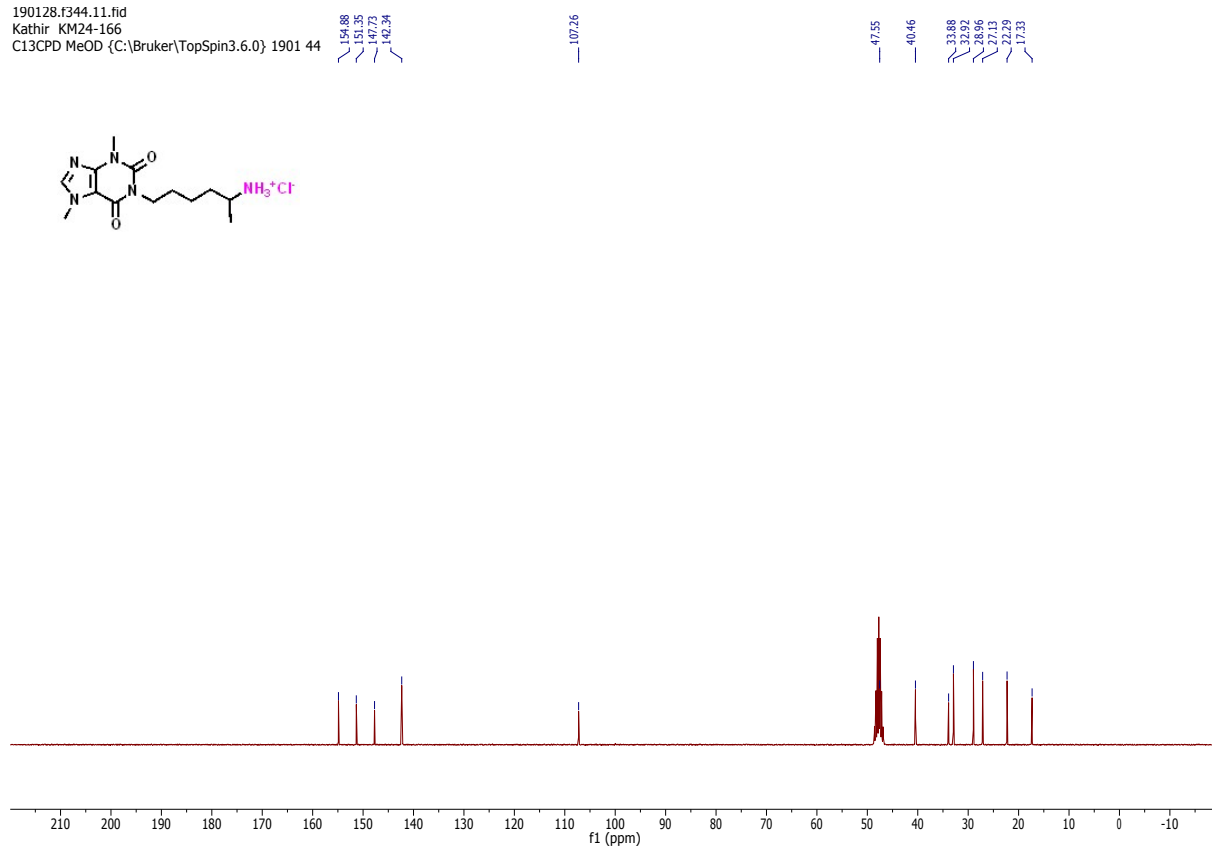
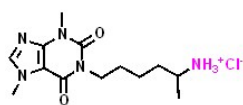
190128.316.11.fid
 Kathir KM24-163
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 16



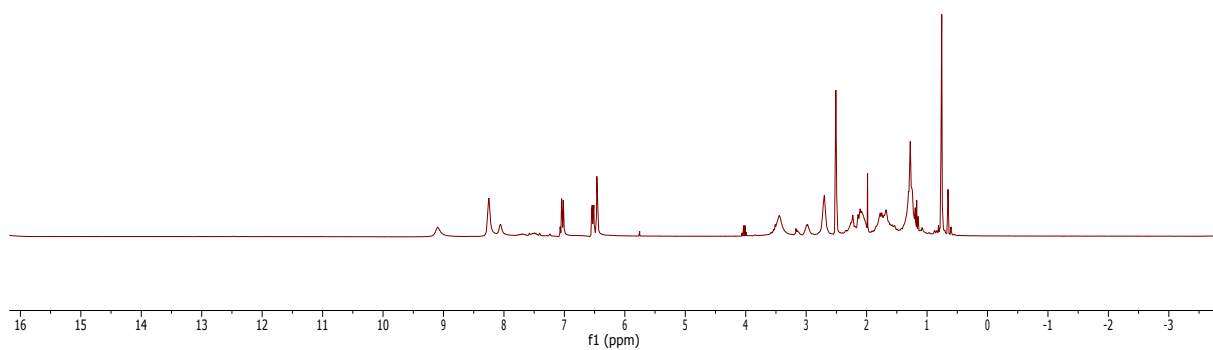
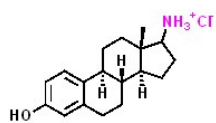
190128.f344.10.fid
 Kathir KM24-166
 PROTON MeOD {C:\Bruker\TopSpin3.6.0} 1901 44



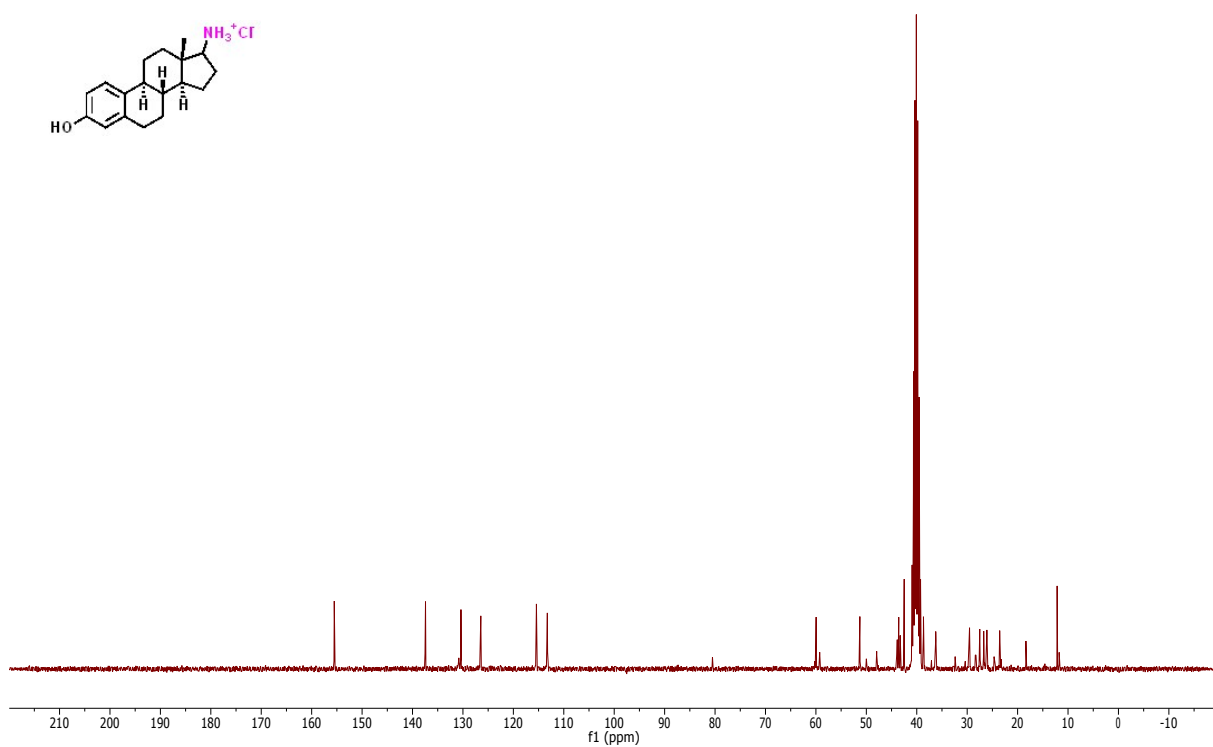
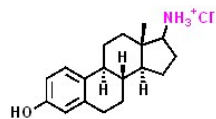
190128.f344.11.fid
 Kathir KM24-166
 C13CPD MeOD {C:\Bruker\TopSpin3.6.0} 1901 44



190128.f345.10.fid
Kathir KM24-165
PROTON DMSO {C:\Bruker\TopSpin3.6.0} 1901 45



190128.f345.11.fid
Kathir KM24-165
C13CPD DMSO {C:\Bruker\TopSpin3.6.0} 1901 45

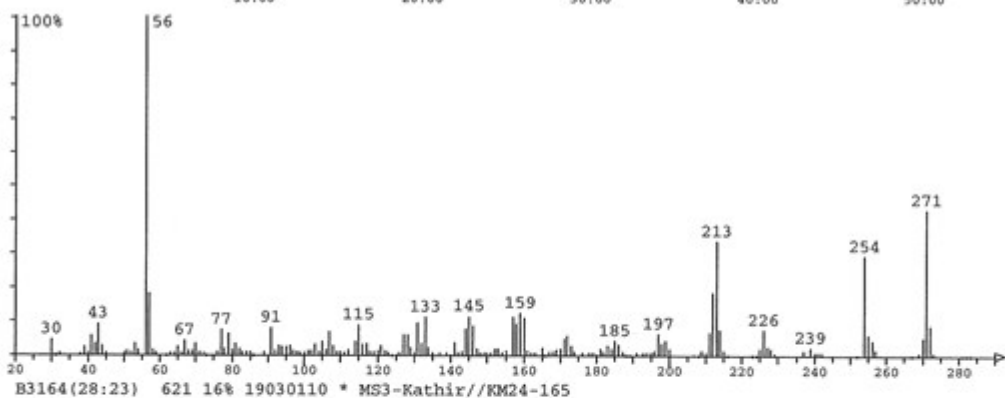
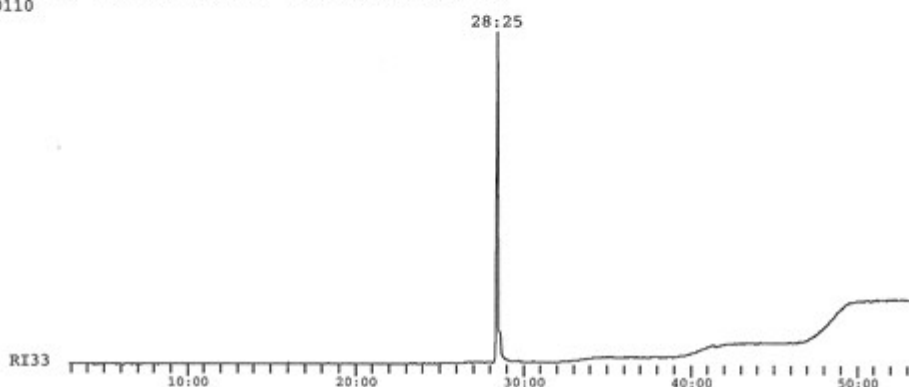
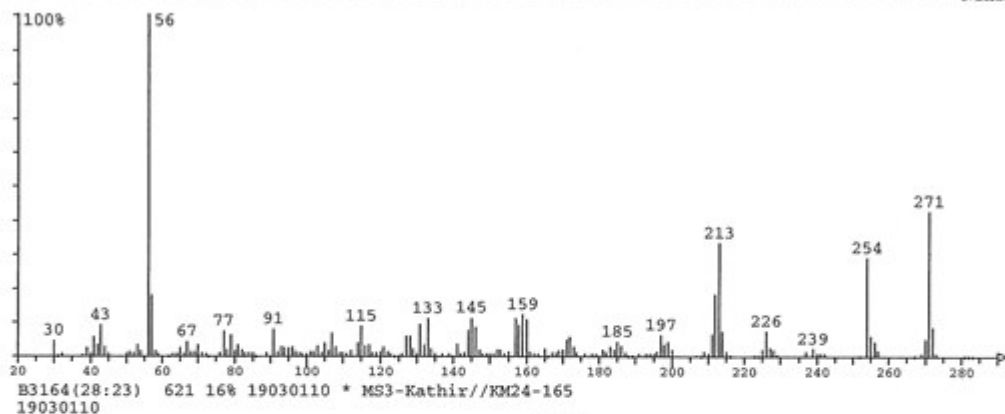


tarlin's KM 24-165

HK(EI)

File : D:\Xcalibur\data\1903\19030502hrei-av2.RAW
Full ms [251.500 - 285.500] - Range: 271.000 - 271.500
Scan No. 1 of 1

Mass	Absolute Intensity	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
271.19292	84857	26.1	271.19307	-0.5	-0.1	7.0	C ₁₈ H ₂₅ O ₁ N ₁

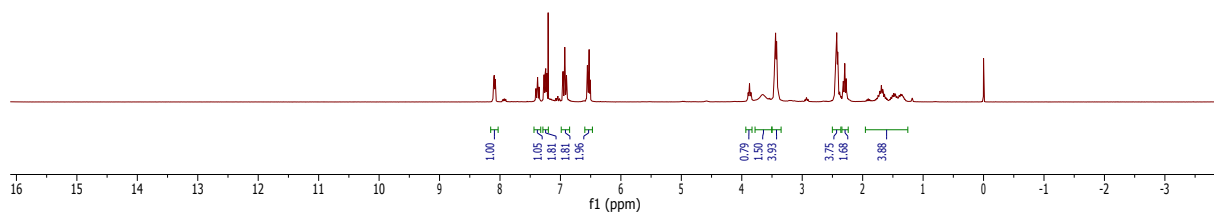
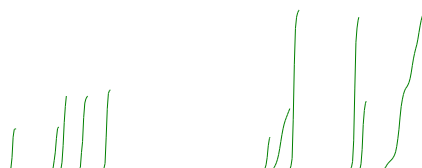
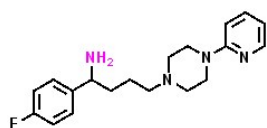


30	4.38	67	3.97	95	2.28	118	0.75	147	1.67	174	0.81	213	33.42
32	0.62	68	1.12	96	2.68	119	0.82	148	0.63	176	0.57	214	7.19
39	2.26	69	0.99	97	1.03	120	1.07	151	0.54	178	0.54	215	1.13
40	0.57	70	3.16	98	0.70	121	2.61	152	1.72	179	0.51	225	1.62
41	5.51	71	0.66	99	0.56	122	1.15	153	1.62	181	1.66	226	7.19
42	3.19	72	0.64	100	0.58	123	0.52	154	0.59	182	0.83	227	2.25
43	8.88	76	0.71	101	1.17	126	0.47	155	1.05	183	2.55	228	1.67
44	2.40	77	7.05	102	0.97	127	5.78	157	10.85	184	1.71	237	0.95
45	0.61	78	1.68	103	2.92	128	5.79	158	9.04	185	3.89	239	1.97
50	0.61	79	5.94	104	0.67	129	1.94	159	12.16	186	2.94	240	0.65
51	0.95	80	1.29	105	3.84	131	9.27	160	10.75	187	0.70	241	0.48
52	0.75	81	3.00	106	1.33	132	3.06	161	1.14	191	0.50	242	0.53
53	3.03	82	1.56	107	6.62	133	10.83	163	0.63	195	0.48	254	28.82
54	1.39	83	0.83	108	2.42	134	1.95	165	1.83	196	1.05	255	5.70
56	100.00	84	0.81	109	0.88	139	0.52	167	0.80	197	6.13	256	4.02
57	17.98	85	0.71	110	0.93	141	3.53	168	0.68	198	3.07	257	1.25
58	1.33	89	0.77	112	1.25	142	0.64	169	1.49	199	4.11	269	0.64
59	0.61	91	7.84	114	3.65	143	0.95	170	1.64	200	1.66	270	5.01
63	0.61	92	0.98	115	8.69	144	7.52	171	4.43	209	1.04	271	42.53
65	2.18	93	2.60	116	2.69	145	11.08	172	5.44	211	6.32	272	8.47
66	0.54	94	2.31	117	3.27	146	8.48	173	2.66	212	18.22	273	0.54

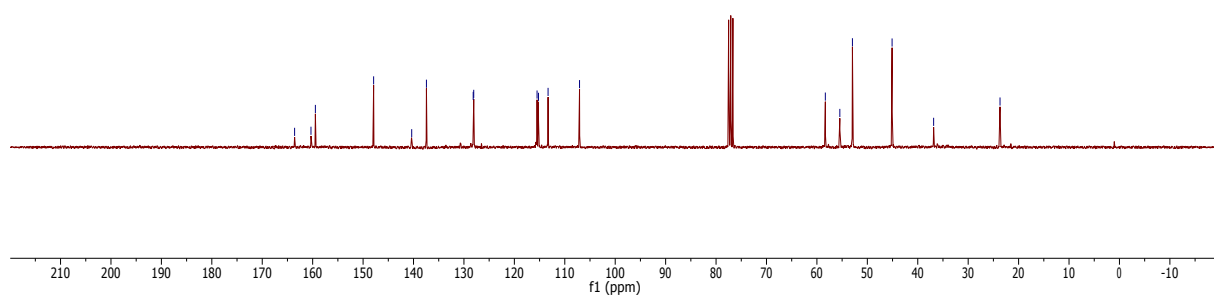
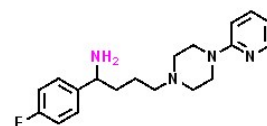
B3164(28:23)621 16% 19030110 * MS3-Kathir//KM24-165

lim: 0.44%

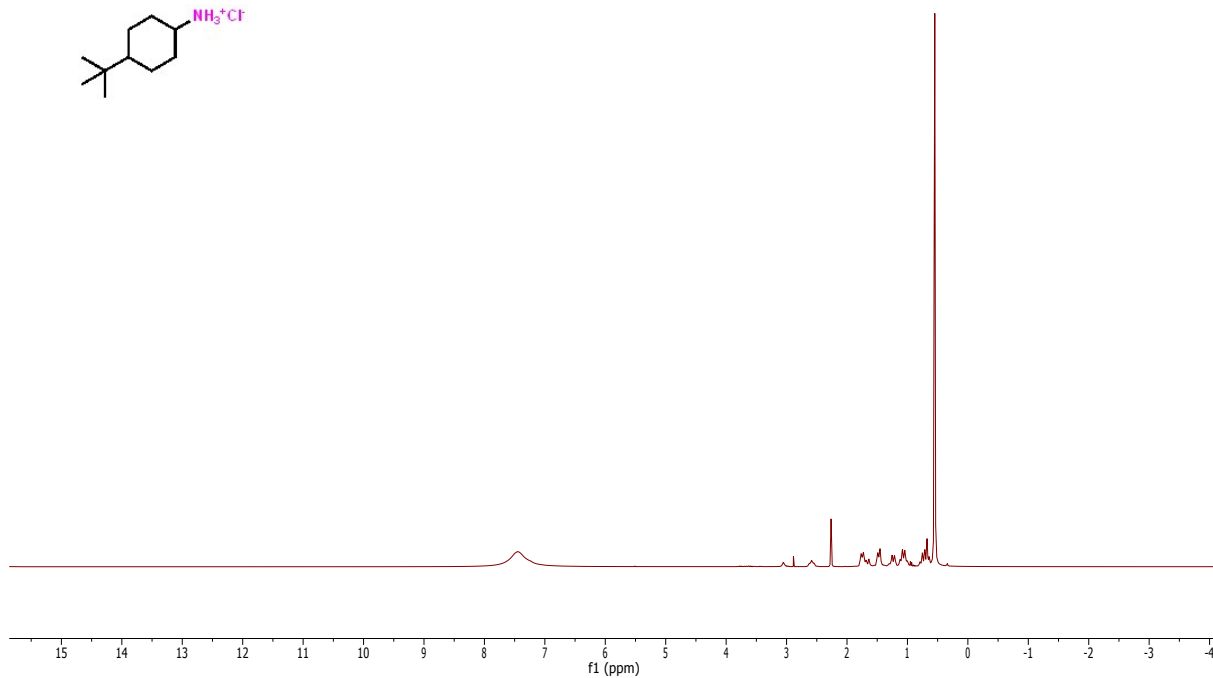
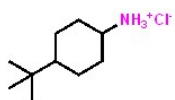
190128.f343.10.fid
 Kathir KM24-164
 PROTON CDCl₃ {C:\Bruker\TopSpin3.6.0} 1901 43



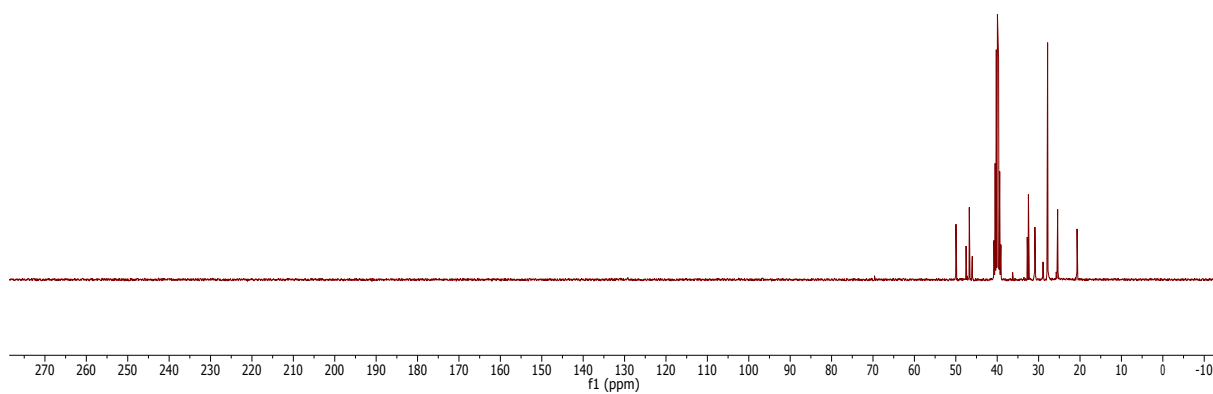
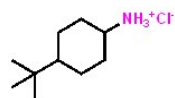
190128.f343.11.fid
 Kathir KM24-164
 C13CPD CDCl₃ {C:\Bruker\TopSpin3.6.0} 1901 43



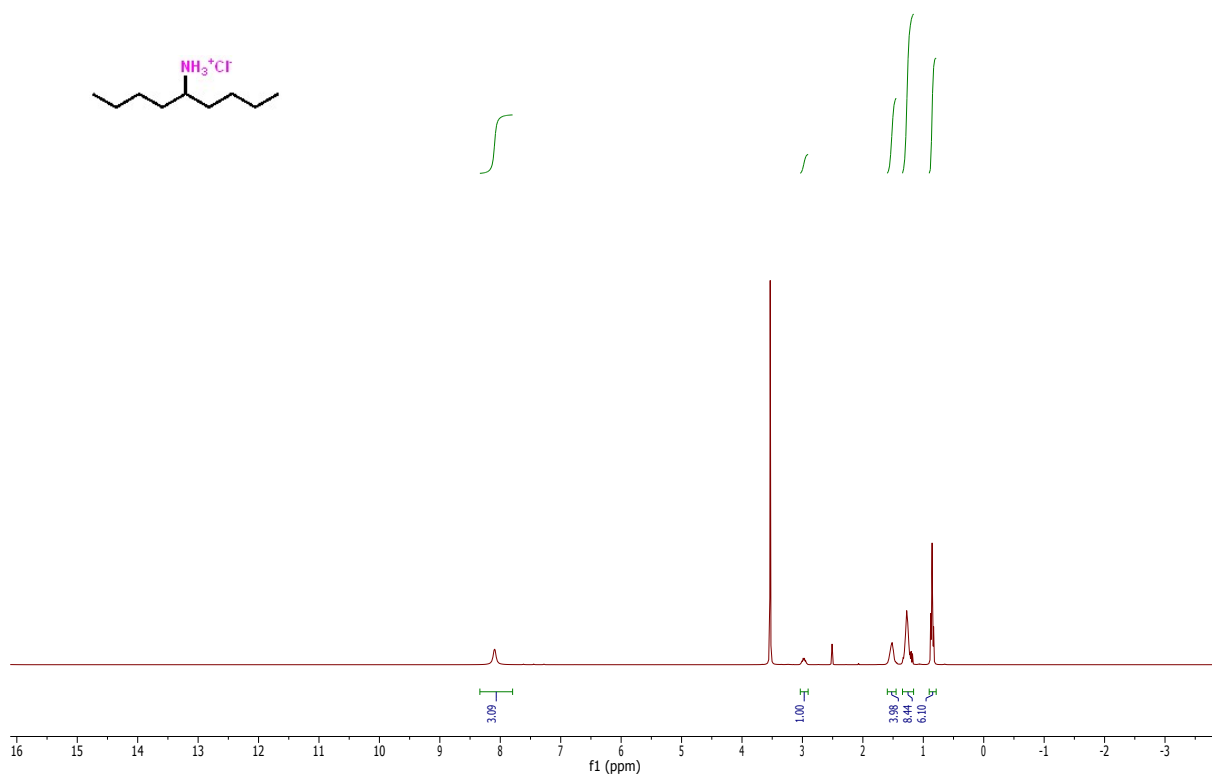
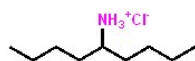
190128.319.10.fid
Kathir KM24-194
Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 19



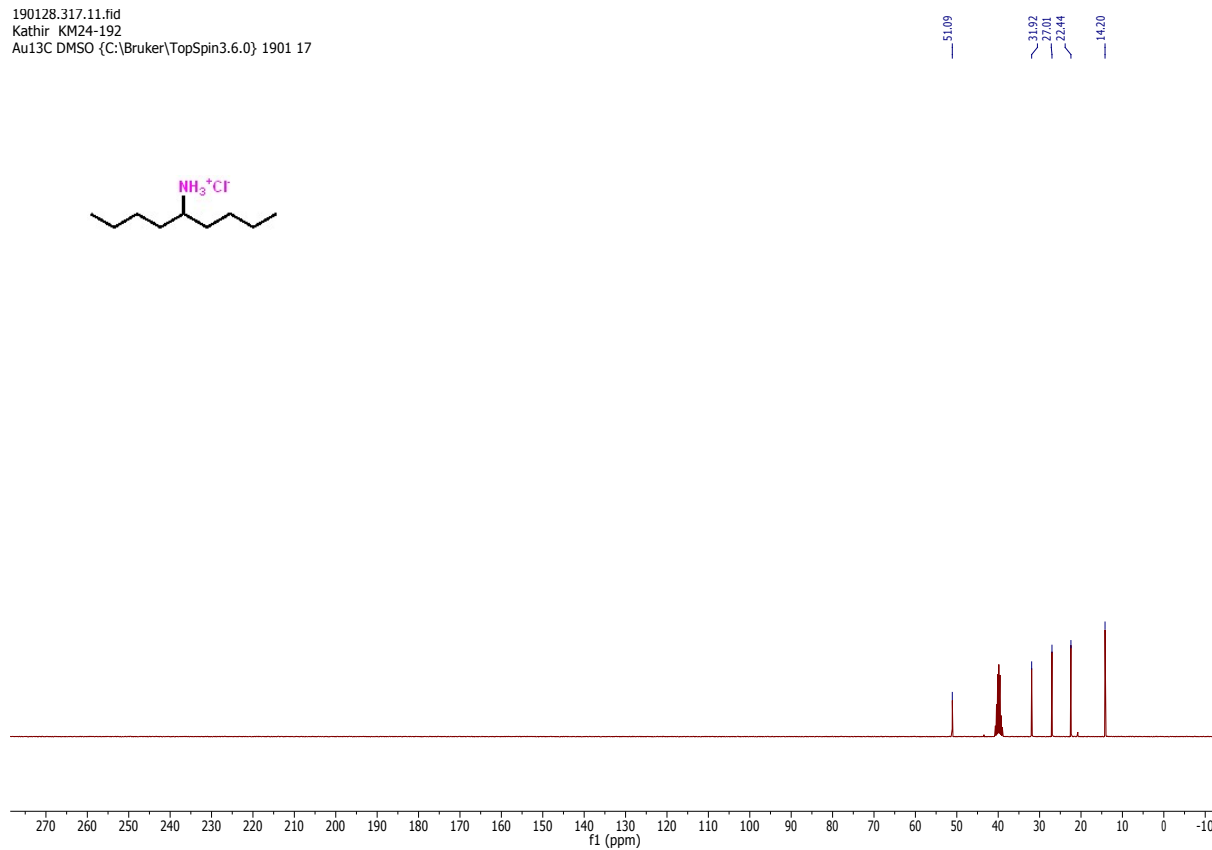
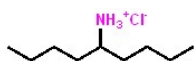
190128.319.11.fid
Kathir KM24-194
Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 19



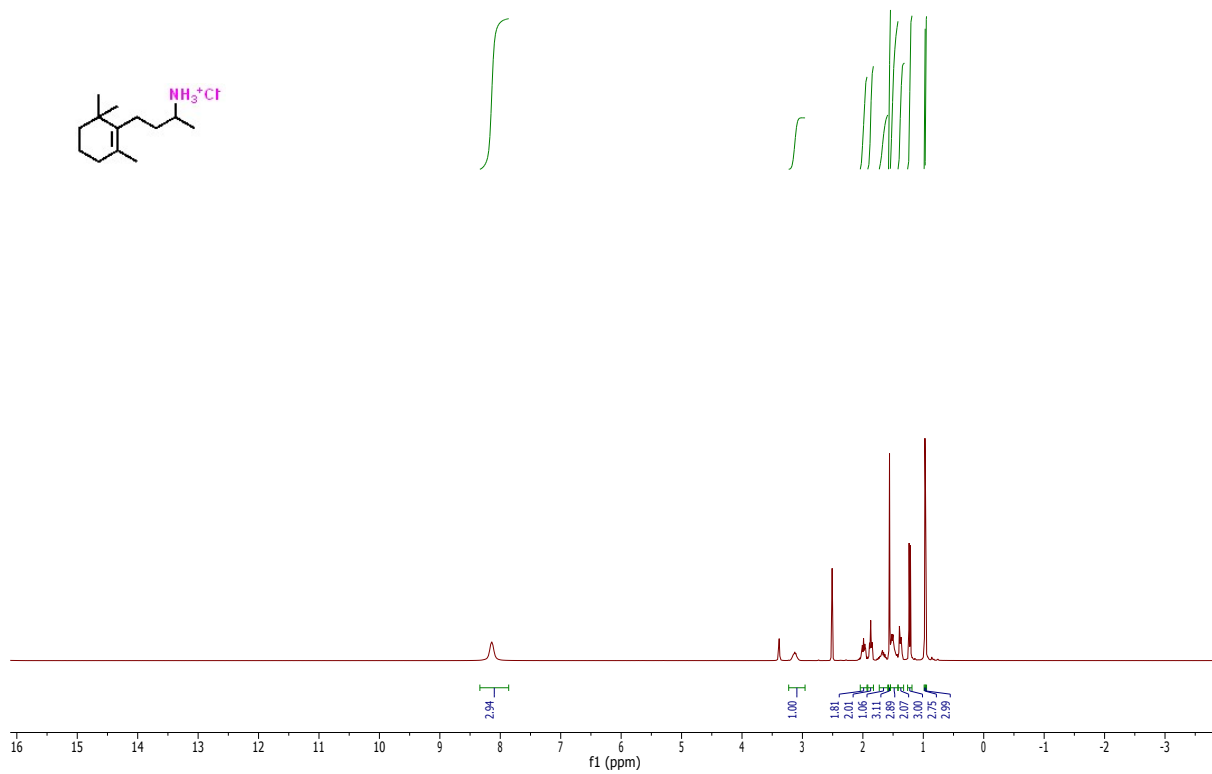
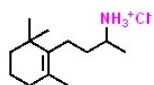
190128.317.10.fid
 Kathir KM24-192
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 17



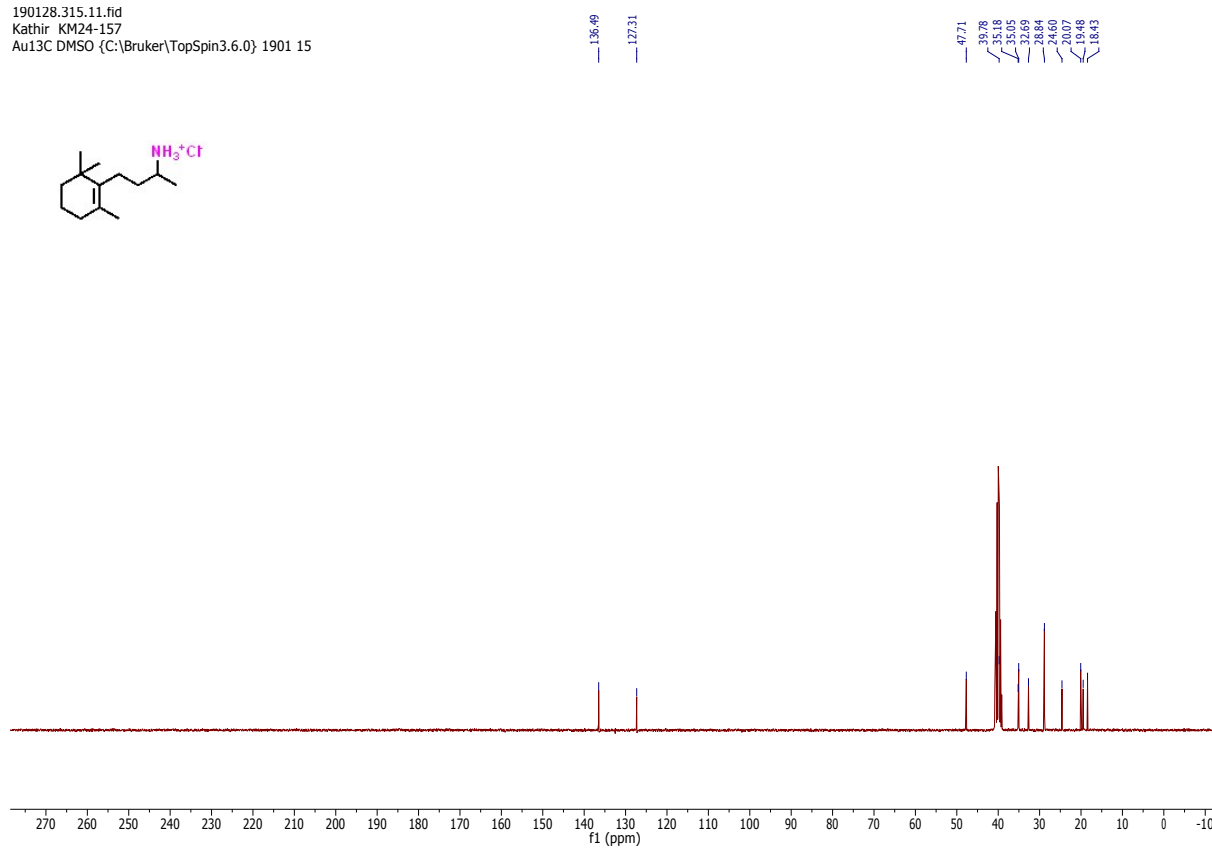
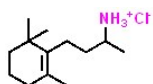
190128.317.11.fid
 Kathir KM24-192
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 17



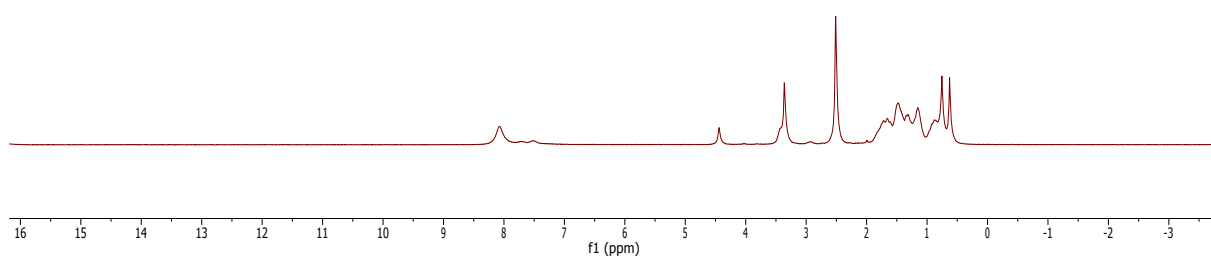
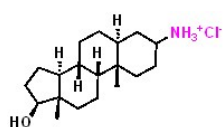
190128.315.10.fid
 Kathir KM24-157
 Au1H DMSO {C:\Bruker\TopSpin3.6.0} 1901 15



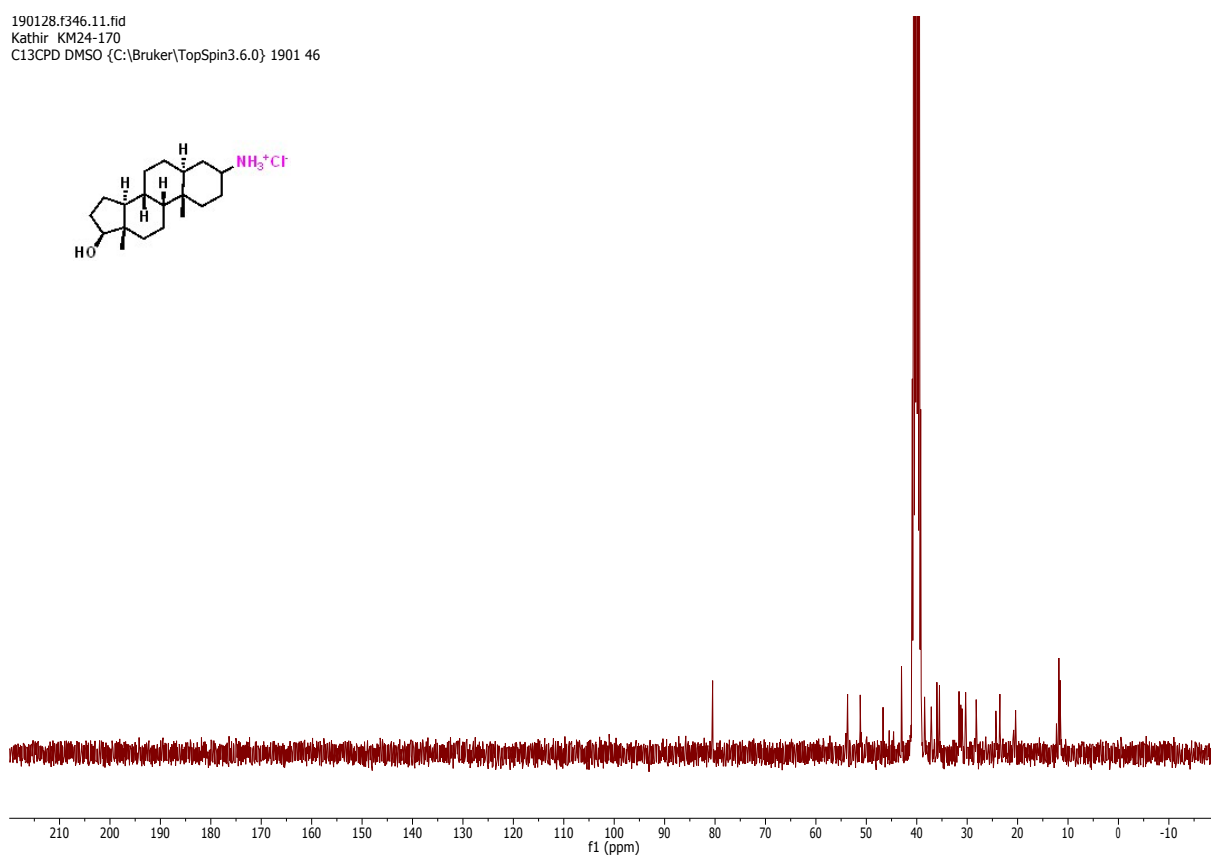
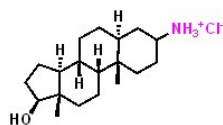
190128.315.11.fid
 Kathir KM24-157
 Au13C DMSO {C:\Bruker\TopSpin3.6.0} 1901 15



190128.f346.10.fid
Kathir KM24-170
PROTON DMSO {C:\Bruker\TopSpin3.6.0} 1901 46

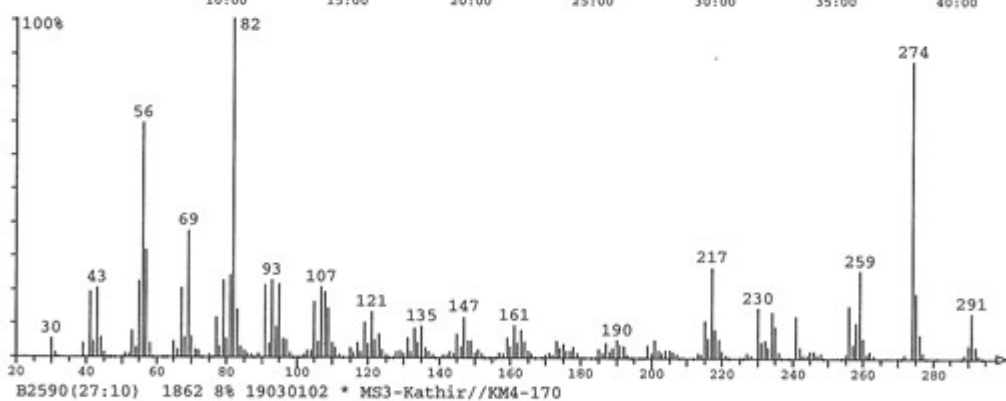
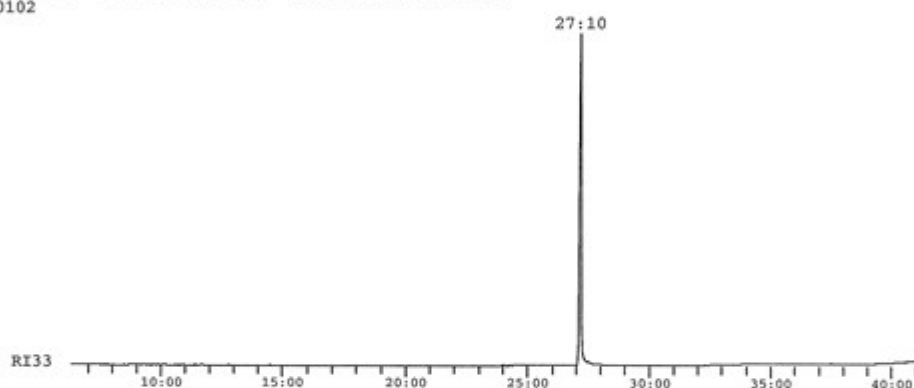
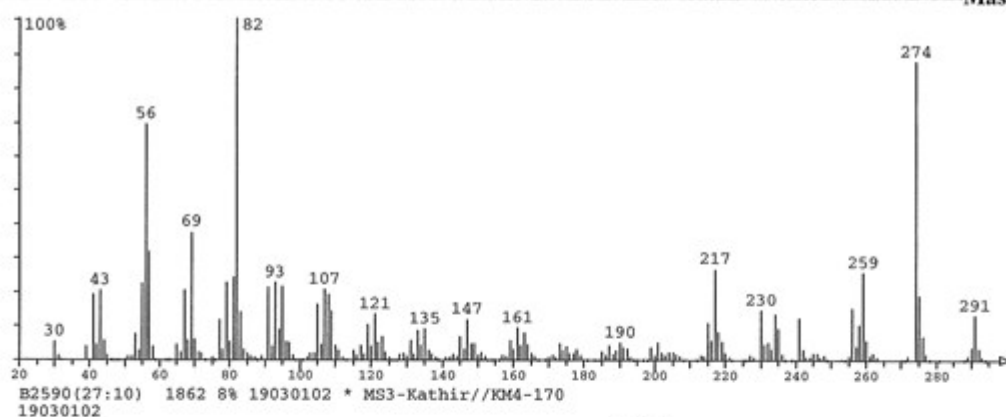


190128.f346.11.fid
Kathir KM24-170
C13CPD DMSO {C:\Bruker\TopSpin3.6.0} 1901 46



kalit fm 24 - 70 HR(EI)

File : D:\Xcalibur\data\1903\19030503hrei-av2.RAW
Full ms [277.500 - 309.500] - Range: 291.000 - 291.500
Scan No. 1 of 1
Mass Absolute Relative Theoretical Delta Delta RDB Composition
Intensity Intensity Mass [ppm] [mmu]
291.25493 85391 7.6 291.25567 -2.5 -0.7 4.0 C₁₉ H₂₃ O₂ N₁

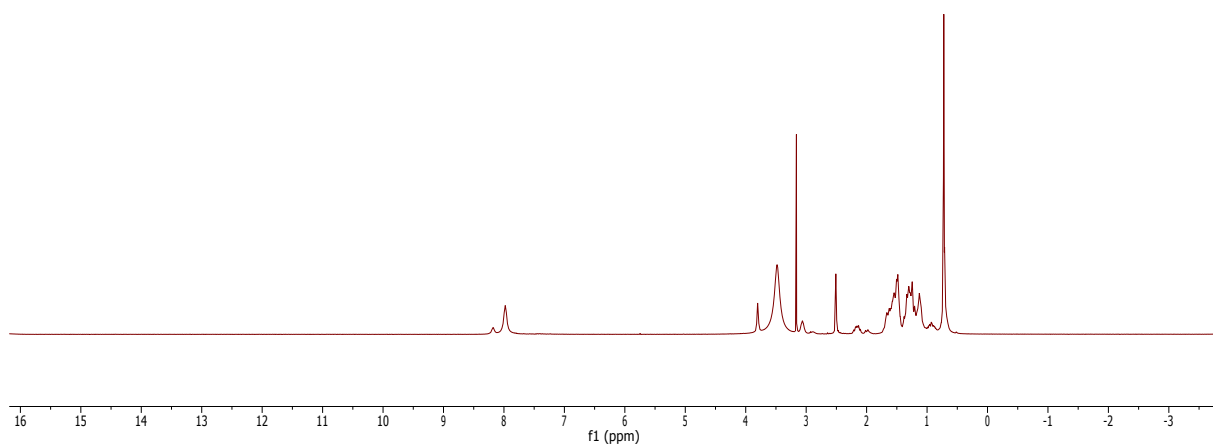
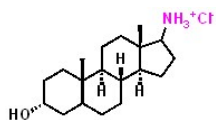


30	5.20	72	1.58	105	16.23	132	1.45	163	7.63	201	4.79	235	8.91
31	1.05	77	11.61	106	4.36	133	8.46	164	4.30	202	2.09	236	1.51
39	3.64	78	2.96	107	20.56	134	4.09	165	1.62	203	1.13	241	12.08
41	19.11	79	22.65	108	18.99	135	8.83	171	1.11	204	2.01	242	2.94
42	4.23	80	5.23	109	14.20	136	2.41	173	4.60	205	1.88	245	1.69
43	20.32	81	23.88	110	3.99	137	1.43	174	2.54	206	1.52	246	1.74
44	5.52	82	100.00	111	2.67	143	1.49	175	3.81	207	0.85	248	1.03
45	1.20	83	13.78	115	2.43	144	0.81	176	1.66	213	1.14	256	14.92
53	7.50	84	2.92	116	1.06	145	6.67	177	1.59	214	0.94	257	3.62
54	2.61	85	1.75	117	3.98	146	2.77	178	2.93	215	10.80	258	10.20
55	22.25	89	0.90	118	1.37	147	11.67	179	1.05	216	5.44	259	25.51
56	69.19	91	21.21	119	10.16	148	4.64	185	2.27	217	26.48	260	5.33
57	31.60	92	3.78	120	3.61	149	4.62	186	1.00	218	7.97	261	0.81
58	3.68	93	22.46	121	13.37	150	1.04	187	3.90	219	5.18	262	1.53
65	4.32	94	8.60	122	5.01	151	2.08	188	1.40	220	1.53	274	87.50
66	2.04	95	21.26	123	6.51	157	1.02	189	2.49	227	1.17	275	18.78
67	20.19	96	5.19	124	1.90	158	0.80	190	4.80	230	14.56	276	6.52
68	5.39	97	4.80	128	1.48	159	5.53	191	3.43	231	4.25	277	1.36
69	37.21	98	1.10	129	1.67	160	2.80	192	3.20	232	4.77	290	3.56
70	5.88	103	1.57	130	0.80	161	9.27	199	3.41	233	2.92	291	13.09
71	2.04	104	1.55	131	5.57	162	3.86	200	1.22	234	13.36	292	2.99

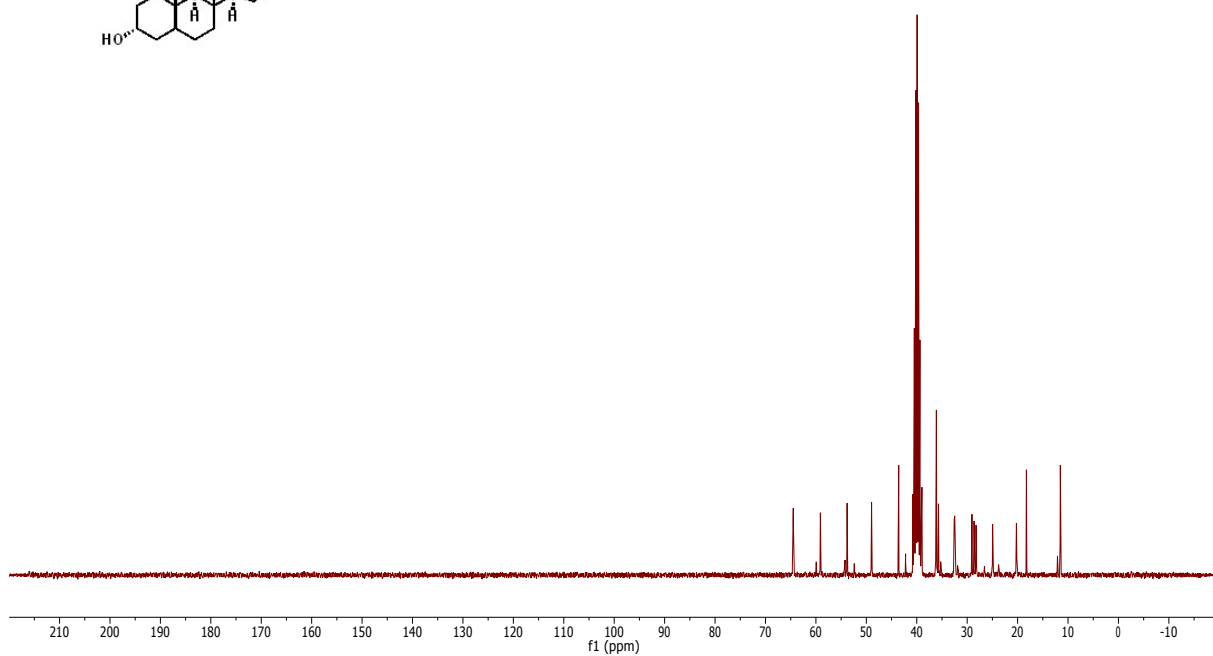
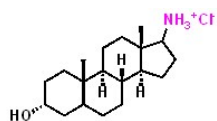
B2590(27:10)1862 8% 19030102 * MS3-Kathir//KM4-170

lim: 0.79%

190128.f347.10.fid
Kathir KM24-171
PROTON DMSO {C:\Bruker\TopSpin3.6.0} 1901 47



190128.f347.11.fid
Kathir KM24-171
C13CPD DMSO {C:\Bruker\TopSpin3.6.0} 1901 47



Karl's KM 24-177

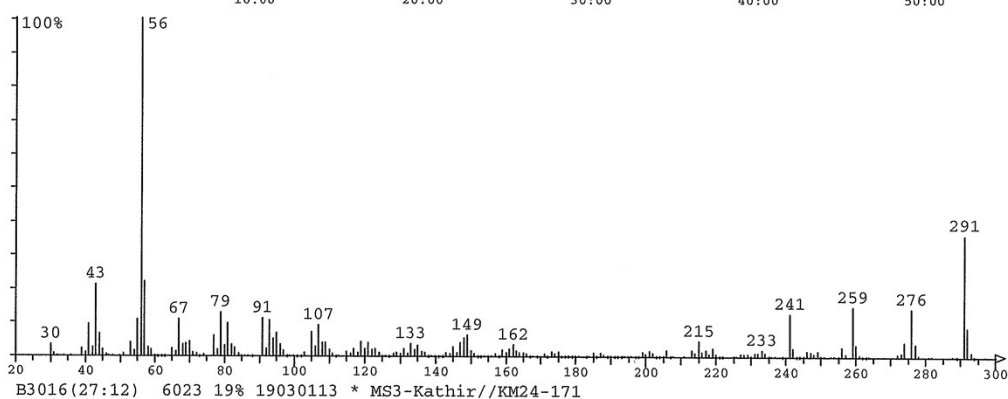
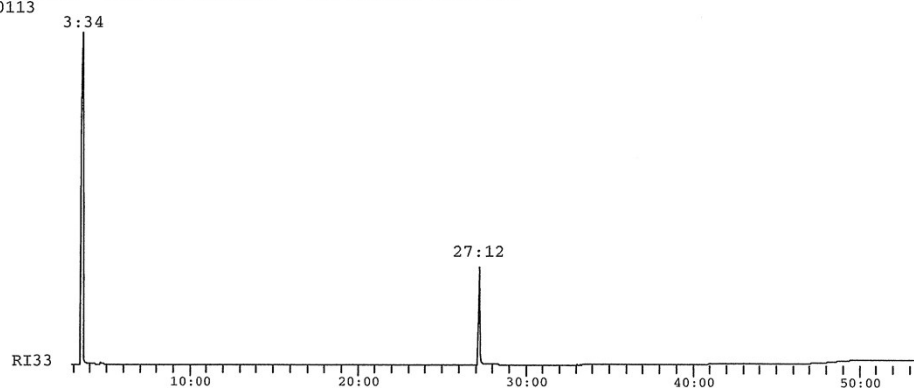
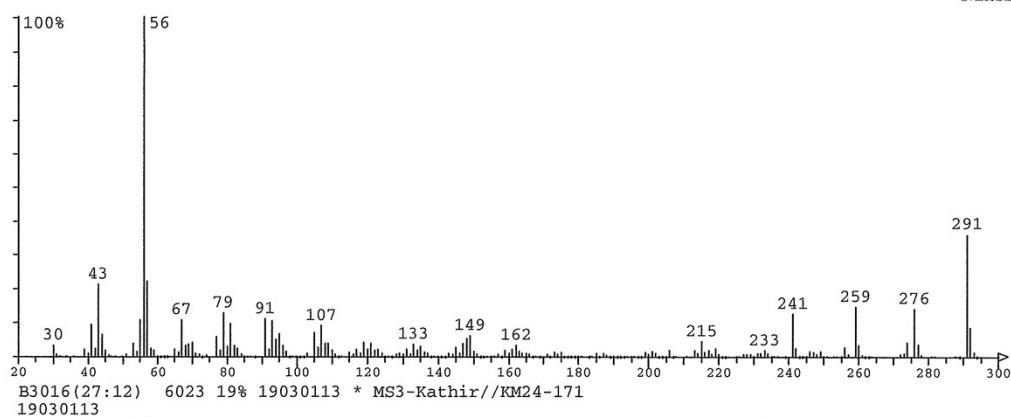
HR (EI)

File : D:\Xcalibur\data\1903\19030504hrei-av2.RAW

Full ms [277.500 - 309.500] - Range: 291.000 - 291.500

Scan No. 1 of 1

Mass	Absolute Intensity	Relative Intensity	Theoretical Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
291.25494	670829	47.5	291.25567	-2.5	-0.7	4.0	C ₁₉ H ₃₃ O ₁ N ₁

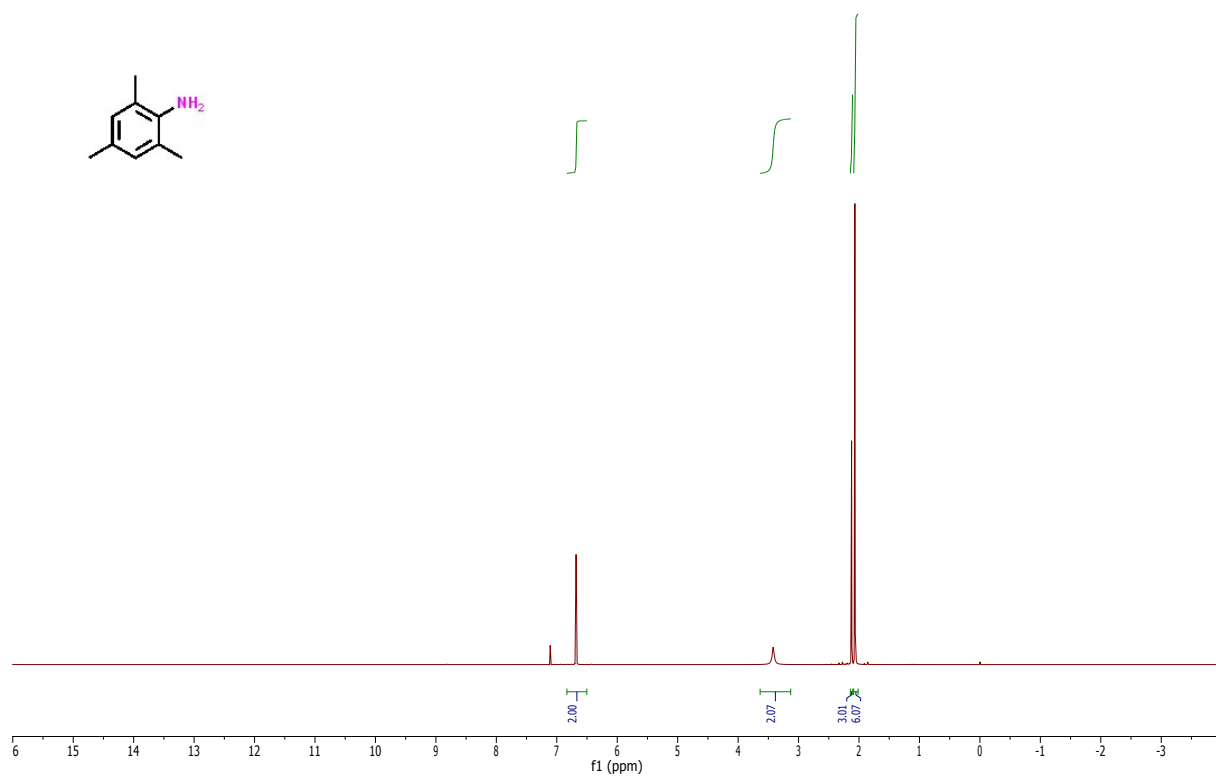
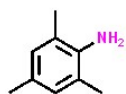


30	3.11	68	3.00	97	1.33	129	0.89	160	0.87	202	0.74	243	0.31
31	0.52	69	3.41	98	0.32	130	0.38	161	2.00	203	0.30	246	1.30
39	2.05	70	4.08	103	0.80	131	2.06	162	3.00	206	1.58	247	1.01
40	0.82	71	0.76	105	6.87	132	0.65	163	1.25	207	0.34	248	0.65
41	9.14	72	0.42	106	2.44	133	3.38	164	0.69	213	1.64	249	1.41
42	2.24	74	0.37	107	8.82	134	1.54	165	0.84	214	0.69	250	0.32
43	21.13	77	5.83	108	3.58	135	2.92	166	0.61	215	4.23	256	2.50
44	6.22	78	1.59	109	3.65	136	1.17	171	0.48	216	1.06	257	0.65
45	1.77	79	12.60	110	1.59	137	0.68	173	1.17	217	1.60	259	14.37
46	0.36	80	2.84	111	0.65	143	0.67	174	0.63	218	0.50	260	3.04
51	0.45	81	9.64	115	1.06	144	0.38	175	0.97	219	2.28	261	0.36
53	3.65	82	3.22	116	0.49	145	2.67	176	0.35	220	0.44	272	0.45
54	1.27	83	2.24	117	2.02	146	0.83	185	0.84	227	0.43	273	0.67
55	10.67	84	0.58	118	0.76	147	3.69	186	0.25	228	0.45	274	3.94
56	100.00	88	0.29	119	3.99	148	5.29	187	0.75	229	0.41	276	13.74
57	21.85	91	11.02	120	1.93	149	5.96	188	0.36	231	0.81	277	3.56
58	2.19	92	2.06	121	3.80	150	1.41	189	0.35	232	0.74	278	0.37
59	1.61	93	10.39	122	1.67	151	0.47	192	0.27	233	1.69	289	0.34
65	2.00	94	4.94	123	2.09	157	0.51	199	1.07	234	0.91	291	35.76
66	1.10	95	6.69	124	0.89	158	0.30	200	0.41	241	12.38	292	8.24
67	10.76	96	3.00	128	0.56	159	1.72	201	1.44	242	2.35	293	0.96

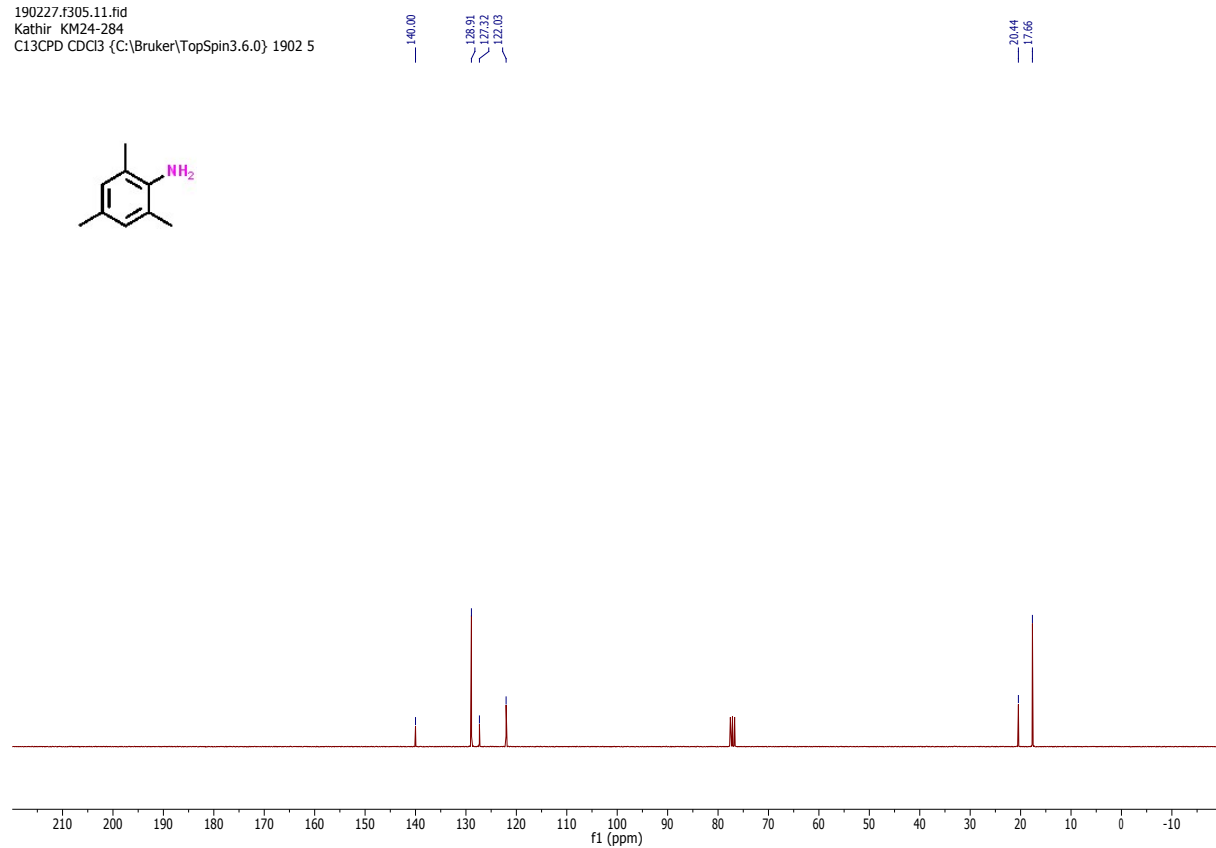
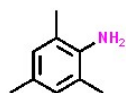
B3016(27:12)6023 19% 19030113 * MS3-Kathir//KM24-171

lim: 0.25%

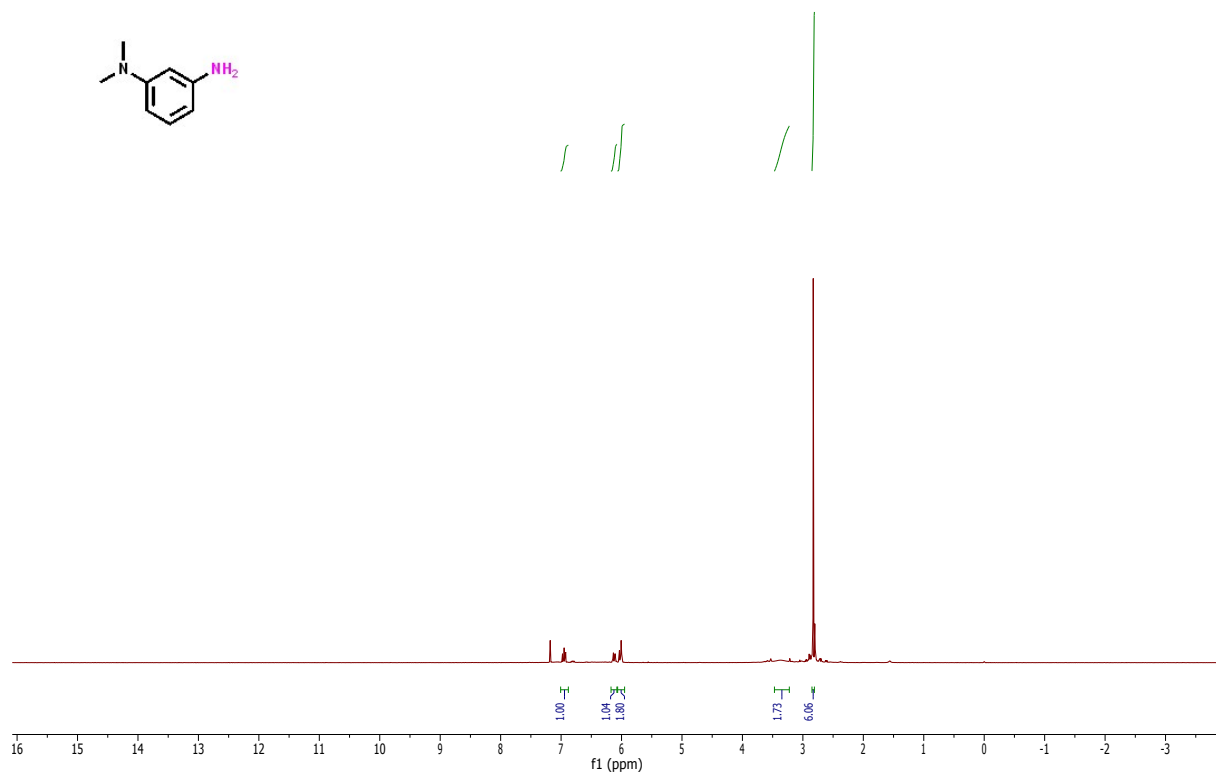
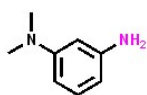
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Kathir KM24-284
PROTON CDCl₃ {C:\Bruker\TopSpin3.6.0} 1902 5



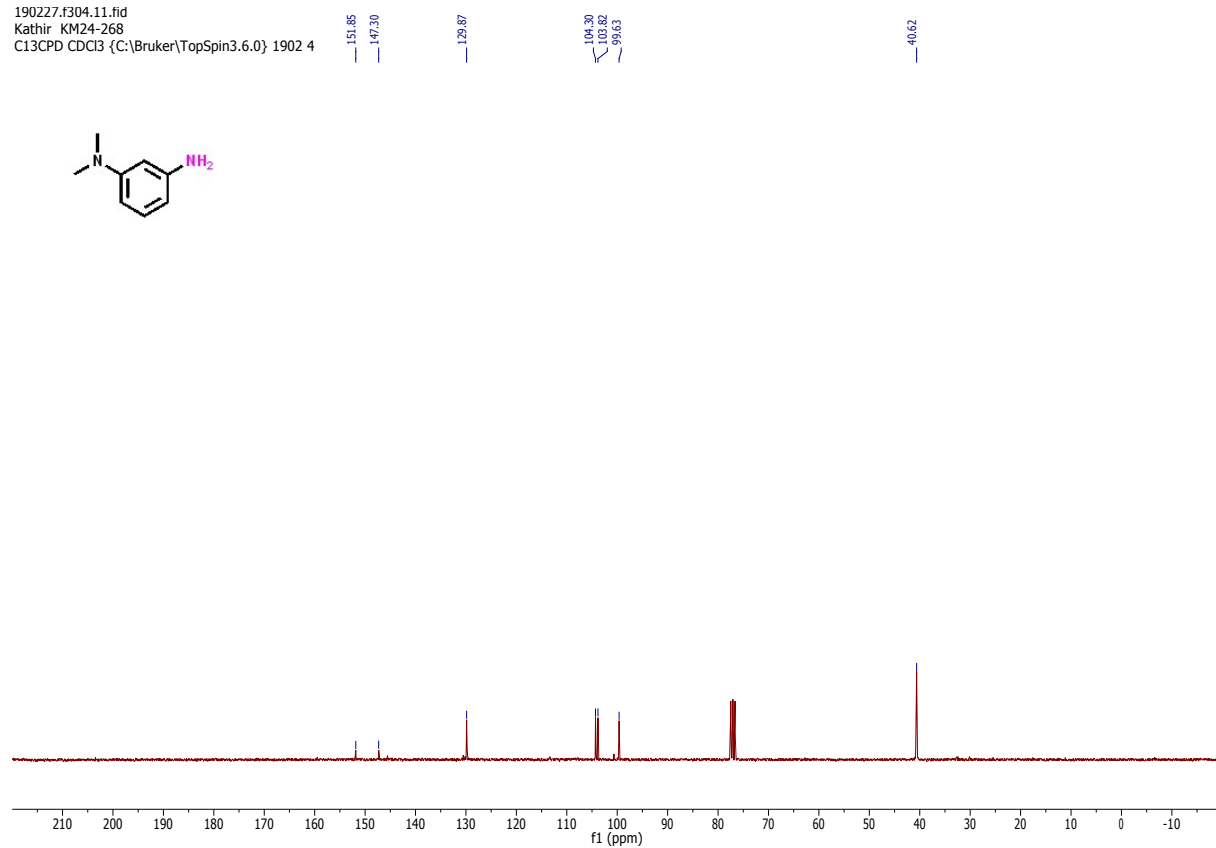
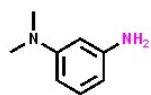
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Kathir KM24-284
Cl₃CPD CDCl₃ {C:\Bruker\TopSpin3.6.0} 1902 5



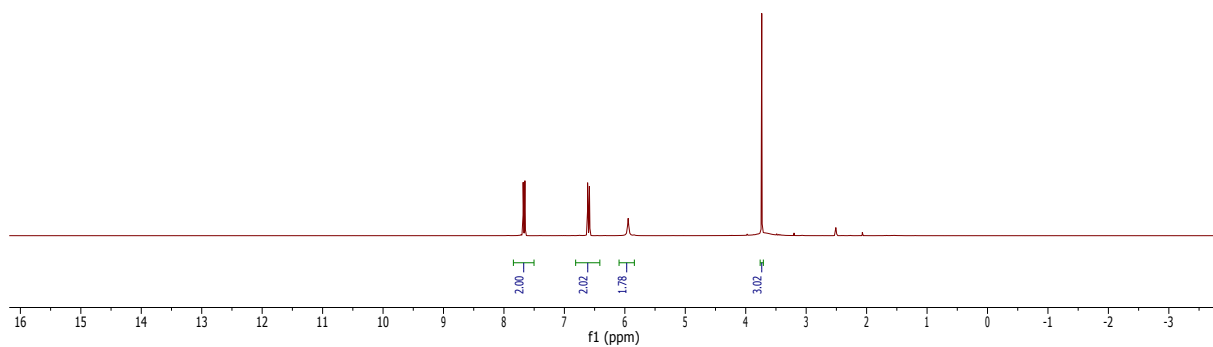
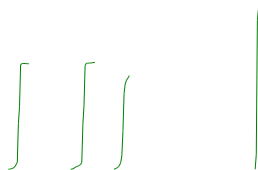
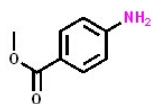
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 Kathir KM24-268
 PROTON CDCl3 {C:\Bruker\TopSpin3.6.0} 1902 4



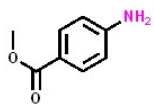
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 Kathir KM24-268
 C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 1902 4



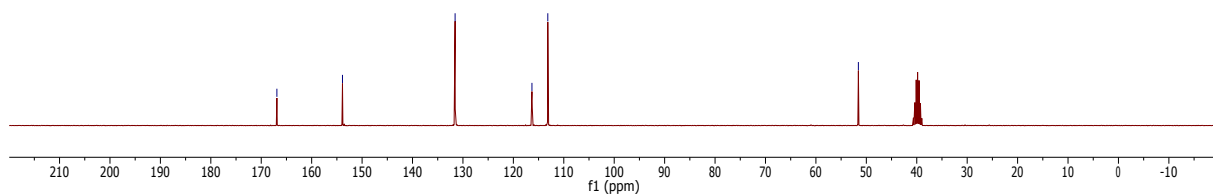
190227.f306.10.fid
 Kathir KM24-94
 PROTON DMSO {C:\Bruker\TopSpin3.6.0} 1902 6



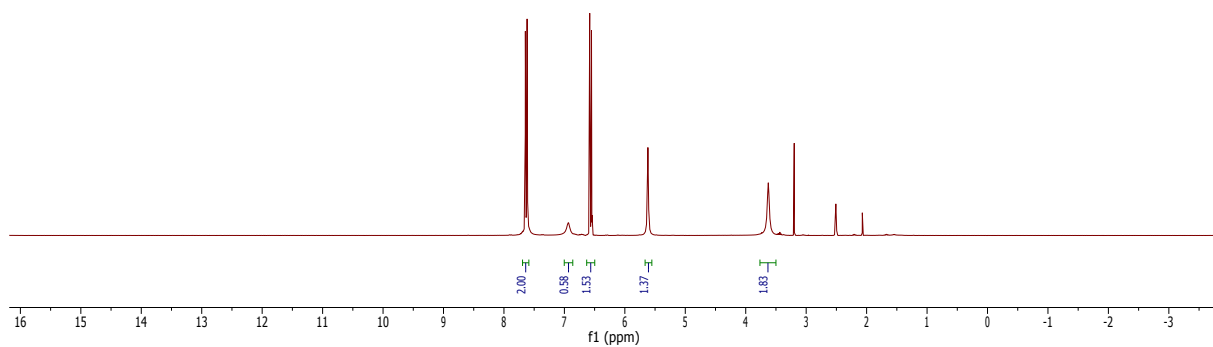
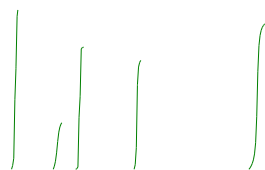
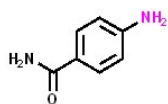
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 Kathir KM24-94
 C13CPD DMSO {C:\Bruker\TopSpin3.6.0} 1902 6



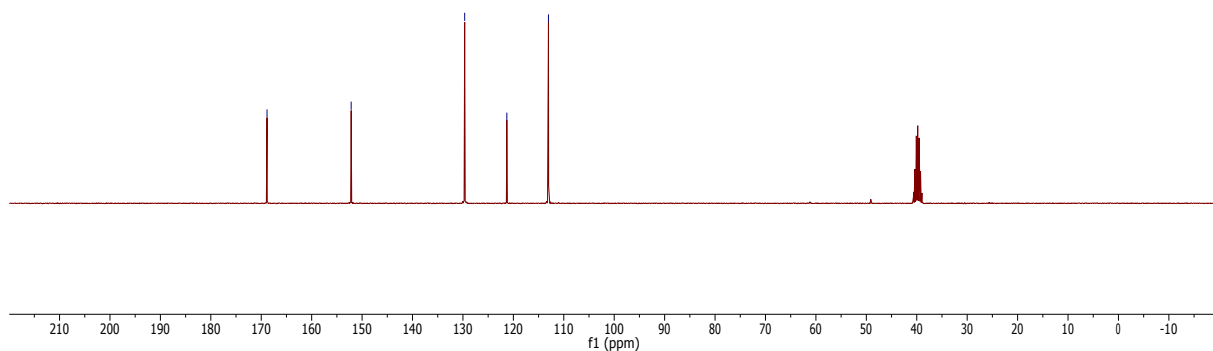
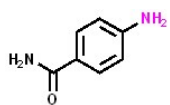
166.90
 153.89
 131.55
 116.31
 113.17
 51.58



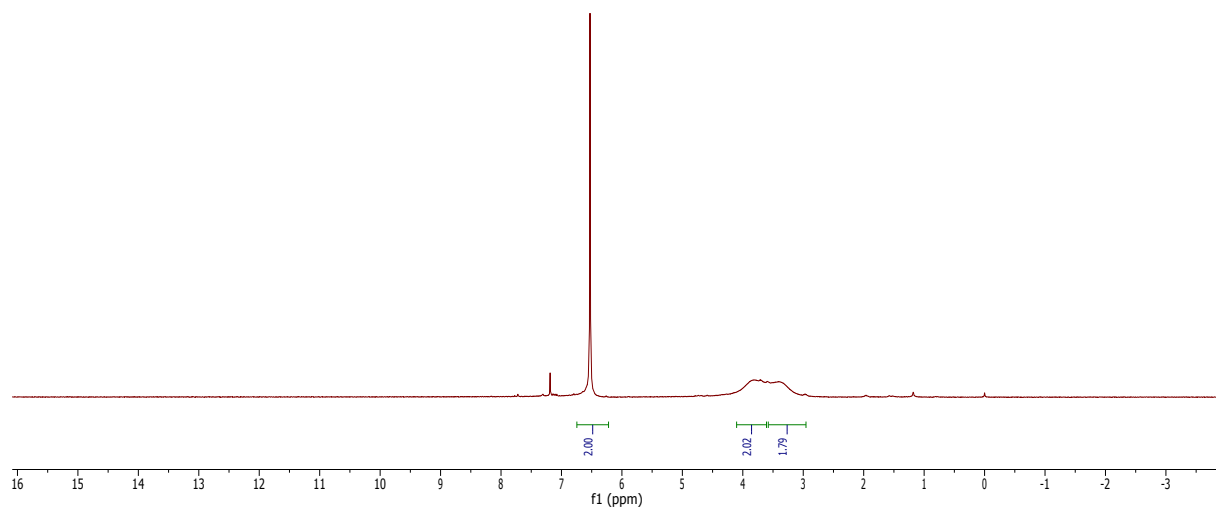
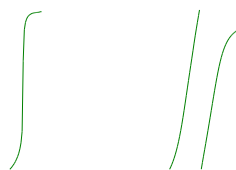
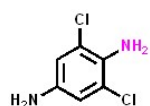
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 Kathir KM24-239
 PROTON DMSO {C:\Bruker\TopSpin3.6.0} 1902 7



190227.f307.11.fid
 Kathir KM24-239
 C13CPD DMSO {C:\Bruker\TopSpin3.6.0} 1902 7

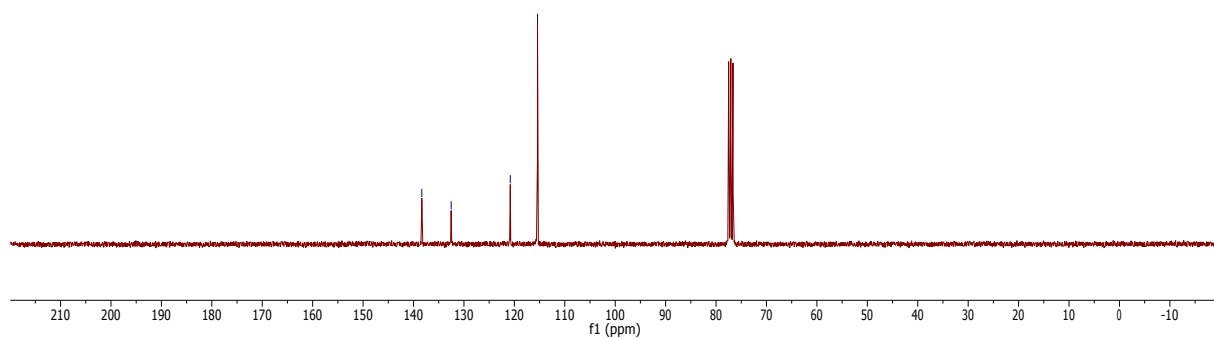
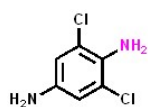


190227.f302.10.fid
 Kathir KM24-237
 PROTON CDCl3 {C:\Bruker\TopSpin3.6.0} 1902 2

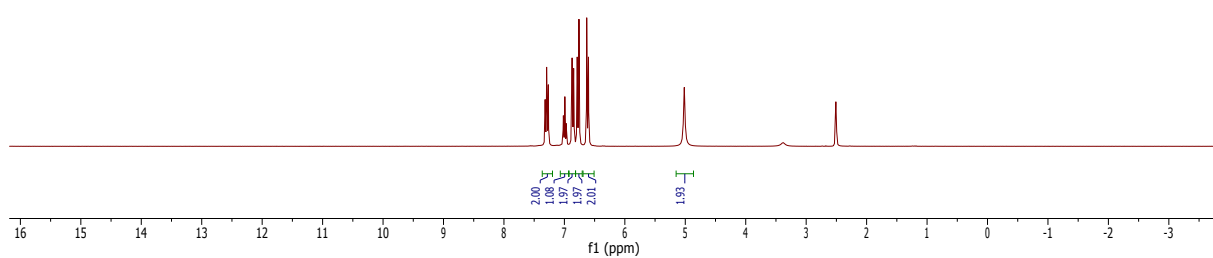
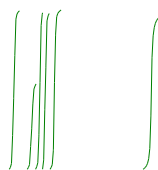
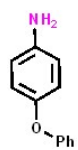


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 Kathir KM24-237
 C13CPD CDCl3 {C:\Bruker\TopSpin3.6.0} 1902 2

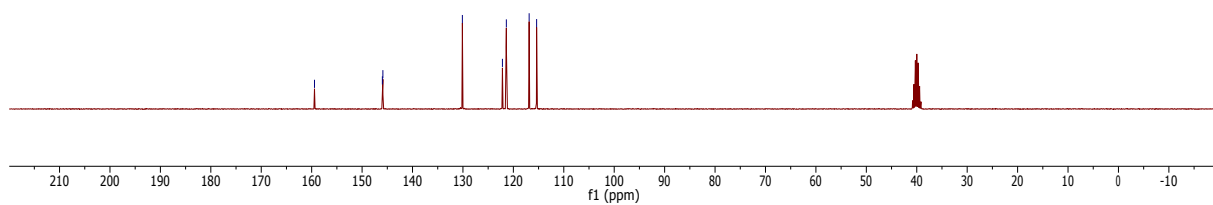
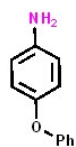
138.36
 132.53
 120.81
 115.41



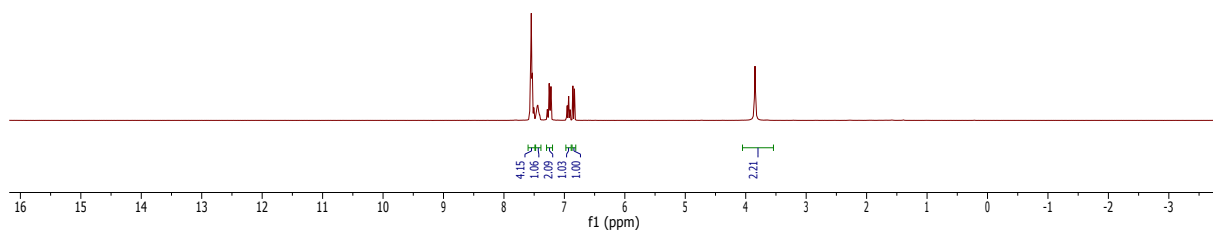
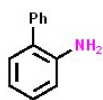
190301.f343.10.fid
 Kathir KM24-227
 PROTON DMSO {C:\Bruker\TopSpin3.6.0} 1903 43



190301.f343.11.fid
 Kathir KM24-227
 C13CPD DMSO {C:\Bruker\TopSpin3.6.0} 1903 43

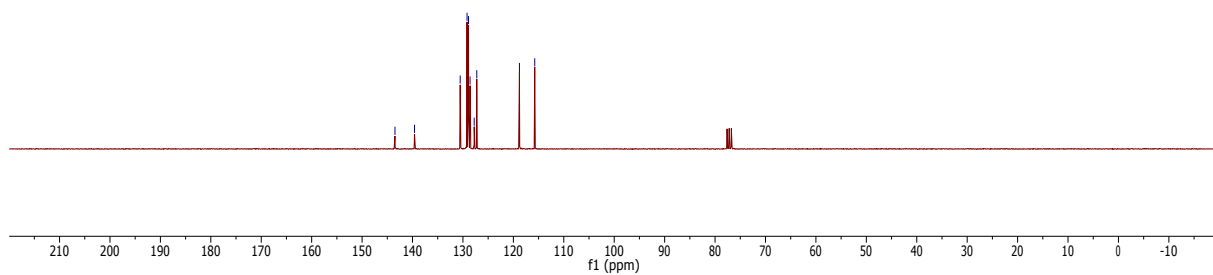
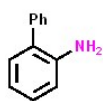


190227.f303.10.fid
Kathir KM24-266
PROTON CDCl₃ {C:\Bruker\TopSpin3.6.0} 1902 3

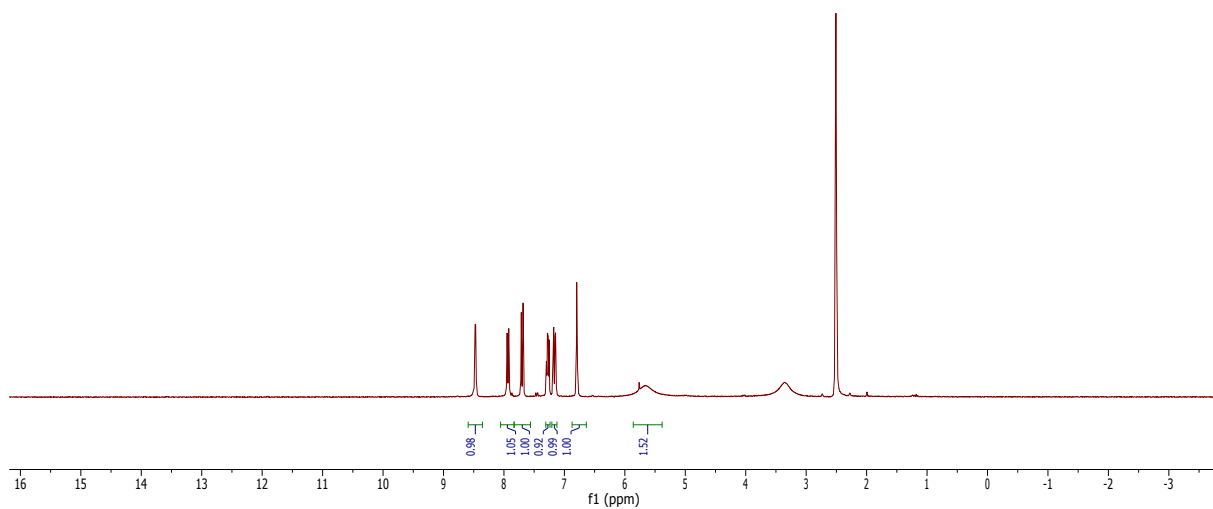
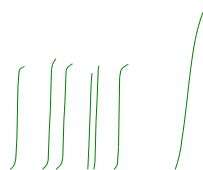
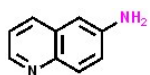


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Kathir KM24-266
C13CPD CDCl₃ {C:\Bruker\TopSpin3.6.0} 1902 3

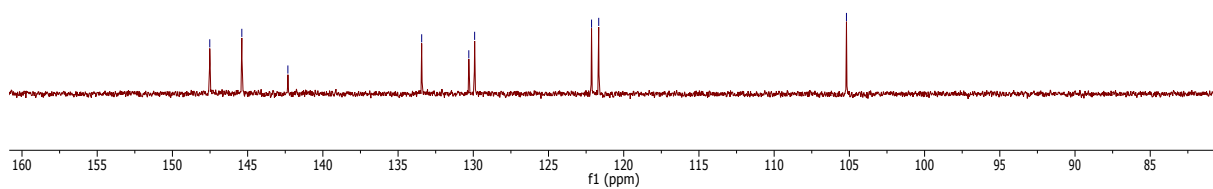
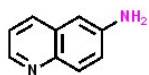
143.48
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129.19
128.90
128.59
127.77
127.26
118.80
115.76



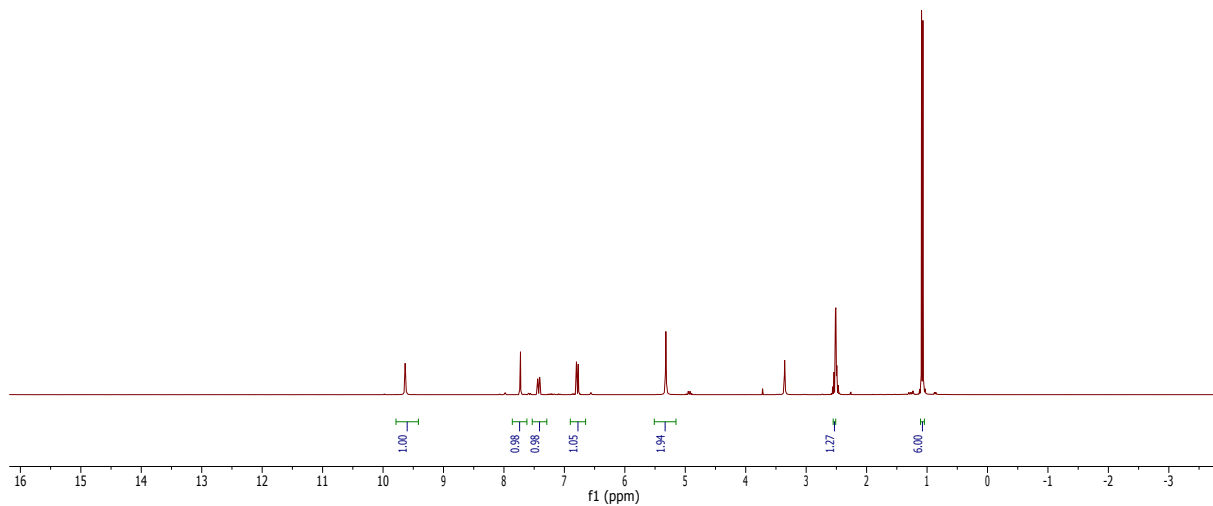
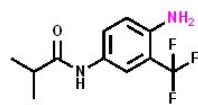
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 Kathir KM24-262
 PROTON DMSO {C:\Bruker\TopSpin3.6.0} 1903 41



190301.f341.11.fid
 Kathir KM24-262
 C13CPD DMSO {C:\Bruker\TopSpin3.6.0} 1903 41



190301.f342.10.fid
 Kathir KM24-264
 PROTON DMSO {C:\Bruker\TopSpin3.6.0} 1903 42



190301.f342.11.fid
 Kathir KM24-264
 C13CPD DMSO {C:\Bruker\TopSpin3.6.0} 1903 42

125.11

142.48

138.85

128.79

127.24

123.64

117.61

117.50

117.45

117.35

111.30

110.91

110.13

35.21

19.97

