Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplemental Information

Regiospecific Deoxygenative Deuteration of Ketones *via* HOME Chemistry

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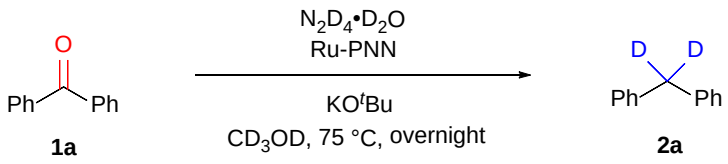
I. General Methods

All reagents and solvents were purchased from commercial sources (Sigma-Aldrich) and used without further purification unless otherwise stated. Ru-PNN was purchased from Sigma-Aldrich, and N_2D_4•D_2O (98% purity) was purchased from Alfa Chemistry. All reactions were carried out under a nitrogen atmosphere unless otherwise stated. Column chromatography was performed on silica gel (200-300 mesh) and visualized with ultraviolet light. Diethyl ether and pentane were used as eluents. ^1H, ^2D and ^{19}F NMR spectra were taken on Bruker AV400, Varian Mercury 400, and Varian/Agilent QANUC 500 with TMS as an internal standard and $CDCl_3$ as solvent unless otherwise stated. ^{13}C NMR spectra were taken on QANUC 800 with 10 seconds relaxation delay to visualize the methylene signal.[1] GC-MS analyses were performed with a Thermo TRACE 1300 ISQ LT spectrometer.

II. Optimization of Reaction Conditions

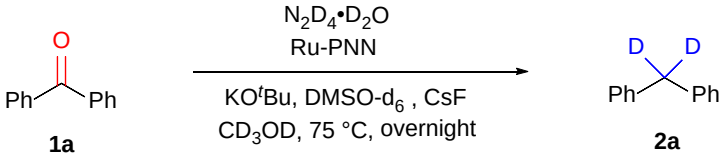
1) Table S1. Screening additive and deuterium hydrazine purity in CD_3OD[a]



entry	additive	N_2D_4•D_2O purtity (%D)	yield(%)[b]	%D[c]
1	DMSO	90	67	78
2	DMSO	98	83	91
3	dDMSO	98	89	94
4	-	98	87	95
5	dDMSO, CsF	98	83	96
6	CsF	98	79	96
7[d]	dDMSO, CsF	98	73	96

[a] **1a** (36.5 mg, 0.2 mmol, 1.0 equiv), N_2D_4·D_2O (50 µL, 1.0 mmol, 5.0 equiv), CD_3OD (0.2 mL), Ru-PNN (4.5 mg, 0.006 mmol, 3 mol%), KOtBu (44.8 mg, 0.4 mmol, 2.0 equiv), additive: DMSO (2.6 µL, 0.04 mmol, 20 mol%), DMSO-d_6 (2.6 µL, 0.04 mmol, 20 mol%), CsF (15 mg, 0.1 mmol, 50 mol%), 75°C, overnight, under N_2. [b] Yields were determined by crude ^1H NMR using mesitylene as an internal standard. [c] Deuterium contents were determined by crude ^2D NMR using $CDCl_3$ as an internal standard. [d]Dry CD_3OD was used from ampoule.

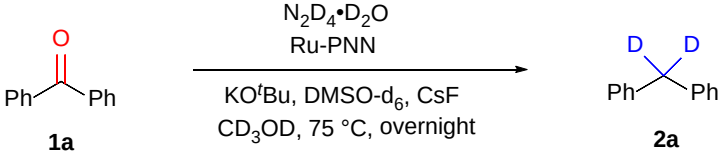
2) Table S2. Screening the amount of CsF in CD_3OD[a]



entry	CsF (equiv)	yield(%)[b]	%D[c]
1	0.5	73	96
2	1	73	92
3	1.5	65	92

[a] **1a** (36.5 mg, 0.2 mmol, 1.0 equiv), $N_2D_4 \cdot D_2O$ (50 µL, 1.0 mmol, 5.0 equiv), dry CD_3OD (0.2 mL), Ru-PNN (4.5 mg, 0.006 mmol, 3 mol%), KOtBu (44.8 mg, 0.4 mmol, 2.0 equiv), additive: DMSO-d_6 (2.6 µL, 0.04 mmol, 20 mol%), CsF (15 mg, 0.1 mmol, 50 mol%), 75°C, overnight, under N_2. [b] Yields were determined by crude ^{1}H NMR using mesitylene as an internal standard. [c] Deuterium contents were determined by crude ^{2}D NMR using $CDCl_3$ as an internal standard.

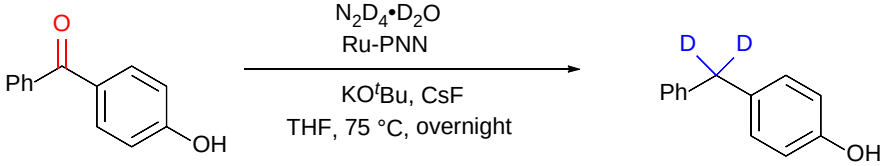
3) Table S3. Screening additive in CD_3OD[a]



entry	D_2O (µl)	yield(%)[b]	%D[c]
1	10	67	95
2	20	63	96
3	30	75	96

[a] **1a** (36.5 mg, 0.2 mmol, 1.0 equiv), $N_2D_4 \cdot D_2O$ (50 µL, 1.0 mmol, 5.0 equiv), dry CD_3OD (0.2 mL), Ru-PNN (4.5 mg, 0.006 mmol, 3 mol%), KOtBu (44.8 mg, 0.4 mmol, 2.0 equiv), additive: DMSO-d_6 (2.6 µL, 0.04 mmol, 20 mol%), CsF (15 mg, 0.1 mmol, 50 mol%), 75°C, overnight, under N_2. [b] Yields were determined by crude ^{1}H NMR using mesitylene as an internal standard. [c] Deuterium contents were determined by crude ^{2}D NMR using $CDCl_3$ as an internal standard.

4) Table S4. Screening co-solvent with 4-hydroxybenzophenone[a]

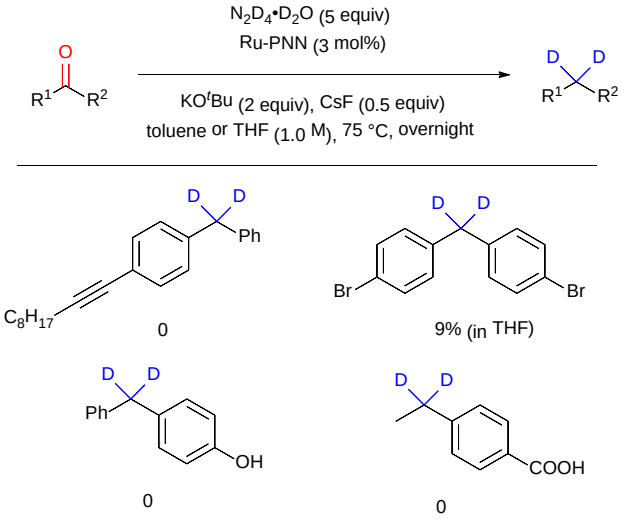


entry	Co-solvent	yield(%)[b]
1	d_6-DMSO	0
2	D_2O	4
3	CD_3OD	0

[a] Ketone (39.6 mg, 0.2 mmol, 1.0 equiv), $N_2D_4 \cdot D_2O$ (50 µL, 1.0 mmol, 5.0 equiv), dry THF (0.1 mL), co-solvent (0.1 ml), Ru-PNN (4.5 mg, 0.006 mmol, 3 mol%), KOtBu (44.8 mg, 0.4 mmol, 2.0 equiv), CsF (15 mg, 0.1 mmol, 50 mol%), 75°C, overnight, under N_2. [b] Yields were determined by crude ^{1}H NMR using mesitylene as an internal standard.

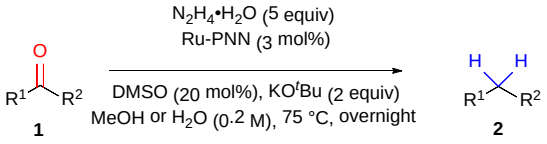
III. Other Substrates

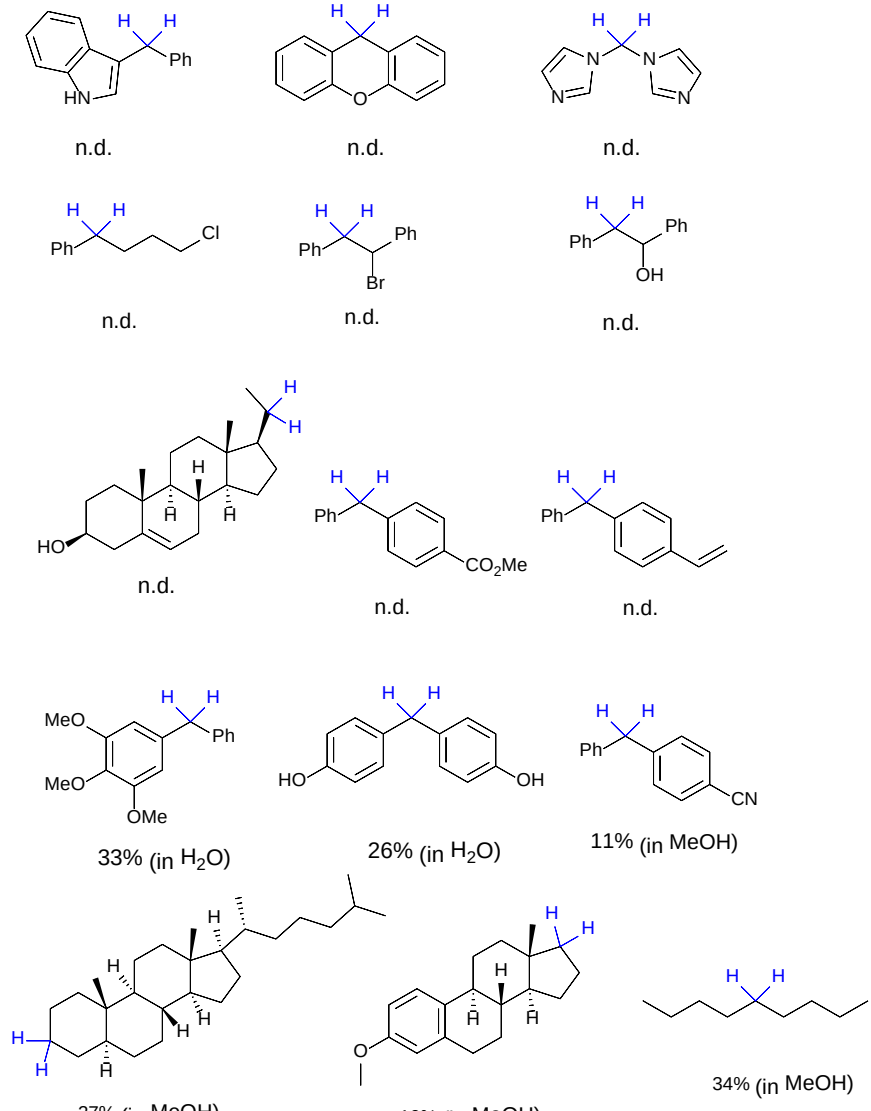
Scheme S1. Substrates not tolerated[a, b]



[a] **1** (0.2 mmol, 1.0 equiv), $N_2D_4 \cdot D_2O$ (50 µL, 1.0 mmol, 5.0 equiv), dry toluene or dry THF (0.2 mL), Ru-PNN (4.5 mg, 0.006 mmol, 3 mol%), KOtBu (44.8 mg, 0.4 mmol, 2.0 equiv), additive: CsF (15 mg, 0.1 mmol, 50 mol%), 75°C, overnight, under N_2. [b] Yields were determined by crude ^{1}H NMR using mesitylene as an internal standard.

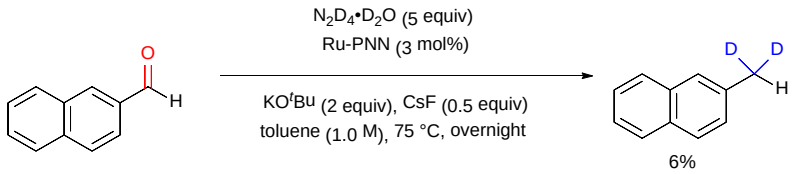
Scheme S2. Substrates not tolerated for previous deoxygenation[a]





[a] **1** (0.2 mmol, 1.0 equiv), $N_2H_4 \cdot H_2O$ (50 µL, 1.0 mmol, 5.0 equiv), methanol or water (0.2 mL), Ru-PNN (4.5 mg, 0.006 mmol, 3 mol%), KOtBu (44.8 mg, 0.4 mmol, 2.0 equiv), additive: DMSO (2.6 µL, 0.04 mmol, 20 mol%), 75°C, overnight, under N_2. [b] Yields were determined by crude ^{1}H NMR using mesitylene as an internal standard.

Scheme S3. Investigation of aldehyde[a, b]



[a] Aldehyde (0.2 mmol, 1.0 equiv), $N_2D_4 \cdot D_2O$ (50 µL, 1.0 mmol, 5.0 equiv), dry toluene (0.2 mL), Ru-PNN (4.5 mg, 0.006 mmol, 3 mol%), KOtBu (44.8 mg, 0.4 mmol, 2.0 equiv), additive: CsF (15 mg, 0.1 mmol, 50 mol%), 75°C, overnight, under N_2. [b] Yields were determined by crude ^{1}H NMR using mesitylene as an internal standard.

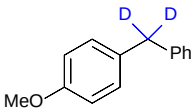
IV. General Procedure for the Deoxygenation of Ketones

A 10 mL V-shape frame-dry microwave vial with a magnetic stir-bar was transferred to glovebox and charged with Ru-PNN (4.5 mg, 0.006 mmol, 3 mol%), KOtBu (44.8 mg, 0.4 mmol, 2.0 equiv) ketone (0.2 mmol, 1.0 equiv), and CsF (15.0 mg, 0.1 mmol, 0.5 equiv). Dry toluene or THF was charged via a 1 mL plastic syringe, and deuterium hydrazine monohydrate (50 µL, 1.0 mmol, 5.0 equiv) was charged via Hamilton microliter syringe. The tube was sealed with an aluminum cap adapted with a septum and taken out from the glovebox. The tube was placed in a preheated oil bath at 75 °C and the mixture was stirred under an N_2 atmosphere overnight. The reaction mixture was cooled to room temperature, diluted with diethyl ether, filtered through anhydrous $MgSO_4$ followed by silica gel, concentrated, and charged with mesitylene (9.2 µL, 0.067 mmol, 0.33 equiv), DMSO-d_6 (14.1 µL, 0.2 mmol, 1.0 equiv). The ^{1}H and ^{2}D NMR data was taken, and the crude mixture was purified by column chromatography on silica gel under argon eluting with pentane: Et_2O (10:1). The solvent was frozen in an ice-water bath and gently evacuated by vacuum to afford the products.

V. Characterization of Products

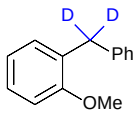
diphenylmethane-d2

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 – 7.24 (m, 5H), 7.24 – 7.16 (m, 5H). ^{2}D NMR (77 MHz, $CDCl_3$) δ 3.98. ^{13}C NMR (201 MHz, $CDCl_3$) δ 141.2, 129.1, 128.6, 126.2, 43.0 – 40.7 (m, $J_{D\text{-}C}$=20.1 Hz). IR wavenumber (cm^{-1}) 3082.6, 3059.3, 3024.3, 1509.7, 1493.2, 1447.1, 696.2. HRMS calc. for $C_{13}H_{10}D$ [M-D]-: 168.0918; found, 168.0915.



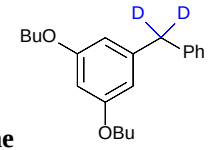
1-methoxy-4-(phenylmethyl-d2)benzene

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 – 7.27 (m, 2H), 7.23 – 7.14 (m, 3H), 7.14 – 7.07 (m, 2H), 6.87 – 6.80 (m, 2H), 3.78 (s, 3H). ^{2}D NMR (77 MHz, $CDCl_3$) δ 3.91. ^{13}C NMR (201 MHz, $CDCl_3$) δ 158.1, 141.7 (d, $J_{D\text{-}C}$ = 7.3 Hz), 133.4 (d, $J_{D\text{-}C}$ = 6.4 Hz), 130.0, 128.9, 128.6, 126.1, 114.0 (d, $J_{D\text{-}C}$ = 22.6 Hz), 55.4, 42.9 – 39.3 (m, $J_{D\text{-}C}$=20.1 Hz). IR wavenumber (cm^{-1}) 3059.1, 3024.7, 2999.9, 2952.7, 2931.7, 2904.5, 2833.6, 1493.0, 1472.1, 1294.3. HRMS calc. for $C_{14}H_{13}D_2O$ [M+H]+: 201.12430; found, 201.12379.



1-methoxy-2-(phenylmethyl-d2)benzene

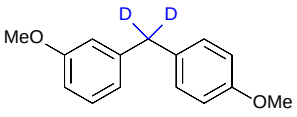
^{1}H NMR (800 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 2H), 7.22 – 7.16 (m, 3H), 7.14 – 7.05 (m, 2H), 6.86 – 6.80 (m, 2H), 3.78 (s, 3H). ^{2}D NMR (61 MHz, $CDCl_3$) δ 3.92. ^{13}C NMR (201 MHz, $CDCl_3$) δ 158.1, 141.7, 133.3, 130.0, 129.0, 128.6, 128.5, 126.1, 114.0, 113.9, 55.4, 41.2 – 40.2 (m, $J_{D\text{-}C}$=20.1 Hz). IR wavenumber (cm^{-1}) 3025.4, 2953.8, 2833.5, 1509.4, 1491.1, 1089.6, 1006.5. HRMS calc. for $C_{14}H_{13}D_2O$ [M+H]+: 201.12430; found, 201.12382.



1,3-dibutoxy-5-(phenylmethyl-d2)benzene

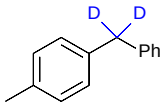
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35 – 7.09 (m, 5H), 6.96 (d, *J* = 8.2 Hz, 1H), 6.44 (d, *J* = 2.4 Hz, 1H), 6.39 (dd, *J* = 8.2, 2.4 Hz, 1H), 3.92 (dt, *J* = 7.5, 6.5 Hz, 4H), 1.82 – 1.63 (m, 4H), 1.54 – 1.35 (m, 4H), 0.95 (dt, *J* = 17.5, 7.4 Hz, 6H). ^{13}C NMR (201 MHz, $CDCl_3$) δ 159.0, 157.8, 141.8, 130.6, 129.0, 128.3, 125.7, 122.2, 104.6, 99.9, 67.9, 67.7, 35.7 – 34.6 (m, J_{D-C}=20.1 Hz), 31.6, 31.5, 19.4, 14.0, 14.0. ^{2}D NMR (61 MHz, $CDCl_3$) δ 3.88. IR wavenumber (cm^{-1}) 3024.3, 2957.4, 2932.2, 2870.5, 1643.2, 1610.3, 1503.9, 1173.3, 1126.8. HRMS calc. for $C_{21}H_{27}D_2O_2$ [M+H]+: 315.2288; found, 315.2280.

1-methoxy-3-((4-methoxyphenyl)methyl-d2)benzene



^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (td, *J* = 7.7, 0.8 Hz, 1H), 7.15 – 7.07 (m, 2H), 6.87 – 6.80 (m, 2H), 6.80 – 6.69 (m, 3H), 3.78 (s, 3H), 3.77 (s, 3H). ^{2}D NMR (61 MHz, $CDCl_3$) δ 3.88. ^{13}C NMR (201 MHz, $CDCl_3$) δ 159.8, 158.1, 143.3, 133.1, 130.0, 129.5, 121.4, 114.8, 114.0, 111.4, 55.4, 55.3, 40.3 – 41.0 (m, J_{D-C}=20.1 Hz). IR wavenumber (cm^{-1}) 3025.5, 2999.0, 2954.8, 2905.6, 2833.5, 1509.6, 1486.0, 1243.4, 1007.9. HRMS calc. for $C_{15}H_{14}D_2O_2$ [M]+: 230.1270; found, 230.1277.

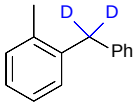
1-methyl-4-(phenylmethyl-d2)benzene



(with deuterium at p-methyl group)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 2H), 7.19 (ddt, *J* = 7.0, 3.4, 1.5 Hz, 3H), 7.10 (d, *J* = 0.9 Hz, 4H), 2.32 (s, 3H), [-CH_2D, -CHD_2: 2.32 – 2.30 (m, 1H), 2.29 (q, *J* = 2.2 Hz, 0H)]. ^{2}D NMR (61 MHz, $CDCl_3$) δ 3.94, [-CH_2D, -CHD_2, -CD_3: 2.37, 2.34, 2.30]. ^{13}C NMR (201 MHz, $CDCl_3$) δ 141.5, 138.2, 135.7, 129.3, 129.0, 128.9, 128.6, 126.1, 41.9 – 40.6 (m, J_{D-C}=20.1 Hz), 21.2, [substrates with deuterium at p-methyl group: 141.5, 138.2, 135.7 – 135.6 (m), 21.0 – 20.3 (m)]. IR wavenumber (cm^{-1}) 3022.5, 2921.1, 1512.1, 1492.8, 1008.4. HRMS calc. for $C_{14}H_{12}D_2$ [M]+: 184.1216; found, 184.1211. [HRMS calc. for $C_{14}H_{11}D_3$ [M]+: 185.1278; found, 185.1276.]

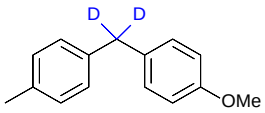
1-methyl-2-(phenylmethyl-d2)benzene



(with deuterium at o-methyl group)

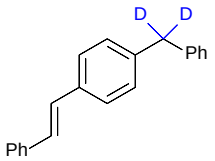
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.24 (m, 2H), 7.22 – 7.08 (m, 7H), 2.25 (s, 3H), [-CH_2D, -CHD_2: 2.24 – 2.22 (m, 0H)]. ^{2}D NMR (61 MHz, $CDCl_3$) δ 3.98, [-CH_2D, -CHD_2, -CD_3:2.30, 2.27, 2.23]. ^{13}C NMR (201 MHz, $CDCl_3$) δ 140.5, 139.0, 136.8, 130.4, 130.1, 128.9, 128.5, 126.6, 126.1, 126.1, 39.5 – 38.7 (m, J_{D-C}=20.1 Hz), 19.8, [substrates with deuterium at o-methyl group: 140.5, 139.0, 136.7, 19.7 – 19.4 (m)]. IR wavenumber (cm^{-1}) 3059.1, 3023.6, 2952.1, 2833.4, 1509.8, 1491.7, 1090.0, 1031.9. HRMS calc. for $C_{14}H_{12}D_2$ [M]+: 184.1216; found, 184.1202. [HRMS calc. for $C_{14}H_{11}D_3$ [M]+: 185.1278; found, 185.1268.]

1-methoxy-4-(p-tolylmethyl-d2)benzene

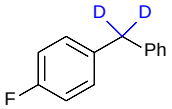


(with deuterium at p-methyl group)

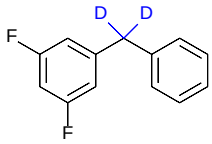
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 – 7.04 (m, 6H), 6.87 – 6.79 (m, 2H), 3.79 (s, 3H), 2.32 (s, 3H), [-CH_2D, -CHD_2: 2.30 (dt, *J* = 6.5, 2.2 Hz, 1H)]. ^{2}D NMR (61 MHz, $CDCl_3$) δ 3.88, [-CH_2D, -CHD_2, -CD_3:2.37, 2.33, 2.30]. ^{13}C NMR (201 MHz, $CDCl_3$) δ 158.0, 138.6, 135.6, 133.6, 129.9, 129.3, 128.8, 114.0, 55.4, 40.5 – 40.0 (m, J_{D-C}=20.1 Hz), 21.1 [substrates with deuterium at p-methyl group: 138.7, 135.5 – 135.5 (m), 133.7, 21.0 –20.1 (m)]. IR wavenumber (cm^{-1}) 2998.8, 2952.6, 2905.6, 2833.7, 1509.1, 1242.5, 1111.3, 1036.1. HRMS calc. for $C_{15}H_{14}D_2O$ [M]+: 214.1321; found, 214.1313. [HRMS calc. for $C_{15}H_{13}D_3O$ [M]+: 215.1384; found, 215.1378.]

(E)-1-(phenylmethyl-d2)-4-styrylbenzene 

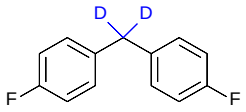
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.47 (m, 2H), 7.47 – 7.41 (m, 2H), 7.35 (t, *J* = 7.7 Hz, 2H), 7.32 – 7.24 (m, 3H), 7.24 – 7.17 (m, 5H), 7.07 (d, *J* = 1.6 Hz, 2H). ^{2}D NMR (61 MHz, $CDCl_3$) δ 3.98. ^{13}C NMR (201 MHz, $CDCl_3$) δ 141.1, 140.8, 137.6, 135.4, 129.4, 129.0, 128.8, 128.7, 128.6, 128.3, 127.6, 126.8, 126.6, 126.3. IR wavenumber (cm^{-1}) 3078.7, 3051.0, 3021.2, 1509.4, 1491.8, 1447.2, 960.2, 945.1. HRMS calc. for $C_{21}H_{17}D_2$ [M+H]+: 273.1607; found, 273.1620.

1-fluoro-4-(phenylmethyl-d2)benzene 

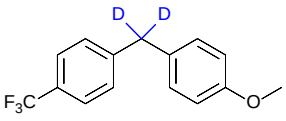
^{1}H NMR (800 MHz, $CDCl_3$) δ 7.25 – 7.20 (m, 2H), 7.16 – 7.12 (m, 1H), 7.11 – 7.08 (m, 2H), 7.07 – 6.97 (m, 2H), 6.91 – 6.88 (m, 2H). ^{2}D NMR (61 MHz, $CDCl_3$) δ 3.95. ^{13}C NMR (201 MHz, $CDCl_3$) δ 161.6 (d, $J_{C\text{-}F}$= 244.0 Hz), 141.0 (d, $J_{C\text{-}F}$= 7.1 Hz), 136.8, 130.4 (d, $J_{C\text{-}F}$= 7.8 Hz), 129.0, 128.7, 126.4, 115.4 (d, $J_{C\text{-}F}$= 21.3 Hz), 41.2 – 40.3 (m, $J_{D\text{-}C}$=20.1 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -117.42. IR wavenumber (cm^{-1}) 2955.2, 2927.0, 2856.3, 1082.80, 1032.2. HRMS calc. for $C_{13}H_9DF$ [M-D]-: 186.08238; found, 186.08229.

1,3-difluoro-5-(phenylmethyl-d2)benzene 

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.30 (m, 3H), 7.29 – 7.23 (m, 1H), 7.22 – 7.16 (m, 2H), 6.79 – 6.68 (m, 2H). ^{2}D NMR (77 MHz, $CDCl_3$) δ 3.94. ^{13}C NMR (201 MHz, $CDCl_3$) δ 163.2 (dd, $J_{C\text{-}F}$= 248.2, 12.9 Hz), 145.1 (t, $J_{C\text{-}F}$= 8.4 Hz), 139.5, 129.1, 128.9, 126.8, 111.8 (dd, $J_{C\text{-}F}$= 20.4, 4.3 Hz), 102.1 – 101.1 (m), 42.3 – 40.7 (m, $J_{D\text{-}C}$=20.1 Hz). ^{19}F NMR (471 MHz, $CDCl_3$) δ -110.39, -110.66. IR wavenumber (cm^{-1}) 2955.3, 2928.9, 2857.0, 1082.0, 1032.1. HRMS calc. for $C_{13}H_8D_2F_2$ [M]+: 206.0871; found, 206.0864.

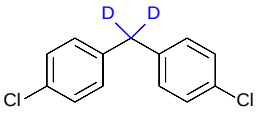
bis(4-fluorophenyl)methane-d2 

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.11 (dd, *J* = 8.5, 5.3 Hz, 4H), 7.03 – 6.89 (m, 4H). ^{2}D NMR (77 MHz, $CDCl_3$) δ 3.90. ^{19}F NMR (471 MHz, $CDCl_3$) δ -117.15. ^{13}C NMR (201 MHz, $CDCl_3$) δ 161.63 (d, $J_{C\text{-}F}$= 244.3 Hz), 136.67, 130.33 (d, $J_{C\text{-}F}$= 7.9 Hz), 115.45 (d, $J_{C\text{-}F}$= 21.3 Hz), 40.6 – 39.9 (m, $J_{D\text{-}C}$=20.1 Hz). IR wavenumber (cm^{-1}) 3050.7, 3021.7, 1507.6, 1492.3. HRMS calc. for $C_{13}H_7D_2F_2$ [M-H]-: 205.0792; found, 205.0795.

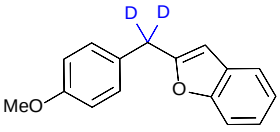
1-methoxy-4-((4-(trifluoromethyl)phenyl)methyl-d2)benzene 

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 11.7 Hz, 2H), 7.14 – 7.04 (m, 2H), 6.84 (d, *J* = 8.6 Hz, 2H), 3.79 (s, 3H). ^{2}D NMR (61 MHz, $CDCl_3$) δ 4.04. ^{19}F NMR (376 MHz, cdcl$_3$) δ -62.36. ^{13}C NMR (201 MHz, $CDCl_3$) δ 158.4, 145.8, 132.2, 130.0, 129.2, 128.6, 128.5, 125.5 (q, $J_{C\text{-}F}$= 3.7 Hz), 114.2, 55.4, 41.2 – 40.2 (m,

$J_{D\text{-}C}$=20.1 Hz). IR wavenumber (cm^{-1}) 3059.7, 3025.6, 1264.4, 1246.0. HRMS calc. for $C_{15}H_{11}D_2F_3O$ [M]+: 268.1039; found, 268.1049.

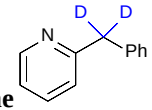
bis(4-chlorophenyl)methane-d2 

^{1}H NMR (800 MHz, $CDCl_3$) δ 7.26 (d, *J* = 8.2 Hz, 4H), 7.09 (d, *J* = 8.5 Hz, 4H). ^{2}D NMR (61 MHz, $CDCl_3$) δ 3.90. ^{13}C NMR (201 MHz, $CDCl_3$) δ 139.1, 132.3, 130.3, 128.8, 40.7 – 39.7 (m, $J_{D\text{-}C}$=20.1 Hz). IR wavenumber (cm^{-1}) 3026.9, 2925.9, 1489.5, 1088.8, 1006.6. HRMS calc. for $C_{13}H_8DCl_2$ [M-D]-: 236.01386; found, 236.01342.

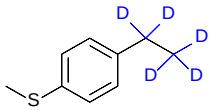
2-((4-methoxyphenyl)methyl-d2)benzofuran 

(with deuterium at furan)

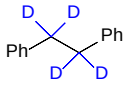
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 – 7.37 (m, 2H), 7.33 – 7.09 (m, 4H), 6.87 (d, *J* = 8.7 Hz, 2H), 6.35 (s, 1H), 3.80 (s, 3H). ^{2}D NMR (77 MHz, $CDCl_3$) δ 4.03. ^{13}C NMR (201 MHz, $CDCl_3$) δ 158.5, 155.0, 129.9, 129.2, 128.8, 128.8, 123.3, 122.5, 120.4, 114.0, 110.9, 103.1, 55.3, 30.2 – 29.7 (m, $J_{D\text{-}C}$=20.1 Hz). IR wavenumber (cm^{-1}) 2954.1, 2926.1, 2835.8, 1508.9, 1453.3, 1235.6, 1174.4. HRMS calc. for $C_{16}H_{13}D_2O_2$ [M+H]+: 241.1192; found, 241.1185.

2-(phenylmethyl-d2)pyridine 

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (dd, *J* = 5.3, 2.1 Hz, 1H), 7.56 (td, *J* = 7.7, 1.9 Hz, 1H), 7.38 – 7.24 (m, 4H), 7.24 – 7.14 (m, 1H), 7.14 – 6.98 (m, 2H). ^{2}D NMR (61 MHz, $CDCl_3$) δ 4.15. ^{13}C NMR (201 MHz, $CDCl_3$) δ 161.1, 149.5, 139.6, 136.7, 129.2, 128.7, 126.5, 123.2, 121.4, 44.9 – 43.8 (m, $J_{D\text{-}C}$=20.1 Hz). IR wavenumber (cm^{-1}) 2959.1, 2869.8, 1090.5, 635.7. HRMS calc. for $C_{12}H_{10}D_2N$ [M+H]+: 172.10898; found, 172.10857.

(4-(ethyl-d5)phenyl)(methyl)sulfane 

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 – 7.17 (m, 2H), 7.16 – 7.09 (m, 2H), 2.47 (s, 3H). ^{2}D NMR (61 MHz, $CDCl_3$) δ 2.57, 1.18. ^{13}C NMR (201 MHz, $CDCl_3$) δ 141.6, 135.1, 128.6, 127.5, 30.5, 16.6. IR wavenumber (cm^{-1}) 2955.5, 2928.7, 2856.8, 1081.6. HRMS calc. for $C_9H_6D_5S$ [M-H]-: 156.0890; found, 156.0888.

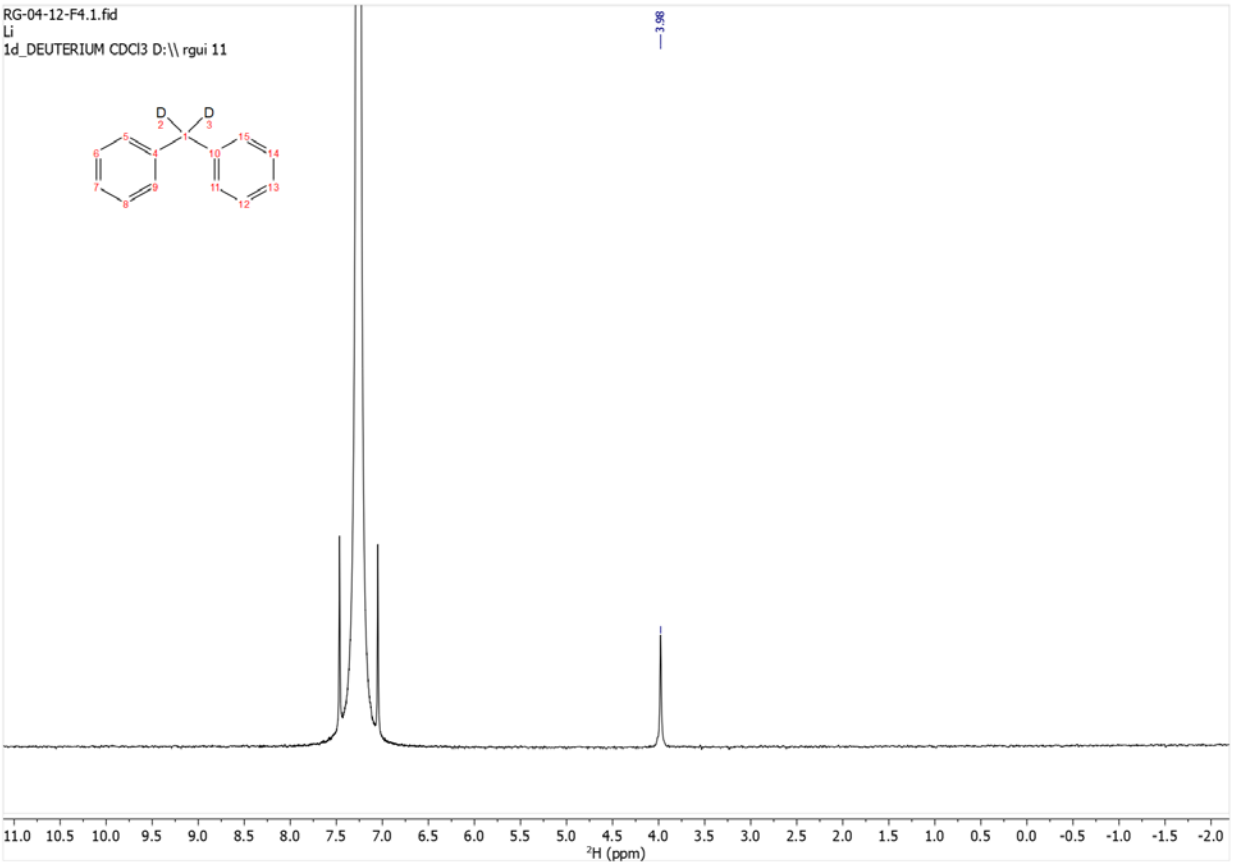
1,2-diphenylethane-1,1,2,2-d4 

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 5H), 7.23 – 7.10 (m, 5H). ^{2}D NMR (61 MHz, $CDCl_3$) δ 2.90. ^{13}C NMR (201 MHz, $CDCl_3$) δ 141.9, 128.6, 128.5, 126.1, 37.9 – 37.4 (m, $J_{D\text{-}C}$=20.1 Hz). IR wavenumber (cm^{-1}) 1084.6, 1006.2. HRMS calc. for $C_9H_6D_5S$ [M-H]-: 156.0890; found, 156.0888. HRMS calc. for $C_{14}H_{10}D_3$ [M-D]-: 184.1200; found, 184.1198.

VI. References

1. G. Facey, *Finding "Lost" Deuterated ^{13}C Signals.*

VII. Copies of IR, HRMS, ^{1}H NMR, ^{2}D NMR, ^{13}C NMR, and ^{19}F NMR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1d_DEUTERIUM CDCl3 D:\\ rgui 11
D
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3.98
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0
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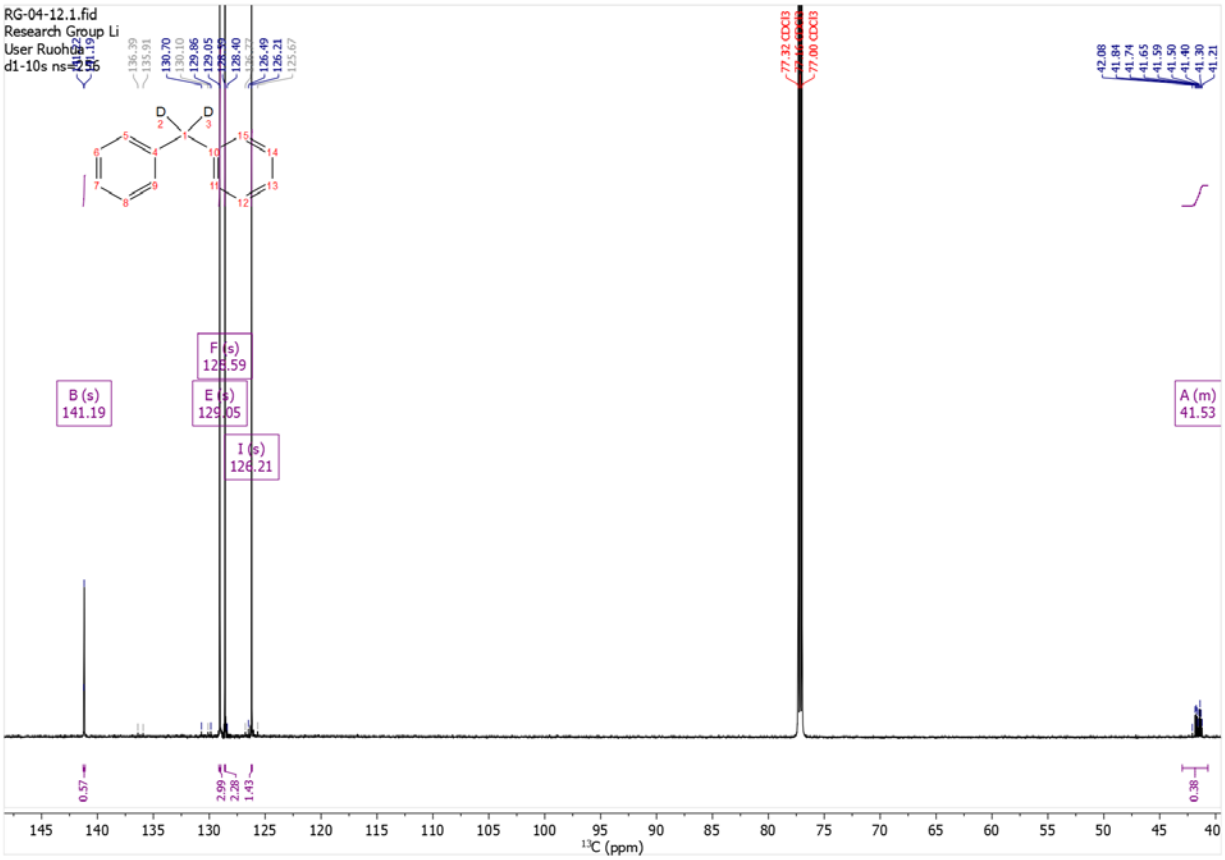
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User Ruohan
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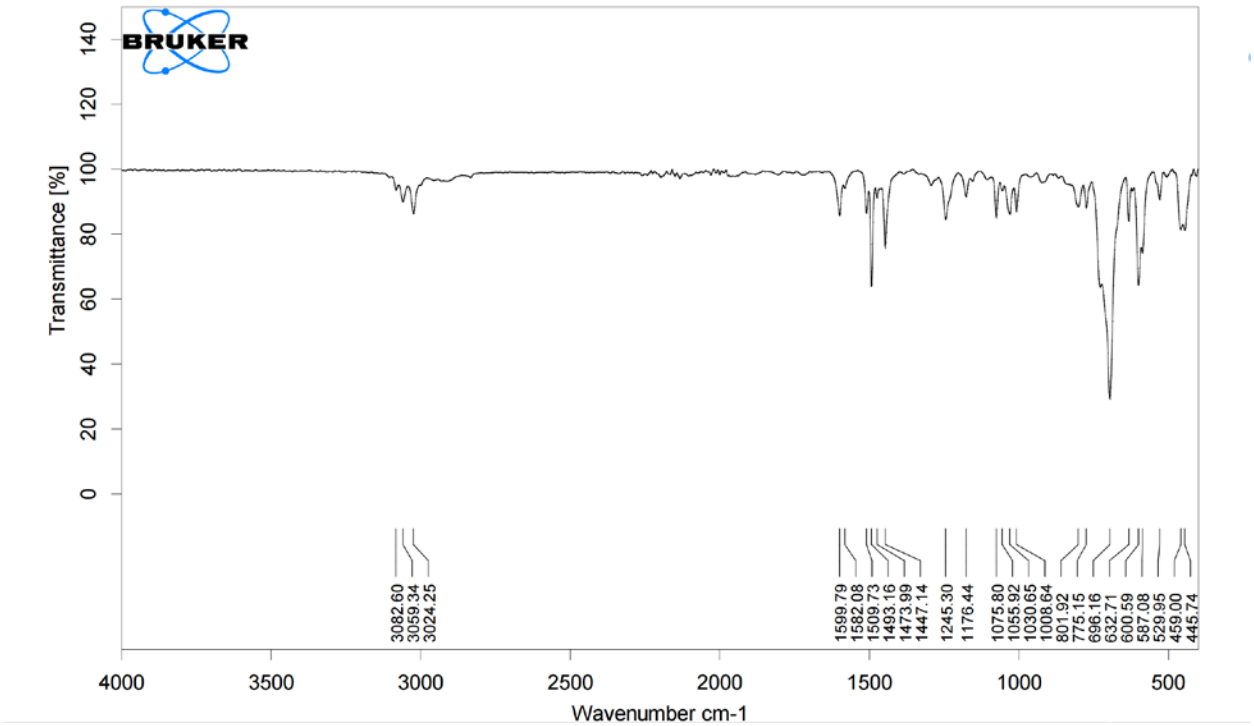
BRUKER
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1075.80
1055.92
1030.65
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632.71
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587.08
529.95
459.00
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Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Li\2022-09-13 Li-Gui RG-04-12 APCI +ve.d	Acquisition Date	9/13/2022 3:06:06 PM
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Sample Name	2022-09-13 Li-Gui RG-04-12 APCI +ve	Instrument	maXis impact 282001.00044
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
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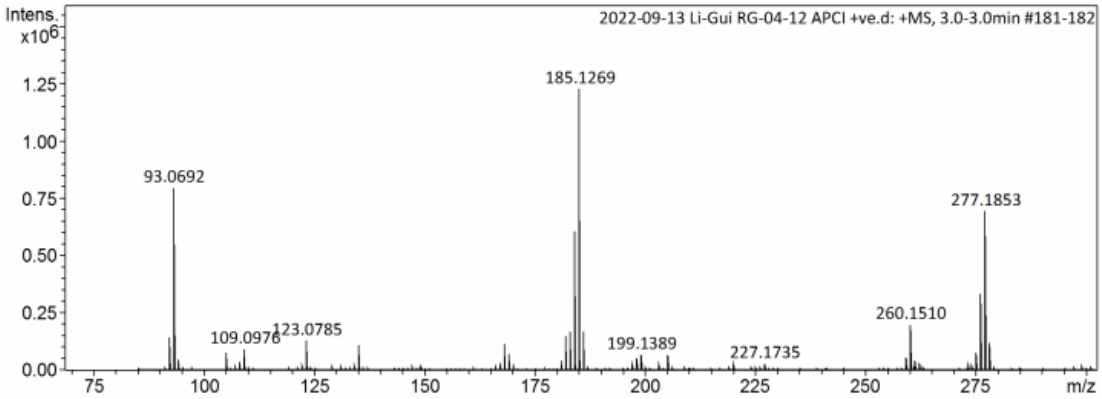

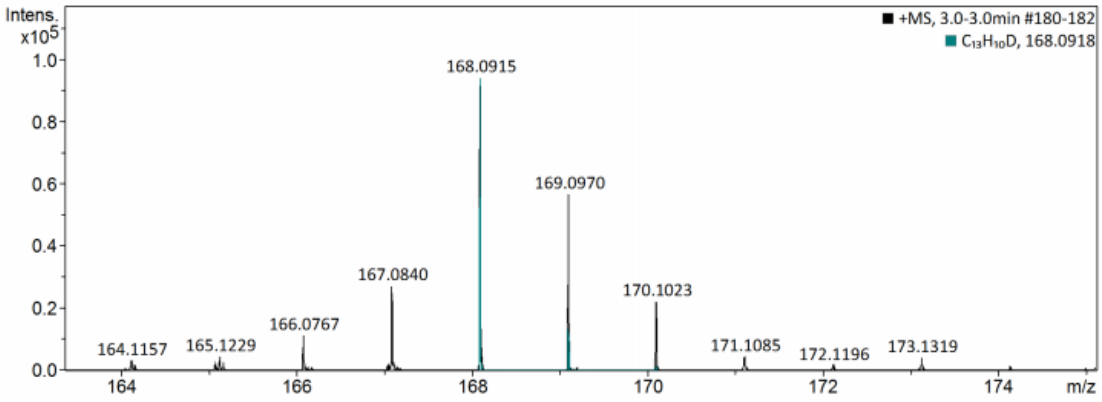

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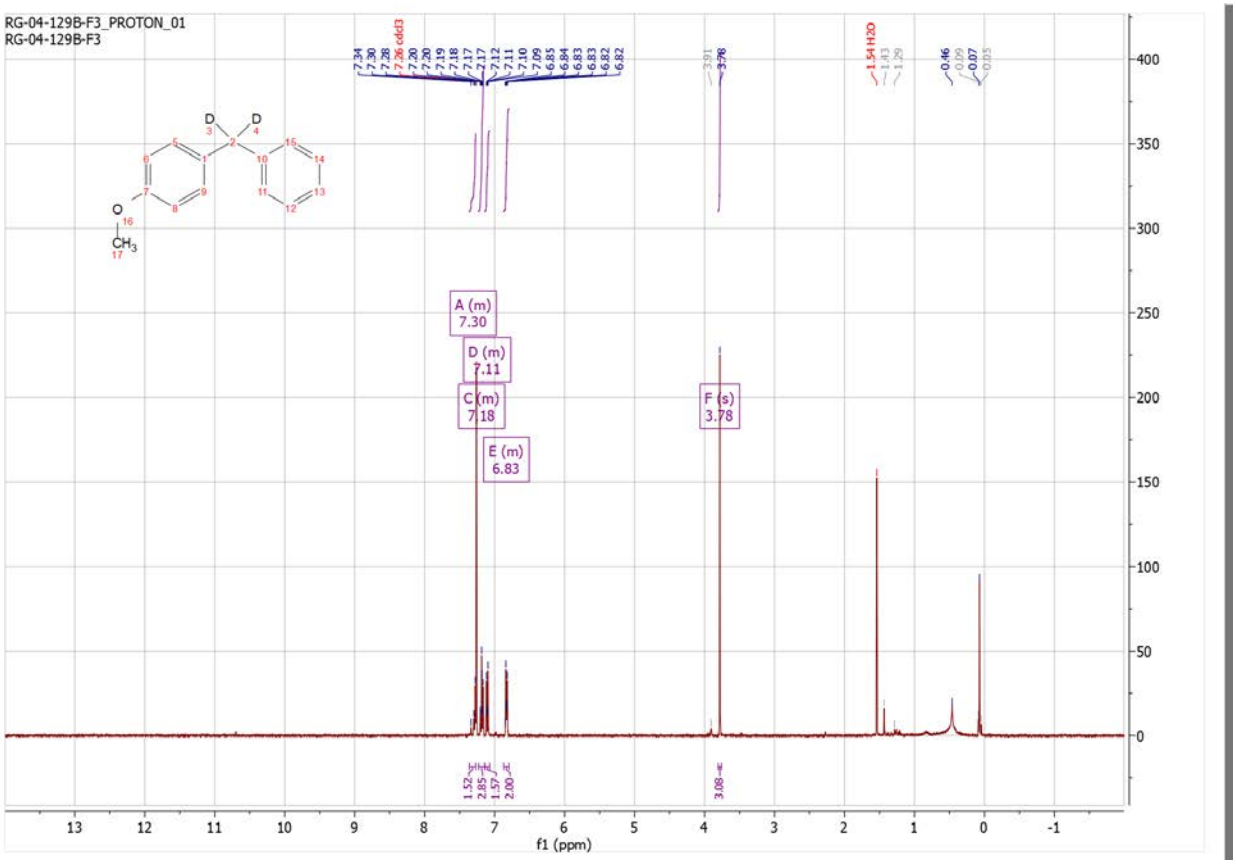
	2	C13H8D2	168.0903	-7.3	295.9	2	60.41	9.0	odd	ok
169.0970	1	C13H9D2	169.0981	6.1	148.1	1	100.00	8.5	even	ok
	2	C8H13N2O2	169.0972	0.6	173.8	2	26.40	3.5	even	ok
	3	C8H11DN2O2	169.0956	-8.5	173.9	3	12.83	4.0	odd	ok
	4	C6H11N5O	169.0958	-7.3	180.5	4	8.86	4.0	odd	ok
170.1023	1	C13H14	170.1090	39.6	31.4	1	0.20	7.0	odd	ok
	2	C13H12D	170.1075	30.5	31.5	2	2.43	7.5	even	ok
	3	C13H10D2	170.1059	21.4	31.6	3	17.54	8.0	odd	ok
	4	C12H12N	170.0964	-34.4	35.5	4	0.79	7.5	even	ok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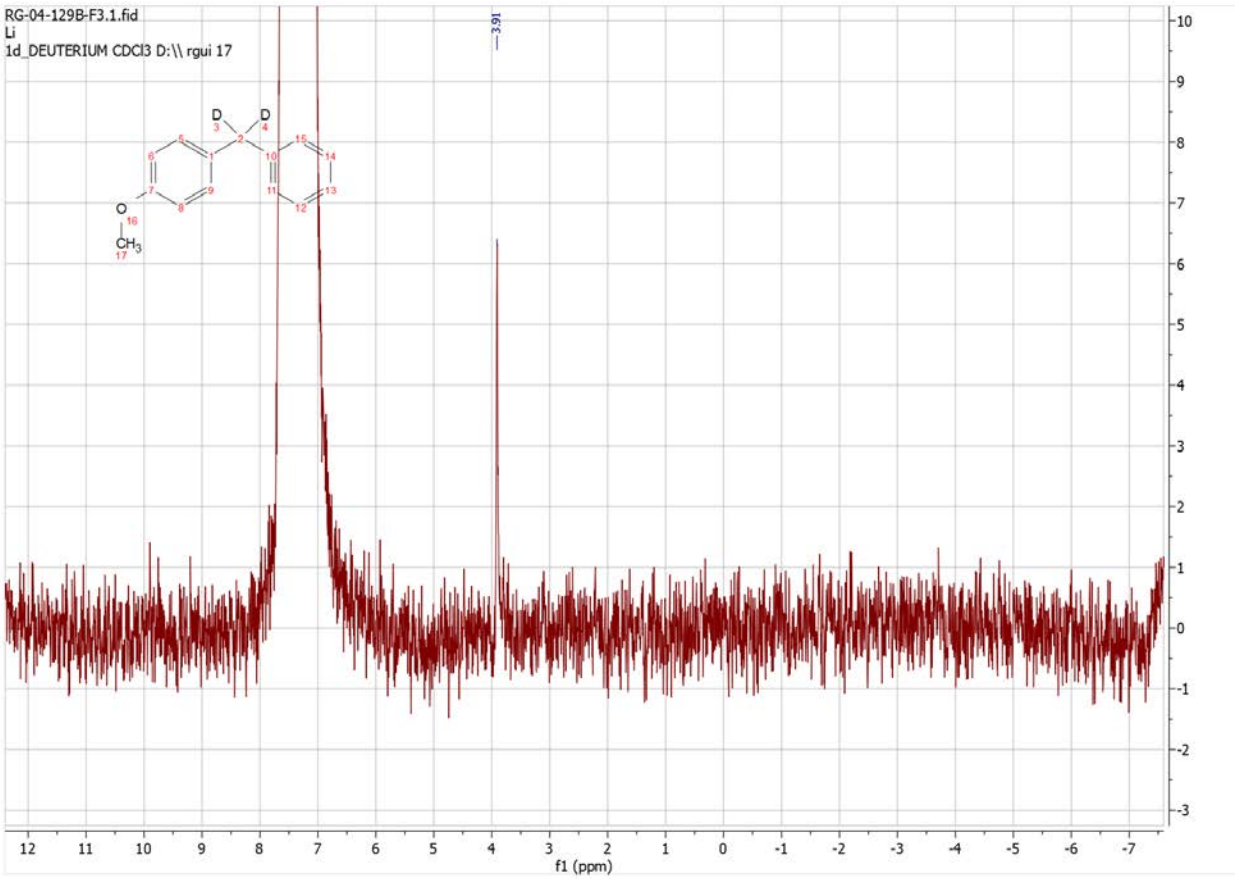
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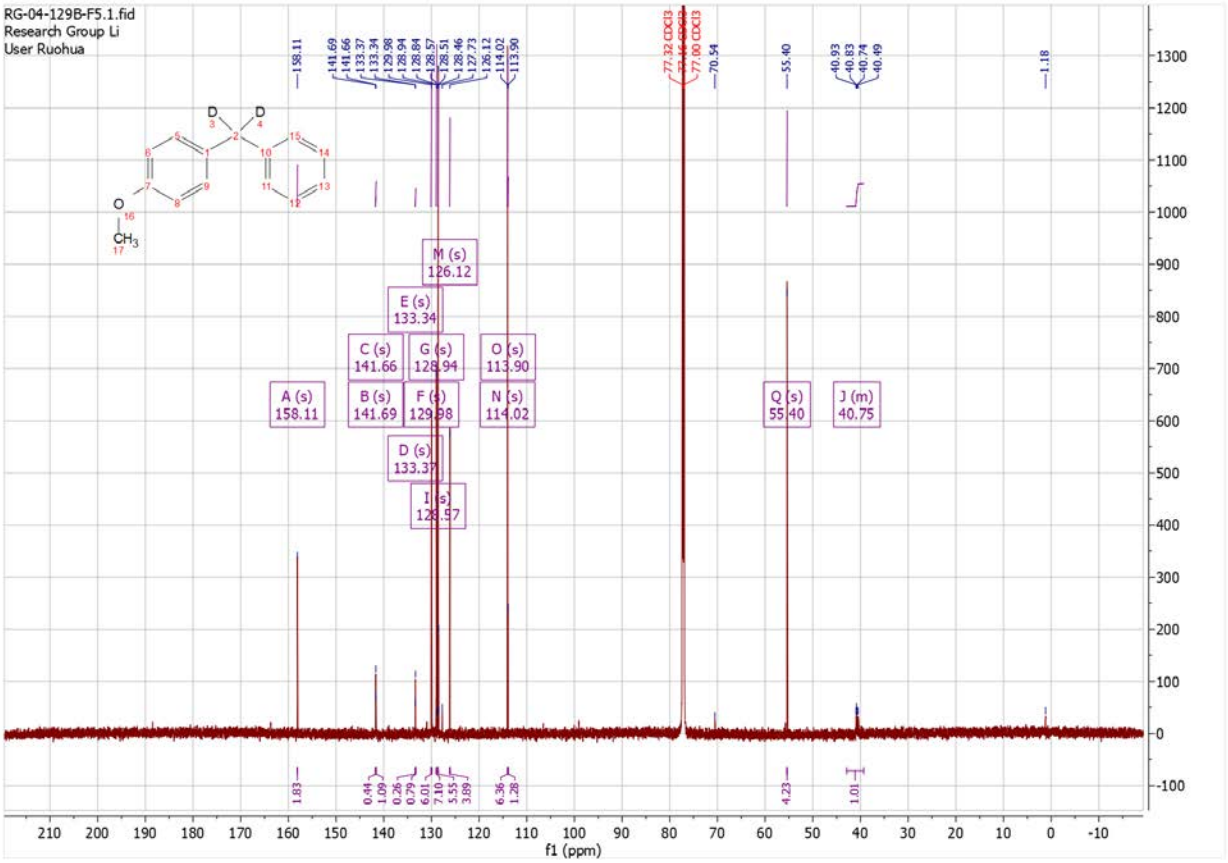
f1 (ppm)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Research Group Li
User Ruohua
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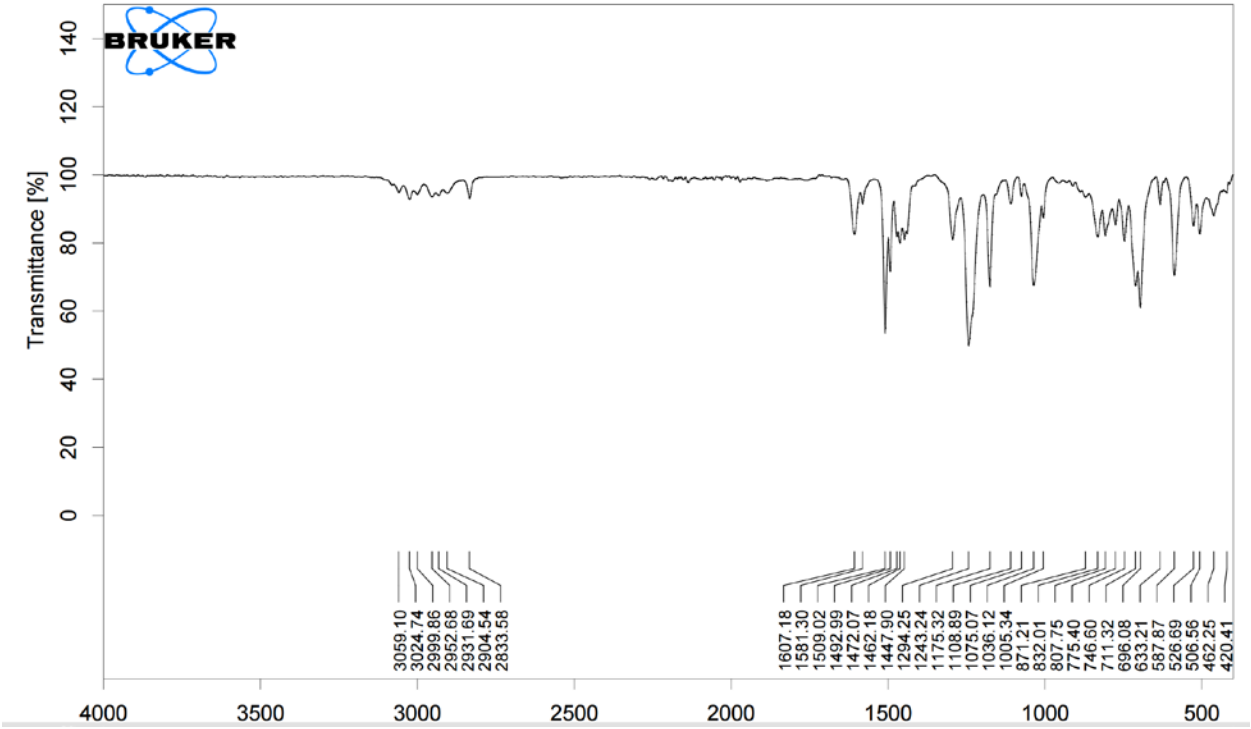
f1 (ppm)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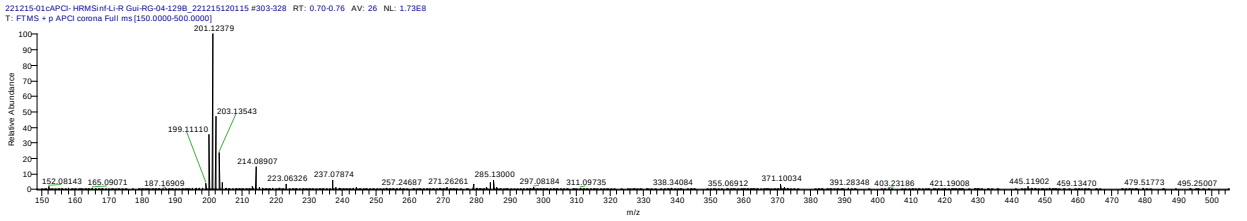

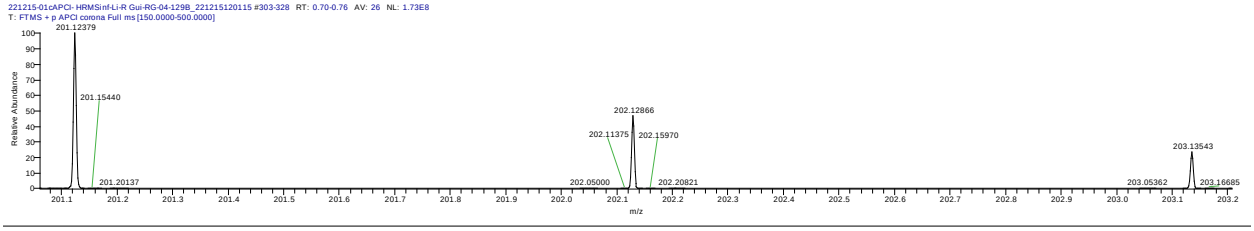

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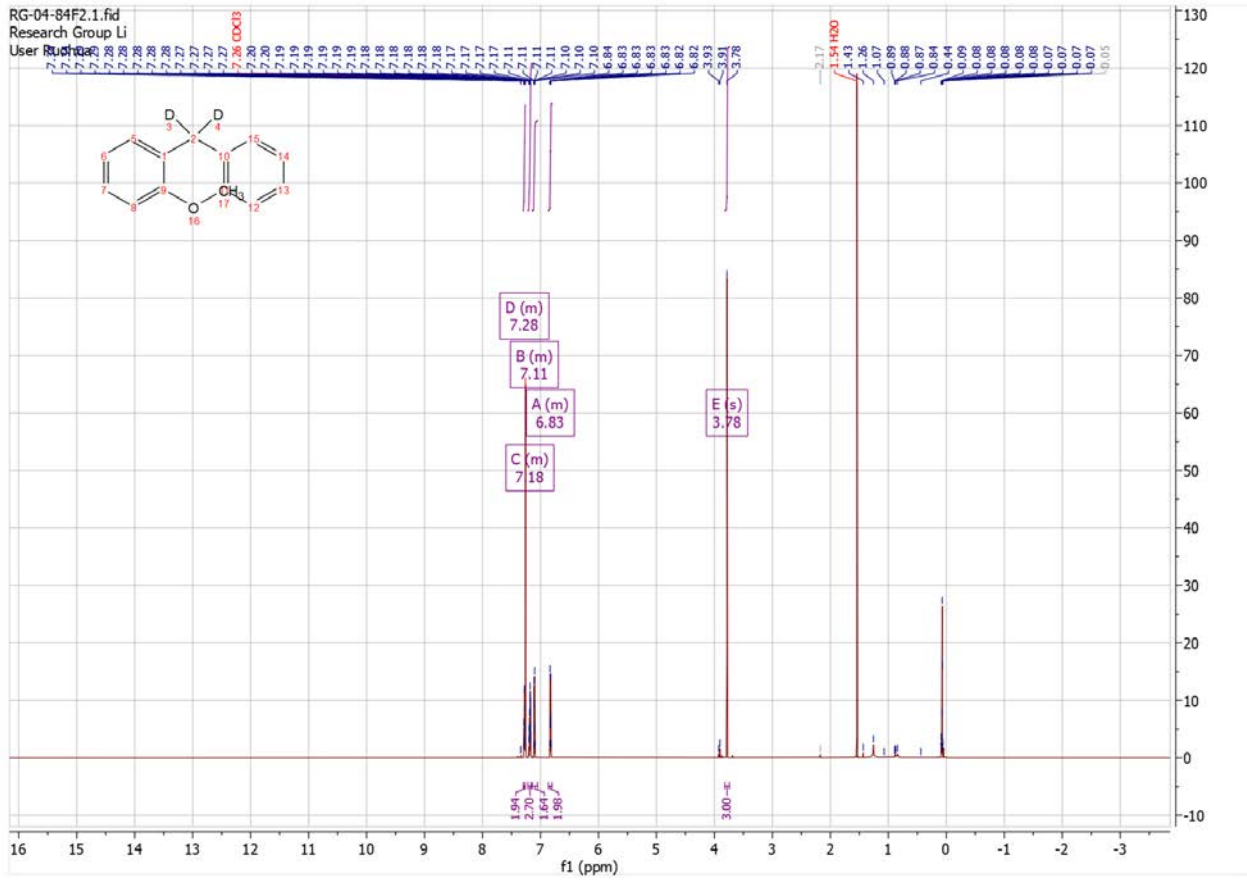

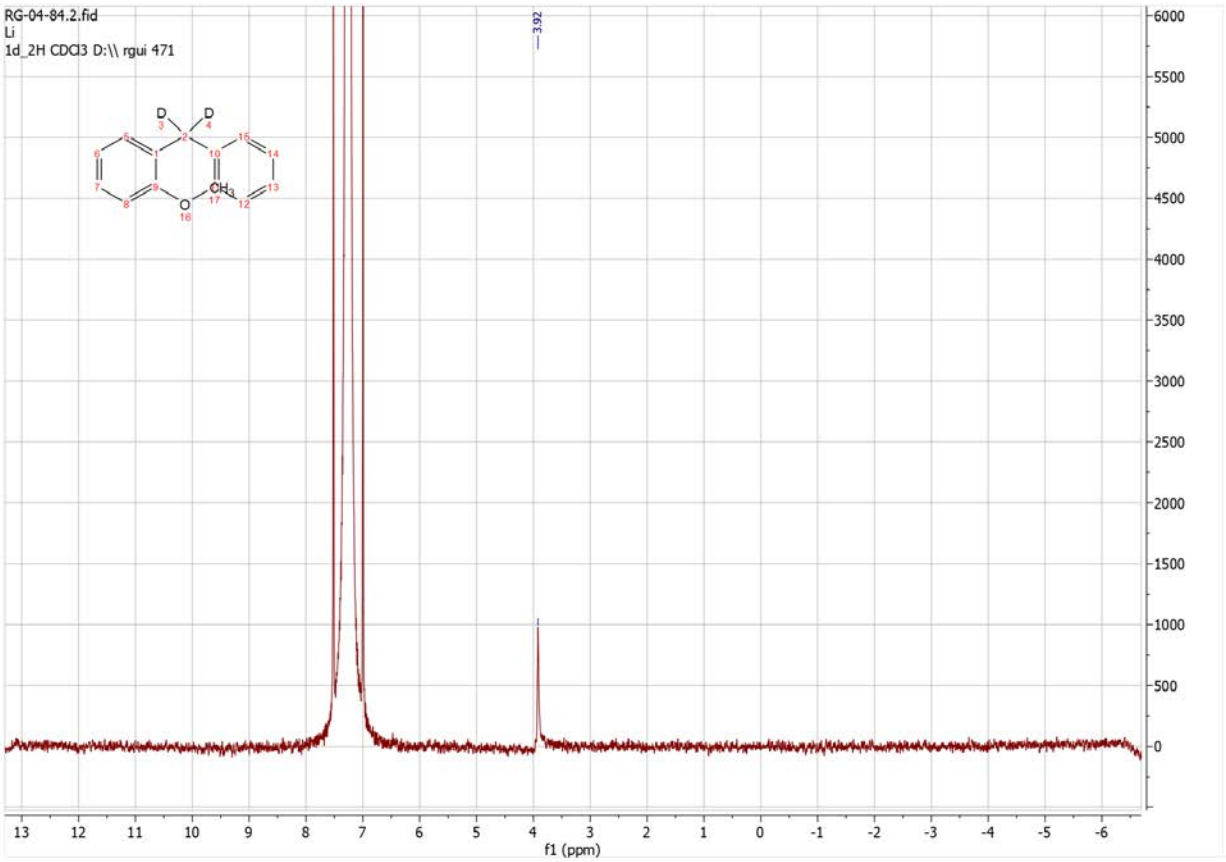
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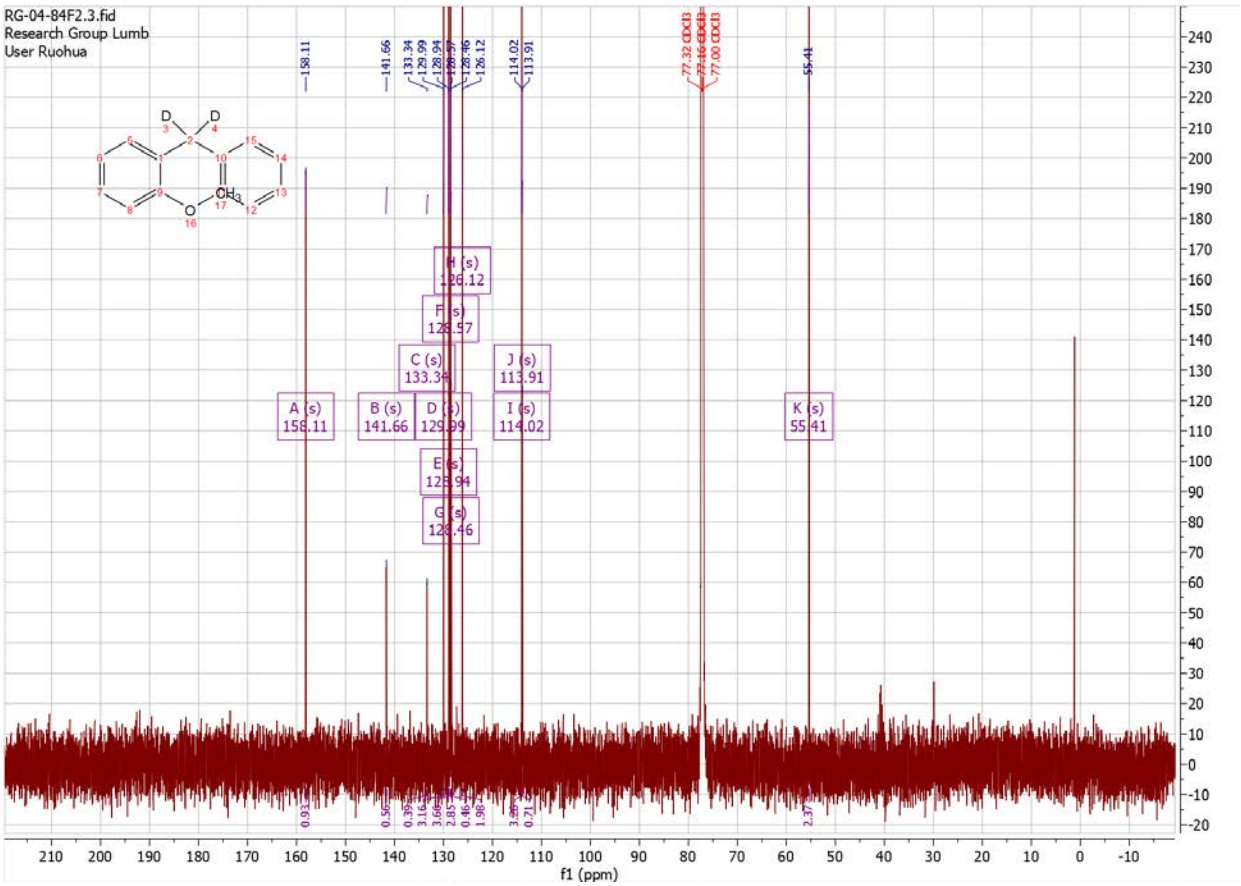
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User Ruohua
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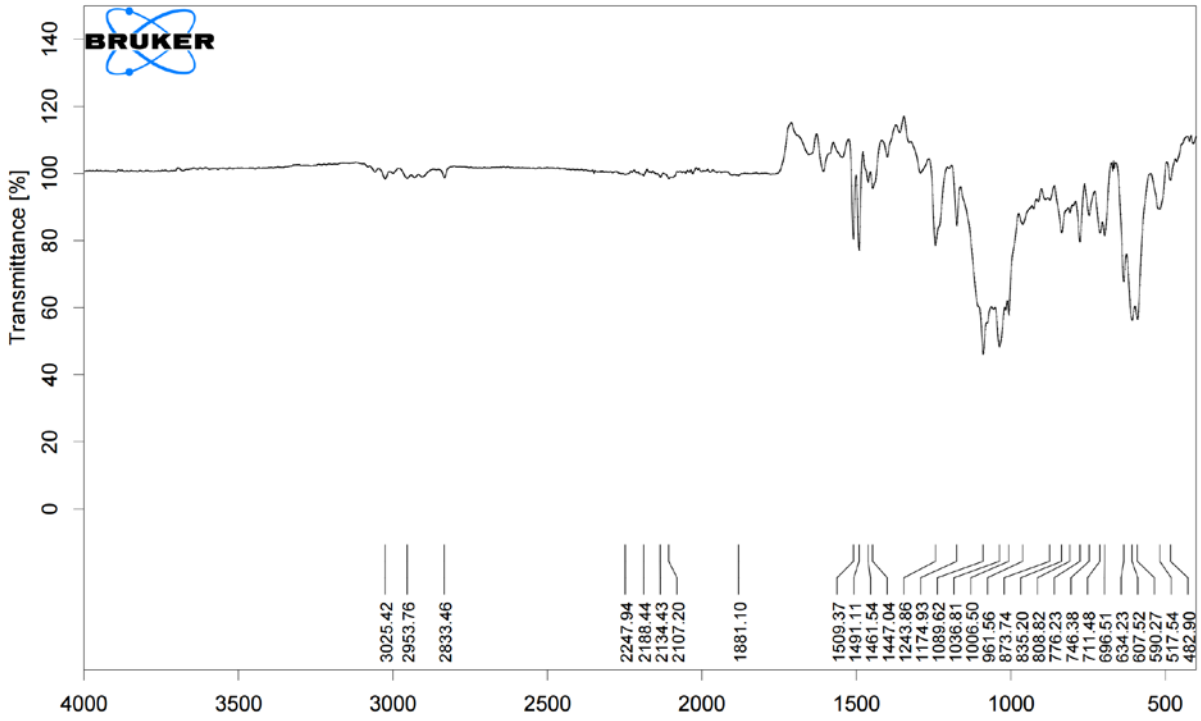
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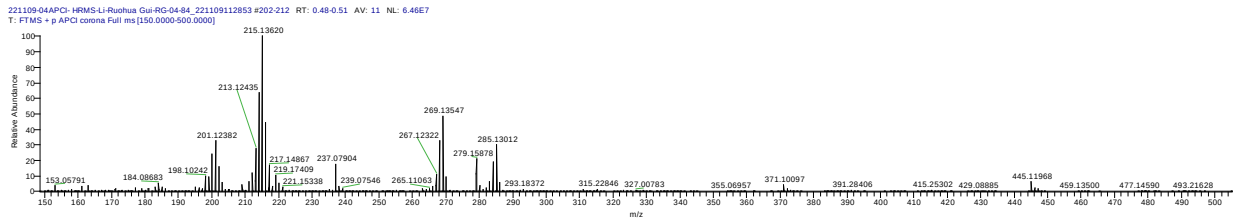

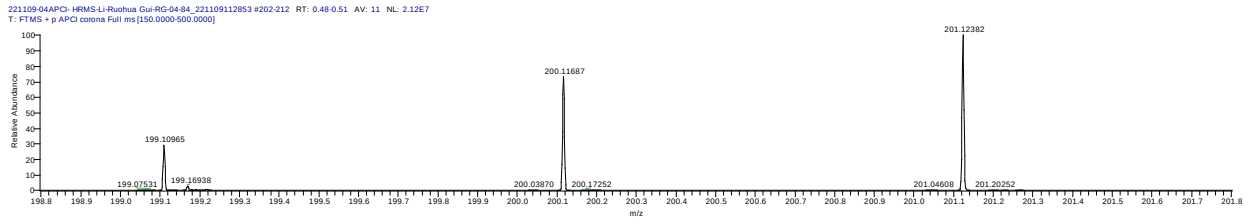

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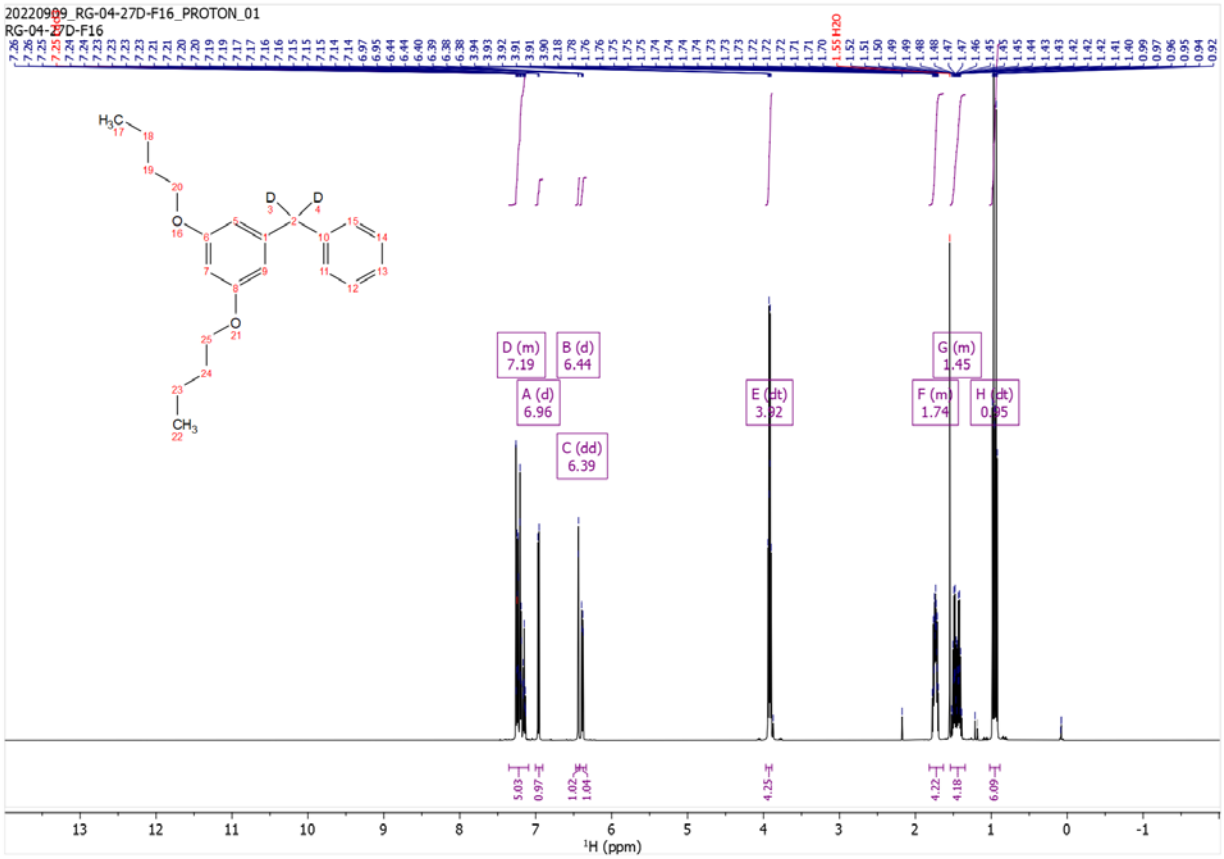
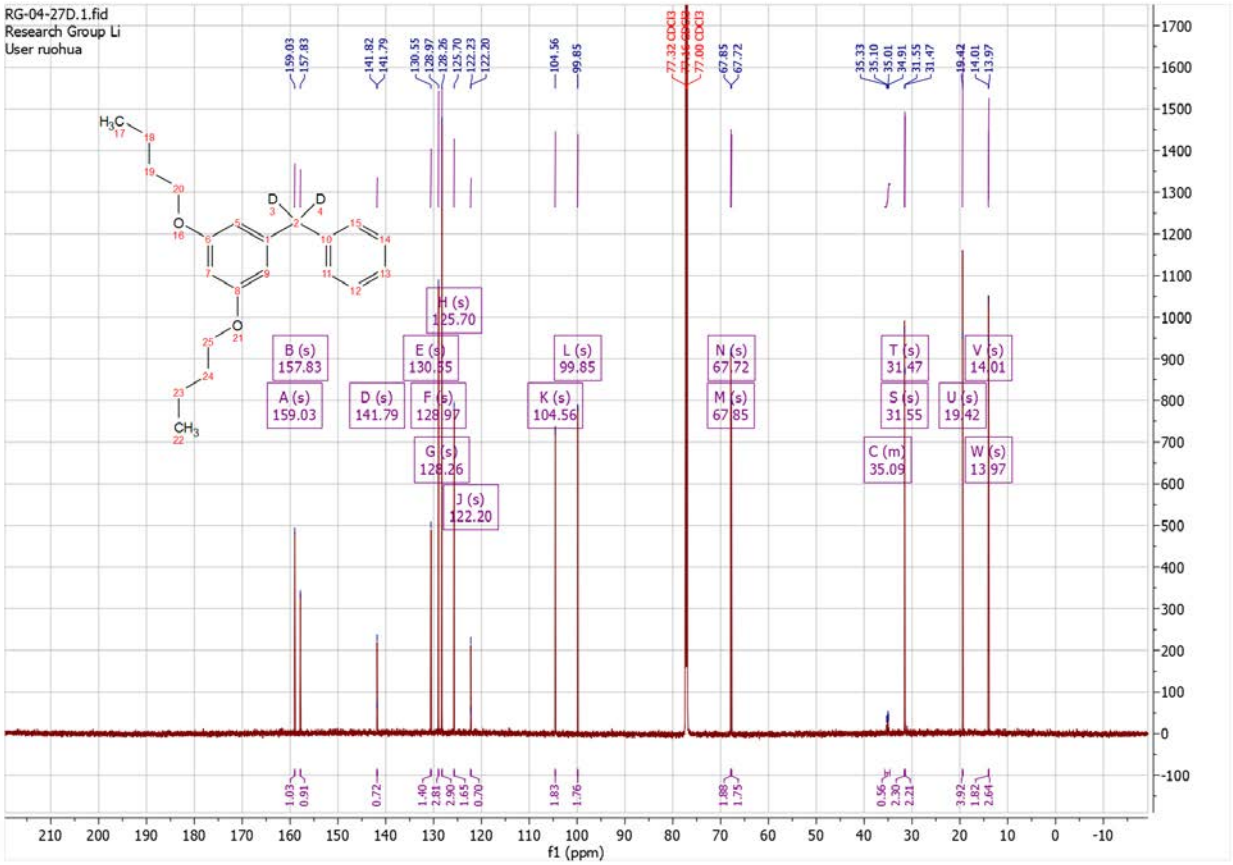
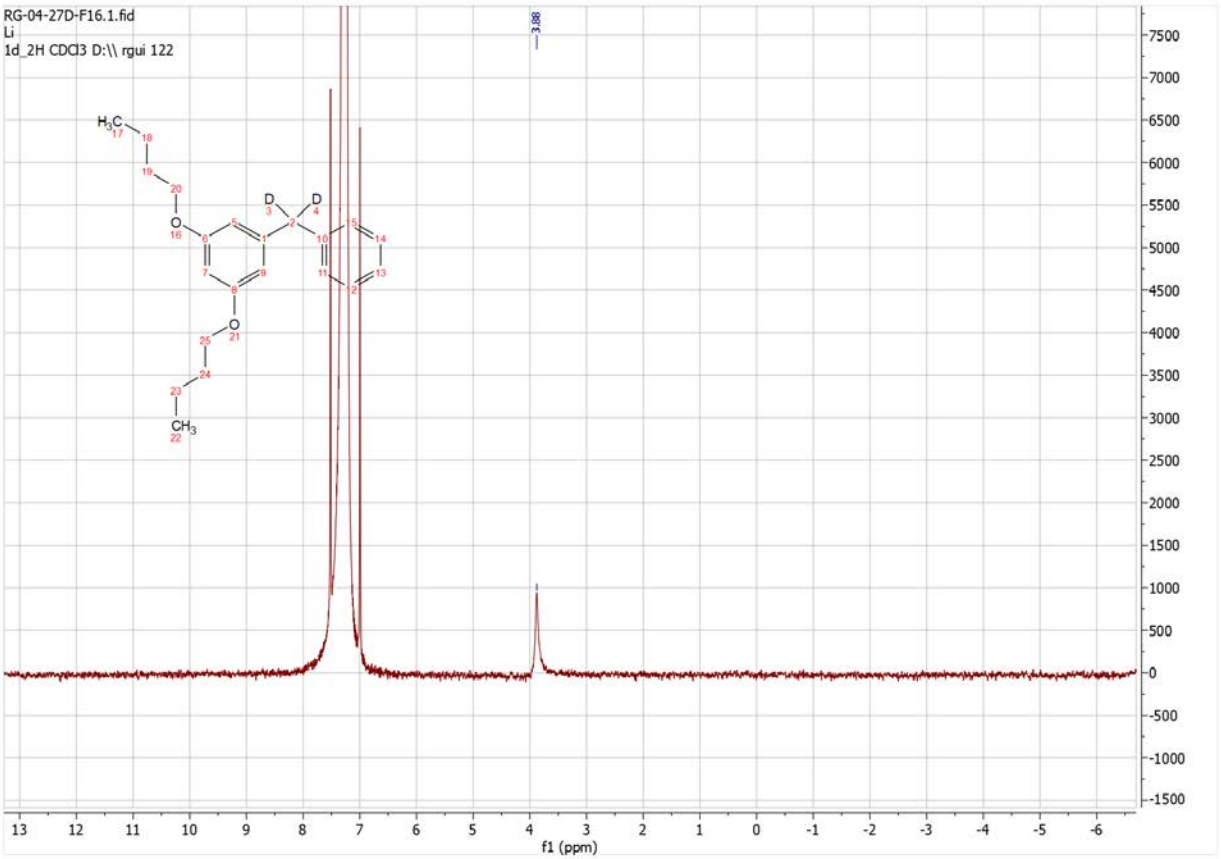
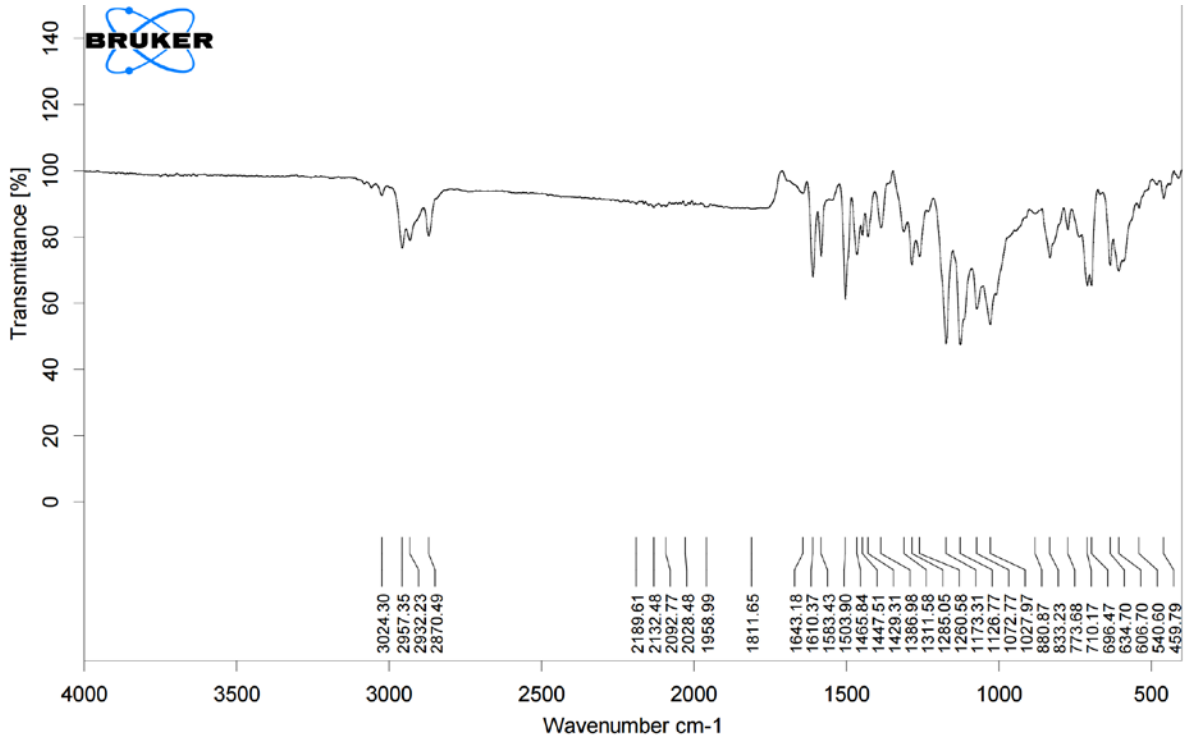
m/z= 201.11330-201.12523

m/z	Intensity	Relative	Resolution	Charge	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
201.12382	21188554.0	100.00	37415.57	1.00	201.12430	-2.38	7.5	$C_{14}H_{13}{}^{2}H_{2}O$




RG-04-27D.1.fid
Research Group Li
User ruohua
f1 (ppm)


RG-04-27D-F16.1.fid
Li
1d_2H CDCl3 D:\\ rgui 122
3.88
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1
3024.30
2957.35
2932.23
2870.49
2189.61
2132.48
2092.77
2028.48
1958.99
1811.65
1643.18
1610.37
1583.43
1503.90
1465.84
1447.51
1429.31
1386.98
1311.58
1285.05
1260.58
1173.31
1126.77
1072.77
1027.97
880.87
833.23
773.68
710.17
696.47
634.70
606.70
540.60
459.79

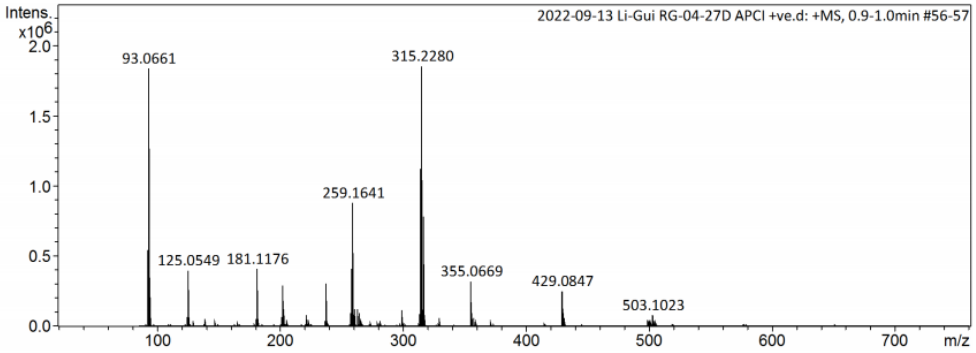
Mass Spectrum SmartFormula Report

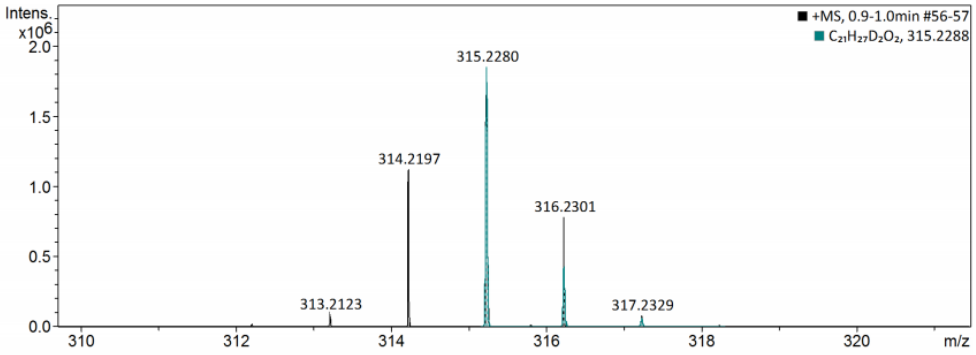
Analysis Info

Analysis Name	D:\Data\Li\2022-09-13 Li-Gui RG-04-27D APCI +ve.d	Acquisition Date	9/13/2022 4:34:19 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-09-13 Li-Gui RG-04-27D APCI +ve	Instrument	maXis impact 282001.00044
Comment			

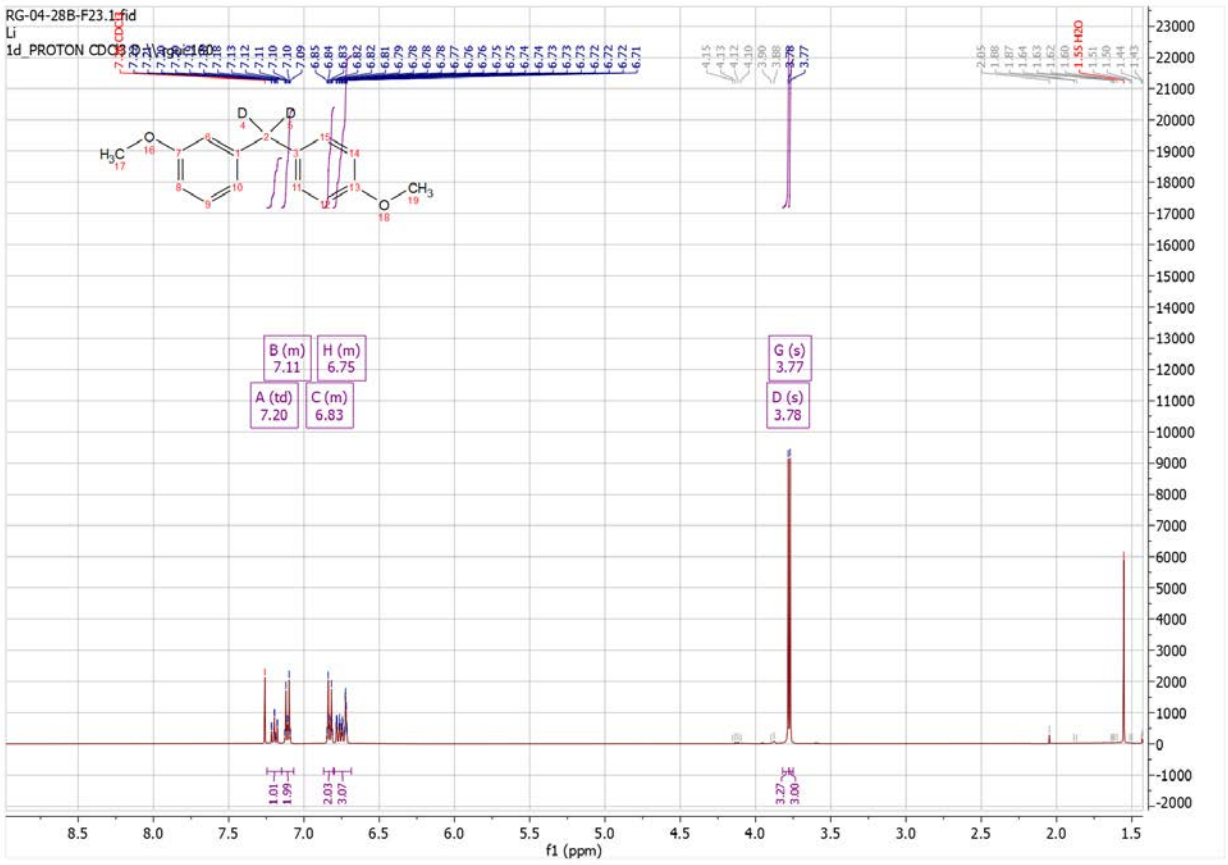
Acquisition Parameter

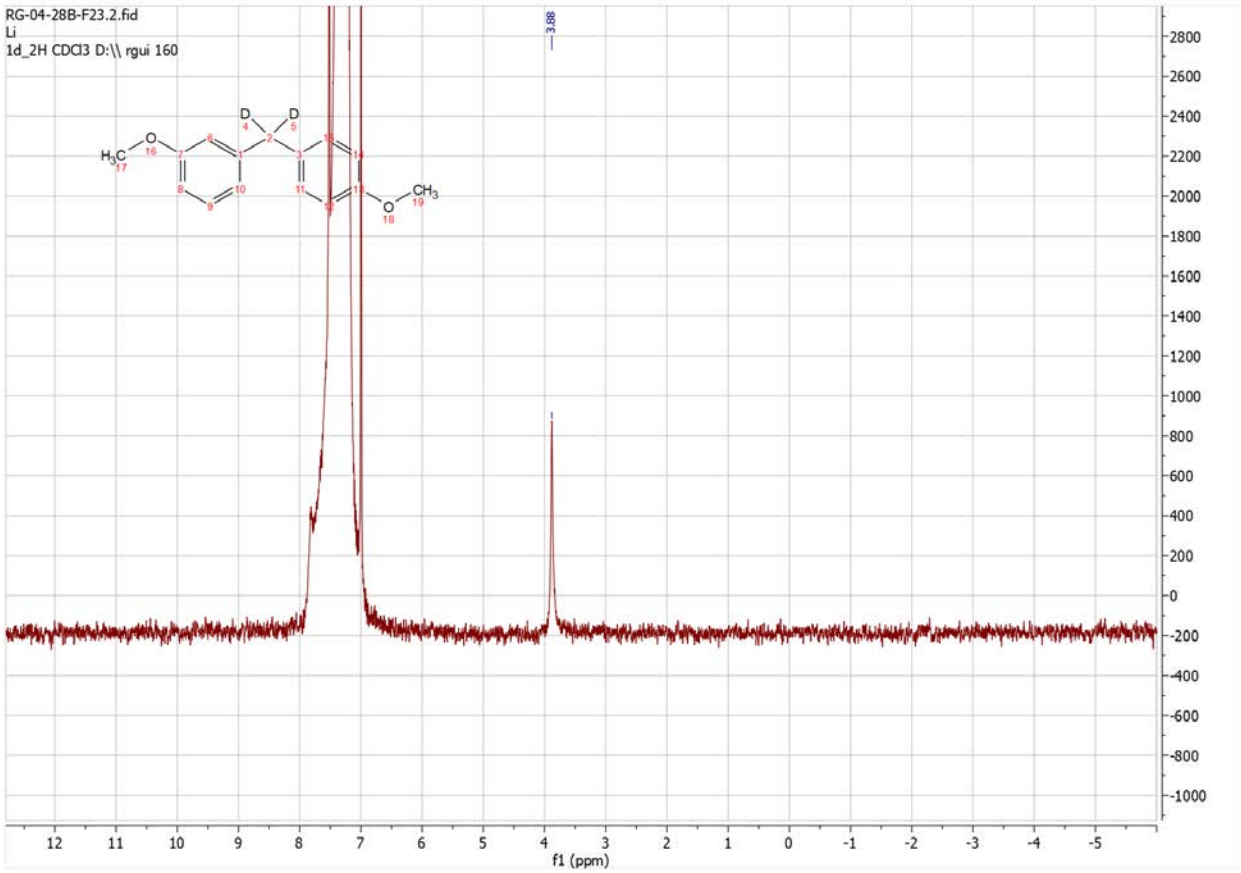
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

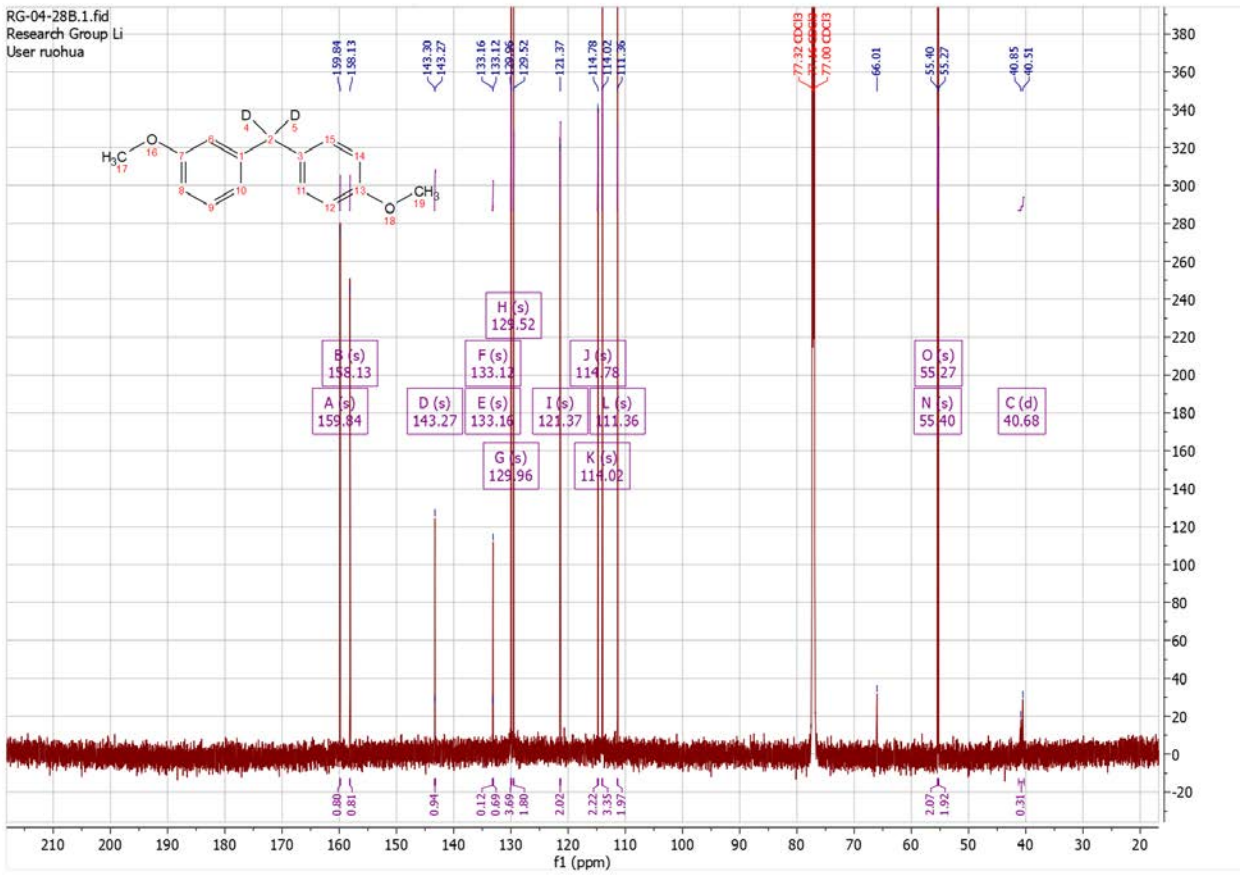


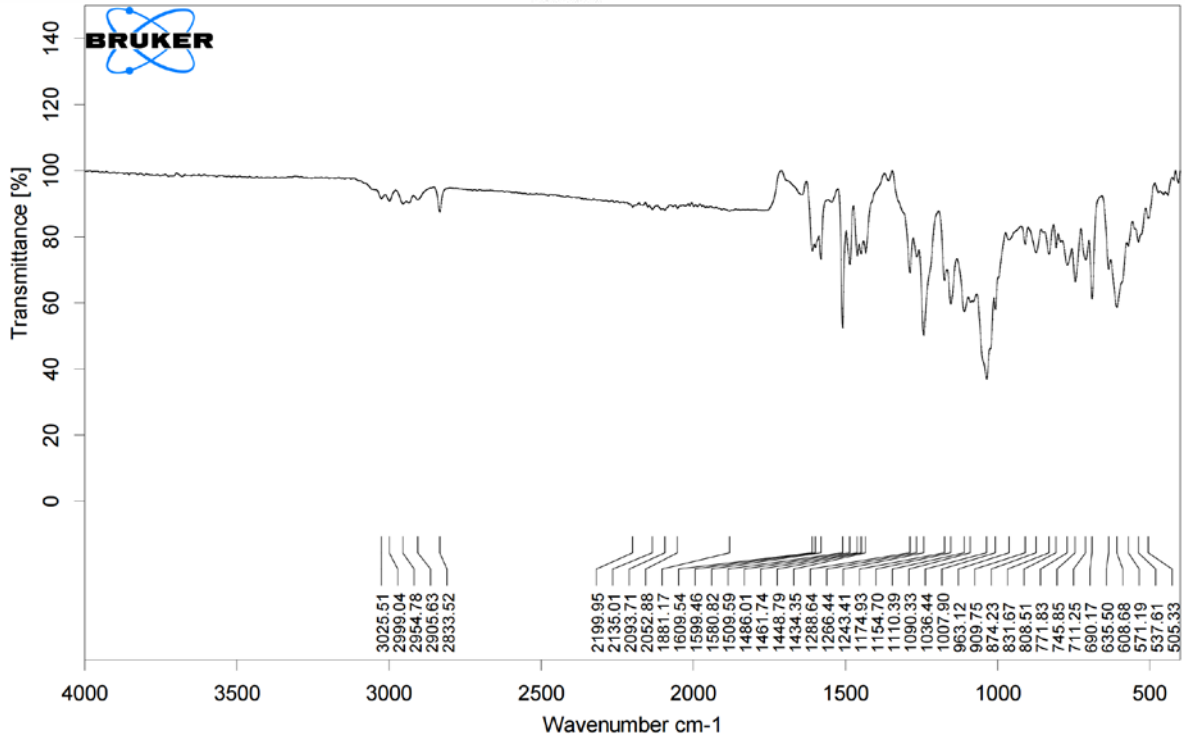


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
314.2197	1	C21H26D2O2	314.2209	3.8	547.6	1	65.61	8.0	odd	ok
	2	C21H24D3O2	314.2194	-1.1	547.7	2	100.00	8.5	even	ok
	3	C19H26DN3O	314.2211	4.5	553.9	3	14.42	8.0	odd	ok
	4	C19H24D2N3O	314.2196	-0.5	554.0	4	27.36	8.5	even	ok
	5	C17H24DN6	314.2198	0.2	560.2	5	7.00	8.5	even	ok
	6	C17H22D2N6	314.2182	-4.7	560.3	6	3.19	9.0	odd	ok
	7	C16H30N2O4	314.2200	0.9	570.3	7	0.64	3.0	odd	ok
	8	C16H28DN2O4	314.2185	-4.1	570.4	8	0.36	3.5	even	ok
	9	C14H28N5O3	314.2187	-3.4	576.6	9	0.10	3.5	even	ok
315.2280	1	C21H27D2O2	315.2288	2.5	110.1	1	97.82	7.5	even	ok


RG-04-28B-F23.1.fid
Li
1d_PROTON CDCl3 2 1 1 qge 160
B (m) 7.11
H (m) 6.75
A (td) 7.20
C (m) 6.83
G (s) 3.77
D (s) 3.78
1.01
1.99
2.03
3.07
3.27
3.00
f1 (ppm)


RG-04-28B-F23.2.fid
Li
1d_2H CDCl3 D:\\ rgui 160
3.888
f1 (ppm)


RG-04-28B.1.fid
Research Group Li
User ruohua
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1

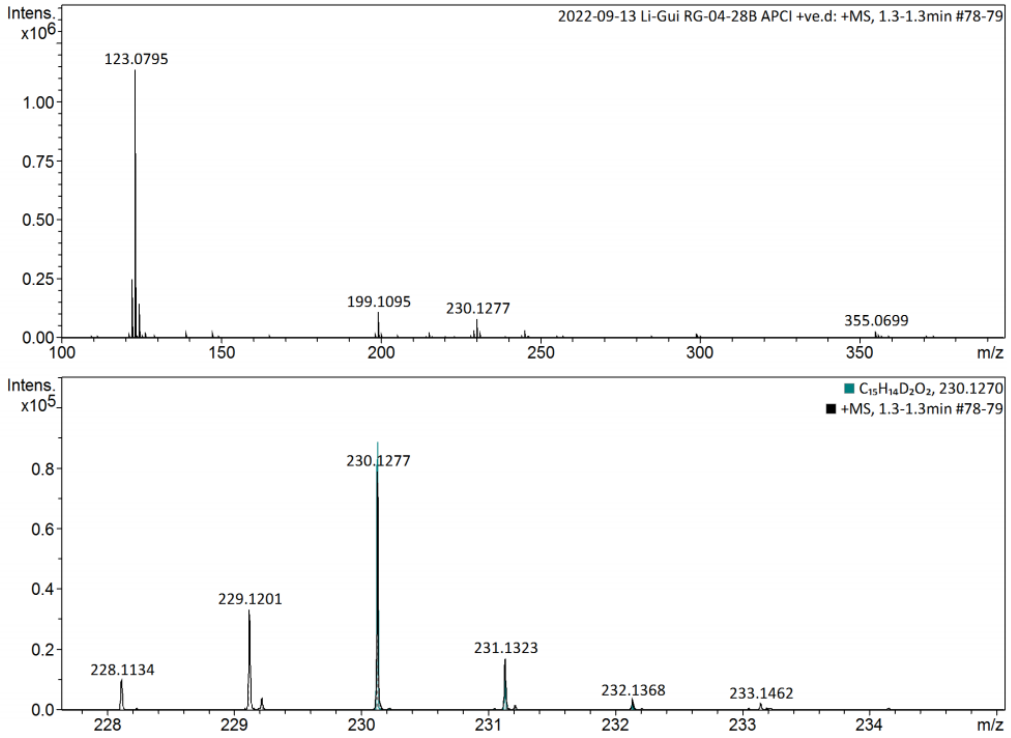
Mass Spectrum SmartFormula Report

Analysis Info

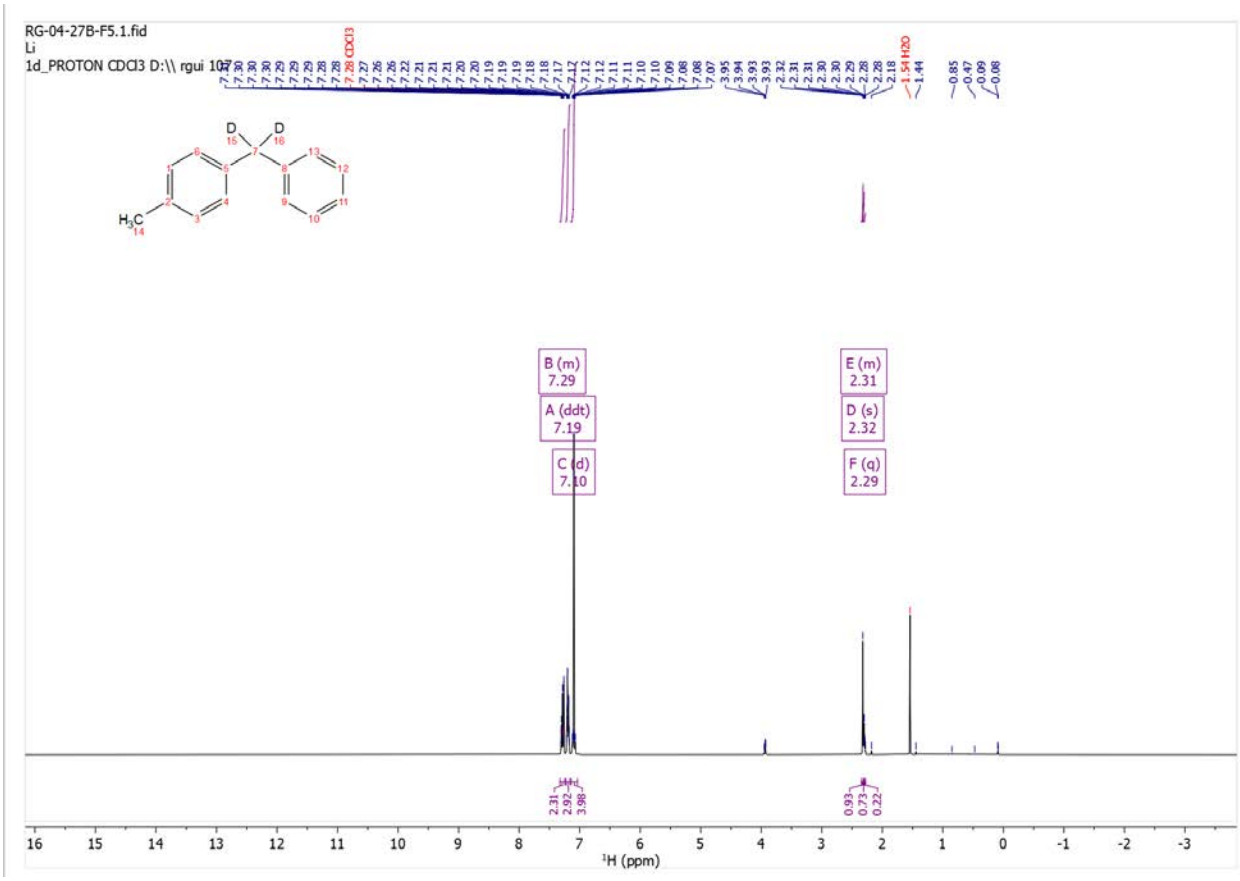
Analysis Name	D:\Data\Li\2022-09-13 Li-Gui RG-04-28B APCI +ve.d	Acquisition Date	9/13/2022 2:50:02 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-09-13 Li-Gui RG-04-28B APCI +ve	Instrument	maXis impact 282001.00044
Comment			

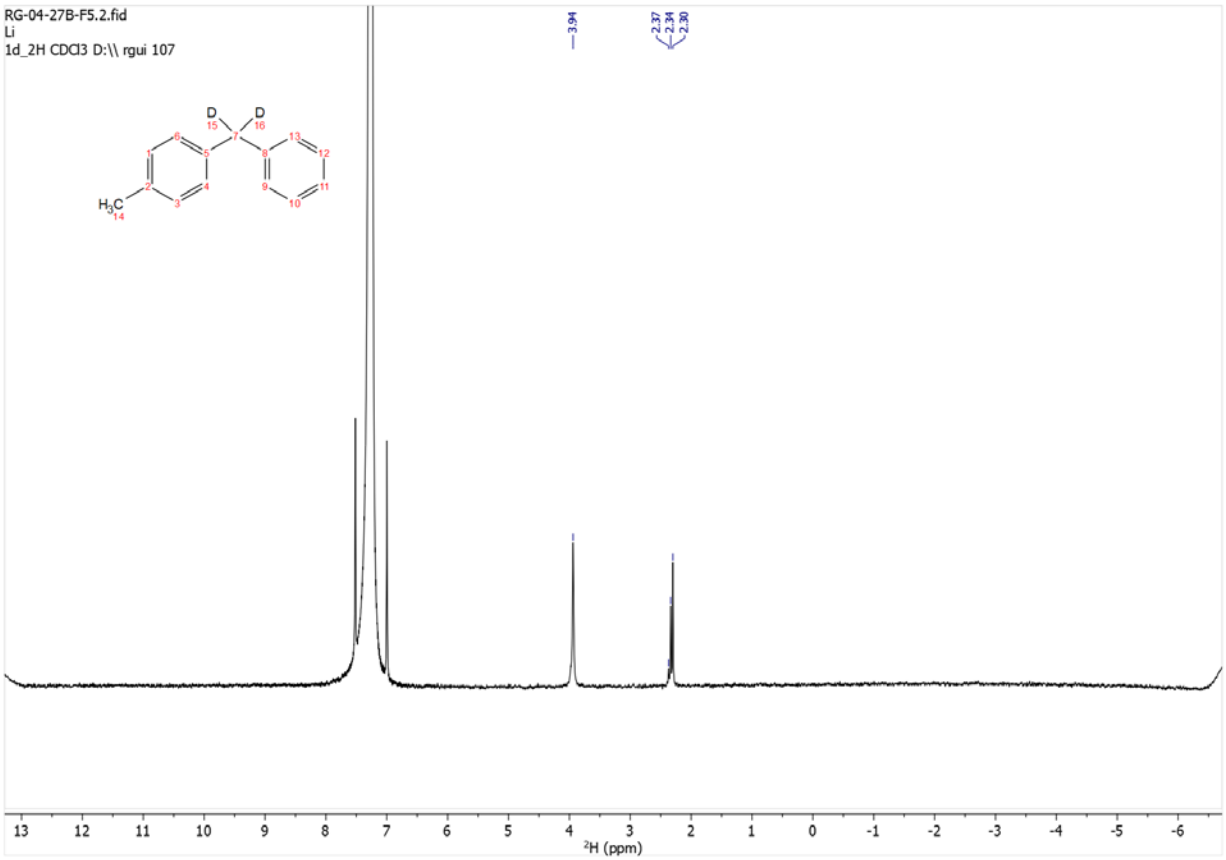
Acquisition Parameter

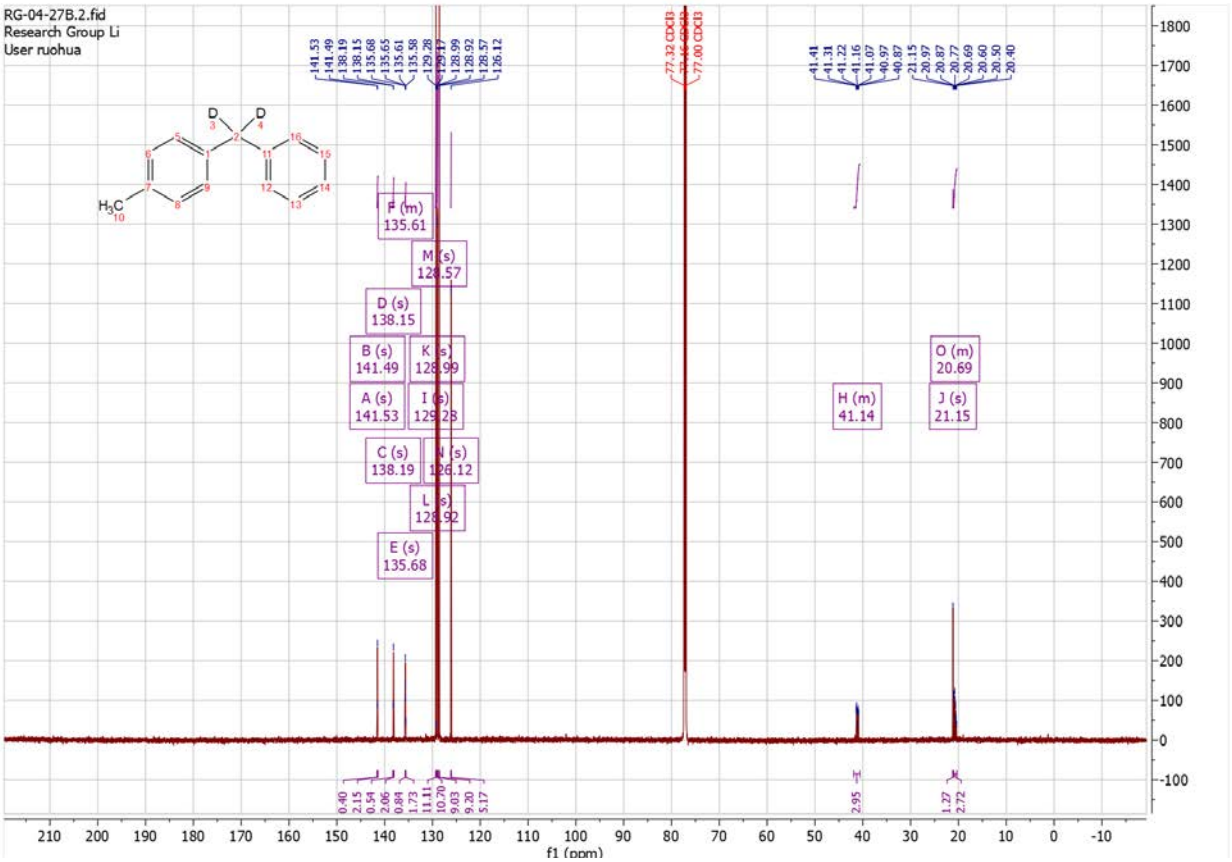
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

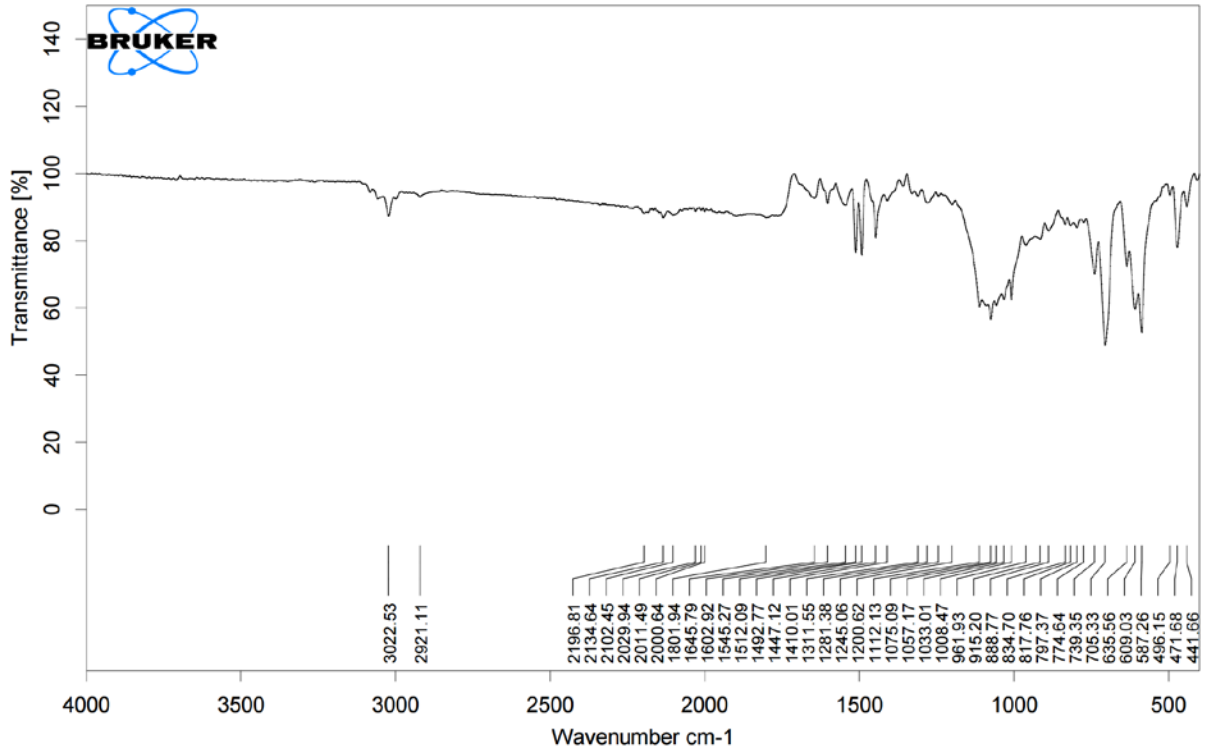


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
123.0795	1	C8H9DO	123.0789	-5.1	21.7	1	100.00	4.0	odd	ok
	2	C6H9N3	123.0791	-3.4	28.3	2	95.21	4.0	odd	ok
199.1095	1	C12H13N3	199.1104	4.4	4.6	1	89.29	8.0	odd	ok
	2	C12H11DN3	199.1089	-3.3	4.7	2	100.00	8.5	even	ok
	3	C14H11D2O	199.1086	-4.4	4.8	3	89.53	8.5	even	ok
	4	C14H13DO	199.1102	3.4	4.9	4	99.08	8.0	odd	ok
	1	C12H16NaO	199.1093	-0.9	8.7	1	100.00	4.5	even	ok
230.1277	1	C15H16DO2	230.1286	3.9	31.8	1	87.47	7.5	even	ok
	2	C15H14D2O2	230.1270	-2.8	31.9	2	100.00	8.0	odd	ok
	3	C13H16N3O	230.1288	4.8	38.5	3	65.36	7.5	even	ok


RG-04-27B-F5.1.fid
Li
1d_PROTON CDCl3 D:\\ rgui 107
CDCl3
H2O
D
15
D
16
H3C
14
B (m)
7.29
A (ddt)
7.19
C (d)
7.10
E (m)
2.31
D (s)
2.32
F (q)
2.29
2.31
2.92
3.98
0.93
0.73
0.22
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
¹H (ppm)


RG-04-27B-F5.2.fid
Li
1d_2H CDCl3 D:\\ rgui 107
D
15
D
16
H3C
14
3.94
2.37
2.34
2.30
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6
2H (ppm)


RG-04-27B.2.fid
Research Group Li
User ruohua
F (m)
135.61
M (s)
128.57
D (s)
138.15
B (s)
141.49
K (s)
128.99
A (s)
141.53
I (s)
129.28
C (s)
138.19
N (s)
126.12
L (s)
128.92
E (s)
135.68
O (m)
20.69
H (m)
41.14
J (s)
21.15
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1
3022.53
2921.11

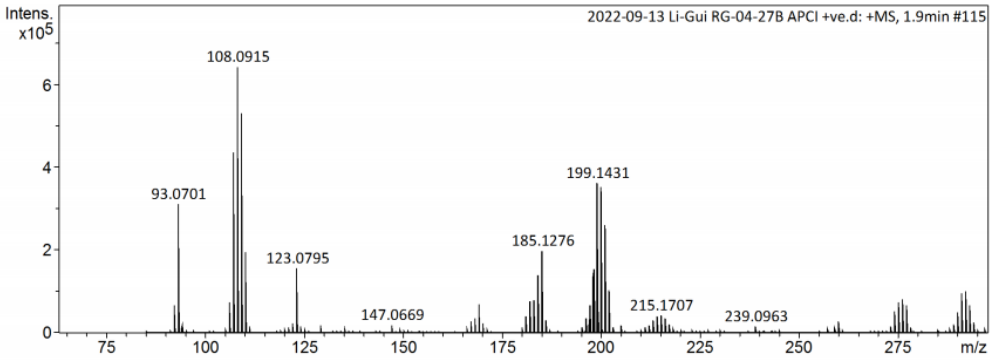
Mass Spectrum SmartFormula Report

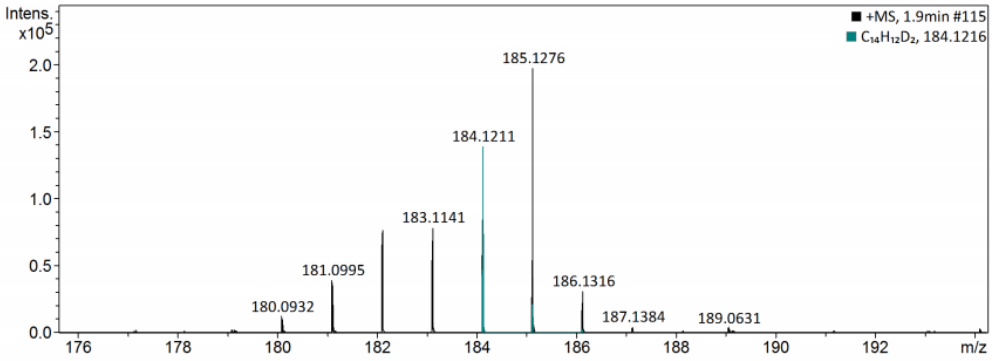
Analysis Info

Analysis Name	D:\Data\Li\2022-09-13 Li-Gui RG-04-27B APCI +ve.d	Acquisition Date	9/13/2022 3:27:05 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-09-13 Li-Gui RG-04-27B APCI +ve	Instrument	maXis impact 282001.00044
Comment			

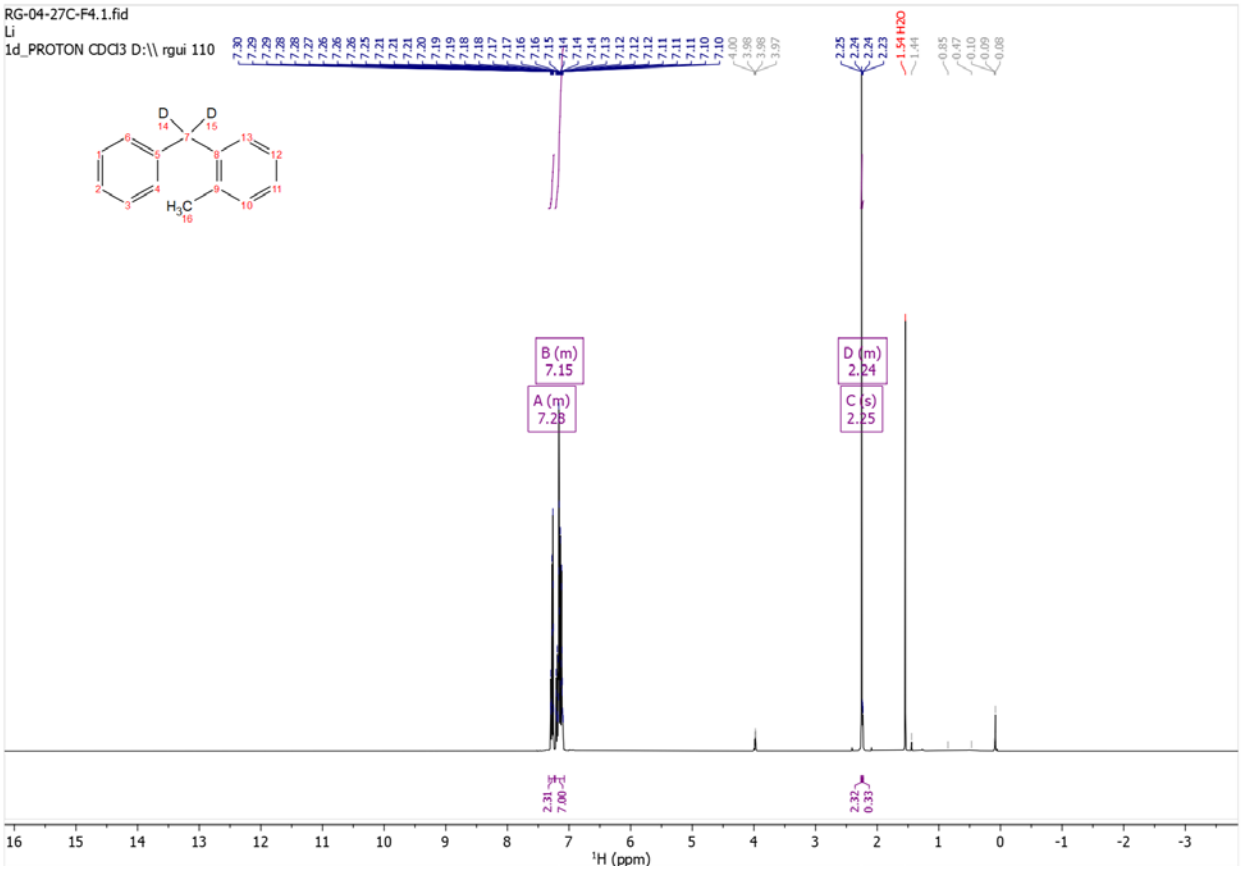
Acquisition Parameter

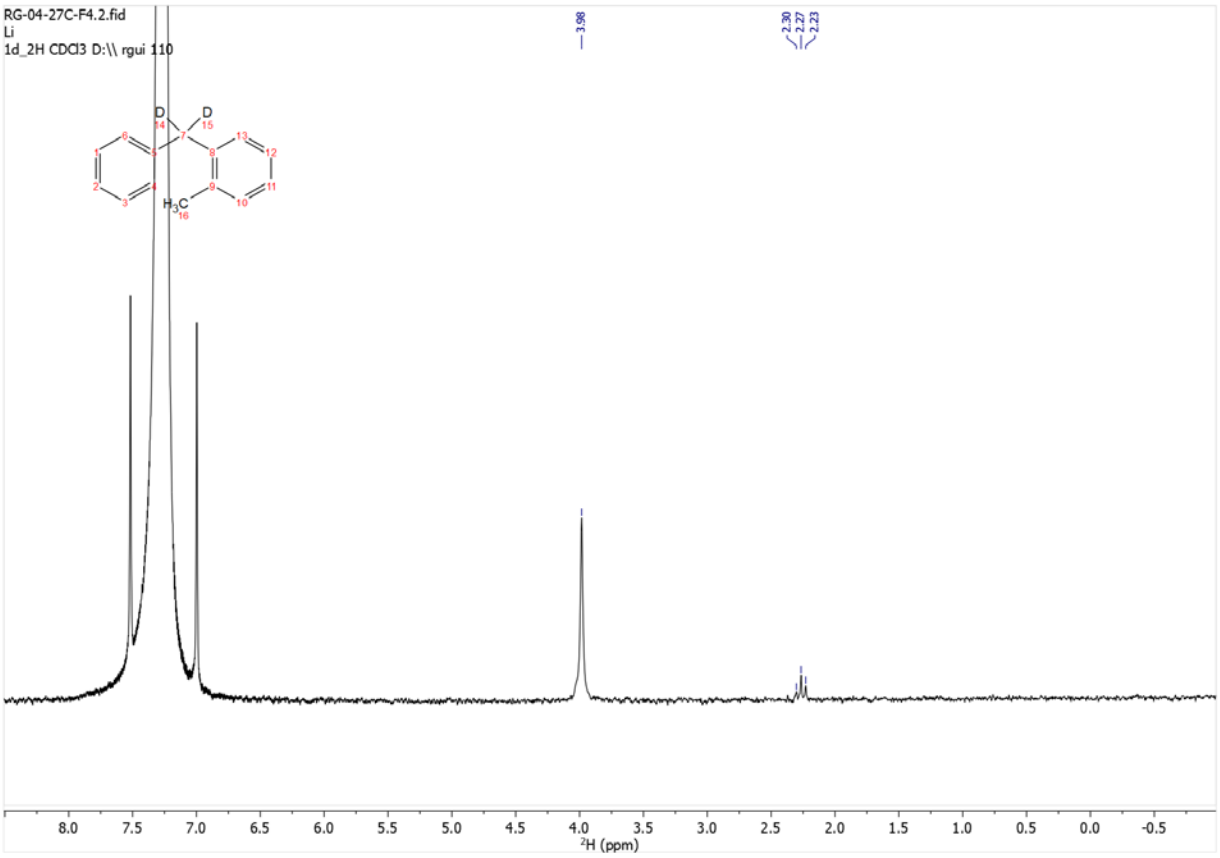
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

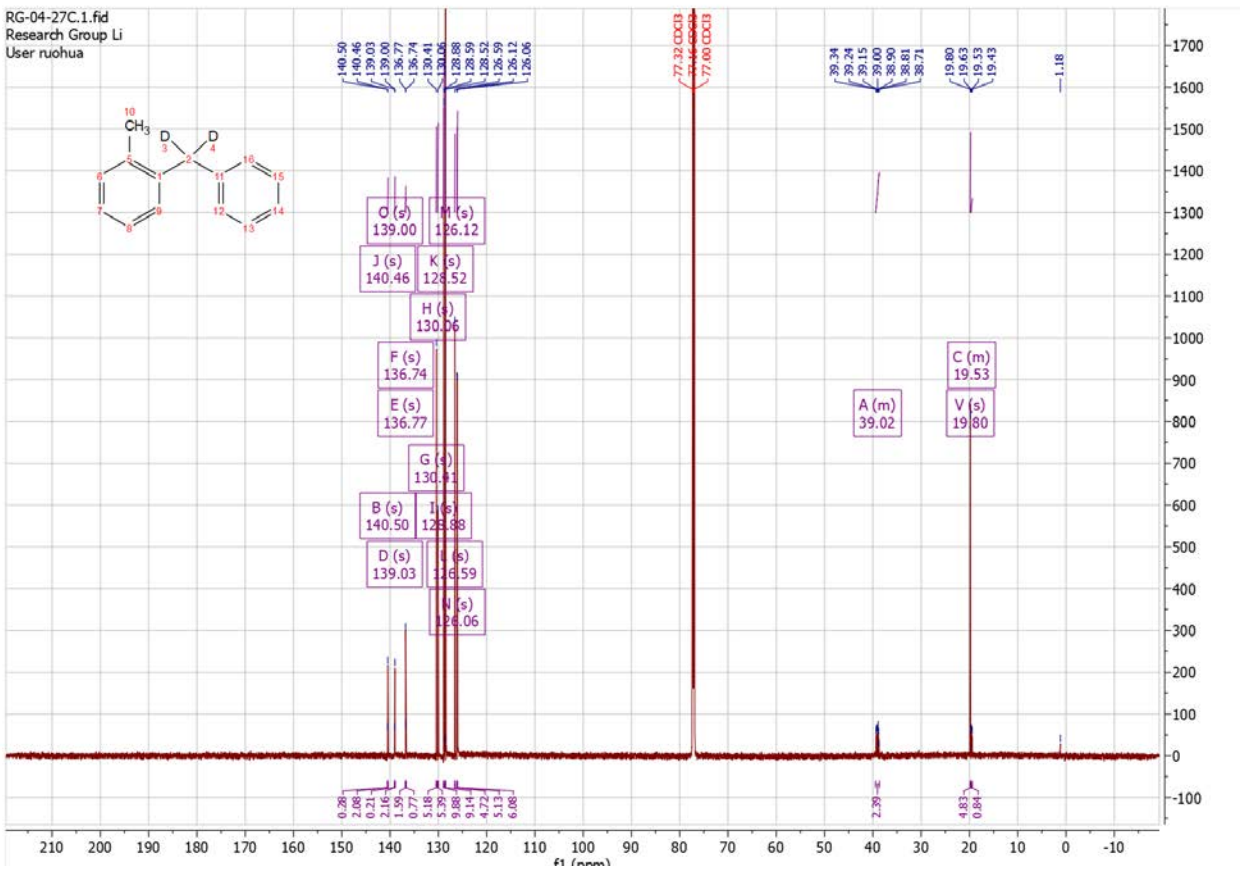


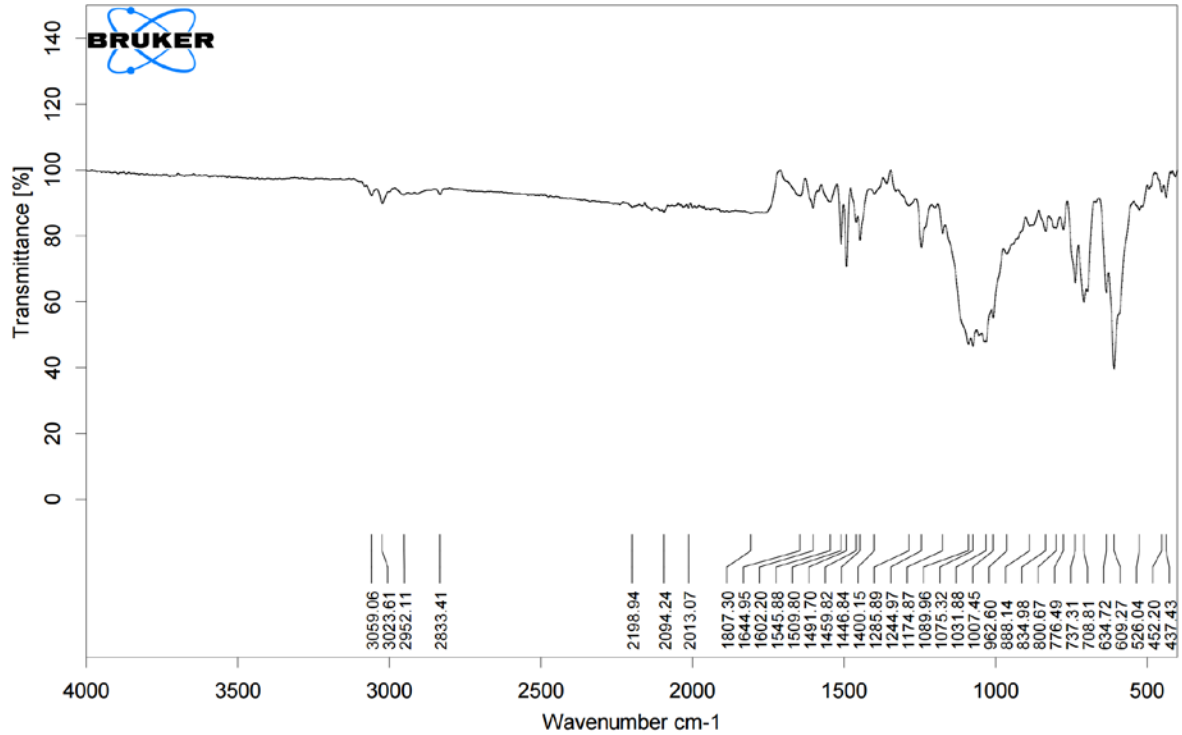


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
182.1067	1	C14H12D	182.1075	4.2	670.8	1	100.00	8.5	even	ok
	2	C14H10D2	182.1059	-4.3	670.9	2	96.49	9.0	odd	ok
	3	C9H14N2O2	182.1050	-9.4	681.3	3	3.19	4.0	odd	ok
183.1141	1	C14H13D	183.1153	6.6	741.1	1	64.75	8.0	odd	ok
	2	C14H11D2	183.1137	-1.9	741.2	2	100.00	8.5	even	ok
	3	C9H15N2O2	183.1128	-6.9	753.5	3	1.50	3.5	even	ok
184.1211	1	C14H12D2	184.1216	2.5	524.7	1	100.00	8.0	odd	ok
	2	C14H10D3	184.1200	-5.9	524.9	2	70.22	8.5	even	ok
	3	C9H16N2O2	184.1206	-2.5	549.5	3	0.47	3.0	odd	ok
	4	C7H14N5O	184.1193	-9.8	555.9	4	0.05	3.5	even	ok


RG-04-27C-F4.1.fid
Li
1d_PROTON CDCl3 D:\\ rgui 110
B (m)
7.15
A (m)
7.23
D (m)
2.24
C (s)
2.25
H2O
1.54
2.31
7.00
2.32
0.33
¹H (ppm)


RG-04-27C-F4.2.fid
Li
1d_2H CDCl3 D:\\ rgui 110
3.98
2.30
2.27
2.23
D
D
H3C
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
2H (ppm)


RG-04-27C.1.fid
Research Group Li
User ruohua
O (s) 139.00
M (s) 126.12
J (s) 140.46
K (s) 128.52
H (s) 130.06
F (s) 136.74
E (s) 136.77
G (s) 130.41
B (s) 140.50
I (s) 128.88
D (s) 139.03
L (s) 126.59
N (s) 126.06
A (m) 39.02
C (m) 19.53
V (s) 19.80
77.32 CDCl3
77.16 CDCl3
77.00 CDCl3
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1
3059.06
3023.61
2952.11
2833.41
2198.94
2094.24
2013.07
1807.30
1644.95
1602.20
1545.88
1509.80
1491.70
1459.82
1446.84
1400.15
1285.89
1244.97
1174.87
1089.96
1075.32
1031.88
1007.45
982.60
888.14
834.98
800.67
776.49
737.31
708.81
634.72
609.27
526.04
452.20
437.43

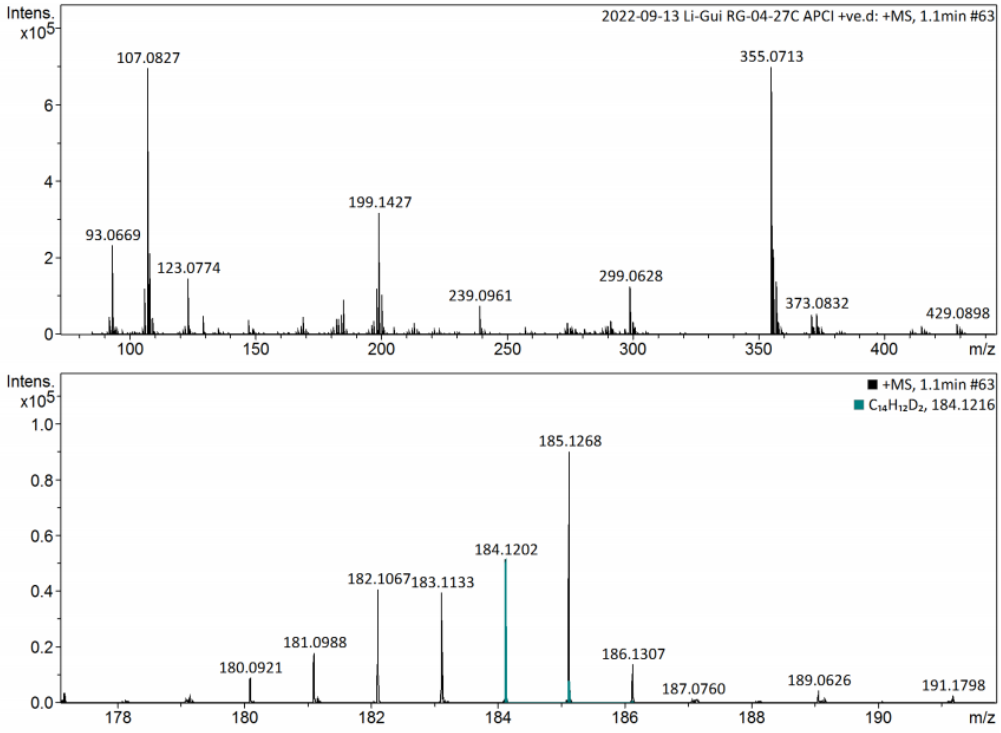
Mass Spectrum SmartFormula Report

Analysis Info

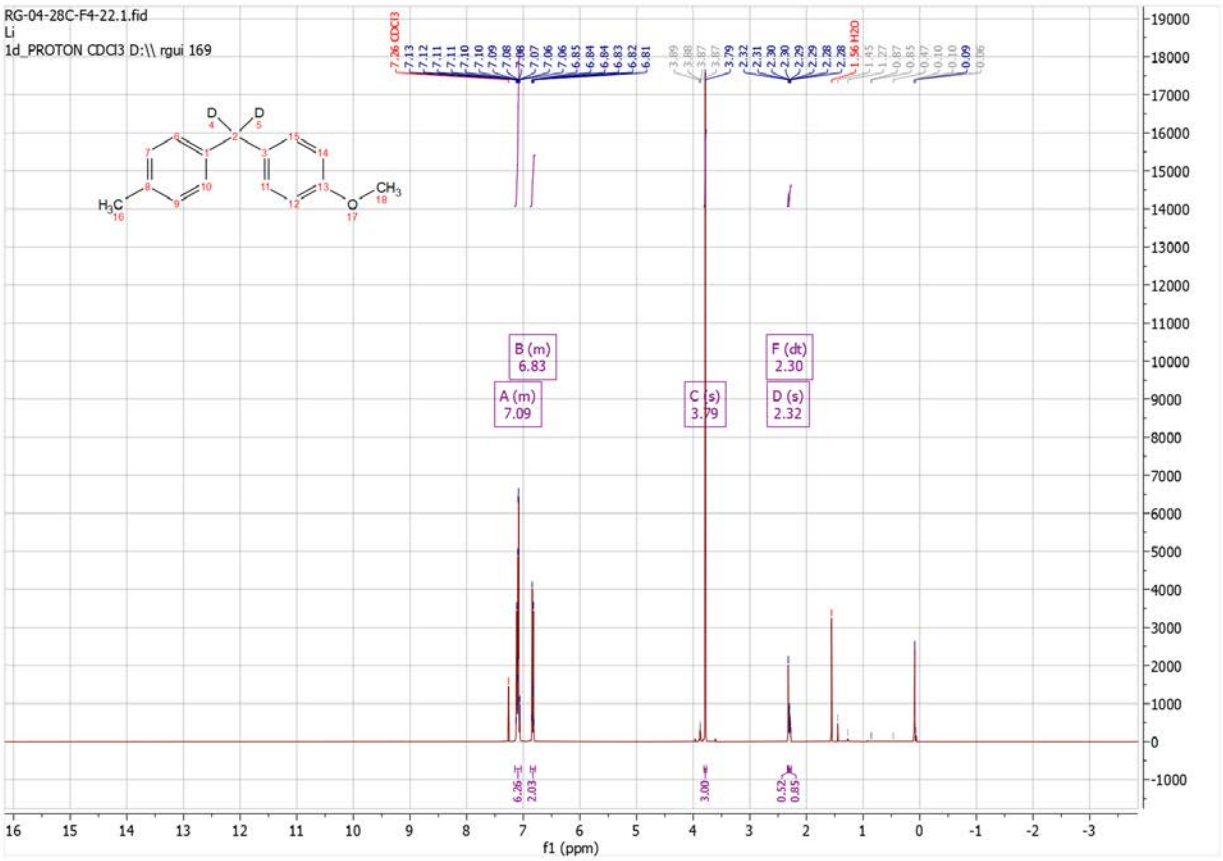
Analysis Name	D:\Data\Li\2022-09-13 Li-Gui RG-04-27C APCI +ve.d	Acquisition Date	9/13/2022 3:34:36 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-09-13 Li-Gui RG-04-27C APCI +ve	Instrument	maXis impact 282001.00044
Comment			

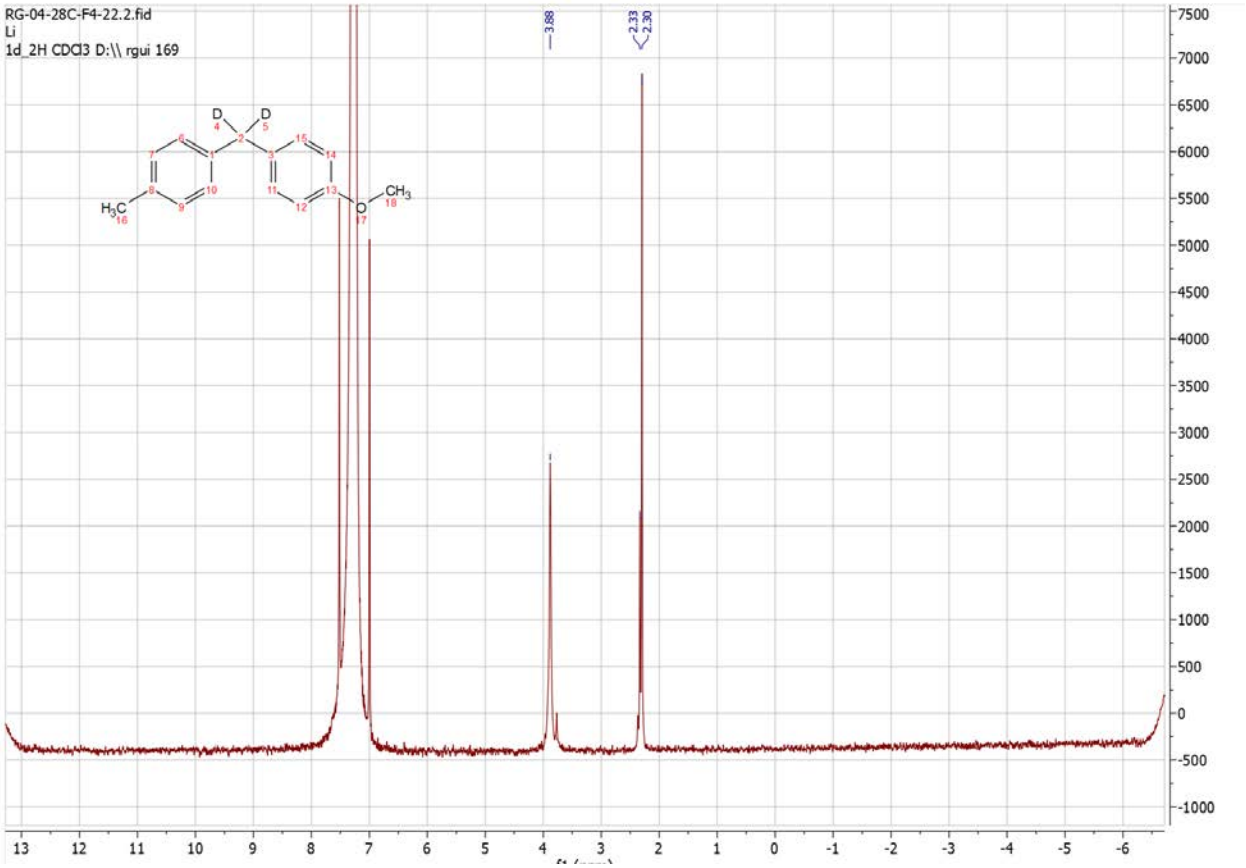
Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

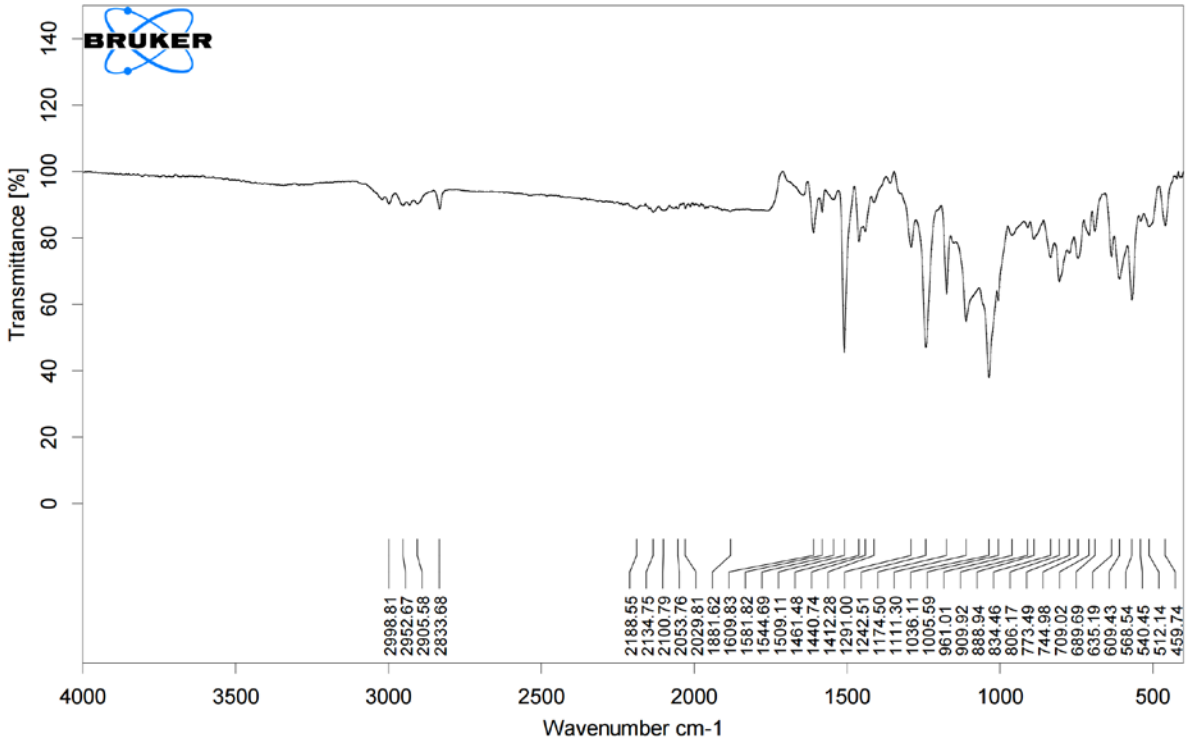


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
182.1067	1	C14H12D	182.1075	4.2	682.3	1	100.00	8.5	even	ok
	2	C14H10D2	182.1059	-4.3	682.4	2	96.41	9.0	odd	ok
	3	C9H14N2O2	182.1050	-9.4	697.1	3	0.92	4.0	odd	ok
183.1133	1	C14H11D2	183.1137	2.6	700.1	1	100.00	8.5	even	ok
	2	C14H9D3	183.1122	-5.9	700.1	2	71.65	9.0	odd	ok
	3	C9H15N2O2	183.1128	-2.5	710.2	3	5.67	3.5	even	ok
	4	C7H13N5O	183.1115	-9.8	714.1	4	0.83	4.0	odd	ok
184.1202	1	C14H12D2	184.1216	7.6	554.8	1	53.16	8.0	odd	ok
	2	C14H10D3	184.1200	-0.8	555.0	2	100.00	8.5	even	ok
	3	C9H16N2O2	184.1206	2.5	578.3	3	0.42	3.0	odd	ok


RG-04-28C-F4-22.1.fid
Li
1d_PROTON CDCl3 D:\\ rgui 169
B (m)
6.83
A (m)
7.09
C (s)
3.79
F (dt)
2.30
D (s)
2.32
f1 (ppm)


RG-04-28C-F4-22.2.fid
Li
1d_2H CDCl3 D:\\ rgui 169
3.88
2.33
2.30
D
D
CH3
H3C
O


RG-04-28C.1.fid
Research Group Li
User ruohua
D (s)
135.58
L (s)
129.25
I (s)
133.64
C (s)
138.61
A (s)
158.04
B (s)
138.65
P (s)
113.98
H (s)
133.67
K (s)
129.90
M (s)
128.80
E (m)
135.51
Q (s)
55.39
F (m)
40.23
G (m)
20.54
B1 (s)
21.14
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1
2998.81
2952.67
2905.58
2833.68
2188.55
2134.75
2100.79
2053.76
2029.81
1881.62
1609.83
1581.82
1544.69
1509.11
1461.48
1440.74
1412.28
1291.00
1242.51
1174.50
1111.30
1036.11
1005.59
961.01
909.92
888.94
834.46
806.17
773.49
744.98
709.02
689.69
635.19
609.43
568.54
540.45
512.14
459.74

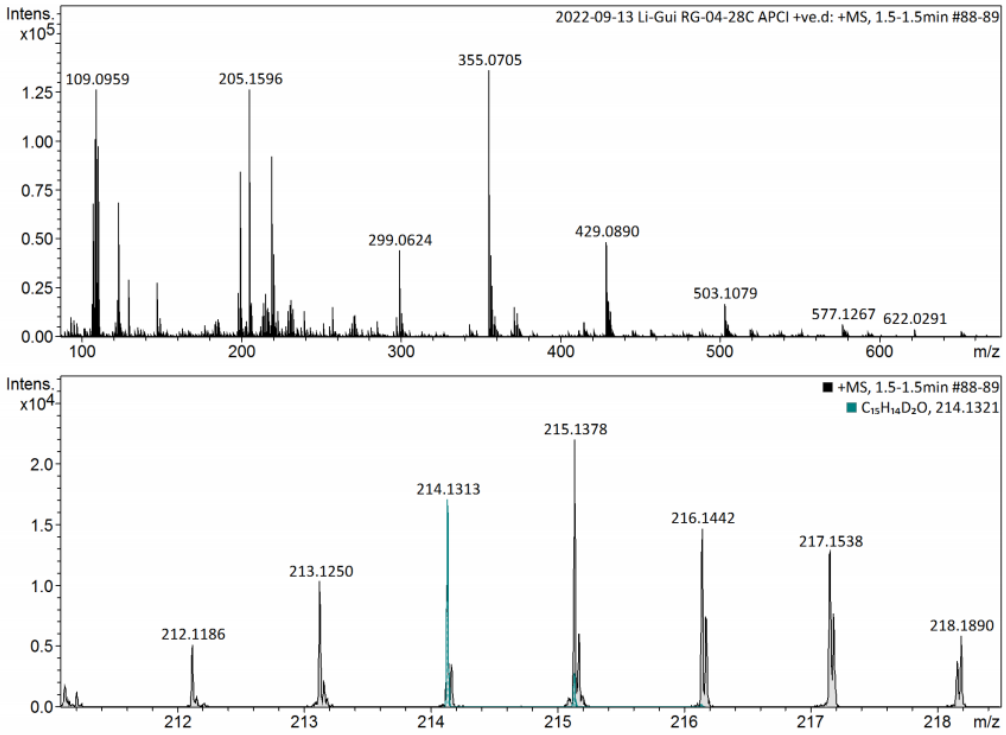
Mass Spectrum SmartFormula Report

Analysis Info

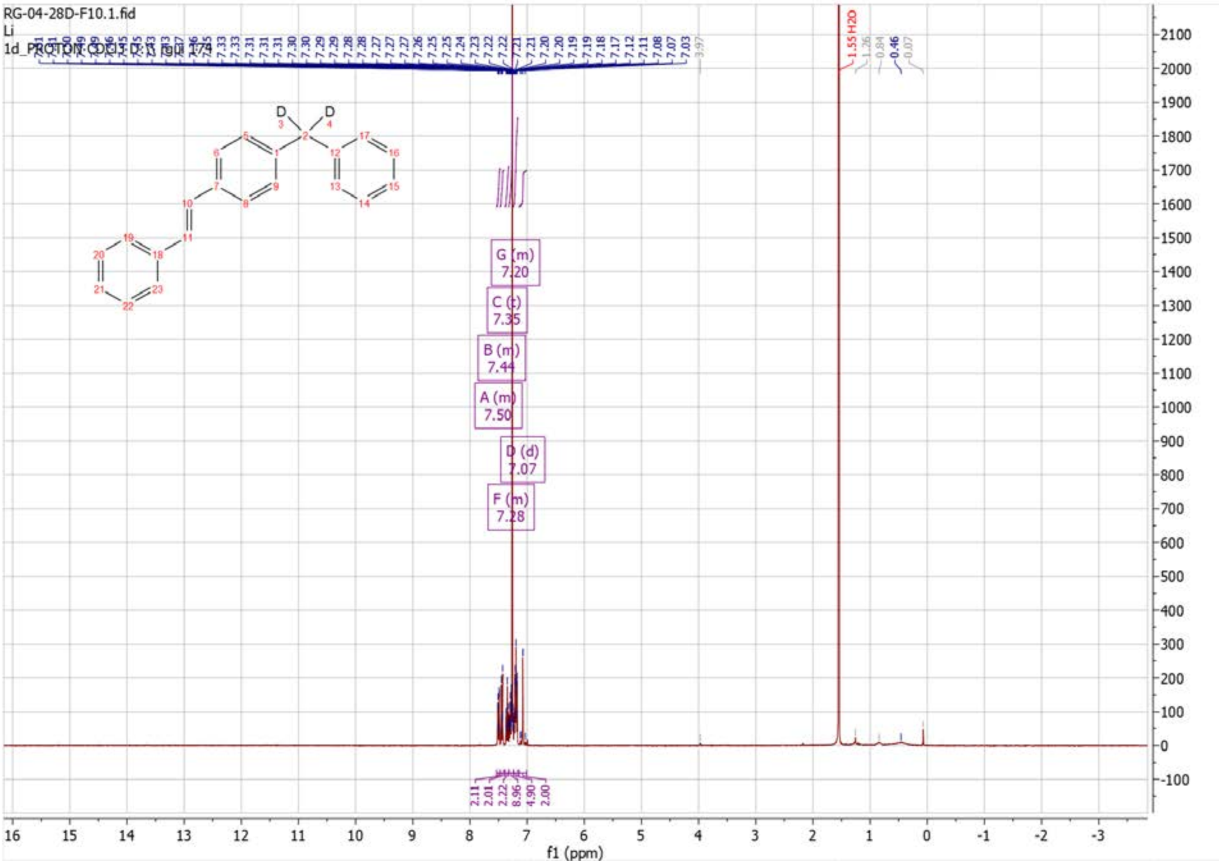
Analysis Name	D:\Data\Li\2022-09-13 Li-Gui RG-04-28C APCI +ve.d	Acquisition Date	9/13/2022 4:25:47 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-09-13 Li-Gui RG-04-28C APCI +ve	Instrument	maXis impact 282001.00044
Comment			

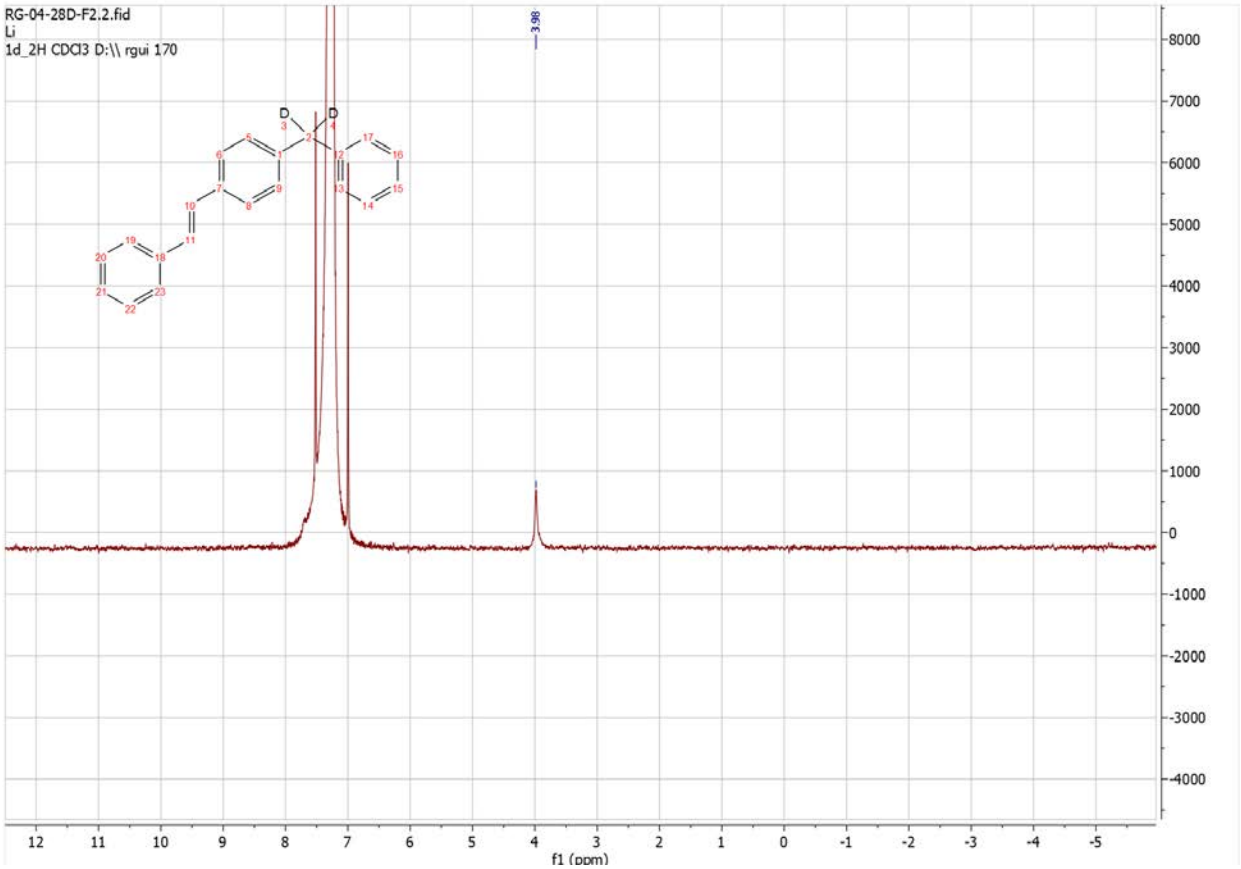
Acquisition Parameter

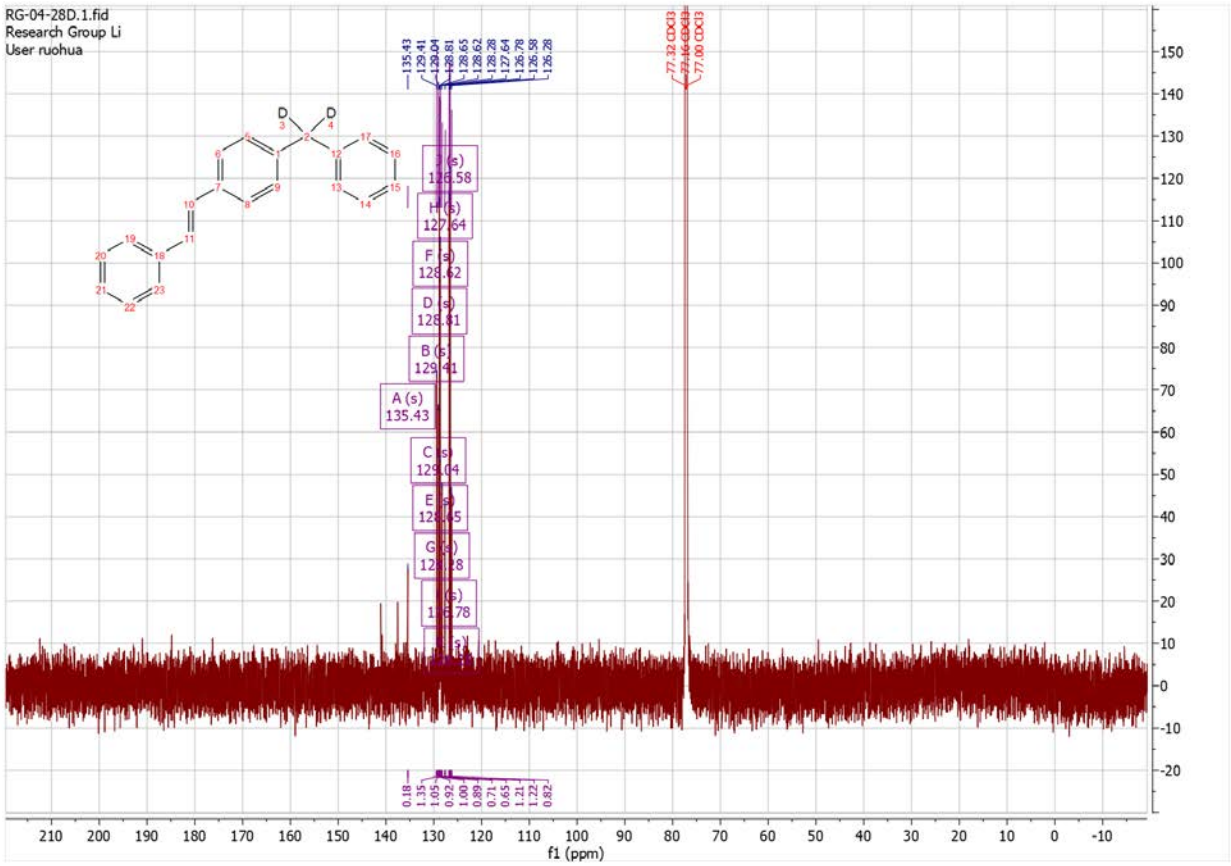
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

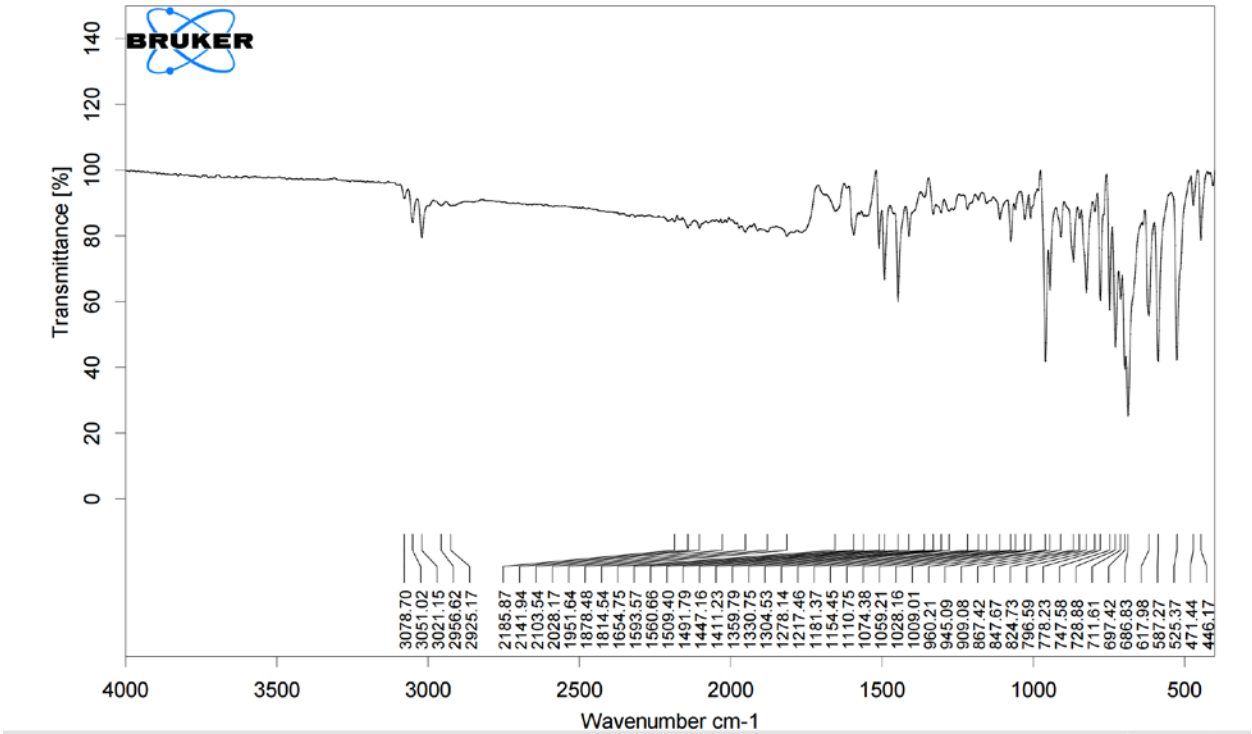


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
123.0778	1	C8H7D2O	123.0773	-3.8	6.5	1	100.00	4.5	even	ok
	2	C6H7DN3	123.0776	-2.1	12.2	2	99.01	4.5	even	ok
199.1091	1	C14H11D2O	199.1086	-2.5	25.8	1	100.00	8.5	even	ok
	2	C12H11DN3	199.1089	-1.5	30.9	2	97.43	8.5	even	ok
205.1596	1	C14H21O	205.1587	-4.5	12.1	1	100.00	4.5	even	ok
213.1250	1	C15H15DO	213.1258	4.1	736.4	1	92.27	8.0	odd	ok
	2	C15H13D2O	213.1243	-3.2	736.5	2	100.00	8.5	even	ok
	3	C13H15N3	213.1260	5.1	741.1	3	20.14	8.0	odd	ok
	4	C13H13DN3	213.1245	-2.2	741.2	4	27.14	8.5	even	ok
214.1313	1	C15H14D2O	214.1321	3.7	626.2	1	100.00	8.0	odd	ok


RG-04-28D-F10.1.fid
Li
G (m)
7.20
C (t)
7.35
B (m)
7.44
A (m)
7.50
D (d)
7.07
F (m)
7.28
f1 (ppm)


RG-04-28D-F2.2.fid
Li
1d_2H CDCl3 D:\\ rgui 170
3.98
D
D
f1 (ppm)


RG-04-28D.1.fid
Research Group Li
User ruohua
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1

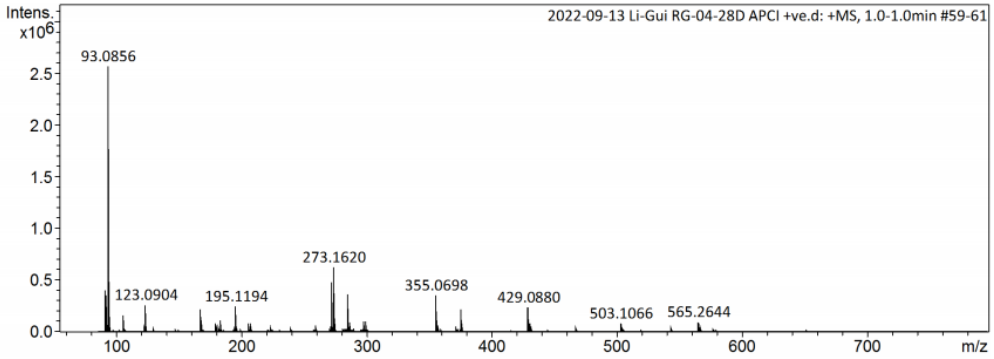
Mass Spectrum SmartFormula Report

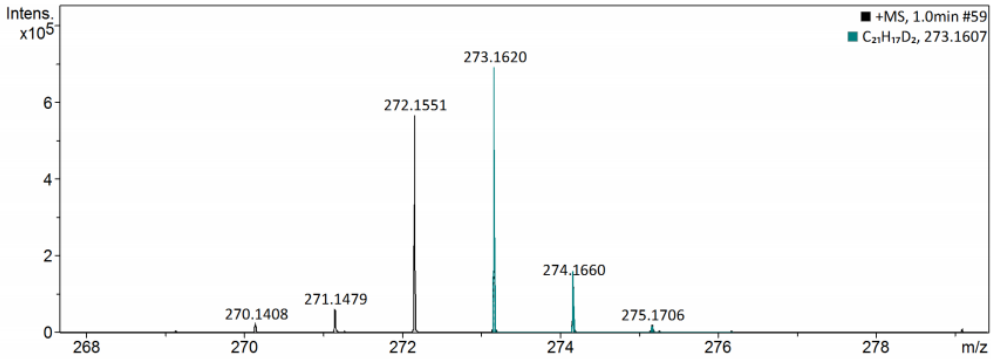
Analysis Info

Analysis Name	D:\Data\Li\2022-09-13 Li-Gui RG-04-28D APCI +ve.d	Acquisition Date	9/13/2022 3:44:01 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-09-13 Li-Gui RG-04-28D APCI +ve	Instrument	maXis impact 282001.00044
Comment			

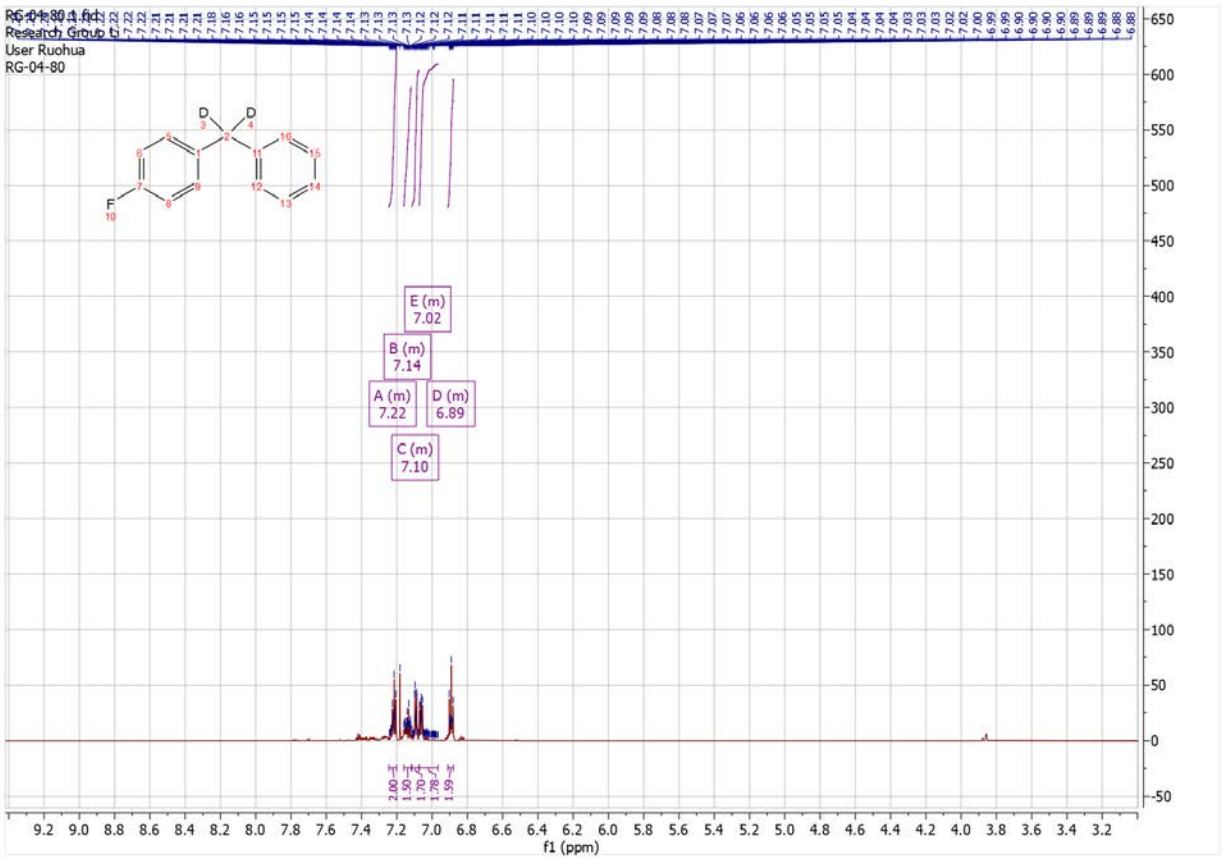
Acquisition Parameter

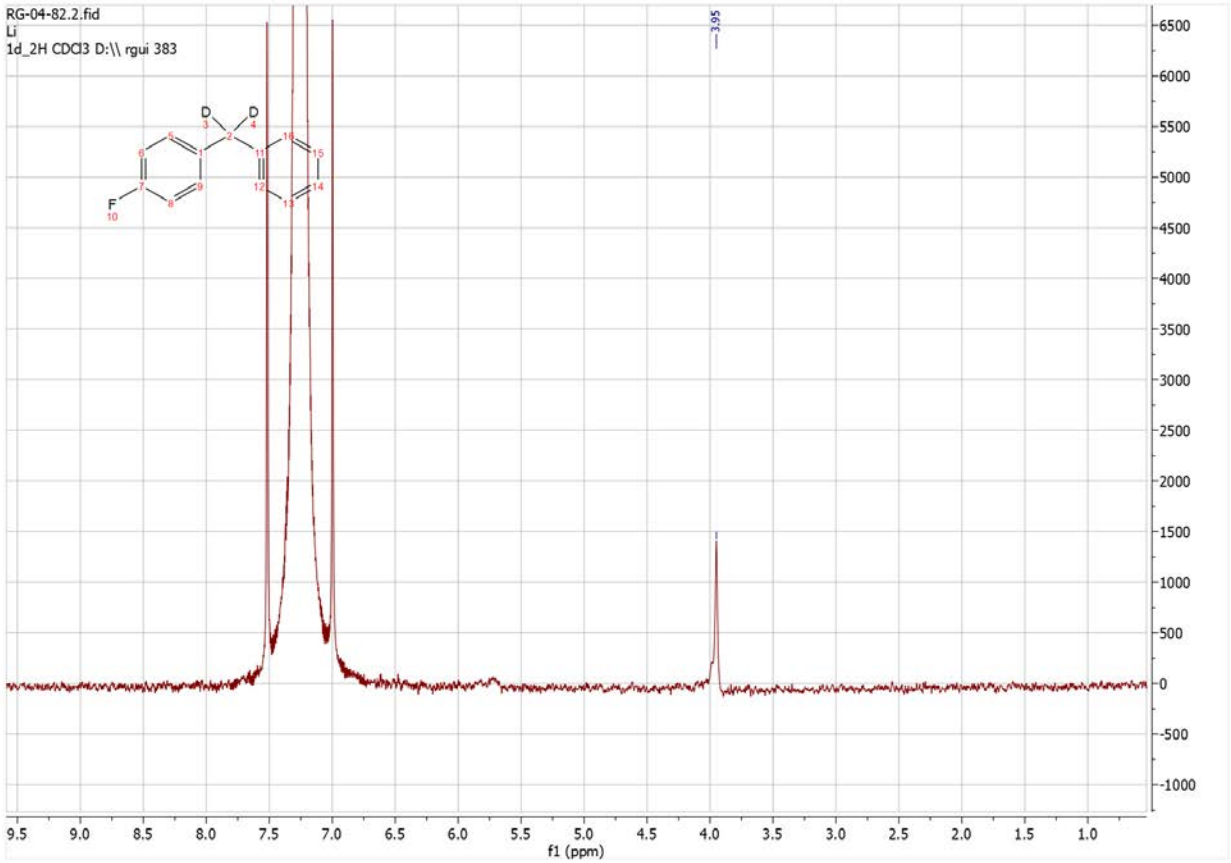
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

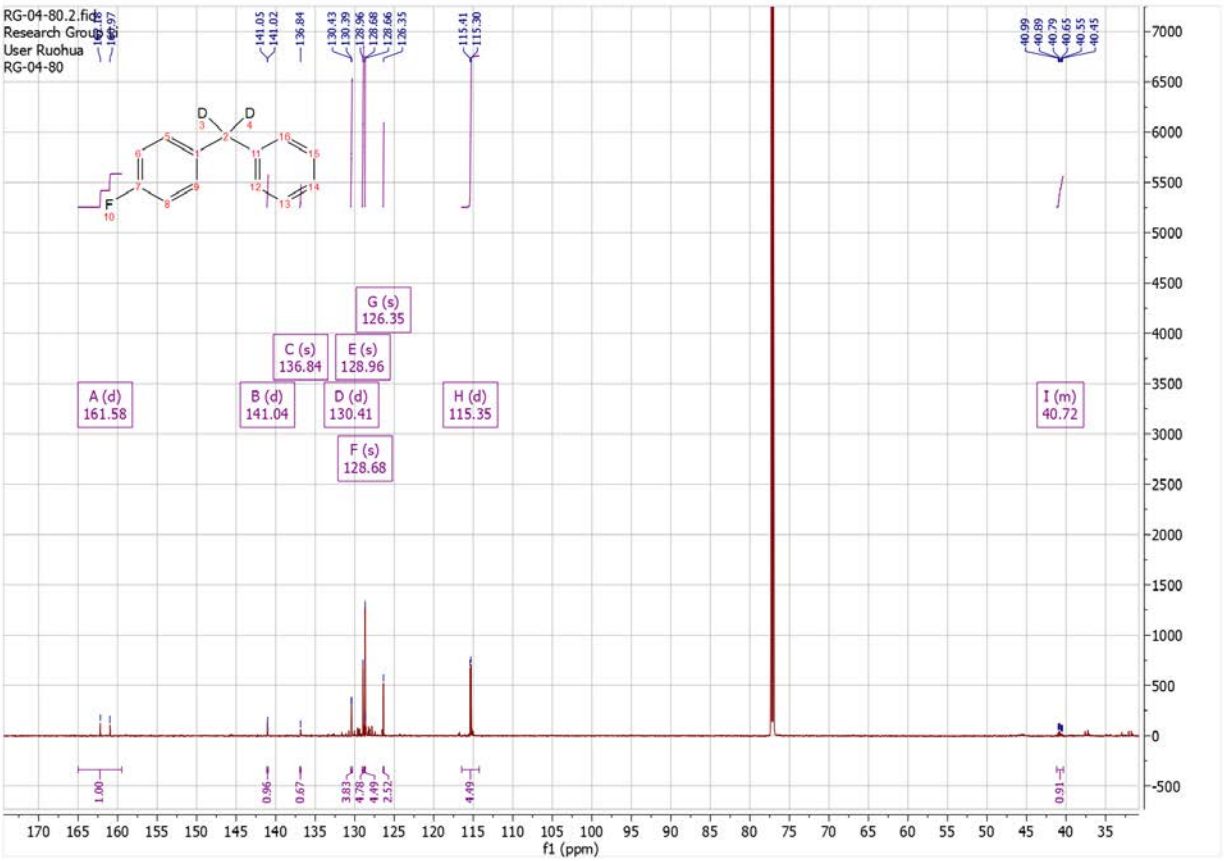


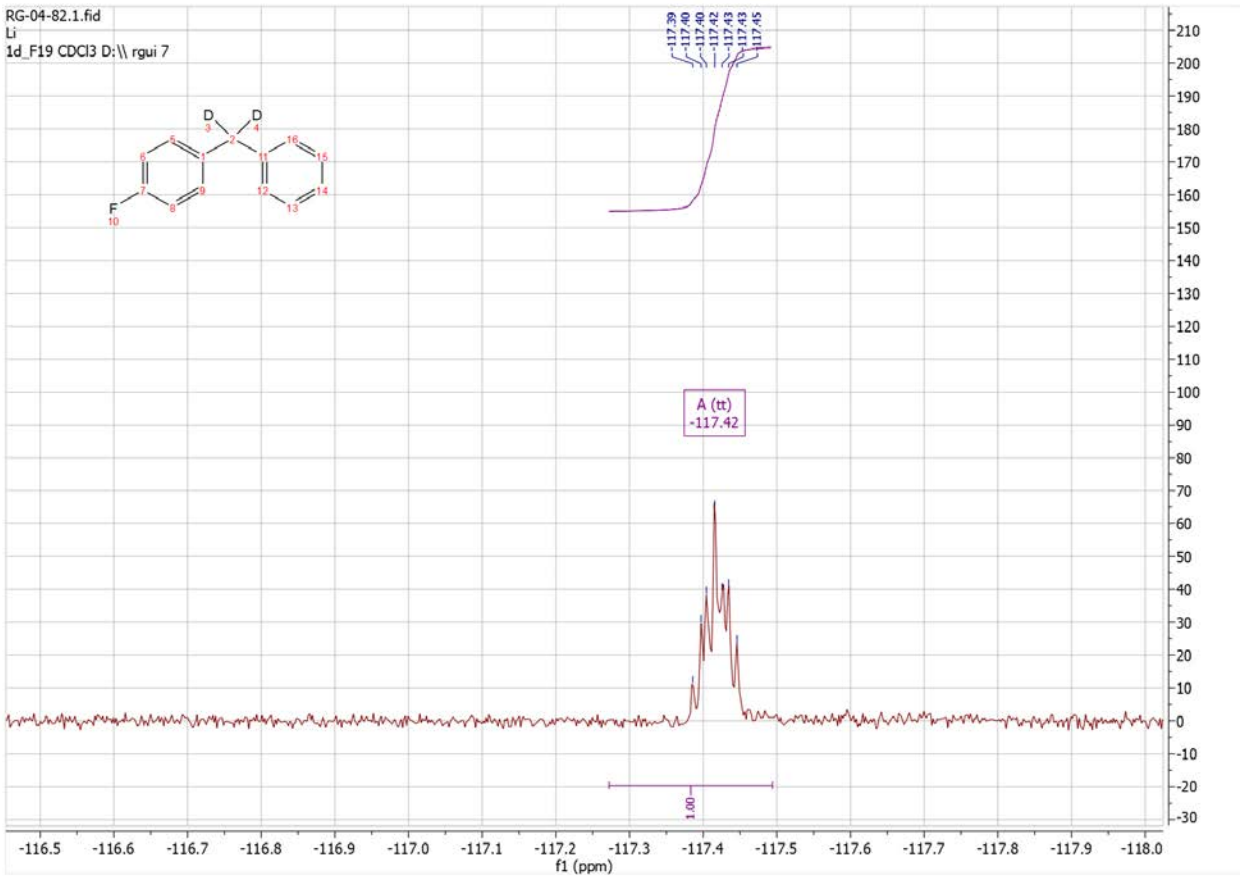


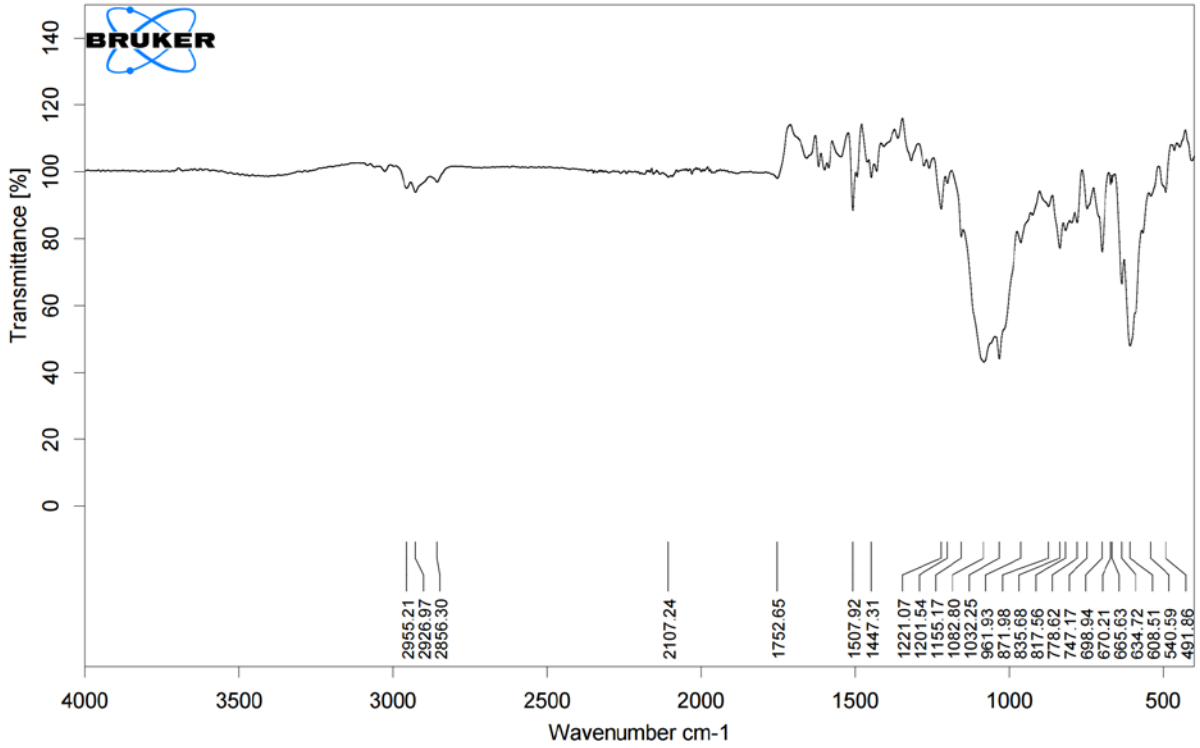
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
272.1551	1	C21H18D	272.1544	-2.6	467.9	1	100.00	12.5	even	ok
	2	C21H16D2	272.1529	-8.3	468.0	2	34.87	13.0	odd	ok
	3	C13H12D3N7	272.1572	7.6	503.2	3	0.04	10.0	odd	ok
	4	C14H18D3O5	272.1572	7.6	509.0	4	0.01	4.5	even	ok
	5	C12H18D2N3O4	272.1574	8.3	515.5	5	0.00	4.5	even	ok
	6	C12H16D3N3O4	272.1558	2.6	515.6	6	0.01	5.0	odd	ok
	7	C10H18DN6O3	272.1576	9.1	522.0	7	0.00	4.5	even	ok
	8	C10H16D2N6O3	272.1560	3.4	522.2	8	0.00	5.0	odd	ok
	9	C10H14D3N6O3	272.1545	-2.3	522.3	9	0.00	5.5	even	ok
	10	C8H16DN9O2	272.1562	4.1	528.7	10	0.00	5.0	odd	ok

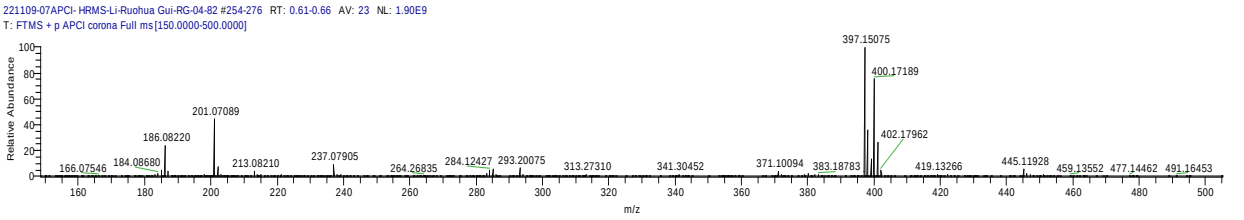

RG-04-80-1.fid
Research Group 1
User Ruohua
RG-04-80
E (m)
7.02
B (m)
7.14
A (m)
7.22
D (m)
6.89
C (m)
7.10
f1 (ppm)

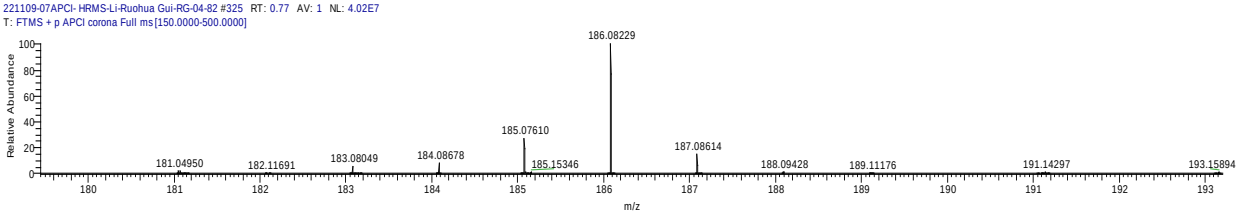

RG-04-82.2.fid
Li
1d_2H CDCl3 D:\\ rgui 383
3.95
f1 (ppm)


RG-04-80.2.fid
Research Group
User Ruohua
RG-04-80
A (d)
161.58
B (d)
141.04
C (s)
136.84
D (d)
130.41
E (s)
128.96
F (s)
128.68
G (s)
126.35
H (d)
115.35
I (m)
40.72
f1 (ppm)


RG-04-82.1.fid
Li
1d_F19 CDCl3 D:\\ rgui 7
D
D
F
-117.39
-117.40
-117.40
-117.42
-117.43
-117.43
-117.45
A (tt)
-117.42
1.00
-116.5
-116.6
-116.7
-116.8
-116.9
-117.0
-117.1
-117.2
-117.3
-117.4
-117.5
-117.6
-117.7
-117.8
-117.9
-118.0
f1 (ppm)

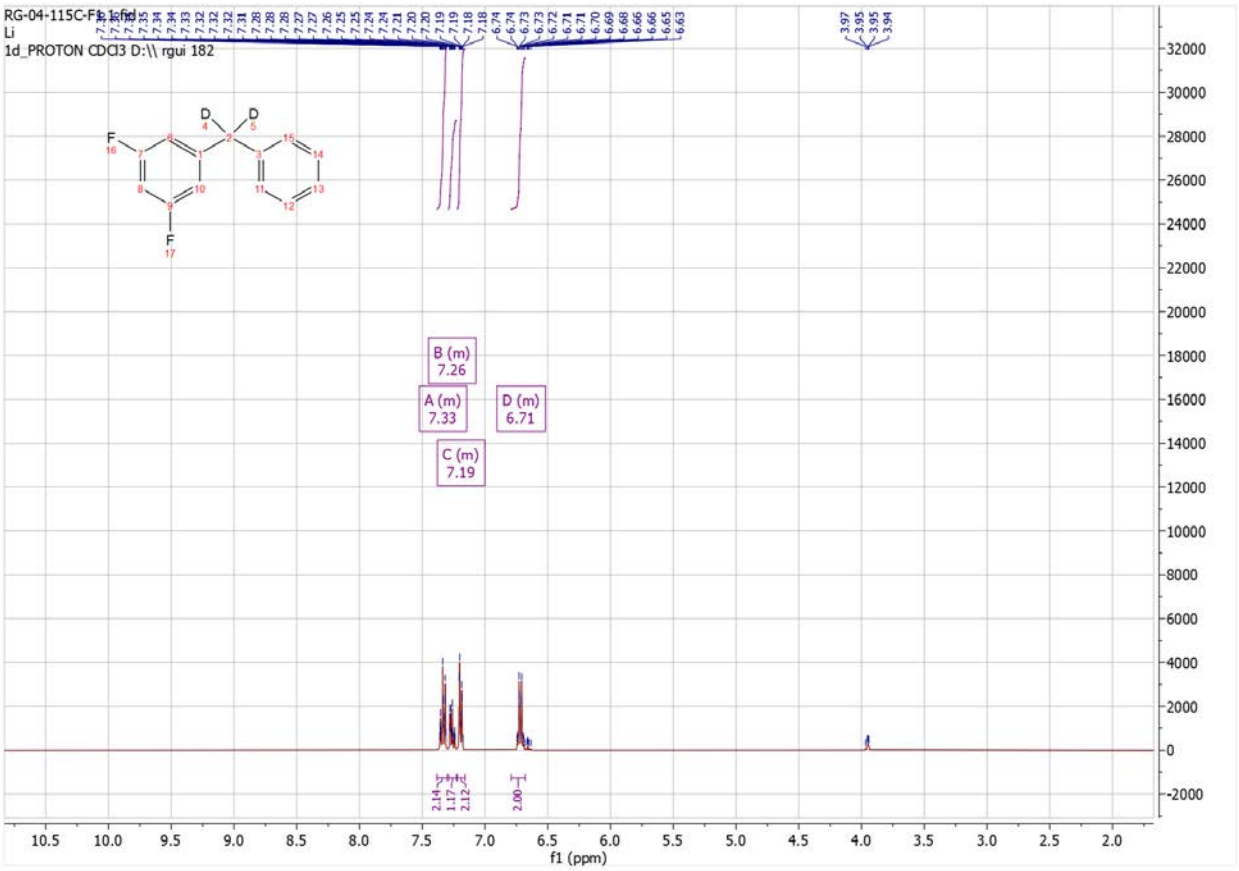

BRUKER
Transmittance [%]
0
20
40
60
80
100
120
140
2955.21
2926.97
2856.30
2107.24
1752.65
1507.92
1447.31
1221.07
1201.54
1155.17
1082.80
1032.25
961.93
871.98
835.68
817.56
778.62
747.17
698.94
670.21
665.63
634.72
608.51
540.59
491.88
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber cm-1

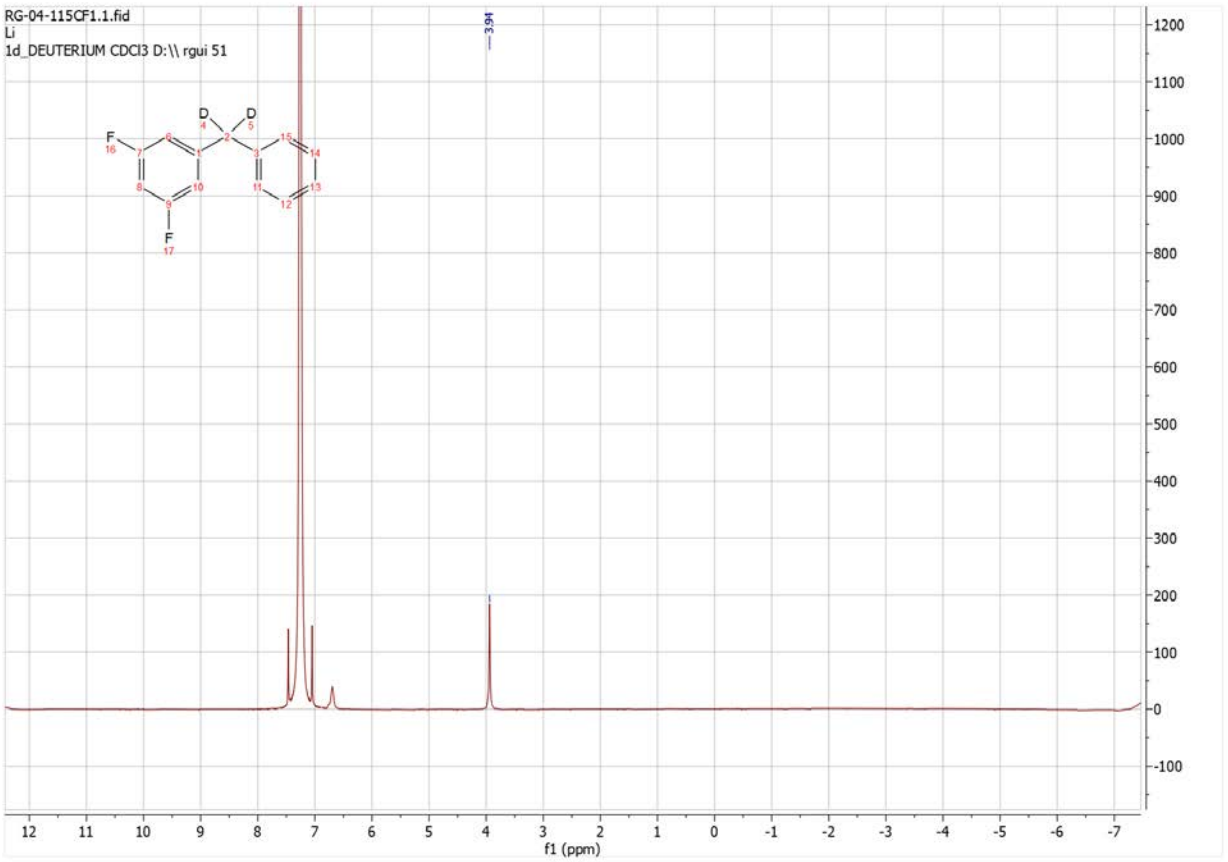




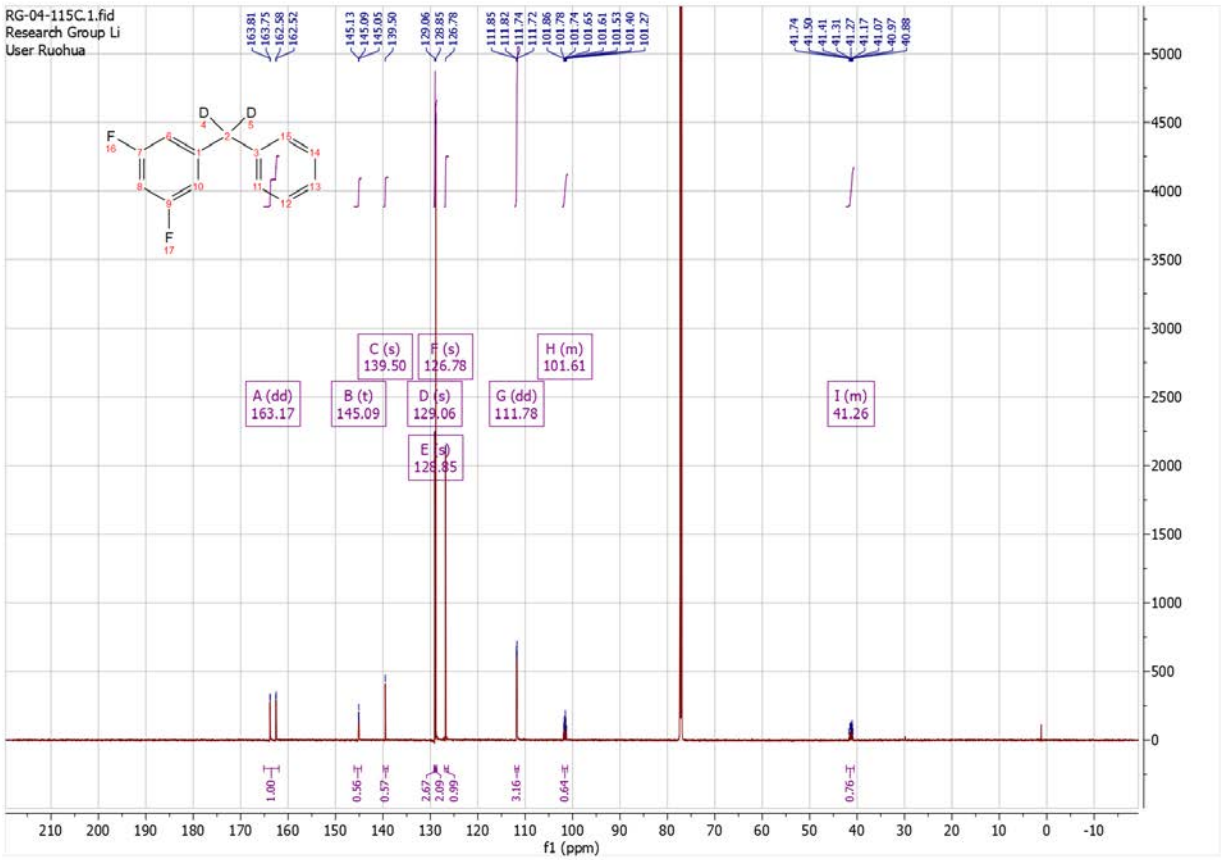
m/z	Intensity	Relative	Resolution	Charge	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
186.08229	40231092.0	100.00	41506.00	1.00	186.08238	-0.49	8.5	$C_{13}H_9{}^2HF$

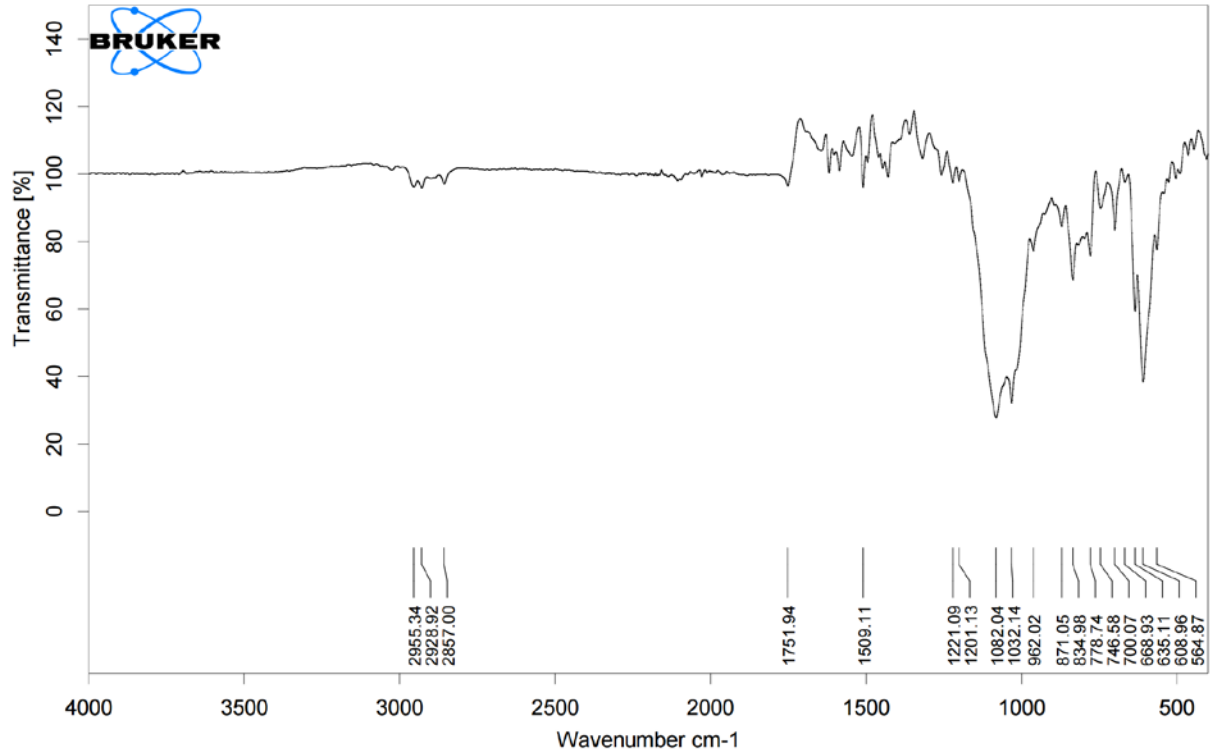
m/z	Intensity	Relative	Resolution	Charge	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
185.07610	10931645.0	100.00	41702.00	0.00	185.07611	-0.05	8.5	$C_{13}H_{10}F$


RG-04-115C-F1_1.fid
Li
1d_PROTON CDCl3 D:\\ rgui 182
B (m)
7.26
A (m)
7.33
D (m)
6.71
C (m)
7.19
2.14
1.17
2.12
2.00
f1 (ppm)


RG-04-115CF1.1.fid
Li
1d_DEUTERIUM CDCl3 D:\\ rgui 51
3.94
f1 (ppm)


RG-04-115CF1.2.fid
Li
1d_F19CPD CDCl3 D:\\ rgui 51
-110.39
-110.66
B (s)
-110.66
A (s)
-110.39
1.00
7.97
f1 (ppm)


RG-04-115C.1.fid
Research Group Li
User Ruohua
C (s) 139.50
F (s) 126.78
H (m) 101.61
A (dd) 163.17
B (t) 145.09
D (s) 129.06
G (dd) 111.78
I (m) 41.26
E (s) 126.85
f1 (ppm)


BRUKER
Transmittance [%]
2955.34
2928.92
2857.00
1751.94
1509.11
1221.09
1201.13
1082.04
1032.14
962.02
871.05
834.98
778.74
746.58
700.07
668.93
635.11
608.96
564.87
Wavenumber cm-1

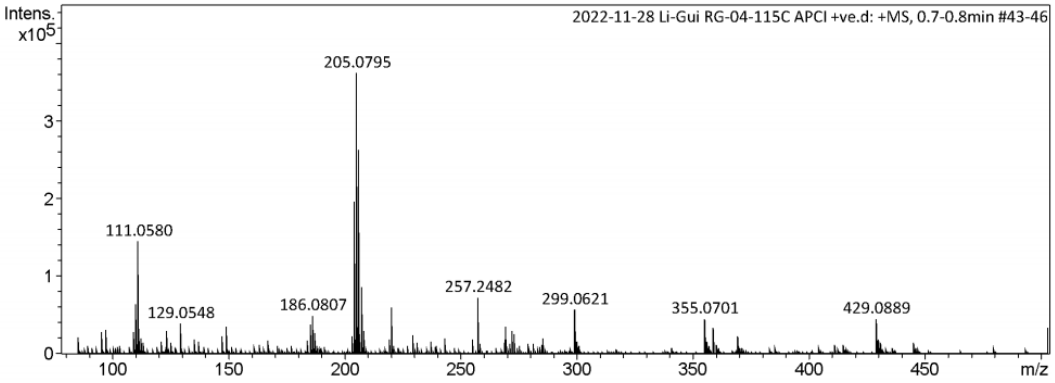
Mass Spectrum SmartFormula Report

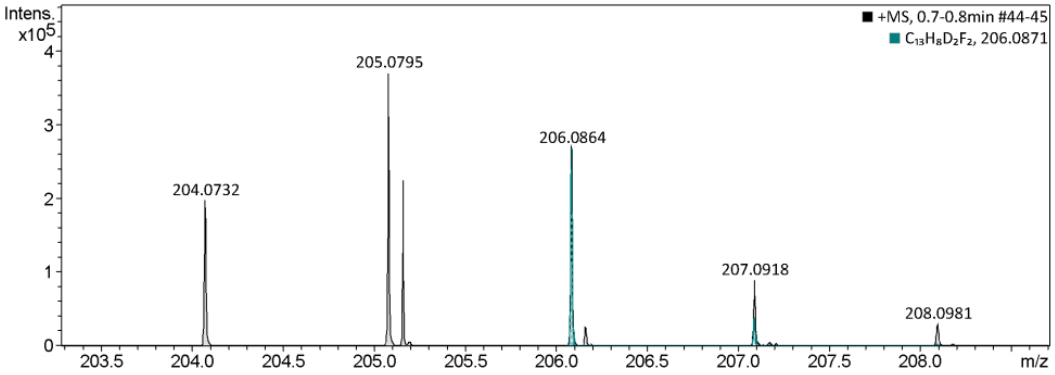
Analysis Info

Analysis Name	D:\Data\Li\2022-11-28 Li-Gui RG-04-115C APCI +ve.d	Acquisition Date	11/28/2022 2:42:22 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-11-28 Li-Gui RG-04-115C APCI +ve	Instrument	maXis impact 282001.00044
Comment			

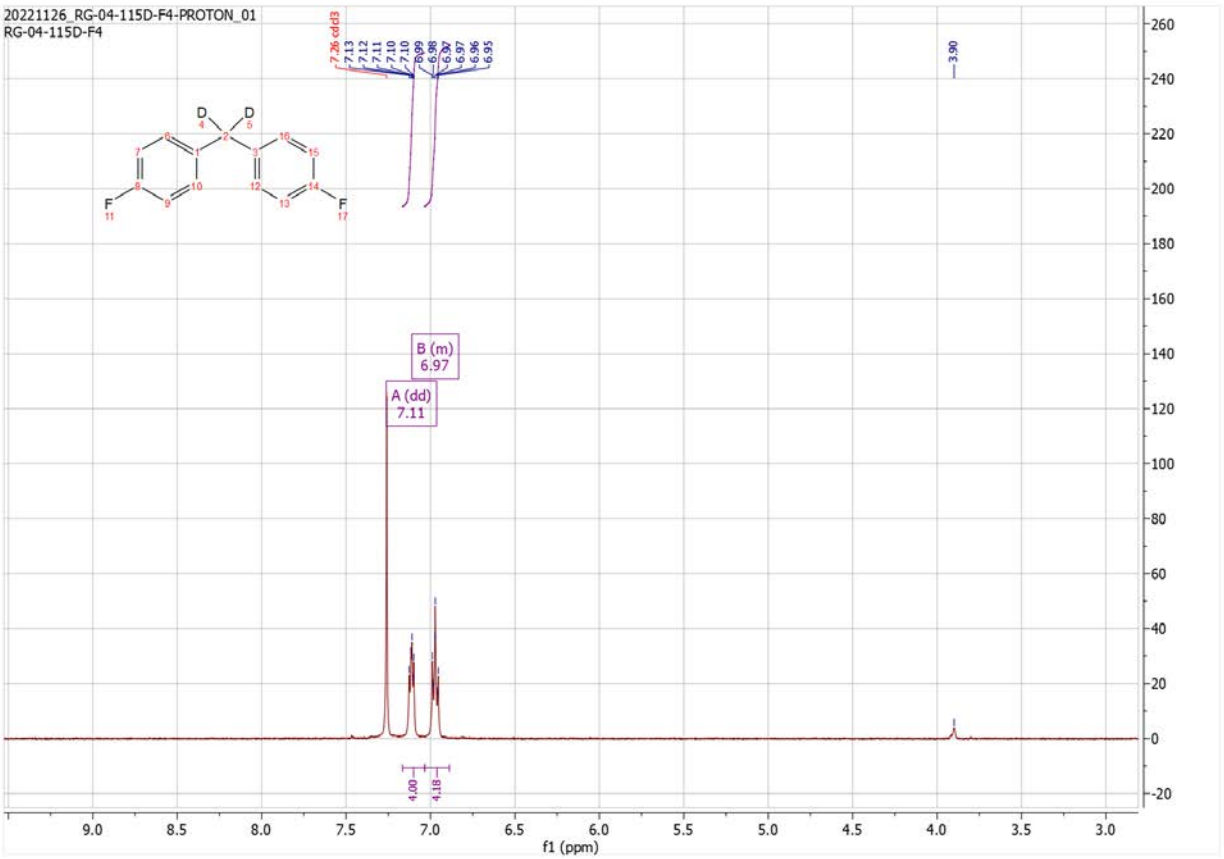
Acquisition Parameter

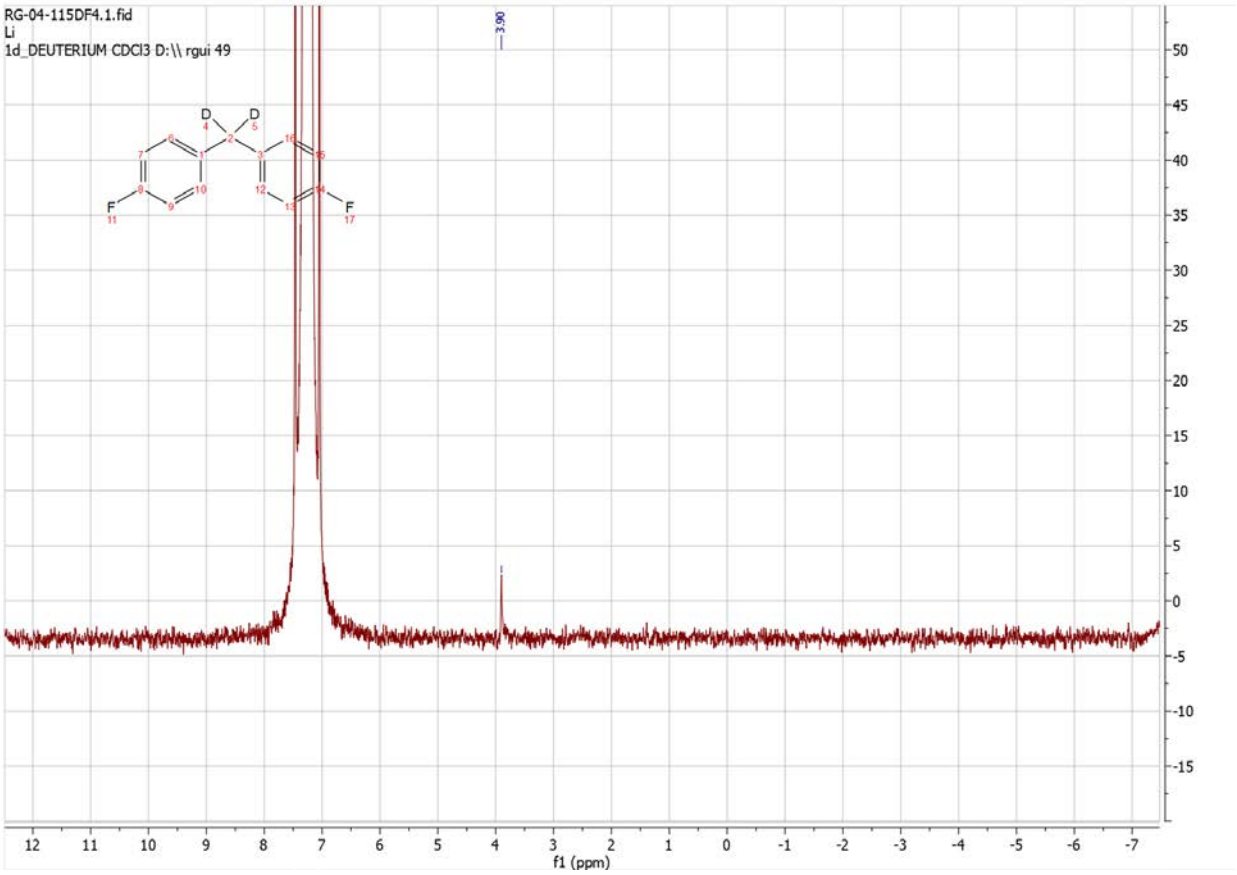
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

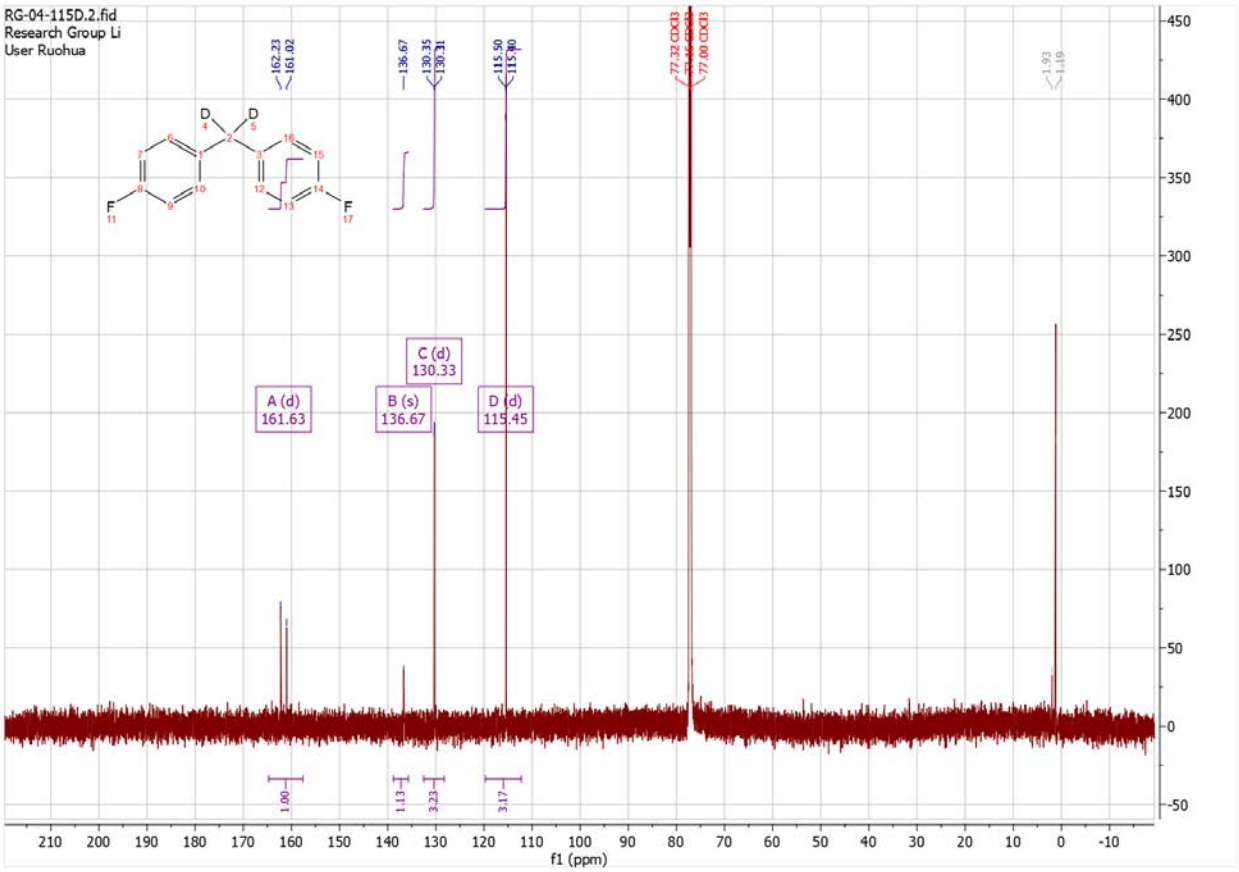


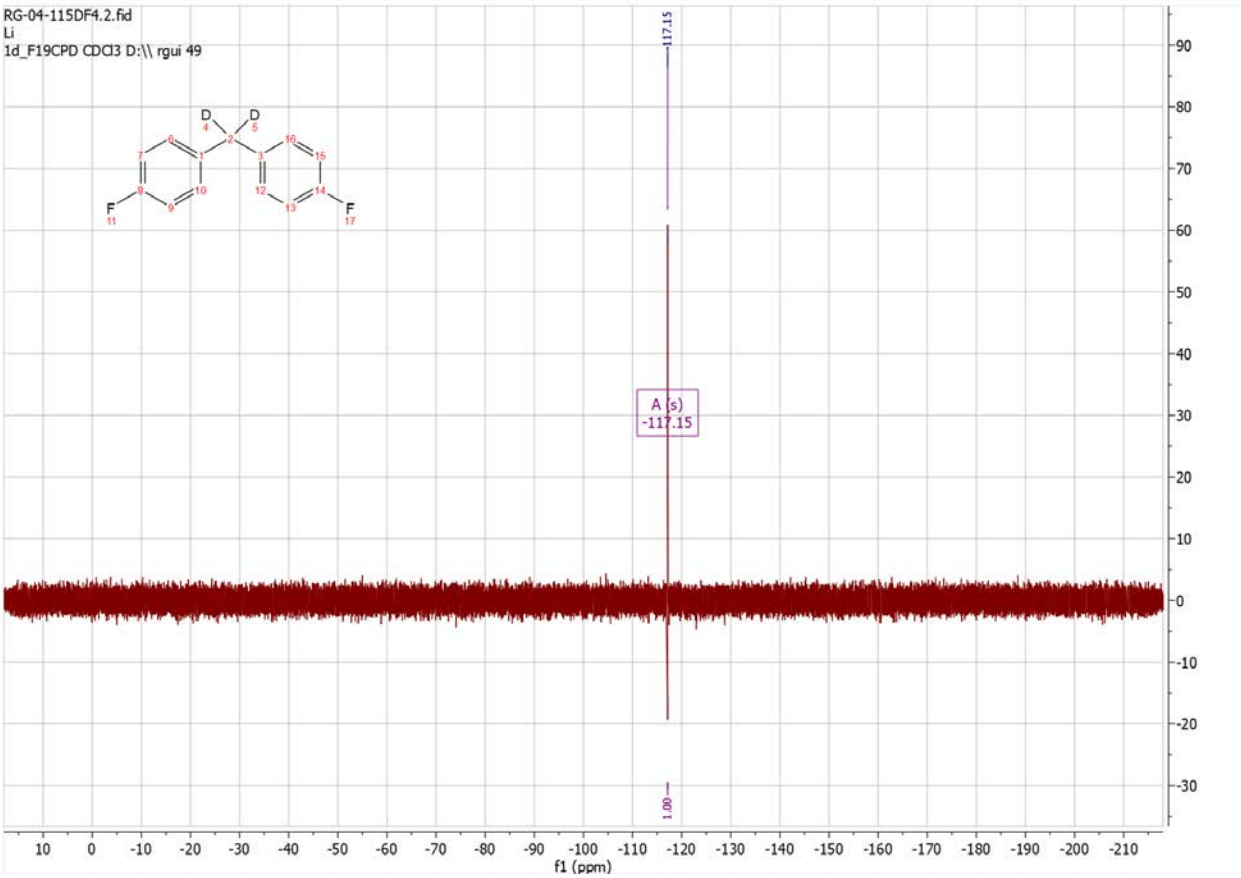


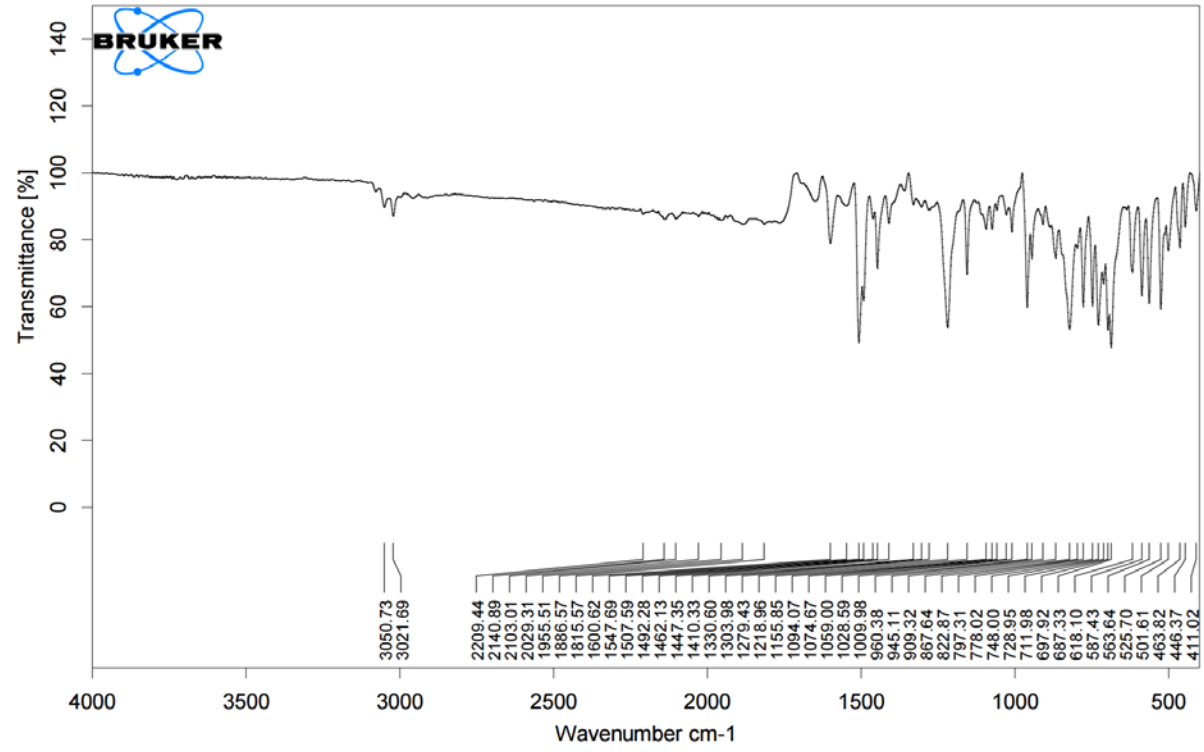
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
204.0732	1	C13H8DF2	204.0730	-1.3	699.2	1	100.00	8.5	even	ok
205.0795	1	C13H7D2F2	205.0792	-1.5	361.2	1	100.00	8.5	even	ok
206.0864	1	C13H8D2F2	206.0871	3.3	123.4	1	100.00	8.0	odd	ok
	2	C8H12F2N2O2	206.0861	-1.2	147.4	2	28.77	3.0	odd	ok
207.0918	1	C8H11DF2N2O2	207.0924	3.1	140.5	1	100.00	3.0	odd	ok
	2	C8H9D2F2N2O2	207.0909	-4.4	140.7	2	86.70	3.5	even	ok
	3	C6H11F2N5O	207.0926	4.1	147.1	3	59.06	3.0	odd	ok
	4	C6H9DF2N5O	207.0911	-3.4	147.3	4	63.65	3.5	even	ok
	5	C4H9F2N8	207.0913	-2.4	148.5	5	65.13	3.5	even	ok


20221126_RG-04-115D-F4-PROTON_01
RG-04-115D-F4
7.26 cdcl3
7.13
7.12
7.11
7.10
7.10
6.99
6.98
6.97
6.97
6.96
6.95
3.90
D
D
F
F
B (m)
6.97
A (dd)
7.11
4.00
4.18
f1 (ppm)


RG-04-115DF4.1.fid
Li
1d_DEUTERIUM CDCl3 D:\\ rgui 49
3.90
f1 (ppm)


RG-04-115D.2.fid
Research Group Li
User Ruohua
A (d)
161.63
B (s)
136.67
C (d)
130.33
D (d)
115.45
f1 (ppm)


RG-04-115DF4.2.fid
Li
1d_F19CPD CDCl3 D:\\ rgui 49
D
D
F
F
A (s)
-117.15
-117.15
1.00
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1
3050.73
3021.69
2209.44
2140.89
2103.01
2029.31
1955.51
1886.57
1815.57
1600.62
1547.69
1507.59
1492.28
1462.13
1447.35
1410.33
1330.60
1303.98
1279.43
1218.96
1155.85
1094.07
1074.67
1059.00
1028.59
1009.98
960.38
945.11
909.32
867.64
822.87
797.31
778.02
748.00
728.95
711.98
697.92
687.33
618.10
587.43
563.64
525.70
501.61
463.82
446.37
411.02

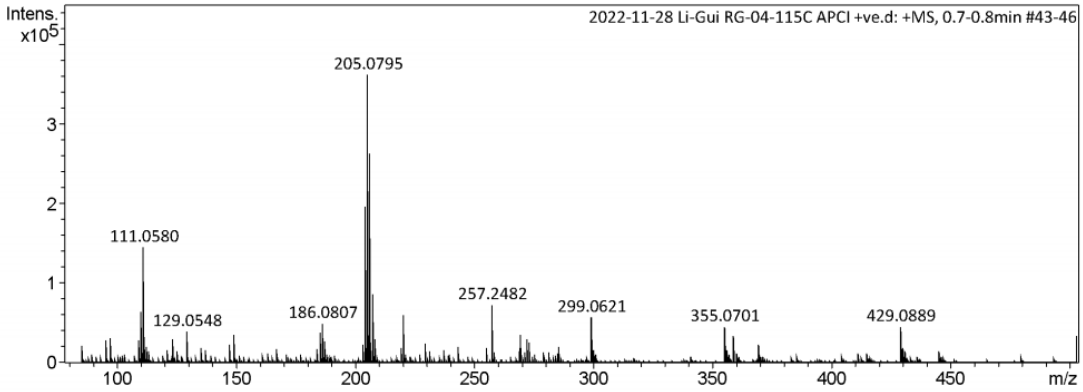
Mass Spectrum SmartFormula Report

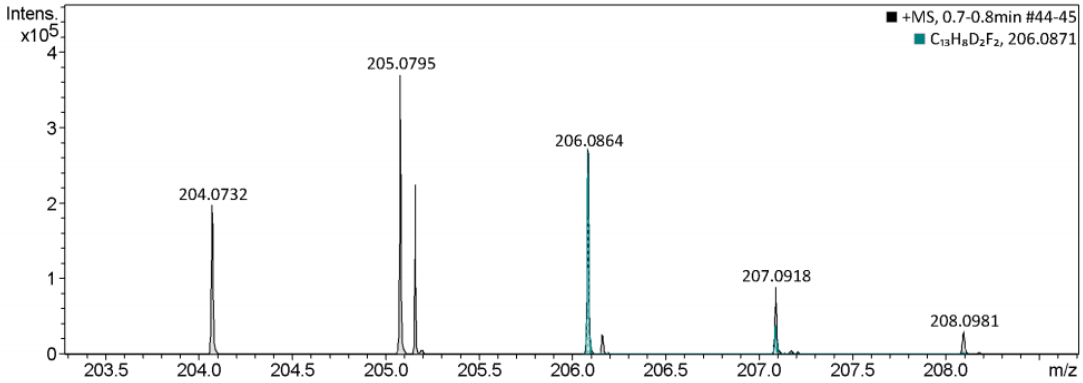
Analysis Info

Analysis Name	D:\Data\Li\2022-11-28 Li-Gui RG-04-115C APCI +ve.d	Acquisition Date	11/28/2022 2:42:22 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-11-28 Li-Gui RG-04-115C APCI +ve	Instrument	maXis impact 282001.00044
Comment			

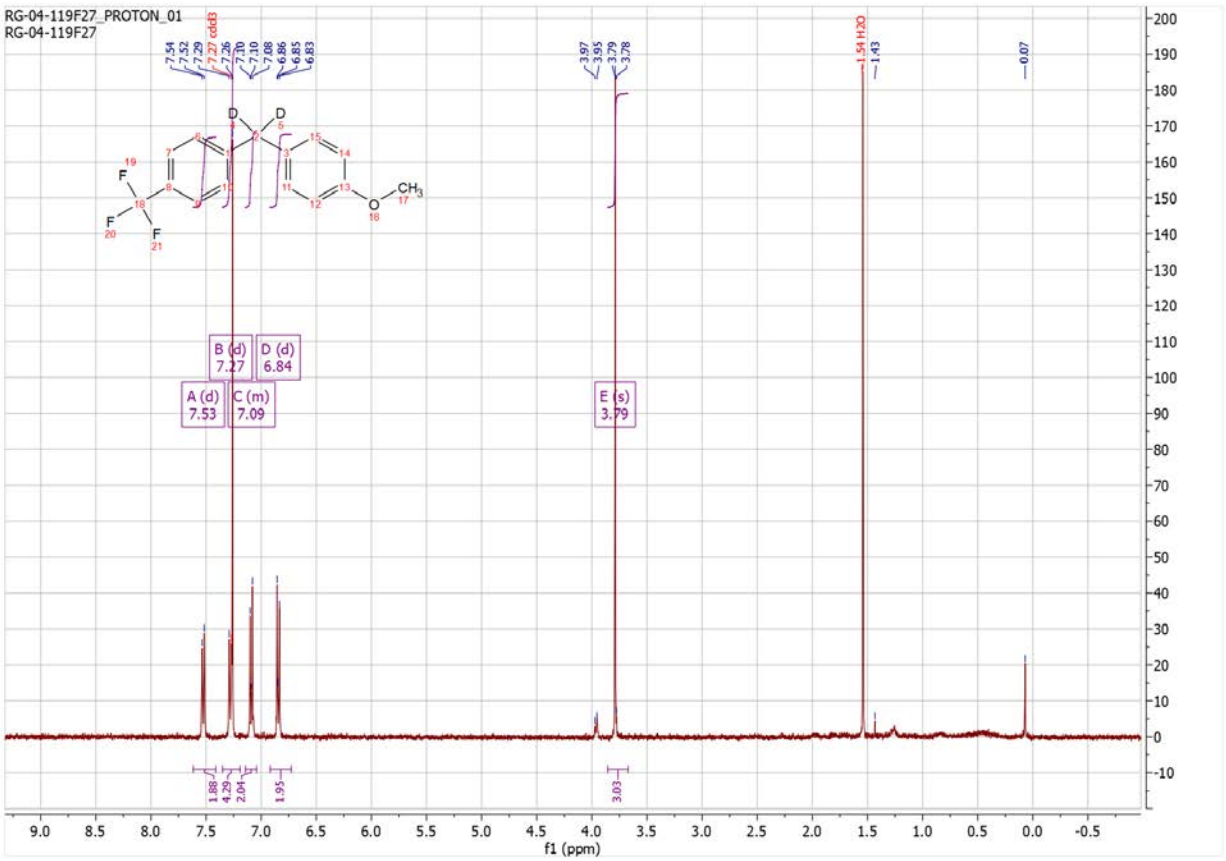
Acquisition Parameter

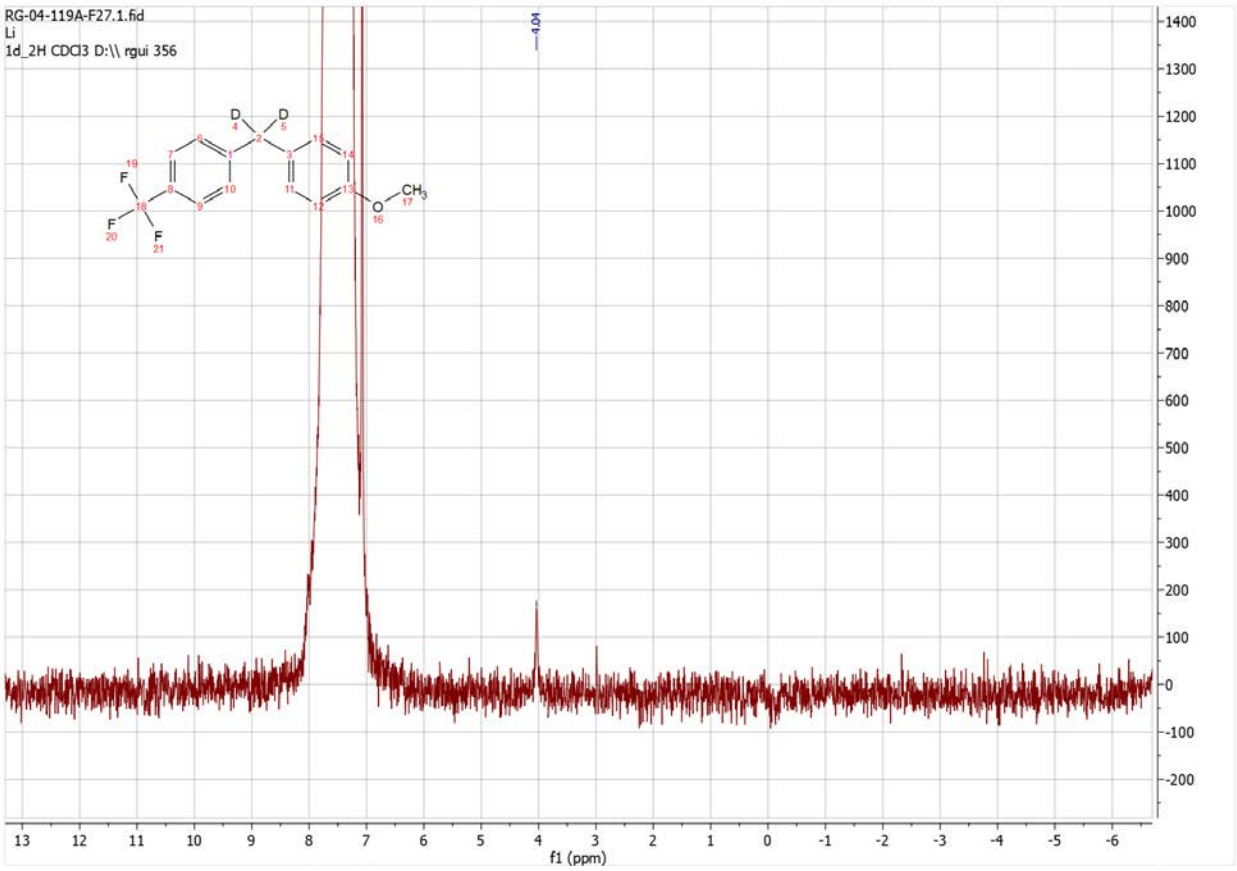
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

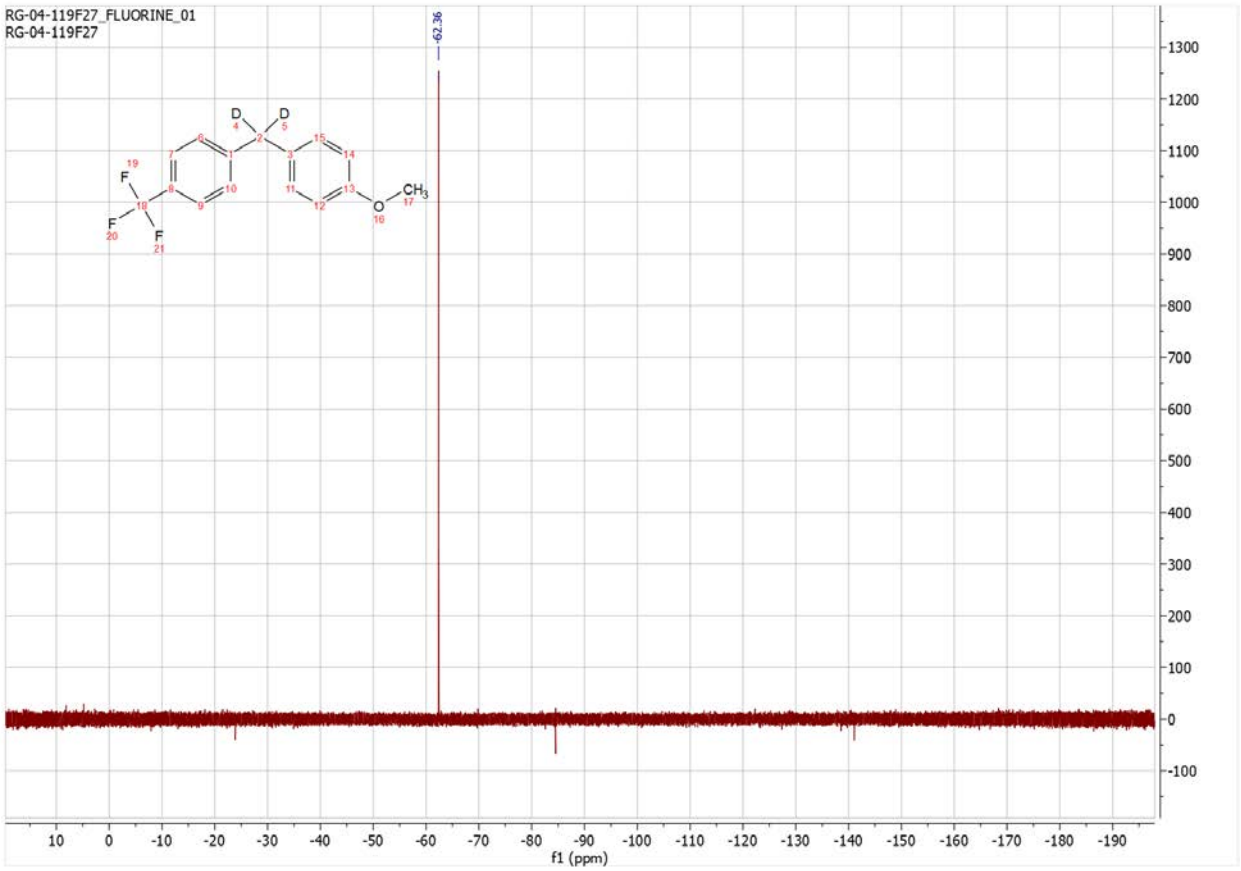


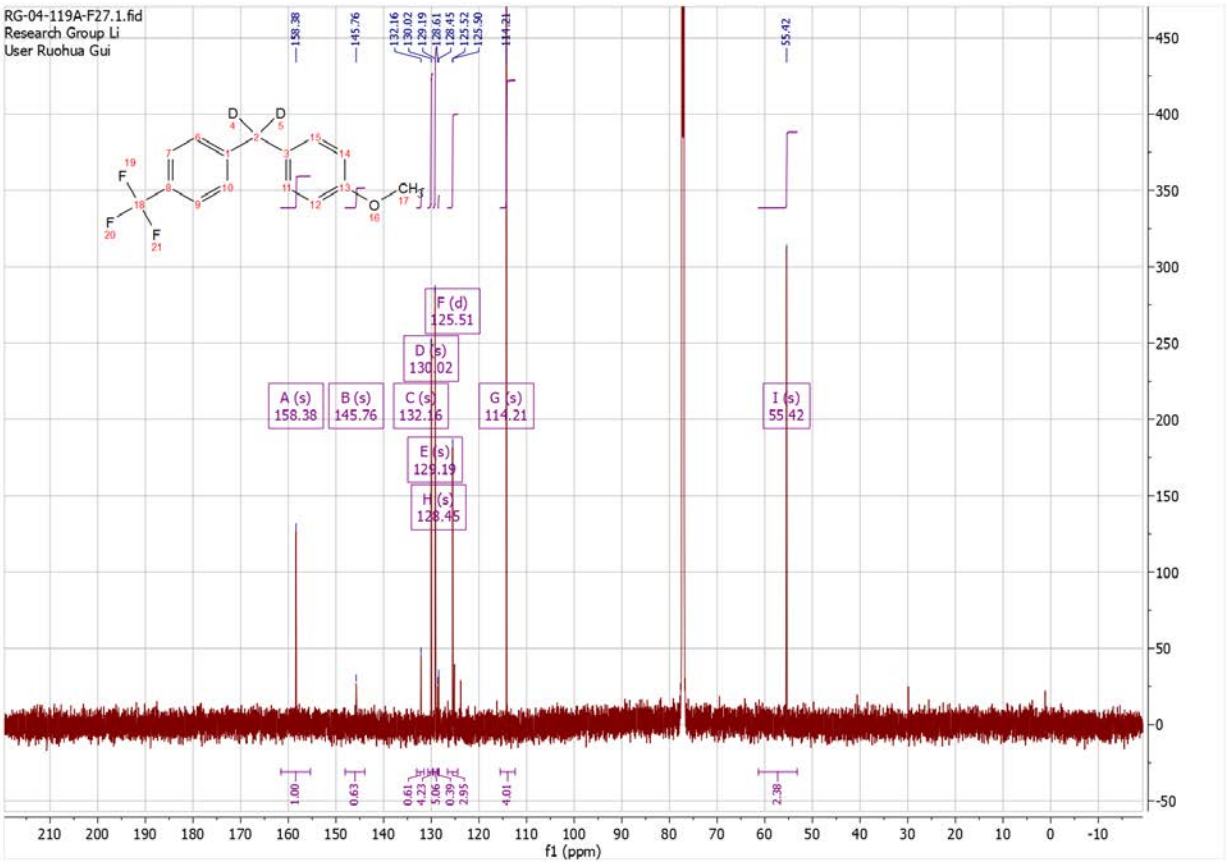


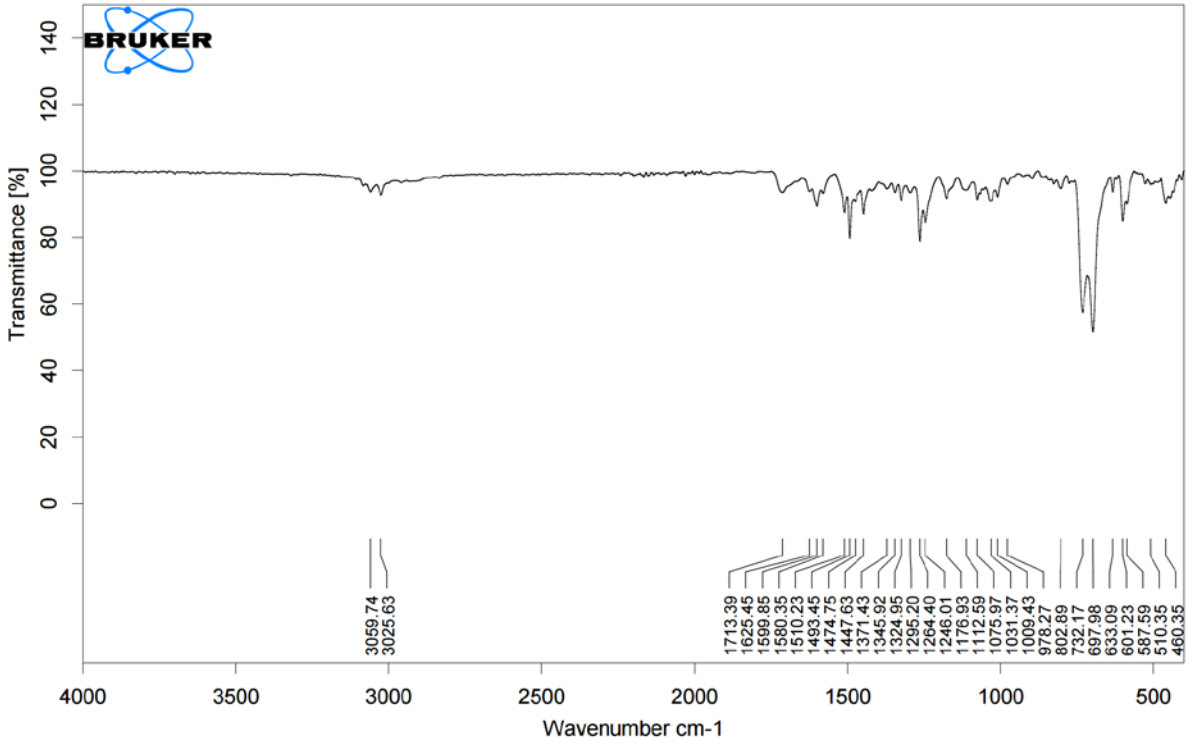
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
204.0732	1	C13H8DF2	204.0730	-1.3	699.2	1	100.00	8.5	even	ok
205.0795	1	C13H7D2F2	205.0792	-1.5	361.2	1	100.00	8.5	even	ok
206.0864	1	C13H8D2F2	206.0871	3.3	123.4	1	100.00	8.0	odd	ok
	2	C8H12F2N2O2	206.0861	-1.2	147.4	2	28.77	3.0	odd	ok
207.0918	1	C8H11DF2N2O2	207.0924	3.1	140.5	1	100.00	3.0	odd	ok
	2	C8H9D2F2N2O2	207.0909	-4.4	140.7	2	86.70	3.5	even	ok
	3	C6H11F2N5O	207.0926	4.1	147.1	3	59.06	3.0	odd	ok
	4	C6H9DF2N5O	207.0911	-3.4	147.3	4	63.65	3.5	even	ok
	5	C4H9F2N8	207.0913	-2.4	148.5	5	65.13	3.5	even	ok


RG-04-119F27_PROTON_01
RG-04-119F27
7.54
7.52
7.29
7.27 cddB
7.26
7.10
7.08
6.86
6.85
6.83
3.97
3.95
3.79
3.78
1.54 H2O
1.43
0.07
B (d) 7.27
D (d) 6.84
A (d) 7.53
C (m) 7.09
E (s) 3.79
1.88
4.29
2.04
1.95
3.03
f1 (ppm)


RG-04-119A-F27.1.fid
Li
1d_2H CDCl3 D:\\ rgui 356
4.04
D
D
F
F
F
O
CH3
f1 (ppm)


RG-04-119F27_FLUORINE_01
RG-04-119F27
-62.36
D
D
F
F
F
CH3
O
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
f1 (ppm)


RG-04-119A-F27.1.fid
Research Group Li
User Ruohua Gui
158.38
145.76
132.16
130.02
129.19
128.61
128.45
125.52
125.50
114.21
55.42
F (d)
125.51
D (s)
130.02
A (s)
158.38
B (s)
145.76
C (s)
132.16
G (s)
114.21
I (s)
55.42
E (s)
129.19
H (s)
128.45
1.00
0.63
0.61
4.23
5.06
0.39
2.95
4.01
2.38
f1 (ppm)


BRUKER
Transmittance [%]
3059.74
3025.63
1713.39
1625.45
1599.85
1580.35
1510.23
1493.45
1474.75
1447.63
1371.43
1345.92
1324.95
1295.20
1264.40
1246.01
1176.93
1112.59
1075.97
1031.37
1009.43
978.27
802.89
732.17
697.98
633.09
601.23
587.59
510.35
460.35
Wavenumber cm-1

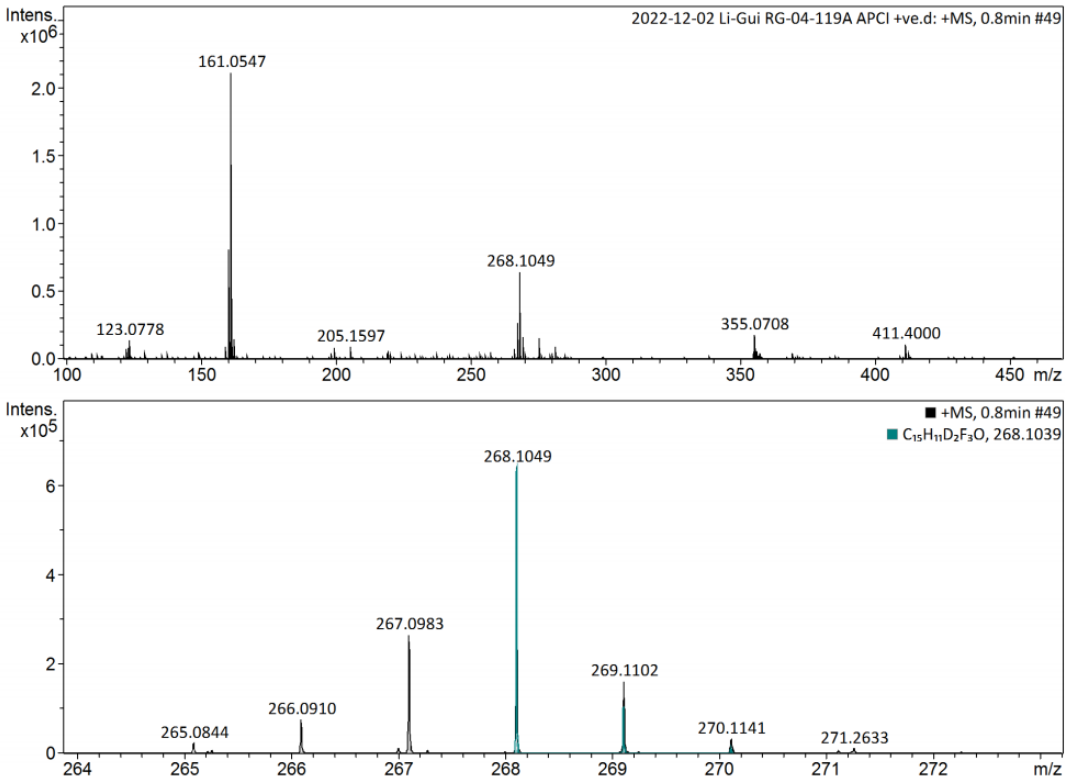
Mass Spectrum SmartFormula Report

Analysis Info

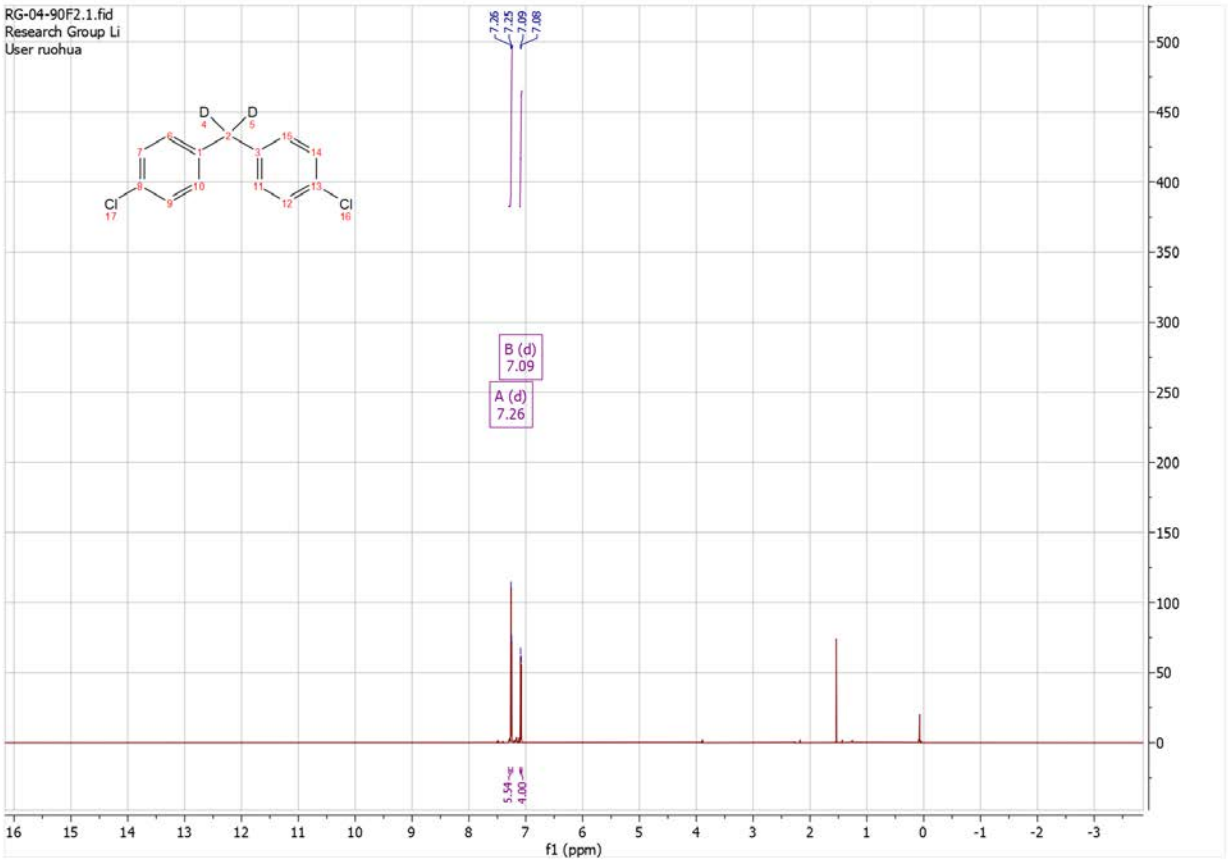
Analysis Name	D:\Data\Li\2022-12-02 Li-Gui RG-04-119A APCI +ve.d	Acquisition Date	12/2/2022 10:17:32 AM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-12-02 Li-Gui RG-04-119A APCI +ve	Instrument	maXis impact 282001.00044
Comment			

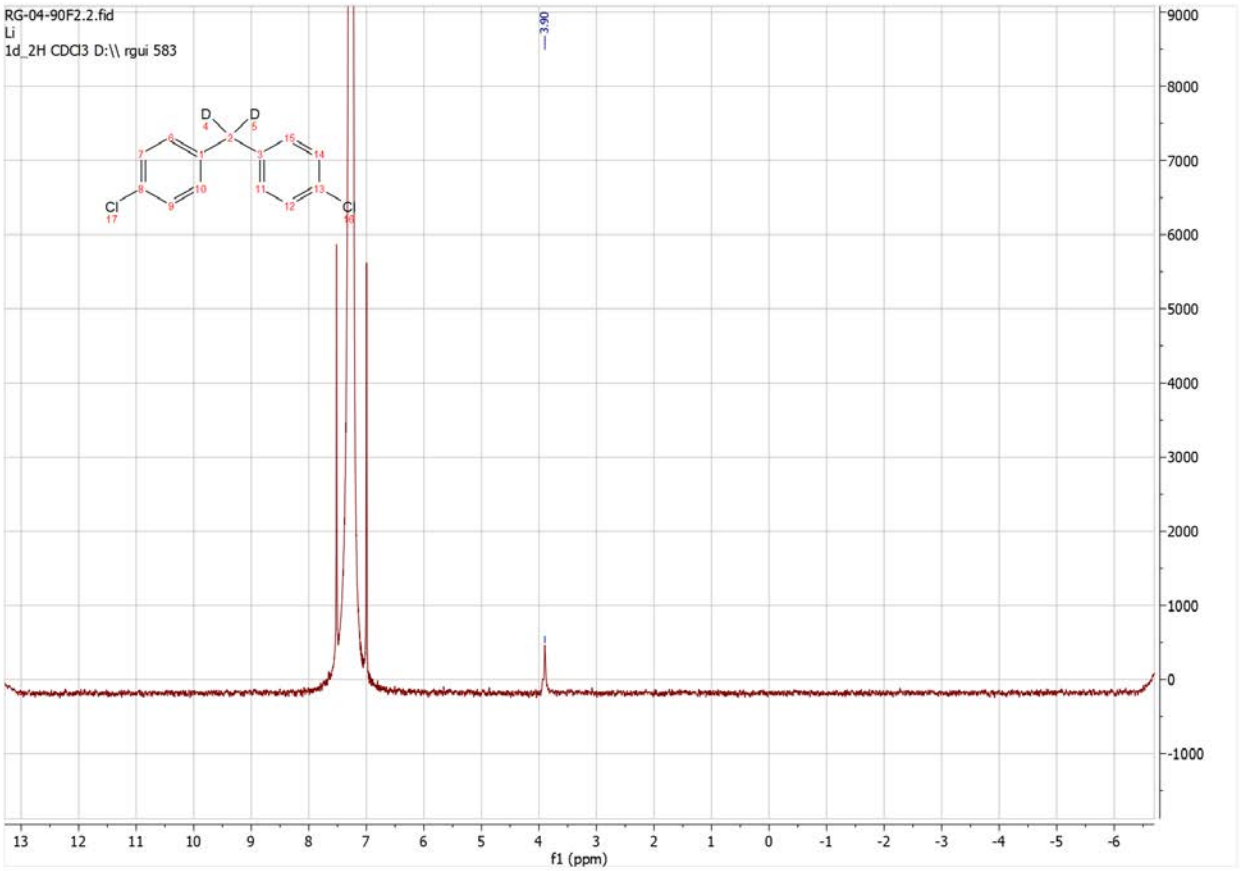
Acquisition Parameter

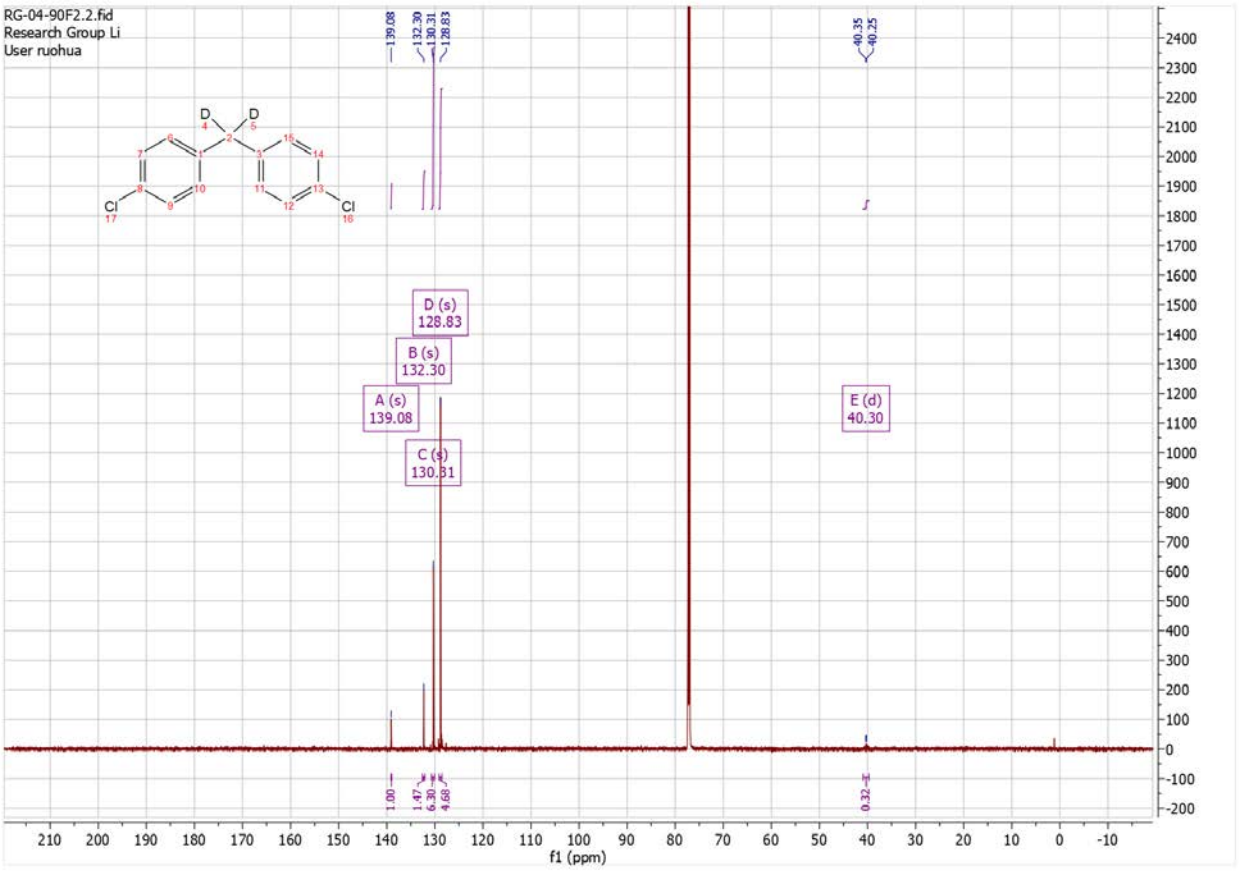
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

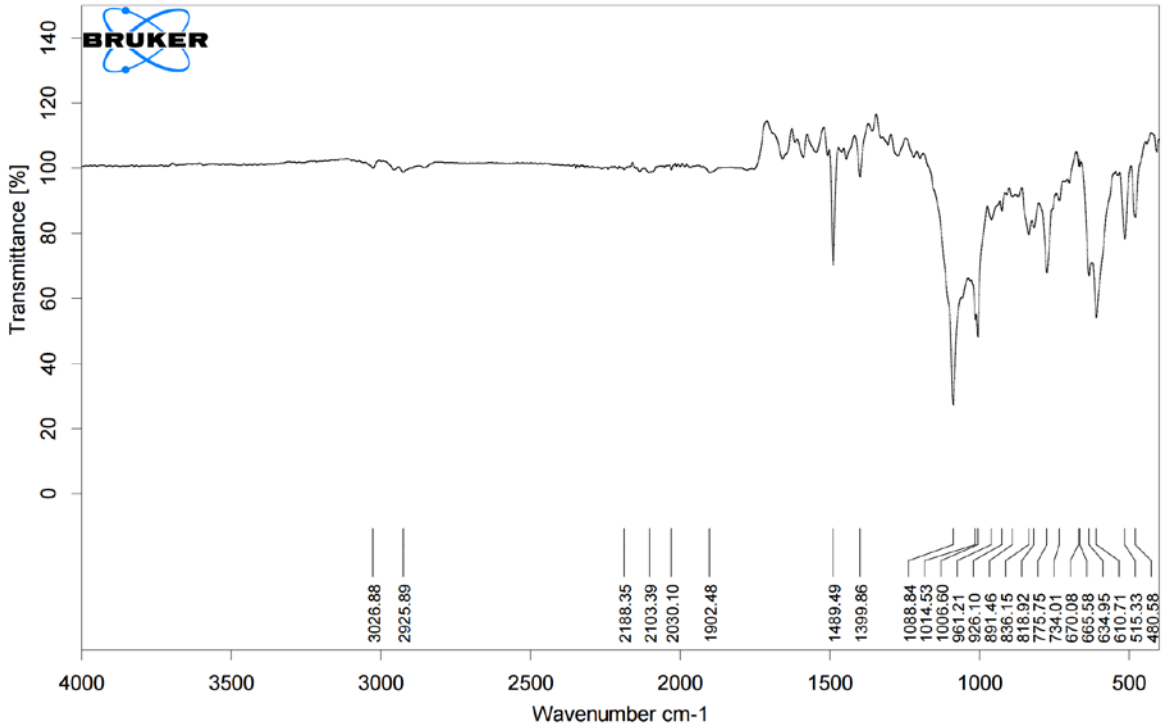


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
267.0983	1	C15H14F3O	267.0991	3.0	605.0	1	99.92	7.5	even	ok
	2	C15H12DF3O	267.0976	-2.8	605.1	2	100.00	8.0	odd	ok
	3	C13H12F3N3	267.0978	-2.0	610.7	3	28.30	8.0	odd	ok
	4	C4H10D2F3N6O4	267.0992	3.3	650.8	4	0.00	0.5	even	ok
268.1049	1	C15H13DF3O	268.1054	1.8	53.6	1	100.00	7.5	even	ok
	2	C15H11D2F3O	268.1039	-4.0	53.7	2	73.48	8.0	odd	ok
	3	C13H13F3N3	268.1056	2.6	60.3	3	72.44	7.5	even	ok
	4	C13H11DF3N3	268.1041	-3.2	60.4	4	66.18	8.0	odd	ok
269.1102	1	C15H12D2F3O	269.1117	5.7	20.5	1	56.01	7.5	even	ok
	2	C13H12DF3N3	269.1119	6.4	27.2	2	41.79	7.5	even	ok

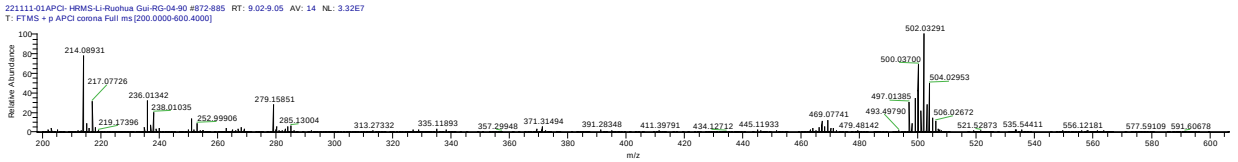

RG-04-90F2.1.fid
Research Group Li
User ruohua
D
D
Cl
Cl
7.26
7.25
7.09
7.08
B (d)
7.09
A (d)
7.26
5.54
4.00
f1 (ppm)

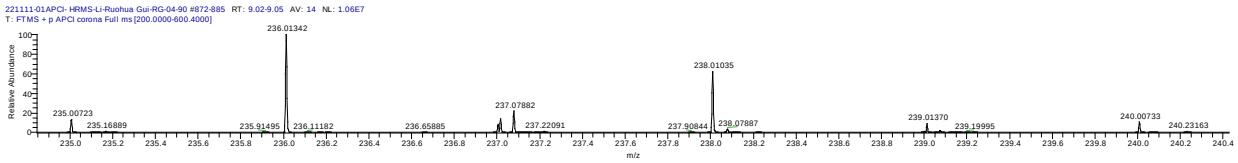

RG-04-90F2.2.fid
Li
1d_2H CDCl3 D:\\ rgui 583
3.90
f1 (ppm)


RG-04-90F2.2.fid
Research Group Li
User ruohua
D (s)
128.83
B (s)
132.30
A (s)
139.08
C (s)
130.31
E (d)
40.30
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1
3026.88
2925.89
2188.35
2103.39
2030.10
1902.48
1489.49
1399.86
1088.84
1014.53
1006.60
961.21
926.10
891.46
836.15
818.92
775.75
734.01
670.08
665.58
634.95
610.71
515.33
480.58

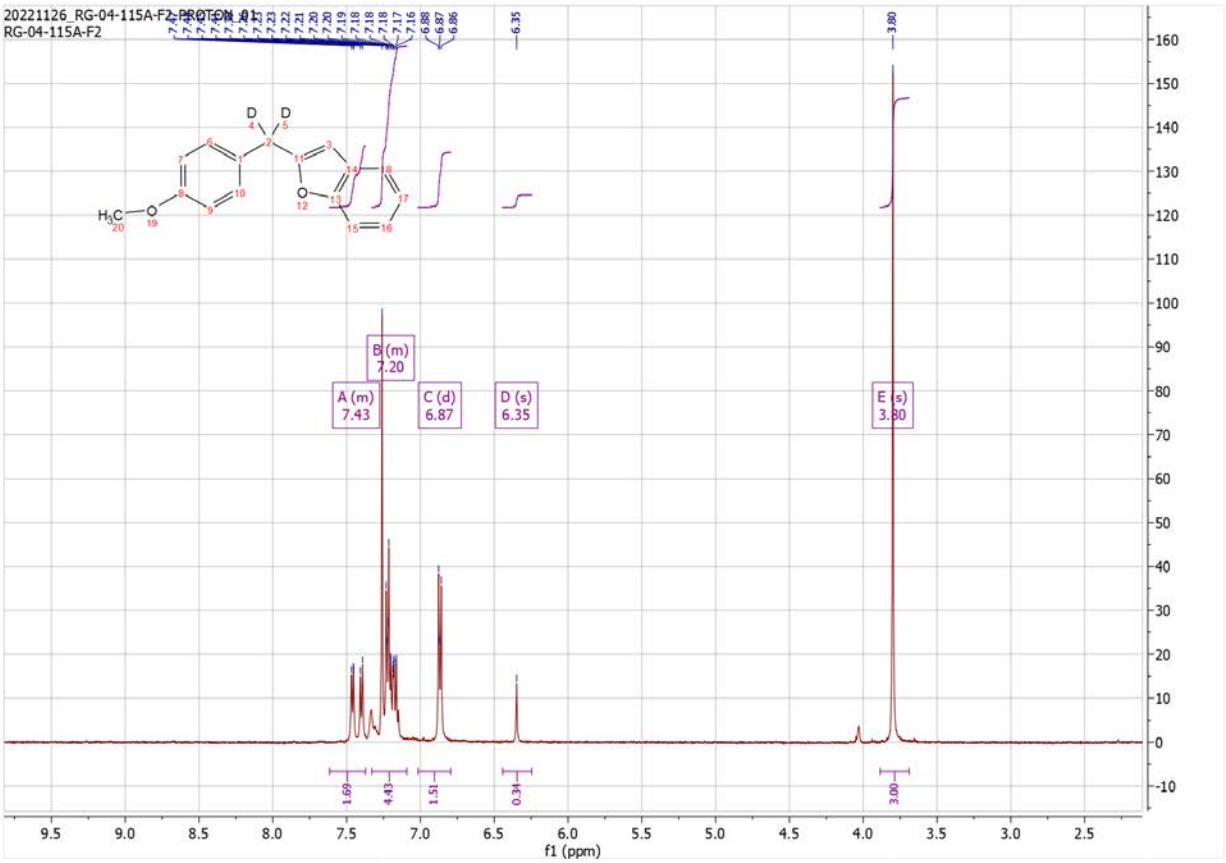
221111-01APCI- HRMS-Li-Ruohua Gui-RG-... 11/11/22 09:08:25

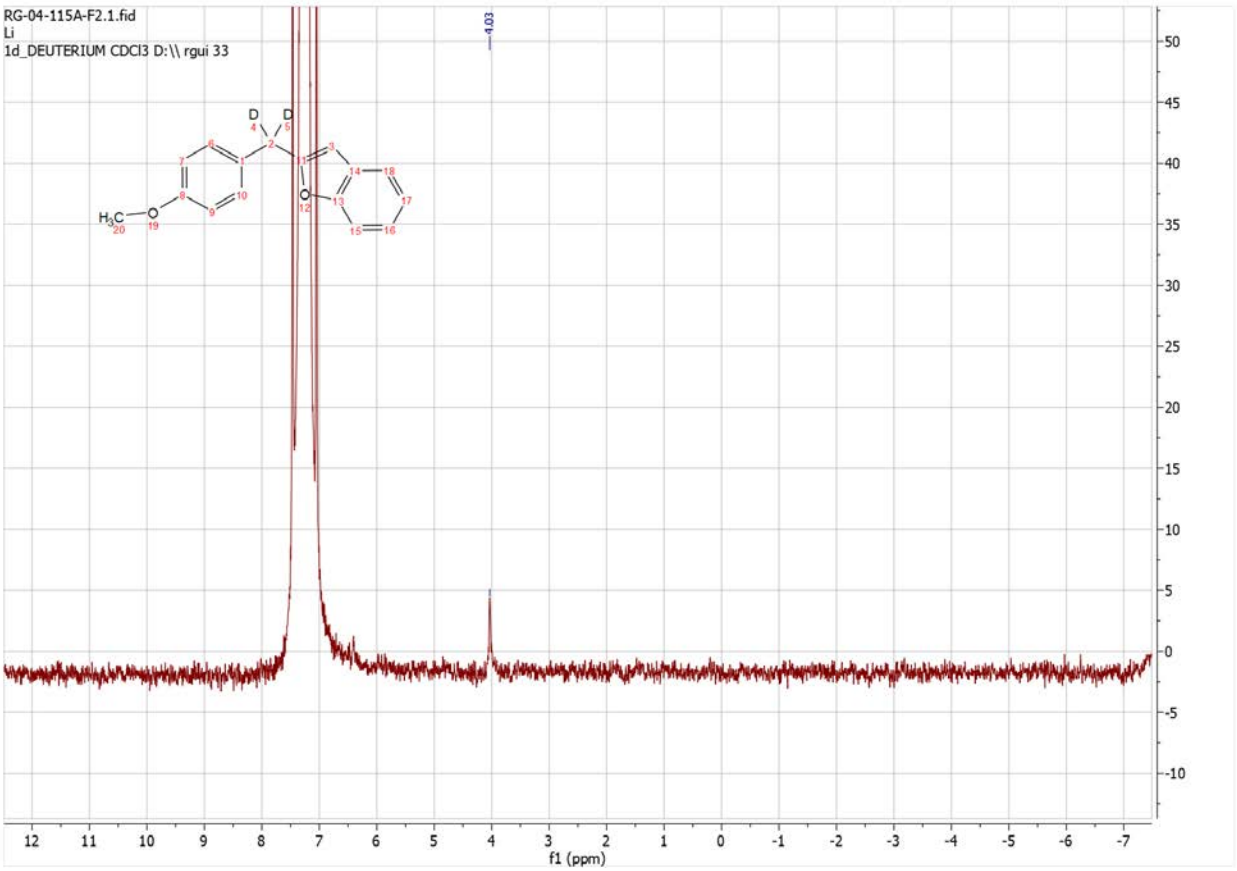


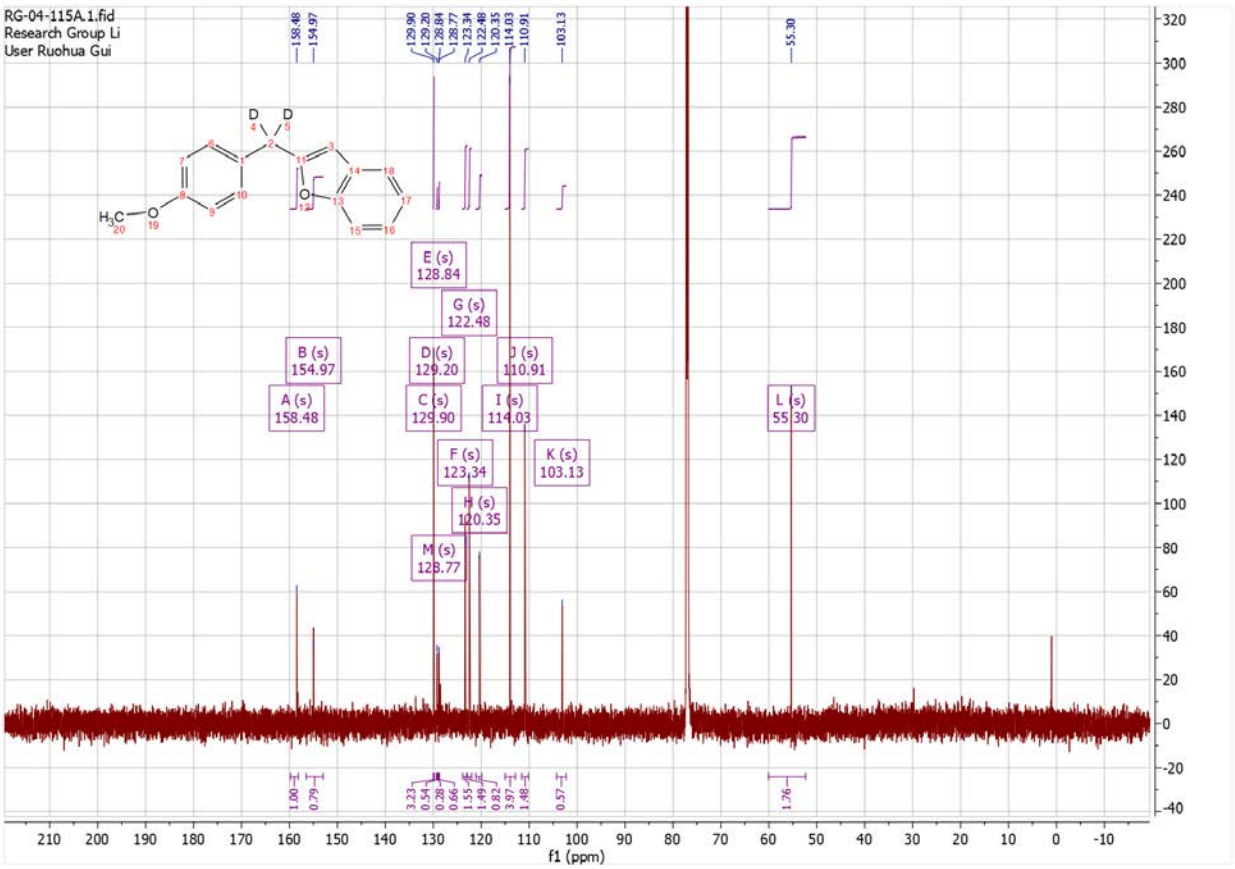


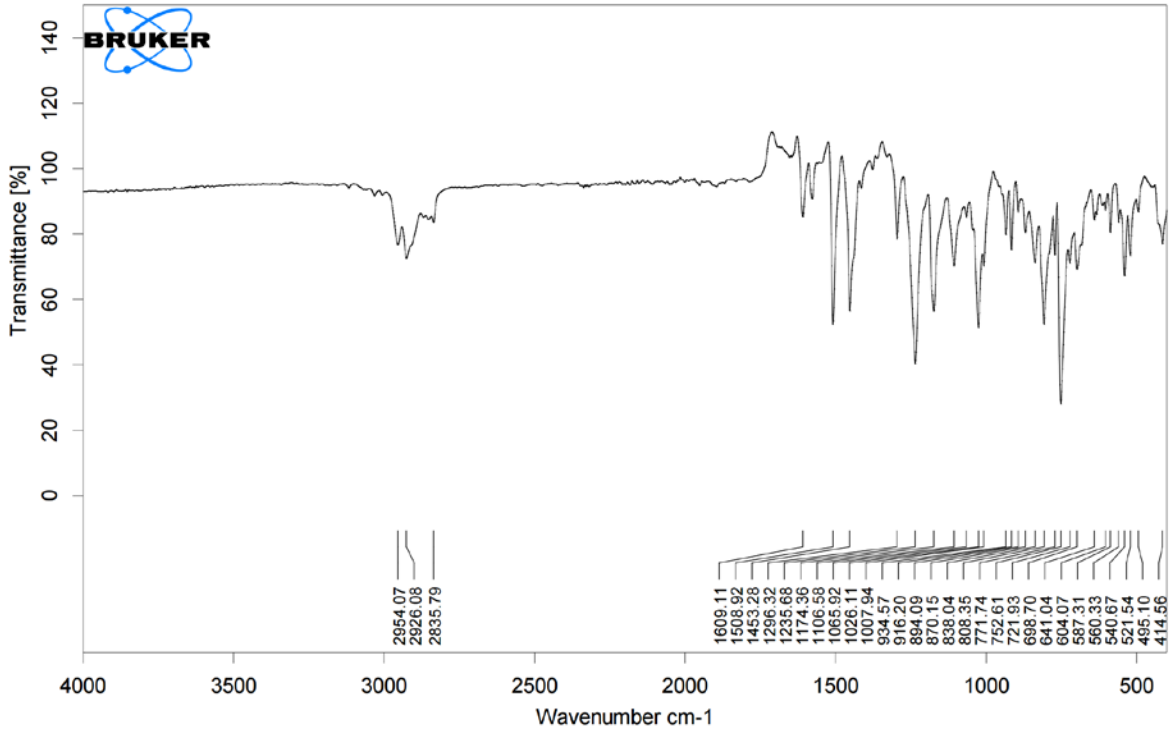
m/z	Intensity	Relative	Resolution	Charge	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
236.01342	10869240.0	100.00	35771.10	1.00	236.01386	-1.88	8.5	$C_{13}H_8{}^2HCl_2$
					236.01231	4.68	9.0	$C_{13}H_6{}^2H_2Cl_2$

m/z	Intensity	Relative	Resolution	Charge	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
238.01035	6929178.5	100.00	35112.48	1.00	238.01039	-0.15	13.5	$C_{13}{}^2H_2O_4N$
					238.01091	-2.34	8.5	$C_{13}H_8{}^2HCl^{37}Cl$
					238.00936	4.16	9.0	$C_{13}H_6{}^2H_2Cl^{37}Cl$




RG-04-115A-F2.1.fid
Li
1d_DEUTERIUM CDCl3 D:\\ rgui 33
4.03
D
D
H3C
O
f1 (ppm)


RG-04-115A.1.fid
Research Group Li
User Ruohua Gui
158.48
154.97
129.90
129.20
128.84
128.77
123.34
122.48
120.35
114.03
110.91
103.13
55.30
E (s) 128.84
G (s) 122.48
B (s) 154.97
D (s) 129.20
J (s) 110.91
A (s) 158.48
C (s) 129.90
I (s) 114.03
L (s) 55.30
F (s) 123.34
K (s) 103.13
H (s) 120.35
M (s) 128.77
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1
2954.07
2926.08
2835.79
1609.11
1508.92
1453.28
1296.32
1235.68
1174.36
1106.58
1065.92
1026.11
1007.94
934.57
916.20
894.09
870.15
838.04
808.35
771.74
752.61
721.93
698.70
641.04
604.07
587.31
560.33
540.67
521.54
495.10
414.56

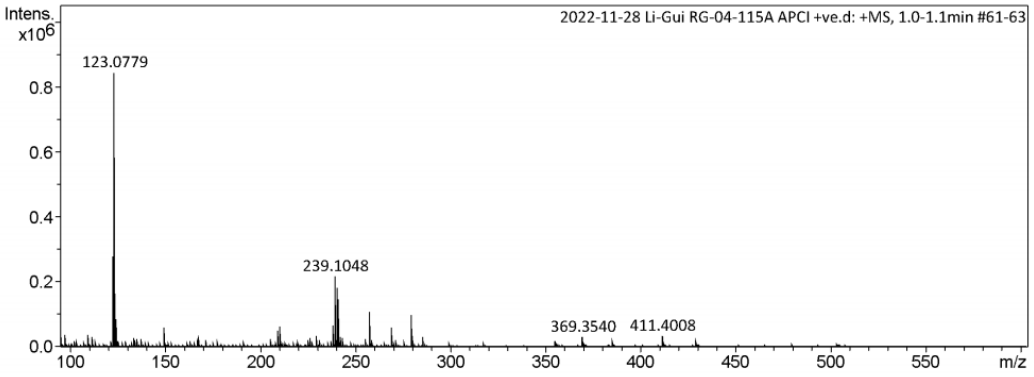
Mass Spectrum SmartFormula Report

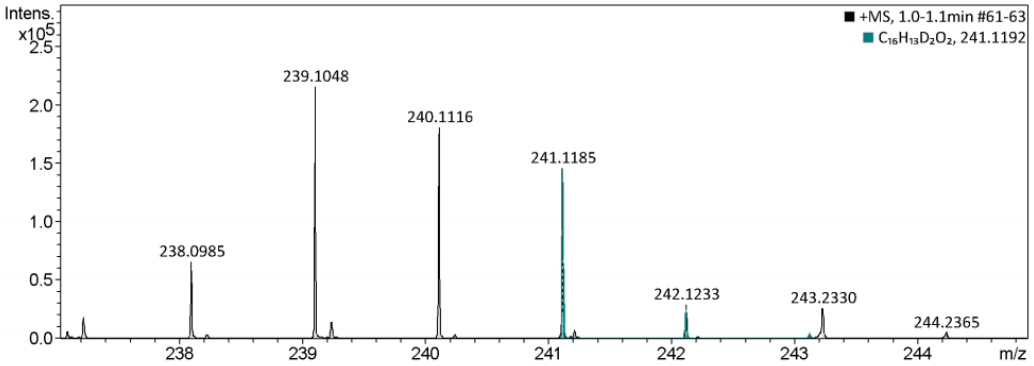
Analysis Info

Analysis Name	D:\Data\Li\2022-11-28 Li-Gui RG-04-115A APCI +ve.d	Acquisition Date	11/28/2022 2:37:18 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-11-28 Li-Gui RG-04-115A APCI +ve	Instrument	maXis impact 282001.00044
Comment			

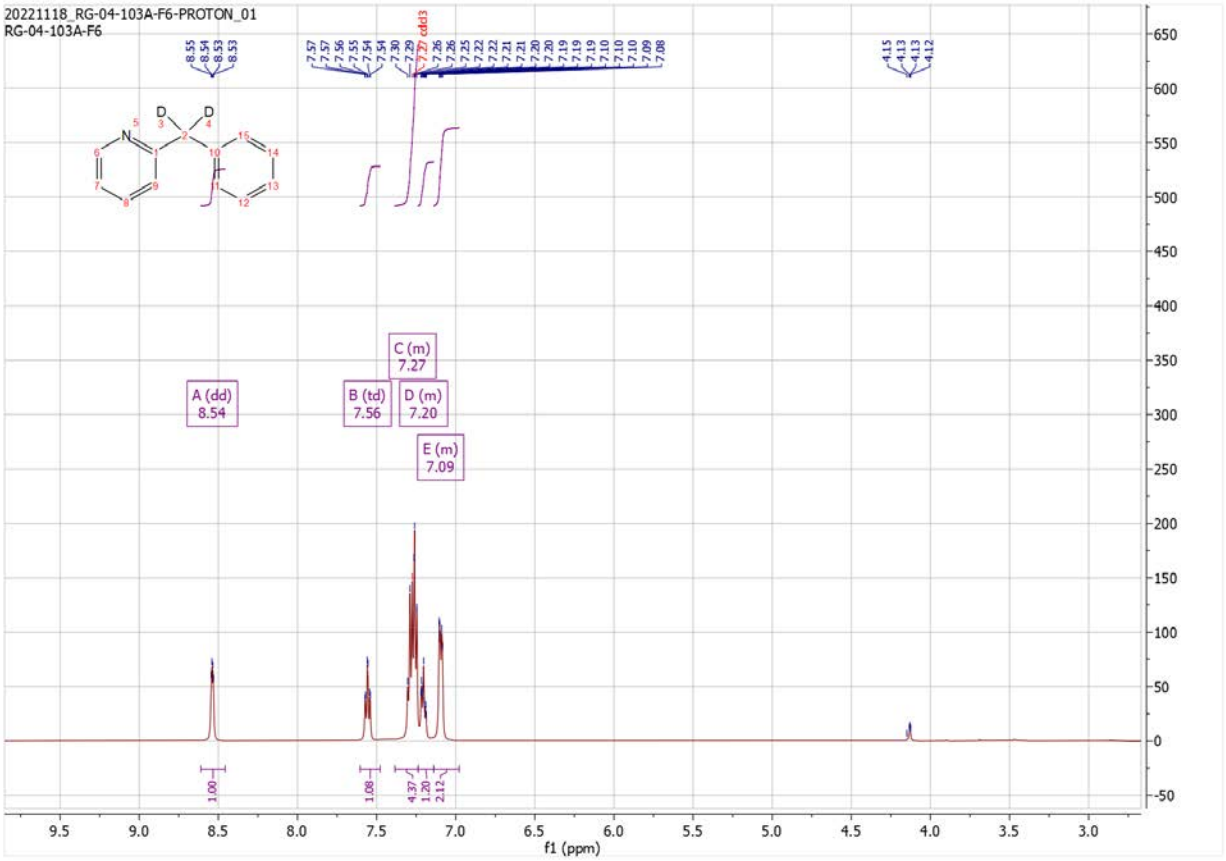
Acquisition Parameter

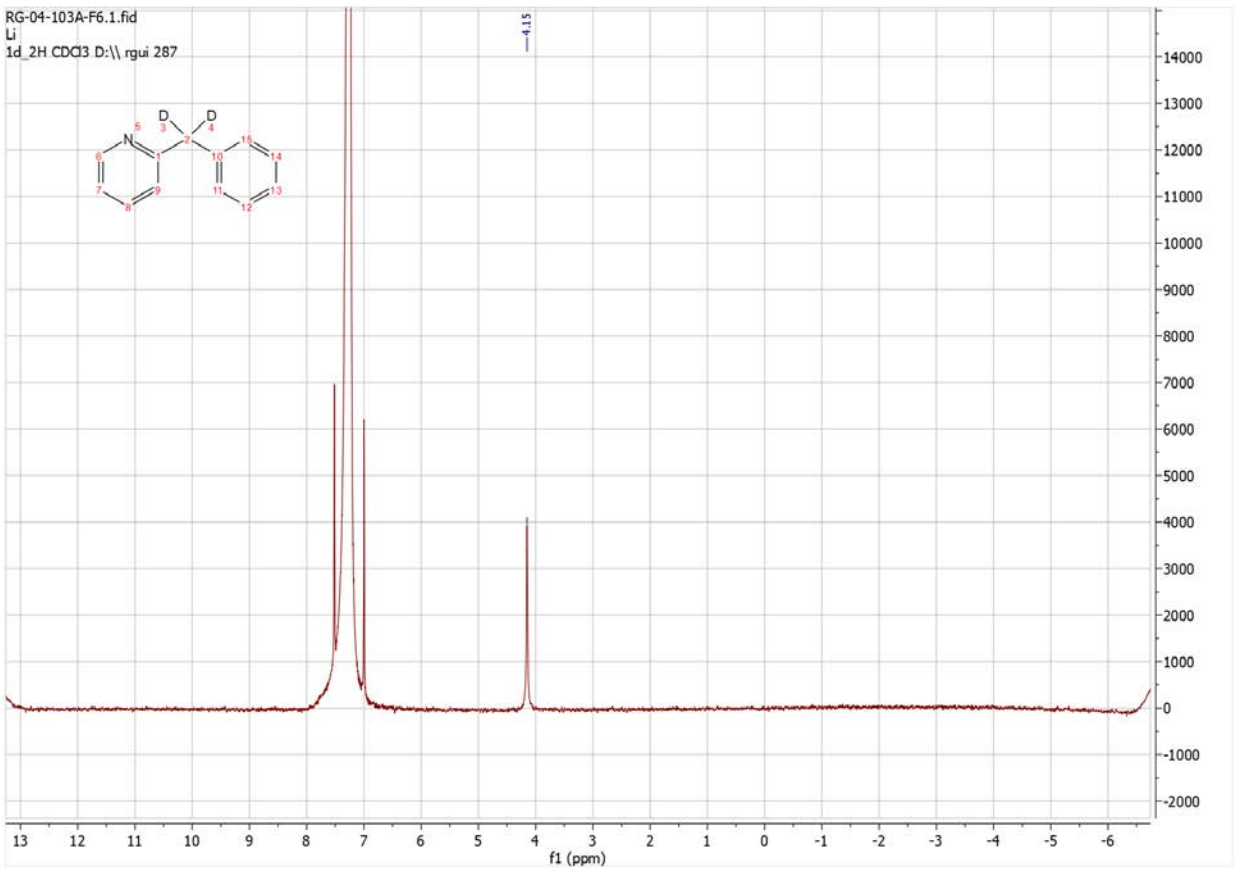
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

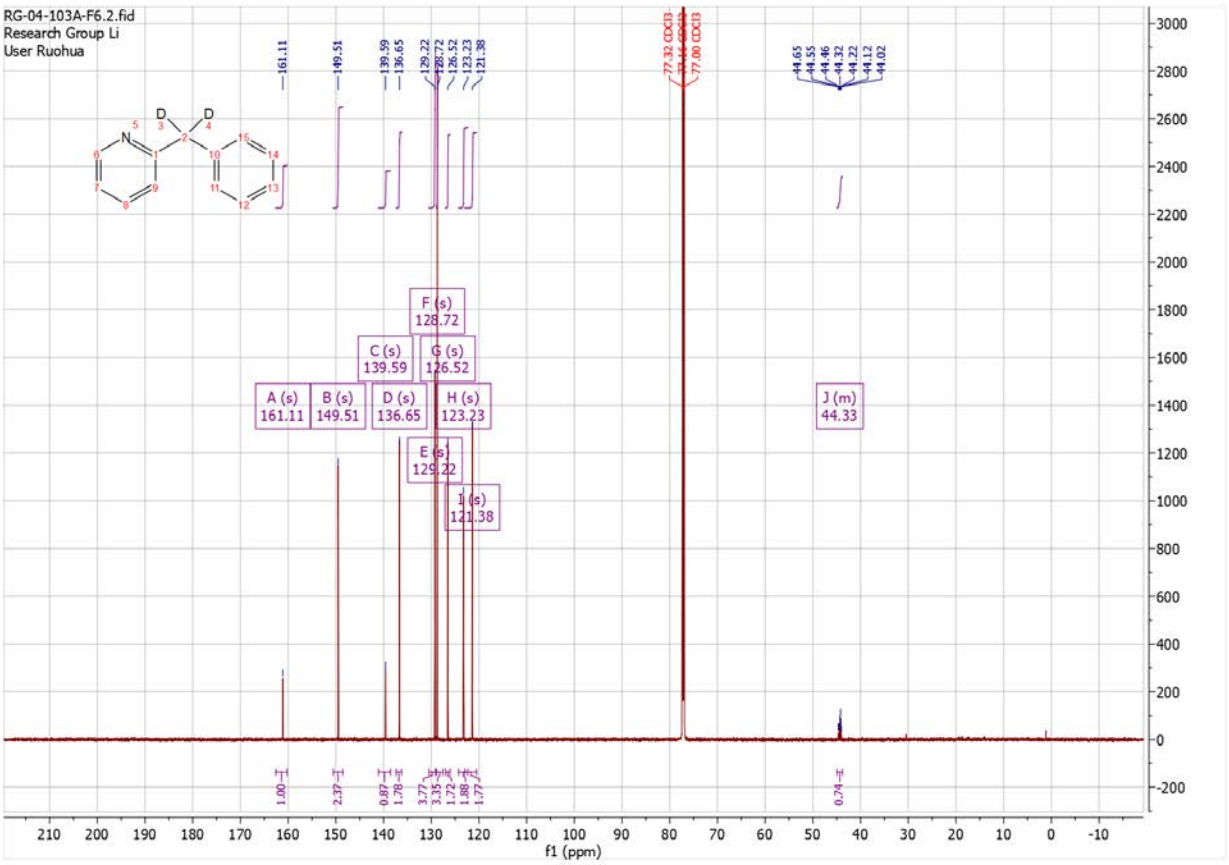


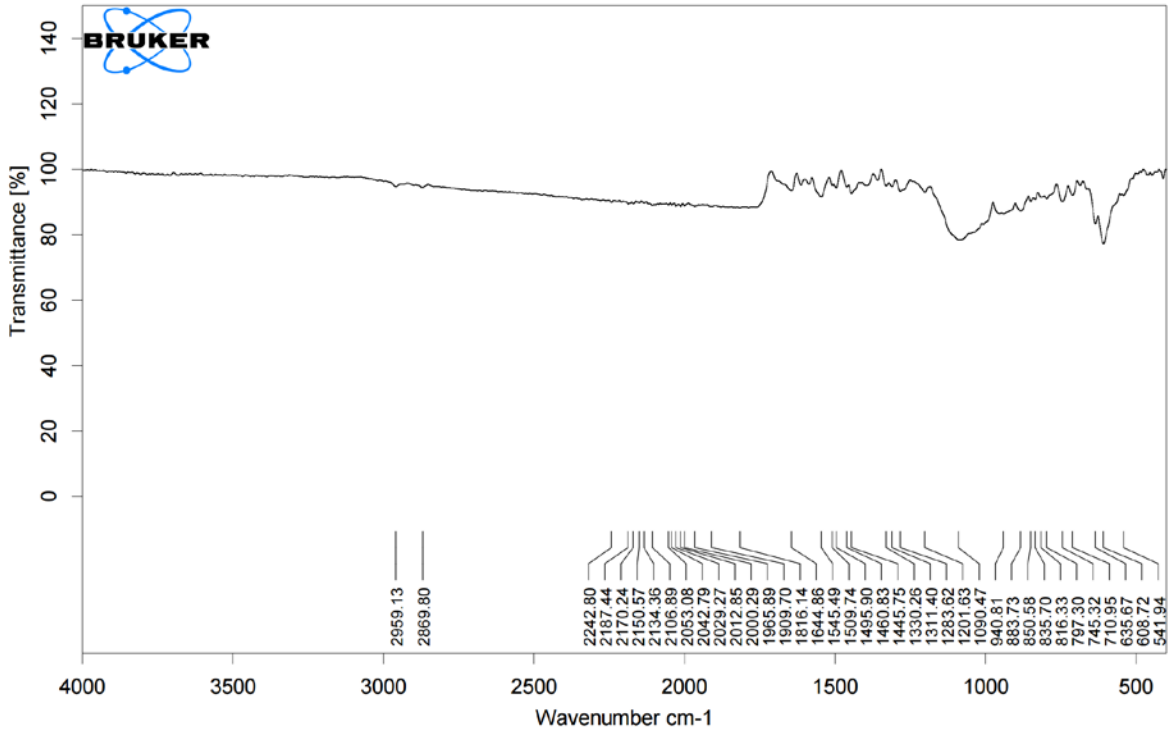


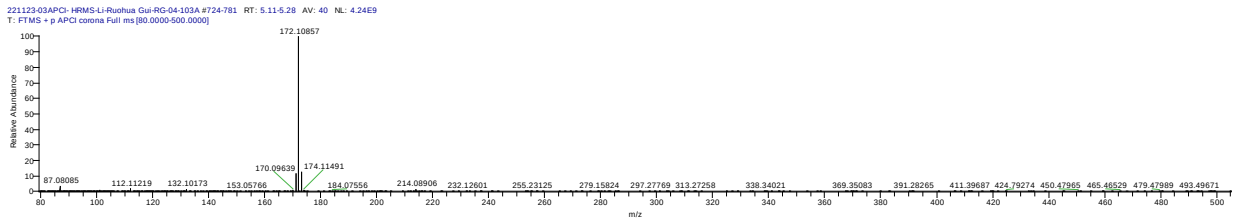
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e¯ Conf	N-Rule
238.0985	1	C4H4D2N13	238.0989	1.7	661.6	1	100.00	8.5	even	ok
	2	C14H12N3O	238.0975	-4.3	787.8	2	0.00	10.5	even	ok
239.1048	1	C16H13DO2	239.1051	1.5	538.8	1	100.00	10.0	odd	ok
	2	C16H11D2O2	239.1036	-5.0	538.9	2	62.45	10.5	even	ok
	3	C14H13N3O	239.1053	2.3	544.9	3	23.95	10.0	odd	ok
	4	C14H11DN3O	239.1038	-4.1	545.0	4	18.60	10.5	even	ok
	5	C12H11N6	239.1040	-3.3	551.1	5	5.46	10.5	even	ok
240.1116	1	C16H12D2O2	240.1114	-1.0	374.6	1	100.00	10.0	odd	ok
	2	C14H12DN3O	240.1116	-0.2	381.3	2	38.87	10.0	odd	ok
	3	C12H12N6	240.1118	0.7	388.0	3	12.96	10.0	odd	ok

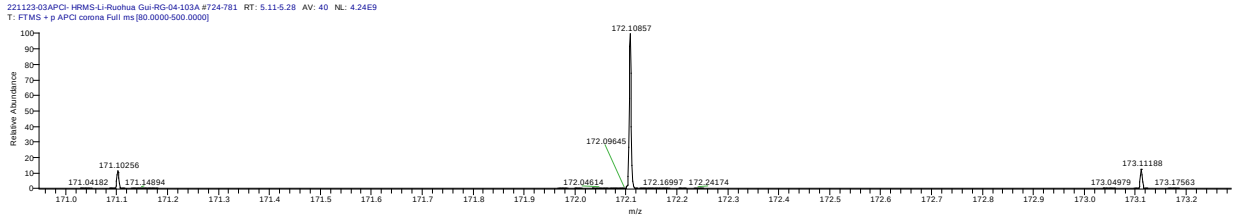

20221118_RG-04-103A-F6-PROTON_01
RG-04-103A-F6
A (dd)
8.54
B (td)
7.56
C (m)
7.27
D (m)
7.20
E (m)
7.09
1.00
1.08
4.37
1.20
2.12
f1 (ppm)


RG-04-103A-F6.1.fid
Li
1d_2H CDCl3 D:\\ rgui 287
D
D
N
4.15
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 -4 -5 -6
f1 (ppm)


RG-04-103A-F6.2.fid
Research Group Li
User Ruohua
F (s) 128.72
C (s) 139.59
G (s) 126.52
A (s) 161.11
B (s) 149.51
D (s) 136.65
H (s) 123.23
E (s) 129.22
I (s) 121.38
J (m) 44.33
f1 (ppm)

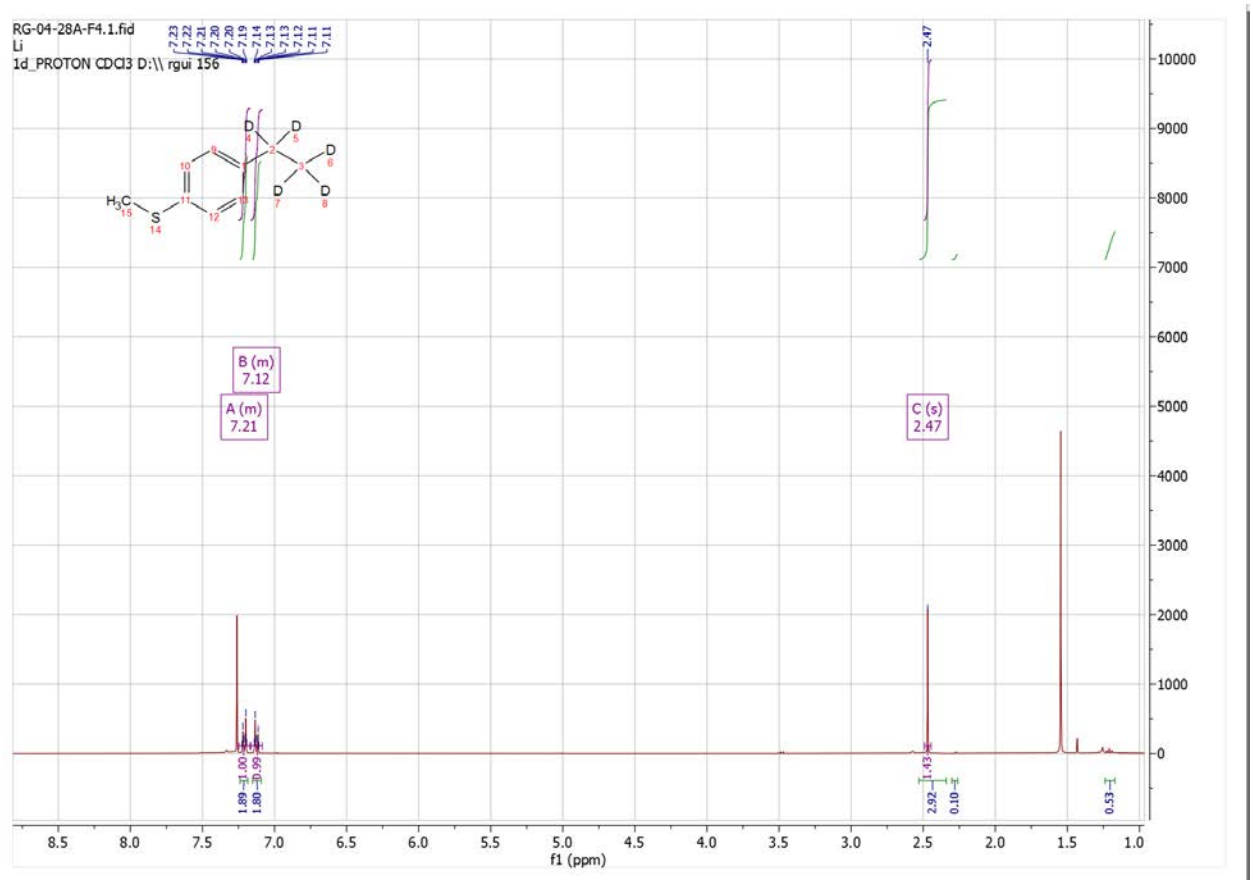

BRUKER
Transmittance [%]
Wavenumber cm-1
2959.13
2869.80
2242.80
2187.44
2170.24
2150.57
2134.36
2106.89
2053.08
2042.79
2029.27
2012.85
2000.29
1965.89
1909.70
1816.14
1644.86
1545.49
1509.74
1495.90
1460.83
1445.75
1330.26
1311.40
1283.62
1201.63
1090.47
940.81
883.73
850.58
835.70
816.33
797.30
745.32
710.95
635.67
608.72
541.94

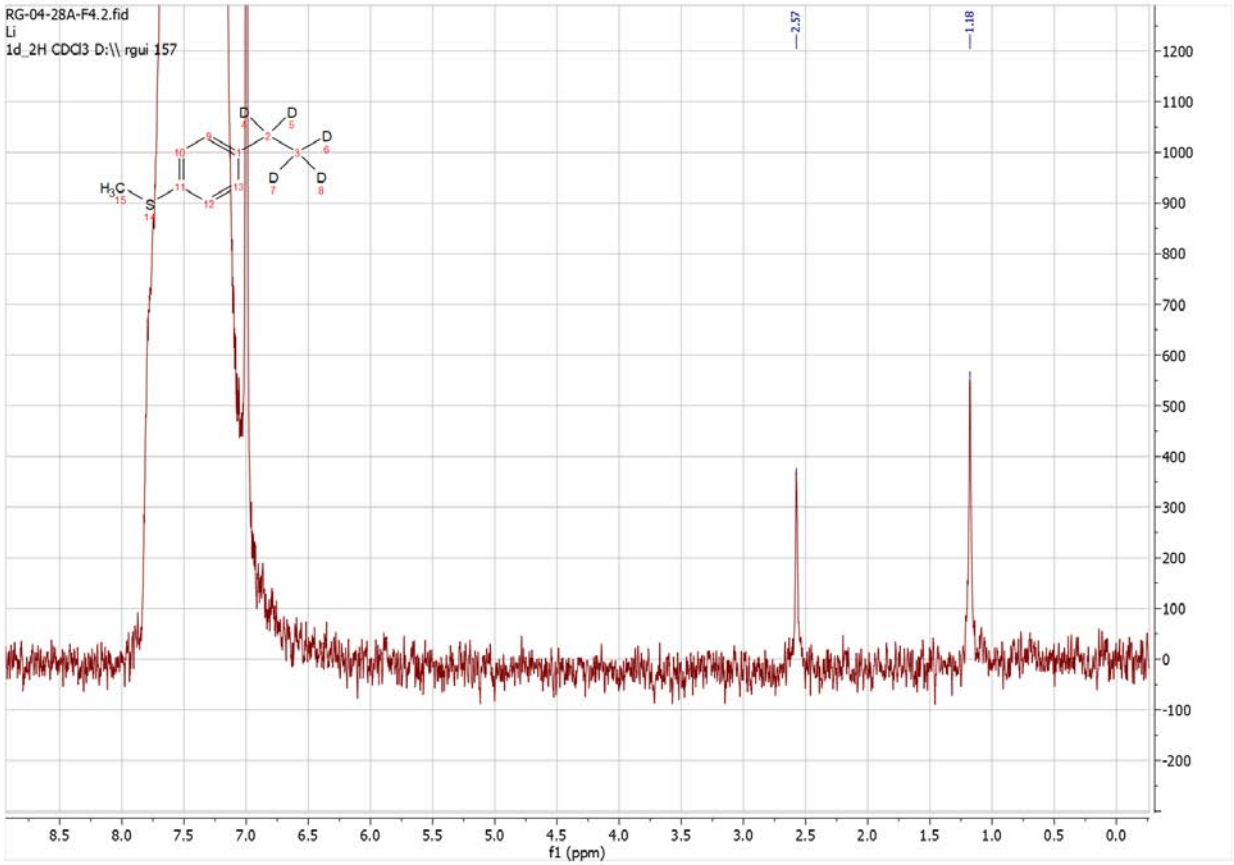


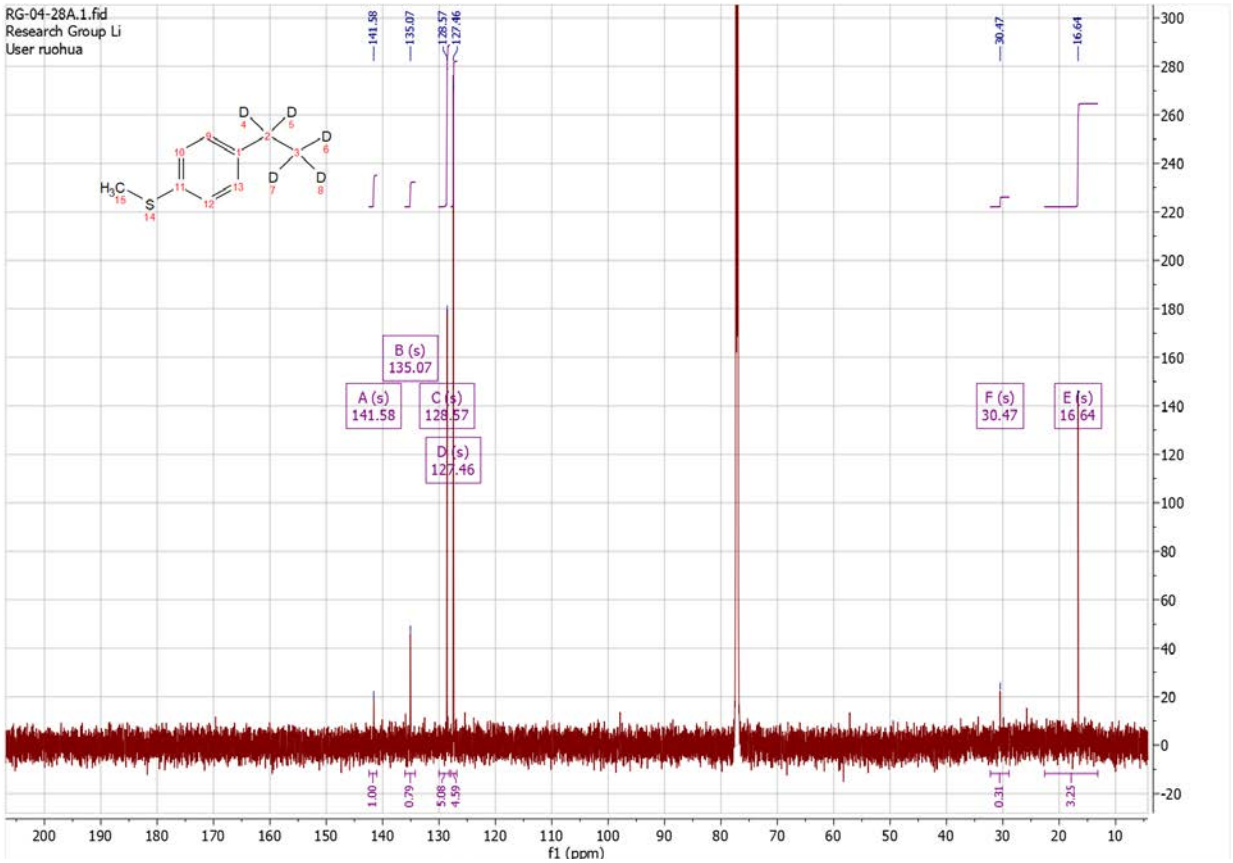


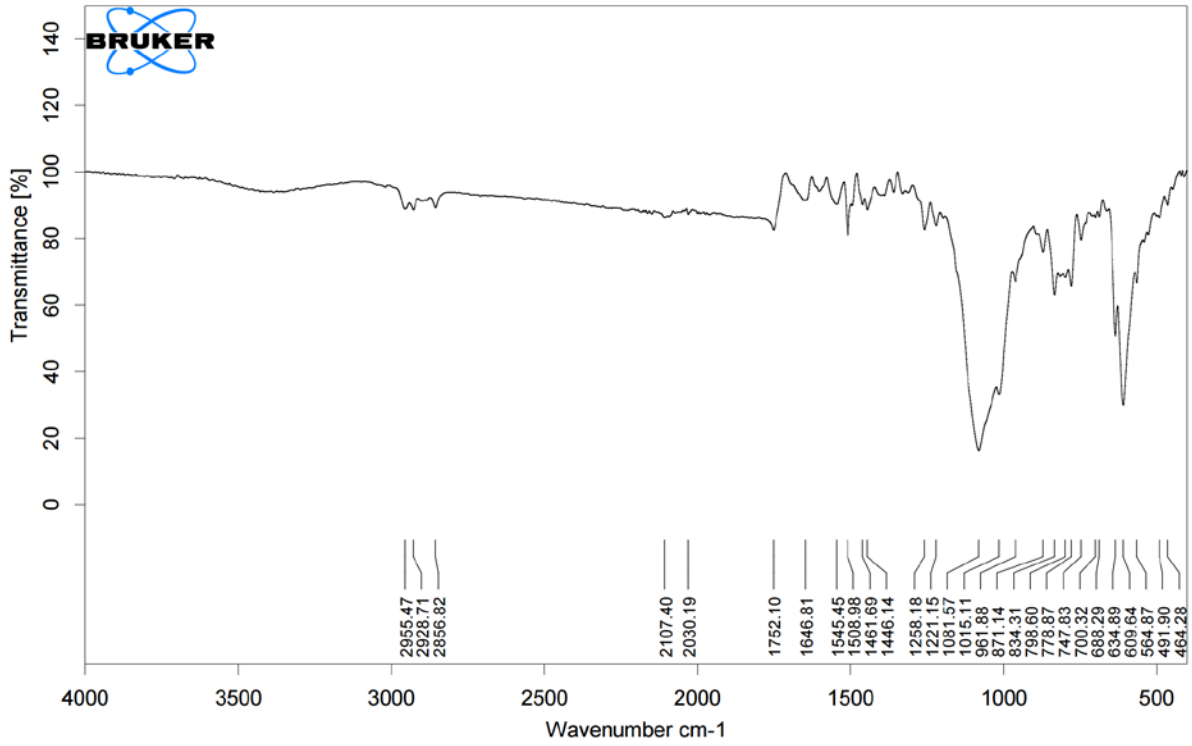
221123-03APCI- HRMS-Li-Ruohua Gui-RG-04-103A#724-781 RT: 5.11-5.28 AV: 40
T: FTMS + p APCI corona Full ms [80.0000-500.0000]
m/z= 172.10017-172.11565

m/z	Intensity	Relative	Resolution	Charge	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
172.10857	4290112000.0	100.00	40540.30	1.00	172.10898	-2.41	7.5	$C_{12}H_{10}{}^{2}H_{2}N$




RG-04-28A-F4.2.fid
Li
1d_2H CDCl3 D:\\ rgui 157
2.57
1.18
f1 (ppm)


RG-04-28A.1.fid
Research Group Li
User ruohua
141.58
135.07
128.57
127.46
30.47
16.64
B (s)
135.07
A (s)
141.58
C (s)
128.57
D (s)
127.46
F (s)
30.47
E (s)
16.64
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1
2955.47
2928.71
2856.82
2107.40
2030.19
1752.10
1646.81
1545.45
1508.98
1461.69
1446.14
1258.18
1221.15
1081.57
1015.11
961.88
871.14
834.31
798.60
778.87
747.83
700.32
688.29
634.89
609.64
564.87
491.90
464.28

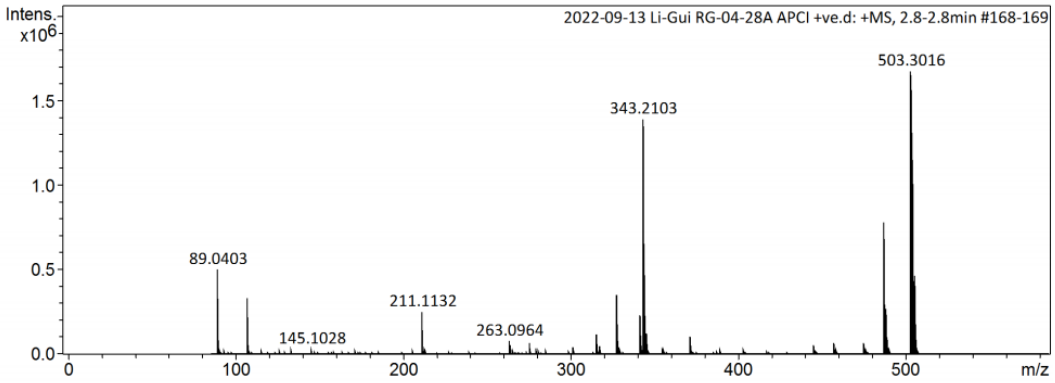
Mass Spectrum SmartFormula Report

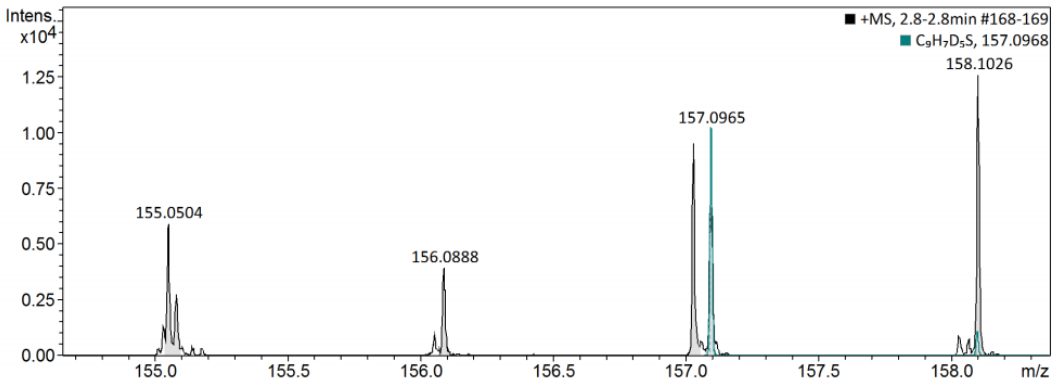
Analysis Info

Analysis Name	D:\Data\Li\2022-09-13 Li-Gui RG-04-28A APCI +ve.d	Acquisition Date	9/13/2022 4:19:34 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2022-09-13 Li-Gui RG-04-28A APCI +ve	Instrument	maXis impact 282001.00044
Comment			

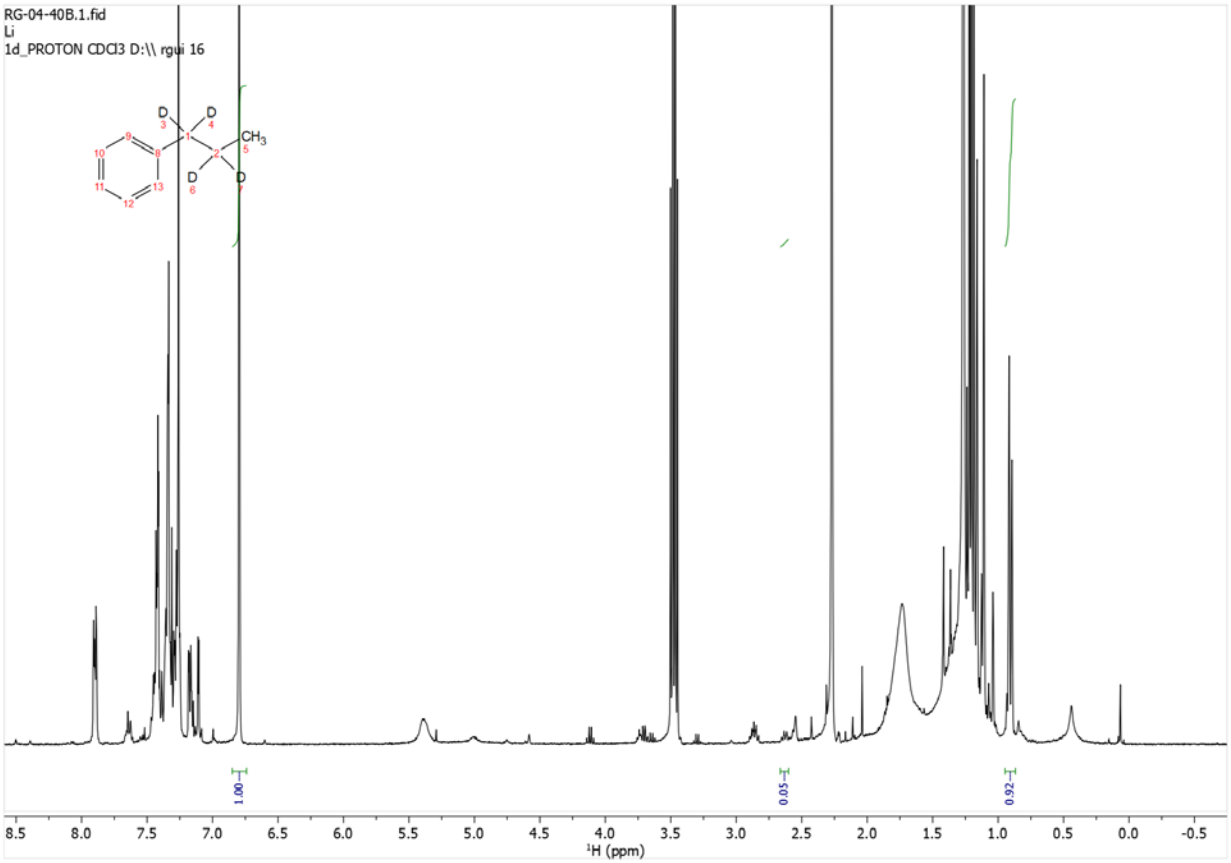
Acquisition Parameter

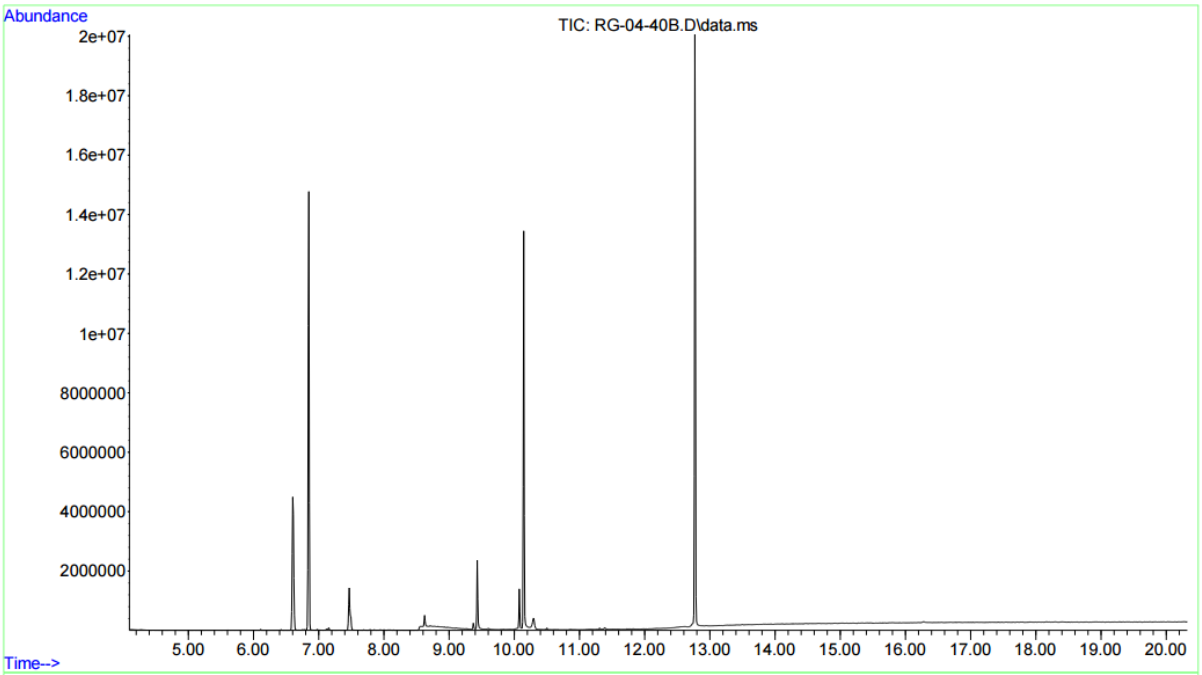
Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1250 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C

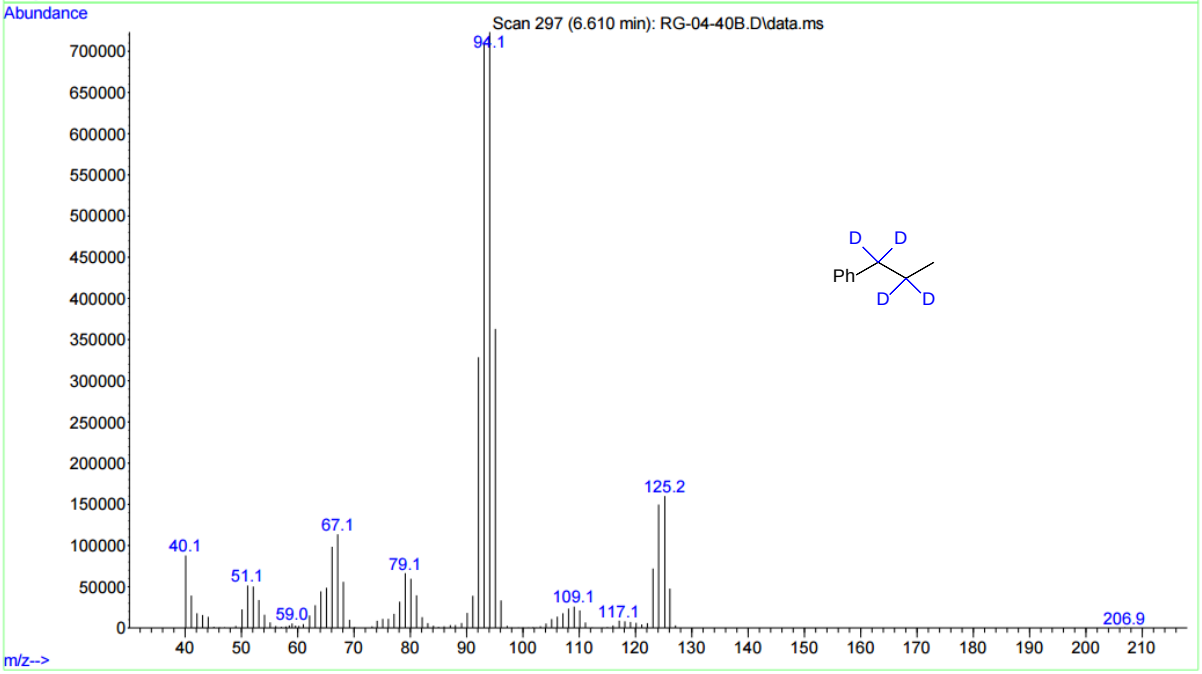


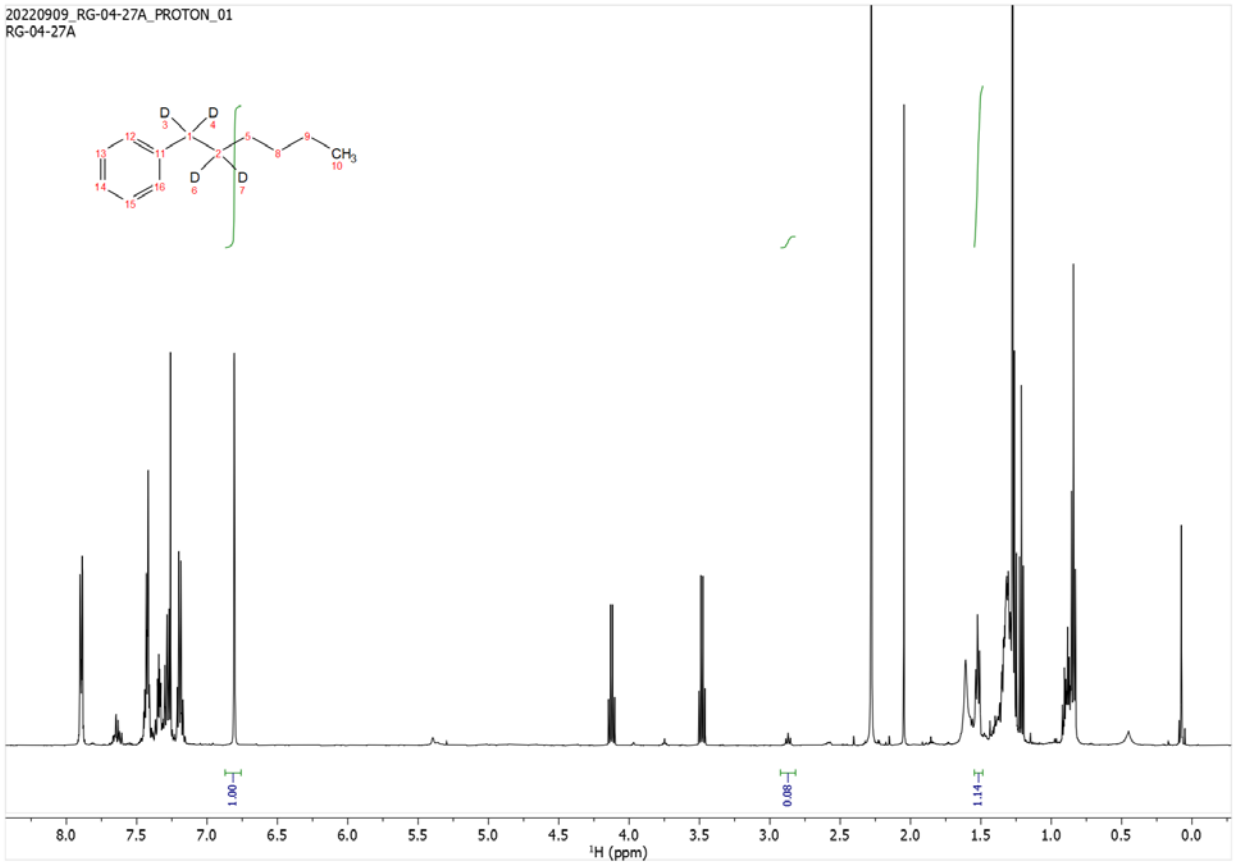


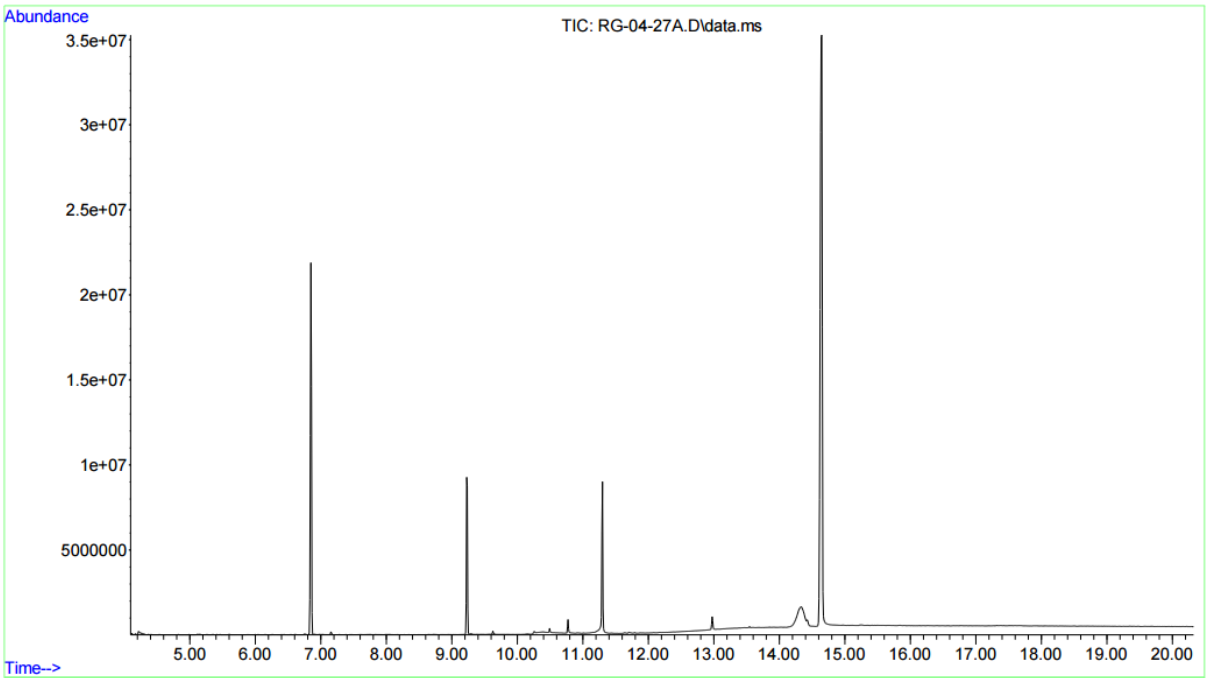
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
156.0888	1	C9H6D5S	156.0890	1.0	627.0	1	100.00	4.5	even	ok
	2	C12H6D3	156.0887	-0.8	799.6	2	0.00	8.5	even	ok
	3	C7H12N2O2	156.0893	3.2	812.9	3	0.00	3.0	odd	ok
157.0300	1	C7H7DO2S	157.0302	1.3	n.a.	1	100.00	4.0	odd	ok
	2	C3H3D3O7	157.0296	-2.5	n.a.	2	92.34	1.0	odd	ok
	3	C5H7N3OS	157.0304	2.6	n.a.	3	91.17	4.0	odd	ok
157.0965	1	C9H7D5S	157.0968	1.8	528.6	1	100.00	4.0	odd	ok
158.1026	1	C9H8D5S	158.1046	12.8	n.a.	1	100.00	3.5	even	ok
	2	C8H16NS	158.0998	-17.8	n.a.	2	50.81	1.5	even	ok

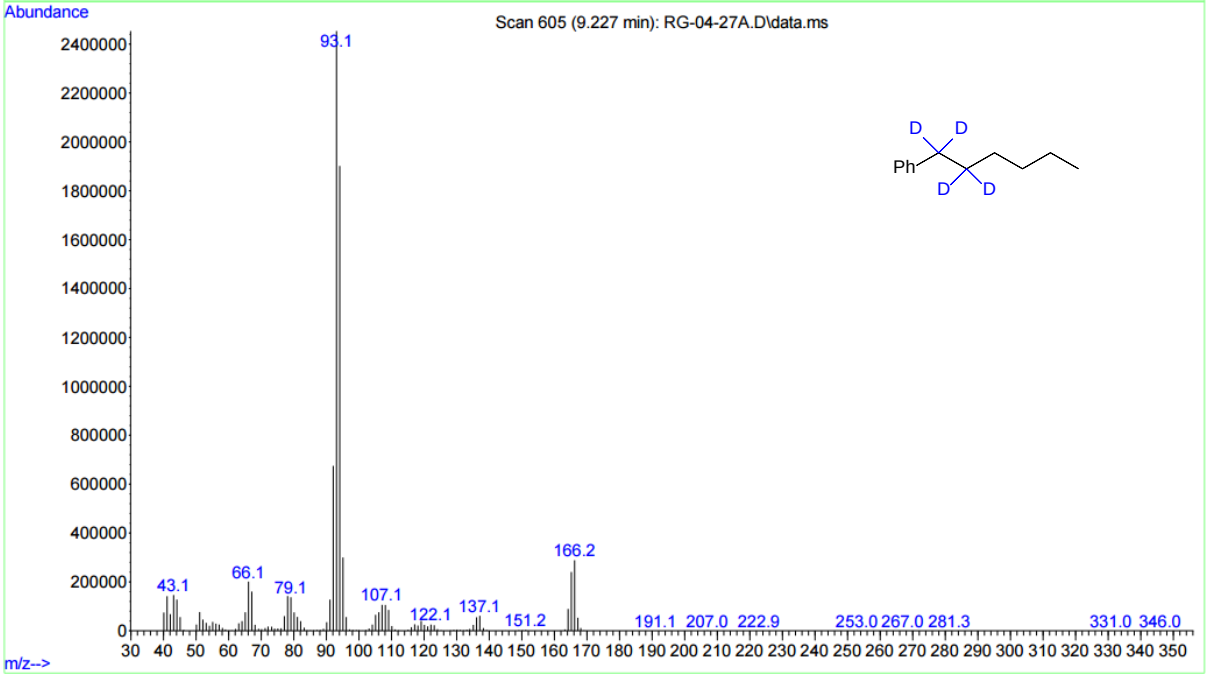

RG-04-40B.1.fid
Li
1d_PROTON CDCl3 D:\\ rgui 16
D
3
D
4
CH3
5
D
6
D
7
1
2
8
9
10
11
12
13
1.00
0.05
0.92
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
¹H (ppm)


Abundance
TIC: RG-04-40B.D\data.ms
2e+07
1.8e+07
1.6e+07
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
5.00
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
16.00
17.00
18.00
19.00
20.00
Time-->

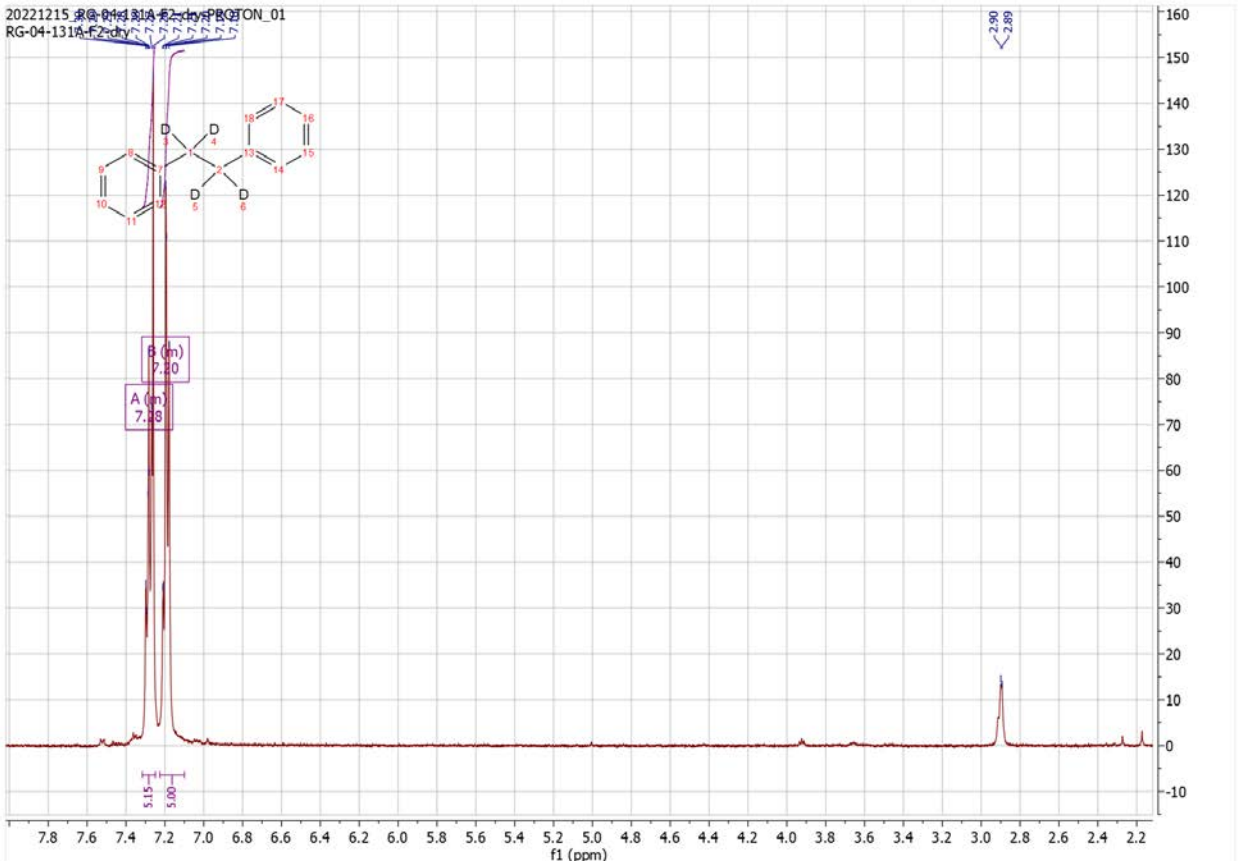

Abundance
Scan 297 (6.610 min): RG-04-40B.D\data.ms
94.1
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
125.2
67.1
40.1
79.1
51.1
109.1
117.1
59.0
206.9
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
m/z-->
D
D
Ph
D
D

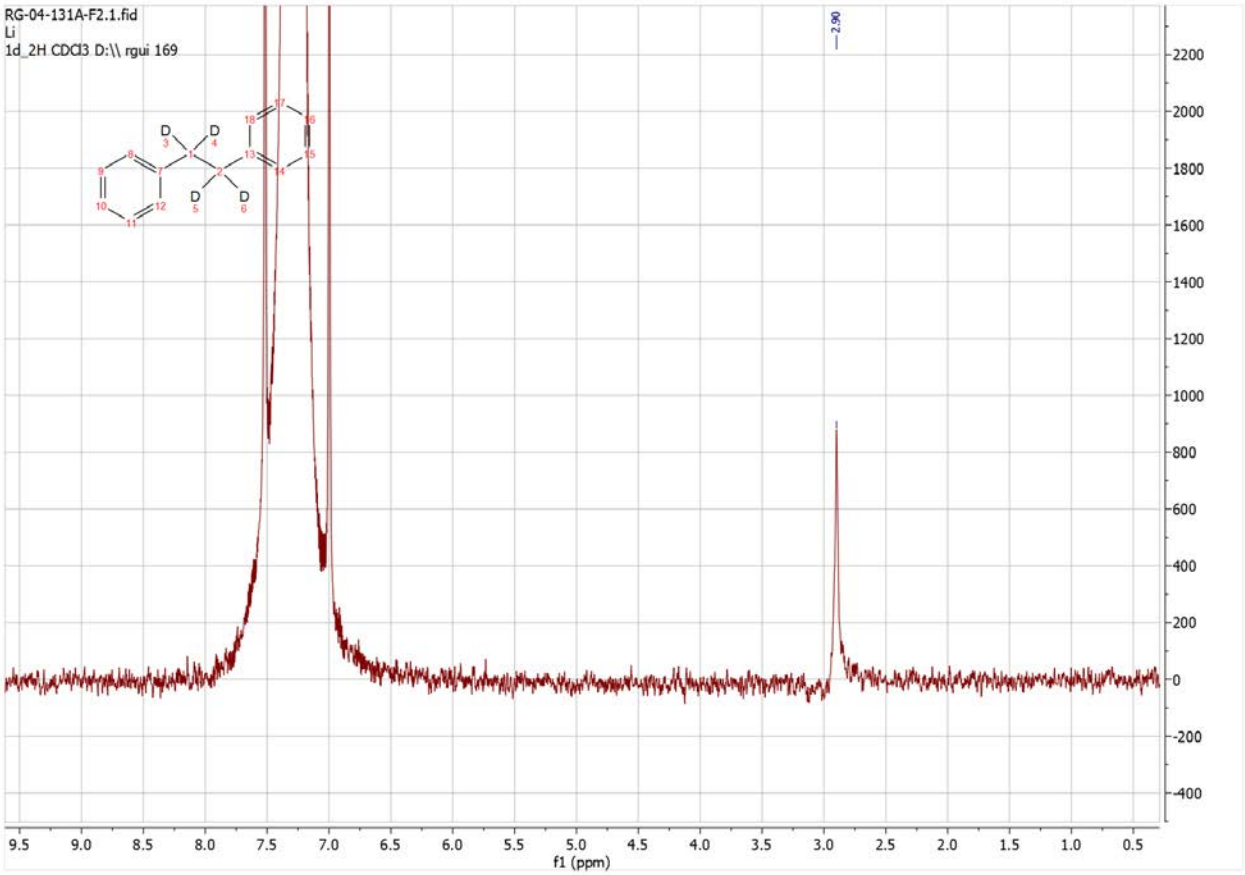

20220909_RG-04-27A_PROTON_01
RG-04-27A
D
D
D
D
CH3
1.00
0.08
1.14
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
¹H (ppm)

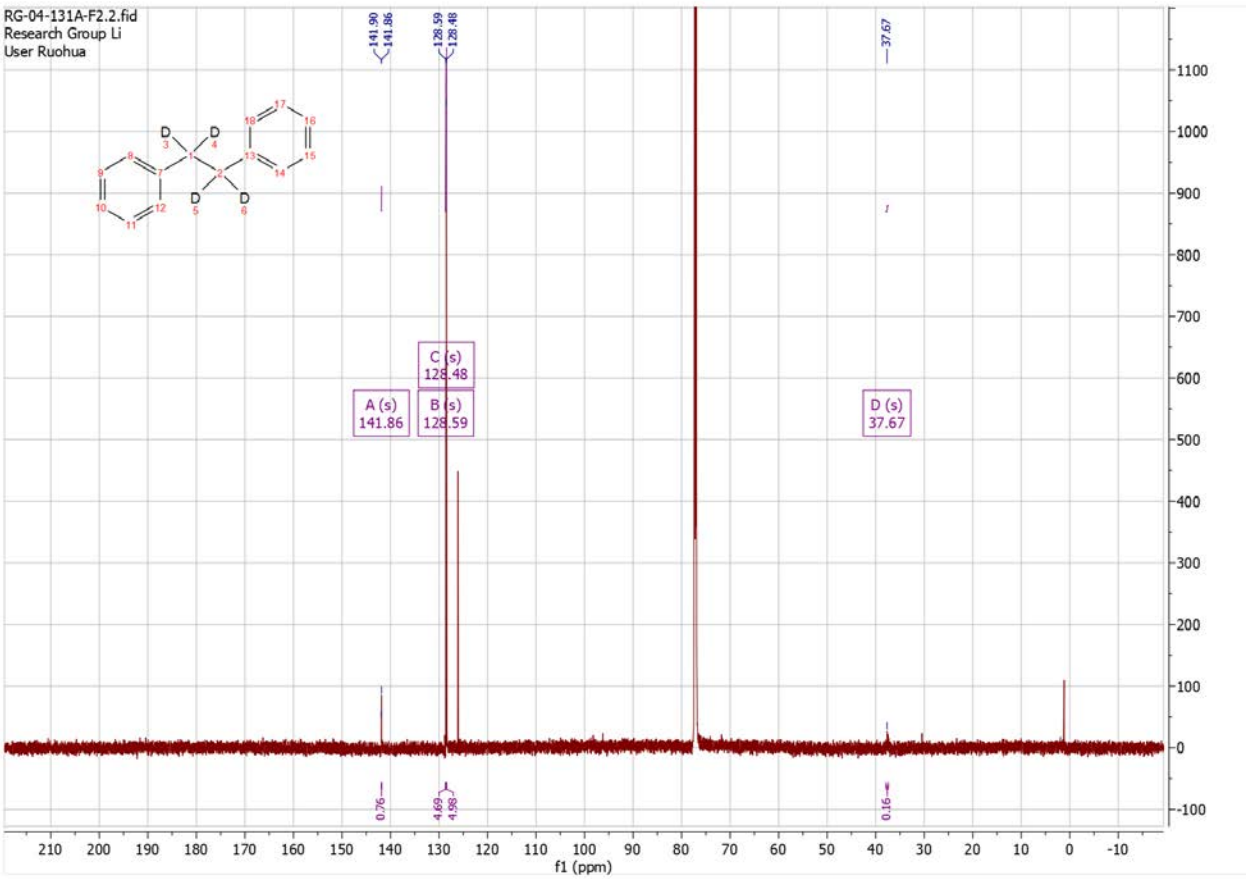

Abundance
TIC: RG-04-27A.D\data.ms
3.5e+07
3e+07
2.5e+07
2e+07
1.5e+07
1e+07
5000000
5.00 6.00 7.00 8.00 9.00 10.00 11.00 12.00 13.00 14.00 15.00 16.00 17.00 18.00 19.00 20.00
Time-->

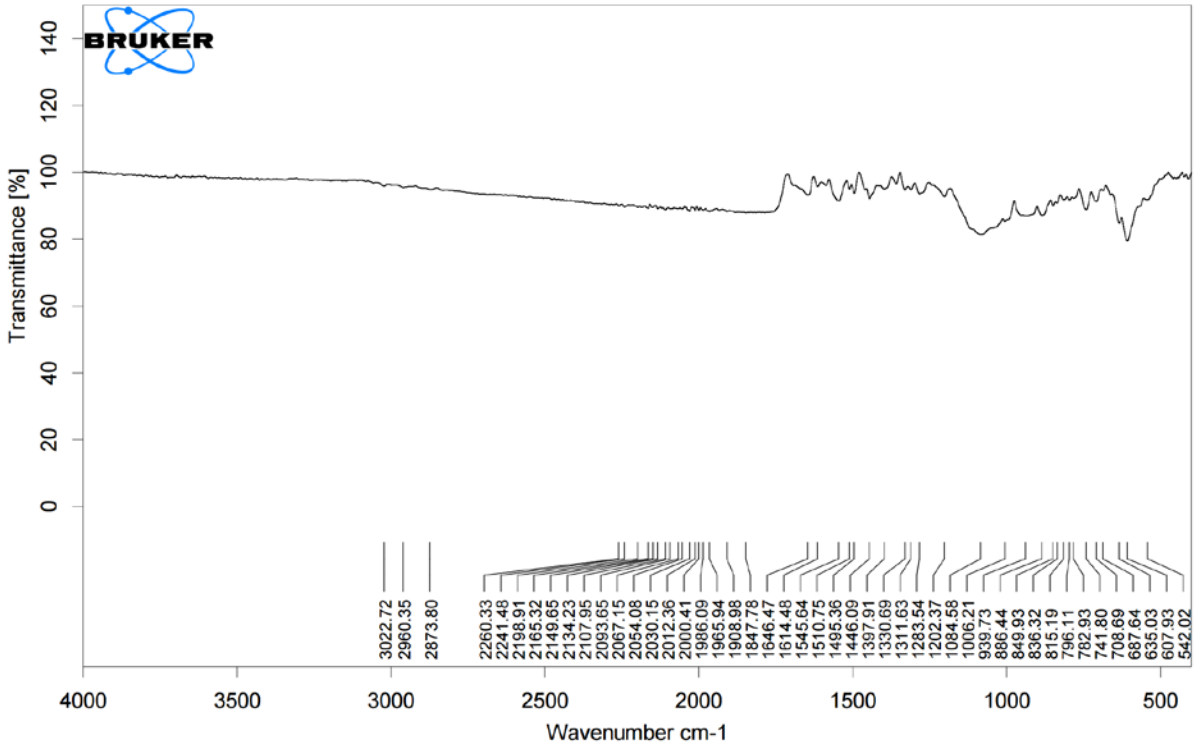

Abundance
Scan 605 (9.227 min): RG-04-27A.D\data.ms
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
93.1
166.2
43.1
66.1
79.1
107.1
122.1
137.1
151.2
191.1 207.0 222.9
253.0 267.0 281.3
331.0 346.0
30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350
m/z-->

D
D
Ph
D
D


20221215_RG-04-131A-F2-dry_PROTON_01
RG-04-131A-F2-dry
B (m)
7.20
A (m)
7.28
5.15
5.00
2.90
2.89
f1 (ppm)


RG-04-131A-F2.1.fid
Li
1d_2H CDCl3 D:\\ rgui 169
2.90
f1 (ppm)


RG-04-131A-F2.2.fid
Research Group Li
User Ruohua
141.90
141.86
128.59
128.48
37.67
C (s)
128.48
A (s)
141.86
B (s)
128.59
D (s)
37.67
0.76
4.69
4.98
0.16
f1 (ppm)


BRUKER
Transmittance [%]
Wavenumber cm-1
3022.72
2960.35
2873.80
2260.33
2241.48
2198.91
2165.32
2149.65
2134.23
2107.95
2093.65
2067.15
2054.08
2030.15
2012.36
2000.41
1986.09
1965.94
1908.98
1847.78
1646.47
1614.48
1545.64
1510.75
1495.36
1446.09
1397.91
1330.69
1311.63
1283.54
1202.37
1084.58
1006.21
939.73
886.44
849.93
836.32
815.19
796.11
782.93
741.80
708.69
687.64
635.03
607.93
542.02

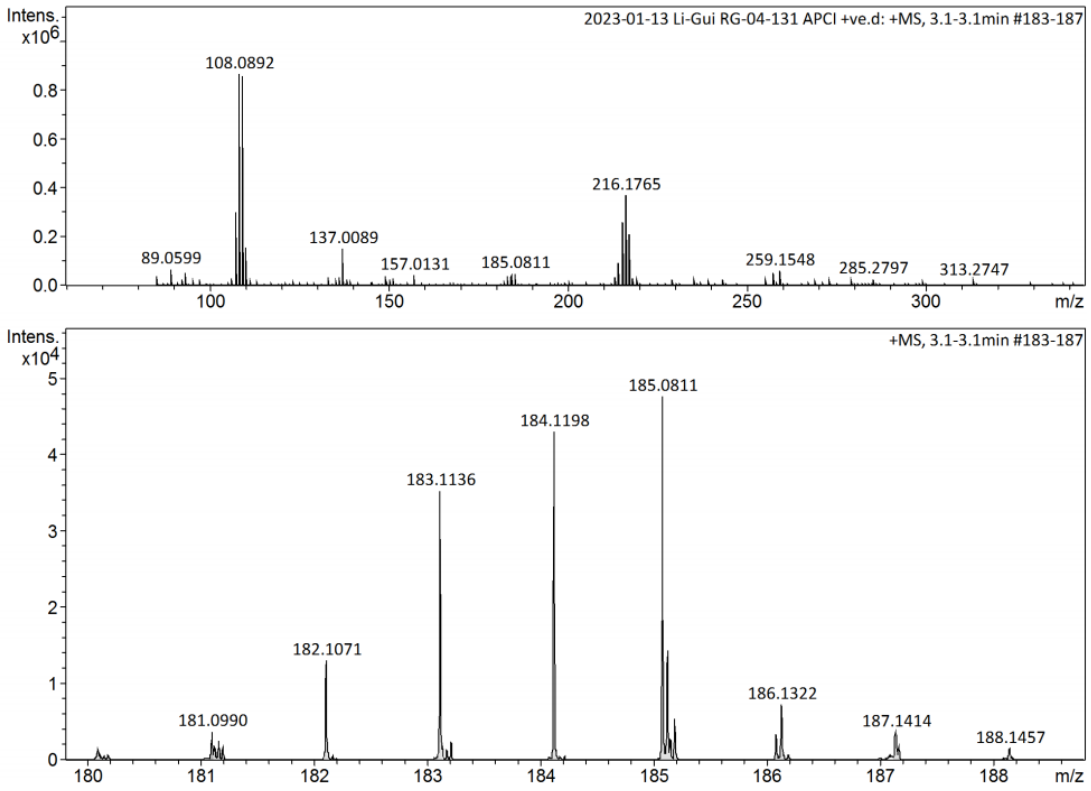
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\Li\2023-01-13 Li-Gui RG-04-131 APCI +ve.d	Acquisition Date	1/13/2023 12:46:48 PM
Method	APCI_Tune_pos_Low_AW Small.m	Operator	Alex
Sample Name	2023-01-13 Li-Gui RG-04-131 APCI +ve	Instrument	maXis impact 282001.00044
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	4.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	150 °C
Scan Begin	90 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.5 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	4000 nA	Set APCI Heater	450 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
	2	C14H12D	182.1075	1.7	798.7	2	100.00	8.5	even	ok
	3	C14H10D2	182.1059	-6.8	798.8	3	59.43	9.0	odd	ok
	4	C10H4D6NO2	182.1083	6.1	810.4	4	1.48	6.5	even	ok
183.1136	1	C14H11D2	183.1137	0.5	533.4	1	100.00	8.5	even	ok
184.1198	1	C14H12D2	184.1216	9.4	138.3	1	41.92	8.0	odd	ok
	2	C14H10D3	184.1200	1.0	138.4	2	100.00	8.5	even	ok
	3	C14H8D4	184.1185	-7.4	138.5	3	53.39	9.0	odd	ok
185.0811	1	C8HD6N2O3	185.0828	8.9	14.8	7	47.08	6.5	even	ok
	2	C10H7DN4	185.0806	-2.8	30.3	10	64.97	9.0	odd	ok
	3	C10H9N4	185.0822	5.6	30.5	11	48.92	8.5	even	ok
	4	C12H7D2NO	185.0804	-3.9	36.9	12	49.56	9.0	odd	ok
	5	C12H9DNO	185.0820	4.5	37.1	13	46.40	8.5	even	ok
186.1322	1	C14H10D4	186.1341	10.3	227.5	1	40.14	8.0	odd	ok
	2	C14H8D5	186.1326	1.9	227.6	2	100.00	8.5	even	ok
	3	C14H6D6	186.1310	-6.4	227.7	3	63.72	9.0	odd	ok