

1-(4-[[3,5-bis([[3,5-dimethyl-4-(4-methyl-3,5-dioxo-1,2,4-triazolidin-1-yl)-phenoxy]methyl)])phenyl]methoxy}-2,6-dimethyl-phenyl)-4-methyl-1,2,4-triazolidine-3,5-dione

Gary W. Breton* and James Alexander Bowron, Jr.

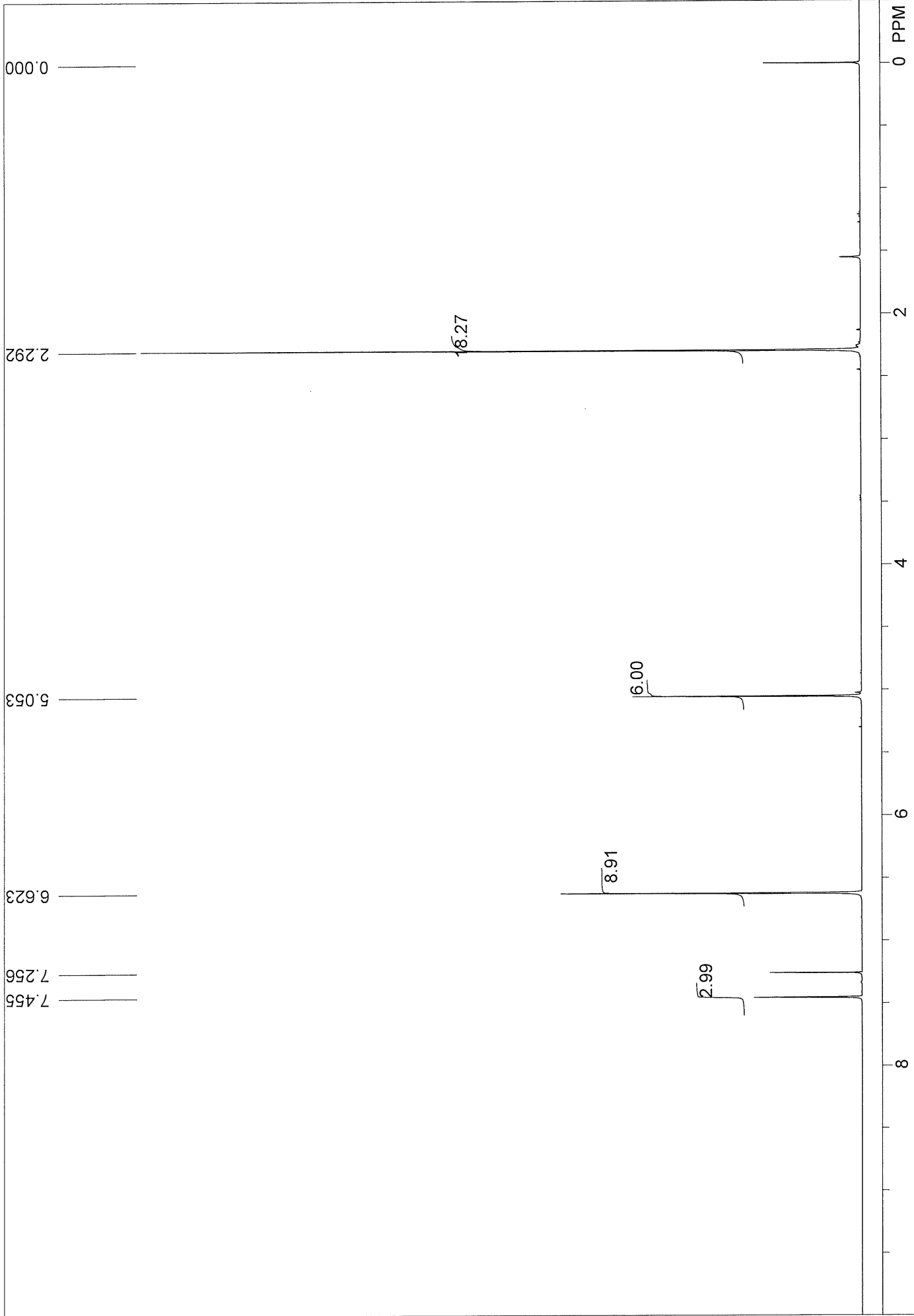
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Supplementary Materials

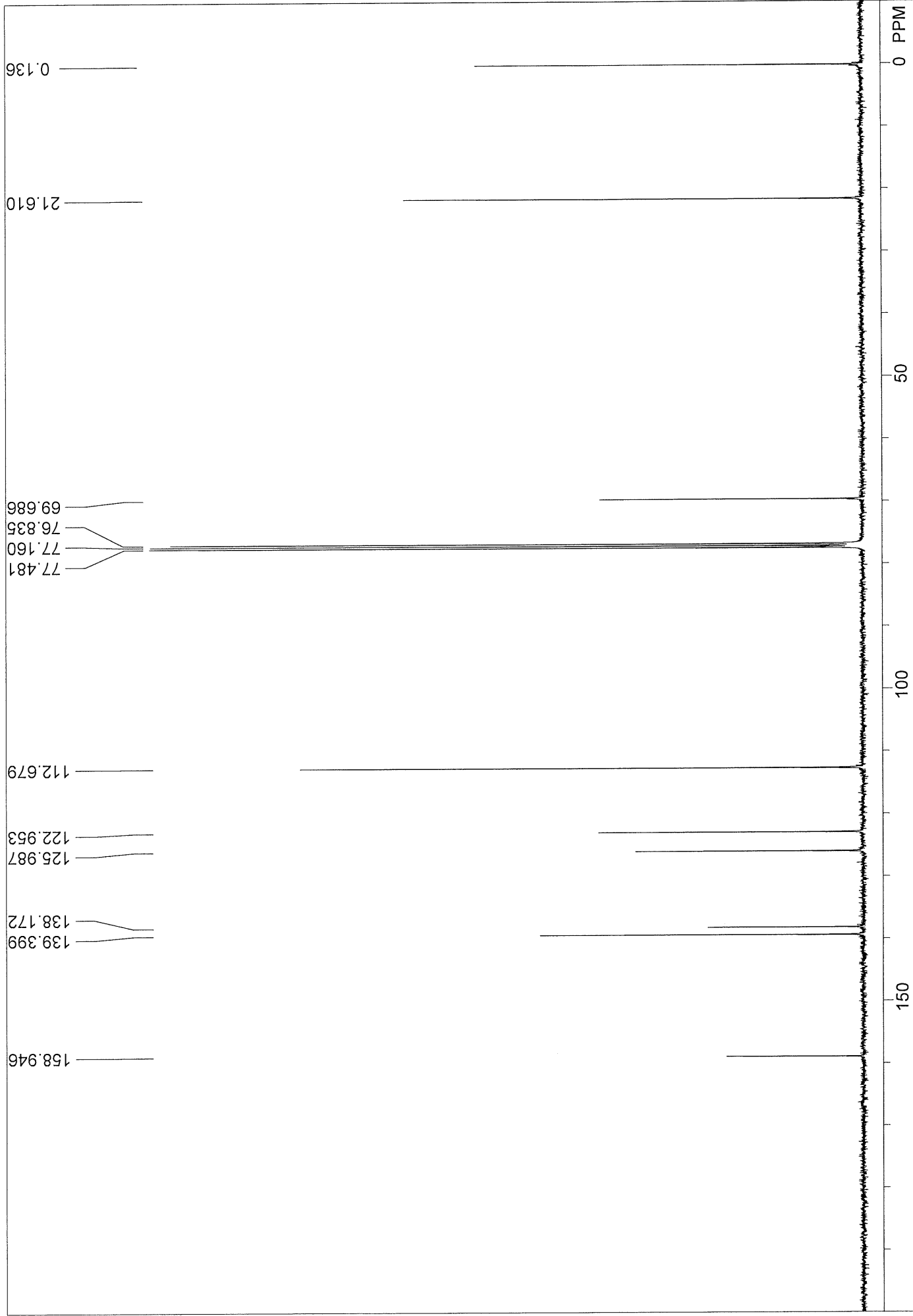
Data for Compound 9

1,3,5-tris[(3,5-dimethylphenoxy)methyl]benzene

- ^1H NMR spectrum
- ^{13}C NMR spectrum
- IR spectrum
- HRMS spectra

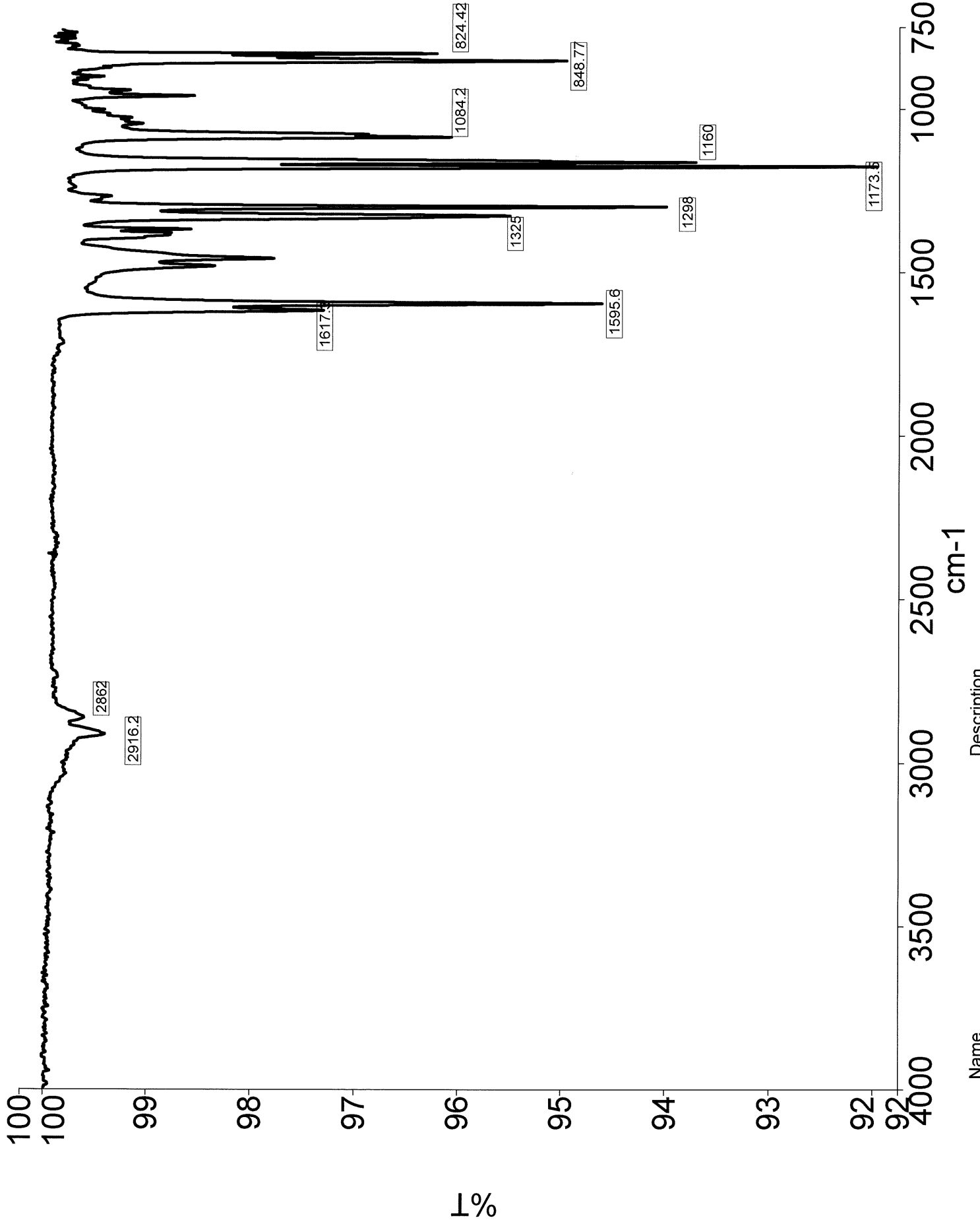


S#375718 (single_pulse) USER: chemlab -- DATE: Dec 2, 2022 10:28:25
 F1: 399.784 F2: 399.784 OF1: 2002.8 PTS1d: 16384
 EX: 10_single_pulse. Nuts - ~~11~~ bromomethylbenzene-~~1,4~~ diethylphenol-tertbutoxide compound (run 2, new compound) B
 PD: 5.0 sec PW: 6.8 us



S#382486 (single pulse decoupled gated NOE)

F1: 100.535	F2: 399.784	SW1: 31407	OF1: 10058.1	PTS1d: 32768	USER: chemlab -- DATE: Apr 5, 2022 11:28:53
EX: 10 single_pulse	PW: 3.3 us	PD: 2.0 sec Nuts - trist	phenol-terbutoxide compound (run 2, new compound) C13		



Breton021222

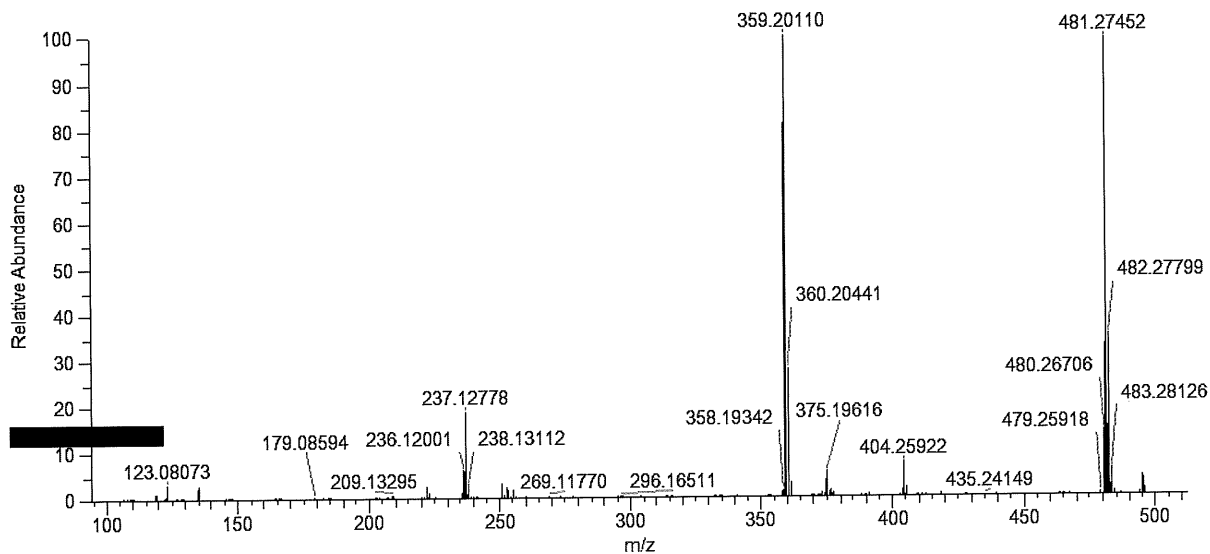
GB2022_4

Peak Mass	Display Formula	RDB	Delta [ppm]	Delta [mmu]	Theo. mass	Combined Score	MS Cov. [%]
481.27452	C ₃₃ H ₃₇ O ₃	15.5	1.65	0.8	481.27372	97.64	99.91
481.27452	C ₂₁ H ₄₁ O ₁₀ N ₂	2.5	-2.19	-1.05	481.27557	68.87	71.21
481.27452	C ₁₇ H ₃₇ O ₈ N ₈	3.5	3.39	1.63	481.27289	67.59	70.79
481.27452	C ₂₂ H ₃₇ O ₆ N ₆	7.5	-4.97	-2.39	481.27691	67.4	70.79

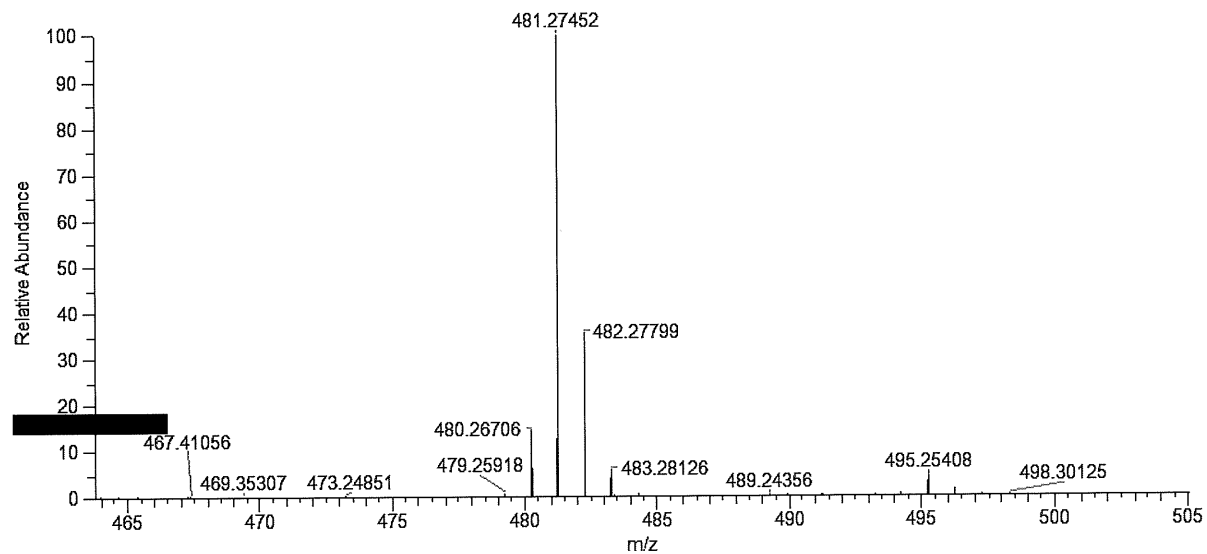
Peak Mass	Display Formula	RDB	Delta [ppm]	Delta [mmu]	Theo. mass	Combined Score	MS Cov. [%]
359.2011	C ₂₅ H ₂₇ O ₂	12.5	1.51	0.54	359.2006	96.92	99.81
359.2011	C ₁₃ H ₃₁ O ₉ N ₂	-0.5	-3.64	-1.31	359.2024	73.46	76.75
359.2011	C ₉ H ₂₇ O ₇ N ₈	0.5	3.83	1.38	359.1997	72.95	76.6

Peak Mass	Display Formula	RDB	Delta [ppm]	Delta [mmu]	Theo. mass	Combined Score	MS Cov. [%]
237.12778	C ₁₇ H ₁₇ O	9.5	1.65	0.39	237.12739	95.14	97.37

EX5331 #18-38 RT: 0.16-0.33 AV: 21 SB: 4 0.03-0.05 NL: 6.28E8
T: FTMS + p APCI corona Full ms [100.0000-500.0000]



EX5331 #18-38 RT: 0.16-0.33 AV: 21 SB: 4 0.03-0.05 NL: 6.21E+008
T: FTMS + p APCI corona Full ms [100.0000-500.0000]

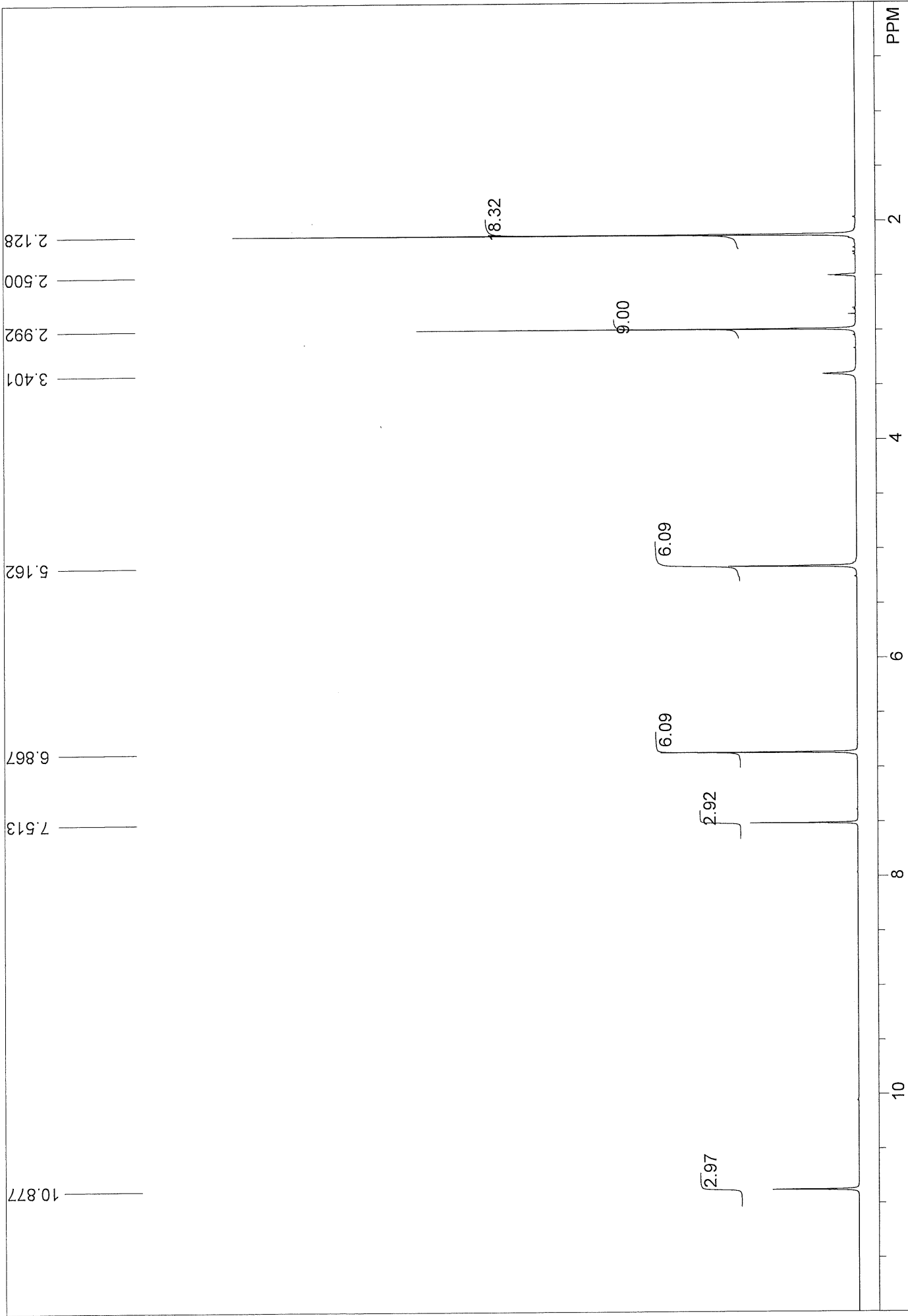


m/z	Intensity	Relative
123.0807	19726853	3.070217
135.0807	18618461	2.897711
222.1043	15553277	2.420657
236.12	38578203	6.004174
237.1278	1.19E+08	18.47726
238.1311	19921914	3.100576
251.1435	19690402	3.064544
253.1227	14418917	2.244109
255.1383	11683409	1.818364
359.2011	6.43E+08	100
360.2044	1.74E+08	27.15387
361.2077	20246876	3.151152
375.1962	35007770	5.448485
404.2592	47070483	7.325882
405.2625	13300258	2.070005
480.2671	90989510	14.16128
481.2745	6.31E+08	98.22267
482.278	2.19E+08	34.12309
483.2813	36647360	5.703665
495.2541	26122728	4.065648

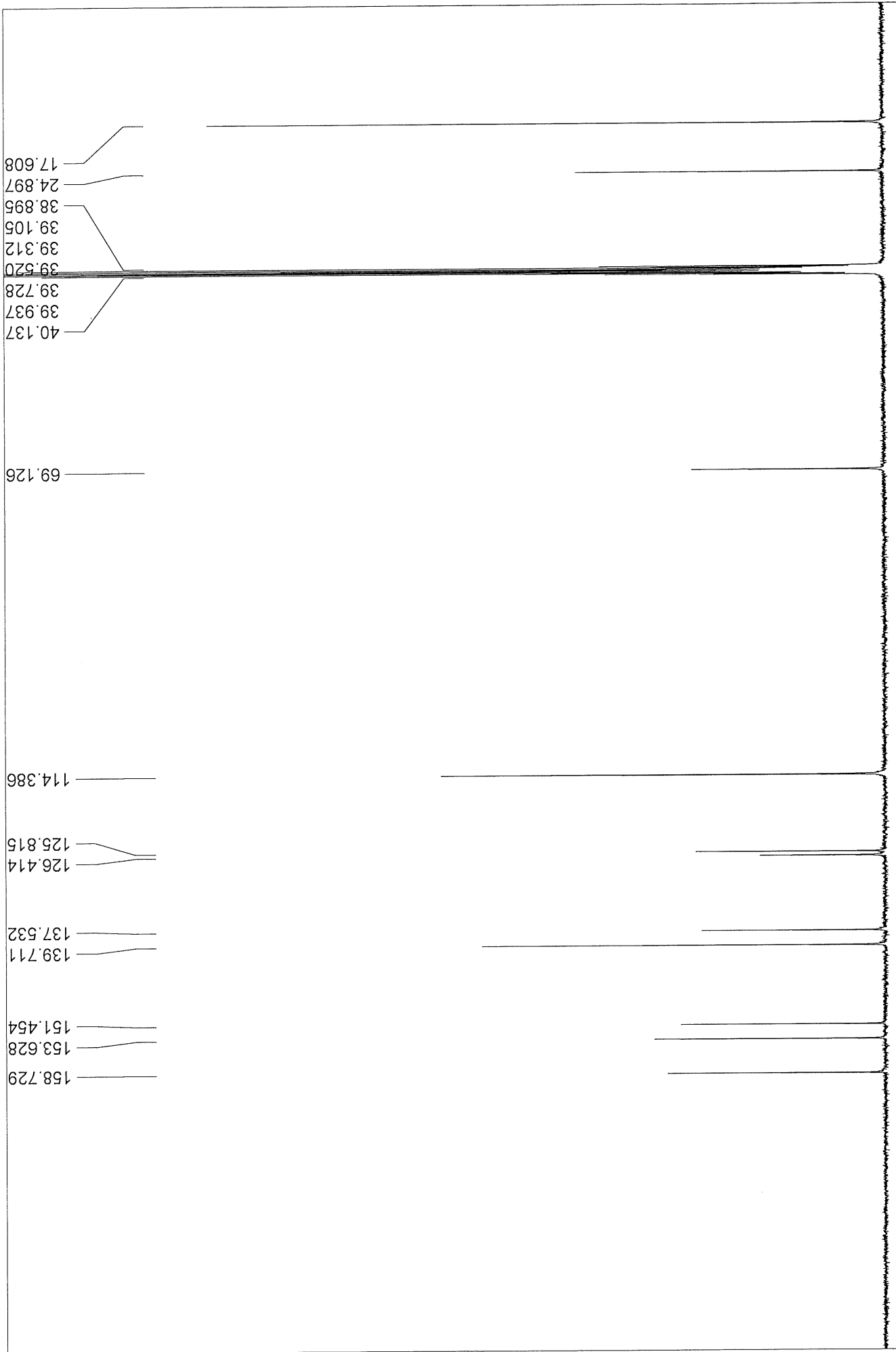
Data for Compound 8

1-(4-{[3,5-bis({[3,5-dimethyl-4-(4-methyl-3,5-dioxo-1,2,4-triazolidin-1-yl)-phenoxy]methyl})phenyl]methoxy}-2,6-dimethylphenyl)-4-methyl-1,2,4-triazolidine-3,5-dione

- ¹H NMR spectrum
- ¹³C NMR spectrum
- DEPT spectrum
- IR spectrum
- HRMS spectra



S#311853 (single_pulse) USER: chemlab -- DATE: Nov 30, 2022 08:41:43
 F1: 399.784 F2: 399.784 PTS1d: 16384
 OF1: 2014.6
 EX: 10_single_pulse. PW: 6.8 us, 45deg PD: 5.0 sec ~~NAME: trisbromomethylphenol~~ phenol-tertbutoxide compound MeTAD adduct B



S#314413 (single pulse decoupled gated NOE)
 USER: chemlab -- DATE: Nov 30, 2022 10:41:15
 F1: 100.535 F2: 399.784 SW1: 31407 PTS1d: 32768
 OF1: 10004.7
 EX: 10 single_pulse Nuts - ~~Nuts~~ methylphenol-terbutoxide compound MeTAD adduct (C13) B
 PD: 2.0 sec PD: 2.0 sec
 PW: 3.3 us, 30deg

Methyl



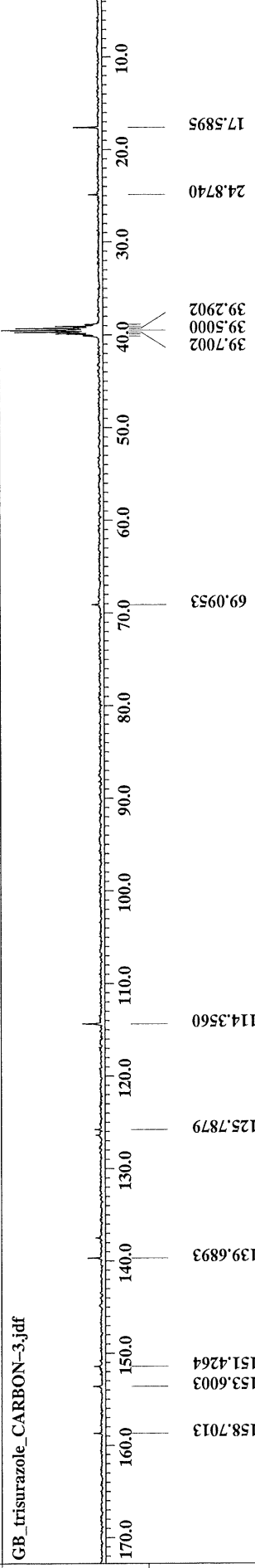
Methylene



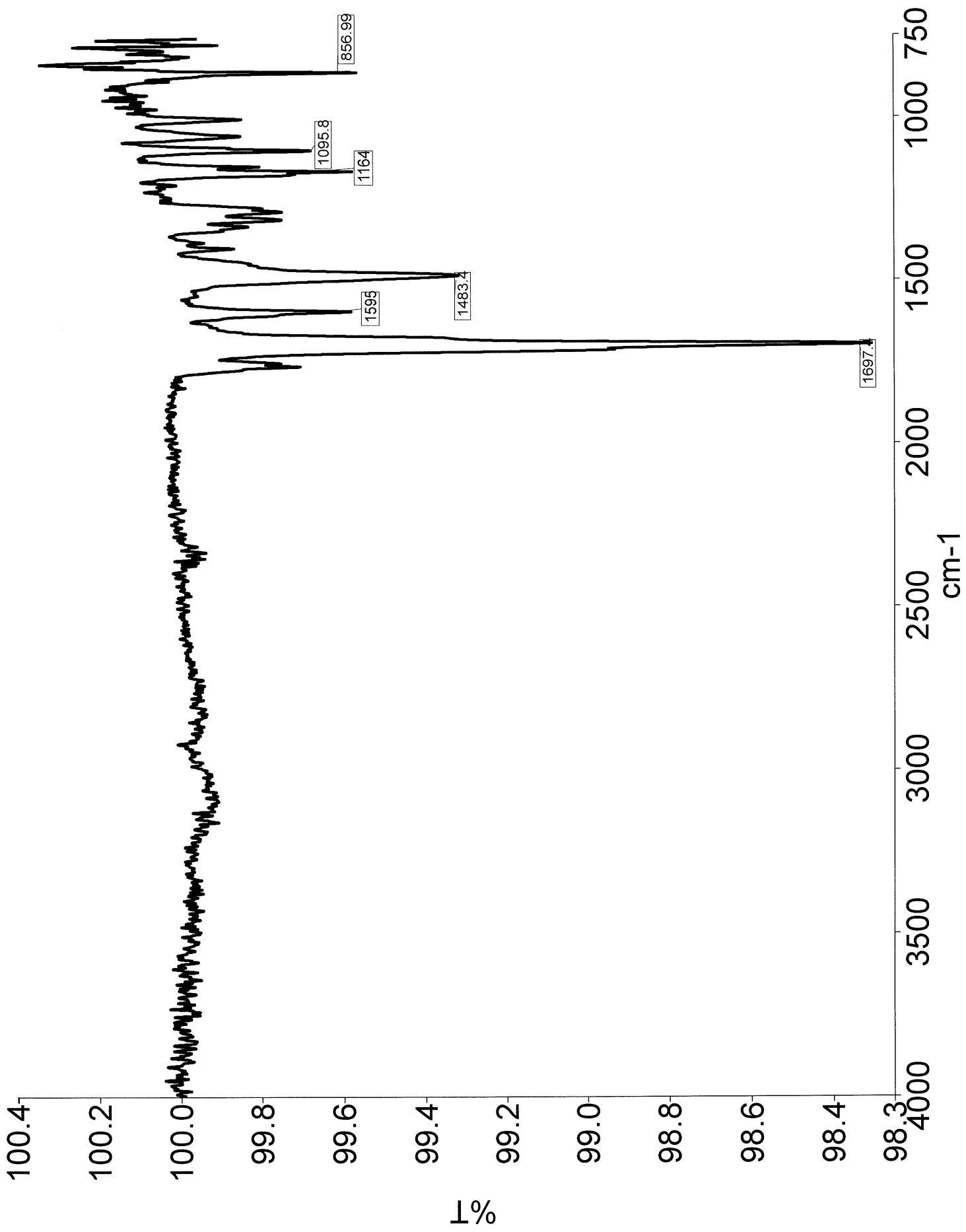
Methine



All Carbons



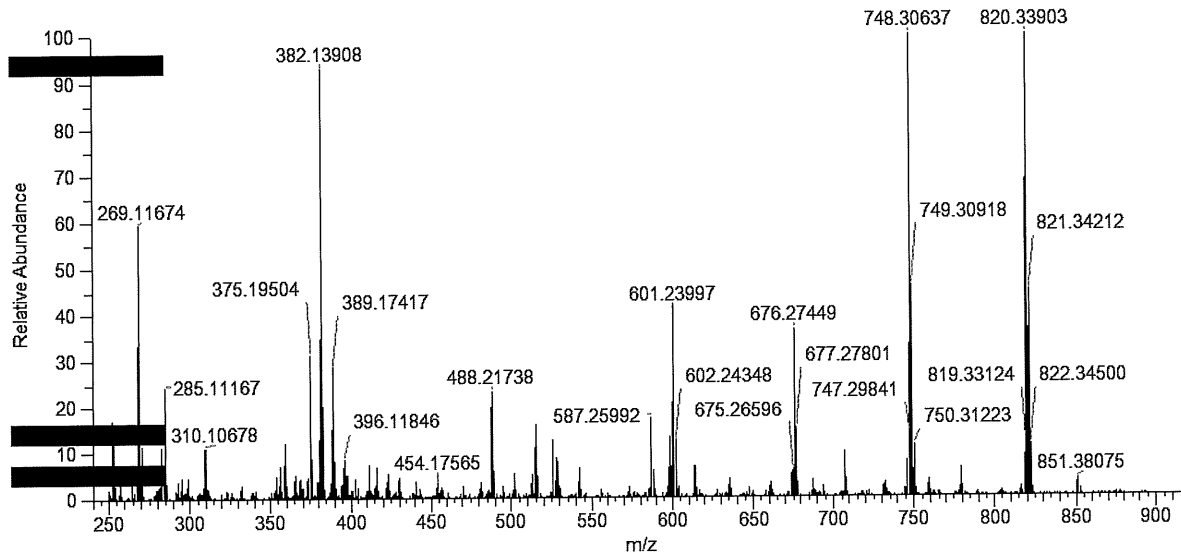
X : parts per Million : 13C



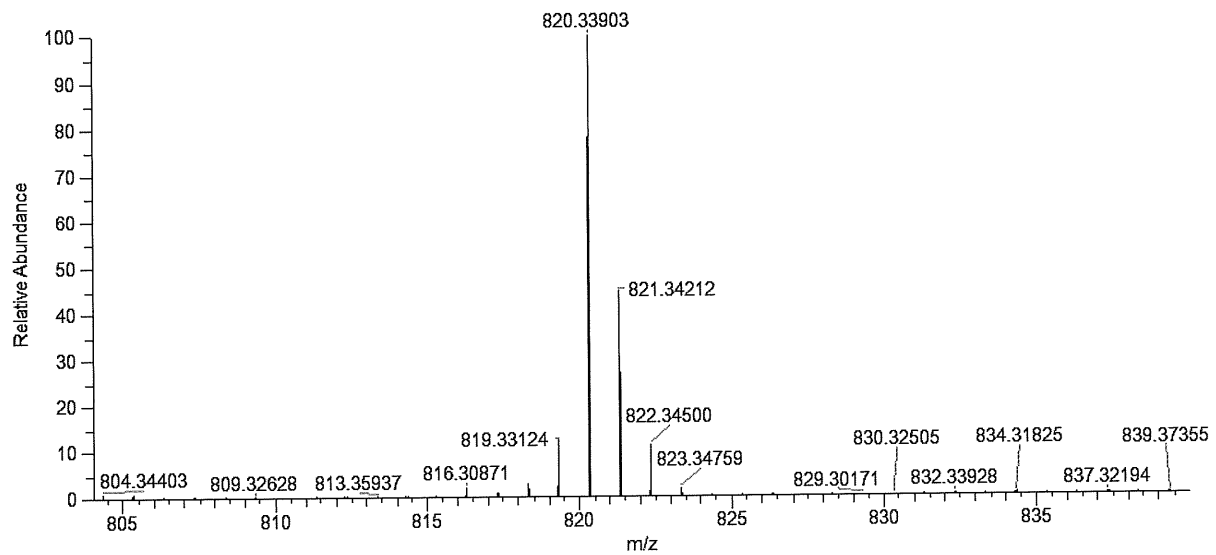
GB2022_5

Peak Mass	Display Formula	RDB	Delta [ppm]	Delta [mmu]	Theo. mass	Combined Score	MS Cov. [%]
820.33903	C ₄₁ H ₅₀ O ₁₃ N ₅	19.5	-1.14	-0.93	820.33996	95.83	98.72
820.33903	C ₄₂ H ₄₆ O ₉ N ₉	24.5	-2.77	-2.27	820.3413	95.62	98.72
820.33903	C ₃₆ H ₅₀ O ₁₅ N ₇	15.5	3.77	3.09	820.33594	94.6	98.52
820.33903	C ₄₉ H ₄₂ O ₄ N ₉	33.5	4.39	3.6	820.33543	60.43	63.43

EX5332 #169-171 RT: 1.47-1.49 AV: 3 SB: 4 1.41-1.44 NL: 2.46E6
T: FTMS + p APCI corona Full ms [250.0000-900.0000]



EX5332 #169-171 RT: 1.47-1.49 AV: 3 SB: 4 1.41-1.44 NL: 2.46E+006
T: FTMS + p APCI corona Full ms [250.0000-900.0000]



m/z	Intensity	Relative
253.1218	426252.9	17.11627
269.1167	1503517	60.374
285.1117	610453.2	24.51286
375.195	779376	31.29599
382.1391	2339542	93.94476
383.1424	494114.3	19.84125
389.1742	704761.1	28.29982
488.2174	577730.7	23.19889
515.2282	387846	15.57403
587.2599	433044.9	17.389
598.2394	329516.8	13.23181
600.2549	325902.4	13.08667
601.24	1026860	41.23378
676.2745	902353.8	36.23419
677.278	371949.4	14.9357
747.2984	342649.9	13.75917
748.3064	2486776	99.85697
749.3092	1124016	45.13509
820.339	2490338	100
821.3421	1098958	44.12886