LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100421\
Data File : BM032321.D
Acq On : 04 Oct 2021 13:28
Operator : CG/JU
Sample : M3702-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
PT-ACIDS-WP

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM032321.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.578	121	126	133	rVB	173665	241026	1.44%	0.114%
2	5.207	396	403	423	rBV	6686504	9585129	57.32%	4.549%
3	6.648	643	648	654	rVB	178124	256133	1.53%	0.122%
4	6.837	670	680	682	rBV	5524626	11156530	66.72%	5.295%
5	6.860	682	684	697	rVB	6363016	7898957	47.24%	3.749%
6	7.207	734	743	752	rBV	6504263	10496266	62.77%	4.981%
7	7.637	805	816	824	rVB2	1227354	2012108	12.03%	0.955%
8	7.889	852	859	868	rBV	260501	444634	2.66%	0.211%
9	8.095	887	894	900	rBV	4843953	7285067	43.56%	3.457%
10	8.201	907	912	916	rBV	168825	249621	1.49%	0.118%
11	8.431	941	951	961	rVV	8305972	13901641	83.13%	6.598%
12	8.795	1004	1013	1019	rBV	3900339	6374514	38.12%	3.025%
13	9.548	1132	1141	1147	rBV	4362248	6917684	41.37%	3.283%
14	9.625	1147	1154	1170	rVB	8213775	13303563	79.56%	6.314%
15	10.083	1225	1232	1244	rBV	5330536	8487228	50.75%	4.028%
16	10.425	1283	1290	1298	rBV	1574098	2496600	14.93%	1.185%
17	10.613	1310	1322	1334	rBV	7778252	13127936	78.51%	6.230%
18	11.725	1503	1511	1524	rVB	4846942	7833601	46.85%	3.718%
19	12.713	1672	1679	1685	rBV	4535593	6734197	40.27%	3.196%
20	12.783	1685	1691	1704	rVV	4630254	6695206	40.04%	3.177%
21	12.901	1704	1711	1718	rVB	8997402	13438958	80.37%	6.378%
22	13.730	1843	1852	1861	rBV	88467	241138	1.44%	0.114%
23	14.283	1939	1946	1952	rBV	2272922	3160539	18.90%	1.500%
24	14.513	1976	1985	1997	rBV	5031196	7944484	47.51%	3.770%
25	14.913	2048	2053	2059	rBV	123868	168651	1.01%	0.080%
26	15.401	2130	2136	2151	rBV	3627040	4842492	28.96%	2.298%
27	15.771	2192	2199	2216	rVB	6570563	9756267	58.34%	4.630%
28	16.677	2347	2353	2367	rBV	5519443	7507904	44.90%	3.563%
29	17.012	2403	2410	2419	rBV	2671350	3674842	21.98%	1.744%
30	19.630	2848	2855	2859	rBV	12271088	16722308	100.00%	7.936%
31	20.383	2979	2983	2989	rBV	674932	720858	4.31%	0.342%
32	21.177	3113	3118	3124	rBV	2885630	3640137	21.77%	1.728%
33	23.336	3479	3485	3495	rVB2	1883934	3390704	20.28%	1.609%

Sum of corrected areas: 210706923

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Instrument :
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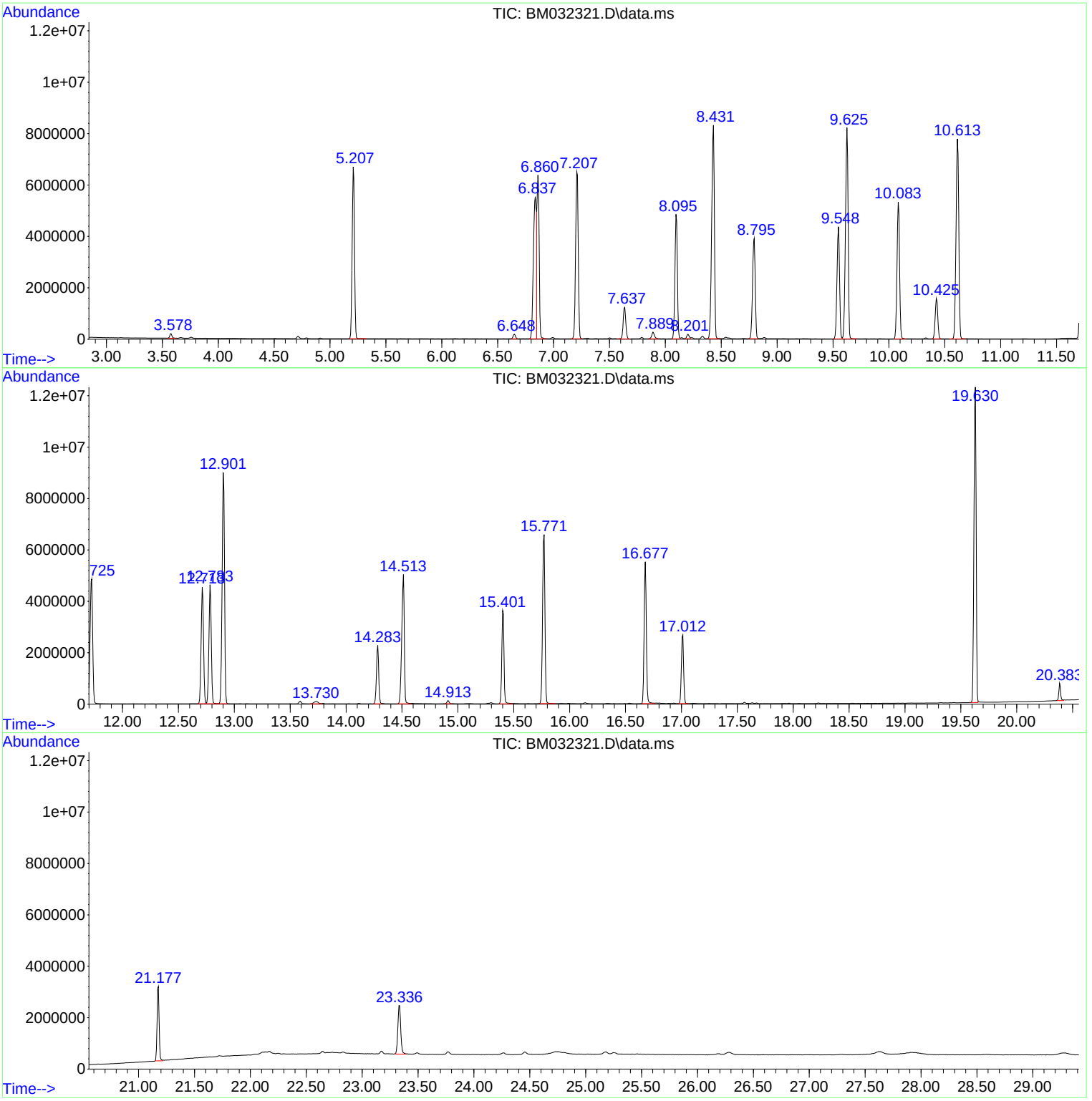
ClientSampleId :
PT-ACIDS-WP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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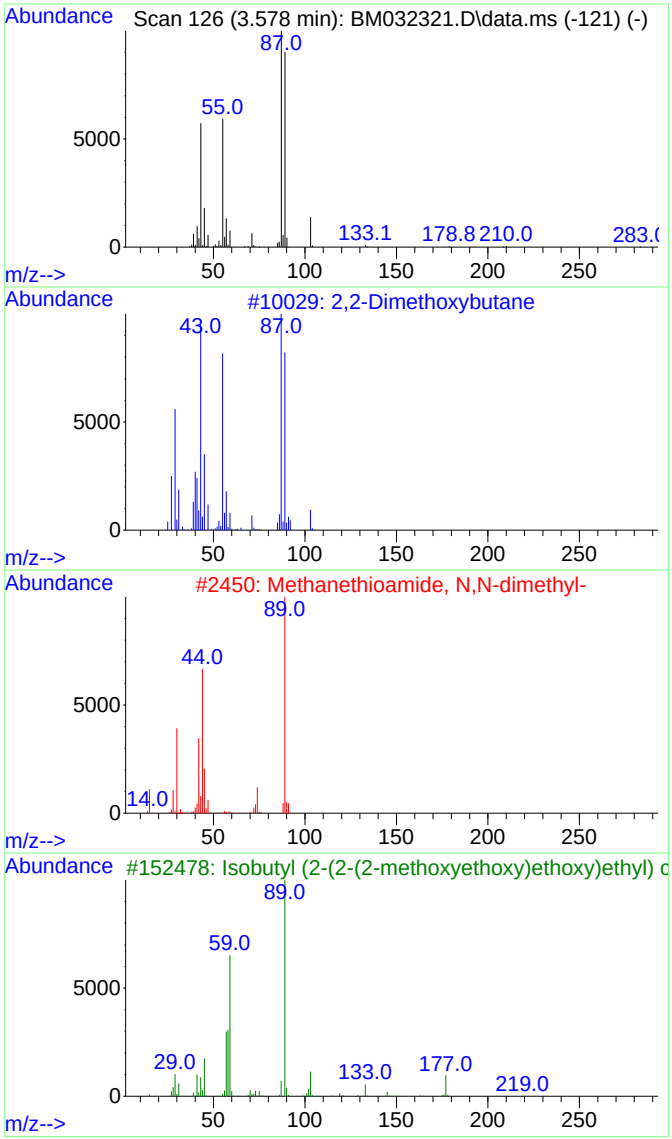
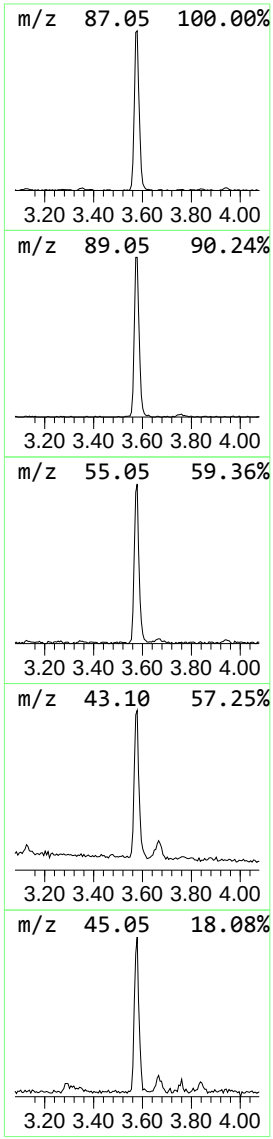
Peak Number 1 2,2-Dimethoxybutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.578	2.40 ng	241026	1,4-Dichlorobenzene-d4	7.637

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethoxybutane	118	C6H14O2	003453-99-4	74
2	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	59
3	Isobutyl (2-(2-(2-methoxyethoxy)...	264	C12H24O6	1000378-28-5	45
4	Isobutyl 2,5,8,11-tetraoxatridec...	308	C14H28O7	1000378-27-9	45
5	Propane, 2,2',2''-[methylidynetr...	190	C10H22O3	004447-60-3	42





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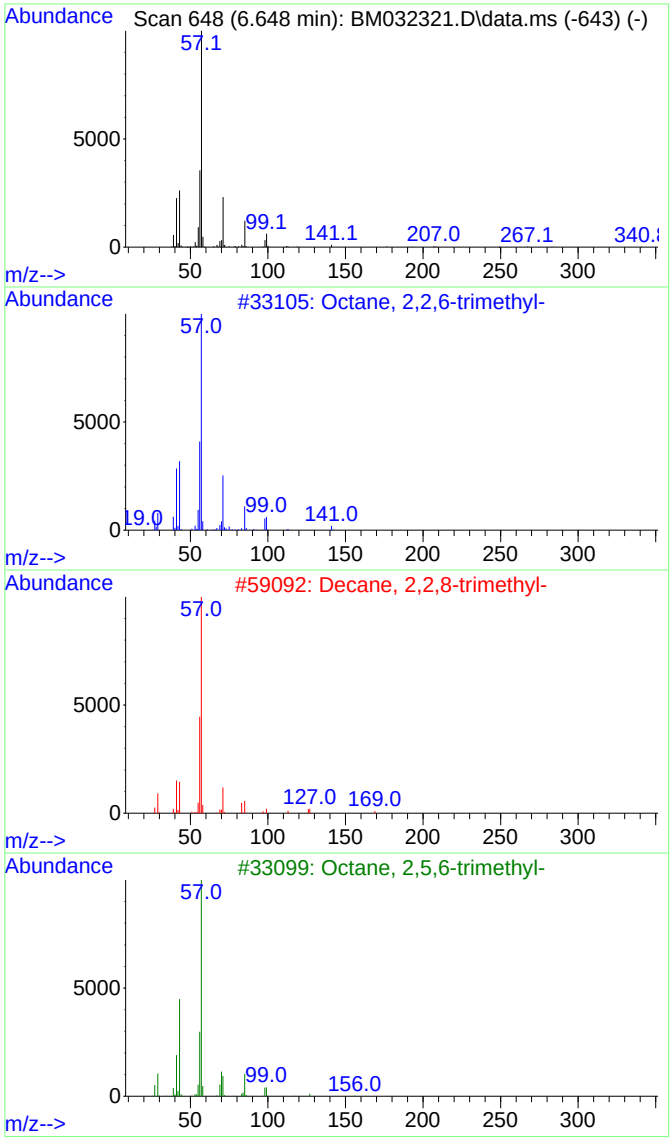
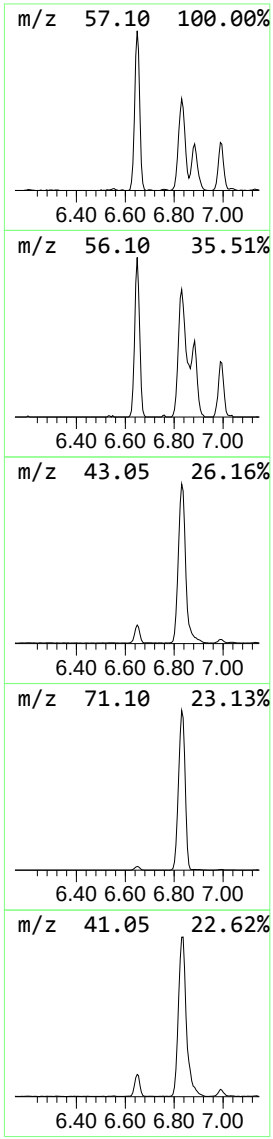
Peak Number 2 Octane, 2,2,6-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.648	2.55 ng	256133	1,4-Dichlorobenzene-d4	7.637

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	74
2	Decane, 2,2,8-trimethyl-	184	C13H28	062238-01-1	72
3	Octane, 2,5,6-trimethyl-	156	C11H24	062016-14-2	64
4	Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	64
5	Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	64





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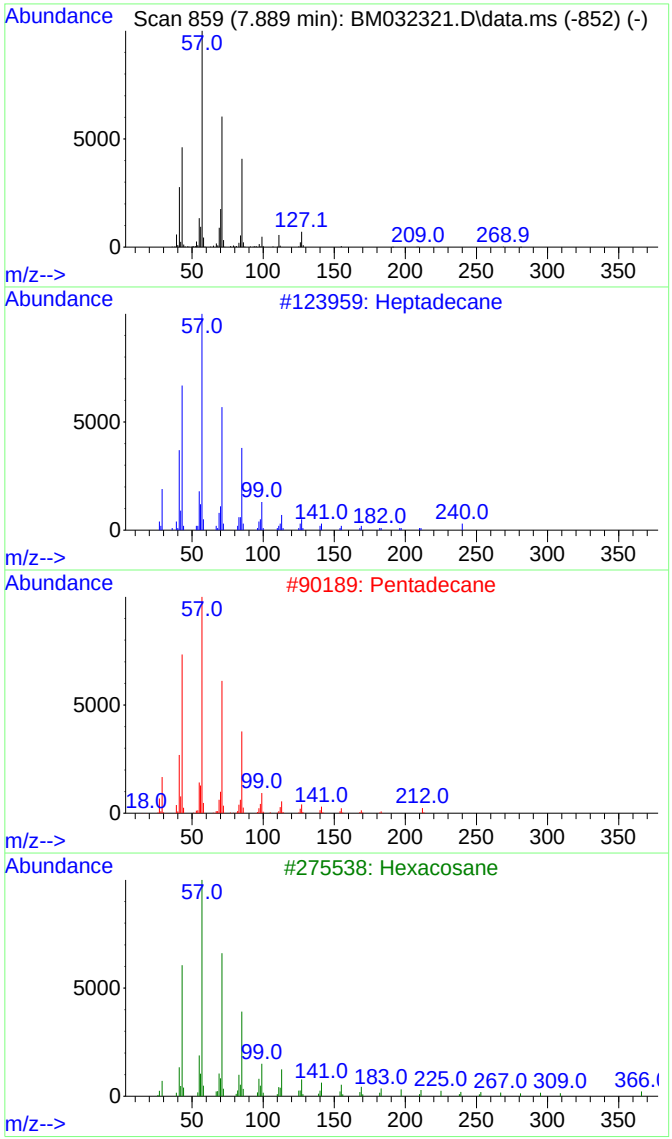
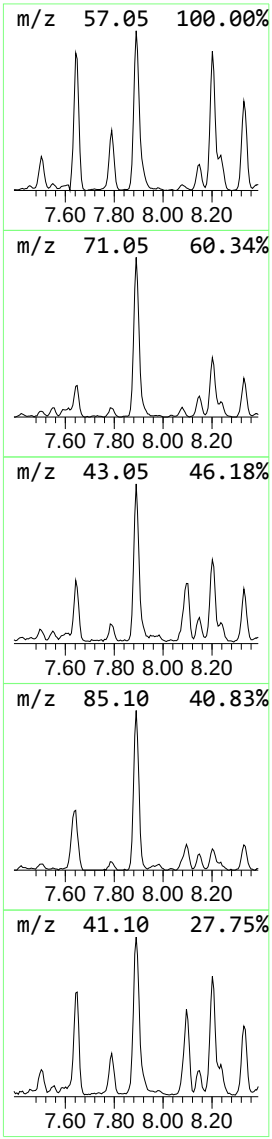
Peak Number 3 Heptadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.889	4.42 ng	444634	1,4-Dichlorobenzene-d4	7.637

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	78
2	Pentadecane	212	C15H32	000629-62-9	78
3	Hexacosane	366	C26H54	000630-01-3	72
4	Pentacosane	352	C25H52	000629-99-2	72
5	Decane, 2,3,8-trimethyl-	184	C13H28	062238-14-6	72





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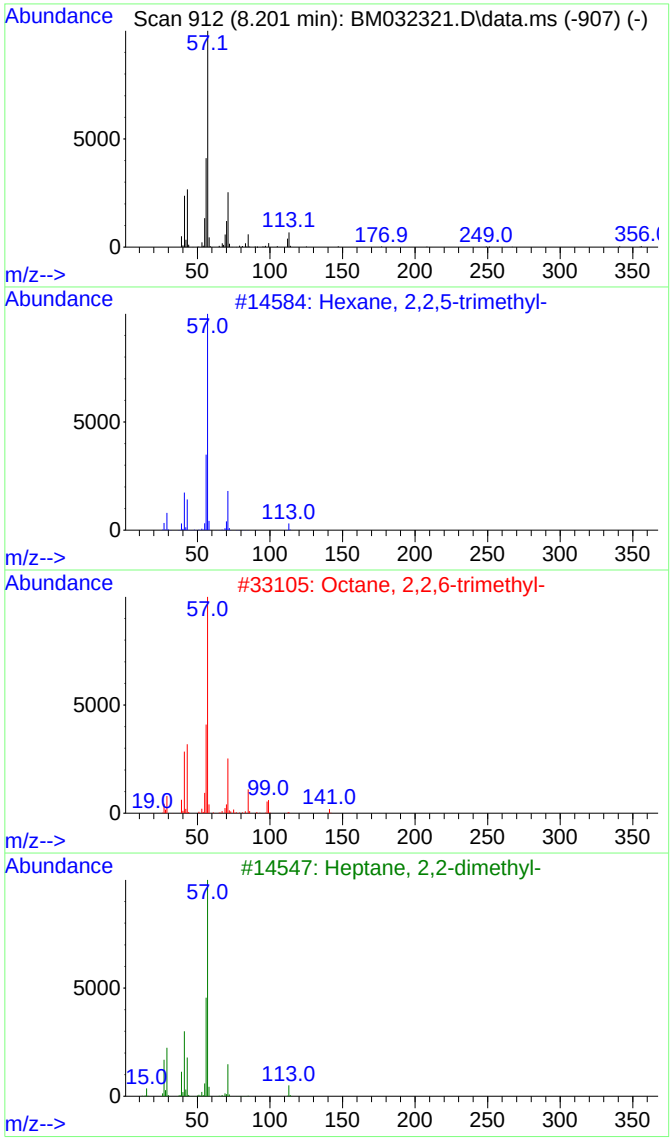
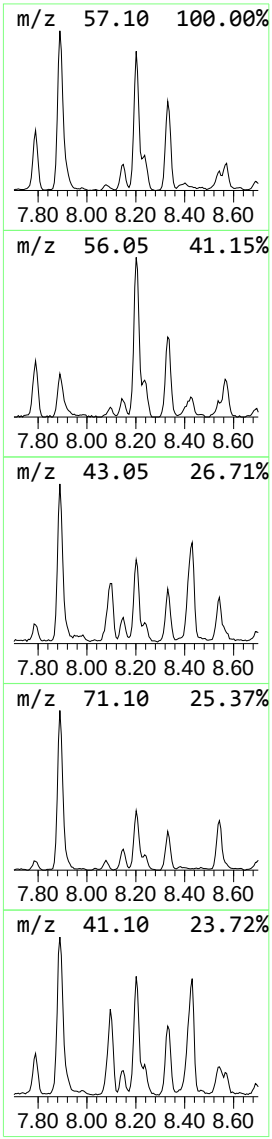
Peak Number 4 Hexane, 2,2,5-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.201	2.48 ng	249621	1,4-Dichlorobenzene-d4	7.637

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	64
2	Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	59
3	Heptane, 2,2-dimethyl-	128	C9H20	001071-26-7	59
4	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	56
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	53





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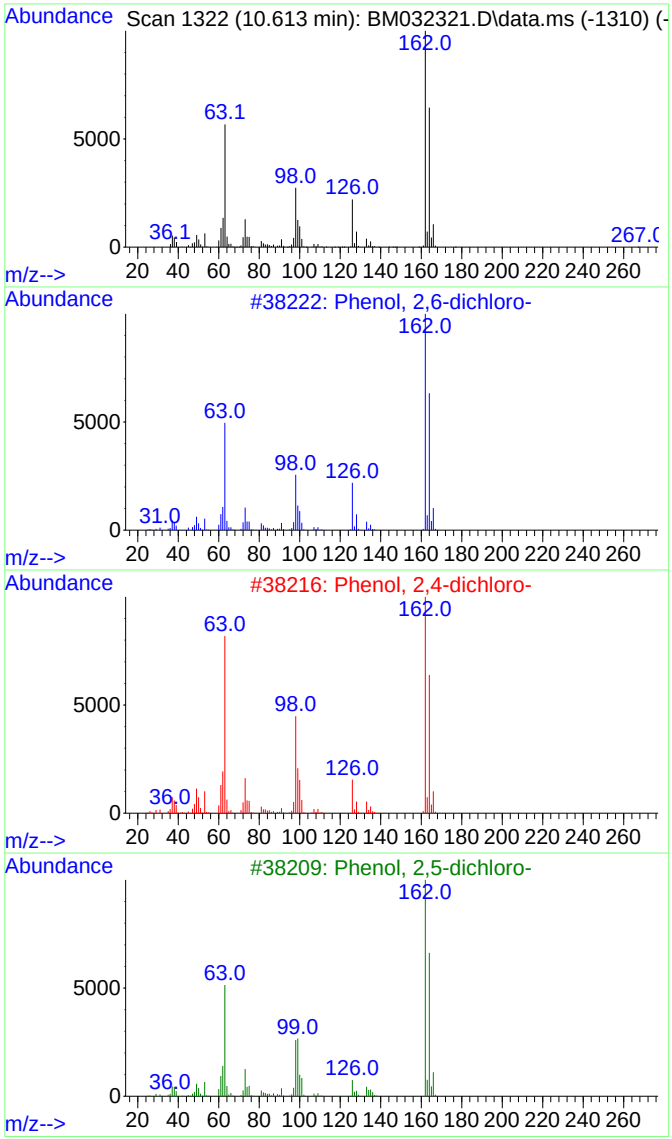
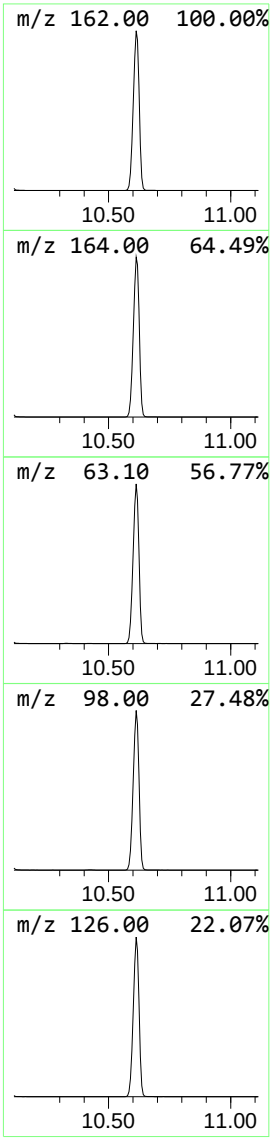
Peak Number 5 Phenol, 2,6-dichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.613	105.17 ng	13127900	Naphthalene-d8	10.425

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-dichloro-	162	C6H4Cl2O	000087-65-0	98
2	Phenol, 2,4-dichloro-	162	C6H4Cl2O	000120-83-2	97
3	Phenol, 2,5-dichloro-	162	C6H4Cl2O	000583-78-8	94
4	Phenol, 2,3-dichloro-	162	C6H4Cl2O	000576-24-9	94
5	Phenol, 3,5-dichloro-	162	C6H4Cl2O	000591-35-5	64





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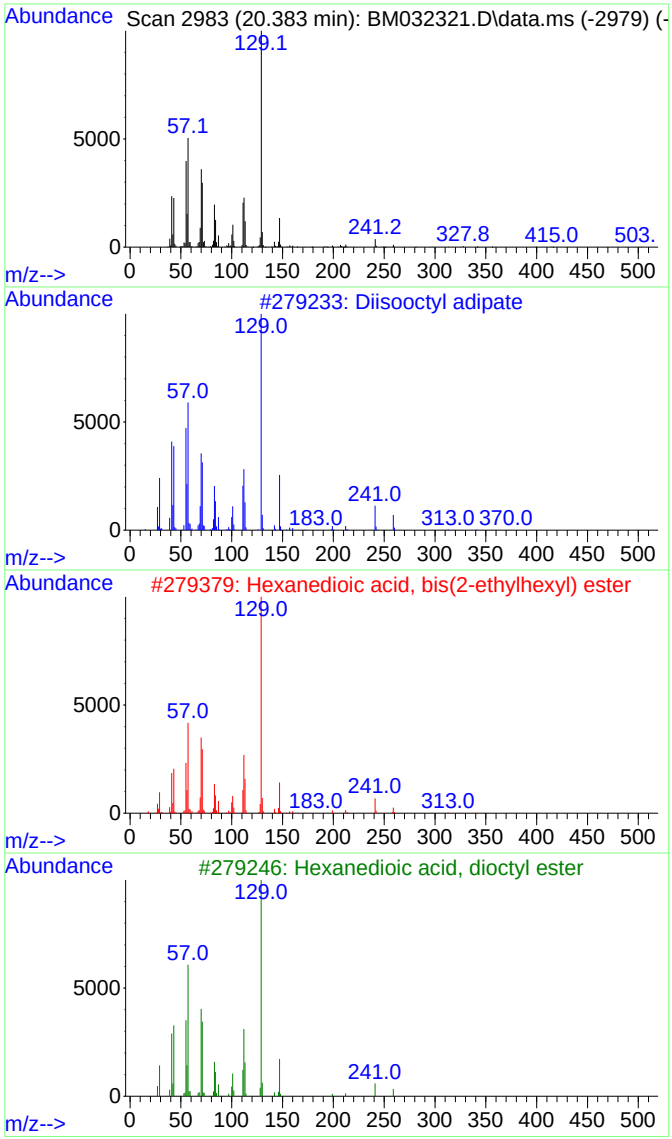
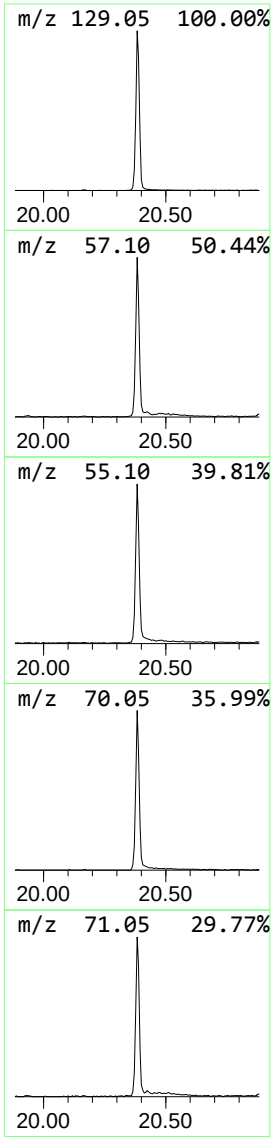
Peak Number 6 Diisooctyl adipate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.383	3.96 ng	720858	Chrysene-d12	21.177

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisooctyl adipate	370	C22H42O4	001330-86-5	90
2	Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	87
3	Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	70
4	Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	53
5	Adipic acid, di(oct-4-yl ester)	370	C22H42O4	1000160-80-1	50





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2,2-Dimethoxybu...	3.578	2.4	ng	241026	1	7.637	2012110	20.0
Octane, 2,2,6-t...	6.648	2.5	ng	256133	1	7.637	2012110	20.0
Heptadecane	7.889	4.4	ng	444634	1	7.637	2012110	20.0
Hexane, 2,2,5-t...	8.201	2.5	ng	249621	1	7.637	2012110	20.0
Phenol, 2,6-dic...	10.613	105.2	ng	13127900	2	10.425	2496600	20.0
Diisooctyl adipate	20.383	4.0	ng	720858	5	21.177	3640140	20.0