LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032502.D
Acq On : 13 Oct 2021 18:52
Operator : CG/JU
Sample : M4142-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2186-2187

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: BM032502.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.178	392	398	412	rVB	2203937	3027089	35.29%	4.472%
2	5.649	470	478	491	rBV4	39968	126039	1.47%	0.186%
3	6.790	666	672	686	rBV	1269008	1959634	22.85%	2.895%
4	7.601	802	810	818	rBV	865017	1366254	15.93%	2.018%
5	7.684	818	824	843	rVV	389536	812302	9.47%	1.200%
6	8.754	999	1006	1018	rBV	2631921	4156194	48.45%	6.140%
7	10.166	1241	1246	1254	rVB	919784	1370156	15.97%	2.024%
8	10.389	1276	1284	1297	rVB	1111406	1880698	21.93%	2.779%
9	10.542	1305	1310	1318	rVB4	51300	105081	1.23%	0.155%
10	10.913	1365	1373	1380	rBV	601554	1058146	12.34%	1.563%
11	11.389	1447	1454	1459	rBV5	66415	131377	1.53%	0.194%
12	11.442	1459	1463	1470	rVB6	55756	97968	1.14%	0.145%
13	12.148	1579	1583	1589	rVB	64320	116358	1.36%	0.172%
14	12.366	1616	1620	1628	rBV9	41824	97219	1.13%	0.144%
15	12.866	1699	1705	1717	rBV	5860573	8577513	100.00%	12.672%
16	13.172	1748	1757	1763	rBV	2557586	4712177	54.94%	6.962%
17	13.630	1831	1835	1840	rBV5	75238	134176	1.56%	0.198%
18	14.248	1934	1940	1950	rBV3	2010448	3375441	39.35%	4.987%
19	15.630	2172	2175	2181	rVB3	176333	267205	3.12%	0.395%
20	15.736	2187	2193	2197	rBV	3794657	5315442	61.97%	7.853%
21	15.783	2197	2201	2211	rVB	1434729	1986208	23.16%	2.934%
22	16.507	2320	2324	2332	rVB2	630808	988359	11.52%	1.460%
23	16.618	2339	2343	2353	rBV	904063	1383519	16.13%	2.044%
24	16.977	2399	2404	2414	rVB	1682776	2343415	27.32%	3.462%
25	17.330	2460	2464	2469	rBV	857727	1155385	13.47%	1.707%
26	17.795	2539	2543	2551	rVB	820145	1107716	12.91%	1.637%
27	17.877	2553	2557	2567	rBV	1156565	1673700	19.51%	2.473%
28	19.154	2771	2774	2785	rVB	988253	1402506	16.35%	2.072%
29	19.601	2845	2850	2856	rVB	6136500	8165212	95.19%	12.063%
30	21.148	3109	3113	3118	rVB	1759099	2076927	24.21%	3.068%
31	21.859	3230	3234	3245	rVB	2734612	3492589	40.72%	5.160%
32	23.289	3472	3477	3487	rVB2	1296636	2312762	26.96%	3.417%
33	23.577	3522	3526	3540	rVB	490043	912161	10.63%	1.348%

Sum of corrected areas: 67686928

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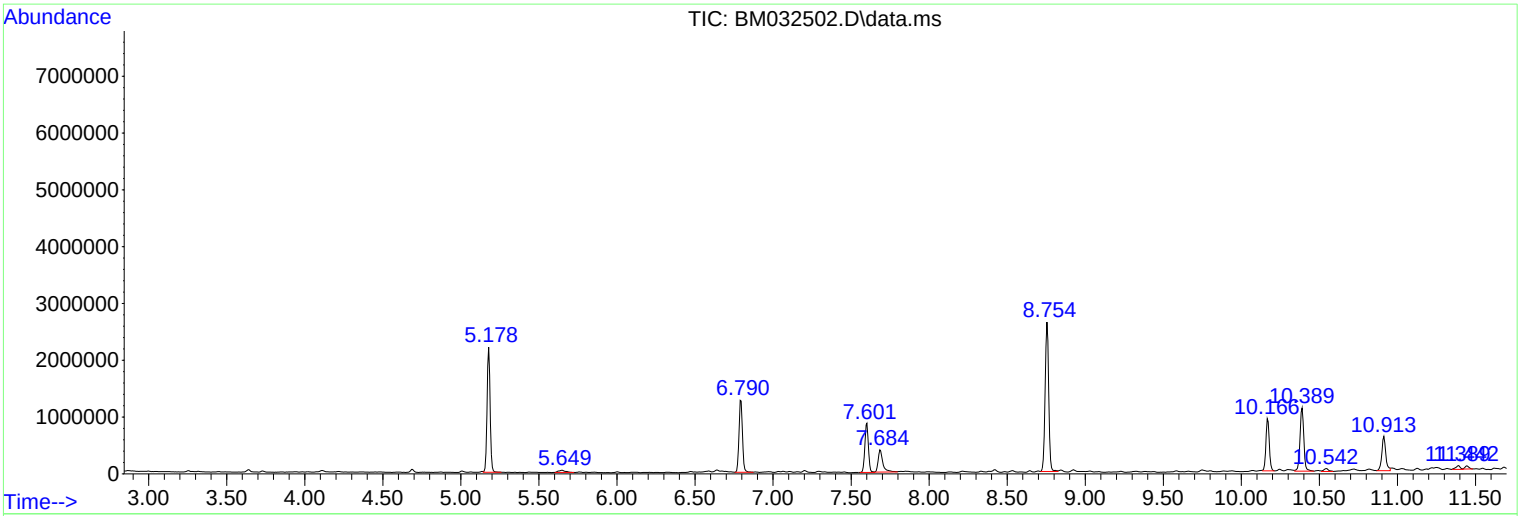
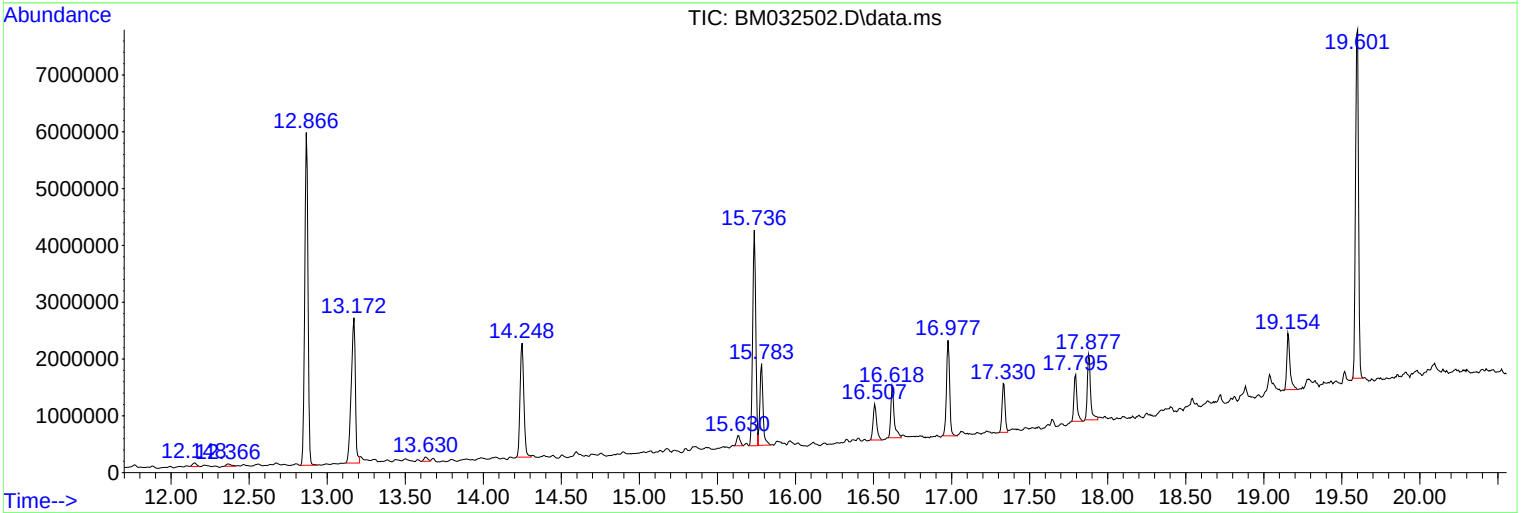
Misc :
ALS Vial : 17 Sample Multiplier: 1

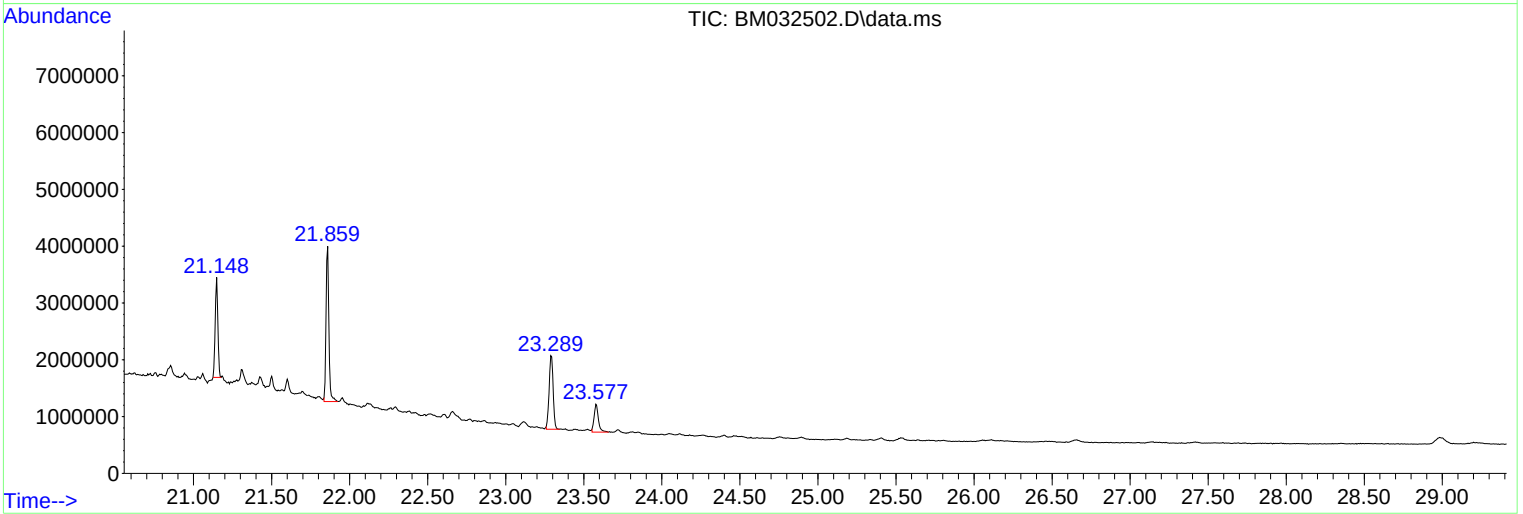
Instrument :
BNA_M
ClientSampleId :
2186-2187

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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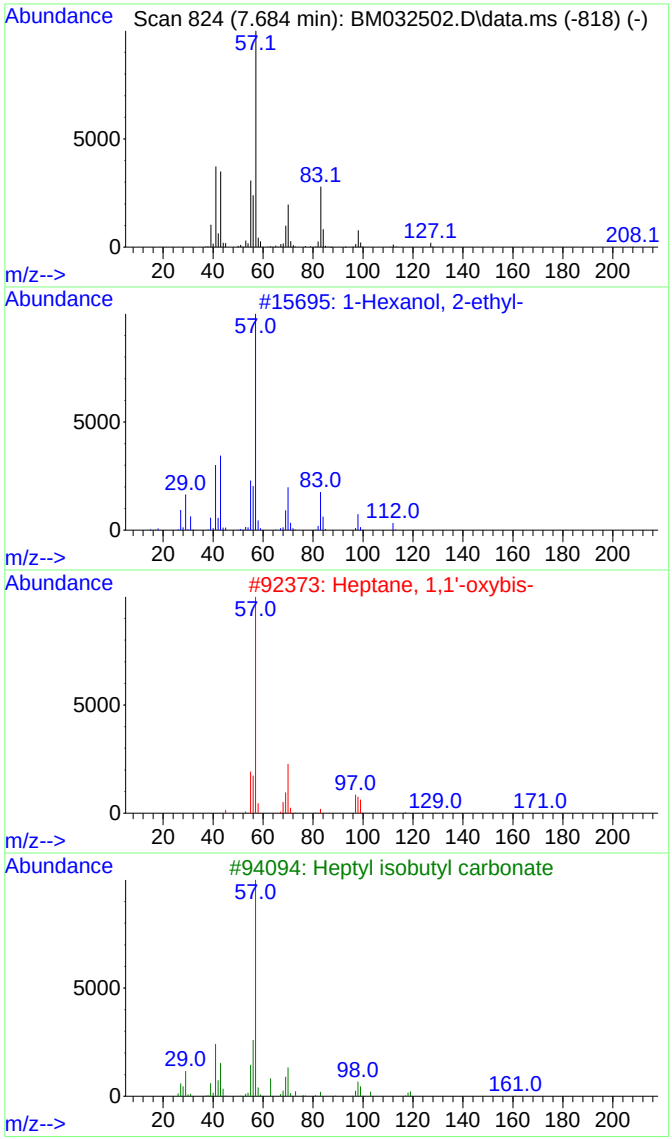
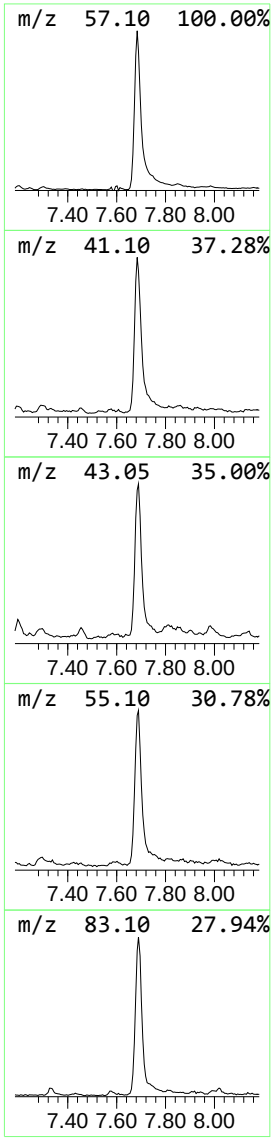
****

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.684	11.89 ng	812302	1,4-Dichlorobenzene-d4	7.601

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	42
4	Methanamine, N-heptylidene-	127	C8H17N	006898-71-1	38
5	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	38





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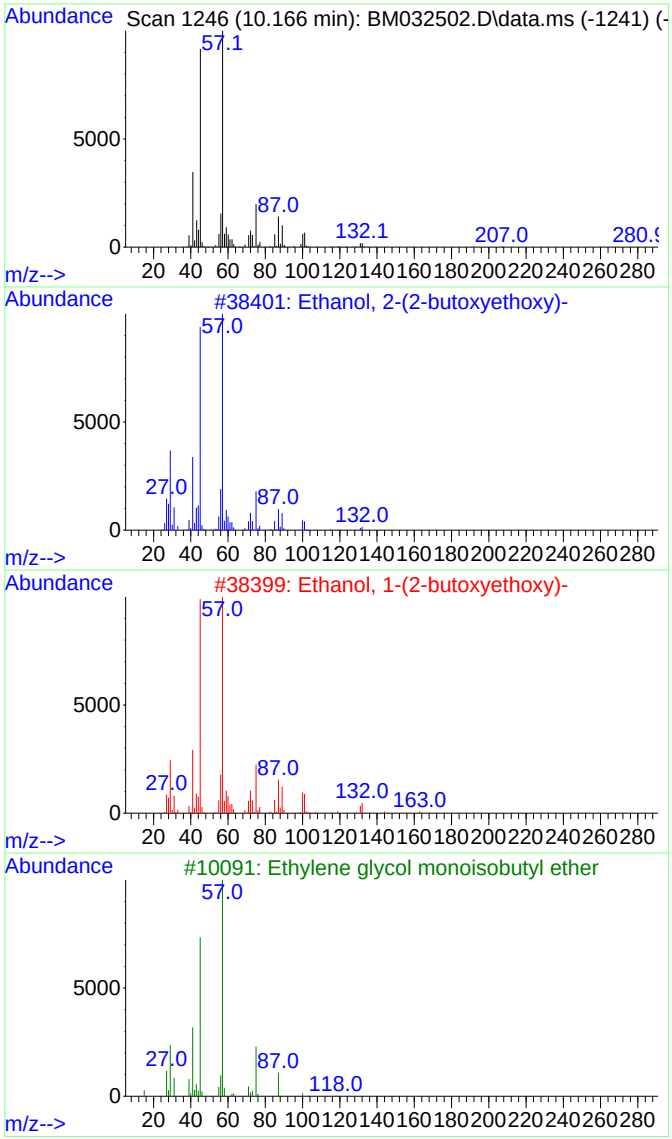
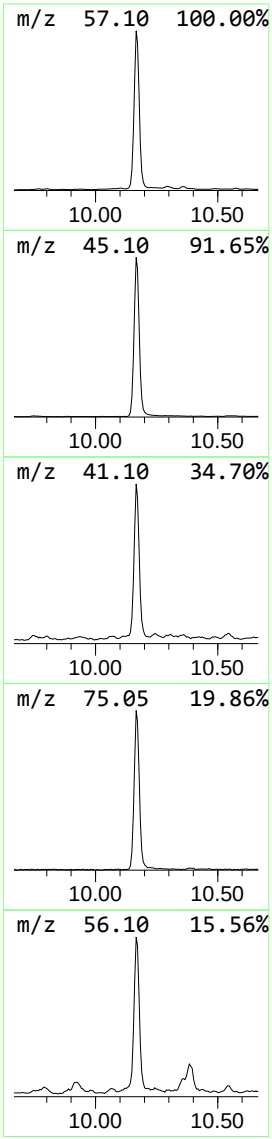
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.166	14.57 ng	1370160	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52





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Sample : M4142-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2186-2187

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
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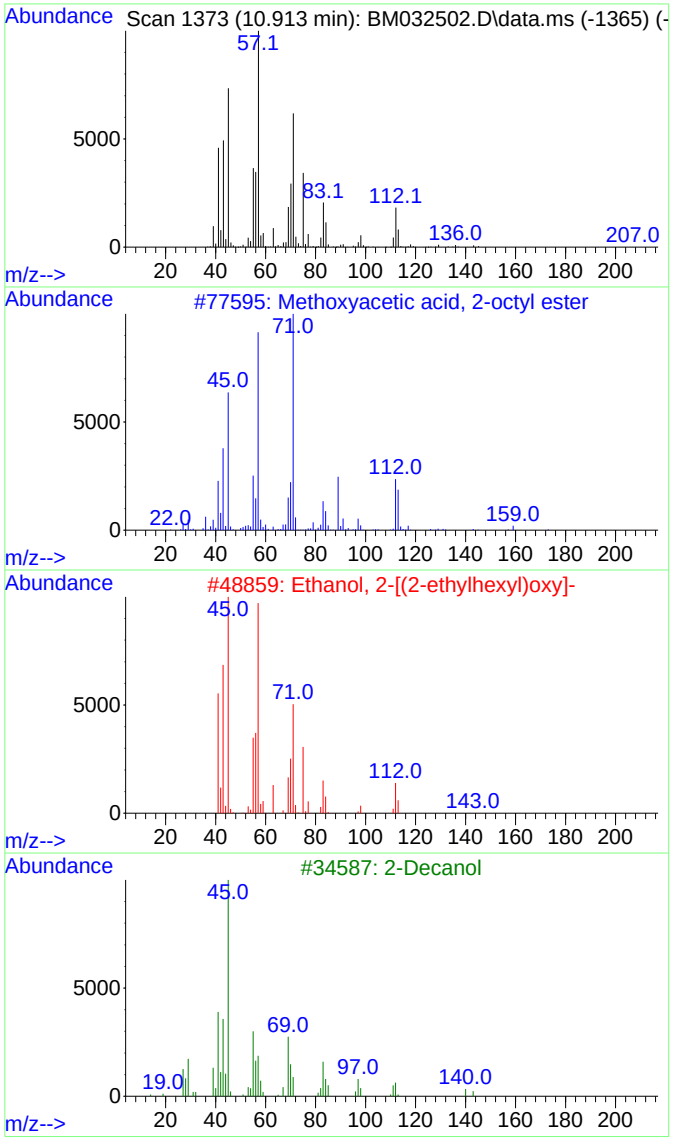
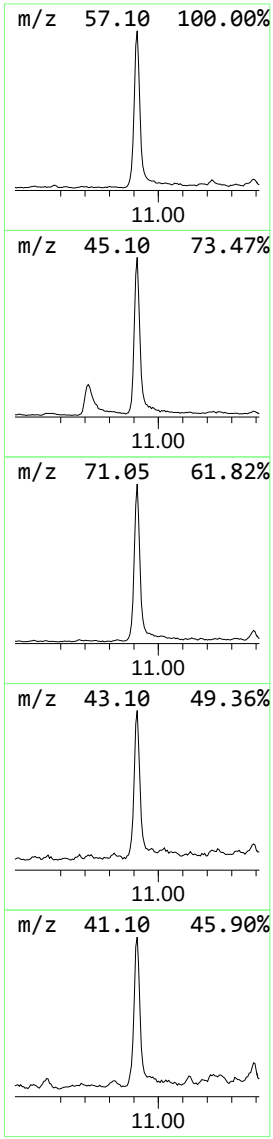
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Methoxyacetic acid, 2-octyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.913	11.25 ng	1058150	Naphthalene-d8	10.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 2-octyl ester	202	C11H22O3	1000282-69-6	50
2	Ethanol, 2-[(2-ethylhexyl)oxy]-	174	C10H22O2	001559-35-9	50
3	2-Decanol	158	C10H22O	001120-06-5	47
4	Methoxyacetic acid, 2-ethylhexyl...	202	C11H22O3	1000282-41-4	43
5	Isoamyl lactate	160	C8H16O3	019329-89-6	43





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Instrument : BNA_M
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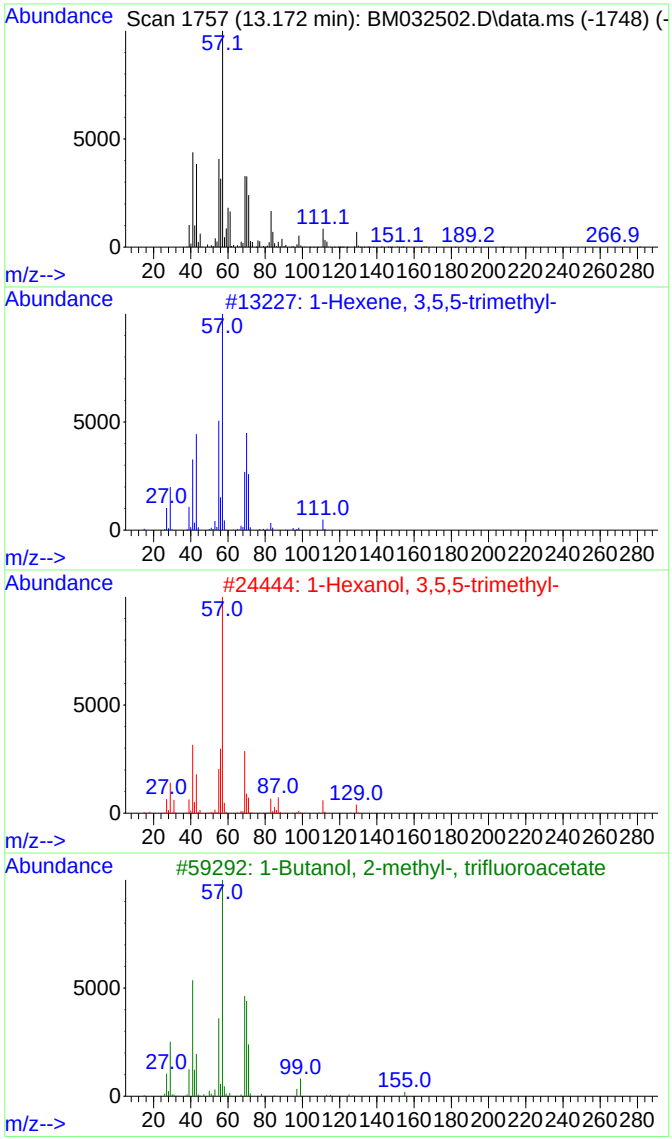
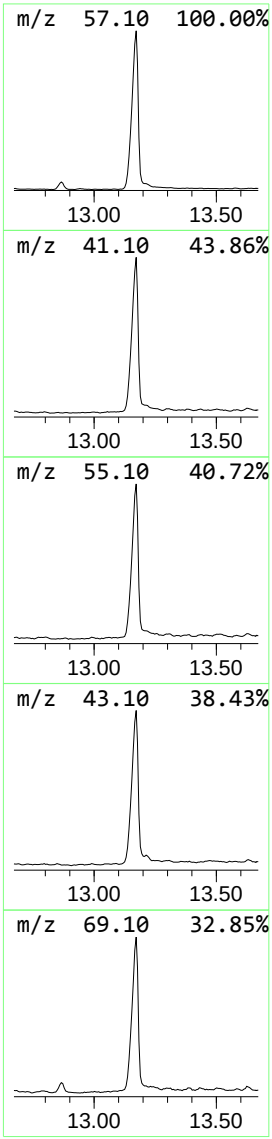
Peak Number 4 unknown13.172 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.172	27.92 ng	4712180	Acenaphthene-d10	14.248

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene, 3,5,5-trimethyl-	126	C9H18	004316-65-8	47
2	1-Hexanol, 3,5,5-trimethyl-	144	C9H20O	003452-97-9	43
3	1-Butanol, 2-methyl-, trifluoroa...	184	C7H11F3O2	340034-47-1	43
4	1-Butoxy-2-ethylhexane	186	C12H26O	062625-25-6	43
5	2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	43





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TIC Library : C:\Database\NIST20.L
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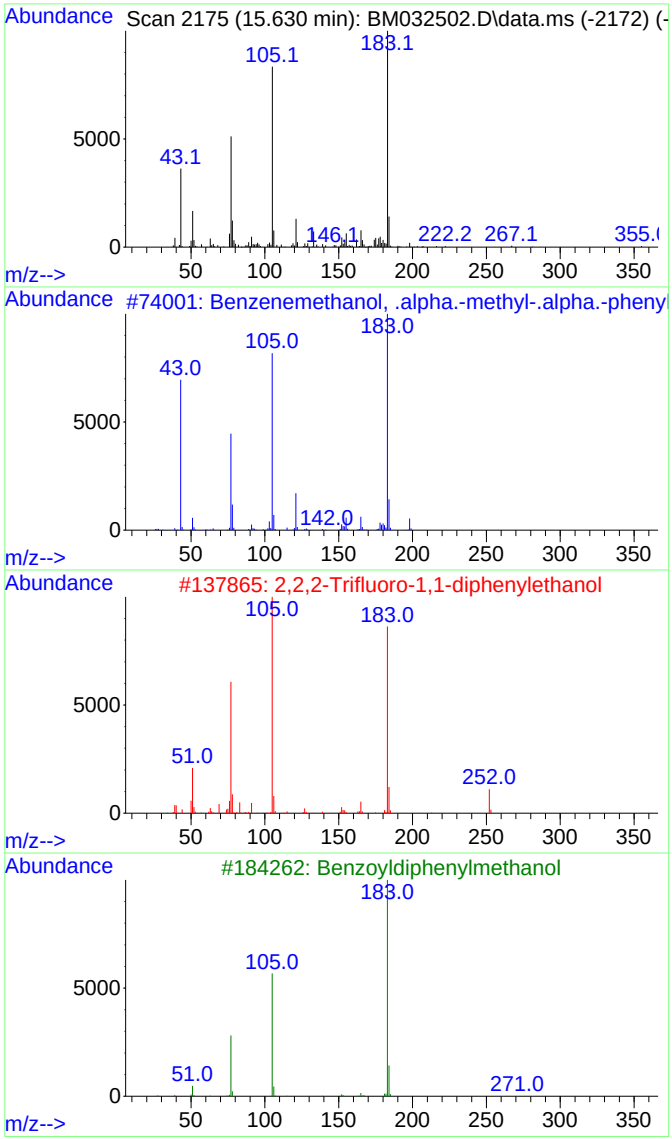
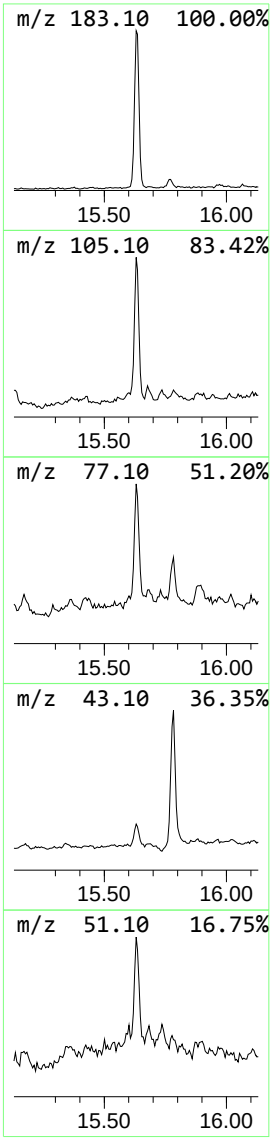
****

Peak Number 5 Benzenemethanol, .alpha.-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.630	2.28 ng	267205	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, .alpha.-methyl-...	198	C14H14O	000599-67-7	80
2	2,2,2-Trifluoro-1,1-diphenylethanol	252	C14H11F3O	000379-18-0	72
3	Benzoyldiphenylmethanol	288	C20H16O2	004237-46-1	64
4	Acetic acid, 2-hydroxy-2,2-diphe...	346	C22H18O4	102706-04-7	64
5	Benzenemethanol, .alpha.-[3-(met...	270	C17H18OS	053634-88-1	53





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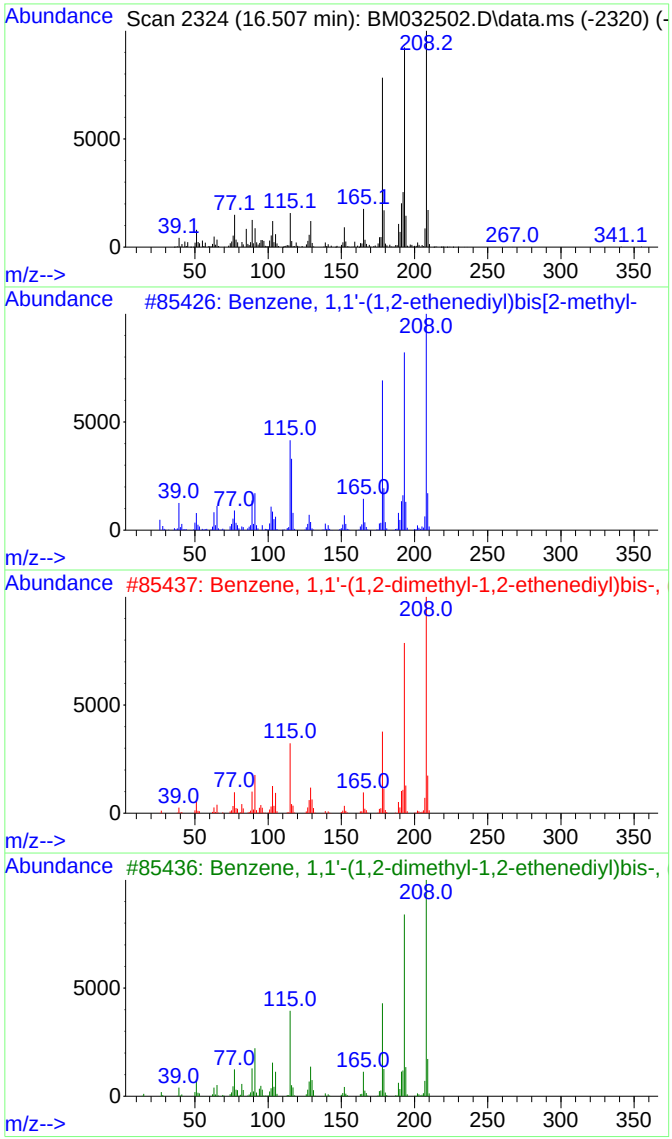
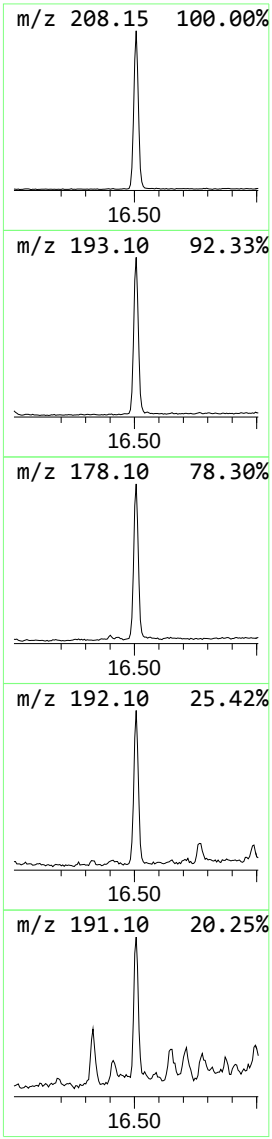
****
Peak Number 6 Benzene, 1,1'-(1,2-ethenedi... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.507	8.44 ng	988359	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,2-ethenediyl)bi...	208	C16H16	010311-74-7	93
2	Benzene, 1,1'-(1,2-dimethyl-1,2-...	208	C16H16	000782-06-9	89
3	Benzene, 1,1'-(1,2-dimethyl-1,2-...	208	C16H16	000782-05-8	86
4	3-(2-Methoxyethyl)-1H,4H,5H,6H,7...	208	C12H20N2O	1000436-13-7	70
5	1,2,5,6-Tetramethylacenaphthylene	208	C16H16	132118-73-1	52





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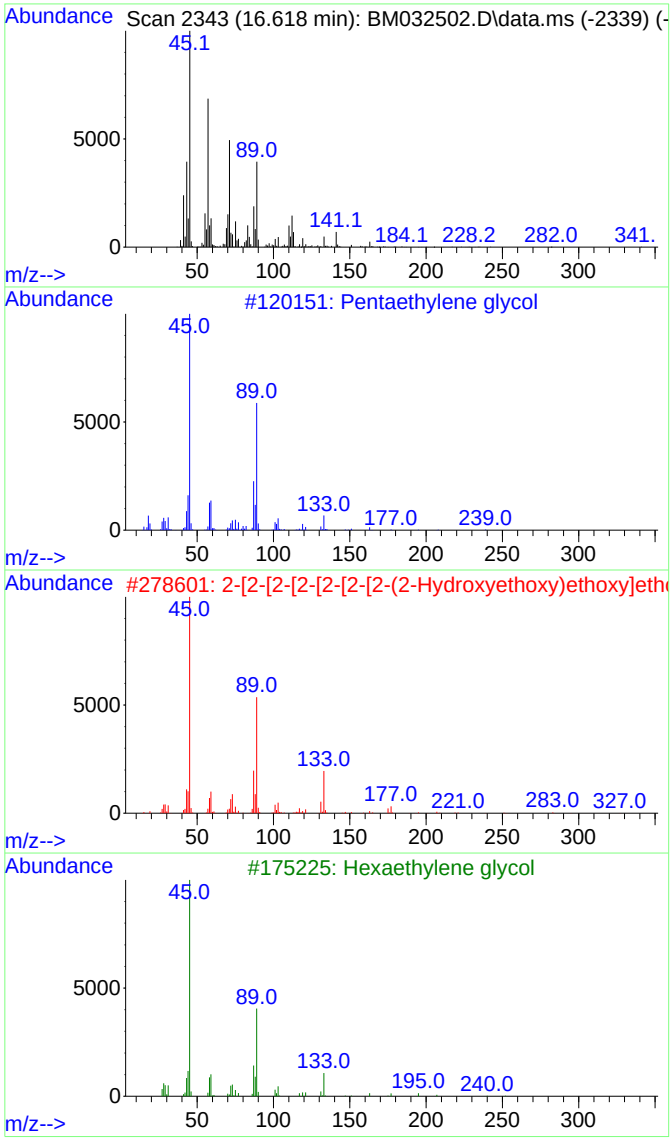
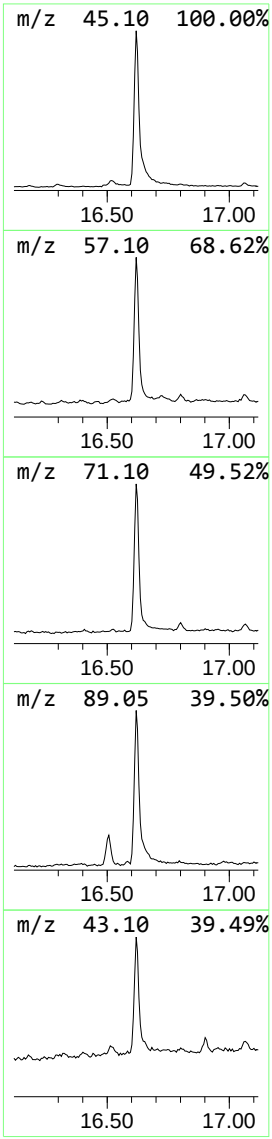
****

Peak Number 7 Pentaethylene glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.618	11.81 ng	1383520	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	62
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	52
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	52
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	52
5	Diisopropyl ether	102	C6H14O	000108-20-3	38





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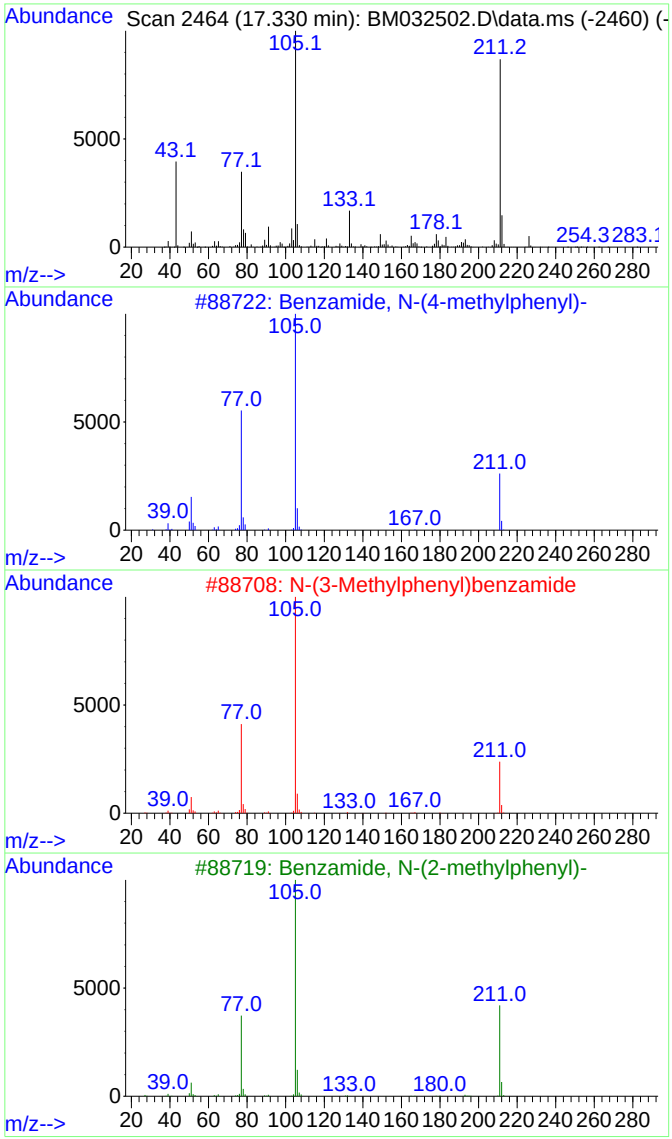
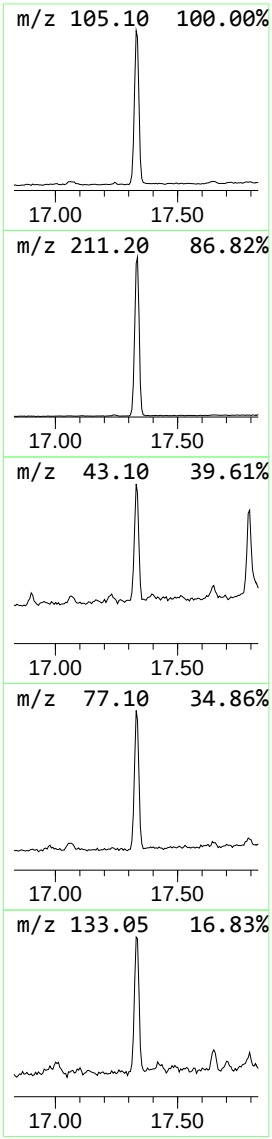
****
Peak Number 8 Benzamide, N-(4-methylphenyl)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.330	9.86 ng	1155390	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzamide, N-(4-methylphenyl)-	211	C14H13NO	000582-78-5	83
2	N-(3-Methylphenyl)benzamide	211	C14H13NO	000582-77-4	83
3	Benzamide, N-(2-methylphenyl)-	211	C14H13NO	000584-70-3	83
4	N-Benzylbenzamide	211	C14H13NO	001485-70-7	81
5	Benzamide, N-methyl-N-phenyl-	211	C14H13NO	001934-92-5	80





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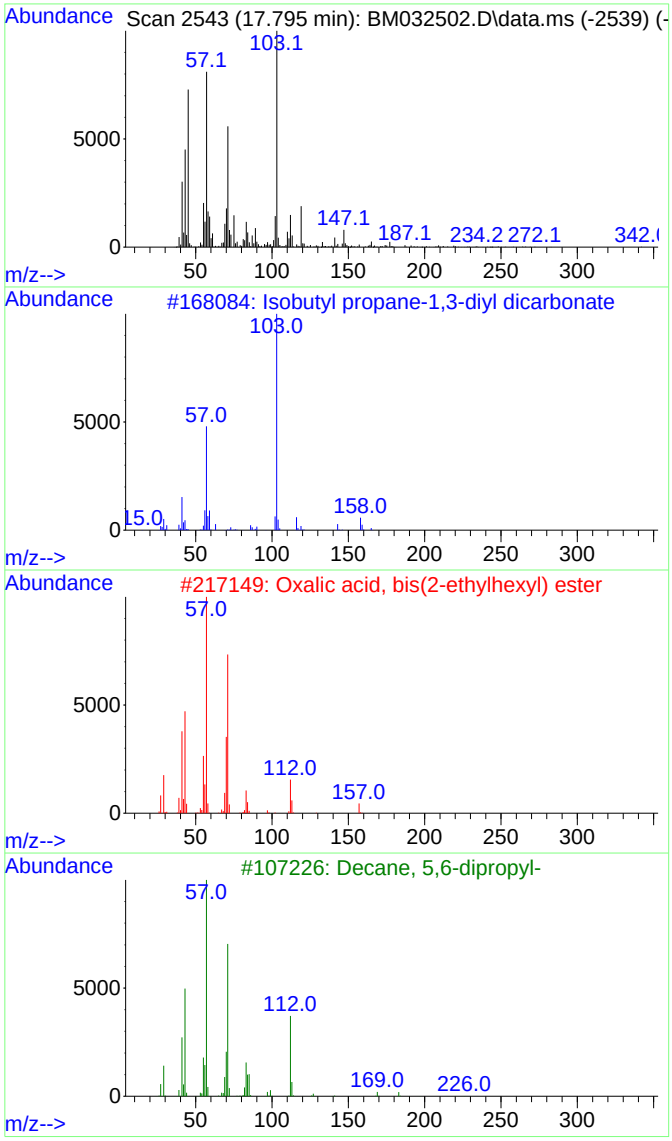
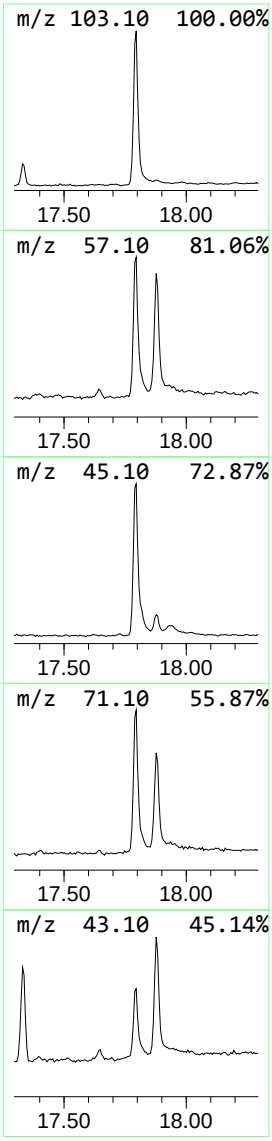
Peak Number 9 unknown17.795 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.795	9.45 ng	1107720	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl propane-1,3-diyl dicarb...	276	C13H24O6	1010373-68-1	38
2	Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	18
3	Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	15
4	Heptane, 3-[(ethenyloxy)methyl]-	156	C10H20O	000103-44-6	15
5	Oxalic acid, 2-ethylhexyl tetrad...	398	C24H46O4	1000309-39-7	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032502.D
Acq On : 13 Oct 2021 18:52
Operator : CG/JU
Sample : M4142-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
2186-2187

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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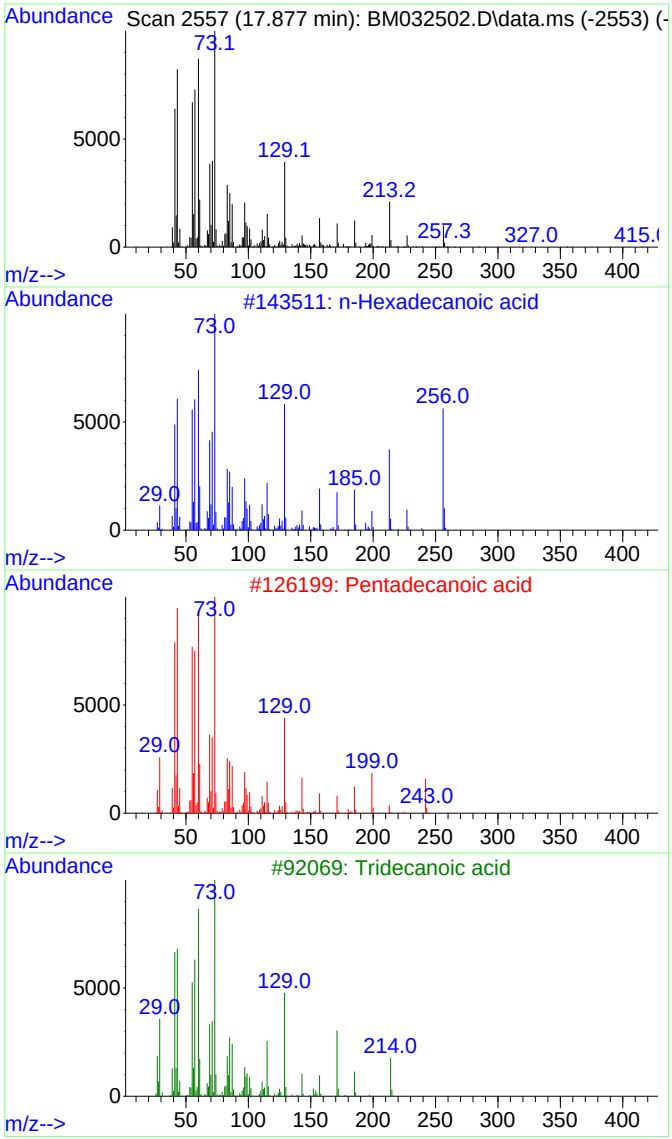
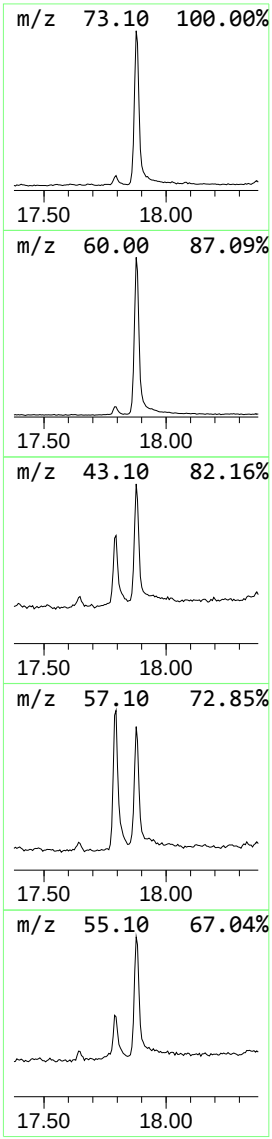
Peak Number 10 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.877	14.28 ng	1673700	Phenanthrene-d10	16.977

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	70





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Data File : BM032502.D
Acq On : 13 Oct 2021 18:52
Operator : CG/JU
Sample : M4142-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2186-2187

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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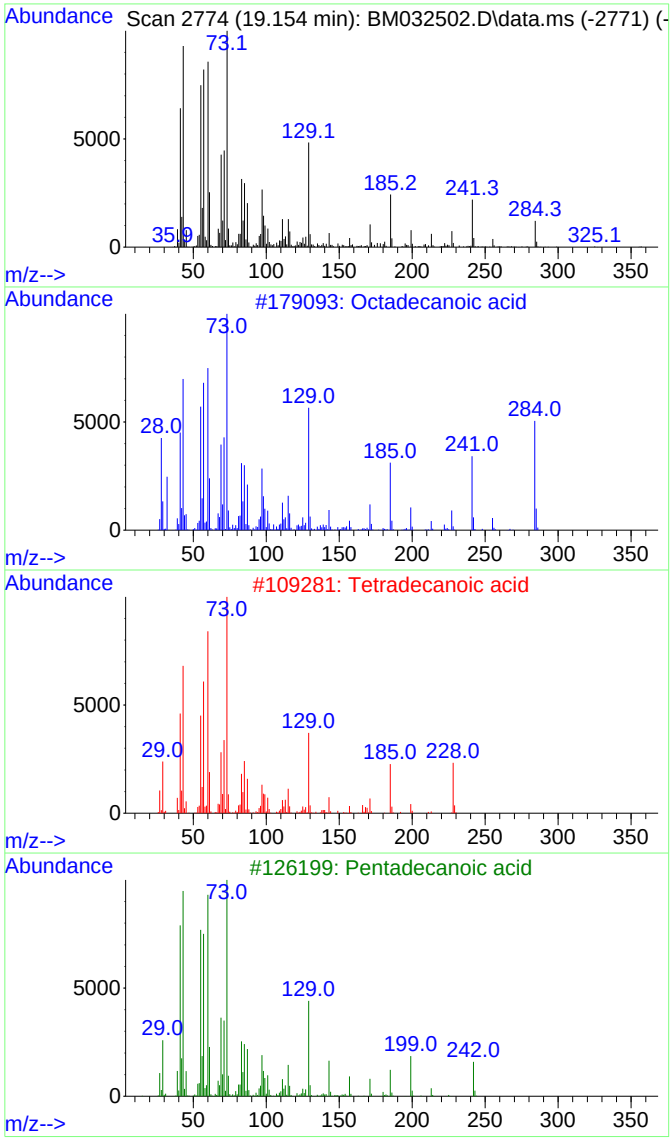
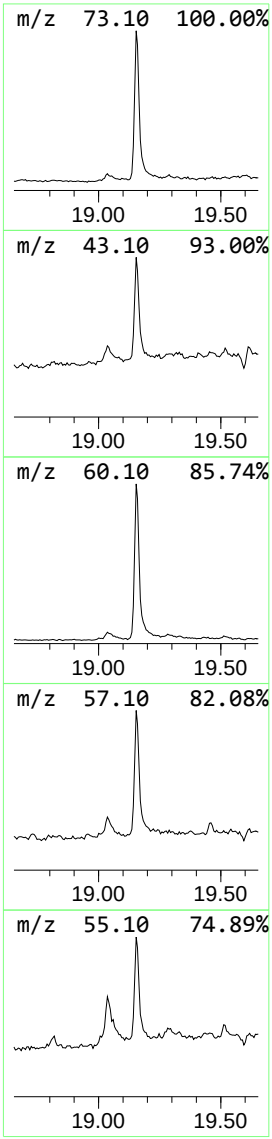
Peak Number 11 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.154	13.51 ng	1402510	Chrysene-d12	21.148

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Data File : BM032502.D
Acq On : 13 Oct 2021 18:52
Operator : CG/JU
Sample : M4142-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2186-2187

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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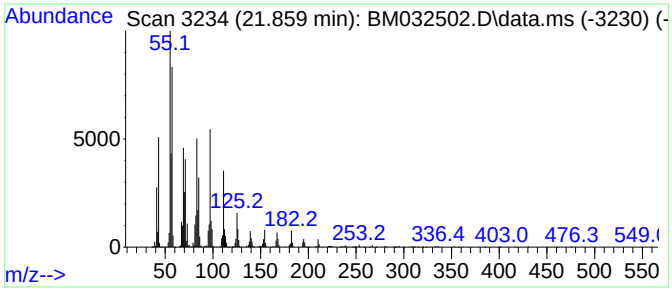
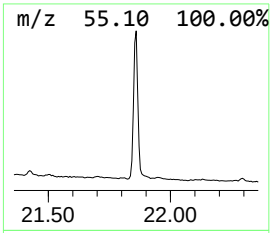
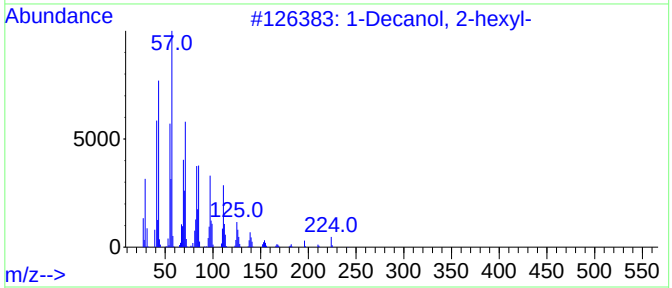
Peak Number 12 1-Decanol, 2-hexyl- Concentration Rank 1

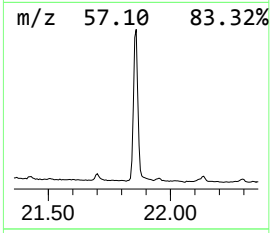
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.859	33.63 ng	3492590	Chrysene-d12	21.148

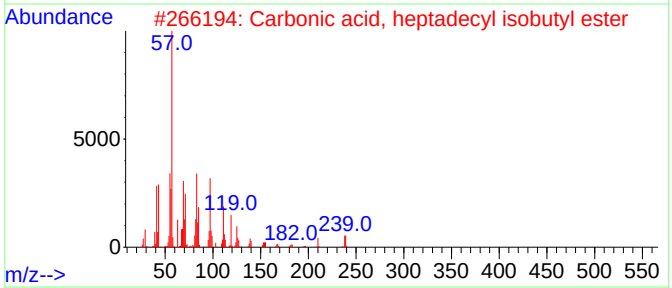
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	92
2	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87

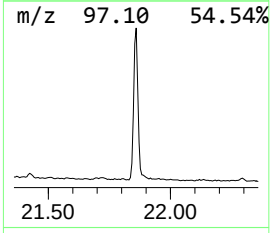


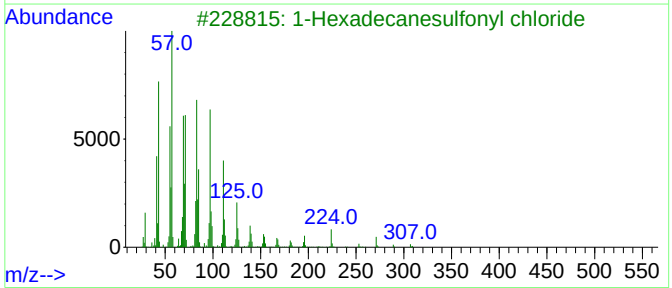


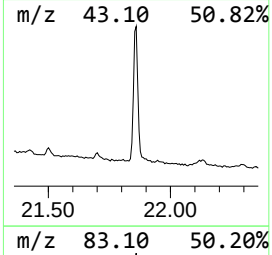


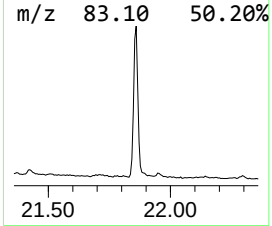












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Data File : BM032502.D
Acq On : 13 Oct 2021 18:52
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Instrument :
BNA_M
ClientSampleId :
2186-2187

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

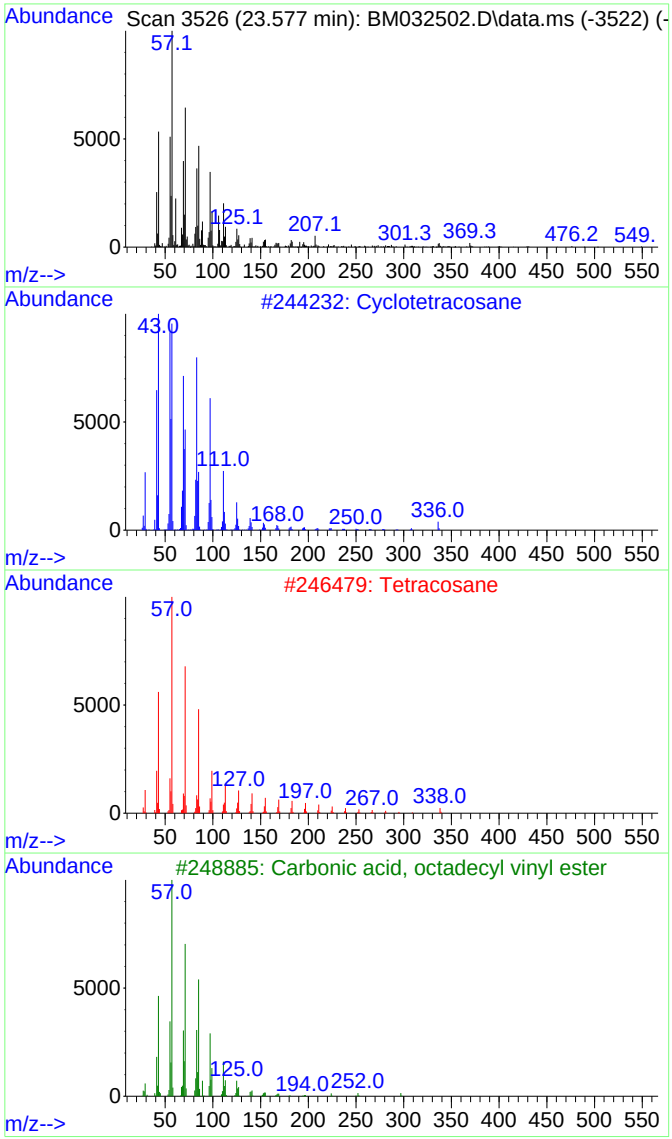
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

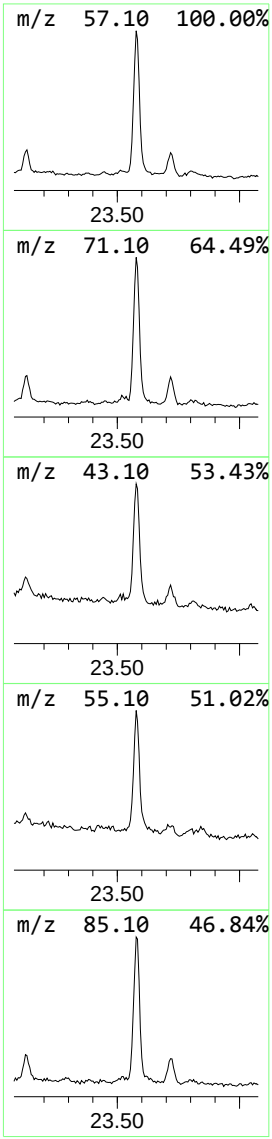
****

Peak Number 13 Cyclotetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.577	7.89 ng	912161	Perylene-d12	23.289

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	90
2	Tetracosane	338	C24H50	000646-31-1	89
3	Carbonic acid, octadecyl vinyl e...	340	C21H40O3	1000382-54-4	81
4	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	76
5	Isobutyl tetracosyl ether	410	C28H58O	1000406-33-2	76





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032502.D
Acq On : 13 Oct 2021 18:52
Operator : CG/JU
Sample : M4142-04
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 2186-2187

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Hexanol, 2-et...	7.684	11.9	ng	812302	1	7.601	1366250	20.0
Ethanol, 2-(2-b...	10.166	14.6	ng	1370160	2	10.389	1880700	20.0
Methoxyacetic a...	10.913	11.3	ng	1058150	2	10.389	1880700	20.0
unknown13.172	13.172	27.9	ng	4712180	3	14.248	3375440	20.0
Benzenemethanol...	15.630	2.3	ng	267205	4	16.977	2343420	20.0
Benzene, 1,1'-(...	16.507	8.4	ng	988359	4	16.977	2343420	20.0
Pentaethylene g...	16.618	11.8	ng	1383520	4	16.977	2343420	20.0
Benzamide, N-(4...	17.330	9.9	ng	1155390	4	16.977	2343420	20.0
unknown17.795	17.795	9.4	ng	1107720	4	16.977	2343420	20.0
n-Hexadecanoic ...	17.877	14.3	ng	1673700	4	16.977	2343420	20.0
Octadecanoic acid	19.154	13.5	ng	1402510	5	21.148	2076930	20.0
1-Decanol, 2-he...	21.859	33.6	ng	3492590	5	21.148	2076930	20.0
Cyclotetracosane	23.577	7.9	ng	912161	6	23.289	2312760	20.0