LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031621\
Data File : BM029155.D
Acq On : 16 Mar 2021 19:06
Operator : CG/JU
Sample : M1677-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D2470-D2800(WATER)

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-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.093	353	358	365	rBB	45719	62802	7.48%	1.632%
2	5.199	371	376	377	rBV	60324	70482	8.40%	1.832%
3	5.228	377	381	392	rVB	160976	307208	36.61%	7.983%
4	5.599	438	444	452	rBB	111155	160050	19.07%	4.159%
5	5.693	456	460	467	rBB	6098	8640	1.03%	0.225%
6	6.728	630	636	642	rBV	6714	11679	1.39%	0.303%
7	6.828	648	653	663	rBB	36007	63316	7.54%	1.645%
8	7.610	781	786	793	rBB	31036	43991	5.24%	1.143%
9	7.681	793	798	807	rBB	16244	23134	2.76%	0.601%
10	7.928	834	840	847	rBB	128196	197988	23.59%	5.145%
11	8.787	980	986	993	rBV	109287	170575	20.33%	4.433%
12	8.981	1009	1019	1025	rBB	17174	37344	4.45%	0.970%
13	9.804	1149	1159	1171	rBB5	10326	19186	2.29%	0.499%
14	10.398	1254	1260	1266	rBV	39921	61391	7.32%	1.595%
15	12.892	1678	1684	1693	rBV	276954	389133	46.37%	10.112%
16	13.228	1736	1741	1747	rBV	28506	42527	5.07%	1.105%
17	14.263	1911	1917	1926	rVB2	205991	330543	39.39%	8.590%
18	15.786	2166	2176	2186	rBB	195280	263861	31.44%	6.857%
19	17.033	2382	2388	2393	rBV	81221	107730	12.84%	2.799%
20	17.933	2536	2541	2549	rBV	54223	72292	8.61%	1.879%
21	18.004	2550	2553	2560	rVB3	6292	9485	1.13%	0.246%
22	18.674	2662	2667	2673	rBV	7298	9717	1.16%	0.253%
23	19.215	2755	2759	2768	rBV	26985	38168	4.55%	0.992%
24	19.668	2830	2836	2845	rBV	707267	839224	100.00%	21.808%
25	20.215	2925	2929	2935	rVB2	11096	16727	1.99%	0.435%
26	20.698	3008	3011	3015	rBV3	7788	8589	1.02%	0.223%
27	20.921	3045	3049	3059	rVB	72841	100398	11.96%	2.609%
28	21.027	3064	3067	3071	rVB	9389	10212	1.22%	0.265%
29	21.215	3094	3099	3105	rBV	129463	152361	18.15%	3.959%
30	21.457	3137	3140	3145	rVB2	12440	13392	1.60%	0.348%
31	21.880	3209	3212	3218	rBV4	7014	10661	1.27%	0.277%
32	23.351	3456	3462	3472	rVB2	92431	161019	19.19%	4.184%
33	23.898	3550	3555	3563	rVB4	16076	34381	4.10%	0.893%

Sum of corrected areas: 3848206

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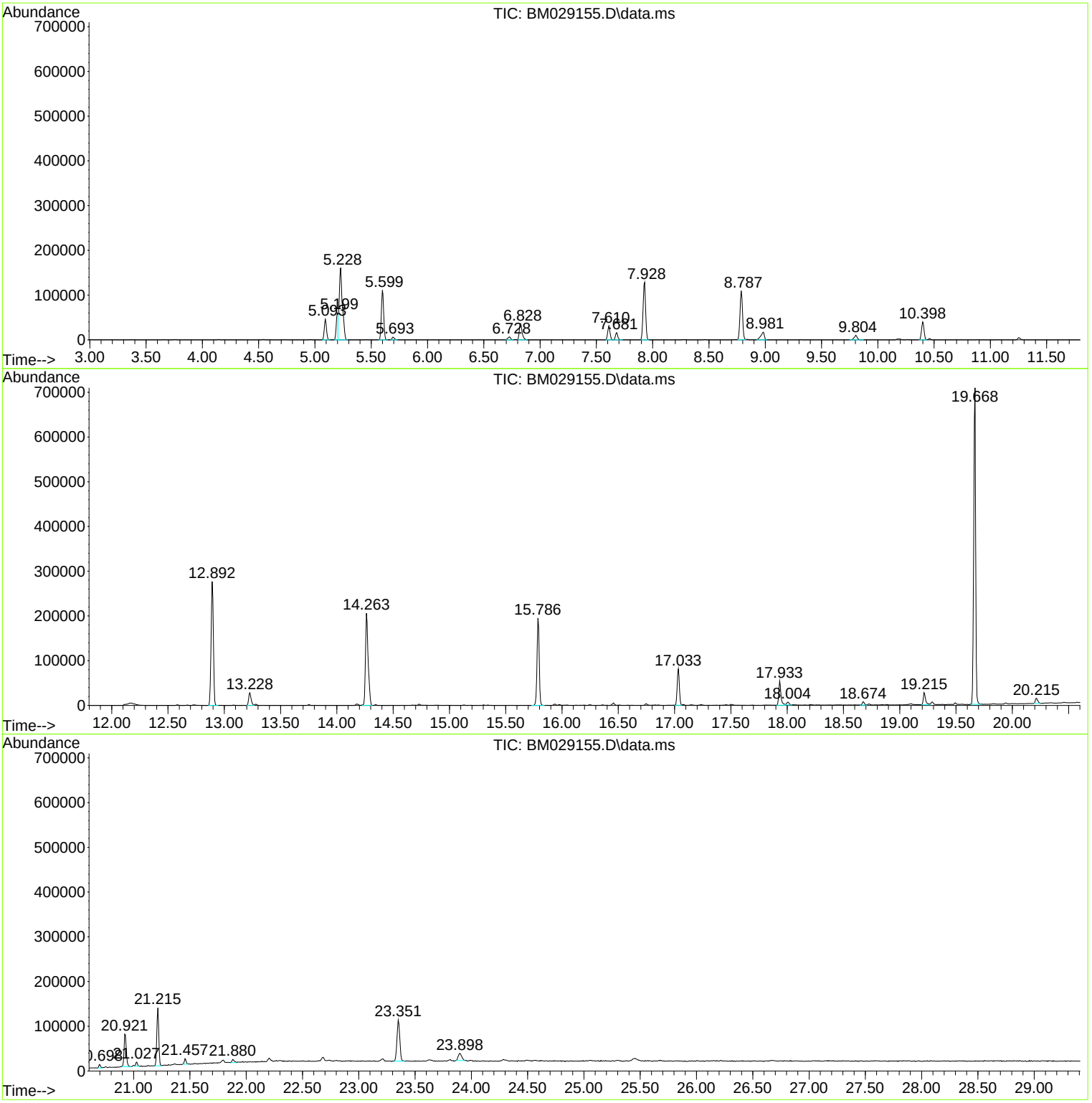
D2470-D2800(WATER)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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TIC Library : C:\DATABASE\NIST11.L
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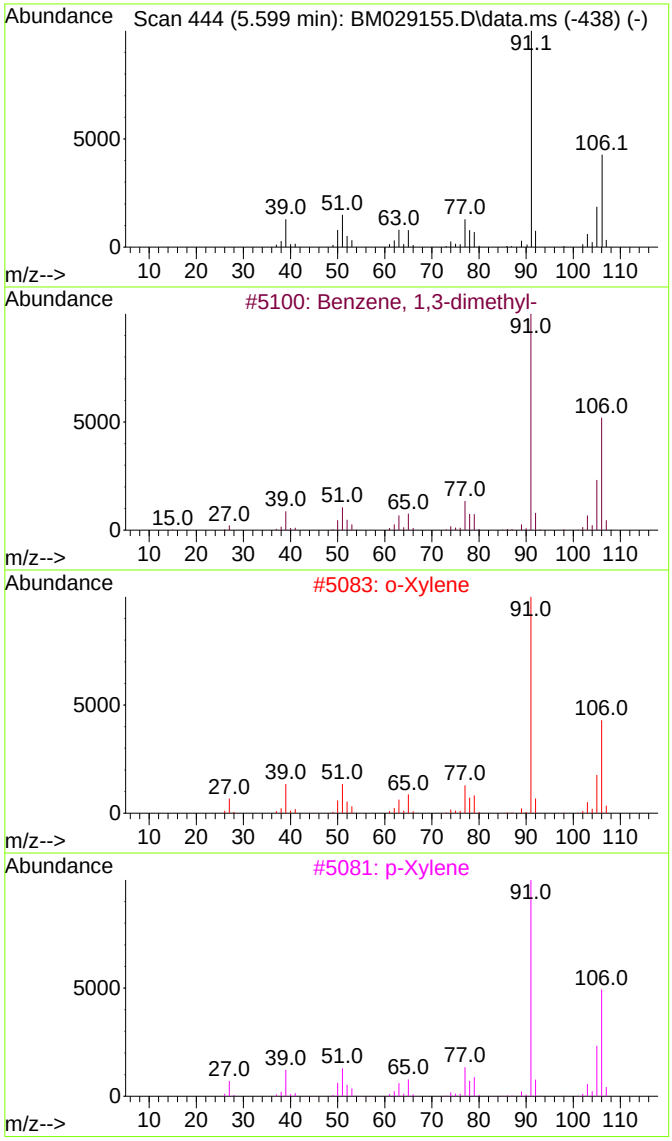
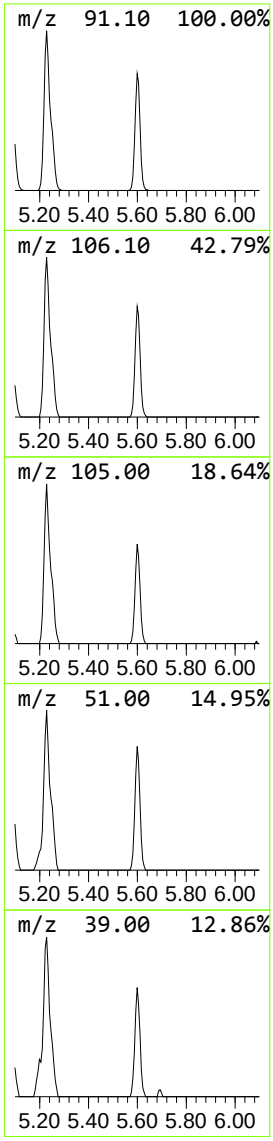
****
Peak Number 2 Benzene, 1,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.599	72.76 ng	160050	1,4-Dichlorobenzene-d4	7.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	97
2	o-Xylene	106	C8H10	000095-47-6	97
3	p-Xylene	106	C8H10	000106-42-3	97
4	Ethylbenzene	106	C8H10	000100-41-4	90
5	1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	76





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Data File : BM029155.D
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Instrument :
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ClientSampleId :
D2470-D2800(WATER)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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TIC Library : C:\DATABASE\NIST11.L
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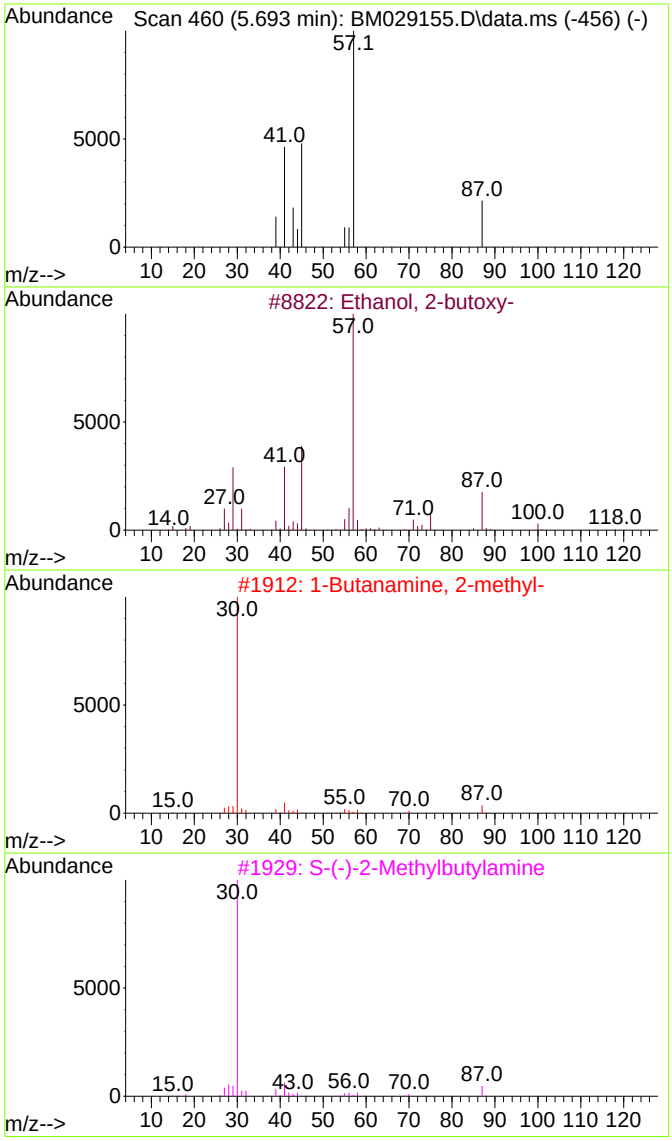
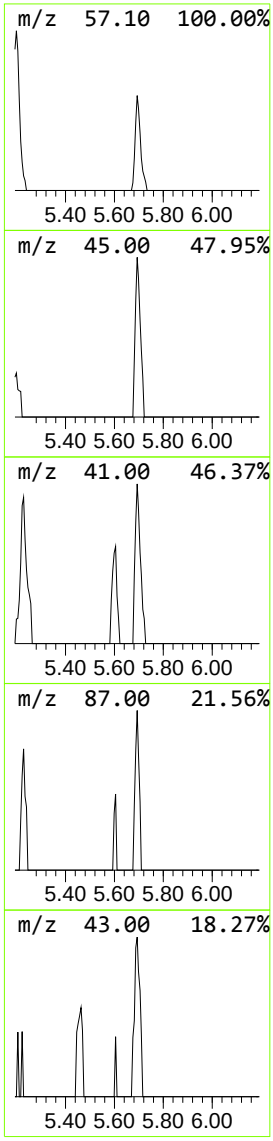
****
Peak Number 3 unknown5.693 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.693	3.93 ng	8640	1,4-Dichlorobenzene-d4	7.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	40
2	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7
3	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	7
4	1-Pentanamine	87	C5H13N	000110-58-7	5
5	Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	4





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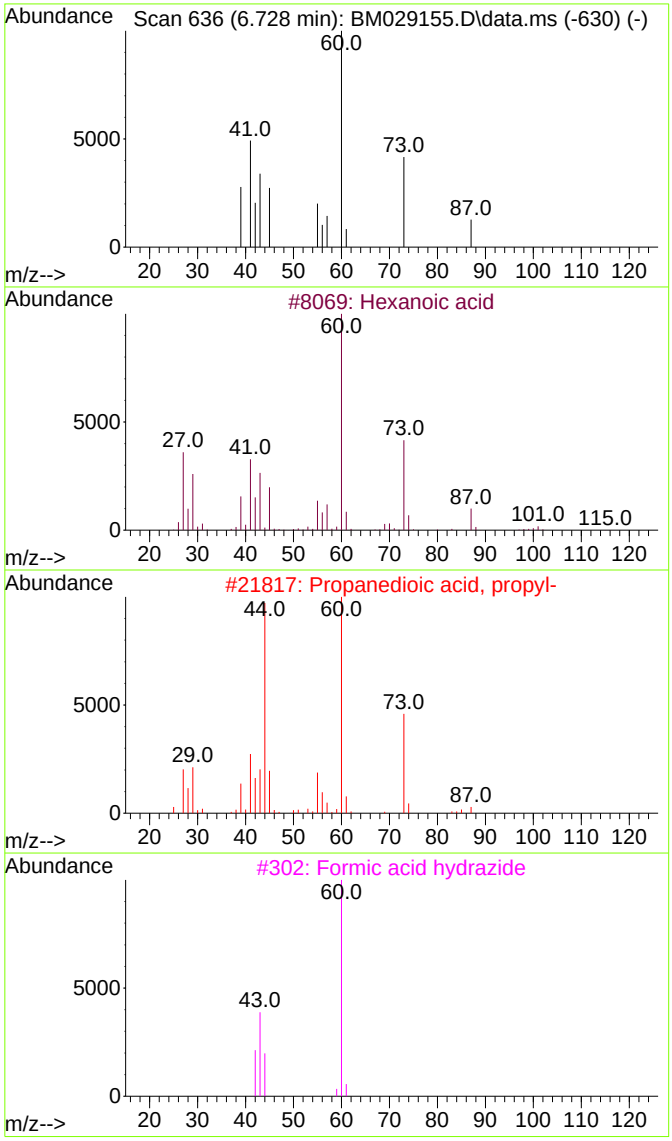
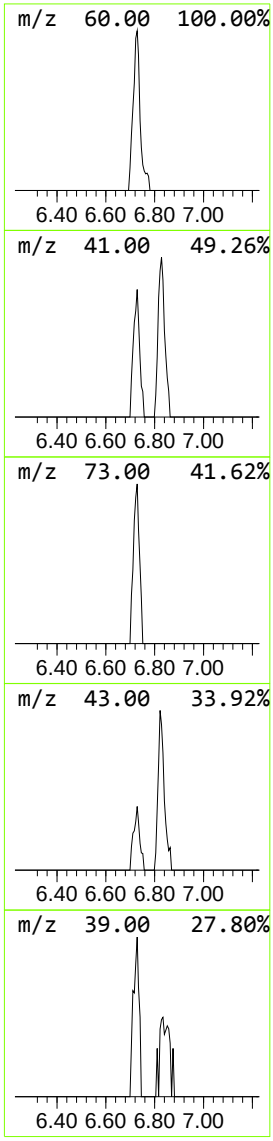
****

Peak Number 4 Hexanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.728	5.31 ng	11679	1,4-Dichlorobenzene-d4	7.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid	116	C6H12O2	000142-62-1	83
2	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	40
3	Formic acid hydrazide	60	CH4N2O	000624-84-0	38
4	Pentanoic acid	102	C5H10O2	000109-52-4	10
5	1-Octanamine	129	C8H19N	000111-86-4	9





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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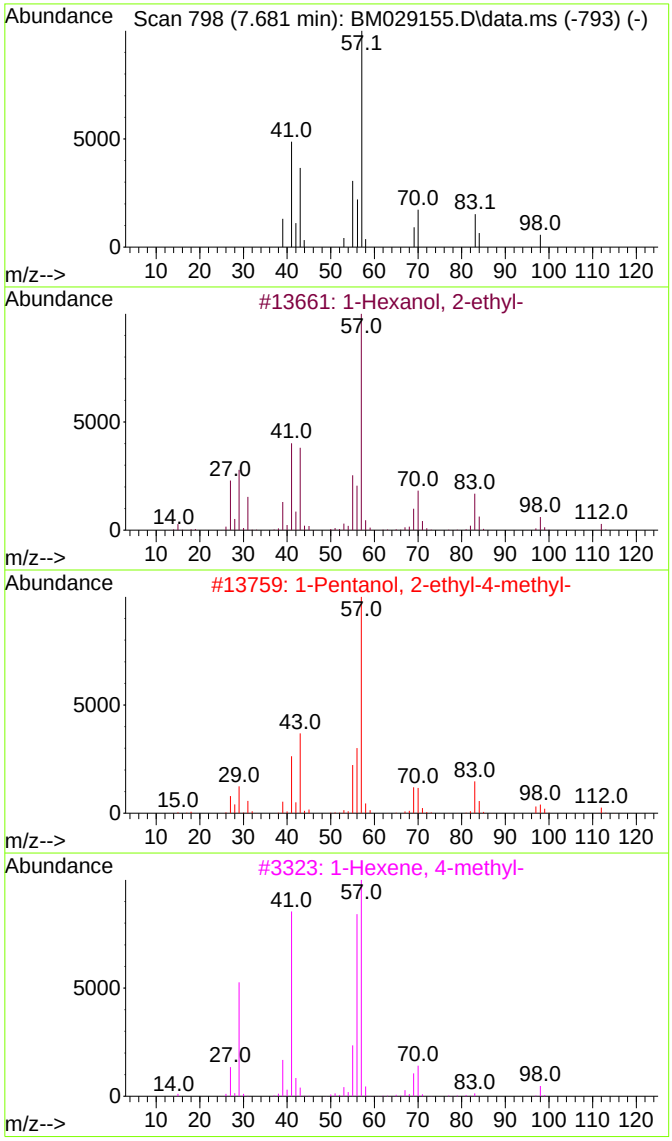
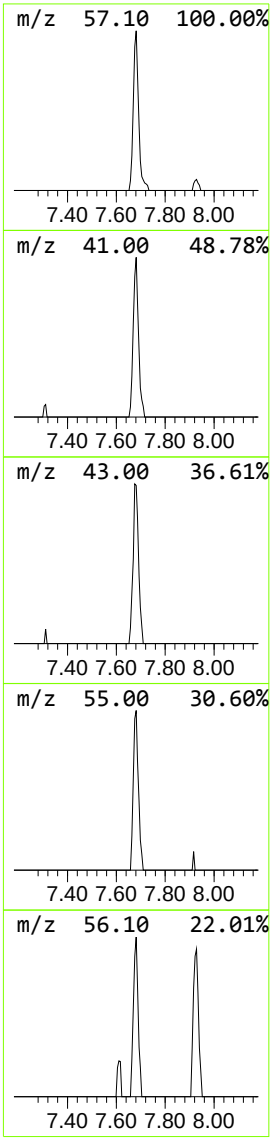
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.681	10.52 ng	23134	1,4-Dichlorobenzene-d4	7.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	72
3	1-Hexene, 4-methyl-	98	C7H14	003769-23-1	47
4	Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	36
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	33





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Instrument :
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ClientSampleId :
D2470-D2800(WATER)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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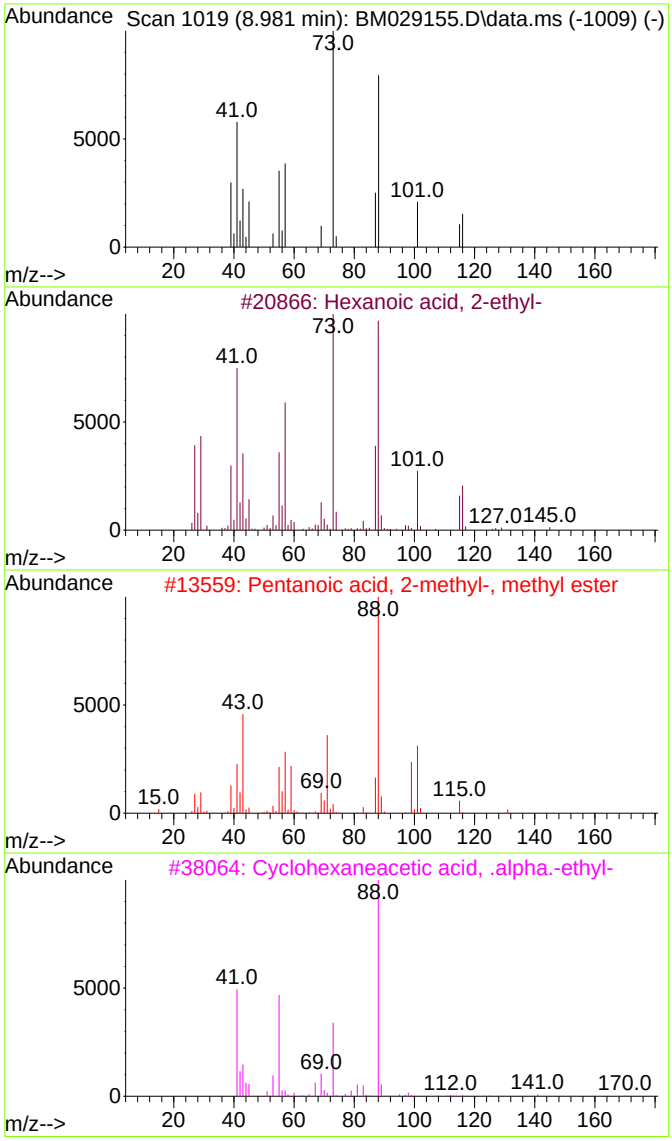
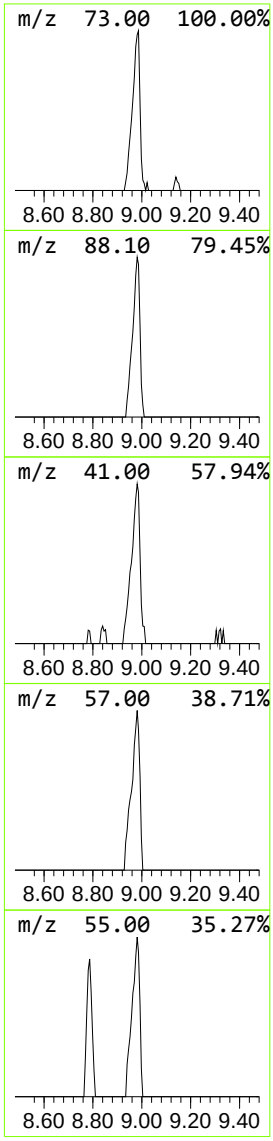
****
Peak Number 7 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.981	16.98 ng	37344	1,4-Dichlorobenzene-d4	7.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2	Pentanoic acid, 2-methyl-, methy...	130	C7H14O2	002177-77-7	33
3	Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	28
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	28
5	3-Heptanol, 3-methyl-	130	C8H18O	005582-81-1	16





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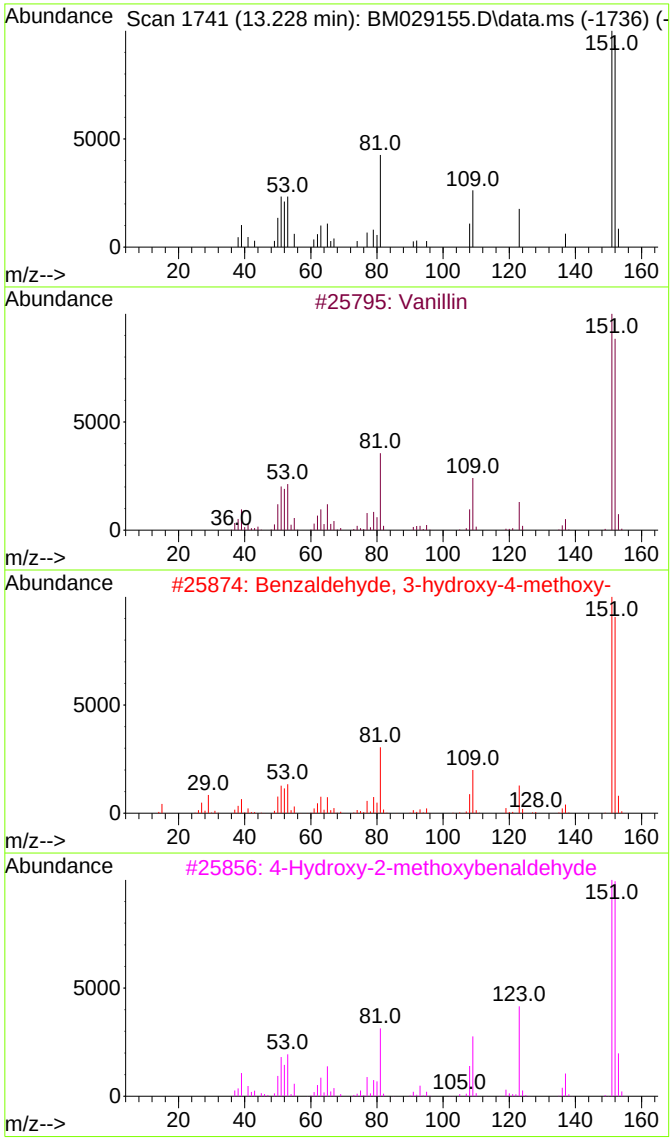
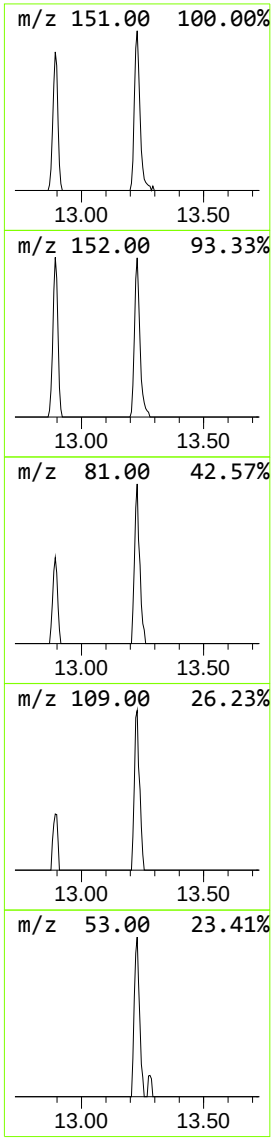
****

Peak Number 8 Vanillin Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.228	2.57 ng	42527	Acenaphthene-d10	14.281

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	97
2	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	94
3	4-Hydroxy-2-methoxybenaldehyde	152	C8H8O3	018278-34-7	53
4	Benzaldehyde, 3-(chloroacetoxy)-...	228	C10H9ClO4	066267-38-7	50
5	7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	49





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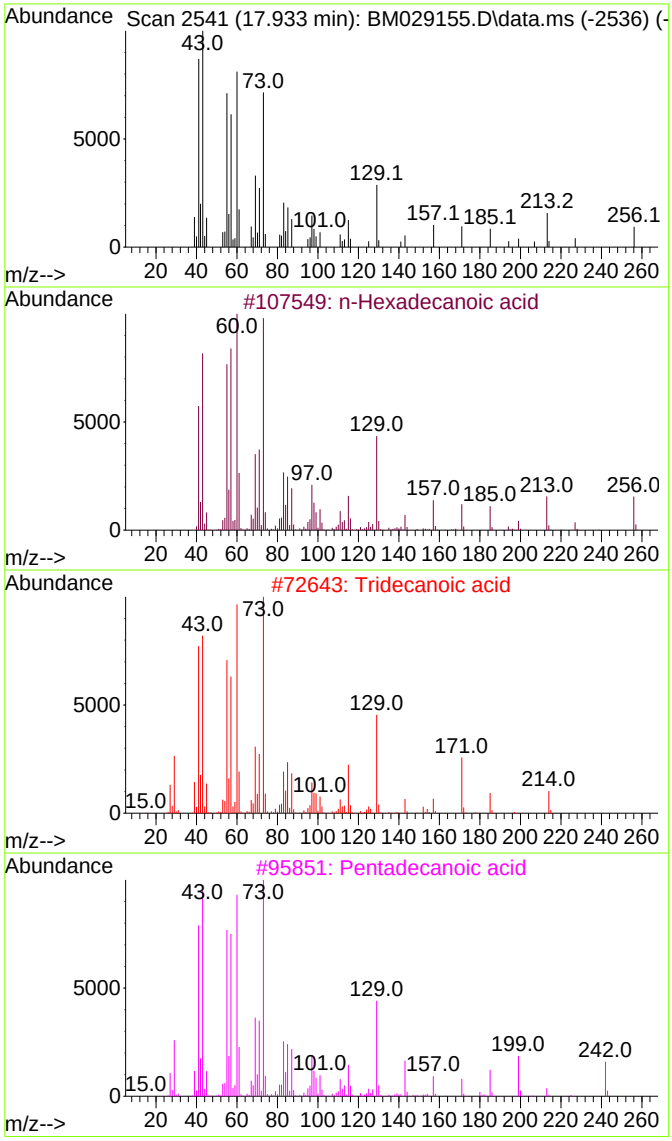
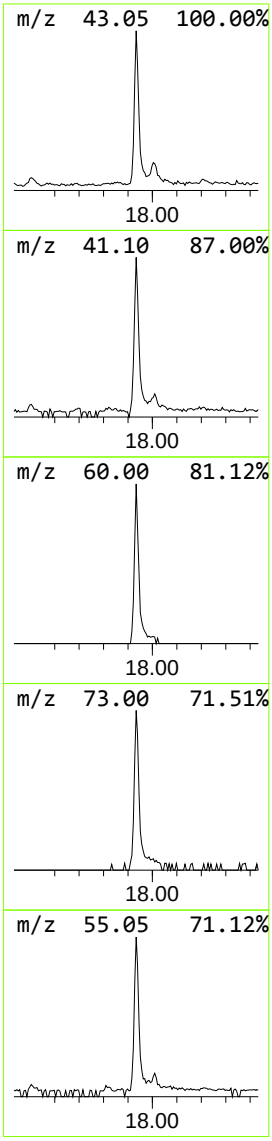
Peak Number 9 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.933	13.42 ng	72292	Phenanthrene-d10	17.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	50





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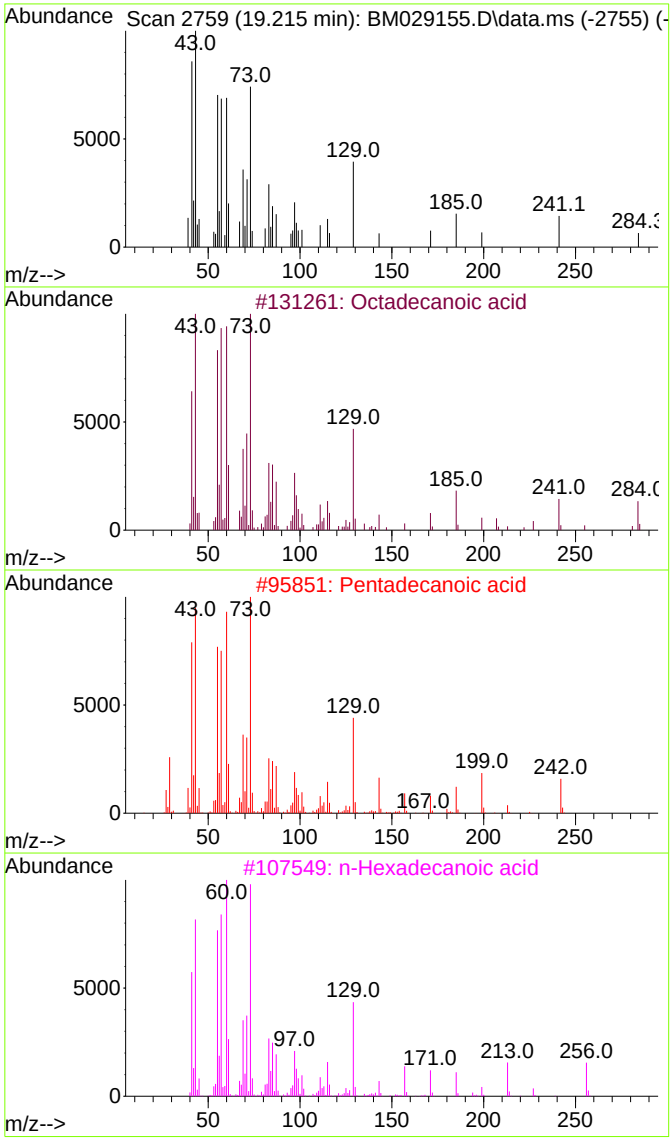
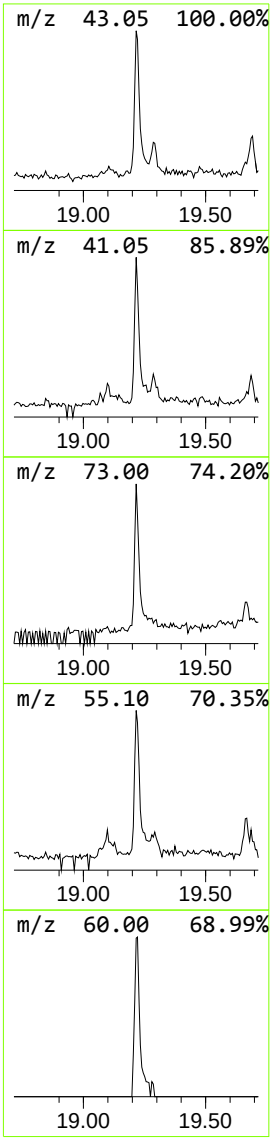
Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.215	5.01 ng	38168	Chrysene-d12	21.215

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





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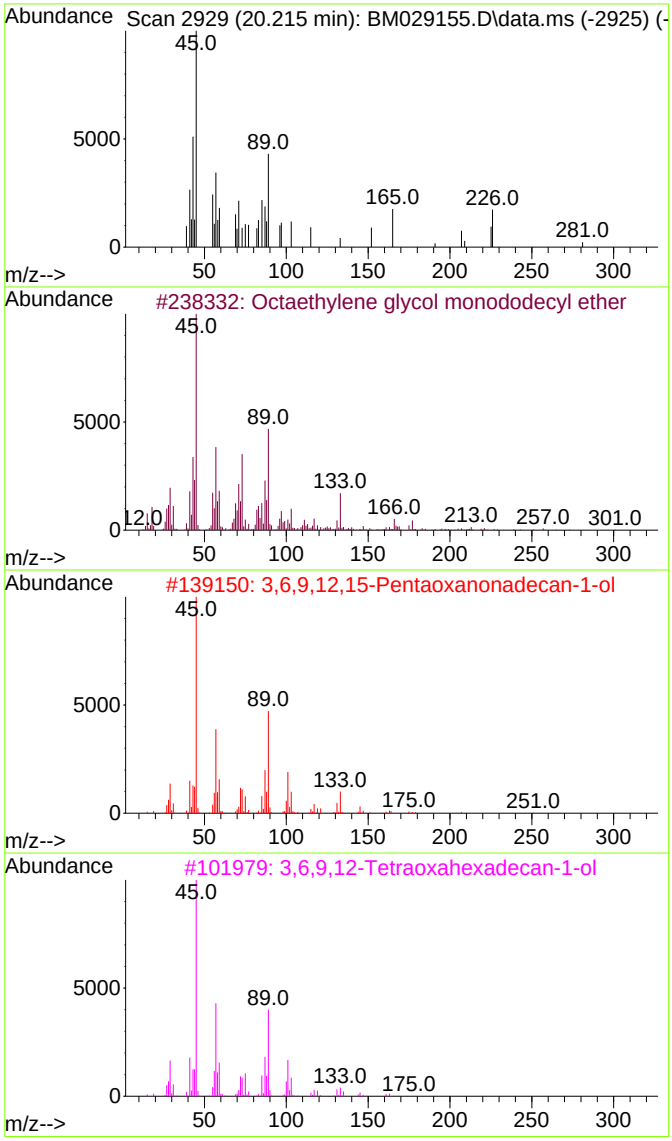
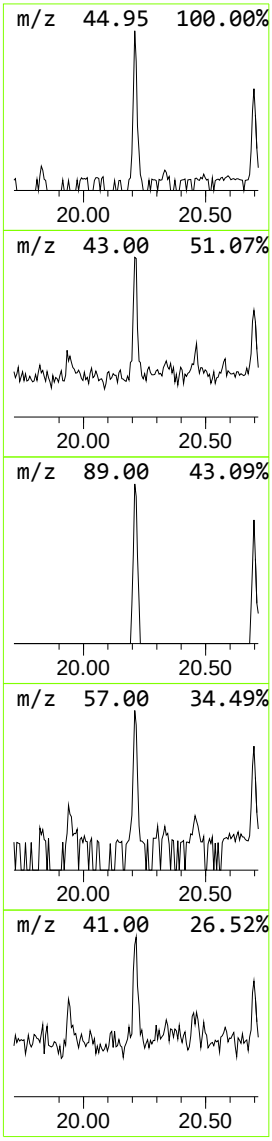
****
Peak Number 11 Octaethylene glycol monodod... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.215	2.20 ng	16727	Chrysene-d12	21.215

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octaethylene glycol monododecyl ...	538	C28H58O9	003055-98-9	53
2	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	52
3	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	52
4	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	50
5	Tetraethylene glycol monododecyl...	362	C20H42O5	005274-68-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031621\
Data File : BM029155.D
Acq On : 16 Mar 2021 19:06
Operator : CG/JU
Sample : M1677-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
D2470-D2800(WATER)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

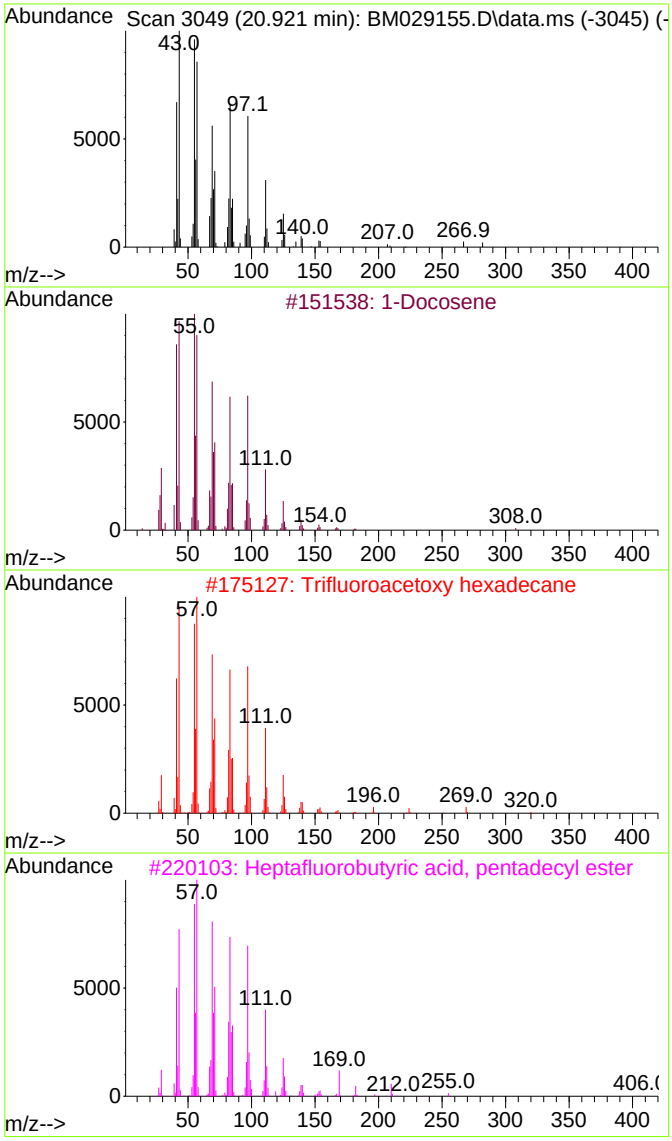
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

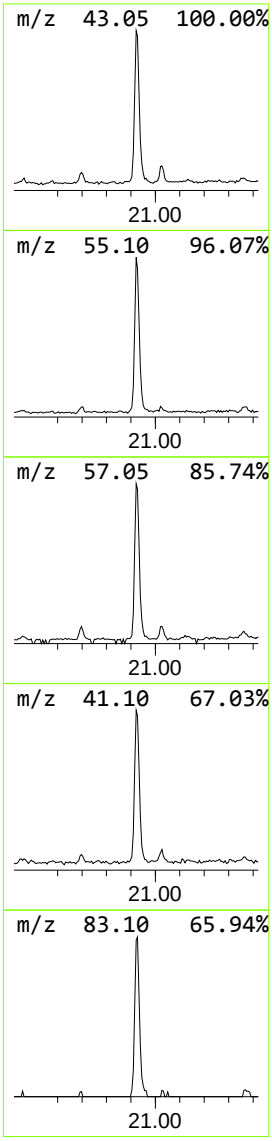
****

Peak Number 12 1-Docosene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.921	13.18 ng	100398	Chrysene-d12	21.215

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031621\
Data File : BM029155.D
Acq On : 16 Mar 2021 19:06
Operator : CG/JU
Sample : M1677-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
D2470-D2800(WATER)

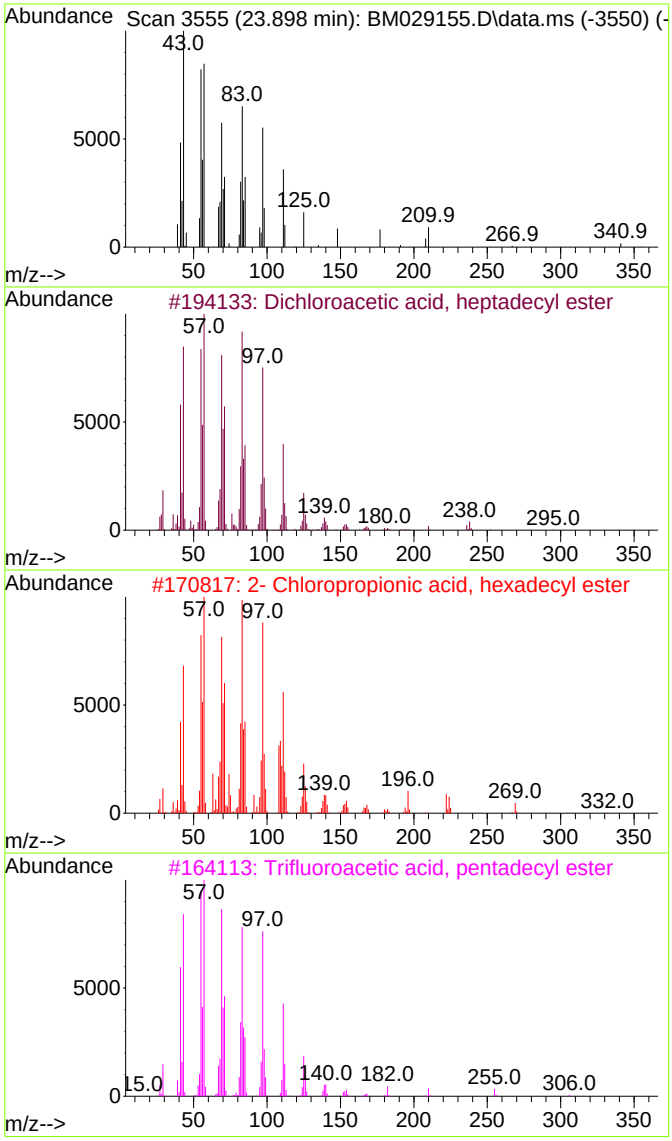
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

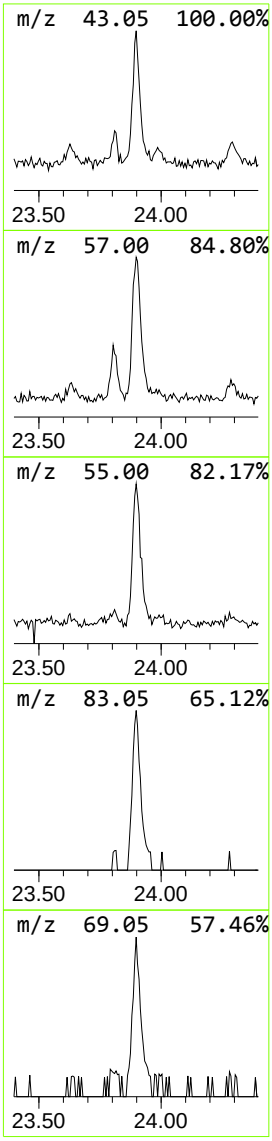
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 Dichloroacetic acid, heptad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.898	4.27 ng	34381	Perylene-d12	23.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	90
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
4	Cyclopentane, decyl-	210	C15H30	001795-21-7	90
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031621\
Data File : BM029155.D
Acq On : 16 Mar 2021 19:06
Operator : CG/JU
Sample : M1677-03
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D2470-D2800(WATER)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzene, 1,3-di...	5.599	72.8	ng	160050	1	7.610	43991	20.0
unknown5.693	5.693	3.9	ng	8640	1	7.610	43991	20.0
Hexanoic acid	6.728	5.3	ng	11679	1	7.610	43991	20.0
1-Hexanol, 2-et...	7.681	10.5	ng	23134	1	7.610	43991	20.0
Hexanoic acid, ...	8.981	17.0	ng	37344	1	7.610	43991	20.0
Vanillin	13.228	2.6	ng	42527	3	14.281	330543	20.0
n-Hexadecanoic ...	17.933	13.4	ng	72292	4	17.033	107730	20.0
Octadecanoic acid	19.215	5.0	ng	38168	5	21.215	152361	20.0
Octaethylene gl...	20.215	2.2	ng	16727	5	21.215	152361	20.0
1-Docosene	20.921	13.2	ng	100398	5	21.215	152361	20.0
Dichloroacetic ...	23.898	4.3	ng	34381	6	23.351	161019	20.0