LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008101.D
Acq On : 23 Nov 2021 17:55
Operator : CG/JU
Sample : M4786-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-279

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_P\Methods\8270E-BP111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	13	rBV	546404	755391	13.61%	1.789%
2	4.946	326	333	343	rBV	178941	254851	4.59%	0.604%
3	5.411	405	412	426	rBV	1833104	2748149	49.51%	6.510%
4	6.999	673	682	698	rBV	1760473	2988735	53.85%	7.080%
5	7.822	815	822	829	rVB	589243	949909	17.11%	2.250%
6	8.046	852	860	867	rBV2	49550	77149	1.39%	0.183%
7	8.981	1010	1019	1030	rBV	1150236	1956021	35.24%	4.634%
8	10.405	1254	1261	1274	rBV	136087	259599	4.68%	0.615%
9	10.616	1289	1297	1308	rBV	822530	1389787	25.04%	3.292%
10	12.275	1572	1579	1588	rBV	56949	110974	2.00%	0.263%
11	13.087	1709	1717	1728	rBV	2598541	3932770	70.86%	9.316%
12	13.387	1760	1768	1786	rBV	308012	675527	12.17%	1.600%
13	14.463	1944	1951	1958	rBV	1317461	1931344	34.80%	4.575%
14	15.292	2083	2092	2106	rBV	109307	233373	4.20%	0.553%
15	15.957	2199	2205	2214	rBV	2380188	3454339	62.24%	8.183%
16	16.887	2358	2363	2370	rBV2	40762	86432	1.56%	0.205%
17	17.222	2413	2420	2425	rBV	1668812	2420295	43.61%	5.733%
18	17.263	2425	2427	2431	rVB	65481	72429	1.30%	0.172%
19	17.898	2531	2535	2541	rVB3	52791	67008	1.21%	0.159%
20	18.004	2548	2553	2559	rBV6	31439	64577	1.16%	0.153%
21	18.122	2568	2573	2581	rBV	472964	644564	11.61%	1.527%
22	18.281	2596	2600	2604	rBV2	42463	63312	1.14%	0.150%
23	18.851	2692	2697	2709	rBV	325044	551820	9.94%	1.307%
24	19.239	2758	2763	2770	rBV	476188	647911	11.67%	1.535%
25	19.357	2779	2783	2791	rBV	215812	295341	5.32%	0.700%
26	19.586	2815	2822	2831	rVB	342066	546798	9.85%	1.295%
27	19.792	2851	2857	2862	rBV	4469594	5550429	100.00%	13.148%
28	20.380	2952	2957	2967	rBV	850082	1325350	23.88%	3.140%
29	20.539	2982	2984	2987	rVB	73627	67641	1.22%	0.160%
30	21.033	3065	3068	3076	rBV2	253266	348295	6.28%	0.825%
31	21.322	3111	3117	3121	rBV	1629958	2268956	40.88%	5.375%
32	21.663	3171	3175	3195	rBV	1224028	1926095	34.70%	4.563%
33	23.127	3419	3424	3438	rBV	719501	1535458	27.66%	3.637%
34	23.721	3518	3525	3536	rVB2	964303	2013987	36.29%	4.771%

Sum of corrected areas: 42214616

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BNA_P
ClientSampleId :
RO-279

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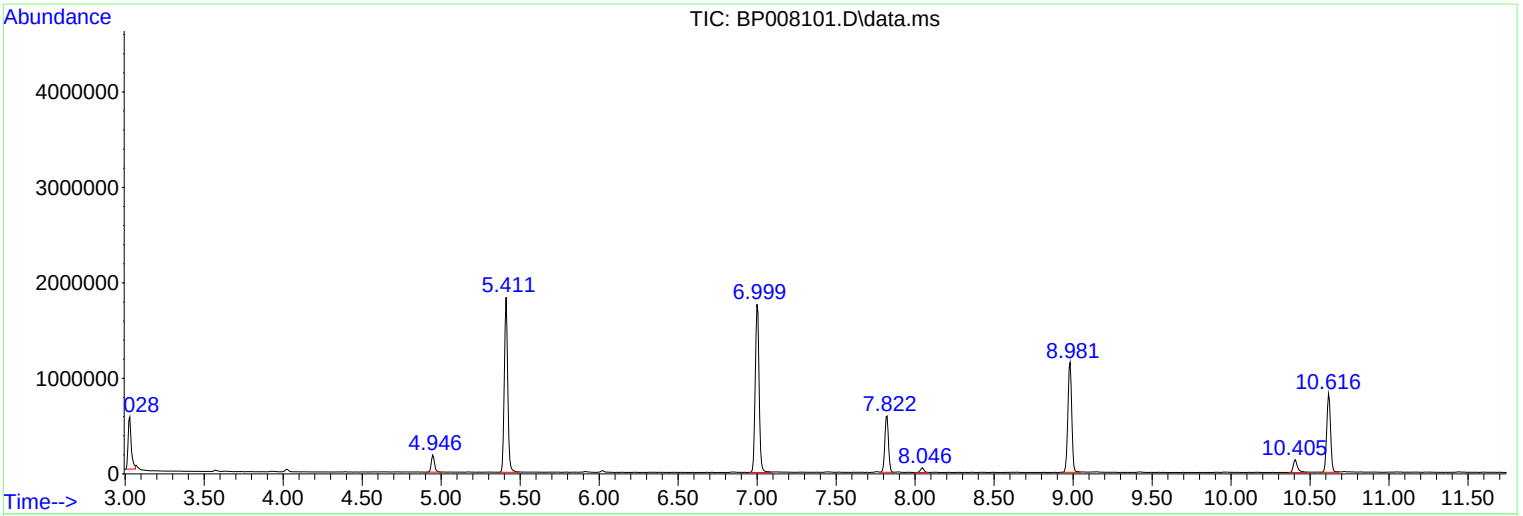
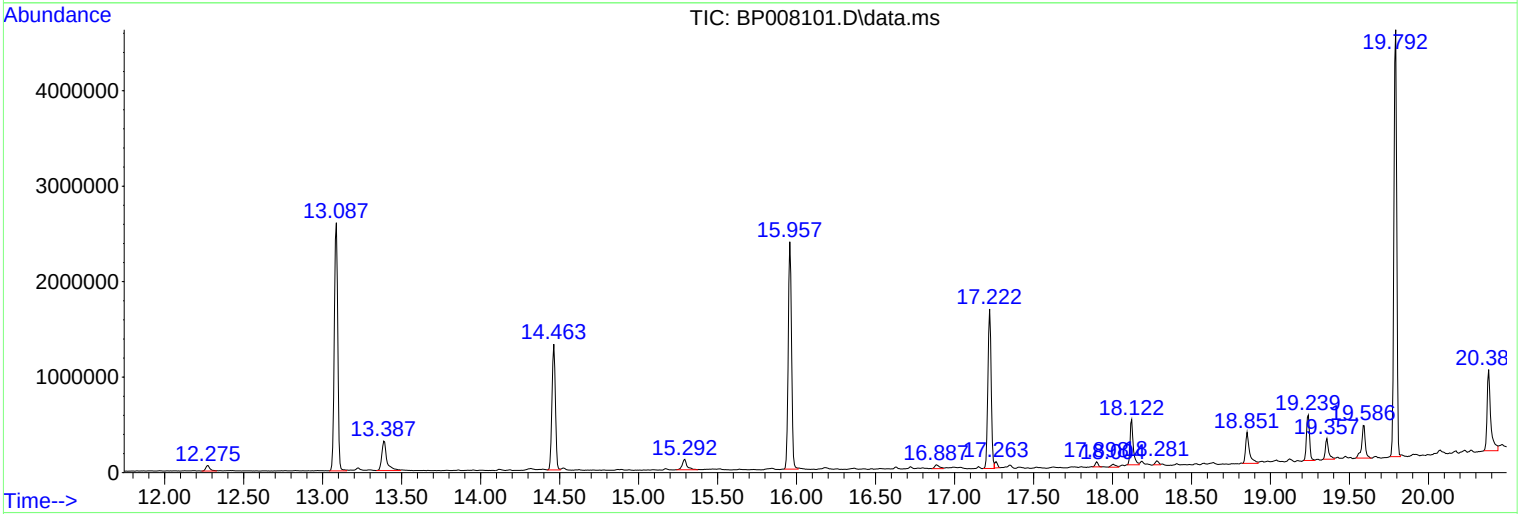
ALS Vial : 9 Sample Multiplier: 1

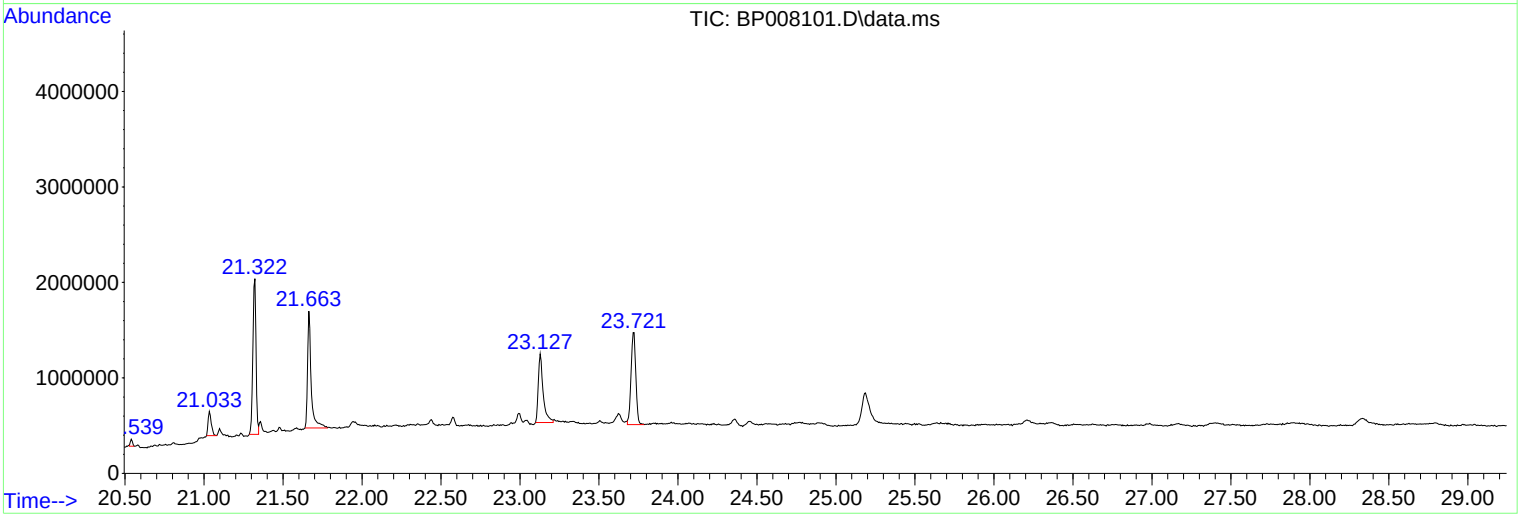
Instrument :
BNA_P
ClientSampleId :
RO-279

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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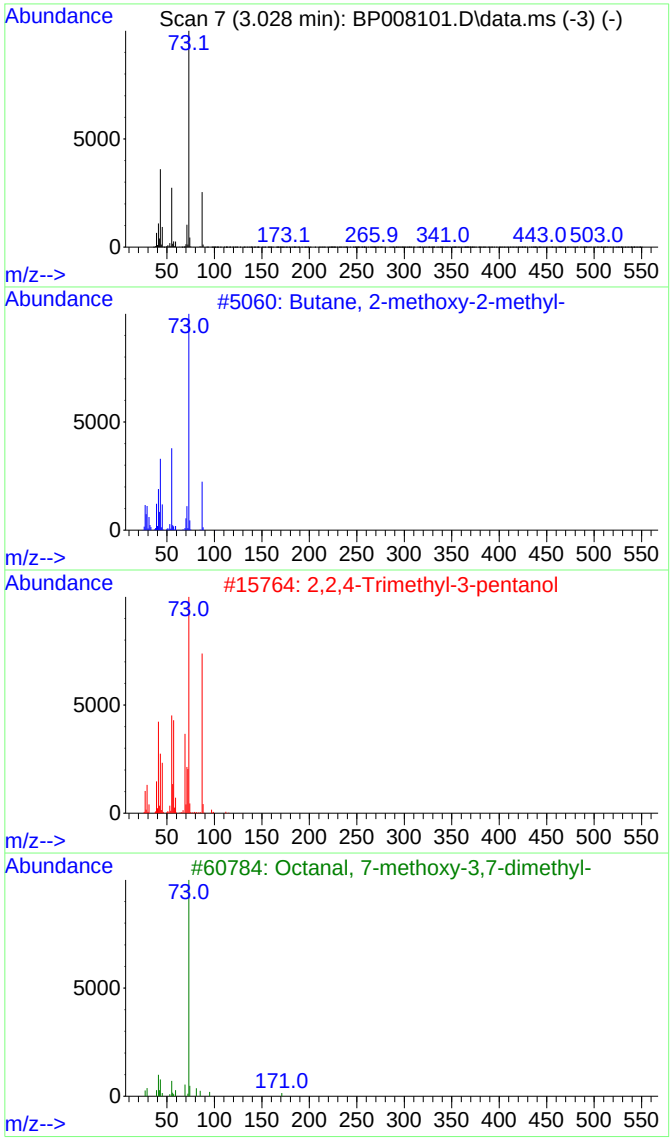
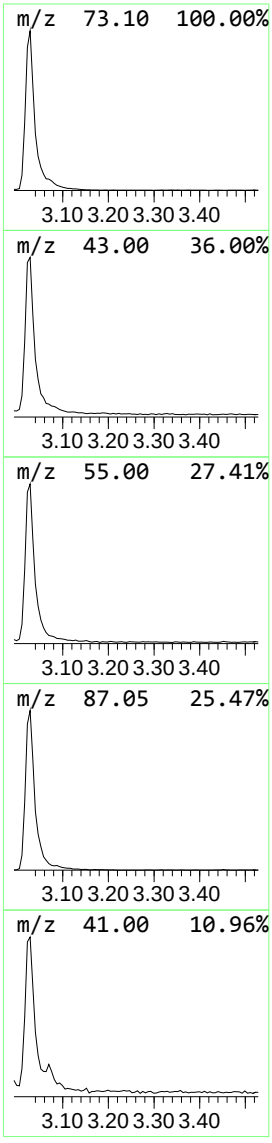
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	15.90 ng	755391	1,4-Dichlorobenzene-d4	7.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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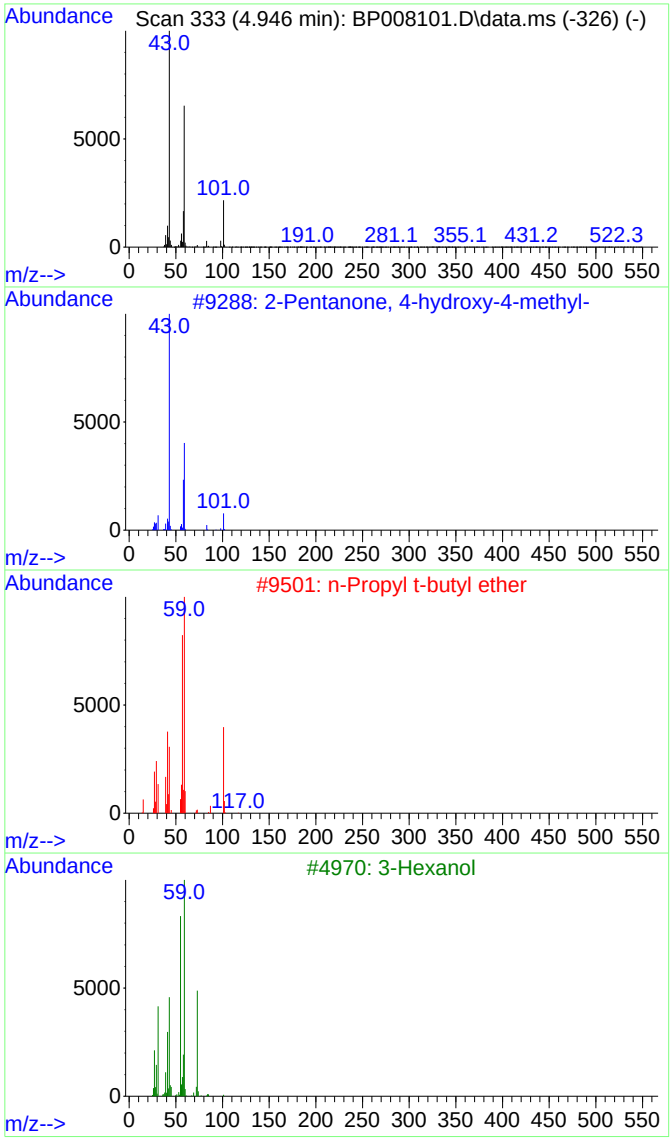
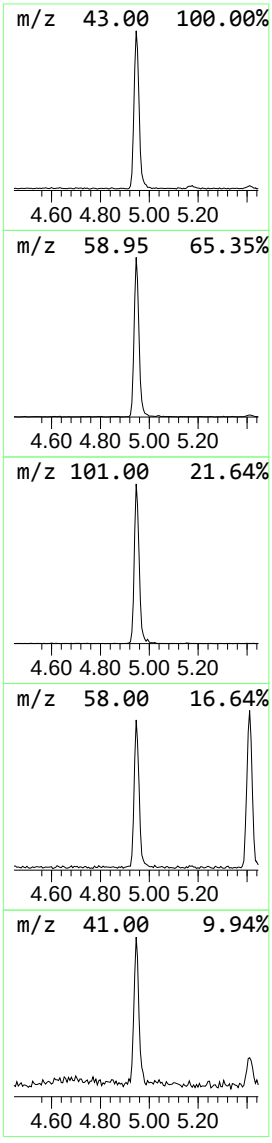
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	5.37 ng	254851	1,4-Dichlorobenzene-d4	7.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
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TIC Library : C:\Database\NIST20.L
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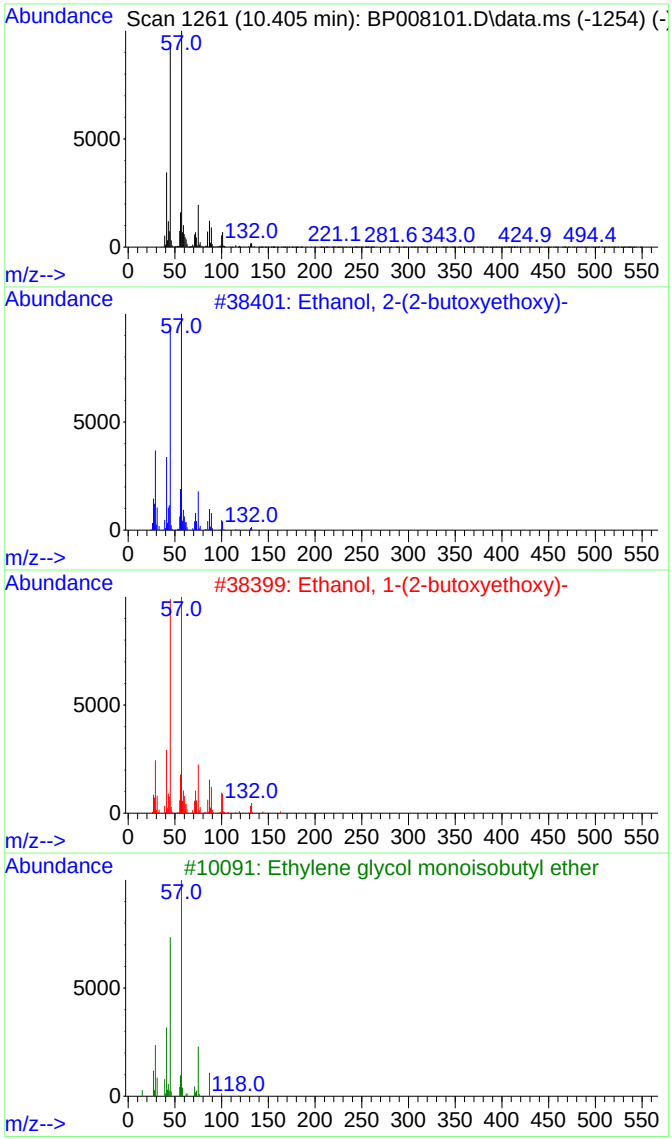
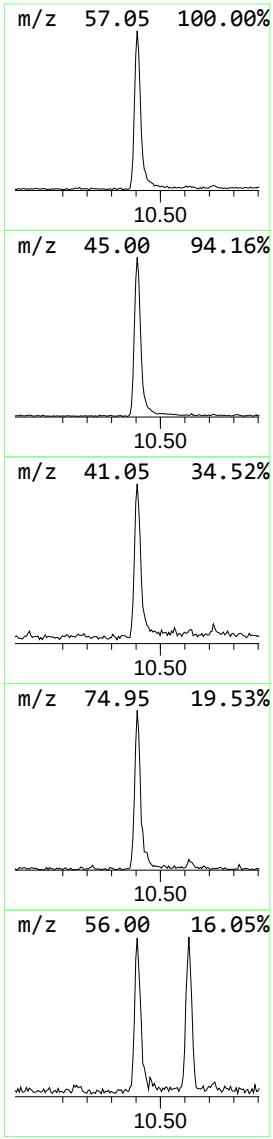
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.405	3.74 ng	259599	Naphthalene-d8	10.616

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	50





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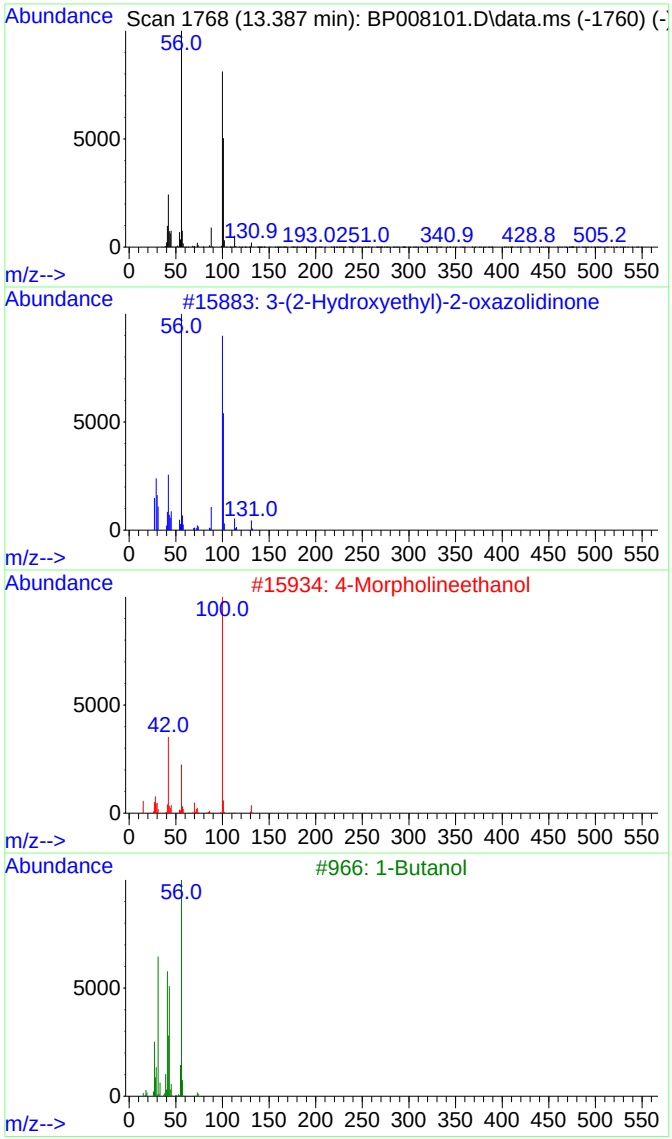
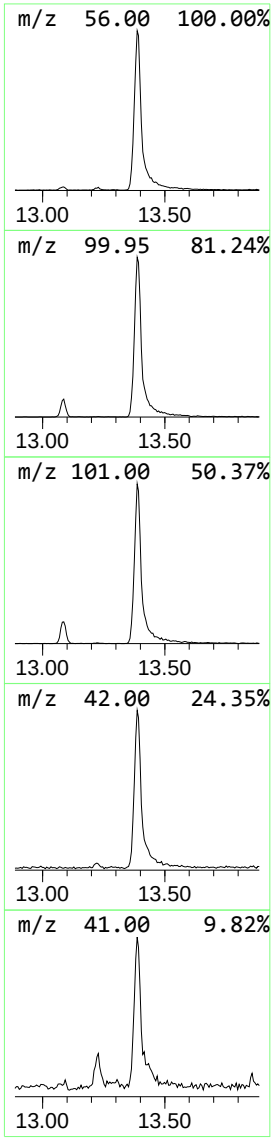
****
Peak Number 4 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.387	7.00 ng	675527	Acenaphthene-d10	14.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	83
2	4-Morpholineethanol	131	C6H13NO2	000622-40-2	35
3	1-Butanol	74	C4H10O	000071-36-3	27
4	N-(3-Hydoxypropyl)morpholine	145	C7H15NO2	1000425-83-2	17
5	Aminothiazole	100	C3H4N2S	000096-50-4	12





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

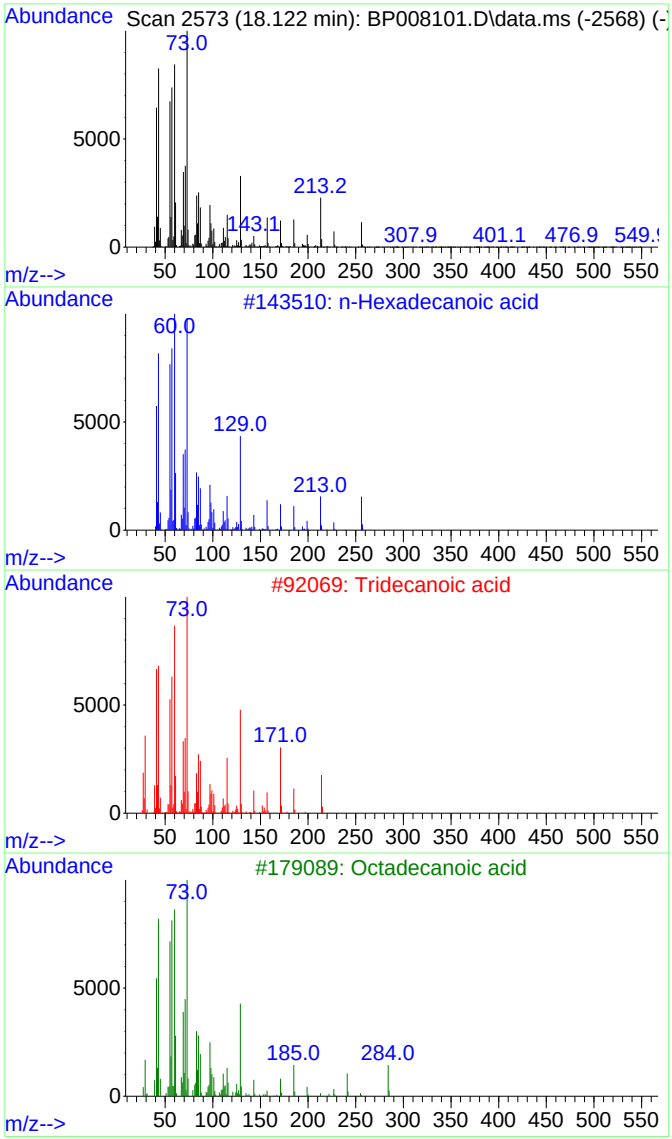
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

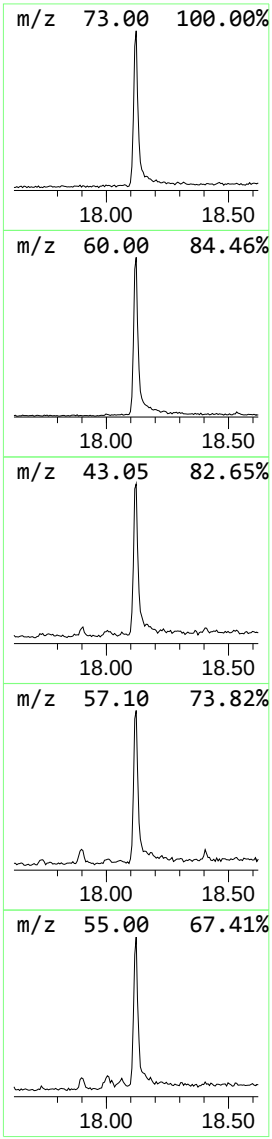
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.122	5.33 ng	644564	Phenanthrene-d10	17.222

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	96
3	Octadecanoic acid	284	C18H36O2	000057-11-4	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	64





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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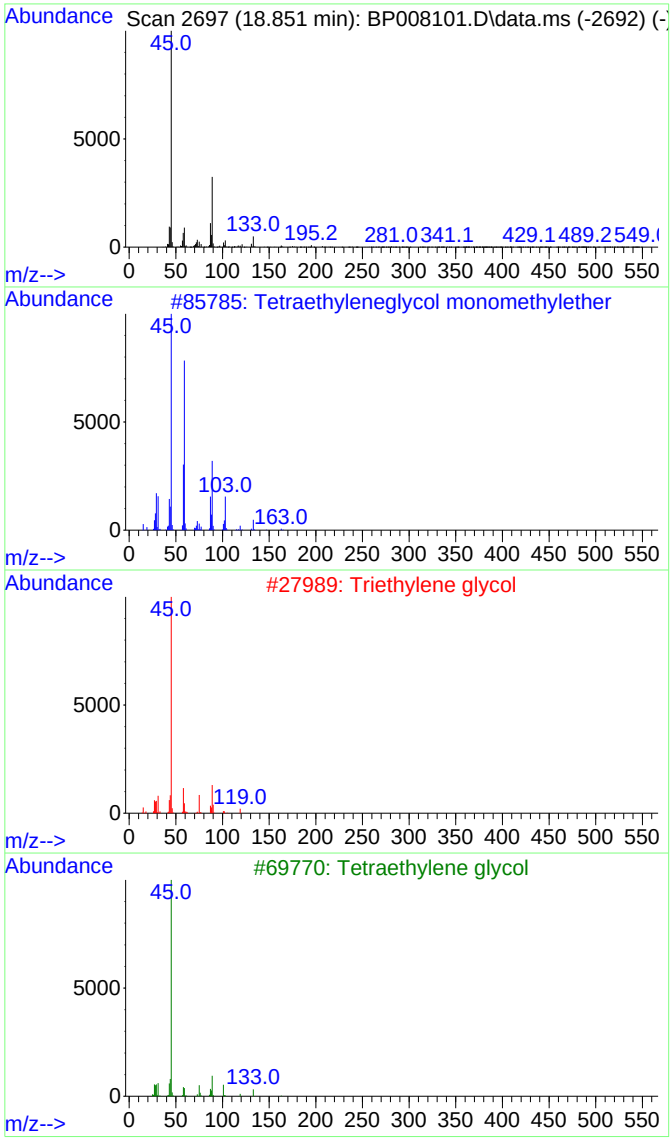
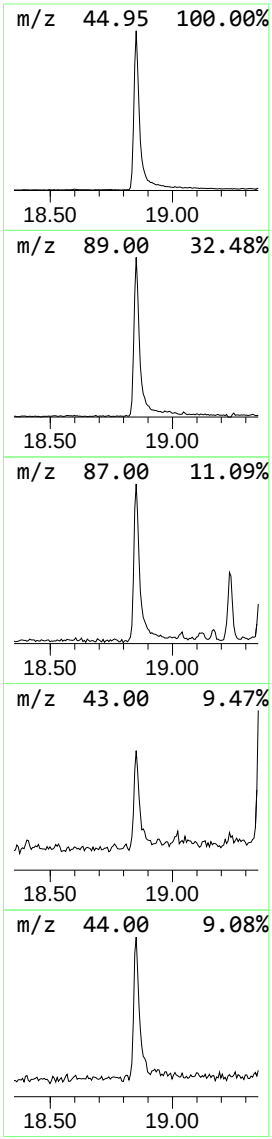
****

Peak Number 6 Tetraethyleneglycol monomet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.851	4.56 ng	551820	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetraethyleneglycol monomethylether	208	C9H20O5	023783-42-8	78
2	Triethylene glycol	150	C6H14O4	000112-27-6	78
3	Tetraethylene glycol	194	C8H18O5	000112-60-7	72
4	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	72
5	Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	64





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

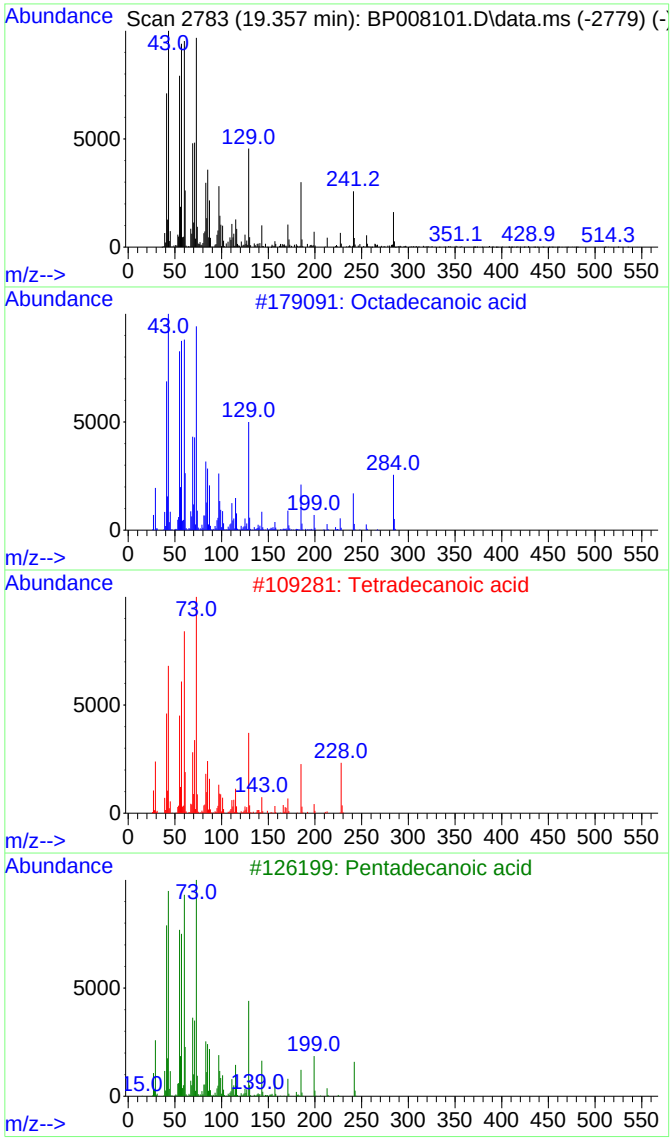
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

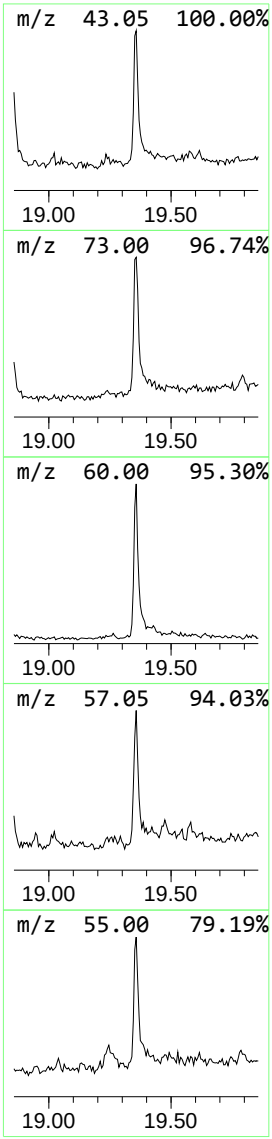
****

Peak Number 7 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.357	2.60 ng	295341	Chrysene-d12	21.322

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	74
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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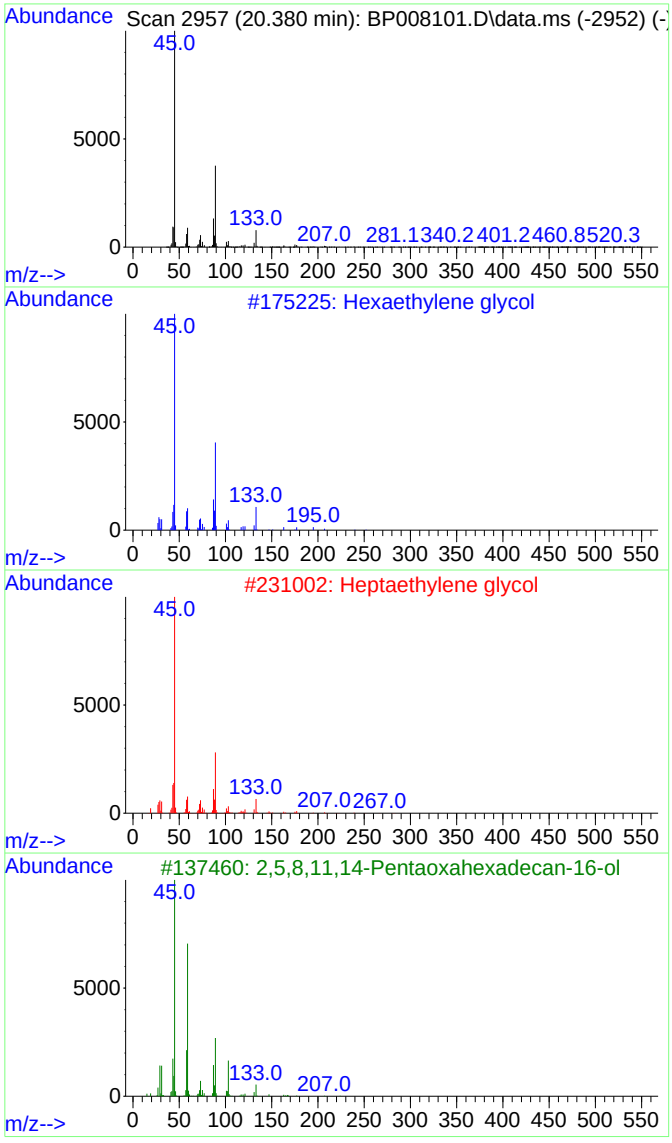
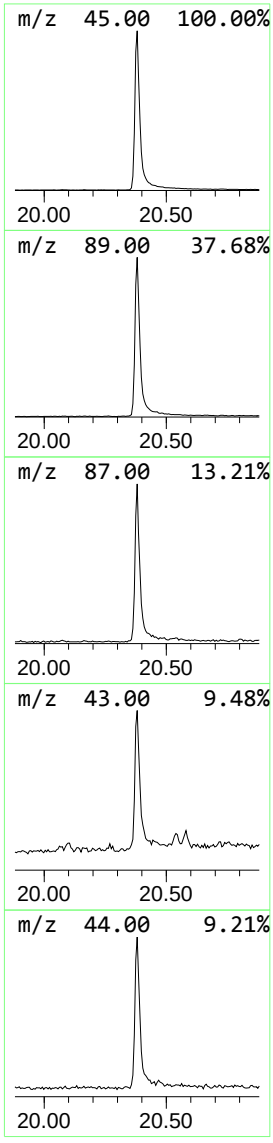
****

Peak Number 8 Hexaethylene glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.380	11.68 ng	1325350	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	83
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	78
3	2,5,8,11,14-Pentaoxahexadecan-16-ol	252	C11H24O6	023778-52-1	78
4	Acetaldehyde, tetramer	176	C8H16O4	000108-62-3	72
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	64





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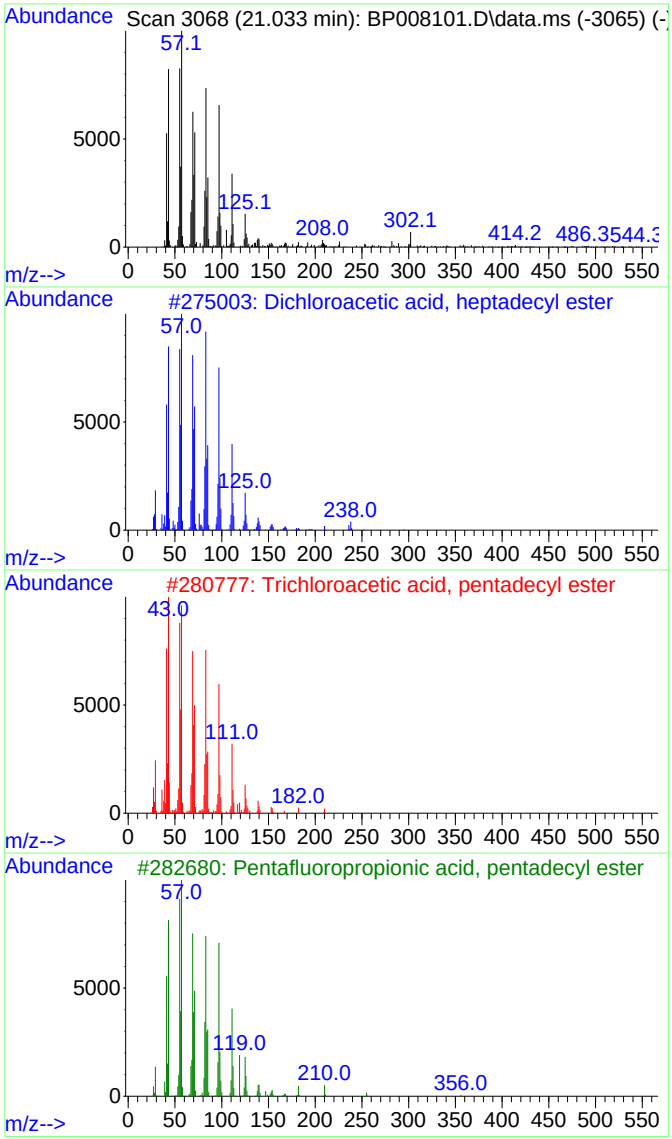
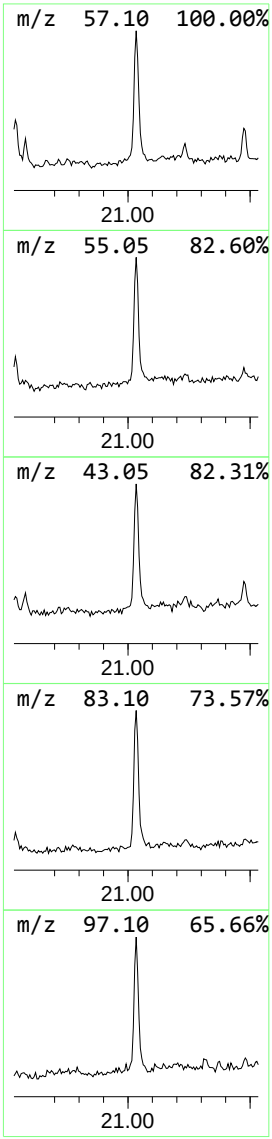
****
Peak Number 9 Dichloroacetic acid, heptad... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	3.07 ng	348295	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	94
5	1-Hexacosene	364	C26H52	018835-33-1	93





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Data File : BP008101.D
Acq On : 23 Nov 2021 17:55
Operator : CG/JU
Sample : M4786-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-279

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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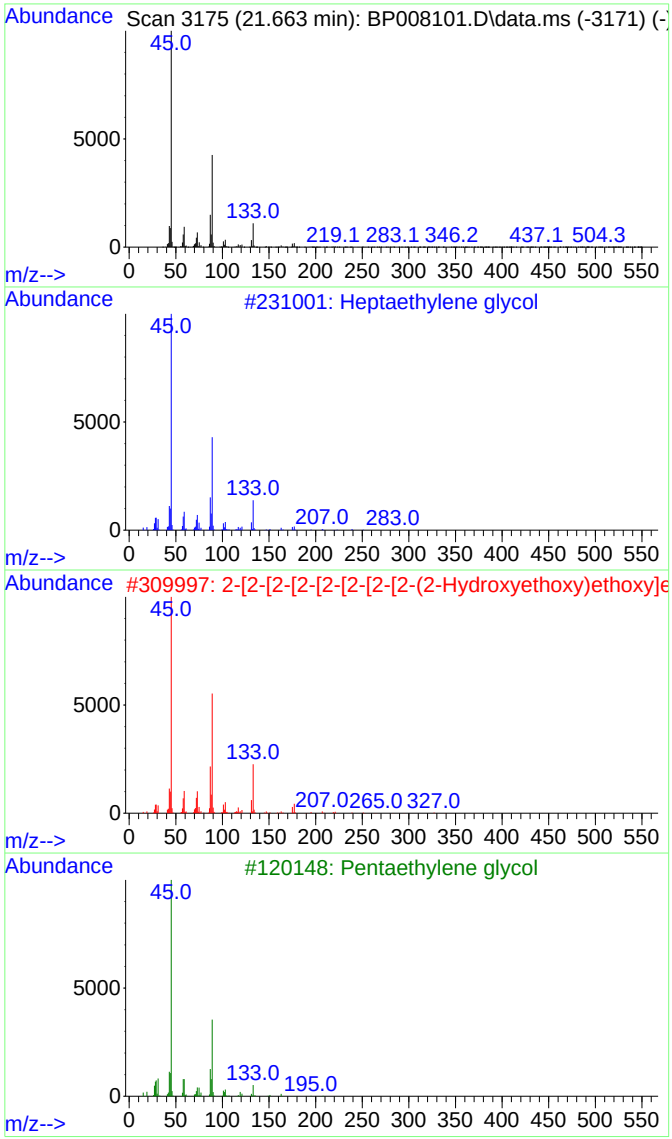
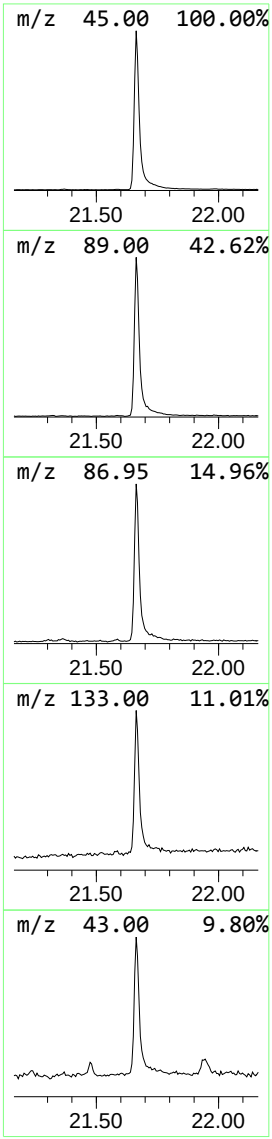
Peak Number 10 Heptaethylene glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.663	16.98 ng	1926100	Chrysene-d12	21.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	91
2	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	003386-18-3	91
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	64
4	Acetaldehyde, tetramer	176	C8H16O4	000108-62-3	64
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008101.D
Acq On : 23 Nov 2021 17:55
Operator : CG/JU
Sample : M4786-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-279

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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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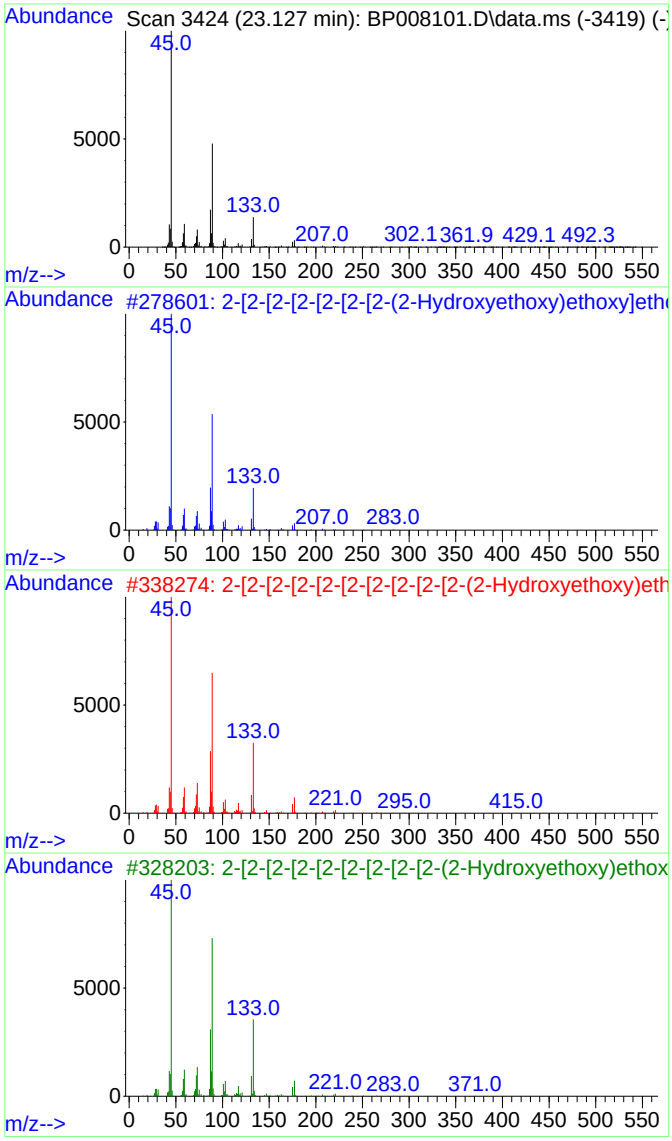
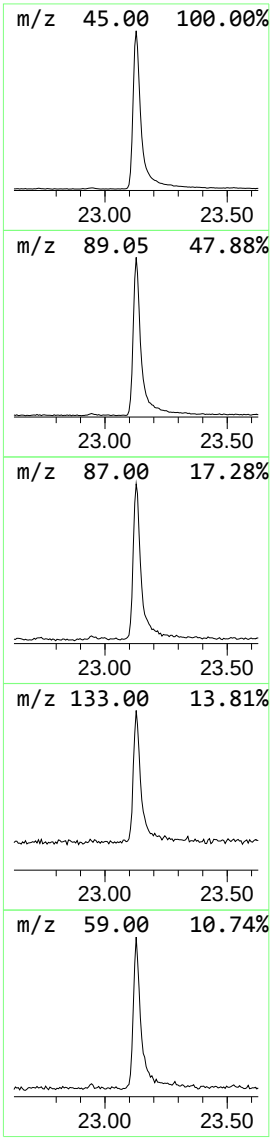
Peak Number 11 unknown23.127 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.127	15.25 ng	1535460	Perylene-d12	23.716

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
2	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	006809-70-7	91
3	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	005579-66-8	91
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	90
5	Heptaethylene glycol	326	C14H30O8	005617-32-3	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP112321\
Data File : BP008101.D
Acq On : 23 Nov 2021 17:55
Operator : CG/JU
Sample : M4786-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
RO-279

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP111921.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
Butane, 2-metho...	3.028	15.9	ng	755391	1	7.822	949909	20.0
2-Pentanone, 4-...	4.946	5.4	ng	254851	1	7.822	949909	20.0
Ethanol, 2-(2-b...	10.405	3.7	ng	259599	2	10.616	1389790	20.0
3-(2-Hydroxyeth...	13.387	7.0	ng	675527	3	14.463	1931340	20.0
n-Hexadecanoic ...	18.122	5.3	ng	644564	4	17.222	2420300	20.0
Tetraethylenegl...	18.851	4.6	ng	551820	4	17.222	2420300	20.0
Octadecanoic acid	19.357	2.6	ng	295341	5	21.322	2268960	20.0
Hexaethylene gl...	20.380	11.7	ng	1325350	5	21.322	2268960	20.0
Dichloroacetic ...	21.033	3.1	ng	348295	5	21.322	2268960	20.0
Heptaethylene g...	21.663	17.0	ng	1926100	5	21.322	2268960	20.0
unknown23.127	23.127	15.3	ng	1535460	6	23.716	2013990	20.0