LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
Data File : BG057813.D
Acq On : 22 Jun 2023 17:14
Operator : CG/JU
Sample : 03238-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-4

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_G\Methods\8270-BG061923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057813.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.188	9	17	20	rBV	179242	349009	13.29%	3.057%
2	3.217	20	22	35	rVB	42223	59474	2.26%	0.521%
3	5.491	403	409	419	rVB	334981	520685	19.83%	4.561%
4	7.077	670	679	689	rBV	255576	414354	15.78%	3.629%
5	7.923	816	823	830	rBV	99934	165569	6.31%	1.450%
6	9.081	1010	1020	1031	rBV	394676	681018	25.93%	5.965%
7	9.187	1031	1038	1045	rBV2	20549	33160	1.26%	0.290%
8	10.720	1289	1299	1307	rBV	154182	270674	10.31%	2.371%
9	13.176	1710	1717	1725	rBV	1012354	1616918	61.58%	14.163%
10	14.557	1945	1952	1961	rVB	272849	430332	16.39%	3.769%
11	15.908	2176	2182	2188	rBV	193944	268851	10.24%	2.355%
12	16.043	2198	2205	2219	rBV	981311	1516431	57.75%	13.282%
13	17.301	2412	2419	2425	rVB	394739	595972	22.70%	5.220%
14	18.188	2564	2570	2580	rBV	96805	146104	5.56%	1.280%
15	19.463	2782	2787	2792	rBV2	24287	34621	1.32%	0.303%
16	19.915	2858	2864	2870	rBV	1998580	2625914	100.00%	23.000%
17	21.202	3078	3083	3093	rBV	138200	196097	7.47%	1.718%
18	21.284	3093	3097	3102	rVB	26086	36375	1.39%	0.319%
19	21.549	3135	3142	3150	rVB	405109	640941	24.41%	5.614%
20	22.353	3274	3279	3285	rBV3	16341	35941	1.37%	0.315%
21	24.698	3667	3678	3693	rBV2	247817	723682	27.56%	6.339%
22	25.967	3889	3894	3906	rVB8	18040	54740	2.08%	0.479%

Sum of corrected areas: 11416862

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Misc :
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Instrument :
BNA_G
ClientSampleId :
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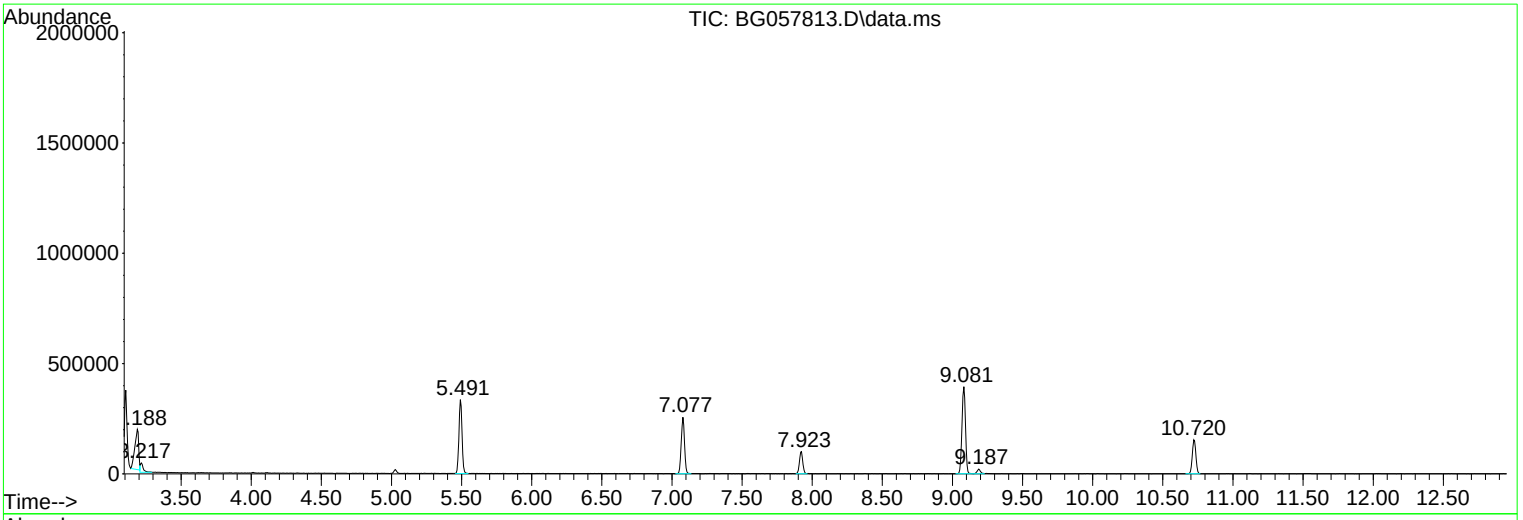
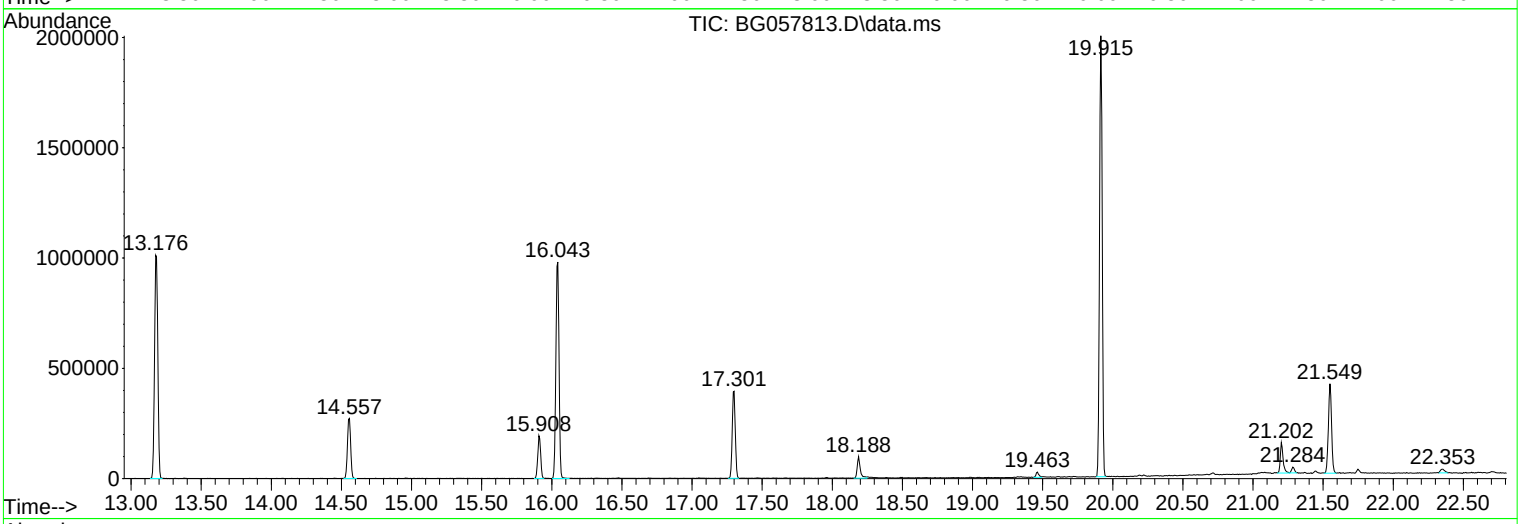
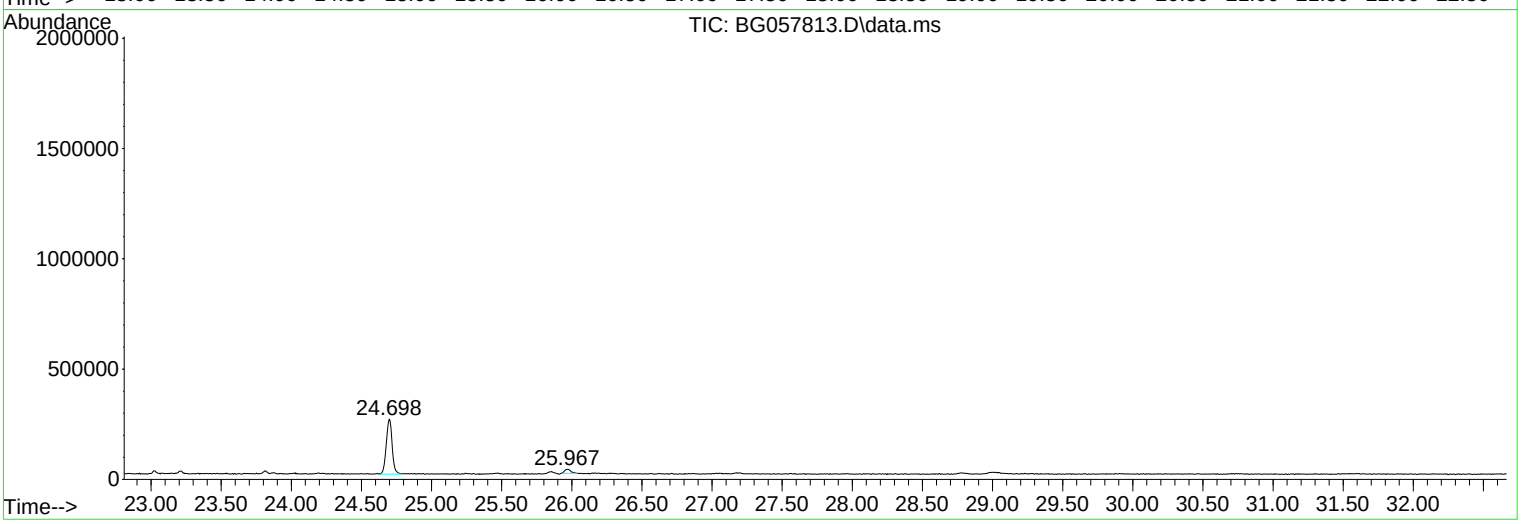
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

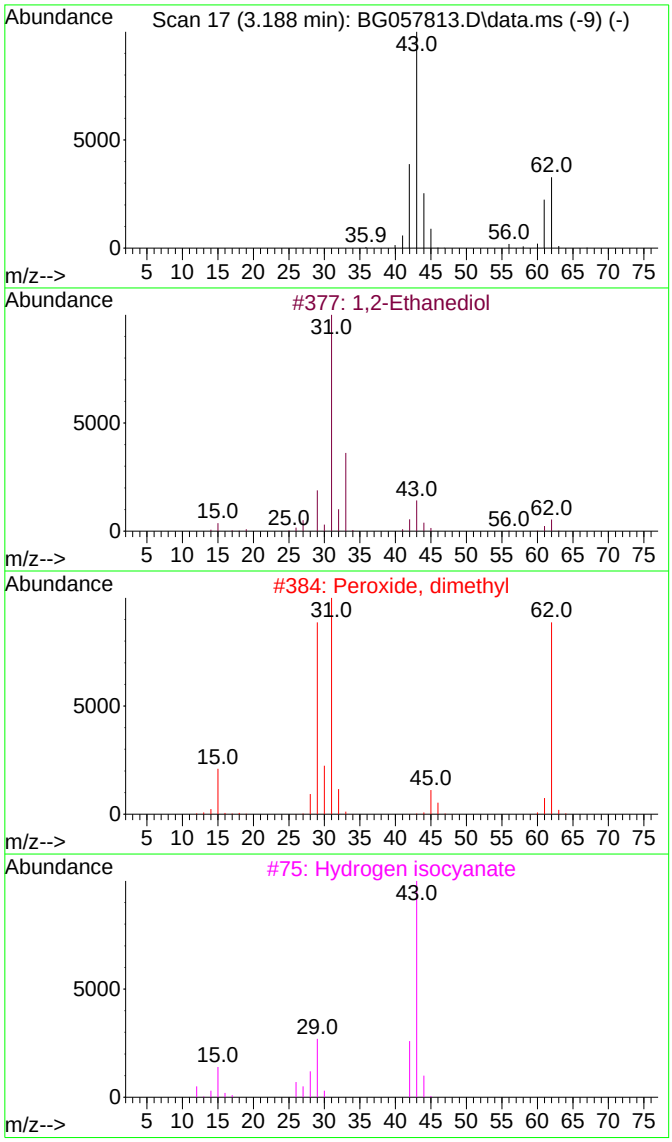
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

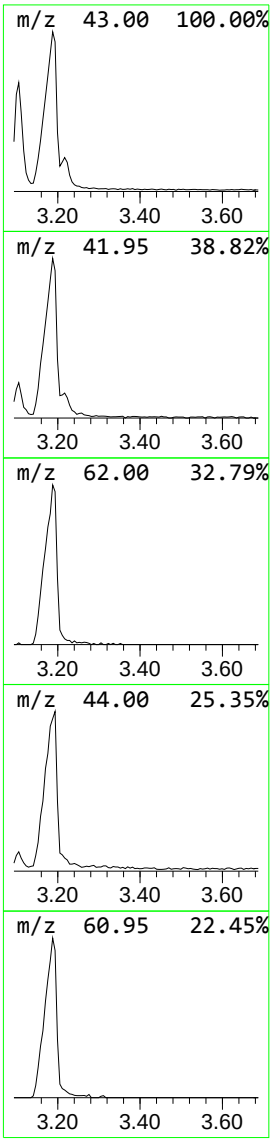
****

Peak Number 1 unknown3.188 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.188	42.16 ng	349009	1,4-Dichlorobenzene-d4	7.923

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Ethanediol	62	C2H6O2	000107-21-1	7
2	Peroxide, dimethyl	62	C2H6O2	000690-02-8	5
3	Hydrogen isocyanate	43	CHNO	000075-13-8	3
4	Monoethanolamine	61	C2H7NO	000141-43-5	3
5	2-(2-Aminoethanesulfonyl)propane	151	C5H13NO2S	320337-16-4	2





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Data File : BG057813.D
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Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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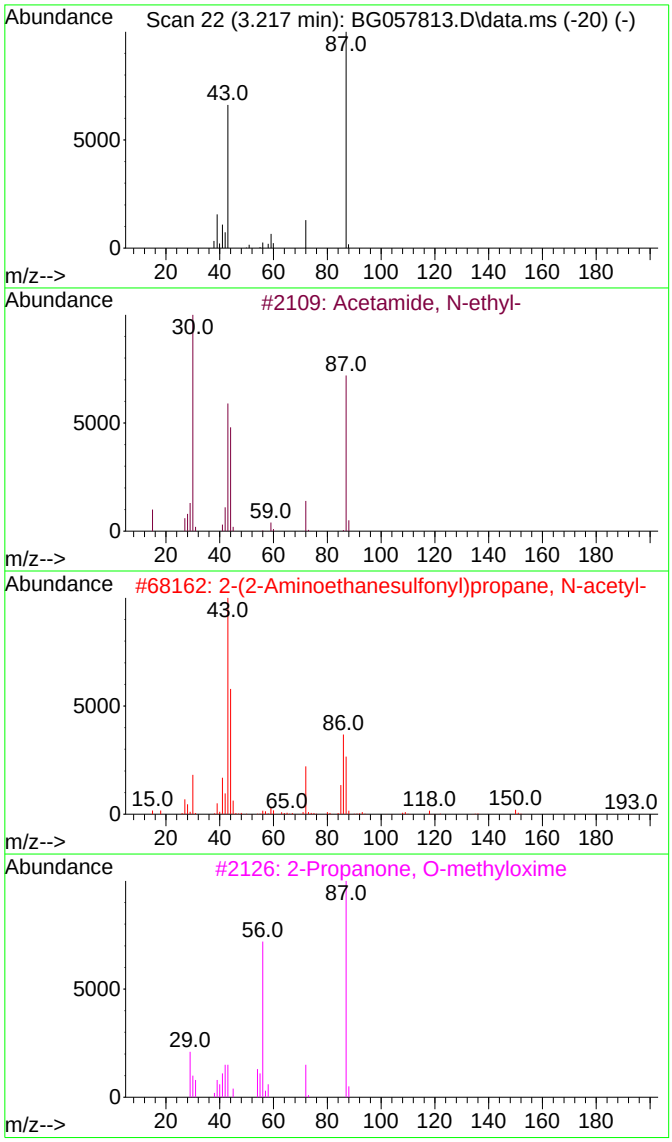
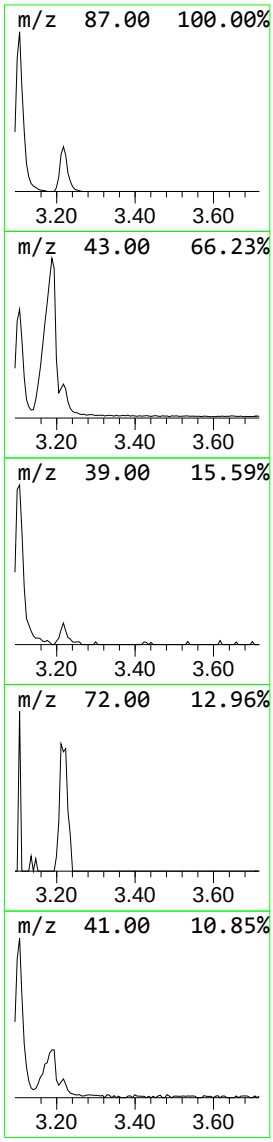
Peak Number 2 unknown3.217 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.217	7.18 ng	59474	1,4-Dichlorobenzene-d4	7.923

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
2	2-(2-Aminoethanesulfonyl)propane...	193	C7H15NO3S	1863983-02-1	9
3	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	7
4	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	7
5	N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	5





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Operator : CG/JU
Sample : 03238-04
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
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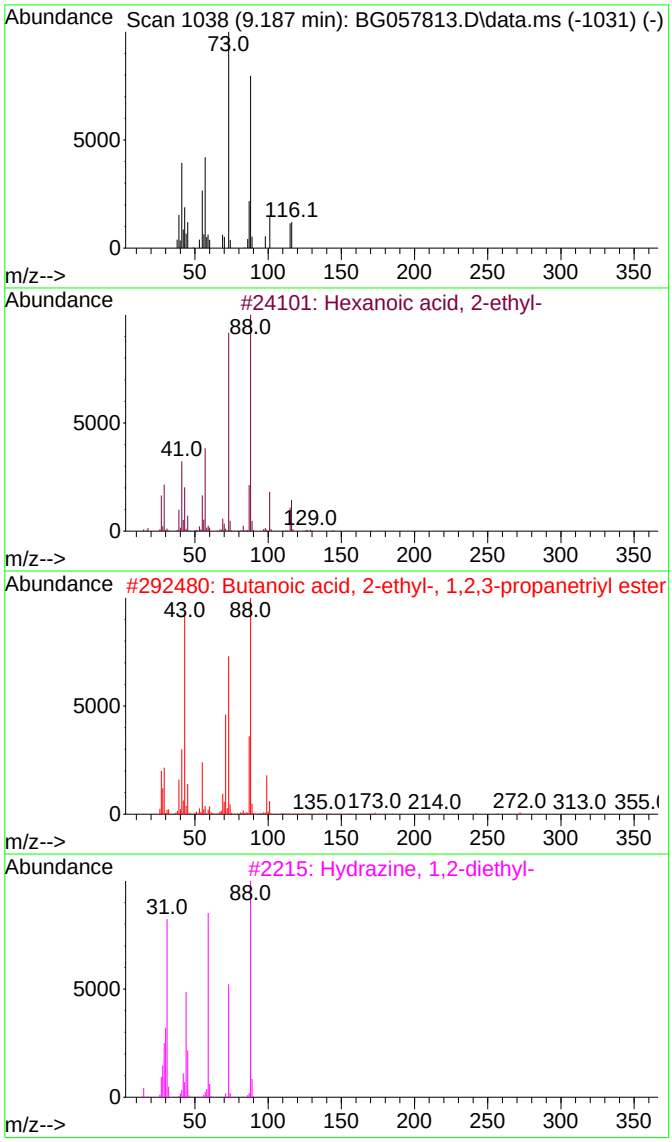
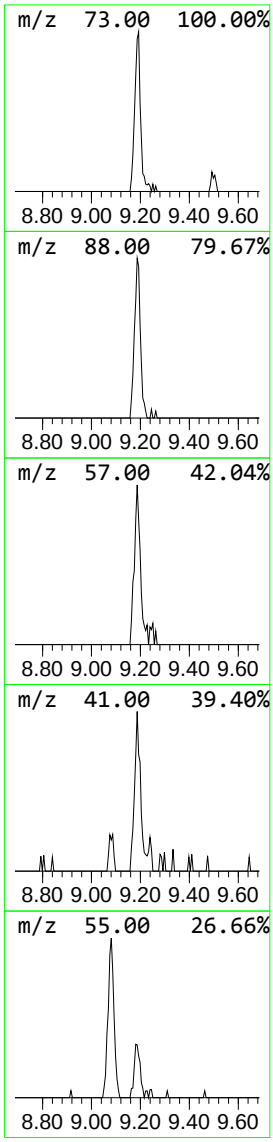
Peak Number 3 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.187	4.01 ng	33160	1,4-Dichlorobenzene-d4	7.923

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
3	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	50
4	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
5	Hydroxypivalic acid	118	C5H10O3	004835-90-9	40





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BNA_G
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MW-4

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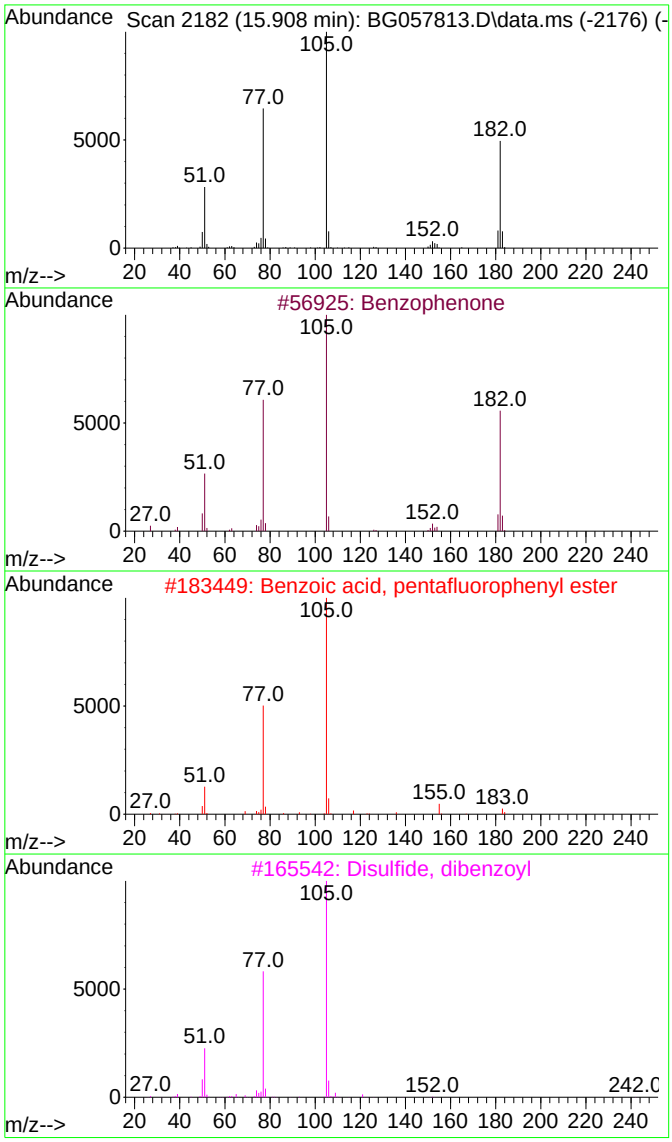
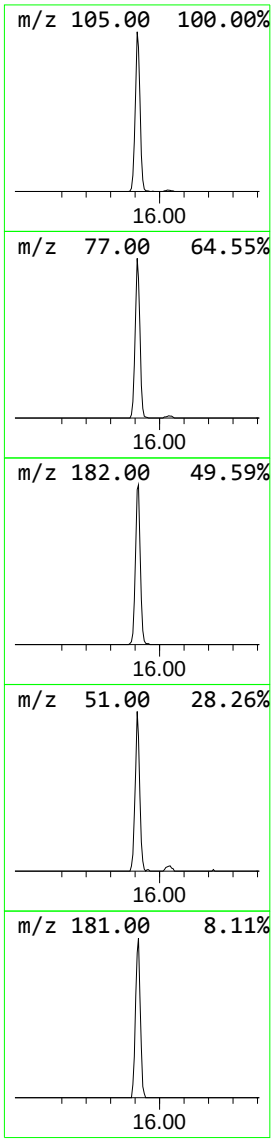
Peak Number 4 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.908	12.50 ng	268851	Acenaphthene-d10	14.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	50
3	Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
4	Azobenzene	182	C12H10N2	000103-33-3	47
5	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47





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BNA_G
ClientSampleId :
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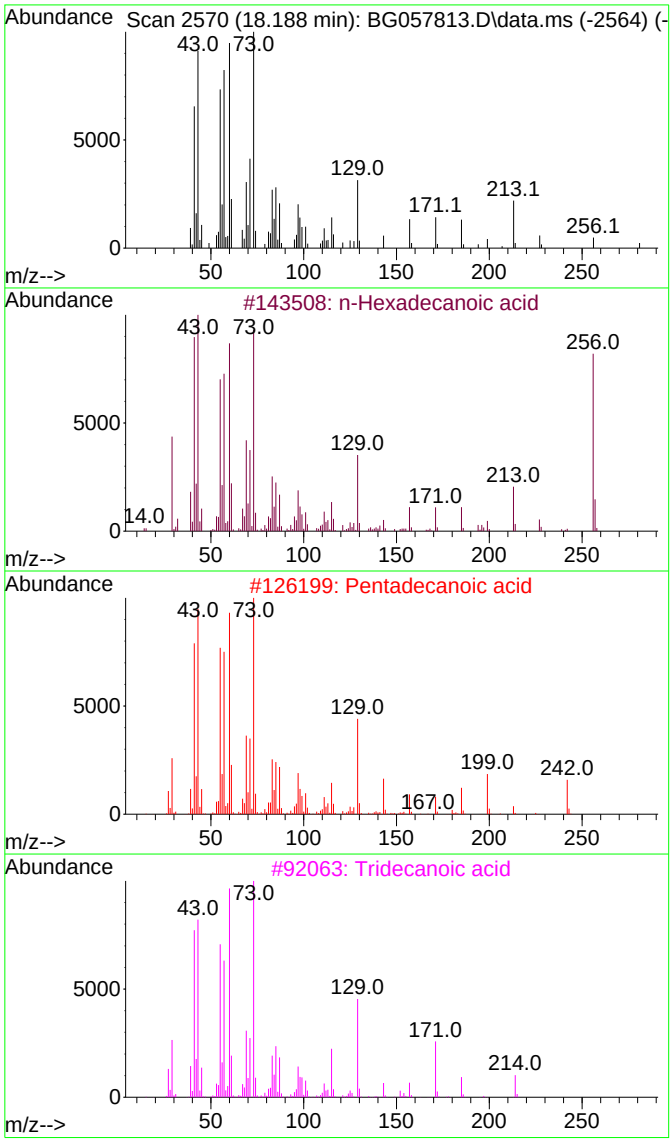
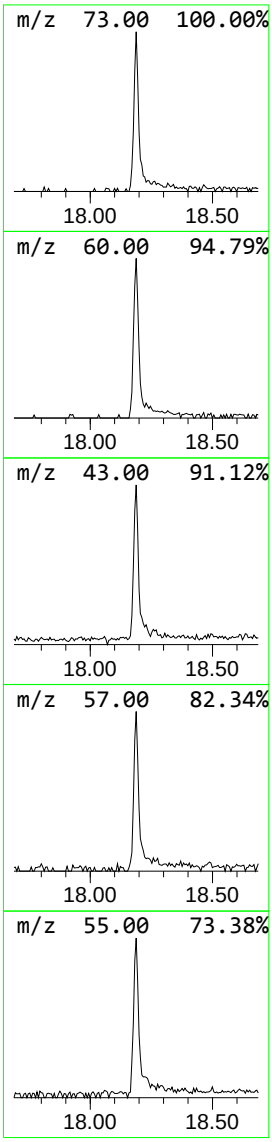
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.188	4.90 ng	146104	Phenanthrene-d10	17.301

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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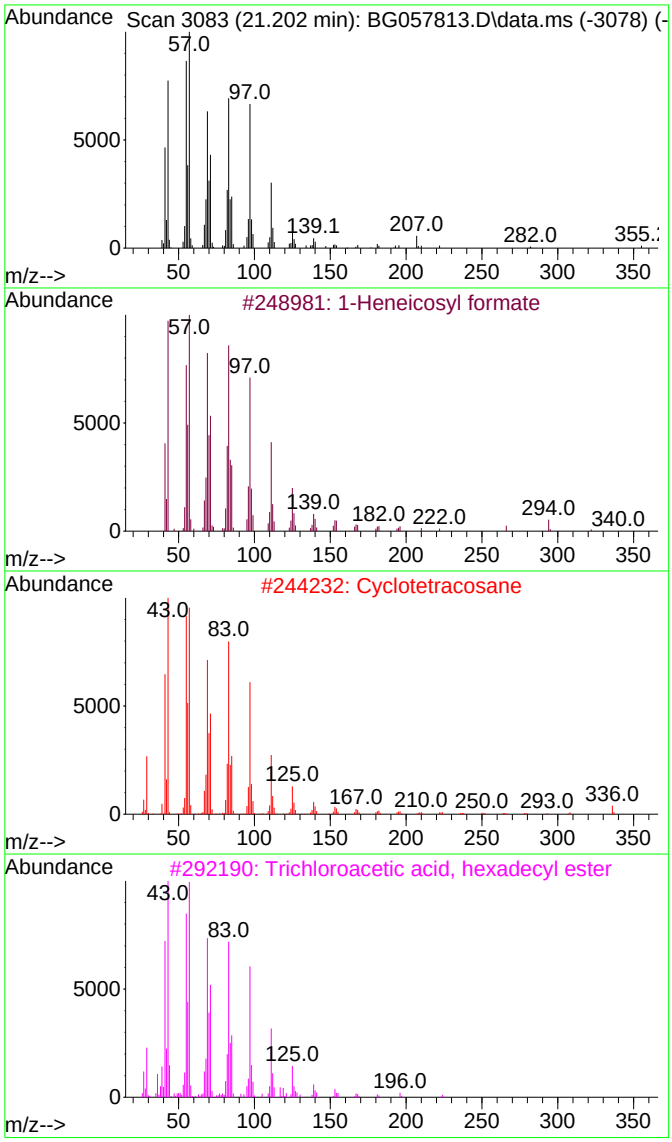
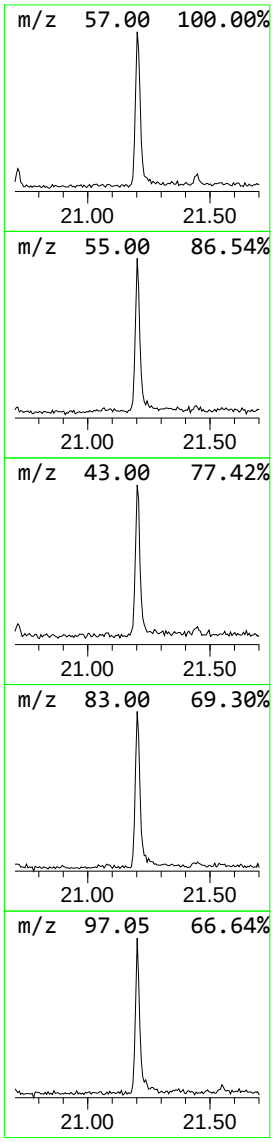
Peak Number 6 1-Heneicosyl formate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.202	6.12 ng	196097	Chrysene-d12	21.549

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	Cyclotetracosane	336	C24H48	000297-03-0	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

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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
unknown3.188	3.188	42.2	ng	349009	1	7.923	165569	20.0
unknown3.217	3.217	7.2	ng	59474	1	7.923	165569	20.0
Hexanoic acid, ...	9.187	4.0	ng	33160	1	7.923	165569	20.0
Benzophenone	15.908	12.5	ng	268851	3	14.557	430332	20.0
n-Hexadecanoic ...	18.188	4.9	ng	146104	4	17.301	595972	20.0
1-Heneicosyl fo...	21.202	6.1	ng	196097	5	21.549	640941	20.0