LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012621\
Data File : BG048011.D
Acq On : 26 Jan 2021 17:52
Operator : CG/JU
Sample : M1219-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : IDW-BR2-AQ-012121-02

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-BG012521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048011.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.220	313	320	328	rVB	52473	76612	2.01%	0.458%
2	5.608	378	386	393	rBV2	24156	45446	1.19%	0.272%
3	5.684	393	399	407	rVB	323361	537623	14.09%	3.214%
4	7.277	663	670	681	rVB2	202472	411434	10.78%	2.460%
5	8.129	809	815	821	rBV	146417	249001	6.53%	1.489%
6	9.292	1005	1013	1022	rBV	515236	903990	23.70%	5.405%
7	10.708	1245	1254	1259	rBV2	28329	51763	1.36%	0.309%
8	10.943	1288	1294	1300	rBV	193864	344811	9.04%	2.062%
9	13.381	1701	1709	1717	rVB	1436931	2170883	56.91%	12.979%
10	14.392	1873	1881	1889	rBV	70534	112897	2.96%	0.675%
11	14.750	1933	1942	1950	rBV	371045	574218	15.05%	3.433%
12	15.549	2073	2078	2083	rBV3	25879	43462	1.14%	0.260%
13	16.231	2186	2194	2206	rBV	835423	1532846	40.18%	9.164%
14	17.400	2387	2393	2398	rVB5	42360	70434	1.85%	0.421%
15	17.494	2402	2409	2415	rBV	522739	789923	20.71%	4.723%
16	17.770	2452	2456	2458	rBV	32917	39276	1.03%	0.235%
17	18.446	2566	2571	2576	rBV	59607	78516	2.06%	0.469%
18	18.822	2633	2635	2641	rVB5	44122	67936	1.78%	0.406%
19	18.887	2642	2646	2652	rBV2	44400	70806	1.86%	0.423%
20	19.145	2685	2690	2694	rBV	364607	449650	11.79%	2.688%
21	19.227	2700	2704	2709	rVB	101803	125172	3.28%	0.748%
22	19.298	2712	2716	2721	rBV	33705	42907	1.12%	0.257%
23	19.774	2793	2797	2805	rBV	484008	604165	15.84%	3.612%
24	20.097	2846	2852	2857	rBV	2881364	3814890	100.00%	22.808%
25	20.303	2883	2887	2892	rBV	57645	77098	2.02%	0.461%
26	20.778	2964	2968	2973	rVB	116992	147497	3.87%	0.882%
27	20.996	3001	3005	3010	rBV	488583	628550	16.48%	3.758%
28	21.049	3010	3014	3017	rVB	113050	141067	3.70%	0.843%
29	21.113	3022	3025	3030	rVB2	43546	56361	1.48%	0.337%
30	21.401	3069	3074	3082	rVB	406834	593552	15.56%	3.549%
31	21.560	3097	3101	3107	rVB	62036	85885	2.25%	0.513%
32	21.766	3130	3136	3143	rVB	541389	890871	23.35%	5.326%
33	22.594	3275	3277	3290	rVB9	40184	103109	2.70%	0.616%
34	25.056	3687	3696	3704	rBV2	297452	793423	20.80%	4.744%

Sum of corrected areas: 16726074

Instrument :
BNA_G
ClientSampleId :
IDW-BR2-AQ-012121-02

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012621\
Data File : BG048011.D
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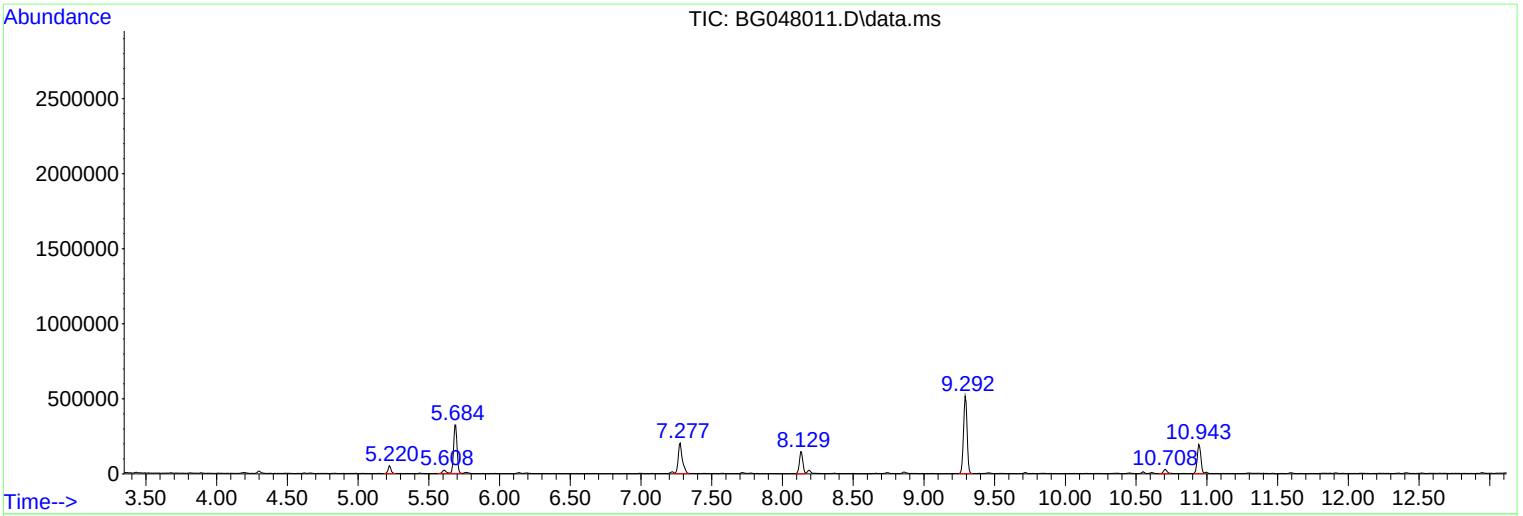
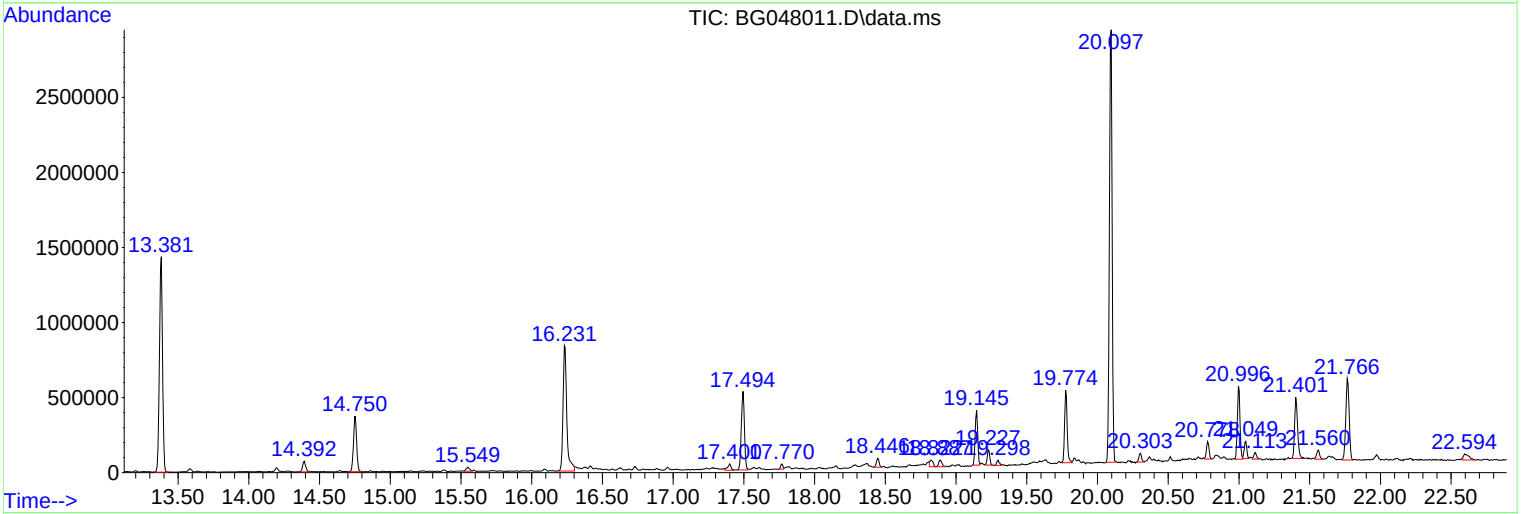
Misc :
ALS Vial : 4 Sample Multiplier: 1

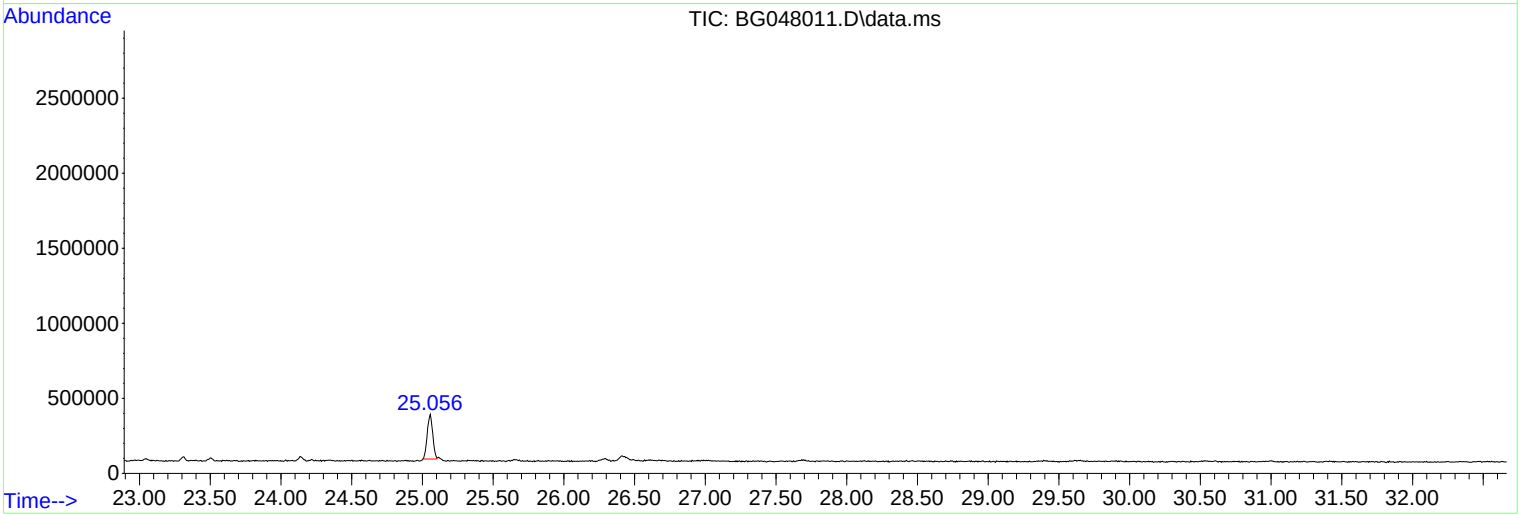
Instrument :
BNA_G
ClientSampleId :
IDW-BR2-AQ-012121-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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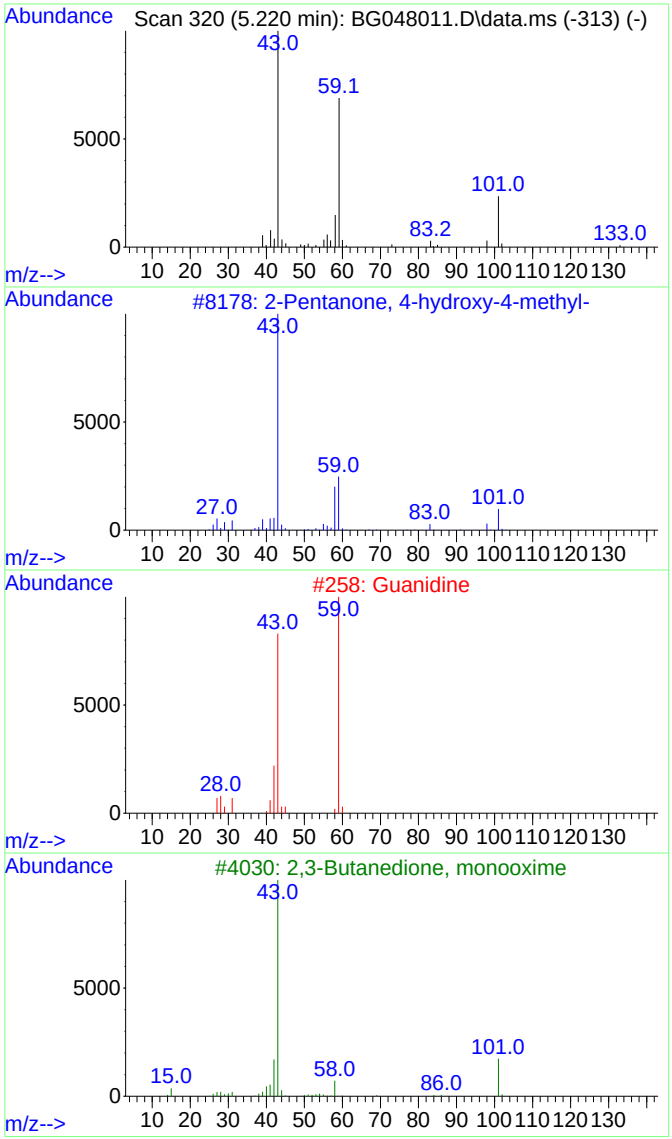
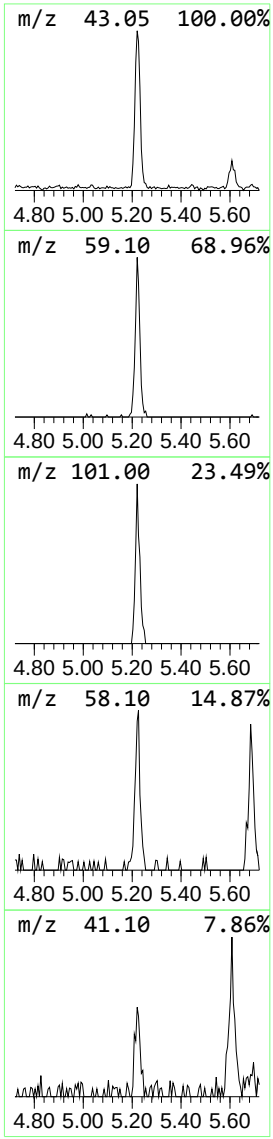
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.220	6.15 ng	76612	1,4-Dichlorobenzene-d4	8.129

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Guanidine	59	CH5N3	000113-00-8	49
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33
5	Tetraglyme	222	C10H22O5	000143-24-8	28





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Misc :
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Instrument : BNA_G
ClientSampleId : IDW-BR2-AQ-012121-02

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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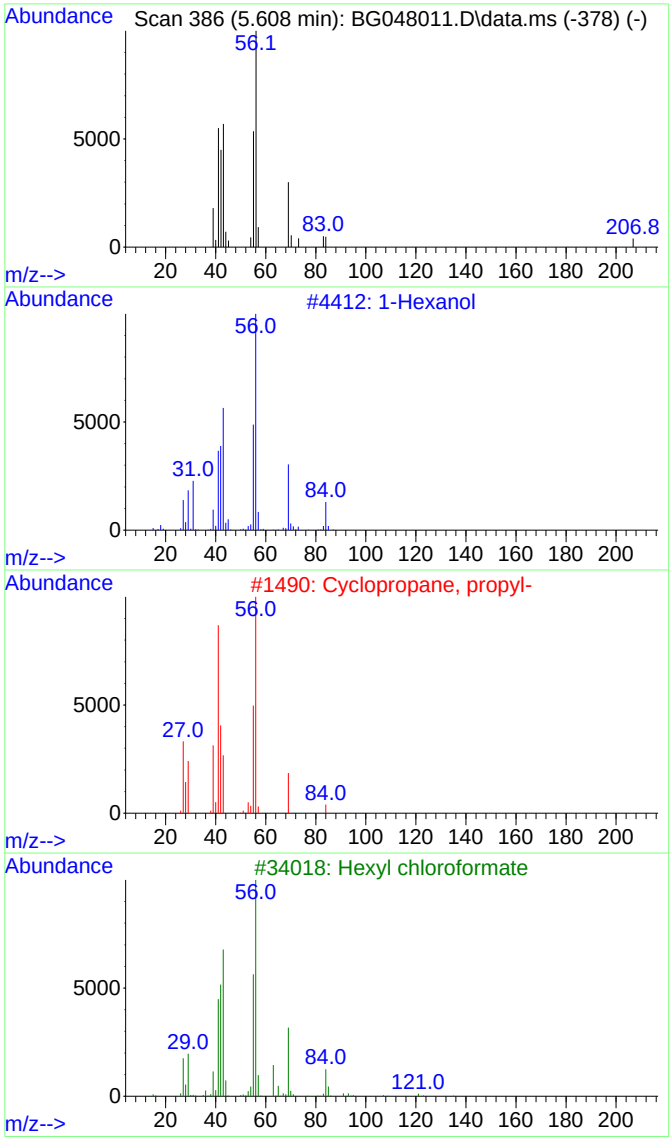
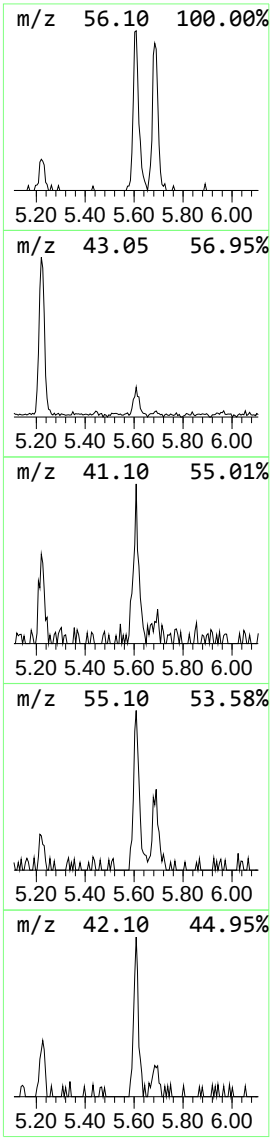
****

Peak Number 2 1-Hexanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.608	3.65 ng	45446	1,4-Dichlorobenzene-d4	8.129

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	78
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	72
3	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	72
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	64
5	Cyclohexane	84	C6H12	000110-82-7	59





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Instrument : BNA_G
ClientSampleId : IDW-BR2-AQ-012121-02

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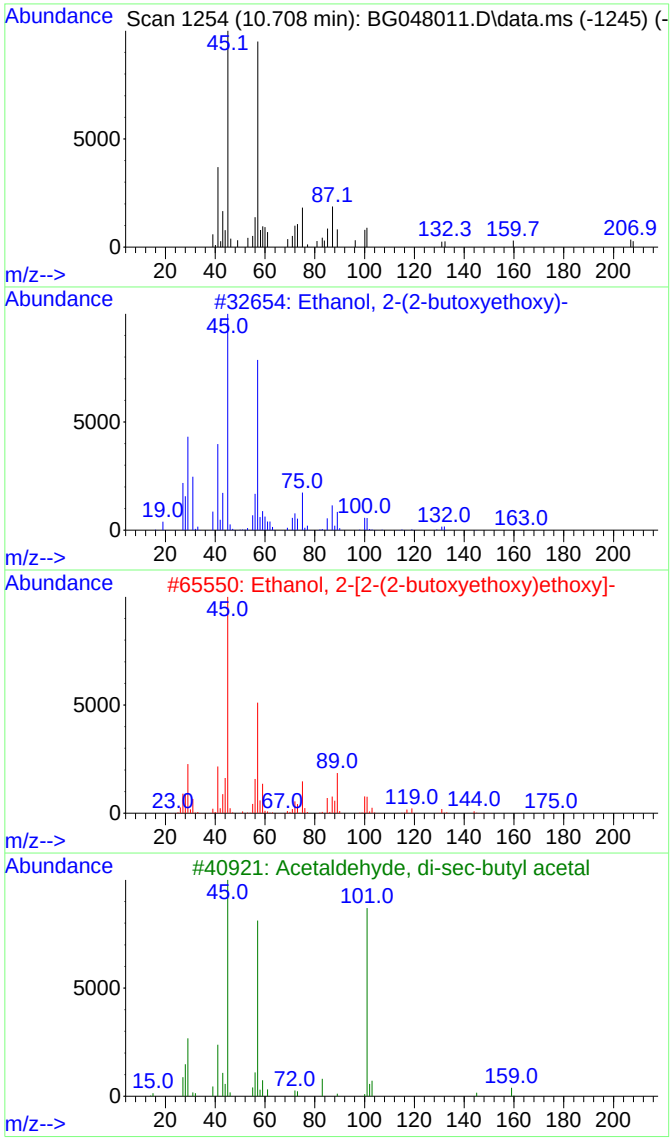
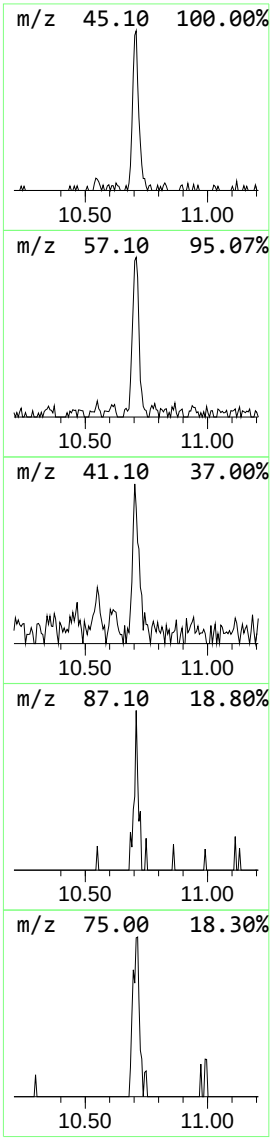
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.708	3.00 ng	51763	Naphthalene-d8	10.943

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	64
2	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
3	Acetaldehyde, di-sec-butyl acetal	174	C10H22O2	005314-41-0	53
4	Di-sec-butyl ether	130	C8H18O	006863-58-7	53
5	Hexaethylene glycol	282	C12H26O7	002615-15-8	45





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Sample : M1219-02
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ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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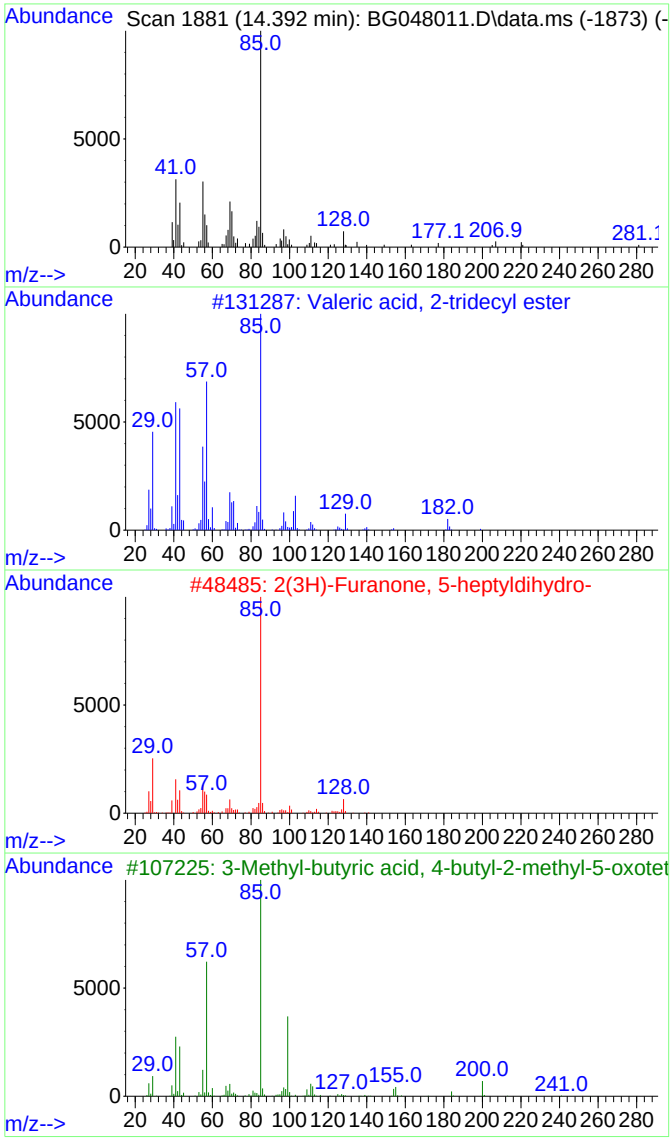
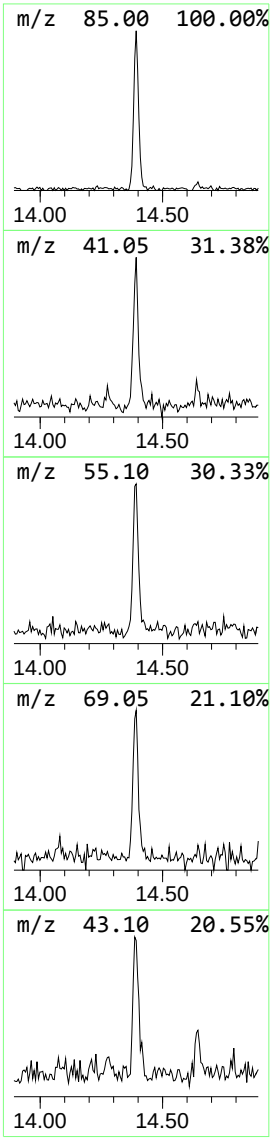
****
Peak Number 4 Valeric acid, 2-tridecyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	3.93 ng	112897	Acenaphthene-d10	14.750

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Valeric acid, 2-tridecyl ester	284	C18H36O2	055193-13-0	72
2	2(3H)-Furanone, 5-heptyldihydro-	184	C11H20O2	000104-67-6	72
3	3-Methyl-butyric acid, 4-butyl-2...	256	C14H24O4	1000192-62-1	64
4	Sulfurous acid, decyl hexyl ester	306	C16H34O3S	1000309-13-2	64
5	2(3H)-Furanone, 5-hexyldihydro-	170	C10H18O2	000706-14-9	64





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Instrument :
BNA_G
ClientSampleId :
IDW-BR2-AQ-012121-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
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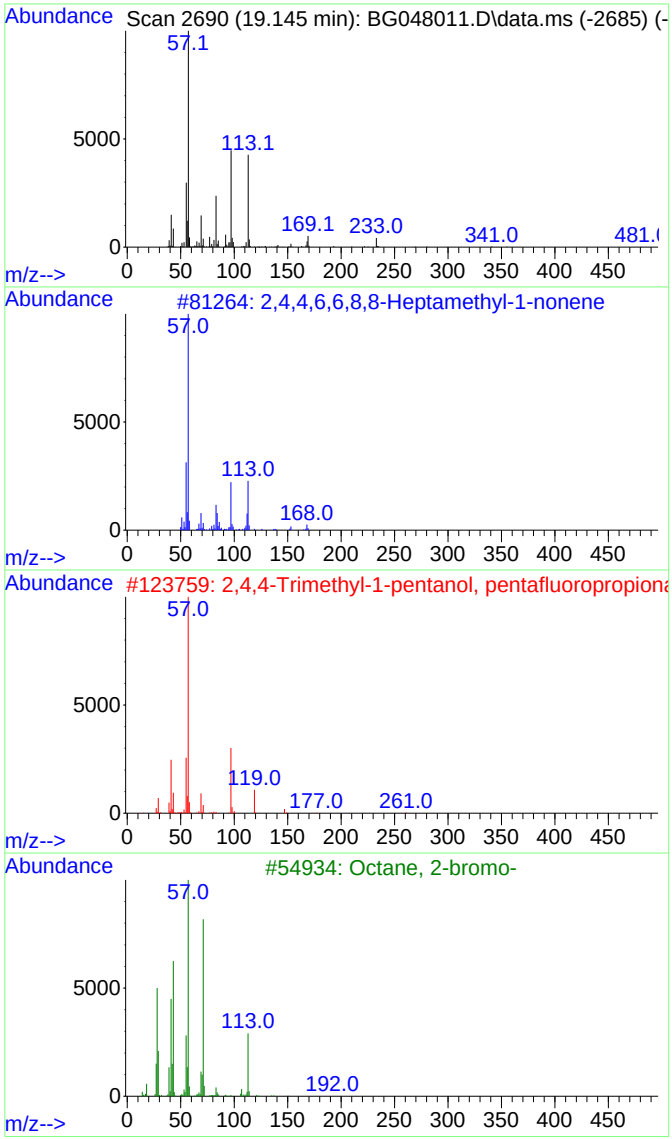
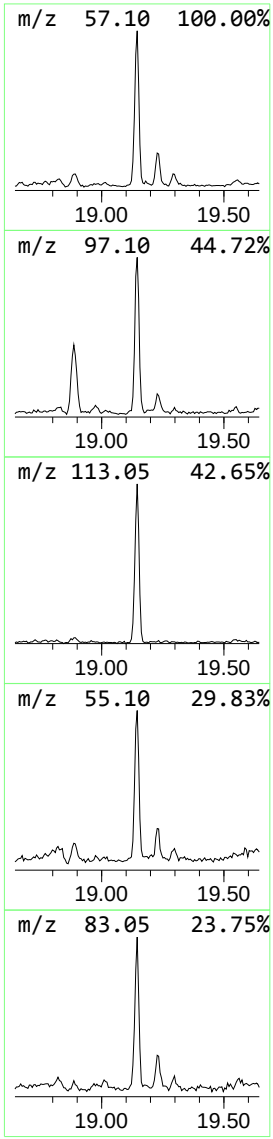
****

Peak Number 5 unknown19.145 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.145	11.38 ng	449650	Phenanthrene-d10	17.494

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	43
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	35
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
4	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	32
5	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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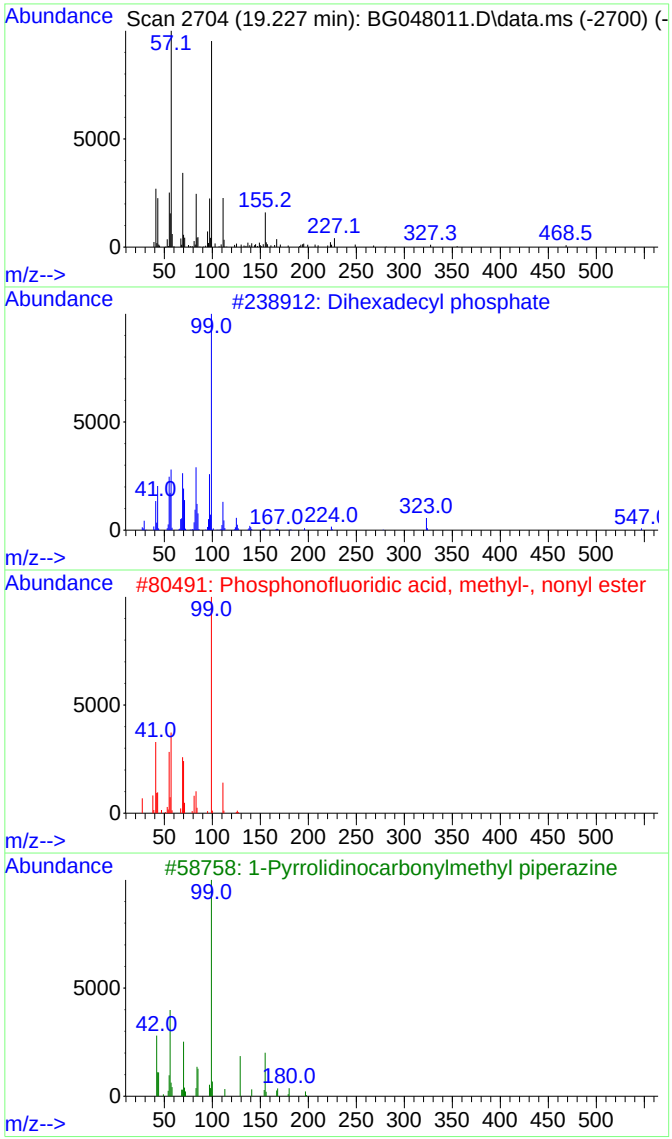
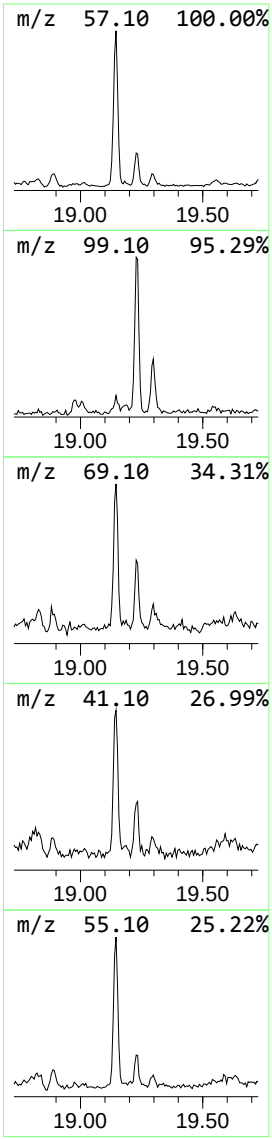
****

Peak Number 6 unknown19.227 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.227	3.17 ng	125172	Phenanthrene-d10	17.494

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dihexadecyl phosphate	546	C32H67O4P	002197-63-9	42
2	Phosphonofluoridic acid, methyl-...	224	C10H22FO2P	211192-74-4	25
3	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	23
4	Hexanoic acid, 4-tridecyl ester	298	C19H38O2	1000279-29-3	23
5	D-Gulonic acid, .gamma.-lactone,...	254	C10H16B2O6	074128-60-2	23





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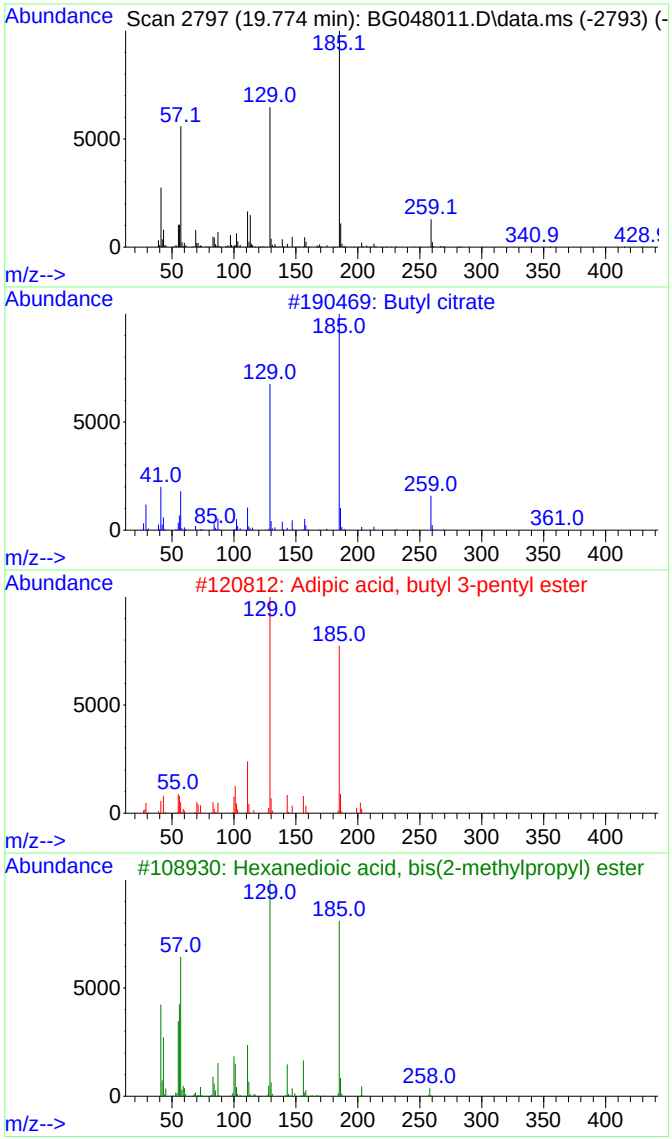
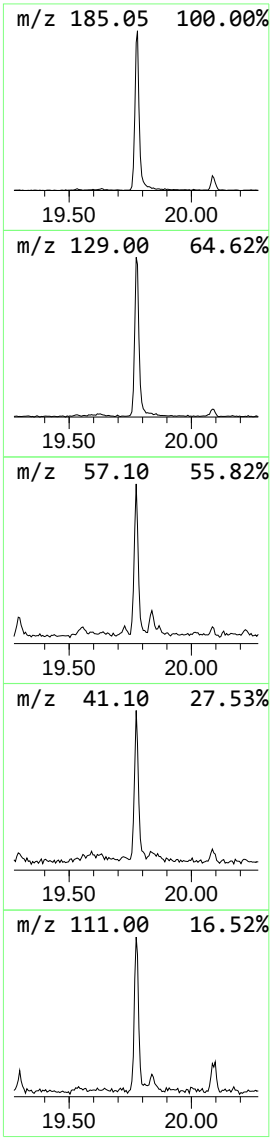
****

Peak Number 7 Butyl citrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.774	13.56 ng	604165	Chrysene-d12	21.766

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Adipic acid, butyl 3-pentyl ester	272	C15H28O4	1000324-60-5	64
3	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	50
4	Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	45
5	Dibutyl adipate	258	C14H26O4	000105-99-7	45





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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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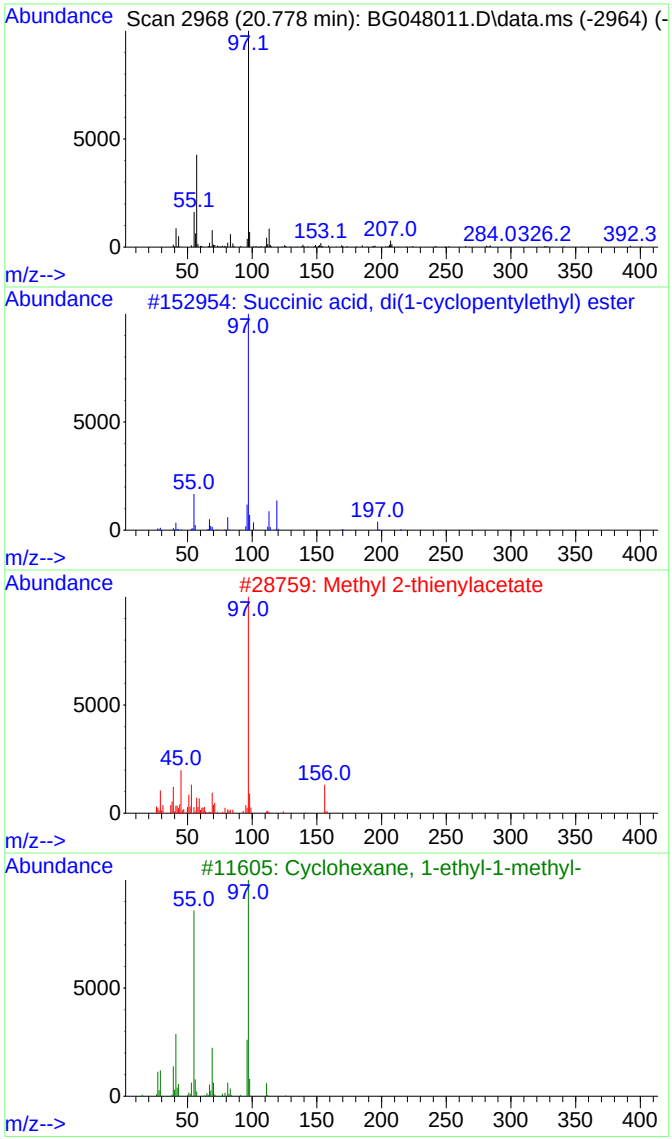
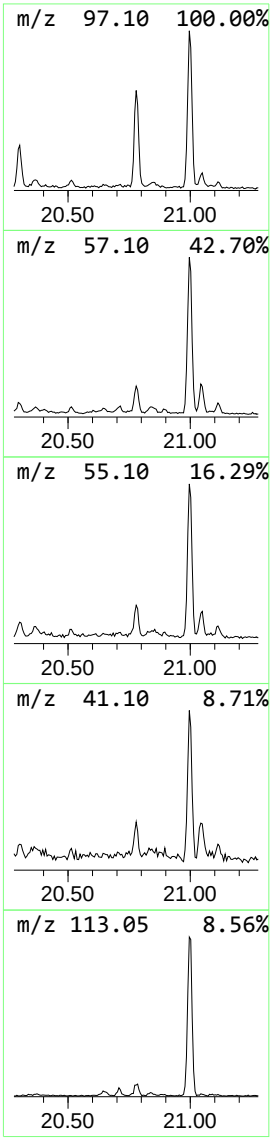
****
Peak Number 8 Succinic acid, di(1-cyclope... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.779	3.31 ng	147497	Chrysene-d12	21.766

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Succinic acid, di(1-cyclopentyle...	310	C18H30O4	1000330-21-8	50
2	Methyl 2-thienylacetate	156	C7H8O2S	019432-68-9	50
3	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	45
4	Ethanone, 1,2-di-2-furanyl-2-hyd...	192	C10H8O4	000552-86-3	39
5	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	39





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Sample : M1219-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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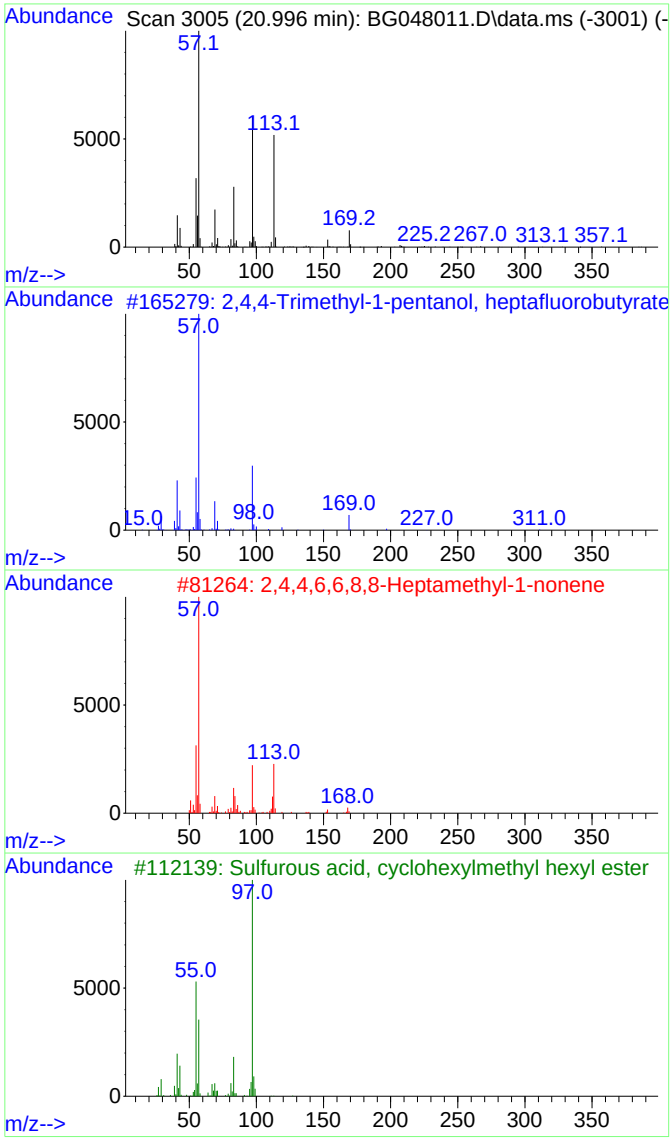
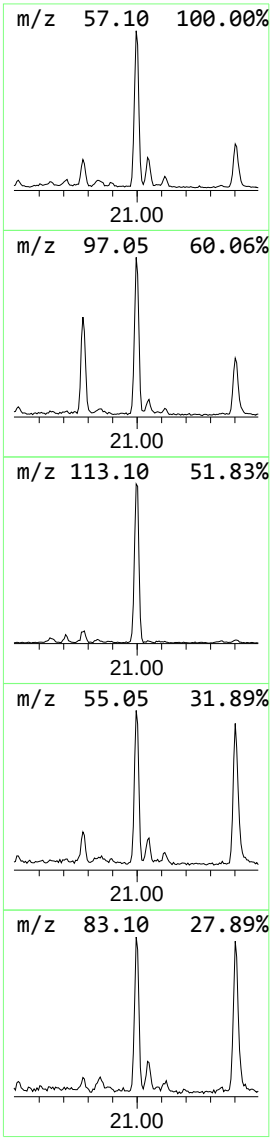
Peak Number 9 unknown20.996 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.996	14.11 ng	628550	Chrysene-d12	21.766

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	38
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38
3	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	37
4	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	37
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012621\
Data File : BG048011.D
Acq On : 26 Jan 2021 17:52
Operator : CG/JU
Sample : M1219-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : IDW-BR2-AQ-012121-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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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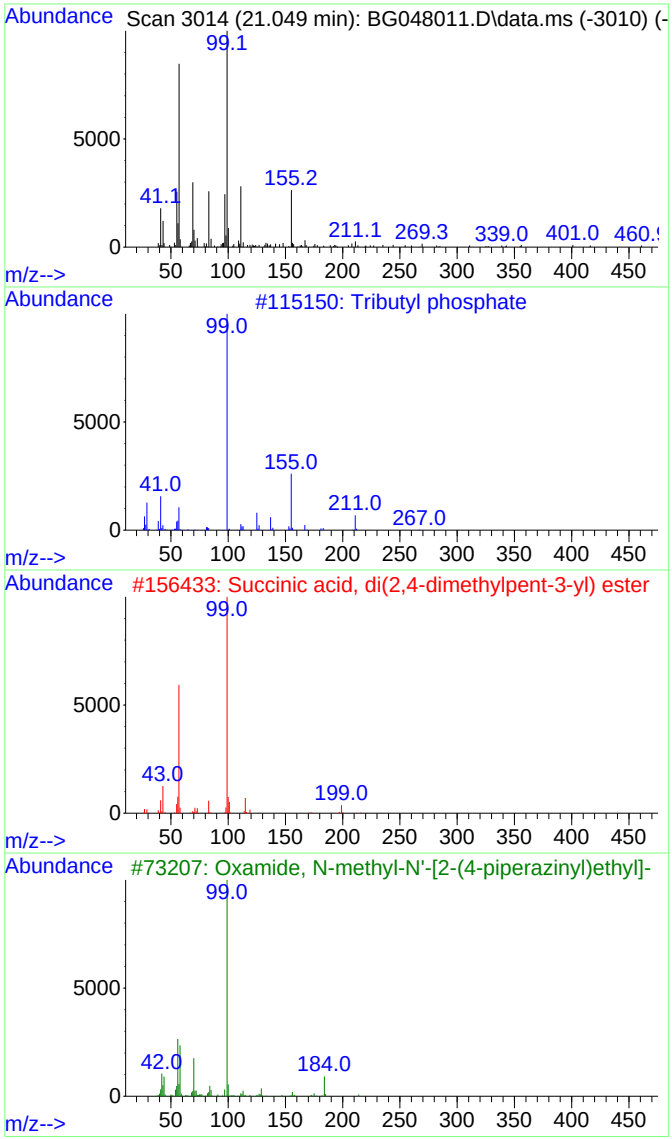
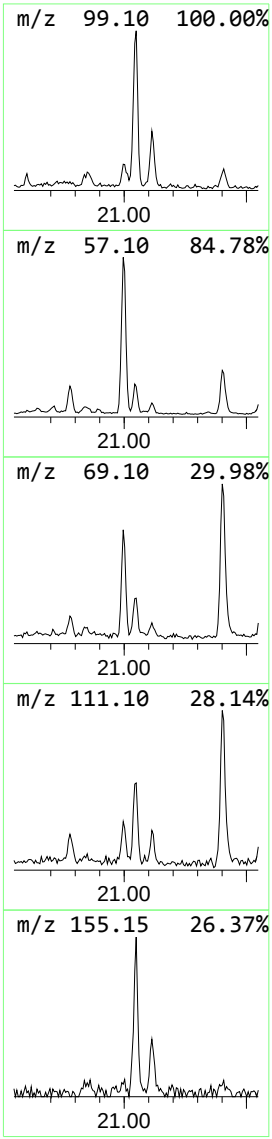
Peak Number 10 unknown21.049 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.049	3.17 ng	141067	Chrysene-d12	21.766

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	47
2	Succinic acid, di(2,4-dimethylpe...	314	C18H34O4	1000349-36-7	43
3	Oxamide, N-methyl-N'-[2-(4-piper...	214	C9H18N4O2	294877-47-7	35
4	Tetrahydrofuran-2-one, 3-[2-pent...	168	C10H16O2	1000132-08-6	35
5	Hexanoic acid, 6-tridecyl ester	298	C19H38O2	1000279-29-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012621\
Data File : BG048011.D
Acq On : 26 Jan 2021 17:52
Operator : CG/JU
Sample : M1219-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : IDW-BR2-AQ-012121-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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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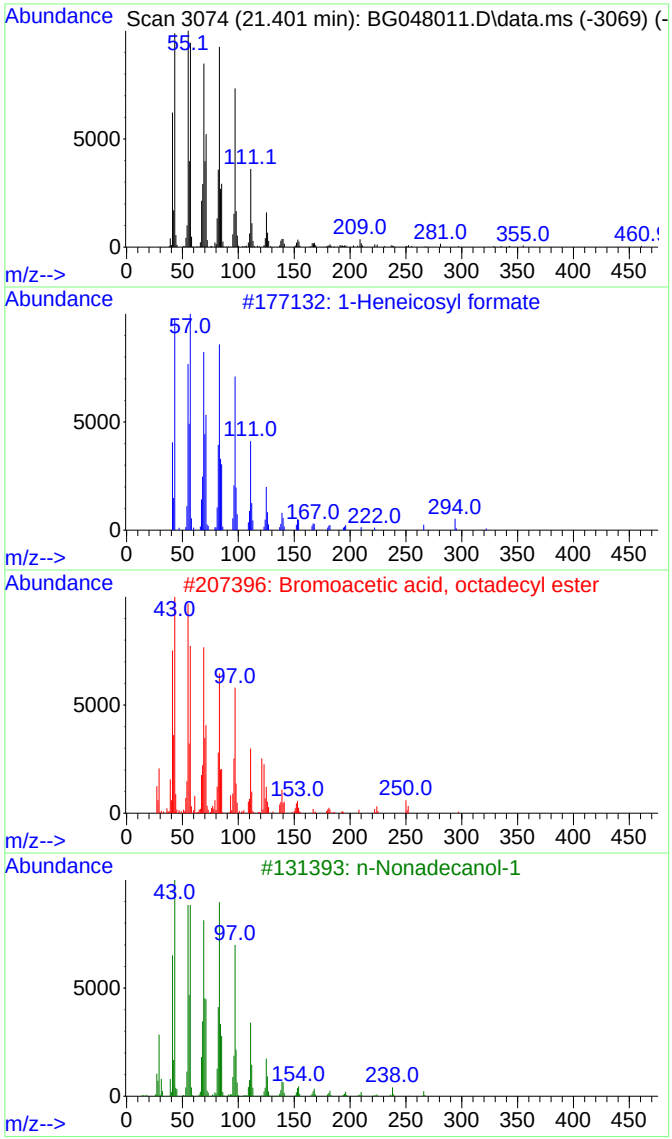
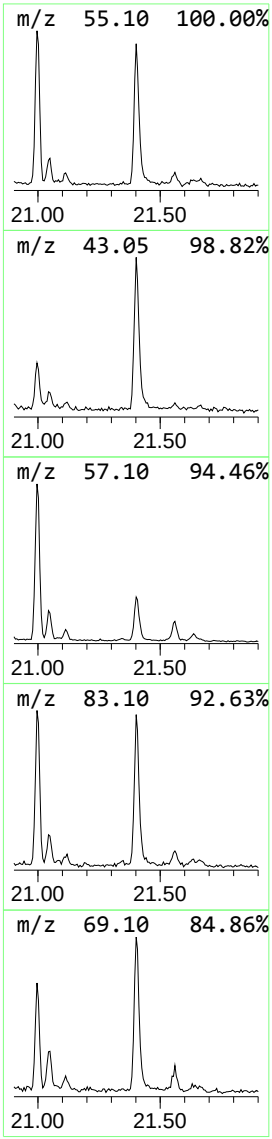
Peak Number 11 1-Heneicosyl formate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.401	13.33 ng	593552	Chrysene-d12	21.766

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012621\
Data File : BG048011.D
Acq On : 26 Jan 2021 17:52
Operator : CG/JU
Sample : M1219-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : IDW-BR2-AQ-012121-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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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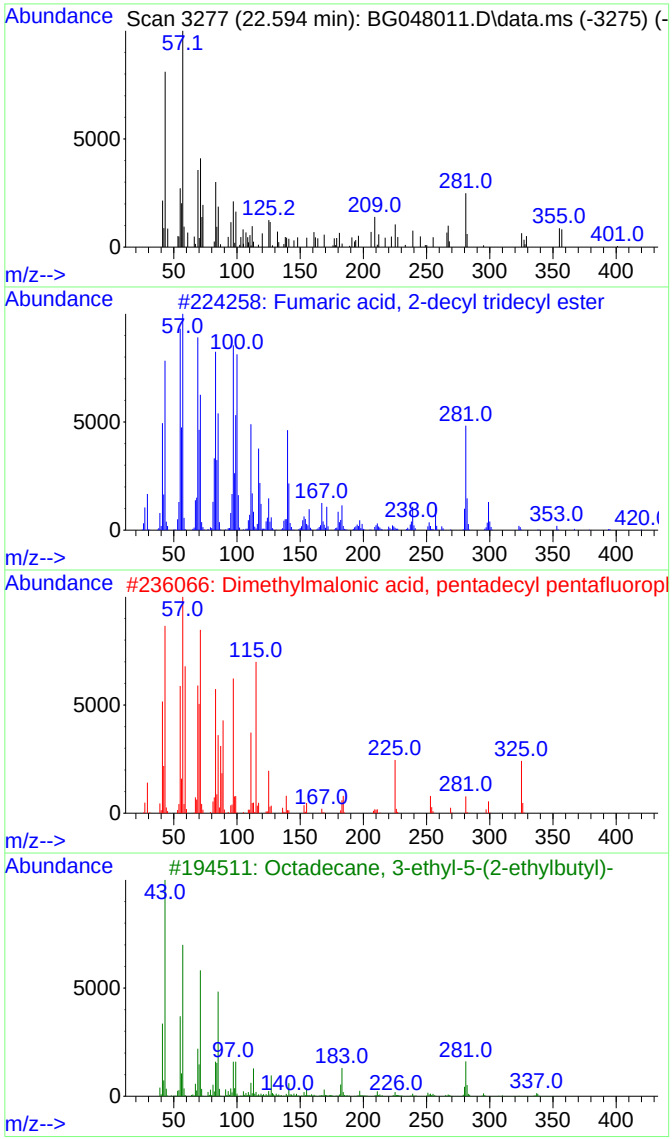
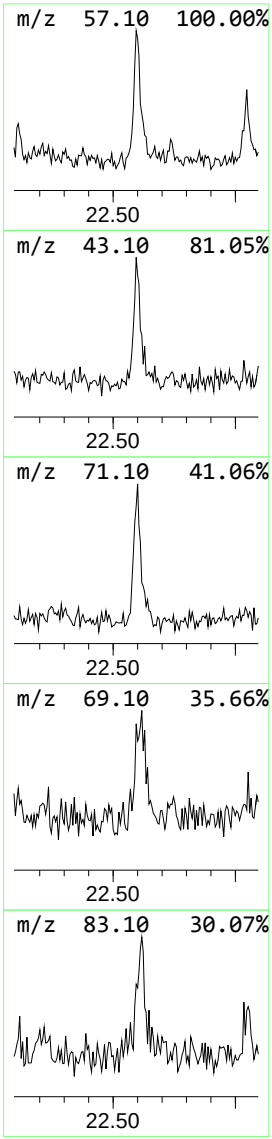
Peak Number 12 unknown22.594 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.594	2.31 ng	103109	Chrysene-d12	21.766

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 2-decyl tridecyl e...	438	C27H50O4	1000348-59-4	37
2	Dimethylmalonic acid, pentadecyl...	508	C26H37F5O4	1000363-67-2	25
3	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	25
4	13,17,21-Trimethylheptatriacontane	563	C40H82	058668-40-9	25
5	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	23





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012621\
Data File : BG048011.D
Acq On : 26 Jan 2021 17:52
Operator : CG/JU
Sample : M1219-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : IDW-BR2-AQ-012121-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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
2-Pentanone, 4-...	5.220	6.2	ng	76612	1	8.129	249001	20.0
1-Hexanol	5.608	3.6	ng	45446	1	8.129	249001	20.0
Ethanol, 2-(2-b...	10.708	3.0	ng	51763	2	10.943	344811	20.0
Valeric acid, 2...	14.392	3.9	ng	112897	3	14.750	574218	20.0
unknown19.145	19.145	11.4	ng	449650	4	17.494	789923	20.0
unknown19.227	19.227	3.2	ng	125172	4	17.494	789923	20.0
Butyl citrate	19.774	13.6	ng	604165	5	21.766	890871	20.0
Succinic acid, ...	20.779	3.3	ng	147497	5	21.766	890871	20.0
unknown20.996	20.996	14.1	ng	628550	5	21.766	890871	20.0
unknown21.049	21.049	3.2	ng	141067	5	21.766	890871	20.0
1-Heneicosyl fo...	21.401	13.3	ng	593552	5	21.766	890871	20.0
unknown22.594	22.594	2.3	ng	103109	5	21.766	890871	20.0