LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048946.D
Acq On : 14 Jun 2021 12:40
Operator : CG/JU
Sample : M2678-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0216-COMP-K(DISCRETE-CL-16)

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-BG061121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048946.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.166	17	22	34	rVB	227659	366290	13.20%	2.410%
2	3.290	38	43	52	rVB	102202	147192	5.30%	0.969%
3	5.199	362	368	375	rBV	74479	125310	4.52%	0.825%
4	5.663	440	447	455	rBV	818565	1337133	48.18%	8.799%
5	5.740	456	460	472	rVB	30626	69542	2.51%	0.458%
6	7.261	711	719	727	rBV	841242	1489021	53.66%	9.798%
7	8.119	859	865	871	rVB	144288	244708	8.82%	1.610%
8	9.288	1056	1064	1073	rVB	521892	951136	34.27%	6.259%
9	10.704	1298	1305	1317	rBV2	306373	515527	18.58%	3.392%
10	10.945	1339	1346	1357	rVB	191415	356537	12.85%	2.346%
11	13.384	1754	1761	1773	rVB	1195724	1945955	70.12%	12.805%
12	14.758	1987	1995	2004	rBV	307324	515348	18.57%	3.391%
13	16.157	2228	2233	2238	rBV2	66011	96296	3.47%	0.634%
14	16.245	2241	2248	2260	rVB	1021339	1573521	56.70%	10.354%
15	17.508	2457	2463	2471	rBV	413562	648632	23.37%	4.268%
16	17.626	2478	2483	2489	rVB2	53862	81976	2.95%	0.539%
17	18.172	2570	2576	2581	rVB2	82323	128206	4.62%	0.844%
18	18.390	2609	2613	2619	rBV2	50738	72711	2.62%	0.478%
19	19.341	2766	2775	2778	rBV5	38002	71530	2.58%	0.471%
20	19.664	2826	2830	2836	rBV6	27375	46879	1.69%	0.308%
21	20.117	2901	2907	2913	rVB	2044253	2775076	100.00%	18.261%
22	20.875	3033	3036	3043	rBV	33780	43047	1.55%	0.283%
23	21.439	3127	3132	3137	rBV3	52122	89393	3.22%	0.588%
24	21.692	3171	3175	3183	rVB	68753	102067	3.68%	0.672%
25	21.803	3187	3194	3201	rVV2	390683	678652	24.46%	4.466%
26	23.031	3399	3403	3409	rVB3	35857	57599	2.08%	0.379%
27	25.140	3752	3762	3772	rBV2	227676	667216	24.04%	4.391%

Sum of corrected areas: 15196500

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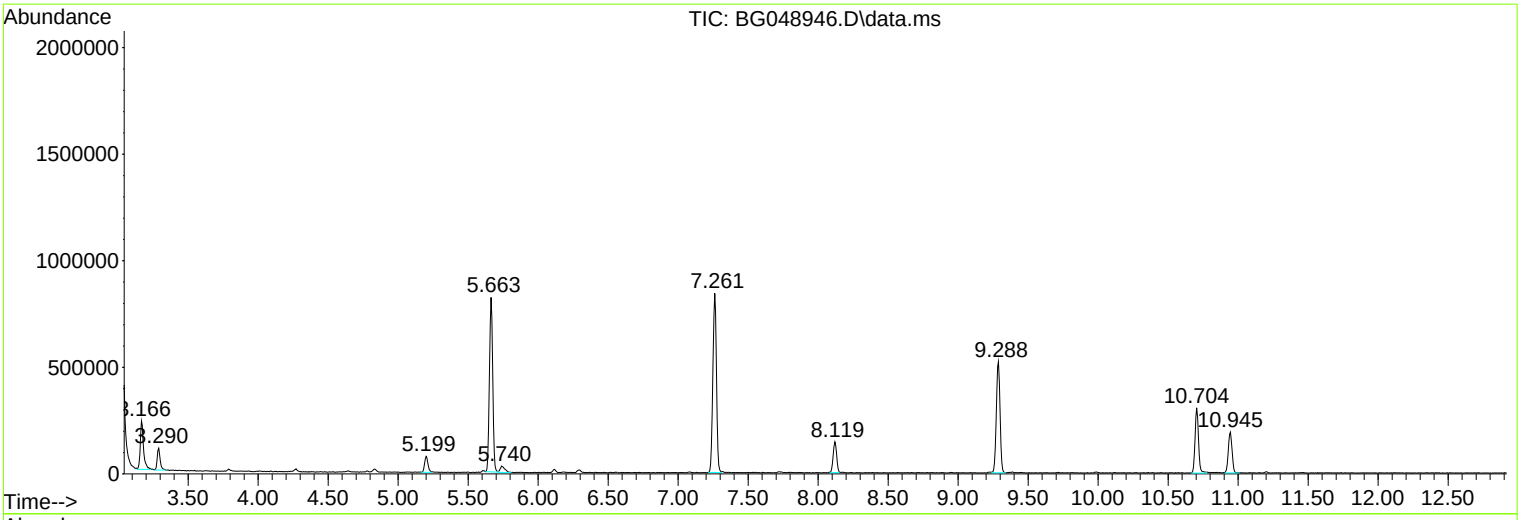
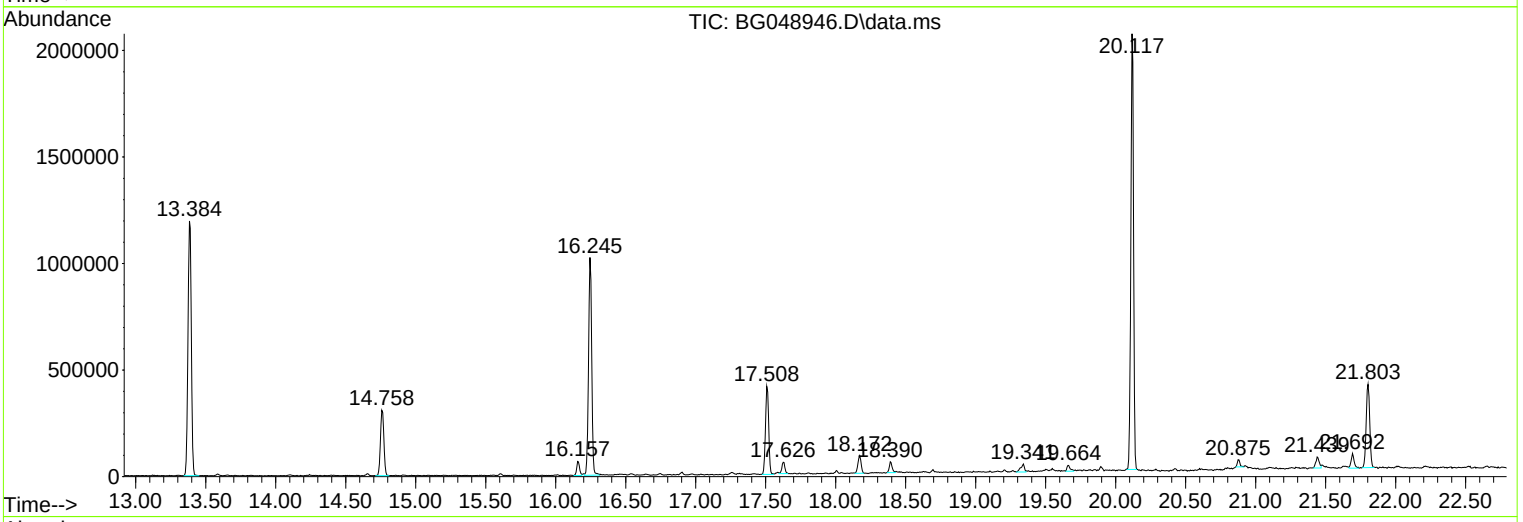
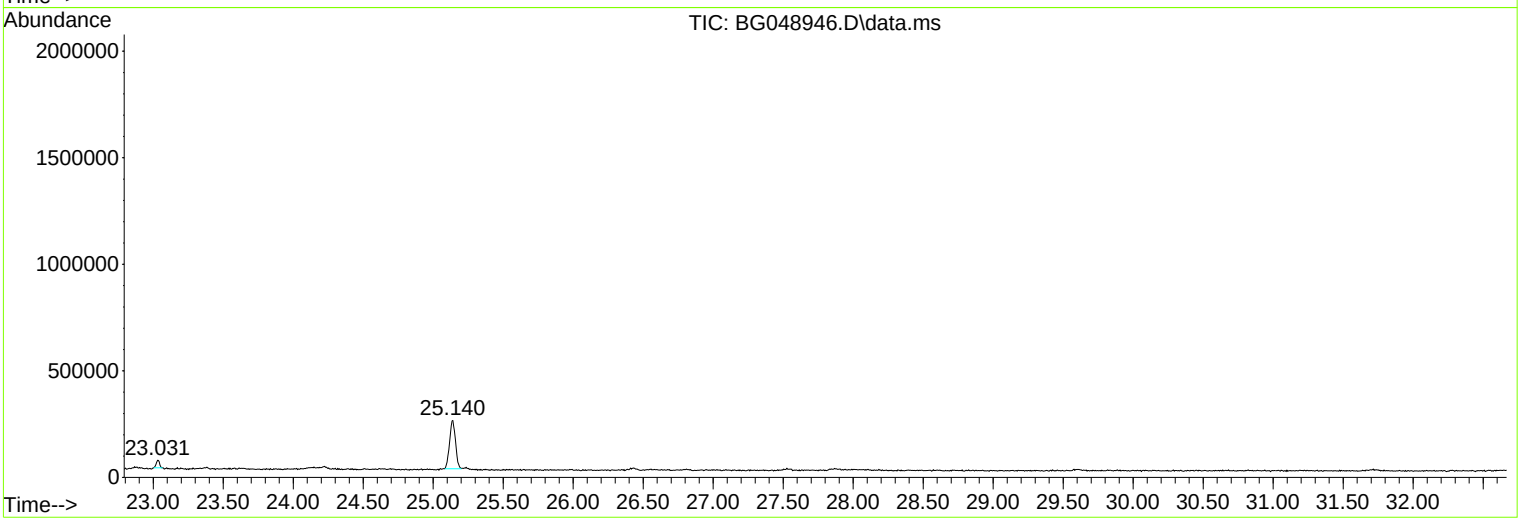
0216-COMP-K(DISCRETE-CL-16)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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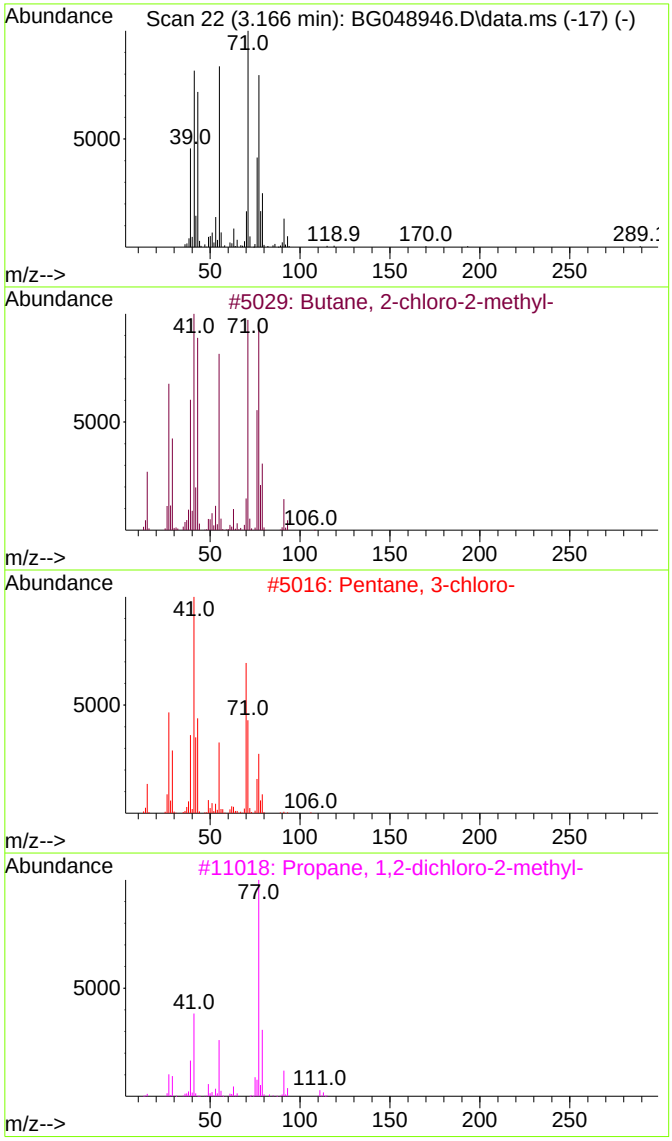
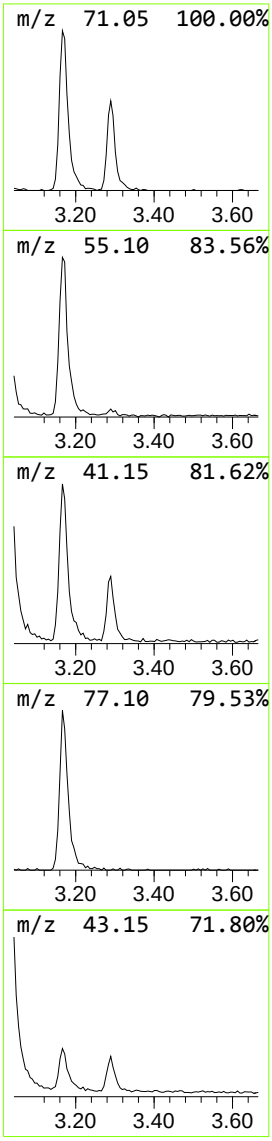
****
Peak Number 1 Butane, 2-chloro-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.166	29.94 ng	366290	1,4-Dichlorobenzene-d4	8.119

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-chloro-2-methyl-	106	C5H11Cl	000594-36-5	91
2	Pentane, 3-chloro-	106	C5H11Cl	000616-20-6	38
3	Propane, 1,2-dichloro-2-methyl-	126	C4H8Cl2	000594-37-6	27
4	2-Penten-1-ol, 2-methyl-, (E)-	100	C6H12O	016958-19-3	16
5	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	16





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Operator : CG/JU
Sample : M2678-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0216-COMP-K(DISCRETE-CL-16)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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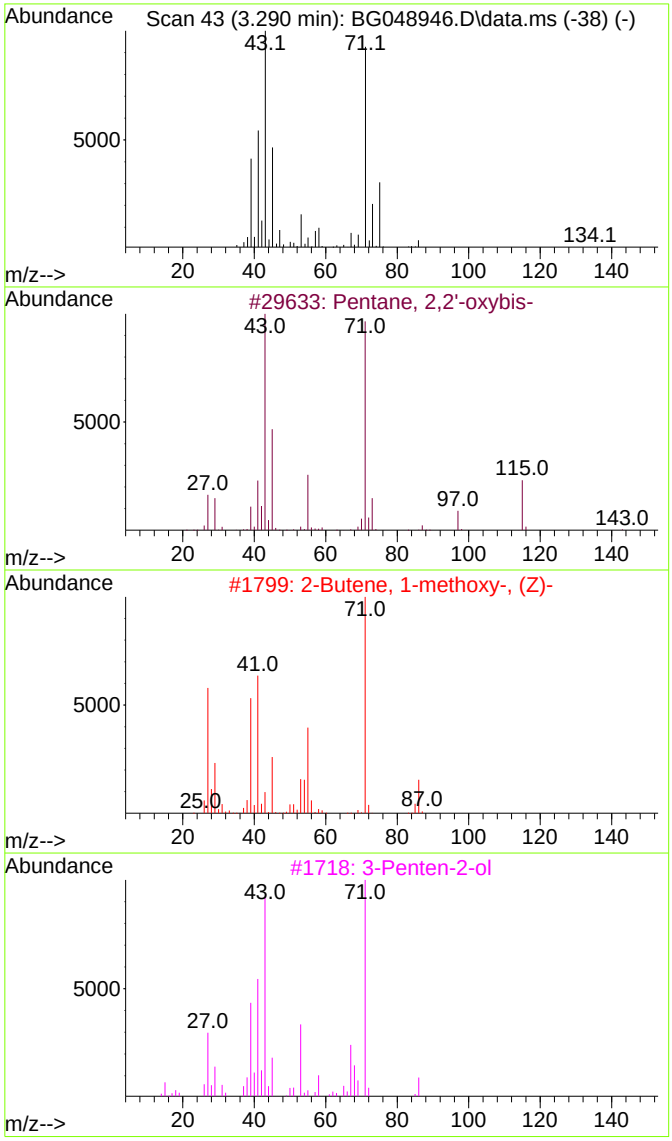
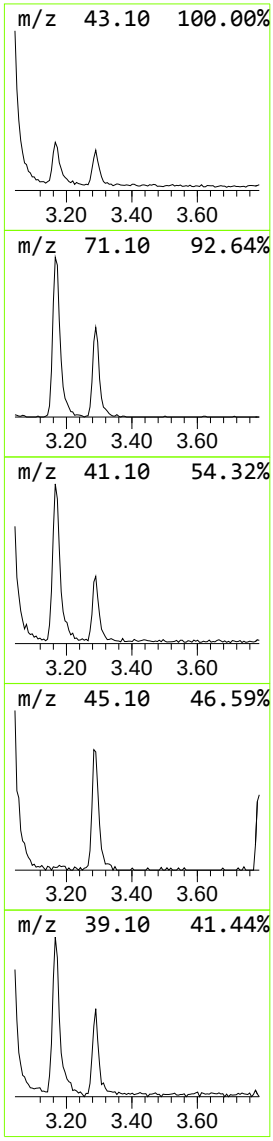
****

Peak Number 2 unknown3.290 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.290	12.03 ng	147192	1,4-Dichlorobenzene-d4	8.119

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	47
2	2-Butene, 1-methoxy-, (Z)-	86	C5H10O	010034-16-9	38
3	3-Penten-2-ol	86	C5H10O	001569-50-2	38
4	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	37
5	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	37





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Instrument :
BNA_G
ClientSampleId :
0216-COMP-K(DISCRETE-CL-16)

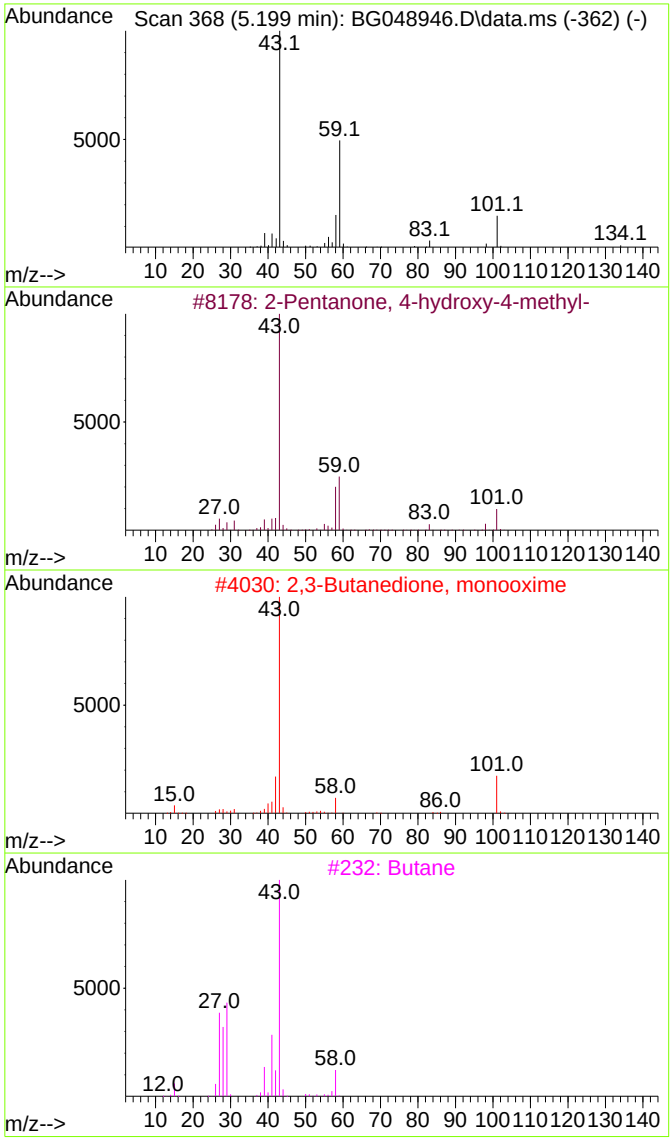
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

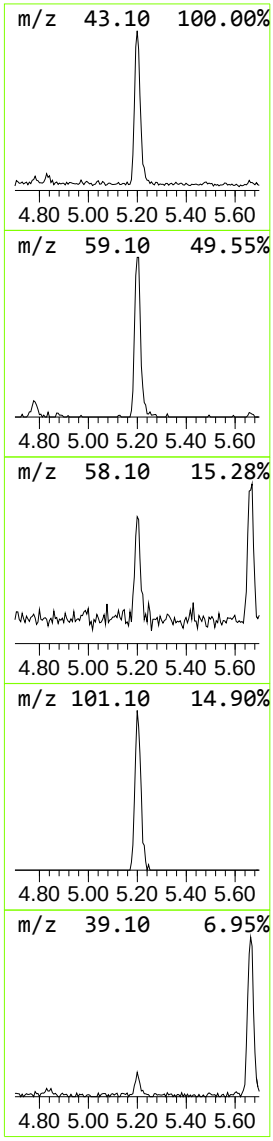
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.199	10.24 ng	125310	1,4-Dichlorobenzene-d4	8.119

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Butane	58	C4H10	000106-97-8	9
4	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0216-COMP-K(DISCRETE-CL-16)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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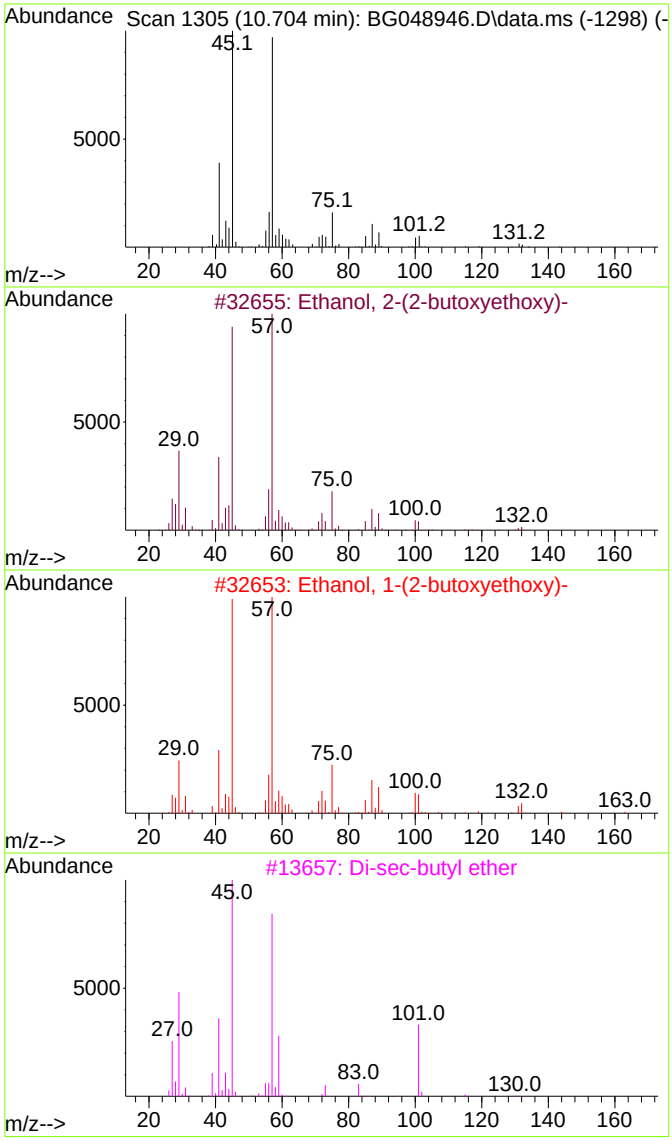
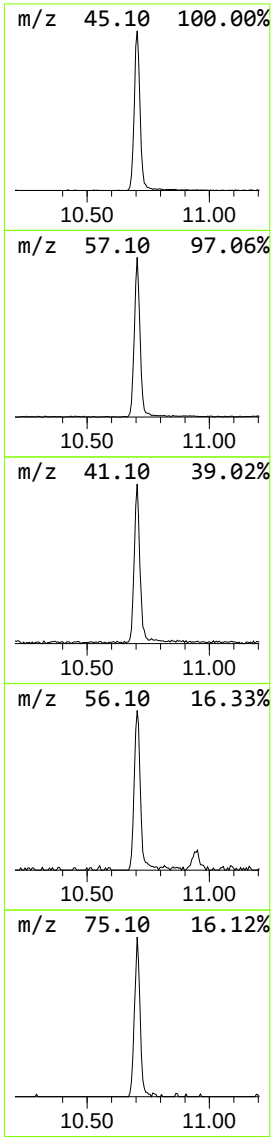
****

Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.704	28.92 ng	515527	Naphthalene-d8	10.945

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	78
3	Di-sec-butyl ether	130	C8H18O	006863-58-7	59
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	50





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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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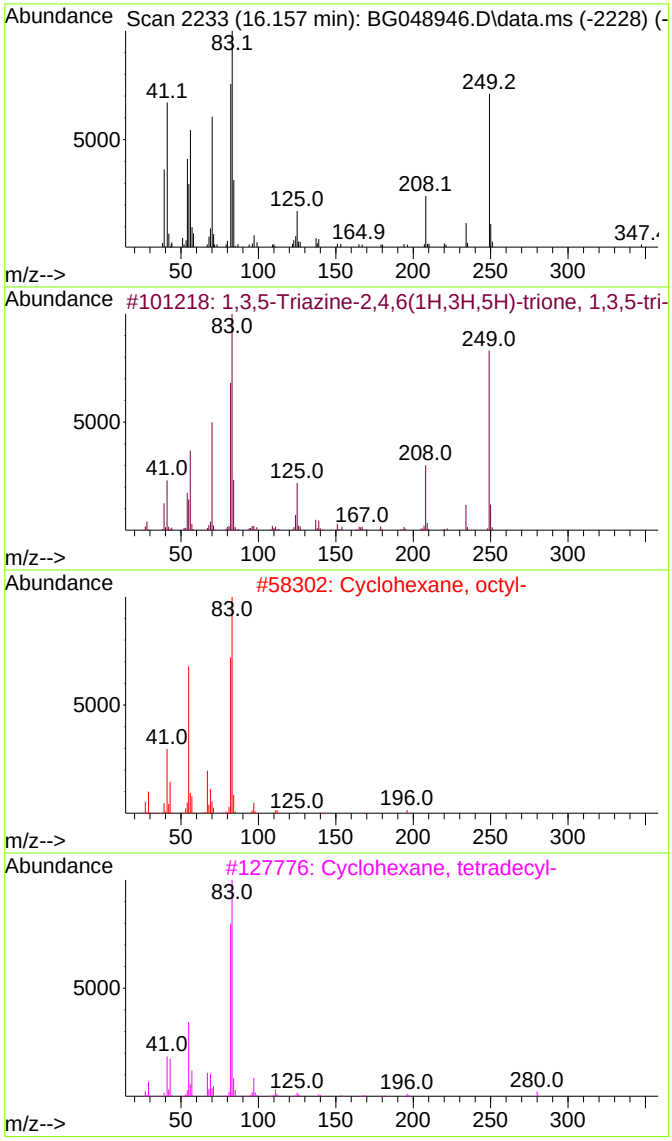
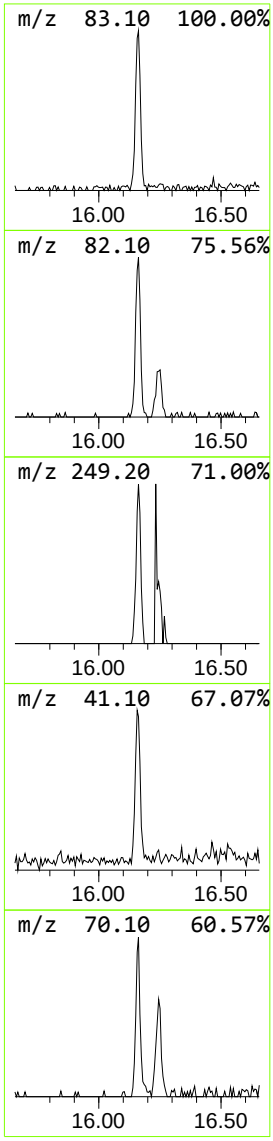
****
Peak Number 6 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.157	2.97 ng	96296	Phenanthrene-d10	17.508

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	96
2	Cyclohexane, octyl-	196	C14H28	001795-15-9	38
3	Cyclohexane, tetradecyl-	280	C20H40	001795-18-2	35
4	Cyclohexane, (4-methylpentyl)-	168	C12H24	061142-20-9	35
5	Cyclohexane, decyl-	224	C16H32	001795-16-0	35





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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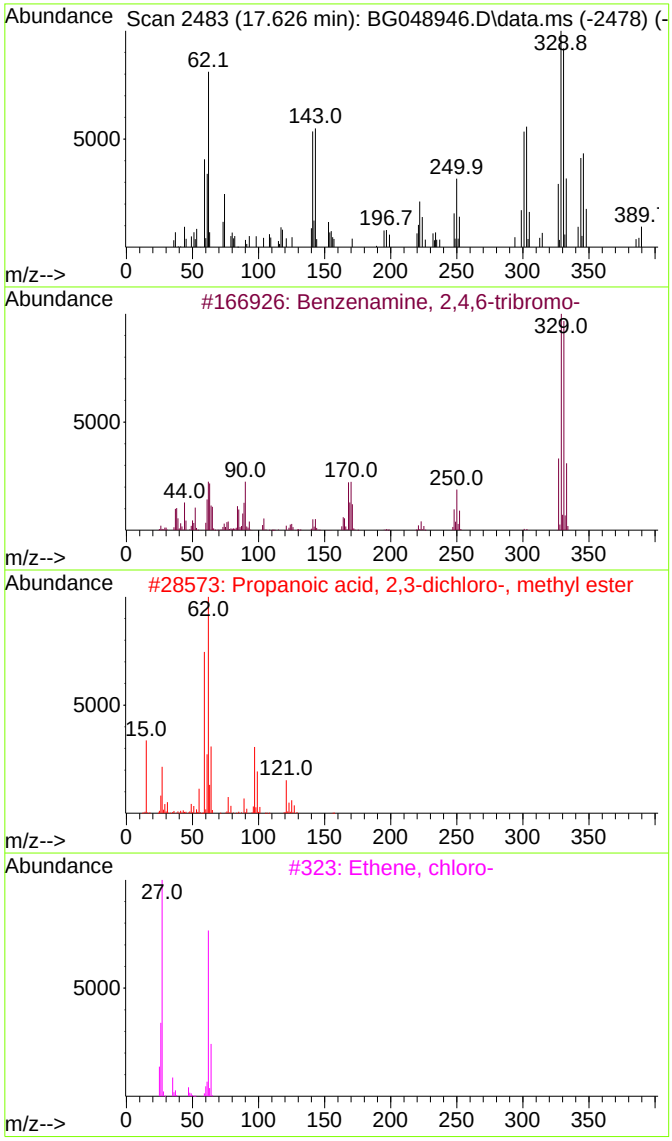
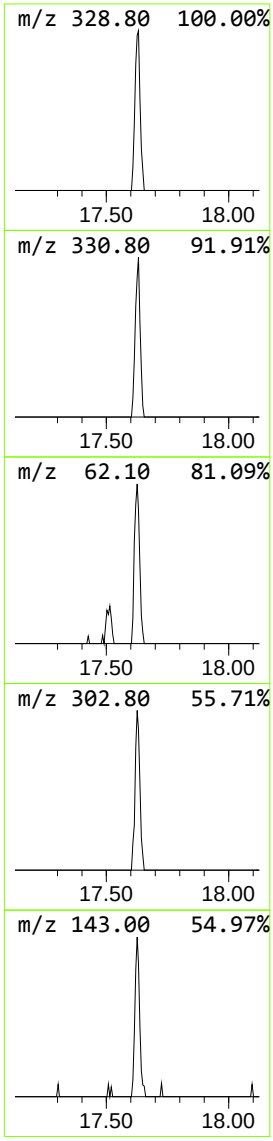
****

Peak Number 7 unknown17.626 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.626	2.53 ng	81976	Phenanthrene-d10	17.508

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	42
2	Propanoic acid, 2,3-dichloro-, m...	156	C4H6Cl2O2	003674-09-7	17
3	Ethene, chloro-	62	C2H3Cl	000075-01-4	9
4	Ethane, 1,2-dichloro-	98	C2H4Cl2	000107-06-2	9
5	Dimethyl sulfide	62	C2H6S	000075-18-3	9





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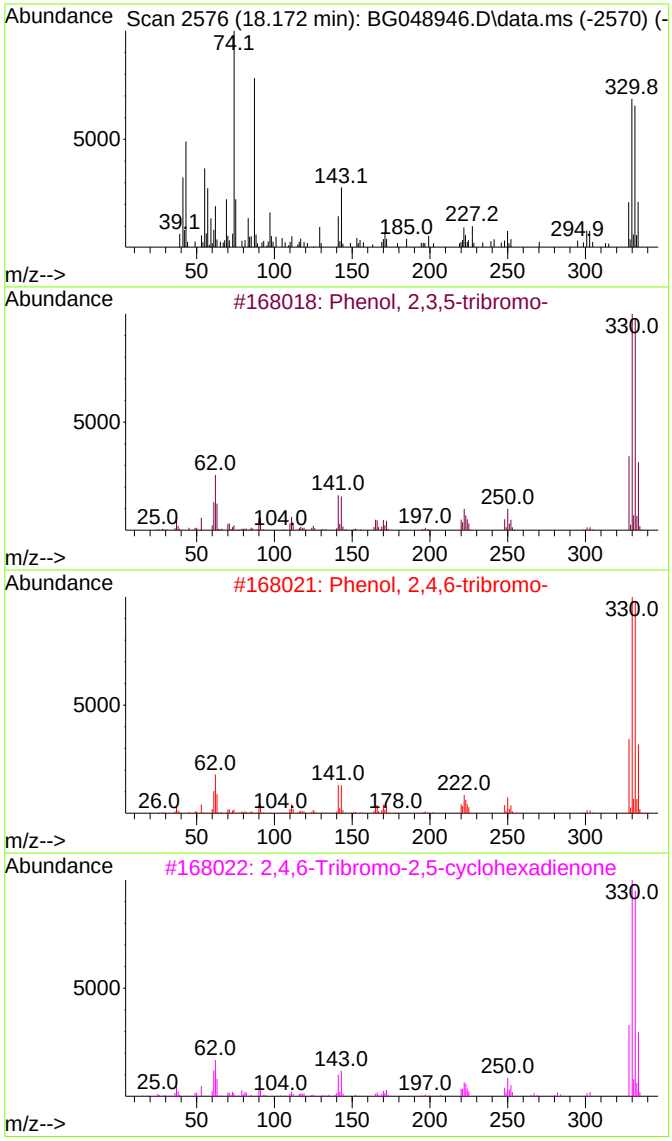
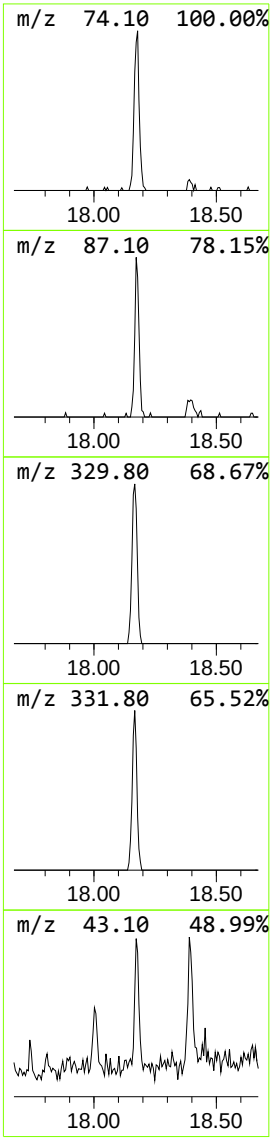
****

Peak Number 8 Phenol, 2,3,5-tribromo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.172	3.95 ng	128206	Phenanthrene-d10	17.508

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,3,5-tribromo-	328	C6H3Br3O	057383-81-0	97
2	Phenol, 2,4,6-tribromo-	328	C6H3Br3O	000118-79-6	96
3	2,4,6-Tribromo-2,5-cyclohexadienone	328	C6H3Br3O	020244-61-5	95
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	42
5	Methyl stearate	298	C19H38O2	000112-61-8	41





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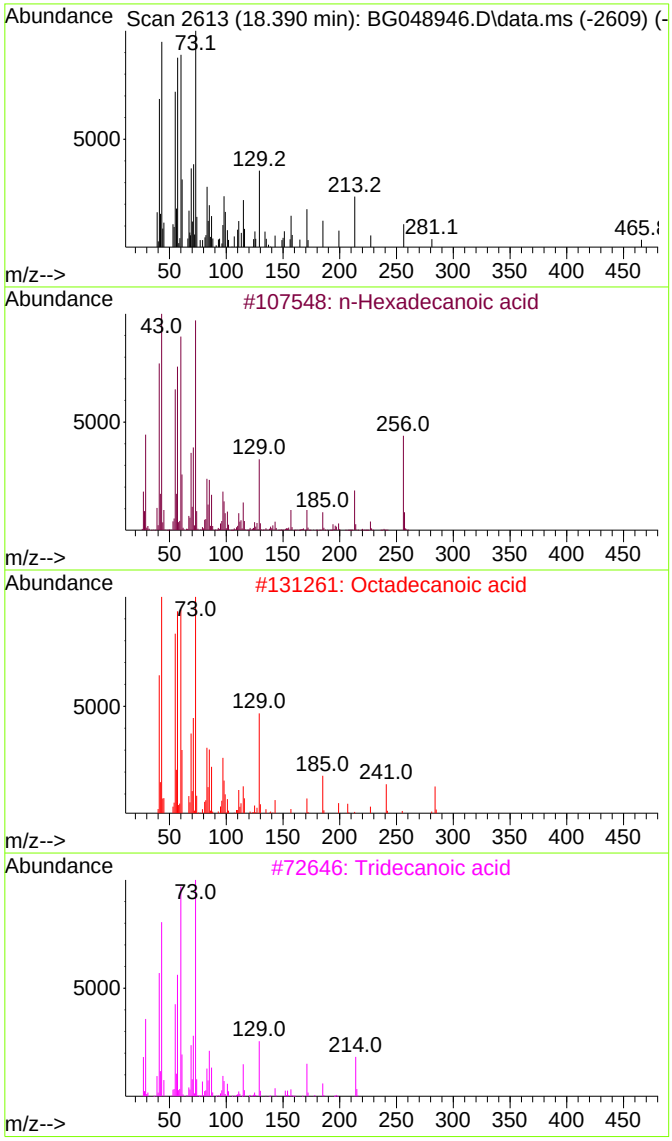
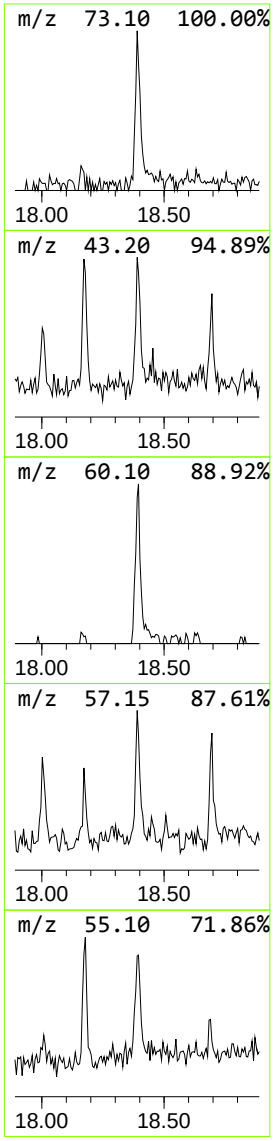
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.390	2.24 ng	72711	Phenanthrene-d10	17.508

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Octadecanoic acid	284	C18H36O2	000057-11-4	74
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





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Operator : CG/JU
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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-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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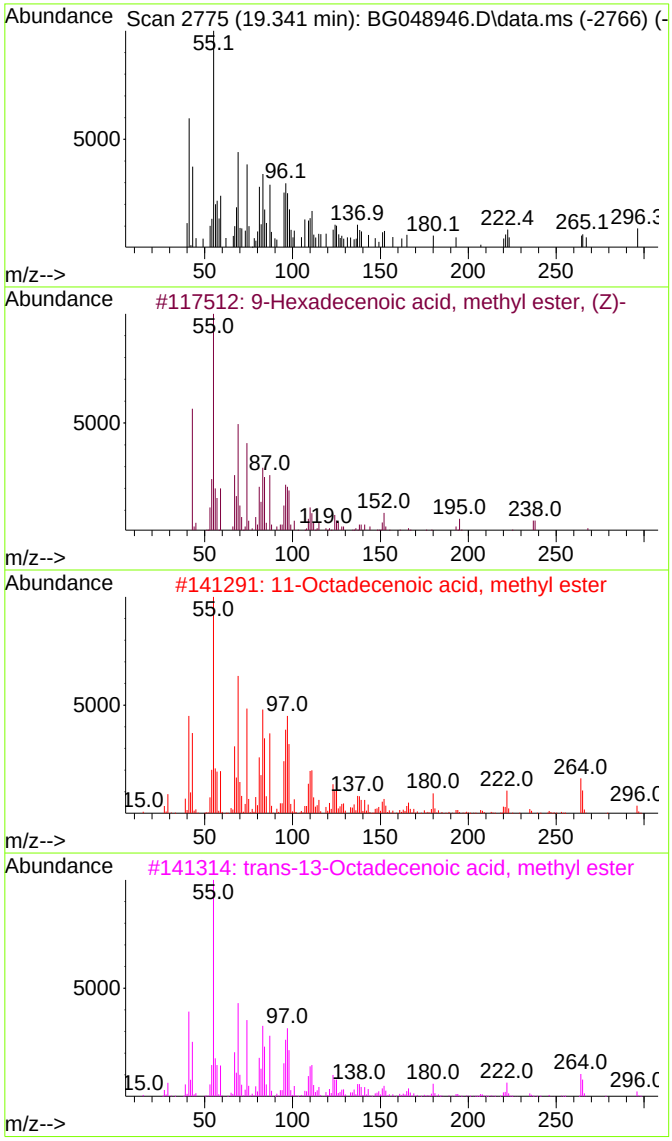
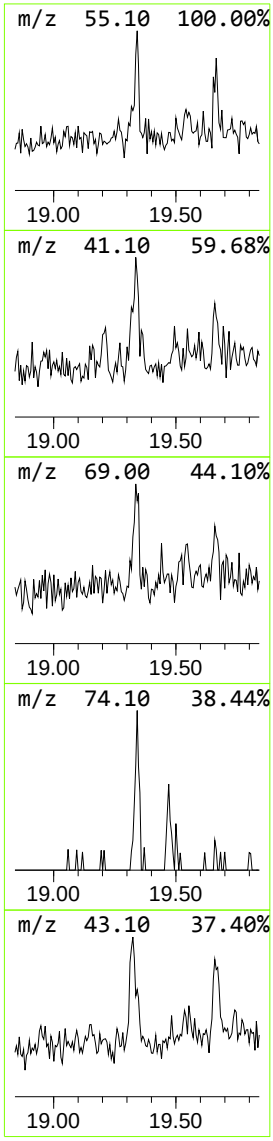
****
Peak Number 10 9-Hexadecenoic acid, methyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.341	2.21 ng	71530	Phenanthrene-d10	17.508

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	72
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	72
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	72
4	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	62
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048946.D
Acq On : 14 Jun 2021 12:40
Operator : CG/JU
Sample : M2678-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0216-COMP-K(DISCRETE-CL-16)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

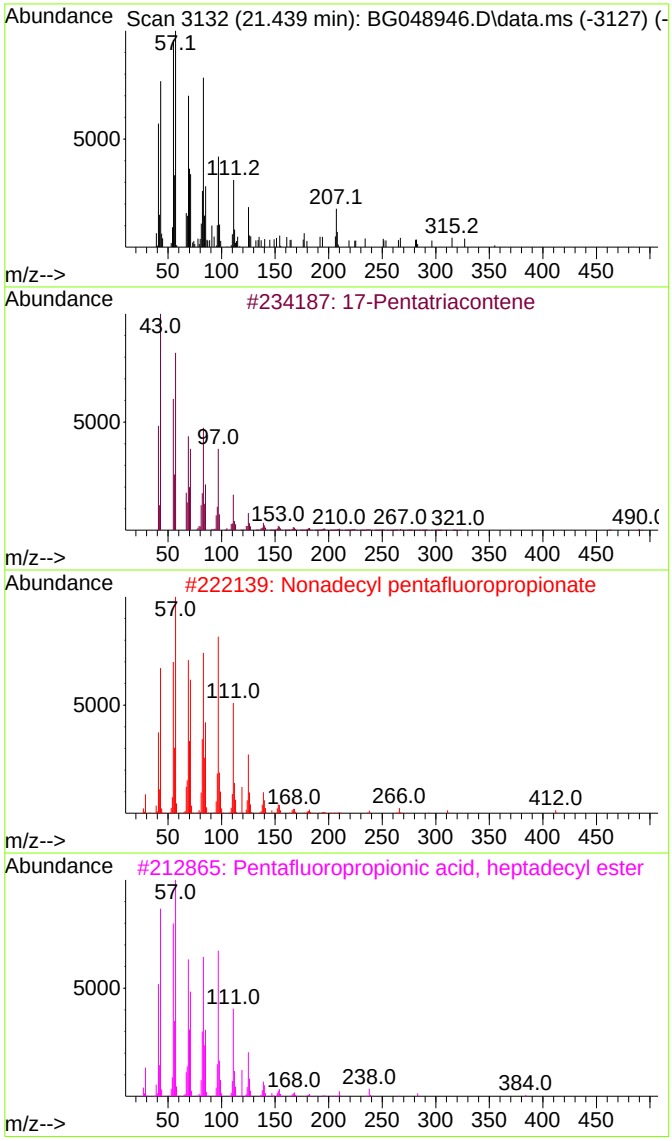
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

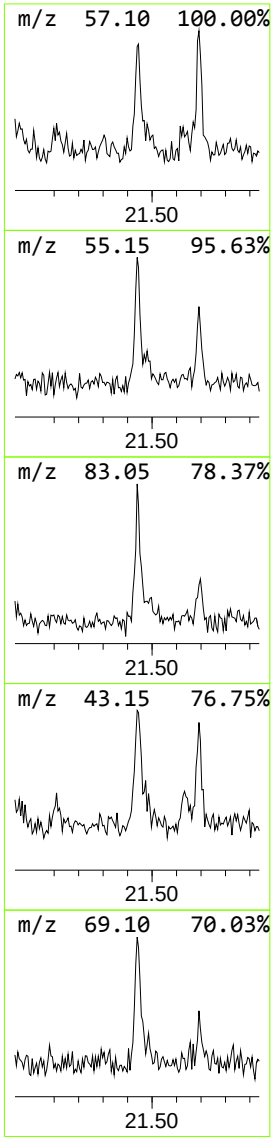
****

Peak Number 11 17-Pentatriacontene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.439	2.63 ng	89393	Chrysene-d12	21.803

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	64
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	53
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	53
4	Cyclohexadecane	224	C16H32	000295-65-8	50
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061421\
Data File : BG048946.D
Acq On : 14 Jun 2021 12:40
Operator : CG/JU
Sample : M2678-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0216-COMP-K(DISCRETE-CL-16)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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
Butane, 2-chlor...	3.166	29.9	ng	366290	1	8.119	244708	20.0
unknown3.290	3.290	12.0	ng	147192	1	8.119	244708	20.0
2-Pentanone, 4-...	5.199	10.2	ng	125310	1	8.119	244708	20.0
Ethanol, 2-(2-b...	10.704	28.9	ng	515527	2	10.945	356537	20.0
1,3,5-Triazine-...	16.157	3.0	ng	96296	4	17.508	648632	20.0
unknown17.626	17.626	2.5	ng	81976	4	17.508	648632	20.0
Phenol, 2,3,5-t...	18.172	4.0	ng	128206	4	17.508	648632	20.0
n-Hexadecanoic ...	18.390	2.2	ng	72711	4	17.508	648632	20.0
9-Hexadecenoic ...	19.341	2.2	ng	71530	4	17.508	648632	20.0
17-Pentatriacon...	21.439	2.6	ng	89393	5	21.803	678652	20.0