LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048048.D
Acq On : 28 Jan 2021 4:22
Operator : CG/JU
Sample : M1226-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0051-045-COMP-E-ELUTRIATE

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: BG048048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.676	391	398	409	rBV	584722	953802	23.00%	4.570%
2	7.268	661	669	680	rBV	432716	768355	18.53%	3.681%
3	8.126	808	815	820	rBV	181439	301469	7.27%	1.444%
4	9.283	1005	1012	1021	rBV	586122	1056067	25.47%	5.060%
5	10.934	1285	1293	1300	rBV	232516	411852	9.93%	1.973%
6	13.373	1699	1708	1715	rBV	1565997	2422129	58.42%	11.605%
7	14.189	1842	1847	1853	rBV	102986	150525	3.63%	0.721%
8	14.272	1857	1861	1870	rVB2	32127	41979	1.01%	0.201%
9	14.748	1935	1942	1951	rVB	393854	621360	14.99%	2.977%
10	14.953	1970	1977	1981	rBV	59346	82834	2.00%	0.397%
11	16.228	2187	2194	2205	rBV	1496131	2228558	53.75%	10.678%
12	17.491	2402	2409	2415	rVB	513785	793690	19.14%	3.803%
13	17.762	2448	2455	2460	rBV	749098	948607	22.88%	4.545%
14	18.150	2511	2521	2526	rBV7	40467	73523	1.77%	0.352%
15	18.373	2553	2559	2567	rBV	722830	981775	23.68%	4.704%
16	18.443	2567	2571	2577	rVB	49278	70936	1.71%	0.340%
17	19.137	2684	2689	2694	rBV	172769	218826	5.28%	1.048%
18	19.225	2700	2704	2709	rBV2	49952	60769	1.47%	0.291%
19	19.489	2745	2749	2751	rBV2	39075	44337	1.07%	0.212%
20	19.636	2769	2774	2786	rBV	515015	697840	16.83%	3.344%
21	19.765	2792	2796	2803	rVB3	58036	100687	2.43%	0.482%
22	20.088	2845	2851	2856	rBV	3061013	4146198	100.00%	19.866%
23	20.294	2883	2886	2891	rVB	34814	45566	1.10%	0.218%
24	20.770	2964	2967	2973	rVB	75839	103748	2.50%	0.497%
25	20.993	3000	3005	3009	rBV	335930	408853	9.86%	1.959%
26	21.040	3009	3013	3017	rVB	77578	96094	2.32%	0.460%
27	21.399	3069	3074	3085	rBV	457419	707634	17.07%	3.390%
28	21.551	3097	3100	3106	rVB	34721	42413	1.02%	0.203%
29	21.763	3130	3136	3143	rVB	573813	932784	22.50%	4.469%
30	22.597	3273	3278	3289	rVB8	38666	104090	2.51%	0.499%
31	24.119	3534	3537	3544	rVB6	23915	45623	1.10%	0.219%
32	25.047	3686	3695	3711	rVB	336001	986913	23.80%	4.729%
33	26.387	3915	3923	3935	rBV6	68160	221503	5.34%	1.061%

Sum of corrected areas: 20871339

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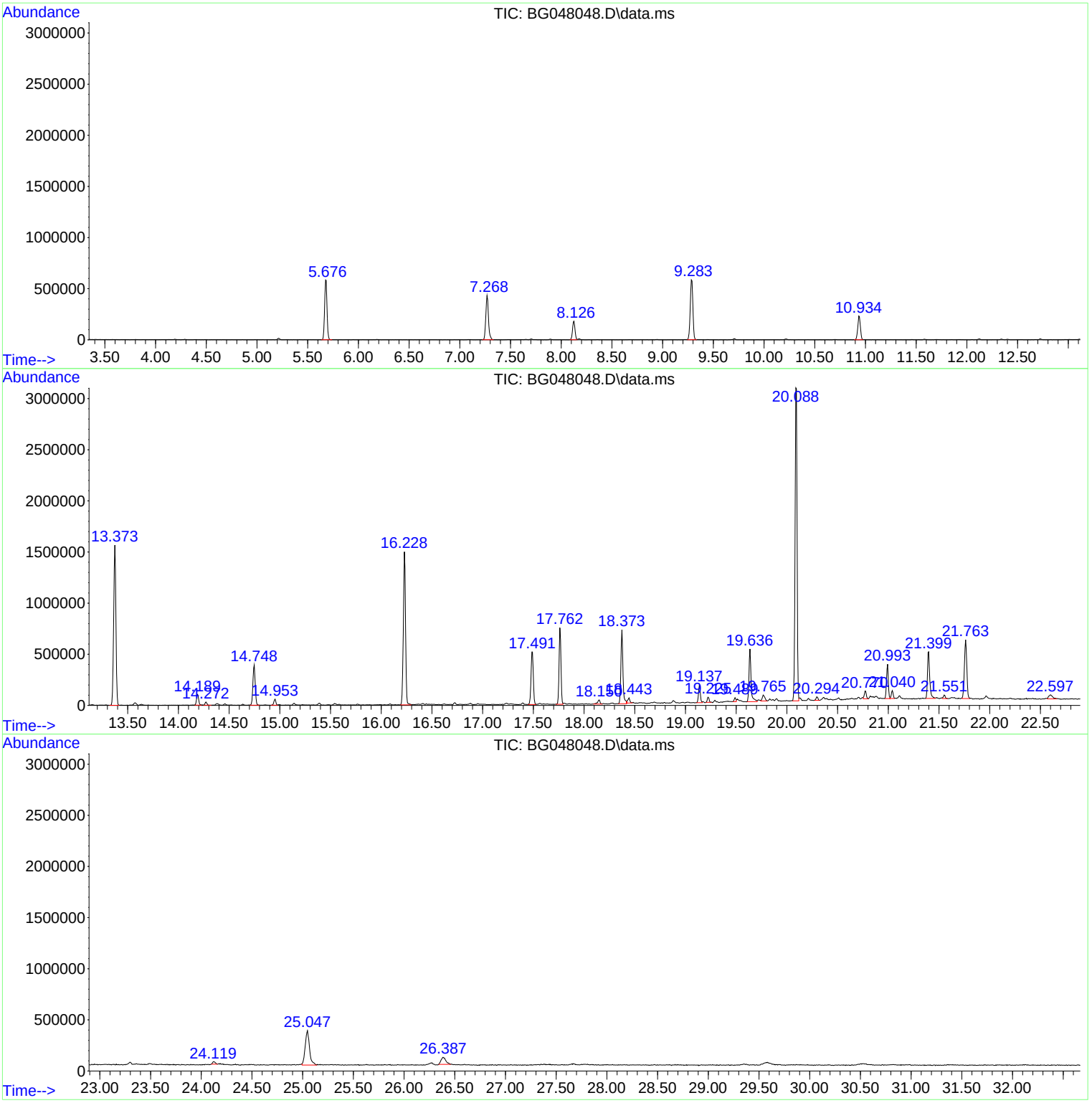
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0051-045-COMP-E-ELUTRIATE

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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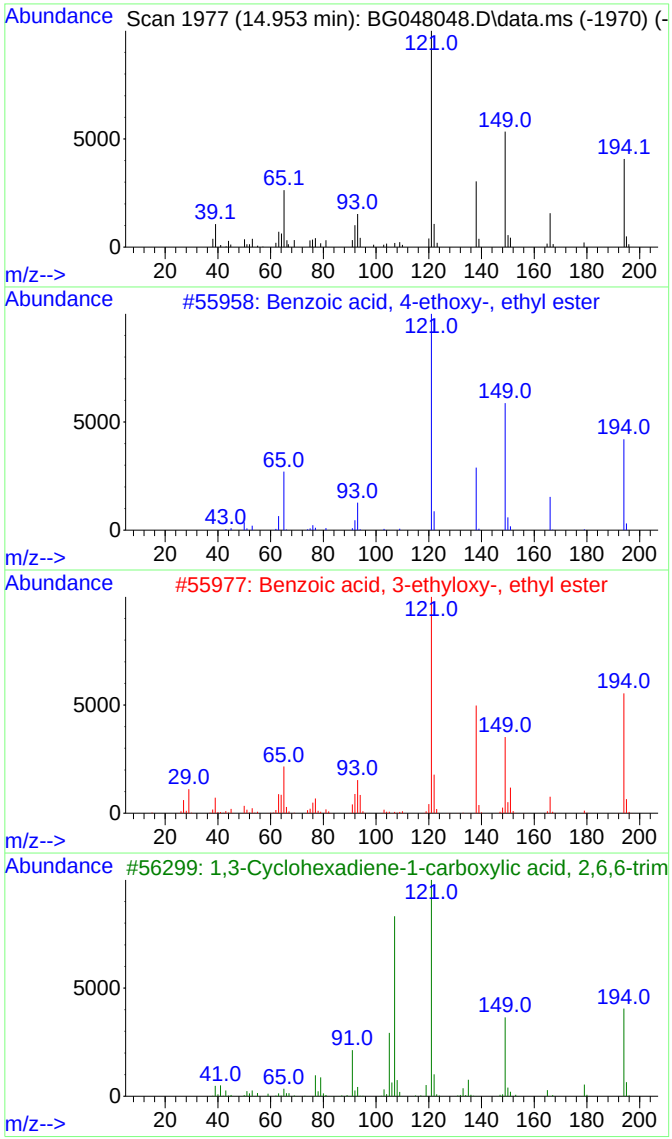
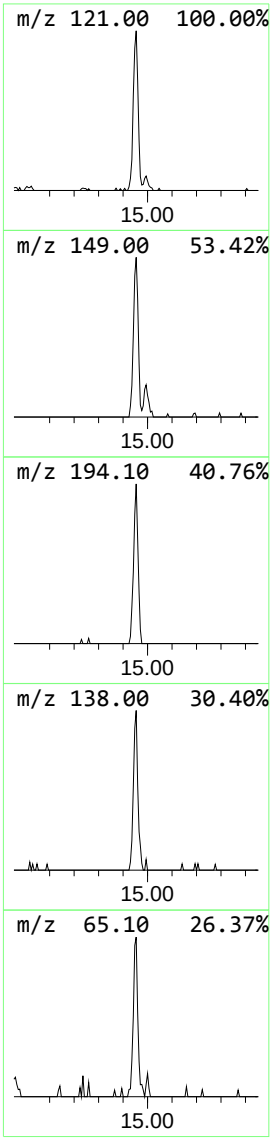
****
Peak Number 1 Benzoic acid, 4-ethoxy-, et... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.953	2.67 ng	82834	Acenaphthene-d10	14.748

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 4-ethoxy-, ethyl e...	194	C11H14O3	023676-09-7	96
2	Benzoic acid, 3-ethyloxy-, ethyl...	194	C11H14O3	1000374-55-3	55
3	1,3-Cyclohexadiene-1-carboxylic ...	194	C12H18O2	035044-59-8	53
4	4-Ethoxybenzhydrazide	180	C9H12N2O2	058586-81-5	50
5	4-(3-Hydroxyphenyl)-4-oxobutyric...	194	C10H10O4	056872-07-2	49





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Sample : M1226-08
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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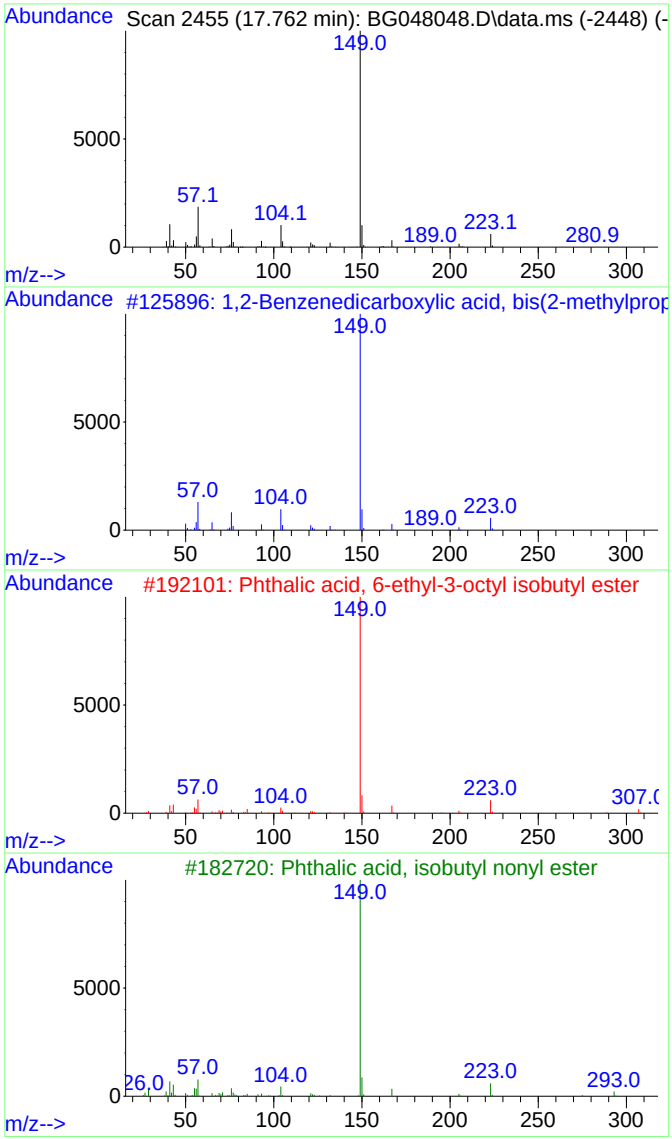
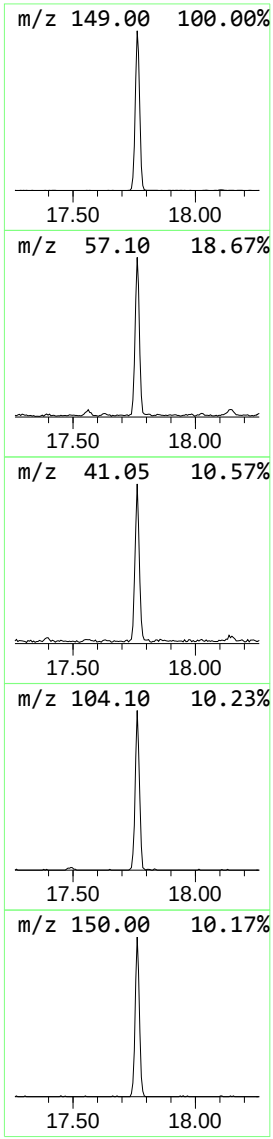
****
Peak Number 2 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.762	23.90 ng	948607	Phenanthrene-d10	17.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2	Phthalic acid, 6-ethyl-3-octyl i...	362	C22H34O4	1000315-17-9	83
3	Phthalic acid, isobutyl nonyl ester	348	C21H32O4	1000309-04-4	83
4	Phthalic acid, isobutyl octyl ester	334	C20H30O4	1000309-04-5	78
5	Phthalic acid, isobutyl pent-2-e...	286	C17H18O4	1000315-45-6	78





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Instrument :
BNA_G
ClientSampleId :
0051-045-COMP-E-ELUTRIATE

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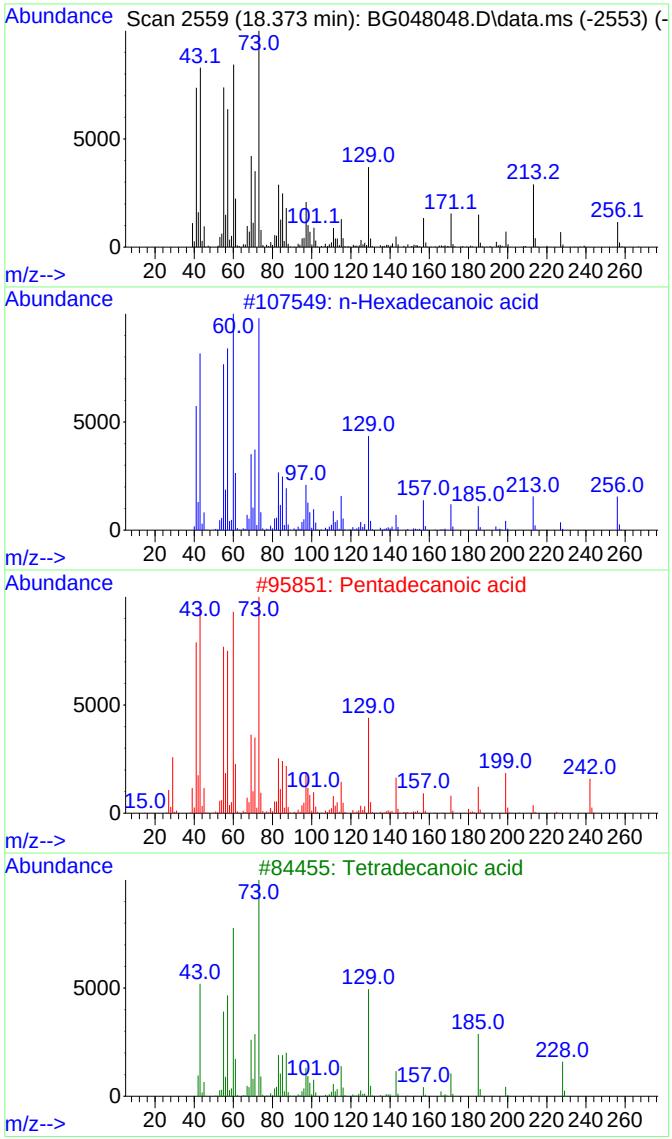
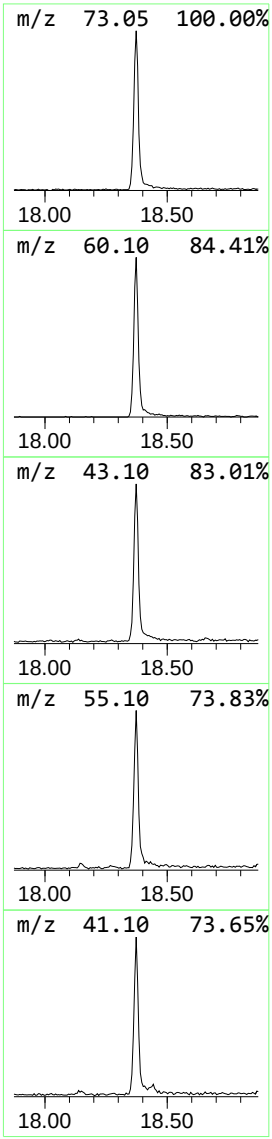
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.373	24.74 ng	981775	Phenanthrene-d10	17.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Isopropyl palmitate	298	C19H38O2	000142-91-6	50
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	47





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0051-045-COMP-E-ELUTRIATE

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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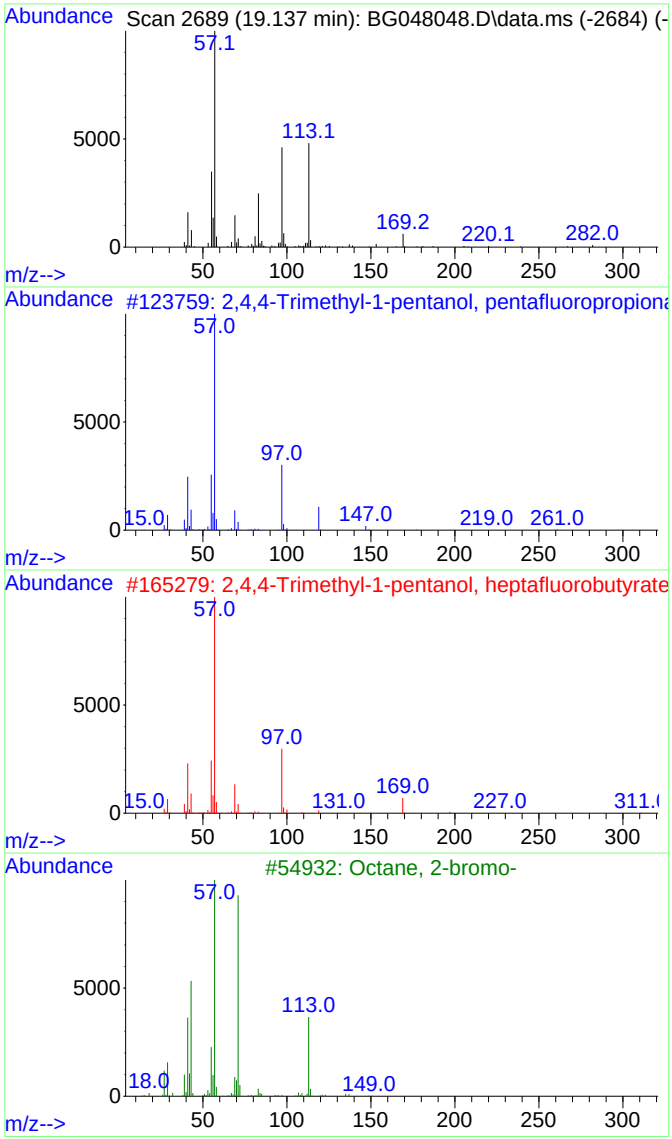
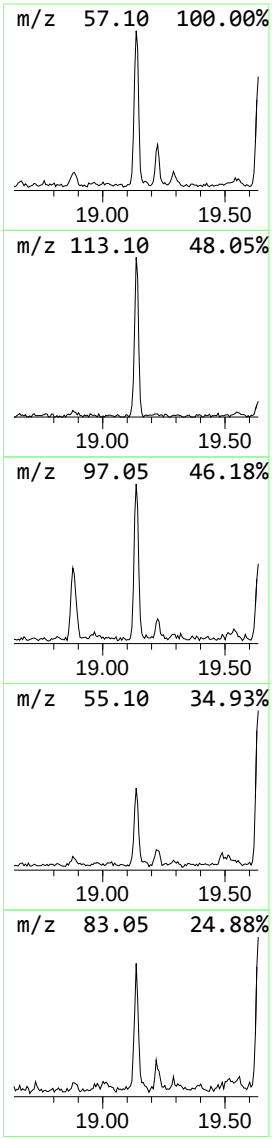
****

Peak Number 4 unknown19.137 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.137	5.51 ng	218826	Phenanthrene-d10	17.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	43
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	37
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
4	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	27





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Instrument :
BNA_G
ClientSampleId :
0051-045-COMP-E-ELUTRIATE

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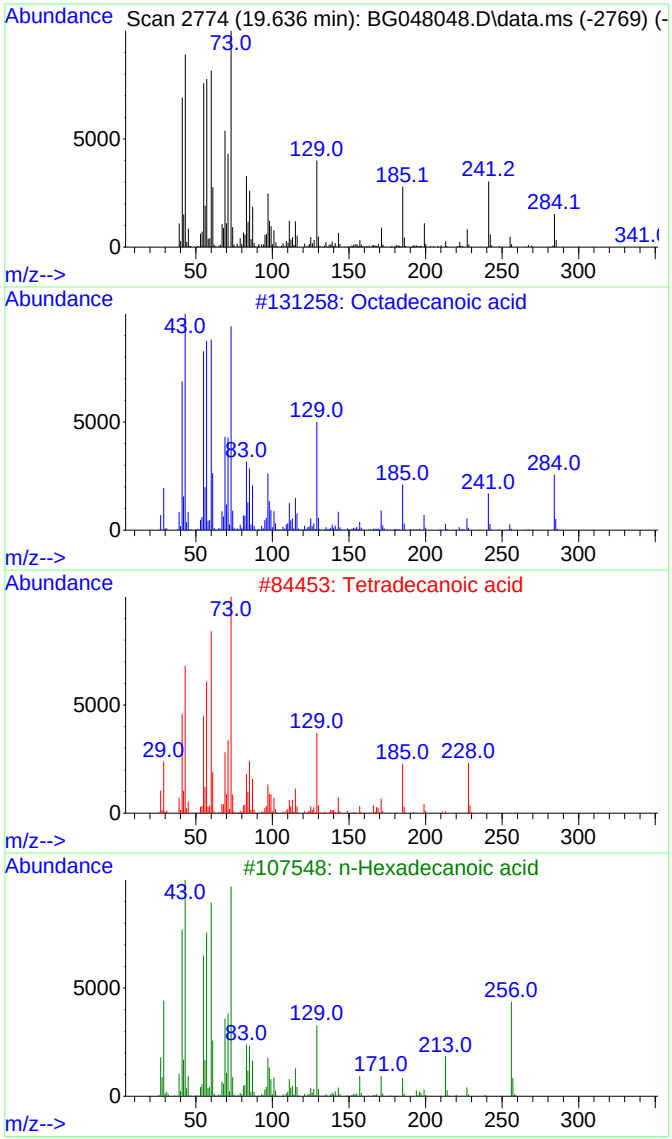
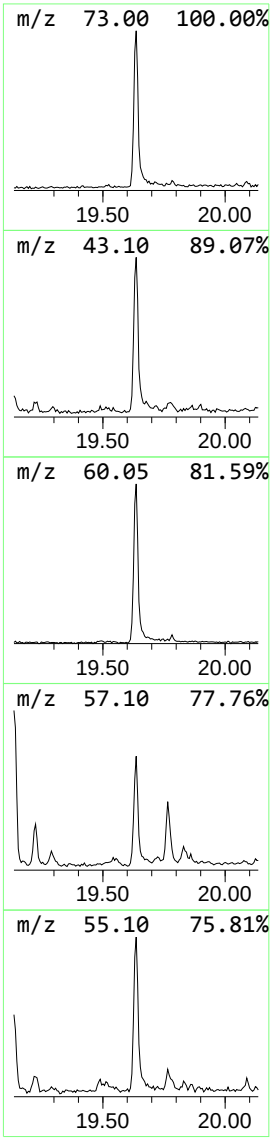
****

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.636	14.96 ng	697840	Chrysene-d12	21.763

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	74
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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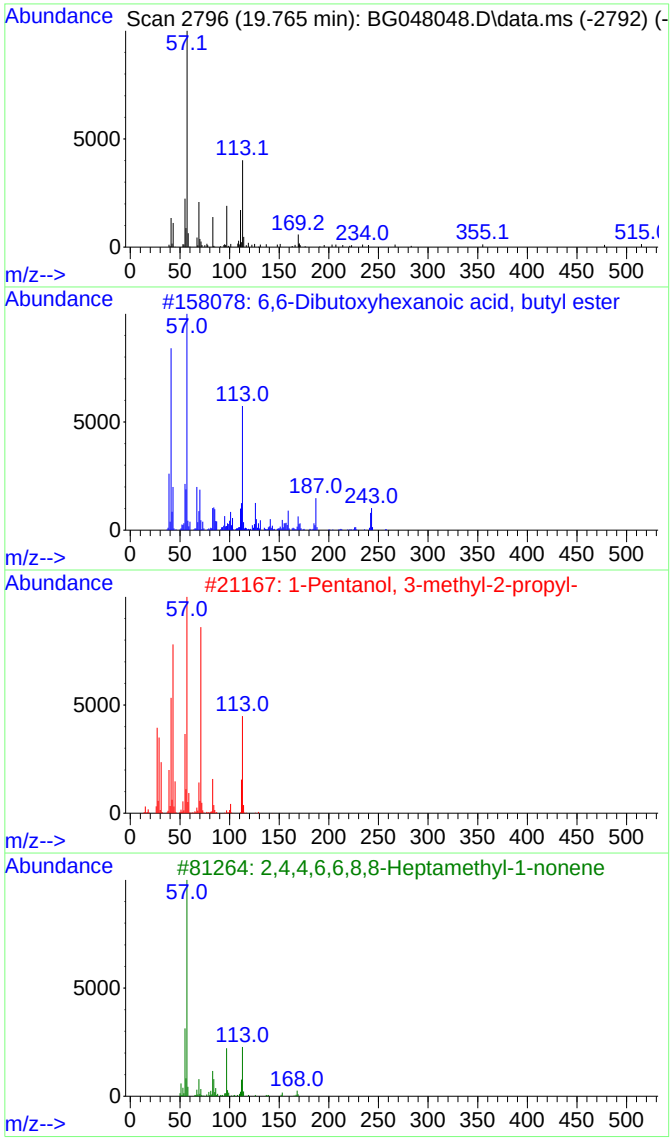
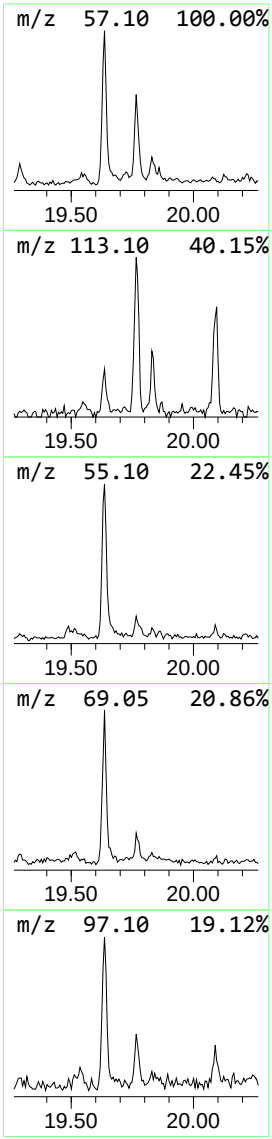
Peak Number 6 unknown19.765 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.765	2.16 ng	100687	Chrysene-d12	21.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,6-Dibutoxyhexanoic acid, butyl...	316	C18H36O4	1000280-29-0	33
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	23
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	17
5	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	17





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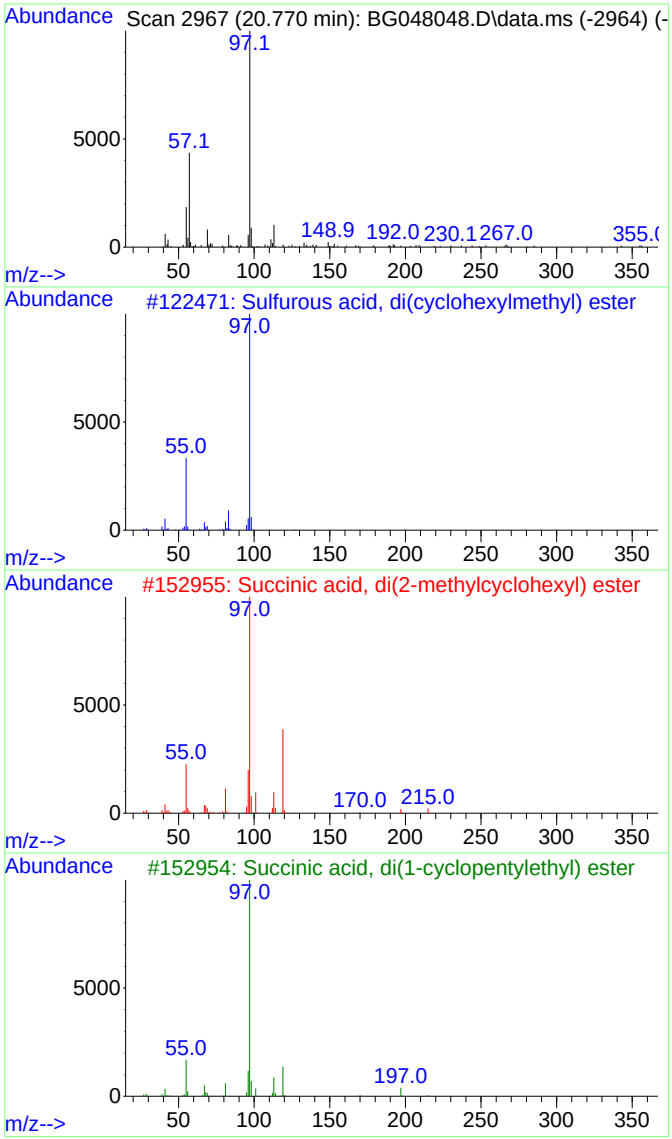
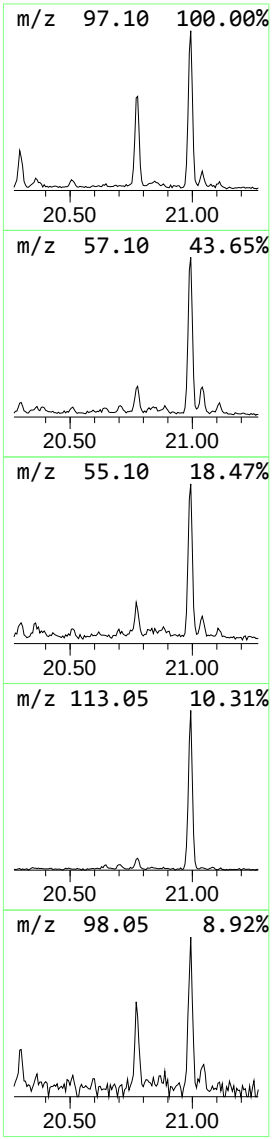
****

Peak Number 7 unknown20.770 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.770	2.22 ng	103748	Chrysene-d12	21.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, di(cyclohexylmet...	274	C14H26O3S	1000309-22-7	42
2	Succinic acid, di(2-methylcycloh...	310	C18H30O4	1000329-83-0	38
3	Succinic acid, di(1-cyclopentyle...	310	C18H30O4	1000330-21-8	38
4	2-Ethoxy-4-methyl-pent-2-enoic acid	158	C8H14O3	1000190-08-8	36
5	2-Thiophenylacetic acid, 2,5-dic...	286	C12H8Cl2O2S	1000325-71-9	36





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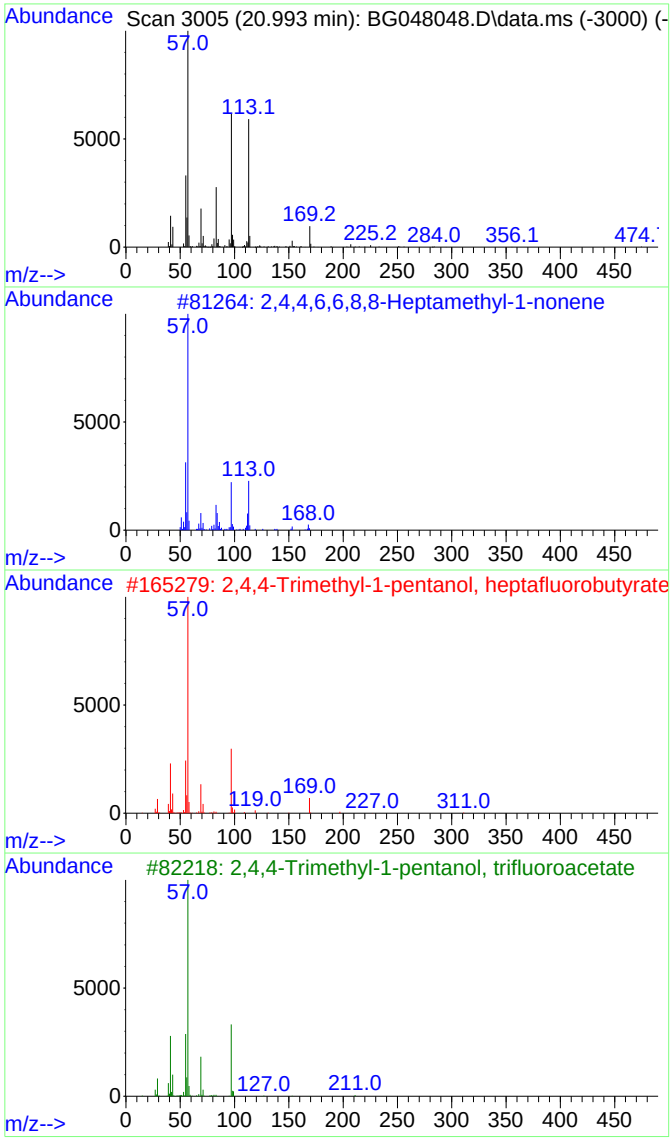
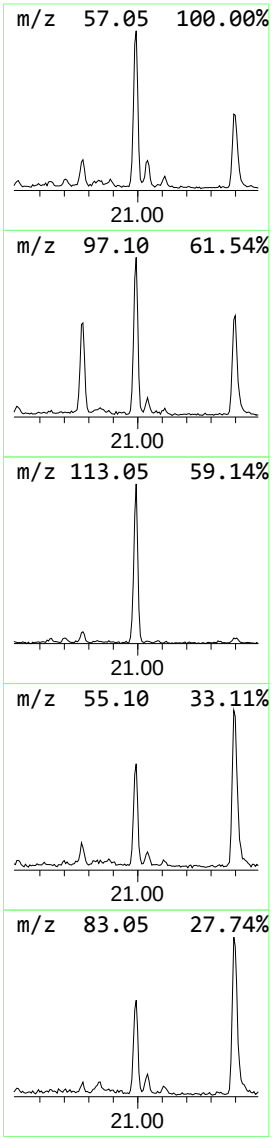
****
Peak Number 8 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.993	8.77 ng	408853	Chrysene-d12	21.763

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	64
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	38
3	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	25
4	Silane, butyldichloromethyl-	170	C5H12Cl2Si	018147-23-4	22
5	Sulfurous acid, cyclohexylmethyl...	374	C21H42O3S	1000309-22-2	16





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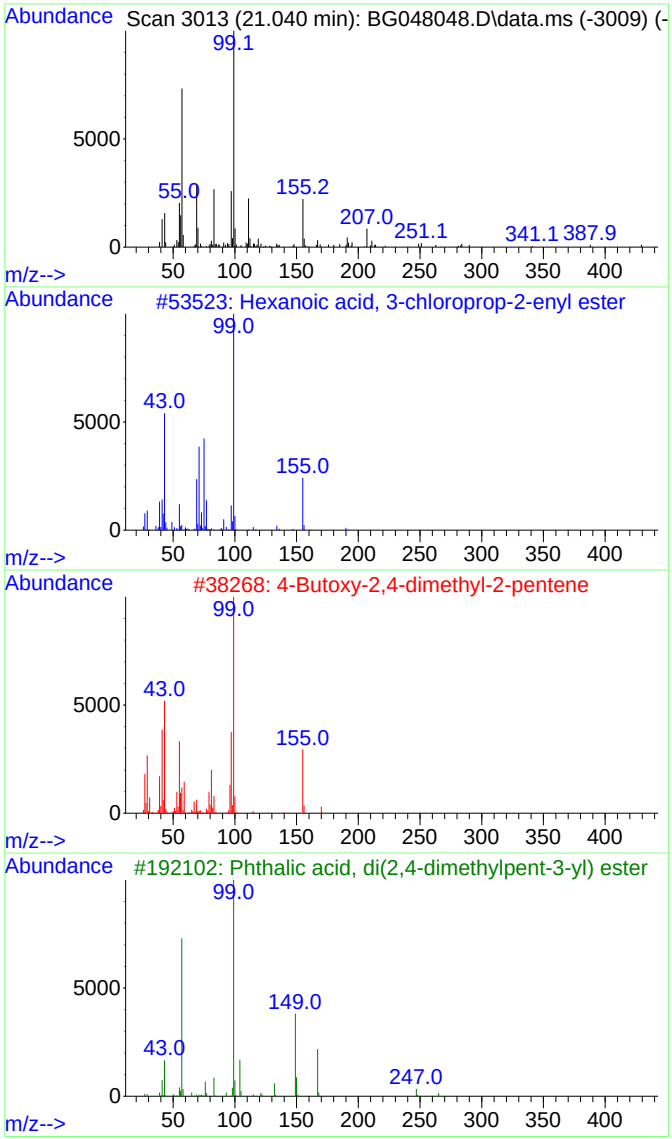
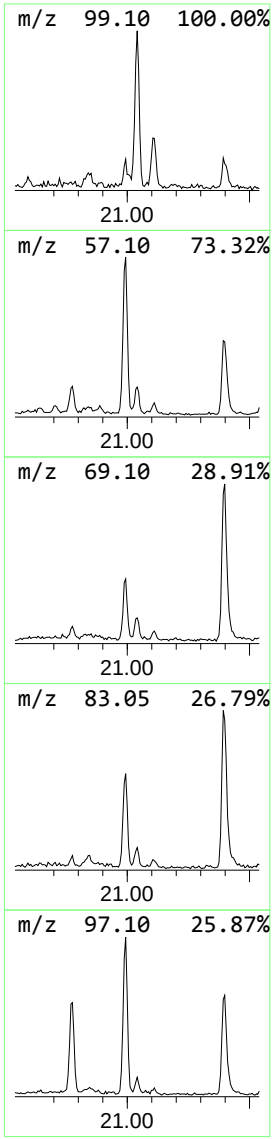
****

Peak Number 9 unknown21.040 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.040	2.06 ng	96094	Chrysene-d12	21.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	46
2	4-Butoxy-2,4-dimethyl-2-pentene	170	C11H22O	1000159-08-7	40
3	Phthalic acid, di(2,4-dimethylpe...	362	C22H34O4	1000356-85-5	37
4	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	37
5	Succinic acid, di(2,4-dimethylpe...	314	C18H34O4	1000349-36-7	37





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Data File : BG048048.D
Acq On : 28 Jan 2021 4:22
Operator : CG/JU
Sample : M1226-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0051-045-COMP-E-ELUTRIATE

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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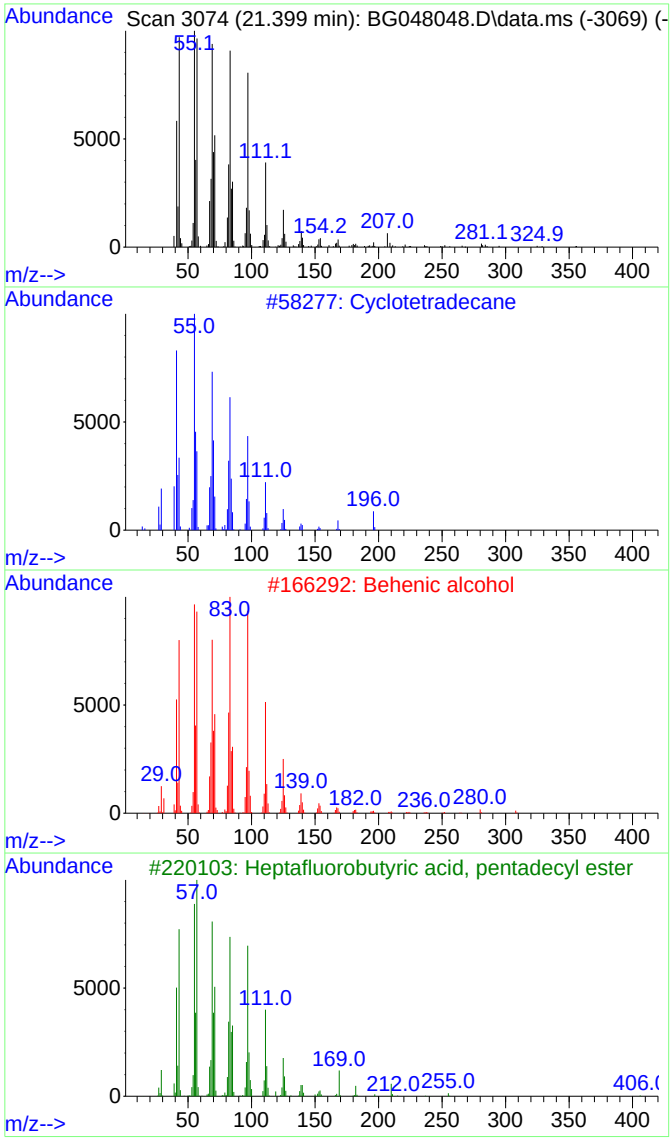
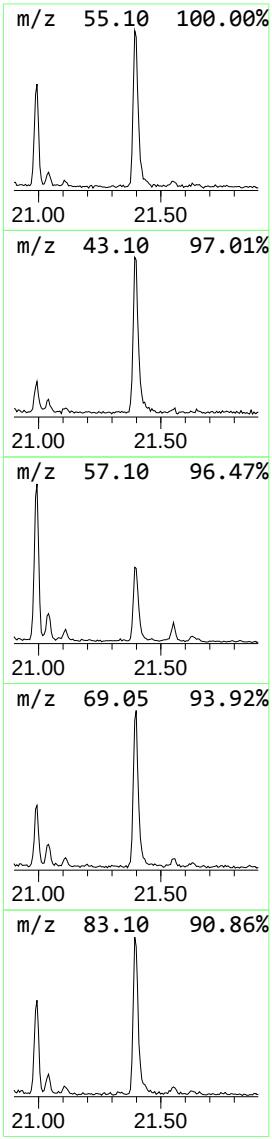
Peak Number 10 Cyclotetradecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.399	15.17 ng	707634	Chrysene-d12	21.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	98
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048048.D
Acq On : 28 Jan 2021 4:22
Operator : CG/JU
Sample : M1226-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0051-045-COMP-E-ELUTRIATE

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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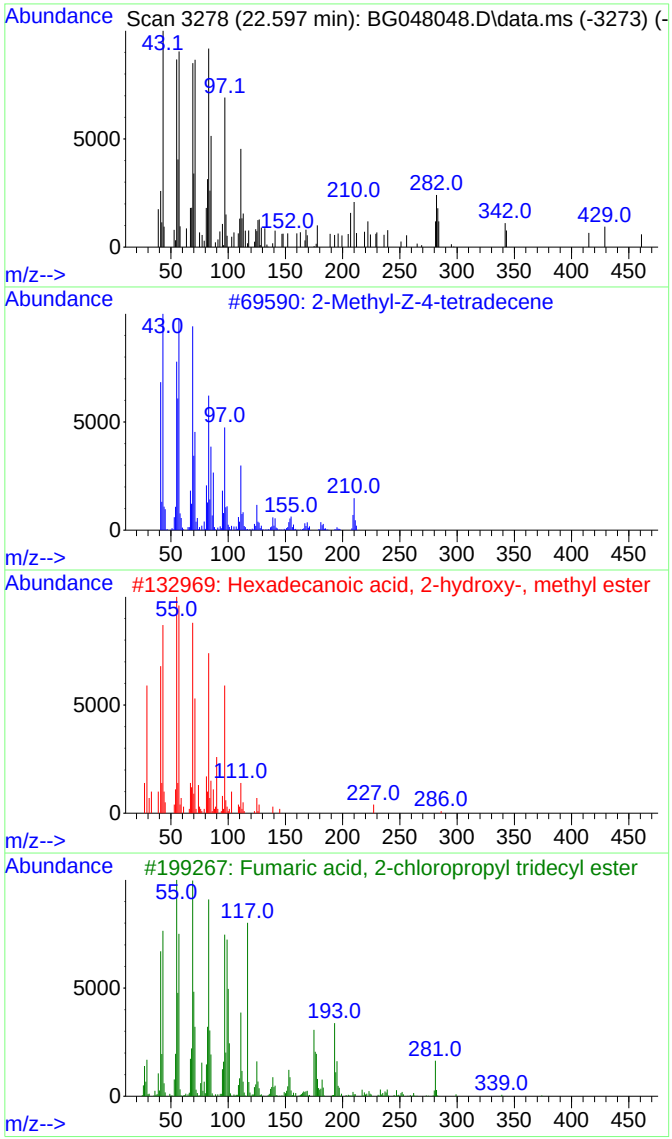
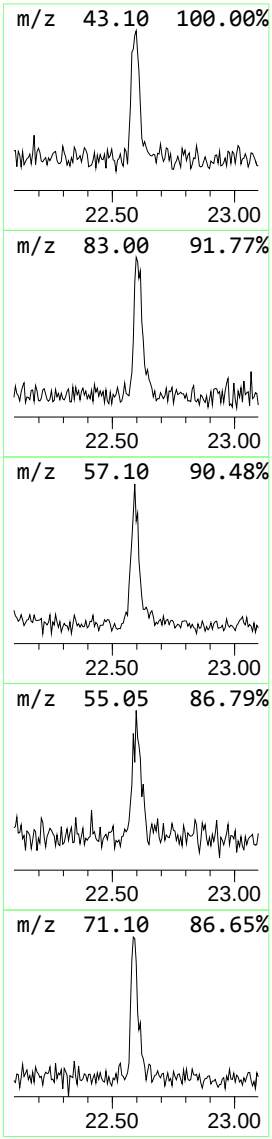
Peak Number 11 2-Methyl-Z-4-tetradecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.597	2.23 ng	104090	Chrysene-d12	21.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-Z-4-tetradecene	210	C15H30	1000130-78-3	70
2	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	47
3	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	46
4	Methyl 2-hydroxy-eicosanoate	342	C21H42O3	1000336-20-4	43
5	Fumaric acid, 2,4,6-trichlorophe...	476	C23H31Cl3O4	1000348-27-7	40





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048048.D
Acq On : 28 Jan 2021 4:22
Operator : CG/JU
Sample : M1226-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0051-045-COMP-E-ELUTRIATE

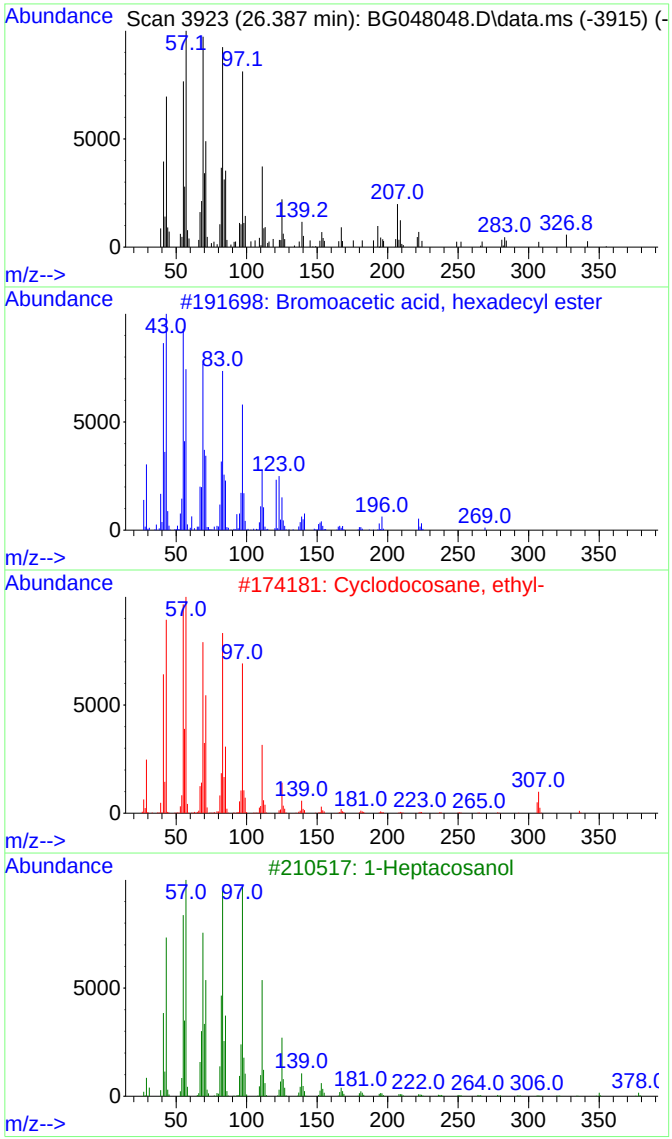
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

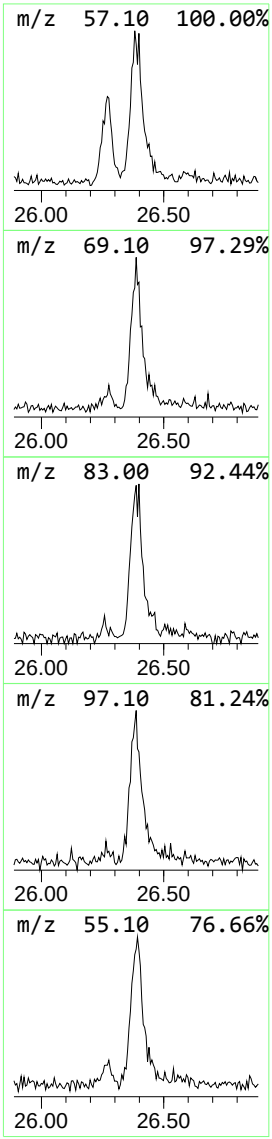
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 Bromoacetic acid, hexadecyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.387	4.49 ng	221503	Perylene-d12	25.047

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
2	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	62
3	1-Heptacosanol	396	C27H56O	002004-39-9	62
4	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	53
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048048.D
Acq On : 28 Jan 2021 4:22
Operator : CG/JU
Sample : M1226-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0051-045-COMP-E-ELUTRIATE

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
Benzoic acid, 4...	14.953	2.7	ng	82834	3	14.748	621360	20.0
1,2-Benzenedica...	17.762	23.9	ng	948607	4	17.491	793690	20.0
n-Hexadecanoic ...	18.373	24.7	ng	981775	4	17.491	793690	20.0
unknown19.137	19.137	5.5	ng	218826	4	17.491	793690	20.0
Octadecanoic acid	19.636	15.0	ng	697840	5	21.763	932784	20.0
unknown19.765	19.765	2.2	ng	100687	5	21.763	932784	20.0
unknown20.770	20.770	2.2	ng	103748	5	21.763	932784	20.0
2,4,4,6,6,8,8-H...	20.993	8.8	ng	408853	5	21.763	932784	20.0
unknown21.040	21.040	2.1	ng	96094	5	21.763	932784	20.0
Cyclotetradecane	21.399	15.2	ng	707634	5	21.763	932784	20.0
2-Methyl-Z-4-te...	22.597	2.2	ng	104090	5	21.763	932784	20.0
Bromoacetic aci...	26.387	4.5	ng	221503	6	25.047	986913	20.0