LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110422\
Data File : BG055455.D
Acq On : 4 Nov 2022 15:39
Operator : CG/JU
Sample : N5306-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221166-COMP-01-MODIFIED-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-BG110122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.274	330	338	348	rBV	22056	35899	1.73%	0.418%
2	5.756	414	420	437	rBV	206831	356750	17.19%	4.150%
3	7.383	690	697	709	rBV	162177	299865	14.45%	3.488%
4	8.229	834	841	853	rBV	82262	140473	6.77%	1.634%
5	9.410	1033	1042	1056	rBV	245423	439691	21.19%	5.115%
6	10.809	1273	1280	1299	rBV	132118	248419	11.97%	2.890%
7	11.061	1316	1323	1331	rBV	114895	197600	9.52%	2.299%
8	13.476	1725	1734	1745	rBV	782224	1155417	55.68%	13.441%
9	13.723	1768	1776	1784	rBV	47997	71629	3.45%	0.833%
10	14.851	1961	1968	1976	rBV	202968	306633	14.78%	3.567%
11	16.332	2214	2220	2233	rVB	619372	969478	46.72%	11.278%
12	17.583	2427	2433	2439	rBV	285879	413738	19.94%	4.813%
13	18.212	2534	2540	2546	rBV2	55562	84727	4.08%	0.986%
14	18.435	2573	2578	2590	rBV	63185	111144	5.36%	1.293%
15	19.364	2732	2736	2740	rVB	99729	111165	5.36%	1.293%
16	19.493	2752	2758	2762	rBV	36947	43435	2.09%	0.505%
17	19.693	2788	2792	2799	rBV2	18147	28554	1.38%	0.332%
18	20.157	2865	2871	2880	rBV	1555950	2075232	100.00%	24.141%
19	20.427	2911	2917	2921	rBV2	27078	48932	2.36%	0.569%
20	20.768	2971	2975	2979	rBV	43353	48719	2.35%	0.567%
21	20.926	2998	3002	3006	rBV	17111	22157	1.07%	0.258%
22	21.449	3085	3091	3103	rBV3	63683	197268	9.51%	2.295%
23	21.855	3153	3160	3167	rBV2	299409	510234	24.59%	5.935%
24	22.002	3181	3185	3190	rVB	17463	23186	1.12%	0.270%
25	22.624	3287	3291	3296	rBV3	14402	22667	1.09%	0.264%
26	23.347	3408	3414	3419	rVB4	14494	27323	1.32%	0.318%
27	23.547	3442	3448	3454	rVB	34328	63580	3.06%	0.740%
28	25.227	3724	3734	3747	rVB2	187765	542521	26.14%	6.311%

Sum of corrected areas: 8596436

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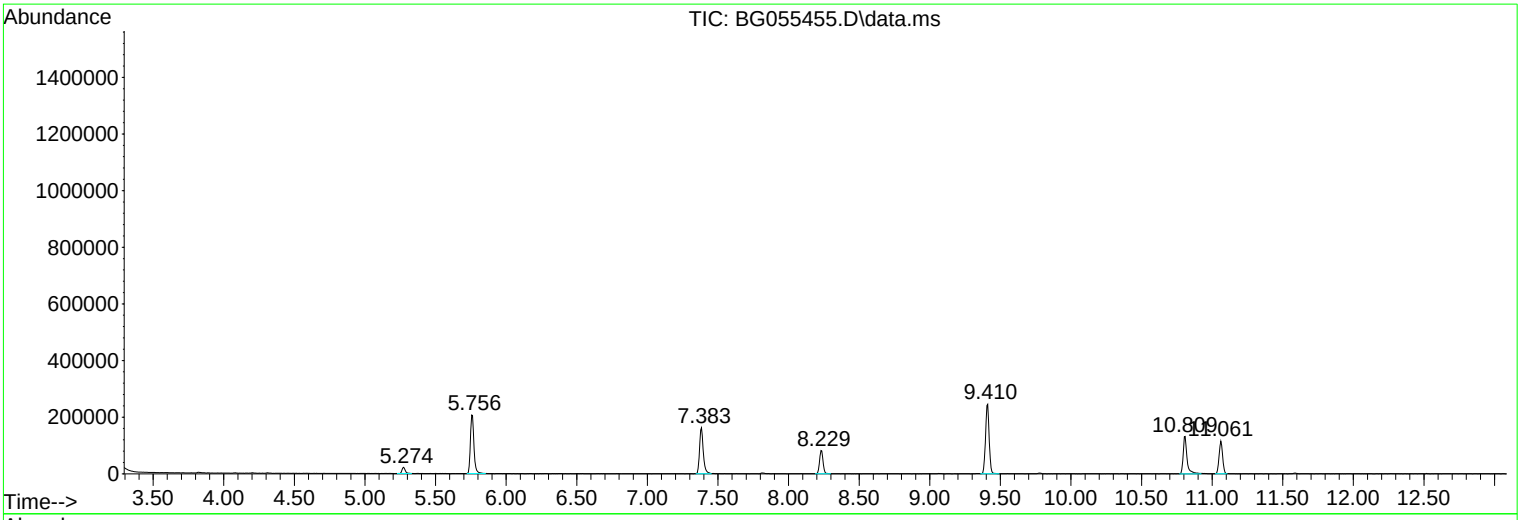
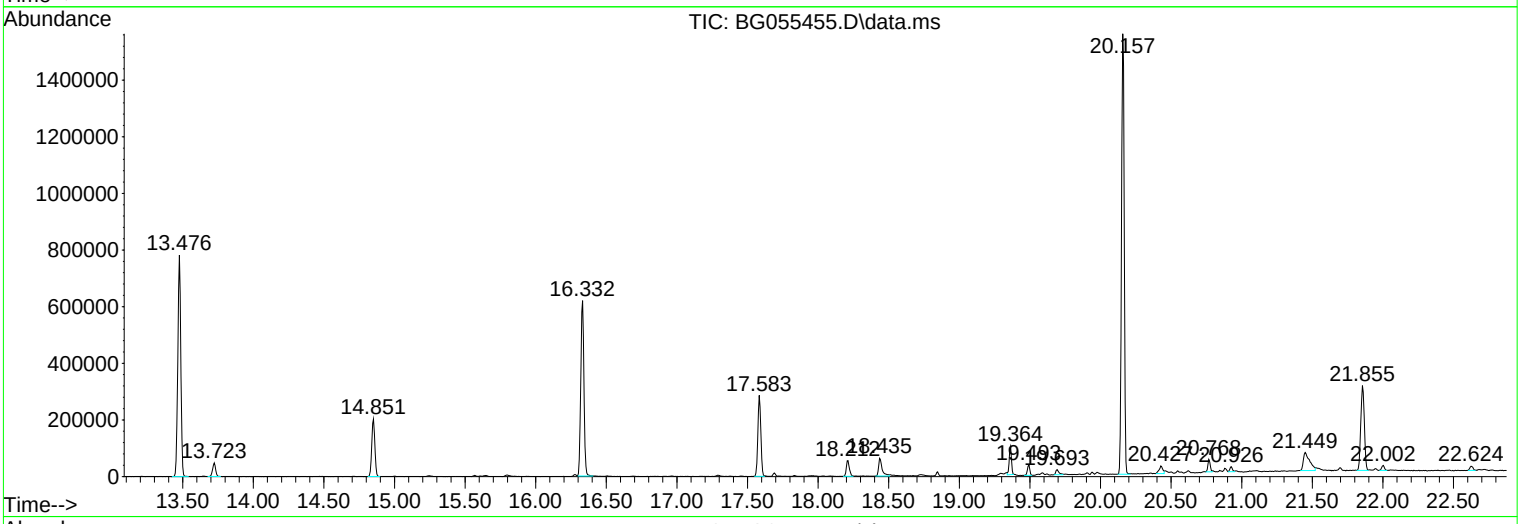
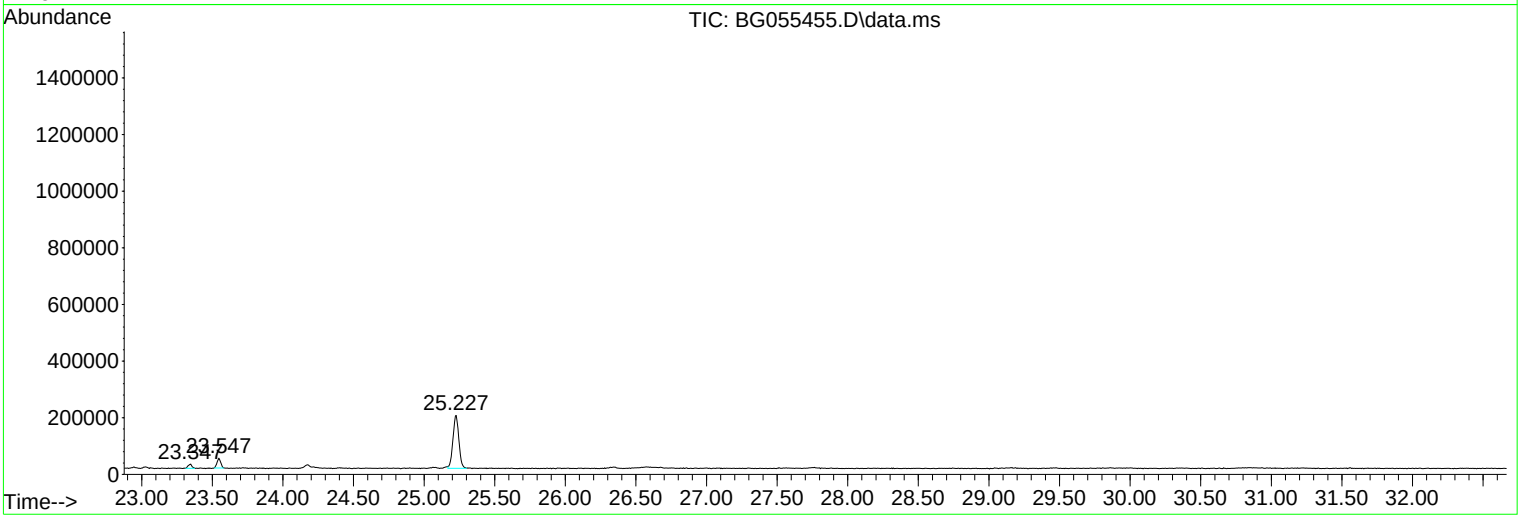
ClientSampleId :
20221166-COMP-01-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.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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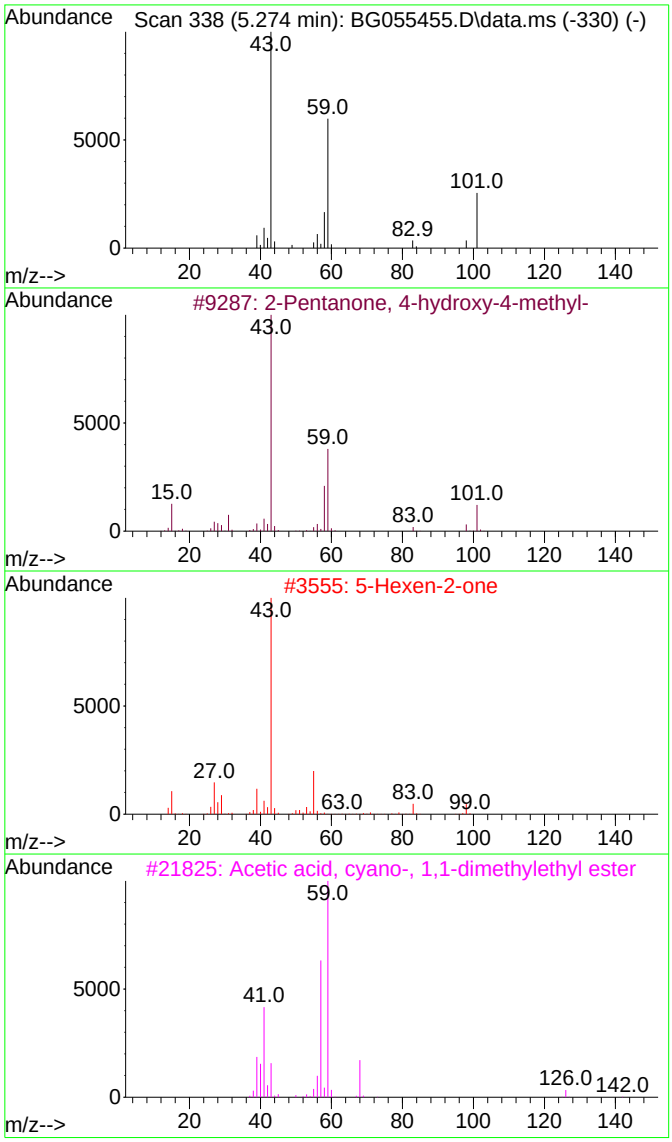
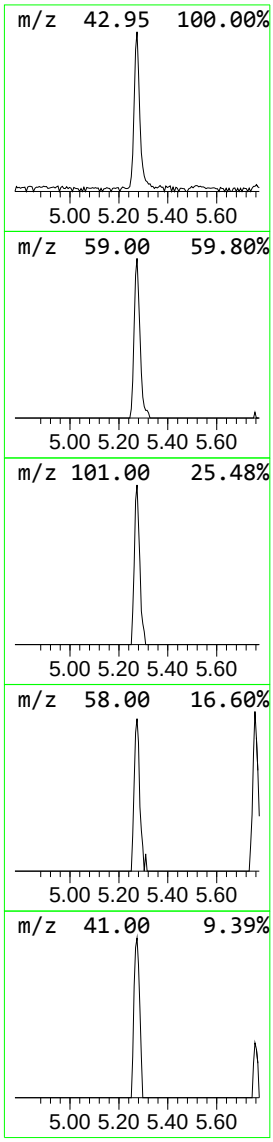
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.274	5.11 ng	35899	1,4-Dichlorobenzene-d4	8.229

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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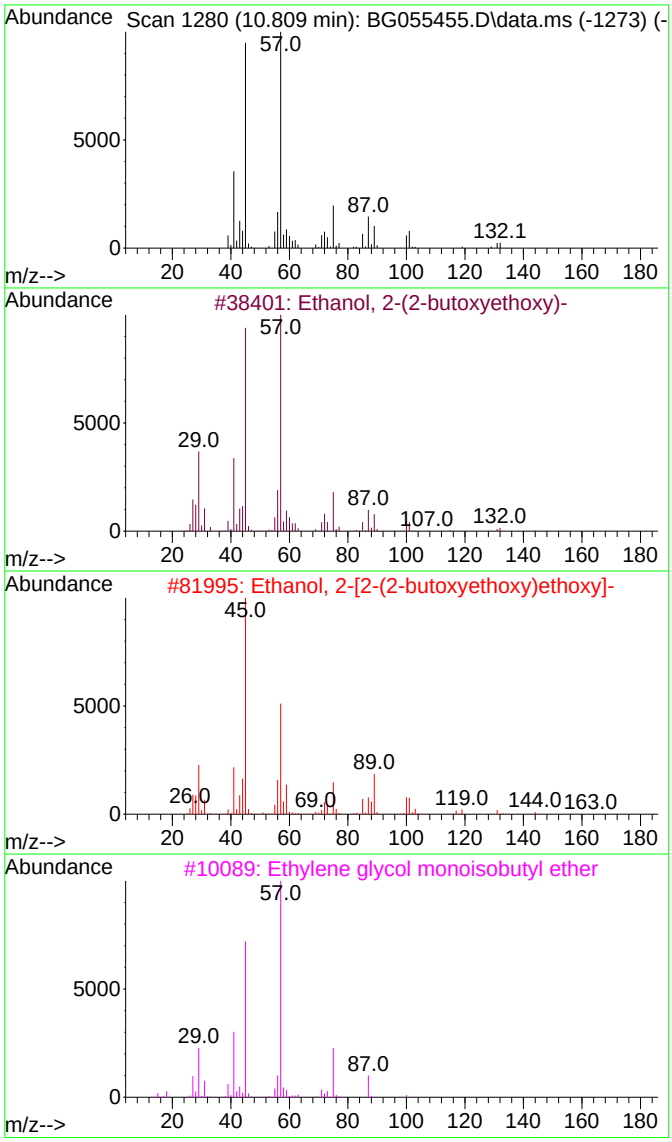
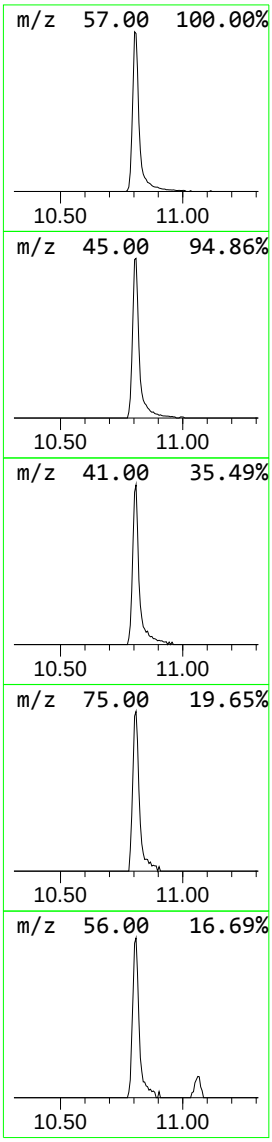
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.809	25.14 ng	248419	Naphthalene-d8	11.062

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	72
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	58
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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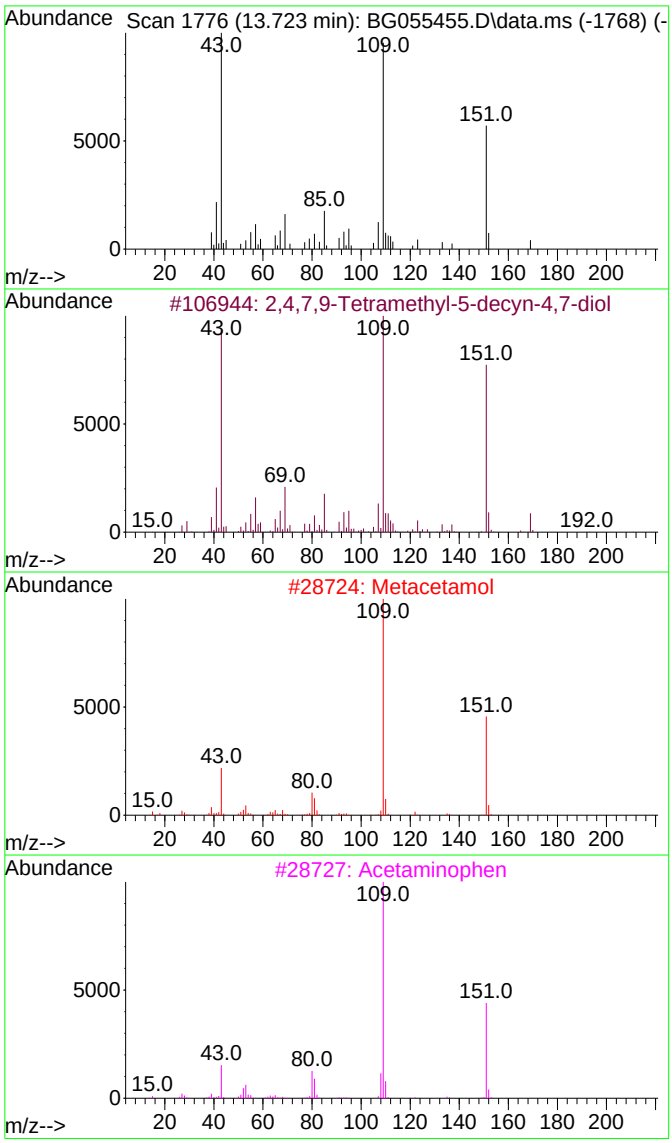
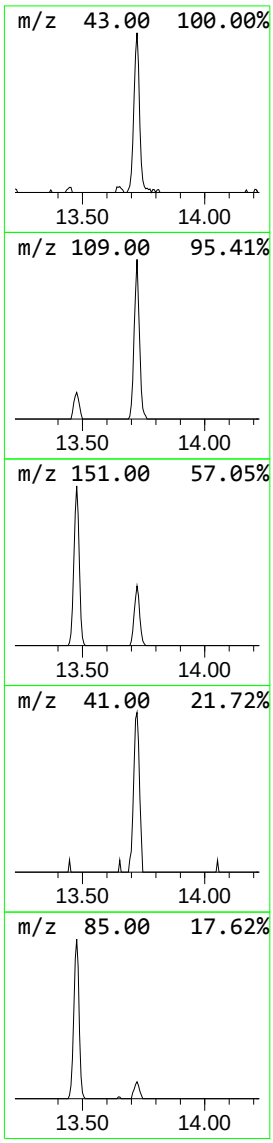
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.723	4.67 ng	71629	Acenaphthene-d10	14.851

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	53
3	Acetaminophen	151	C8H9NO2	000103-90-2	53
4	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53





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Sample : N5306-01
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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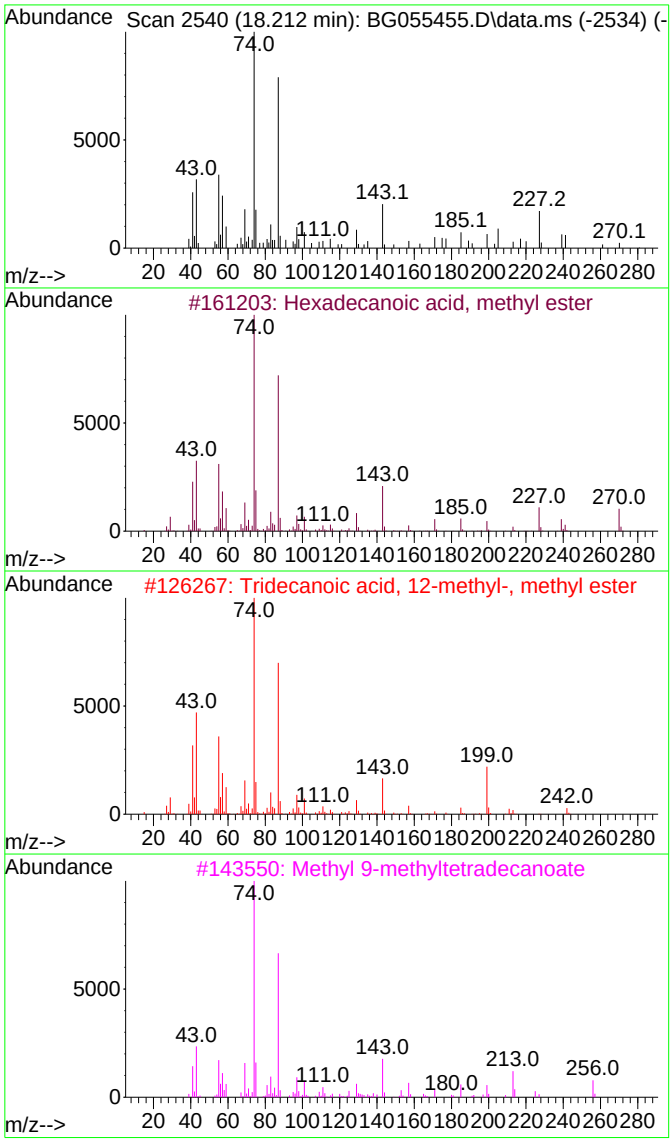
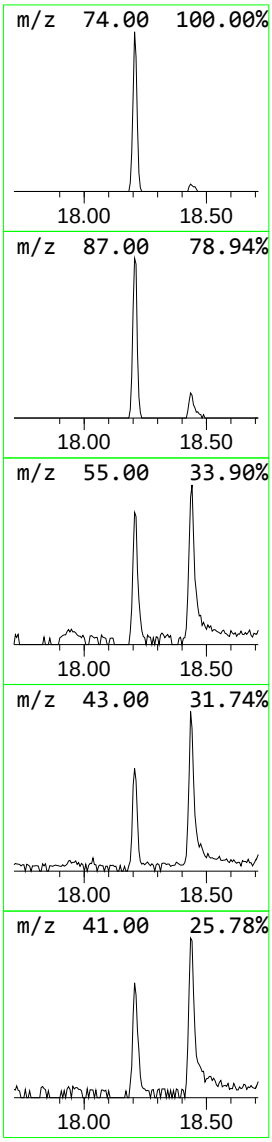
****
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	4.10 ng	84727	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80
3	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	80
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	72
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	72





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Sample : N5306-01
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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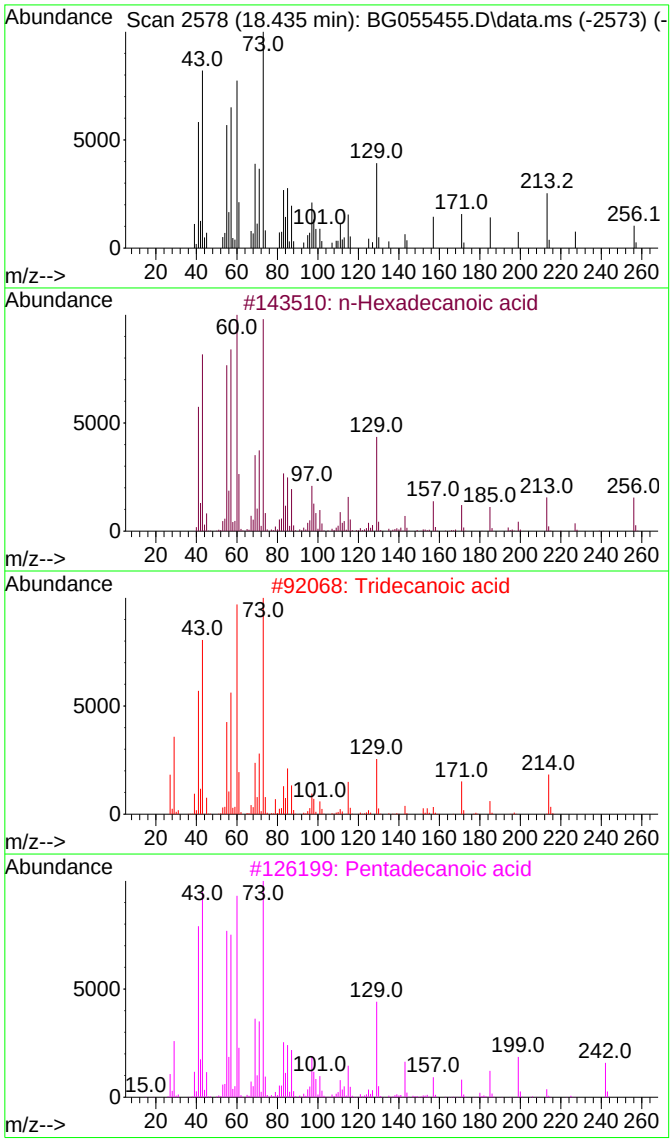
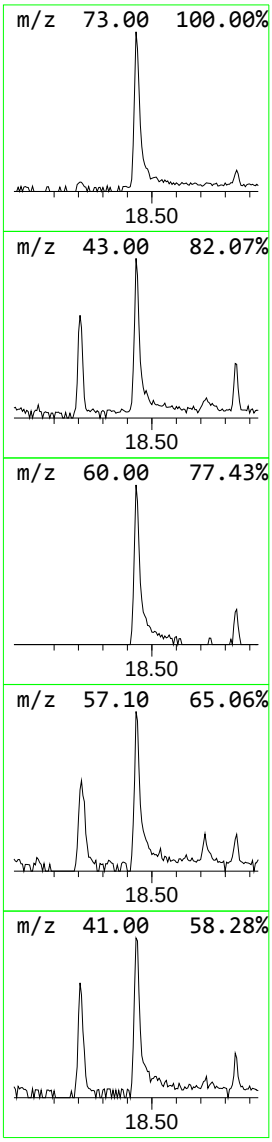
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.435	5.37 ng	111144	Phenanthrene-d10	17.583

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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TIC Library : C:\Database\NIST20.L
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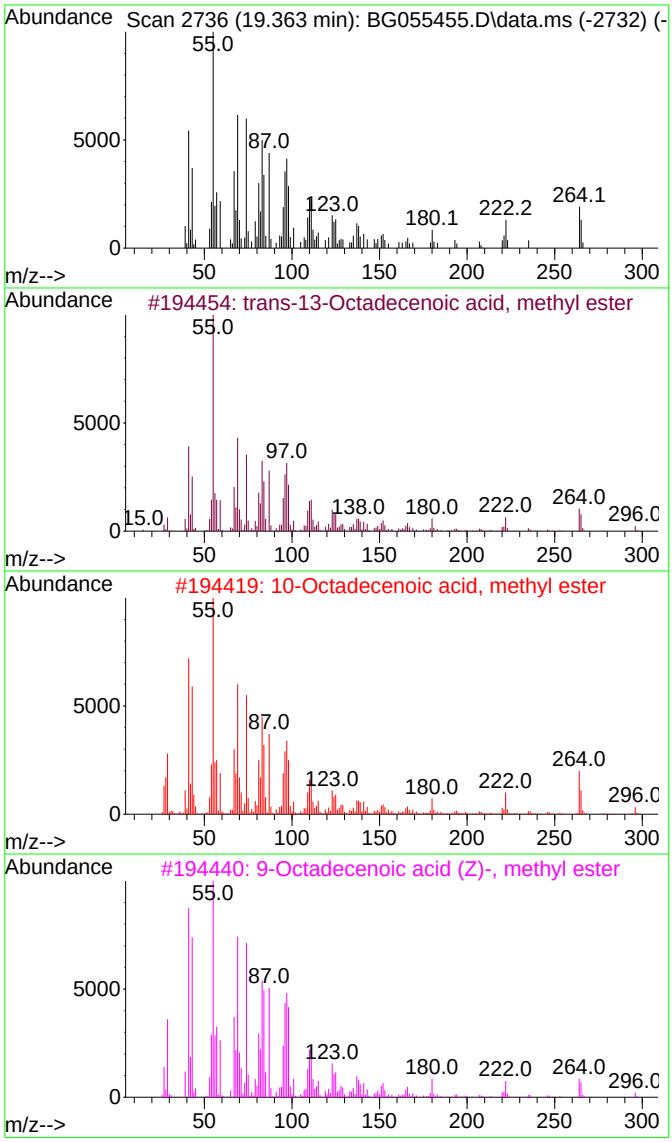
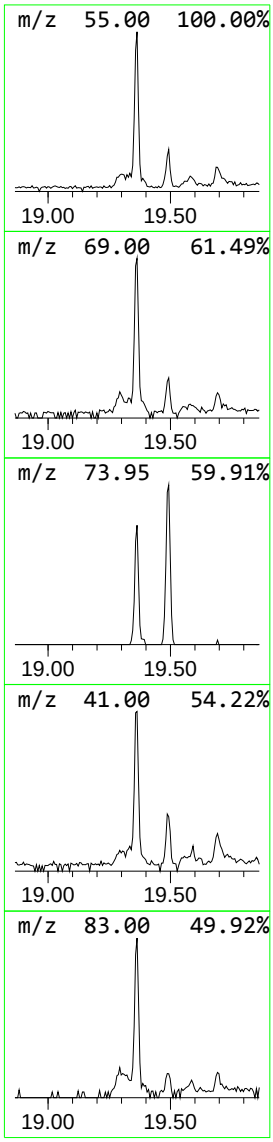
****
Peak Number 6 trans-13-Octadecenoic acid,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.363	5.37 ng	111165	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	93
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	91





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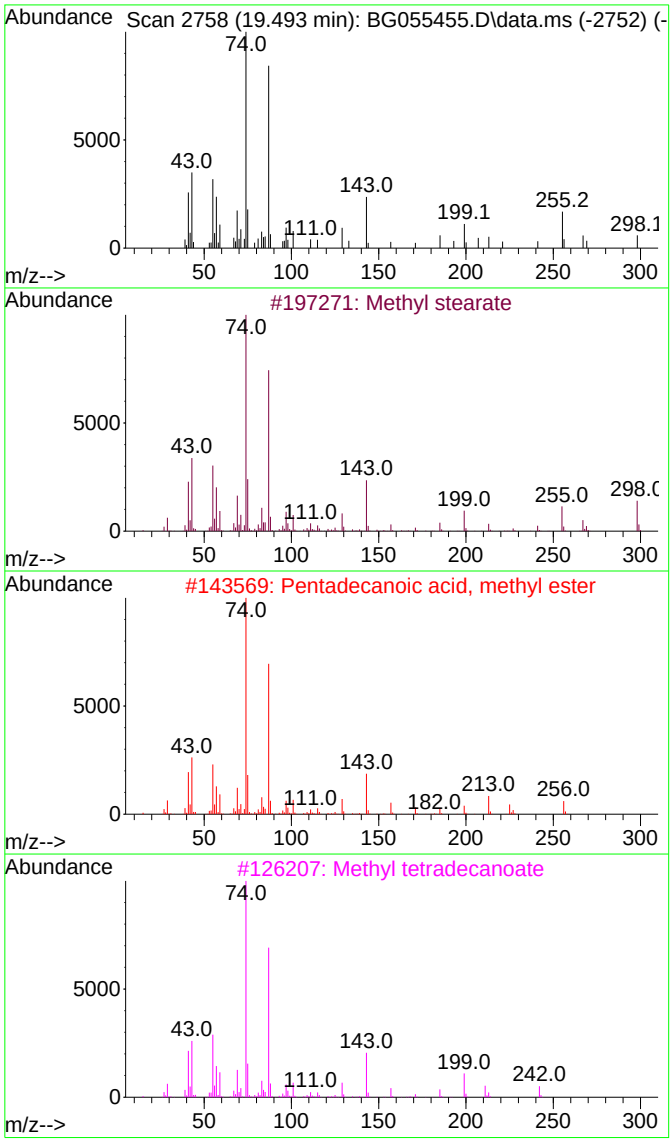
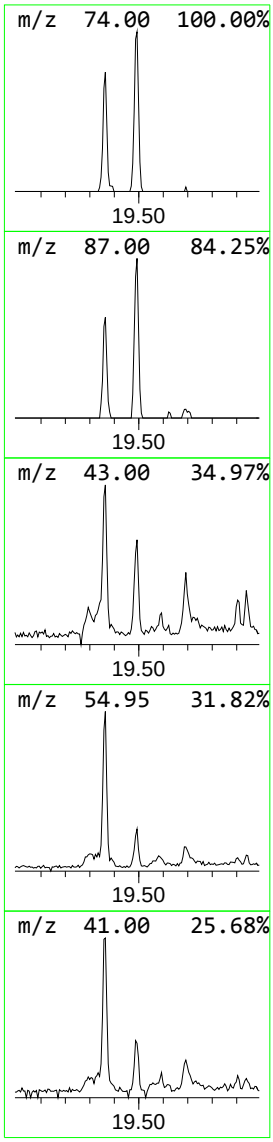
****

Peak Number 7 Methyl stearate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.493	2.10 ng	43435	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	95
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	86
5	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	86





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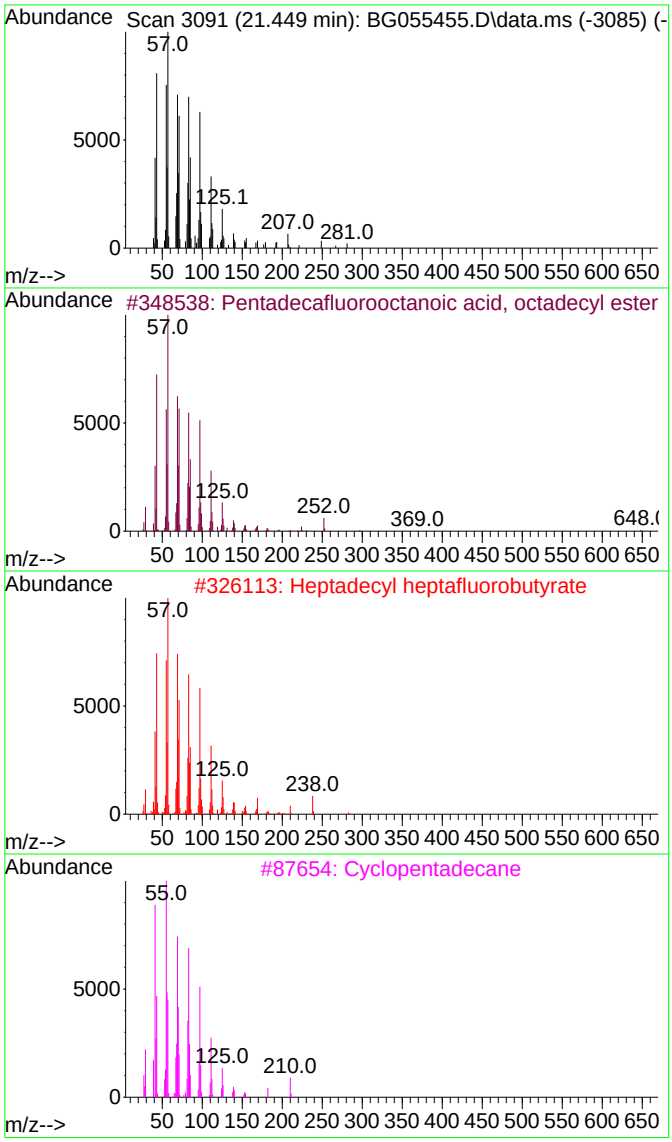
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

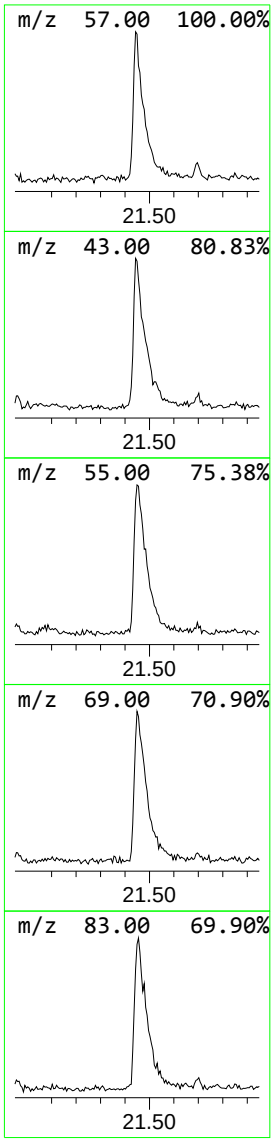
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.449	7.73 ng	197268	Chrysene-d12	21.855

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3	Cyclopentadecane	210	C15H30	000295-48-7	93
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91





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Instrument :
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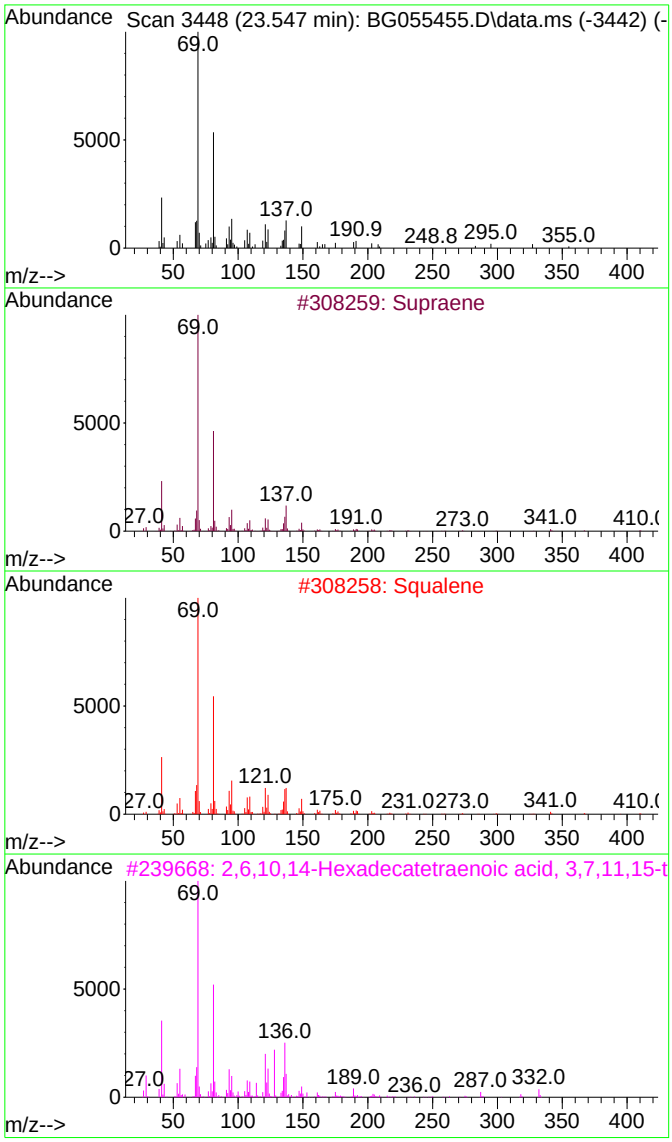
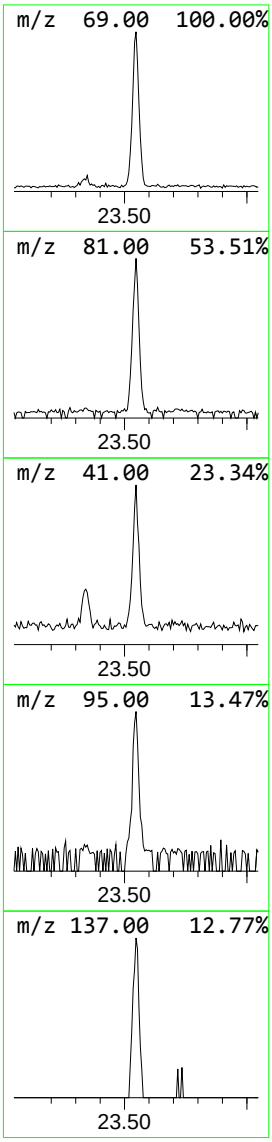
****

Peak Number 9 Supraene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.547	2.34 ng	63580	Perylene-d12	25.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Squalene	410	C30H50	000111-02-4	83
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	64
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	1,6,10,14-Hexadecatetraen-3-ol, ...	290	C20H34O	001113-21-9	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110422\
Data File : BG055455.D
Acq On : 4 Nov 2022 15:39
Operator : CG/JU
Sample : N5306-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221166-COMP-01-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.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
2-Pentanone, 4-...	5.274	5.1	ng	35899	1	8.229	140473	20.0
Ethanol, 2-(2-b...	10.809	25.1	ng	248419	2	11.062	197600	20.0
2,4,7,9-Tetrame...	13.723	4.7	ng	71629	3	14.851	306633	20.0
Hexadecanoic ac...	18.212	4.1	ng	84727	4	17.583	413738	20.0
n-Hexadecanoic ...	18.435	5.4	ng	111144	4	17.583	413738	20.0
trans-13-Octade...	19.363	5.4	ng	111165	4	17.583	413738	20.0
Methyl stearate	19.493	2.1	ng	43435	4	17.583	413738	20.0
Pentadecafluoro...	21.449	7.7	ng	197268	5	21.855	510234	20.0
Supraene	23.547	2.3	ng	63580	6	25.227	542521	20.0