LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055445.D
Acq On : 3 Nov 2022 20:08
Operator : CG/JU
Sample : N5306-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221173-COMP-08-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: BG055445.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.277	332	338	348	rBV	21335	34969	1.67%	0.406%
2	5.759	414	420	435	rBV	224736	377876	18.01%	4.385%
3	7.380	690	696	708	rBV	166285	301472	14.37%	3.498%
4	8.232	833	841	850	rBV	87445	146529	6.98%	1.700%
5	9.407	1033	1041	1055	rBV	287666	512156	24.41%	5.943%
6	10.806	1271	1279	1293	rBV	144204	251900	12.00%	2.923%
7	11.064	1315	1323	1332	rBV	117697	209345	9.98%	2.429%
8	13.479	1726	1734	1743	rBV	847699	1337033	63.72%	15.515%
9	13.726	1770	1776	1782	rBV	42289	67365	3.21%	0.782%
10	14.848	1961	1967	1976	rVB	207022	323115	15.40%	3.750%
11	16.329	2213	2219	2235	rBV	696424	1097901	52.32%	12.740%
12	17.586	2426	2433	2439	rBV	282493	427823	20.39%	4.965%
13	18.209	2534	2539	2547	rBV3	47827	73331	3.49%	0.851%
14	18.438	2573	2578	2587	rBV3	15634	27266	1.30%	0.316%
15	19.360	2731	2735	2739	rVB2	77979	88648	4.22%	1.029%
16	19.490	2752	2757	2762	rVB	37402	42960	2.05%	0.499%
17	20.160	2865	2871	2877	rBV	1666022	2098337	100.00%	24.350%
18	21.452	3087	3091	3105	rBV9	21695	73483	3.50%	0.853%
19	21.858	3153	3160	3167	rBV	315777	514234	24.51%	5.967%
20	23.550	3442	3448	3456	rVB	35798	68598	3.27%	0.796%
21	25.224	3724	3733	3746	rVB2	190354	543121	25.88%	6.303%

Sum of corrected areas: 8617462

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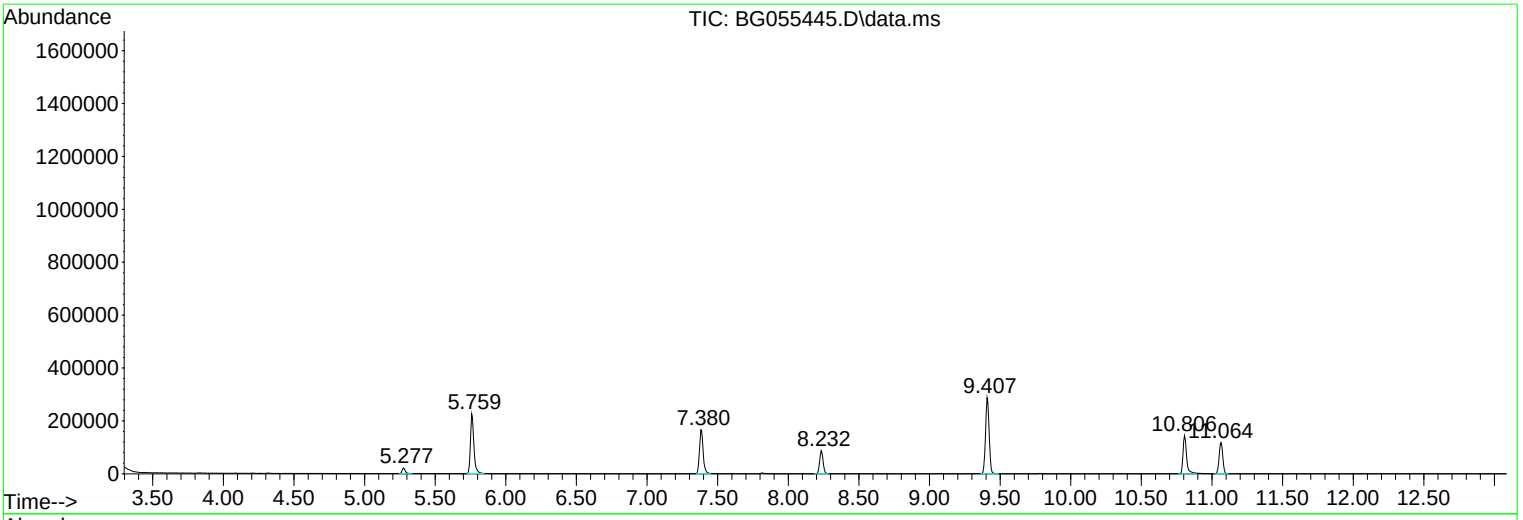
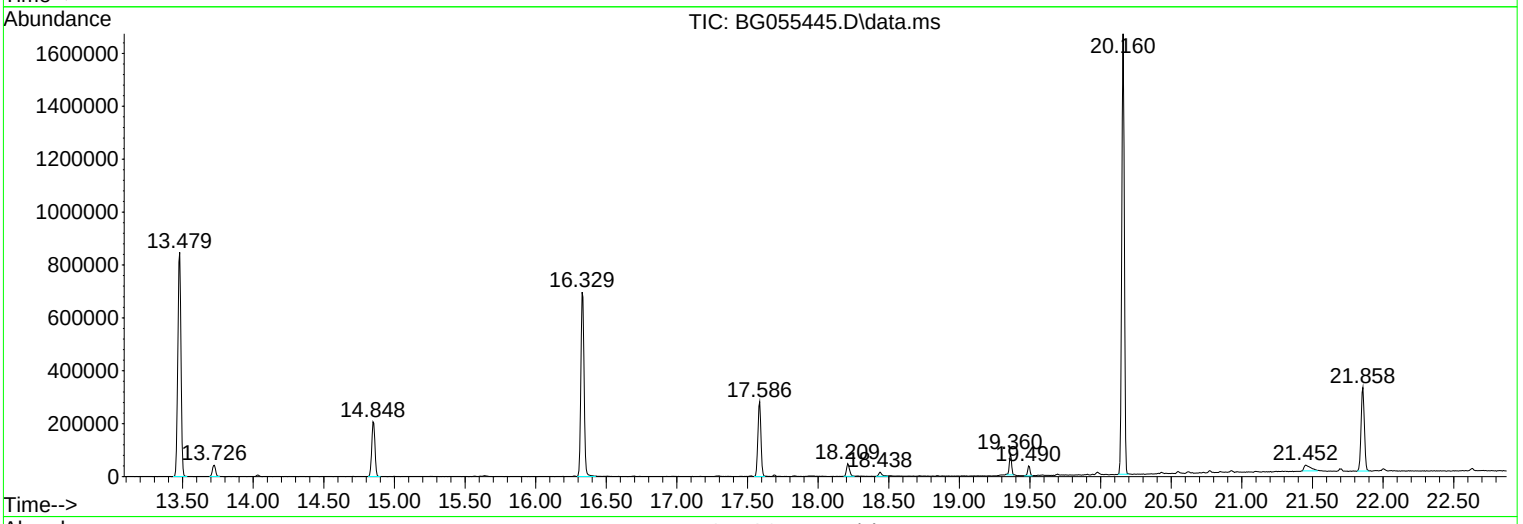
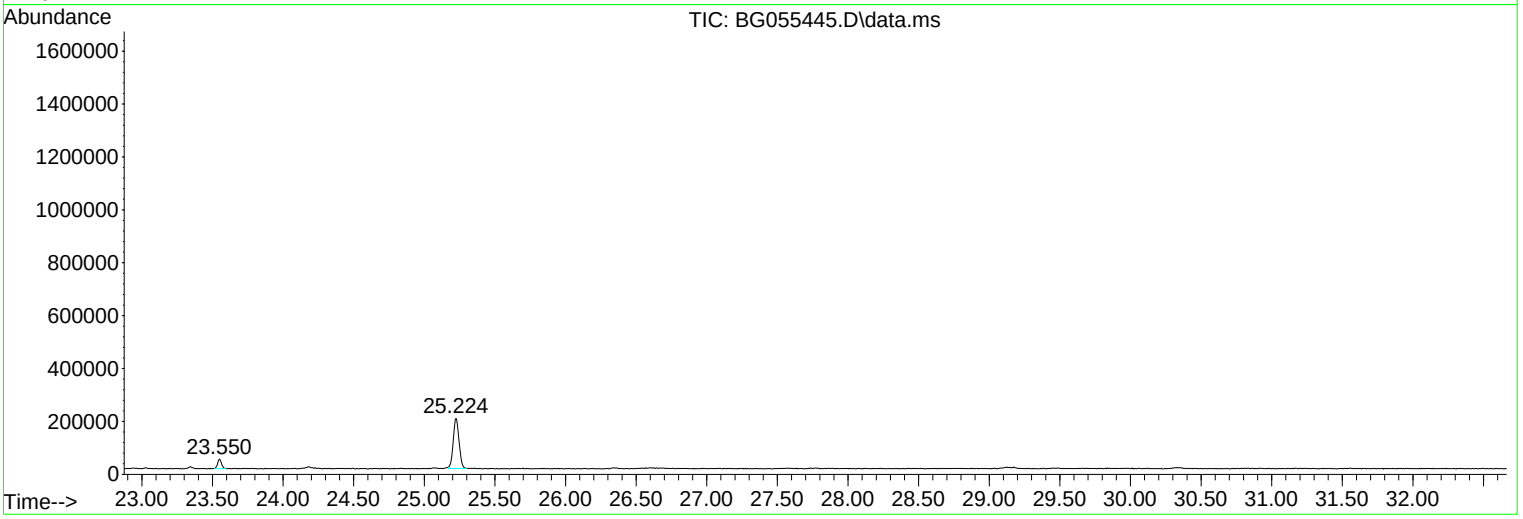
Instrument :
BNA_G
ClientSampleId :
20221173-COMP-08-MODIFIED-ELUTRIATE

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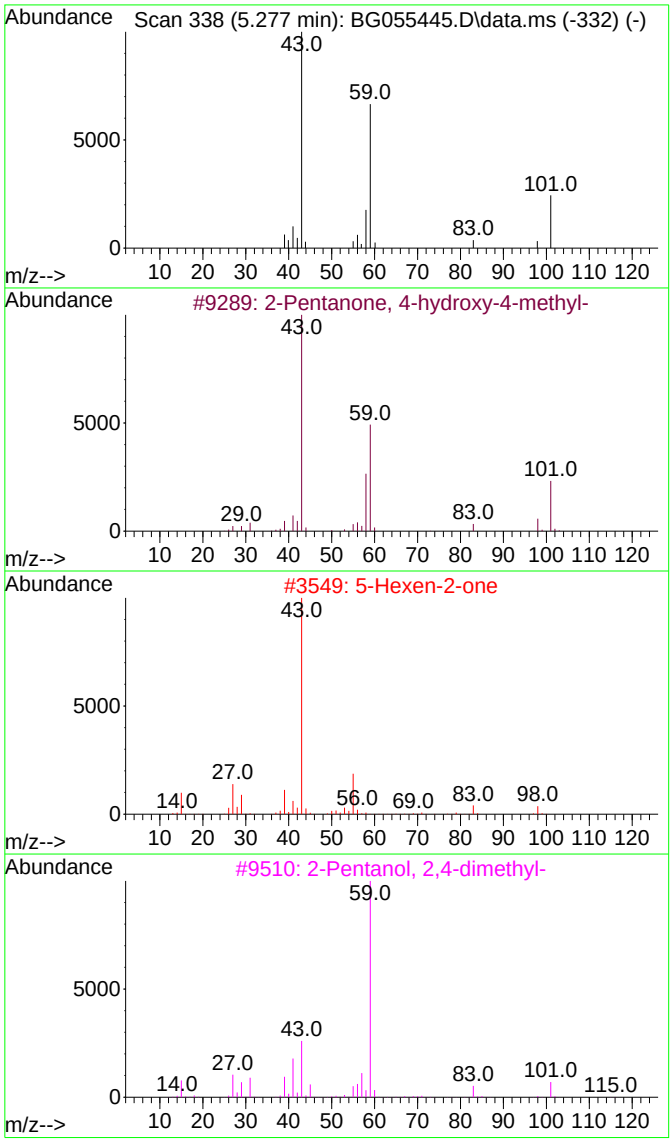
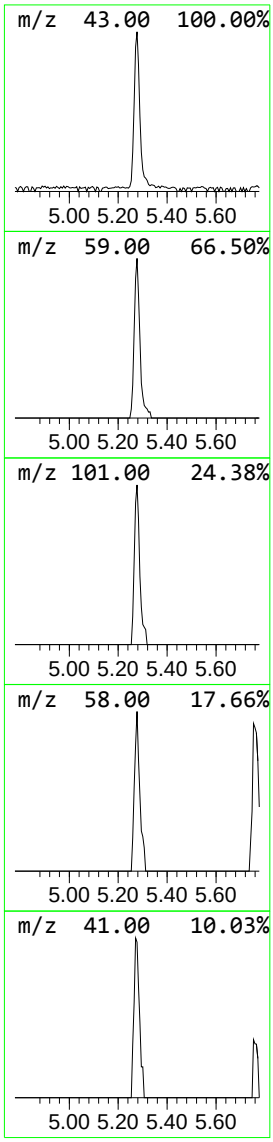
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.277	4.77 ng	34969	1,4-Dichlorobenzene-d4	8.232

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9
4	Hexanamide	115	C6H13NO	000628-02-4	9
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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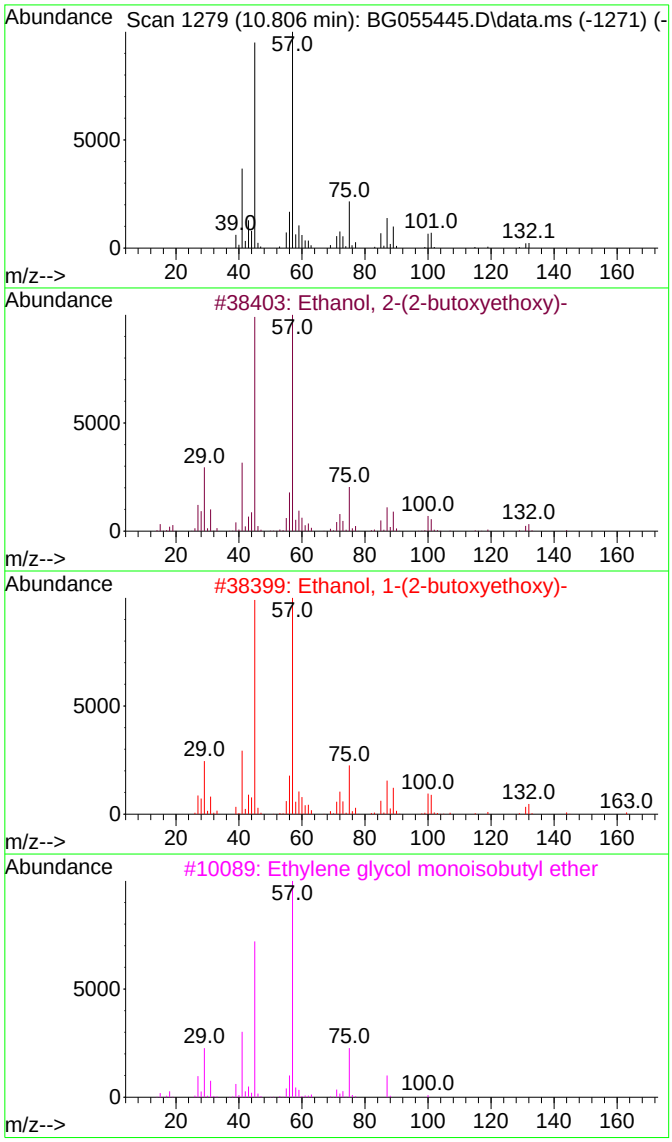
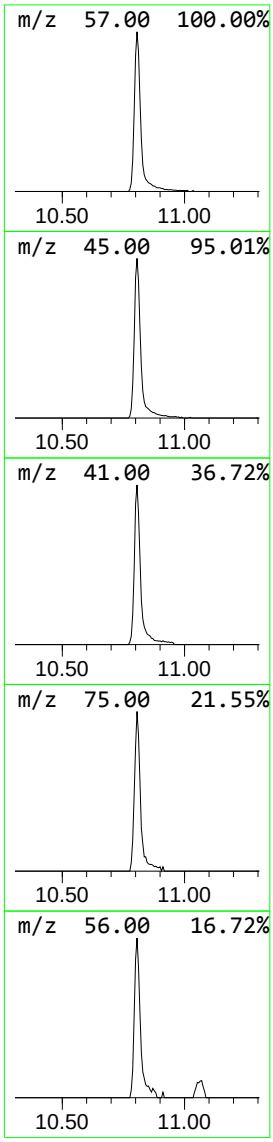
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.806	24.07 ng	251900	Naphthalene-d8	11.064

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	83
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





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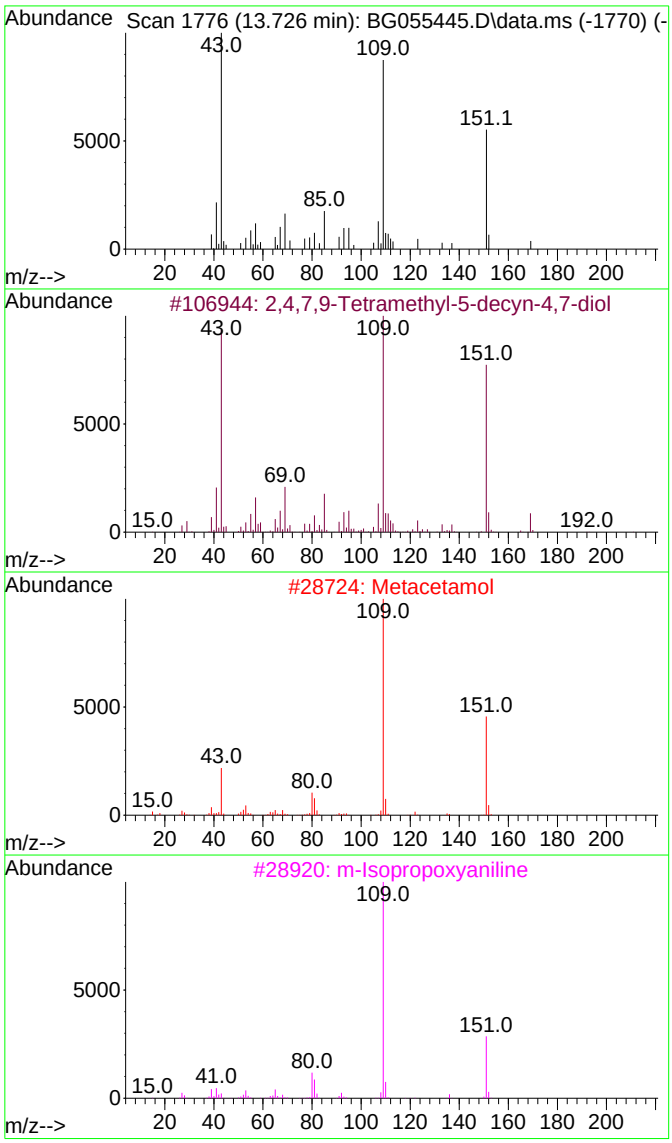
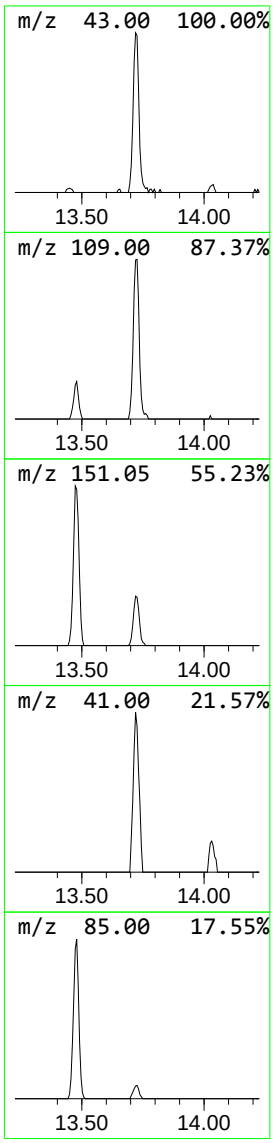
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.726	4.17 ng	67365	Acenaphthene-d10	14.848

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	58
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	58
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
5	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53





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Operator : CG/JU
Sample : N5306-04
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Instrument :
BNA_G
ClientSampleId :
20221173-COMP-08-MODIFIED-ELUTRIATE

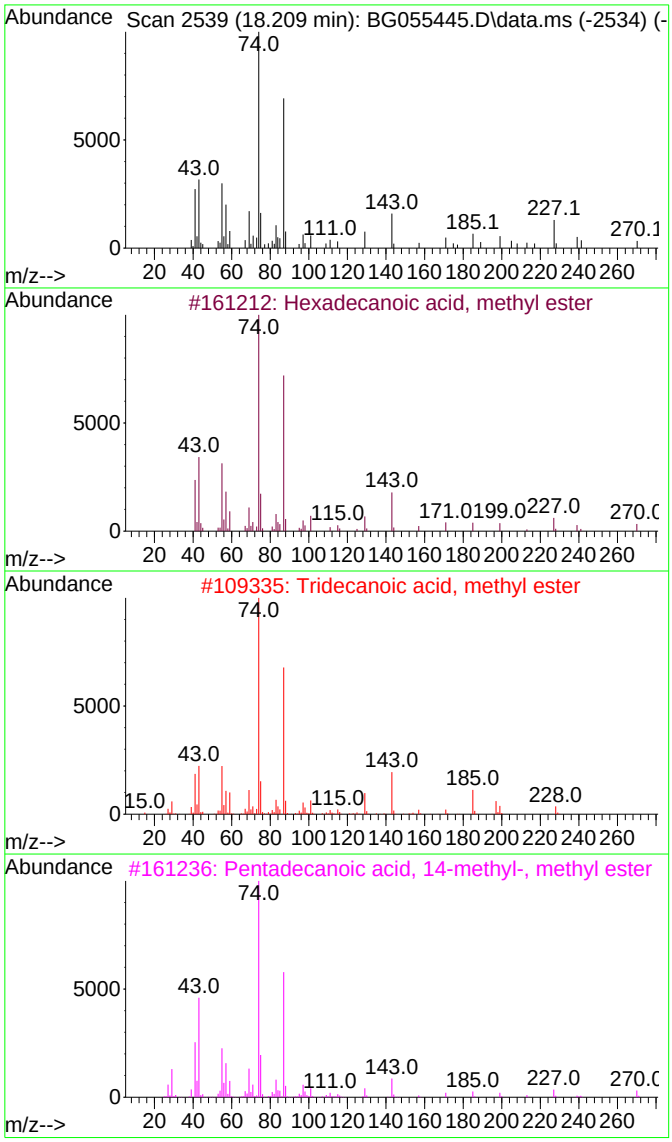
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

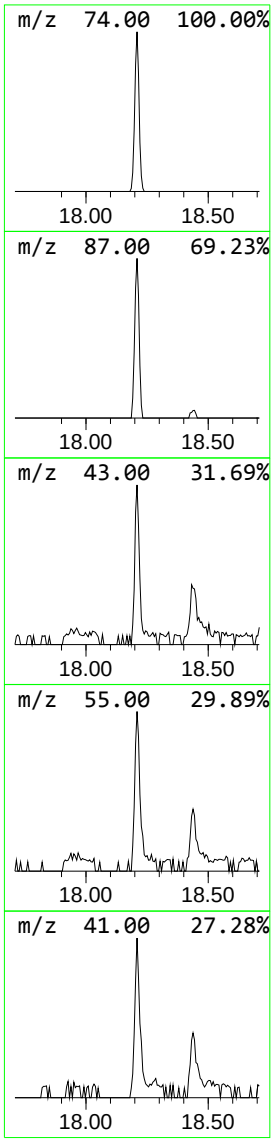
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.209	3.43 ng	73331	Phenanthrene-d10	17.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	72
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	64





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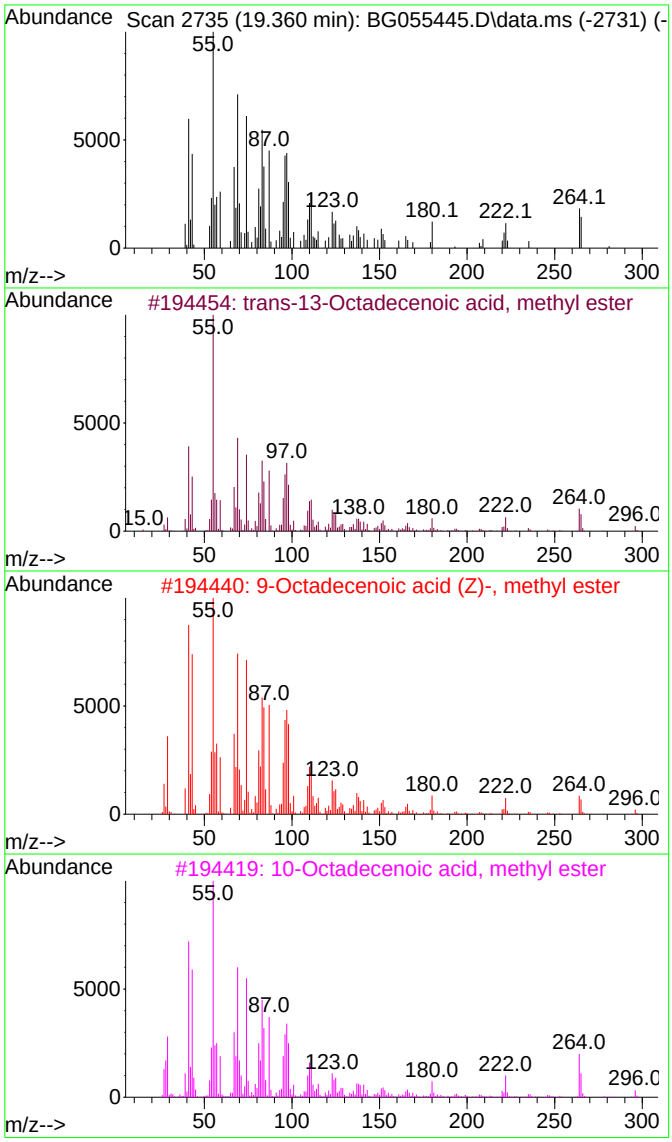
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

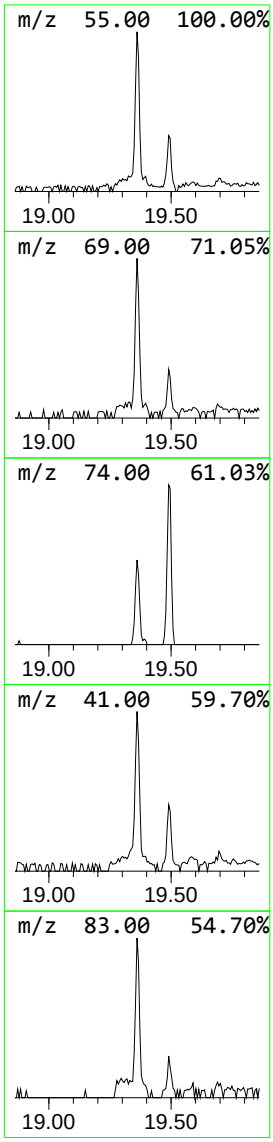
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 trans-13-Octadecenoic acid,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.360	4.14 ng	88648	Phenanthrene-d10	17.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	87





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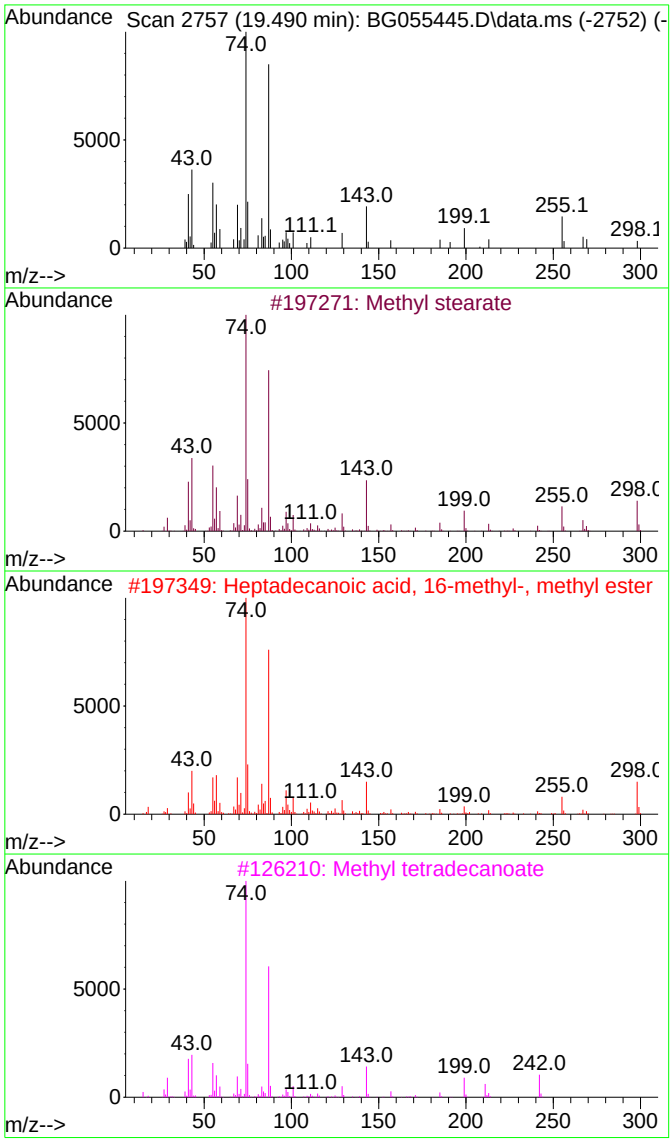
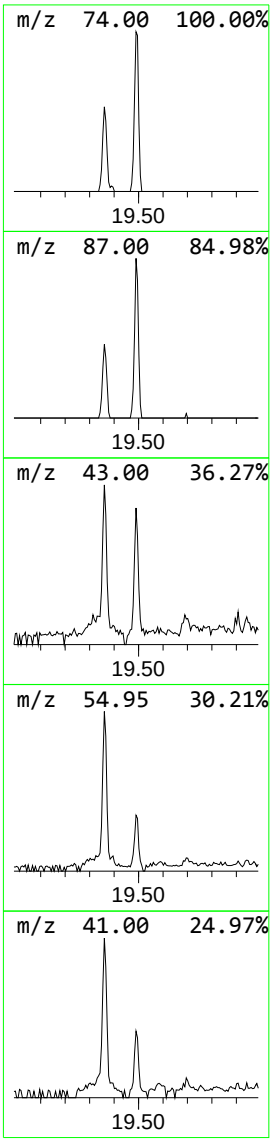
****

Peak Number 6 Methyl stearate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.490	2.01 ng	42960	Phenanthrene-d10	17.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	91
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	86
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80





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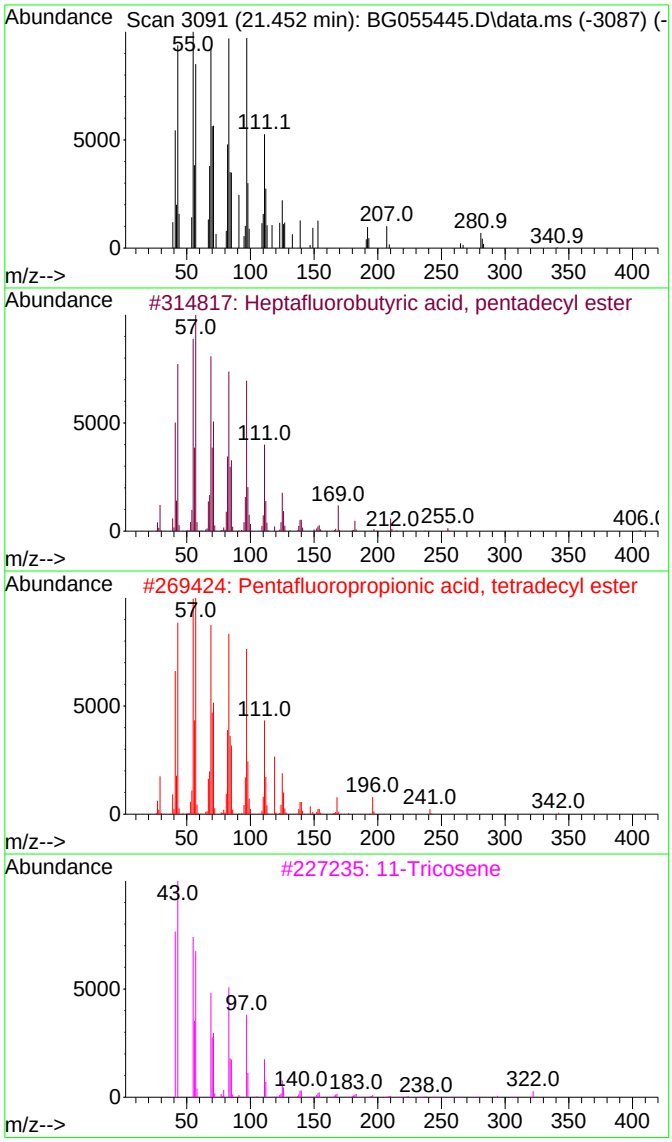
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

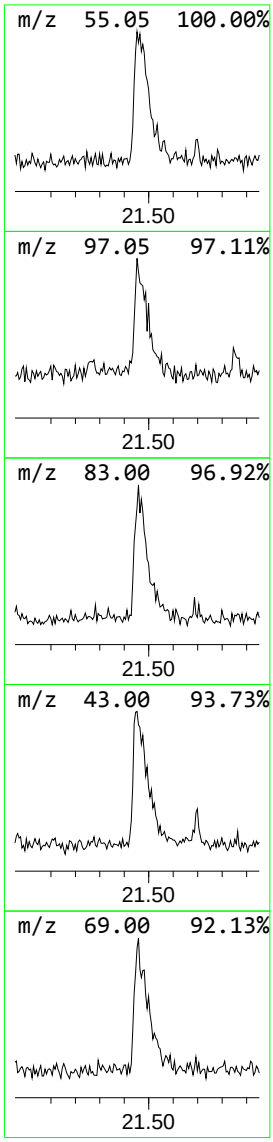
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.452	2.86 ng	73483	Chrysene-d12	21.858

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
3	11-Tricosene	322	C23H46	052078-56-5	91
4	1-Tetracosene	336	C24H48	010192-32-2	91
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





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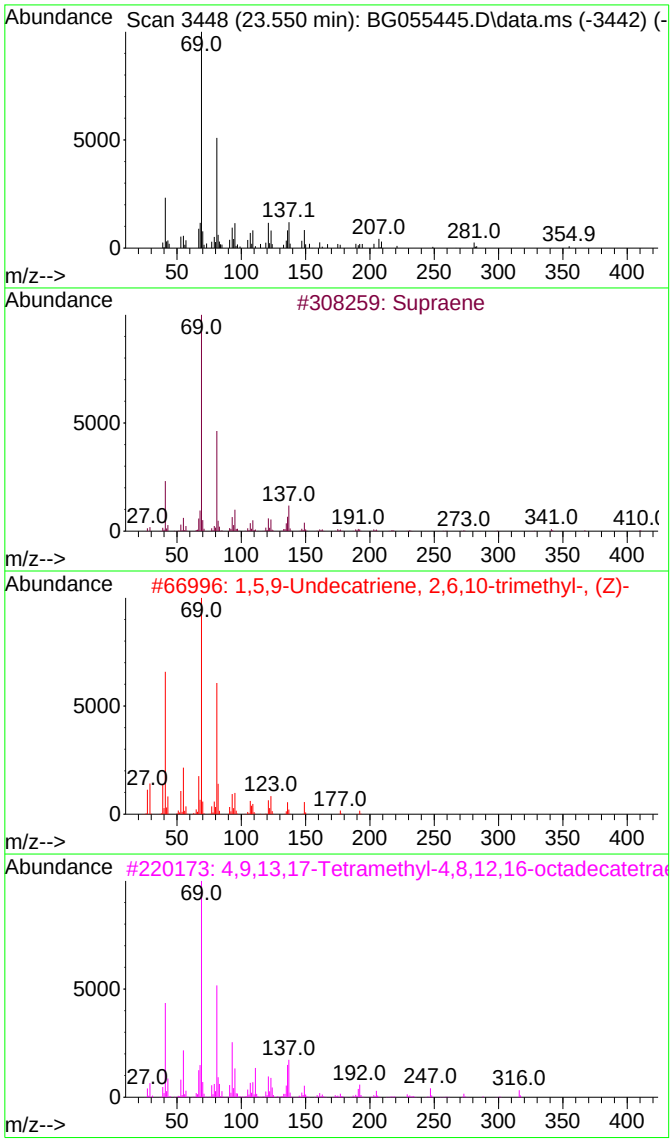
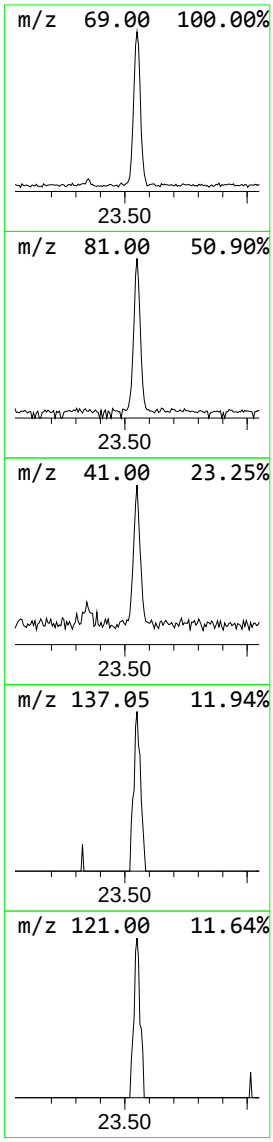
****

Peak Number 8 Supraene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.550	2.53 ng	68598	Perylene-d12	25.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	90
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	78
4	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	64
5	trans-Farnesol	222	C15H26O	000106-28-5	59





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
2-Pentanone, 4-...	5.277	4.8	ng	34969	1	8.232	146529	20.0
Ethanol, 2-(2-b...	10.806	24.1	ng	251900	2	11.064	209345	20.0
2,4,7,9-Tetrame...	13.726	4.2	ng	67365	3	14.848	323115	20.0
Hexadecanoic ac...	18.209	3.4	ng	73331	4	17.586	427823	20.0
trans-13-Octade...	19.360	4.1	ng	88648	4	17.586	427823	20.0
Methyl stearate	19.490	2.0	ng	42960	4	17.586	427823	20.0
Heptafluorobuty...	21.452	2.9	ng	73483	5	21.858	514234	20.0
Supraene	23.550	2.5	ng	68598	6	25.224	543121	20.0