LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055448.D
Acq On : 3 Nov 2022 22:14
Operator : CG/JU
Sample : N5306-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221167-COMP-02-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: BG055448.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	333	338	346	rBV	29541	44945	2.27%	0.469%
2	5.762	414	421	433	rBV	239518	391779	19.80%	4.086%
3	7.384	690	697	711	rBV	214658	392376	19.83%	4.092%
4	8.236	835	842	847	rBV	88075	147064	7.43%	1.534%
5	9.411	1034	1042	1054	rBV	235151	423622	21.41%	4.418%
6	10.809	1273	1280	1293	rBV	246390	433652	21.91%	4.523%
7	11.062	1316	1323	1332	rVB	126769	219417	11.09%	2.288%
8	13.476	1725	1734	1746	rVB	763348	1154005	58.32%	12.035%
9	13.723	1769	1776	1784	rBV	82396	126005	6.37%	1.314%
10	14.851	1960	1968	1978	rVB	226937	344635	17.42%	3.594%
11	16.332	2214	2220	2234	rBV	653599	989559	50.01%	10.320%
12	17.583	2427	2433	2440	rBV	303593	454077	22.95%	4.736%
13	18.212	2534	2540	2547	rBV	82621	117256	5.93%	1.223%
14	18.441	2573	2579	2590	rBV	93663	164229	8.30%	1.713%
15	19.364	2732	2736	2740	rVB	159891	181384	9.17%	1.892%
16	19.493	2753	2758	2762	rVB	44523	49727	2.51%	0.519%
17	19.587	2765	2774	2779	rBV10	11014	30426	1.54%	0.317%
18	19.693	2784	2792	2805	rBV2	23281	47217	2.39%	0.492%
19	20.157	2865	2871	2877	rBV	1477357	1978793	100.00%	20.637%
20	20.433	2911	2918	2922	rBV4	13288	26964	1.36%	0.281%
21	20.774	2972	2976	2980	rBV2	17374	23492	1.19%	0.245%
22	21.449	3086	3091	3113	rBV2	93214	309450	15.64%	3.227%
23	21.855	3154	3160	3168	rVB2	307288	524143	26.49%	5.466%
24	22.625	3287	3291	3296	rBV4	12378	22593	1.14%	0.236%
25	23.553	3441	3449	3459	rVB	205598	423583	21.41%	4.418%
26	25.227	3724	3734	3747	rVB2	189757	568067	28.71%	5.924%

Sum of corrected areas: 9588460

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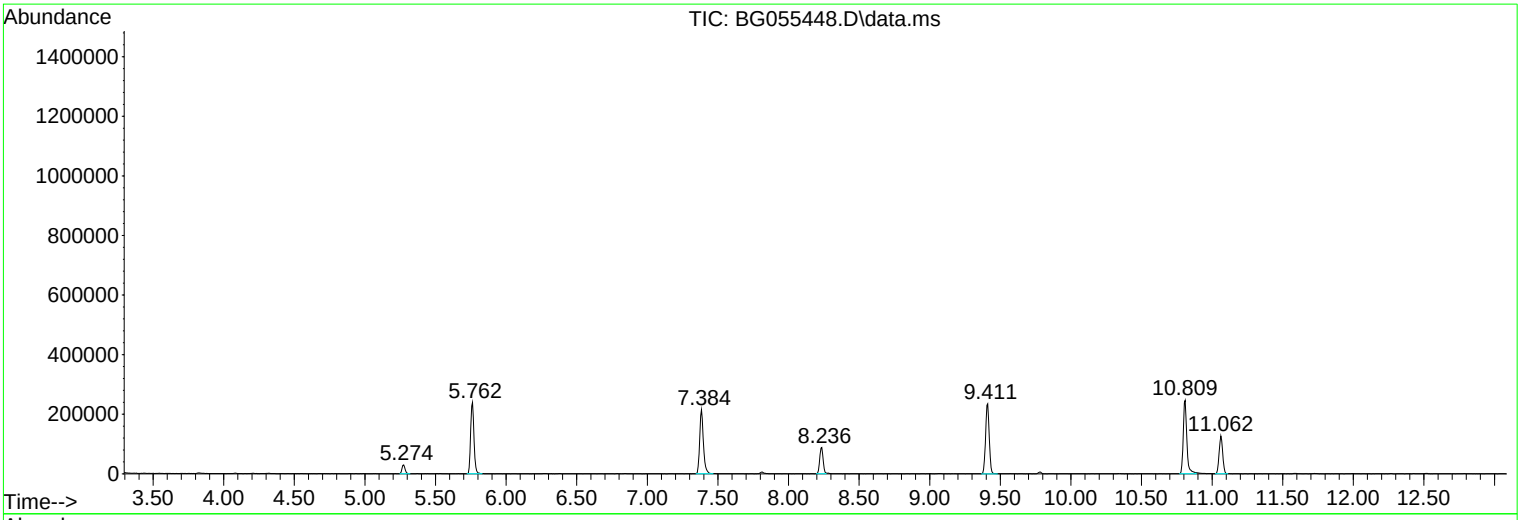
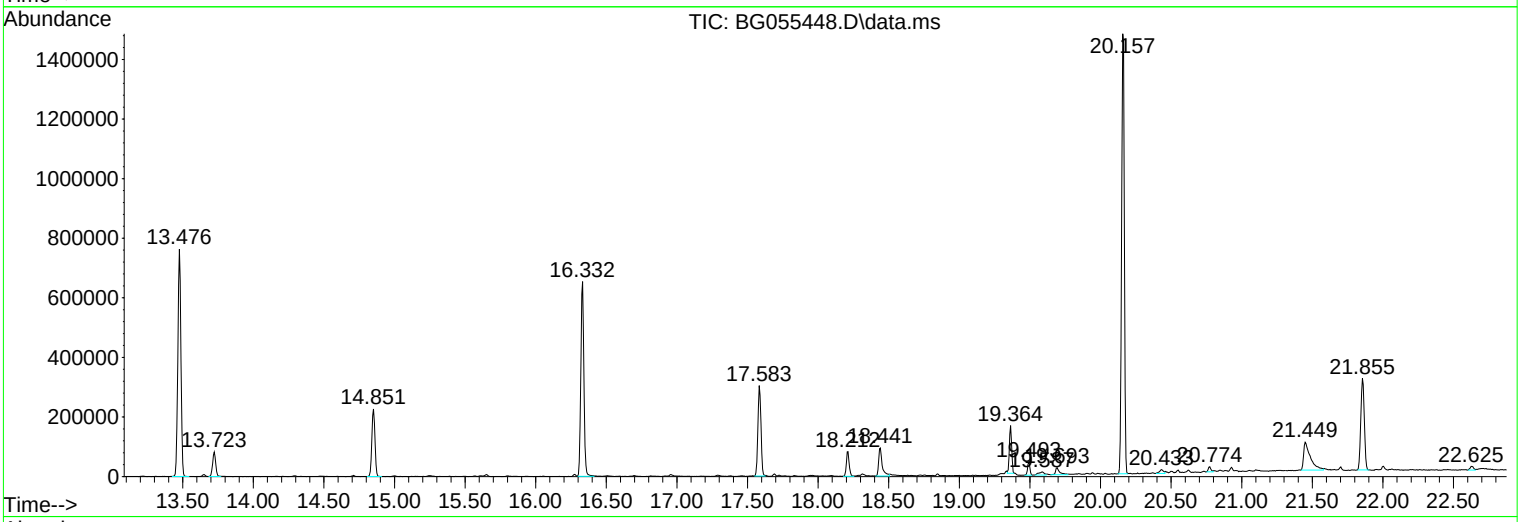
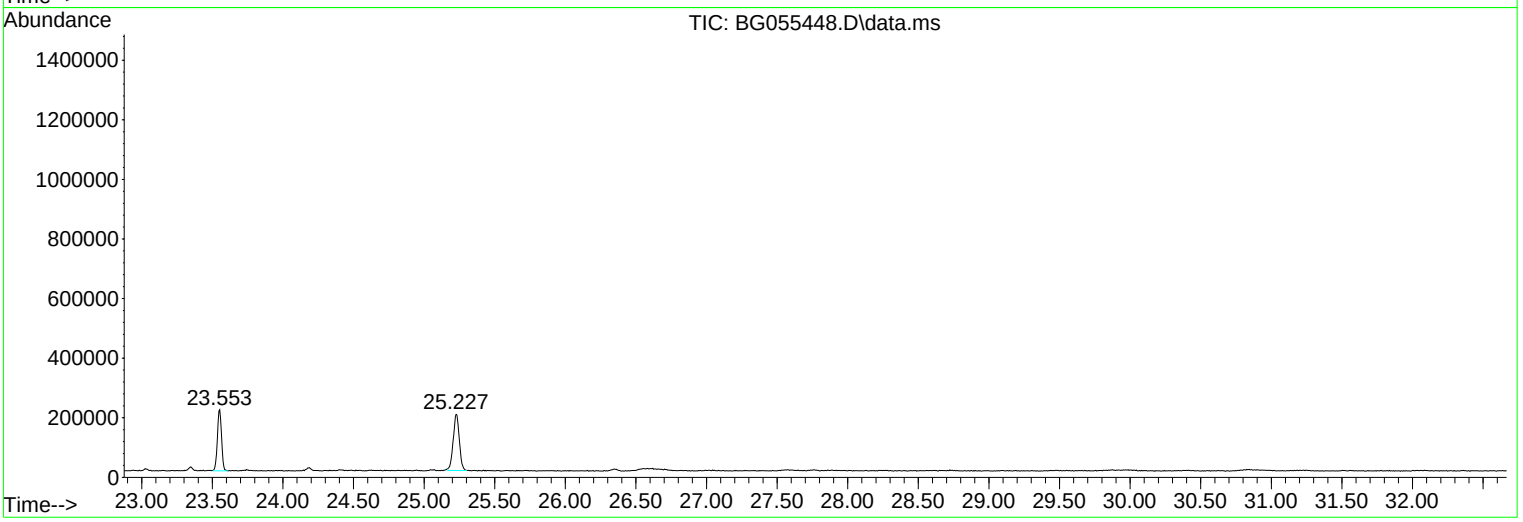
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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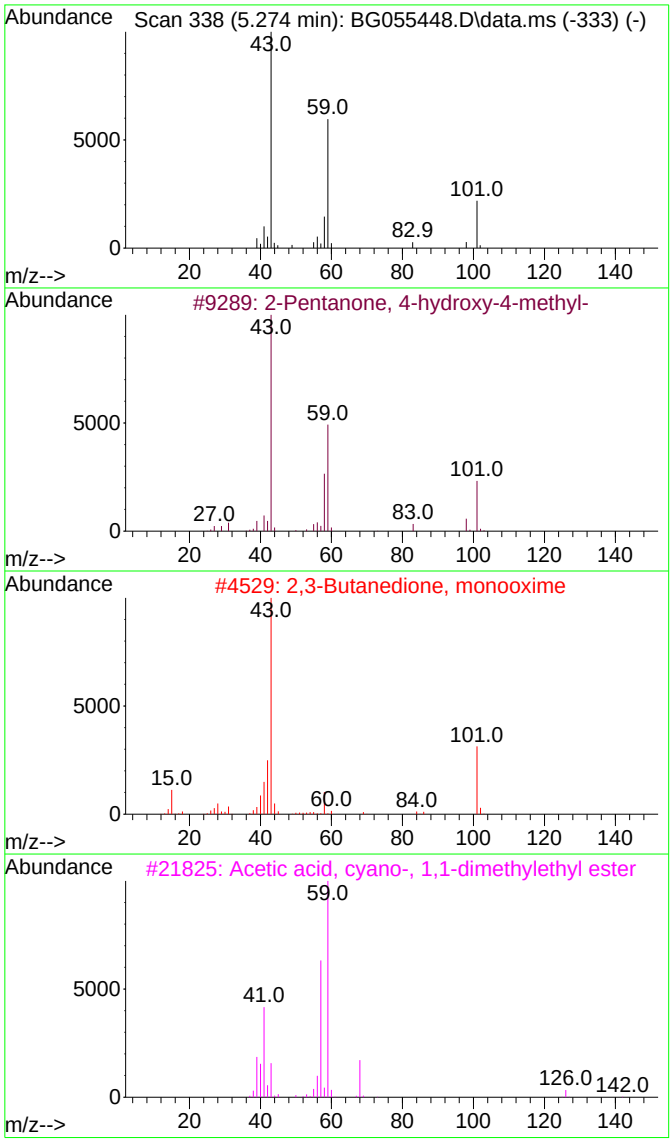
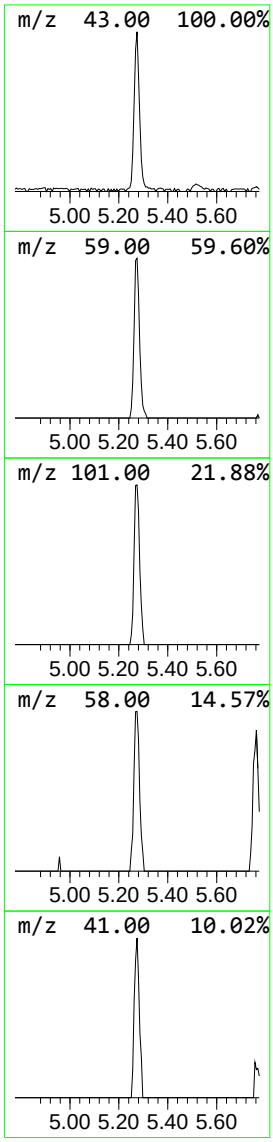
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.274	6.11 ng	44945	1,4-Dichlorobenzene-d4	8.236

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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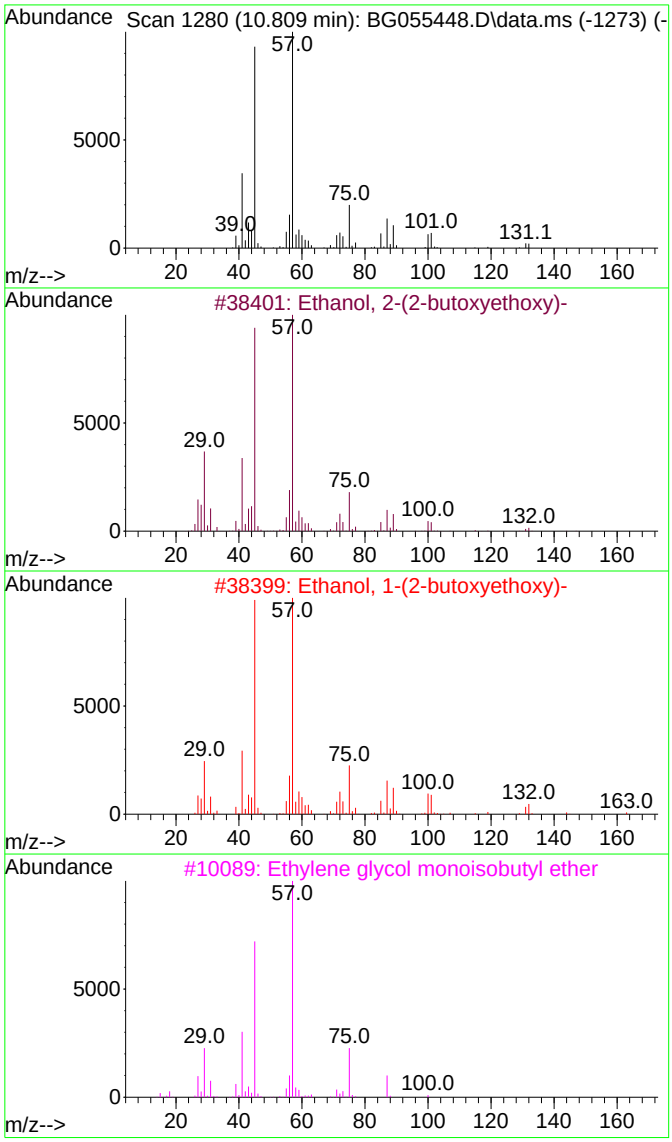
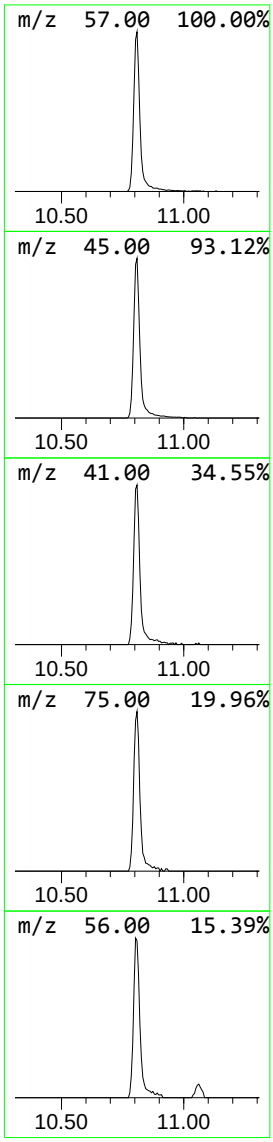
****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.809	39.53 ng	433652	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, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
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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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110122.M
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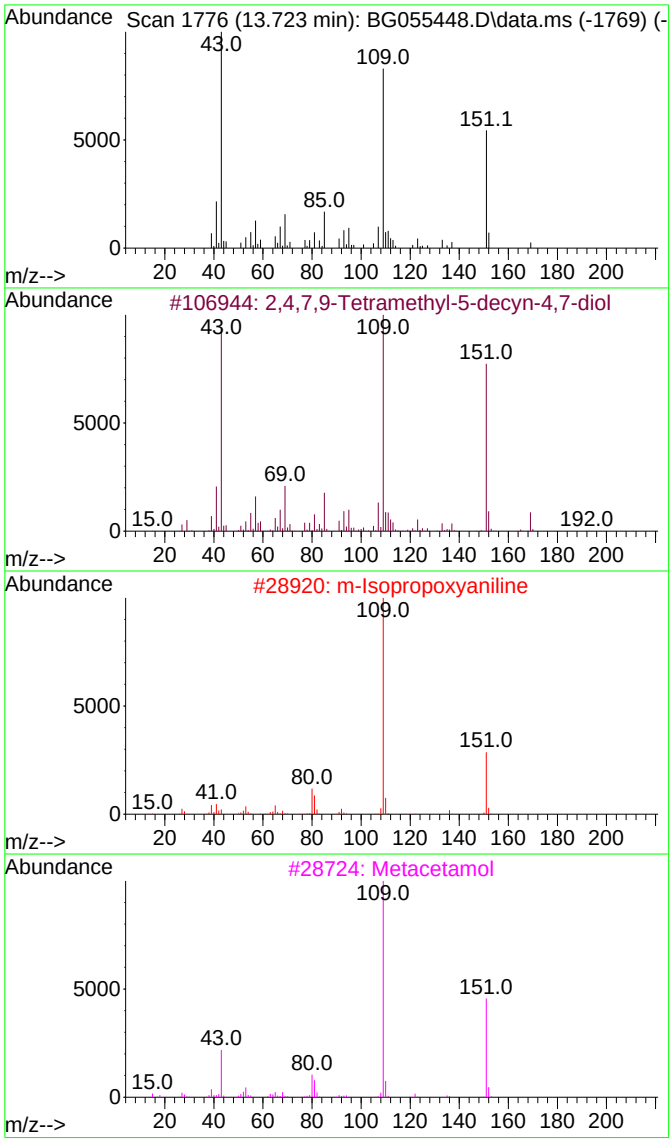
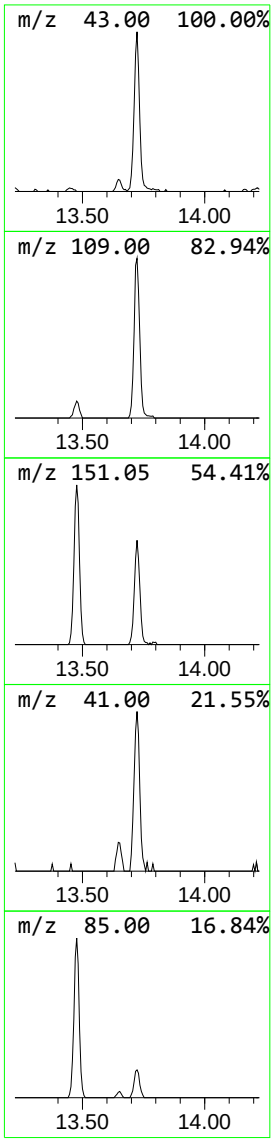
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.723	7.31 ng	126005	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	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	58
3	Metacetamol	151	C8H9NO2	000621-42-1	53
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
5	6,6-Dimethylhepta-2,4-diene	124	C9H16	1000195-03-3	38





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TIC Library : C:\Database\NIST20.L
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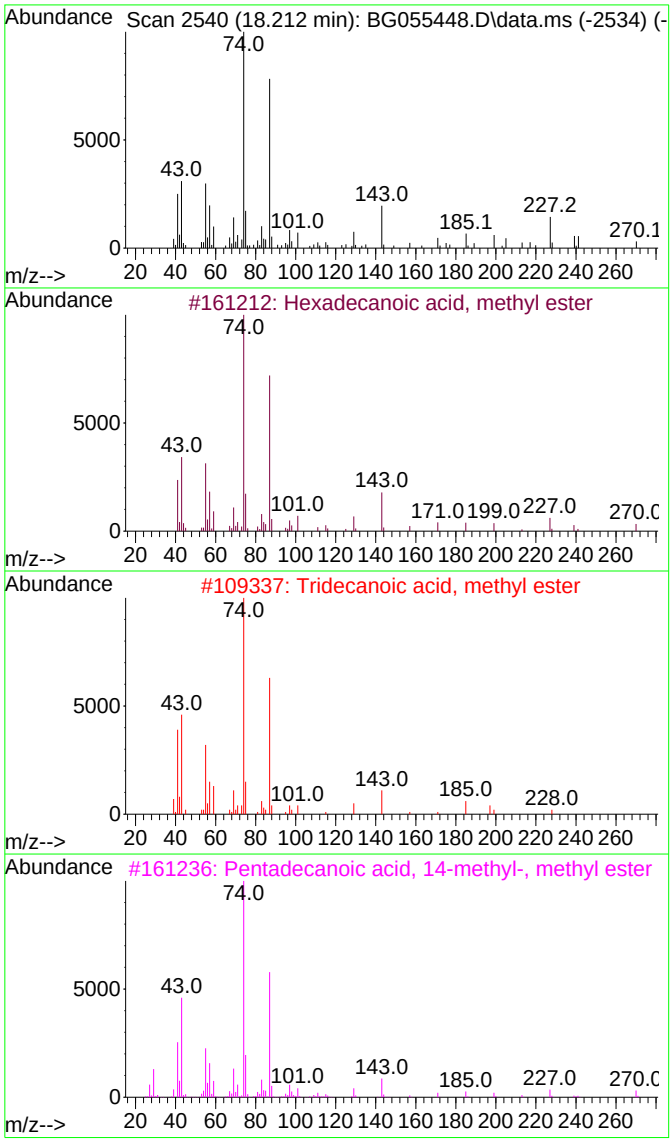
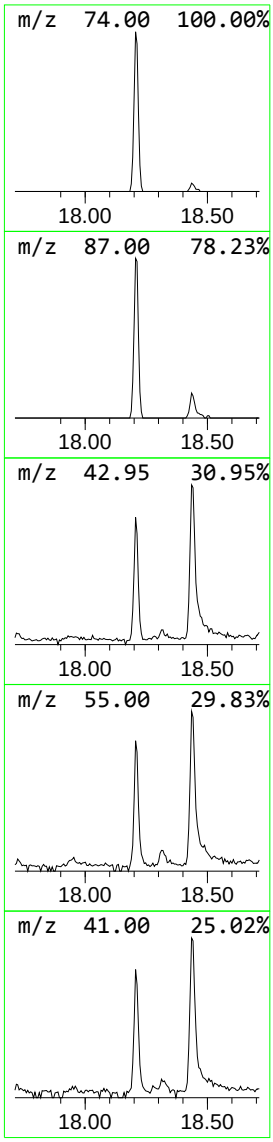
****
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	5.16 ng	117256	Phenanthrene-d10	17.583

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	90
4	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	80
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	72





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Misc :
ALS Vial : 17 Sample Multiplier: 1

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BNA_G
ClientSampleId :
DISSOLVED-20221167-COMP-02-MODIFIED-ELUTRIATE

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TIC Library : C:\Database\NIST20.L
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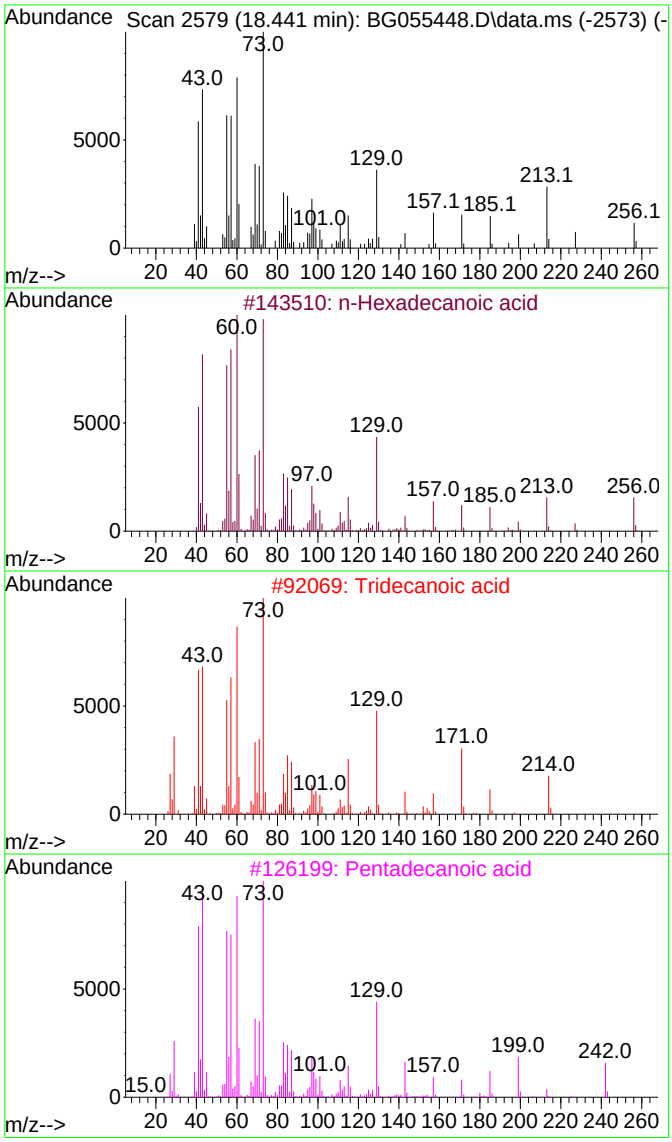
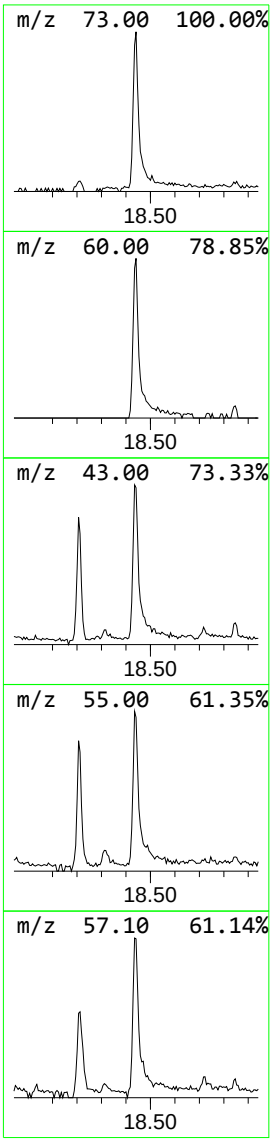
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.441	7.23 ng	164229	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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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TIC Library : C:\Database\NIST20.L
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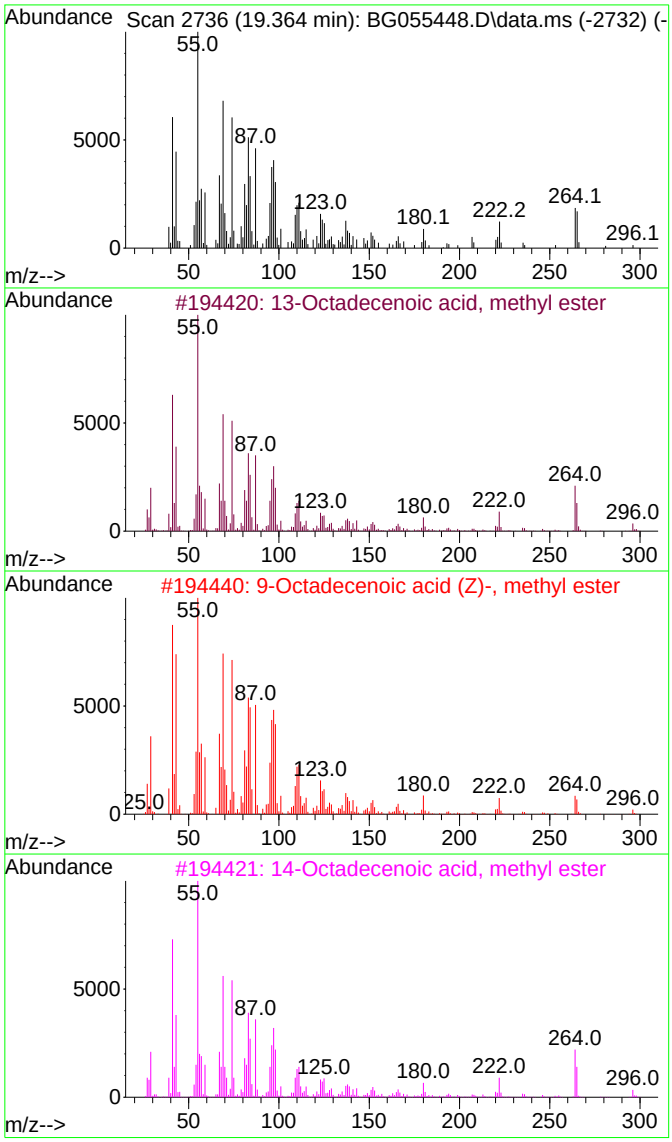
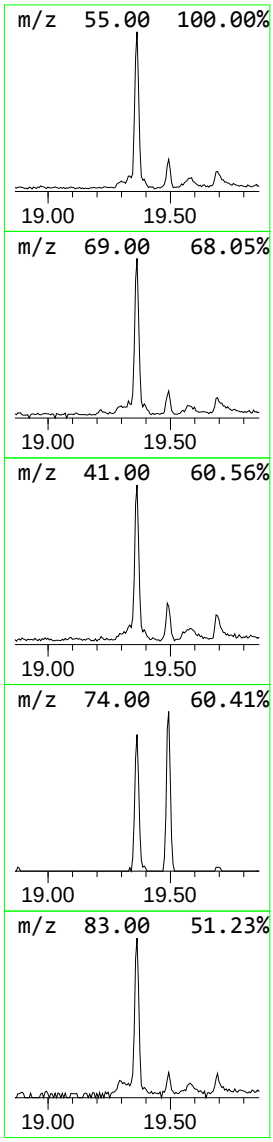
****
Peak Number 6 13-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.364	7.99 ng	181384	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	98
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	97
5	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	94





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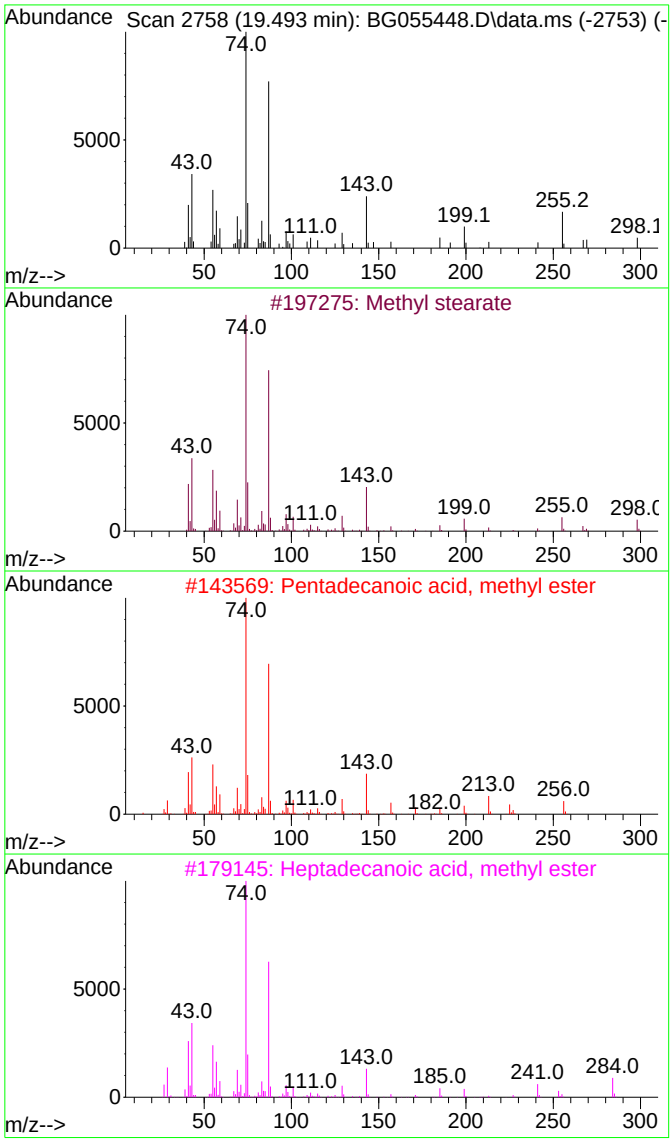
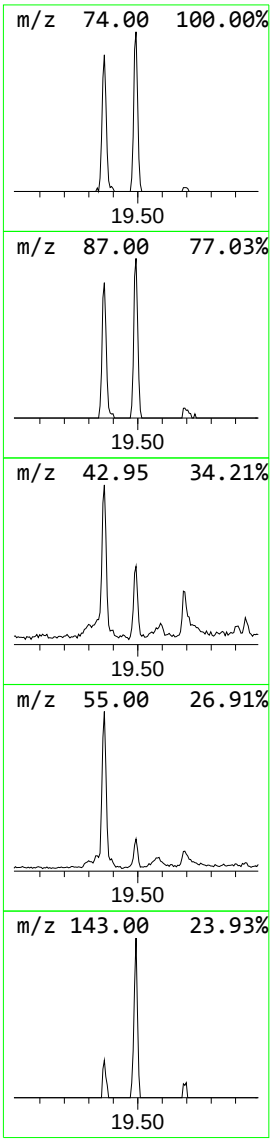
****

Peak Number 7 Methyl stearate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.493	2.19 ng	49727	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
3	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	80
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	72





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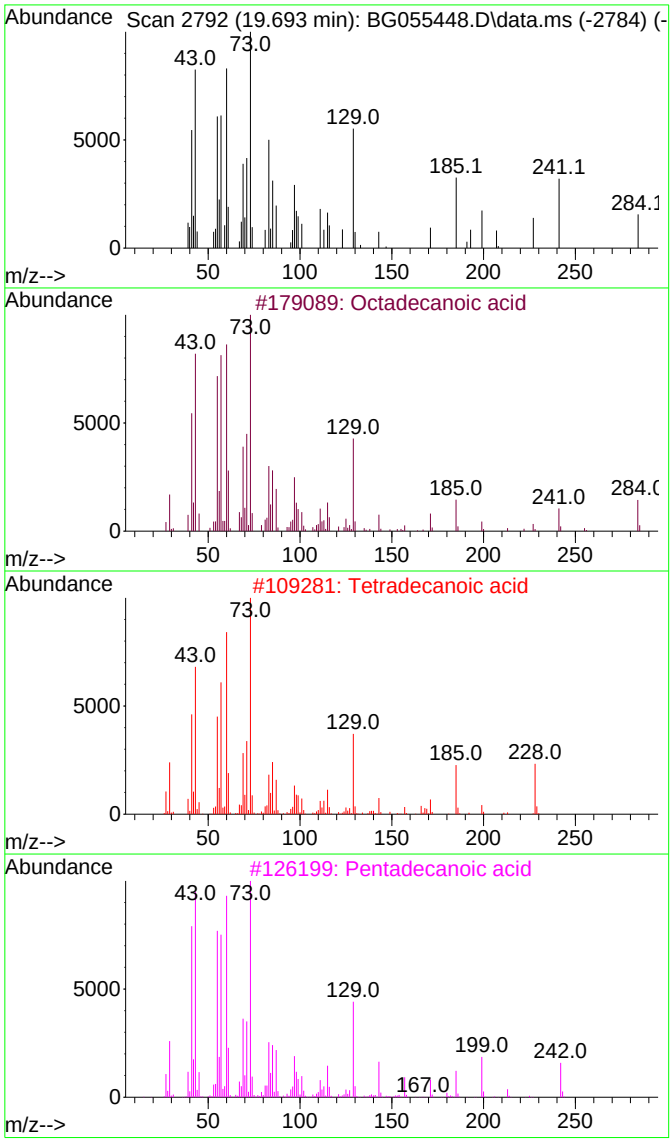
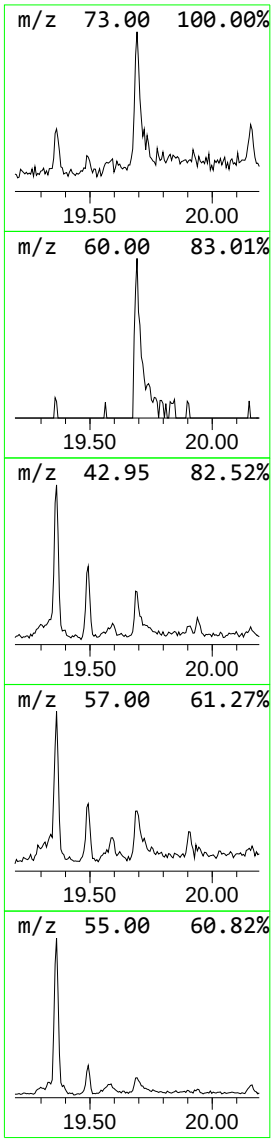
****

Peak Number 8 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.693	2.08 ng	47217	Phenanthrene-d10	17.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	87
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
5	Dodecanoic acid	200	C12H24O2	000143-07-7	46





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
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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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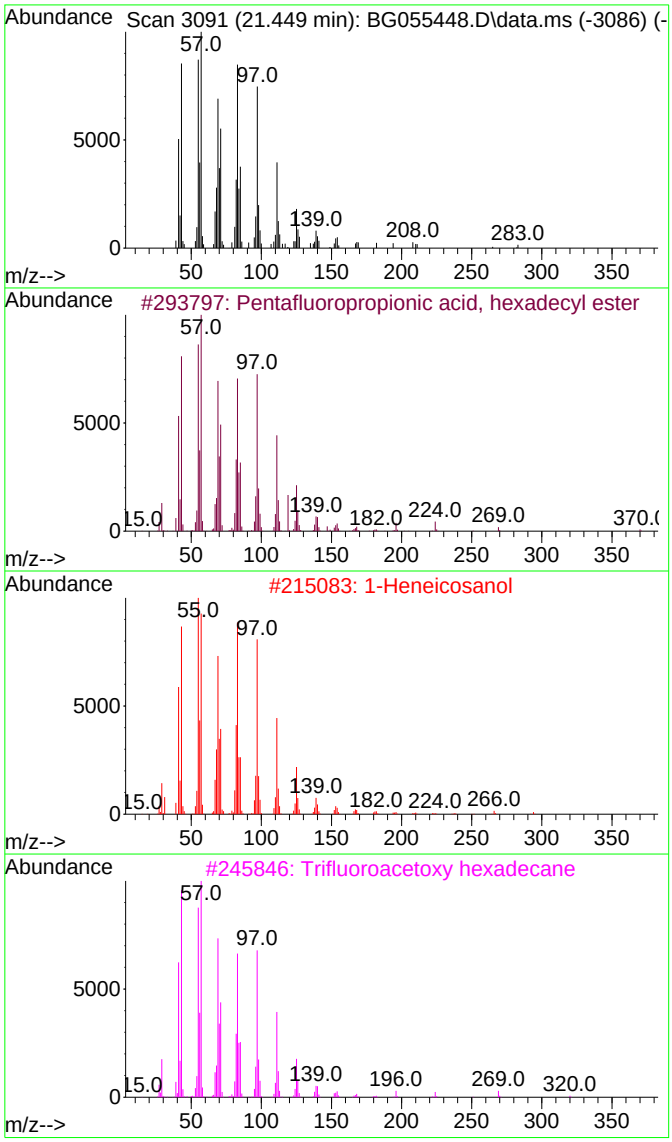
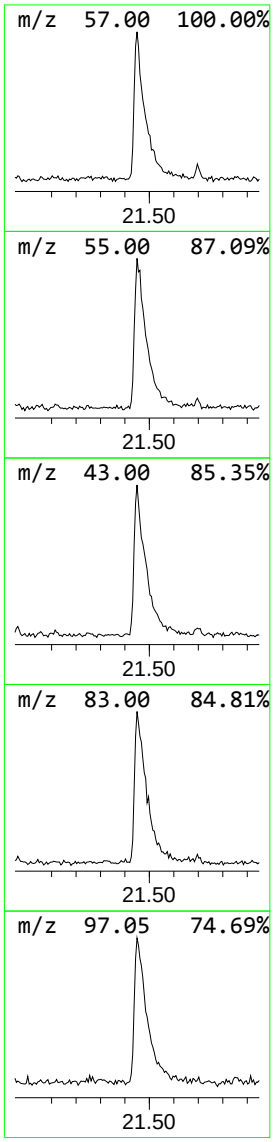
****
Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.449	11.81 ng	309450	Chrysene-d12	21.855

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055448.D
Acq On : 3 Nov 2022 22:14
Operator : CG/JU
Sample : N5306-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221167-COMP-02-MODIFIED-ELUTRIATE

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

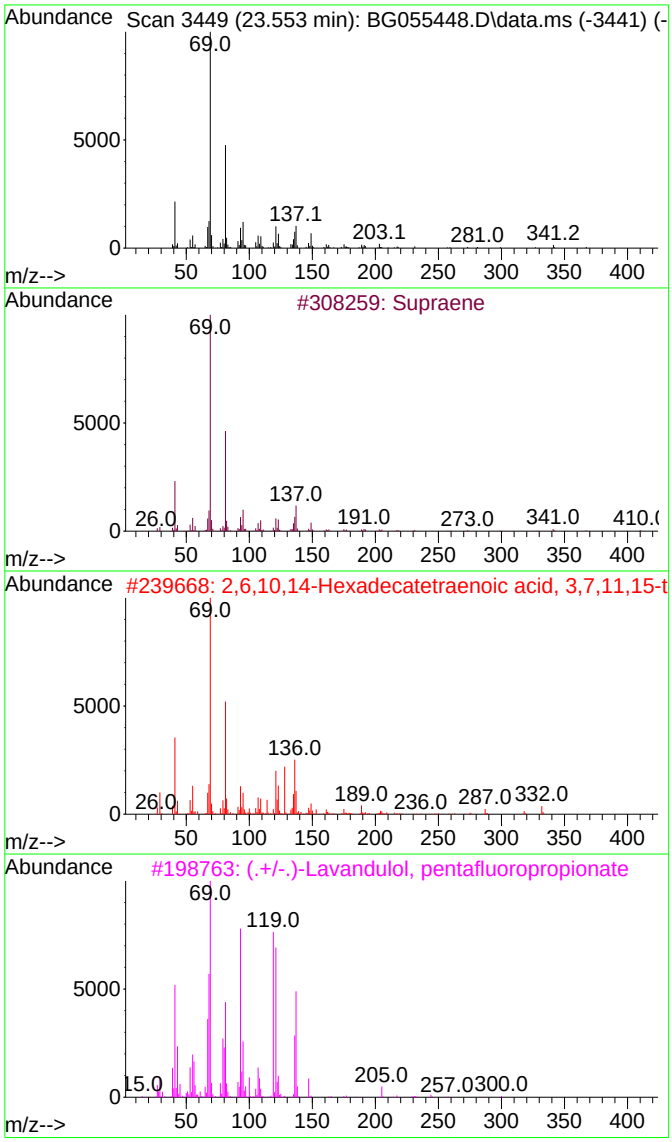
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

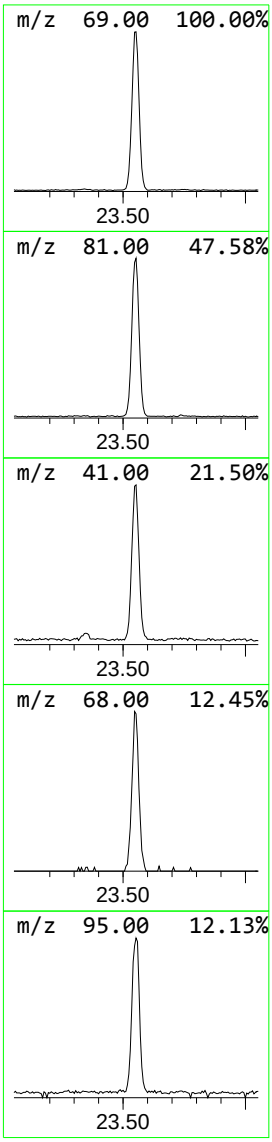
****

Peak Number 10 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.553	14.91 ng	423583	Perylene-d12	25.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
3	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
4	trans-Farnesol	222	C15H26O	000106-28-5	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG110322\
Data File : BG055448.D
Acq On : 3 Nov 2022 22:14
Operator : CG/JU
Sample : N5306-07
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DISSOLVED-20221167-COMP-02-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	6.1	ng	44945	1	8.236	147064	20.0
Ethanol, 2-(2-b...	10.809	39.5	ng	433652	2	11.062	219417	20.0
2,4,7,9-Tetrame...	13.723	7.3	ng	126005	3	14.851	344635	20.0
Hexadecanoic ac...	18.212	5.2	ng	117256	4	17.583	454077	20.0
n-Hexadecanoic ...	18.441	7.2	ng	164229	4	17.583	454077	20.0
13-Octadecenoic...	19.364	8.0	ng	181384	4	17.583	454077	20.0
Methyl stearate	19.493	2.2	ng	49727	4	17.583	454077	20.0
Octadecanoic acid	19.693	2.1	ng	47217	4	17.583	454077	20.0
Pentafluoroprop...	21.449	11.8	ng	309450	5	21.855	524143	20.0
Supraene	23.553	14.9	ng	423583	6	25.227	568067	20.0