LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053809.D
Acq On : 3 Jun 2022 12:21
Operator : CG/JU
Sample : N3138-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-3-053122

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-BG060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053809.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.783	64	67	74	rBV	14351	23800	1.58%	0.250%
2	5.651	379	385	396	rVB	337132	584486	38.89%	6.147%
3	7.238	647	655	665	rBV	357388	633537	42.15%	6.663%
4	8.090	793	800	807	rVB	100266	177515	11.81%	1.867%
5	9.247	987	997	1005	rBV	217322	403123	26.82%	4.239%
6	10.898	1269	1278	1286	rBV	140778	279259	18.58%	2.937%
7	12.320	1514	1520	1526	rBV3	15484	25709	1.71%	0.270%
8	13.342	1686	1694	1700	rBV	605298	1013254	67.41%	10.656%
9	13.542	1721	1728	1736	rBV2	19233	32869	2.19%	0.346%
10	14.611	1906	1910	1916	rVB3	11904	17274	1.15%	0.182%
11	14.711	1918	1927	1935	rBV	234117	390936	26.01%	4.111%
12	16.192	2173	2179	2187	rBV	488309	760660	50.61%	8.000%
13	16.421	2214	2218	2221	rBV3	11413	19359	1.29%	0.204%
14	17.455	2387	2394	2398	rBV	291113	460785	30.66%	4.846%
15	17.496	2398	2401	2408	rVV	42680	64913	4.32%	0.683%
16	17.584	2411	2416	2423	rVB	11937	21222	1.41%	0.223%
17	17.831	2453	2458	2469	rBV7	15315	34856	2.32%	0.367%
18	17.954	2475	2479	2483	rBV3	9882	15238	1.01%	0.160%
19	18.125	2503	2508	2513	rBV	98481	125920	8.38%	1.324%
20	18.348	2540	2546	2560	rBV2	115312	226955	15.10%	2.387%
21	18.524	2571	2576	2578	rBV5	10676	15581	1.04%	0.164%
22	18.642	2593	2596	2605	rVB5	12565	17652	1.17%	0.186%
23	19.200	2686	2691	2695	rBV2	52713	73478	4.89%	0.773%
24	19.259	2696	2701	2703	rVV	167288	217909	14.50%	2.292%
25	19.288	2703	2706	2717	rVB	270258	395382	26.31%	4.158%
26	19.423	2724	2729	2734	rBV	69353	85148	5.67%	0.895%
27	19.506	2734	2743	2752	rBV2	105496	229011	15.24%	2.408%
28	19.611	2757	2761	2778	rBV	98751	202246	13.46%	2.127%
29	19.864	2795	2804	2811	rVB	84585	159880	10.64%	1.681%
30	20.064	2831	2838	2849	rVB	1094810	1503031	100.00%	15.807%
31	20.358	2883	2888	2889	rBV4	14645	23771	1.58%	0.250%
32	20.516	2912	2915	2919	rVB2	11607	15040	1.00%	0.158%
33	20.816	2962	2966	2970	rBV7	8721	17001	1.13%	0.179%
34	21.380	3058	3062	3071	rVB4	56979	102070	6.79%	1.073%
35	21.732	3114	3122	3127	rBV	311958	598581	39.82%	6.295%
36	21.944	3155	3158	3164	rVB4	18771	25665	1.71%	0.270%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053809.D
Acq On : 3 Jun 2022 12:21
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-3-053122

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-BG060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.965	3498	3502	3506	rBV3	17086	32827	2.18%	0.345%
38	24.999	3669	3678	3688	rBV2	172554	482849	32.13%	5.078%

Sum of corrected areas: 9508792

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ClientSampleId :
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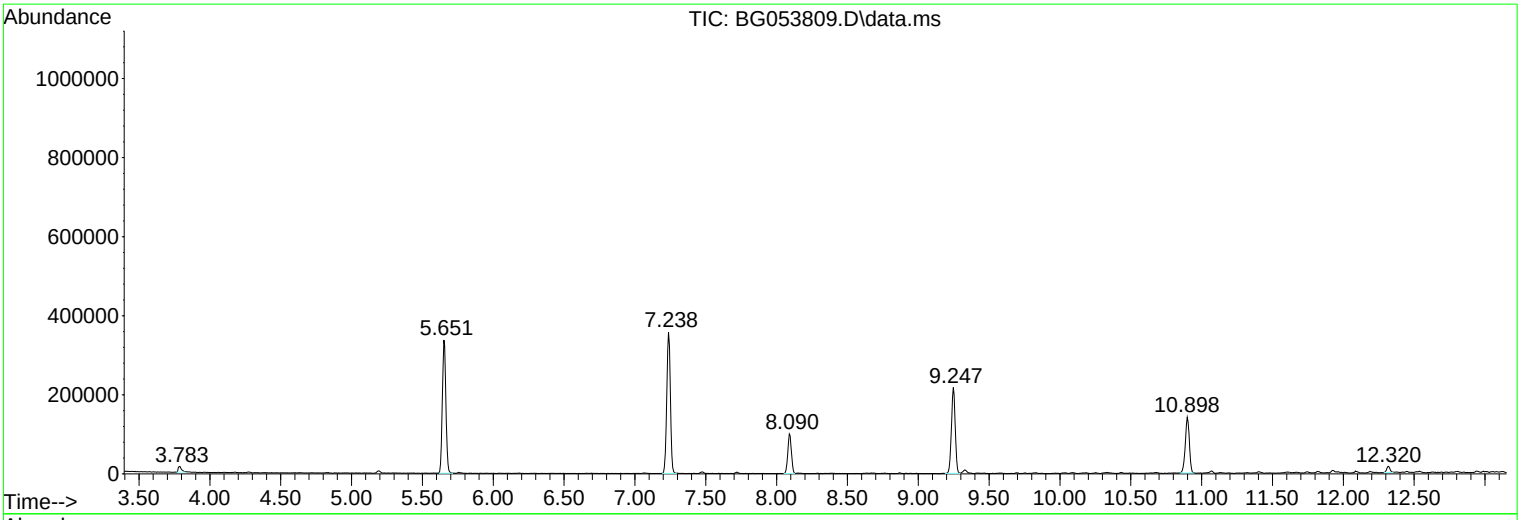
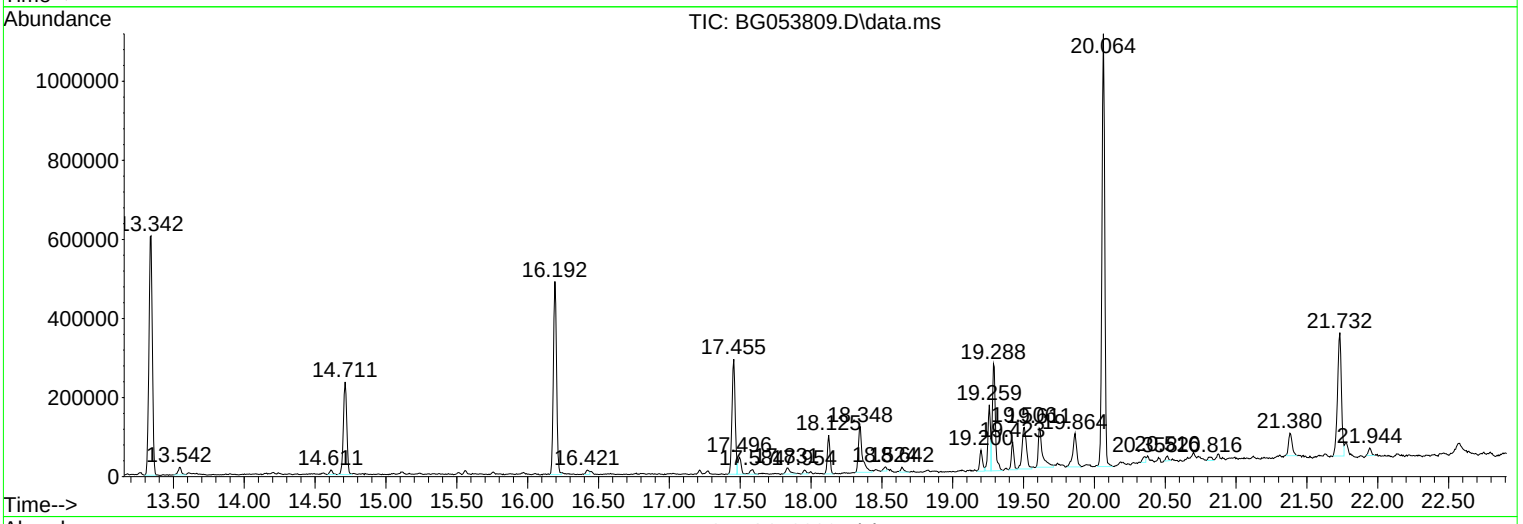
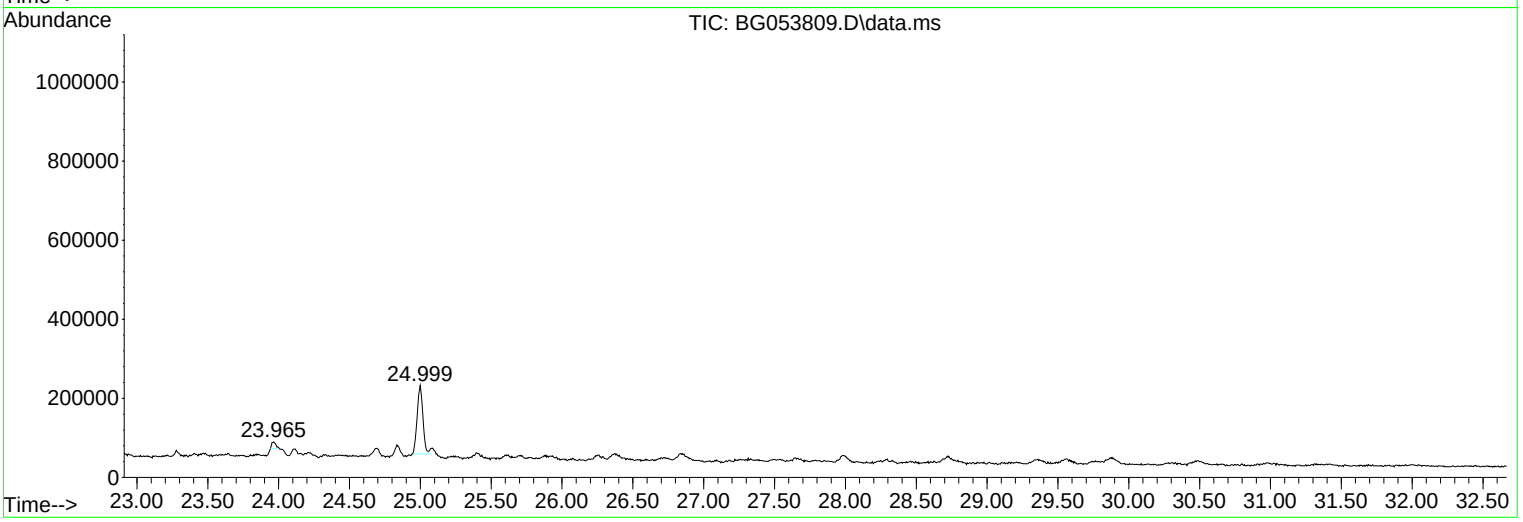
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053809.D
Acq On : 3 Jun 2022 12:21
Operator : CG/JU
Sample : N3138-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

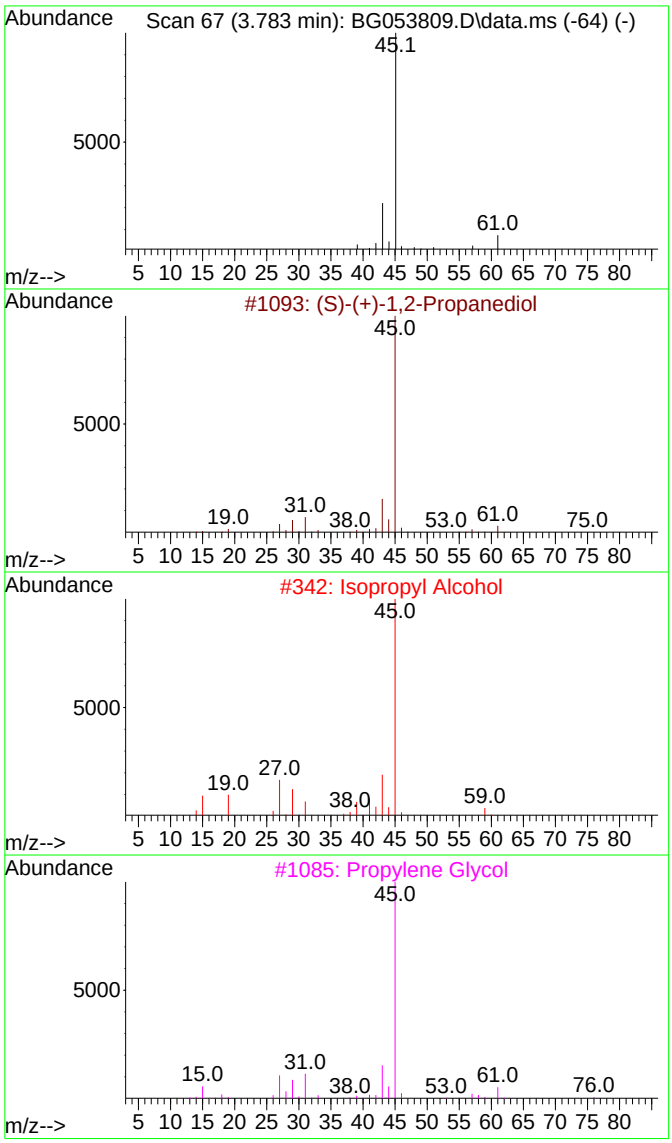
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

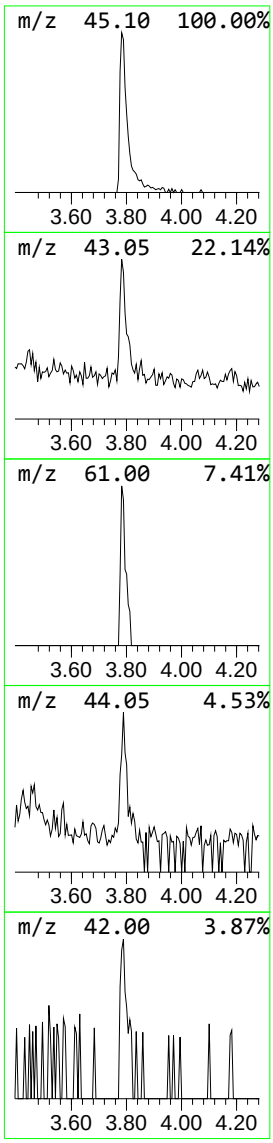
****

Peak Number 1 unknown3.783 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.783	2.68 ng	23800	1,4-Dichlorobenzene-d4	8.095

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Formamide	45	CH3NO	000075-12-7	5





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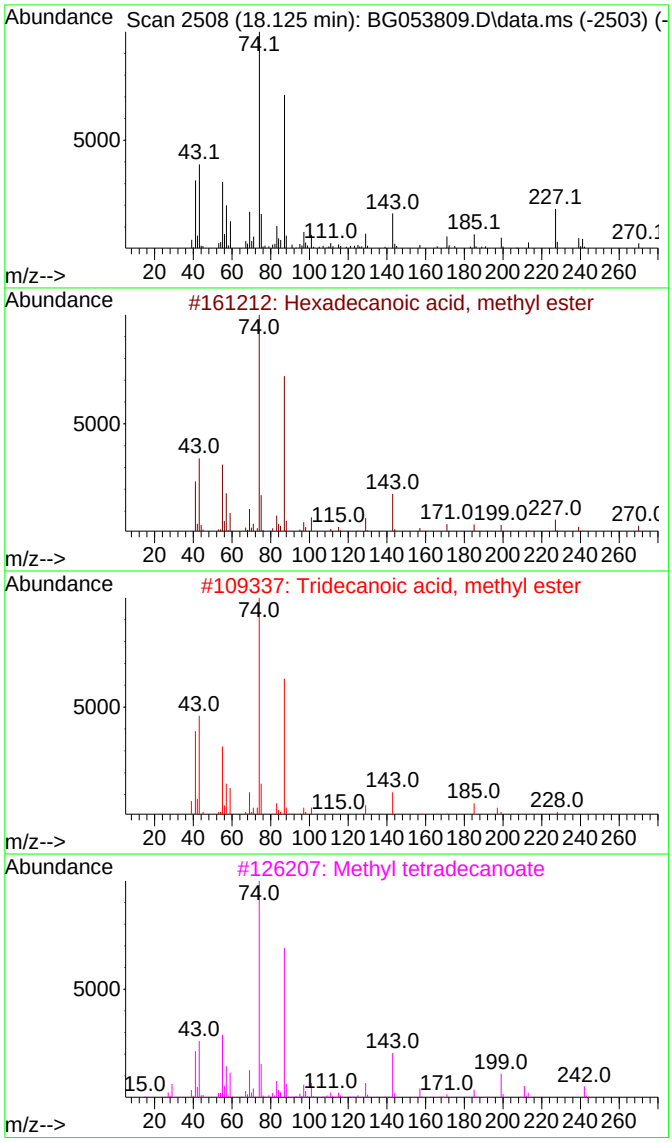
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

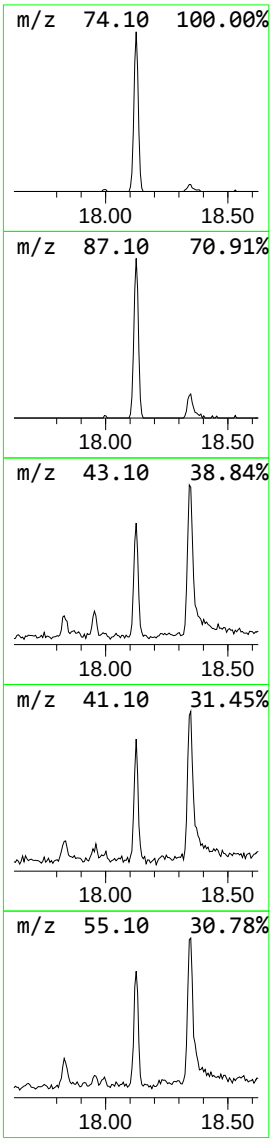
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.125	5.47 ng	125920	Phenanthrene-d10	17.455

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	95
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	94
4	Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	80
5	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053809.D
Acq On : 3 Jun 2022 12:21
Operator : CG/JU
Sample : N3138-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-3-053122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

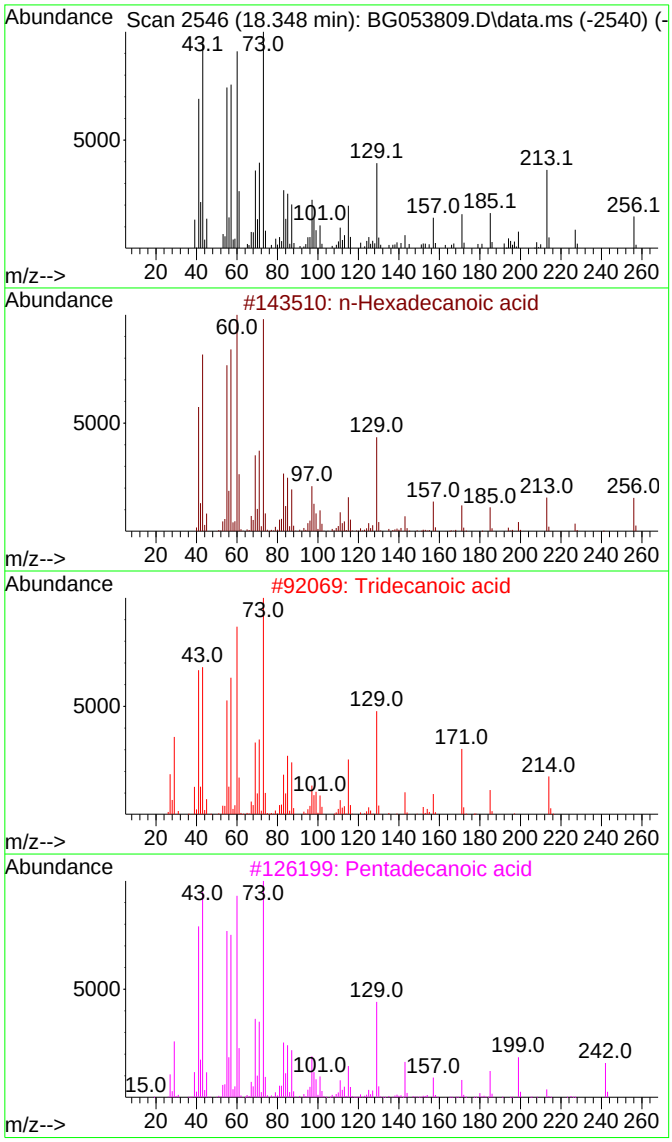
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

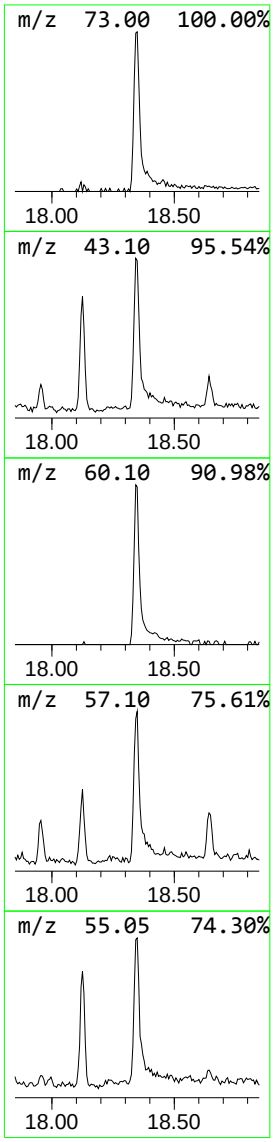
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.348	9.85 ng	226955	Phenanthrene-d10	17.455

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	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Undecanoic acid	186	C11H22O2	000112-37-8	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053809.D
Acq On : 3 Jun 2022 12:21
Operator : CG/JU
Sample : N3138-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-3-053122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

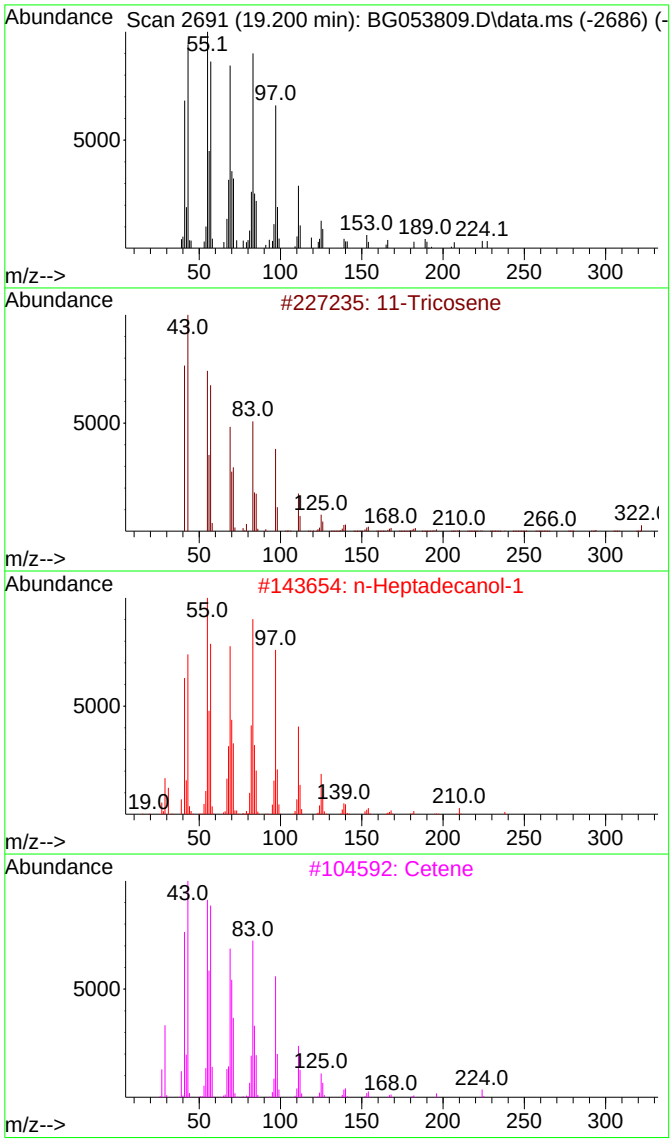
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

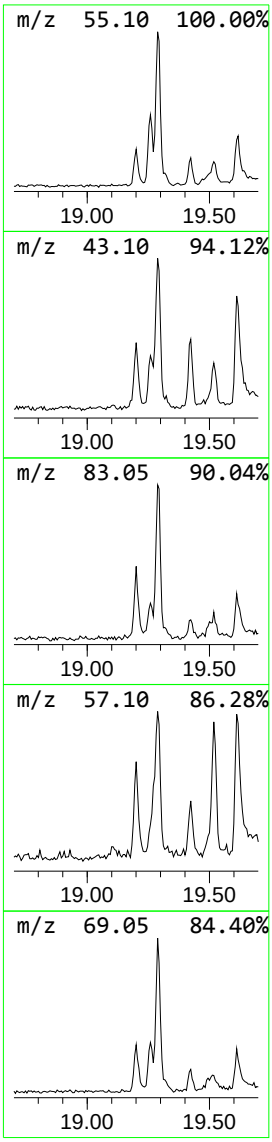
****

Peak Number 4 11-Tricosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.200	3.19 ng	73478	Phenanthrene-d10	17.455

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	91
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
3	Cetene	224	C16H32	000629-73-2	90
4	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	90
5	Cyclohexadecane	224	C16H32	000295-65-8	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053809.D
Acq On : 3 Jun 2022 12:21
Operator : CG/JU
Sample : N3138-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-3-053122

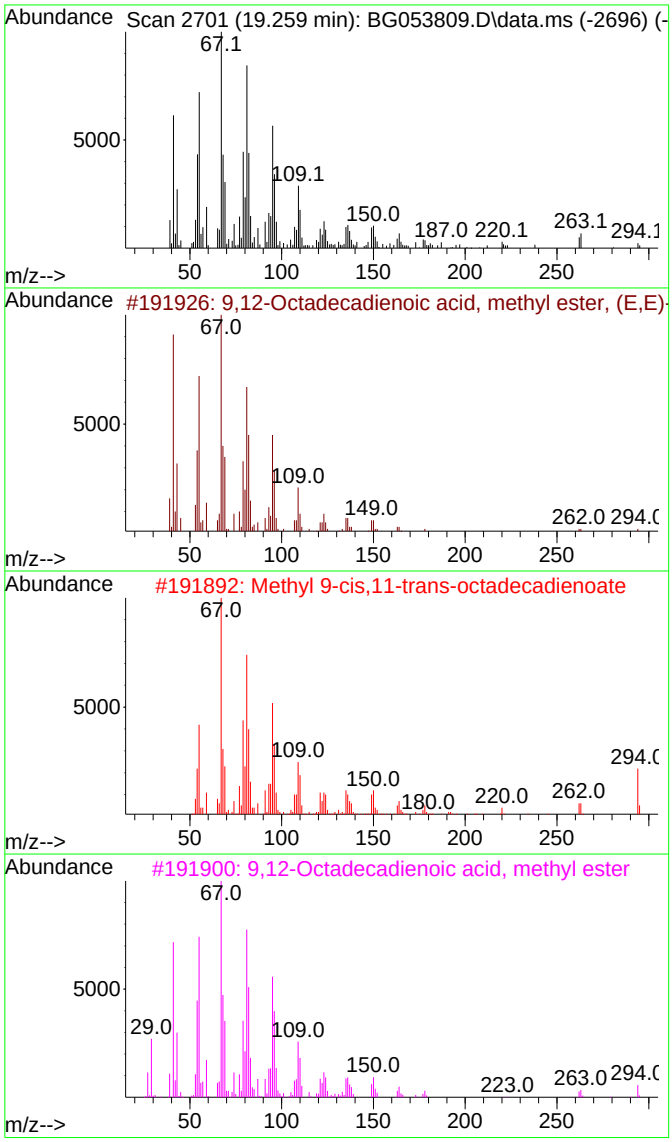
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

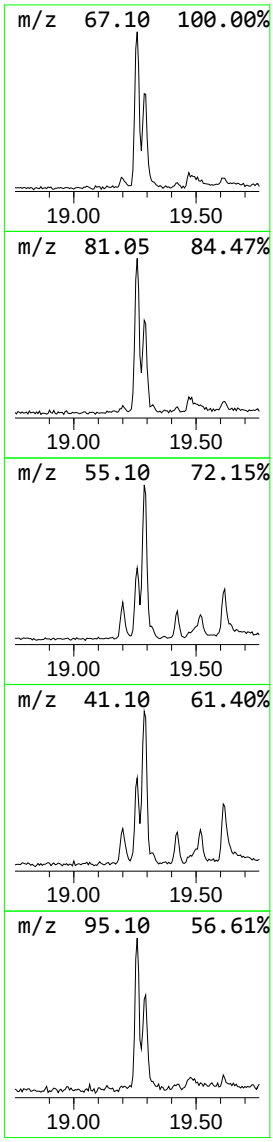
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.259	9.46 ng	217909	Phenanthrene-d10	17.455

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	96
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	94
4	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	91
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	91





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Data File : BG053809.D
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Operator : CG/JU
Sample : N3138-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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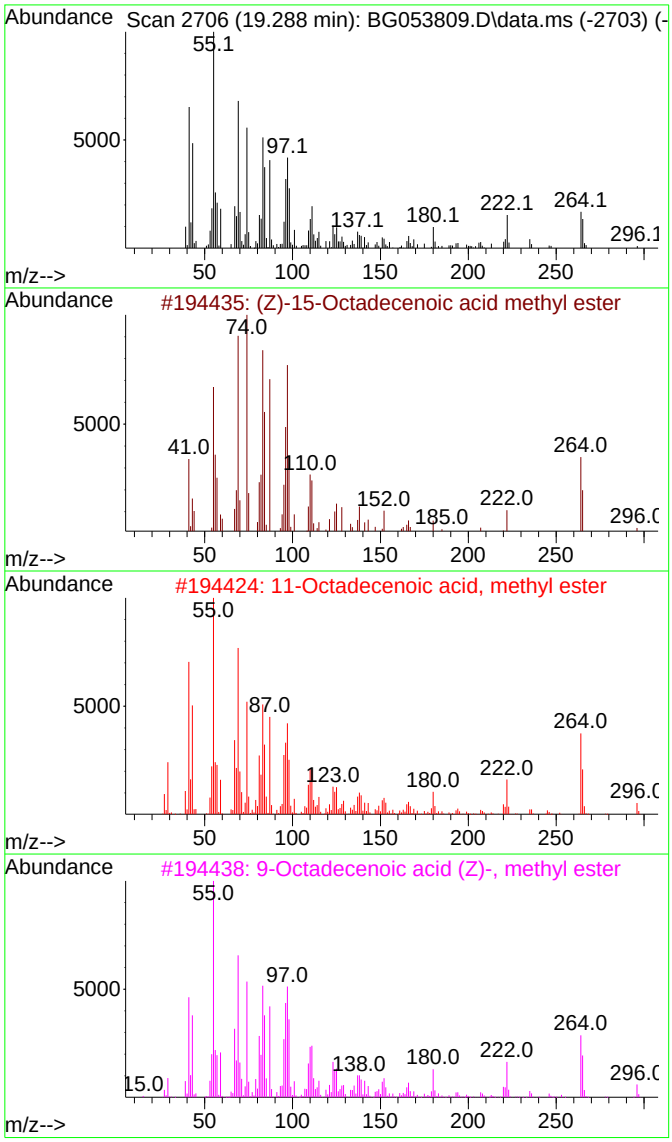
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

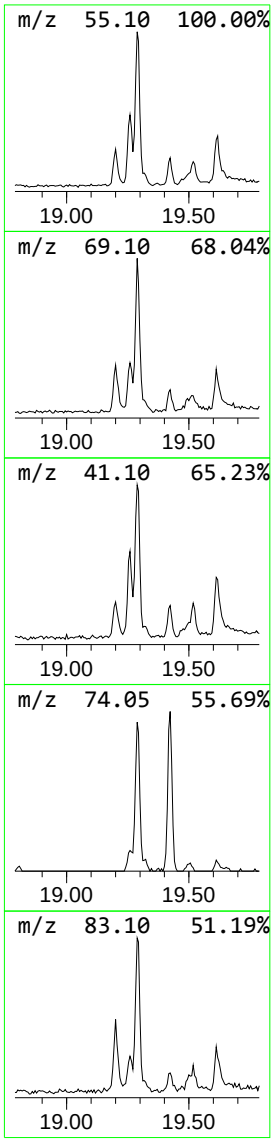
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (Z)-15-Octadecenoic acid me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.288	17.16 ng	395382	Phenanthrene-d10	17.455

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93
2	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	91
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	91
4	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	90
5	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	87





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

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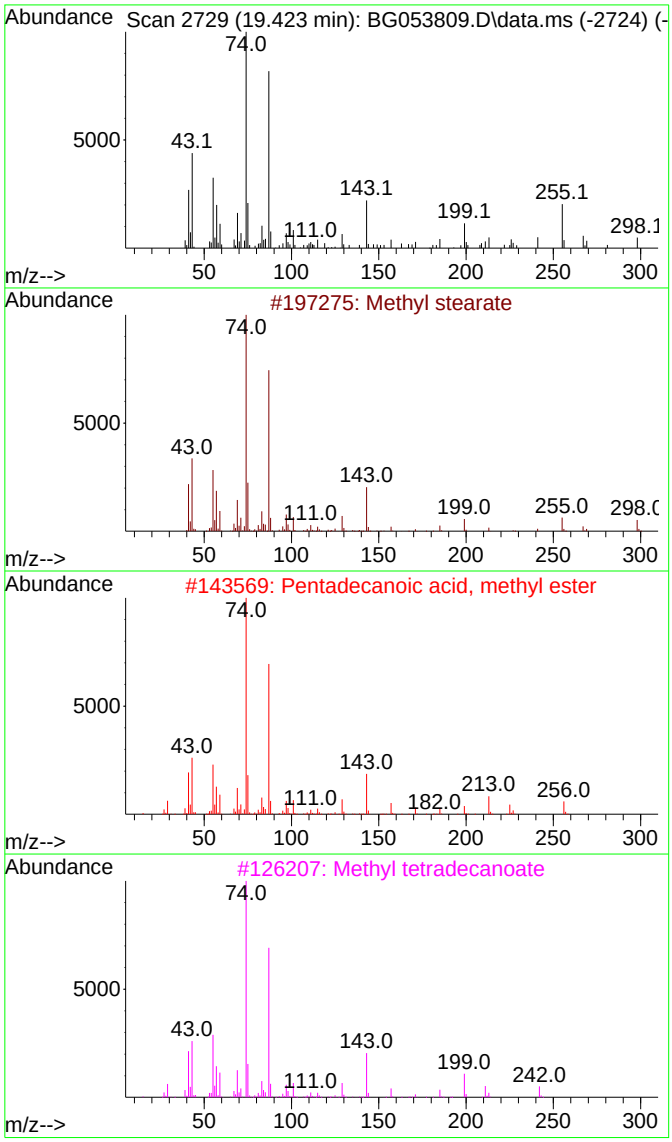
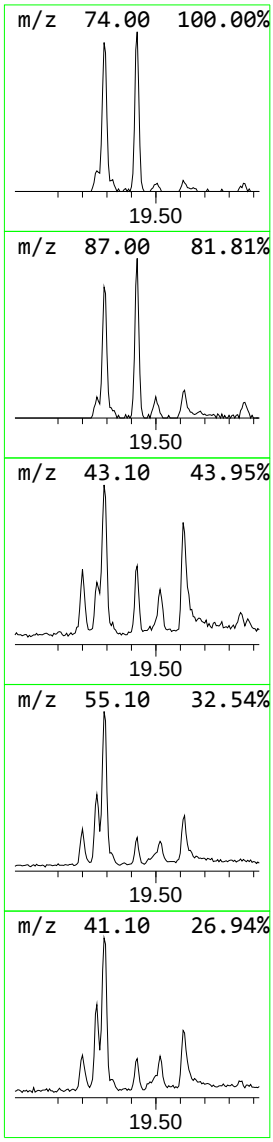
Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.423	3.70 ng	85148	Phenanthrene-d10	17.455

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	96
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	80
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053809.D
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Sample : N3138-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-3-053122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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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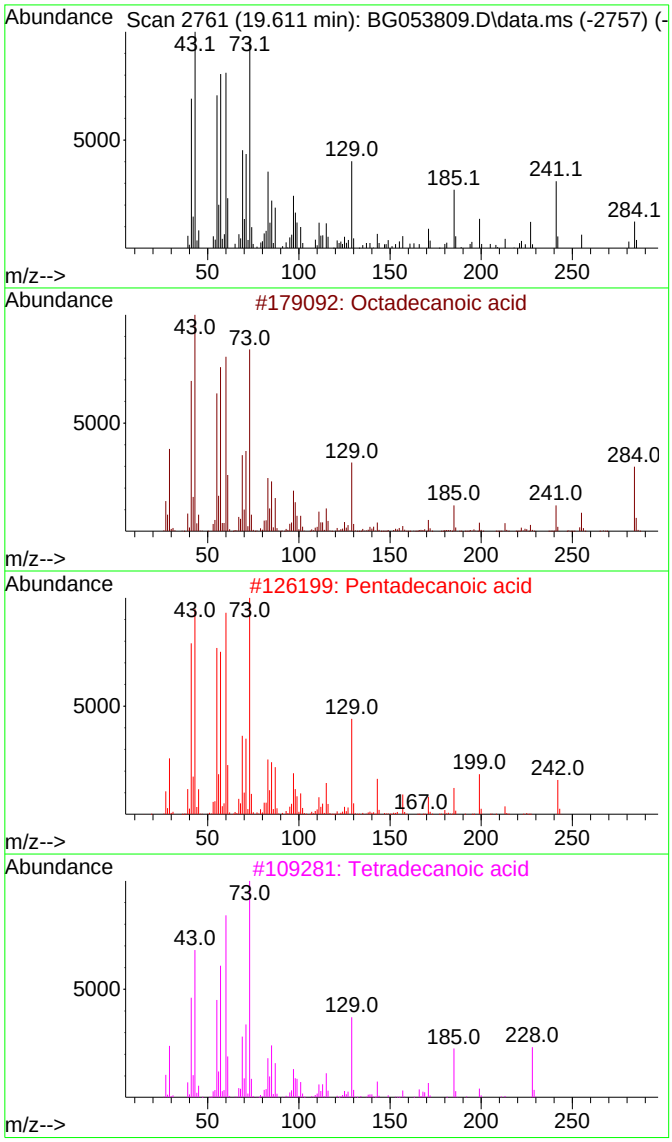
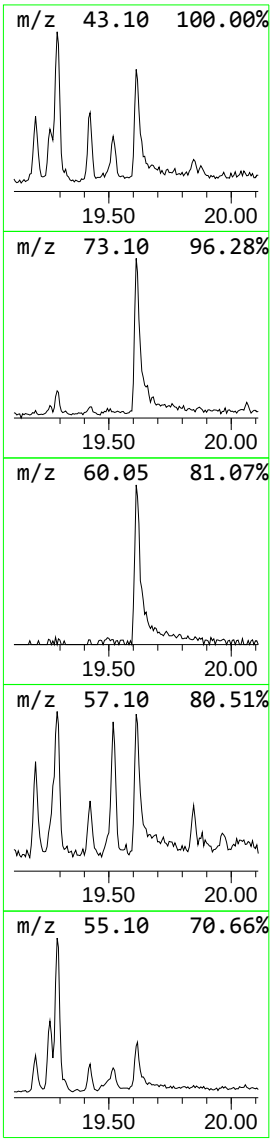
Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.611	6.76 ng	202246	Chrysene-d12	21.732

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	78
5	n-Decanoic acid	172	C10H20O2	000334-48-5	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053809.D
Acq On : 3 Jun 2022 12:21
Operator : CG/JU
Sample : N3138-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-3-053122

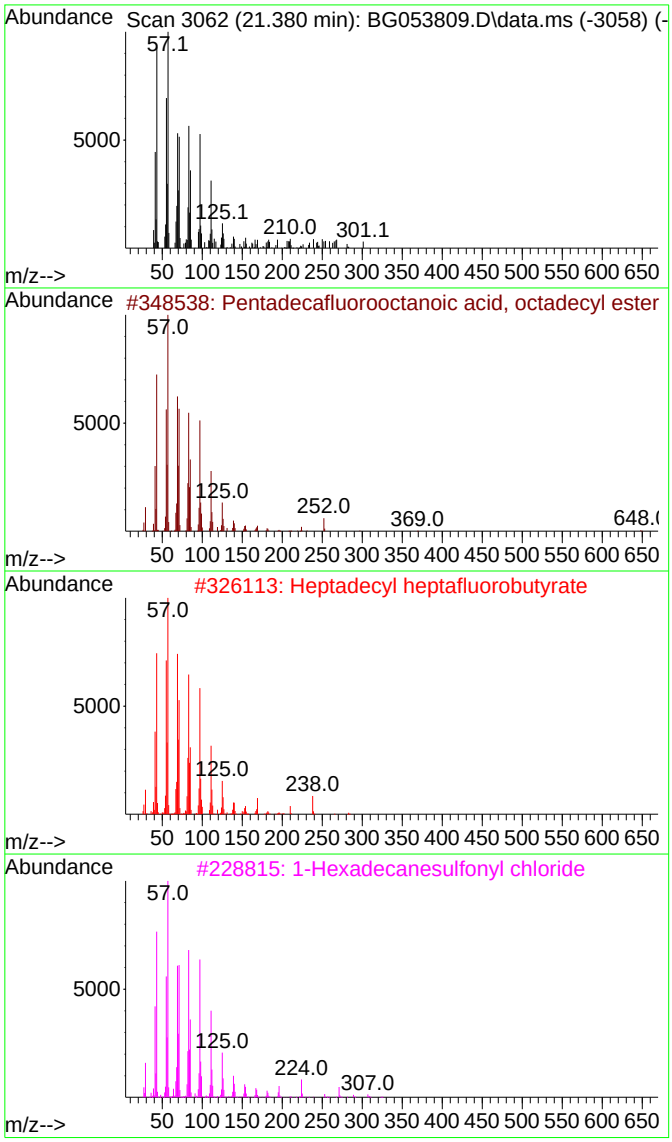
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

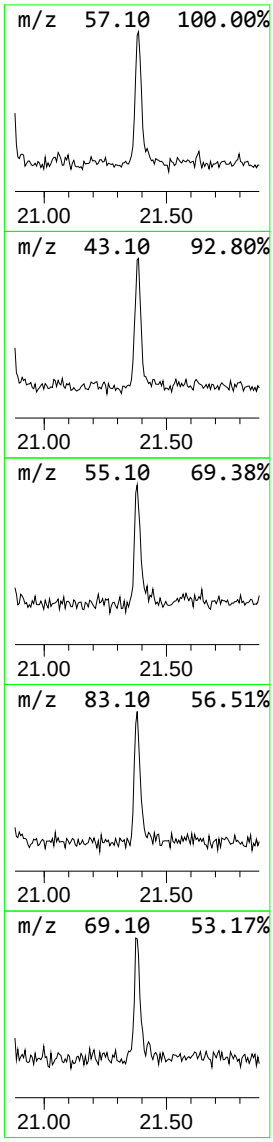
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Pentadecafluorooctanoic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.380	3.41 ng	102070	Chrysene-d12	21.732

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
3	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	87
5	Cyclopentadecane	210	C15H30	000295-48-7	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053809.D
Acq On : 3 Jun 2022 12:21
Operator : CG/JU
Sample : N3138-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
OR-3-053122

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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
unknown3.783	3.783	2.7	ng	23800	1	8.095	177515	20.0
Hexadecanoic ac...	18.125	5.5	ng	125920	4	17.455	460785	20.0
n-Hexadecanoic ...	18.348	9.8	ng	226955	4	17.455	460785	20.0
11-Tricosene	19.200	3.2	ng	73478	4	17.455	460785	20.0
9,12-Octadecadi...	19.259	9.5	ng	217909	4	17.455	460785	20.0
(Z)-15-Octadece...	19.288	17.2	ng	395382	4	17.455	460785	20.0
Methyl stearate	19.423	3.7	ng	85148	4	17.455	460785	20.0
Octadecanoic acid	19.611	6.8	ng	202246	5	21.732	598581	20.0
Pentadecafluoro...	21.380	3.4	ng	102070	5	21.732	598581	20.0