LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059857.D
Acq On : 24 Nov 2023 13:51
Operator : MA/JU
Sample : 05412-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-1

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-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059857.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.809	406	412	420	rBV	573964	919987	35.93%	8.825%
2	7.442	682	690	698	rVB	402349	731979	28.59%	7.022%
3	8.318	833	839	846	rVB3	101233	176104	6.88%	1.689%
4	9.516	1035	1043	1049	rBV	248830	443066	17.30%	4.250%
5	11.167	1317	1324	1332	rVB	144364	241573	9.43%	2.317%
6	13.570	1727	1733	1740	rVB	688200	1052989	41.12%	10.101%
7	13.770	1760	1767	1774	rBV3	83104	139561	5.45%	1.339%
8	14.951	1961	1968	1976	rVB	207544	327748	12.80%	3.144%
9	16.438	2213	2221	2228	rBV	683334	1067952	41.71%	10.245%
10	17.060	2314	2327	2335	rBV	67348	252429	9.86%	2.422%
11	17.701	2429	2436	2442	rBV	366806	587743	22.95%	5.638%
12	18.512	2569	2574	2582	rBV	227456	307763	12.02%	2.952%
13	18.841	2624	2630	2635	rBV10	31435	57212	2.23%	0.549%
14	19.769	2785	2788	2792	rBV2	107609	128572	5.02%	1.233%
15	19.916	2810	2813	2815	rBV4	18572	25787	1.01%	0.247%
16	20.274	2868	2874	2880	rBV	1975416	2560486	100.00%	24.562%
17	21.038	3002	3004	3008	rVB5	31117	34336	1.34%	0.329%
18	21.555	3089	3092	3100	rVB8	66654	105029	4.10%	1.008%
19	21.819	3135	3137	3144	rVB3	68344	101637	3.97%	0.975%
20	22.025	3166	3172	3178	rVB	311849	533635	20.84%	5.119%
21	22.601	3268	3270	3278	rVB8	37965	82706	3.23%	0.793%
22	23.535	3427	3429	3432	rBV4	33966	44259	1.73%	0.425%
23	25.591	3773	3779	3788	rVB2	169676	474045	18.51%	4.547%
24	29.364	4419	4421	4423	rBV3	24868	27804	1.09%	0.267%

Sum of corrected areas: 10424402

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
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Instrument :
BNA_G
ClientSampleId :
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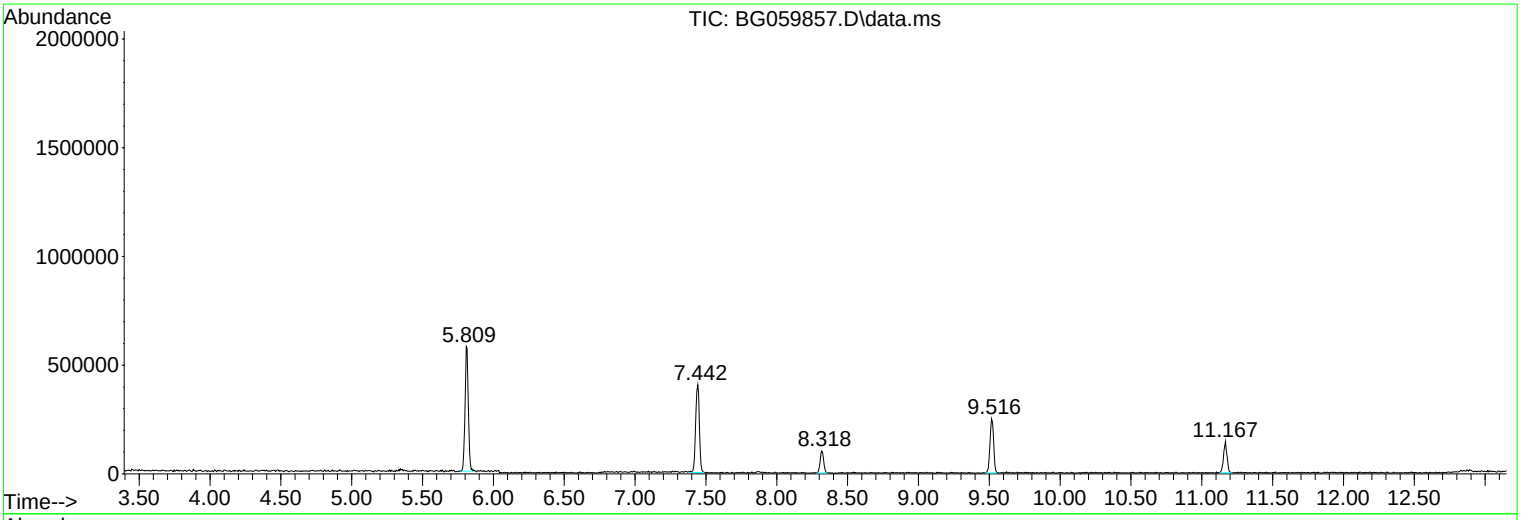
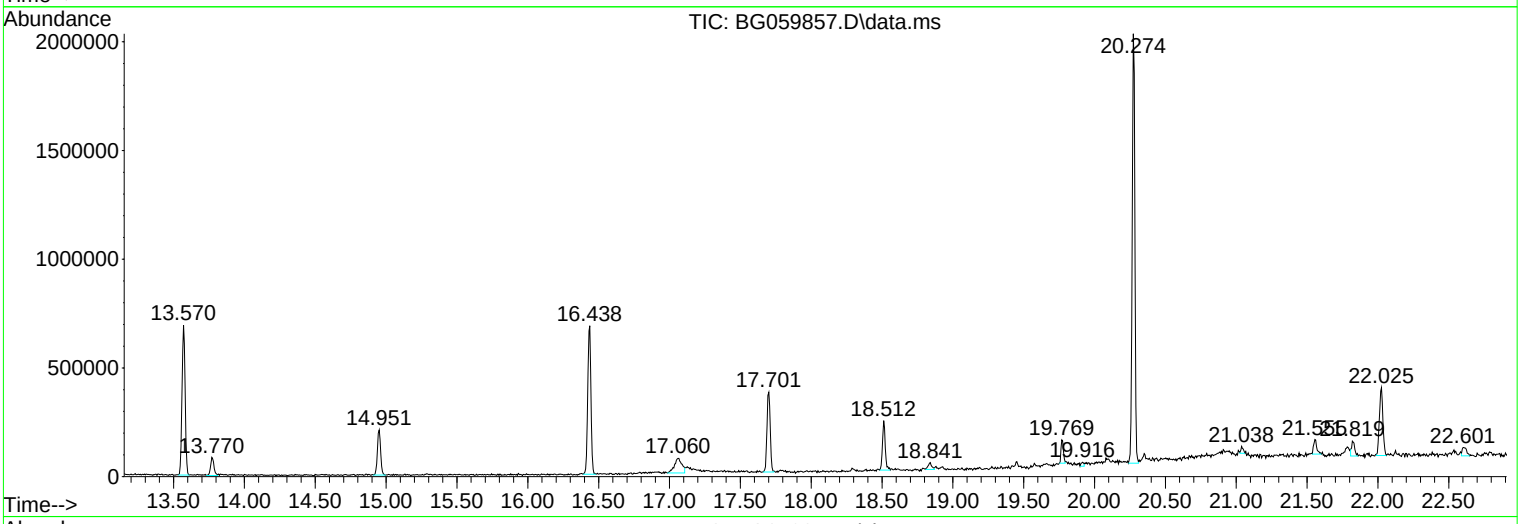
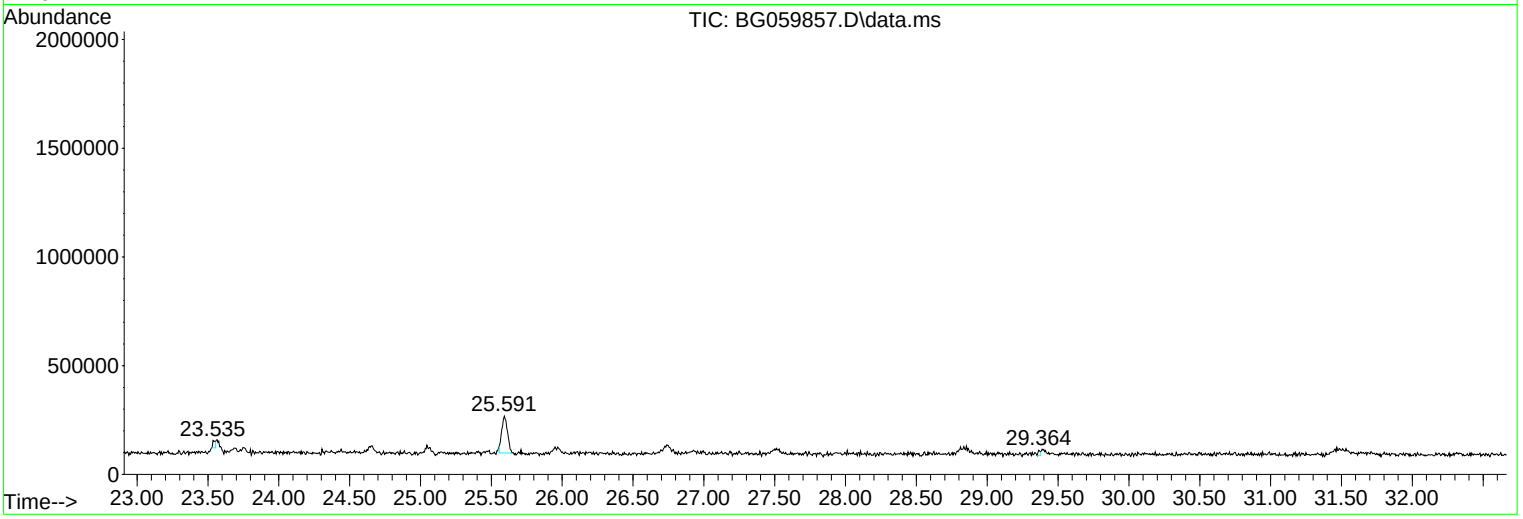
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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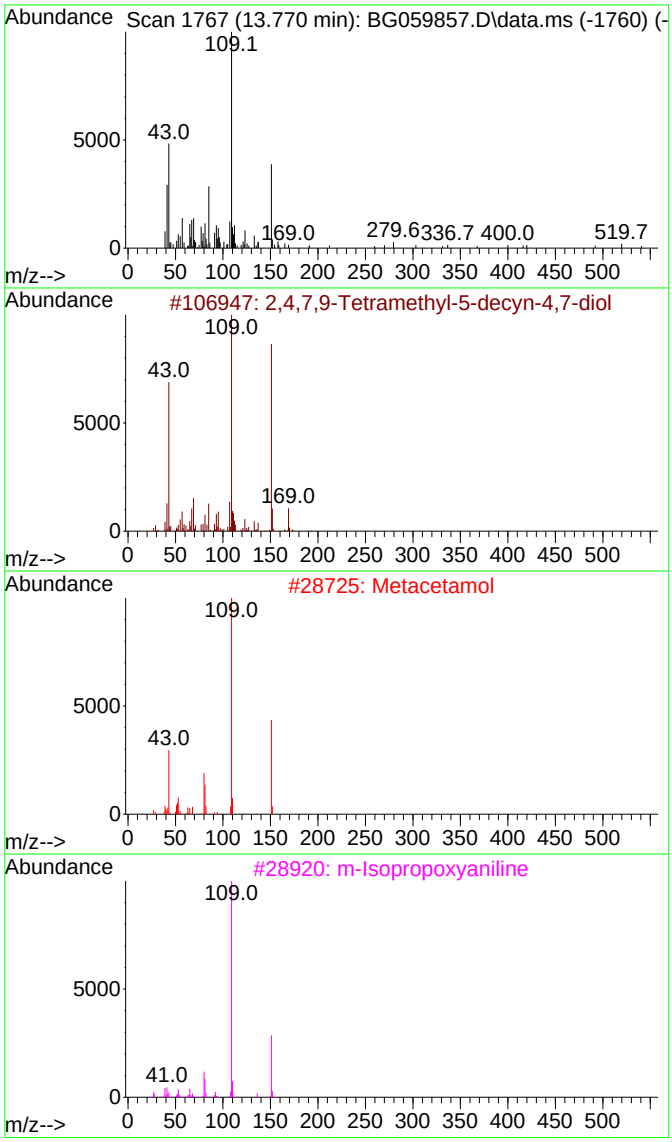
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

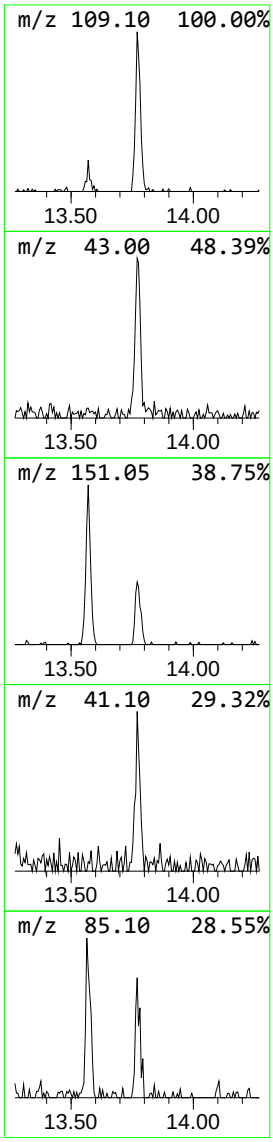
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.770	8.52 ng	139561	Acenaphthene-d10	14.951

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	72
2	Metacetamol	151	C8H9NO2	000621-42-1	64
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	64
4	Acetaminophen	151	C8H9NO2	000103-90-2	64
5	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	59





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Operator : MA/JU
Sample : 05412-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

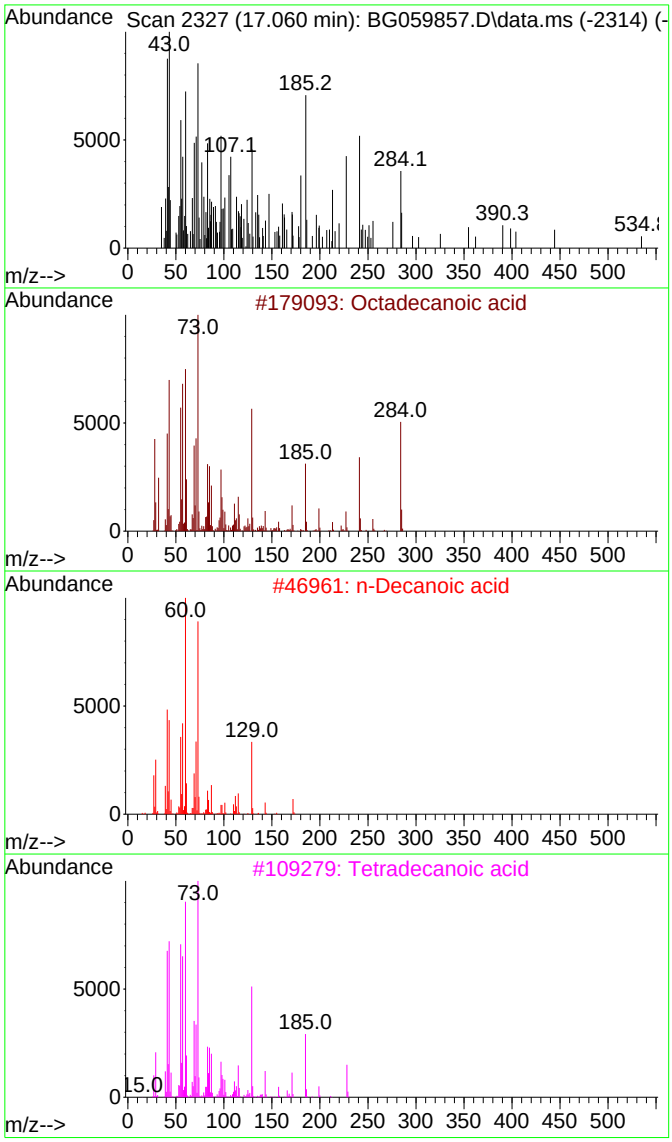
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

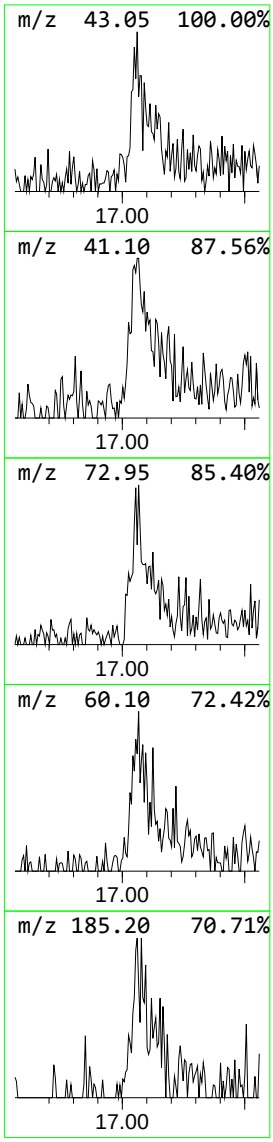
****

Peak Number 2 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.060	8.59 ng	252429	Phenanthrene-d10	17.701

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	50
2	n-Decanoic acid	172	C10H20O2	000334-48-5	25
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	22
4	4-Methyl-5-(oxolan-2-yl)-1,2,4-t...	185	C7H11N3OS	1000409-63-4	18
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059857.D
Acq On : 24 Nov 2023 13:51
Operator : MA/JU
Sample : 05412-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

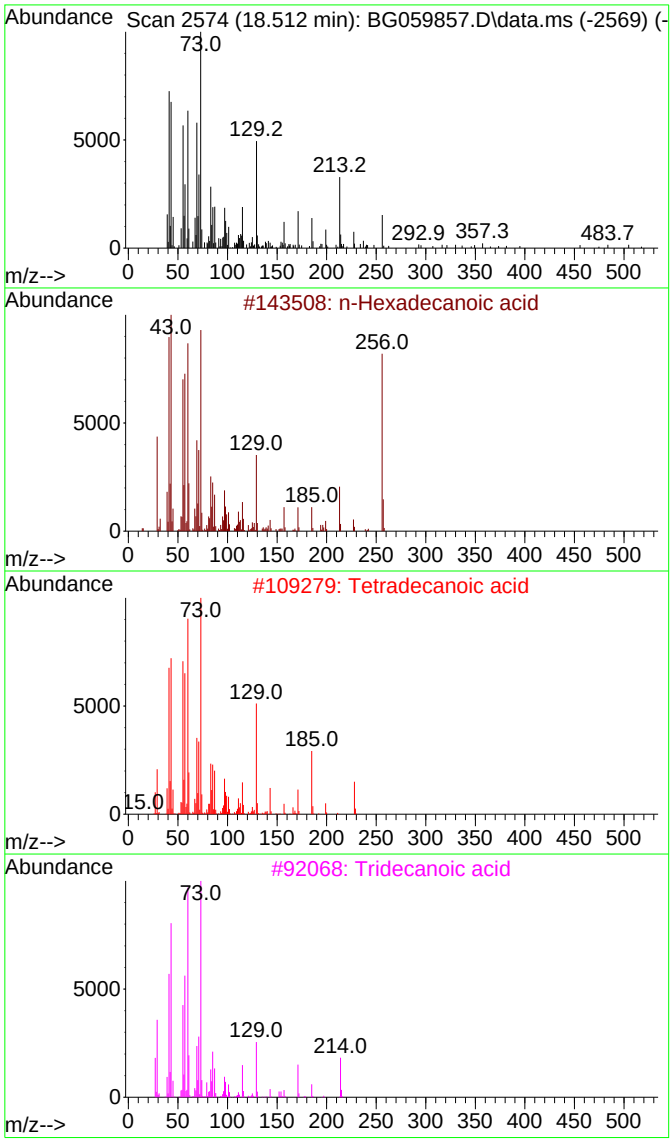
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

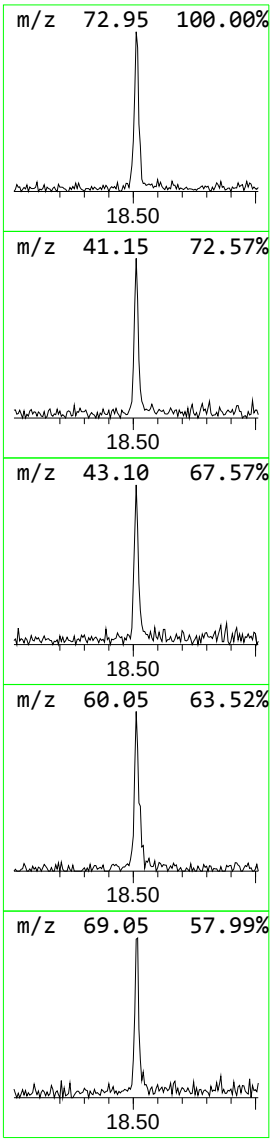
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.512	10.47 ng	307763	Phenanthrene-d10	17.701

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
3	Tridecanoic acid	214	C13H26O2	000638-53-9	50
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





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Operator : MA/JU
Sample : 05412-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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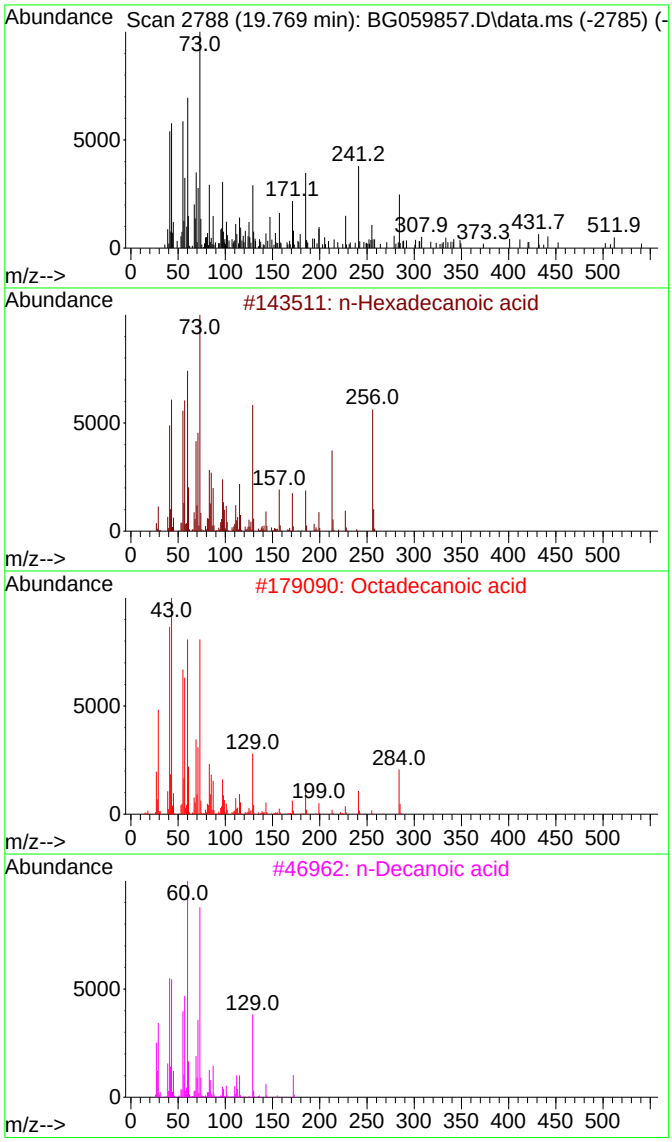
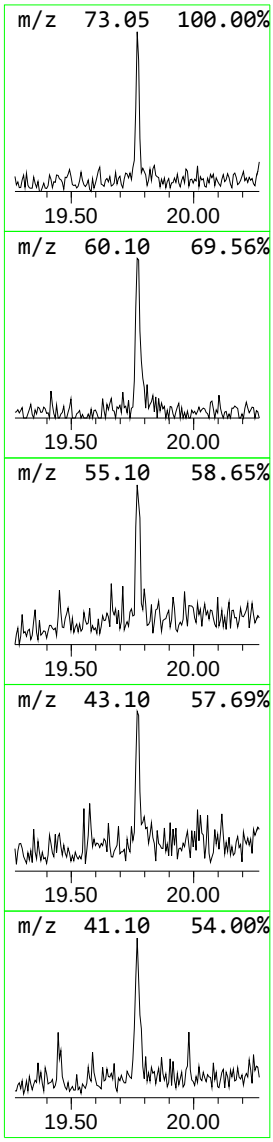
Peak Number 4 unknown19.769 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.769	4.38 ng	128572	Phenanthrene-d10	17.701

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	55
2	Octadecanoic acid	284	C18H36O2	000057-11-4	52
3	n-Decanoic acid	172	C10H20O2	000334-48-5	42
4	Nonanoic acid	158	C9H18O2	000112-05-0	38
5	Undecanoic acid	186	C11H22O2	000112-37-8	38





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Sample : 05412-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
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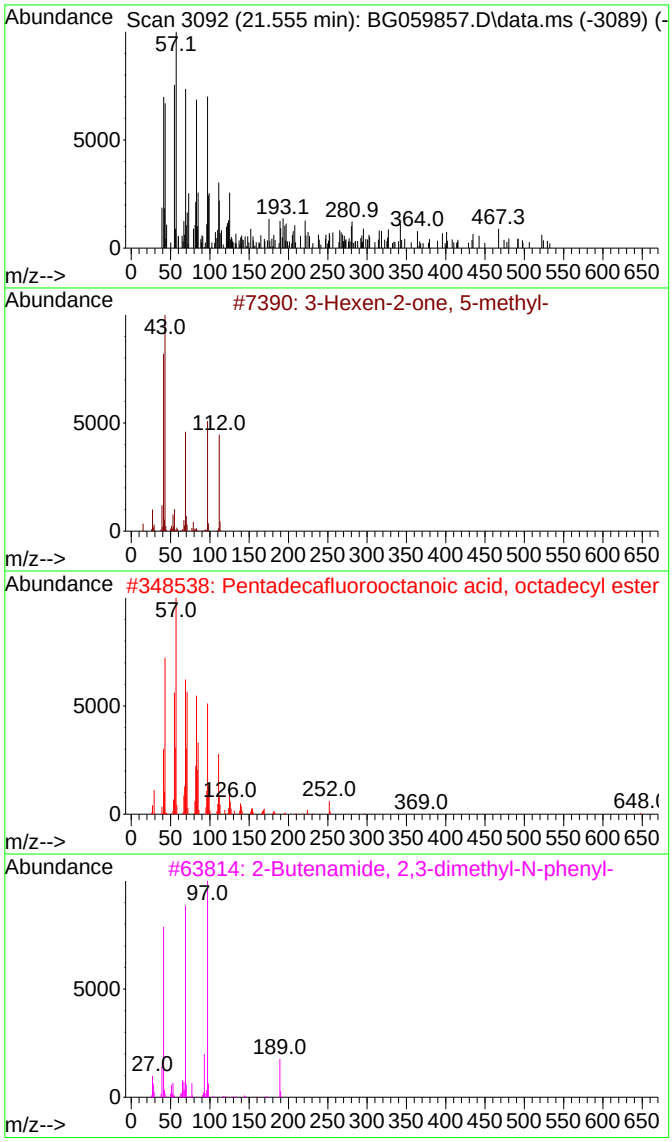
TIC Integration Parameters: LSCINT.P

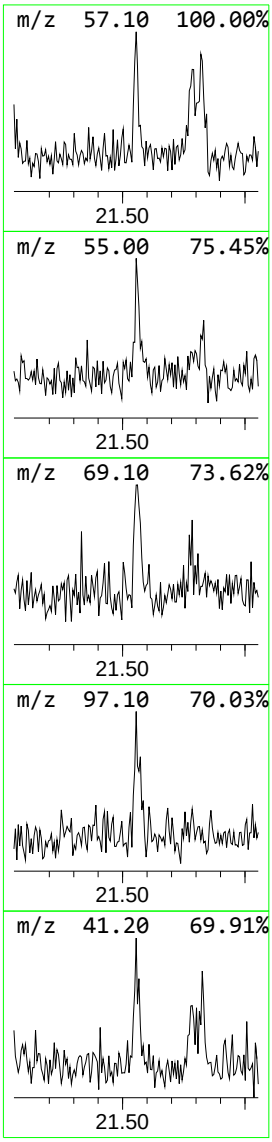
****

Peak Number 5 3-Hexen-2-one, 5-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.555	3.94 ng	105029	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one, 5-methyl-	112	C7H12O	005166-53-0	68
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	64
3	2-Butenamide, 2,3-dimethyl-N-phe...	189	C12H15NO	024735-54-4	64
4	Fumaric acid, hexadecyl 2-methyl...	394	C24H42O4	1000330-55-5	64
5	1-Heptadecene	238	C17H34	006765-39-5	64





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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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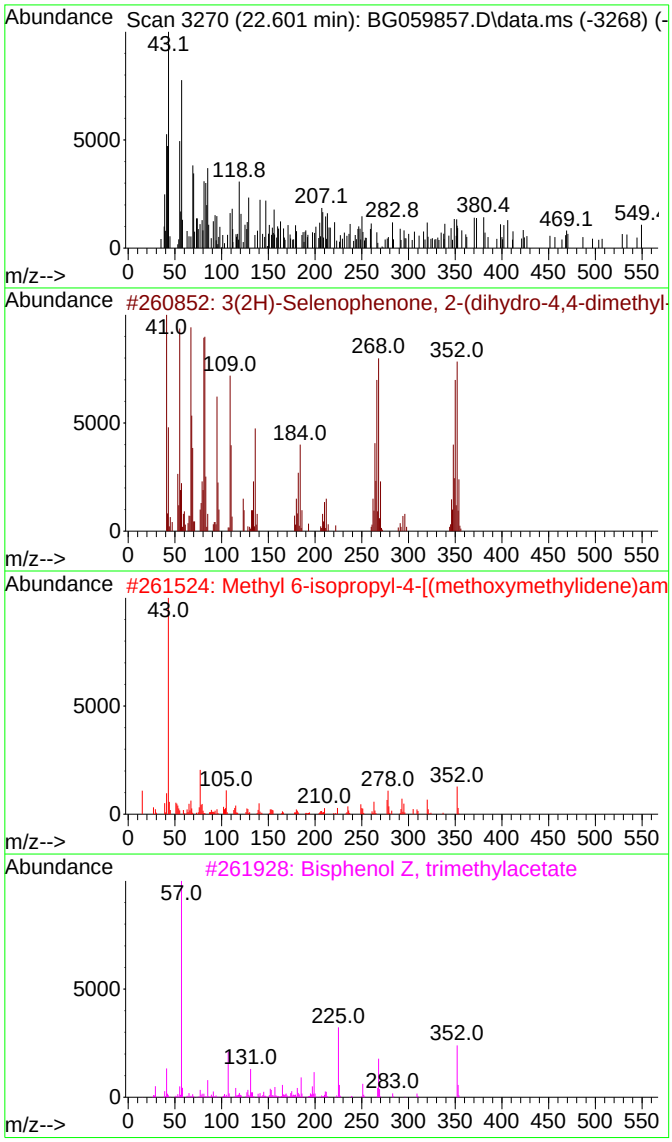
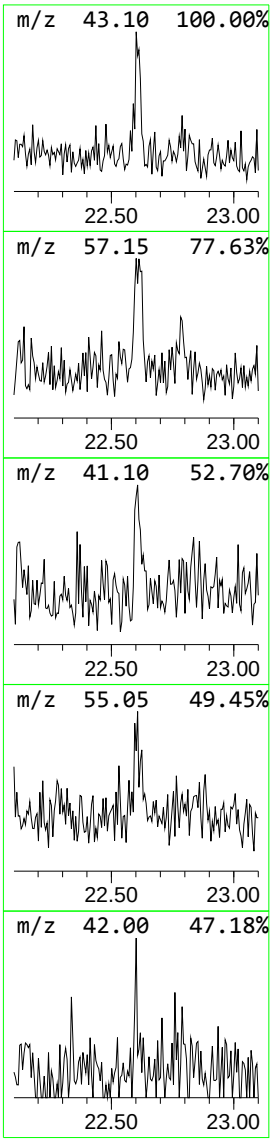
Peak Number 6 unknown22.601 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.601	3.10 ng	82706	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3(2H)-Selenophenone, 2-(dihydro-...	352	C12H16O2Se2	056009-21-3	10
2	Methyl 6-isopropyl-4-[(methoxyme...	352	C20H20N2O4	1000489-18-2	10
3	Bisphenol Z, trimethylacetate	352	C23H28O3	1000462-23-2	9
4	.alpha.-Dihydroequilenin diacetate	352	C22H24O4	1000251-91-9	9
5	Eicosane, 2,6,10,14,18-pentamethyl-	352	C25H52	051794-16-2	9





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
2,4,7,9-Tetrame...	13.770	8.5	ng	139561	3	14.951	327748	20.0
Octadecanoic acid	17.060	8.6	ng	252429	4	17.701	587743	20.0
n-Hexadecanoic ...	18.512	10.5	ng	307763	4	17.701	587743	20.0
unknown19.769	19.769	4.4	ng	128572	4	17.701	587743	20.0
3-Hexen-2-one, ...	21.555	3.9	ng	105029	5	22.019	533635	20.0
unknown22.601	22.601	3.1	ng	82706	5	22.019	533635	20.0