LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061112.D
Acq On : 3 May 2024 18:54
Operator : MA/JU
Sample : P2362-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : INSIDE

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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061112.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.153	23	28	40	rVB	160898	266131	15.39%	3.030%
2	3.670	112	116	124	rBV	17113	28685	1.66%	0.327%
3	5.526	425	432	440	rBV	364245	580729	33.59%	6.613%
4	7.107	693	701	712	rBV	394845	692309	40.04%	7.883%
5	7.935	835	842	849	rBV	114220	189292	10.95%	2.155%
6	9.087	1026	1038	1049	rBV	256146	462052	26.72%	5.261%
7	10.732	1310	1318	1325	rBV	148811	264390	15.29%	3.011%
8	13.188	1727	1736	1742	rBV	707071	1113225	64.38%	12.676%
9	14.563	1962	1970	1980	rVB	240337	363182	21.00%	4.136%
10	14.780	1999	2007	2015	rVB4	9927	23078	1.33%	0.263%
11	16.055	2217	2224	2235	rBV	667727	994708	57.53%	11.327%
12	17.312	2429	2438	2448	rBV	300347	451944	26.14%	5.146%
13	18.211	2584	2591	2600	rBV2	74130	119920	6.94%	1.366%
14	19.363	2783	2787	2791	rBV2	12768	20799	1.20%	0.237%
15	19.480	2804	2807	2813	rBV5	18183	33939	1.96%	0.386%
16	19.616	2827	2830	2836	rVB3	21870	29002	1.68%	0.330%
17	19.727	2845	2849	2852	rBV2	12568	20392	1.18%	0.232%
18	19.933	2878	2884	2889	rBV	1313735	1729129	100.00%	19.690%
19	20.691	3008	3013	3016	rBV7	14100	29465	1.70%	0.336%
20	21.237	3102	3106	3116	rBV2	85749	169063	9.78%	1.925%
21	21.566	3156	3162	3168	rBV2	284357	500291	28.93%	5.697%
22	22.406	3296	3305	3317	rBV7	40819	149061	8.62%	1.697%
23	23.828	3543	3547	3553	rVB3	48736	85394	4.94%	0.972%
24	24.698	3687	3695	3710	rBV2	96922	359326	20.78%	4.092%
25	25.849	3884	3891	3898	rBV3	39635	106370	6.15%	1.211%

Sum of corrected areas: 8781876

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ClientSampleId :
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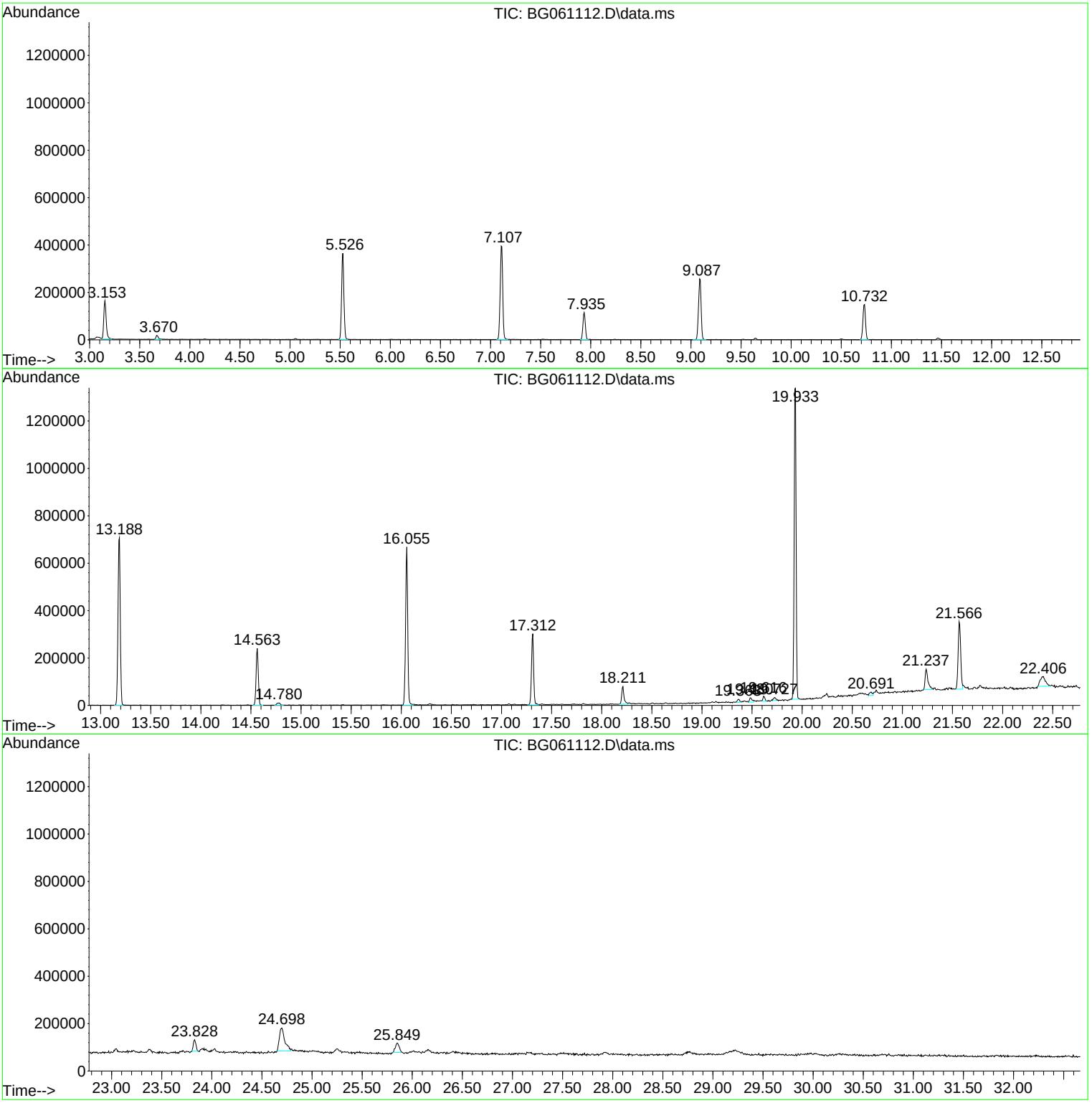
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050324\
Data File : BG061112.D
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Operator : MA/JU
Sample : P2362-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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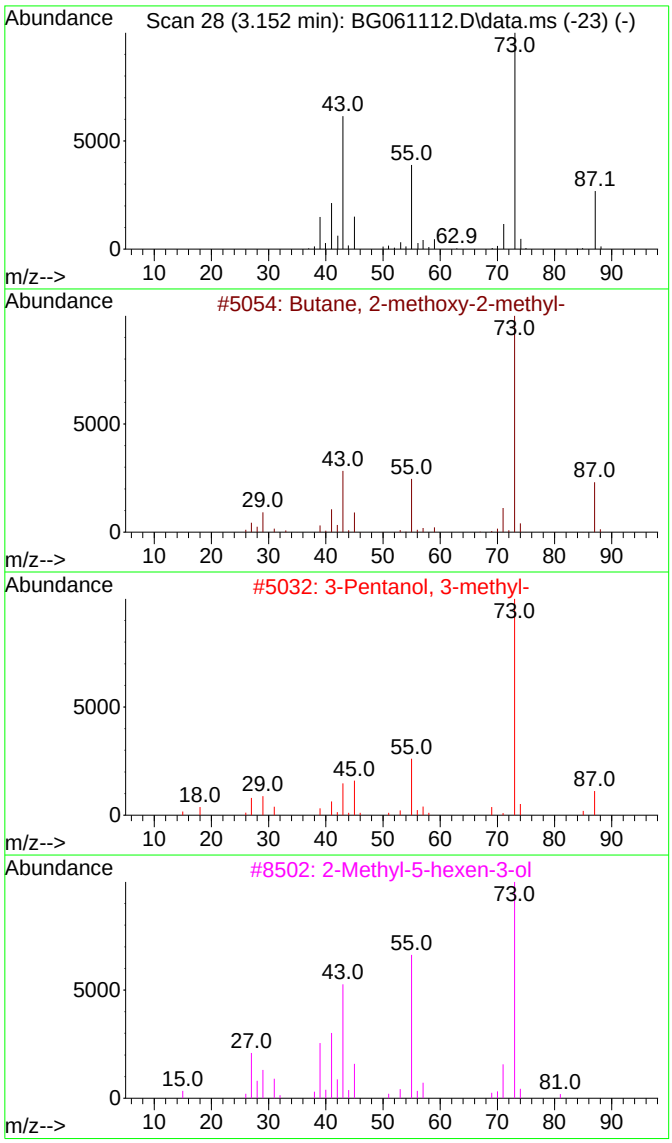
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

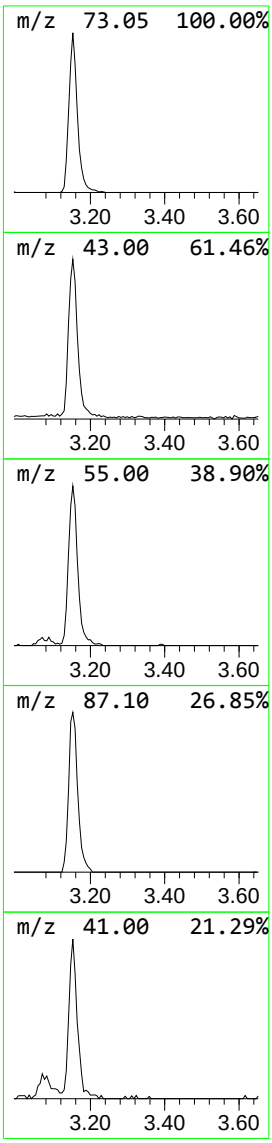
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.152	28.12 ng	266131	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	4-Penten-2-ol, acetate	128	C7H12O2	1000352-31-5	12





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Data File : BG061112.D
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Operator : MA/JU
Sample : P2362-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

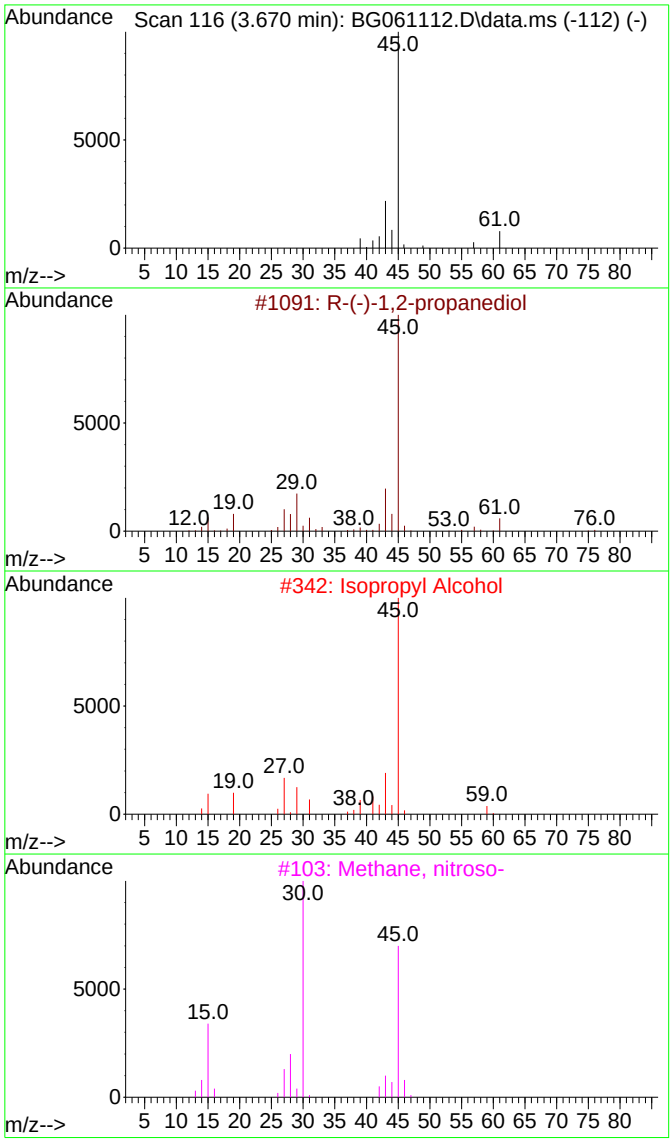
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

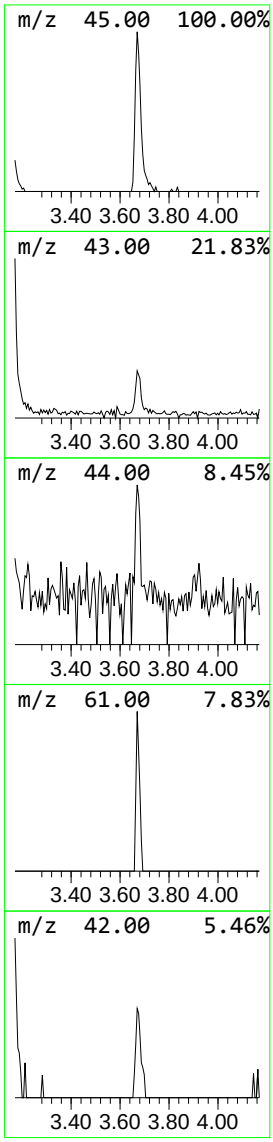
****

Peak Number 2 unknown3.670 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.670	3.03 ng	28685	1,4-Dichlorobenzene-d4	7.935

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Propylene Glycol	76	C3H8O2	000057-55-6	4
5	2-Butanol, (R)-	74	C4H10O	014898-79-4	4





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Acq On : 3 May 2024 18:54
Operator : MA/JU
Sample : P2362-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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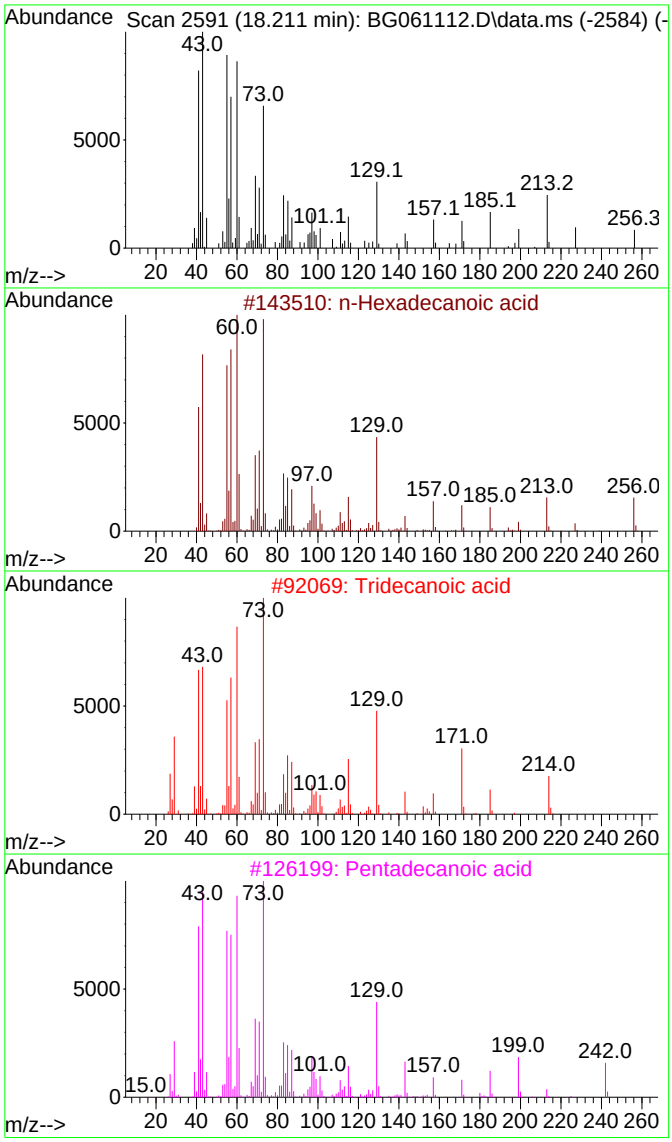
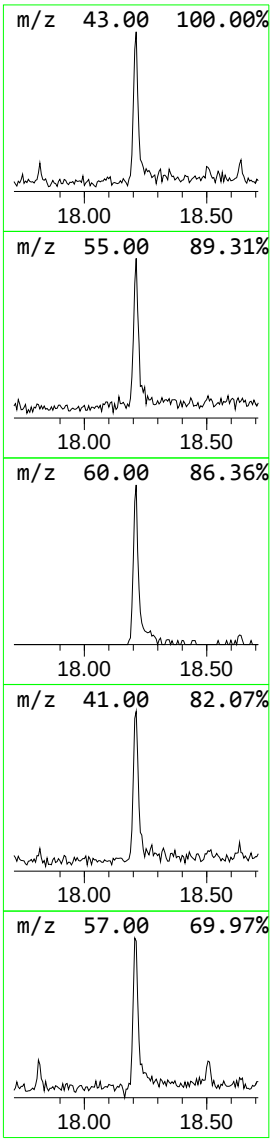
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.211	5.31 ng	119920	Phenanthrene-d10	17.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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Sample : P2362-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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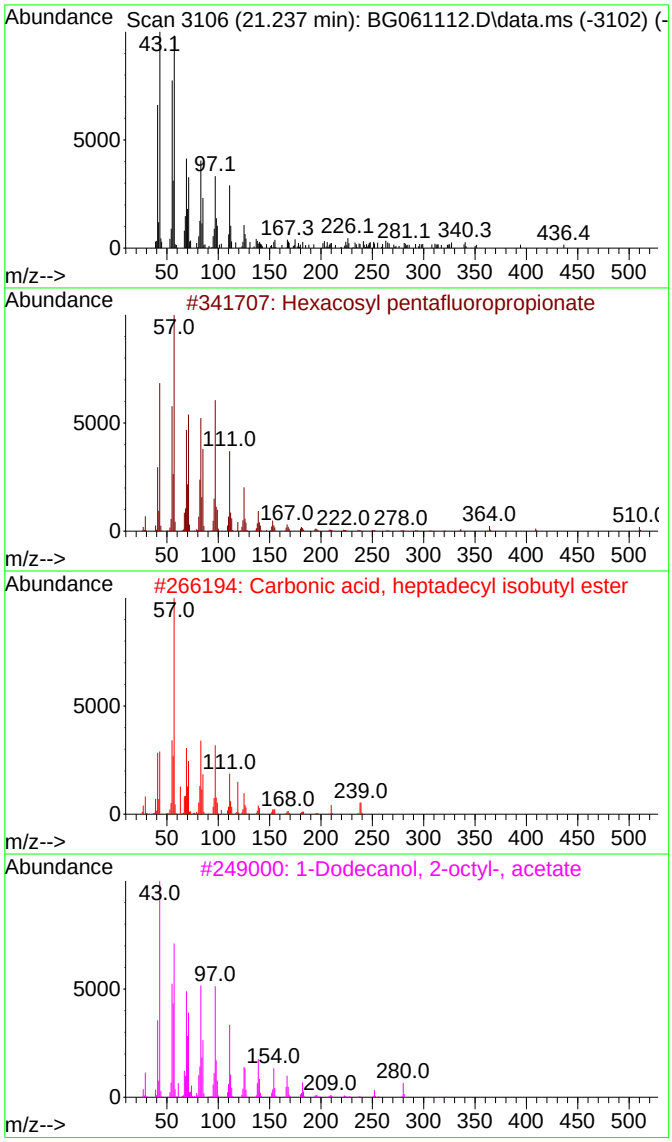
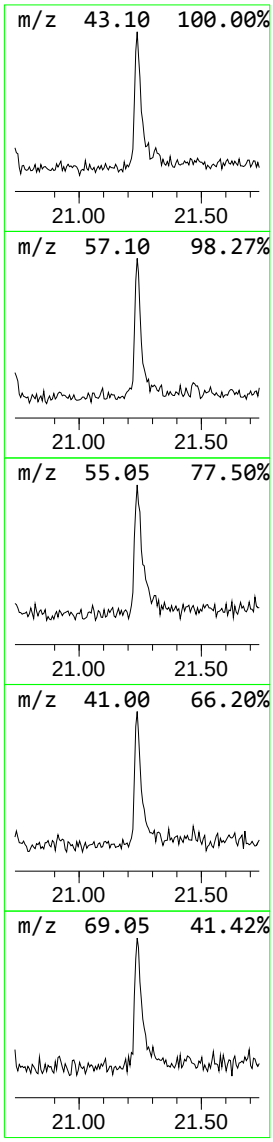
****
Peak Number 4 Hexacosyl pentafluoropropio... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.237	6.76 ng	169063	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	87
2	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	87
3	1-Dodecanol, 2-octyl-, acetate	340	C22H44O2	074051-84-6	87
4	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	83
5	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	83





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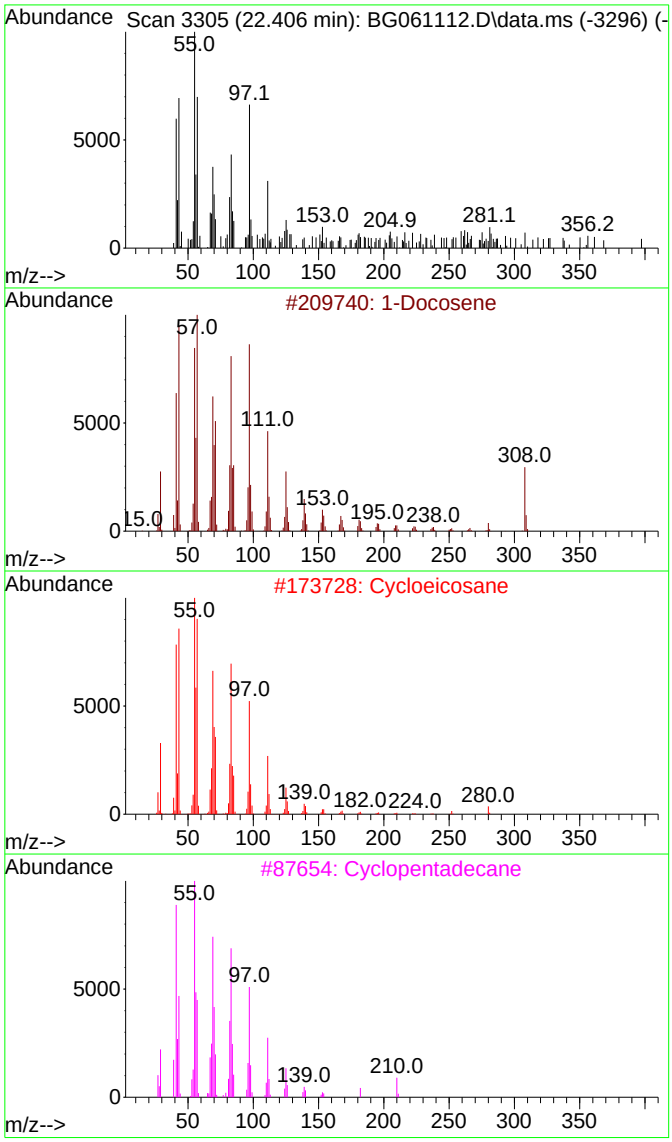
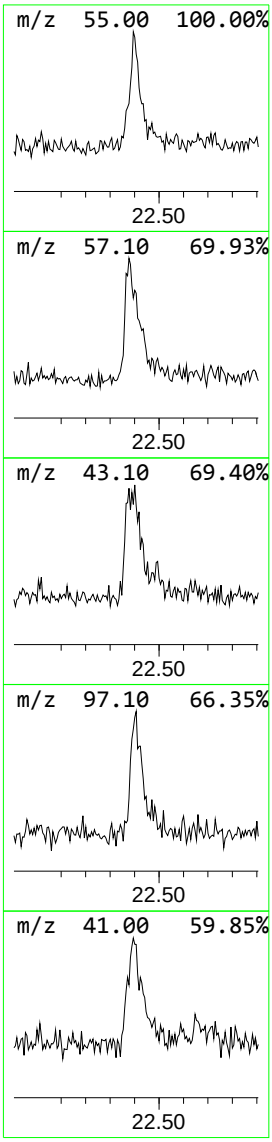
****

Peak Number 5 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.406	5.96 ng	149061	Chrysene-d12	21.566

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	86
2	Cycloeicosane	280	C20H40	000296-56-0	64
3	Cyclopentadecane	210	C15H30	000295-48-7	64
4	11-Tricosene	322	C23H46	052078-56-5	64
5	9-Tricosene, (Z)-	322	C23H46	027519-02-4	50





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Sample : P2362-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
INSIDE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

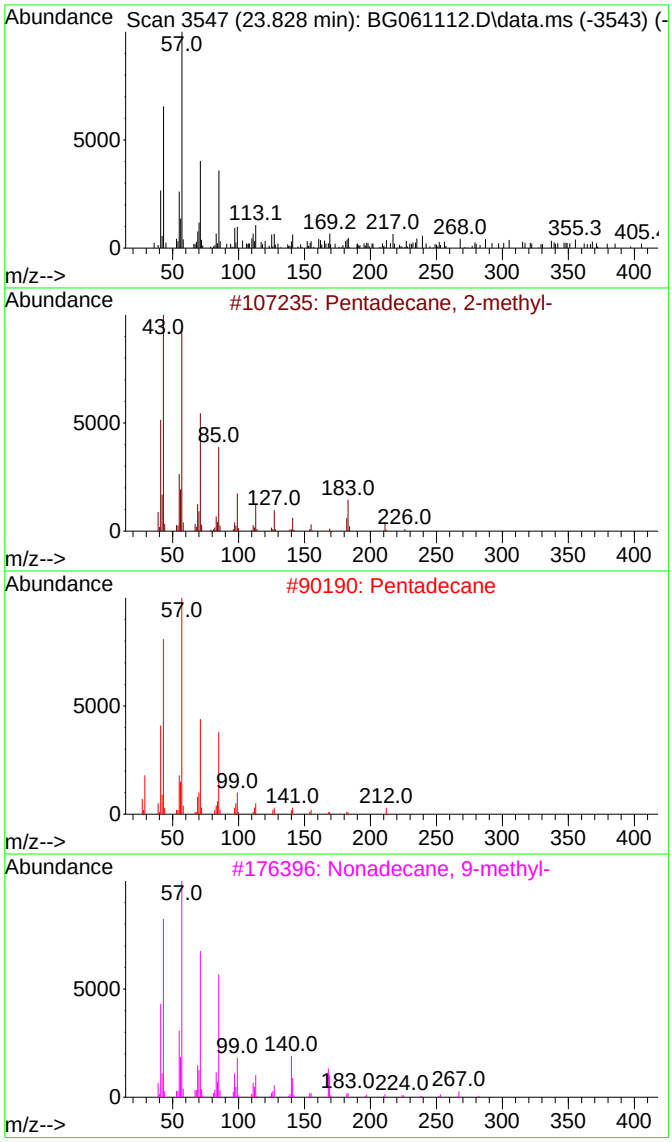
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

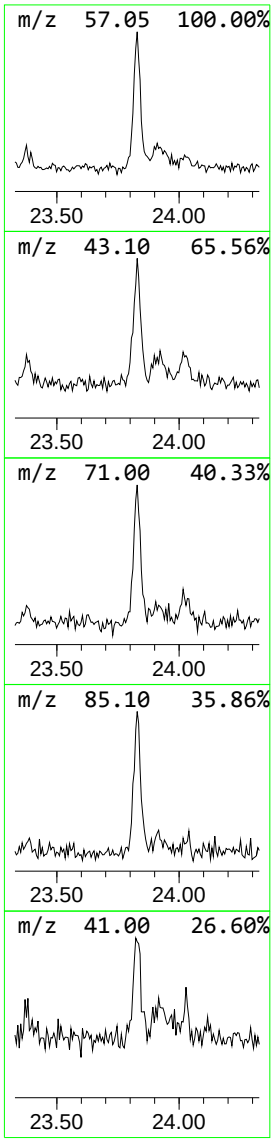
****

Peak Number 6 Pentadecane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.828	4.75 ng	85394	Perylene-d12	24.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	64
2	Pentadecane	212	C15H32	000629-62-9	64
3	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	58
4	Octacosane	394	C28H58	000630-02-4	58
5	Hexacosane	366	C26H54	000630-01-3	58





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Sample : P2362-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

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

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

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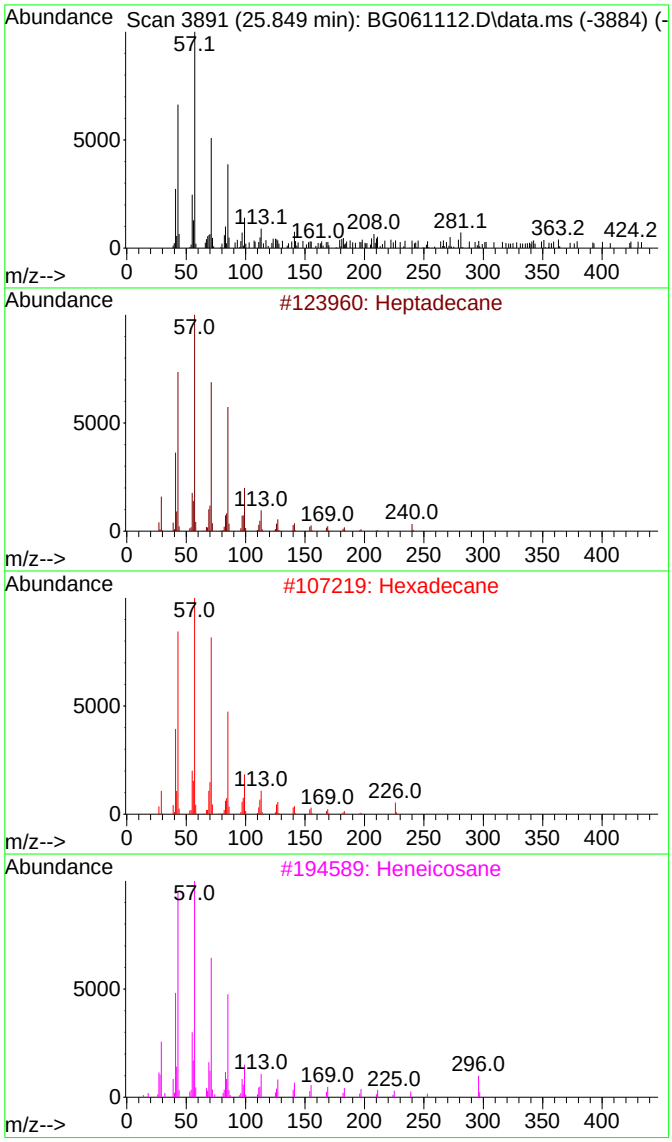
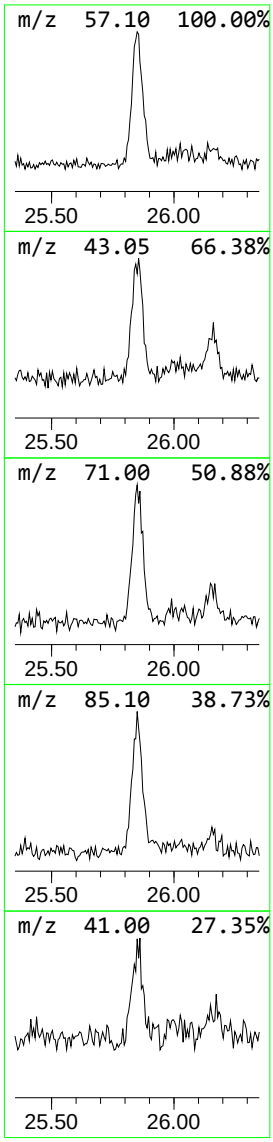
Peak Number 7 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.849	5.92 ng	106370	Perylene-d12	24.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Hexadecane	226	C16H34	000544-76-3	81
3	Heneicosane	296	C21H44	000629-94-7	81
4	Tetradecane	198	C14H30	000629-59-4	74
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	74





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
Butane, 2-metho...	3.152	28.1	ng	266131	1	7.935	189292	20.0
unknown3.670	3.670	3.0	ng	28685	1	7.935	189292	20.0
n-Hexadecanoic ...	18.211	5.3	ng	119920	4	17.312	451944	20.0
Hexacosyl penta...	21.237	6.8	ng	169063	5	21.566	500291	20.0
1-Docosene	22.406	6.0	ng	149061	5	21.566	500291	20.0
Pentadecane, 2-...	23.828	4.8	ng	85394	6	24.692	359326	20.0
Heptadecane	25.849	5.9	ng	106370	6	24.692	359326	20.0