LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011819\
Data File : BG039217.D
Acq On : 18 Jan 2019 15:55
Operator : JU/SJ
Sample : K1157-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-06-011519

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-BG010919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.097	336	342	351	rVB	23318	40955	2.82%	0.444%
2	5.567	415	422	434	rBV	389983	655001	45.06%	7.094%
3	7.177	685	696	706	rBV	404737	731799	50.35%	7.925%
4	7.542	750	758	767	rBV	366158	632810	43.54%	6.853%
5	8.006	829	837	849	rBB	61911	108588	7.47%	1.176%
6	8.329	885	892	900	rBV	309928	517163	35.58%	5.601%
7	9.187	1029	1038	1051	rBV	230813	436746	30.05%	4.730%
8	10.826	1309	1317	1324	rBV	89017	164196	11.30%	1.778%
9	13.270	1725	1733	1744	rBV	809373	1266043	87.10%	13.711%
10	14.093	1867	1873	1881	rBV	45012	66829	4.60%	0.724%
11	14.651	1961	1968	1976	rBV2	147670	235153	16.18%	2.547%
12	16.143	2215	2222	2234	rBV	579950	872068	60.00%	9.444%
13	17.395	2429	2435	2440	rBV2	163179	255935	17.61%	2.772%
14	17.442	2440	2443	2448	rVB	24991	34083	2.34%	0.369%
15	18.258	2575	2582	2589	rBV4	33886	61408	4.22%	0.665%
16	19.451	2776	2785	2792	rBV	59584	87278	6.00%	0.945%
17	19.780	2836	2841	2843	rBV3	11448	15339	1.06%	0.166%
18	19.810	2843	2846	2853	rVB	53235	76275	5.25%	0.826%
19	20.003	2873	2879	2885	rBV	1095542	1453528	100.00%	15.742%
20	20.268	2916	2924	2926	rBV6	8987	17166	1.18%	0.186%
21	21.267	3087	3094	3103	rBV3	73550	124249	8.55%	1.346%
22	21.666	3152	3162	3168	rBV2	190792	379850	26.13%	4.114%
23	21.719	3168	3171	3175	rVB	23630	34851	2.40%	0.377%
24	21.807	3182	3186	3193	rVB2	22340	35395	2.44%	0.383%
25	22.407	3284	3288	3291	rBV2	34006	53384	3.67%	0.578%
26	23.094	3399	3405	3412	rVB2	35231	66865	4.60%	0.724%
27	23.288	3434	3438	3443	rVB7	9495	16286	1.12%	0.176%
28	23.899	3531	3542	3549	rBV	69375	176456	12.14%	1.911%
29	23.964	3551	3553	3560	rVB4	13664	27004	1.86%	0.292%
30	24.627	3659	3666	3672	rBV2	10533	26354	1.81%	0.285%
31	24.774	3682	3691	3695	rBV3	18027	48972	3.37%	0.530%
32	24.839	3695	3702	3708	rVV2	23444	70579	4.86%	0.764%
33	24.933	3708	3718	3728	rVB	112209	316676	21.79%	3.430%
34	25.967	3885	3894	3904	rBV3	27024	81835	5.63%	0.886%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011819\
Data File : BG039217.D
Acq On : 18 Jan 2019 15:55
Operator : JU/SJ
Sample : K1157-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-06-011519

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-BG010919.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	26.108	3912	3918	3922	rBV8	7902	19861	1.37%	0.215%
36	27.313	4114	4123	4129	rBV5	10386	26658	1.83%	0.289%

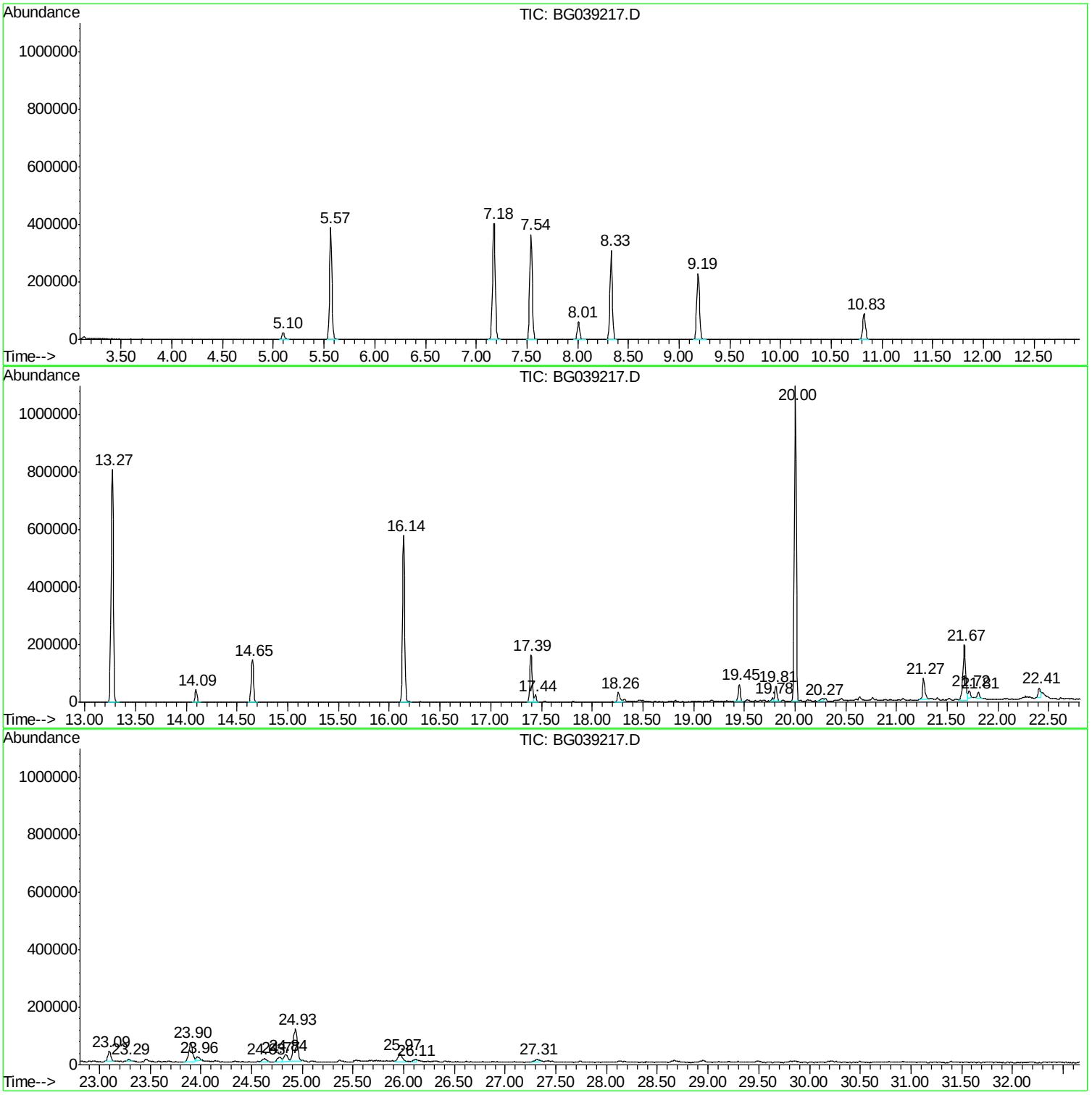
Sum of corrected areas: 9233638

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011819\
Data File : BG039217.D
Acq On : 18 Jan 2019 15:55
Operator : JU/SJ
Sample : K1157-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-06-011519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011819\
Data File : BG039217.D
Acq On : 18 Jan 2019 15:55
Operator : JU/SJ
Sample : K1157-11
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-06-011519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

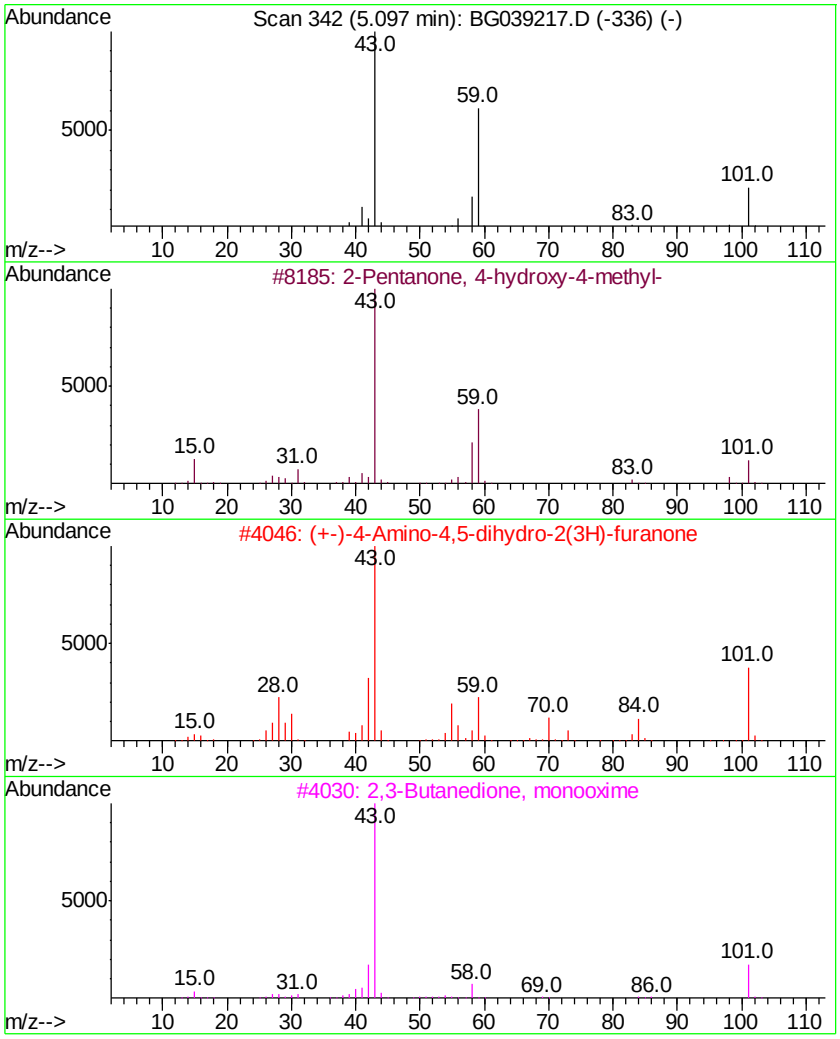
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

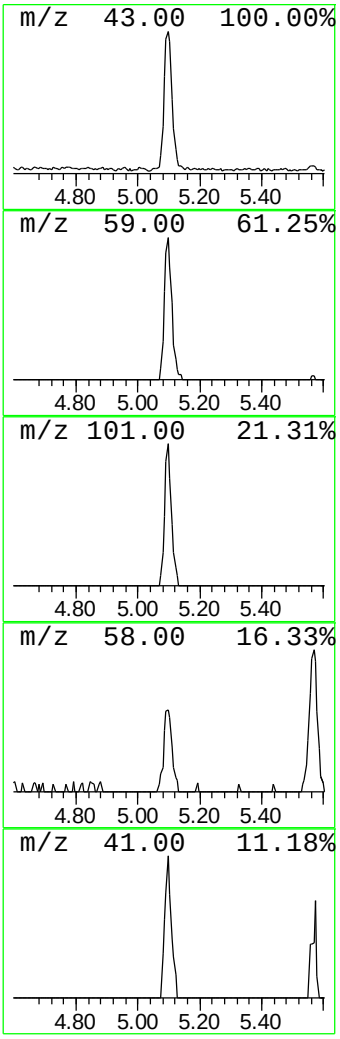
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	7.54 ng	40955	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011819\
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Operator : JU/SJ
Sample : K1157-11
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Instrument : BNA_G
ClientSampleId : WC-06-011519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

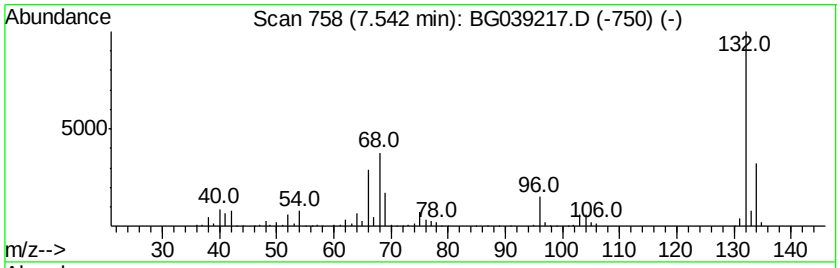
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

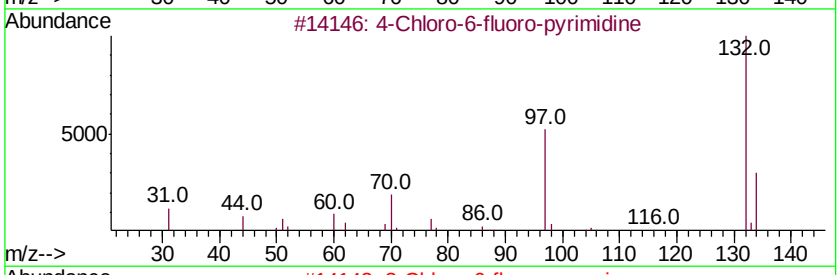
****

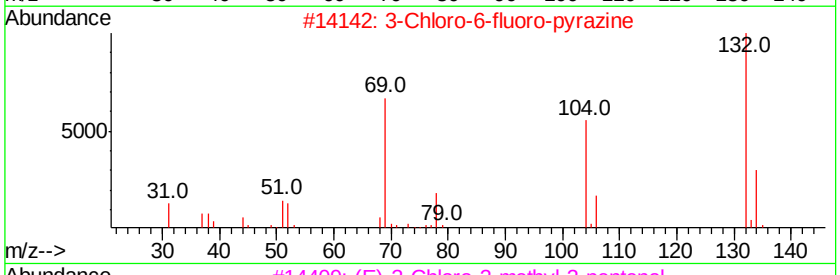
Peak Number 2 unknown7.54 Concentration Rank 1

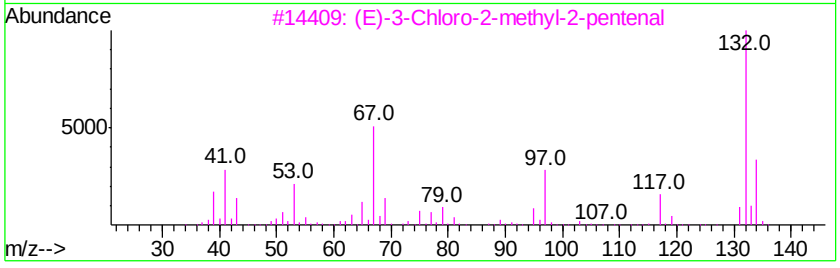
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	116.55 ng	632810	1,4-Dichlorobenzene-d4	8.01

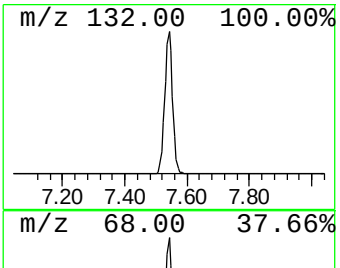
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
5	5-Aminoindole	132	C8H8N2	005192-03-0	16

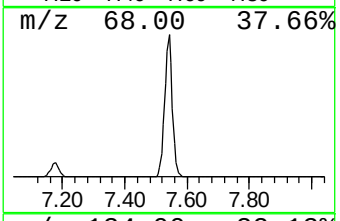


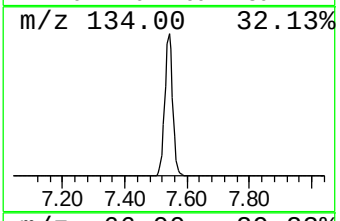


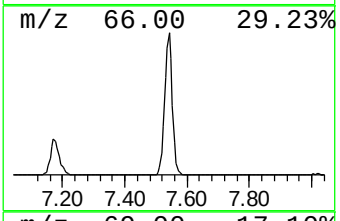


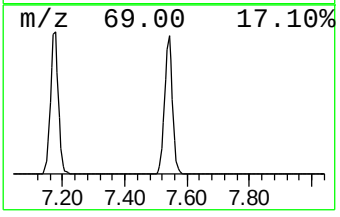












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Instrument : BNA_G
ClientSampleId : WC-06-011519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

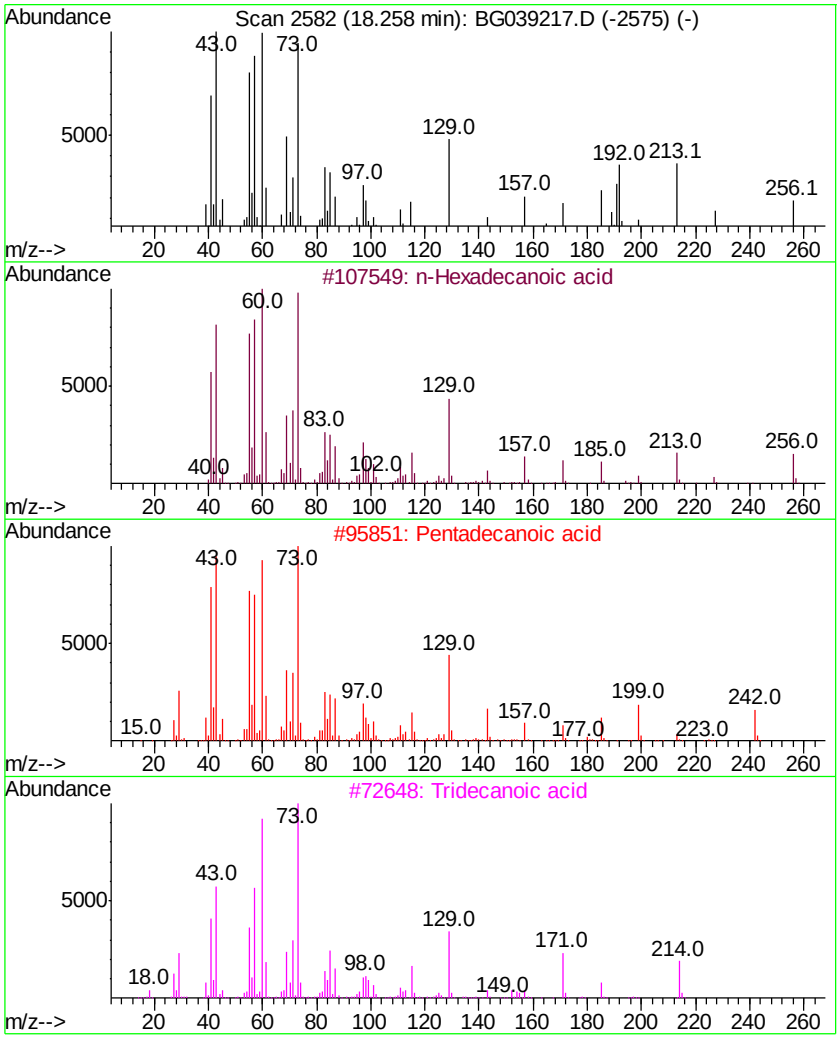
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

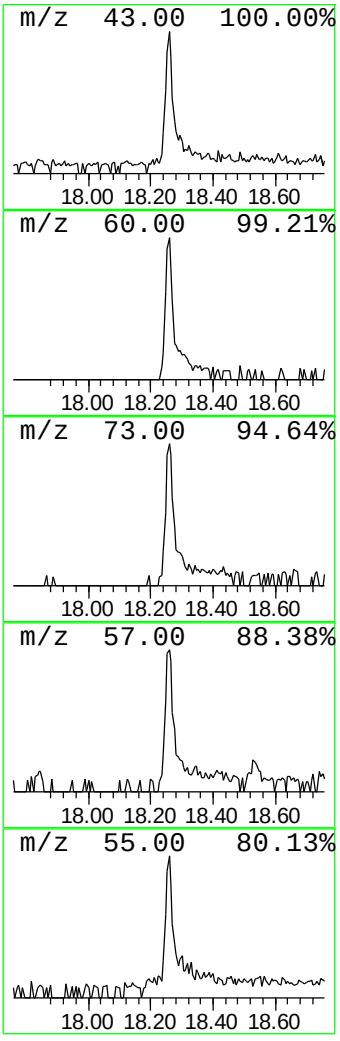
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	4.80 ng	61408	Phenanthrene-d10	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
3	Tridecanoic acid	214	C13H26O2	000638-53-9	50
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	43





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Misc :
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Instrument : BNA_G
ClientSampleId : WC-06-011519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

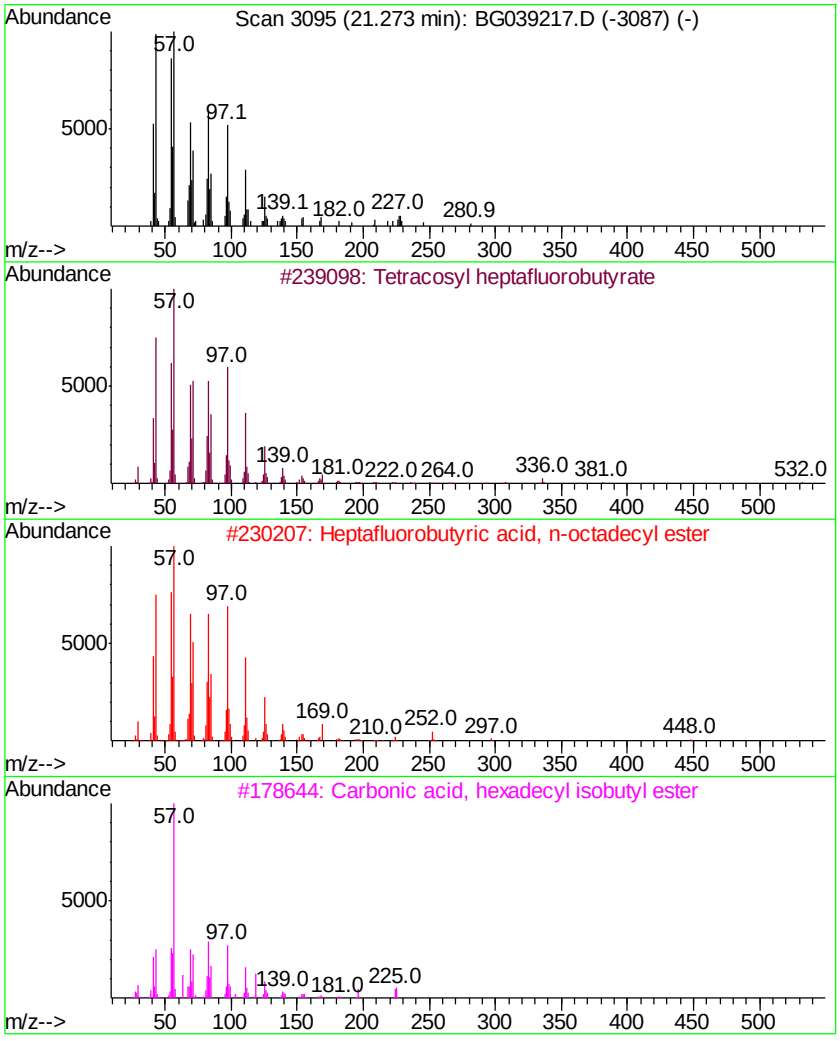
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

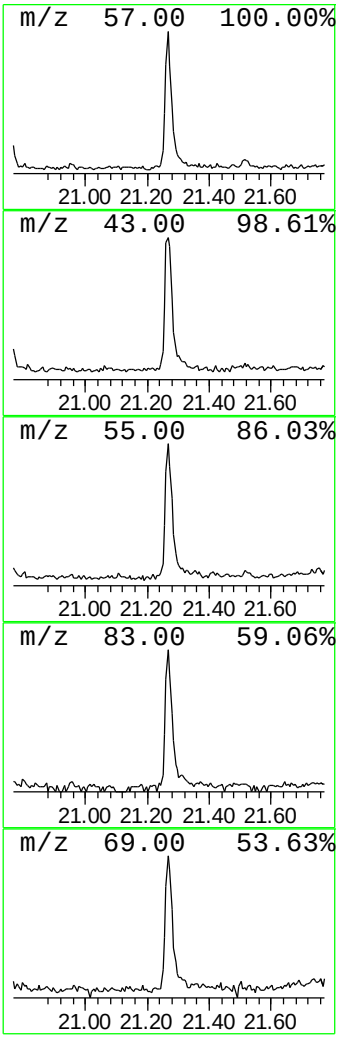
****

Peak Number 5 Tetracosyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.27	6.54 ng	124249	Chrysene-d12	21.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Carbonic acid, hexadecyl isobutyl...	342	C21H42O3	1000314-61-3	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011819\
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Instrument : BNA_G
ClientSampleId : WC-06-011519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

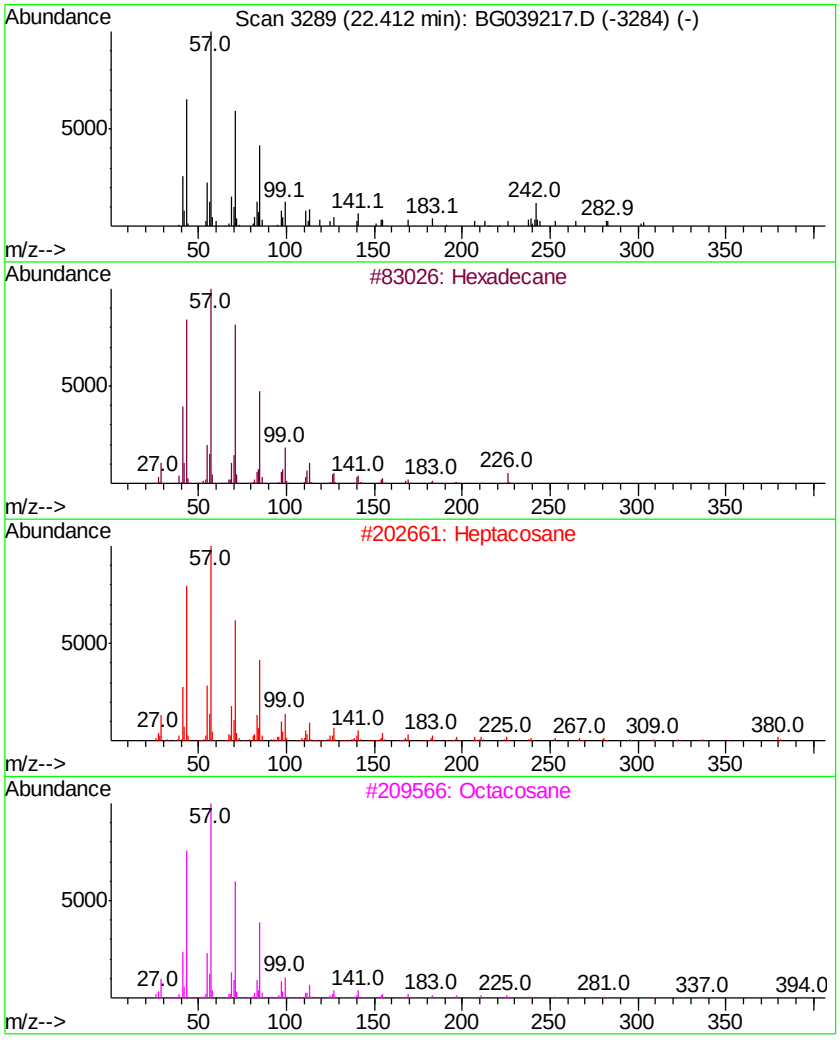
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

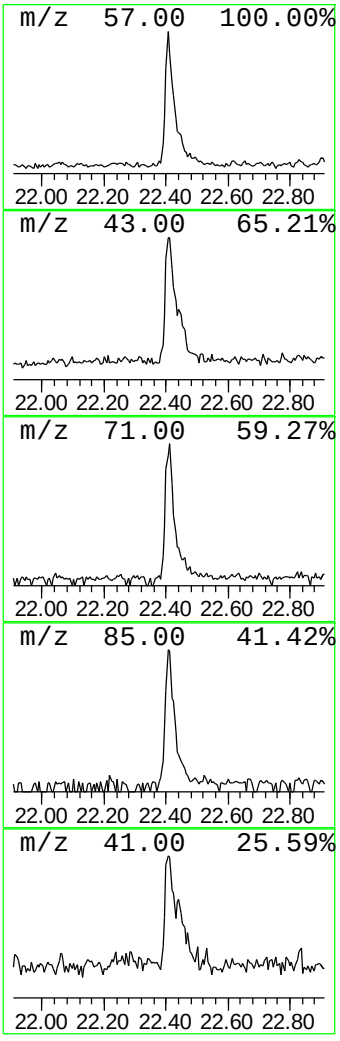
****

Peak Number 6 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	2.81 ng	53384	Chrysene-d12	21.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Heptacosane	380	C27H56	000593-49-7	81
3	Octacosane	394	C28H58	000630-02-4	81
4	Hexacosane	366	C26H54	000630-01-3	81
5	Hentriacontane	437	C31H64	000630-04-6	74





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Instrument : BNA_G
ClientSampleId : WC-06-011519

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

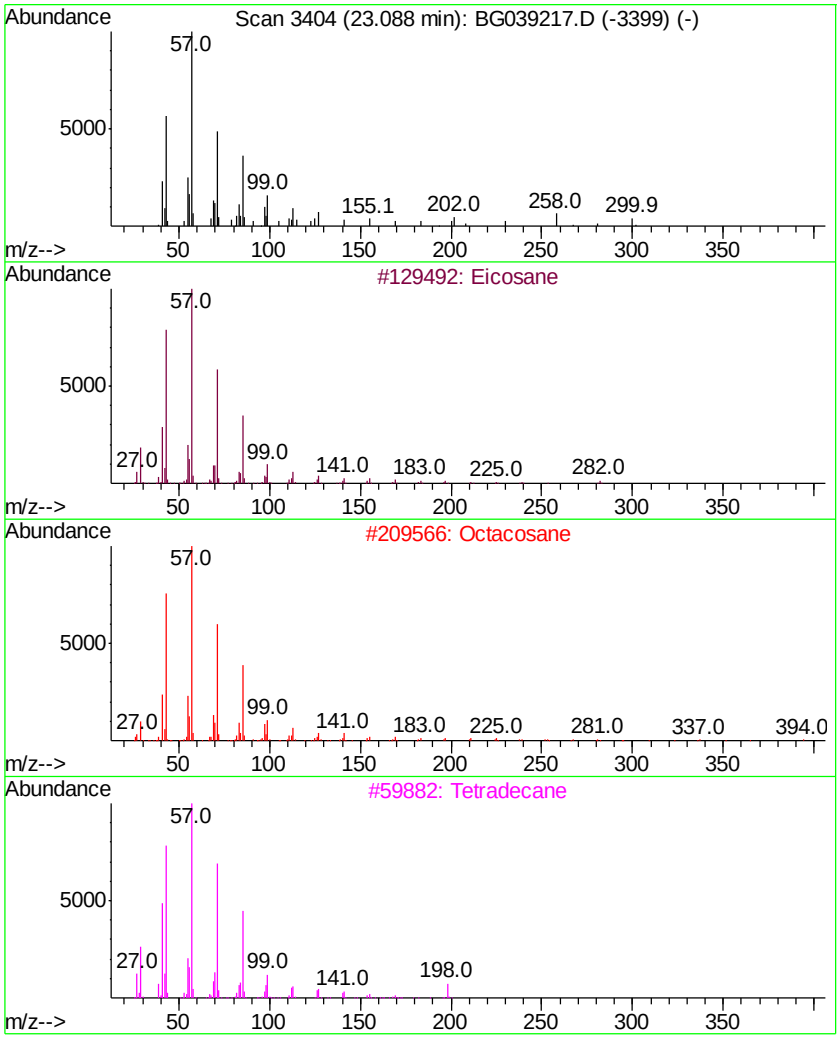
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

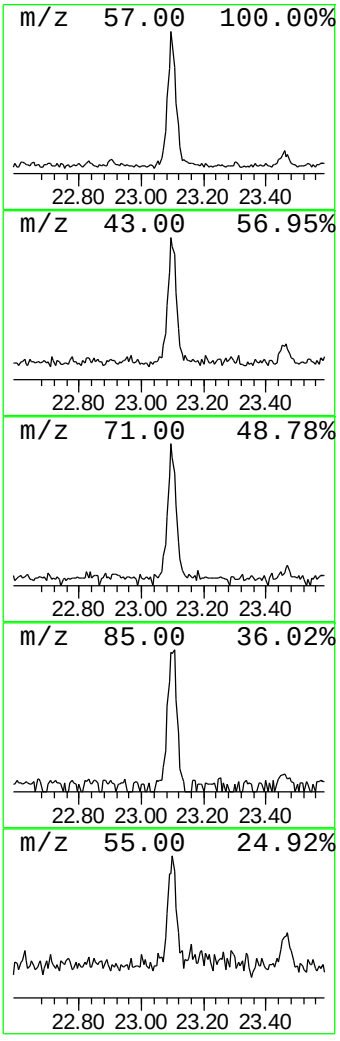
****

Peak Number 7 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.09	3.52 ng	66865	Chrysene-d12	21.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Octacosane	394	C28H58	000630-02-4	81
3	Tetradecane	198	C14H30	000629-59-4	74
4	2-methyloctacosane	408	C29H60	1000376-72-8	74
5	Tetracosane	338	C24H50	000646-31-1	74





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	7.5	ng	40955	1	8.01	108588	20.0
unknown7.54	7.54	116.6	ng	632810	1	8.01	108588	20.0
n-Hexadecanoic acid	18.26	4.8	ng	61408	4	17.39	255935	20.0
Tetracosyl heptaf...	21.27	6.5	ng	124249	5	21.67	379850	20.0
Hexadecane	22.41	2.8	ng	53384	5	21.67	379850	20.0
Eicosane	23.09	3.5	ng	66865	5	21.67	379850	20.0