LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039468.D
Acq On : 12 Feb 2019 17:52
Operator : JU/SJ
Sample : K1462-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

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-BG012919.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	3.226	17	23	31	rBV	79936	154187	5.04%	0.770%
2	3.296	31	35	49	rVB	49465	86493	2.83%	0.432%
3	5.252	362	368	377	rVB	53313	87973	2.87%	0.440%
4	5.711	439	446	456	rVB	941317	1471381	48.08%	7.351%
5	7.308	710	718	728	rBV	1002392	1762697	57.59%	8.806%
6	7.696	775	784	793	rBV	924397	1573266	51.40%	7.860%
7	8.172	858	865	873	rBV	178369	306732	10.02%	1.532%
8	8.495	911	920	929	rBV	595821	1041366	34.03%	5.203%
9	9.347	1055	1065	1076	rBV	579697	1028080	33.59%	5.136%
10	10.992	1338	1345	1356	rBV	272355	479809	15.68%	2.397%
11	13.418	1751	1758	1765	rBV	1322241	2076997	67.86%	10.377%
12	14.234	1890	1897	1903	rBV	109799	151979	4.97%	0.759%
13	14.792	1986	1992	2002	rBV3	470988	759967	24.83%	3.797%
14	16.279	2238	2245	2258	rBV	1321689	1999468	65.33%	9.989%
15	17.536	2453	2459	2470	rBV2	642917	997704	32.60%	4.985%
16	18.393	2597	2605	2623	rBV2	55999	111609	3.65%	0.558%
17	20.132	2895	2901	2908	rBV	2262499	3060533	100.00%	15.290%
18	21.425	3115	3121	3129	rBV	138173	207438	6.78%	1.036%
19	21.830	3182	3190	3199	rBV2	658895	1122403	36.67%	5.608%
20	21.989	3212	3217	3227	rVB	29627	50869	1.66%	0.254%
21	22.617	3320	3324	3340	rVB4	36144	89503	2.92%	0.447%
22	23.346	3441	3448	3454	rBV2	46920	87832	2.87%	0.439%
23	24.191	3585	3592	3599	rVB2	45723	93980	3.07%	0.470%
24	25.208	3753	3765	3782	rVB	371298	1157575	37.82%	5.783%
25	26.388	3958	3966	3976	rVB5	20317	56092	1.83%	0.280%

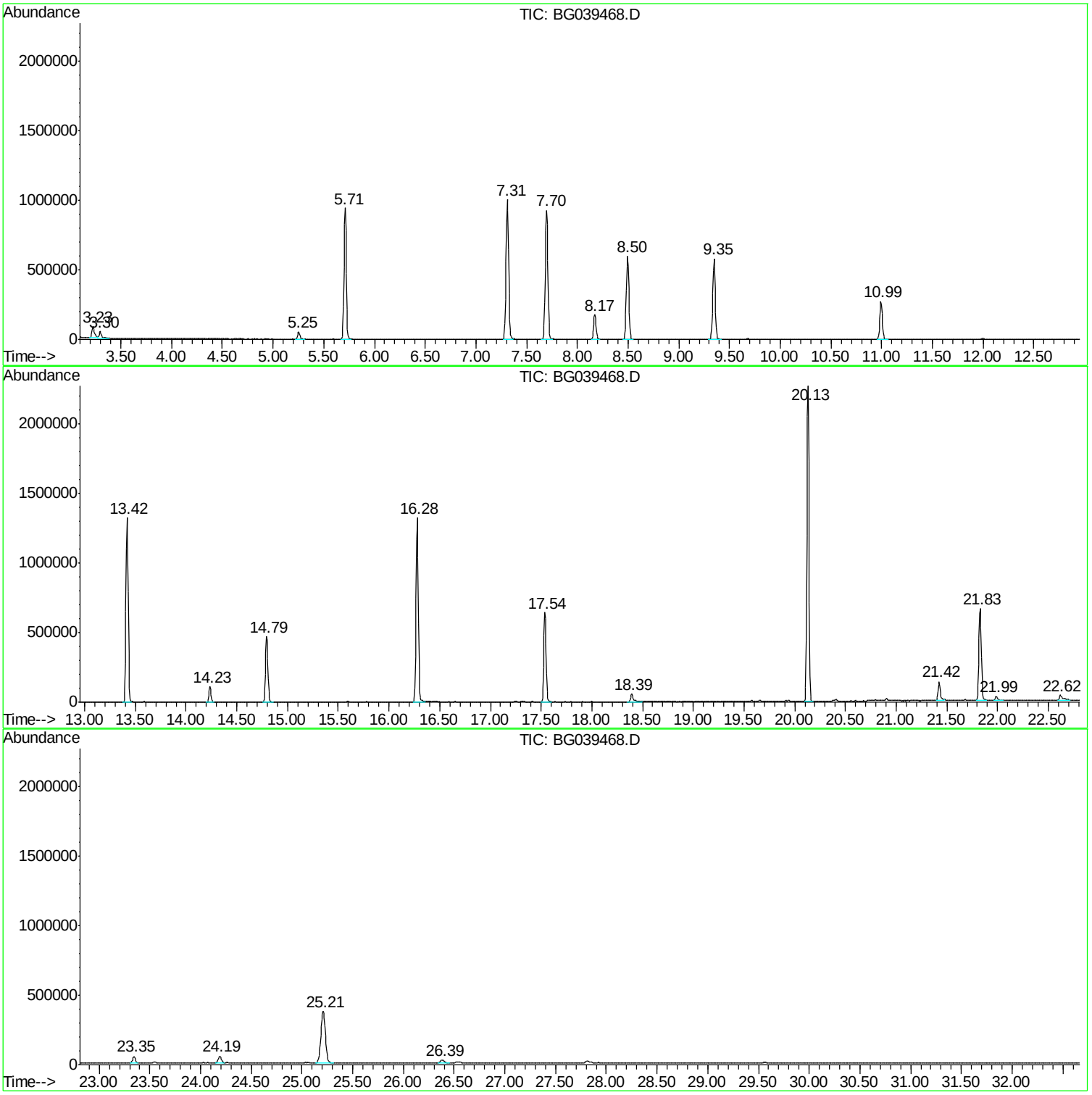
Sum of corrected areas: 20015933

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039468.D
Acq On : 12 Feb 2019 17:52
Operator : JU/SJ
Sample : K1462-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.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\BG021219\
Data File : BG039468.D
Acq On : 12 Feb 2019 17:52
Operator : JU/SJ
Sample : K1462-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

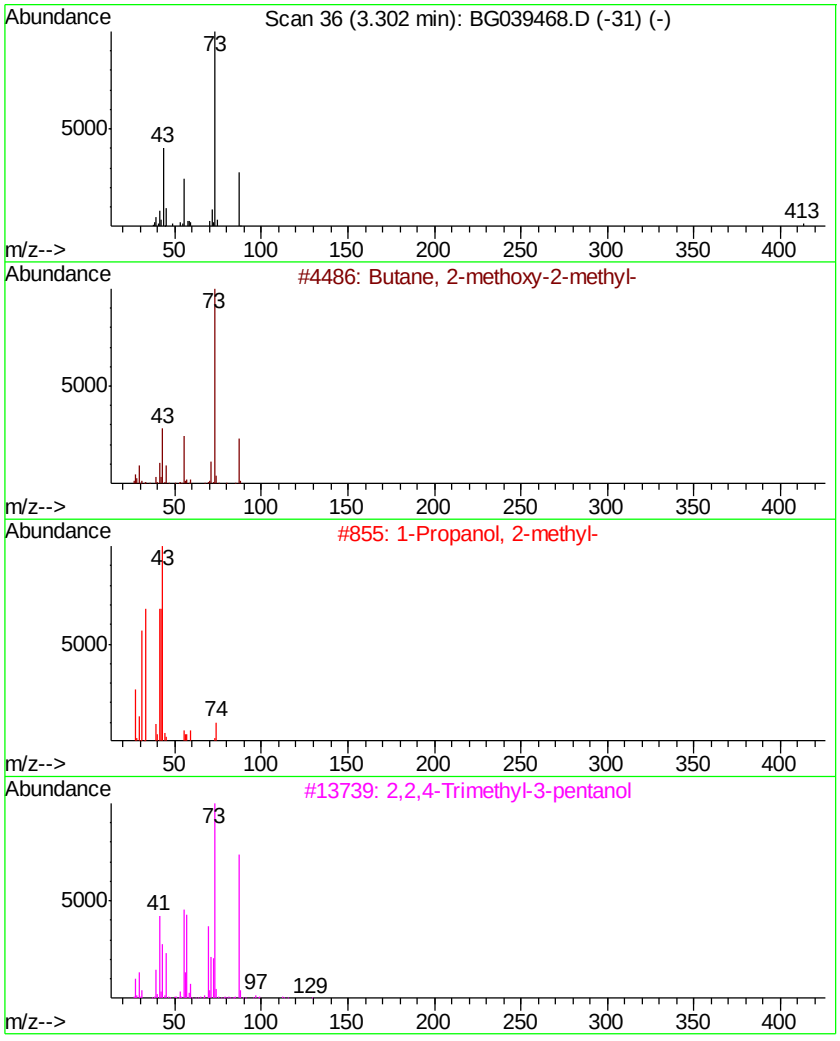
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

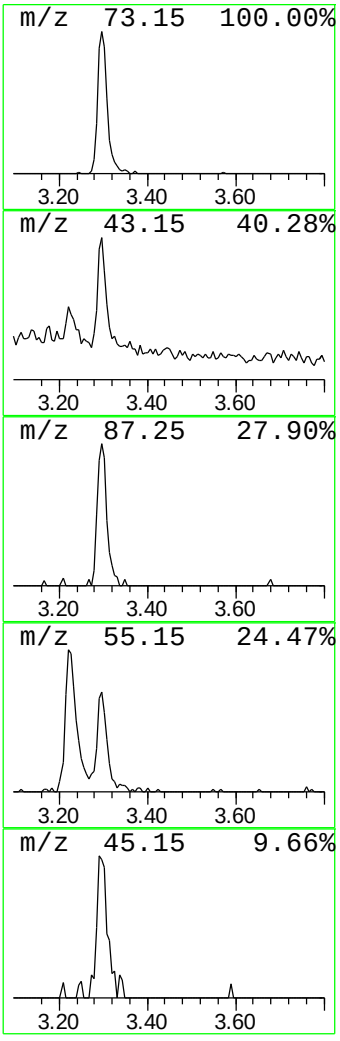
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.30	5.64 ng	86493	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	50
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	7
5	(R)-3-Pyrrolidinol	87	C4H9NO	002799-21-5	7





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039468.D
Acq On : 12 Feb 2019 17:52
Operator : JU/SJ
Sample : K1462-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

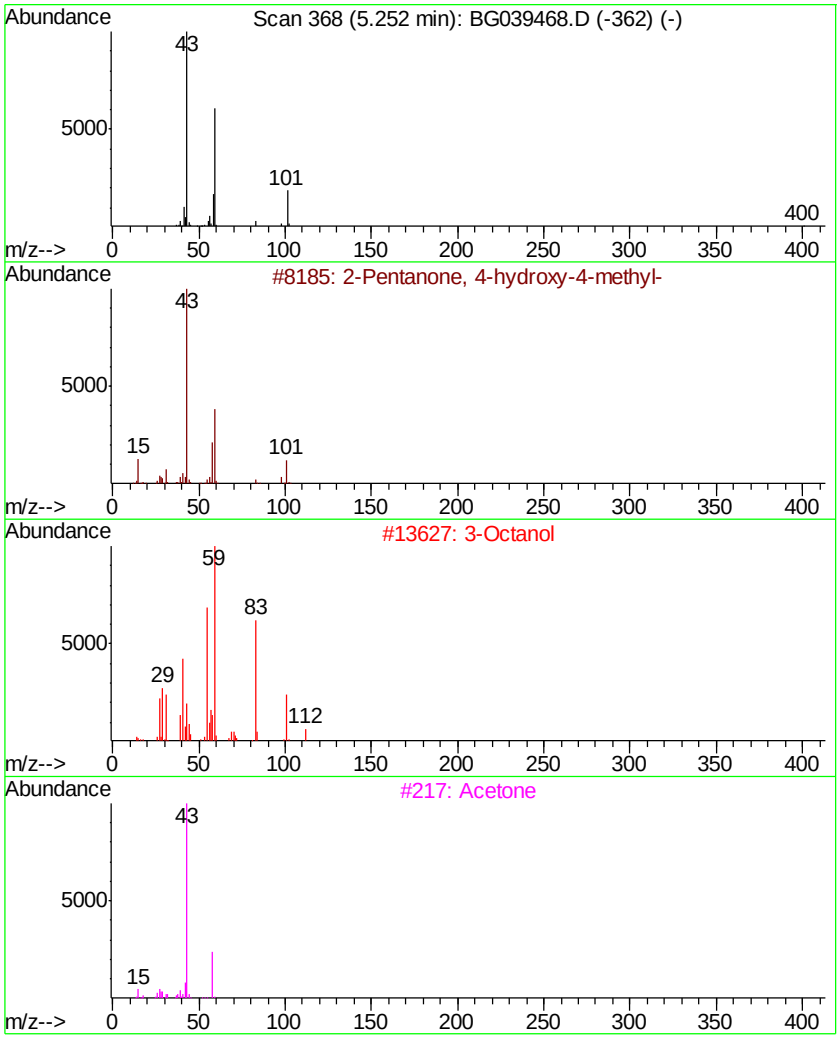
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

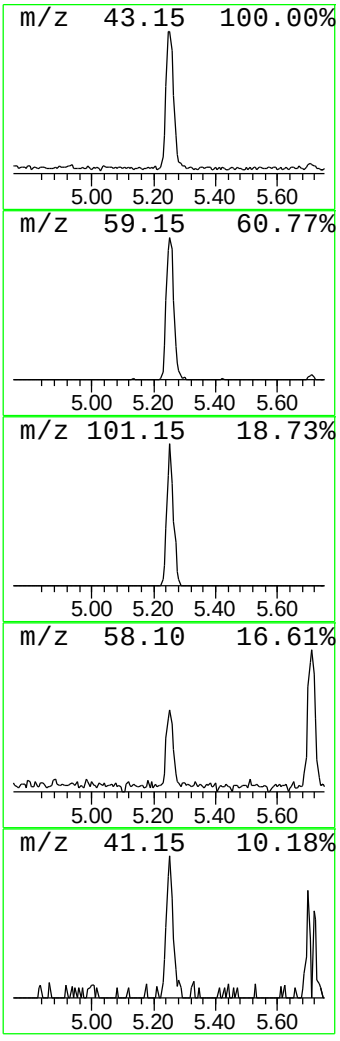
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.25	5.74 ng	87973	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Octanol	130	C8H18O	000589-98-0	33
3	Acetone	58	C3H6O	000067-64-1	22
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	.alpha.-Hydroxyisobutyric acid, ...	146	C6H10O4	1000374-31-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039468.D
Acq On : 12 Feb 2019 17:52
Operator : JU/SJ
Sample : K1462-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

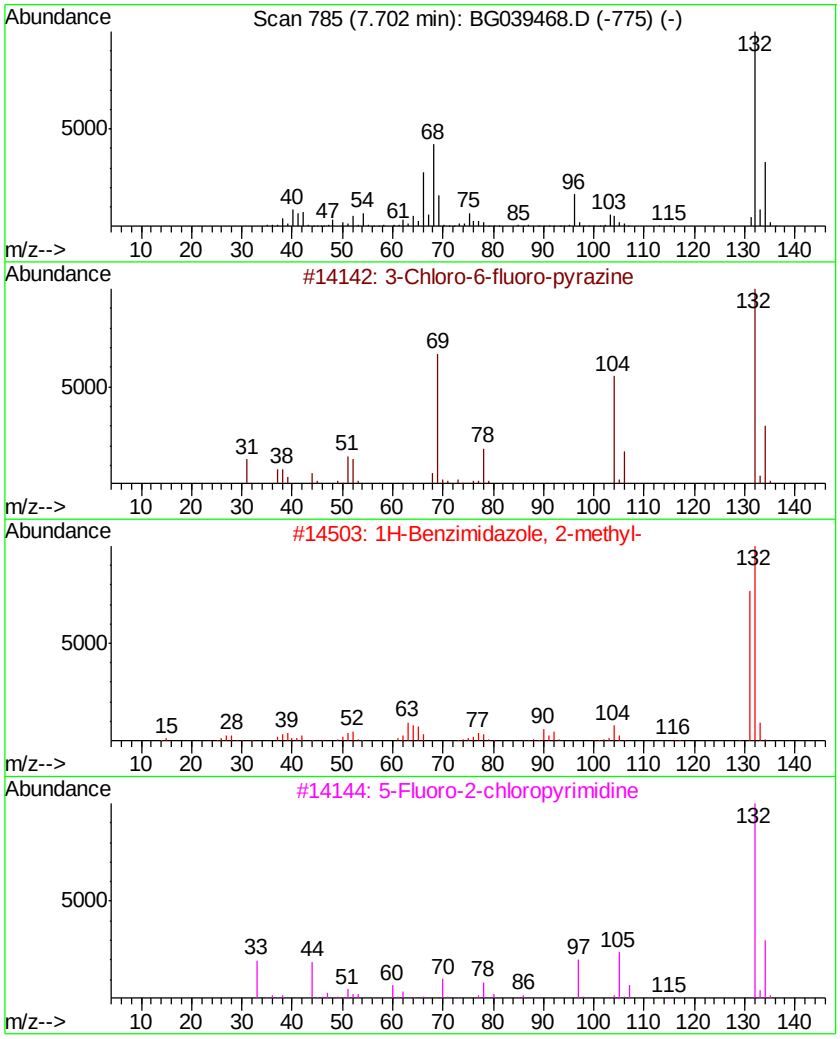
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

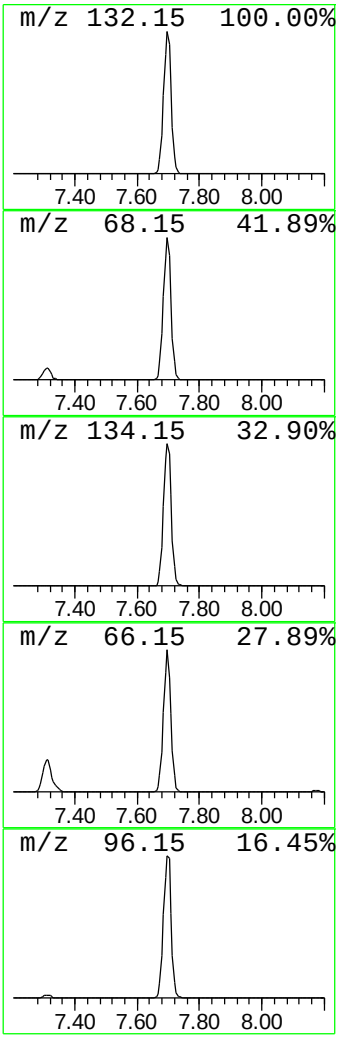
****

Peak Number 4 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	102.58 ng	1573270	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039468.D
Acq On : 12 Feb 2019 17:52
Operator : JU/SJ
Sample : K1462-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

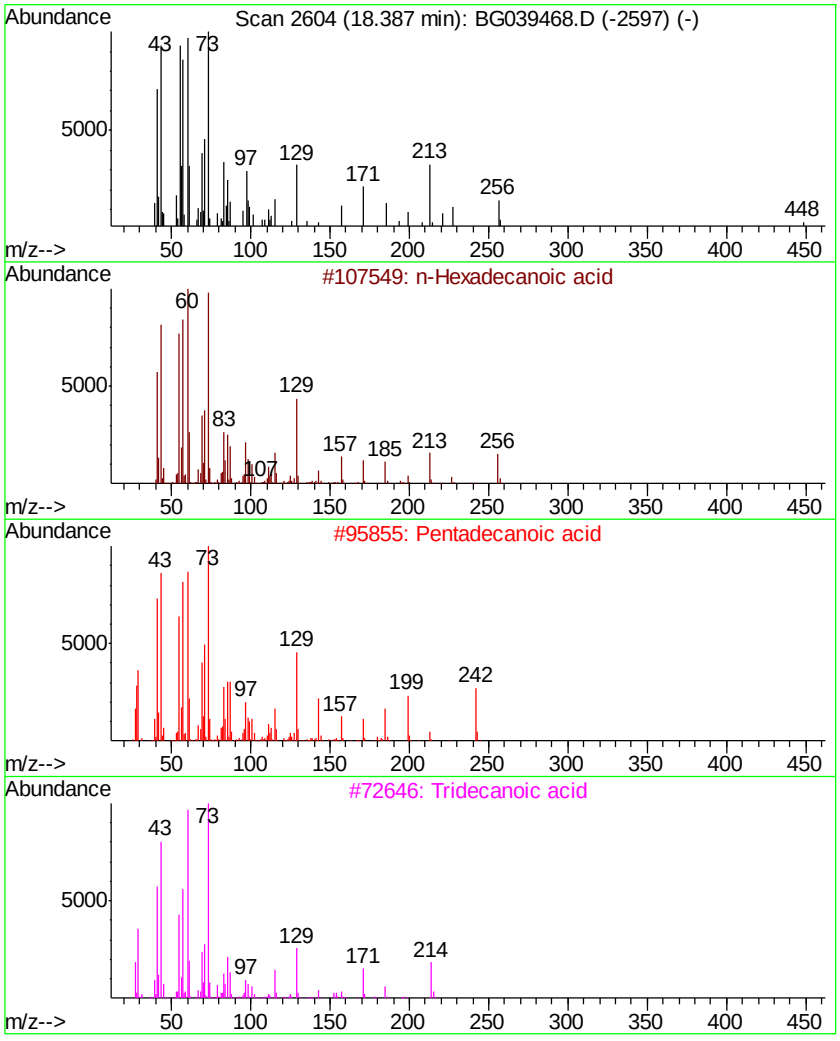
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

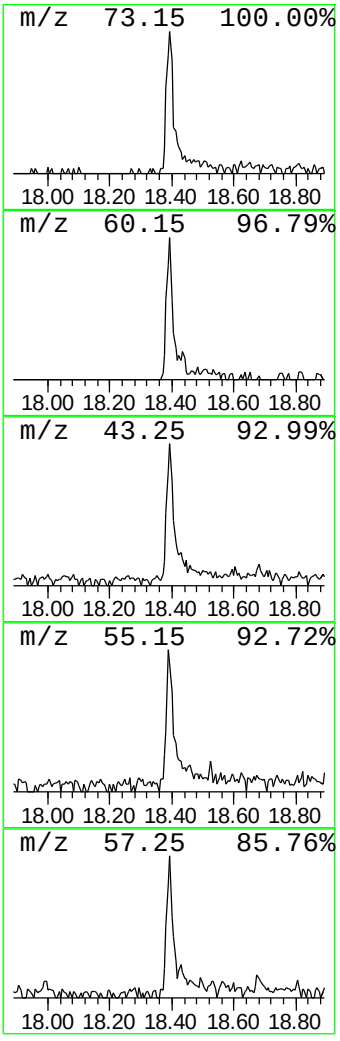
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	2.24 ng	111609	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG021219\
Data File : BG039468.D
Acq On : 12 Feb 2019 17:52
Operator : JU/SJ
Sample : K1462-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

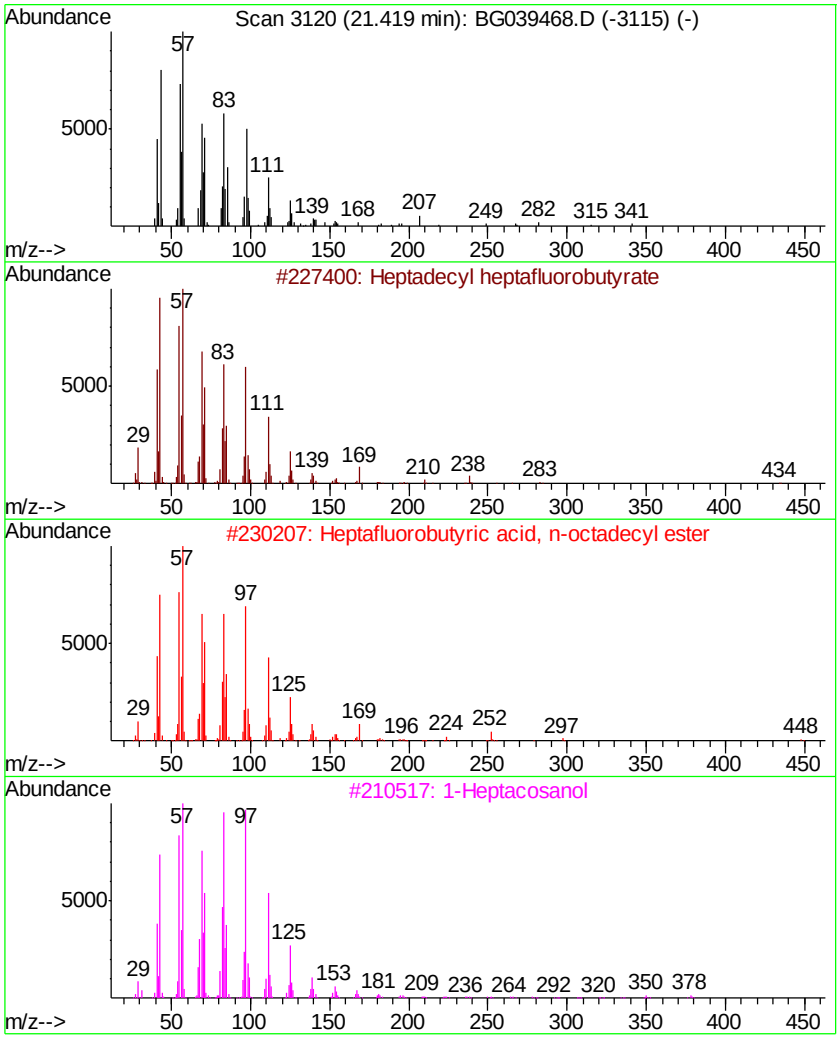
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

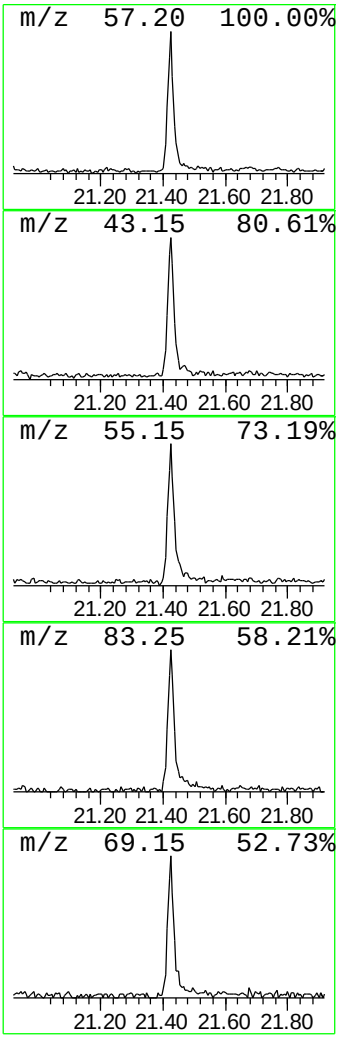
****

Peak Number 7 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.42	3.70 ng	207438	Chrysene-d12	21.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG021219\
Data File : BG039468.D
Acq On : 12 Feb 2019 17:52
Operator : JU/SJ
Sample : K1462-19
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
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
Butane, 2-methoxy...	3.30	5.6	ng	86493	1	8.17	306732	20.0
2-Pentanone, 4-hy...	5.25	5.7	ng	87973	1	8.17	306732	20.0
unknown7.70	7.70	102.6	ng	1573270	1	8.17	306732	20.0
n-Hexadecanoic acid	18.39	2.2	ng	111609	4	17.54	997704	20.0
Heptadecyl heptaf...	21.42	3.7	ng	207438	5	21.83	1122400	20.0