LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG022719\
Data File : BG039632.D
Acq On : 27 Feb 2019 13:21
Operator : JU/SJ
Sample : K1594-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(4-5)

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	3.217	17	22	31	rBV	93122	187946	5.66%	0.926%
2	3.293	31	35	47	rVB	57473	87620	2.64%	0.432%
3	5.713	440	447	461	rVB	942866	1537020	46.33%	7.575%
4	7.311	710	719	730	rBV	978868	1762315	53.12%	8.685%
5	7.693	776	784	792	rBV	932566	1620737	48.85%	7.988%
6	8.163	858	864	874	rVB	171136	304058	9.16%	1.499%
7	8.492	911	920	927	rBV	621432	1082199	32.62%	5.334%
8	9.344	1055	1065	1078	rBV	563895	1017225	30.66%	5.013%
9	10.989	1336	1345	1354	rBV	255644	439171	13.24%	2.164%
10	13.415	1750	1758	1768	rBV	1257843	1944828	58.62%	9.585%
11	14.231	1890	1897	1903	rBV	101576	149431	4.50%	0.736%
12	14.789	1983	1992	2001	rBV3	416545	660442	19.91%	3.255%
13	16.276	2238	2245	2257	rBV	1291367	1989684	59.97%	9.806%
14	17.533	2452	2459	2473	rBV	578042	900517	27.14%	4.438%
15	18.384	2599	2604	2610	rBV2	81715	122004	3.68%	0.601%
16	19.647	2815	2819	2825	rBV6	21595	37170	1.12%	0.183%
17	20.123	2894	2900	2910	rBV	2425937	3317673	100.00%	16.351%
18	20.887	3027	3030	3036	rBV3	31056	38837	1.17%	0.191%
19	21.410	3114	3119	3137	rBV3	63531	175764	5.30%	0.866%
20	21.668	3157	3163	3169	rVB	122954	173557	5.23%	0.855%
21	21.821	3182	3189	3201	rVB2	600692	1025153	30.90%	5.052%
22	21.968	3209	3214	3219	rBV	53177	75268	2.27%	0.371%
23	22.596	3315	3321	3327	rBV	59953	100316	3.02%	0.494%
24	23.313	3436	3443	3451	rBV	73013	142916	4.31%	0.704%
25	23.513	3469	3477	3485	rBV2	21355	51106	1.54%	0.252%
26	24.159	3579	3587	3595	rBV2	60548	132445	3.99%	0.653%
27	25.193	3747	3763	3780	rVB3	317889	1107069	33.37%	5.456%
28	26.327	3949	3956	3969	rVB5	35516	107997	3.26%	0.532%

Sum of corrected areas: 20290468

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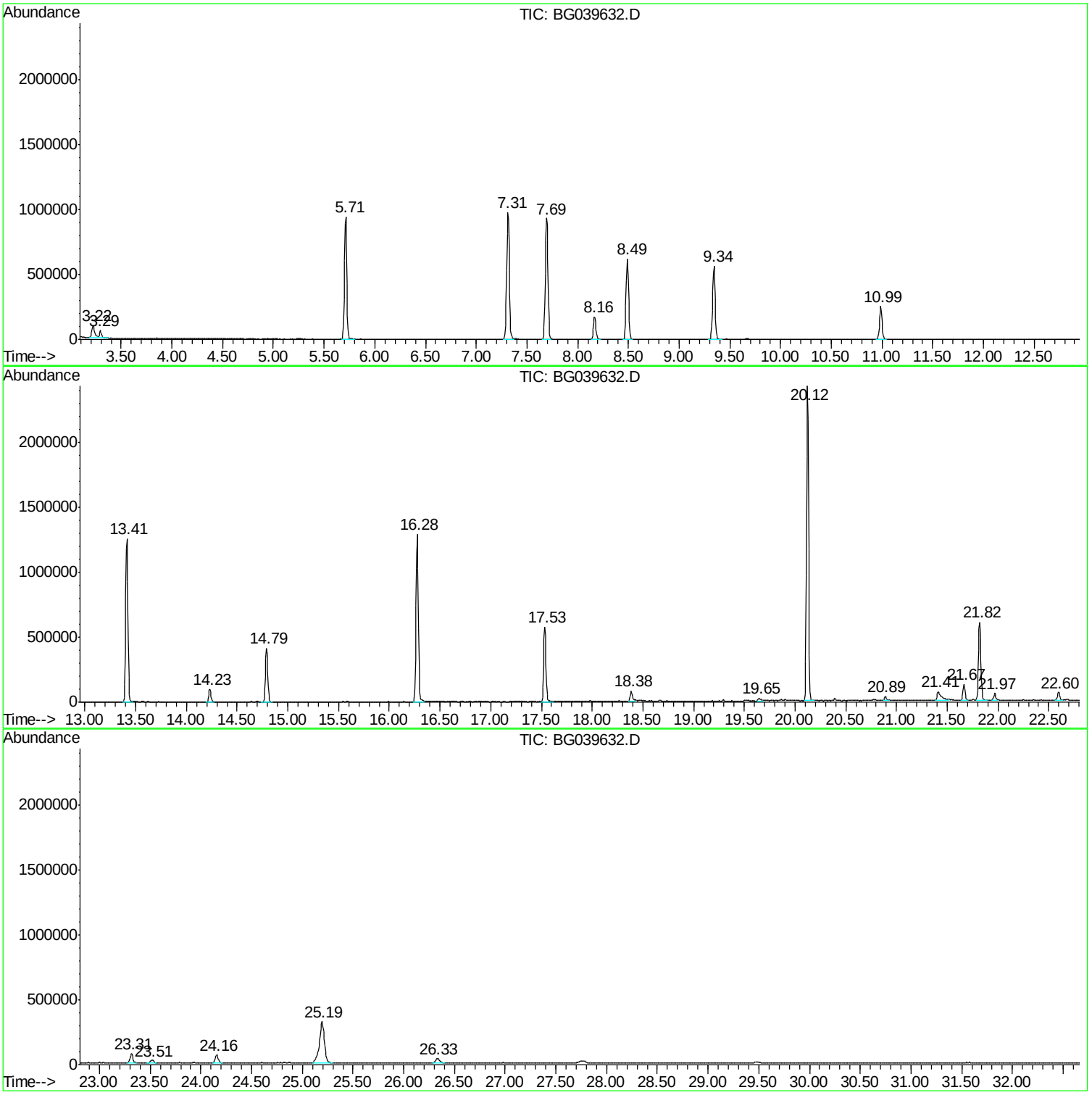
Instrument :
BNA_G
ClientSampleId :
B-1(4-5)

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

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Data File : BG039632.D
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Operator : JU/SJ
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Instrument : BNA_G
ClientSampleId : B-1(4-5)

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

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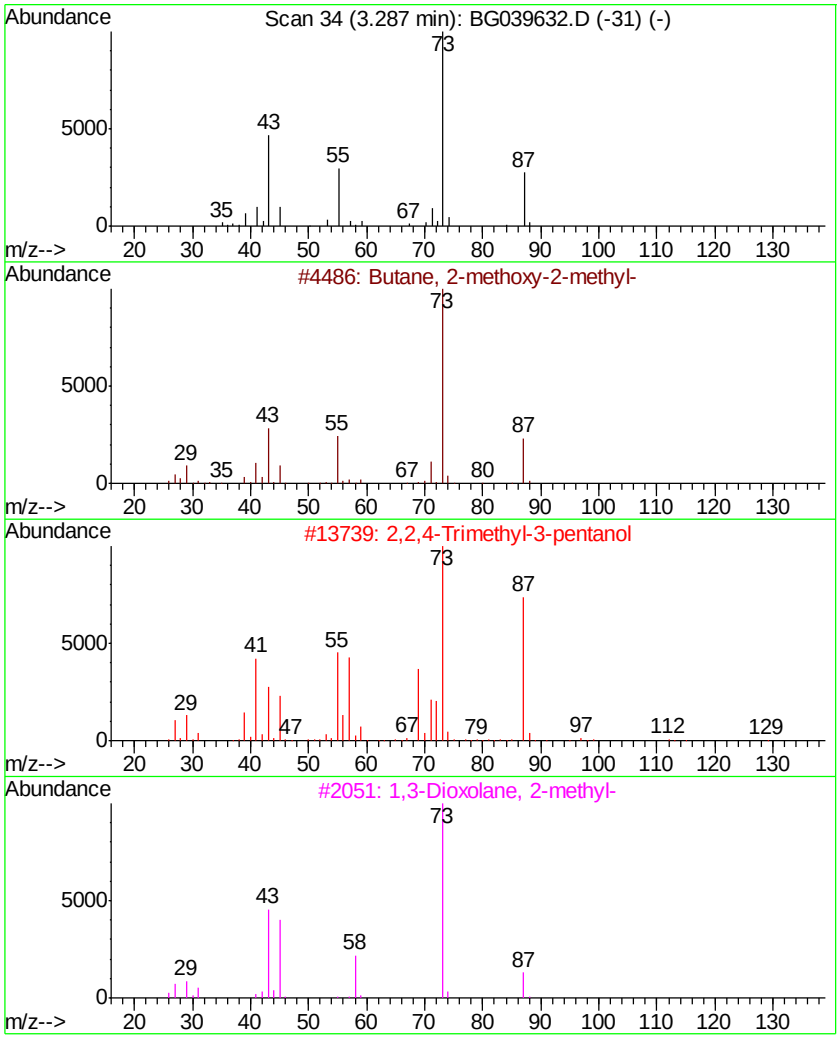
TIC Integration Parameters: LSCINT.P

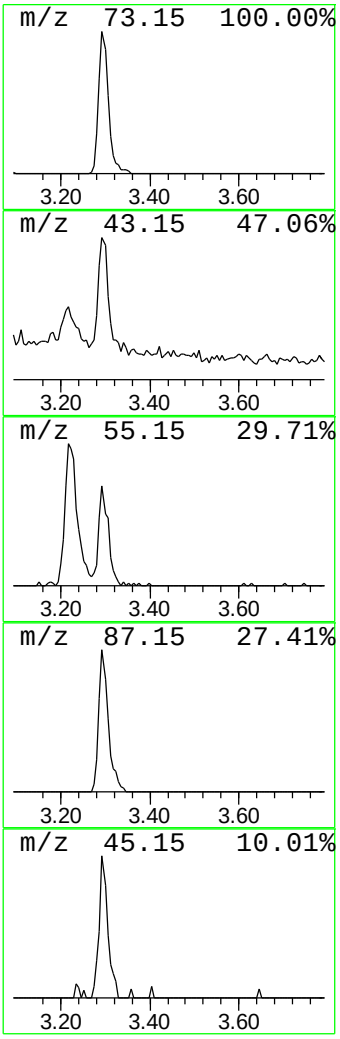
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.29	5.76 ng	87620	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





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Data File : BG039632.D
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Operator : JU/SJ
Sample : K1594-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(4-5)

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

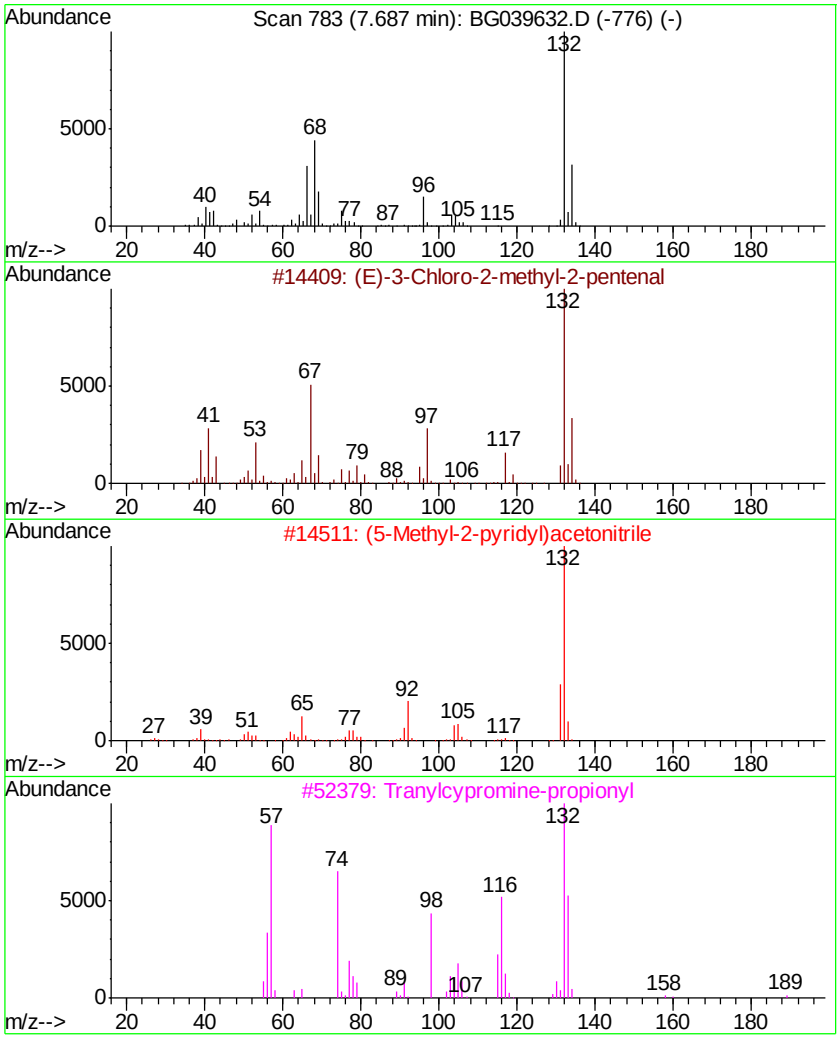
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

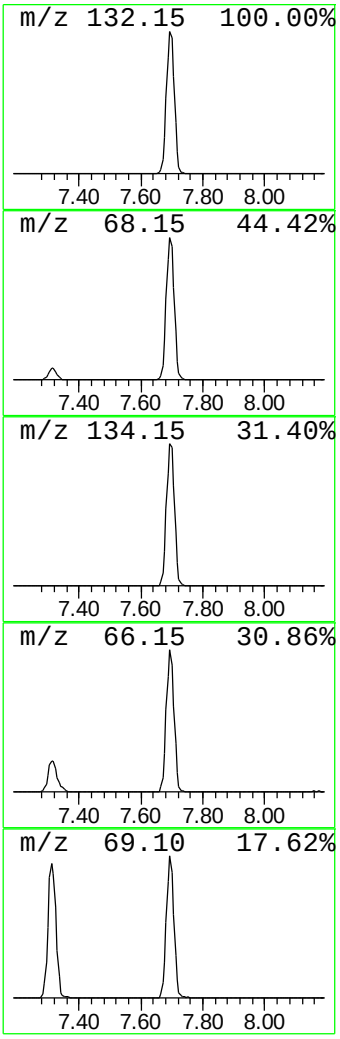
****

Peak Number 3 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	106.61 ng	1620740	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : B-1(4-5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012919.M
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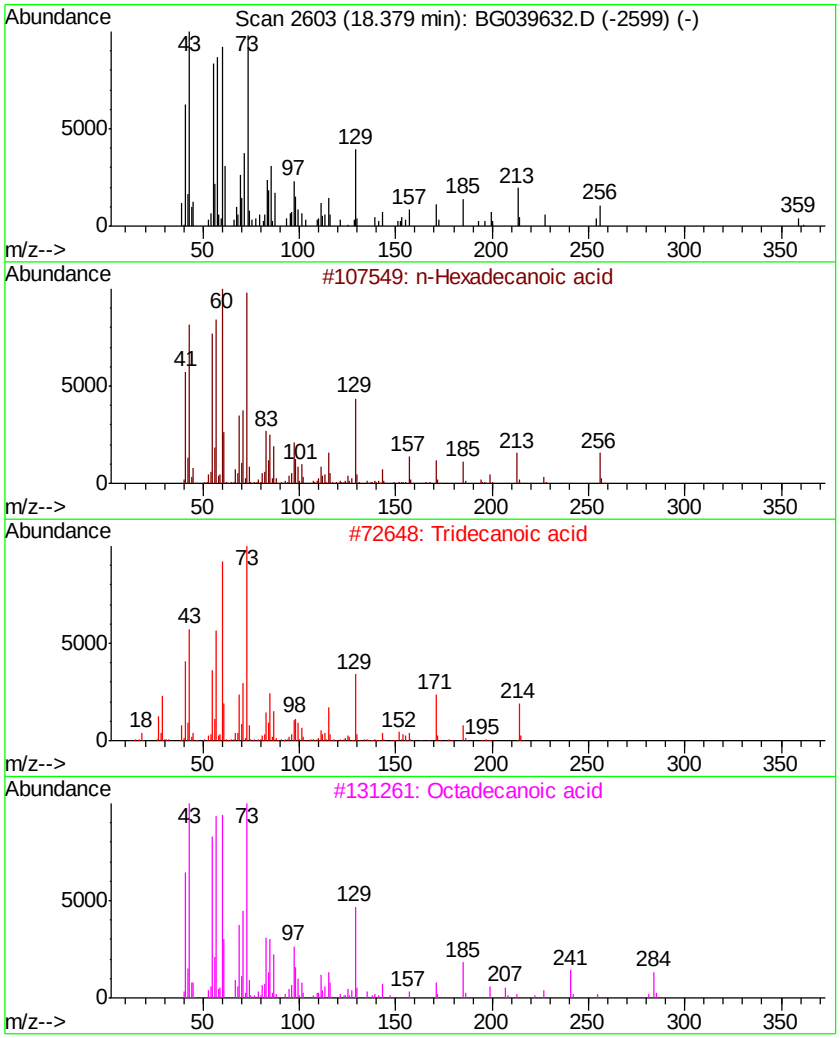
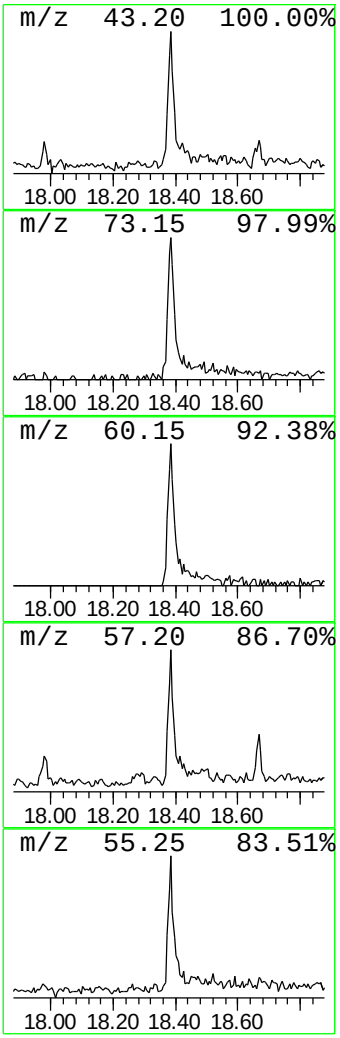
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	2.71 ng	122004	Phenanthrene-d10	17.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	68
3	Octadecanoic acid	284	C18H36O2	000057-11-4	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	53





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : B-1(4-5)

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

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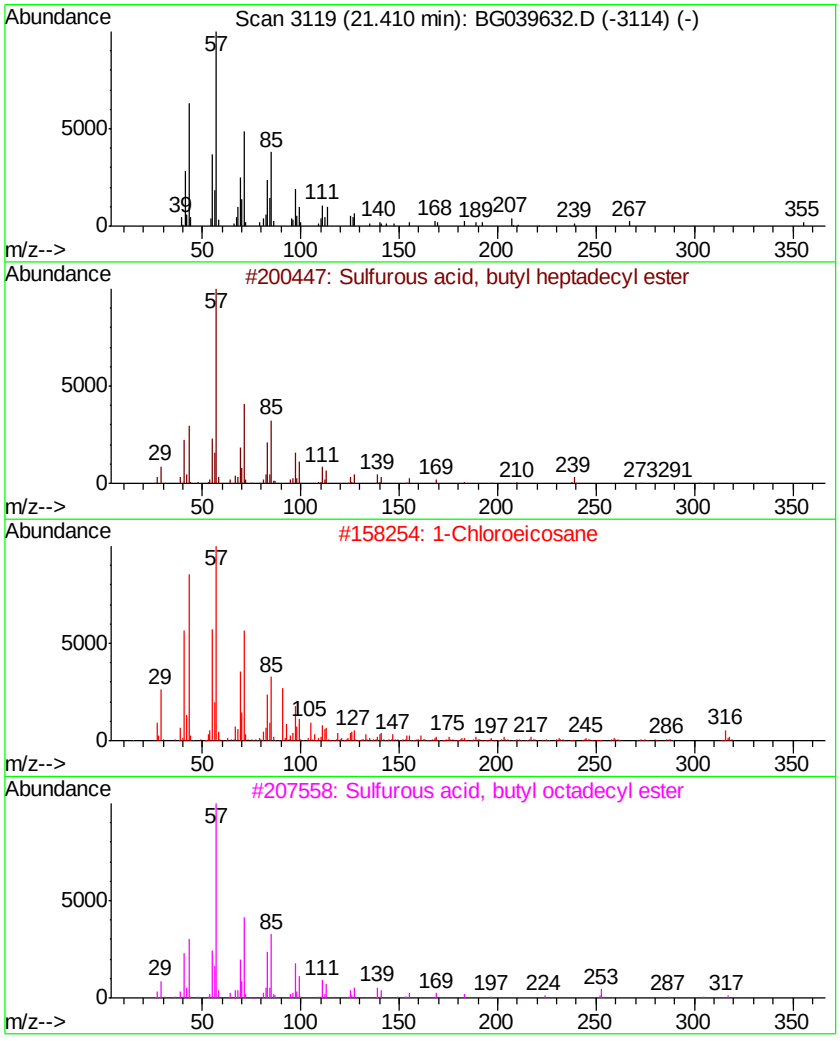
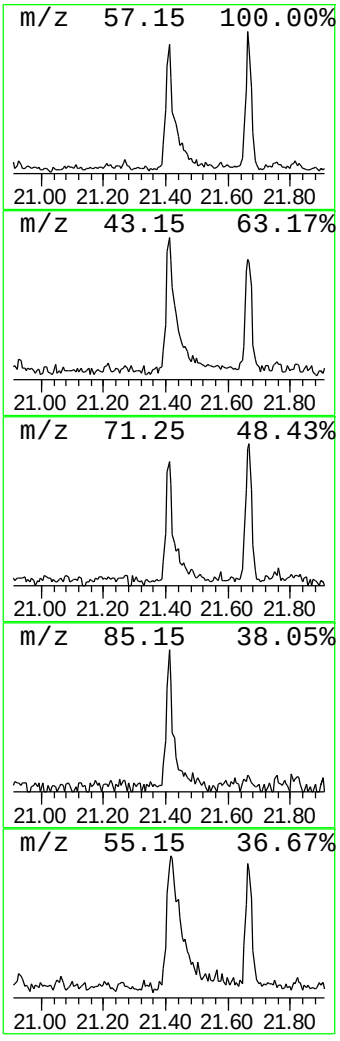
Peak Number 6 Sulfurous acid, butyl hepta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.41	3.43 ng	175764	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
2	1-Chloroeicosane	316	C20H41Cl	042217-02-7	91
3	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	90
4	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	90
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	86





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : B-1(4-5)

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TIC Library : C:\Database\NIST11.L
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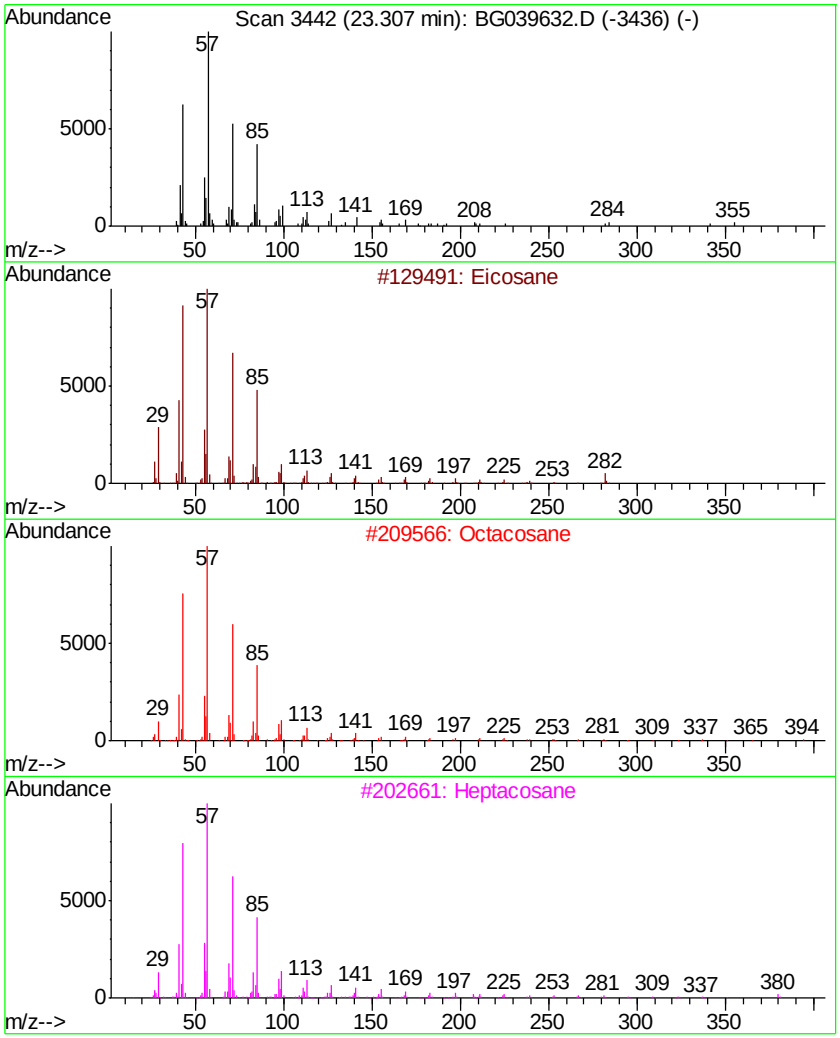
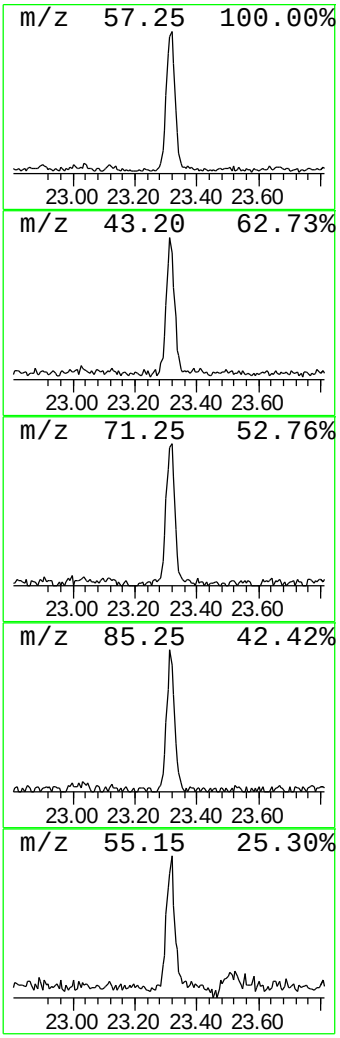
****

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	2.79 ng	142916	Chrysene-d12	21.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Octacosane	394	C28H58	000630-02-4	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Hexacosane	366	C26H54	000630-01-3	90





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TIC Library : C:\Database\NIST11.L
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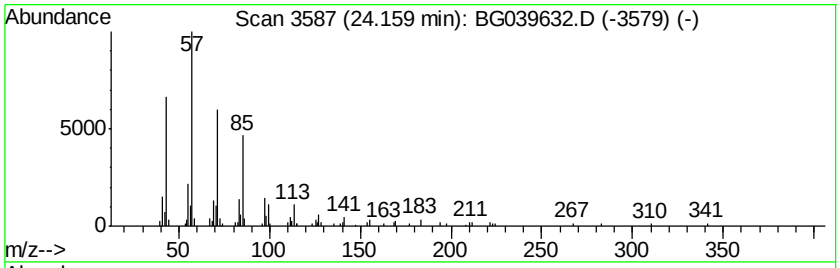
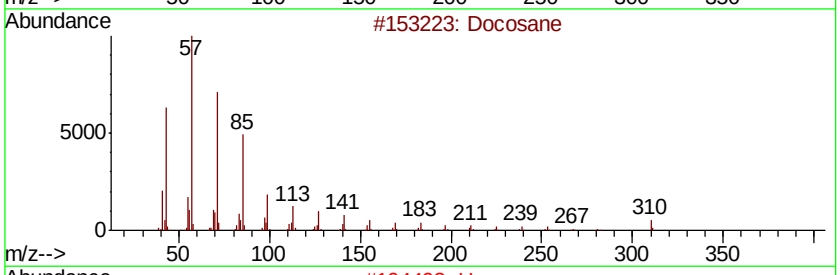
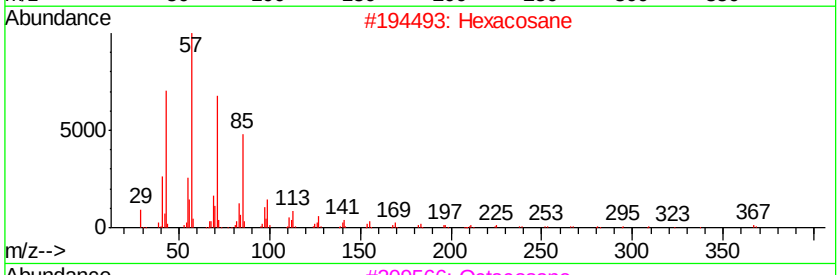
Peak Number 8 Docosane Concentration Rank 8

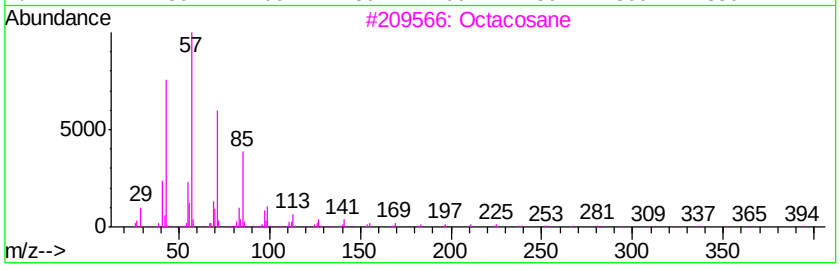
R.T.	EstConc	Area	Relative to ISTD	R.T.
24.16	2.39 ng	132445	Perylene-d12	25.19

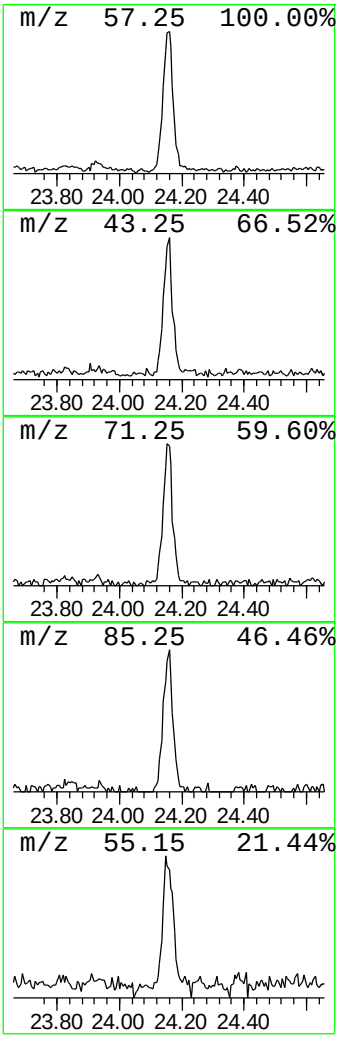
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	94
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	87
5	Tetracosane	338	C24H50	000646-31-1	87











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG022719\
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Instrument : BNA_G
ClientSampleId : B-1(4-5)

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...	3.29	5.8	ng	87620	1	8.17	304058	20.0
unknown7.69	7.69	106.6	ng	1620740	1	8.17	304058	20.0
n-Hexadecanoic acid	18.38	2.7	ng	122004	4	17.53	900517	20.0
Sulfurous acid, b...	21.41	3.4	ng	175764	5	21.82	1025150	20.0
Eicosane	23.31	2.8	ng	142916	5	21.82	1025150	20.0
Docosane	24.16	2.4	ng	132445	6	25.19	1107070	20.0