LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011719\
Data File : BG039192.D
Acq On : 17 Jan 2019 18:40
Operator : JU/SJ
Sample : K1149-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SW001-190114-01

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	3.135	4	8	17	rVB	31200	44803	1.74%	0.455%
2	5.567	415	422	432	rBV	197291	329962	12.81%	3.348%
3	7.171	687	695	707	rBV2	131317	257707	10.01%	2.615%
4	7.542	751	758	768	rBV	316688	557401	21.64%	5.655%
5	8.017	831	839	845	rBV	76388	133762	5.19%	1.357%
6	8.335	886	893	906	rBV	281669	502252	19.50%	5.096%
7	8.793	965	971	979	rBV	22074	41040	1.59%	0.416%
8	9.193	1031	1039	1048	rBV	252920	446659	17.34%	4.532%
9	10.832	1310	1318	1322	rBV	99348	185176	7.19%	1.879%
10	10.879	1322	1326	1335	rVB	75564	137894	5.35%	1.399%
11	13.276	1726	1734	1742	rBV	850390	1292669	50.19%	13.115%
12	13.517	1767	1775	1785	rVB	41906	71512	2.78%	0.726%
13	14.657	1962	1969	1976	rVB2	191382	307987	11.96%	3.125%
14	15.732	2150	2152	2161	rVB2	18456	27992	1.09%	0.284%
15	16.149	2216	2223	2240	rBV	709826	1121884	43.56%	11.383%
16	17.406	2429	2437	2442	rBV	276276	445696	17.31%	4.522%
17	18.264	2575	2583	2588	rBV4	19171	33343	1.29%	0.338%
18	20.009	2873	2880	2886	rBV	2046724	2575466	100.00%	26.131%
19	21.284	3091	3097	3101	rBV5	18063	35531	1.38%	0.360%
20	21.678	3157	3164	3173	rVB2	330887	554753	21.54%	5.628%
21	22.418	3283	3290	3295	rBV3	19270	35686	1.39%	0.362%
22	23.112	3401	3408	3416	rVB2	28712	58595	2.28%	0.595%
23	23.300	3433	3440	3448	rVB2	37609	67692	2.63%	0.687%
24	23.905	3536	3543	3551	rVB3	26934	58069	2.25%	0.589%
25	24.851	3696	3704	3710	rBV4	19311	49700	1.93%	0.504%
26	24.945	3710	3720	3735	rVB2	164719	482929	18.75%	4.900%

Sum of corrected areas: 9856160

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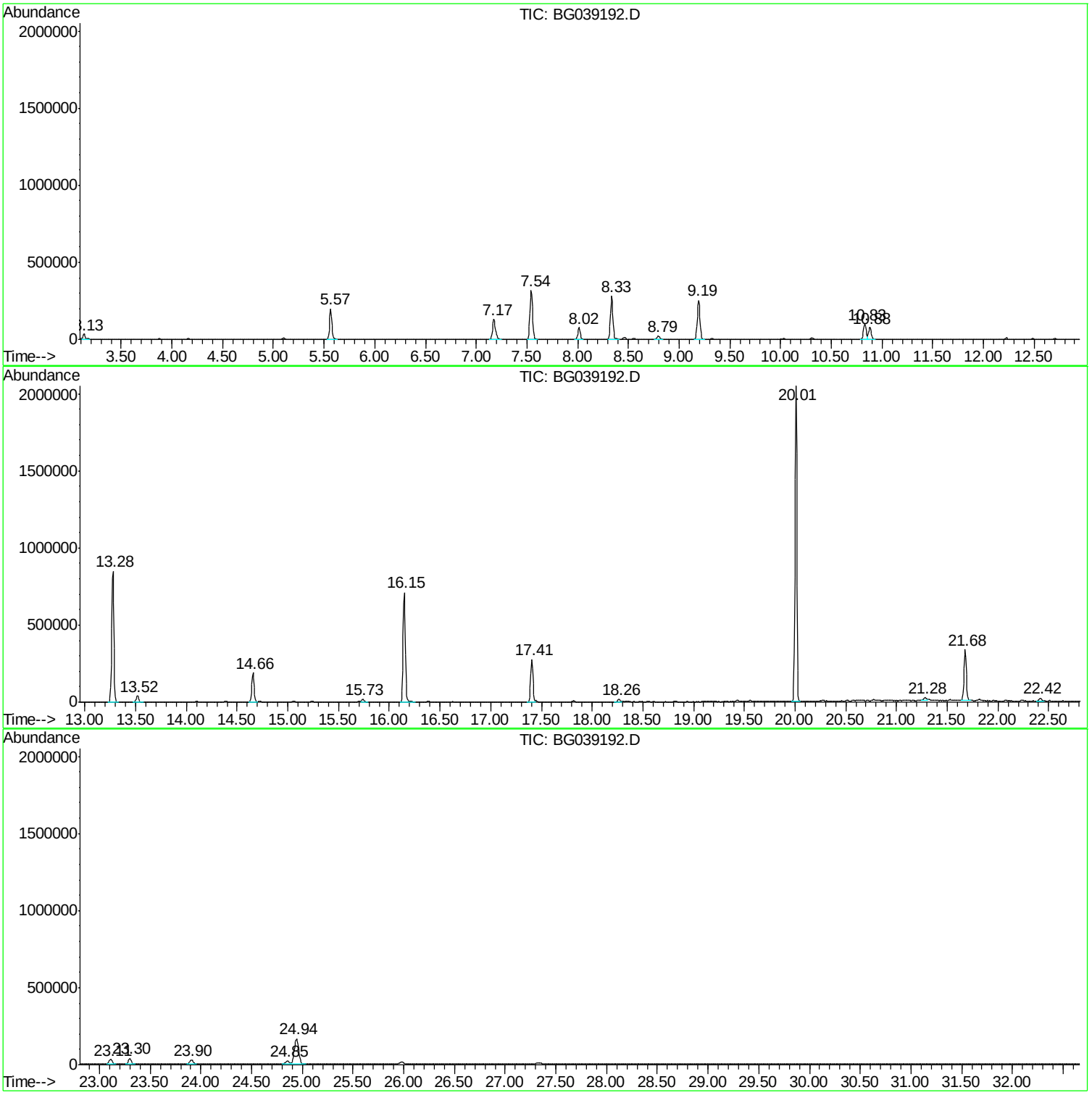
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SW001-190114-01

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\BG011719\
Data File : BG039192.D
Acq On : 17 Jan 2019 18:40
Operator : JU/SJ
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Misc :
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Instrument : BNA_G
ClientSampleId : SW001-190114-01

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

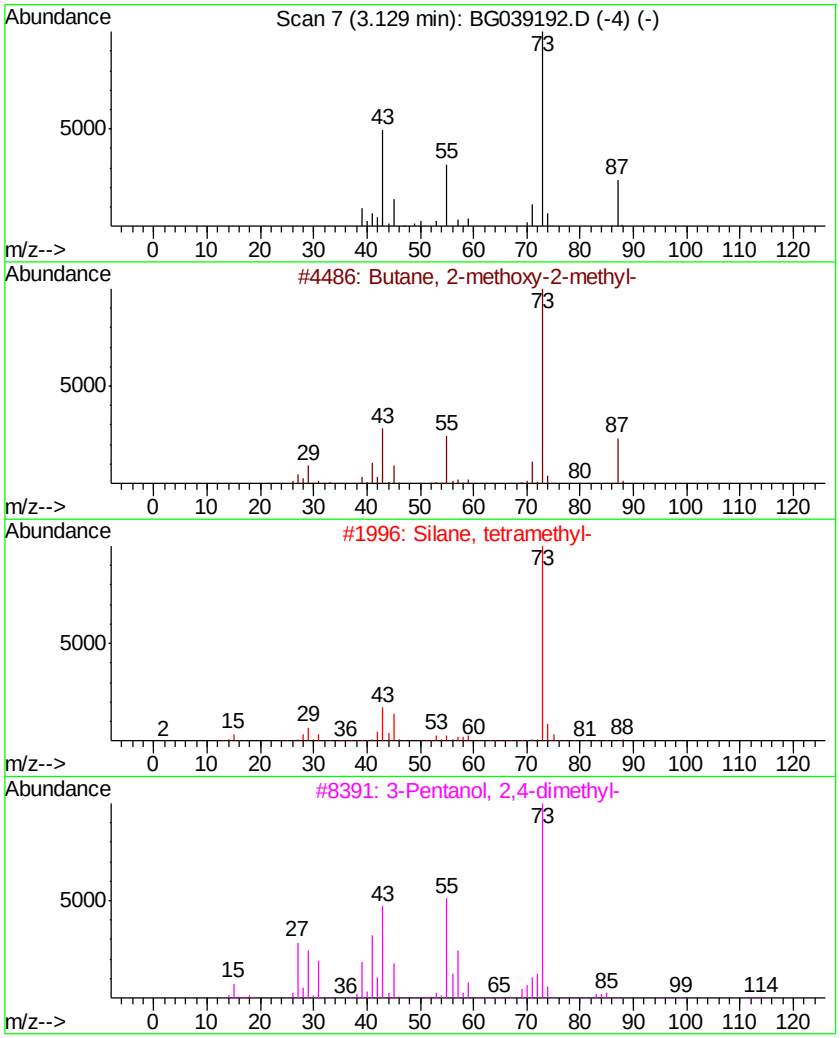
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

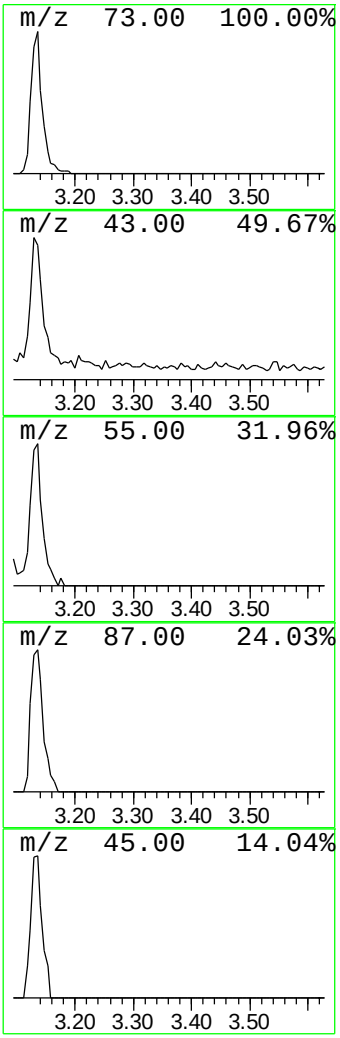
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	6.70 ng	44803	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011719\
Data File : BG039192.D
Acq On : 17 Jan 2019 18:40
Operator : JU/SJ
Sample : K1149-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SW001-190114-01

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

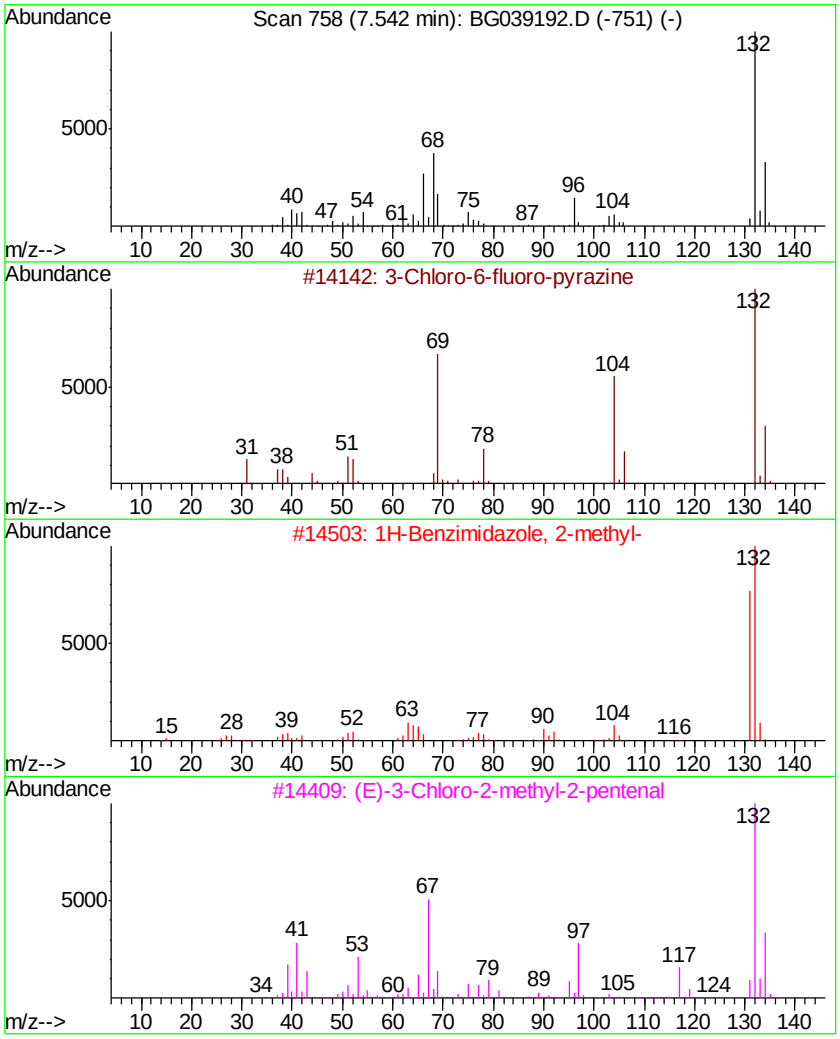
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

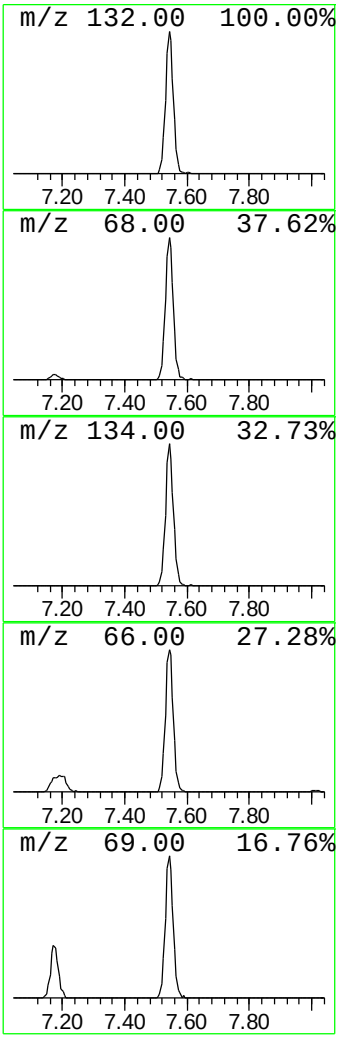
****

Peak Number 2 unknown7.54 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	83.34 ng	557401	1,4-Dichlorobenzene-d4	8.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
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	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011719\
Data File : BG039192.D
Acq On : 17 Jan 2019 18:40
Operator : JU/SJ
Sample : K1149-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SW001-190114-01

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

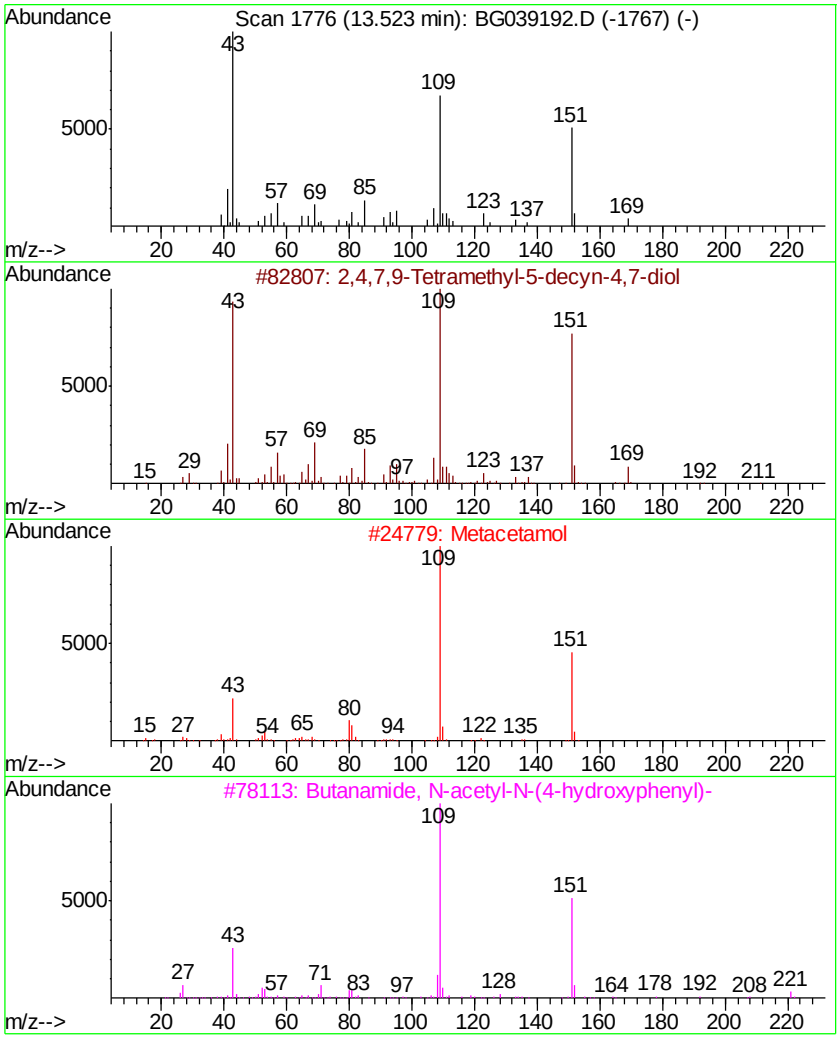
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

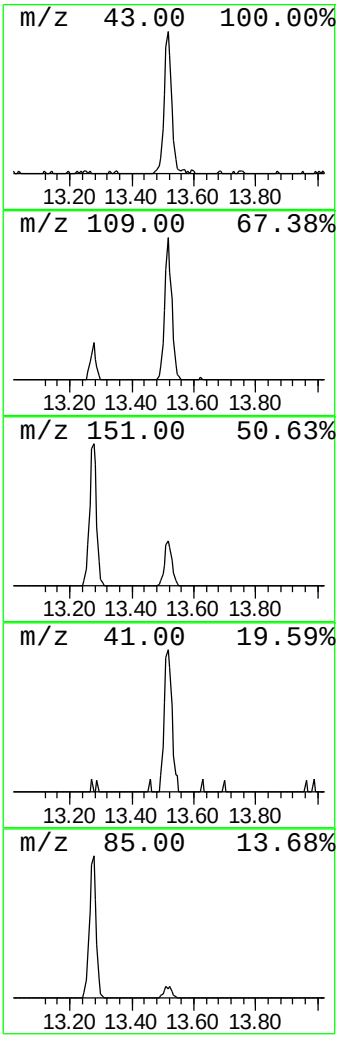
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.52	4.64 ng	71512	Acenaphthene-d10	14.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	64
2	Metacetamol	151	C8H9NO2	000621-42-1	59
3	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	50
4	(-)-10-Camphorsulfonyl chloride	250	C10H15ClO3S	039262-22-1	50
5	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011719\
Data File : BG039192.D
Acq On : 17 Jan 2019 18:40
Operator : JU/SJ
Sample : K1149-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SW001-190114-01

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
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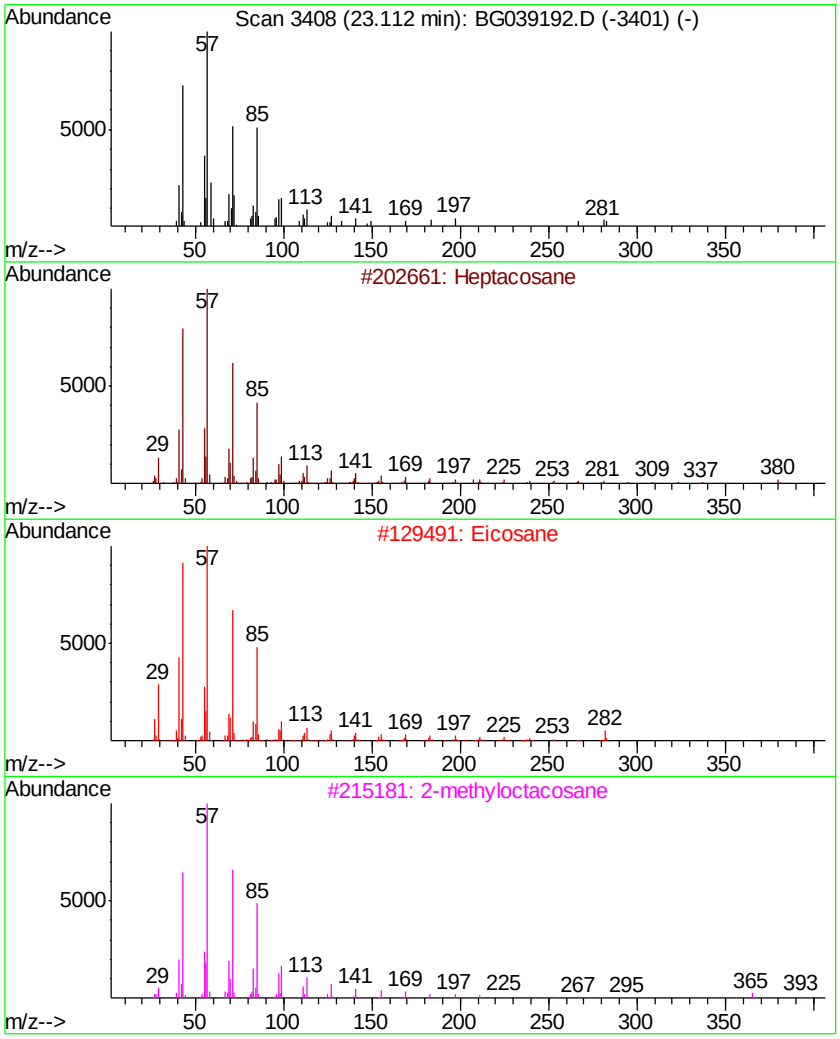
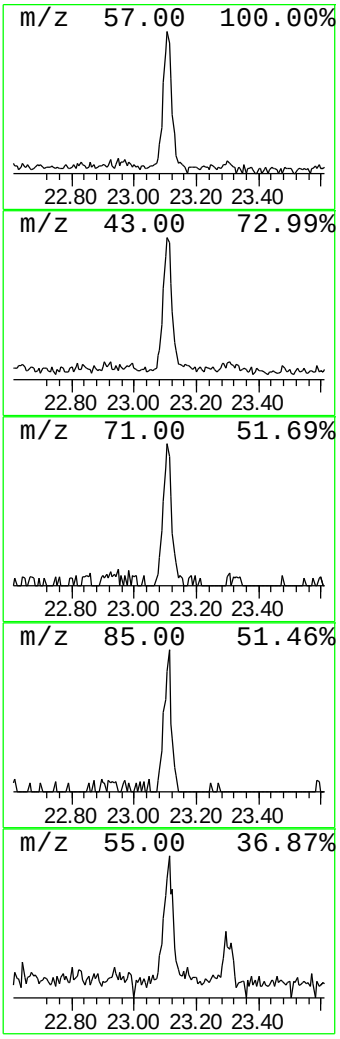
****

Peak Number 5 Heptacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.11	2.11 ng	58595	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	74
2	Eicosane	282	C20H42	000112-95-8	68
3	2-methyloctacosane	408	C29H60	1000376-72-8	68
4	Hexacosane	366	C26H54	000630-01-3	68
5	Heptadecane	240	C17H36	000629-78-7	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011719\
Data File : BG039192.D
Acq On : 17 Jan 2019 18:40
Operator : JU/SJ
Sample : K1149-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SW001-190114-01

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

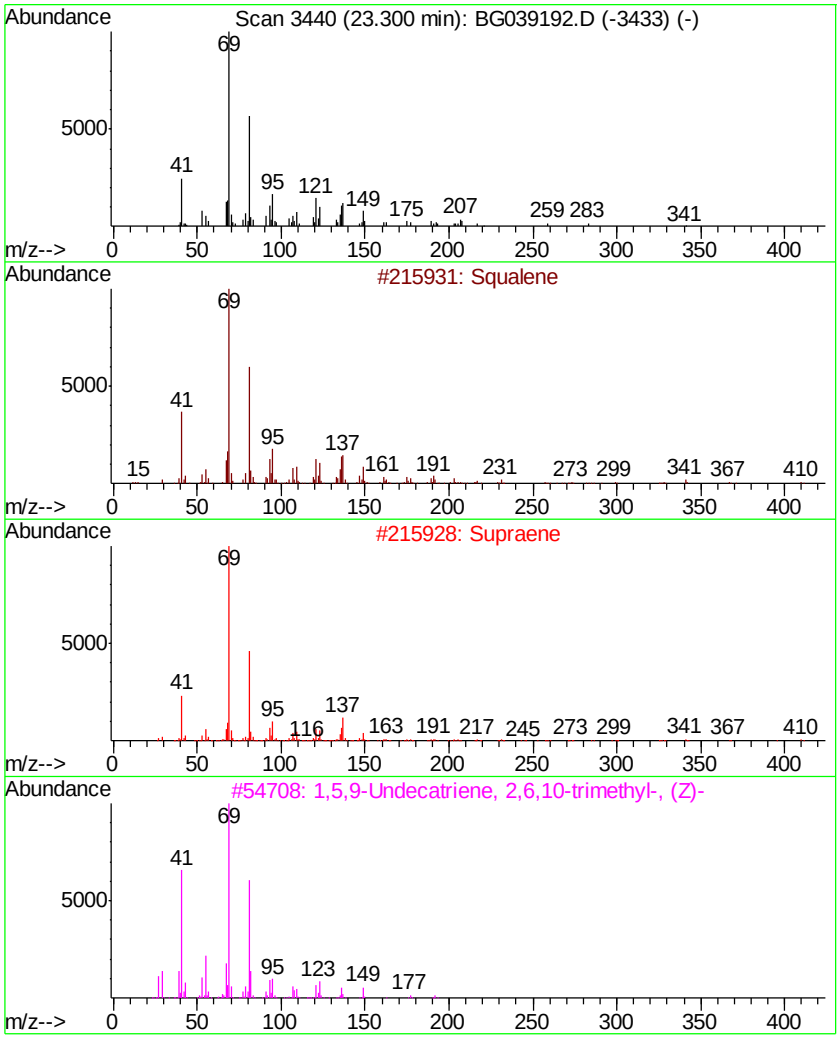
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

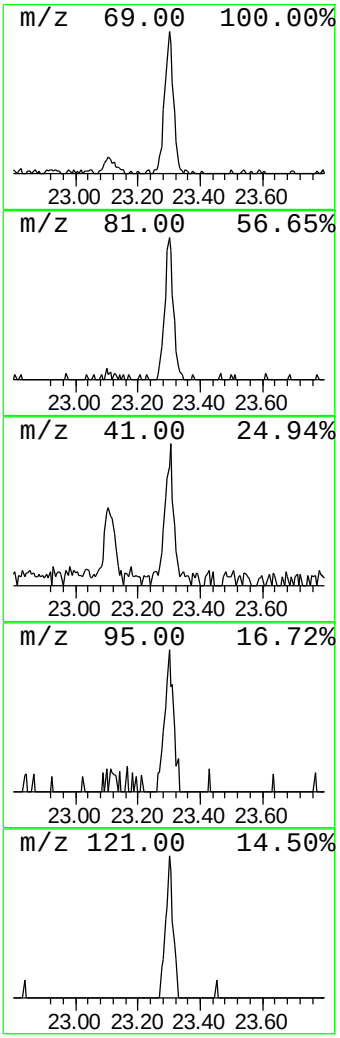
****

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.30	2.44 ng	67692	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	86
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	4-Aza-5-thiatricyclo[5.2.1.0(3,7...	283	C14H21NO3S	1000156-44-2	43





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Sample : K1149-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SW001-190114-01

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

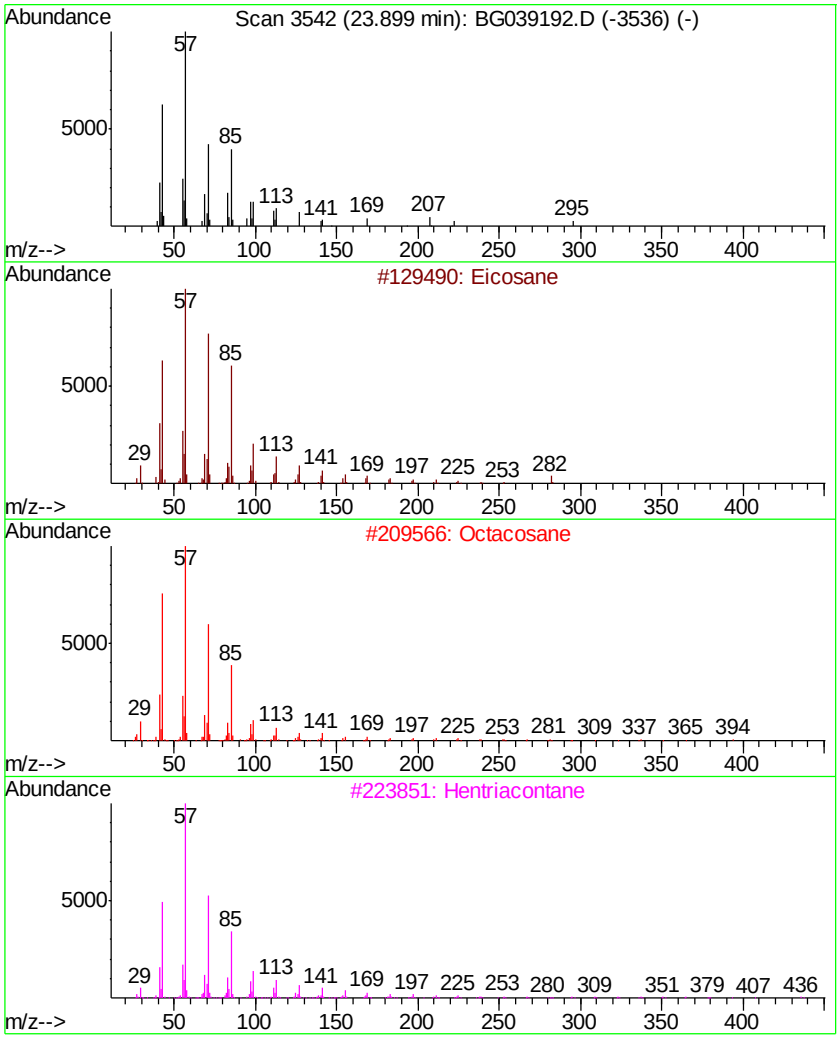
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

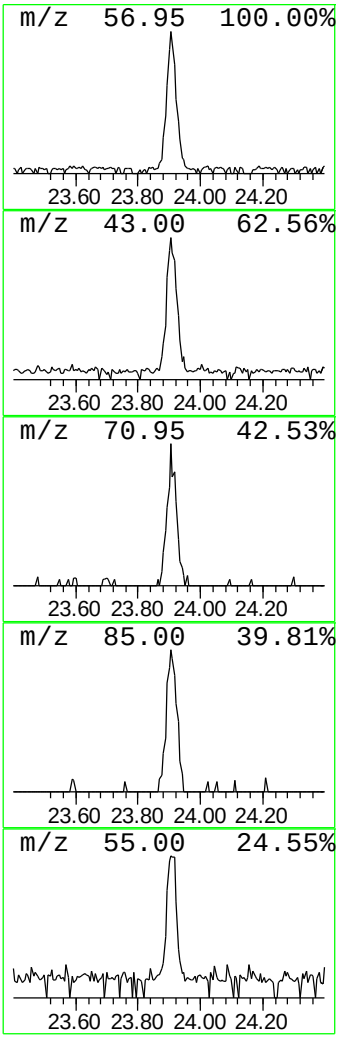
****

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.90	2.40 ng	58069	Perylene-d12	24.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Octacosane	394	C28H58	000630-02-4	90
3	Hentriacontane	437	C31H64	000630-04-6	86
4	Heneicosane	296	C21H44	000629-94-7	83
5	Heptacosane	380	C27H56	000593-49-7	81





Library Search Compound Report

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Misc :
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Instrument : BNA_G
ClientSampleId : SW001-190114-01

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

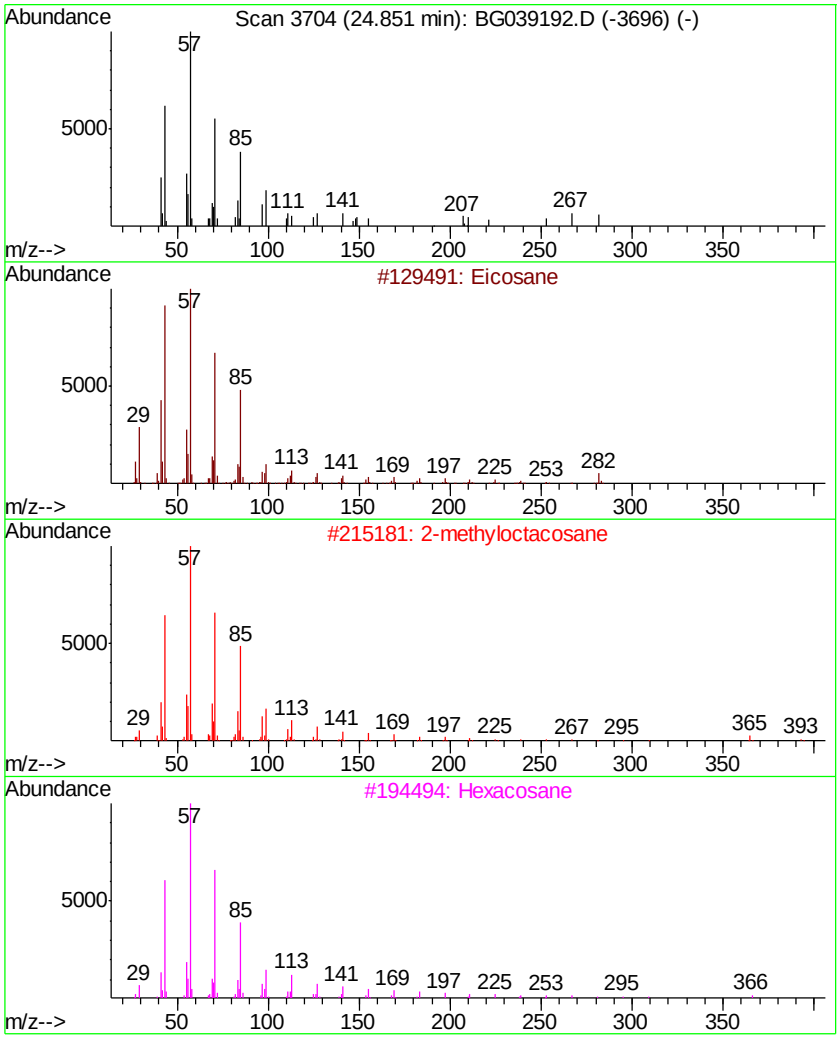
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

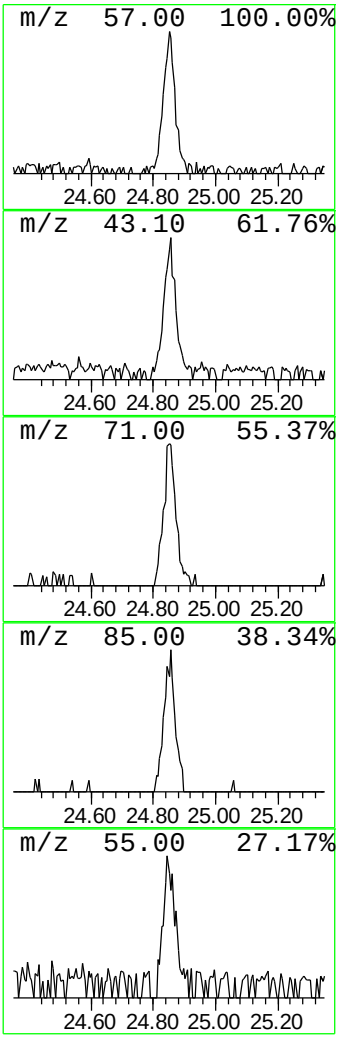
****

Peak Number 8 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.85	2.06 ng	49700	Perylene-d12	24.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	80
3	Hexacosane	366	C26H54	000630-01-3	80
4	Hentriacontane	437	C31H64	000630-04-6	80
5	Octacosane	394	C28H58	000630-02-4	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011719\
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ClientSampleId : SW001-190114-01

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.13	6.7	ng	44803	1	8.01	133762	20.0
unknown7.54	7.54	83.3	ng	557401	1	8.01	133762	20.0
2,4,7,9-Tetrameth...	13.52	4.6	ng	71512	3	14.66	307987	20.0
Heptacosane	23.11	2.1	ng	58595	5	21.68	554753	20.0
Squalene	23.30	2.4	ng	67692	5	21.68	554753	20.0
Eicosane	23.90	2.4	ng	58069	6	24.94	482929	20.0
2-methyloctacosane	24.85	2.1	ng	49700	6	24.94	482929	20.0