LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044029.D
Acq On : 14 Jan 2020 2:14
Operator : JU
Sample : L1103-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-1(4-6)

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-BG123019.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	3.129	3	7	29	rVB	428305	766544	13.28%	2.105%
2	5.050	328	334	347	rBV	320321	536456	9.30%	1.473%
3	5.526	407	415	431	rBV	1490610	2488485	43.12%	6.835%
4	7.113	677	685	700	rBV	1605389	2897068	50.20%	7.957%
5	7.483	740	748	761	rBV	1565857	2791554	48.37%	7.667%
6	7.947	818	827	836	rBV	409541	717582	12.43%	1.971%
7	8.270	872	882	891	rBV	1231999	2174069	37.67%	5.971%
8	9.099	1015	1023	1035	rBV	919407	1695056	29.37%	4.656%
9	10.744	1296	1303	1318	rBV	532603	998686	17.30%	2.743%
10	13.200	1714	1721	1734	rBV	2443385	3954050	68.51%	10.860%
11	14.028	1854	1862	1873	rBV	221070	332831	5.77%	0.914%
12	14.575	1948	1955	1968	rBV	872073	1394912	24.17%	3.831%
13	16.061	2201	2208	2222	rBV	1966459	3078607	53.34%	8.456%
14	17.318	2415	2422	2434	rBV	1081364	1661773	28.79%	4.564%
15	19.939	2861	2868	2877	rBV	3814539	5771201	100.00%	15.851%
16	20.620	2979	2984	2990	rVB2	36841	60487	1.05%	0.166%
17	21.237	3084	3089	3098	rBV	376117	598919	10.38%	1.645%
18	21.572	3139	3146	3158	rBV	1023402	1744288	30.22%	4.791%
19	21.784	3178	3182	3190	rVB2	50564	74836	1.30%	0.206%
20	22.383	3280	3284	3291	rBV3	58086	109618	1.90%	0.301%
21	23.059	3394	3399	3407	rVB	50680	88985	1.54%	0.244%
22	23.241	3424	3430	3442	rVB	92837	217201	3.76%	0.597%
23	23.846	3527	3533	3540	rBV3	47888	104776	1.82%	0.288%
24	24.692	3666	3677	3704	rBV	473555	1944333	33.69%	5.340%
25	25.615	3829	3834	3844	rVB4	37735	110287	1.91%	0.303%
26	25.891	3875	3881	3888	rVB5	36503	96391	1.67%	0.265%

Sum of corrected areas: 36408995

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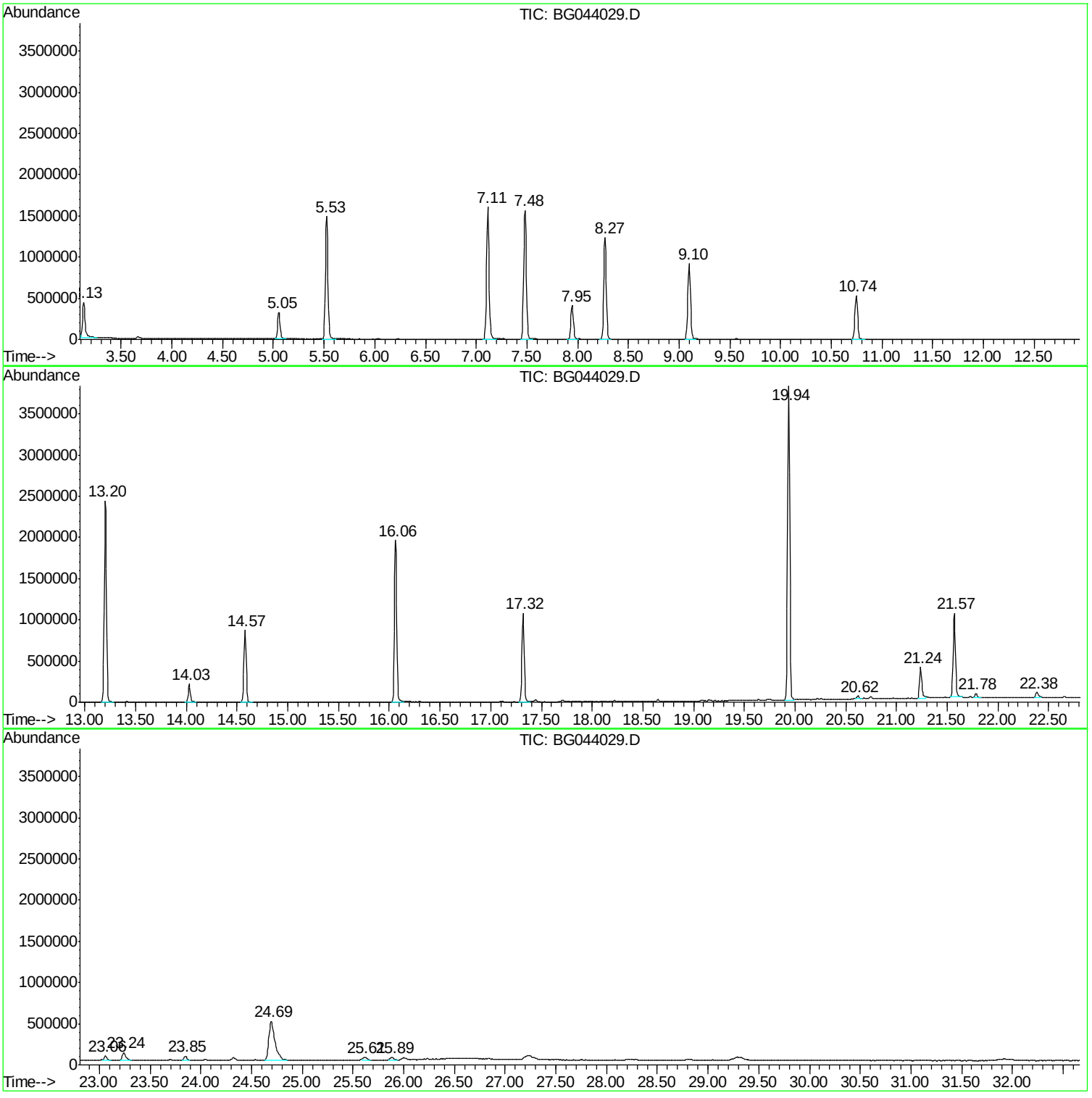
Sample : L1103-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-1(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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\BG011320\
Data File : BG044029.D
Acq On : 14 Jan 2020 2:14
Operator : JU
Sample : L1103-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-1(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

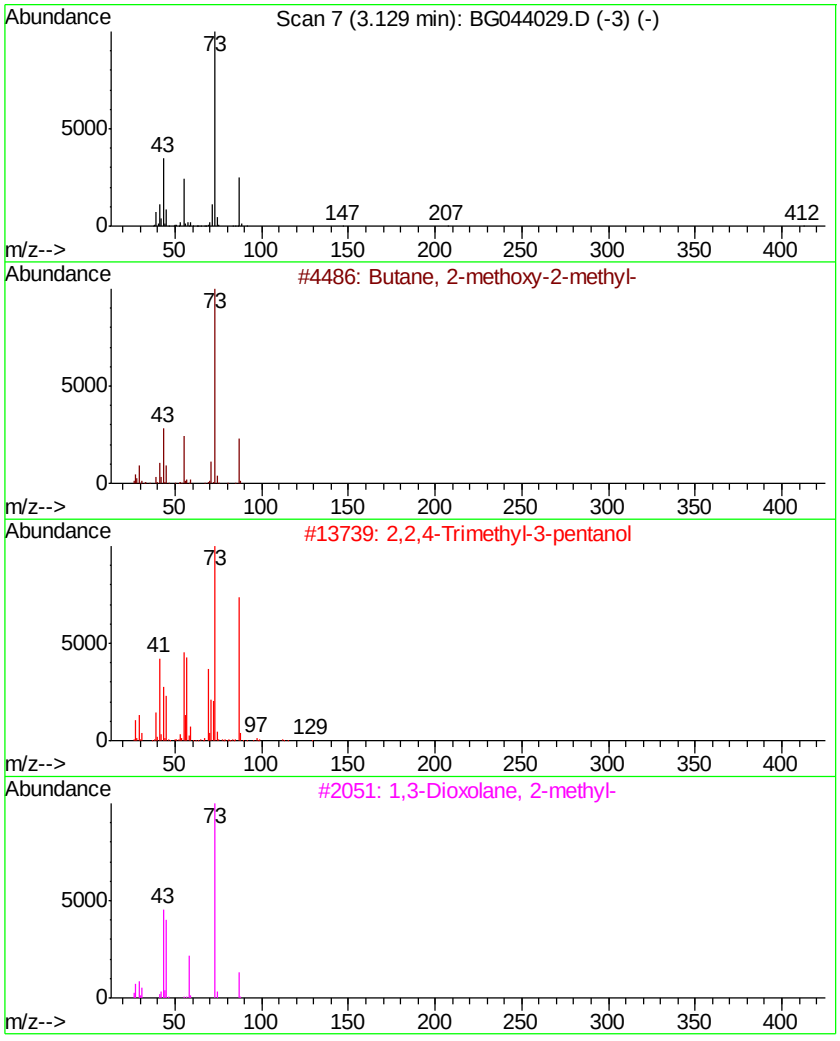
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

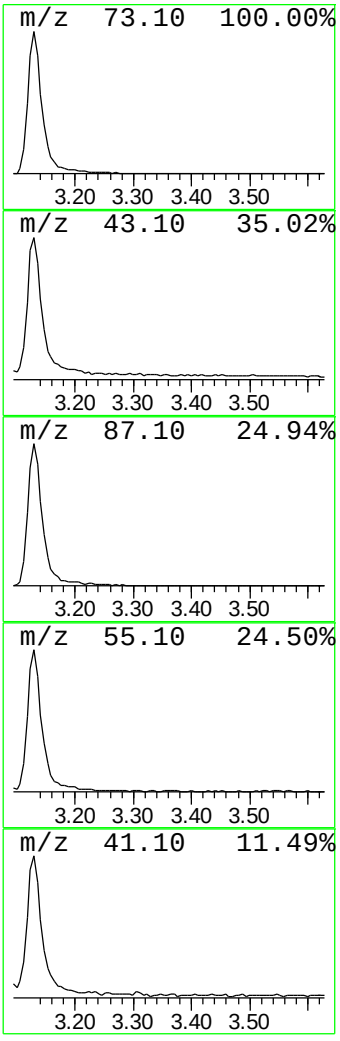
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	21.36 ng	766544	1,4-Dichlorobenzene-d4	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044029.D
Acq On : 14 Jan 2020 2:14
Operator : JU
Sample : L1103-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-1(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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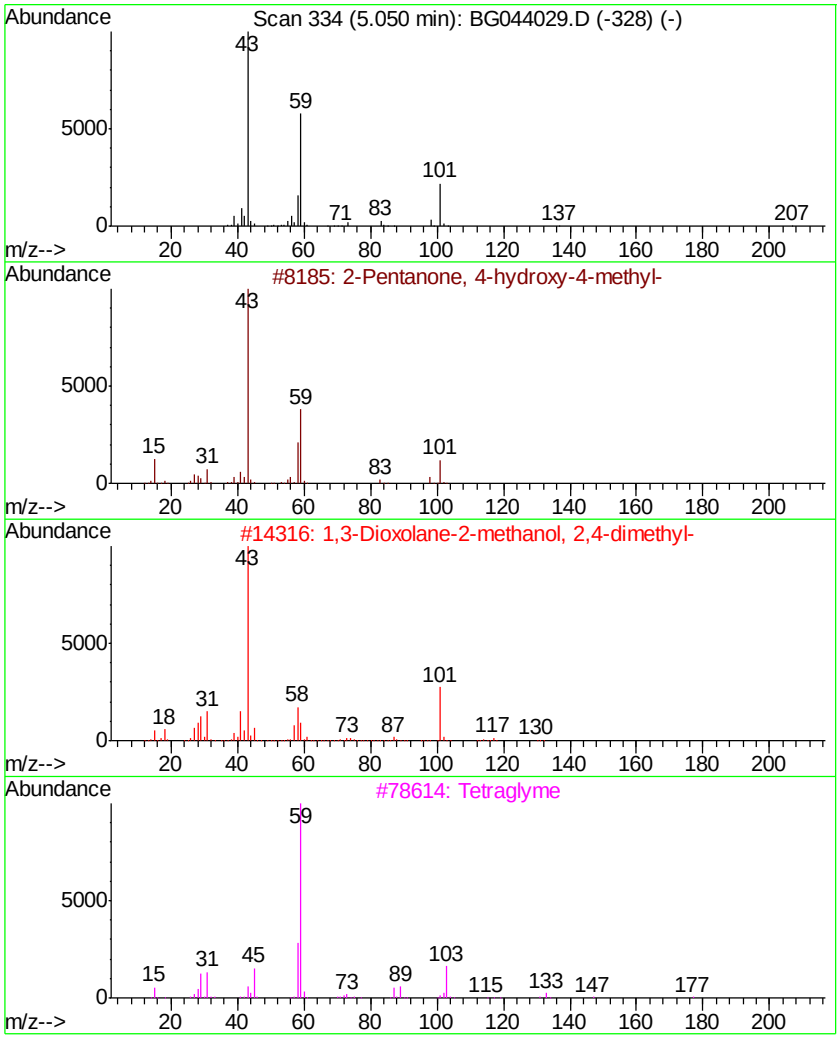
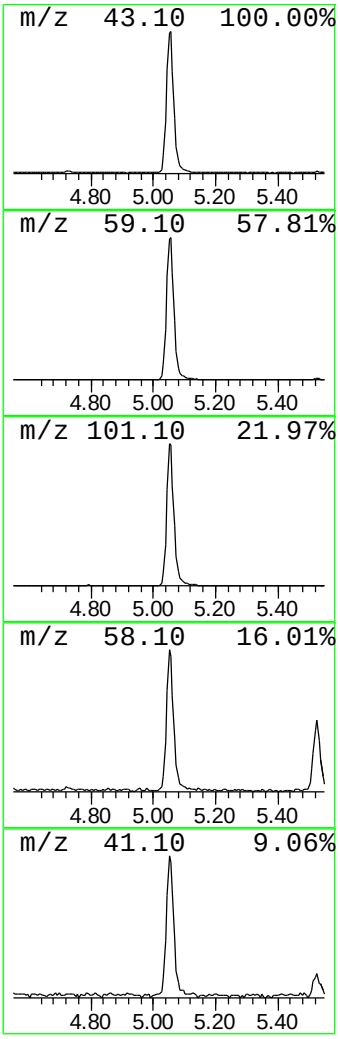
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	14.95 ng	536456	1,4-Dichlorobenzene-d4	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
3	Tetraglyme	222	C10H22O5	000143-24-8	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetone	58	C3H6O	000067-64-1	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044029.D
Acq On : 14 Jan 2020 2:14
Operator : JU
Sample : L1103-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-1(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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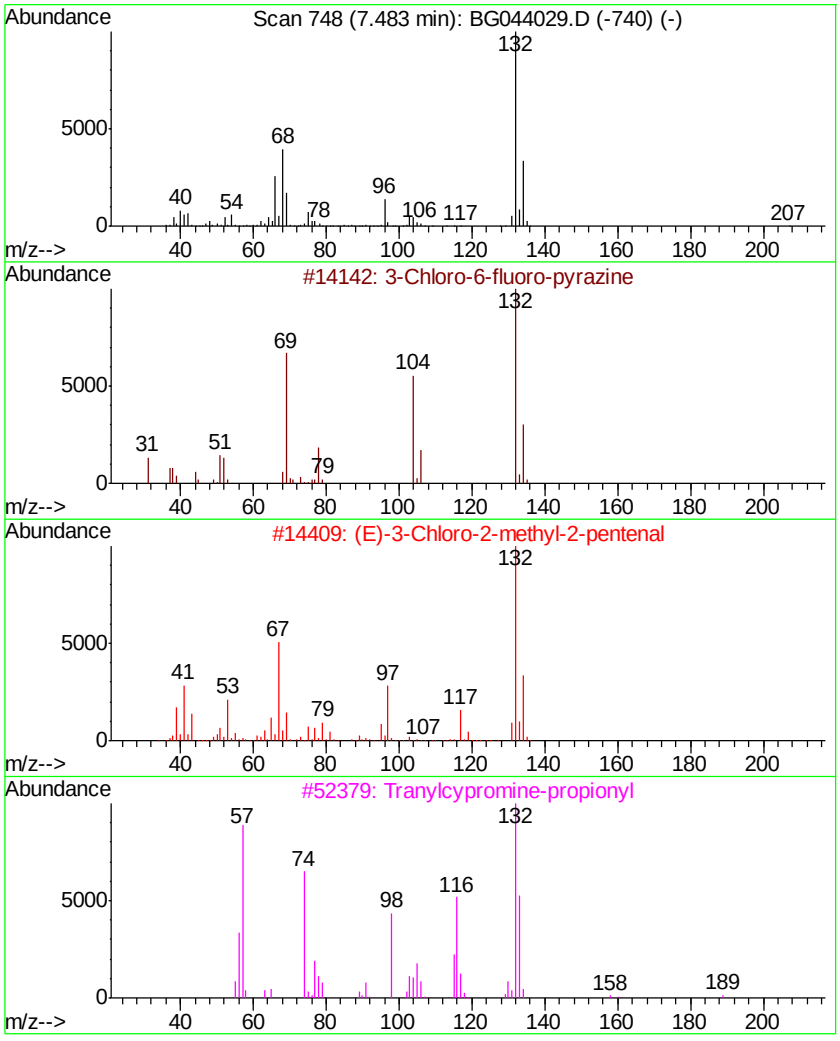
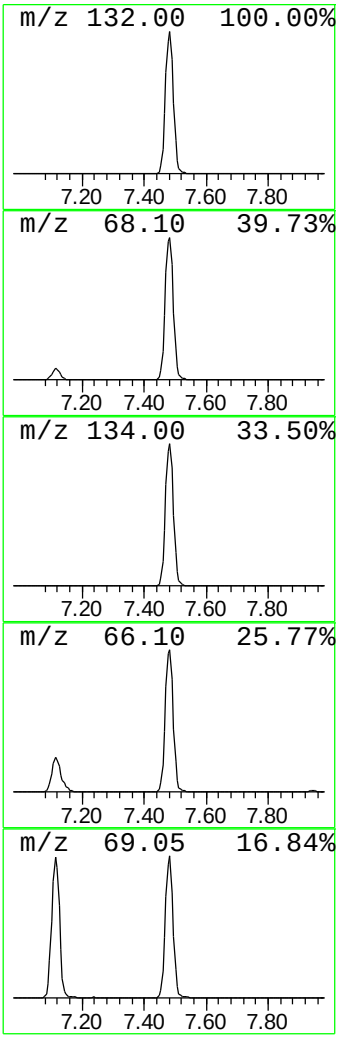
Peak Number 3 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	77.80 ng	2791550	1,4-Dichlorobenzene-d4	7.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044029.D
Acq On : 14 Jan 2020 2:14
Operator : JU
Sample : L1103-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-1(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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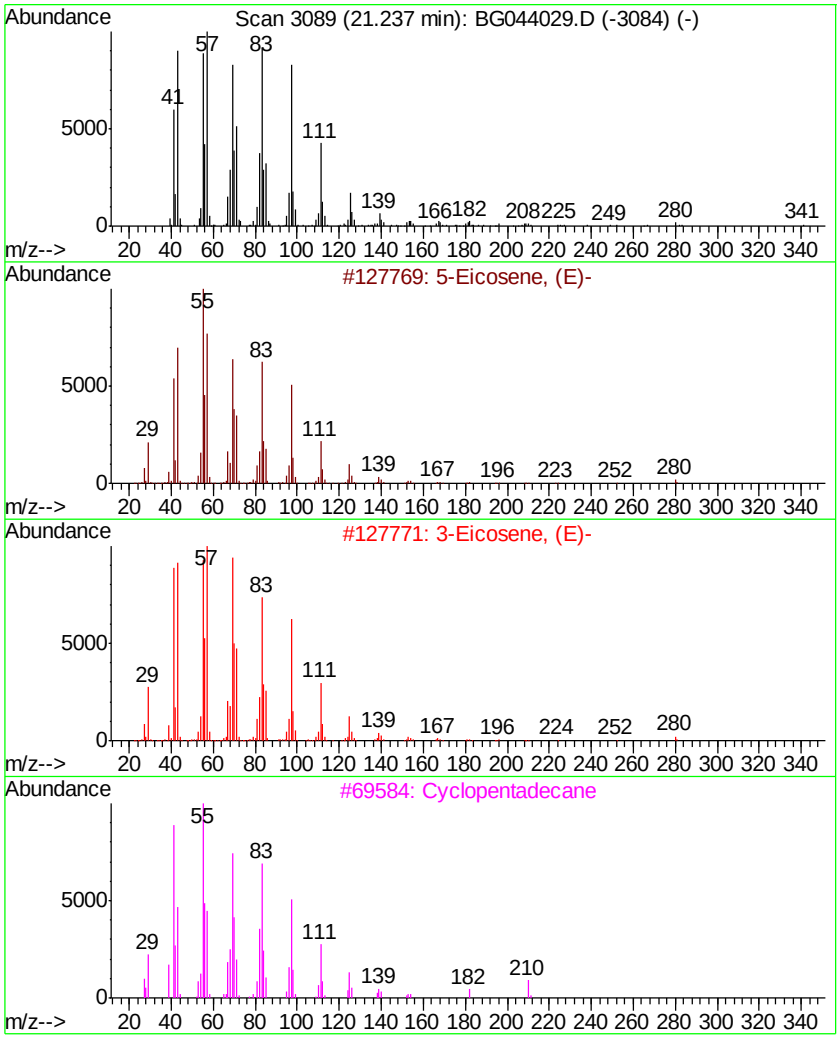
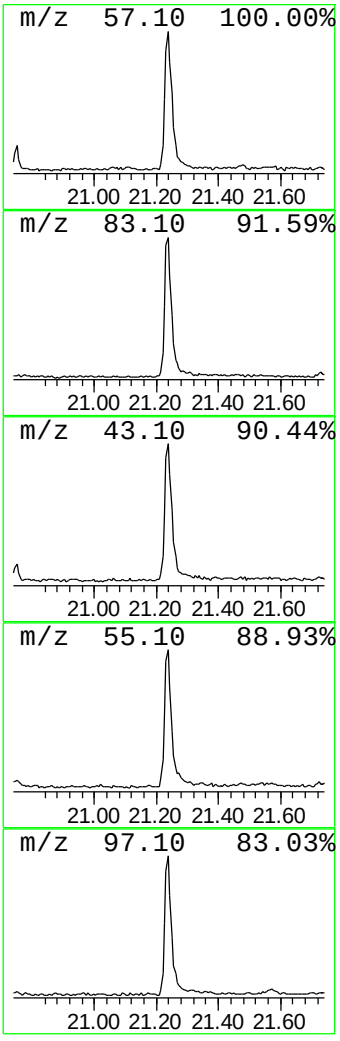
Peak Number 5 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.24	6.87 ng	598919	Chrysene-d12	21.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	96
3	Cyclopentadecane	210	C15H30	000295-48-7	95
4	Cetene	224	C16H32	000629-73-2	95
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	95





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044029.D
Acq On : 14 Jan 2020 2:14
Operator : JU
Sample : L1103-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-1(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

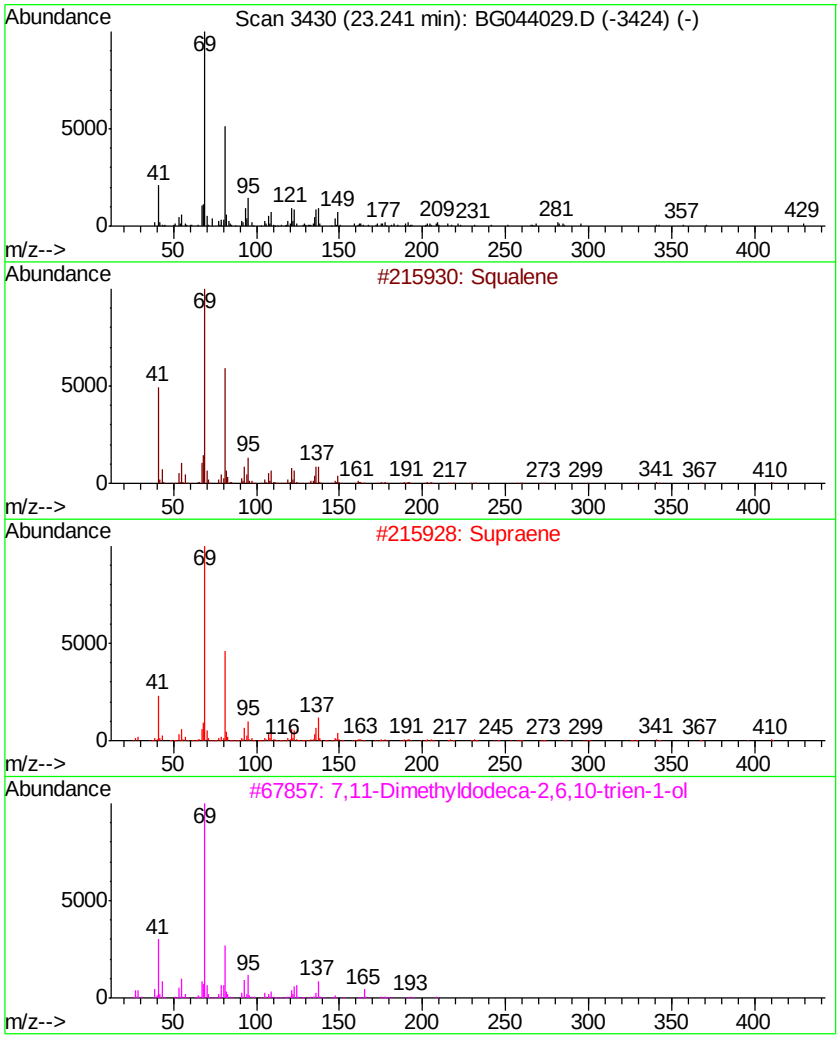
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

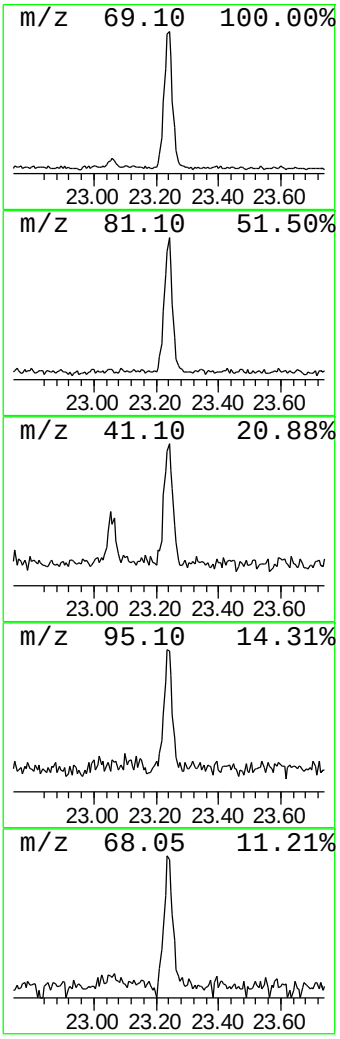
****

Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.24	2.23 ng	217201	Perylene-d12	24.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	83
2	Supraene	410	C30H50	007683-64-9	83
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
5	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011320\
Data File : BG044029.D
Acq On : 14 Jan 2020 2:14
Operator : JU
Sample : L1103-10
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-1(4-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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	21.4	ng	766544	1	7.95	717582	20.0
2-Pentanone, 4-hy...	5.05	14.9	ng	536456	1	7.95	717582	20.0
unknown7.48	7.48	77.8	ng	2791550	1	7.95	717582	20.0
5-Eicosene, (E)-	21.24	6.9	ng	598919	5	21.57	1744290	20.0
Squalene	23.24	2.2	ng	217201	6	24.69	1944330	20.0