LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044030.D
Acq On : 14 Jan 2020 2:53
Operator : JU
Sample : L1103-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(3-5)

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-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	18	rVB	432818	727490	14.40%	2.160%
2	5.056	328	335	349	rVB	321752	535820	10.60%	1.591%
3	5.527	407	415	430	rBV	1475342	2439463	48.27%	7.242%
4	7.113	675	685	703	rBV	1533399	2772625	54.86%	8.231%
5	7.483	739	748	761	rBV	1501642	2689802	53.23%	7.985%
6	7.947	818	827	836	rBV	371635	658706	13.03%	1.956%
7	8.270	874	882	891	rBV	1168210	2058776	40.74%	6.112%
8	9.099	1015	1023	1034	rBV	877248	1601145	31.68%	4.753%
9	10.750	1292	1304	1316	rBV	482293	903408	17.88%	2.682%
10	13.200	1713	1721	1735	rBV	2156400	3541520	70.08%	10.514%
11	14.028	1856	1862	1874	rBV	182220	283798	5.62%	0.843%
12	14.575	1947	1955	1970	rVB	754643	1234662	24.43%	3.665%
13	16.061	2200	2208	2224	rBV	1800900	2799379	55.39%	8.311%
14	17.319	2415	2422	2432	rBV	958841	1454884	28.79%	4.319%
15	17.712	2483	2489	2501	rBV	29582	56786	1.12%	0.169%
16	19.933	2861	2867	2880	rBV	3711176	5053636	100.00%	15.003%
17	21.232	3083	3088	3102	rBV	328848	568724	11.25%	1.688%
18	21.567	3138	3145	3156	rBV	971789	1580009	31.26%	4.691%
19	22.377	3279	3283	3289	rVB3	49430	84124	1.66%	0.250%
20	23.047	3392	3397	3406	rBV2	58057	107044	2.12%	0.318%
21	23.229	3422	3428	3437	rVB	166401	312819	6.19%	0.929%
22	23.834	3525	3531	3537	rVB	66365	126097	2.50%	0.374%
23	24.681	3665	3675	3684	rBV3	555031	1611134	31.88%	4.783%
24	24.751	3685	3687	3695	rVB2	75134	130201	2.58%	0.387%
25	25.844	3868	3873	3885	rVB4	61678	161572	3.20%	0.480%
26	25.967	3887	3894	3904	rVB4	20928	69688	1.38%	0.207%
27	27.160	4092	4097	4109	rVB4	43037	121156	2.40%	0.360%

Sum of corrected areas: 33684468

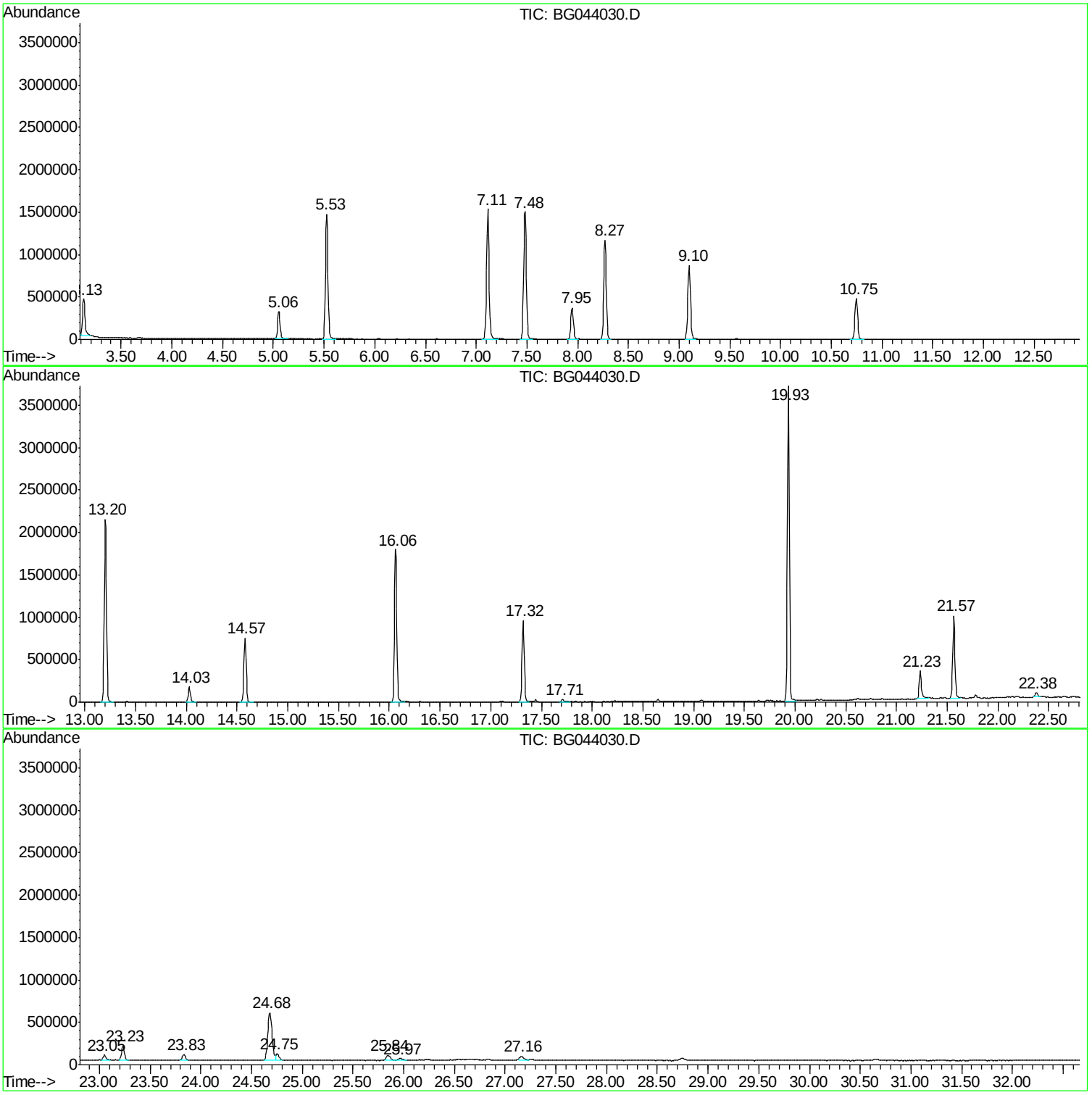
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044030.D
Acq On : 14 Jan 2020 2:53
Operator : JU
Sample : L1103-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(3-5)

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 : BG044030.D
Acq On : 14 Jan 2020 2:53
Operator : JU
Sample : L1103-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(3-5)

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

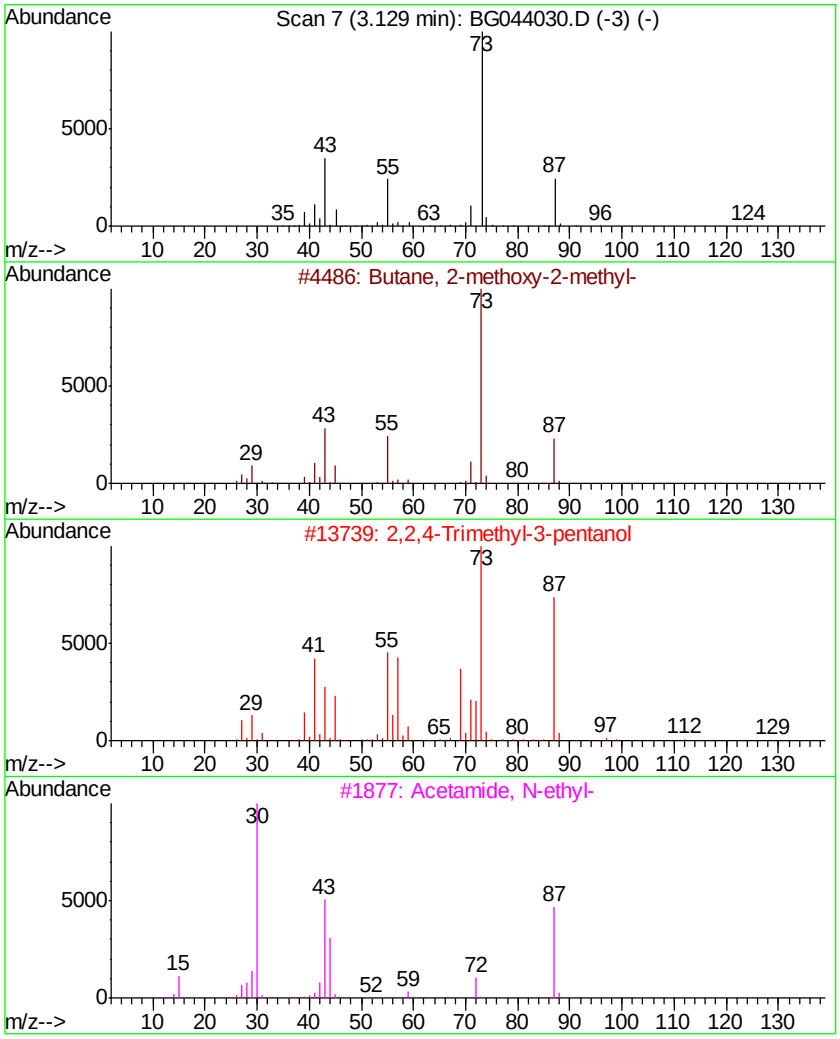
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

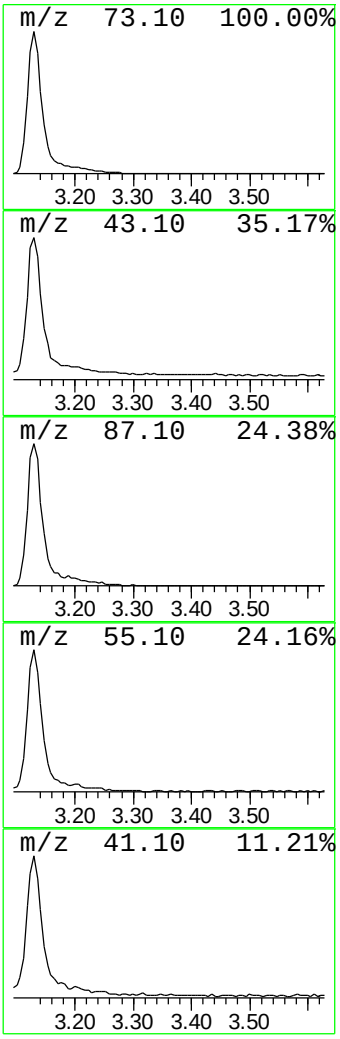
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	22.09 ng	727490	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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044030.D
Acq On : 14 Jan 2020 2:53
Operator : JU
Sample : L1103-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(3-5)

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

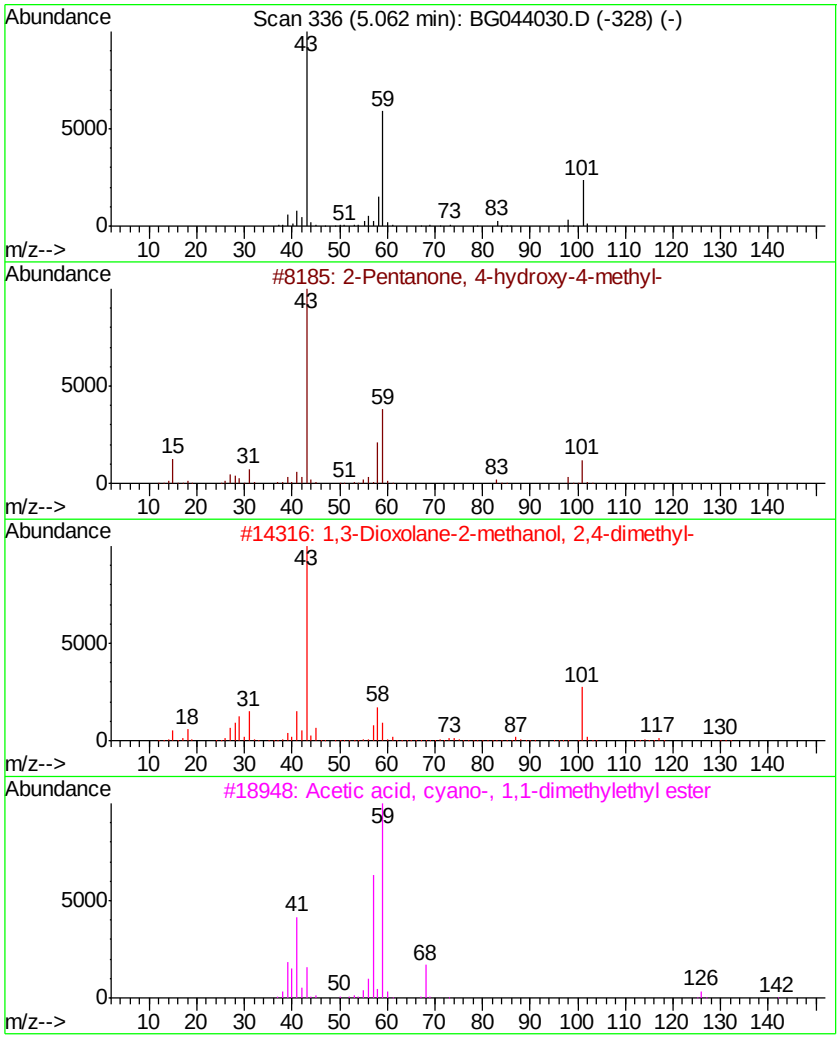
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

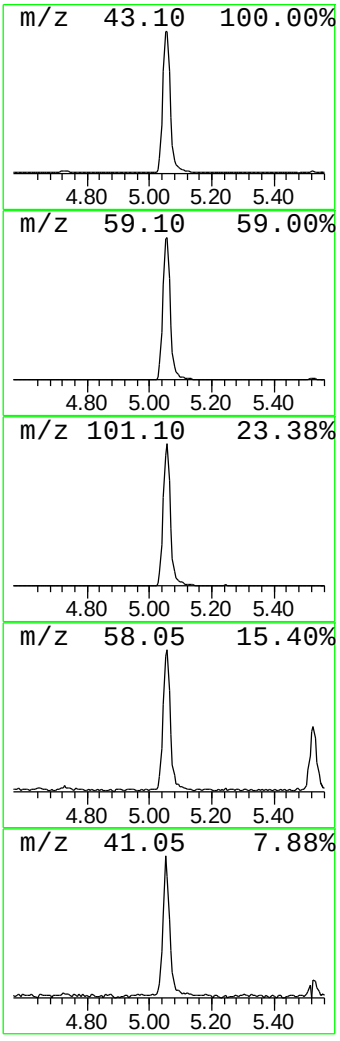
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	16.27 ng	535820	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	50
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044030.D
Acq On : 14 Jan 2020 2:53
Operator : JU
Sample : L1103-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(3-5)

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

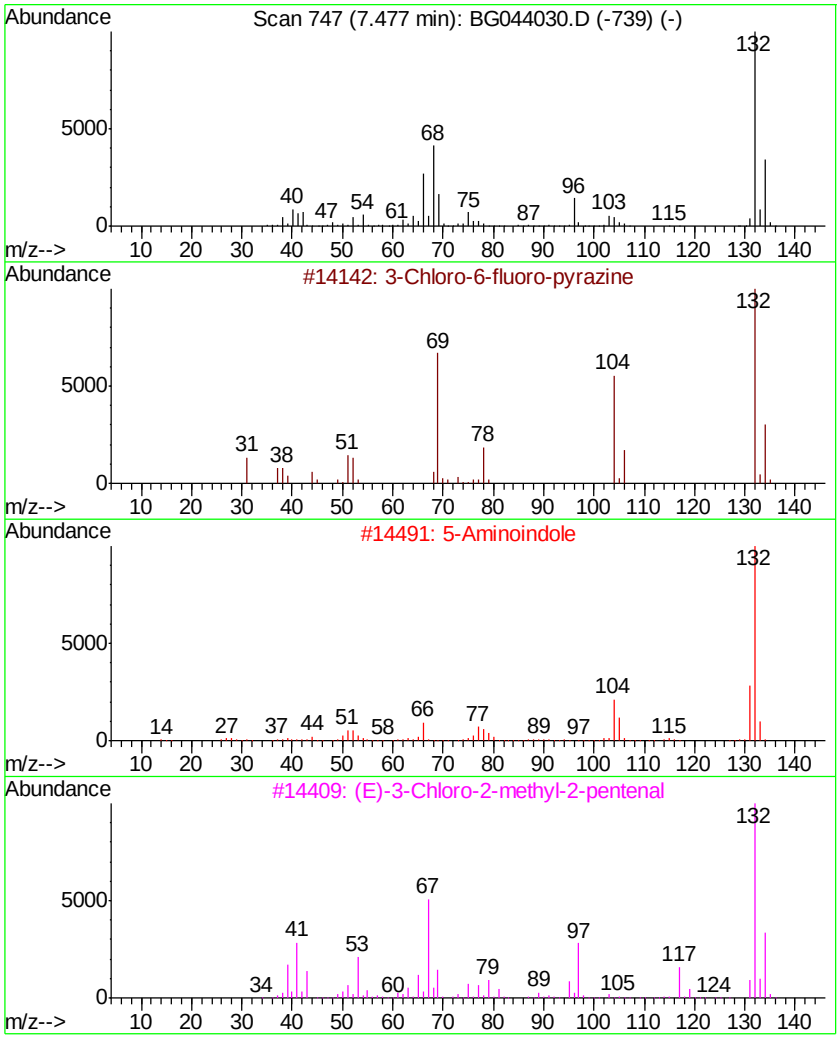
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

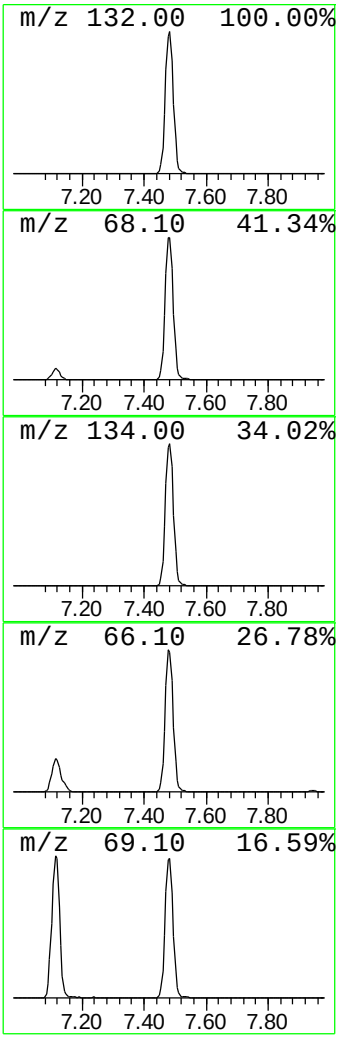
****

Peak Number 3 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	81.67 ng	2689800	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	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044030.D
Acq On : 14 Jan 2020 2:53
Operator : JU
Sample : L1103-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(3-5)

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

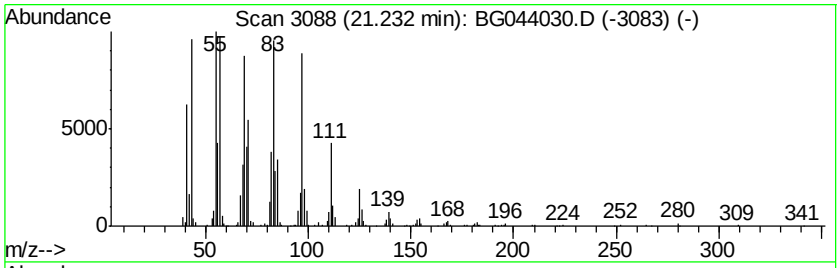
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

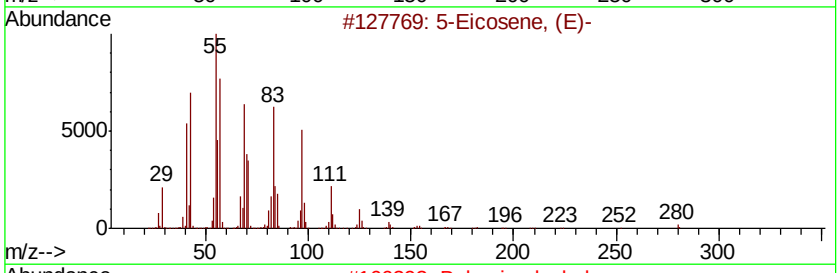
****

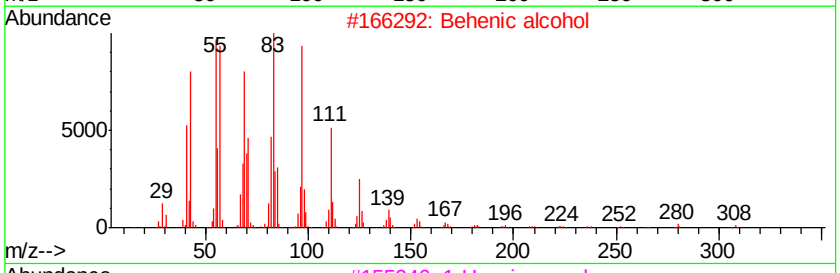
Peak Number 5 5-Eicosene, (E)- Concentration Rank 5

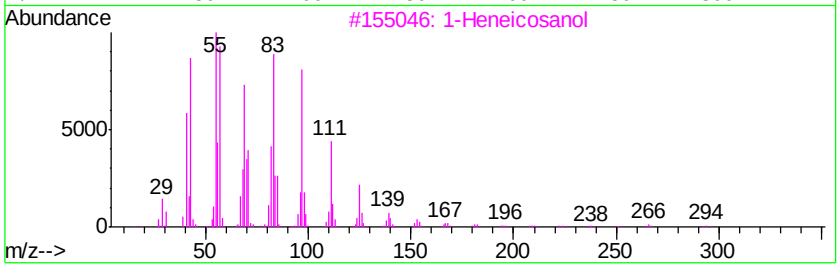
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.23	7.20 ng	568724	Chrysene-d12	21.57

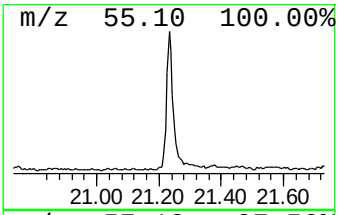
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	1-Heptacosanol	396	C27H56O	002004-39-9	94

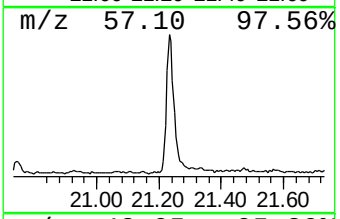


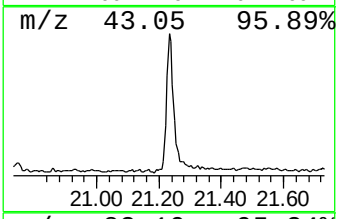


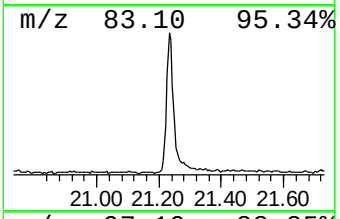


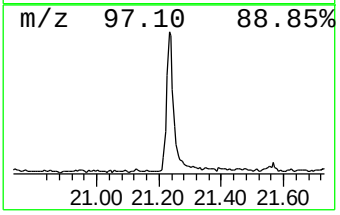












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044030.D
Acq On : 14 Jan 2020 2:53
Operator : JU
Sample : L1103-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(3-5)

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

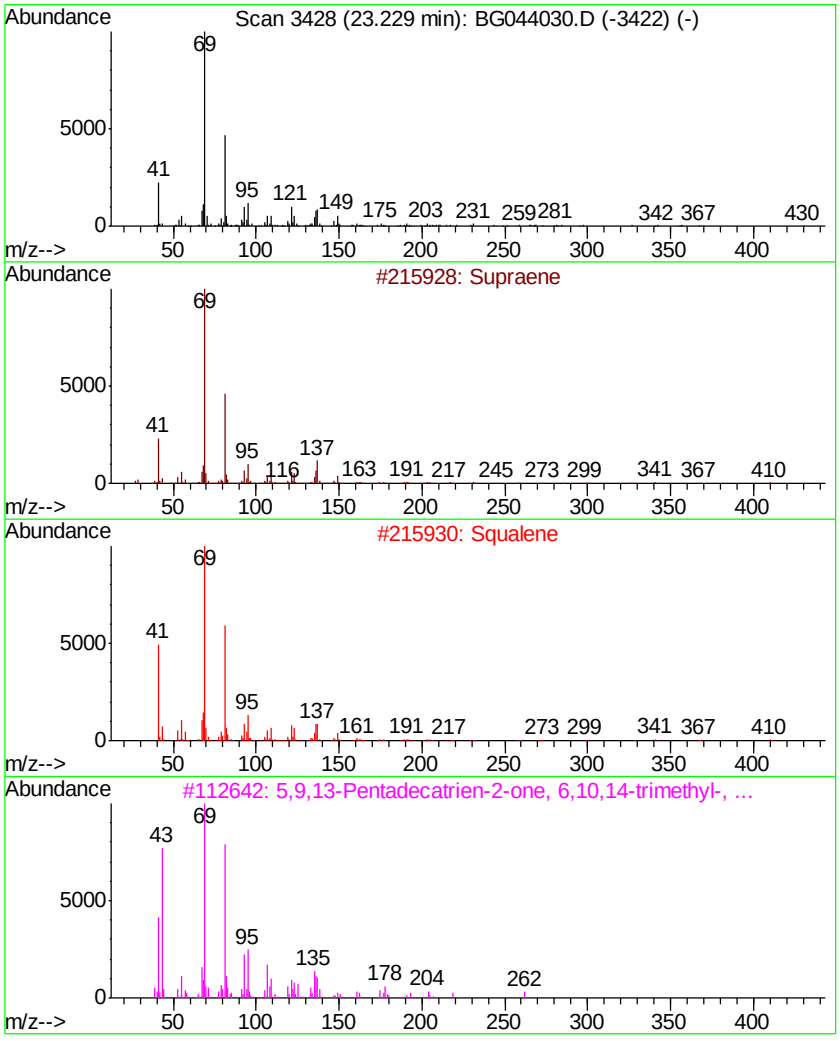
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

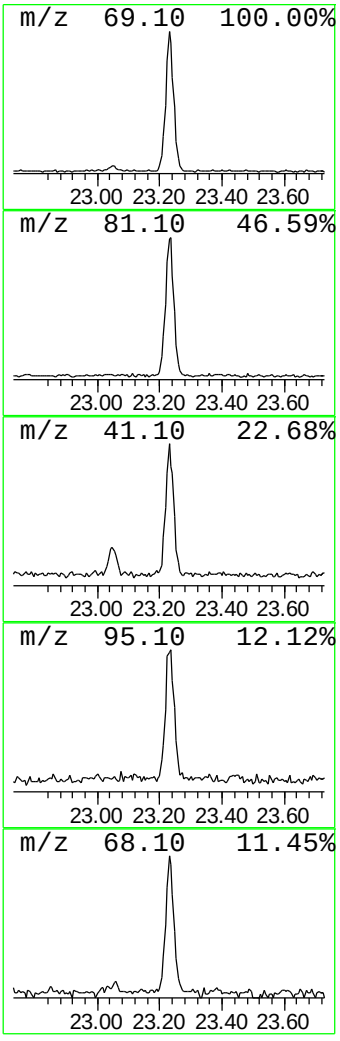
****

Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.23	3.88 ng	312819	Perylene-d12	24.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	72
4	trans-Farnesol	222	C15H26O	000106-28-5	72
5	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
Data File : BG044030.D
Acq On : 14 Jan 2020 2:53
Operator : JU
Sample : L1103-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(3-5)

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

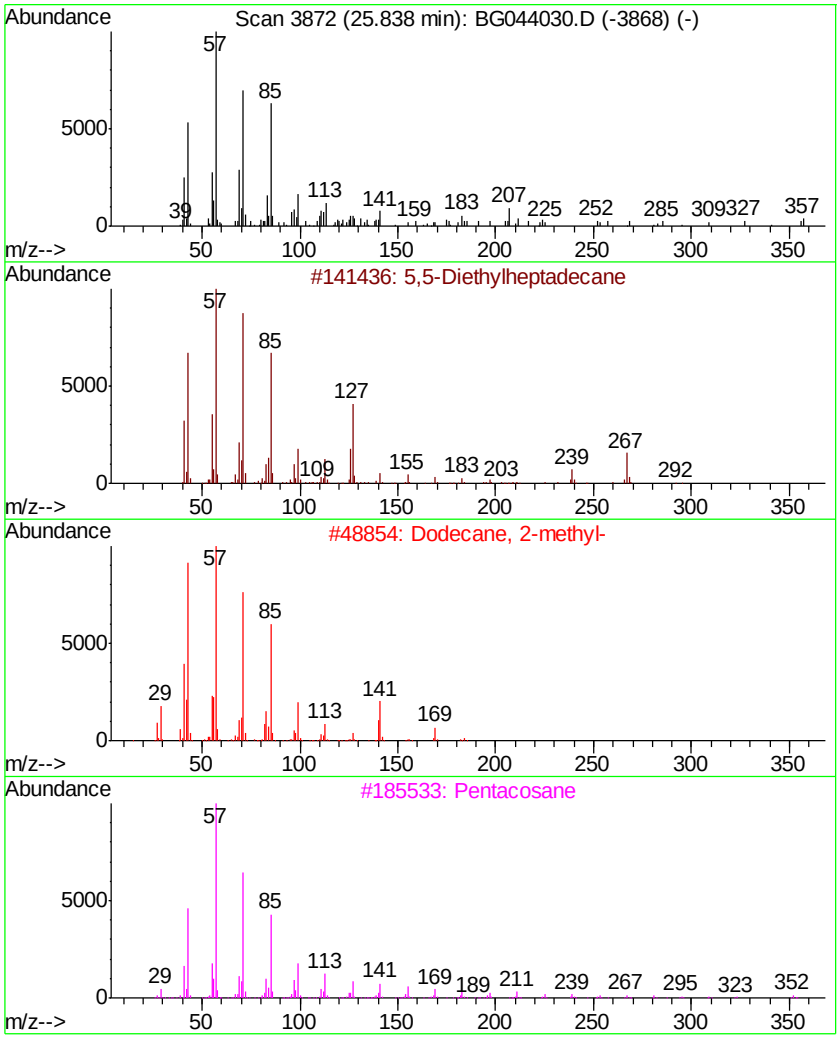
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

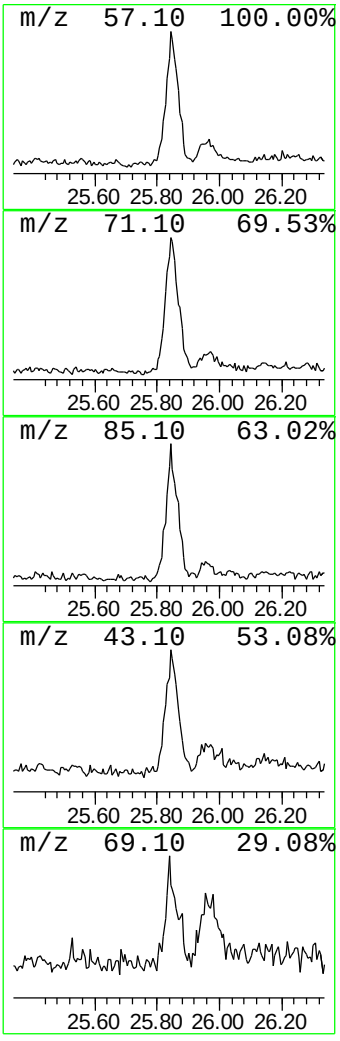
****

Peak Number 7 5,5-Diethylheptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.84	2.01 ng	161572	Perylene-d12	24.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,5-Diethylheptadecane	296	C21H44	1000360-41-7	90
2	Dodecane, 2-methyl-	184	C13H28	001560-97-0	87
3	Pentacosane	352	C25H52	000629-99-2	86
4	Tetratetracontane	619	C44H90	007098-22-8	68
5	Decane, 1-iodo-	268	C10H21I	002050-77-3	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011320\
Data File : BG044030.D
Acq On : 14 Jan 2020 2:53
Operator : JU
Sample : L1103-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-18(3-5)

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	22.1	ng	727490	1	7.95	658706	20.0
2-Pentanone, 4-hy...	5.06	16.3	ng	535820	1	7.95	658706	20.0
unknown7.48	7.48	81.7	ng	2689800	1	7.95	658706	20.0
5-Eicosene, (E)-	21.23	7.2	ng	568724	5	21.57	1580010	20.0
Supraene	23.23	3.9	ng	312819	6	24.68	1611130	20.0
5,5-Diethylheptad...	25.84	2.0	ng	161572	6	24.68	1611130	20.0