LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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	31	rVB	311242	656469	14.25%	2.158%
2	5.050	328	334	345	rBV	273144	445414	9.67%	1.464%
3	5.520	406	414	429	rBV	1164443	1977336	42.92%	6.500%
4	7.113	677	685	701	rBV	1230221	2252739	48.89%	7.405%
5	7.477	739	747	759	rBV	1243107	2198263	47.71%	7.226%
6	7.941	818	826	836	rBV	363962	625339	13.57%	2.056%
7	8.264	873	881	890	rBV	954152	1678020	36.42%	5.516%
8	9.093	1015	1022	1035	rBV	715484	1316704	28.58%	4.328%
9	10.744	1294	1303	1315	rBV	454270	861876	18.71%	2.833%
10	13.200	1712	1721	1736	rBV	1811265	2979956	64.68%	9.796%
11	14.022	1856	1861	1873	rBV	90190	154322	3.35%	0.507%
12	14.575	1948	1955	1966	rBV	725117	1166203	25.31%	3.834%
13	16.061	2200	2208	2223	rBV	1533451	2387984	51.83%	7.850%
14	17.318	2415	2422	2432	rBV	918040	1402744	30.44%	4.611%
15	19.933	2860	2867	2879	rBV	3463911	4607549	100.00%	15.146%
16	21.231	3083	3088	3097	rBV	386921	664153	14.41%	2.183%
17	21.466	3124	3128	3134	rVB	53815	76770	1.67%	0.252%
18	21.566	3137	3145	3154	rBV	963501	1690333	36.69%	5.556%
19	21.778	3176	3181	3188	rVB	69268	95240	2.07%	0.313%
20	22.371	3277	3282	3292	rBV2	140052	264677	5.74%	0.870%
21	22.642	3323	3328	3336	rBV	39725	78039	1.69%	0.257%
22	23.041	3391	3396	3403	rVB	112590	199191	4.32%	0.655%
23	23.229	3421	3428	3436	rBV3	166674	335808	7.29%	1.104%
24	23.817	3523	3528	3535	rBV2	93346	211192	4.58%	0.694%
25	23.887	3536	3540	3553	rVB5	41641	105354	2.29%	0.346%
26	24.263	3600	3604	3614	rVB3	44828	107670	2.34%	0.354%
27	24.674	3664	3674	3682	rBV2	597328	1699526	36.89%	5.587%
28	25.832	3865	3871	3881	rVB4	64812	182341	3.96%	0.599%

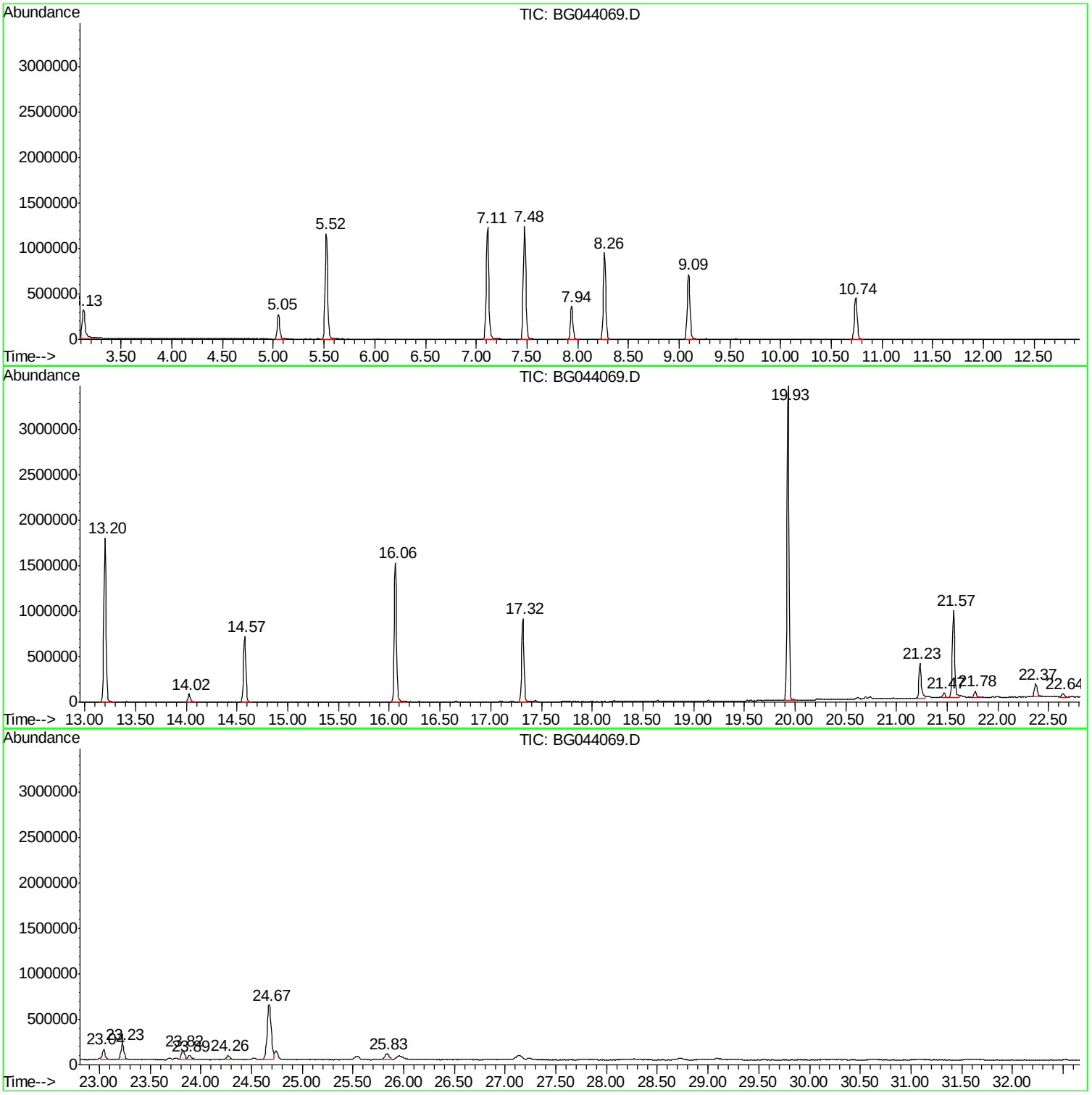
Sum of corrected areas: 30421212

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FESB-33-(3.5-4)

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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Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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

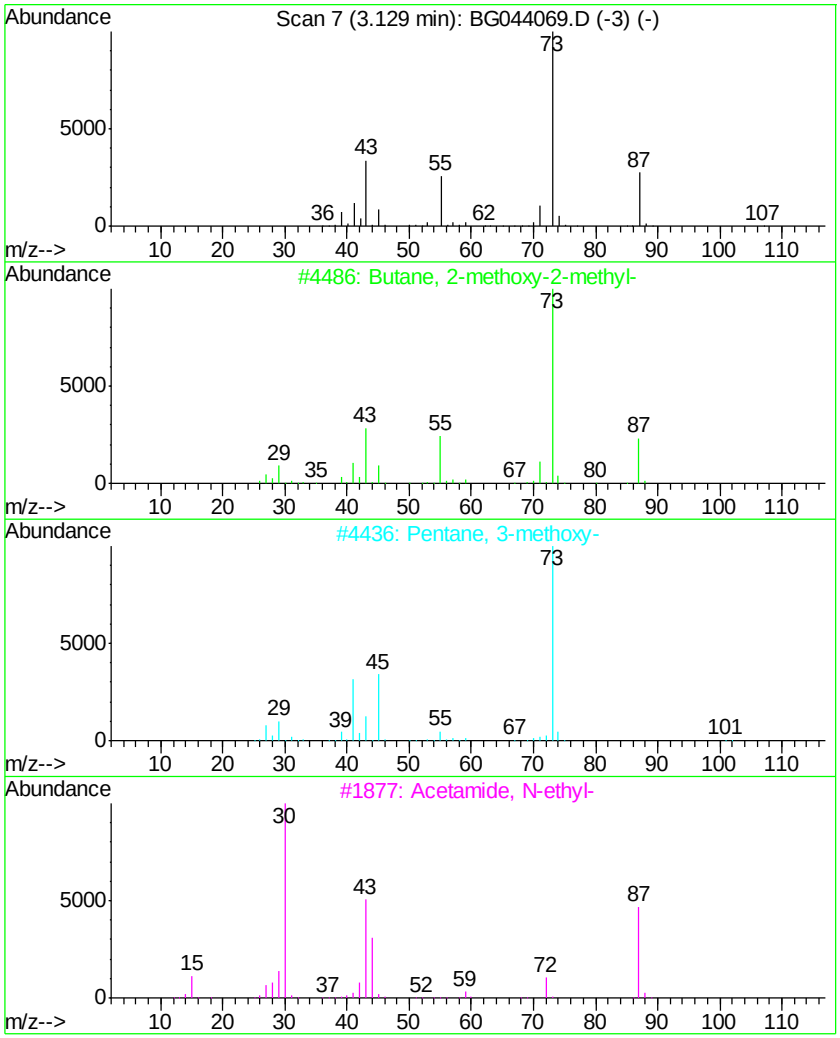
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

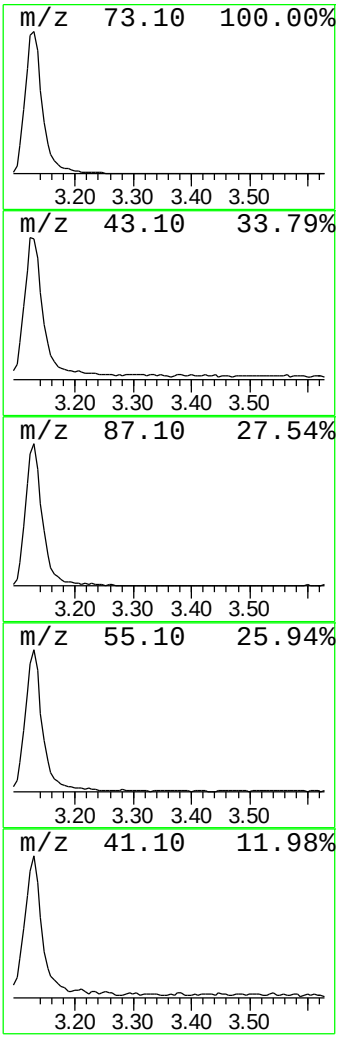
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	21.00 ng	656469	1,4-Dichlorobenzene-d4	7.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	1-Propene-1-thiol	74	C3H6S	000925-89-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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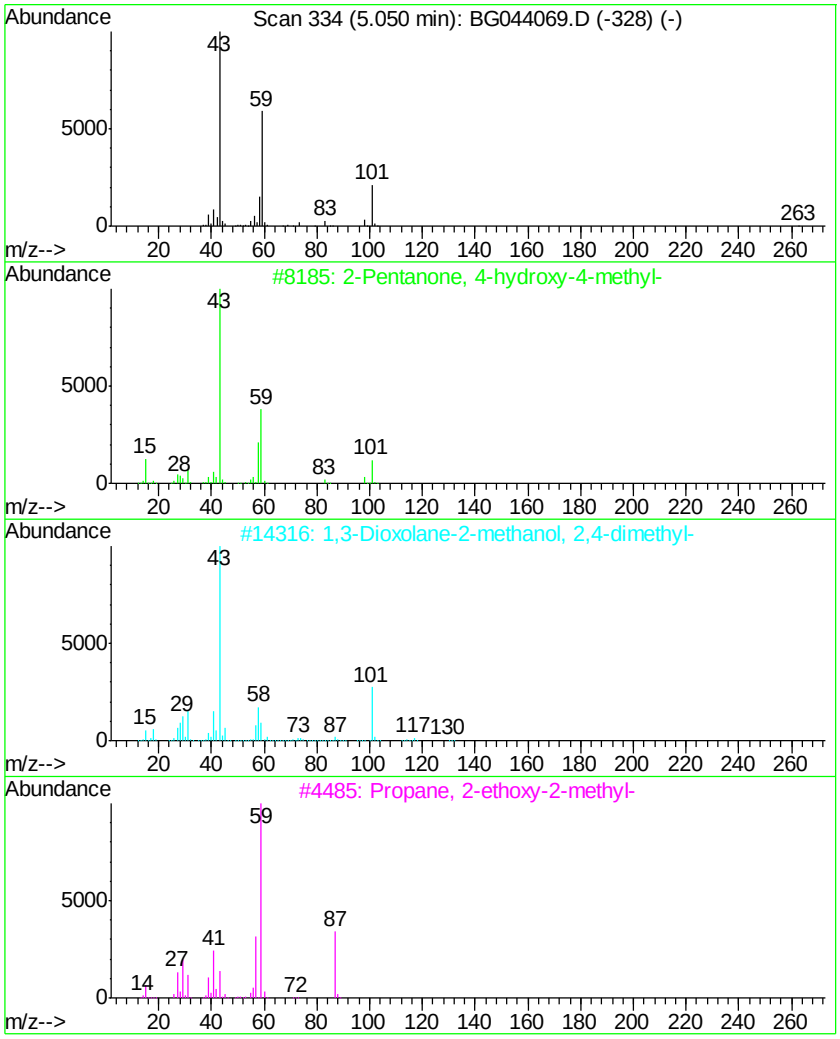
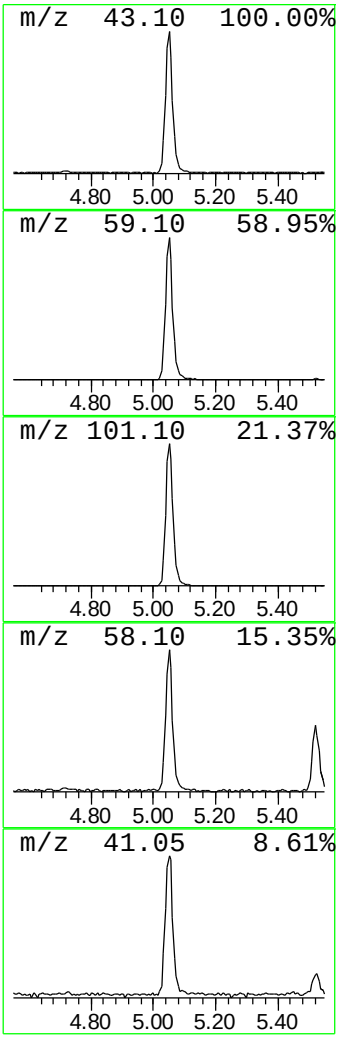
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	14.25 ng	445414	1,4-Dichlorobenzene-d4	7.94

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	25
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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
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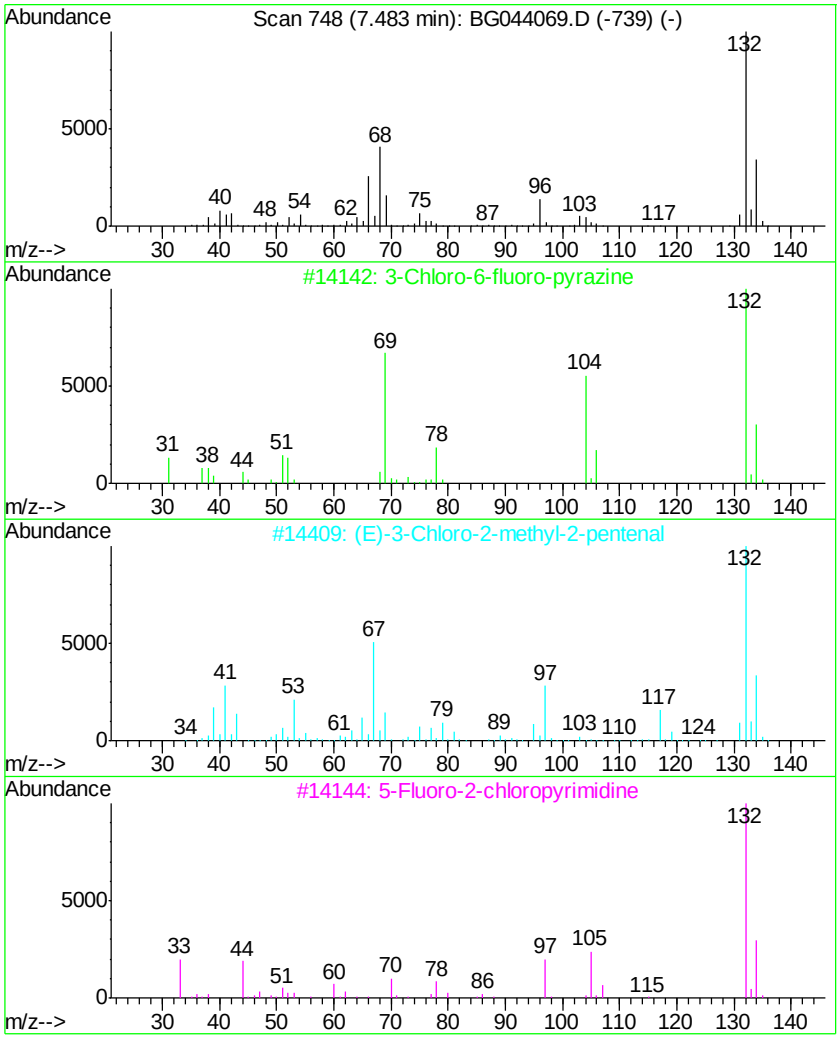
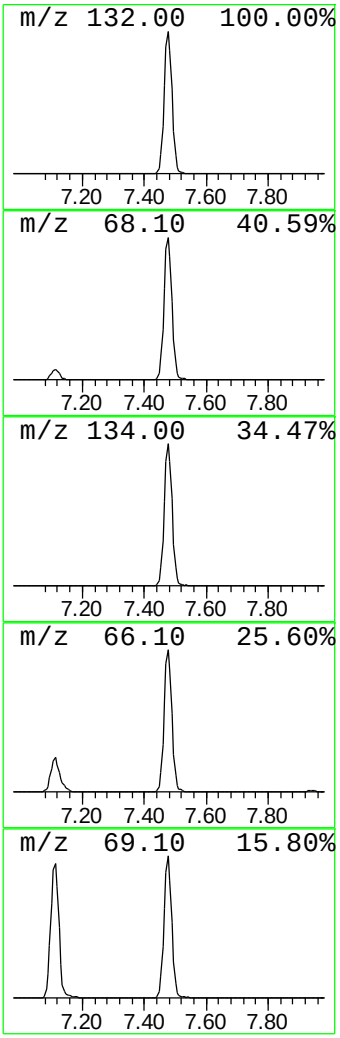
Peak Number 3 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	70.31 ng	2198260	1,4-Dichlorobenzene-d4	7.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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
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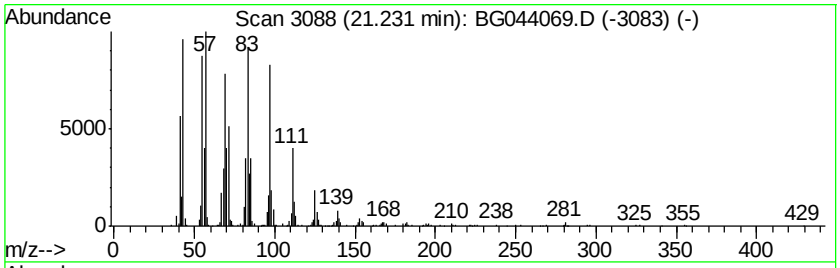
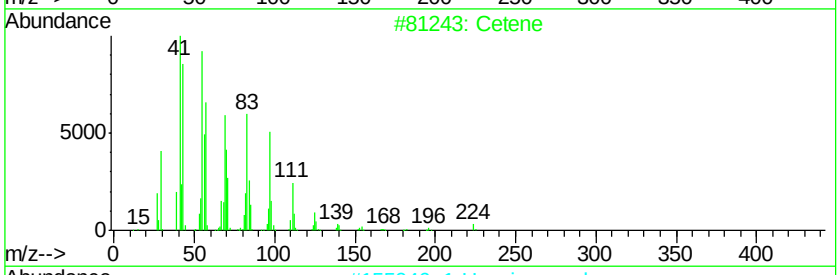
****

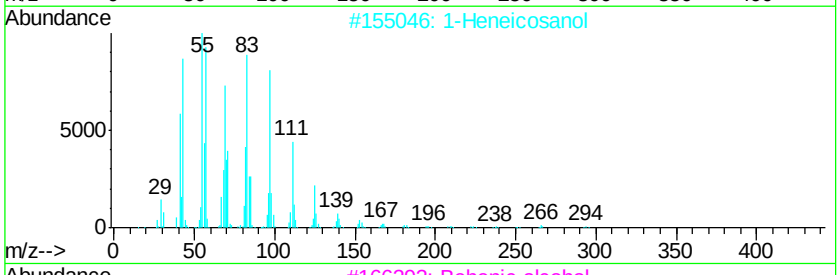
Peak Number 5 Cetene Concentration Rank 5

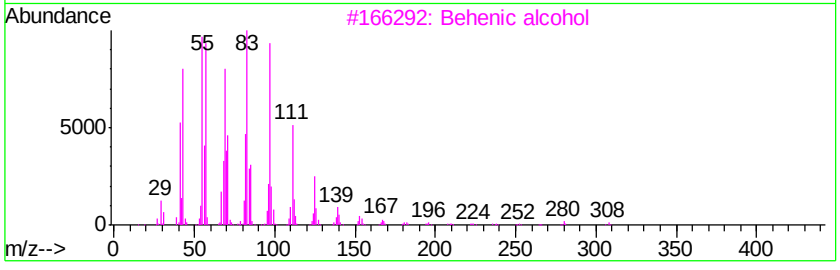
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.23	7.86 ng	664153	Chrysene-d12	21.56

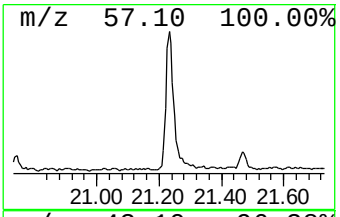
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93

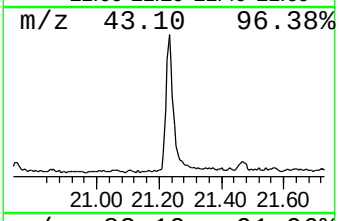


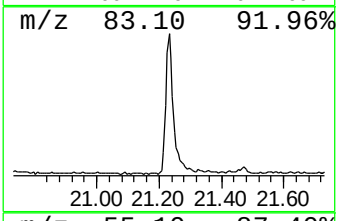


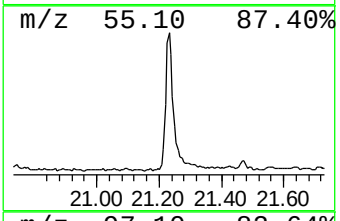


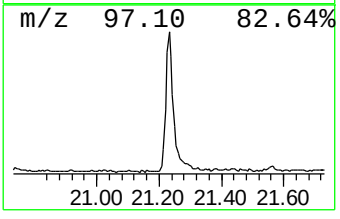












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Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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

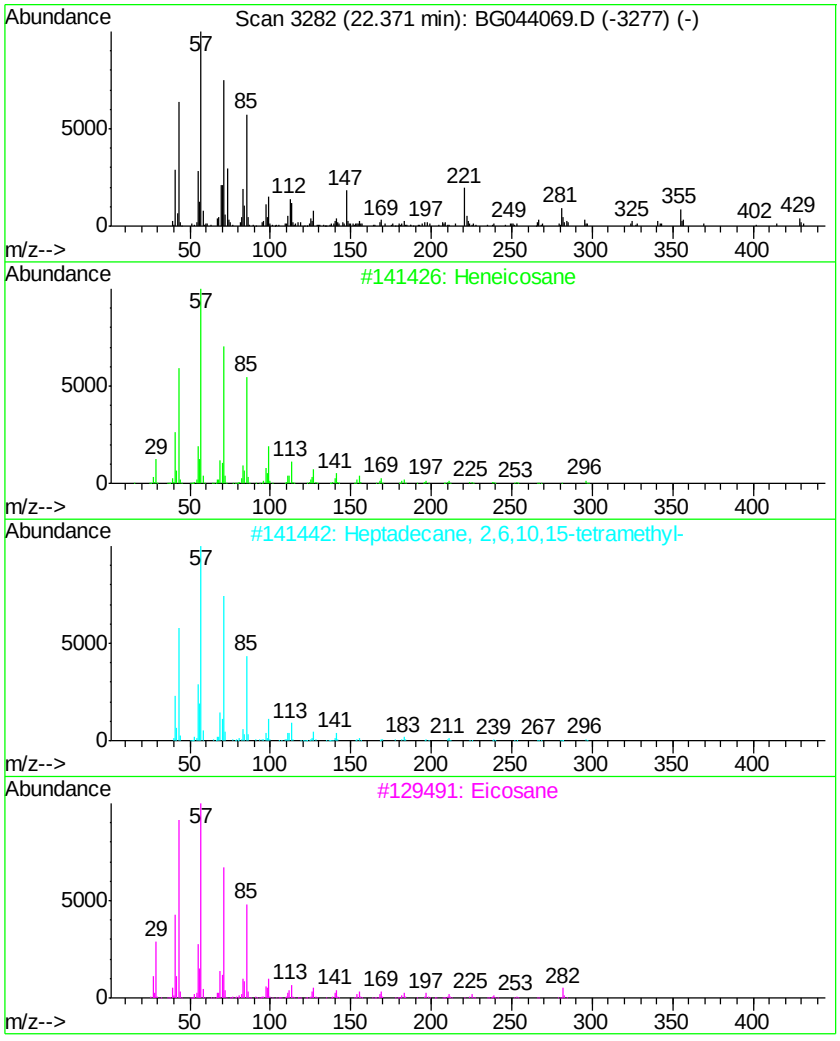
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

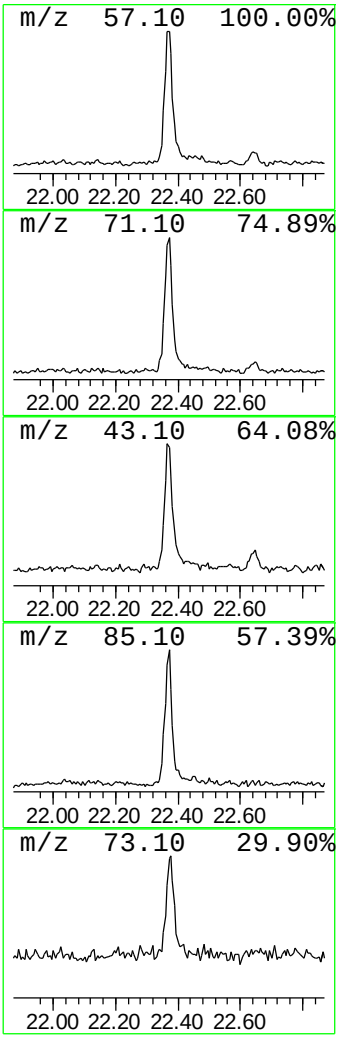
****

Peak Number 6 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	3.13 ng	264677	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	78
3	Eicosane	282	C20H42	000112-95-8	78
4	Octadecane	254	C18H38	000593-45-3	60
5	Hexacosane	366	C26H54	000630-01-3	60





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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

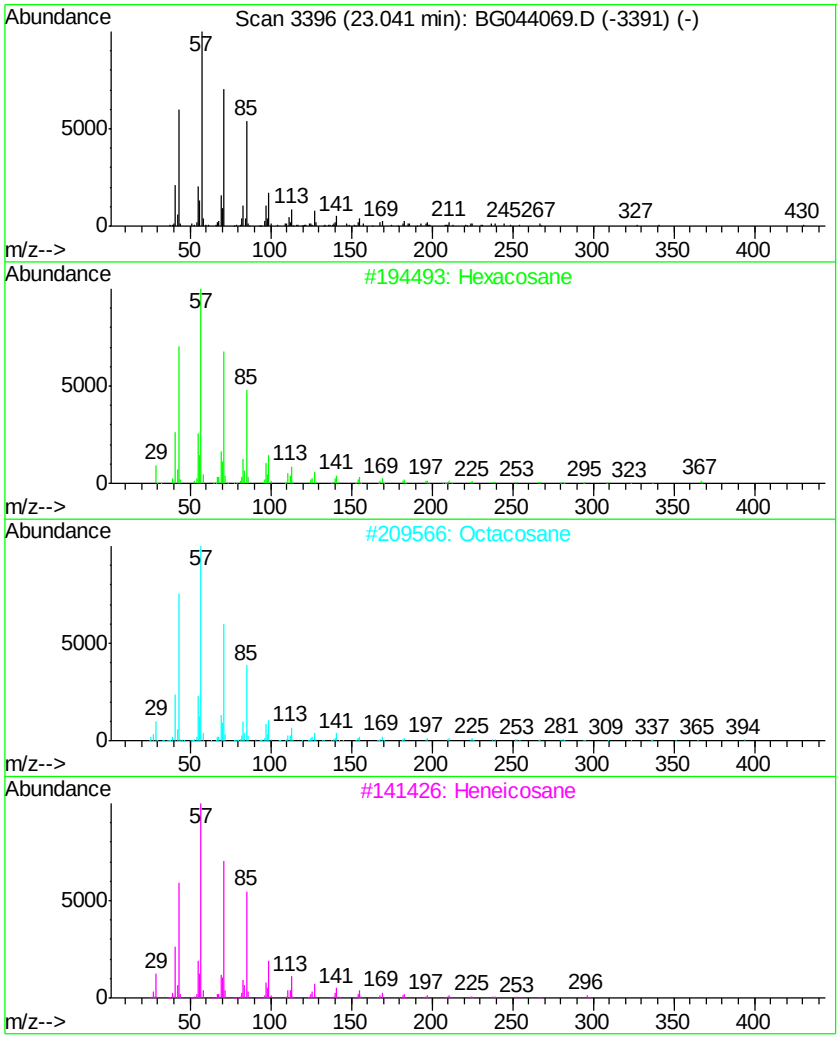
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

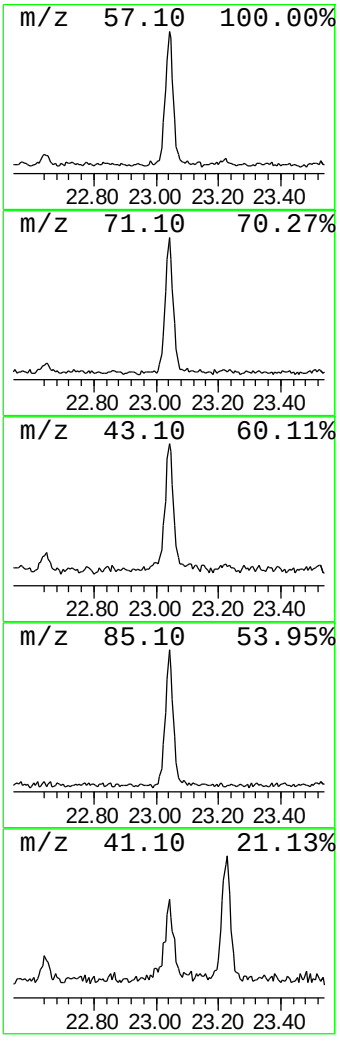
****

Peak Number 7 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.04	2.36 ng	199191	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Octacosane	394	C28H58	000630-02-4	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Tetracosane	338	C24H50	000646-31-1	86





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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

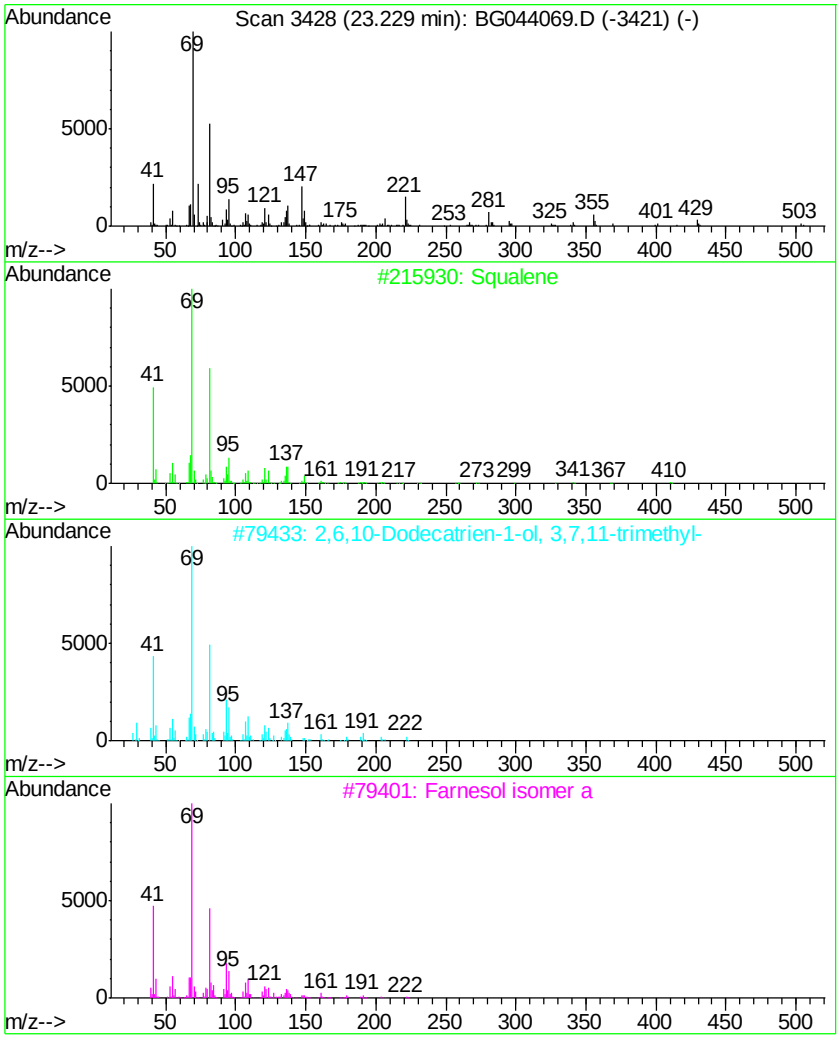
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

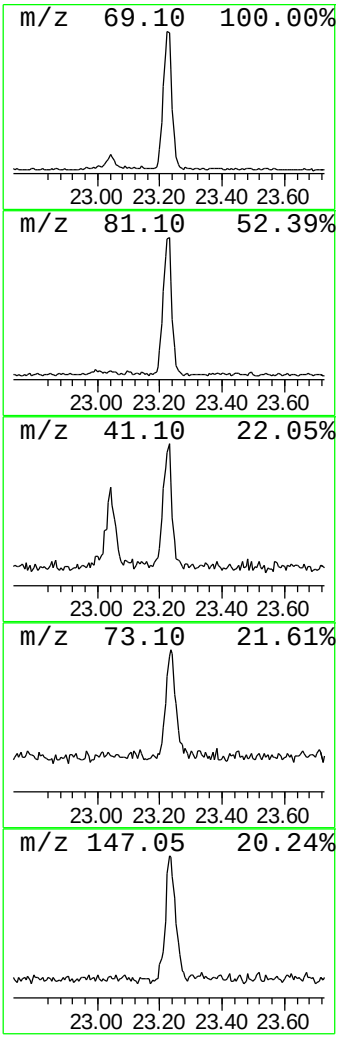
****

Peak Number 8 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.23	3.95 ng	335808	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	55
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	49
3	Farnesol isomer a	222	C15H26O	1000108-92-4	49
4	Supraene	410	C30H50	007683-64-9	49
5	trans-Farnesol	222	C15H26O	000106-28-5	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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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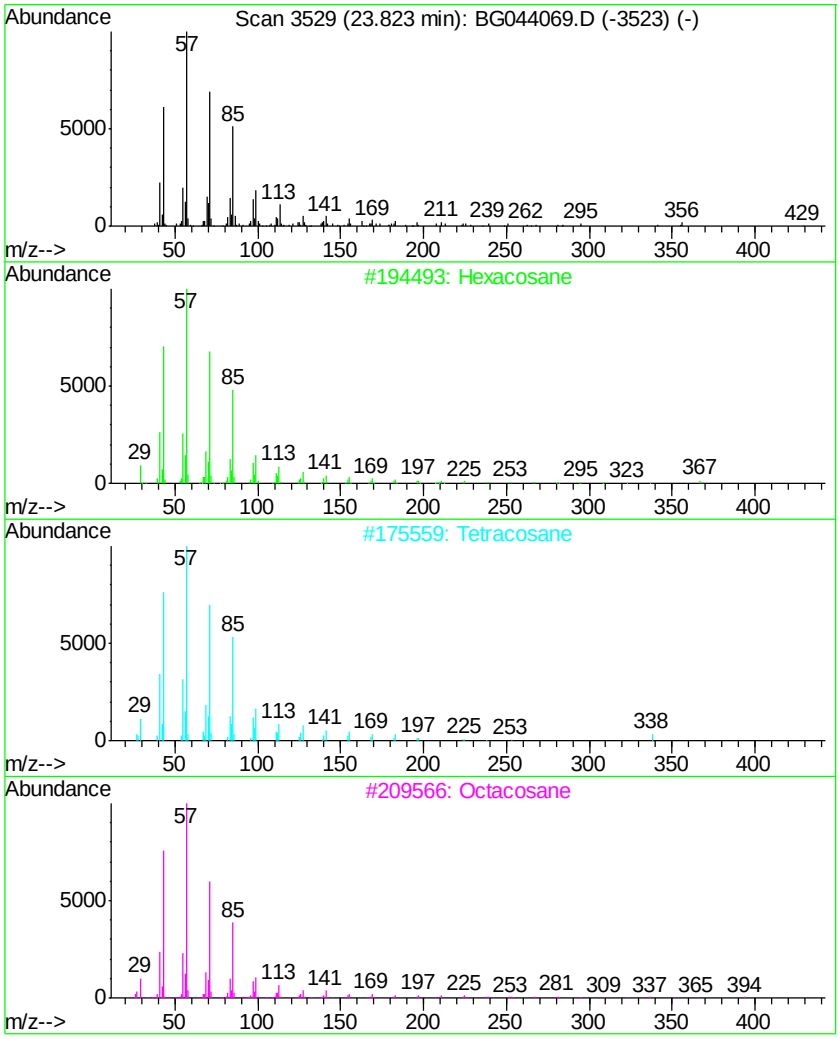
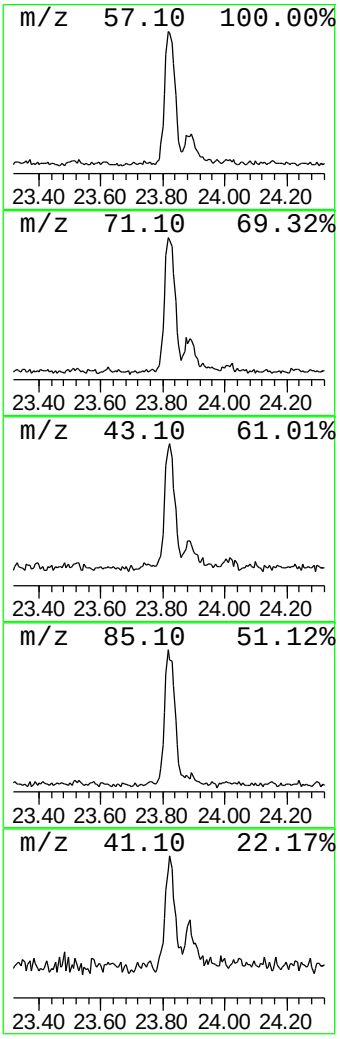
Peak Number 9 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.82	2.49 ng	211192	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Tetracosane	338	C24H50	000646-31-1	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Heptacosane	380	C27H56	000593-49-7	86
5	Heptadecane	240	C17H36	000629-78-7	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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

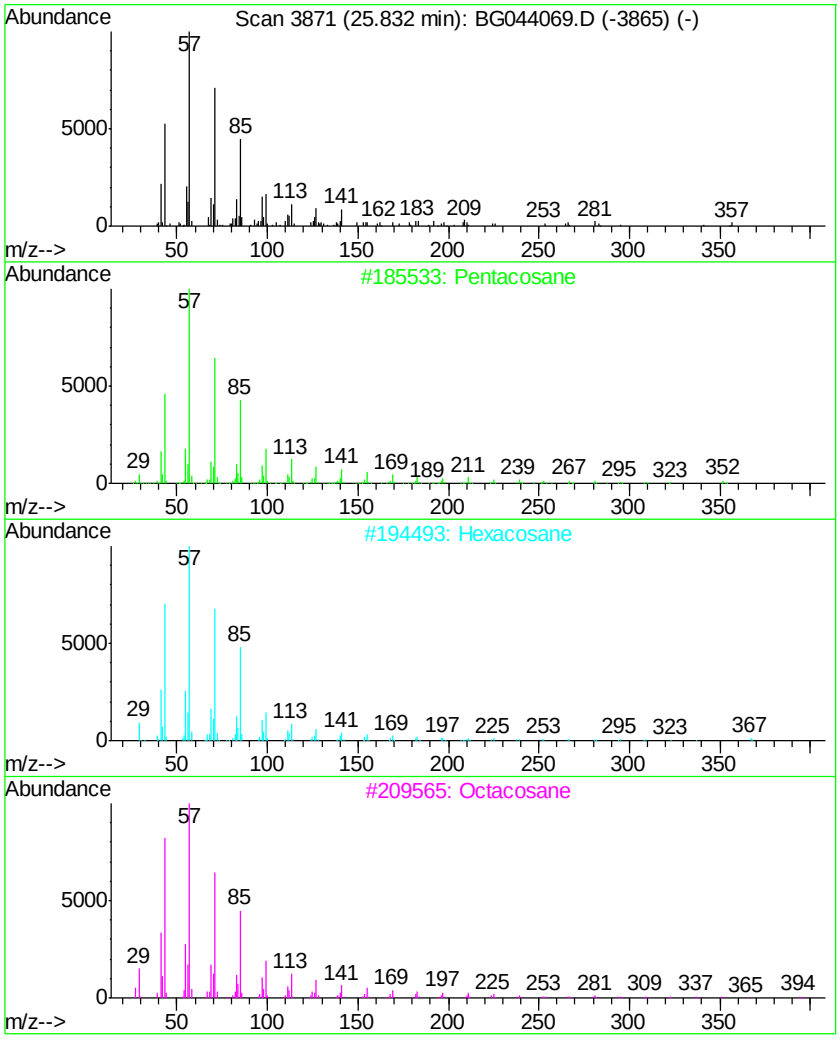
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

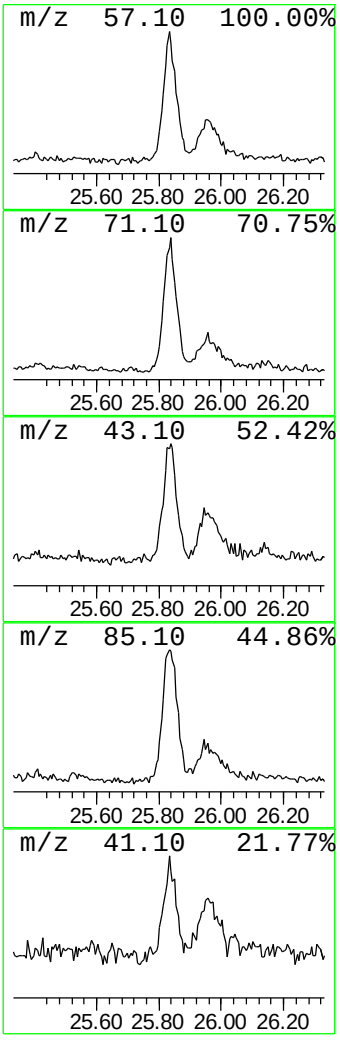
****

Peak Number 10 Pentacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.83	2.15 ng	182341	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptacosane	380	C27H56	000593-49-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011620\
Data File : BG044069.D
Acq On : 16 Jan 2020 15:22
Operator : JU
Sample : L1125-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-33-(3.5-4)

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	21.0	ng	656469	1	7.94	625339	20.0
2-Pentanone, 4-hy...	5.05	14.3	ng	445414	1	7.94	625339	20.0
unknown7.48	7.48	70.3	ng	2198260	1	7.94	625339	20.0
Cetene	21.23	7.9	ng	664153	5	21.56	1690330	20.0
Heneicosane	22.37	3.1	ng	264677	5	21.56	1690330	20.0
Hexacosane	23.04	2.4	ng	199191	5	21.56	1690330	20.0
Squalene	23.23	4.0	ng	335808	6	24.67	1699530	20.0
Tetracosane	23.82	2.5	ng	211192	6	24.67	1699530	20.0
Pentacosane	25.83	2.1	ng	182341	6	24.67	1699530	20.0