LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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	3.122	3	6	27	rVB	389170	706357	17.01%	2.557%
2	5.049	327	334	343	rBV	273570	435616	10.49%	1.577%
3	5.519	407	414	430	rBV	1158203	1907956	45.96%	6.906%
4	7.112	674	685	702	rBV	1226654	2145246	51.67%	7.765%
5	7.476	738	747	757	rBV	1214975	2107279	50.76%	7.627%
6	7.940	817	826	834	rBV	322864	546654	13.17%	1.979%
7	8.263	874	881	890	rBV	925690	1637343	39.44%	5.926%
8	9.092	1014	1022	1034	rBV	668066	1257266	30.28%	4.551%
9	10.743	1295	1303	1314	rBV	408474	743389	17.91%	2.691%
10	13.199	1714	1721	1734	rBV	1709971	2709831	65.27%	9.808%
11	14.027	1855	1862	1872	rVB	87249	138613	3.34%	0.502%
12	14.573	1948	1955	1969	rBV2	647124	1017819	24.52%	3.684%
13	16.060	2201	2208	2219	rBV	1434200	2217508	53.41%	8.026%
14	17.317	2414	2422	2433	rBV	787871	1222461	29.45%	4.425%
15	18.216	2568	2575	2579	rBV4	26218	44303	1.07%	0.160%
16	19.932	2861	2867	2879	rBV	3058383	4151475	100.00%	15.026%
17	21.230	3084	3088	3100	rVB	402425	632327	15.23%	2.289%
18	21.565	3138	3145	3159	rBV	898907	1553562	37.42%	5.623%
19	21.777	3177	3181	3186	rVB2	39772	56458	1.36%	0.204%
20	22.370	3278	3282	3294	rVB3	71333	161167	3.88%	0.583%
21	23.040	3392	3396	3403	rVB2	80475	143845	3.46%	0.521%
22	23.228	3422	3428	3436	rVB	212463	390642	9.41%	1.414%
23	23.821	3524	3529	3537	rVB2	81945	167499	4.03%	0.606%
24	24.673	3665	3674	3683	rBV2	536016	1533925	36.95%	5.552%

Sum of corrected areas: 27628541

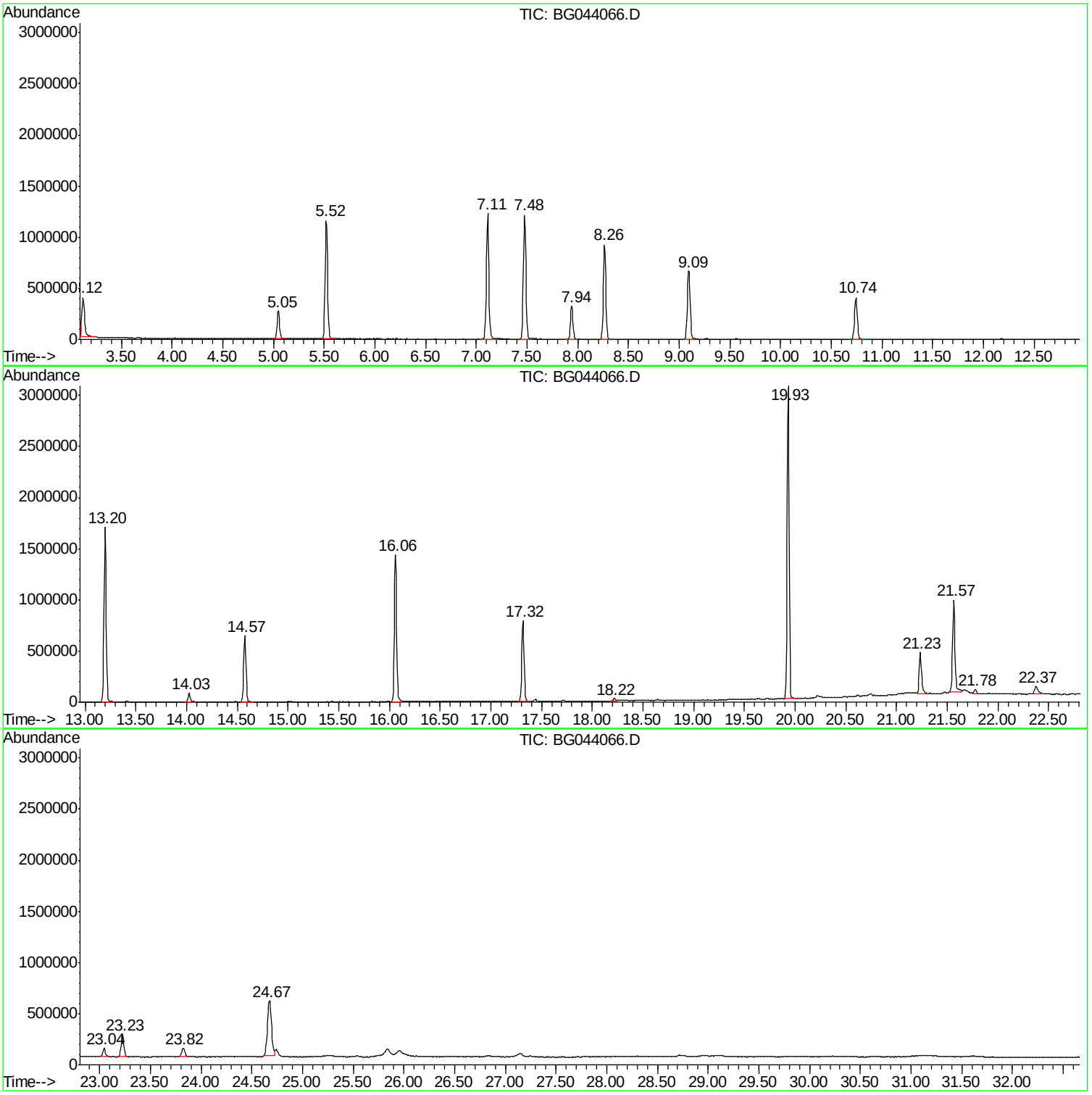
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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

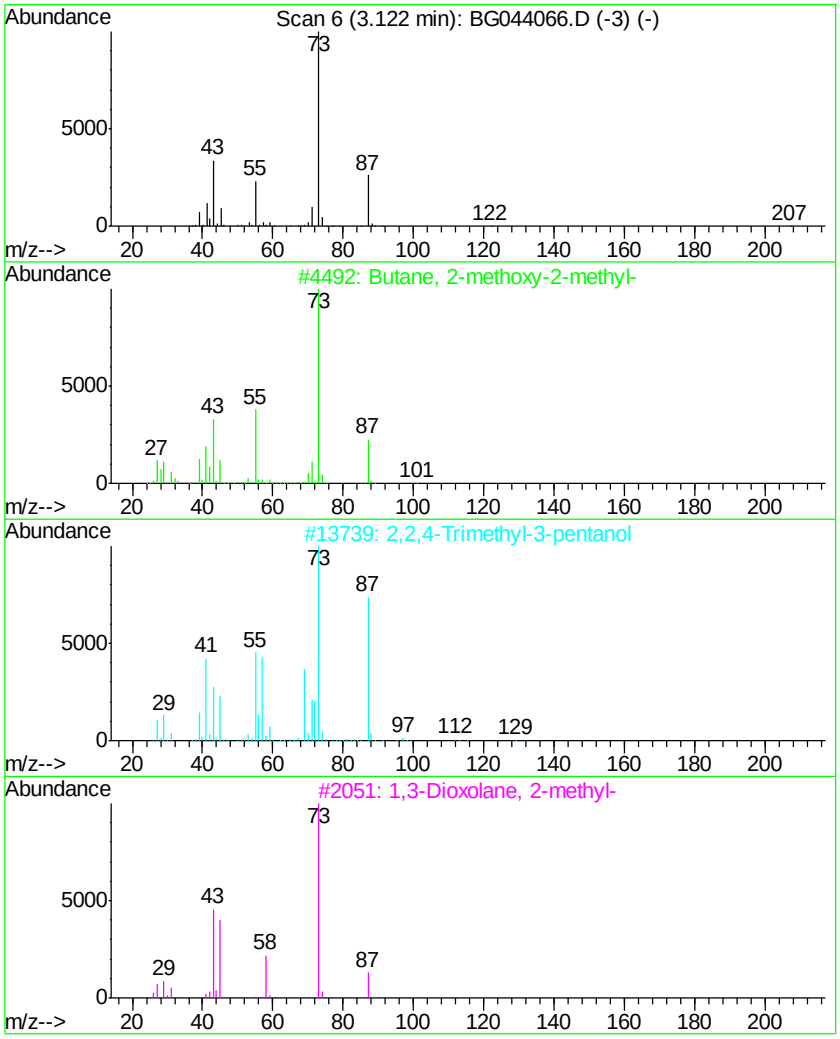
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

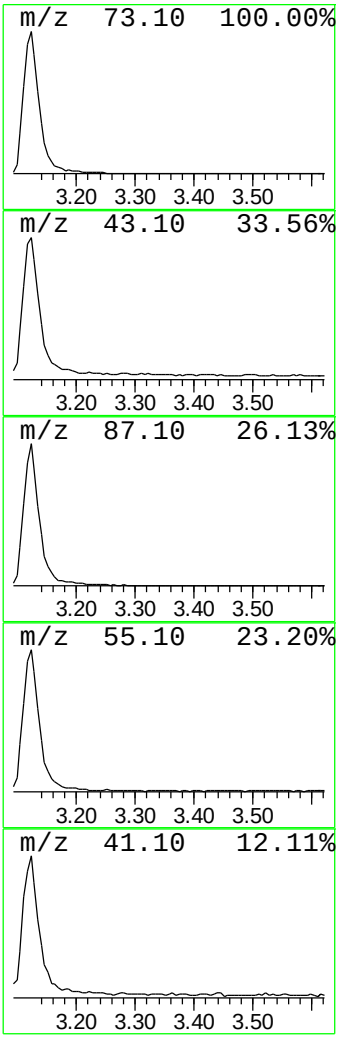
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	25.84 ng	706357	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	64
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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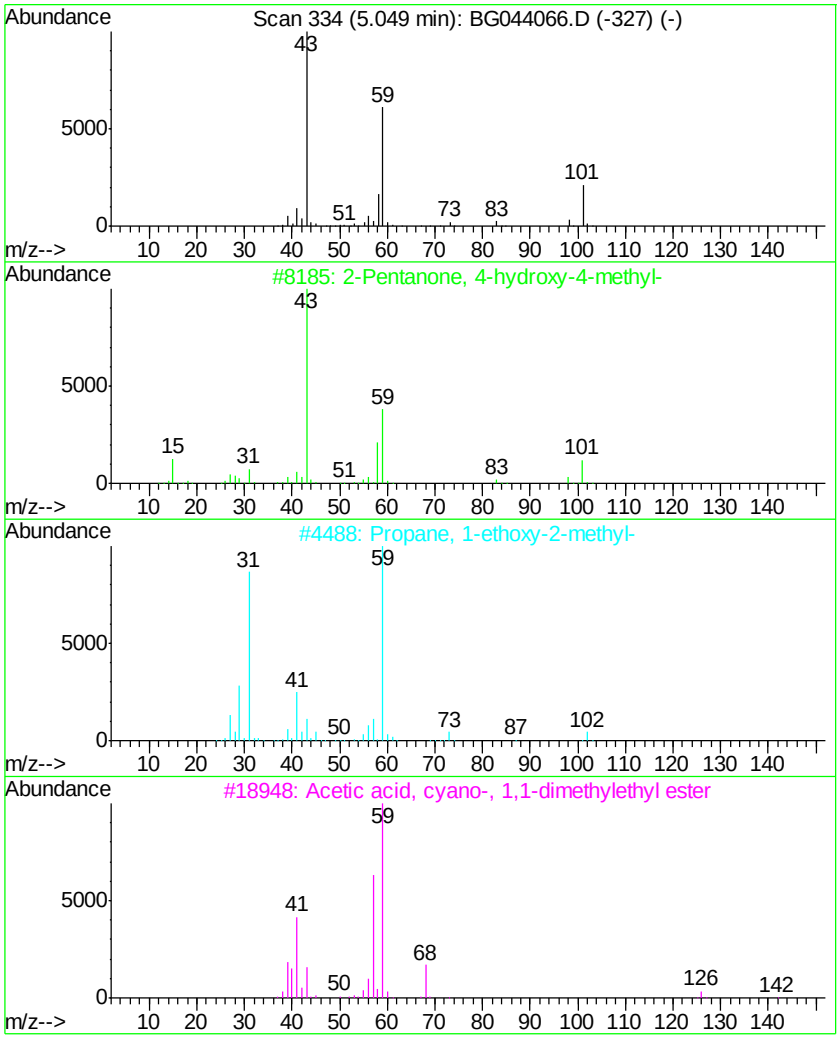
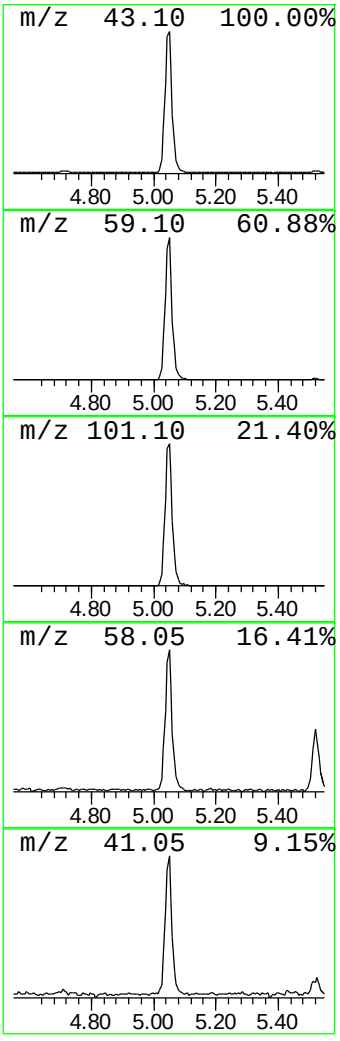
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	15.94 ng	435616	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	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	23
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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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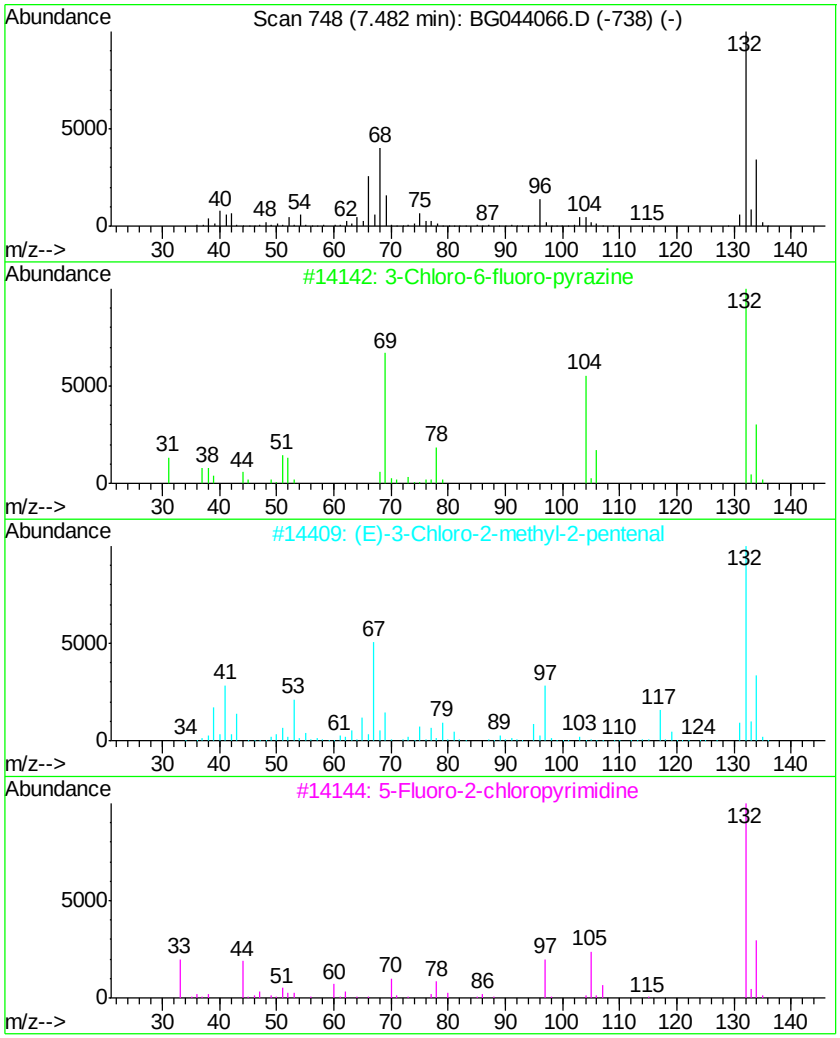
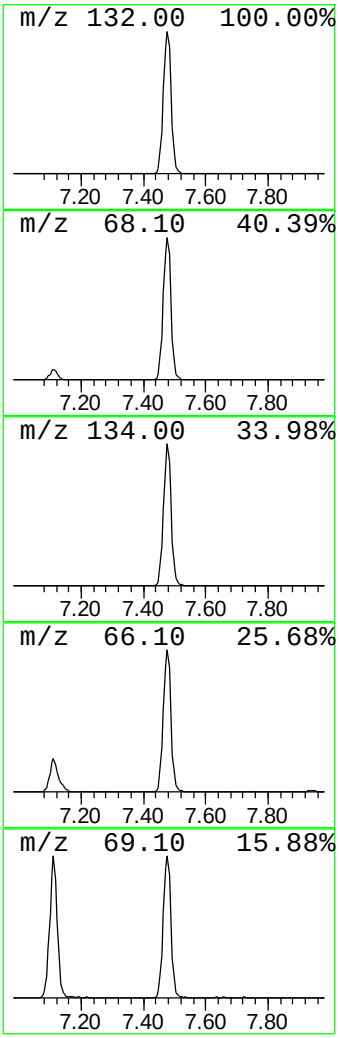
Peak Number 3 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	77.10 ng	2107280	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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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

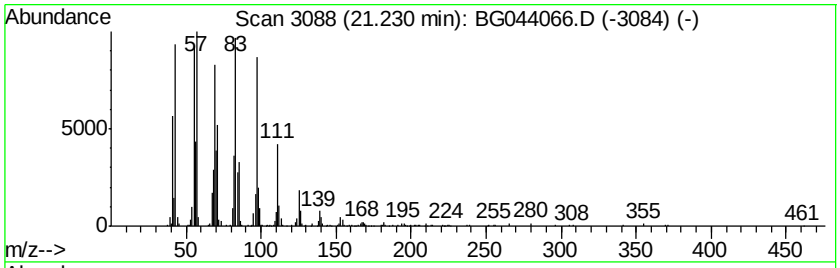
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

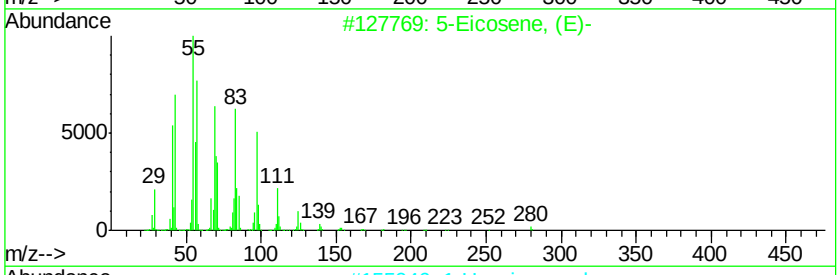
****

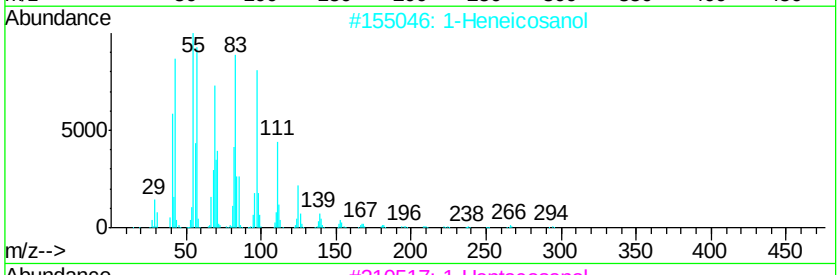
Peak Number 5 5-Eicosene, (E)- Concentration Rank 5

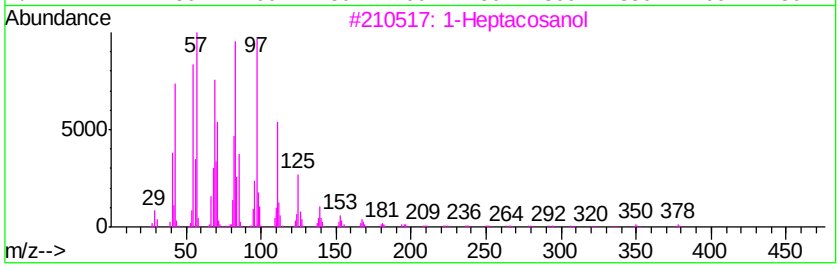
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.23	8.14 ng	632327	Chrysene-d12	21.57

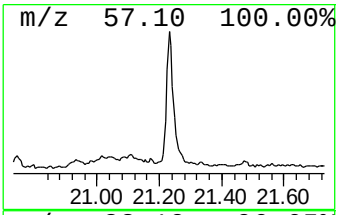
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94

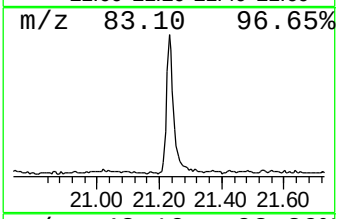


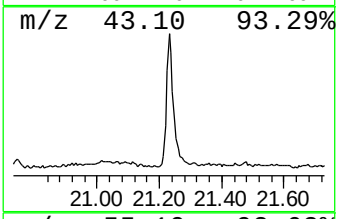


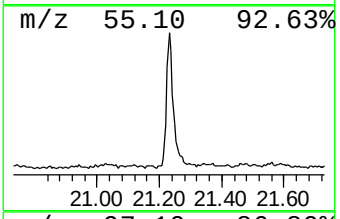


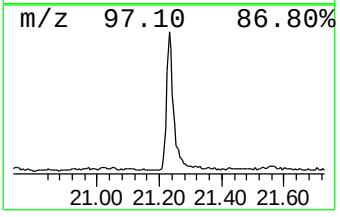












Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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

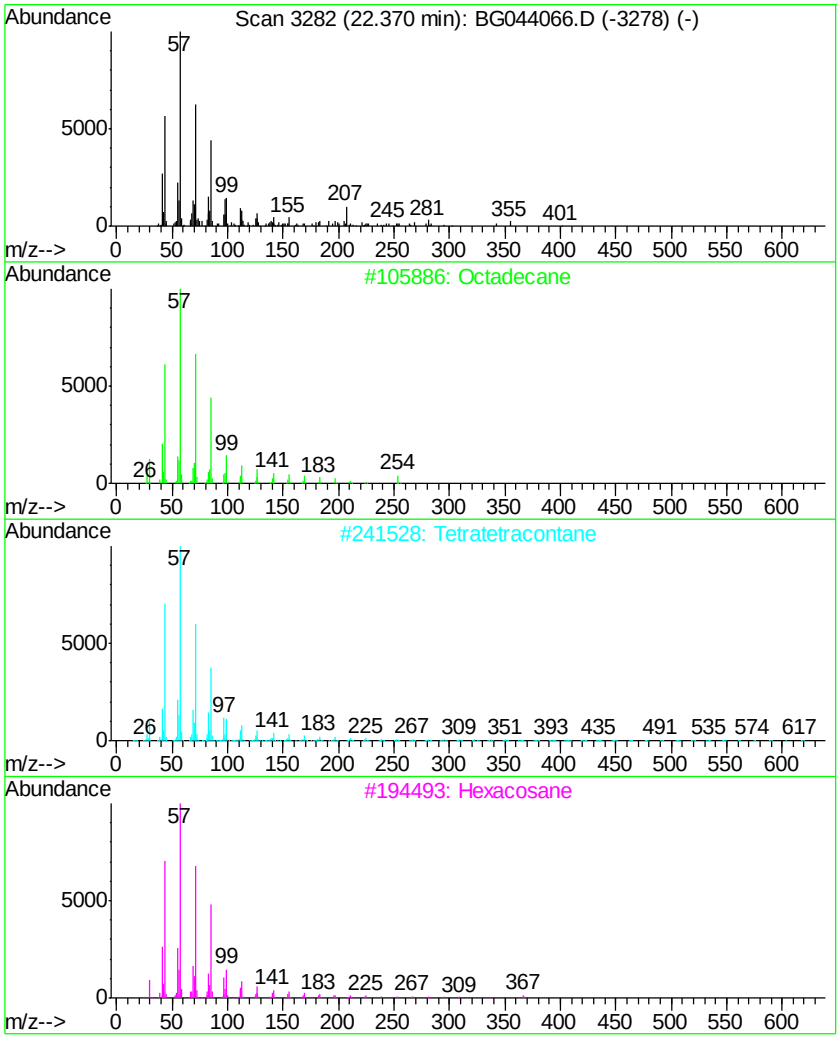
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

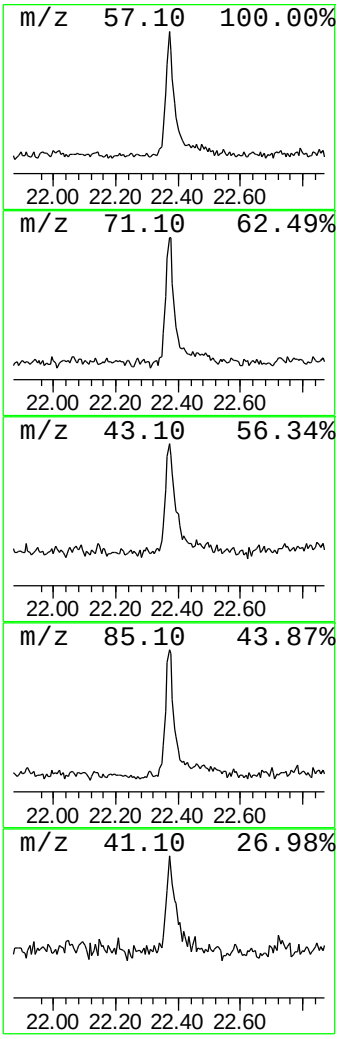
****

Peak Number 6 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	2.07 ng	161167	Chrysene-d12	21.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	94
2	Tetratetracontane	619	C44H90	007098-22-8	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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

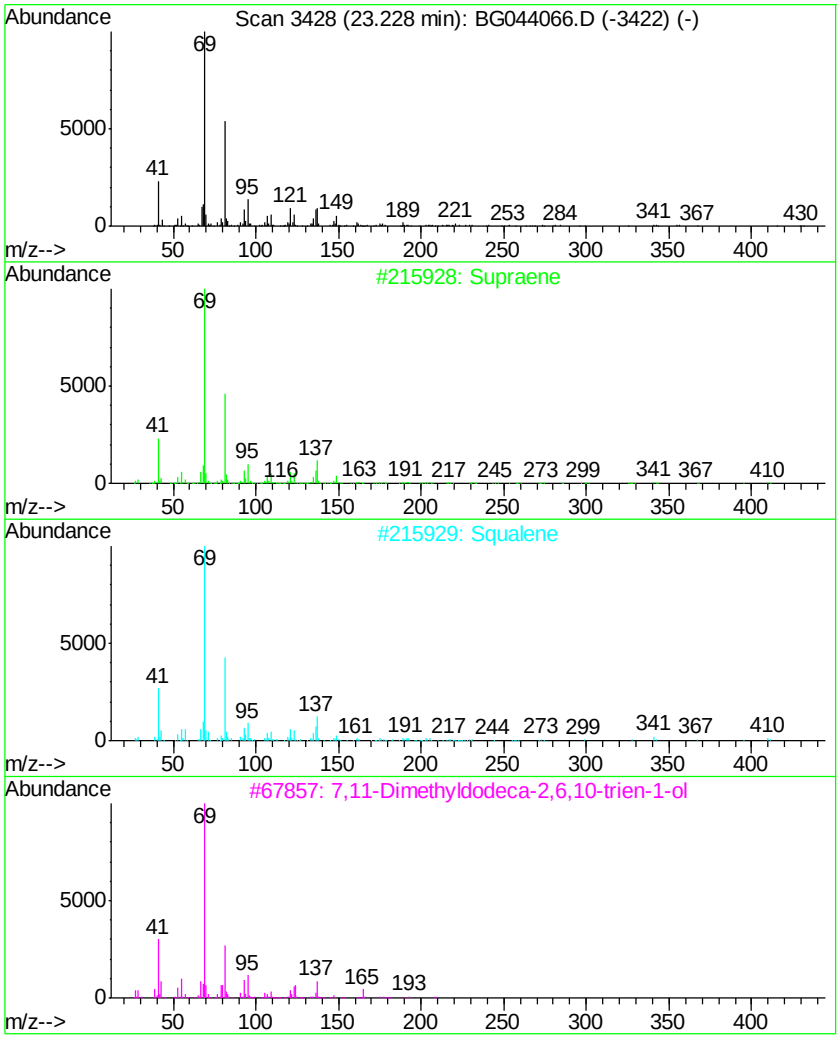
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

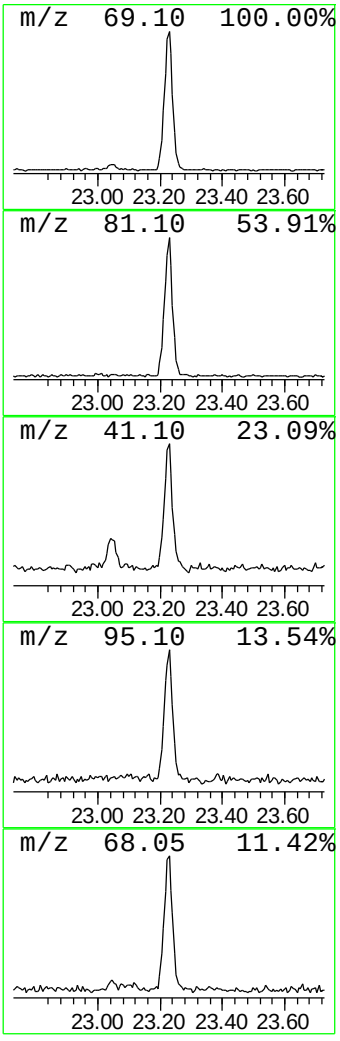
****

Peak Number 7 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.23	5.09 ng	390642	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	72
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
5	trans-Farnesol	222	C15H26O	000106-28-5	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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

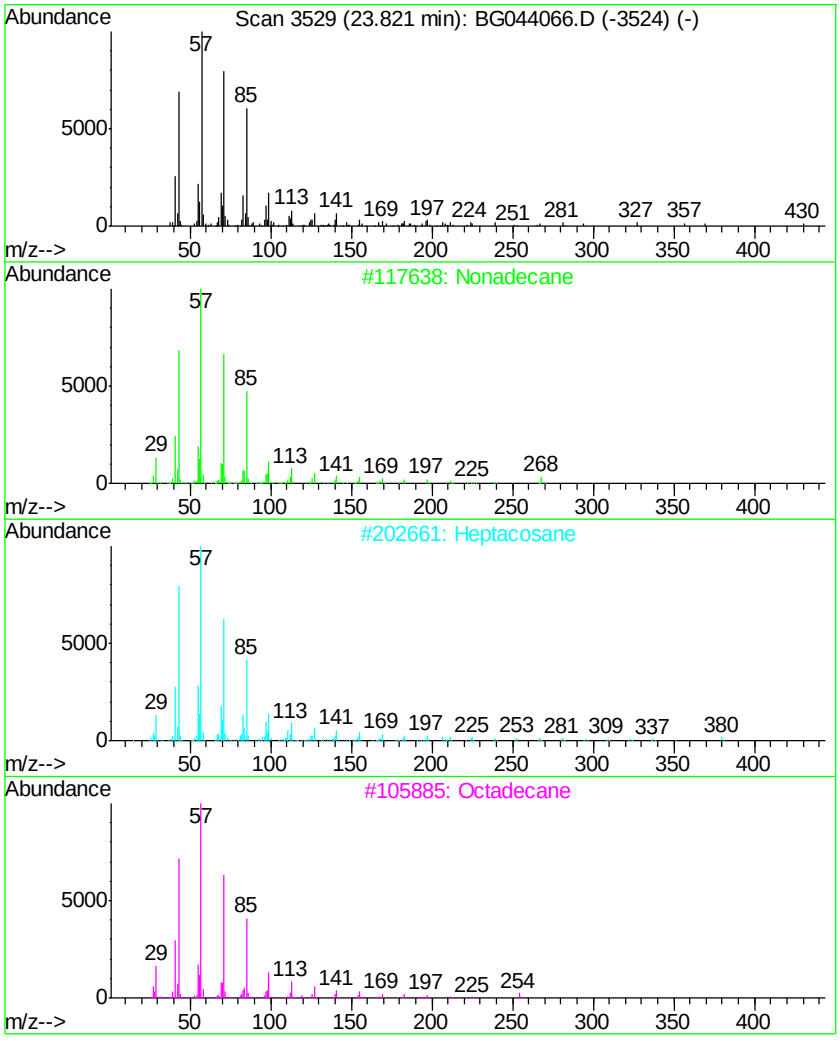
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

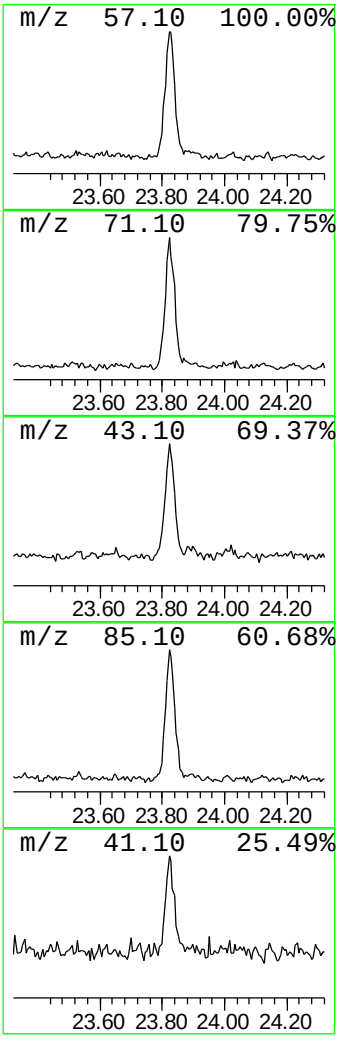
****

Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.82	2.18 ng	167499	Perylene-d12	24.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	86
2	Heptacosane	380	C27H56	000593-49-7	81
3	Octadecane	254	C18H38	000593-45-3	80
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011620\
Data File : BG044066.D
Acq On : 16 Jan 2020 13:25
Operator : JU
Sample : L1125-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : FESB-28-(1.5-2)

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...	3.12	25.8	ng	706357	1	7.94	546654	20.0
2-Pentanone, 4-hy...	5.05	15.9	ng	435616	1	7.94	546654	20.0
unknown7.48	7.48	77.1	ng	2107280	1	7.94	546654	20.0
5-Eicosene, (E)-	21.23	8.1	ng	632327	5	21.57	1553560	20.0
Octadecane	22.37	2.1	ng	161167	5	21.57	1553560	20.0
Supraene	23.23	5.1	ng	390642	6	24.67	1533930	20.0
Nonadecane	23.82	2.2	ng	167499	6	24.67	1533930	20.0