LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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	1.667	6	7	12	rVV	35294	49828	2.61%	0.288%
2	1.781	15	17	24	rVV	322614	446975	23.46%	2.585%
3	1.884	24	26	46	rVB	57793	118303	6.21%	0.684%
4	4.844	283	285	293	rBV	74932	109814	5.76%	0.635%
5	5.290	321	324	326	rBV	1720541	1905519	100.00%	11.020%
6	6.341	413	416	419	rBV2	1566372	1802604	94.60%	10.425%
7	6.456	424	426	429	rBV	1768035	1734397	91.02%	10.030%
8	6.684	444	446	449	rBV	629416	527164	27.67%	3.049%
9	6.844	457	460	462	rBV	1619358	1610727	84.53%	9.315%
10	7.256	493	496	498	rBV	1120440	1107147	58.10%	6.403%
11	7.382	501	507	512	rVB2	24706	39705	2.08%	0.230%
12	7.976	556	559	561	rBV	563497	641102	33.64%	3.708%
13	9.050	650	653	655	rBV	2049972	1851049	97.14%	10.705%
14	9.450	686	688	690	rBV	623821	528128	27.72%	3.054%
15	9.668	705	707	709	rBV	48063	41046	2.15%	0.237%
16	9.725	709	712	714	rBV	635892	618587	32.46%	3.577%
17	10.136	739	748	749	rBV	14674	25140	1.32%	0.145%
18	10.159	749	750	752	rVB	68818	65346	3.43%	0.378%
19	10.376	766	769	773	rBV	24060	43706	2.29%	0.253%
20	10.513	778	781	783	rBV	695574	815494	42.80%	4.716%
21	10.639	790	792	796	rBV	58044	98714	5.18%	0.571%
22	10.822	806	808	813	rBV3	10168	21062	1.11%	0.122%
23	11.085	829	831	832	rBV	28747	38353	2.01%	0.222%
24	11.199	839	841	843	rBV	645260	526218	27.62%	3.043%
25	12.788	977	980	982	rBV	1145311	1403153	73.64%	8.115%
26	13.268	1016	1022	1024	rBV5	6224	21524	1.13%	0.124%
27	13.634	1051	1054	1056	rBV	11929	19807	1.04%	0.115%
28	13.702	1057	1060	1064	rVV2	39387	78322	4.11%	0.453%
29	13.828	1069	1071	1074	rVV	566611	515176	27.04%	2.979%
30	13.931	1078	1080	1082	rVV	40462	40743	2.14%	0.236%
31	14.662	1142	1144	1146	rBV	41249	45980	2.41%	0.266%
32	15.211	1189	1192	1198	rBV	334429	400516	21.02%	2.316%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
08-B5(0-8)C

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:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 17291349

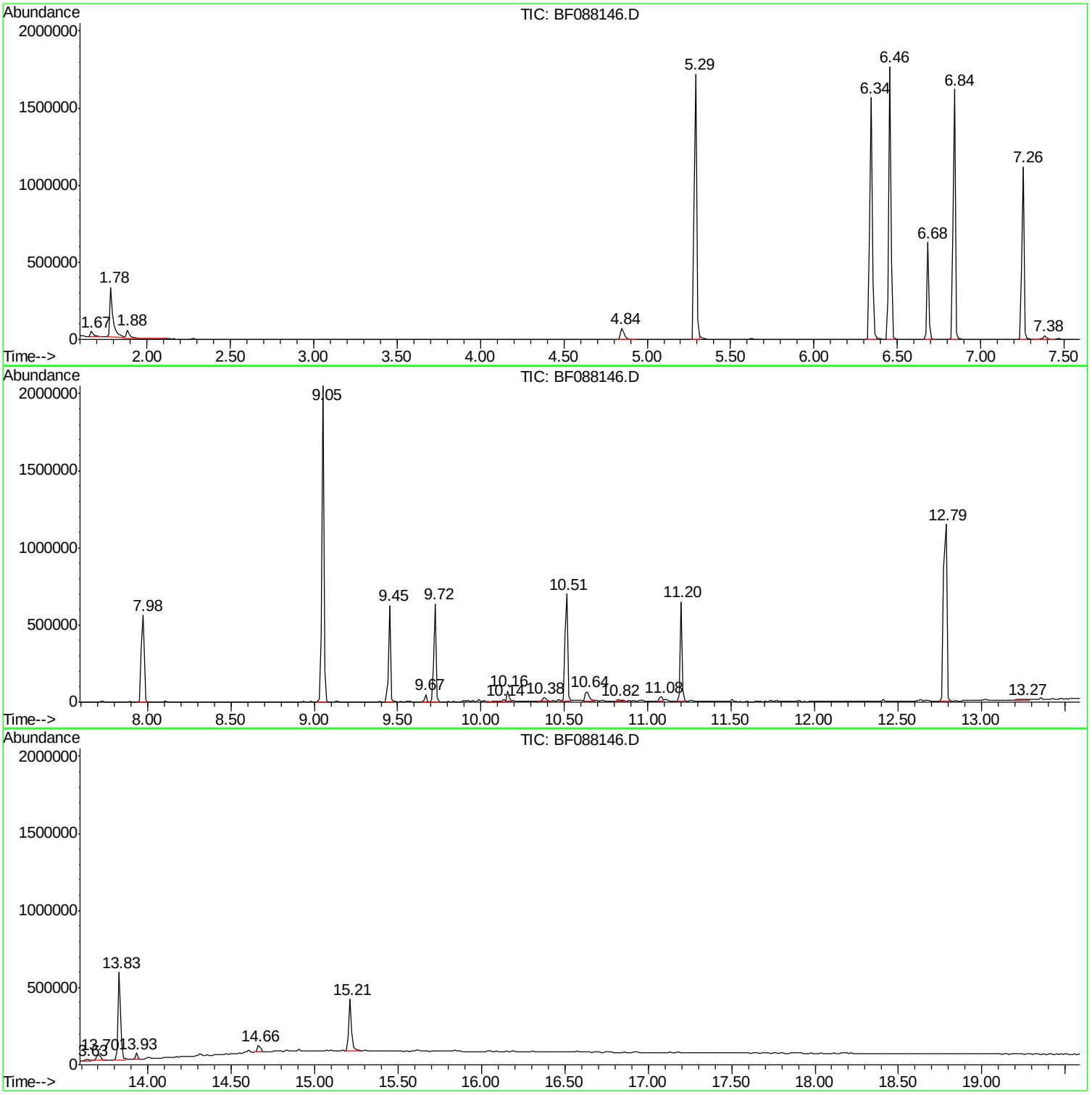
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

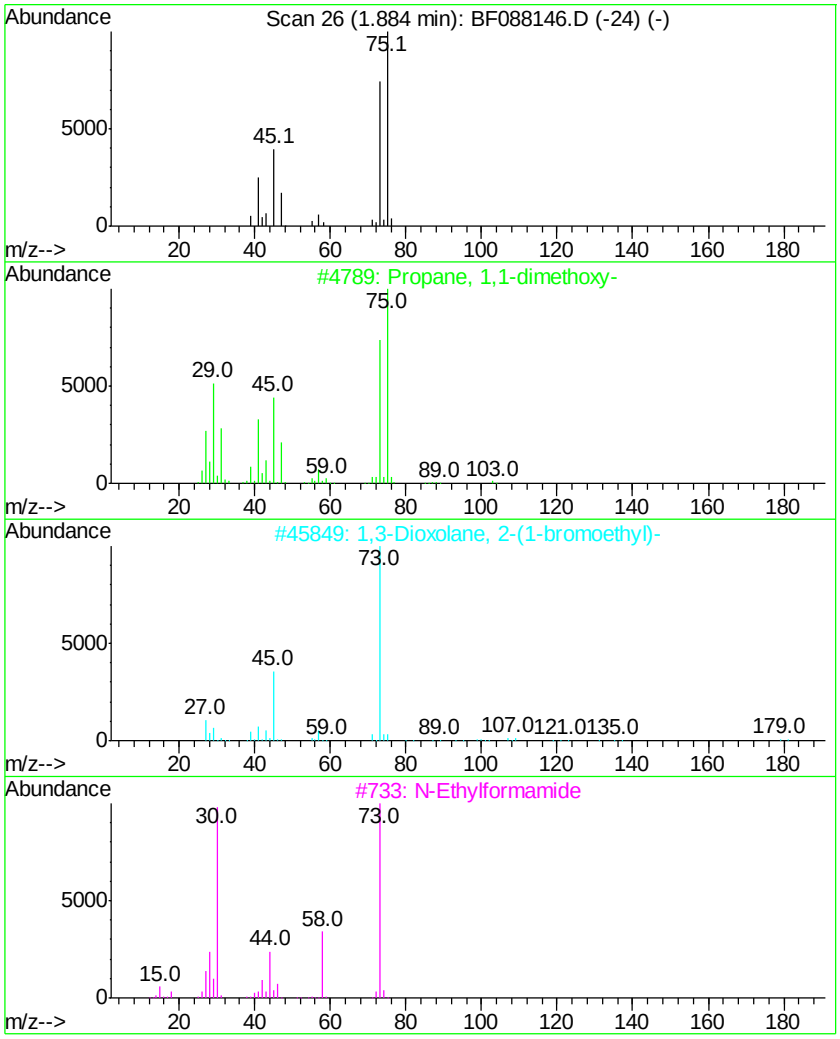
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

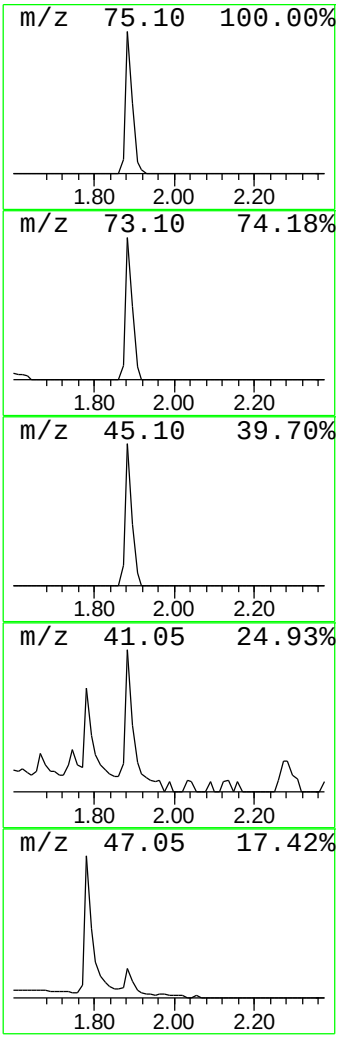
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.88	4.49 ng	118303	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	12
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

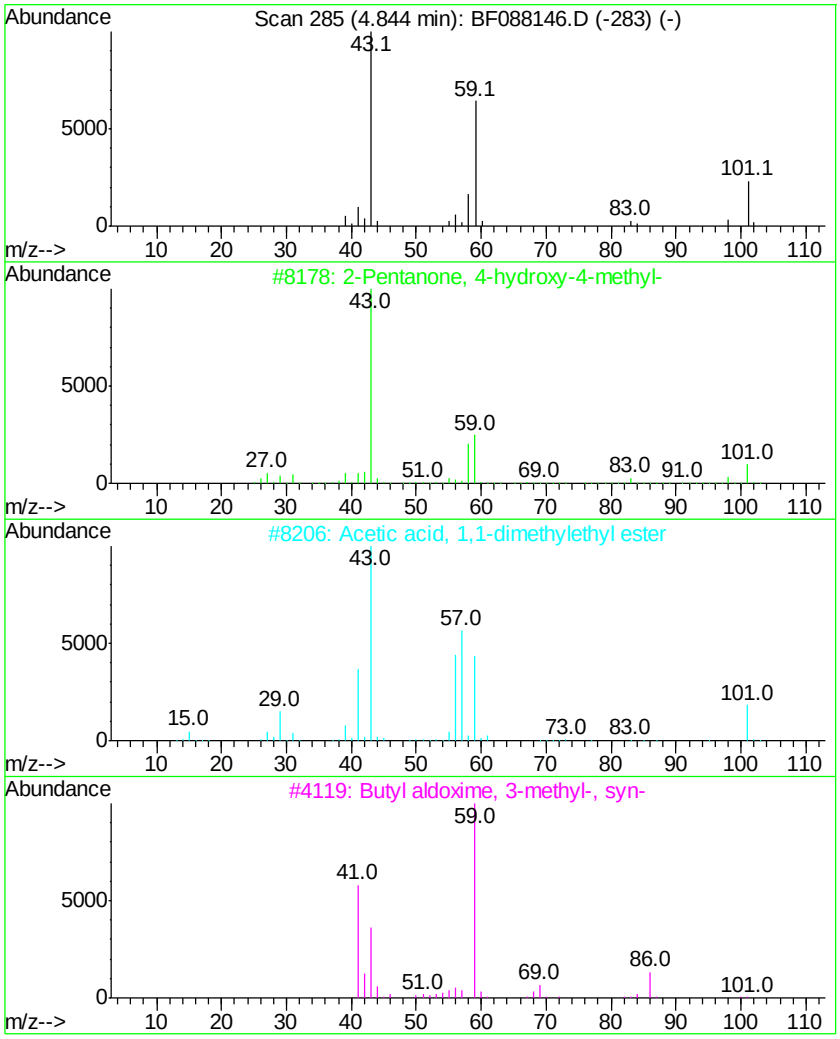
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

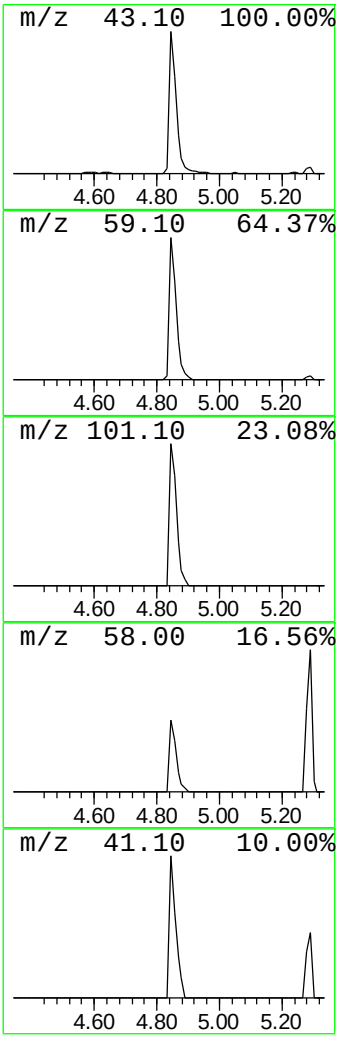
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	4.17 ng	109814	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4	3-Hexanol	102	C6H14O	000623-37-0	25
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

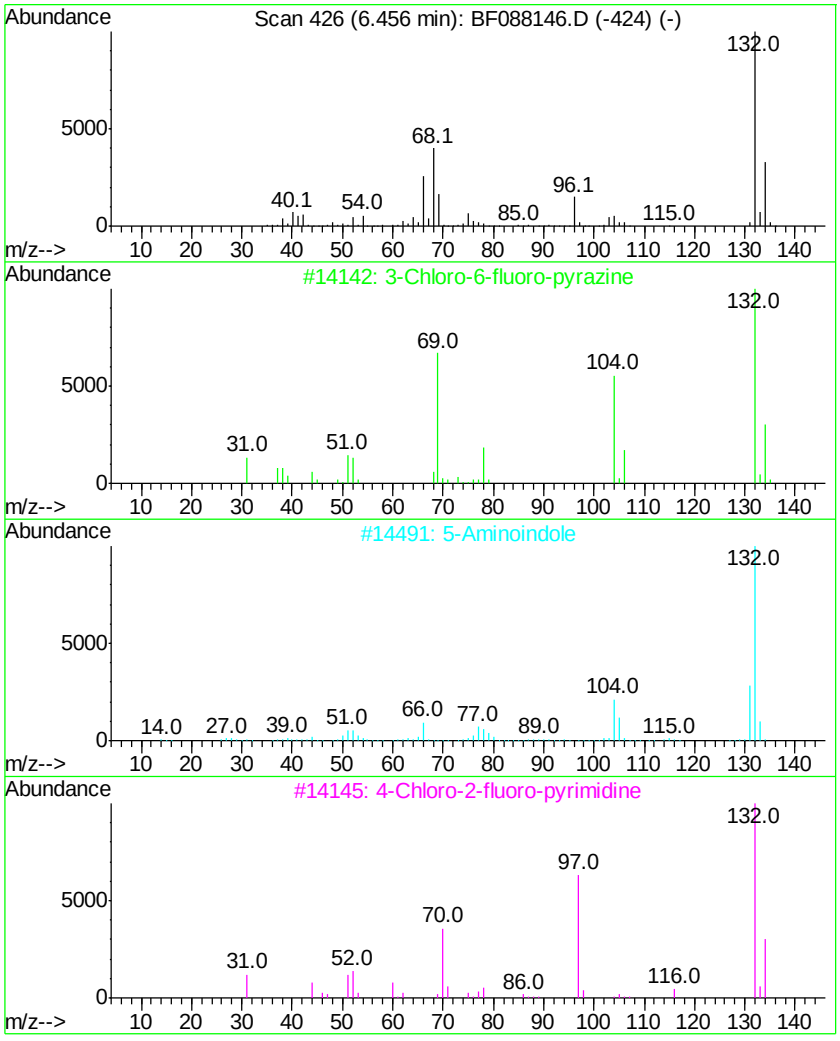
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

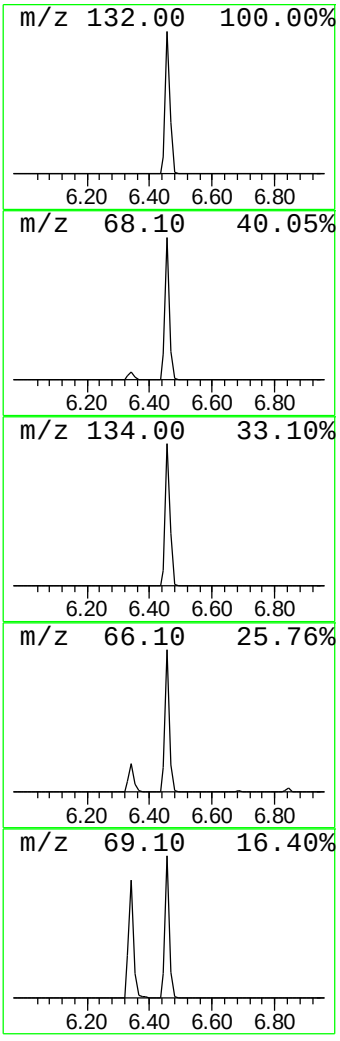
****

Peak Number 4 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	65.80 ng	1734400	1,4-Dichlorobenzene-d4	6.68

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	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

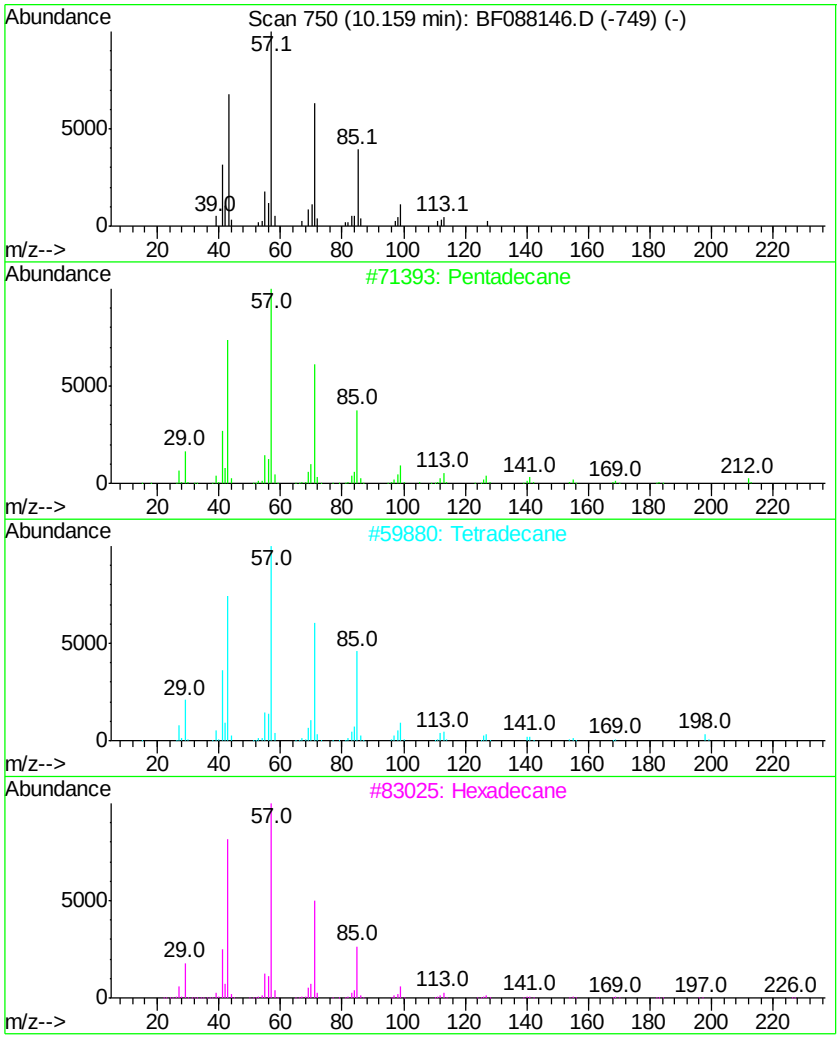
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

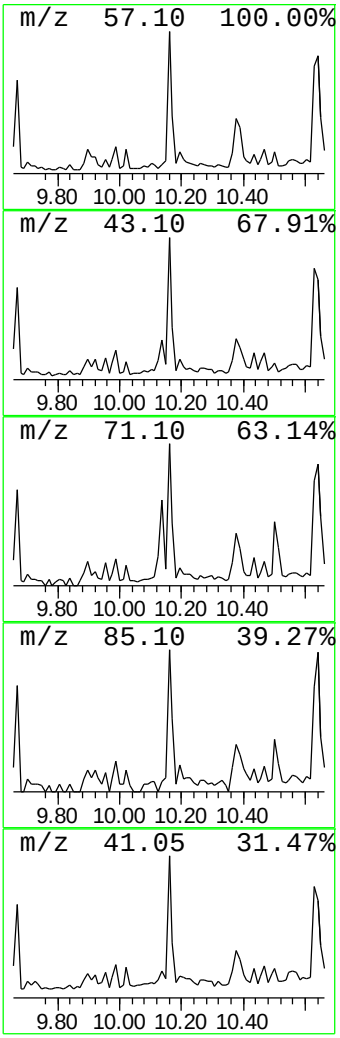
****

Peak Number 6 Pentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	2.11 ng	65346	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Hexadecane	226	C16H34	000544-76-3	80
4	Tridecane	184	C13H28	000629-50-5	78
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

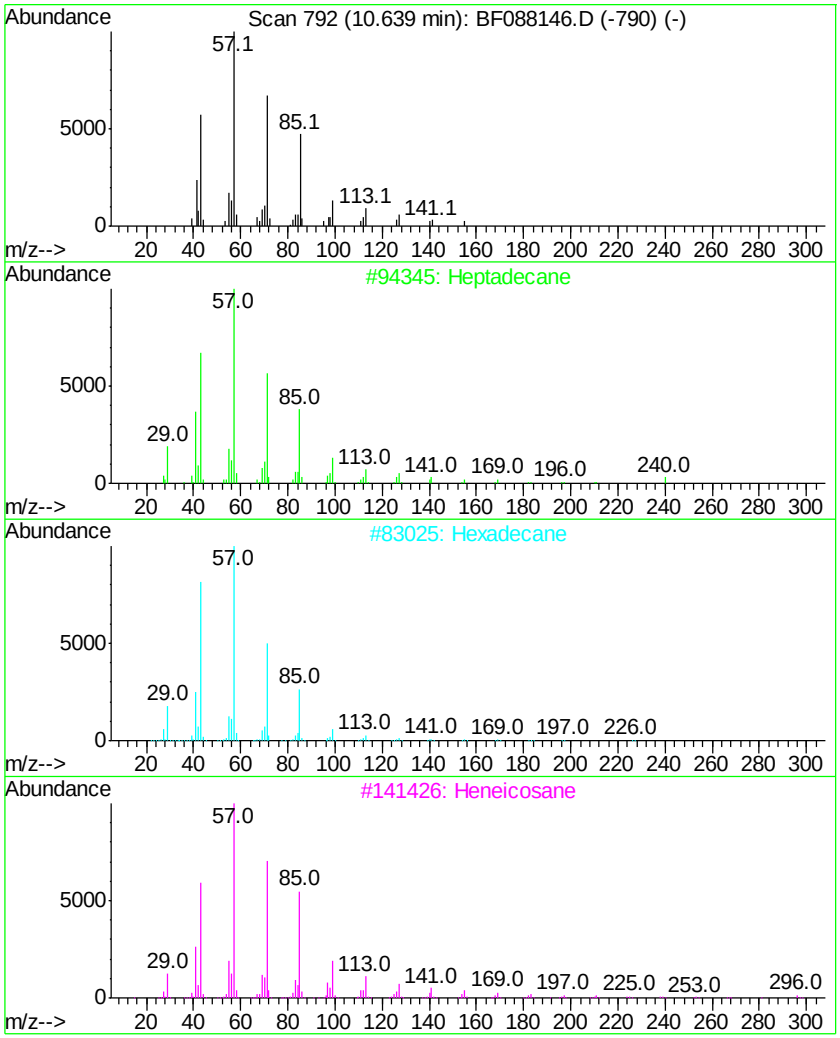
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

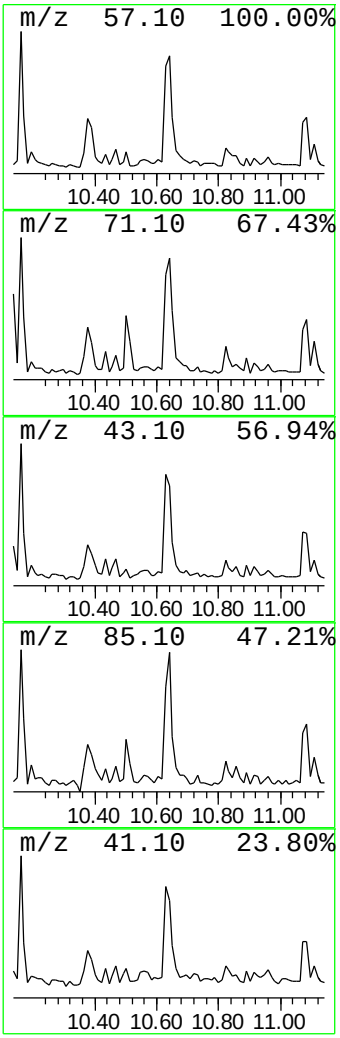
****

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	3.75 ng	98714	Phenanthrene-d10	11.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Eicosane	282	C20H42	000112-95-8	86
5	Octadecane	254	C18H38	000593-45-3	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

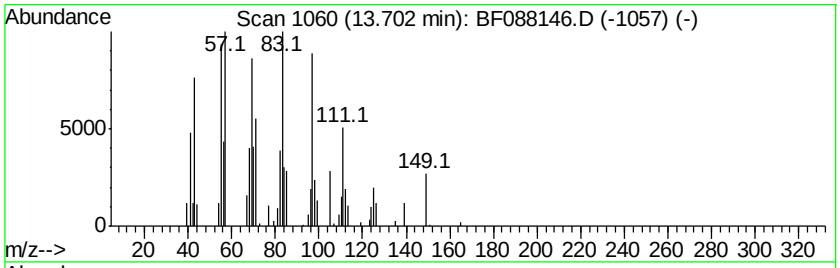
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

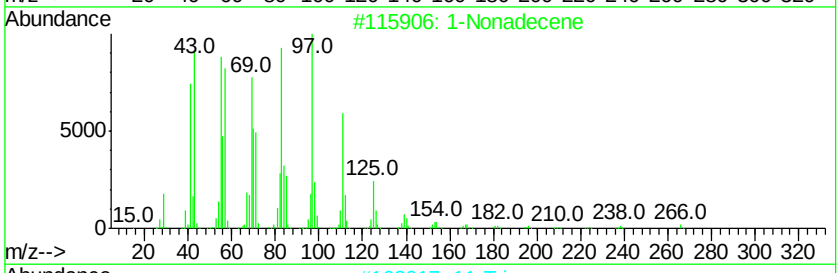
****

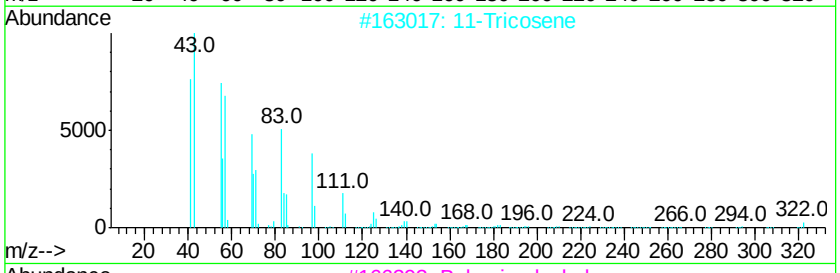
Peak Number 8 1-Nonadecene Concentration Rank 7

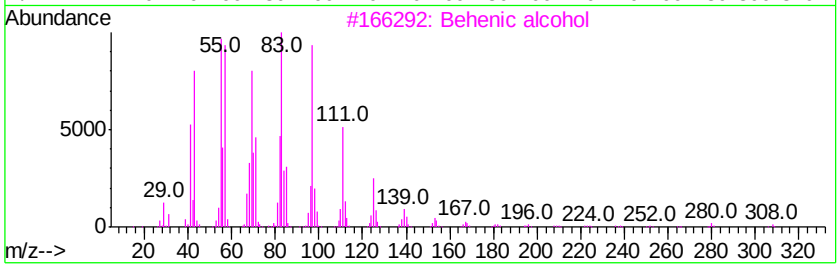
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	3.04 ng	78322	Chrysene-d12	13.83

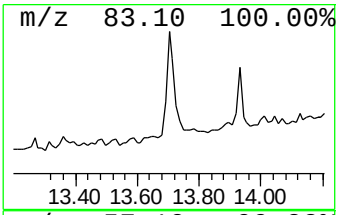
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	94
2	11-Tricosene	322	C23H46	052078-56-5	91
3	Behenic alcohol	326	C22H46O	000661-19-8	90
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	90
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	90

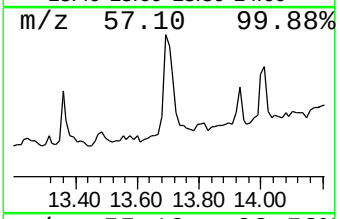


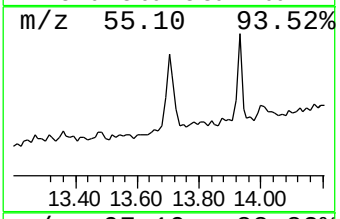


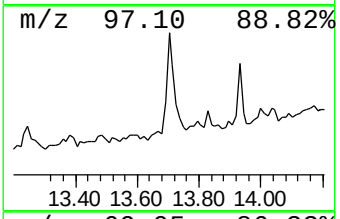


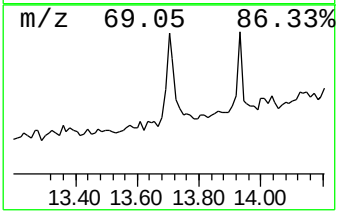












Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

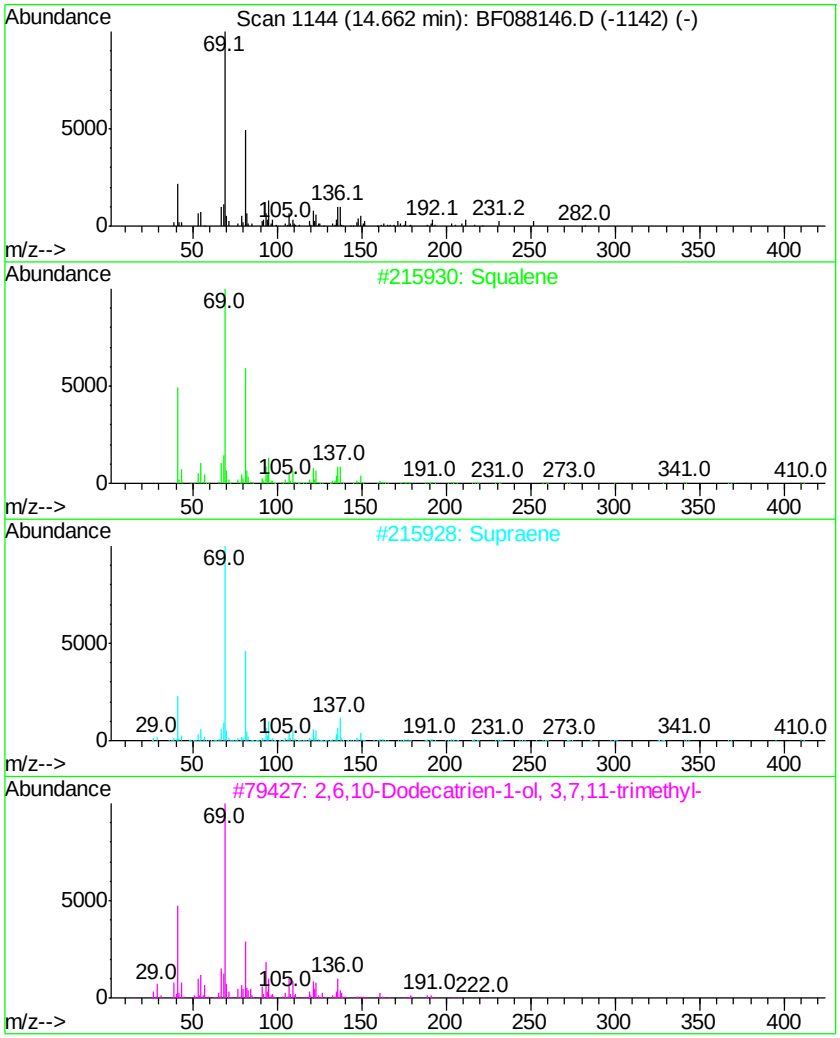
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

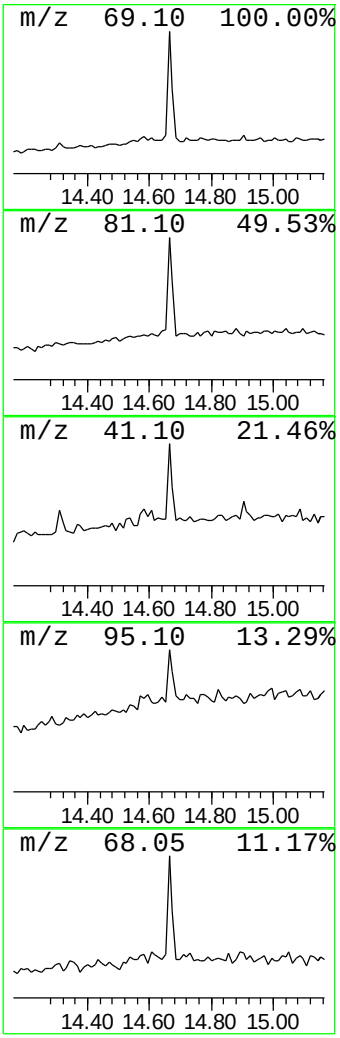
****

Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.30 ng	45980	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	86
2	Supraene	410	C30H50	007683-64-9	80
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088146.D
Acq On : 18 Jun 2016 21:01
Operator : UM/SJ
Sample : H3580-11
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B5(0-8)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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
Propane, 1,1-dime...	1.88	4.5	ng	118303	1	6.68	527164	20.0
2-Pentanone, 4-hy...	4.84	4.2	ng	109814	1	6.68	527164	20.0
unknown6.46	6.46	65.8	ng	1734400	1	6.68	527164	20.0
Pentadecane	10.16	2.1	ng	65346	3	9.72	618587	20.0
Heptadecane	10.64	3.8	ng	98714	4	11.20	526218	20.0
1-Nonadecene	13.70	3.0	ng	78322	5	13.83	515176	20.0
Squalene	14.66	2.3	ng	45980	6	15.21	400516	20.0