LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088144.D
Acq On : 18 Jun 2016 20:04
Operator : UM/SJ
Sample : H3580-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(0-6)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	5	7	15	rVV	111297	185987	9.57%	0.980%
2	1.781	15	17	24	rVV	880107	1318654	67.86%	6.947%
3	1.884	24	26	51	rVB	83615	306605	15.78%	1.615%
4	4.844	283	285	295	rBB	95601	134587	6.93%	0.709%
5	5.290	321	324	326	rBV	1758512	1869825	96.22%	9.850%
6	6.342	413	416	419	rBV2	1541910	1915343	98.56%	10.090%
7	6.456	424	426	429	rBV	1723632	1740864	89.58%	9.171%
8	6.684	444	446	449	rBV	638842	530087	27.28%	2.793%
9	6.844	457	460	462	rBV	1781472	1686968	86.81%	8.887%
10	7.256	493	496	498	rBV	1052534	1042828	53.66%	5.494%
11	7.382	502	507	512	rVB2	11955	26165	1.35%	0.138%
12	7.896	550	552	556	rBV	13266	20929	1.08%	0.110%
13	7.976	556	559	561	rBV	582961	646161	33.25%	3.404%
14	9.050	650	653	655	rBV	2166294	1943257	100.00%	10.237%
15	9.450	685	688	690	rBV	715721	604785	31.12%	3.186%
16	9.668	705	707	709	rBV	49540	43567	2.24%	0.230%
17	9.725	709	712	714	rBV	685211	641254	33.00%	3.378%
18	10.136	741	748	749	rBV	16143	28173	1.45%	0.148%
19	10.159	749	750	752	rVB	77235	71899	3.70%	0.379%
20	10.376	766	769	773	rBV	27587	53505	2.75%	0.282%
21	10.513	778	781	783	rBV	624129	738781	38.02%	3.892%
22	10.639	790	792	796	rBV	62534	110852	5.70%	0.584%
23	10.822	806	808	813	rBV3	11578	24340	1.25%	0.128%
24	11.085	829	831	832	rBV	30854	43898	2.26%	0.231%
25	11.199	839	841	843	rBV	648690	539182	27.75%	2.840%
26	12.788	977	980	982	rBV	1414802	1559871	80.27%	8.218%
27	13.359	1028	1030	1034	rBV2	12179	23982	1.23%	0.126%
28	13.702	1057	1060	1065	rBV	68277	120691	6.21%	0.636%
29	13.828	1069	1071	1074	rBV	516775	496302	25.54%	2.615%
30	14.011	1084	1087	1088	rBV	18212	25036	1.29%	0.132%
31	14.308	1111	1113	1115	rBV	25887	32350	1.66%	0.170%
32	14.662	1142	1144	1147	rVB	43356	52888	2.72%	0.279%
33	15.211	1190	1192	1197	rBV	324381	402631	20.72%	2.121%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088144.D
Acq On : 18 Jun 2016 20:04
Operator : UM/SJ
Sample : H3580-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(0-6)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: 18982247

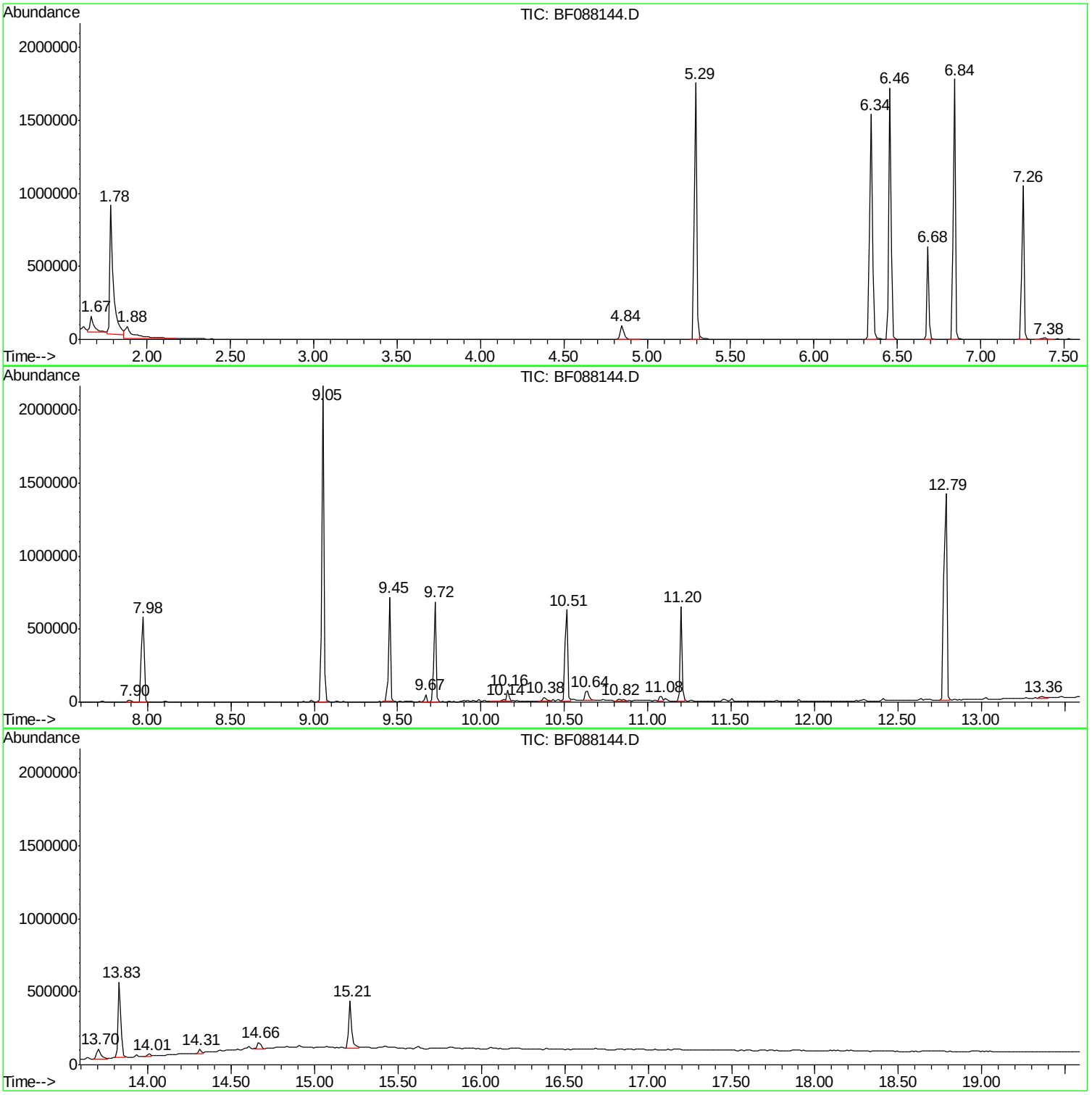
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088144.D
Acq On : 18 Jun 2016 20:04
Operator : UM/SJ
Sample : H3580-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(0-6)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 : BF088144.D
Acq On : 18 Jun 2016 20:04
Operator : UM/SJ
Sample : H3580-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(0-6)C

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

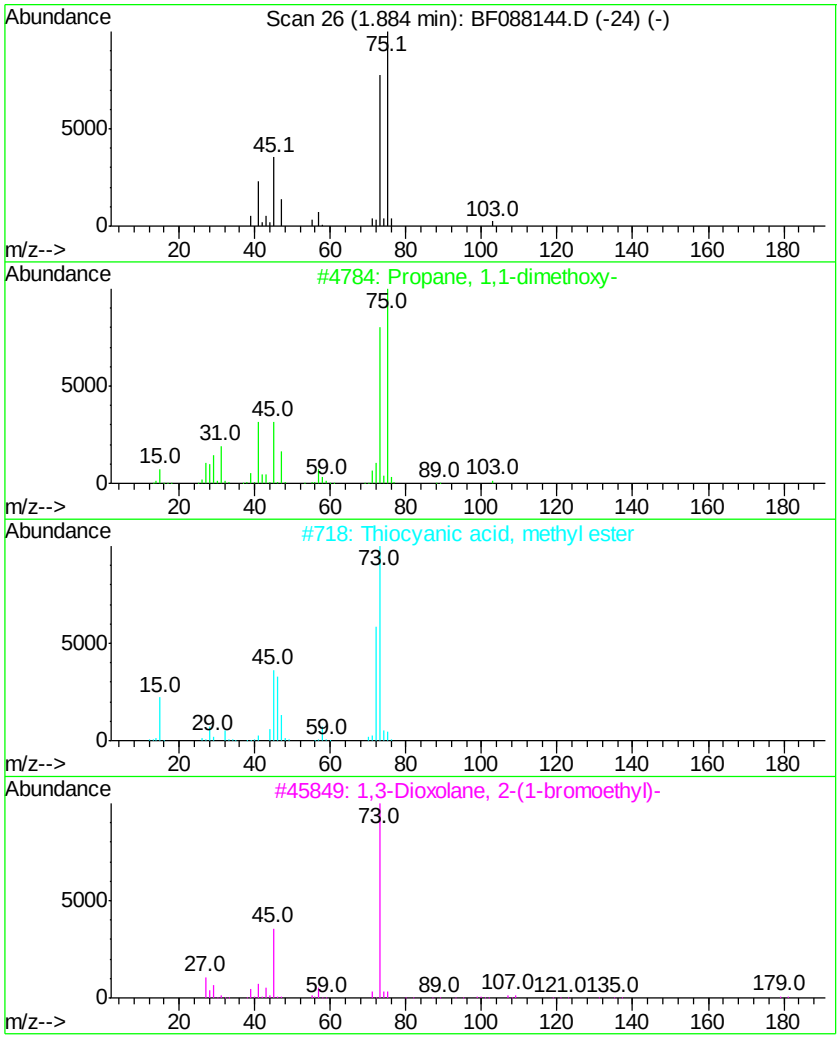
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

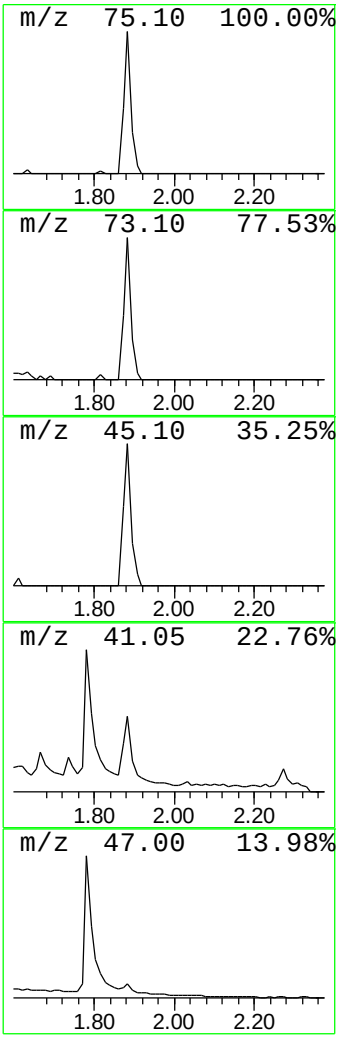
****

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.88	11.57 ng	306605	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	83
2	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	16
3	1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	10
4	Glycine	75	C2H5NO2	000056-40-6	9
5	Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088144.D
Acq On : 18 Jun 2016 20:04
Operator : UM/SJ
Sample : H3580-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(0-6)C

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

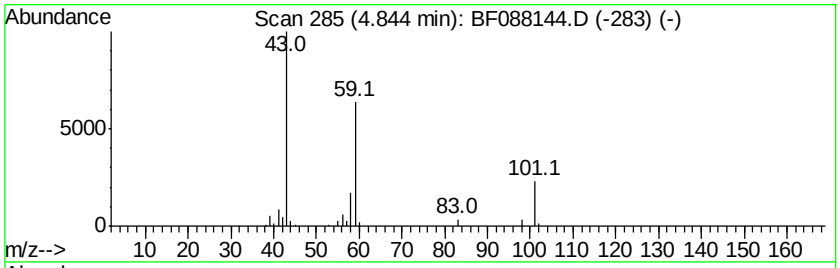
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

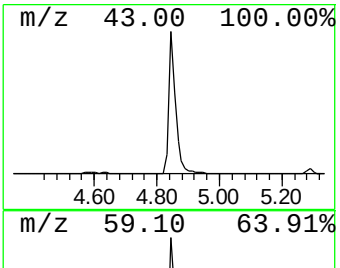
****

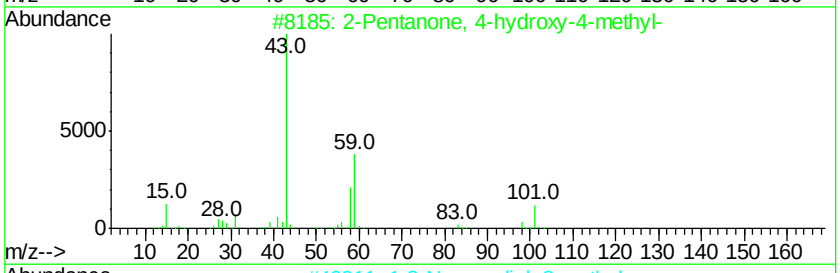
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

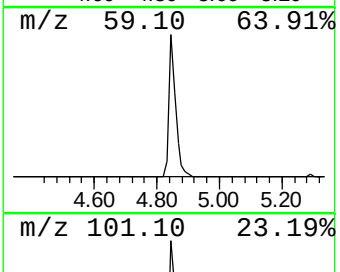
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.84	5.08 ng	134587	1,4-Dichlorobenzene-d4	6.68

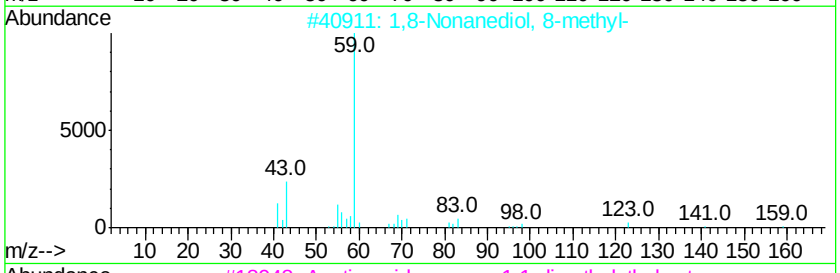
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9

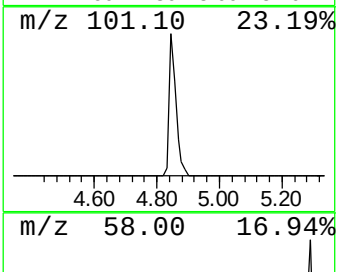


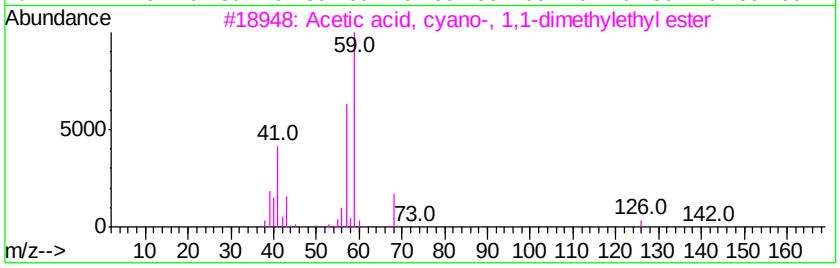


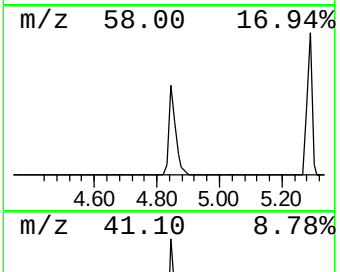


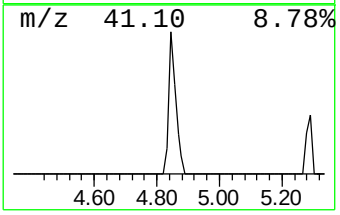












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Instrument : BNA_F
ClientSampleId : 08-B4(0-6)C

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

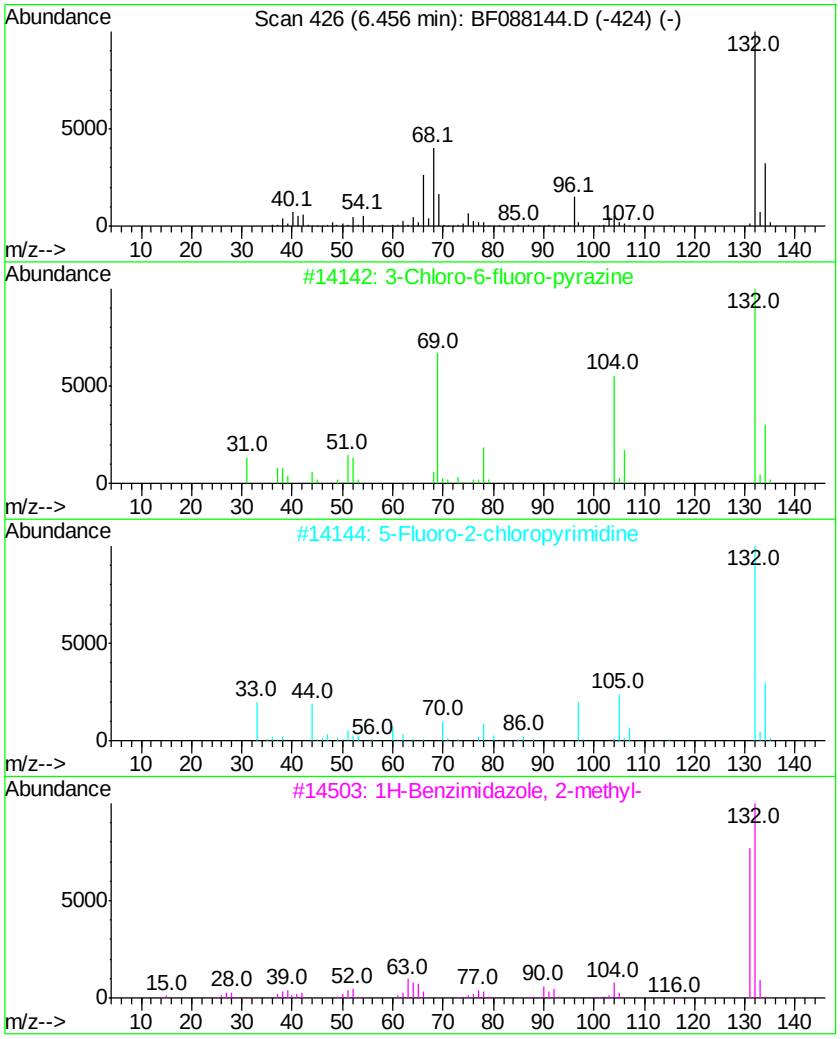
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

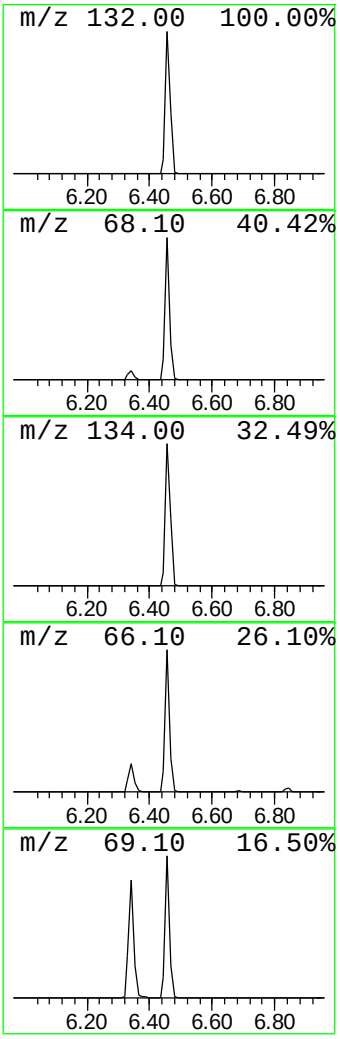
****

Peak Number 5 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	65.68 ng	1740860	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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

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Data File : BF088144.D
Acq On : 18 Jun 2016 20:04
Operator : UM/SJ
Sample : H3580-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(0-6)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
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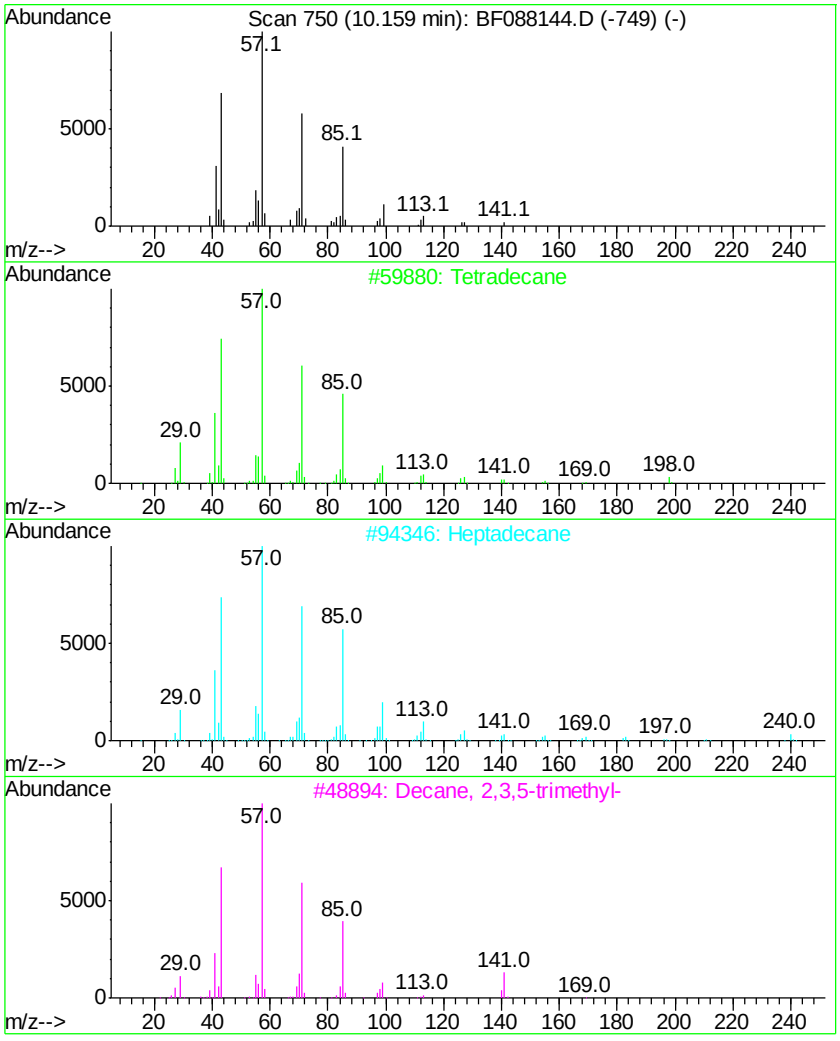
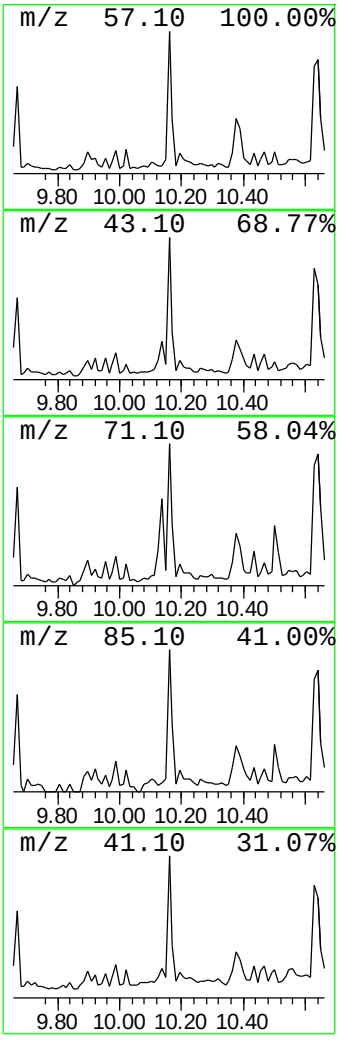
****

Peak Number 7 Tetradecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	2.24 ng	71899	Acenaphthene-d10	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	90
2	Heptadecane	240	C17H36	000629-78-7	83
3	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
4	Hexadecane	226	C16H34	000544-76-3	80
5	Tridecane	184	C13H28	000629-50-5	64





Library Search Compound Report

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Operator : UM/SJ
Sample : H3580-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(0-6)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
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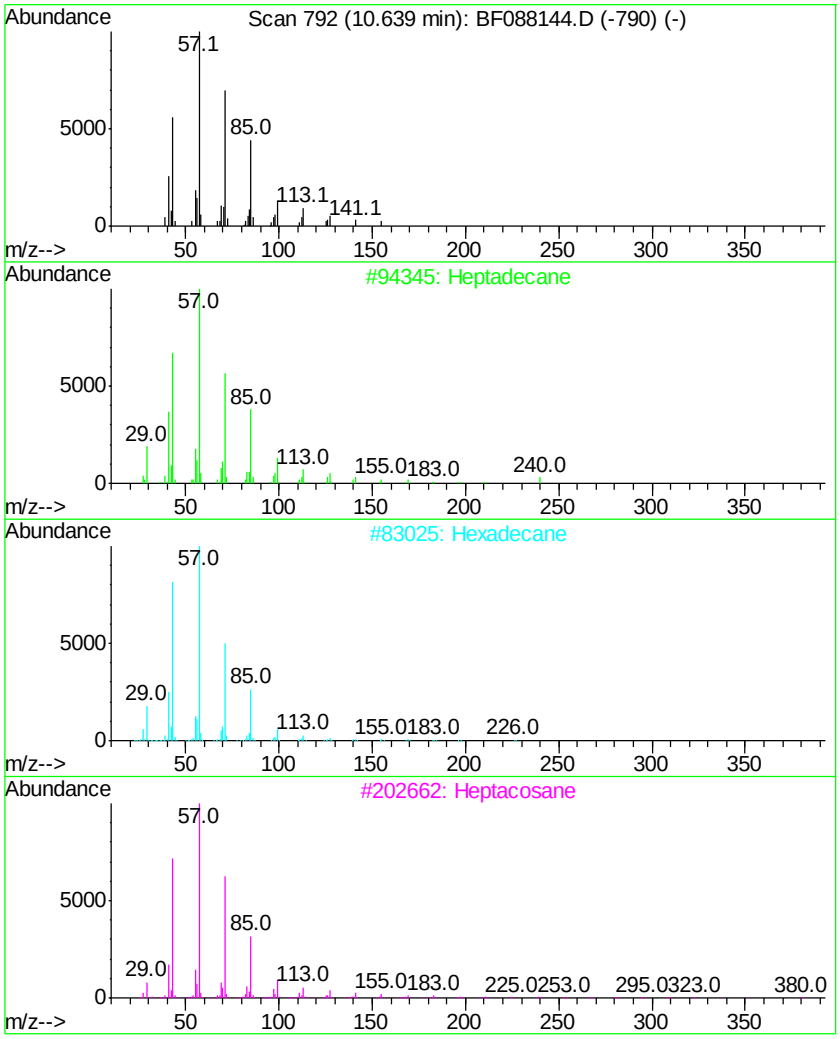
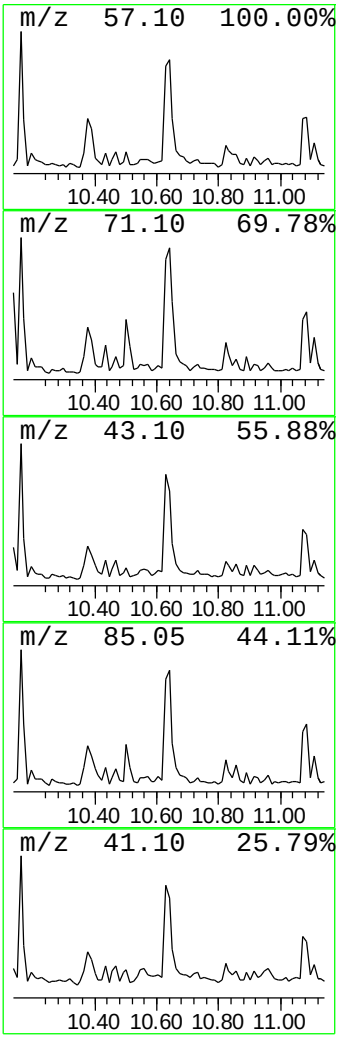
****

Peak Number 8 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	4.11 ng	110852	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	Heptacosane	380	C27H56	000593-49-7	90
4	Pentadecane	212	C15H32	000629-62-9	86
5	Octacosane	394	C28H58	000630-02-4	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061816\
Data File : BF088144.D
Acq On : 18 Jun 2016 20:04
Operator : UM/SJ
Sample : H3580-07
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 08-B4(0-6)C

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

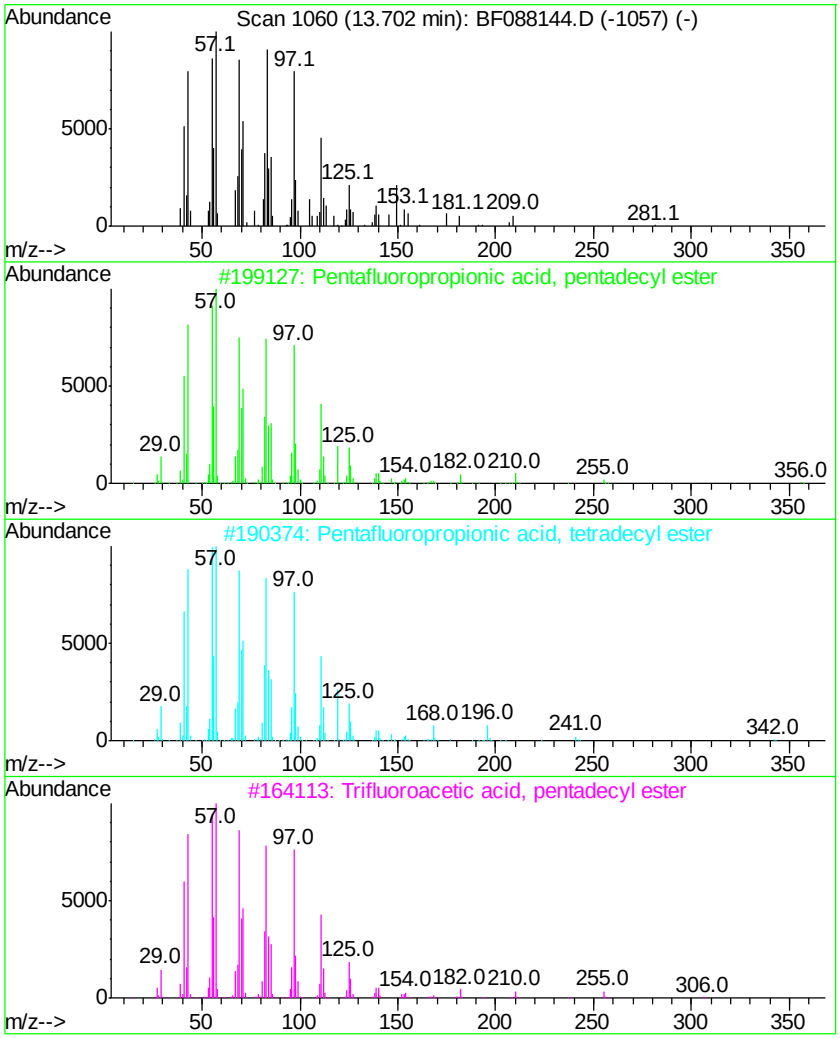
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

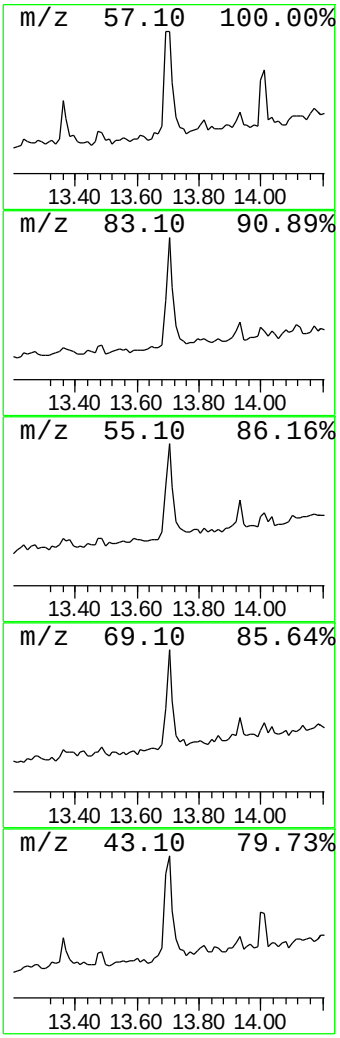
****

Peak Number 9 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	4.86 ng	120691	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95





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Misc :
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Instrument : BNA_F
ClientSampleId : 08-B4(0-6)C

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

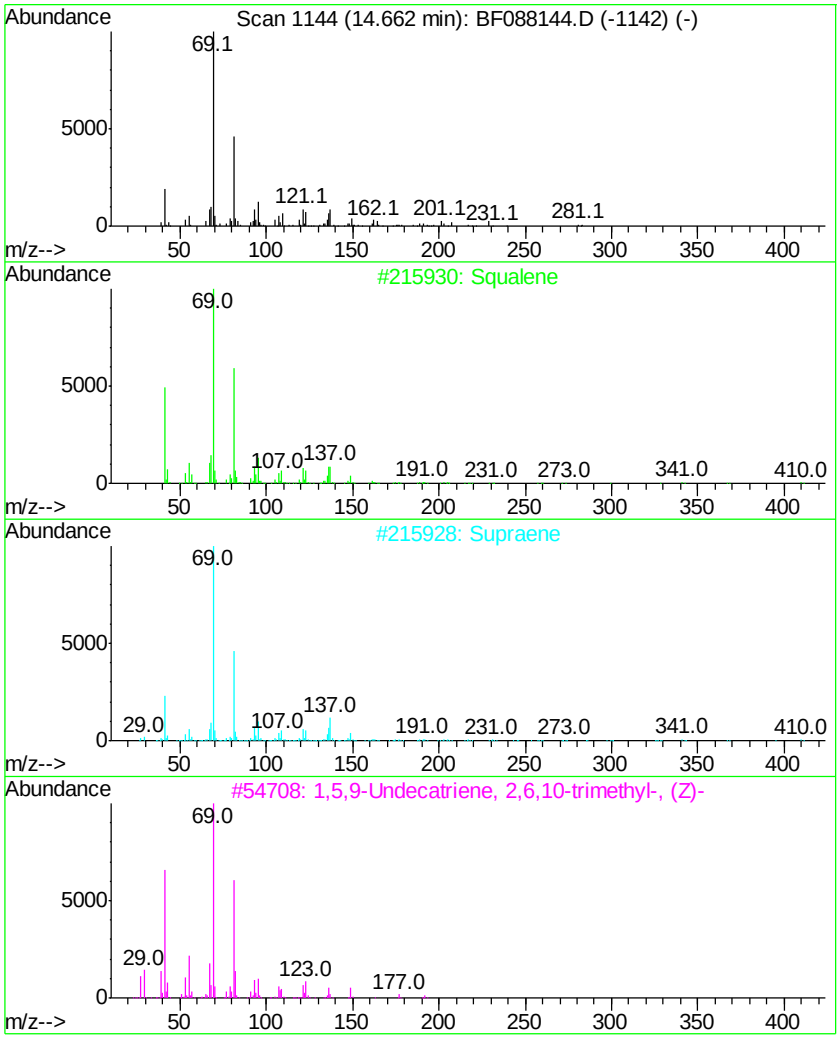
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

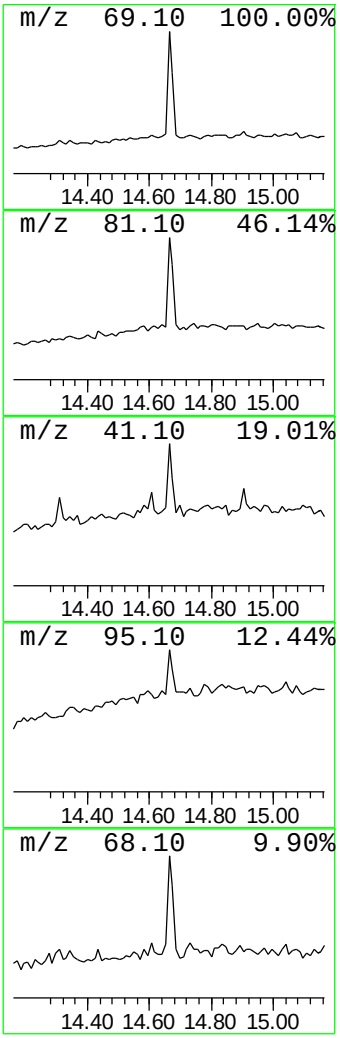
****

Peak Number 10 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	2.63 ng	52888	Perylene-d12	15.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	90
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	78
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061816\
Data File : BF088144.D
Acq On : 18 Jun 2016 20:04
Operator : UM/SJ
Sample : H3580-07
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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	11.6	ng	306605	1	6.68	530087	20.0
2-Pentanone, 4-hy...	4.84	5.1	ng	134587	1	6.68	530087	20.0
unknown6.46	6.46	65.7	ng	1740860	1	6.68	530087	20.0
Tetradecane	10.16	2.2	ng	71899	3	9.72	641254	20.0
Heptadecane	10.64	4.1	ng	110852	4	11.20	539182	20.0
Pentafluoropropio...	13.70	4.9	ng	120691	5	13.83	496302	20.0
Squalene	14.66	2.6	ng	52888	6	15.21	402631	20.0