LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088597.D
Acq On : 2 Jul 2016 2:35
Operator : UM/SJ
Sample : H3816-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-COMP

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-BF063016.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	3	7	9	rVB	4652550	6986830	100.00%	17.820%
2	1.735	12	13	23	rVB	584577	904263	12.94%	2.306%
3	1.861	23	24	39	rVB	2333007	5509837	78.86%	14.053%
4	2.055	39	41	76	rVB2	141554	765094	10.95%	1.951%
5	3.118	125	134	137	rBV	218681	786359	11.25%	2.006%
6	4.981	294	297	302	rVB	178413	235221	3.37%	0.600%
7	5.404	331	334	337	rBV	2408067	2506708	35.88%	6.393%
8	6.444	422	425	427	rBV	2679358	3017816	43.19%	7.697%
9	6.570	434	436	439	rBV	2016354	2819515	40.35%	7.191%
10	6.810	455	457	459	rBV	856896	799714	11.45%	2.040%
11	6.970	468	471	473	rVB	1428794	1981910	28.37%	5.055%
12	7.370	503	506	508	rBV	1751959	1675390	23.98%	4.273%
13	8.090	567	569	572	rBV	1193980	1001835	14.34%	2.555%
14	9.165	661	663	666	rBV	2011839	2765914	39.59%	7.054%
15	9.565	695	698	700	rBV	375158	343329	4.91%	0.876%
16	9.839	720	722	725	rVB	979364	948803	13.58%	2.420%
17	10.628	788	791	793	rBV	1515971	1455318	20.83%	3.712%
18	11.199	839	841	843	rBV	110929	115123	1.65%	0.294%
19	11.314	849	851	853	rVB2	599839	785629	11.24%	2.004%
20	11.382	853	857	861	rVB3	33620	74837	1.07%	0.191%
21	11.634	877	879	881	rVB	67483	88108	1.26%	0.225%
22	12.902	987	990	992	rBV	2224959	1980902	28.35%	5.052%
23	13.382	1030	1032	1038	rBV2	45781	86871	1.24%	0.222%
24	13.817	1067	1070	1079	rBV	112048	167937	2.40%	0.428%
25	13.942	1079	1081	1084	rBV	884135	800546	11.46%	2.042%
26	15.348	1201	1204	1206	rBV	473760	604078	8.65%	1.541%

Sum of corrected areas: 39207887

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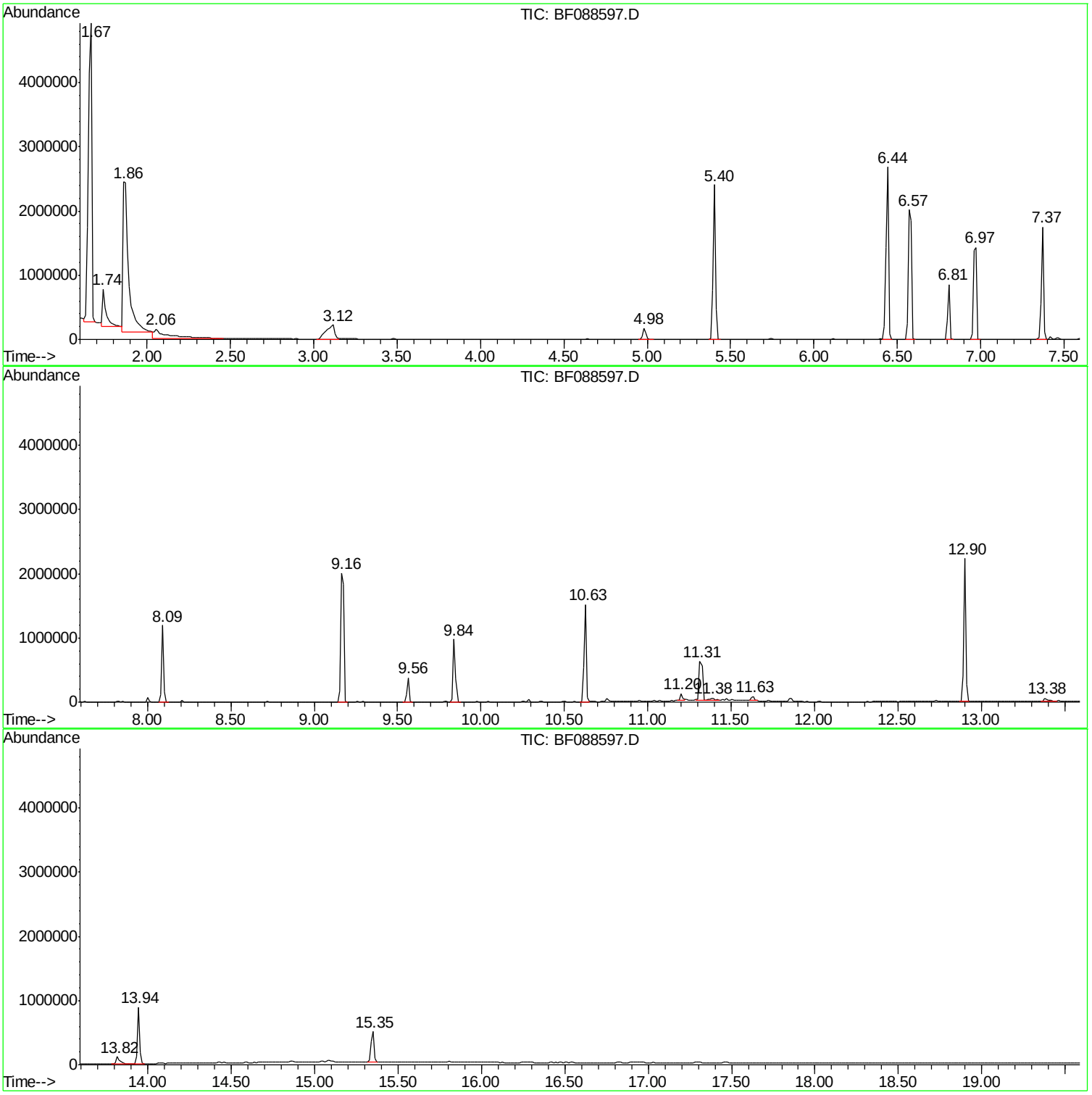
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-04-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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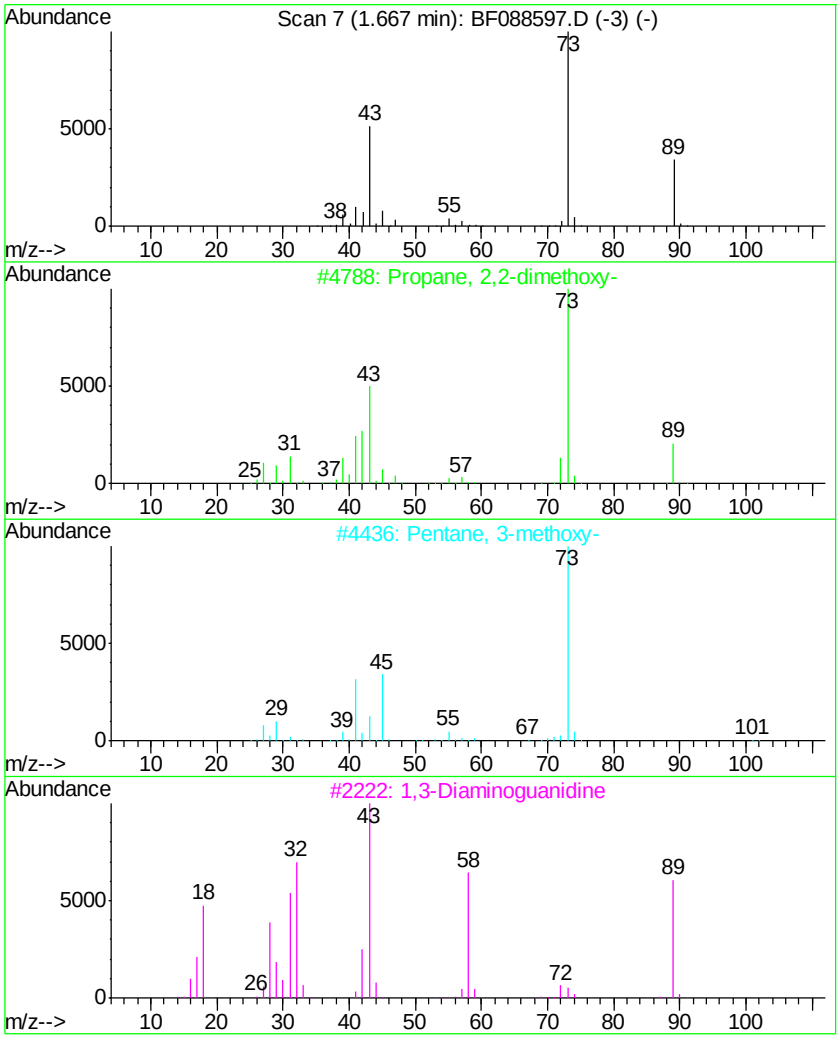
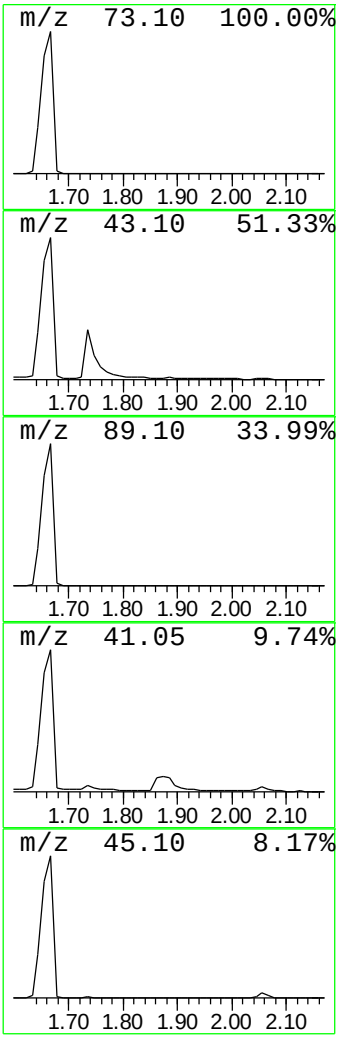
Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	174.73 ng	6986830	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Instrument : BNA_F
ClientSampleId : SB-04-COMP

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TIC Library : C:\Database\NIST11.L
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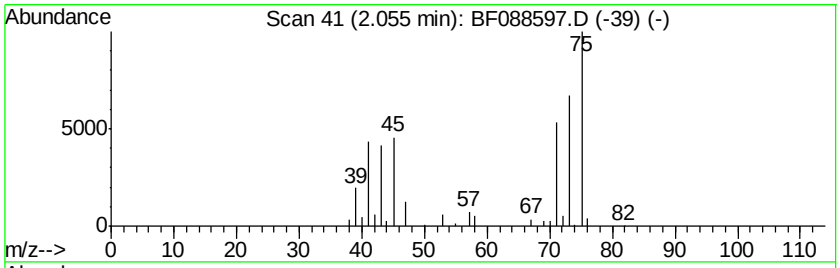
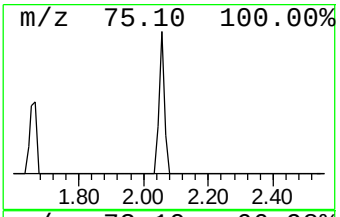
****

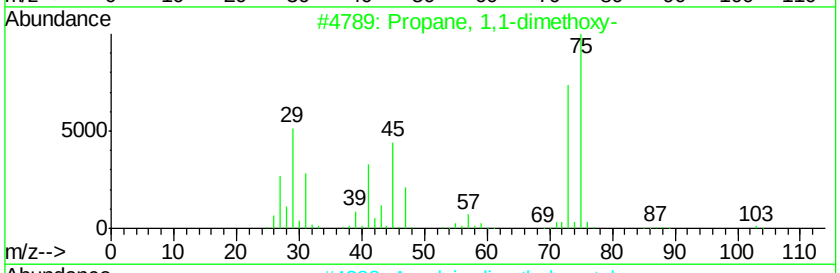
Peak Number 4 unknown2.06 Concentration Rank 7

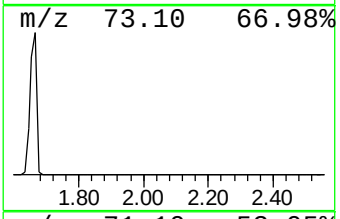
R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	19.13 ng	765094	1,4-Dichlorobenzene-d4	6.81

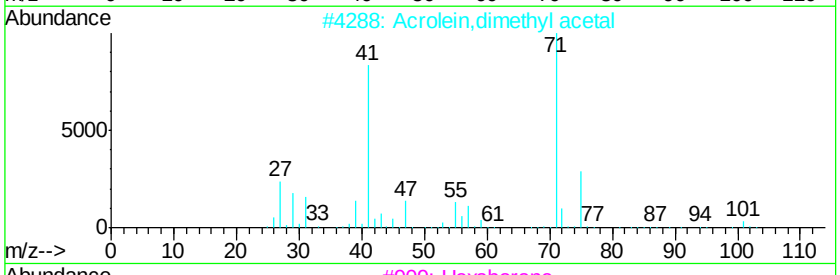
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	36
2	Acrolein,dimethyl acetal	102	C5H10O2	006044-68-4	10
3	Hexaborane	76	B6H10	023777-80-2	10
4	2(3H)-Furanone, dihydro-3-hydrox...	130	C6H10O3	000079-50-5	9
5	5H-Tetrazole-5-thione, 1-[2-(dim...	173	C5H11N5S	061607-68-9	9

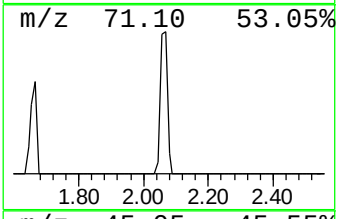


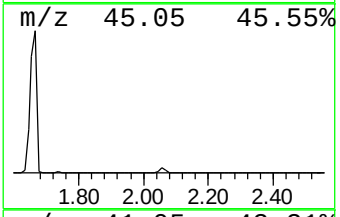


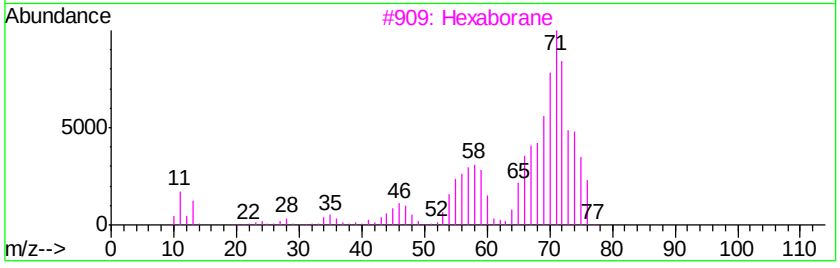


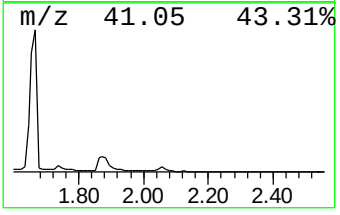












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Instrument : BNA_F
ClientSampleId : SB-04-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

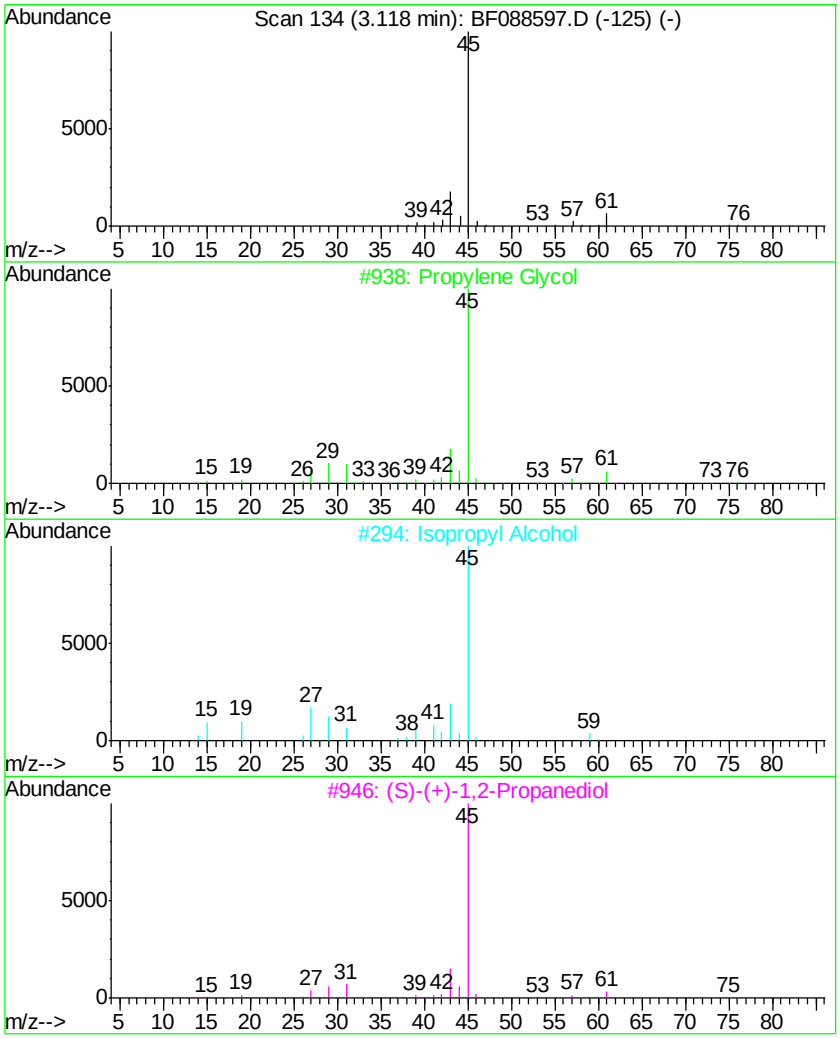
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

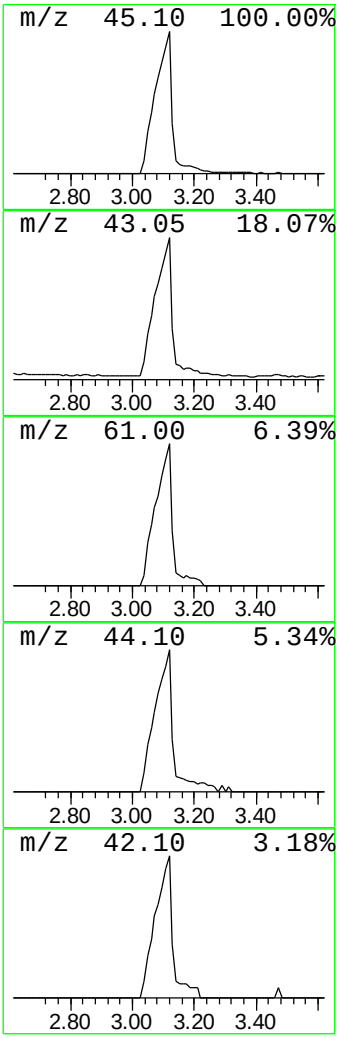
****

Peak Number 5 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.12	19.67 ng	786359	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	86
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
4	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9





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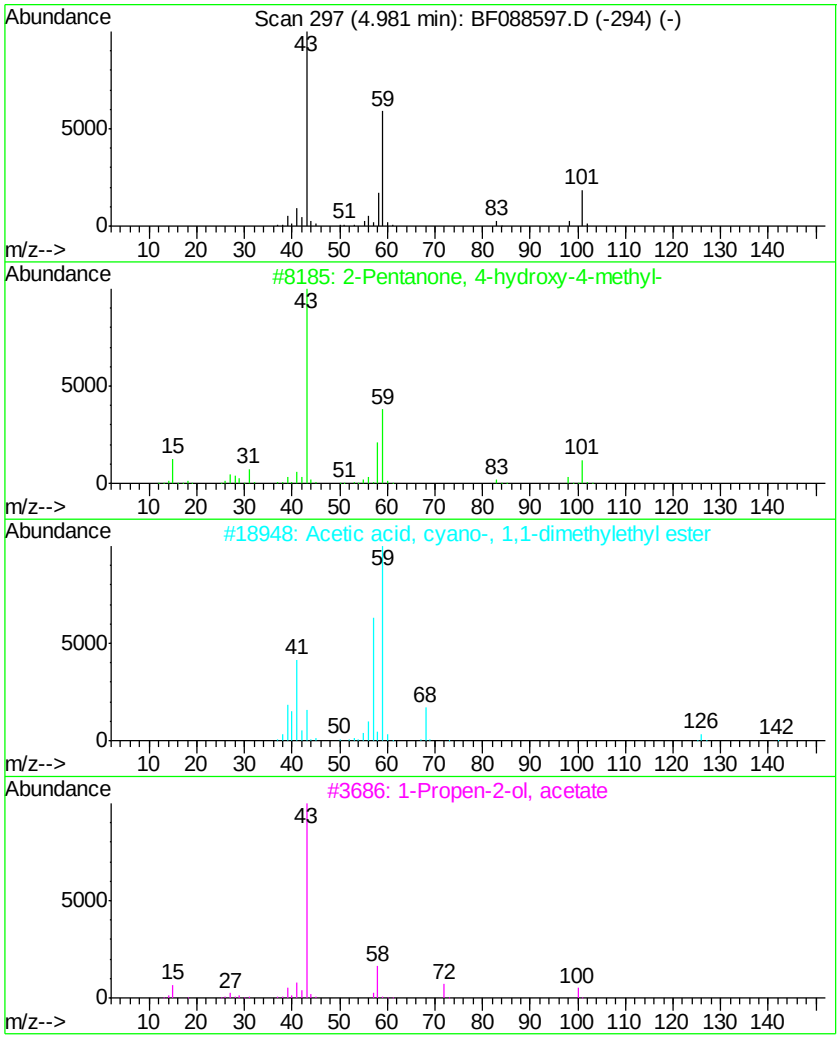
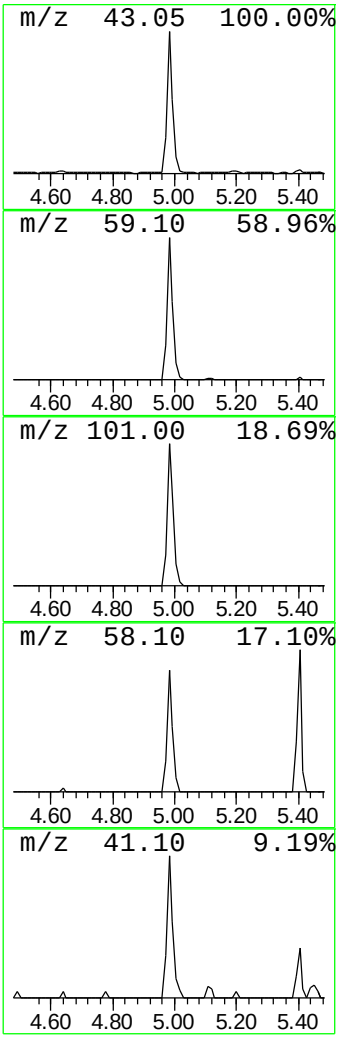
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	5.88 ng	235221	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

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Operator : UM/SJ
Sample : H3816-14
Misc :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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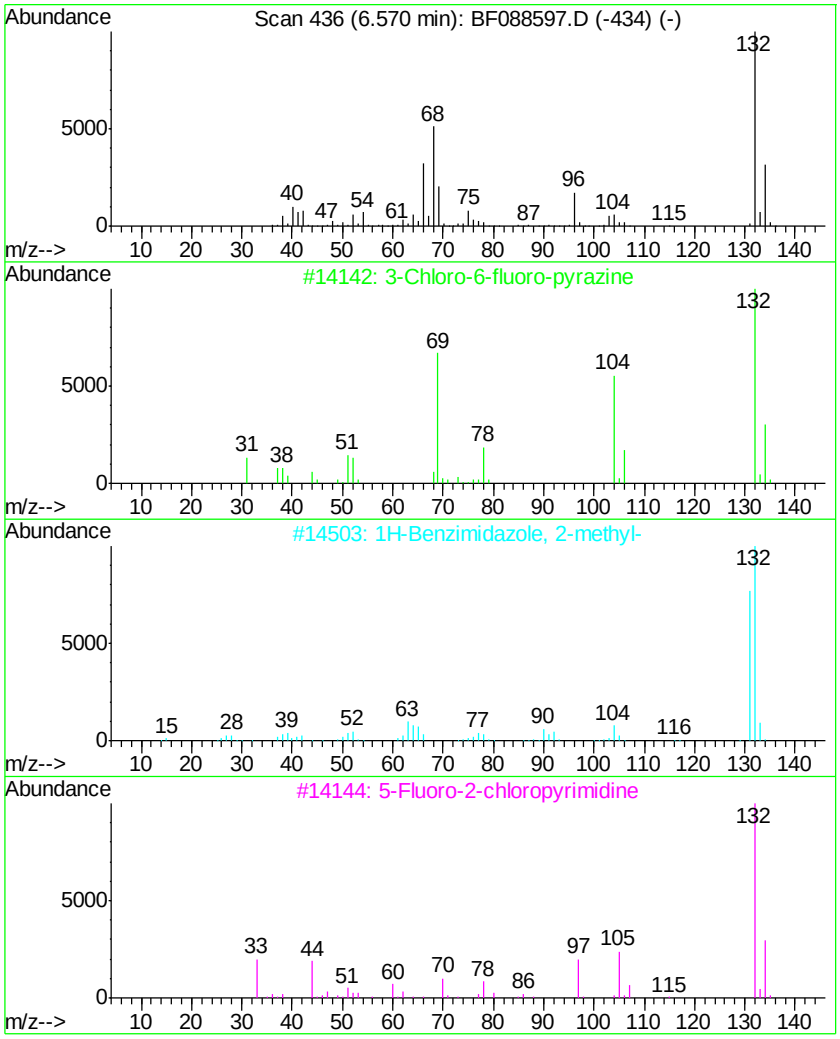
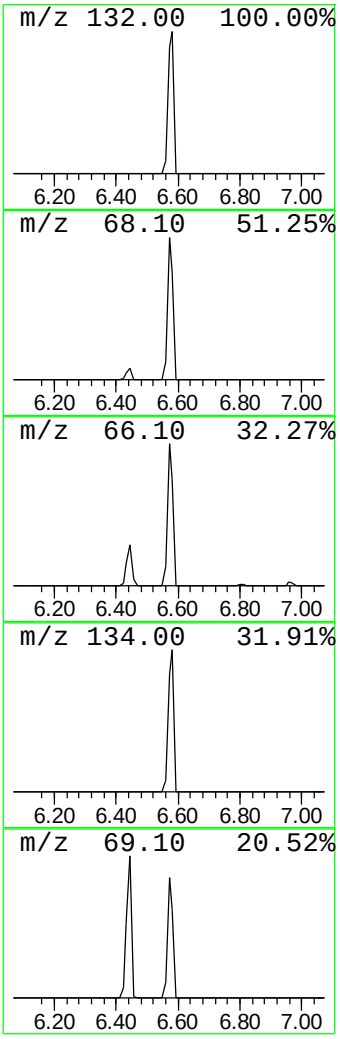
Peak Number 7 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	70.51 ng	2819520	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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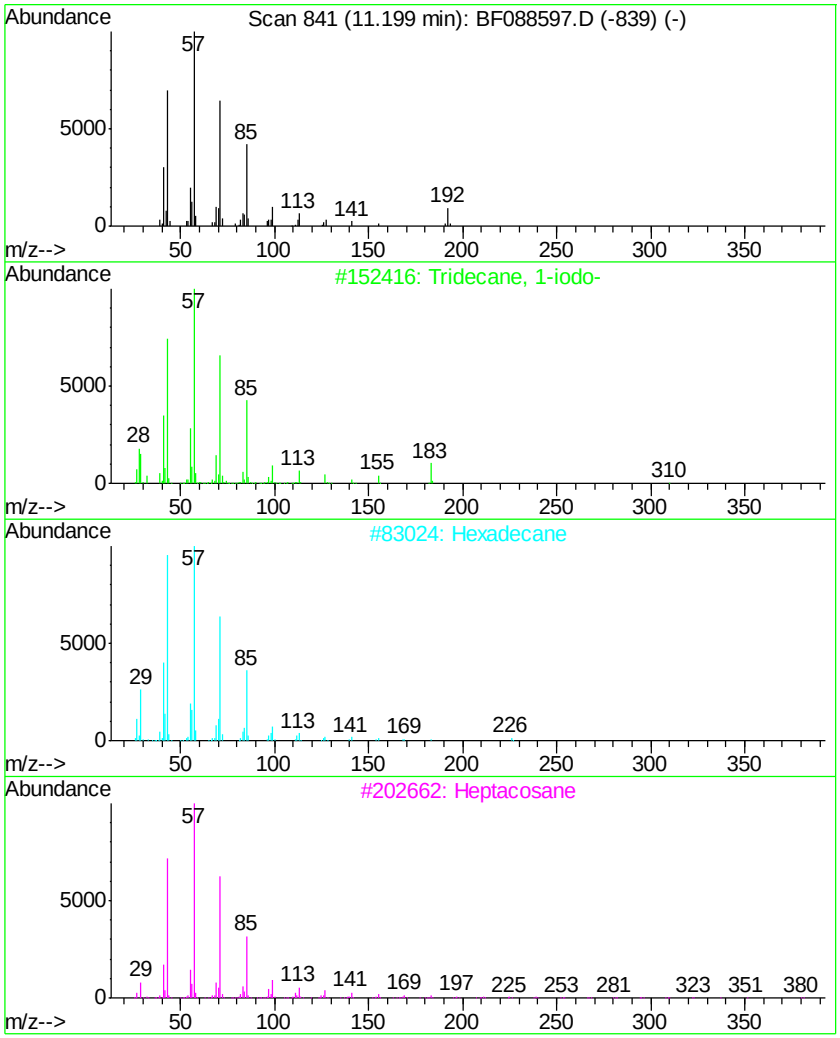
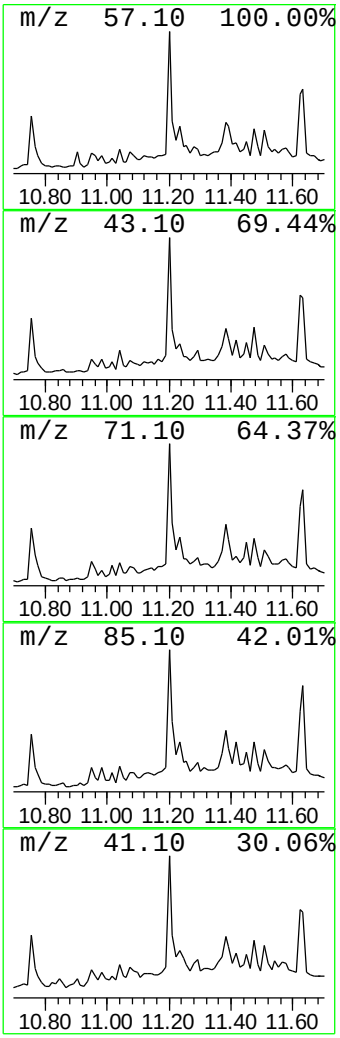
Peak Number 9 Tridecane, 1-iodo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	2.93 ng	115123	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
2	Hexadecane	226	C16H34	000544-76-3	78
3	Heptacosane	380	C27H56	000593-49-7	78
4	Eicosane	282	C20H42	000112-95-8	72
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	64





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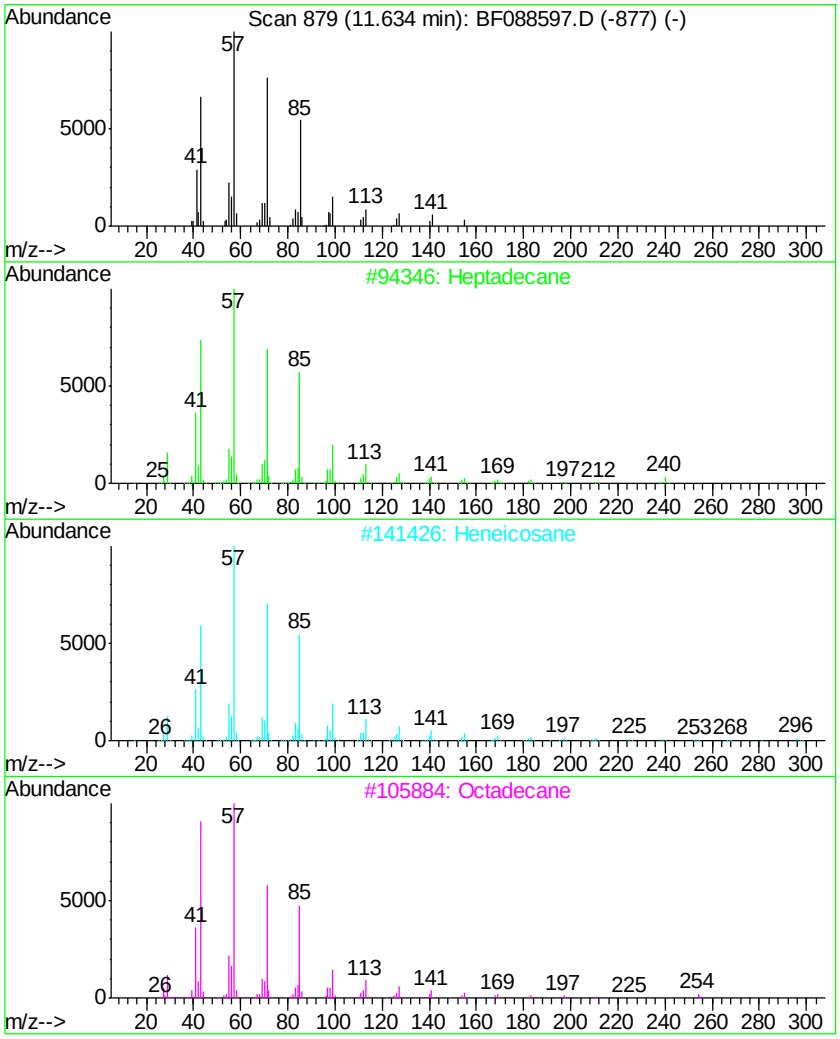
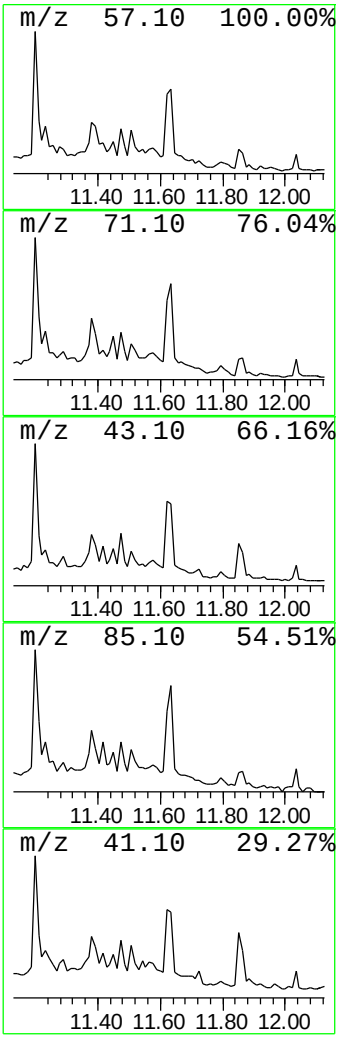
Peak Number 10 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.63	2.24 ng	88108	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Heptacosane	380	C27H56	000593-49-7	90
5	Hexadecane	226	C16H34	000544-76-3	90





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TIC Library : C:\Database\NIST11.L
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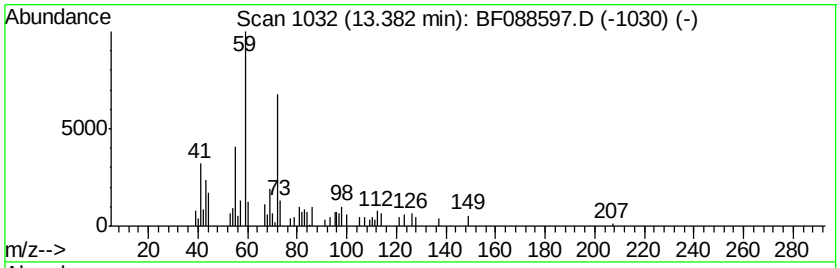
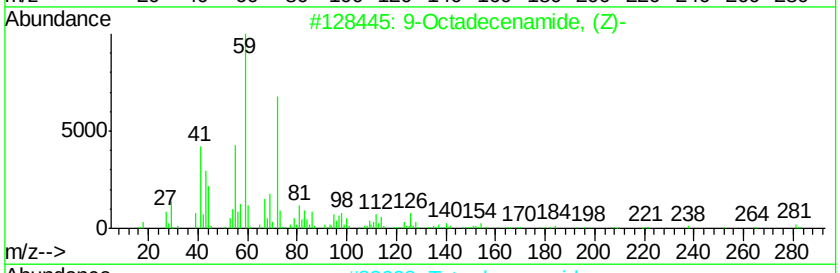
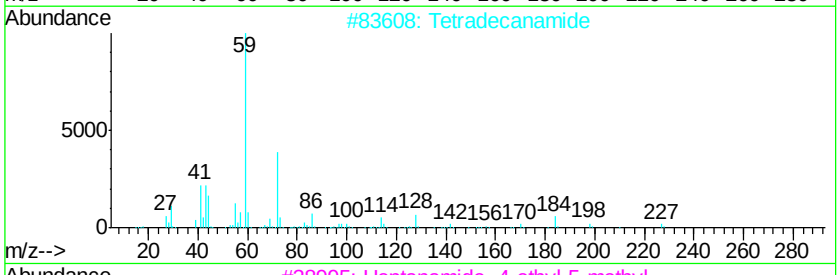
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 12

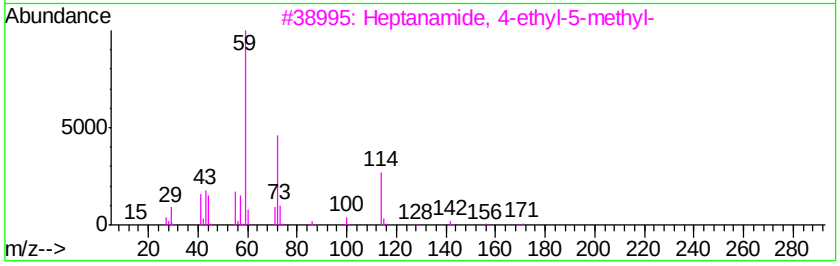
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	2.17 ng	86871	Chrysene-d12	13.94

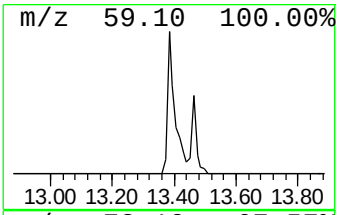
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Tetradecanamide	227	C14H29NO	000638-58-4	72
3	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
4	Dodecanamide	199	C12H25NO	001120-16-7	59
5	Silane, octyl-	144	C8H20Si	000871-92-1	47

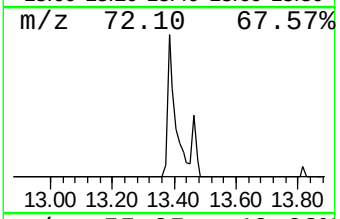


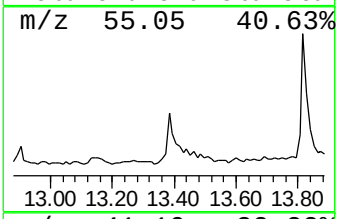


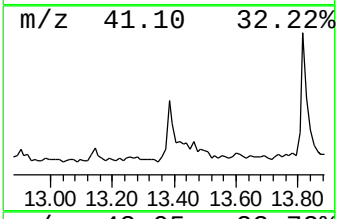


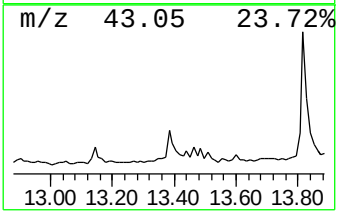












Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088597.D
Acq On : 2 Jul 2016 2:35
Operator : UM/SJ
Sample : H3816-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

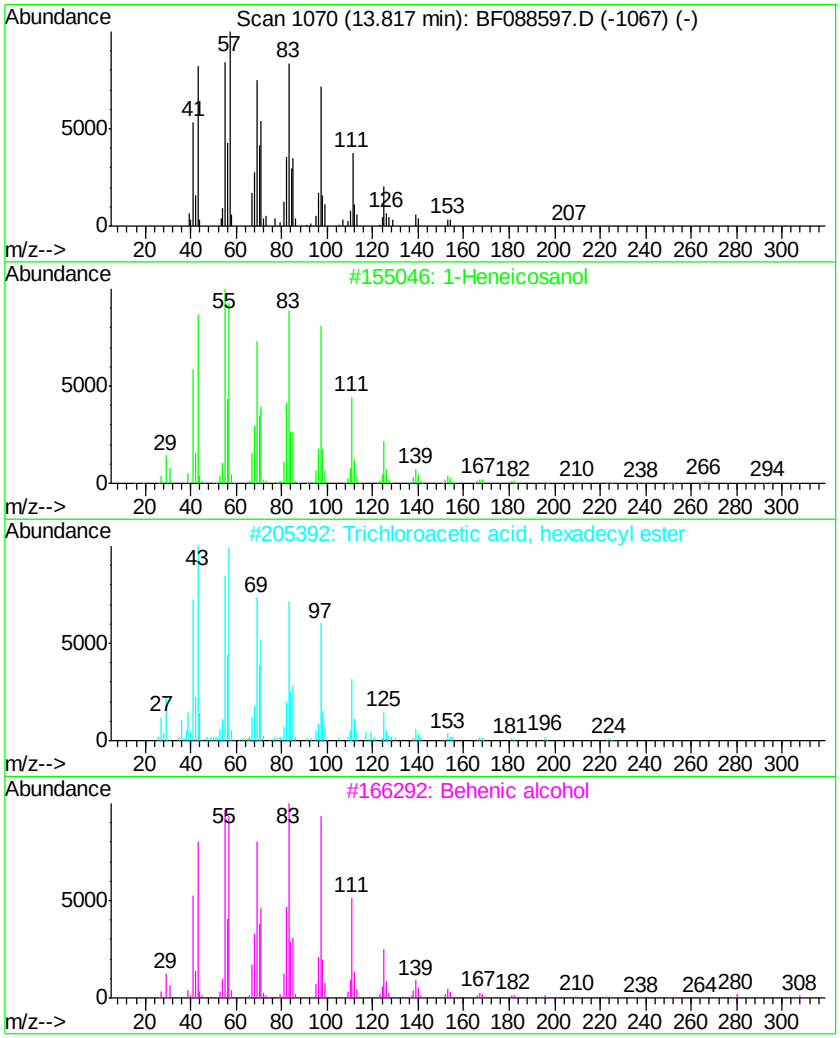
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

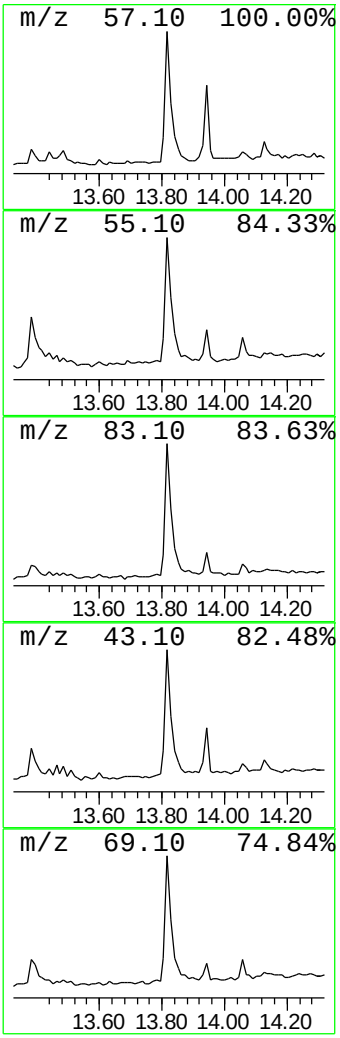
****

Peak Number 12 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.20 ng	167937	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
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	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088597.D
Acq On : 2 Jul 2016 2:35
Operator : UM/SJ
Sample : H3816-14
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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, 2,2-dime...	1.67	174.7	ng	6986830	1	6.81	799714	20.0
unknown2.06	2.06	19.1	ng	765094	1	6.81	799714	20.0
Propylene Glycol	3.12	19.7	ng	786359	1	6.81	799714	20.0
2-Pentanone, 4-hy...	4.98	5.9	ng	235221	1	6.81	799714	20.0
unknown6.57	6.57	70.5	ng	2819520	1	6.81	799714	20.0
Tridecane, 1-iodo-	11.20	2.9	ng	115123	4	11.32	785629	20.0
Heptadecane	11.63	2.2	ng	88108	4	11.32	785629	20.0
9-Octadecenamide,...	13.38	2.2	ng	86871	5	13.94	800546	20.0
1-Heneicosanol	13.82	4.2	ng	167937	5	13.94	800546	20.0