LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070116\
Data File : BF088596.D
Acq On : 2 Jul 2016 2:05
Operator : UM/SJ
Sample : H3816-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-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	4	7	10	rVB	4544087	6485353	100.00%	16.134%
2	1.735	12	13	23	rVB	599554	931523	14.36%	2.317%
3	1.861	23	24	40	rVB	2598610	5673552	87.48%	14.115%
4	2.055	40	41	75	rVB2	117550	682783	10.53%	1.699%
5	3.130	127	135	137	rBV	216725	807621	12.45%	2.009%
6	4.981	294	297	301	rVB	167196	239033	3.69%	0.595%
7	5.404	331	334	337	rBV	2347530	2553018	39.37%	6.351%
8	6.444	422	425	427	rVB	2593263	2984995	46.03%	7.426%
9	6.570	433	436	439	rBV	2075458	2781702	42.89%	6.920%
10	6.810	454	457	459	rBV	933362	854812	13.18%	2.127%
11	6.970	468	471	473	rVB	1630825	2241377	34.56%	5.576%
12	7.370	503	506	508	rBV	1790328	1741872	26.86%	4.333%
13	8.090	566	569	571	rVV	1234552	1057905	16.31%	2.632%
14	9.165	660	663	666	rBV	2146051	2849889	43.94%	7.090%
15	9.565	695	698	700	rBV	306052	306930	4.73%	0.764%
16	9.839	720	722	724	rBV	1012888	987675	15.23%	2.457%
17	10.628	788	791	793	rBV	1412808	1442824	22.25%	3.589%
18	11.199	839	841	843	rBV	96399	99176	1.53%	0.247%
19	11.313	849	851	854	rBV	632007	846363	13.05%	2.106%
20	11.393	855	858	861	rVB2	33797	67262	1.04%	0.167%
21	11.633	876	879	882	rVB	59588	83032	1.28%	0.207%
22	11.851	896	898	900	rBV	64389	77047	1.19%	0.192%
23	12.525	954	957	959	rBV	214278	182731	2.82%	0.455%
24	12.754	974	977	979	rBV	167194	209292	3.23%	0.521%
25	12.902	988	990	993	rVB	2082342	1893422	29.20%	4.710%
26	13.816	1066	1070	1077	rBV2	154844	232056	3.58%	0.577%
27	13.942	1078	1081	1087	rVB	868057	964575	14.87%	2.400%
28	14.457	1121	1126	1129	rBV4	45755	116220	1.79%	0.289%
29	14.948	1166	1169	1174	rBV	74041	156270	2.41%	0.389%
30	15.279	1196	1198	1201	rBV	51521	66367	1.02%	0.165%
31	15.348	1201	1204	1206	rBV	372539	579863	8.94%	1.443%

Sum of corrected areas: 40196540

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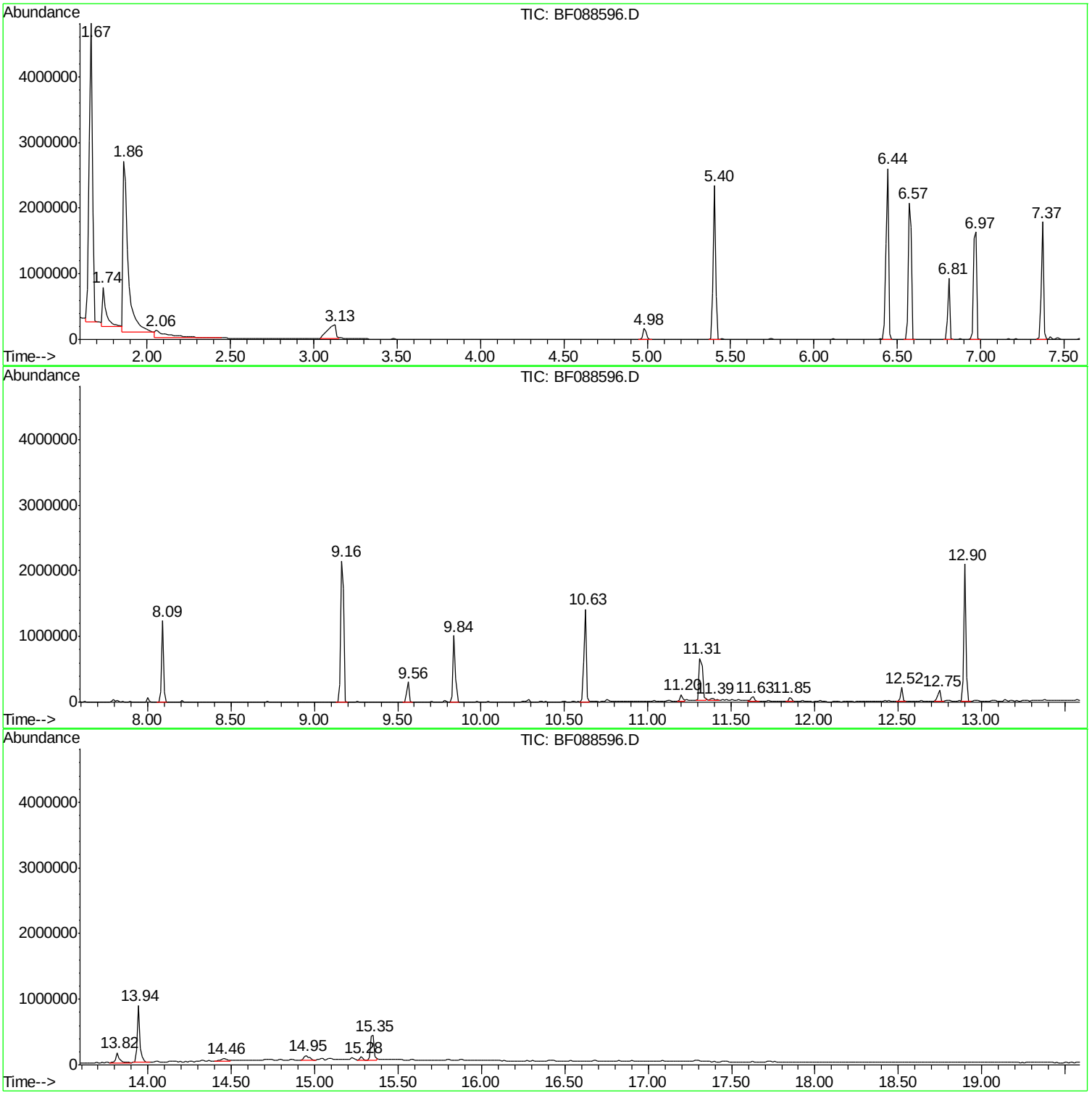
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-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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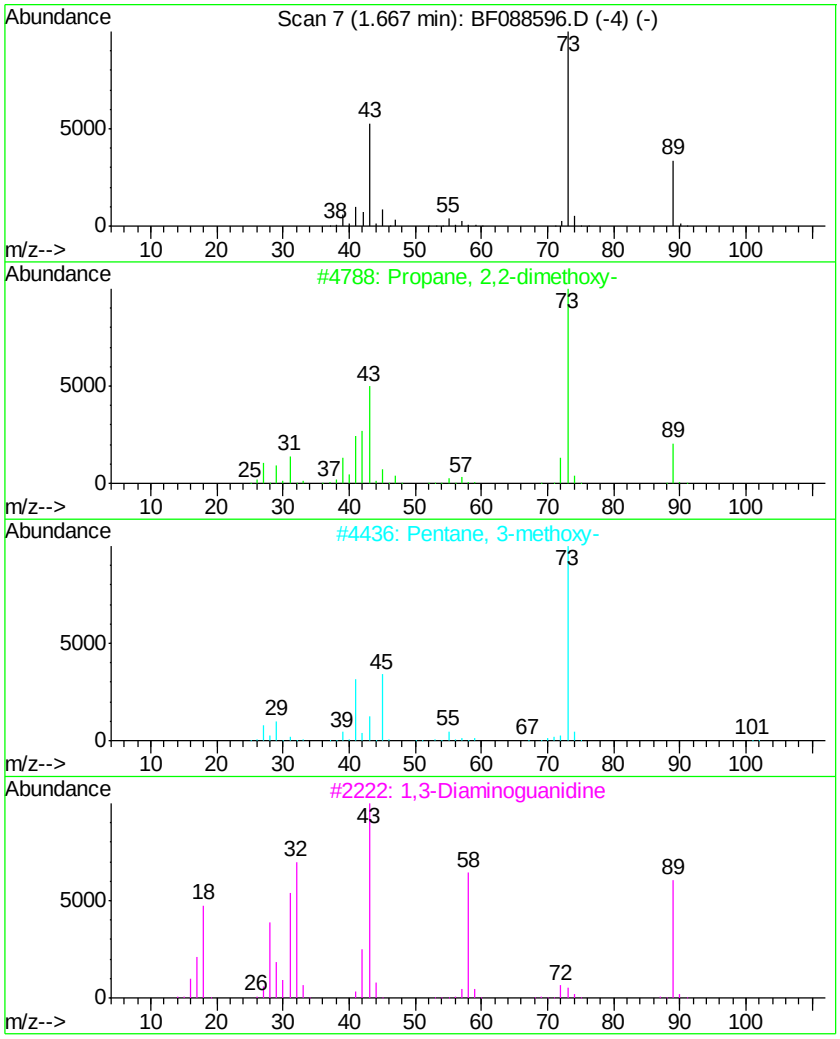
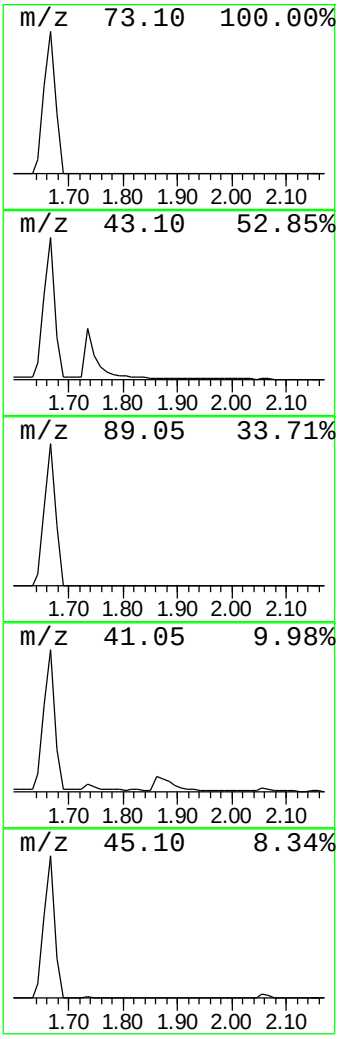
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.67	151.74 ng	6485350	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	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : SB-05-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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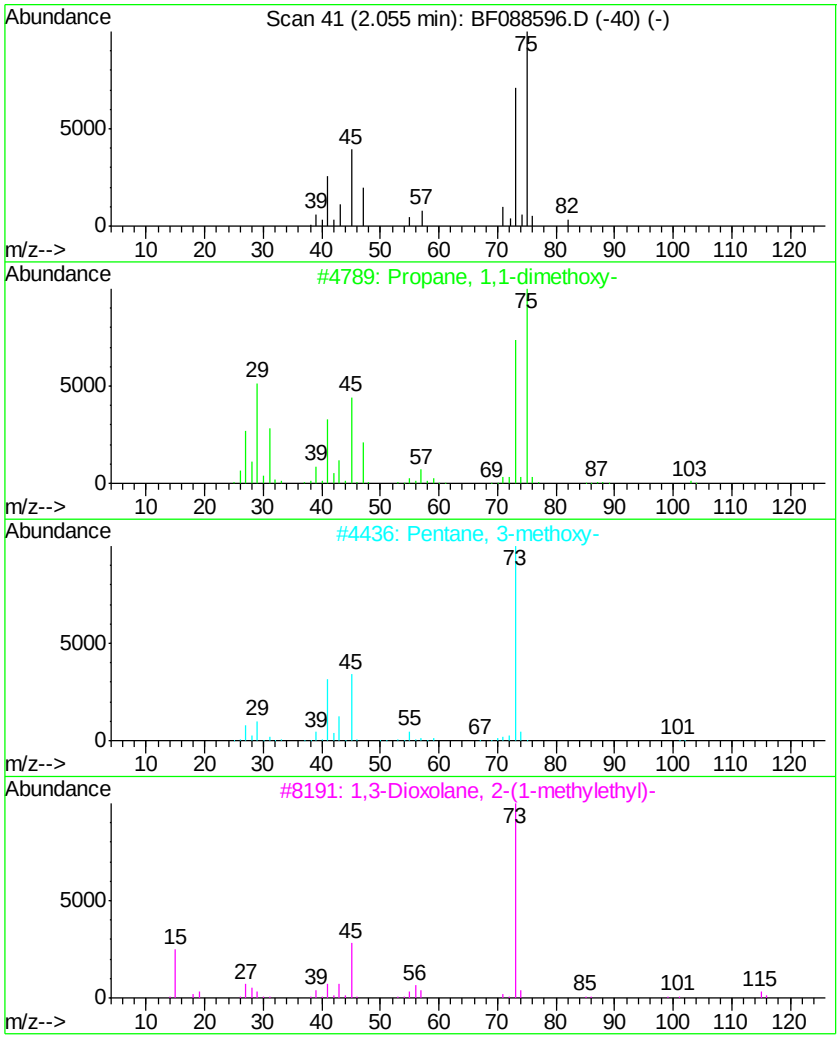
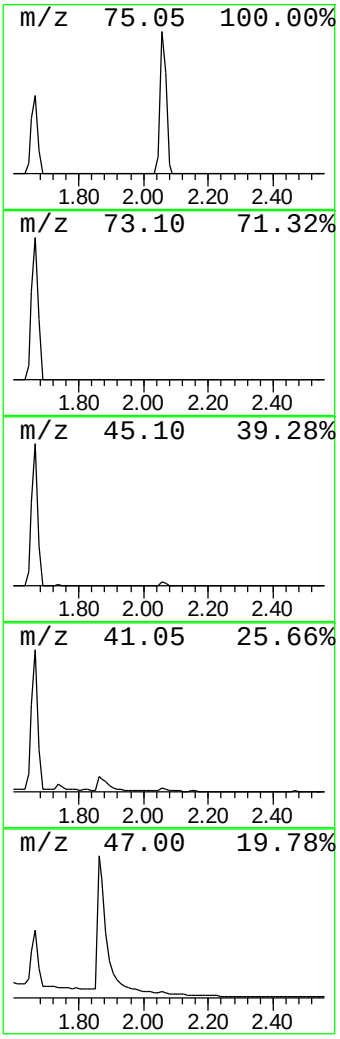
Peak Number 4 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.06	15.98 ng	682783	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	78
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
4	Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
5	Glycine	75	C2H5NO2	000056-40-6	7





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Sample : H3816-12
Misc :
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Instrument : BNA_F
ClientSampleId : SB-05-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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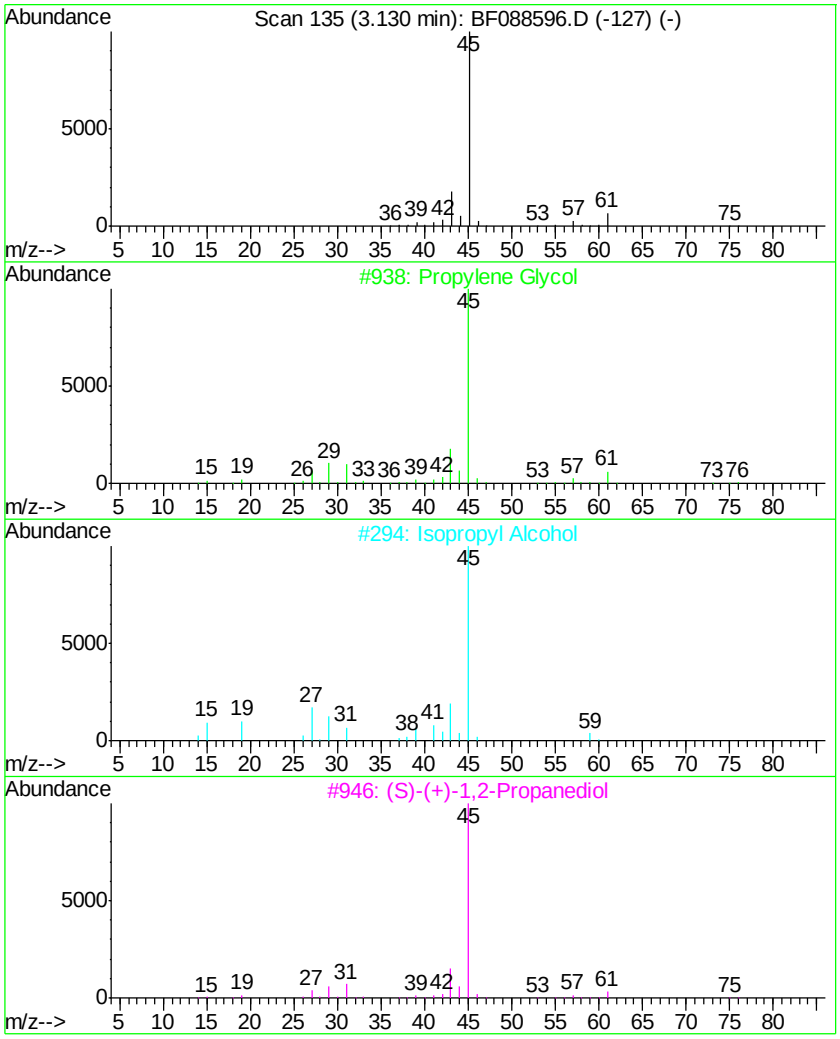
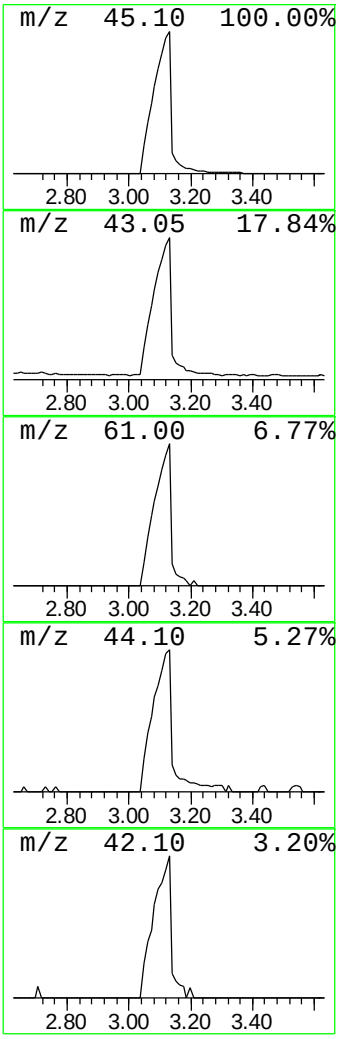
Peak Number 5 Propylene Glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	18.90 ng	807621	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
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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ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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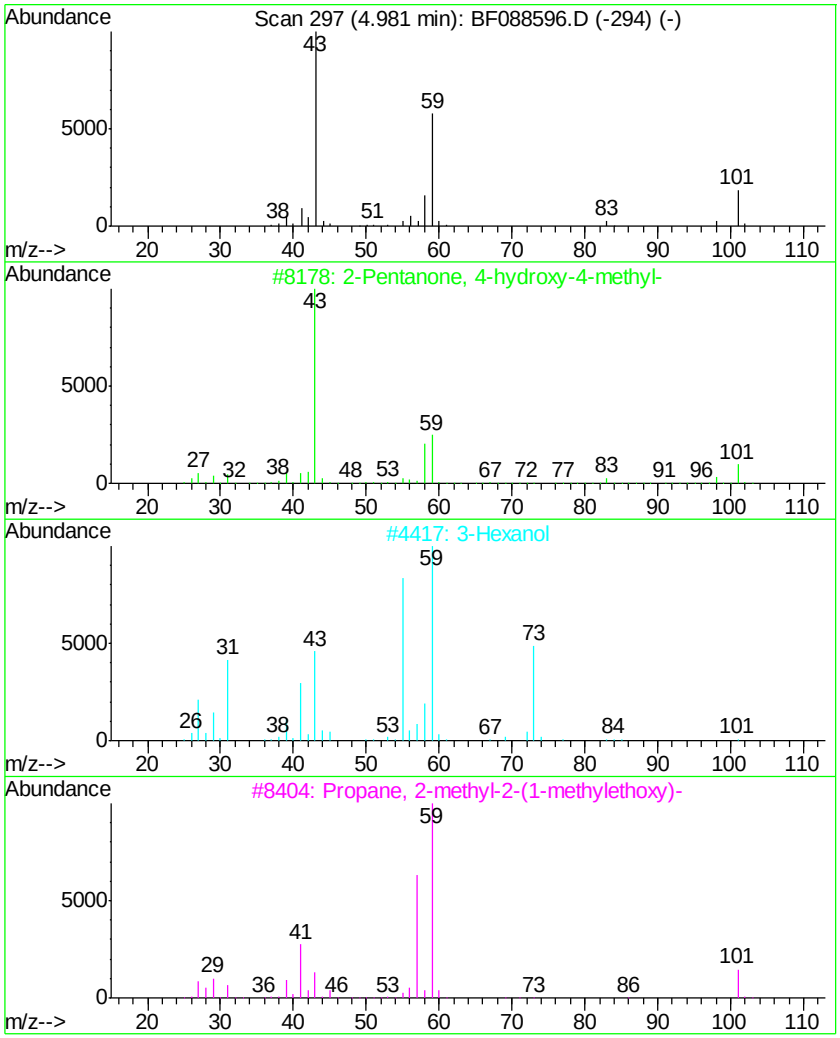
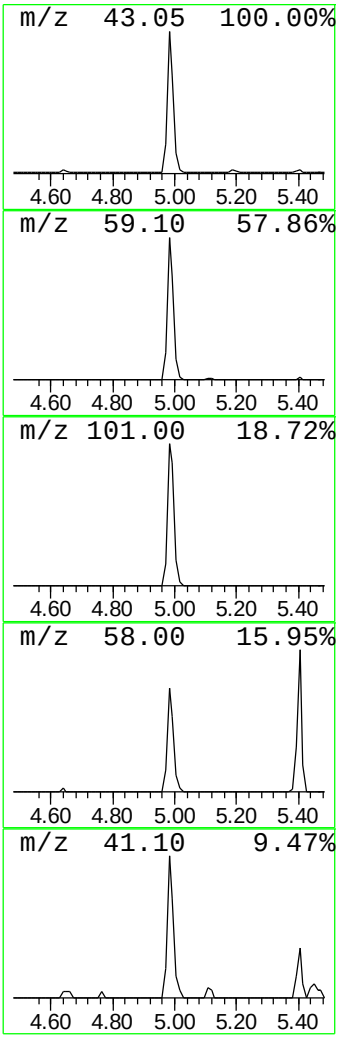
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	5.59 ng	239033	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	3-Hexanol	102	C6H14O	000623-37-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Sample : H3816-12
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-05-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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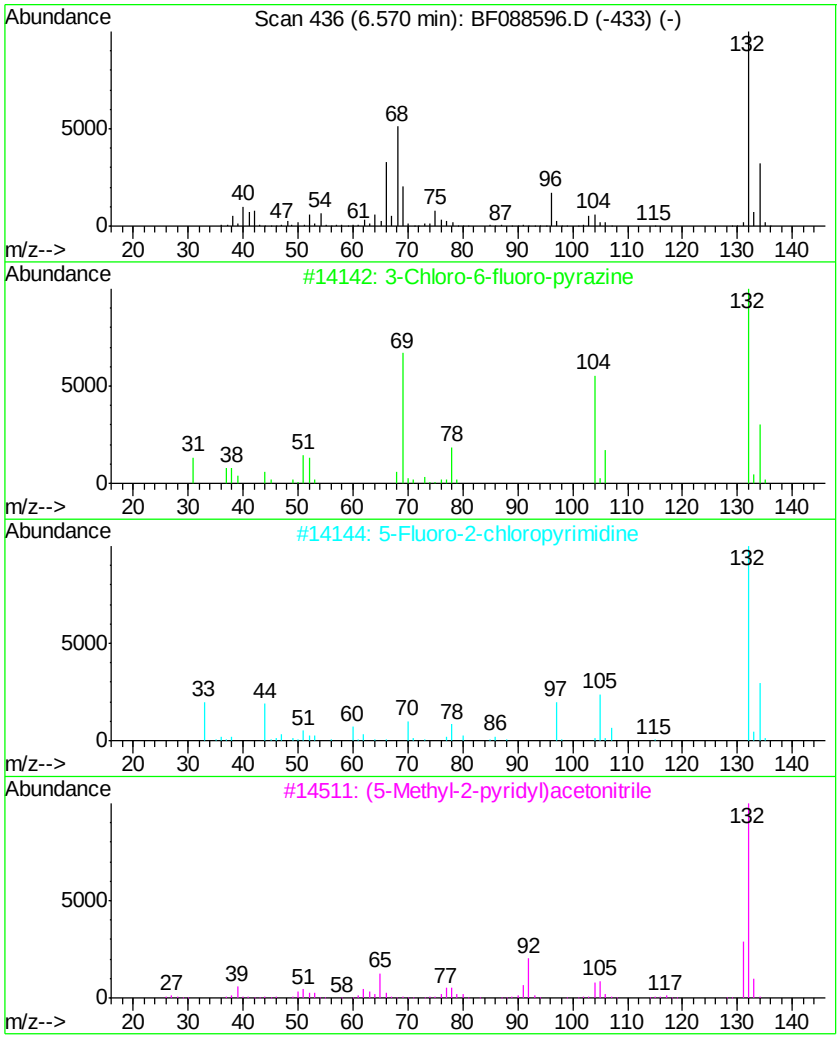
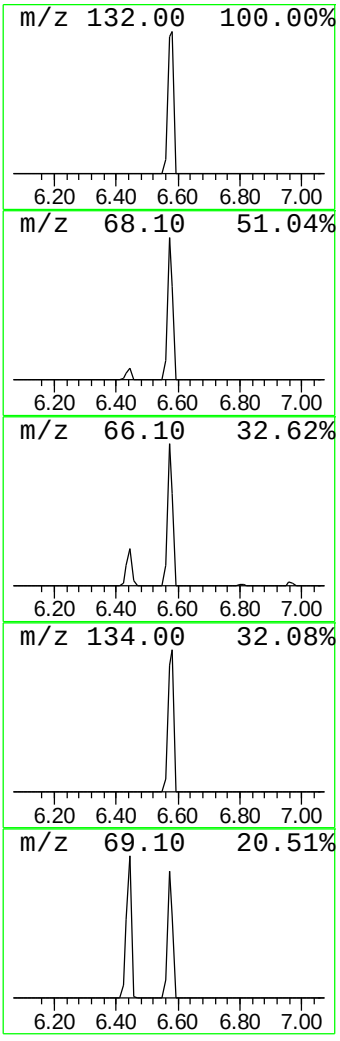
Peak Number 7 unknown6.57 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	65.08 ng	2781700	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

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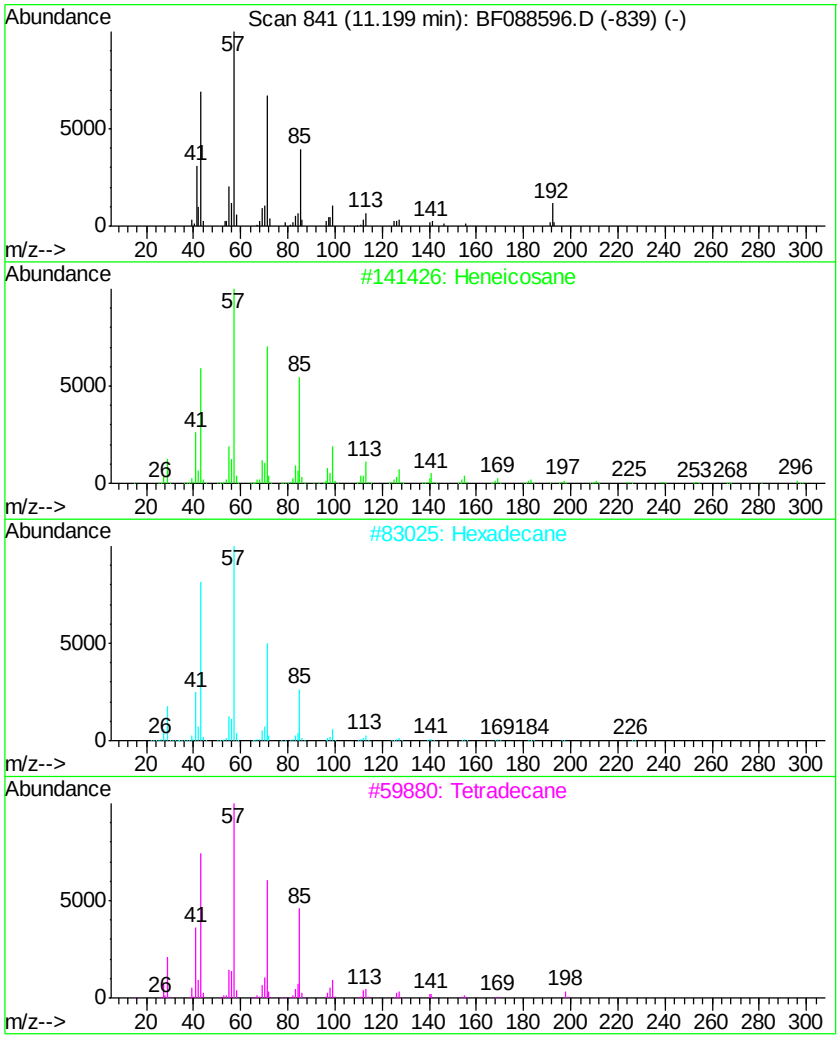
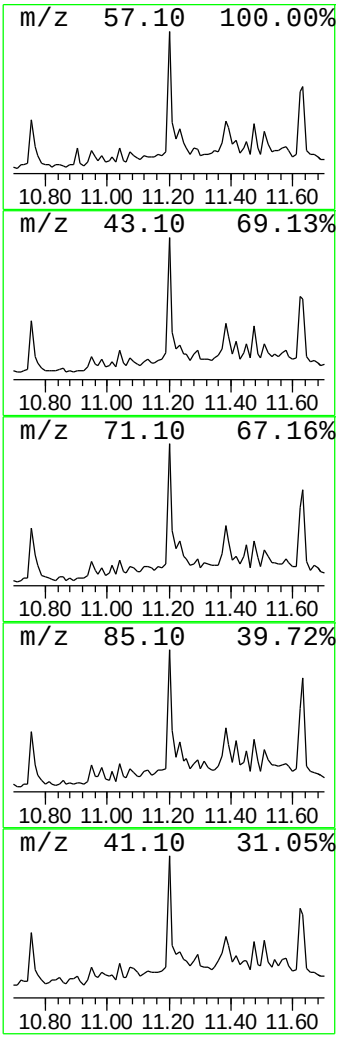
Peak Number 9 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.20	2.34 ng	99176	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tetradecane	198	C14H30	000629-59-4	83
4	Eicosane	282	C20H42	000112-95-8	80
5	Eicosane, 10-methyl-	296	C21H44	054833-23-7	80





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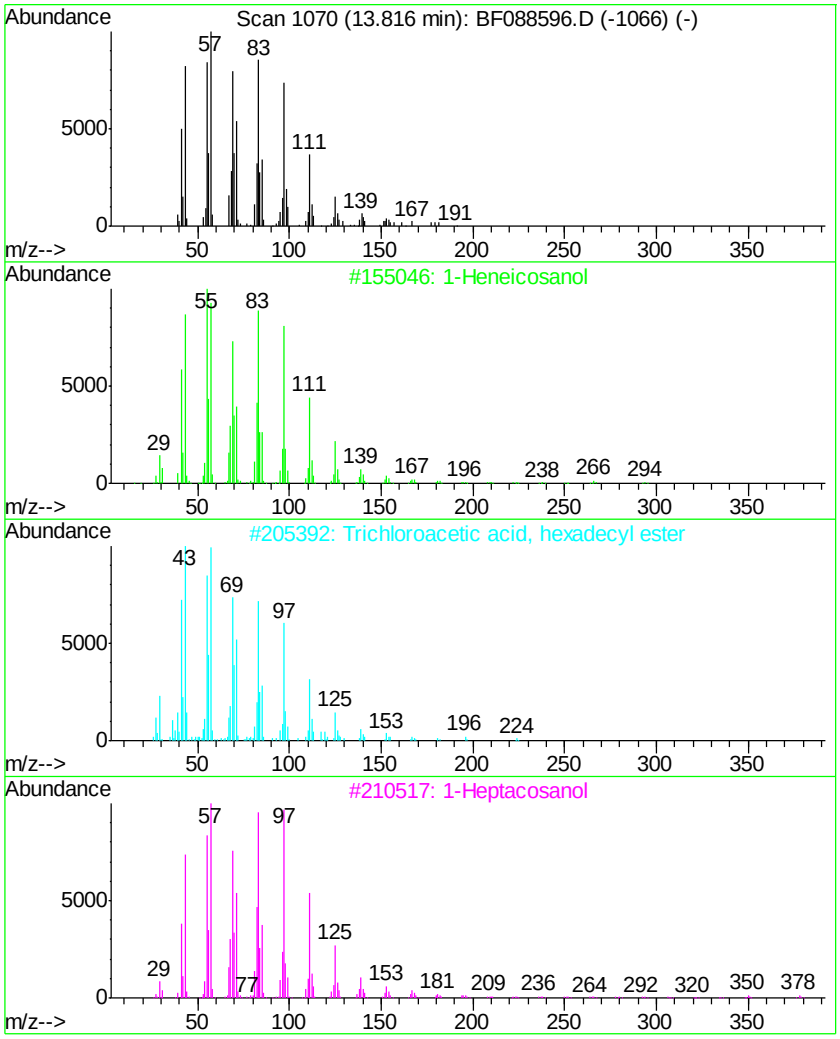
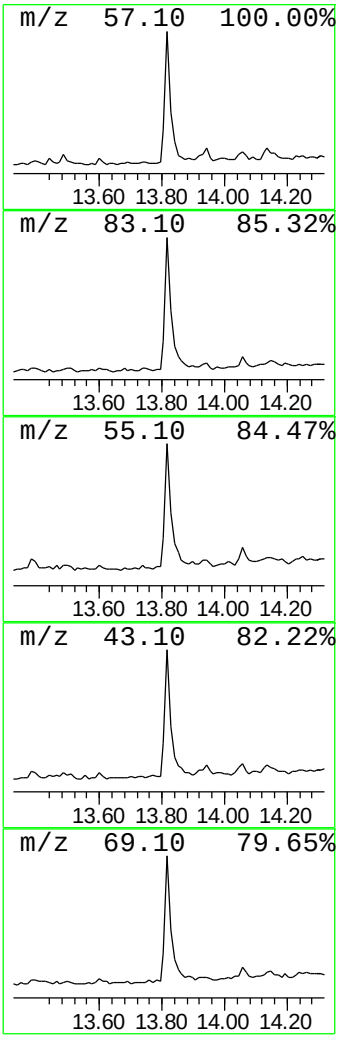
****

Peak Number 10 1-Heneicosanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.81 ng	232056	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





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TIC Library : C:\Database\NIST11.L
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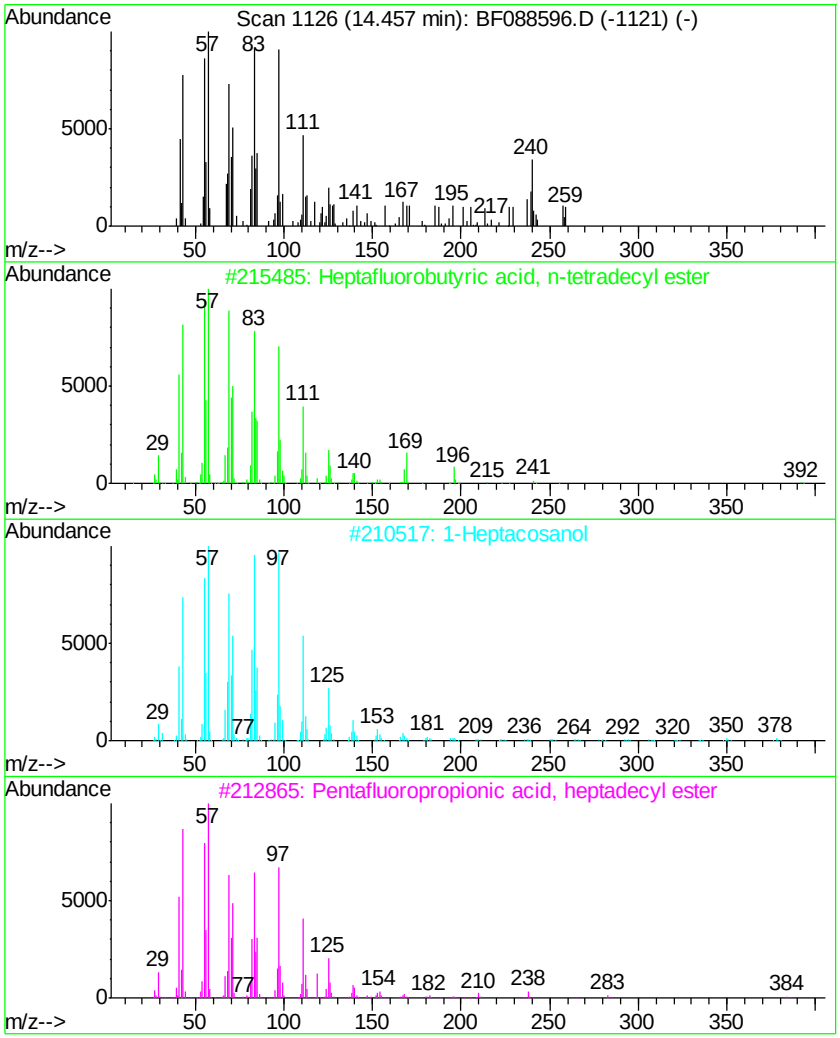
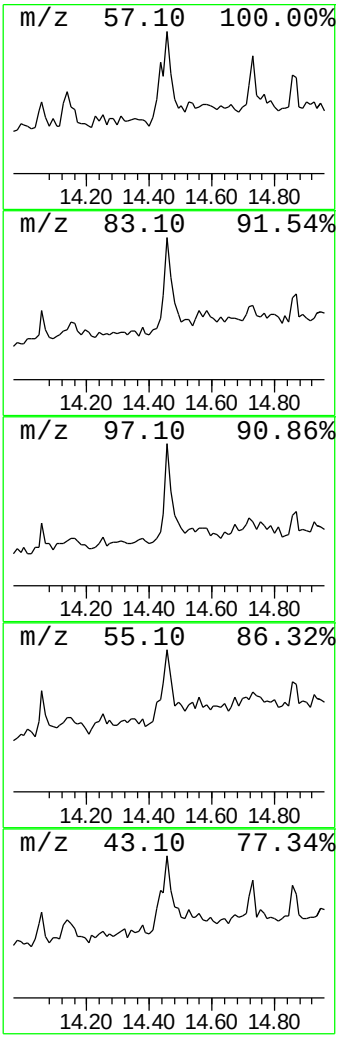
Peak Number 11 Heptafluorobutyric acid, n-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.41 ng	116220	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87
2	1-Heptacosanol	396	C27H56O	002004-39-9	87
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87
5	Octacosanol	410	C28H58O	000557-61-9	87





Tentatively Identified Compound (LSC) summary

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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	151.7	ng	6485350	1	6.81	854812	20.0
Propane, 1,1-dime...	2.06	16.0	ng	682783	1	6.81	854812	20.0
Propylene Glycol	3.13	18.9	ng	807621	1	6.81	854812	20.0
2-Pentanone, 4-hy...	4.98	5.6	ng	239033	1	6.81	854812	20.0
unknown6.57	6.57	65.1	ng	2781700	1	6.81	854812	20.0
Heneicosane	11.20	2.3	ng	99176	4	11.31	846363	20.0
1-Heneicosanol	13.82	4.8	ng	232056	5	13.94	964575	20.0
Heptafluorobutyri...	14.46	2.4	ng	116220	5	13.94	964575	20.0