LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF088998.D
Acq On : 14 Jul 2016 21:20
Operator : UM/SJ
Sample : H3996-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : U2-B2(6-12)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-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	1.655	5	6	15	rVB	152906	308434	16.73%	1.866%
2	1.781	15	17	23	rVV	1138321	1491689	80.90%	9.025%
3	1.861	23	24	53	rVB	81186	311895	16.92%	1.887%
4	2.821	106	108	121	rVB	11471	26704	1.45%	0.162%
5	4.833	282	284	290	rBB	111012	192188	10.42%	1.163%
6	5.279	320	323	326	rBV	1309323	1597773	86.66%	9.667%
7	6.342	412	416	418	rBV	1650700	1843803	100.00%	11.155%
8	6.456	423	426	428	rBV	1713363	1623041	88.03%	9.820%
9	6.684	444	446	448	rBV	468682	372883	20.22%	2.256%
10	6.845	457	460	462	rBB	1511264	1400172	75.94%	8.471%
11	7.256	493	496	498	rBV	1100045	1119894	60.74%	6.775%
12	7.965	556	558	561	rBV	329920	445025	24.14%	2.692%
13	9.050	650	653	655	rBV	2019465	1832805	99.40%	11.089%
14	9.439	685	687	690	rVB	219231	196480	10.66%	1.189%
15	9.713	709	711	714	rBB	477051	456276	24.75%	2.761%
16	10.502	777	780	782	rBV	986445	888138	48.17%	5.373%
17	11.085	828	831	832	rBV	20677	29871	1.62%	0.181%
18	11.188	838	840	842	rVB	437201	391222	21.22%	2.367%
19	11.256	842	846	851	rVB3	8423	20928	1.14%	0.127%
20	12.777	976	979	981	rBV	1259044	1200500	65.11%	7.263%
21	13.679	1056	1058	1065	rBV	68523	93774	5.09%	0.567%
22	13.817	1067	1070	1072	rBV	317358	389735	21.14%	2.358%
23	15.177	1187	1189	1192	rBV	269894	295357	16.02%	1.787%

Sum of corrected areas: 16528587

LSC Report - Integrated Chromatogram

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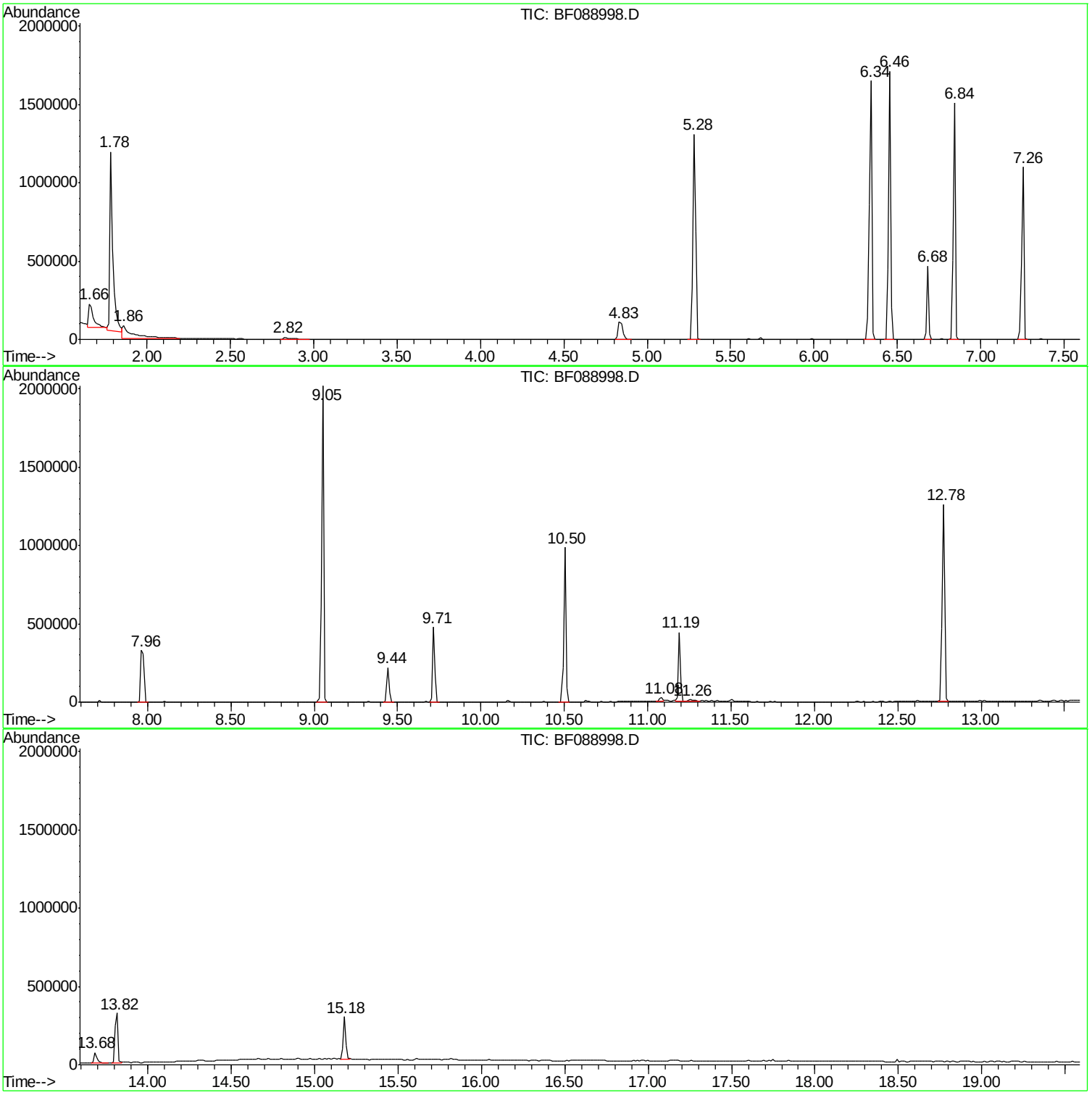
ClientSampleId : U2-B2(6-12)C

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF088998.D
Acq On : 14 Jul 2016 21:20
Operator : UM/SJ
Sample : H3996-11
Misc :
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Instrument : BNA_F
ClientSampleId : U2-B2(6-12)C

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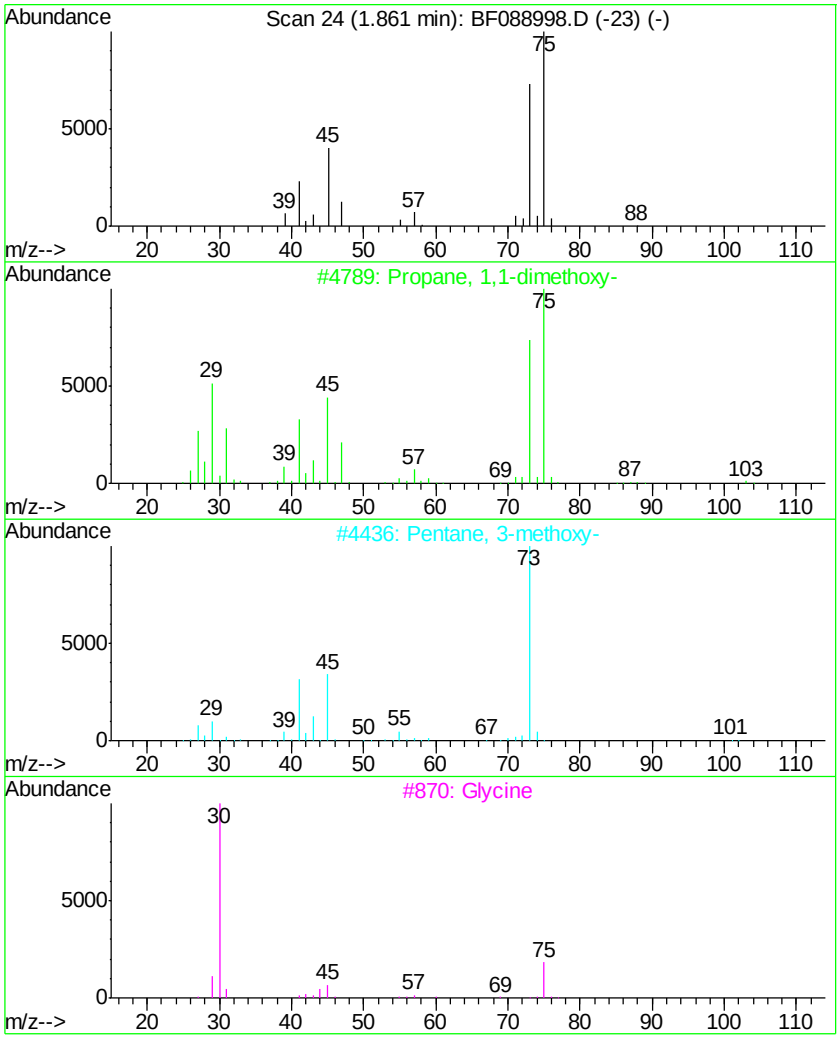
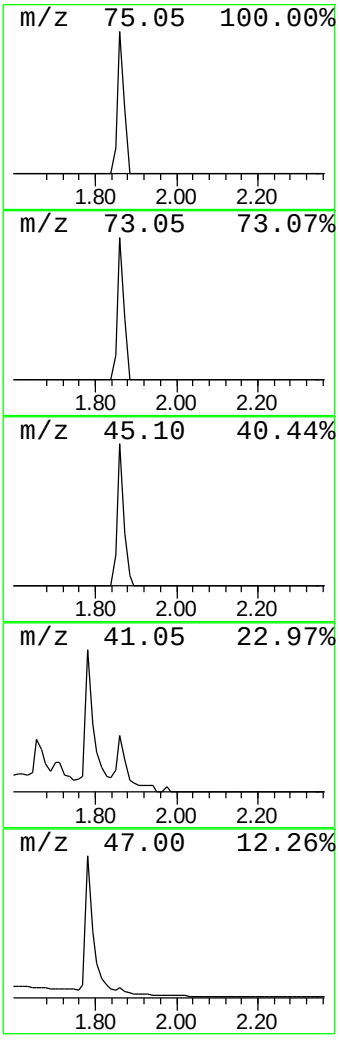
Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.86	16.73 ng	311895	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	72
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3	Glycine	75	C2H5NO2	000056-40-6	7
4	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	7
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	4





Library Search Compound Report

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : U2-B2(6-12)C

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

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TIC Integration Parameters: LSCINT.P

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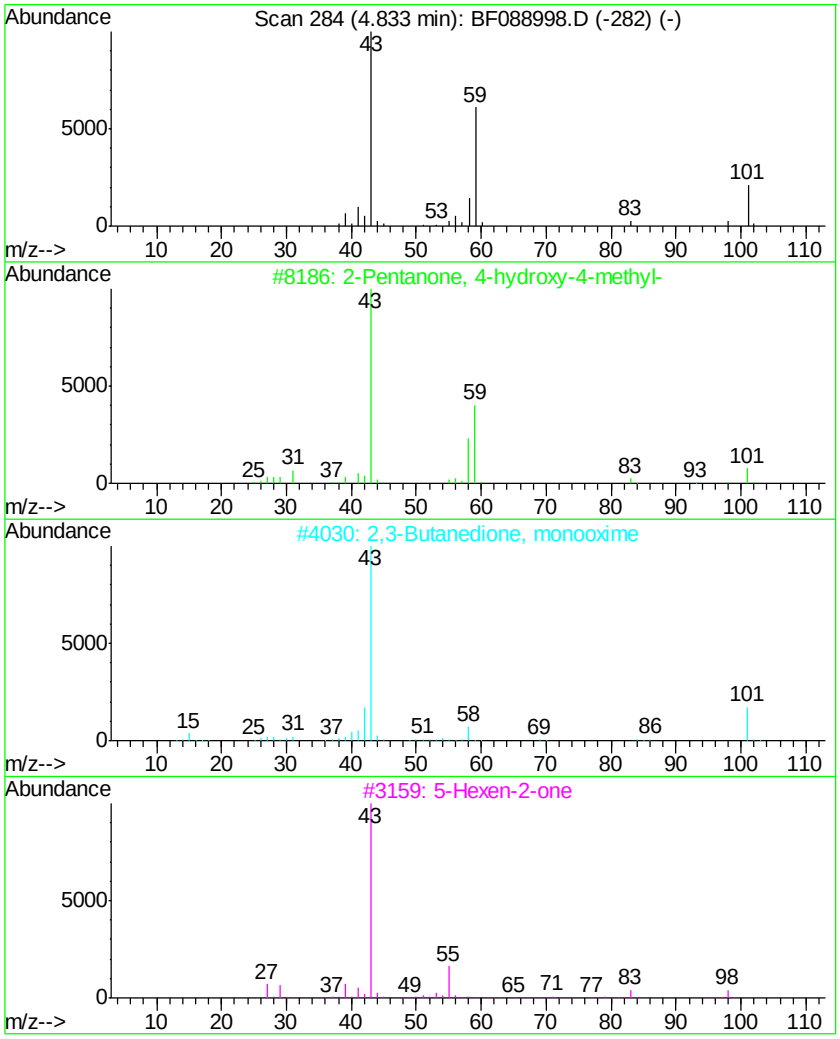
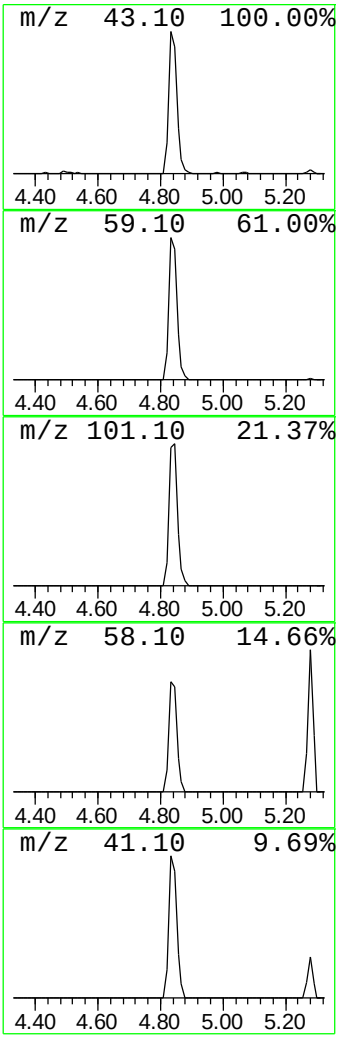
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	10.31 ng	192188	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	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Operator : UM/SJ
Sample : H3996-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : U2-B2(6-12)C

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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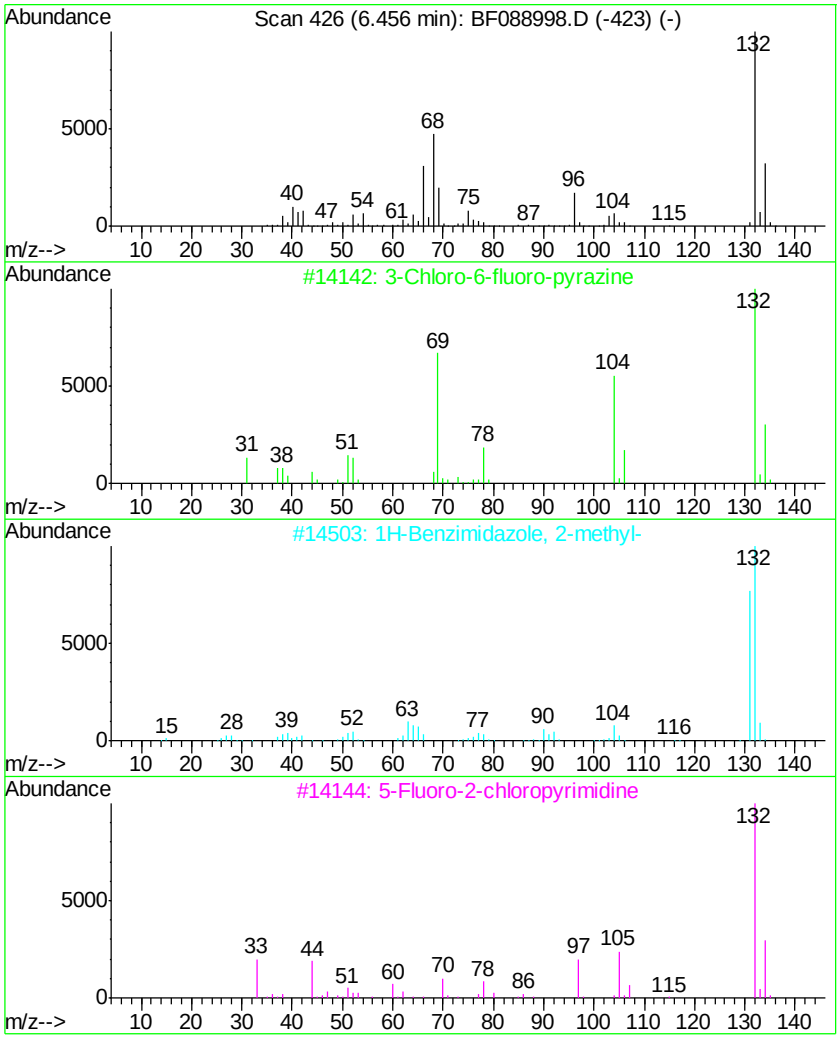
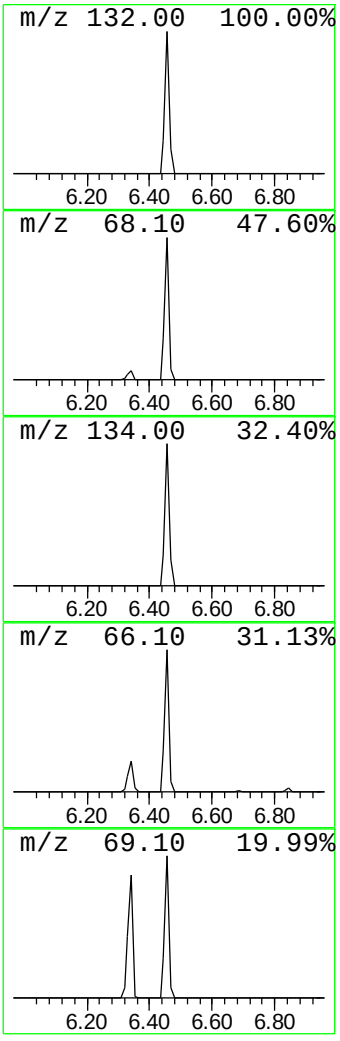
Peak Number 5 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	87.05 ng	1623040	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	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10





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ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : U2-B2(6-12)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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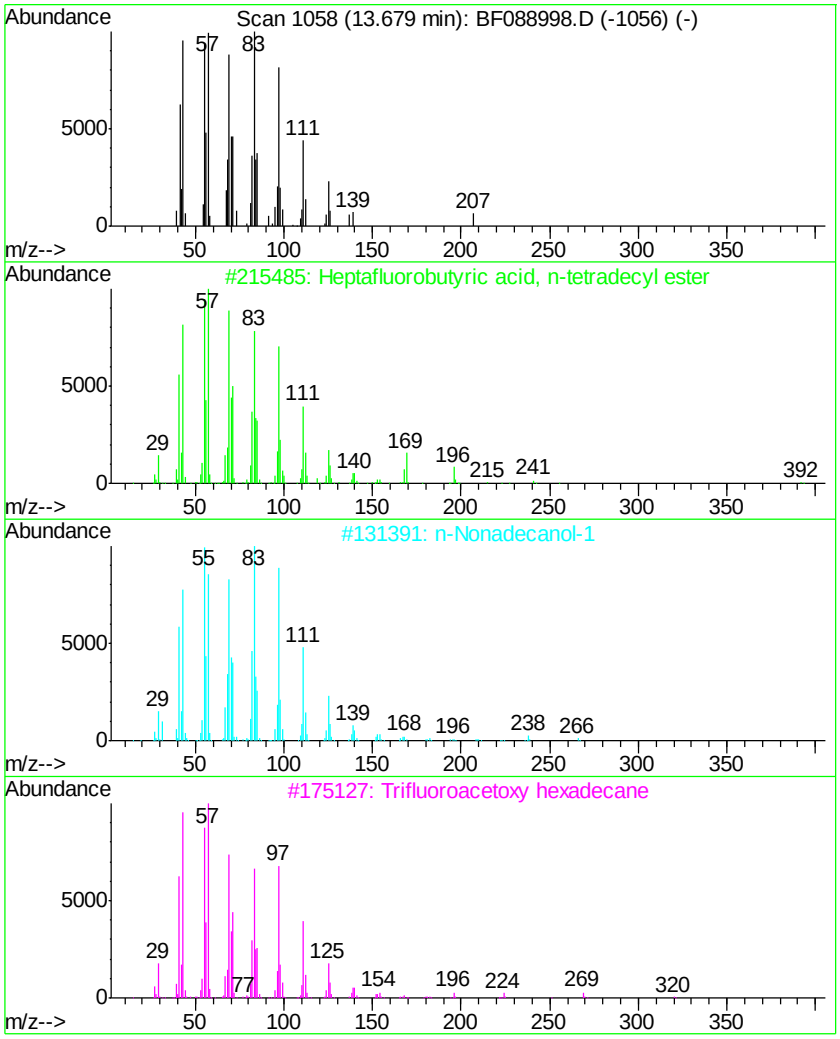
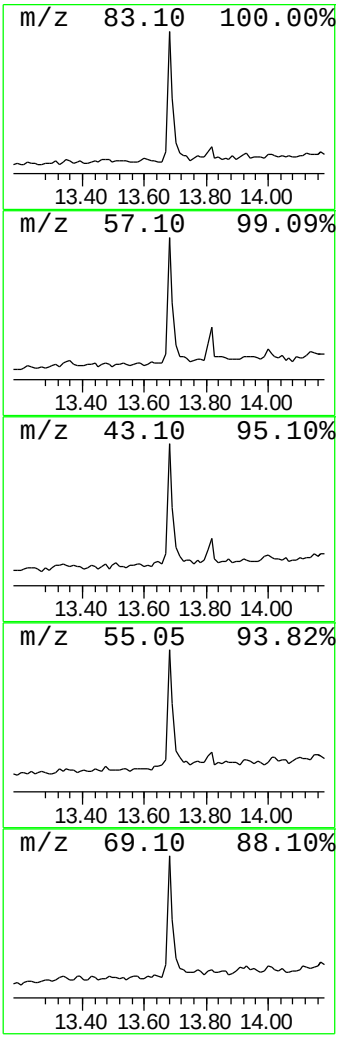
Peak Number 7 Heptafluorobutyric acid, n-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	4.81 ng	93774	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071416\
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Operator : UM/SJ
Sample : H3996-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : U2-B2(6-12)C

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, 1,1-dime...	1.86	16.7	ng	311895	1	6.68	372883	20.0
2-Pentanone, 4-hy...	4.83	10.3	ng	192188	1	6.68	372883	20.0
unknown6.46	6.46	87.0	ng	1623040	1	6.68	372883	20.0
Heptafluorobutyri...	13.68	4.8	ng	93774	5	13.82	389735	20.0