LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102250.D
Acq On : 20 Jan 2018 6:26
Operator : SJ/JU
Sample : J1114-17
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-29-2.0-2.5

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-BF010918.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	4.928	477	483	494	rVB	176376	272459	7.59%	0.883%
2	5.334	547	552	555	rBV	3352487	3568988	99.43%	11.570%
3	6.363	721	727	730	rBV	3208660	3589622	100.00%	11.637%
4	6.493	744	749	752	rBV	3660685	3589441	99.99%	11.636%
5	6.716	784	787	791	rBV	1055081	883972	24.63%	2.866%
6	6.875	810	814	817	rBV	3158391	2750008	76.61%	8.915%
7	7.287	878	884	887	rBV	2280177	2316348	64.53%	7.509%
8	7.998	1001	1005	1009	rBV	1344444	1161798	32.37%	3.766%
9	9.081	1183	1189	1192	rBV	3443235	3349891	93.32%	10.860%
10	9.469	1252	1255	1258	rBV	256907	209481	5.84%	0.679%
11	9.686	1288	1292	1295	rVB	130954	108218	3.01%	0.351%
12	9.751	1299	1303	1307	rVB	1314542	1186669	33.06%	3.847%
13	10.181	1373	1376	1379	rVB	175928	152397	4.25%	0.494%
14	10.404	1409	1414	1416	rBV	47205	56762	1.58%	0.184%
15	10.545	1431	1438	1441	rBV	2032144	1946950	54.24%	6.312%
16	10.657	1454	1457	1466	rBV	157290	161178	4.49%	0.523%
17	11.104	1530	1533	1536	rBV	66997	53445	1.49%	0.173%
18	11.233	1551	1555	1559	rBV	1137964	1018004	28.36%	3.300%
19	12.645	1792	1795	1798	rBV	183380	150457	4.19%	0.488%
20	12.822	1821	1825	1829	rBV	2341488	2222221	61.91%	7.204%
21	13.351	1911	1915	1918	rBV	123873	104060	2.90%	0.337%
22	13.716	1973	1977	1984	rBV	184575	197561	5.50%	0.640%
23	13.868	1999	2003	2007	rBV	835909	789416	21.99%	2.559%
24	14.351	2079	2085	2091	rBV3	61355	95466	2.66%	0.309%
25	14.963	2185	2189	2191	rBV2	31572	35918	1.00%	0.116%
26	15.292	2240	2245	2249	rBV	708985	821133	22.88%	2.662%
27	15.727	2314	2319	2323	rBV3	38301	55451	1.54%	0.180%

Sum of corrected areas: 30847314

LSC Report - Integrated Chromatogram

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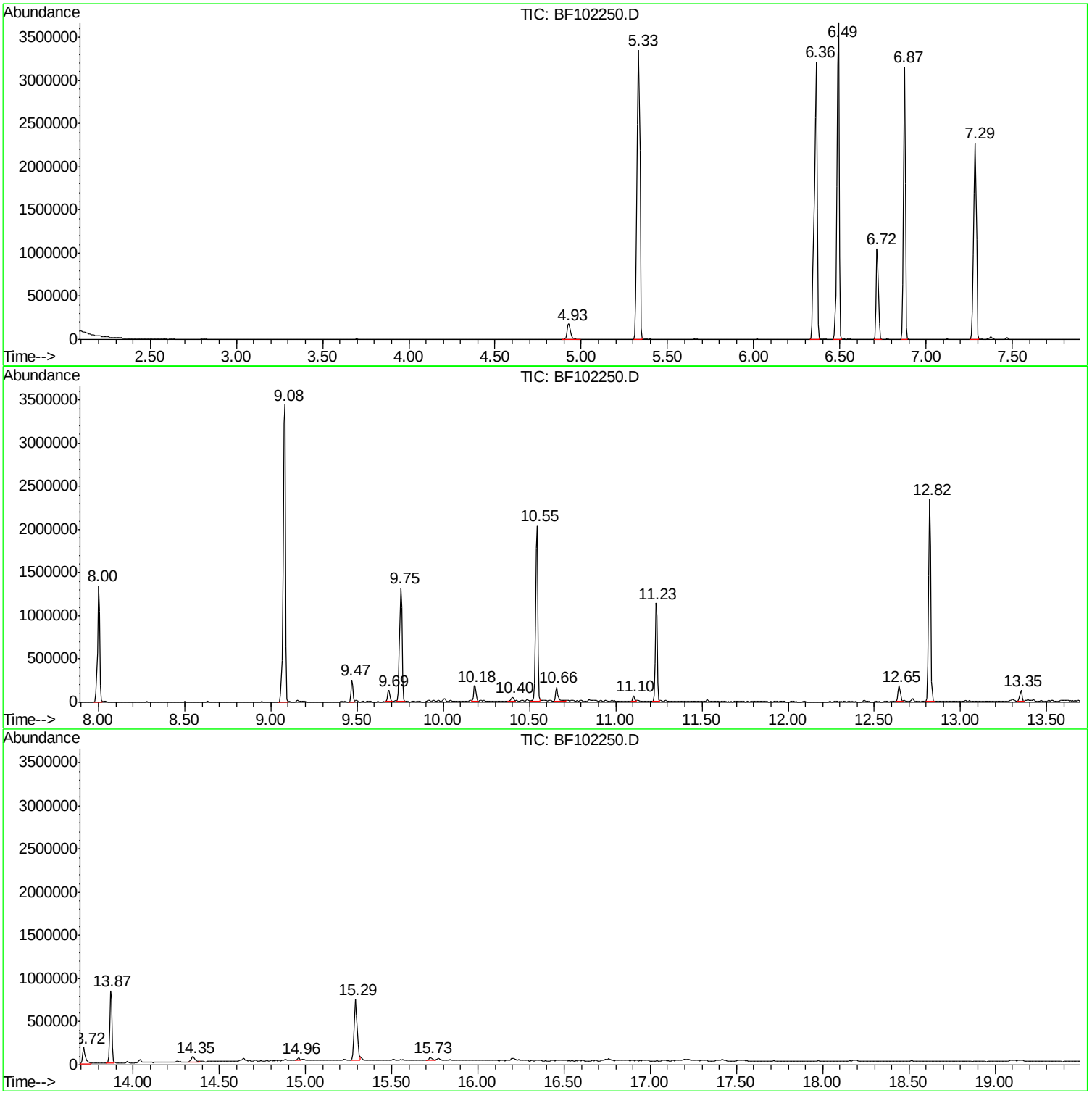
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-29-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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\BF011918\
Data File : BF102250.D
Acq On : 20 Jan 2018 6:26
Operator : SJ/JU
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

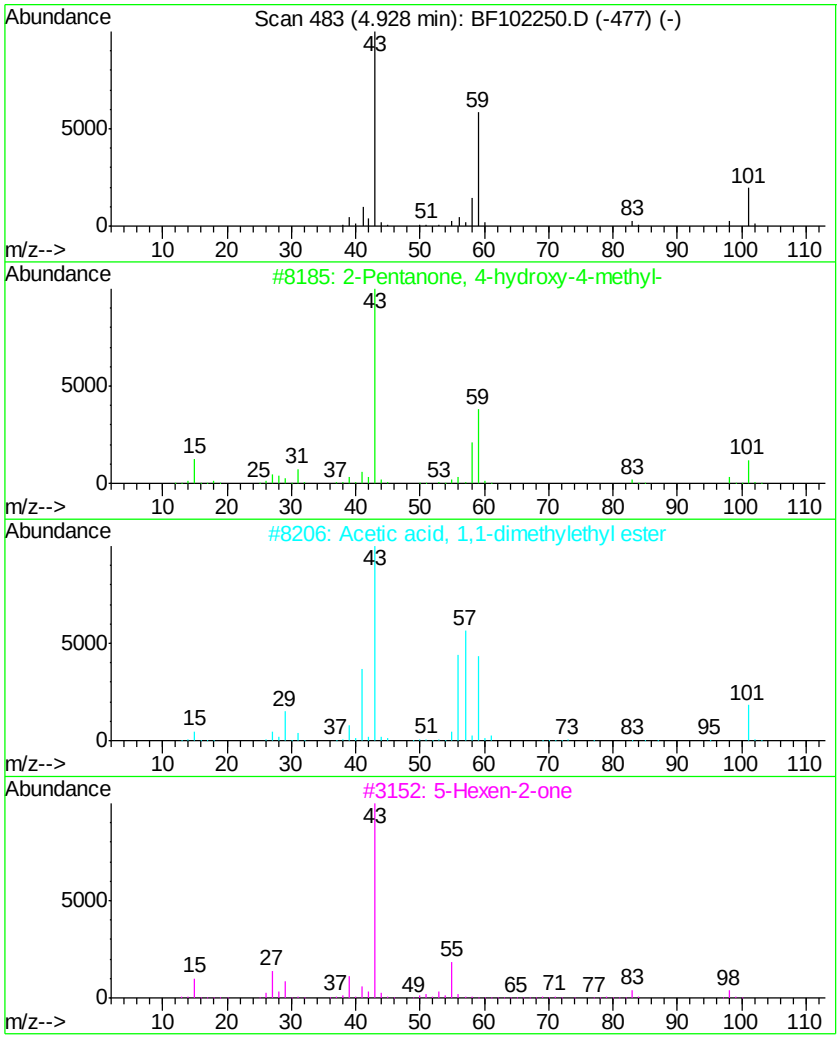
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

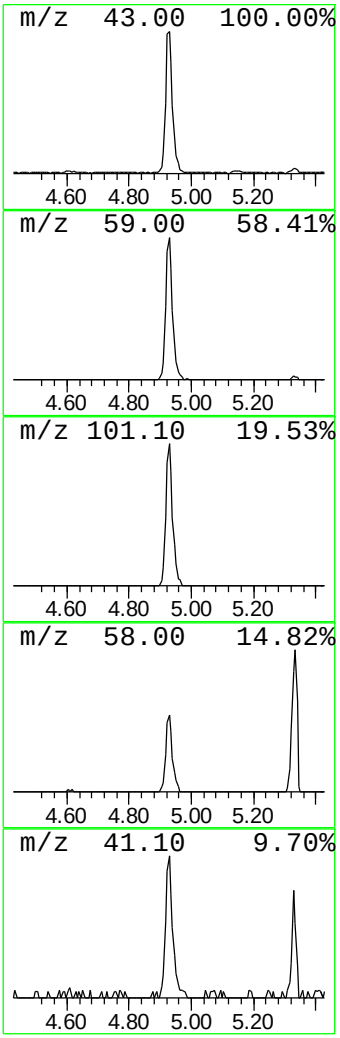
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	6.16 ng	272459	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Acq On : 20 Jan 2018 6:26
Operator : SJ/JU
Sample : J1114-17
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-29-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

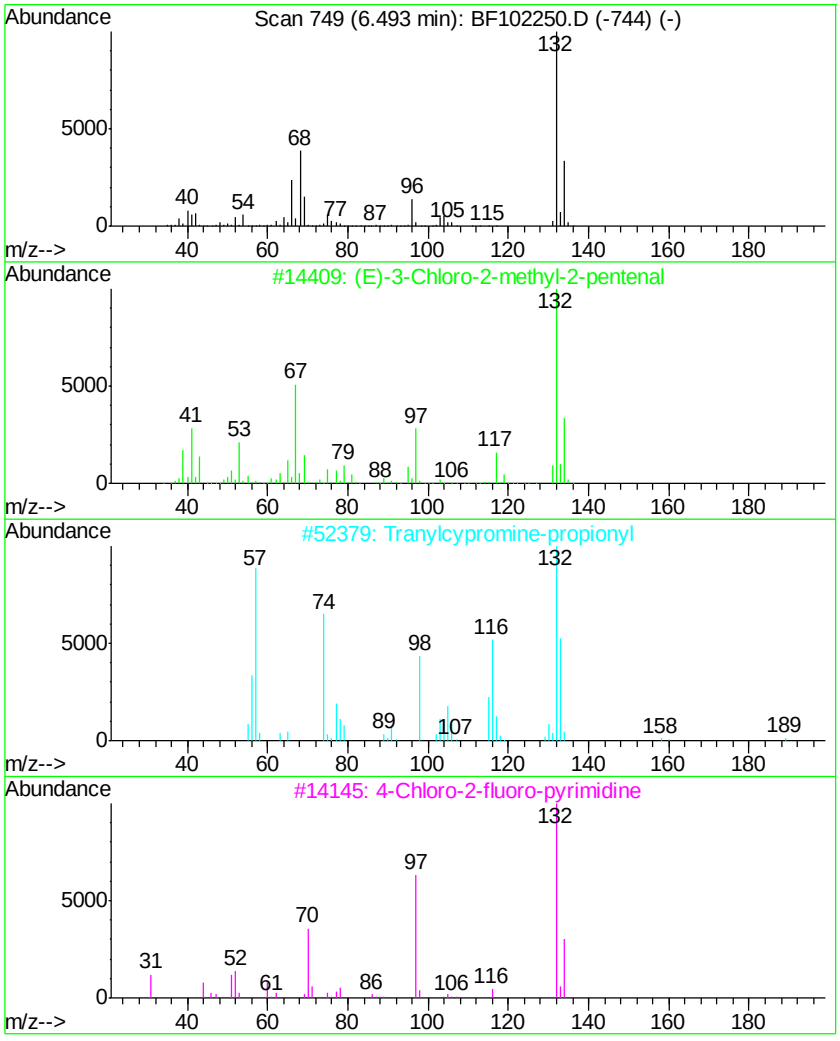
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

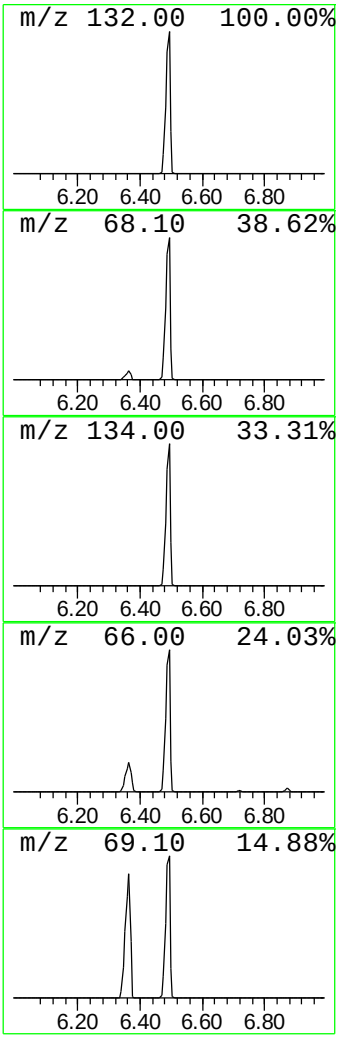
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	81.21 ng	3589440	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





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Data File : BF102250.D
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Operator : SJ/JU
Sample : J1114-17
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-29-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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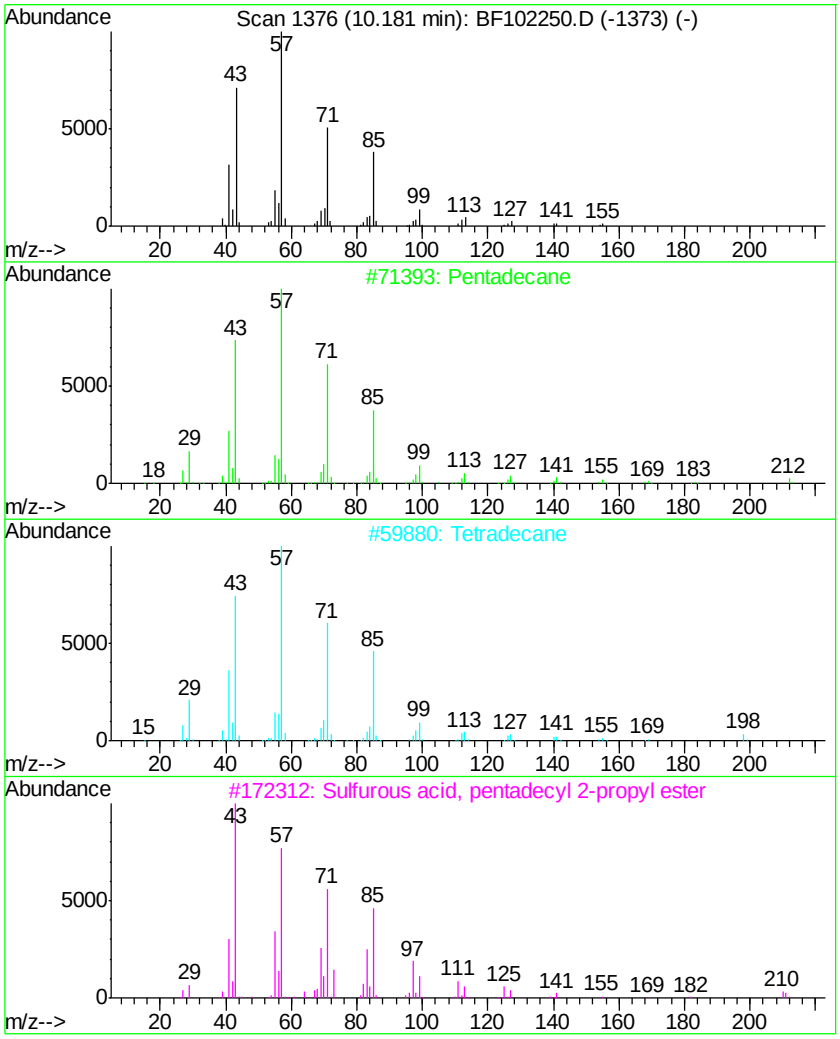
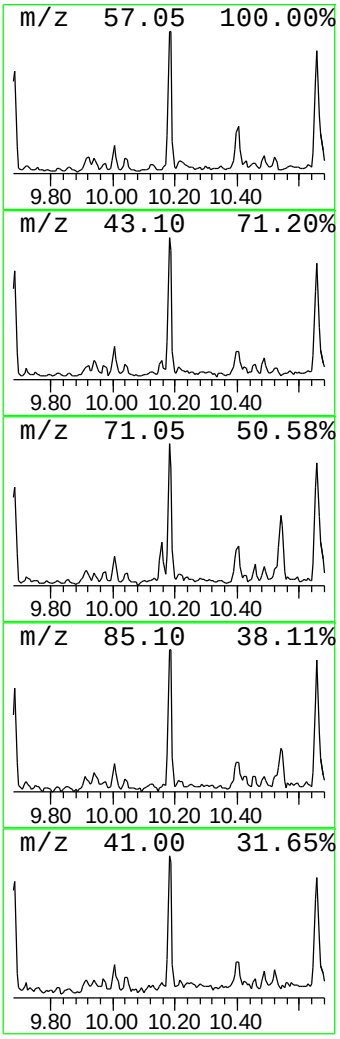
Peak Number 4 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	2.57 ng	152397	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	78
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5	Hexadecane	226	C16H34	000544-76-3	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102250.D
Acq On : 20 Jan 2018 6:26
Operator : SJ/JU
Sample : J1114-17
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-29-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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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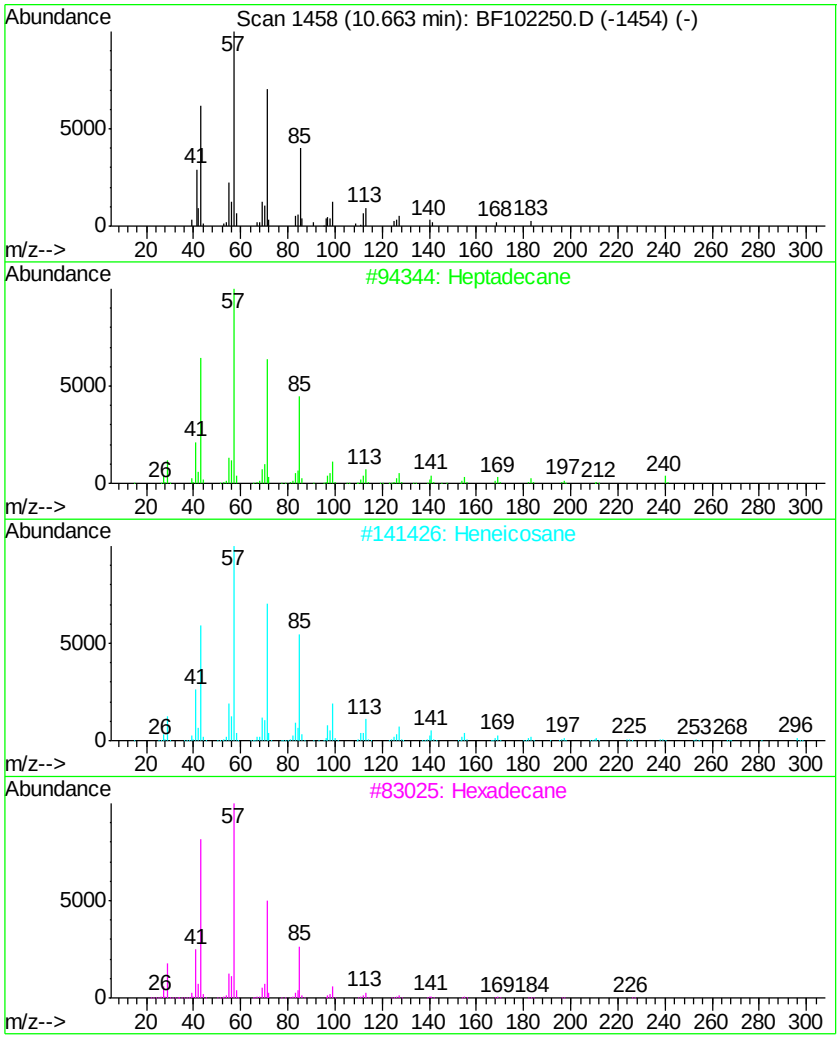
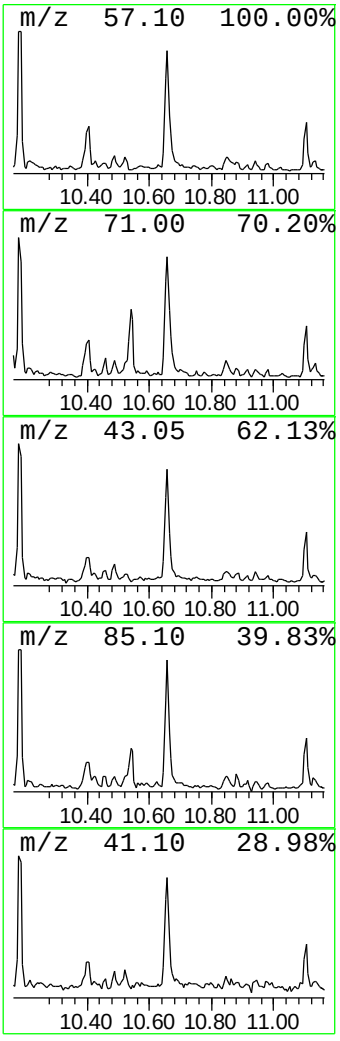
Peak Number 5 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.17 ng	161178	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
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Operator : SJ/JU
Sample : J1114-17
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-29-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

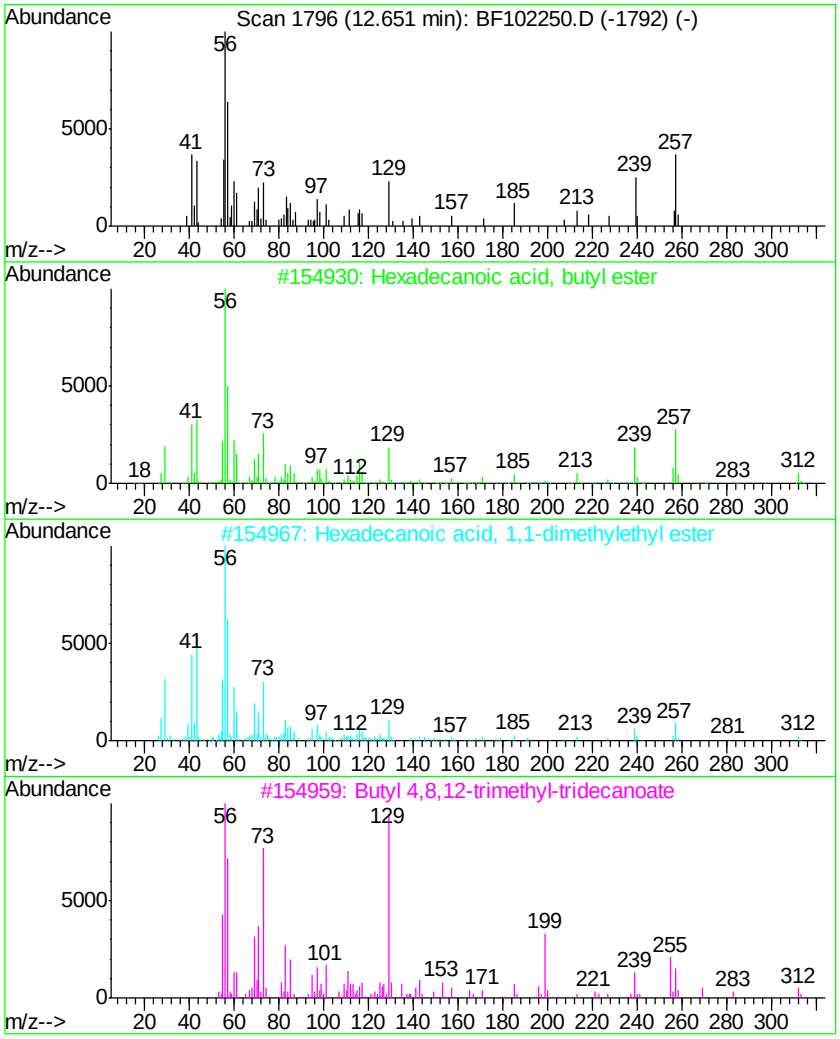
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

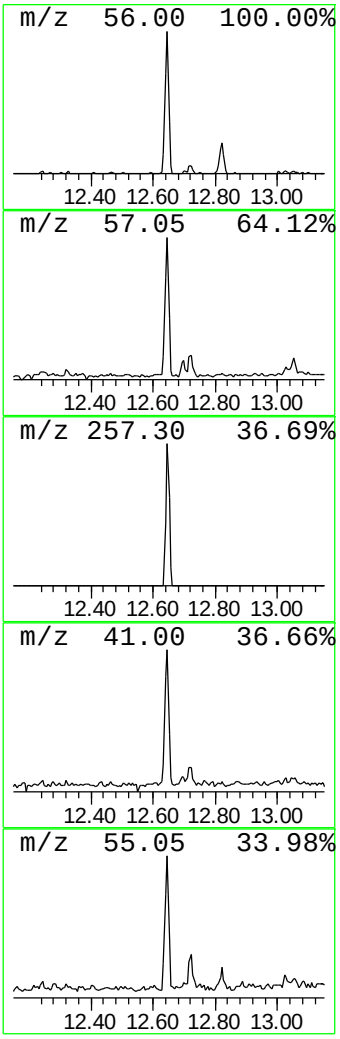
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	3.81 ng	150457	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	80
3	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	45
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	35





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

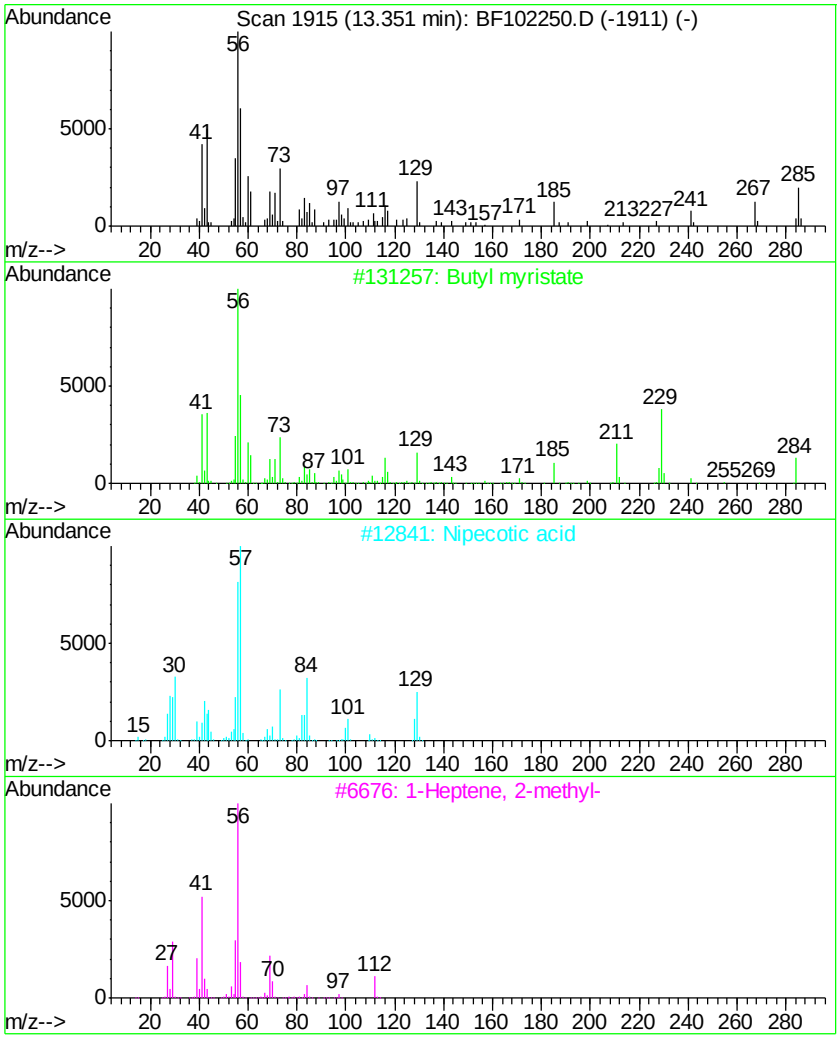
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

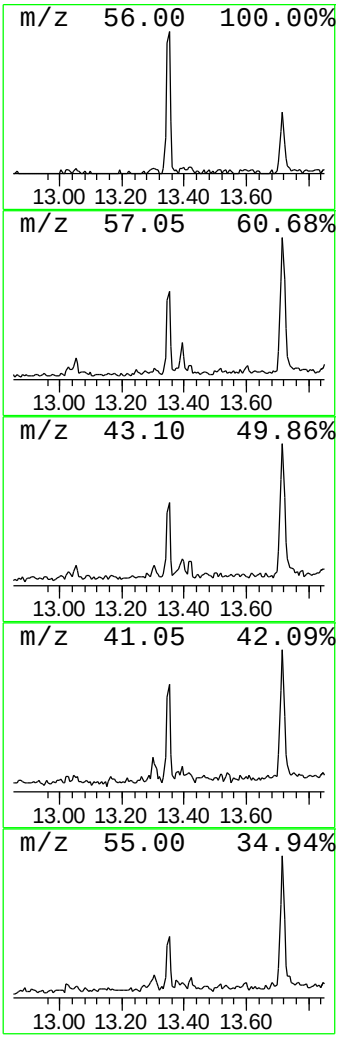
****

Peak Number 7 Butyl myristate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	2.64 ng	104060	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	68
2	Nipecotic acid	129	C6H11NO2	000498-95-3	47
3	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5	Cycloheptylamine	113	C7H15N	005452-35-7	27





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Instrument : BNA_F
ClientSampleId : SB-29-2.0-2.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

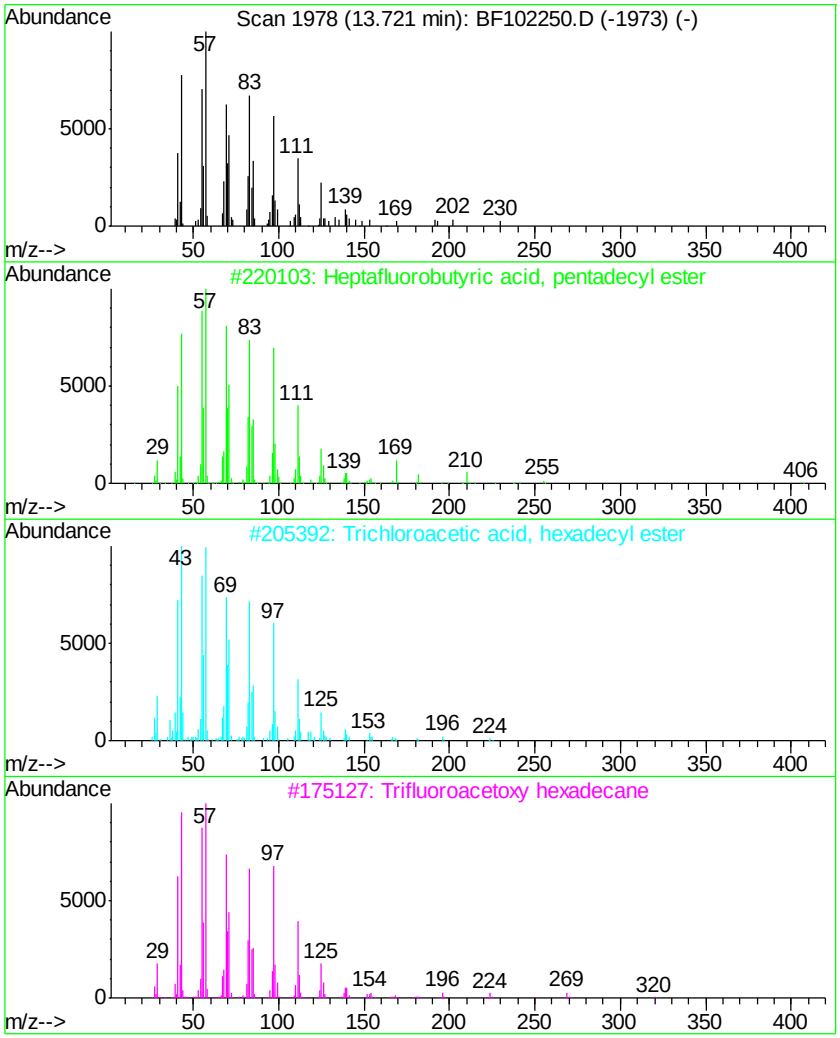
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

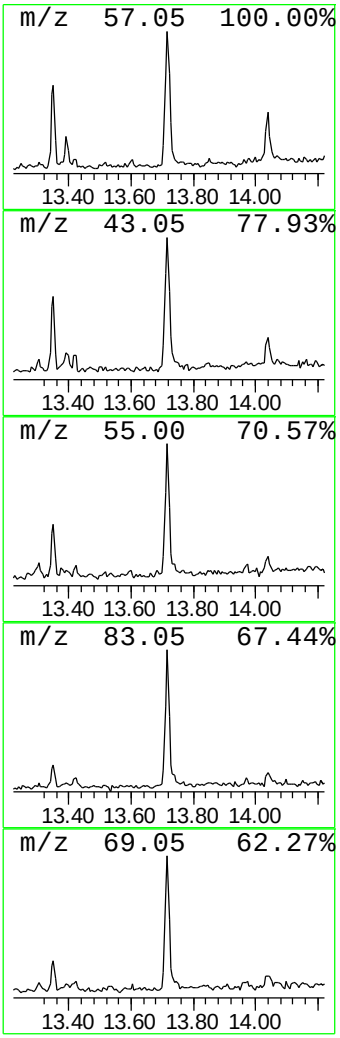
****

Peak Number 8 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.01 ng	197561	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.93	6.2	ng	272459	1	6.72	883972	20.0
unknown6.49	6.49	81.2	ng	3589440	1	6.72	883972	20.0
Pentadecane	10.18	2.6	ng	152397	3	9.75	1186670	20.0
Heptadecane	10.66	3.2	ng	161178	4	11.23	1018000	20.0
Hexadecanoic acid...	12.65	3.8	ng	150457	5	13.87	789416	20.0
Butyl myristate	13.35	2.6	ng	104060	5	13.87	789416	20.0
Heptafluorobutyri...	13.72	5.0	ng	197561	5	13.87	789416	20.0