LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102321.D
Acq On : 23 Jan 2018 1:12
Operator : SJ/JU
Sample : J1238-18
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-06-9.5-10.0

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-BF012218.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	4.922	478	482	492	rVB	161092	224079	7.32%	0.894%
2	5.334	547	552	555	rBV	2948289	2949308	96.32%	11.768%
3	6.369	723	728	744	rBV	2819966	3061943	100.00%	12.217%
4	6.492	744	749	752	rBV	3247130	3011078	98.34%	12.014%
5	6.716	784	787	796	rBV	828296	699013	22.83%	2.789%
6	6.875	810	814	817	rBV	2523227	2189157	71.50%	8.735%
7	7.286	879	884	887	rBV	1975173	1800751	58.81%	7.185%
8	7.998	1002	1005	1019	rVB	1070602	926234	30.25%	3.696%
9	9.074	1184	1188	1192	rBV	2565434	2425772	79.22%	9.679%
10	9.157	1199	1202	1204	rBV	62438	52249	1.71%	0.208%
11	9.474	1251	1256	1258	rBV	407891	373391	12.19%	1.490%
12	9.686	1288	1292	1295	rBV	148777	127479	4.16%	0.509%
13	9.751	1300	1303	1309	rVB	958362	883766	28.86%	3.526%
14	10.180	1373	1376	1380	rVB	144887	120265	3.93%	0.480%
15	10.404	1409	1414	1416	rBV	35399	43537	1.42%	0.174%
16	10.545	1434	1438	1441	rBV	1640408	1461007	47.72%	5.829%
17	10.657	1453	1457	1466	rVB	116903	121810	3.98%	0.486%
18	11.104	1530	1533	1536	rBV	41577	35511	1.16%	0.142%
19	11.239	1552	1556	1563	rBV	892547	724696	23.67%	2.892%
20	12.645	1792	1795	1798	rBV2	58596	49542	1.62%	0.198%
21	12.827	1821	1826	1829	rBV	1836764	1714054	55.98%	6.839%
22	13.027	1857	1860	1863	rBV2	36657	35023	1.14%	0.140%
23	13.351	1912	1915	1917	rBV	42527	32758	1.07%	0.131%
24	13.715	1974	1977	1987	rBV	464797	458033	14.96%	1.828%
25	13.874	2000	2004	2008	rBV	708168	694851	22.69%	2.772%
26	13.974	2018	2021	2024	rVB4	43326	42405	1.38%	0.169%
27	14.039	2029	2032	2034	rBV2	35406	35623	1.16%	0.142%
28	14.351	2081	2085	2093	rBV	159993	196471	6.42%	0.784%
29	15.303	2242	2247	2257	rBV	427145	573094	18.72%	2.287%

Sum of corrected areas: 25062900

LSC Report - Integrated Chromatogram

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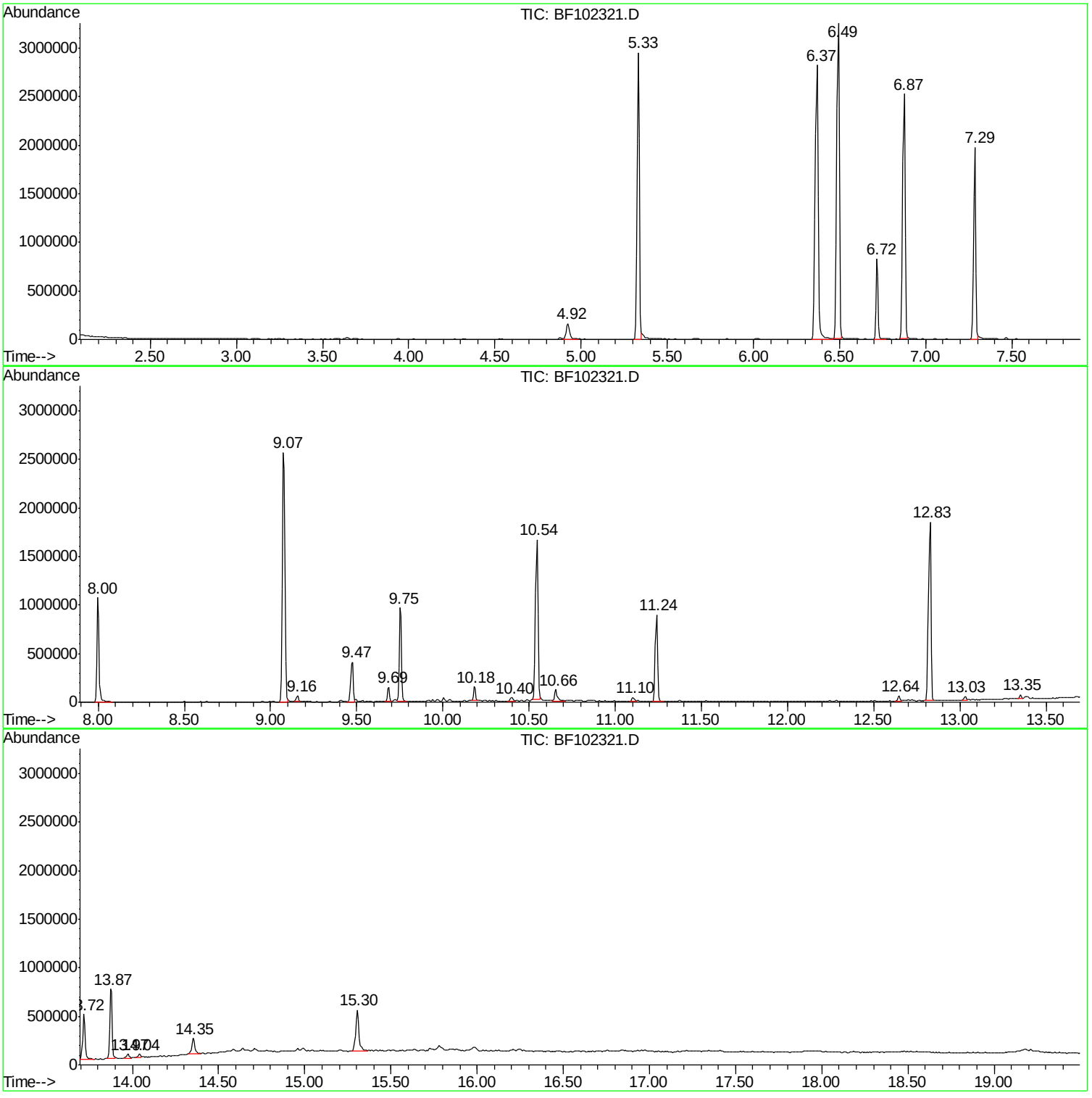
Operator : SJ/JU
Sample : J1238-18
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-06-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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Acq On : 23 Jan 2018 1:12
Operator : SJ/JU
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ClientSampleId : SB-06-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

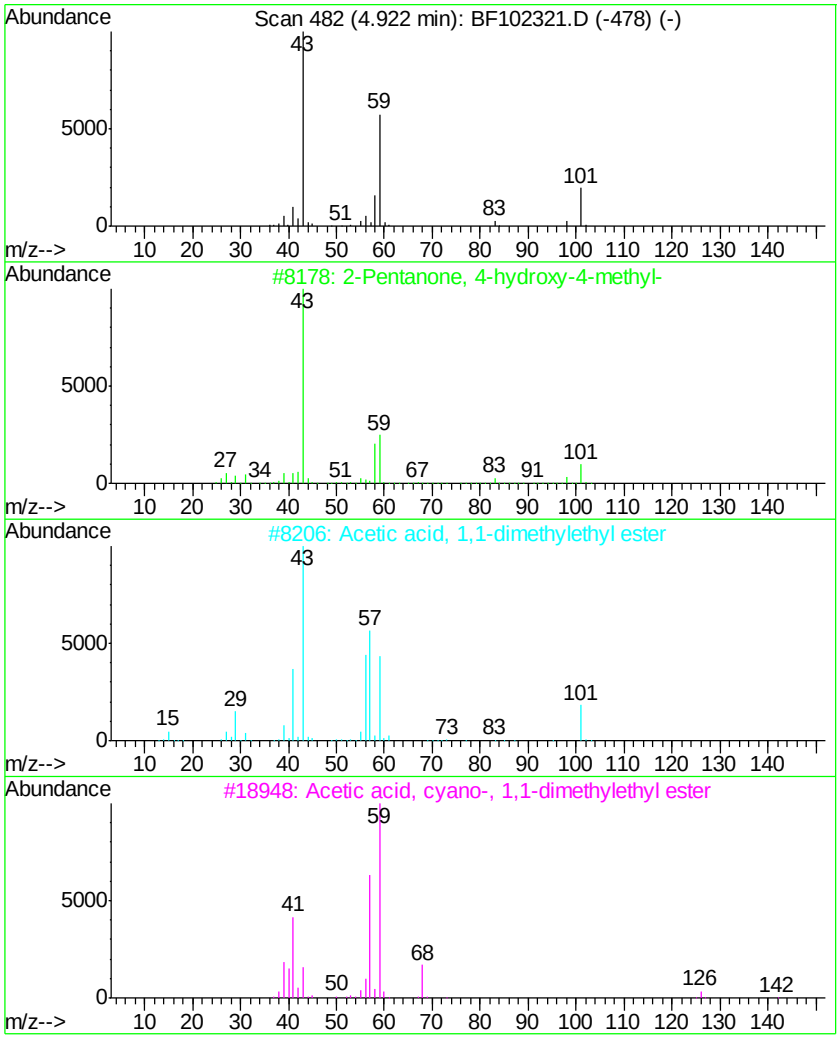
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

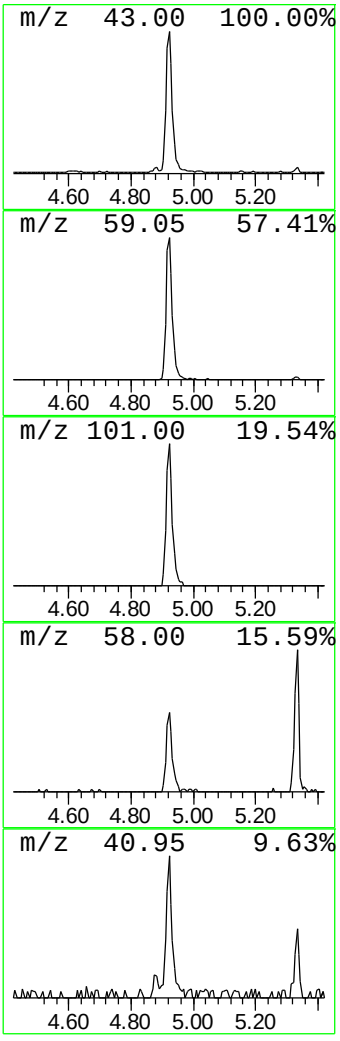
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	6.41 ng	224079	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Operator : SJ/JU
Sample : J1238-18
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-06-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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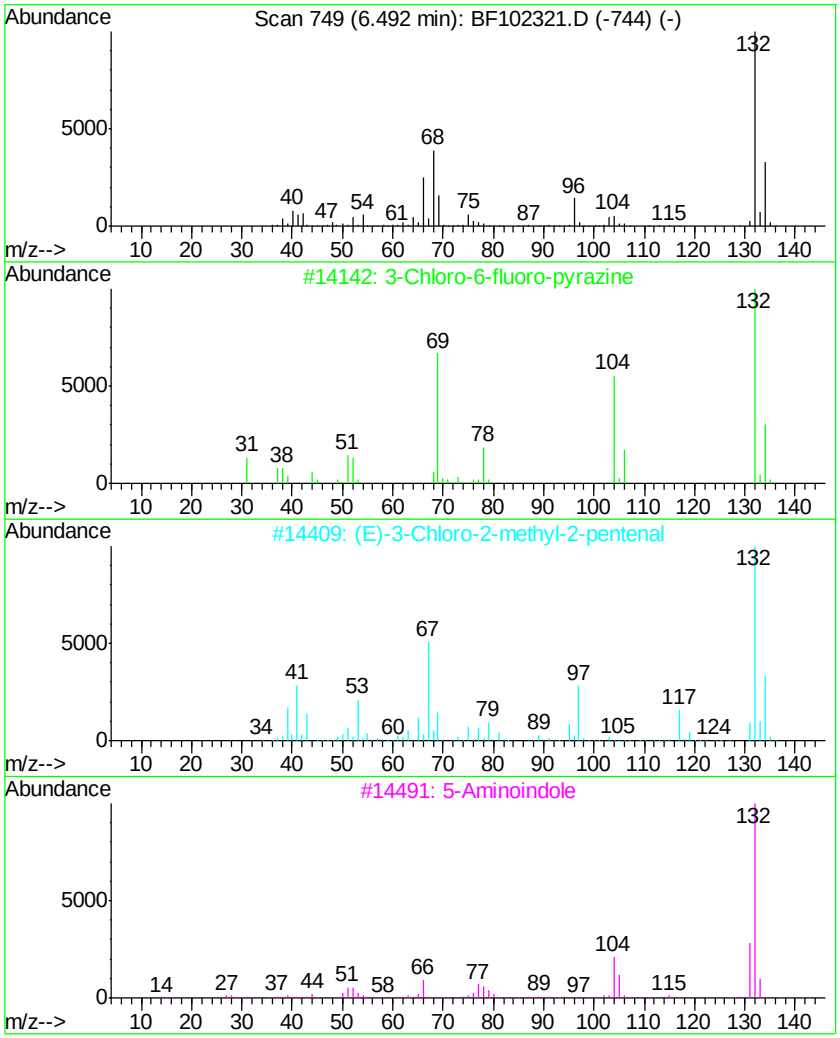
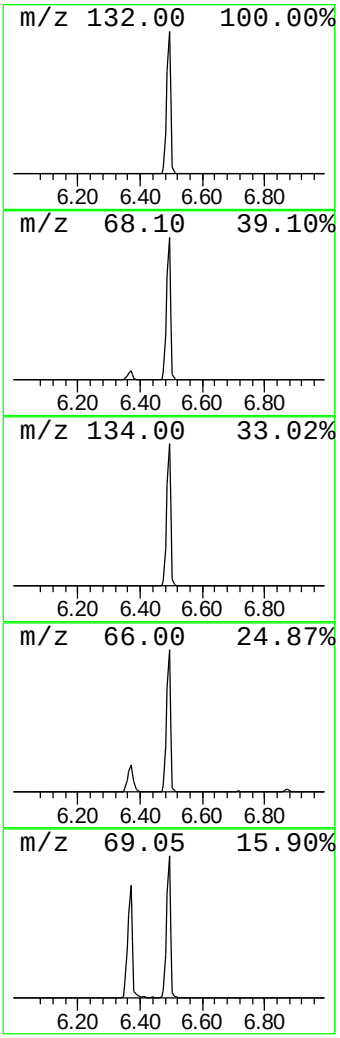
Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	86.15 ng	3011080	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Acq On : 23 Jan 2018 1:12
Operator : SJ/JU
Sample : J1238-18
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-06-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

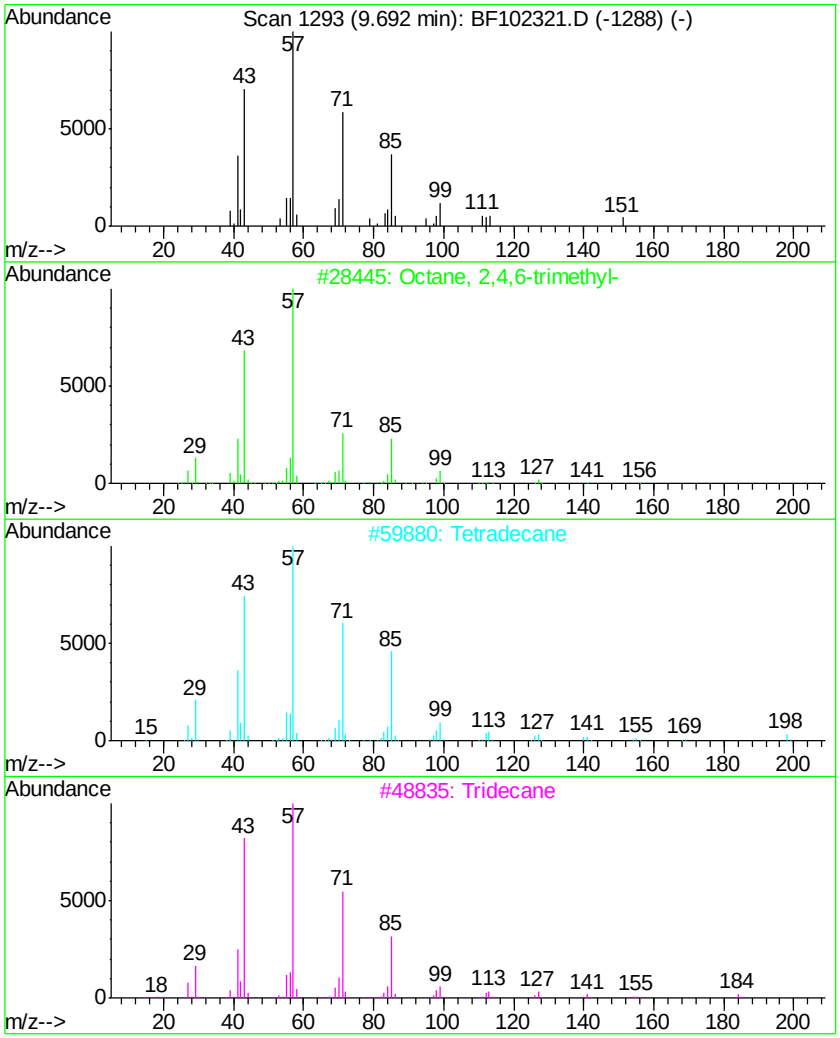
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

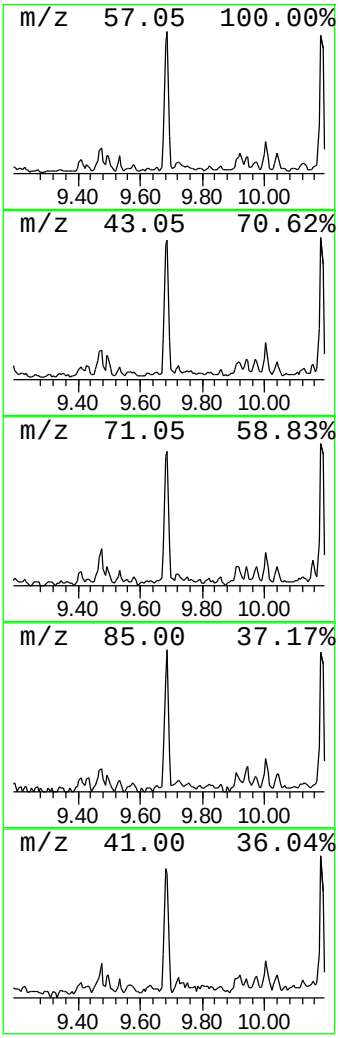
****

Peak Number 4 Octane, 2,4,6-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.69	2.88 ng	127479	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	90
2	Tetradecane	198	C14H30	000629-59-4	90
3	Tridecane	184	C13H28	000629-50-5	83
4	Hexadecane	226	C16H34	000544-76-3	83
5	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102321.D
Acq On : 23 Jan 2018 1:12
Operator : SJ/JU
Sample : J1238-18
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-06-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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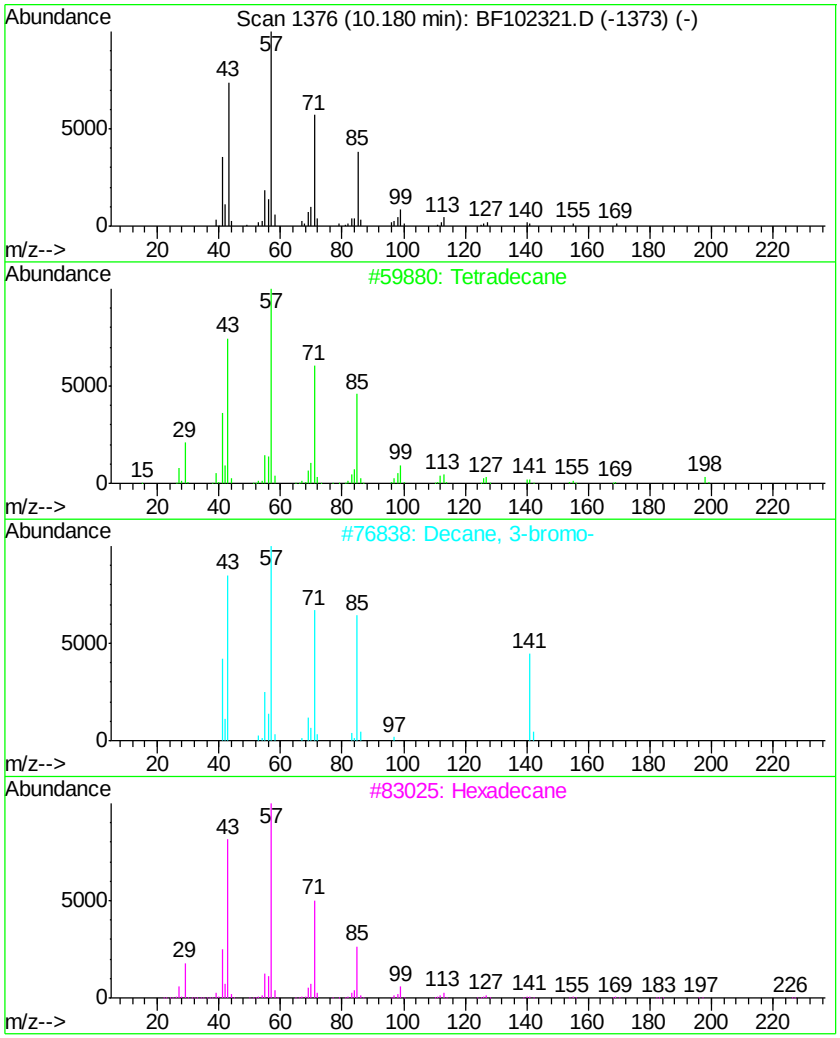
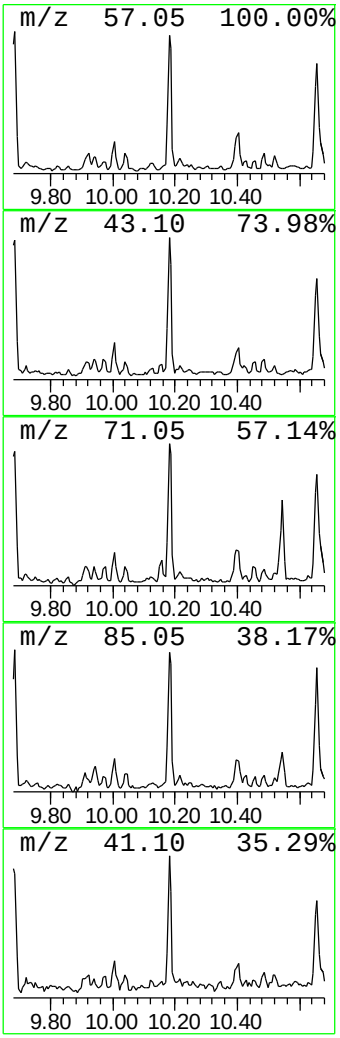
Peak Number 5 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.18	2.72 ng	120265	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	78
2	Decane, 3-bromo-	220	C10H21Br	030571-71-2	72
3	Hexadecane	226	C16H34	000544-76-3	72
4	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5	Tridecane	184	C13H28	000629-50-5	50





Library Search Compound Report

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Acq On : 23 Jan 2018 1:12
Operator : SJ/JU
Sample : J1238-18
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ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-06-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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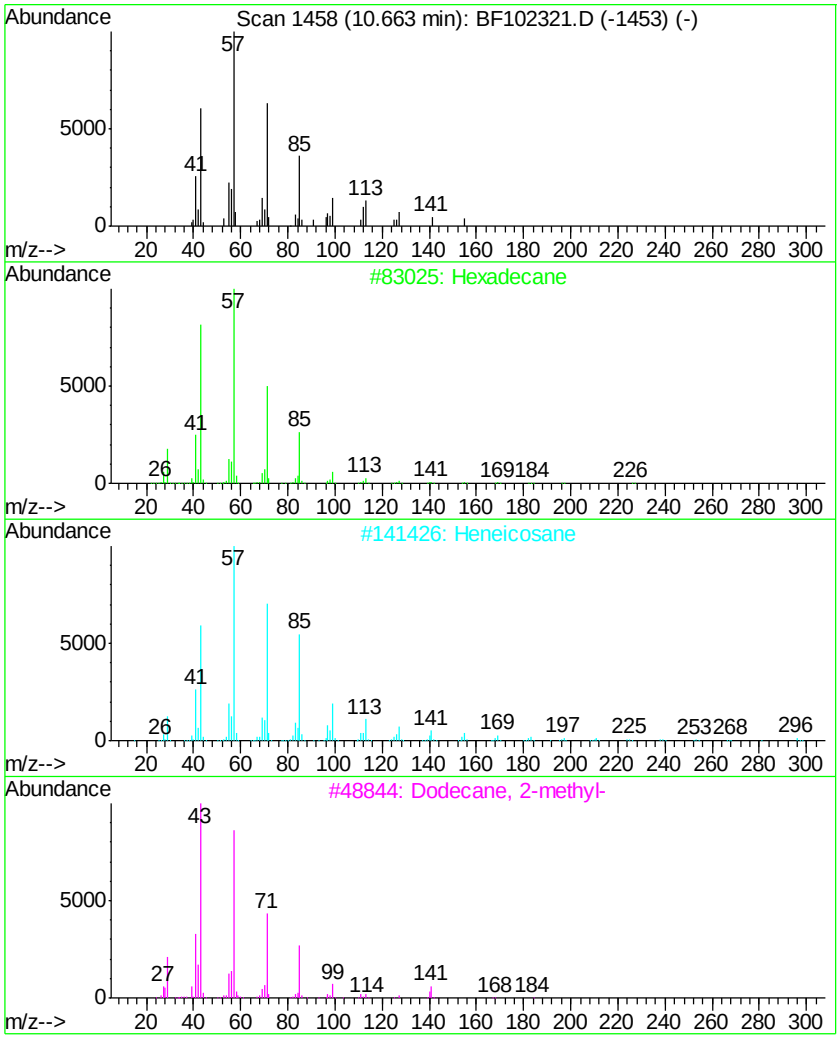
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

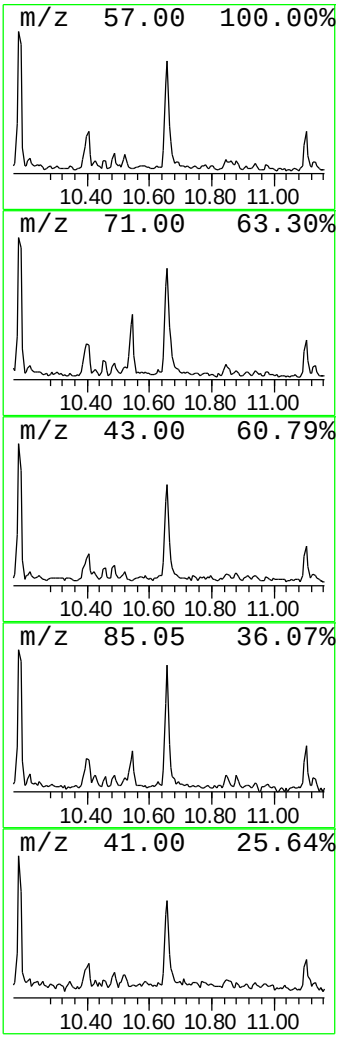
****

Peak Number 6 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	3.36 ng	121810	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heneicosane	296	C21H44	000629-94-7	87
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	86
4	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
5	Heptadecane	240	C17H36	000629-78-7	83





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Sample : J1238-18
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-06-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

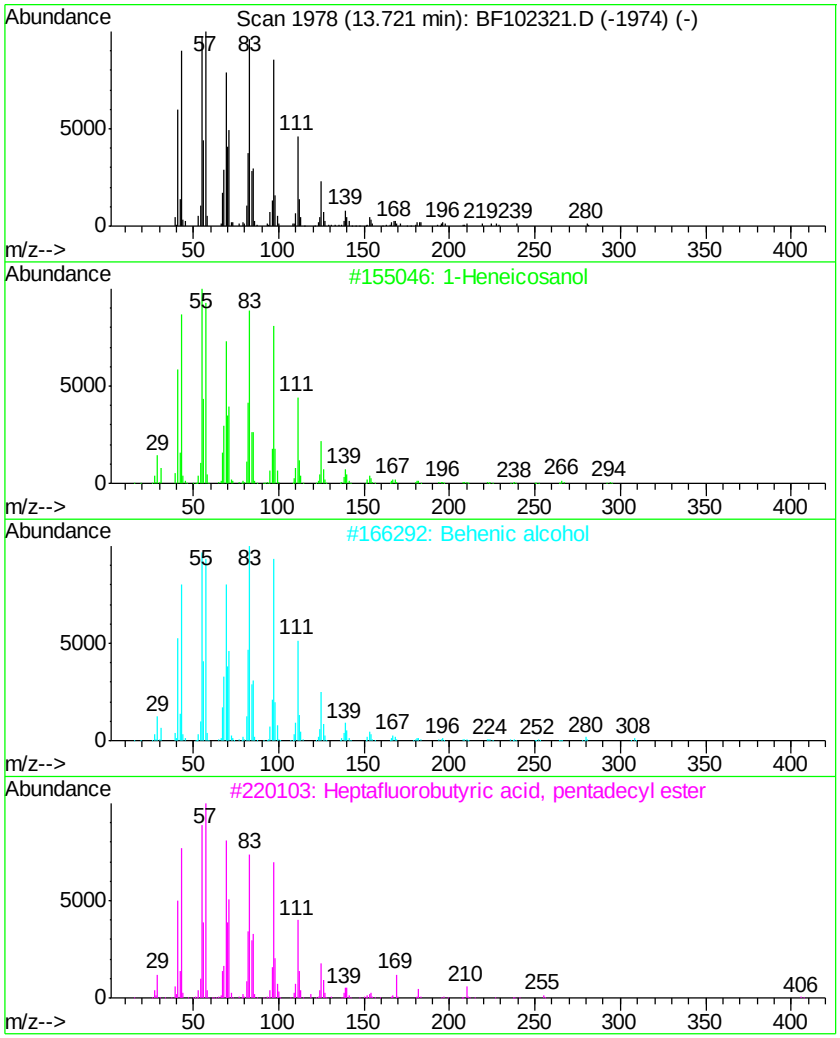
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

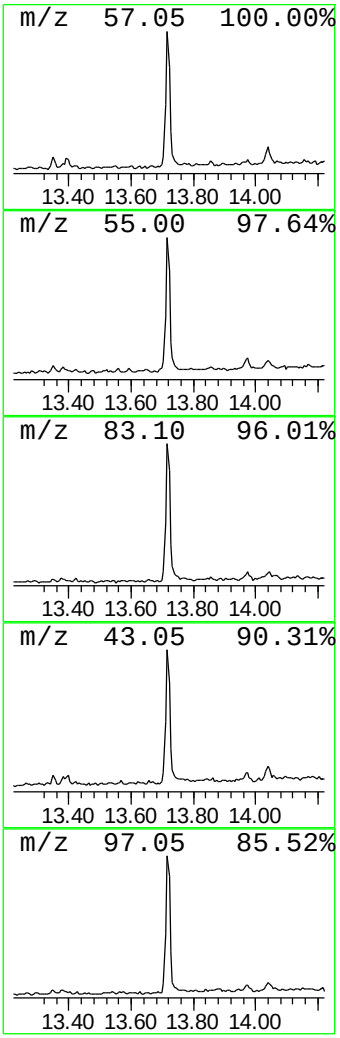
****

Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	13.18 ng	458033	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

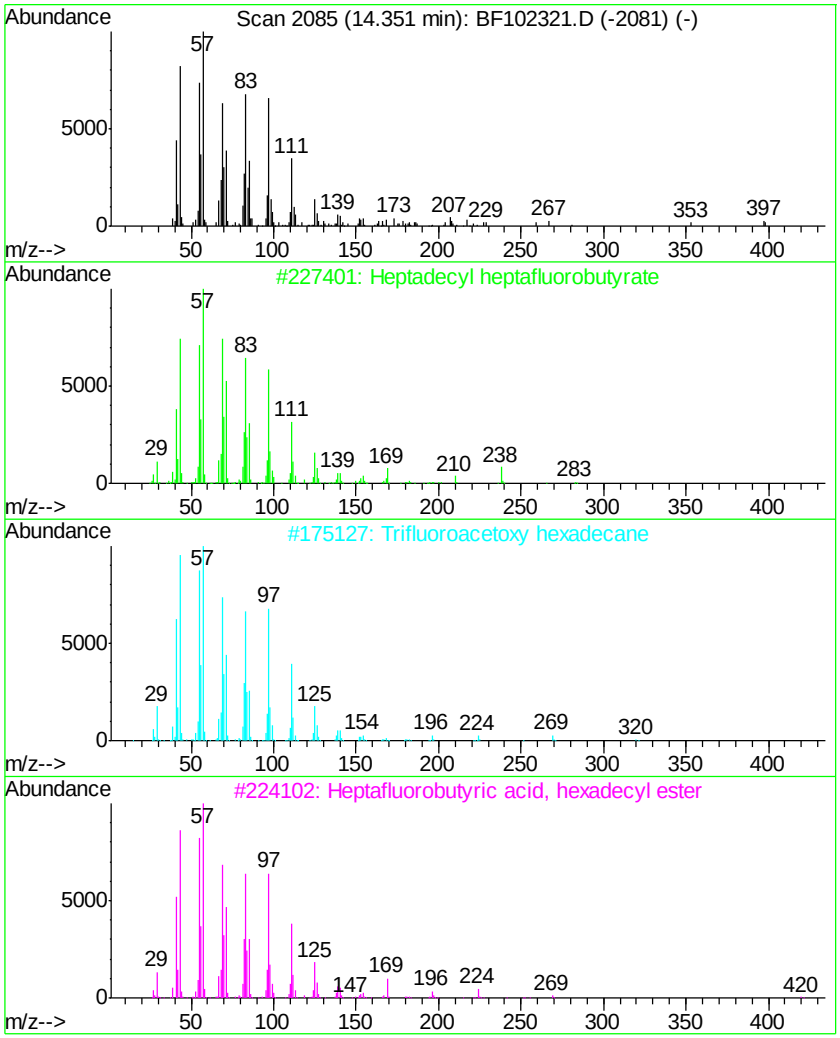
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

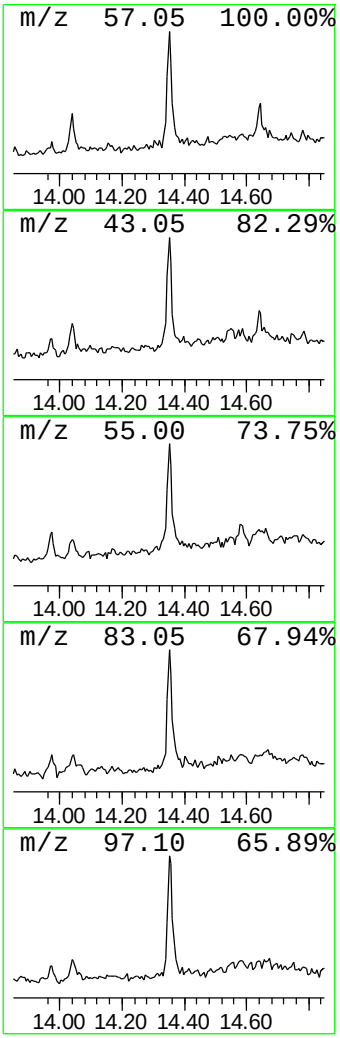
****

Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	5.66 ng	196471	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	93
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	6.4	ng	224079	1	6.72	699013	20.0
unknown6.49	6.49	86.2	ng	3011080	1	6.72	699013	20.0
Octane, 2,4,6-tri...	9.69	2.9	ng	127479	3	9.75	883766	20.0
Tetradecane	10.18	2.7	ng	120265	3	9.75	883766	20.0
Hexadecane	10.66	3.4	ng	121810	4	11.24	724696	20.0
1-Heneicosanol	13.72	13.2	ng	458033	5	13.87	694851	20.0
Heptadecyl heptaf...	14.35	5.7	ng	196471	5	13.87	694851	20.0