LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100364.D
Acq On : 10 Nov 2017 2:00
Operator : SJ/JU
Sample : I6379-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-(1-4)

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-BF110817.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	5.140	514	519	530	rVB	713023	962683	23.97%	2.723%
2	5.528	579	585	588	rBV	3429120	3838111	95.55%	10.858%
3	6.528	748	755	758	rBV	3578450	4016761	100.00%	11.363%
4	6.675	774	780	783	rBV	3716545	3865855	96.24%	10.936%
5	6.904	815	819	822	rBV	1246140	1032667	25.71%	2.921%
6	7.057	841	845	849	rVB	2945589	2858436	71.16%	8.086%
7	7.463	909	914	917	rBV	2499414	2515583	62.63%	7.116%
8	8.181	1032	1036	1040	rBV	1464834	1336088	33.26%	3.780%
9	8.733	1126	1130	1134	rBV	209550	168157	4.19%	0.476%
10	9.257	1214	1219	1223	rBV	4075774	3919244	97.57%	11.087%
11	9.645	1283	1285	1289	rVB	110095	81191	2.02%	0.230%
12	9.939	1331	1335	1339	rVB	1618388	1366771	34.03%	3.866%
13	10.651	1451	1456	1459	rBV	745179	594591	14.80%	1.682%
14	10.727	1464	1469	1472	rBV	2399899	2275562	56.65%	6.437%
15	11.421	1582	1587	1590	rBV	1321959	1231869	30.67%	3.485%
16	11.939	1672	1675	1683	rBV	225092	208517	5.19%	0.590%
17	12.633	1790	1793	1798	rBV	60555	61058	1.52%	0.173%
18	12.727	1805	1809	1817	rBV	120510	148448	3.70%	0.420%
19	13.010	1852	1857	1860	rBV	3026152	2743144	68.29%	7.760%
20	13.892	2004	2007	2013	rBV2	152184	153481	3.82%	0.434%
21	14.062	2032	2036	2039	rBV	1079969	979396	24.38%	2.771%
22	14.527	2112	2115	2119	rBV	51192	57789	1.44%	0.163%
23	15.545	2283	2288	2296	rVB	757635	933885	23.25%	2.642%

Sum of corrected areas: 35349287

LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
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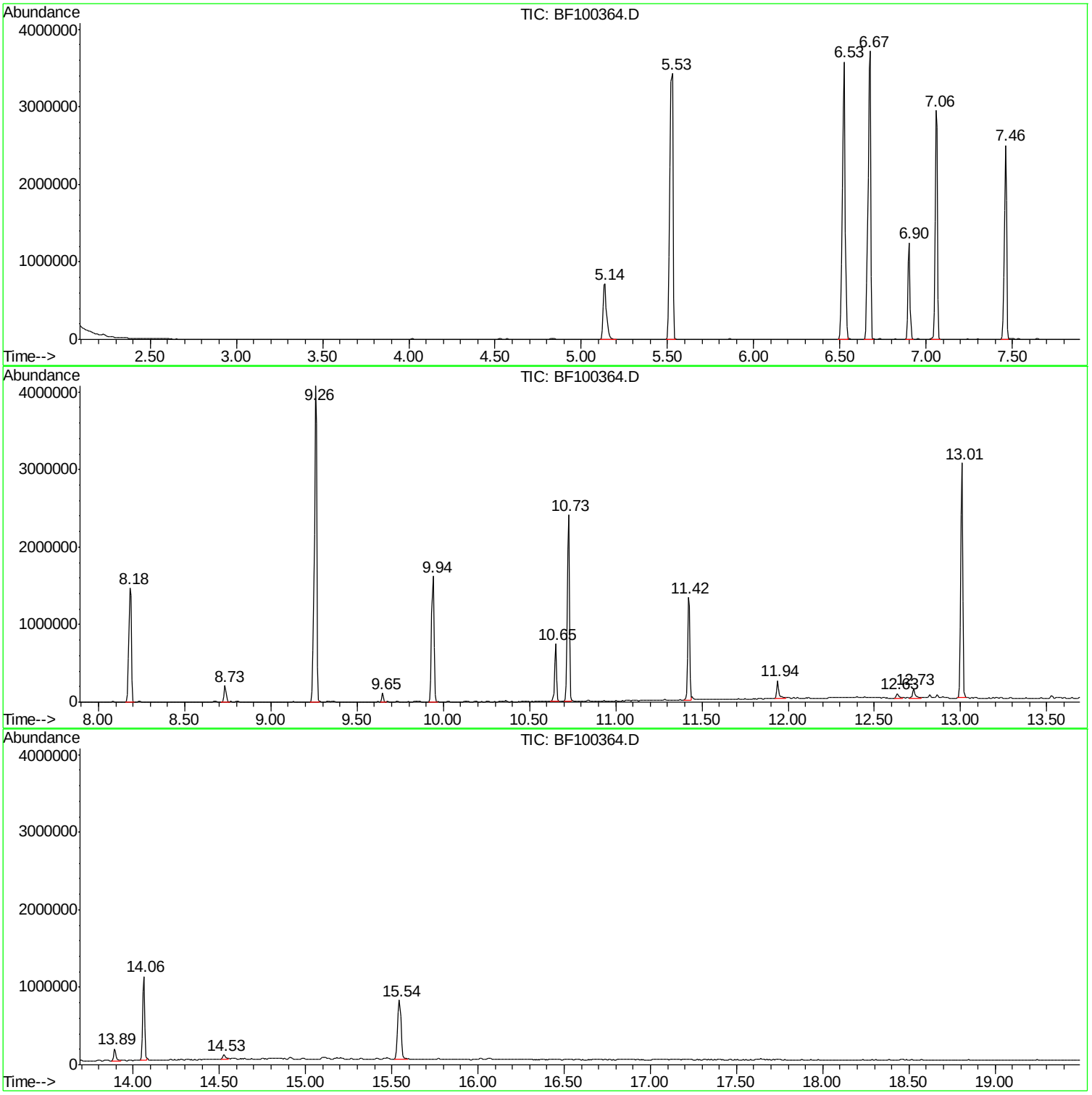
Acq On : 10 Nov 2017 2:00
Operator : SJ/JU
Sample : I6379-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-2-(1-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100364.D
Acq On : 10 Nov 2017 2:00
Operator : SJ/JU
Sample : I6379-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-(1-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

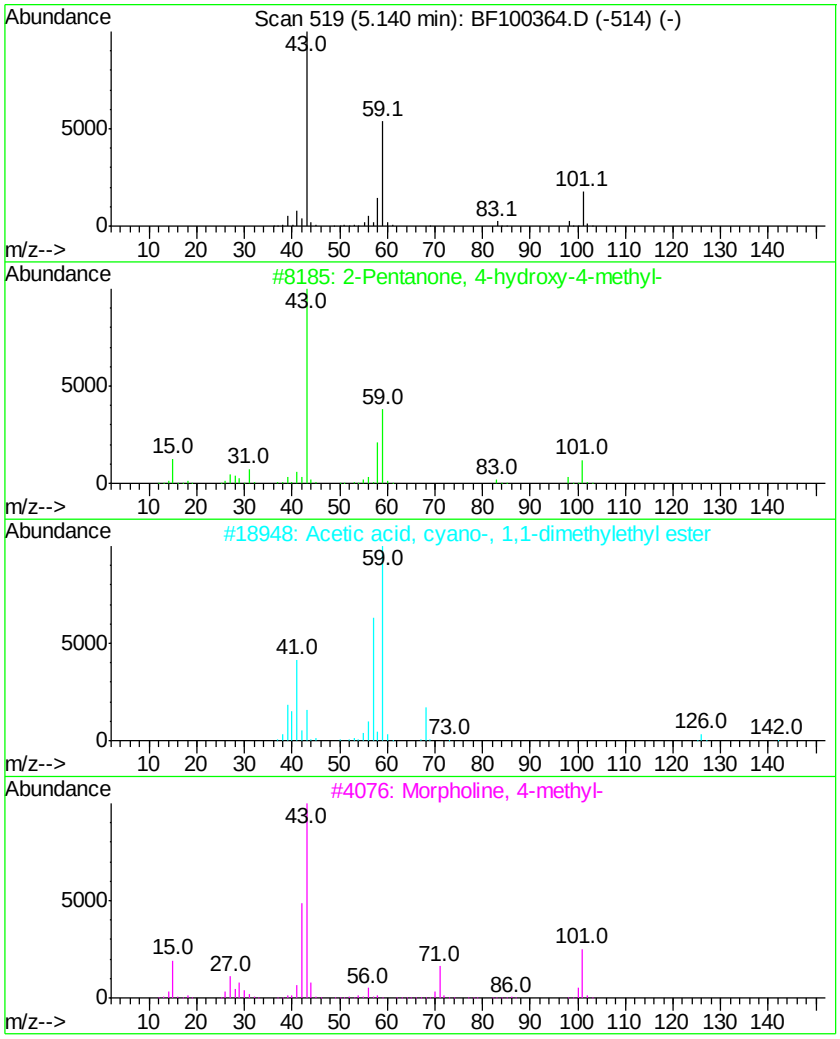
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

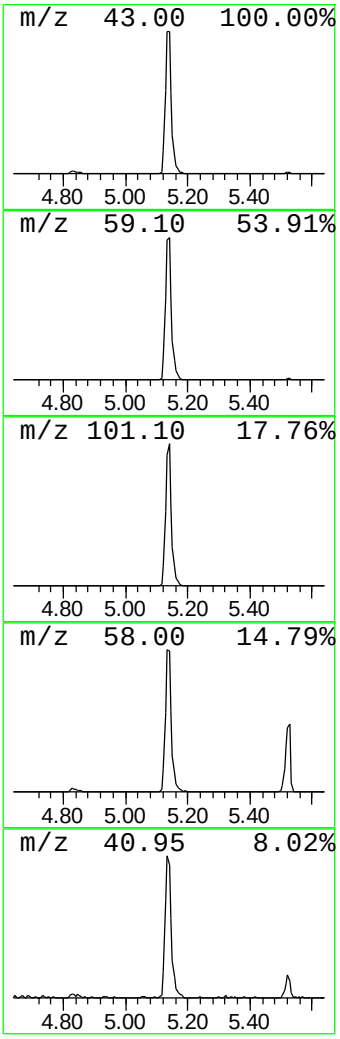
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	18.64 ng	962683	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Library Search Compound Report

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Acq On : 10 Nov 2017 2:00
Operator : SJ/JU
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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-(1-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

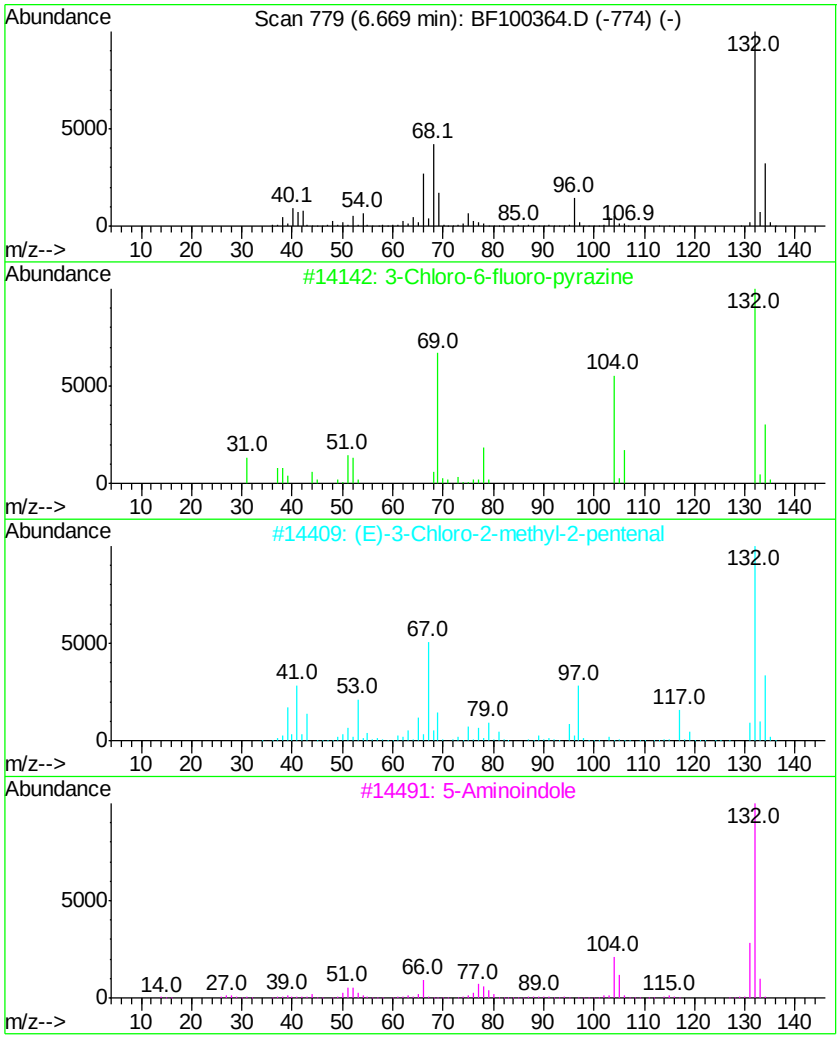
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

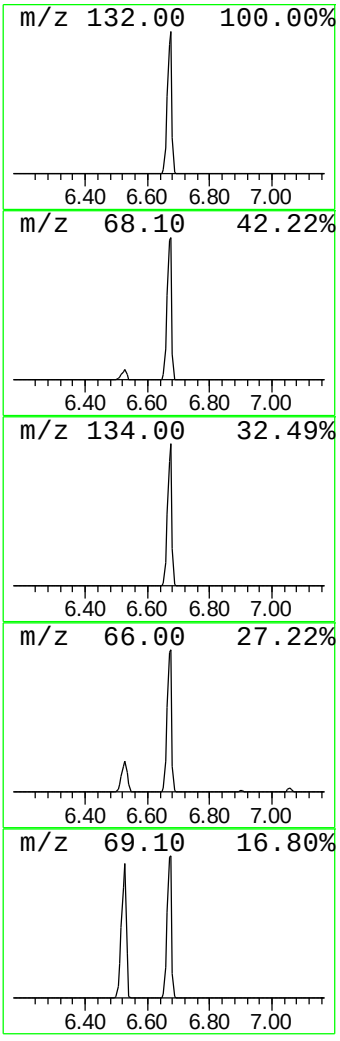
****

Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	74.87 ng	3865860	1,4-Dichlorobenzene-d4	6.90

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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Data File : BF100364.D
Acq On : 10 Nov 2017 2:00
Operator : SJ/JU
Sample : I6379-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-(1-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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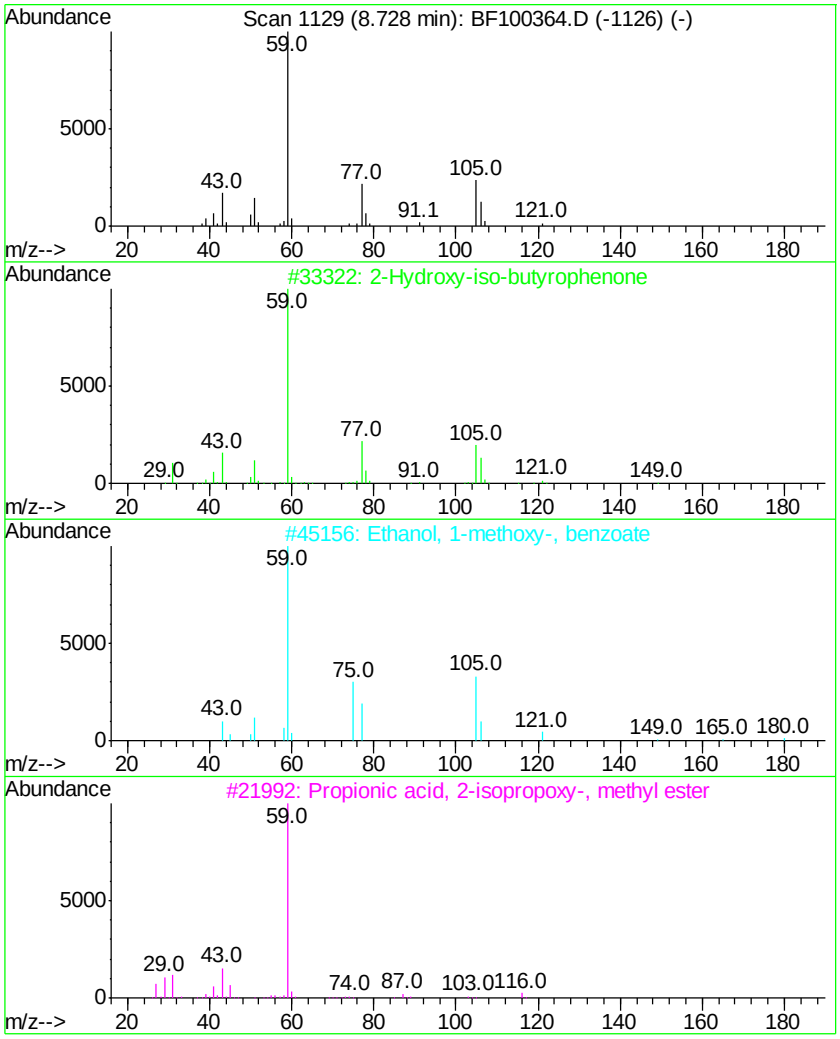
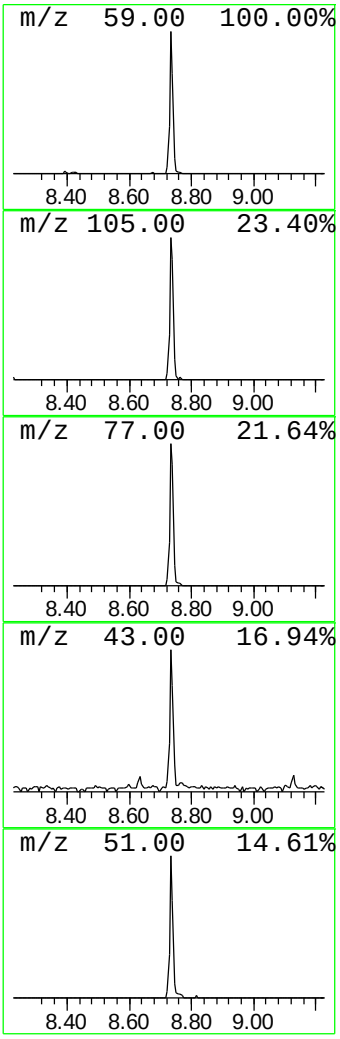
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	2.52 ng	168157	Naphthalene-d8	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	72
3	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
5	Guanidine	59	CH5N3	000113-00-8	7





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100364.D
Acq On : 10 Nov 2017 2:00
Operator : SJ/JU
Sample : I6379-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-(1-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

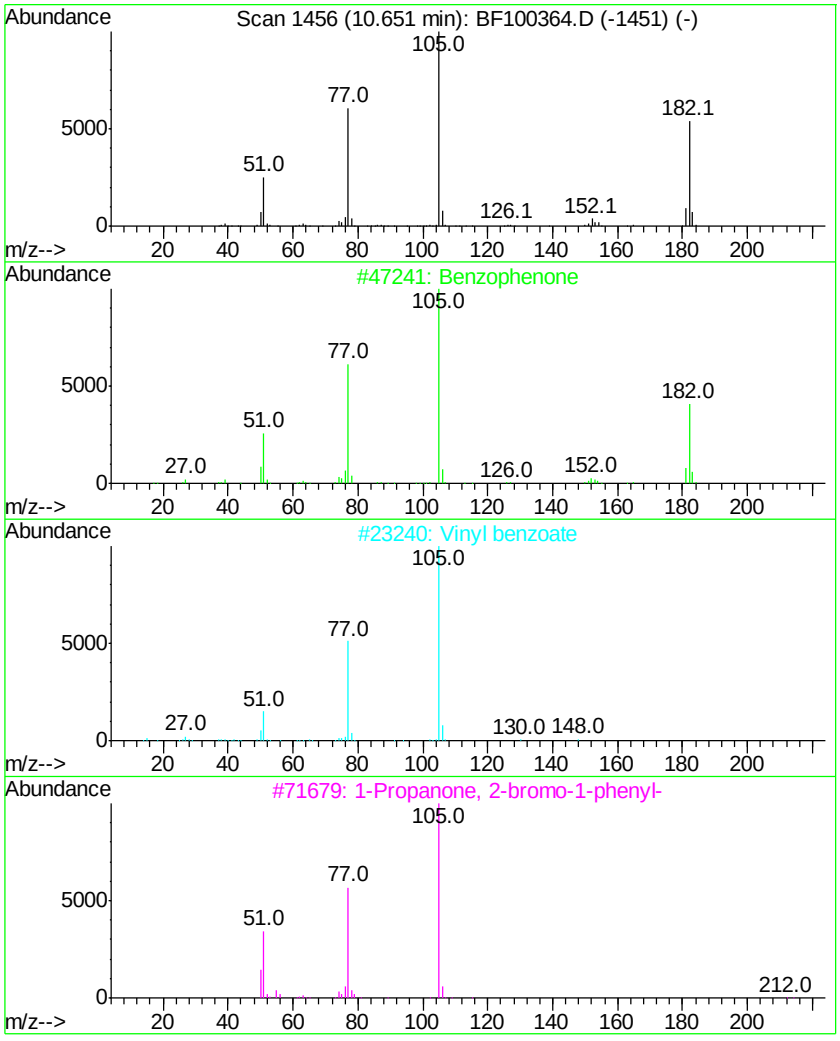
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

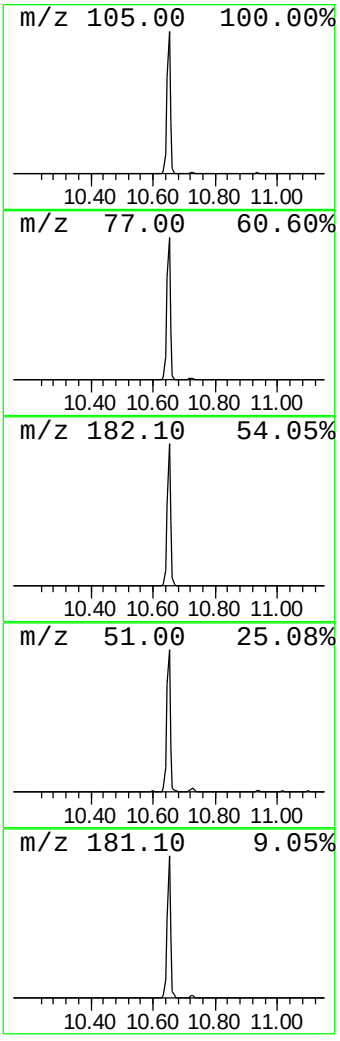
****

Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	8.70 ng	594591	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Vinyl benzoate	148	C9H8O2	000769-78-8	47
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47
5	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100364.D
Acq On : 10 Nov 2017 2:00
Operator : SJ/JU
Sample : I6379-04
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-(1-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

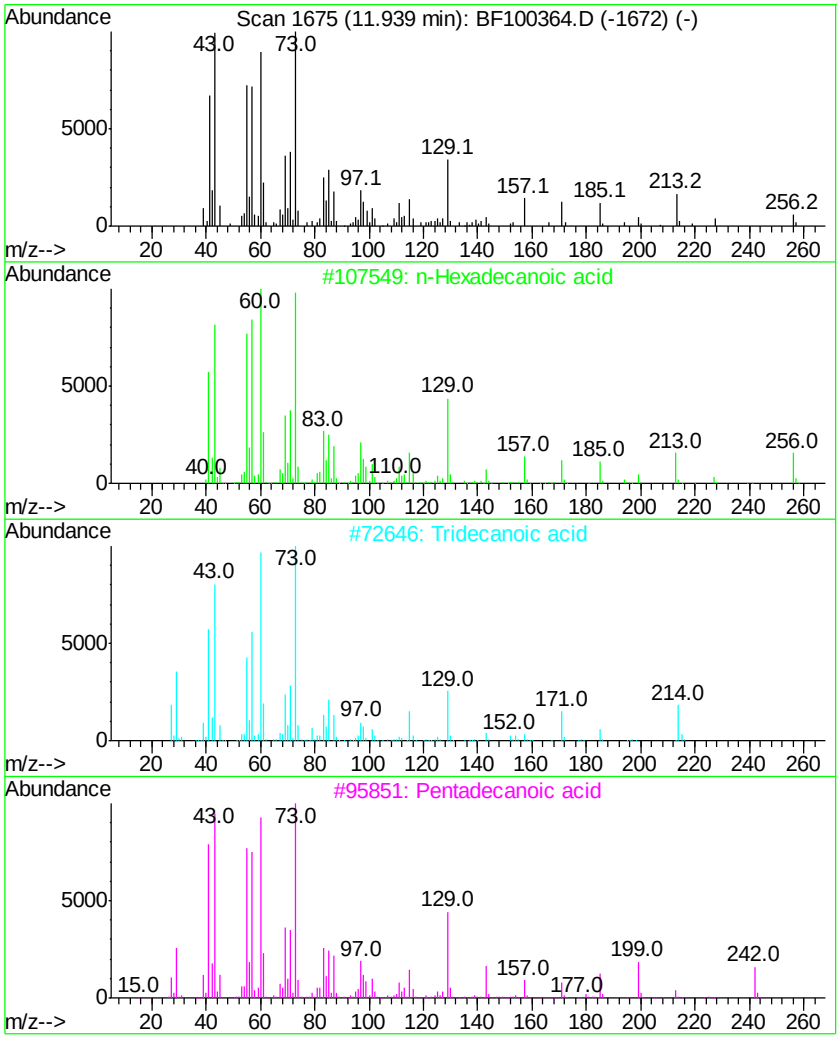
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

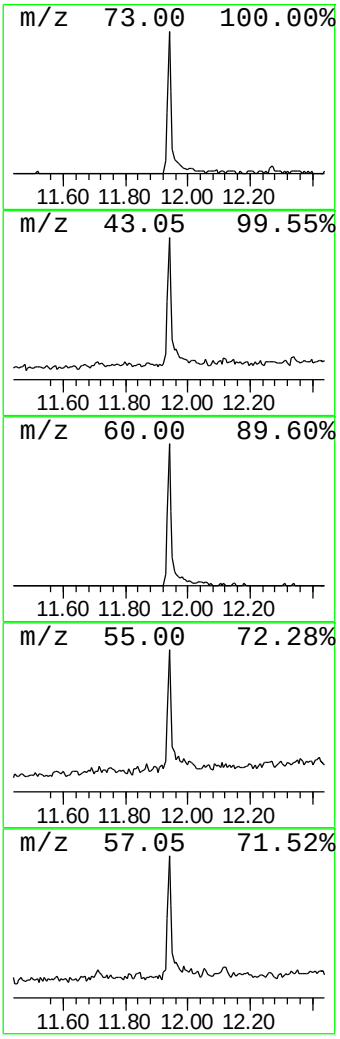
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	3.39 ng	208517	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Dodecanoic acid	200	C12H24O2	000143-07-7	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	62





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Operator : SJ/JU
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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-2-(1-4)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
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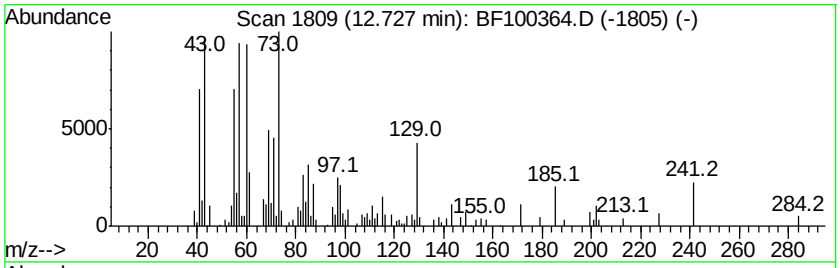
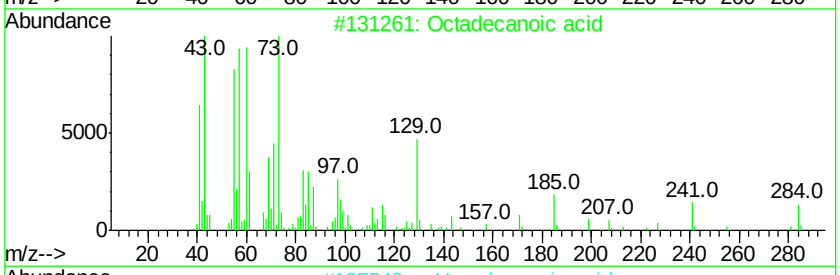
****

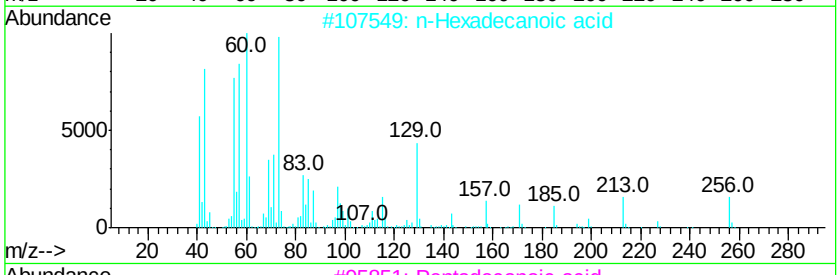
Peak Number 7 Octadecanoic acid Concentration Rank 8

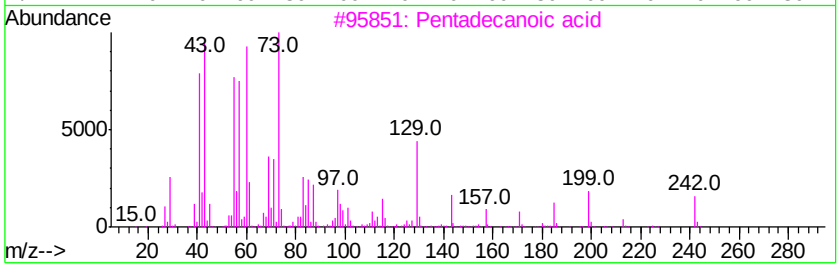
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.41 ng	148448	Phenanthrene-d10	11.42

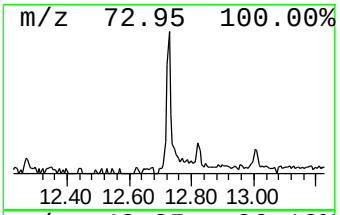
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18

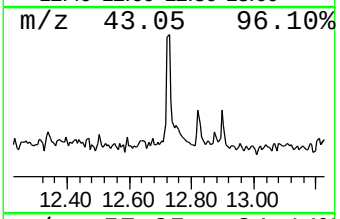


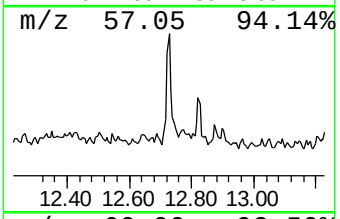


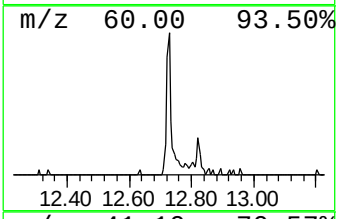


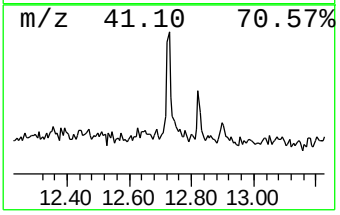












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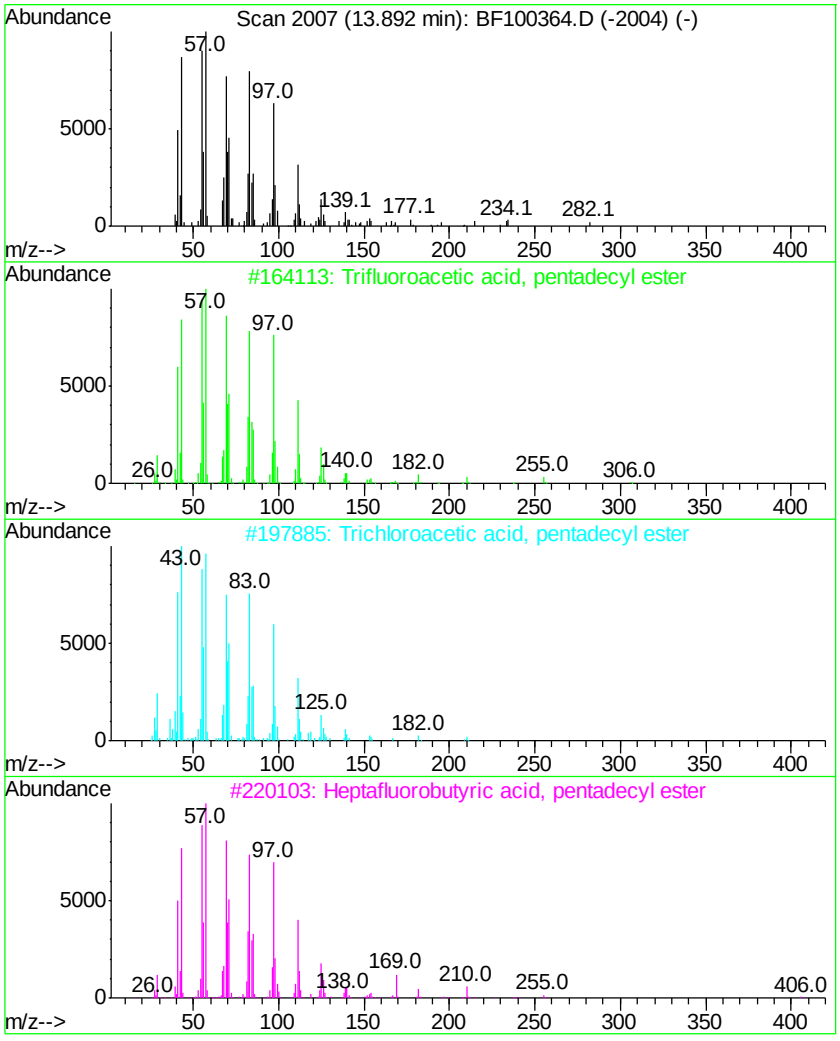
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

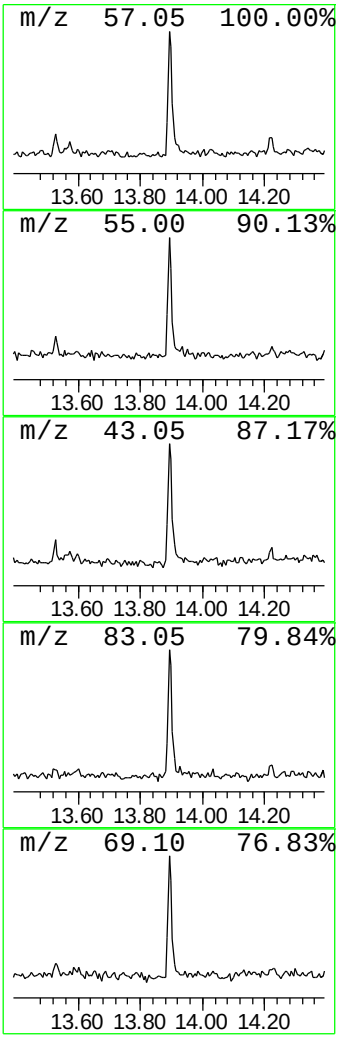
****

Peak Number 8 Trifluoroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	3.13 ng	153481	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91





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...	5.14	18.6	ng	962683	1	6.90	1032670	20.0
unknown6.67	6.67	74.9	ng	3865860	1	6.90	1032670	20.0
2-Hydroxy-iso-but...	8.73	2.5	ng	168157	2	8.18	1336090	20.0
Benzophenone	10.65	8.7	ng	594591	3	9.94	1366770	20.0
n-Hexadecanoic acid	11.94	3.4	ng	208517	4	11.42	1231870	20.0
Octadecanoic acid	12.73	2.4	ng	148448	4	11.42	1231870	20.0
Trifluoroacetic a...	13.89	3.1	ng	153481	5	14.06	979396	20.0