LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
Data File : BF100403.D
Acq On : 10 Nov 2017 20:44
Operator : SJ/JU
Sample : I6388-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-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-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	4.522	410	414	421	rVB	39501	46699	1.56%	0.167%
2	5.134	513	518	526	rVB	439625	540516	18.04%	1.928%
3	5.522	579	584	587	rBV	2888540	2880439	96.14%	10.276%
4	6.528	749	755	758	rBV	2837144	2939853	98.12%	10.488%
5	6.669	775	779	783	rBV	2813720	2864201	95.59%	10.218%
6	6.904	815	819	822	rBV	1176064	976157	32.58%	3.482%
7	7.057	841	845	849	rBV	2464578	2226658	74.32%	7.943%
8	7.169	857	864	869	rVB4	13385	32085	1.07%	0.114%
9	7.463	909	914	917	rBV	1972016	1751545	58.46%	6.248%
10	8.186	1033	1037	1040	rVB	1351051	1218766	40.68%	4.348%
11	8.733	1127	1130	1134	rBV	125774	106473	3.55%	0.380%
12	9.257	1215	1219	1222	rBV	3361340	2996233	100.00%	10.689%
13	9.645	1282	1285	1293	rBV	220417	206247	6.88%	0.736%
14	9.939	1331	1335	1346	rVB	1382515	1181123	39.42%	4.214%
15	10.651	1452	1456	1459	rBV	309302	257440	8.59%	0.918%
16	10.727	1464	1469	1472	rBV	1493329	1415298	47.24%	5.049%
17	11.427	1584	1588	1591	rBV	1082441	1006209	33.58%	3.590%
18	11.939	1671	1675	1681	rBV	278667	267337	8.92%	0.954%
19	12.633	1790	1793	1794	rBV2	55697	51001	1.70%	0.182%
20	12.727	1805	1809	1817	rBV	247798	273598	9.13%	0.976%
21	12.886	1830	1836	1849	rVB	570749	829812	27.70%	2.960%
22	13.010	1853	1857	1860	rBV	2402422	2146945	71.65%	7.659%
23	13.468	1930	1935	1942	rBV3	44744	80772	2.70%	0.288%
24	13.892	2005	2007	2011	rBV	121419	123315	4.12%	0.440%
25	14.062	2032	2036	2040	rBV	1043775	907613	30.29%	3.238%
26	15.545	2284	2288	2297	rVB	523673	705403	23.54%	2.516%

Sum of corrected areas: 28031738

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
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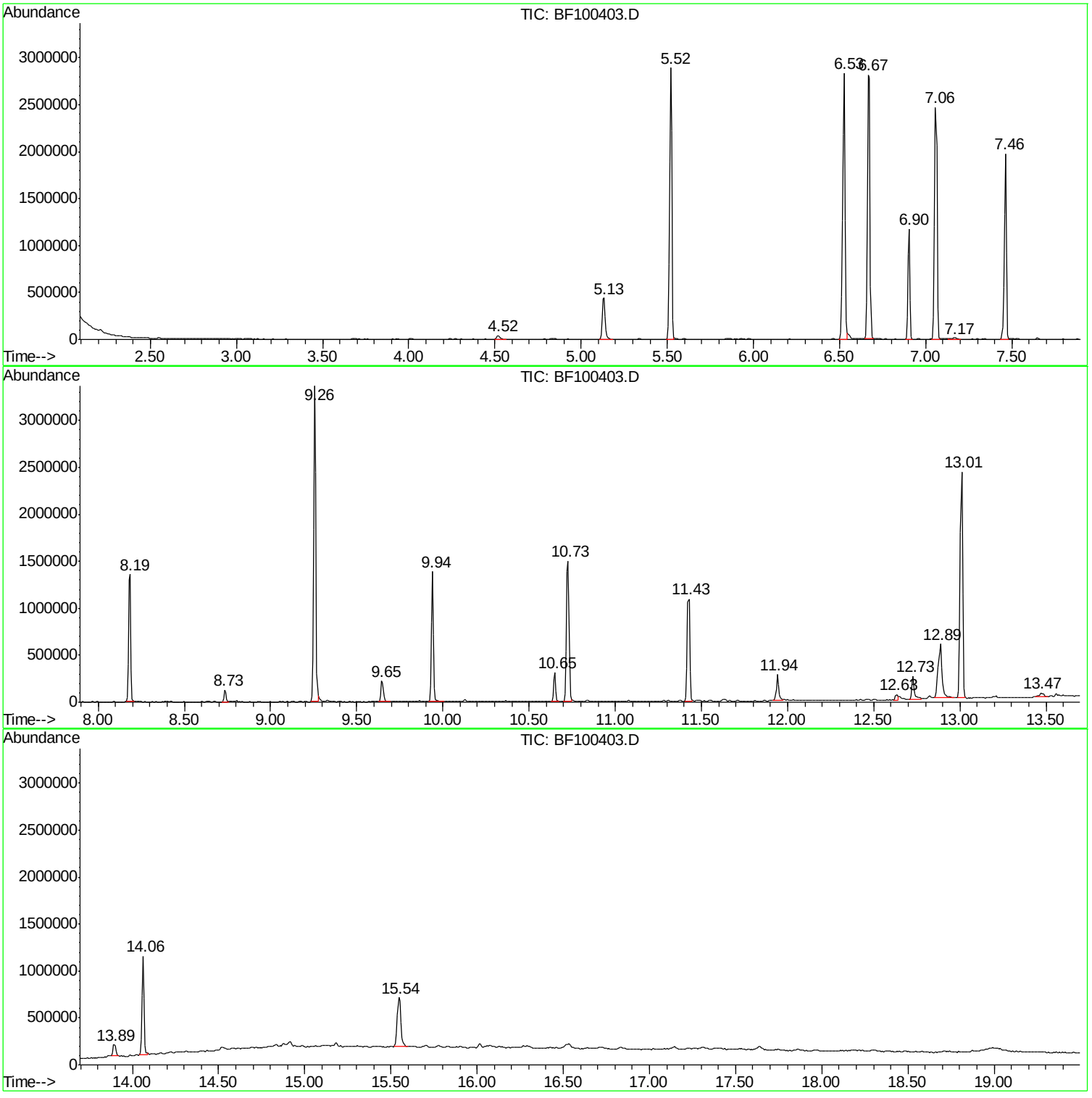
Operator : SJ/JU
Sample : I6388-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-5

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



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Data File : BF100403.D
Acq On : 10 Nov 2017 20:44
Operator : SJ/JU
Sample : I6388-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-5

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

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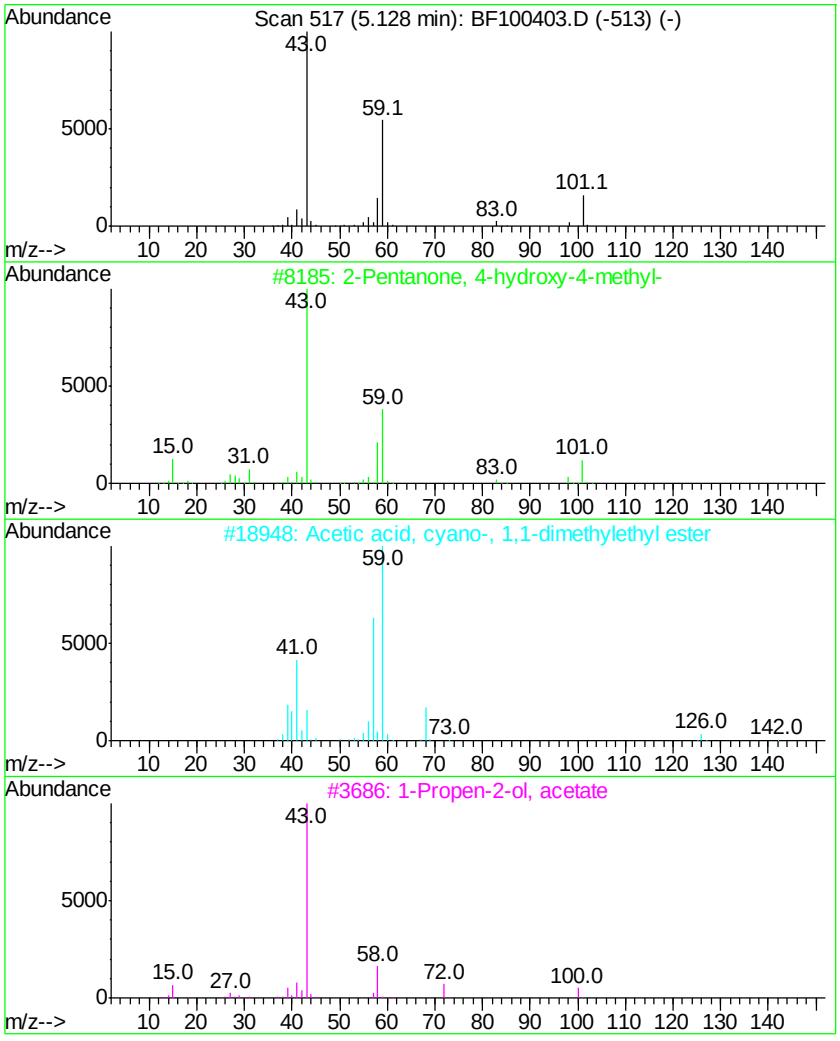
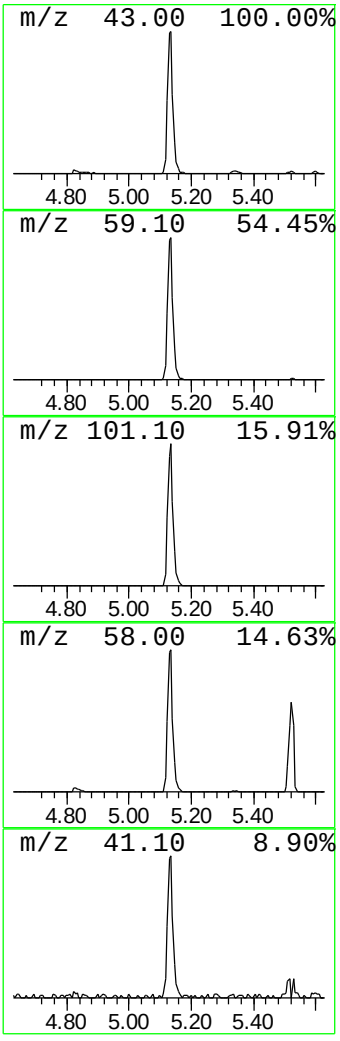
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	11.07 ng	540516	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	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

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Acq On : 10 Nov 2017 20:44
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Misc :
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Instrument : BNA_F
ClientSampleId : 3N-5

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

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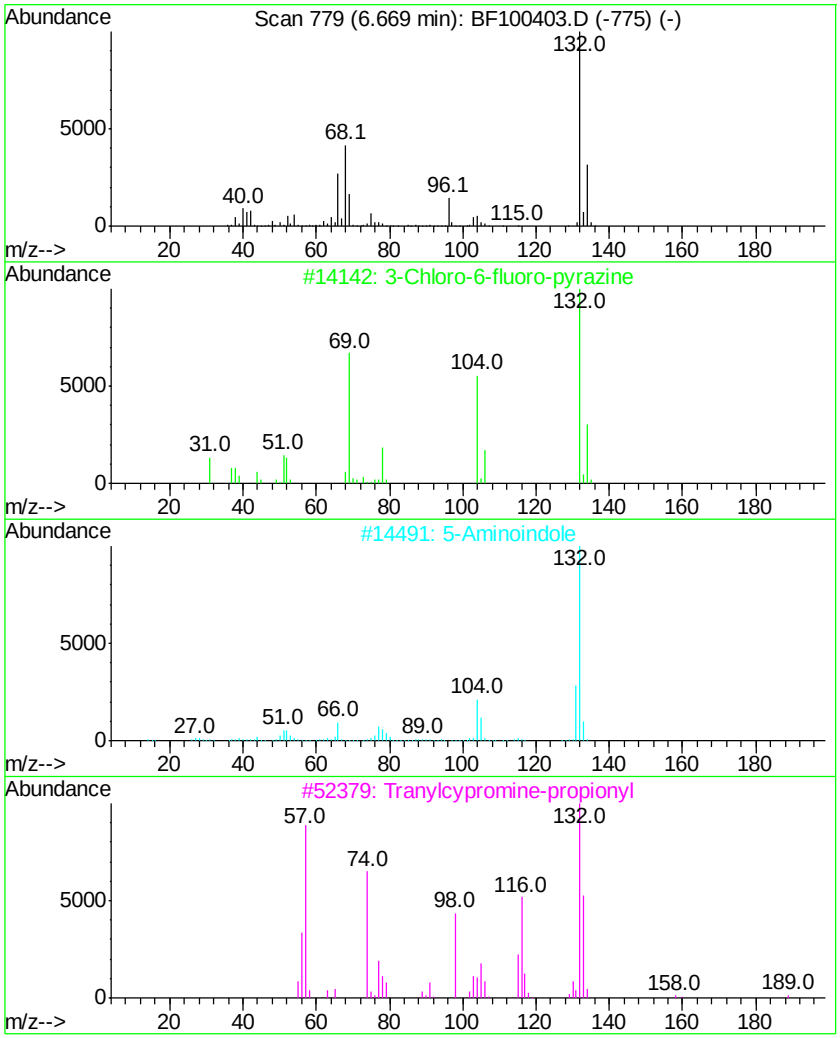
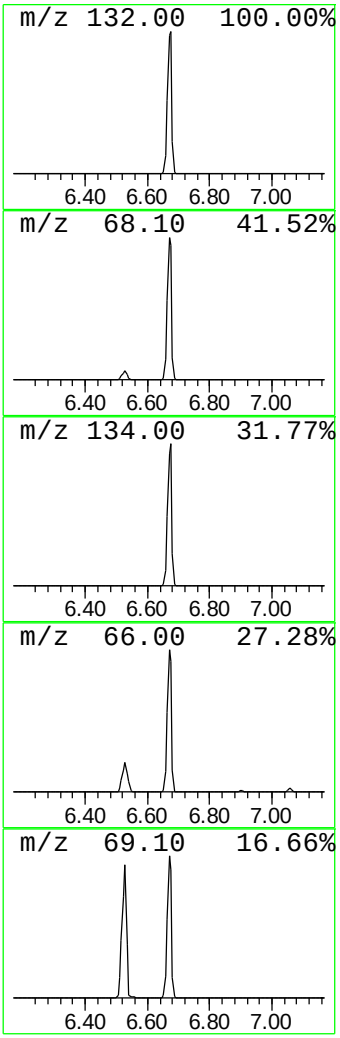
Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	58.68 ng	2864200	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	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	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 : BF100403.D
Acq On : 10 Nov 2017 20:44
Operator : SJ/JU
Sample : I6388-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-5

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

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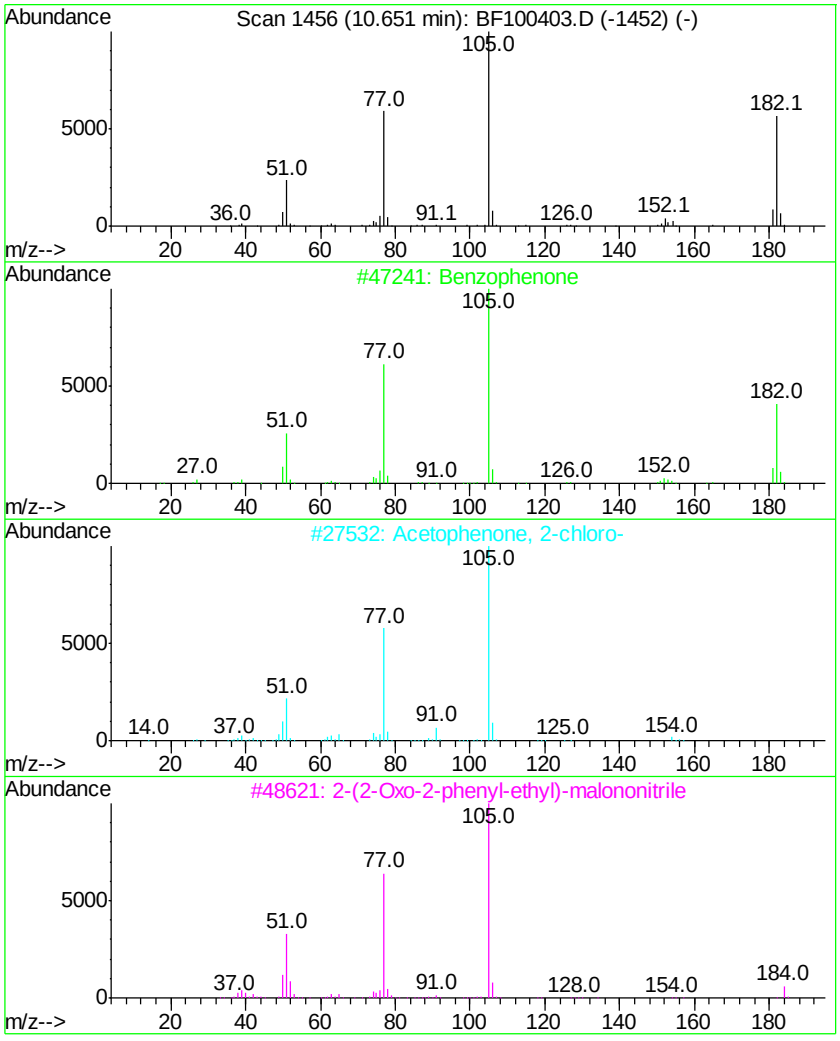
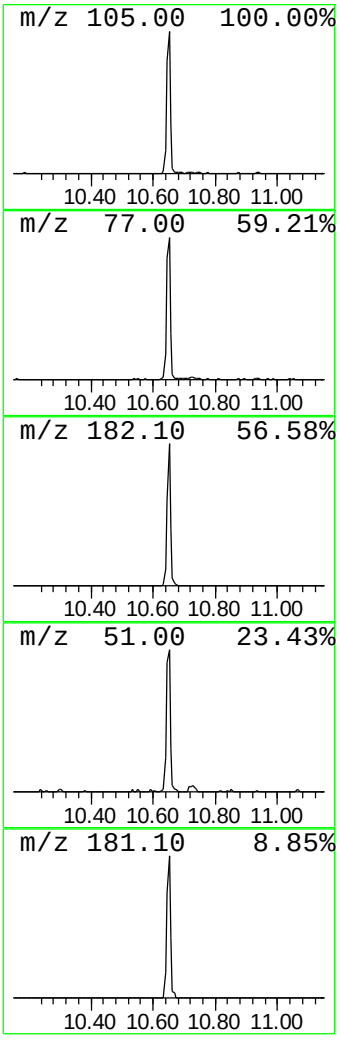
Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	4.36 ng	257440	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
4	Benzoyl bromide	184	C7H5BrO	000618-32-6	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





Library Search Compound Report

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Acq On : 10 Nov 2017 20:44
Operator : SJ/JU
Sample : I6388-09
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-5

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

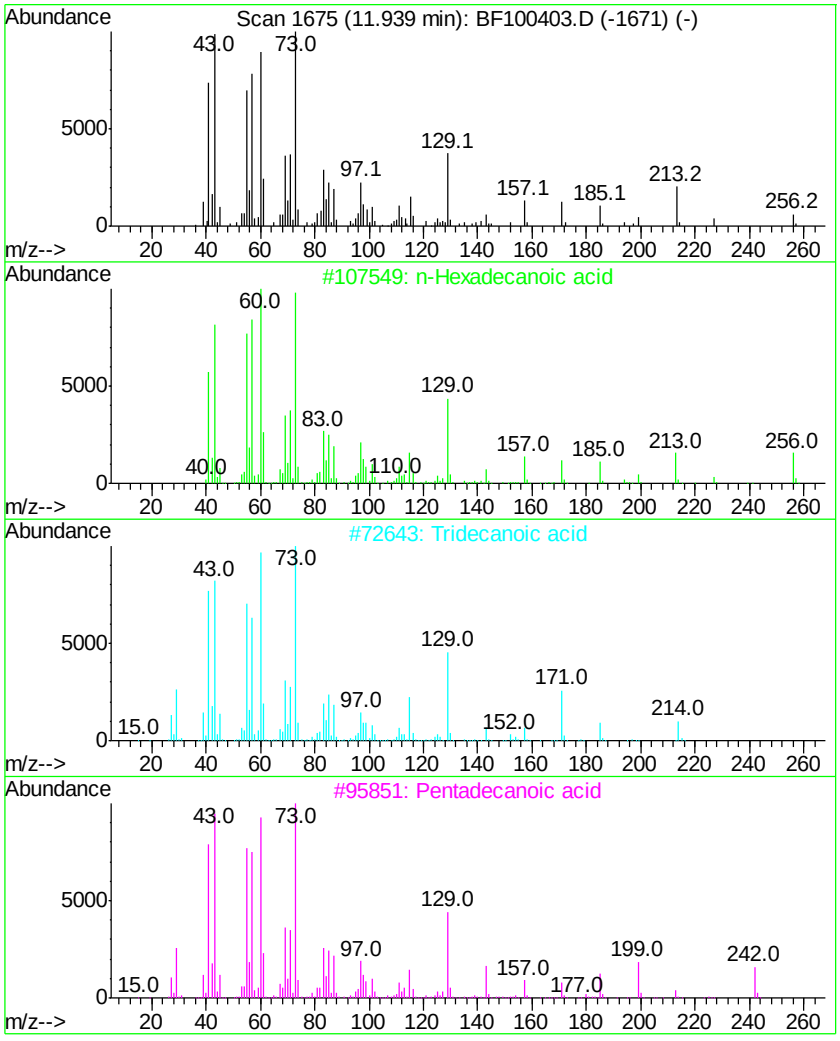
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

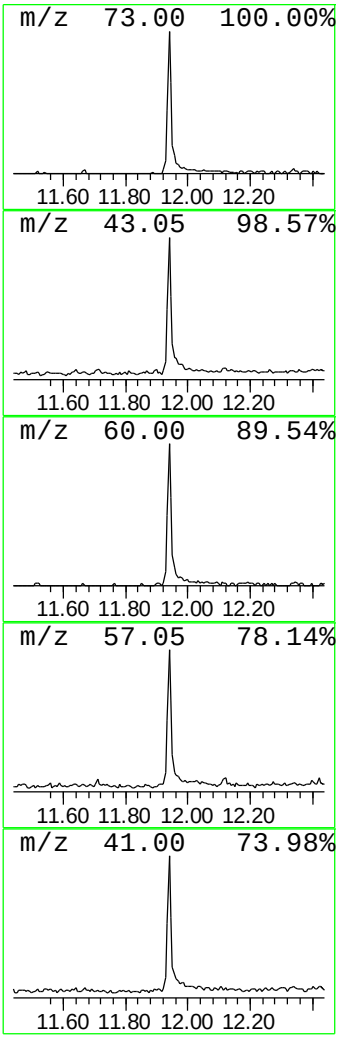
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	5.31 ng	267337	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Lactose	342	C12H22O11	000063-42-3	38





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111017\
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-5

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

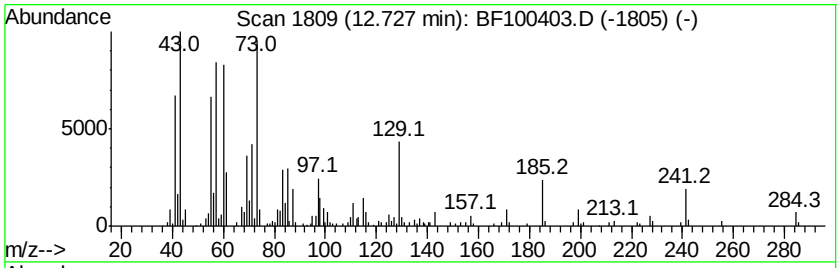
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

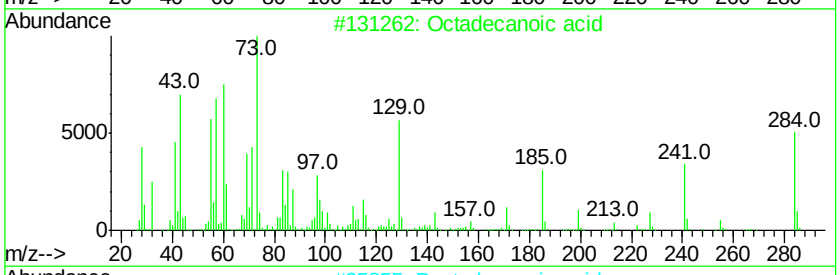
****

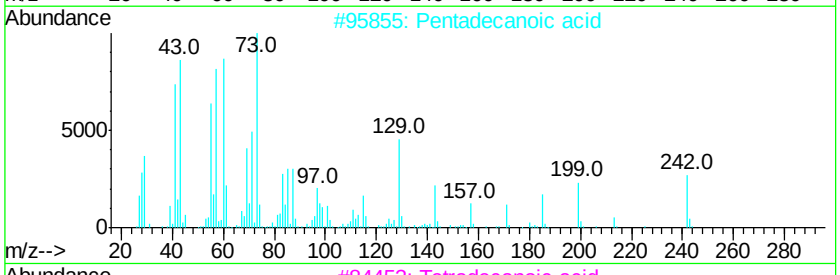
Peak Number 6 Octadecanoic acid Concentration Rank 5

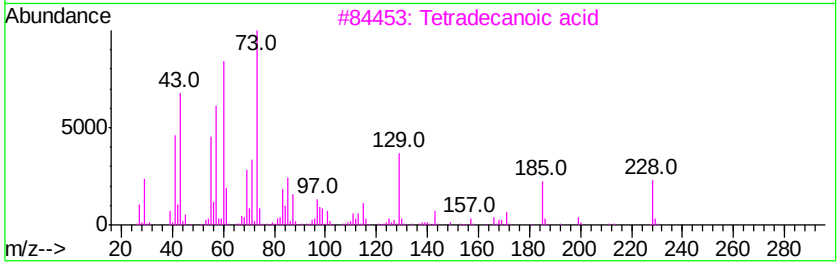
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	5.44 ng	273598	Phenanthrene-d10	11.43

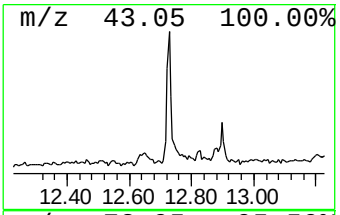
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	70
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64

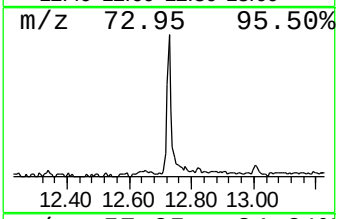


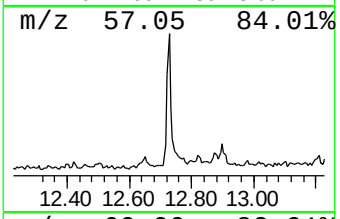


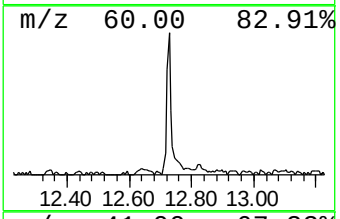


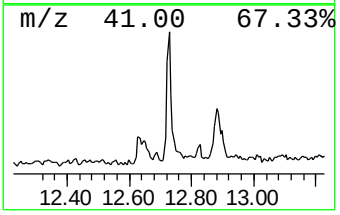












Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : 3N-5

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

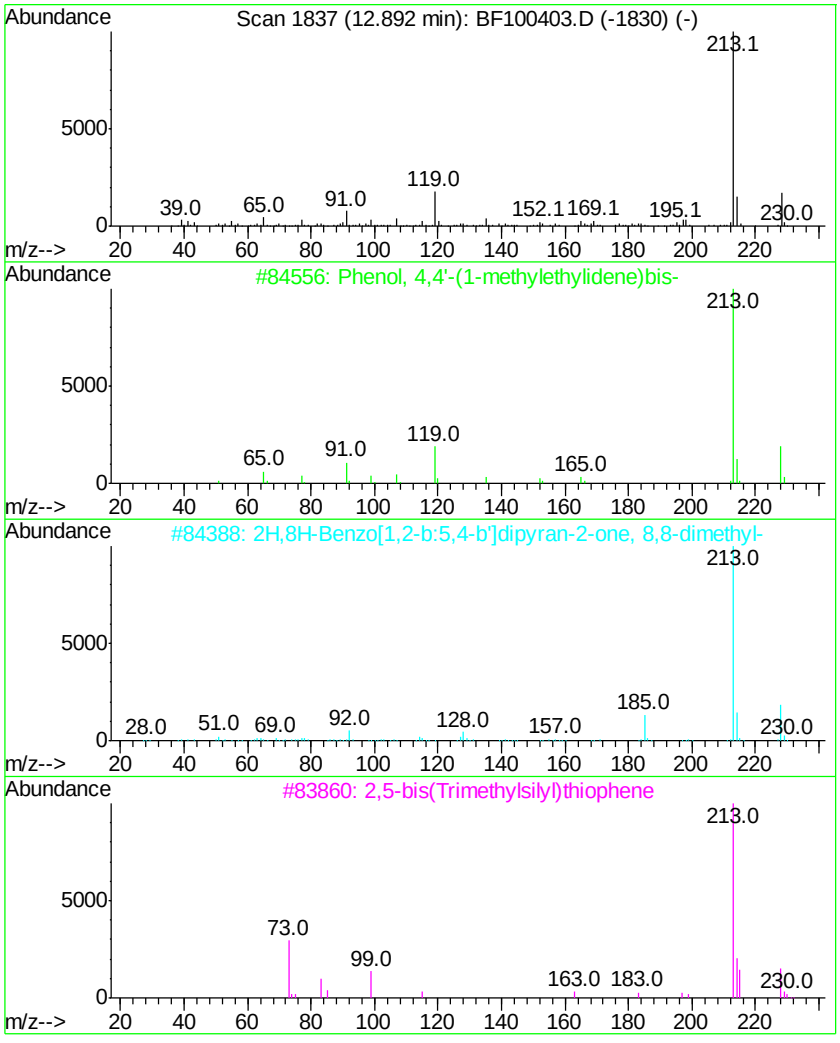
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

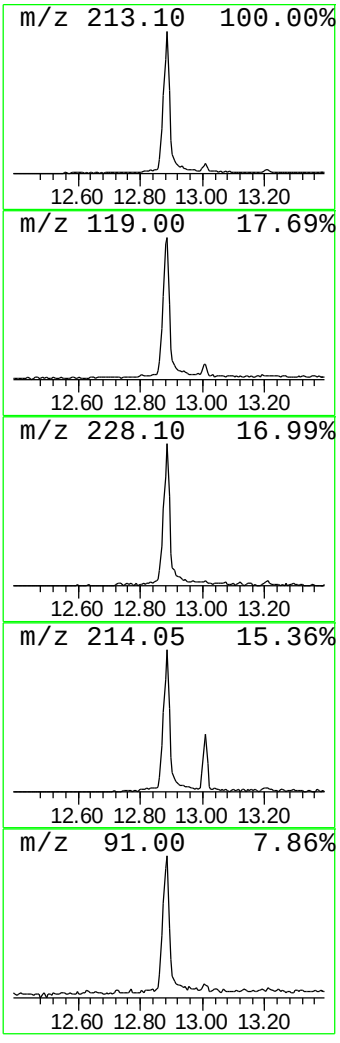
****

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	18.29 ng	829812	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	52
3	2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	50
4	2-Bromo-7-(methylamino)tropone	213	C8H8BrNO	103539-25-9	47
5	Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	45





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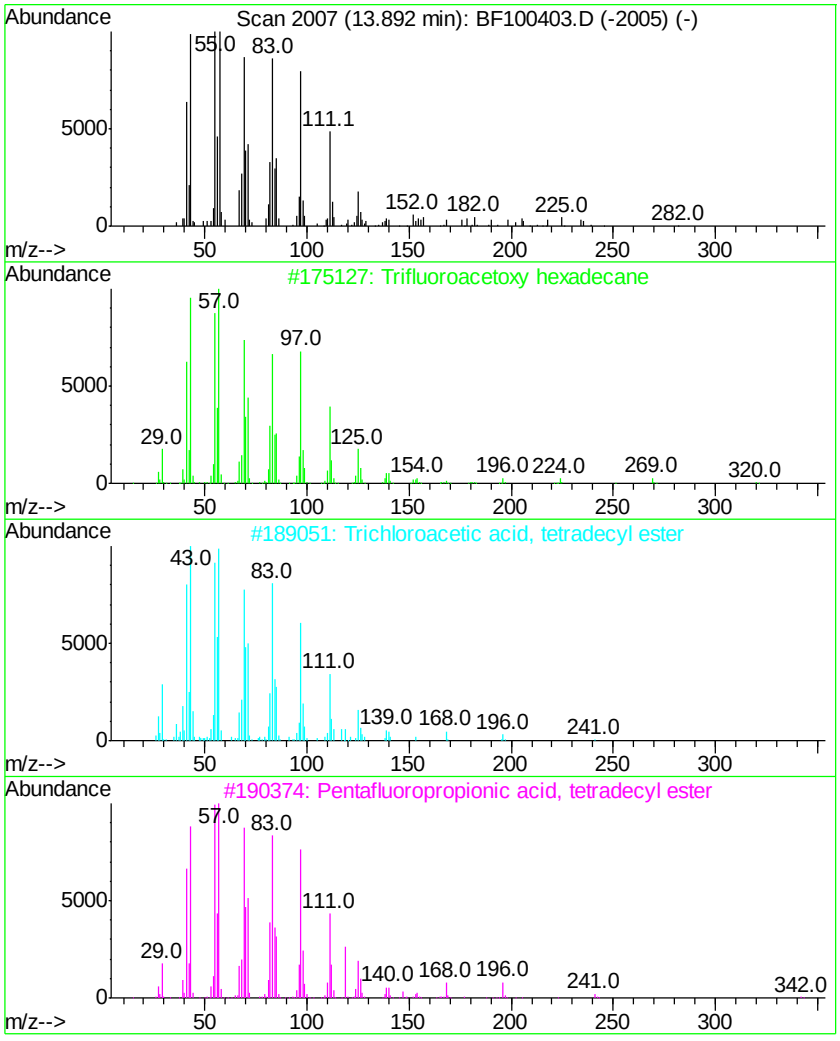
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

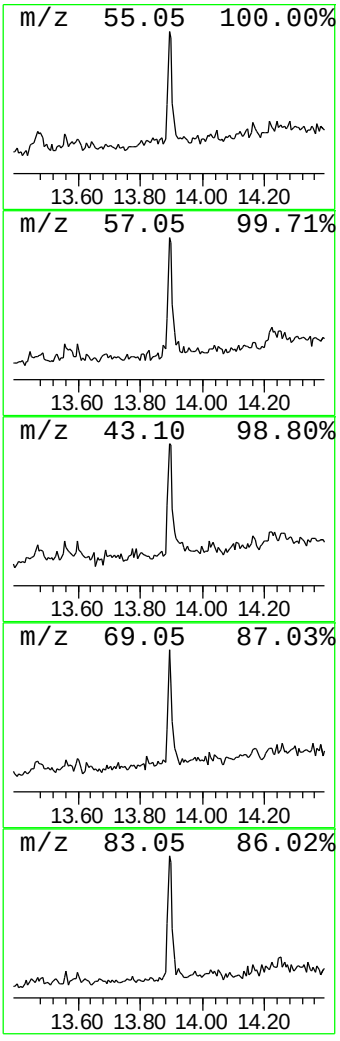
****

Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	2.72 ng	123315	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	87
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	81
5	1-Heneicosanol	312	C21H44O	015594-90-8	81





Tentatively Identified Compound (LSC) summary

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Data File : BF100403.D
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Operator : SJ/JU
Sample : I6388-09
Misc :
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Instrument : BNA_F
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.13	11.1	ng	540516	1	6.90	976157	20.0
unknown6.67	6.67	58.7	ng	2864200	1	6.90	976157	20.0
Benzophenone	10.65	4.4	ng	257440	3	9.94	1181120	20.0
n-Hexadecanoic acid	11.94	5.3	ng	267337	4	11.43	1006210	20.0
Octadecanoic acid	12.73	5.4	ng	273598	4	11.43	1006210	20.0
Phenol, 4,4'-(1-m...	12.89	18.3	ng	829812	5	14.06	907613	20.0
Trifluoroacetoxy ...	13.89	2.7	ng	123315	5	14.06	907613	20.0