LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-25(0-10)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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	2.228	20	24	42	rVB	93427	188994	13.91%	1.549%
2	5.175	522	525	536	rBV	29333	42244	3.11%	0.346%
3	5.563	587	591	612	rBV	1114563	1216902	89.54%	9.971%
4	6.569	758	762	782	rBV	1300636	1359123	100.00%	11.136%
5	6.710	782	786	793	rBV	1525844	1311401	96.49%	10.745%
6	6.939	822	825	832	rBV	407123	391798	28.83%	3.210%
7	7.098	848	852	868	rBV	1066643	933411	68.68%	7.648%
8	7.510	918	922	940	rBV	738097	817135	60.12%	6.695%
9	8.228	1040	1044	1061	rBV	455075	534008	39.29%	4.375%
10	9.298	1222	1226	1242	rBV	1350346	1291076	94.99%	10.579%
11	9.692	1289	1293	1303	rVB	90603	98022	7.21%	0.803%
12	9.986	1339	1343	1355	rBV	545982	583254	42.91%	4.779%
13	10.775	1473	1477	1489	rBV	756549	774224	56.96%	6.344%
14	11.480	1593	1597	1604	rBV	497414	526076	38.71%	4.310%
15	11.980	1679	1682	1687	rBV2	29993	33368	2.46%	0.273%
16	13.057	1861	1865	1869	rBV	1073239	916783	67.45%	7.512%
17	13.527	1941	1945	1949	rBV3	24220	24038	1.77%	0.197%
18	13.933	2011	2014	2020	rBV	78230	94590	6.96%	0.775%
19	14.127	2043	2047	2054	rBV	460210	445581	32.78%	3.651%
20	14.557	2117	2120	2124	rBV4	26533	35257	2.59%	0.289%
21	14.874	2171	2174	2176	rBV	23251	21935	1.61%	0.180%
22	15.221	2231	2233	2237	rVB	40701	39072	2.87%	0.320%
23	15.615	2297	2300	2303	rBV	31431	35048	2.58%	0.287%
24	15.657	2303	2307	2312	rVB	274885	342807	25.22%	2.809%
25	16.068	2373	2377	2383	rVB2	40271	65129	4.79%	0.534%
26	16.357	2421	2426	2433	rVB9	24569	57149	4.20%	0.468%
27	16.815	2499	2504	2507	rBV6	13750	26260	1.93%	0.215%

Sum of corrected areas: 12204685

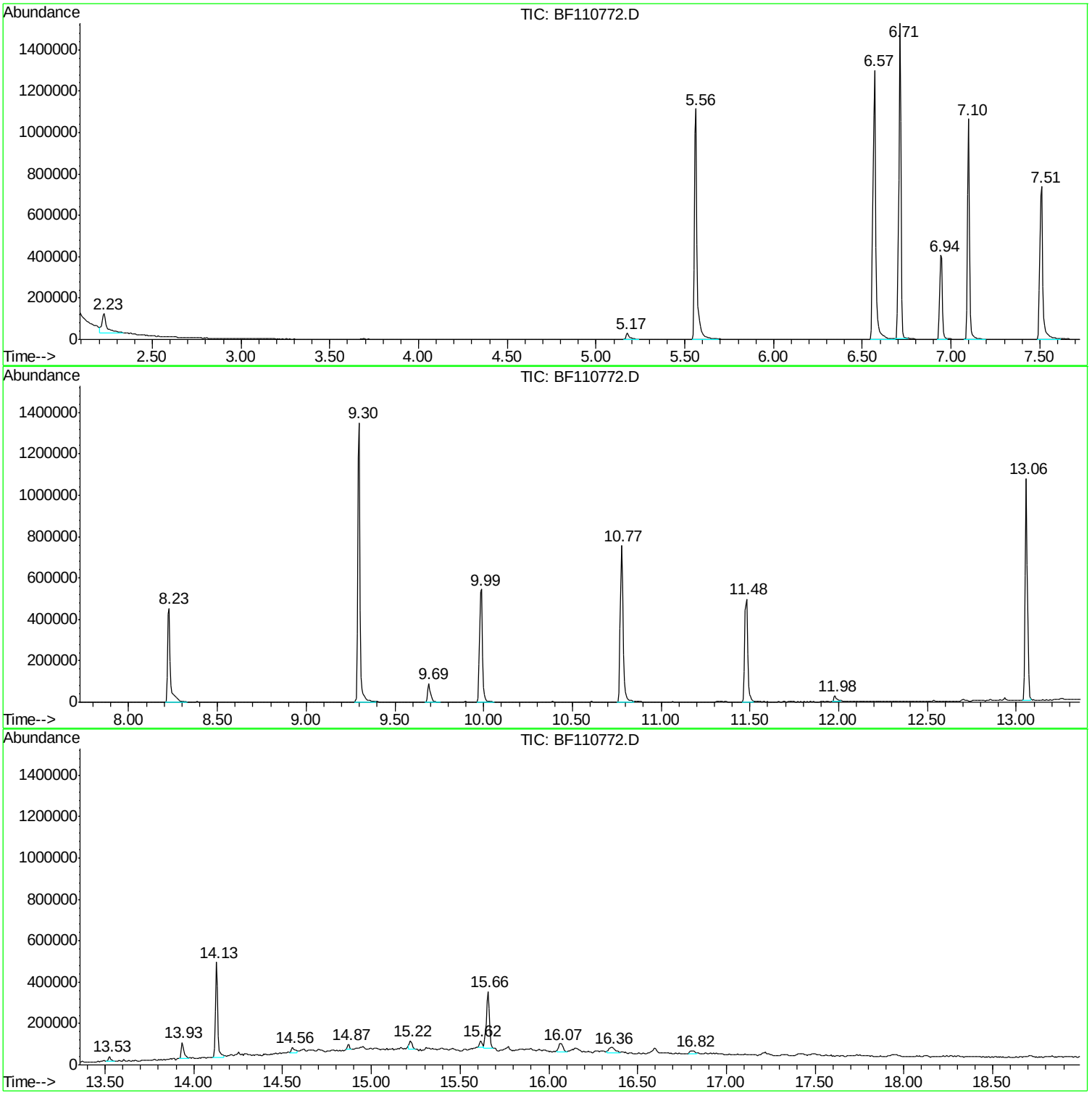
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-25(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-25(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

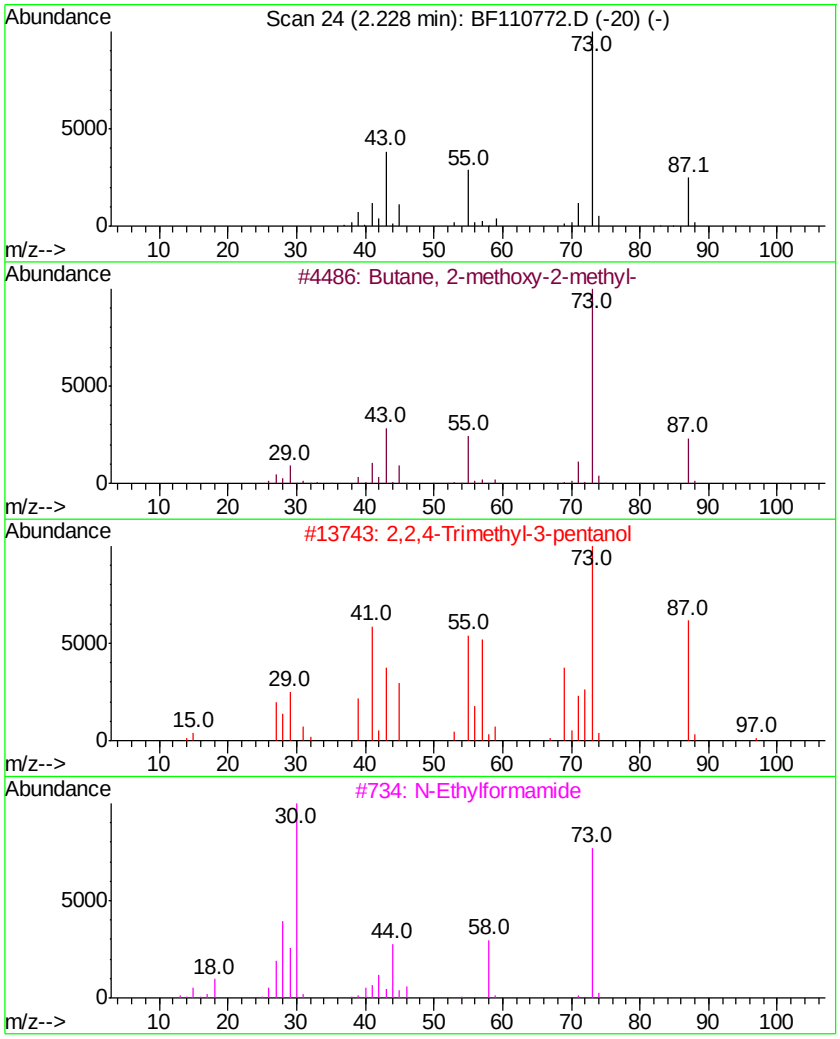
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

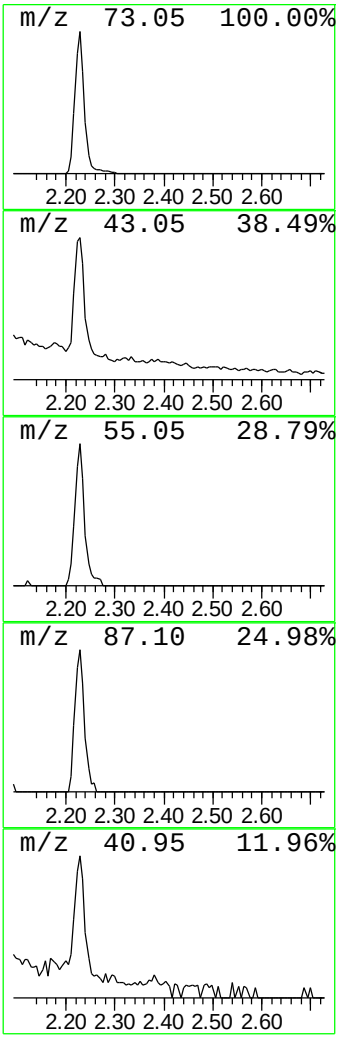
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	9.65 ng	188994	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-25(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.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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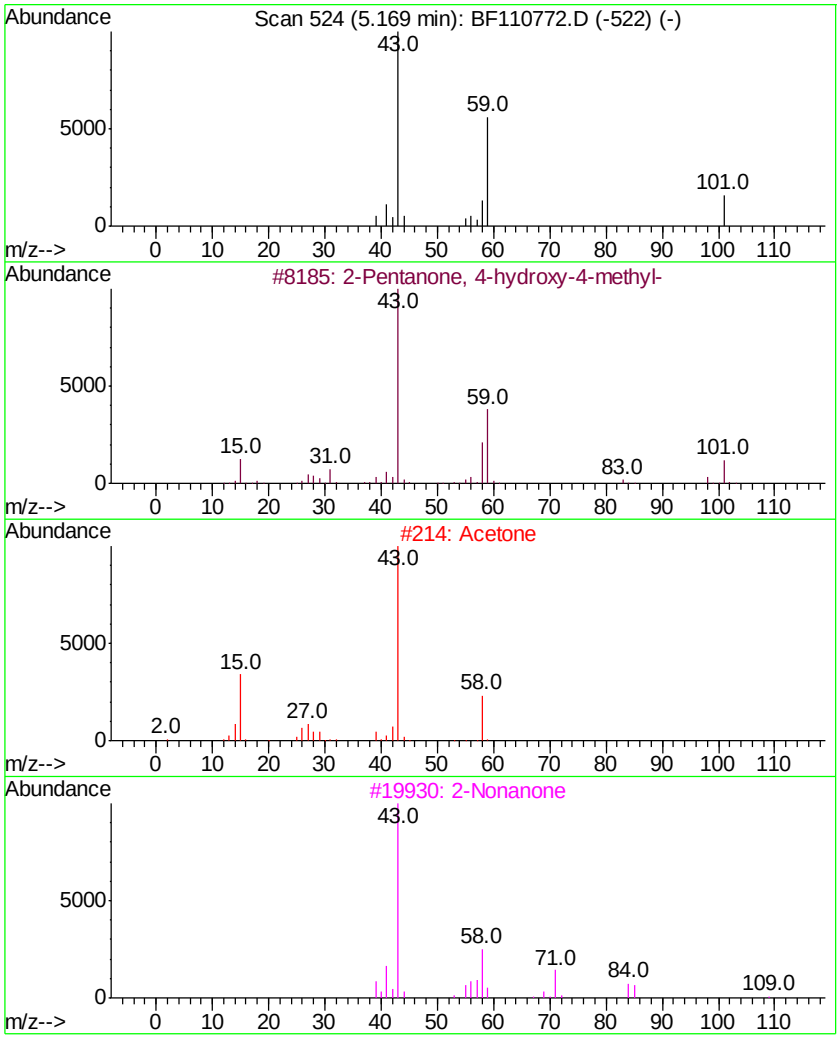
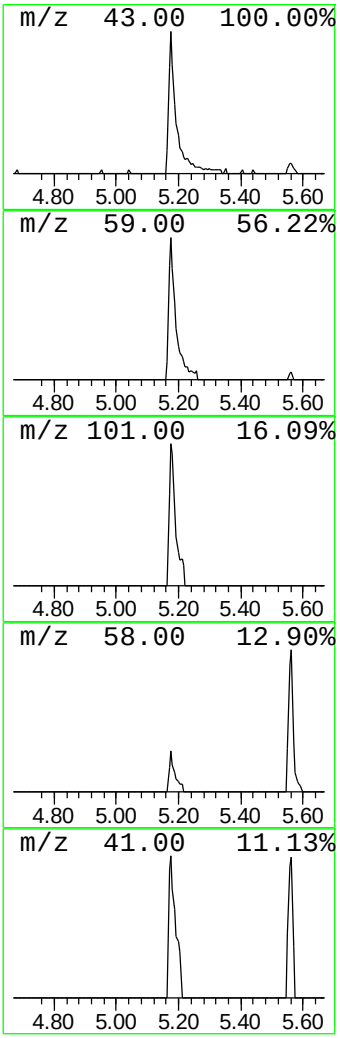
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	2.16 ng	42244	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2	Acetone	58	C3H6O	000067-64-1	16
3	2-Nonanone	142	C9H18O	000821-55-6	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-25(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

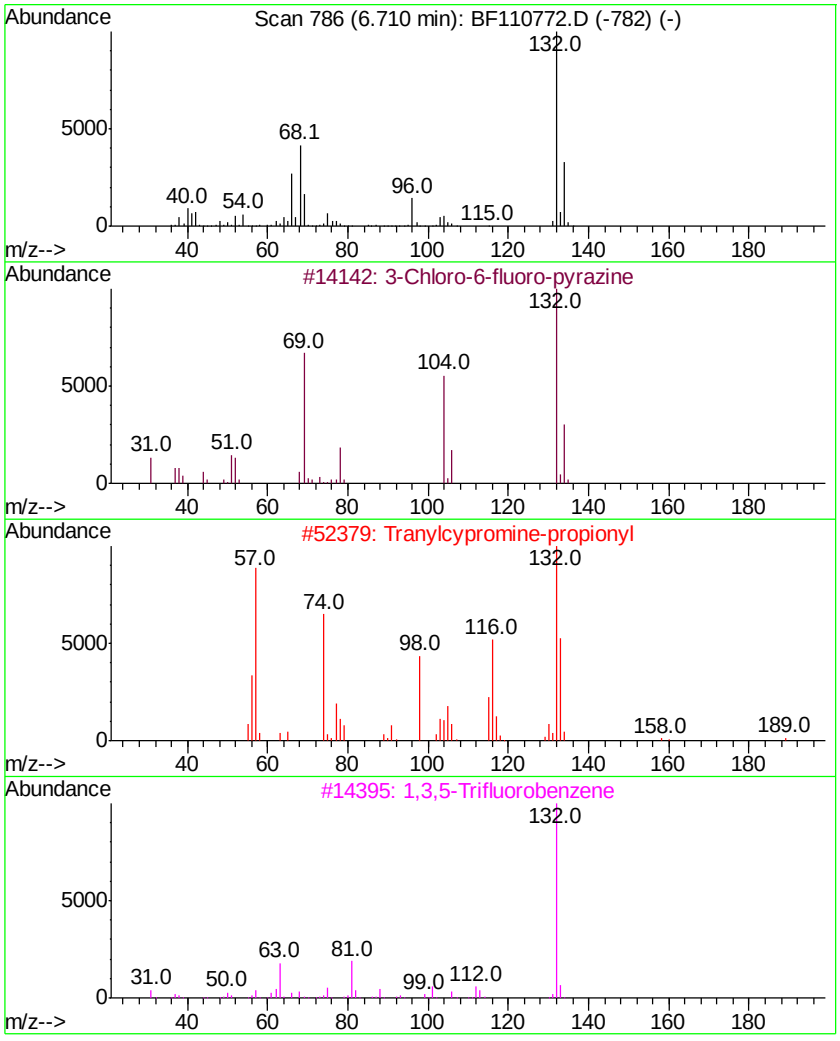
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

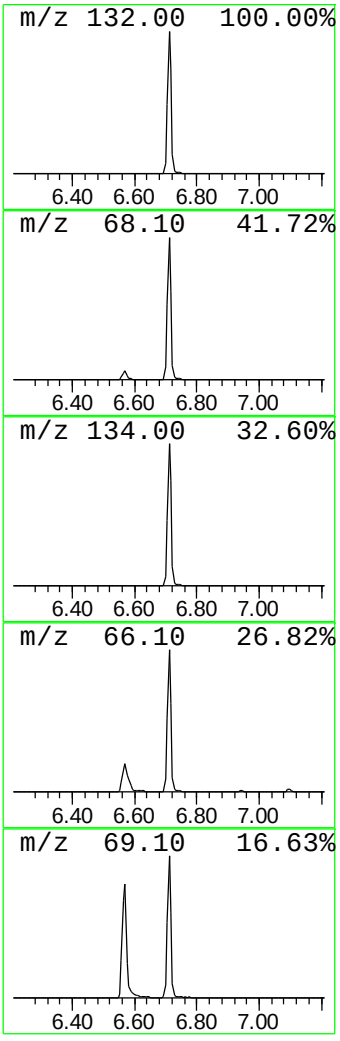
****

Peak Number 3 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	66.94 ng	1311400	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
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





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-25(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

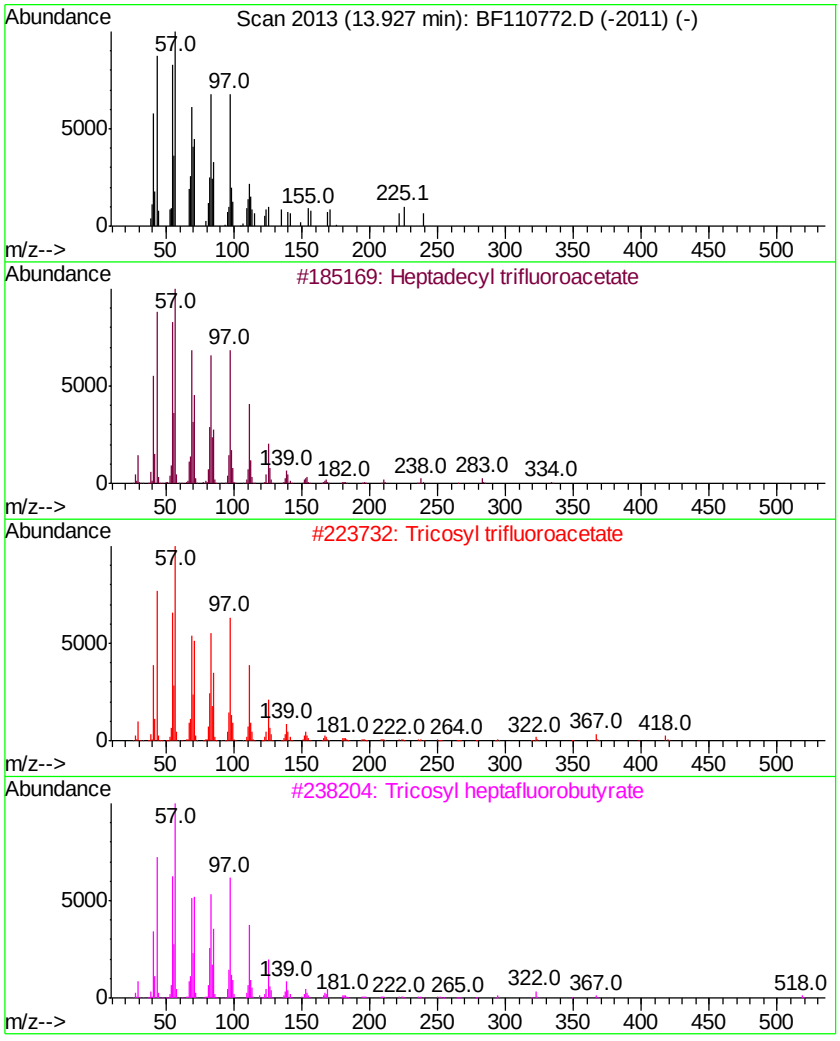
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

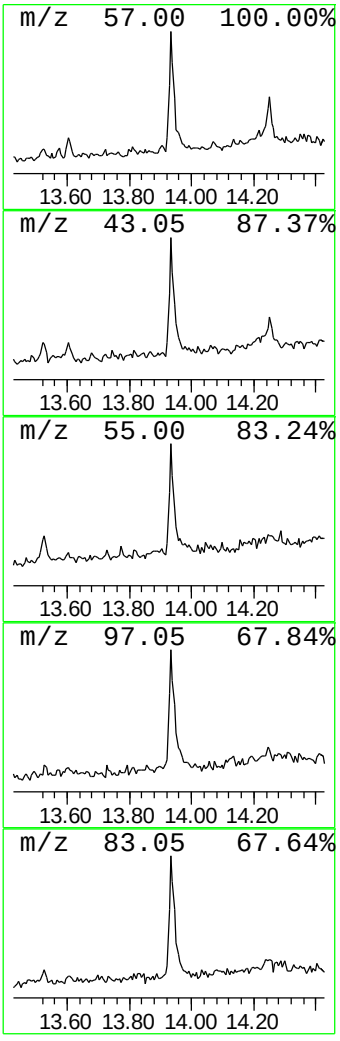
****

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	4.25 ng	94590	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
2	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
3	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	91
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-25(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

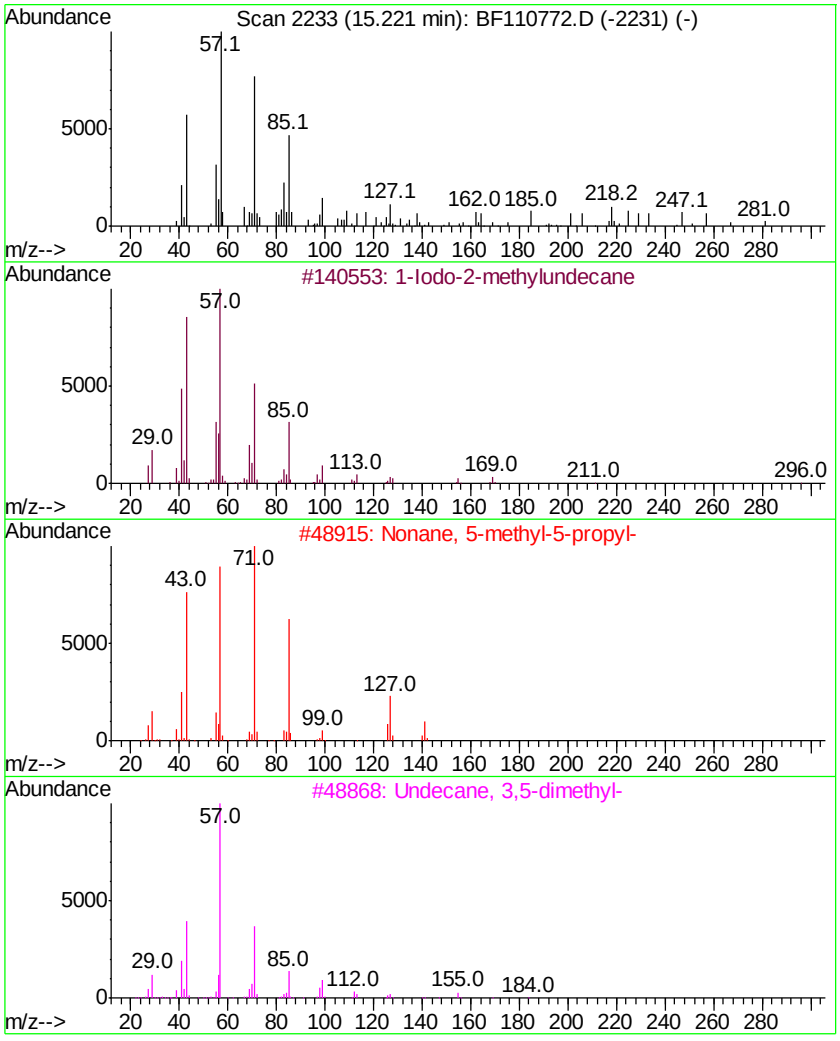
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

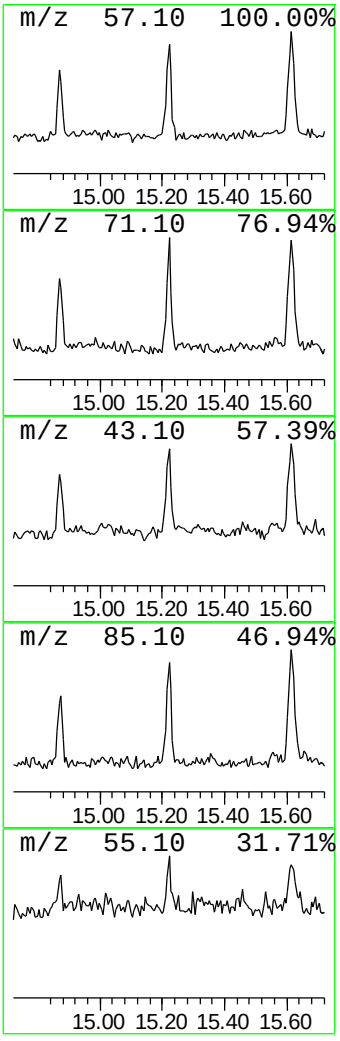
****

Peak Number 6 1-Iodo-2-methylundecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	2.28 ng	39072	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	59
2	Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	59
3	Undecane, 3,5-dimethyl-	184	C13H28	017312-81-1	53
4	Decane, 3-methyl-	156	C11H24	013151-34-3	53
5	Nonane, 1-iodo-	254	C9H19I	004282-42-2	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-25(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

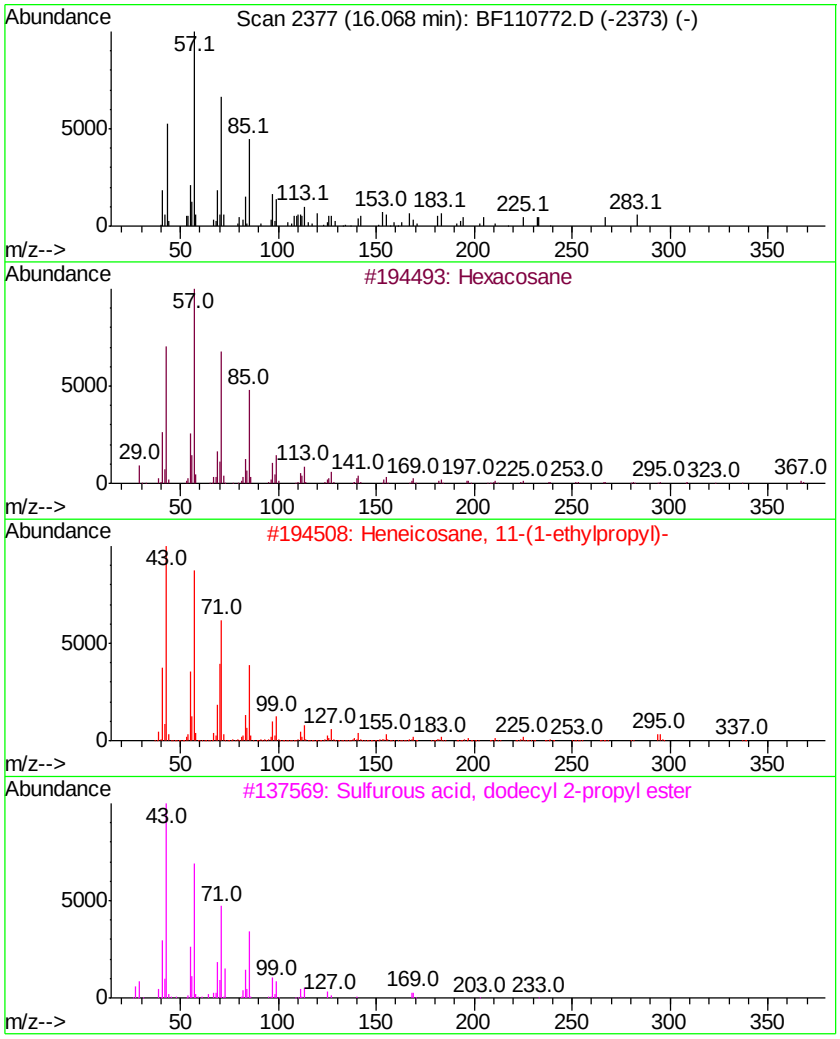
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

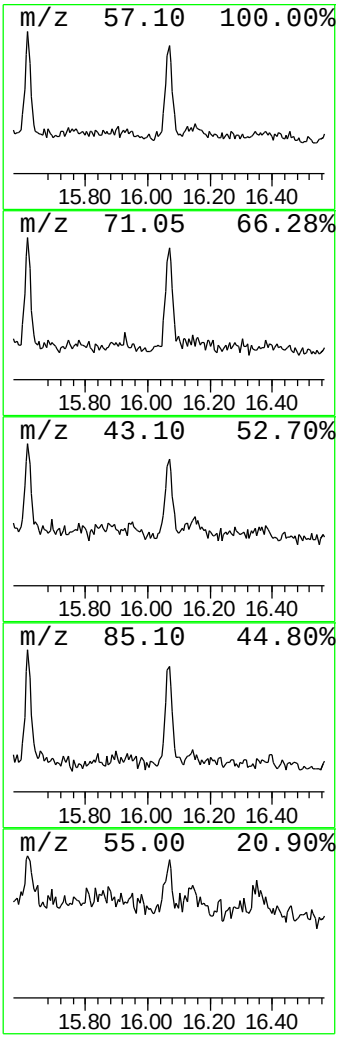
****

Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	3.80 ng	65129	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	83
2	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	80
3	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	80
4	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	72
5	Hentriacontane	437	C31H64	000630-04-6	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-25(0-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

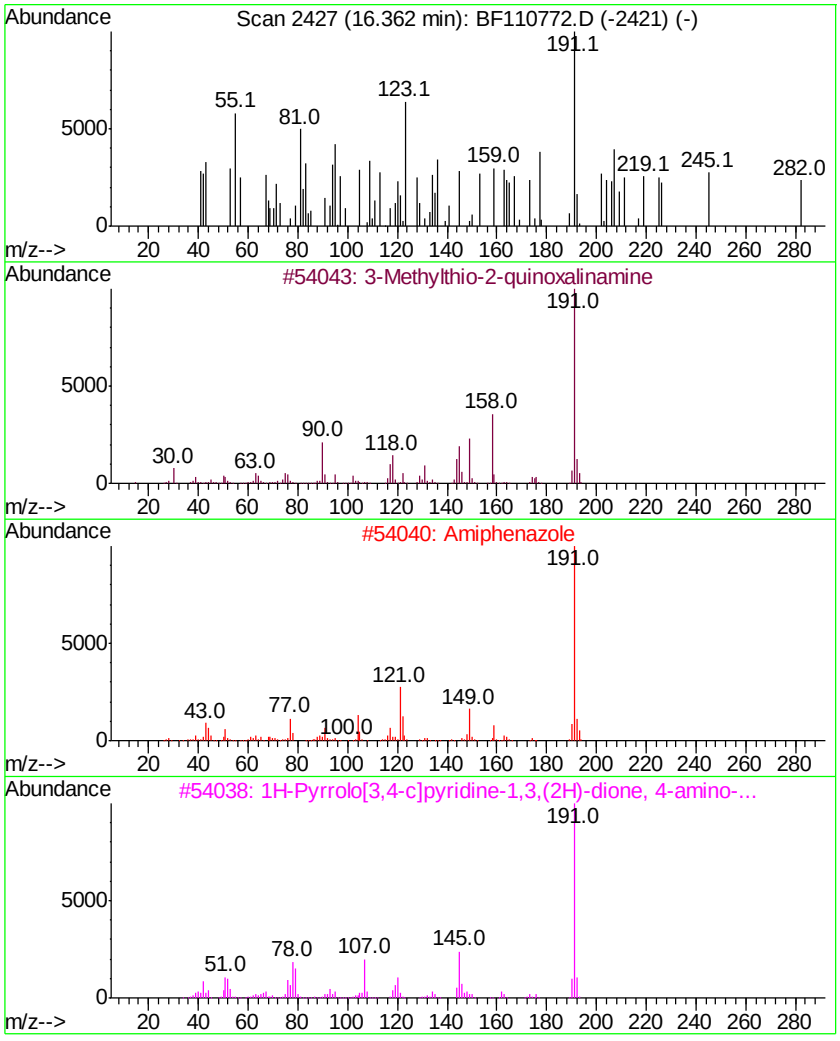
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

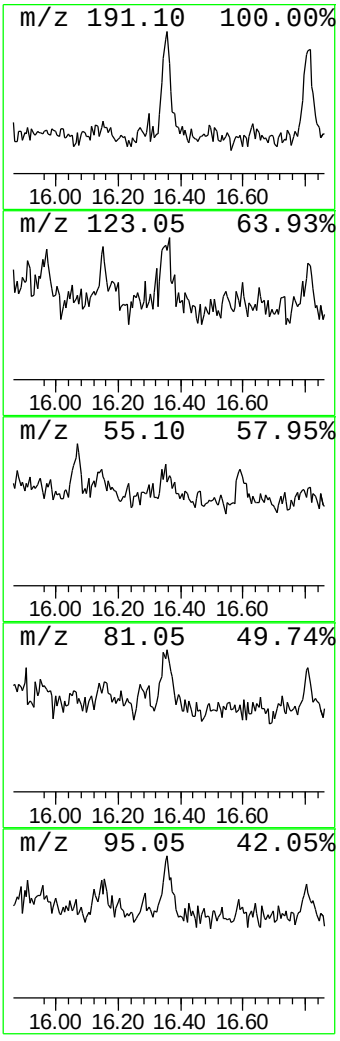
****

Peak Number 8 unknown16.36 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.36	3.33 ng	57149	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Methylthio-2-quinoxalinamine	191	C9H9N3S	090349-86-3	35
2	Amiphenazole	191	C9H9N3S	000490-55-1	27
3	1H-Pyrrolo[3,4-c]pyridine-1,3,(2...	191	C9H9N3O2	298688-32-1	27
4	Propenamide, 3-(3-methoxyphenyl)...	191	C11H13NO2	1000259-85-9	18
5	4-Fluoro-3-trifluoromethylbenzoi...	418	C23H34F4O2	1000338-69-2	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111418\
Data File : BF110772.D
Acq On : 14 Nov 2018 18:50
Operator : JU/SJ
Sample : J5940-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-25(0-10)

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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
Butane, 2-methoxy...	2.23	9.7	ng	188994	1	6.95	391798	20.0
2-Pentanone, 4-hy...	5.17	2.2	ng	42244	1	6.95	391798	20.0
unknown6.71	6.71	66.9	ng	1311400	1	6.95	391798	20.0
Heptadecyl triflu...	13.93	4.3	ng	94590	5	14.13	445581	20.0
1-Iodo-2-methylun...	15.22	2.3	ng	39072	6	15.66	342807	20.0
Hexacosane	16.07	3.8	ng	65129	6	15.66	342807	20.0
unknown16.36	16.36	3.3	ng	57149	6	15.66	342807	20.0