LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107603.D
Acq On : 23 Jul 2018 22:01
Operator : JU/SJ
Sample : J3991-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1-A

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-BF072018.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	5.213	485	489	499	rVB	587742	680336	16.82%	1.831%
2	5.613	552	557	578	rBV	3194311	4044480	100.00%	10.888%
3	6.607	722	726	746	rBV	3176941	3956969	97.84%	10.652%
4	6.748	746	750	768	rVB	3895861	4023915	99.49%	10.832%
5	6.978	785	789	796	rBV	1066368	1135159	28.07%	3.056%
6	7.131	811	815	835	rBV	3250529	3227012	79.79%	8.687%
7	7.537	880	884	909	rBV	1888758	2422763	59.90%	6.522%
8	8.260	1003	1007	1027	rBV	1238107	1342878	33.20%	3.615%
9	9.331	1185	1189	1204	rBV	3670273	3704041	91.58%	9.971%
10	9.436	1204	1207	1218	rVB	115405	129520	3.20%	0.349%
11	9.725	1252	1256	1268	rBV	531657	477196	11.80%	1.285%
12	10.019	1302	1306	1316	rBV	1318513	1224206	30.27%	3.296%
13	10.813	1437	1441	1454	rBV	2390318	2433829	60.18%	6.552%
14	11.513	1556	1560	1569	rBV	1320279	1415327	34.99%	3.810%
15	12.019	1643	1646	1648	rBV3	62248	58517	1.45%	0.158%
16	12.730	1764	1767	1772	rBV	133981	138590	3.43%	0.373%
17	12.966	1802	1807	1813	rBV2	127550	230448	5.70%	0.620%
18	13.066	1821	1824	1825	rBV3	59692	59180	1.46%	0.159%
19	13.101	1826	1830	1836	rVB	4172208	3907847	96.62%	10.520%
20	13.977	1977	1979	1983	rBV	203168	181799	4.49%	0.489%
21	14.166	2007	2011	2023	rBV	1299493	1416034	35.01%	3.812%
22	15.707	2268	2273	2281	rVB	611425	937473	23.18%	2.524%

Sum of corrected areas: 37147519

LSC Report - Integrated Chromatogram

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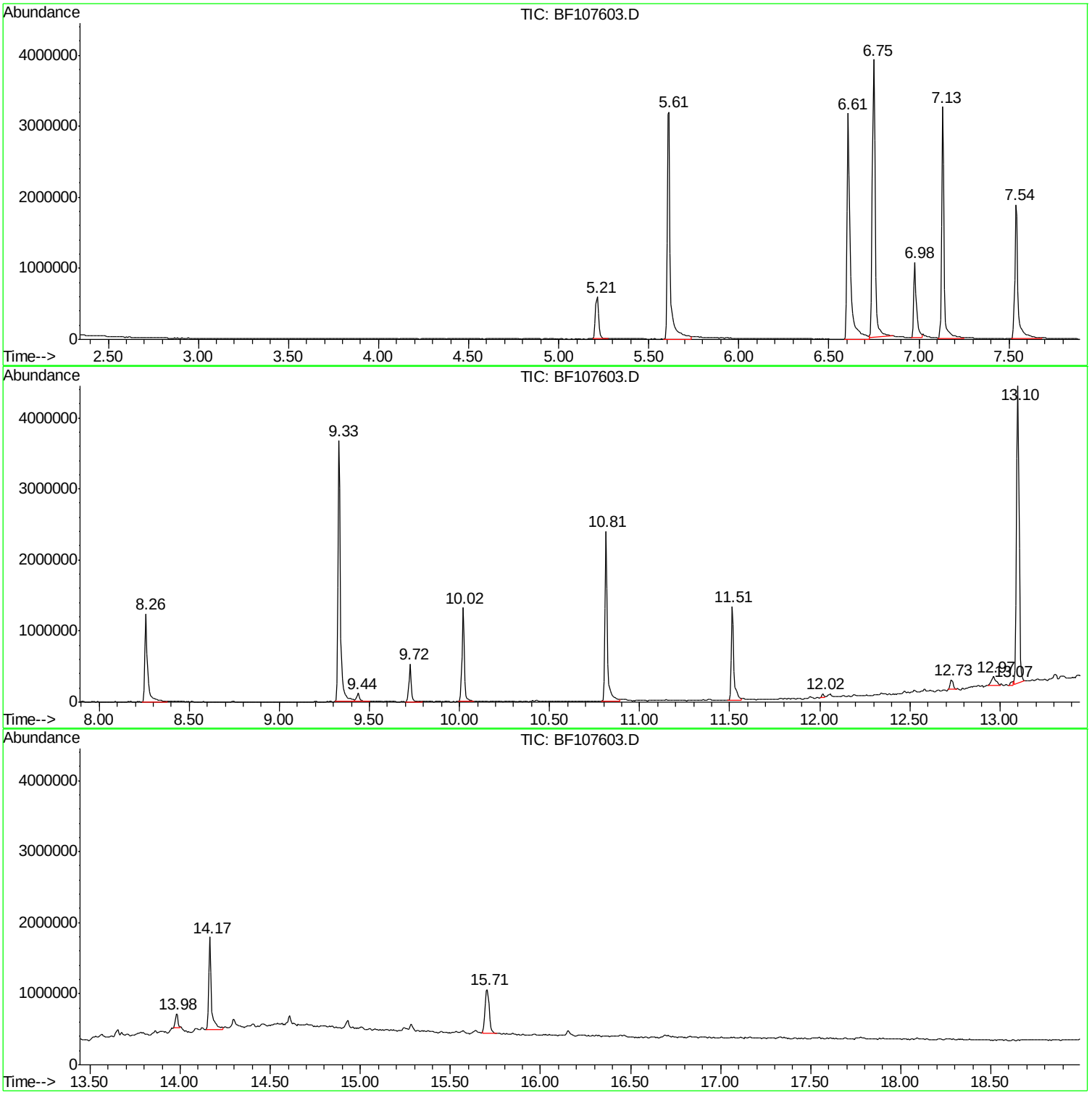
Instrument : BNA_F
ClientSampleId : SB-1-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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

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Instrument : BNA_F
ClientSampleId : SB-1-A

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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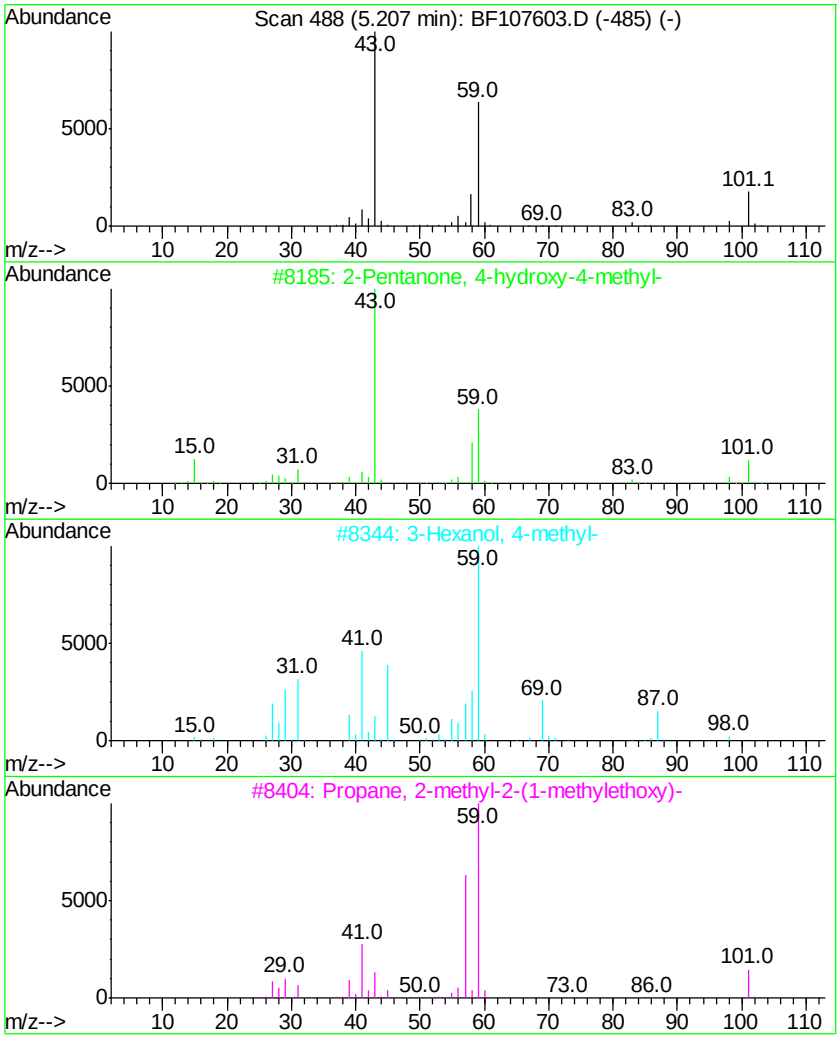
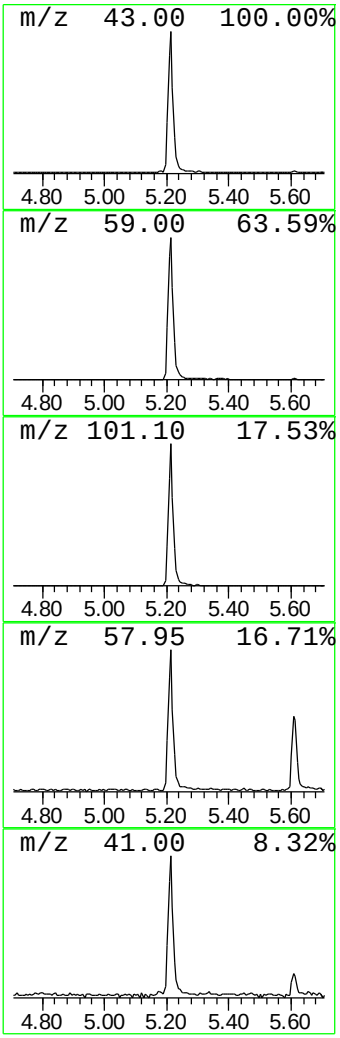
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	11.99 ng	680336	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Acetone	58	C3H6O	000067-64-1	9





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Instrument : BNA_F
ClientSampleId : SB-1-A

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

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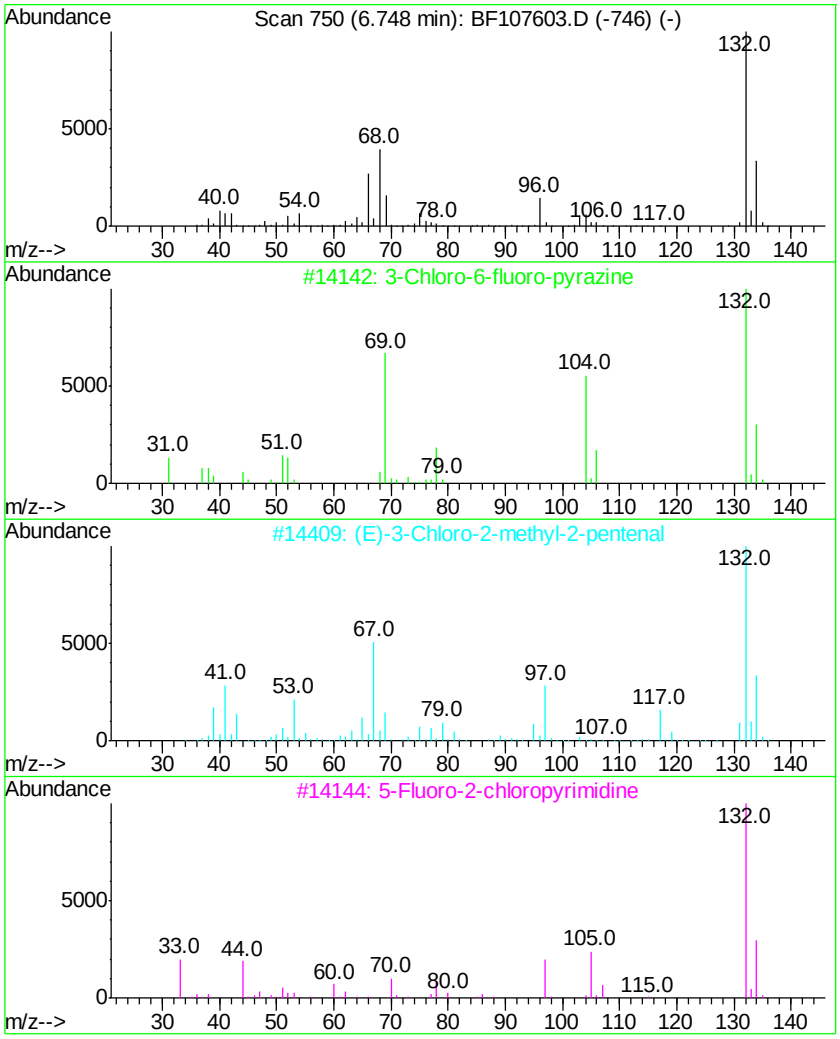
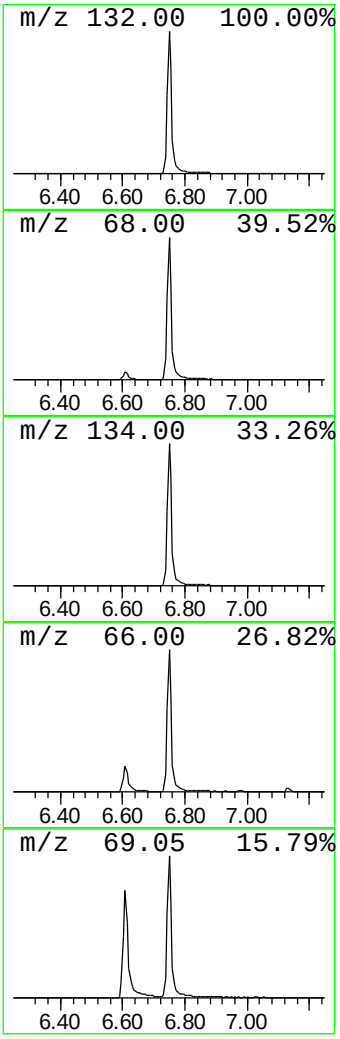
Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	70.90 ng	4023920	1,4-Dichlorobenzene-d4	6.98

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-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

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Operator : JU/SJ
Sample : J3991-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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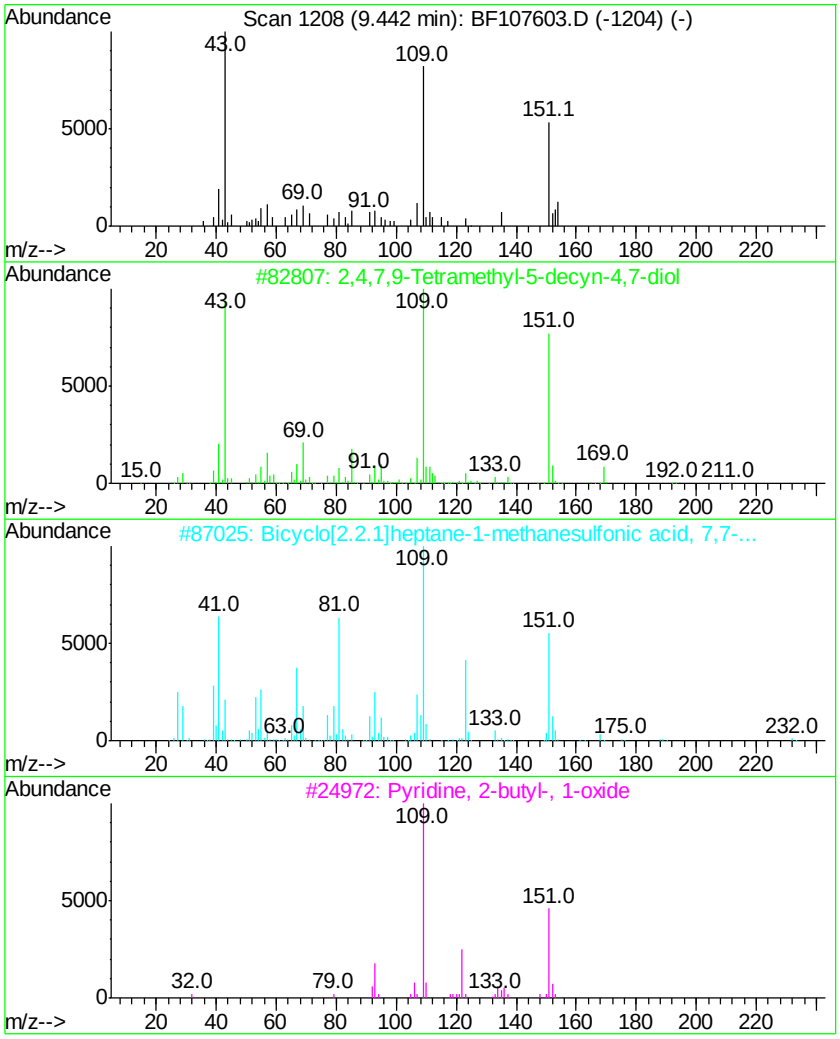
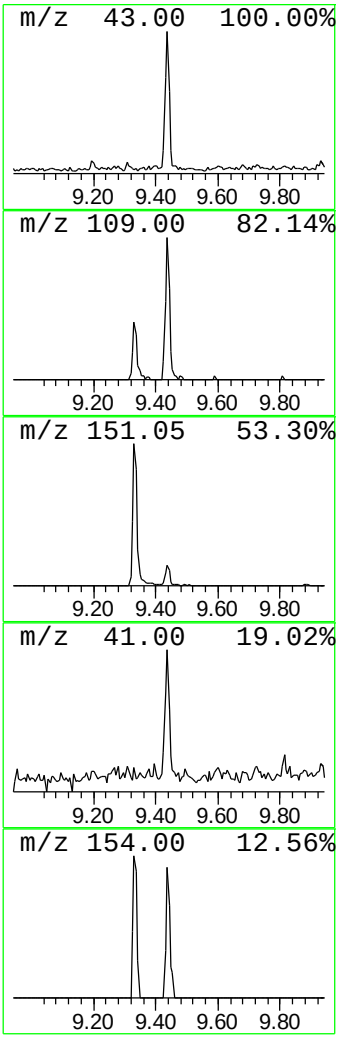
Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.44	2.12 ng	129520	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	72
2	Bicyclo[2.2.1]heptane-1-methanes...	232	C10H16O4S	005872-08-2	59
3	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	50
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	47
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	47





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ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-1-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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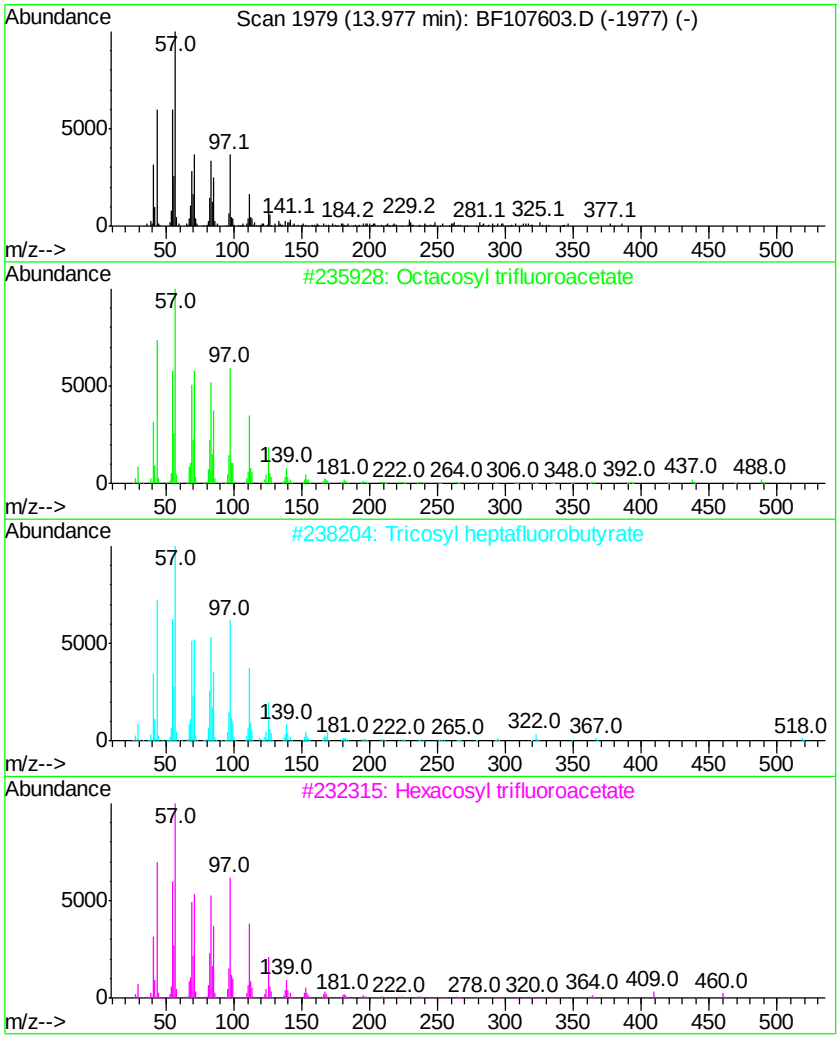
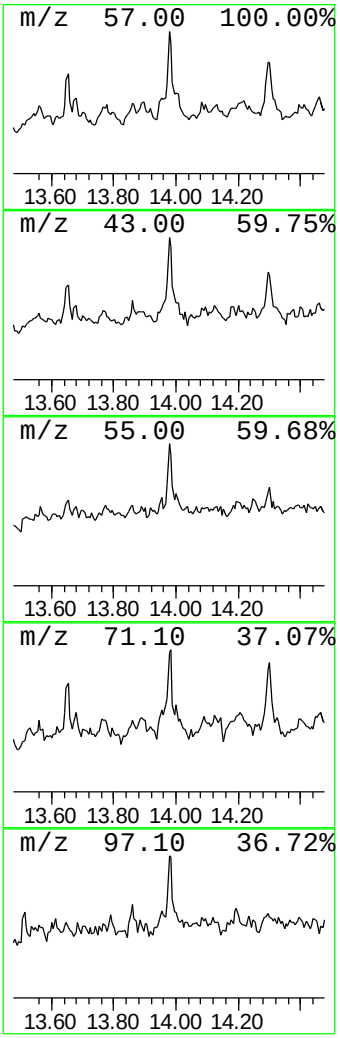
Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	2.57 ng	181799	Chrysene-d12	14.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	90
3	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	90
4	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	90
5	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	90





Tentatively Identified Compound (LSC) summary

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Misc :
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Instrument : BNA_F
ClientSampleId : SB-1-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
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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...	5.21	12.0	ng	680336	1	6.98	1135160	20.0
unknown6.75	6.75	70.9	ng	4023920	1	6.98	1135160	20.0
2,4,7,9-Tetrameth...	9.44	2.1	ng	129520	3	10.02	1224210	20.0
Octacosyl trifluo...	13.98	2.6	ng	181799	5	14.17	1416030	20.0