LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106409.D
Acq On : 13 Jun 2018 23:25
Operator : JU/SJ
Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48971

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-BF061118.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	4.331	334	339	343	rBV	37245	43707	1.16%	0.144%
2	5.190	481	485	492	rVB	160037	168938	4.46%	0.556%
3	5.613	553	557	563	rBV	1526547	1680251	44.40%	5.535%
4	6.613	723	727	735	rBV	1001618	1219738	32.23%	4.018%
5	6.748	746	750	753	rBV	3005699	2761530	72.98%	9.097%
6	6.966	783	787	790	rBV	1089830	892422	23.58%	2.940%
7	7.125	809	814	817	rVB	2754236	2588090	68.39%	8.525%
8	7.531	871	883	886	rBV	2365934	2358861	62.34%	7.770%
9	8.248	1001	1005	1008	rBV	1470942	1168754	30.89%	3.850%
10	8.360	1021	1024	1030	rBV	101717	96453	2.55%	0.318%
11	8.525	1049	1052	1054	rVB	86718	66851	1.77%	0.220%
12	8.842	1103	1106	1113	rVB5	93557	142279	3.76%	0.469%
13	9.325	1183	1188	1191	rBV	4001013	3784094	100.00%	12.465%
14	9.425	1202	1205	1209	rVB2	71316	78334	2.07%	0.258%
15	9.589	1226	1233	1236	rBV4	38536	68312	1.81%	0.225%
16	9.654	1241	1244	1248	rBV4	67926	89879	2.38%	0.296%
17	9.713	1251	1254	1256	rBV	459165	325410	8.60%	1.072%
18	9.772	1261	1264	1268	rVB	103762	102876	2.72%	0.339%
19	9.919	1286	1289	1294	rVB	137046	114298	3.02%	0.377%
20	9.972	1294	1298	1300	rBV2	27040	43677	1.15%	0.144%
21	10.007	1300	1304	1308	rVB	1529605	1298065	34.30%	4.276%
22	10.207	1336	1338	1341	rVB	50674	44460	1.17%	0.146%
23	10.266	1346	1348	1352	rVB3	46530	49223	1.30%	0.162%
24	10.419	1369	1374	1377	rVB2	193440	187299	4.95%	0.617%
25	10.548	1393	1396	1404	rVB10	31006	65530	1.73%	0.216%
26	10.636	1404	1411	1414	rBV2	121045	160464	4.24%	0.529%
27	10.801	1434	1439	1442	rBV	2580465	2466089	65.17%	8.123%
28	10.895	1452	1455	1459	rBV	128386	113499	3.00%	0.374%
29	11.342	1528	1531	1534	rBV2	80754	69850	1.85%	0.230%
30	11.495	1554	1557	1561	rBV	1334647	1226308	32.41%	4.040%
31	11.666	1583	1586	1589	rVB	131567	100444	2.65%	0.331%
32	11.772	1601	1604	1610	rVB	32487	38816	1.03%	0.128%
33	12.013	1641	1645	1653	rBV2	359628	462235	12.22%	1.523%
34	12.801	1776	1779	1786	rBV	116046	143842	3.80%	0.474%

LSC Area Percent Report

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Acq On : 13 Jun 2018 23:25
Operator : JU/SJ
Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48971

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-BF061118.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.966	1804	1807	1810	rVB	114322	94579	2.50%	0.312%
36	13.083	1823	1827	1831	rBV	3364516	3440735	90.93%	11.334%
37	13.630	1917	1920	1924	rVB	320300	249852	6.60%	0.823%
38	13.966	1974	1977	1982	rBV	188213	182067	4.81%	0.600%
39	14.142	2003	2007	2011	rBV	1018279	954262	25.22%	3.143%
40	14.601	2083	2085	2092	rBV7	22720	45188	1.19%	0.149%
41	15.001	2150	2153	2158	rVB	88772	92489	2.44%	0.305%
42	15.677	2262	2268	2279	rBV	805036	1016241	26.86%	3.348%
43	17.412	2561	2563	2571	rVB8	31927	61456	1.62%	0.202%

Sum of corrected areas: 30357747

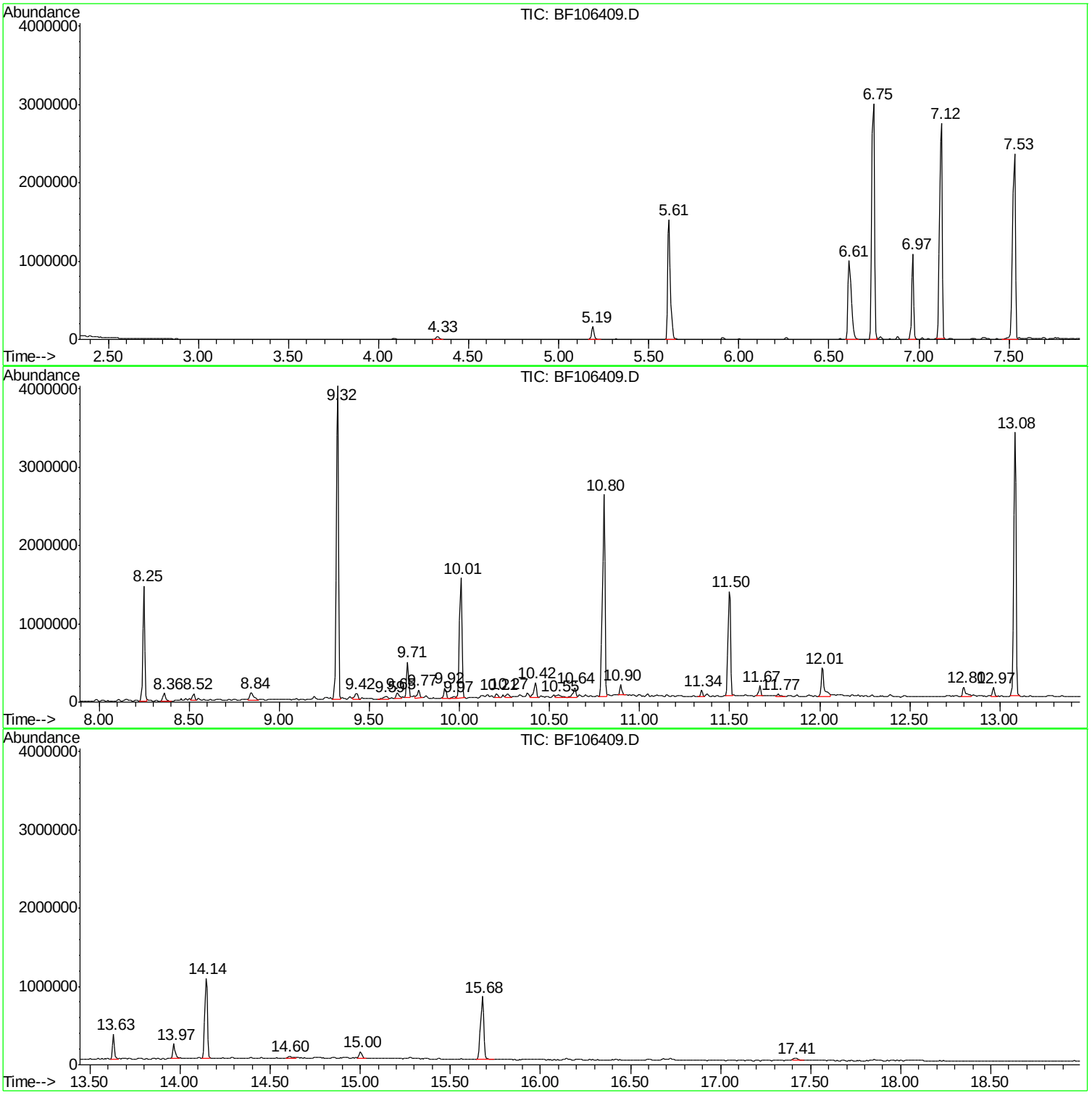
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106409.D
Acq On : 13 Jun 2018 23:25
Operator : JU/SJ
Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106409.D
Acq On : 13 Jun 2018 23:25
Operator : JU/SJ
Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

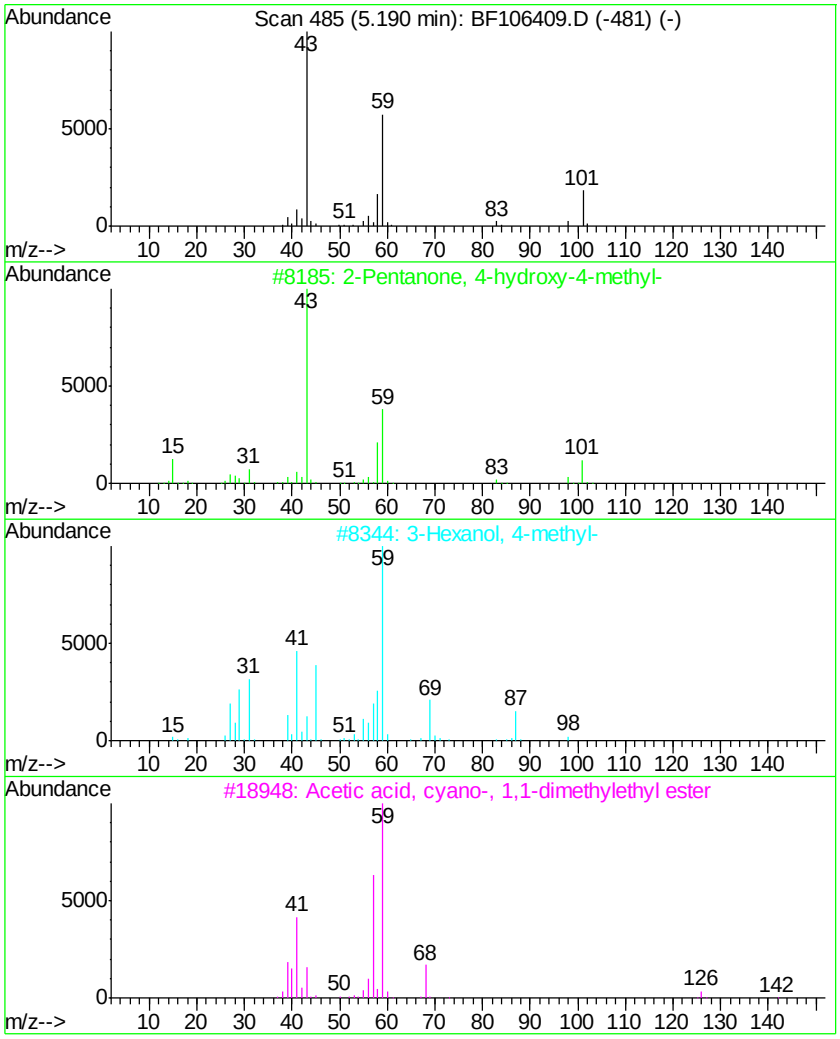
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

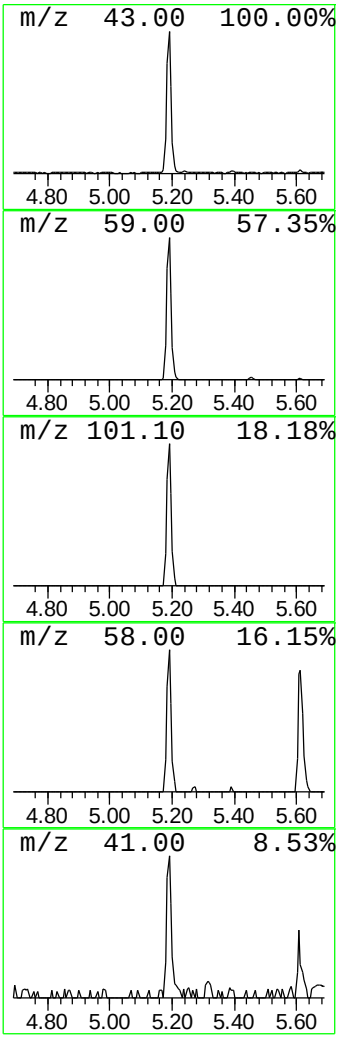
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	3.79 ng	168938	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
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Operator : JU/SJ
Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

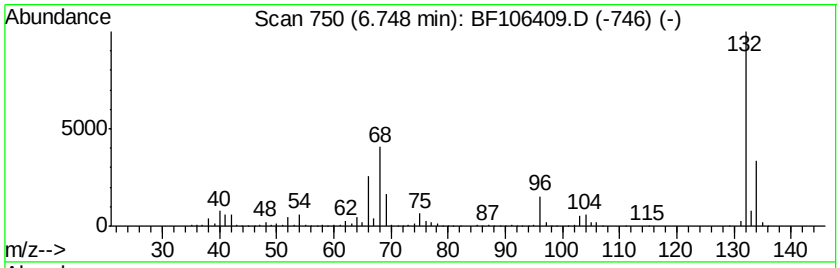
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

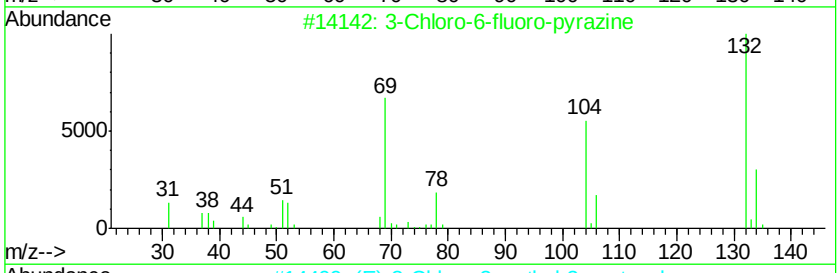
****

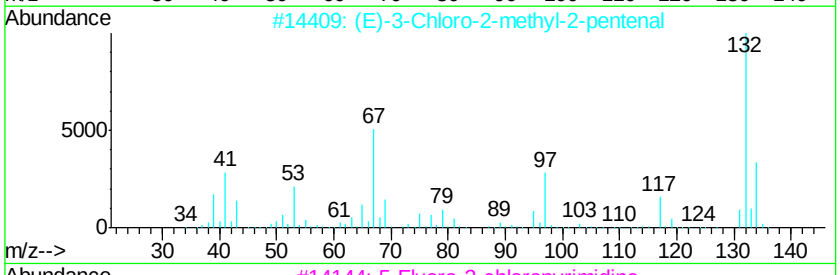
Peak Number 2 unknown6.75 Concentration Rank 1

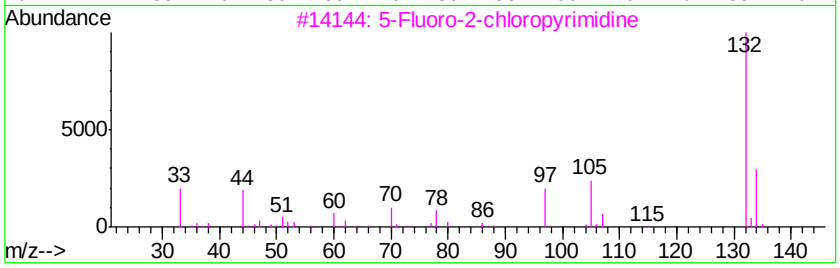
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	61.89 ng	2761530	1,4-Dichlorobenzene-d4	6.97

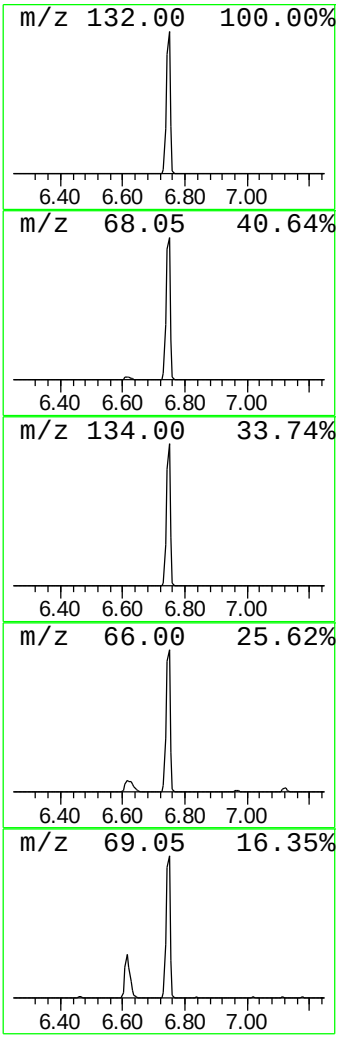
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9











Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106409.D
Acq On : 13 Jun 2018 23:25
Operator : JU/SJ
Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

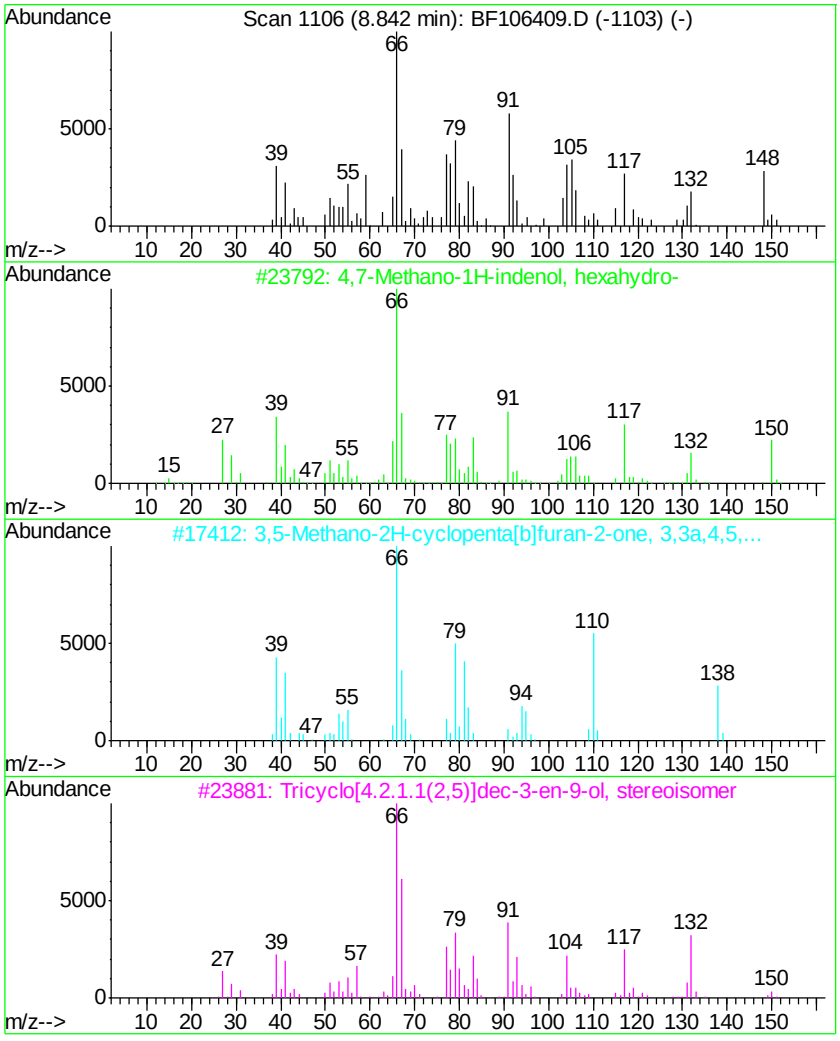
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

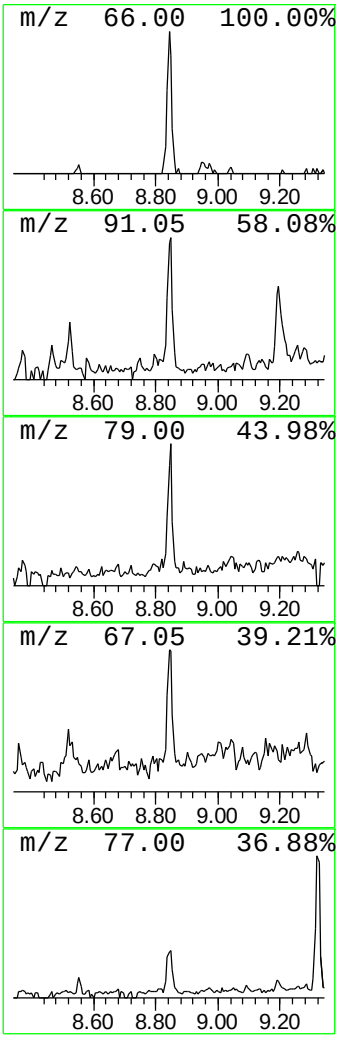
****

Peak Number 4 4,7-Methano-1H-indenol, hex... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.84	2.43 ng	142279	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Methano-1H-indenol, hexahydro-	150	C10H14O	037275-49-3	64
2	3,5-Methano-2H-cyclopenta[b]fura...	138	C8H10O2	1000141-72-9	59
3	Tricyclo[4.2.1.1(2,5)]dec-3-en-9...	150	C10H14O	070220-93-8	59
4	Dicyclopentadiene	132	C10H12	000077-73-6	53
5	4-Nonen-2-yne, (Z)-	122	C9H14	053497-78-2	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106409.D
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Operator : JU/SJ
Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

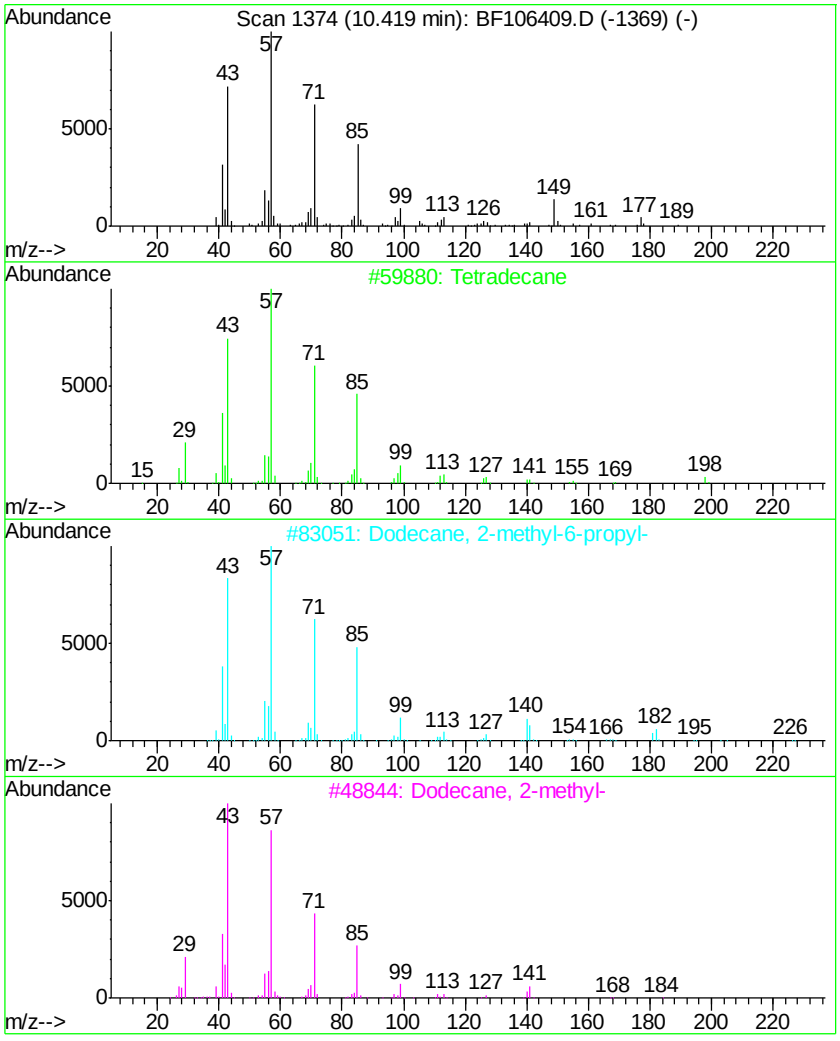
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

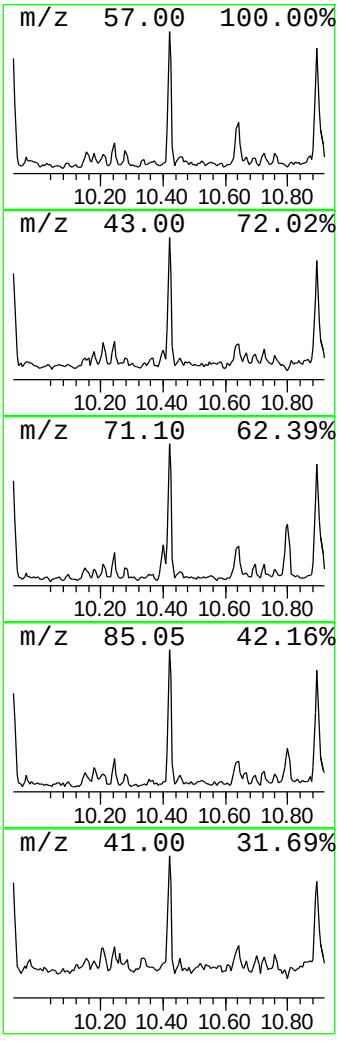
****

Peak Number 5 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	2.89 ng	187299	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	80
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	80
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	72
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	59
5	Hexadecane	226	C16H34	000544-76-3	58





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Instrument : BNA_F
ClientSampleId : N-48971

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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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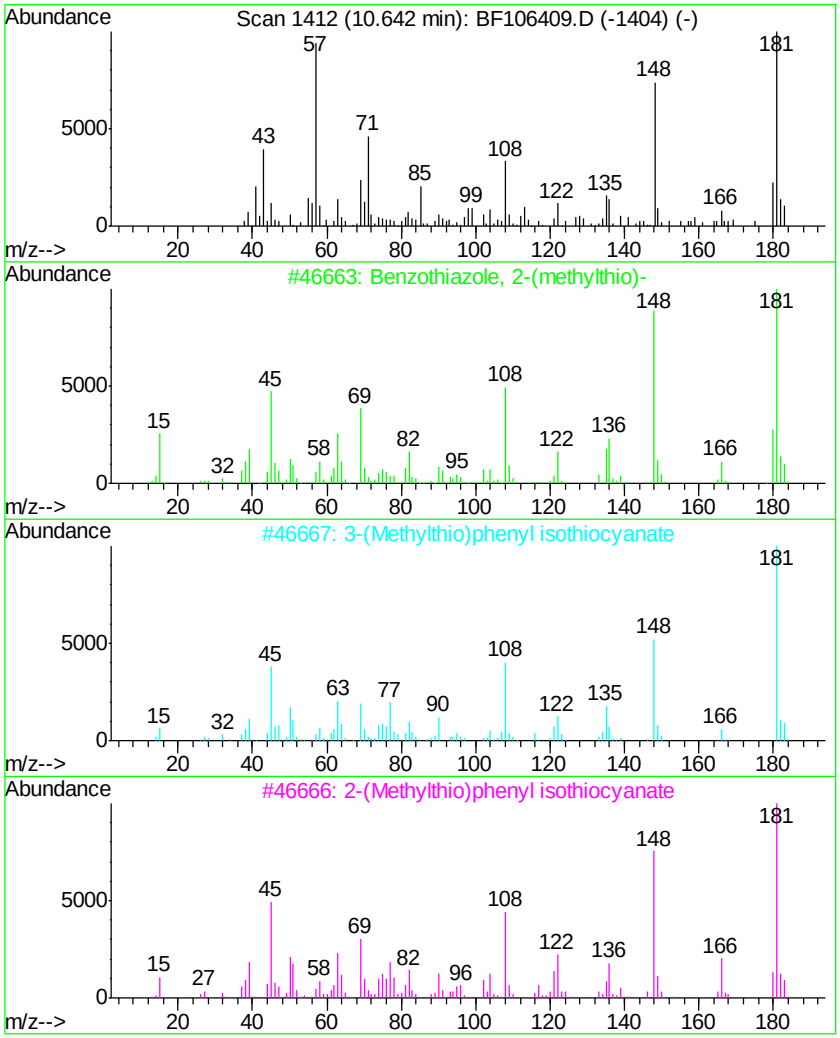
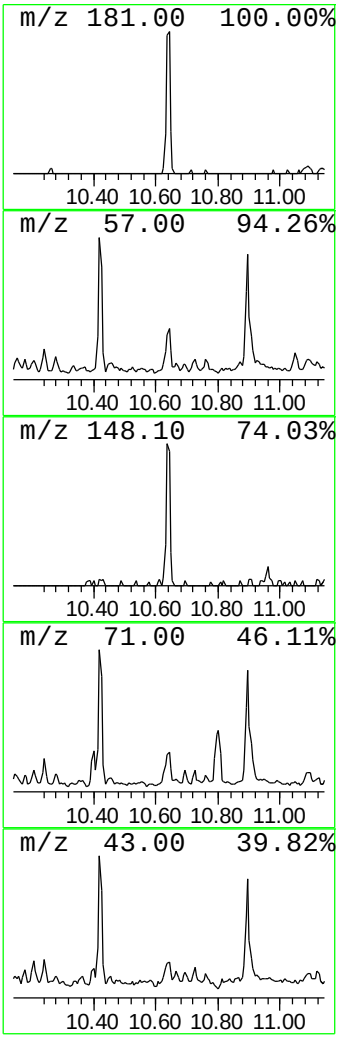
Peak Number 6 Benzothiazole, 2-(methylthio)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	2.47 ng	160464	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	000615-22-5	95
2	3-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-80-3	60
3	2-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-75-6	53
4	4-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	015863-41-9	42
5	Ethyl (p-hydroxyphenyl)carbamate	181	C9H11NO3	007159-95-7	27





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Misc :
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Instrument : BNA_F
ClientSampleId : N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

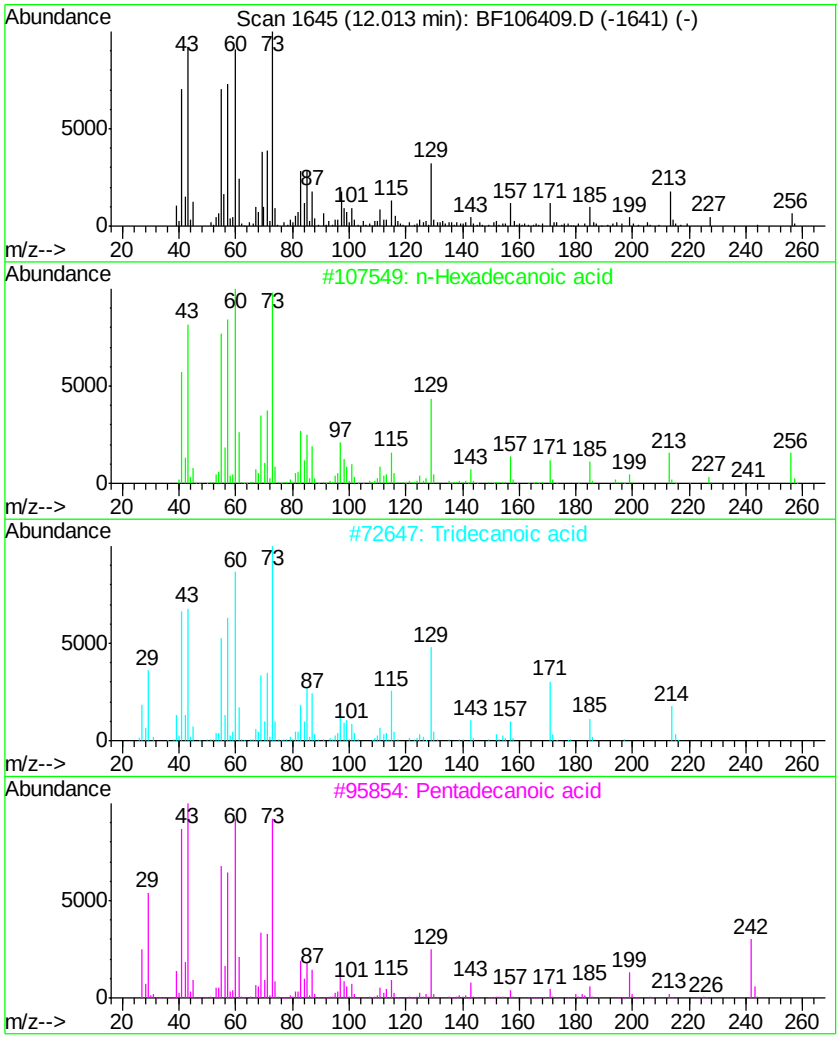
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

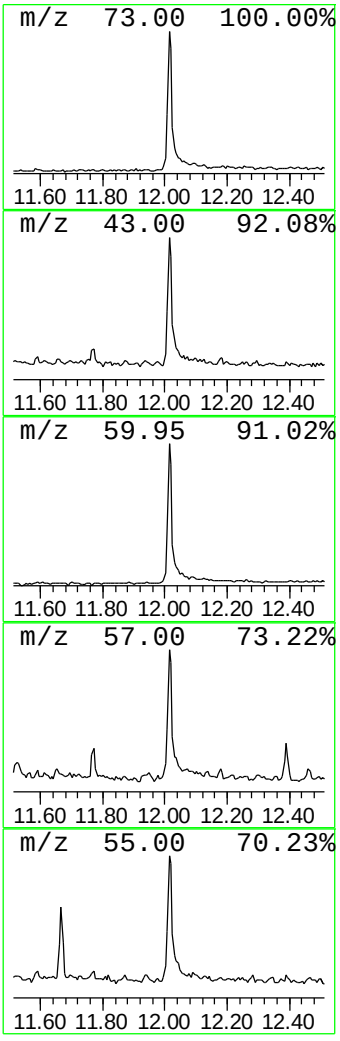
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	7.54 ng	462235	Phenanthrene-d10	11.50

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	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	25





Library Search Compound Report

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Data File : BF106409.D
Acq On : 13 Jun 2018 23:25
Operator : JU/SJ
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Instrument : BNA_F
ClientSampleId : N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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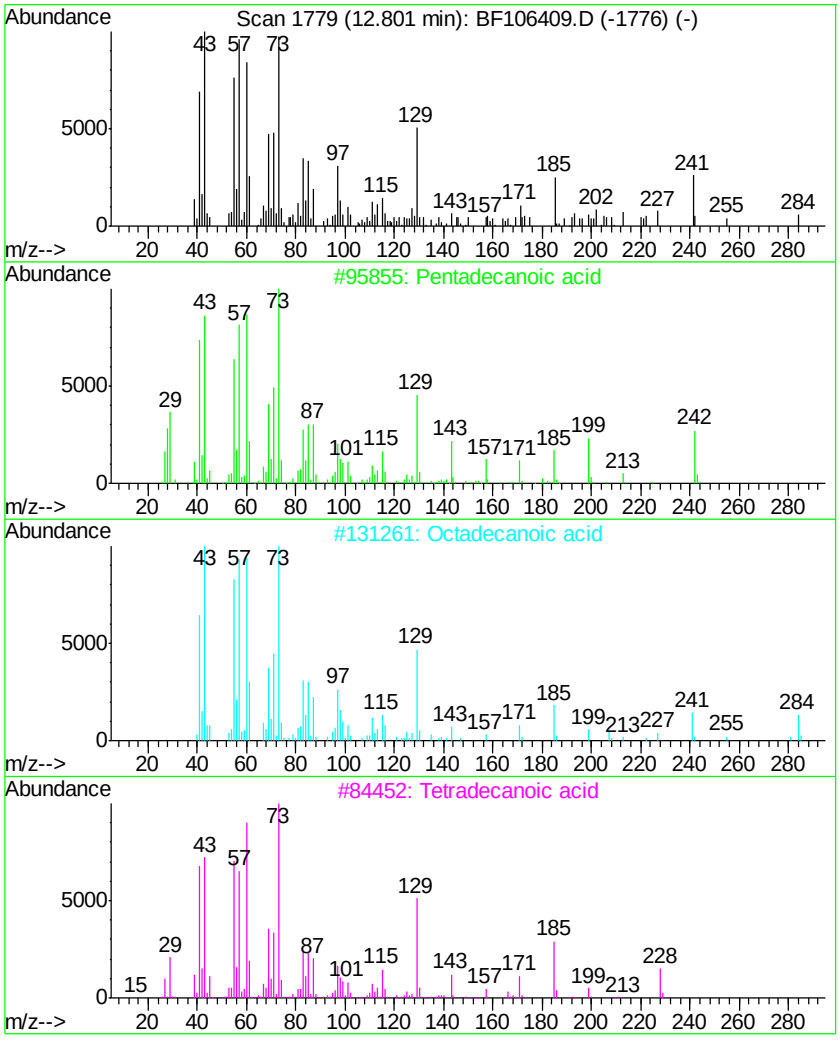
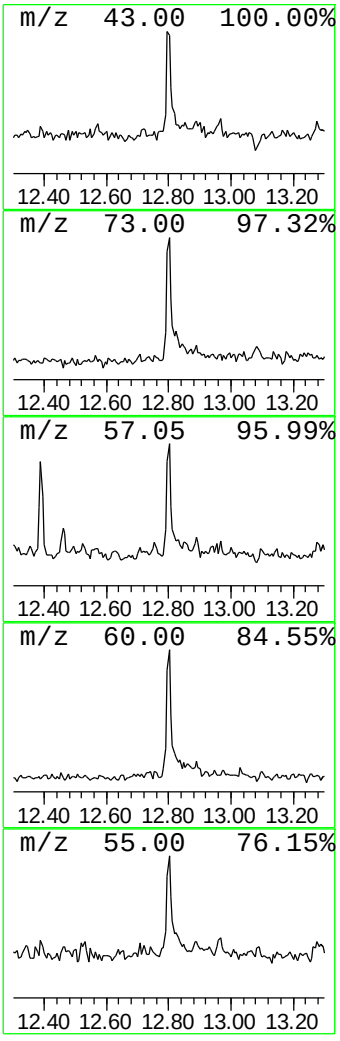
Peak Number 8 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.35 ng	143842	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106409.D
Acq On : 13 Jun 2018 23:25
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Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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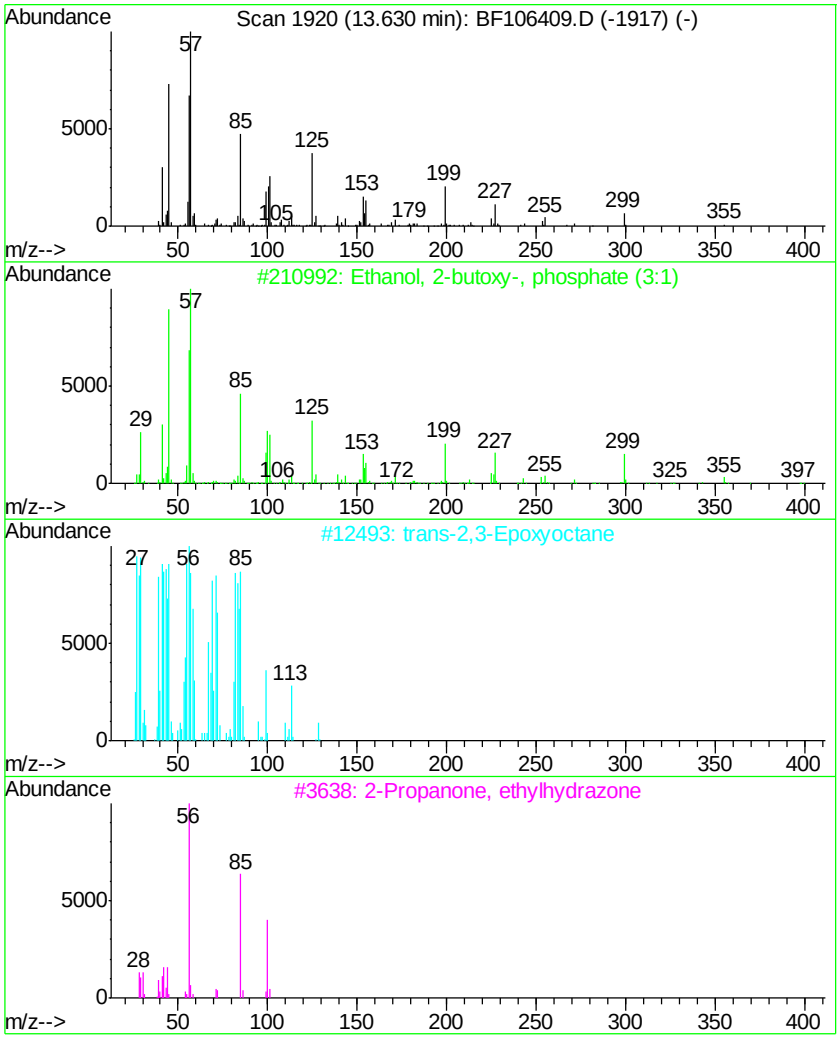
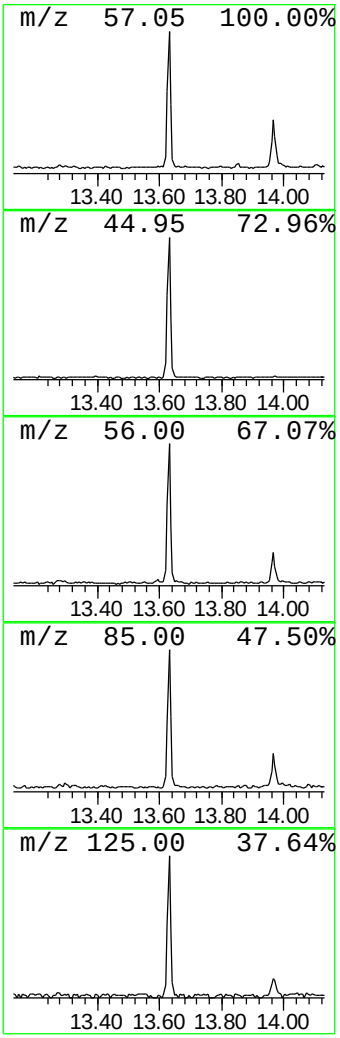
Peak Number 9 Ethanol, 2-butoxy-, phospha... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	5.24 ng	249852	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-, phosphate (3:1)	398	C18H39O7P	000078-51-3	91
2	trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	38
3	2-Propanone, ethylhydrazone	100	C5H12N2	007422-99-3	35
4	Propane, 1,3-dimethoxy-2,2-dimet...	132	C7H16O2	020637-32-5	25
5	3,7,11,15-Tetramethyl-hexadecano...	370	C23H50OSi	078695-20-2	14





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106409.D
Acq On : 13 Jun 2018 23:25
Operator : JU/SJ
Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

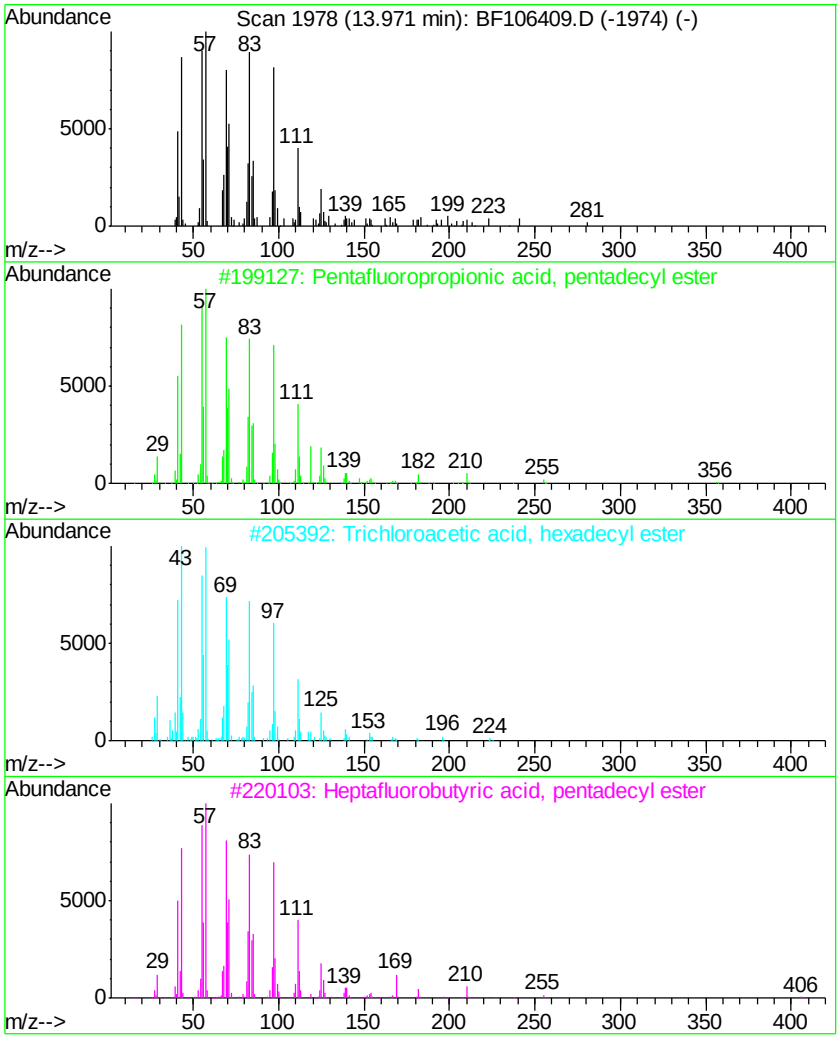
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

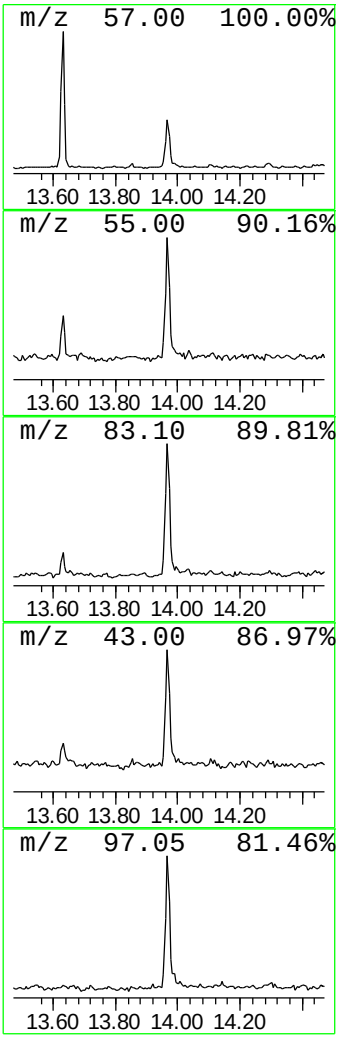
****

Peak Number 10 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.82 ng	182067	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	90
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061318\
Data File : BF106409.D
Acq On : 13 Jun 2018 23:25
Operator : JU/SJ
Sample : J3448-01
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48971

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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...	5.19	3.8	ng	168938	1	6.97	892422	20.0
unknown6.75	6.75	61.9	ng	2761530	1	6.97	892422	20.0
4,7-Methano-1H-in...	8.84	2.4	ng	142279	2	8.25	1168750	20.0
Tetradecane	10.42	2.9	ng	187299	3	10.01	1298070	20.0
Benzothiazole, 2-...	10.64	2.5	ng	160464	3	10.01	1298070	20.0
n-Hexadecanoic acid	12.01	7.5	ng	462235	4	11.50	1226310	20.0
Pentadecanoic acid	12.80	2.4	ng	143842	4	11.50	1226310	20.0
Ethanol, 2-butoxy...	13.63	5.2	ng	249852	5	14.14	954262	20.0
Pentafluoropropio...	13.97	3.8	ng	182067	5	14.14	954262	20.0