LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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	4.325	334	338	345	rVB	43558	53323	1.50%	0.180%
2	5.190	481	485	493	rVB	114302	121947	3.44%	0.411%
3	5.613	553	557	564	rBV	1403396	1568666	44.20%	5.283%
4	6.613	723	727	735	rBV	895008	1130384	31.85%	3.807%
5	6.748	746	750	753	rBV	2968905	2612843	73.62%	8.800%
6	6.784	753	756	760	rVB	40217	38204	1.08%	0.129%
7	6.878	768	772	778	rVB2	36938	41881	1.18%	0.141%
8	6.966	783	787	790	rBV	1111302	871746	24.56%	2.936%
9	7.125	809	814	817	rVB	2645672	2465801	69.48%	8.305%
10	7.354	851	853	857	rBV2	70995	76715	2.16%	0.258%
11	7.531	878	883	886	rVB	2246039	2147879	60.52%	7.234%
12	7.766	918	923	930	rVB5	24137	37797	1.07%	0.127%
13	7.990	958	961	963	rBV2	41310	37413	1.05%	0.126%
14	8.107	978	981	984	rBV	50568	40225	1.13%	0.135%
15	8.142	984	987	991	rBV3	38873	57681	1.63%	0.194%
16	8.248	1001	1005	1008	rBV	1404298	1124080	31.67%	3.786%
17	8.360	1021	1024	1029	rBV	98443	93031	2.62%	0.313%
18	8.525	1049	1052	1054	rVB2	66563	59345	1.67%	0.200%
19	8.660	1070	1075	1080	rVB9	20153	47059	1.33%	0.158%
20	8.842	1103	1106	1113	rBV5	109850	154081	4.34%	0.519%
21	9.266	1173	1178	1180	rBV	72143	83329	2.35%	0.281%
22	9.325	1183	1188	1191	rVB	3867562	3548918	100.00%	11.953%
23	9.431	1201	1206	1208	rVB2	79376	88378	2.49%	0.298%
24	9.595	1226	1234	1236	rBV7	34753	79814	2.25%	0.269%
25	9.654	1241	1244	1248	rBV6	31951	50909	1.43%	0.171%
26	9.713	1251	1254	1256	rBV	576717	424799	11.97%	1.431%
27	9.772	1261	1264	1267	rVV3	62133	75880	2.14%	0.256%
28	9.813	1269	1271	1275	rVB4	45082	42294	1.19%	0.142%
29	9.919	1286	1289	1294	rVB	144940	125986	3.55%	0.424%
30	10.007	1300	1304	1308	rVB2	1418904	1227164	34.58%	4.133%
31	10.154	1326	1329	1332	rBV4	37111	38287	1.08%	0.129%
32	10.207	1335	1338	1342	rVB3	40209	37797	1.07%	0.127%
33	10.266	1346	1348	1353	rVB2	41565	42657	1.20%	0.144%
34	10.378	1365	1367	1370	rBV	55357	47938	1.35%	0.161%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
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Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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	10.419	1372	1374	1378	rVB2	198701	160970	4.54%	0.542%
36	10.542	1393	1395	1404	rVB9	32428	66040	1.86%	0.222%
37	10.642	1406	1412	1414	rBV2	191074	211444	5.96%	0.712%
38	10.701	1419	1422	1424	rBV2	58057	49155	1.39%	0.166%
39	10.801	1435	1439	1442	rBV	2405305	2300589	64.83%	7.748%
40	10.895	1453	1455	1459	rBV	145572	142467	4.01%	0.480%
41	11.183	1502	1504	1509	rBV4	30433	42003	1.18%	0.141%
42	11.342	1528	1531	1534	rBV2	93649	90490	2.55%	0.305%
43	11.495	1554	1557	1561	rBV	1319839	1172233	33.03%	3.948%
44	11.666	1583	1586	1589	rVB	189723	155511	4.38%	0.524%
45	12.013	1642	1645	1649	rBV	269039	280741	7.91%	0.946%
46	12.213	1676	1679	1684	rVB2	50968	53053	1.49%	0.179%
47	12.795	1776	1778	1786	rBV	61006	78051	2.20%	0.263%
48	12.966	1804	1807	1810	rBV	503510	411234	11.59%	1.385%
49	13.083	1823	1827	1830	rBV	3357033	3213081	90.54%	10.822%
50	13.630	1917	1920	1924	rBV	505821	402944	11.35%	1.357%
51	13.966	1974	1977	1981	rBV	137465	131807	3.71%	0.444%
52	14.142	2003	2007	2011	rBV	1096086	951560	26.81%	3.205%
53	15.001	2149	2153	2157	rBV	106395	108643	3.06%	0.366%
54	15.677	2262	2268	2274	rBV	725216	975373	27.48%	3.285%

Sum of corrected areas: 29691640

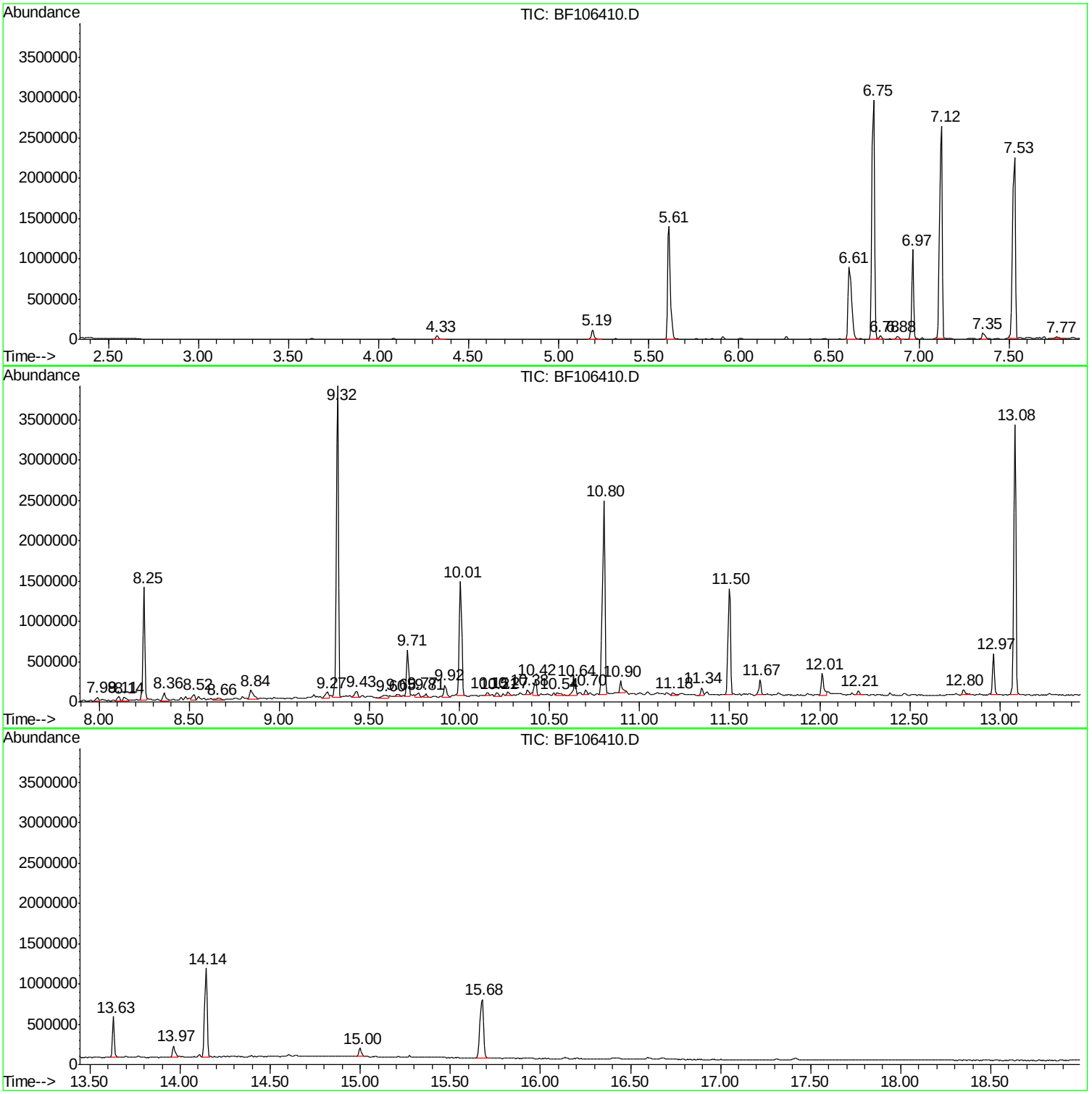
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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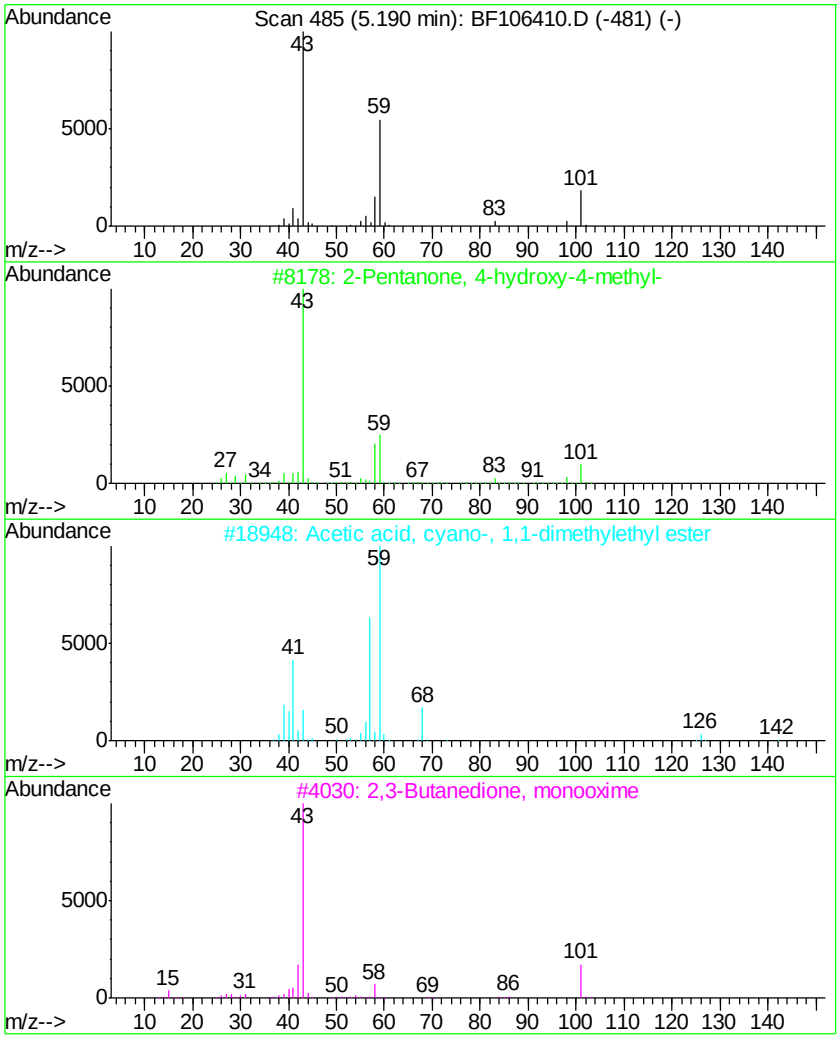
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

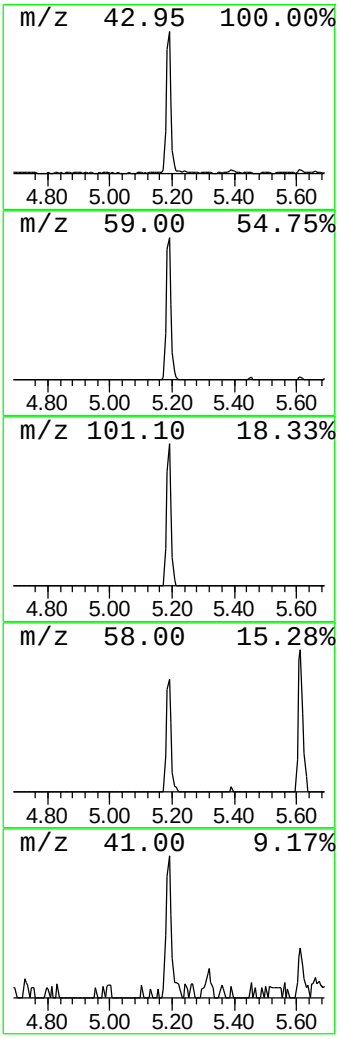
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.80 ng	121947	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	45
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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

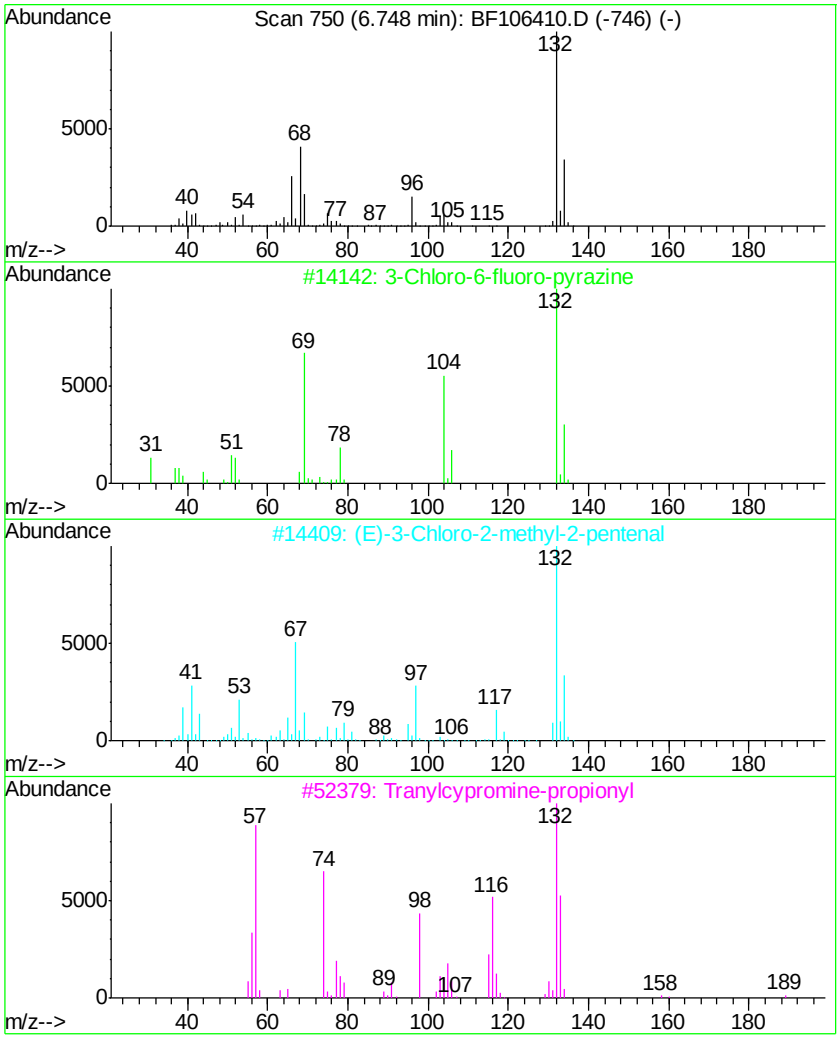
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

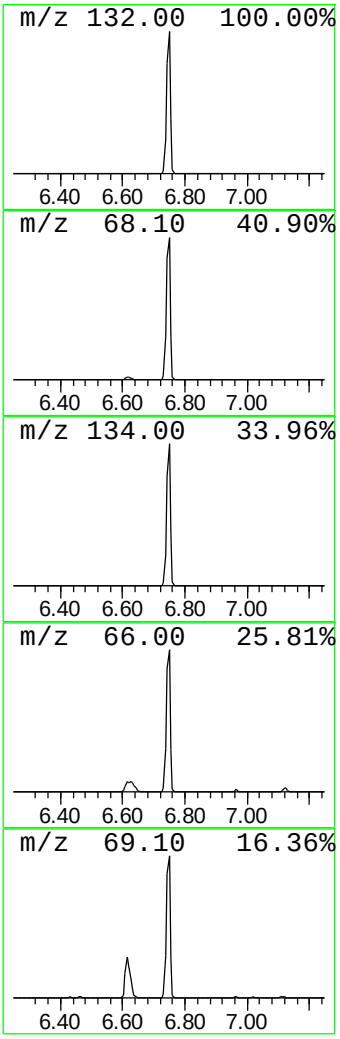
****

Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	59.95 ng	2612840	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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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

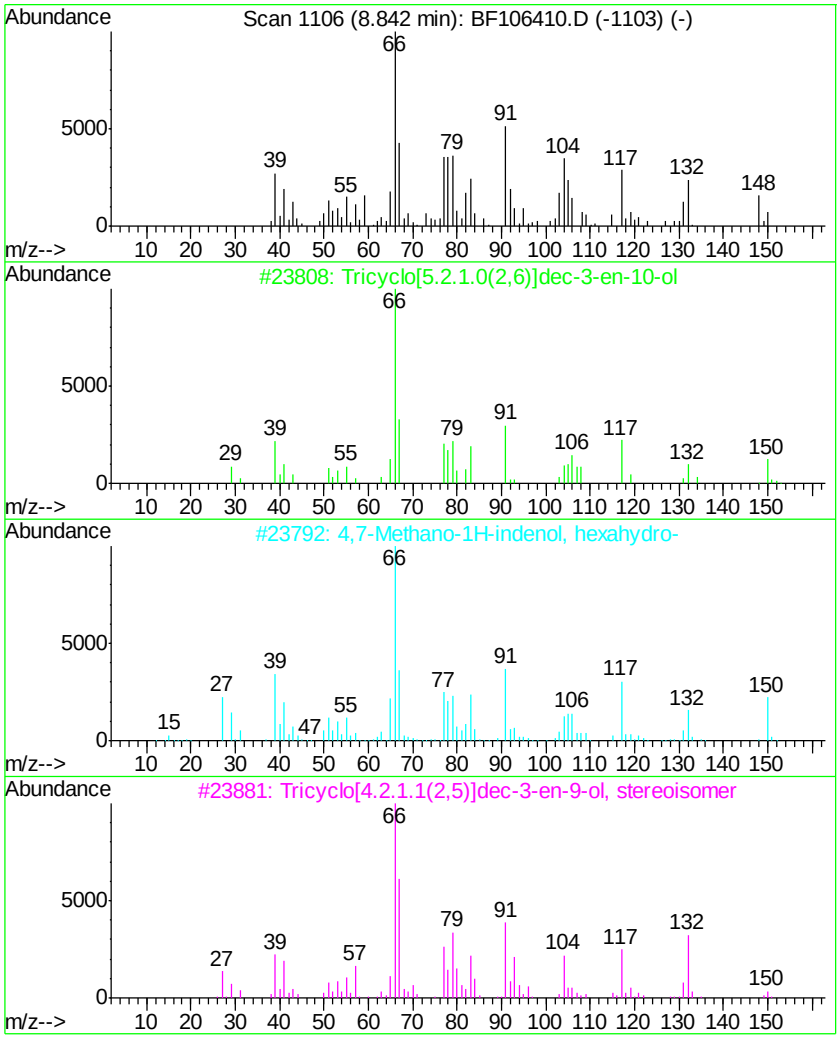
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

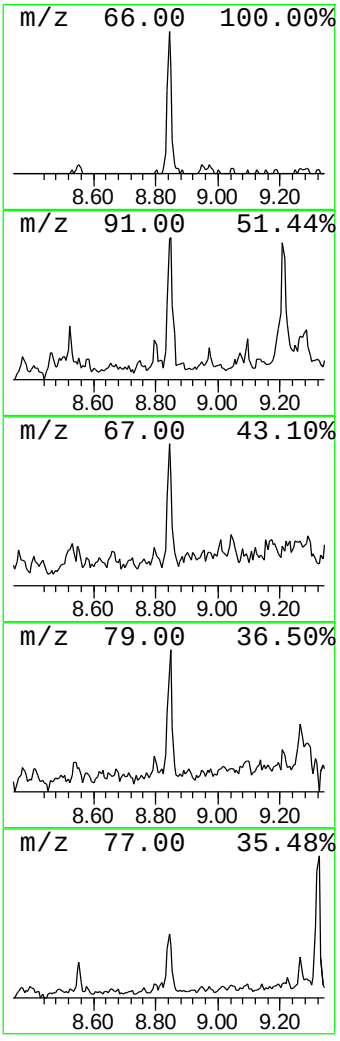
****

Peak Number 4 Tricyclo[5.2.1.0(2,6)]dec-3... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.84	2.74 ng	154081	Naphthalene-d8	8.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[5.2.1.0(2,6)]dec-3-en-1...	150	C10H14O	039852-87-4	64
2	4,7-Methano-1H-indenol, hexahydro-	150	C10H14O	037275-49-3	64
3	Tricyclo[4.2.1.1(2,5)]dec-3-en-9...	150	C10H14O	070220-93-8	64
4	Tricyclo[5.2.1.0(2,6)]dec-3-en-1...	148	C10H12O	1000289-10-5	64
5	Bicyclo[3.2.0]hept-2-ene, 6-meth...	106	C8H10	038695-51-1	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106410.D
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Operator : JU/SJ
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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

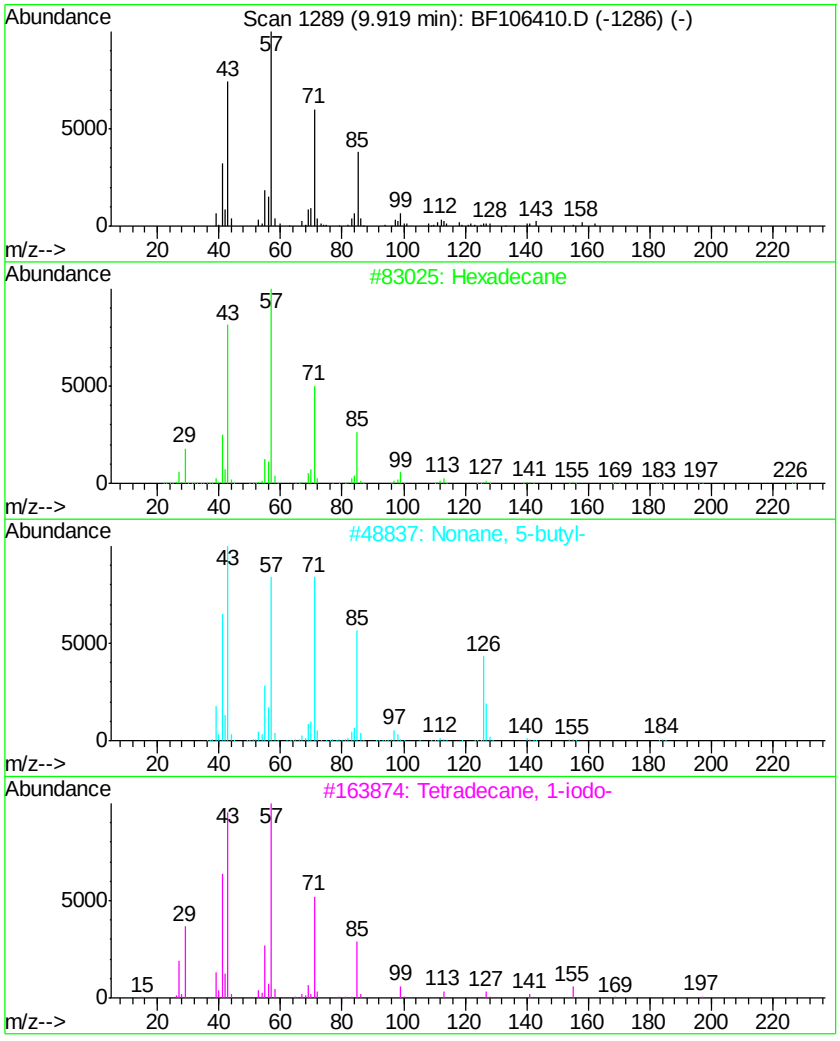
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

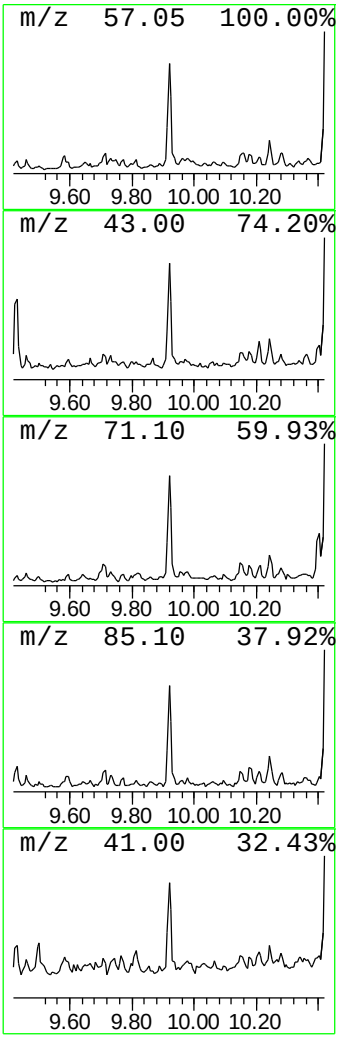
****

Peak Number 5 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	2.05 ng	125986	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	86
2	Nonane, 5-butyl-	184	C13H28	017312-63-9	72
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	64
4	Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	59
5	Decane, 3-bromo-	220	C10H21Br	030571-71-2	53





Library Search Compound Report

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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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

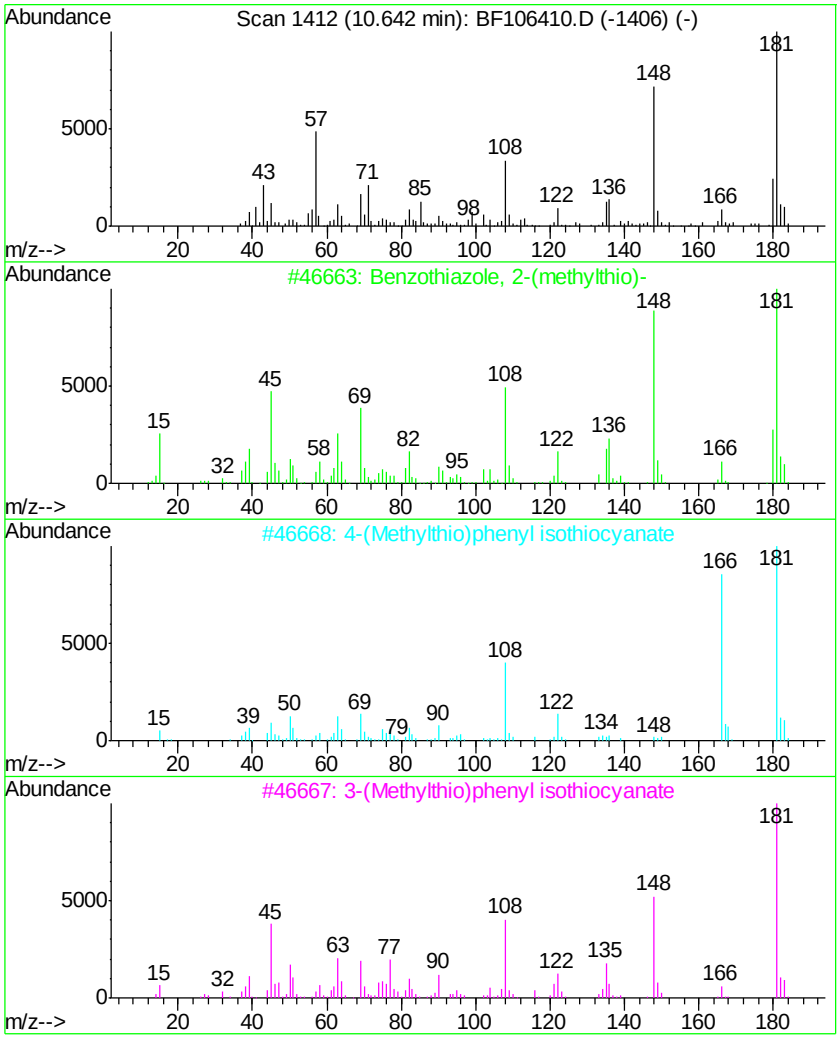
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

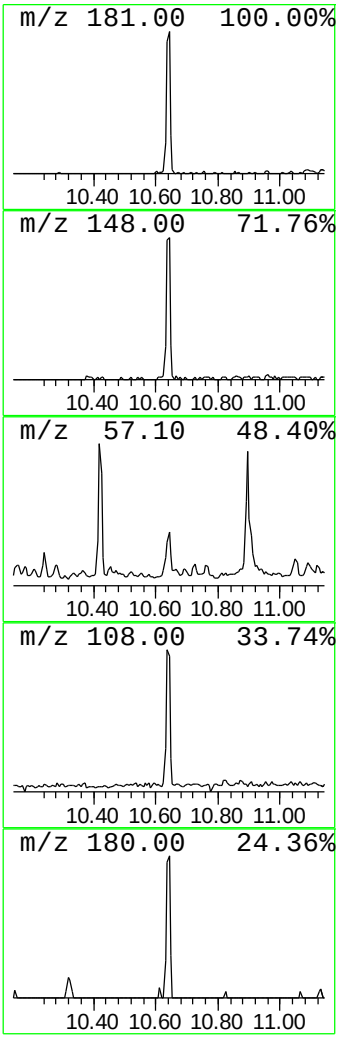
****

Peak Number 7 Benzothiazole, 2-(methylthio)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	3.45 ng	211444	Acenaphthene-d10	10.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole, 2-(methylthio)-	181	C8H7NS2	000615-22-5	96
2	4-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	015863-41-9	78
3	3-(Methylthio)phenyl isothiocyanate	181	C8H7NS2	051333-80-3	68
4	2(3H)-Benzothiazolethione, 3-met...	181	C8H7NS2	002254-94-6	58
5	9-Amino-1-methyl-3,6-diazahomoad...	181	C10H19N3	1000216-24-2	47





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Acq On : 13 Jun 2018 23:53
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Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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

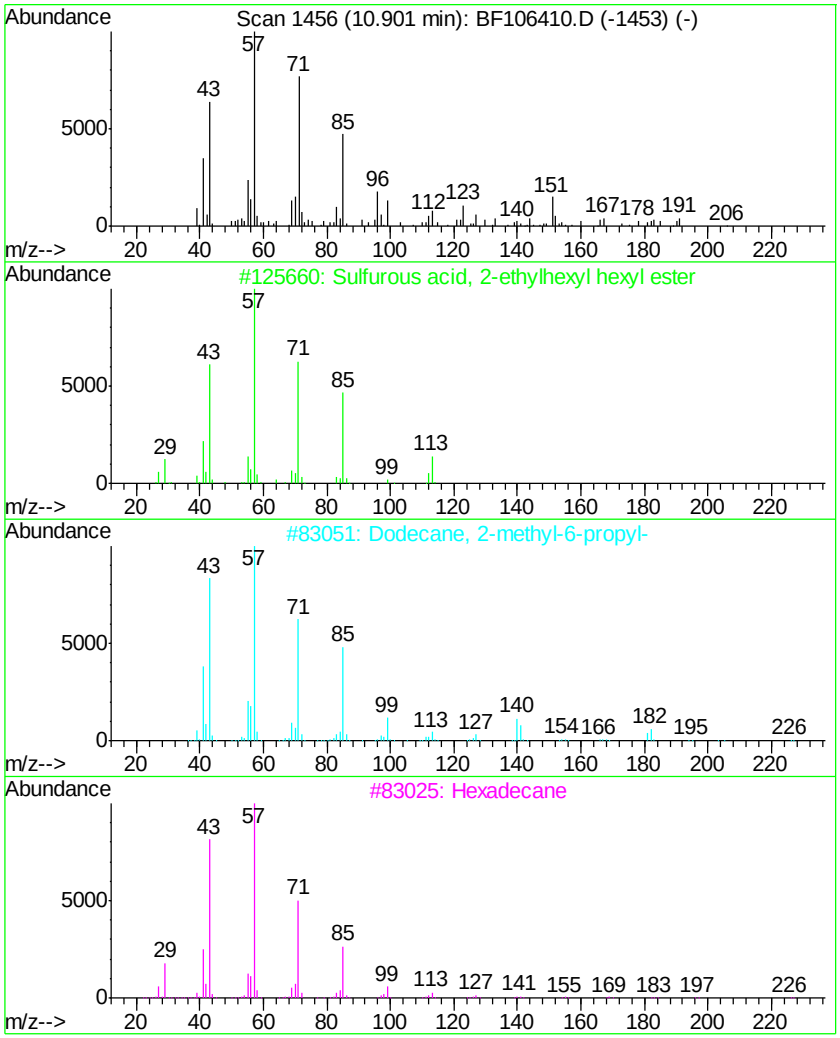
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

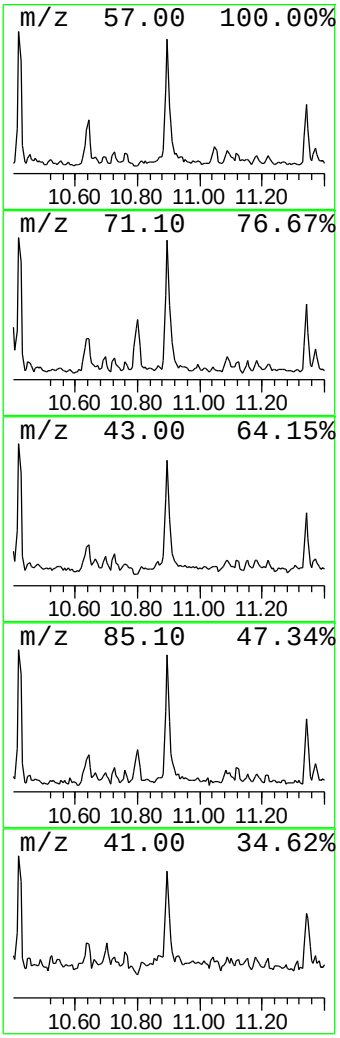
****

Peak Number 8 Sulfurous acid, 2-ethylhexy... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.43 ng	142467	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	90
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
3	Hexadecane	226	C16H34	000544-76-3	80
4	Dodecane, 3-methyl-	184	C13H28	017312-57-1	72
5	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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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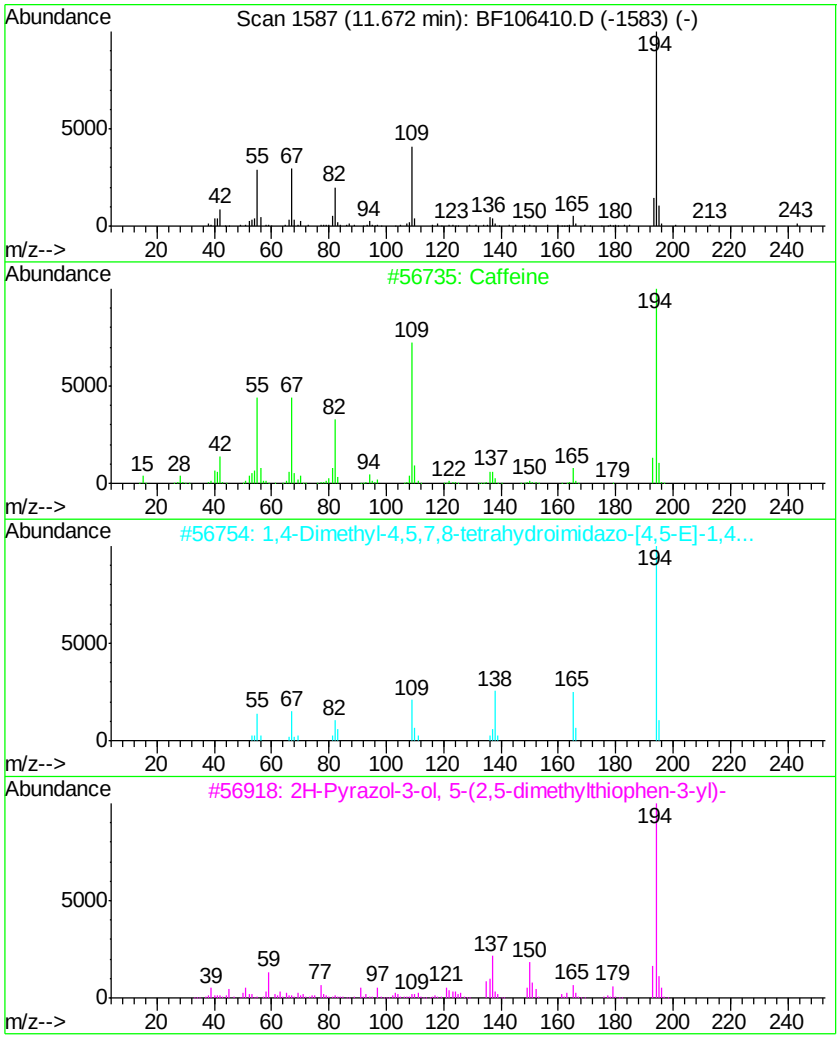
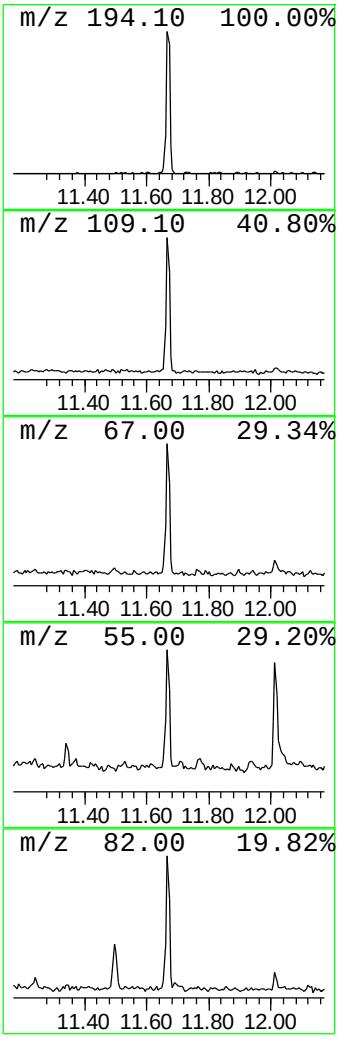
Peak Number 9 Caffeine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	2.65 ng	155511	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	97
2	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	50
3	2H-Pyrazol-3-ol, 5-(2,5-dimethyl...	194	C9H10N2OS	1000304-22-5	43
4	3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	40
5	1H-Benzimidazole, 2-phenyl-	194	C13H10N2	000716-79-0	38





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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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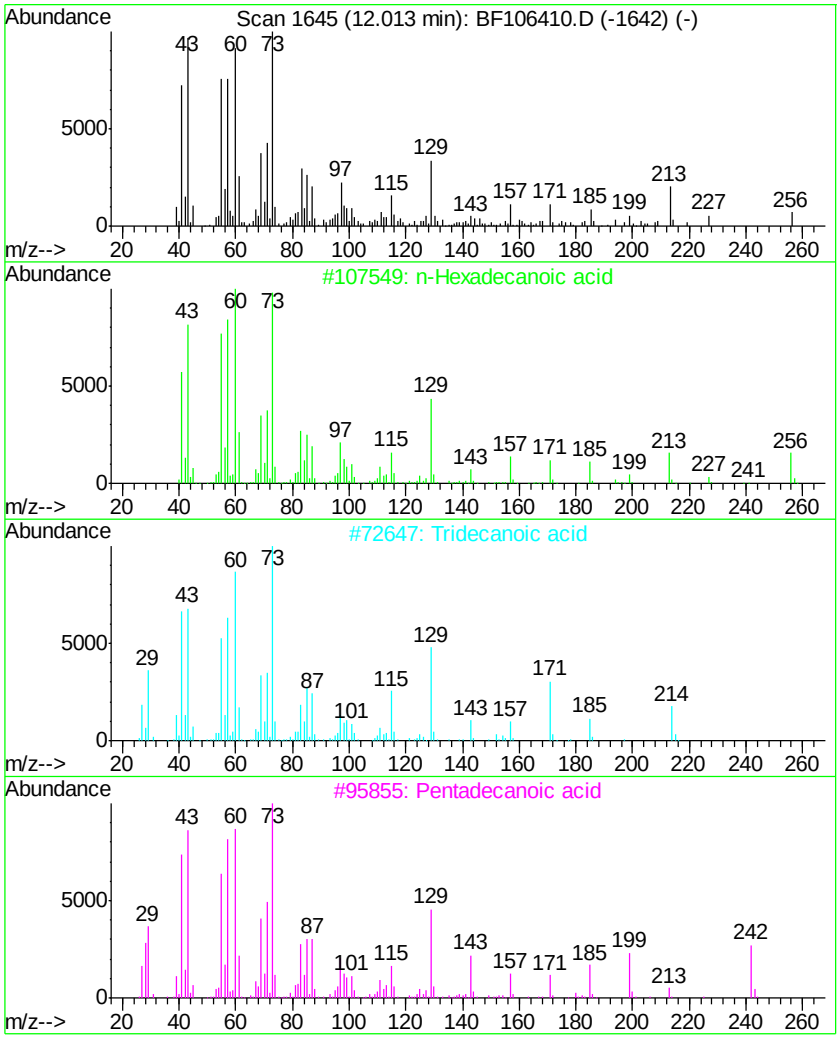
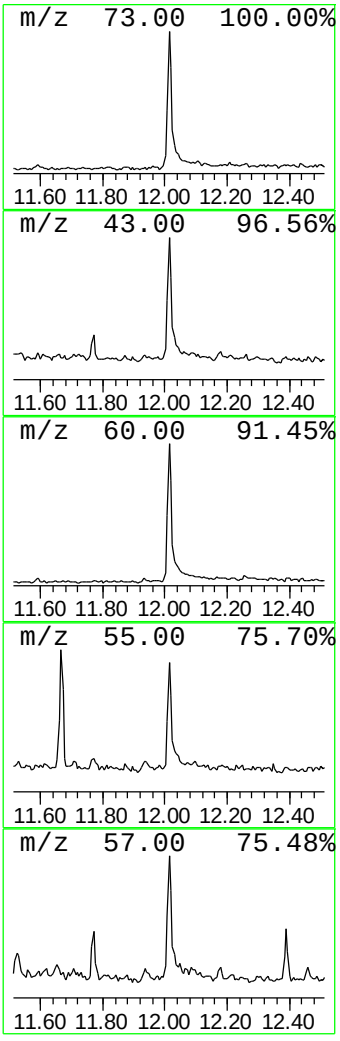
Peak Number 10 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	4.79 ng	280741	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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Oxalic acid, allyl octadecyl ester	382	C23H42O4	1000309-24-5	18





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061318\
Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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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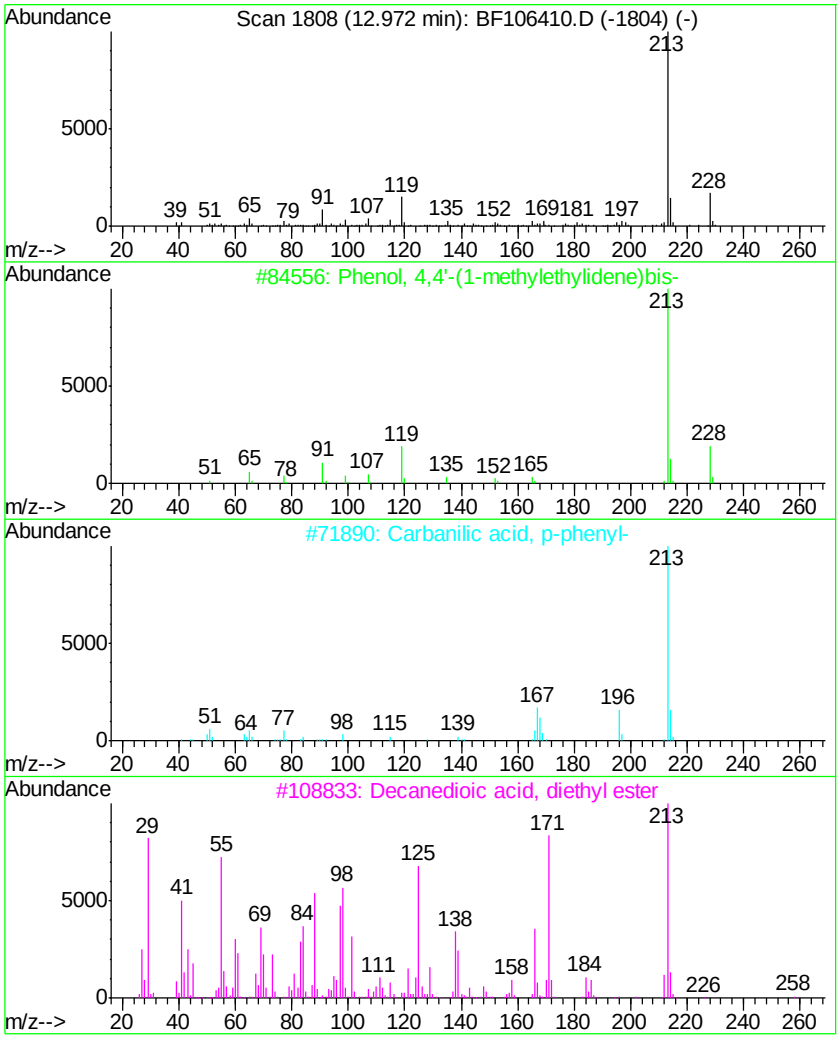
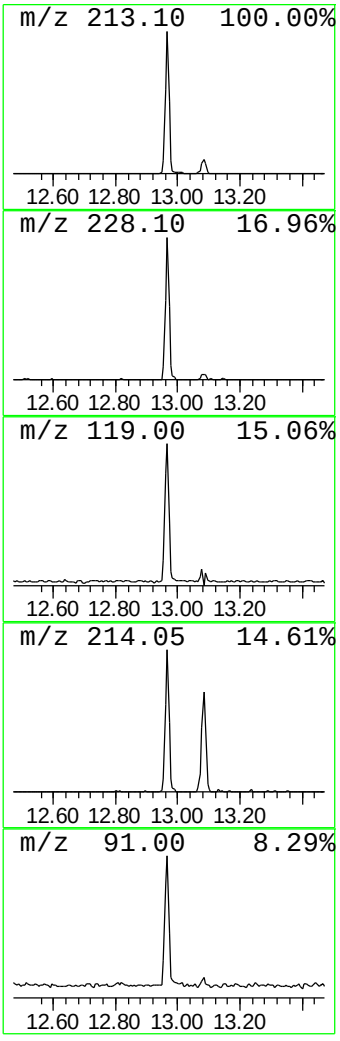
Peak Number 11 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.97	8.64 ng	411234	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	52
3	Decanedioic acid, diethyl ester	258	C14H26O4	000110-40-7	50
4	2-Trimethylsilyl-3-trimethylsily...	228	C8H20N4Si2	1000373-05-5	45
5	Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	45





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Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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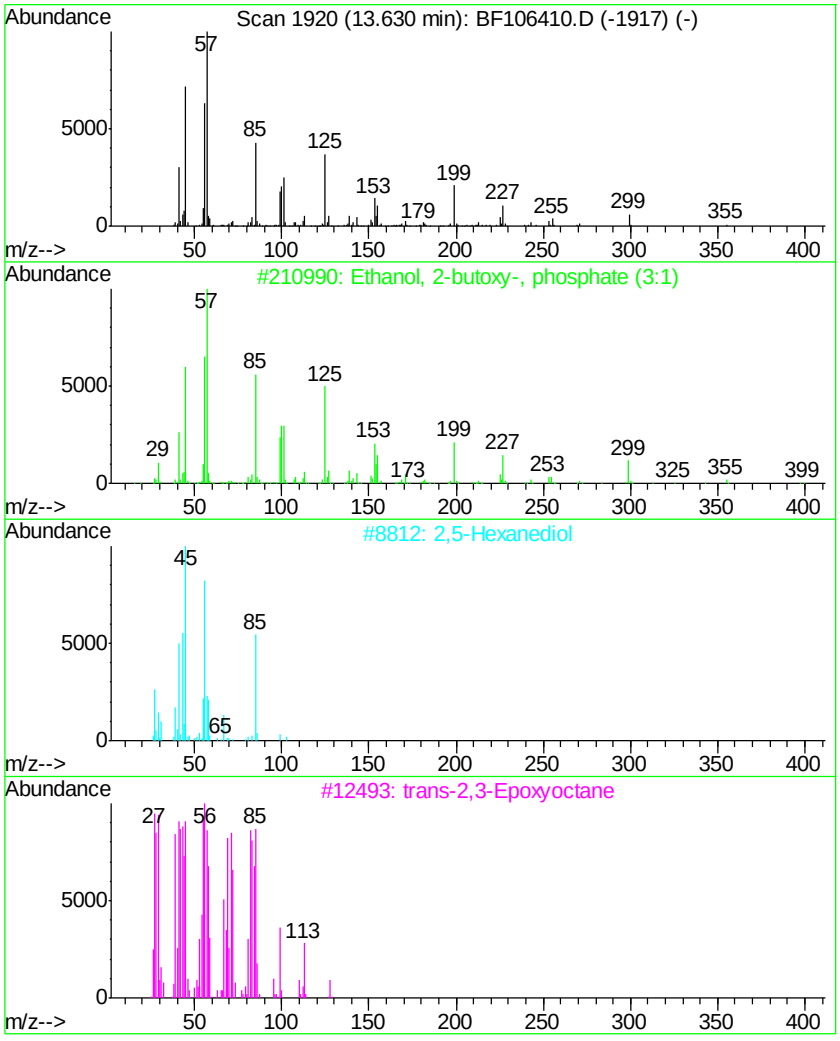
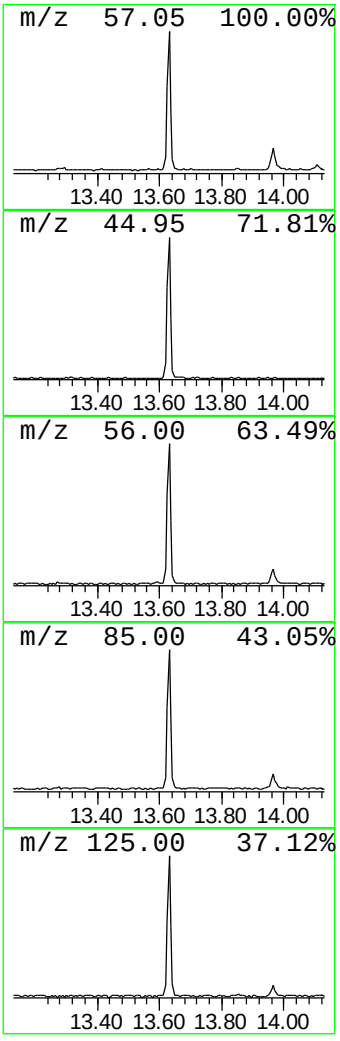
Peak Number 12 Ethanol, 2-butoxy-, phospha... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	8.47 ng	402944	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	90
2	2,5-Hexanediol	118	C6H14O2	002935-44-6	38
3	trans-2,3-Epoxyoctane	128	C8H16O	028180-70-3	38
4	2-Propanone, ethylhydrazone	100	C5H12N2	007422-99-3	25
5	Oxetane, 2,3,4-trimethyl-	100	C6H12O	053778-61-3	22





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Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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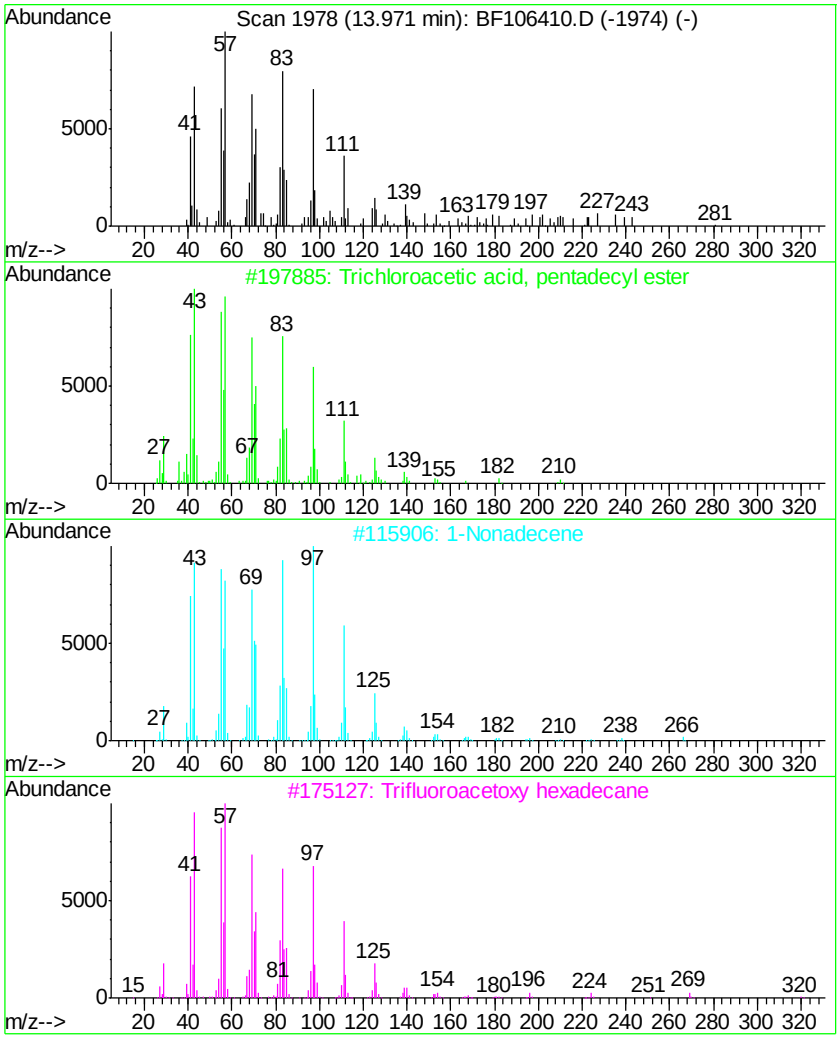
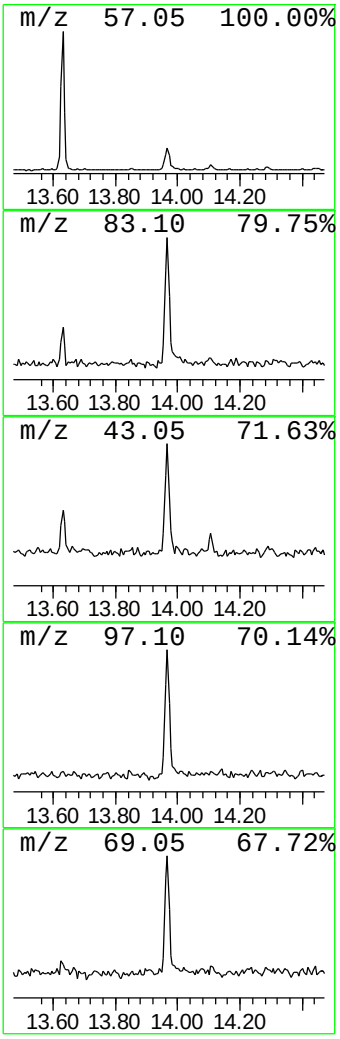
Peak Number 13 Trichloroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.77 ng	131807	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91





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Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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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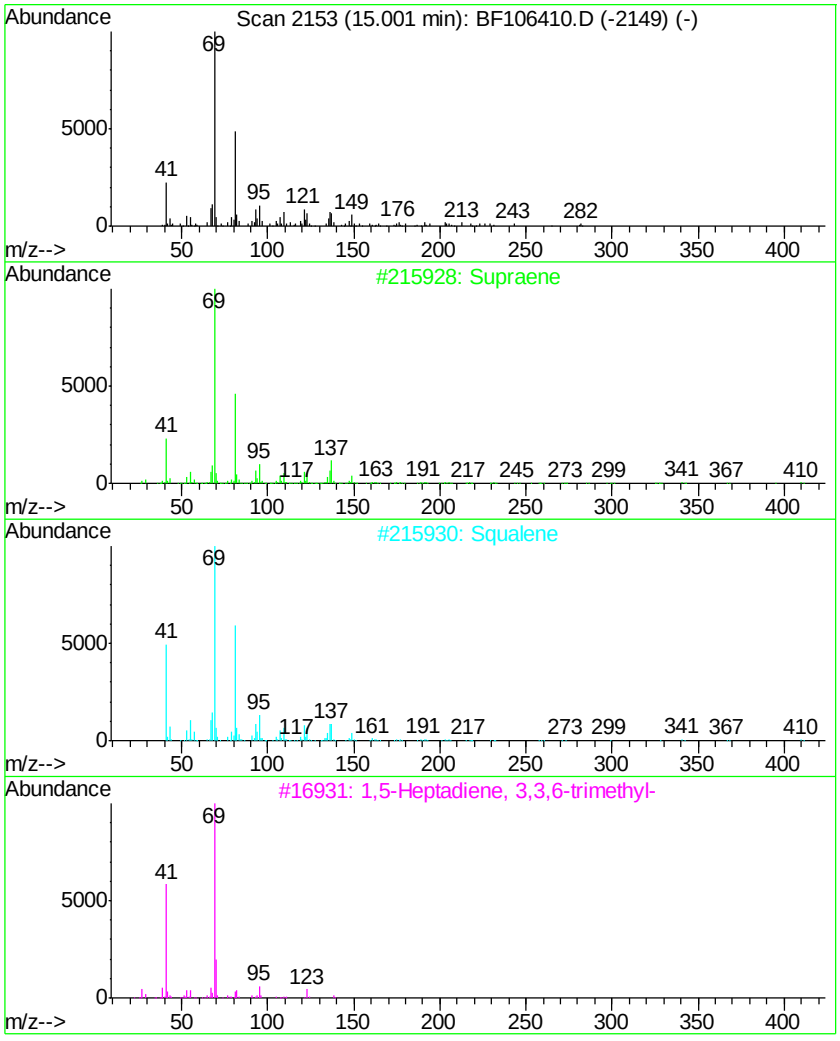
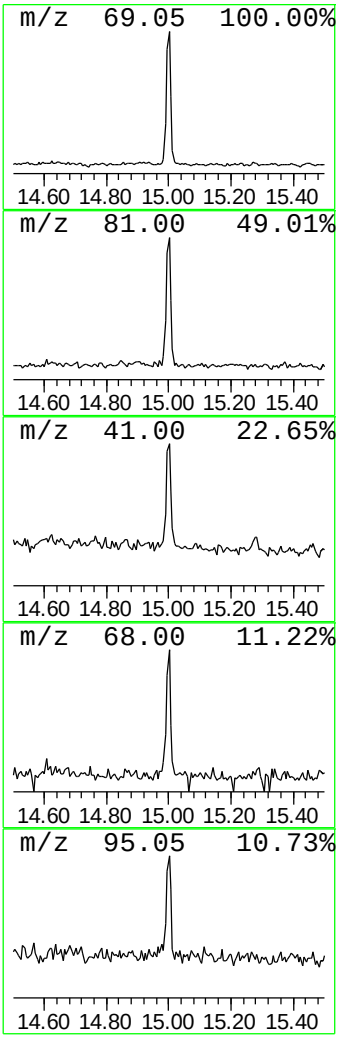
Peak Number 14 Supraene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.00	2.23 ng	108643	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Squalene	410	C30H50	000111-02-4	87
3	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64
4	(.+/-.)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64
5	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64





Tentatively Identified Compound (LSC) summary

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Data File : BF106410.D
Acq On : 13 Jun 2018 23:53
Operator : JU/SJ
Sample : J3448-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : N-48969

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	2.8	ng	121947	1	6.97	871746	20.0
unknown6.75	6.75	60.0	ng	2612840	1	6.97	871746	20.0
Tricyclo[5.2.1.0(...	8.84	2.7	ng	154081	2	8.25	1124080	20.0
Hexadecane	9.92	2.0	ng	125986	3	10.01	1227160	20.0
Benzothiazole, 2-...	10.64	3.5	ng	211444	3	10.01	1227160	20.0
Sulfurous acid, 2...	10.90	2.4	ng	142467	4	11.50	1172230	20.0
Caffeine	11.67	2.6	ng	155511	4	11.50	1172230	20.0
n-Hexadecanoic acid	12.01	4.8	ng	280741	4	11.50	1172230	20.0
Phenol, 4,4'-(1-m...	12.97	8.6	ng	411234	5	14.14	951560	20.0
Ethanol, 2-butoxy...	13.63	8.5	ng	402944	5	14.14	951560	20.0
Trichloroacetic a...	13.97	2.8	ng	131807	5	14.14	951560	20.0
Supraene	15.00	2.2	ng	108643	6	15.68	975373	20.0