LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100801.D
Acq On : 22 Nov 2017 1:33
Operator : SJ/JU
Sample : I6466-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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	5.104	508	513	523	rBB	243663	338610	16.35%	1.804%
2	5.498	574	580	583	rBV	1760345	1794531	86.63%	9.562%
3	6.504	745	751	757	rVB	1687651	1912345	92.31%	10.190%
4	6.645	770	775	778	rBV	1921517	1865193	90.04%	9.938%
5	6.875	810	814	817	rBV	560775	508535	24.55%	2.710%
6	7.028	836	840	843	rBV	1643103	1435850	69.31%	7.651%
7	7.433	904	909	912	rBV	1130274	1173095	56.63%	6.251%
8	8.151	1027	1031	1035	rBV	742849	664472	32.08%	3.540%
9	8.704	1120	1125	1128	rBV	97796	85850	4.14%	0.457%
10	9.227	1209	1214	1217	rBV	2264629	2071607	100.00%	11.038%
11	9.622	1277	1281	1284	rBV2	91229	84036	4.06%	0.448%
12	9.827	1309	1316	1321	rBV	20576	22066	1.07%	0.118%
13	9.910	1326	1330	1334	rVV	830297	702301	33.90%	3.742%
14	10.333	1394	1402	1404	rBV2	20093	24609	1.19%	0.131%
15	10.621	1444	1451	1454	rBV	371898	300730	14.52%	1.602%
16	10.698	1460	1464	1467	rBV	1212681	1060390	51.19%	5.650%
17	10.816	1479	1484	1487	rVB2	22235	29686	1.43%	0.158%
18	11.398	1579	1583	1585	rBV	695605	618730	29.87%	3.297%
19	11.416	1585	1586	1592	rVB	91998	64352	3.11%	0.343%
20	11.915	1664	1671	1676	rBV3	64242	96944	4.68%	0.517%
21	12.010	1683	1687	1689	rBV2	19726	22849	1.10%	0.122%
22	12.610	1786	1789	1792	rBV	146724	120884	5.84%	0.644%
23	12.645	1792	1795	1798	rVB	122500	99055	4.78%	0.528%
24	12.792	1817	1820	1822	rVB	86819	67024	3.24%	0.357%
25	12.839	1822	1828	1831	rBV	111354	124536	6.01%	0.664%
26	12.980	1847	1852	1855	rBV	1509306	1343206	64.84%	7.157%
27	13.162	1881	1883	1887	rVB2	26034	26727	1.29%	0.142%
28	13.498	1938	1940	1943	rVB	52497	46250	2.23%	0.246%
29	13.539	1943	1947	1949	rBV3	20691	24376	1.18%	0.130%
30	13.862	1999	2002	2009	rVB2	110509	134614	6.50%	0.717%
31	14.033	2026	2031	2034	rBV	592259	590669	28.51%	3.147%
32	14.057	2034	2035	2038	rVB	63953	44192	2.13%	0.235%
33	14.186	2054	2057	2060	rBV4	23481	25161	1.21%	0.134%
34	14.492	2106	2109	2115	rBV5	41641	58304	2.81%	0.311%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I6466-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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

35	15.074	2205	2208	2211	rBV	61930	84906	4.10%	0.452%
36	15.133	2216	2218	2221	rVV	34000	35265	1.70%	0.188%
37	15.380	2258	2260	2266	rVB	42226	48624	2.35%	0.259%
38	15.445	2268	2271	2275	rVV	49260	59059	2.85%	0.315%
39	15.509	2278	2282	2291	rVB2	370454	485657	23.44%	2.588%
40	15.727	2316	2319	2323	rBV5	26178	40748	1.97%	0.217%
41	15.956	2355	2358	2362	rVB2	33608	46333	2.24%	0.247%
42	16.215	2398	2402	2415	rVB5	74827	170416	8.23%	0.908%
43	16.650	2473	2476	2488	rVB3	51432	122933	5.93%	0.655%
44	16.986	2530	2533	2541	rVB5	22495	42290	2.04%	0.225%
45	17.574	2629	2633	2637	rBV7	26369	49736	2.40%	0.265%

Sum of corrected areas: 18767746

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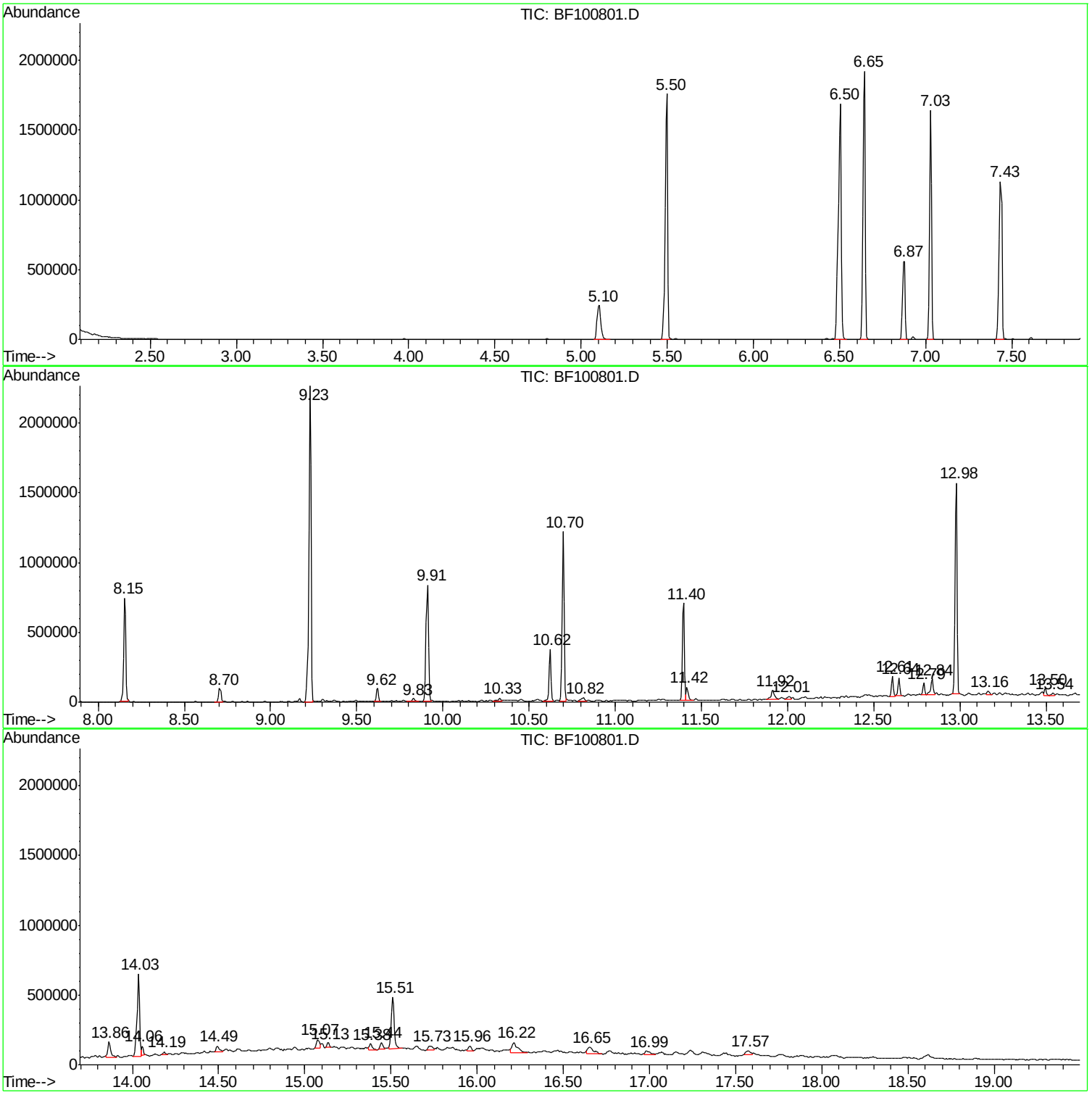
Instrument :
BNA_F
ClientSampleId :
CHAP-4-E(3-4)

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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Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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

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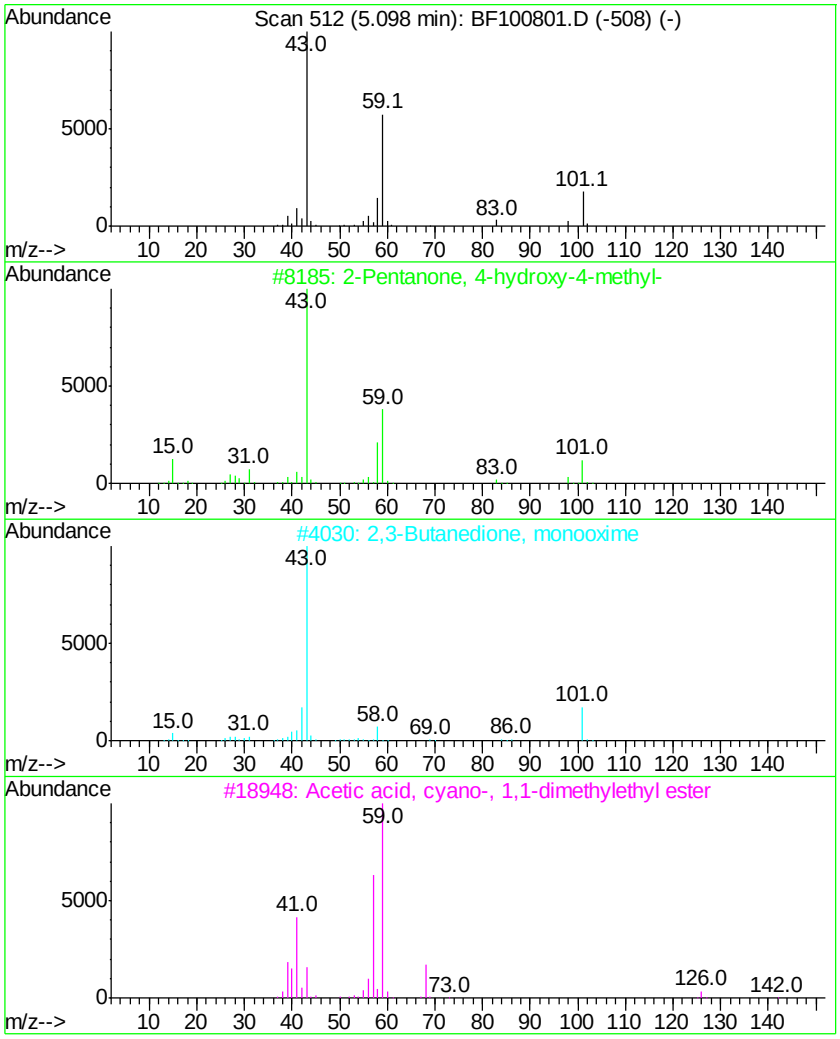
TIC Integration Parameters: LSCINT.P

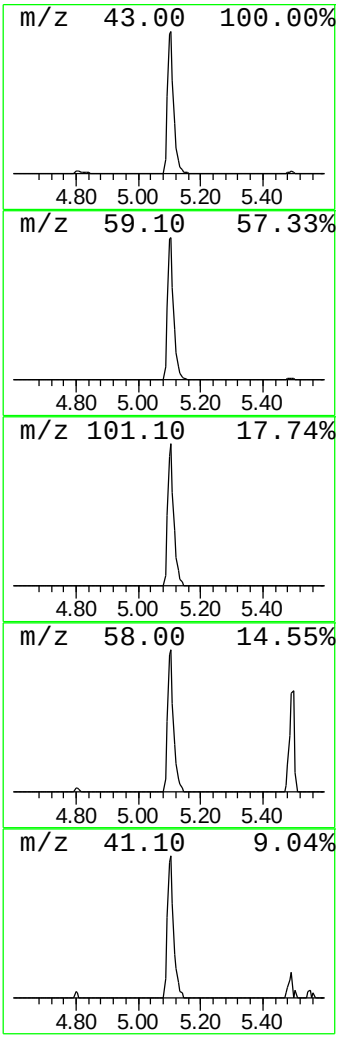
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	13.32 ng	338610	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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Operator : SJ/JU
Sample : I6466-05
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Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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
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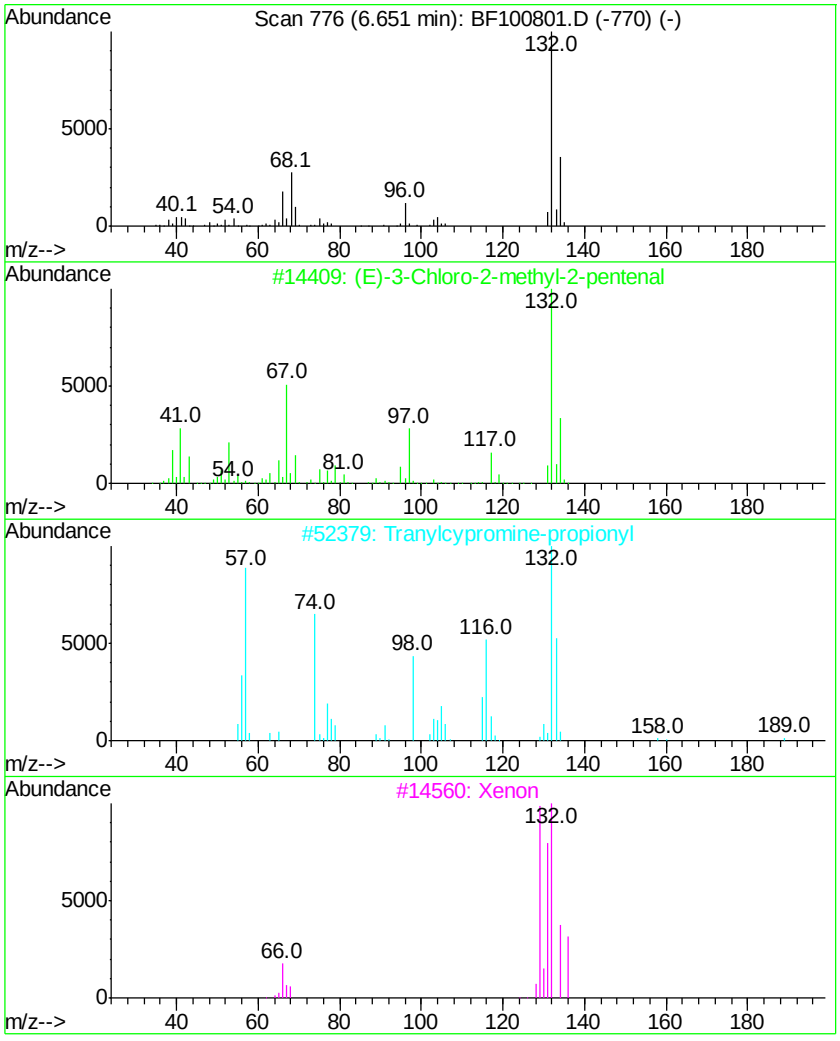
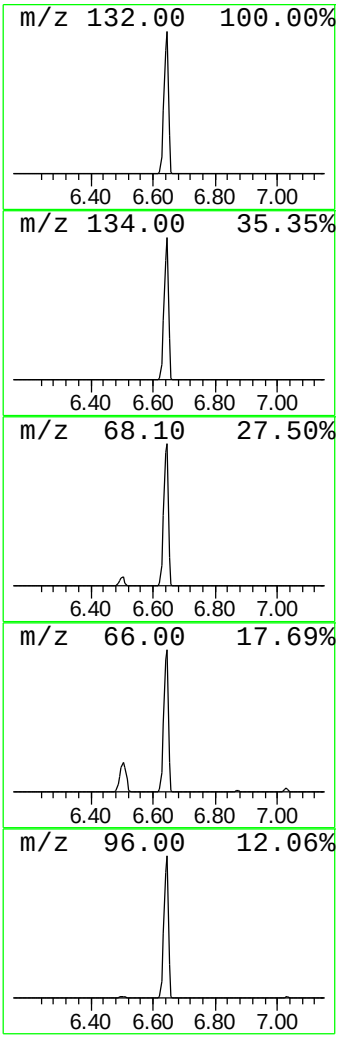
****

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	73.36 ng	1865190	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Xenon	132	Xe	007440-63-3	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Sample : I6466-05
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Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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

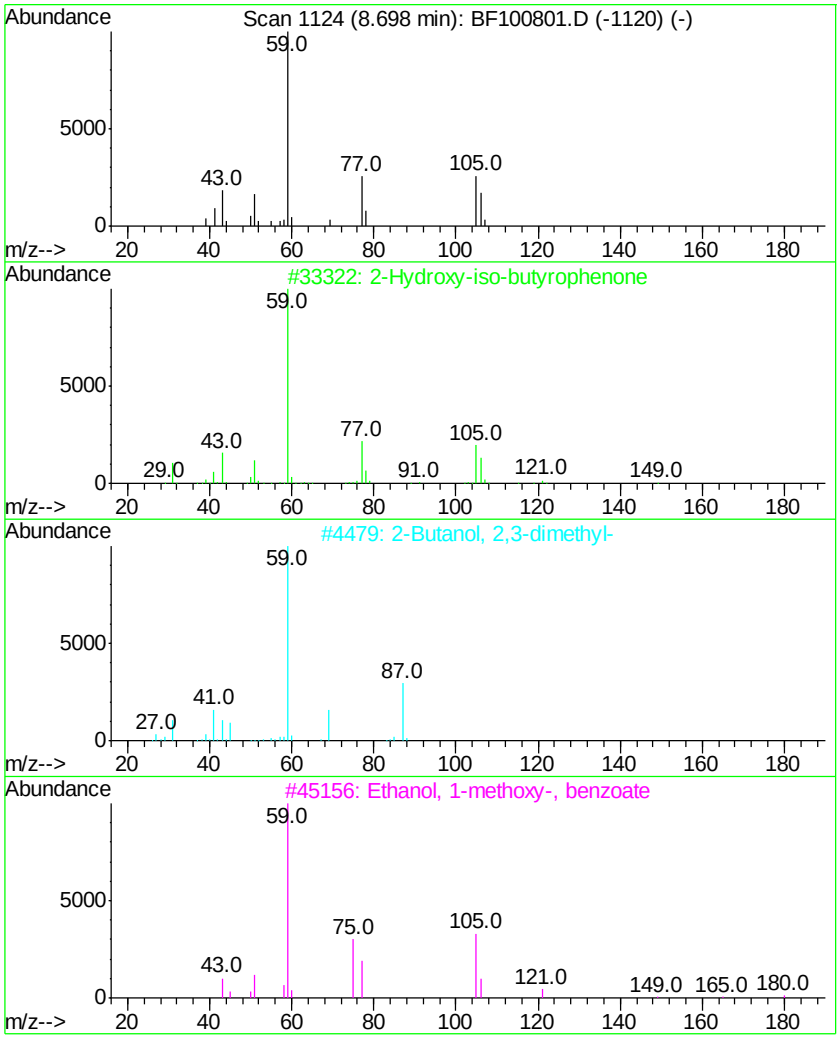
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

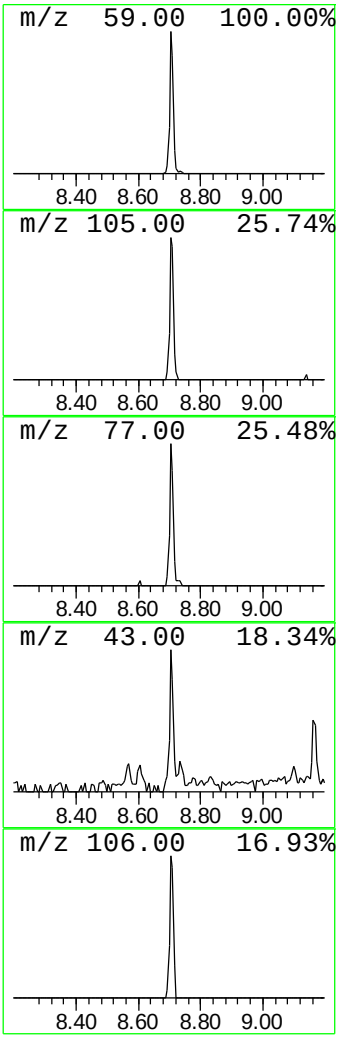
****

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.70	2.58 ng	85850	Naphthalene-d8	8.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	78
2	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	9
3	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	9
4	Guanidine	59	CH5N3	000113-00-8	7
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
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Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
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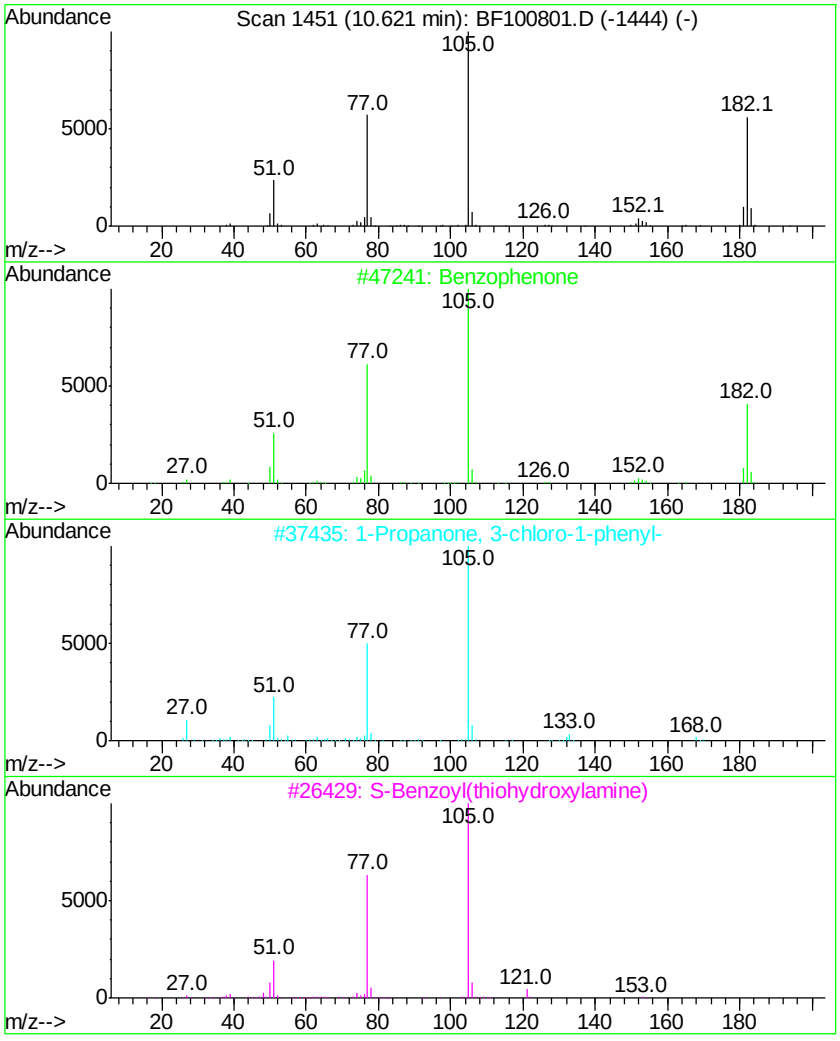
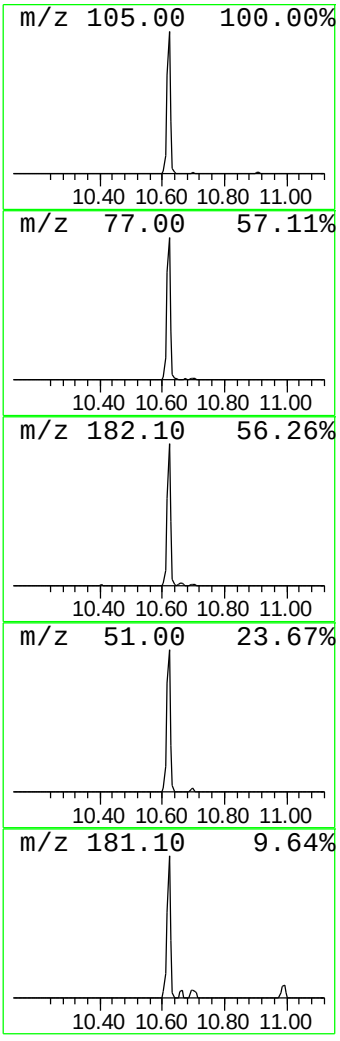
Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.62	8.56 ng	300730	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	43
3	S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	43
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
5	Benzoylformic acid	150	C8H6O3	000611-73-4	43





Library Search Compound Report

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Sample : I6466-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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
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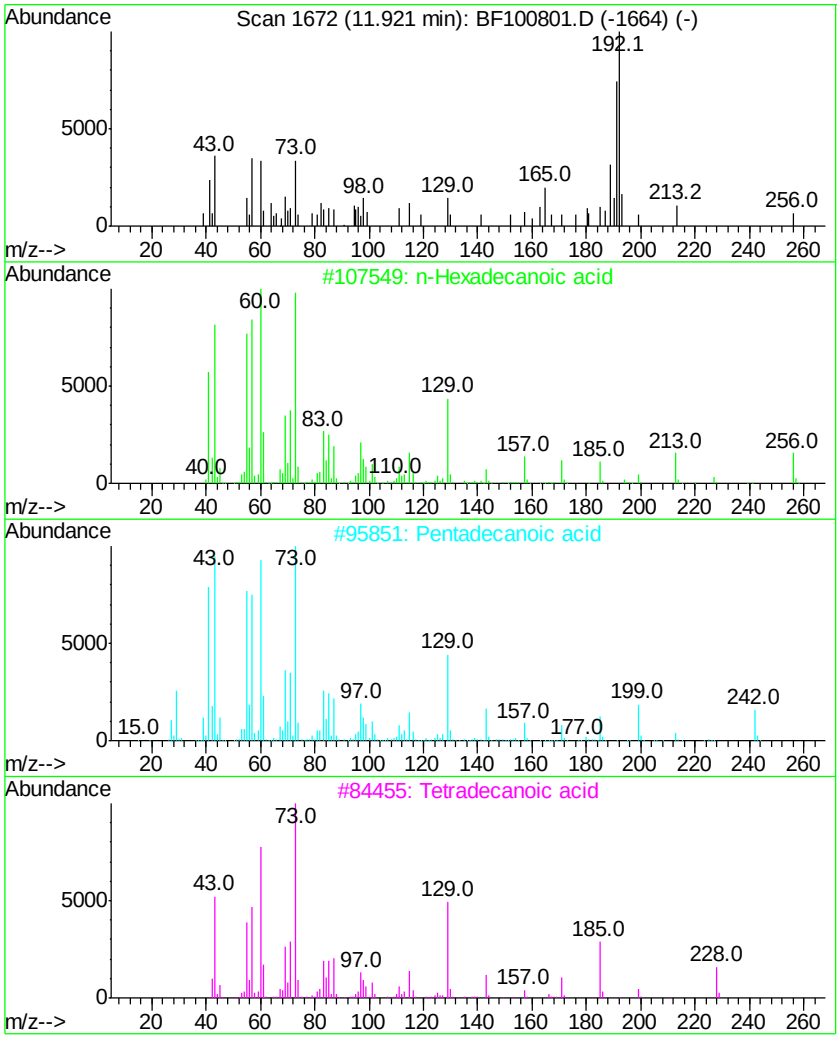
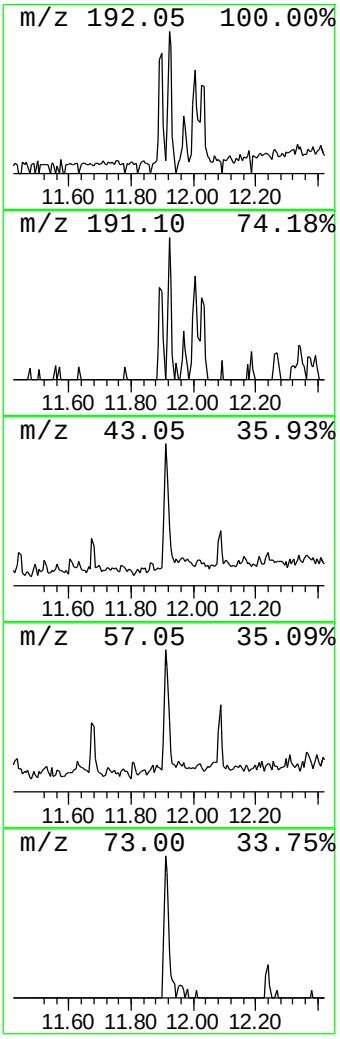
Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.13 ng	96944	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Dodecanoic acid	200	C12H24O2	000143-07-7	49
5	Tridecanoic acid	214	C13H26O2	000638-53-9	49





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ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CHAP-4-E(3-4)

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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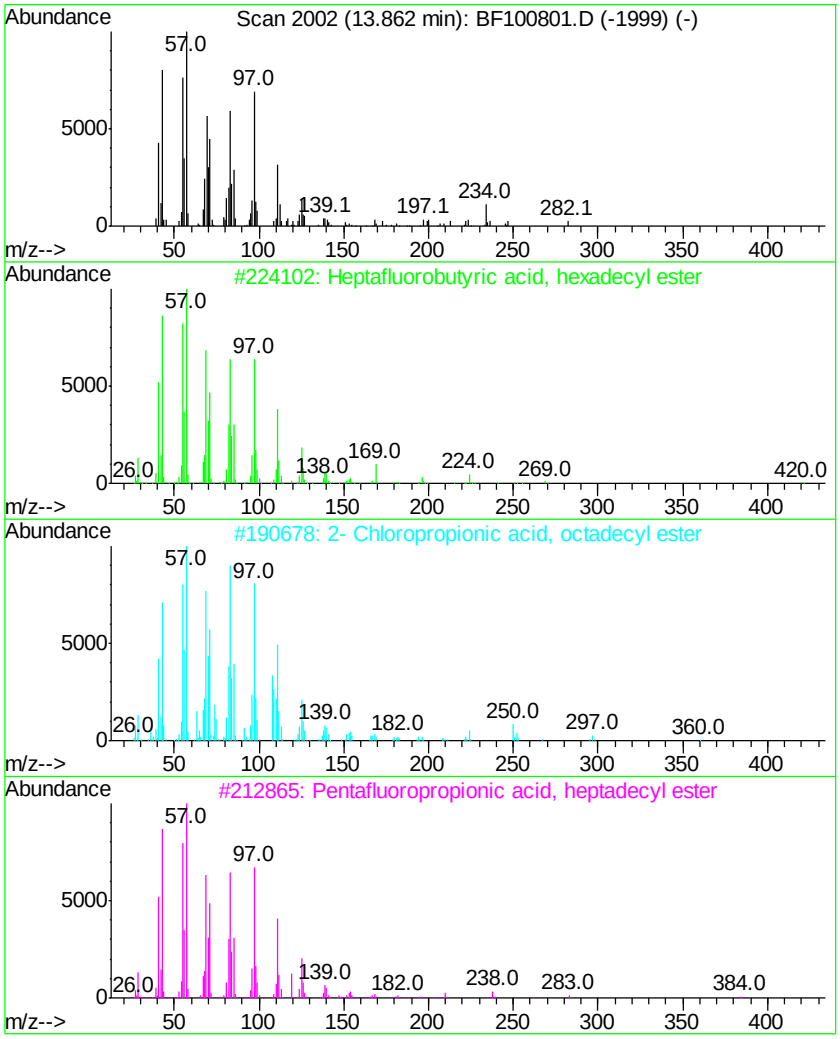
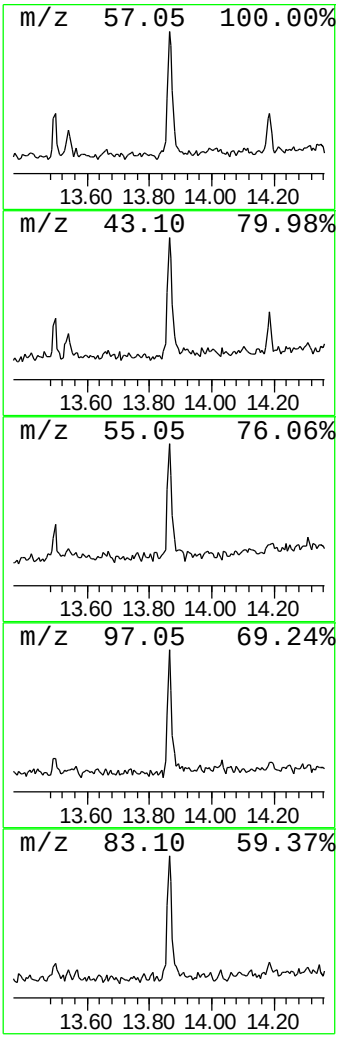
Peak Number 7 Heptafluorobutyric acid, he... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.56 ng	134614	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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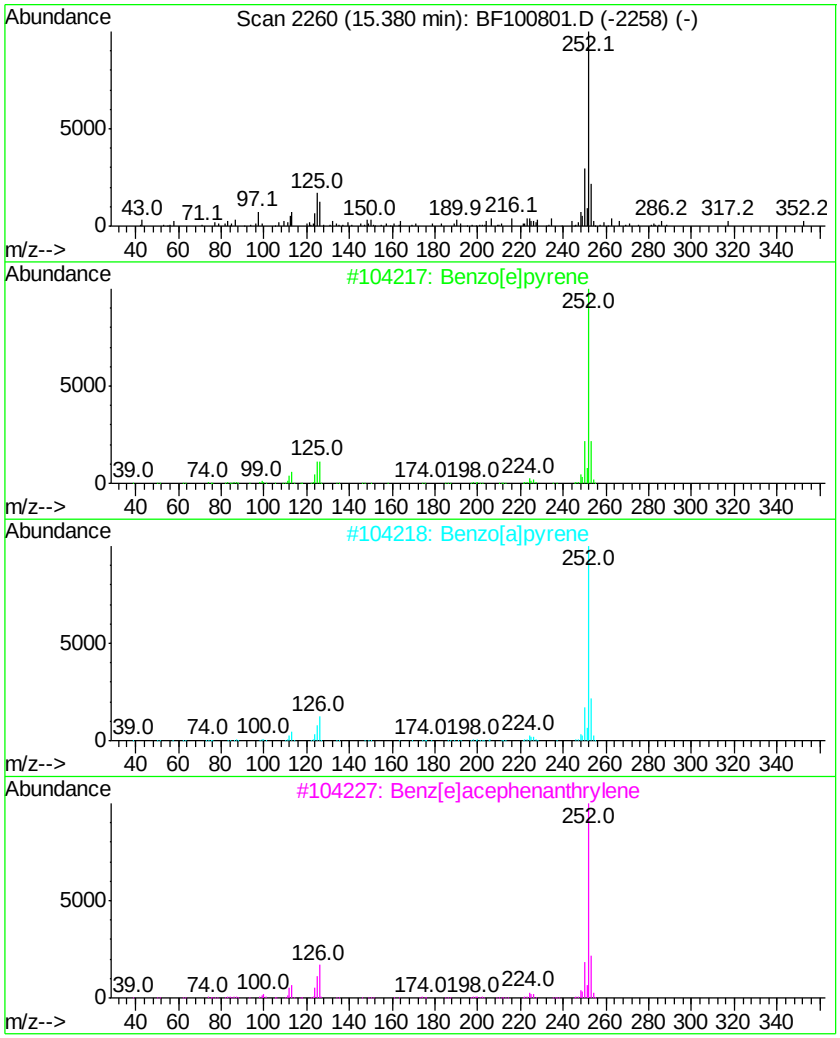
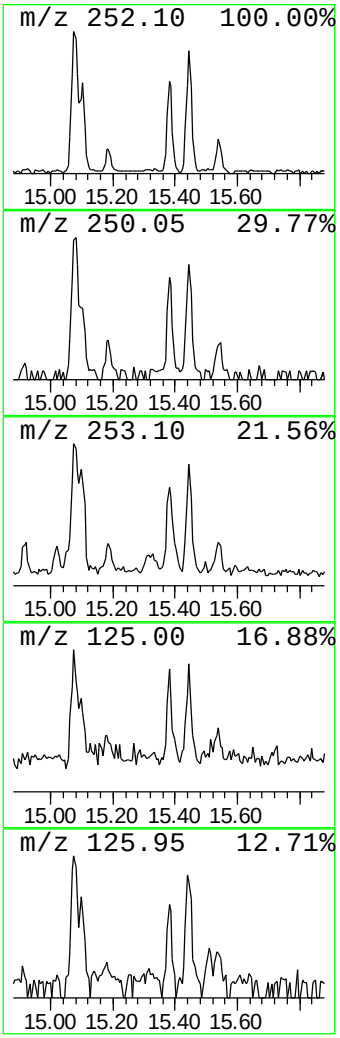
Peak Number 8 Benzo[e]pyrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.38	2.00 ng	48624	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[a]pyrene	252	C20H12	000050-32-8	95
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
5	Perylene	252	C20H12	000198-55-0	95





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Sample : I6466-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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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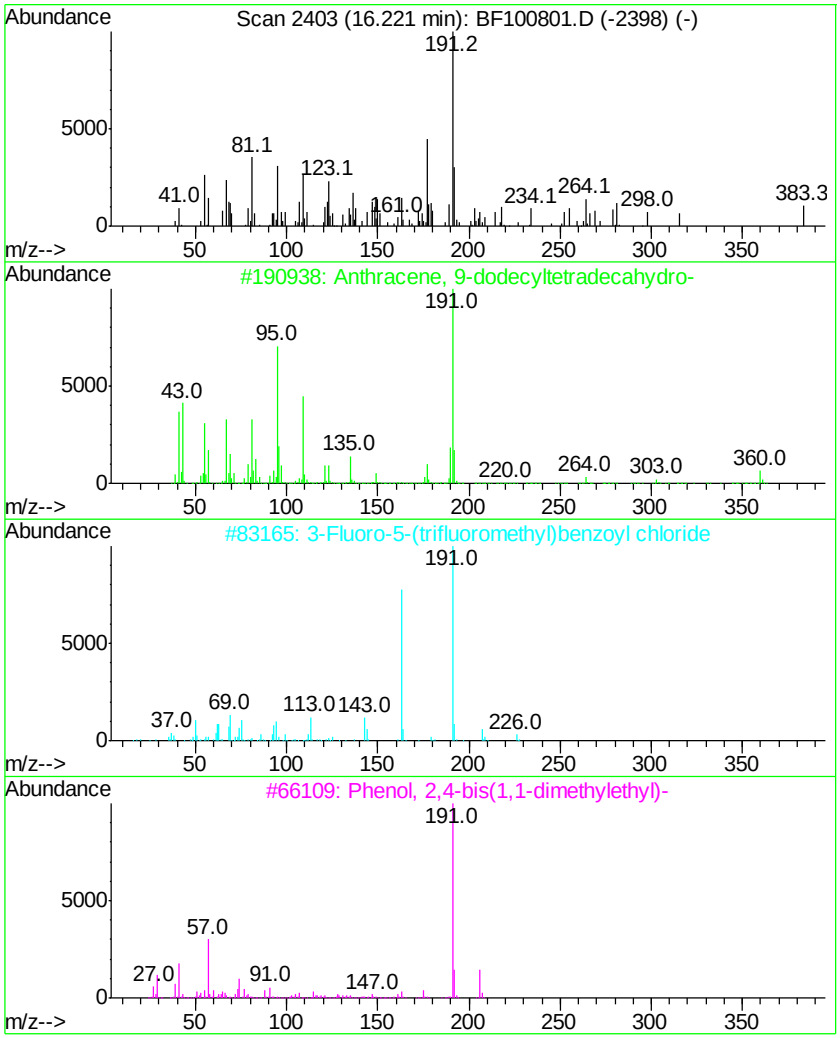
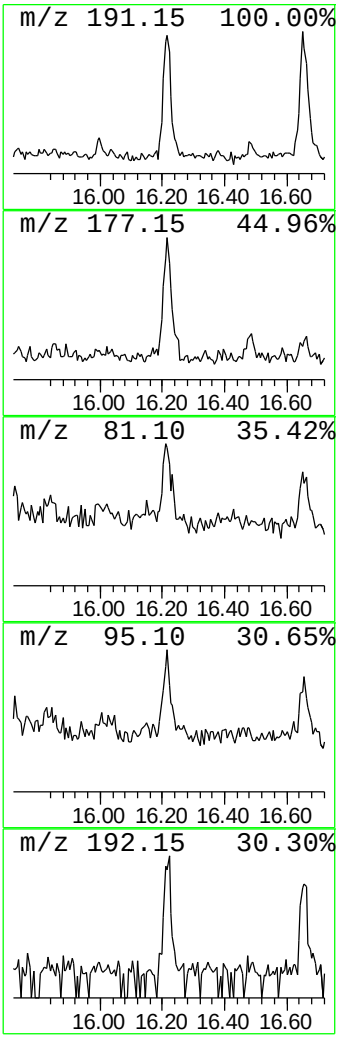
Peak Number 9 unknown16.22 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	7.02 ng	170416	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-dodecyltetradecahv...	360	C26H48	055401-75-7	43
2	3-Fluoro-5-(trifluoromethyl)benz...	226	C8H3ClF4O	171243-30-4	25
3	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	22
4	4-Fluoro-2-trifluoromethylbenzoi...	236	C10H8F4O2	1000338-81-9	22
5	Propenoic acid, 3-(3,4-dimethoxy...	344	C19H24N2O4	1000259-51-5	22





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Sample : I6466-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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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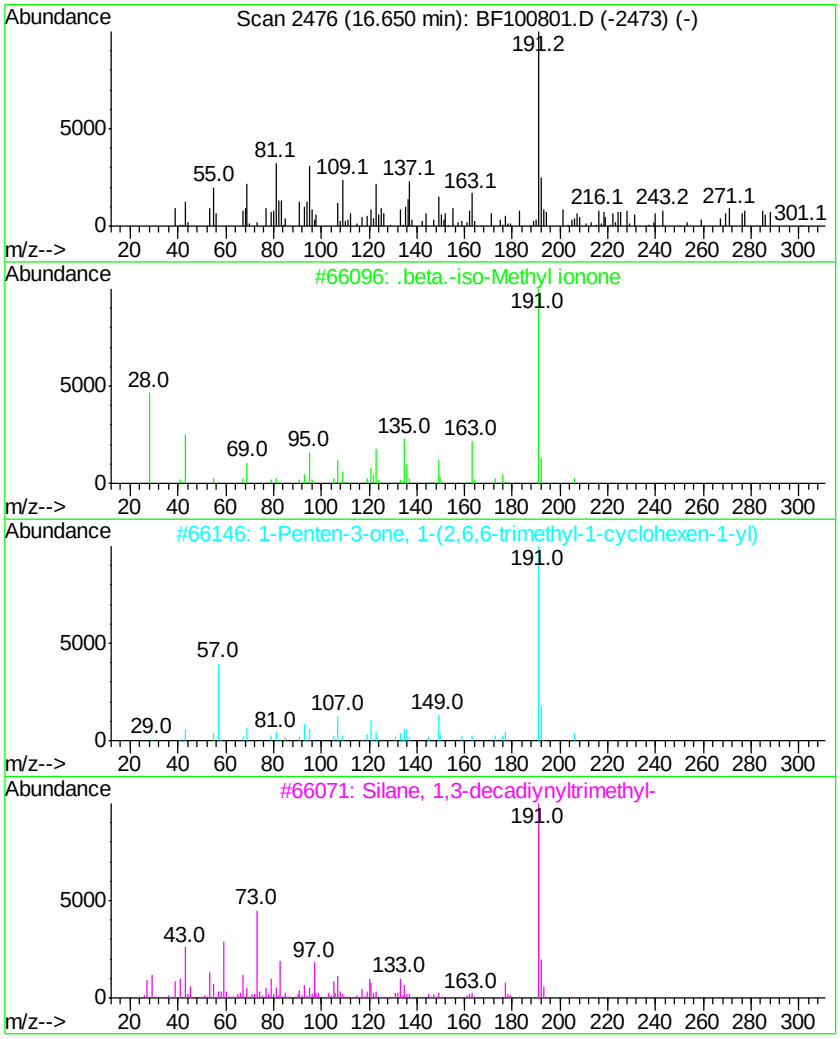
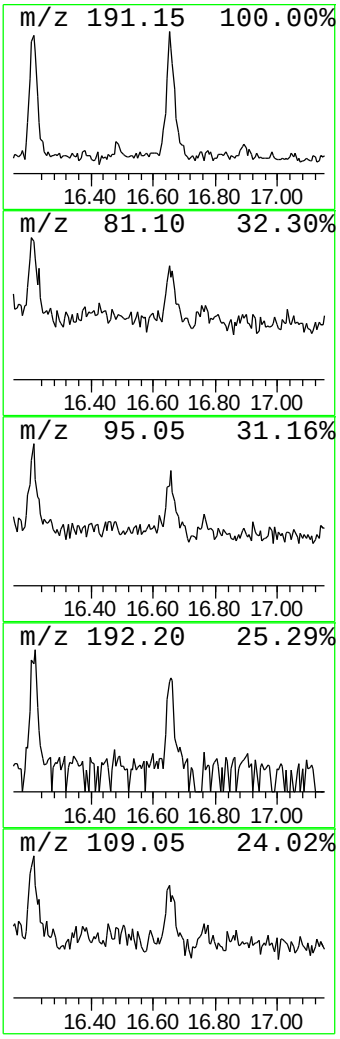
Peak Number 10 .beta.-iso-Methyl ionone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.65	5.06 ng	122933	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	58
2	1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	55
3	Silane, 1,3-decadiynyltrimethyl-	206	C13H22Si	084751-17-7	38
4	3-Buten-2-one, 4-(2,5,6,6-tetram...	206	C14H22O	000079-70-9	38
5	Quinoline, 2-chloro-4,8-dimethyl-	191	C11H10ClN	1000337-72-5	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112117\
Data File : BF100801.D
Acq On : 22 Nov 2017 1:33
Operator : SJ/JU
Sample : I6466-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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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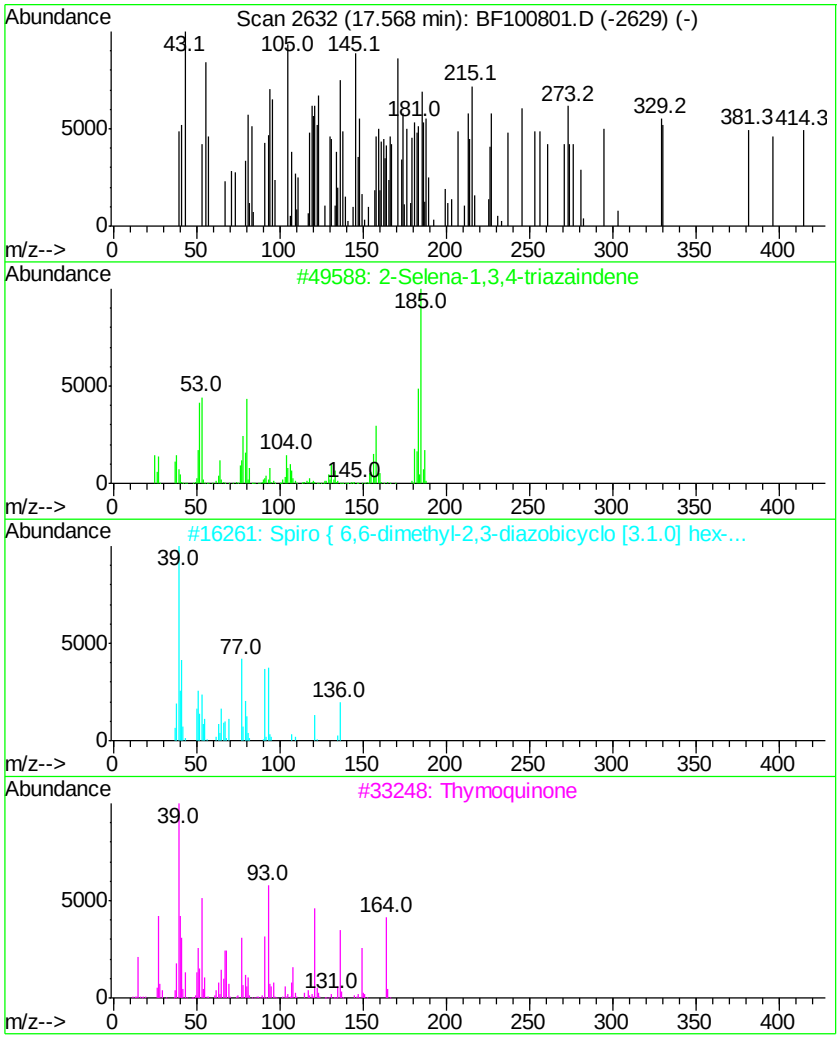
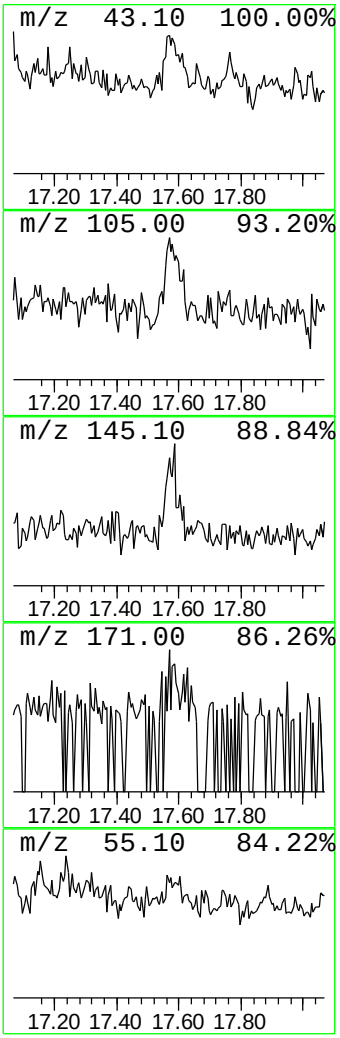
Peak Number 11 unknown17.57 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.57	2.05 ng	49736	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Selena-1,3,4-triazaindene	185	C5H3N3Se	021381-57-7	32
2	Spiro { 6,6-dimethyl-2,3-diazobi...	136	C8H12N2	135485-30-2	14
3	Thymoquinone	164	C10H12O2	000490-91-5	10
4	Sebacic acid, heptyl 2-heptyl ester	398	C24H46O4	1000355-55-3	9
5	Sebacic acid, 3,3-dimethylbut-2-...	384	C23H44O4	1000355-60-1	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112117\
Data File : BF100801.D
Acq On : 22 Nov 2017 1:33
Operator : SJ/JU
Sample : I6466-05
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CHAP-4-E(3-4)

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...	5.10	13.3	ng	338610	1	6.87	508535	20.0
unknown6.65	6.65	73.4	ng	1865190	1	6.87	508535	20.0
2-Hydroxy-iso-but...	8.70	2.6	ng	85850	2	8.15	664472	20.0
Benzophenone	10.62	8.6	ng	300730	3	9.91	702301	20.0
n-Hexadecanoic acid	11.92	3.1	ng	96944	4	11.40	618730	20.0
Heptafluorobutyri...	13.86	4.6	ng	134614	5	14.03	590669	20.0
Benzo[e]pyrene	15.38	2.0	ng	48624	6	15.51	485657	20.0
unknown16.22	16.22	7.0	ng	170416	6	15.51	485657	20.0
.beta.-iso-Methyl...	16.65	5.1	ng	122933	6	15.51	485657	20.0
unknown17.57	17.57	2.0	ng	49736	6	15.51	485657	20.0