LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF030218\
Data File : BF103387.D
Acq On : 3 Mar 2018 1:00
Operator : SJ/JU
Sample : J1724-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-13

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-BF022218.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	2.116	3	5	13	rVB	176744	189230	4.98%	0.512%
2	4.481	403	407	416	rBV	37832	64098	1.69%	0.173%
3	5.110	511	514	526	rVB	111772	155087	4.08%	0.419%
4	5.504	576	581	603	rVB	3426635	3722786	97.94%	10.064%
5	6.516	749	753	772	rBV	3035616	3801216	100.00%	10.276%
6	6.651	772	776	782	rVV	3598243	3521636	92.64%	9.521%
7	6.698	782	784	790	rVB3	46859	47765	1.26%	0.129%
8	6.875	811	814	821	rBV	1143577	997710	26.25%	2.697%
9	7.034	837	841	850	rBV	2798497	2639208	69.43%	7.135%
10	7.445	907	911	926	rBV	2440765	2421638	63.71%	6.547%
11	8.163	1029	1033	1035	rBV	1361697	1228417	32.32%	3.321%
12	8.875	1152	1154	1161	rVB	65227	70332	1.85%	0.190%
13	9.234	1211	1215	1224	rBV	3144782	3091138	81.32%	8.357%
14	9.304	1224	1227	1230	rVV	99461	94319	2.48%	0.255%
15	9.339	1230	1233	1238	rVV2	39702	44895	1.18%	0.121%
16	9.504	1257	1261	1265	rBV2	30434	43587	1.15%	0.118%
17	9.575	1269	1273	1276	rVV2	46137	56179	1.48%	0.152%
18	9.628	1276	1282	1289	rVB	253794	317226	8.35%	0.858%
19	9.692	1289	1293	1298	rBV4	19534	38136	1.00%	0.103%
20	9.781	1304	1308	1313	rBV	83159	102087	2.69%	0.276%
21	9.833	1313	1317	1320	rVB	174259	153093	4.03%	0.414%
22	9.922	1328	1332	1335	rBV	1149541	1062521	27.95%	2.872%
23	9.951	1335	1337	1340	rVB	114506	96535	2.54%	0.261%
24	10.069	1353	1357	1359	rBV4	29737	41146	1.08%	0.111%
25	10.122	1363	1366	1369	rBV2	84535	95408	2.51%	0.258%
26	10.157	1369	1372	1376	rVB3	62116	64836	1.71%	0.175%
27	10.233	1381	1385	1388	rBV	53215	67679	1.78%	0.183%
28	10.333	1396	1402	1405	rBV	193019	190351	5.01%	0.515%
29	10.469	1422	1425	1431	rVB2	72395	85587	2.25%	0.231%
30	10.551	1434	1439	1442	rBV2	80207	84467	2.22%	0.228%
31	10.716	1463	1467	1479	rBV	1404220	1519189	39.97%	4.107%
32	10.804	1479	1482	1493	rVB3	142996	243303	6.40%	0.658%
33	11.016	1513	1518	1521	rBV6	36001	61831	1.63%	0.167%
34	11.169	1542	1544	1549	rVB5	34984	38426	1.01%	0.104%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
ClientSampleId : SP-13

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-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.222	1550	1553	1556	rVV2	44218	49302	1.30%	0.133%
36	11.257	1556	1559	1561	rVV	116970	108815	2.86%	0.294%
37	11.286	1561	1564	1566	rVV2	60538	72247	1.90%	0.195%
38	11.310	1566	1568	1572	rVB	56715	56006	1.47%	0.151%
39	11.416	1582	1586	1588	rBV	930874	946838	24.91%	2.560%
40	11.439	1588	1590	1594	rVV	652697	548908	14.44%	1.484%
41	11.492	1595	1599	1603	rVV	163826	162967	4.29%	0.441%
42	11.651	1621	1626	1629	rBV2	76066	109448	2.88%	0.296%
43	11.680	1629	1631	1633	rVB	54655	41424	1.09%	0.112%
44	11.745	1640	1642	1647	rVB2	35995	38041	1.00%	0.103%
45	11.922	1668	1672	1674	rBV2	207024	250781	6.60%	0.678%
46	11.945	1674	1676	1680	rVB	145732	126676	3.33%	0.342%
47	11.992	1682	1684	1687	rVB	58577	48464	1.27%	0.131%
48	12.027	1687	1690	1693	rBV	160225	191314	5.03%	0.517%
49	12.092	1698	1701	1704	rBV2	49168	46201	1.22%	0.125%
50	12.210	1718	1721	1723	rBV2	83542	76221	2.01%	0.206%
51	12.245	1725	1727	1732	rVB4	68084	74502	1.96%	0.201%
52	12.463	1762	1764	1768	rBV2	92462	124156	3.27%	0.336%
53	12.563	1777	1781	1783	rBV2	68796	86457	2.27%	0.234%
54	12.633	1789	1793	1796	rBV	1168520	1039663	27.35%	2.811%
55	12.863	1826	1832	1838	rBV	1096633	1259181	33.13%	3.404%
56	12.910	1838	1840	1845	rVV2	63533	78089	2.05%	0.211%
57	12.998	1851	1855	1858	rBV	1979013	1873115	49.28%	5.064%
58	13.027	1858	1860	1863	rVB	58046	53801	1.42%	0.145%
59	13.192	1886	1888	1893	rVB2	148318	157384	4.14%	0.425%
60	13.257	1897	1899	1901	rVB	66265	52453	1.38%	0.142%
61	13.710	1973	1976	1979	rVB	87423	87133	2.29%	0.236%
62	13.816	1992	1994	1996	rBV	82599	58250	1.53%	0.157%
63	13.874	2001	2004	2009	rBV4	426067	517386	13.61%	1.399%
64	14.069	2032	2037	2039	rBV2	769832	1096301	28.84%	2.964%
65	14.092	2039	2041	2047	rVB	456991	418530	11.01%	1.131%
66	15.133	2215	2218	2221	rBV	265028	371573	9.78%	1.005%
67	15.580	2291	2294	2297	rVB	283844	316732	8.33%	0.856%

Sum of corrected areas: 36989421

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Misc :
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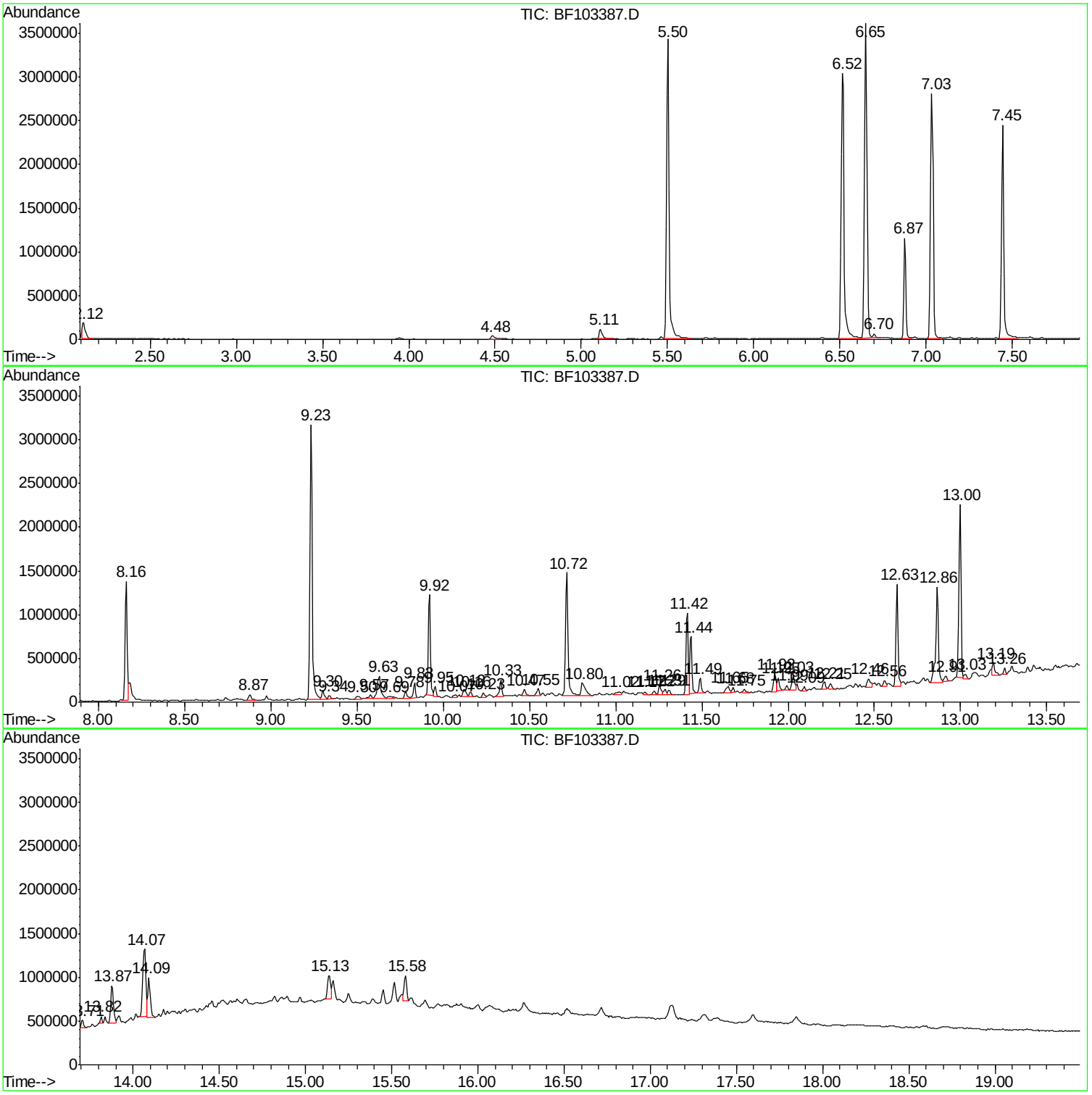
Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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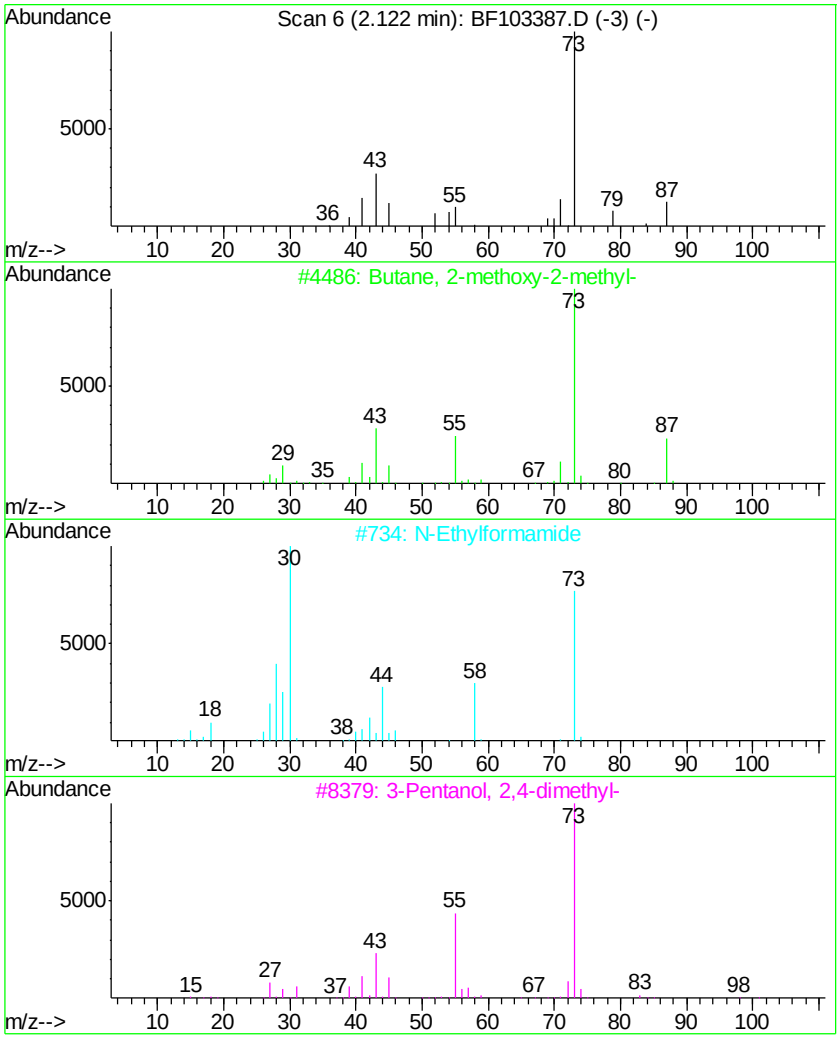
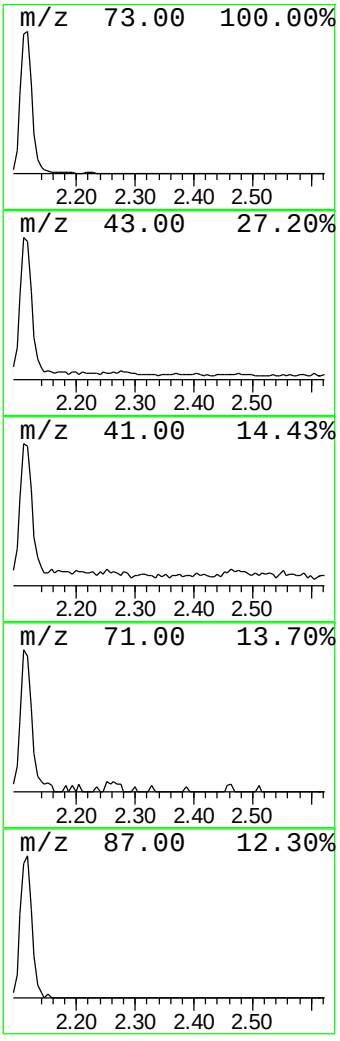
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	3.79 ng	189230	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	N-Ethylformamide	73	C3H7NO	000627-45-2	9
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9
5	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9





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Data File : BF103387.D
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Operator : SJ/JU
Sample : J1724-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

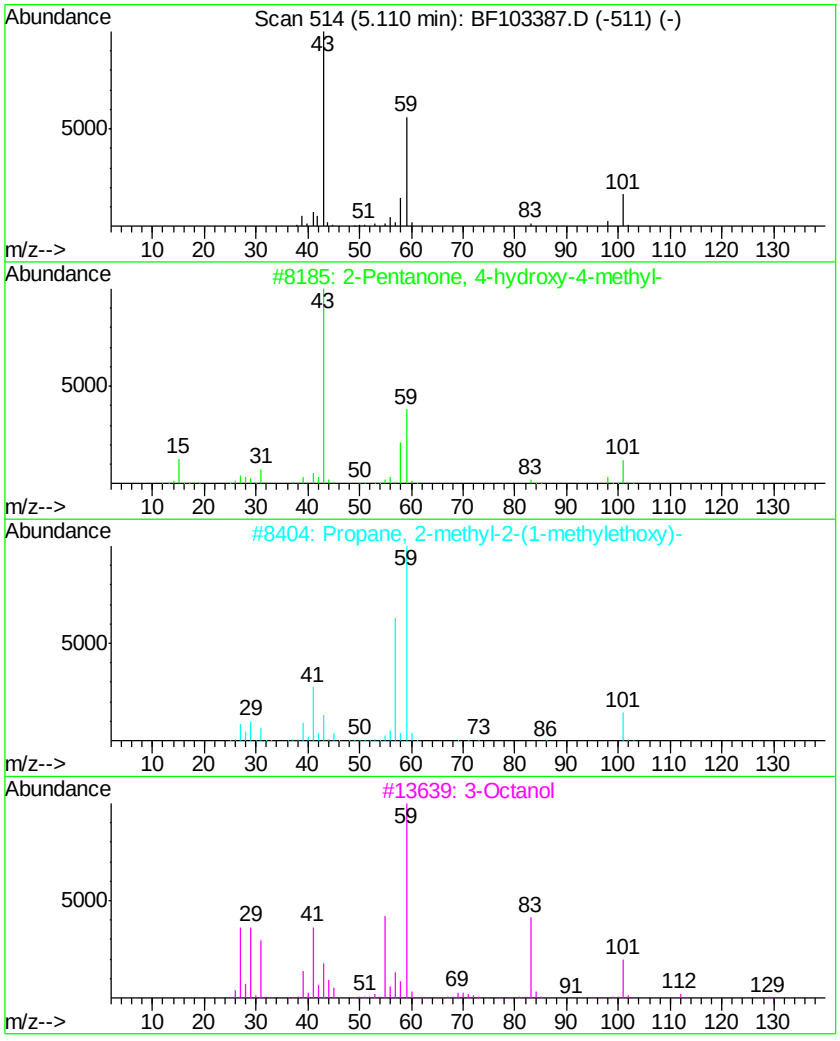
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

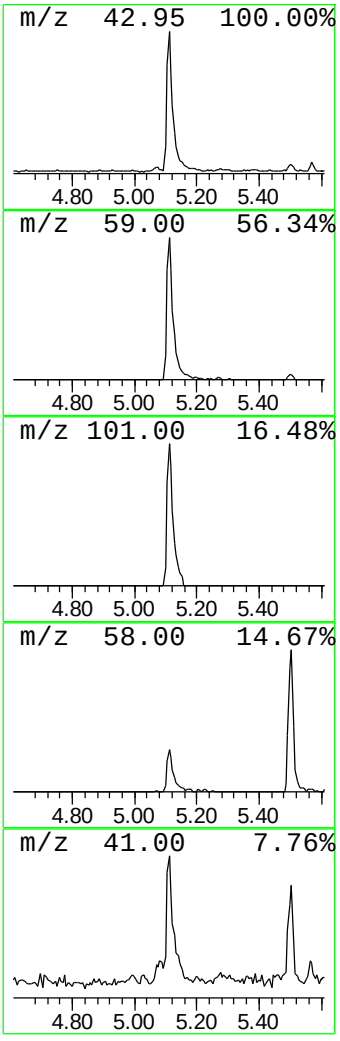
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	3.11 ng	155087	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	53
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Octanol	130	C8H18O	000589-98-0	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23





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Misc :
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Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
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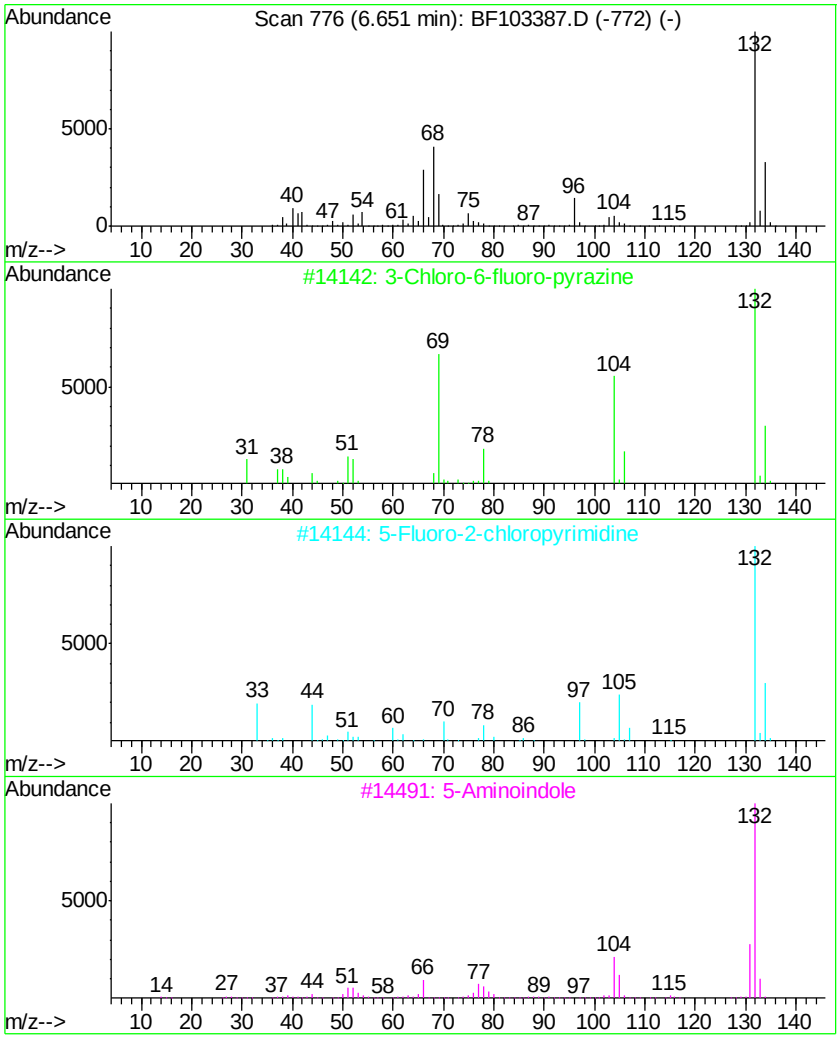
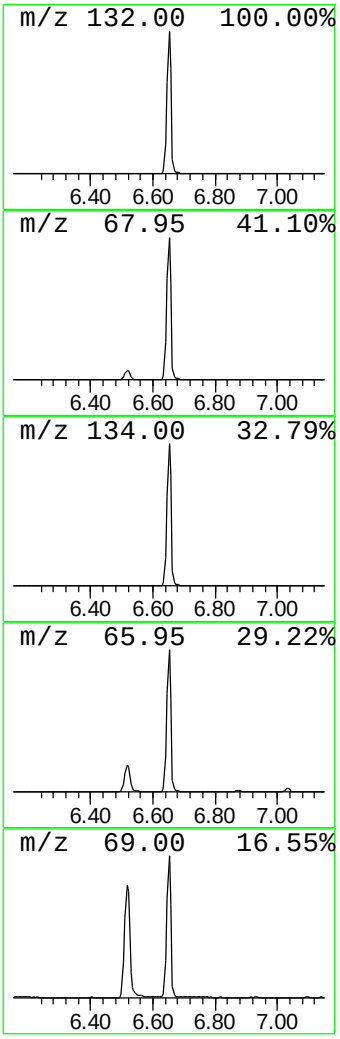
Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	70.59 ng	3521640	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
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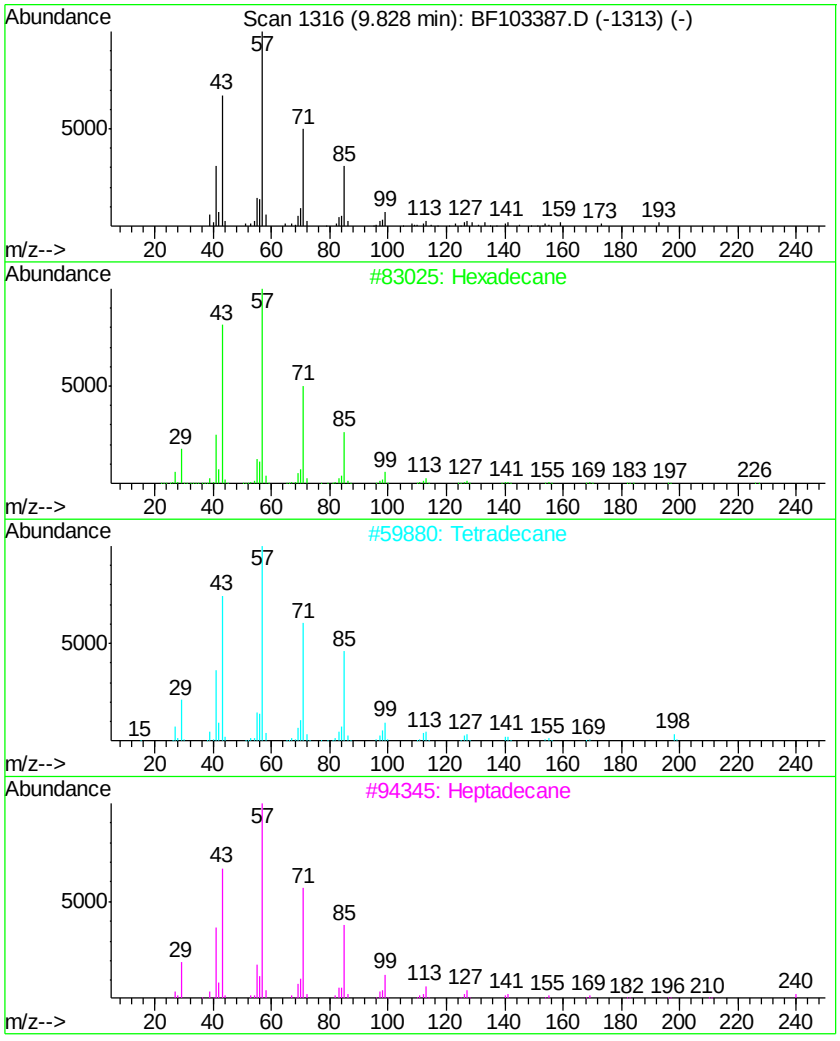
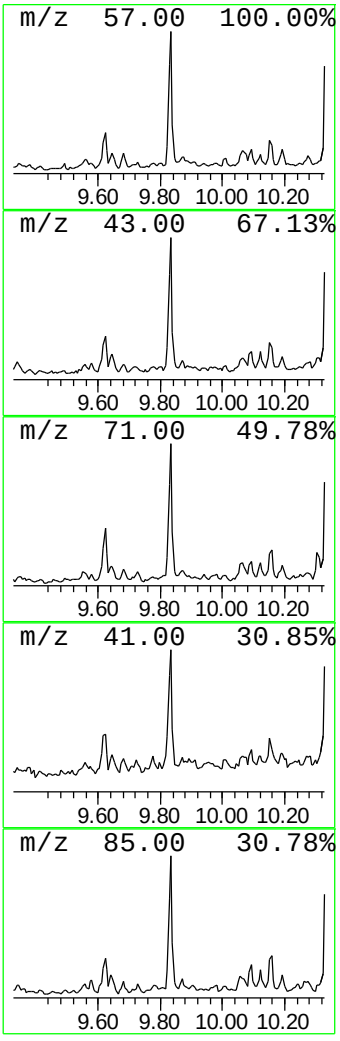
Peak Number 5 Hexadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.88 ng	153093	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Tetradecane	198	C14H30	000629-59-4	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Tetratetracontane	619	C44H90	007098-22-8	83
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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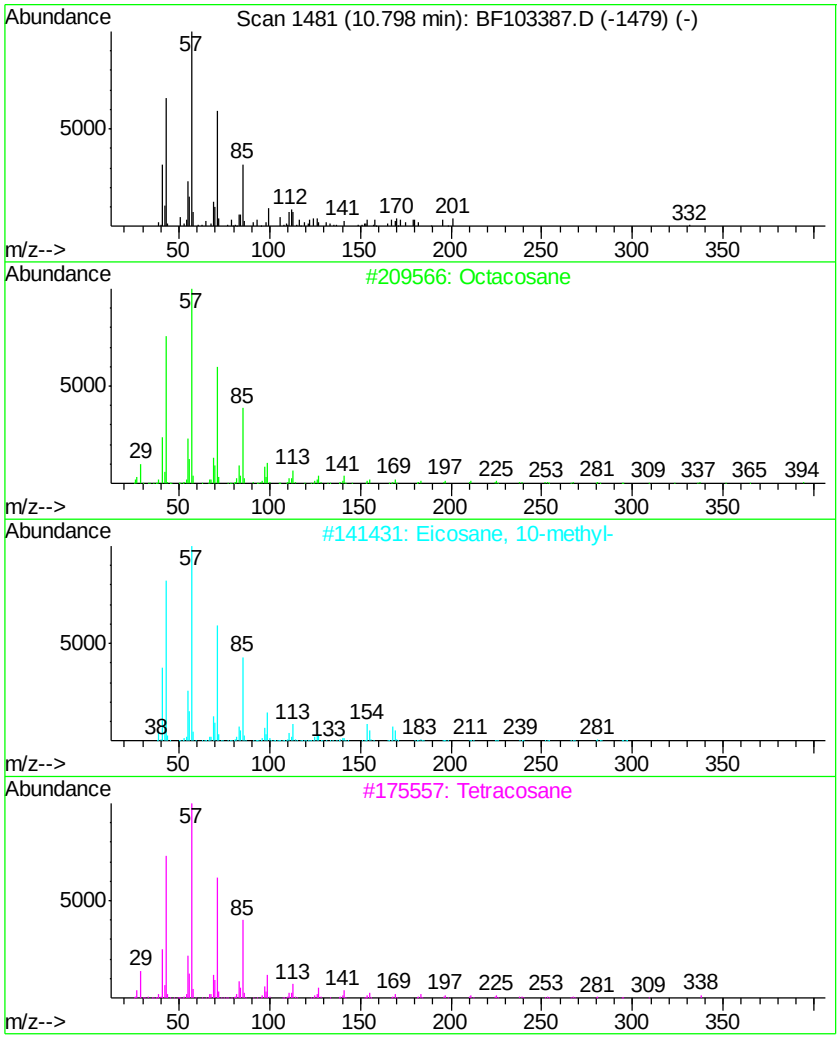
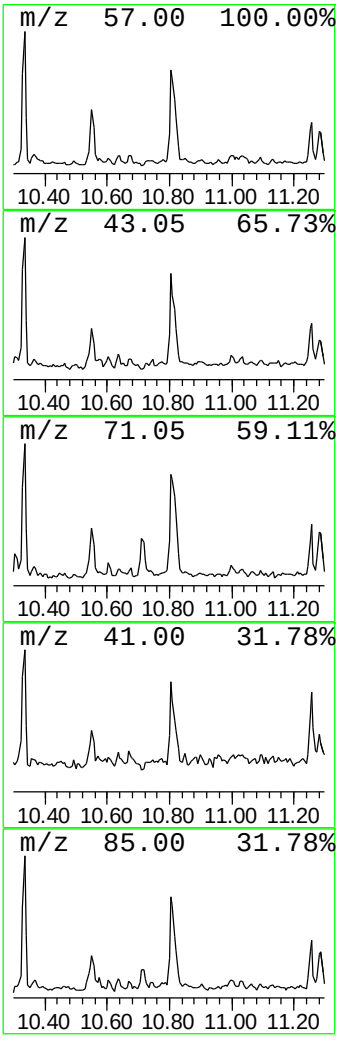
Peak Number 7 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	5.14 ng	243303	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Hexadecane	226	C16H34	000544-76-3	90
5	Heptadecane	240	C17H36	000629-78-7	80





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TIC Library : C:\DATABASE\NIST11.L
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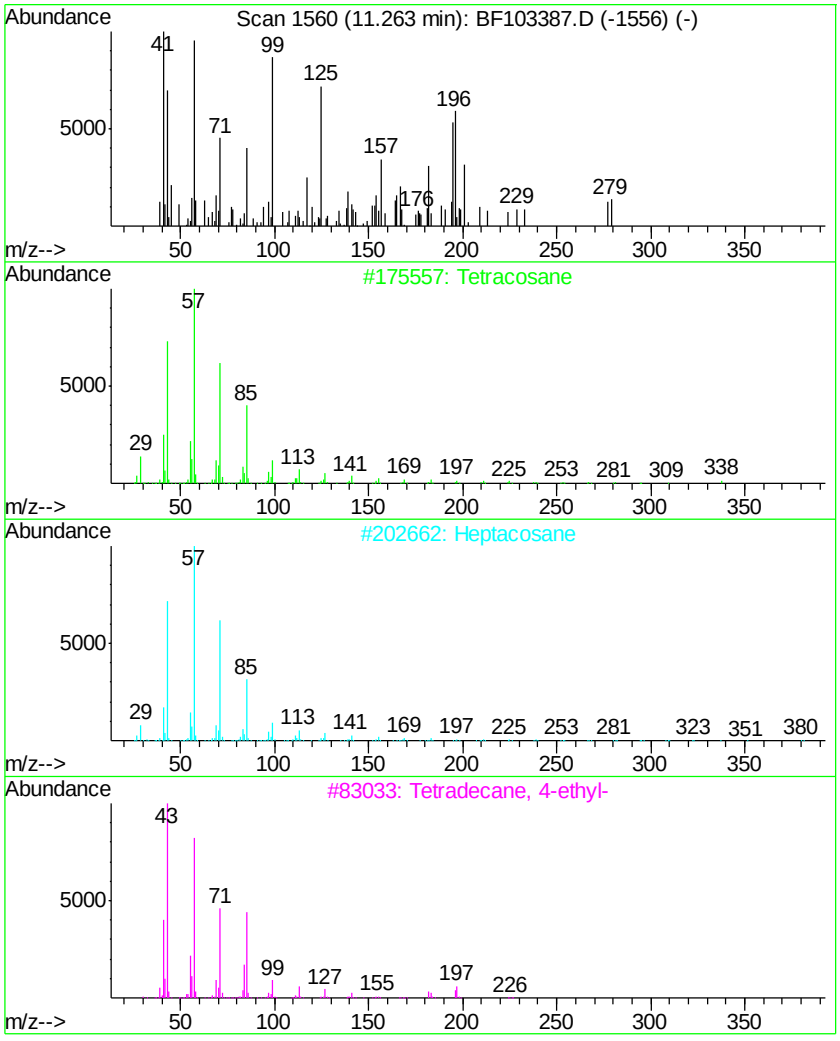
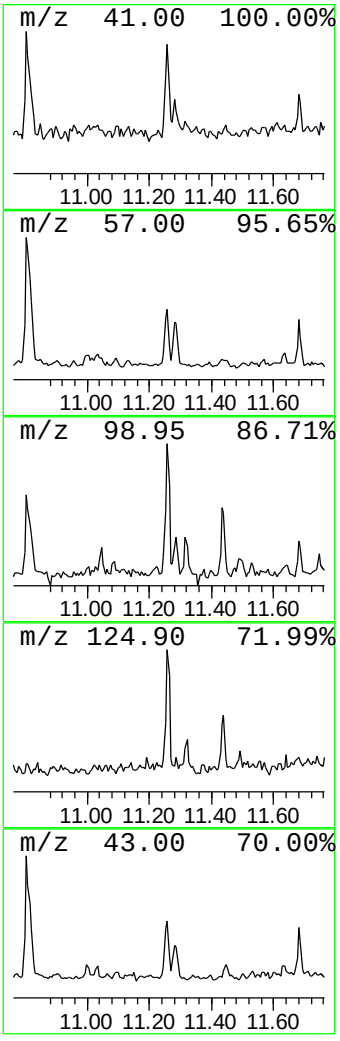
Peak Number 8 unknown11.26 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.26	2.30 ng	108815	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	38
2	Heptacosane	380	C27H56	000593-49-7	38
3	Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	35
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	30
5	Hexadecane	226	C16H34	000544-76-3	30





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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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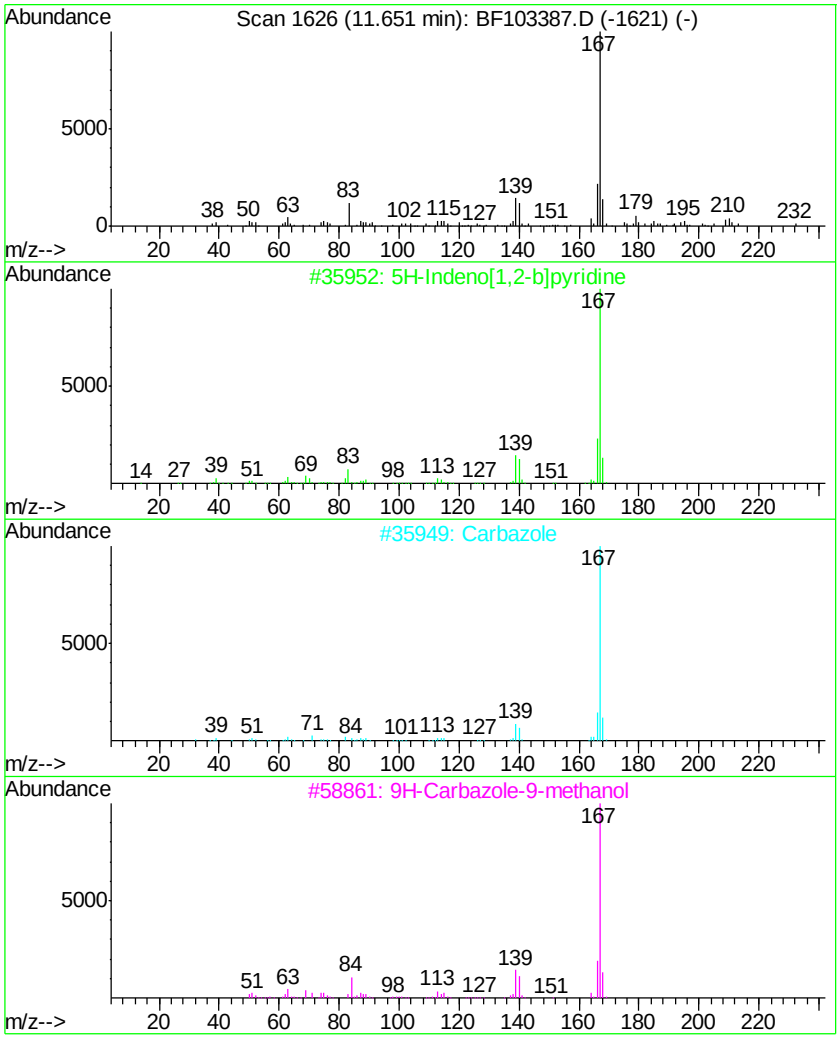
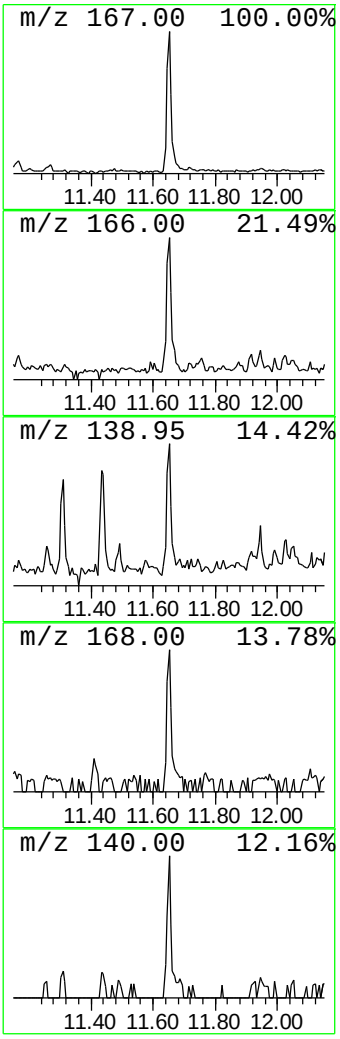
Peak Number 9 5H-Indeno[1,2-b]pyridine Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	2.31 ng	109448	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Indeno[1,2-b]pyridine	167	C12H9N	000244-99-5	87
2	Carbazole	167	C12H9N	000086-74-8	87
3	9H-Carbazole-9-methanol	197	C13H11NO	002409-36-1	83
4	9H-Carbazole, 9-nitroso-	196	C12H8N2O	002788-23-0	83
5	1,1'-Biphenyl, 2-azido-	195	C12H9N3	007599-23-7	83





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Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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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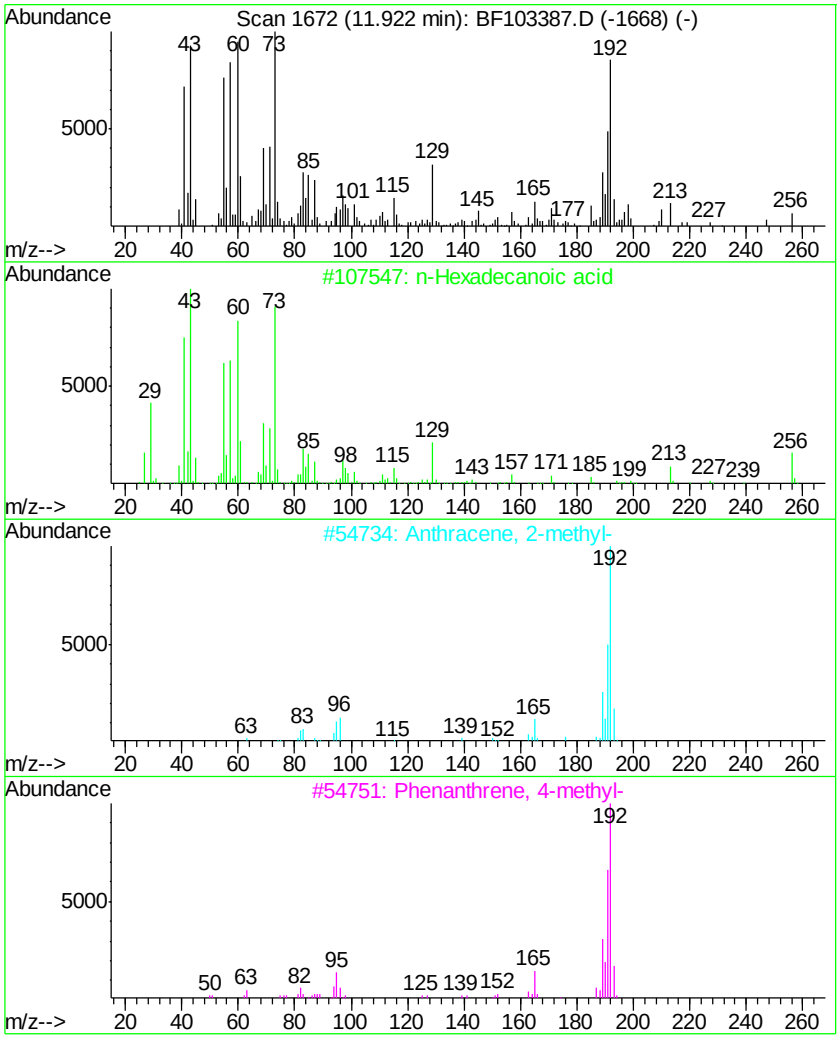
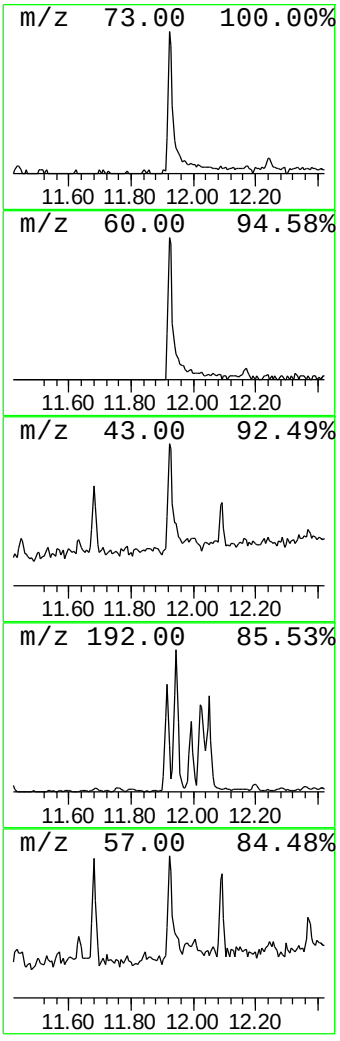
Peak Number 10 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	5.30 ng	250781	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	83
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	74
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	55
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	51





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Acq On : 3 Mar 2018 1:00
Operator : SJ/JU
Sample : J1724-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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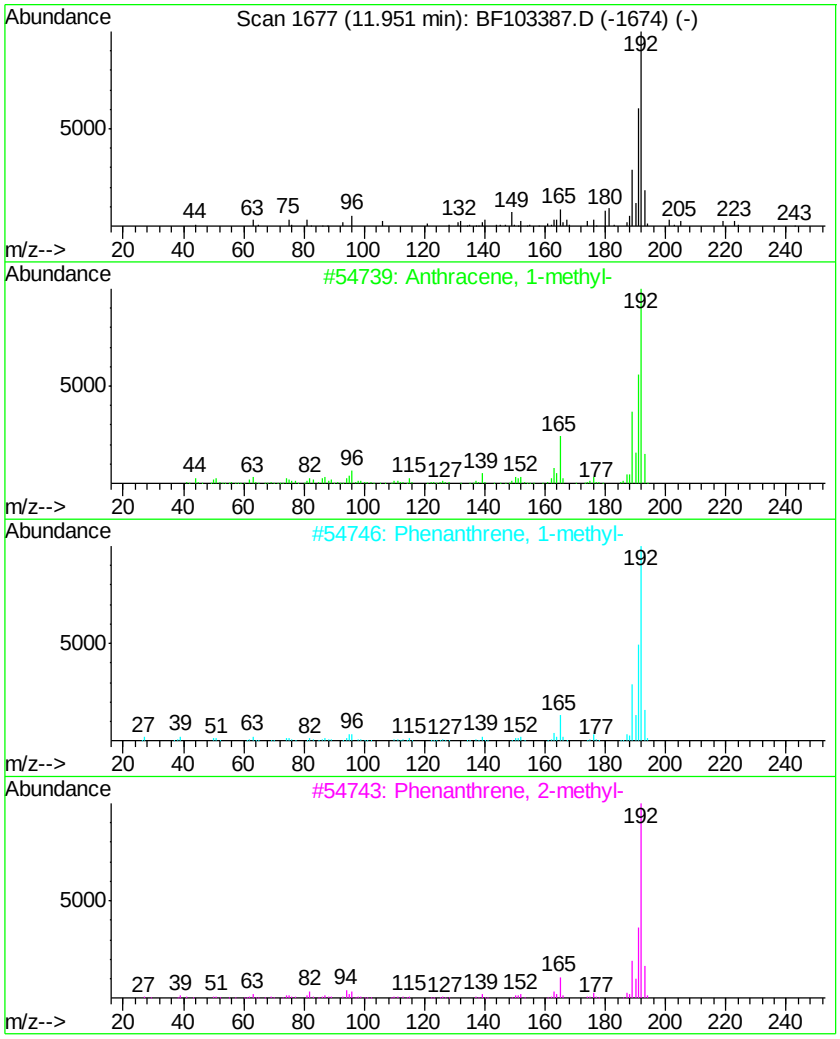
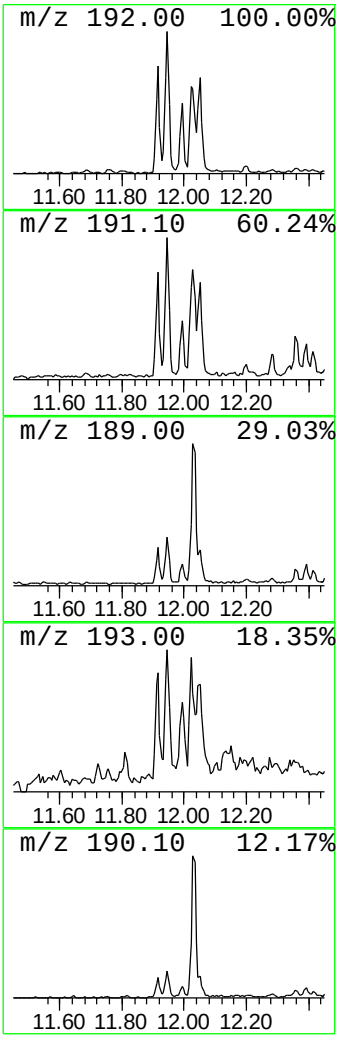
Peak Number 11 Anthracene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	2.68 ng	126676	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	81
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	81





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Sample : J1724-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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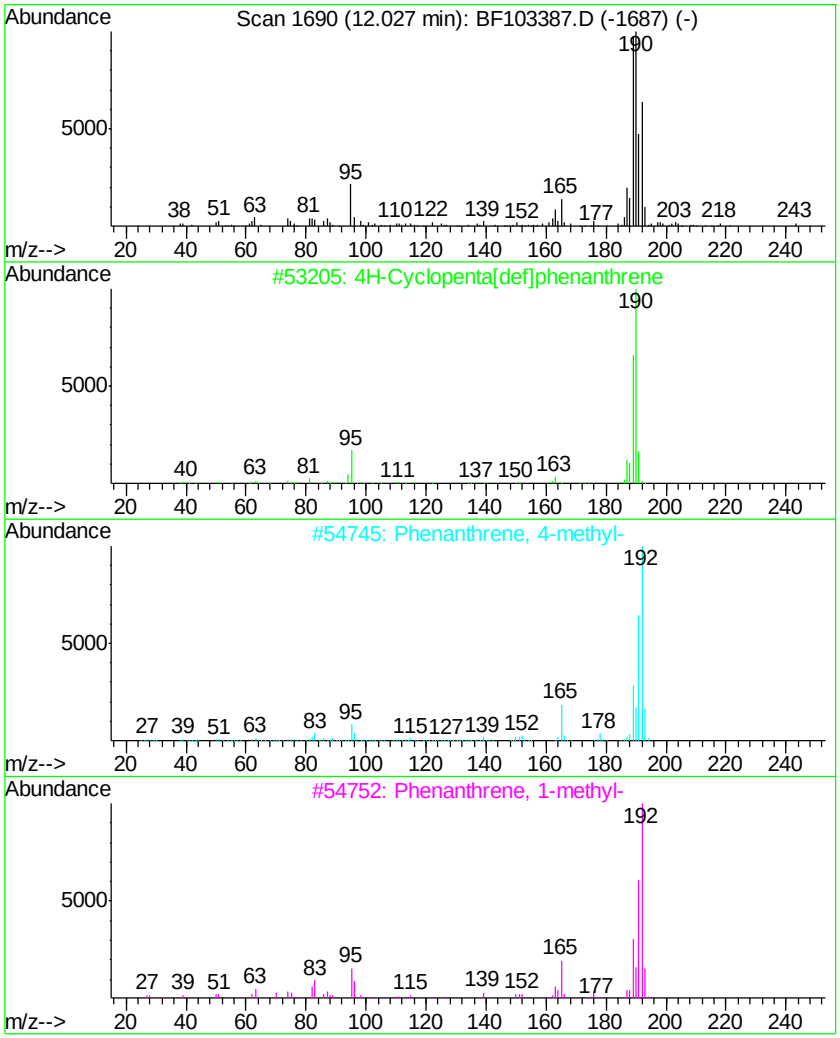
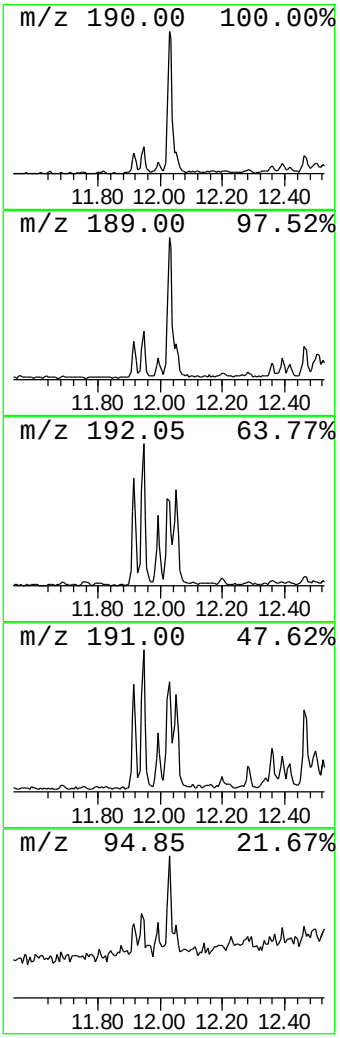
Peak Number 12 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	4.04 ng	191314	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	35
5	1a,9b-Dihydro-1H-cyclopropa[a]an...	192	C15H12	006109-24-6	30





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Acq On : 3 Mar 2018 1:00
Operator : SJ/JU
Sample : J1724-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-13

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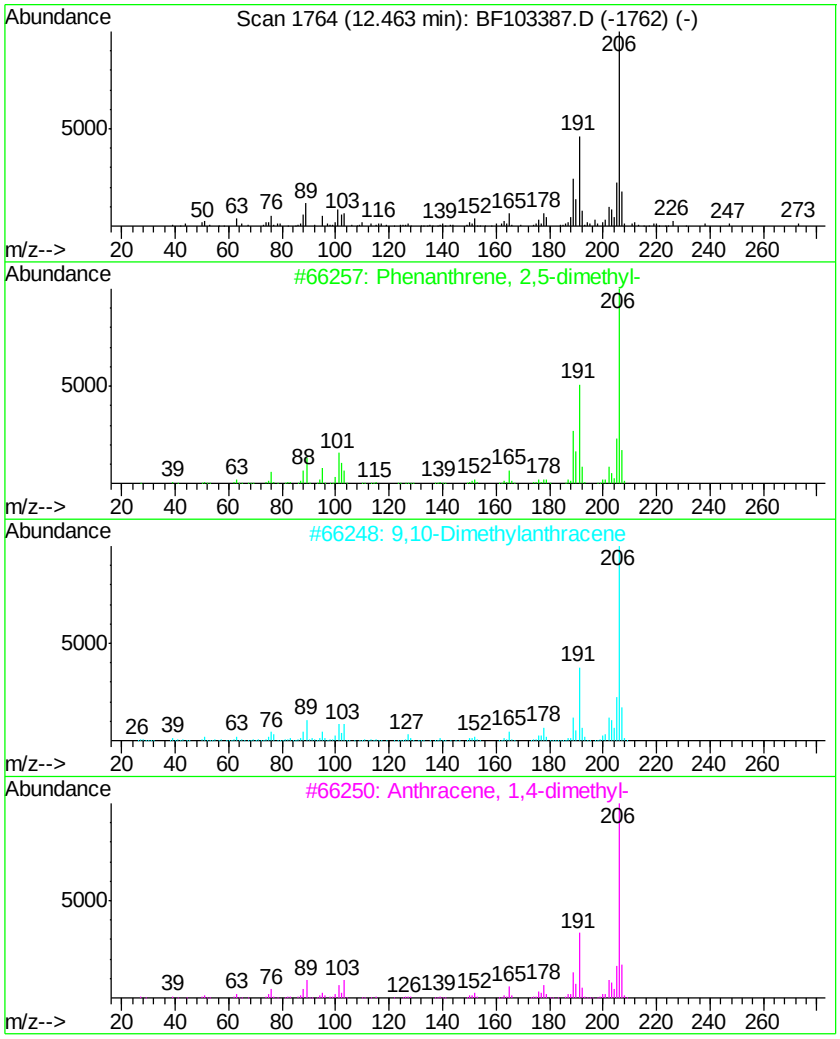
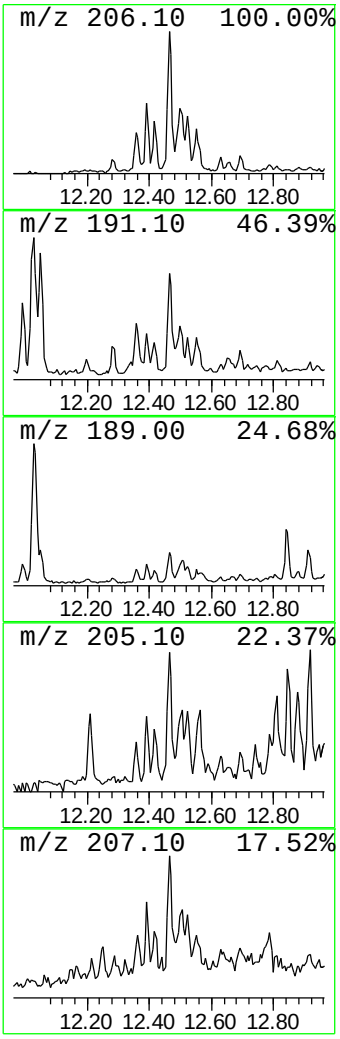
Peak Number 13 Phenanthrene, 2,5-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	2.62 ng	124156	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	97
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	95
3	Anthracene, 1,4-dimethyl-	206	C16H14	000781-92-0	93
4	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	91
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90





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Operator : SJ/JU
Sample : J1724-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Integration Parameters: LSCINT.P

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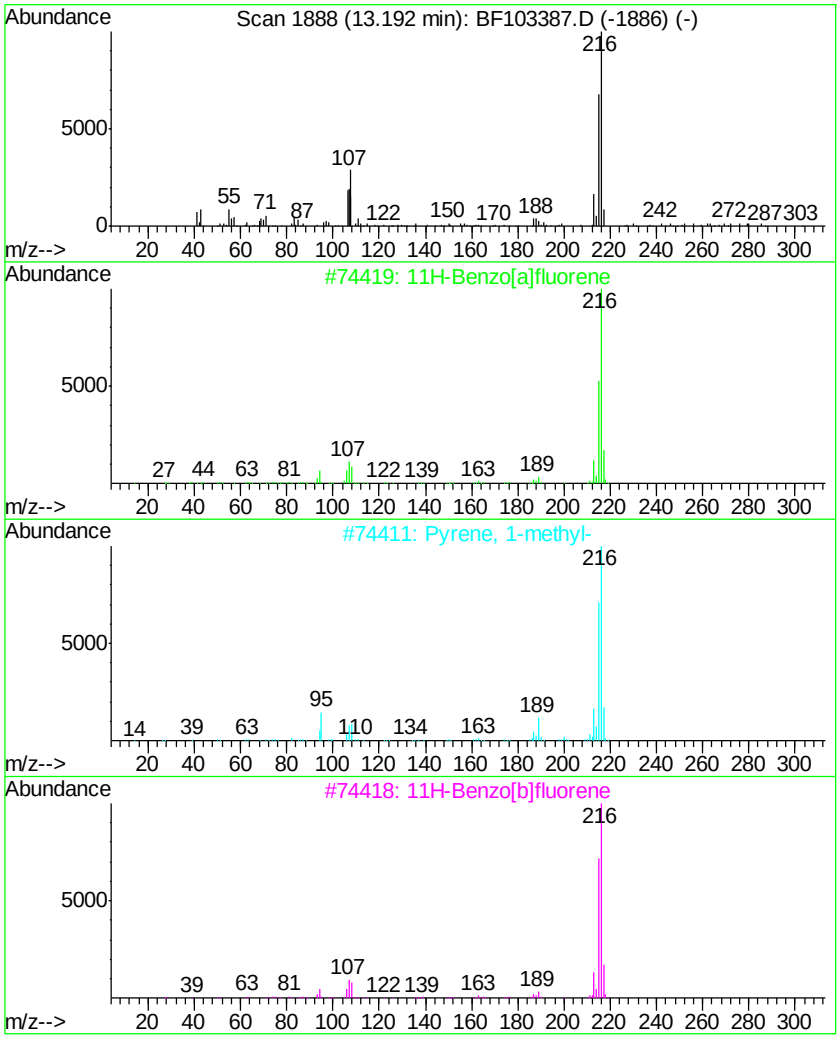
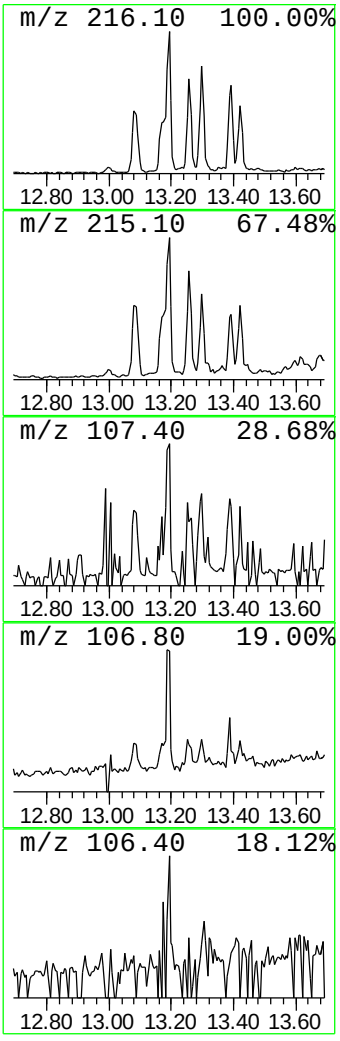
Peak Number 14 11H-Benzo[a]fluorene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.87 ng	157384	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	64
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	59
3	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	59
4	Pyrene, 2-methyl-	216	C17H12	003442-78-2	59
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	53





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Operator : SJ/JU
Sample : J1724-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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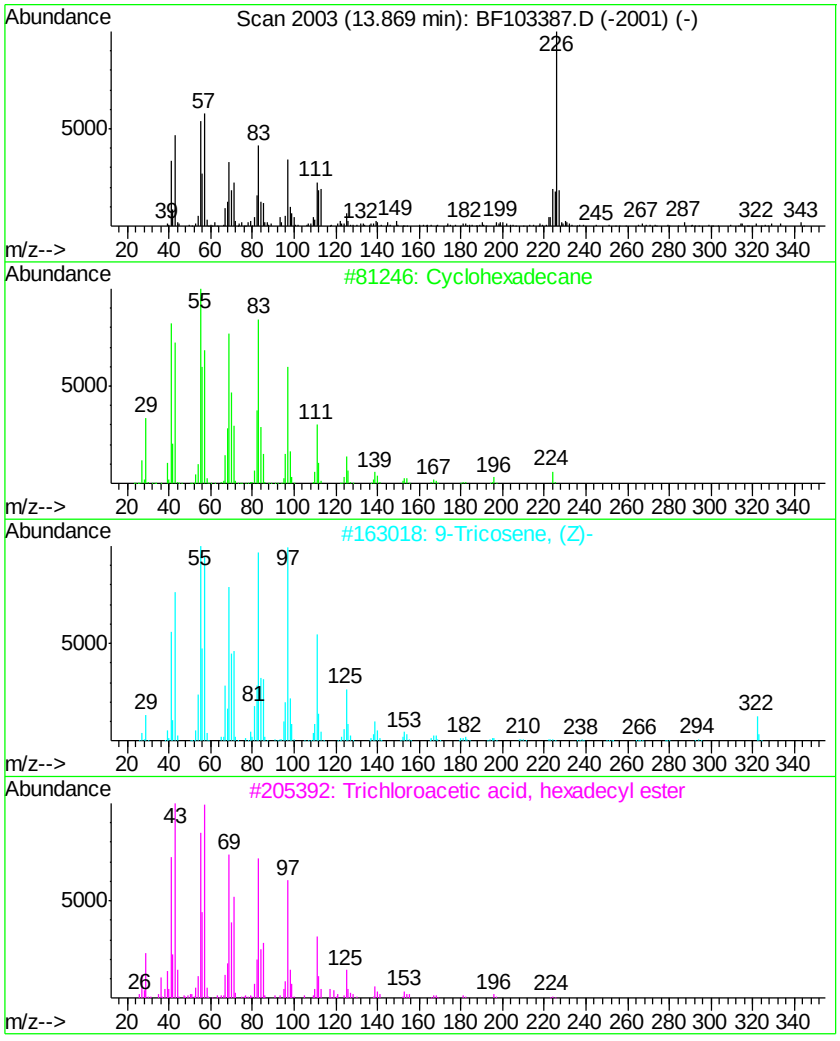
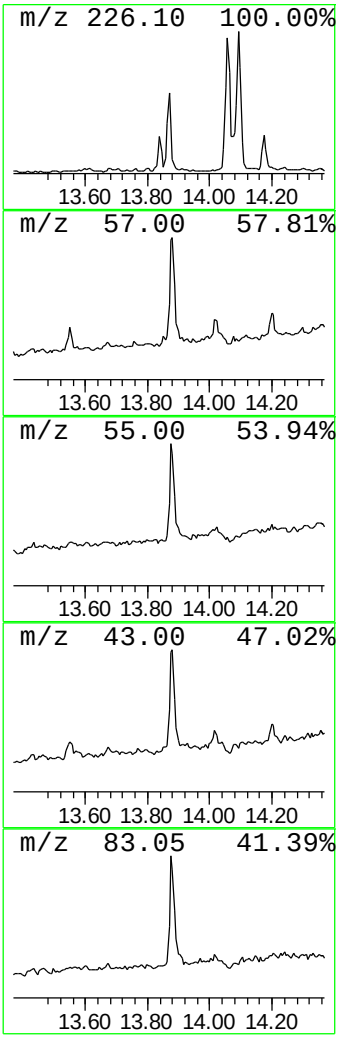
Peak Number 15 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	9.44 ng	517386	Chrysene-d12	14.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	95
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF030218\
Data File : BF103387.D
Acq On : 3 Mar 2018 1:00
Operator : SJ/JU
Sample : J1724-07
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-13

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.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
Butane, 2-methoxy...	2.12	3.8	ng	189230	1	6.87	997710	20.0
2-Pentanone, 4-hy...	5.11	3.1	ng	155087	1	6.87	997710	20.0
unknown6.65	6.65	70.6	ng	3521640	1	6.87	997710	20.0
Hexadecane	9.83	2.9	ng	153093	3	9.92	1062520	20.0
Octacosane	10.80	5.1	ng	243303	4	11.42	946838	20.0
unknown11.26	11.26	2.3	ng	108815	4	11.42	946838	20.0
5H-Indeno[1,2-b]p...	11.65	2.3	ng	109448	4	11.42	946838	20.0
n-Hexadecanoic acid	11.92	5.3	ng	250781	4	11.42	946838	20.0
Anthracene, 1-met...	11.95	2.7	ng	126676	4	11.42	946838	20.0
4H-Cyclopenta[def...	12.03	4.0	ng	191314	4	11.42	946838	20.0
Phenanthrene, 2,5...	12.46	2.6	ng	124156	4	11.42	946838	20.0
11H-Benzo[a]fluorene	13.19	2.9	ng	157384	5	14.07	1096300	20.0
Cyclohexadecane	13.87	9.4	ng	517386	5	14.07	1096300	20.0