LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102564.D
Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

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-BF012218.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	4.916	477	481	488	rBV	65844	91504	2.61%	0.210%
2	5.328	546	551	571	rBV	3122052	3376055	96.27%	7.764%
3	6.363	722	727	743	rBV	2968680	3506917	100.00%	8.065%
4	6.486	743	748	751	rBV	3537252	3359472	95.80%	7.725%
5	6.710	783	786	793	rBV	1140698	954146	27.21%	2.194%
6	6.869	809	813	816	rBV	2913919	2637493	75.21%	6.065%
7	7.281	879	883	886	rBV	2219179	2101562	59.93%	4.833%
8	7.304	886	887	892	rVB	130472	85329	2.43%	0.196%
9	7.733	957	960	963	rBV3	79142	72289	2.06%	0.166%
10	7.992	1001	1004	1010	rVB	1359240	1215246	34.65%	2.795%
11	8.051	1011	1014	1017	rVB	62066	60961	1.74%	0.140%
12	8.280	1046	1053	1058	rBV9	24486	51152	1.46%	0.118%
13	8.410	1071	1075	1077	rBV	80894	65343	1.86%	0.150%
14	8.580	1101	1104	1107	rBV	135866	106526	3.04%	0.245%
15	8.710	1123	1126	1132	rVB	82646	83077	2.37%	0.191%
16	8.804	1139	1142	1145	rVB	45311	37505	1.07%	0.086%
17	9.069	1182	1187	1190	rBV	3907710	3457563	98.59%	7.951%
18	9.145	1197	1200	1202	rBV	108116	76209	2.17%	0.175%
19	9.333	1229	1232	1236	rBV2	29875	38315	1.09%	0.088%
20	9.404	1241	1244	1246	rBV2	33892	37285	1.06%	0.086%
21	9.463	1251	1254	1262	rVB	511401	464686	13.25%	1.069%
22	9.674	1286	1290	1293	rBV	152138	121219	3.46%	0.279%
23	9.745	1298	1302	1305	rVV	1471776	1256020	35.82%	2.888%
24	9.774	1305	1307	1311	rVB	190844	165921	4.73%	0.382%
25	9.951	1335	1337	1341	rVB	75053	69277	1.98%	0.159%
26	9.992	1341	1344	1348	rVB3	42953	45695	1.30%	0.105%
27	10.174	1372	1375	1377	rVB	161088	134579	3.84%	0.309%
28	10.292	1392	1395	1401	rBV	177483	155742	4.44%	0.358%
29	10.386	1408	1411	1415	rBV2	43196	62884	1.79%	0.145%
30	10.539	1433	1437	1446	rVB	1734389	1690995	48.22%	3.889%
31	10.645	1452	1455	1464	rVB	149810	176719	5.04%	0.406%
32	10.839	1484	1488	1491	rBV3	37468	47071	1.34%	0.108%
33	11.092	1526	1531	1533	rBV2	74373	68514	1.95%	0.158%
34	11.127	1533	1537	1542	rVB2	79766	88879	2.53%	0.204%

LSC Area Percent Report

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Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

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-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.233	1551	1555	1557	rBV	1089516	1066177	30.40%	2.452%
36	11.257	1557	1559	1563	rVV	1387813	1100589	31.38%	2.531%
37	11.304	1564	1567	1571	rVV	343827	348254	9.93%	0.801%
38	11.345	1571	1574	1580	rVB	35266	46582	1.33%	0.107%
39	11.468	1590	1595	1601	rBV	155173	181039	5.16%	0.416%
40	11.521	1601	1604	1609	rVV3	40860	51076	1.46%	0.117%
41	11.733	1637	1640	1642	rBV	112287	97718	2.79%	0.225%
42	11.763	1642	1645	1648	rVB	141446	129549	3.69%	0.298%
43	11.845	1656	1659	1661	rBV	222259	215105	6.13%	0.495%
44	11.863	1661	1662	1668	rVB	69839	61486	1.75%	0.141%
45	11.921	1668	1672	1674	rBV3	34937	38815	1.11%	0.089%
46	12.027	1687	1690	1693	rVB	89163	68085	1.94%	0.157%
47	12.063	1693	1696	1701	rBV	60415	68228	1.95%	0.157%
48	12.280	1730	1733	1736	rBV	47550	54716	1.56%	0.126%
49	12.316	1736	1739	1742	rVV3	45702	49863	1.42%	0.115%
50	12.374	1745	1749	1753	rBV3	36267	54097	1.54%	0.124%
51	12.445	1755	1761	1765	rBV	1537649	1408078	40.15%	3.238%
52	12.592	1781	1786	1789	rBV3	50805	66867	1.91%	0.154%
53	12.674	1794	1800	1805	rBV	1210349	1334393	38.05%	3.069%
54	12.721	1805	1808	1814	rVB	59073	71046	2.03%	0.163%
55	12.815	1817	1824	1827	rBV	2361009	2249800	64.15%	5.174%
56	12.886	1833	1836	1841	rVB3	62078	101879	2.91%	0.234%
57	12.974	1848	1851	1853	rBV2	62621	77671	2.21%	0.179%
58	13.004	1853	1856	1859	rVB	191994	175321	5.00%	0.403%
59	13.068	1864	1867	1870	rBV	177325	157186	4.48%	0.361%
60	13.104	1870	1873	1876	rBV2	99768	103282	2.95%	0.238%
61	13.198	1886	1889	1892	rBV2	51504	40025	1.14%	0.092%
62	13.227	1892	1894	1898	rBV2	45287	54994	1.57%	0.126%
63	13.380	1916	1920	1922	rBV4	40310	55359	1.58%	0.127%
64	13.515	1940	1943	1949	rVB	50403	53867	1.54%	0.124%
65	13.621	1958	1961	1963	rBV	100885	95611	2.73%	0.220%
66	13.645	1963	1965	1967	rVV	115158	98431	2.81%	0.226%
67	13.674	1967	1970	1971	rVV	82515	86703	2.47%	0.199%
68	13.710	1973	1976	1985	rVB3	290446	391665	11.17%	0.901%
69	13.868	1995	2003	2006	rBV2	1100291	1752162	49.96%	4.029%
70	13.898	2006	2008	2016	rVV	663707	585719	16.70%	1.347%
71	13.974	2016	2021	2024	rVV2	168632	188245	5.37%	0.433%

LSC Area Percent Report

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
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Start Thrs: 0.2 Max Peaks: 100
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Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	14.021	2027	2029	2035	rVV4	71659	108364	3.09%	0.249%
73	14.068	2035	2037	2041	rVV2	56285	80191	2.29%	0.184%
74	14.104	2041	2043	2046	rVB	72452	61057	1.74%	0.140%
75	14.221	2060	2063	2065	rBV	59940	57860	1.65%	0.133%
76	14.257	2067	2069	2072	rVB	106991	89674	2.56%	0.206%
77	14.351	2079	2085	2088	rBV4	107083	196671	5.61%	0.452%
78	14.404	2092	2094	2096	rVB	79886	67480	1.92%	0.155%
79	14.568	2120	2122	2126	rBV4	41557	62419	1.78%	0.144%
80	14.739	2149	2151	2154	rBV	45769	51232	1.46%	0.118%
81	14.892	2173	2177	2184	rBV	567905	1075266	30.66%	2.473%
82	14.992	2192	2194	2198	rVB	123050	123205	3.51%	0.283%
83	15.180	2222	2226	2232	rVB	357844	450826	12.86%	1.037%
84	15.239	2232	2236	2242	rBV	513152	646182	18.43%	1.486%
85	15.304	2242	2247	2250	rBV	738673	910877	25.97%	2.095%
86	15.715	2313	2317	2321	rVB4	70613	99835	2.85%	0.230%
87	16.698	2479	2484	2493	rVB	202424	412924	11.77%	0.950%
88	17.115	2551	2555	2562	rVB	133014	249752	7.12%	0.574%

Sum of corrected areas: 43485648

LSC Report - Integrated Chromatogram

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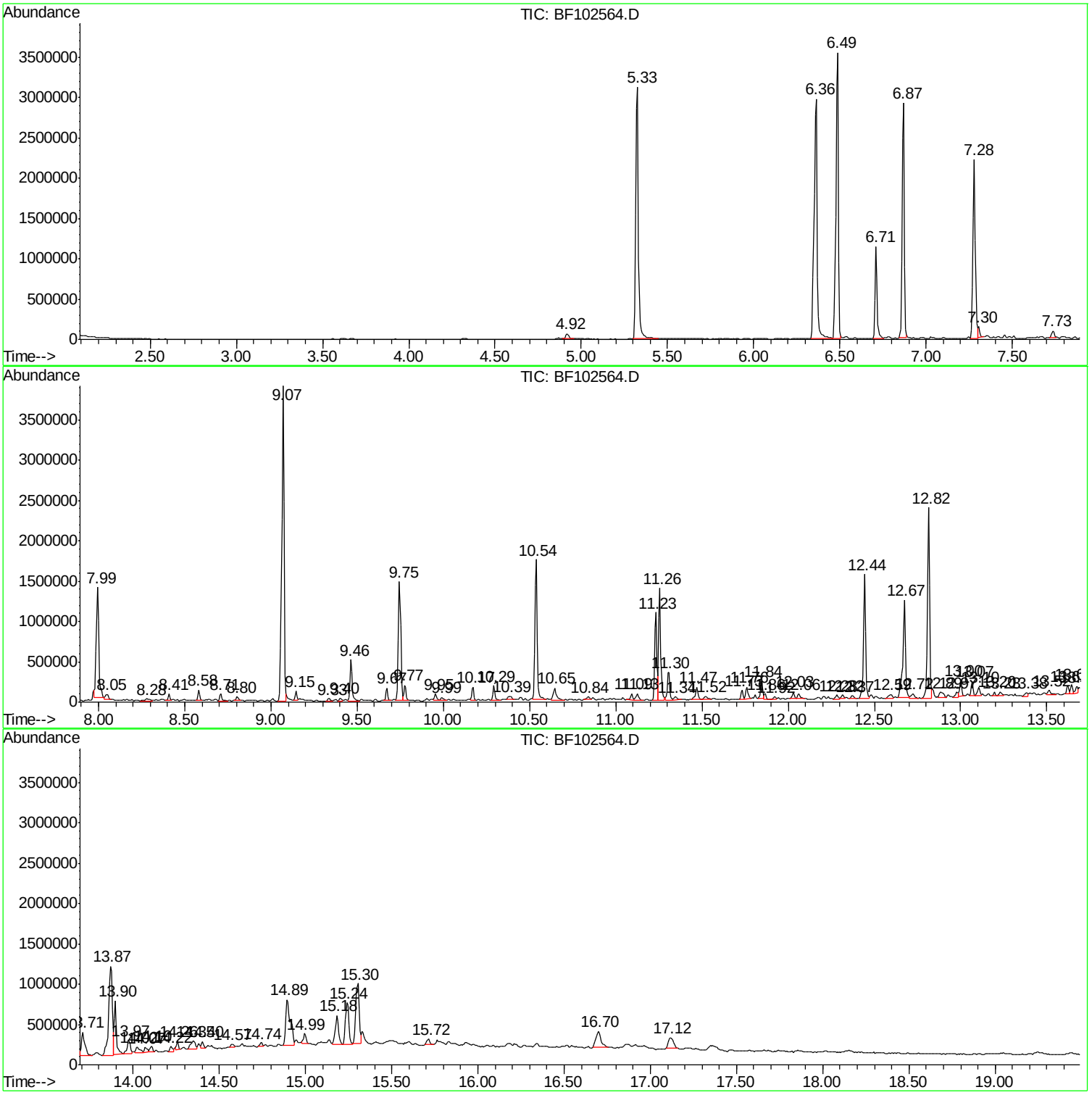
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102564.D
Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

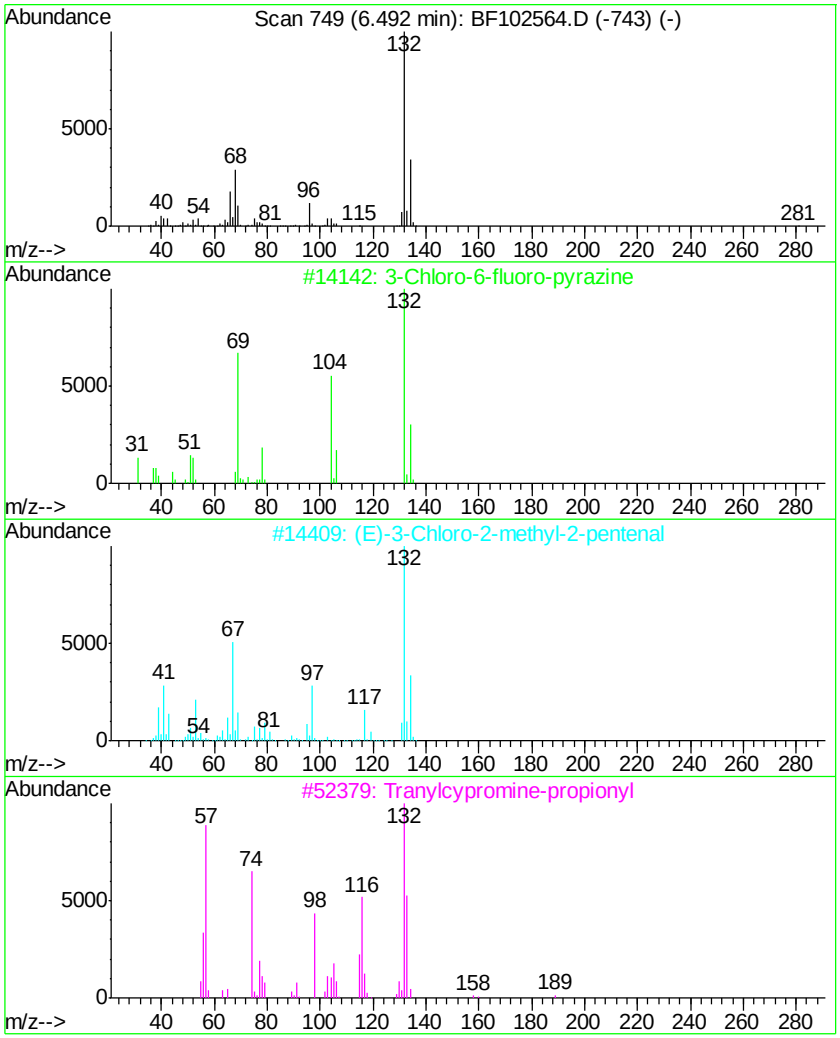
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

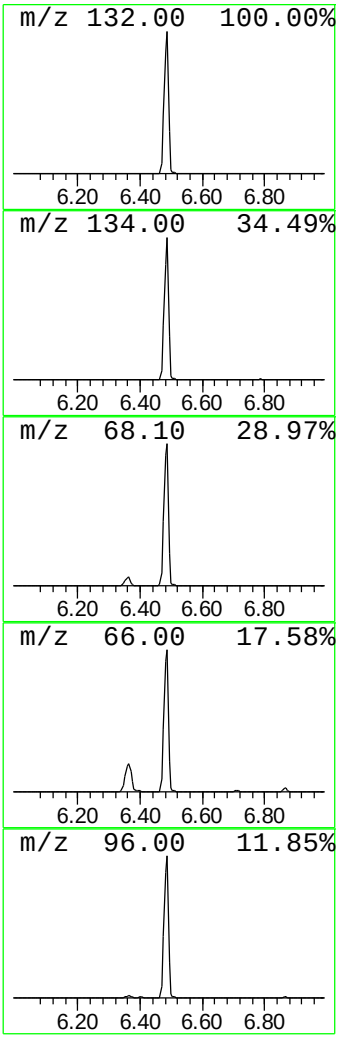
****

Peak Number 1 unknown Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	70.42 ng	3359470	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





Library Search Compound Report

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Data File : BF102564.D
Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

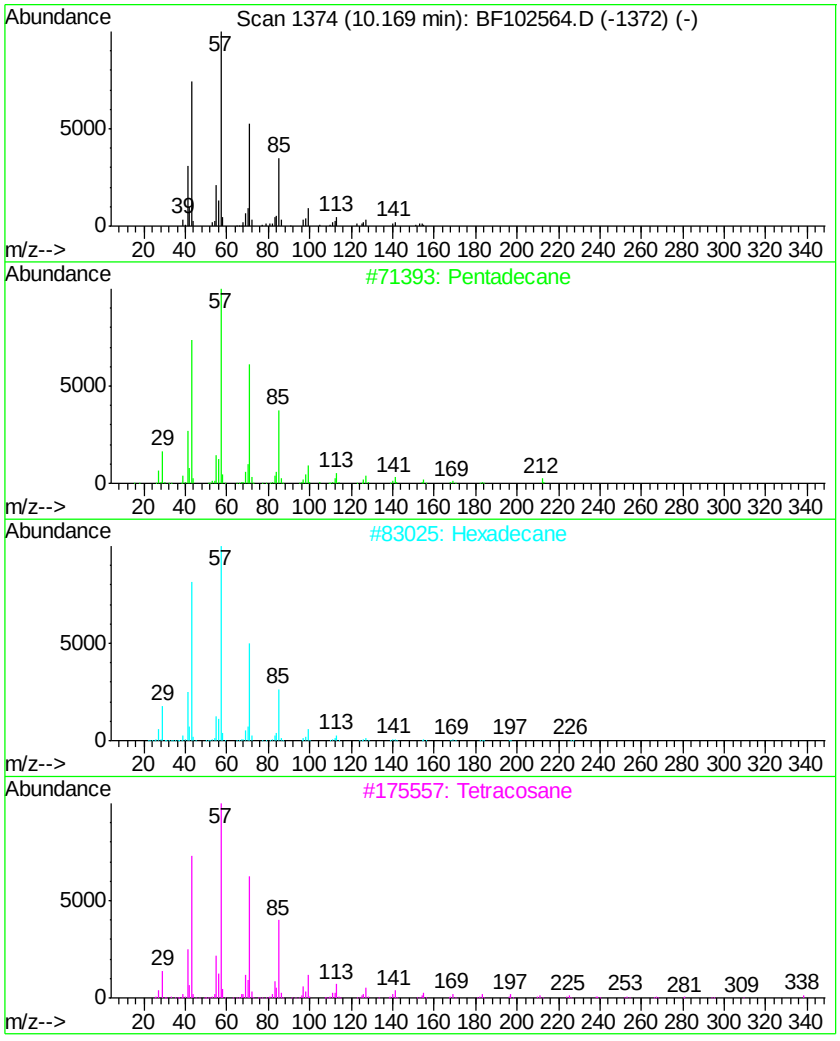
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

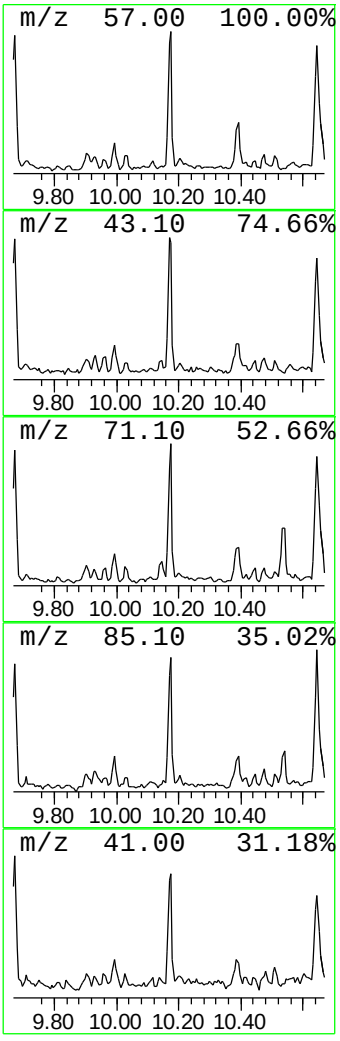
****

Peak Number 3 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.17	2.14 ng	134579	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Tridecane	184	C13H28	000629-50-5	86
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86





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Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
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Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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TIC Library : C:\DATABASE\NIST11.L
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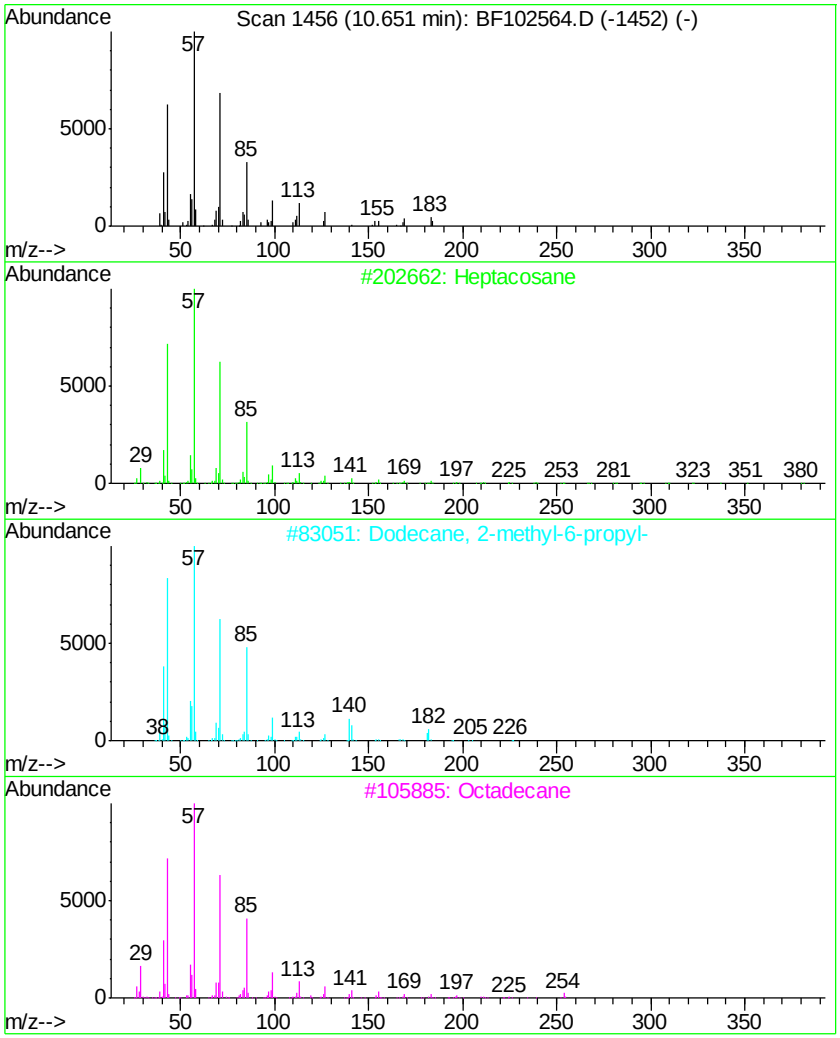
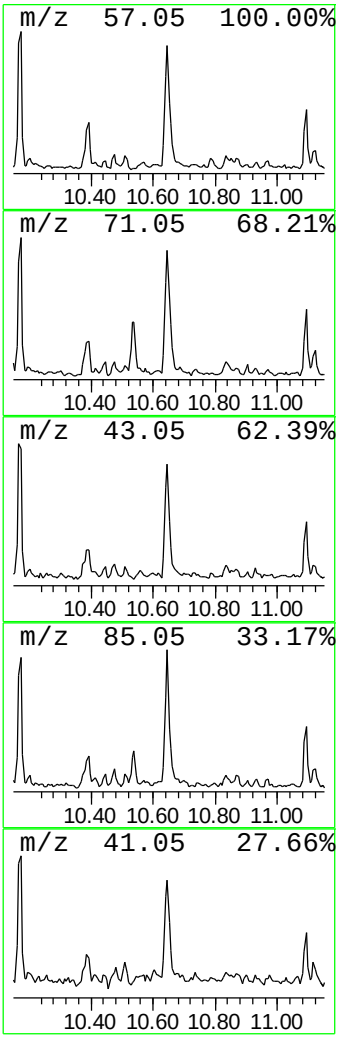
Peak Number 4 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	3.32 ng	176719	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
3	Octadecane	254	C18H38	000593-45-3	78
4	Heptadecane	240	C17H36	000629-78-7	78
5	Pentadecane	212	C15H32	000629-62-9	72





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ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
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TIC Library : C:\DATABASE\NIST11.L
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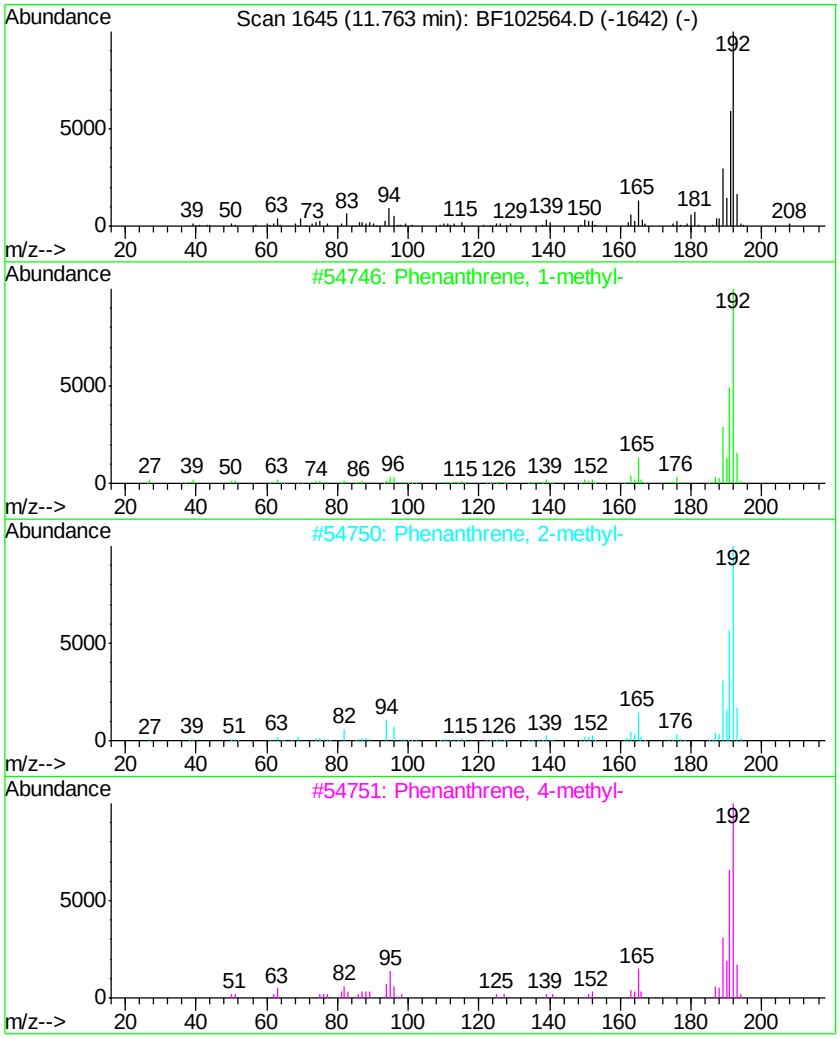
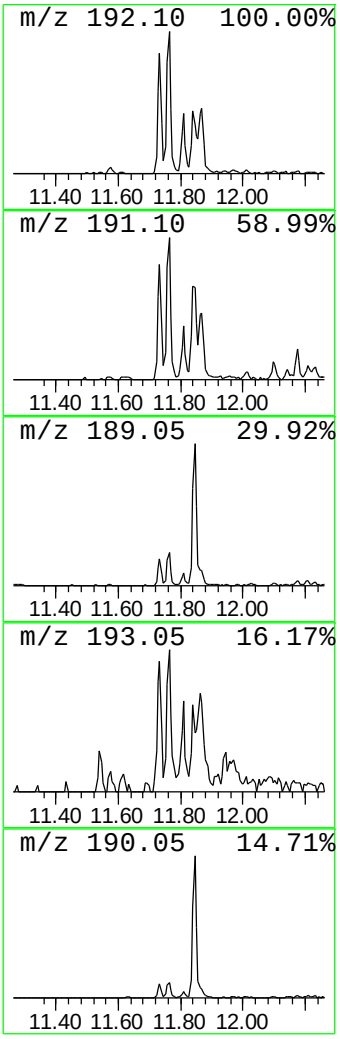
Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	2.43 ng	129549	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	94
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	94
5	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	93





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Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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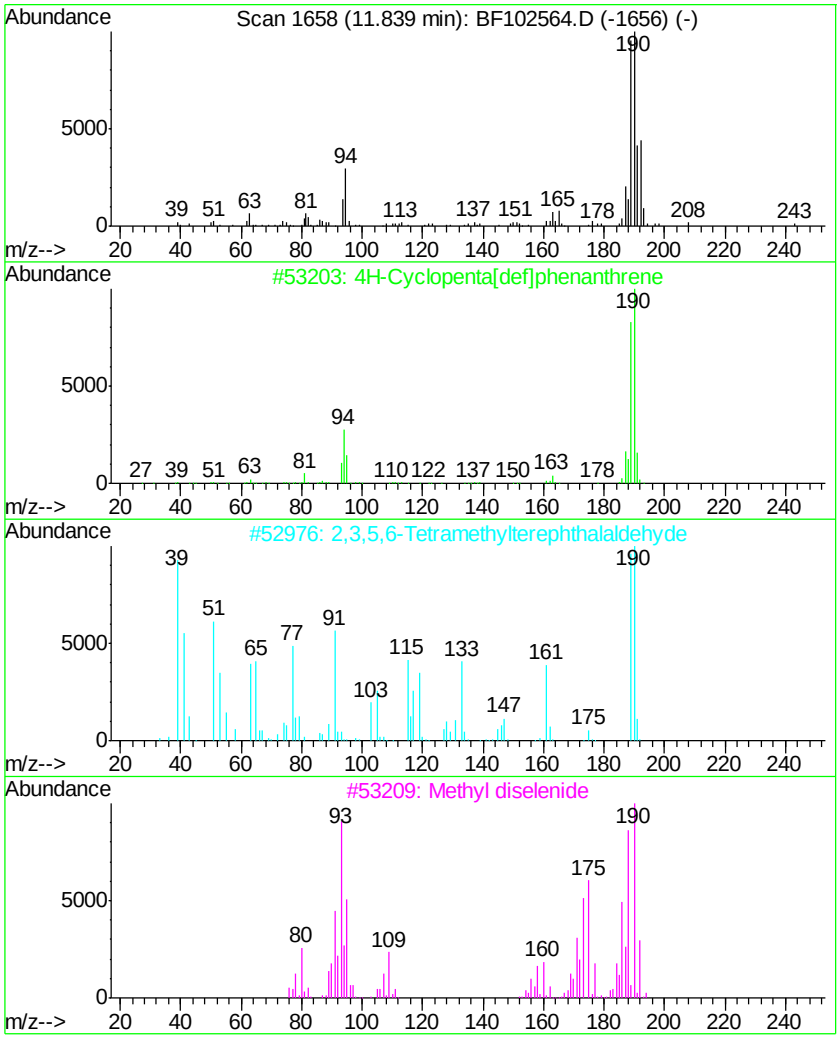
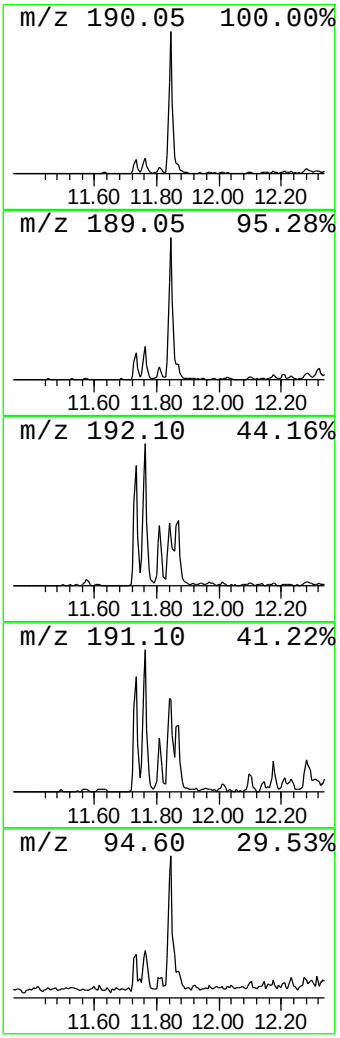
Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	4.04 ng	215105	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	93
2	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
3	Methyl diselenide	190	C2H6Se2	007101-31-7	45
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
5	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
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Sample : J1290-18
Misc :
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Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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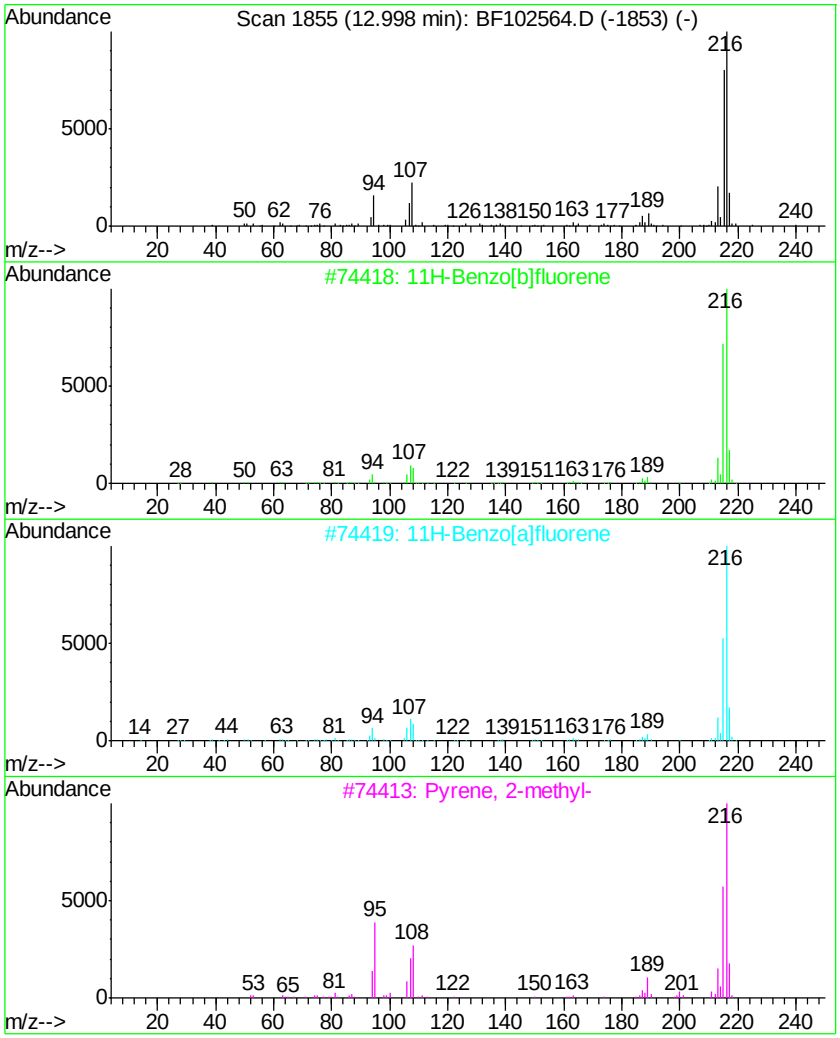
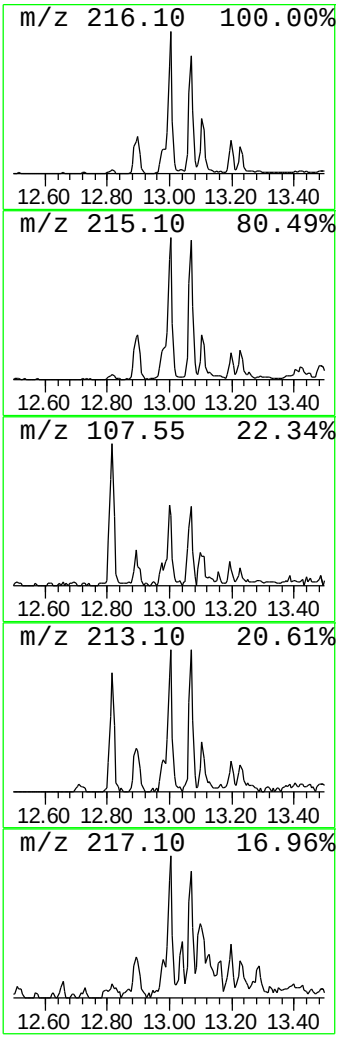
Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.00	2.00 ng	175321	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	87
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102564.D
Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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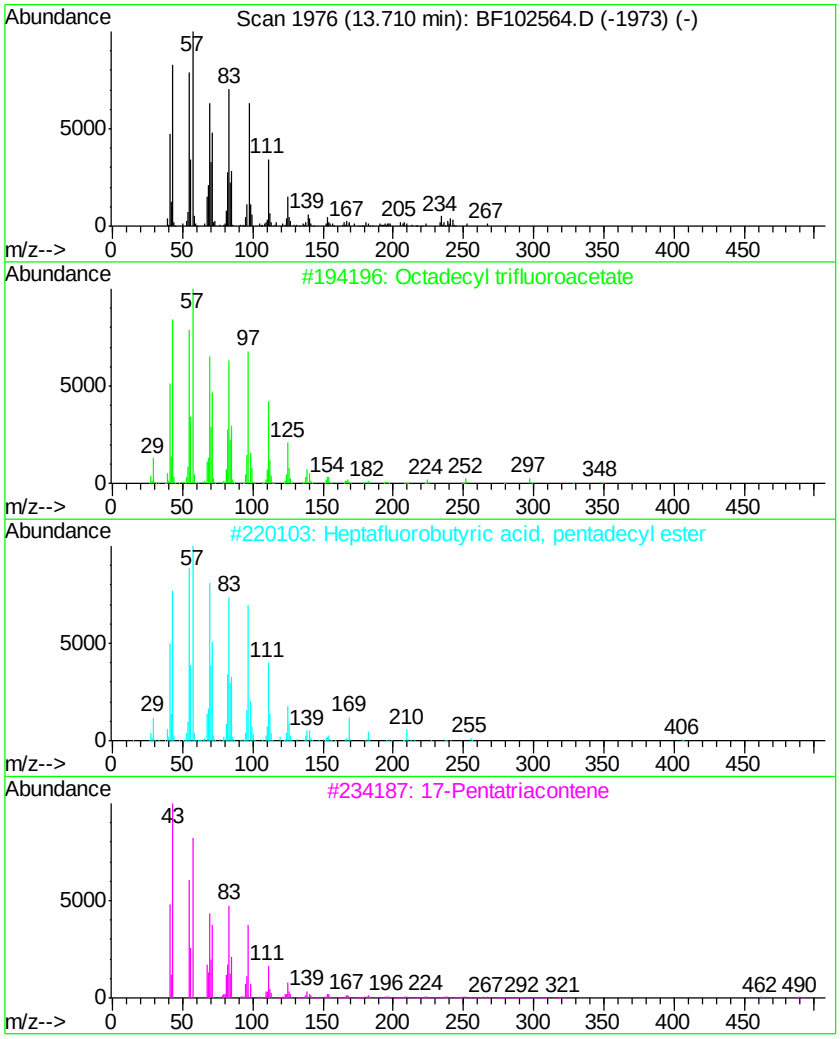
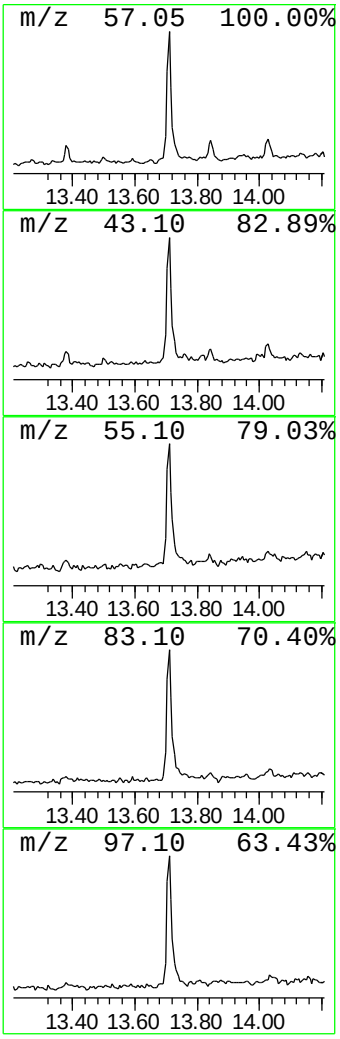
Peak Number 8 Octadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.71	4.47 ng	391665	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
3	17-Pentatriacontene	491	C35H70	006971-40-0	90
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	87





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Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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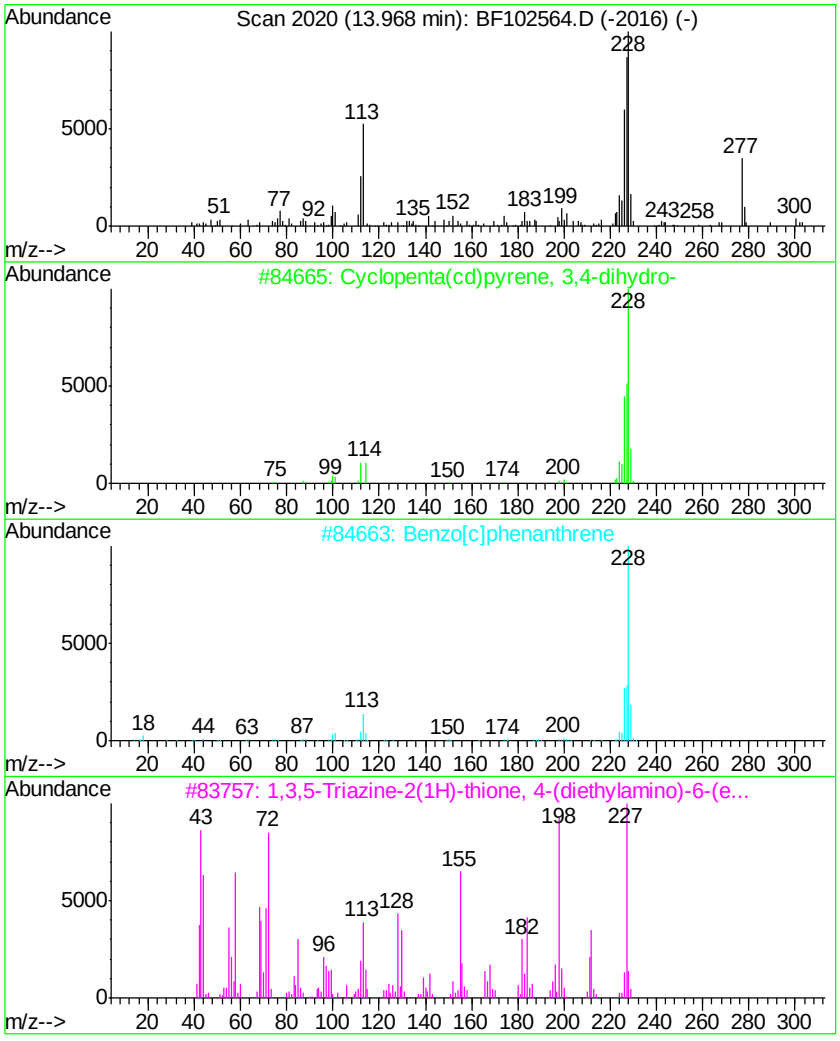
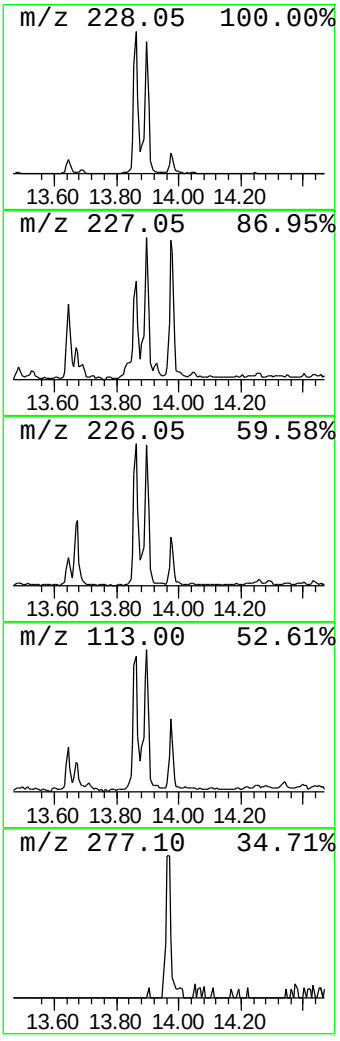
Peak Number 9 Cyclopenta(cd)pyrene, 3,4-d... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.15 ng	188245	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(cd)pyrene, 3,4-dihydro-	228	C18H12	025732-74-5	55
2	Benzo[c]phenanthrene	228	C18H12	000195-19-7	52
3	1,3,5-Triazine-2(1H)-thione, 4-(...	227	C9H17N5S	023613-02-7	46
4	Diphenylvinylphosphine oxide	228	C14H13OP	002096-78-8	43
5	Triphenylene	228	C18H12	000217-59-4	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012818\
Data File : BF102564.D
Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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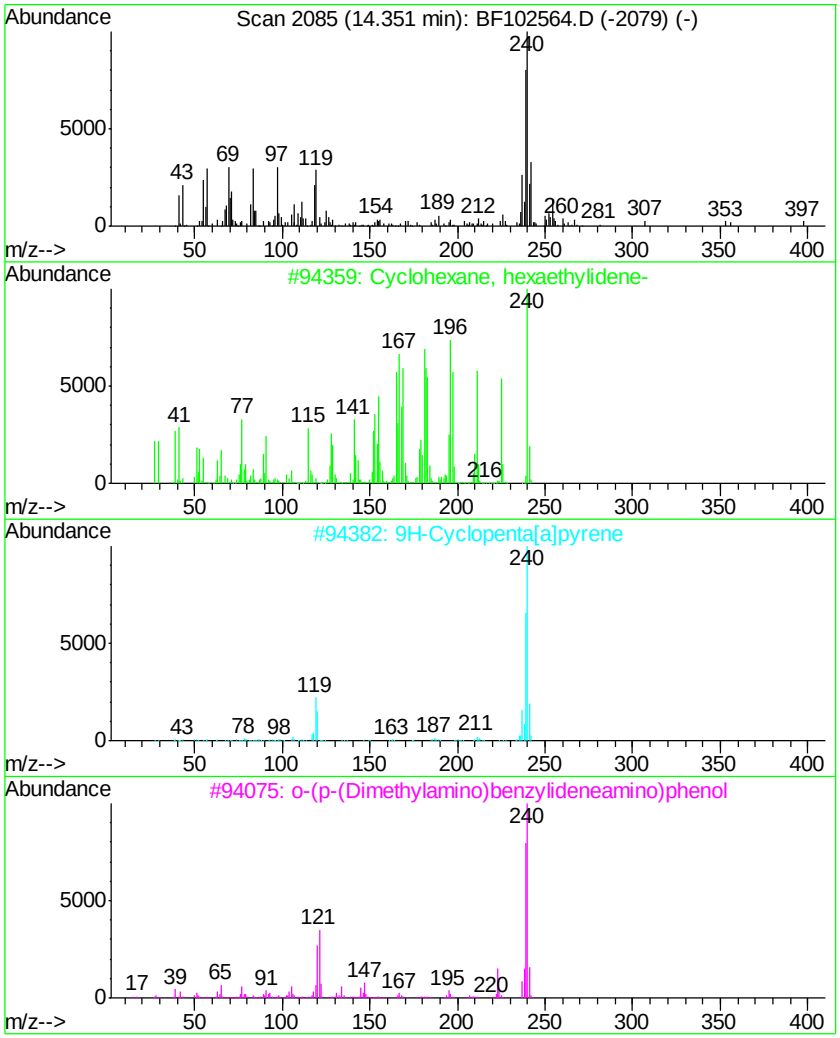
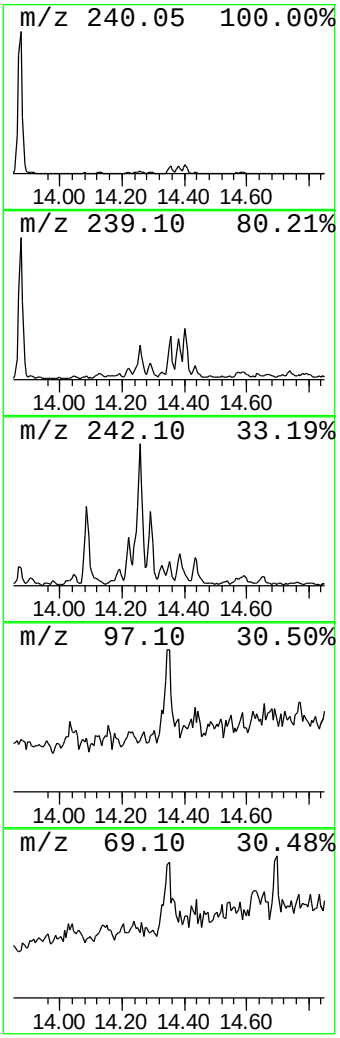
Peak Number 10 Cyclohexane, hexaethylidene- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	2.24 ng	196671	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, hexaethylidene-	240	C18H24	001482-93-5	91
2	9H-Cyclopenta[a]pyrene	240	C19H12	050861-05-7	53
3	o-(p-(Dimethylamino)benzylidenea...	240	C15H16N2O	023837-35-6	47
4	Pyrrolo[2,3-f]quinolin-7-one, 2,...	240	C15H16N2O	1000302-73-0	47
5	3-Pyridinemethanamine, N-[[4-(di...	239	C15H17N3	1000350-96-8	38





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Data File : BF102564.D
Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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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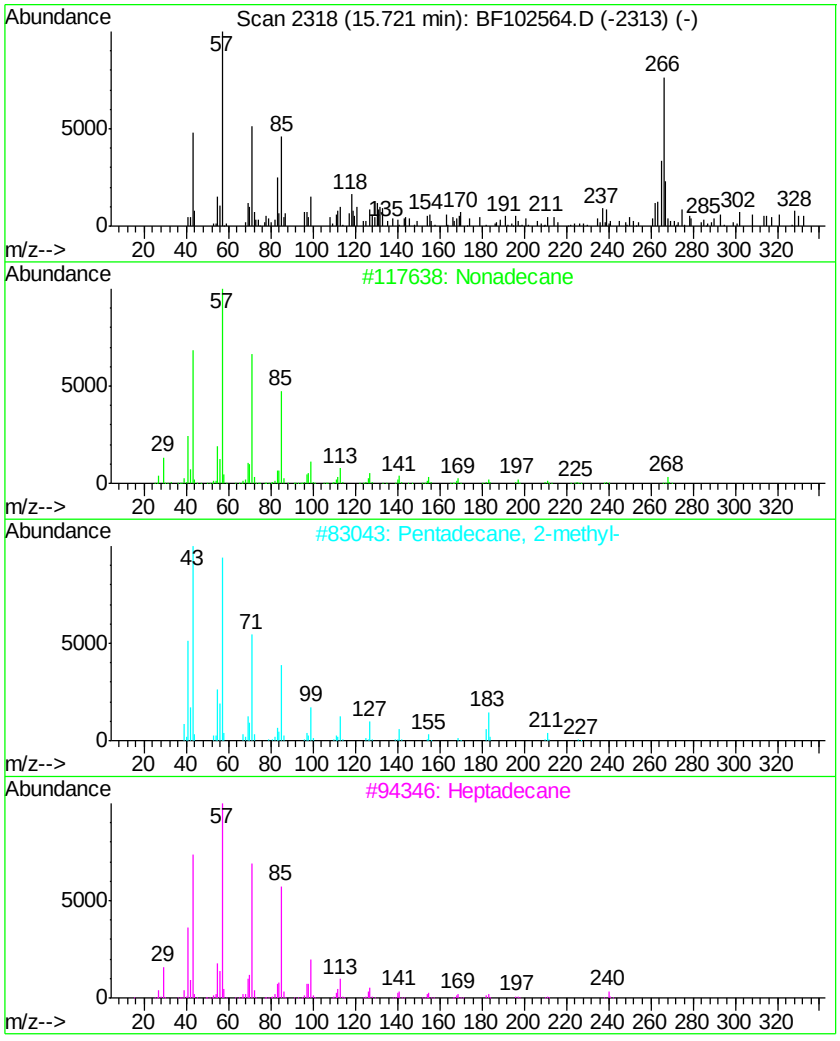
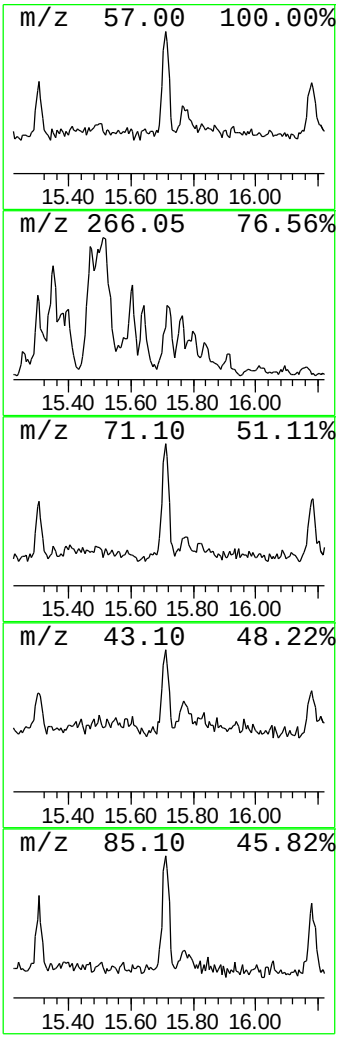
Peak Number 13 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.19 ng	99835	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	50
2	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	49
3	Heptadecane	240	C17H36	000629-78-7	49
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	46
5	Docosane	310	C22H46	000629-97-0	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012818\
Data File : BF102564.D
Acq On : 28 Jan 2018 18:21
Operator : SJ/JU
Sample : J1290-18
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-46-9.5-10.0

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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
unknown	6.49	70.4	ng	3359470	1	6.71	954146	20.0
Pentadecane	10.17	2.1	ng	134579	3	9.75	1256020	20.0
Heptacosane	10.65	3.3	ng	176719	4	11.23	1066180	20.0
Phenanthrene, 1-m...	11.76	2.4	ng	129549	4	11.23	1066180	20.0
4H-Cyclopenta[def...	11.84	4.0	ng	215105	4	11.23	1066180	20.0
11H-Benzo[b]fluorene	13.00	2.0	ng	175321	5	13.87	1752160	20.0
Octadecyl trifluo...	13.71	4.5	ng	391665	5	13.87	1752160	20.0
Cyclopenta(cd)pyr...	13.97	2.1	ng	188245	5	13.87	1752160	20.0
Cyclohexane, hexa...	14.35	2.2	ng	196671	5	13.87	1752160	20.0
Nonadecane	15.72	2.2	ng	99835	6	15.30	910877	20.0