LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099637.D
Acq On : 19 Oct 2017 00:29
Operator : SJ/JU
Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

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-BF092317.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	5.040	499	502	512	rBV	112967	126006	14.46%	0.969%
2	5.451	569	572	590	rBV	843788	837461	96.13%	6.439%
3	6.469	741	745	758	rBV	849027	817062	93.79%	6.282%
4	6.598	764	767	774	rBV	1045734	871163	100.00%	6.698%
5	6.828	803	806	814	rBV	620457	490131	56.26%	3.769%
6	6.981	829	832	844	rBB	827590	685296	78.66%	5.269%
7	7.392	898	902	912	rBV	524734	459831	52.78%	3.536%
8	8.110	1020	1024	1027	rBV	700606	597595	68.60%	4.595%
9	8.822	1142	1145	1148	rBV	27039	22264	2.56%	0.171%
10	8.922	1159	1162	1167	rVB	17791	16142	1.85%	0.124%
11	9.180	1202	1206	1209	rBV	1045097	858606	98.56%	6.602%
12	9.451	1248	1252	1254	rBV2	8656	10028	1.15%	0.077%
13	9.522	1261	1264	1267	rBV	13679	13768	1.58%	0.106%
14	9.575	1270	1273	1280	rVB2	22418	24408	2.80%	0.188%
15	9.722	1295	1298	1304	rBV	29827	30449	3.50%	0.234%
16	9.863	1318	1322	1325	rBV	629652	521018	59.81%	4.006%
17	9.892	1325	1327	1330	rVB	24442	20170	2.32%	0.155%
18	10.069	1353	1357	1360	rVB2	13519	14017	1.61%	0.108%
19	10.175	1372	1375	1378	rBV	9536	10339	1.19%	0.079%
20	10.410	1412	1415	1421	rVB	23990	24346	2.79%	0.187%
21	10.651	1453	1456	1467	rBV	446543	386477	44.36%	2.972%
22	10.763	1470	1475	1478	rBV3	9709	15074	1.73%	0.116%
23	10.957	1503	1508	1511	rBV4	10491	11164	1.28%	0.086%
24	11.198	1546	1549	1552	rBV	13310	14832	1.70%	0.114%
25	11.351	1571	1575	1577	rBV	620230	508801	58.40%	3.912%
26	11.374	1577	1579	1583	rVB	171057	131449	15.09%	1.011%
27	11.427	1585	1588	1591	rBV	69124	55258	6.34%	0.425%
28	11.592	1611	1616	1619	rBV4	10917	16960	1.95%	0.130%
29	11.680	1629	1631	1636	rVB3	7984	9996	1.15%	0.077%
30	11.851	1657	1660	1663	rBV	44295	52592	6.04%	0.404%
31	11.880	1663	1665	1670	rVV	67580	57686	6.62%	0.444%
32	11.927	1670	1673	1676	rVV	33313	30674	3.52%	0.236%
33	11.963	1676	1679	1682	rVV2	75844	85850	9.85%	0.660%
34	11.986	1682	1683	1688	rVB	34209	22587	2.59%	0.174%

LSC Area Percent Report

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

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-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.145	1706	1710	1713	rBV	40216	35313	4.05%	0.272%
36	12.186	1713	1717	1721	rVB3	21323	23461	2.69%	0.180%
37	12.327	1738	1741	1743	rBV	16895	13168	1.51%	0.101%
38	12.351	1743	1745	1748	rVB	16590	13228	1.52%	0.102%
39	12.410	1750	1755	1757	rBV2	51924	87931	10.09%	0.676%
40	12.433	1757	1759	1762	rVV2	48293	47848	5.49%	0.368%
41	12.498	1765	1770	1772	rBV2	49673	58339	6.70%	0.449%
42	12.563	1778	1781	1785	rBV	613464	548960	63.01%	4.221%
43	12.627	1790	1792	1795	rVV4	18335	15036	1.73%	0.116%
44	12.663	1795	1798	1800	rVV	25343	23083	2.65%	0.177%
45	12.716	1803	1807	1809	rVV3	31041	36919	4.24%	0.284%
46	12.739	1809	1811	1814	rVV3	18988	19037	2.19%	0.146%
47	12.798	1814	1821	1826	rVV2	472214	572596	65.73%	4.403%
48	12.845	1826	1829	1833	rVB2	36251	40598	4.66%	0.312%
49	12.927	1838	1843	1847	rVV	887285	855767	98.23%	6.580%
50	12.957	1847	1848	1852	rVB2	17935	15202	1.75%	0.117%
51	13.010	1853	1857	1863	rBV4	47696	88602	10.17%	0.681%
52	13.121	1869	1876	1879	rBV	101214	155667	17.87%	1.197%
53	13.186	1885	1887	1890	rBV	70547	57063	6.55%	0.439%
54	13.227	1890	1894	1896	rBV2	75021	81778	9.39%	0.629%
55	13.321	1907	1910	1912	rBV	39943	31516	3.62%	0.242%
56	13.351	1912	1915	1921	rVB2	48778	61788	7.09%	0.475%
57	13.639	1961	1964	1967	rBV	46333	44837	5.15%	0.345%
58	13.745	1979	1982	1984	rBV	54463	45626	5.24%	0.351%
59	13.768	1984	1986	1988	rVB	47837	36069	4.14%	0.277%
60	13.815	1991	1994	1997	rVV2	99962	121873	13.99%	0.937%
61	13.845	1997	1999	2002	rVB	41629	39155	4.49%	0.301%
62	13.992	2019	2024	2027	rBV2	673709	868368	99.68%	6.677%
63	14.021	2027	2029	2033	rVB	250190	199919	22.95%	1.537%
64	14.098	2040	2042	2045	rBV	32573	30862	3.54%	0.237%
65	15.033	2198	2201	2204	rBV	175902	235776	27.06%	1.813%
66	15.339	2250	2253	2257	rVB	87764	95377	10.95%	0.733%
67	15.404	2260	2264	2268	rVB	136884	170798	19.61%	1.313%
68	15.462	2270	2274	2278	rVB	316593	384531	44.14%	2.957%

Sum of corrected areas: 13005591

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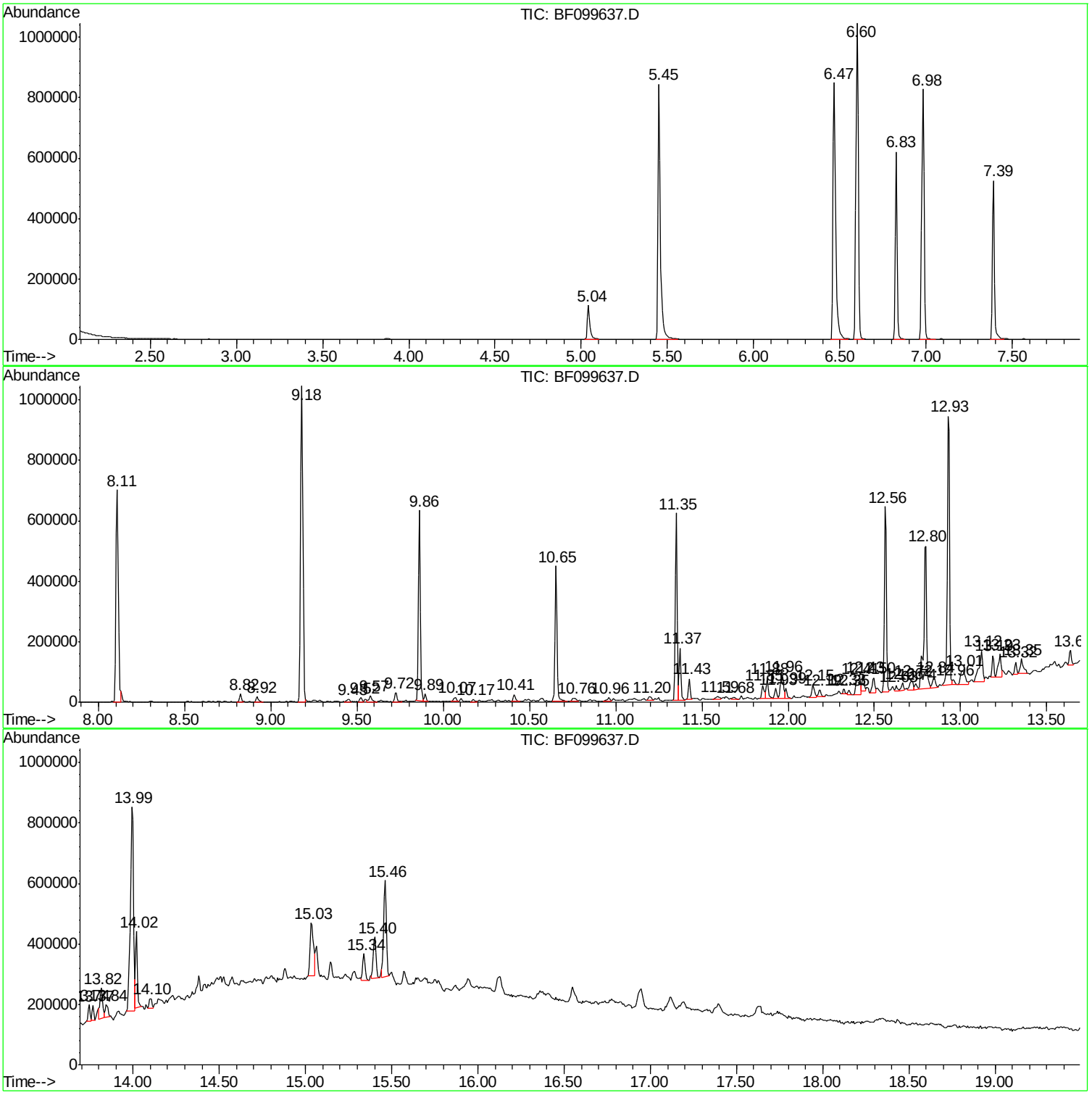
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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\BF101817\
Data File : BF099637.D
Acq On : 19 Oct 2017 00:29
Operator : SJ/JU
Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

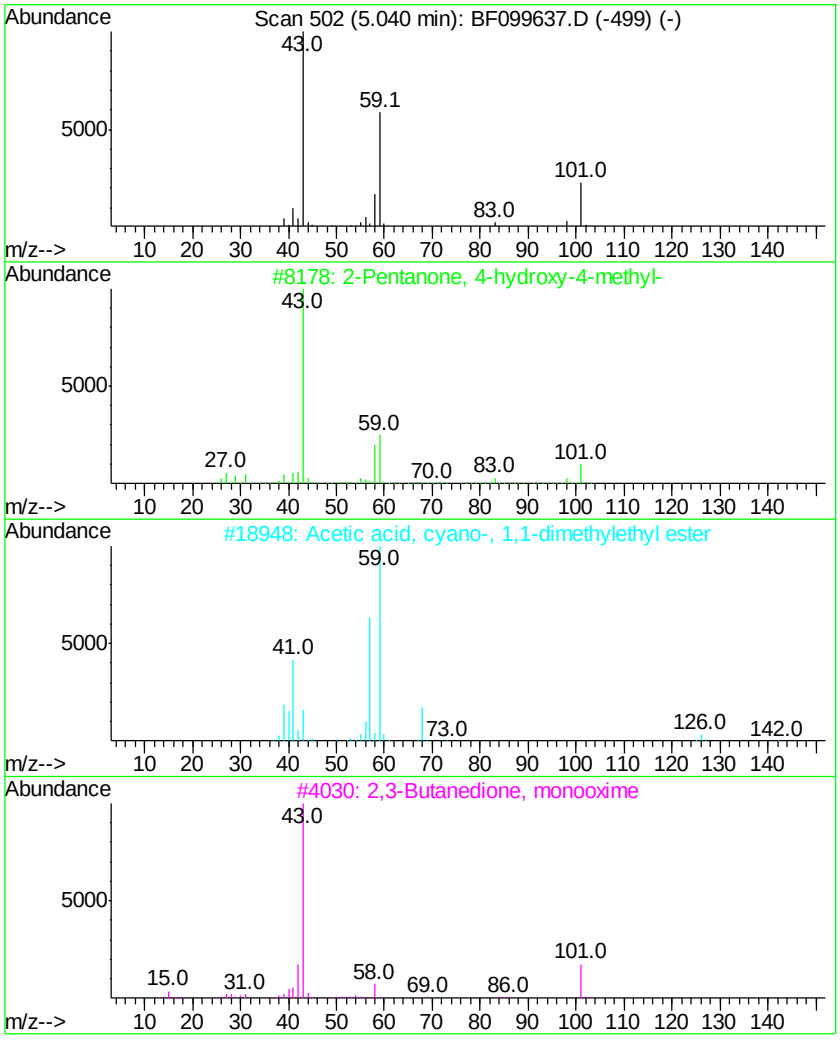
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

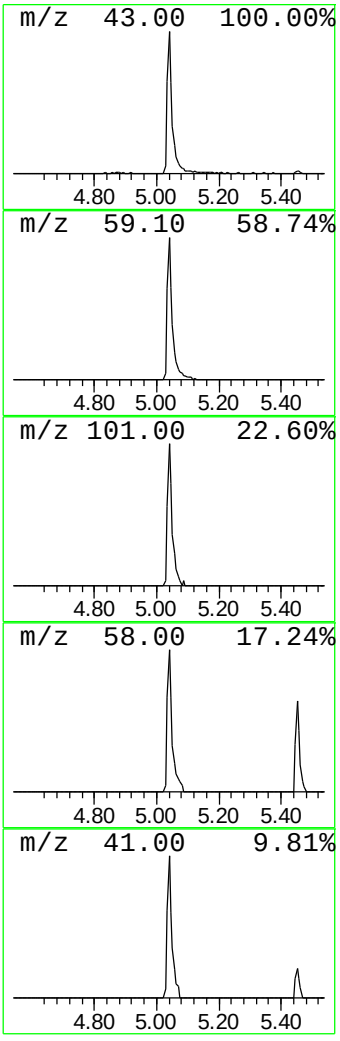
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	5.14 ng	126006	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : SJ/JU
Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

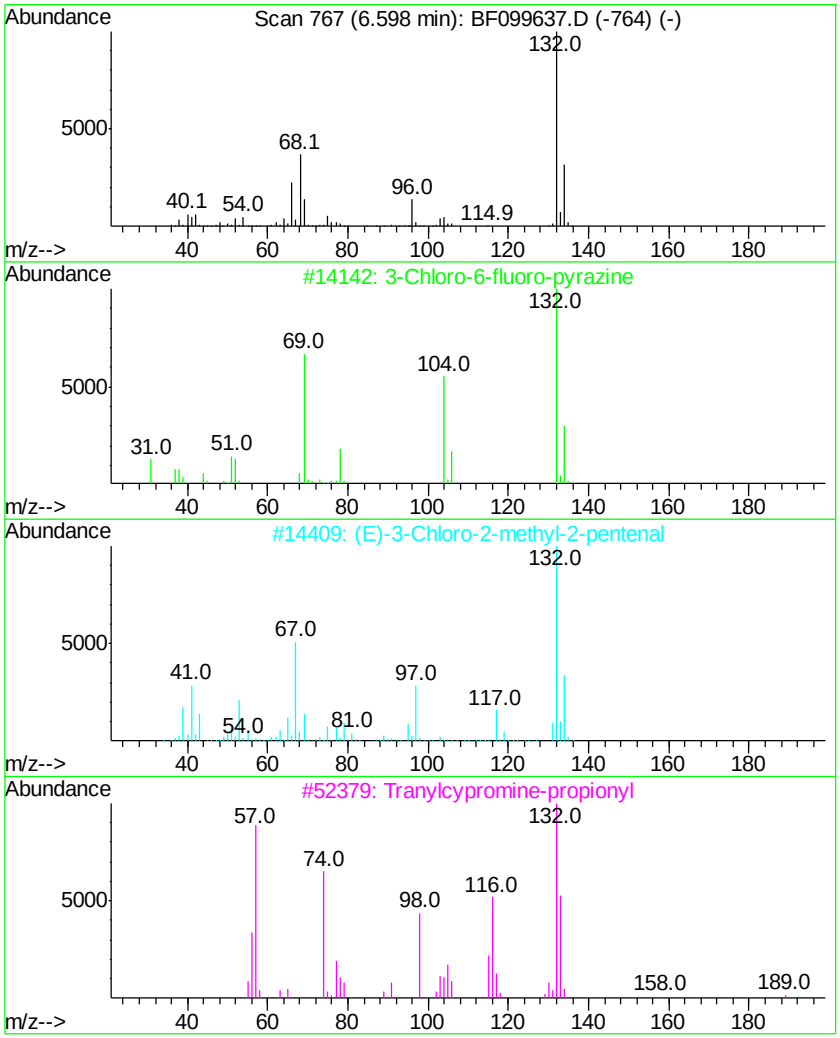
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

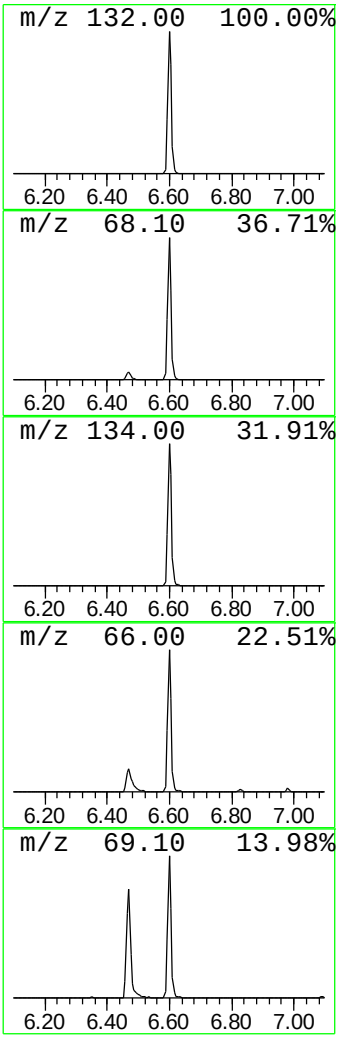
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	35.55 ng	871163	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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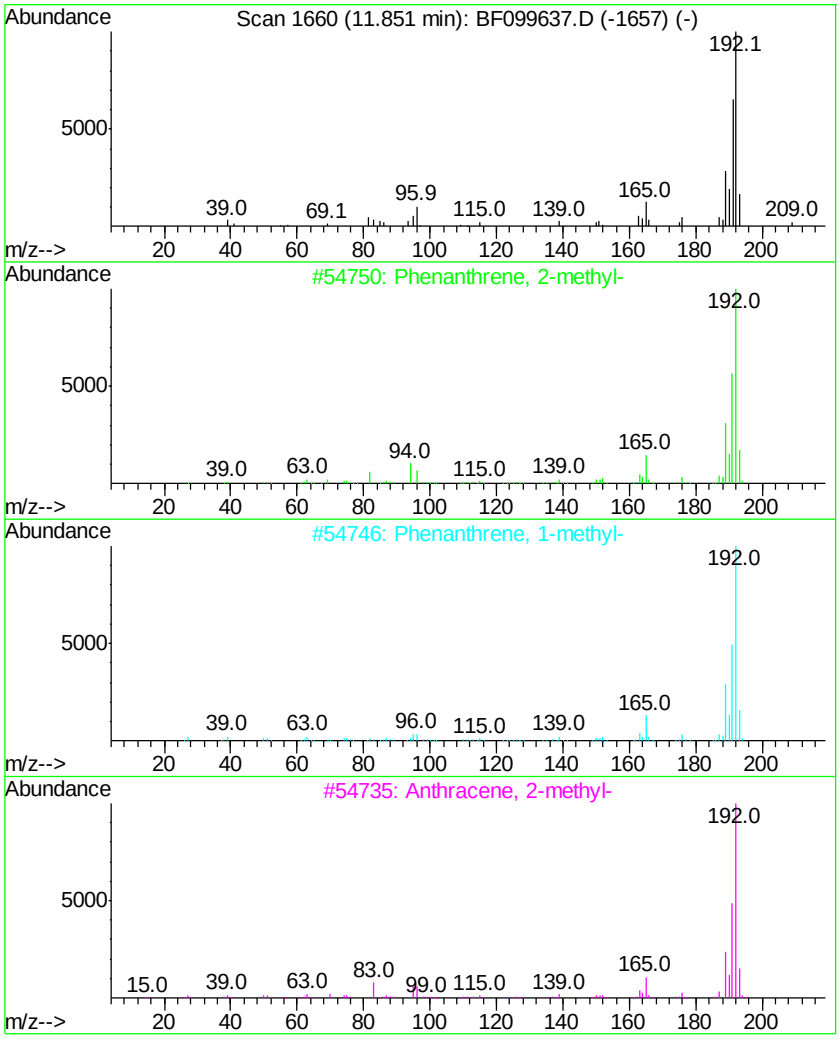
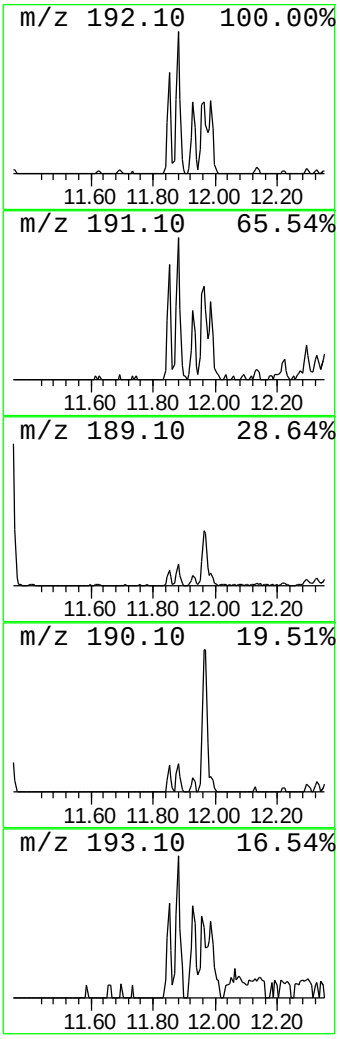
Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	2.07 ng	52592	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	94
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	93
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	90
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87





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Acq On : 19 Oct 2017 00:29
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Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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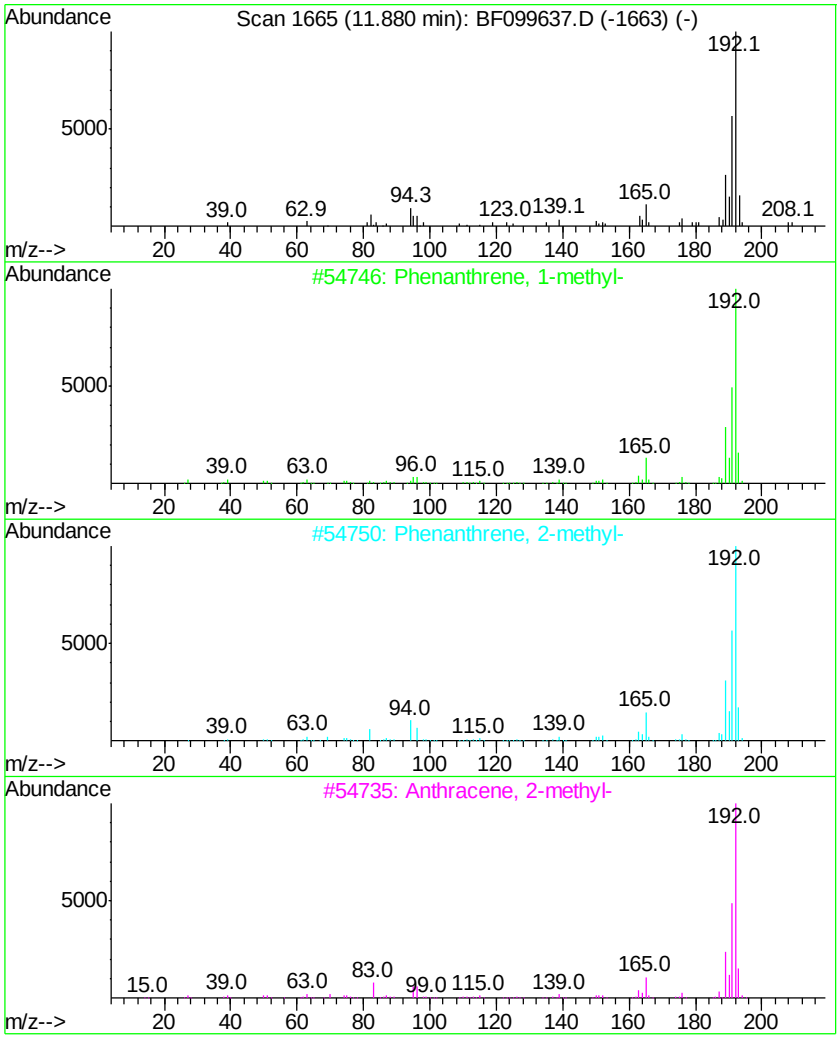
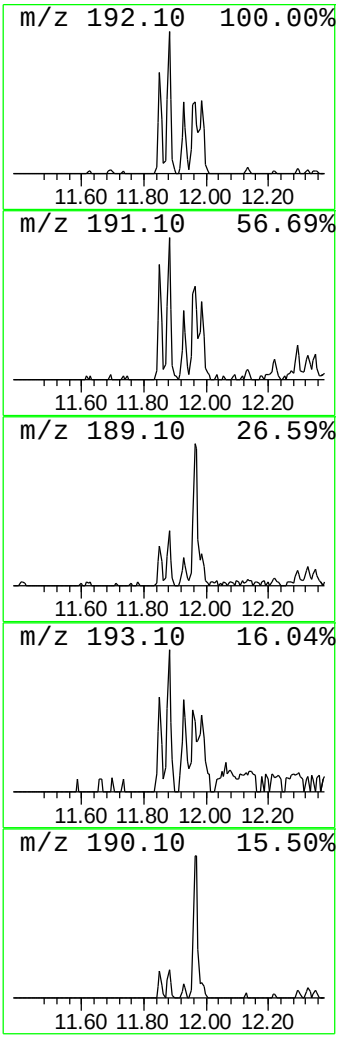
Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	2.27 ng	57686	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	97
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	94
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	93





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Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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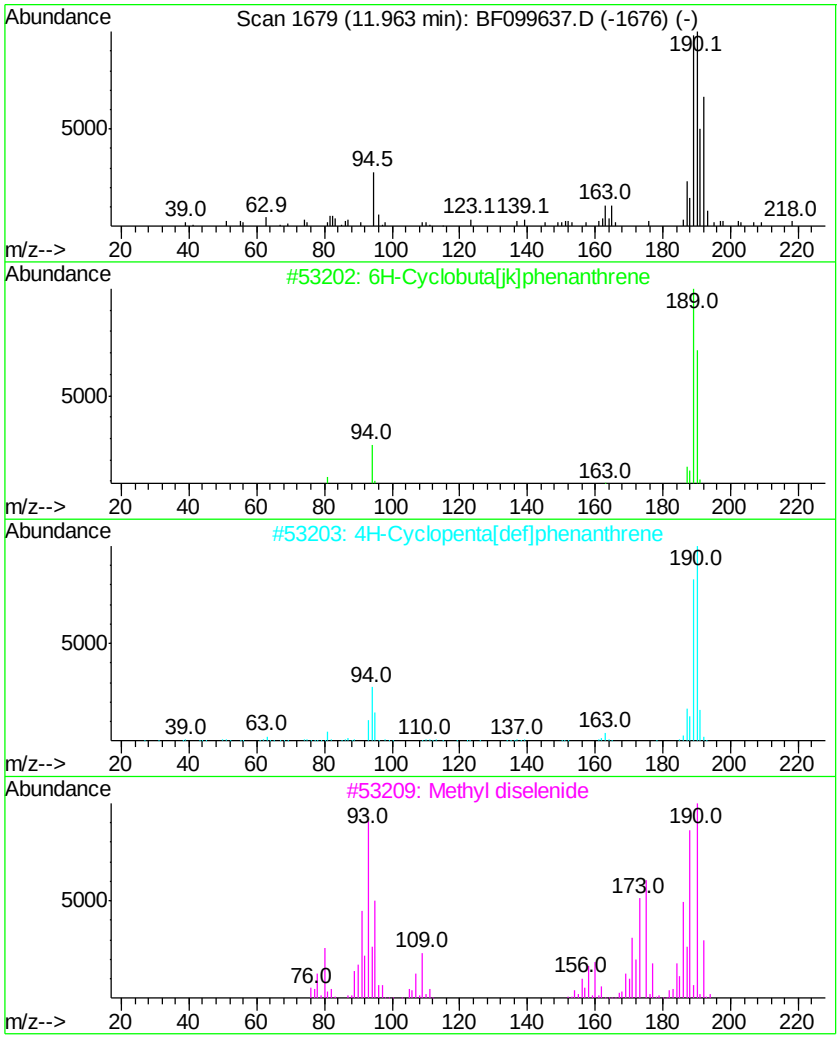
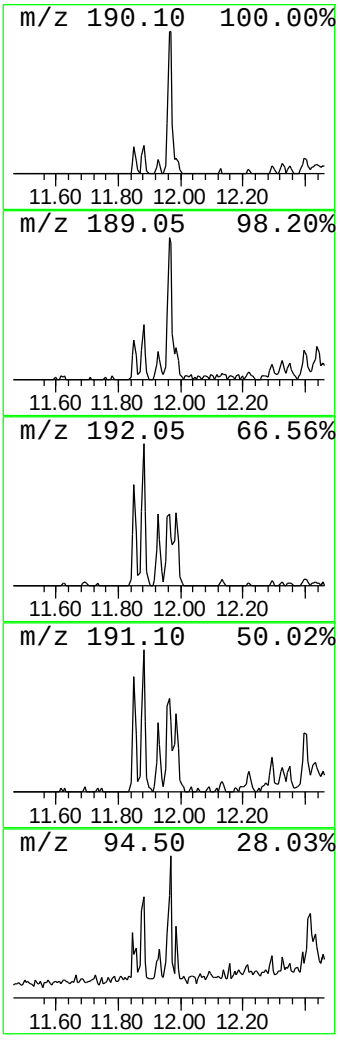
Peak Number 6 6H-Cyclobuta[jk]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	3.37 ng	85850	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	58
2	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
3	Methyl diselenide	190	C2H6Se2	007101-31-7	45
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	43
5	3,5-Dichlorobenzoic acid	190	C7H4Cl2O2	000051-36-5	30





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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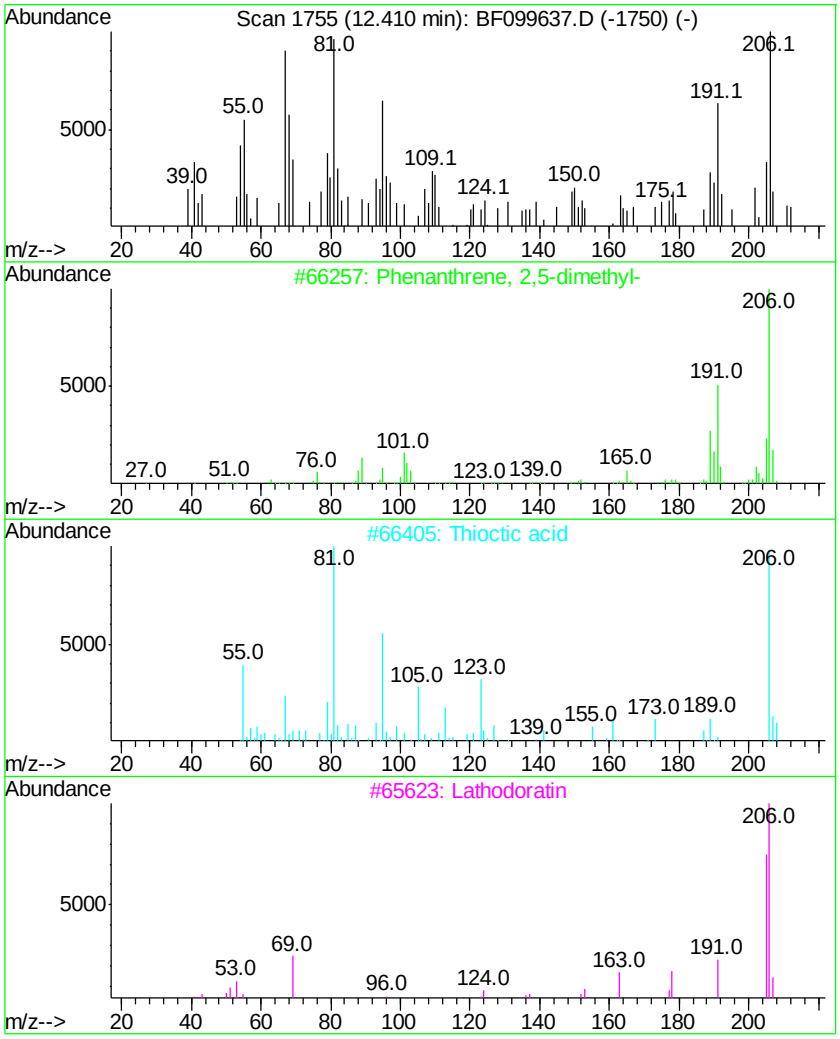
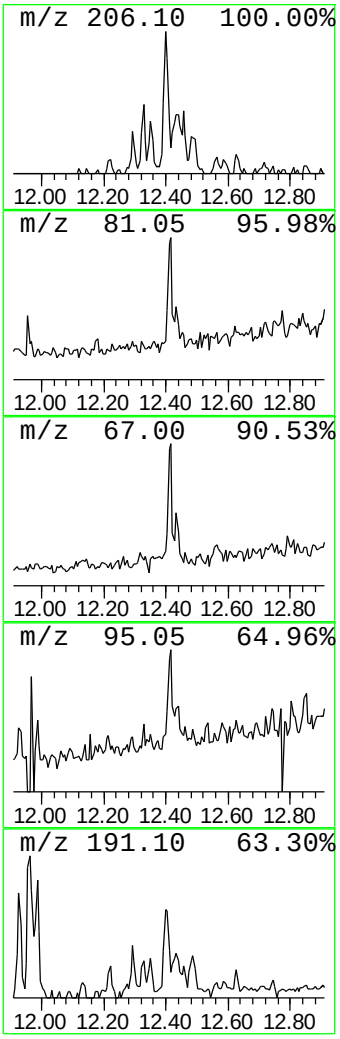
Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	3.46 ng	87931	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	55
2	Thioctic acid	206	C8H14O2S2	001077-28-7	46
3	Lathodoratin	206	C11H10O4	076693-50-0	44
4	9,10-Dimethylanthracene	206	C16H14	000781-43-1	42
5	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099637.D
Acq On : 19 Oct 2017 00:29
Operator : SJ/JU
Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

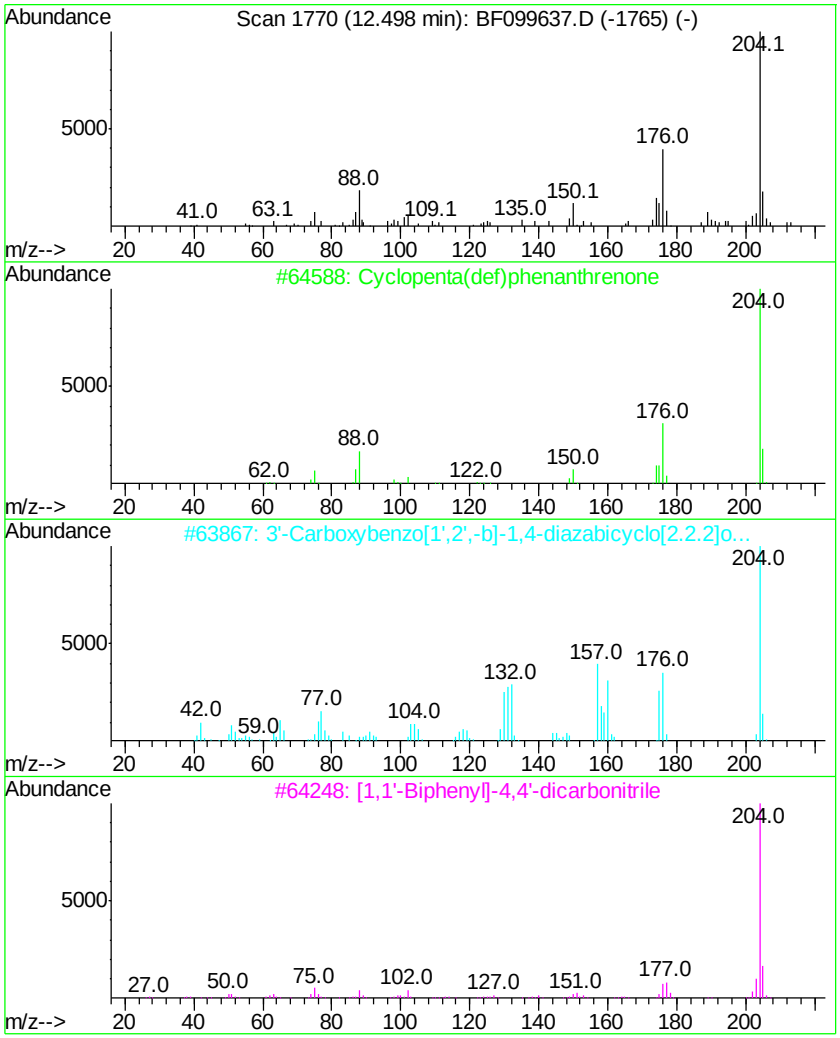
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

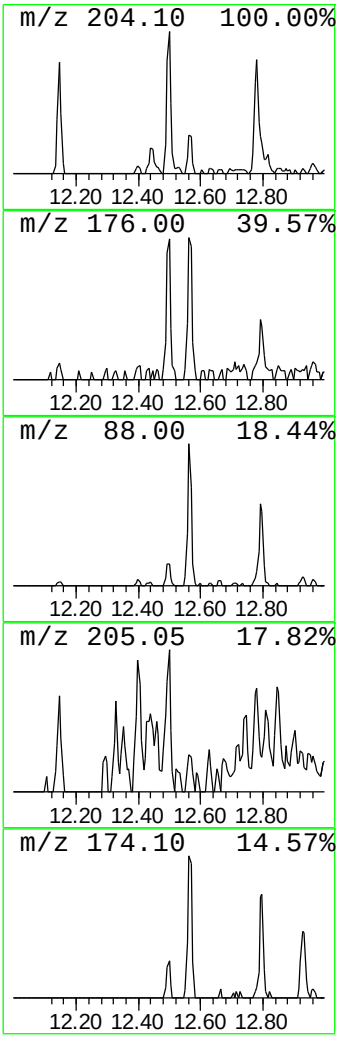
****

Peak Number 8 Cyclopenta(def)phenanthrenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	2.29 ng	58339	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenta(def)phenanthrenone	204	C15H8O	005737-13-3	97
2	3'-Carboxybenzo[1',2',-b]-1,4-di...	204	C11H12N2O2	138023-41-3	59
3	[1,1'-Biphenyl]-4,4'-dicarbonitrile	204	C14H8N2	001591-30-6	53
4	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	49
5	(E)-Ethyl 3-oxo-2-(pyrid-2-yl)me...	219	C12H13NO3	1000147-59-7	45





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Acq On : 19 Oct 2017 00:29
Operator : SJ/JU
Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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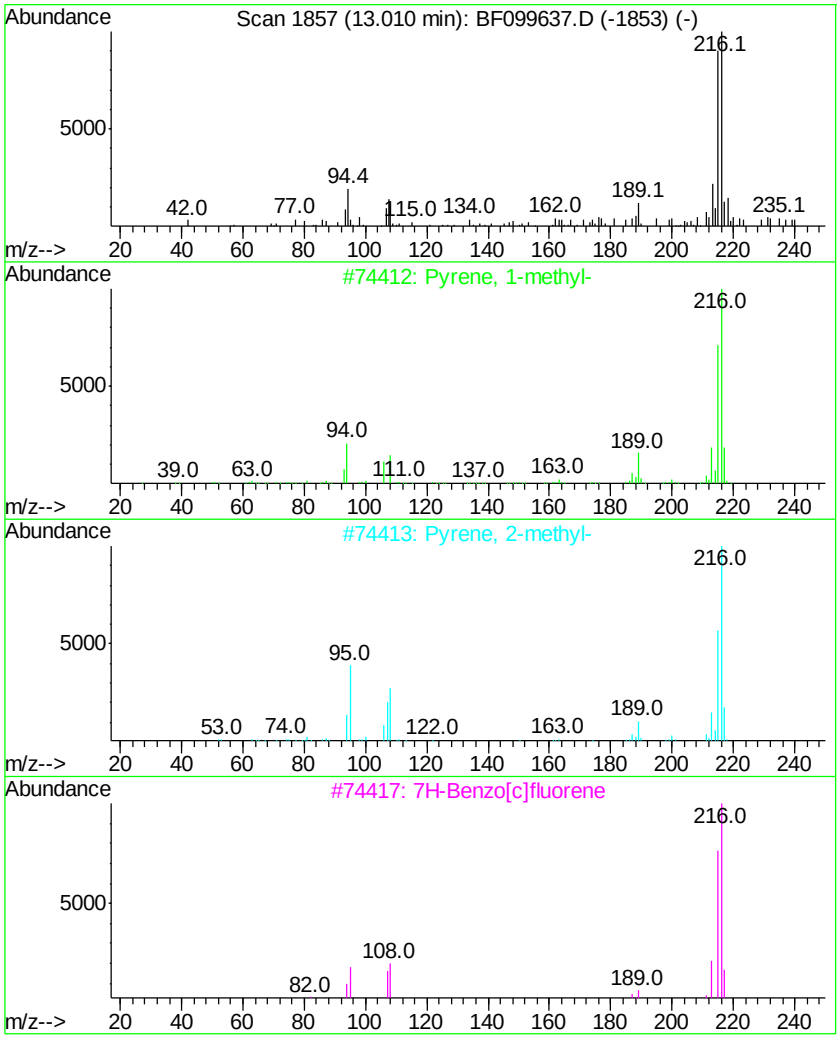
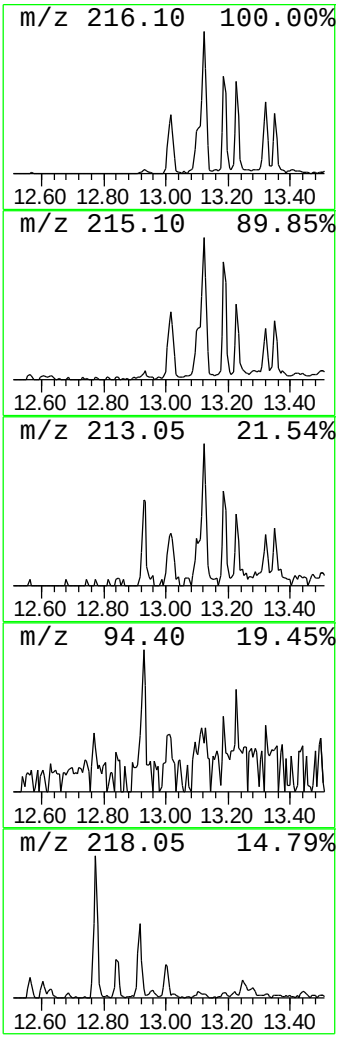
Peak Number 9 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.01	2.04 ng	88602	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 1-methyl-	216	C17H12	002381-21-7	76
2	Pyrene, 2-methyl-	216	C17H12	003442-78-2	76
3	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	59
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	59
5	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	58





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ClientSampleId : SU-03-101717

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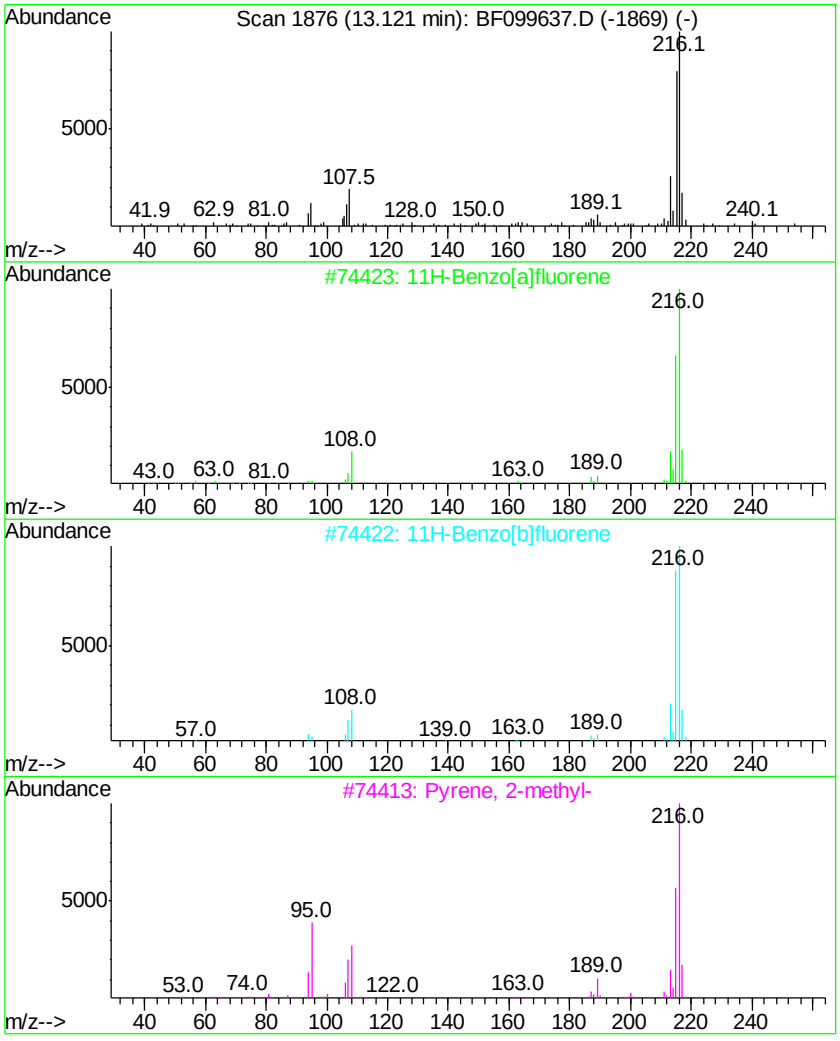
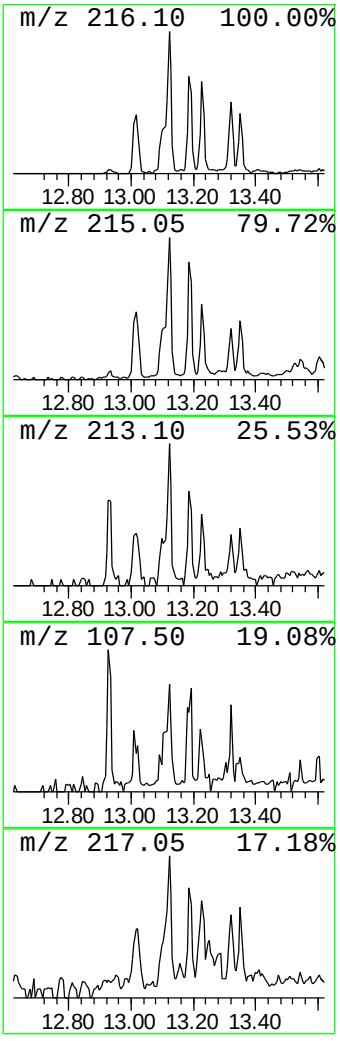
Peak Number 10 11H-Benzo[a]fluorene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	3.59 ng	155667	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	93
2	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	93
3	Pyrene, 2-methyl-	216	C17H12	003442-78-2	89
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	81
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099637.D
Acq On : 19 Oct 2017 00:29
Operator : SJ/JU
Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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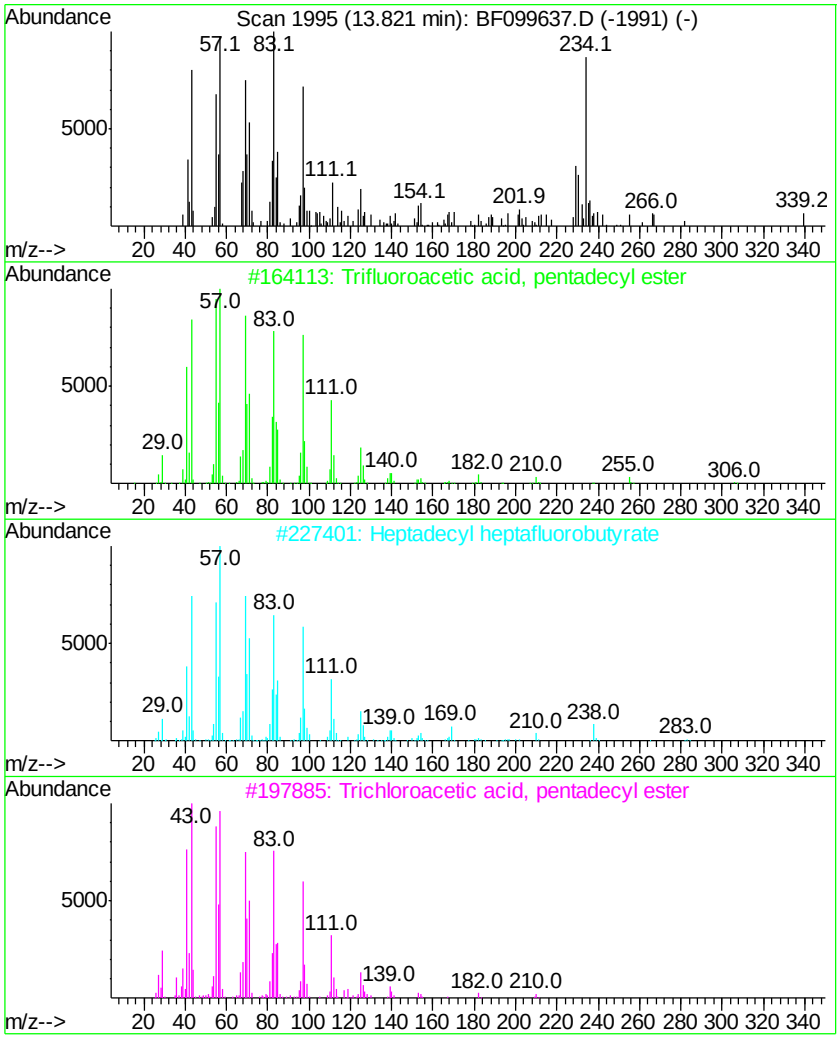
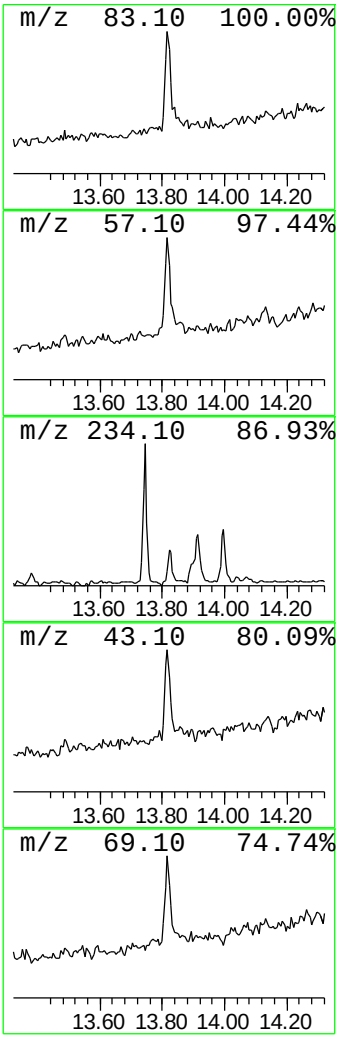
Peak Number 11 Trifluoroacetic acid, penta... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	2.81 ng	121873	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	64
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	60
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	60
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	46





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Operator : SJ/JU
Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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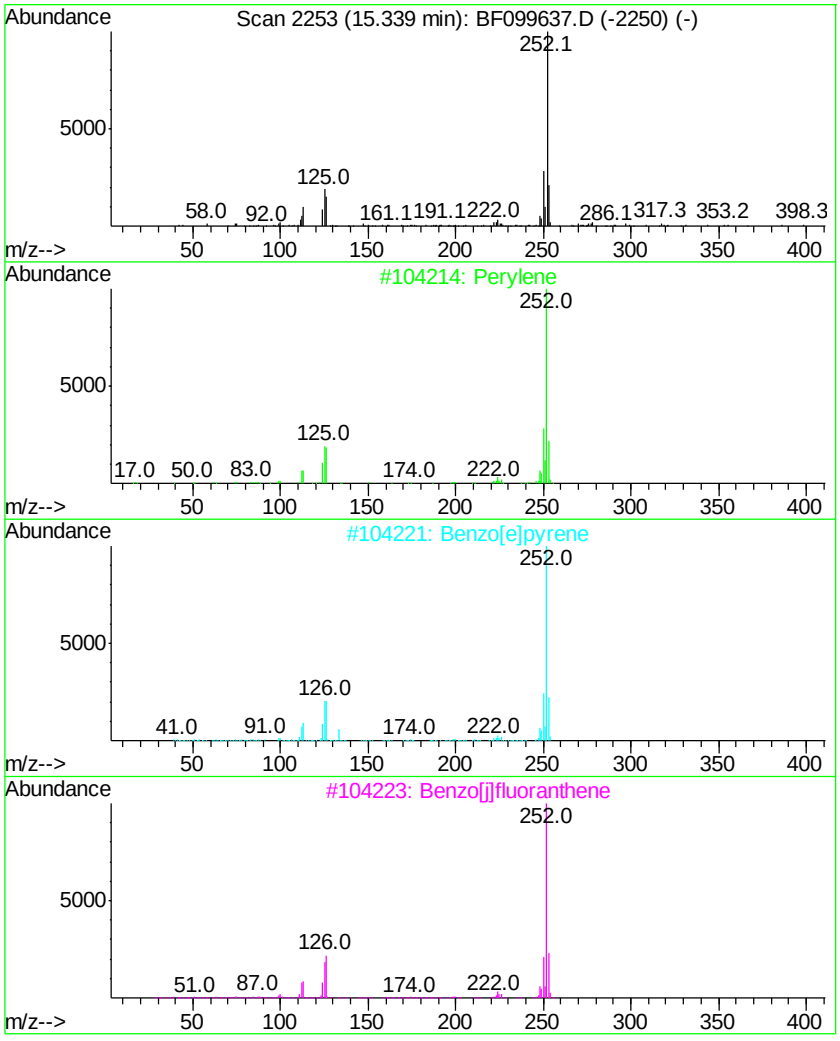
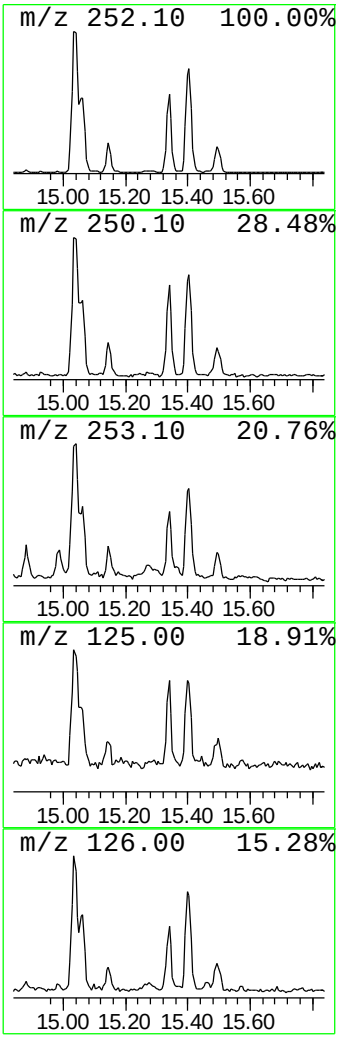
Peak Number 12 Perylene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	4.96 ng	95377	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	98
2	Benzo[e]pyrene	252	C20H12	000192-97-2	97
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	97
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
5	Benzo[a]pyrene	252	C20H12	000050-32-8	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101817\
Data File : BF099637.D
Acq On : 19 Oct 2017 00:29
Operator : SJ/JU
Sample : I5943-01 2X
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SU-03-101717

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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...	5.04	5.1	ng	126006	1	6.83	490131	20.0
unknown6.60	6.60	35.5	ng	871163	1	6.83	490131	20.0
Phenanthrene, 2-m...	11.85	2.1	ng	52592	4	11.35	508801	20.0
Phenanthrene, 1-m...	11.88	2.3	ng	57686	4	11.35	508801	20.0
6H-Cyclobuta[jk]p...	11.96	3.4	ng	85850	4	11.35	508801	20.0
Phenanthrene, 2,5...	12.41	3.5	ng	87931	4	11.35	508801	20.0
Cyclopenta(def)ph...	12.50	2.3	ng	58339	4	11.35	508801	20.0
Pyrene, 1-methyl-	13.01	2.0	ng	88602	5	14.00	868368	20.0
11H-Benzo[a]fluorene	13.12	3.6	ng	155667	5	14.00	868368	20.0
Trifluoroacetic a...	13.82	2.8	ng	121873	5	14.00	868368	20.0
Perylene	15.34	5.0	ng	95377	6	15.46	384531	20.0