LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133707.D
Acq On : 12 Jun 2023 16:51
Operator : CG\JU
Sample : 03044-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133707.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	498	502	509	rBV	18216	24490	1.43%	0.141%
2	5.445	566	571	574	rBV	1704315	1522809	89.18%	8.798%
3	6.457	738	743	746	rBV	1593552	1573370	92.14%	9.090%
4	6.828	803	806	810	rBV	535647	466580	27.32%	2.696%
5	7.392	898	902	905	rBV	1182523	1020299	59.75%	5.895%
6	8.116	1021	1025	1028	rBV	730995	586772	34.36%	3.390%
7	9.192	1204	1208	1211	rBV	2175618	1707543	100.00%	9.865%
8	9.869	1316	1323	1326	rBV	753740	606879	35.54%	3.506%
9	9.904	1326	1329	1333	rVB	49362	43118	2.53%	0.249%
10	10.074	1354	1358	1362	rBV2	31149	28554	1.67%	0.165%
11	10.416	1412	1416	1422	rVB	41755	36761	2.15%	0.212%
12	10.580	1440	1444	1448	rVB	167953	153981	9.02%	0.890%
13	10.657	1453	1457	1461	rBV	1217187	1032725	60.48%	5.967%
14	10.969	1504	1510	1512	rBV5	14974	24415	1.43%	0.141%
15	11.216	1547	1552	1556	rBV4	14951	27324	1.60%	0.158%
16	11.257	1556	1559	1564	rVB	24644	24873	1.46%	0.144%
17	11.357	1573	1576	1578	rBV	659442	552353	32.35%	3.191%
18	11.380	1578	1580	1584	rVV	462867	371224	21.74%	2.145%
19	11.433	1584	1589	1592	rVB	104942	90823	5.32%	0.525%
20	11.586	1609	1615	1618	rBV2	32950	38787	2.27%	0.224%
21	11.863	1656	1662	1663	rBV	61496	64067	3.75%	0.370%
22	11.886	1663	1666	1670	rVV2	216401	214643	12.57%	1.240%
23	11.933	1670	1674	1677	rVV2	35606	46511	2.72%	0.269%
24	11.974	1677	1681	1683	rVV2	97886	111388	6.52%	0.644%
25	11.992	1683	1684	1688	rVB	44648	32822	1.92%	0.190%
26	12.157	1709	1712	1714	rBV	45191	40346	2.36%	0.233%
27	12.180	1714	1716	1720	rVB2	33835	29242	1.71%	0.169%
28	12.410	1751	1755	1758	rBV	43788	47213	2.76%	0.273%
29	12.451	1758	1762	1764	rVV2	30878	35458	2.08%	0.205%
30	12.498	1767	1770	1776	rVB2	31090	35734	2.09%	0.206%
31	12.574	1779	1783	1786	rBV	663219	548513	32.12%	3.169%
32	12.668	1796	1799	1802	rBV2	47182	44982	2.63%	0.260%
33	12.804	1815	1822	1825	rBV	588498	583331	34.16%	3.370%
34	12.851	1827	1830	1835	rVB3	33109	44282	2.59%	0.256%
35	12.921	1838	1842	1843	rBV2	32856	32918	1.93%	0.190%
36	12.945	1843	1846	1853	rVB	1290941	1201345	70.36%	6.941%

LSC Area Percent Report

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Acq On : 12 Jun 2023 16:51
Operator : CG\JU
Sample : 03044-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

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:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.021	1854	1859	1862	rBV2	37924	64020	3.75%	0.370%
38	13.104	1870	1873	1874	rBV2	25836	23645	1.38%	0.137%
39	13.133	1875	1878	1880	rVB	76096	74465	4.36%	0.430%
40	13.180	1880	1886	1887	rBV2	27985	35042	2.05%	0.202%
41	13.198	1887	1889	1892	rVB	58676	42918	2.51%	0.248%
42	13.233	1892	1895	1898	rBV2	62041	66391	3.89%	0.384%
43	13.327	1909	1911	1914	rBV	33814	25110	1.47%	0.145%
44	13.357	1914	1916	1920	rBV2	32820	31189	1.83%	0.180%
45	13.521	1939	1944	1948	rBV4	39710	65739	3.85%	0.380%
46	13.639	1961	1964	1968	rVB	40525	41388	2.42%	0.239%
47	13.751	1978	1983	1986	rBV2	53225	73562	4.31%	0.425%
48	13.780	1986	1988	1990	rVV	53856	47539	2.78%	0.275%
49	13.804	1990	1992	1993	rVV	44985	39059	2.29%	0.226%
50	13.845	1996	1999	2007	rVB2	148870	177950	10.42%	1.028%
51	14.004	2018	2026	2028	rBV2	635311	827530	48.46%	4.781%
52	14.027	2028	2030	2036	rVB	282028	268829	15.74%	1.553%
53	14.110	2041	2044	2047	rVV	57806	53109	3.11%	0.307%
54	14.168	2051	2054	2057	rVV4	40964	52197	3.06%	0.302%
55	14.233	2060	2065	2067	rVV2	20515	29491	1.73%	0.170%
56	14.392	2089	2092	2094	rVB	59528	56577	3.31%	0.327%
57	14.427	2095	2098	2100	rVB	31210	29547	1.73%	0.171%
58	14.480	2103	2107	2110	rVV3	59552	77298	4.53%	0.447%
59	14.515	2110	2113	2115	rVV3	34423	40347	2.36%	0.233%
60	14.539	2115	2117	2120	rVB3	34406	31744	1.86%	0.183%
61	14.780	2155	2158	2162	rBV	34289	33641	1.97%	0.194%
62	15.039	2198	2202	2205	rBV	278236	379994	22.25%	2.195%
63	15.115	2213	2215	2218	rBV2	31902	29398	1.72%	0.170%
64	15.145	2218	2220	2224	rVB	53775	55074	3.23%	0.318%
65	15.339	2249	2253	2260	rVB	154968	225216	13.19%	1.301%
66	15.404	2260	2264	2269	rVB	252715	286651	16.79%	1.656%
67	15.468	2270	2275	2278	rBV	402499	508644	29.79%	2.939%
68	15.498	2278	2280	2287	rVB2	88431	107440	6.29%	0.621%
69	16.921	2517	2522	2530	rVB2	97328	188878	11.06%	1.091%
70	17.103	2548	2553	2557	rBV2	21915	48771	2.86%	0.282%
71	17.362	2593	2597	2604	rVB	73969	123597	7.24%	0.714%

Sum of corrected areas: 17308465

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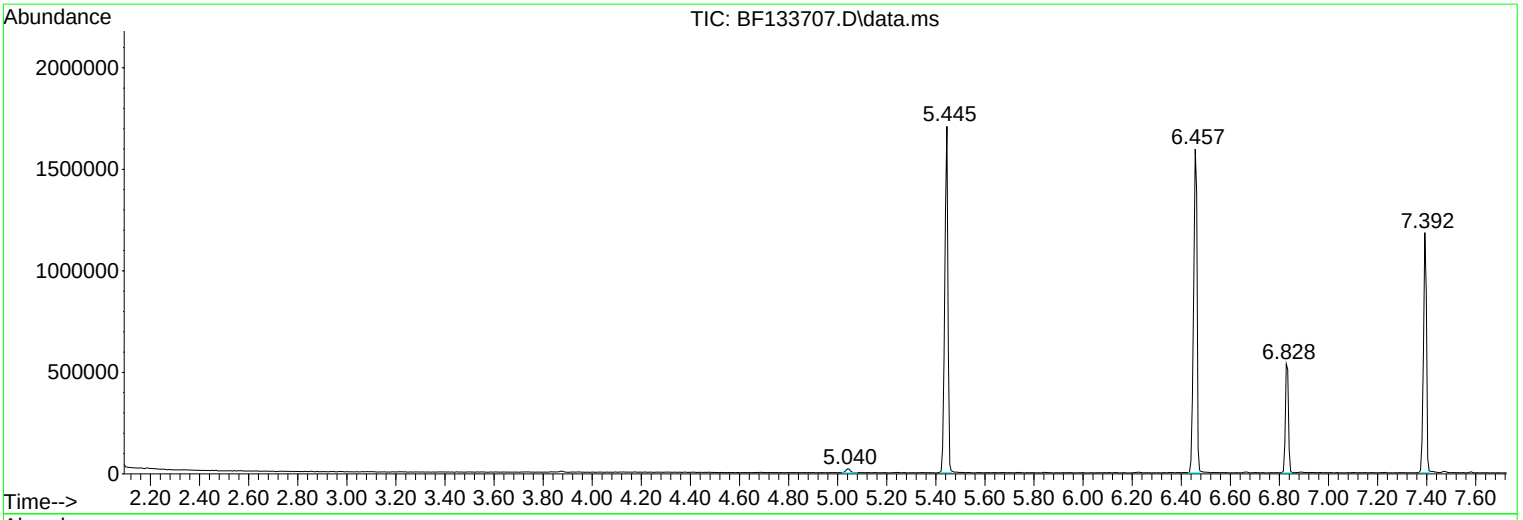
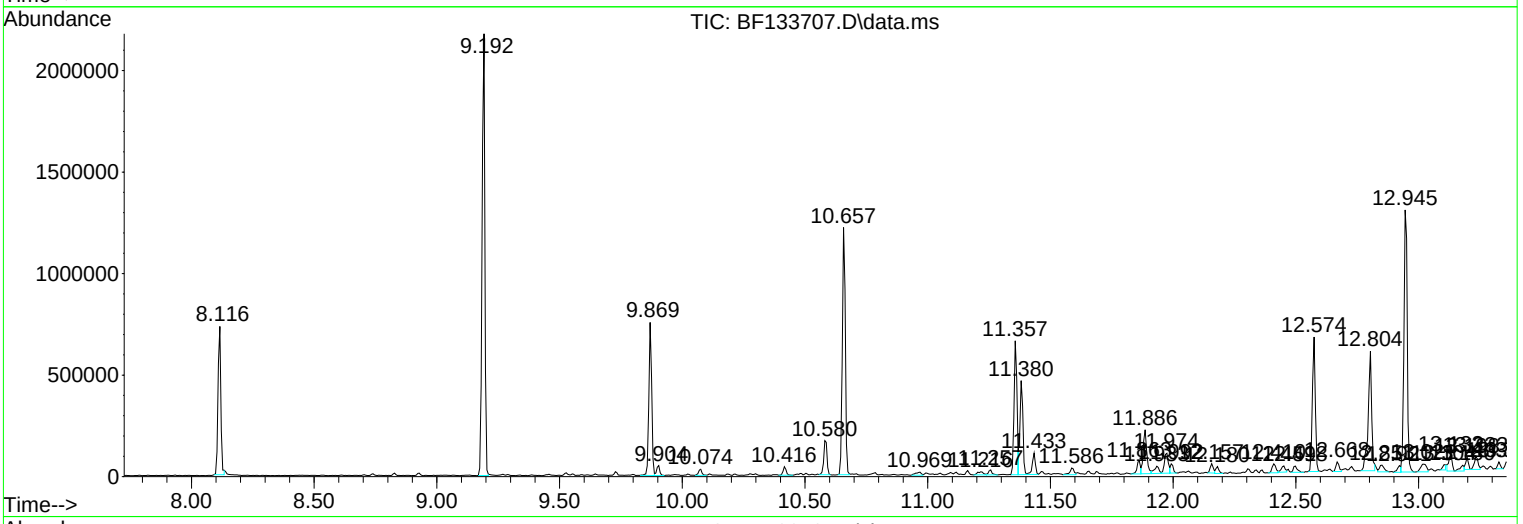
Misc :
ALS Vial : 8 Sample Multiplier: 1

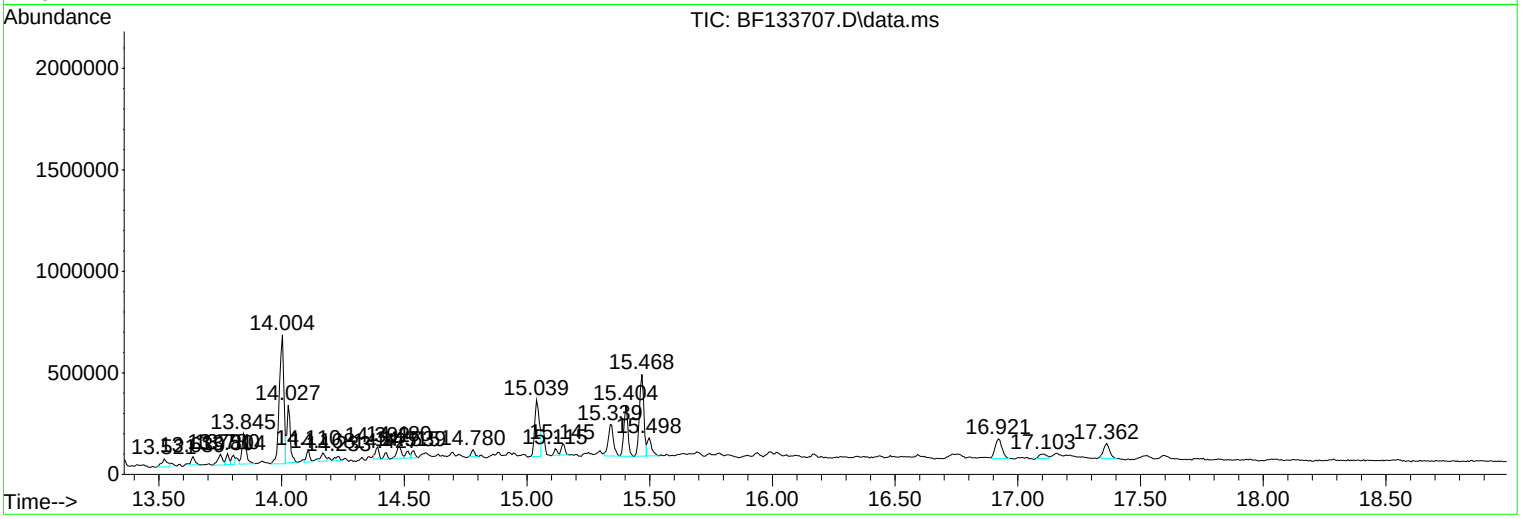
Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BF133707.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

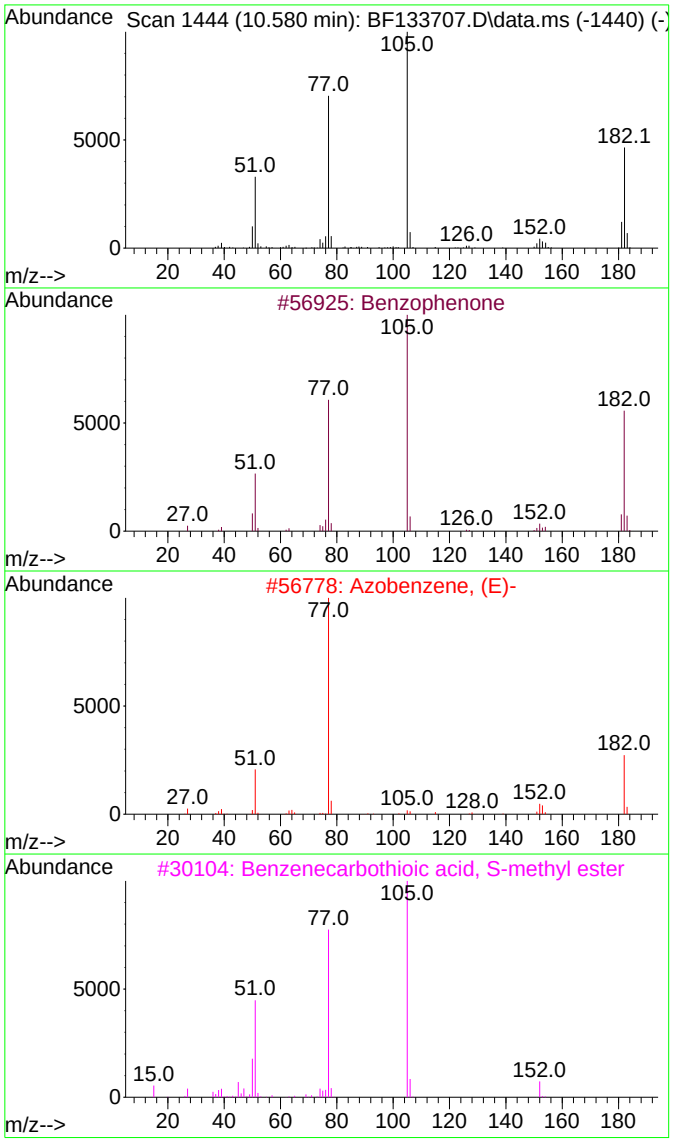
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

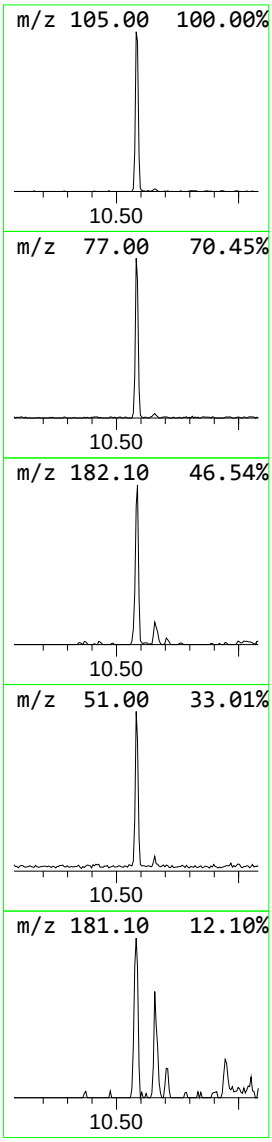
****

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.580	5.07 ng	153981	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Azobenzene, (E)-	182	C12H10N2	017082-12-1	53
3	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

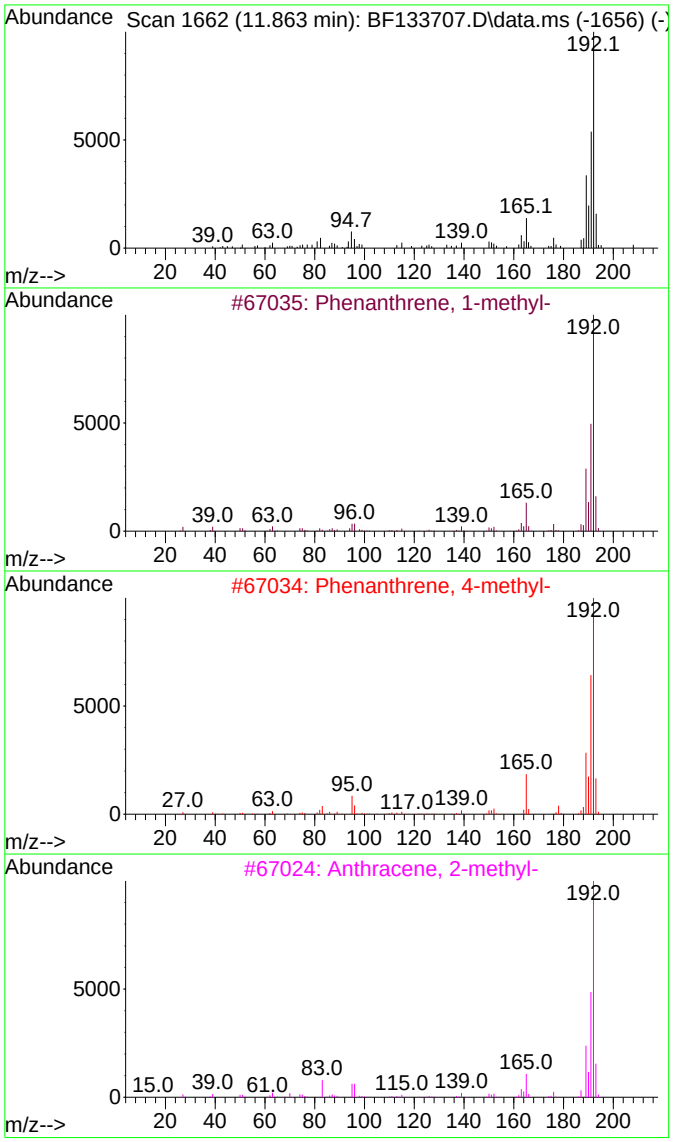
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

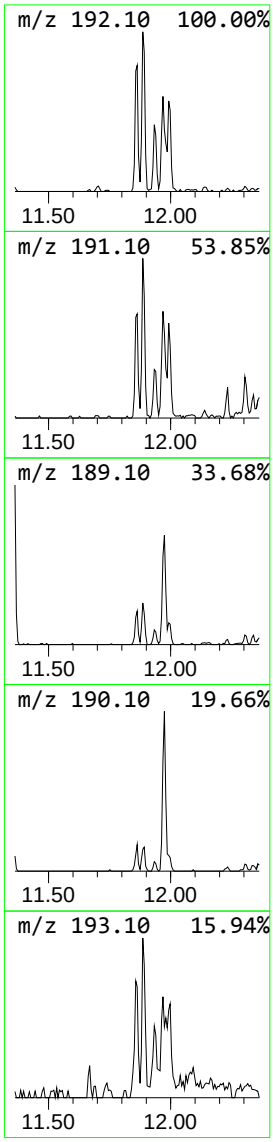
****

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.863	2.32 ng	64067	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
4	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133707.D
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

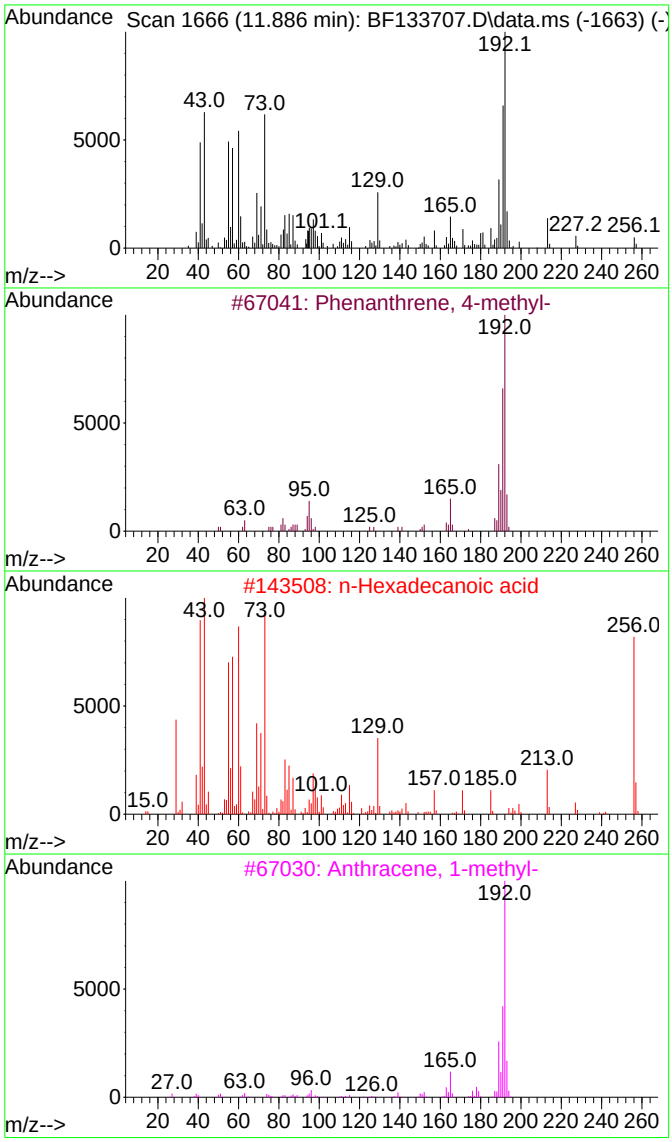
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

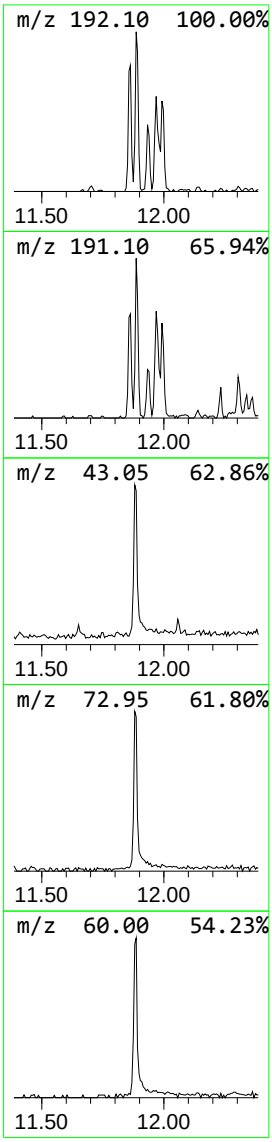
****

Peak Number 3 Phenanthrene, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.886	7.77 ng	214643	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	87
4	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	78
5	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	70





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SB-02-0-2.0

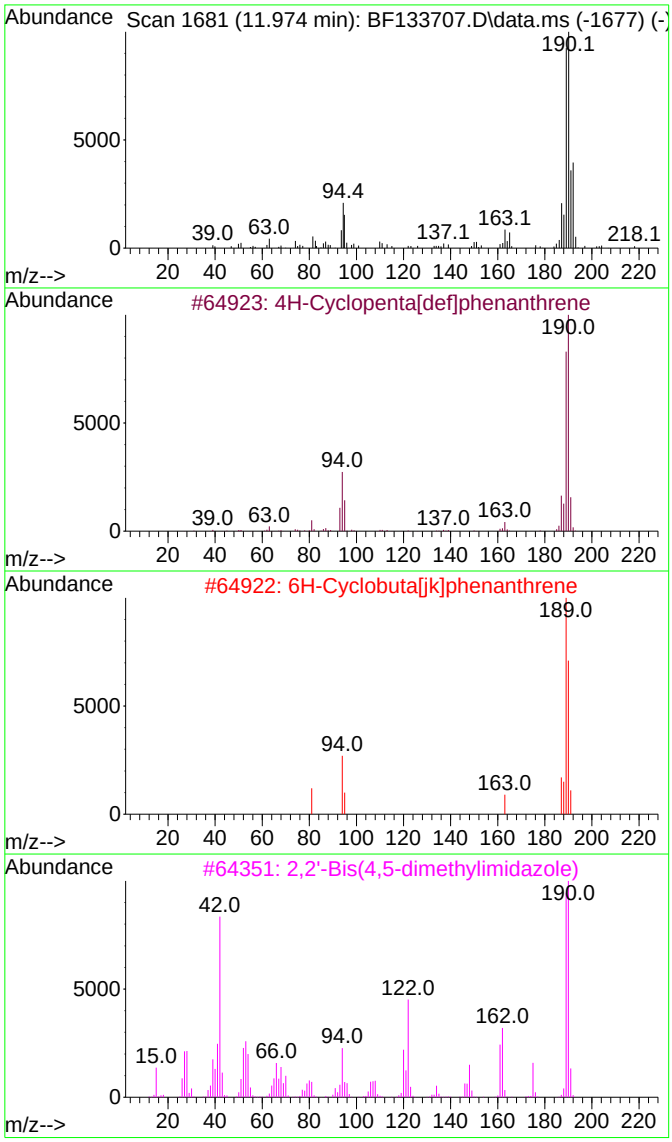
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

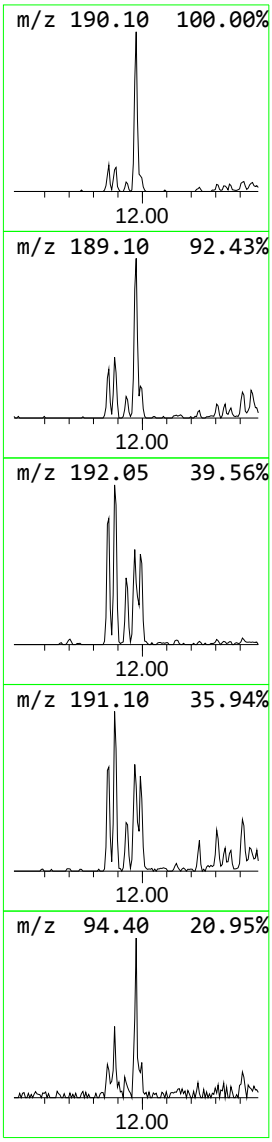
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.974	4.03 ng	111388	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	59
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
4	Pyrimidine, 6-oxo-4-(3-fluorophe...	190	C10H7FN2O	085979-55-1	37
5	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133707.D
Acq On : 12 Jun 2023 16:51
Operator : CG\JU
Sample : 03044-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

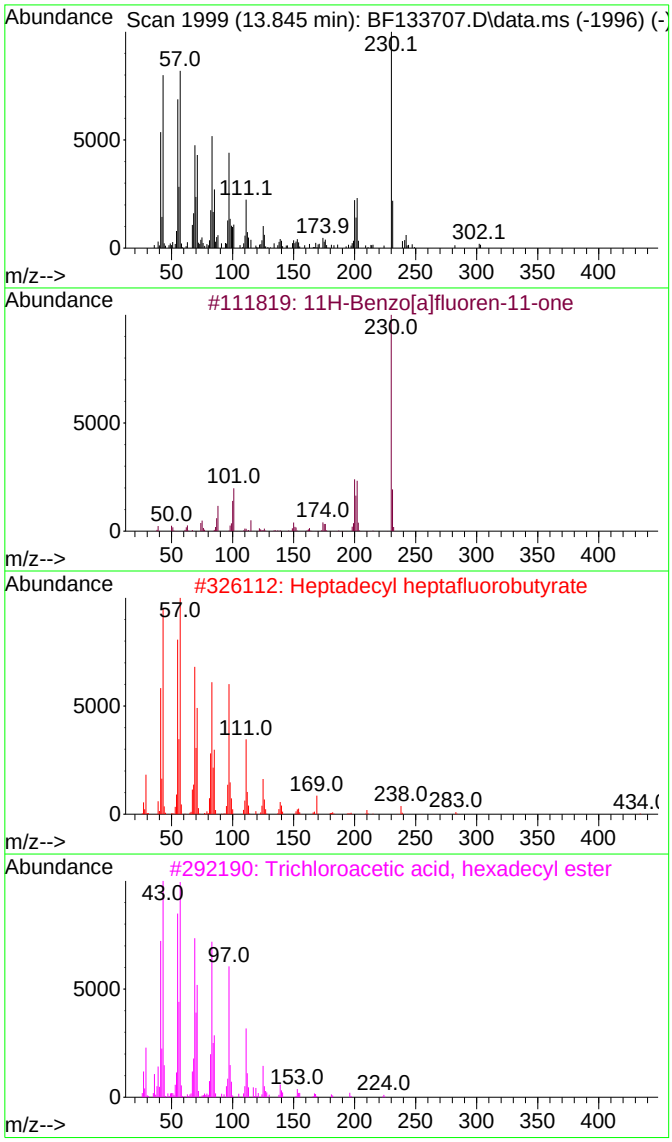
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

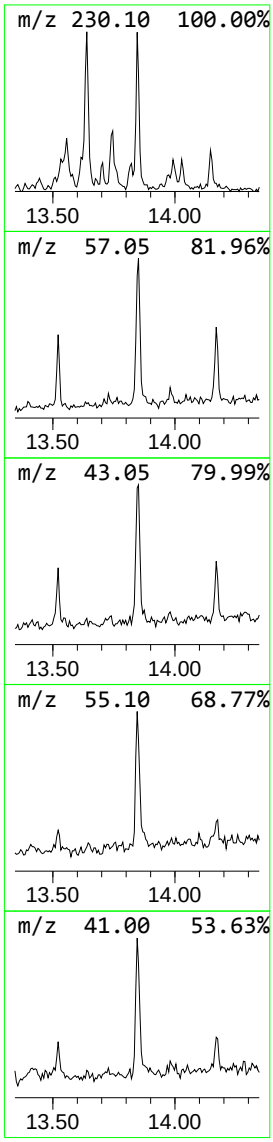
****

Peak Number 5 11H-Benzo[a]fluoren-11-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.845	4.30 ng	177950	Chrysene-d12	14.004

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	94
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	84
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	64
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133707.D
Acq On : 12 Jun 2023 16:51
Operator : CG\JU
Sample : 03044-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

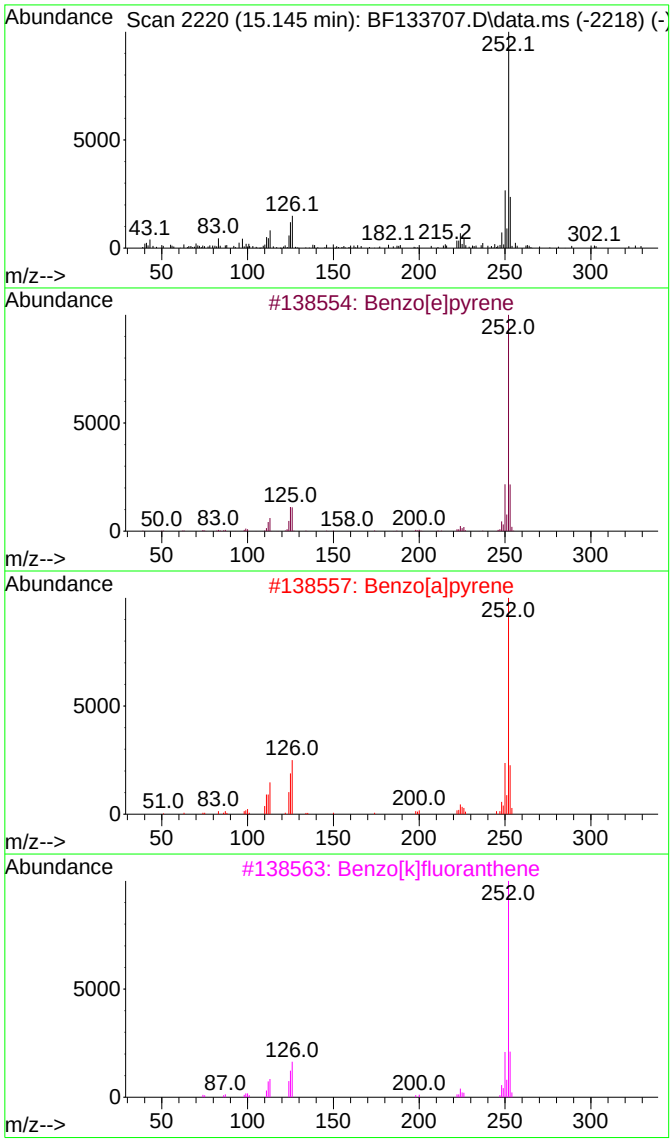
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

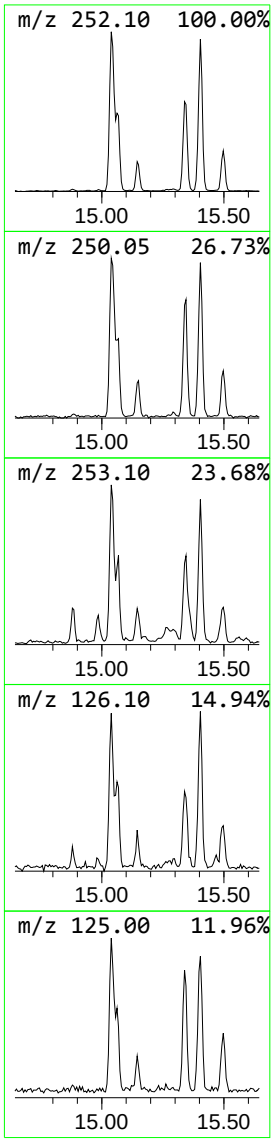
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.145	2.17 ng	55074	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	90
2	Benzo[a]pyrene	252	C20H12	000050-32-8	90
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
5	Perylene	252	C20H12	000198-55-0	81





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133707.D
Acq On : 12 Jun 2023 16:51
Operator : CG\JU
Sample : 03044-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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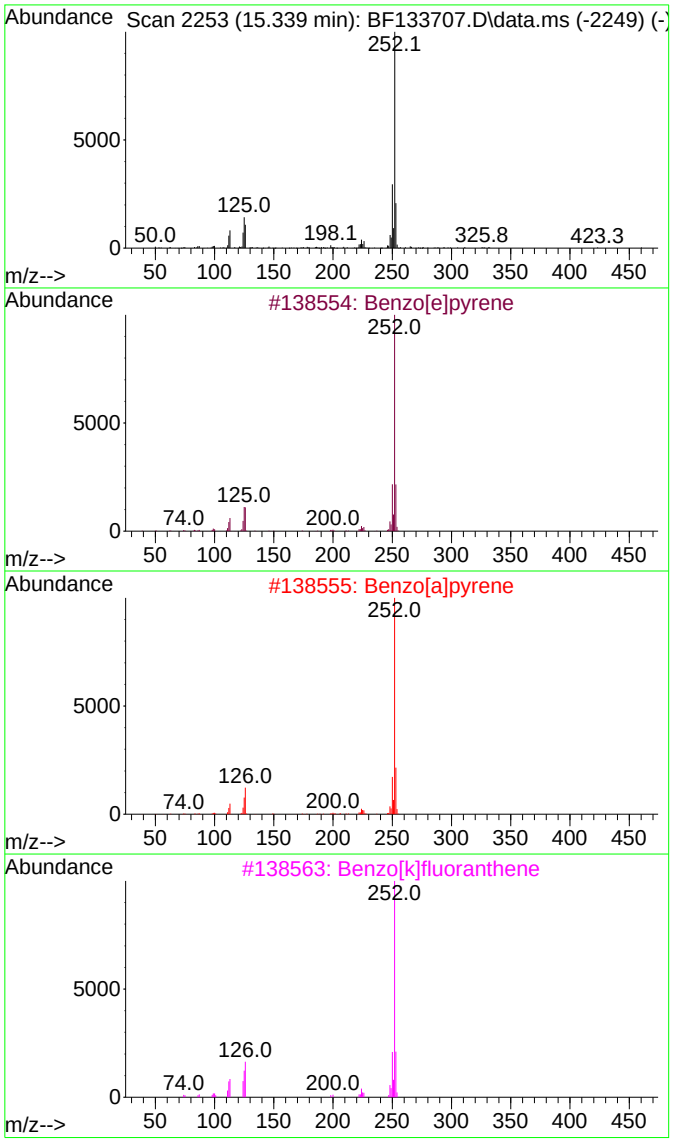
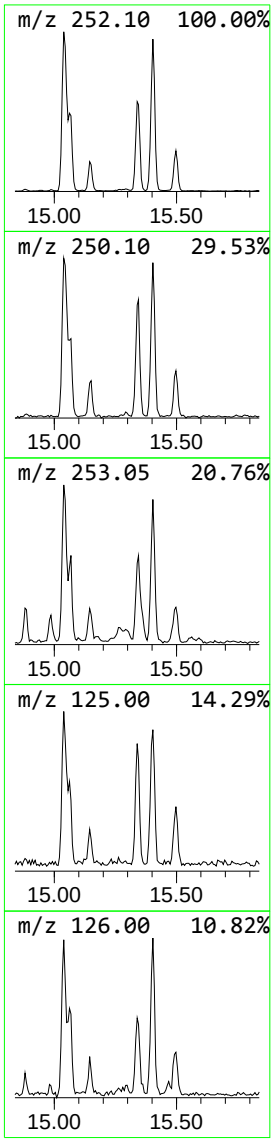
Peak Number 7 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.339	8.86 ng	225216	Perylene-d12	15.468

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[a]pyrene	252	C20H12	000050-32-8	91
3	Benzo[k]fluoranthene	252	C20H12	000207-08-9	90
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	90
5	Perylene	252	C20H12	000198-55-0	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061223\
Data File : BF133707.D
Acq On : 12 Jun 2023 16:51
Operator : CG\JU
Sample : 03044-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-02-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Benzophenone	10.580	5.1	ng	153981	3	9.869	606879	20.0
Phenanthrene, 1...	11.863	2.3	ng	64067	4	11.357	552353	20.0
Phenanthrene, 4...	11.886	7.8	ng	214643	4	11.357	552353	20.0
4H-Cyclopenta[d...	11.974	4.0	ng	111388	4	11.357	552353	20.0
11H-Benzo[a]flu...	13.845	4.3	ng	177950	5	14.004	827530	20.0
Benzo[e]pyrene	15.145	2.2	ng	55074	6	15.468	508644	20.0
Perylene	15.339	8.9	ng	225216	6	15.468	508644	20.0