

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060724\
 Data File : BF138163.D
 Acq On : 07 Jun 2024 16:35
 Operator : CG\JU
 Sample : P2704-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WCS-TPU

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-BF060524.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF138163.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.228	18	24	30	rVB	4005894	5154770	66.02%	7.227%
2	3.434	225	229	241	rBV	98018	181522	2.32%	0.254%
3	5.528	580	585	588	rBV	6241678	6028007	77.20%	8.451%
4	6.528	749	755	758	rBV	6345549	6247024	80.01%	8.758%
5	6.904	815	819	822	rBV	3022997	2270027	29.07%	3.183%
6	7.463	909	914	917	rBV	4211760	4012827	51.39%	5.626%
7	7.716	954	957	960	rBV	215598	152001	1.95%	0.213%
8	8.086	1016	1020	1025	rBV	94126	97099	1.24%	0.136%
9	8.186	1033	1037	1040	rBV	3989973	3078859	39.43%	4.317%
10	8.492	1086	1089	1098	rVB	216918	231543	2.97%	0.325%
11	9.263	1215	1220	1223	rBV	9159425	7808052	100.00%	10.947%
12	9.939	1329	1335	1338	rBV	4565809	3607801	46.21%	5.058%
13	9.969	1338	1340	1344	rVV	474893	377794	4.84%	0.530%
14	10.039	1347	1352	1356	rVV3	121805	168344	2.16%	0.236%
15	10.139	1366	1369	1373	rBV	479025	413179	5.29%	0.579%
16	10.486	1424	1428	1433	rBV	619867	538501	6.90%	0.755%
17	10.639	1452	1454	1459	rVB	168288	153860	1.97%	0.216%
18	10.727	1465	1469	1472	rBV	5338678	4685392	60.01%	6.569%
19	10.845	1485	1489	1496	rVB4	68937	109052	1.40%	0.153%
20	11.033	1514	1521	1523	rBV3	118271	150840	1.93%	0.211%
21	11.157	1538	1542	1544	rBV3	66133	88472	1.13%	0.124%
22	11.268	1558	1561	1563	rBV	86863	92585	1.19%	0.130%
23	11.321	1567	1570	1578	rVB	231768	215072	2.75%	0.302%
24	11.427	1584	1588	1590	rBV	3647712	3300146	42.27%	4.627%
25	11.445	1590	1591	1595	rVV	1552230	1222964	15.66%	1.715%
26	11.498	1595	1600	1603	rVB	1048637	842565	10.79%	1.181%
27	11.927	1667	1673	1675	rBV	231719	268717	3.44%	0.377%
28	11.951	1675	1677	1681	rVV2	457525	401221	5.14%	0.563%
29	11.998	1681	1685	1688	rVV2	185761	189159	2.42%	0.265%
30	12.039	1688	1692	1694	rVV	455096	485001	6.21%	0.680%
31	12.057	1694	1695	1700	rVV	154304	123689	1.58%	0.173%
32	12.121	1700	1706	1710	rVB3	57625	98636	1.26%	0.138%
33	12.221	1720	1723	1729	rVB	197361	170525	2.18%	0.239%
34	12.474	1762	1766	1769	rBV	114826	128172	1.64%	0.180%
35	12.515	1769	1773	1778	rVB	112424	146251	1.87%	0.205%
36	12.639	1790	1794	1797	rBV	2425774	2135833	27.35%	2.994%

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37	12.863	1826	1832	1838	rVB2	1722844	2006133	25.69%	2.813%
38	12.915	1838	1841	1846	rVB2	93247	115372	1.48%	0.162%
39	12.986	1849	1853	1854	rBV	91322	105008	1.34%	0.147%
40	13.010	1854	1857	1860	rVV	6450835	5357025	68.61%	7.511%
41	13.086	1864	1870	1873	rBV3	86139	144014	1.84%	0.202%
42	13.192	1885	1888	1892	rVB	282524	248185	3.18%	0.348%
43	13.257	1895	1899	1902	rBV	271884	255987	3.28%	0.359%
44	13.292	1902	1905	1908	rBV2	137842	148726	1.90%	0.209%
45	13.492	1935	1939	1946	rBV	555162	520416	6.67%	0.730%
46	13.862	2000	2002	2008	rVB3	78171	93460	1.20%	0.131%
47	14.062	2028	2036	2038	rBV2	2023915	2434258	31.18%	3.413%
48	14.086	2038	2040	2043	rVB	568042	434226	5.56%	0.609%
49	14.168	2051	2054	2057	rVB	185996	155478	1.99%	0.218%
50	14.445	2097	2101	2104	rBV	104152	118102	1.51%	0.166%
51	14.539	2114	2117	2120	rBV2	126089	111619	1.43%	0.156%
52	14.592	2124	2126	2130	rVB2	89159	88109	1.13%	0.124%
53	15.104	2209	2213	2217	rBV	471402	788287	10.10%	1.105%
54	15.215	2230	2232	2237	rVB	120496	119796	1.53%	0.168%
55	15.415	2262	2266	2271	rVB	261609	306146	3.92%	0.429%
56	15.474	2272	2276	2281	rBV	367312	421541	5.40%	0.591%
57	15.545	2283	2288	2291	rBV	1189024	1463115	18.74%	2.051%
58	17.021	2535	2539	2550	rVB2	151613	344517	4.41%	0.483%
59	17.474	2611	2616	2623	rVB2	79990	170780	2.19%	0.239%

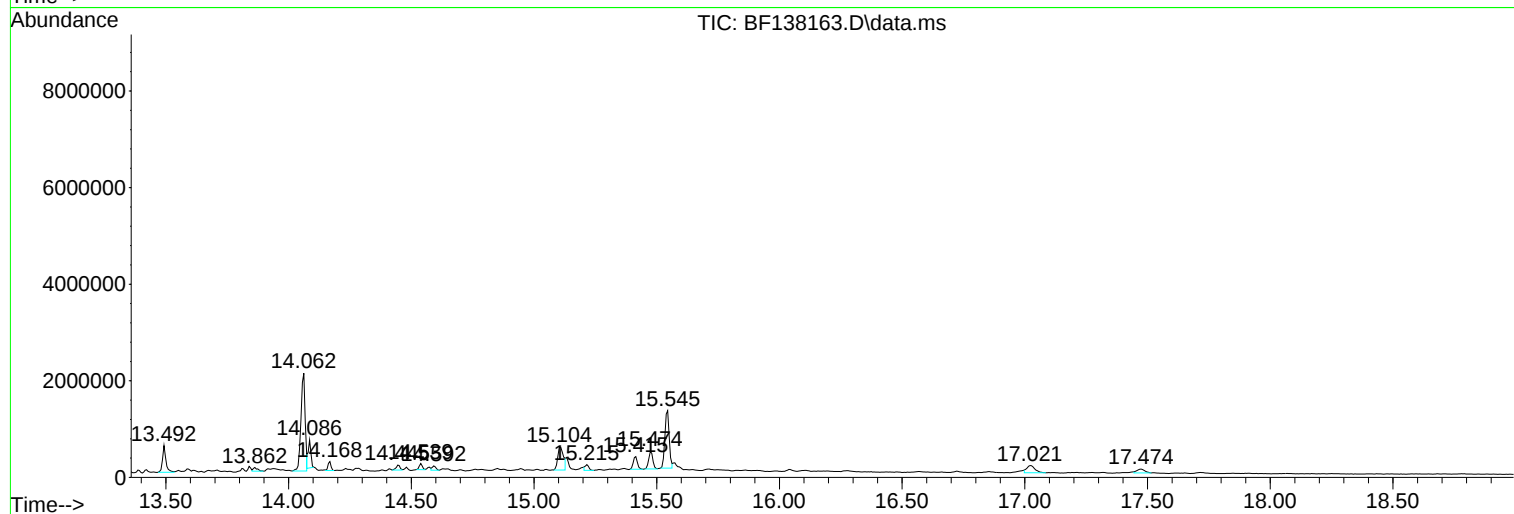
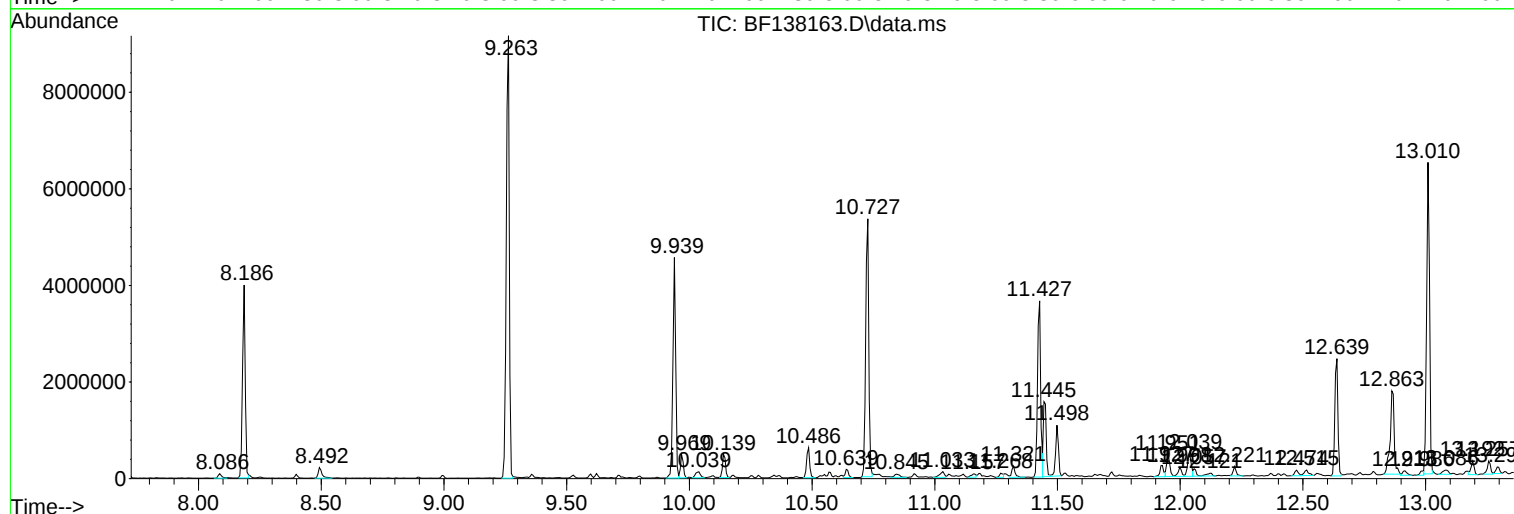
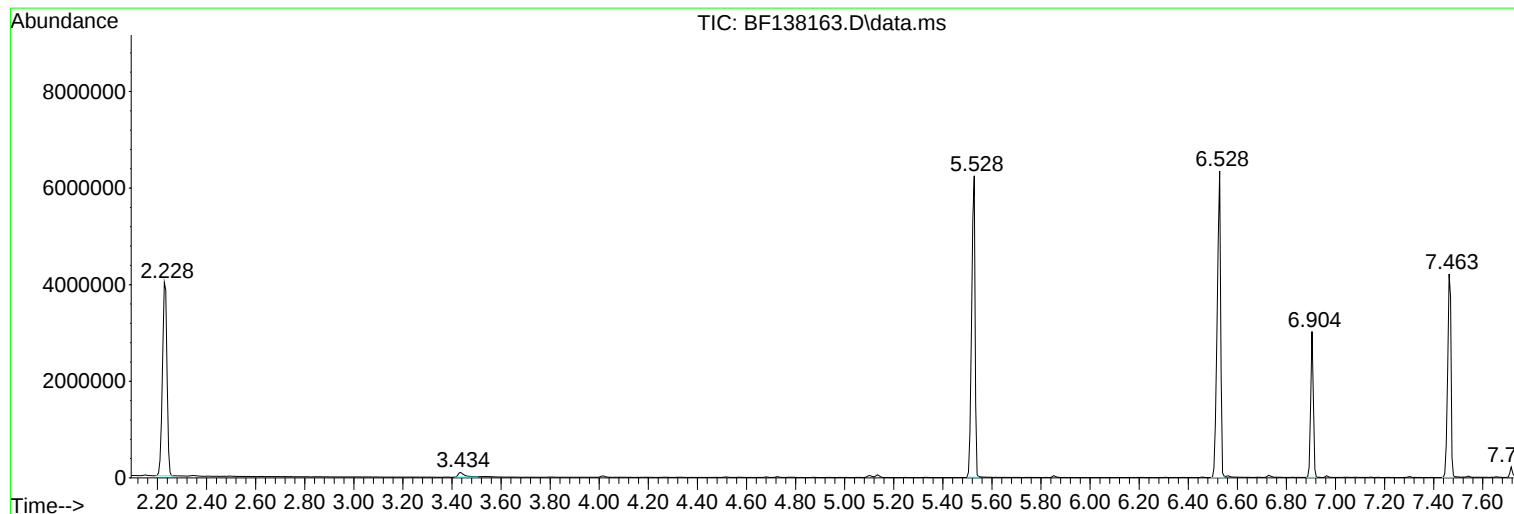
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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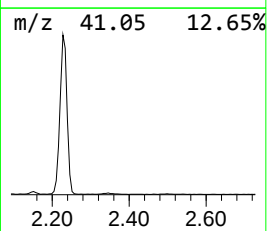
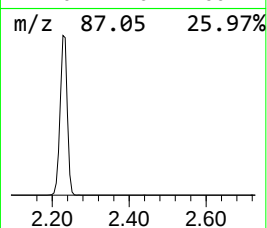
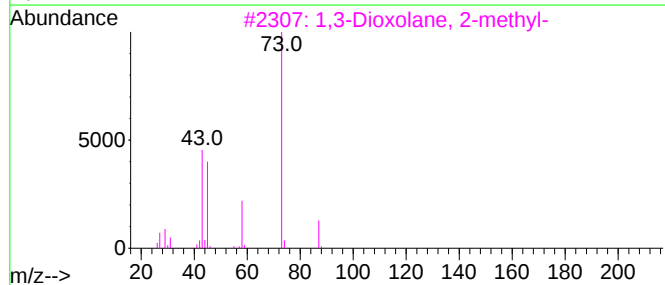
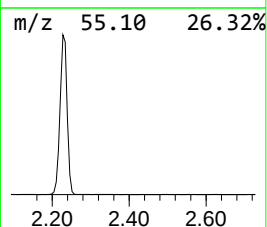
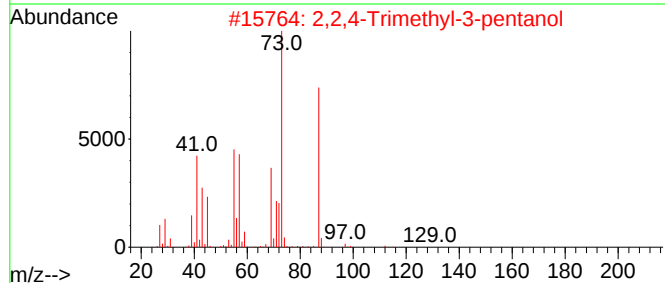
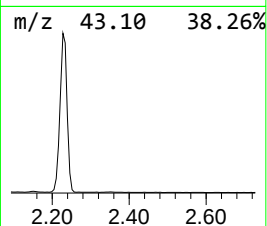
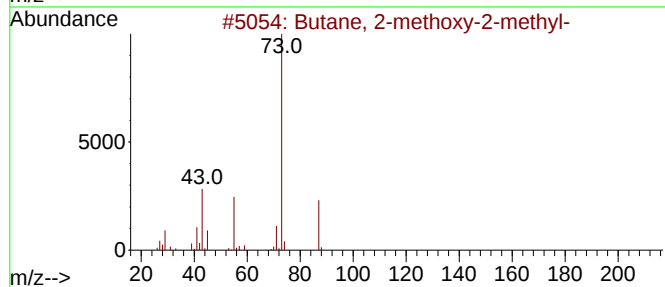
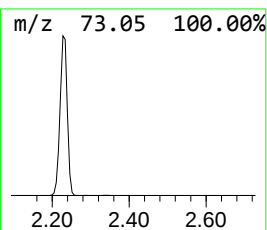
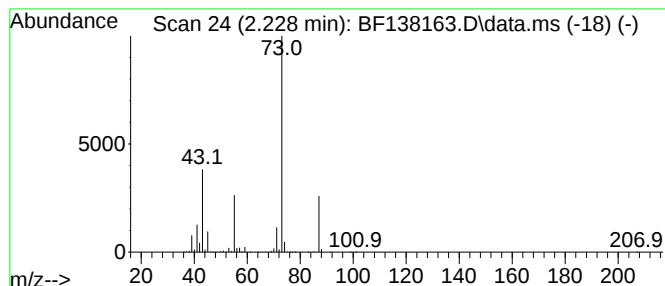
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.228	45.42 ng	5154770	1,4-Dichlorobenzene-d4	6.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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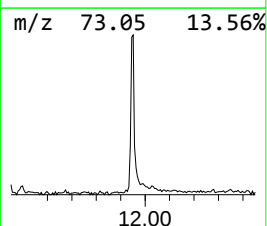
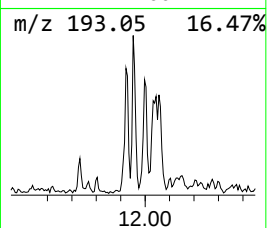
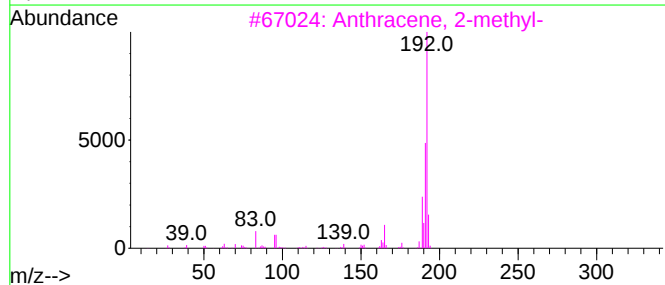
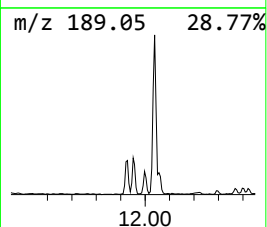
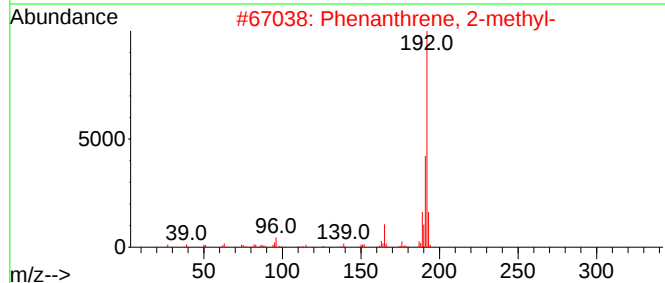
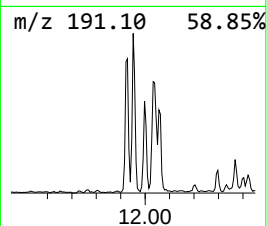
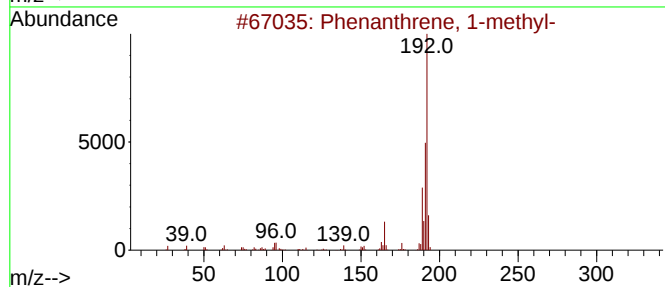
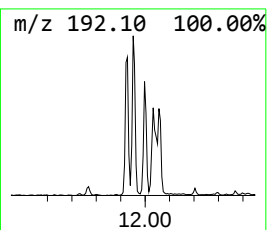
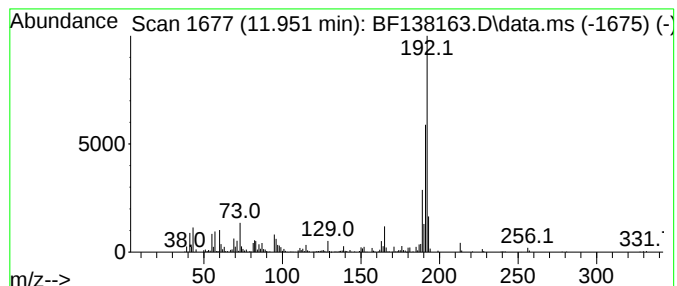
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Phenanthrene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	2.43 ng	401221	Phenanthrene-d10	11.427

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	97
4		Anthracene, 1-methyl-	192	C15H12	000610-48-0	96
5		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	95



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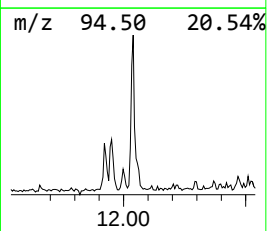
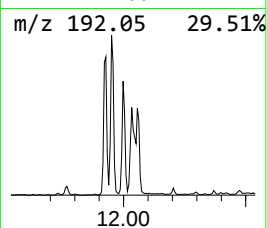
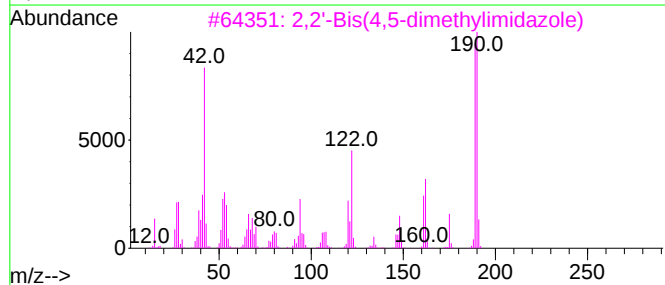
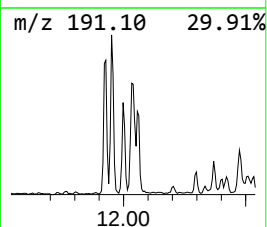
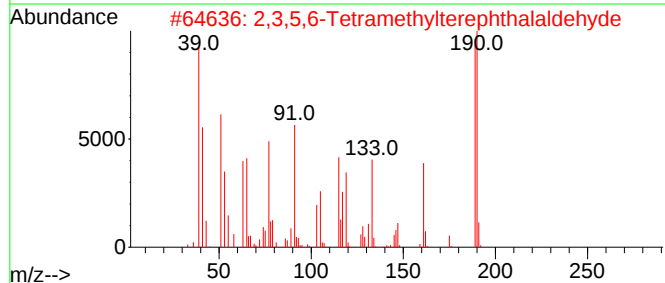
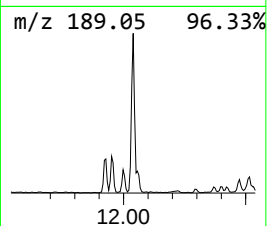
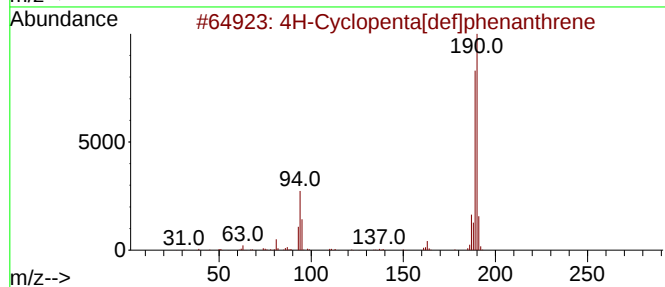
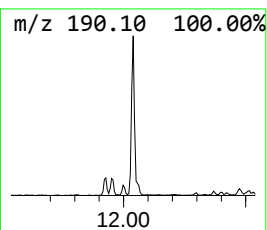
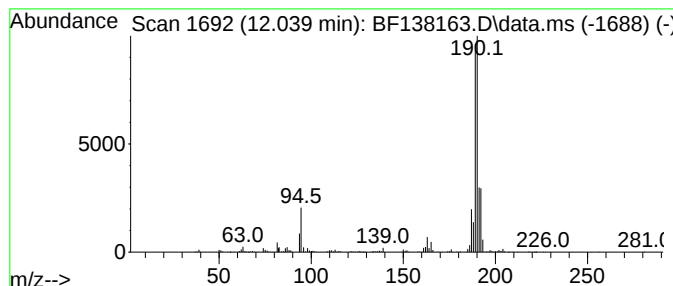
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 4H-Cyclopenta[def]phenanthrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.039	2.94 ng	485001	Phenanthrene-d10	11.427	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	87
2	2,3,5,6-Tetramethylterephthalald...	190	C12H14O2	007072-01-7	50
3	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	45
4	1,4-Naphthalenedione, 2,5-dihydr...	190	C10H6O4	004923-55-1	25
5	2,4(1H,3H)-Pyrimidinedione, 5-br...	190	C4H3BrN2O2	000051-20-7	16



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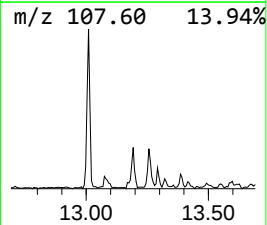
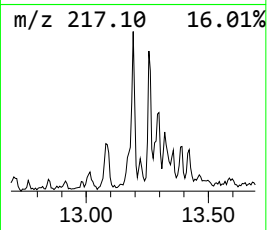
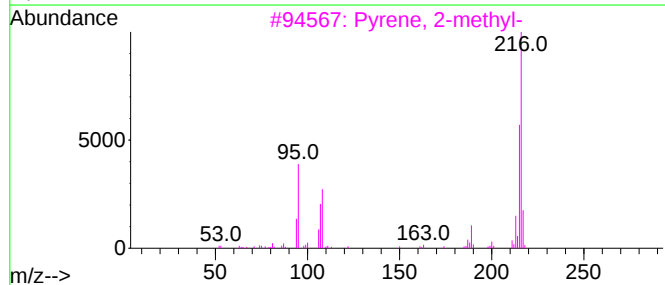
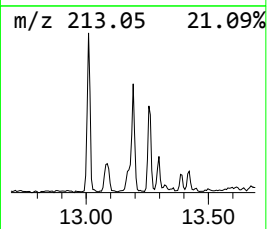
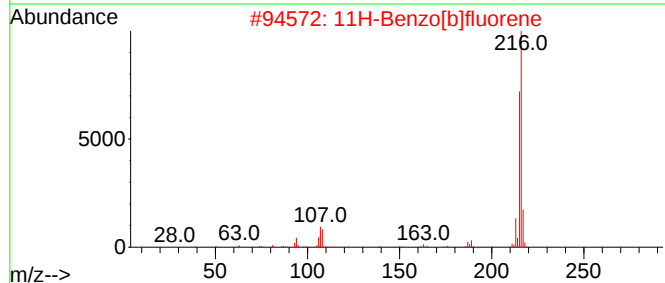
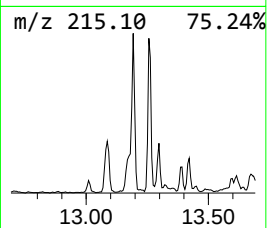
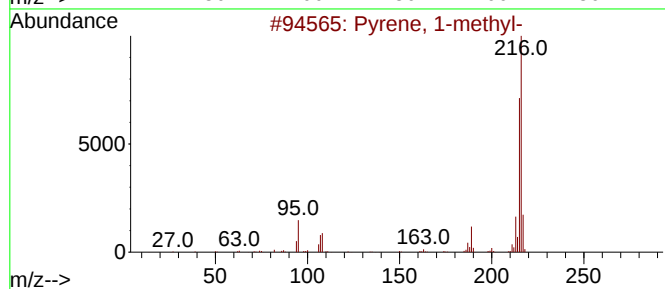
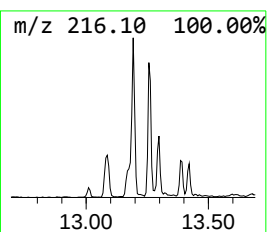
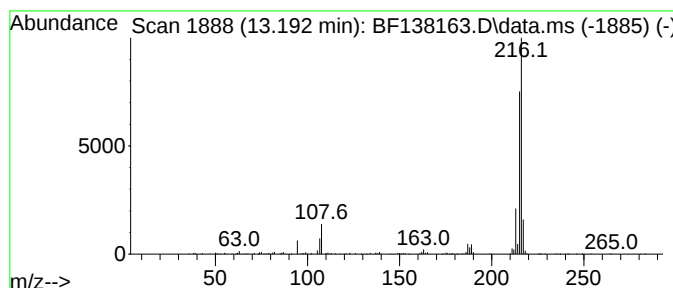
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pyrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.192	2.04 ng	248185	Chrysene-d12	14.062

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	90
2			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
3			Pyrene, 2-methyl-	216	C17H12	003442-78-2	76
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	74
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	64



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ClientSampleId :
WCS-TPU

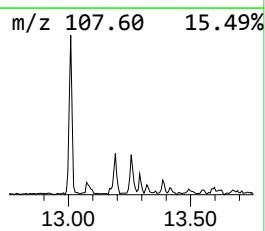
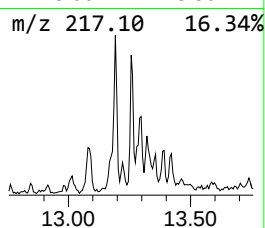
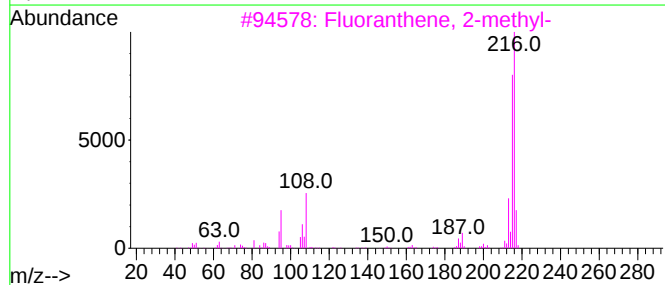
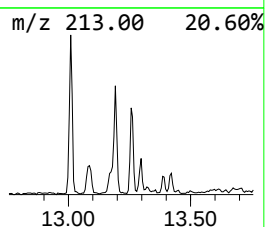
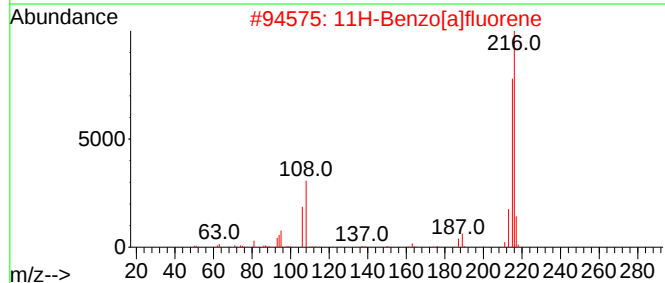
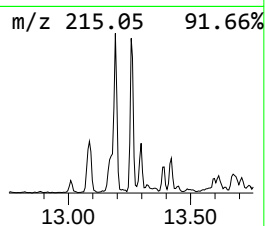
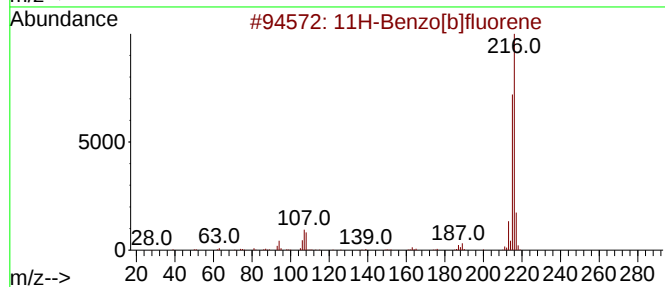
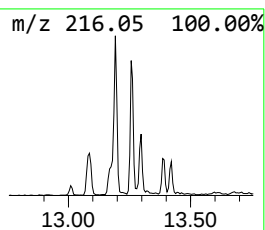
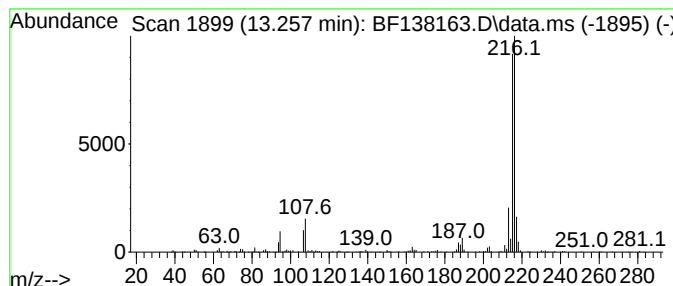
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.257	2.10 ng	255987	Chrysene-d12	14.062

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[b]fluorene	216	C17H12	000243-17-4	94
2			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
3			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
4			Pyrene, 1-methyl-	216	C17H12	002381-21-7	86
5			7H-Benzo[c]fluorene	216	C17H12	000205-12-9	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060724\
Data File : BF138163.D
Acq On : 07 Jun 2024 16:35
Operator : CG\JU
Sample : P2704-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

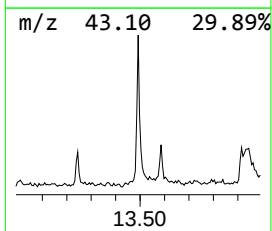
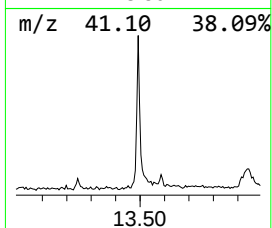
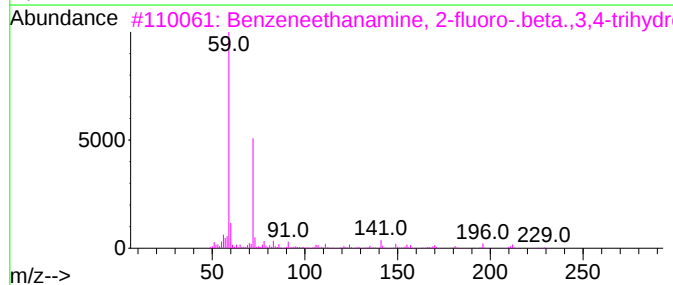
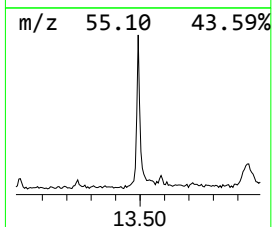
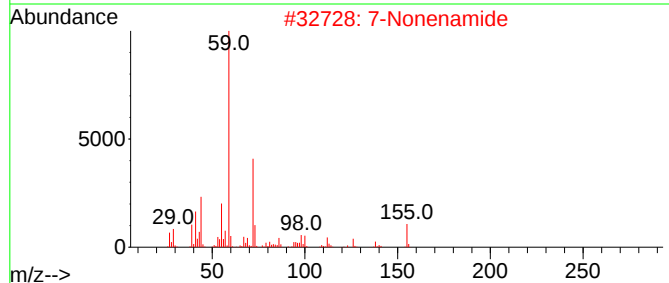
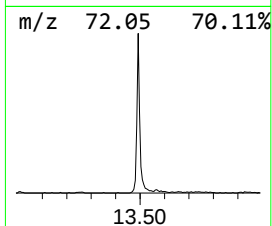
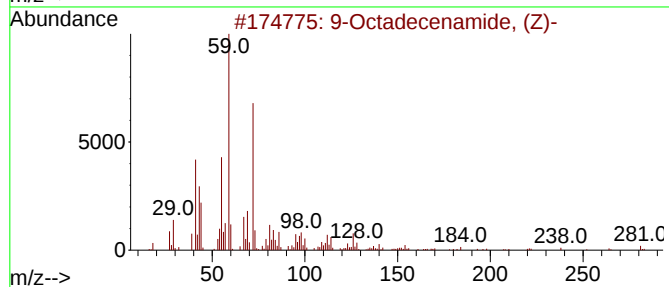
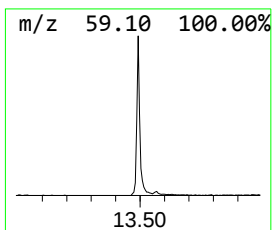
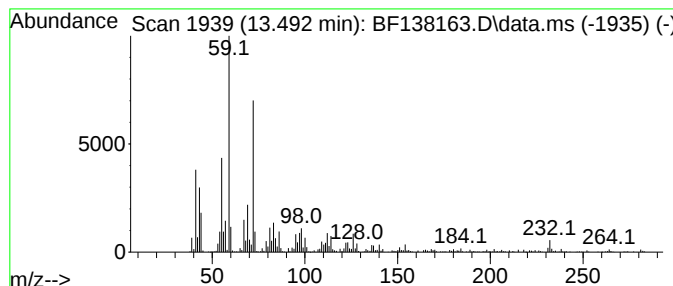
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ClientSampleId :
WCS-TPU

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.492	4.28 ng	520416	Chrysene-d12		14.062	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	99
2	7-Nonenamide		155	C9H17NO	090949-53-4	72
3	Benzeneethanamine, 2-fluoro-.bet...		229	C11H16FN03	061338-98-5	64
4	Octanamide		143	C8H17NO	000629-01-6	59
5	Dodecanamide		199	C12H25NO	001120-16-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060724\
Data File : BF138163.D
Acq On : 07 Jun 2024 16:35
Operator : CG\JU
Sample : P2704-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPU

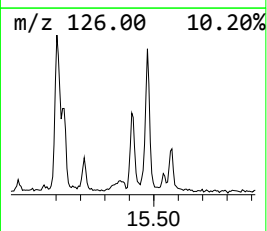
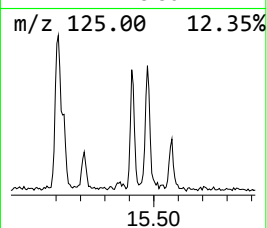
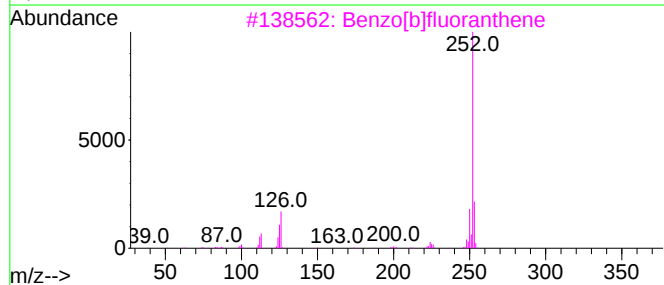
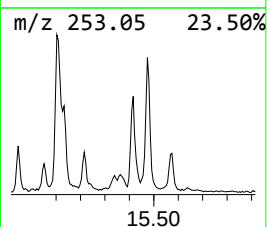
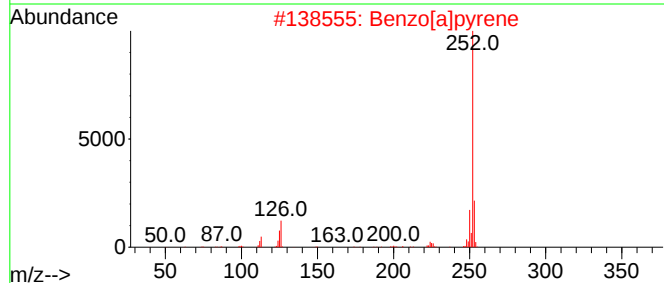
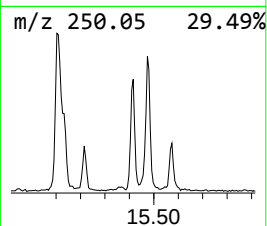
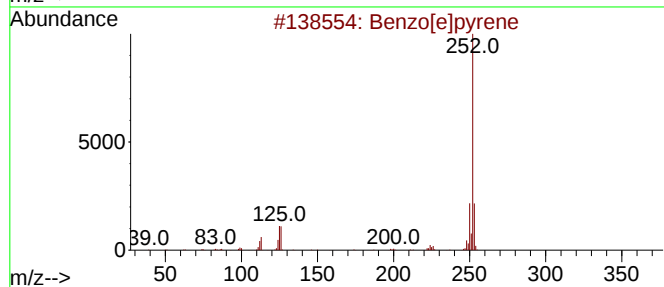
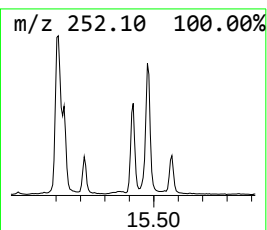
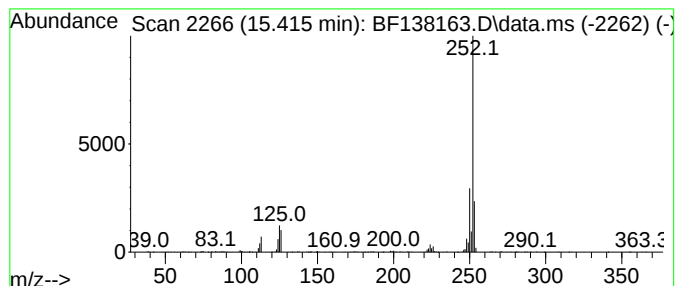
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.415	4.18 ng	306146	Perylene-d12	15.545

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	96
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5			Perylene	252	C20H12	000198-55-0	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060724\
Data File : BF138163.D
Acq On : 07 Jun 2024 16:35
Operator : CG\JU
Sample : P2704-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WCS-TPU

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060524.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.228	45.4	ng	5154770	1	6.904	2270030	20.0
Phenanthrene, 1...	11.951	2.4	ng	401221	4	11.427	3300150	20.0
4H-Cyclopenta[d...	12.039	2.9	ng	485001	4	11.427	3300150	20.0
Pyrene, 1-methyl-	13.192	2.0	ng	248185	5	14.062	2434260	20.0
11H-Benzo[b]flu...	13.257	2.1	ng	255987	5	14.062	2434260	20.0
9-Octadecenamid...	13.492	4.3	ng	520416	5	14.062	2434260	20.0
Benzo[e]pyrene	15.415	4.2	ng	306146	6	15.545	1463120	20.0