

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
 Data File : BF137601.D
 Acq On : 14 Mar 2024 20:26
 Operator : CG\JU
 Sample : P1746-16
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-05-0-2.0-DUP

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-BF022924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137601.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.075	164	168	170	rBV	18712	30814	1.19%	0.108%
2	5.328	548	551	568	rBV	2514551	2460635	95.35%	8.617%
3	6.357	723	726	744	rBV	2554415	2488780	96.45%	8.716%
4	6.728	785	789	801	rBV	820099	818108	31.70%	2.865%
5	7.287	881	884	888	rBV	1670276	1412710	54.75%	4.947%
6	7.322	888	890	898	rVB	351578	337397	13.07%	1.182%
7	8.004	1003	1006	1013	rBV	1168439	1045266	40.51%	3.660%
8	8.328	1058	1061	1070	rBV	35187	58307	2.26%	0.204%
9	9.081	1185	1189	1201	rBV	3126782	2580502	100.00%	9.037%
10	9.616	1277	1280	1286	rBV	76904	74490	2.89%	0.261%
11	9.681	1288	1291	1296	rBV	161324	135874	5.27%	0.476%
12	9.757	1300	1304	1308	rBV	1319521	1105948	42.86%	3.873%
13	9.857	1317	1321	1328	rVB2	69685	90356	3.50%	0.316%
14	10.545	1434	1438	1452	rBV	1339555	1366609	52.96%	4.786%
15	10.669	1455	1459	1464	rVB3	29192	37657	1.46%	0.132%
16	11.239	1552	1556	1558	rBV	1177296	988256	38.30%	3.461%
17	11.263	1558	1560	1567	rVV	402791	373697	14.48%	1.309%
18	11.316	1567	1569	1573	rVB	51460	46329	1.80%	0.162%
19	11.480	1594	1597	1604	rBV2	23255	42364	1.64%	0.148%
20	11.639	1620	1624	1631	rVB2	34641	40501	1.57%	0.142%
21	11.739	1637	1641	1644	rBV2	96769	105454	4.09%	0.369%
22	11.775	1644	1647	1651	rBV2	252646	312684	12.12%	1.095%
23	11.851	1657	1660	1662	rBV2	113463	115886	4.49%	0.406%
24	11.880	1662	1665	1670	rVB2	146458	147656	5.72%	0.517%
25	12.039	1688	1692	1694	rBV	51933	52142	2.02%	0.183%
26	12.063	1694	1696	1700	rVB	54495	48427	1.88%	0.170%
27	12.286	1731	1734	1737	rBV	74580	82270	3.19%	0.288%
28	12.327	1737	1741	1743	rVV4	47367	68771	2.67%	0.241%
29	12.375	1746	1749	1753	rBV	69479	73912	2.86%	0.259%
30	12.445	1758	1761	1765	rBV	981047	943402	36.56%	3.304%
31	12.486	1765	1768	1775	rVB3	71953	120160	4.66%	0.421%
32	12.545	1775	1778	1783	rBV	67810	86706	3.36%	0.304%
33	12.674	1795	1800	1803	rBV	986952	936626	36.30%	3.280%
34	12.727	1807	1809	1813	rVB2	47097	48469	1.88%	0.170%
35	12.798	1818	1821	1822	rBV2	40862	38079	1.48%	0.133%
36	12.822	1822	1825	1832	rVB	2451614	2158225	83.64%	7.558%

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37	12.898	1833	1838	1842	rVV4	77845	113848	4.41%	0.399%
38	12.980	1849	1852	1854	rBV3	69864	88556	3.43%	0.310%
39	13.004	1854	1856	1859	rVB	123978	107230	4.16%	0.376%
40	13.074	1860	1868	1870	rBV2	71182	112789	4.37%	0.395%
41	13.110	1870	1874	1877	rVV	105465	111531	4.32%	0.391%
42	13.198	1886	1889	1892	rVB	65158	54024	2.09%	0.189%
43	13.233	1892	1895	1898	rBV2	57039	56800	2.20%	0.199%
44	13.298	1904	1906	1913	rVB6	19217	38057	1.47%	0.133%
45	13.404	1921	1924	1926	rBV4	37276	40619	1.57%	0.142%
46	13.516	1940	1943	1947	rVB	101587	104099	4.03%	0.365%
47	13.621	1956	1961	1964	rBV	120656	153758	5.96%	0.538%
48	13.651	1964	1966	1968	rVV	95789	95682	3.71%	0.335%
49	13.674	1968	1970	1972	rVV	86195	86890	3.37%	0.304%
50	13.727	1976	1979	1986	rVB2	218611	284244	11.02%	0.995%
51	13.869	1998	2003	2006	rBV2	1216212	1661088	64.37%	5.817%
52	13.898	2006	2008	2014	rVB	584248	541728	20.99%	1.897%
53	13.974	2019	2021	2024	rVB	47874	40010	1.55%	0.140%
54	14.021	2026	2029	2031	rBV	56452	65483	2.54%	0.229%
55	14.045	2031	2033	2036	rVB4	42903	37326	1.45%	0.131%
56	14.221	2061	2063	2065	rBV2	39984	40351	1.56%	0.141%
57	14.263	2065	2070	2073	rVV	111264	144574	5.60%	0.506%
58	14.292	2073	2075	2080	rVB2	59074	63828	2.47%	0.224%
59	14.351	2082	2085	2088	rVV3	83952	73696	2.86%	0.258%
60	14.380	2088	2090	2093	rBV3	43811	41617	1.61%	0.146%
61	14.580	2122	2124	2127	rVB2	73098	66971	2.60%	0.235%
62	14.645	2132	2135	2137	rBV2	54938	52866	2.05%	0.185%
63	14.716	2145	2147	2149	rBV	40618	45412	1.76%	0.159%
64	14.886	2172	2176	2179	rBV	557546	784815	30.41%	2.748%
65	14.992	2191	2194	2198	rVB	97729	100424	3.89%	0.352%
66	15.174	2221	2225	2232	rBV	320928	415504	16.10%	1.455%
67	15.233	2232	2235	2241	rVB	450188	523608	20.29%	1.834%
68	15.292	2241	2245	2249	rBV	818405	1023532	39.66%	3.584%
69	16.674	2475	2480	2489	rVB2	147918	297438	11.53%	1.042%
70	17.092	2546	2551	2559	rVB	111886	213482	8.27%	0.748%

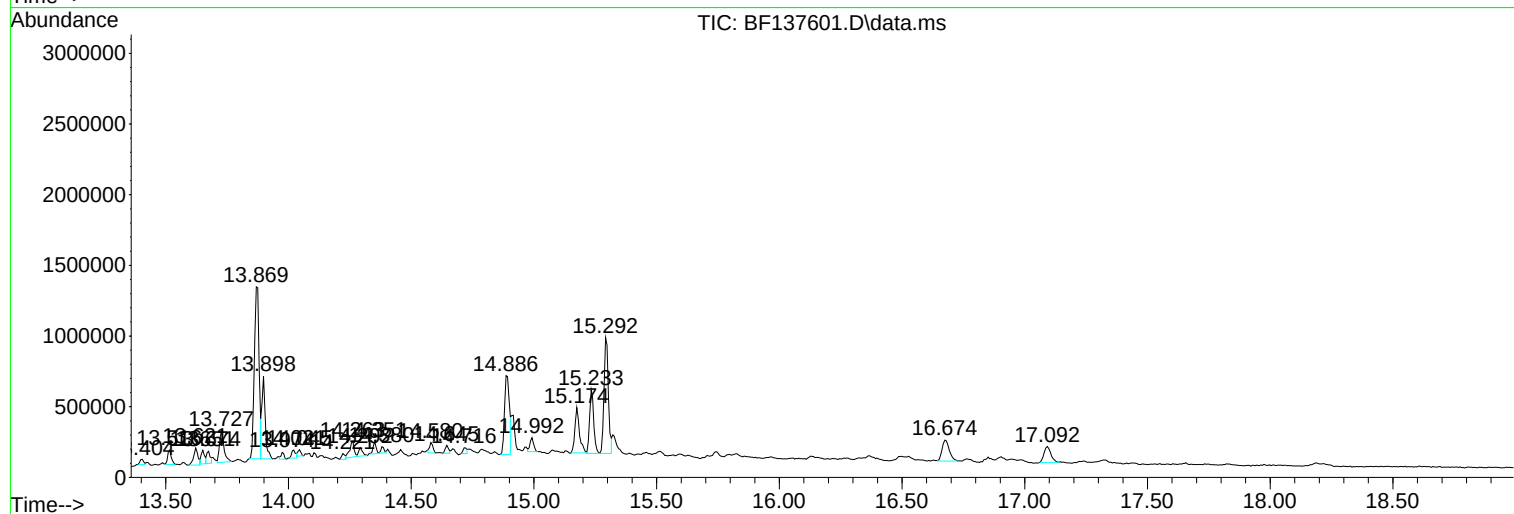
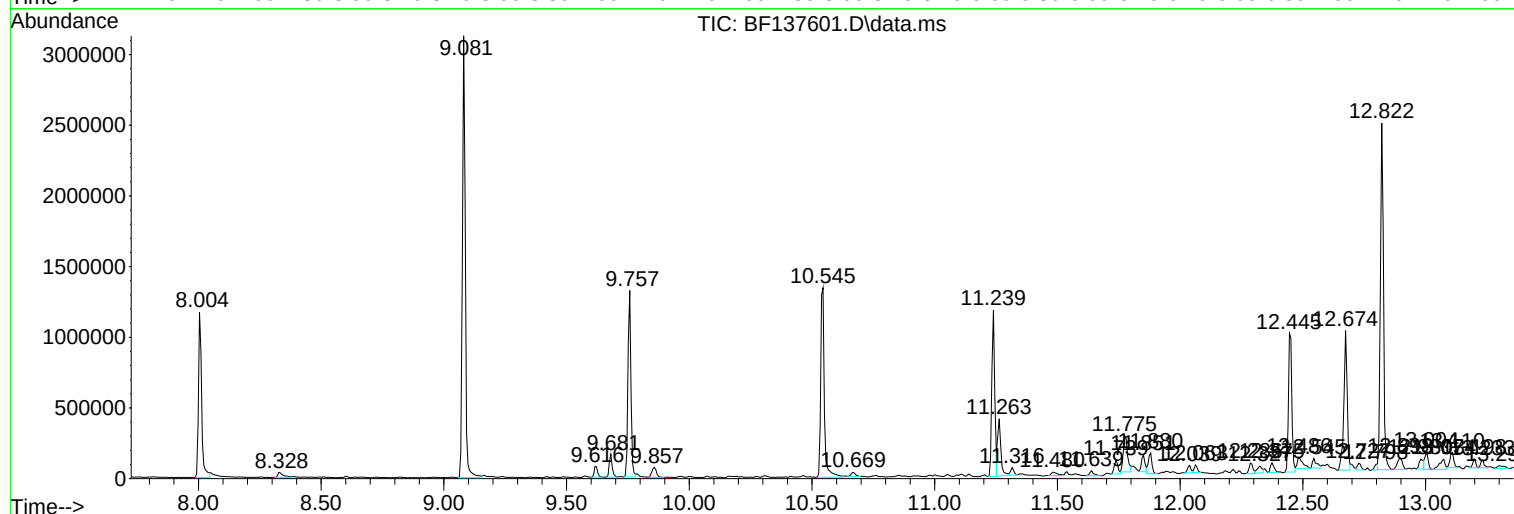
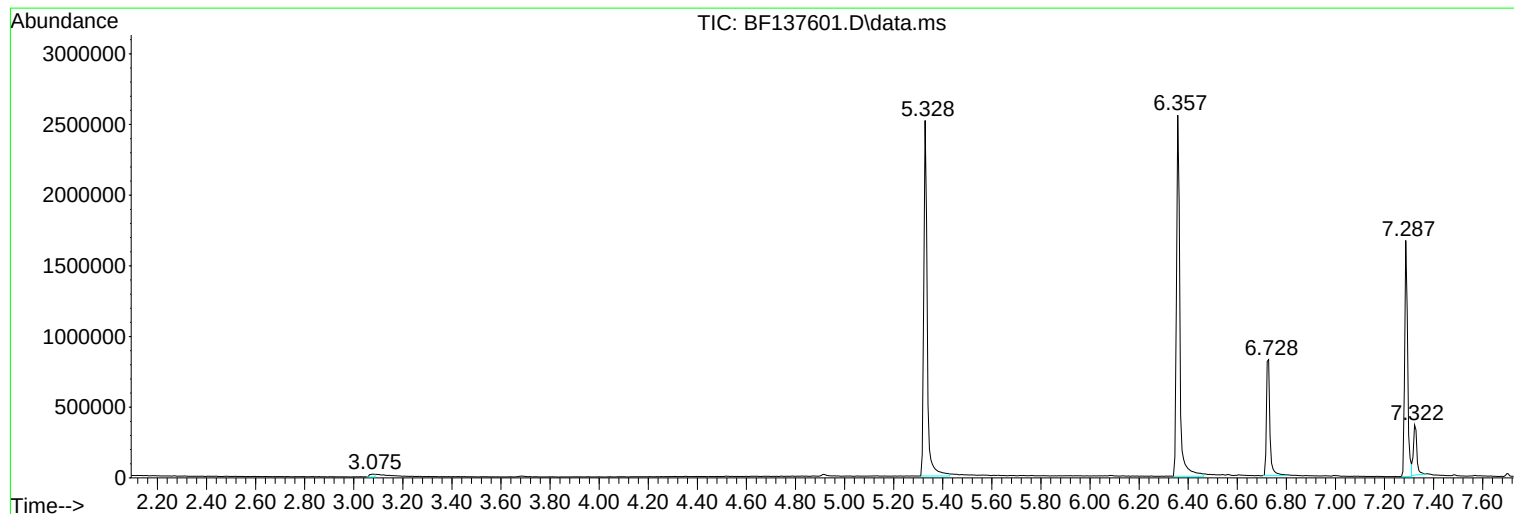
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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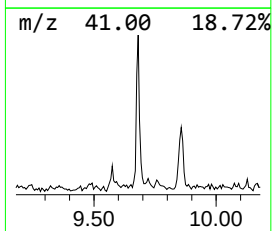
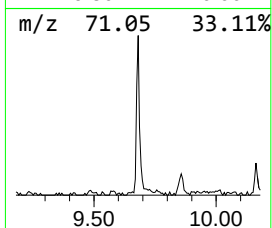
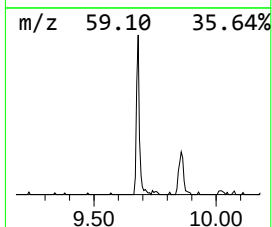
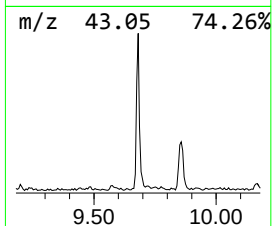
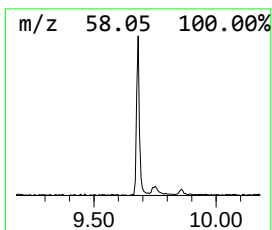
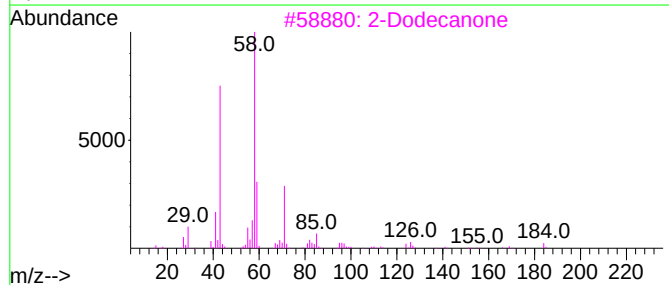
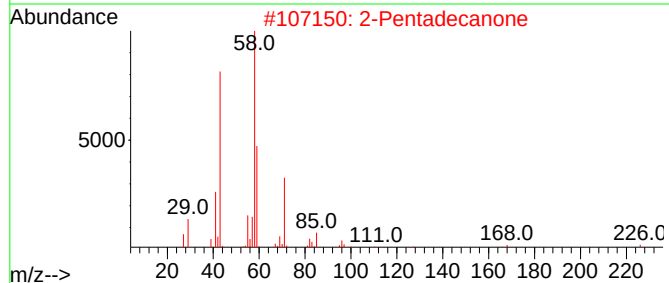
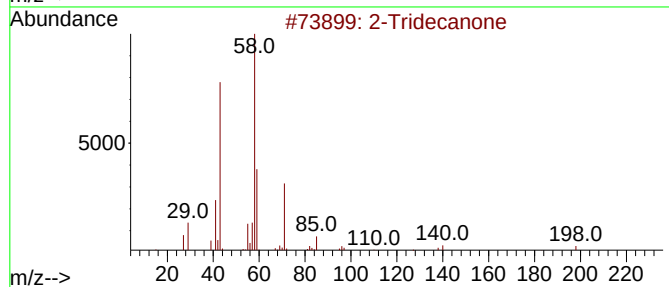
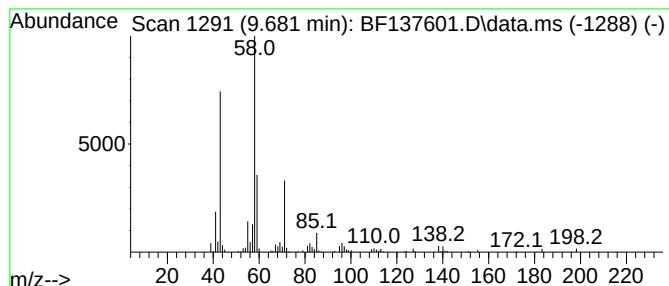
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Tridecanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.681	2.46 ng	135874	Acenaphthene-d10	9.757

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Tridecanone	198	C13H26O	000593-08-8	95	
2	2-Pentadecanone	226	C15H30O	002345-28-0	91	
3	2-Dodecanone	184	C12H24O	006175-49-1	83	
4	2-Decanone	156	C10H20O	000693-54-9	83	
5	2-Tetradecanone	212	C14H28O	002345-27-9	64	



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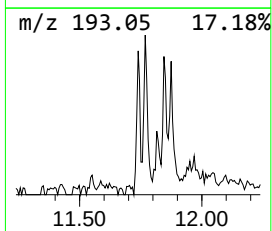
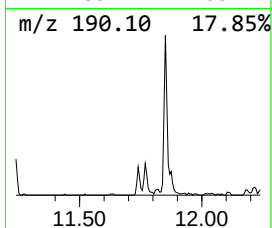
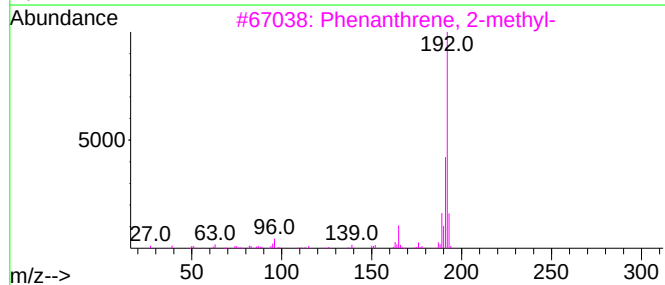
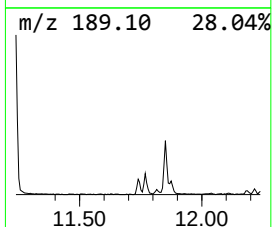
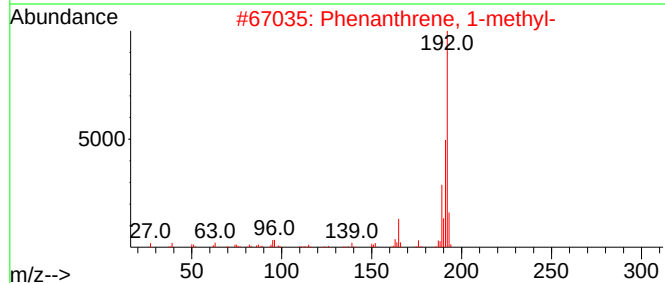
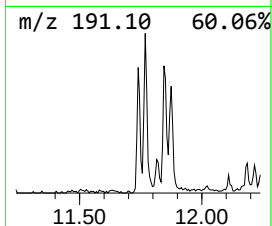
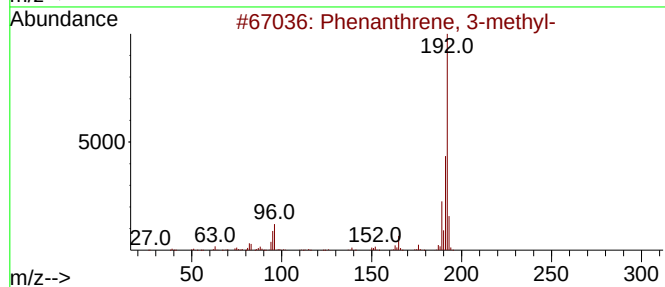
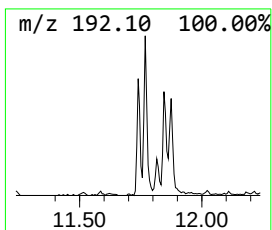
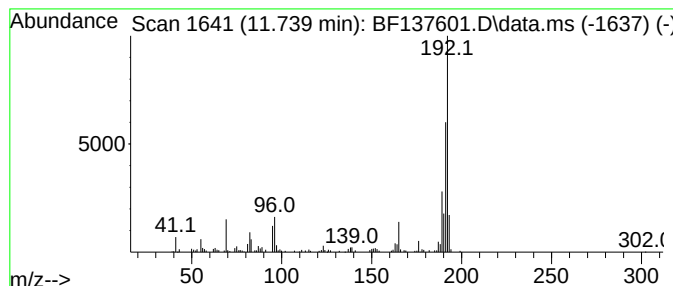
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Phenanthrene, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.739	2.13 ng	105454	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	95
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	95
3			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	94
4			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	94
5			1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	93



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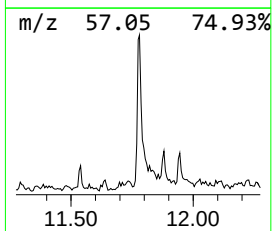
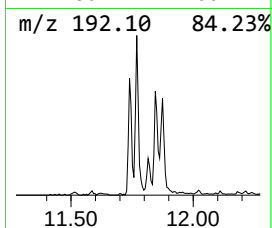
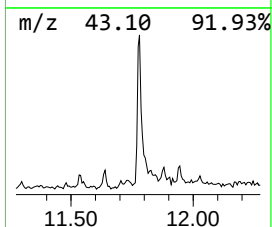
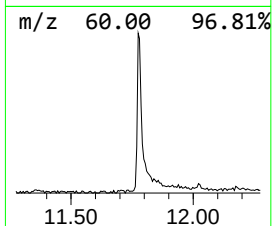
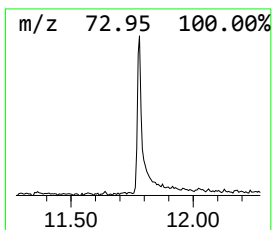
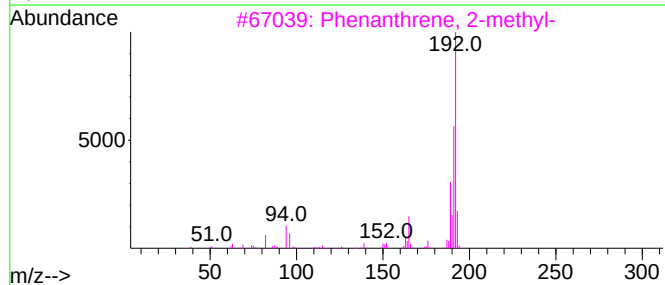
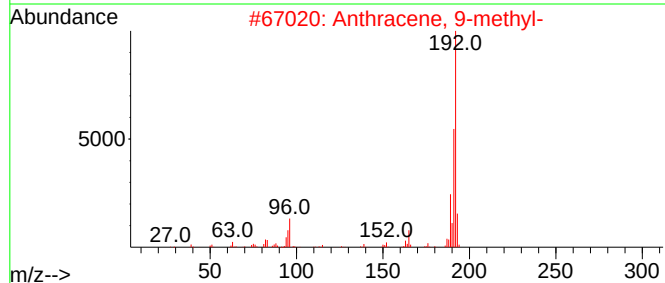
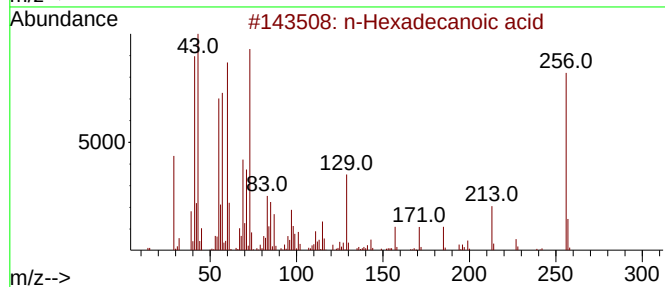
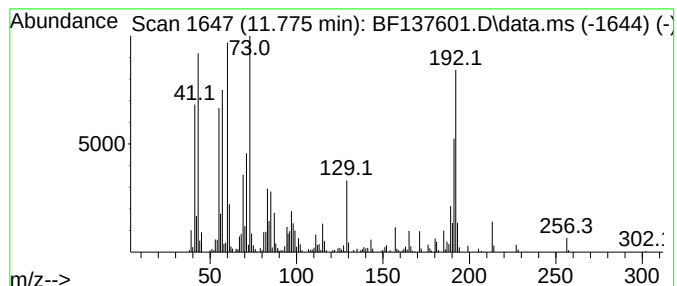
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.775	6.33 ng	312684	Phenanthrene-d10	11.239	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Anthracene, 9-methyl-	192	C15H12	000779-02-2	74
3	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	70
4	Octadecanoic acid	284	C18H36O2	000057-11-4	55
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	51



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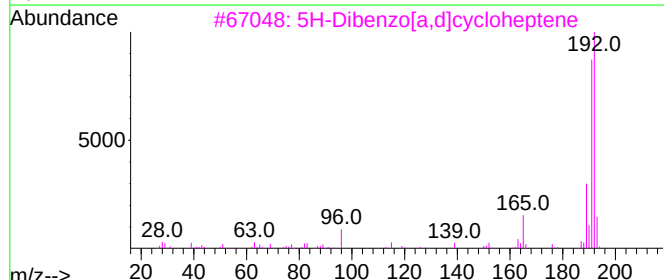
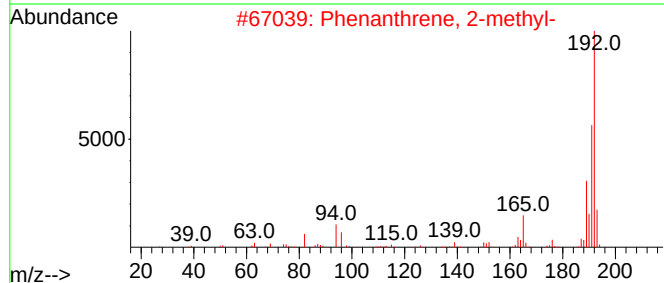
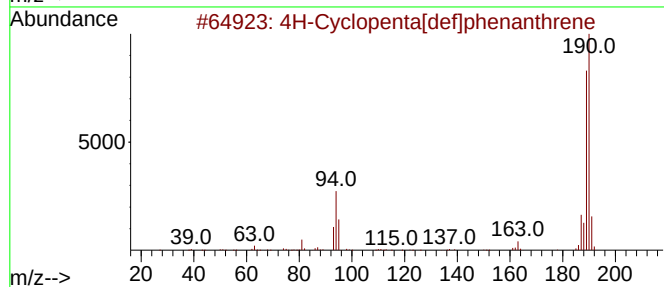
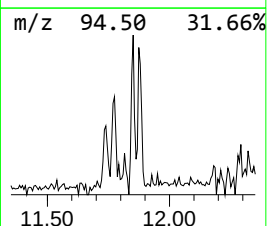
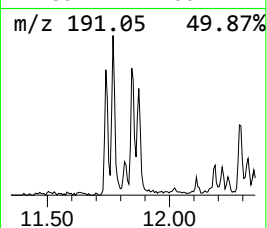
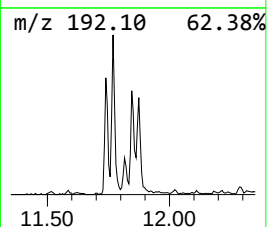
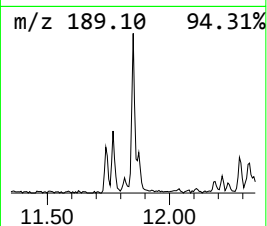
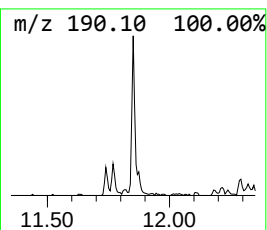
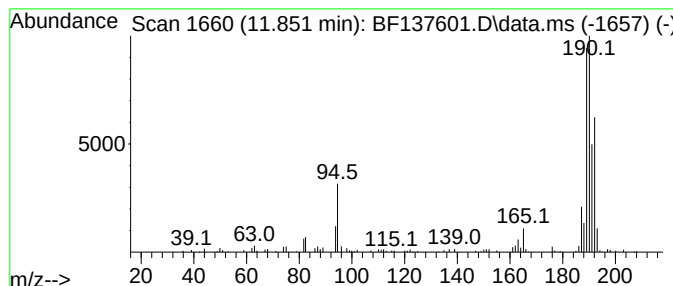
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.851	2.35 ng	115886	Phenanthrene-d10	11.239

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	58
2		Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	38
3		5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	35
4		Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	35
5		Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137601.D
Acq On : 14 Mar 2024 20:26
Operator : CG\JU
Sample : P1746-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-0-2.0-DUP

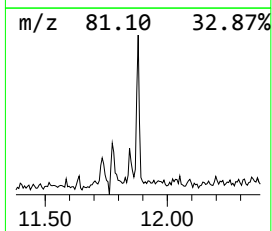
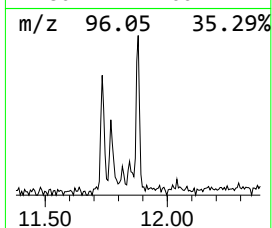
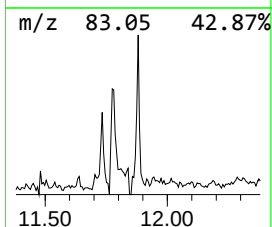
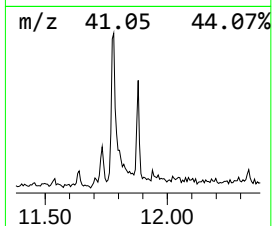
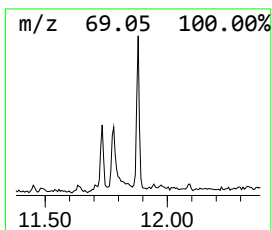
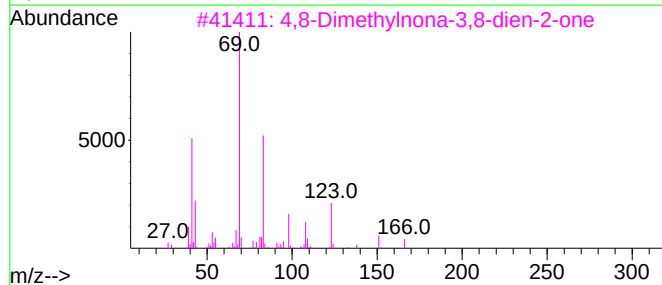
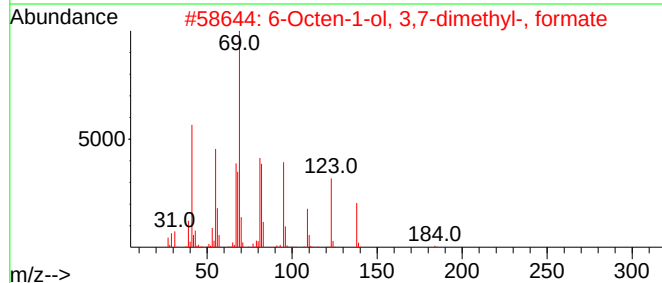
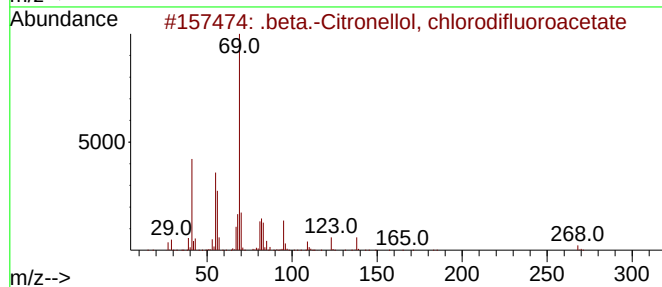
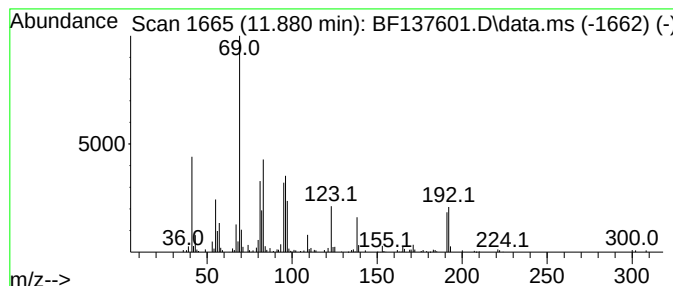
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown11.880 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	2.99 ng	147656	Phenanthrene-d10	11.239

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	beta.-Citronellol, chlorodifluo...	268	C12H19ClF2O2	1000376-20-8	38	
2	6-Octen-1-ol, 3,7-dimethyl-, for...	184	C11H20O2	000105-85-1	37		
3	4,8-Dimethylnona-3,8-dien-2-one	166	C11H18O	872858-42-9	37		
4	6-Octenoic acid, 3,7-dimethyl-, ...	308	C20H36O2	082766-40-3	35		
5	3,7-Dimethyloct-6-en-1-yl dodeca...	338	C22H42O2	072934-07-7	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137601.D
Acq On : 14 Mar 2024 20:26
Operator : CG\JU
Sample : P1746-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-0-2.0-DUP

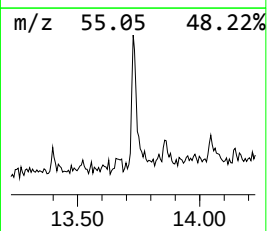
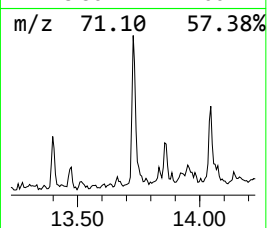
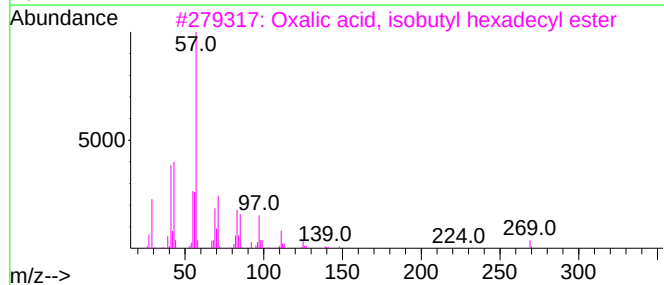
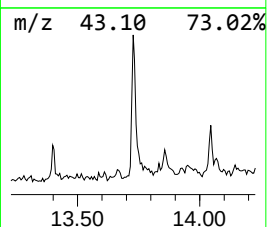
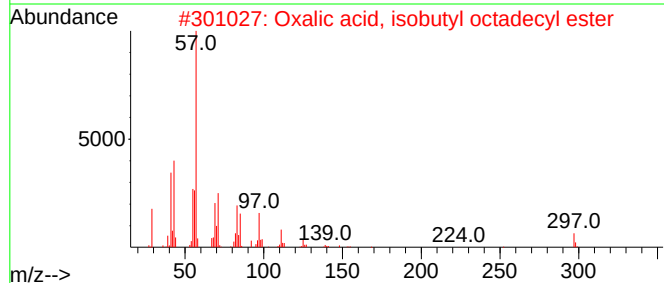
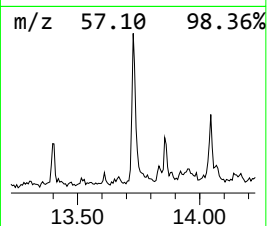
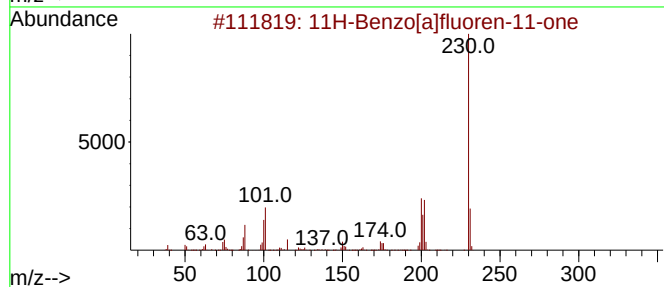
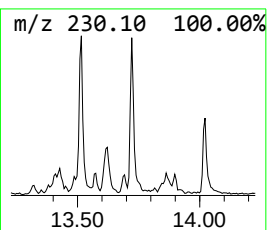
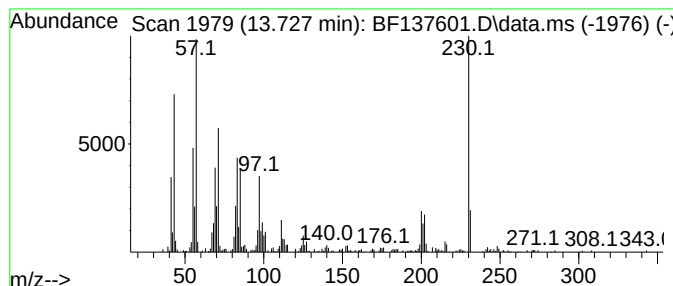
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 11H-Benzo[a]fluoren-11-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	3.42 ng	284244	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	52
2			Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	50
3			Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	45
4			Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	45
5			Propionic acid, 3-iodo-, heptade...	438	C20H39IO2	1000406-24-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137601.D
Acq On : 14 Mar 2024 20:26
Operator : CG\JU
Sample : P1746-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-0-2.0-DUP

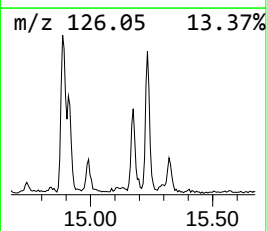
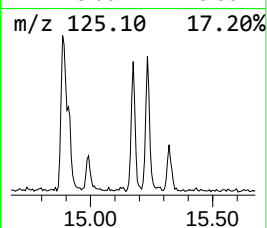
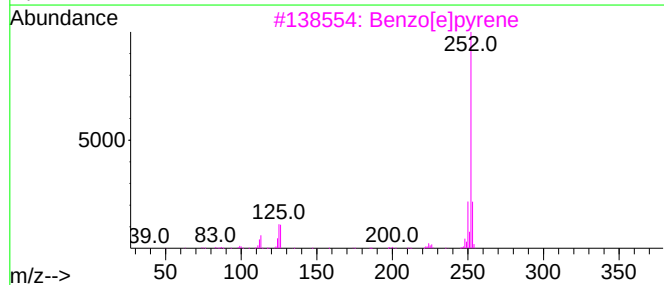
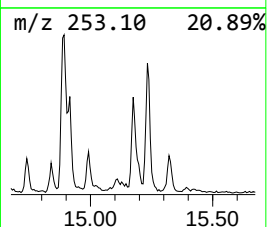
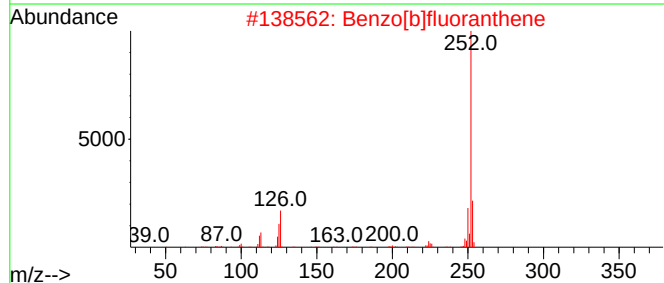
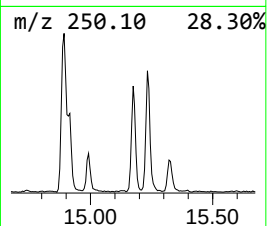
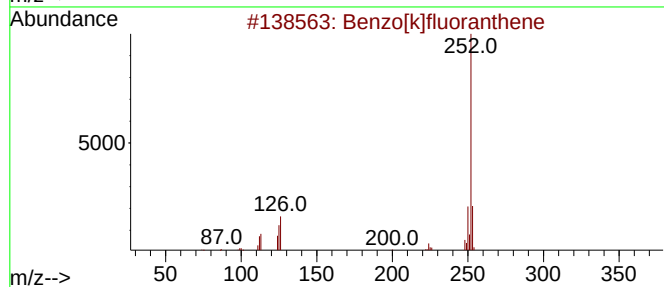
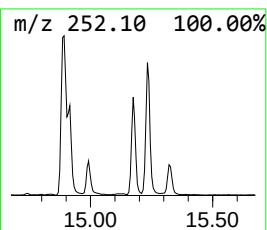
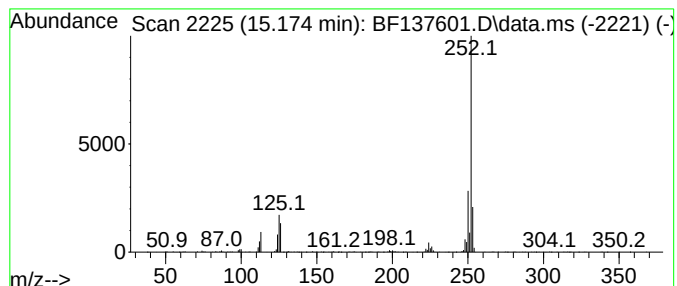
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	8.12 ng	415504	Perylene-d12	15.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	99
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	99
3			Benzo[e]pyrene	252	C20H12	000192-97-2	98
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	96
5			Perylene	252	C20H12	000198-55-0	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031424\
Data File : BF137601.D
Acq On : 14 Mar 2024 20:26
Operator : CG\JU
Sample : P1746-16
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-05-0-2.0-DUP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Tridecanone	9.681	2.5	ng	135874	3	9.757	1105950	20.0
Phenanthrene, 3...	11.739	2.1	ng	105454	4	11.239	988256	20.0
n-Hexadecanoic ...	11.775	6.3	ng	312684	4	11.239	988256	20.0
4H-Cyclopenta[d...	11.851	2.4	ng	115886	4	11.239	988256	20.0
unknown11.880	11.880	3.0	ng	147656	4	11.239	988256	20.0
11H-Benzo[a]flu...	13.727	3.4	ng	284244	5	13.874	1661090	20.0
Benzo[e]pyrene	15.174	8.1	ng	415504	6	15.292	1023530	20.0