

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
 Data File : BF124381.D
 Acq On : 18 Jun 2021 19:05
 Operator : JU/CG
 Sample : M2749-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PP-01_4.5-5.0

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-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	489	493	501	rBV	44584	53749	4.43%	0.512%
2	5.404	561	564	579	rBV	780349	801971	66.08%	7.643%
3	6.428	735	738	751	rBV	839703	834174	68.74%	7.950%
4	6.781	795	798	803	rVB	249972	194460	16.02%	1.853%
5	7.351	891	895	898	rBV	716224	573867	47.29%	5.469%
6	8.069	1013	1017	1020	rBV	276377	250674	20.66%	2.389%
7	9.145	1196	1200	1203	rBV	1460864	1106671	91.19%	10.547%
8	9.822	1311	1315	1318	rBV	423672	316960	26.12%	3.021%
9	9.851	1318	1320	1324	rVB	26701	22066	1.82%	0.210%
10	10.369	1405	1408	1412	rBB	22232	18978	1.56%	0.181%
11	10.616	1446	1450	1453	rBV	897430	765458	63.07%	7.295%
12	11.122	1532	1536	1540	rVB	24342	20299	1.67%	0.193%
13	11.310	1564	1568	1570	rBV	430642	348794	28.74%	3.324%
14	11.333	1570	1572	1576	rVV	376962	293116	24.15%	2.794%
15	11.386	1576	1581	1584	rVB	74097	59445	4.90%	0.567%
16	11.545	1603	1608	1615	rBV2	33258	35234	2.90%	0.336%
17	11.810	1650	1653	1656	rBV	44004	38526	3.17%	0.367%
18	11.839	1656	1658	1663	rVV	62811	56860	4.69%	0.542%
19	11.892	1663	1667	1669	rVV	17600	17781	1.47%	0.169%
20	11.922	1669	1672	1675	rVV	60911	67998	5.60%	0.648%
21	11.945	1675	1676	1680	rVB	33019	22877	1.89%	0.218%
22	12.104	1701	1703	1707	rBV	26419	24961	2.06%	0.238%
23	12.139	1707	1709	1713	rVB2	30048	26375	2.17%	0.251%
24	12.257	1724	1729	1733	rBV4	11399	14789	1.22%	0.141%
25	12.363	1742	1747	1749	rBV	29357	26837	2.21%	0.256%
26	12.398	1749	1753	1755	rVV3	18723	25091	2.07%	0.239%
27	12.457	1759	1763	1766	rVB3	29990	31723	2.61%	0.302%
28	12.527	1771	1775	1778	rBV	499432	418310	34.47%	3.987%
29	12.675	1795	1800	1803	rBV3	17377	19401	1.60%	0.185%
30	12.757	1808	1814	1819	rBV	403666	431199	35.53%	4.110%
31	12.810	1819	1823	1828	rVV6	19031	32161	2.65%	0.307%
32	12.898	1832	1838	1841	rVB	1429860	1213605	100.00%	11.566%
33	12.974	1847	1851	1855	rVB2	27649	39460	3.25%	0.376%
34	13.069	1863	1867	1868	rBV3	23314	34080	2.81%	0.325%
35	13.086	1868	1870	1874	rVB	43332	35901	2.96%	0.342%
36	13.151	1879	1881	1883	rBV	23083	20323	1.67%	0.194%

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37	13.186	1883	1887	1890	rBV3	43407	48504	4.00%	0.462%
38	13.280	1900	1903	1906	rVB	22649	19316	1.59%	0.184%
39	13.310	1906	1908	1912	rBV3	21377	24071	1.98%	0.229%
40	13.474	1931	1936	1938	rBV4	8503	14921	1.23%	0.142%
41	13.598	1954	1957	1961	rVB	48037	41382	3.41%	0.394%
42	13.704	1970	1975	1978	rBV	40757	48998	4.04%	0.467%
43	13.733	1978	1980	1982	rVV	29408	20929	1.72%	0.199%
44	13.757	1982	1984	1986	rVV	23886	22218	1.83%	0.212%
45	13.810	1990	1993	1996	rVB	38616	39725	3.27%	0.379%
46	13.874	1996	2004	2006	rBV6	15565	32592	2.69%	0.311%
47	13.957	2011	2018	2021	rBV2	375205	494415	40.74%	4.712%
48	13.980	2021	2022	2026	rVB	162249	109712	9.04%	1.046%
49	14.063	2034	2036	2039	rVB	19970	15085	1.24%	0.144%
50	14.116	2042	2045	2049	rBV6	16594	28522	2.35%	0.272%
51	14.186	2055	2057	2061	rVB2	17210	17017	1.40%	0.162%
52	14.345	2081	2084	2086	rBV	37241	26035	2.15%	0.248%
53	14.421	2093	2097	2099	rBV5	11757	19600	1.62%	0.187%
54	14.469	2103	2105	2107	rBV3	16791	14161	1.17%	0.135%
55	14.839	2165	2168	2170	rBV4	19633	18194	1.50%	0.173%
56	14.998	2190	2195	2197	rBV	145469	193961	15.98%	1.849%
57	15.057	2202	2205	2210	rVV7	12677	20440	1.68%	0.195%
58	15.104	2210	2213	2217	rVB	30238	32864	2.71%	0.313%
59	15.198	2224	2229	2234	rBV6	10445	28209	2.32%	0.269%
60	15.292	2241	2245	2250	rBV	82043	93932	7.74%	0.895%
61	15.357	2252	2256	2260	rVB	109670	140054	11.54%	1.335%
62	15.416	2261	2266	2270	rBV2	212511	268060	22.09%	2.555%
63	15.445	2270	2271	2276	rVB2	26910	29086	2.40%	0.277%
64	15.845	2336	2339	2344	rVB4	13162	18761	1.55%	0.179%
65	15.974	2357	2361	2365	rVB6	10242	15127	1.25%	0.144%
66	16.339	2421	2423	2431	rVB6	14007	23301	1.92%	0.222%
67	16.674	2476	2480	2484	rBV6	10627	18028	1.49%	0.172%
68	16.868	2508	2513	2521	rBV3	57882	98082	8.08%	0.935%
69	16.933	2521	2524	2530	rVB6	9401	16578	1.37%	0.158%
70	17.045	2537	2543	2547	rBV5	13807	26679	2.20%	0.254%
71	17.098	2547	2552	2557	rVV6	11666	24896	2.05%	0.237%
72	17.304	2582	2587	2595	rVB4	39945	75366	6.21%	0.718%
73	17.562	2625	2631	2636	rBV6	8992	19732	1.63%	0.188%

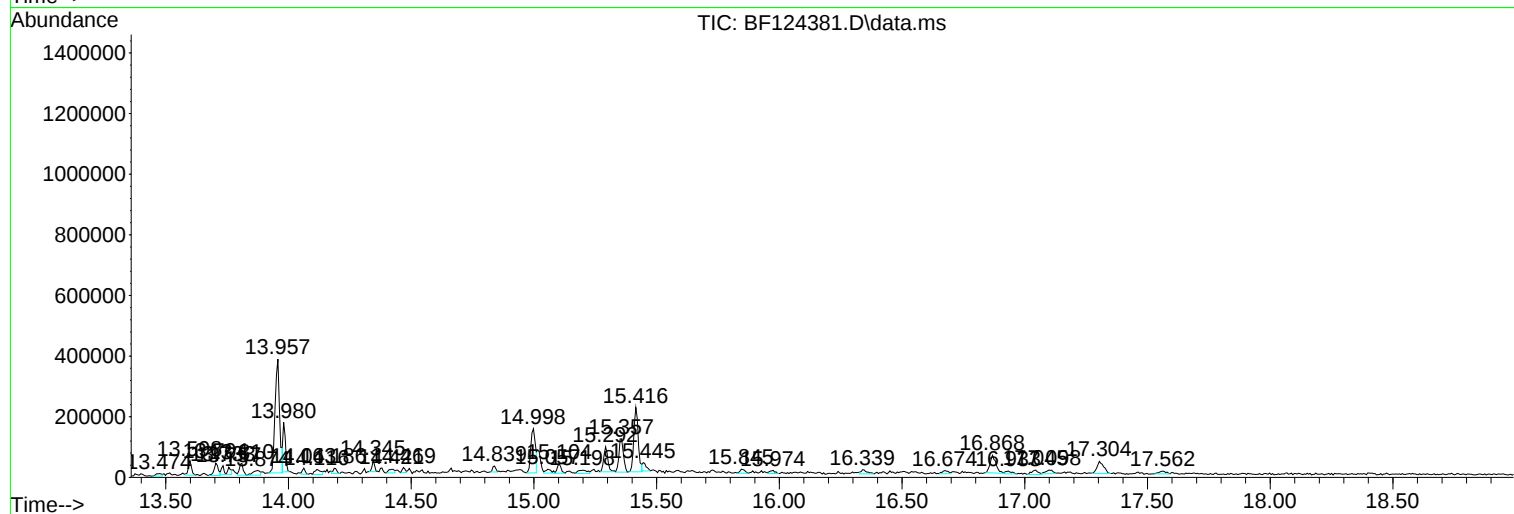
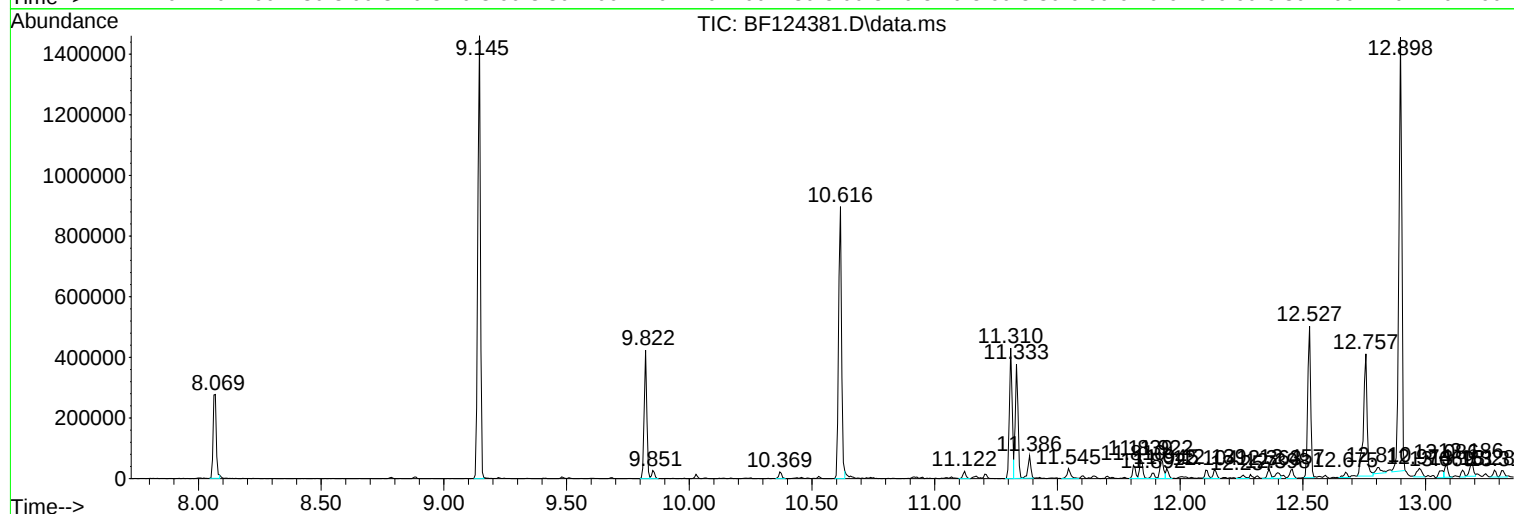
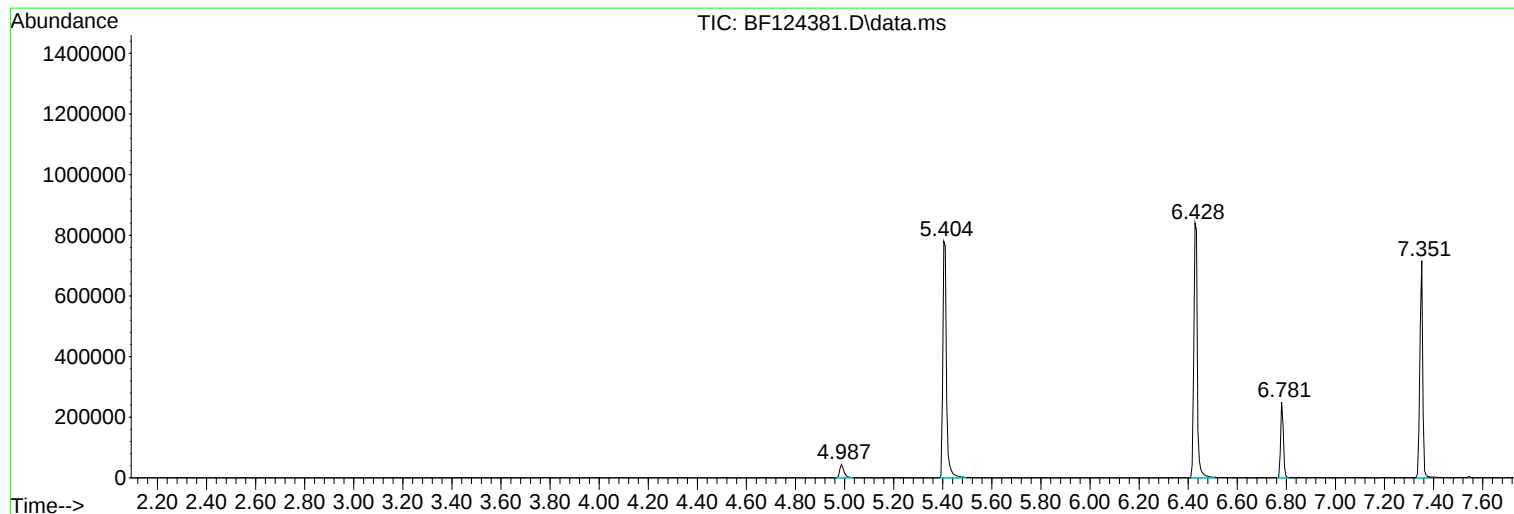
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PP-01 4.5-5.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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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Sample : M2749-05
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Instrument :
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ClientSampleId :
PP-01_4.5-5.0

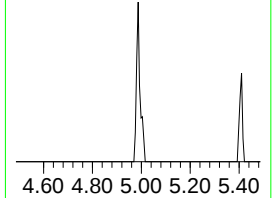
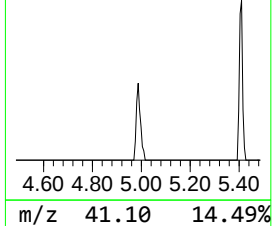
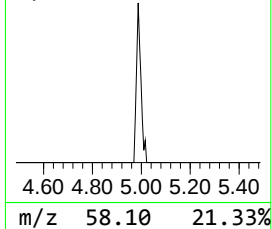
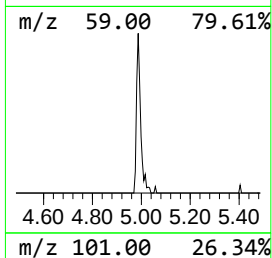
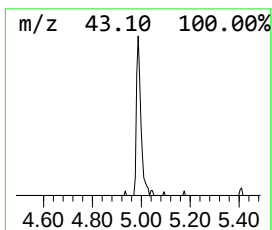
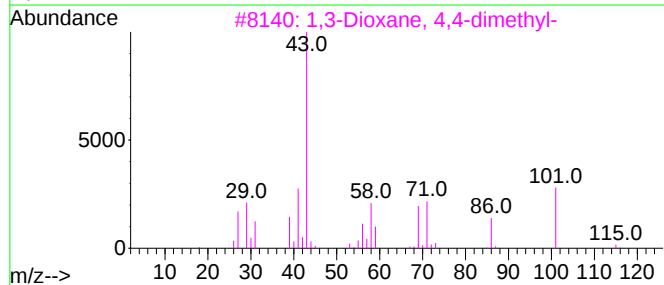
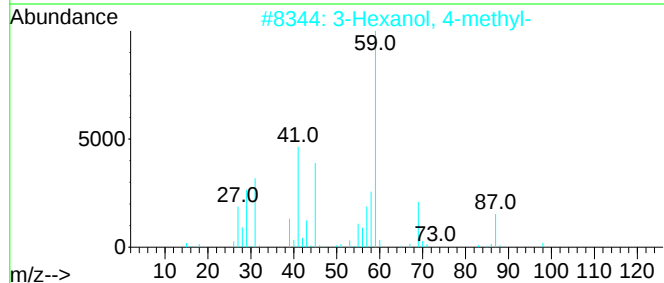
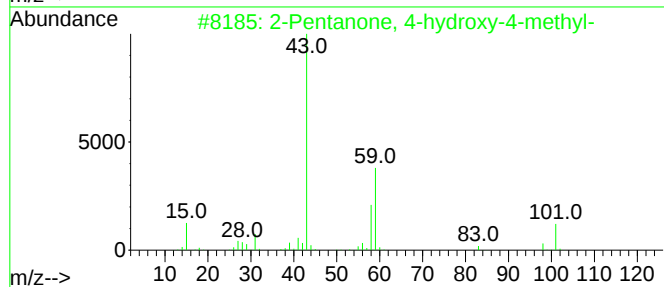
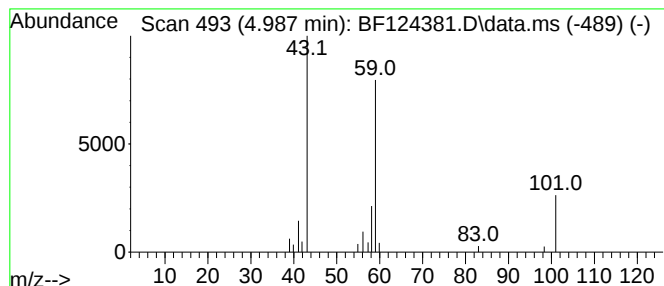
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	5.53 ng	53749	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	36		
3	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	17		
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9		



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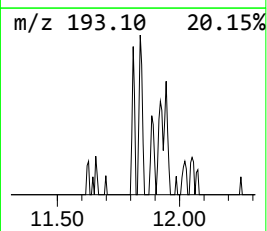
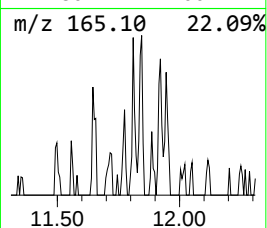
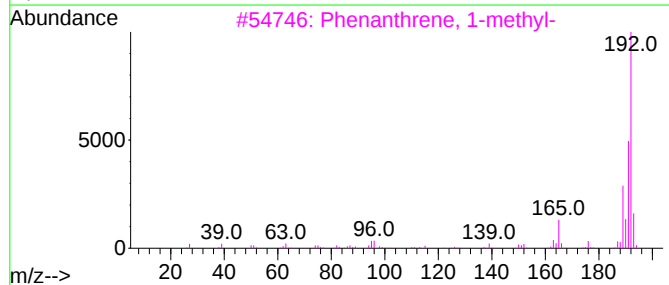
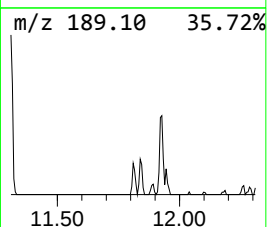
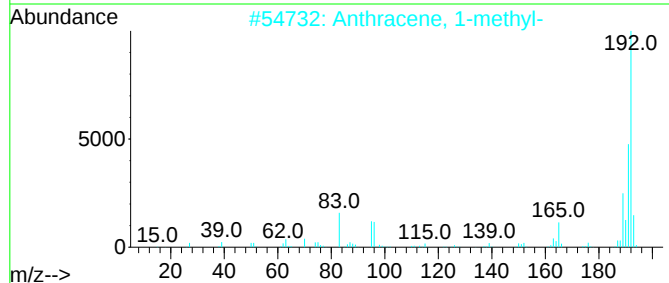
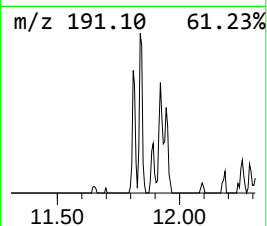
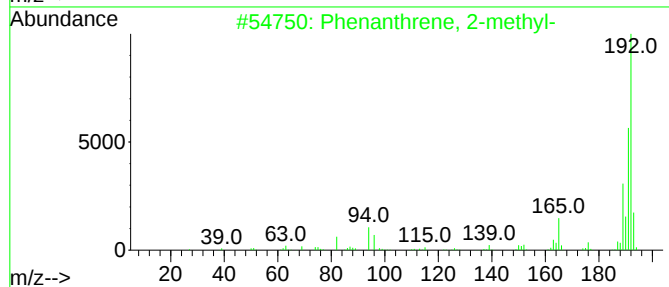
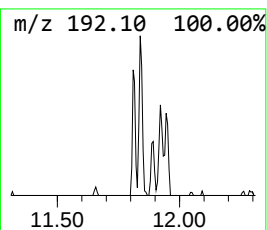
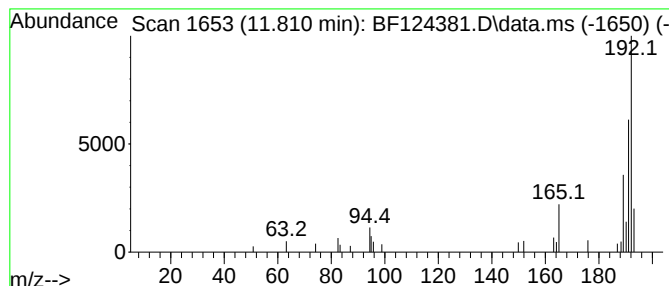
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenanthrene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	2.21 ng	38526	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	93
2			Anthracene, 1-methyl-	192	C15H12	000610-48-0	91
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4			Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	90
5			Naphtho[2,3-b]norbornadiene	192	C15H12	107426-38-0	87



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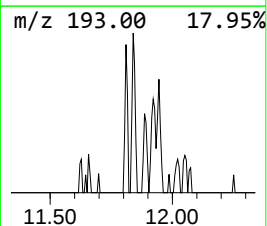
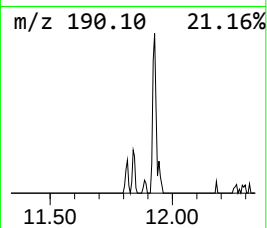
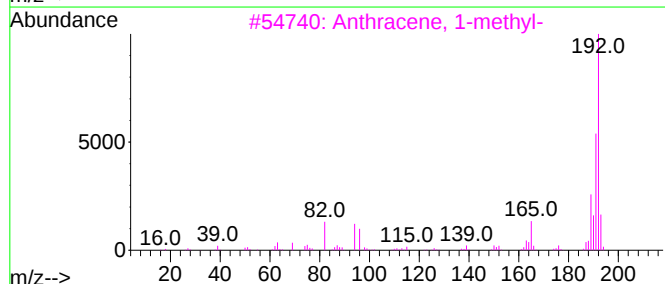
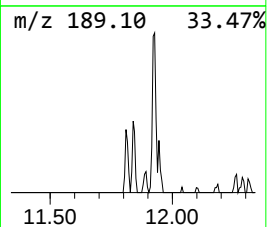
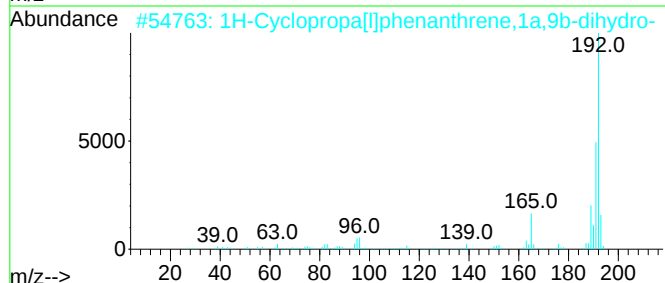
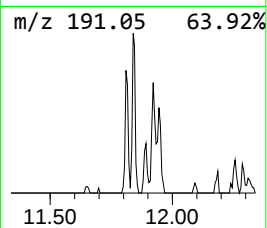
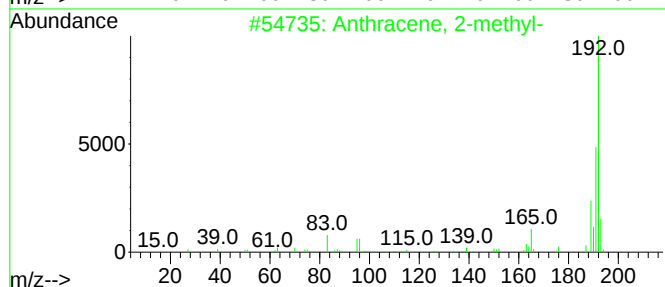
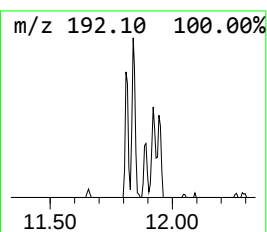
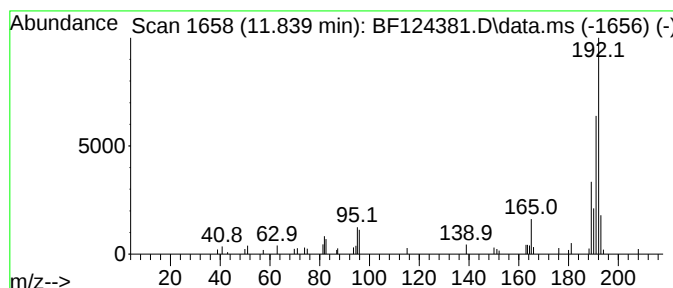
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Anthracene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.839	3.26 ng	56860	Phenanthrene-d10	11.310	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
2	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	91
3	Anthracene, 1-methyl-	192	C15H12	000610-48-0	89
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	87
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	81



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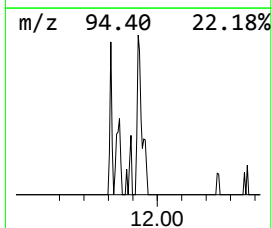
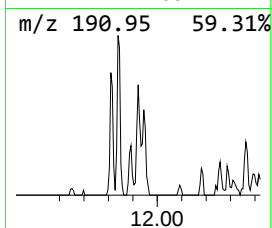
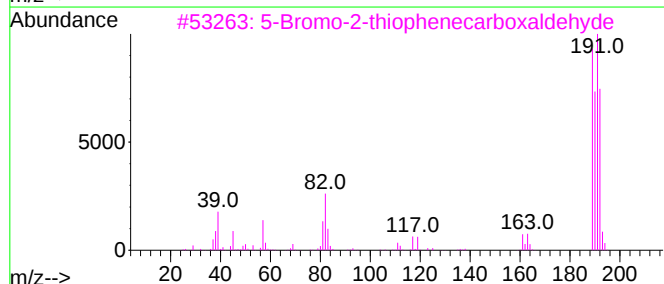
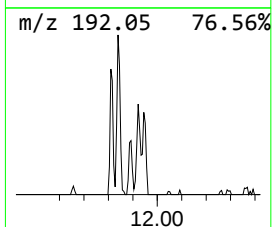
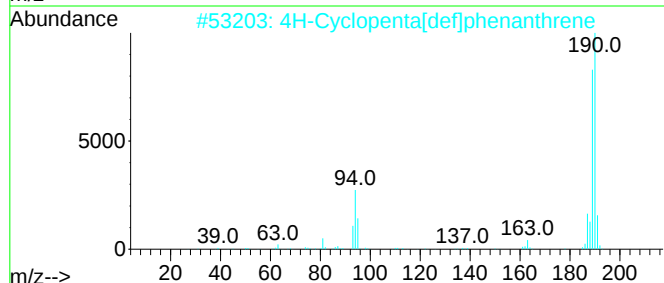
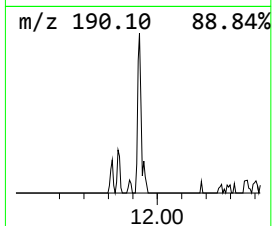
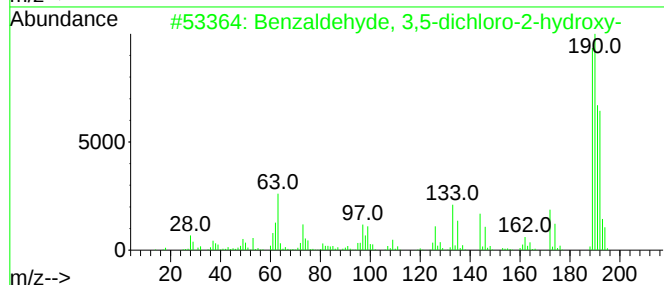
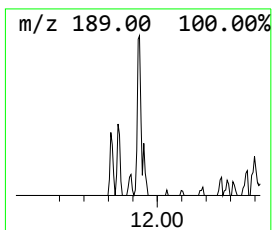
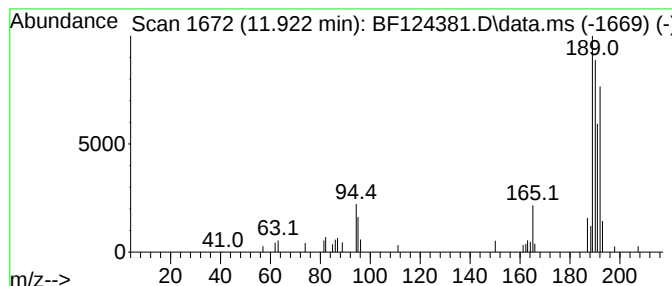
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzaldehyde, 3,5-dichloro-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.90 ng	67998	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	72
2			4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
3			5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	53
4			6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	47
5			Benzene, 1,1'-(2-cyclopropen-1-y...	192	C15H12	022825-21-4	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124381.D
Acq On : 18 Jun 2021 19:05
Operator : JU/CG
Sample : M2749-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

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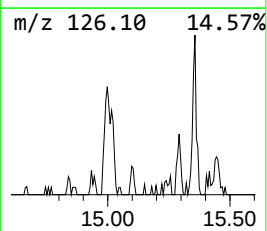
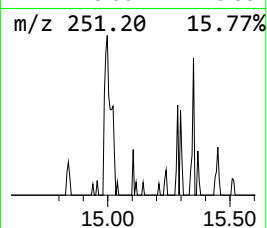
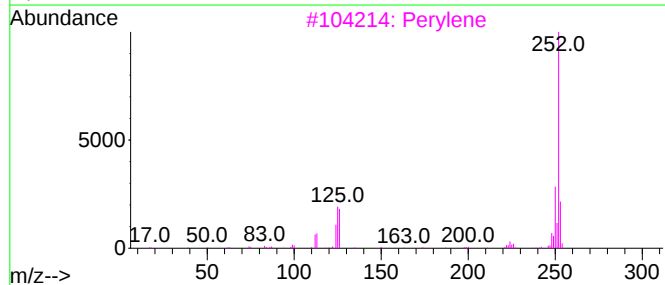
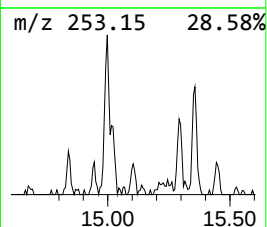
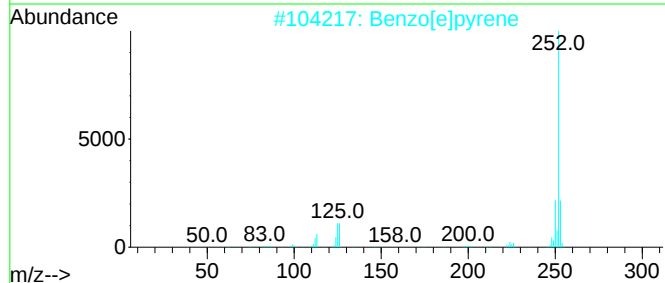
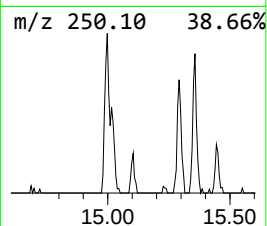
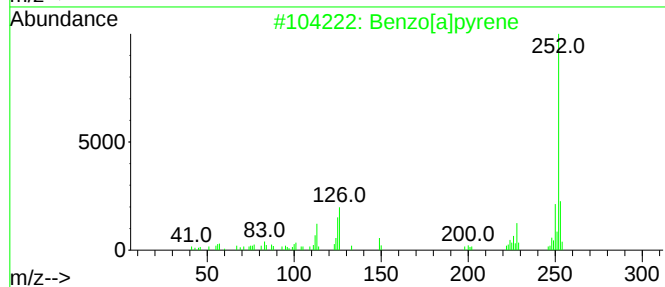
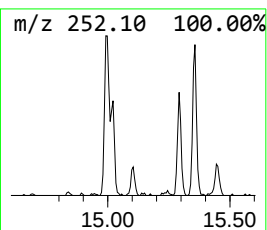
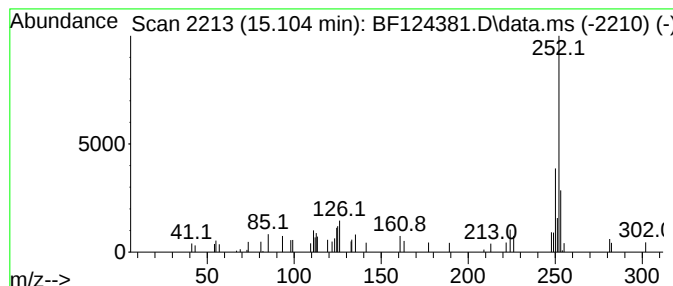
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.104	2.45 ng	32864	Perylene-d12	15.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	52
2			Benzo[e]pyrene	252	C20H12	000192-97-2	52
3			Perylene	252	C20H12	000198-55-0	47
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	47
5			1-Phenyl-3-(4-methoxyphenyl)-2-p...	252	C16H16N2O	003314-43-0	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124381.D
Acq On : 18 Jun 2021 19:05
Operator : JU/CG
Sample : M2749-05
Misc :
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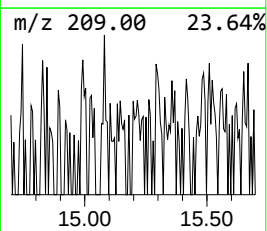
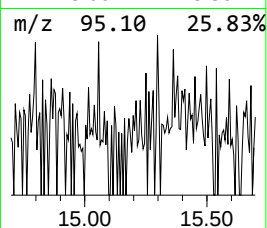
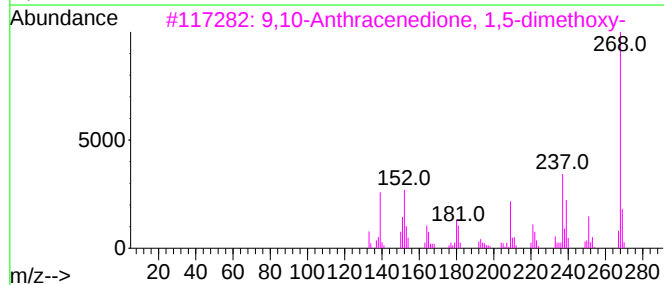
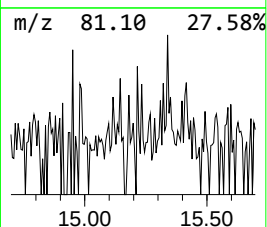
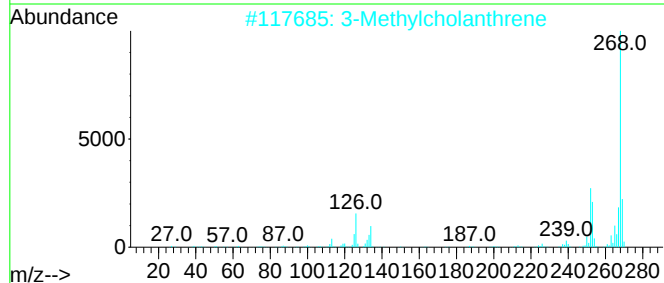
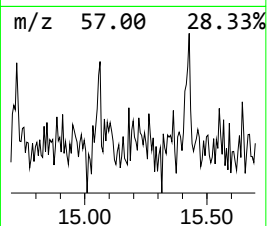
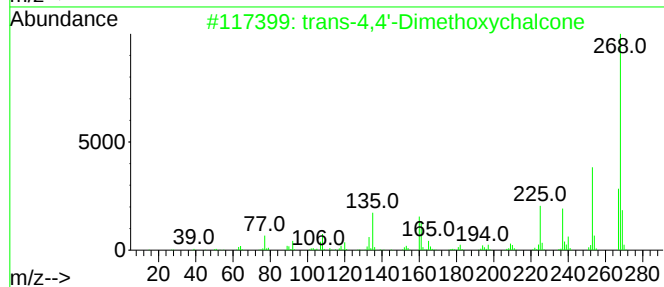
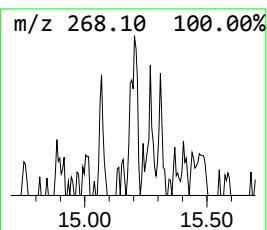
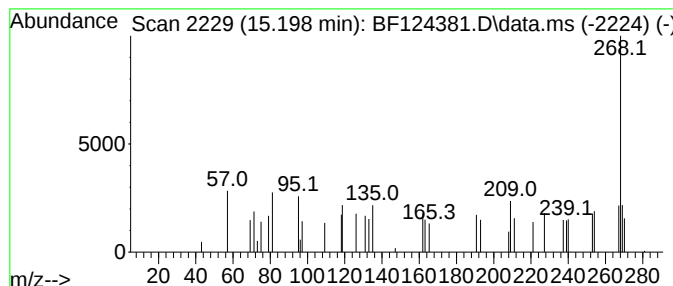
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 trans-4,4'-Dimethoxychalcone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.198	2.10 ng	28209	Perylene-d12	15.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-4,4'-Dimethoxychalcone	268	C17H16O3	041564-67-4	50
2	3-Methylcholanthrene	268	C21H16	000056-49-5	49
3	9,10-Anthracenedione, 1,5-dimeth...	268	C16H12O4	006448-90-4	47
4	3-Hydroxy-cis-D-homoestra-1,3,5(...	268	C18H20O2	021547-08-0	47
5	4H-1-Benzopyran-4-one, 7-hydroxy...	268	C16H12O4	000487-24-1	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124381.D
Acq On : 18 Jun 2021 19:05
Operator : JU/CG
Sample : M2749-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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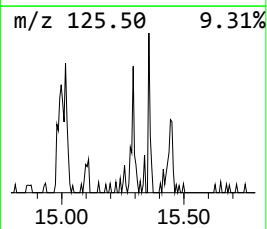
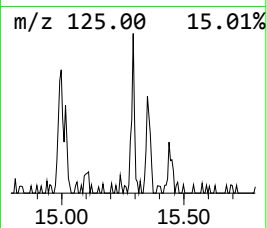
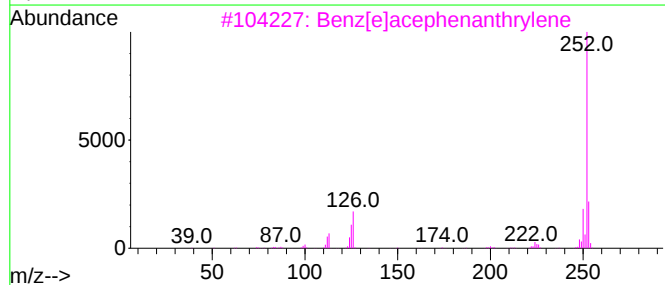
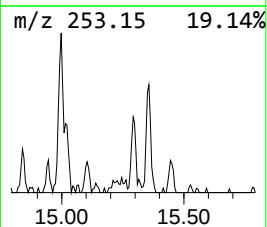
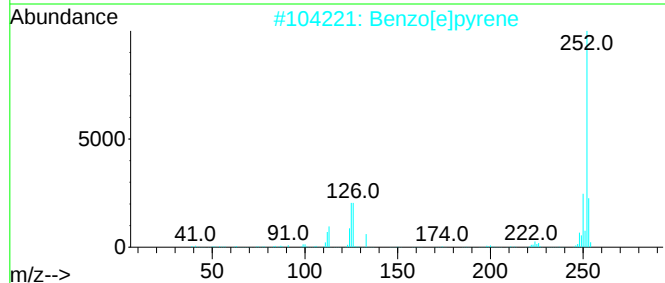
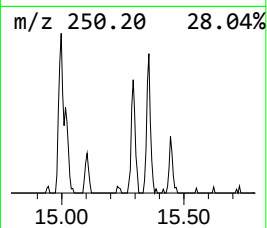
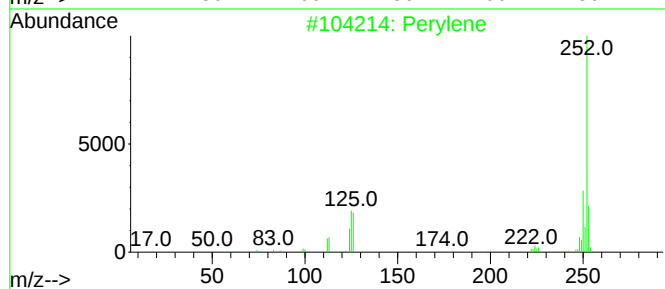
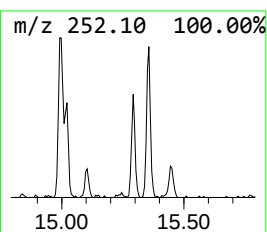
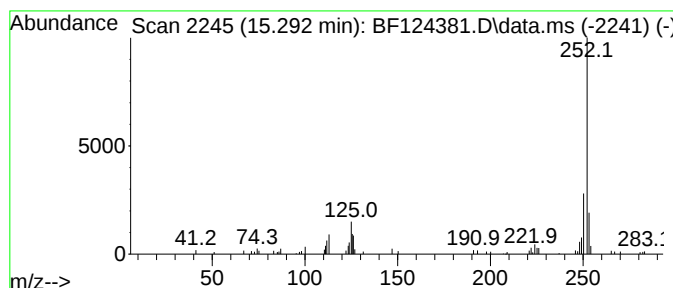
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.292	7.01 ng	93932	Perylene-d12	15.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	91
2			Benzo[e]pyrene	252	C20H12	000192-97-2	87
3			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
4			Benzo[k]fluoranthene	252	C20H12	000207-08-9	76
5			Benzo[a]pyrene	252	C20H12	000050-32-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061821\
Data File : BF124381.D
Acq On : 18 Jun 2021 19:05
Operator : JU/CG
Sample : M2749-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PP-01_4.5-5.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	5.5	ng	53749	1	6.781	194460	20.0
Phenanthrene, 2...	11.810	2.2	ng	38526	4	11.310	348794	20.0
Anthracene, 2-m...	11.839	3.3	ng	56860	4	11.310	348794	20.0
Benzaldehyde, 3...	11.922	3.9	ng	67998	4	11.310	348794	20.0
Benzo[e]pyrene	15.104	2.5	ng	32864	6	15.416	268060	20.0
trans-4,4'-Dime...	15.198	2.1	ng	28209	6	15.416	268060	20.0
Perylene	15.292	7.0	ng	93932	6	15.416	268060	20.0