

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090718\
 Data File : BF108868.D
 Acq On : 7 Sep 2018 18:39
 Operator : JU/SJ
 Sample : J4825-18MSD
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP1-WS-COMP-18MSD

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF090518.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	4.437	353	357	361	rBV	145205	162775	2.69%	0.284%
2	4.943	436	443	451	rBV	175237	240695	3.98%	0.420%
3	5.354	507	513	516	rBV	5107848	5270965	87.24%	9.203%
4	6.378	681	687	690	rBV	5149870	5474305	90.61%	9.558%
5	6.507	704	709	712	rBV	5245257	5476682	90.65%	9.562%
6	6.572	717	720	722	rBV	99746	92736	1.53%	0.162%
7	6.737	745	748	752	rBV	1636611	1278135	21.16%	2.232%
8	6.895	771	775	778	rBV	4834438	4266861	70.62%	7.450%
9	7.301	838	844	846	rBV	3489279	3589530	59.41%	6.267%
10	8.019	962	966	969	rBV	1985224	1597497	26.44%	2.789%
11	9.095	1144	1149	1152	rBV	6519905	6041628	100.00%	10.549%
12	9.483	1212	1215	1218	rBV	1509278	1304450	21.59%	2.278%
13	9.766	1259	1263	1267	rBV2	1865682	1646915	27.26%	2.876%
14	9.801	1267	1269	1272	rVB	88609	70389	1.17%	0.123%
15	10.307	1353	1355	1360	rVB	86764	76872	1.27%	0.134%
16	10.554	1392	1397	1400	rBV	3080683	3055873	50.58%	5.336%
17	11.242	1511	1514	1516	rBV	1528480	1346235	22.28%	2.351%
18	11.266	1516	1518	1522	rVV	991677	780503	12.92%	1.363%
19	11.319	1522	1527	1530	rVB	246501	212835	3.52%	0.372%
20	11.466	1547	1552	1555	rBV2	71679	90707	1.50%	0.158%
21	11.742	1596	1599	1602	rBV	147274	132986	2.20%	0.232%
22	11.777	1602	1605	1609	rVV2	231059	332482	5.50%	0.581%
23	11.819	1609	1612	1615	rVV2	94157	92295	1.53%	0.161%
24	11.854	1615	1618	1621	rVV	237759	272478	4.51%	0.476%
25	11.877	1621	1622	1625	rVB	124022	69109	1.14%	0.121%
26	12.036	1647	1649	1651	rBV	90973	85066	1.41%	0.149%
27	12.295	1689	1693	1696	rBV	95210	120770	2.00%	0.211%
28	12.371	1704	1706	1712	rVB3	77978	97657	1.62%	0.171%
29	12.448	1716	1719	1723	rVB	1267028	1111433	18.40%	1.941%
30	12.566	1737	1739	1743	rBV3	46556	77510	1.28%	0.135%
31	12.677	1753	1758	1761	rBV	1260984	1213272	20.08%	2.118%
32	12.795	1776	1778	1780	rBV	65824	65895	1.09%	0.115%
33	12.830	1780	1784	1787	rVV	4358289	3967152	65.66%	6.927%
34	12.901	1793	1796	1798	rBV	70106	74995	1.24%	0.131%

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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

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35	13.007	1812	1814	1817	rVB	145289	128207	2.12%	0.224%
36	13.071	1823	1825	1828	rBV	126600	104509	1.73%	0.182%
37	13.107	1828	1831	1835	rBV	164030	188757	3.12%	0.330%
38	13.201	1845	1847	1850	rVB	95349	75199	1.24%	0.131%
39	13.230	1850	1852	1856	rBV	98376	87176	1.44%	0.152%
40	13.507	1897	1899	1906	rVB	115822	102846	1.70%	0.180%
41	13.648	1921	1923	1925	rBV	105407	76966	1.27%	0.134%
42	13.713	1932	1934	1936	rBV	110355	99098	1.64%	0.173%
43	13.736	1936	1938	1943	rVB2	255204	273139	4.52%	0.477%
44	13.871	1956	1961	1963	rBV2	1678584	2023869	33.50%	3.534%
45	13.895	1963	1965	1968	rVB	689620	500534	8.28%	0.874%
46	14.630	2087	2090	2093	rBV3	230382	242155	4.01%	0.423%
47	14.877	2129	2132	2135	rBV	565979	797353	13.20%	1.392%
48	14.977	2147	2149	2152	rVB	211979	198331	3.28%	0.346%
49	15.165	2177	2181	2186	rVB	373880	465440	7.70%	0.813%
50	15.218	2187	2190	2195	rBV	528858	536964	8.89%	0.938%
51	15.283	2196	2201	2204	rBV	990034	1168537	19.34%	2.040%
52	16.636	2427	2431	2438	rVB2	222988	414968	6.87%	0.725%

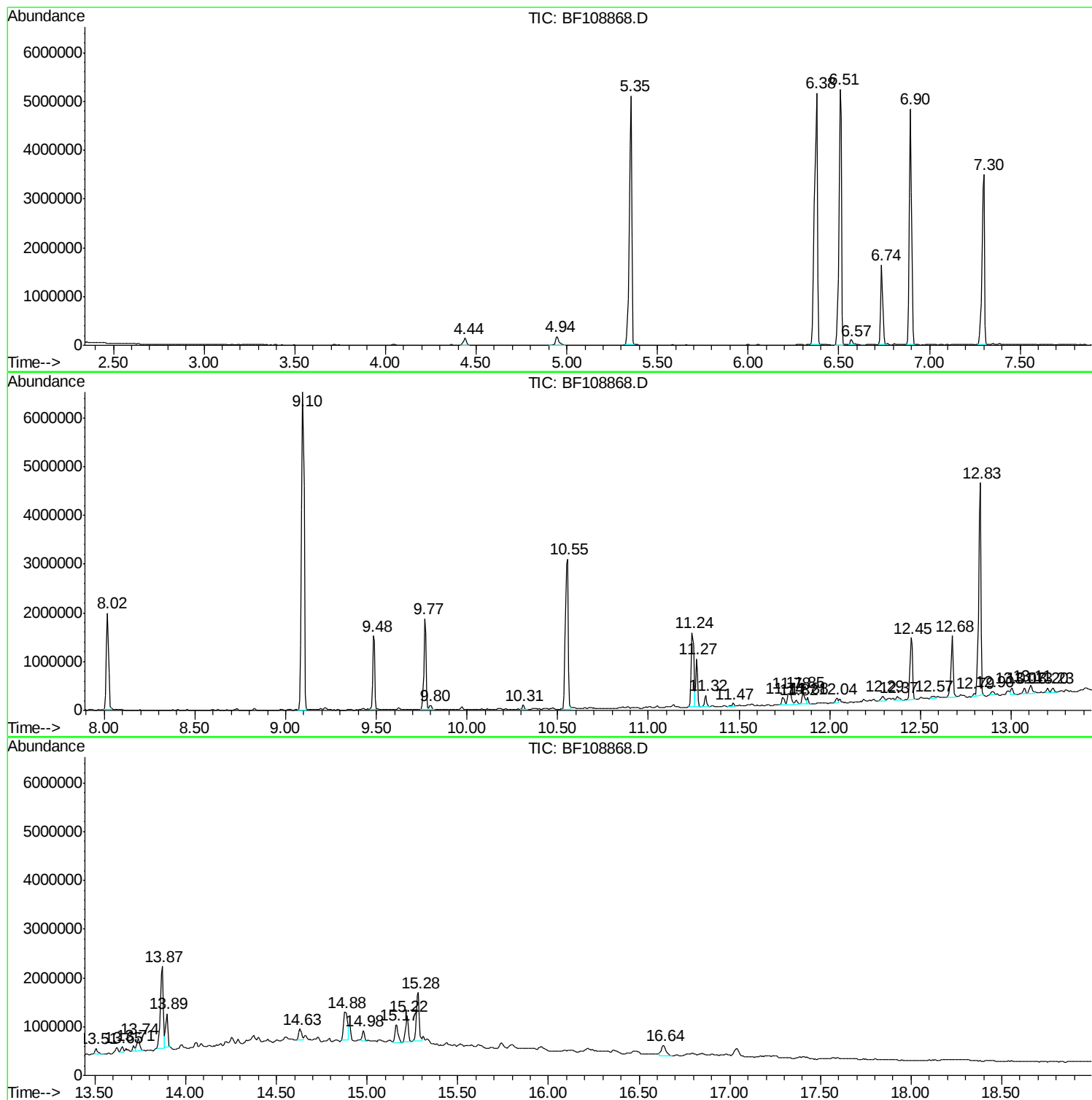
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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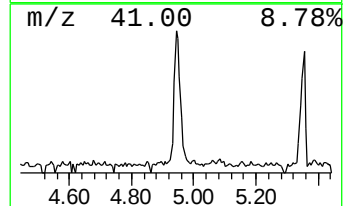
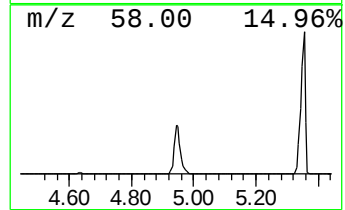
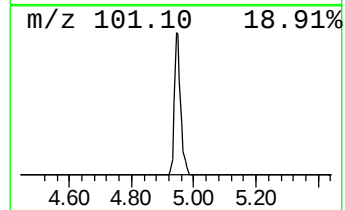
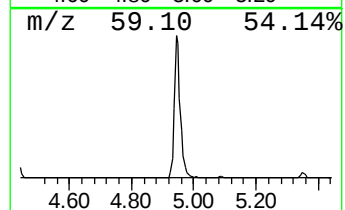
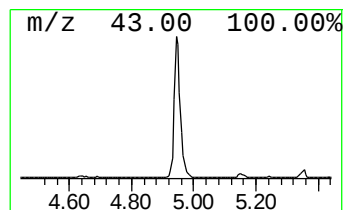
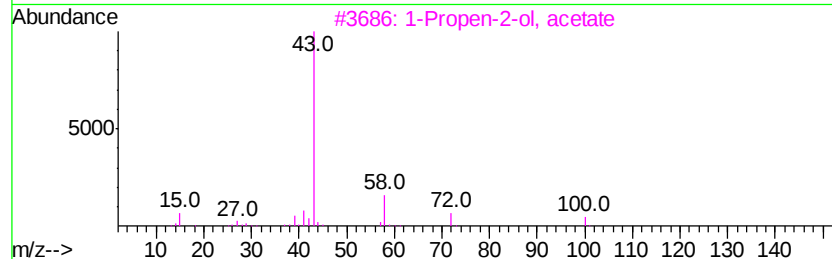
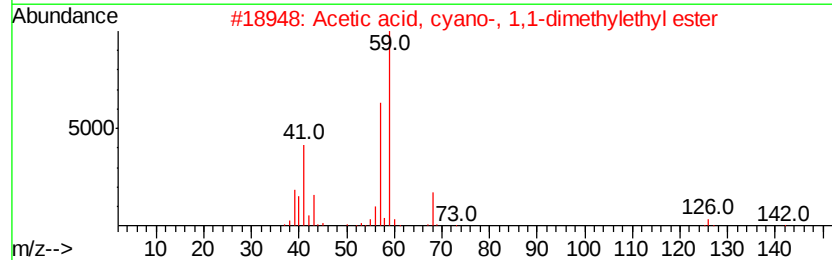
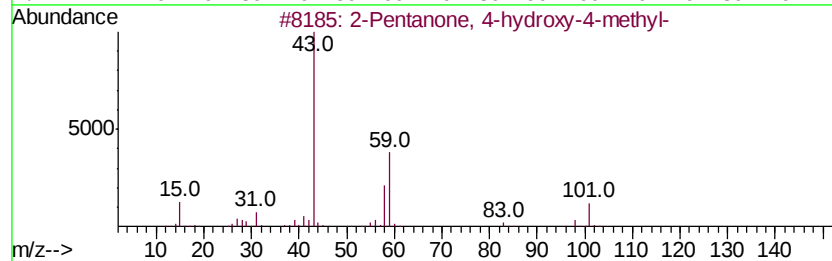
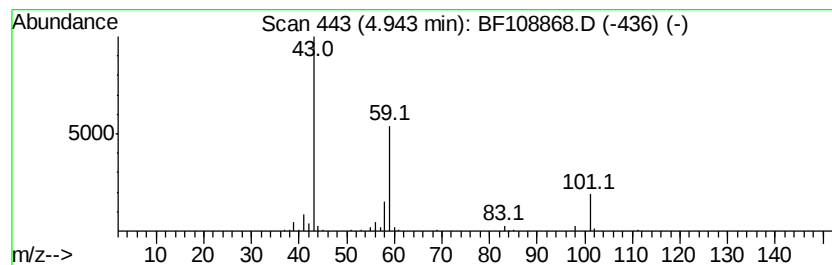
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	3.77 ng	240695	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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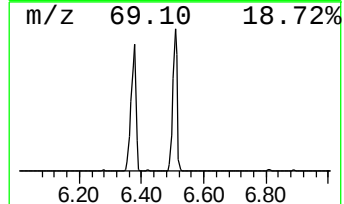
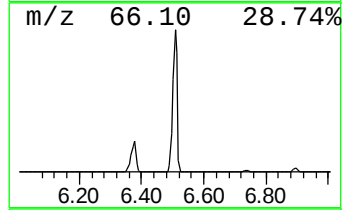
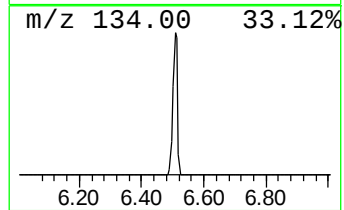
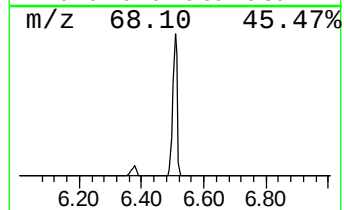
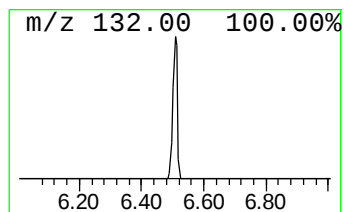
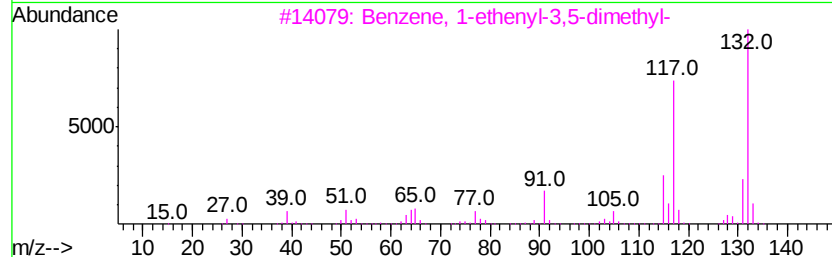
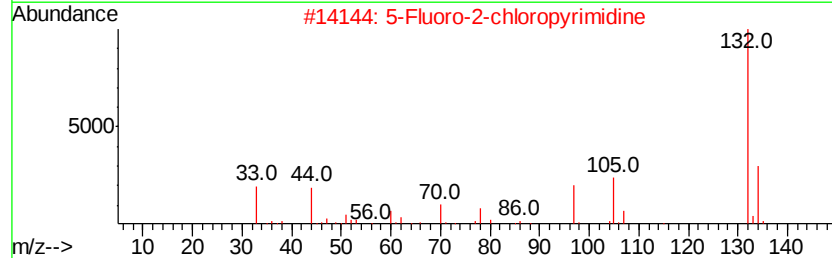
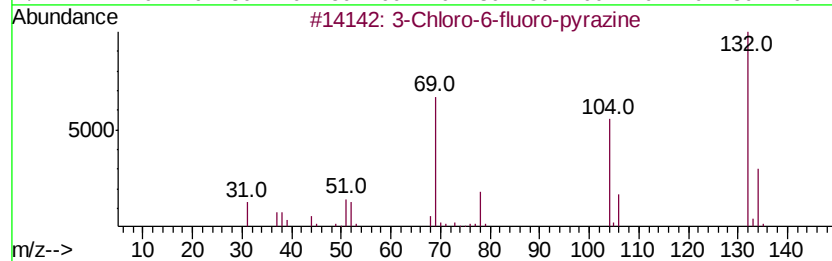
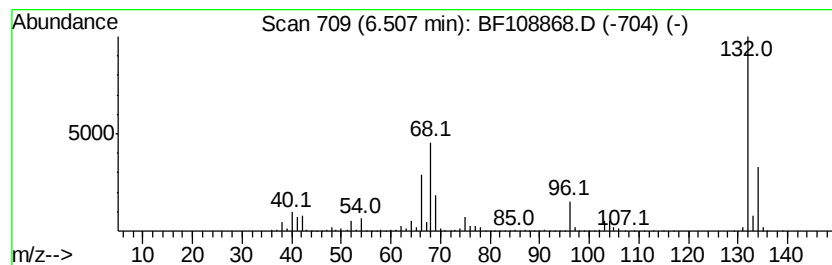
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Peak Number 3 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	85.70 ng	5476680	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12	
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9	
4	Xenon	132	Xe	007440-63-3	9	
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	



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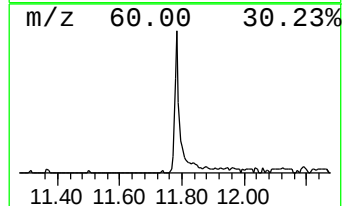
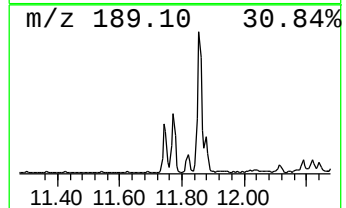
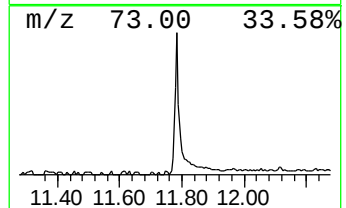
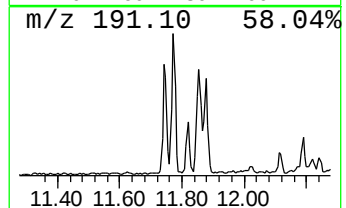
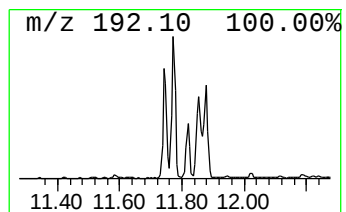
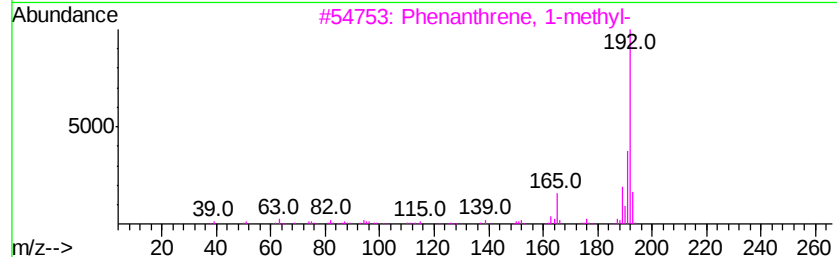
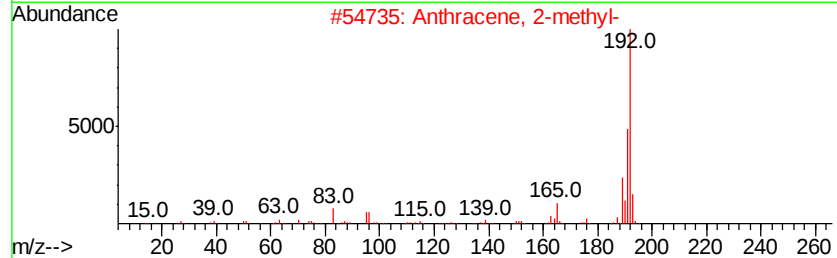
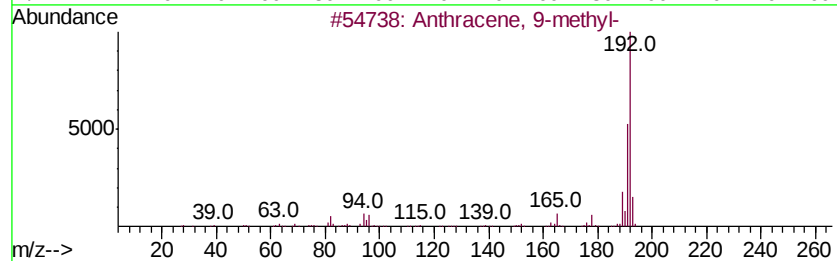
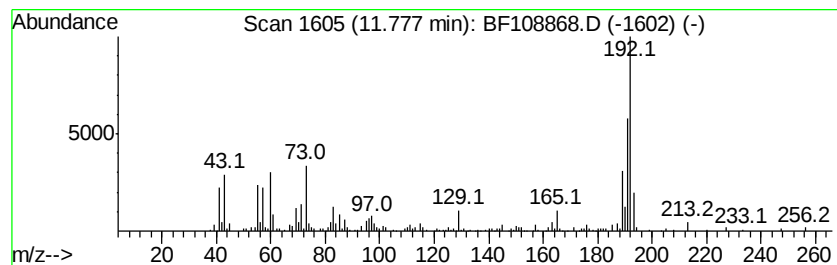
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Anthracene, 9-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.78	4.94 ng	332482	Phenanthrene-d10		11.24
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	92
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	91
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	91
4	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	90
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	83



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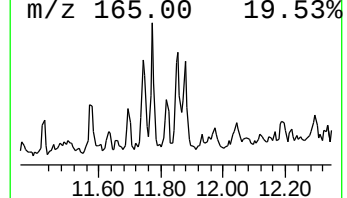
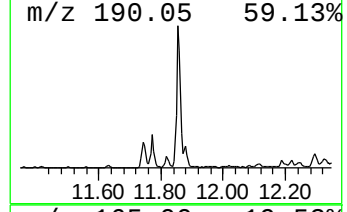
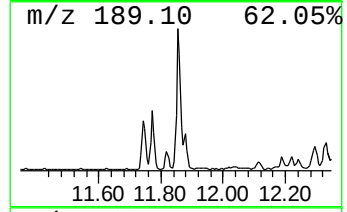
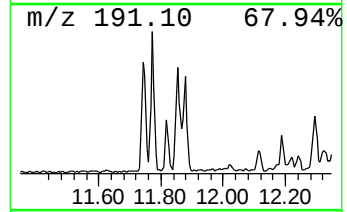
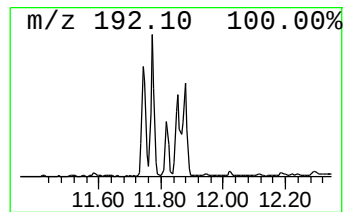
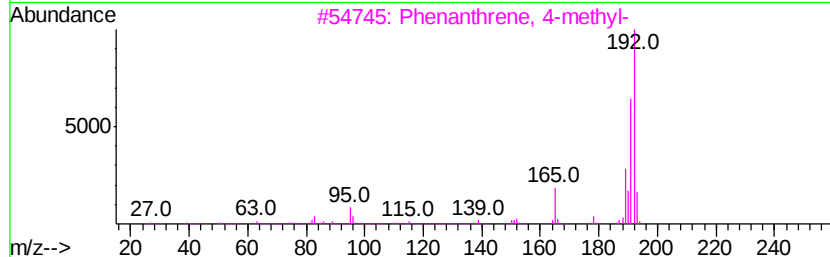
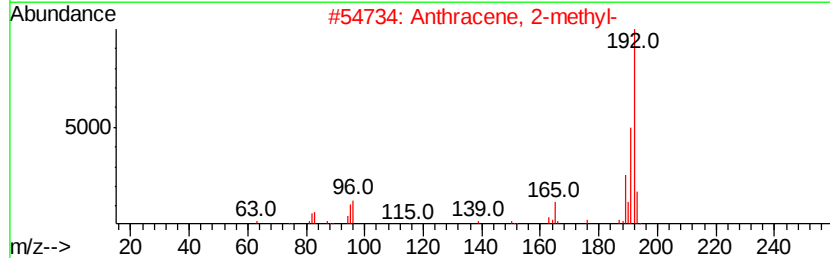
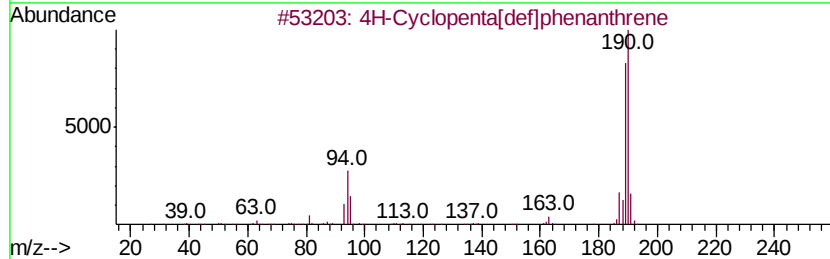
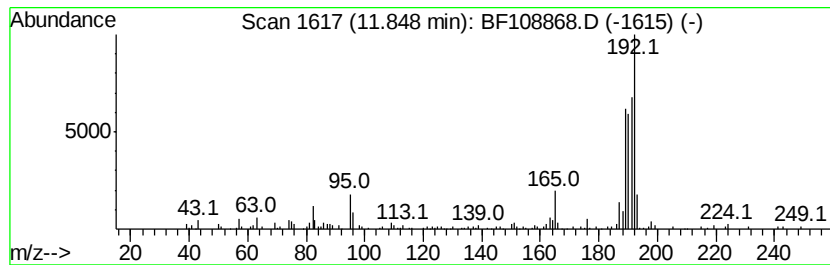
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.85	4.05 ng	272478	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	60
2	Anthracene, 2-methyl-	192	C15H12	000613-12-7	46
3	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	42
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	42
5	Anthracene, 9-methyl-	192	C15H12	000779-02-2	41



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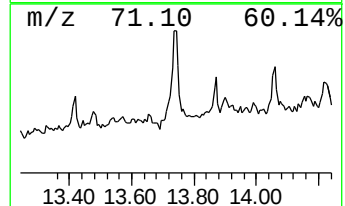
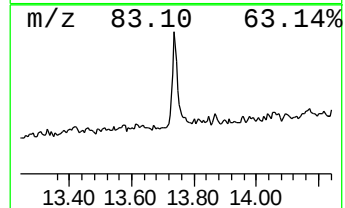
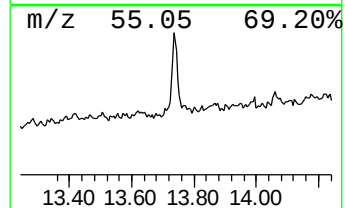
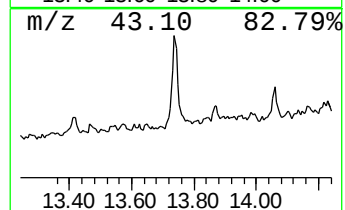
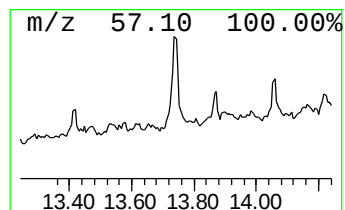
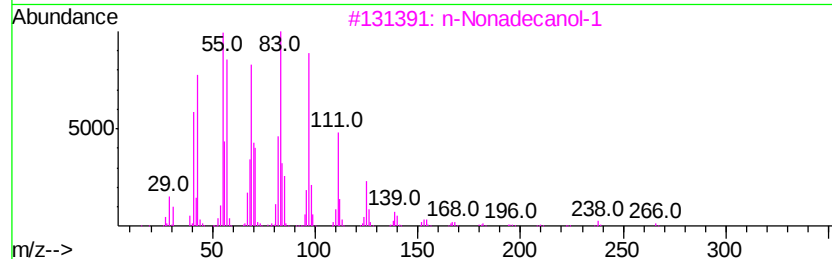
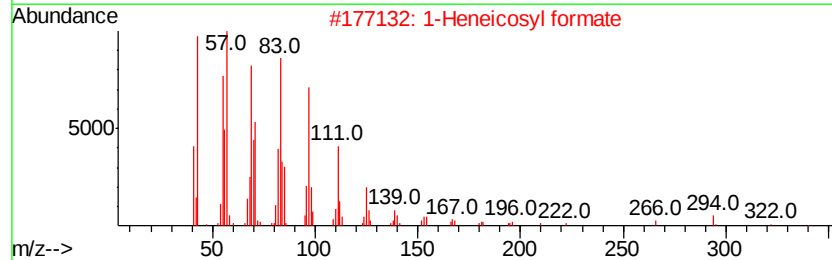
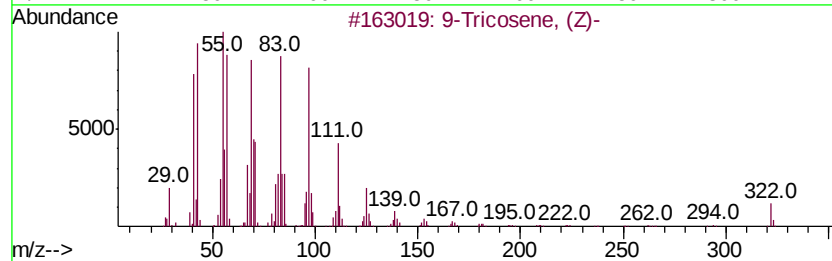
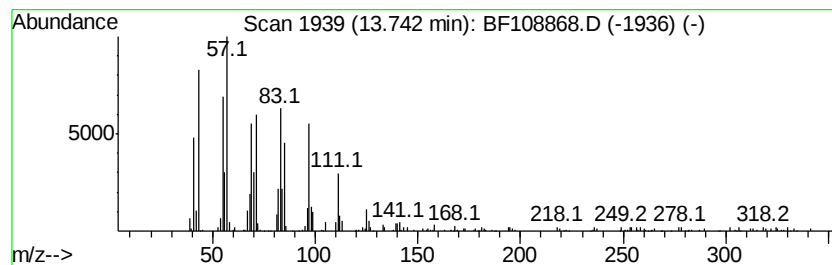
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Tricosene, (Z)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.74	2.70 ng	273139	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Tricosene, (Z)-	322	C23H46	027519-02-4	94
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4		Behenic alcohol	326	C22H46O	000661-19-8	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108868.D
Acq On : 7 Sep 2018 18:39
Operator : JU/SJ
Sample : J4825-18MSD
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-WS-COMP-18MSD

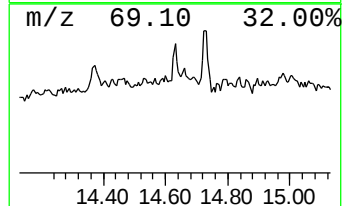
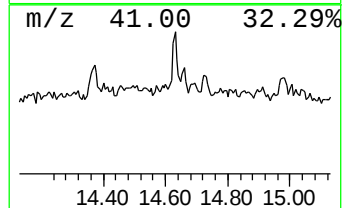
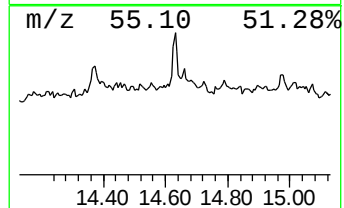
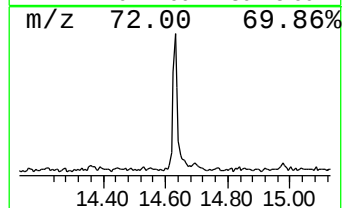
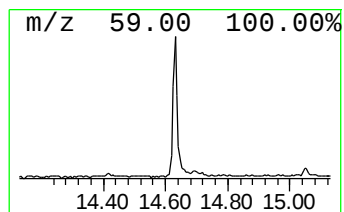
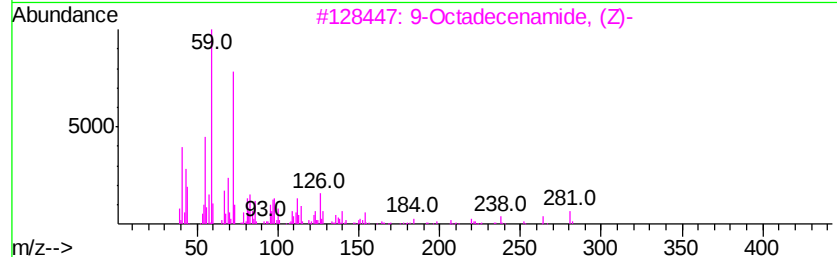
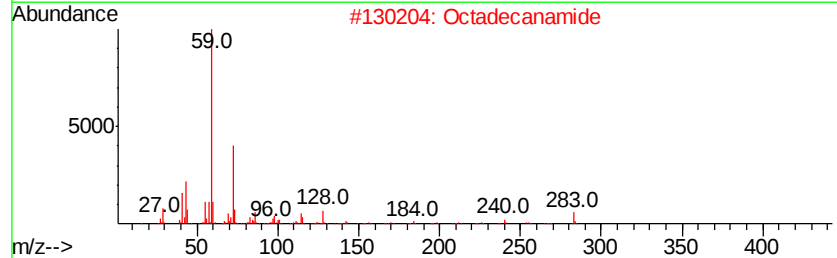
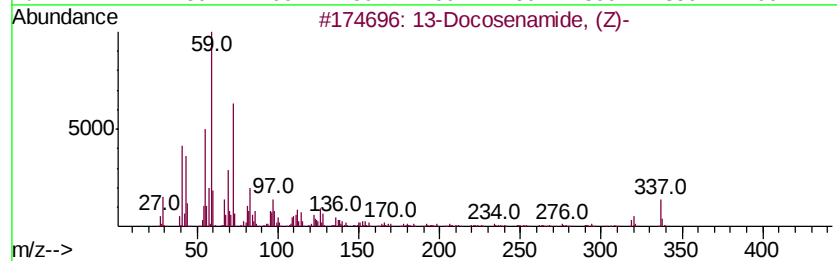
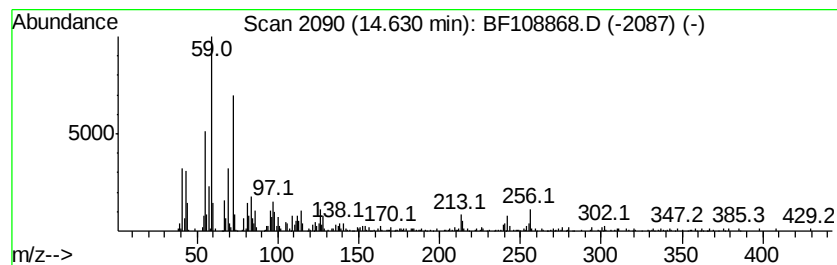
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 13-Docosenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	4.14 ng	242155	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	90
2		Octadecanamide	283	C18H37NO	000124-26-5	80
3		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	74
4		Hexadecanamide	255	C16H33NO	000629-54-9	64
5		Decanamide-	171	C10H21NO	002319-29-1	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090718\
Data File : BF108868.D
Acq On : 7 Sep 2018 18:39
Operator : JU/SJ
Sample : J4825-18MSD
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-WS-COMP-18MSD

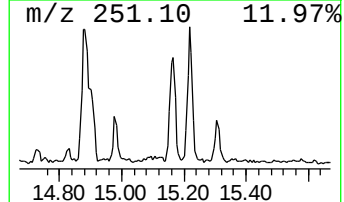
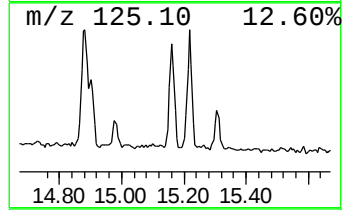
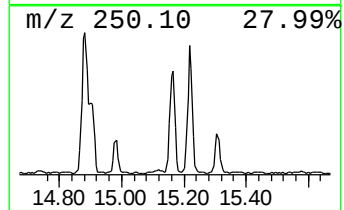
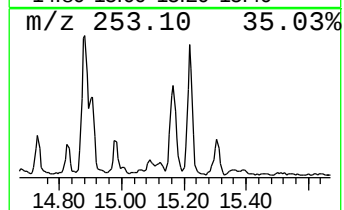
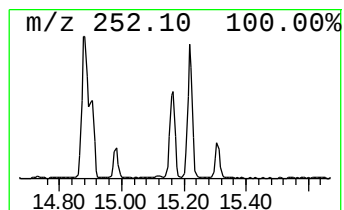
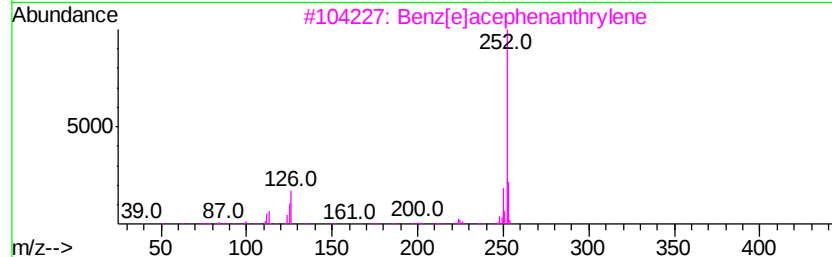
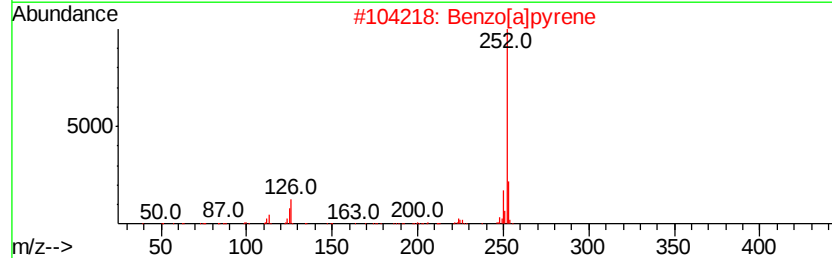
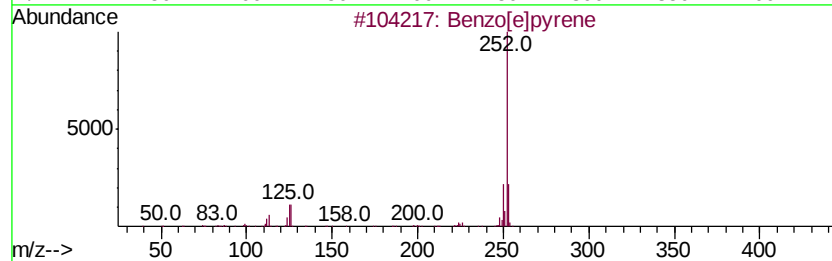
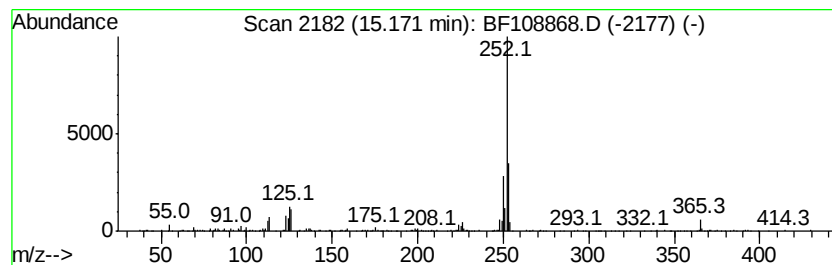
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzo[e]pyrene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	7.97 ng	465440	Perylene-d12	15.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[e]pyrene	252	C20H12	000192-97-2	99
2		Benzo[a]pyrene	252	C20H12	000050-32-8	98
3		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	96
4		Perylene	252	C20H12	000198-55-0	90
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	89



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090718\
Data File : BF108868.D
Acq On : 7 Sep 2018 18:39
Operator : JU/SJ
Sample : J4825-18MSD
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
EP1-WS-COMP-18MSD

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF090518.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-hy...	4.94	3.8	ng	240695	1	6.74	1278140	20.0
unknown6.51	6.51	85.7	ng	5476680	1	6.74	1278140	20.0
Anthracene, 9-met...	11.78	4.9	ng	332482	4	11.24	1346240	20.0
4H-Cyclopenta[def...	11.85	4.0	ng	272478	4	11.24	1346240	20.0
9-Tricosene, (Z)-	13.74	2.7	ng	273139	5	13.87	2023870	20.0
13-Docosenamide, ...	14.63	4.1	ng	242155	6	15.28	1168540	20.0
Benzo[e]pyrene	15.17	8.0	ng	465440	6	15.28	1168540	20.0