

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
 Data File : BF118138.D
 Acq On : 7 Dec 2019 19:26
 Operator : JU
 Sample : K6147-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :

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-BF120619.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	2.481	57	67	73	rVB	83405	117225	4.23%	0.191%
2	5.075	503	508	515	rVB	341377	398232	14.35%	0.649%
3	5.481	573	577	580	rBV	2185707	1954246	70.44%	3.184%
4	6.498	745	750	753	rBV	2346931	2150213	77.50%	3.503%
5	6.639	769	774	777	rBV	2611843	2366807	85.31%	3.856%
6	6.698	781	784	788	rVB	86362	71756	2.59%	0.117%
7	6.869	809	813	816	rBV	809641	724626	26.12%	1.181%
8	7.022	835	839	843	rBV	2179556	1828155	65.89%	2.979%
9	7.428	904	908	911	rBV	1485524	1346859	48.55%	2.194%
10	7.539	924	927	930	rVB	57948	45455	1.64%	0.074%
11	8.151	1028	1031	1033	rBV	1113669	947357	34.15%	1.544%
12	8.175	1033	1035	1039	rVV	982126	724616	26.12%	1.181%
13	8.869	1149	1153	1159	rBV	552540	447031	16.11%	0.728%
14	8.969	1166	1170	1178	rVB	246709	218362	7.87%	0.356%
15	9.233	1210	1215	1218	rBV	3060874	2774415	100.00%	4.520%
16	9.333	1229	1232	1237	rVB	190648	169788	6.12%	0.277%
17	9.427	1245	1248	1253	rVB	61789	54320	1.96%	0.089%
18	9.498	1256	1260	1264	rVV	76439	99828	3.60%	0.163%
19	9.569	1269	1272	1275	rBV	91522	92596	3.34%	0.151%
20	9.622	1279	1281	1285	rVV	245673	208912	7.53%	0.340%
21	9.686	1290	1292	1299	rVB2	47087	54484	1.96%	0.089%
22	9.774	1303	1307	1312	rVB	178903	151548	5.46%	0.247%
23	9.916	1324	1331	1333	rBV	1320759	1174442	42.33%	1.914%
24	9.945	1333	1336	1340	rVB	600882	458954	16.54%	0.748%
25	10.069	1352	1357	1360	rBV2	36195	44179	1.59%	0.072%
26	10.116	1362	1365	1370	rVB	448223	409737	14.77%	0.668%
27	10.339	1396	1403	1406	rBV4	36189	53074	1.91%	0.086%
28	10.369	1406	1408	1410	rBV	63096	44800	1.61%	0.073%
29	10.427	1410	1418	1420	rBV4	31396	47004	1.69%	0.077%
30	10.463	1420	1424	1430	rVB	383273	322787	11.63%	0.526%
31	10.521	1430	1434	1437	rBV2	64668	78258	2.82%	0.128%
32	10.621	1448	1451	1455	rBV3	133755	134558	4.85%	0.219%
33	10.669	1455	1459	1461	rVV	185364	198821	7.17%	0.324%
34	10.704	1462	1465	1475	rVB2	2062015	1936866	69.81%	3.156%

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35	10.786	1475	1479	1481	rBV3	50642	78022	2.81%	0.127%
36	10.816	1481	1484	1485	rBV	119345	113527	4.09%	0.185%
37	10.833	1485	1487	1489	rVV	999284	763213	27.51%	1.244%
38	10.857	1489	1491	1493	rVV	278458	207834	7.49%	0.339%
39	10.886	1493	1496	1498	rVV	1932301	1566549	56.46%	2.552%
40	10.921	1498	1502	1505	rVV2	2295646	2592464	93.44%	4.224%
41	10.957	1505	1508	1510	rVV	2034190	1856725	66.92%	3.025%
42	10.980	1510	1512	1514	rVV	1224211	911221	32.84%	1.485%
43	11.010	1514	1517	1518	rVV	610623	686608	24.75%	1.119%
44	11.021	1518	1519	1520	rVV	708306	423067	15.25%	0.689%
45	11.033	1520	1521	1524	rVV	773780	617575	22.26%	1.006%
46	11.068	1524	1527	1530	rVV3	1685815	1942035	70.00%	3.164%
47	11.104	1530	1533	1535	rVV	1829706	1544070	55.65%	2.516%
48	11.121	1535	1536	1538	rVV	604892	539450	19.44%	0.879%
49	11.145	1538	1540	1545	rVV2	1162844	962893	34.71%	1.569%
50	11.216	1548	1552	1557	rVV3	154028	235514	8.49%	0.384%
51	11.268	1558	1561	1562	rVV	111924	123820	4.46%	0.202%
52	11.286	1562	1564	1570	rVV2	162882	309482	11.15%	0.504%
53	11.333	1570	1572	1574	rVV	93708	91818	3.31%	0.150%
54	11.357	1574	1576	1579	rVB	102396	84876	3.06%	0.138%
55	11.410	1581	1585	1587	rVV	1074594	1051829	37.91%	1.714%
56	11.433	1587	1589	1592	rVV	1632193	1214138	43.76%	1.978%
57	11.480	1594	1597	1600	rVV	420886	361058	13.01%	0.588%
58	11.516	1600	1603	1606	rVB4	37513	47291	1.70%	0.077%
59	11.633	1618	1623	1630	rBV	132951	191500	6.90%	0.312%
60	11.698	1631	1634	1639	rVV3	50356	76839	2.77%	0.125%
61	11.910	1664	1670	1671	rBV	176781	173364	6.25%	0.282%
62	11.933	1671	1674	1680	rVV2	898822	855842	30.85%	1.394%
63	11.986	1680	1683	1686	rVV2	79970	77453	2.79%	0.126%
64	12.021	1686	1689	1692	rVV	231319	246008	8.87%	0.401%
65	12.045	1692	1693	1697	rVB	107881	66557	2.40%	0.108%
66	12.104	1698	1703	1705	rBV4	50340	88789	3.20%	0.145%
67	12.204	1718	1720	1723	rBV	168143	142575	5.14%	0.232%
68	12.233	1723	1725	1728	rVB2	119912	103421	3.73%	0.169%
69	12.333	1740	1742	1744	rBV2	41383	44396	1.60%	0.072%
70	12.357	1744	1746	1748	rVV	60875	50132	1.81%	0.082%
71	12.386	1748	1751	1753	rVV	84310	72644	2.62%	0.118%

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72	12.463	1761	1764	1767	rVV	139200	159794	5.76%	0.260%
73	12.492	1767	1769	1772	rVV3	92878	100841	3.63%	0.164%
74	12.545	1775	1778	1783	rVV	120059	160300	5.78%	0.261%
75	12.627	1788	1792	1795	rBV	2638507	2346022	84.56%	3.822%
76	12.657	1795	1797	1801	rVV3	120056	167470	6.04%	0.273%
77	12.721	1805	1808	1815	rBV3	443071	508417	18.33%	0.828%
78	12.857	1825	1831	1834	rBV2	1937418	2305427	83.10%	3.756%
79	12.910	1837	1840	1843	rVB3	154539	210673	7.59%	0.343%
80	12.998	1851	1855	1858	rVB	2470276	1939728	69.91%	3.160%
81	13.068	1865	1867	1872	rBV3	90643	129994	4.69%	0.212%
82	13.186	1884	1887	1892	rVB2	251606	328649	11.85%	0.535%
83	13.251	1896	1898	1901	rVB	171990	126904	4.57%	0.207%
84	13.286	1901	1904	1907	rBV2	189223	223674	8.06%	0.364%
85	13.380	1918	1920	1923	rBV	104241	78524	2.83%	0.128%
86	13.445	1929	1931	1934	rBV2	87282	65794	2.37%	0.107%
87	13.539	1945	1947	1950	rBV	178613	177386	6.39%	0.289%
88	13.621	1959	1961	1966	rVB	284861	255891	9.22%	0.417%
89	13.698	1971	1974	1982	rVV2	198425	347125	12.51%	0.566%
90	13.809	1988	1993	1995	rBV4	307738	510802	18.41%	0.832%
91	13.833	1995	1997	1999	rVV	185735	185405	6.68%	0.302%
92	13.857	1999	2001	2005	rVV4	199927	319214	11.51%	0.520%
93	14.057	2028	2035	2038	rBV3	1428319	2504601	90.27%	4.081%
94	14.086	2038	2040	2043	rVB	938725	831385	29.97%	1.355%
95	15.121	2211	2216	2219	rBV	1051545	1642670	59.21%	2.676%
96	15.427	2265	2268	2274	rVB	542166	722840	26.05%	1.178%
97	15.492	2275	2279	2285	rBV	744307	1162093	41.89%	1.893%
98	15.556	2287	2290	2294	rVV	444434	538210	19.40%	0.877%
99	17.068	2542	2547	2556	rVB2	287045	600166	21.63%	0.978%
100	17.521	2620	2624	2632	rVB	193000	360144	12.98%	0.587%

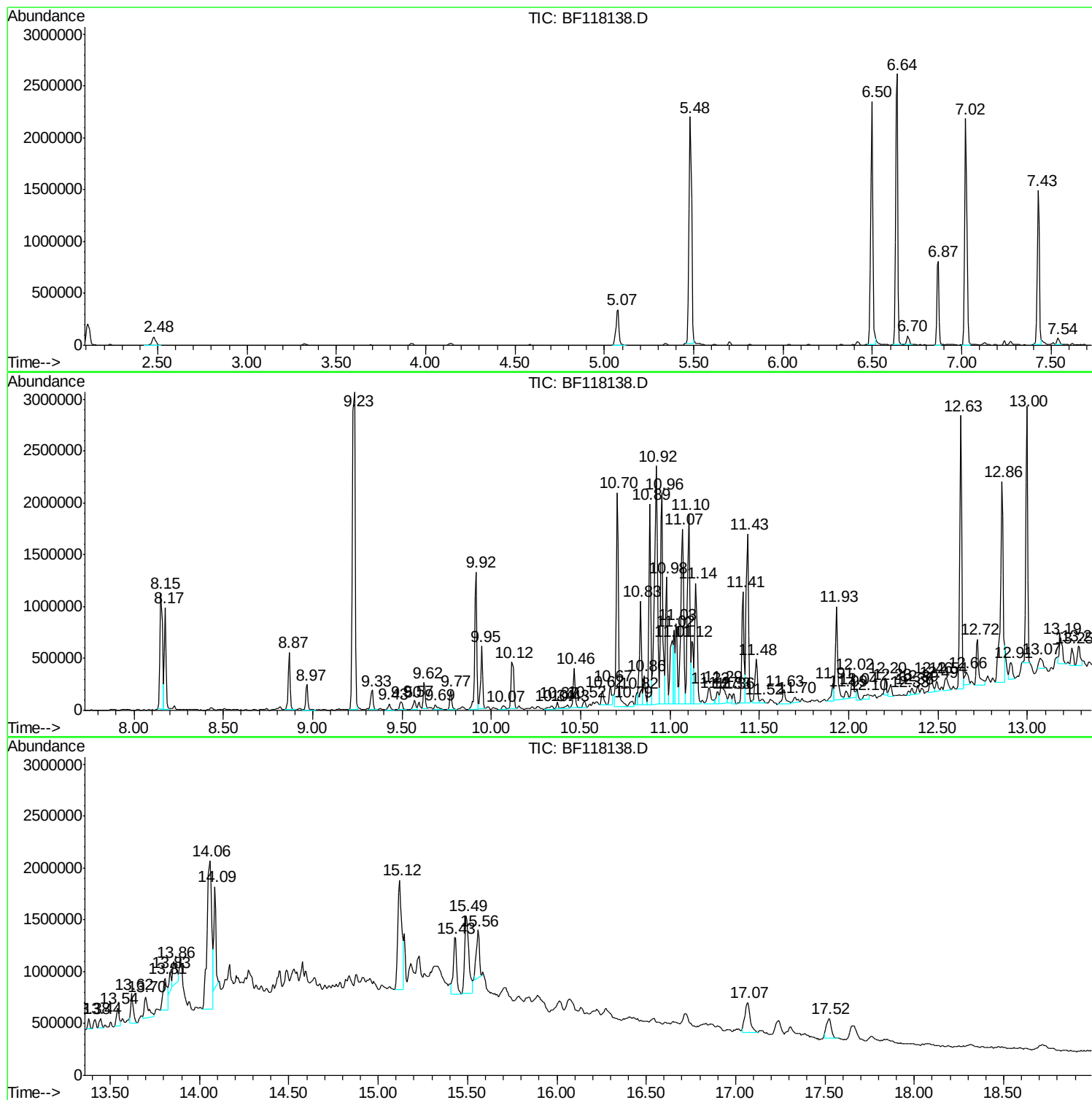
Sum of corrected areas: 61375053

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Instrument :
BNA_F
ClientSampled :

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.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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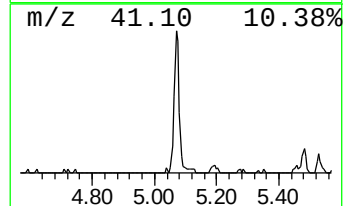
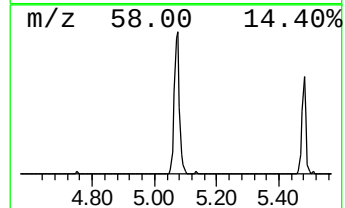
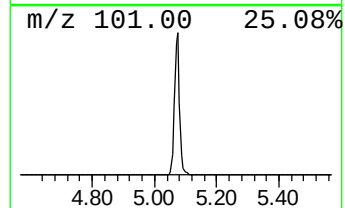
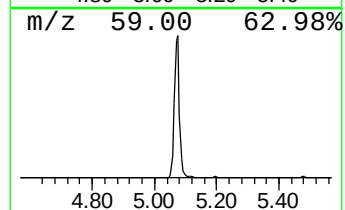
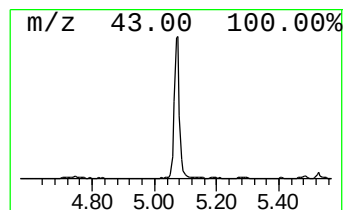
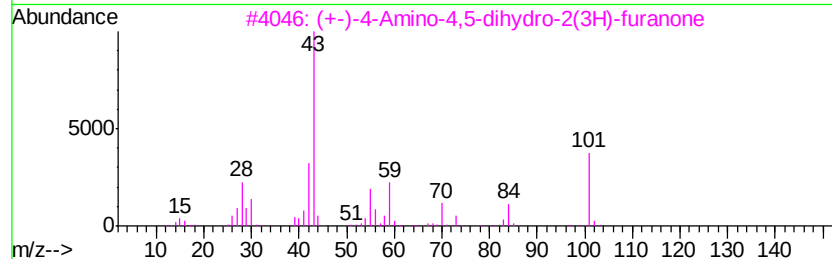
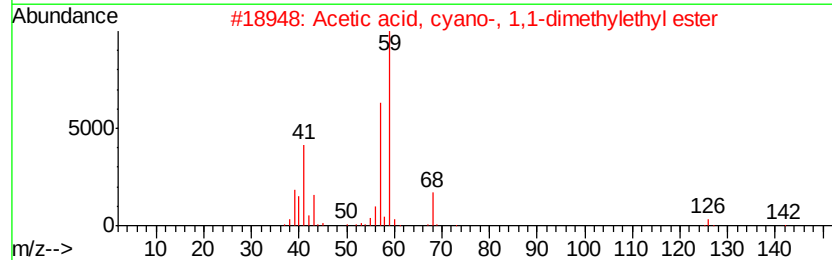
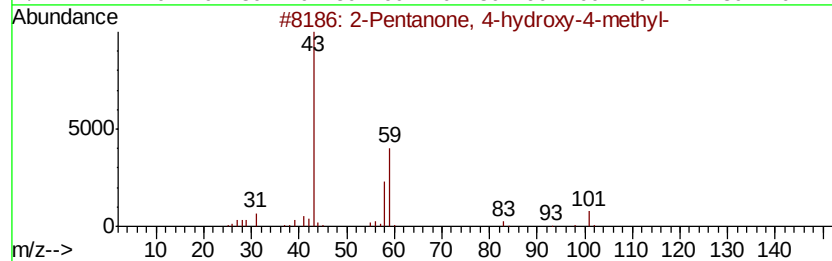
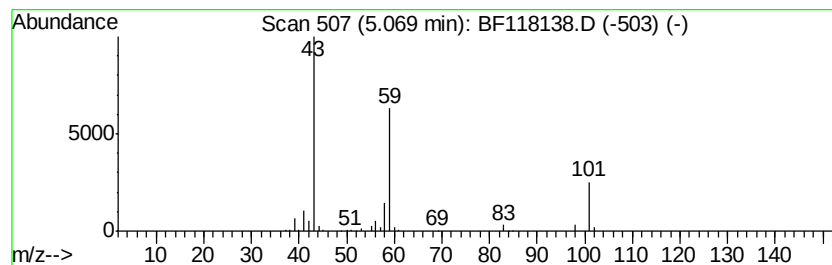
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	10.99 ng	398232	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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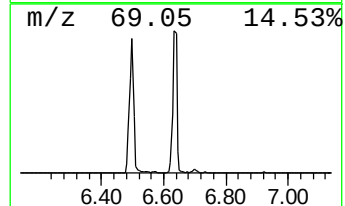
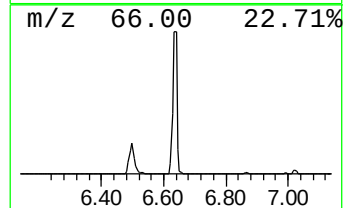
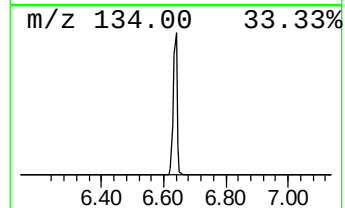
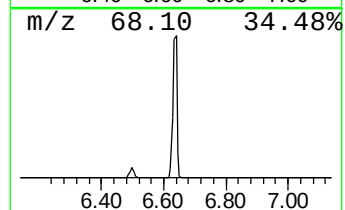
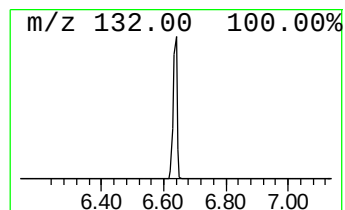
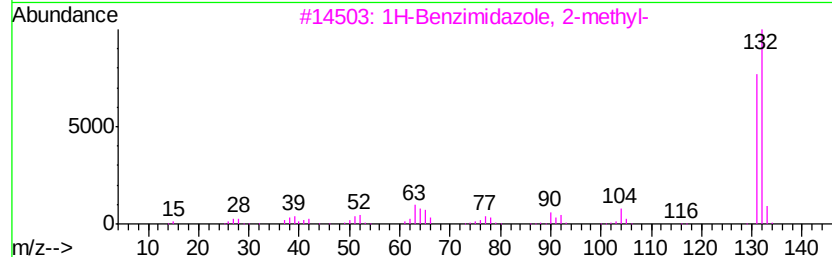
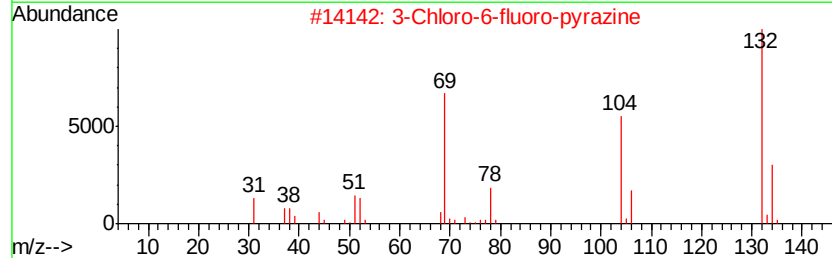
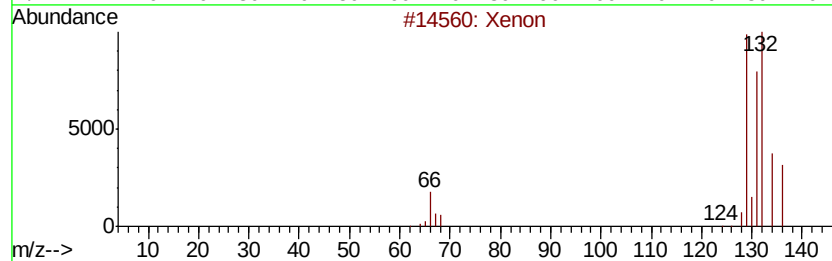
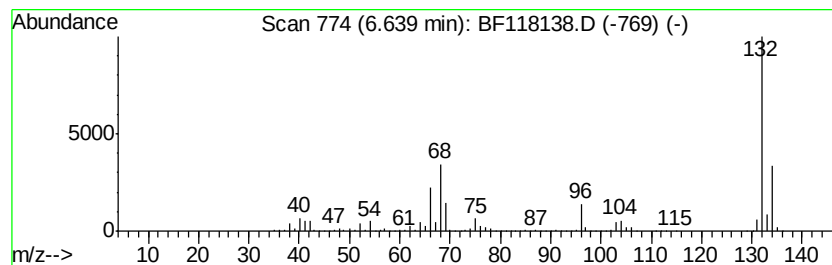
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Peak Number 2 Xenon Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	65.32 ng	2366810	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Xenon	132	Xe	007440-63-3	50
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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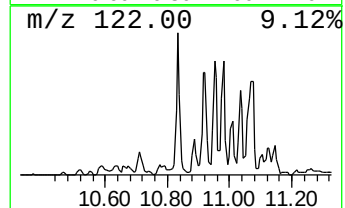
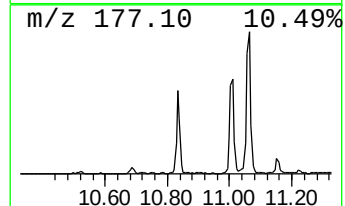
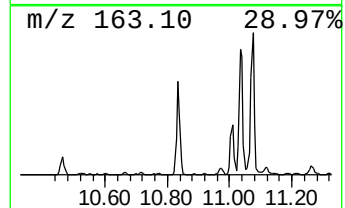
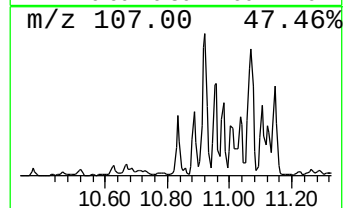
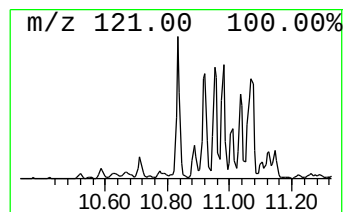
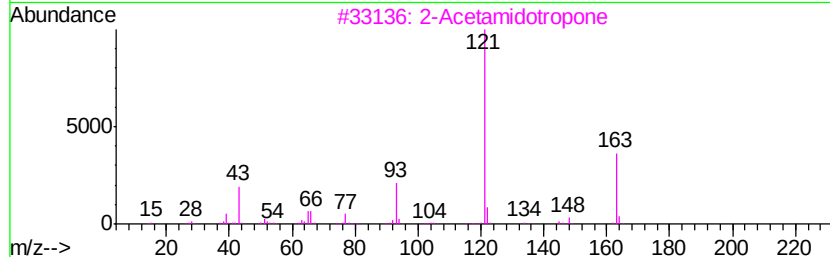
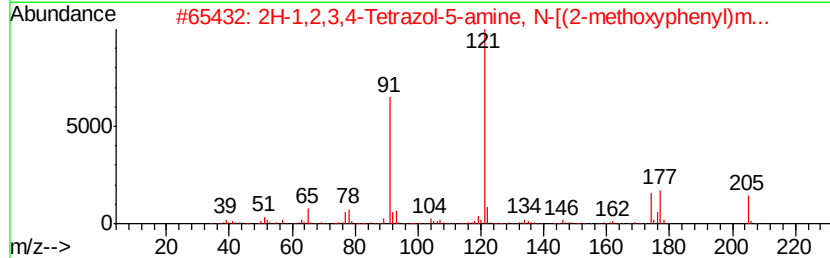
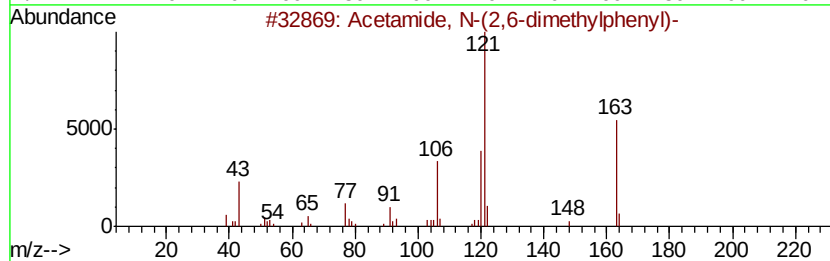
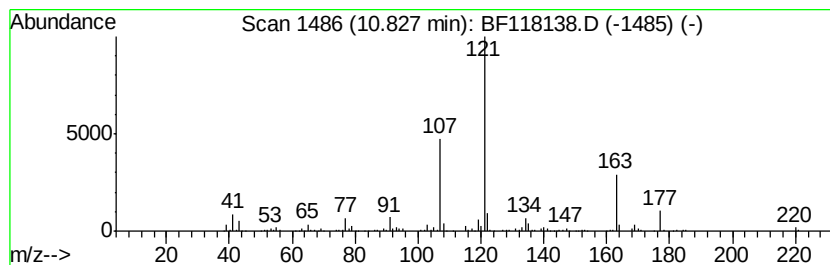
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Peak Number 4 Acetamide, N-(2,6-dimethylp... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.83	14.51 ng	763213	Phenanthrene-d10	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2,6-dimethylphenyl)-	163	C10H13NO	002198-53-0	50
2	2H-1,2,3,4-Tetrazol-5-amine, N-[...]	205	C9H11N5O	1000337-56-1	47
3	2-Acetamidotropone	163	C9H9NO2	006422-12-4	47
4	p-Sec-butylphenyl acetate	192	C12H16O2	003245-24-7	43
5	Benorilate	313	C17H15NO5	005003-48-5	38



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Operator : JU
Sample : K6147-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :

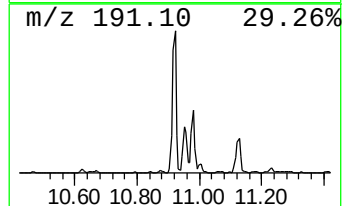
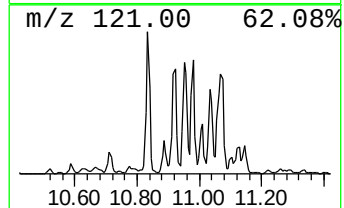
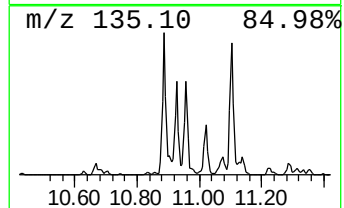
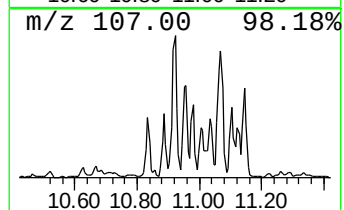
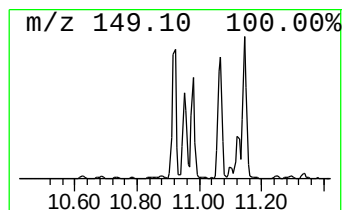
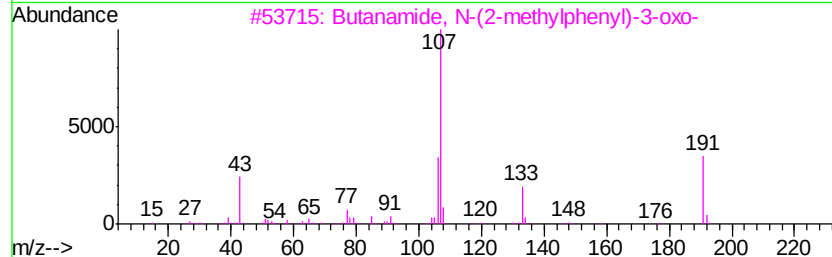
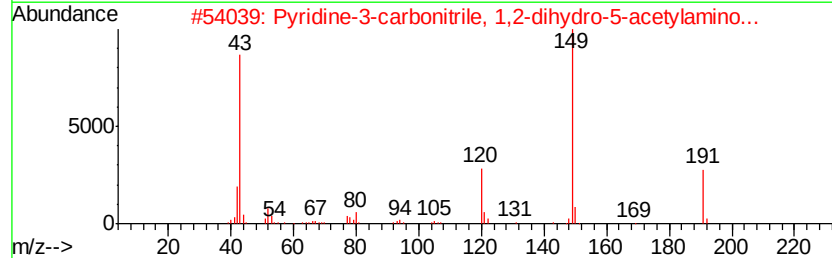
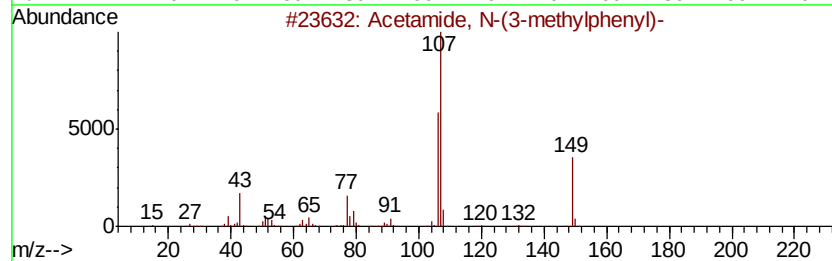
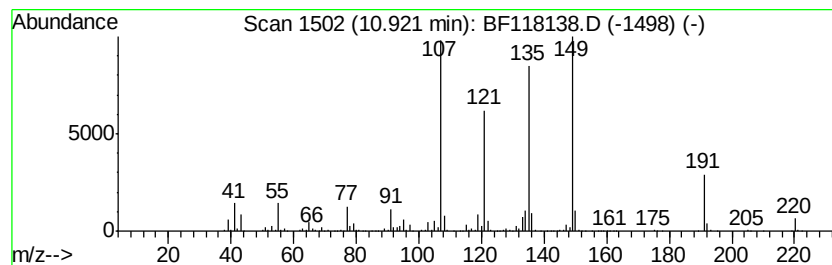
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown10.92 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.92	49.29 ng	2592460	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	43
2		Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	30
3		Butanamide, N-(2-methylphenyl)-3...	191	C11H13NO2	000093-68-5	25
4		Phenol, 4-butyl-	150	C10H14O	001638-22-8	18
5		Benzestrol	298	C20H26O2	000085-95-0	18



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
Data File : BF118138.D
Acq On : 7 Dec 2019 19:26
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Sample : K6147-07
Misc :
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ClientSampleId :

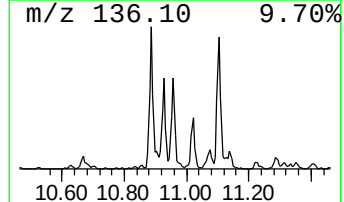
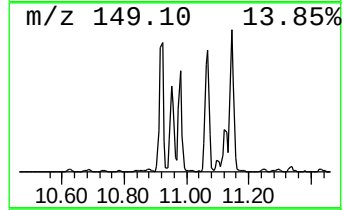
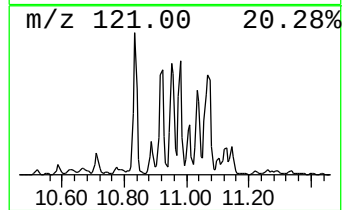
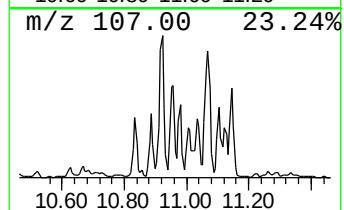
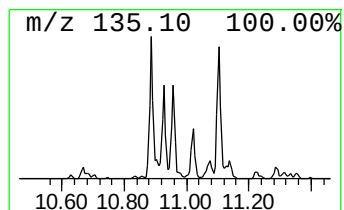
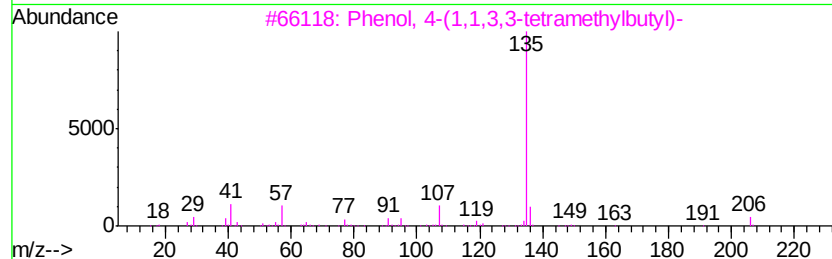
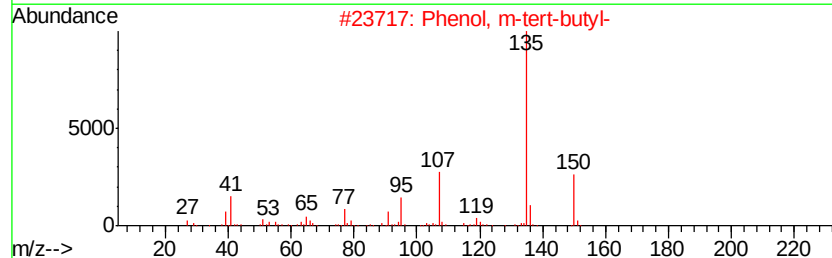
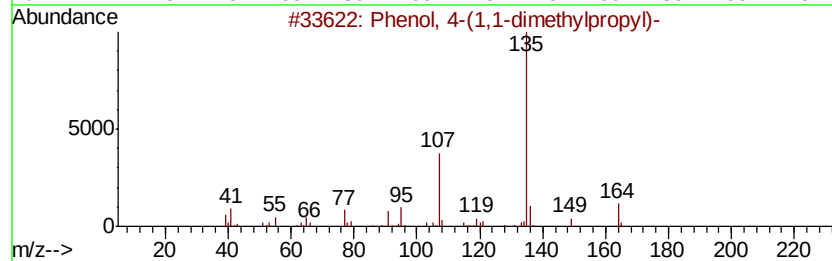
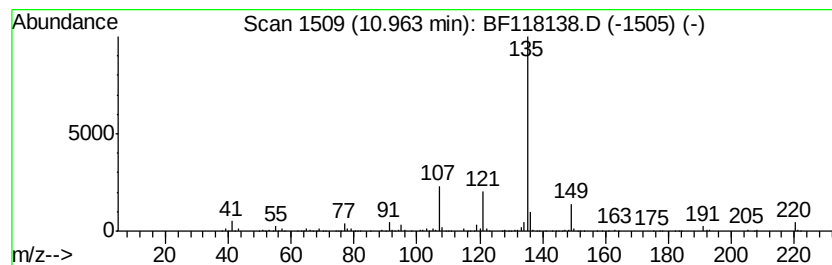
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	35.30 ng	1856730	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	64
2		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	58
3		Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	53
4		Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	53
5		Hexestrol	270	C18H22O2	005635-50-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
Data File : BF118138.D
Acq On : 7 Dec 2019 19:26
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Sample : K6147-07
Misc :
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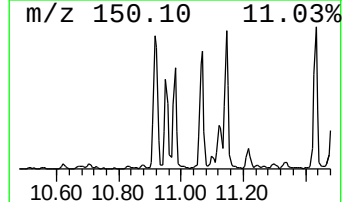
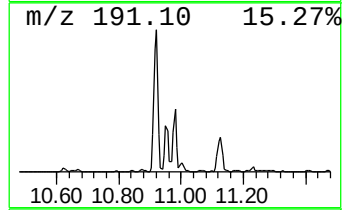
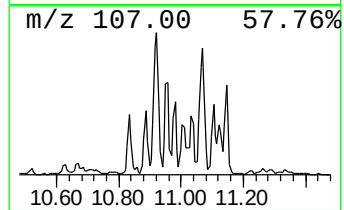
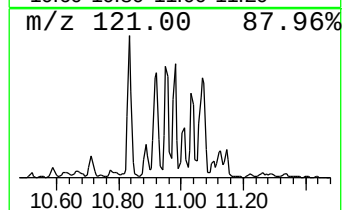
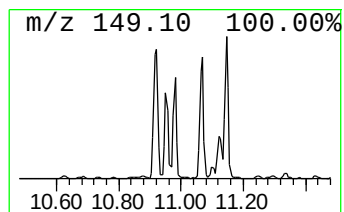
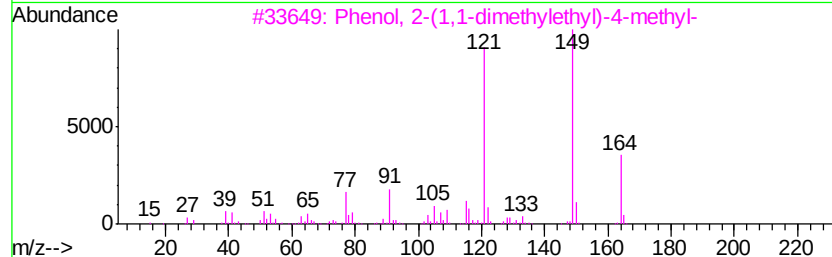
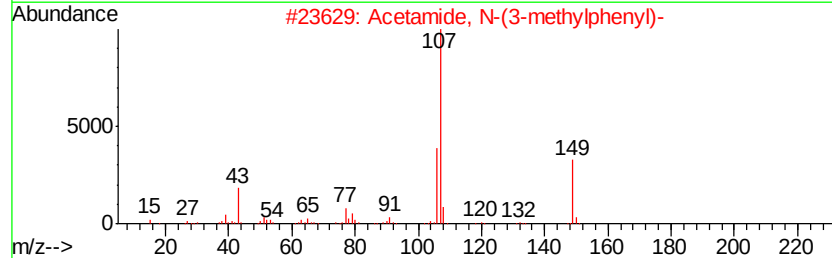
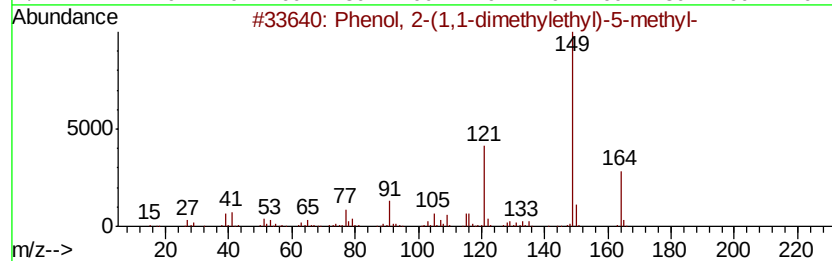
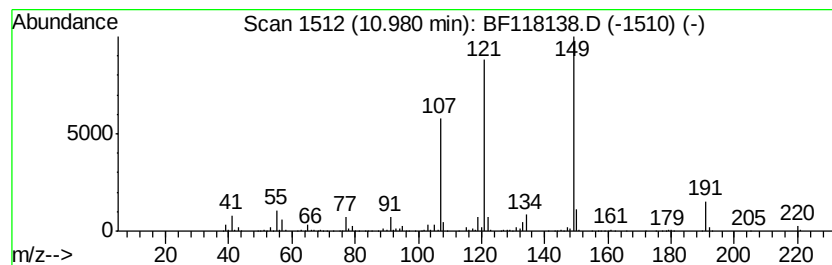
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 2-(1,1-dimethylethy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	17.33 ng	911221	Phenanthrene-d10	11.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	59
2		Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	46
3		Phenol, 2-(1,1-dimethylethyl)-4-...	164	C11H16O	002409-55-4	45
4		Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	38
5		1-(2,6-Dimethyl-4-propoxyphenyl)...	220	C14H20O2	1000190-22-3	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
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Sample : K6147-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

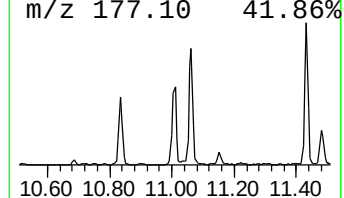
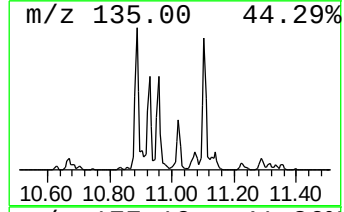
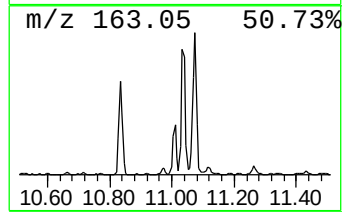
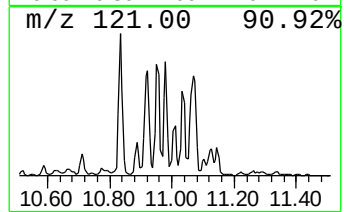
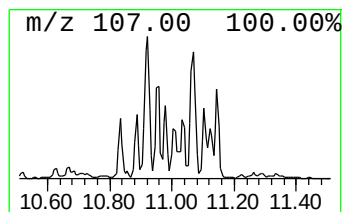
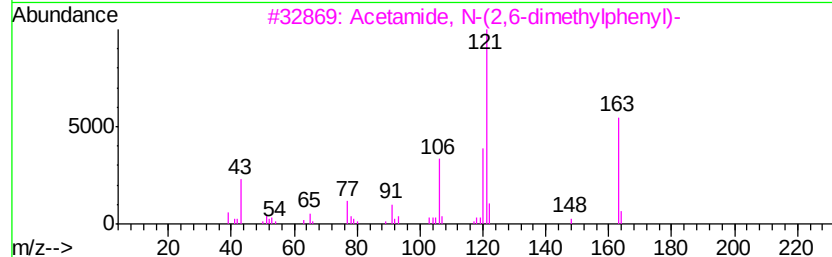
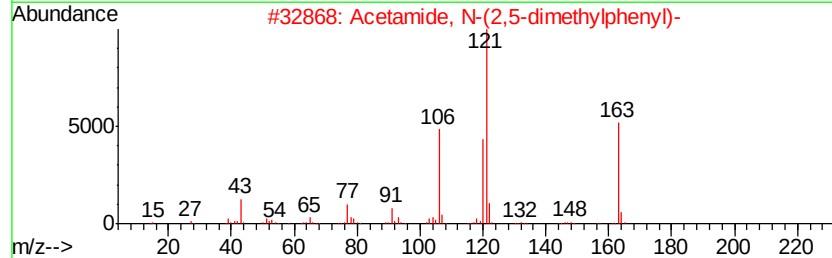
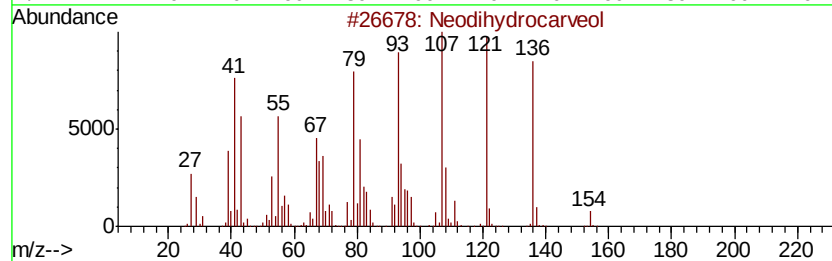
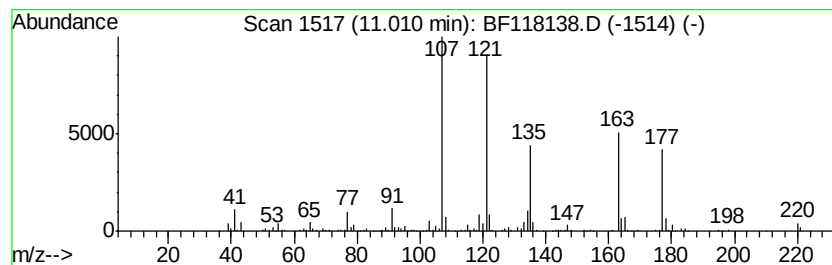
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown11.01 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.01	13.06 ng	686608	Phenanthrene-d10	11.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Neodihydrocarveol	154	C10H18O	018675-34-8	38
2	Acetamide, N-(2,5-dimethylphenyl)-	163	C10H13NO	002050-44-4	30
3	Acetamide, N-(2,6-dimethylphenyl)-	163	C10H13NO	002198-53-0	30
4	Propanamide, N-(3-methylphenyl)-...	177	C11H15NO	1000307-32-0	30
5	p-Propionotoluidide	163	C10H13NO	002759-55-9	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
Data File : BF118138.D
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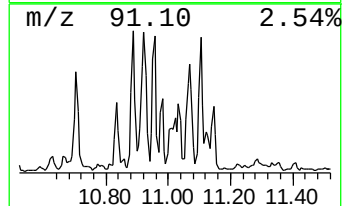
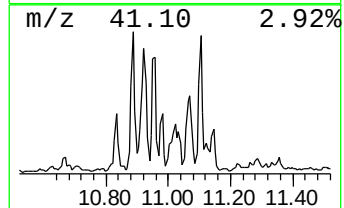
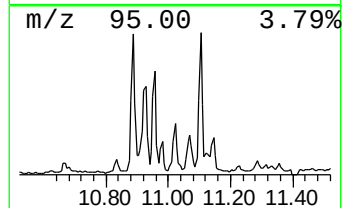
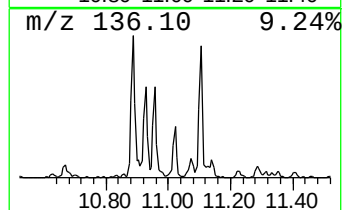
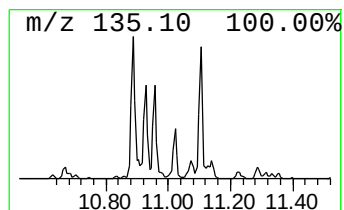
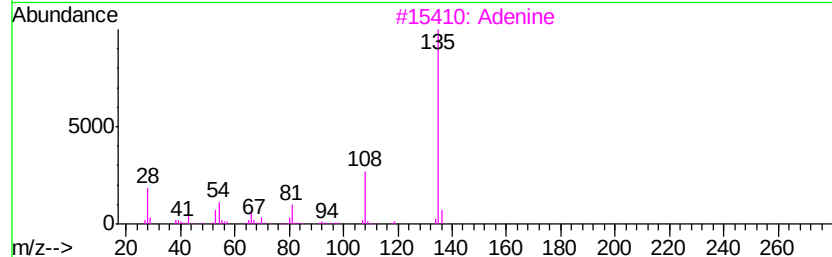
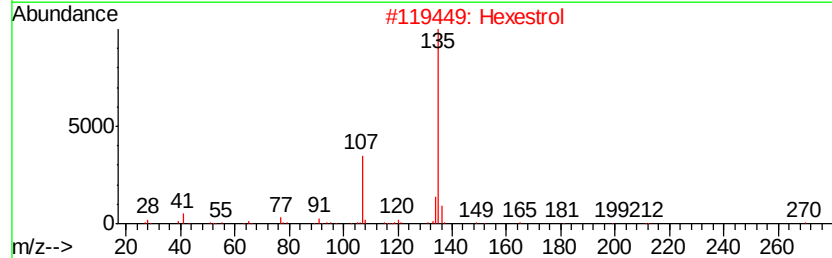
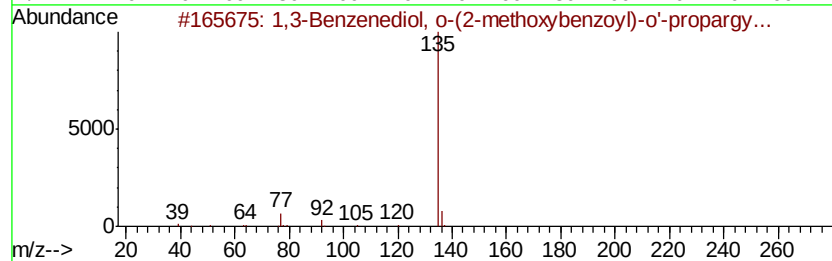
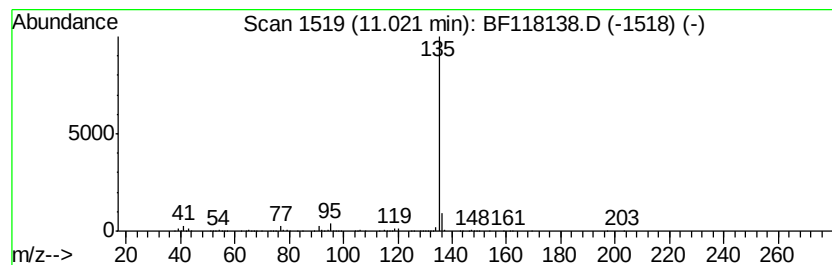
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown11.02 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	8.04 ng	423067	Phenanthrene-d10	11.41

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenediol, o-(2-methoxyben...	326	C18H14O6	1000330-77-3	40
2			Hexestrol	270	C18H22O2	000084-16-2	40
3			Adenine	135	C5H5N5	000073-24-5	9
4			Thioimidodicarbonic diamide	135	C2H5N3S2	000541-53-7	9
5			1,3-Benzenediol, o-(2-furoyl)-o'...	338	C19H14O6	1000330-77-5	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF120719\
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :

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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 11 1,2-Dimethyl-5-nitroadamantane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.03	11.74 ng	617575	Phenanthrene-d10	11.41

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	43
2			Tricyclo[3.3.1.1(3,7)]decane, 1...	242	C12H19Br	000941-37-7	37
3			3-(4-Methoxyphenyl)propionic aci...	208	C12H16O3	022767-72-2	27
4			2-Propanone, 1-(4-methoxyphenyl)-	164	C10H12O2	000122-84-9	27
5			Carbonic acid, isobutyl 4-isopro...	236	C14H20O3	1000331-40-6	27

