

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
 Data File : BF102228.D
 Acq On : 19 Jan 2018 20:37
 Operator : SJ/JU
 Sample : J1189-06
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 4-2

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:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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	2.451	57	62	70	rVB	39980	59864	1.16%	0.110%
2	3.051	156	164	171	rBV	62502	115740	2.25%	0.212%
3	3.575	248	253	262	rBV	66989	108299	2.11%	0.199%
4	3.698	268	274	279	rVB	132133	189066	3.68%	0.347%
5	4.263	366	370	374	rBV	70284	86882	1.69%	0.159%
6	4.916	476	481	492	rBV	421998	589021	11.46%	1.080%
7	5.287	537	544	547	rBV	240787	254985	4.96%	0.468%
8	5.328	547	551	555	rVB	2756601	2990776	58.19%	5.486%
9	5.557	586	590	594	rBV2	320228	409428	7.97%	0.751%
10	5.657	603	607	612	rBV	251071	214120	4.17%	0.393%
11	5.763	621	625	628	rBV	156188	124748	2.43%	0.229%
12	6.004	660	666	676	rBV3	111551	187143	3.64%	0.343%
13	6.316	714	719	721	rBV	93952	93113	1.81%	0.171%
14	6.357	721	726	730	rVV	2610485	3109954	60.50%	5.704%
15	6.392	730	732	741	rVV2	179717	198221	3.86%	0.364%
16	6.486	744	748	752	rVV	3110535	3110424	60.51%	5.705%
17	6.545	754	758	770	rVB2	227574	258776	5.03%	0.475%
18	6.716	784	787	791	rBV	1057873	867661	16.88%	1.592%
19	6.775	794	797	800	rBV2	96561	91468	1.78%	0.168%
20	6.875	810	814	817	rBV	2644873	2251308	43.80%	4.130%
21	6.992	831	834	839	rVB3	47588	60965	1.19%	0.112%
22	7.286	879	884	887	rVB	1920105	1916744	37.29%	3.516%
23	7.380	893	900	902	rBV3	65007	105755	2.06%	0.194%
24	7.433	906	909	912	rVB	169934	150895	2.94%	0.277%
25	7.539	923	927	930	rVB	2264842	2043622	39.76%	3.749%
26	7.675	948	950	953	rVB	73518	55200	1.07%	0.101%
27	7.745	957	962	965	rVV2	366117	315080	6.13%	0.578%
28	7.904	986	989	993	rBV	64655	59482	1.16%	0.109%
29	7.998	1001	1005	1008	rBV	1371062	1179600	22.95%	2.164%
30	8.769	1132	1136	1141	rBV	702954	581832	11.32%	1.067%
31	9.075	1183	1188	1195	rVB	3086864	2922758	56.86%	5.361%
32	9.216	1210	1212	1216	rVB	75613	62762	1.22%	0.115%
33	9.474	1251	1256	1259	rBV	988968	849704	16.53%	1.559%
34	9.686	1288	1292	1294	rBV2	87522	75259	1.46%	0.138%

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35	9.751	1296	1303	1307	rBV2	1435069	1253365	24.38%	2.299%
36	10.016	1342	1348	1355	rBV	204082	234972	4.57%	0.431%
37	10.157	1368	1372	1375	rBV	445852	412776	8.03%	0.757%
38	10.180	1375	1376	1380	rVB	115483	87699	1.71%	0.161%
39	10.404	1410	1414	1417	rBV	492232	407278	7.92%	0.747%
40	10.545	1433	1438	1441	rBV	1931236	2019171	39.28%	3.704%
41	10.604	1444	1448	1454	rVV	641269	599898	11.67%	1.100%
42	10.657	1454	1457	1463	rVB2	108990	112751	2.19%	0.207%
43	10.786	1476	1479	1484	rBV	211638	194639	3.79%	0.357%
44	11.104	1531	1533	1535	rBV	73987	55755	1.08%	0.102%
45	11.233	1551	1555	1558	rBV	1270367	1184045	23.04%	2.172%
46	11.463	1590	1594	1598	rBV3	54895	64867	1.26%	0.119%
47	11.527	1603	1605	1608	rVB	73966	57344	1.12%	0.105%
48	11.580	1608	1614	1616	rBV4	61091	101630	1.98%	0.186%
49	11.610	1616	1619	1624	rVB2	104069	107553	2.09%	0.197%
50	11.733	1636	1640	1642	rBV2	41093	62619	1.22%	0.115%
51	11.774	1643	1647	1649	rVV	562622	537491	10.46%	0.986%
52	11.810	1649	1653	1656	rVV	4625642	5140057	100.00%	9.428%
53	11.851	1656	1660	1662	rVB3	47034	55929	1.09%	0.103%
54	11.939	1671	1675	1677	rBV2	64935	64625	1.26%	0.119%
55	12.204	1717	1720	1724	rVB	226461	209736	4.08%	0.385%
56	12.363	1743	1747	1751	rBV3	117778	175899	3.42%	0.323%
57	12.492	1766	1769	1772	rBV3	111576	86991	1.69%	0.160%
58	12.545	1772	1778	1782	rVV3	66686	122889	2.39%	0.225%
59	12.598	1782	1787	1791	rVV4	74770	94518	1.84%	0.173%
60	12.651	1793	1796	1798	rVV	105511	103797	2.02%	0.190%
61	12.704	1801	1805	1812	rVB2	122362	170170	3.31%	0.312%
62	12.821	1821	1825	1828	rBV	2377876	2289043	44.53%	4.199%
63	12.862	1828	1832	1835	rVB	1898143	1785930	34.75%	3.276%
64	13.104	1869	1873	1875	rBV	155061	152055	2.96%	0.279%
65	13.180	1882	1886	1889	rBV	1978847	1758652	34.21%	3.226%
66	13.210	1889	1891	1894	rVB	315541	281567	5.48%	0.516%
67	13.298	1903	1906	1908	rBV	371061	311622	6.06%	0.572%
68	13.321	1908	1910	1913	rVB	114432	100631	1.96%	0.185%
69	13.492	1937	1939	1943	rBV3	63573	67357	1.31%	0.124%
70	13.715	1973	1977	1983	rBV2	501766	515634	10.03%	0.946%
71	13.862	1997	2002	2006	rBV2	3349666	3976759	77.37%	7.294%

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72	14.074	2035	2038	2040	rBV	103672	95682	1.86%	0.176%
73	14.121	2043	2046	2049	rBV	104241	100412	1.95%	0.184%
74	14.162	2050	2053	2058	rVV2	97760	151645	2.95%	0.278%
75	14.262	2067	2070	2074	rBV	223696	219443	4.27%	0.403%
76	14.362	2083	2087	2094	rVB3	281492	325477	6.33%	0.597%
77	14.421	2094	2097	2102	rBV3	343169	402883	7.84%	0.739%
78	14.462	2102	2104	2106	rBV2	119090	96389	1.88%	0.177%
79	14.709	2143	2146	2149	rVB3	90416	95645	1.86%	0.175%
80	15.292	2241	2245	2253	rVB	615326	745761	14.51%	1.368%
81	15.774	2324	2327	2336	rVB3	74141	136528	2.66%	0.250%
82	17.639	2641	2644	2654	rVB5	89289	191297	3.72%	0.351%
83	17.850	2673	2680	2689	rVB5	190658	552930	10.76%	1.014%
84	18.009	2701	2707	2717	rVB3	155230	399566	7.77%	0.733%
85	18.921	2854	2862	2870	rBV3	127756	355624	6.92%	0.652%

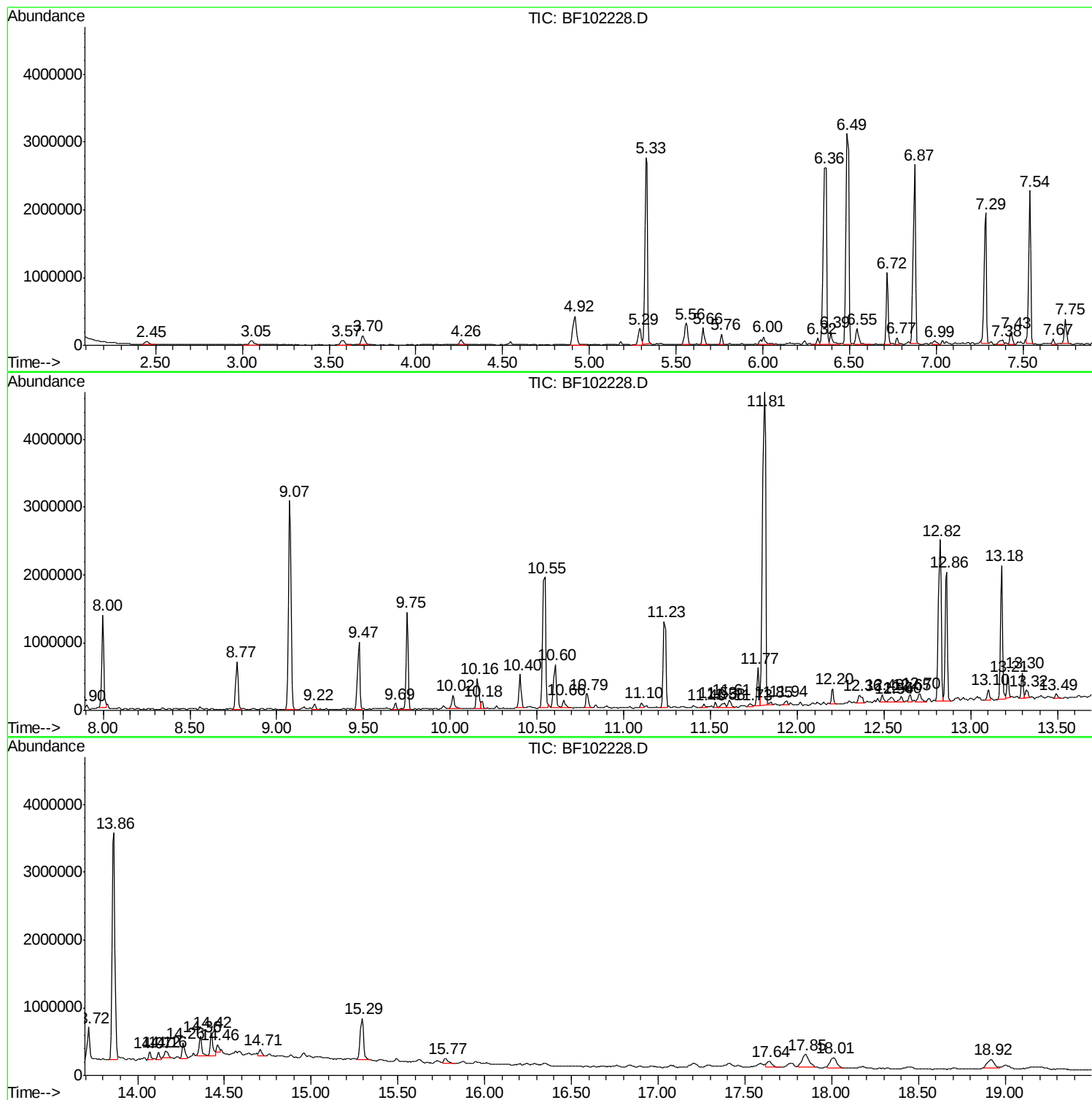
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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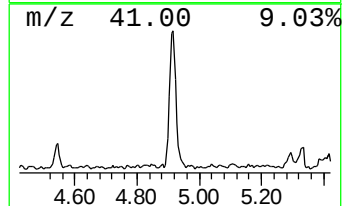
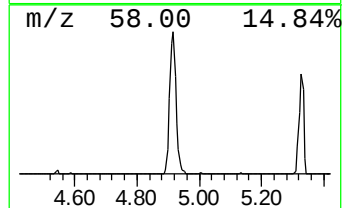
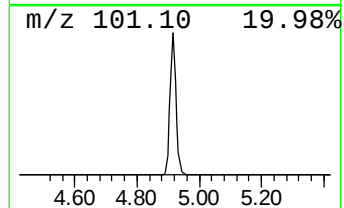
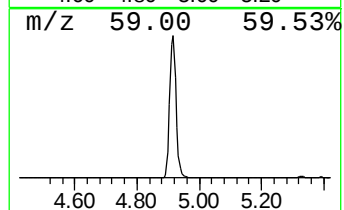
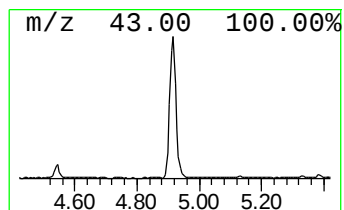
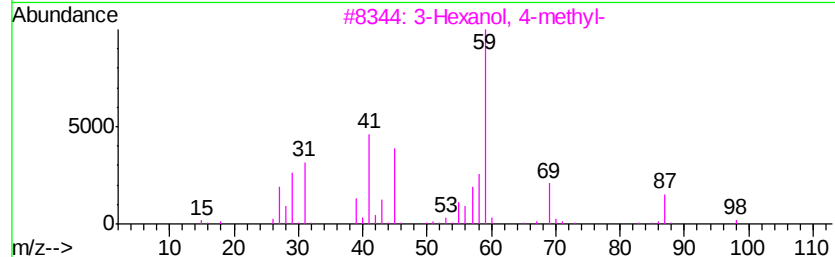
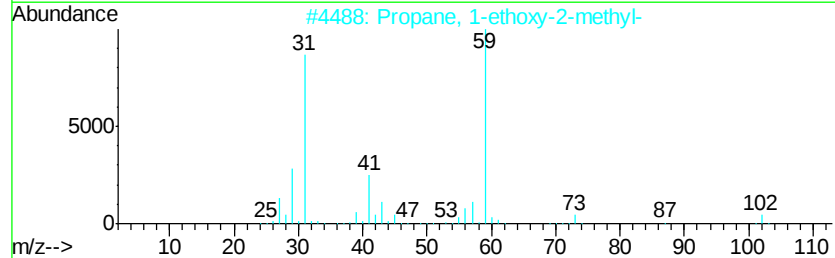
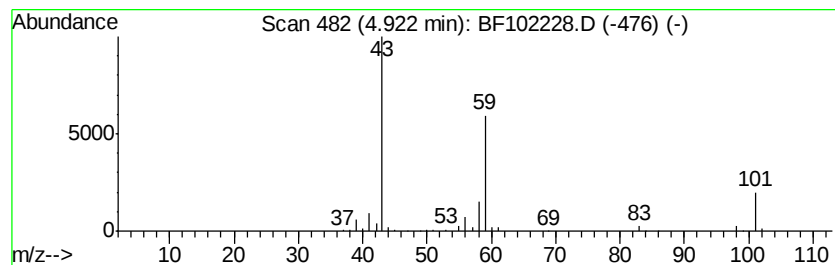
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	13.58 ng	589021	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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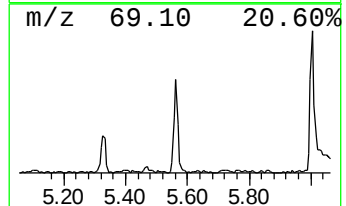
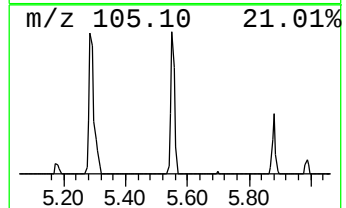
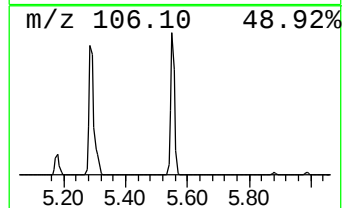
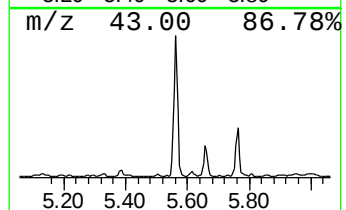
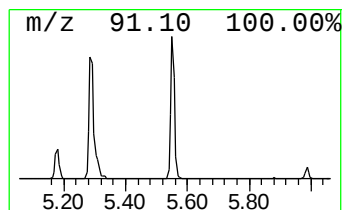
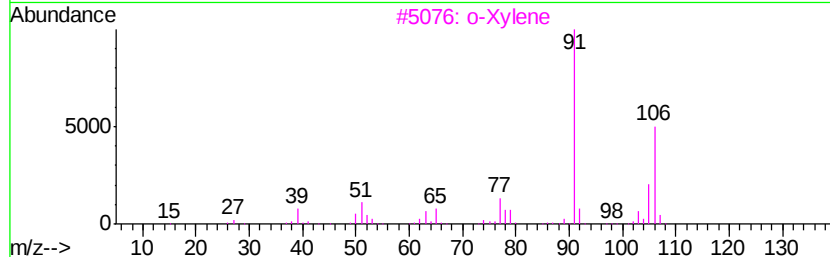
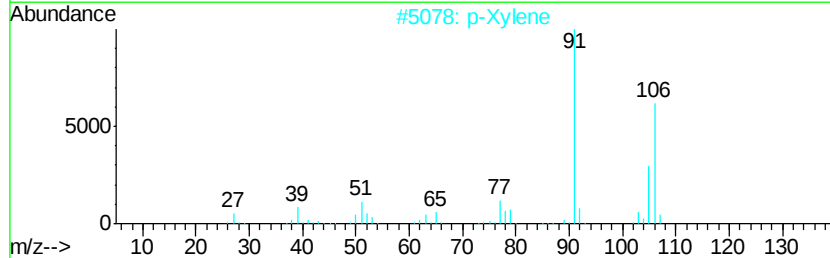
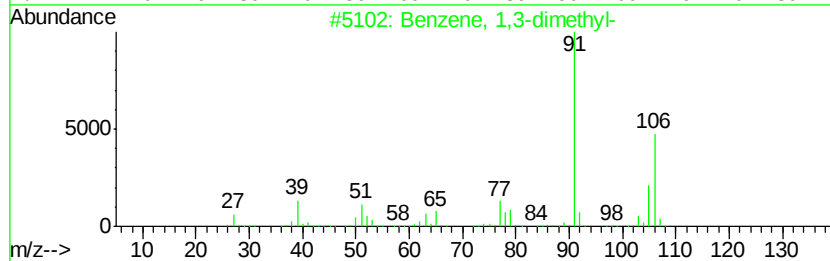
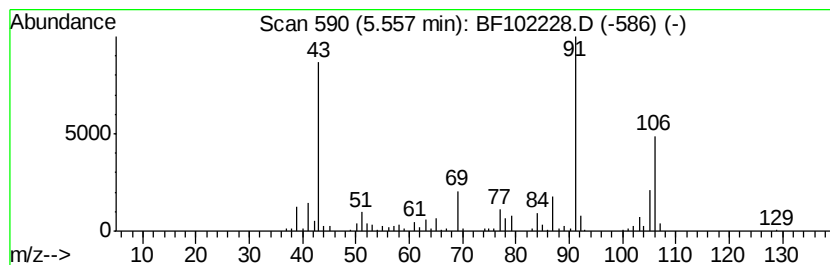
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.56	9.44 ng	409428	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3-dimethyl-	106	C8H10	000108-38-3	95
2		p-Xylene	106	C8H10	000106-42-3	95
3		o-Xylene	106	C8H10	000095-47-6	94
4		1,3-Cyclopentadiene, 5-(1-methyl...	106	C8H10	002175-91-9	74
5		Ethylbenzene	106	C8H10	000100-41-4	62



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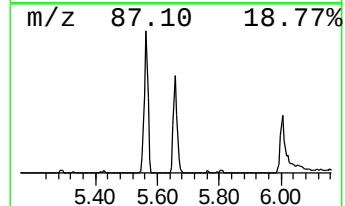
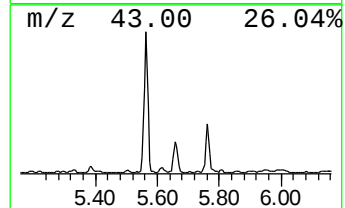
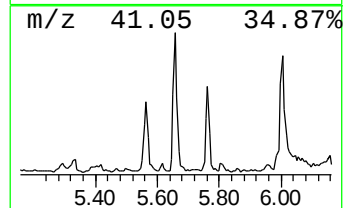
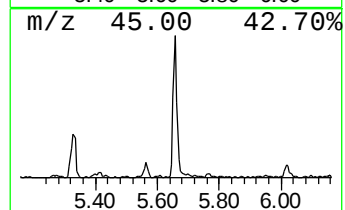
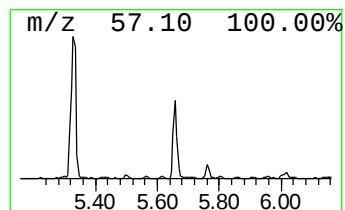
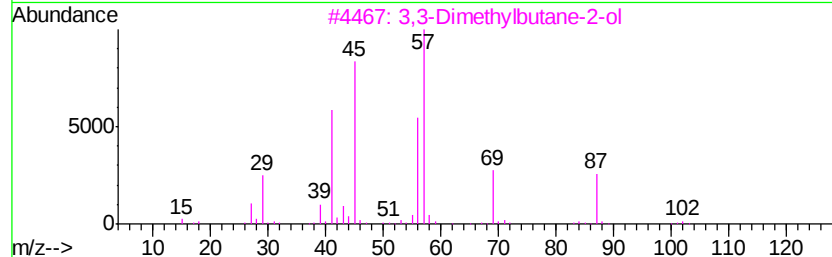
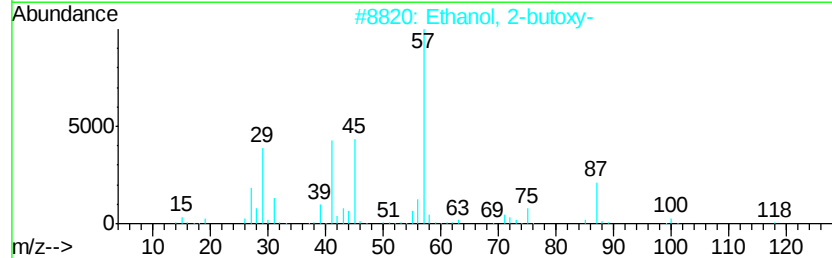
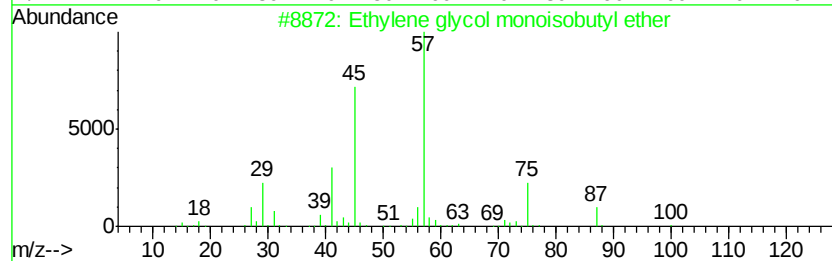
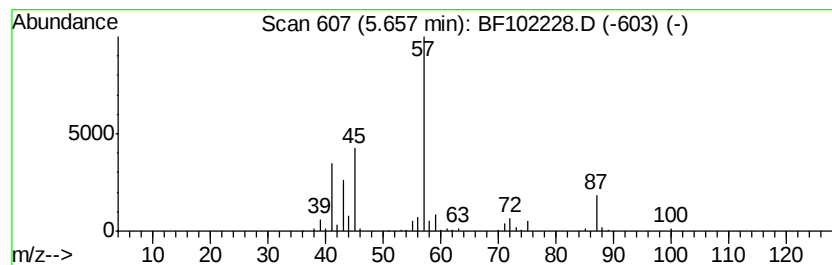
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethylene glycol monoisobuty... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.66	4.94 ng	214120	1,4-Dichlorobenzene-d4	6.72

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
2		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	50
3		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	33
4		Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	27
5		Propanoic acid, 2-hydroxyethyl e...	118	C5H10O3	024567-27-9	12



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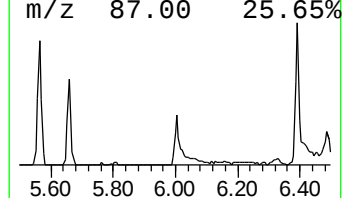
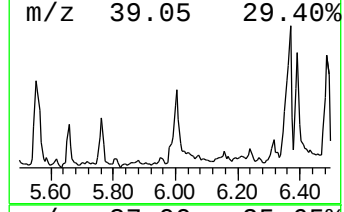
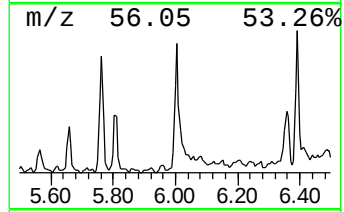
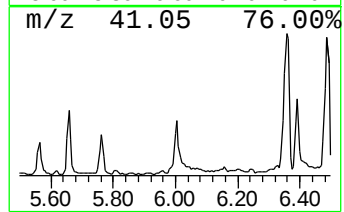
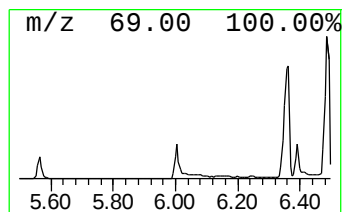
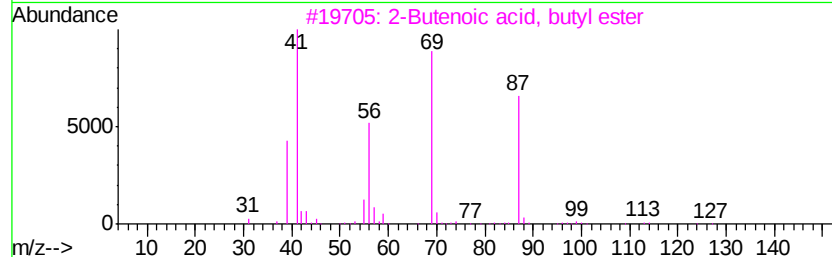
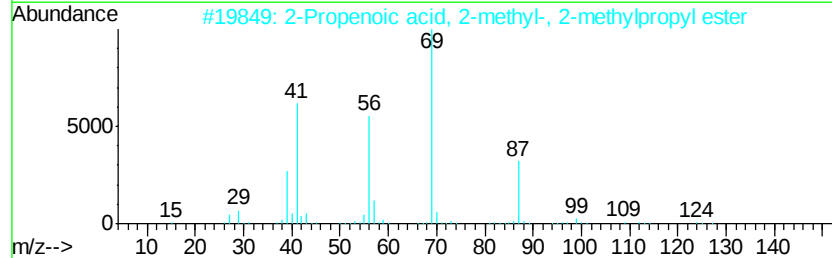
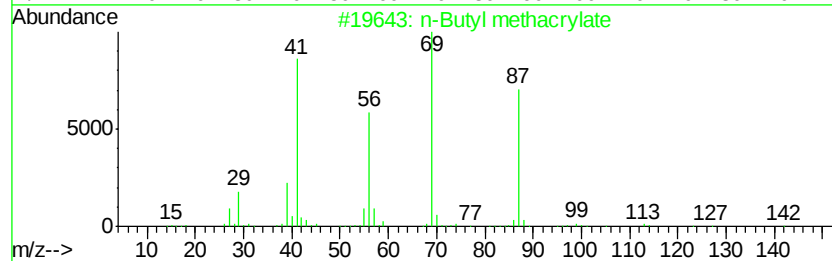
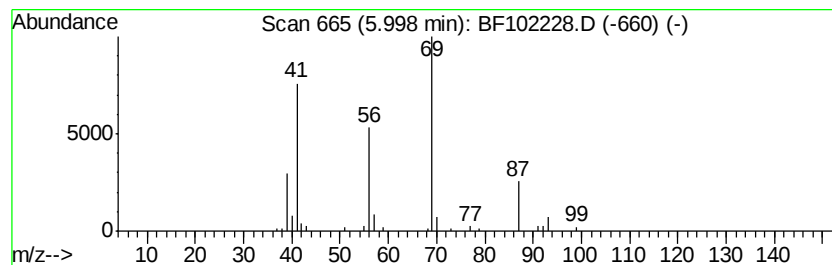
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Butyl methacrylate Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.00	4.31 ng	187143	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Butyl methacrylate	142	C8H14O2	000097-88-1	83
2		2-Propenoic acid, 2-methyl-, 2-m...	142	C8H14O2	000097-86-9	83
3		2-Butenoic acid, butyl ester	142	C8H14O2	007299-91-4	74
4		4-Hexen-3-one	98	C6H10O	002497-21-4	37
5		Vinyl crotonate	112	C6H8O2	014861-06-4	32



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102228.D
Acq On : 19 Jan 2018 20:37
Operator : SJ/JU
Sample : J1189-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

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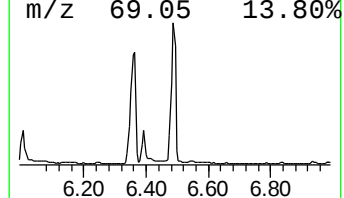
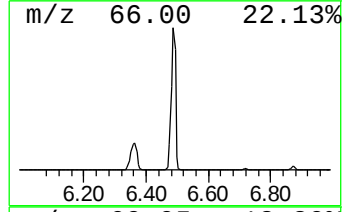
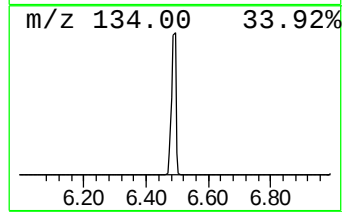
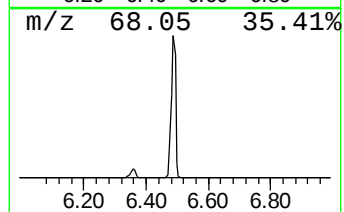
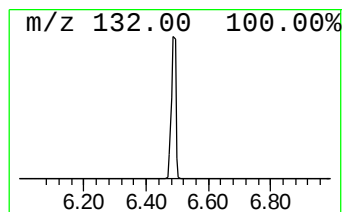
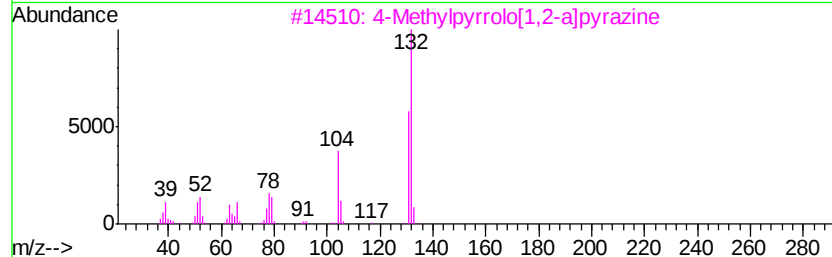
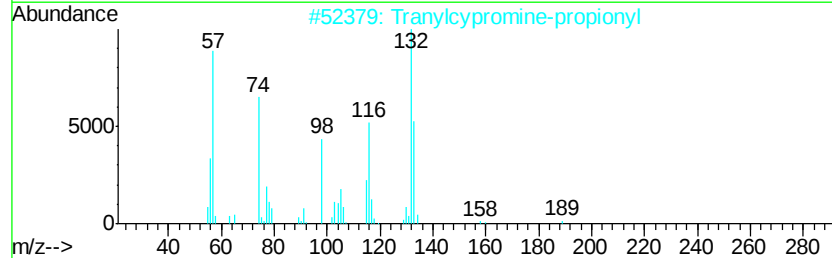
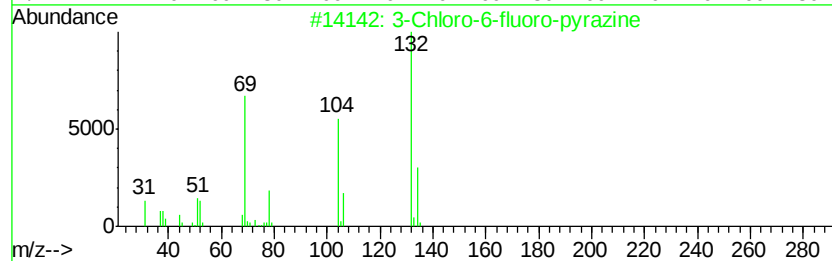
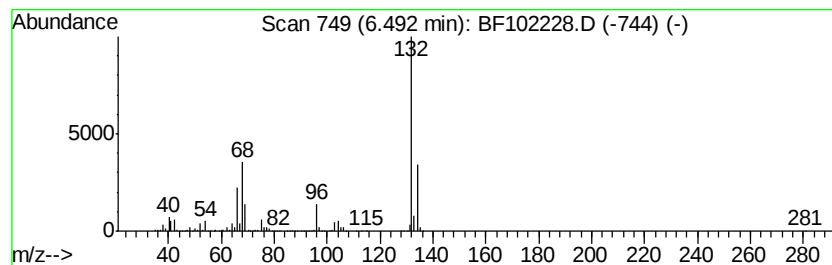
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	71.70 ng	3110420	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
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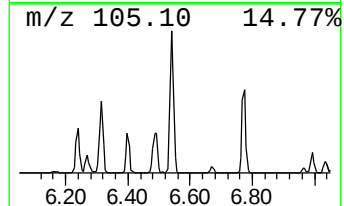
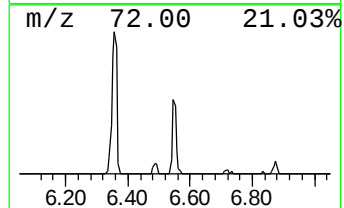
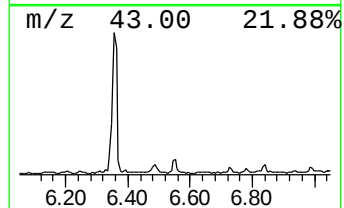
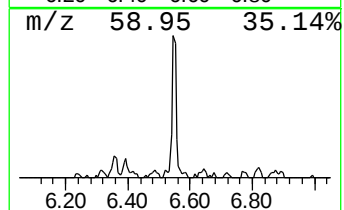
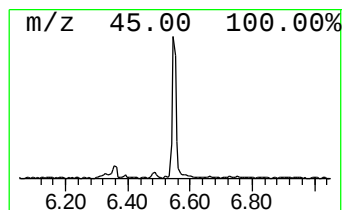
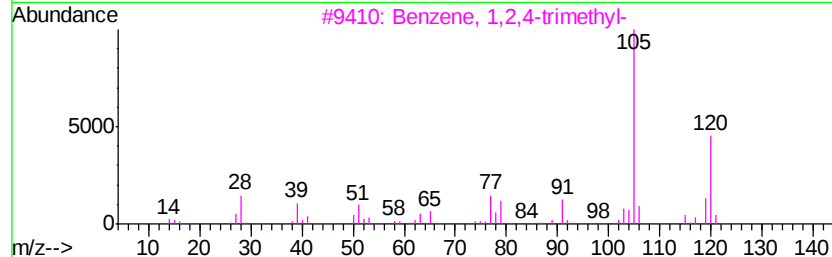
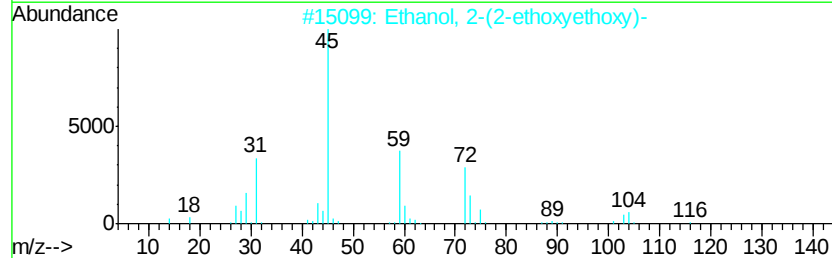
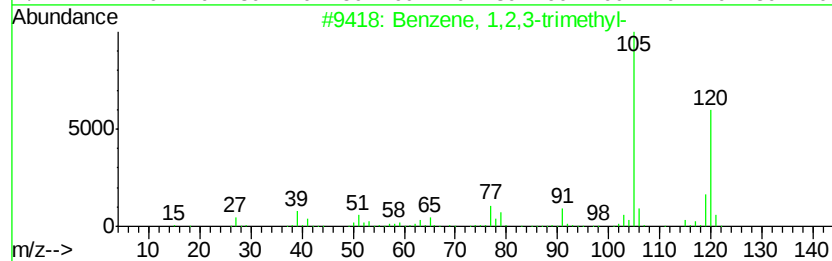
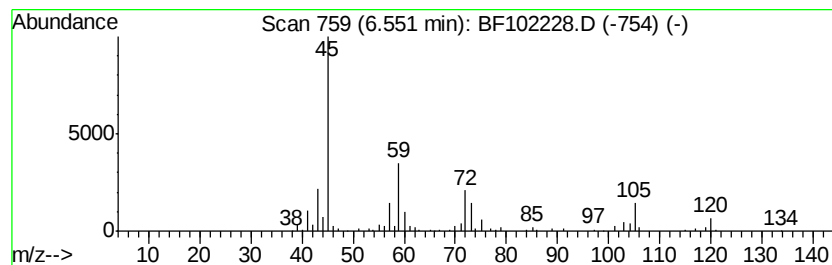
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	5.96 ng	258776	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	64
2		Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	58
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	43
4		Methoxyacetic acid, 2-methylprop...	146	C7H14O3	1000282-40-9	35
5		Mesitylene	120	C9H12	000108-67-8	35



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Misc :
ALS Vial : 4 Sample Multiplier: 1

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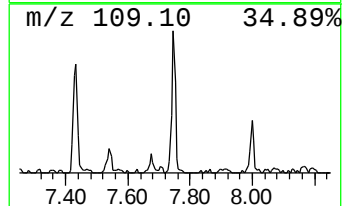
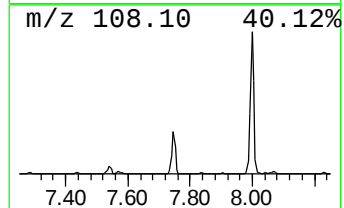
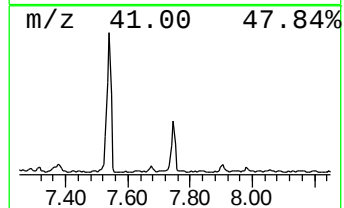
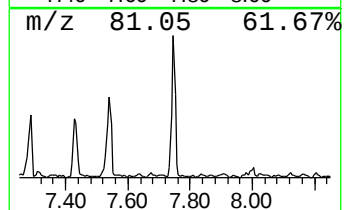
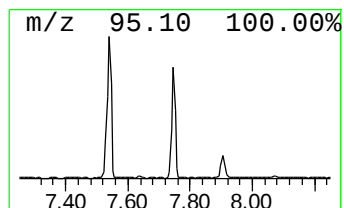
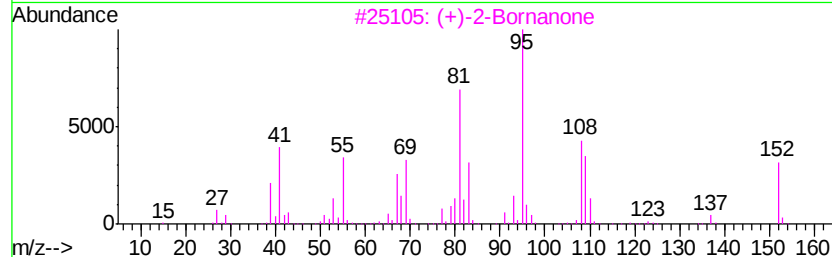
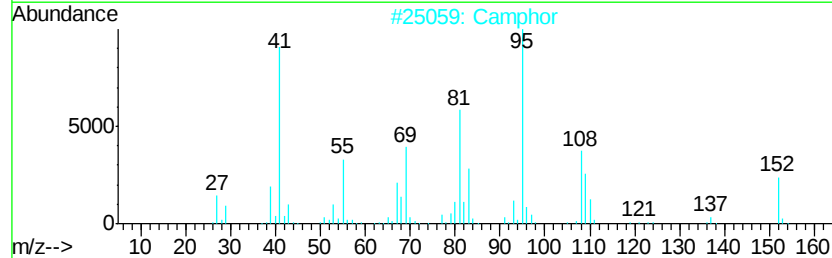
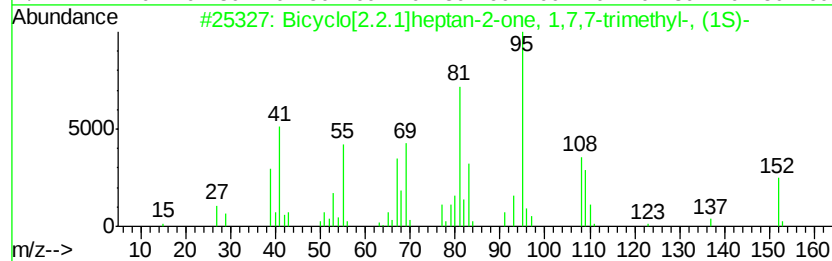
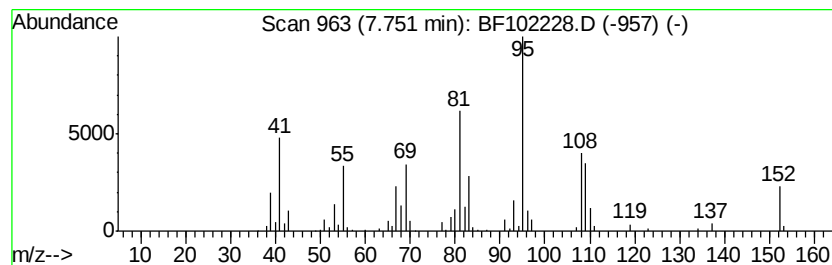
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	5.34 ng	315080	Naphthalene-d8	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	97
2		Camphor	152	C10H16O	000076-22-2	97
3		(+)-2-Bornanone	152	C10H16O	000464-49-3	97
4		1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	46
5		5-Hepten-2-ol, 6-methyl-	128	C8H16O	001569-60-4	43



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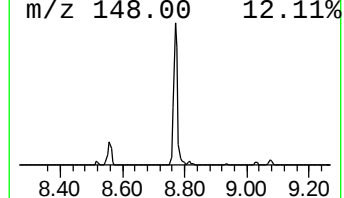
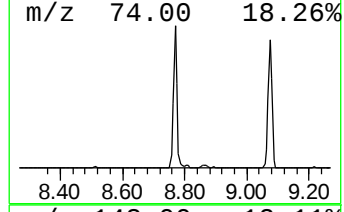
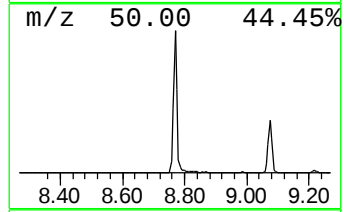
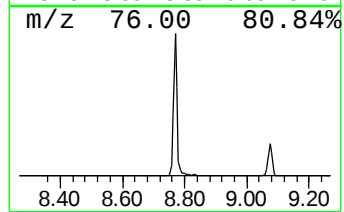
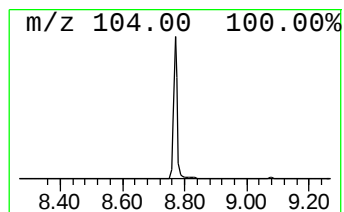
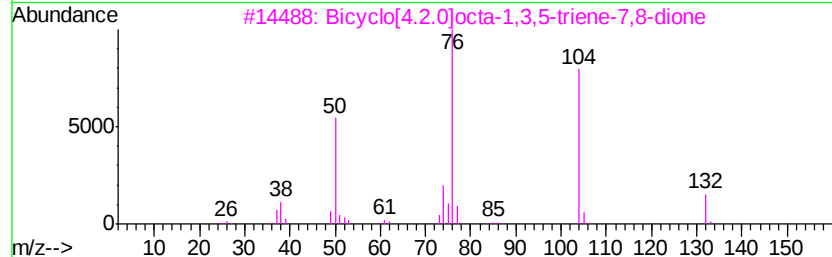
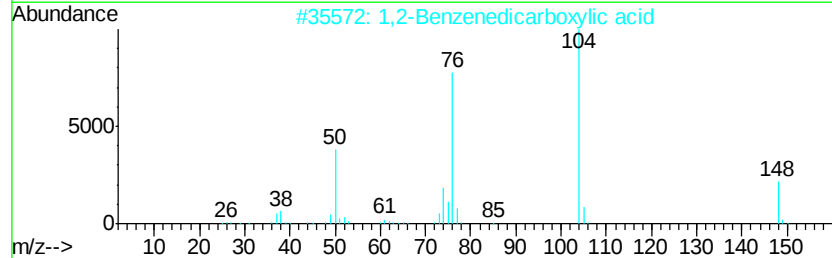
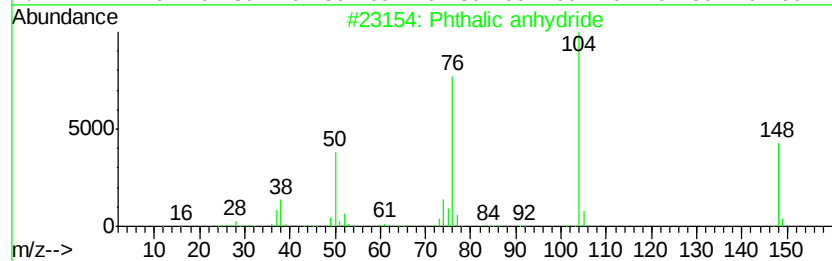
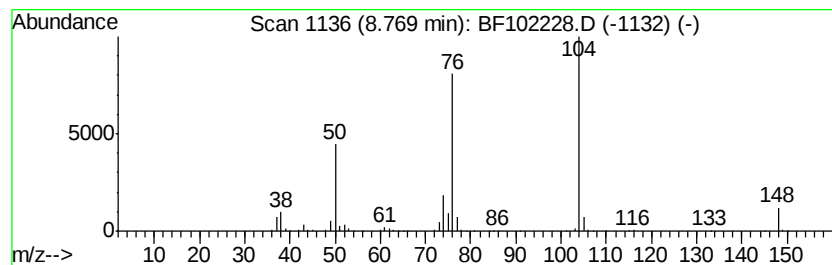
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Phthalic anhydride Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.77	9.86 ng	581832	Naphthalene-d8	8.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic anhydride	148	C8H4O3	000085-44-9	94
2			1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	90
3			Bicyclo[4.2.0]octa-1,3,5-triene-...	132	C8H4O2	006383-11-5	86
4			Phthalamic acid	165	C8H7NO3	000088-97-1	83
5			Methyl hydrogen phthalate	180	C9H8O4	004376-18-5	72



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
 Data File : BF102228.D
 Acq On : 19 Jan 2018 20:37
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 Misc :
 ALS Vial : 4 Sample Multiplier: 1

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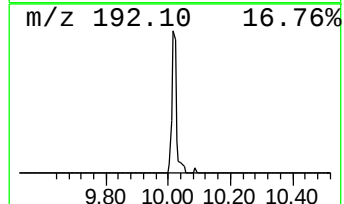
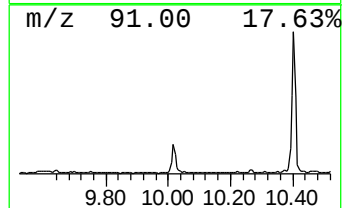
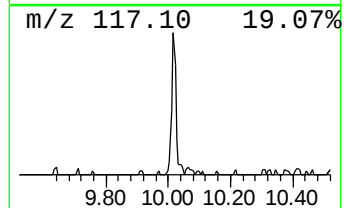
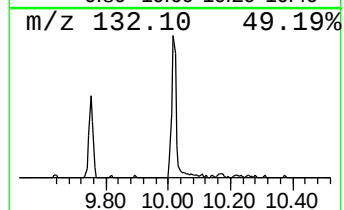
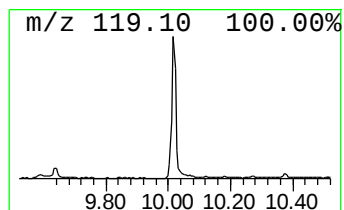
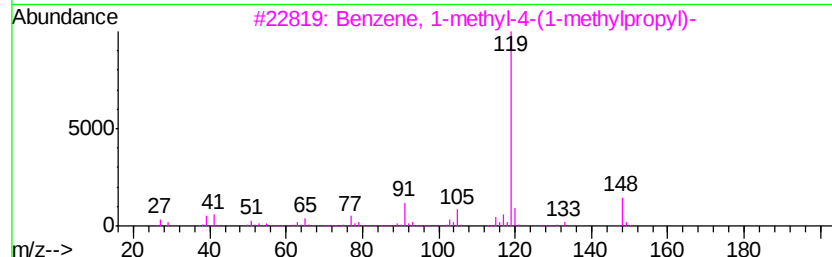
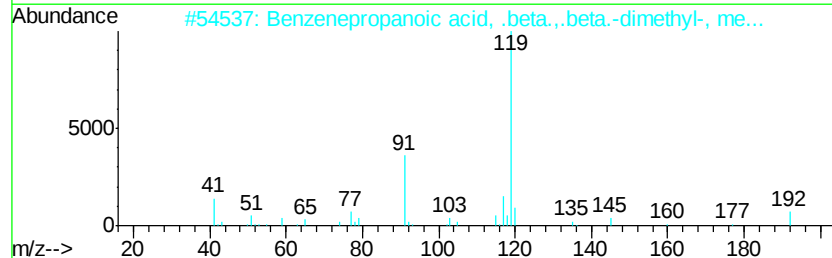
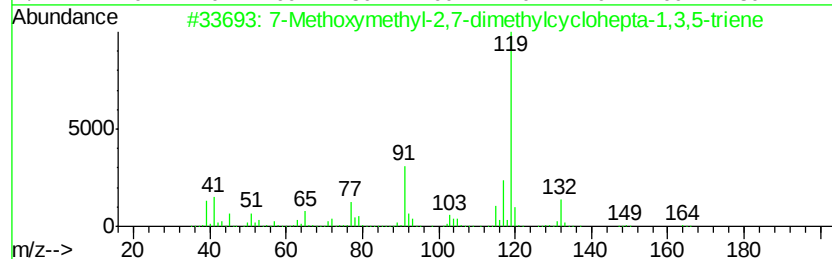
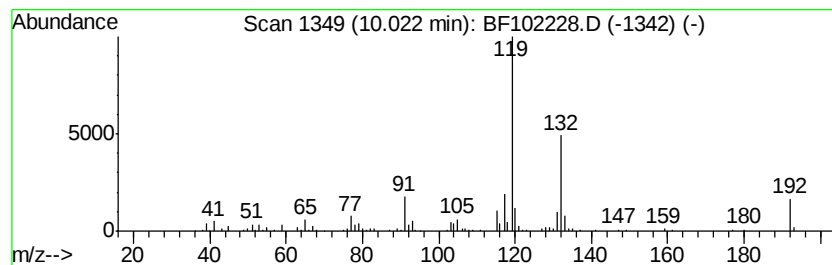
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 12 7-Methoxymethyl-2,7-dimethy... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.02	3.75 ng	234972	Acenaphthene-d10	9.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Methoxymethyl-2,7-dimethylcyclo...	164	C11H16O	073992-48-0	59
2		Benzenepropanoic acid, .beta.,.b...	192	C12H16O2	025080-84-6	47
3		Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	47
4		Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	43
5		o-Cymene	134	C10H14	000527-84-4	43



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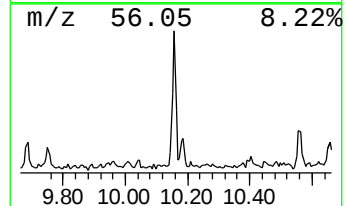
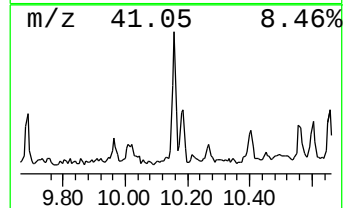
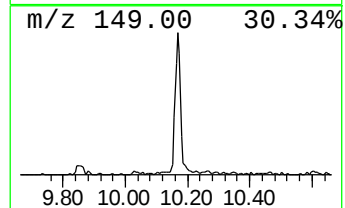
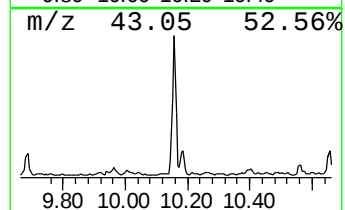
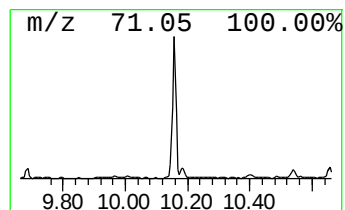
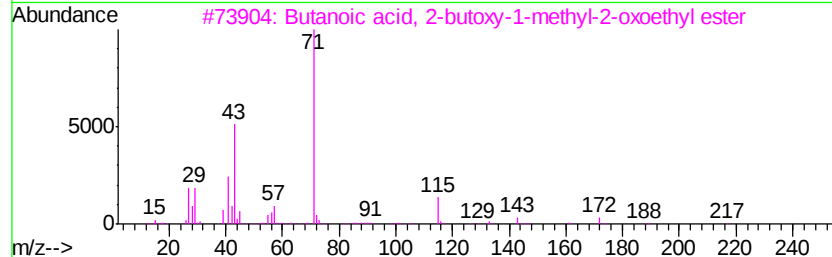
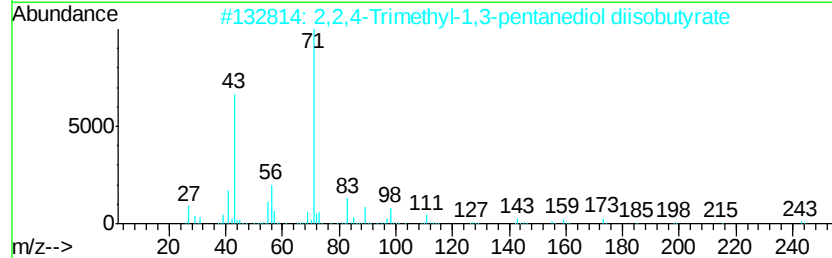
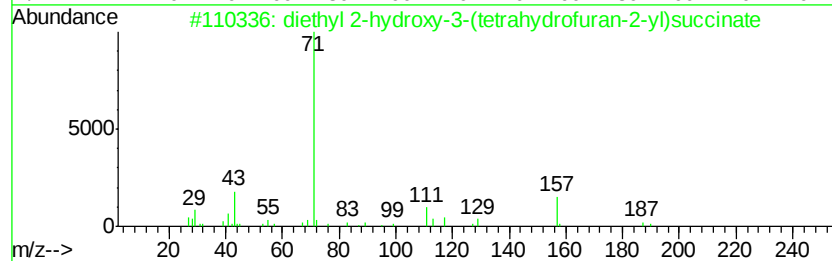
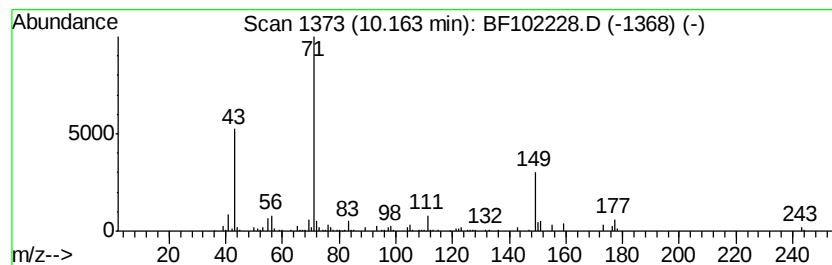
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 diethyl 2-hydroxy-3-(tetrahydrofuran-2-yl)succinate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.16	6.59 ng	412776	Acenaphthene-d10	9.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			diethyl 2-hydroxy-3-(tetrahydrofuran-2-yl)succinate	260	C12H20O6	1000365-67-1	59
2			2,2,4-Trimethyl-1,3-pentanediol	286	C16H30O4	006846-50-0	50
3			Butanoic acid, 2-butoxy-1-methyl-	216	C11H20O4	007492-70-8	50
4			Pentanoic acid, 2,2,4-trimethyl-	286	C16H30O4	1000140-77-5	43
5			4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	42



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Misc :
ALS Vial : 4 Sample Multiplier: 1

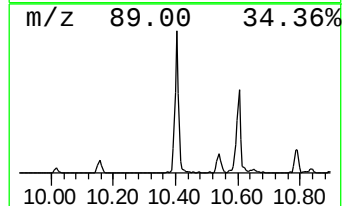
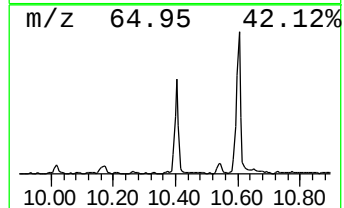
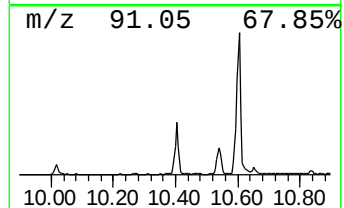
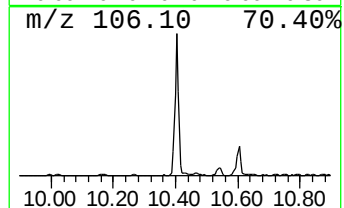
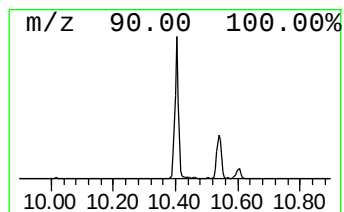
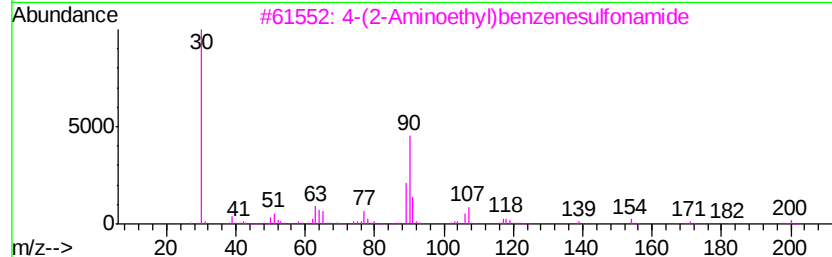
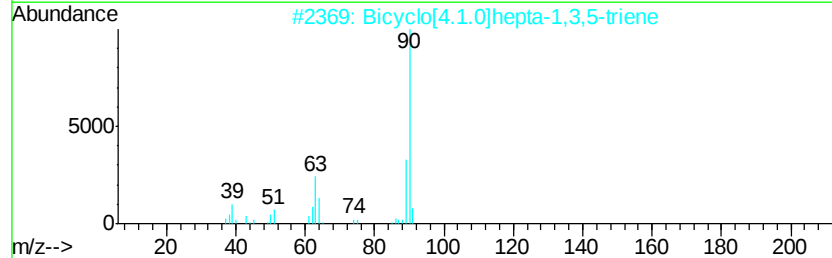
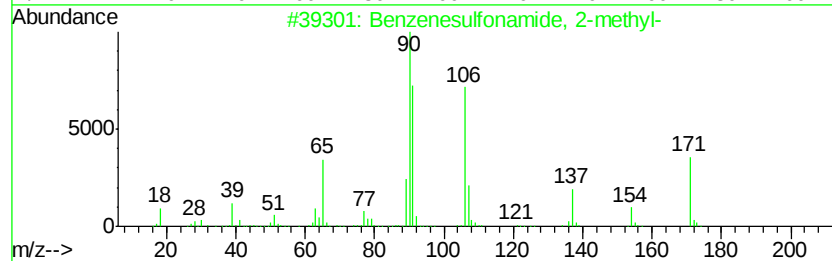
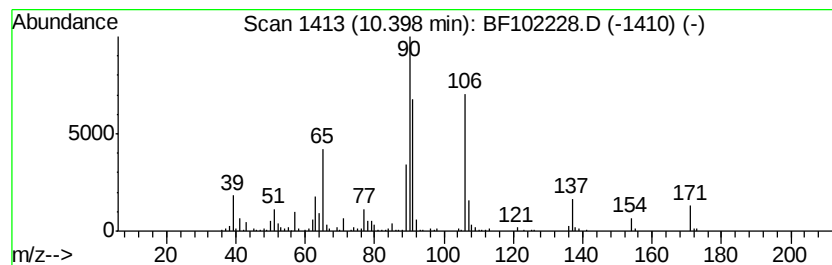
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzenesulfonamide, 2-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.40	6.50 ng	407278	Acenaphthene-d10	9.75	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	95
2	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	43
3	4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	38
4	Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	35
5	Benzene, 1-methyl-3-nitro-	137	C7H7NO2	000099-08-1	22



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102228.D
Acq On : 19 Jan 2018 20:37
Operator : SJ/JU
Sample : J1189-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
4-2

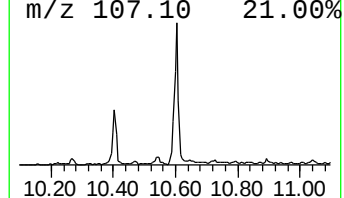
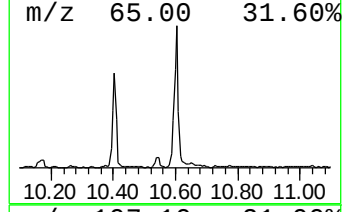
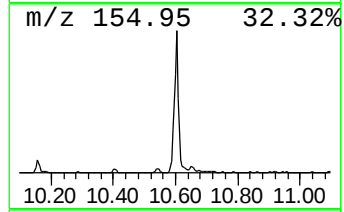
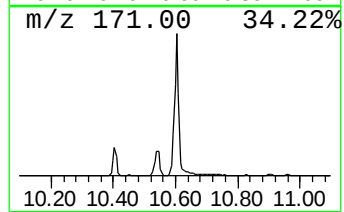
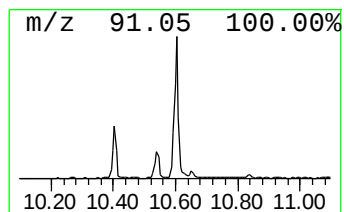
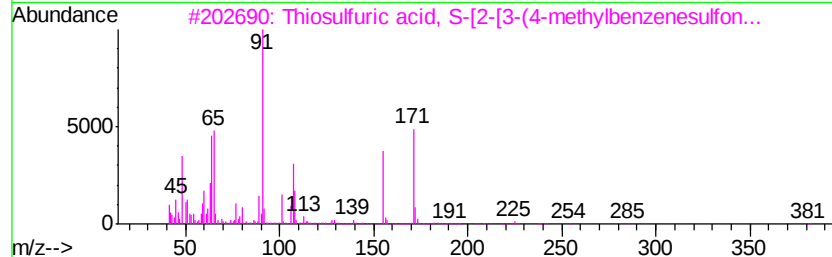
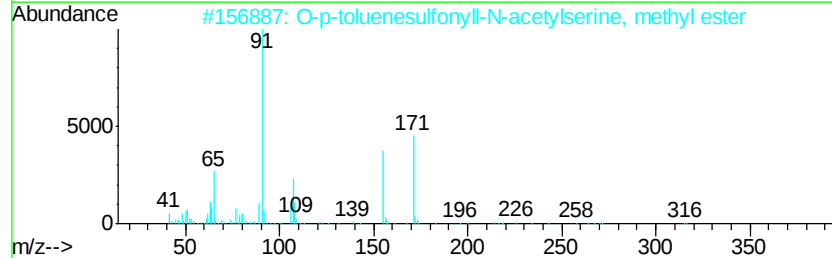
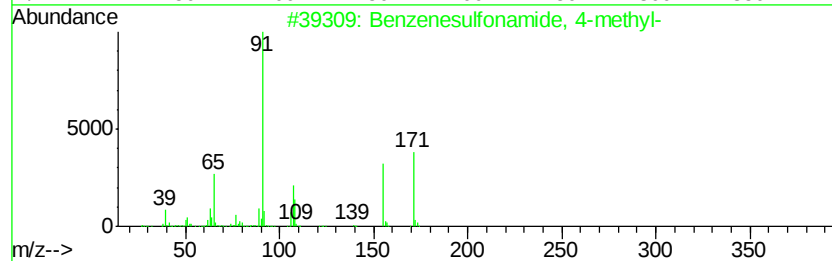
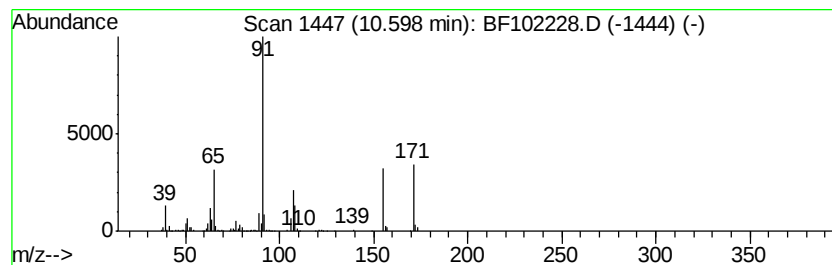
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzenesulfonamide, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	10.13 ng	599898	Phenanthrene-d10	11.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	98
2		O-p-toluenesulfonyl-N-acetylser...	315	C13H17NO6S	1000126-44-8	72
3		Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	64
4		Tolbutamide	270	C12H18N2O3S	000064-77-7	50
5		N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	47



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102228.D
Acq On : 19 Jan 2018 20:37
Operator : SJ/JU
Sample : J1189-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

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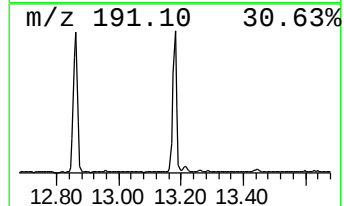
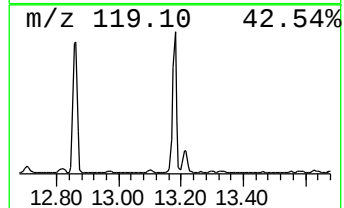
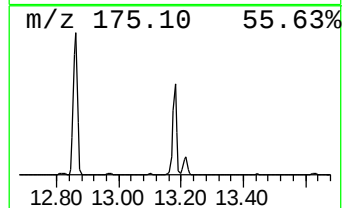
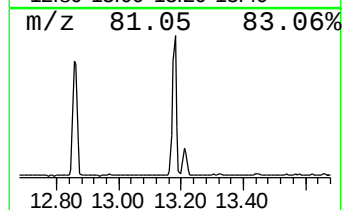
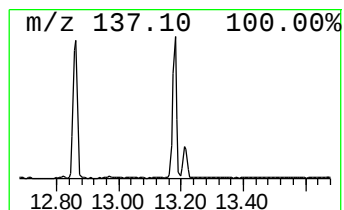
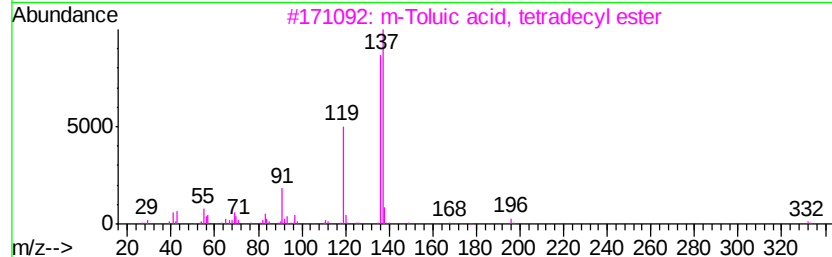
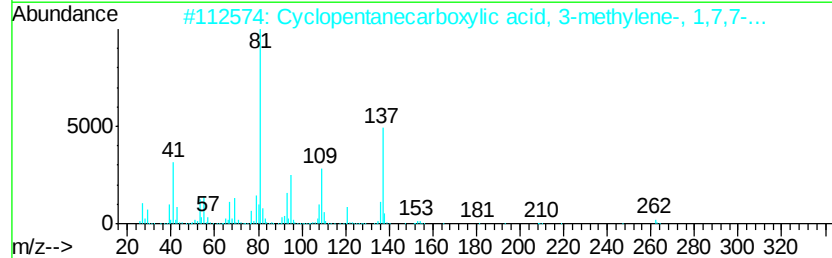
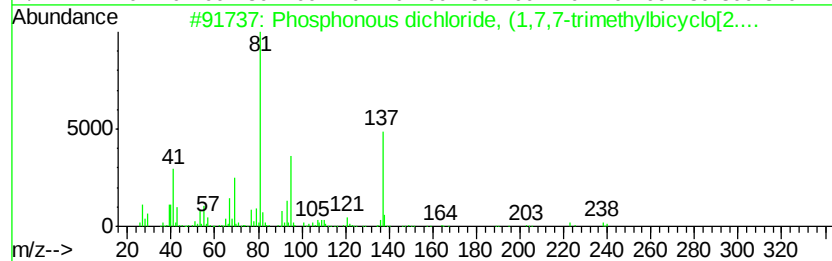
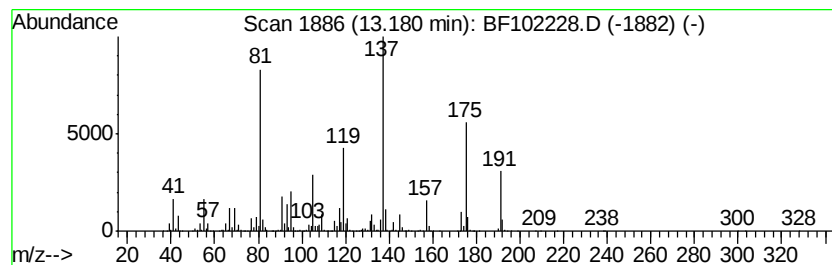
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown13.18 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.18	8.84 ng	1758650	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosphonous dichloride, (1,7,7-t...	238	C10H17Cl2P	074630-16-3	32
2			Cyclopentanecarboxylic acid, 3-m...	262	C17H26O2	074793-59-2	17
3			m-Toluic acid, tetradecyl ester	332	C22H36O2	1000292-36-0	16
4			m-Toluic acid, hexadecyl ester	360	C24H40O2	1000292-36-2	12
5			Cyclopentanecarboxylic acid, 3-i...	290	C19H30O2	1000151-83-4	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102228.D
Acq On : 19 Jan 2018 20:37
Operator : SJ/JU
Sample : J1189-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

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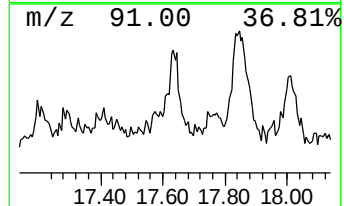
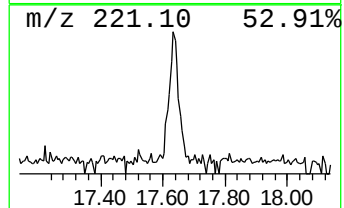
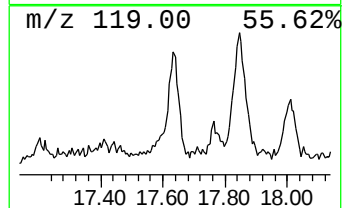
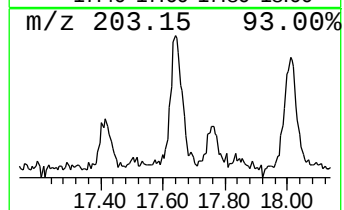
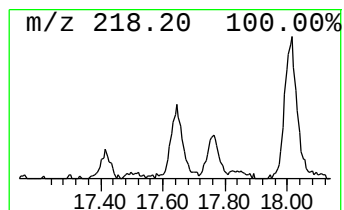
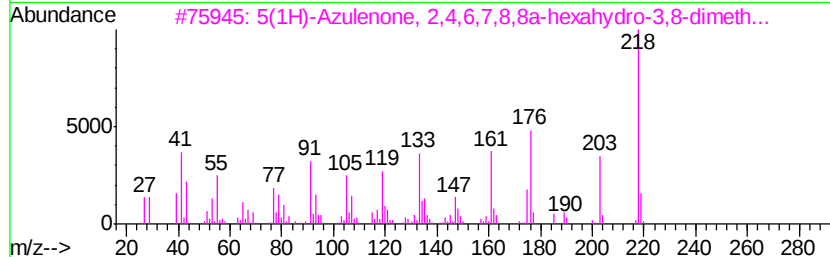
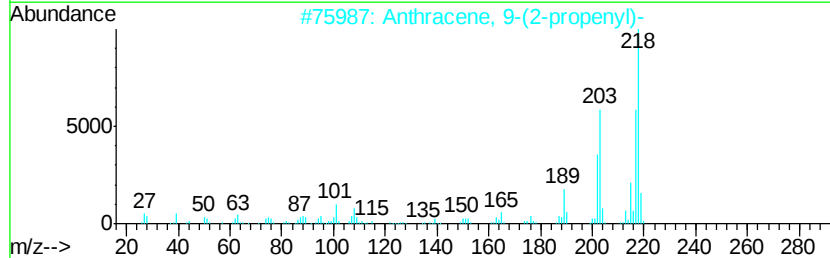
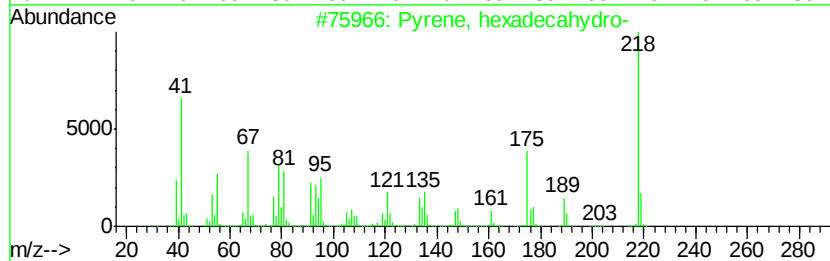
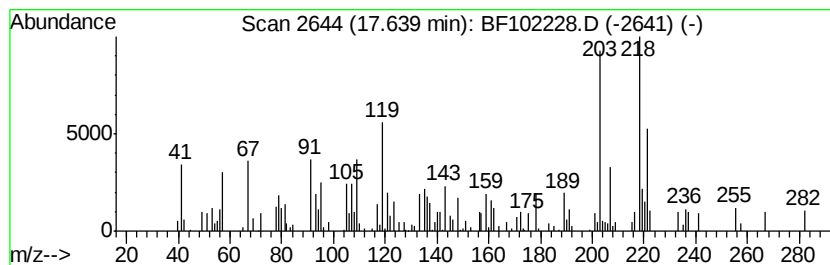
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Pyrene, hexadecahydro- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.64	5.13 ng	191297	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	53
2		Anthracene, 9-(2-propenyl)-	218	C17H14	023707-65-5	27
3		5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	27
4		Tetrachloro-o-benzoquinone	244	C6Cl4O2	002435-53-2	18
5		4-(p-N,N-dimethylaminophenylimin...	218	C13H18N2O	1000100-07-8	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102228.D
Acq On : 19 Jan 2018 20:37
Operator : SJ/JU
Sample : J1189-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

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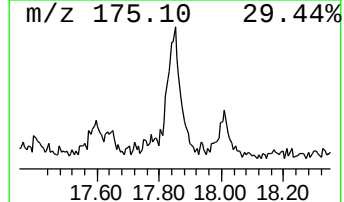
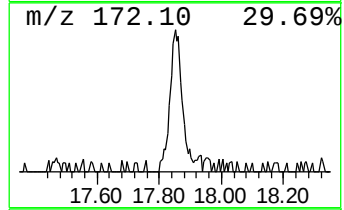
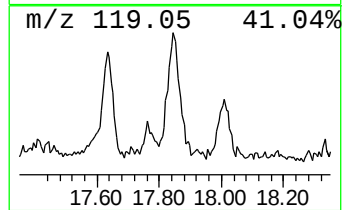
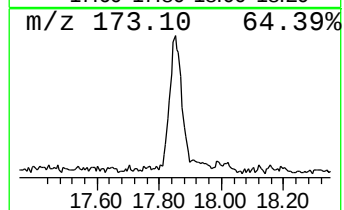
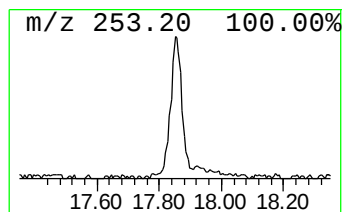
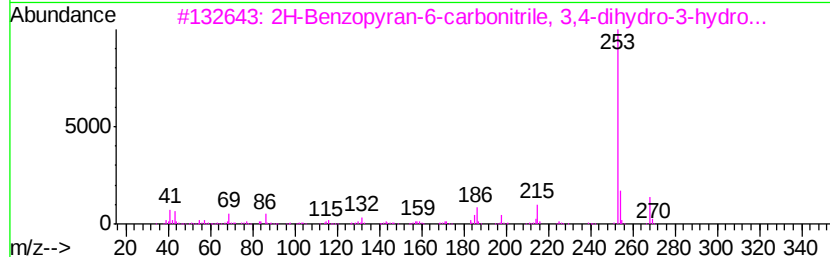
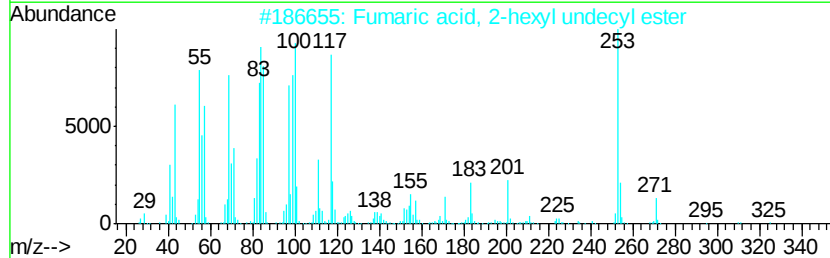
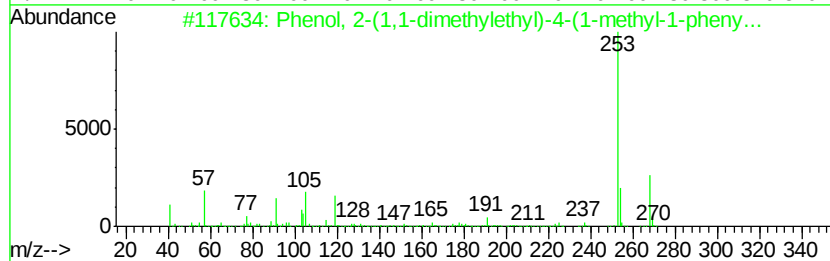
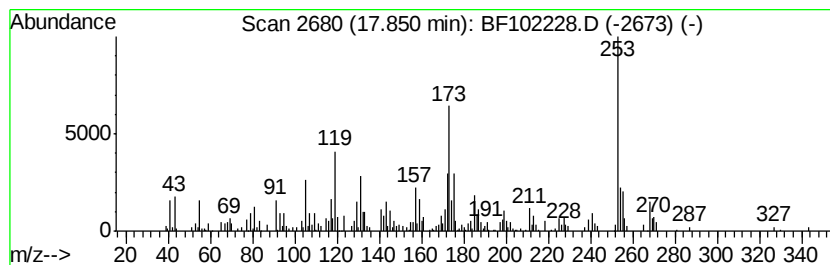
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown17.85 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	14.83 ng	552930	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2-(1,1-dimethylethyl)-4-...	268	C19H24O	056187-92-9	35
2		Fumaric acid, 2-hexyl undecyl ester	354	C21H38O4	1000348-74-9	30
3		2H-Benzopyran-6-carbonitrile, 3,...	286	C16H18N2O3	150871-62-8	27
4		Phthalic acid, di(3,4-dimethylph...	374	C24H22O4	1000309-82-6	22
5		Musk ambrette (artificial)	268	C12H16N2O5	000083-66-9	22



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
Data File : BF102228.D
Acq On : 19 Jan 2018 20:37
Operator : SJ/JU
Sample : J1189-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
4-2

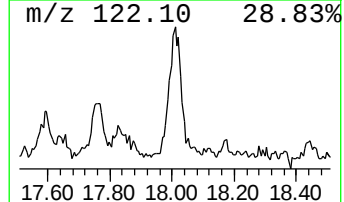
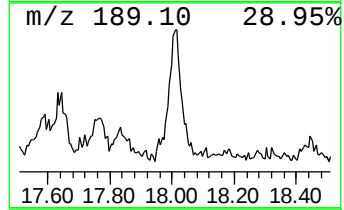
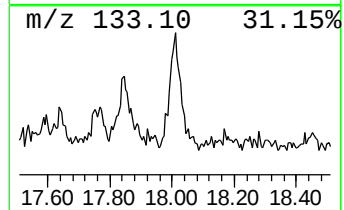
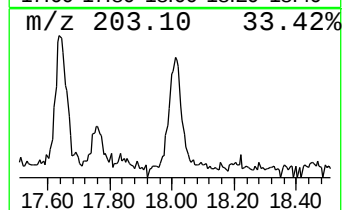
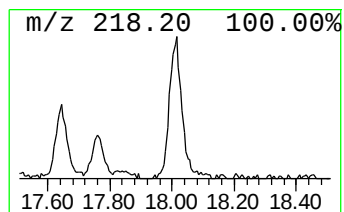
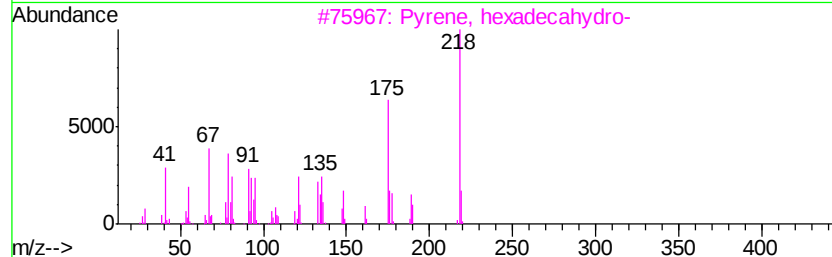
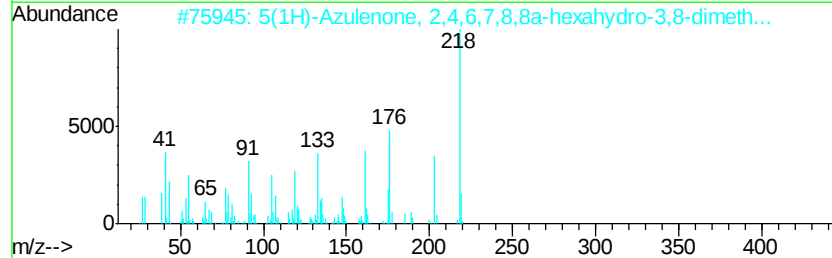
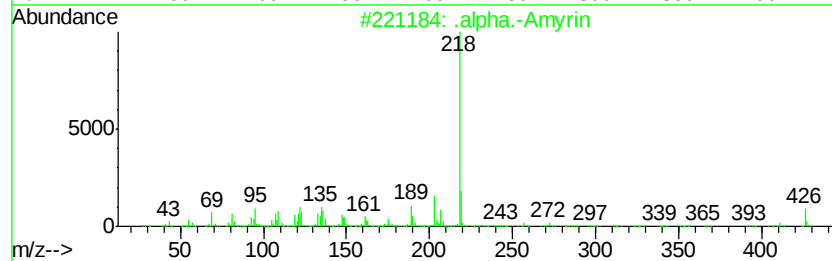
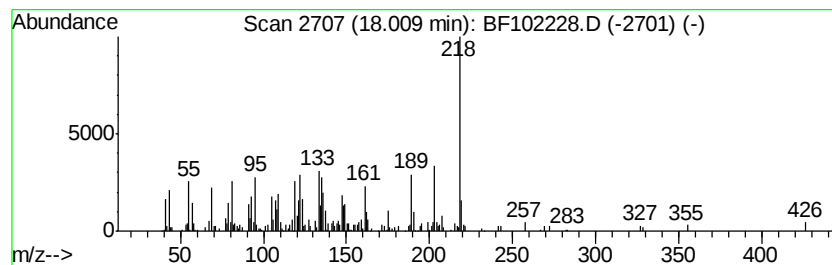
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 .alpha.-Amyrin Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.01	10.72 ng	399566	Perylene-d12	15.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.alpha.-Amyrin	426	C30H50O	000638-95-9	95
2		5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	64
3		Pvrene, hexadecahydro-	218	C16H26	002435-85-0	46
4		2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	43
5		9-Oxabicyclo[4.3.0]non-6-en-8-on...	218	C13H14O3	1000160-28-8	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011918\
Data File : BF102228.D
Acq On : 19 Jan 2018 20:37
Operator : SJ/JU
Sample : J1189-06
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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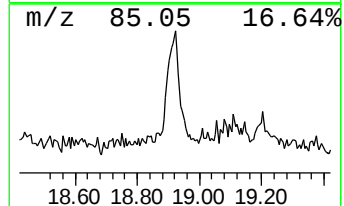
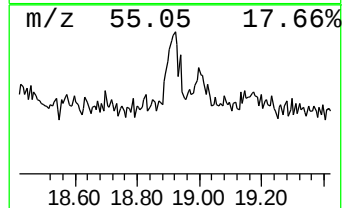
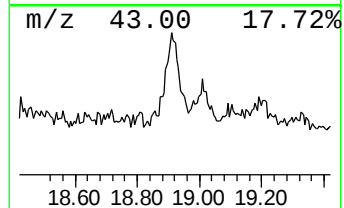
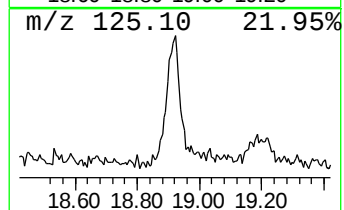
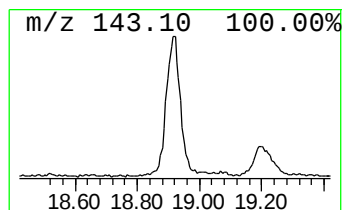
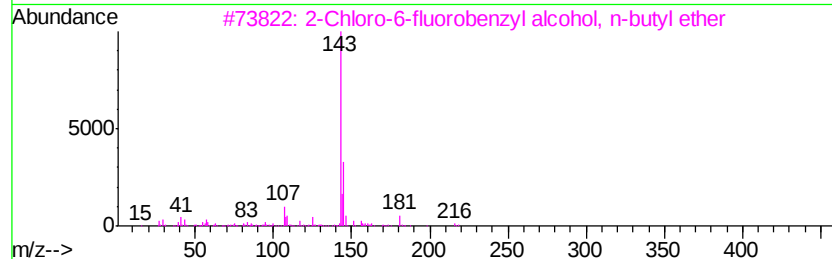
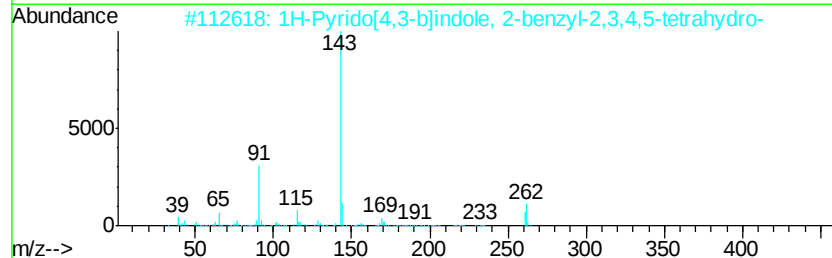
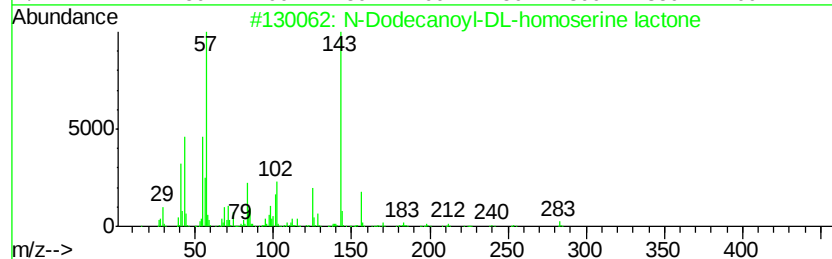
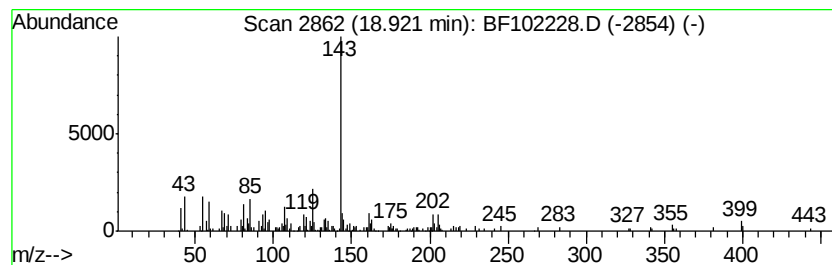
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown18.32 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.92	9.54 ng	355624	Perylene-d12	15.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Dodecanoyl-DL-homoserine lactone	283	C16H29NO3	018627-38-8	40
2			1H-Pyrido[4,3-b]indole, 2-benzyl...	262	C18H18N2	1000303-43-2	38
3			2-Chloro-6-fluorobenzyl alcohol,...	216	C11H14ClFO	1000378-14-6	38
4			6-Aza-2-thiothymine	143	C4H5N3OS	000615-76-9	38
5			2,3-Dimethyl-5-methylamino-1,3,4...	143	C5H9N3S	1000288-97-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011918\
 Data File : BF102228.D
 Acq On : 19 Jan 2018 20:37
 Operator : SJ/JU
 Sample : J1189-06
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 4-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF010918.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...	4.92	13.6	ng	589021	1	6.72	867661	20.0
Benzene, 1,3-dime...	5.56	9.4	ng	409428	1	6.72	867661	20.0
Ethylene glycol m...	5.66	4.9	ng	214120	1	6.72	867661	20.0
n-Butyl methacrylate	6.00	4.3	ng	187143	1	6.72	867661	20.0
unknown6.49	6.49	71.7	ng	3110420	1	6.72	867661	20.0
Benzene, 1,2,3-tr...	6.55	6.0	ng	258776	1	6.72	867661	20.0
Bicyclo[2.2.1]hep...	7.75	5.3	ng	315080	2	8.00	1179600	20.0
Phthalic anhydride	8.77	9.9	ng	581832	2	8.00	1179600	20.0
7-Methoxymethyl-2...	10.02	3.8	ng	234972	3	9.75	1253370	20.0
diethyl 2-hydroxy...	10.16	6.6	ng	412776	3	9.75	1253370	20.0
Benzenesulfonamid...	10.40	6.5	ng	407278	3	9.75	1253370	20.0
Benzenesulfonamid...	10.60	10.1	ng	599898	4	11.23	1184050	20.0
unknown13.18	13.18	8.8	ng	1758650	5	13.87	3976760	20.0
Pyrene, hexadecah...	17.64	5.1	ng	191297	6	15.29	745761	20.0
unknown17.85	17.85	14.8	ng	552930	6	15.29	745761	20.0
.alpha.-Amyrin	18.01	10.7	ng	399566	6	15.29	745761	20.0
unknown18.32	18.92	9.5	ng	355624	6	15.29	745761	20.0