

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
 Data File : BM016279.D
 Acq On : 09 Aug 2018 13:37
 Operator : SJ/JU
 Sample : J4356-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-12

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_M\METHODS\8270-BM072318.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	3.452	24	28	33	rBV2	45241	61348	1.73%	0.196%
2	4.040	124	128	141	rVB3	27605	47931	1.35%	0.153%
3	4.657	227	233	244	rVB	443145	608598	17.16%	1.946%
4	5.051	294	300	310	rVB	74362	112231	3.16%	0.359%
5	5.187	318	323	331	rVB	53840	81584	2.30%	0.261%
6	5.663	395	404	421	rBV	513039	819279	23.10%	2.619%
7	6.334	512	518	523	rBV	46037	70427	1.99%	0.225%
8	7.145	647	656	660	rBV2	22193	39017	1.10%	0.125%
9	7.304	677	683	702	rVB	286170	547234	15.43%	1.750%
10	7.610	728	735	738	rBV2	25927	44521	1.26%	0.142%
11	7.663	738	744	754	rVB	1140458	1789390	50.45%	5.721%
12	8.134	818	824	840	rBV	231004	421992	11.90%	1.349%
13	8.451	870	878	889	rVB	1113242	1855743	52.32%	5.933%
14	8.945	955	962	968	rBV4	84460	160906	4.54%	0.514%
15	9.204	997	1006	1010	rBV6	23897	66870	1.89%	0.214%
16	9.263	1011	1016	1020	rVB	64419	89986	2.54%	0.288%
17	9.322	1020	1026	1032	rBV	771683	1286363	36.26%	4.113%
18	9.498	1052	1056	1061	rVB5	23692	35719	1.01%	0.114%
19	9.563	1061	1067	1071	rBV2	26731	51747	1.46%	0.165%
20	9.675	1082	1086	1091	rVB3	37013	64082	1.81%	0.205%
21	9.763	1091	1101	1102	rBV6	32836	69521	1.96%	0.222%
22	9.833	1109	1113	1124	rVB3	92951	199726	5.63%	0.639%
23	10.098	1153	1158	1163	rBV4	62813	114051	3.22%	0.365%
24	10.310	1188	1194	1197	rBV6	23433	48286	1.36%	0.154%
25	10.351	1197	1201	1212	rVB8	42296	110507	3.12%	0.353%
26	10.457	1213	1219	1220	rBV5	26764	41580	1.17%	0.133%
27	10.563	1231	1237	1243	rVB8	31068	65559	1.85%	0.210%
28	10.622	1243	1247	1253	rVV5	29136	59355	1.67%	0.190%
29	10.686	1253	1258	1262	rVV5	36240	78001	2.20%	0.249%
30	10.733	1262	1266	1271	rVB6	36168	64930	1.83%	0.208%
31	10.804	1271	1278	1285	rBV7	46474	113081	3.19%	0.362%
32	10.863	1285	1288	1296	rVV8	28763	67394	1.90%	0.215%
33	10.945	1296	1302	1314	rVV	266250	514887	14.52%	1.646%
34	11.051	1316	1320	1324	rVV4	33416	58337	1.64%	0.187%

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35	11.116	1325	1331	1338	rVB2	76602	148666	4.19%	0.475%
36	11.286	1357	1360	1365	rVB7	24635	41161	1.16%	0.132%
37	11.404	1366	1380	1386	rBV10	54507	181244	5.11%	0.579%
38	11.469	1386	1391	1395	rVV5	35212	57322	1.62%	0.183%
39	11.522	1396	1400	1407	rVB8	22325	45272	1.28%	0.145%
40	11.704	1426	1431	1436	rVB5	41659	78638	2.22%	0.251%
41	11.822	1438	1451	1461	rBV7	84363	304741	8.59%	0.974%
42	11.969	1472	1476	1482	rVB8	23892	41944	1.18%	0.134%
43	12.045	1483	1489	1492	rBV5	41803	95984	2.71%	0.307%
44	12.192	1505	1514	1520	rVB4	78926	209468	5.91%	0.670%
45	12.286	1525	1530	1537	rVB3	57705	111282	3.14%	0.356%
46	12.439	1553	1556	1560	rVB5	30863	44954	1.27%	0.144%
47	12.545	1560	1574	1579	rBV3	178888	438106	12.35%	1.401%
48	12.604	1580	1584	1589	rVB4	81741	141000	3.98%	0.451%
49	12.657	1589	1593	1597	rBV5	69165	137934	3.89%	0.441%
50	12.704	1597	1601	1606	rVV7	82755	207514	5.85%	0.663%
51	12.757	1606	1610	1617	rVB5	121540	233207	6.57%	0.746%
52	12.922	1632	1638	1647	rVB6	93118	259027	7.30%	0.828%
53	12.998	1647	1651	1657	rBV8	48312	114301	3.22%	0.365%
54	13.086	1662	1666	1667	rBV3	36000	51422	1.45%	0.164%
55	13.204	1681	1686	1690	rBV5	57102	123928	3.49%	0.396%
56	13.257	1690	1695	1699	rBV	174694	283510	7.99%	0.906%
57	13.386	1711	1717	1723	rBV	1910828	2775479	78.24%	8.874%
58	13.451	1723	1728	1734	rVV3	190449	331412	9.34%	1.060%
59	13.539	1740	1743	1748	rBV5	46873	73745	2.08%	0.236%
60	13.610	1749	1755	1759	rBV8	54155	131787	3.72%	0.421%
61	13.663	1760	1764	1772	rVB5	93430	160431	4.52%	0.513%
62	13.739	1774	1777	1781	rBV5	46258	83303	2.35%	0.266%
63	13.892	1798	1803	1810	rBV5	136675	279149	7.87%	0.892%
64	13.957	1811	1814	1818	rVB5	68333	87938	2.48%	0.281%
65	14.033	1823	1827	1832	rVV4	69207	115102	3.24%	0.368%
66	14.221	1856	1859	1864	rVB2	95374	142238	4.01%	0.455%
67	14.345	1876	1880	1886	rBV	181870	328974	9.27%	1.052%
68	14.610	1922	1925	1927	rBV3	49123	54206	1.53%	0.173%
69	14.768	1947	1952	1964	rVB3	324359	671685	18.94%	2.148%
70	15.186	2019	2023	2026	rBV	135874	191265	5.39%	0.612%
71	15.221	2026	2029	2034	rVB	153978	218471	6.16%	0.698%

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72	15.280	2034	2039	2047	rBV2	185979	353800	9.97%	1.131%
73	15.357	2047	2052	2057	rBV2	226933	370042	10.43%	1.183%
74	15.415	2059	2062	2066	rBV4	72770	111398	3.14%	0.356%
75	15.568	2084	2088	2097	rVB5	176425	368511	10.39%	1.178%
76	16.180	2189	2192	2196	rBV3	75266	90845	2.56%	0.290%
77	16.262	2200	2206	2218	rVB	1626402	2316241	65.30%	7.406%
78	16.480	2240	2243	2246	rVB	101371	104452	2.94%	0.334%
79	16.568	2254	2258	2262	rBV	341277	418058	11.79%	1.337%
80	16.627	2264	2268	2274	rVB2	286512	517297	14.58%	1.654%
81	16.692	2275	2279	2283	rVB2	329264	423966	11.95%	1.356%
82	16.733	2283	2286	2290	rVB	189593	233816	6.59%	0.748%
83	16.780	2292	2294	2296	rBV3	57121	64852	1.83%	0.207%
84	16.839	2301	2304	2307	rVB3	97206	110466	3.11%	0.353%
85	16.892	2308	2313	2319	rBV4	314562	558804	15.75%	1.787%
86	16.957	2320	2324	2328	rBV	301201	381077	10.74%	1.218%
87	17.027	2333	2336	2341	rVB2	174579	231300	6.52%	0.740%
88	17.504	2413	2417	2423	rVB2	362184	490488	13.83%	1.568%
89	18.374	2562	2565	2570	rVB2	276529	327673	9.24%	1.048%
90	19.627	2775	2778	2788	rVB2	178910	227333	6.41%	0.727%
91	20.086	2851	2856	2861	rBV	3105239	3547166	100.00%	11.341%
92	21.639	3116	3120	3124	rVB	450290	589117	16.61%	1.884%
93	23.974	3513	3517	3525	rVB	310652	584604	16.48%	1.869%

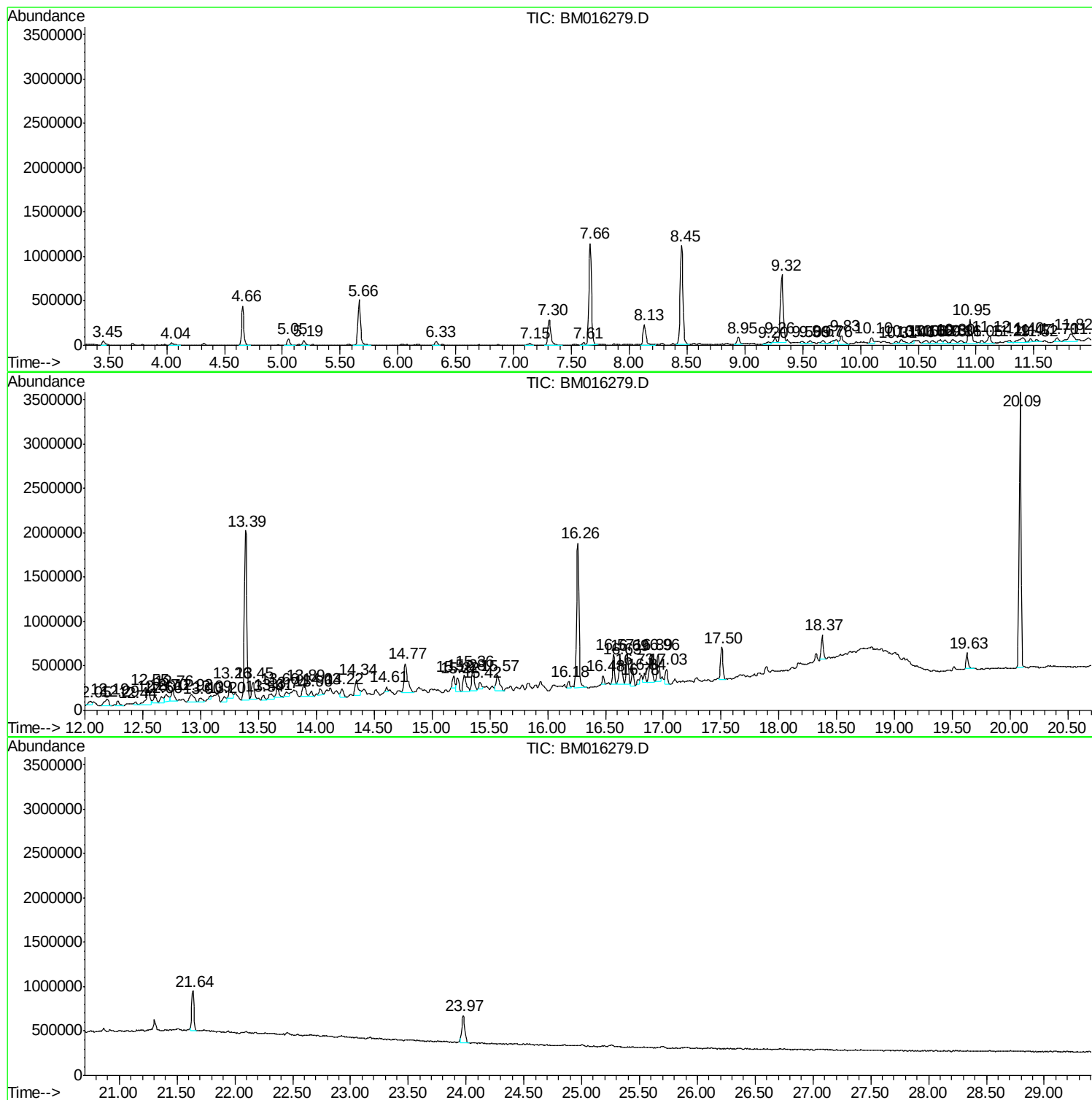
Sum of corrected areas: 31277299

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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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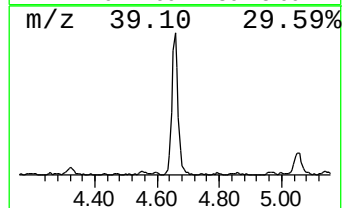
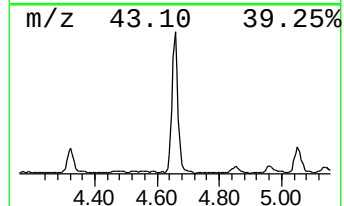
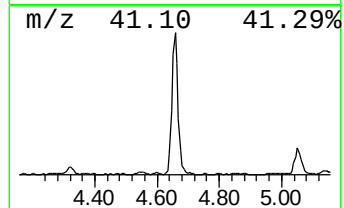
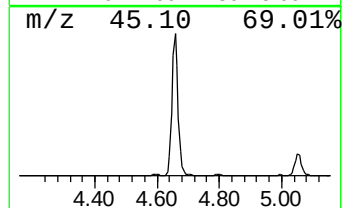
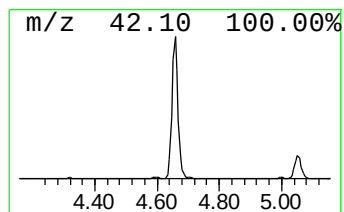
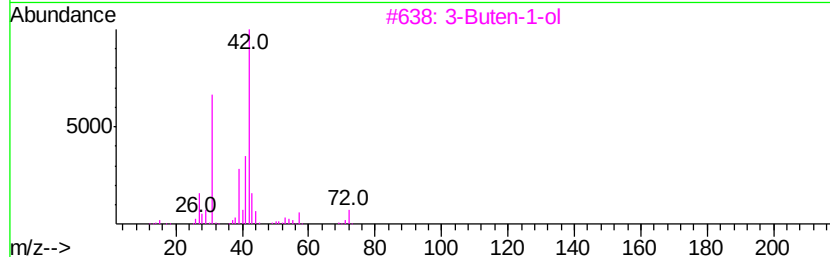
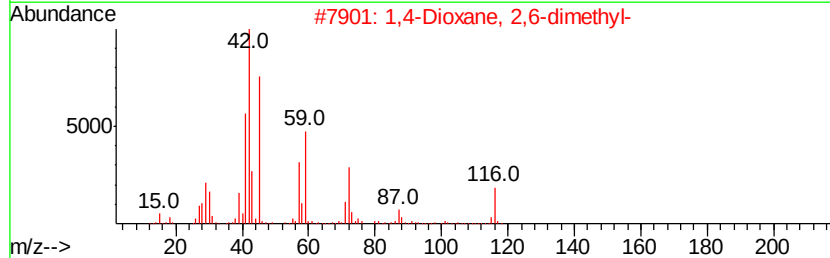
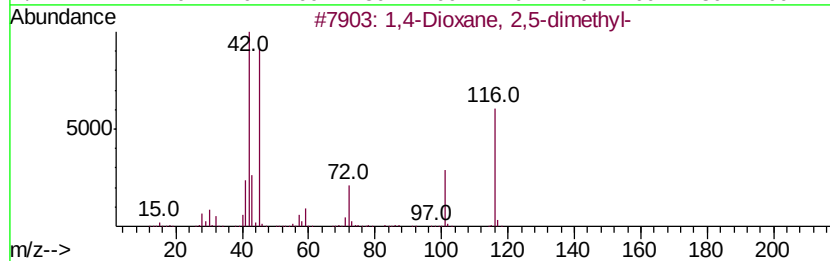
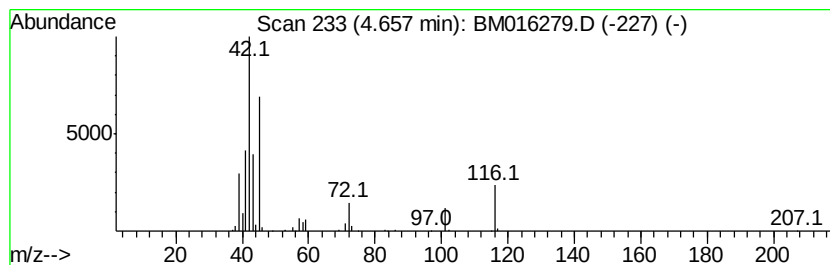
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1,4-Dioxane, 2,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.66	28.84 ng	608598	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Dioxane, 2,5-dimethyl-	116	C6H12O2	015176-21-3	91
2		1,4-Dioxane, 2,6-dimethyl-	116	C6H12O2	010138-17-7	78
3		3-Buten-1-ol	72	C4H8O	000627-27-0	38
4		Oxetane, 2,4-dimethyl-, trans-	86	C5H10O	029424-94-0	17
5		2,3-Butanedione, dioxime	116	C4H8N2O2	000095-45-4	9



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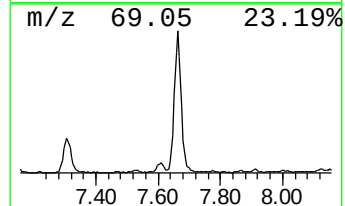
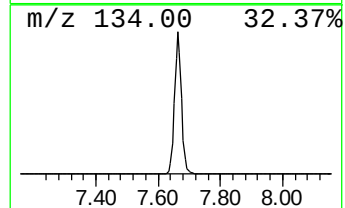
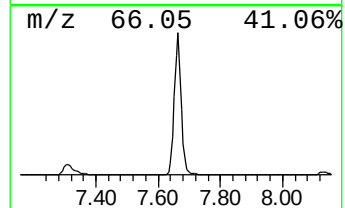
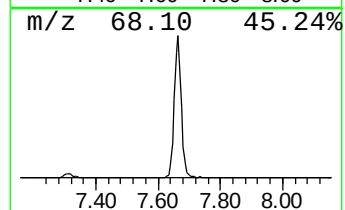
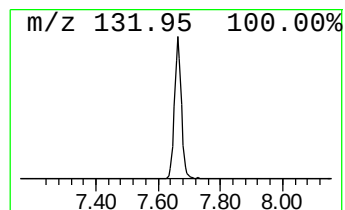
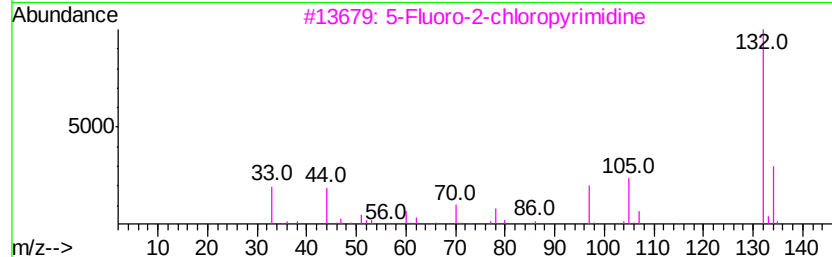
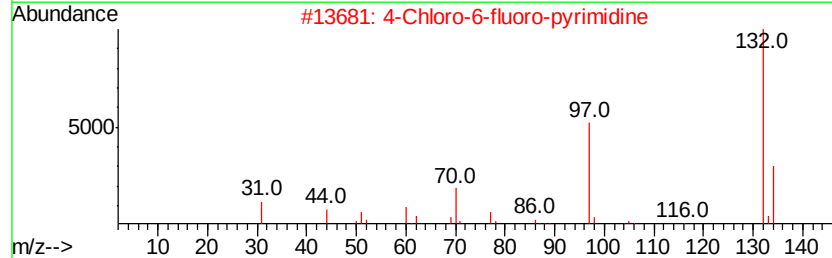
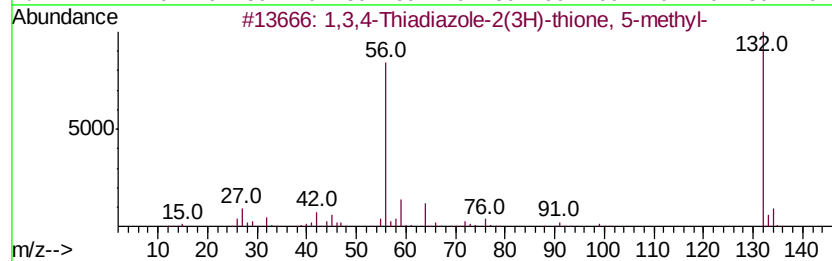
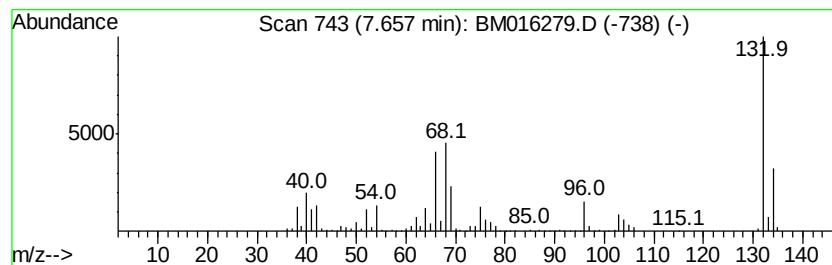
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	84.81 ng	1789390	1,4-Dichlorobenzene-d4	8.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2			4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
4			3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
5			1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12



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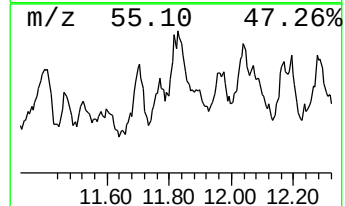
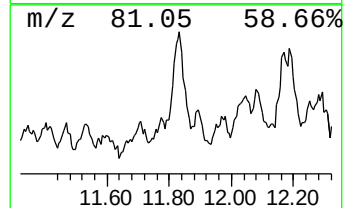
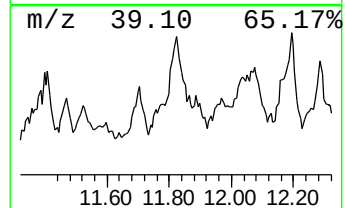
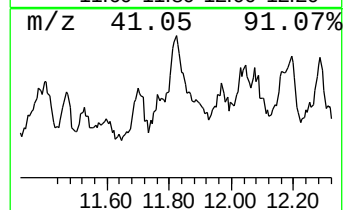
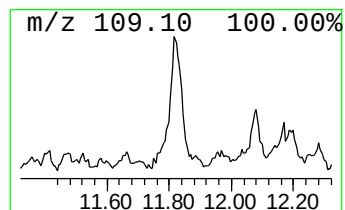
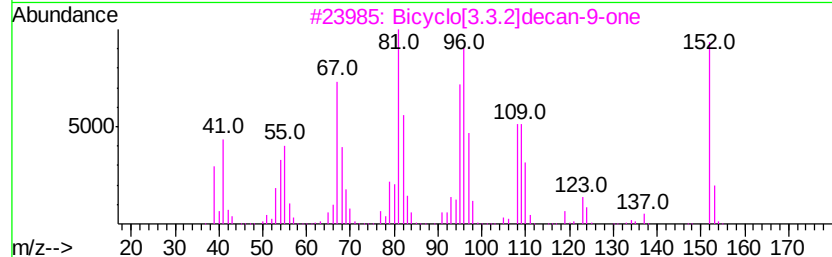
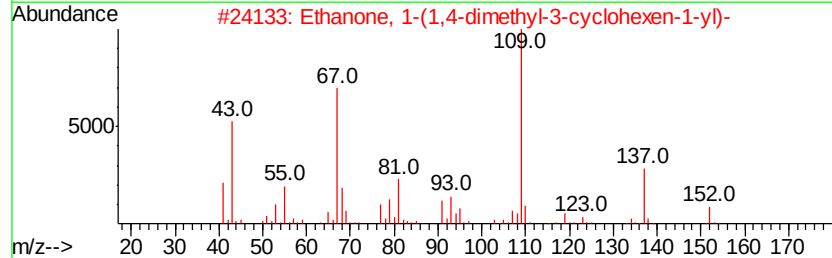
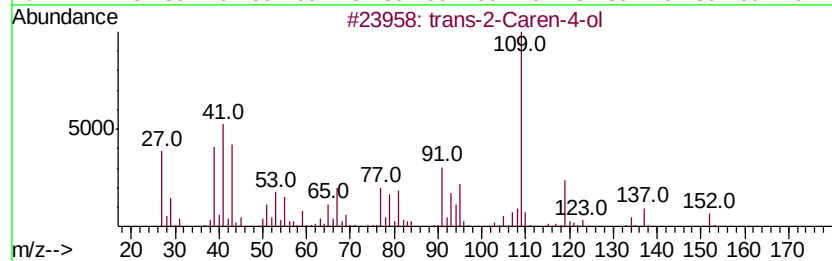
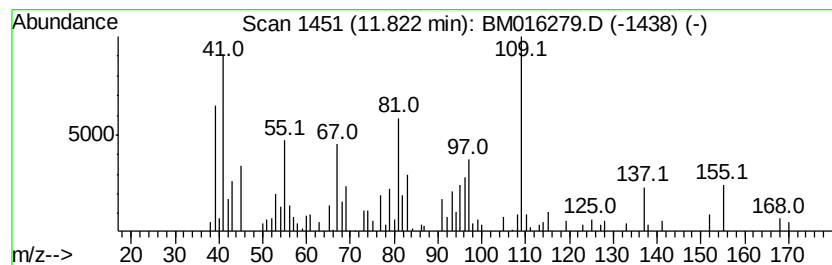
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Peak Number 4 unknown11.82 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.82	11.84 ng	304741	Napthalene-d8	10.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2-Caren-4-ol	152	C10H16O	004017-82-7	45
2	Ethanone, 1-(1,4-dimethyl-3-cycl...	152	C10H16O	043219-68-7	42
3	Bicyclo[3.3.2]decan-9-one	152	C10H16O	028054-91-3	38
4	1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	021391-98-0	30
5	Benzenamine, 3-ethoxy-	137	C8H11NO	000621-33-0	30



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Sample : J4356-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

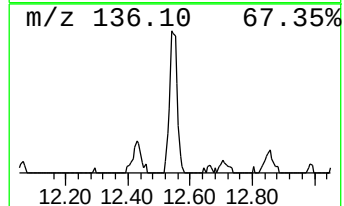
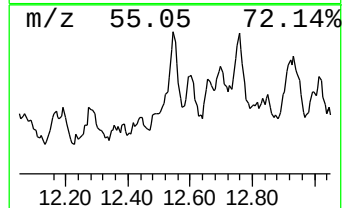
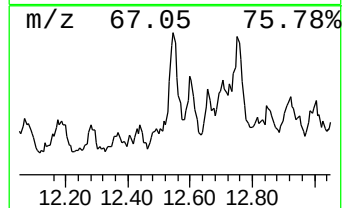
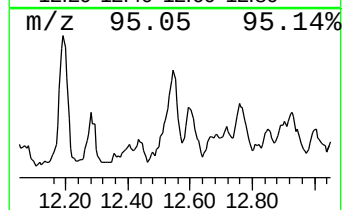
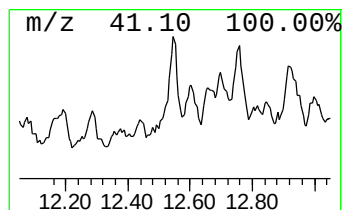
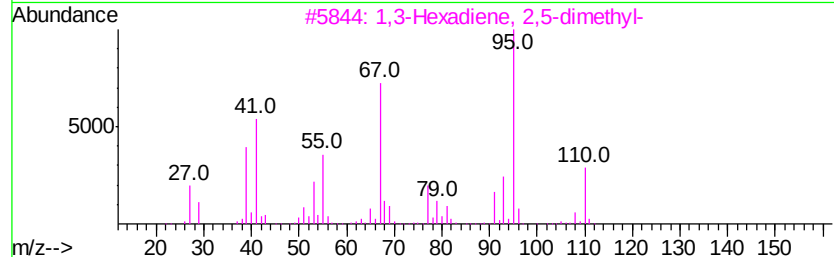
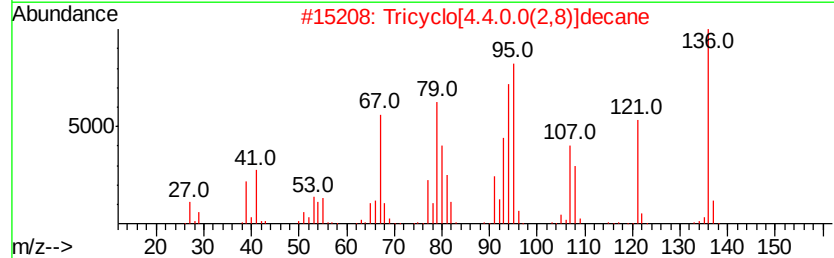
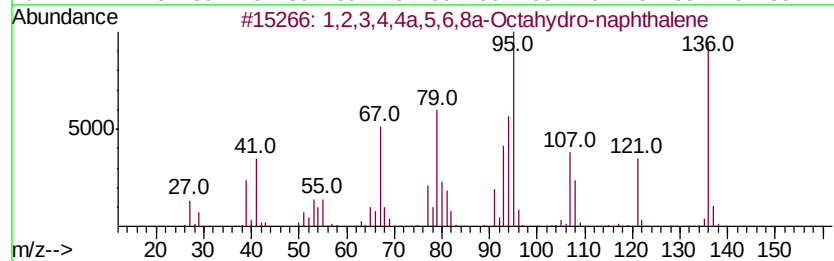
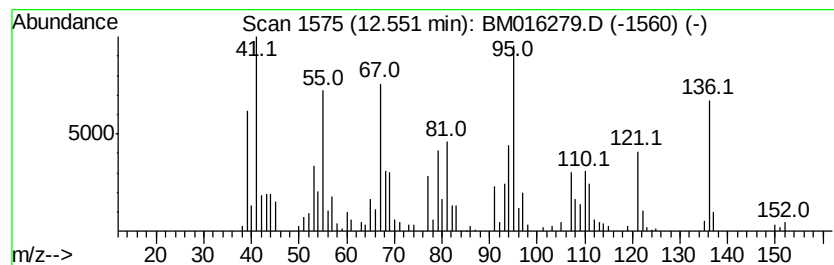
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,2,3,4,4a,5,6,8a-Octahydro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.55	17.02 ng	438106	Naphthalene-d8	10.95	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3,4,4a,5,6,8a-Octahydro-naph...	136	C10H16	031244-58-3	93
2	Tricyclo[4.4.0.0(2,8)]decane	136	C10H16	049700-59-6	60
3	1,3-Hexadiene, 2,5-dimethyl-	110	C8H14	029253-64-3	50
4	2,5-Methano-1H-indene, octahydro-	136	C10H16	019026-94-9	46
5	7-Methylene-9-oxa-bicyclo[3.3.1]...	136	C9H12O	1000193-85-5	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
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Acq On : 09 Aug 2018 13:37
Operator : SJ/JU
Sample : J4356-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

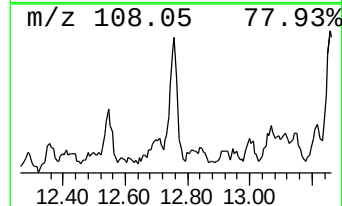
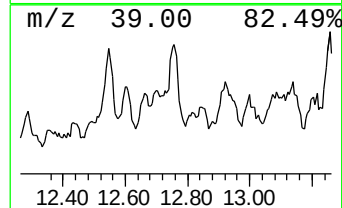
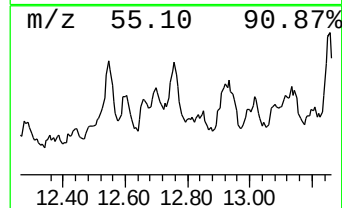
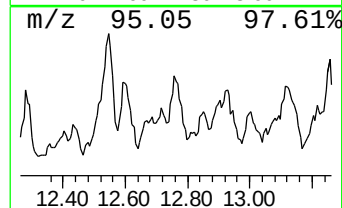
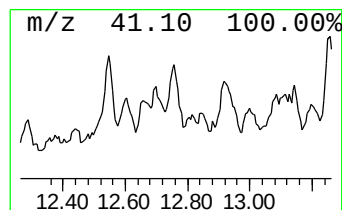
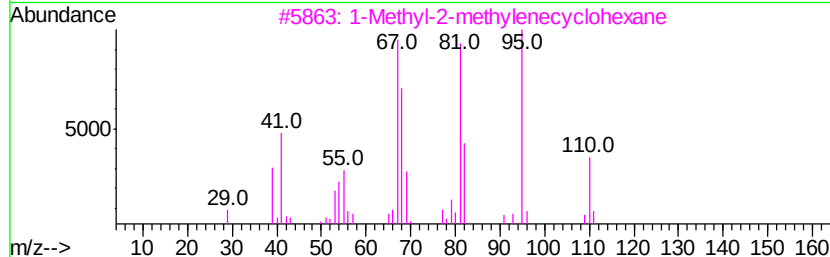
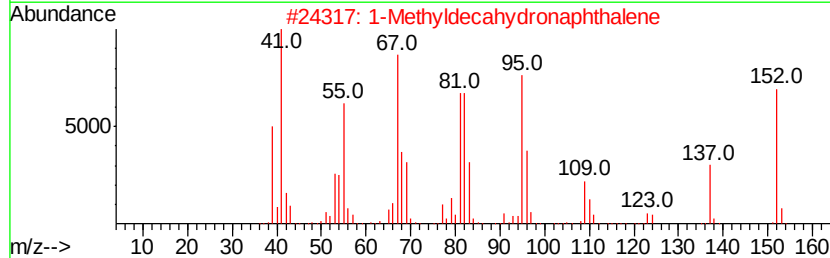
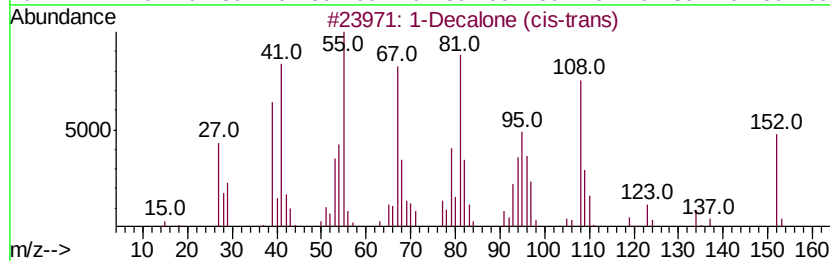
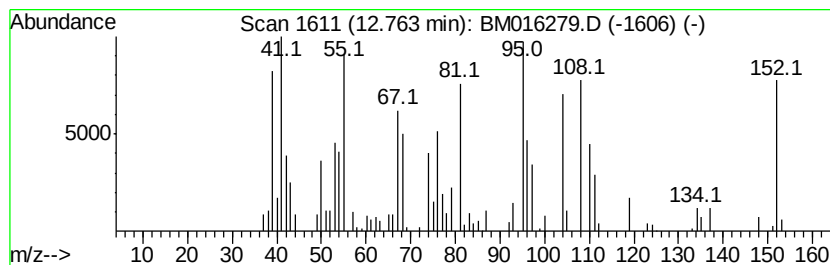
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Decalone (cis-trans) Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.76	9.06 ng	233207	Naphthalene-d8	10.95
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Decalone (cis-trans)	152 C10H16O	004832-16-0	60
2	1-Methyldecahydronaphthalene	152 C11H20	002958-75-0	41
3	1-Methyl-2-methylenecyclohexane	110 C8H14	002808-75-5	41
4	Naphthalene, decahydro-2-methyl-	152 C11H20	002958-76-1	41
5	Bicyclo[2.2.1]heptane, 2-methyl-	110 C8H14	015185-11-2	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016279.D
Acq On : 09 Aug 2018 13:37
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Sample : J4356-03
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ALS Vial : 7 Sample Multiplier: 1

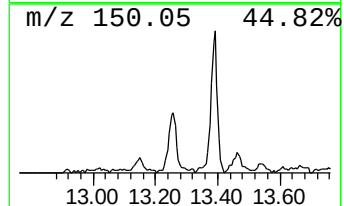
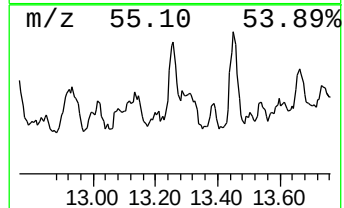
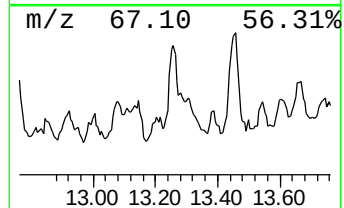
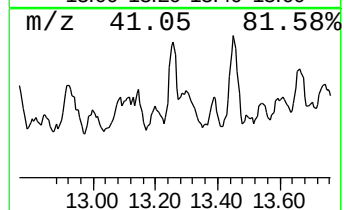
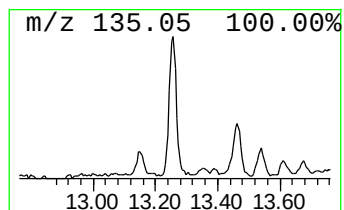
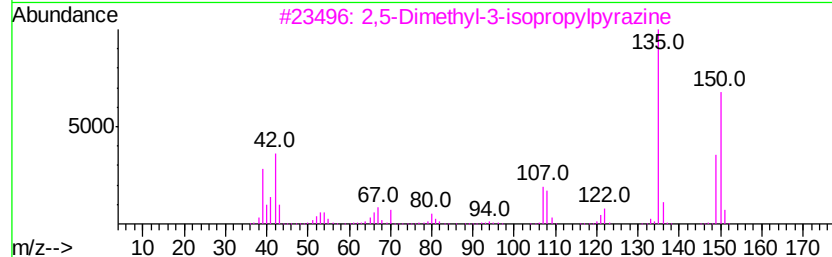
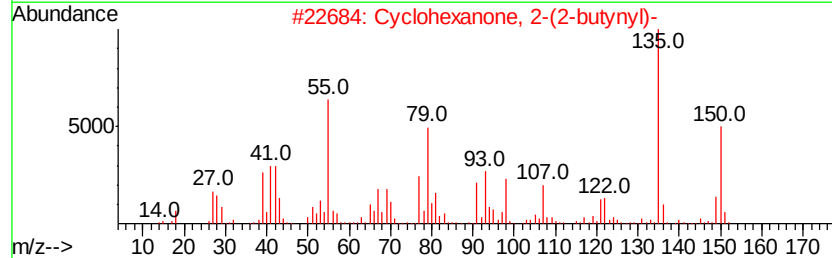
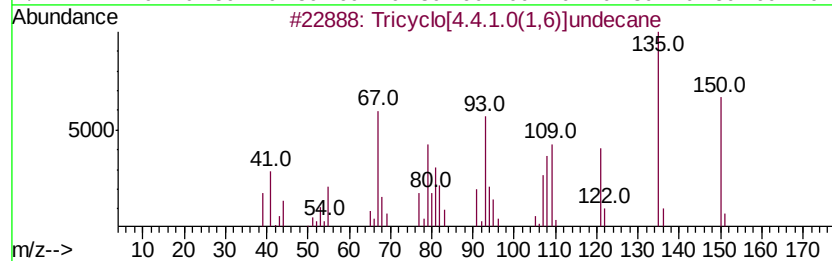
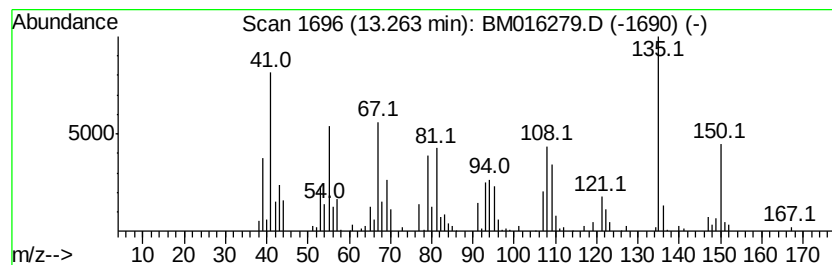
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tricyclo[4.4.1.0(1,6)]undecane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.26	8.44 ng	283510	Acenaphthene-d10		14.77
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricyclo[4.4.1.0(1,6)]undecane	150	C11H18	006571-73-9	87
2	Cyclohexanone, 2-(2-butylnyl)-	150	C10H14O	054166-48-2	55
3	2,5-Dimethyl-3-isopropylpyrazine	150	C9H14N2	013610-20-3	49
4	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	46
5	5-Cyano-1,2,3,4-tetrahydro-4,6-d...	150	C8H10N2O	027036-93-7	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016279.D
Acq On : 09 Aug 2018 13:37
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ALS Vial : 7 Sample Multiplier: 1

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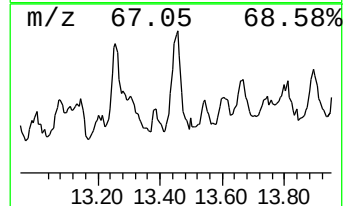
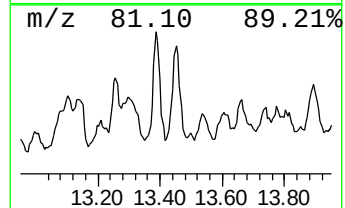
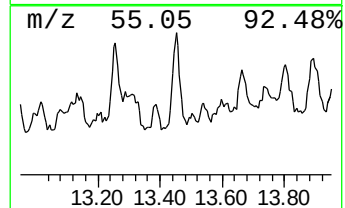
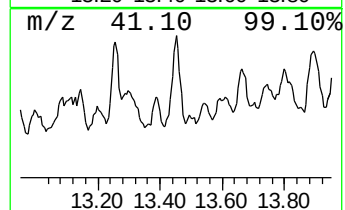
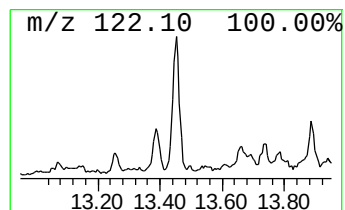
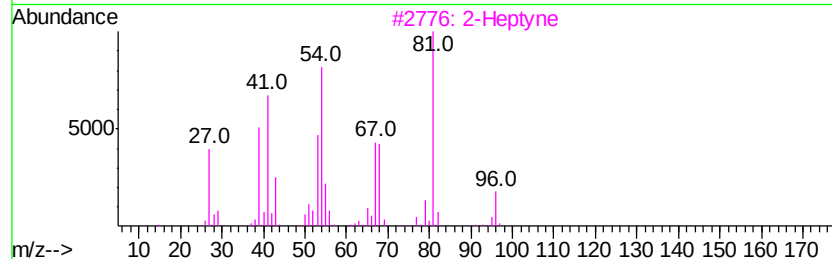
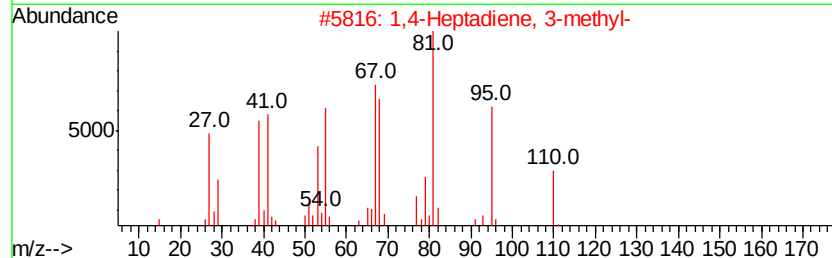
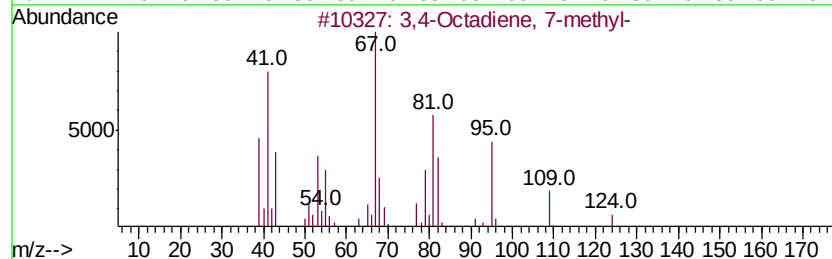
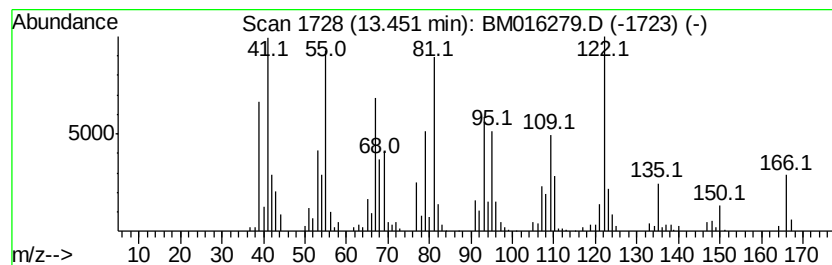
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown13.45 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	9.87 ng	331412	Acenaphthene-d10	14.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	49
2			1,4-Heptadiene, 3-methyl-	110	C8H14	001603-01-6	43
3			2-Heptyne	96	C7H12	001119-65-9	41
4			(E)-2-Butenylcyclopropane	96	C7H12	076588-98-2	41
5			(2R,4R)-p-Mentha-[1(7),8]-diene,...	168	C10H16O2	1000292-74-1	35



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
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Misc :
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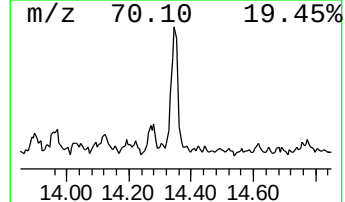
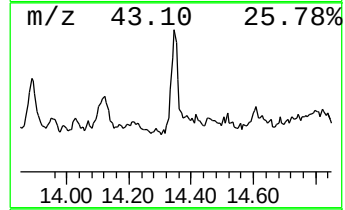
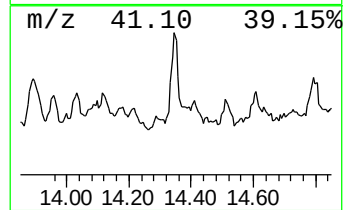
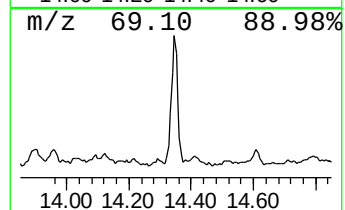
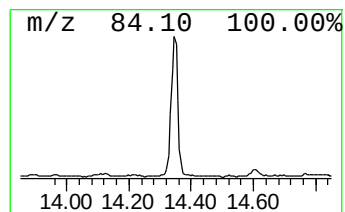
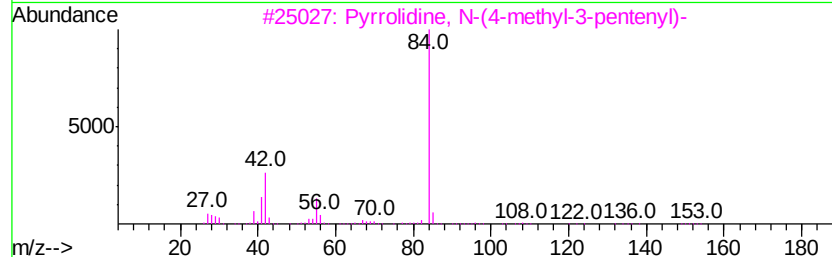
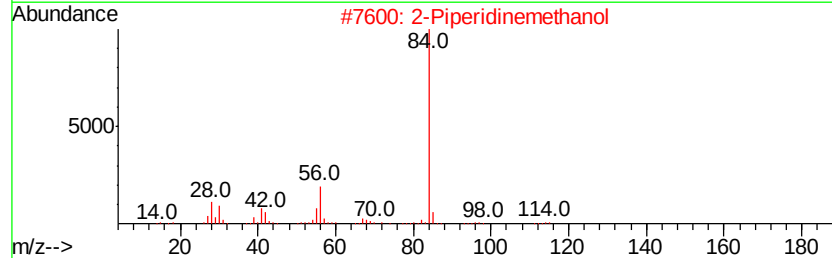
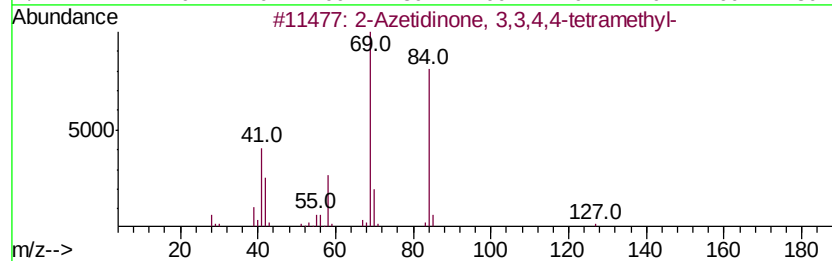
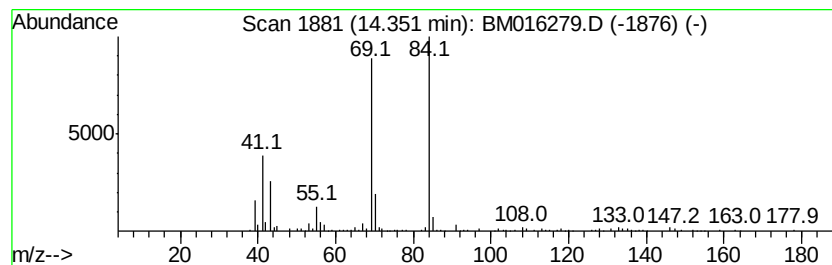
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 2-Azetidinone, 3,3,4,4-tetr... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.35	9.80 ng	328974	Acenaphthene-d10	14.77	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Azetidinone, 3,3,4,4-tetramethyl-	127	C7H13NO	013423-22-8	78
2	2-Piperidinemethanol	115	C6H13NO	003433-37-2	27
3	Pvrrolidine, N-(4-methyl-3-pente...	153	C10H19N	1000161-63-8	25
4	2-Pyrrolidineethanamine, 1-methyl-	128	C7H16N2	051387-90-7	25
5	Phosphonic acid, [1-[(1-methylet...	309	C11H28N03PSi2	055108-64-0	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
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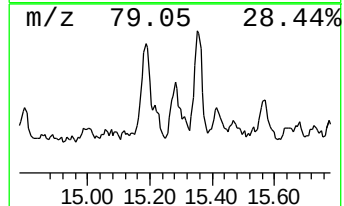
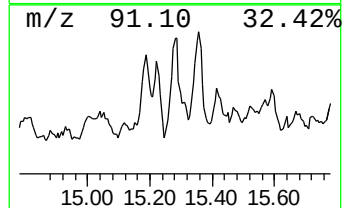
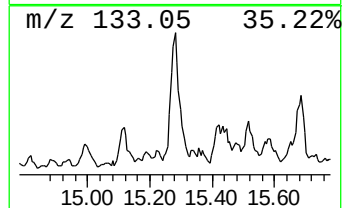
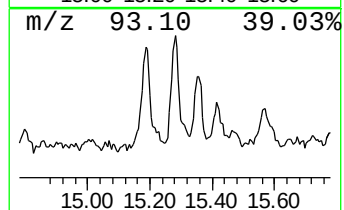
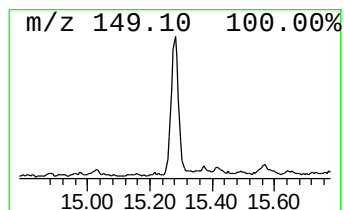
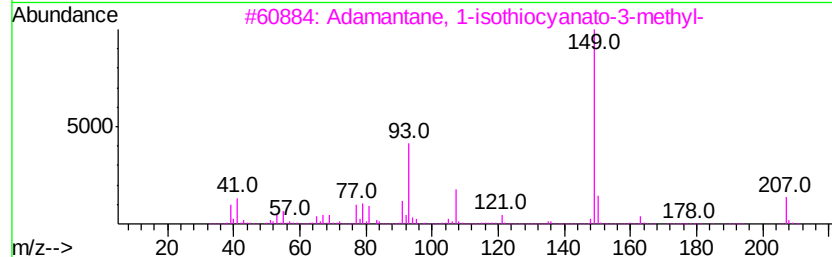
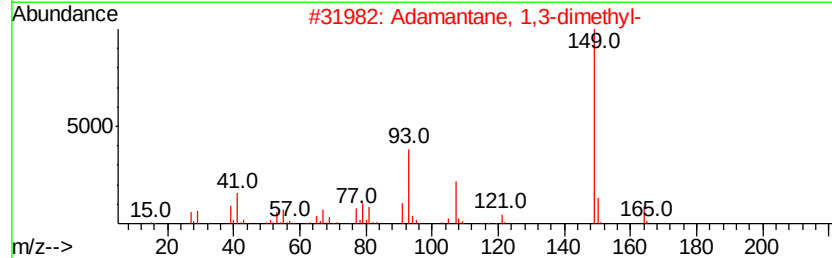
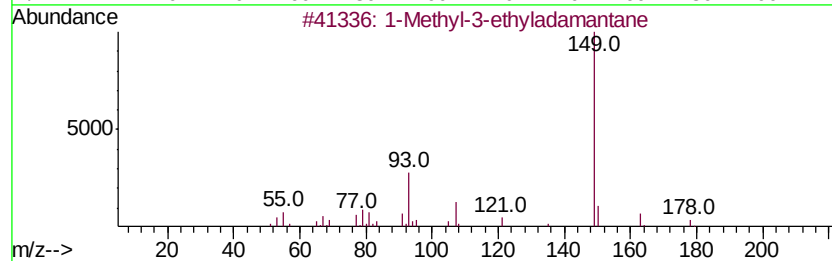
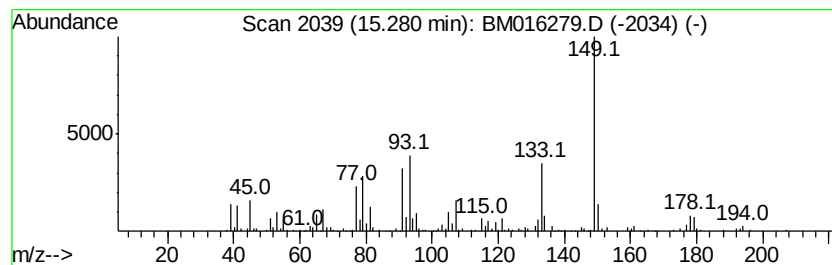
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1-Methyl-3-ethyladamantane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.28	10.53 ng	353800	Acenaphthene-d10	14.77	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	62
2	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	53
3	Adamantane, 1-isothiocyano-3-methyl-	207	C12H17NS	136860-48-5	45
4	Oxazolidine, 3-phenyl-	149	C9H11NO	020503-92-8	43
5	Cis-1,4-dimethyladamantane	164	C12H20	024145-89-9	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016279.D
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Sample : J4356-03
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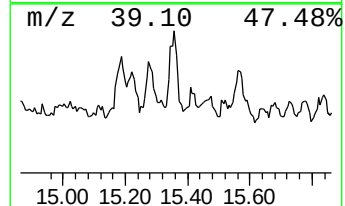
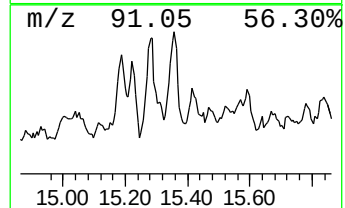
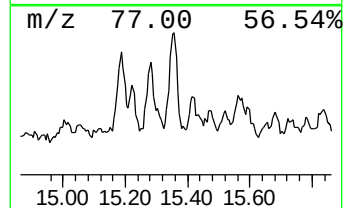
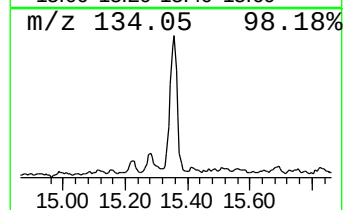
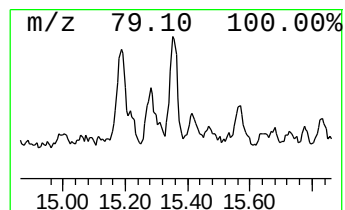
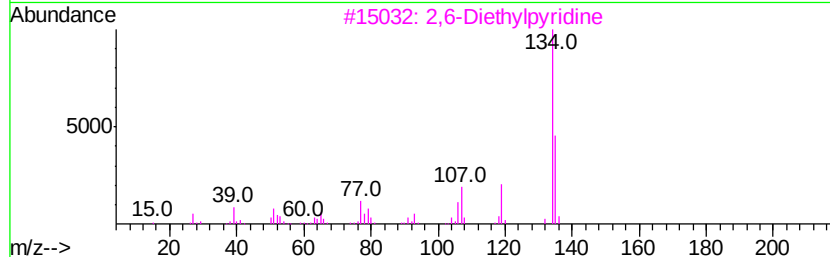
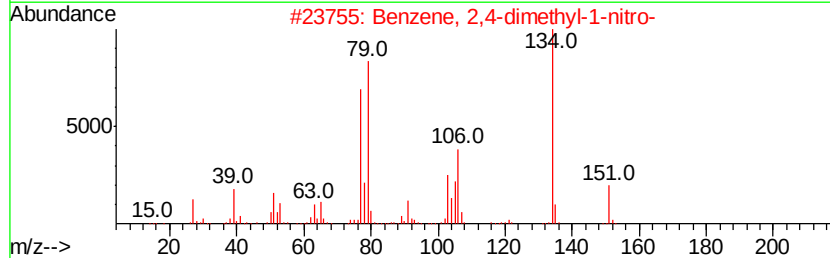
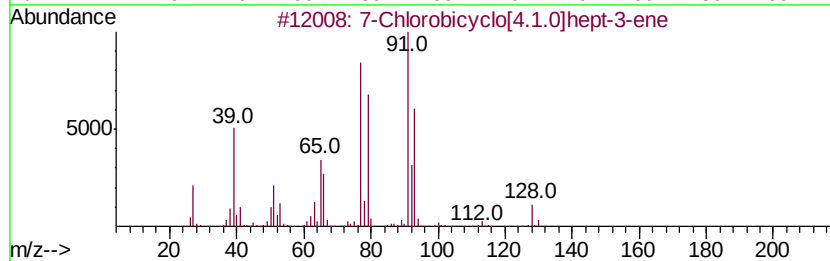
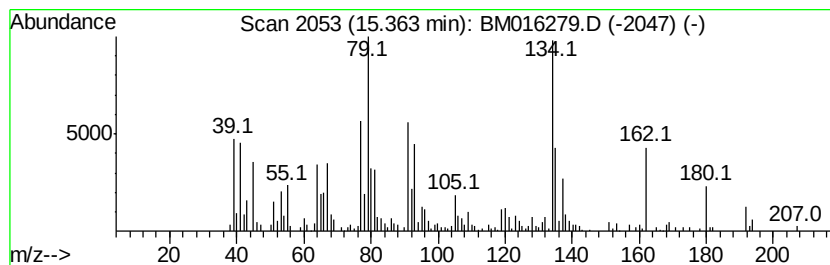
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown15.36 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	11.02 ng	370042	Acenaphthene-d10	14.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-Chlorobicyclo[4.1.0]hept-3-ene	128	C7H9Cl	1000195-01-7	38
2		Benzene, 2,4-dimethyl-1-nitro-	151	C8H9NO2	000089-87-2	38
3		2,6-Diethylpyridine	135	C9H13N	000935-28-4	25
4		Sydnone, 3-(4-methoxyphenyl)-	192	C9H8N2O3	003815-80-3	22
5		cis-4,5-Bis(cyanomethyl)cyclohexene	160	C10H12N2	025886-61-7	22



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016279.D
Acq On : 09 Aug 2018 13:37
Operator : SJ/JU
Sample : J4356-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
MW-12

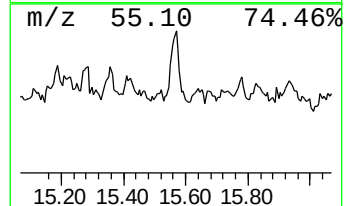
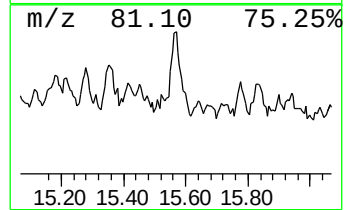
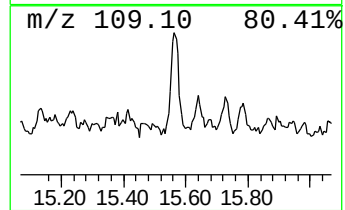
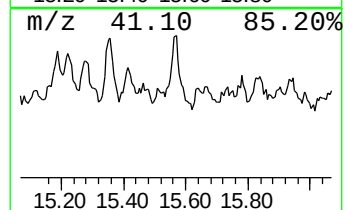
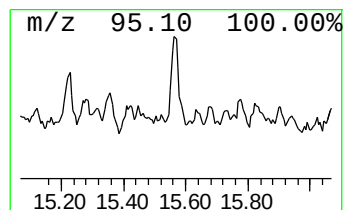
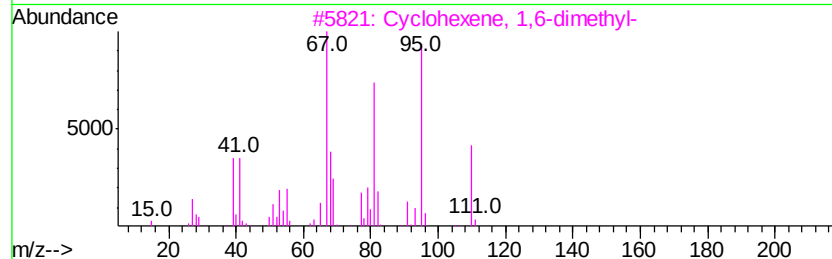
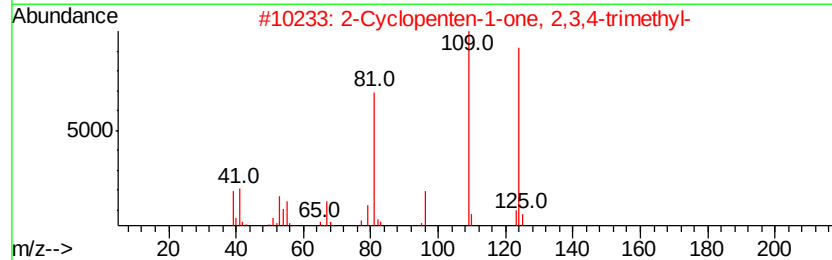
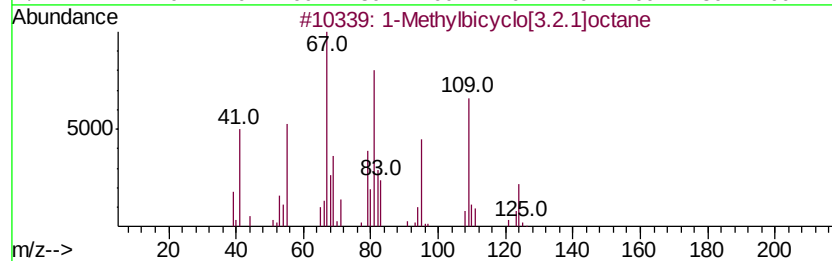
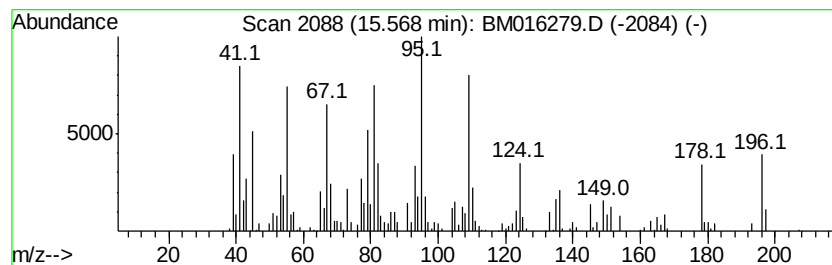
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown15.57 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.57	10.97 ng	368511	Acenaphthene-d10	14.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Methylbicyclo[3.2.1]octane	124	C9H16	119972-41-7	49
2		2-Cyclopenten-1-one, 2,3,4-trime...	124	C8H12O	028790-86-5	38
3		Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	38
4		1,1-Dimethyl-4-methylenecyclohexane	124	C9H16	006007-96-1	38
5		4-Methylimidazole-5-butyric acid	168	C8H12N2O2	1000129-14-7	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016279.D
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Sample : J4356-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

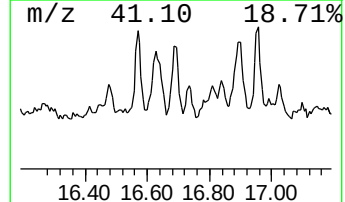
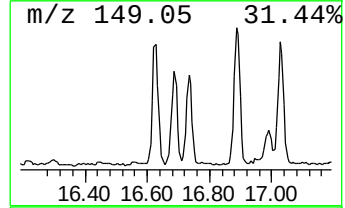
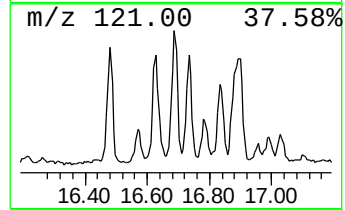
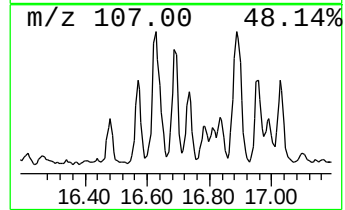
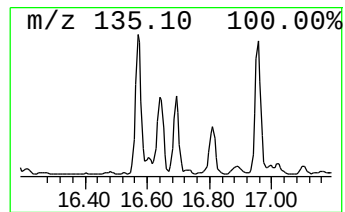
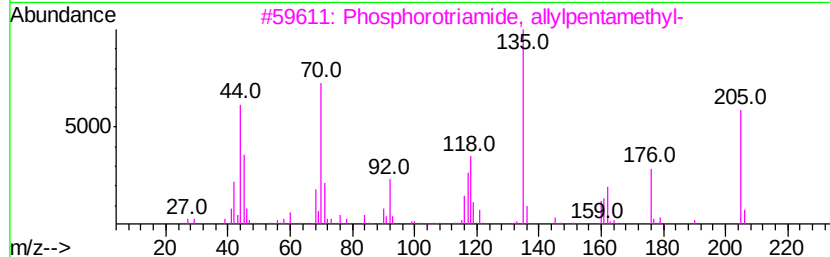
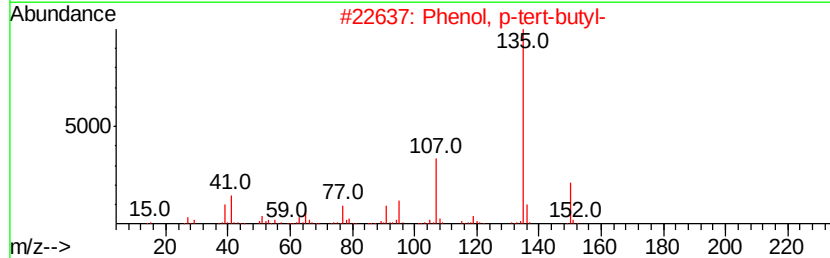
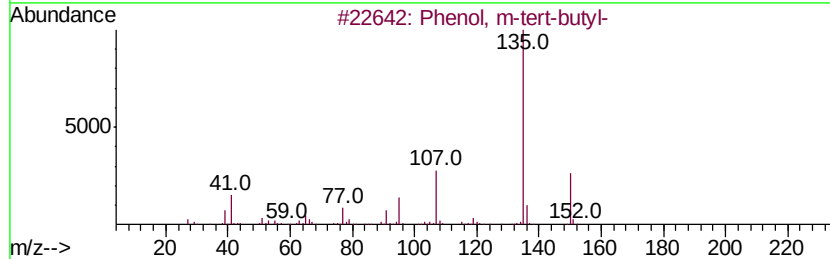
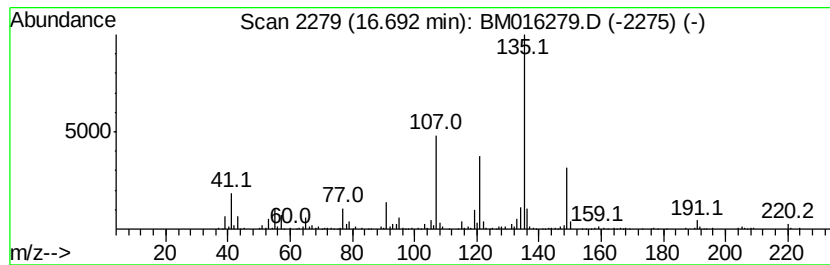
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Phenol, m-tert-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.69	17.29 ng	423966	Phenanthrene-d10	17.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Phenol, m-tert-butyl-	150 C10H14O	000585-34-2 59
2		Phenol, p-tert-butyl-	150 C10H14O	000098-54-4 59
3		Phosphorotriamide, allylpentamet...	205 C8H20N3OP	057041-73-3 55
4		4,6-Bis(4-ethoxybenzylthio)-5-ni...	457 C22H23N3O4S2	325957-76-4 53
5		Propane, 1,3-bis(ethylthio)-	164 C7H16S2	033672-52-5 52



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016279.D
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Sample : J4356-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

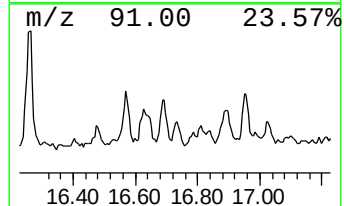
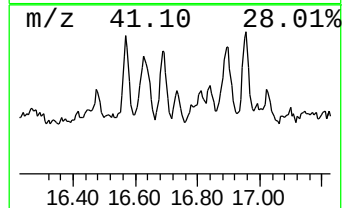
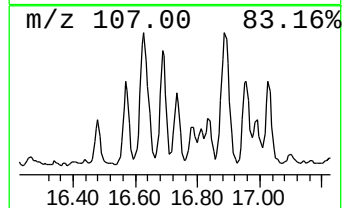
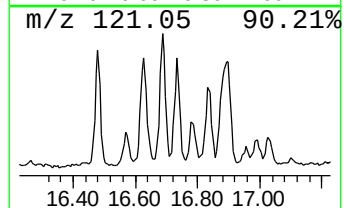
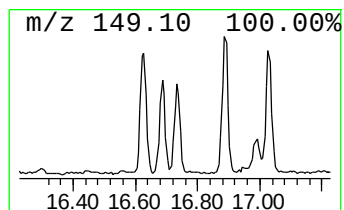
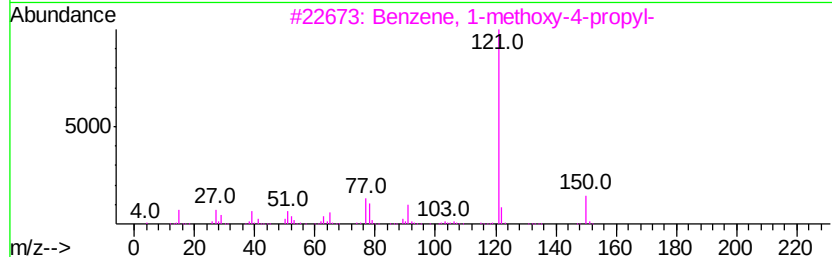
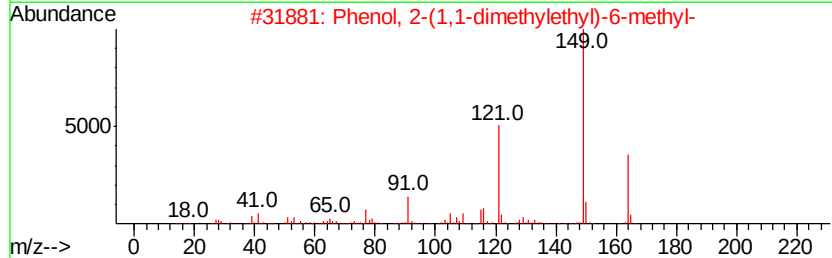
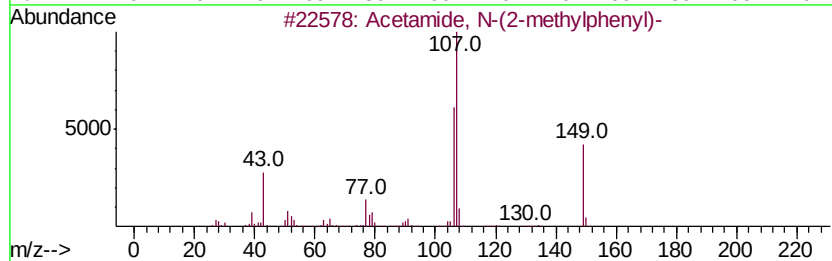
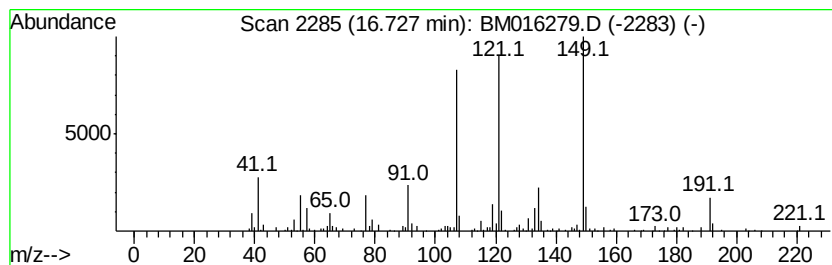
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown16.73 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.73	9.53 ng	233816	Phenanthrene-d10	17.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	49
2	Phenol, 2-(1,1-dimethylethyl)-6-...	164	C11H16O	002219-82-1	43
3	Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	35
4	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	000537-92-8	30
5	3',4'-Formoxylidide	149	C9H11NO	006639-60-7	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016279.D
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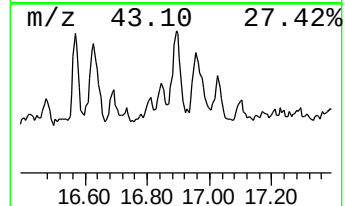
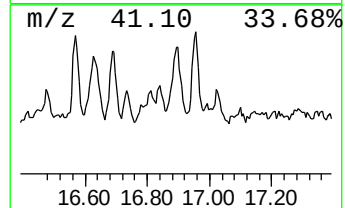
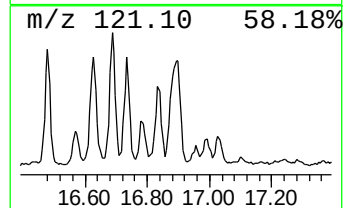
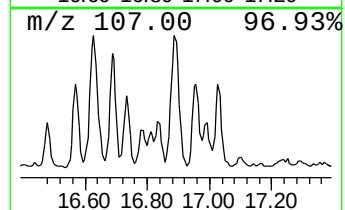
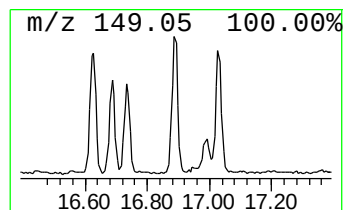
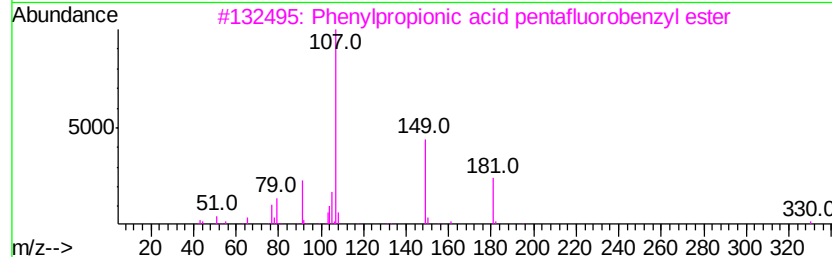
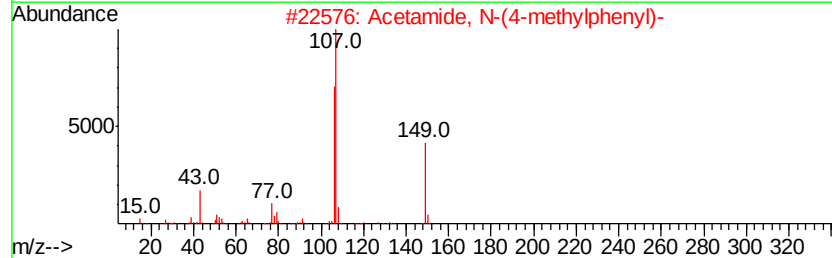
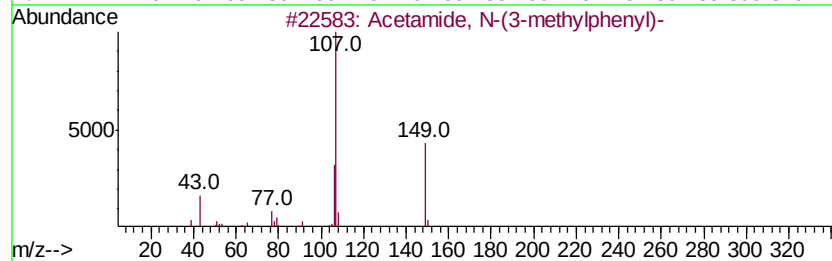
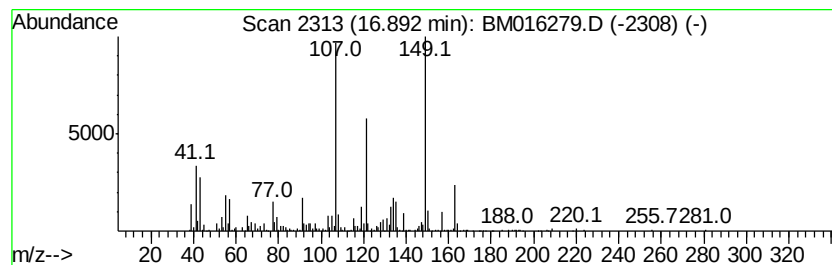
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Acetamide, N-(3-methylphenyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.89	22.79 ng	558804	Phenanthrene-d10	17.50
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Acetamide, N-(3-methylphenyl)-	149 C9H11NO	000537-92-8	64
2	Acetamide, N-(4-methylphenyl)-	149 C9H11NO	000103-89-9	38
3	Phenylpropionic acid pentafluoro...	330 C16H11F5O2	062434-95-1	38
4	1,3-Cyclohexadiene, 1,2,3,4,5,6-...	164 C12H20	1000152-09-6	35
5	3-Keto-4-aza-2,3-dihydrobenzopyran	149 C8H7NO2	1000289-12-0	30



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016279.D
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Sample : J4356-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

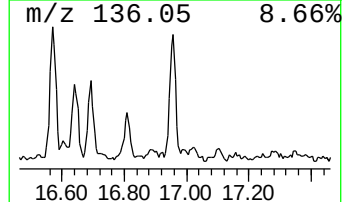
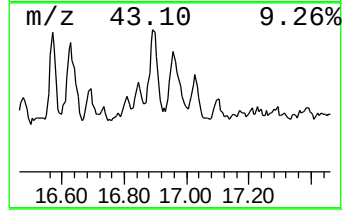
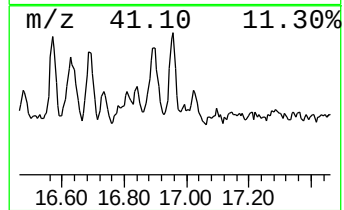
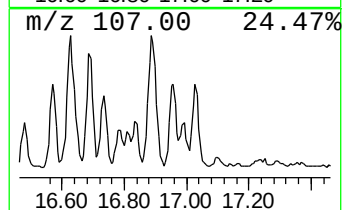
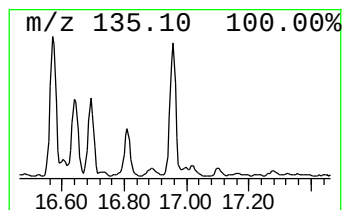
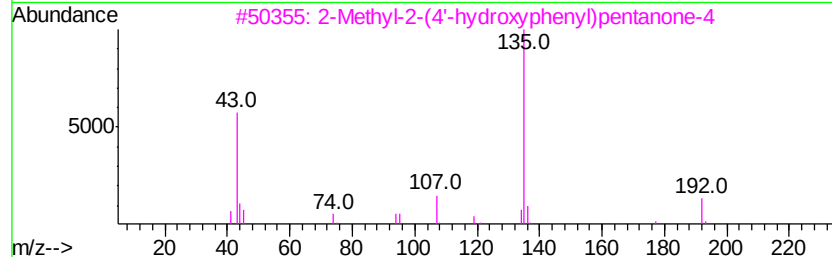
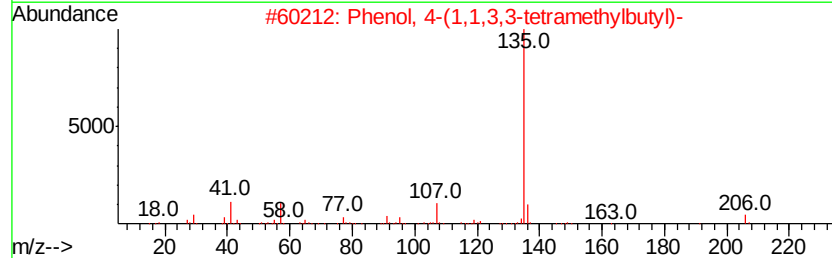
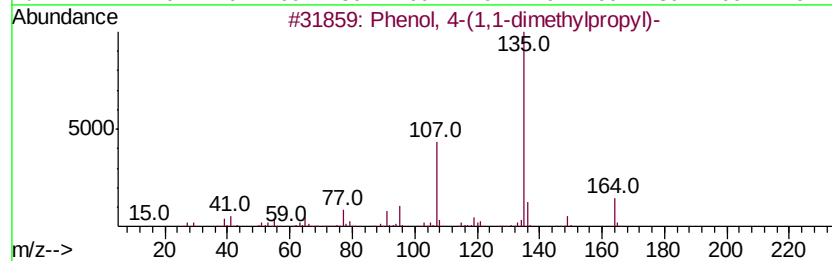
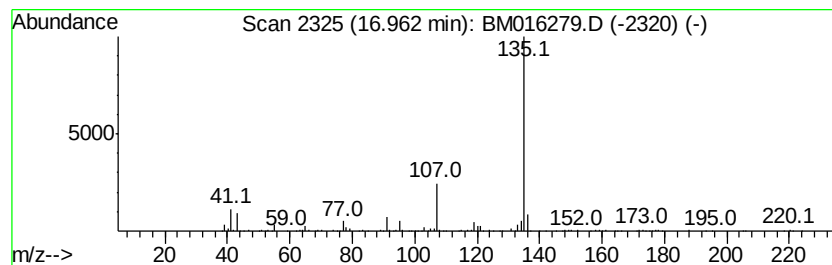
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 Phenol, 4-(1,1-dimethylprop... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.96	15.54 ng	381077	Phenanthrene-d10	17.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	78
2	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	64
3	2-Methyl-2-(4'-hydroxyphenyl)pen...	192	C12H16O2	070205-18-4	64
4	Thymol	150	C10H14O	000089-83-8	59
5	1-Adamantyl bromomethyl ketone	256	C12H17BrO	005122-82-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
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Misc :
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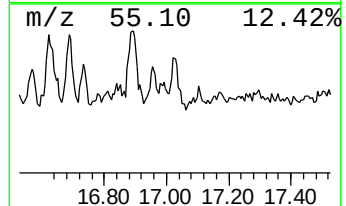
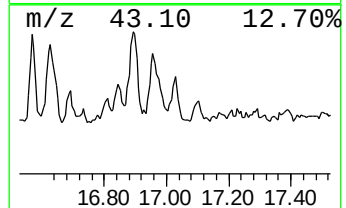
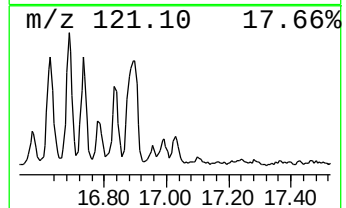
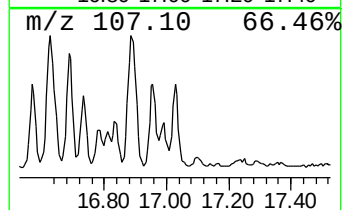
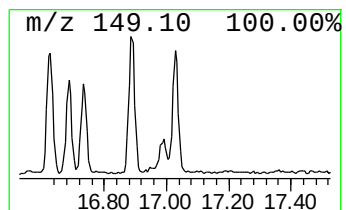
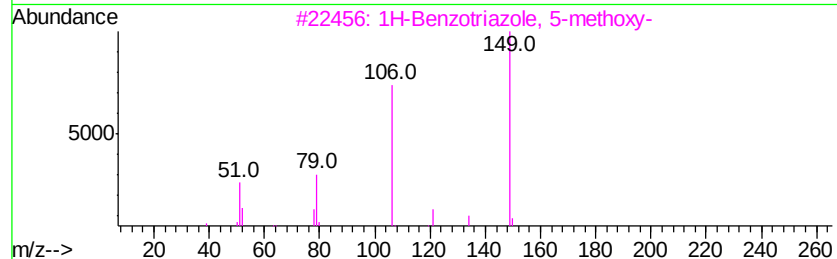
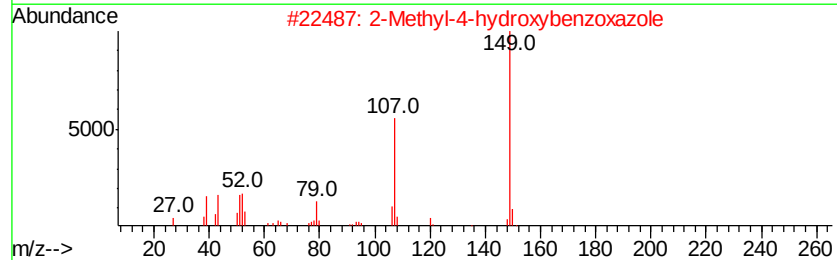
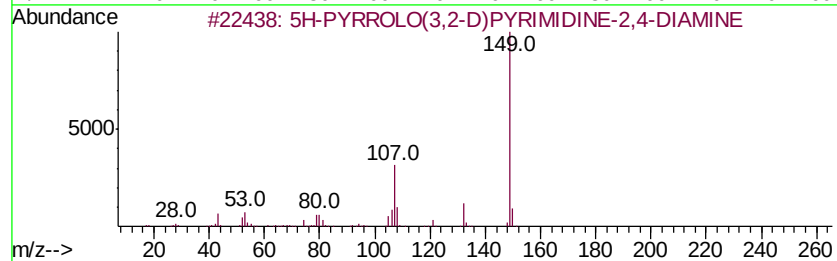
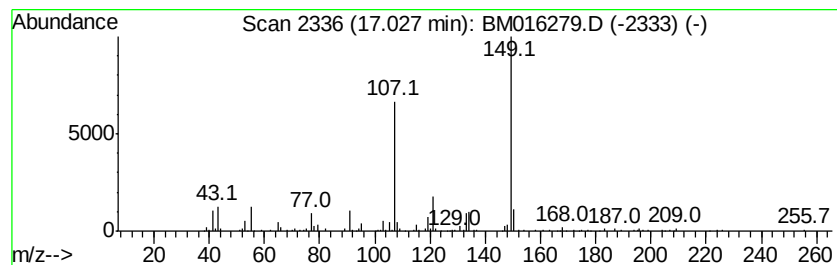
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 5H-PYRROLO(3,2-D)PYRIMIDINE... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.03	9.43 ng	231300	Phenanthrene-d10	17.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-PYRROLO(3,2-D)PYRIMIDINE-2,4-...	149	C6H7N5	1000244-21-4	64
2	2-Methyl-4-hydroxybenzoxazole	149	C8H7N02	051110-60-2	59
3	1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	50
4	Benzene, 2-methoxy-4-methyl-1-(1...	164	C11H16O	001076-56-8	50
5	1,3-Cyclohexadiene, 1,3,5,5,6,6-...	164	C12H20	1000150-39-4	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080918\
Data File : BM016279.D
Acq On : 09 Aug 2018 13:37
Operator : SJ/JU
Sample : J4356-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-12

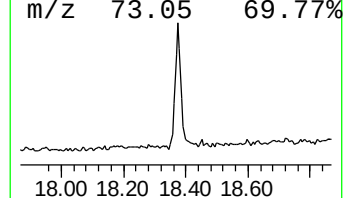
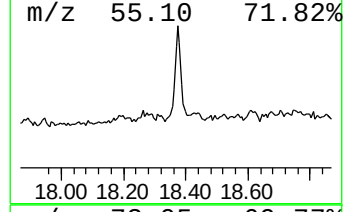
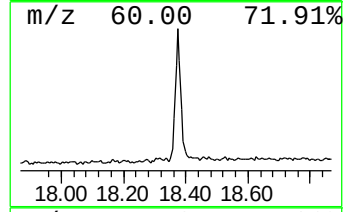
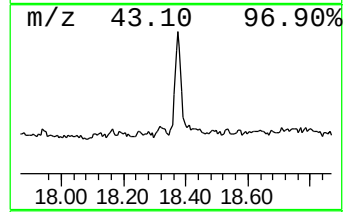
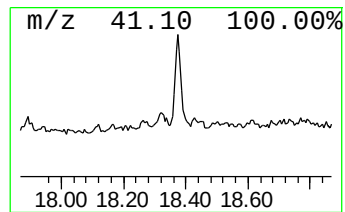
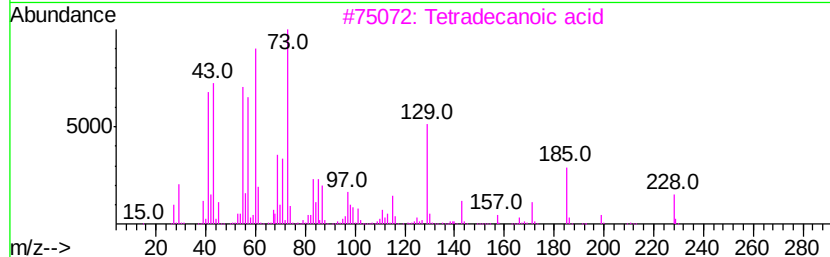
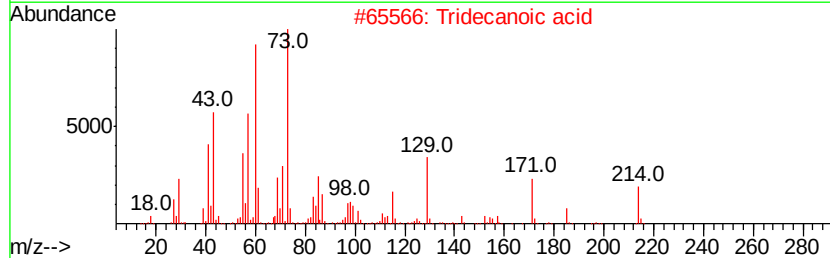
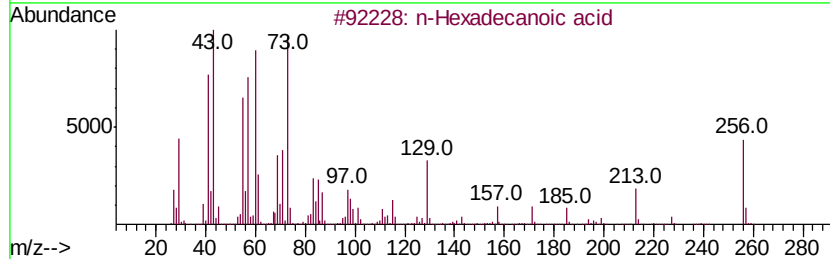
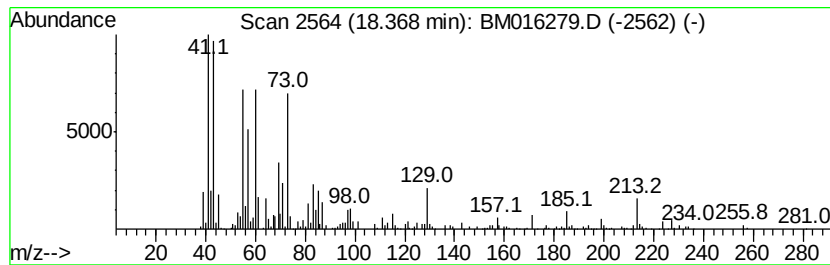
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	13.36 ng	327673	Phenanthrene-d10	17.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Tridecanoic acid	214	C13H26O2	000638-53-9	64
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Dodecanoic acid	200	C12H24O2	000143-07-7	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM080918\
 Data File : BM016279.D
 Acq On : 09 Aug 2018 13:37
 Operator : SJ/JU
 Sample : J4356-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 MW-12

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM072318.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,4-Dioxane, 2,5-...	4.66	28.8	ng	608598	1	8.13	421992	20.0
unknown7.66	7.66	84.8	ng	1789390	1	8.13	421992	20.0
unknown11.82	11.82	11.8	ng	304741	2	10.95	514887	20.0
1,2,3,4,4a,5,6,8a...	12.55	17.0	ng	438106	2	10.95	514887	20.0
1-Decalone (cis-t...	12.76	9.1	ng	233207	2	10.95	514887	20.0
Tricyclo[4.4.1.0(...	13.26	8.4	ng	283510	3	14.77	671685	20.0
unknown13.45	13.45	9.9	ng	331412	3	14.77	671685	20.0
2-Azetidinone, 3,...	14.35	9.8	ng	328974	3	14.77	671685	20.0
1-Methyl-3-ethyla...	15.28	10.5	ng	353800	3	14.77	671685	20.0
unknown15.36	15.36	11.0	ng	370042	3	14.77	671685	20.0
unknown15.57	15.57	11.0	ng	368511	3	14.77	671685	20.0
Phenol, m-tert-bu...	16.69	17.3	ng	423966	4	17.50	490488	20.0
unknown16.73	16.73	9.5	ng	233816	4	17.50	490488	20.0
Acetamide, N-(3-m...	16.89	22.8	ng	558804	4	17.50	490488	20.0
Phenol, 4-(1,1-di...	16.96	15.5	ng	381077	4	17.50	490488	20.0
5H-PYRROLO(3,2-D)...	17.03	9.4	ng	231300	4	17.50	490488	20.0
n-Hexadecanoic acid	18.37	13.4	ng	327673	4	17.50	490488	20.0