

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
 Data File : BF112910.D
 Acq On : 7 Mar 2019 4:49
 Operator : JU/SJ
 Sample : K1705-16
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-028-B101-022719

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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	5.345	549	554	557	rBV	3725952	3536694	90.32%	5.459%
2	6.016	664	668	672	rBV	765899	650286	16.61%	1.004%
3	6.186	690	697	700	rBV	301906	297050	7.59%	0.459%
4	6.369	723	728	734	rBV	3878337	3864697	98.69%	5.966%
5	6.439	737	740	744	rVB	1281556	1025384	26.18%	1.583%
6	6.498	746	750	754	rBV	3922103	3915936	100.00%	6.045%
7	6.692	780	783	786	rVB	123335	95458	2.44%	0.147%
8	6.734	786	790	793	rBV	1263724	1127977	28.80%	1.741%
9	6.857	808	811	813	rBV	168008	131379	3.35%	0.203%
10	6.886	813	816	820	rVB	3295328	2893825	73.90%	4.467%
11	7.286	880	884	897	rBV	2310820	2357186	60.19%	3.639%
12	8.010	1003	1007	1014	rBV	1421358	1338280	34.18%	2.066%
13	8.592	1103	1106	1108	rBV	118641	88051	2.25%	0.136%
14	9.086	1186	1190	1198	rBV	4118761	3790151	96.79%	5.851%
15	9.145	1198	1200	1205	rVV2	71312	117462	3.00%	0.181%
16	9.210	1209	1211	1214	rVV3	78206	80022	2.04%	0.124%
17	9.239	1214	1216	1223	rVB	58674	52822	1.35%	0.082%
18	9.427	1245	1248	1251	rBV2	100951	83552	2.13%	0.129%
19	9.480	1251	1257	1261	rVV	297393	381640	9.75%	0.589%
20	9.527	1261	1265	1269	rVB2	236938	237810	6.07%	0.367%
21	9.763	1302	1305	1308	rVB	1467971	1323508	33.80%	2.043%
22	9.792	1308	1310	1320	rVB4	112820	182188	4.65%	0.281%
23	9.904	1323	1329	1333	rBV3	61130	78854	2.01%	0.122%
24	9.969	1333	1340	1344	rBV4	28349	40958	1.05%	0.063%
25	10.033	1348	1351	1358	rBV	156280	150359	3.84%	0.232%
26	10.174	1370	1375	1378	rBV4	32220	41550	1.06%	0.064%
27	10.304	1395	1397	1404	rVB	56968	57188	1.46%	0.088%
28	10.545	1433	1438	1448	rBV	2469136	2480677	63.35%	3.829%
29	10.616	1448	1450	1454	rVB	58851	53715	1.37%	0.083%
30	11.198	1544	1549	1552	rBV5	34462	49127	1.25%	0.076%
31	11.239	1552	1556	1558	rVV	1390724	1367146	34.91%	2.110%
32	11.257	1558	1559	1564	rVV	293048	255441	6.52%	0.394%
33	11.310	1566	1568	1573	rVB	54727	53418	1.36%	0.082%
34	11.469	1591	1595	1602	rBV2	21146	39722	1.01%	0.061%

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Integrator: RTE

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35	11.704	1630	1635	1638	rBV6	22201	39337	1.00%	0.061%
36	11.739	1638	1641	1643	rVV	59931	56942	1.45%	0.088%
37	11.774	1643	1647	1656	rVV3	677744	801832	20.48%	1.238%
38	11.845	1656	1659	1662	rVV	77894	107610	2.75%	0.166%
39	11.868	1662	1663	1668	rVB	50563	43861	1.12%	0.068%
40	12.051	1692	1694	1700	rVB5	35164	40787	1.04%	0.063%
41	12.286	1728	1734	1737	rBV	54514	72756	1.86%	0.112%
42	12.368	1745	1748	1753	rVB4	34401	42620	1.09%	0.066%
43	12.439	1757	1760	1764	rBV	332428	334421	8.54%	0.516%
44	12.486	1765	1768	1775	rVV7	34980	80137	2.05%	0.124%
45	12.557	1777	1780	1791	rVV2	256580	344023	8.79%	0.531%
46	12.668	1794	1799	1804	rBV	313965	352167	8.99%	0.544%
47	12.815	1820	1824	1828	rBV	3522577	3273759	83.60%	5.053%
48	12.892	1832	1837	1840	rBV4	38328	49363	1.26%	0.076%
49	12.974	1844	1851	1853	rBV6	37865	66779	1.71%	0.103%
50	12.998	1853	1855	1858	rVB	47987	43566	1.11%	0.067%
51	13.045	1859	1863	1864	rBV3	34845	40453	1.03%	0.062%
52	13.063	1864	1866	1869	rVB	54575	41960	1.07%	0.065%
53	13.098	1869	1872	1880	rVB2	68299	73003	1.86%	0.113%
54	13.404	1921	1924	1930	rVB2	100250	108338	2.77%	0.167%
55	13.498	1937	1940	1946	rBV2	48768	76444	1.95%	0.118%
56	13.610	1956	1959	1962	rBV2	29786	41743	1.07%	0.064%
57	13.727	1973	1979	1986	rBV2	519554	690667	17.64%	1.066%
58	13.804	1989	1992	1996	rVV	92517	95166	2.43%	0.147%
59	13.862	1997	2002	2005	rVV	1782651	1907778	48.72%	2.945%
60	13.886	2005	2006	2012	rVB	191232	140392	3.59%	0.217%
61	14.045	2029	2033	2041	rBV3	496816	679060	17.34%	1.048%
62	14.115	2041	2045	2050	rVV5	82764	126200	3.22%	0.195%
63	14.286	2065	2074	2077	rBV	1730658	2020532	51.60%	3.119%
64	14.321	2077	2080	2081	rVV	229217	215173	5.49%	0.332%
65	14.345	2081	2084	2088	rVV3	1559052	2213365	56.52%	3.417%
66	14.398	2091	2093	2096	rVV	1225872	1232392	31.47%	1.902%
67	14.427	2096	2098	2101	rVV2	450872	616940	15.75%	0.952%
68	14.457	2101	2103	2107	rVV	671550	582689	14.88%	0.899%
69	14.498	2107	2110	2115	rVV	633692	659172	16.83%	1.018%
70	14.586	2122	2125	2128	rBV	1499919	1295206	33.08%	1.999%
71	14.645	2131	2135	2140	rVV2	1009470	1231685	31.45%	1.901%

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 Sampling : 1 Min Area: 3 % of largest Peak
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 Stop Thrs : 0 Peak Location: TOP

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72	14.692	2140	2143	2146	rVV2	229914	242070	6.18%	0.374%
73	14.721	2146	2148	2151	rVV	194941	200973	5.13%	0.310%
74	14.774	2151	2157	2160	rVV3	935640	1570064	40.09%	2.424%
75	14.815	2160	2164	2170	rVV4	2035788	3007267	76.80%	4.642%
76	14.892	2171	2177	2181	rVB3	555413	819689	20.93%	1.265%
77	14.939	2181	2185	2186	rBV	355516	398466	10.18%	0.615%
78	14.957	2186	2188	2191	rVV	929871	1040444	26.57%	1.606%
79	14.986	2191	2193	2199	rVB	335219	423405	10.81%	0.654%
80	15.139	2216	2219	2223	rBV2	287738	334495	8.54%	0.516%
81	15.204	2227	2230	2236	rVV	154084	321222	8.20%	0.496%
82	15.268	2236	2241	2245	rVV	1272521	1597924	40.81%	2.467%
83	15.315	2245	2249	2253	rVB	740692	906214	23.14%	1.399%
84	15.498	2277	2280	2283	rVB	81108	91198	2.33%	0.141%
85	15.715	2313	2317	2322	rBV	622086	889234	22.71%	1.373%
86	15.774	2323	2327	2331	rBV4	113493	205334	5.24%	0.317%
87	16.186	2392	2397	2407	rVB2	253201	450513	11.50%	0.695%
88	16.733	2485	2490	2496	rVB	113948	206087	5.26%	0.318%

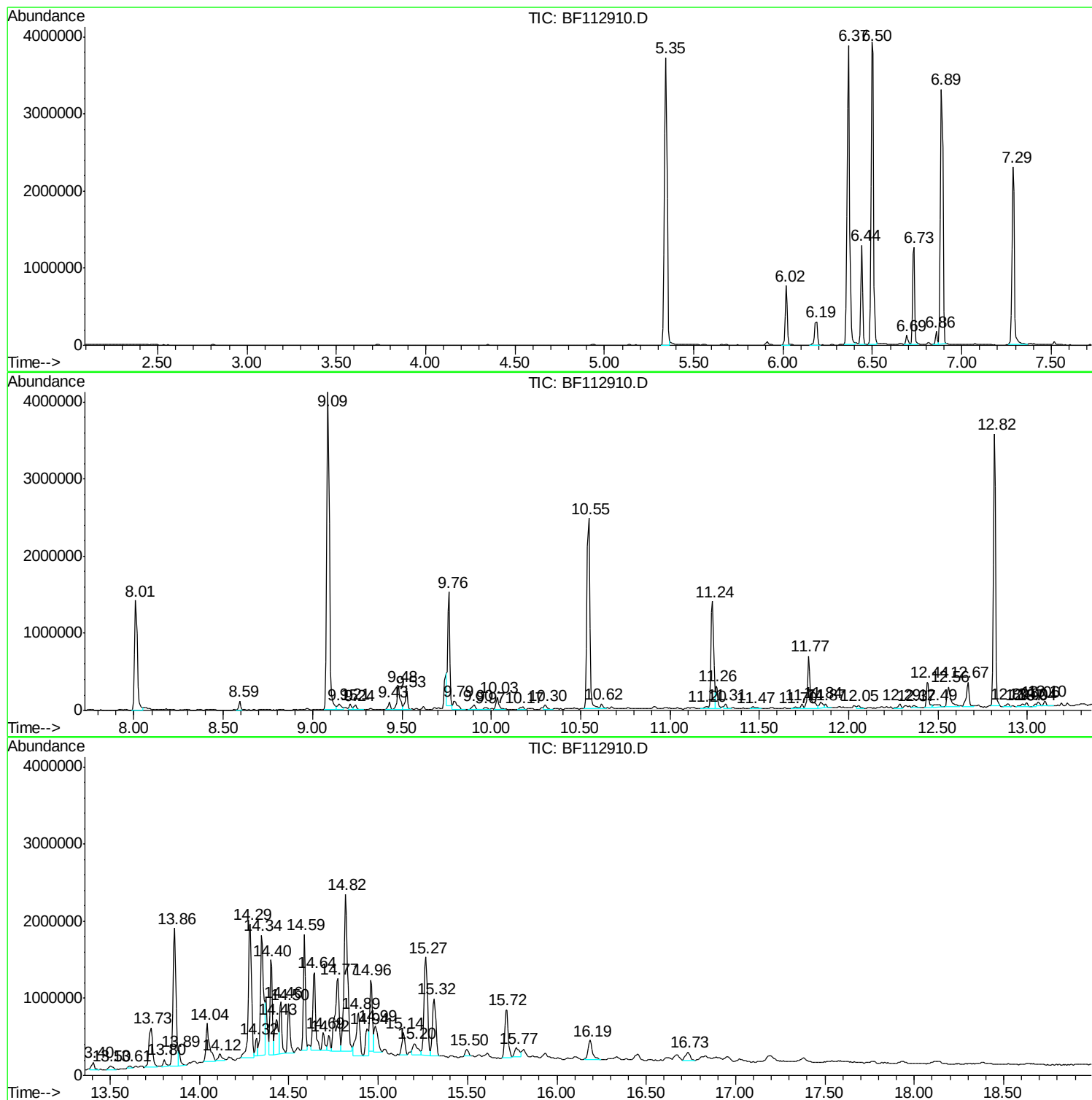
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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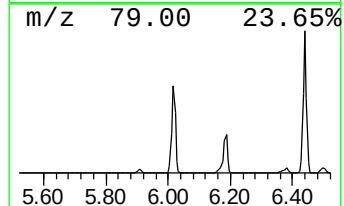
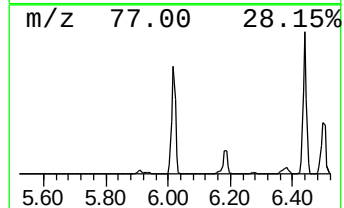
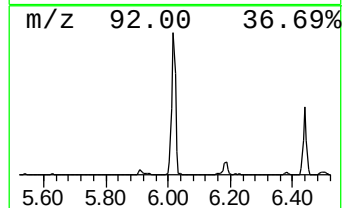
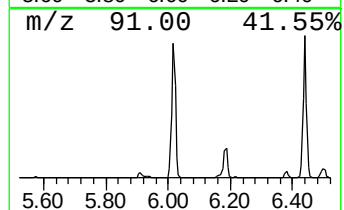
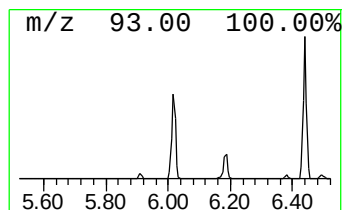
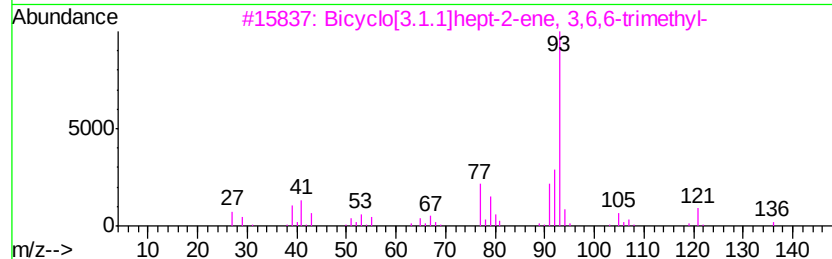
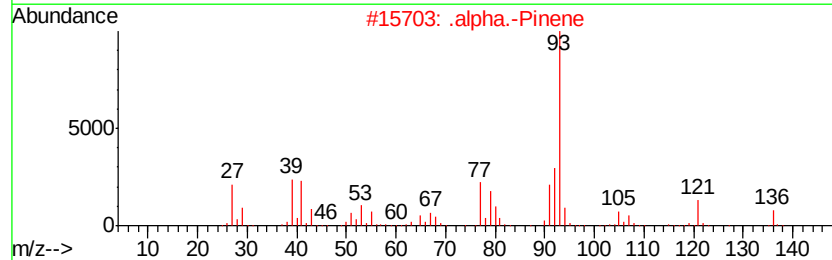
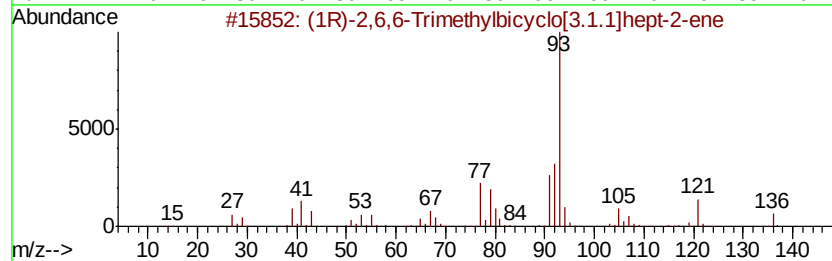
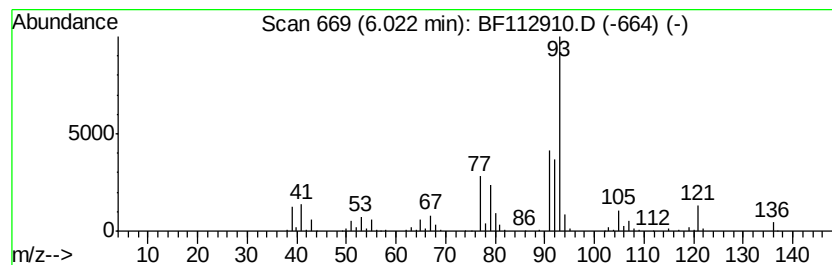
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.02	11.53 ng	650286	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1R)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	136	C10H16	007785-70-8	96
2		.alpha.-Pinene	136	C10H16	000080-56-8	94
3		Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	136	C10H16	004889-83-2	94
4		trans-.beta.-Ocimene	136	C10H16	003779-61-1	91
5		1,3,6-Octatriene, 3,7-dimethyl-, (1E,3E,5E)-	136	C10H16	003338-55-4	91



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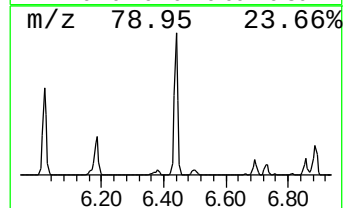
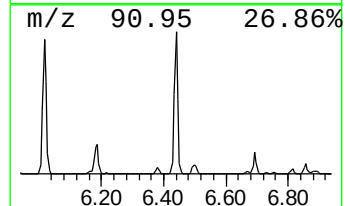
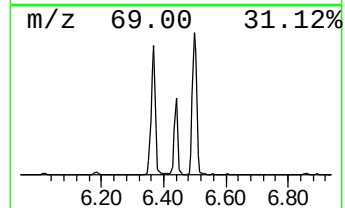
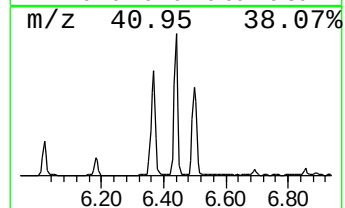
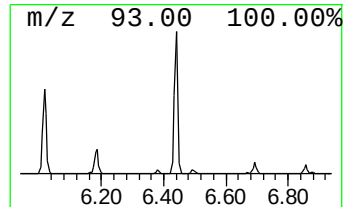
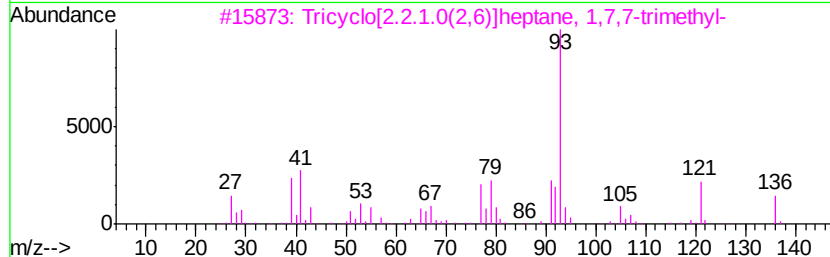
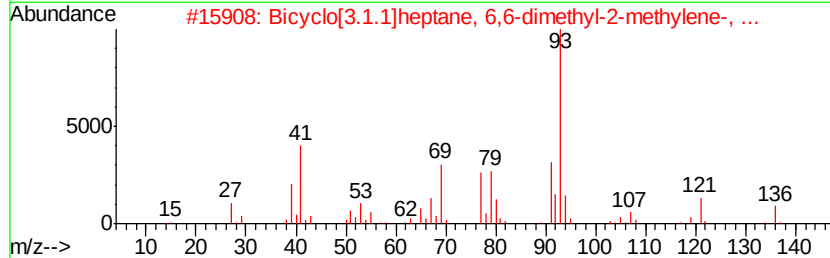
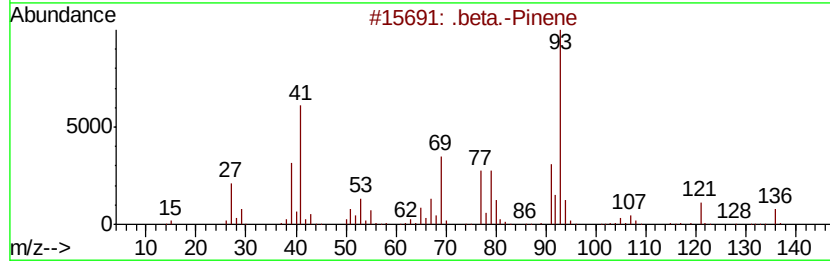
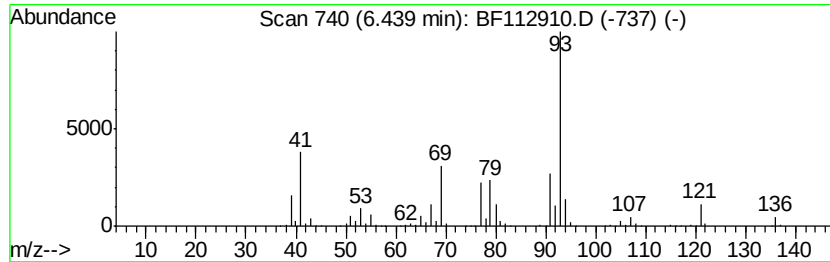
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 .beta.-Pinene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
6.44	18.18 ng	1025380	1,4-Dichlorobenzene-d4	6.73		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Pinene	136	C10H16	000127-91-3	93
2		Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	91
3		Tricvclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
4		Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	86
5		.alpha.-Pinene	136	C10H16	000080-56-8	83



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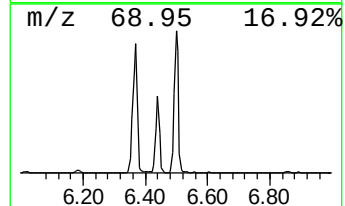
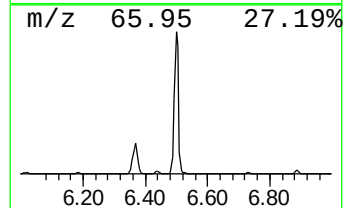
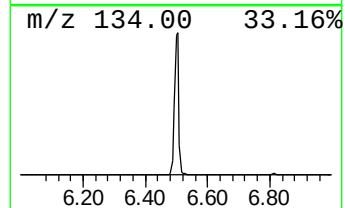
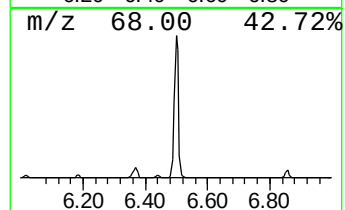
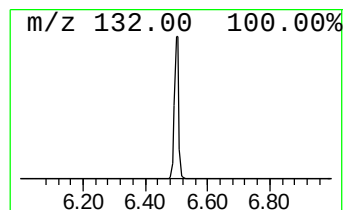
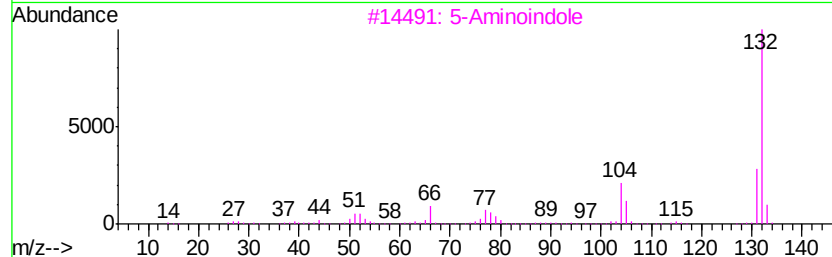
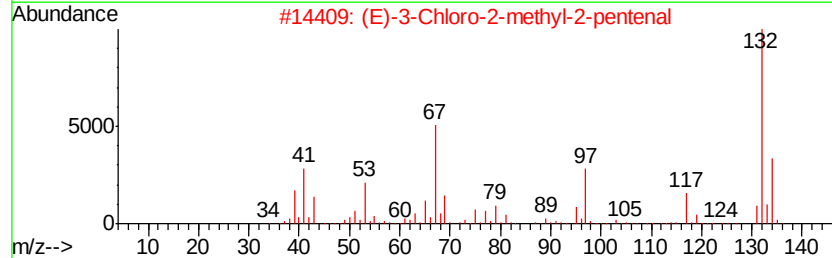
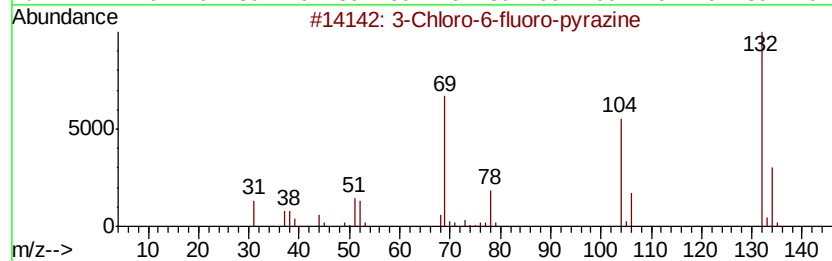
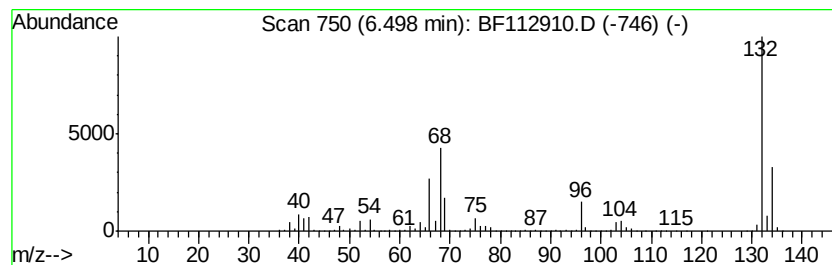
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	69.43 ng	3915940	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Amphetaminil	250	C17H18N2	017590-01-1	10



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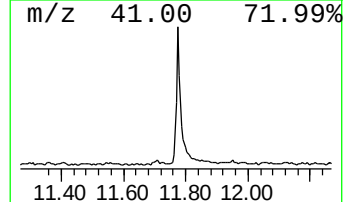
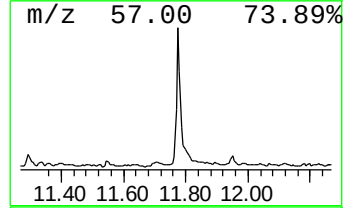
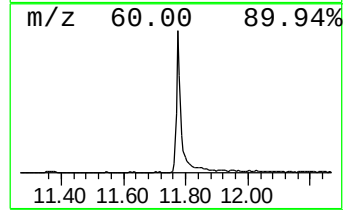
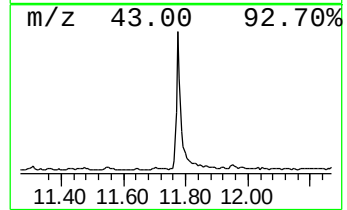
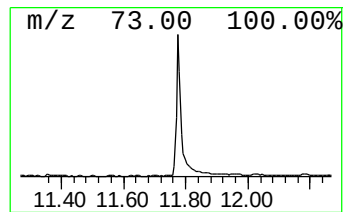
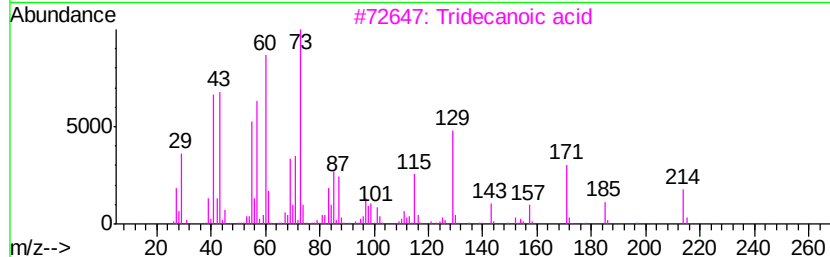
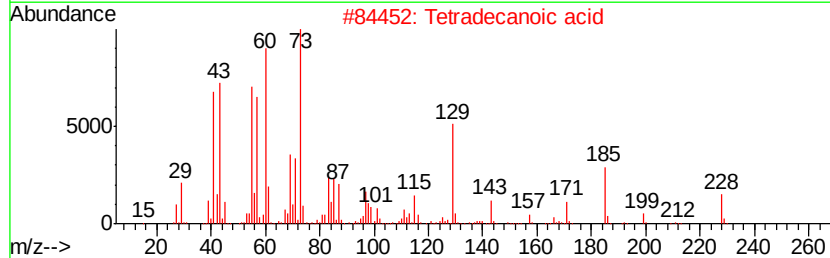
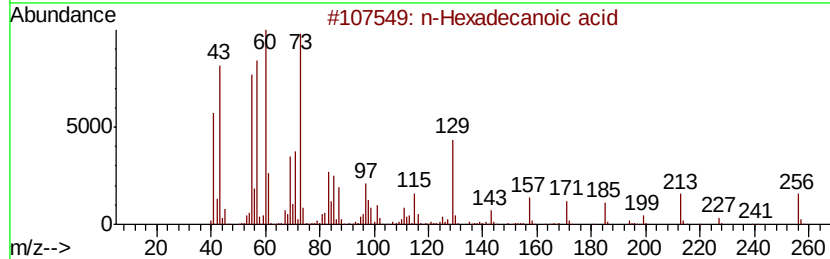
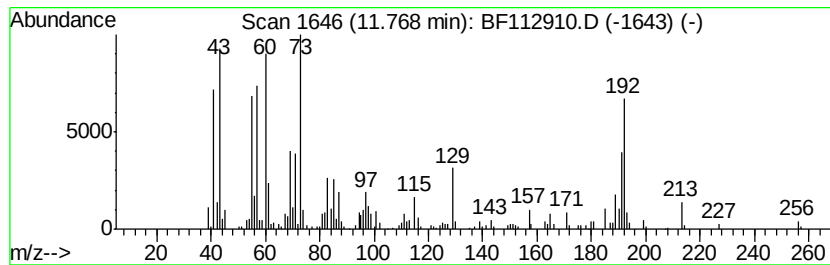
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 5 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	11.73 ng	801832	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3		Tridecanoic acid	214	C13H26O2	000638-53-9	93
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112910.D
Acq On : 7 Mar 2019 4:49
Operator : JU/SJ
Sample : K1705-16
Misc :
ALS Vial : 28 Sample Multiplier: 1

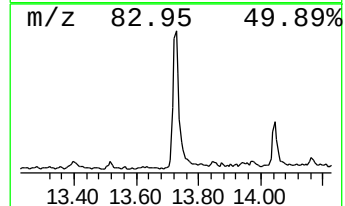
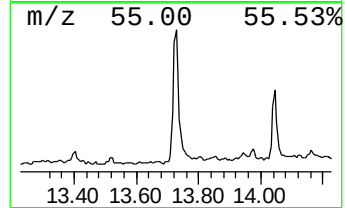
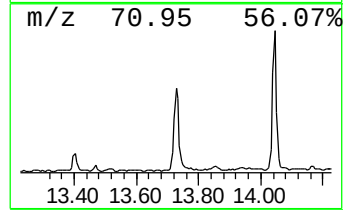
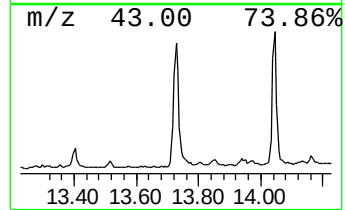
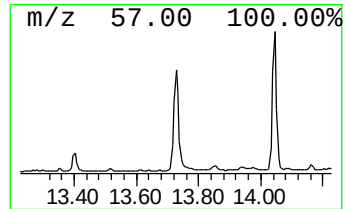
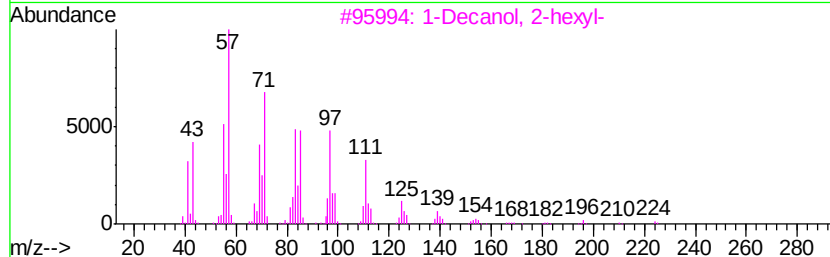
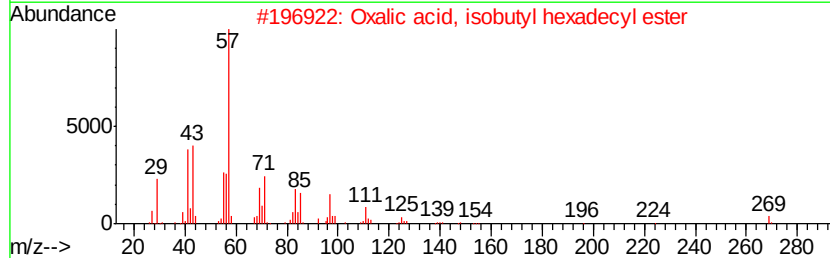
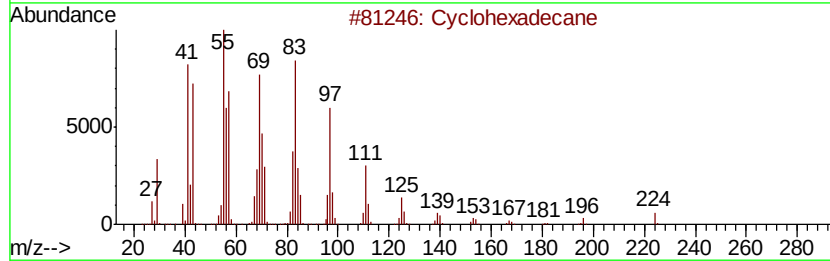
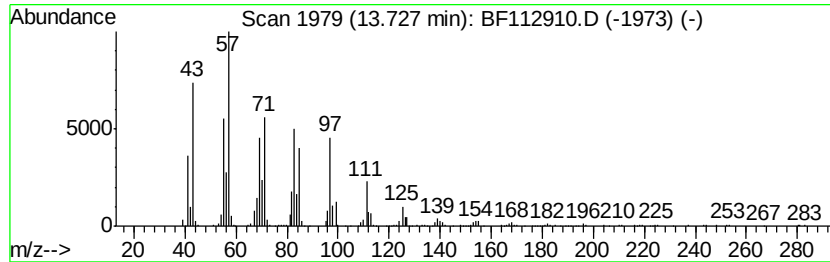
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	7.24 ng	690667	Chrysene-d12	13.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 96
2		Oxalic acid, isobutyl hexadecyl ...	370 C22H42O4	1000309-38-1 91
3		1-Decanol, 2-hexyl-	242 C16H34O	002425-77-6 91
4		Oxalic acid, isobutyl tetradecyl...	342 C20H38O4	1000309-37-9 91
5		1-Hexadecanesulfonyl chloride	324 C16H33ClO2S	038775-38-1 87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112910.D
Acq On : 7 Mar 2019 4:49
Operator : JU/SJ
Sample : K1705-16
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ClientSampleId :
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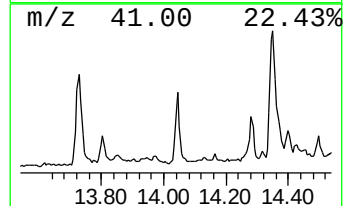
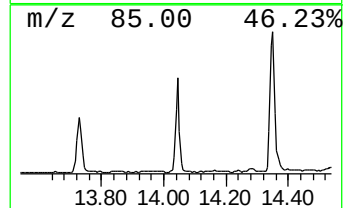
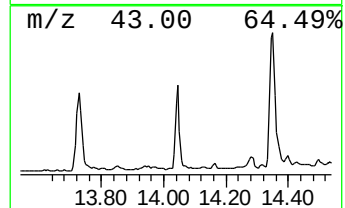
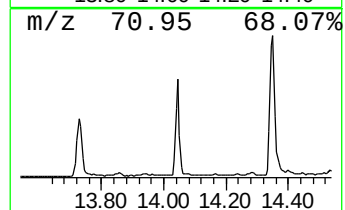
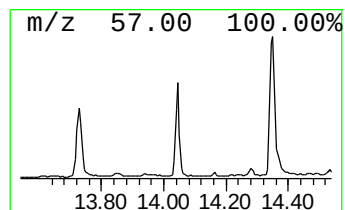
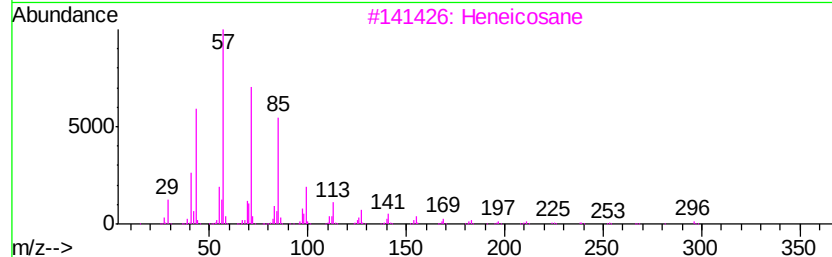
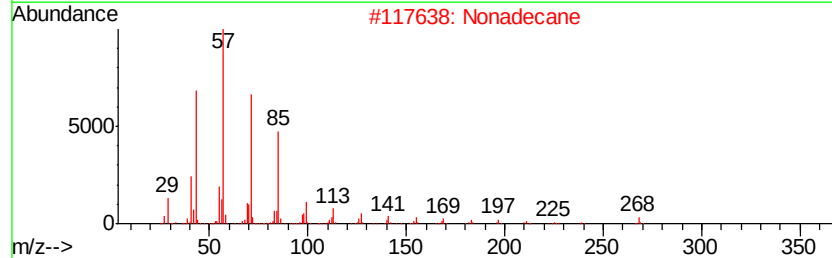
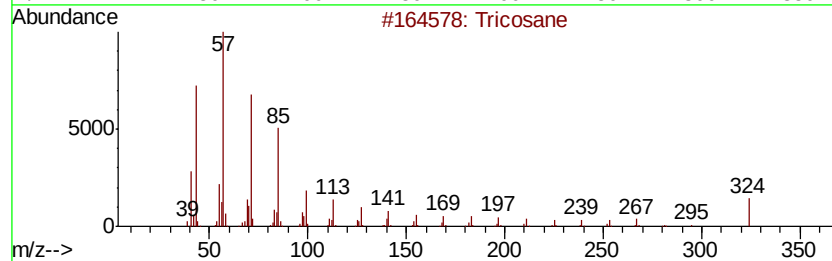
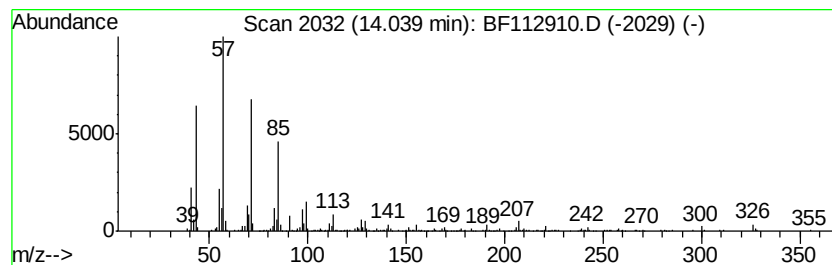
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tricosane Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	7.12 ng	679060	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosane	324	C23H48	000638-67-5	94
2		Nonadecane	268	C19H40	000629-92-5	94
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heptadecane	240	C17H36	000629-78-7	83
5		Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112910.D
Acq On : 7 Mar 2019 4:49
Operator : JU/SJ
Sample : K1705-16
Misc :
ALS Vial : 28 Sample Multiplier: 1

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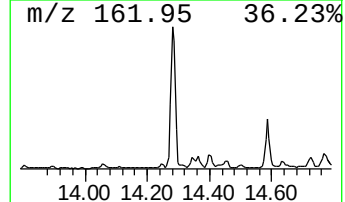
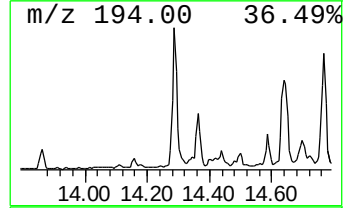
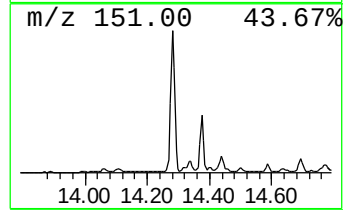
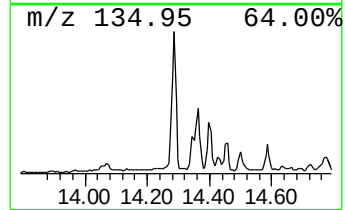
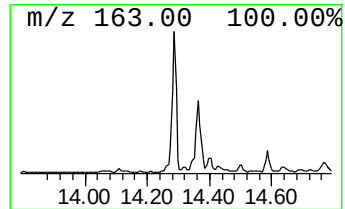
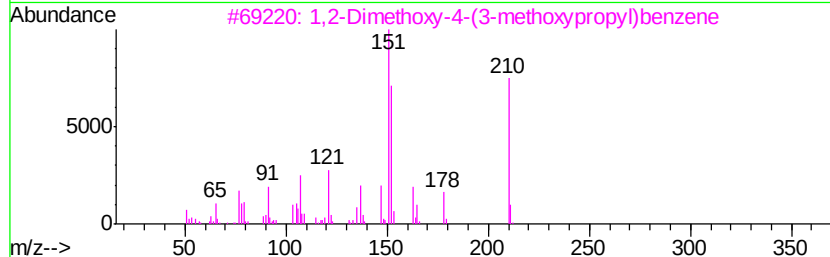
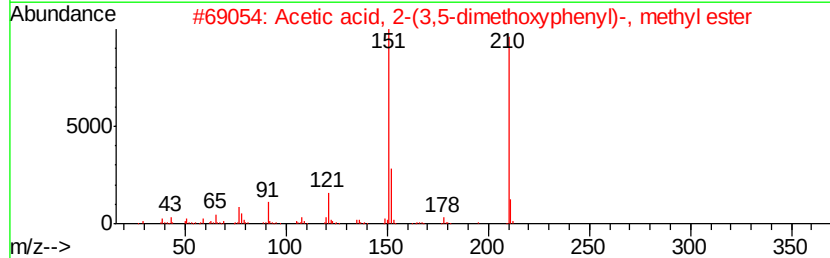
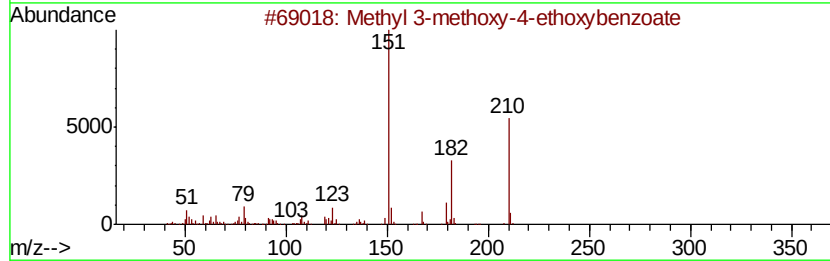
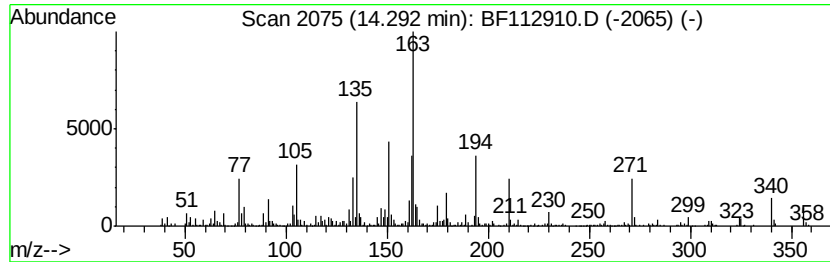
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown14.29 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	21.18 ng	2020530	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methyl 3-methoxy-4-ethoxybenzoate	210	C11H14O4	003535-24-8	35
2		Acetic acid, 2-(3,5-dimethoxyphenyl)-, methyl ester	210	C11H14O4	006512-32-9	25
3		1,2-Dimethoxy-4-(3-methoxypropyl)benzene	210	C12H18O3	1000313-34-9	25
4		1-(2-Ethoxycarbonyl-ethyl)-2-oxo-3-methoxybenzene	270	C14H22O5	1000193-00-6	25
5		Benzeneacetic acid, 3,4-dimethoxyphenyl-, methyl ester	210	C11H14O4	015964-79-1	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
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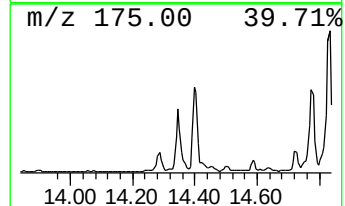
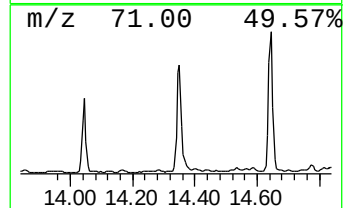
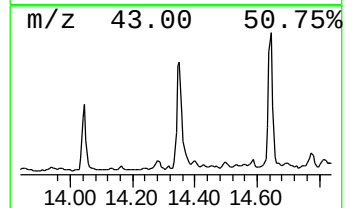
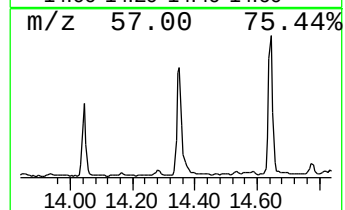
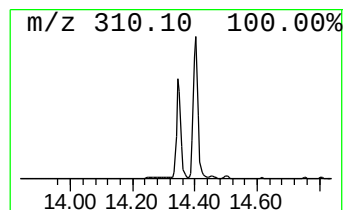
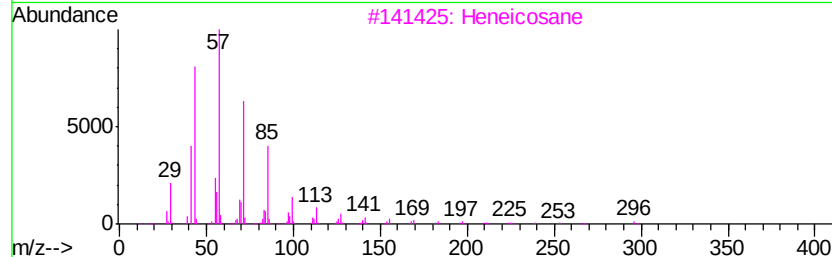
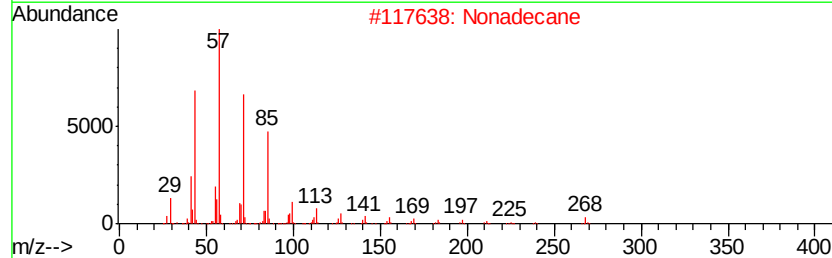
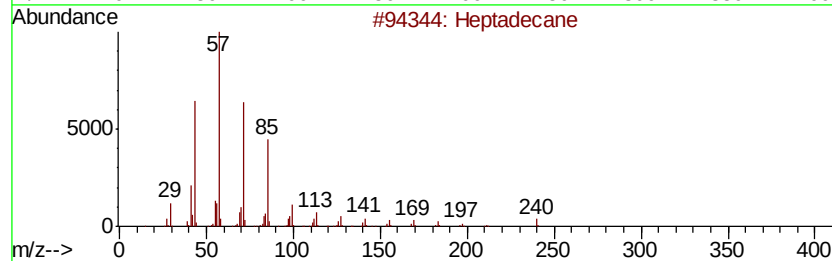
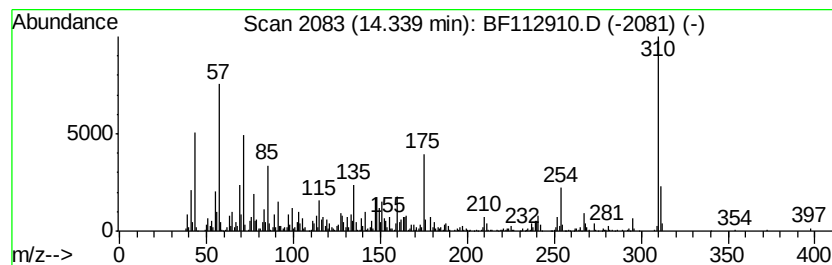
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	23.20 ng	2213370	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecane	240	C17H36	000629-78-7	91
2		Nonadecane	268	C19H40	000629-92-5	78
3		Heneicosane	296	C21H44	000629-94-7	68
4		Eicosane	282	C20H42	000112-95-8	64
5		Ferrocene, 1,2-diacetyl-1',4-(1,...	310	C17H18FeO2	041558-93-4	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
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Acq On : 7 Mar 2019 4:49
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Sample : K1705-16
Misc :
ALS Vial : 28 Sample Multiplier: 1

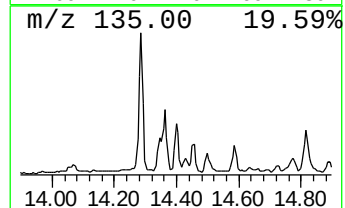
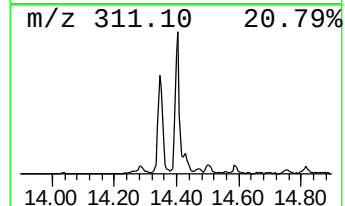
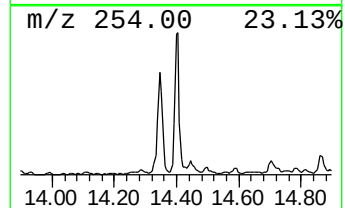
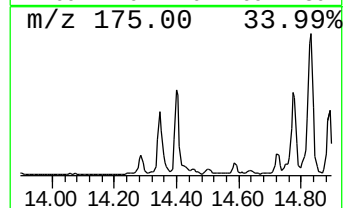
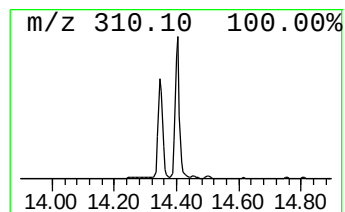
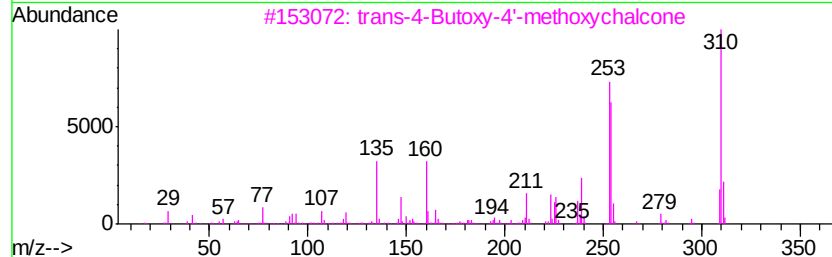
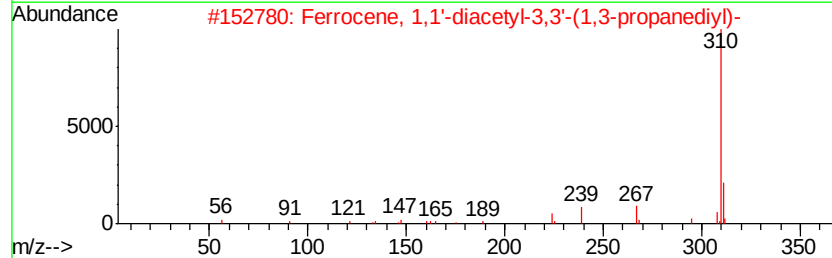
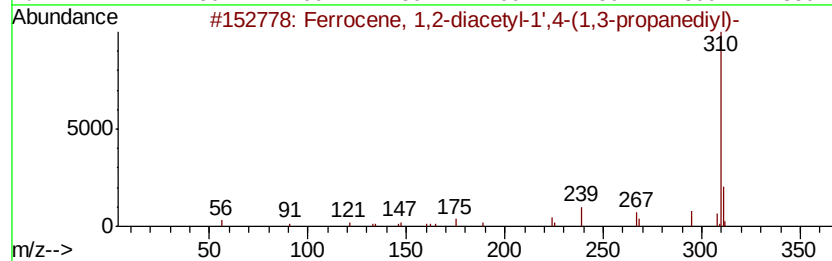
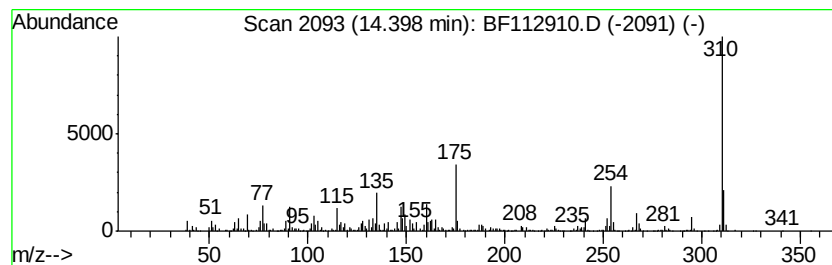
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Ferrocene, 1,2-diacetyl-1',... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.40	12.92 ng	1232390	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ferrocene, 1,2-diacetyl-1',4-(1,...	310	C17H18FeO2	041558-93-4	64
2	Ferrocene, 1,1'-diacetyl-3,3'-(1...	310	C17H18FeO2	041558-92-3	60
3	trans-4-Butoxy-4'-methoxychalcone	310	C20H22O3	131887-84-8	53
4	Ferrocene, 1,1'-diacetyl-2,2'-(1...	310	C17H18FeO2	041558-91-2	49
5	Ferrocene, 1,1'-diacetyl-2,3'-(1...	310	C17H18FeO2	038548-79-7	46



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
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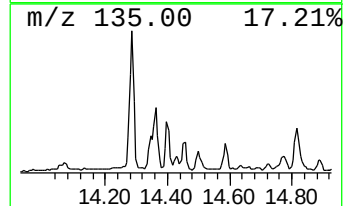
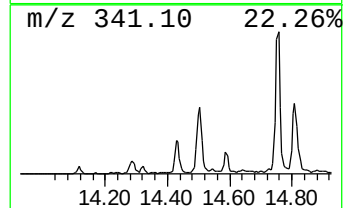
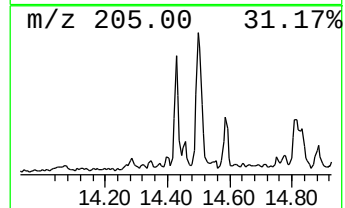
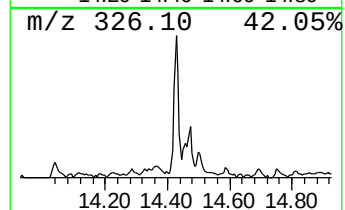
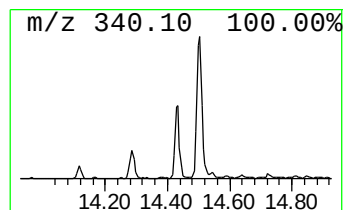
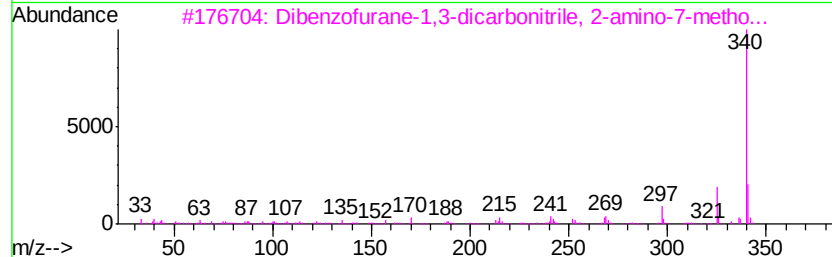
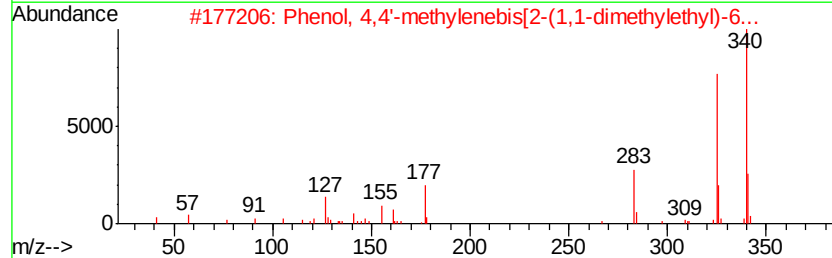
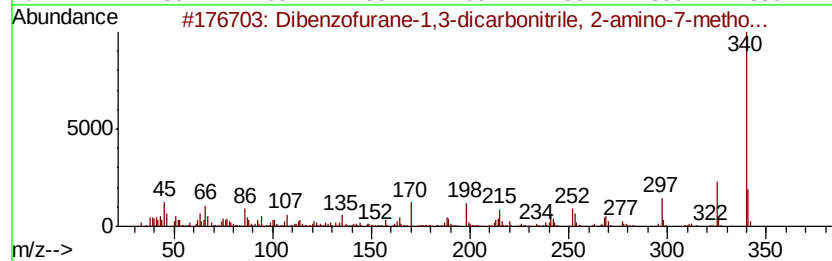
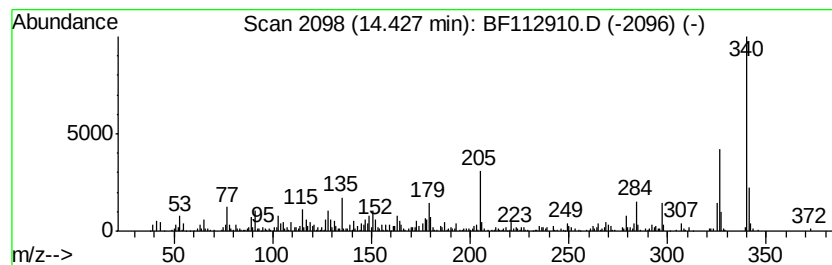
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dibenzofurane-1,3-dicarboni... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	6.47 ng	616940	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dibenzofurane-1,3-dicarbonitrile...	340	C20H12N4O2	330158-97-9	55
2		Phenol, 4,4'-methylenebis[2-(1,1...	340	C23H32O2	000096-65-1	49
3		Dibenzofurane-1,3-dicarbonitrile...	340	C20H12N4O2	328286-70-0	49
4		2,4-Di(2,2,6,6-tetramethyl-1,2,5...	341	C22H35N3	1000311-57-0	43
5		2-Phenyl-4,6-di(2-hydroxyphenyl)...	340	C22H16N2O2	052829-03-5	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112910.D
Acq On : 7 Mar 2019 4:49
Operator : JU/SJ
Sample : K1705-16
Misc :
ALS Vial : 28 Sample Multiplier: 1

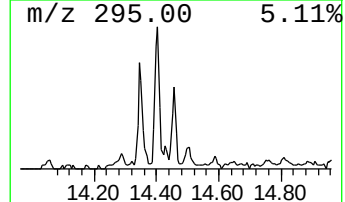
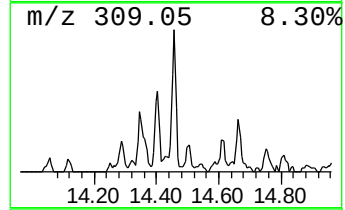
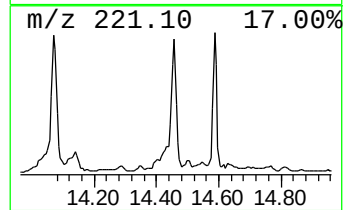
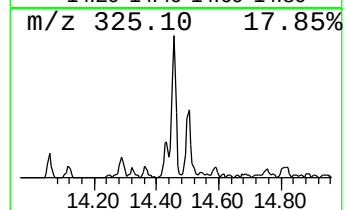
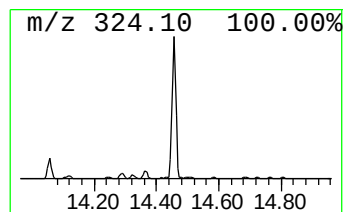
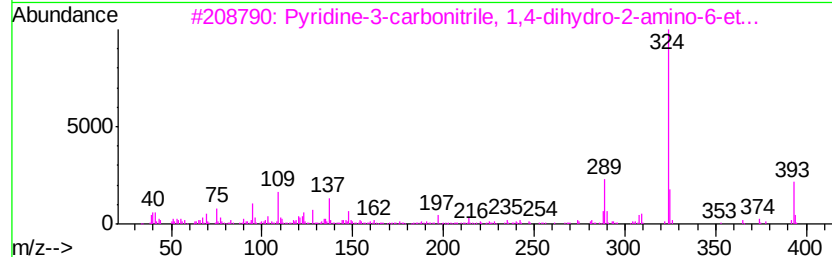
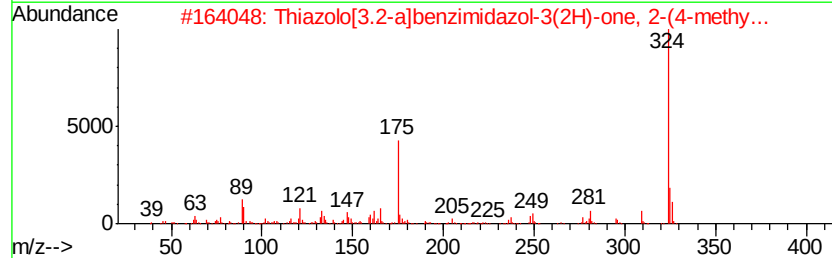
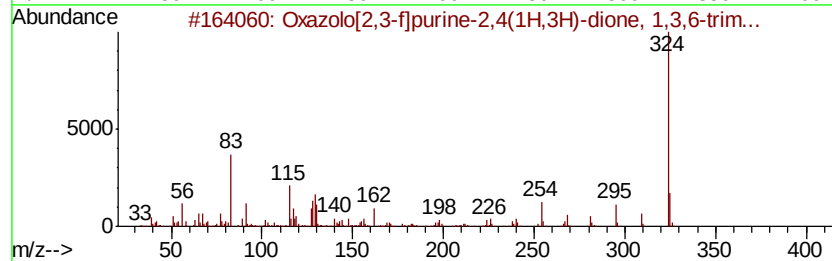
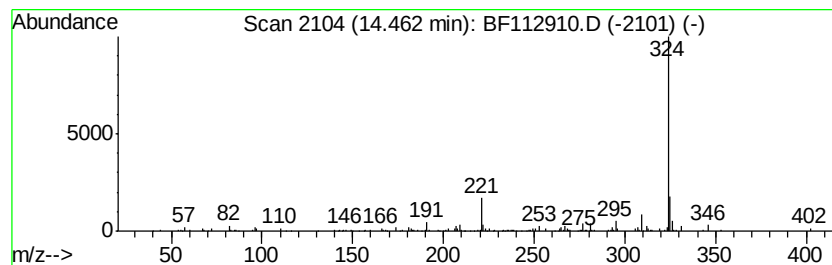
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Oxazolo[2,3-f]purine-2,4(1H... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.46	6.11 ng	582689	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazolo[2,3-f]purine-2,4(1H,3H)-...	324	C17H16N4O3	1000350-27-1	64
2	Thiazolo[3,2-a]benzimidazol-3(2H)...	324	C17H12N2OS2	311783-63-8	53
3	Pvridine-3-carbonitrile, 1,4-dih...	393	C17H14F7N3	1000273-85-8	53
4	Thieno[3,2-e]l[1,2,4]triazolo[1,5...	324	C16H12N4O2S	1000350-80-1	52
5	Thiazolo[3,2-a]benzimidazol-3(2H)...	324	C18H13FN2OS	294878-41-4	45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112910.D
Acq On : 7 Mar 2019 4:49
Operator : JU/SJ
Sample : K1705-16
Misc :
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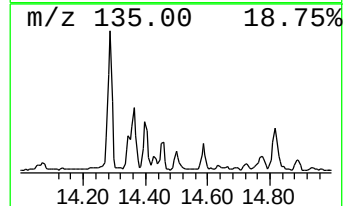
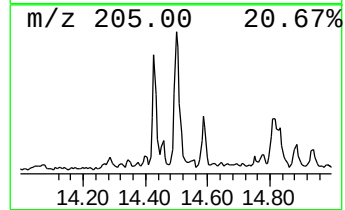
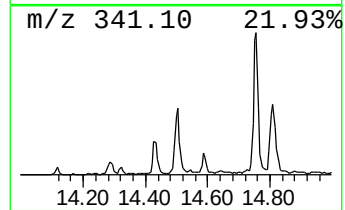
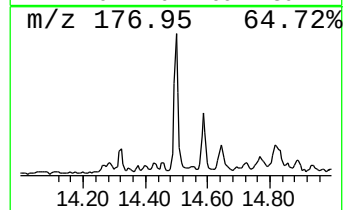
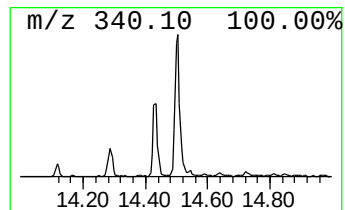
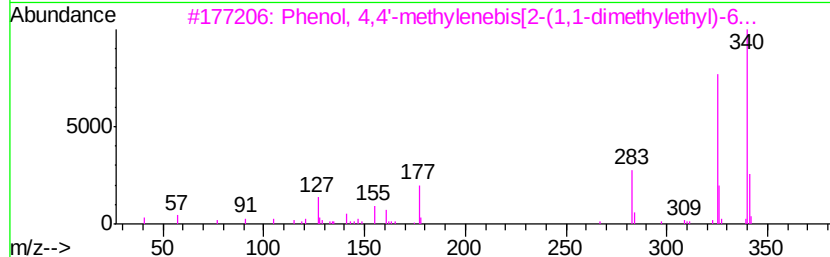
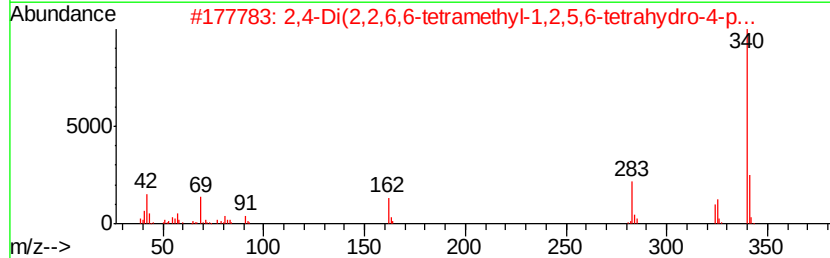
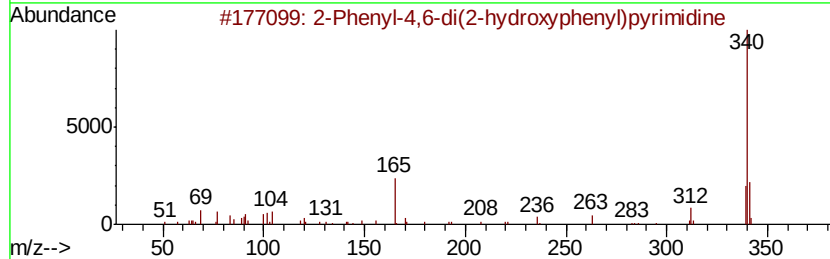
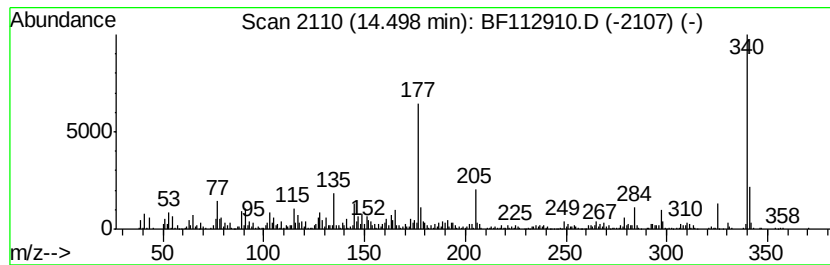
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ClientSampleId :
PST-028-B101-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown14.50 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.50	6.91 ng	659172	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenyl-4,6-di(2-hydroxyphenyl)...	340	C22H16N2O2	052829-03-5	46
2	2,4-Di(2,2,6,6-tetramethyl-1,2,5...	341	C22H35N3	1000311-57-0	46
3	Phenol, 4,4'-methylenebis[2-(1,1...	340	C23H32O2	000096-65-1	46
4	Naphtho[1,8-de]-1,3,2-dioxasilin...	340	C22H16O2Si	006398-61-4	38
5	6,13-Pentacenedione, 5,14-dihydr...	340	C22H12O4	068970-90-1	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112910.D
Acq On : 7 Mar 2019 4:49
Operator : JU/SJ
Sample : K1705-16
Misc :
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Instrument :
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ClientSampleId :
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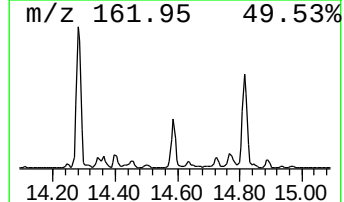
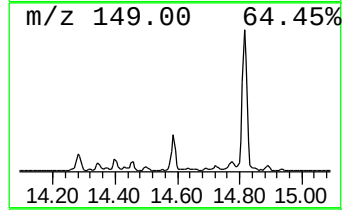
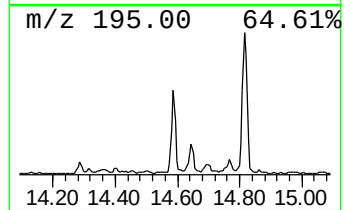
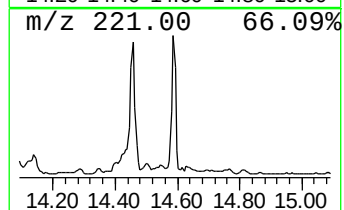
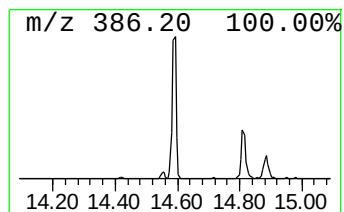
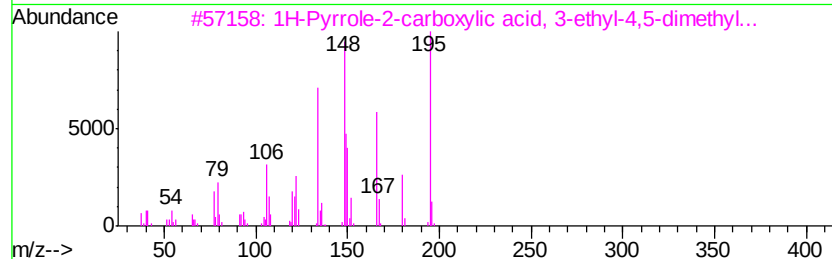
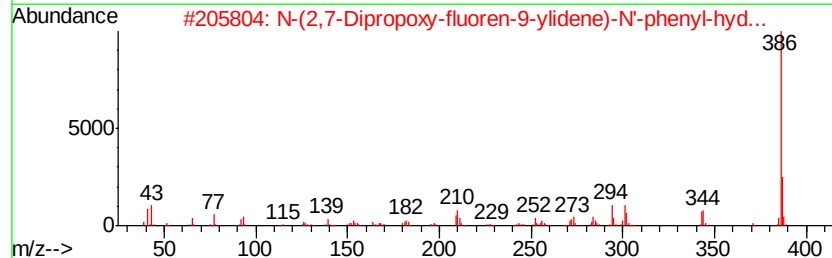
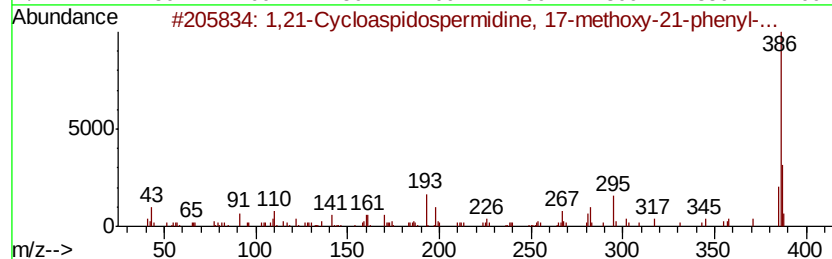
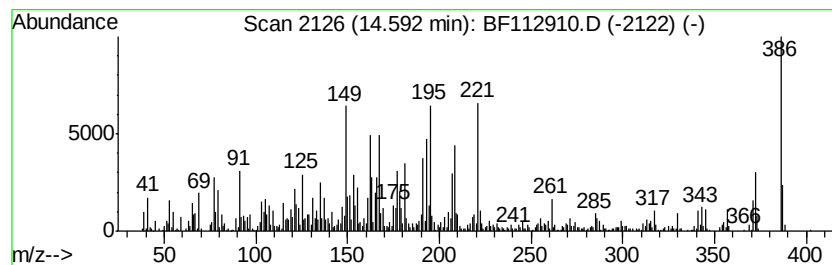
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown14.59 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	16.21 ng	1295210	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,21-Cycloaspidospermidine, 17-m...	386	C26H30N2O	036528-88-8	25
2		N-(2,7-Dipropoxy-fluoren-9-ylide...	386	C25H26N2O2	1000317-92-9	25
3		1H-Pyrrole-2-carboxylic acid, 3-...	195	C11H17N02	034549-93-4	25
4		5H-Pyrrolo[1,2-a]imidazole-3-car...	195	C9H13N3O2	1000338-27-0	18
5		4',6'-Bis(1,1-dimethylethyl)-4,4...	386	C28H34O	1000326-27-6	15



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
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Operator : JU/SJ
Sample : K1705-16
Misc :
ALS Vial : 28 Sample Multiplier: 1

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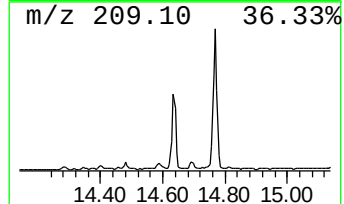
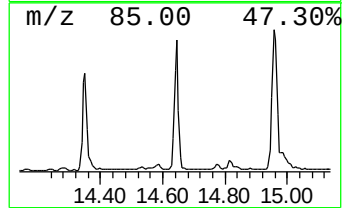
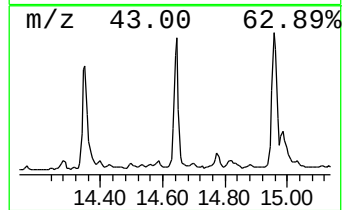
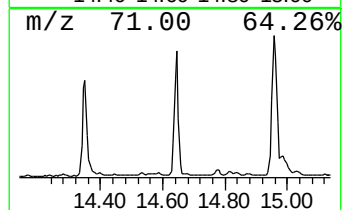
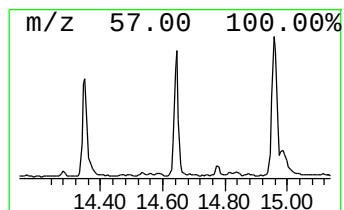
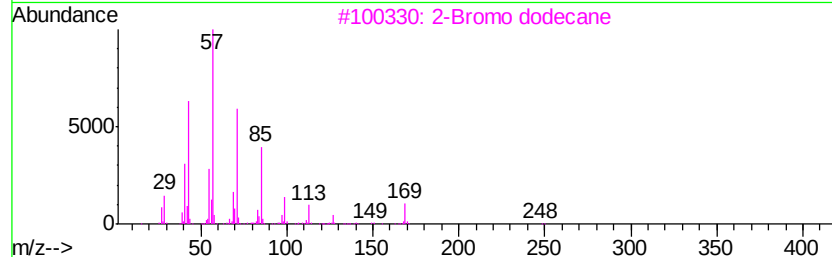
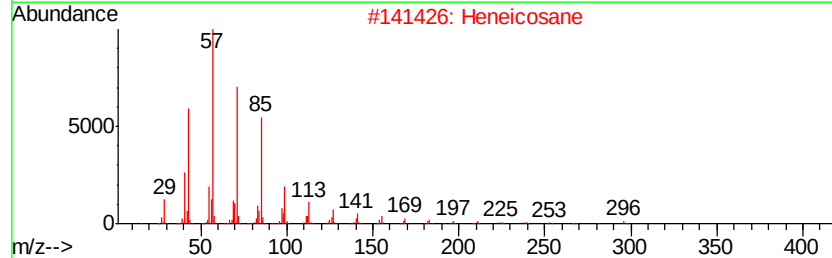
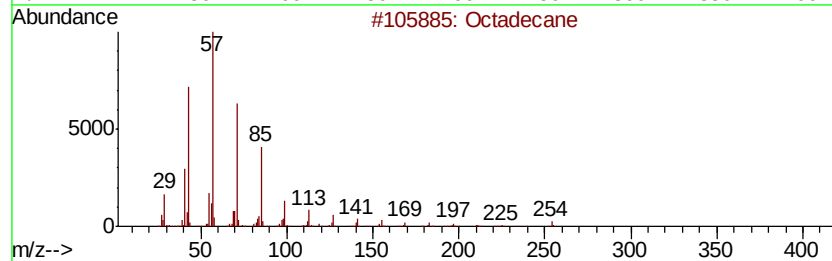
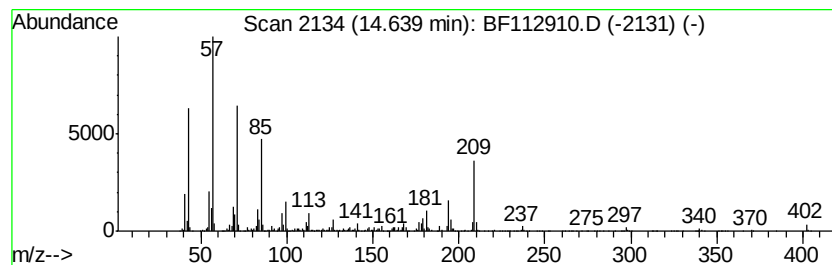
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Octadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	15.42 ng	1231690	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecane	254	C18H38	000593-45-3	95
2		Heneicosane	296	C21H44	000629-94-7	87
3		2-Bromo dodecane	248	C12H25Br	013187-99-0	86
4		Nonadecane, 2-methyl-	282	C20H42	001560-86-7	80
5		Decane, 1-iodo-	268	C10H21I	002050-77-3	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112910.D
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Operator : JU/SJ
Sample : K1705-16
Misc :
ALS Vial : 28 Sample Multiplier: 1

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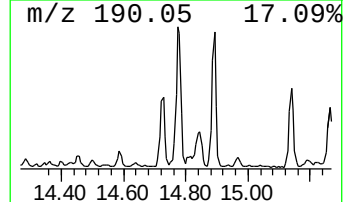
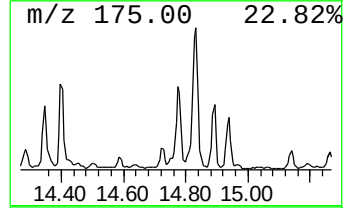
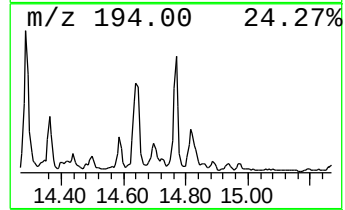
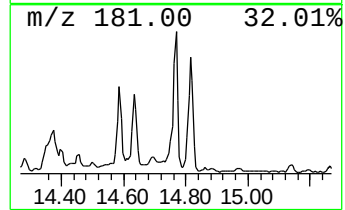
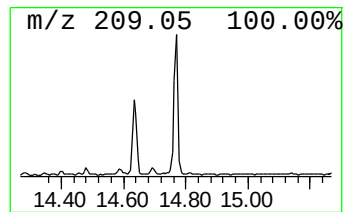
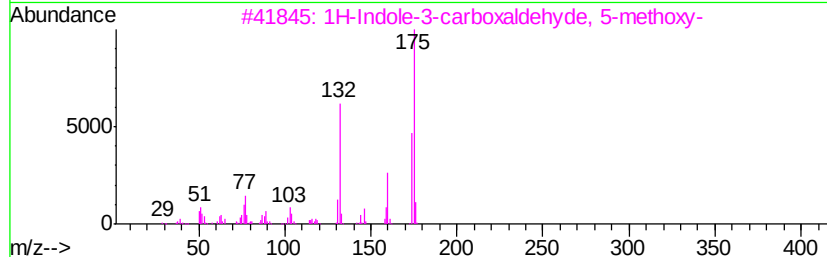
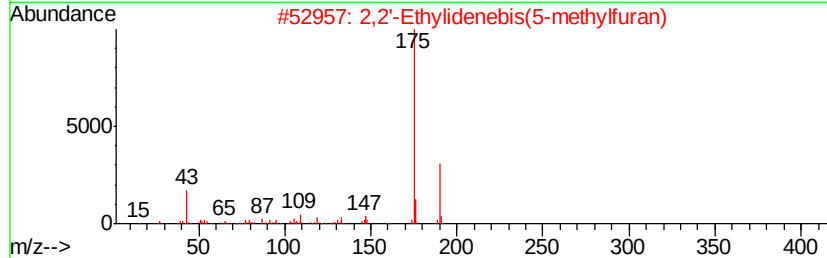
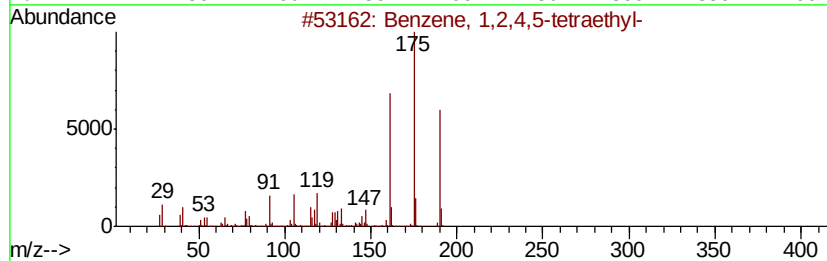
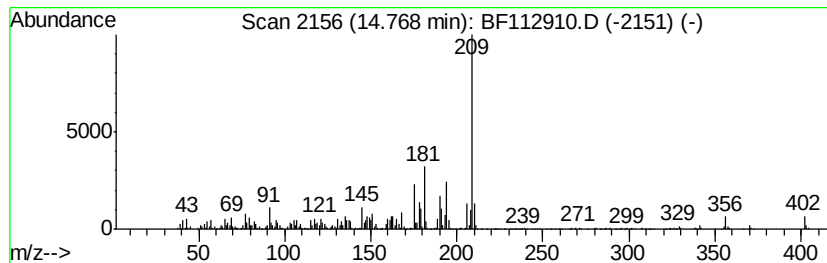
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown14.77 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	19.65 ng	1570060	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,4,5-tetraethyl-	190	C14H22	000635-81-4	38
2		2,2'-Ethylidenebis(5-methylfuran)	190	C12H14O2	003209-79-8	30
3		1H-Indole-3-carboxaldehyde, 5-me...	175	C10H9NO2	010601-19-1	25
4		3,5-Dichloro-4-hydroxybenzoic acid	206	C7H4Cl2O3	003336-41-2	25
5		Benzene, 1,4-dimethyl-2,5-bis(1-...	190	C14H22	010375-96-9	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
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Sample : K1705-16
Misc :
ALS Vial : 28 Sample Multiplier: 1

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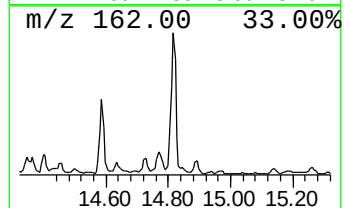
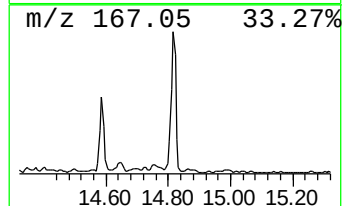
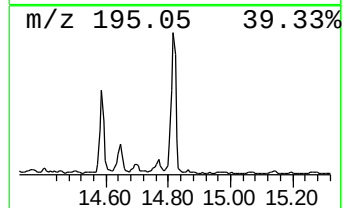
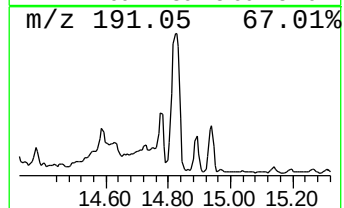
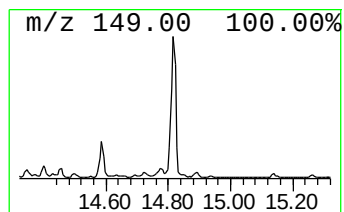
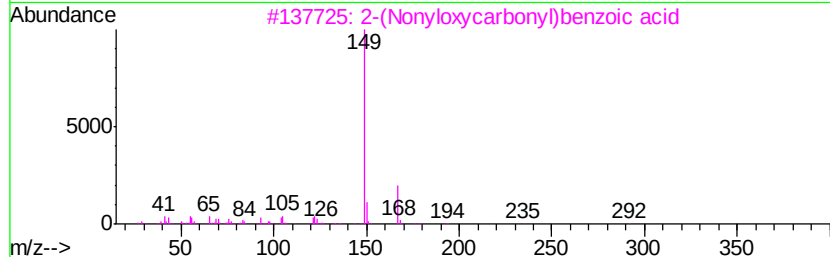
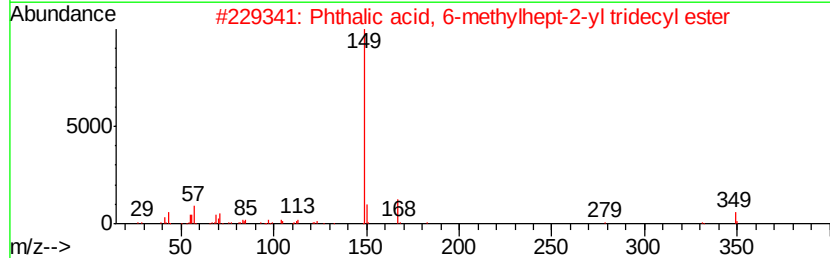
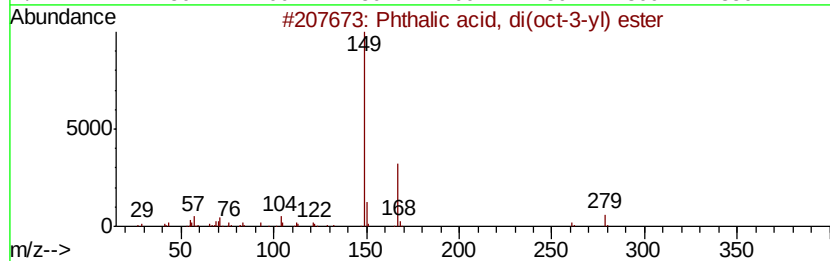
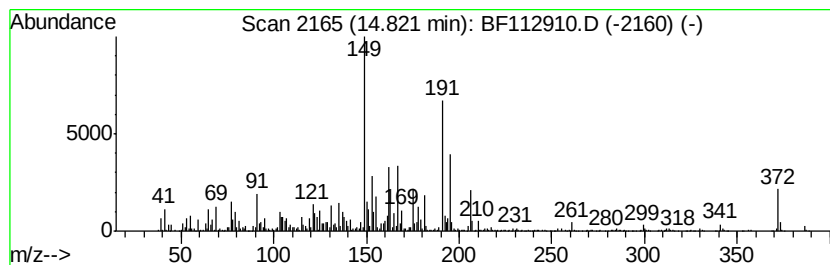
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown14.82 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	37.64 ng	3007270	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phthalic acid, di(oct-3-yl) ester	390	C24H38O4	1000377-72-3	35
2		Phthalic acid, 6-methylhept-2-yl...	460	C29H48O4	1000377-96-7	27
3		2-(Nonylloxycarbonyl)benzoic acid	292	C17H24O4	1000373-89-9	27
4		Phthalic acid, isopropyl propyl ...	250	C14H18O4	1000314-99-7	27
5		Phthalic acid, 3,4-dichloropheny...	422	C22H24Cl2O4	1000315-52-0	27



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112910.D
Acq On : 7 Mar 2019 4:49
Operator : JU/SJ
Sample : K1705-16
Misc :
ALS Vial : 28 Sample Multiplier: 1

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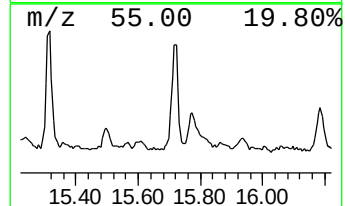
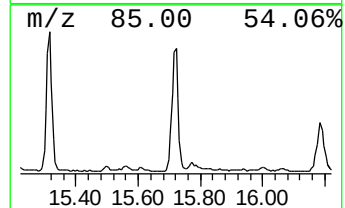
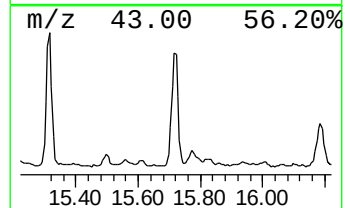
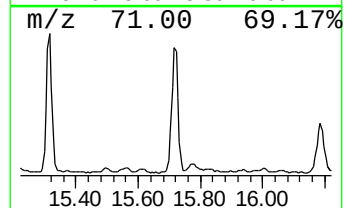
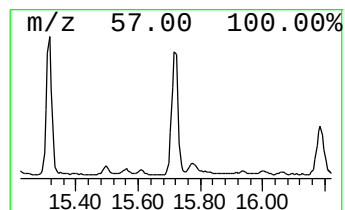
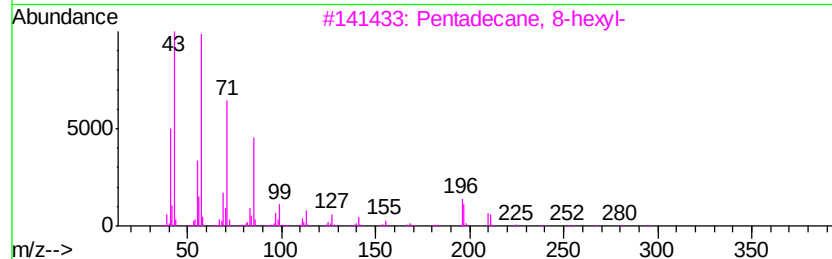
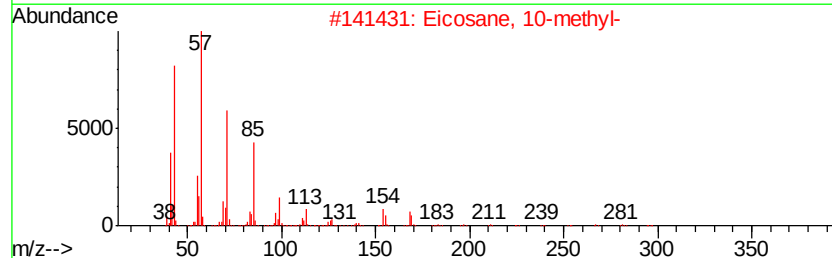
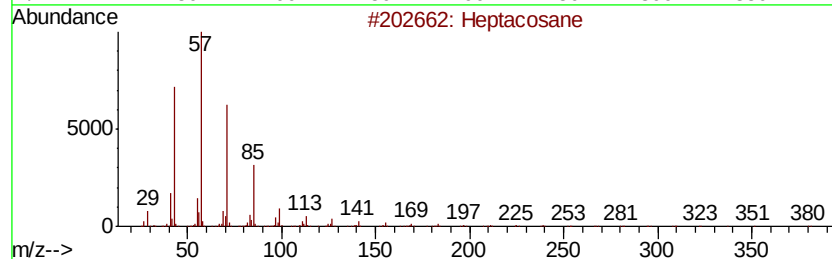
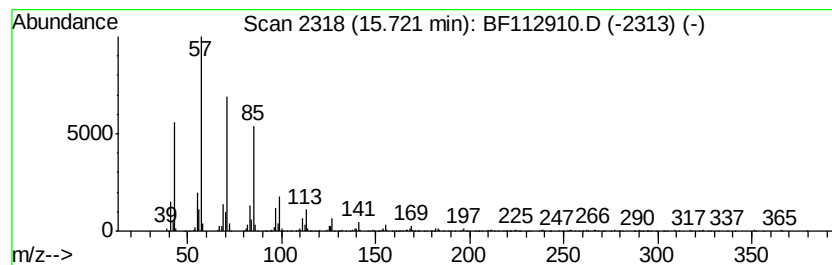
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Heptacosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	11.13 ng	889234	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptacosane	380	C27H56	000593-49-7	95
2		Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	93
4		Heneicosane	296	C21H44	000629-94-7	91
5		Hexadecane	226	C16H34	000544-76-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF030619\
Data File : BF112910.D
Acq On : 7 Mar 2019 4:49
Operator : JU/SJ
Sample : K1705-16
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PST-028-B101-022719

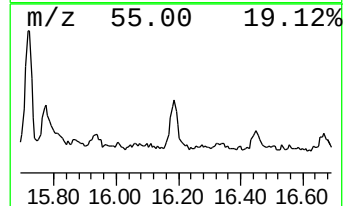
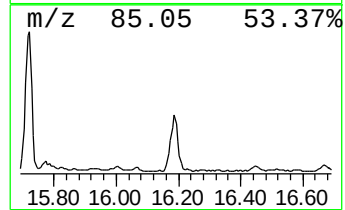
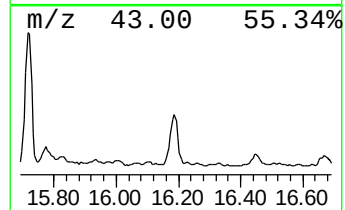
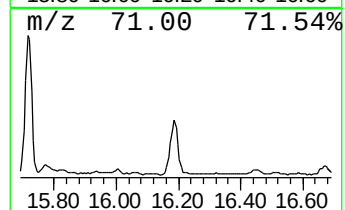
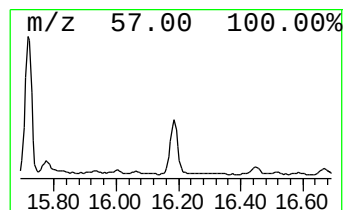
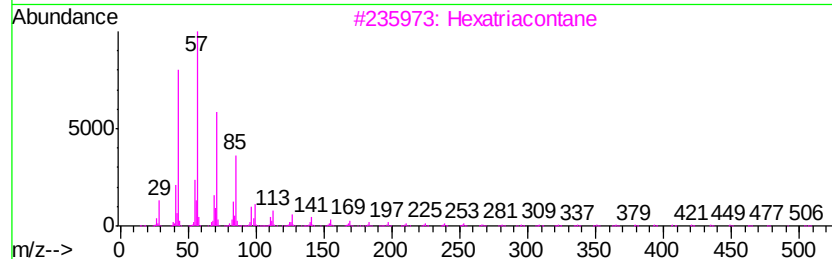
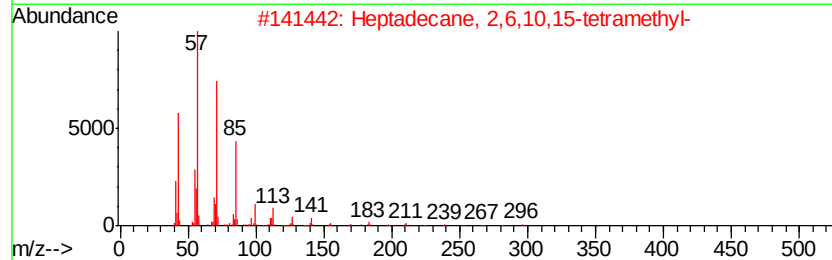
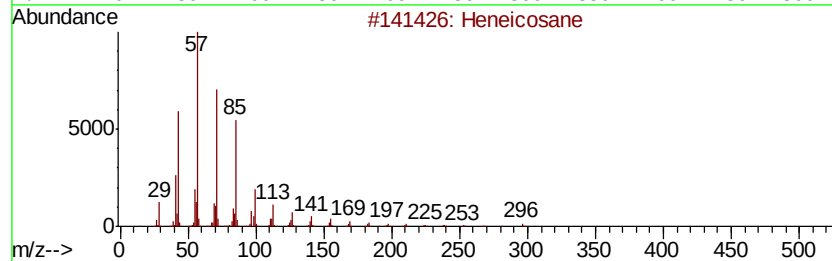
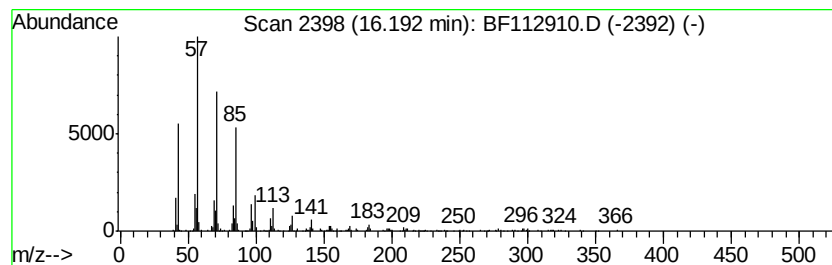
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Heneicosane Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.19	5.64 ng	450513	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	98
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
3			Hexatriacontane	507	C36H74	000630-06-8	91
4			Hexacosane	366	C26H54	000630-01-3	90
5			Tridecane, 7-hexyl-	268	C19H40	007225-66-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030619\
 Data File : BF112910.D
 Acq On : 7 Mar 2019 4:49
 Operator : JU/SJ
 Sample : K1705-16
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PST-028-B101-022719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
(1R)-2,6,6-Trimet...	6.02	11.5	ng	650286	1	6.73	1127980	20.0
.beta.-Pinene	6.44	18.2	ng	1025380	1	6.73	1127980	20.0
unknown6.50	6.50	69.4	ng	3915940	1	6.73	1127980	20.0
n-Hexadecanoic acid	11.77	11.7	ng	801832	4	11.24	1367150	20.0
Cyclohexadecane	13.73	7.2	ng	690667	5	13.86	1907780	20.0
Tricosane	14.04	7.1	ng	679060	5	13.86	1907780	20.0
unknown14.29	14.29	21.2	ng	2020530	5	13.86	1907780	20.0
Heptadecane	14.34	23.2	ng	2213370	5	13.86	1907780	20.0
Ferrocene, 1,2-di...	14.40	12.9	ng	1232390	5	13.86	1907780	20.0
Dibenzofurane-1,3...	14.43	6.5	ng	616940	5	13.86	1907780	20.0
Oxazolo[2,3-f]pur...	14.46	6.1	ng	582689	5	13.86	1907780	20.0
unknown14.50	14.50	6.9	ng	659172	5	13.86	1907780	20.0
unknown14.59	14.59	16.2	ng	1295210	6	15.27	1597920	20.0
Octadecane	14.64	15.4	ng	1231690	6	15.27	1597920	20.0
unknown14.77	14.77	19.6	ng	1570060	6	15.27	1597920	20.0
unknown14.82	14.82	37.6	ng	3007270	6	15.27	1597920	20.0
Heptacosane	15.72	11.1	ng	889234	6	15.27	1597920	20.0
Heneicosane	16.19	5.6	ng	450513	6	15.27	1597920	20.0