

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
 Data File : BM032504.D
 Acq On : 13 Oct 2021 20:05
 Operator : CG/JU
 Sample : M4142-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 2158

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM032504.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.831	140	169	172	rVB	493019	2769898	6.45%	0.556%
2	4.596	272	299	307	rVB3	440913	2021956	4.71%	0.406%
3	4.749	320	325	333	rVB3	314440	568223	1.32%	0.114%
4	5.184	380	399	404	rBV	2317158	4731463	11.01%	0.949%
5	5.401	434	436	437	rVB	814201	559243	1.30%	0.112%
6	5.437	437	442	448	rVB	485685	774421	1.80%	0.155%
7	5.672	471	482	488	rBV2	644394	2200834	5.12%	0.442%
8	6.813	667	676	681	rBV	1620168	3452946	8.04%	0.693%
9	7.066	713	719	726	rVB	4191658	6183973	14.39%	1.241%
10	7.137	726	731	736	rBV	478833	671091	1.56%	0.135%
11	7.195	736	741	746	rVB	772927	1109215	2.58%	0.223%
12	7.484	782	790	794	rBV2	235869	540532	1.26%	0.108%
13	7.595	805	809	816	rVB2	994160	1790737	4.17%	0.359%
14	7.725	827	831	835	rBV2	365892	557650	1.30%	0.112%
15	7.860	849	854	859	rBV3	207927	483808	1.13%	0.097%
16	7.919	859	864	872	rVB	1415562	2174254	5.06%	0.436%
17	7.990	872	876	884	rVB3	343729	644116	1.50%	0.129%
18	8.066	884	889	895	rBV2	324224	525754	1.22%	0.105%
19	8.131	895	900	909	rVB	455772	791317	1.84%	0.159%
20	8.313	918	931	936	rBV	1953682	4204832	9.79%	0.844%
21	8.495	958	962	965	rBV	1041884	1661162	3.87%	0.333%
22	8.695	988	996	1001	rVB2	4803248	8680624	20.20%	1.742%
23	8.760	1001	1007	1018	rVB	2584288	4343933	10.11%	0.872%
24	9.001	1039	1048	1054	rBV	1277298	2355742	5.48%	0.473%
25	9.089	1054	1063	1068	rBV	1117825	2649382	6.17%	0.532%
26	9.301	1090	1099	1103	rVV3	535209	1494849	3.48%	0.300%
27	9.354	1104	1108	1128	rVB3	889958	3555767	8.28%	0.713%
28	9.513	1128	1135	1144	rVB7	192200	646740	1.51%	0.130%
29	9.701	1160	1167	1169	rBV	294045	501033	1.17%	0.101%
30	9.731	1169	1172	1177	rVB2	440924	634673	1.48%	0.127%
31	9.807	1178	1185	1190	rBV	2224608	4193036	9.76%	0.841%
32	9.925	1194	1205	1209	rBV	2322154	5917132	13.77%	1.187%
33	10.107	1232	1236	1243	rVB2	421463	781884	1.82%	0.157%
34	10.195	1245	1251	1256	rBV4	518679	1055477	2.46%	0.212%
35	10.260	1256	1262	1266	rBV	3007842	4532248	10.55%	0.909%
36	10.295	1266	1268	1274	rVB2	565214	792024	1.84%	0.159%

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	10.395	1277	1285	1288	rBV	1752748	3794895	8.83%	0.761%
38	10.560	1304	1313	1314	rBV	1610370	3321232	7.73%	0.666%
39	10.836	1335	1360	1364	rBV	2914424	17794821	41.42%	3.571%
40	10.878	1364	1367	1370	rVB	1355675	1928640	4.49%	0.387%
41	10.989	1381	1386	1390	rVB	670582	994611	2.31%	0.200%
42	11.054	1392	1397	1405	rVB	1336187	2337853	5.44%	0.469%
43	11.248	1423	1430	1438	rBV	3885561	7309980	17.01%	1.467%
44	11.366	1438	1450	1453	rBV5	2153779	6047109	14.07%	1.213%
45	11.472	1463	1468	1471	rBV3	1348789	2875088	6.69%	0.577%
46	11.960	1548	1551	1555	rVV3	1111833	1794012	4.18%	0.360%
47	12.019	1556	1561	1563	rVV3	2219385	3885619	9.04%	0.780%
48	12.054	1563	1567	1572	rVB	4119632	6091392	14.18%	1.222%
49	12.160	1574	1585	1587	rBV	3227064	6352207	14.78%	1.275%
50	12.213	1591	1594	1599	rVB3	1417703	2091660	4.87%	0.420%
51	12.336	1599	1615	1620	rBV3	5083496	23256441	54.13%	4.667%
52	12.401	1623	1626	1628	rVV	1781287	2029206	4.72%	0.407%
53	12.466	1632	1637	1641	rVB	1813892	2370267	5.52%	0.476%
54	12.660	1661	1670	1675	rBV	6676620	13835375	32.20%	2.776%
55	12.825	1675	1698	1701	rBV3	9984174	42964841	100.00%	8.621%
56	13.213	1762	1764	1767	rVB	1312287	1188575	2.77%	0.238%
57	13.254	1767	1771	1773	rBV2	3813564	4781152	11.13%	0.959%
58	13.277	1773	1775	1778	rVB	3624967	3001266	6.99%	0.602%
59	13.324	1780	1783	1785	rBV2	430016	505893	1.18%	0.102%
60	13.360	1785	1789	1794	rBV	2334583	3300521	7.68%	0.662%
61	13.401	1794	1796	1799	rVB3	797716	771653	1.80%	0.155%
62	13.507	1799	1814	1817	rBV6	3455991	13771569	32.05%	2.763%
63	13.595	1818	1829	1835	rVB5	6870493	26586475	61.88%	5.335%
64	13.654	1835	1839	1844	rVB2	2237504	3022472	7.03%	0.606%
65	13.748	1847	1855	1859	rBV	6607901	12253518	28.52%	2.459%
66	13.824	1865	1868	1872	rVB2	1305934	1678445	3.91%	0.337%
67	13.907	1872	1882	1885	rBV2	8678587	24011299	55.89%	4.818%
68	14.219	1932	1935	1938	rBV2	1233037	1630416	3.79%	0.327%
69	14.266	1940	1943	1947	rVB2	1546560	2017414	4.70%	0.405%
70	14.307	1948	1950	1956	rVB3	443708	658987	1.53%	0.132%
71	14.366	1957	1960	1963	rBV2	539667	598593	1.39%	0.120%
72	14.560	1977	1993	1996	rBV3	7707541	28577508	66.51%	5.734%
73	14.583	1996	1997	2000	rVB	2349080	1149114	2.67%	0.231%
74	14.677	2000	2013	2015	rBV3	5610232	16118069	37.51%	3.234%
75	14.707	2015	2018	2022	rBV2	399676	613416	1.43%	0.123%
76	14.795	2022	2033	2037	rVV3	5291504	15074607	35.09%	3.025%

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77	14.871	2037	2046	2049	rVV3	6426304	15560952	36.22%	3.122%
78	14.930	2052	2056	2061	rVB2	4636575	7357333	17.12%	1.476%
79	15.024	2068	2072	2076	rVB	1551471	1754386	4.08%	0.352%
80	15.254	2105	2111	2116	rBV5	518485	1416166	3.30%	0.284%
81	15.371	2117	2131	2134	rVV4	6095818	18646814	43.40%	3.742%
82	15.407	2134	2137	2139	rVV	1256526	1359964	3.17%	0.273%
83	15.507	2139	2154	2158	rVB3	3660048	13136691	30.58%	2.636%
84	15.624	2168	2174	2178	rBV2	3019861	7233084	16.83%	1.451%
85	15.671	2178	2182	2186	rVB	4470847	7373638	17.16%	1.480%
86	15.718	2186	2190	2191	rBV2	925760	1146009	2.67%	0.230%
87	15.760	2191	2197	2201	rVB2	3554703	6298357	14.66%	1.264%
88	15.830	2206	2209	2214	rVV3	840948	1371895	3.19%	0.275%
89	16.336	2291	2295	2298	rBV2	695842	839930	1.95%	0.169%
90	16.371	2298	2301	2303	rBV	701903	854631	1.99%	0.171%
91	16.518	2322	2326	2328	rBV	787040	1092998	2.54%	0.219%
92	16.612	2338	2342	2345	rVB	525064	696571	1.62%	0.140%
93	16.807	2371	2375	2383	rBV3	348775	583793	1.36%	0.117%
94	16.989	2402	2406	2411	rVB	1559394	2073936	4.83%	0.416%
95	17.489	2487	2491	2500	rBV	468864	735516	1.71%	0.148%
96	17.883	2554	2558	2566	rBV	731947	1109954	2.58%	0.223%
97	19.154	2771	2774	2784	rVB	472134	703770	1.64%	0.141%
98	19.601	2844	2850	2855	rBV	7166117	9479023	22.06%	1.902%
99	21.147	3108	3113	3118	rBV	1828149	2225185	5.18%	0.446%
100	23.289	3471	3477	3484	rVB2	1353864	2380607	5.54%	0.478%

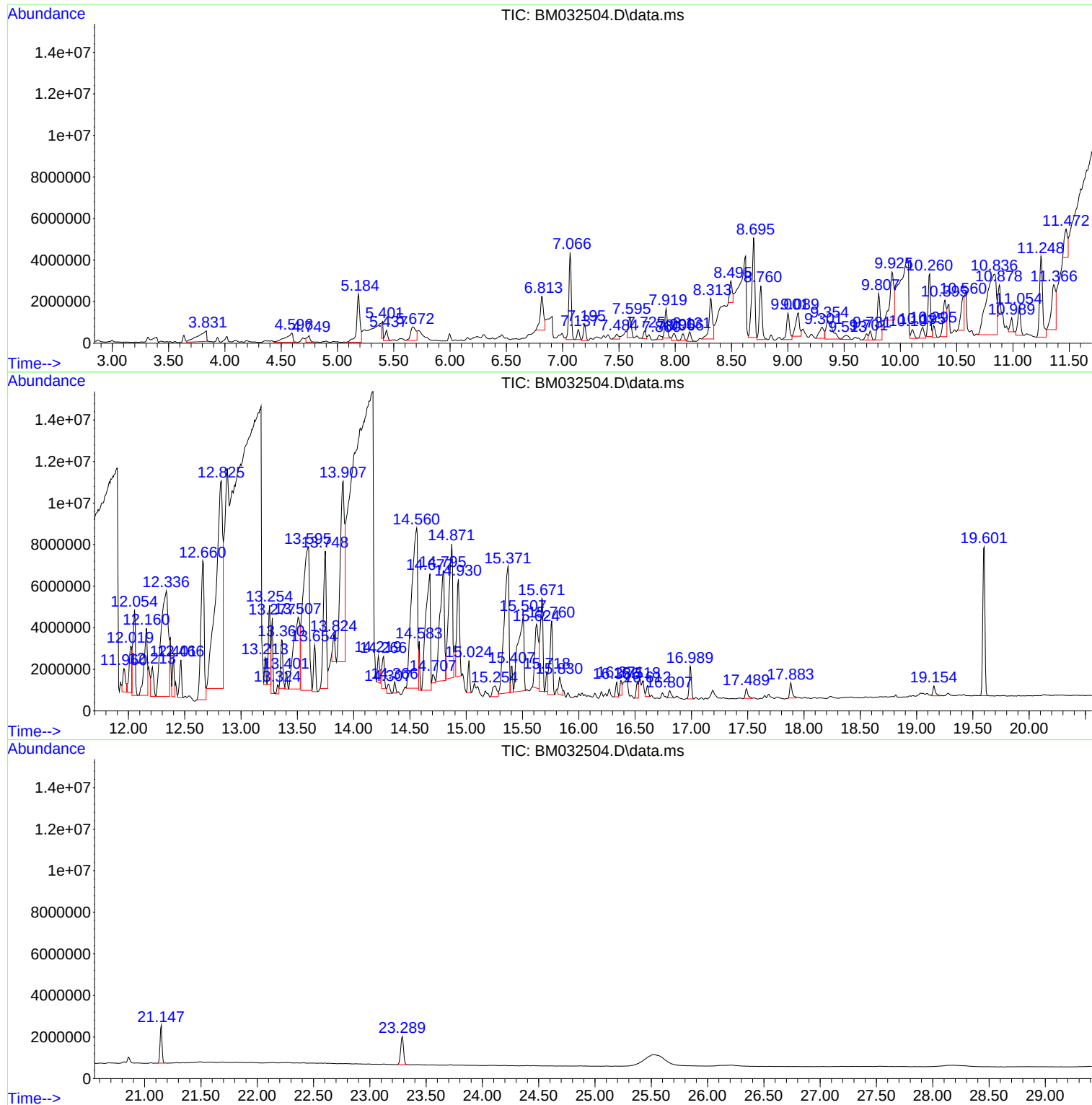
Sum of corrected areas: 498369383

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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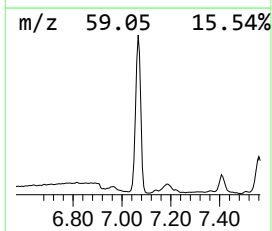
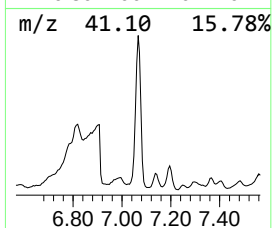
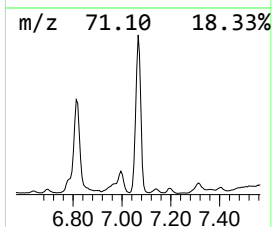
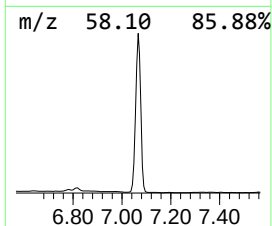
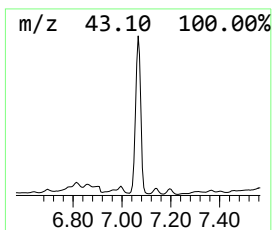
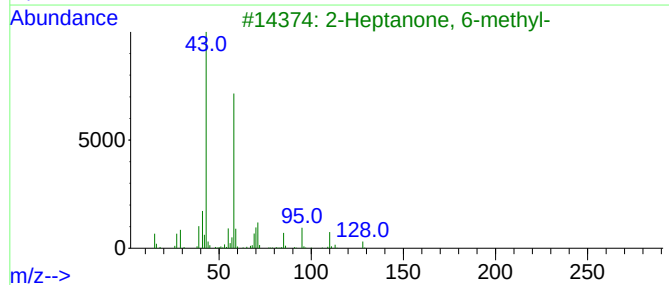
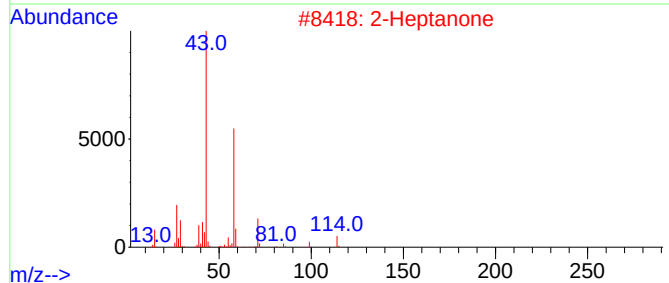
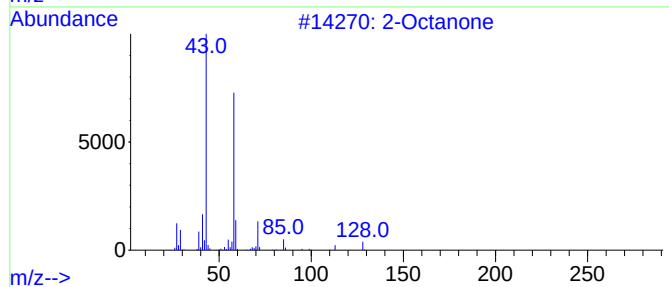
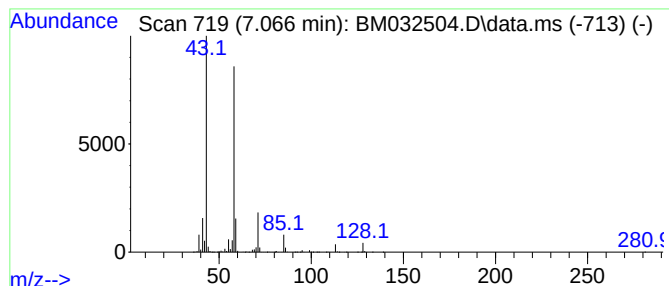
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Octanone Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.066	69.07 ng	6183970	1,4-Dichlorobenzene-d4	7.601

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octanone	128	C8H16O	000111-13-7	91
2			2-Heptanone	114	C7H14O	000110-43-0	78
3			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	64
4			2-Hexanone	100	C6H12O	000591-78-6	64
5			Meclofenoxate	257	C12H16ClNO3	000051-68-3	38



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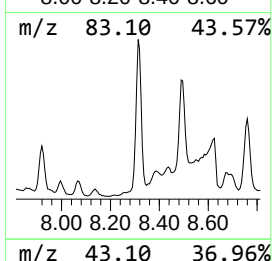
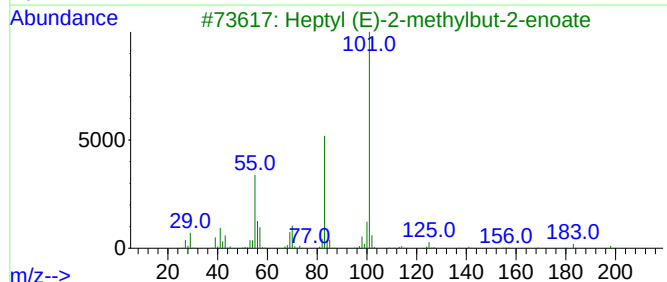
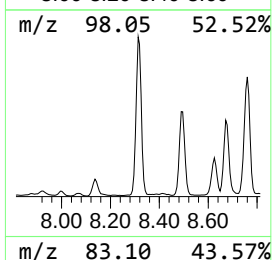
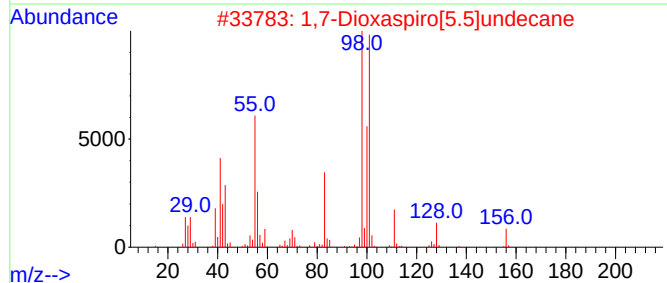
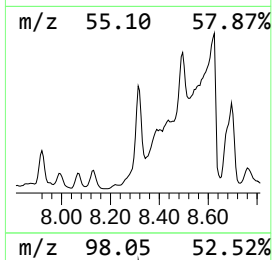
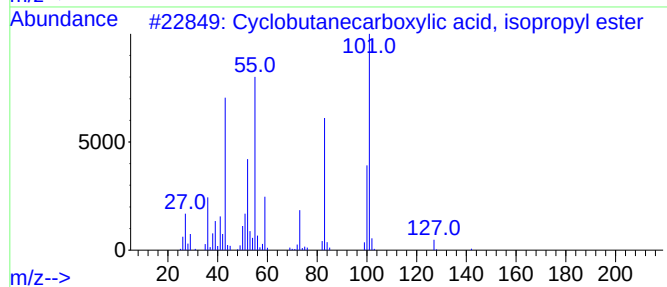
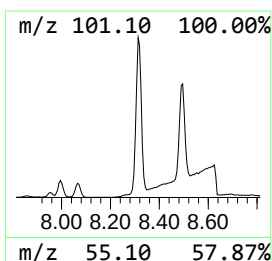
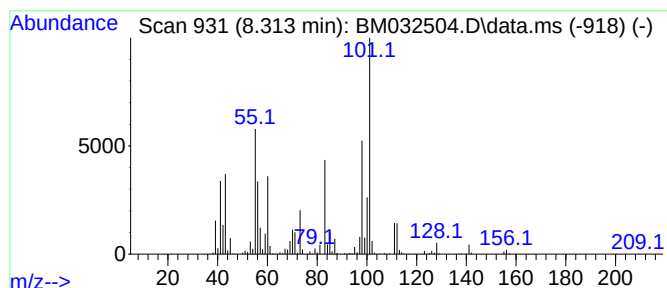
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown8.313 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD		R.T.	
8.313	46.96 ng	4204830	1,4-Dichlorobenzene-d4		7.601	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclobutanecarboxylic acid, isop...		142	C8H14O2	1000282-21-6	46
2	1,7-Dioxaspiro[5.5]undecane		156	C9H16O2	000180-84-7	43
3	Heptyl (E)-2-methylbut-2-enoate		198	C12H22O2	1010373-73-8	38
4	Isopropyl isothiocyanate		101	C4H7NS	002253-73-8	27
5	2-Oxazolidinone, 3-methyl-		101	C4H7NO2	019836-78-3	22



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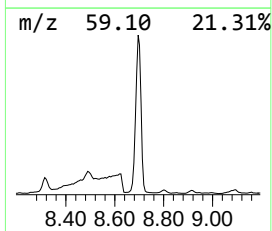
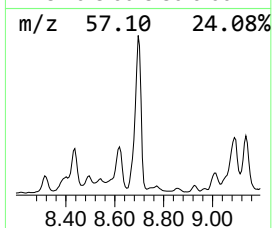
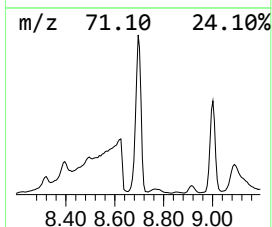
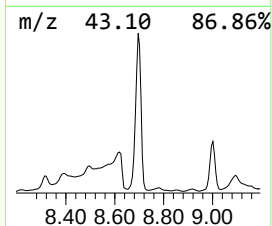
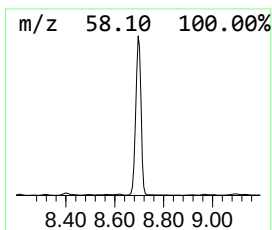
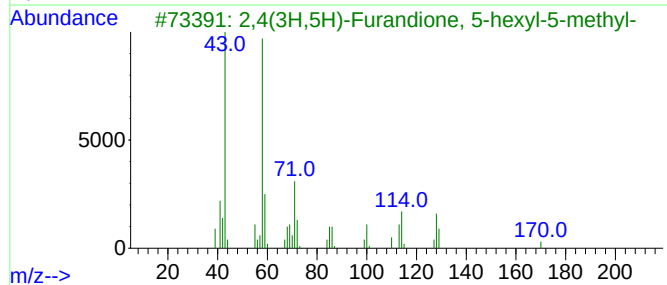
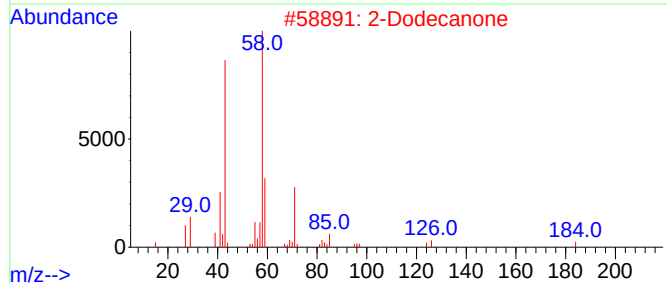
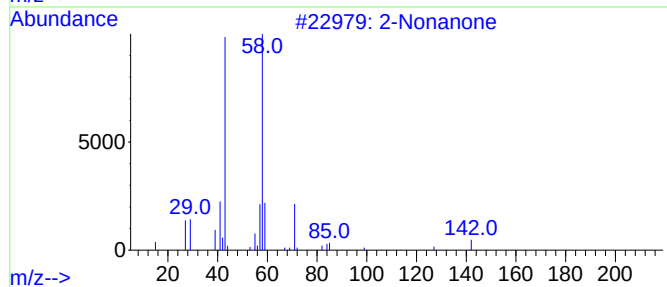
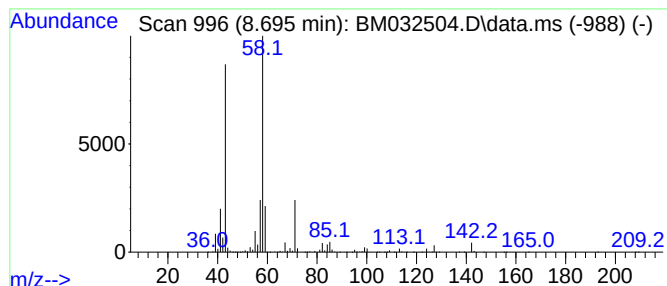
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Nonanone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.695	96.95 ng	8680620	1,4-Dichlorobenzene-d4	7.601

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonanone	142	C9H18O	000821-55-6	91
2			2-Dodecanone	184	C12H24O	006175-49-1	64
3			2,4(3H,5H)-Furandione, 5-hexyl-5...	198	C11H18O3	054852-79-8	64
4			2-Octanone	128	C8H16O	000111-13-7	64
5			trans-2,3-Epoxyonane	142	C9H18O	056820-01-0	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
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Acq On : 13 Oct 2021 20:05
Operator : CG/JU
Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

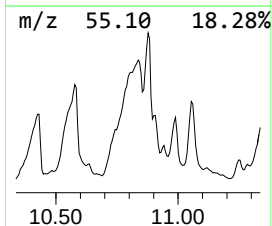
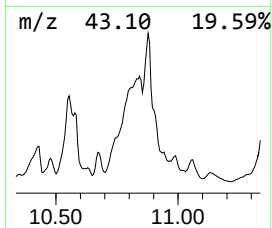
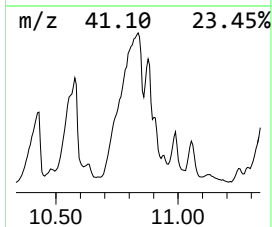
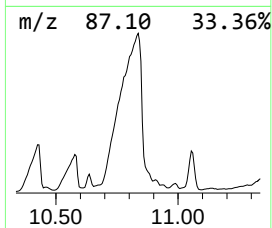
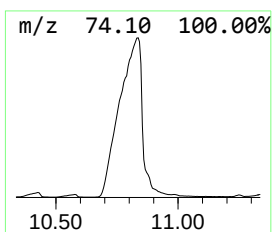
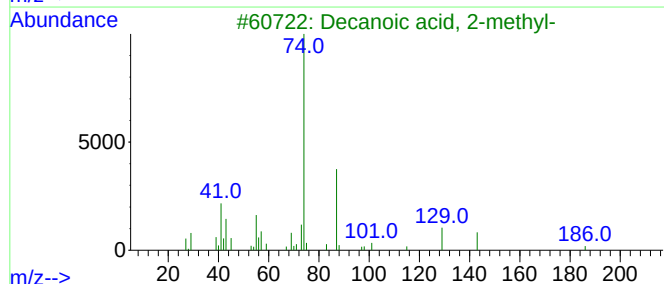
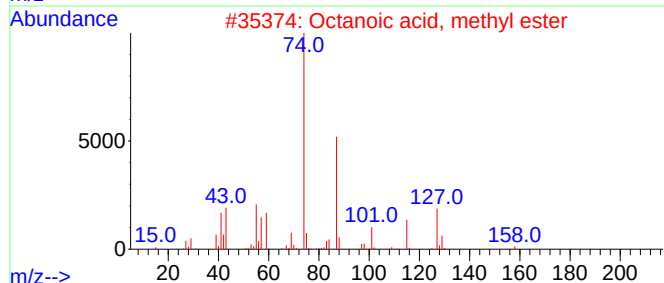
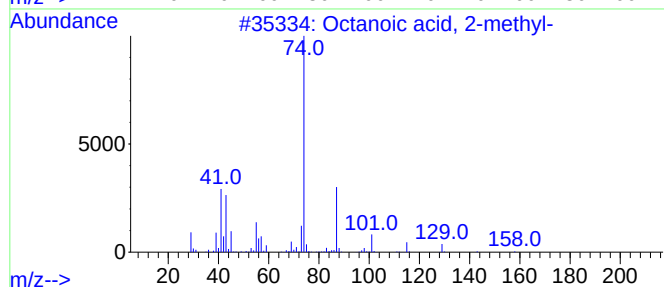
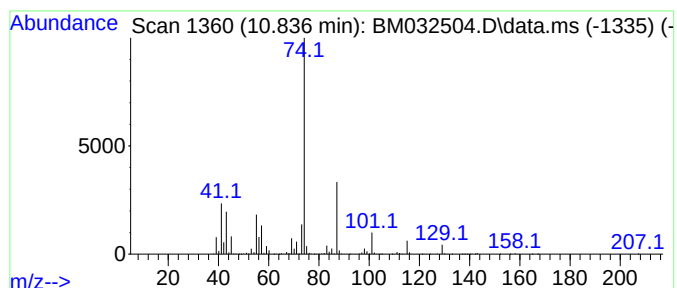
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octanoic acid, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.836	93.78 ng	17794800	Naphthalene-d8	10.389	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	95
2	Octanoic acid, methyl ester	158	C9H18O2	000111-11-5	72
3	Decanoic acid, 2-methyl-	186	C11H22O2	024323-23-7	72
4	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	64
5	Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
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Operator : CG/JU
Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

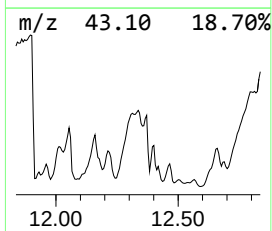
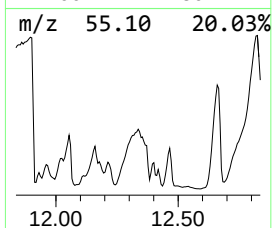
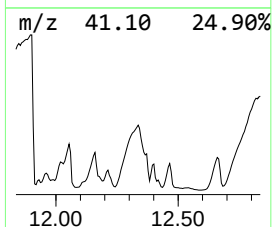
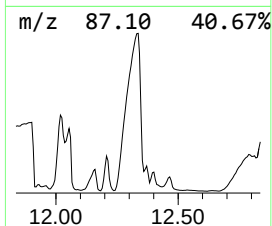
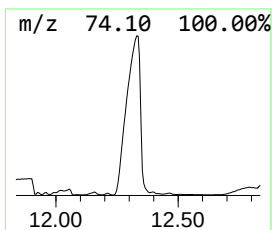
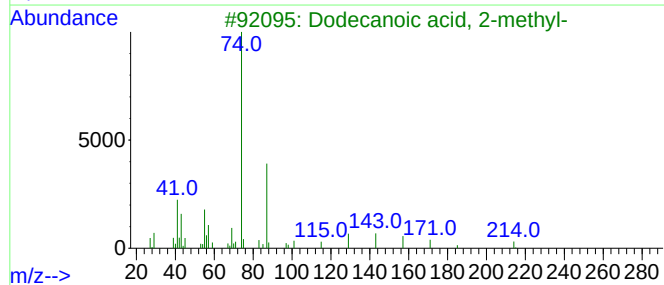
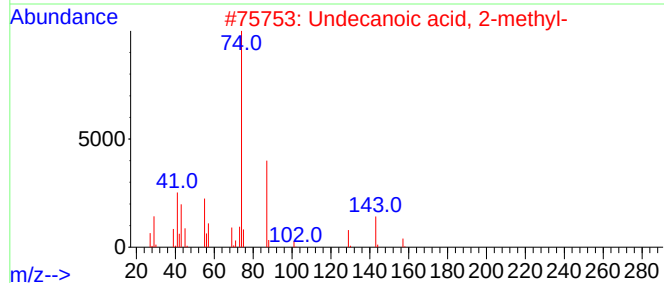
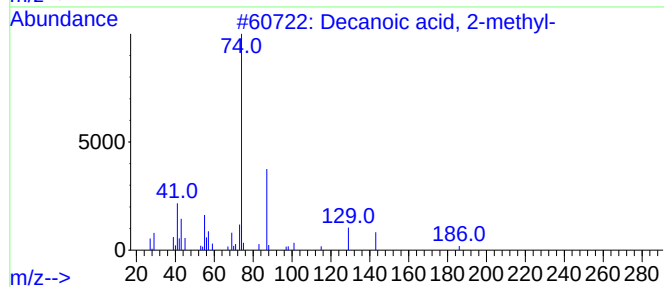
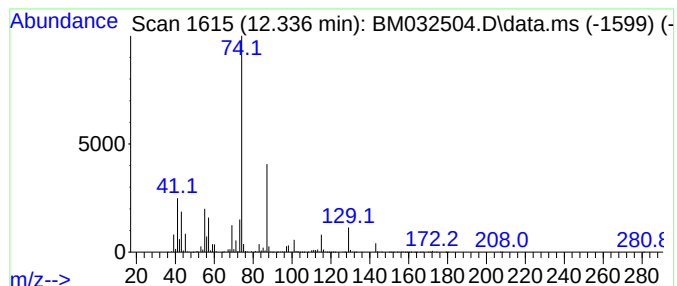
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Decanoic acid, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.336	230.56 ng	23256400	Acenaphthene-d10			14.260
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decanoic acid, 2-methyl-		186	C11H22O2	024323-23-7	90
2	Undecanoic acid, 2-methyl-		200	C12H24O2	024323-25-9	78
3	Dodecanoic acid, 2-methyl-		214	C13H26O2	002874-74-0	72
4	Butanoic acid, 2-methyl-		102	C5H10O2	000116-53-0	64
5	Nonanoic acid, methyl ester		172	C10H20O2	001731-84-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
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Sample : M4142-07
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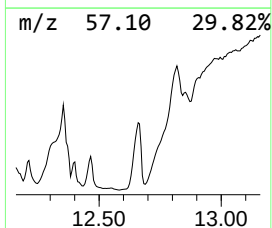
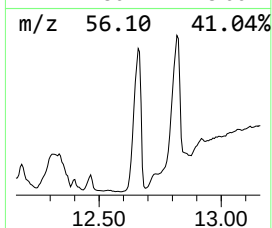
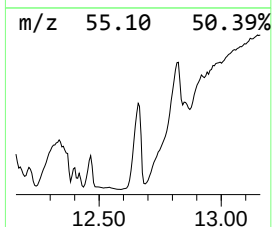
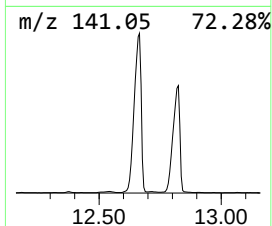
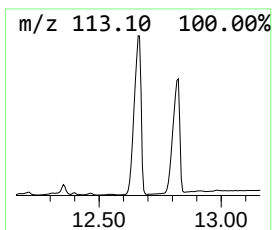
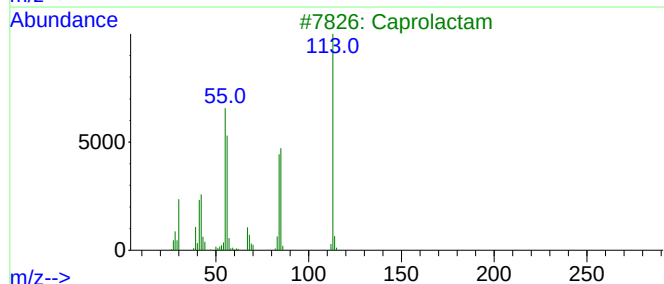
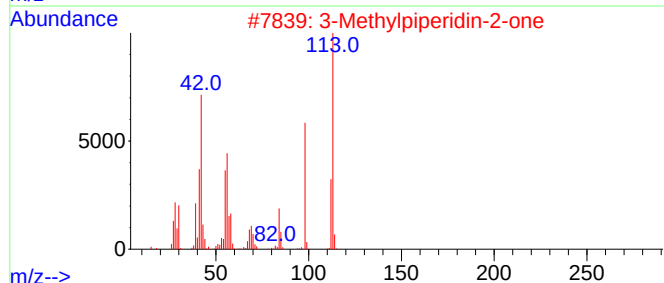
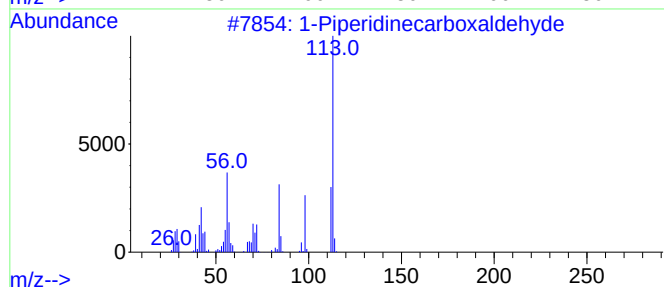
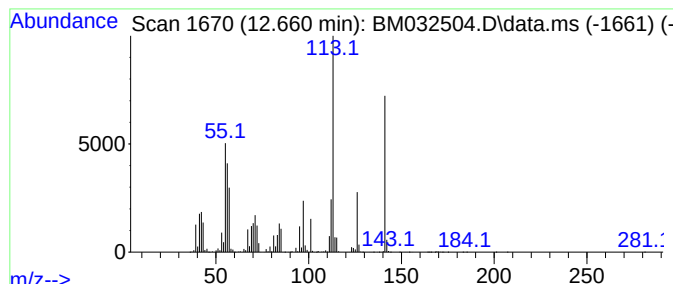
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Piperidinecarboxaldehyde Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.660	137.16 ng	13835400	Acenaphthene-d10		14.260	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Piperidinecarboxaldehyde		113	C6H11NO	002591-86-8	53
2	3-Methylpiperidin-2-one		113	C6H11NO	003768-43-2	49
3	Caprolactam		113	C6H11NO	000105-60-2	43
4	(S)-5-Butyl-5-ethyldihydrofuran-...		170	C10H18O2	1212228-49-3	43
5	./+/-..beta.,.beta.-Dimethyl-.ga...		144	C7H12O3	052398-48-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
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Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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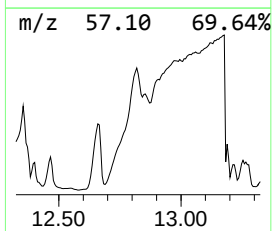
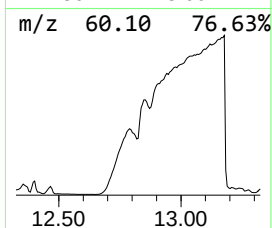
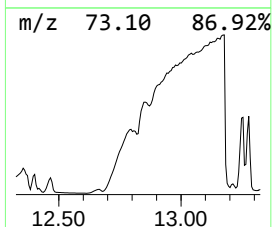
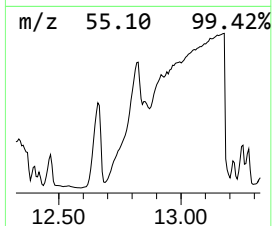
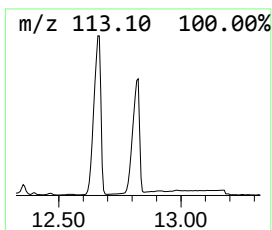
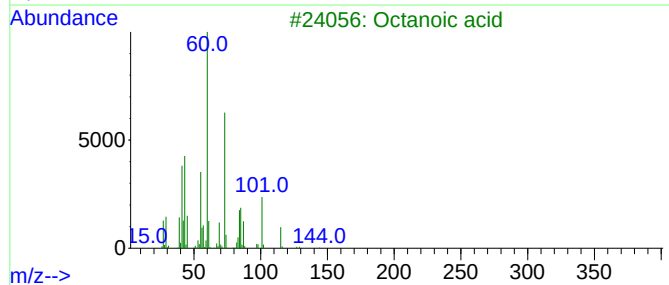
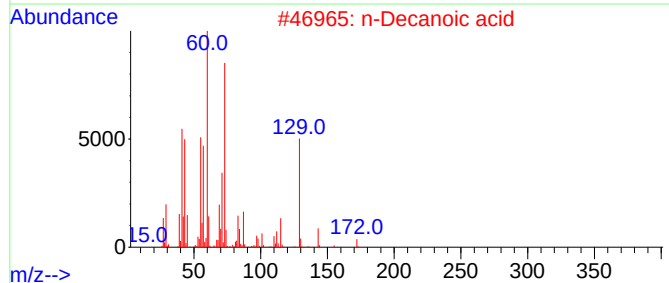
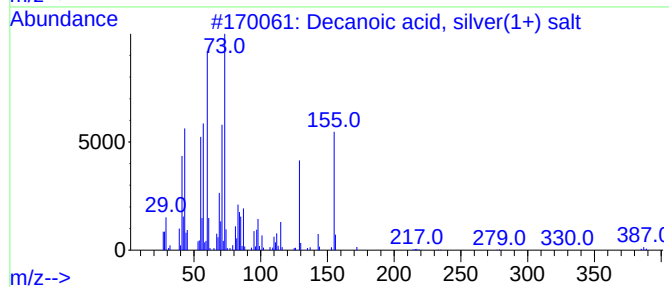
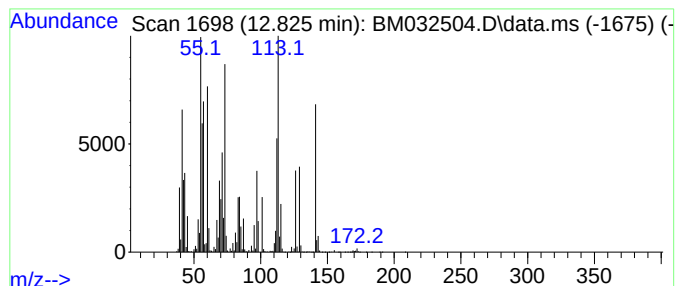
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown12.825 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.825	425.94 ng	42964800	Acenaphthene-d10	14.260

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	30
2			n-Decanoic acid	172	C10H20O2	000334-48-5	27
3			Octanoic acid	144	C8H16O2	000124-07-2	25
4			5-Methylthiophen-3-ylamine	113	C5H7NS	1000311-36-5	14
5			.beta.-Guanidinopropionic acid	131	C4H9N3O2	000353-09-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
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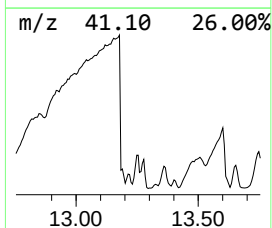
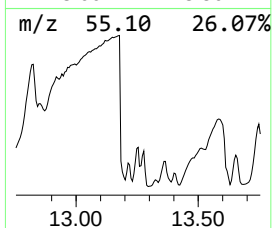
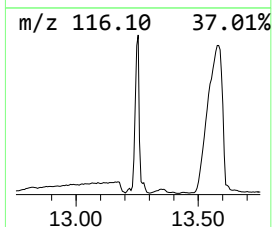
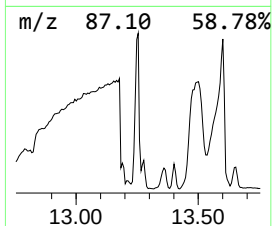
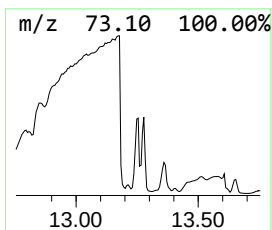
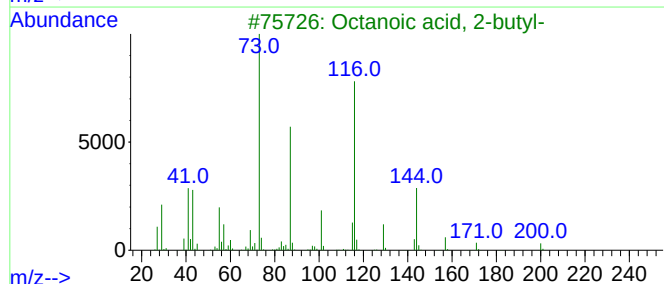
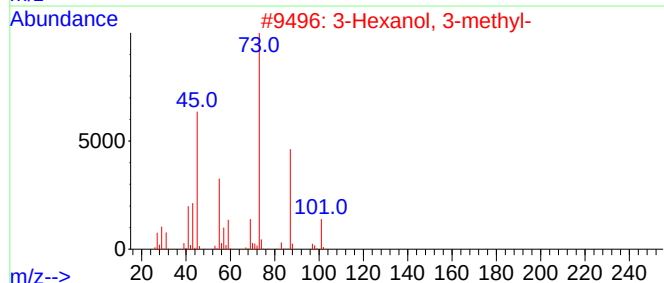
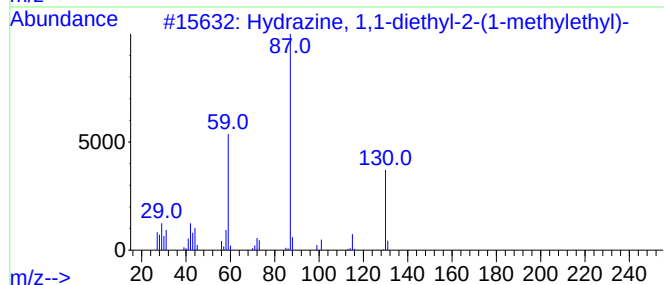
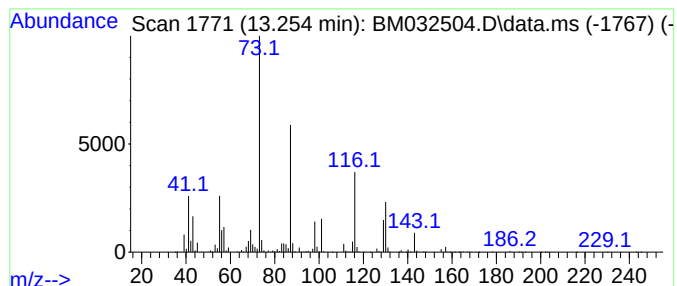
Instrument :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown13.254 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.254	47.40 ng	4781150	Acenaphthene-d10	14.260	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,1-diethyl-2-(1-meth...	130	C7H18N2	067398-39-4	38
2	3-Hexanol, 3-methyl-	116	C7H16O	000597-96-6	38
3	Octanoic acid, 2-butyl-	200	C12H24O2	027610-92-0	37
4	Heptanoic acid, 2-propyl-, methy...	186	C11H22O2	056247-53-1	37
5	.alpha.-D-Glucopyranoside, methy...	319	C14H25NO7	036663-25-9	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
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Misc :
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Instrument :
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ClientSampleId :
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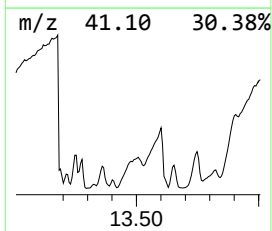
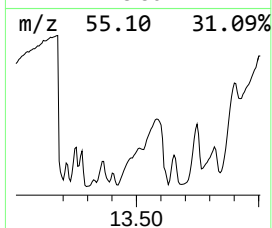
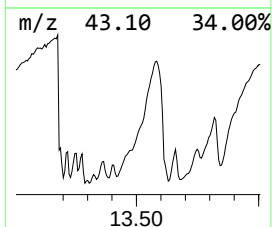
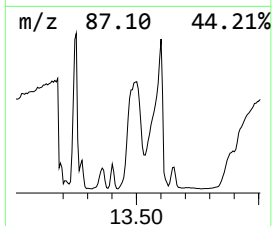
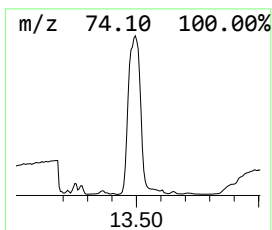
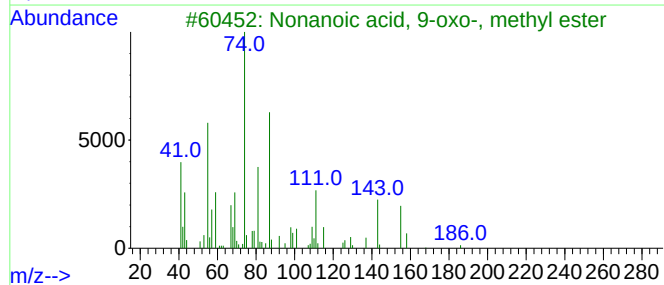
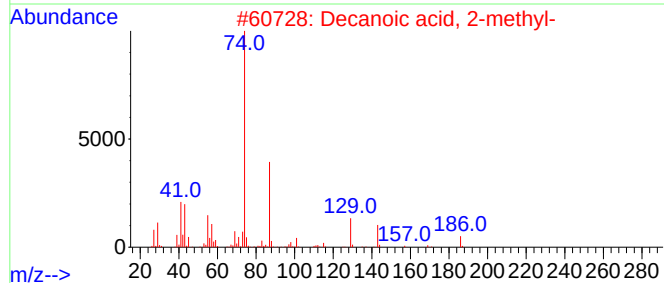
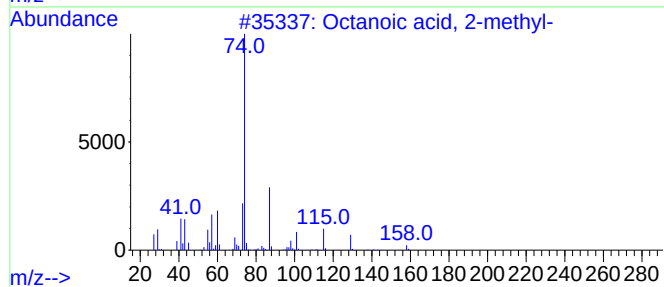
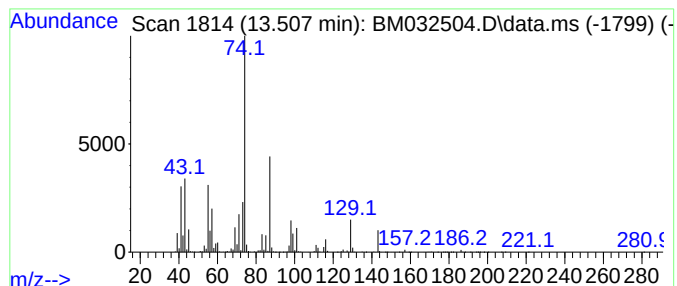
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Nonanoic acid, 9-oxo-, meth... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.507	136.53 ng	13771600	Acenaphthene-d10	14.260

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid, 2-methyl-	158	C9H18O2	003004-93-1	72
2			Decanoic acid, 2-methyl-	186	C11H22O2	024323-23-7	59
3			Nonanoic acid, 9-oxo-, methyl ester	186	C10H18O3	001931-63-1	59
4			Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	53
5			2,3,4-Trimethylpentanoic acid	144	C8H16O2	090435-18-0	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
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Sample : M4142-07
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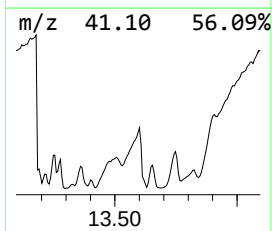
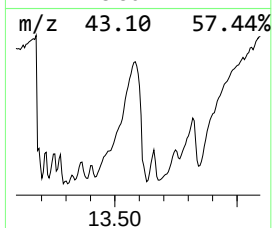
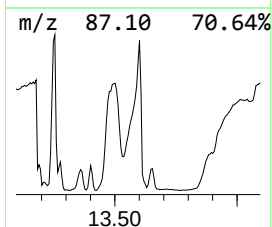
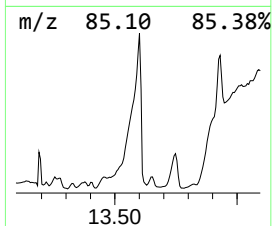
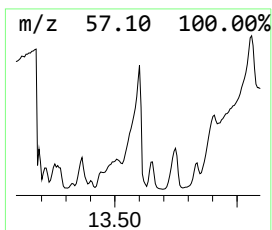
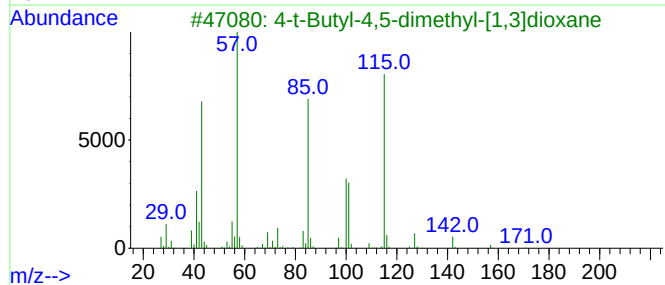
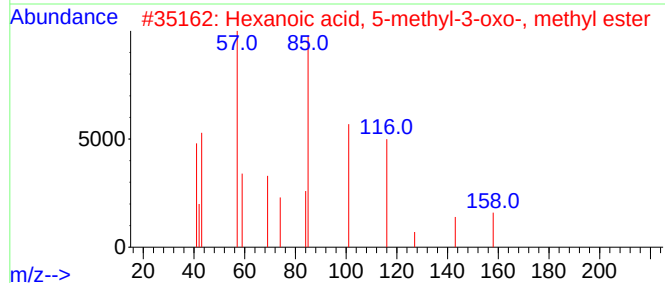
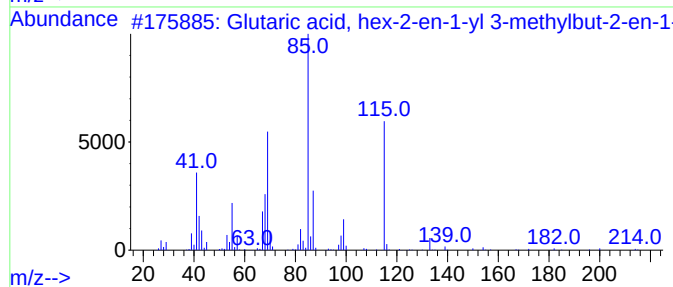
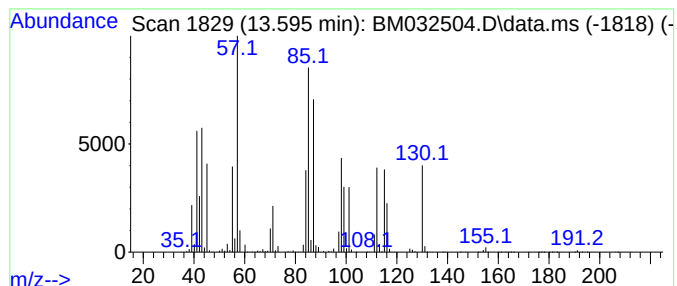
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown13.595 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.595	263.57 ng	26586500	Acenaphthene-d10	14.260

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glutaric acid, hex-2-en-1-yl 3-m...	282	C16H26O4	1000405-32-9	27
2			Hexanoic acid, 5-methyl-3-oxo-, ...	158	C8H14O3	030414-55-2	22
3			4-t-Butyl-4,5-dimethyl-[1,3]dioxane	172	C10H20O2	1000190-70-0	16
4			Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	14
5			Tetradecane, 5-methyl-	212	C15H32	025117-32-2	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
Operator : CG/JU
Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

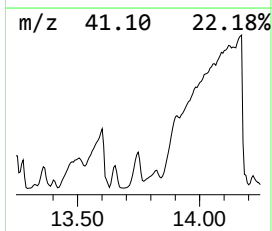
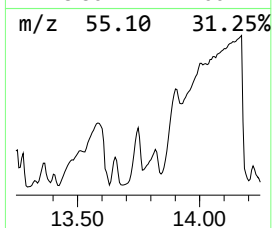
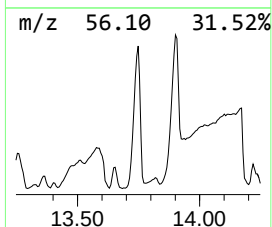
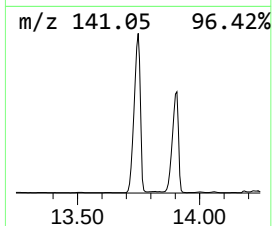
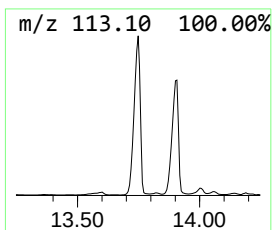
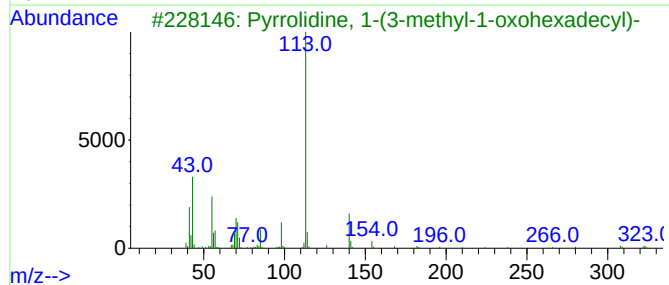
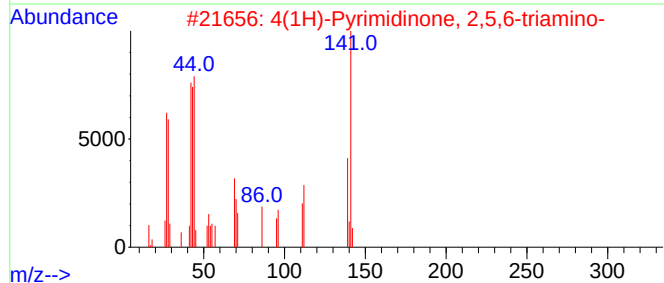
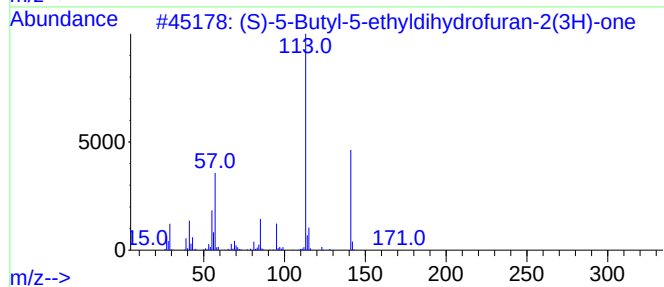
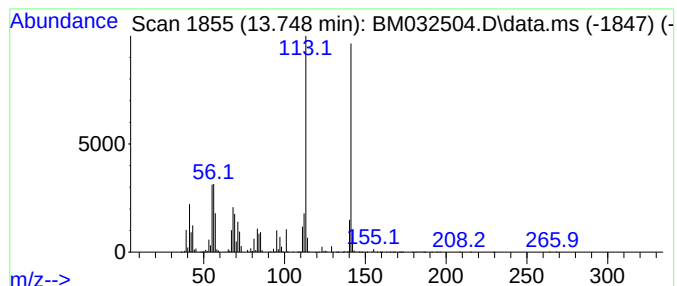
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 (S)-5-Butyl-5-ethyldihydrofuran-2(3H)-one Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.748	121.48 ng	12253500	Acenaphthene-d10	14.260
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		(S)-5-Butyl-5-ethyldihydrofuran-2(3H)-one	170 C10H18O2	1212228-49-3 50
2		4(1H)-Pyrimidinone, 2,5,6-triamino-	141 C4H7N5O	001004-75-7 38
3		Pyrrolidine, 1-(3-methyl-1-oxohexadecyl)-	323 C21H41NO	056630-57-0 38
4		Pyrrolidine, 1-(3-methyl-1-oxohexadecyl)-	337 C22H43NO	1000036-69-5 38
5		4-Methyl-2-piperidone	113 C6H11NO	1000432-34-3 35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
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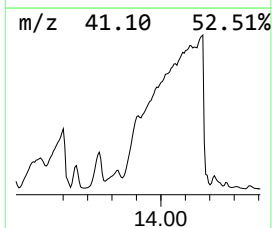
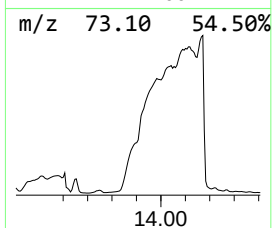
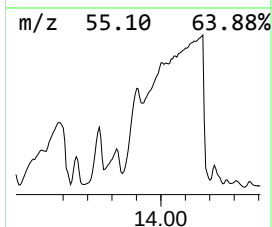
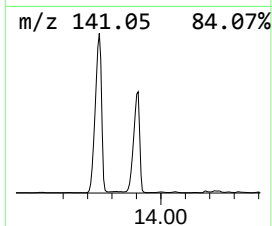
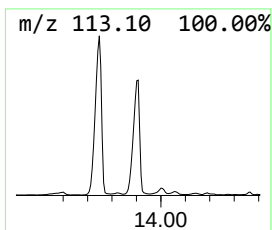
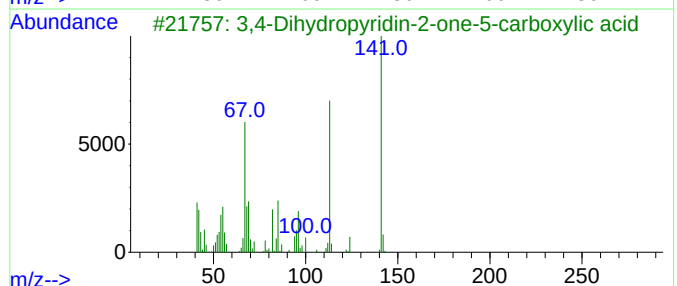
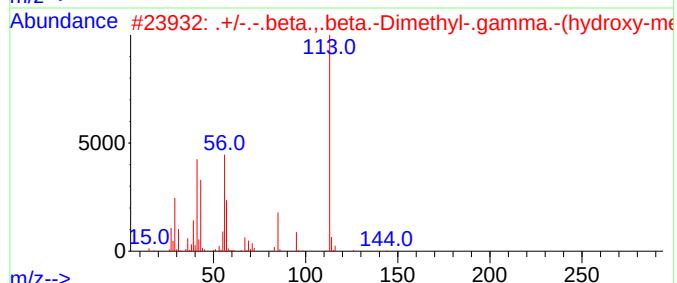
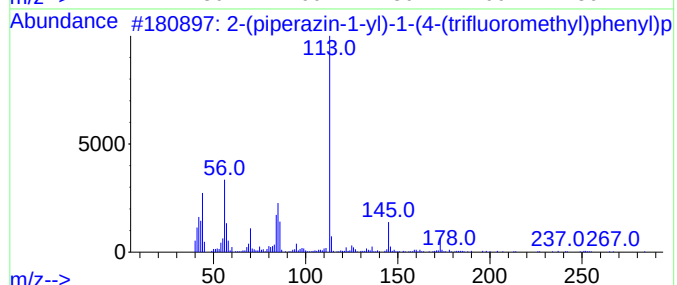
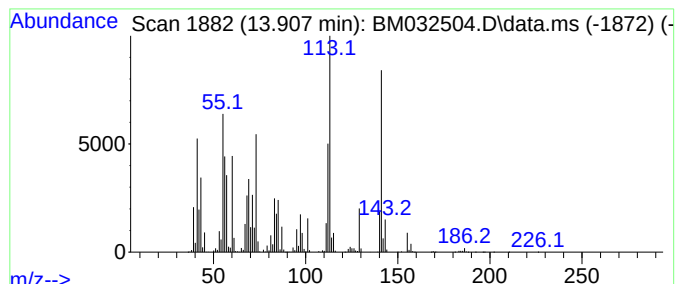
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 unknown13.907 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.907	238.04 ng	24011300	Acenaphthene-d10	14.260

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(piperazin-1-yl)-1-(4-(trifluo...	286	C14H17F3N2O	1000455-09-8	27		
2	./+/-..beta.,.beta.-Dimethyl-.ga...	144	C7H12O3	052398-48-8	27		
3	3,4-Dihydropyridin-2-one-5-carbo...	141	C6H7NO3	005155-13-5	27		
4	Imidazole, 4-aminocarbonyl-5-flu...	261	C9H12FN3O5	056766-95-1	27		
5	4-Ethyl-5-hydroxy-3,5-dimethylfu...	156	C8H12O3	050461-82-0	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
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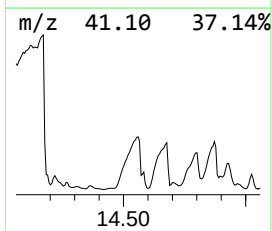
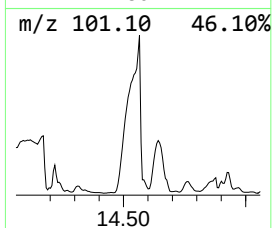
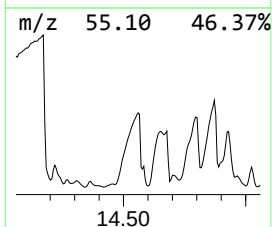
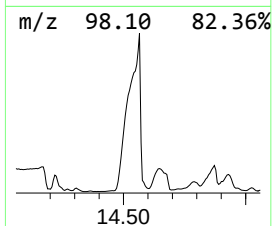
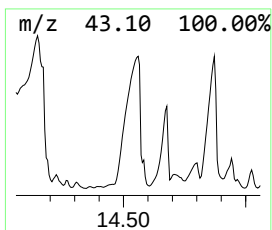
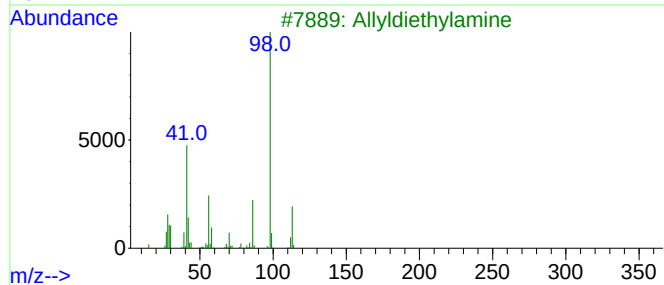
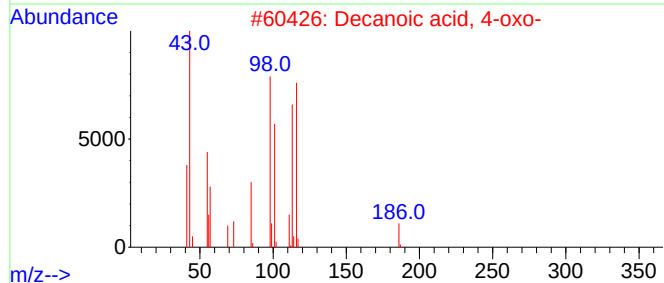
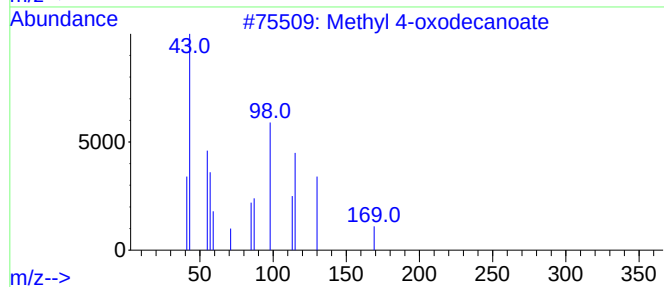
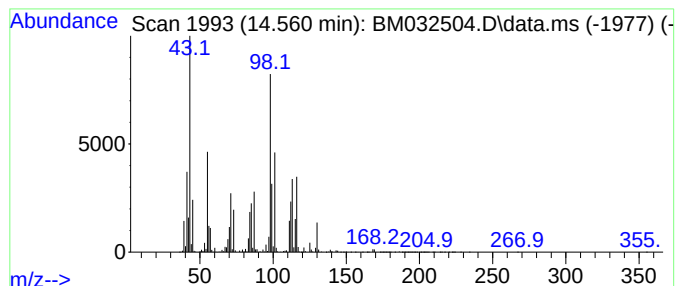
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown14.560 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.560	283.31 ng	28577500	Acenaphthene-d10	14.260	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 4-oxodecanoate	200	C11H20O3	007011-82-7	38
2	Decanoic acid, 4-oxo-	186	C10H18O3	004144-54-1	35
3	Allyldiethylamine	113	C7H15N	005666-17-1	30
4	Fumaric Acid	116	C4H4O4	000110-17-8	25
5	1-((Dicyclohexylphosphorothioyl)...	327	C18H34NPS	1000298-06-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
Operator : CG/JU
Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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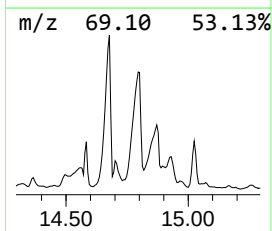
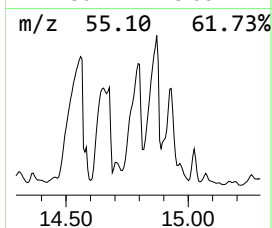
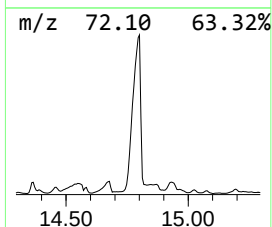
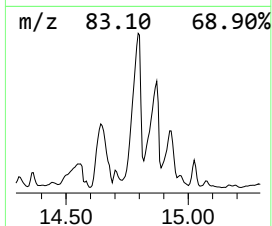
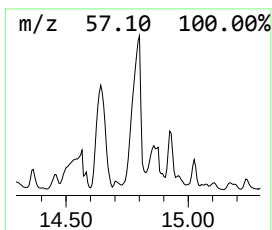
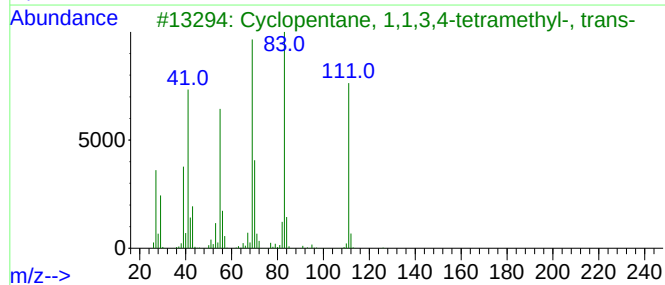
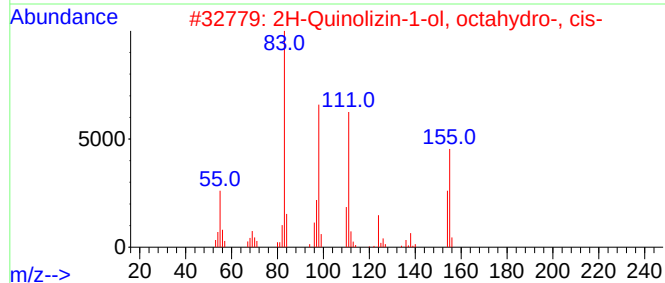
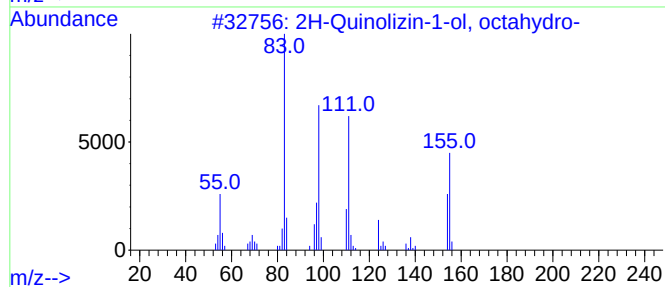
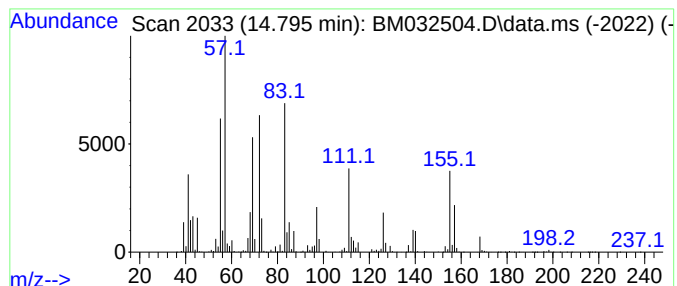
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 unknown14.795 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.795	149.44 ng	15074600	Acenaphthene-d10	14.260

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2H-Quinolizin-1-ol, octahydro-	155	C9H17NO	022525-60-6	43
2		2H-Quinolizin-1-ol, octahydro-, ...	155	C9H17NO	010447-19-5	43
3		Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	22
4		t-Butyl cyclohexaneperoxy-carboxy...	200	C11H20O3	020396-49-0	22
5		3-Octen-2-one	126	C8H14O	001669-44-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
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Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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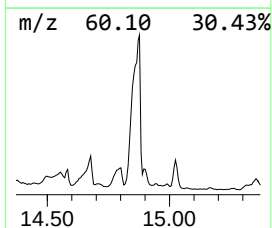
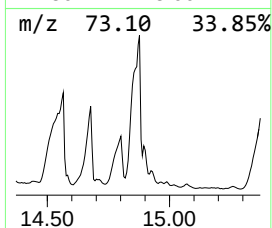
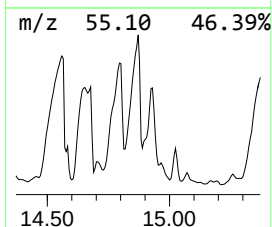
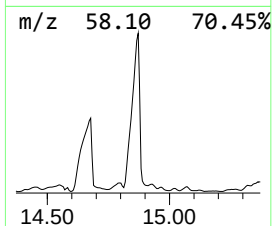
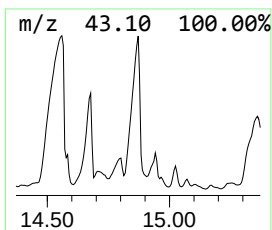
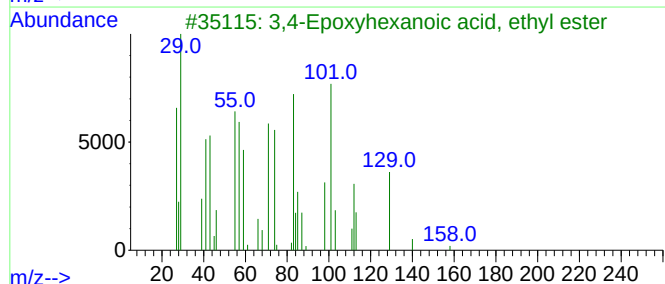
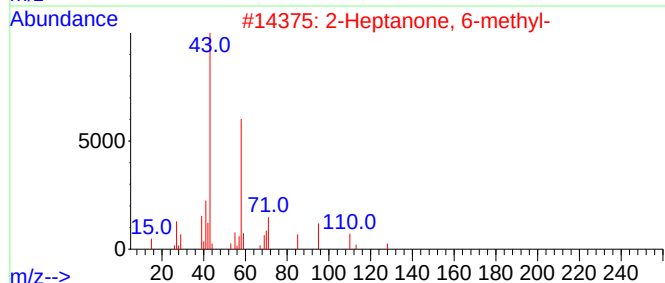
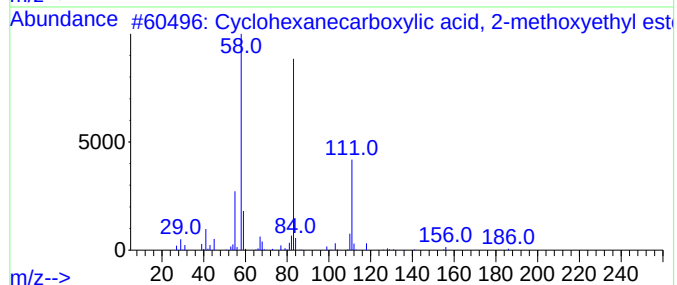
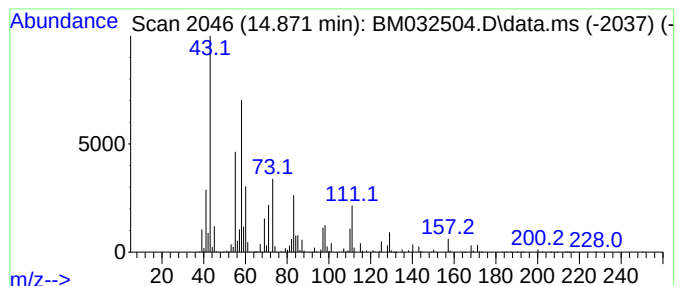
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown14.871 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.871	154.27 ng	15561000	Acenaphthene-d10	14.260

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid, 2-me...	186	C10H18O3	1000330-87-5	35
2			2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	25
3			3,4-Epoxyhexanoic acid, ethyl ester	158	C8H14O3	061454-92-0	25
4			8-Hydroxy-2-octanone	144	C8H16O2	025368-54-1	14
5			2H-Pyran,3,4-dihydro-2-methoxy-4...	128	C7H12O2	038113-08-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
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Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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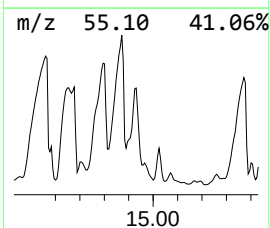
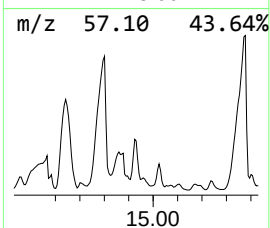
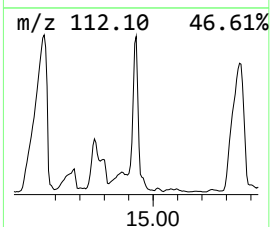
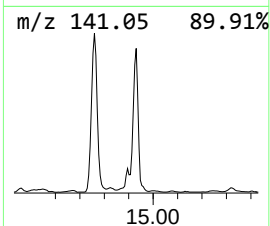
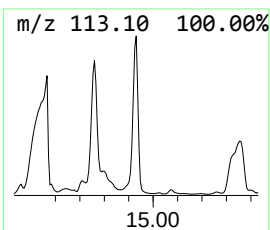
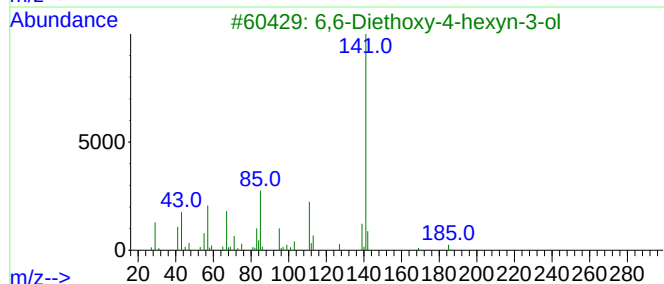
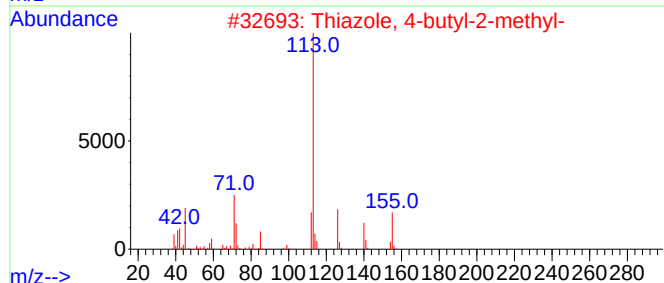
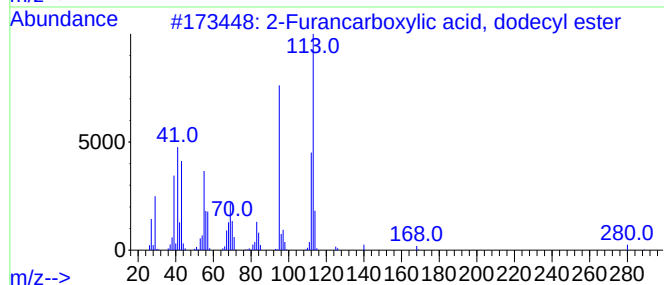
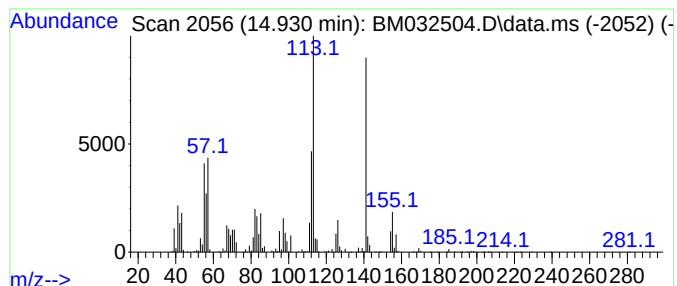
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 unknown14.930 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.930	72.94 ng	7357330	Acenaphthene-d10	14.260

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Furancarboxylic acid, dodecyl ...	280	C17H28O3	116435-27-9	38		
2	Thiazole, 4-butyl-2-methyl-	155	C8H13NS	041981-69-5	38		
3	6,6-Diethoxy-4-hexyn-3-ol	186	C10H18O3	1000434-41-7	30		
4	3,4-Difluorobenzoic acid, 2-trid...	340	C20H30F2O2	1010338-59-9	27		
5	19-Methyl-eicosanoic acid, pyrro...	379	C25H49NO	1000336-08-5	22		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
Operator : CG/JU
Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

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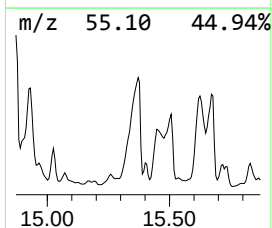
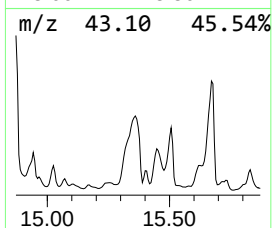
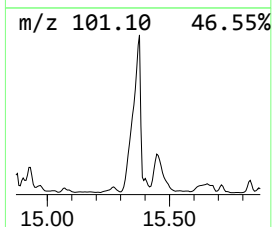
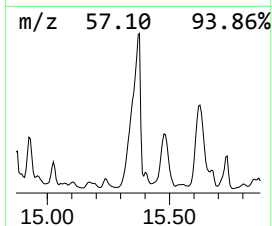
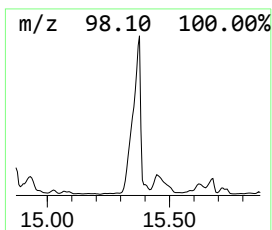
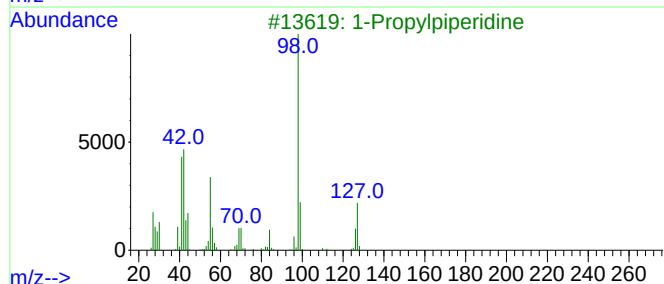
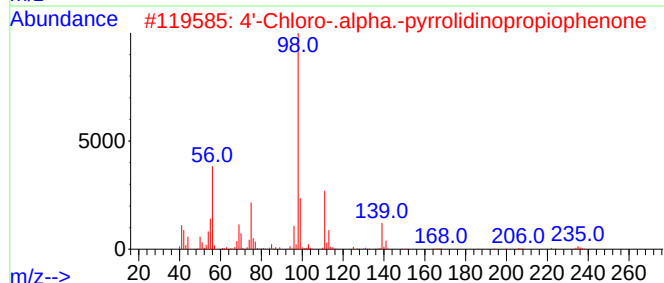
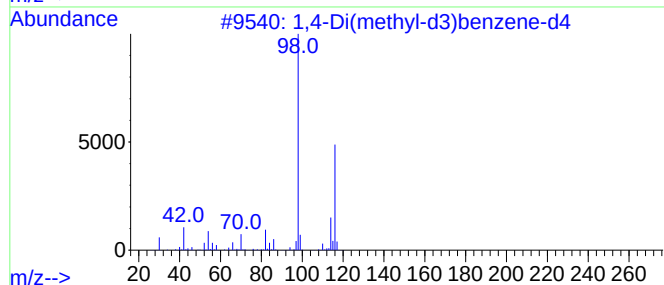
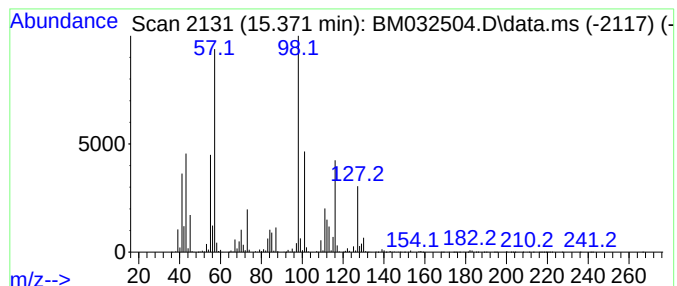
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 unknown15.371 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.371	184.86 ng	18646800	Acenaphthene-d10	14.260

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Di(methyl-d3)benzene-d4	116	C8D10	041051-88-1	35
2			4'-Chloro-.alpha.-pyrrolidinopro...	237	C13H16ClNO	028117-79-5	27
3			1-Propylpiperidine	127	C8H17N	005470-02-0	22
4			rac-(2R,4R)-2,4-Dimethylpiperidine	113	C7H15N	741660-40-2	22
5			Pentanoic acid, 2,2,4,4-tetramet...	172	C10H20O2	035201-72-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
Operator : CG/JU
Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

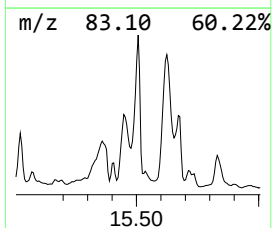
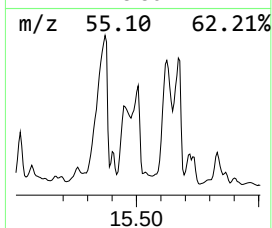
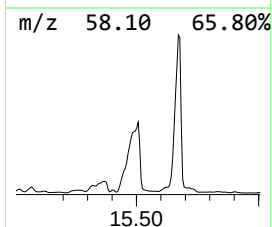
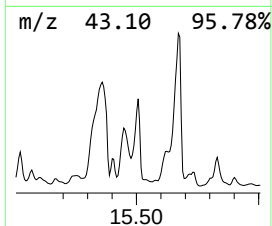
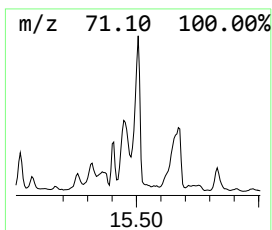
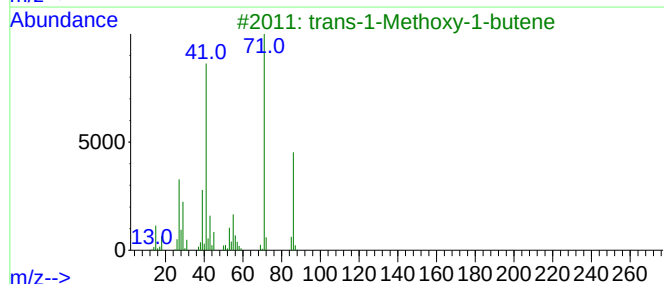
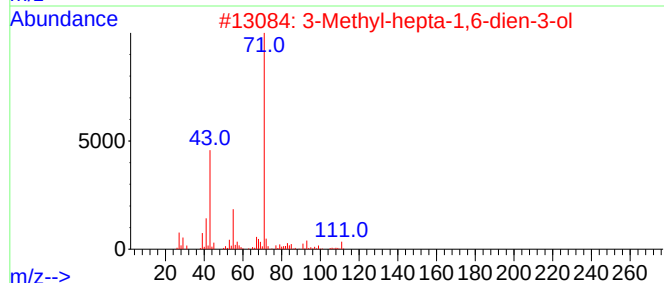
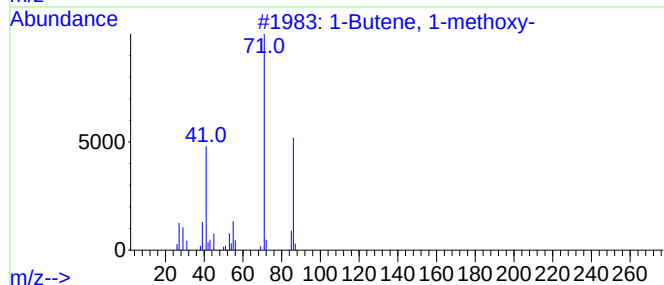
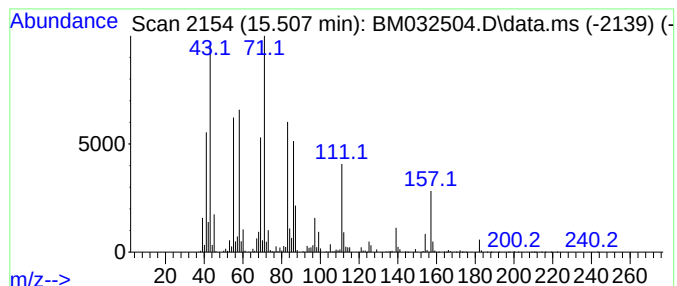
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 unknown15.507 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.507	130.23 ng	13136700	Acenaphthene-d10	14.260
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		1-Butene, 1-methoxy-	86 C5H10O	029512-02-5 30
2		3-Methyl-hepta-1,6-dien-3-ol	126 C8H14O	034780-69-3 27
3		trans-1-Methoxy-1-butene	86 C5H10O	010034-13-6 27
4		Acetic acid, (1,2-dimethyl-1-pro...	128 C7H12O2	003814-41-3 27
5		3-Methoxybut-1-ene	86 C5H10O	017351-24-5 27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
Operator : CG/JU
Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
2158

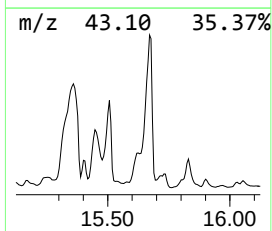
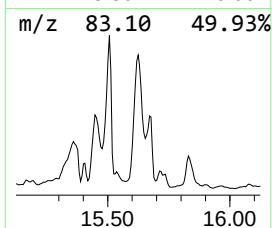
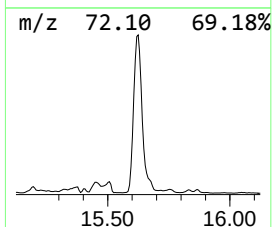
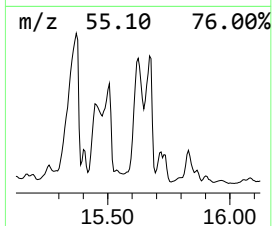
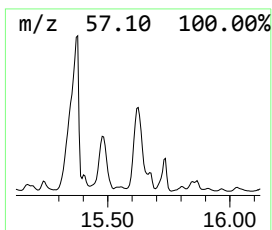
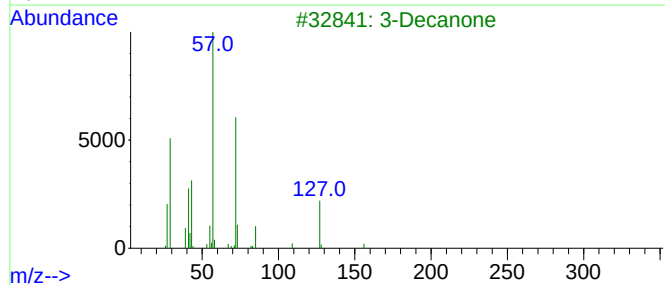
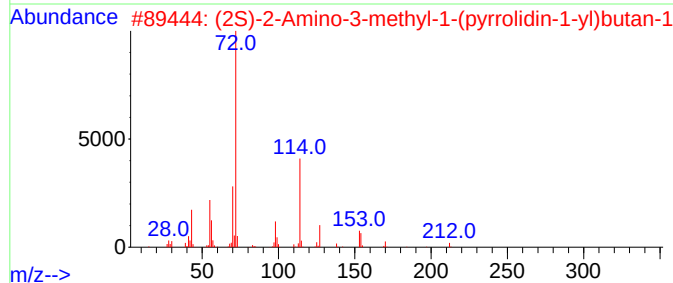
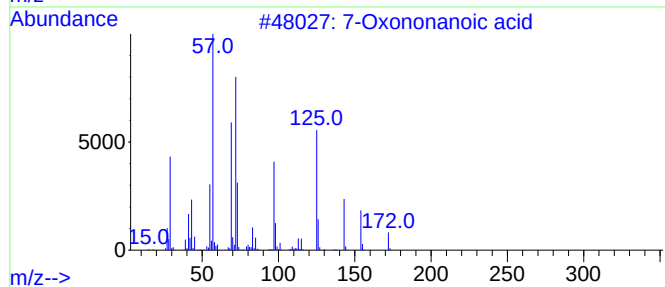
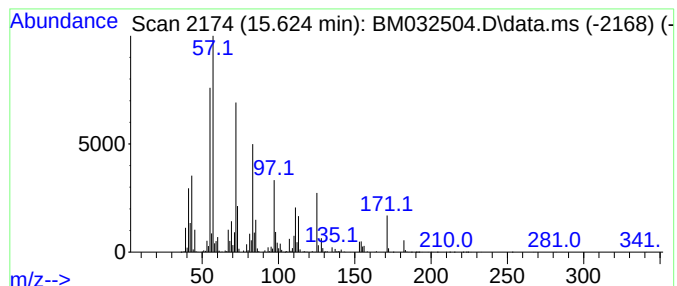
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 unknown15.624 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.624	69.75 ng	7233080	Phenanthrene-d10	16.989

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Oxononanoic acid	172	C9H16O3	020356-92-7	38
2			(2S)-2-Amino-3-methyl-1-(pyrroli...	212	C11H20N2O2	1000502-02-4	14
3			3-Decanone	156	C10H20O	000928-80-3	14
4			Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	14
5			1-Pentene, 2,3,3-trimethyl-	112	C8H16	000560-23-6	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
Data File : BM032504.D
Acq On : 13 Oct 2021 20:05
Operator : CG/JU
Sample : M4142-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
2158

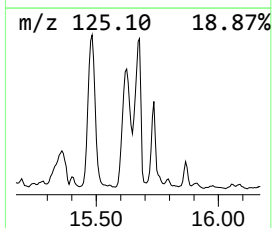
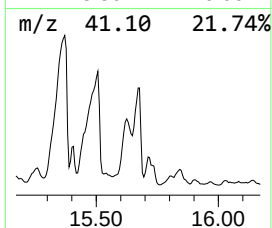
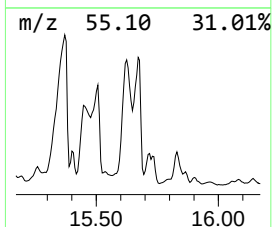
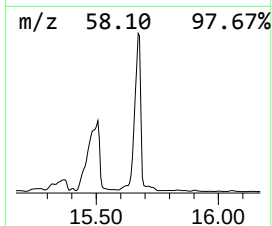
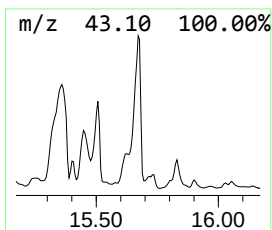
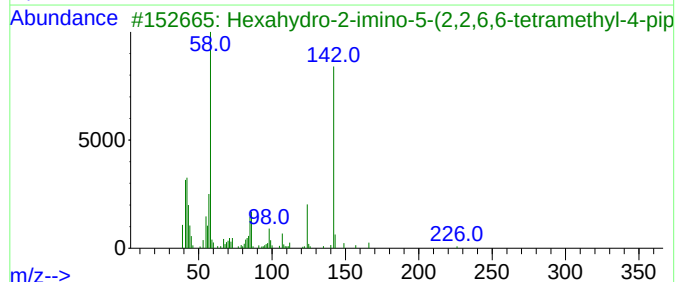
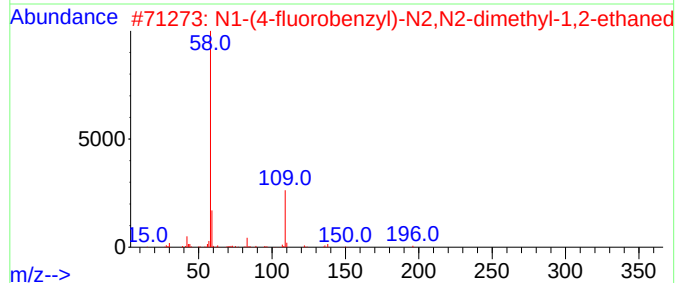
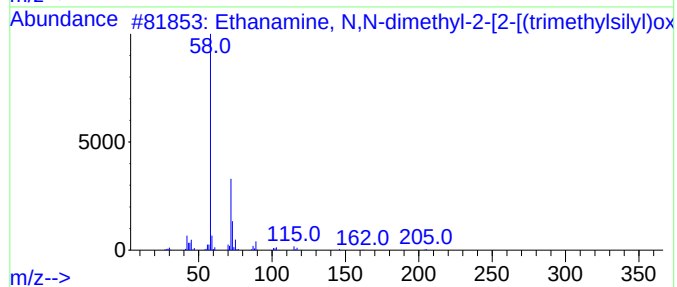
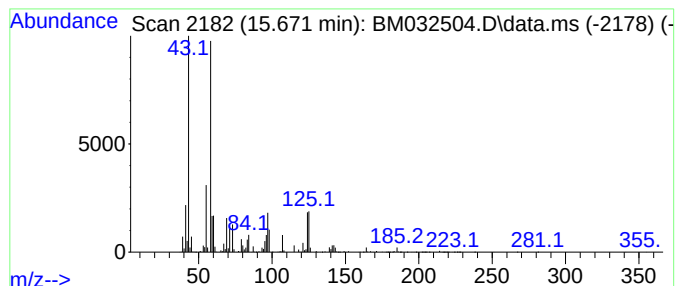
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 unknown15.671 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.671	71.11 ng	7373640	Phenanthrene-d10	16.989

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanamine, N,N-dimethyl-2-[2-(...	205	C9H23NO2Si	1309865-85-7	38
2			N1-(4-fluorobenzyl)-N2,N2-dimeth...	196	C11H17FN2	002714-80-9	37
3			Hexahydro-2-imino-5-(2,2,6,6-tet...	264	C13H24N6	329205-85-8	36
4			8-Oxononanoic acid	172	C9H16O3	025542-64-7	33
5			Cyclobutanecarboxylic acid, 2-di...	171	C9H17NO2	1000331-08-6	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM101321\
 Data File : BM032504.D
 Acq On : 13 Oct 2021 20:05
 Operator : CG/JU
 Sample : M4142-07
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 2158

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Octanone	7.066	69.1	ng	6183970	1	7.601	1790740	20.0
unknown8.313	8.313	47.0	ng	4204830	1	7.601	1790740	20.0
2-Nonanone	8.695	97.0	ng	8680620	1	7.601	1790740	20.0
Octanoic acid, ...	10.836	93.8	ng	17794800	2	10.389	3794900	20.0
Decanoic acid, ...	12.336	230.6	ng	23256400	3	14.260	2017410	20.0
1-Piperidinecar...	12.660	137.2	ng	13835400	3	14.260	2017410	20.0
unknown12.825	12.825	425.9	ng	42964800	3	14.260	2017410	20.0
unknown13.254	13.254	47.4	ng	4781150	3	14.260	2017410	20.0
Nonanoic acid, ...	13.507	136.5	ng	13771600	3	14.260	2017410	20.0
unknown13.595	13.595	263.6	ng	26586500	3	14.260	2017410	20.0
(S)-5-Butyl-5-e...	13.748	121.5	ng	12253500	3	14.260	2017410	20.0
unknown13.907	13.907	238.0	ng	24011300	3	14.260	2017410	20.0
unknown14.560	14.560	283.3	ng	28577500	3	14.260	2017410	20.0
unknown14.795	14.795	149.4	ng	15074600	3	14.260	2017410	20.0
unknown14.871	14.871	154.3	ng	15561000	3	14.260	2017410	20.0
unknown14.930	14.930	72.9	ng	7357330	3	14.260	2017410	20.0
unknown15.371	15.371	184.9	ng	18646800	3	14.260	2017410	20.0
unknown15.507	15.507	130.2	ng	13136700	3	14.260	2017410	20.0
unknown15.624	15.624	69.8	ng	7233080	4	16.989	2073940	20.0
unknown15.671	15.671	71.1	ng	7373640	4	16.989	2073940	20.0