

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
 Data File : BF130319.D
 Acq On : 19 Sep 2022 14:11
 Operator : CG\JU
 Sample : N4628-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HW-54

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_F\Methods\8270-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.840	463	468	475	rBV	118452	156448	3.31%	0.341%
2	5.257	532	539	551	rBV	1398188	1341657	28.38%	2.921%
3	6.292	711	715	720	rVB	934556	835743	17.68%	1.820%
4	6.657	773	777	781	rBV	682978	611055	12.93%	1.331%
5	6.716	784	787	790	rVB	118243	92499	1.96%	0.201%
6	6.816	798	804	806	rBV3	40037	60626	1.28%	0.132%
7	6.981	829	832	837	rBV2	38424	61415	1.30%	0.134%
8	7.063	841	846	849	rBV5	37118	60456	1.28%	0.132%
9	7.228	863	874	877	rBV	1924293	2259837	47.81%	4.921%
10	7.345	891	894	897	rVB3	94973	97724	2.07%	0.213%
11	7.428	906	908	911	rVV3	88201	85970	1.82%	0.187%
12	7.457	911	913	915	rVB	81386	53833	1.14%	0.117%
13	7.604	930	938	944	rBV4	173988	264878	5.60%	0.577%
14	7.681	944	951	954	rBV4	263699	382770	8.10%	0.833%
15	7.739	958	961	964	rVV3	93003	126015	2.67%	0.274%
16	7.781	964	968	971	rVB	168226	218439	4.62%	0.476%
17	7.816	971	974	981	rBV4	48062	67406	1.43%	0.147%
18	7.910	981	990	991	rBV7	157849	318561	6.74%	0.694%
19	7.939	991	995	997	rVV	901315	880605	18.63%	1.917%
20	7.969	997	1000	1009	rVV5	242048	627131	13.27%	1.366%
21	8.039	1009	1012	1016	rVB2	154332	179158	3.79%	0.390%
22	8.110	1017	1024	1026	rVB	328199	452353	9.57%	0.985%
23	8.139	1026	1029	1030	rBV2	111729	111439	2.36%	0.243%
24	8.163	1031	1033	1035	rVV2	124379	147079	3.11%	0.320%
25	8.192	1035	1038	1041	rVV2	257954	400614	8.48%	0.872%
26	8.228	1041	1044	1046	rVV3	231399	263910	5.58%	0.575%
27	8.251	1046	1048	1049	rVV2	134950	107780	2.28%	0.235%
28	8.269	1049	1051	1053	rVB	213626	153160	3.24%	0.333%
29	8.357	1058	1066	1069	rBV2	501877	872183	18.45%	1.899%
30	8.404	1071	1074	1077	rVV3	163743	253164	5.36%	0.551%
31	8.457	1080	1083	1086	rVB3	303505	304522	6.44%	0.663%
32	8.492	1086	1089	1092	rVB4	199430	222341	4.70%	0.484%
33	8.545	1092	1098	1100	rBV3	318521	470655	9.96%	1.025%
34	8.575	1100	1103	1104	rBV	89349	69797	1.48%	0.152%
35	8.592	1104	1106	1109	rBV3	139928	144822	3.06%	0.315%
36	8.704	1119	1125	1127	rBV5	295798	531633	11.25%	1.158%

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.733	1127	1130	1132	rVV	476014	552934	11.70%	1.204%
38	8.769	1132	1136	1138	rVV4	239908	379249	8.02%	0.826%
39	8.804	1138	1142	1145	rVV3	466340	661595	14.00%	1.441%
40	8.845	1145	1149	1151	rVV2	301095	402532	8.52%	0.876%

41	8.892	1151	1157	1159	rVV2	553945	893846	18.91%	1.946%
42	8.922	1159	1162	1165	rVB3	284101	359270	7.60%	0.782%
43	8.963	1165	1169	1174	rBV5	367216	485573	10.27%	1.057%
44	9.022	1174	1179	1181	rVB	4034947	3422065	72.40%	7.451%
45	9.051	1181	1184	1187	rVB2	314300	292348	6.18%	0.637%

46	9.080	1187	1189	1191	rBV3	65021	64413	1.36%	0.140%
47	9.104	1191	1193	1195	rVB2	116207	77597	1.64%	0.169%
48	9.133	1195	1198	1200	rBV2	147605	169751	3.59%	0.370%
49	9.186	1204	1207	1208	rBV2	238541	244651	5.18%	0.533%
50	9.251	1216	1218	1219	rBV	75657	53220	1.13%	0.116%

51	9.275	1219	1222	1225	rVV4	269804	298833	6.32%	0.651%
52	9.333	1228	1232	1236	rBV3	394902	730329	15.45%	1.590%
53	9.386	1236	1241	1243	rVV2	470825	820671	17.36%	1.787%
54	9.410	1243	1245	1247	rVB	463745	395851	8.37%	0.862%
55	9.451	1247	1252	1253	rBV4	227361	280172	5.93%	0.610%

56	9.486	1256	1258	1260	rVB2	135780	93786	1.98%	0.204%
57	9.510	1260	1262	1265	rVB2	199986	172782	3.66%	0.376%
58	9.563	1268	1271	1273	rBV	212356	274595	5.81%	0.598%
59	9.692	1290	1293	1295	rVB	878275	749271	15.85%	1.631%
60	9.727	1296	1299	1302	rVB4	308829	280960	5.94%	0.612%

61	9.763	1302	1305	1307	rVB	453409	400929	8.48%	0.873%
62	9.792	1307	1310	1312	rBV4	183214	218898	4.63%	0.477%
63	9.827	1313	1316	1319	rVB2	431595	402586	8.52%	0.877%
64	9.875	1321	1324	1327	rBV	332272	343794	7.27%	0.749%
65	9.945	1335	1336	1338	rBV2	100910	98154	2.08%	0.214%

66	9.998	1343	1345	1348	rBV2	329906	372297	7.88%	0.811%
67	10.022	1348	1349	1354	rVB	274946	270872	5.73%	0.590%
68	10.080	1354	1359	1362	rBV6	199211	338856	7.17%	0.738%
69	10.116	1363	1365	1369	rBV5	108852	116494	2.46%	0.254%
70	10.157	1369	1372	1375	rVV3	278625	315509	6.67%	0.687%

71	10.210	1379	1381	1384	rVB2	212392	166473	3.52%	0.362%
72	10.239	1384	1386	1389	rVB3	219801	206662	4.37%	0.450%
73	10.292	1391	1395	1398	rBV2	469742	621474	13.15%	1.353%
74	10.316	1398	1399	1403	rVB4	244516	223222	4.72%	0.486%
75	10.404	1411	1414	1417	rBV	266016	293007	6.20%	0.638%

76	10.480	1423	1427	1431	rVB	2021105	1996423	42.24%	4.347%
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77	10.545	1434	1438	1442	rVB	469400	487025	10.30%	1.060%
78	10.663	1455	1458	1459	rBV3	107629	110826	2.34%	0.241%
79	10.680	1459	1461	1466	rVB3	200566	257067	5.44%	0.560%
80	10.757	1471	1474	1475	rBV	81247	70917	1.50%	0.154%
81	10.886	1493	1496	1499	rVB4	117739	123088	2.60%	0.268%
82	10.916	1499	1501	1504	rVB3	83208	60538	1.28%	0.132%
83	11.086	1526	1530	1532	rBV2	101426	159892	3.38%	0.348%
84	11.110	1532	1534	1537	rVB	171583	137355	2.91%	0.299%
85	11.139	1537	1539	1541	rVB2	78016	59542	1.26%	0.130%
86	11.169	1541	1544	1547	rBV	793762	669437	14.16%	1.458%
87	11.574	1610	1613	1616	rBV2	155237	147319	3.12%	0.321%
88	11.704	1632	1635	1636	rBV3	319475	289891	6.13%	0.631%
89	11.733	1636	1640	1646	rVB	1568472	1703864	36.05%	3.710%
90	11.939	1672	1675	1678	rBV4	73749	130728	2.77%	0.285%
91	12.410	1752	1755	1756	rBV	263135	243105	5.14%	0.529%
92	12.521	1765	1774	1777	rVB2	2813061	4726821	100.00%	10.292%
93	12.757	1809	1814	1818	rVB	2656892	2570721	54.39%	5.597%
94	13.215	1890	1892	1894	rBV	81899	88270	1.87%	0.192%
95	13.798	1987	1991	1994	rBV	605938	604048	12.78%	1.315%
96	13.821	1994	1995	2000	rVB	121210	79598	1.68%	0.173%
97	14.204	2057	2060	2068	rVB	148097	265636	5.62%	0.578%
98	15.186	2223	2227	2231	rBV	447967	473191	10.01%	1.030%
99	15.327	2244	2251	2271	rBV	128848	638071	13.50%	1.389%

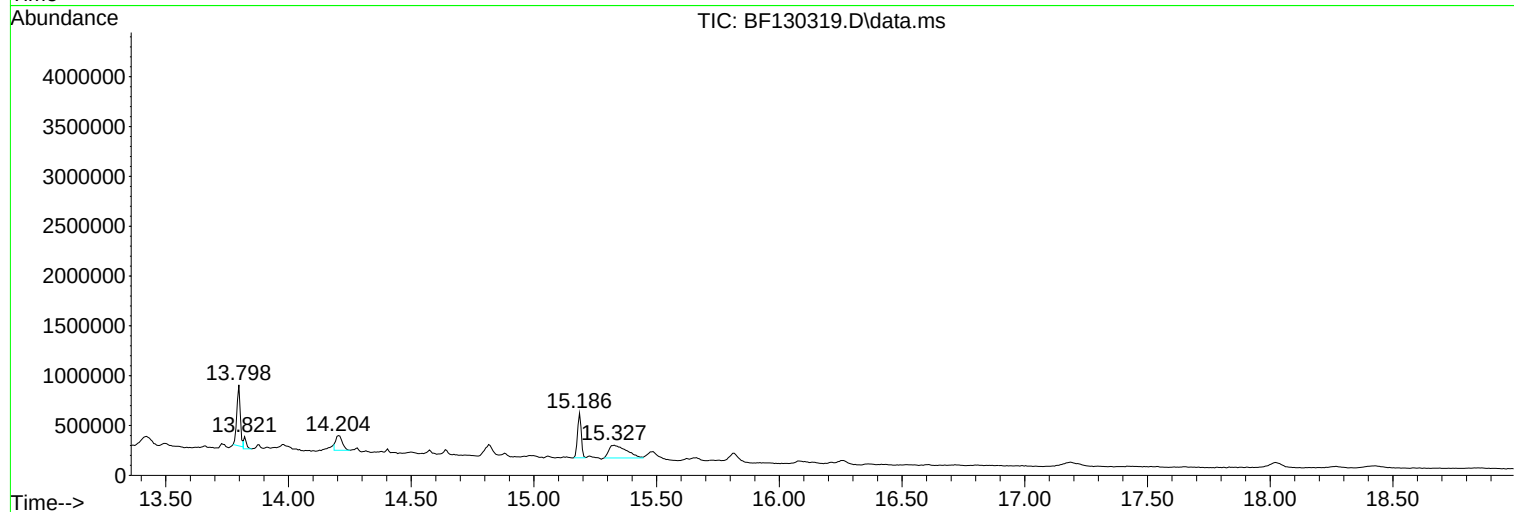
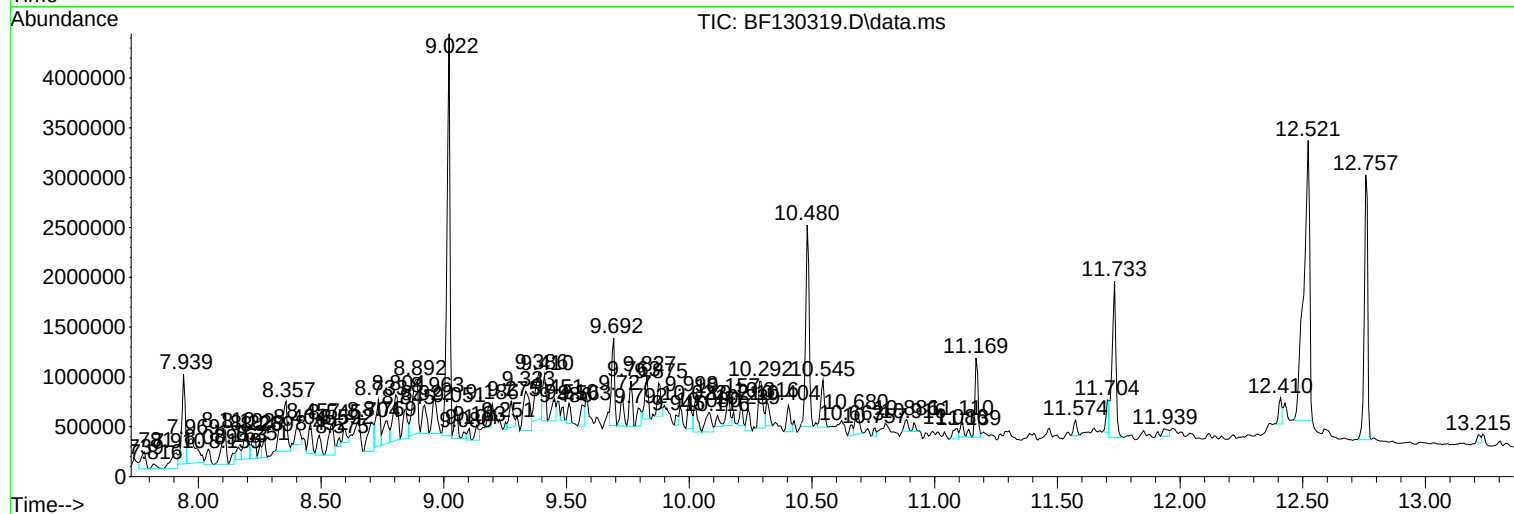
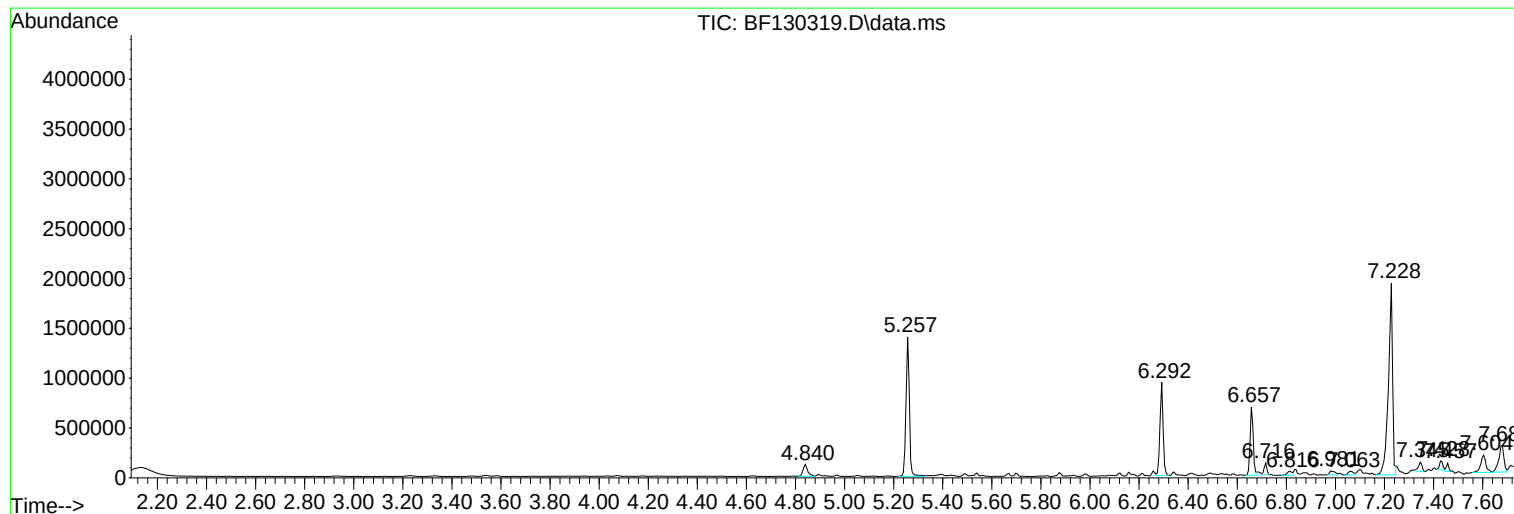
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Instrument :
BNA_F
ClientSampleId :
HW-54

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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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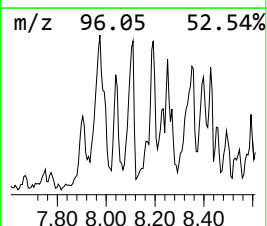
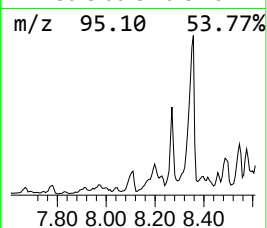
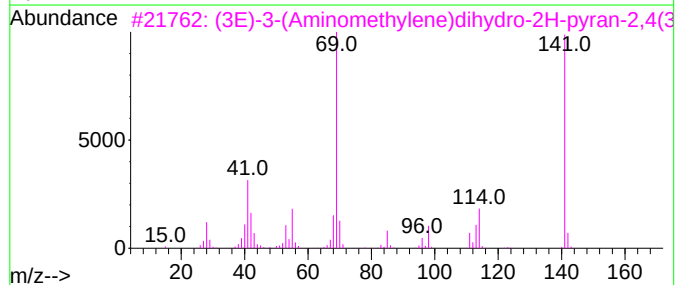
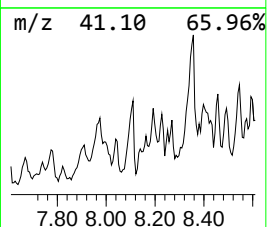
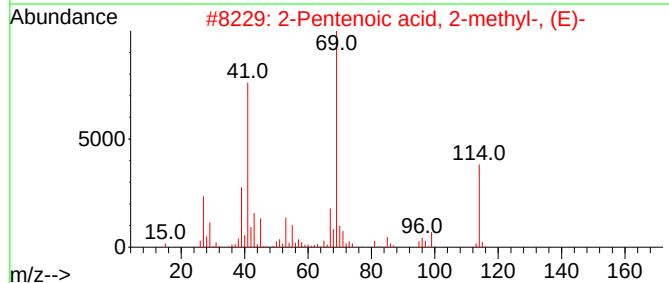
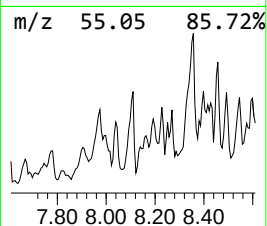
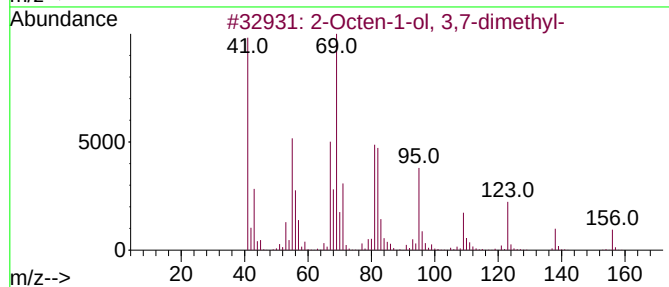
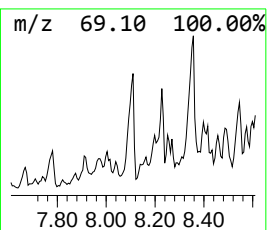
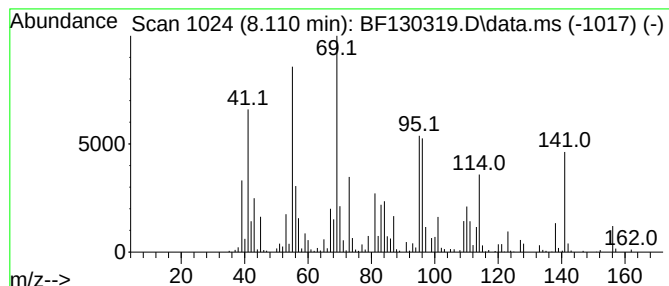
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown8.110 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	10.27 ng	452353	Naphthalene-d8	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octen-1-ol, 3,7-dimethyl-	156	C10H20O	040607-48-5	38
2			2-Pentenoic acid, 2-methyl-, (E)-	114	C6H10O2	016957-70-3	38
3			(3E)-3-(Aminomethylene)dihydro-2...	141	C6H7NO3	022108-77-6	35
4			2-Cyclohexen-1-one, 4-(1-methyle...	138	C9H14O	000500-02-7	35
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	25



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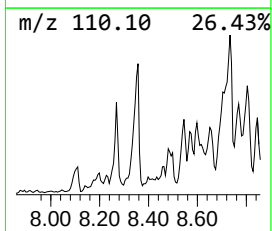
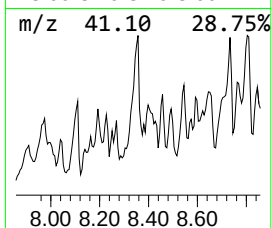
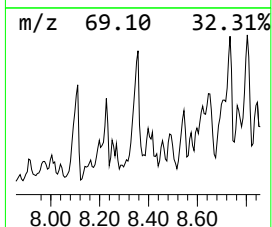
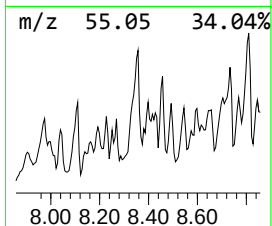
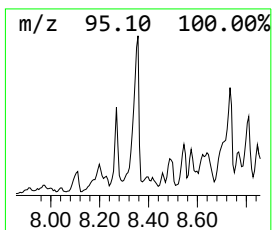
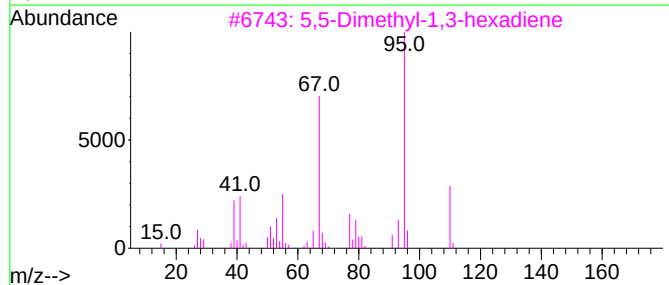
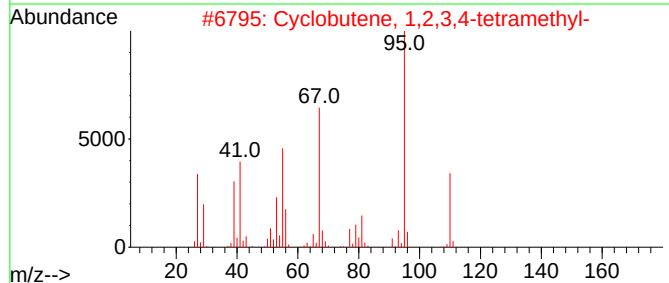
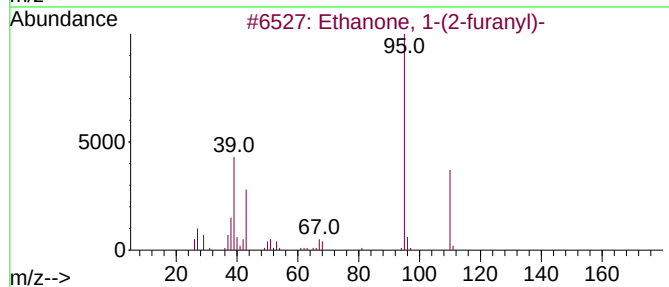
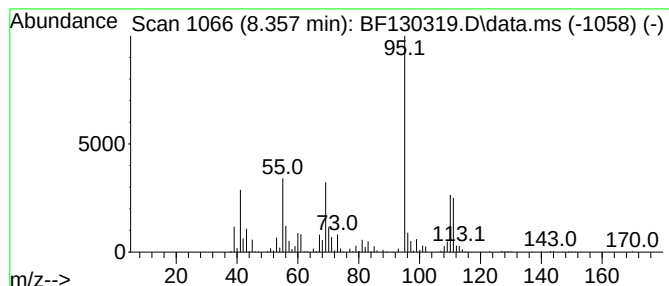
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanone, 1-(2-furanyl)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.357	19.81 ng	872183	Naphthalene-d8	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanone, 1-(2-furanyl)-	110	C6H6O2	001192-62-7	52
2			Cyclobutene, 1,2,3,4-tetramethyl-	110	C8H14	090346-45-5	50
3			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	50
4			1,3-Dimethyl-5-heptafluorobutyryl...	324	C12H15F7O2	1000216-63-8	45
5			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	42



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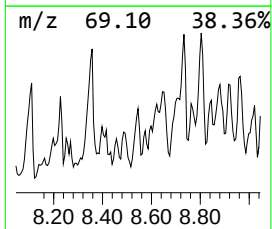
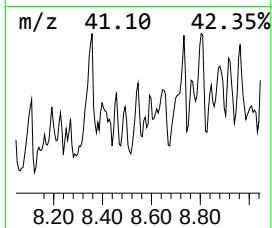
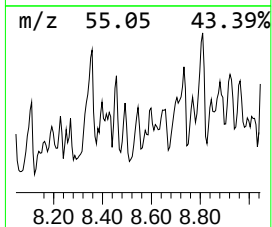
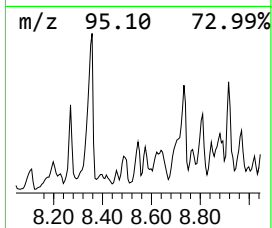
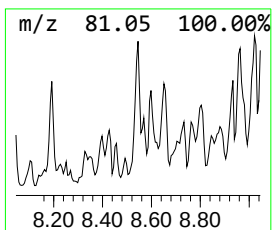
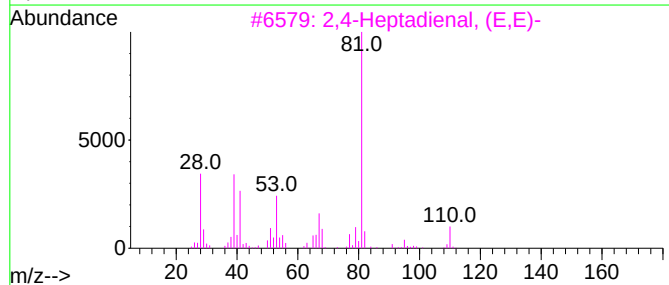
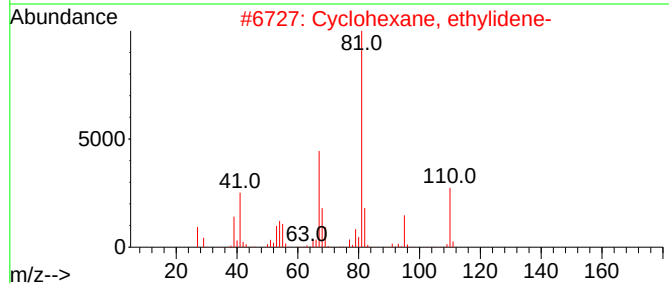
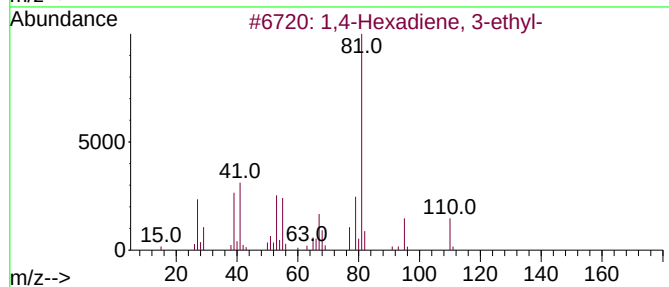
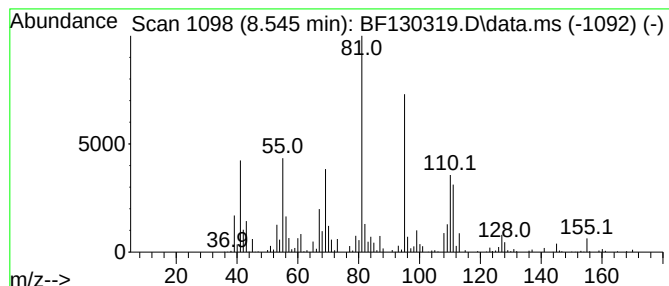
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown8.545 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.545	10.69 ng	470655	Naphthalene-d8	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Hexadiene, 3-ethyl-	110	C8H14	002080-89-9	47
2			Cyclohexane, ethylidene-	110	C8H14	001003-64-1	47
3			2,4-Heptadienal, (E,E)-	110	C7H10O	004313-03-5	43
4			2-Furancarboxylic acid, 2-ethylc...	222	C13H18O3	1000278-83-7	27
5			3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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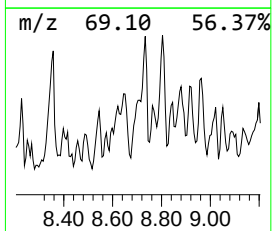
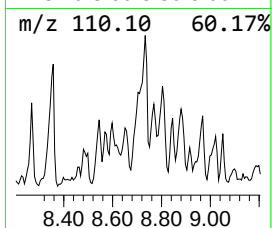
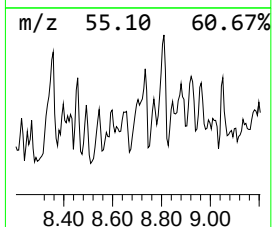
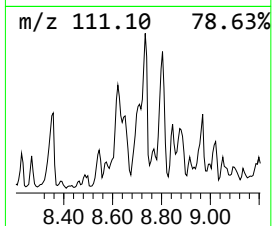
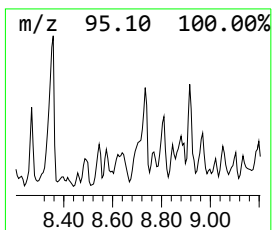
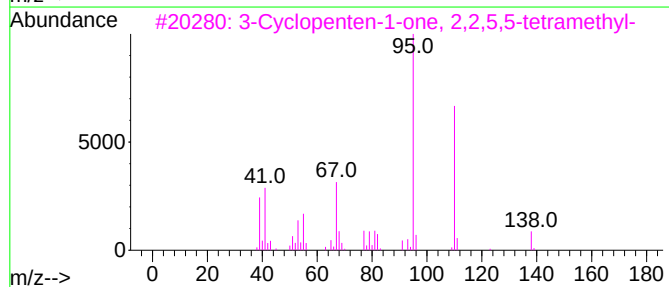
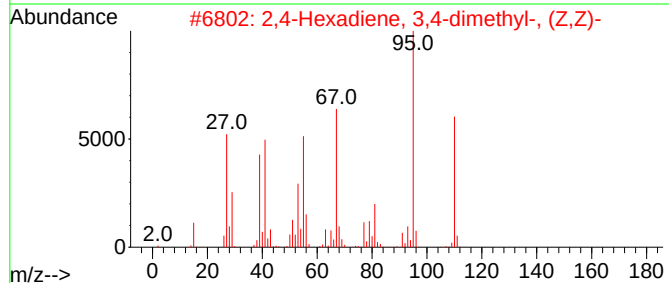
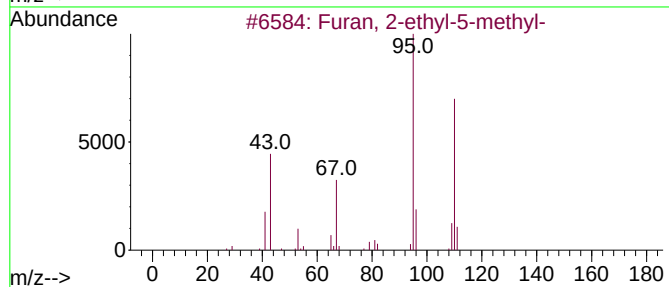
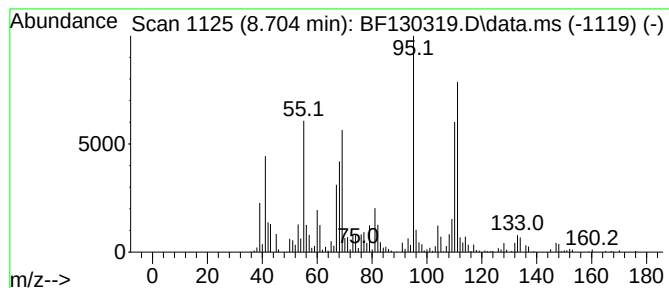
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown8.704 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.704	12.07 ng	531633	Naphthalene-d8	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	43
2			2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	38
3			3-Cyclopenten-1-one, 2,2,5,5-tet...	138	C9H14O	081396-36-3	38
4			1,3-Dimethyl-5-heptafluorobutyry...	324	C12H15F7O2	1000216-63-8	38
5			Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
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Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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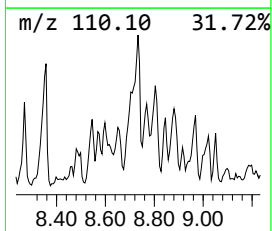
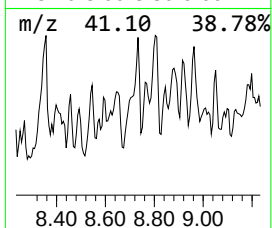
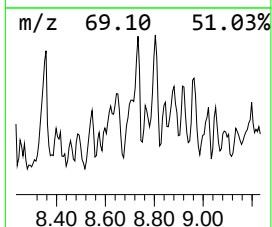
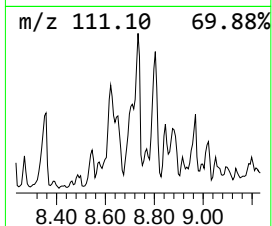
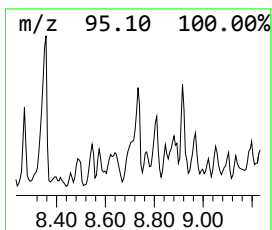
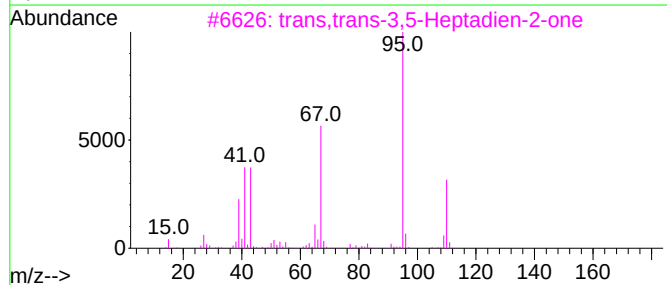
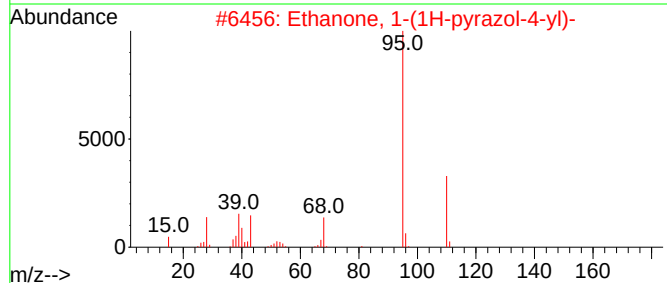
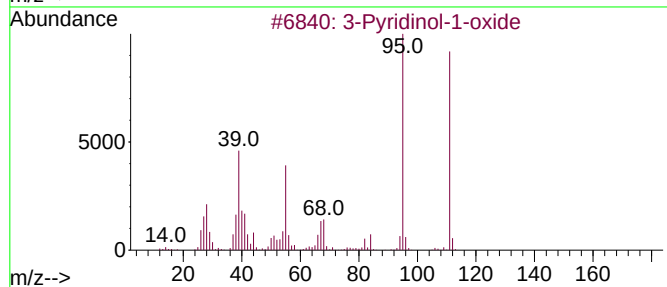
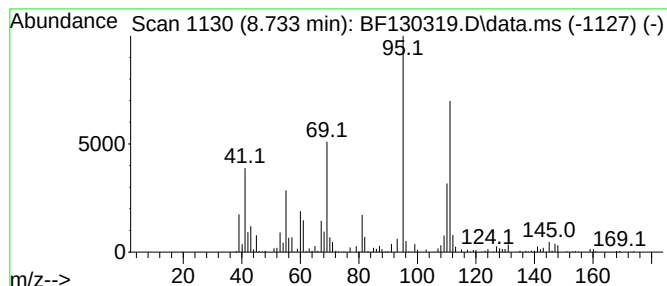
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 3-Pyridinol-1-oxide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.733	12.56 ng	552934	Naphthalene-d8	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pyridinol-1-oxide	111	C5H5NO2	006602-28-4	50
2			Ethanone, 1-(1H-pyrazol-4-yl)-	110	C5H6N2O	025016-16-4	46
3			trans,trans-3,5-Heptadien-2-one	110	C7H10O	018402-90-9	43
4			4,4-Dimethyl-2-cyclopenten-1-one	110	C7H10O	022748-16-9	43
5			Succinic acid, di(3,5-dimethylcy...	338	C20H34O4	1000330-05-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
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Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

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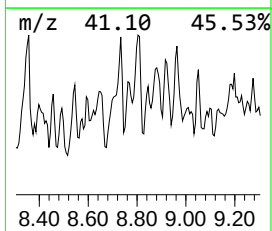
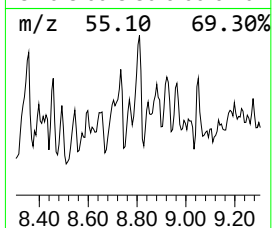
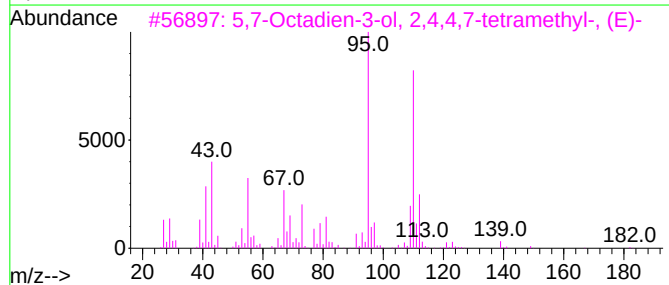
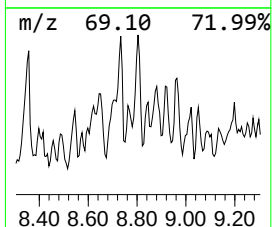
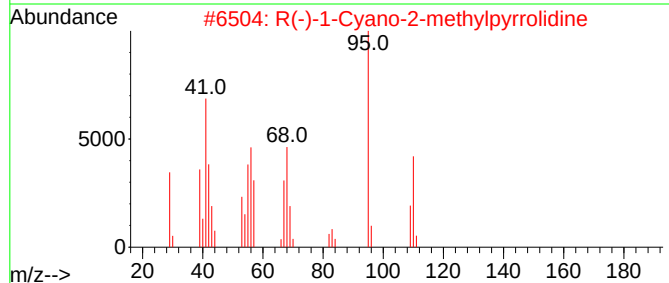
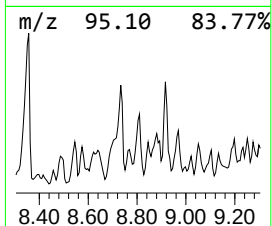
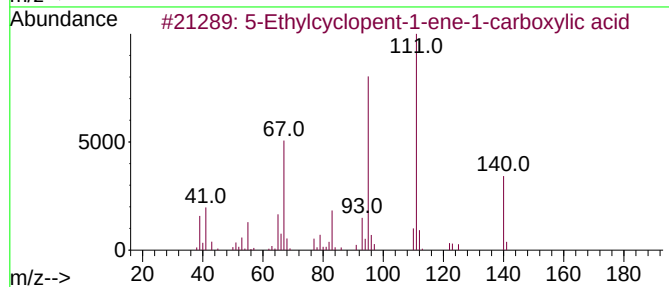
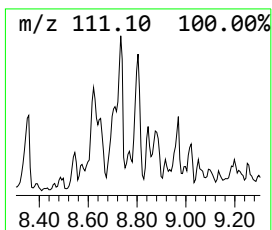
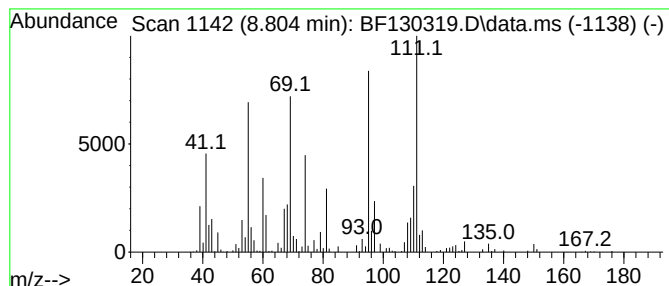
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown8.804 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.804	15.03 ng	661595	Naphthalene-d8	7.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Ethylcyclopent-1-ene-1-carboxy...	140	C8H12O2	036258-07-8	43
2			R(-)-1-Cyano-2-methylpyrrolidine	110	C6H10N2	1000145-01-8	30
3			5,7-Octadien-3-ol, 2,4,4,7-tetra...	182	C12H22O	077142-78-0	27
4			Bicyclo[3.1.0]hexane, 1,5-dimethyl-	110	C8H14	1010142-17-5	25
5			Cyclobutene, 1,2,3,4-tetramethyl-	110	C8H14	090346-45-5	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
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Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

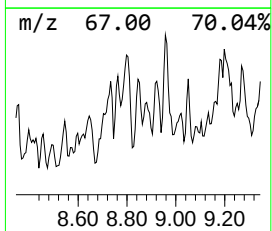
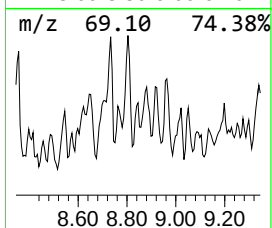
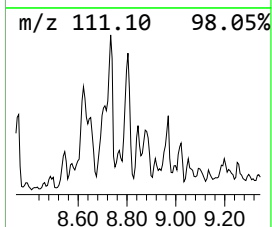
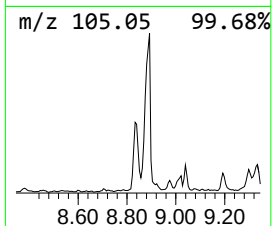
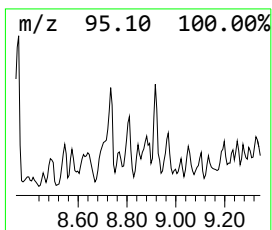
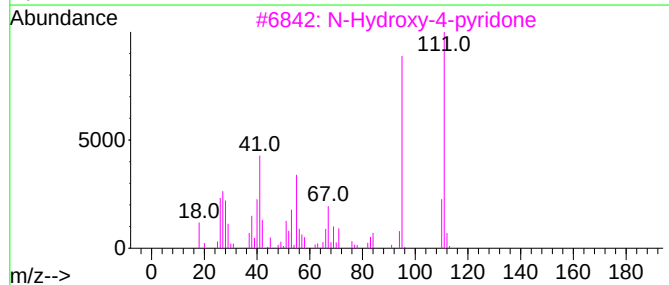
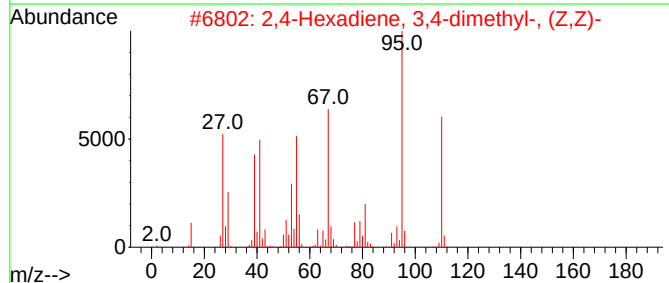
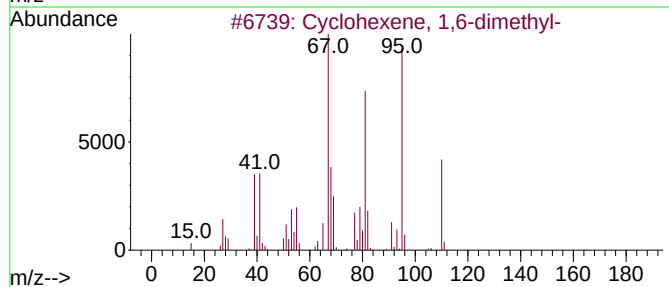
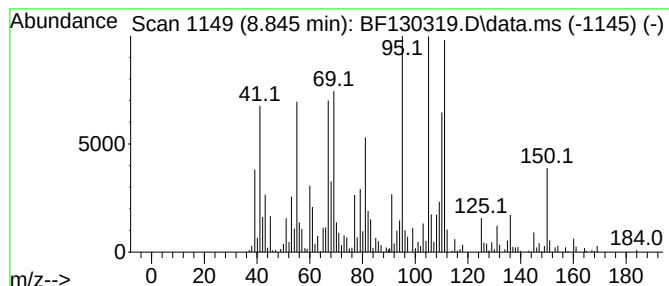
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.845 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.845	10.74 ng	402532	Acenaphthene-d10	9.692	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1,6-dimethyl-	110	C8H14	001759-64-4	38
2	2,4-Hexadiene, 3,4-dimethyl-, (Z...	110	C8H14	021293-01-6	38
3	N-Hydroxy-4-pyridone	111	C5H5NO2	1010426-43-6	38
4	2-Cyclopenten-1-one, 3,4-dimethyl-	110	C7H10O	030434-64-1	30
5	2,4-Hexadiene, 3,4-dimethyl-, (E...	110	C8H14	002417-88-1	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
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Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-54

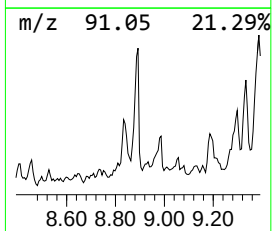
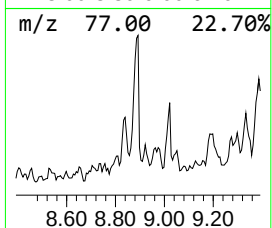
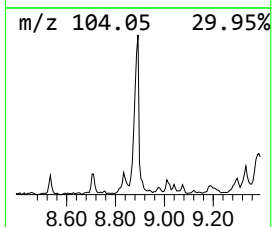
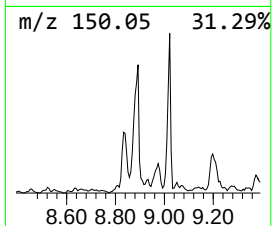
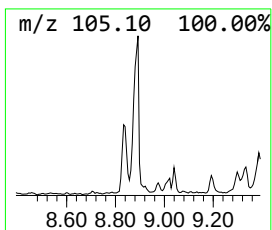
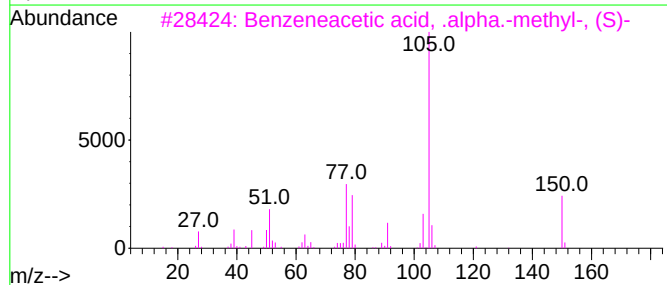
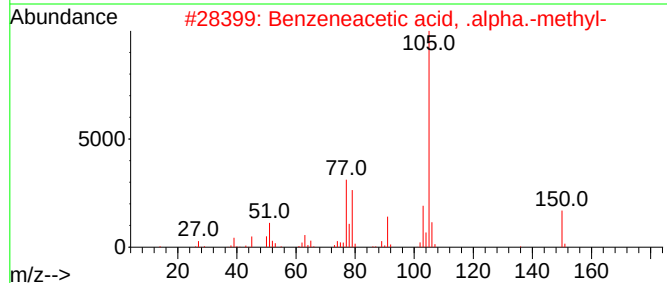
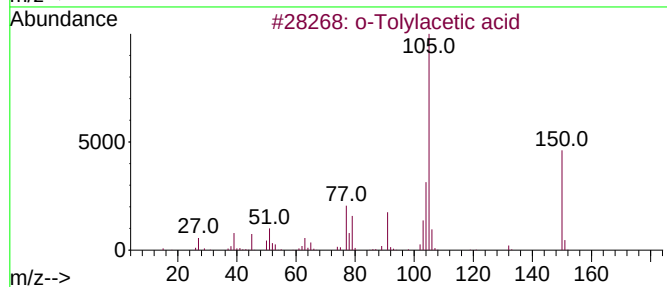
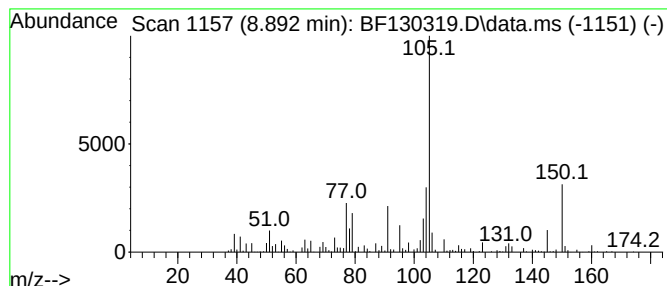
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 o-Tolylacetic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.892	23.86 ng	893846	Acenaphthene-d10	9.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			o-Tolylacetic acid	150	C9H10O2	000644-36-0	70
2			Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	60
3			Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-24-3	55
4			Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-26-5	55
5			p-Tolylacetic acid	150	C9H10O2	000622-47-9	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
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Misc :
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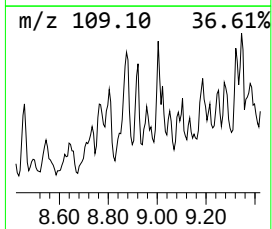
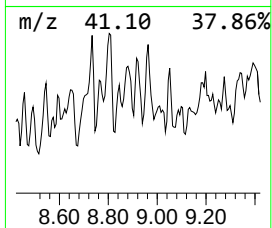
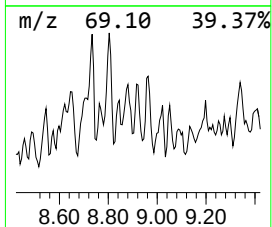
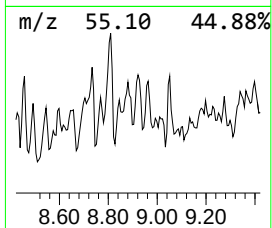
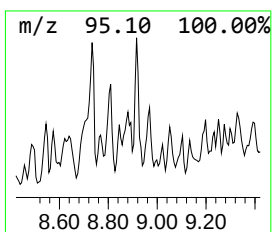
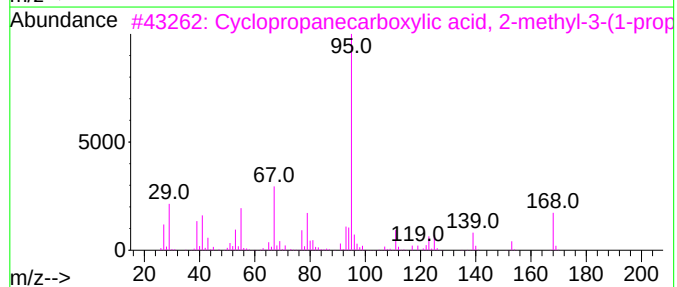
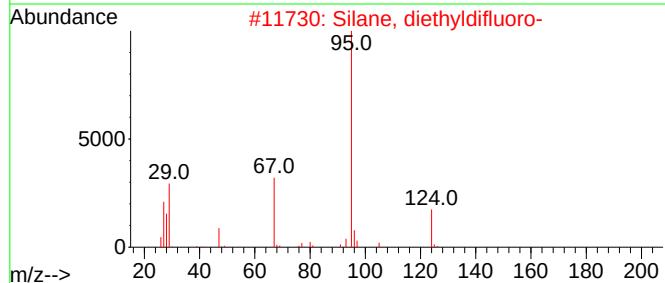
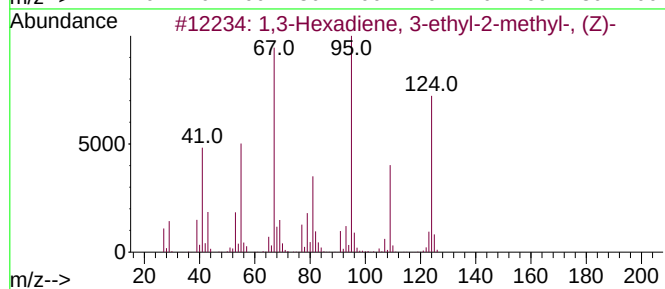
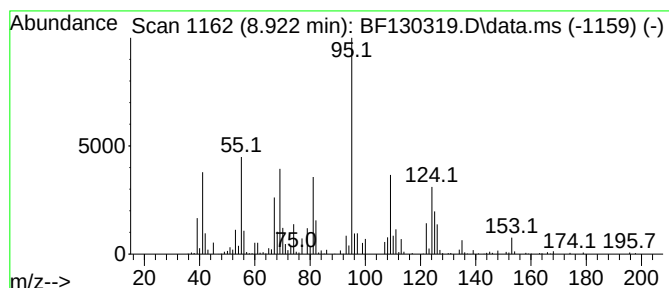
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,3-Hexadiene, 3-ethyl-2-me... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.922	9.59 ng	359270	Acenaphthene-d10	9.692	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexadiene, 3-ethyl-2-methyl-...	124	C9H16	074752-97-9	58
2	Silane, diethyldifluoro-	124	C4H10F2Si	000358-06-5	50
3	Cyclopropanecarboxylic acid, 2-m...	168	C10H16O2	030626-51-8	47
4	Furyl hydroxymethyl ketone	126	C6H6O3	017678-19-2	43
5	2-Decyne	138	C10H18	002384-70-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
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ALS Vial : 7 Sample Multiplier: 1

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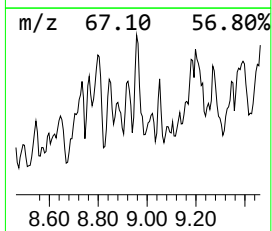
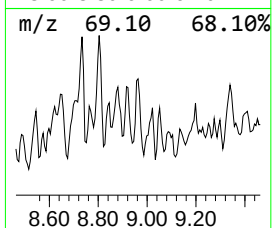
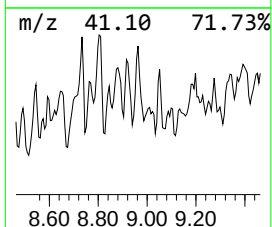
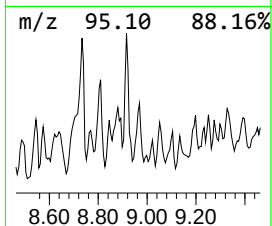
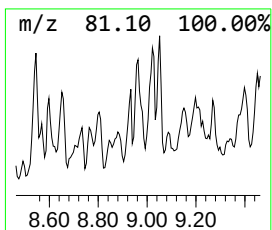
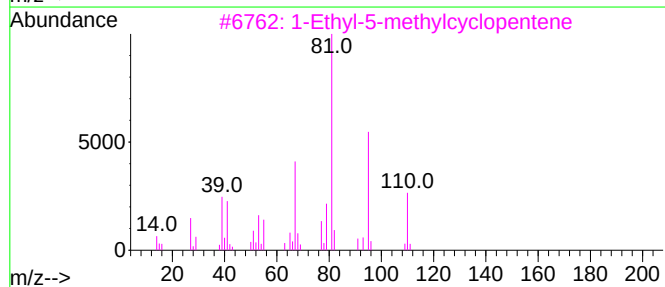
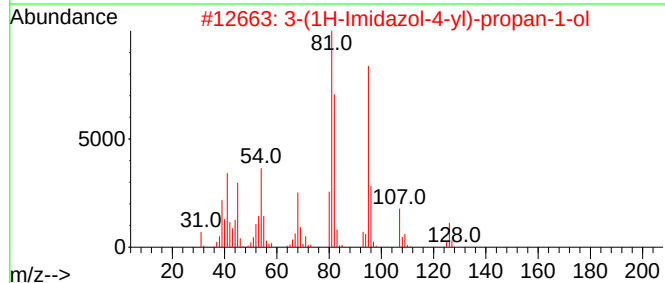
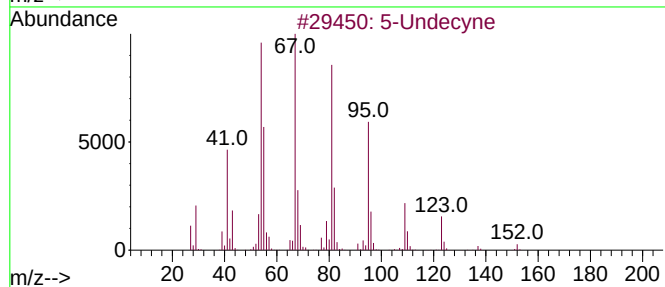
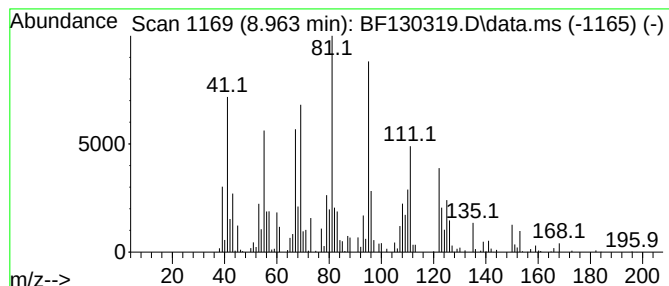
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown8.963 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.963	12.96 ng	485573	Acenaphthene-d10	9.692

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Undecyne	152	C11H20	002294-72-6	49
2	3	(1H-Imidazol-4-yl)-propan-1-ol	126	C6H10N2O	049549-75-9	38
3	1	Ethyl-5-methylcyclopentene	110	C8H14	097797-57-4	30
4	(4R*,5R*,9S*)	-5,9-Dimethylspiro[...]	166	C11H18O	063088-19-7	30
5	5	Dodecyne	166	C12H22	019780-12-2	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-54

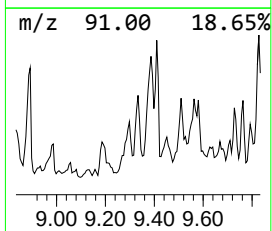
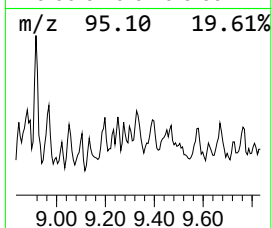
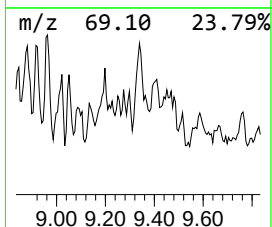
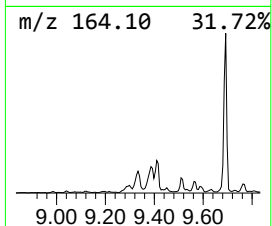
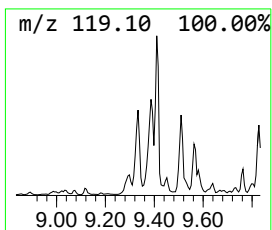
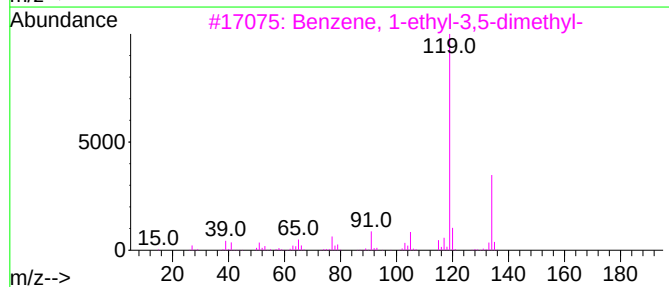
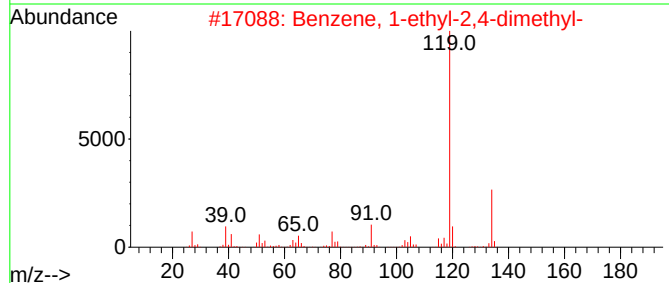
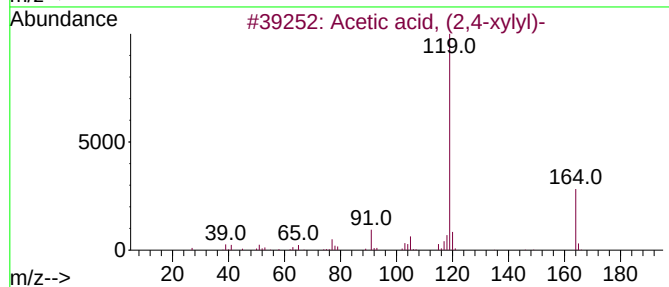
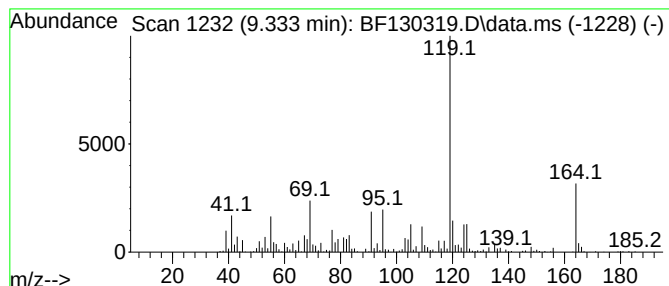
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown9.333 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.333	19.49 ng	730329	Acenaphthene-d10	9.692

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	64
2		Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	43
3		Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	43
4		o-Cymene	134	C10H14	000527-84-4	43
5		Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

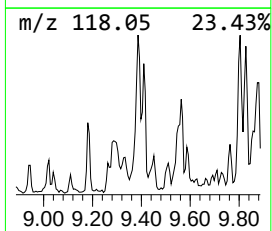
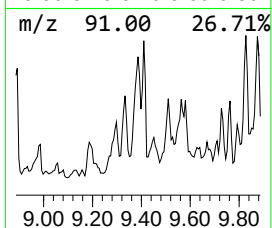
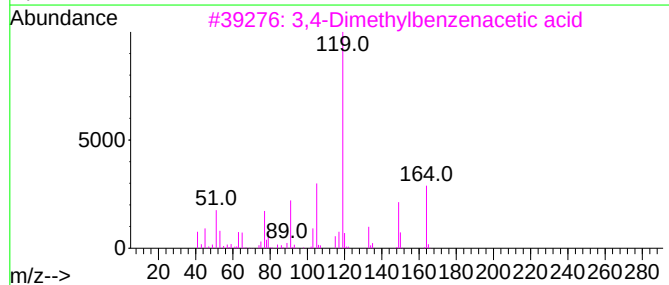
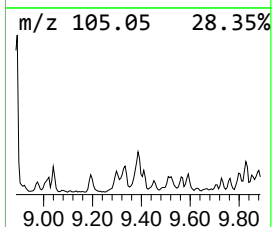
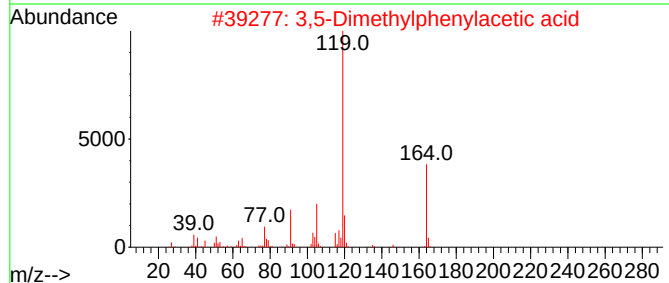
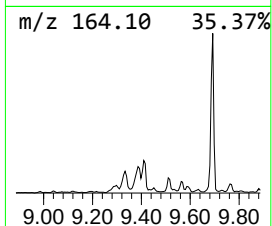
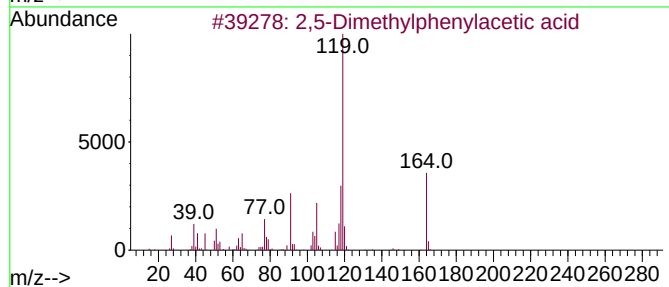
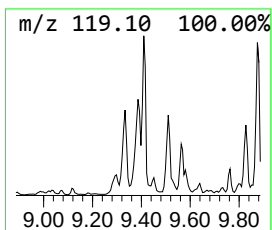
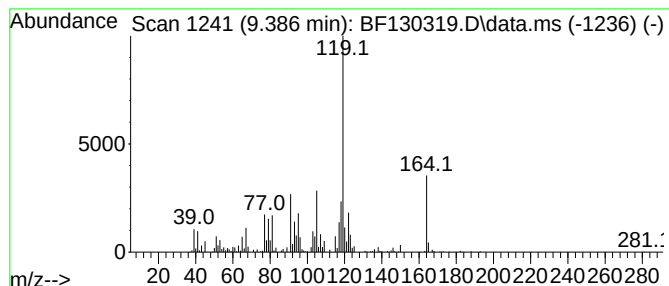
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2,5-Dimethylphenylacetic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.386	21.91 ng	820671	Acenaphthene-d10			9.692
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,5-Dimethylphenylacetic acid		164	C10H12O2	1000342-65-5	87
2	3,5-Dimethylphenylacetic acid		164	C10H12O2	042288-46-0	81
3	3,4-Dimethylbenzenacetic acid		164	C10H12O2	017283-16-8	64
4	Acetic acid, (2,4-xylyl)-		164	C10H12O2	006331-04-0	53
5	Cumene hydroperoxide, TMS deriva...		224	C12H20O2Si	018057-16-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-54

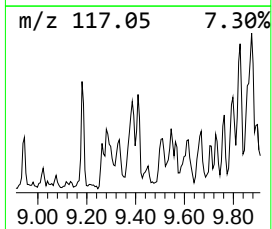
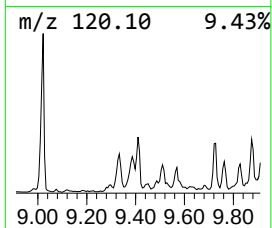
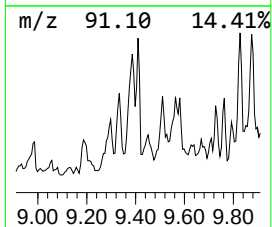
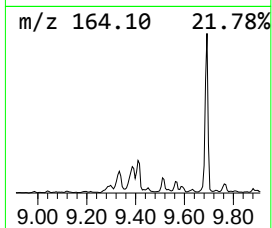
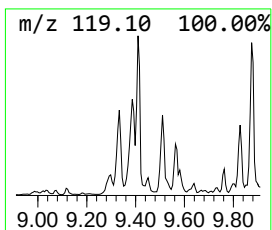
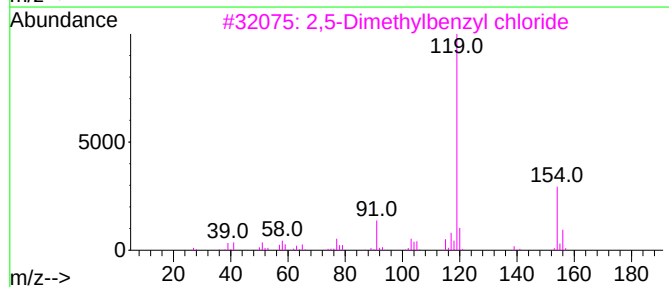
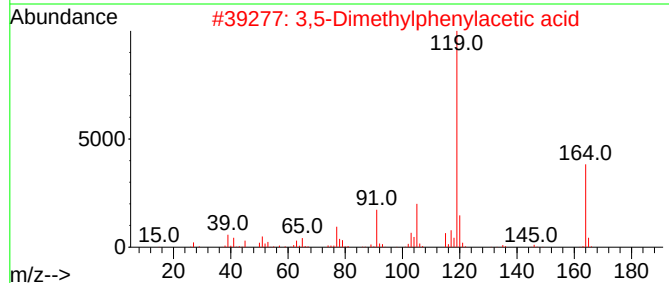
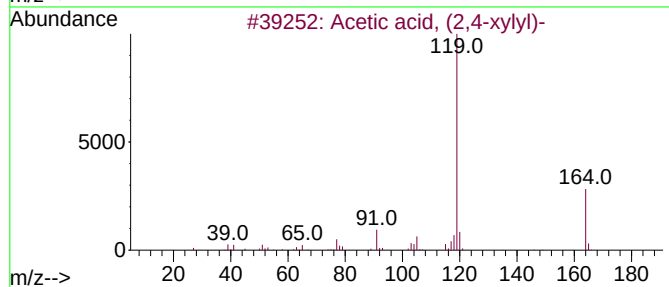
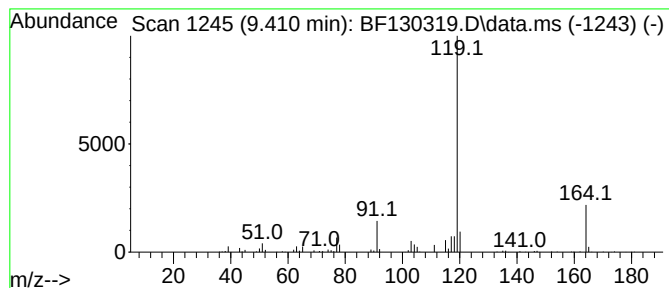
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Acetic acid, (2,4-xylyl)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.410	10.57 ng	395851	Acenaphthene-d10	9.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, (2,4-xylyl)-	164	C10H12O2	006331-04-0	91
2			3,5-Dimethylphenylacetic acid	164	C10H12O2	042288-46-0	86
3			2,5-Dimethylbenzyl chloride	154	C9H11Cl	000824-45-3	72
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-54

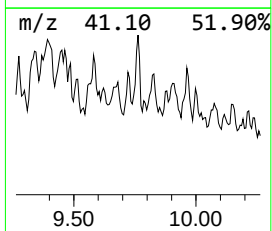
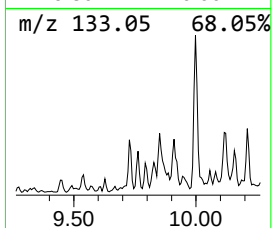
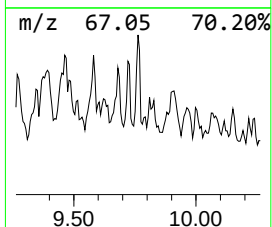
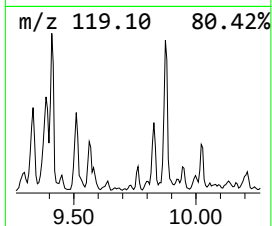
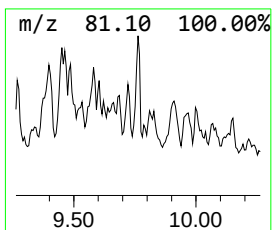
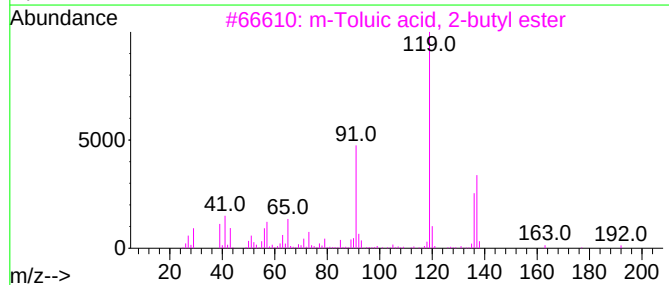
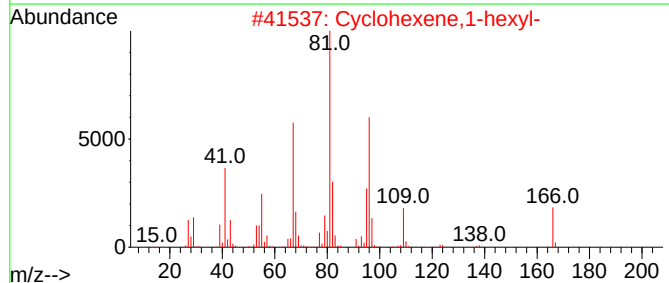
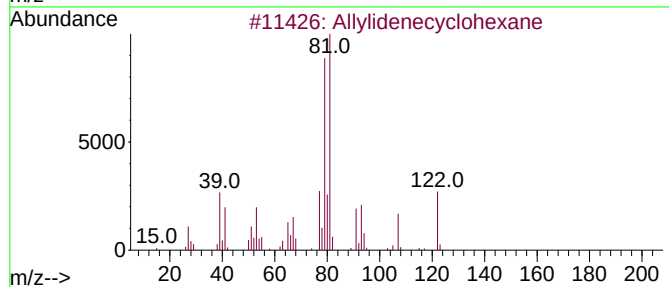
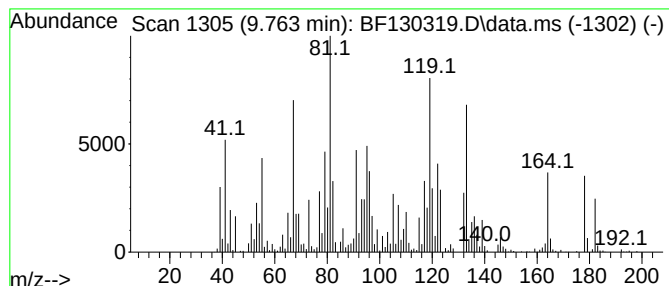
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown9.763 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.763	10.70 ng	400929	Acenaphthene-d10	9.692

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Allylidene cyclohexane	122	C9H14	005664-10-8	35
2		Cyclohexene, 1-hexyl-	166	C12H22	003964-66-7	25
3		m-Toluic acid, 2-butyl ester	192	C12H16O2	005448-57-7	15
4		1,4-Hexadiene, 3-ethyl-	110	C8H14	002080-89-9	11
5		Benzene, isocyanato-	119	C7H5NO	000103-71-9	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-54

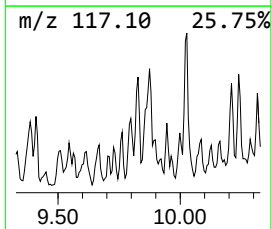
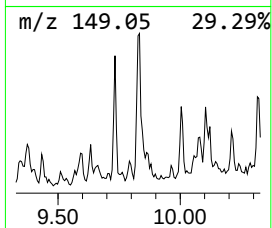
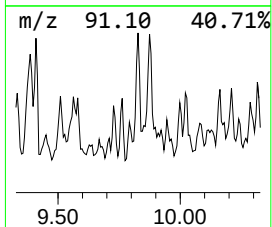
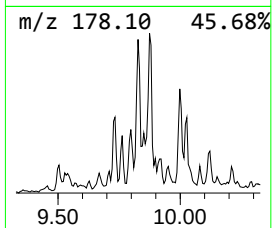
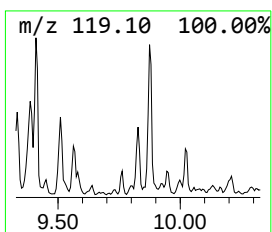
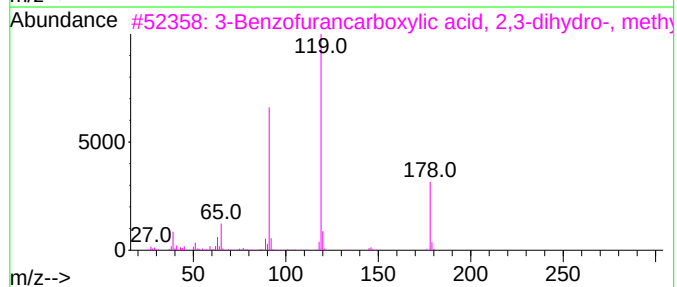
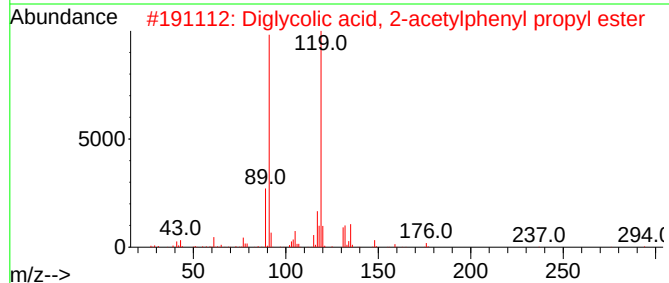
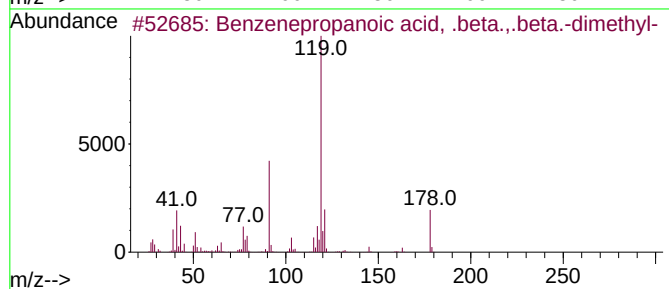
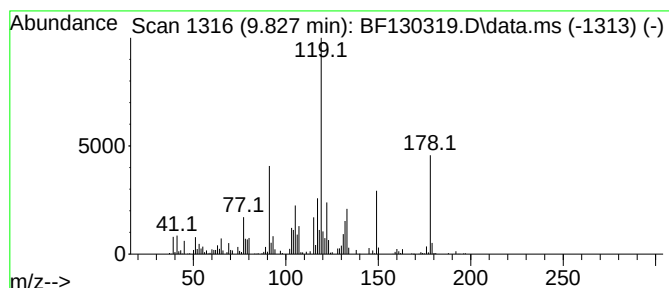
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown9.827 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.827	10.75 ng	402586	Acenaphthene-d10	9.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenepropanoic acid, .beta.,.b...	178	C11H14O2	001010-48-6	49
2			Diglycolic acid, 2-acetylphenyl ...	294	C15H18O6	1010382-71-7	43
3			3-Benzofurancarboxylic acid, 2,3...	178	C10H10O3	039891-56-0	43
4			1-Acetyl-3-phenylurea	178	C9H10N2O2	000102-03-4	43
5			Diglycolic acid, 2-acetylphenyl ...	322	C17H22O6	1000382-72-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-54

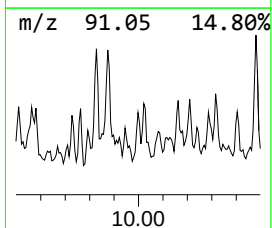
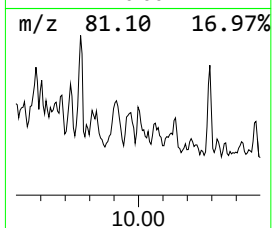
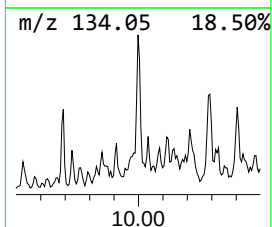
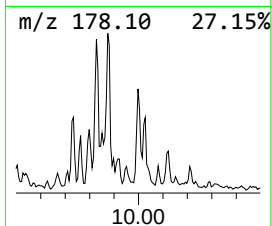
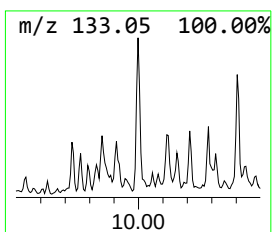
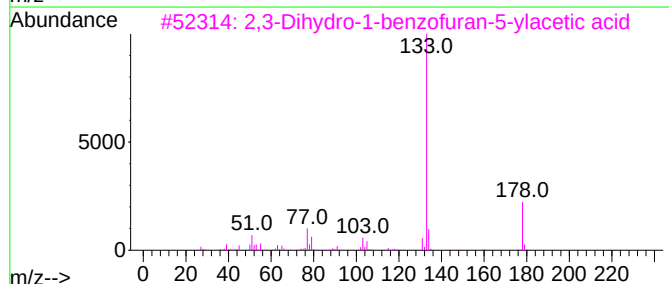
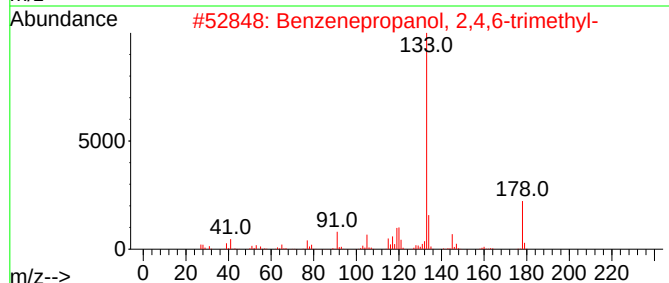
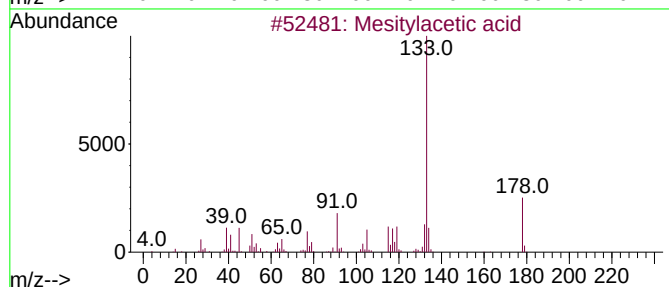
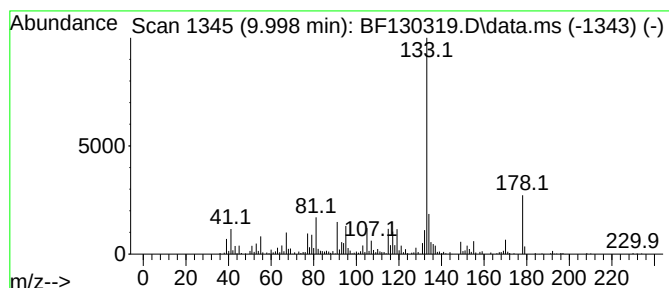
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Mesitylacetic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.998	9.94 ng	372297	Acenaphthene-d10	9.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylacetic acid	178	C11H14O2	004408-60-0	93
2			Benzenepropanol, 2,4,6-trimethyl-	178	C12H18O	027645-07-4	80
3			2,3-Dihydro-1-benzofuran-5-ylace...	178	C10H10O3	069999-16-2	62
4			2,4,6-Trimethylbenzyl mercaptan,...	208	C12H16OS	1439439-12-9	62
5			Benzene, 2,4-dimethyl-1-(1-methy...	162	C12H18	001483-60-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

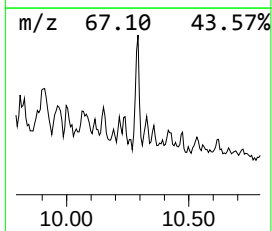
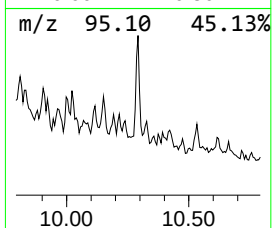
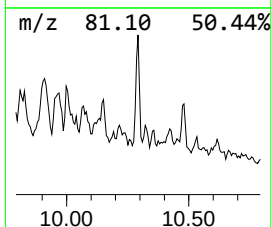
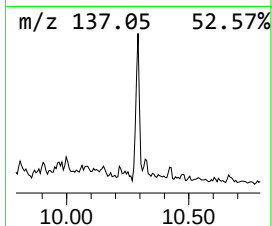
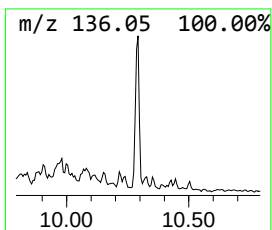
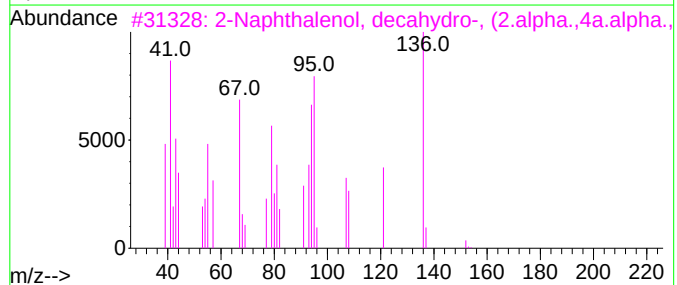
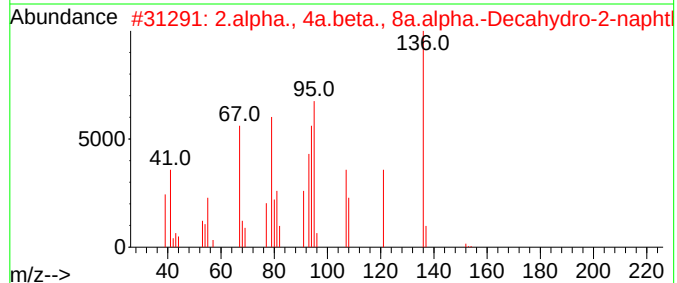
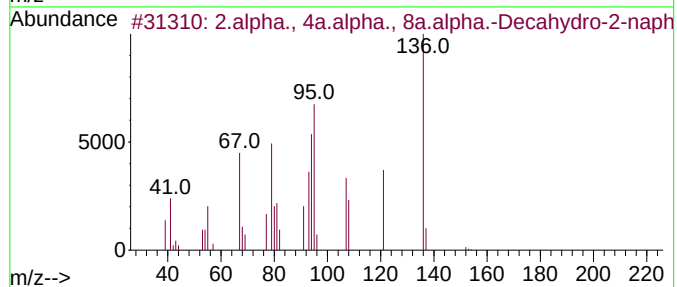
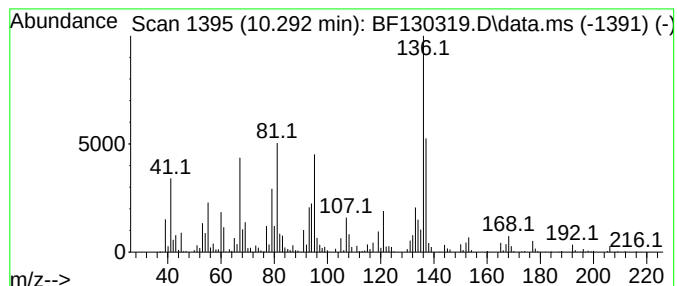
Instrument :
BNA_F
ClientSampleId :
HW-54

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 2.alpha., 4a.alpha., 8a.alp... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.292	16.59 ng	621474	Acenaphthene-d10			9.692
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2.alpha., 4a.alpha., 8a.alpha.-D...		154	C10H18O	001424-36-8	55
2	2.alpha., 4a.beta., 8a.alpha.-De...		154	C10H18O	005779-35-1	55
3	2-Naphthalenol, decahydro-, (2.a...		154	C10H18O	002529-06-8	49
4	3-Benzylsulfonyl-2,6,6-trimethyl...		292	C17H24O2S	1000242-12-7	43
5	5-Cyano-1,2,3,4-tetrahydro-6-met...		136	C7H8N2O	027036-90-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

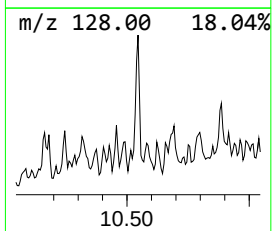
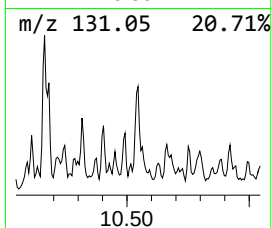
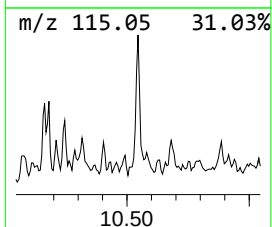
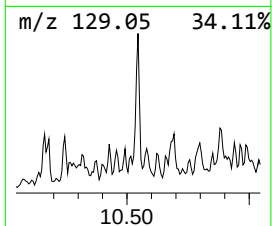
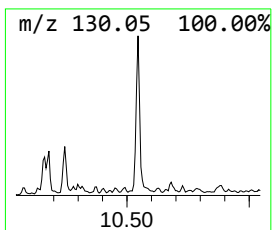
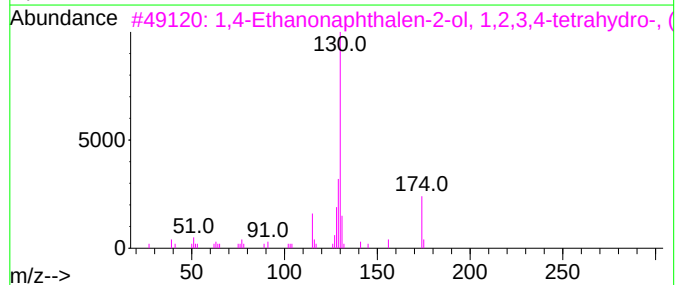
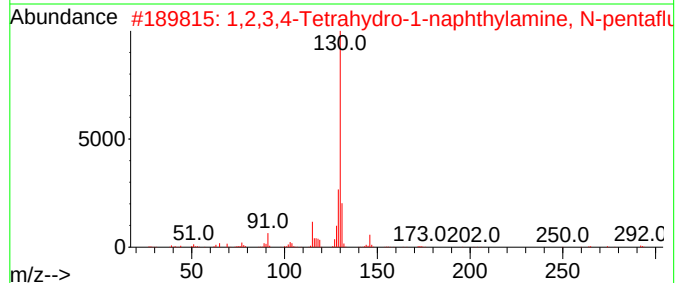
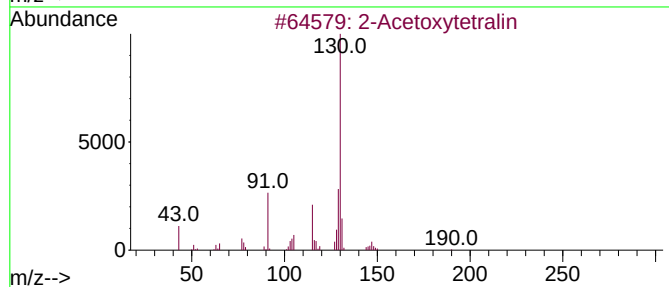
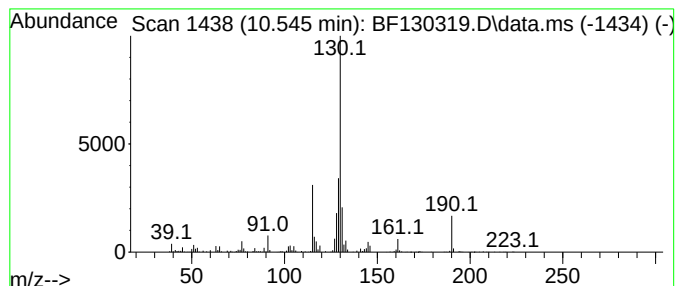
Instrument :
BNA_F
ClientSampleId :
HW-54

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 2-Acetoxytetralin Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.545	14.55 ng	487025	Phenanthrene-d10	11.169
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		2-Acetoxytetralin	190 C12H14O2	1000430-72-6 72
2		1,2,3,4-Tetrahydro-1-naphthylami...	293 C13H12F5NO	1000417-37-5 64
3		1,4-Ethanonaphthalen-2-ol, 1,2,3...	174 C12H14O	013153-78-1 64
4		Acenaphthylene, 1,2,2a,3,4,5-hex...	158 C12H14	000480-72-8 59
5		6-Phenyl-5-hexenoic acid, methyl...	204 C13H16O2	1000281-31-8 59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-54

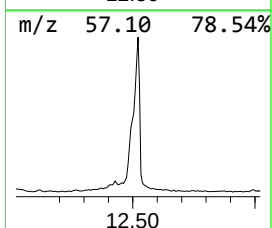
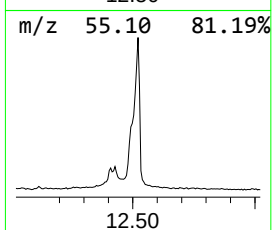
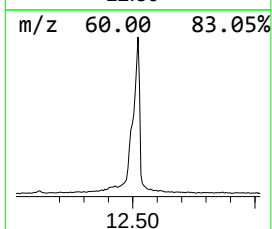
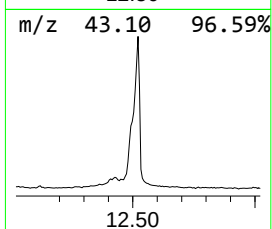
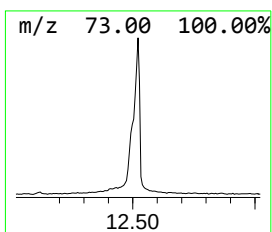
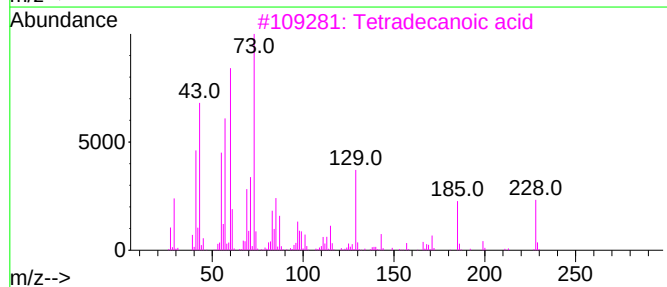
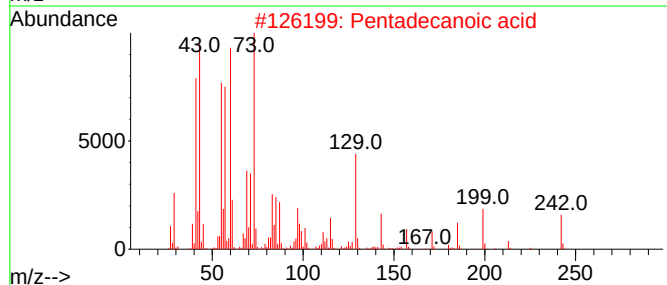
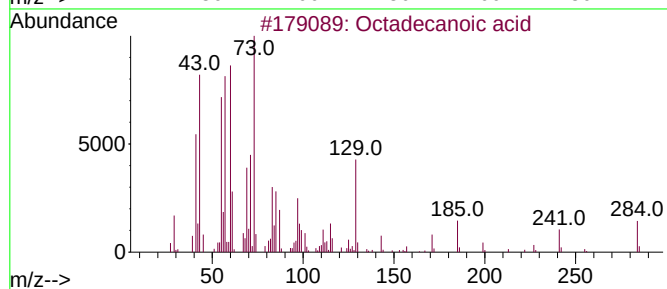
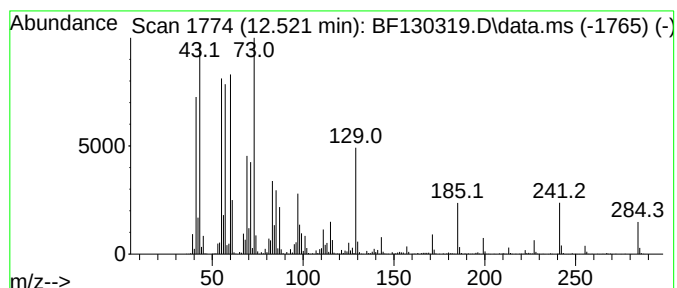
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.521	156.51 ng	4726820	Chrysene-d12	13.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

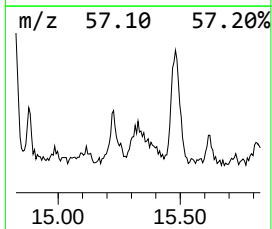
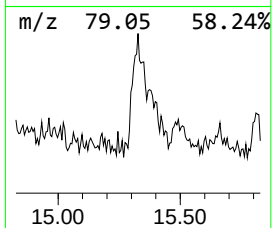
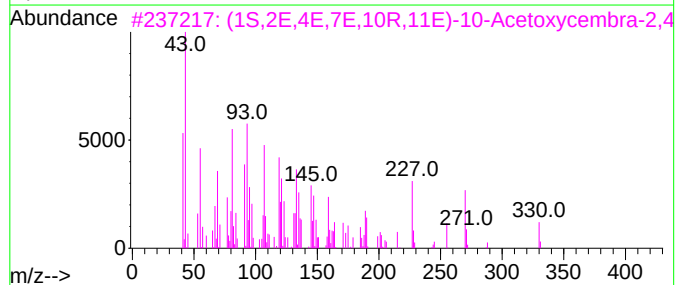
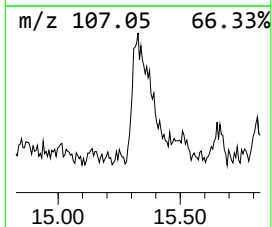
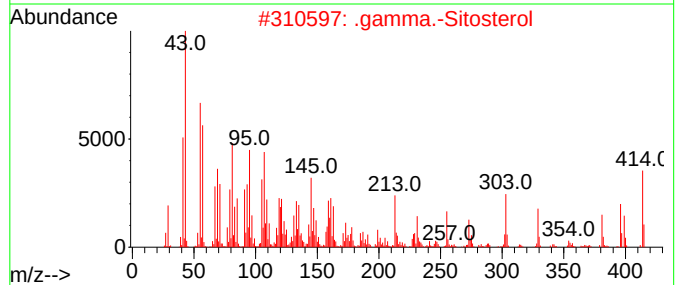
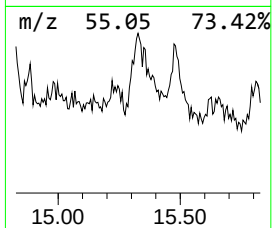
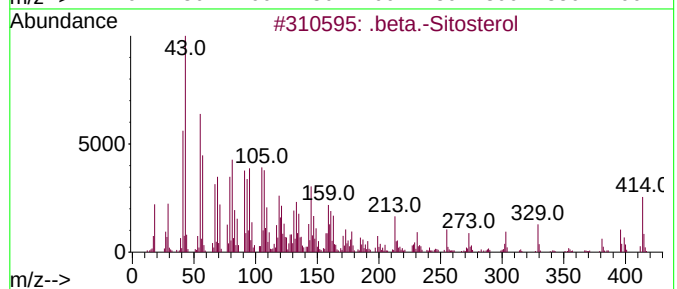
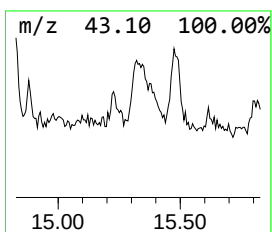
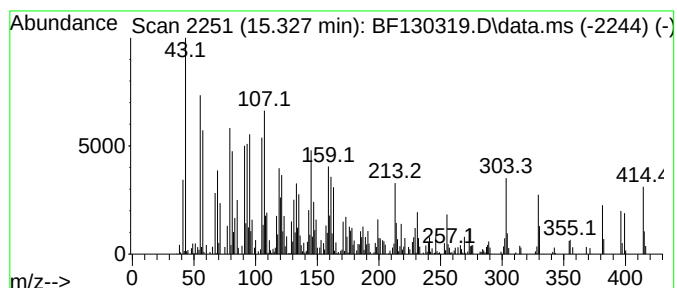
Instrument :
BNA_F
ClientSampleId :
HW-54

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 .beta.-Sitosterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.327	26.97 ng	638071	Perylene-d12	15.186		
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Sitosterol	414	C29H50O	000083-46-5	94
2		.gamma.-Sitosterol	414	C29H50O	000083-47-6	55
3		(1S,2E,4E,7E,10R,11E)-10-Acetoxy...	330	C22H34O2	1000433-18-1	44
4		Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	35
5		(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091922\
Data File : BF130319.D
Acq On : 19 Sep 2022 14:11
Operator : CG\JU
Sample : N4628-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HW-54

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.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
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Ethanone, 1-(2-...	8.357	19.8	ng	872183	2	7.939	880605	20.0
unknown8.545	8.545	10.7	ng	470655	2	7.939	880605	20.0
unknown8.704	8.704	12.1	ng	531633	2	7.939	880605	20.0
3-Pyridinol-1-o...	8.733	12.6	ng	552934	2	7.939	880605	20.0
unknown8.804	8.804	15.0	ng	661595	2	7.939	880605	20.0
unknown8.845	8.845	10.7	ng	402532	3	9.692	749271	20.0
o-Tolylacetic acid	8.892	23.9	ng	893846	3	9.692	749271	20.0
1,3-Hexadiene, ...	8.922	9.6	ng	359270	3	9.692	749271	20.0
unknown8.963	8.963	13.0	ng	485573	3	9.692	749271	20.0
unknown9.333	9.333	19.5	ng	730329	3	9.692	749271	20.0
2,5-Dimethylphe...	9.386	21.9	ng	820671	3	9.692	749271	20.0
Acetic acid, (2...	9.410	10.6	ng	395851	3	9.692	749271	20.0
unknown9.763	9.763	10.7	ng	400929	3	9.692	749271	20.0
unknown9.827	9.827	10.8	ng	402586	3	9.692	749271	20.0
Mesitylacetic acid	9.998	9.9	ng	372297	3	9.692	749271	20.0
2.alpha., 4a.al...	10.292	16.6	ng	621474	3	9.692	749271	20.0
2-Acetoxytetralin	10.545	14.6	ng	487025	4	11.169	669437	20.0
Octadecanoic acid	12.521	156.5	ng	4726820	5	13.798	604048	20.0
.beta.-Sitosterol	15.327	27.0	ng	638071	6	15.186	473191	20.0