

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
 Data File : BF133259.D
 Acq On : 05 May 2023 12:28
 Operator : CG\JU
 Sample : 02597-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1-20230503

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133259.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.169	350	354	362	rVB	456401	542313	9.76%	1.017%
2	4.916	478	481	483	rBV	130358	157648	2.84%	0.296%
3	4.940	483	485	488	rVV	155933	156768	2.82%	0.294%
4	5.016	488	498	499	rVV3	68035	189874	3.42%	0.356%
5	5.040	499	502	507	rVV	161088	162879	2.93%	0.305%
6	5.122	507	516	521	rVB	49767	111962	2.01%	0.210%
7	5.345	550	554	560	rBV	2674487	2626291	47.24%	4.925%
8	6.363	724	727	733	rVB	1999947	1701144	30.60%	3.190%
9	6.534	750	756	758	rBV2	53114	82468	1.48%	0.155%
10	6.722	785	788	792	rBV	1500662	1259065	22.65%	2.361%
11	6.904	816	819	824	rVB	267614	235127	4.23%	0.441%
12	7.134	853	858	869	rBV2	277857	381532	6.86%	0.715%
13	7.222	869	873	879	rBV2	51883	84548	1.52%	0.159%
14	7.292	879	885	888	rBV	3724921	3549977	63.86%	6.657%
15	7.322	888	890	893	rVB	445261	313346	5.64%	0.588%
16	7.404	901	904	906	rBV	75217	76201	1.37%	0.143%
17	7.757	956	964	967	rBV4	1110745	1435627	25.82%	2.692%
18	7.786	967	969	971	rVB	85989	70354	1.27%	0.132%
19	7.845	976	979	981	rVB	122228	118722	2.14%	0.223%
20	7.922	988	992	995	rBV2	87395	105216	1.89%	0.197%
21	7.975	999	1001	1003	rVV3	81854	85144	1.53%	0.160%
22	8.010	1003	1007	1009	rVV	2084246	1870005	33.64%	3.507%
23	8.033	1009	1011	1014	rVV	3294605	2523003	45.38%	4.731%
24	8.081	1014	1019	1024	rVB	277229	299488	5.39%	0.562%
25	8.245	1043	1047	1049	rBV3	60573	78201	1.41%	0.147%
26	8.281	1049	1053	1058	rVB	348032	405892	7.30%	0.761%
27	8.363	1065	1067	1075	rBV2	368856	454061	8.17%	0.851%
28	8.433	1076	1079	1083	rBV3	69338	88002	1.58%	0.165%
29	8.598	1103	1107	1112	rVB3	81166	99637	1.79%	0.187%
30	8.722	1125	1128	1131	rBV	648830	490776	8.83%	0.920%
31	8.751	1131	1133	1135	rBV	146461	125935	2.27%	0.236%
32	8.822	1142	1145	1148	rVB	461400	408954	7.36%	0.767%
33	8.863	1148	1152	1153	rBV3	56676	69144	1.24%	0.130%
34	8.969	1166	1170	1171	rBV2	103764	96378	1.73%	0.181%
35	8.986	1171	1173	1179	rVB3	106125	118998	2.14%	0.223%
36	9.039	1179	1182	1184	rBV	165811	125716	2.26%	0.236%

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Max Peaks: 100

Stop Thrs : 0

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

Peak separation: 5

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.086	1184	1190	1193	rVB	5946129	5559300	100.00%	10.425%
38	9.122	1193	1196	1200	rBV2	54815	59719	1.07%	0.112%
39	9.186	1200	1207	1210	rBV2	136780	249067	4.48%	0.467%
40	9.392	1239	1242	1244	rBV3	50379	64135	1.15%	0.120%
41	9.433	1244	1249	1256	rVV3	534805	829257	14.92%	1.555%
42	9.551	1266	1269	1272	rVB	197929	150713	2.71%	0.283%
43	9.616	1277	1280	1284	rVB4	77113	105723	1.90%	0.198%
44	9.680	1286	1291	1293	rBV3	92467	137363	2.47%	0.258%
45	9.763	1301	1305	1307	rBV	2172548	1810989	32.58%	3.396%
46	9.792	1307	1310	1312	rVV	774162	580610	10.44%	1.089%
47	9.827	1314	1316	1319	rVB	205480	179793	3.23%	0.337%
48	9.904	1326	1329	1332	rBV4	109556	146191	2.63%	0.274%
49	9.933	1332	1334	1336	rVV	183853	153482	2.76%	0.288%
50	9.963	1336	1339	1342	rVB	393464	332435	5.98%	0.623%
51	10.057	1349	1355	1357	rBV2	1114188	1283096	23.08%	2.406%
52	10.169	1370	1374	1379	rVB4	89439	150566	2.71%	0.282%
53	10.304	1394	1397	1402	rVB2	548146	557028	10.02%	1.045%
54	10.475	1423	1426	1428	rBV	282702	217918	3.92%	0.409%
55	10.551	1435	1439	1442	rBV	3393050	3381216	60.82%	6.341%
56	10.692	1461	1463	1467	rVB2	234273	248669	4.47%	0.466%
57	10.763	1473	1475	1478	rBV2	157471	125314	2.25%	0.235%
58	10.904	1496	1499	1502	rBV2	177951	154416	2.78%	0.290%
59	10.933	1502	1504	1506	rVB2	77905	58709	1.06%	0.110%
60	11.004	1514	1516	1518	rBV2	76710	73114	1.32%	0.137%
61	11.045	1521	1523	1525	rBV	178567	139388	2.51%	0.261%
62	11.180	1543	1546	1547	rBV	116236	100266	1.80%	0.188%
63	11.245	1553	1557	1559	rBV	2091748	1791527	32.23%	3.360%
64	11.263	1559	1560	1563	rVB	455311	345426	6.21%	0.648%
65	11.345	1572	1574	1577	rVB3	127755	120899	2.17%	0.227%
66	11.474	1593	1596	1599	rVB	782728	590308	10.62%	1.107%
67	11.633	1620	1623	1626	rBV3	118102	140013	2.52%	0.263%
68	11.792	1647	1650	1657	rVB	1467536	1515637	27.26%	2.842%
69	11.857	1658	1661	1665	rBV3	398070	402084	7.23%	0.754%
70	11.945	1673	1676	1680	rBV	367993	390655	7.03%	0.733%
71	12.298	1734	1736	1739	rVB	157788	119992	2.16%	0.225%
72	12.574	1780	1783	1796	rVB2	1658863	1910671	34.37%	3.583%
73	12.721	1805	1808	1817	rVB	282053	367648	6.61%	0.689%
74	12.833	1823	1827	1830	rVB	4874111	4744992	85.35%	8.898%
75	13.415	1924	1926	1929	rBV2	96936	109259	1.97%	0.205%
76	13.686	1969	1972	1978	rVB	379426	381047	6.85%	0.715%

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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-BF042123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	13.745	1979	1982	1995	rVB	278542	454698	8.18%	0.853%
78	13.874	2001	2004	2008	rVB	1191543	1100704	19.80%	2.064%
79	13.951	2014	2017	2025	rVB3	121871	160897	2.89%	0.302%
80	15.298	2241	2246	2250	rBV	959685	1130418	20.33%	2.120%

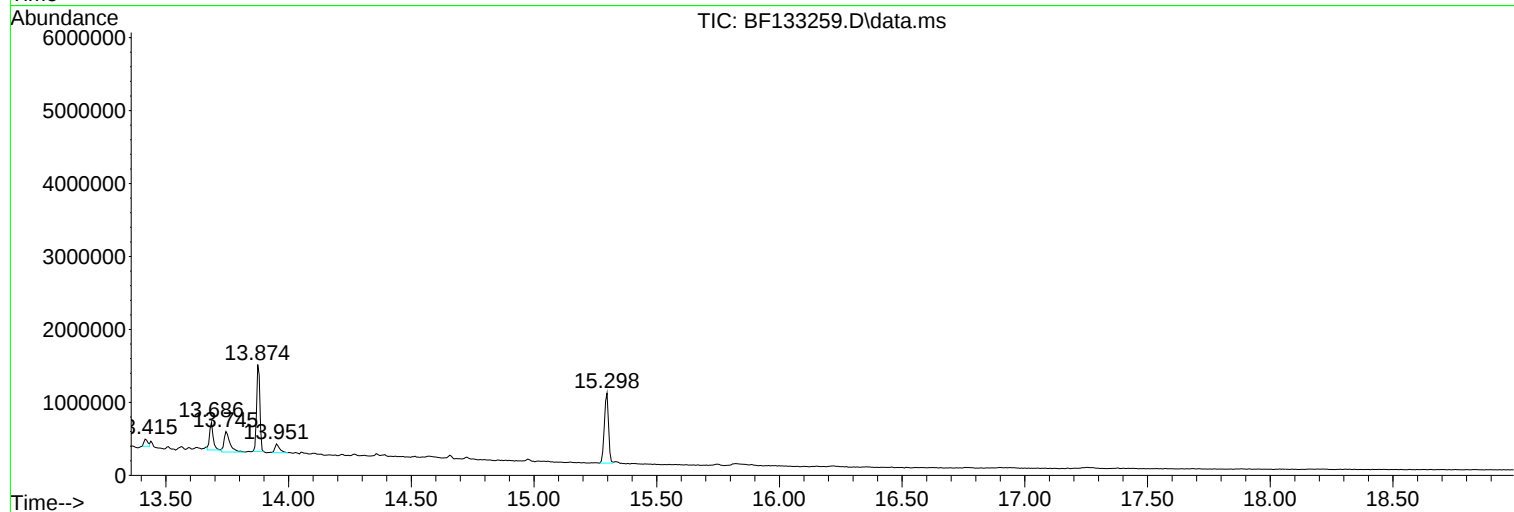
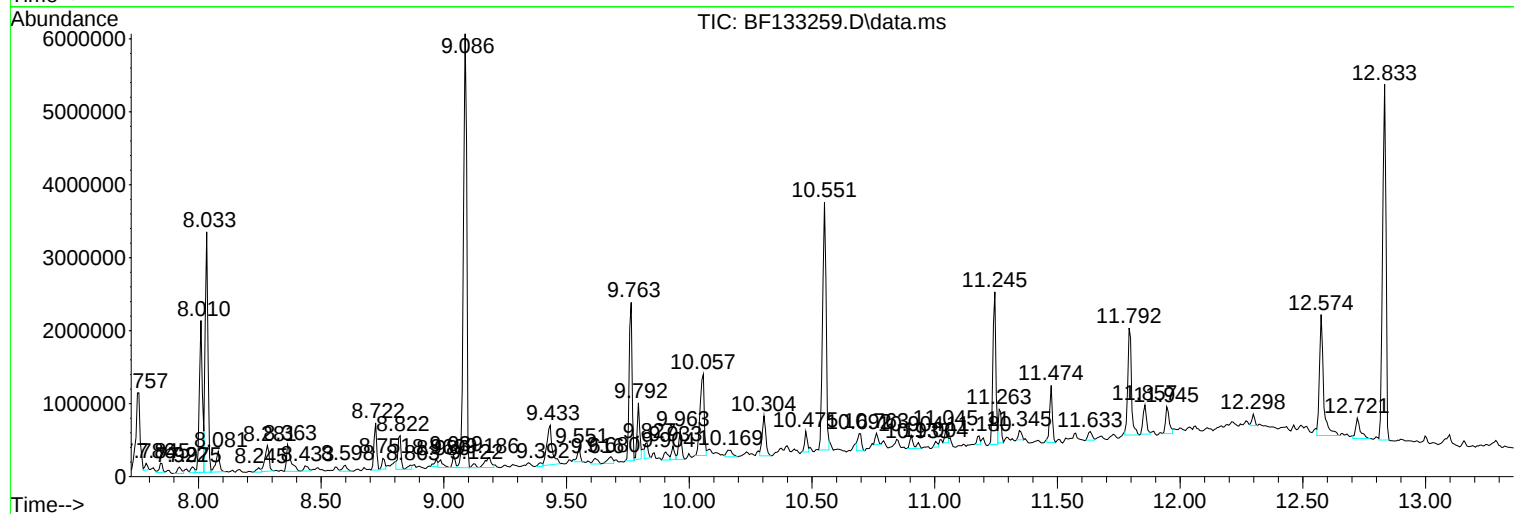
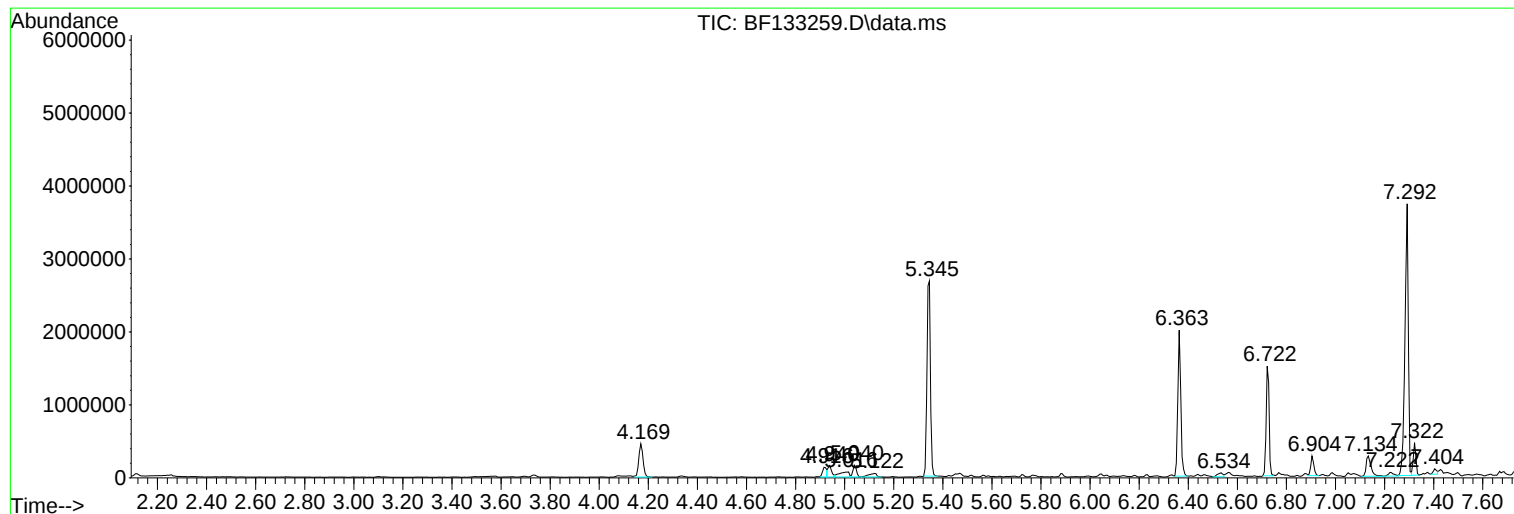
Sum of corrected areas: 53325748

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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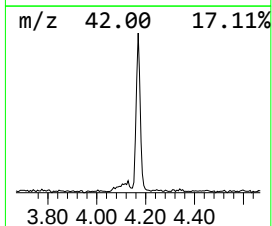
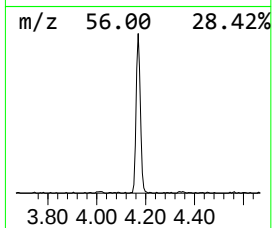
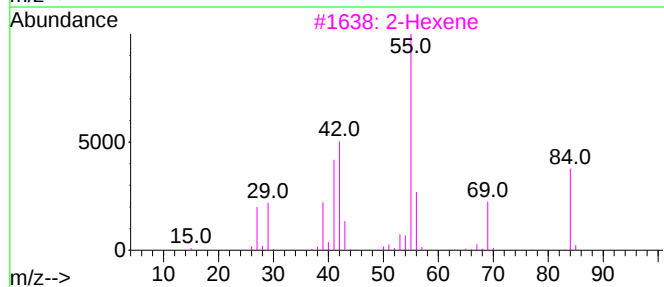
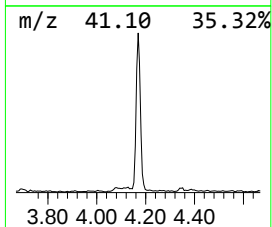
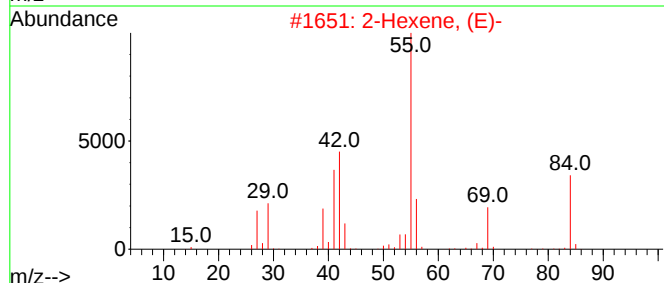
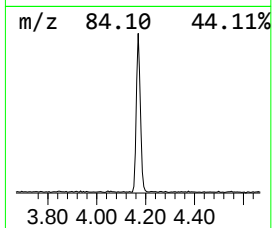
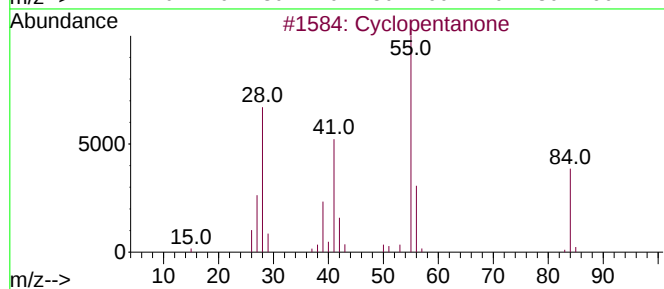
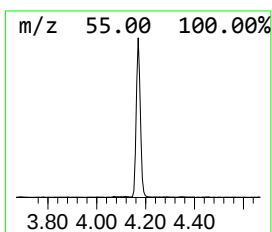
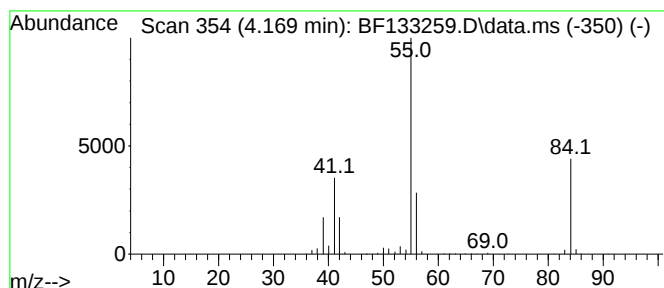
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclopentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.169	8.61 ng	542313	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentanone	84	C5H8O	000120-92-3	91
2			2-Hexene, (E)-	84	C6H12	004050-45-7	64
3			2-Hexene	84	C6H12	000592-43-8	64
4			3-Hexene, (Z)-	84	C6H12	007642-09-3	59
5			2(5H)-Furanone	84	C4H4O2	000497-23-4	53



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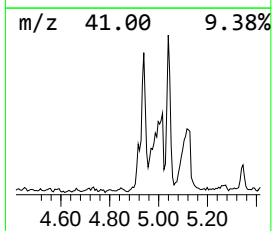
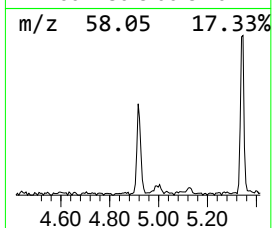
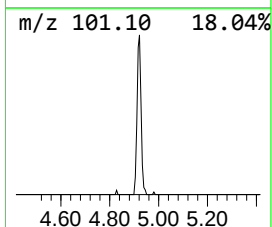
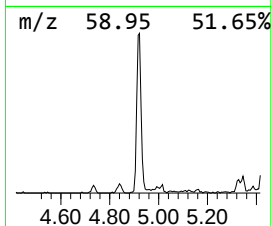
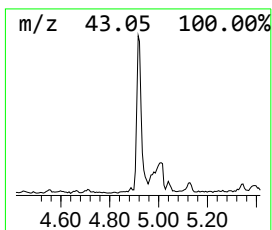
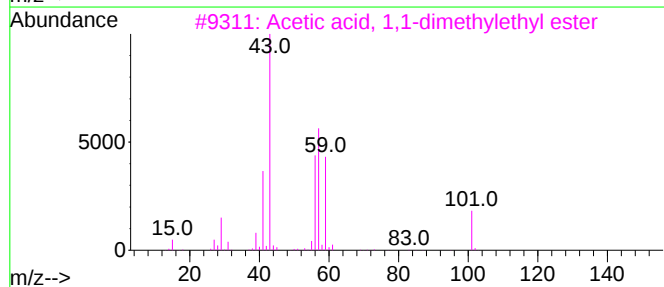
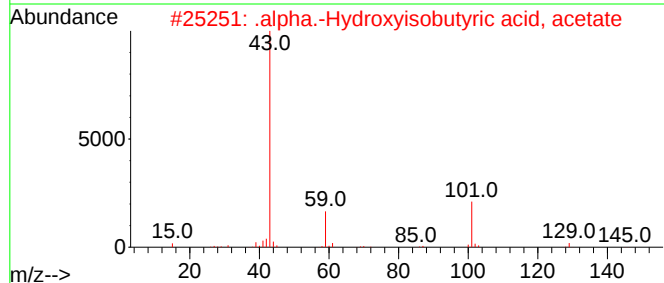
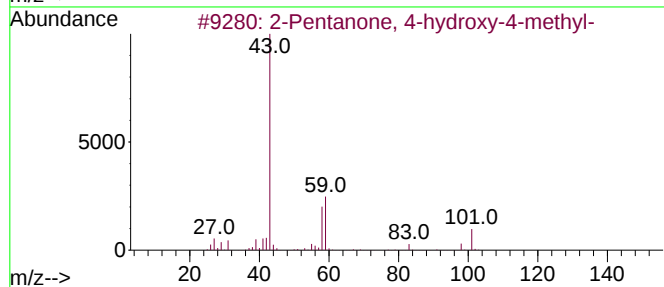
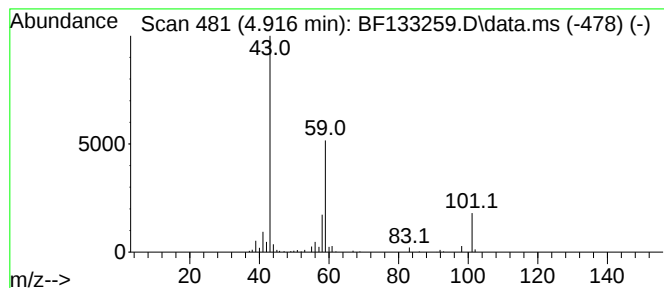
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.916	2.50 ng	157648	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	.alpha.-Hydroxyisobutyric acid, ...	146	C6H10O4	1000374-31-3	45		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
4	3-Octanol	130	C8H18O	000589-98-0	33		
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		



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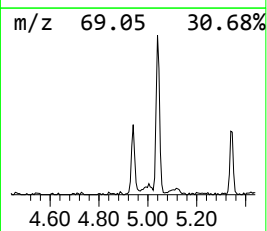
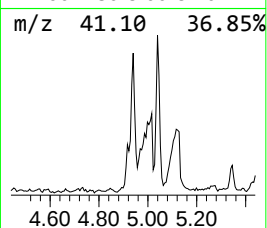
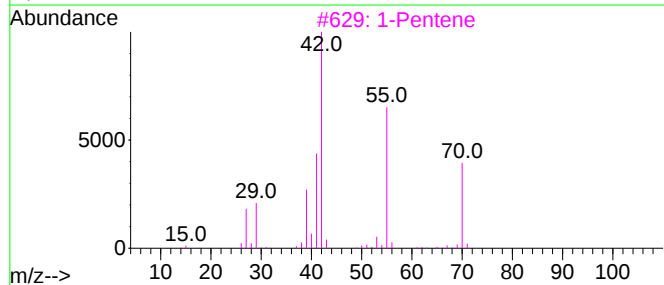
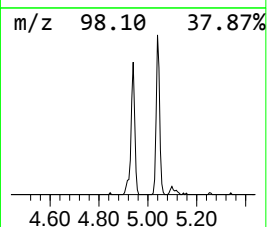
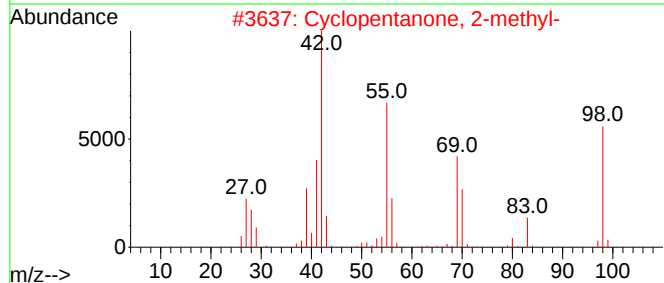
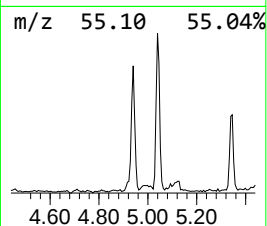
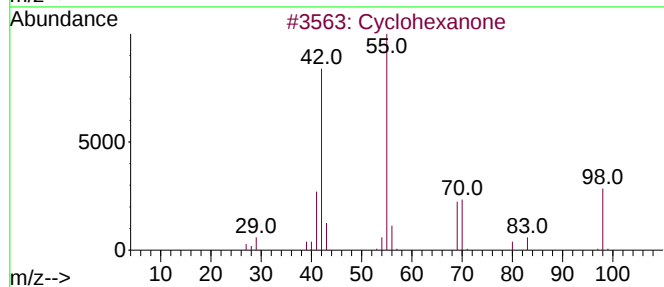
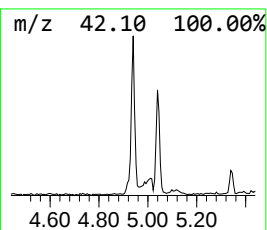
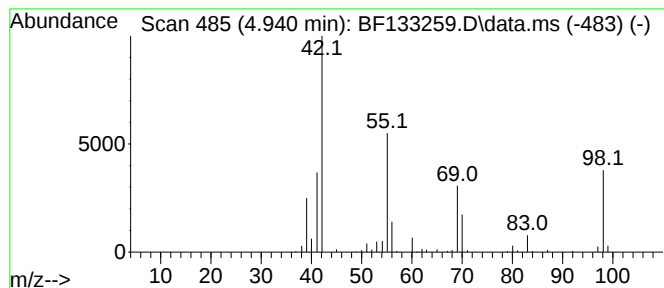
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexanone Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	2.49 ng	156768	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone	98	C6H10O	000108-94-1	72
2			Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	64
3			1-Pentene	70	C5H10	000109-67-1	53
4			Cyclobutane, methyl-	70	C5H10	000598-61-8	50
5			4,5-Dihydro-2-methylimidazole-4-one	98	C4H6N2O	004915-81-5	39



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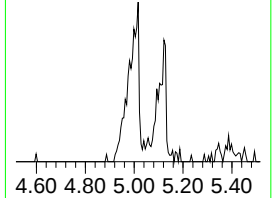
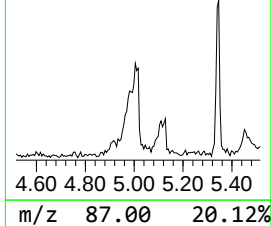
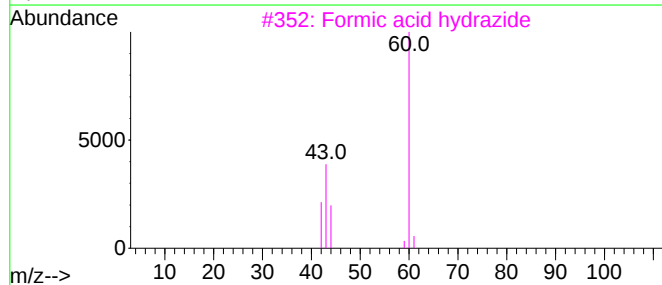
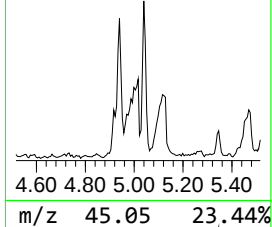
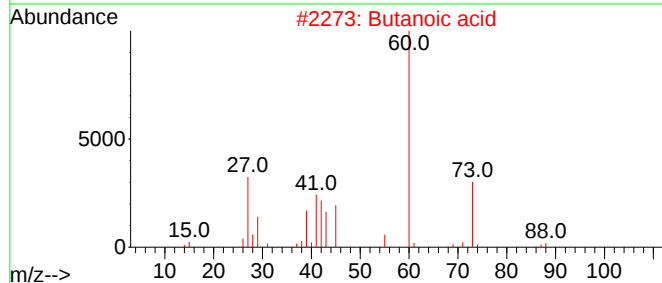
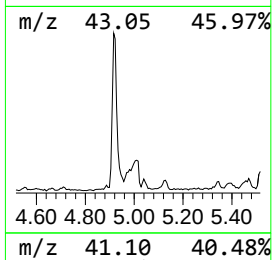
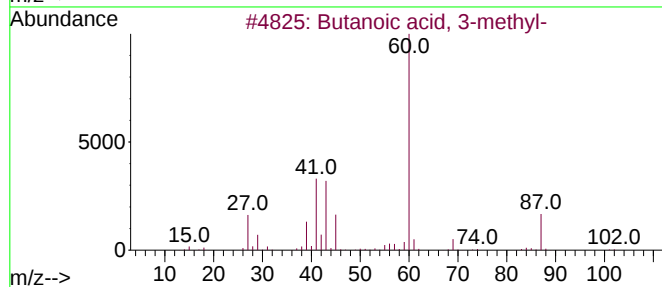
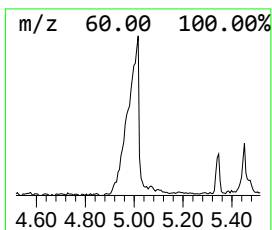
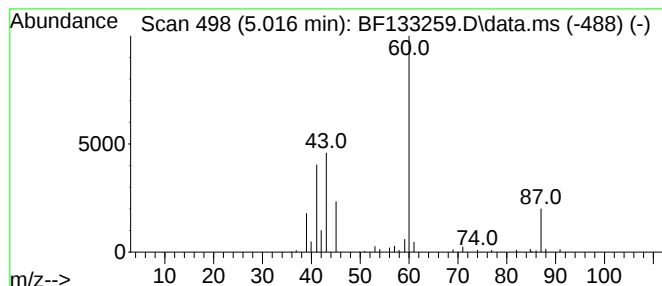
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Butanoic acid, 3-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	3.02 ng	189874	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	72
2			Butanoic acid	88	C4H8O2	000107-92-6	40
3			Formic acid hydrazide	60	CH4N2O	000624-84-0	9
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5			1-Pentanamine	87	C5H13N	000110-58-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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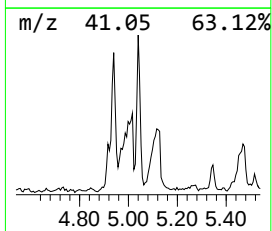
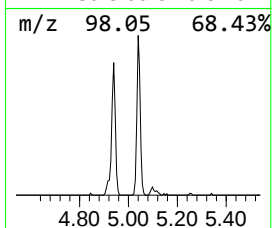
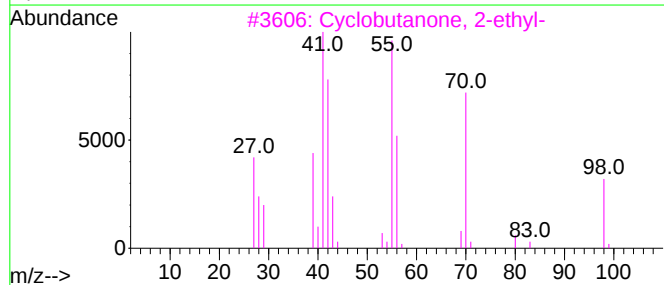
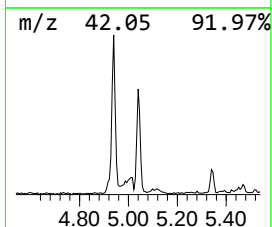
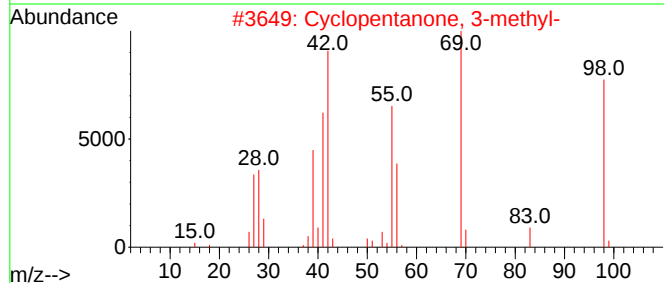
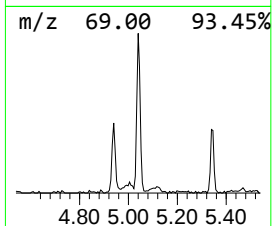
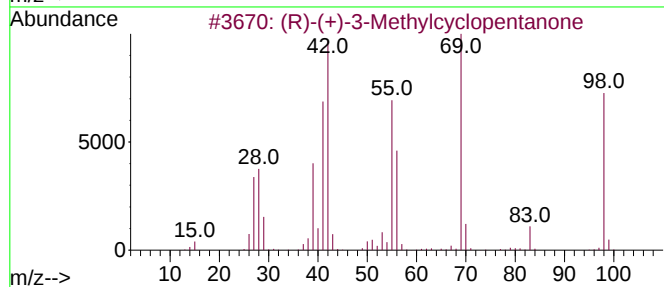
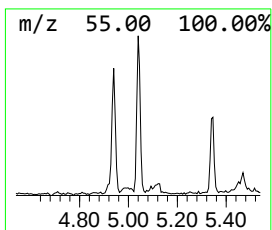
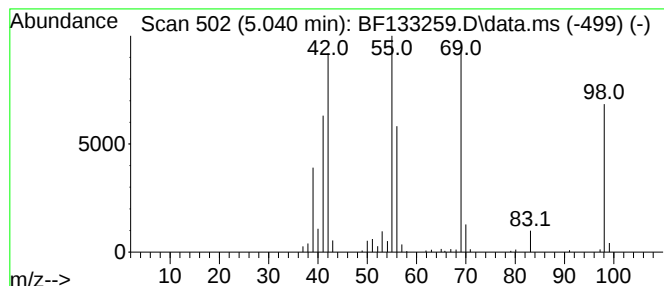
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 (R)-(+)-3-Methylcyclopentanone Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	2.59 ng	162879	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(+)-3-Methylcyclopentanone	98	C6H10O	006672-30-6	97		
2	Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	90		
3	Cyclobutanone, 2-ethyl-	98	C6H10O	010374-14-8	59		
4	1H-Tetrazole, 1,5-dimethyl-	98	C3H6N4	005144-11-6	50		
5	Cyclopentanone, 2-methyl-	98	C6H10O	001120-72-5	46		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1-20230503

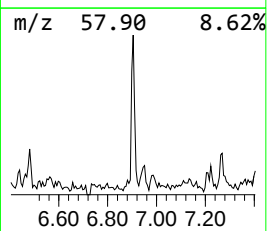
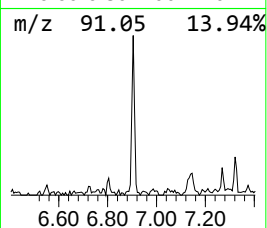
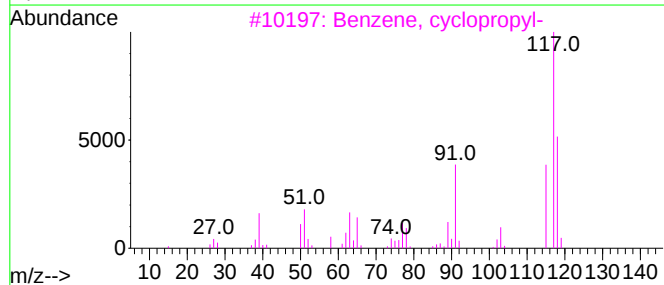
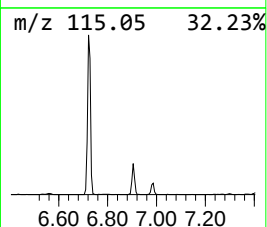
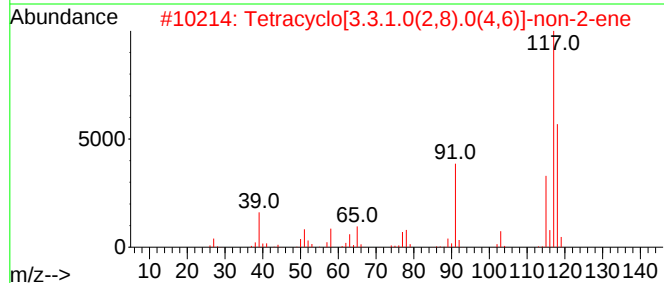
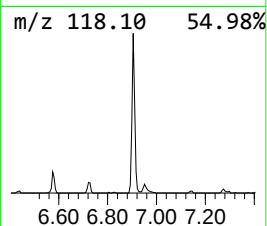
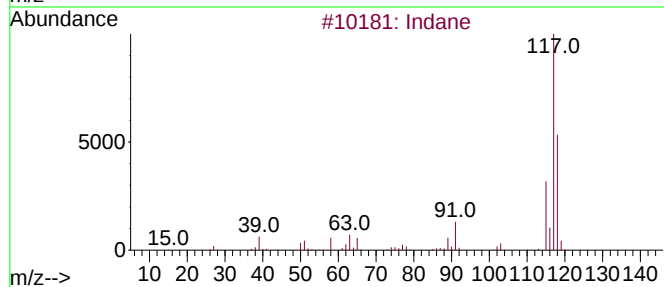
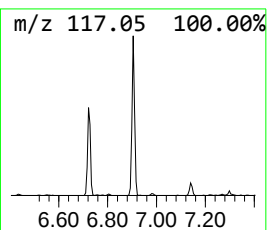
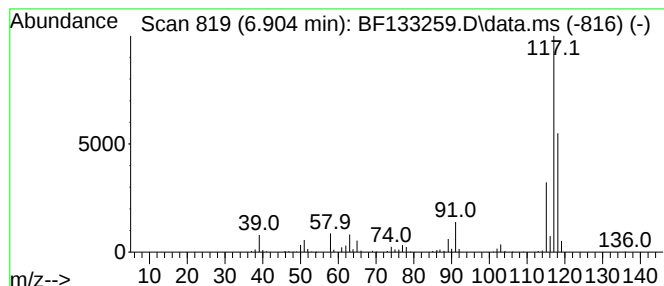
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Indane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.904	3.73 ng	235127	1,4-Dichlorobenzene-d4	6.722

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	95
2			Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	83
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	72
5			Deltacyclene	118	C9H10	007785-10-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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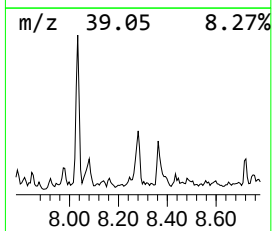
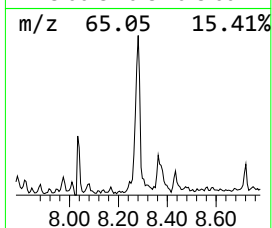
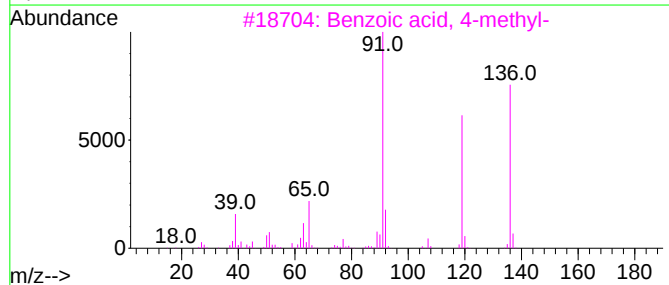
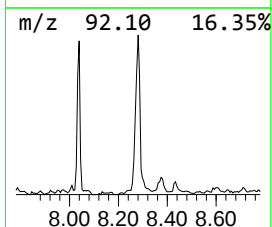
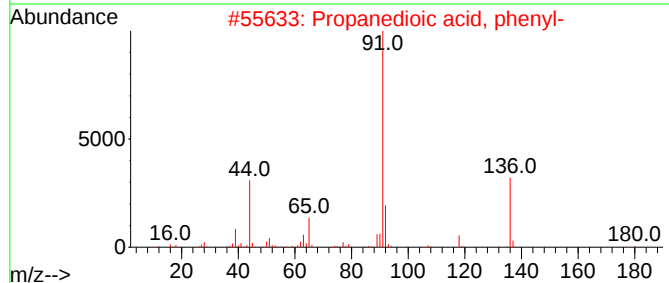
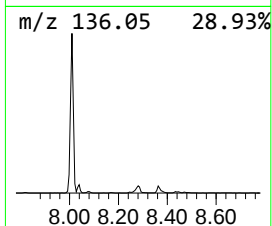
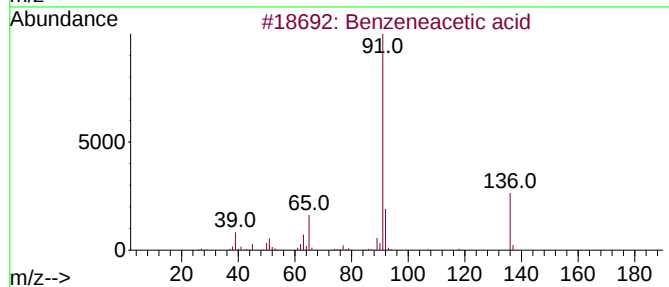
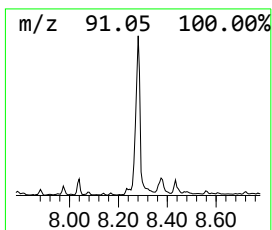
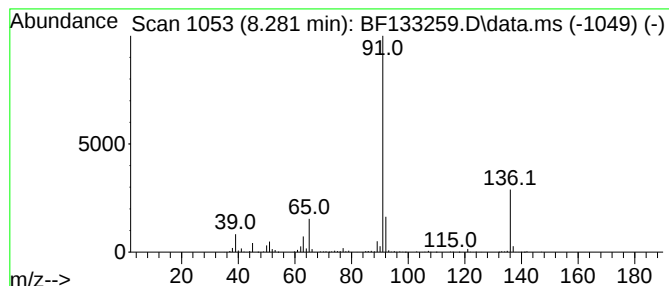
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzeneacetic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.281	4.34 ng	405892	Naphthalene-d8	8.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneacetic acid	136	C8H8O2	000103-82-2	95
2			Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	78
3			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	50
4			Benzene, (iodomethyl)-	218	C7H7I	000620-05-3	50
5			5-Benzyloxy-2-nitrotoluene	243	C14H13NO3	022424-58-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1-20230503

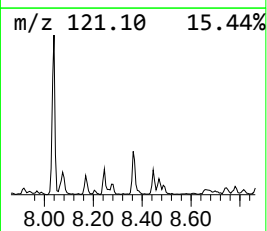
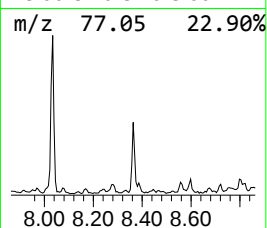
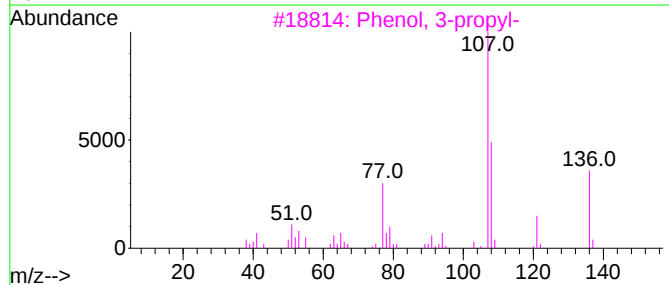
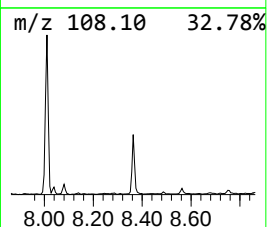
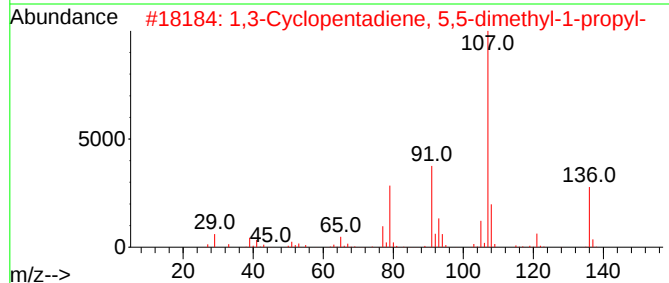
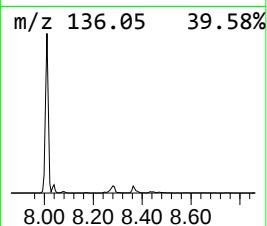
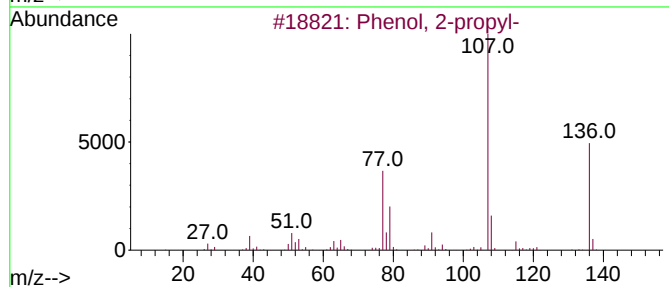
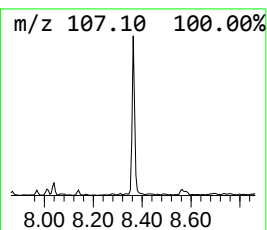
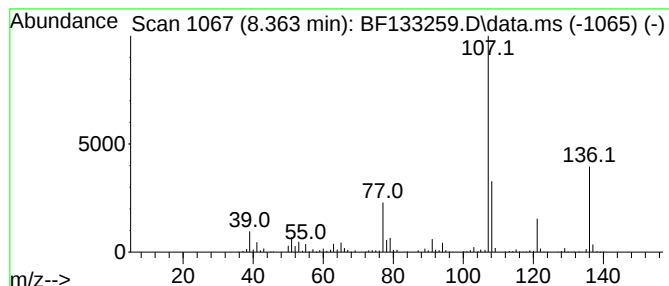
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Phenol, 2-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.363	4.86 ng	454061	Naphthalene-d8	8.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-propyl-	136	C9H12O	000644-35-9	83
2			1,3-Cyclopentadiene, 5,5-dimethy...	136	C10H16	1000163-57-1	72
3			Phenol, 3-propyl-	136	C9H12O	000621-27-2	68
4			Phenol, 4-propyl-	136	C9H12O	000645-56-7	59
5			Benzenemethanol, .alpha.-ethyl-	136	C9H12O	000093-54-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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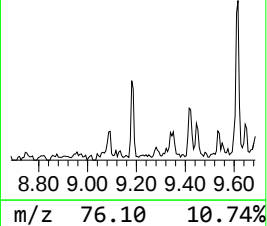
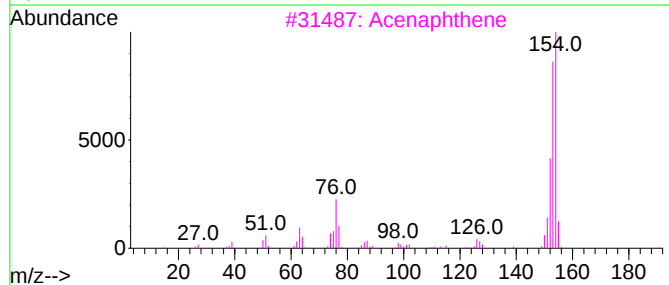
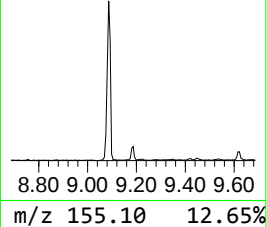
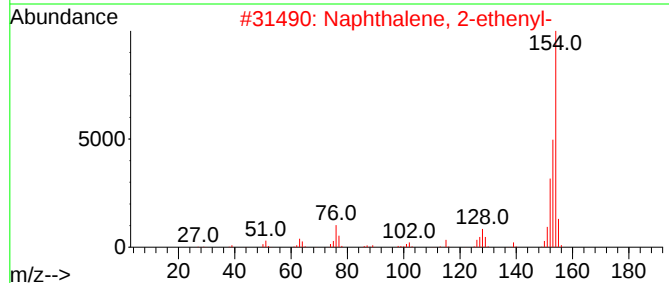
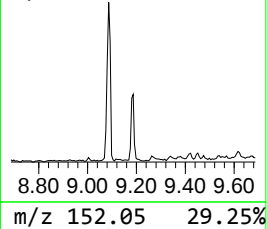
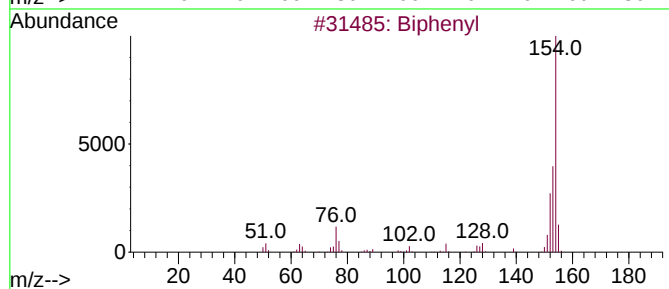
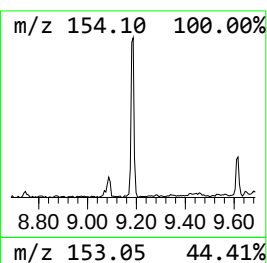
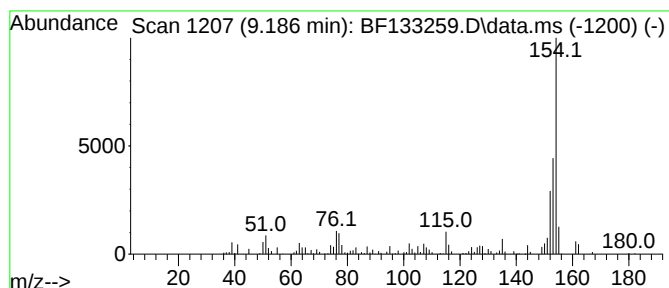
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Biphenyl Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.186	2.75 ng	249067	Acenaphthene-d10	9.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenyl	154	C12H10	000092-52-4	81
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	81
3			Acenaphthene	154	C12H10	000083-32-9	47
4			Propanedinitrile, 2,4,6-cyclohep...	154	C10H6N2	002860-54-0	43
5			1-Isoquinolinecarbonitrile	154	C10H6N2	001198-30-7	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
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ALS Vial : 6 Sample Multiplier: 1

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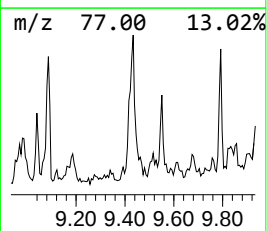
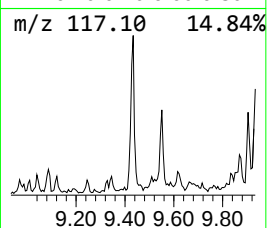
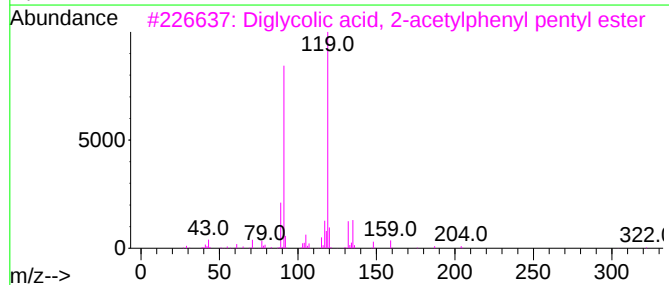
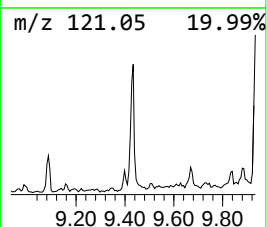
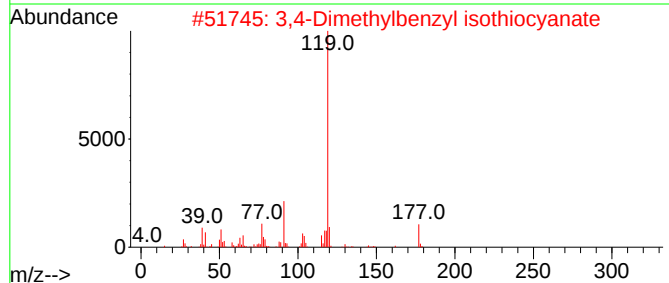
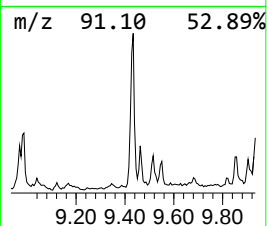
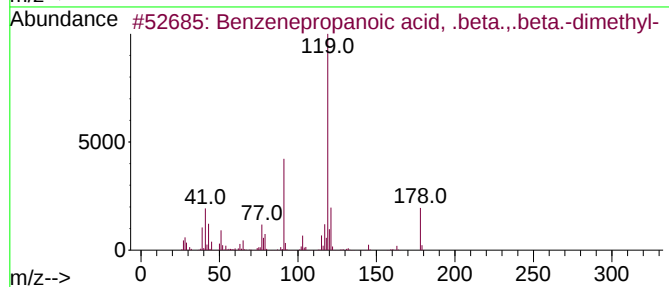
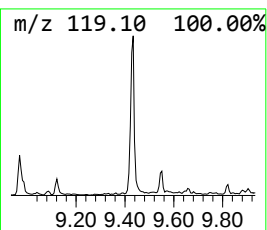
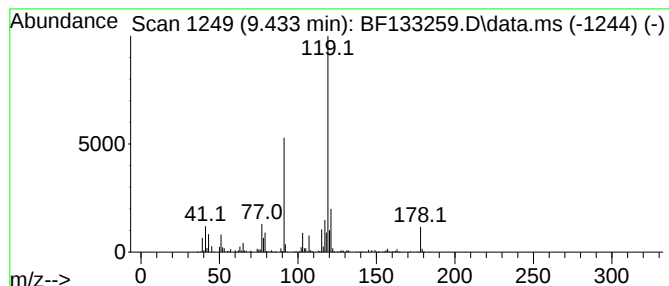
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzenepropanoic acid, .bet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.433	9.16 ng	829257	Acenaphthene-d10	9.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenepropanoic acid, .beta.,.b...	178	C11H14O2	001010-48-6	93
2		3,4-Dimethylbenzyl isothiocyanate	177	C10H11NS	206559-59-3	72
3		Diglycolic acid, 2-acetylphenyl ...	322	C17H22O6	1000382-72-0	72
4		Thiocyanic acid, 1,1,3-trimethyl...	233	C14H19NS	1000293-27-7	64
5		2,5-Dimethylbenzyl chloride	154	C9H11Cl	000824-45-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
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Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

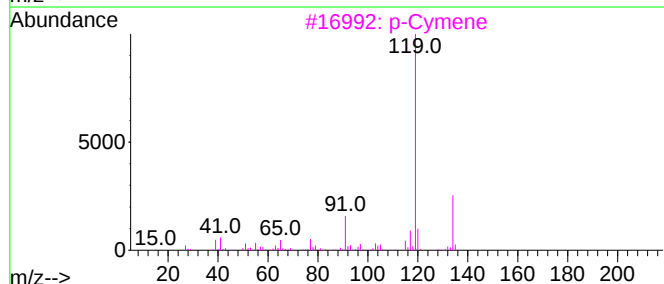
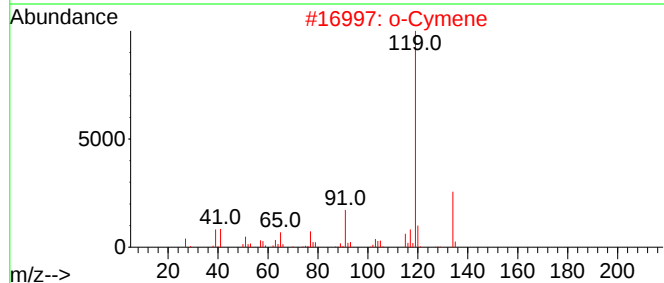
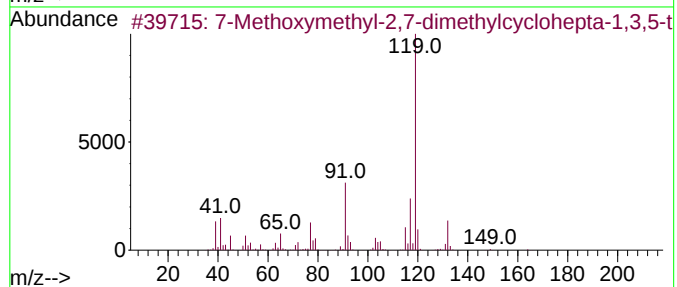
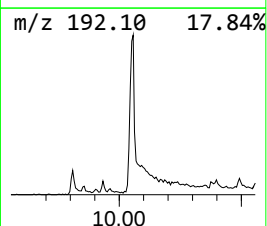
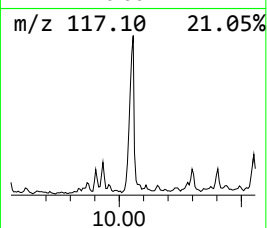
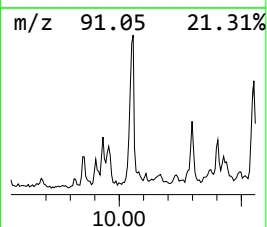
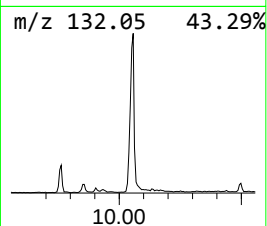
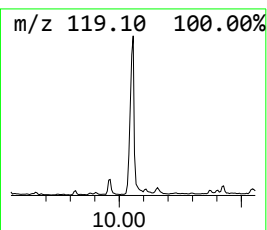
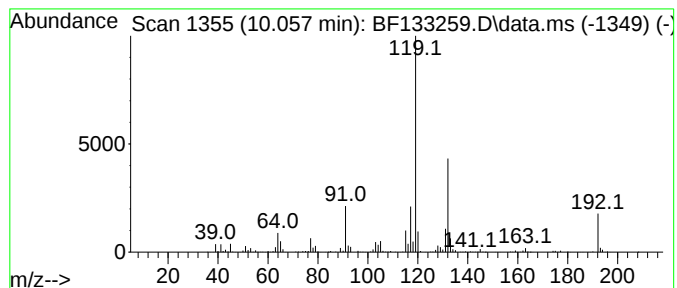
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 7-Methoxymethyl-2,7-dimethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.057	14.17 ng	1283100	Acenaphthene-d10		9.763	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	7-Methoxymethyl-2,7-dimethylcycl...		164	C11H16O	073992-48-0	58
2	o-Cymene		134	C10H14	000527-84-4	55
3	p-Cymene		134	C10H14	000099-87-6	46
4	1-Chloro-2-methyl-2-phenylpropane		168	C10H13Cl	000515-40-2	43
5	Benzonitrile, 3-hydroxy-		119	C7H5NO	000873-62-1	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

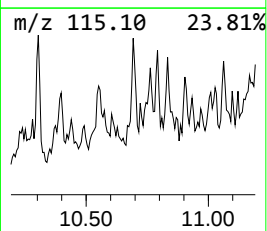
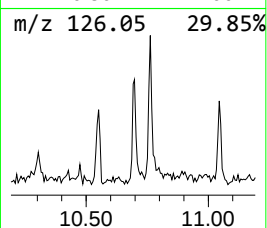
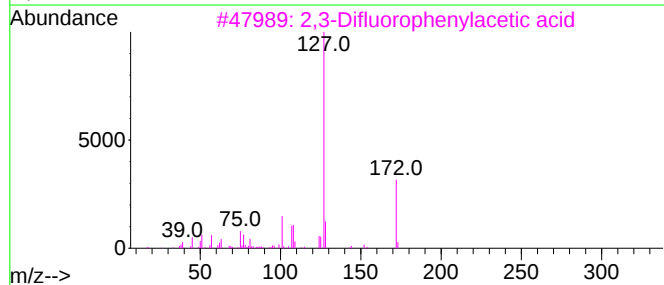
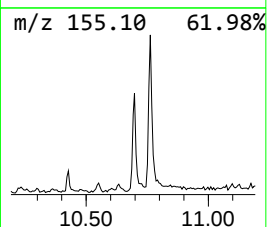
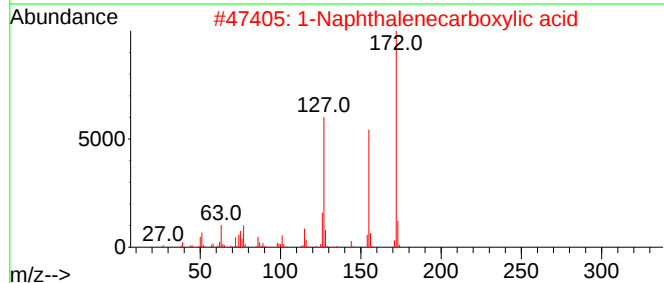
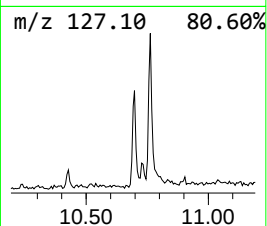
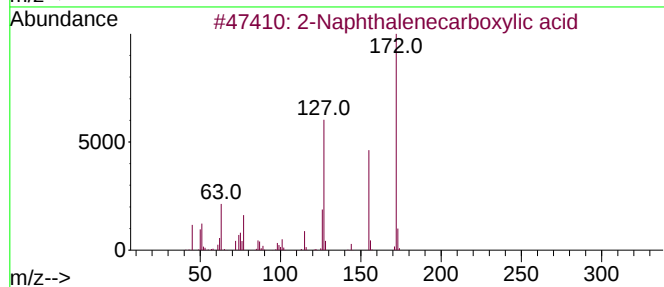
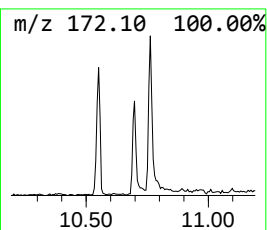
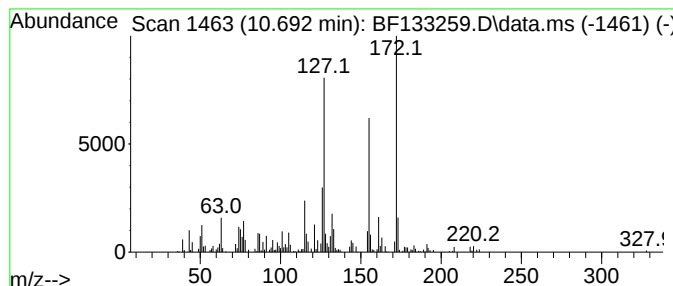
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-Naphthalenecarboxylic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD			R.T.
10.692	2.78 ng	248669	Phenanthrene-d10			11.245
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Naphthalenecarboxylic acid	172	C11H8O2	000093-09-4	95
2		1-Naphthalenecarboxylic acid	172	C11H8O2	000086-55-5	93
3		2,3-Difluorophenylacetic acid	172	C8H6F2O2	000360-03-2	49
4		2,6-Difluorophenylacetic acid	172	C8H6F2O2	085068-28-6	47
5		.alpha.-Naphthoylhydrazine	186	C11H10N2O	043038-45-5	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1-20230503

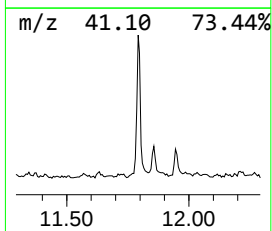
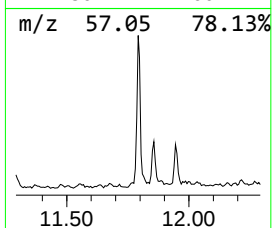
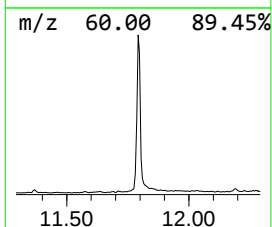
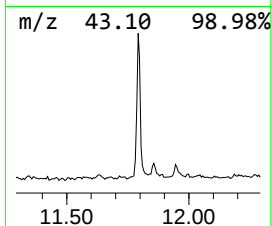
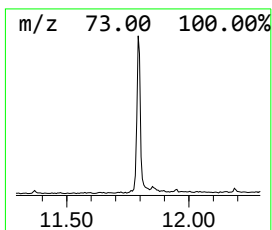
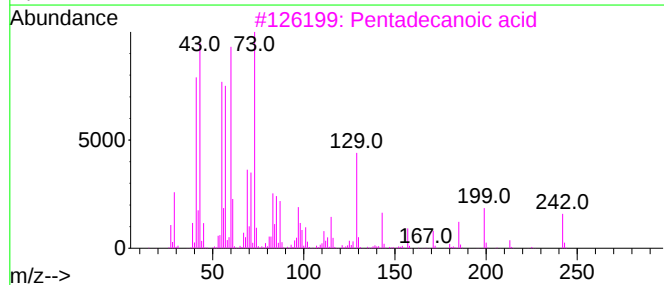
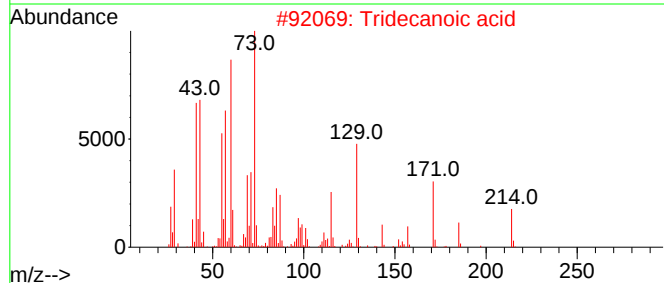
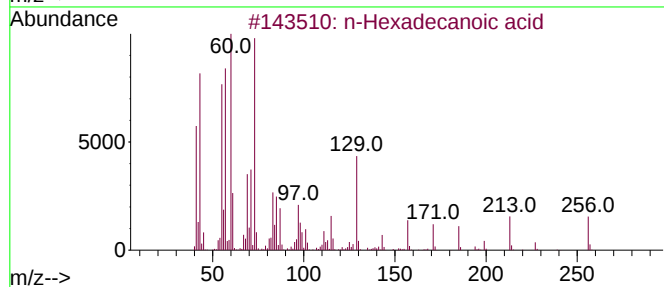
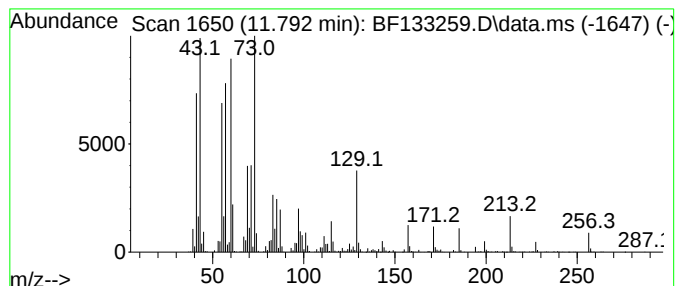
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.792	16.92 ng	1515640	Phenanthrene-d10	11.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Oxalic acid, dodecyl isobutyl ester	314	C18H34O4	1000309-37-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

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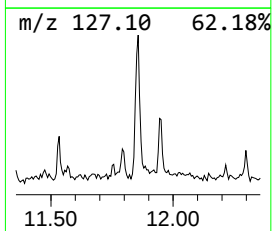
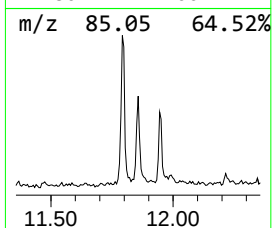
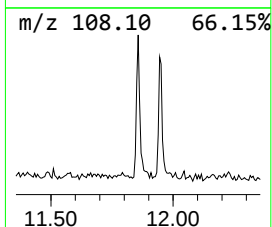
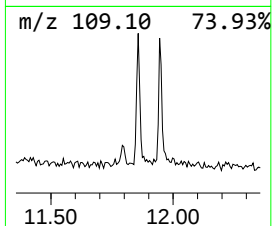
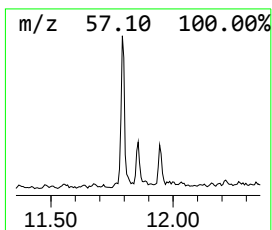
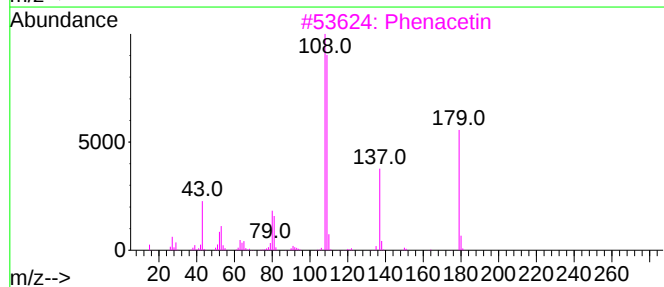
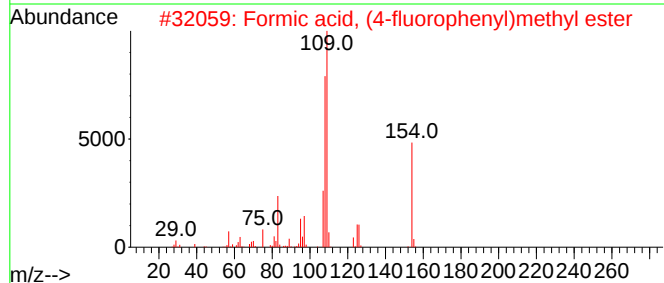
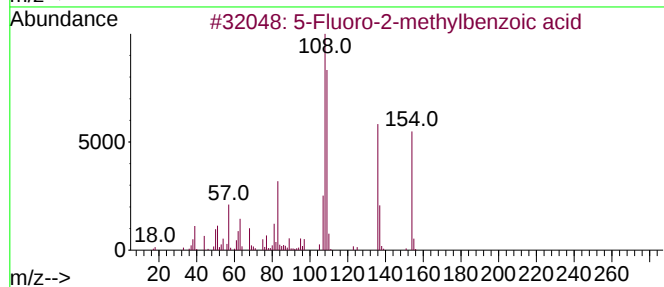
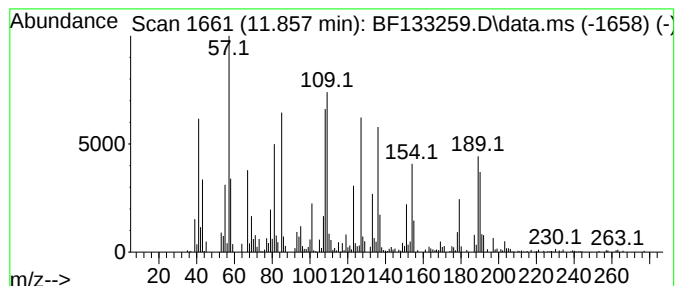
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown11.857 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.857	4.49 ng	402084	Phenanthrene-d10	11.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-methylbenzoic acid	154	C8H7FO2	033184-16-6	45
2			Formic acid, (4-fluorophenyl)met...	154	C8H7FO2	1000368-72-9	38
3			Phenacetin	179	C10H13NO2	000062-44-2	25
4			1-Acetyl-1-methyl-4-methylenecyc...	152	C10H16O	1000424-28-4	20
5			Camphorsulfonic acid	232	C10H16O4S	003144-16-9	15



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
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Sample : 02597-04
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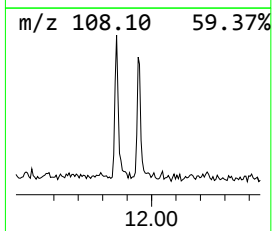
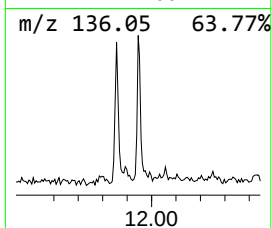
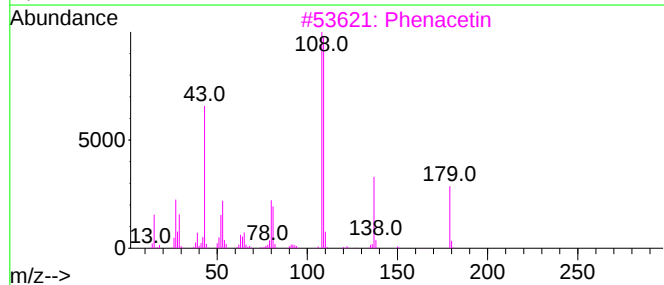
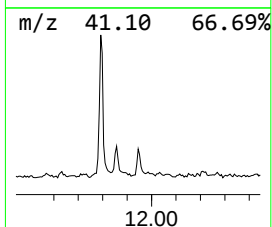
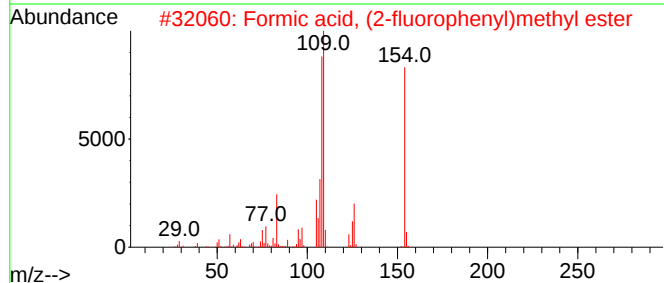
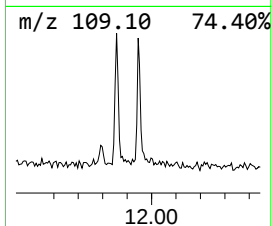
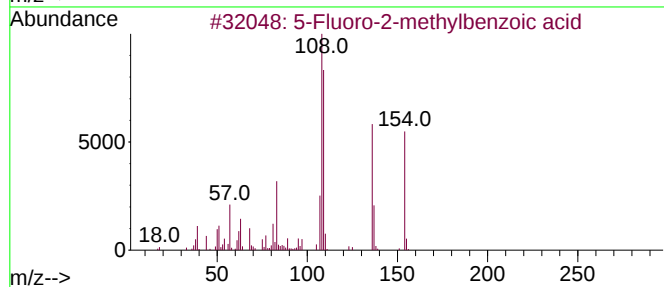
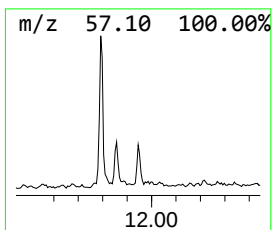
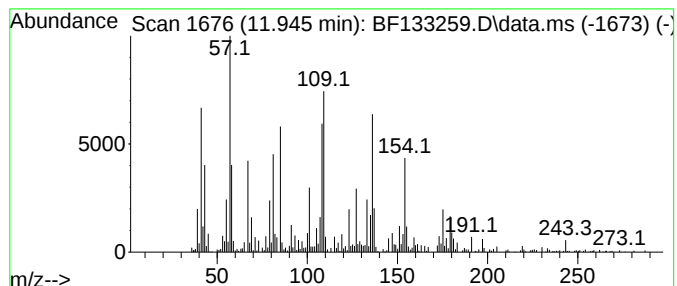
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 5-Fluoro-2-methylbenzoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.945	4.36 ng	390655	Phenanthrene-d10	11.245	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methylbenzoic acid	154	C8H7FO2	033184-16-6	58
2	Formic acid, (2-fluorophenyl)met...	154	C8H7FO2	1000368-73-6	38
3	Phenacetin	179	C10H13NO2	000062-44-2	30
4	[5-(Hydroxymethyl)-2,5,8a-trimet...	238	C15H26O2	1796930-60-3	25
5	Cyclohexanemethanol, 3,3-dimethy...	212	C13H24O2	072541-28-7	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
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ALS Vial : 6 Sample Multiplier: 1

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MW-1-20230503

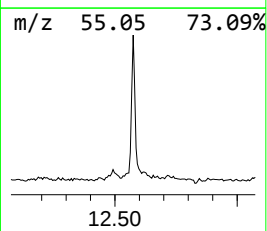
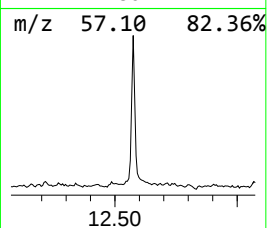
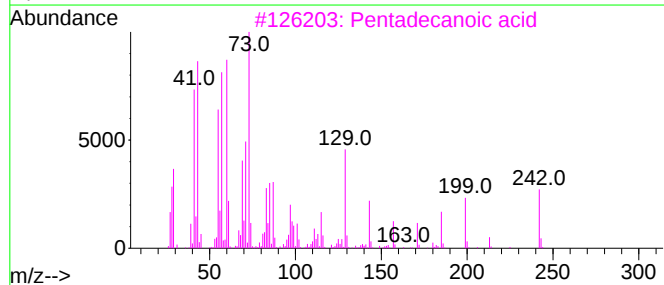
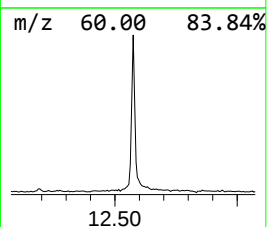
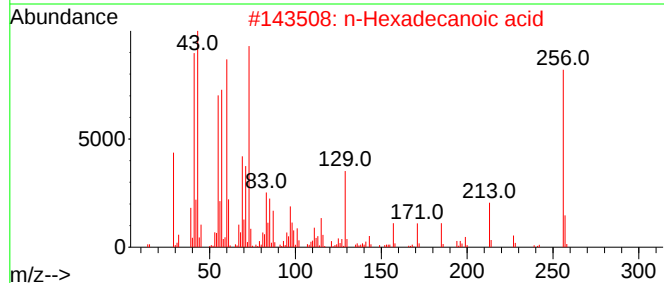
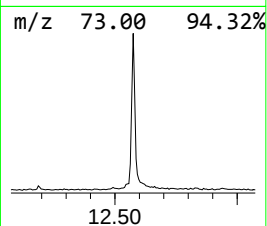
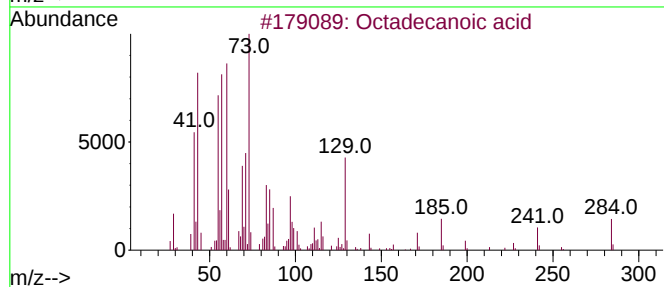
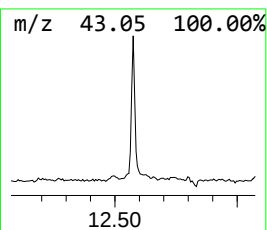
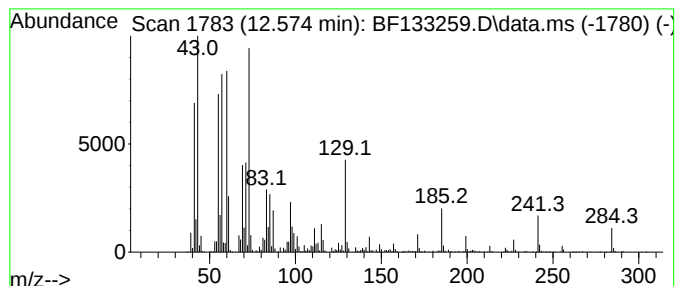
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.574	34.72 ng	1910670	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
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Misc :
ALS Vial : 6 Sample Multiplier: 1

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ClientSampleId :
MW-1-20230503

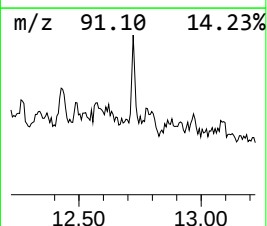
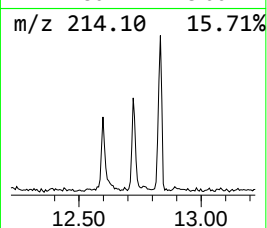
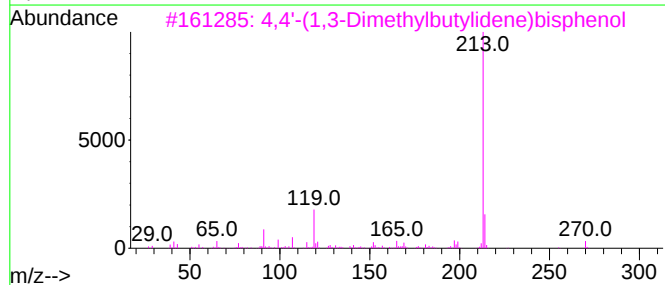
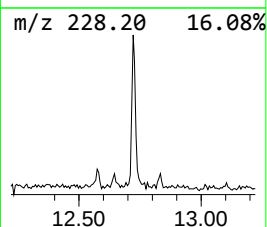
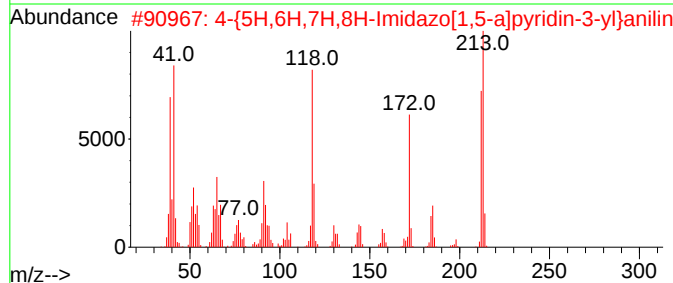
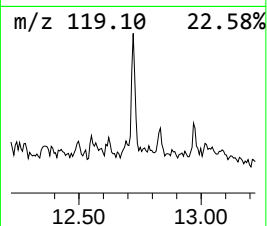
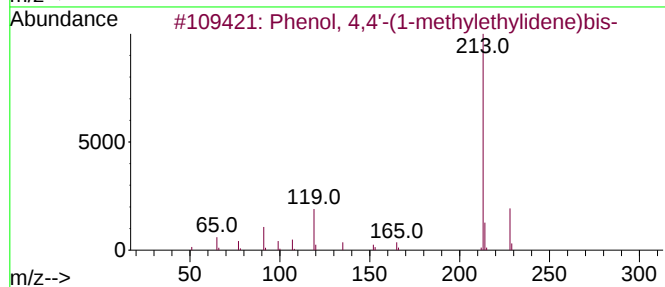
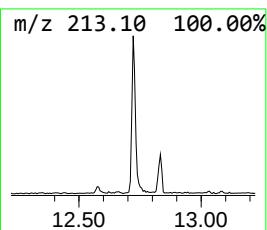
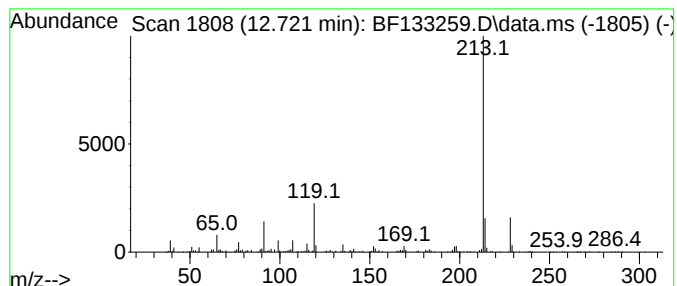
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Phenol, 4,4'-(1-methylethyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.721	6.68 ng	367648	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	95
2			4-{5H,6H,7H,8H-Imidazo[1,5-a]pyr...	213	C13H15N3	1010409-68-6	64
3			4,4'-(1,3-Dimethylbutylidene)bis...	270	C18H22O2	006807-17-6	64
4			3,4'-Isopropylidenediphenol	228	C15H16O2	046765-25-7	60
5			2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1-20230503

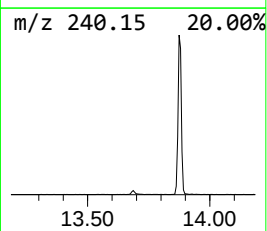
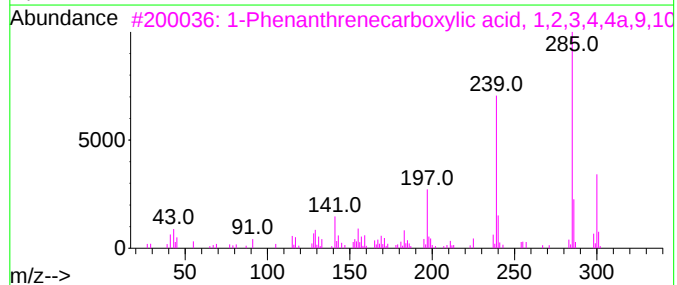
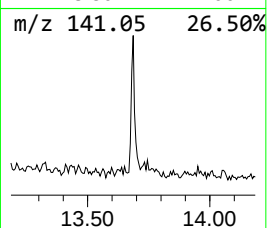
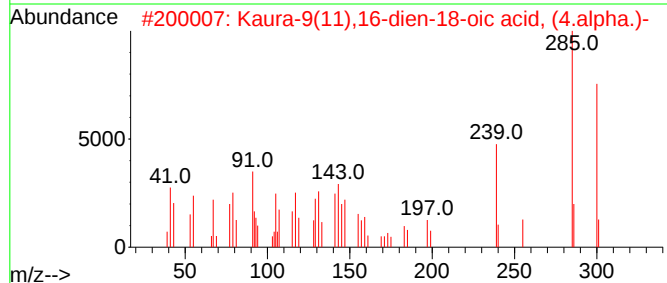
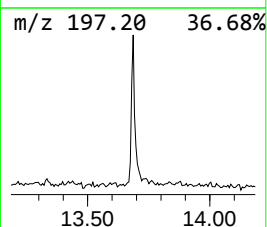
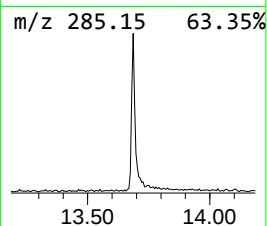
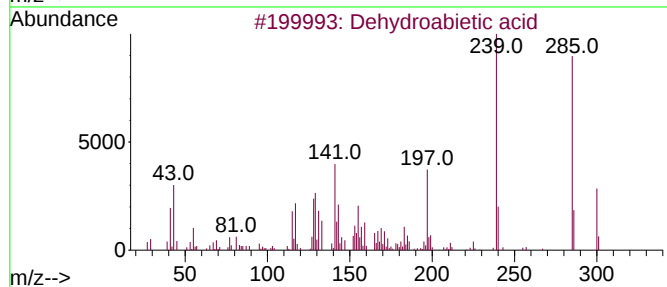
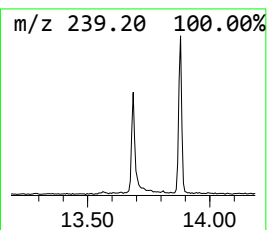
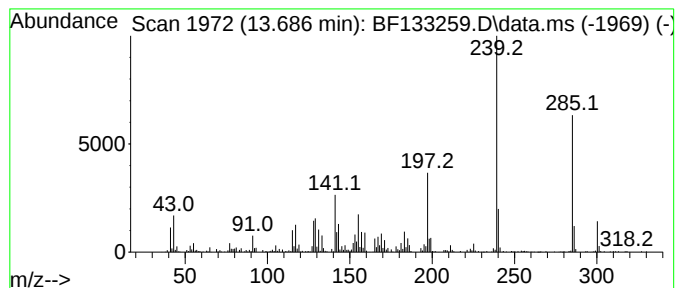
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Dehydroabietic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.686	6.92 ng	381047	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dehydroabietic acid	300	C20H28O2	001740-19-8	95
2			Kaura-9(11),16-dien-18-oic acid,...	300	C20H28O2	022338-67-6	72
3			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	64
4			2-Ethylidene-hydrazono-3-methyl-...	239	C10H10C1N3S	1000148-08-4	41
5			Indole, 3-imidazolo[2,1-b]thiazo...	239	C13H9N3S	292855-05-1	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-1-20230503

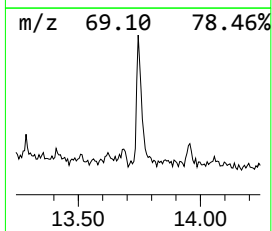
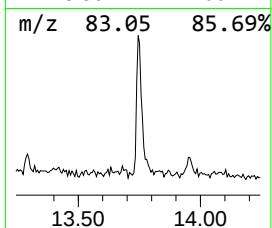
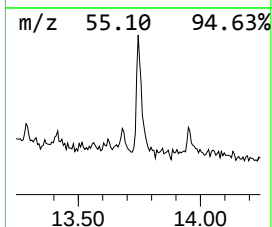
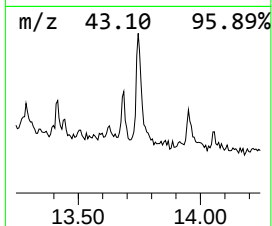
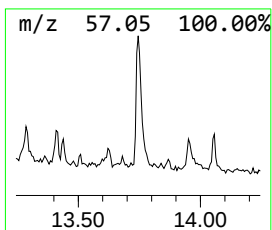
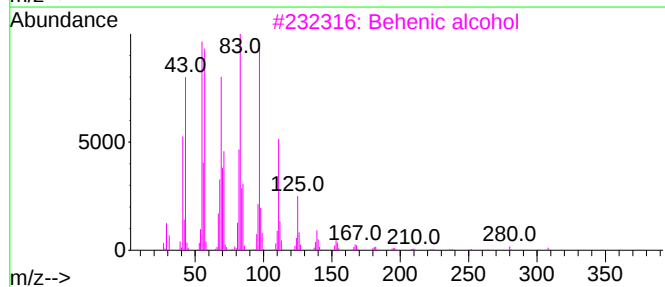
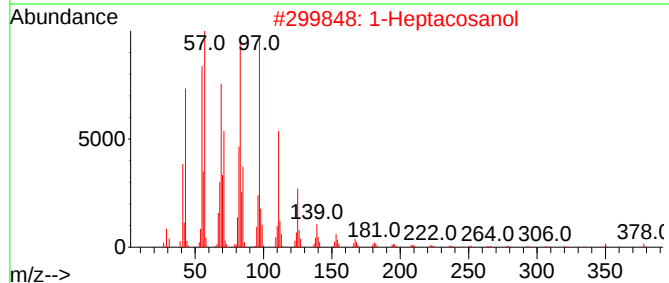
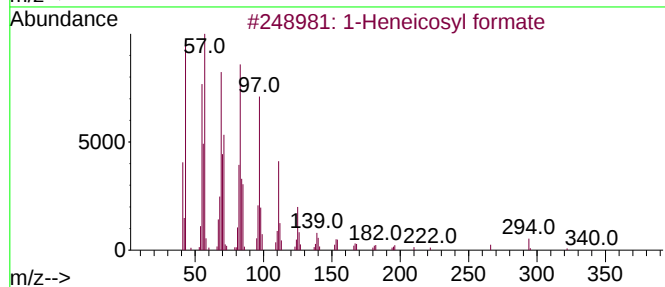
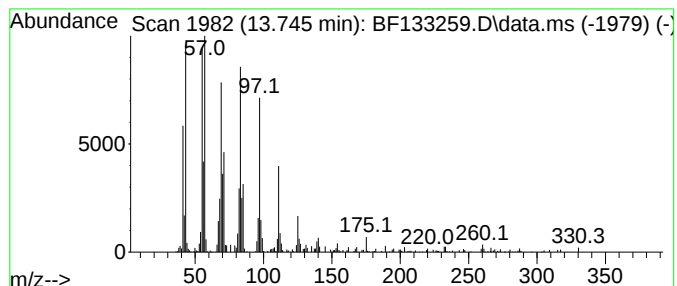
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.745	8.26 ng	454698	Chrysene-d12	13.874

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosyl formate	340	C22H44O2	077899-03-7	95
2		1-Heptacosanol	396	C27H56O	002004-39-9	91
3		Behenic alcohol	326	C22H46O	000661-19-8	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		1-Tetracosene	336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
Data File : BF133259.D
Acq On : 05 May 2023 12:28
Operator : CG\JU
Sample : 02597-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

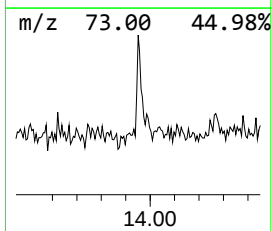
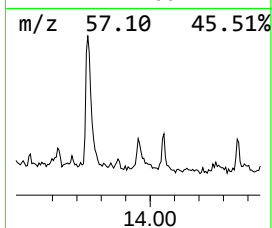
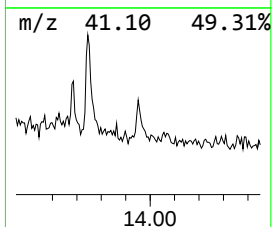
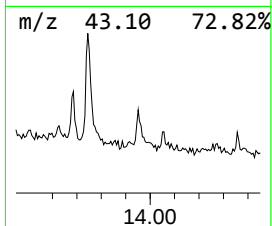
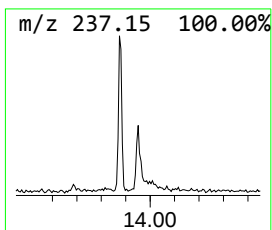
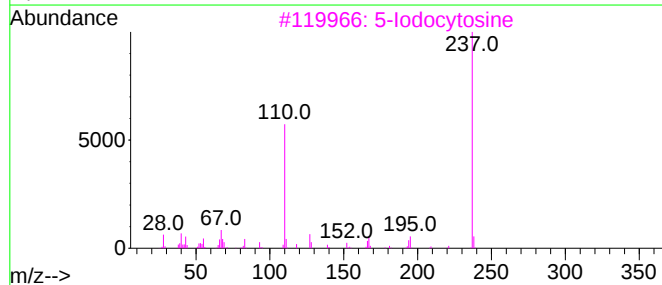
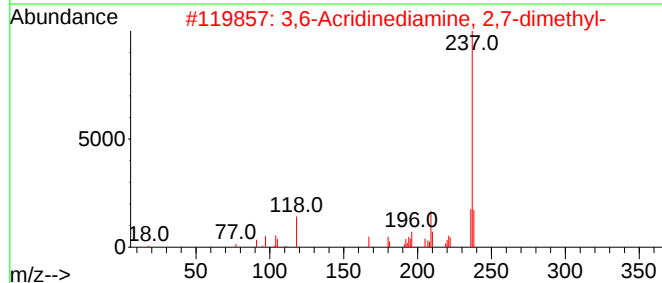
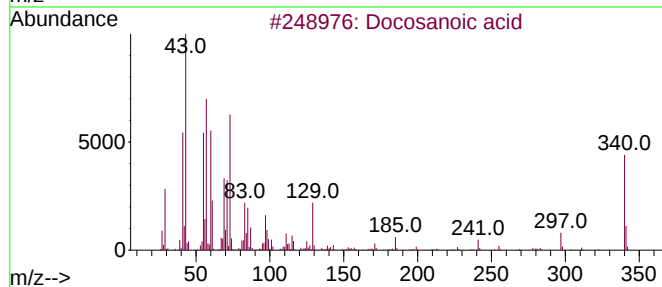
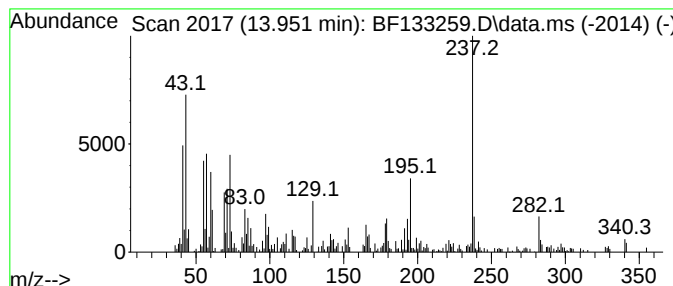
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Docosanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.951	2.92 ng	160897	Chrysene-d12	13.874	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid	340	C22H44O2	000112-85-6	93
2	3,6-Acridinediamine, 2,7-dimethyl-	237	C15H15N3	000092-26-2	49
3	5-Iodocytosine	237	C4H4IN3O	001122-44-7	41
4	9-Acridinecarboxylic acid, methy...	237	C15H11NO2	005132-81-0	38
5	2-p-Tolylisoindole-1,3-dione	237	C15H11NO2	002142-03-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050523\
 Data File : BF133259.D
 Acq On : 05 May 2023 12:28
 Operator : CG\JU
 Sample : 02597-04
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1-20230503

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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
Cyclopentanone	4.169	8.6	ng	542313	1	6.722	1259070	20.0
2-Pentanone, 4-...	4.916	2.5	ng	157648	1	6.722	1259070	20.0
Cyclohexanone	4.940	2.5	ng	156768	1	6.722	1259070	20.0
Butanoic acid, ...	5.016	3.0	ng	189874	1	6.722	1259070	20.0
(R)-(+)-3-Methy...	5.040	2.6	ng	162879	1	6.722	1259070	20.0
Indane	6.904	3.7	ng	235127	1	6.722	1259070	20.0
Benzeneacetic acid	8.281	4.3	ng	405892	2	8.010	1870010	20.0
Phenol, 2-propyl-	8.363	4.9	ng	454061	2	8.010	1870010	20.0
Biphenyl	9.186	2.8	ng	249067	3	9.763	1810990	20.0
Benzenepropanoi...	9.433	9.2	ng	829257	3	9.763	1810990	20.0
7-Methoxymethyl...	10.057	14.2	ng	1283100	3	9.763	1810990	20.0
2-Naphthaleneca...	10.692	2.8	ng	248669	4	11.245	1791530	20.0
n-Hexadecanoic ...	11.792	16.9	ng	1515640	4	11.245	1791530	20.0
unknown11.857	11.857	4.5	ng	402084	4	11.245	1791530	20.0
5-Fluoro-2-meth...	11.945	4.4	ng	390655	4	11.245	1791530	20.0
Octadecanoic acid	12.574	34.7	ng	1910670	5	13.874	1100700	20.0
Phenol, 4,4'-(1...	12.721	6.7	ng	367648	5	13.874	1100700	20.0
Dehydroabietic ...	13.686	6.9	ng	381047	5	13.874	1100700	20.0
1-Heneicosyl fo...	13.745	8.3	ng	454698	5	13.874	1100700	20.0
Docosanoic acid	13.951	2.9	ng	160897	5	13.874	1100700	20.0