

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
 Data File : BF127564.D
 Acq On : 29 Mar 2022 14:38
 Operator : CG\JU
 Sample : N2154-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-4

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-BF032122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127564.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.299	167	172	184	rVB2	23437	48727	1.75%	0.193%
2	3.787	250	255	260	rBV	36661	62215	2.23%	0.247%
3	3.981	279	288	297	rBV2	16828	41812	1.50%	0.166%
4	5.063	469	472	484	rBV	24668	43426	1.56%	0.172%
5	5.228	491	500	508	rBV3	49241	143329	5.15%	0.569%
6	5.328	512	517	526	rVB2	24238	44672	1.60%	0.177%
7	5.463	537	540	555	rBV	1055110	1202158	43.18%	4.773%
8	5.634	566	569	571	rBV	28240	32429	1.16%	0.129%
9	5.675	571	576	581	rVB3	47617	88572	3.18%	0.352%
10	5.787	592	595	609	rVB	150094	195774	7.03%	0.777%
11	6.140	652	655	659	rBV2	63013	73075	2.62%	0.290%
12	6.269	674	677	688	rVB4	34315	71231	2.56%	0.283%
13	6.434	699	705	709	rBV7	16875	33026	1.19%	0.131%
14	6.475	709	712	718	rBV	732979	846159	30.39%	3.360%
15	6.639	738	740	743	rBV2	53518	51915	1.86%	0.206%
16	6.669	743	745	758	rVB2	42371	107644	3.87%	0.427%
17	6.763	758	761	764	rBV	63275	58535	2.10%	0.232%
18	6.834	770	773	777	rBV	588539	518537	18.62%	2.059%
19	6.892	777	783	786	rVV	200512	257087	9.23%	1.021%
20	6.922	786	788	794	rVV2	146580	194508	6.99%	0.772%
21	6.998	797	801	808	rVB7	25649	48643	1.75%	0.193%
22	7.081	811	815	818	rBV	36867	45725	1.64%	0.182%
23	7.245	833	843	846	rBV2	153866	205992	7.40%	0.818%
24	7.310	851	854	858	rVB	66799	75095	2.70%	0.298%
25	7.375	861	865	866	rBV2	100093	87877	3.16%	0.349%
26	7.404	866	870	876	rVV	1869683	1759363	63.19%	6.985%
27	7.451	876	878	883	rVB	53682	50895	1.83%	0.202%
28	7.516	885	889	890	rBV3	44847	51191	1.84%	0.203%
29	7.563	892	897	901	rVV	168086	236635	8.50%	0.940%
30	7.722	911	924	932	rVB	549317	1293918	46.48%	5.137%
31	7.857	944	947	949	rBV2	69921	50615	1.82%	0.201%
32	7.881	949	951	954	rVB4	39363	37290	1.34%	0.148%
33	7.969	954	966	970	rBV	352672	1028533	36.94%	4.084%
34	8.022	973	975	982	rVB	517690	558170	20.05%	2.216%
35	8.092	982	987	988	rBV4	81293	94702	3.40%	0.376%
36	8.116	988	991	993	rVV	762461	613462	22.03%	2.436%

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	8.139	993	995	997	rVB	102043	73815	2.65%	0.293%
38	8.204	1003	1006	1010	rVB3	55904	75117	2.70%	0.298%
39	8.245	1010	1013	1015	rBV3	63568	67763	2.43%	0.269%
40	8.269	1015	1017	1018	rVV	54983	45040	1.62%	0.179%
41	8.292	1018	1021	1025	rVB2	137024	179315	6.44%	0.712%
42	8.333	1025	1028	1030	rBV	290769	326520	11.73%	1.296%
43	8.357	1030	1032	1036	rVB	326154	302057	10.85%	1.199%
44	8.410	1038	1041	1043	rBV2	155708	167454	6.01%	0.665%
45	8.481	1050	1053	1055	rBV	76855	71248	2.56%	0.283%
46	8.510	1055	1058	1062	rVV2	113990	182563	6.56%	0.725%
47	8.545	1062	1064	1066	rVV2	127126	131790	4.73%	0.523%
48	8.569	1066	1068	1070	rVV3	88447	96991	3.48%	0.385%
49	8.598	1070	1073	1078	rVV2	132728	177608	6.38%	0.705%
50	8.639	1078	1080	1084	rVB3	81595	78792	2.83%	0.313%
51	8.686	1085	1088	1091	rBV2	207416	187353	6.73%	0.744%
52	8.722	1091	1094	1098	rVB3	73452	85627	3.08%	0.340%
53	8.769	1100	1102	1108	rVB5	44430	56906	2.04%	0.226%
54	8.828	1108	1112	1114	rBV4	45664	57255	2.06%	0.227%
55	8.851	1114	1116	1119	rBV3	24406	32607	1.17%	0.129%
56	8.939	1129	1131	1135	rBV	50331	54902	1.97%	0.218%
57	8.986	1135	1139	1143	rVB6	55544	73374	2.64%	0.291%
58	9.022	1143	1145	1147	rBV	39509	38437	1.38%	0.153%
59	9.116	1159	1161	1164	rBV	228130	208447	7.49%	0.828%
60	9.192	1169	1174	1177	rVB	3179342	2784100	100.00%	11.054%
61	9.257	1177	1185	1187	rBV2	104479	102685	3.69%	0.408%
62	9.298	1188	1192	1195	rBV2	869064	869959	31.25%	3.454%
63	9.351	1199	1201	1206	rVV	138445	119043	4.28%	0.473%
64	9.398	1206	1209	1213	rVB4	46095	59920	2.15%	0.238%
65	9.457	1214	1219	1222	rBV6	43429	81342	2.92%	0.323%
66	9.516	1226	1229	1233	rVV6	38814	69658	2.50%	0.277%
67	9.575	1237	1239	1244	rVB2	76062	75363	2.71%	0.299%
68	9.633	1246	1249	1257	rVV	423584	434054	15.59%	1.723%
69	9.710	1259	1262	1268	rVB	106210	110061	3.95%	0.437%
70	9.804	1275	1278	1283	rVB	406463	349675	12.56%	1.388%
71	9.869	1286	1289	1293	rVB	815134	679581	24.41%	2.698%
72	10.016	1311	1314	1317	rVB2	67762	65819	2.36%	0.261%
73	10.075	1321	1324	1325	rBV2	37731	39217	1.41%	0.156%
74	10.098	1325	1328	1331	rVB	196055	163815	5.88%	0.650%
75	10.157	1335	1338	1342	rBV	312152	292136	10.49%	1.160%
76	10.257	1352	1355	1357	rBV2	56246	45979	1.65%	0.183%

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77	10.486	1391	1394	1395	rBV	44190	43314	1.56%	0.172%
78	10.504	1395	1397	1400	rVB	92806	68621	2.46%	0.272%
79	10.639	1416	1420	1421	rBV4	41957	43486	1.56%	0.173%
80	10.669	1421	1425	1431	rVB	1749780	1542108	55.39%	6.123%
81	10.986	1474	1479	1483	rVB2	104462	131370	4.72%	0.522%
82	11.122	1500	1502	1507	rVB3	35650	36764	1.32%	0.146%
83	11.222	1516	1519	1522	rVB	56659	40920	1.47%	0.162%
84	11.363	1540	1543	1547	rBV	814115	630051	22.63%	2.502%
85	11.739	1604	1607	1610	rVB	87919	73166	2.63%	0.291%
86	11.880	1628	1631	1636	rBV	79871	79814	2.87%	0.317%
87	11.957	1641	1644	1647	rBV	43861	40949	1.47%	0.163%
88	12.663	1762	1764	1776	rVB4	29785	39341	1.41%	0.156%
89	12.839	1791	1794	1797	rBV	30145	34995	1.26%	0.139%
90	12.945	1808	1812	1816	rBV	2090109	1836424	65.96%	7.291%
91	13.839	1960	1964	1972	rBV	86203	126441	4.54%	0.502%
92	14.015	1990	1994	2004	rBV	434449	454077	16.31%	1.803%
93	15.498	2242	2246	2254	rVB	374183	497798	17.88%	1.976%

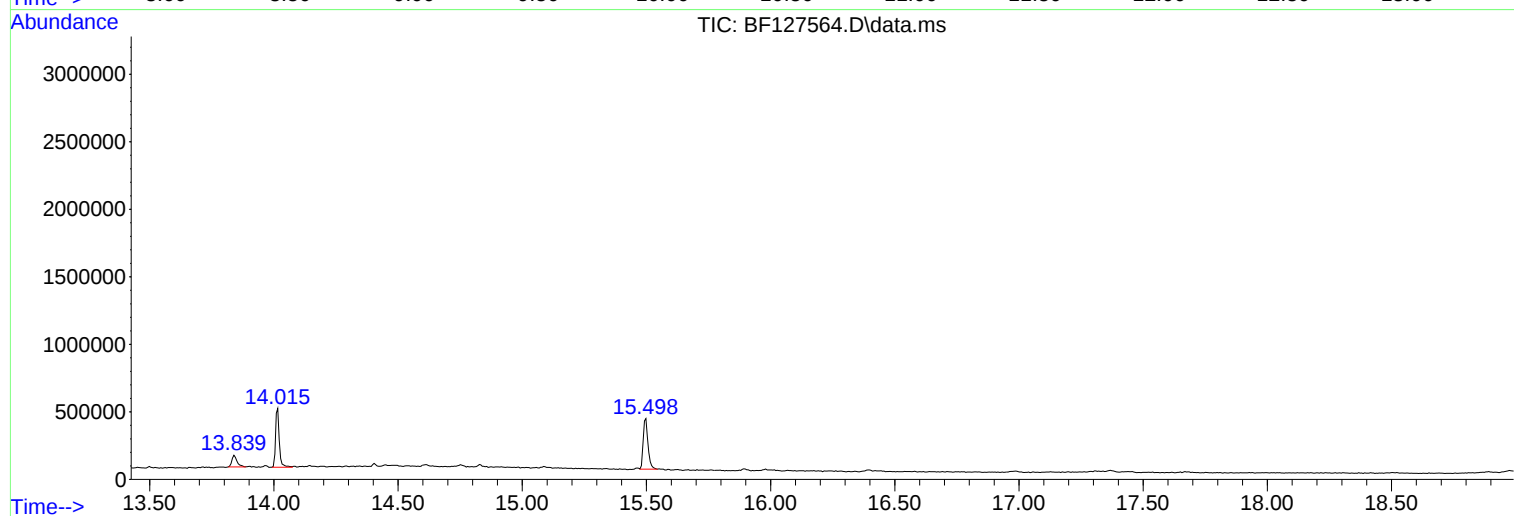
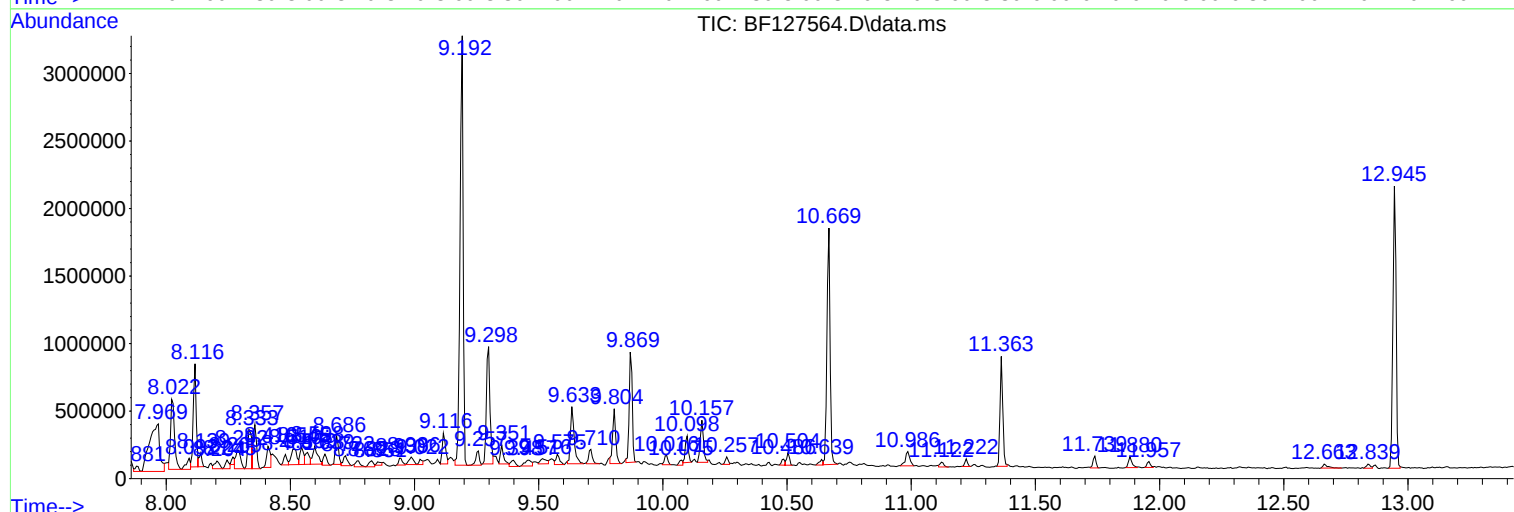
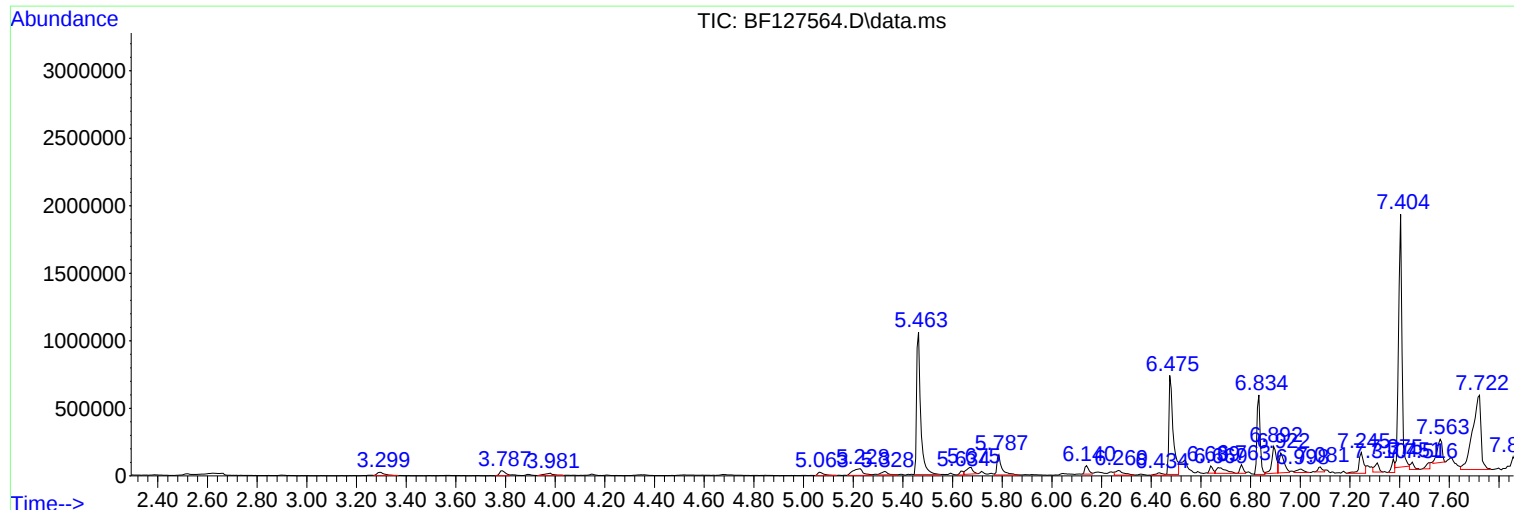
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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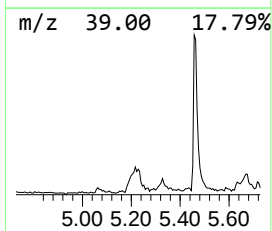
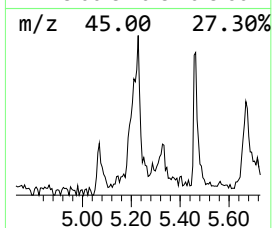
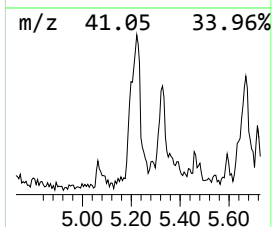
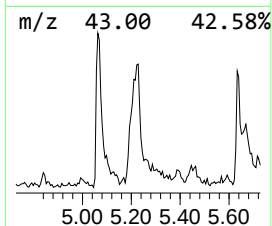
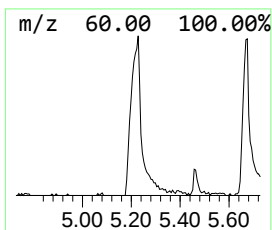
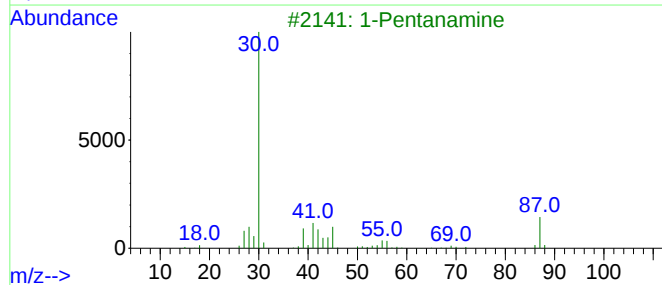
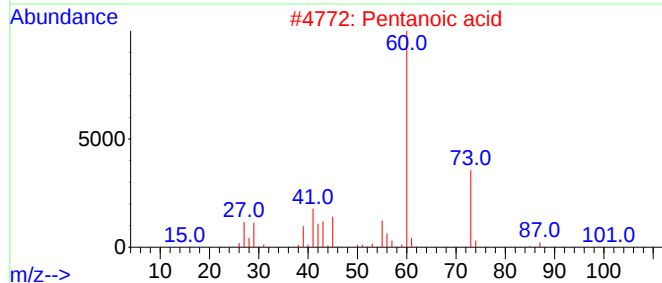
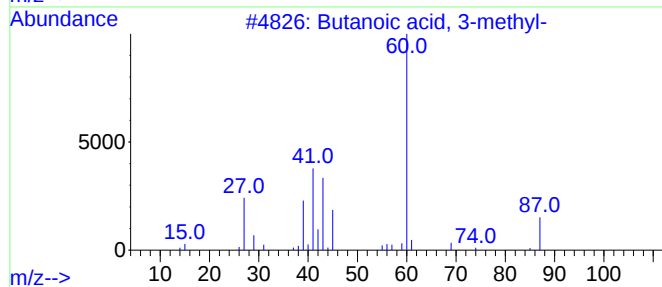
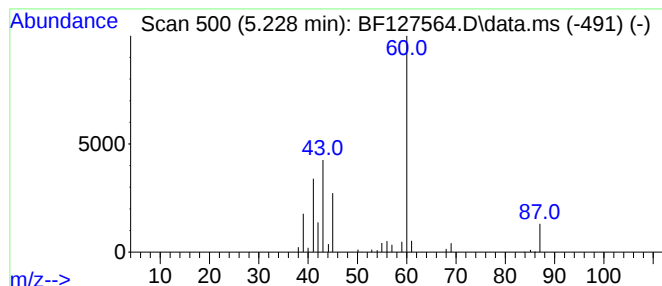
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.228	5.53 ng	143329	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	78
2			Pentanoic acid	102	C5H10O2	000109-52-4	39
3			1-Pentanamine	87	C5H13N	000110-58-7	9
4			Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	9
5			Hexanoic acid	116	C6H12O2	000142-62-1	9



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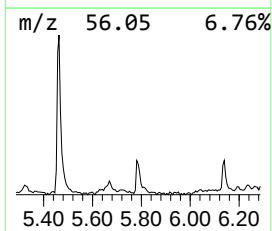
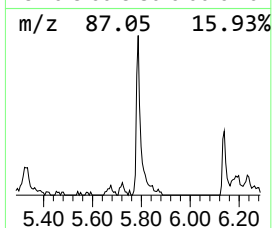
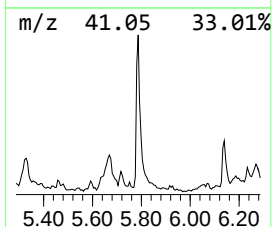
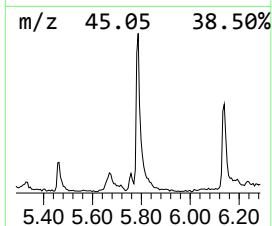
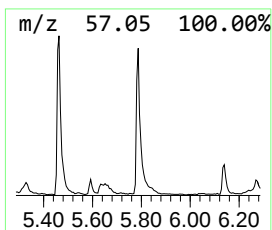
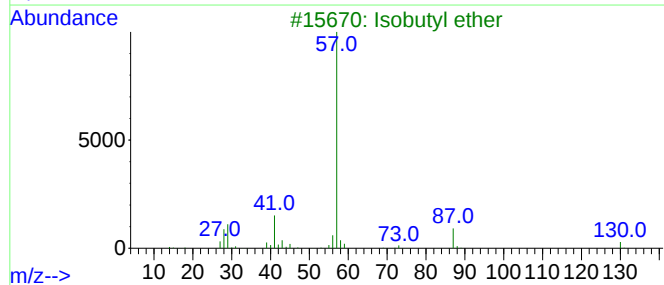
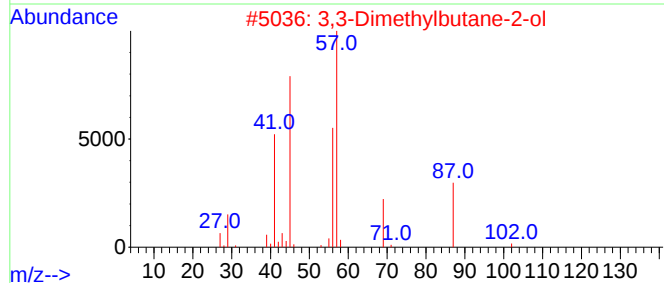
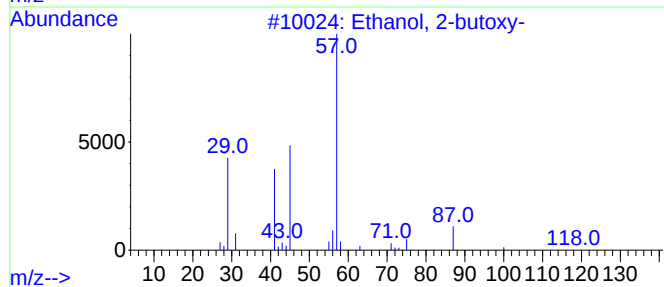
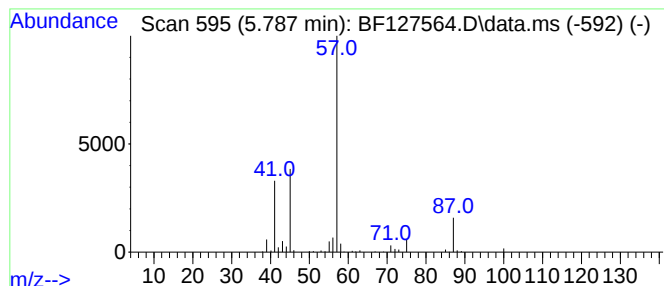
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-butoxy- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.787	7.55 ng	195774	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	83
2			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	40
3			Isobutyl ether	130	C8H18O	000628-55-7	25
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	17
5			n-Butyl ether	130	C8H18O	000142-96-1	16



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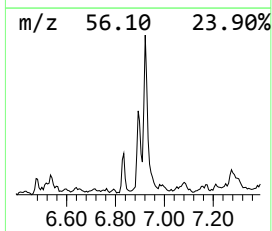
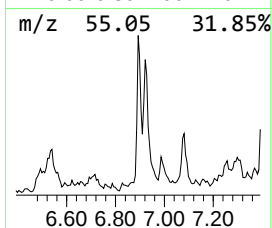
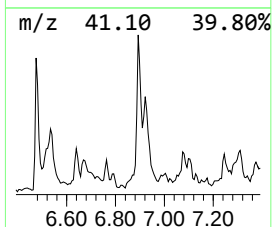
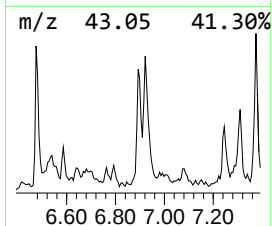
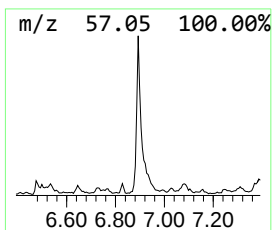
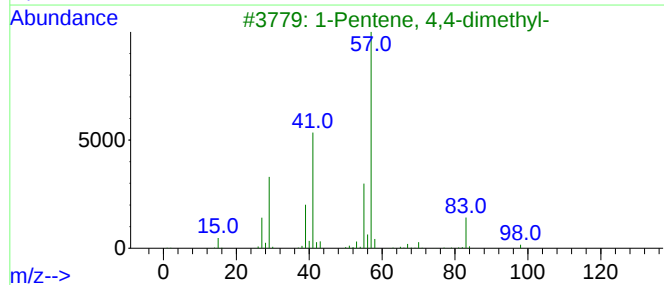
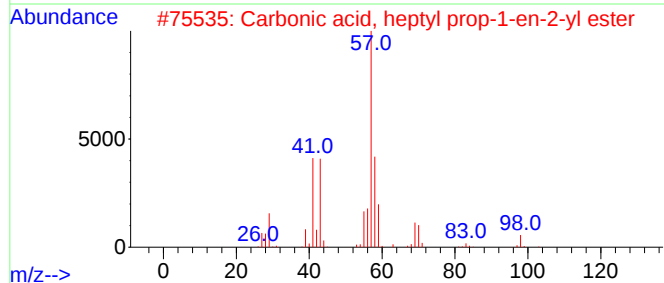
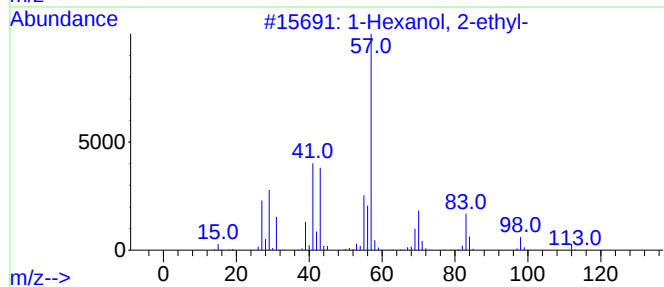
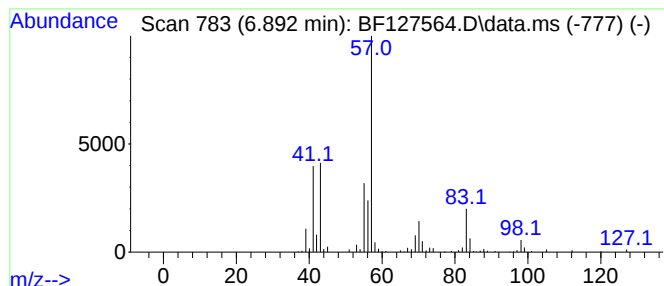
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.892	9.92 ng	257087	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47
3			1-Pentene, 4,4-dimethyl-	98	C7H14	000762-62-9	43
4			Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	43
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	42



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Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
Operator : CG\JU
Sample : N2154-02
Misc :
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Instrument :
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ClientSampleId :
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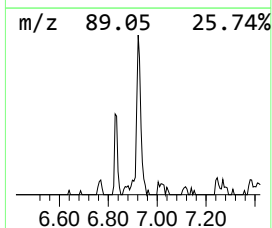
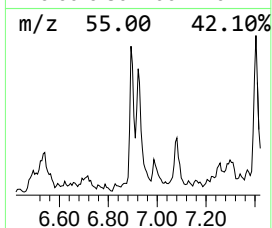
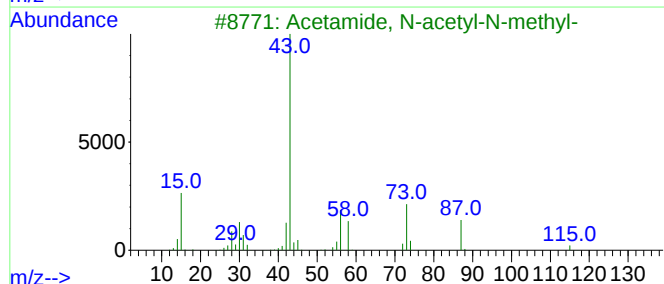
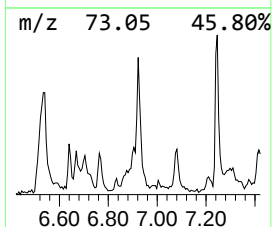
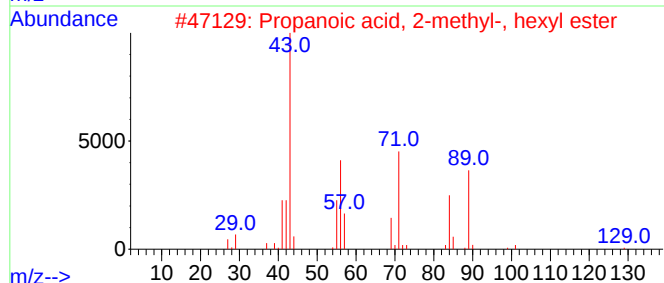
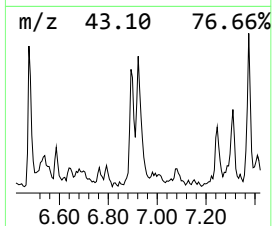
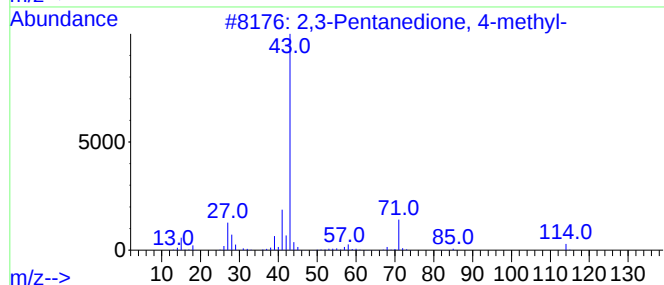
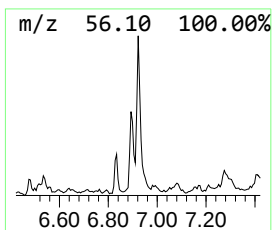
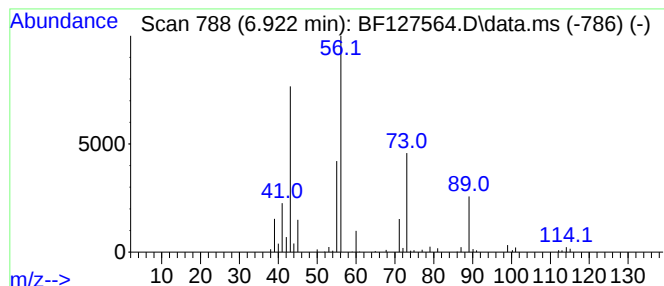
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown6.922 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.922	7.50 ng	194508	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,3-Pentanedione, 4-methyl-	114	C6H10O2	007493-58-5	11
2		Propanoic acid, 2-methyl-, hexyl...	172	C10H20O2	002349-07-7	10
3		Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9
4		1-Butanol	74	C4H10O	000071-36-3	9
5		1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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Misc :
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ClientSampleId :
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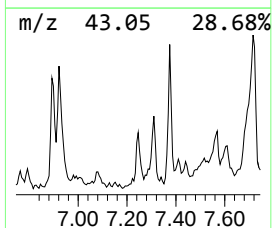
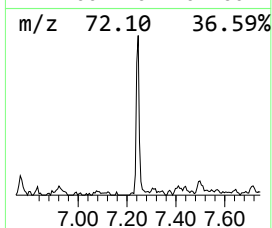
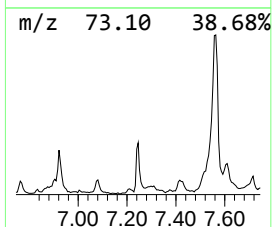
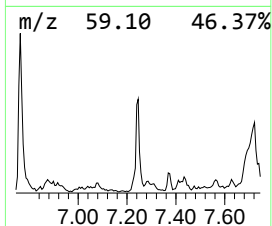
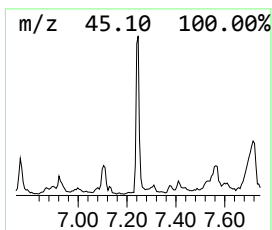
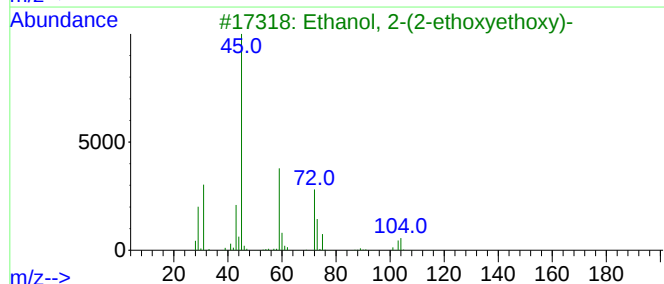
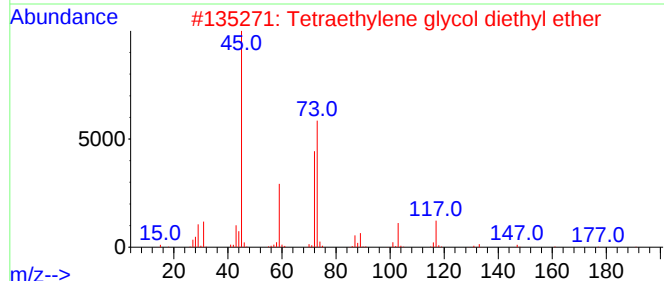
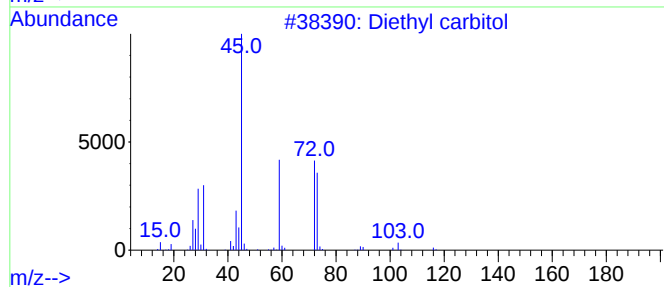
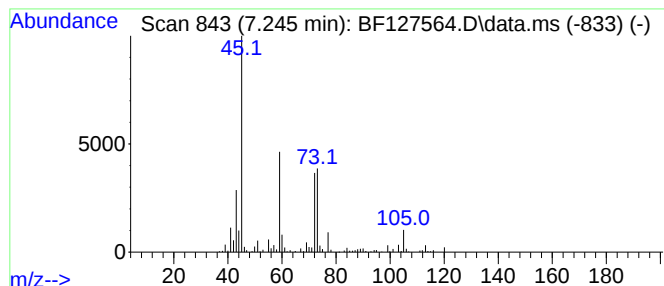
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Diethyl carbitol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.245	7.95 ng	205992	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyl carbitol	162	C8H18O3	000112-36-7	80
2			Tetraethylene glycol diethyl ether	250	C12H26O5	004353-28-0	59
3			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	50
4			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
5			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
Operator : CG\JU
Sample : N2154-02
Misc :
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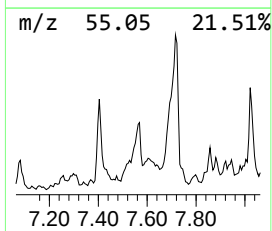
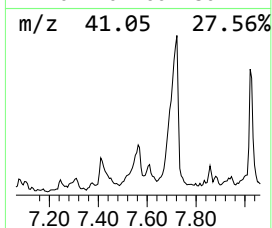
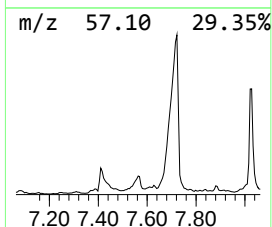
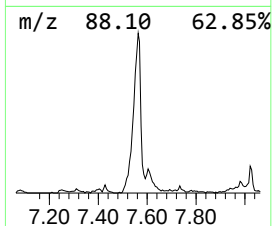
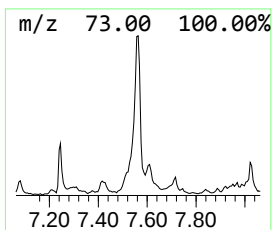
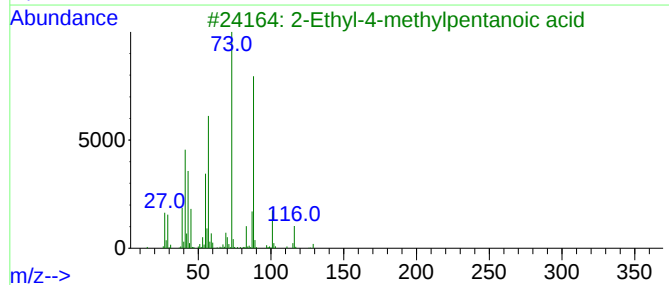
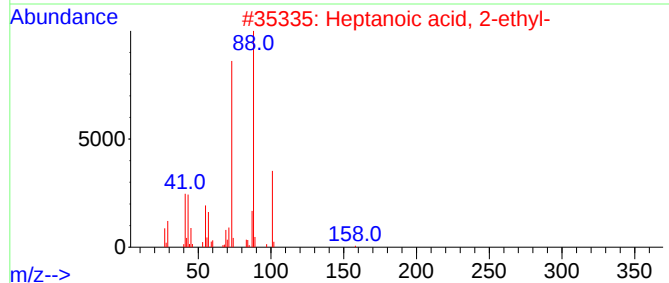
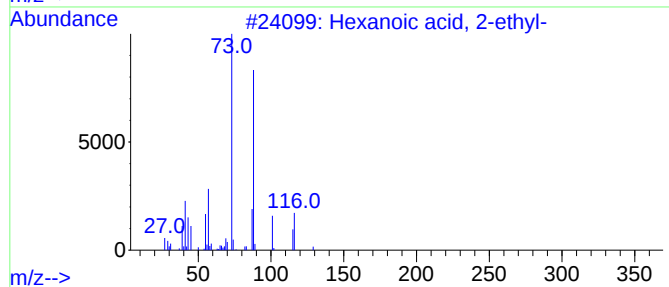
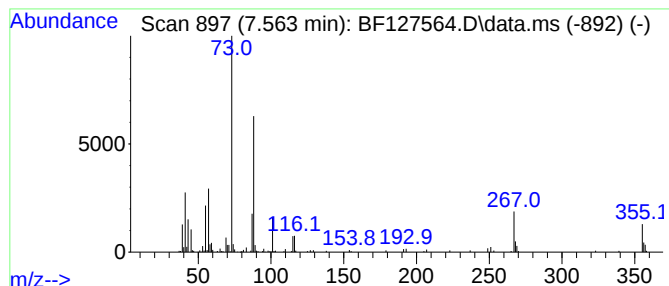
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	7.71 ng	236635	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	52
2			Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	50
3			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	40
4			Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	38
5			Acetic acid, diethyl-	116	C6H12O2	000088-09-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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Sample : N2154-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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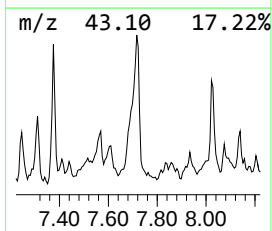
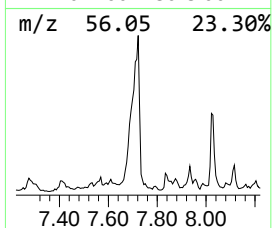
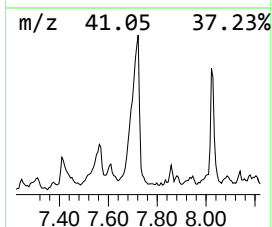
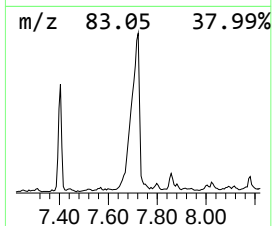
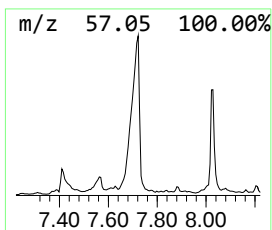
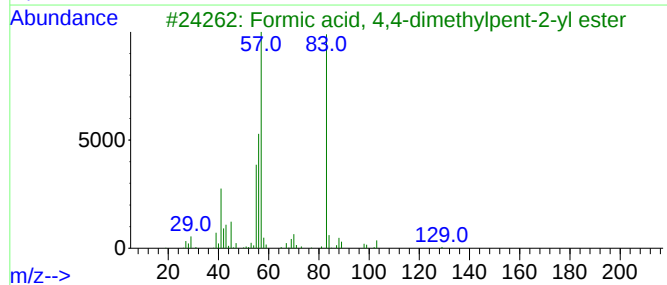
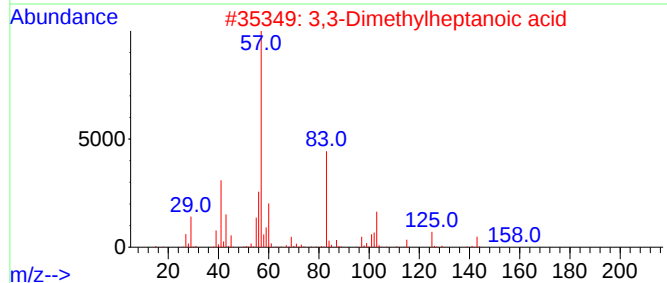
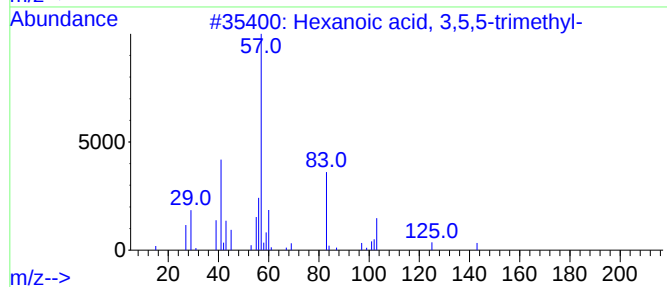
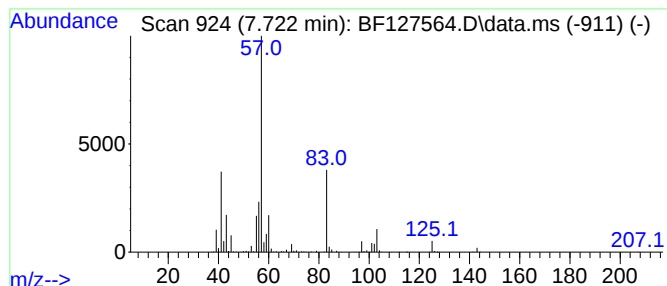
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexanoic acid, 3,5,5-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.722	42.18 ng	1293920	Naphthalene-d8	8.116

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	83
2		3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	56
3		Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	38
4		4,4-Dimethyl-2-pentanol, chlorod...	228	C9H15ClF2O2	1000376-27-0	27
5		Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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Misc :
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Instrument :
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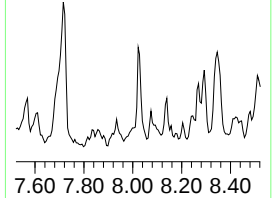
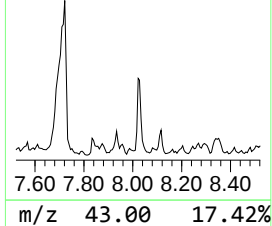
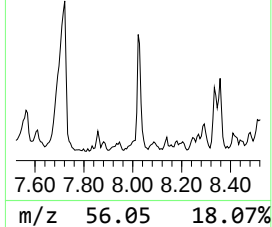
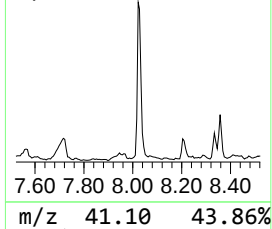
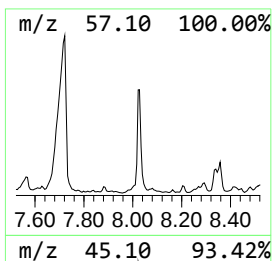
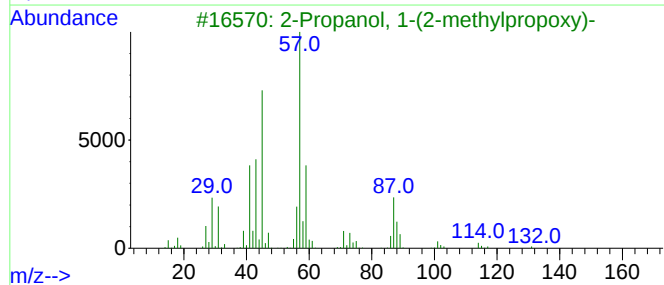
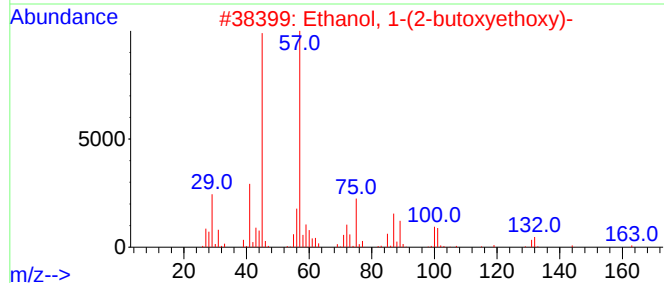
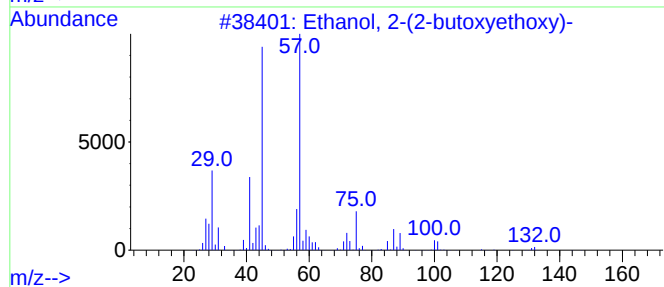
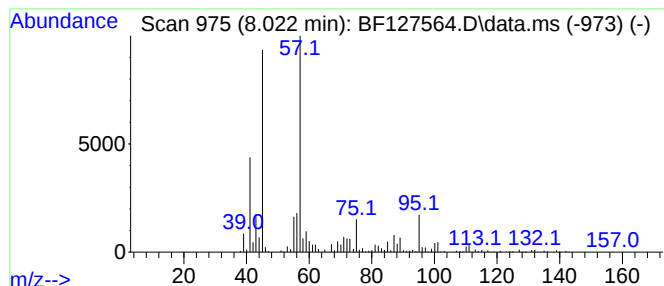
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	18.20 ng	558170	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	86
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3			2-Propanol, 1-(2-methylpropoxy)-	132	C7H16O2	023436-19-3	59
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5			2-Heptanol, 3-methyl-	130	C8H18O	031367-46-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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Misc :
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Instrument :
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ClientSampleId :
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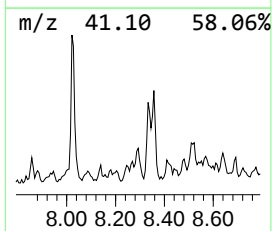
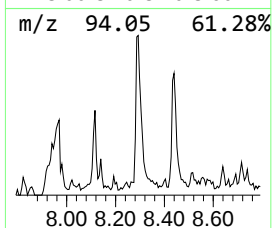
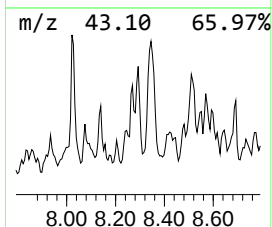
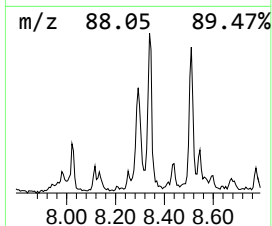
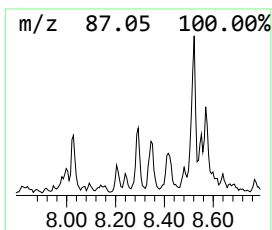
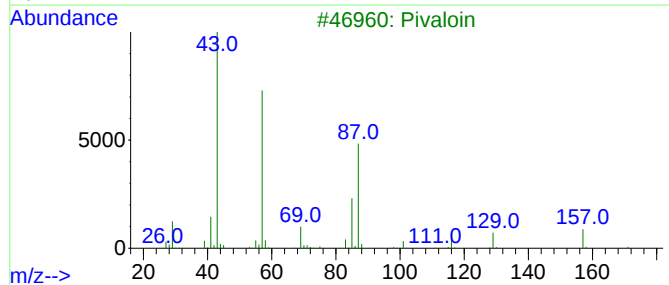
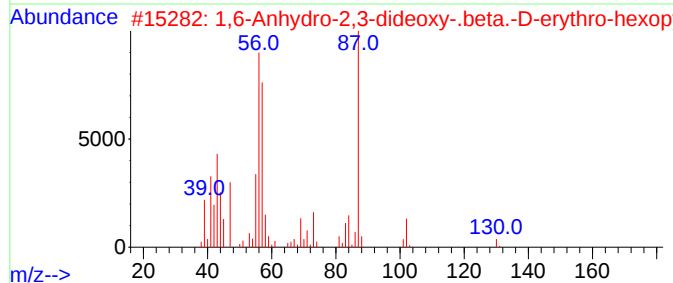
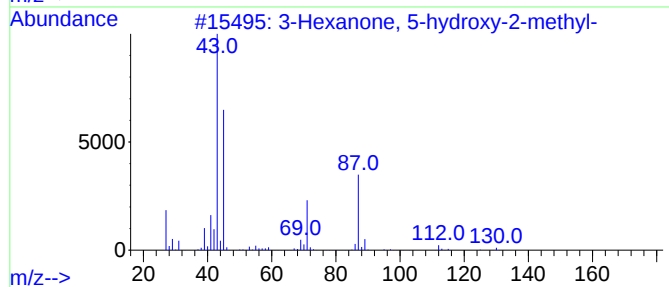
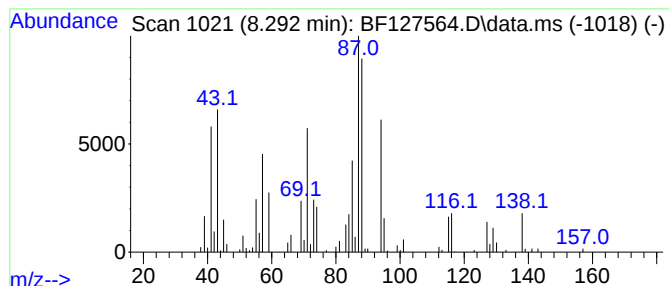
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown8.292 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.292	5.85 ng	179315	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone, 5-hydroxy-2-methyl-	130	C7H14O2	059357-07-2	22		
2	1,6-Anhydro-2,3-dideoxy-.beta.-D...	130	C6H10O3	039726-36-8	18		
3	Pivaloin	172	C10H20O2	000815-66-7	12		
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	12		
5	1-Heptanol, 2-propyl-	158	C10H22O	010042-59-8	10		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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ALS Vial : 9 Sample Multiplier: 1

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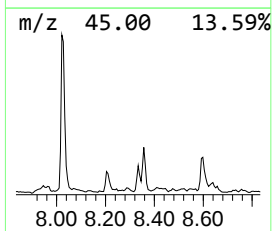
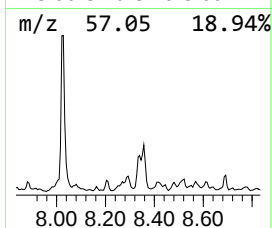
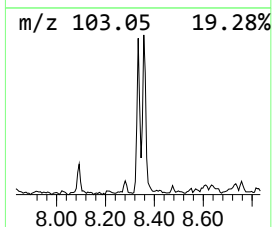
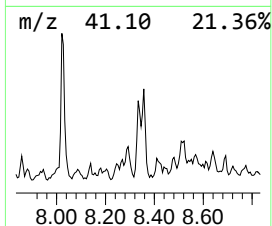
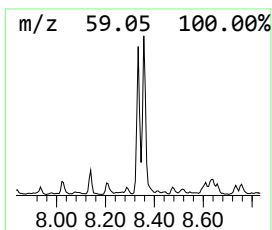
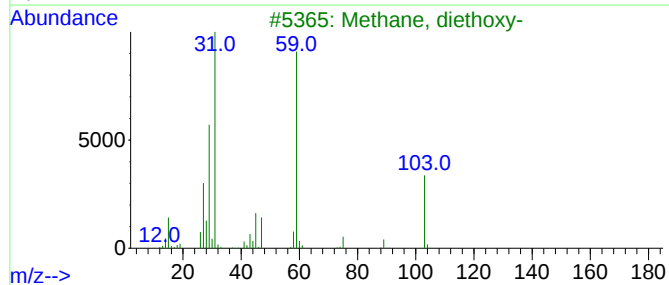
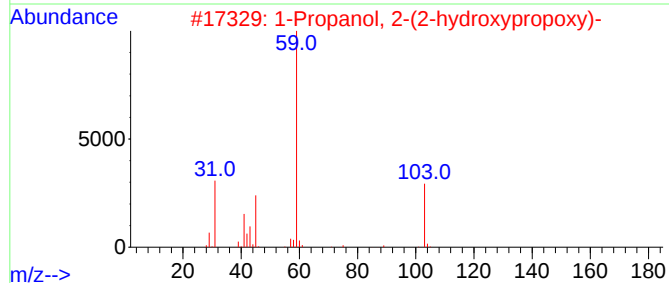
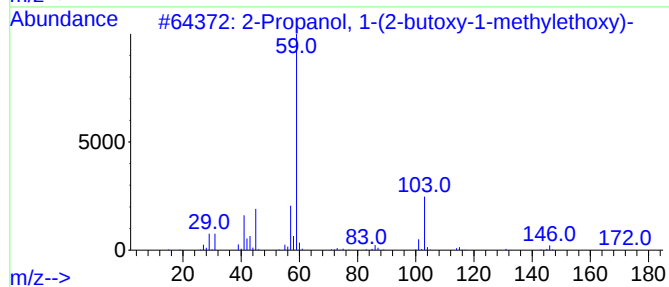
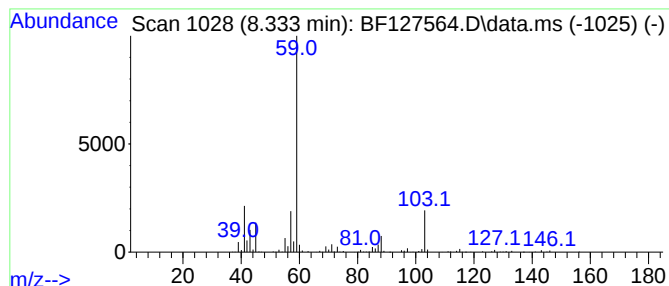
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.333	10.65 ng	326520	Naphthalene-d8	8.116

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3		029911-28-2	78
2	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3		000106-62-7	64
3	Methane, diethoxy-	104	C5H12O2		000462-95-3	64
4	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4		001638-16-0	64
5	4,8,12,16-tetraoxaicosan-1-ol	306	C16H34O5		1010397-63-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
Operator : CG\JU
Sample : N2154-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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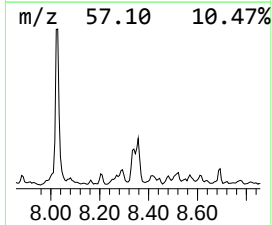
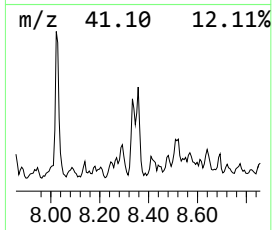
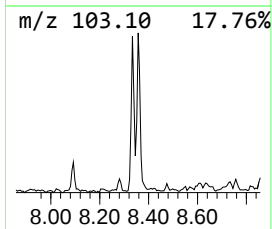
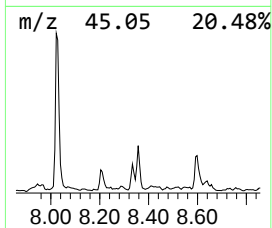
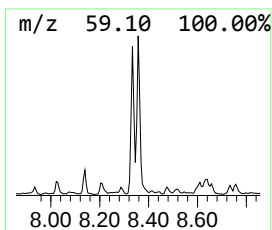
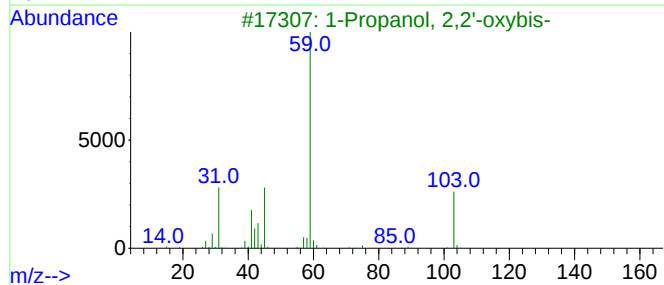
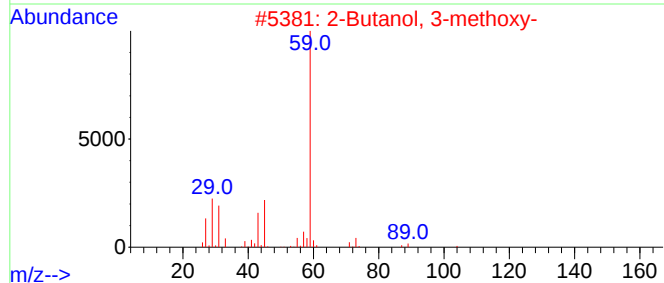
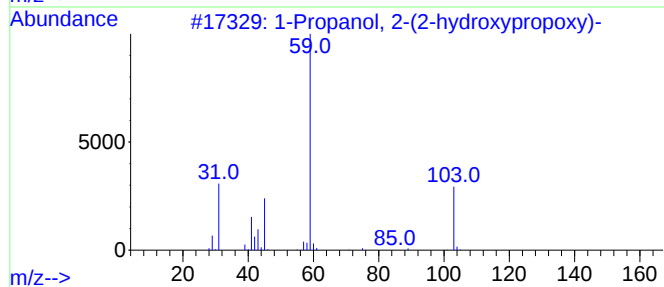
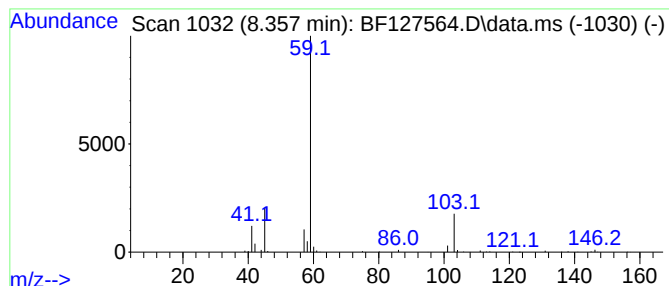
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1-Propanol, 2-(2-hydroxypro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.357	9.85 ng	302057	Naphthalene-d8	8.116

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72	
2	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	72	
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64	
4	Propanedioic acid, oxo-, dimethy...	146	C5H6O5	003298-40-6	59	
5	Methyl 2,5,8,11,14-pentaoxahexad...	280	C12H24O7	1000366-81-5	50	



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
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Acq On : 29 Mar 2022 14:38
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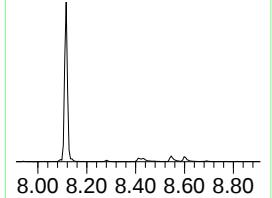
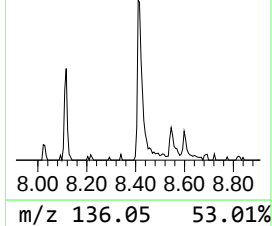
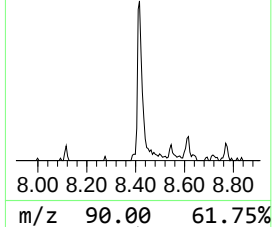
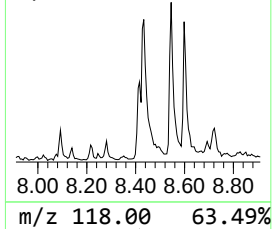
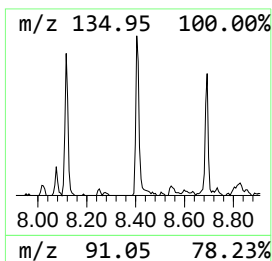
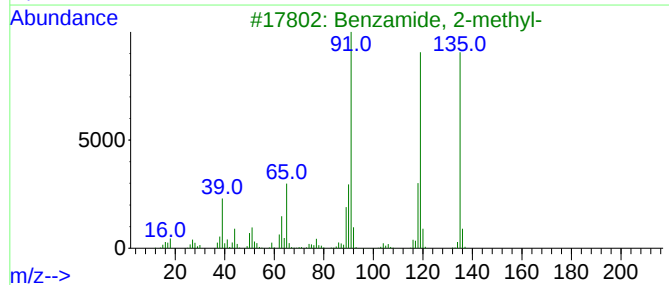
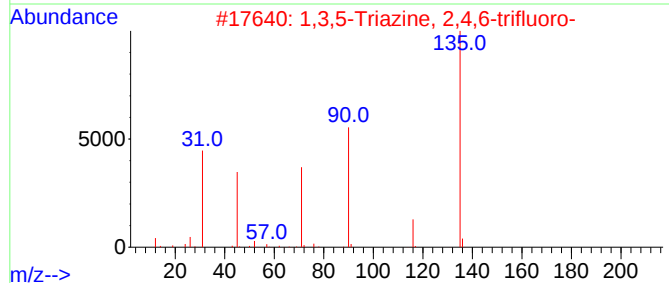
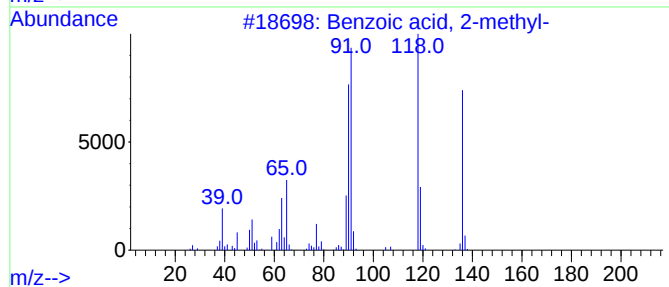
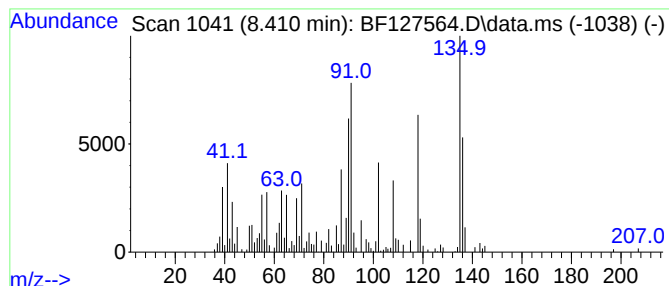
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Benzoic acid, 2-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.410	5.46 ng	167454	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-methyl-	136	C8H8O2	000118-90-1	89
2			1,3,5-Triazine, 2,4,6-trifluoro-	135	C3F3N3	000675-14-9	25
3			Benzamide, 2-methyl-	135	C8H9NO	000527-85-5	22
4			4-Methylphthalic anhydride	162	C9H6O3	019438-61-0	22
5			m-Toluamide	135	C8H9NO	000618-47-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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Sample : N2154-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

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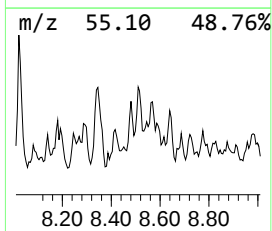
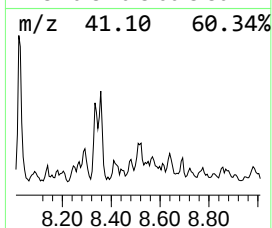
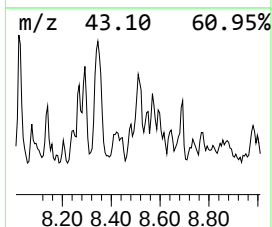
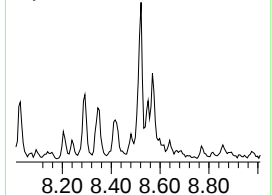
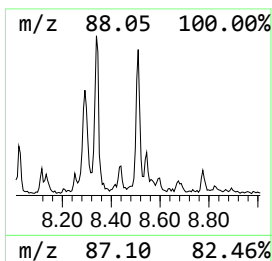
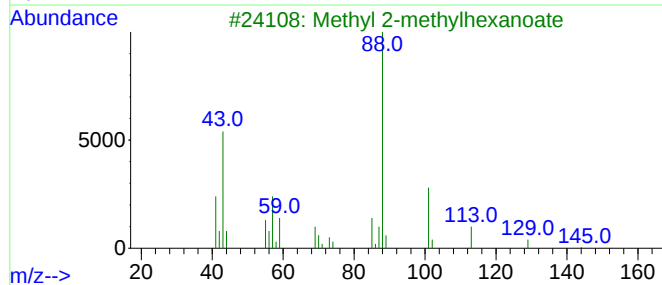
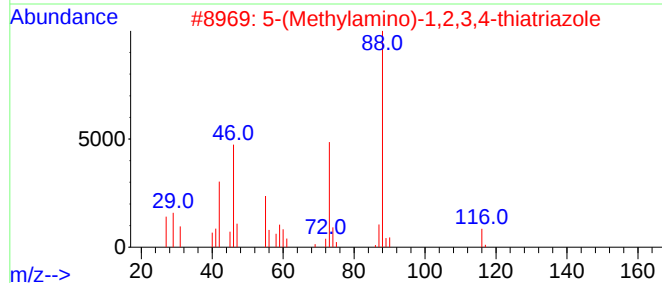
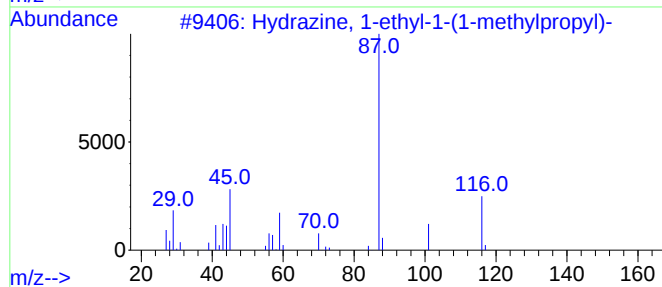
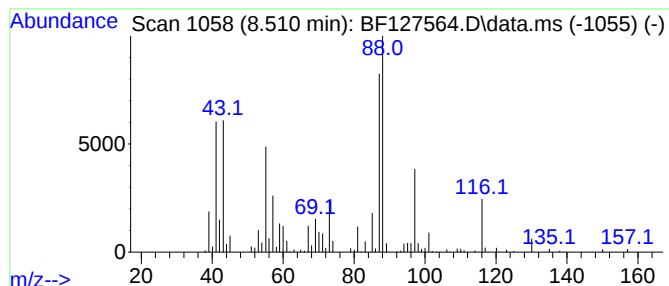
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown8.510 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.510	5.95 ng	182563	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, 1-ethyl-1-(1-methylpr...	116	C6H16N2	020325-97-7	38
2			5-(Methylamino)-1,2,3,4-thiatra...	116	C2H4N4S	052098-72-3	35
3			Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	27
4			Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	27
5			Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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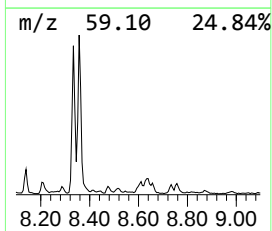
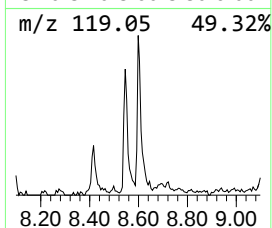
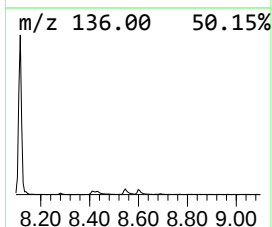
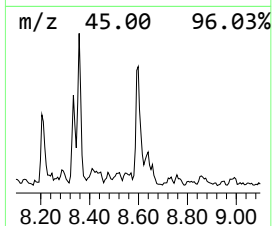
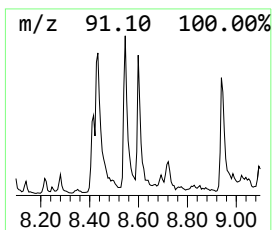
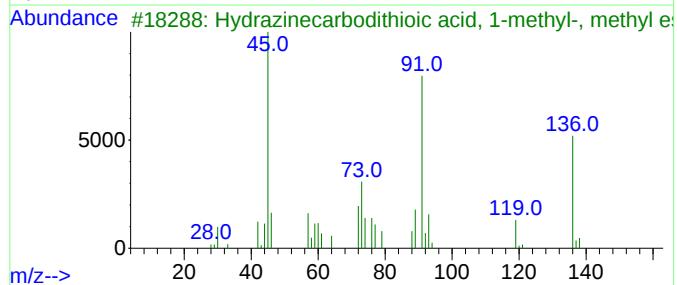
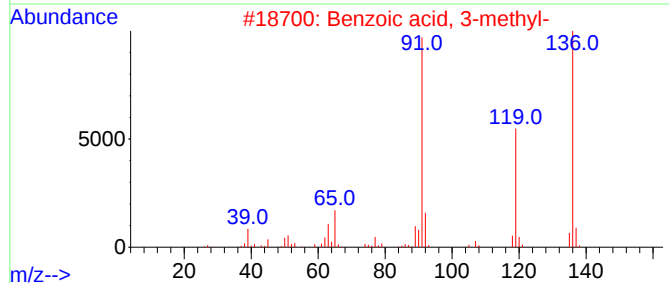
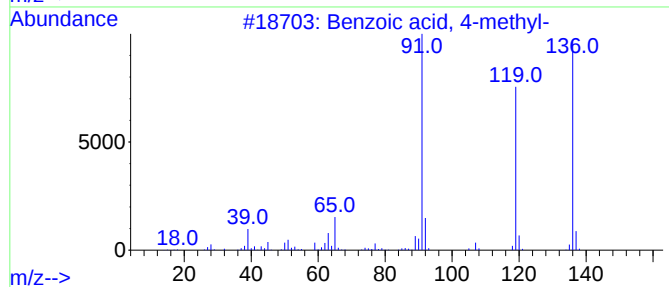
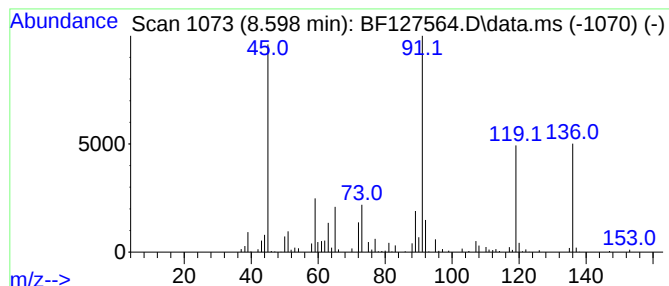
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzoic acid, 4-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.598	5.79 ng	177608	Naphthalene-d8	8.116

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	50
2			Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	38
3			Hydrazinecarbodithioic acid, 1-m...	136	C3H8N2S2	020184-94-5	37
4			3,6,9,12-Tetraoxatetradecan-1-ol	222	C10H22O5	005650-20-4	32
5			Benzeneacetic acid	136	C8H8O2	000103-82-2	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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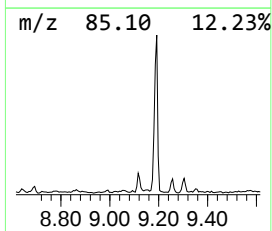
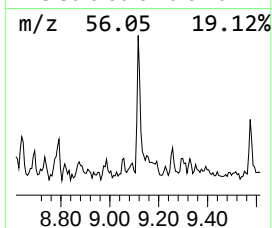
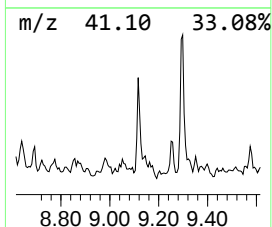
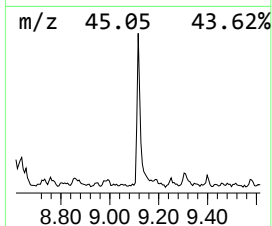
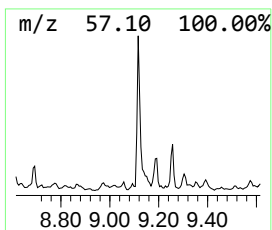
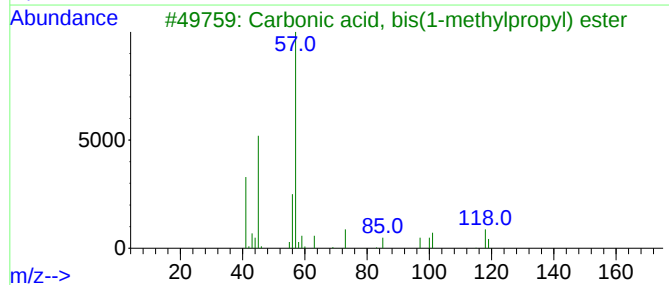
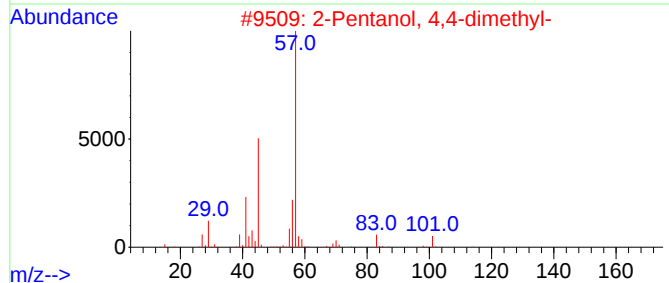
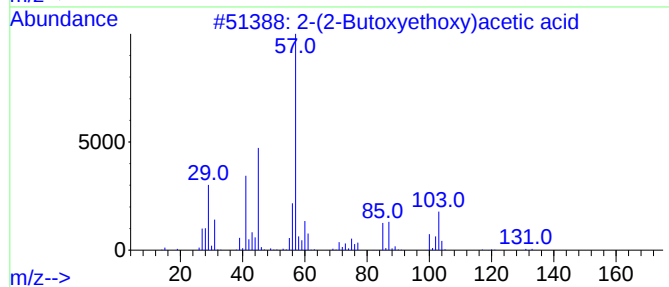
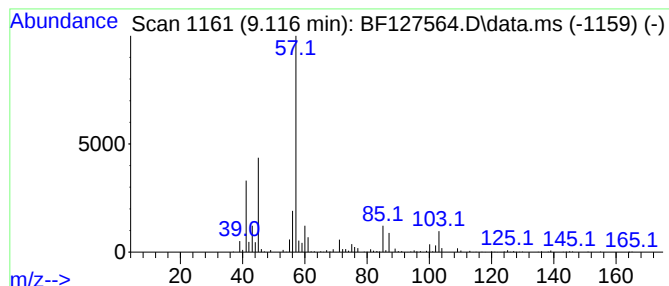
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2-(2-Butoxyethoxy)acetic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.116	6.13 ng	208447	Acenaphthene-d10	9.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-(2-Butoxyethoxy)acetic acid	176	C8H16O4	082941-26-2	72
2		2-Pentanol, 4,4-dimethyl-	116	C7H16O	006144-93-0	50
3		Carbonic acid, bis(1-methylpropy...	174	C9H18O3	000623-63-2	42
4		Propanoic acid, 2,2-dimethyl-, h...	200	C12H24O2	017660-61-6	38
5		Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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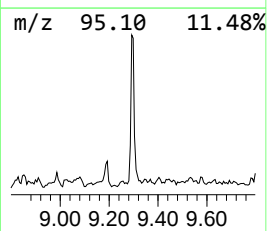
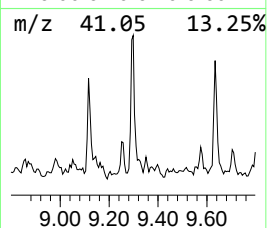
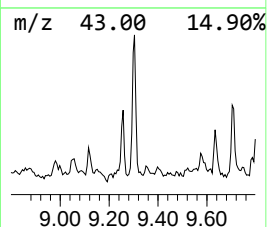
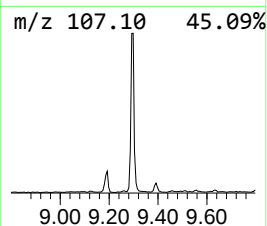
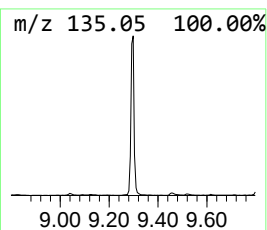
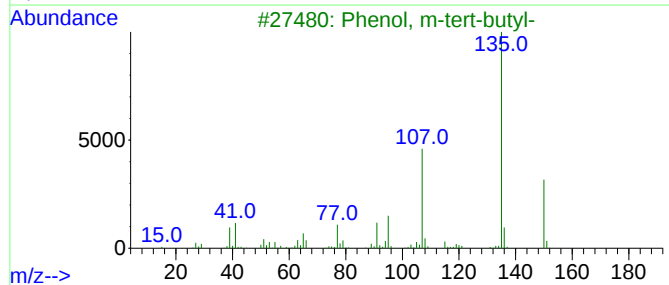
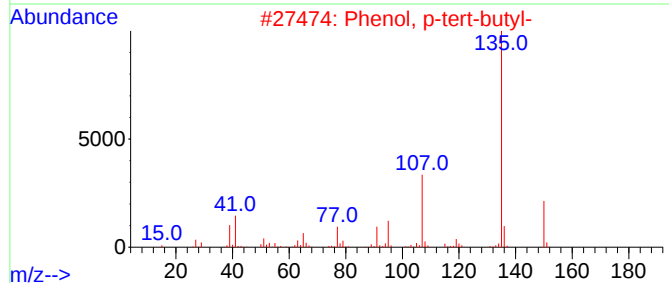
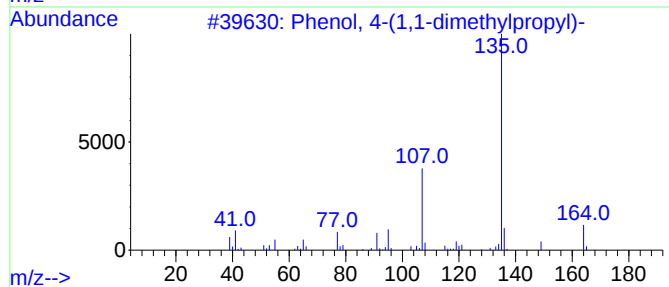
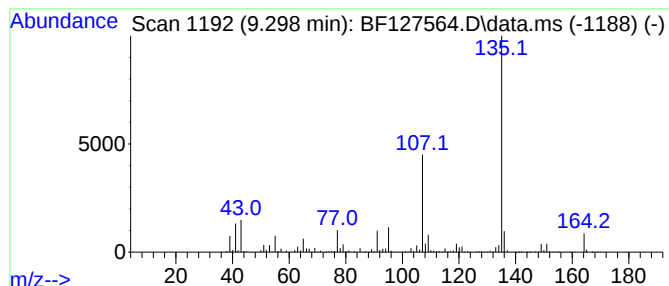
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Phenol, 4-(1,1-dimethylprop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.298	25.60 ng	869959	Acenaphthene-d10	9.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	96
2		Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3		Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	78
4		Hexestrol, 0-isopropoxyxycarbonyl-	356	C22H28O4	1000487-68-4	64
5		4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId :
MW-4

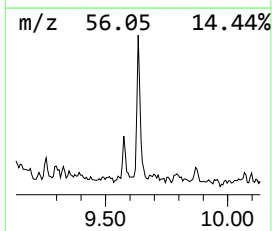
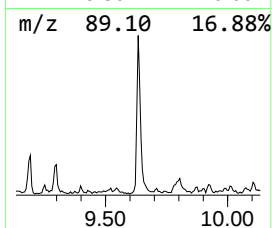
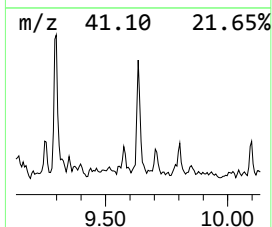
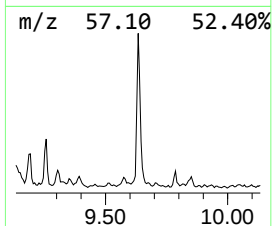
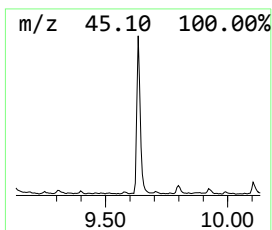
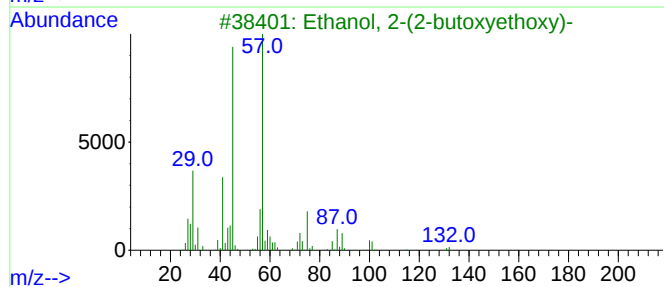
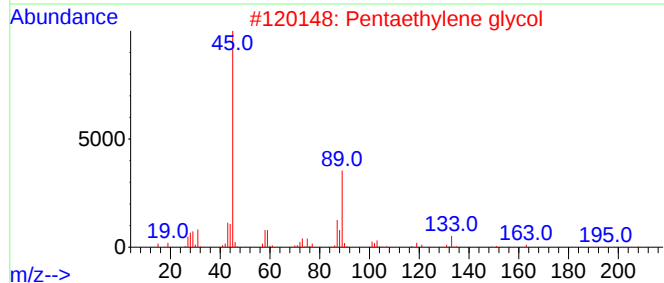
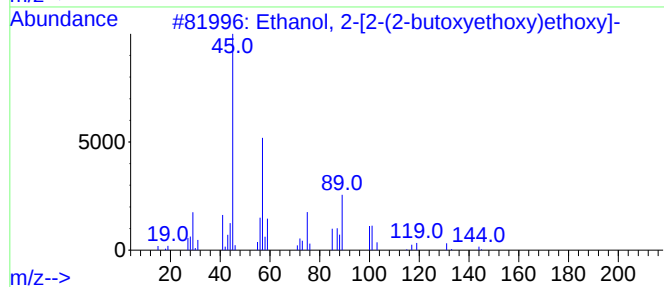
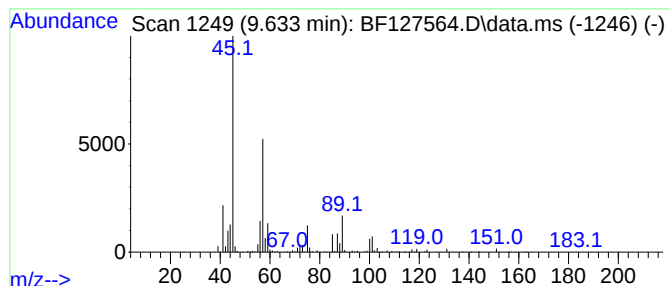
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Ethanol, 2-[2-(2-butoxyetho... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.633	12.77 ng	434054	Acenaphthene-d10	9.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	91
2		Pentaethylene glycol	238	C10H22O6	004792-15-8	72
3		Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
4		Triethylene glycol	150	C6H14O4	000112-27-6	72
5		Hexaethylene glycol	282	C12H26O7	002615-15-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
Operator : CG\JU
Sample : N2154-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

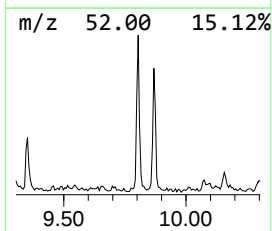
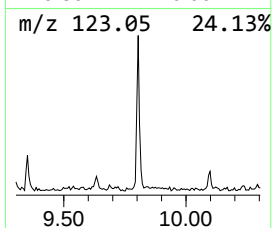
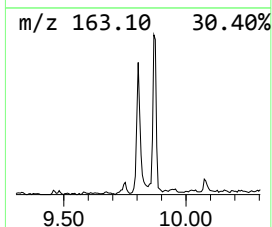
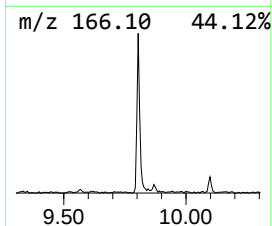
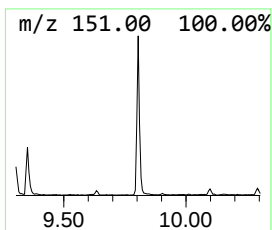
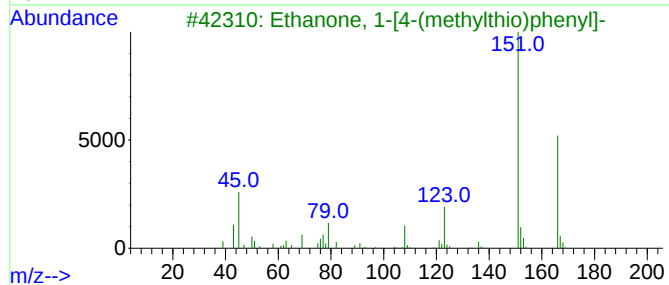
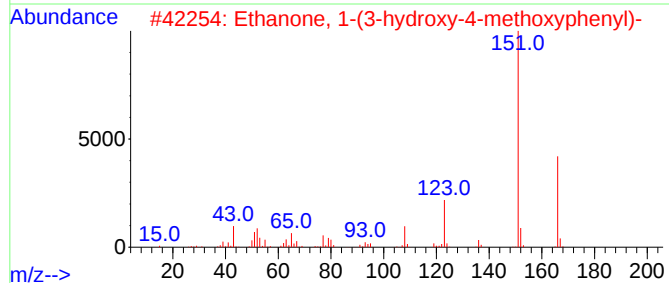
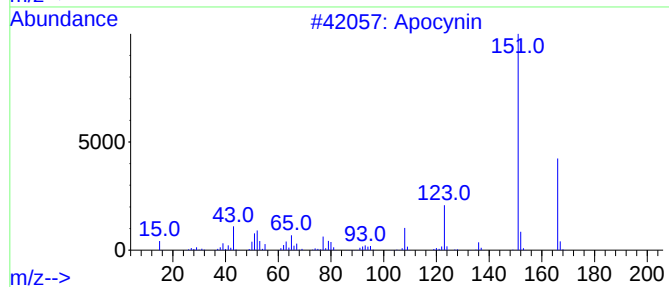
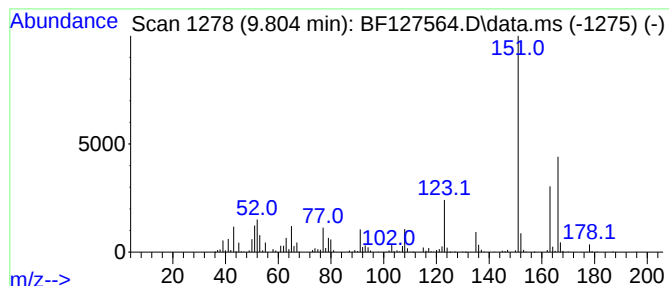
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Apocynin Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.804	10.29 ng	349675	Acenaphthene-d10	9.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Apocynin		166	C9H10O3	000498-02-2	95
2	Ethanone, 1-(3-hydroxy-4-methoxy...		166	C9H10O3	006100-74-9	94
3	Ethanone, 1-[4-(methylthio)phenyl]-		166	C9H10O3	001778-09-2	68
4	t-Butylhydroquinone		166	C10H14O2	001948-33-0	59
5	Benzene, 4-ethyl-1,2-dimethoxy-		166	C10H14O2	005888-51-7	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
Operator : CG\JU
Sample : N2154-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

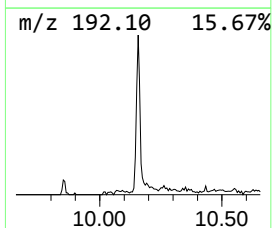
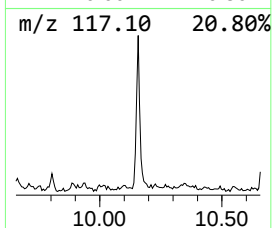
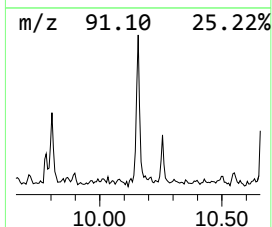
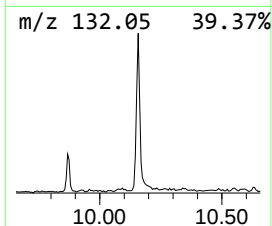
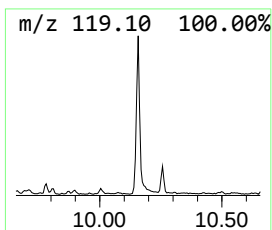
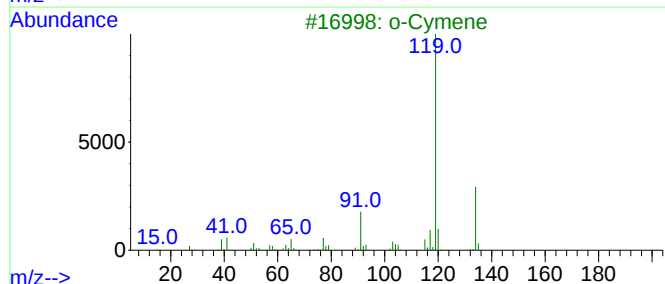
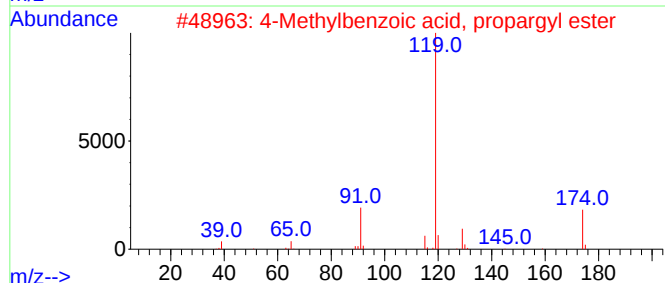
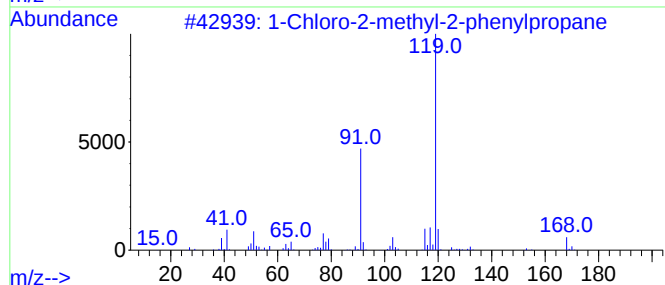
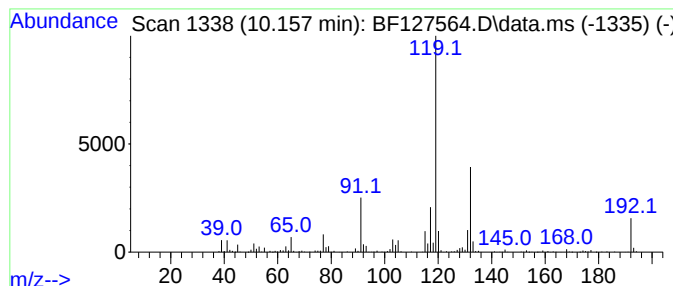
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown10.157 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.157	8.60 ng	292136	Acenaphthene-d10	9.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	47
2		4-Methylbenzoic acid, propargyl ...	174	C11H10O2	1000325-59-9	43
3		o-Cymene	134	C10H14	000527-84-4	43
4		1,3,5-Cycloheptatriene, 3,7,7-tr...	134	C10H14	003479-89-8	43
5		p-Cymene	134	C10H14	000099-87-6	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
Data File : BF127564.D
Acq On : 29 Mar 2022 14:38
Operator : CG\JU
Sample : N2154-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

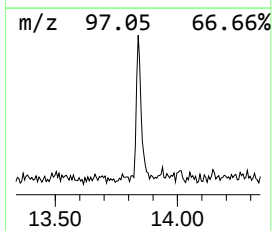
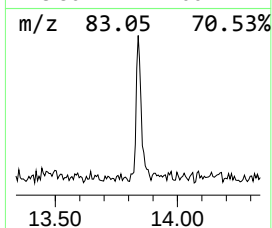
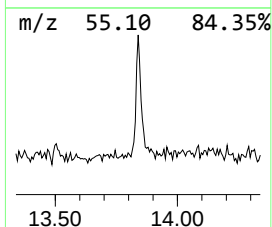
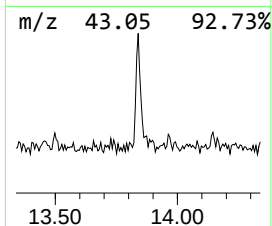
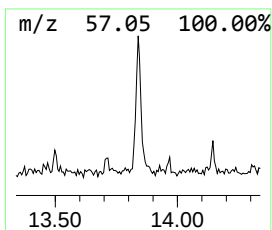
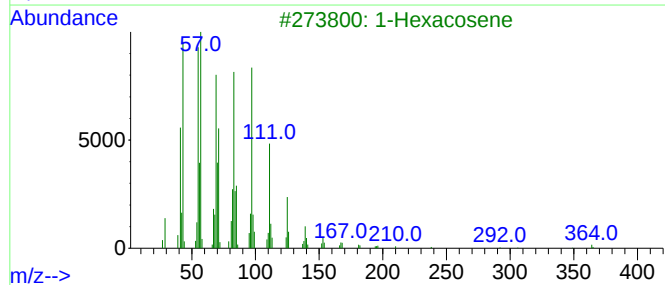
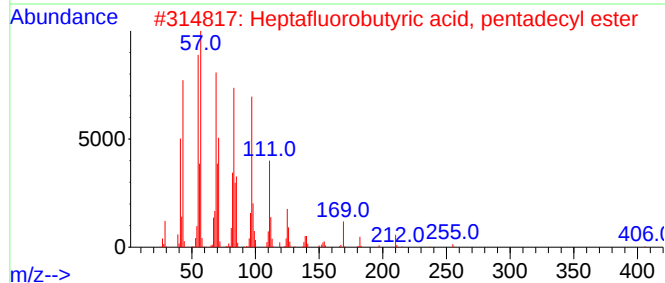
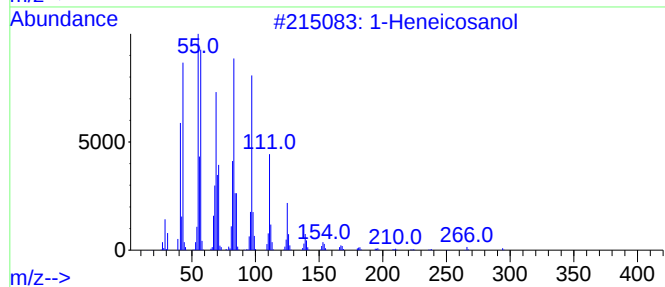
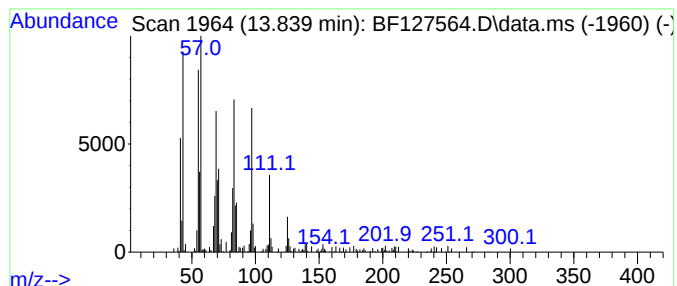
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 1-Heneicosanol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.839	5.57 ng	126441	Chrysene-d12	14.015

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3		1-Hexacosene	364	C26H52	018835-33-1	91
4		13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	91
5		1-Tetracosene	336	C24H48	010192-32-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032922\
 Data File : BF127564.D
 Acq On : 29 Mar 2022 14:38
 Operator : CG\JU
 Sample : N2154-02
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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
Butanoic acid, ...	5.228	5.5	ng	143329	1	6.834	518537	20.0
Ethanol, 2-butoxy-	5.787	7.5	ng	195774	1	6.834	518537	20.0
1-Hexanol, 2-et...	6.892	9.9	ng	257087	1	6.834	518537	20.0
unknown6.922	6.922	7.5	ng	194508	1	6.834	518537	20.0
Diethyl carbitol	7.245	8.0	ng	205992	1	6.834	518537	20.0
Hexanoic acid, ...	7.563	7.7	ng	236635	2	8.116	613462	20.0
Hexanoic acid, ...	7.722	42.2	ng	1293920	2	8.116	613462	20.0
Ethanol, 2-(2-b...	8.022	18.2	ng	558170	2	8.116	613462	20.0
unknown8.292	8.292	5.8	ng	179315	2	8.116	613462	20.0
2-Propanol, 1-(...	8.333	10.7	ng	326520	2	8.116	613462	20.0
1-Propanol, 2-(...	8.357	9.8	ng	302057	2	8.116	613462	20.0
Benzoic acid, 2...	8.410	5.5	ng	167454	2	8.116	613462	20.0
unknown8.510	8.510	6.0	ng	182563	2	8.116	613462	20.0
Benzoic acid, 4...	8.598	5.8	ng	177608	2	8.116	613462	20.0
2-(2-Butoxyetho...	9.116	6.1	ng	208447	3	9.869	679581	20.0
Phenol, 4-(1,1-...	9.298	25.6	ng	869959	3	9.869	679581	20.0
Ethanol, 2-[2-(...	9.633	12.8	ng	434054	3	9.869	679581	20.0
Apocynin	9.804	10.3	ng	349675	3	9.869	679581	20.0
unknown10.157	10.157	8.6	ng	292136	3	9.869	679581	20.0
1-Heneicosanol	13.839	5.6	ng	126441	5	14.015	454077	20.0