

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
 Data File : BF124980.D
 Acq On : 7 Aug 2021 18:25
 Operator : JU/CG
 Sample : M3289-13
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 25082

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-BF080421.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124980.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.040	498	502	506	rBB	43735	49005	32.66%	2.903%
2	5.445	567	571	574	rBV	130412	108563	72.36%	6.432%
3	5.839	636	638	641	rBB	9816	7283	4.85%	0.432%
4	6.457	739	743	746	rBV	121046	112537	75.01%	6.668%
5	6.828	803	806	809	rBB	42061	30023	20.01%	1.779%
6	7.392	898	902	904	rBB	88518	72866	48.57%	4.317%
7	8.010	1004	1007	1010	rBV	32508	25210	16.80%	1.494%
8	8.110	1021	1024	1027	rBB	56418	41047	27.36%	2.432%
9	8.851	1147	1150	1152	rBV3	2561	2061	1.37%	0.122%
10	8.910	1157	1160	1162	rBV2	2288	2202	1.47%	0.130%
11	8.992	1173	1174	1180	rBV2	1954	2963	1.97%	0.176%
12	9.063	1184	1186	1187	rBV	3052	2062	1.37%	0.122%
13	9.104	1187	1193	1196	rVV3	4695	7768	5.18%	0.460%
14	9.139	1196	1199	1203	rVB4	2652	2999	2.00%	0.178%
15	9.186	1203	1207	1210	rBV	198541	150026	100.00%	8.889%
16	9.257	1215	1219	1223	rBV4	22904	25033	16.69%	1.483%
17	9.310	1223	1228	1229	rBV3	5713	6493	4.33%	0.385%
18	9.369	1233	1238	1241	rVB4	8395	10409	6.94%	0.617%
19	9.416	1241	1246	1247	rBV5	4442	6581	4.39%	0.390%
20	9.522	1261	1264	1269	rBV7	6101	8735	5.82%	0.518%
21	9.569	1269	1272	1276	rVB	28767	25106	16.73%	1.487%
22	9.604	1276	1278	1279	rBV2	4088	3142	2.09%	0.186%
23	9.627	1279	1282	1286	rBV4	17138	20262	13.51%	1.200%
24	9.663	1286	1288	1289	rBV2	3569	2623	1.75%	0.155%
25	9.680	1289	1291	1294	rVB4	8101	6137	4.09%	0.364%
26	9.727	1297	1299	1301	rBV2	28494	23004	15.33%	1.363%
27	9.751	1301	1303	1305	rVV2	14146	11462	7.64%	0.679%
28	9.774	1305	1307	1310	rVB2	48561	39317	26.21%	2.329%
29	9.816	1310	1314	1316	rBV4	16057	21973	14.65%	1.302%
30	9.863	1316	1322	1325	rVB2	61597	76258	50.83%	4.518%
31	9.904	1326	1329	1332	rBV4	11008	12907	8.60%	0.765%
32	9.998	1343	1345	1347	rVB2	6410	4016	2.68%	0.238%
33	10.086	1358	1360	1363	rVB4	13081	13625	9.08%	0.807%
34	10.198	1374	1379	1383	rBV7	23780	36582	24.38%	2.167%
35	10.233	1383	1385	1389	rVV4	17697	18524	12.35%	1.098%
36	10.269	1389	1391	1394	rVV3	29154	26009	17.34%	1.541%

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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-BF080421.M
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37	10.404	1412	1414	1417	rBV4	8751	10000	6.67%	0.592%
38	10.657	1453	1457	1460	rBV	99801	95289	63.51%	5.646%
39	11.357	1573	1576	1579	rBV	53911	47493	31.66%	2.814%
40	11.898	1666	1668	1671	rVB3	31446	26881	17.92%	1.593%

41	12.568	1780	1782	1785	rVB	14451	10784	7.19%	0.639%
42	12.798	1819	1821	1824	rVB	12321	10054	6.70%	0.596%
43	12.939	1842	1845	1848	rVB	122056	98049	65.35%	5.809%
44	13.257	1897	1899	1900	rBV2	3708	2862	1.91%	0.170%
45	13.498	1938	1940	1941	rBV2	3575	2331	1.55%	0.138%

46	13.833	1992	1997	2002	rBV4	13887	19350	12.90%	1.146%
47	13.992	2020	2024	2026	rBV	33719	30206	20.13%	1.790%
48	14.015	2026	2028	2030	rVB2	6198	4082	2.72%	0.242%
49	14.139	2048	2049	2051	rBV2	2689	2183	1.46%	0.129%
50	14.268	2069	2071	2073	rVB3	2438	1963	1.31%	0.116%

51	14.474	2099	2106	2109	rBV3	24727	37975	25.31%	2.250%
52	14.545	2116	2118	2121	rVB3	2586	2422	1.61%	0.143%
53	14.592	2124	2126	2130	rVV4	1475	2131	1.42%	0.126%
54	14.745	2150	2152	2156	rBV5	2394	3128	2.08%	0.185%
55	14.833	2163	2167	2169	rVB4	3053	3914	2.61%	0.232%

56	14.898	2176	2178	2183	rVB2	10111	9388	6.26%	0.556%
57	15.021	2196	2199	2203	rBV	5157	5977	3.98%	0.354%
58	15.086	2207	2210	2213	rBV	14917	16519	11.01%	0.979%
59	15.115	2213	2215	2222	rVB4	13031	17552	11.70%	1.040%
60	15.245	2235	2237	2240	rBV3	2214	1961	1.31%	0.116%

61	15.327	2248	2251	2258	rVB6	3173	3537	2.36%	0.210%
62	15.392	2259	2262	2263	rVB3	2865	2217	1.48%	0.131%
63	15.451	2268	2272	2278	rVB2	30137	38839	25.89%	2.301%
64	15.509	2278	2282	2285	rBV4	2055	3069	2.05%	0.182%
65	15.662	2305	2308	2314	rVB3	7647	9929	6.62%	0.588%

66	15.892	2342	2347	2353	rVB2	40139	56661	37.77%	3.357%
67	15.951	2353	2357	2364	rBV3	6090	13427	8.95%	0.796%
68	16.009	2364	2367	2371	rVV4	3468	4379	2.92%	0.259%
69	16.133	2384	2388	2390	rBV3	2168	2672	1.78%	0.158%
70	16.386	2423	2431	2434	rBV3	3984	6372	4.25%	0.378%

71	16.539	2453	2457	2460	rVB3	1485	2074	1.38%	0.123%
72	16.674	2477	2480	2486	rVB2	6268	10144	6.76%	0.601%
73	16.968	2522	2530	2537	rBV3	17350	34087	22.72%	2.020%
74	17.056	2542	2545	2546	rVV	3041	2333	1.56%	0.138%
75	17.074	2546	2548	2551	rVV2	3140	3743	2.49%	0.222%

76	17.150	2555	2561	2567	rVB4	3887	7455	4.97%	0.442%
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Peak separation: 5

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	17.227	2572	2574	2581	rVB2	1165	1951	1.30%	0.116%
78	17.662	2646	2648	2652	rVB	1767	1959	1.31%	0.116%
79	18.750	2828	2833	2834	rBV2	2554	3408	2.27%	0.202%
80	18.762	2834	2835	2838	rVB2	2701	2268	1.51%	0.134%

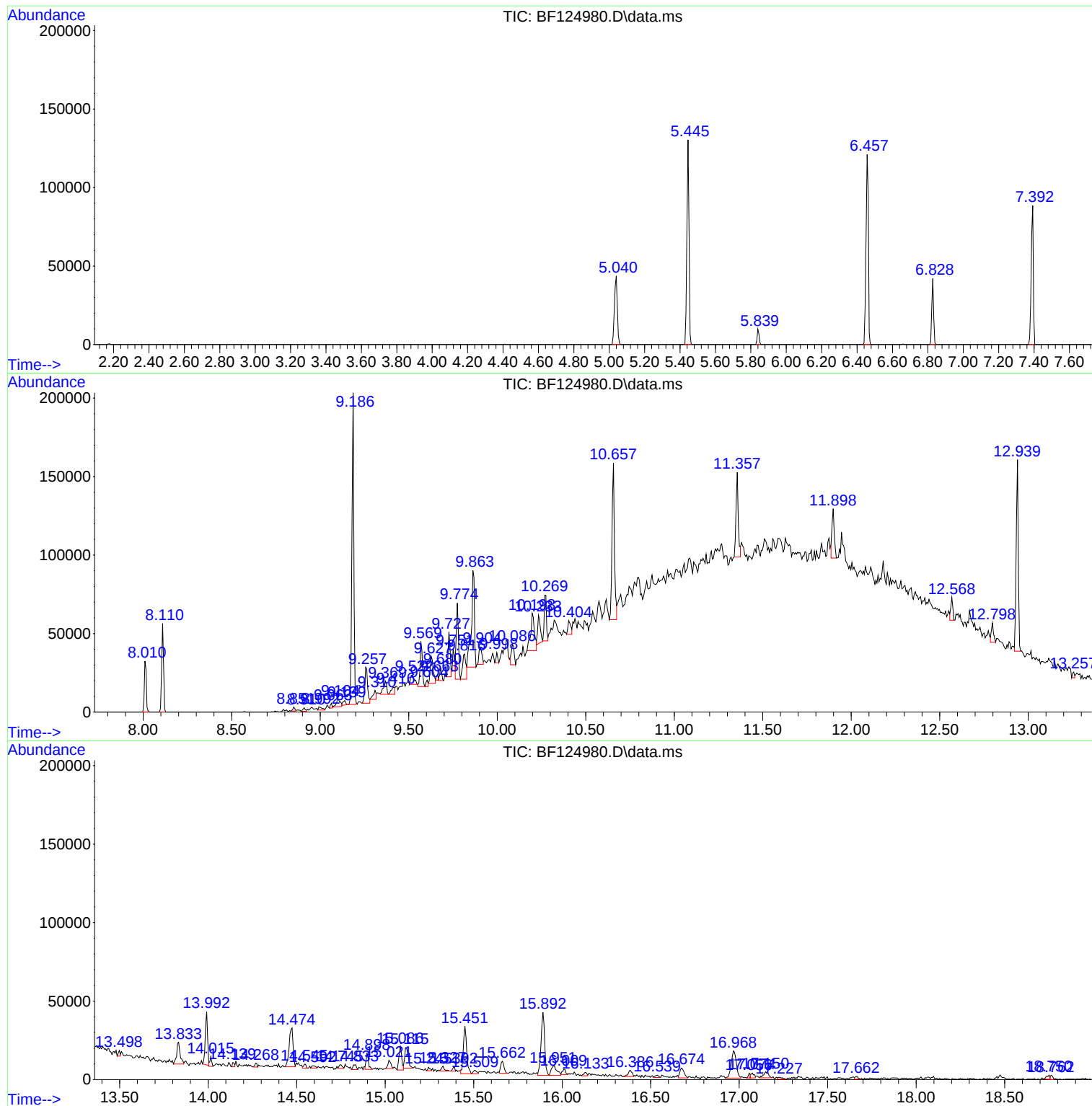
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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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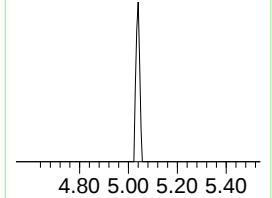
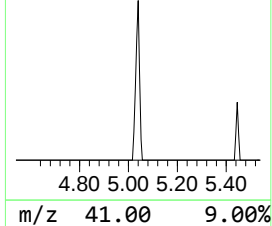
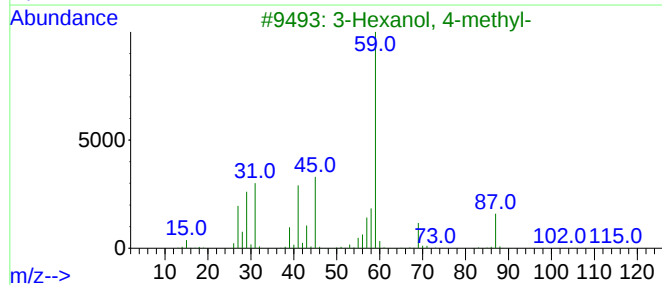
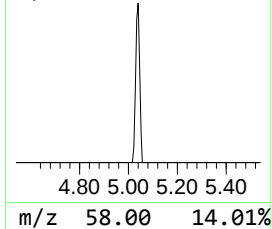
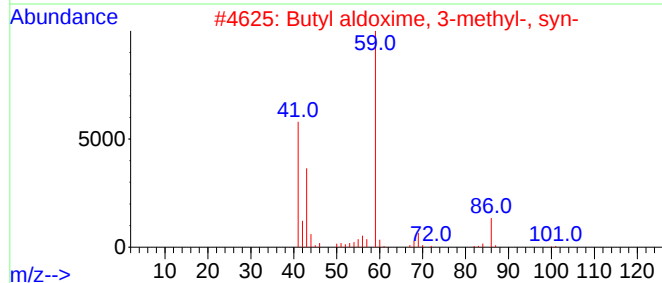
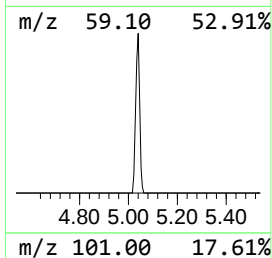
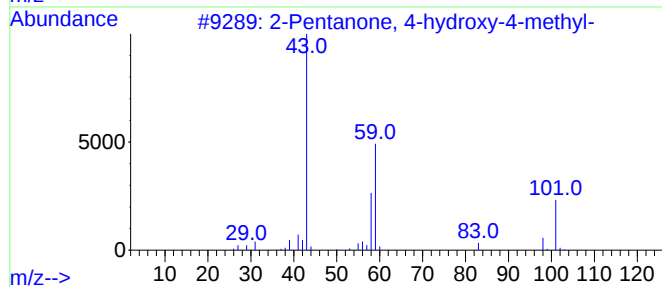
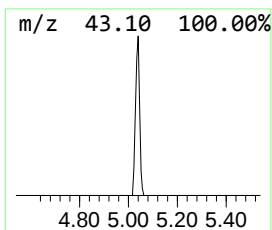
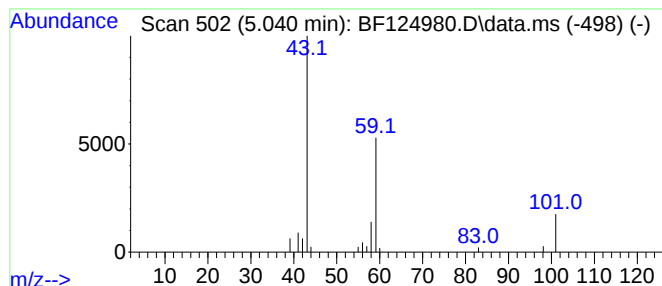
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	32.65 ng	49005	1,4-Dichlorobenzene-d4	6.828

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		
5	Silane, trimethyl-	74	C3H10Si	000993-07-7	9		



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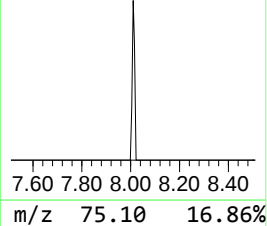
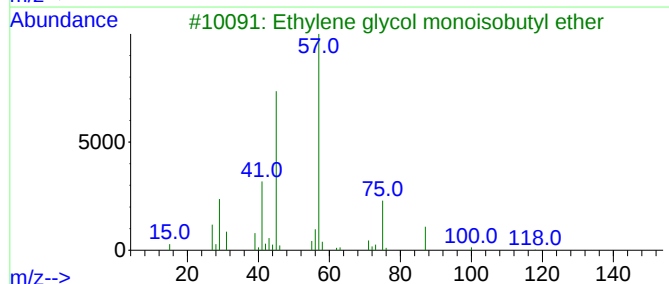
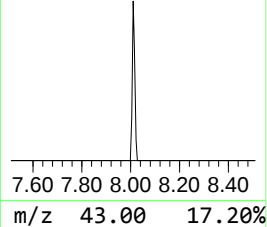
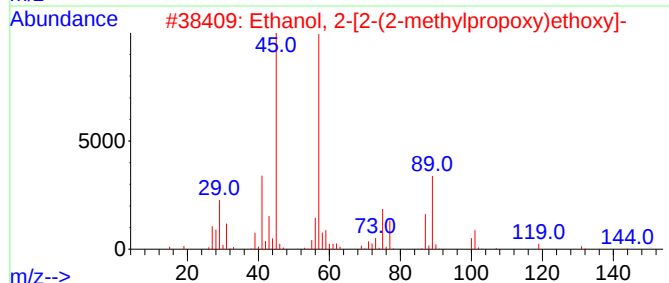
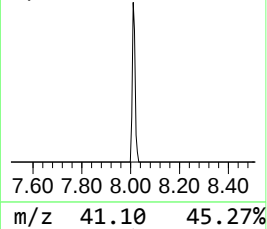
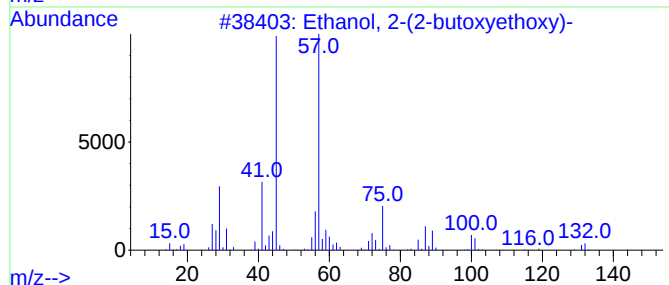
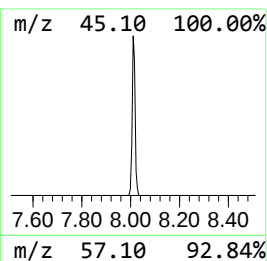
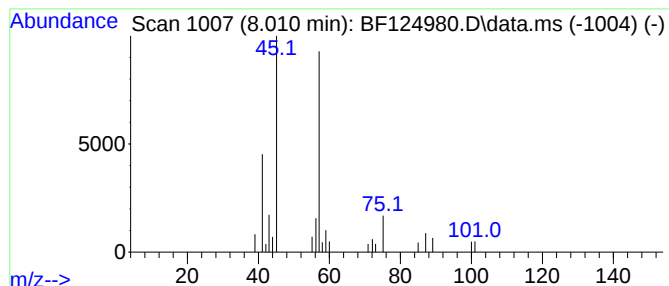
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.010	12.28 ng	25210	Naphthalene-d8	8.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40
4			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	38
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	37



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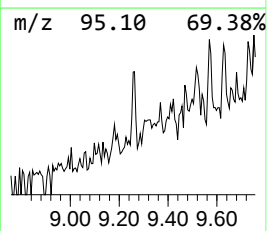
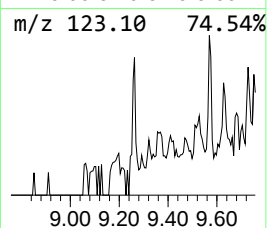
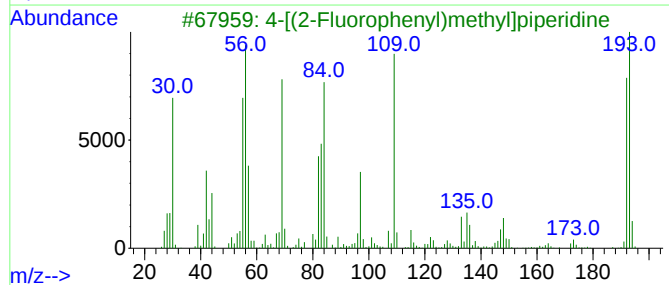
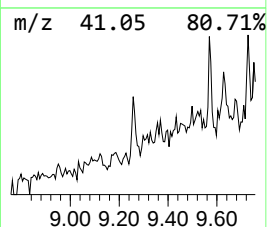
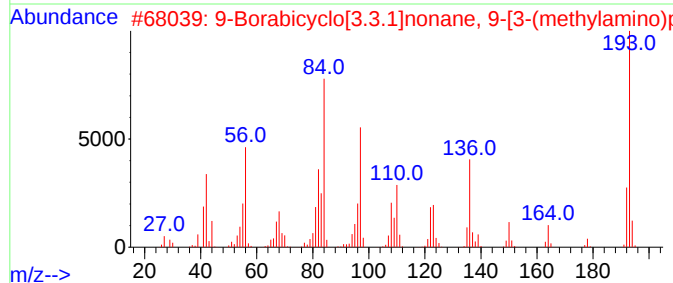
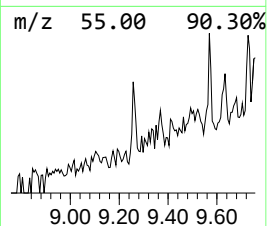
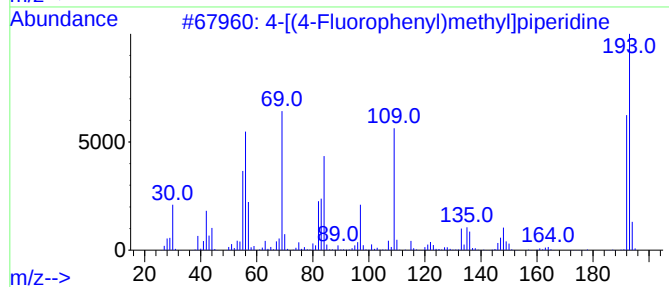
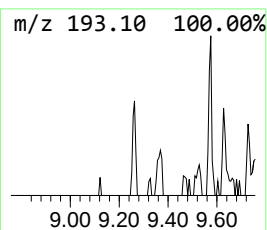
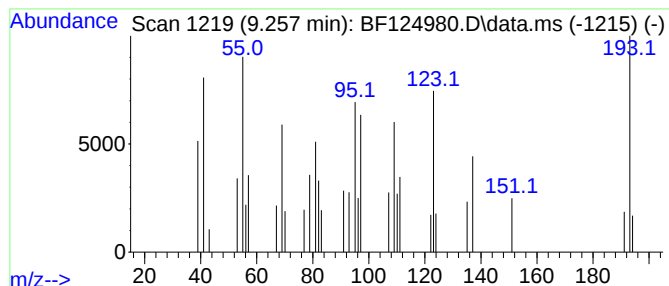
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown9.257 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	6.57 ng	25033	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	30		
2	9-Borabicyclo[3.3.1]nonane, 9-[3...	193	C12H24BN	1010162-56-0	30		
3	4-[(2-Fluorophenyl)methyl]piperi...	193	C12H16FN	194288-97-6	27		
4	Cyclohexanone, 2,5-dimethyl-2-(1...	166	C11H18O	006711-26-8	12		
5	Butanoic acid, 3-methyl-, 3,7-di...	240	C15H28O2	068922-10-1	12		



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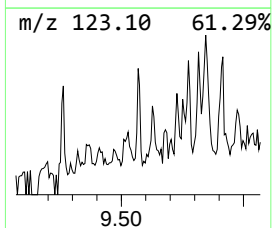
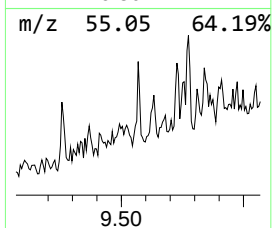
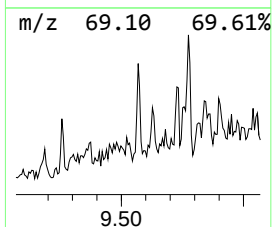
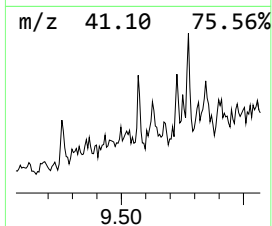
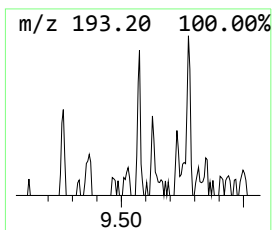
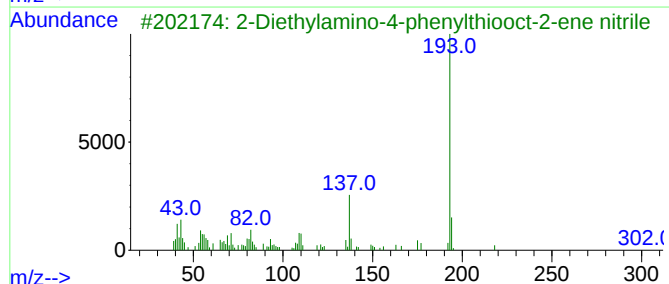
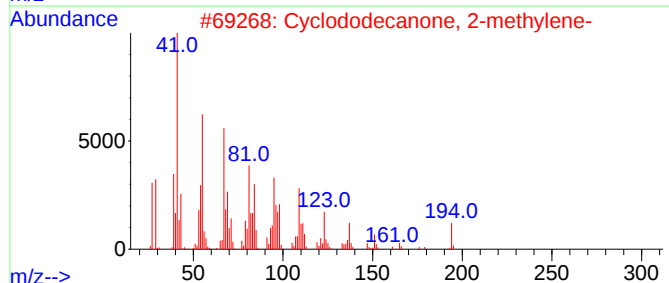
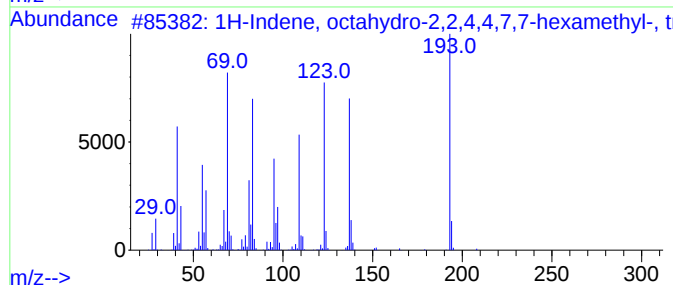
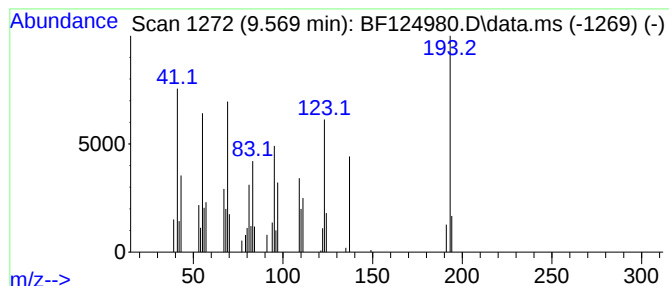
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1H-Indene, octahydro-2,2,4,... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.569	6.58 ng	25106	Acenaphthene-d10		9.863	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Indene, octahydro-2,2,4,4,7,7...		208	C15H28	054832-83-6	53
2	Cyclododecanone, 2-methylene-		194	C13H22O	003045-76-9	38
3	2-Diethylamino-4-phenylthiooct-2...		302	C18H26N2S	1000090-57-0	35
4	4-Amino-N-hydroxypyrazolo[3,2-c]...		193	C6H7N7O	1000443-50-2	22
5	6-Nitroundec-5-ene		199	C11H21NO2	1000192-40-3	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
Operator : JU/CG
Sample : M3289-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

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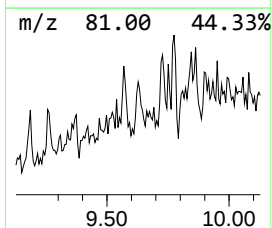
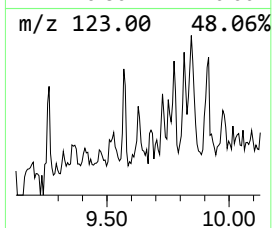
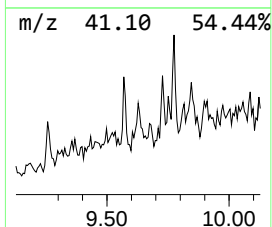
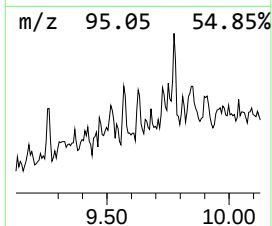
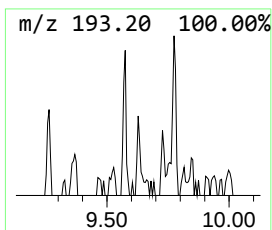
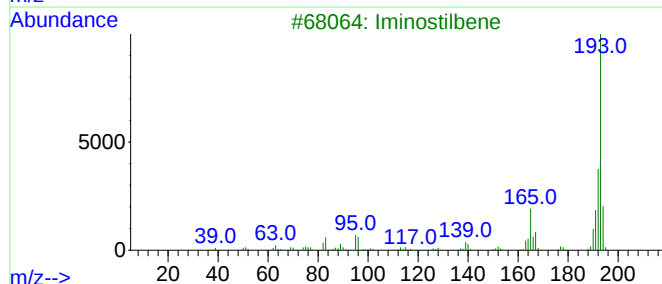
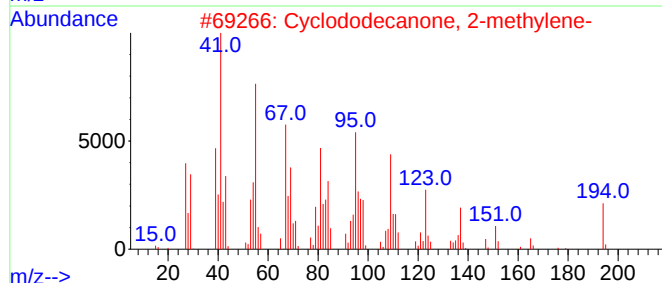
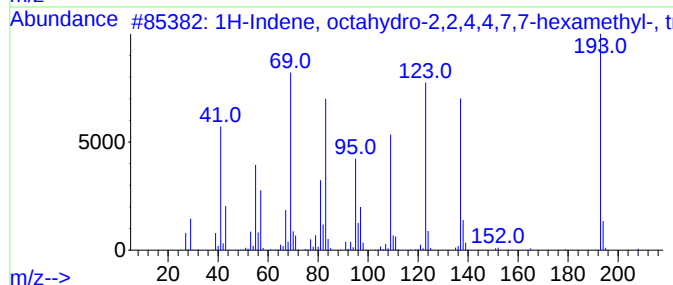
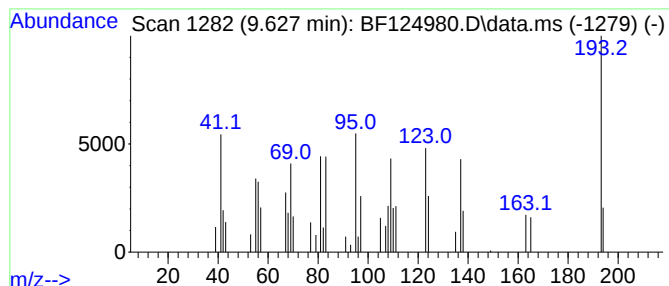
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.627 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.627	5.31 ng	20262	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, octahydro-2,2,4,7,7...	208	C15H28	054832-83-6	53
2			Cyclododecanone, 2-methylene-	194	C13H22O	003045-76-9	43
3			Iminostilbene	193	C14H11N	000256-96-2	14
4			Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	14
5			1-Anthracenamine	193	C14H11N	000610-49-1	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
Operator : JU/CG
Sample : M3289-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

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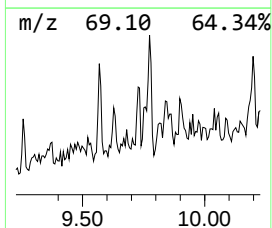
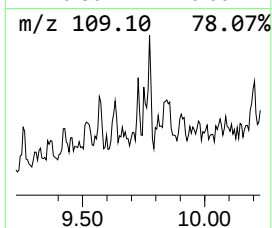
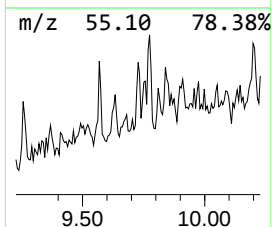
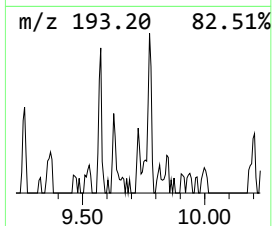
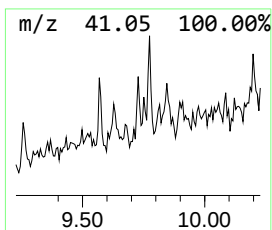
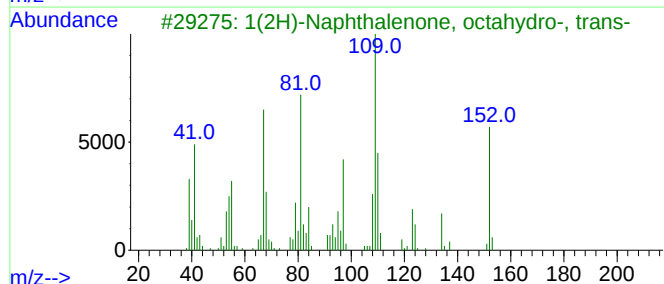
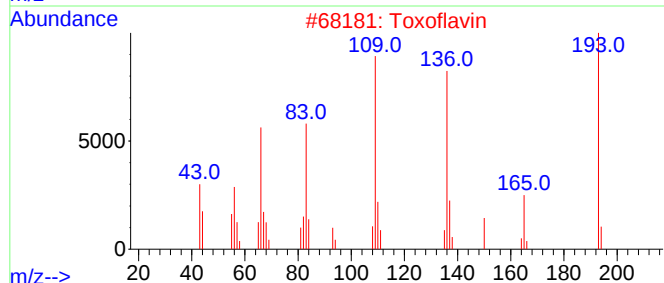
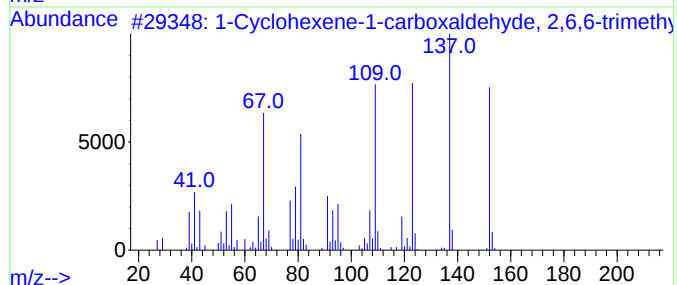
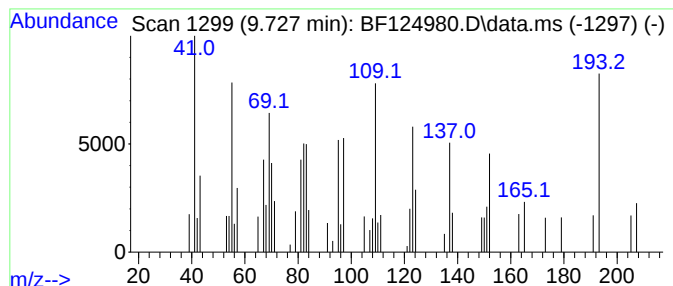
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown9.727 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.727	6.03 ng	23004	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	000432-25-7	38
2			Toxoflavin	193	C7H7N5O2	000084-82-2	38
3			1(2H)-Naphthalenone, octahydro-,...	152	C10H16O	021370-71-8	30
4			Acetaldehyde, (3,3-dimethylcyclo...	152	C10H16O	026532-24-1	30
5			Bicyclo[3.1.0]hexan-2-one, 4-met...	152	C10H16O	002506-61-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
Operator : JU/CG
Sample : M3289-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

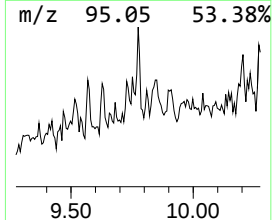
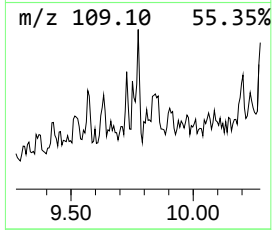
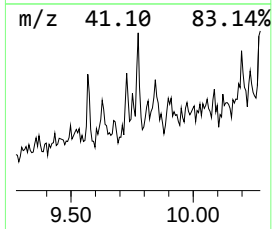
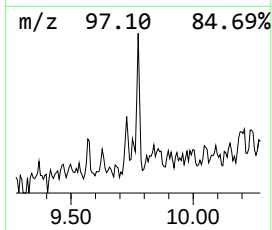
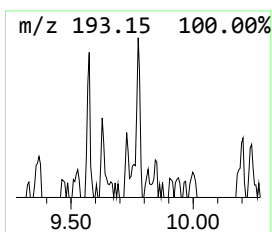
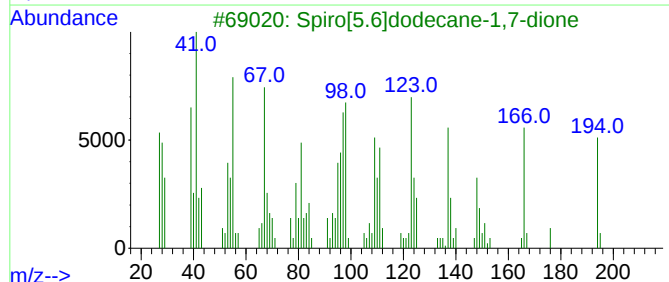
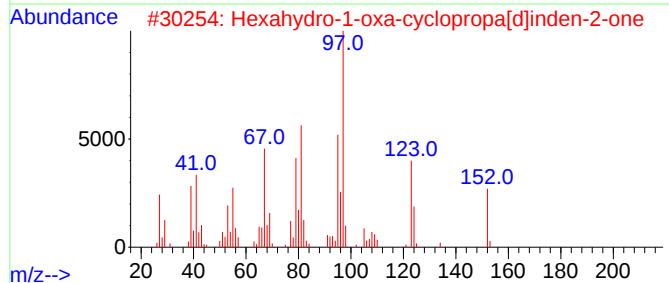
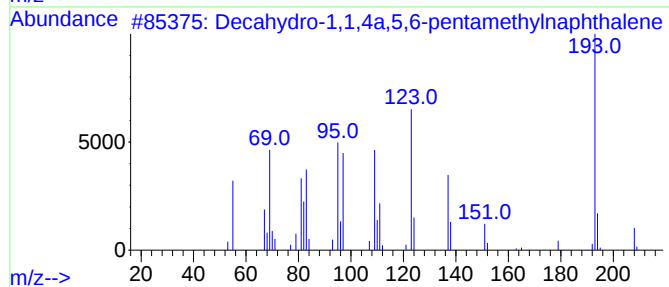
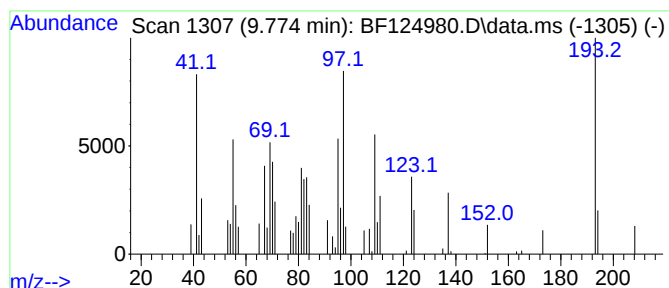
Instrument :
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ClientSampled :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Decahydro-1,1,4a,5,6-pentam... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.774	10.31 ng	39317	Acenaphthene-d10			9.863
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Decahydro-1,1,4a,5,6-pentamethyl...		208	C15H28	080655-44-3	89
2	Hexahydro-1-oxa-cyclopropa[d]ind...		152	C9H12O2	037643-23-5	46
3	Spiro[5.6]dodecane-1,7-dione		194	C12H18O2	050803-80-0	38
4	2-Hexyl-2-cyclopenten-1-one		166	C11H18O	000095-41-0	35
5	Benzenamine, 4-(hexyloxy)-		193	C12H19NO	039905-57-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
Operator : JU/CG
Sample : M3289-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

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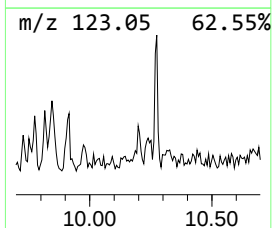
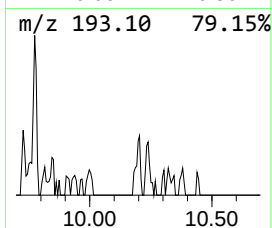
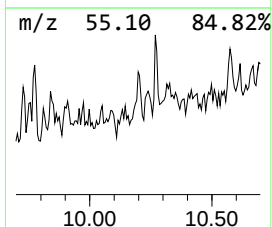
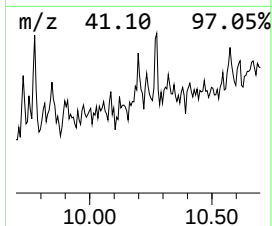
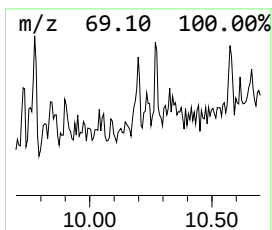
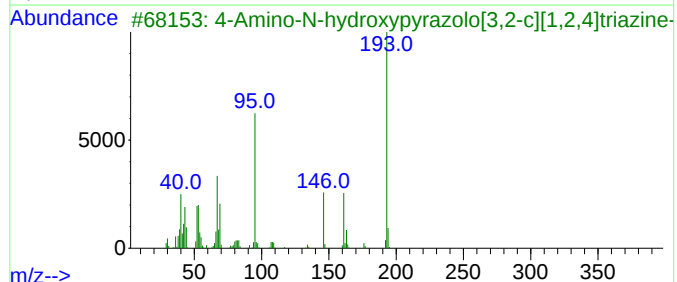
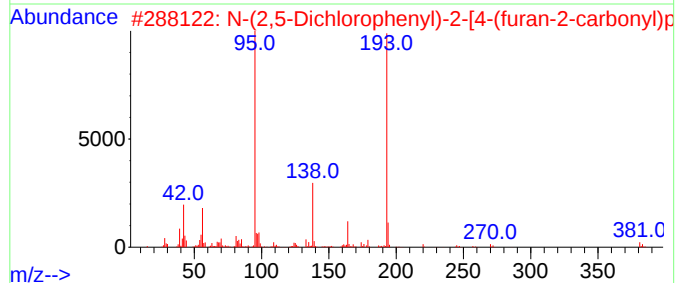
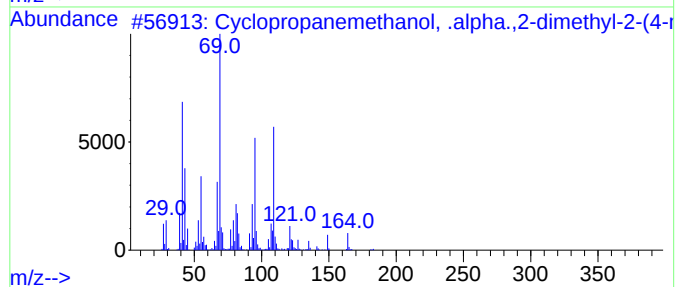
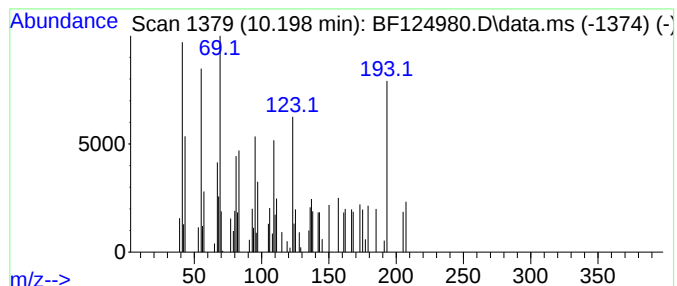
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.198 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.198	9.59 ng	36582	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	16
2			N-(2,5-Dichlorophenyl)-2-[4-(fur...	381	C17H17Cl2N3O3	1010482-48-3	14
3			4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	14
4			4-[(4-Fluorophenyl)methyl]piperi...	193	C12H16FN	092822-02-1	14
5			Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
Operator : JU/CG
Sample : M3289-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

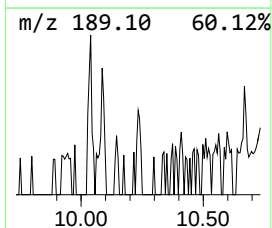
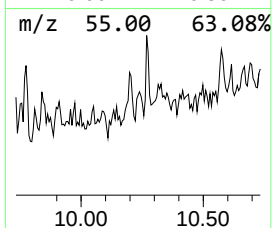
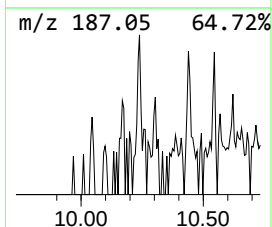
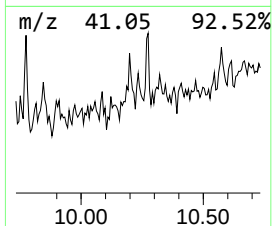
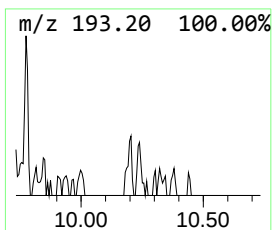
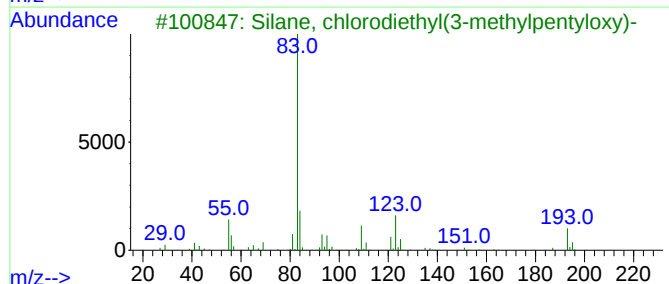
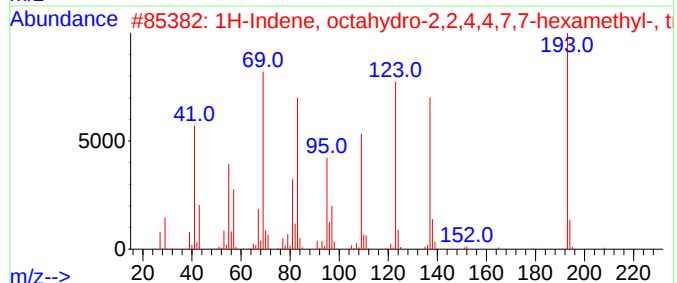
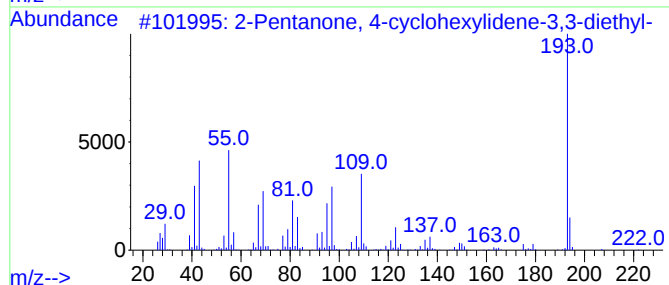
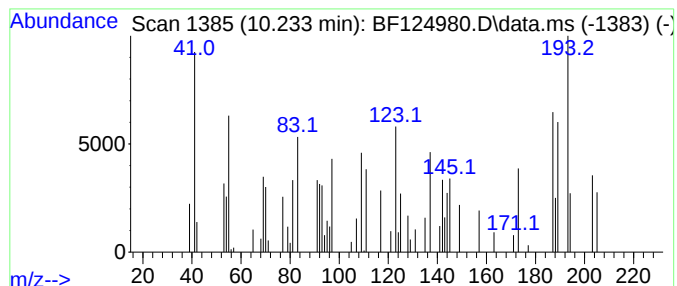
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown10.233 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.233	4.86 ng	18524	Acenaphthene-d10	9.863	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	22
2	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	16
3	Silane, chlorodiethyl(3-methylpe...	222	C10H23ClOSi	1000363-50-1	16
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	12
5	N-(4-Fluorophenyl)succinamic acid	211	C10H10FNO3	199461-14-8	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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Sample : M3289-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

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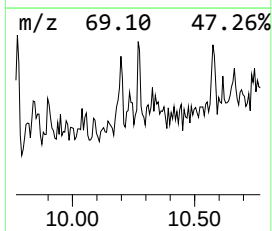
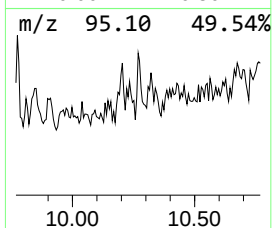
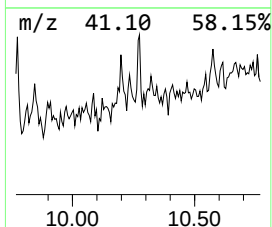
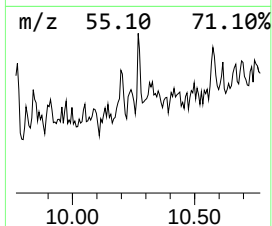
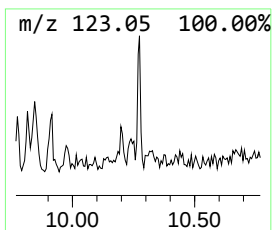
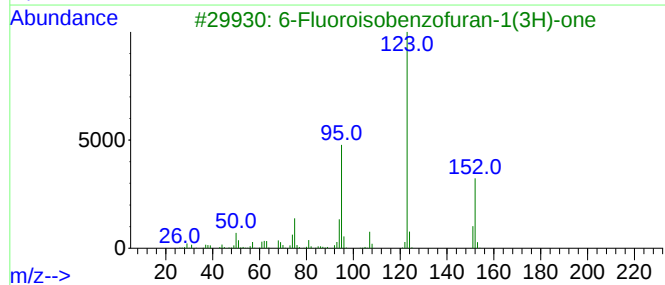
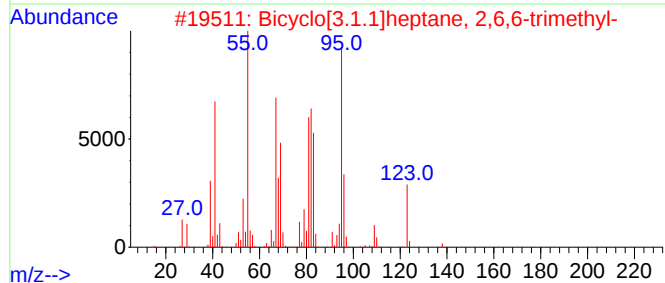
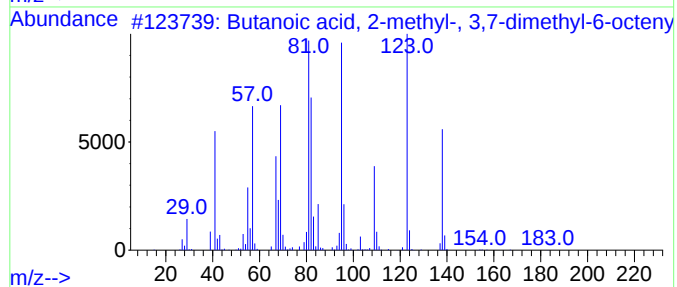
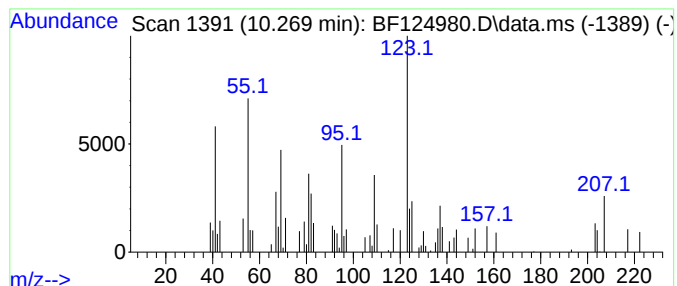
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown10.269 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.269	6.82 ng	26009	Acenaphthene-d10	9.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-, 3,7-di...	240	C15H28O2	085409-36-5	43
2			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	38
3			6-Fluoroisobenzofuran-1(3H)-one	152	C8H5FO2	023932-84-5	38
4			Pyridine-3-carboxylic acid, 1-[(...	290	C15H18N2O4	1010310-27-9	32
5			3-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000279-04-9	32



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Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
Operator : JU/CG
Sample : M3289-13
Misc :
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Instrument :
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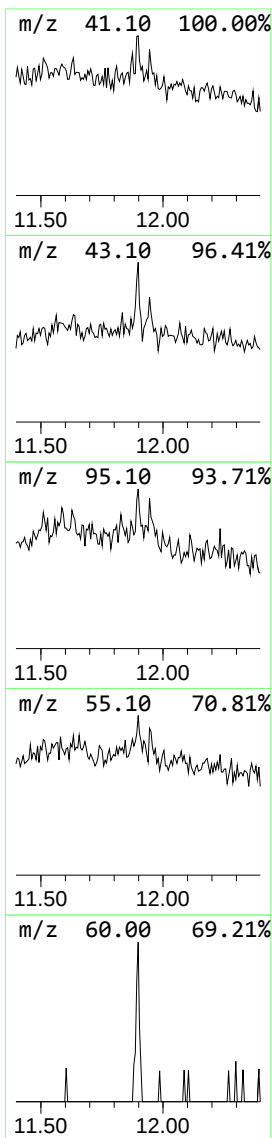
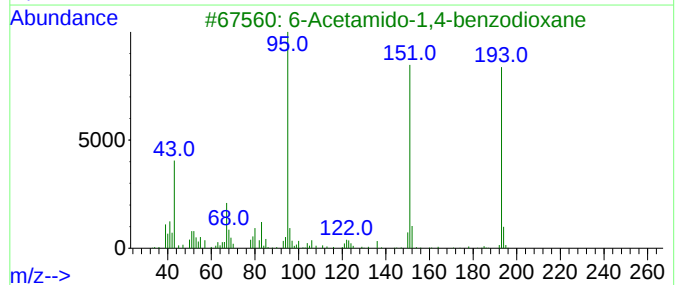
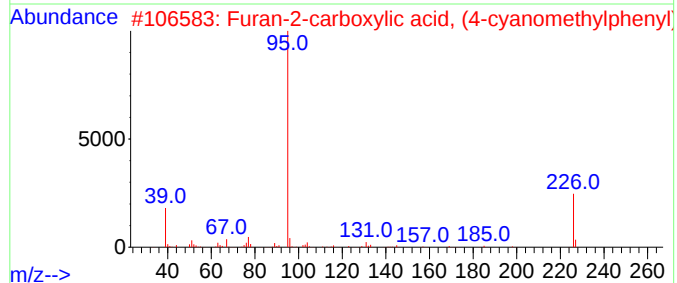
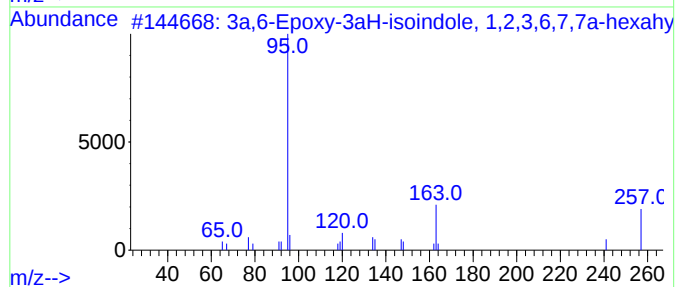
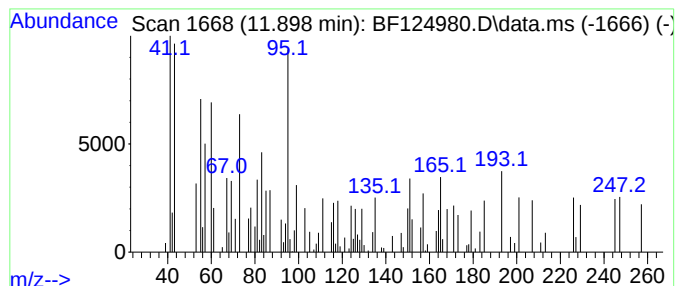
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown11.898 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	11.32 ng	26881	Phenanthrene-d10	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3a,6-Epoxy-3aH-isoindole, 1,2,3,...	257	C16H19NO2	071840-22-7	27
2			Furan-2-carboxylic acid, (4-cyan...	226	C13H10N2O2	1000303-28-7	25
3			6-Acetamido-1,4-benzodioxane	193	C10H11NO3	063546-19-0	22
4			Furoylglycine, TMS derivative	241	C10H15NO4Si	071428-92-7	12
5			Cyclopropanecarboxylic acid, 2-m...	168	C10H16O2	030626-51-8	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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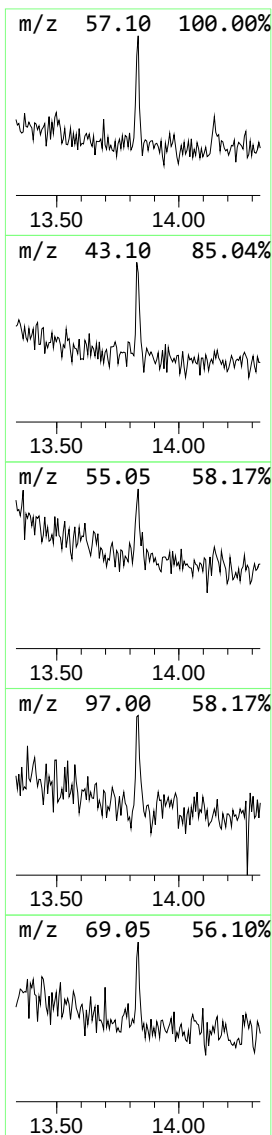
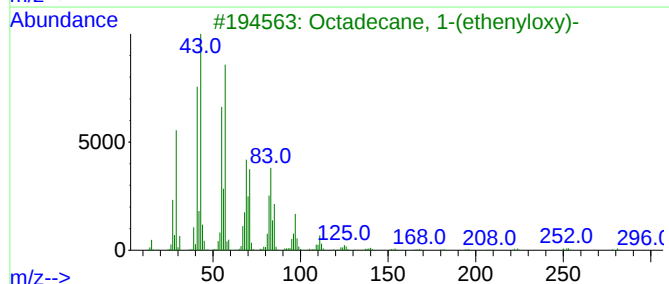
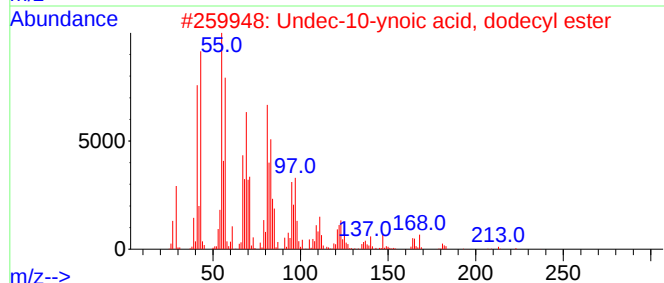
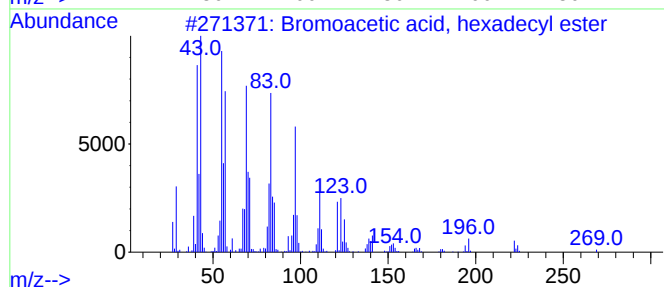
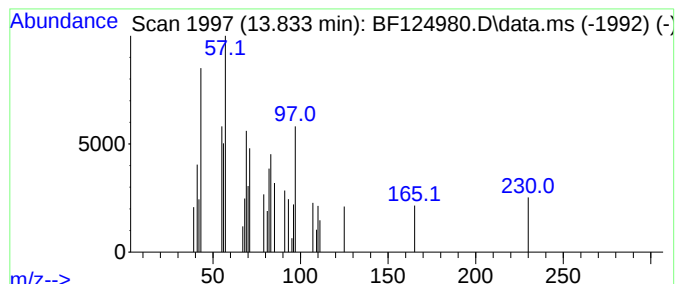
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown13.833 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.833	12.81 ng	19350	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	43
2			Undec-10-ynoic acid, dodecyl ester	350	C23H42O2	1010406-16-5	38
3			Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	38
4			Hexadecane, 1,1-bis(dodecyloxy)-	595	C40H82O2	056554-64-4	35
5			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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ClientSampleId :
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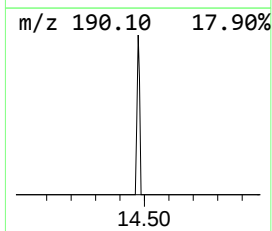
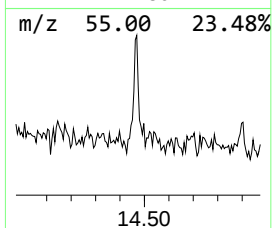
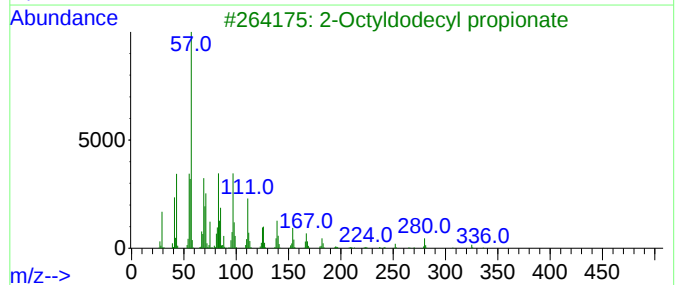
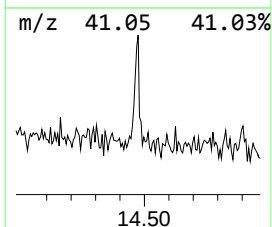
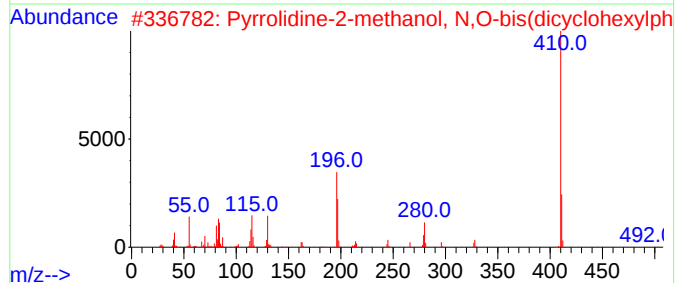
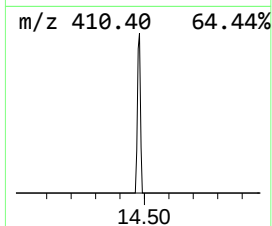
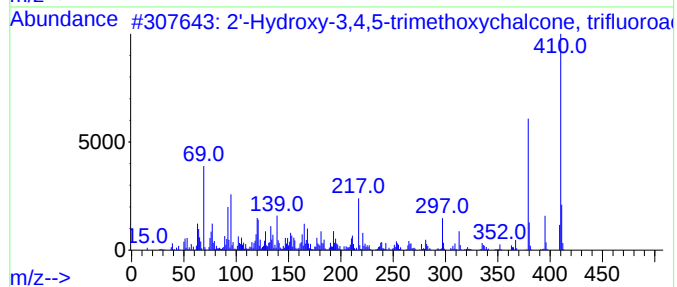
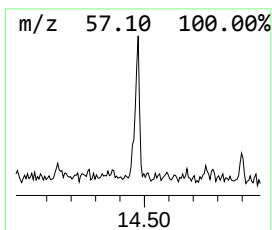
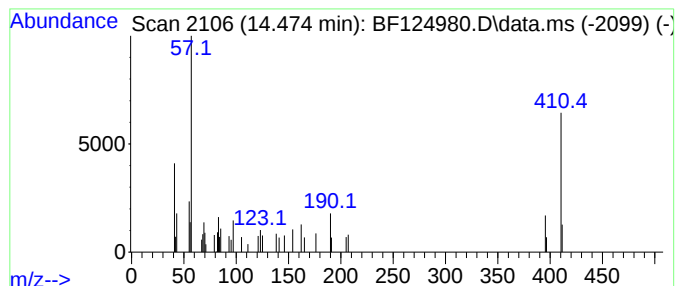
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown14.474 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.474	25.14 ng	37975	Chrysene-d12	13.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2'-Hydroxy-3,4,5-trimethoxychalc...	410	C20H17F3O6	1000449-43-8	38		
2	Pyrrolidine-2-methanol, N,O-bis(...	493	C29H53NOP2	112150-34-2	9		
3	2-Octyldodecyl propionate	354	C23H46O2	1000368-55-1	9		
4	Isobutyl undecyl carbonate	272	C16H32O3	1000372-78-8	9		
5	Spiro[3H-indole-3,3'-pyrrolidine...	410	C17H13F7N2O2	066012-92-8	7		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
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Sample : M3289-13
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ALS Vial : 7 Sample Multiplier: 1

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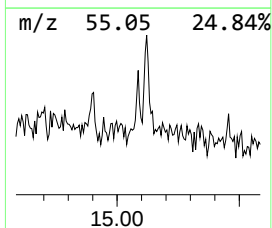
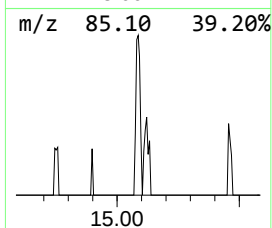
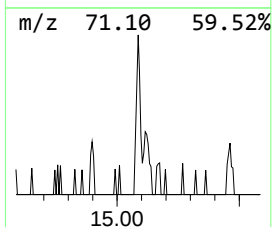
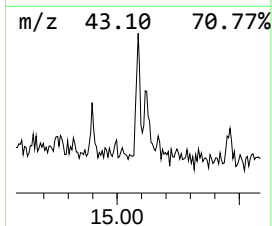
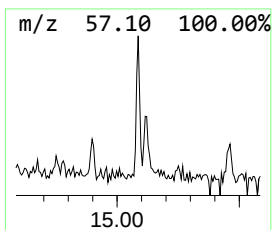
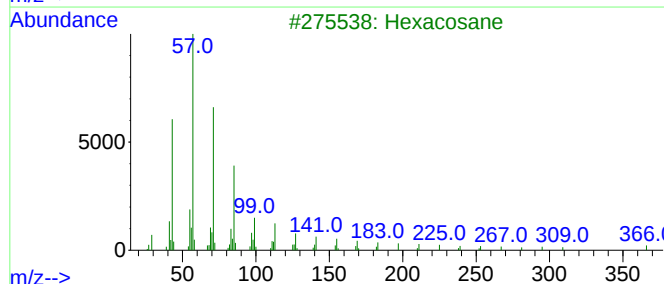
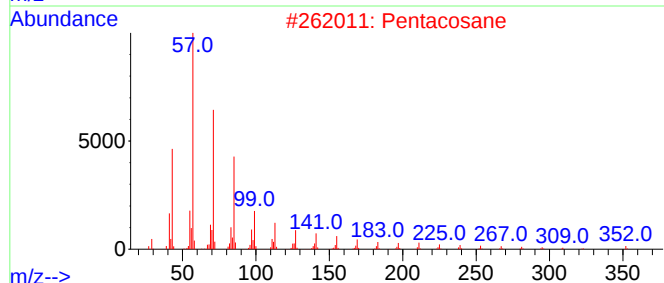
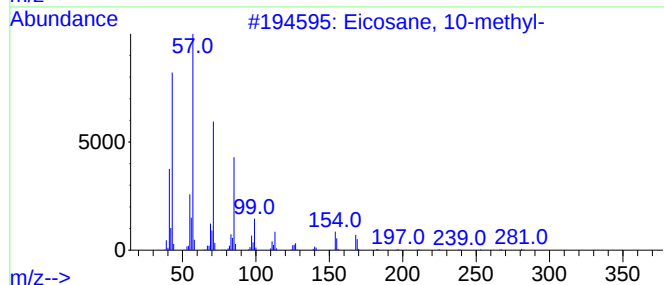
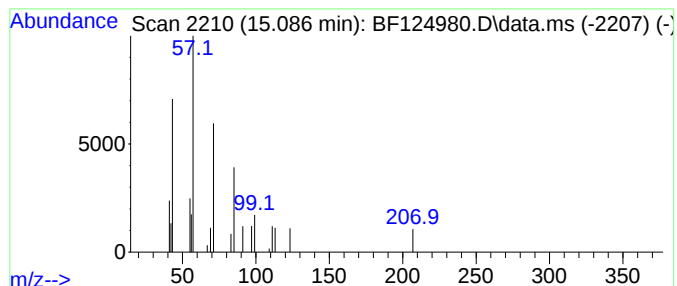
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Eicosane, 10-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.086	8.51 ng	16519	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 10-methyl-	296	C21H44	054833-23-7	64
2			Pentacosane	352	C25H52	000629-99-2	59
3			Hexacosane	366	C26H54	000630-01-3	59
4			Tetracosane	338	C24H50	000646-31-1	59
5			Heptadecane	240	C17H36	000629-78-7	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
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Sample : M3289-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

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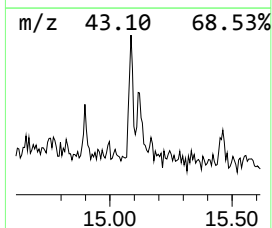
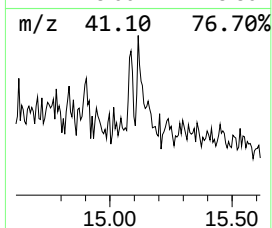
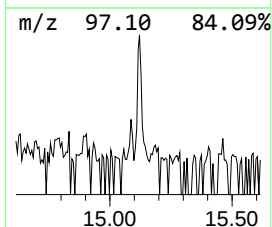
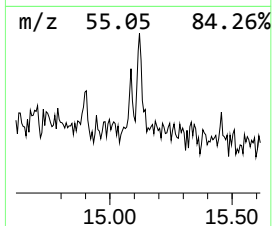
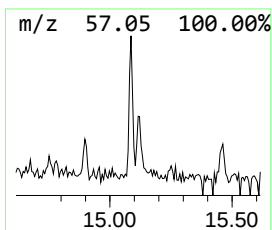
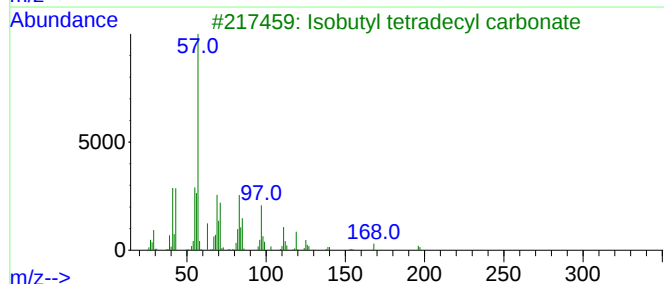
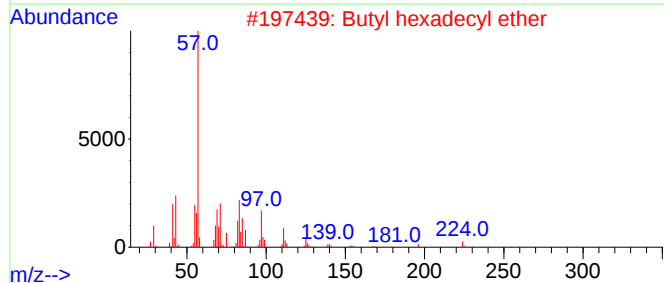
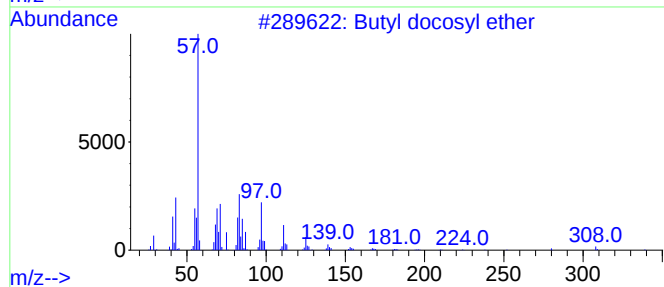
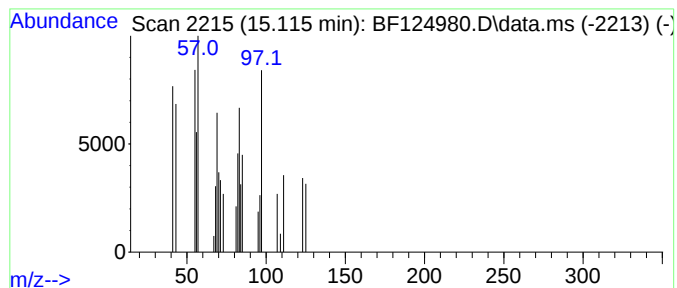
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Butyl docosyl ether Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.115	9.04 ng	17552	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl docosyl ether	382	C26H54O	1000406-40-8	50
2			Butyl hexadecyl ether	298	C20H42O	1010406-40-5	50
3			Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	47
4			Butyl eicosyl ether	354	C24H50O	1000406-40-7	47
5			Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
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ClientSampleId :
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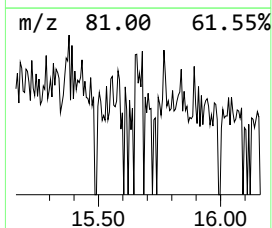
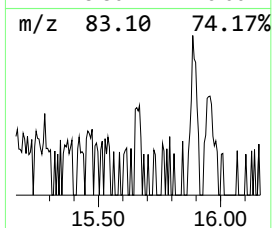
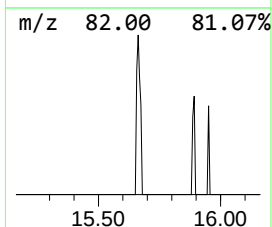
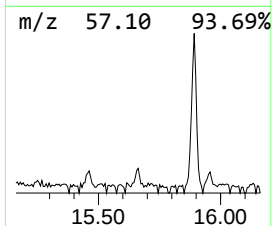
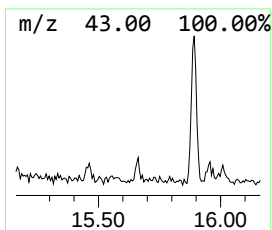
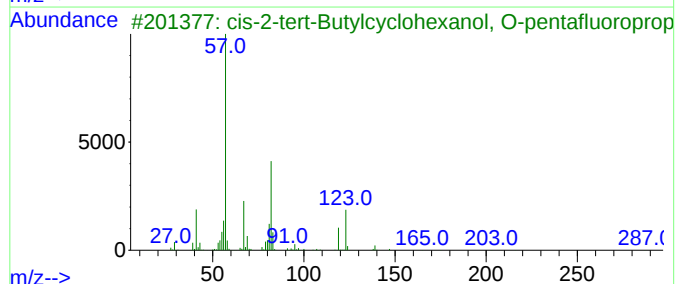
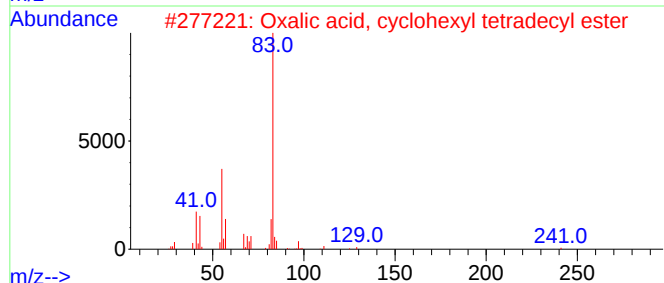
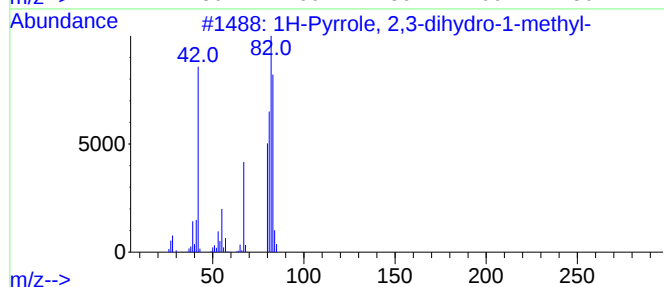
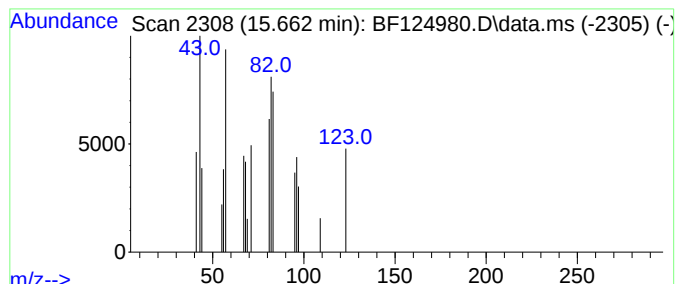
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown15.662 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.662	5.11 ng	9929	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	25
2			Oxalic acid, cyclohexyl tetradec...	368	C22H40O4	1000309-31-5	23
3			cis-2-tert-Butylcyclohexanol, O-...	302	C13H19F5O2	1000467-24-6	23
4			1-Heptadecyne	236	C17H32	026186-00-5	16
5			Bicyclo[4.1.0]heptane, 3-methyl-	110	C8H14	041977-47-3	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
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ALS Vial : 7 Sample Multiplier: 1

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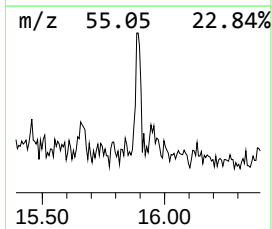
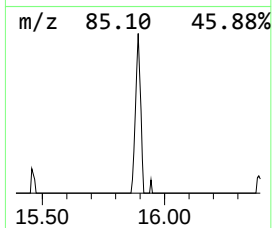
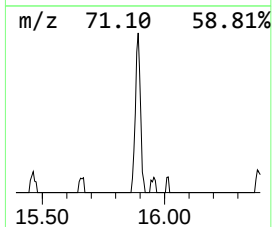
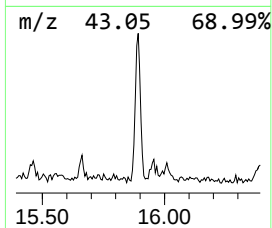
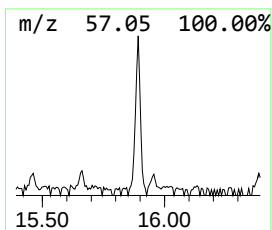
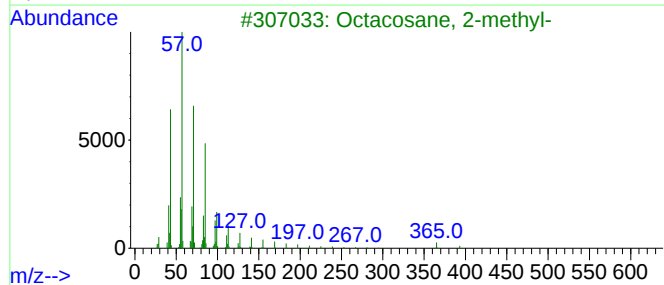
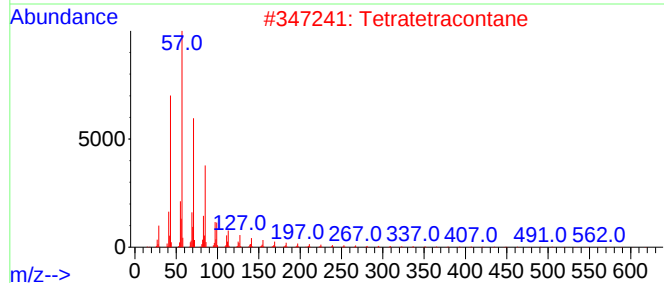
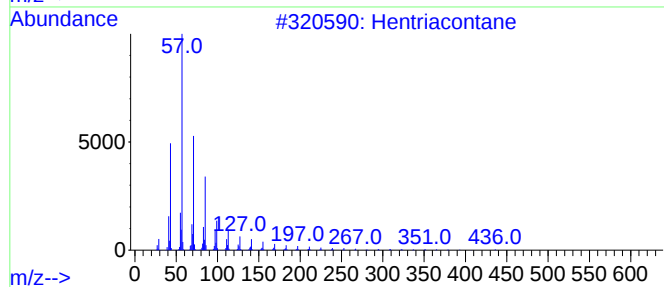
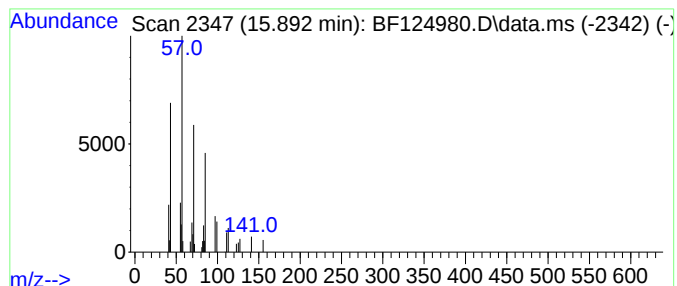
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Hentriacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.892	29.18 ng	56661	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hentriacontane	437	C31H64	000630-04-6	91
2			Tetratetracontane	619	C44H90	007098-22-8	91
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4			Octacosane	394	C28H58	000630-02-4	87
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
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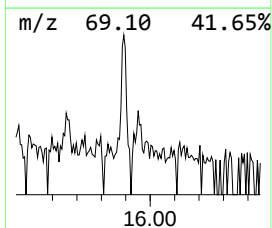
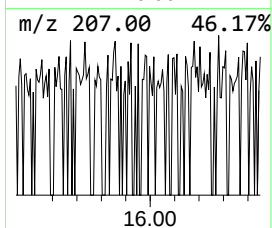
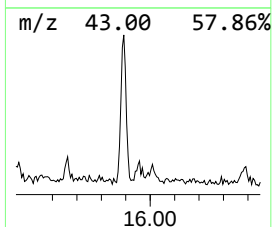
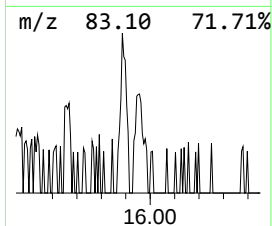
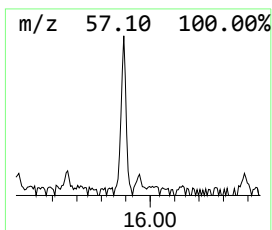
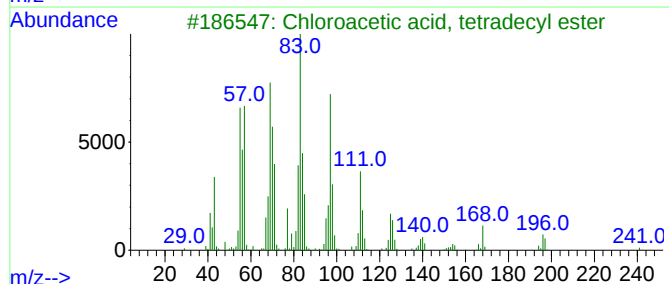
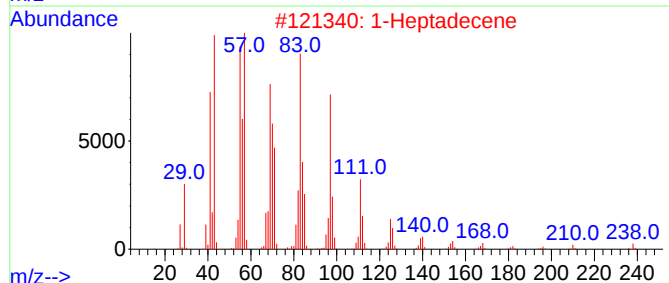
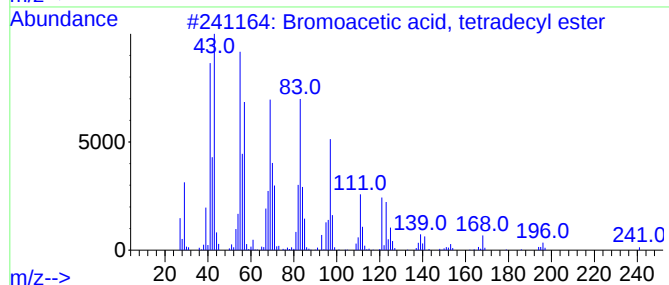
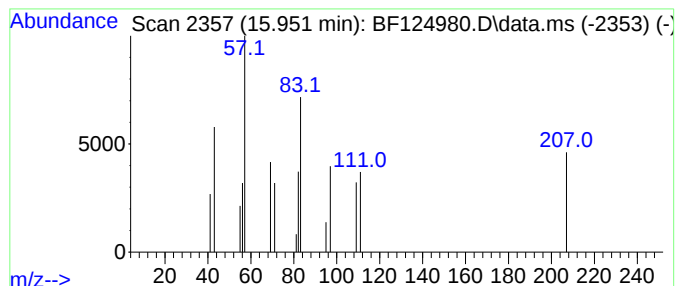
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Bromoacetic acid, tetradecyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.951	6.91 ng	13427	Perylene-d12	15.451

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, tetradecyl ester	334	C16H31BrO2	018992-01-3	50
2		1-Heptadecene	238	C17H34	006765-39-5	47
3		Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	47
4		1-Tricosene	322	C23H46	018835-32-0	38
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
Operator : JU/CG
Sample : M3289-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
25082

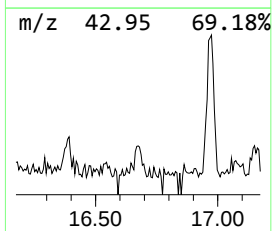
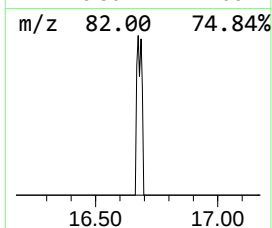
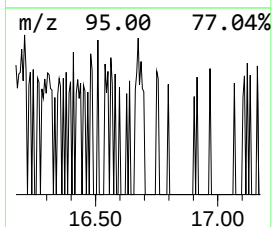
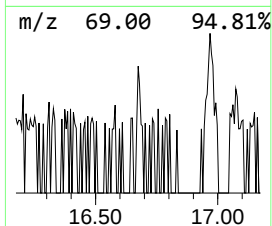
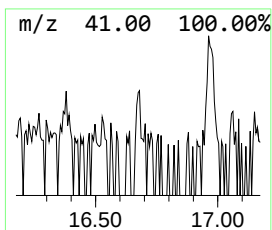
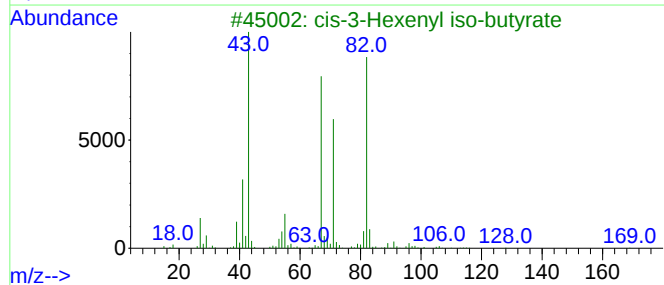
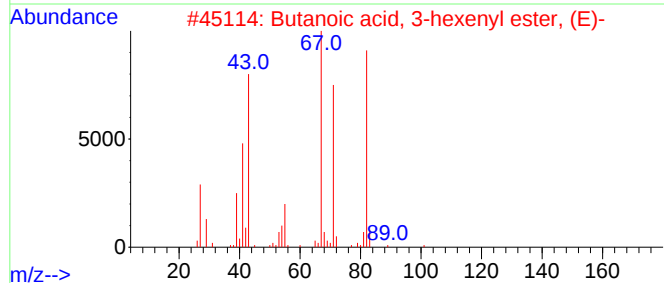
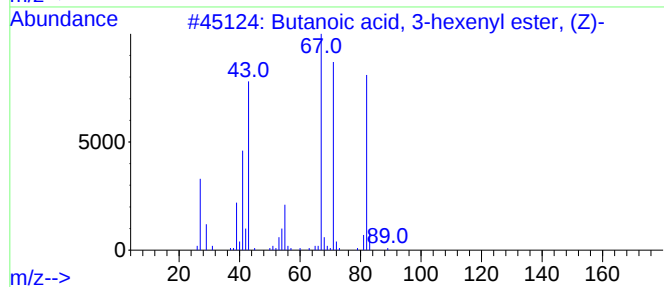
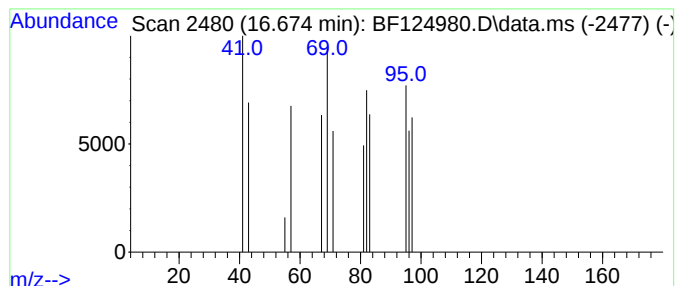
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown16.674 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.674	5.22 ng	10144	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-hexenyl ester, ...	170	C10H18O2	016491-36-4	12
2			Butanoic acid, 3-hexenyl ester, ...	170	C10H18O2	053398-84-8	12
3			cis-3-Hexenyl iso-butyrate	170	C10H18O2	041519-23-7	12
4			3-Heptyne	96	C7H12	002586-89-2	9
5			1H-Imidazole, 2-ethyl-	96	C5H8N2	001072-62-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
Data File : BF124980.D
Acq On : 7 Aug 2021 18:25
Operator : JU/CG
Sample : M3289-13
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
25082

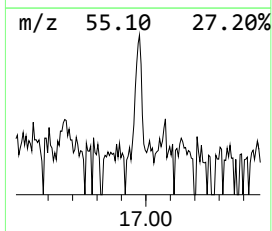
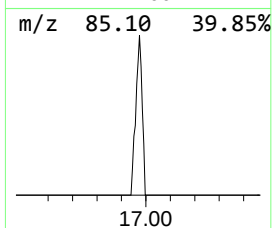
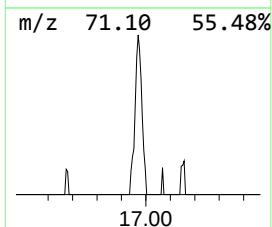
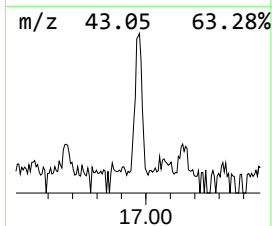
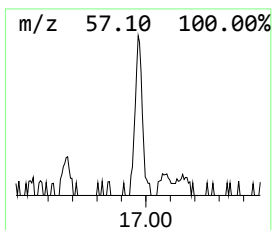
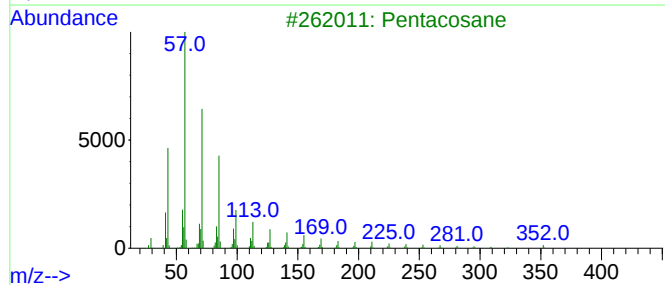
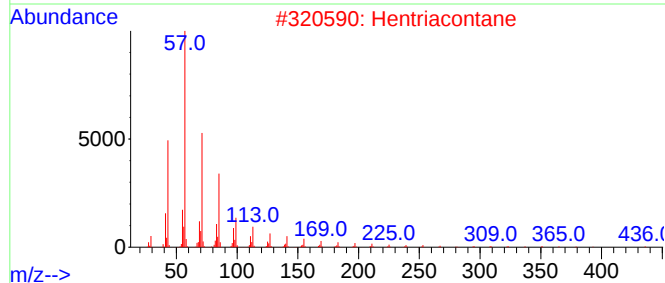
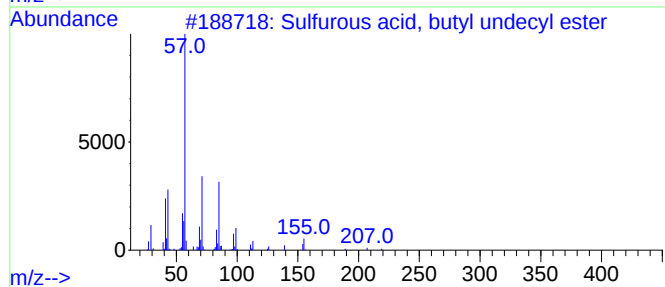
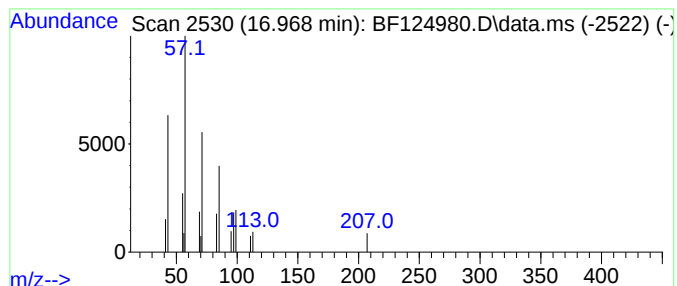
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Sulfurous acid, butyl undec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.968	17.55 ng	34087	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl undecyl ester	292	C15H32O3S	1000309-17-8	78
2			Hentriacontane	437	C31H64	000630-04-6	78
3			Pentacosane	352	C25H52	000629-99-2	72
4			Tetratetracontane	619	C44H90	007098-22-8	72
5			Hexatriacontane	507	C36H74	000630-06-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF080721\
 Data File : BF124980.D
 Acq On : 7 Aug 2021 18:25
 Operator : JU/CG
 Sample : M3289-13
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 25082

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080421.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.040	32.6	ng	49005	1	6.828	30023	20.0
Ethanol, 2-(2-b...	8.010	12.3	ng	25210	2	8.110	41047	20.0
unknown9.257	9.257	6.6	ng	25033	3	9.863	76258	20.0
1H-Indene, octa...	9.569	6.6	ng	25106	3	9.863	76258	20.0
unknown9.627	9.627	5.3	ng	20262	3	9.863	76258	20.0
unknown9.727	9.727	6.0	ng	23004	3	9.863	76258	20.0
Decahydro-1,1,4...	9.774	10.3	ng	39317	3	9.863	76258	20.0
unknown10.198	10.198	9.6	ng	36582	3	9.863	76258	20.0
unknown10.233	10.233	4.9	ng	18524	3	9.863	76258	20.0
unknown10.269	10.269	6.8	ng	26009	3	9.863	76258	20.0
unknown11.898	11.898	11.3	ng	26881	4	11.357	47493	20.0
unknown13.833	13.833	12.8	ng	19350	5	13.992	30206	20.0
unknown14.474	14.474	25.1	ng	37975	5	13.992	30206	20.0
Eicosane, 10-me...	15.086	8.5	ng	16519	6	15.451	38839	20.0
Butyl docosyl e...	15.115	9.0	ng	17552	6	15.451	38839	20.0
unknown15.662	15.662	5.1	ng	9929	6	15.451	38839	20.0
Hentriacontane	15.892	29.2	ng	56661	6	15.451	38839	20.0
Bromoacetic aci...	15.951	6.9	ng	13427	6	15.451	38839	20.0
unknown16.674	16.674	5.2	ng	10144	6	15.451	38839	20.0
Sulfurous acid,...	16.968	17.6	ng	34087	6	15.451	38839	20.0