

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
 Data File : BF124753.D
 Acq On : 24 Jul 2021 18:12
 Operator : JU/CG
 Sample : M3117-01 2X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NJ-CLEAN-1

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-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124753.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	5	9	12	rBB	5417	6054	7.94%	0.978%
2	5.081	506	509	511	rBB	3318	3203	4.20%	0.517%
3	5.481	573	577	580	rBB	72015	62638	82.17%	10.118%
4	6.487	745	748	751	rBB	74438	64714	84.90%	10.453%
5	6.869	810	813	816	rBB	51081	38576	50.61%	6.231%
6	7.428	905	908	911	rBB	51747	42716	56.04%	6.900%
7	8.051	1011	1014	1017	rBV	22748	15462	20.28%	2.498%
8	8.157	1028	1032	1035	rBB	59183	50391	66.11%	8.140%
9	9.228	1211	1214	1217	rBV	108199	76228	100.00%	12.313%
10	9.910	1327	1330	1333	rBB	67004	48140	63.15%	7.776%
11	10.692	1460	1463	1466	rBB	36546	26277	34.47%	4.245%
12	11.392	1579	1582	1586	rBV	43098	36077	47.33%	5.827%
13	11.910	1669	1670	1672	rBB	2110	1148	1.51%	0.185%
14	12.980	1848	1852	1855	rBB	55103	46312	60.75%	7.481%
15	13.886	2001	2006	2013	rVB2	3408	5401	7.09%	0.872%
16	14.033	2028	2031	2034	rBV	34717	29577	38.80%	4.778%
17	14.115	2043	2045	2047	rVB	1149	1034	1.36%	0.167%
18	14.192	2054	2058	2063	rBV3	945	2177	2.86%	0.352%
19	14.327	2078	2081	2082	rBV2	1330	1272	1.67%	0.205%
20	14.498	2107	2110	2113	rBV3	1825	2258	2.96%	0.365%
21	14.586	2123	2125	2128	rBV2	1065	1091	1.43%	0.176%
22	14.721	2145	2148	2149	rBV2	905	1131	1.48%	0.183%
23	14.810	2161	2163	2165	rBV	1239	1213	1.59%	0.196%
24	14.886	2174	2176	2179	rVB3	1999	1471	1.93%	0.238%
25	14.939	2184	2185	2187	rBV	1546	1363	1.79%	0.220%
26	15.010	2192	2197	2198	rVV2	772	1175	1.54%	0.190%
27	15.151	2215	2221	2224	rBV2	1803	2118	2.78%	0.342%
28	15.504	2276	2281	2285	rBV2	17976	21858	28.67%	3.531%
29	15.668	2303	2309	2310	rBV2	1235	2056	2.70%	0.332%
30	15.739	2315	2321	2326	rVB	1418	3237	4.25%	0.523%
31	15.980	2354	2362	2364	rBV3	1628	2342	3.07%	0.378%
32	16.068	2374	2377	2378	rBV	1592	1420	1.86%	0.229%
33	16.356	2425	2426	2430	rVB2	991	1098	1.44%	0.177%
34	16.480	2443	2447	2452	rBV2	754	1534	2.01%	0.248%
35	16.880	2512	2515	2518	rVB	808	1216	1.60%	0.196%
36	17.439	2607	2610	2614	rVB3	1255	2165	2.84%	0.350%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.474	2614	2616	2620	rBV	1322	1805	2.37%	0.292%
38	17.562	2629	2631	2635	rBV	1052	1640	2.15%	0.265%
39	17.733	2657	2660	2661	rBV2	1018	1071	1.40%	0.173%
40	17.803	2668	2672	2676	rVB3	880	1370	1.80%	0.221%
41	17.962	2698	2699	2703	rVB3	1191	1030	1.35%	0.166%
42	18.421	2775	2777	2782	rVB2	1193	1640	2.15%	0.265%
43	18.574	2799	2803	2805	rVB2	849	1086	1.42%	0.175%
44	18.615	2805	2810	2812	rBV2	1031	1407	1.85%	0.227%
45	18.692	2818	2823	2827	rVB2	1112	1890	2.48%	0.305%

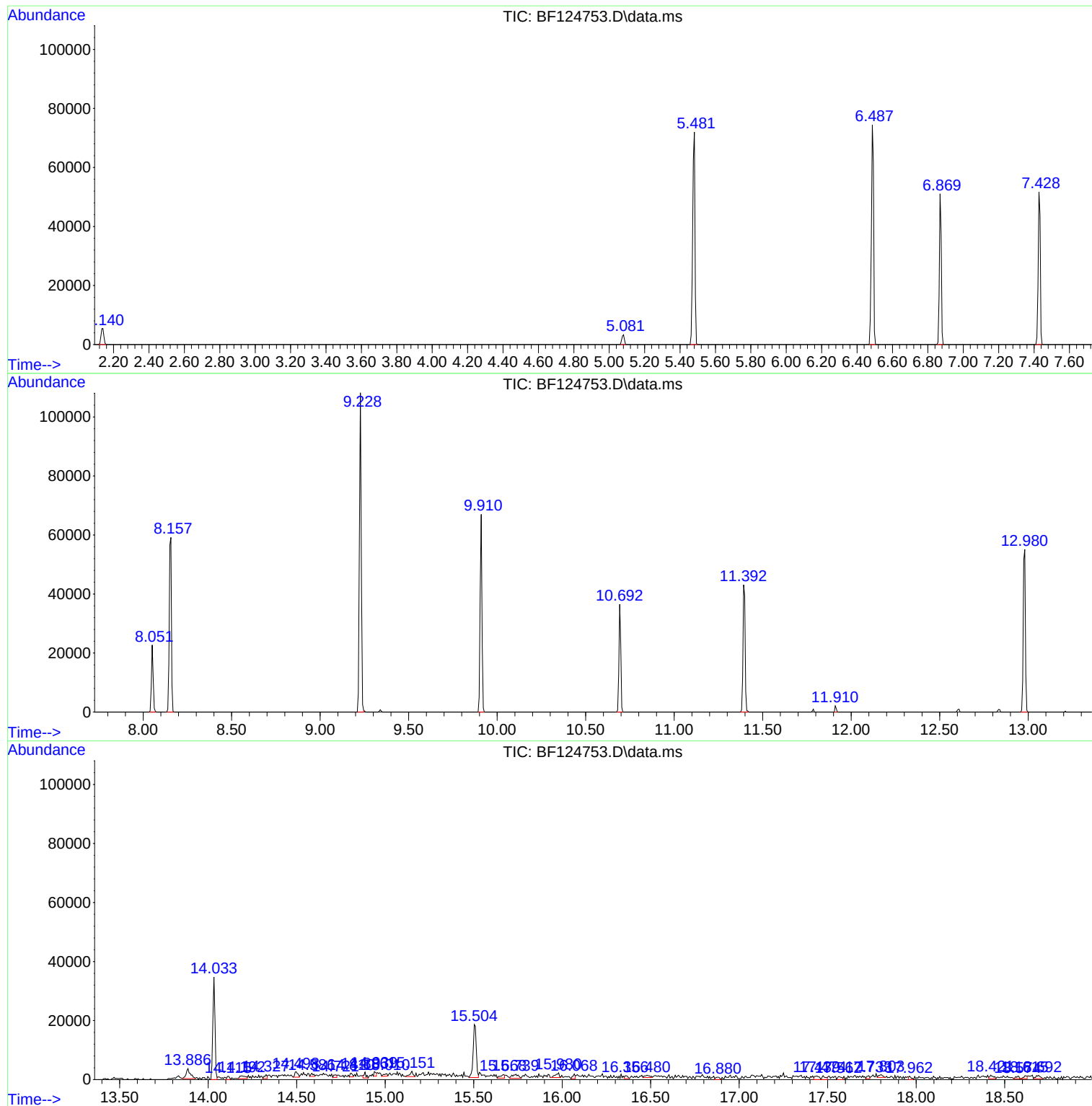
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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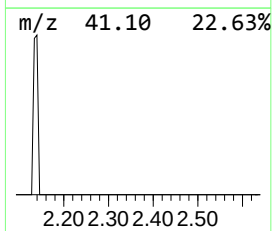
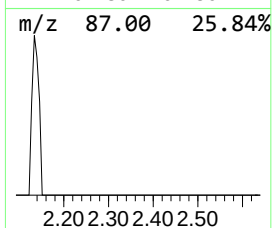
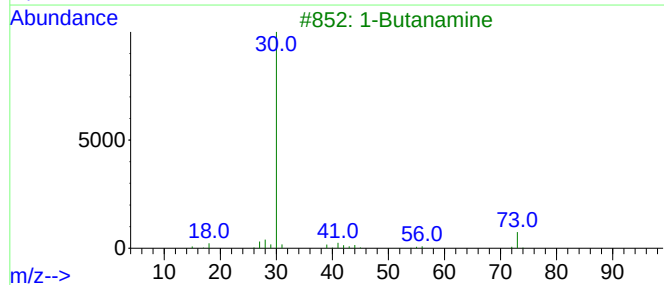
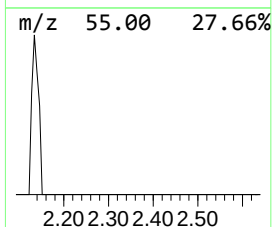
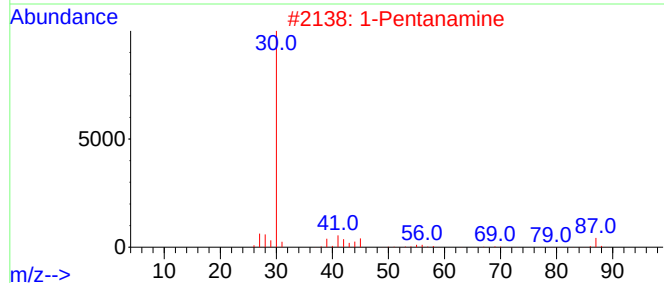
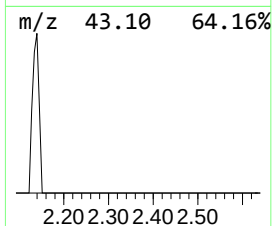
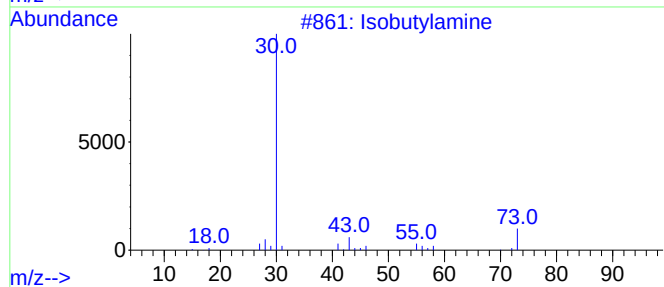
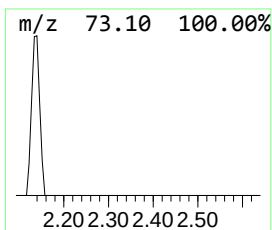
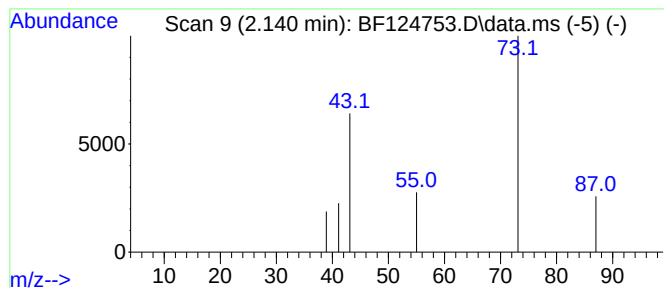
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.140 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	3.14 ng	6054	1,4-Dichlorobenzene-d4	6.869

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutylamine	73	C4H11N	000078-81-9	5
2		1-Pentanamine	87	C5H13N	000110-58-7	4
3		1-Butanamine	73	C4H11N	000109-73-9	3
4		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	3
5		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	2



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ALS Vial : 18 Sample Multiplier: 1

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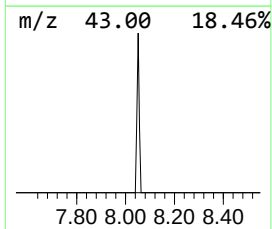
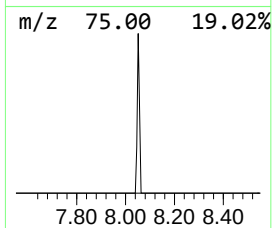
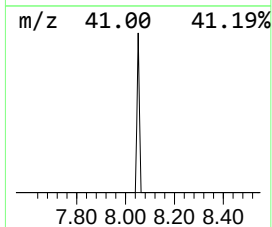
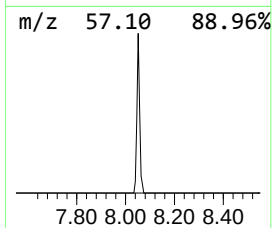
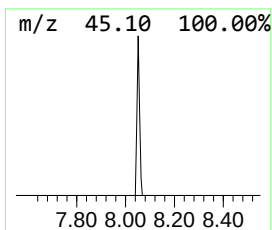
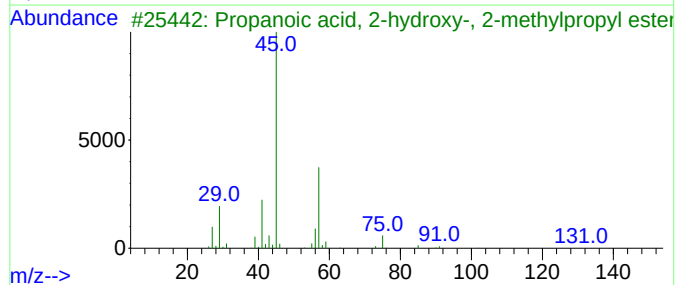
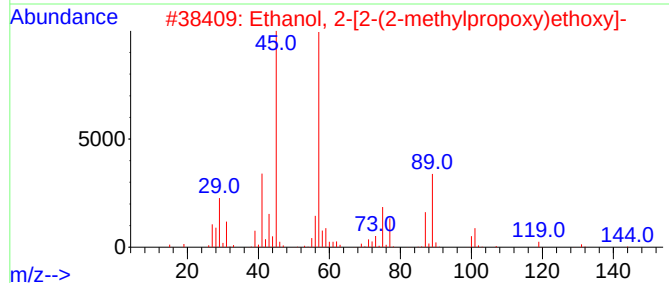
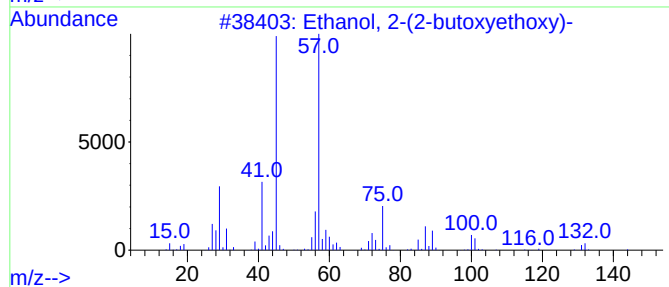
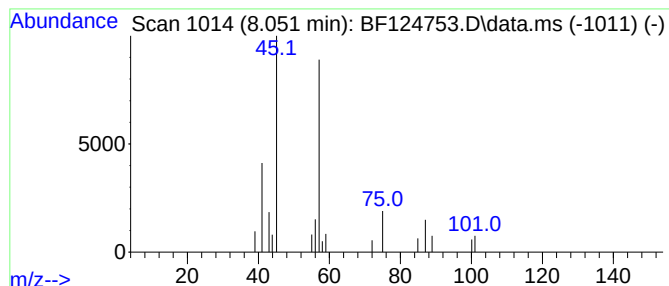
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	6.14 ng	15462	Naphthalene-d8	8.157

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	64
3			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	42
4			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	39
5			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	39



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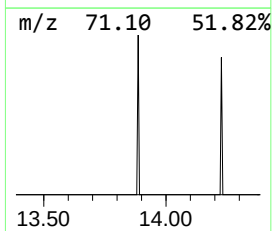
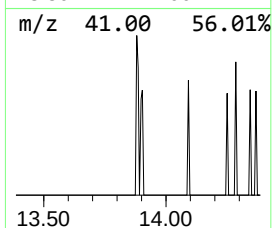
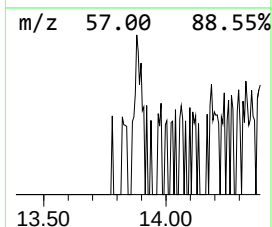
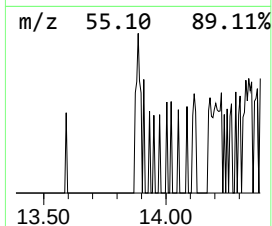
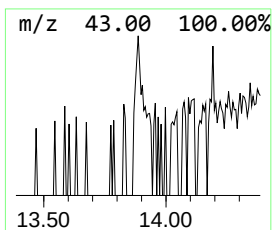
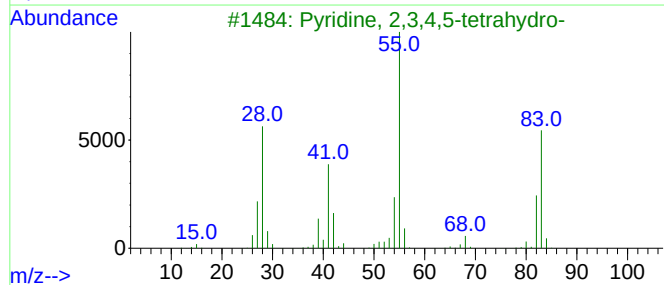
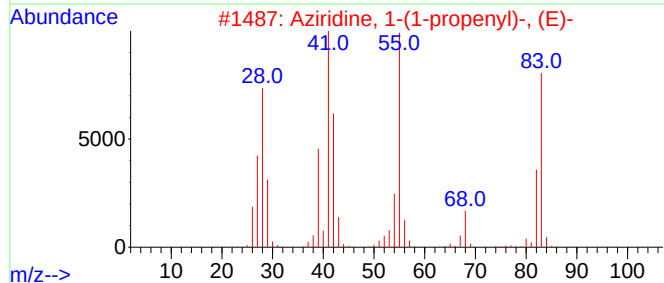
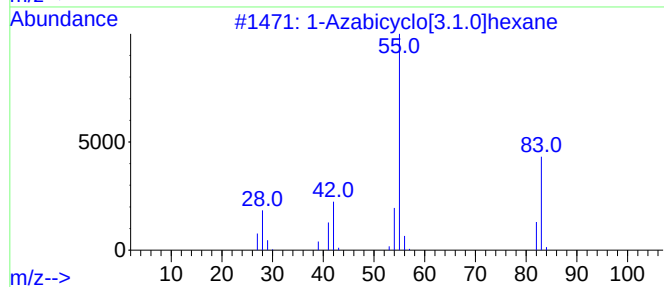
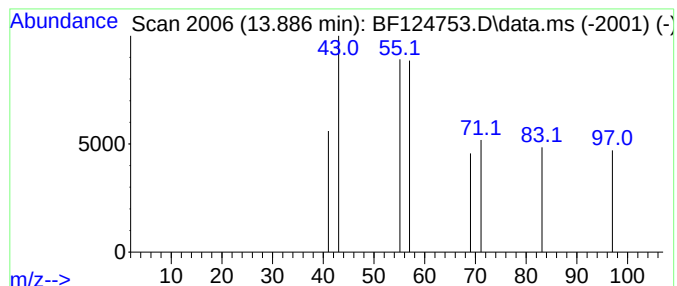
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown13.886 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.65 ng	5401	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Azabicyclo[3.1.0]hexane	83	C5H9N	000285-76-7	4
2			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	4
3			Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4
4			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	4
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	4



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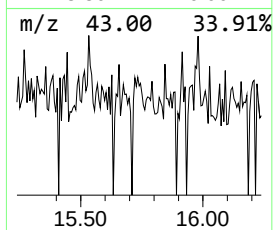
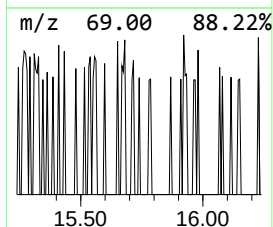
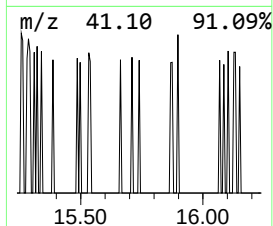
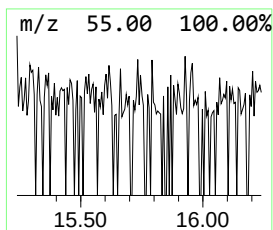
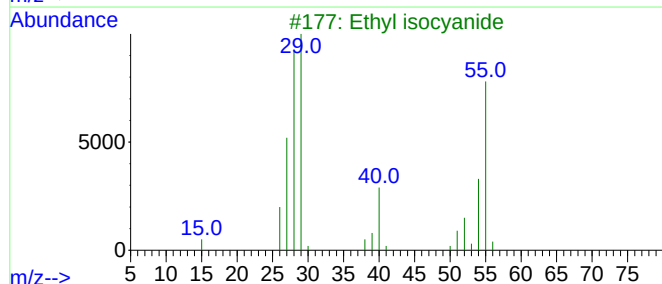
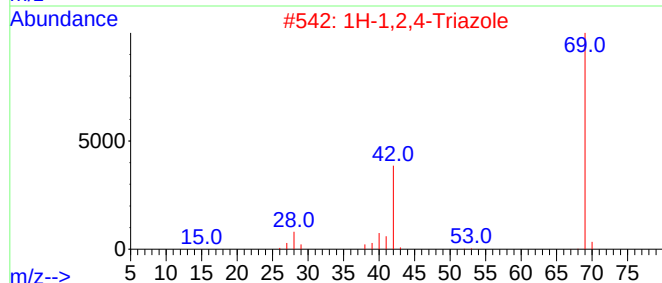
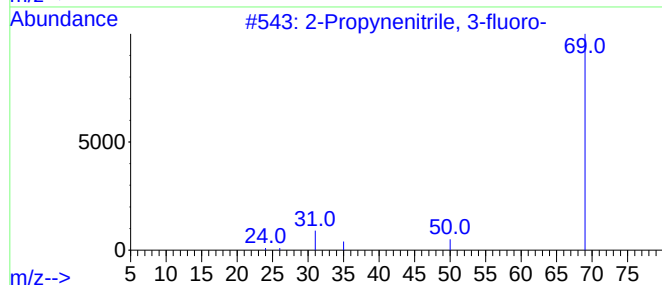
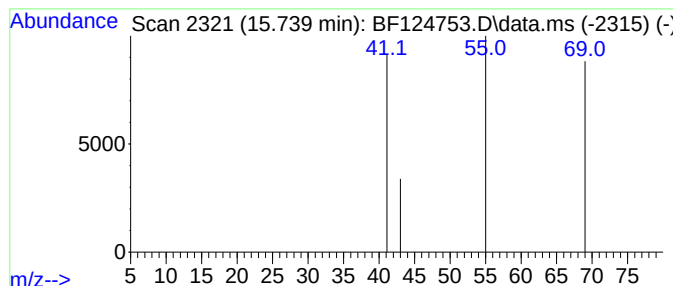
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown15.739 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	2.96 ng	3237	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propynenitrile, 3-fluoro-			69	C3FN	032038-83-8	2
2	1H-1,2,4-Triazole			69	C2H3N3	000288-88-0	2
3	Ethyl isocyanide			55	C3H5N	000624-79-3	1
4	Borane, ethylisopropylmethyl-			98	C6H15B	1000154-39-8	1
5	3-Butyn-2-ol			70	C4H6O	002028-63-9	1



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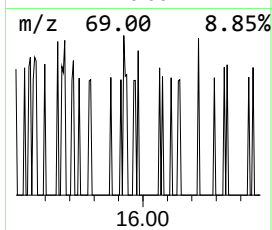
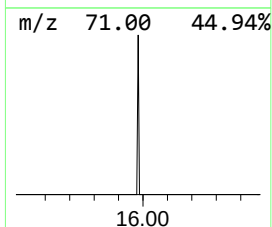
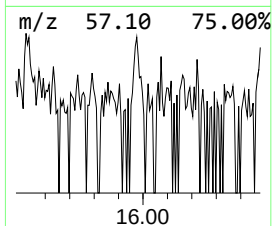
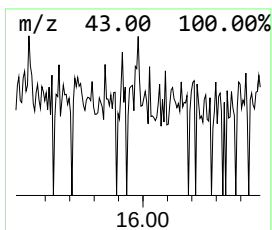
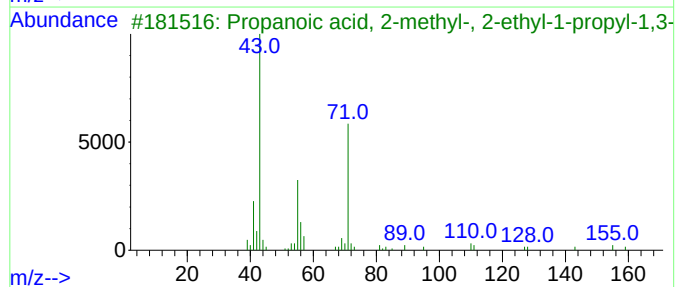
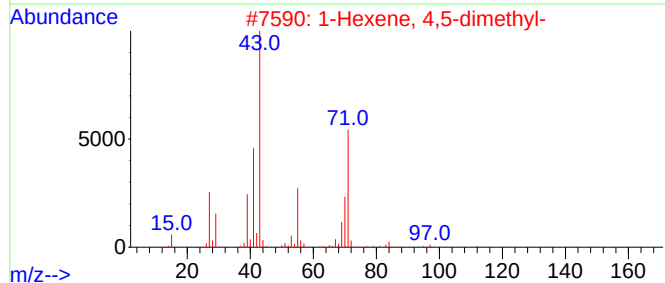
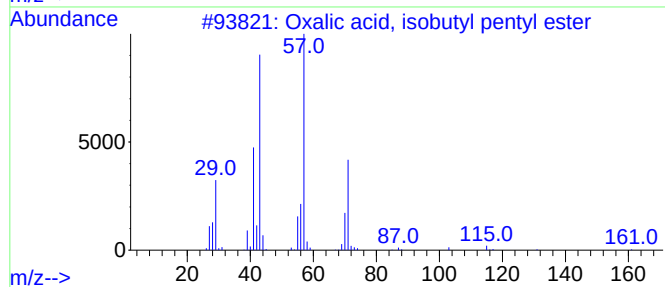
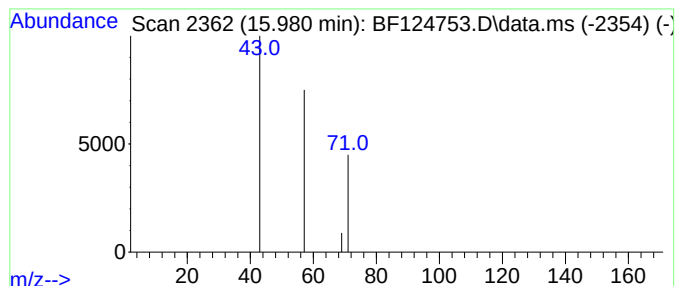
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown15.980 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.980	2.14 ng	2342	Perylene-d12	15.509

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	2
2			1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	2
3			Propanoic acid, 2-methyl-, 2-eth...	286	C16H30O4	074367-30-9	2
4			Cyanoic acid, ethyl ester	71	C3H5NO	000627-48-5	2
5			Methane, isocyanato-	57	C2H3NO	000624-83-9	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124753.D
Acq On : 24 Jul 2021 18:12
Operator : JU/CG
Sample : M3117-01 2X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.140	2.140	3.1	ng	6054	1	6.869	38576	20.0
Ethanol, 2-(2-b...	8.051	6.1	ng	15462	2	8.157	50391	20.0
unknown13.886	13.886	3.6	ng	5401	5	14.033	29577	20.0
unknown15.739	15.739	3.0	ng	3237	6	15.509	21858	20.0
unknown15.980	15.980	2.1	ng	2342	6	15.509	21858	20.0