

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
 Data File : BF124771.D
 Acq On : 26 Jul 2021 18:38
 Operator : JU/CG
 Sample : M3117-09
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NJ-CLEAN-9

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: BF124771.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	7	11	15	rBB	10737	11394	9.73%	1.306%
2	2.493	65	69	73	rBB2	4825	6077	5.19%	0.697%
3	5.093	508	511	513	rBB	2004	2152	1.84%	0.247%
4	5.487	574	578	581	rBV	113519	100473	85.84%	11.517%
5	6.498	745	750	753	rBB	114280	102661	87.71%	11.768%
6	6.875	811	814	817	rBB	41855	29352	25.08%	3.364%
7	7.434	905	909	912	rBB	77373	65925	56.32%	7.557%
8	8.057	1012	1015	1020	rBB	24238	20322	17.36%	2.329%
9	8.157	1028	1032	1035	rBB	55085	38776	33.13%	4.445%
10	9.234	1211	1215	1218	rBV	143002	117047	100.00%	13.417%
11	9.910	1327	1330	1333	rBB	48535	37095	31.69%	4.252%
12	10.698	1461	1464	1467	rBB	71728	53432	45.65%	6.125%
13	11.398	1580	1583	1586	rBV	41257	30732	26.26%	3.523%
14	11.916	1669	1671	1673	rBB	4105	2737	2.34%	0.314%
15	12.610	1787	1789	1792	rBB	5504	3682	3.15%	0.422%
16	12.839	1826	1828	1832	rBB	4390	3632	3.10%	0.416%
17	12.986	1849	1853	1856	rBB	121656	94535	80.77%	10.836%
18	13.210	1889	1891	1894	rBV2	2085	1975	1.69%	0.226%
19	13.516	1941	1943	1946	rBV2	1273	2121	1.81%	0.243%
20	13.551	1946	1949	1952	rVB2	2046	2686	2.29%	0.308%
21	13.886	2002	2006	2008	rBV3	4139	5752	4.91%	0.659%
22	14.039	2028	2032	2035	rBV	34510	29469	25.18%	3.378%
23	14.133	2046	2048	2051	rBV2	1290	1532	1.31%	0.176%
24	14.180	2051	2056	2057	rVV3	1696	2516	2.15%	0.288%
25	14.198	2057	2059	2061	rVB2	2872	2370	2.02%	0.272%
26	14.498	2107	2110	2113	rBV3	4084	4468	3.82%	0.512%
27	14.716	2146	2147	2150	rBV3	1502	1697	1.45%	0.195%
28	14.792	2158	2160	2161	rBV2	1713	1706	1.46%	0.196%
29	14.810	2161	2163	2168	rVB3	2285	3036	2.59%	0.348%
30	14.963	2186	2189	2192	rBV3	1799	1665	1.42%	0.191%
31	15.074	2205	2208	2213	rBV4	1948	3591	3.07%	0.412%
32	15.151	2219	2221	2224	rVB3	3129	3322	2.84%	0.381%
33	15.180	2224	2226	2228	rBV3	1920	2073	1.77%	0.238%
34	15.263	2238	2240	2243	rVB3	1497	1605	1.37%	0.184%
35	15.386	2258	2261	2264	rVB3	1604	1941	1.66%	0.222%
36	15.451	2269	2272	2274	rVB3	1826	1871	1.60%	0.214%

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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

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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37	15.515	2280	2283	2287	rBV2	15557	17299	14.78%	1.983%
38	15.668	2305	2309	2311	rBV4	2285	2842	2.43%	0.326%
39	15.745	2320	2322	2327	rVB5	1557	1809	1.55%	0.207%
40	15.851	2336	2340	2342	rBV3	1357	2382	2.04%	0.273%
41	15.921	2349	2352	2355	rVB5	1321	1672	1.43%	0.192%
42	15.974	2359	2361	2365	rVV2	2529	2800	2.39%	0.321%
43	16.021	2368	2369	2373	rVB4	2040	2068	1.77%	0.237%
44	16.057	2373	2375	2377	rBV2	1535	1622	1.39%	0.186%
45	16.227	2403	2404	2409	rVB4	2480	1994	1.70%	0.229%
46	16.368	2426	2428	2432	rVB2	1437	1584	1.35%	0.182%
47	16.445	2437	2441	2445	rBV4	1034	1672	1.43%	0.192%
48	16.480	2445	2447	2448	rBV2	2414	1841	1.57%	0.211%
49	16.498	2448	2450	2452	rBV3	1356	1414	1.21%	0.162%
50	16.592	2462	2466	2469	rBV3	1269	1806	1.54%	0.207%
51	16.768	2494	2496	2499	rVB4	1505	1721	1.47%	0.197%
52	17.262	2577	2580	2583	rVB3	2088	2125	1.82%	0.244%
53	17.433	2607	2609	2610	rBV2	1895	1369	1.17%	0.157%
54	17.457	2611	2613	2620	rVB5	1759	2605	2.23%	0.299%
55	17.504	2620	2621	2624	rBV3	1181	1363	1.16%	0.156%
56	17.633	2640	2643	2647	rVB4	1210	1919	1.64%	0.220%
57	17.745	2659	2662	2664	rBV3	1460	1714	1.46%	0.196%
58	17.892	2683	2687	2689	rBV4	2091	2394	2.05%	0.274%
59	17.915	2689	2691	2692	rBV3	1901	1557	1.33%	0.178%
60	18.009	2705	2707	2710	rVB3	1766	1617	1.38%	0.185%
61	18.209	2739	2741	2744	rVB3	2043	1874	1.60%	0.215%
62	18.268	2749	2751	2752	rVB	2304	1431	1.22%	0.164%
63	18.280	2752	2753	2757	rBV3	1970	1760	1.50%	0.202%
64	18.409	2770	2775	2776	rVB4	2237	2906	2.48%	0.333%
65	18.433	2776	2779	2781	rBV3	1809	1685	1.44%	0.193%
66	18.474	2784	2786	2789	rVB3	1512	1490	1.27%	0.171%
67	18.574	2801	2803	2808	rBV5	1681	2948	2.52%	0.338%
68	18.803	2840	2842	2844	rBV2	2154	1701	1.45%	0.195%

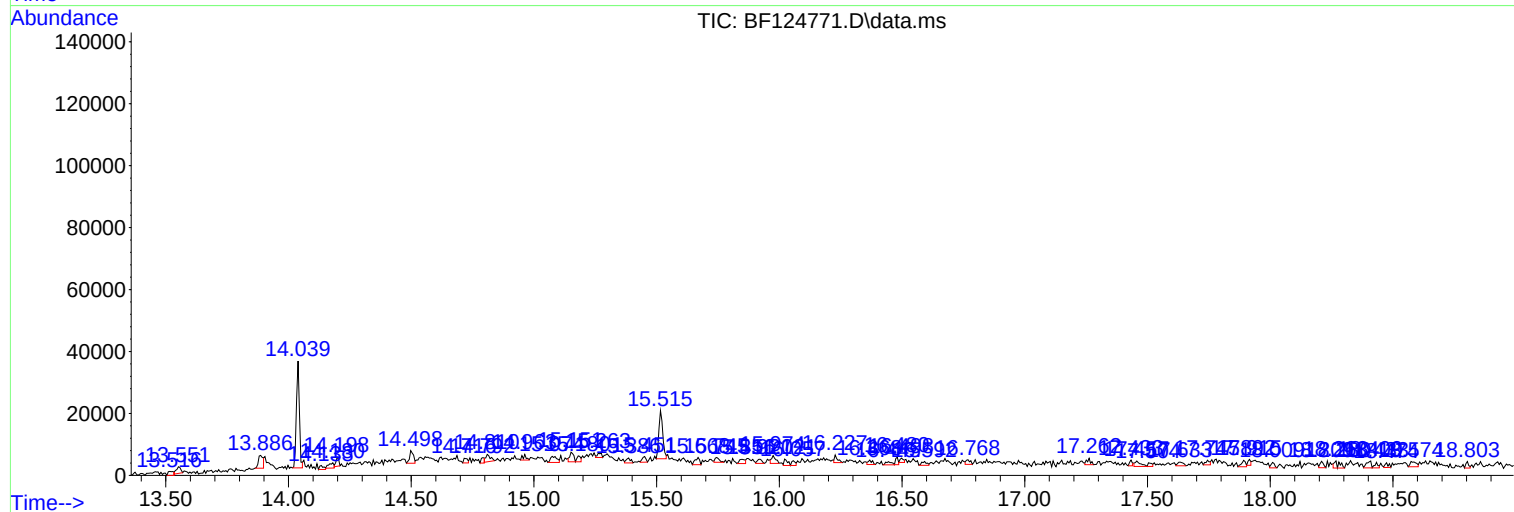
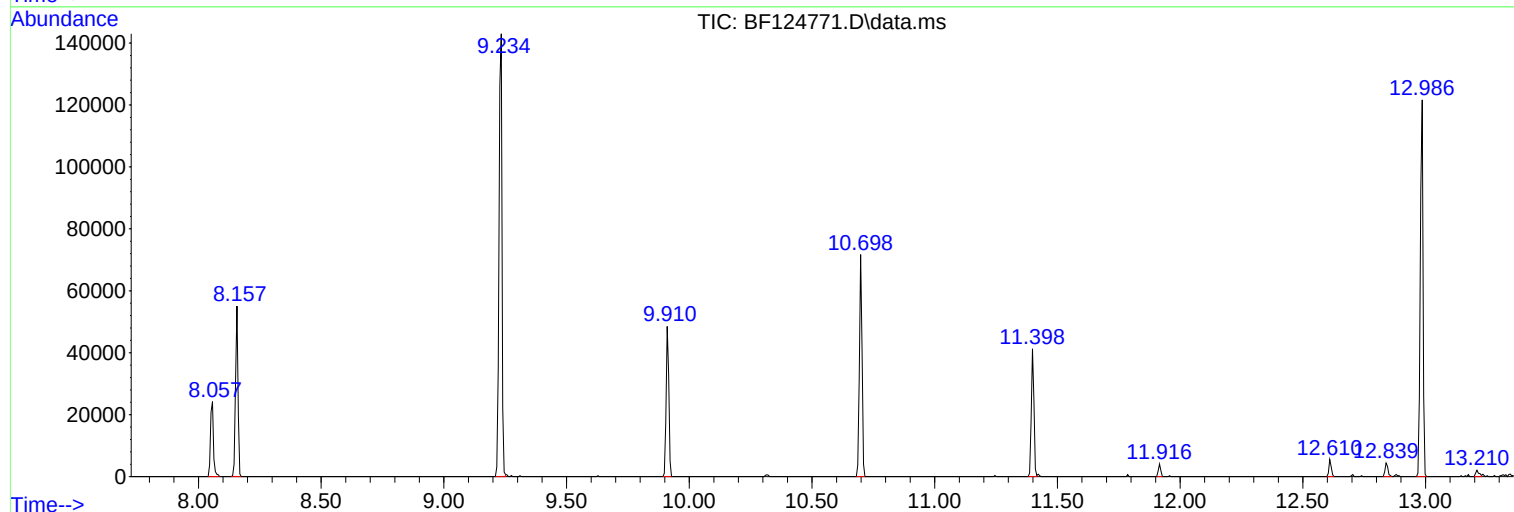
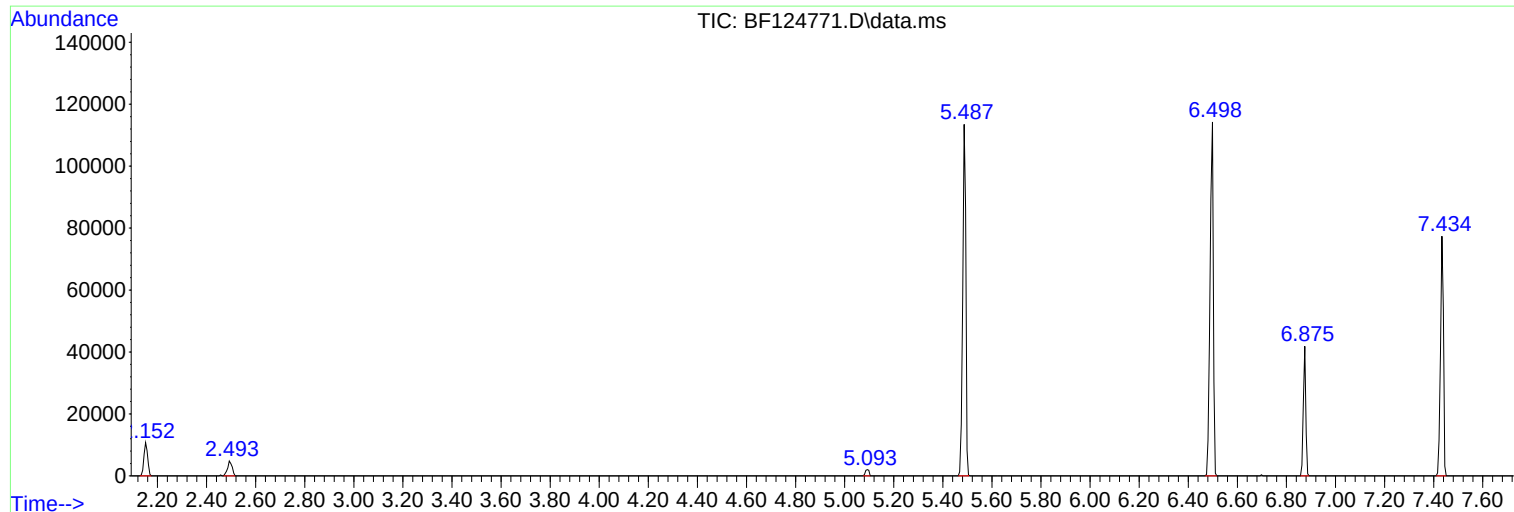
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ALS Vial : 9 Sample Multiplier: 1

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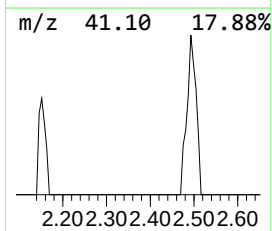
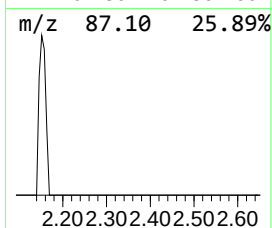
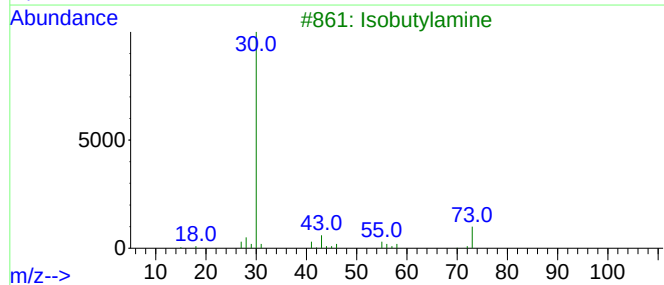
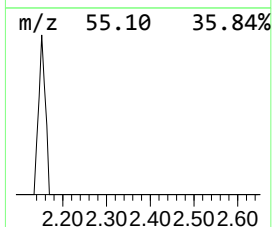
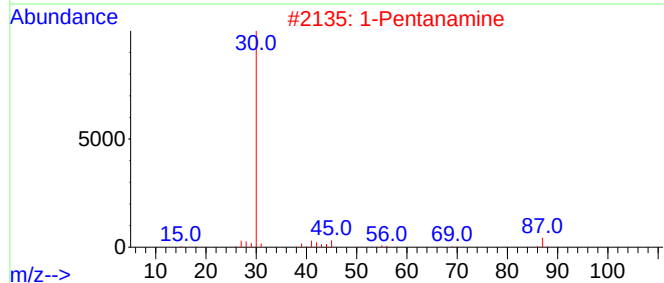
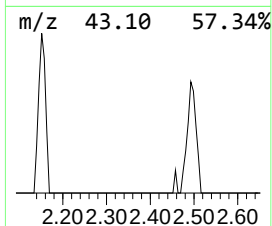
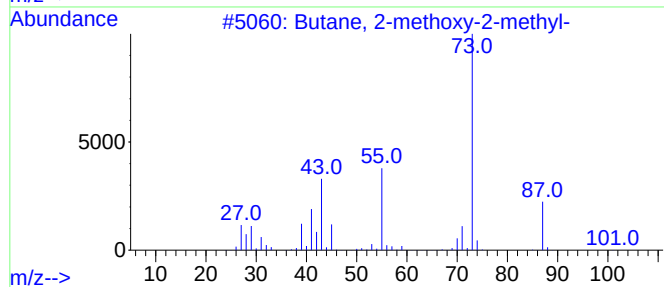
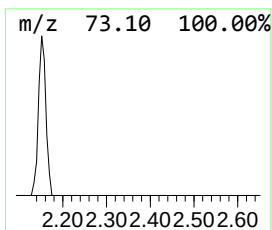
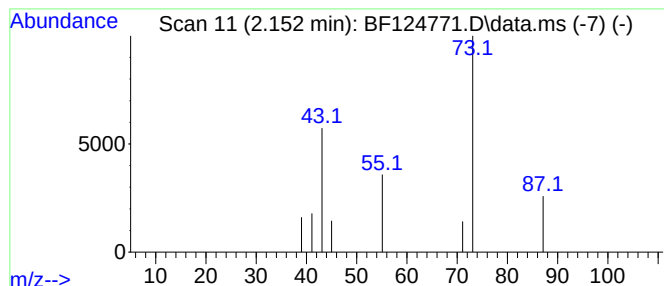
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.152	7.76 ng	11394	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			1-Pentanamine	87	C5H13N	000110-58-7	4
3			Isobutylamine	73	C4H11N	000078-81-9	4
4			2-Pentanol, acetate	130	C7H14O2	000626-38-0	4
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	4



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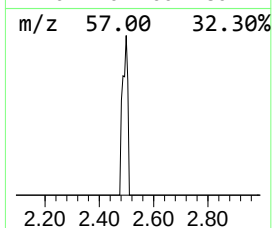
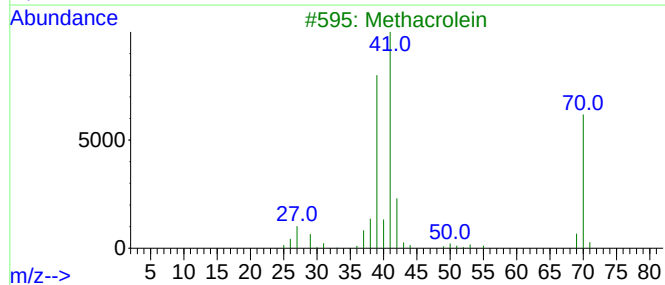
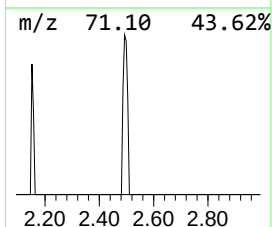
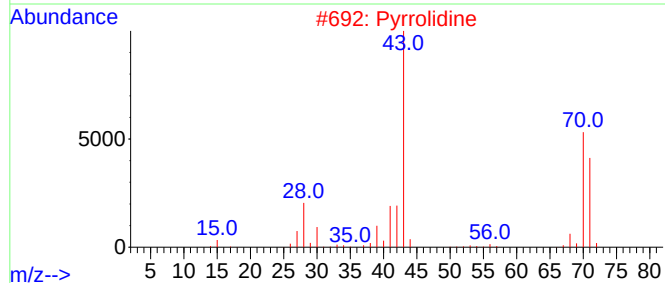
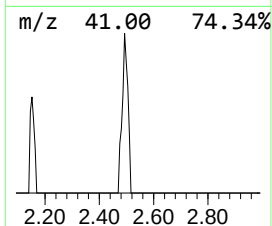
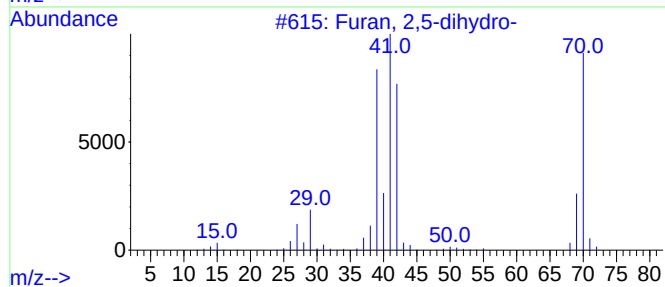
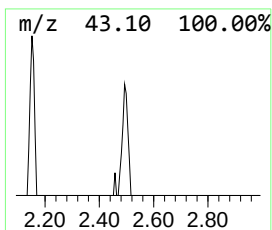
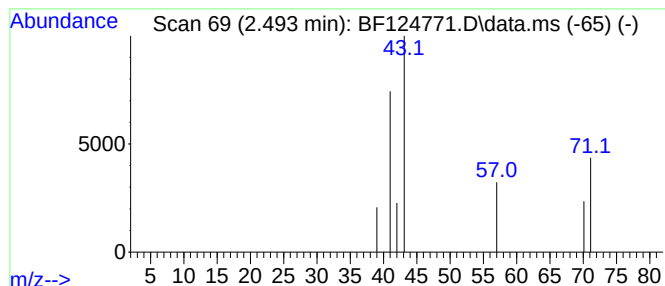
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown2.493 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.493	4.14 ng	6077	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7
2			Pyrrolidine	71	C4H9N	000123-75-1	7
3			Methacrolein	70	C4H6O	000078-85-3	4
4			Ethoxyacetylene	70	C4H6O	000927-80-0	4
5			2-Butenal	70	C4H6O	004170-30-3	4



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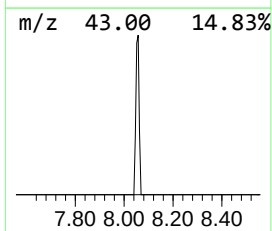
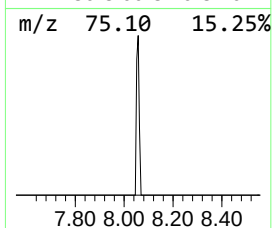
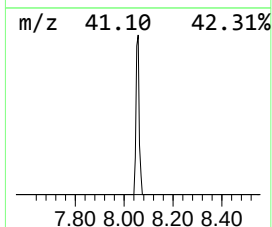
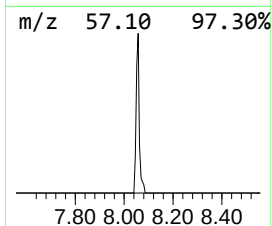
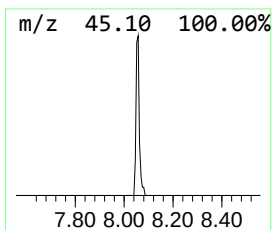
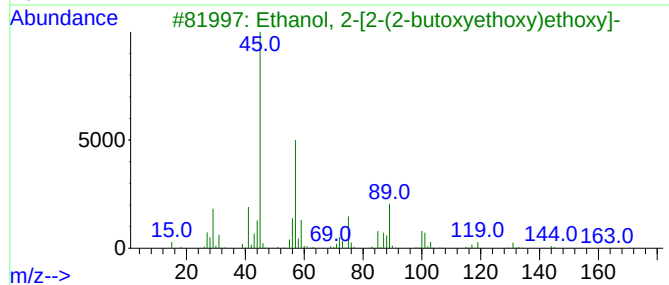
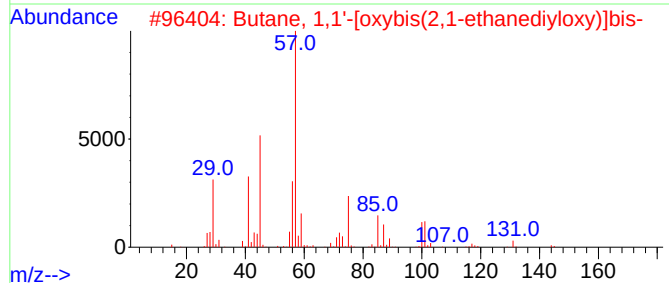
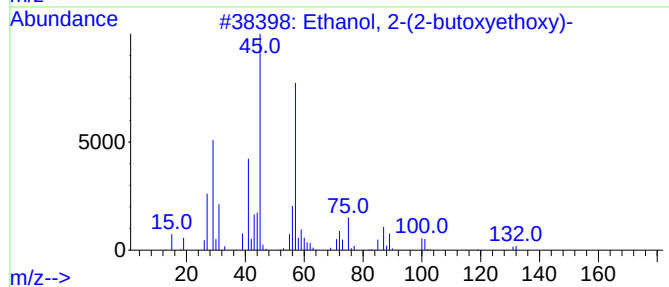
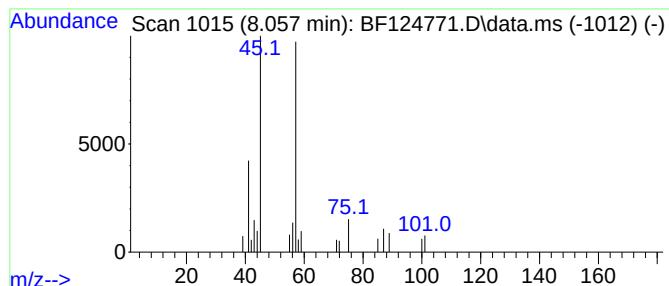
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.057	10.48 ng	20322	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	56
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
5			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45



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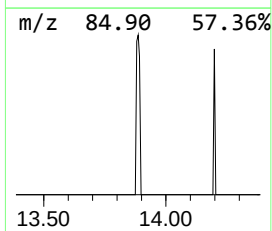
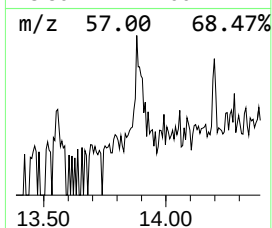
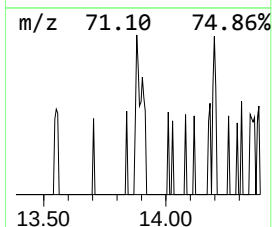
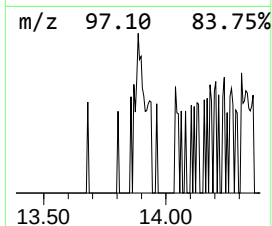
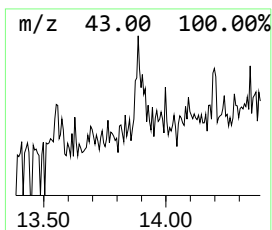
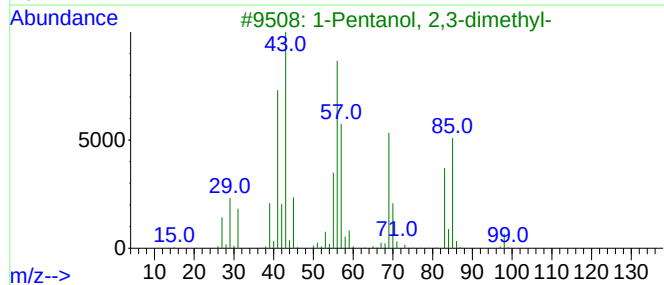
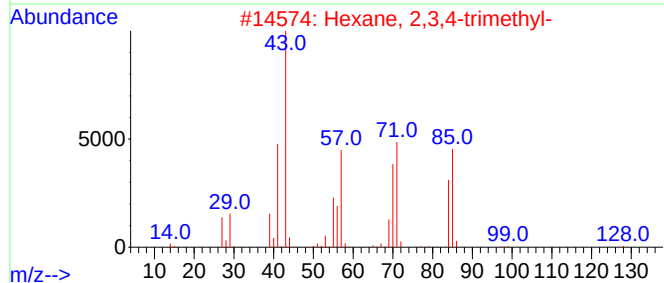
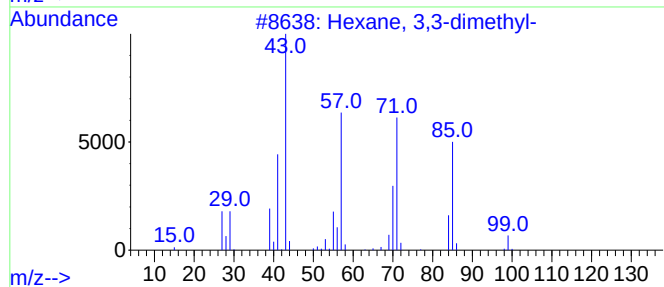
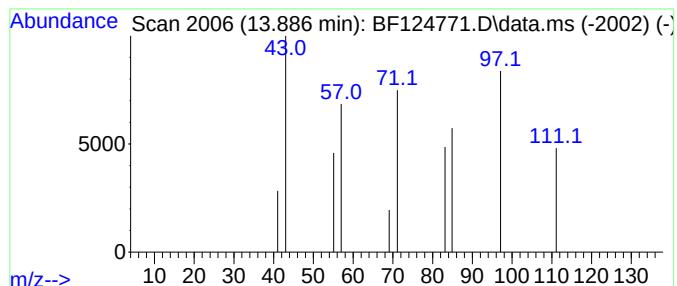
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown13.886 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.90 ng	5752	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	9
2			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	9
3			1-Pentanol, 2,3-dimethyl-	116	C7H16O	010143-23-4	9
4			Oxalic acid, isohexyl neopentyl ...	244	C13H24O4	1000309-73-0	9
5			Isoxazole, 4,5-dimethyl-	97	C5H7NO	007064-40-6	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampled :
NJ-CLEAN-9

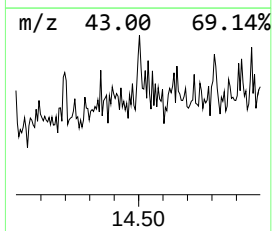
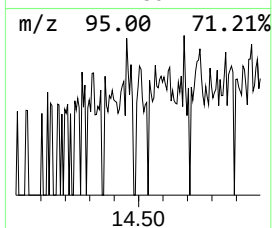
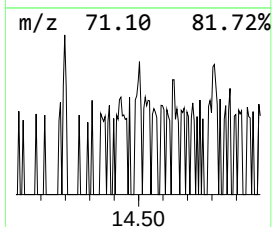
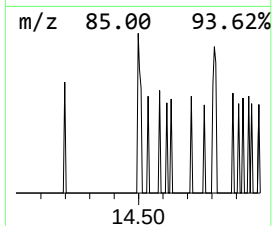
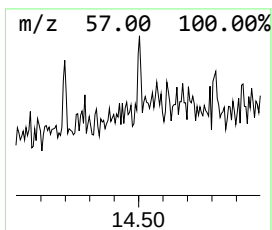
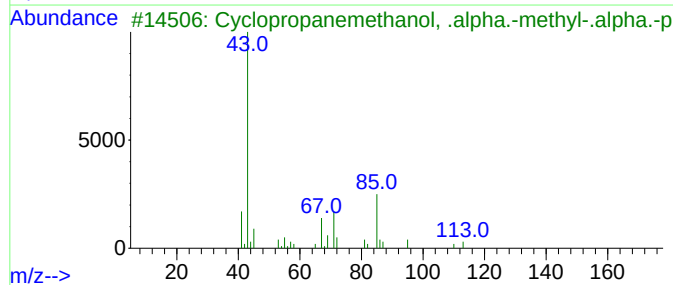
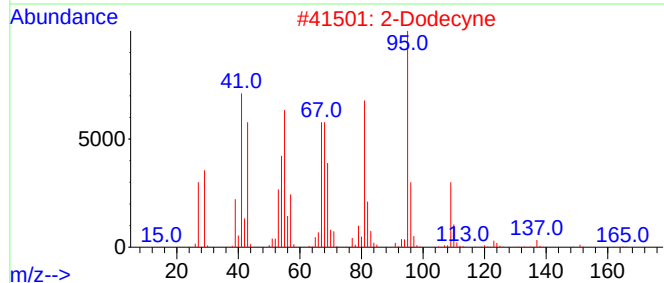
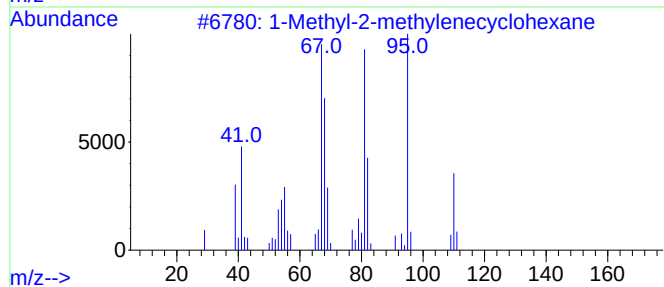
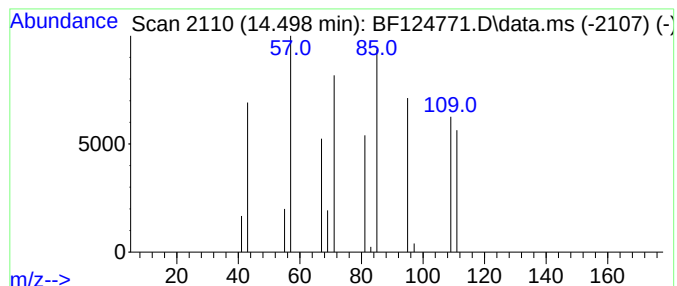
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.498 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	3.03 ng	4468	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	9		
2	2-Dodecyne	166	C12H22	000629-49-2	9		
3	Cyclopropanemethanol, .alpha.-me...	128	C8H16O	024230-08-8	9		
4	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	5		
5	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	4		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

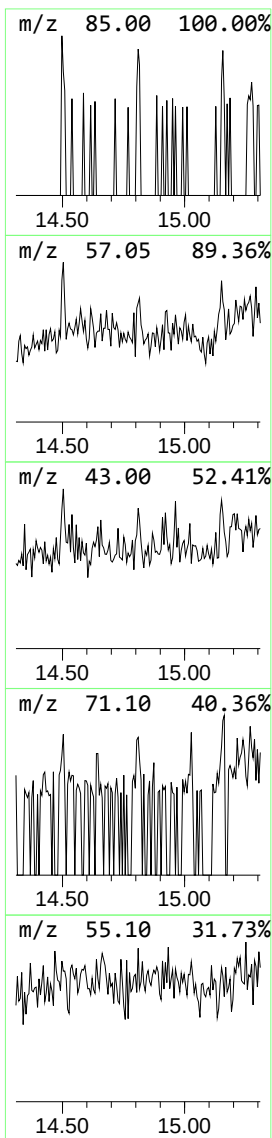
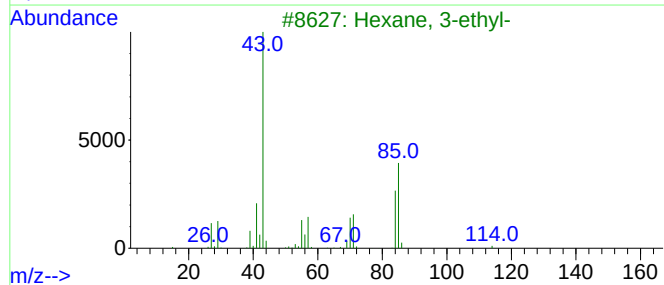
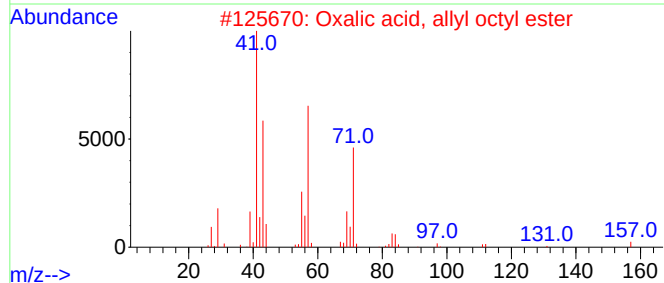
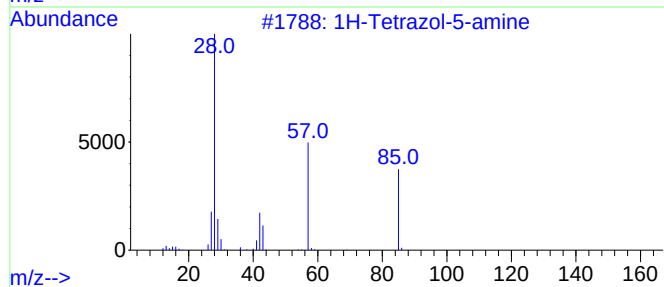
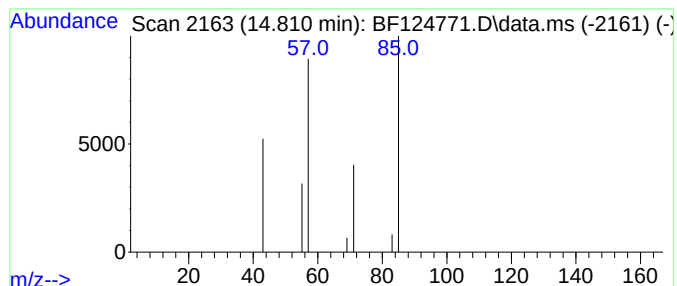
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.810 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.810	3.51 ng	3036	Perylene-d12		15.515	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Tetrazol-5-amine		85	CH3N5	004418-61-5	4
2	Oxalic acid, allyl octyl ester		242	C13H22O4	1000309-23-6	4
3	Hexane, 3-ethyl-		114	C8H18	000619-99-8	4
4	Azetidine, 1,2-dimethyl-		85	C5H11N	051764-32-0	4
5	Azetidine, 1-methyl-		71	C4H9N	004923-79-9	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

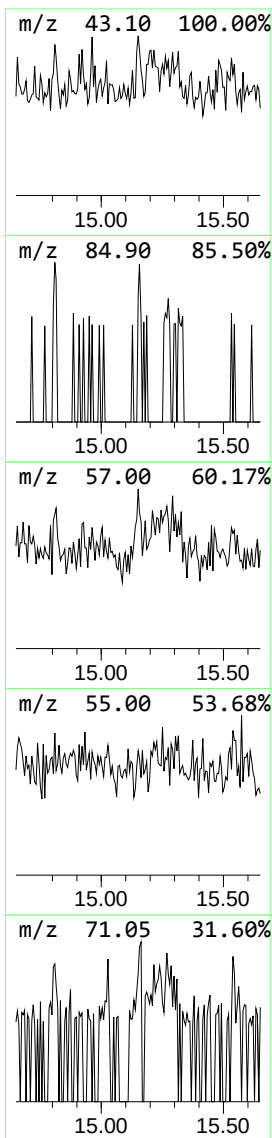
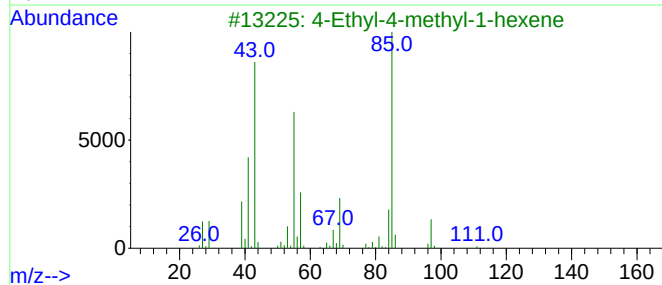
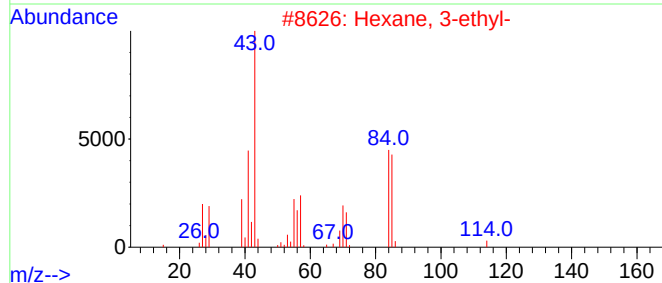
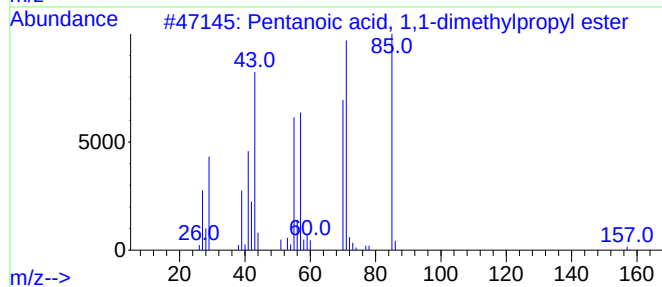
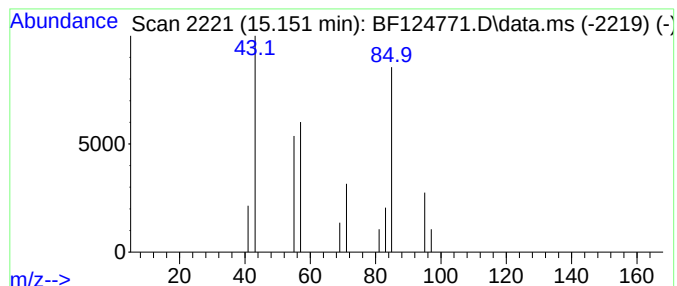
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.151 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.151	3.84 ng	3322	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid, 1,1-dimethylprop...	172	C10H20O2	117421-32-6	9
2	Hexane, 3-ethyl-	114	C8H18	000619-99-8	9
3	4-Ethyl-4-methyl-1-hexene	126	C9H18	090674-67-2	9
4	1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	5
5	Oxalic acid, cyclobutyl dodecyl ...	312	C18H32O4	1000309-70-3	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
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Misc :
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Instrument :
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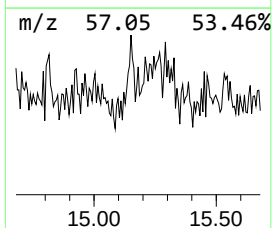
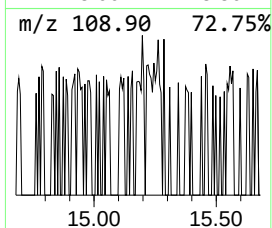
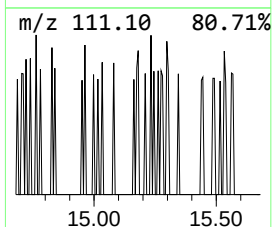
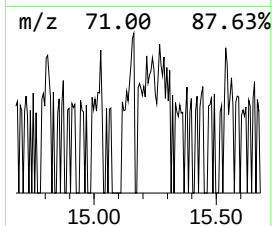
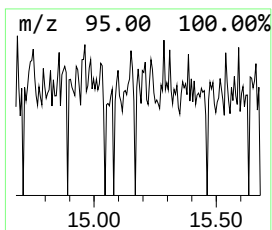
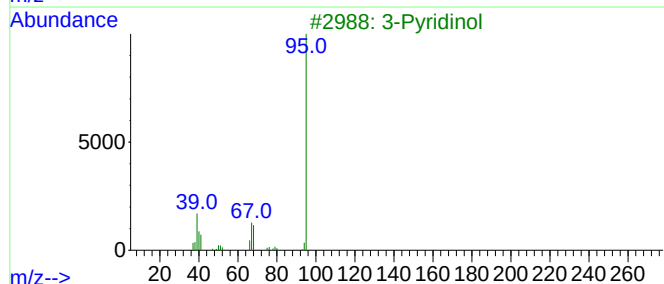
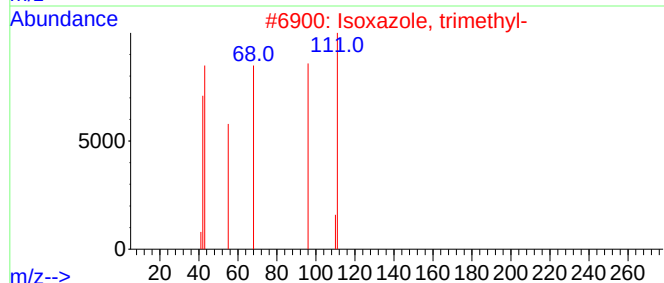
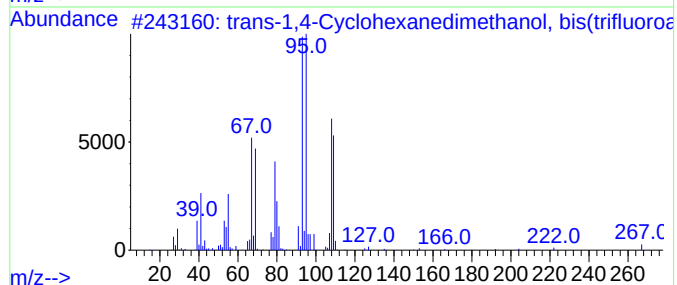
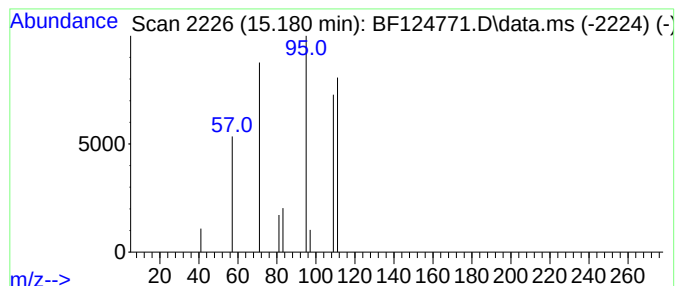
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown15.180 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	2.40 ng	2073	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-1,4-Cyclohexanedimethanol,...	336	C12H14F6O4	1000384-28-8	4
2			Isoxazole, trimethyl-	111	C6H9NO	010557-82-1	3
3			3-Pyridinol	95	C5H5NO	000109-00-2	3
4			Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	3
5			4(1H)-Pyridone	95	C5H5NO	000108-96-3	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
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Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

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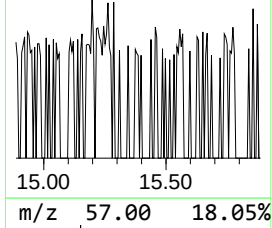
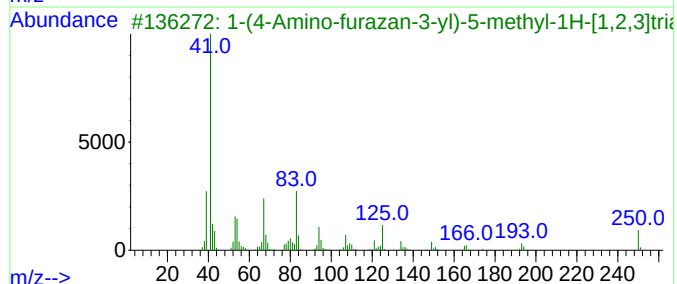
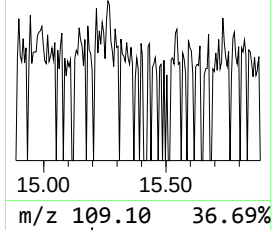
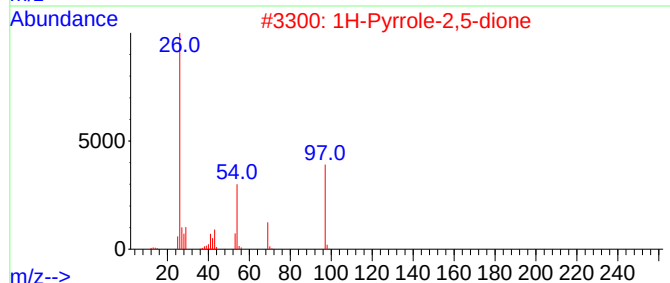
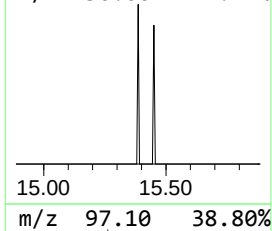
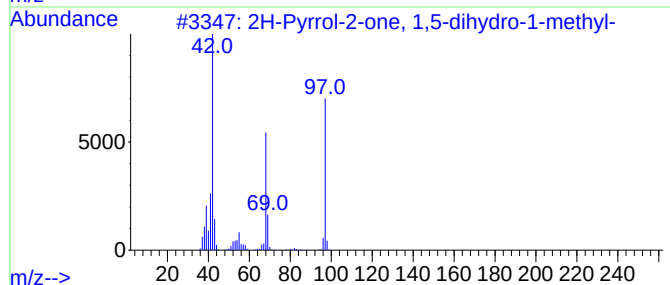
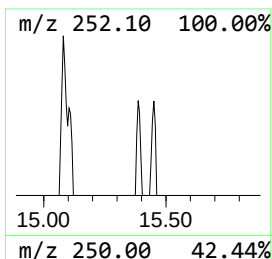
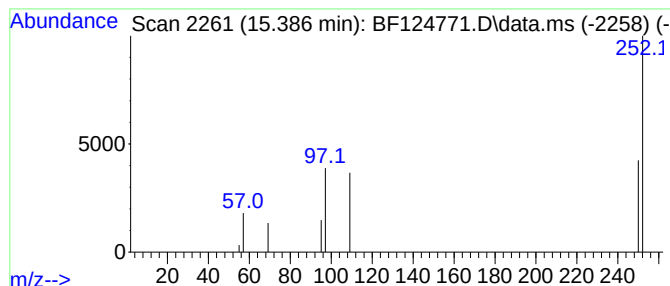
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown15.386 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.386	2.24 ng	1941	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Pyrrol-2-one, 1,5-dihydro-1-m...	97	C5H7NO	013950-21-5	4
2			1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	4
3			1-(4-Amino-furazan-3-yl)-5-methy...	250	C9H10N6O3	1000300-81-0	4
4			Cyclopropane, 1,1-dimethyl-2-chl...	186	C9H11ClS	095104-10-2	4
5			Z-7-Octadecen-1-ol acetate	310	C20H38O2	1010131-08-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
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ALS Vial : 9 Sample Multiplier: 1

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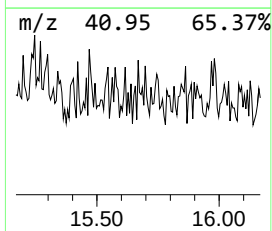
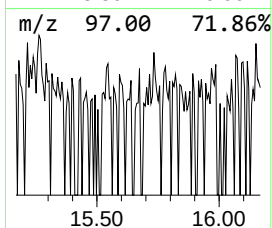
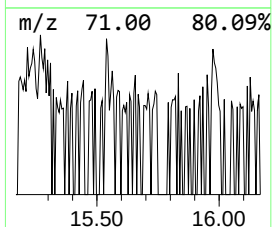
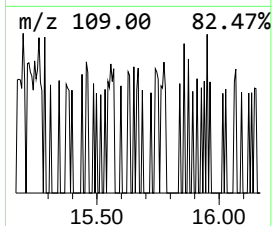
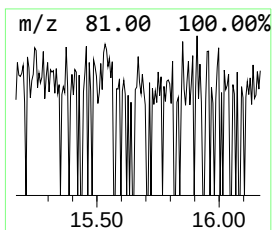
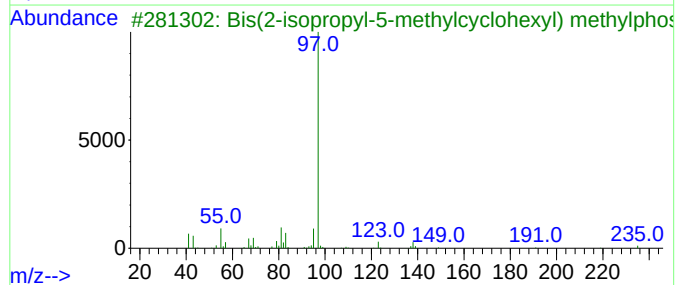
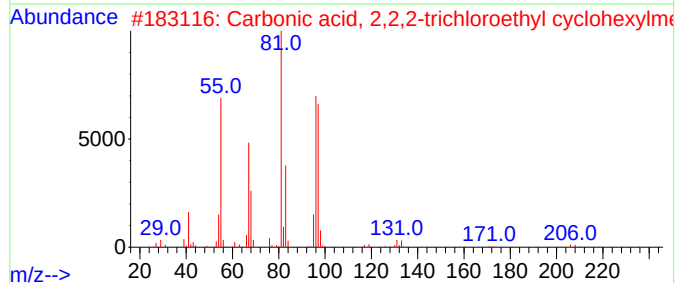
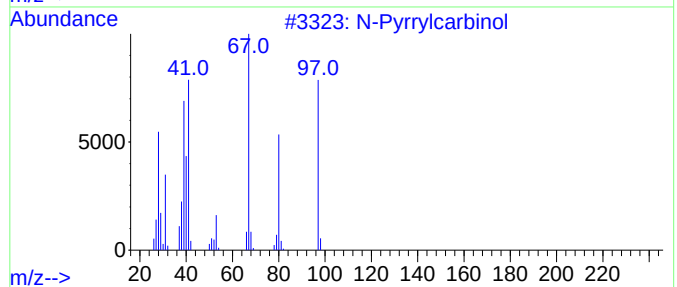
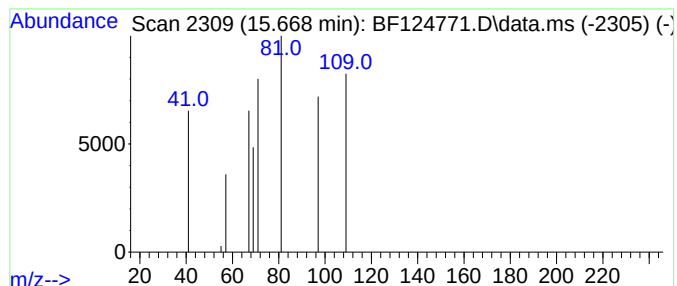
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.668 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.668	3.29 ng	2842	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Pyrrylcarbinol	97	C5H7NO	092776-61-9	9
2			Carbonic acid, 2,2,2-trichloroet...	288	C10H15Cl3O3	1000357-89-8	4
3			Bis(2-isopropyl-5-methylcyclohex...	372	C21H41O3P	1000510-36-8	4
4			Bis(2-isopropyl-5-methylcyclohex...	372	C21H41O3P	1000510-36-7	4
5			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
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Misc :
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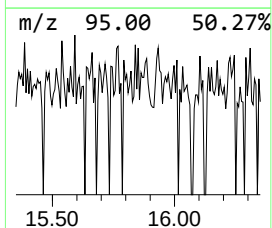
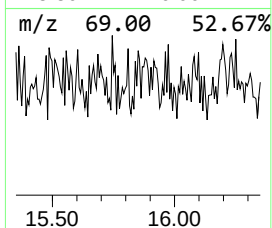
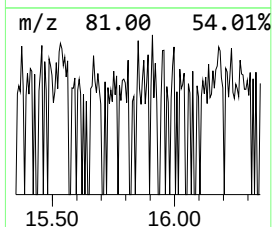
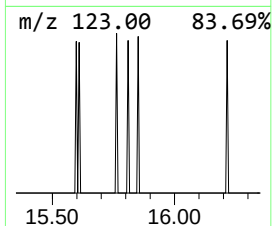
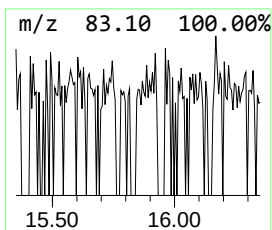
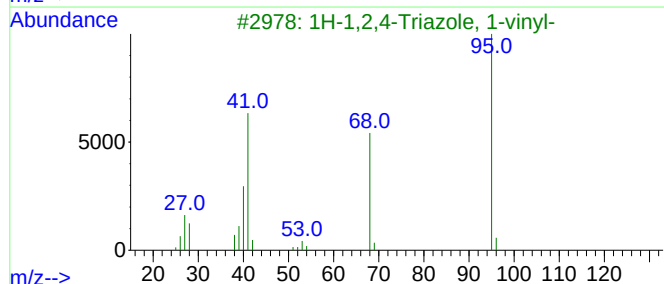
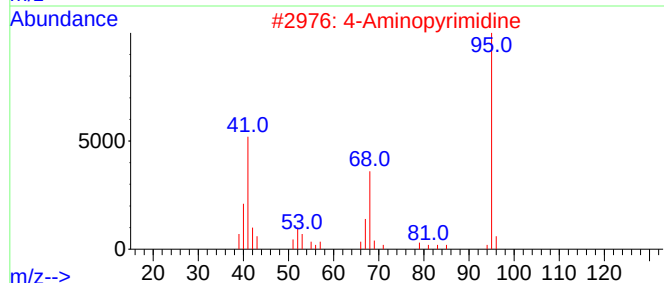
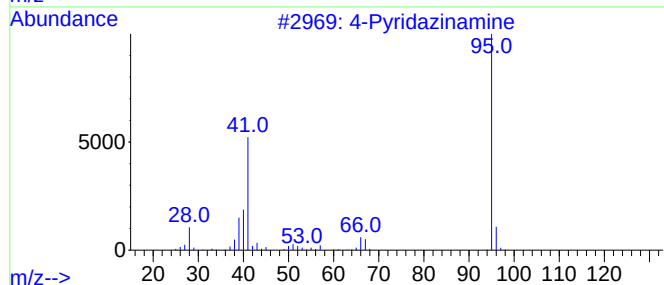
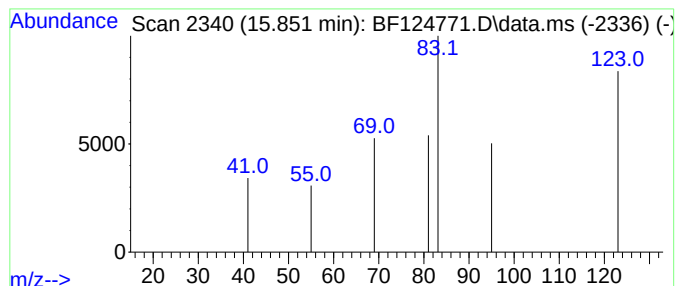
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown15.851 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.851	2.75 ng	2382	Perylene-d12		15.515	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	4-Pyridazinamine		95	C4H5N3	020744-39-2	4
2	4-Aminopyrimidine		95	C4H5N3	000591-54-8	4
3	1H-1,2,4-Triazole, 1-vinyl-		95	C4H5N3	002764-83-2	4
4	5-Aminopyrimidine		95	C4H5N3	000591-55-9	3
5	Pyridine, 1-oxide		95	C5H5NO	000694-59-7	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
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Misc :
ALS Vial : 9 Sample Multiplier: 1

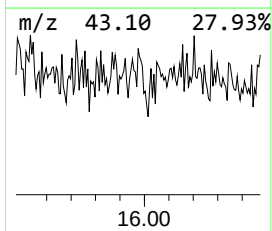
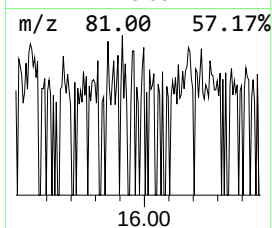
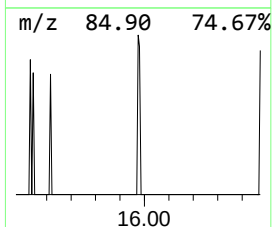
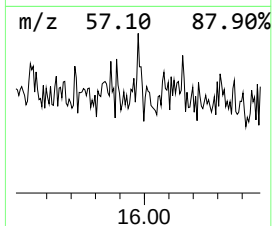
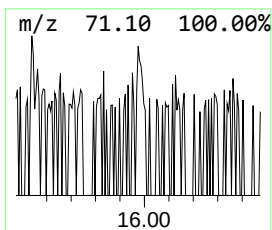
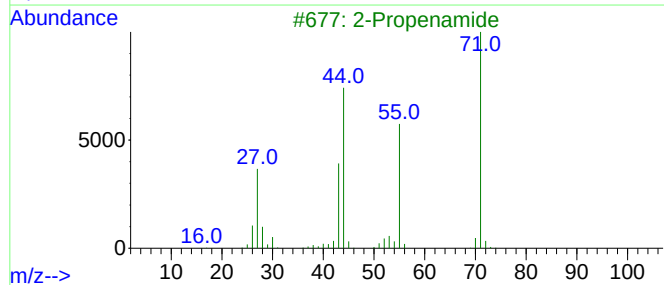
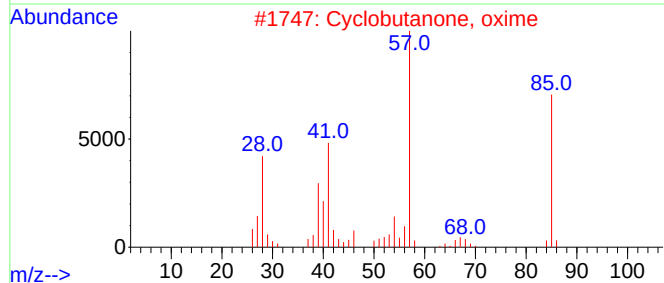
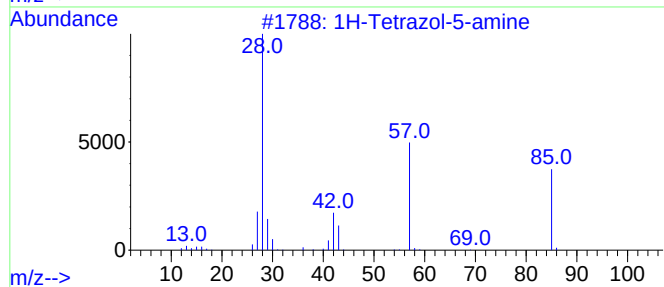
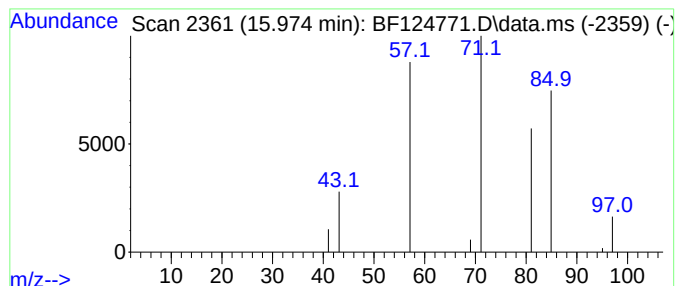
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ClientSampleId :
NJ-CLEAN-9

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 12 unknown15.974 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.974	3.24 ng	2800	Perylene-d12		15.515	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Tetrazol-5-amine		85	CH3N5	004418-61-5	7
2	Cyclobutanone, oxime		85	C4H7NO	002972-05-6	4
3	2-Propenamide		71	C3H5NO	000079-06-1	4
4	Cyanic acid, ethyl ester		71	C3H5NO	000627-48-5	4
5	7-Octen-4-one, 2,6-dimethyl-		154	C10H18O	001879-00-1	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

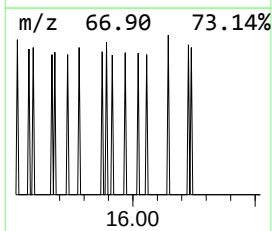
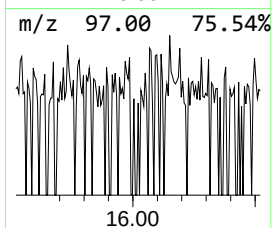
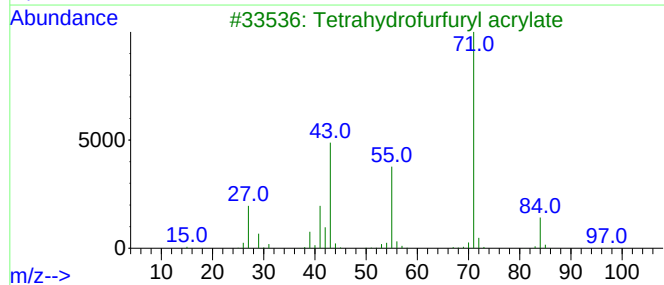
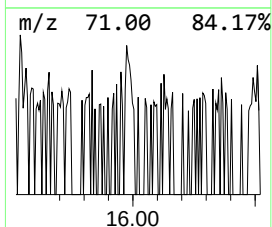
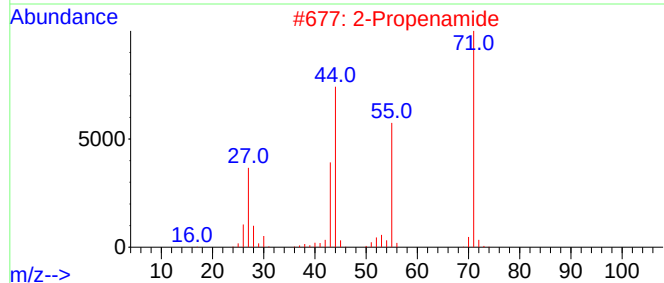
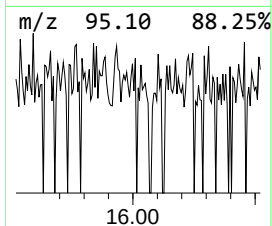
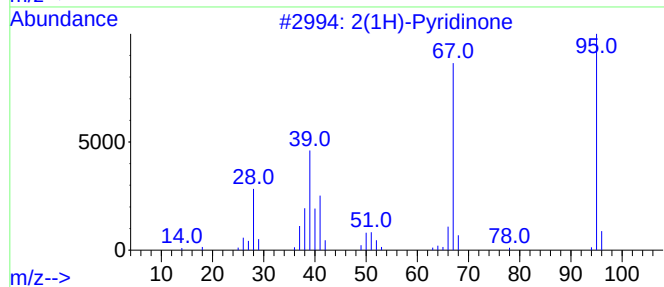
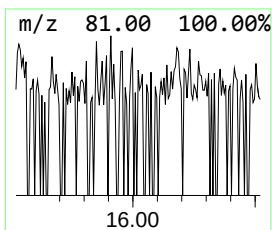
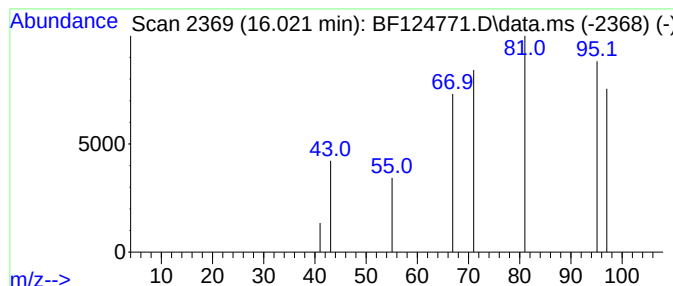
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown16.021 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.021	2.39 ng	2068	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyridinone		95	C5H5NO	000142-08-5	5
2	2-Propenamide		71	C3H5NO	000079-06-1	4
3	Tetrahydrofurfuryl acrylate		156	C8H12O3	002399-48-6	4
4	3-Pyridinol		95	C5H5NO	000109-00-2	3
5	1H-Pyrrole-2,5-dione		97	C4H3NO2	000541-59-3	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

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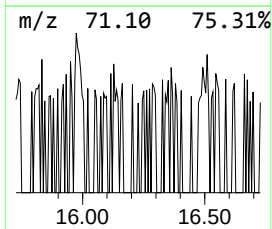
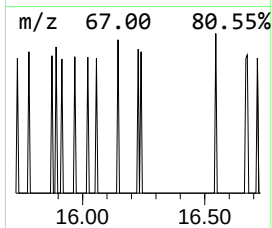
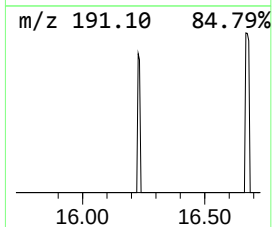
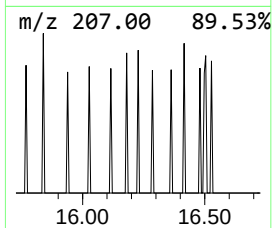
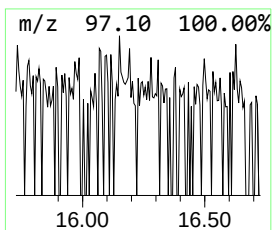
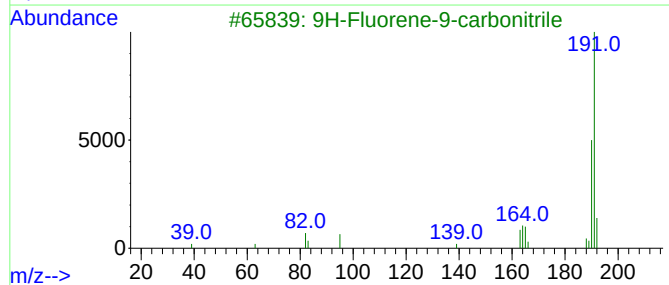
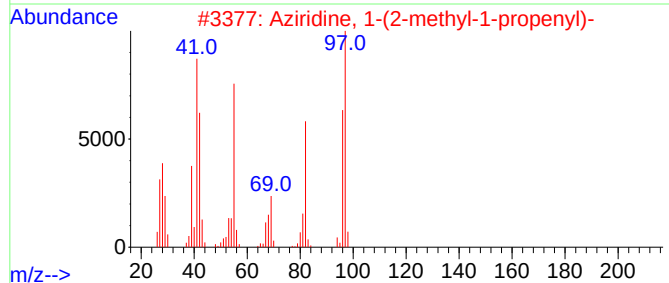
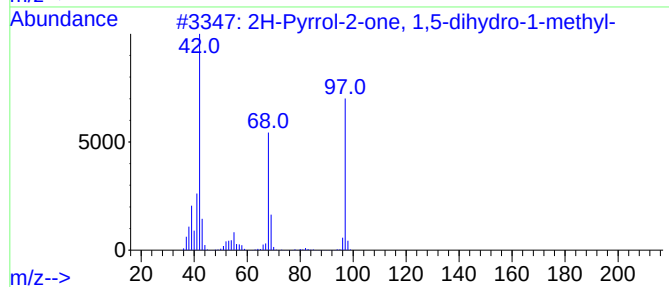
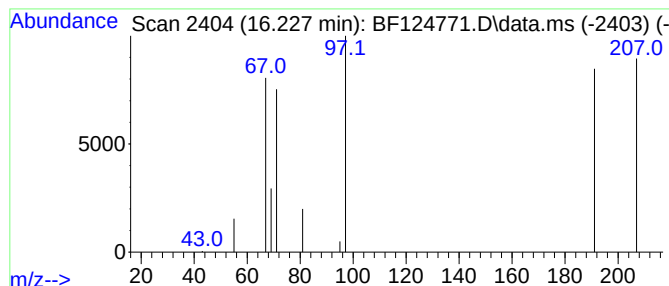
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown16.227 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.227	2.31 ng	1994	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-Pyrrol-2-one, 1,5-dihydro-1-m...	97	C5H7NO	013950-21-5	7
2			Aziridine, 1-(2-methyl-1-propenyl)-	97	C6H11N	080839-93-6	4
3			9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	4
4			5-Amino-1,3,6-trimethyl-1,3-dihy...	191	C10H13N3O	073778-94-6	4
5			4(1H)-Pteridinone, 2-amino-6,7-d...	191	C8H9N5O	000611-55-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

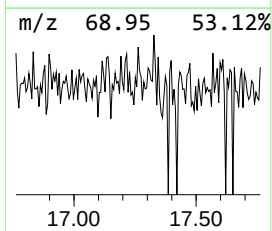
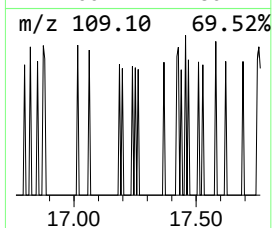
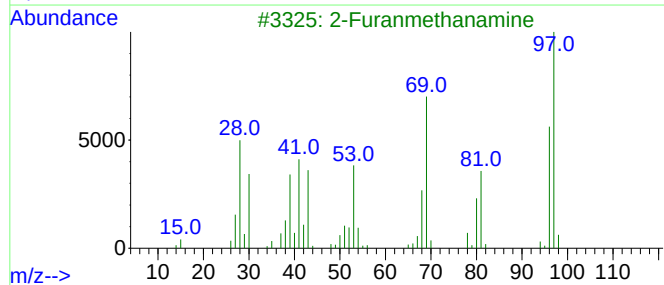
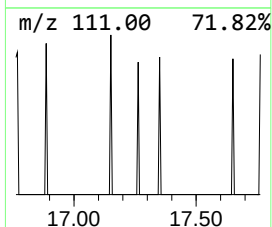
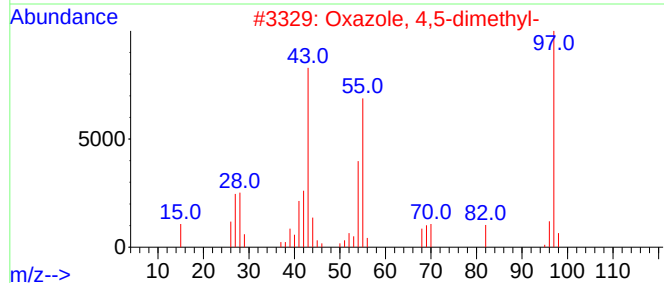
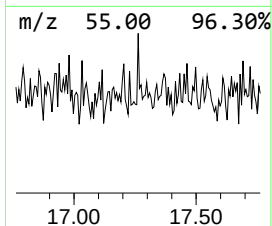
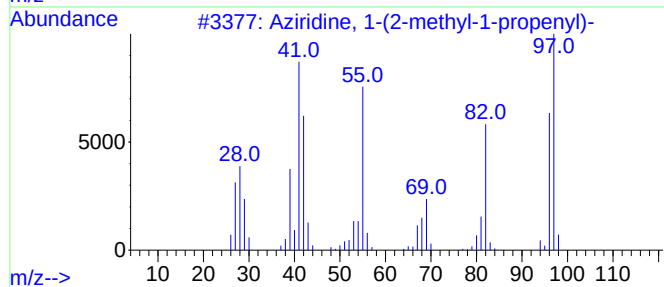
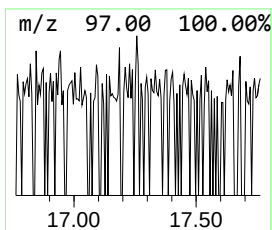
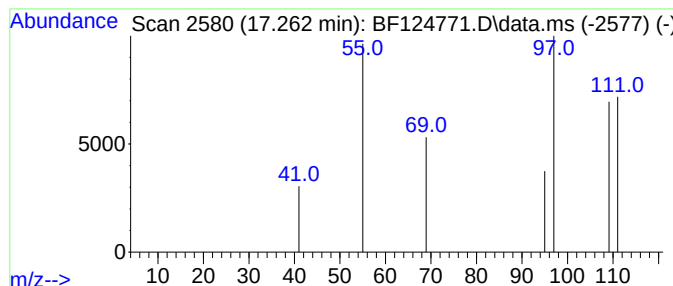
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 unknown17.262 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.262	2.46 ng	2125	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aziridine, 1-(2-methyl-1-propenyl)-	97	C6H11N	080839-93-6	4
2			Oxazole, 4,5-dimethyl-	97	C5H7NO	020662-83-3	4
3			2-Furanmethanamine	97	C5H7NO	000617-89-0	4
4			2,5-Dimethyl-1-pyrroline	97	C6H11N	000822-64-0	4
5			2(1H)-Pyridinone, 3,4-dihydro-	97	C5H7NO	057147-25-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

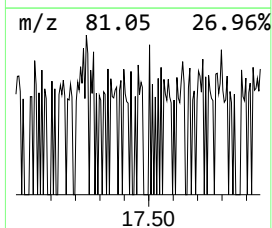
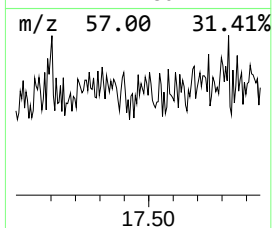
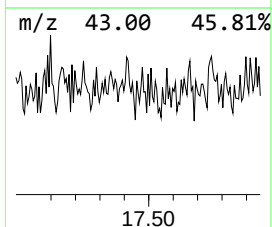
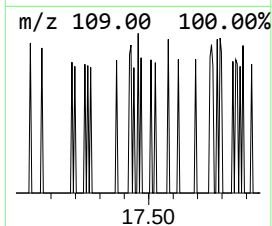
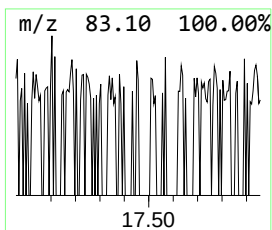
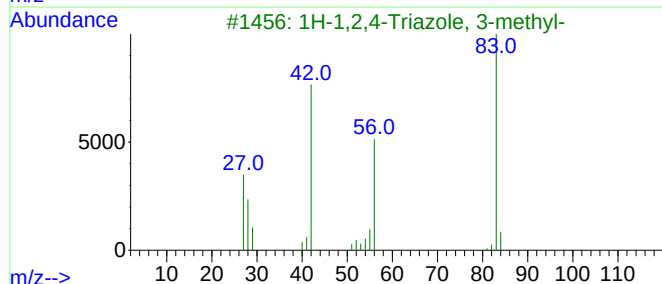
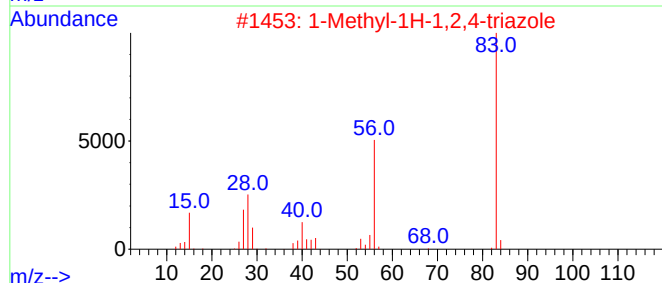
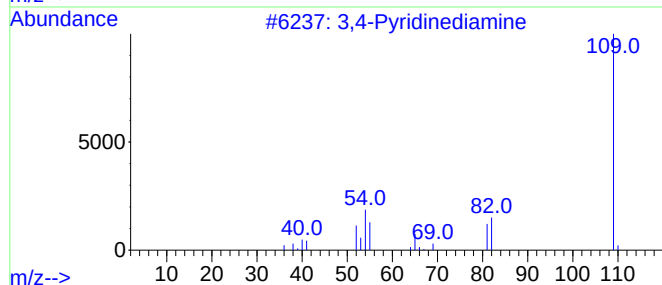
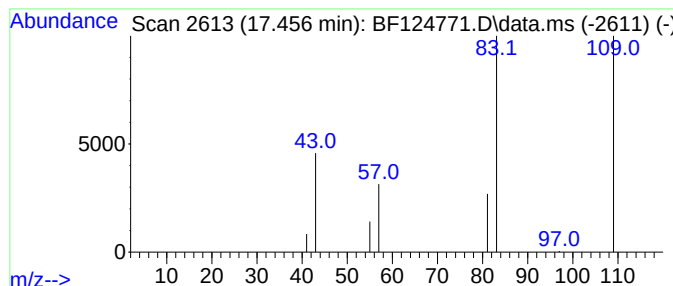
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown17.456 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.456	3.01 ng	2605	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3,4-Pyridinediamine	109	C5H7N3	000054-96-6	5
2		1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	4
3		1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	4
4		4H-1,2,4-Triazole, 4-methyl-	83	C3H5N3	010570-40-8	4
5		1H-Imidazol-2-amine	83	C3H5N3	007720-39-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

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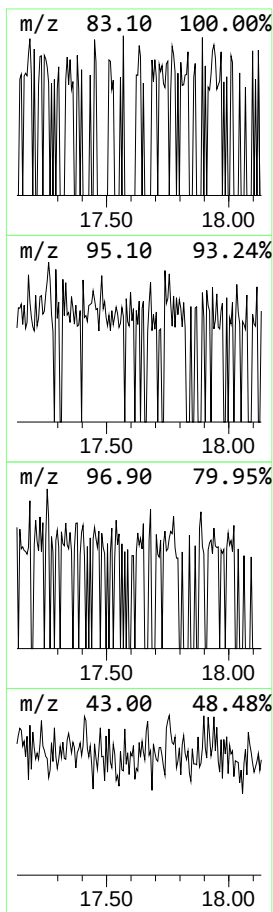
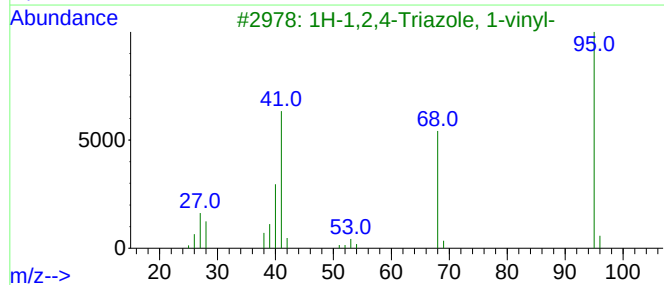
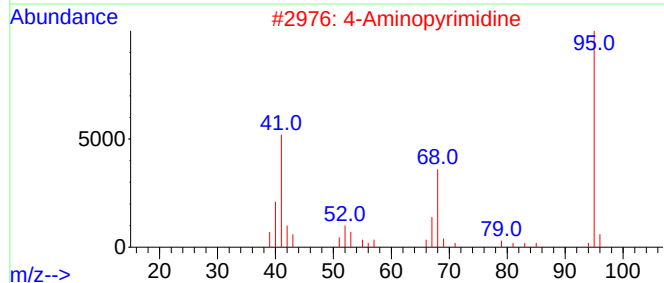
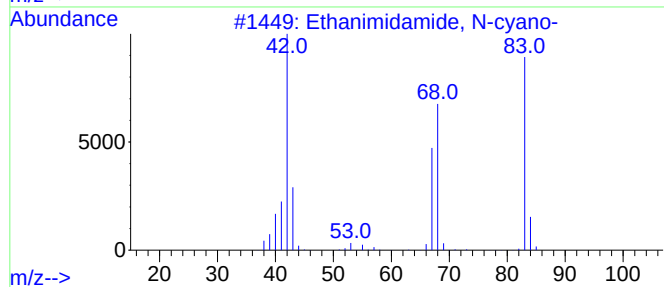
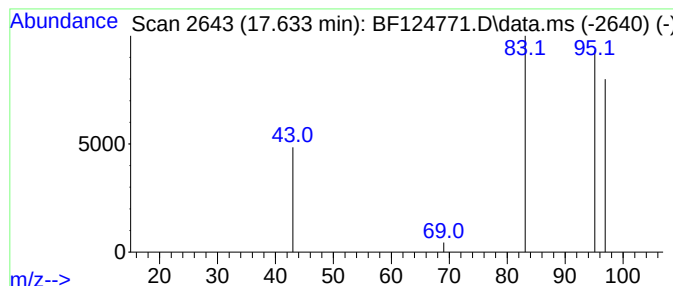
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown17.633 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.633	2.22 ng	1919	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanimidamide, N-cyano-	83	C3H5N3	056563-07-6	4
2			4-Aminopyrimidine	95	C4H5N3	000591-54-8	4
3			1H-1,2,4-Triazole, 1-vinyl-	95	C4H5N3	002764-83-2	4
4			2-Pyrimidinamine	95	C4H5N3	000109-12-6	3
5			3-Pyridinol	95	C5H5NO	000109-00-2	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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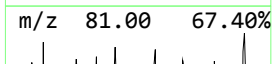
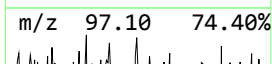
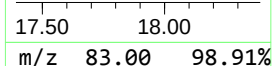
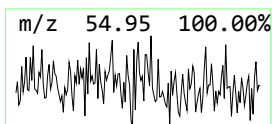
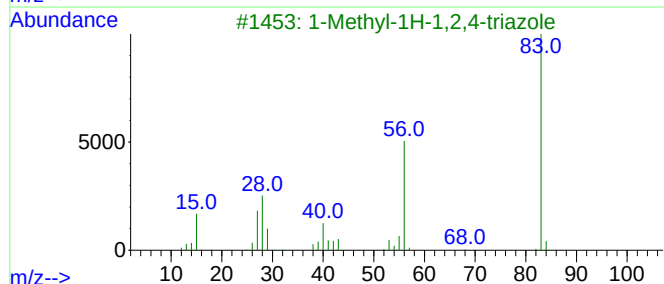
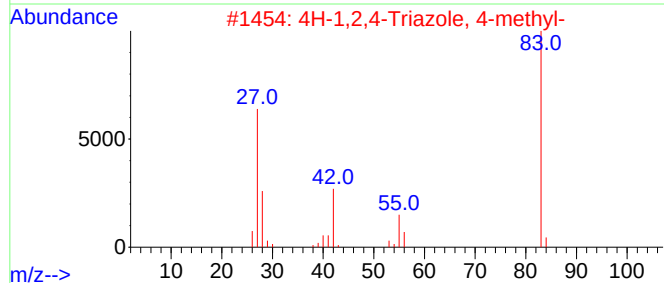
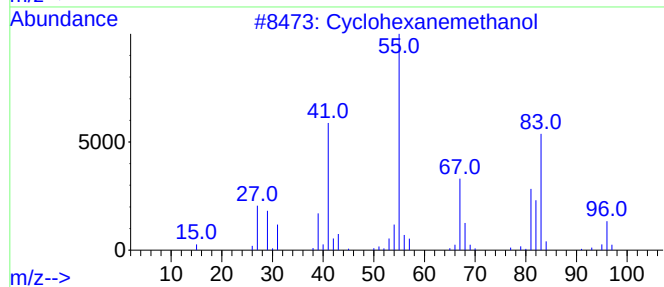
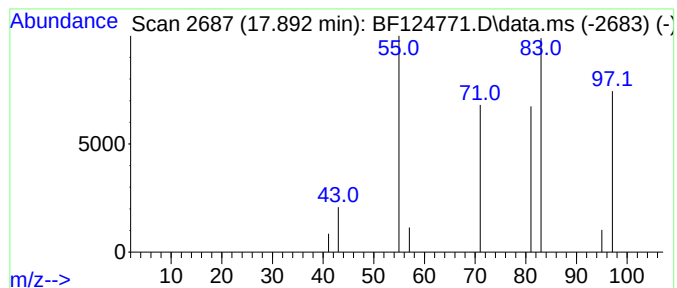
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 unknown17.892 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.892	2.77 ng	2394	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethanol	114	C7H14O	000100-49-2	4
2			4H-1,2,4-Triazole, 4-methyl-	83	C3H5N3	010570-40-8	3
3			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	3
4			3-Aminopyrazole	83	C3H5N3	001820-80-0	3
5			1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

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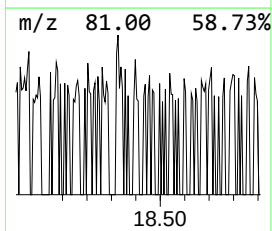
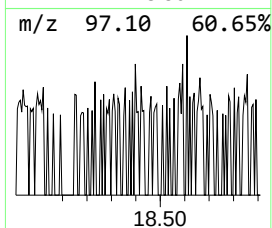
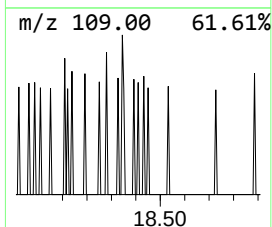
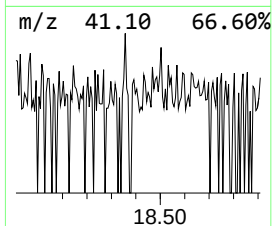
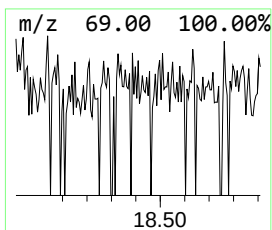
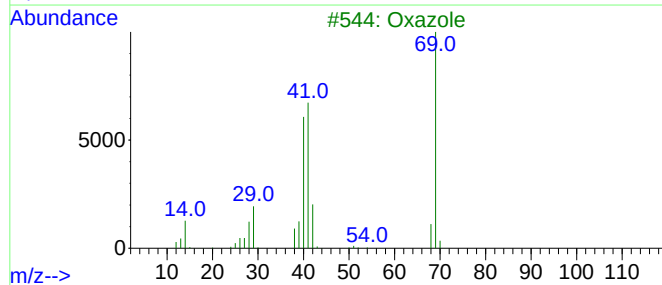
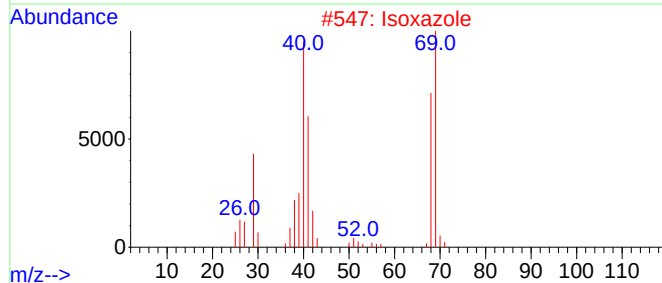
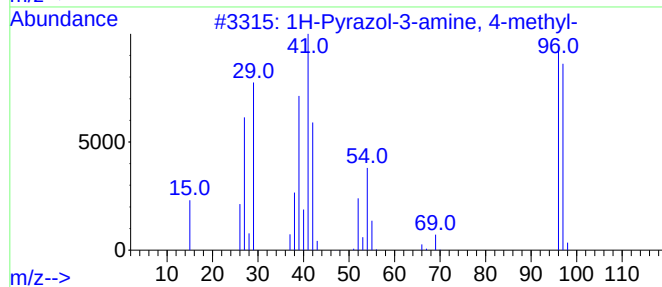
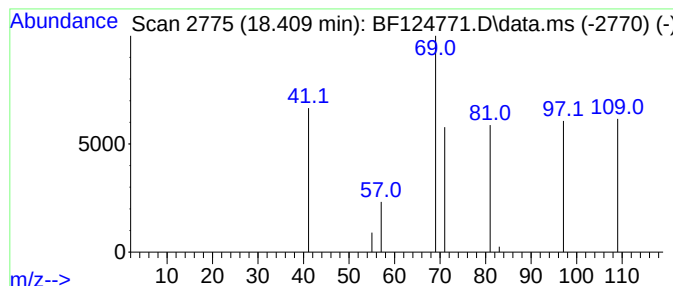
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 unknown18.409 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.409	3.36 ng	2906	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Pyrazol-3-amine, 4-methyl-	97	C4H7N3	064781-79-9	4
2		Isoxazole	69	C3H3NO	000288-14-2	4
3		Oxazole	69	C3H3NO	000288-42-6	4
4		Oxazole, 2,4-dimethyl-	97	C5H7NO	007208-05-1	3
5		4H-1,2,4-Triazole, 4-ethyl-	97	C4H7N3	043183-55-7	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

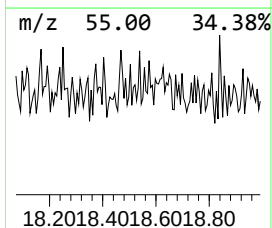
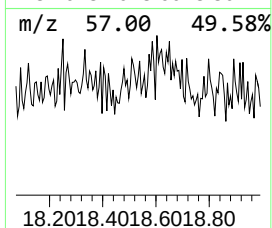
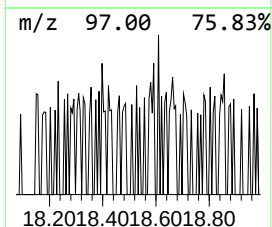
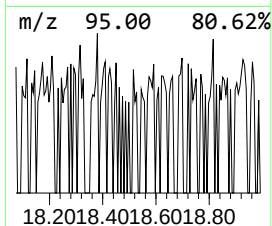
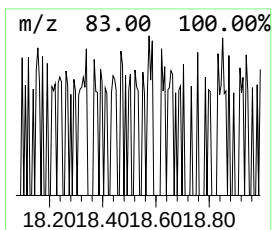
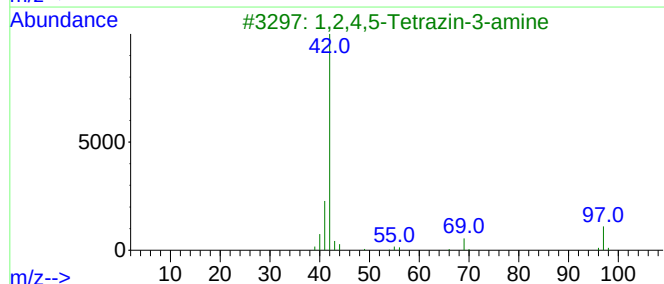
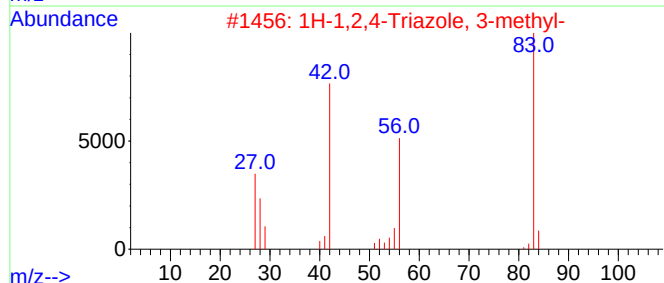
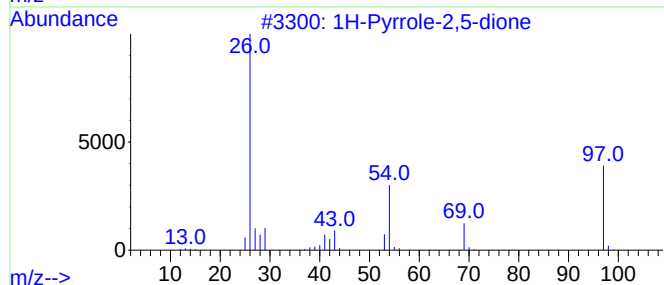
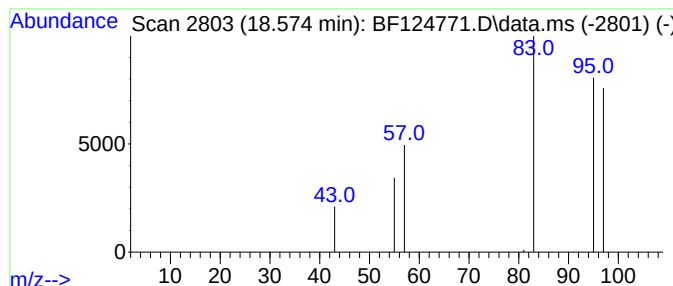
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown18.574 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.574	3.41 ng	2948	Perylene-d12	15.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1H-Pyrrole-2,5-dione	97	C4H3NO2	000541-59-3	3
2		1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	3
3		1,2,4,5-Tetrazin-3-amine	97	C2H3N5	079329-74-1	3
4		Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	3
5		2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072621\
Data File : BF124771.D
Acq On : 26 Jul 2021 18:38
Operator : JU/CG
Sample : M3117-09
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-9

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.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
Butane, 2-metho...	2.152	7.8	ng	11394	1	6.875	29352	20.0
unknown2.493	2.493	4.1	ng	6077	1	6.875	29352	20.0
Ethanol, 2-(2-b...	8.057	10.5	ng	20322	2	8.157	38776	20.0
unknown13.886	13.886	3.9	ng	5752	5	14.039	29469	20.0
unknown14.498	14.498	3.0	ng	4468	5	14.039	29469	20.0
unknown14.810	14.810	3.5	ng	3036	6	15.515	17299	20.0
unknown15.151	15.151	3.8	ng	3322	6	15.515	17299	20.0
unknown15.180	15.180	2.4	ng	2073	6	15.515	17299	20.0
unknown15.386	15.386	2.2	ng	1941	6	15.515	17299	20.0
unknown15.668	15.668	3.3	ng	2842	6	15.515	17299	20.0
unknown15.851	15.851	2.8	ng	2382	6	15.515	17299	20.0
unknown15.974	15.974	3.2	ng	2800	6	15.515	17299	20.0
unknown16.021	16.021	2.4	ng	2068	6	15.515	17299	20.0
unknown16.227	16.227	2.3	ng	1994	6	15.515	17299	20.0
unknown17.262	17.262	2.5	ng	2125	6	15.515	17299	20.0
unknown17.456	17.456	3.0	ng	2605	6	15.515	17299	20.0
unknown17.633	17.633	2.2	ng	1919	6	15.515	17299	20.0
unknown17.892	17.892	2.8	ng	2394	6	15.515	17299	20.0
unknown18.409	18.409	3.4	ng	2906	6	15.515	17299	20.0
unknown18.574	18.574	3.4	ng	2948	6	15.515	17299	20.0