

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
 Data File : BF124754.D
 Acq On : 24 Jul 2021 18:45
 Operator : JU/CG
 Sample : M3117-03 2X
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 NJ-CLEAN-3

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: BF124754.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.134	5	8	11	rBB	4607	4643	7.05%	0.761%
2	5.075	506	508	511	rBB	1667	1588	2.41%	0.260%
3	5.481	573	577	580	rBB	68434	59467	90.32%	9.753%
4	6.493	745	749	752	rBB	70968	60208	91.45%	9.875%
5	6.869	811	813	816	rBB	48599	40286	61.19%	6.607%
6	7.428	905	908	911	rBB	44024	38582	58.60%	6.328%
7	8.051	1012	1014	1018	rBB	20441	14874	22.59%	2.439%
8	8.157	1028	1032	1035	rBB	64586	49631	75.38%	8.140%
9	9.228	1211	1214	1217	rBV	94620	65839	100.00%	10.798%
10	9.628	1278	1282	1284	rBB	2515	2448	3.72%	0.401%
11	9.910	1327	1330	1333	rBB	61343	44355	67.37%	7.275%
12	10.692	1461	1463	1466	rBB	35193	24718	37.54%	4.054%
13	11.398	1579	1583	1586	rBB	40739	35191	53.45%	5.772%
14	11.916	1669	1671	1672	rBB	2874	2001	3.04%	0.328%
15	12.980	1848	1852	1855	rBB	55057	42890	65.14%	7.034%
16	13.886	2003	2006	2017	rBB3	3479	7945	12.07%	1.303%
17	13.974	2019	2021	2023	rBV	1109	1103	1.68%	0.181%
18	14.033	2028	2031	2034	rBV	33827	29043	44.11%	4.763%
19	14.127	2043	2047	2048	rBV	1103	1225	1.86%	0.201%
20	14.192	2055	2058	2063	rBV	1996	3243	4.93%	0.532%
21	14.292	2073	2075	2079	rVB2	687	930	1.41%	0.153%
22	14.339	2079	2083	2086	rVB2	921	1129	1.71%	0.185%
23	14.433	2094	2099	2100	rBV4	780	1026	1.56%	0.168%
24	14.498	2108	2110	2113	rVB2	2386	2118	3.22%	0.347%
25	14.727	2148	2149	2153	rBV3	1283	1320	2.00%	0.216%
26	14.804	2160	2162	2167	rBV2	2468	3152	4.79%	0.517%
27	14.886	2173	2176	2179	rBV	1234	1478	2.24%	0.242%
28	15.021	2196	2199	2202	rBV2	1271	1058	1.61%	0.174%
29	15.074	2205	2208	2211	rBV2	1185	1102	1.67%	0.181%
30	15.151	2215	2221	2224	rVB3	2879	3450	5.24%	0.566%
31	15.186	2224	2227	2229	rBV2	1329	1282	1.95%	0.210%
32	15.357	2255	2256	2261	rVB	1025	1275	1.94%	0.209%
33	15.510	2277	2282	2285	rBV	18137	20824	31.63%	3.415%
34	15.604	2297	2298	2303	rVB	1316	1417	2.15%	0.232%
35	15.651	2303	2306	2308	rBV2	1312	1565	2.38%	0.257%
36	15.751	2322	2323	2325	rVB2	1365	950	1.44%	0.156%

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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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37	15.780	2325	2328	2329	rBV	1048	1054	1.60%	0.173%
38	15.792	2329	2330	2334	rVV	1012	1106	1.68%	0.181%
39	15.968	2358	2360	2361	rBV	2318	1484	2.25%	0.243%
40	15.980	2361	2362	2364	rVV2	2321	1517	2.30%	0.249%
41	16.033	2368	2371	2372	rVB2	1526	1139	1.73%	0.187%
42	16.068	2375	2377	2380	rBV3	834	966	1.47%	0.158%
43	16.245	2405	2407	2410	rVB2	1096	1073	1.63%	0.176%
44	16.492	2444	2449	2451	rBV2	2195	2832	4.30%	0.464%
45	16.533	2453	2456	2459	rBV2	1797	2190	3.33%	0.359%
46	16.627	2469	2472	2476	rBV2	998	1866	2.83%	0.306%
47	16.668	2476	2479	2481	rVB3	1383	1559	2.37%	0.256%
48	16.968	2527	2530	2531	rVB2	1489	1379	2.09%	0.226%
49	16.980	2531	2532	2534	rBV2	1439	928	1.41%	0.152%
50	17.086	2546	2550	2554	rBV2	1682	2622	3.98%	0.430%
51	17.257	2578	2579	2582	rVV2	1255	997	1.51%	0.164%
52	17.315	2585	2589	2590	rVB3	1382	1317	2.00%	0.216%
53	17.568	2630	2632	2635	rBV2	757	965	1.47%	0.158%
54	17.668	2646	2649	2650	rBV2	1375	1577	2.40%	0.259%
55	17.786	2666	2669	2671	rBV	1358	964	1.46%	0.158%
56	17.868	2682	2683	2687	rVB3	894	995	1.51%	0.163%
57	18.027	2705	2710	2713	rVB2	961	1770	2.69%	0.290%
58	18.215	2737	2742	2743	rVB3	1089	1102	1.67%	0.181%
59	18.415	2775	2776	2782	rVB2	917	1206	1.83%	0.198%
60	18.539	2793	2797	2800	rBV2	1150	1763	2.68%	0.289%
61	18.633	2809	2813	2814	rBV	1080	992	1.51%	0.163%
62	18.874	2852	2854	2858	rVB	894	1011	1.54%	0.166%

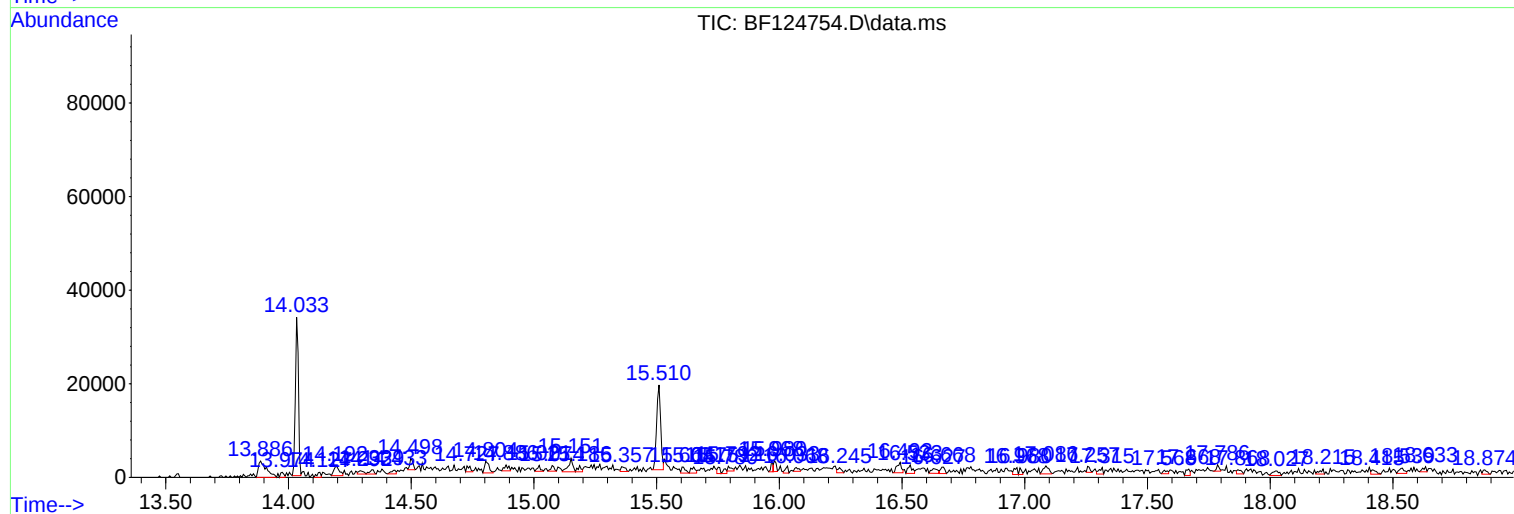
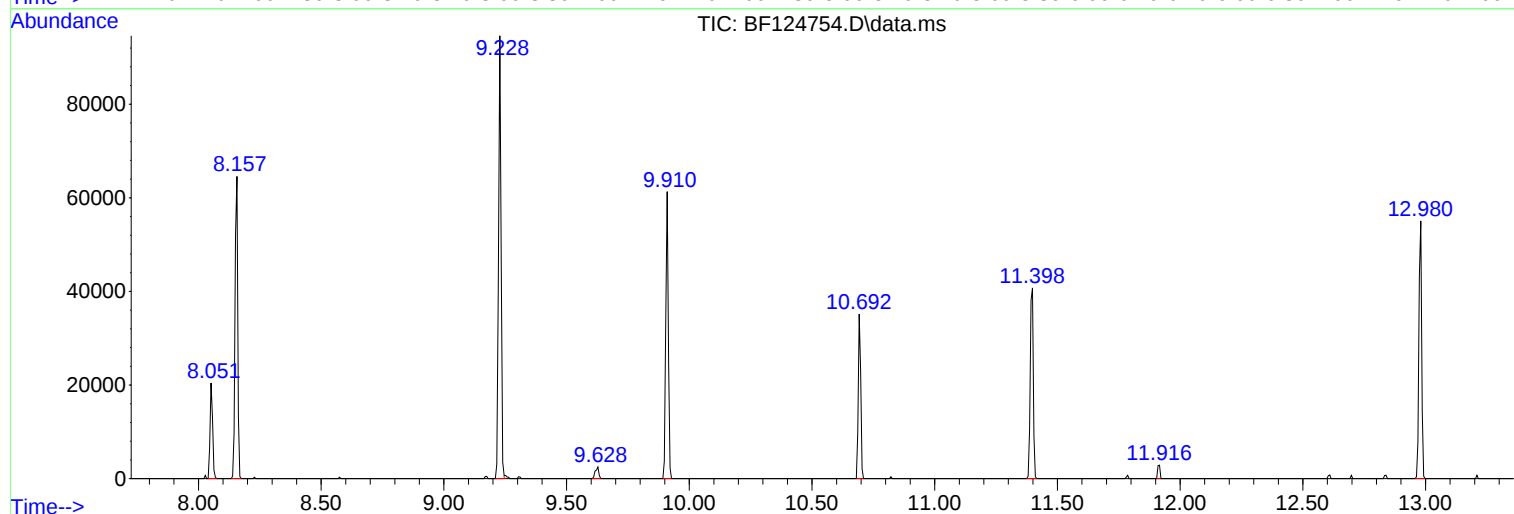
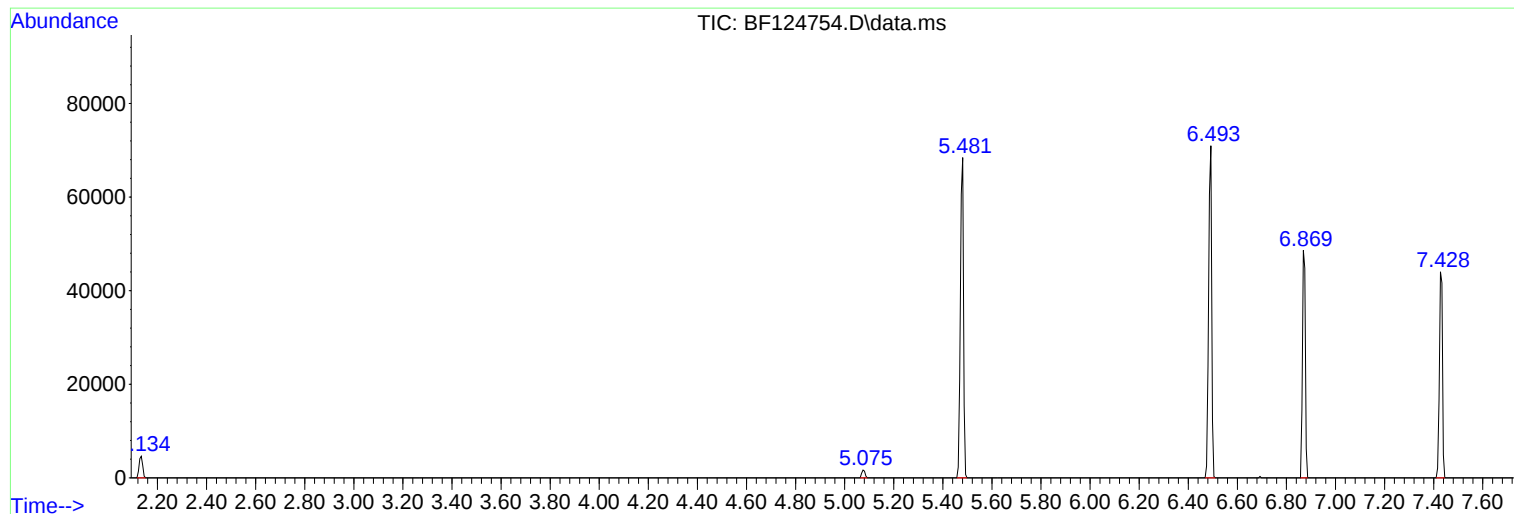
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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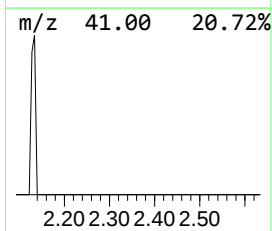
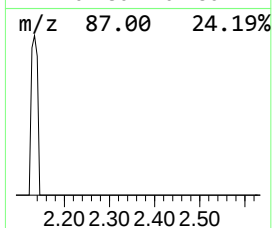
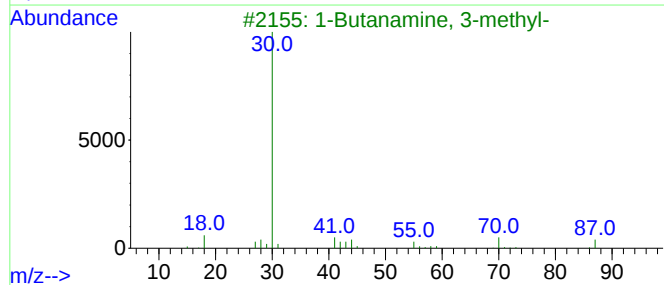
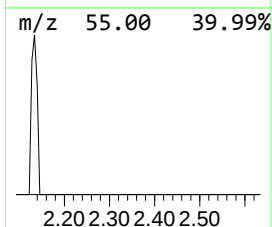
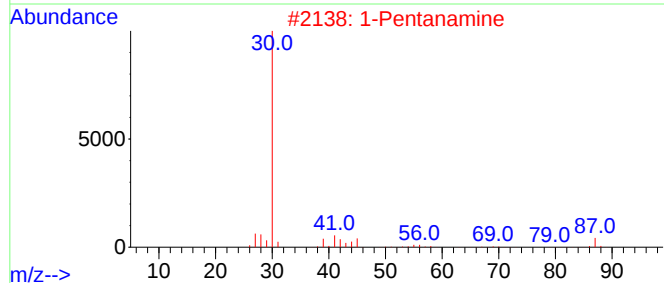
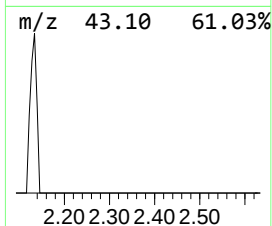
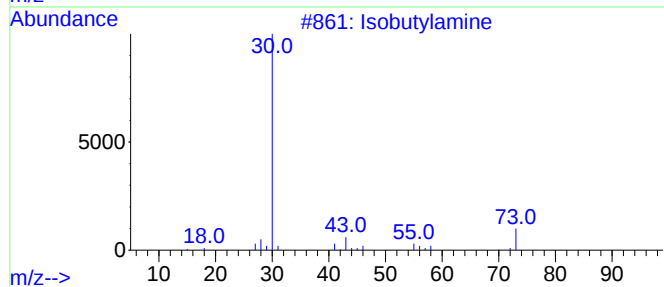
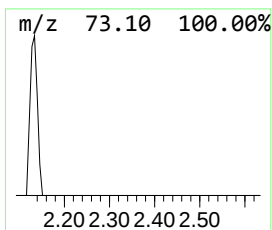
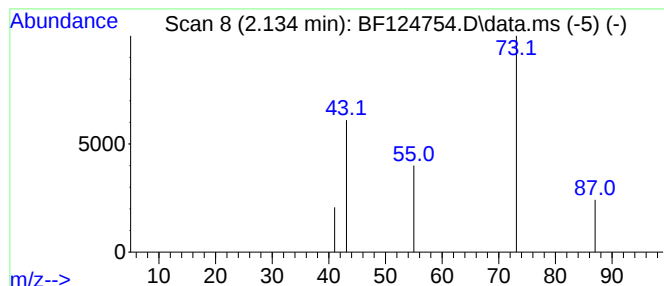
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.134 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.134	2.31 ng	4643	1,4-Dichlorobenzene-d4	6.875

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



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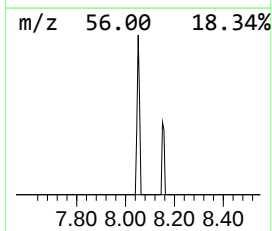
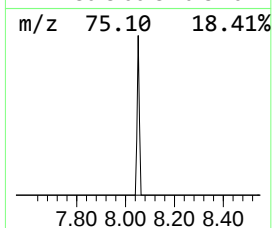
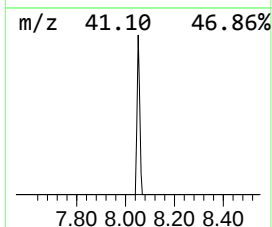
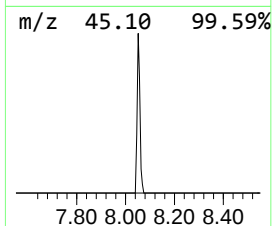
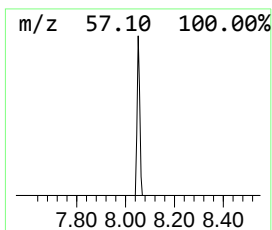
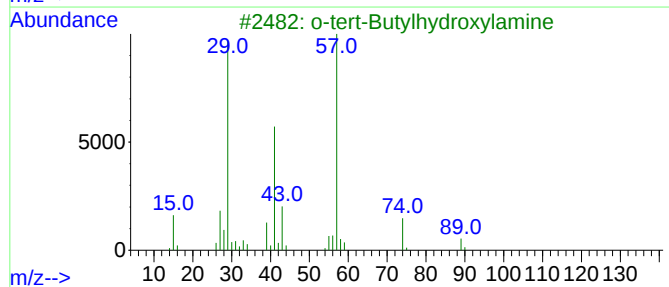
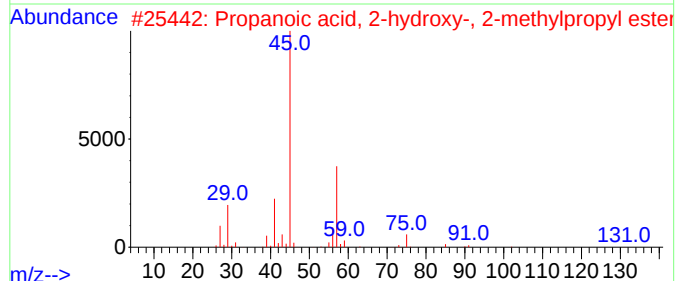
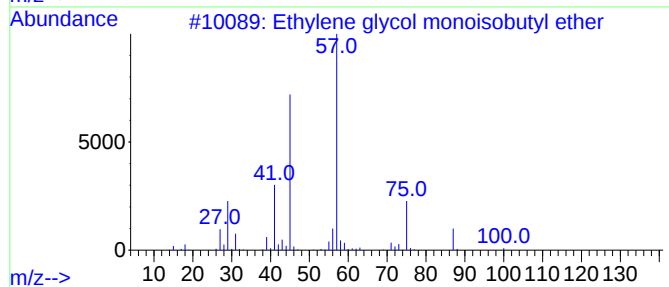
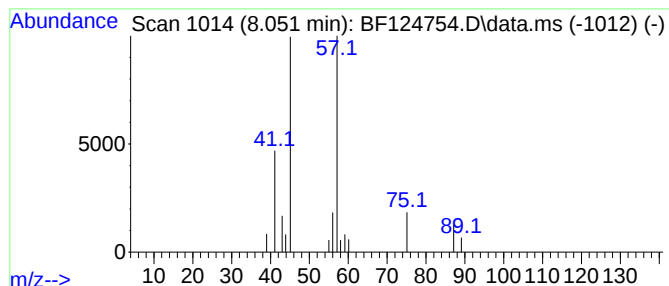
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown8.051 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	5.99 ng	14874	Naphthalene-d8	8.157

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	40
2			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	38
3			o-tert-Butylhydroxylamine	89	C4H11NO	1000322-43-1	9
4			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	9



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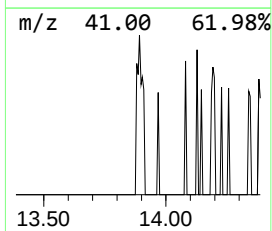
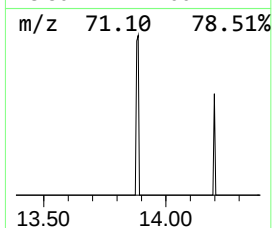
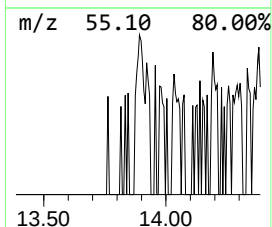
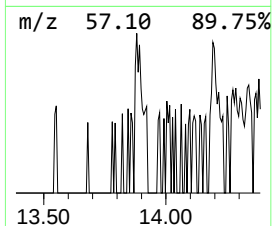
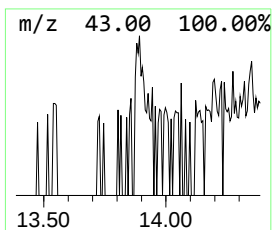
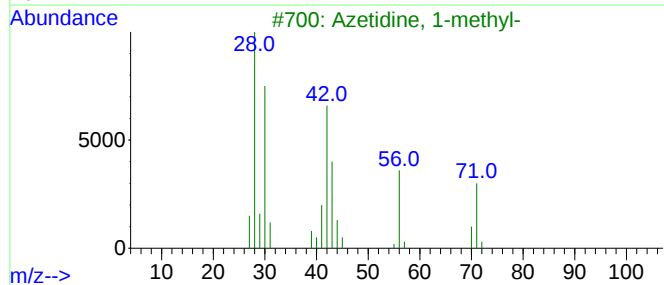
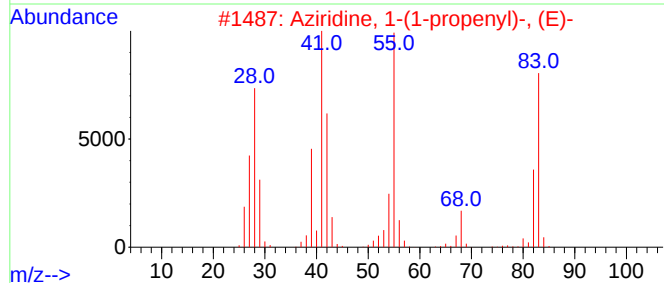
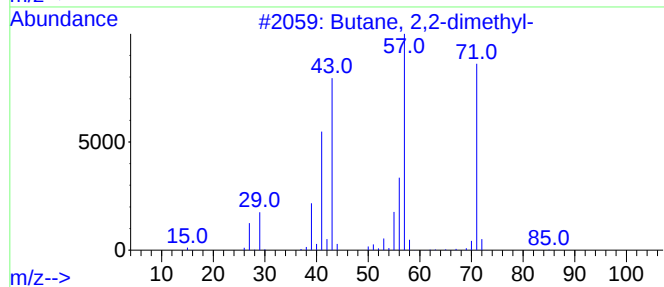
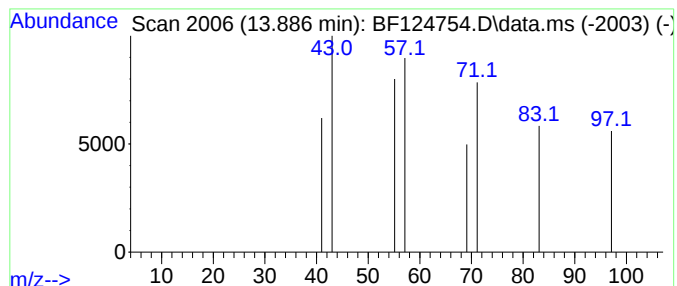
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown13.886 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	5.47 ng	7945	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	9
2			Aziridine, 1-(1-propenyl)-, (E)-	83	C5H9N	080839-91-4	7
3			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	5
4			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	5
5			Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	4



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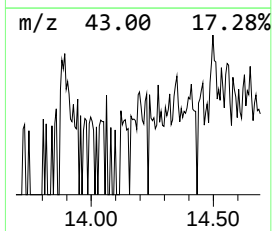
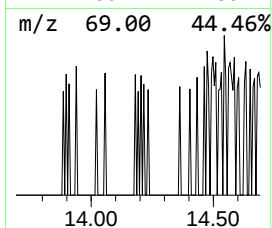
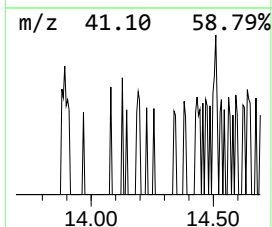
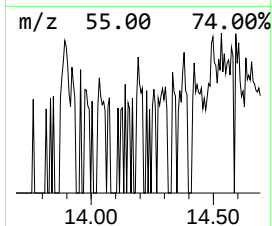
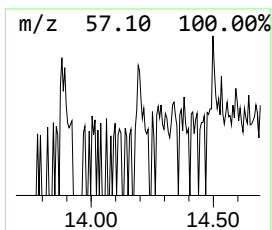
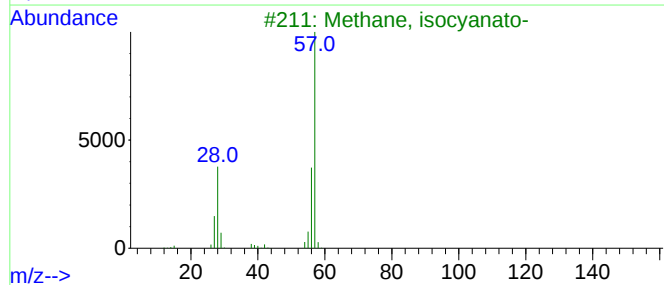
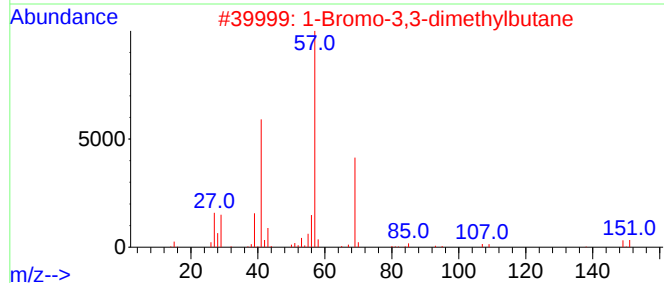
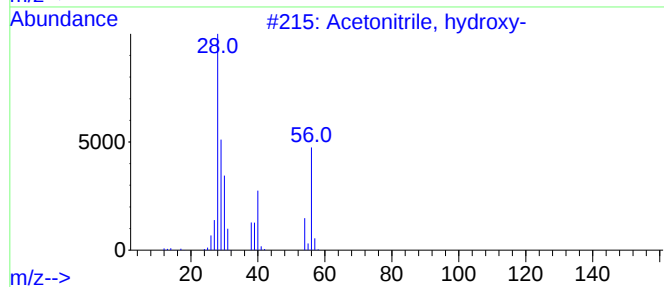
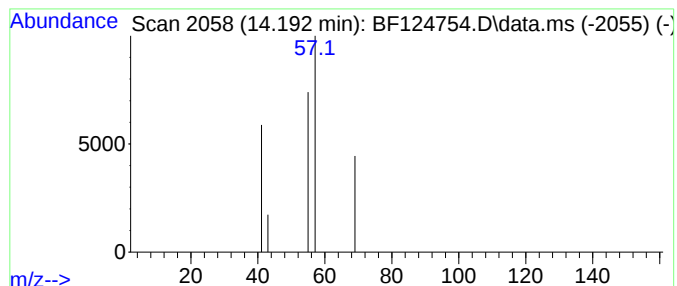
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown14.192 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	2.23 ng	3243	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	3
2			1-Bromo-3,3-dimethylbutane	164	C6H13Br	001647-23-0	2
3			Methane, isocyanato-	57	C2H3NO	000624-83-9	1
4			Carbamic acid, (trifluoromethyl)...	185	C6H10F3NO2	063689-57-6	1
5			Azetidine	57	C3H7N	000503-29-7	1



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-3

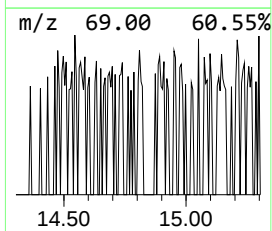
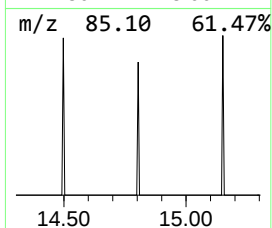
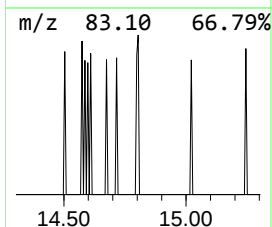
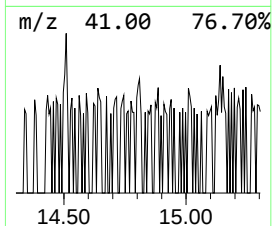
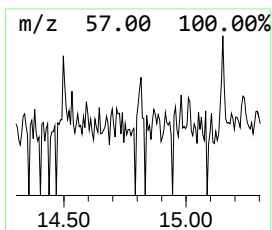
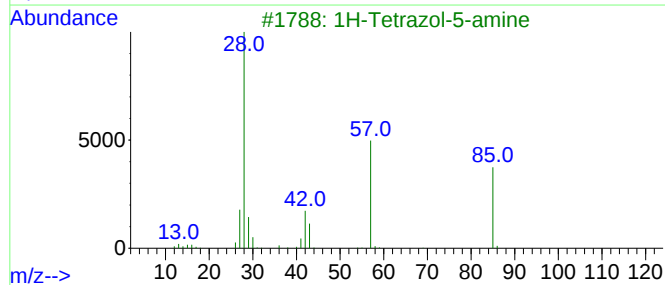
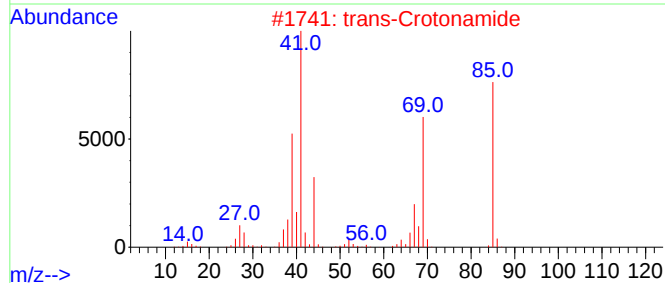
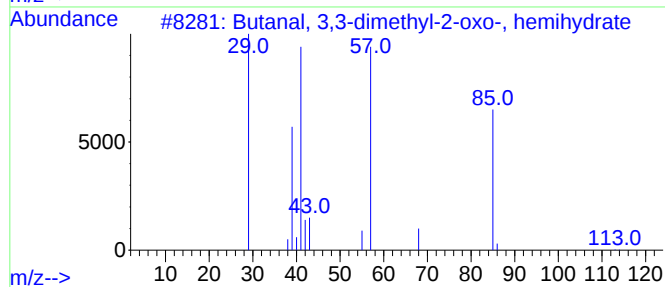
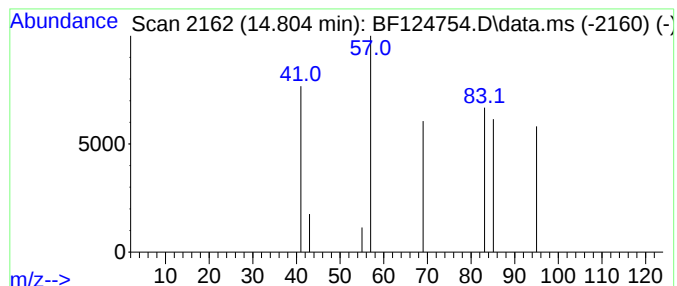
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown14.804 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.804	3.03 ng	3152	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 3,3-dimethyl-2-oxo-, he...	114	C6H10O2	077572-68-0	9
2			trans-Crotonamide	85	C4H7NO	000625-37-6	7
3			1H-Tetrazol-5-amine	85	CH3N5	004418-61-5	7
4			5H-Tetrazol-5-amine	85	CH3N5	1000273-02-0	5
5			Methacrylamide	85	C4H7NO	000079-39-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124754.D
Acq On : 24 Jul 2021 18:45
Operator : JU/CG
Sample : M3117-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

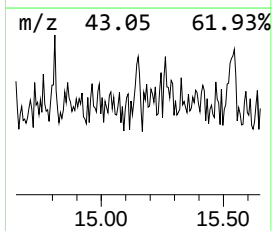
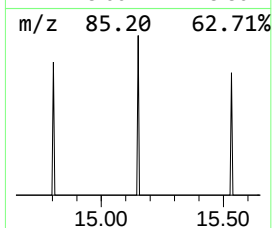
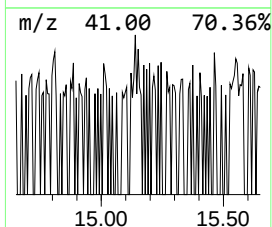
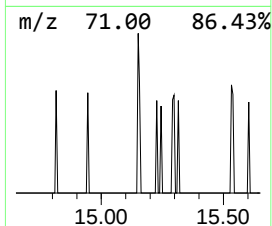
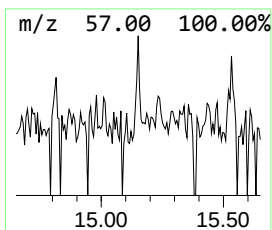
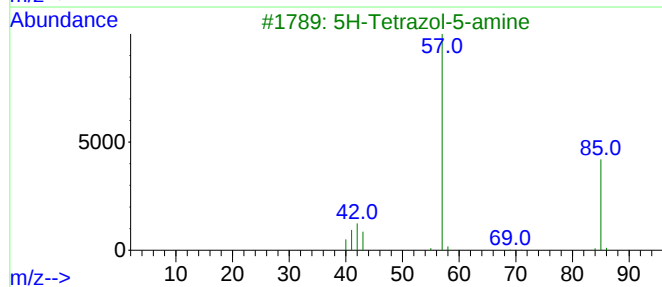
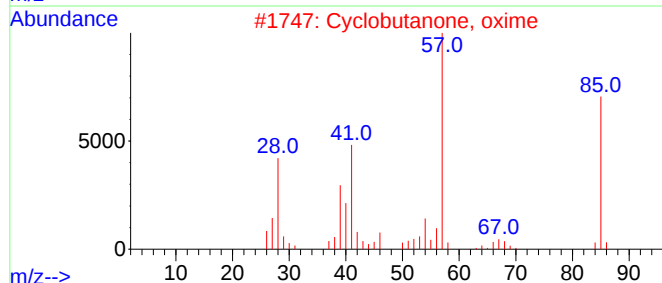
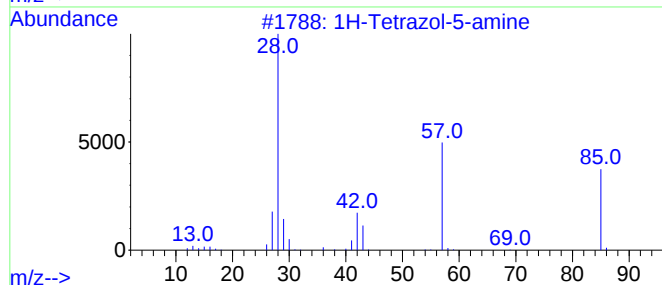
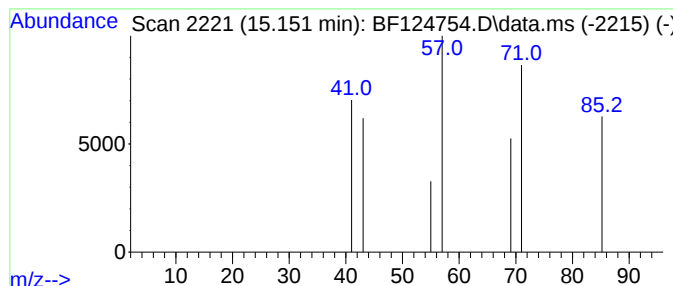
Instrument :
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ClientSampleId :
NJ-CLEAN-3

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 6 unknown15.151 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.151	3.31 ng	3450	Perylene-d12		15.510	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1H-Tetrazol-5-amine		85	CH3N5	004418-61-5	4
2	Cyclobutanone, oxime		85	C4H7NO	002972-05-6	4
3	5H-Tetrazol-5-amine		85	CH3N5	1000273-02-0	4
4	2-Propenamide		71	C3H5NO	000079-06-1	4
5	Octane, 4-methyl-		128	C9H20	002216-34-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124754.D
Acq On : 24 Jul 2021 18:45
Operator : JU/CG
Sample : M3117-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NJ-CLEAN-3

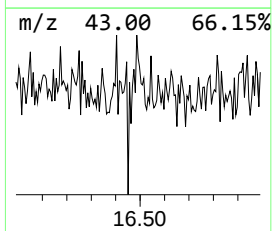
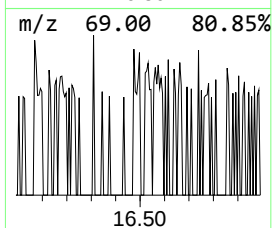
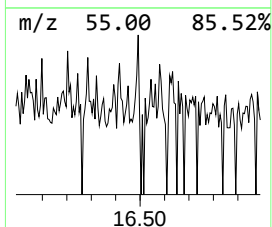
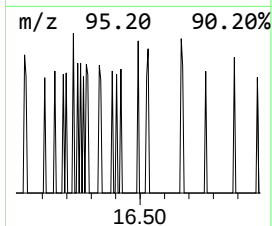
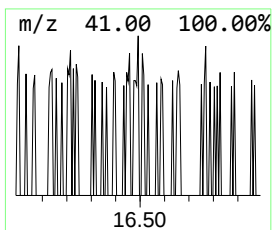
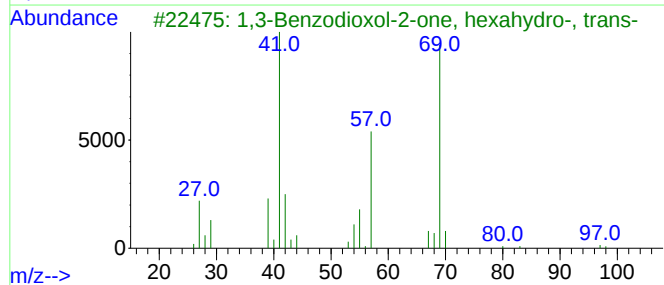
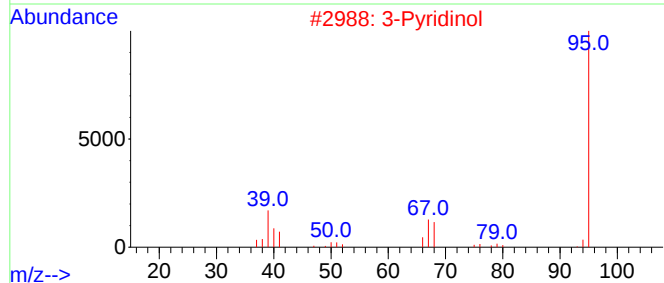
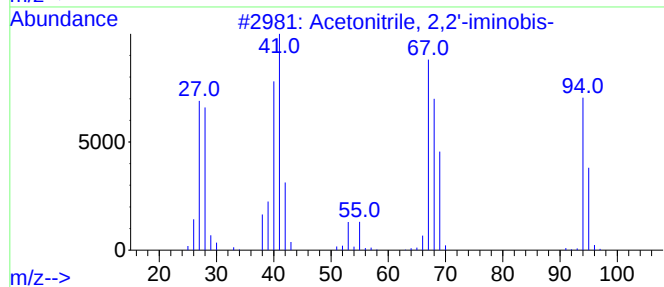
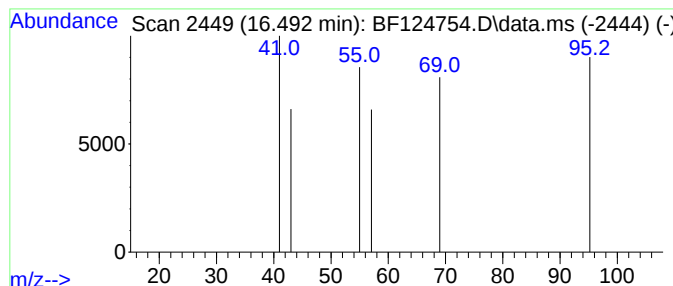
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.492 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.492	2.72 ng	2832	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	4
2			3-Pyridinol	95	C5H5NO	000109-00-2	2
3			1,3-Benzodioxol-2-one, hexahydro...	142	C7H10O3	020192-66-9	2
4			4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
5			Hexanal, 5,5-dimethyl-	128	C8H16O	055320-58-6	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124754.D
Acq On : 24 Jul 2021 18:45
Operator : JU/CG
Sample : M3117-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

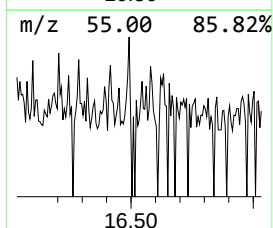
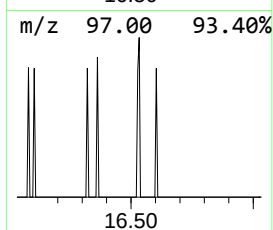
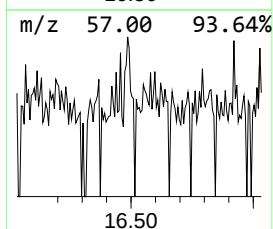
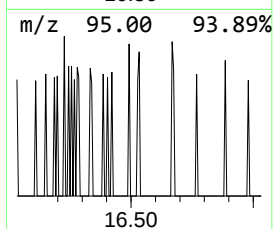
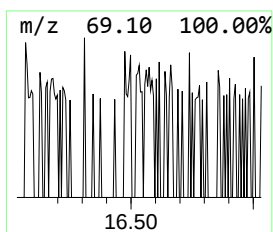
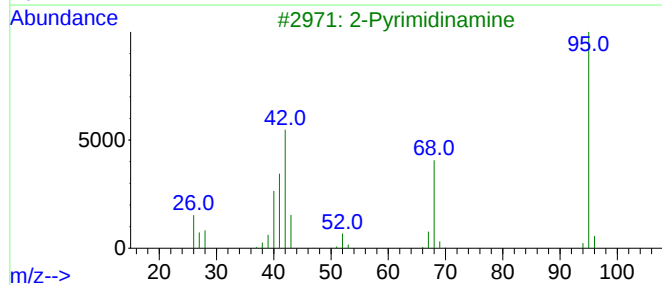
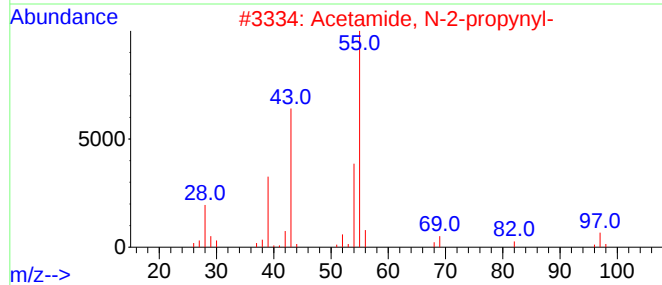
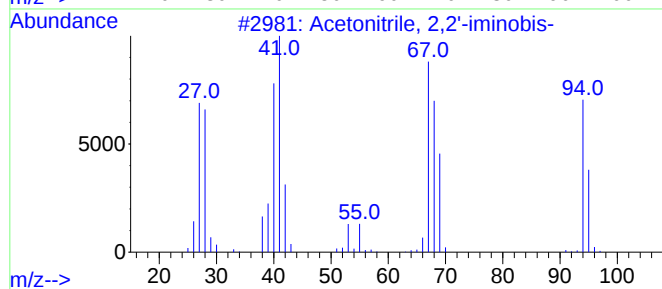
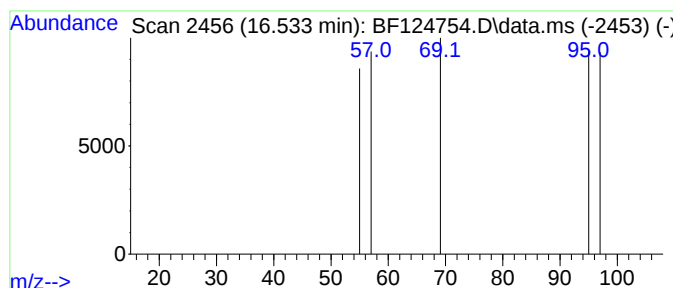
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.533 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.533	2.10 ng	2190	Perylene-d12	15.510	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, 2,2'-iminobis-	95	C4H5N3	000628-87-5	4
2	Acetamide, N-2-propynyl-	97	C5H7NO	065881-41-6	3
3	2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
4	5-Aminopyrimidine	95	C4H5N3	000591-55-9	2
5	2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124754.D
Acq On : 24 Jul 2021 18:45
Operator : JU/CG
Sample : M3117-03 2X
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NJ-CLEAN-3

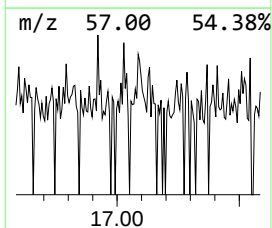
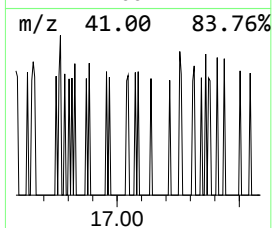
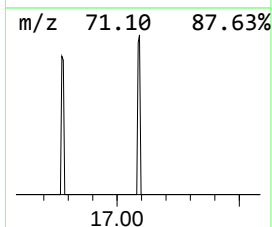
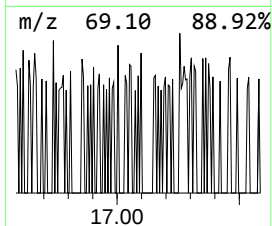
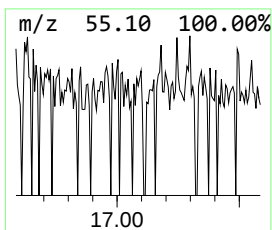
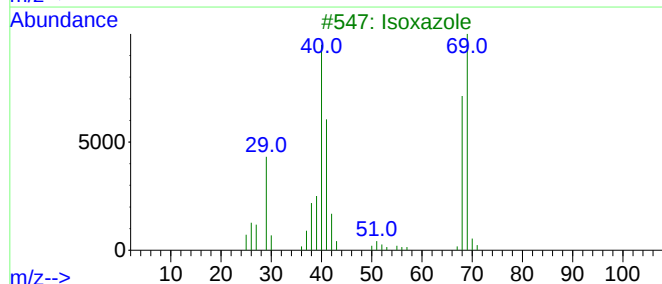
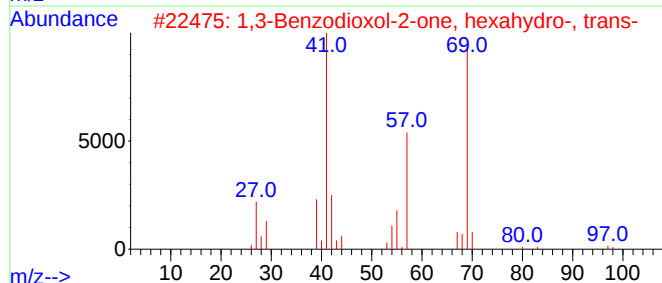
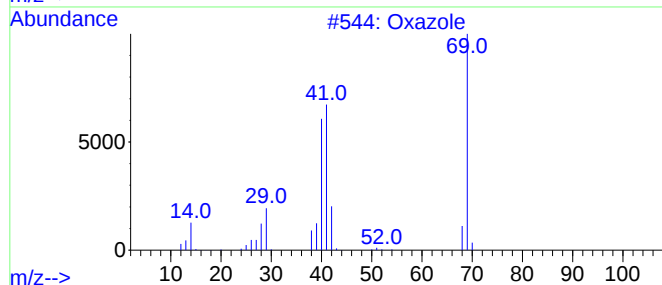
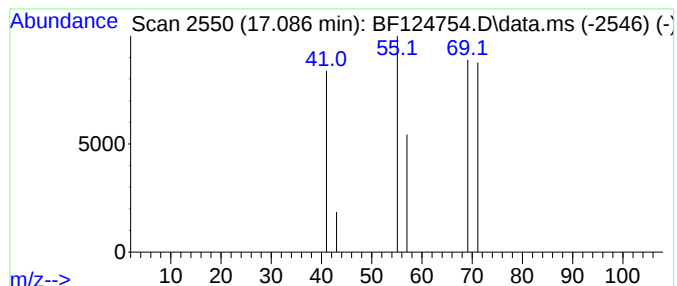
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown17.086 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.086	2.52 ng	2622	Perylene-d12	15.510

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxazole	69	C3H3NO	000288-42-6	4
2			1,3-Benzodioxol-2-one, hexahydro...	142	C7H10O3	020192-66-9	2
3			Isoxazole	69	C3H3NO	000288-14-2	2
4			2-Propenamide	71	C3H5NO	000079-06-1	2
5			2-Propynenitrile, 3-fluoro-	69	C3FN	032038-83-8	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072421\
Data File : BF124754.D
Acq On : 24 Jul 2021 18:45
Operator : JU/CG
Sample : M3117-03 2X
Misc :
ALS Vial : 19 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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
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unknown8.051	8.051	6.0	ng	14874	2	8.157	49631	20.0
unknown13.886	13.886	5.5	ng	7945	5	14.033	29043	20.0
unknown14.192	14.192	2.2	ng	3243	5	14.033	29043	20.0
unknown14.804	14.804	3.0	ng	3152	6	15.510	20824	20.0
unknown15.151	15.151	3.3	ng	3450	6	15.510	20824	20.0
unknown16.492	16.492	2.7	ng	2832	6	15.510	20824	20.0
unknown16.533	16.533	2.1	ng	2190	6	15.510	20824	20.0
unknown17.086	17.086	2.5	ng	2622	6	15.510	20824	20.0