

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
 Data File : BF124813.D
 Acq On : 28 Jul 2021 1:58
 Operator : JU/CG
 Sample : M3194-01 10X
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JC-03-072621

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: BF124813.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.475	573	576	579	rBB	8890	7412	13.46%	1.678%
2	6.486	745	748	751	rBB	12362	8469	15.38%	1.918%
3	6.869	810	813	816	rBB	47433	34457	62.59%	7.802%
4	7.428	905	908	910	rBB	8611	6175	11.22%	1.398%
5	8.151	1028	1031	1034	rBV	62807	47323	85.95%	10.716%
6	9.227	1211	1214	1217	rBB	13283	10888	19.78%	2.465%
7	9.910	1327	1330	1333	rBV	73994	55056	100.00%	12.467%
8	10.692	1461	1463	1466	rBB	6191	4275	7.76%	0.968%
9	11.398	1579	1583	1586	rBV	60482	51689	93.88%	11.704%
10	12.486	1766	1768	1770	rVB	2242	1654	3.00%	0.375%
11	12.851	1826	1830	1832	rBB	816	974	1.77%	0.221%
12	12.974	1849	1851	1854	rBB	11443	8794	15.97%	1.991%
13	13.204	1888	1890	1893	rBV2	1296	1037	1.88%	0.235%
14	13.292	1904	1905	1909	rBV2	1011	995	1.81%	0.225%
15	13.339	1909	1913	1915	rVV	1126	1212	2.20%	0.274%
16	13.421	1922	1927	1930	rBV	1385	2476	4.50%	0.561%
17	13.545	1944	1948	1949	rBV	1485	1340	2.43%	0.303%
18	13.674	1968	1970	1972	rBV	989	1089	1.98%	0.247%
19	13.757	1982	1984	1987	rVB2	1027	1210	2.20%	0.274%
20	13.786	1987	1989	1990	rBV	957	896	1.63%	0.203%
21	13.874	2003	2004	2006	rVV2	1799	941	1.71%	0.213%
22	13.892	2006	2007	2011	rVB3	1235	1118	2.03%	0.253%
23	13.980	2020	2022	2024	rBV2	1332	1306	2.37%	0.296%
24	14.033	2028	2031	2034	rVV	40261	34342	62.38%	7.776%
25	14.068	2034	2037	2040	rVB3	660	1006	1.83%	0.228%
26	14.192	2054	2058	2061	rVB3	1929	2611	4.74%	0.591%
27	14.327	2078	2081	2082	rBV2	1128	1196	2.17%	0.271%
28	14.357	2084	2086	2088	rVV3	1518	1043	1.89%	0.236%
29	14.380	2088	2090	2092	rVV2	1176	1257	2.28%	0.285%
30	14.398	2092	2093	2096	rVB2	1293	986	1.79%	0.223%
31	14.551	2118	2119	2121	rBV2	1190	871	1.58%	0.197%
32	14.604	2127	2128	2131	rBV2	1392	1228	2.23%	0.278%
33	14.715	2144	2147	2149	rVB4	1310	1322	2.40%	0.299%
34	14.774	2154	2157	2158	rVB	1500	1179	2.14%	0.267%
35	14.792	2158	2160	2161	rBV2	1125	1113	2.02%	0.252%
36	14.804	2161	2162	2166	rVB4	1606	1675	3.04%	0.379%

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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
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37	14.886	2173	2176	2178	rVB3	2870	2395	4.35%	0.542%
38	14.921	2180	2182	2183	rBV2	1314	834	1.51%	0.189%
39	14.939	2183	2185	2186	rBV2	829	829	1.51%	0.188%
40	14.951	2186	2187	2189	rVB2	1569	791	1.44%	0.179%
41	14.968	2189	2190	2192	rBV2	1283	1051	1.91%	0.238%
42	15.080	2207	2209	2211	rVB2	1297	912	1.66%	0.207%
43	15.109	2213	2214	2216	rVB2	2018	831	1.51%	0.188%
44	15.145	2216	2220	2223	rBV3	2921	3242	5.89%	0.734%
45	15.221	2228	2233	2235	rBV4	2070	3421	6.21%	0.775%
46	15.280	2242	2243	2245	rBV	1668	1343	2.44%	0.304%
47	15.357	2255	2256	2260	rBV4	1089	1130	2.05%	0.256%
48	15.404	2263	2264	2267	rVB2	1313	805	1.46%	0.182%
49	15.439	2269	2270	2274	rBV3	1077	1404	2.55%	0.318%
50	15.468	2274	2275	2278	rBV4	1989	1465	2.66%	0.332%
51	15.509	2278	2282	2290	rVB2	26873	35488	64.46%	8.036%
52	15.609	2297	2299	2300	rBV2	999	825	1.50%	0.187%
53	15.662	2304	2308	2314	rVB6	2249	3708	6.73%	0.840%
54	15.721	2314	2318	2319	rBV2	1838	1356	2.46%	0.307%
55	15.745	2319	2322	2324	rVB4	2396	3091	5.61%	0.700%
56	15.768	2324	2326	2327	rBV2	2367	1924	3.49%	0.436%
57	15.786	2327	2329	2332	rVB3	1466	1330	2.42%	0.301%
58	15.915	2349	2351	2352	rBV	1662	1108	2.01%	0.251%
59	15.968	2356	2360	2361	rVV2	1737	2070	3.76%	0.469%
60	15.998	2363	2365	2367	rVB3	1316	871	1.58%	0.197%
61	16.033	2367	2371	2372	rBV2	1553	2097	3.81%	0.475%
62	16.133	2387	2388	2390	rVB	1655	957	1.74%	0.217%
63	16.151	2390	2391	2392	rBV	2058	1023	1.86%	0.232%
64	16.215	2398	2402	2408	rBV3	4591	8219	14.93%	1.861%
65	16.262	2408	2410	2411	rVB2	1318	914	1.66%	0.207%
66	16.286	2411	2414	2417	rBV4	690	892	1.62%	0.202%
67	16.339	2421	2423	2424	rBV	1151	982	1.78%	0.222%
68	16.386	2428	2431	2432	rBV2	1139	864	1.57%	0.196%
69	16.445	2439	2441	2444	rVB3	1039	943	1.71%	0.214%
70	16.486	2446	2448	2451	rVV	1357	1966	3.57%	0.445%
71	16.539	2455	2457	2459	rVB3	1568	1017	1.85%	0.230%
72	16.668	2473	2479	2484	rBV2	4265	7517	13.65%	1.702%
73	16.733	2487	2490	2493	rBV3	1196	1575	2.86%	0.357%
74	16.768	2493	2496	2499	rVV3	1066	1161	2.11%	0.263%
75	16.821	2504	2505	2508	rVB2	1091	869	1.58%	0.197%
76	16.845	2508	2509	2511	rBV2	1679	1278	2.32%	0.289%

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77	16.909	2516	2520	2521	rBV3	1005	1044	1.90%	0.236%
78	16.956	2527	2528	2531	rVB3	1118	1118	2.03%	0.253%
79	17.133	2554	2558	2561	rBV3	940	1532	2.78%	0.347%
80	17.203	2567	2570	2572	rBV2	1298	1348	2.45%	0.305%
81	17.245	2575	2577	2583	rVV6	2706	4244	7.71%	0.961%
82	17.333	2586	2592	2596	rVV5	1801	4066	7.39%	0.921%
83	17.398	2600	2603	2604	rBV2	1312	1027	1.87%	0.233%
84	17.421	2604	2607	2609	rVB3	1229	1610	2.92%	0.365%
85	17.439	2609	2610	2612	rBV	1432	1022	1.86%	0.231%
86	17.533	2623	2626	2627	rVB	1009	854	1.55%	0.193%
87	17.598	2635	2637	2640	rVB	1152	1105	2.01%	0.250%
88	17.721	2654	2658	2659	rVB2	1207	1342	2.44%	0.304%
89	17.762	2659	2665	2666	rBV	858	1452	2.64%	0.329%
90	17.786	2666	2669	2676	rVB3	1213	2868	5.21%	0.649%
91	18.097	2720	2722	2724	rVB2	904	838	1.52%	0.190%
92	18.150	2729	2731	2734	rVB2	1304	1177	2.14%	0.267%
93	18.197	2734	2739	2741	rBV2	1332	2239	4.07%	0.507%
94	18.250	2747	2748	2750	rBV2	1682	1286	2.34%	0.291%
95	18.303	2754	2757	2758	rVB	1195	975	1.77%	0.221%
96	18.386	2769	2771	2774	rVB	1452	1074	1.95%	0.243%
97	18.421	2774	2777	2778	rBV	1047	977	1.77%	0.221%
98	18.509	2787	2792	2793	rBV3	820	1061	1.93%	0.240%
99	18.739	2828	2831	2836	rVB	1075	1344	2.44%	0.304%
100	18.797	2840	2841	2844	rVB	1121	904	1.64%	0.205%

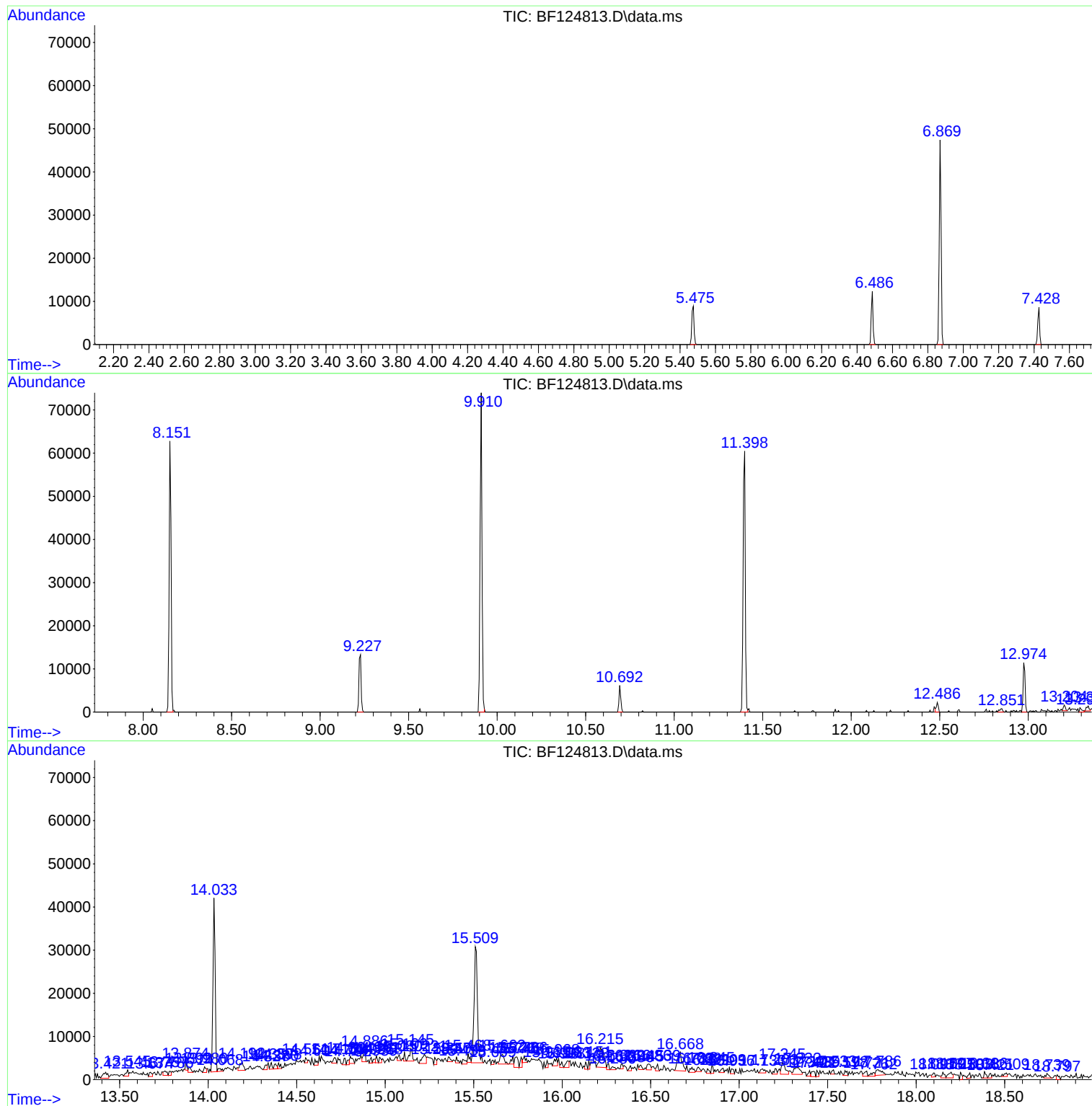
Sum of corrected areas: 441620

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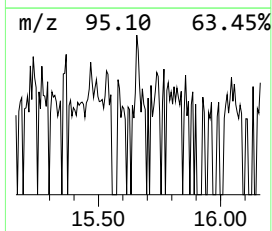
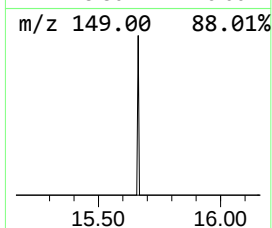
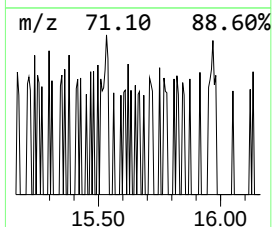
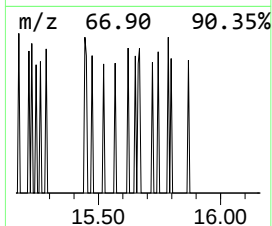
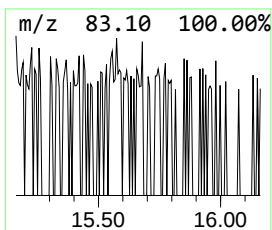
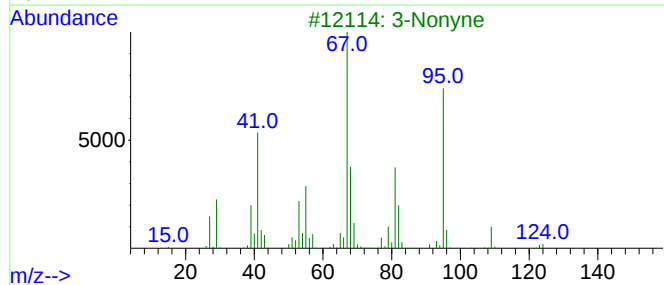
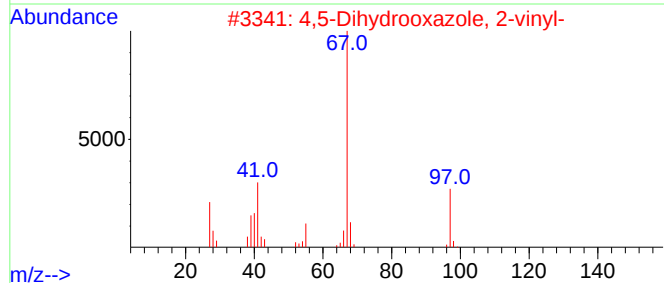
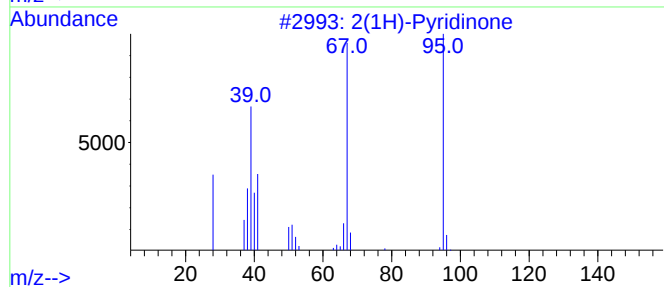
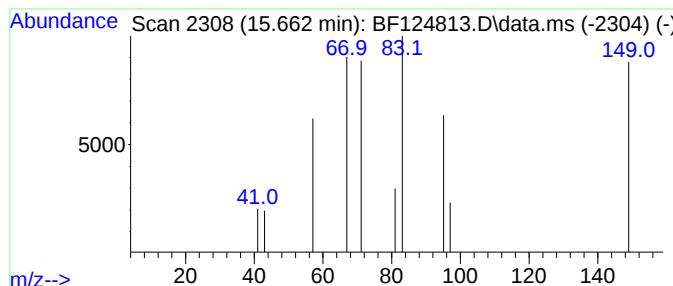
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown15.662 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.662	2.09 ng	3708	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyridinone			95	C5H5NO	000142-08-5	5
2	4,5-Dihydrooxazole, 2-vinyl-			97	C5H7NO	013670-33-2	4
3	3-Nonyne			124	C9H16	020184-89-8	4
4	6,7-Dimethyl-triazolo(4,3-b)(1,2...			149	C6H7N5	061139-73-9	4
5	Spiro[2.3]hexane-5-carboxylic ac...			278	C18H30O2	1000152-25-7	4



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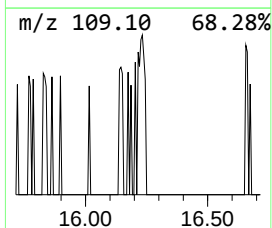
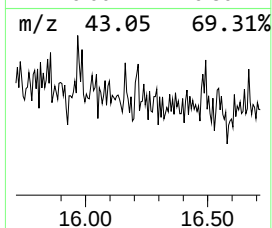
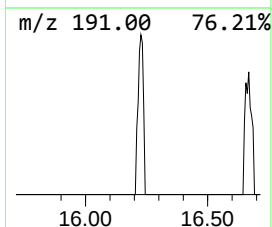
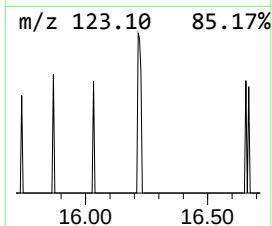
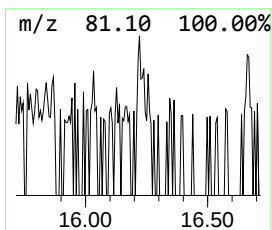
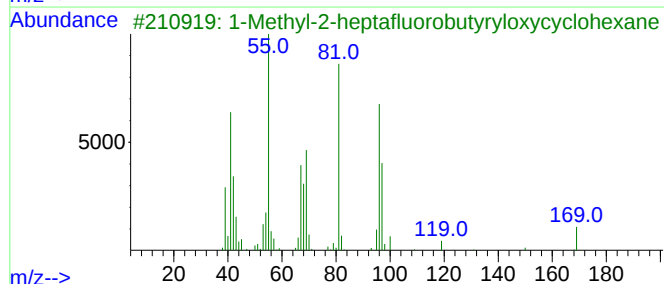
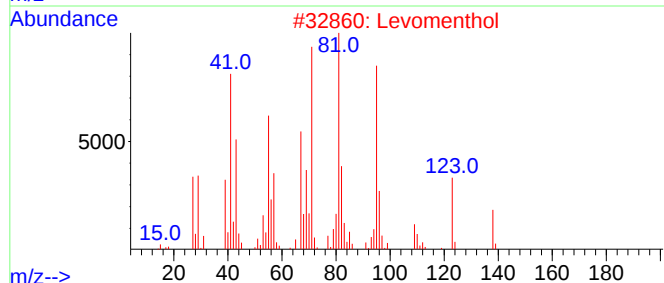
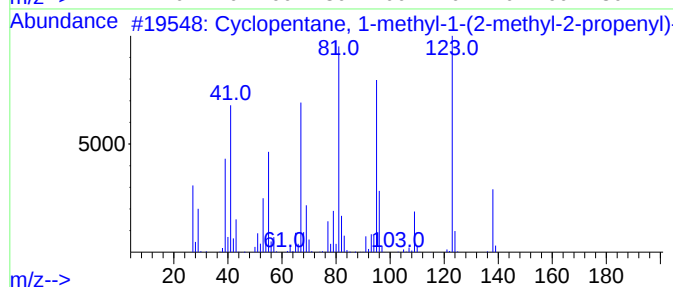
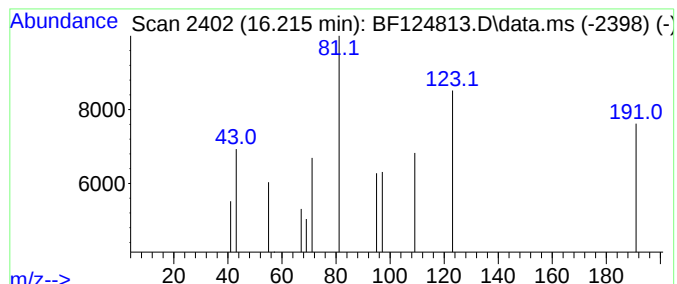
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown16.215 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	4.63 ng	8219	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	37
2			Levomenthol	156	C10H20O	002216-51-5	23
3			1-Methyl-2-heptafluorobutyryloxy...	310	C11H13F7O2	1000216-64-0	10
4			Carbonic acid, 2,2,2-trichloroet...	288	C10H15Cl3O3	1000357-89-8	10
5			(2,4-Dimethylcyclohexyl)methyl a...	184	C11H20O2	1000497-97-0	9



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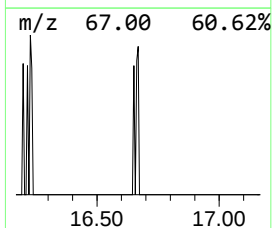
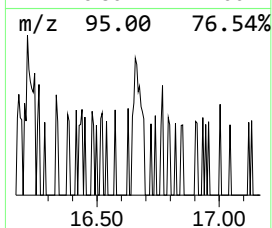
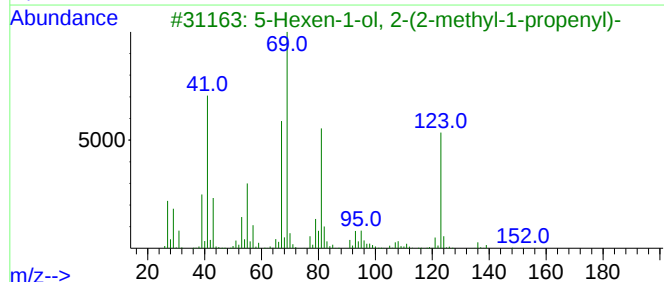
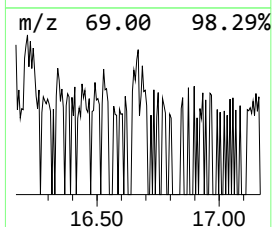
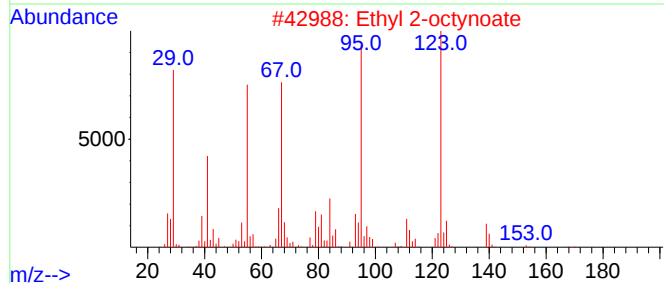
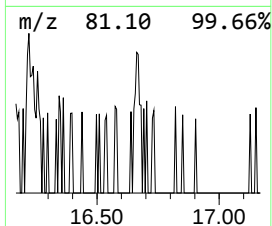
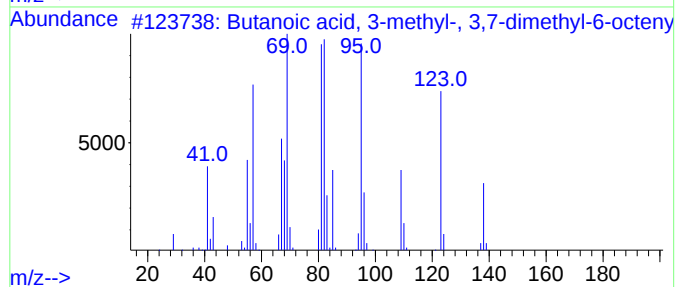
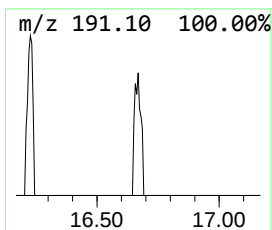
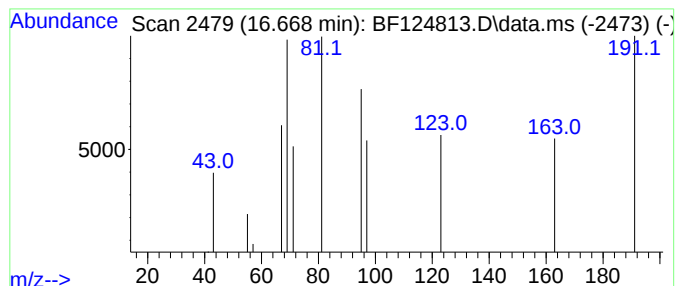
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown16.668 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.668	4.24 ng	7517	Perylene-d12	15.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-, 3,7-di...	240	C15H28O2	068922-10-1	25
2	Ethyl 2-octynoate	168	C10H16O2	010519-20-7	9
3	5-Hexen-1-ol, 2-(2-methyl-1-prop...	154	C10H18O	018675-19-9	9
4	1-Hexadecen-3-ol, 3,5,11,15-tetr...	296	C20H40O	1000262-55-5	9
5	Isophytol	296	C20H40O	000505-32-8	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124813.D
Acq On : 28 Jul 2021 1:58
Operator : JU/CG
Sample : M3194-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-072621

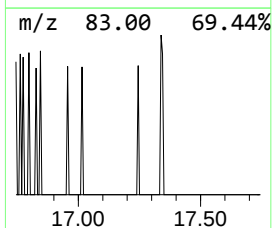
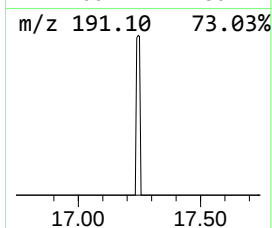
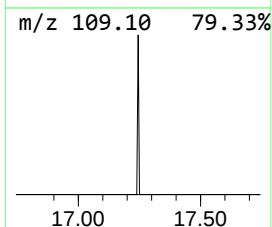
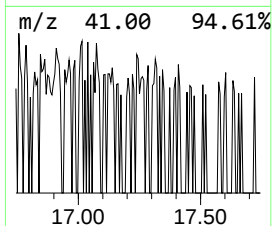
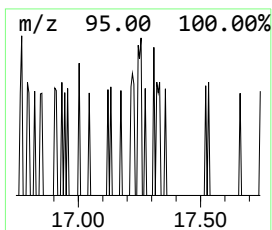
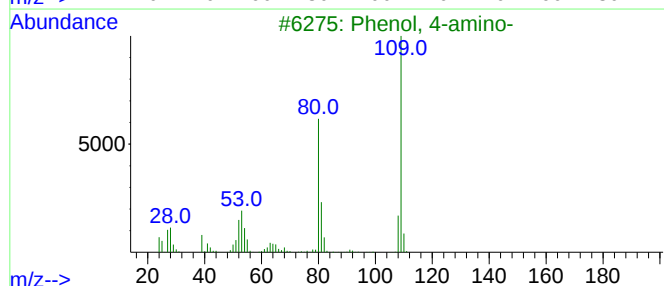
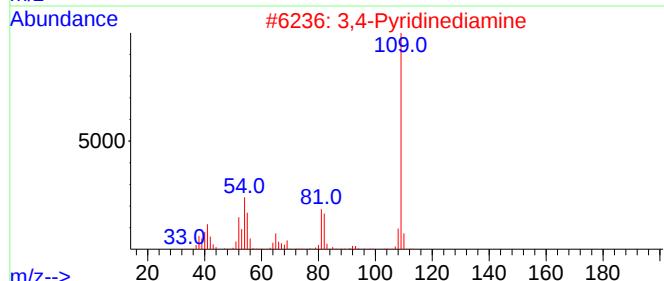
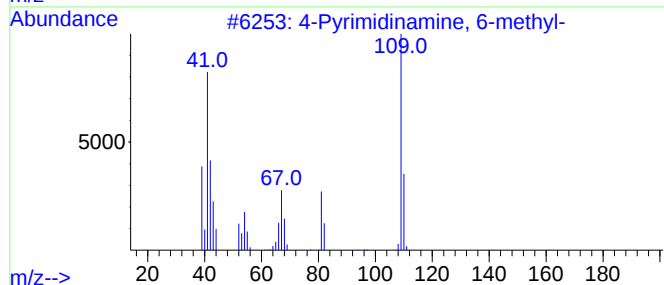
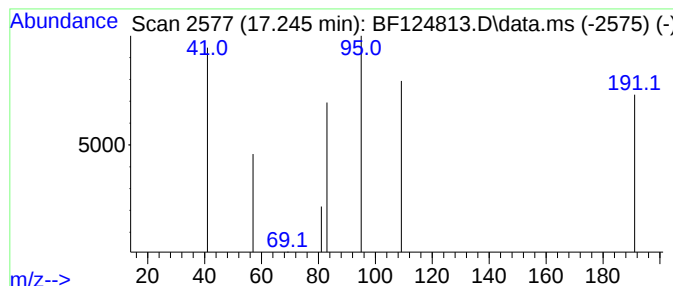
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown17.245 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.245	2.39 ng	4244	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pyrimidinamine, 6-methyl-			109	C5H7N3	003435-28-7	7
2	3,4-Pyridinediamine			109	C5H7N3	000054-96-6	4
3	Phenol, 4-amino-			109	C6H7NO	000123-30-8	4
4	Phenol, 3-amino-			109	C6H7NO	000591-27-5	4
5	2,3-Pyridinediamine			109	C5H7N3	000452-58-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072721\
Data File : BF124813.D
Acq On : 28 Jul 2021 1:58
Operator : JU/CG
Sample : M3194-01 10X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-072621

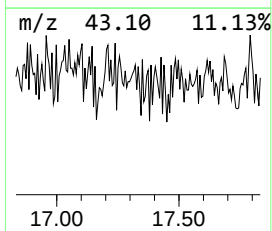
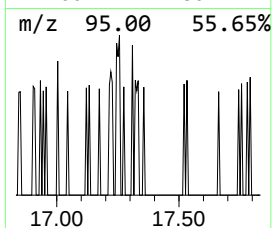
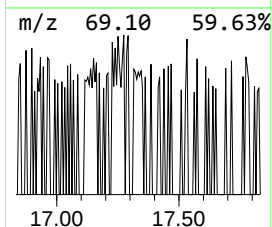
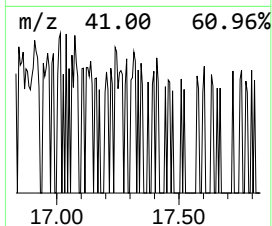
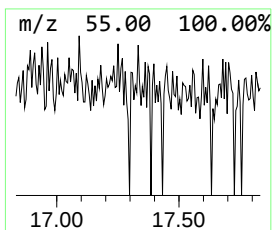
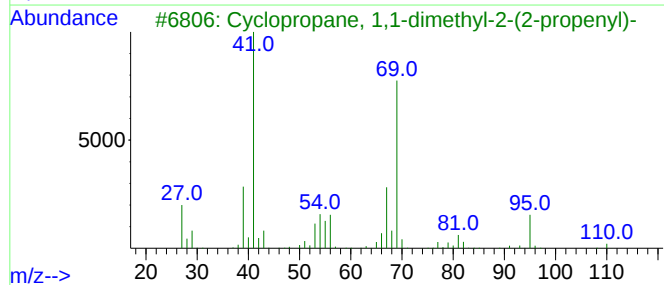
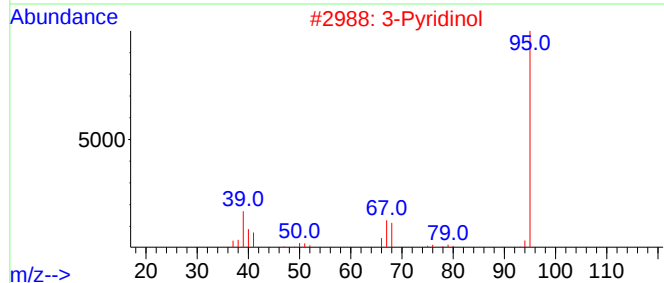
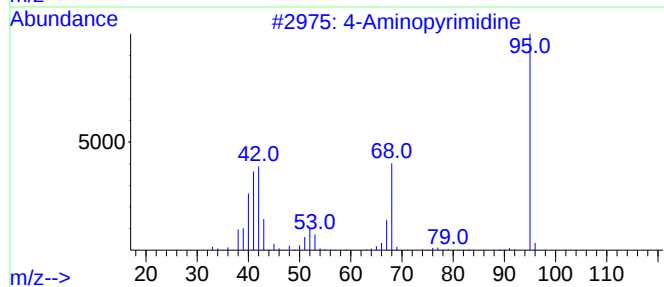
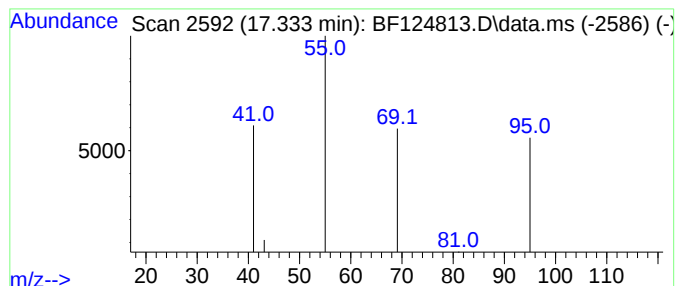
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown17.333 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.333	2.29 ng	4066	Perylene-d12	15.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
2			3-Pyridinol	95	C5H5NO	000109-00-2	2
3			Cyclopropane, 1,1-dimethyl-2-(2-...	110	C8H14	036939-15-8	2
4			1,5-Heptadiene, 2-methyl-, (Z)-	110	C8H14	041044-64-8	1
5			Ethyl isocyanide	55	C3H5N	000624-79-3	1



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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-03-072621

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
unknown15.662	15.662	2.1	ng	3708	6	15.515	35488	20.0
unknown16.215	16.215	4.6	ng	8219	6	15.515	35488	20.0
unknown16.668	16.668	4.2	ng	7517	6	15.515	35488	20.0
unknown17.245	17.245	2.4	ng	4244	6	15.515	35488	20.0
unknown17.333	17.333	2.3	ng	4066	6	15.515	35488	20.0