

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016694.D
 Acq On : 03 Oct 2021 06:24
 Operator : CG/JU
 Sample : M3892-09
 Misc :
 ALS Vial : 62 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-824-N-SO-0-0.5-092221

Integration Parameters: rteint.p

Integrator: RTE

Smothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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_N\METHODS\8270-SIM-BN100121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016694.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.277	127	130	144	rVB	21358	67052	2.03%	0.231%
2	4.581	158	163	167	rBV	14181	34717	1.05%	0.119%
3	4.821	185	189	196	rVB	54504	104897	3.18%	0.361%
4	5.042	209	213	220	rBV	18443	45607	1.38%	0.157%
5	5.273	234	238	253	rVB	17973	44944	1.36%	0.155%
6	6.333	348	353	361	rVB	126507	290934	8.81%	1.000%
7	6.656	381	388	391	rBV2	11922	33200	1.01%	0.114%
8	6.822	403	406	413	rVB	17833	36196	1.10%	0.124%
9	7.080	430	434	444	rVB	216597	480213	14.54%	1.651%
10	7.633	489	494	500	rVB	53162	109653	3.32%	0.377%
11	7.937	521	527	534	rVB	152446	281680	8.53%	0.968%
12	8.784	598	605	609	rBV	27017	68236	2.07%	0.235%
13	9.697	666	677	680	rBV	77084	221730	6.72%	0.762%
14	10.191	713	716	723	rBV	131069	243228	7.37%	0.836%
15	10.407	729	733	735	rBV	106624	189377	5.74%	0.651%
16	10.457	735	737	739	rVB2	31834	52894	1.60%	0.182%
17	12.003	922	931	939	rBV	41071	66325	2.01%	0.228%
18	12.074	939	947	965	rVB	37344	60907	1.84%	0.209%
19	12.296	986	997	1011	rBV	42103	64086	1.94%	0.220%
20	12.886	1071	1074	1077	rBV2	84906	136468	4.13%	0.469%
21	13.190	1093	1098	1101	rVB	141598	258218	7.82%	0.888%
22	13.584	1127	1129	1132	rBV	64386	101565	3.08%	0.349%
23	13.749	1138	1142	1145	rVB	71824	112839	3.42%	0.388%
24	13.990	1157	1161	1164	rBV	60316	105051	3.18%	0.361%
25	14.129	1166	1172	1179	rBV2	69665	133023	4.03%	0.457%
26	14.269	1179	1183	1185	rBV	148999	229926	6.96%	0.791%
27	14.332	1185	1188	1192	rVB2	93914	165376	5.01%	0.569%
28	14.523	1198	1203	1206	rBV3	15585	48340	1.46%	0.166%
29	14.751	1218	1221	1224	rVB	60052	93895	2.84%	0.323%
30	15.093	1243	1248	1250	rBV2	58758	108433	3.28%	0.373%
31	15.170	1250	1254	1256	rVB2	28170	50719	1.54%	0.174%
32	15.322	1263	1266	1269	rBV2	79148	116263	3.52%	0.400%
33	15.626	1287	1290	1292	rBV2	51636	99572	3.02%	0.342%
34	15.728	1295	1298	1300	rVV2	34764	84663	2.56%	0.291%
35	15.766	1300	1301	1305	rVB	39710	55322	1.68%	0.190%
36	16.007	1317	1320	1322	rVB2	101729	136018	4.12%	0.468%

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37	16.081	1322	1326	1332	rVB2	36608	64531	1.95%	0.222%
38	16.421	1352	1354	1357	rBV2	28783	49758	1.51%	0.171%
39	16.592	1365	1368	1372	rVB	36109	64763	1.96%	0.223%
40	17.018	1400	1403	1404	rBV	132349	192456	5.83%	0.662%
41	17.066	1404	1407	1410	rVV	933828	1436704	43.51%	4.940%
42	17.151	1410	1414	1417	rVB	196153	320149	9.70%	1.101%
43	17.431	1432	1437	1440	rBV2	122750	194596	5.89%	0.669%
44	17.796	1465	1467	1472	rBV2	19588	49949	1.51%	0.172%
45	17.894	1472	1475	1477	rBV2	27774	55395	1.68%	0.190%
46	17.955	1477	1480	1483	rVB3	52586	118133	3.58%	0.406%
47	18.418	1560	1566	1571	rBV	48125	68014	2.06%	0.234%
48	19.098	1687	1703	1709	rBV	2319035	3301860	100.00%	11.352%
49	19.137	1709	1711	1717	rVB	49583	52903	1.60%	0.182%
50	19.247	1728	1733	1738	rVB2	53670	66635	2.02%	0.229%
51	19.460	1766	1776	1787	rBV	2075888	2914267	88.26%	10.020%
52	19.679	1815	1820	1823	rBV	76578	98249	2.98%	0.338%
53	19.703	1823	1825	1833	rVB	40374	50331	1.52%	0.173%
54	20.006	1885	1886	1888	rBV	30179	42986	1.30%	0.148%
55	20.112	1893	1896	1898	rVV2	26512	55330	1.68%	0.190%
56	20.335	1914	1917	1919	rVB2	37194	50944	1.54%	0.175%
57	20.378	1919	1921	1923	rBV	38540	51181	1.55%	0.176%
58	20.707	1947	1952	1956	rBV3	63513	141570	4.29%	0.487%
59	20.803	1958	1961	1964	rBV	31625	43657	1.32%	0.150%
60	20.866	1964	1967	1970	rBV3	36930	87960	2.66%	0.302%
61	20.919	1970	1972	1973	rBV	141196	157609	4.77%	0.542%
62	20.973	1973	1977	1979	rVB2	156006	309592	9.38%	1.064%
63	21.174	1993	1996	1997	rBV	145371	215272	6.52%	0.740%
64	21.217	1997	2000	2002	rVV	1279036	1829709	55.41%	6.291%
65	21.270	2002	2005	2009	rVB	1231171	1808106	54.76%	6.216%
66	21.387	2014	2016	2022	rBV2	145313	235213	7.12%	0.809%
67	21.589	2033	2035	2038	rBV2	30574	47389	1.44%	0.163%
68	21.737	2046	2049	2051	rBV3	17638	40228	1.22%	0.138%
69	21.790	2051	2054	2056	rVV	34756	65184	1.97%	0.224%
70	21.875	2056	2062	2064	rVV2	162519	360708	10.92%	1.240%
71	21.939	2064	2068	2070	rVV2	54889	162629	4.93%	0.559%
72	21.981	2070	2072	2074	rVV	66805	130141	3.94%	0.447%
73	22.024	2074	2076	2079	rVV	165178	264575	8.01%	0.910%
74	22.098	2080	2083	2089	rVB2	57534	115029	3.48%	0.395%
75	22.258	2096	2098	2101	rBV	26238	49679	1.50%	0.171%
76	22.396	2109	2111	2113	rVB2	46151	47836	1.45%	0.164%

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77	22.560	2148	2157	2175	rBV2	108171	171051	5.18%	0.588%
78	22.728	2199	2206	2217	rVB2	47119	73358	2.22%	0.252%
79	22.814	2218	2231	2239	rBV	935262	2040796	61.81%	7.016%
80	22.899	2250	2256	2271	rVB	297156	492341	14.91%	1.693%
81	22.985	2272	2281	2312	rVB2	154530	298786	9.05%	1.027%
82	23.293	2359	2371	2387	rBV	566228	1016217	30.78%	3.494%
83	23.389	2387	2399	2417	rVB	675093	1289302	39.05%	4.433%
84	23.491	2418	2429	2435	rBV	121445	233841	7.08%	0.804%
85	23.536	2435	2442	2458	rVB	187123	371494	11.25%	1.277%
86	23.748	2494	2504	2515	rBV2	49316	110103	3.33%	0.379%
87	24.094	2597	2605	2616	rVB	48287	98860	2.99%	0.340%
88	24.186	2620	2632	2655	rVV	112048	268235	8.12%	0.922%
89	24.368	2677	2685	2695	rBV2	23553	44266	1.34%	0.152%
90	25.093	2887	2897	2909	rVB3	18926	44504	1.35%	0.153%
91	25.179	2913	2922	2936	rVB5	15549	42898	1.30%	0.147%
92	25.323	2955	2964	2994	rVB2	36542	111697	3.38%	0.384%
93	25.480	2997	3010	3018	rBV2	56440	154045	4.67%	0.530%
94	25.689	3063	3071	3080	rBV	19860	39693	1.20%	0.136%
95	25.774	3080	3096	3119	rVB2	312460	958435	29.03%	3.295%
96	25.911	3122	3136	3155	rBV4	33233	112490	3.41%	0.387%
97	26.055	3167	3178	3192	rVB2	47773	129159	3.91%	0.444%
98	26.148	3193	3205	3234	rVB	54684	169466	5.13%	0.583%
99	26.476	3281	3301	3332	rBV	217343	737540	22.34%	2.536%
100	26.849	3397	3410	3438	rVB2	39659	134541	4.07%	0.463%

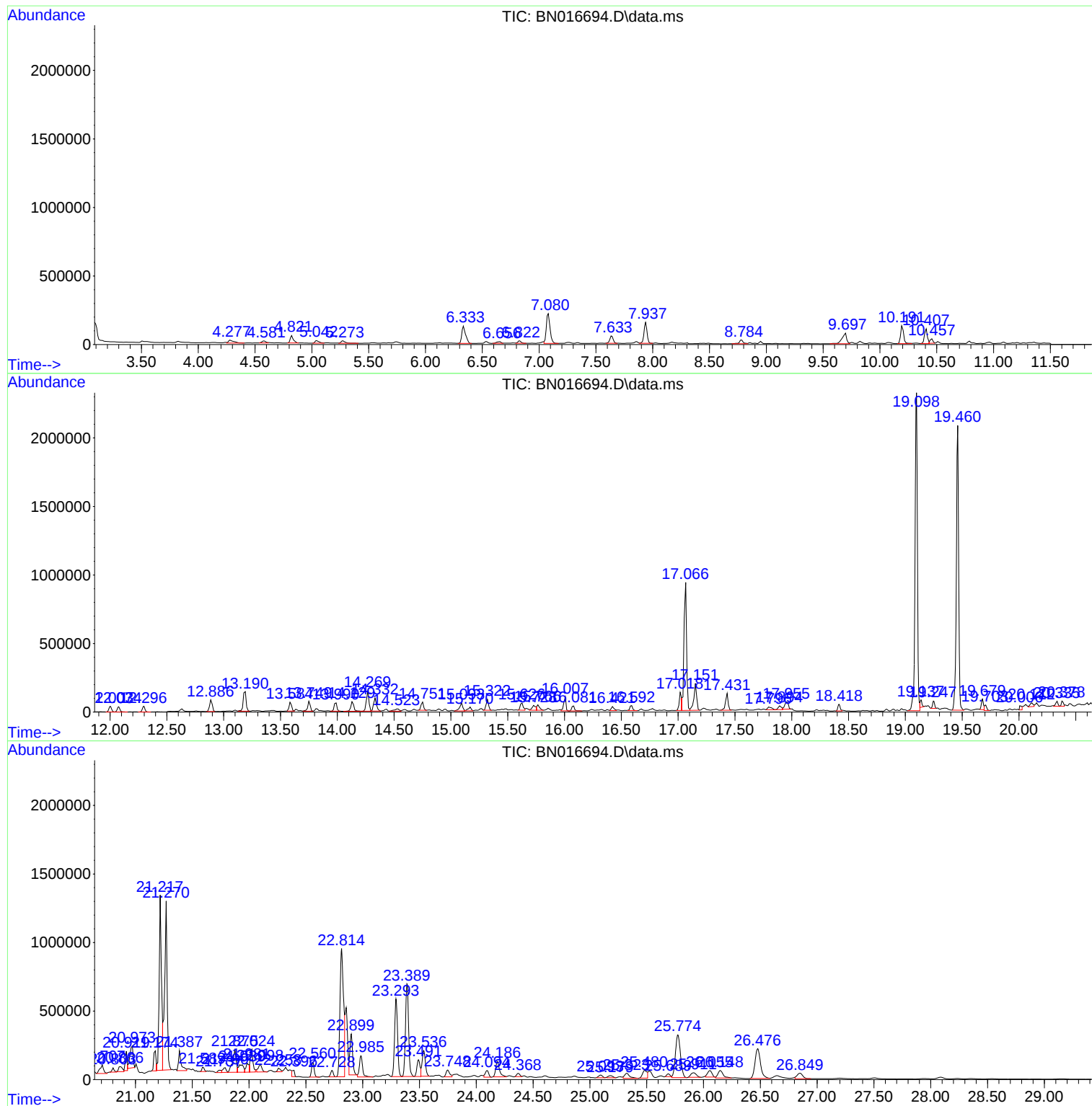
Sum of corrected areas: 29085905

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.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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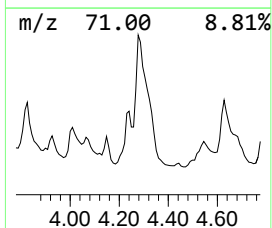
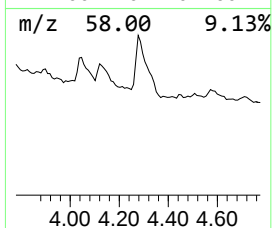
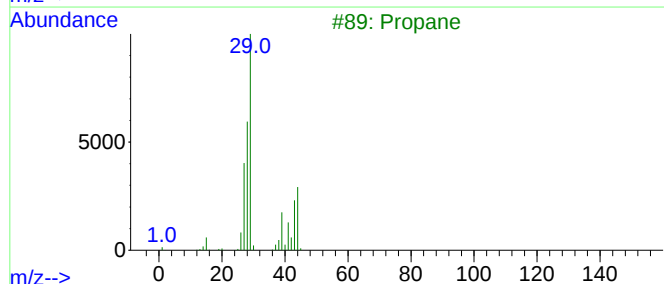
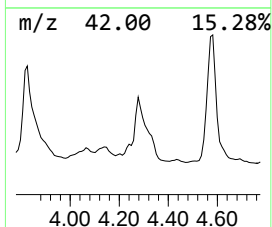
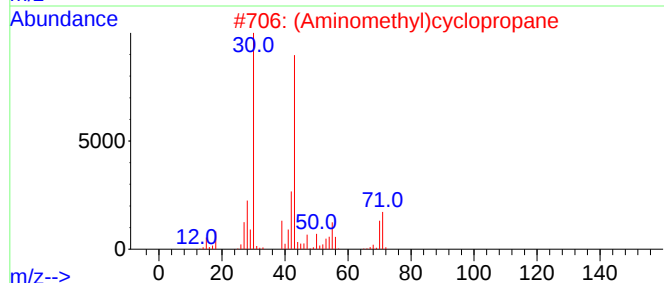
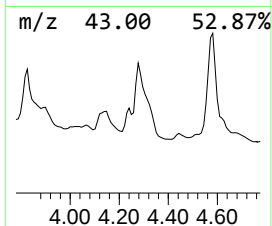
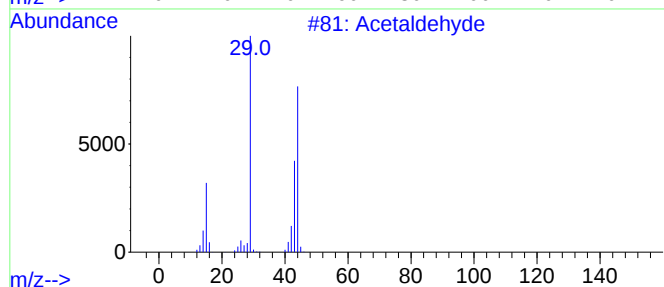
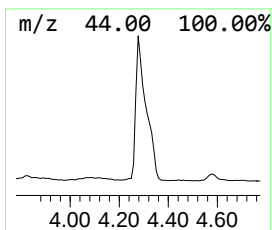
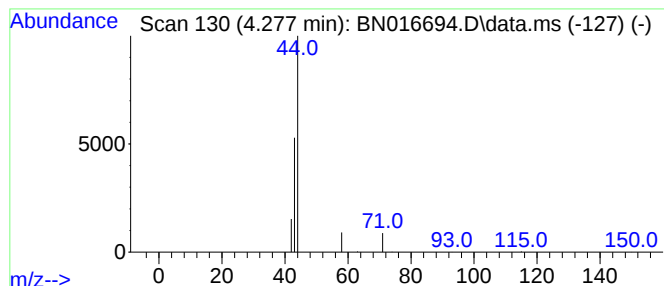
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetaldehyde Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.277	0.24 ng	67052	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	7
2			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	5
3			Propane	44	C3H8	000074-98-6	4
4			Butane	58	C4H10	000106-97-8	4
5			Ethylene oxide	44	C2H4O	000075-21-8	4



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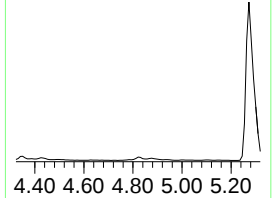
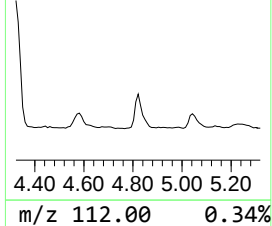
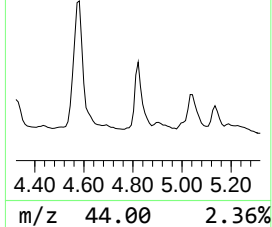
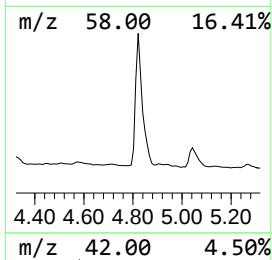
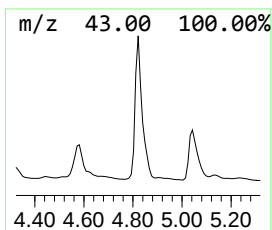
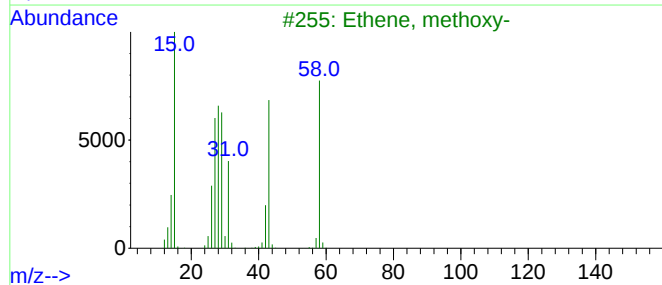
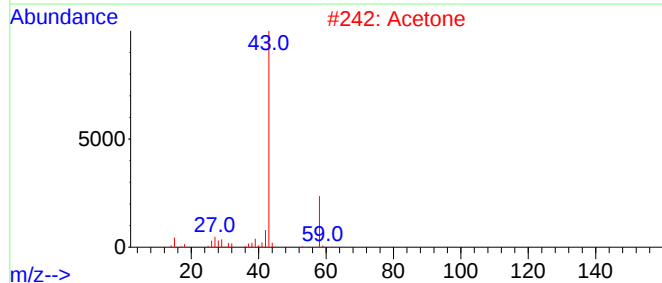
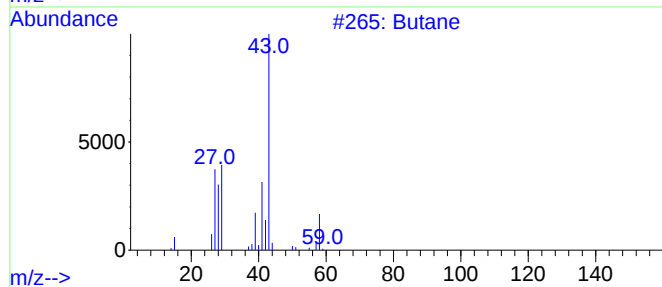
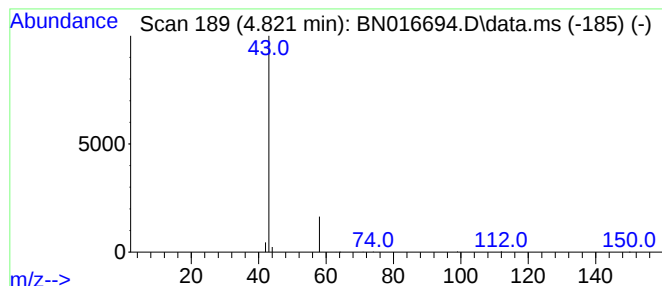
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.38 ng	104897	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	4
2			Acetone	58	C3H6O	000067-64-1	4
3			Ethene, methoxy-	58	C3H6O	000107-25-5	3
4			Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	2



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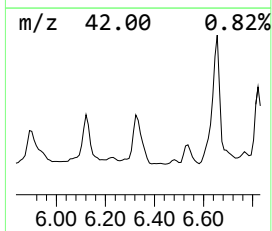
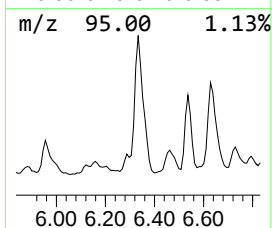
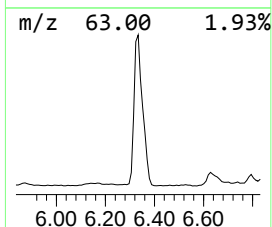
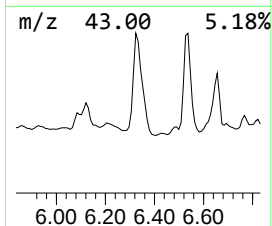
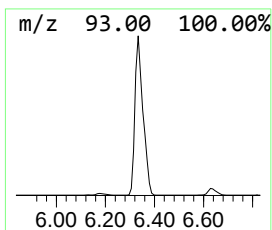
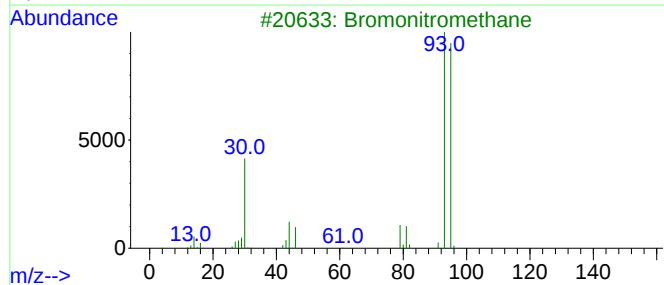
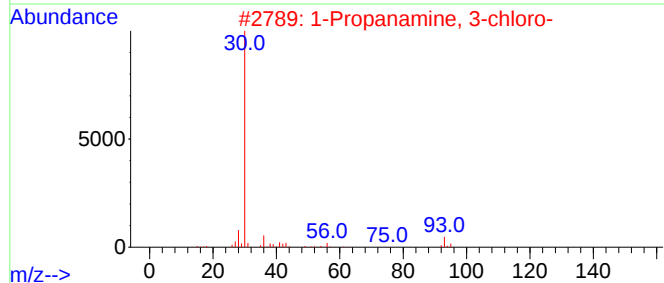
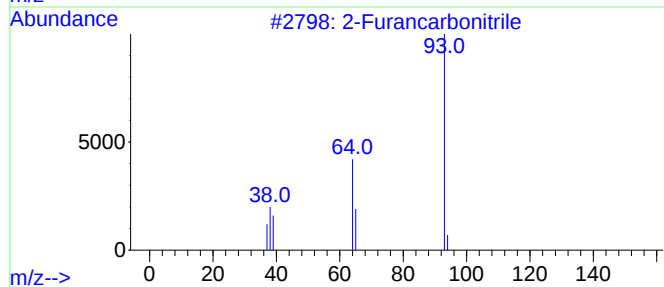
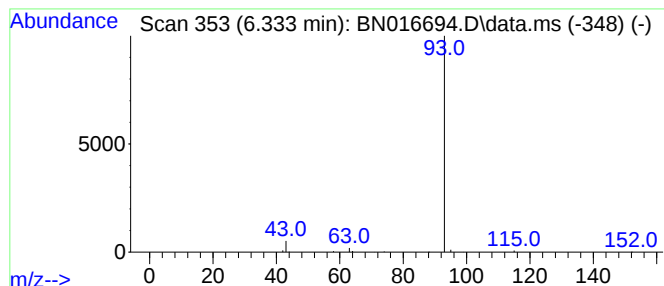
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Furancarbonitrile Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.333	1.06 ng	290934	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Furancarbonitrile	93	C5H3NO	000617-90-3	2
2			1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	1
3			Bromonitromethane	139	CH2BrNO2	000563-70-2	1
4			4-(2-Aminoethyl)pyridine	122	C7H10N2	013258-63-4	1
5			Ethanone, 1-cyclopropyl-2-(4-pyr...	161	C10H11NO	006580-95-6	1



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Data File : BN016694.D
Acq On : 03 Oct 2021 06:24
Operator : CG/JU
Sample : M3892-09
Misc :
ALS Vial : 62 Sample Multiplier: 1

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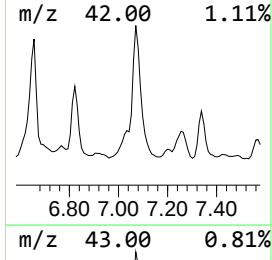
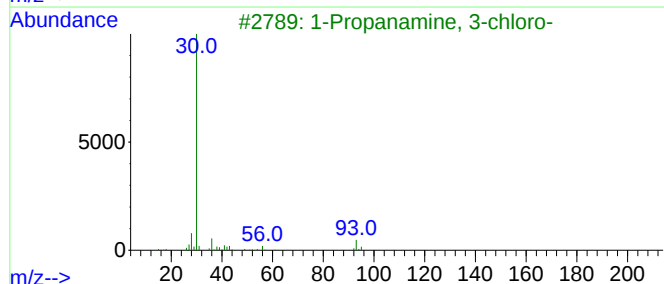
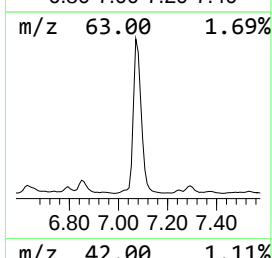
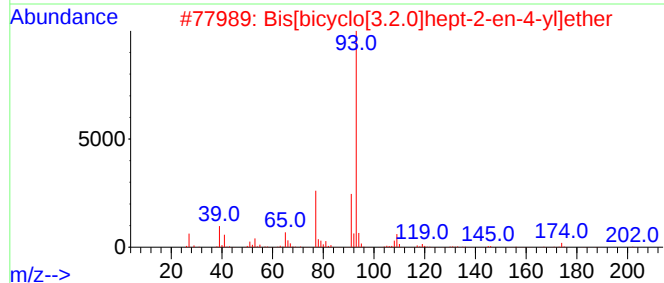
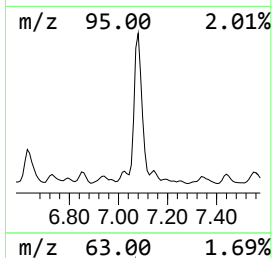
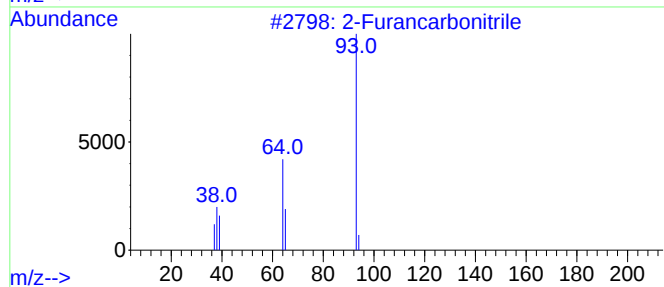
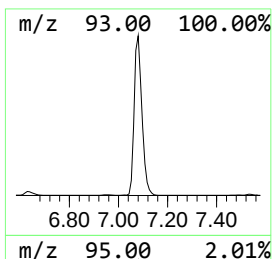
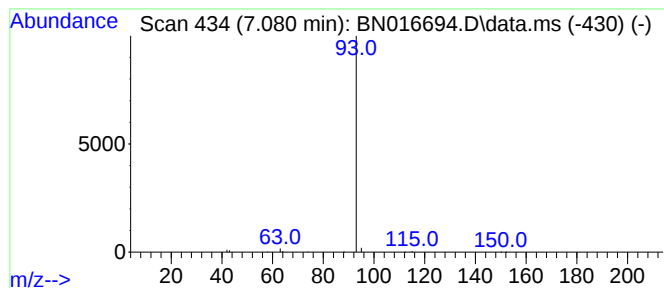
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Furancarbonitrile Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.080	1.75 ng	480213	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Furancarbonitrile	93	C5H3NO	000617-90-3	2
2			Bis[bicyclo[3.2.0]hept-2-en-4-yl]...	202	C14H18O	1000153-89-5	1
3			1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	1
4			Bromonitromethane	139	CH2BrNO2	000563-70-2	1
5			4-(2-Aminoethyl)pyridine	122	C7H10N2	013258-63-4	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Sample : M3892-09
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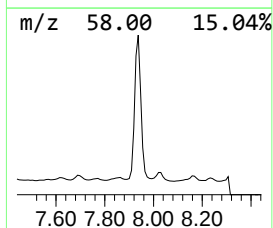
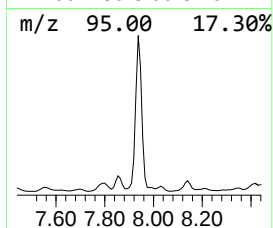
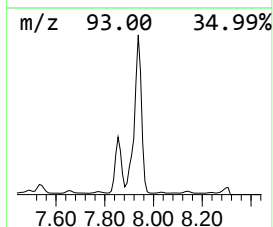
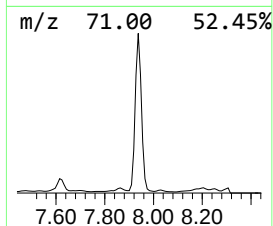
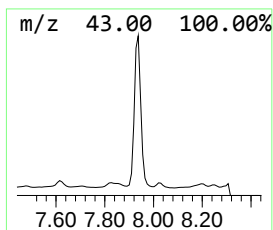
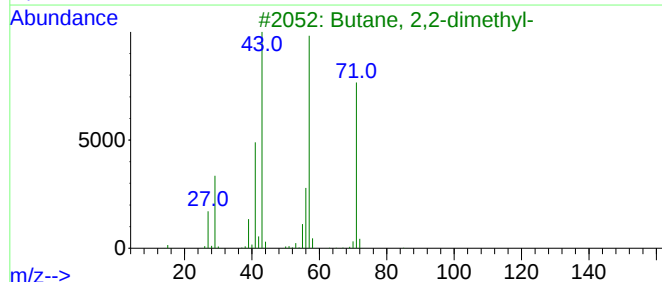
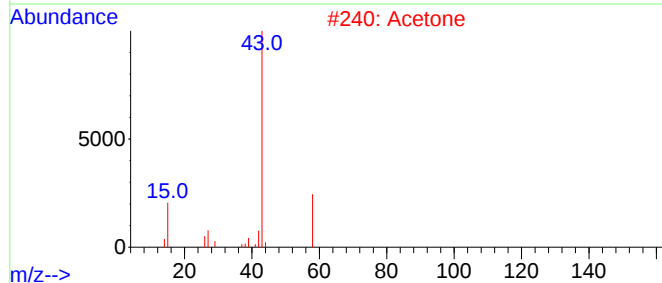
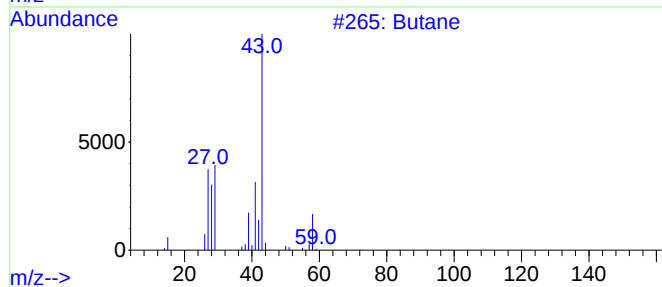
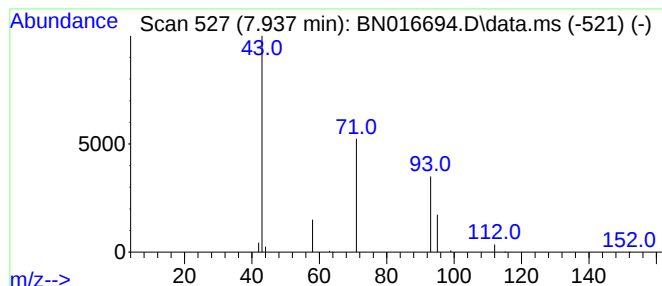
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.937	1.03 ng	281680	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	4
2			Acetone	58	C3H6O	000067-64-1	4
3			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	4
4			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	4
5			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
Acq On : 03 Oct 2021 06:24
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Misc :
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ClientSampleId :
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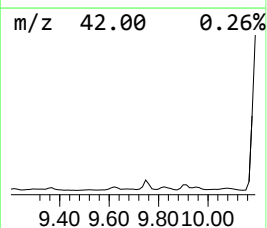
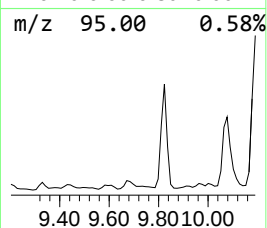
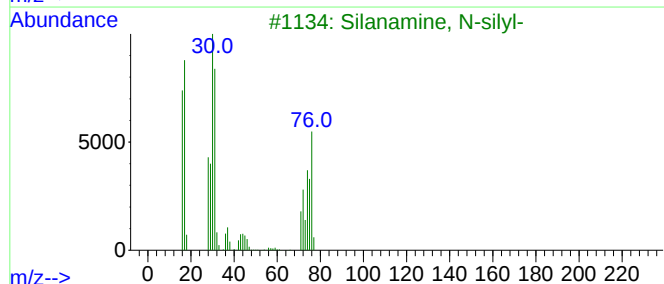
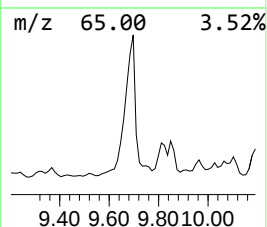
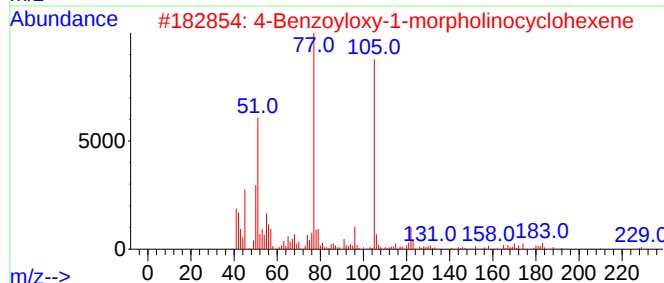
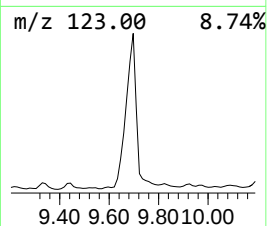
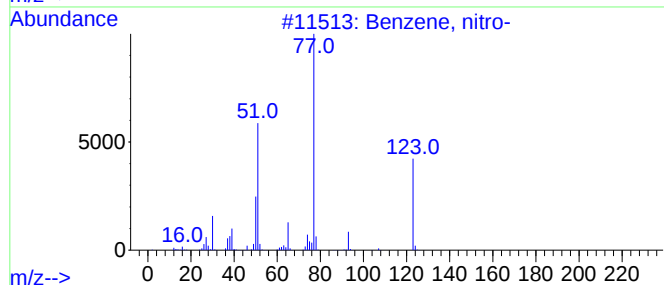
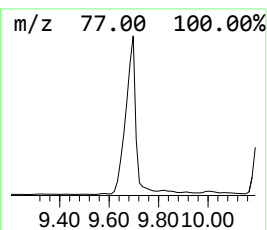
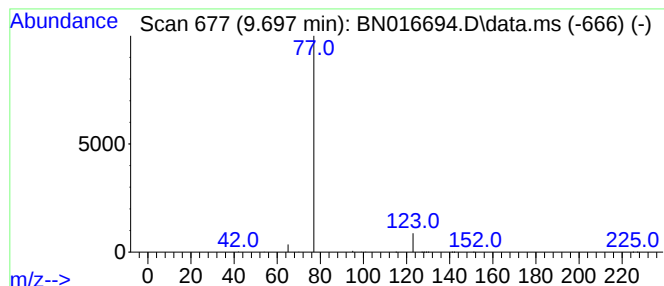
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, nitro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.697	0.47 ng	221730	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, nitro-	123	C6H5NO2	000098-95-3	2
2			4-Benzoyloxy-1-morpholinocyclohe...	287	C17H21NO3	037138-56-0	1
3			Silanamine, N-silyl-	77	H7NSi2	005702-11-4	1
4			Mercaptamine	77	C2H7NS	000060-23-1	1
5			Propane, 1,2-dichloro-2-methyl-	126	C4H8Cl2	000594-37-6	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
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Sample : M3892-09
Misc :
ALS Vial : 62 Sample Multiplier: 1

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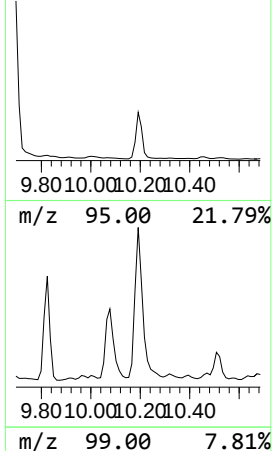
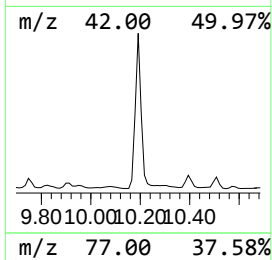
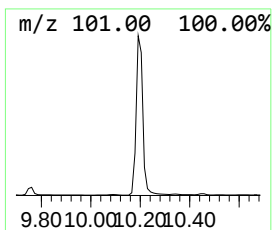
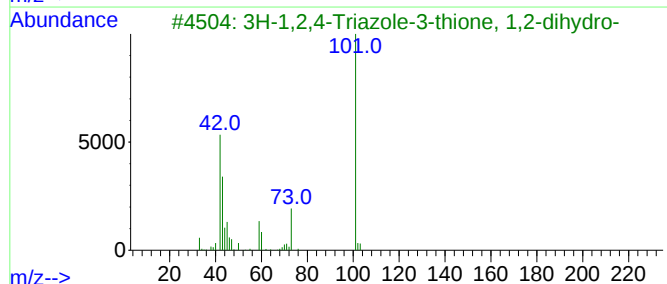
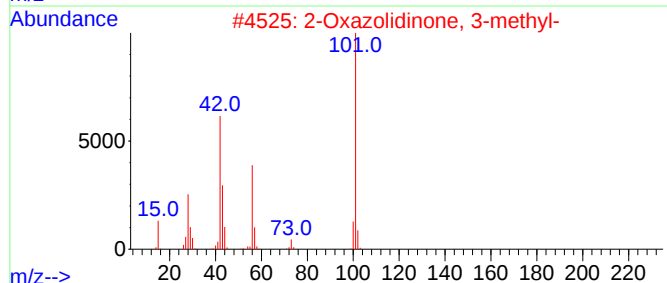
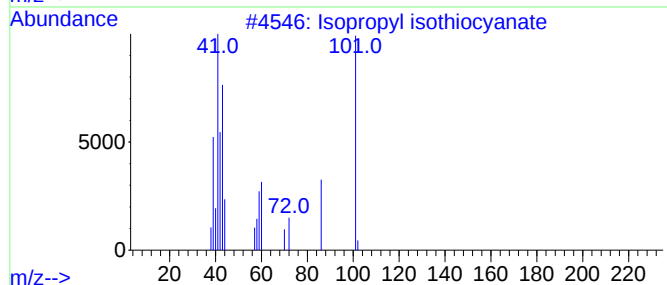
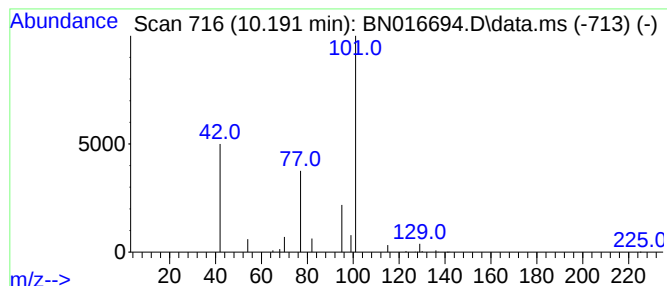
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Isopropyl isothiocyanate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.51 ng	243228	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9
2			2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
3			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5			3-Aminopropionitrile	70	C3H6N2	000151-18-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
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Operator : CG/JU
Sample : M3892-09
Misc :
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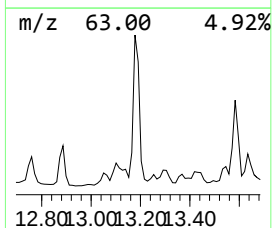
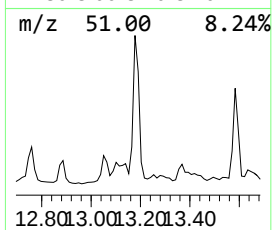
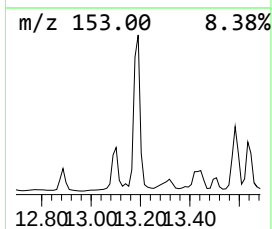
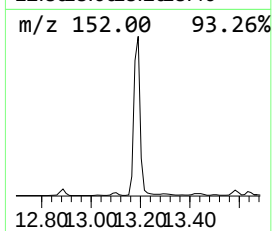
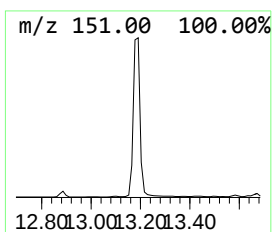
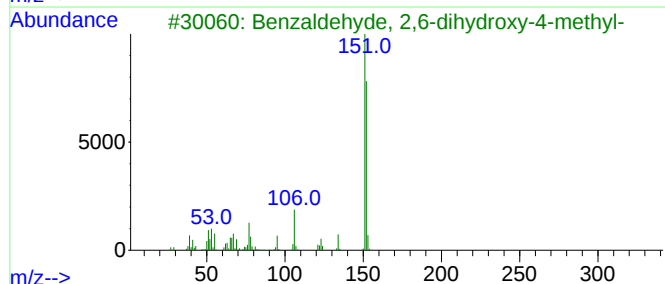
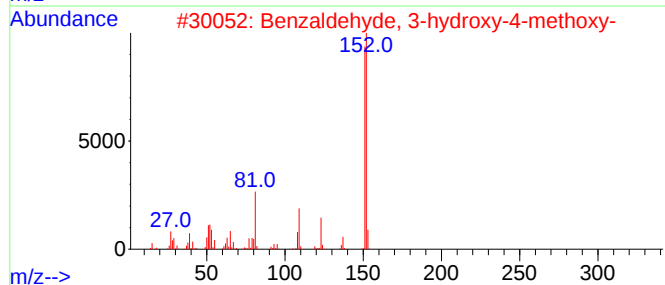
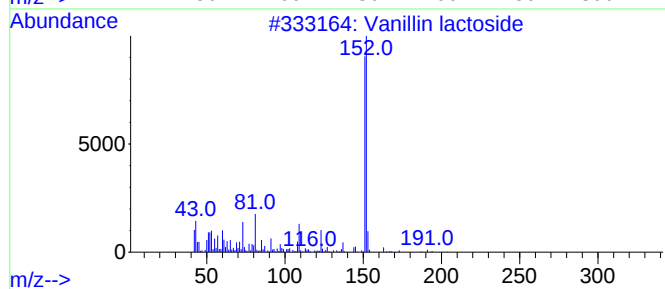
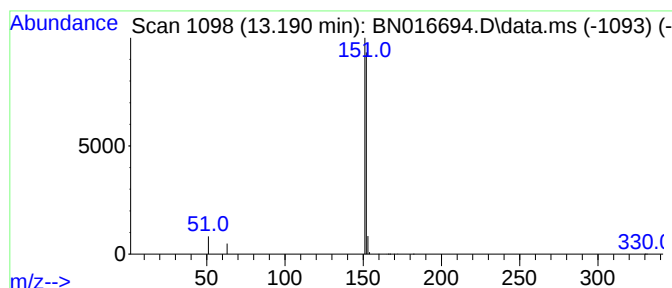
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Vanillin lactoside Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.190	0.45 ng	258218	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Vanillin lactoside	476	C20H28O13	1000129-94-7	64
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	64
3			Benzaldehyde, 2,6-dihydroxy-4-me...	152	C8H8O3	000526-37-4	64
4			Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	000673-22-3	9
5			Vanillin	152	C8H8O3	000121-33-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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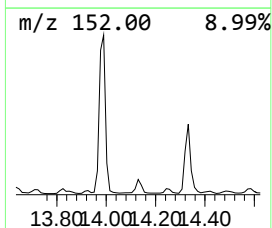
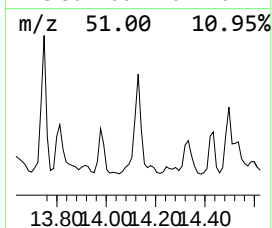
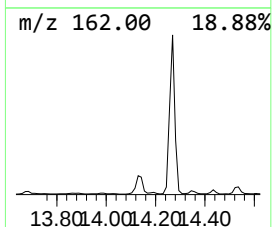
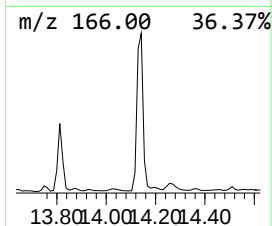
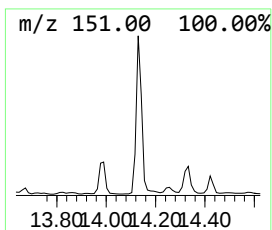
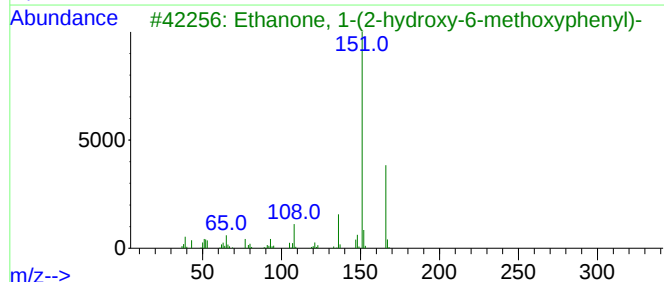
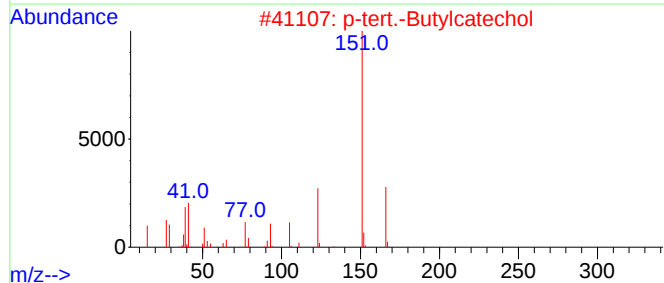
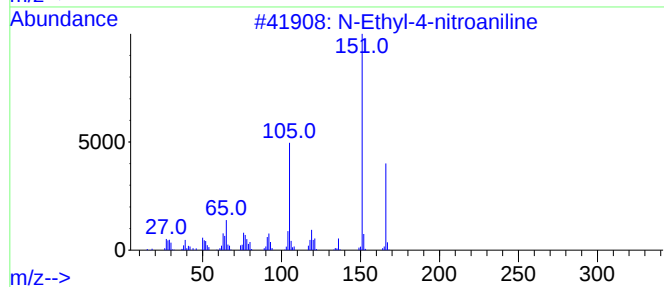
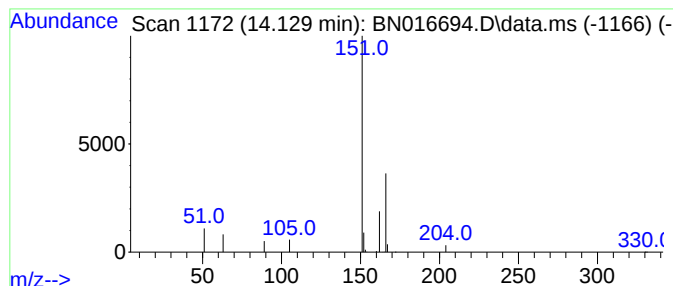
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 N-Ethyl-4-nitroaniline Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.129	0.23 ng	133023	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-Ethyl-4-nitroaniline	166	C8H10N2O2	003665-80-3	64
2			p-tert.-Butylcatechol	166	C10H14O2	000098-29-3	64
3			Ethanone, 1-(2-hydroxy-6-methoxy...	166	C9H10O3	000703-23-1	64
4			Apocynin	166	C9H10O3	000498-02-2	45
5			Ethanone, 1-(2-hydroxy-4-methoxy...	166	C9H10O3	000552-41-0	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
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ALS Vial : 62 Sample Multiplier: 1

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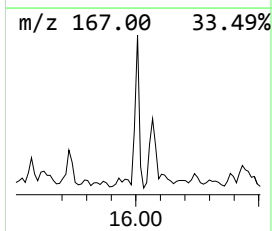
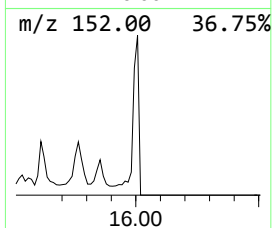
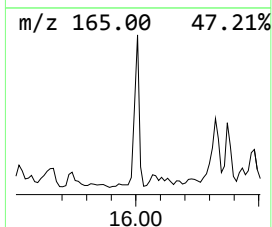
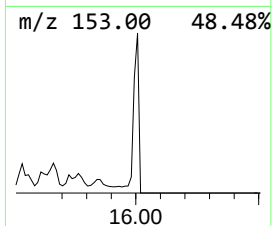
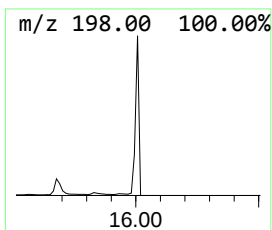
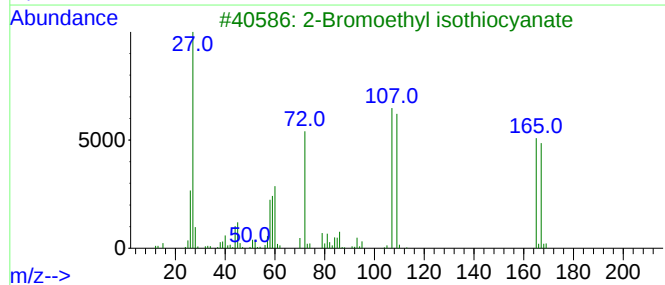
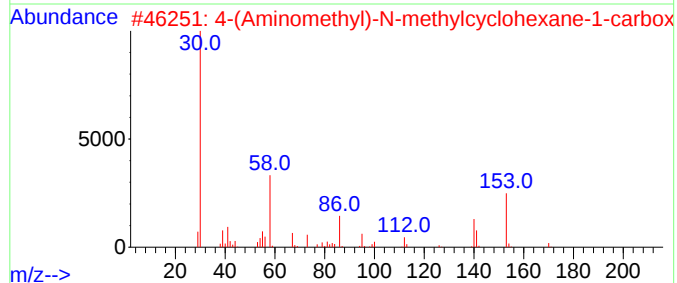
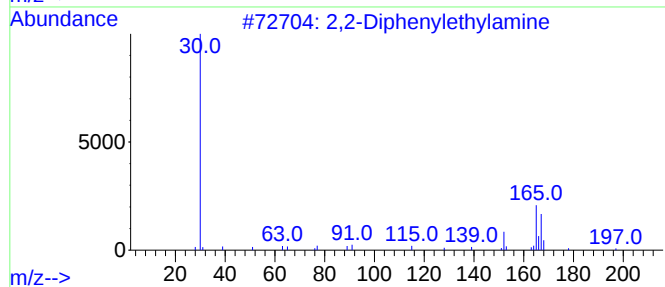
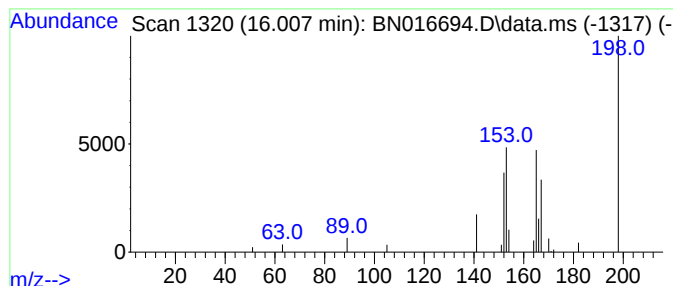
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,2-Diphenylethylamine Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.007	0.28 ng	136018	Phenanthrene-d10	17.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2-Diphenylethylamine	197	C14H15N	003963-62-0	16
2			4-(Aminomethyl)-N-methylcyclohex...	170	C9H18N2O	1000459-82-8	5
3			2-Bromoethyl isothiocyanate	165	C3H4BrNS	001483-41-6	5
4			2H-Azepin-2-one, hexahydro-3-(2-...	153	C9H15NO	029559-34-0	5
5			Methyl 2-(dimethylhydrazono)-3,3...	198	C6H9F3N2O2	1000489-35-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
Acq On : 03 Oct 2021 06:24
Operator : CG/JU
Sample : M3892-09
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-0-0.5-092221

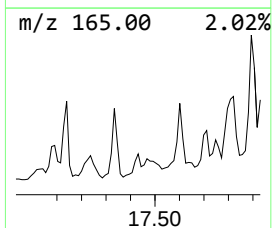
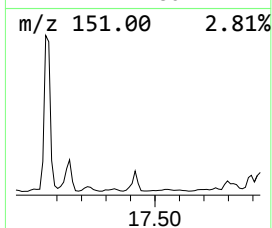
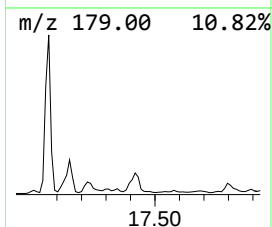
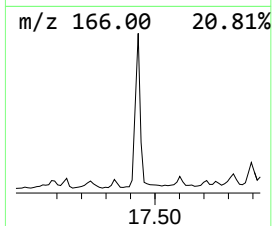
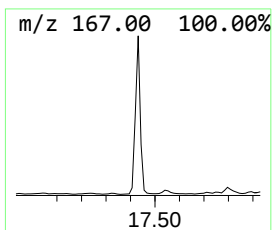
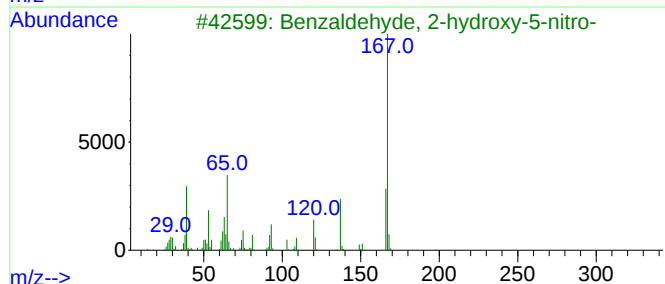
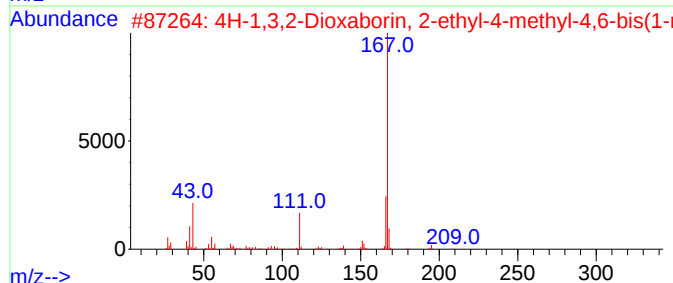
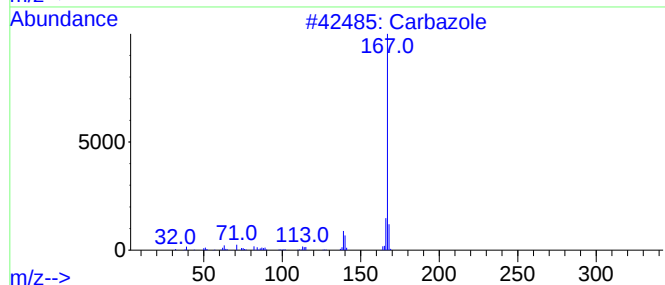
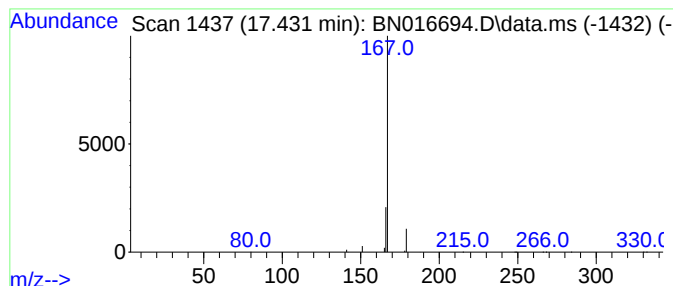
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Carbazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.40 ng	194596	Phenanthrene-d10	17.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbazole	167	C12H9N	000086-74-8	9
2			4H-1,3,2-Dioxaborin, 2-ethyl-4-m...	210	C12H23B02	074421-11-7	9
3			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5N04	000097-51-8	5
4			benzaldehyde, 2-hydroxy-4-nitro-	167	C7H5N04	1000404-52-2	5
5			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Sample : M3892-09
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ClientSampleId :
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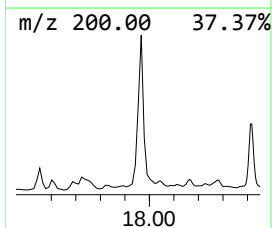
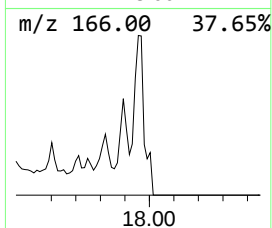
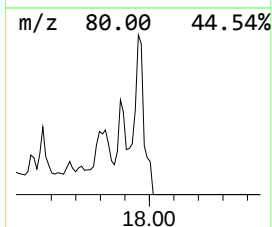
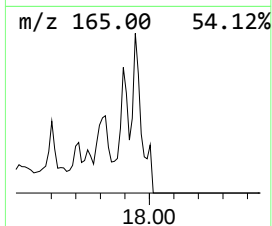
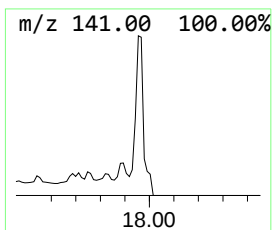
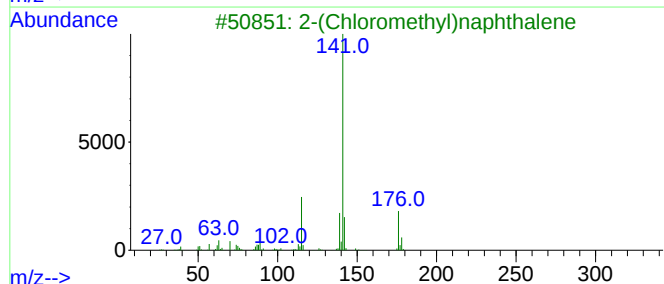
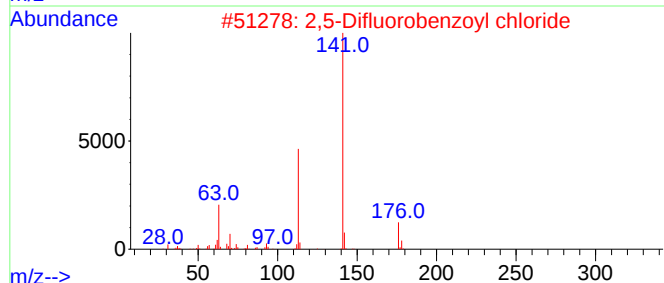
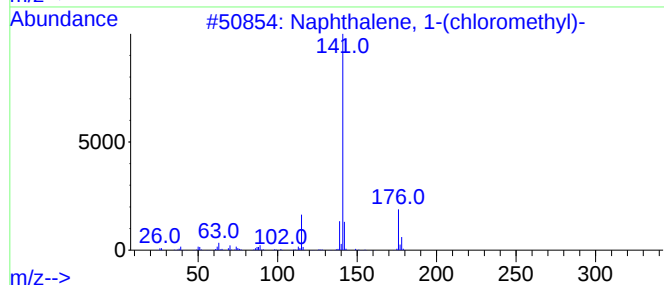
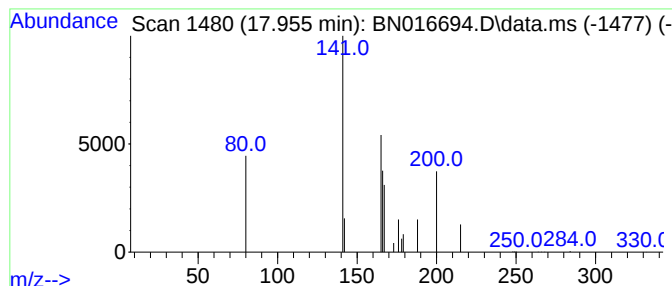
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Naphthalene, 1-(chloromethyl)- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.955	0.25 ng	118133	Phenanthrene-d10	17.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-(chloromethyl)-	176	C11H9Cl	000086-52-2	12
2			2,5-Difluorobenzoyl chloride	176	C7H3ClF2O	035730-09-7	12
3			2-(Chloromethyl)naphthalene	176	C11H9Cl	002506-41-4	12
4			3,5-Difluorobenzoyl chloride	176	C7H3ClF2O	129714-97-2	12
5			1-Naphthalenepropionic acid	200	C13H12O2	003243-42-3	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Misc :
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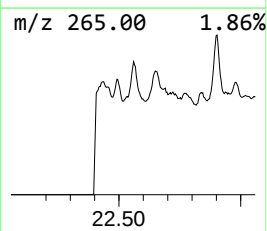
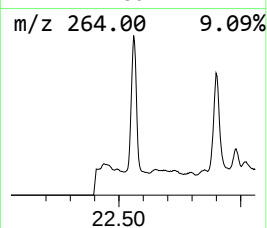
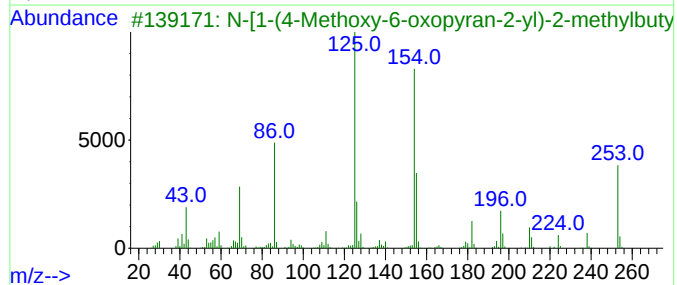
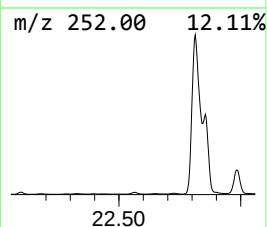
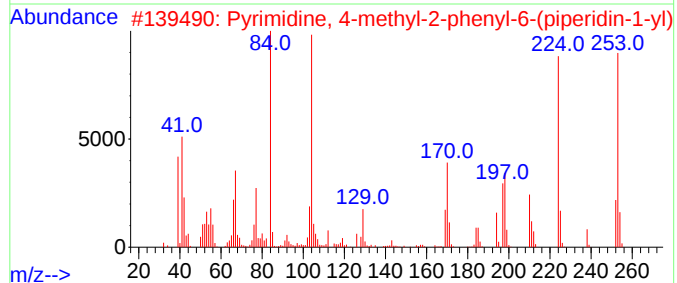
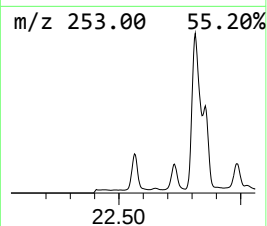
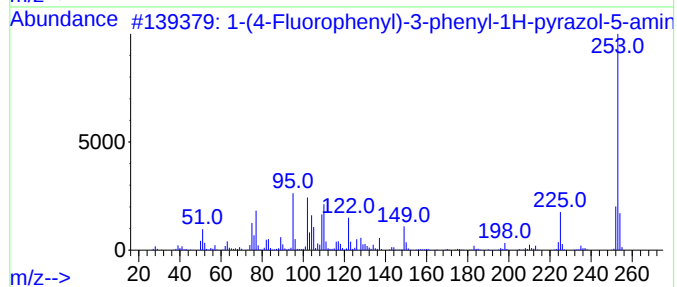
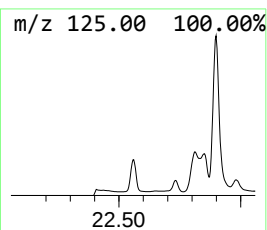
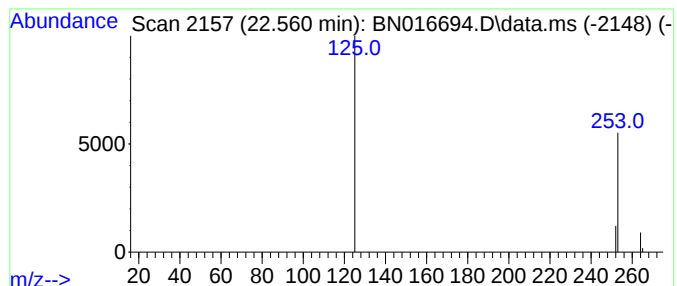
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-(4-Fluorophenyl)-3-phenyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.560	0.29 ng	171051	Perylene-d12	23.488	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Fluorophenyl)-3-phenyl-1H-p...	253	C15H12FN3	072411-51-9	5
2	Pyrimidine, 4-methyl-2-phenyl-6-...	253	C16H19N3	1000302-39-3	5
3	N-[1-(4-Methoxy-6-oxopyran-2-yl)]...	253	C13H19NO4	1246066-80-7	5
4	Chalcone, 4-nitro-, (E)-	253	C15H11NO3	002960-55-6	5
5	2-Nitro-3-phenylthiocyclohexanol	253	C12H15NO3S	1000188-56-1	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
Acq On : 03 Oct 2021 06:24
Operator : CG/JU
Sample : M3892-09
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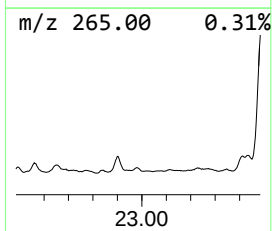
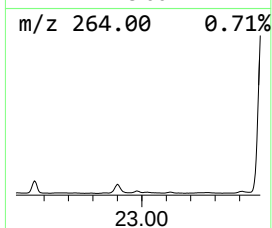
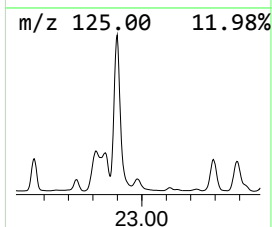
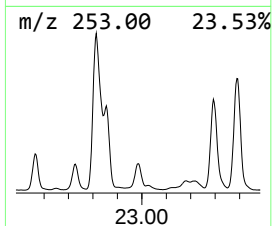
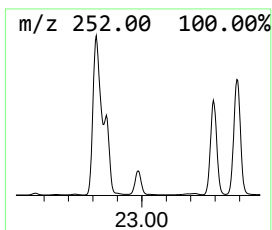
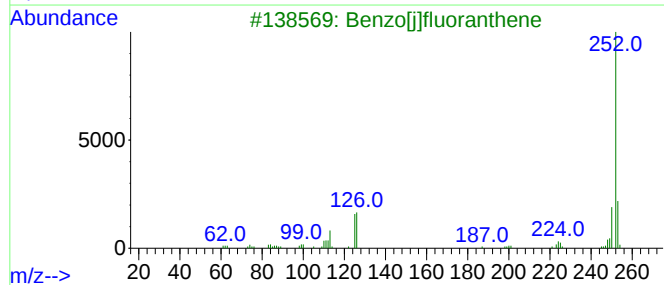
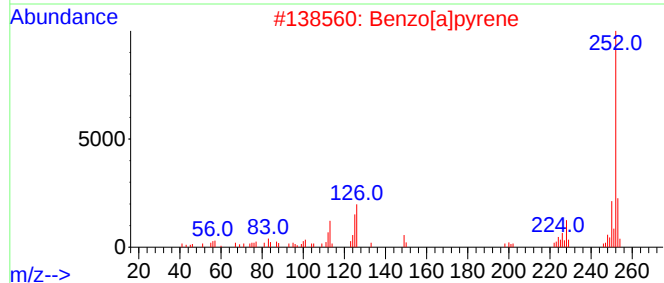
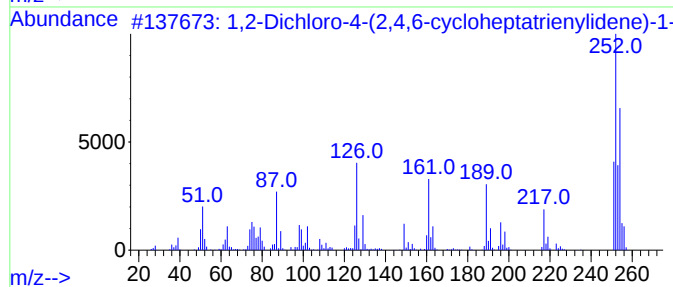
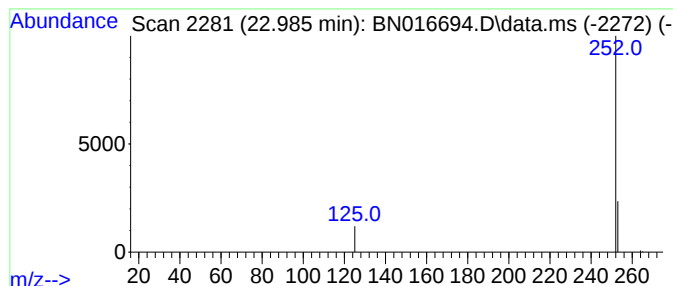
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1,2-Dichloro-4-(2,4,6-cyclo... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.985	0.51 ng	298786	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Dichloro-4-(2,4,6-cyclohepta...	252	C12H6Cl2O2	033548-00-4	9
2			Benzo[a]pyrene	252	C20H12	000050-32-8	9
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
5			1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
Acq On : 03 Oct 2021 06:24
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Sample : M3892-09
Misc :
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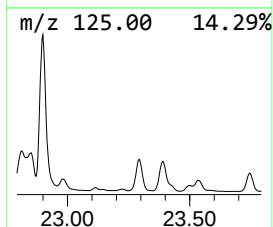
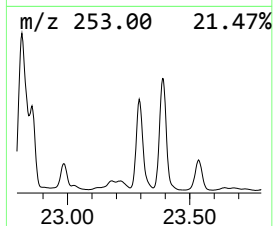
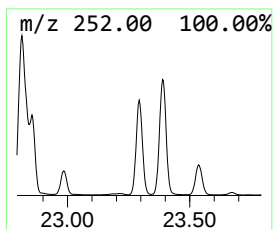
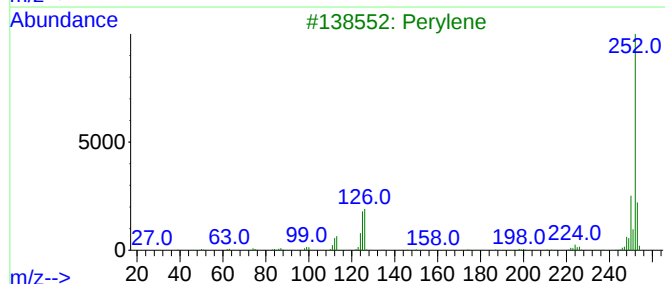
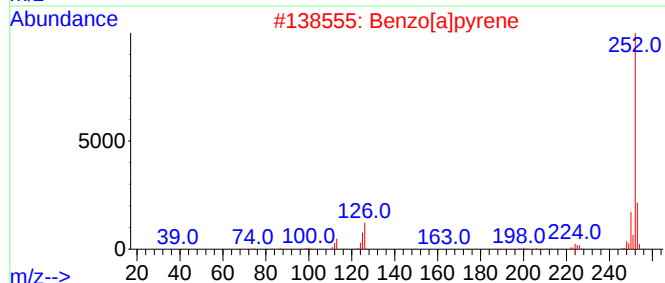
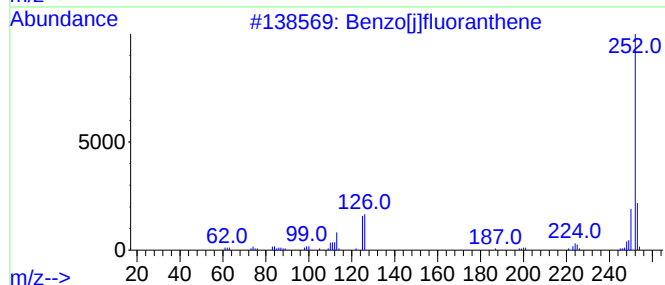
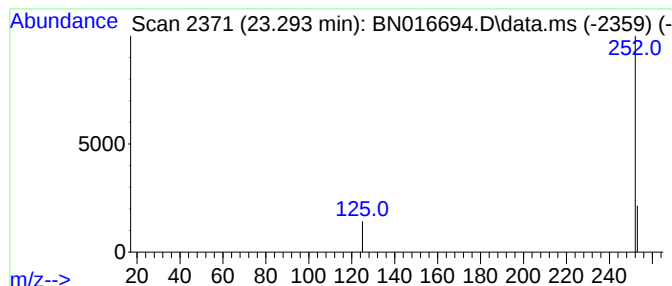
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzo[j]fluoranthene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.293	1.74 ng	1016220	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
2			Benzo[a]pyrene	252	C20H12	000050-32-8	9
3			Perylene	252	C20H12	000198-55-0	9
4			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
5			1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
Acq On : 03 Oct 2021 06:24
Operator : CG/JU
Sample : M3892-09
Misc :
ALS Vial : 62 Sample Multiplier: 1

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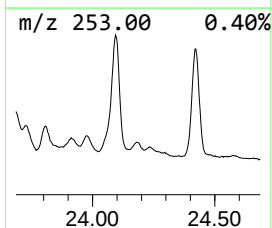
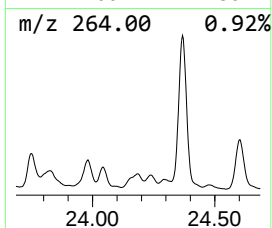
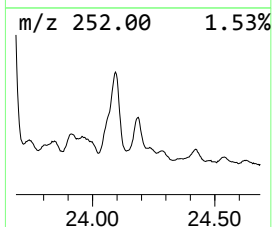
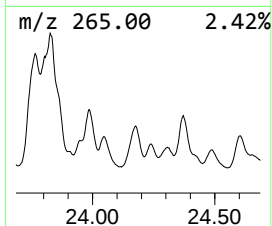
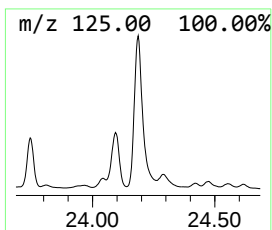
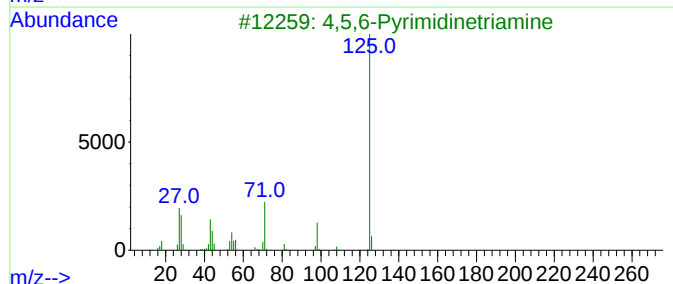
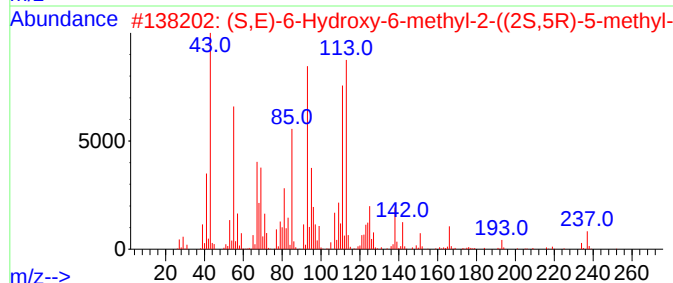
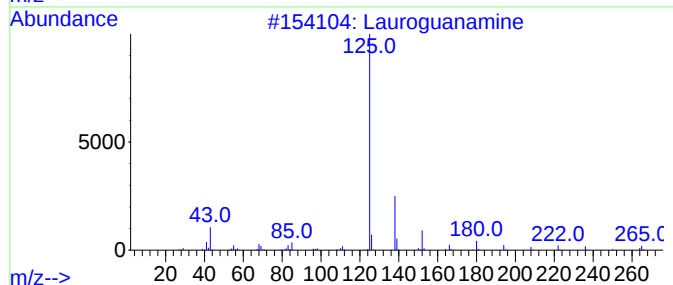
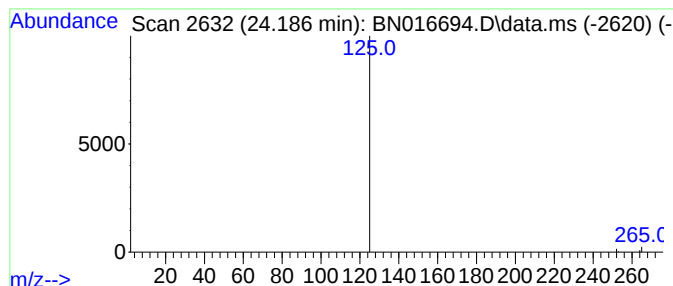
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Lauroguanamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.186	0.46 ng	268235	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Lauroguanamine	265	C14H27N5	002533-34-8	5
2			(S,E)-6-Hydroxy-6-methyl-2-((2S,...	252	C15H24O3	088243-64-5	3
3			4,5,6-Pyrimidinetriamine	125	C4H7N5	000118-70-7	2
4			2-Amino-4-hydroxy-6-methylpyrimi...	125	C5H7N3O	003977-29-5	2
5			Pyridine, 4-methoxy-1-oxide-	125	C6H7NO2	001122-96-9	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
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ALS Vial : 62 Sample Multiplier: 1

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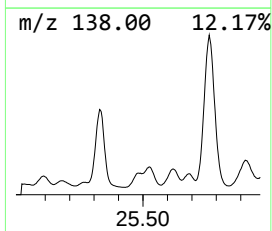
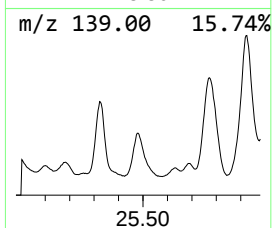
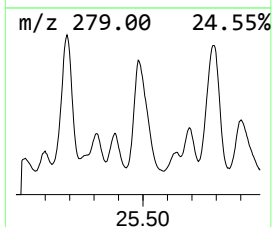
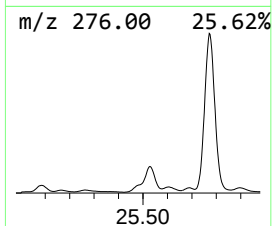
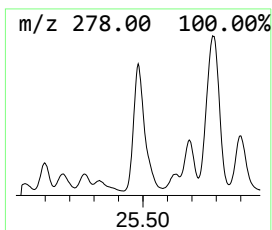
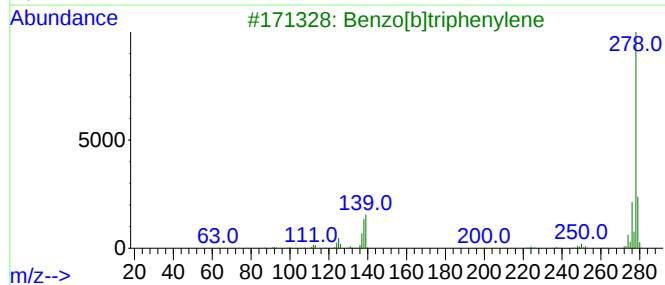
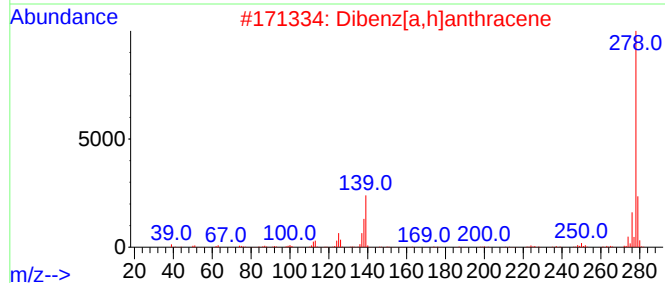
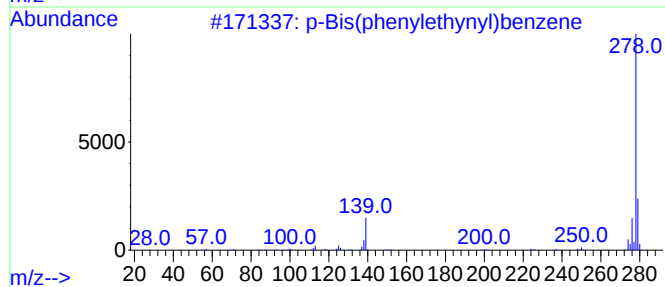
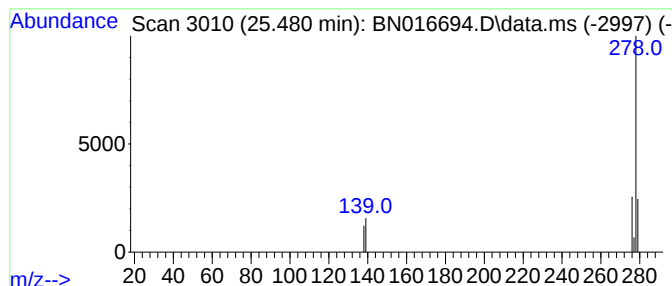
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 p-Bis(phenylethynyl)benzene Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.480	0.26 ng	154045	Perylene-d12	23.488

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		p-Bis(phenylethynyl)benzene	278	C22H14	001849-27-0	72
2		Dibenz[a,h]anthracene	278	C22H14	000053-70-3	64
3		Benzo[b]triphenylene	278	C22H14	000215-58-7	64
4		Pentaphene	278	C22H14	000222-93-5	64
5		Naphtho[1,2-a]anthracene	278	C22H14	000195-06-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
Acq On : 03 Oct 2021 06:24
Operator : CG/JU
Sample : M3892-09
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-0-0.5-092221

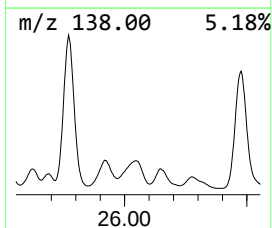
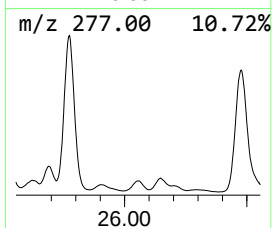
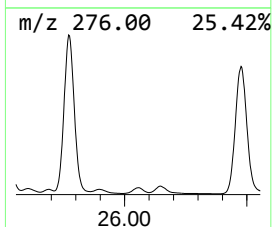
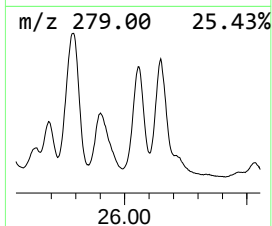
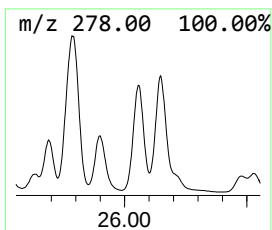
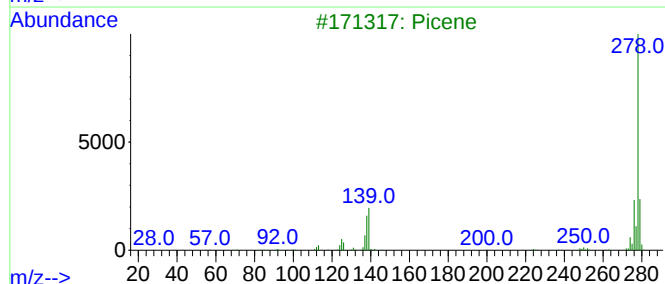
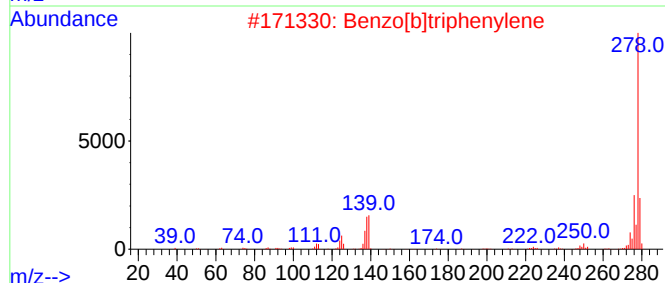
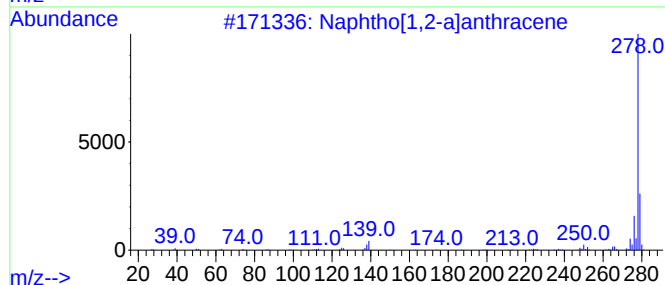
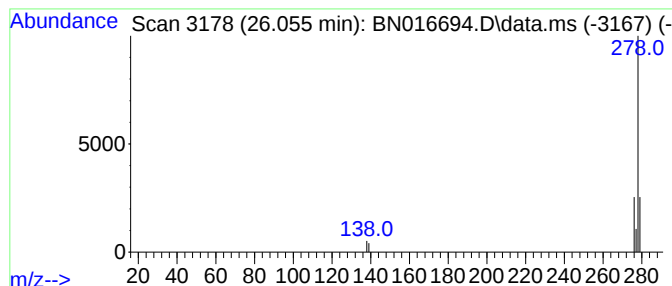
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Naphtho[1,2-a]anthracene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.055	0.22 ng	129159	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphtho[1,2-a]anthracene	278	C22H14	000195-06-2	72
2			Benzo[b]triphenylene	278	C22H14	000215-58-7	72
3			Picene	278	C22H14	000213-46-7	72
4			Benzo[b]chrysene	278	C22H14	000214-17-5	72
5			Dibenz[a,h]anthracene	278	C22H14	000053-70-3	56



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
Acq On : 03 Oct 2021 06:24
Operator : CG/JU
Sample : M3892-09
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-0-0.5-092221

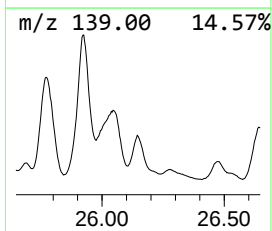
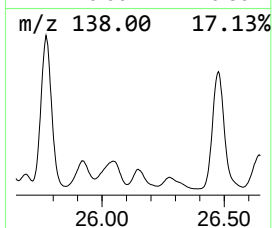
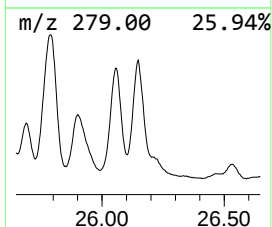
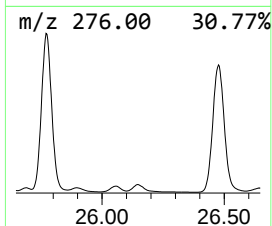
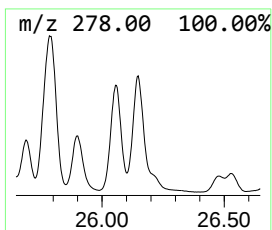
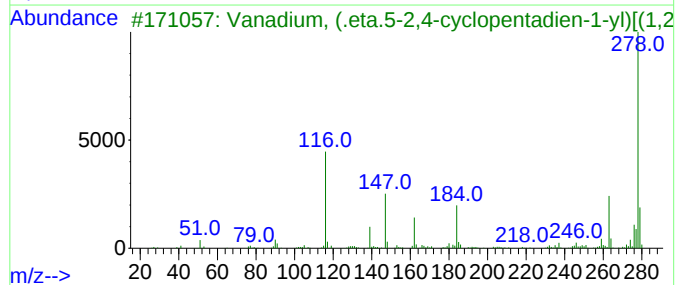
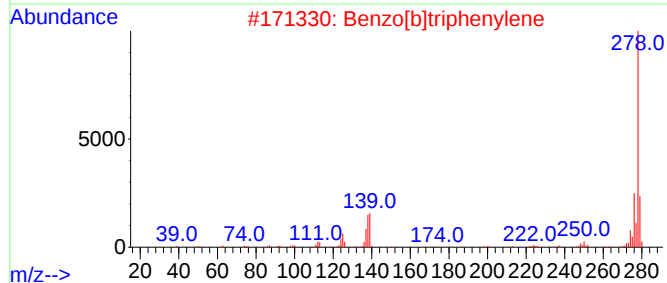
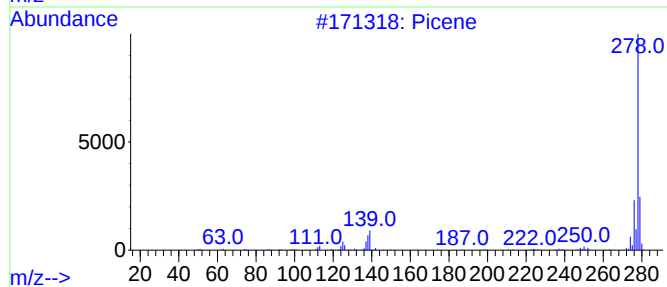
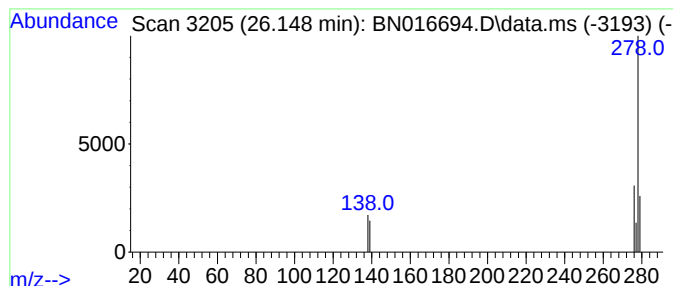
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Picene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.148	0.29 ng	169466	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Picene	278	C22H14	000213-46-7	80
2			Benzo[b]triphenylene	278	C22H14	000215-58-7	80
3			Vanadium, (.eta.5-2,4-cyclopenta...	278	C17H23V	126948-97-8	78
4			Benzo[b]chrysene	278	C22H14	000214-17-5	72
5			Benz[a]anthracene-7,12-dicarboni...	278	C20H10N2	035215-32-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016694.D
Acq On : 03 Oct 2021 06:24
Operator : CG/JU
Sample : M3892-09
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-824-N-SO-0-0.5-092221

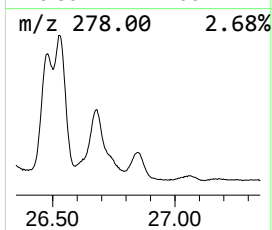
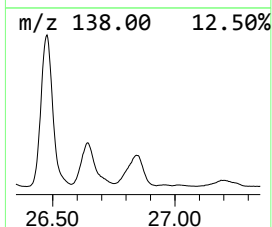
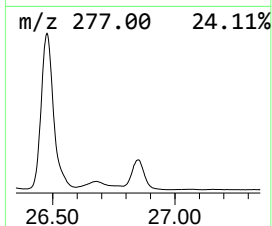
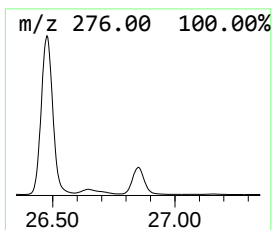
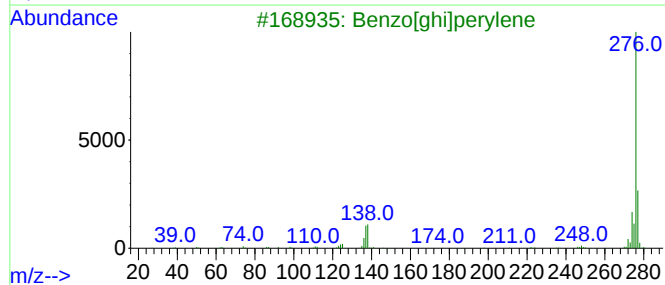
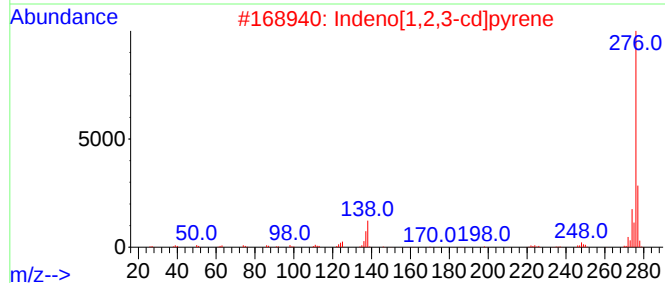
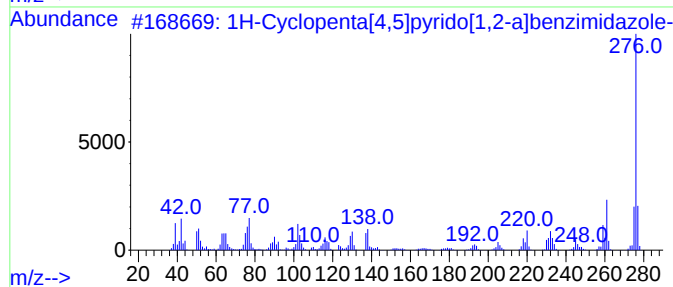
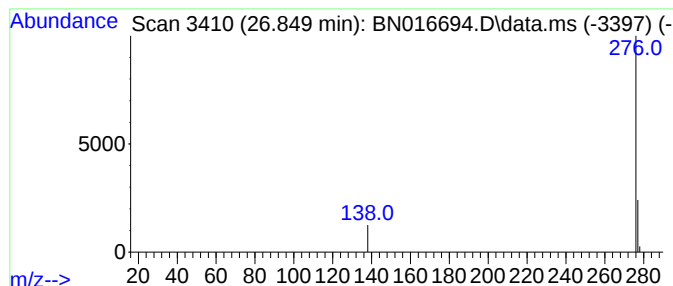
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 1H-Cyclopenta[4,5]pyrido[1,... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.849	0.23 ng	134541	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Cyclopenta[4,5]pyrido[1,2-a]b...	276	C17H16N4	329707-31-5	83
2			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	83
3			Benzo[ghi]perylene	276	C22H12	000191-24-2	83
4			propanedinitrile, 2-(2,6-di-2-fu...	276	C16H8N2O3	1000397-07-0	83
5			(4-Methoxy-3-methyl-phenyl)-naph...	276	C18H16N2O	1000190-44-9	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016694.D
 Acq On : 03 Oct 2021 06:24
 Operator : CG/JU
 Sample : M3892-09
 Misc :
 ALS Vial : 62 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.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
Acetaldehyde	4.277	0.2	ng	67052	1	7.642	109653	0.4
Butane	4.821	0.4	ng	104897	1	7.642	109653	0.4
2-Furancarboxit...	6.333	1.1	ng	290934	1	7.642	109653	0.4
2-Furancarboxit...	7.080	1.8	ng	480213	1	7.642	109653	0.4
Butane	7.937	1.0	ng	281680	1	7.642	109653	0.4
Benzene, nitro-	9.697	0.5	ng	221730	2	10.407	189377	0.4
Isopropyl isoth...	10.191	0.5	ng	243228	2	10.407	189377	0.4
Vanillin lactoside	13.190	0.4	ng	258218	3	14.269	229926	0.4
N-Ethyl-4-nitro...	14.129	0.2	ng	133023	3	14.269	229926	0.4
2,2-Diphenyleth...	16.007	0.3	ng	136018	4	17.018	192456	0.4
Carbazole	17.431	0.4	ng	194596	4	17.018	192456	0.4
Naphthalene, 1-...	17.955	0.2	ng	118133	4	17.018	192456	0.4
1-(4-Fluorophen...	22.560	0.3	ng	171051	6	23.488	233841	0.4
1,2-Dichloro-4-...	22.985	0.5	ng	298786	6	23.488	233841	0.4
Benzo[j]fluoran...	23.293	1.7	ng	1016220	6	23.488	233841	0.4
Lauroguanamine	24.186	0.5	ng	268235	6	23.488	233841	0.4
p-Bis(phenyleth...	25.480	0.3	ng	154045	6	23.488	233841	0.4
Naphtho[1,2-a]a...	26.055	0.2	ng	129159	6	23.488	233841	0.4
Picene	26.148	0.3	ng	169466	6	23.488	233841	0.4
1H-Cyclopenta[4...	26.849	0.2	ng	134541	6	23.488	233841	0.4