

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016700.D
 Acq On : 03 Oct 2021 10:00
 Operator : CG/JU
 Sample : M3892-11
 Misc :
 ALS Vial : 68 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-825-N-SO-0-0.5-092221

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : 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: BN016700.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.821	185	189	196	rVB	43241	82492	1.12%	0.143%
2	5.042	209	213	221	rBV	33686	83148	1.13%	0.144%
3	5.743	285	289	296	rVB	29709	74187	1.01%	0.128%
4	6.333	348	353	361	rVB	786186	1798680	24.44%	3.113%
5	6.628	381	385	395	rVB	51300	136135	1.85%	0.236%
6	7.080	429	434	444	rVB	838592	1830862	24.88%	3.169%
7	7.532	479	483	488	rVV	162958	306302	4.16%	0.530%
8	7.642	488	495	500	rVB	45199	96795	1.32%	0.168%
9	7.854	513	518	521	rBV	53642	99301	1.35%	0.172%
10	7.937	521	527	533	rVB	279414	547571	7.44%	0.948%
11	8.168	546	552	558	rBV	36777	76752	1.04%	0.133%
12	9.709	671	678	681	rBV2	110424	407694	5.54%	0.706%
13	9.824	684	687	691	rVB3	55172	112631	1.53%	0.195%
14	10.191	712	716	720	rBV	102659	208361	2.83%	0.361%
15	10.407	729	733	734	rBV	95291	165531	2.25%	0.286%
16	10.457	734	737	740	rVB2	333863	605682	8.23%	1.048%
17	12.003	923	931	939	rBV	48422	75402	1.02%	0.130%
18	12.078	939	948	963	rVB	112916	181257	2.46%	0.314%
19	12.296	988	997	1007	rVB	50957	78935	1.07%	0.137%
20	12.632	1049	1054	1059	rBV	62412	114411	1.55%	0.198%
21	12.886	1071	1074	1077	rBV2	89578	149298	2.03%	0.258%
22	13.190	1096	1098	1101	rVB	282630	406953	5.53%	0.704%
23	13.583	1127	1129	1132	rBV	139409	244465	3.32%	0.423%
24	13.748	1141	1142	1145	rVB	79156	110092	1.50%	0.191%
25	13.989	1158	1161	1164	rBV	681094	1070530	14.55%	1.853%
26	14.129	1167	1172	1176	rBV2	79596	168012	2.28%	0.291%
27	14.269	1179	1183	1186	rBV	130904	223298	3.03%	0.386%
28	14.332	1186	1188	1192	rVB3	128960	266143	3.62%	0.461%
29	14.763	1219	1222	1224	rVB	71769	122087	1.66%	0.211%
30	15.093	1245	1248	1250	rBV	140114	201060	2.73%	0.348%
31	15.169	1250	1254	1257	rVB2	188617	312941	4.25%	0.542%
32	15.322	1264	1266	1270	rBV	120572	212393	2.89%	0.368%
33	15.626	1287	1290	1292	rBV2	70174	137623	1.87%	0.238%
34	15.740	1296	1299	1300	rVV	68156	149937	2.04%	0.259%
35	15.766	1300	1301	1305	rVB	106012	145422	1.98%	0.252%
36	16.007	1317	1320	1322	rVB2	131625	171630	2.33%	0.297%

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016700.D
 Acq On : 03 Oct 2021 10:00
 Operator : CG/JU
 Sample : M3892-11
 Misc :
 ALS Vial : 68 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-825-N-SO-0-0.5-092221

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : 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

37	16.080	1322	1326	1332	rBV	67476	113706	1.54%	0.197%
38	16.591	1365	1368	1372	rVB2	140071	206103	2.80%	0.357%
39	17.030	1400	1404	1405	rBV	97205	228802	3.11%	0.396%
40	17.066	1405	1407	1410	rVV	1797670	2429845	33.02%	4.205%
41	17.151	1410	1414	1417	rVB	690523	1106273	15.03%	1.915%
42	17.431	1432	1437	1440	rBV	276758	403096	5.48%	0.698%
43	17.796	1465	1467	1471	rVB2	48710	104542	1.42%	0.181%
44	17.894	1471	1475	1477	rBV2	71704	148315	2.02%	0.257%
45	17.955	1477	1480	1483	rVB3	69690	142030	1.93%	0.246%
46	18.417	1560	1566	1572	rBV	136862	184469	2.51%	0.319%
47	19.103	1692	1704	1713	rBV	5048089	7359688	100.00%	12.738%
48	19.251	1729	1734	1739	rVB2	286379	372984	5.07%	0.646%
49	19.366	1746	1757	1767	rVB3	71880	198482	2.70%	0.344%
50	19.465	1767	1777	1787	rBV	4187328	6297152	85.56%	10.899%
51	19.678	1815	1820	1823	rVV	100289	139500	1.90%	0.241%
52	19.708	1823	1826	1835	rVB	88701	130953	1.78%	0.227%
53	19.927	1864	1870	1875	rBV4	45063	83186	1.13%	0.144%
54	20.112	1893	1896	1899	rBV2	73557	181189	2.46%	0.314%
55	20.346	1912	1918	1920	rBV3	47735	146924	2.00%	0.254%
56	20.463	1926	1929	1933	rBV	352571	541722	7.36%	0.938%
57	20.537	1933	1936	1939	rBV2	51340	112904	1.53%	0.195%
58	20.718	1950	1953	1957	rVB	273484	409931	5.57%	0.709%
59	20.824	1960	1963	1965	rVV	215271	348535	4.74%	0.603%
60	20.866	1965	1967	1970	rVV2	210576	406828	5.53%	0.704%
61	20.919	1970	1972	1974	rVV	385110	603086	8.19%	1.044%
62	20.962	1974	1976	1979	rVV2	352857	734015	9.97%	1.270%
63	21.015	1979	1981	1984	rVB	270528	339248	4.61%	0.587%
64	21.174	1994	1996	1997	rBV	139640	173414	2.36%	0.300%
65	21.227	1997	2001	2003	rVV	2659705	4184730	56.86%	7.243%
66	21.280	2003	2006	2012	rVB	2914143	4421823	60.08%	7.653%
67	21.397	2015	2017	2020	rBV	163266	313518	4.26%	0.543%
68	21.610	2034	2037	2042	rVB3	112021	258281	3.51%	0.447%
69	21.790	2052	2054	2057	rVB	85837	135660	1.84%	0.235%
70	21.854	2057	2060	2064	rVV3	168792	381240	5.18%	0.660%
71	21.928	2064	2067	2071	rVV2	116917	237495	3.23%	0.411%
72	21.992	2071	2073	2075	rVV	131841	221793	3.01%	0.384%
73	22.024	2075	2076	2079	rVV	175354	206791	2.81%	0.358%
74	22.109	2080	2084	2087	rVB	120659	216955	2.95%	0.375%
75	22.268	2096	2099	2102	rBV	67610	110470	1.50%	0.191%
76	22.396	2109	2111	2113	rVB2	80714	80173	1.09%	0.139%

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016700.D
 Acq On : 03 Oct 2021 10:00
 Operator : CG/JU
 Sample : M3892-11
 Misc :
 ALS Vial : 68 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-825-N-SO-0-0.5-092221

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : 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

77	22.574	2151	2161	2177	rVB2	115619	202734	2.75%	0.351%
78	22.738	2202	2209	2220	rVB2	61758	96774	1.31%	0.167%
79	22.827	2221	2235	2243	rBV	1833211	4162289	56.56%	7.204%
80	22.995	2273	2284	2313	rVB	391503	723146	9.83%	1.252%
81	23.303	2362	2374	2390	rVB	902613	1663762	22.61%	2.880%
82	23.399	2390	2402	2419	rVB	920433	1699398	23.09%	2.941%
83	23.498	2421	2431	2436	rBV2	78600	146942	2.00%	0.254%
84	23.546	2437	2445	2461	rVB	253695	512765	6.97%	0.887%
85	23.755	2497	2506	2518	rBV3	39743	99092	1.35%	0.172%
86	24.183	2621	2631	2644	rBV	71197	152883	2.08%	0.265%
87	25.103	2888	2900	2912	rVB4	31729	77254	1.05%	0.134%
88	25.487	2999	3012	3020	rBV2	80414	214938	2.92%	0.372%
89	25.778	3082	3097	3120	rVB2	370850	1109931	15.08%	1.921%
90	25.911	3123	3136	3161	rVB3	41445	130992	1.78%	0.227%
91	26.058	3166	3179	3193	rVV	59463	162669	2.21%	0.282%
92	26.151	3194	3206	3272	rVB2	76941	285037	3.87%	0.493%
93	26.483	3284	3303	3333	rVB	213742	662508	9.00%	1.147%
94	26.849	3399	3410	3434	rVB2	27010	86418	1.17%	0.150%

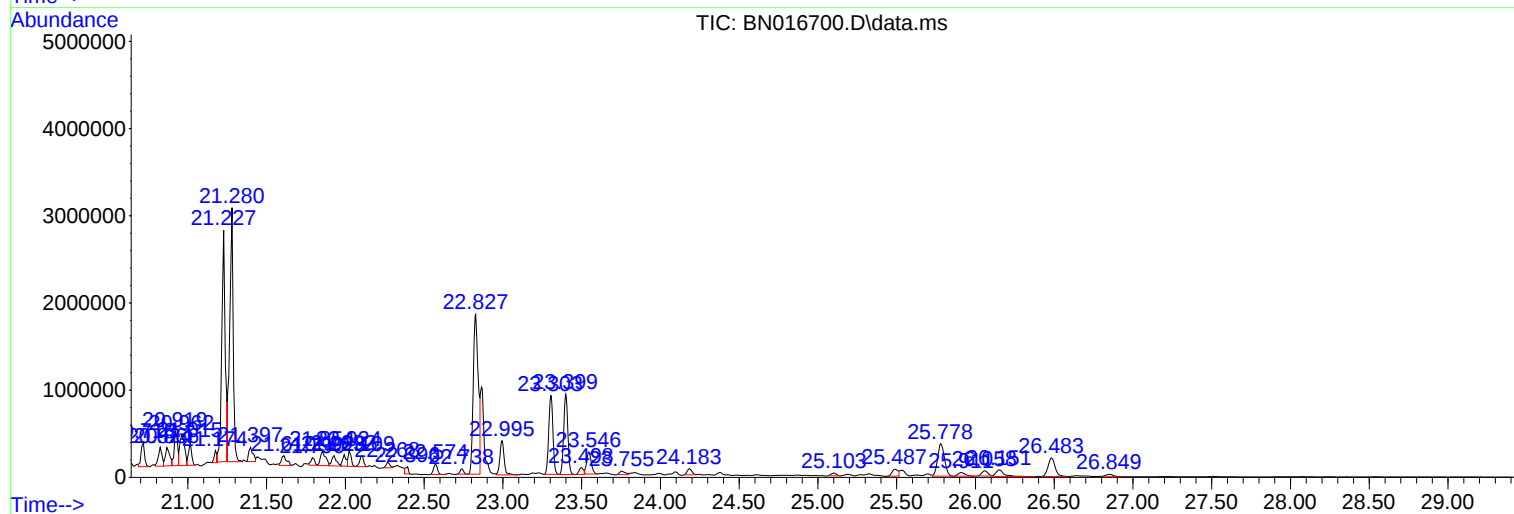
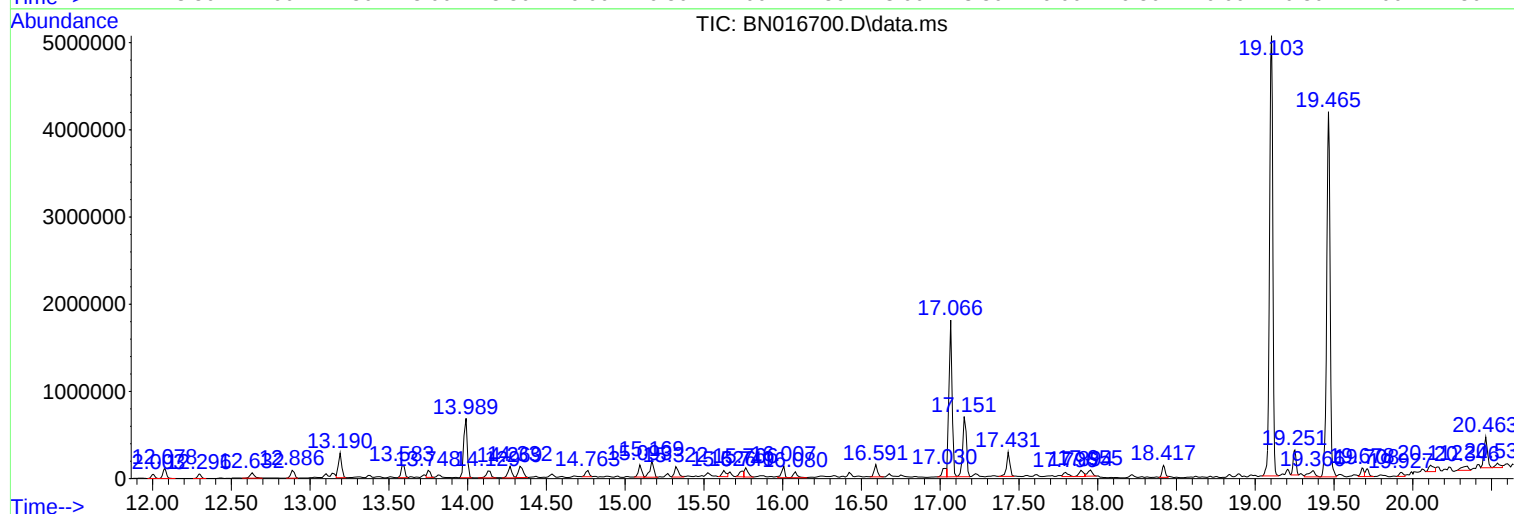
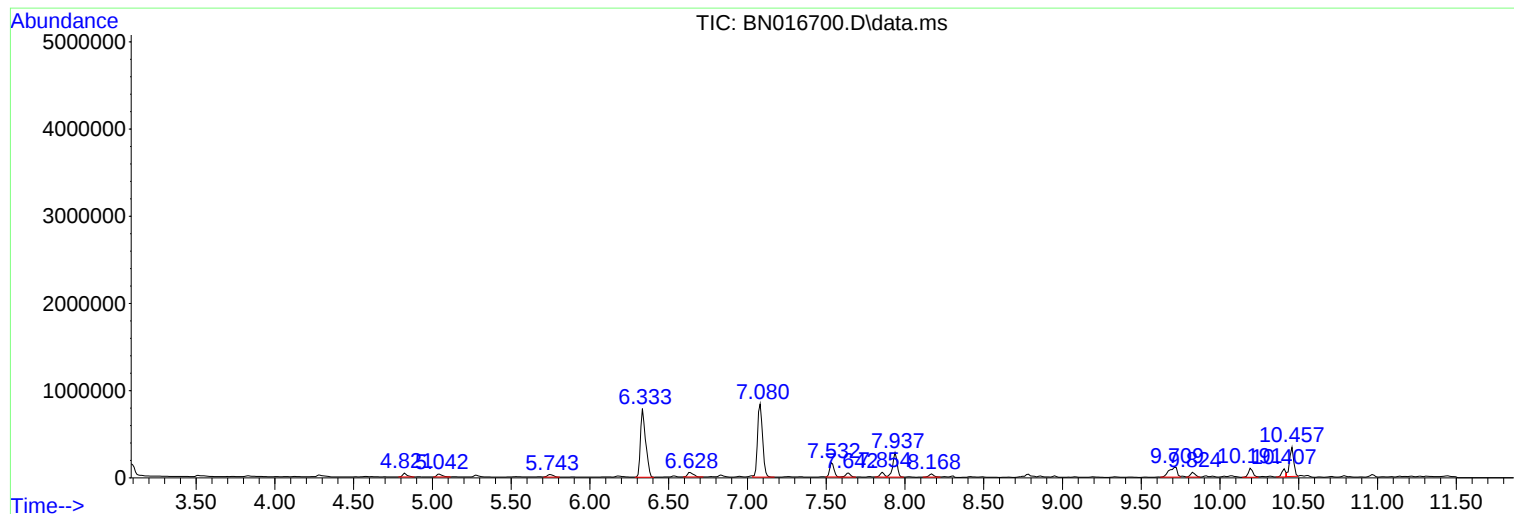
Sum of corrected areas: 57779396

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

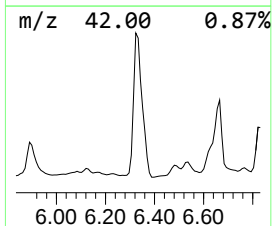
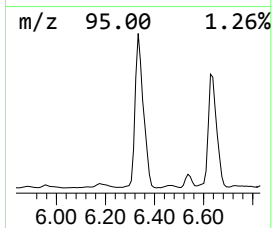
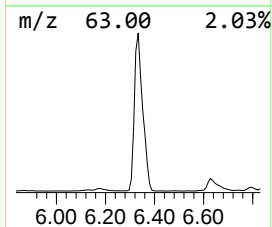
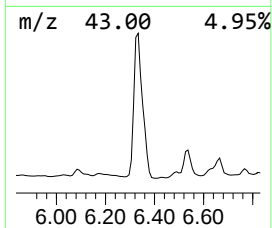
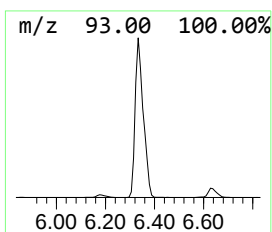
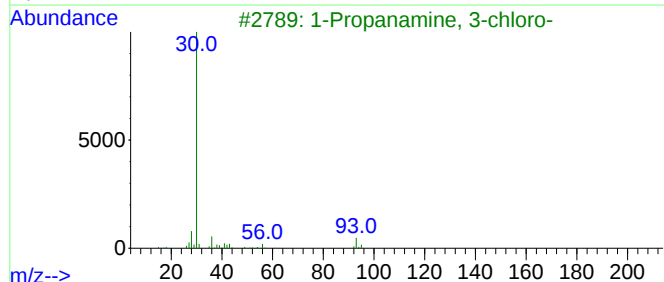
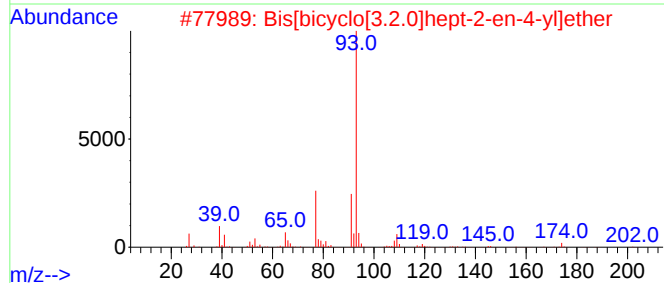
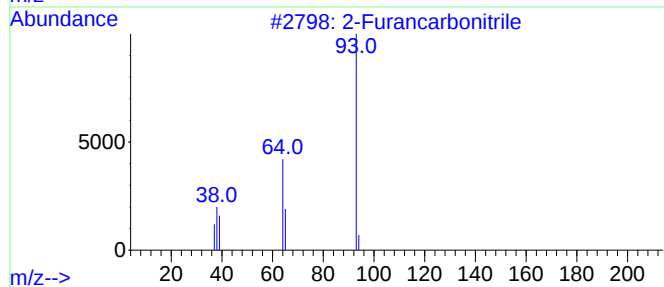
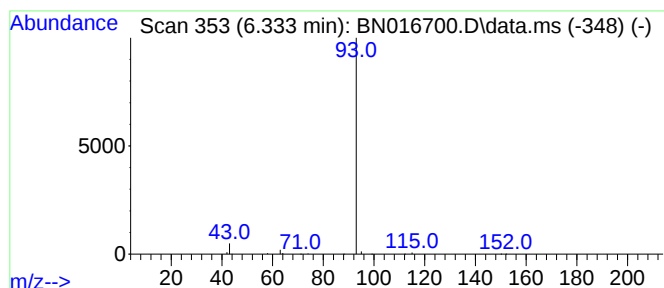
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Furancarbonitrile Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.333	7.43 ng	1798680	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\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

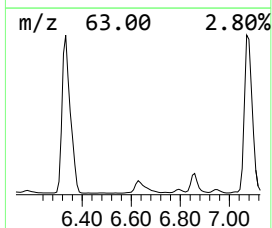
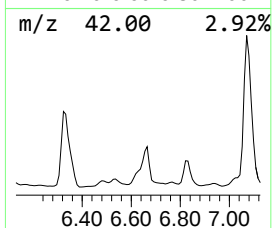
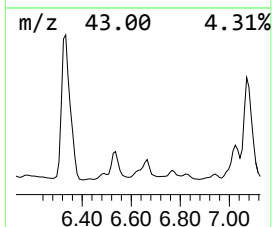
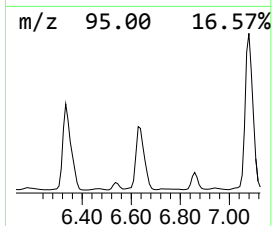
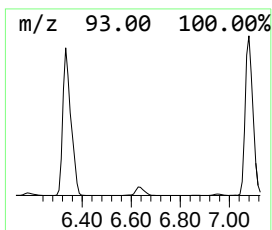
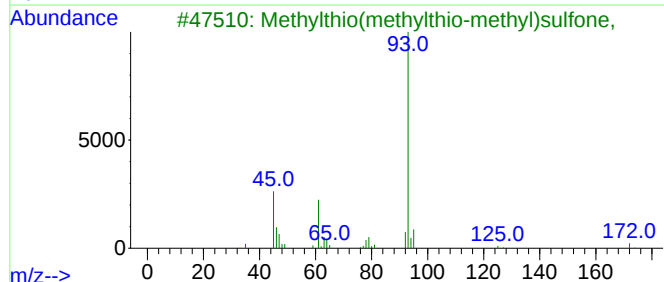
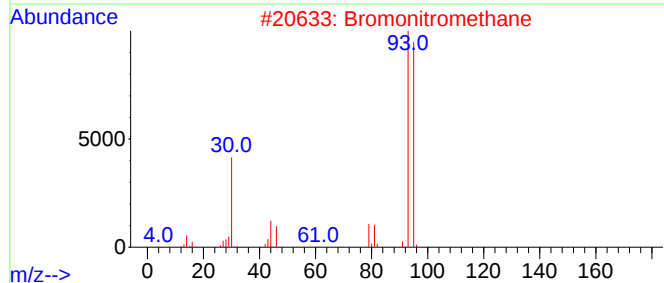
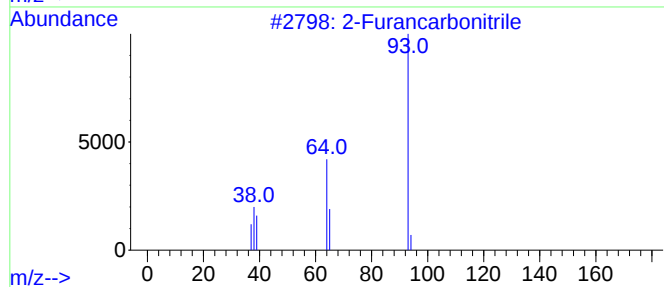
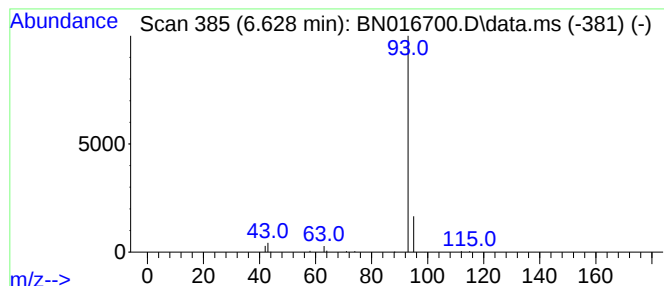
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Furancarbonitrile Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.628	0.56 ng	136135	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			Bromonitromethane	139	CH2BrNO2	000563-70-2	1
3			Methylthio(methylthio-methyl)sul...	172	C3H8O2S3	058000-45-6	1
4			1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	1
5			4-(2-Aminoethyl)pyridine	122	C7H10N2	013258-63-4	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

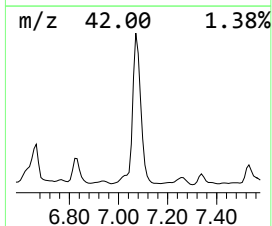
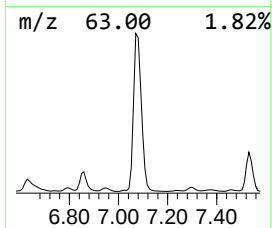
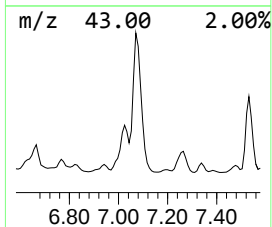
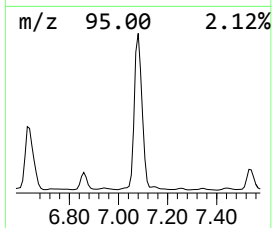
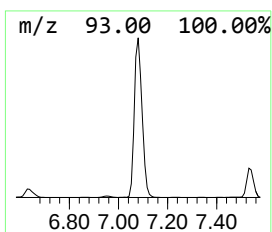
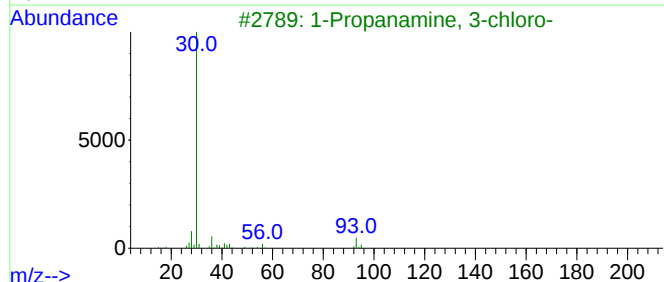
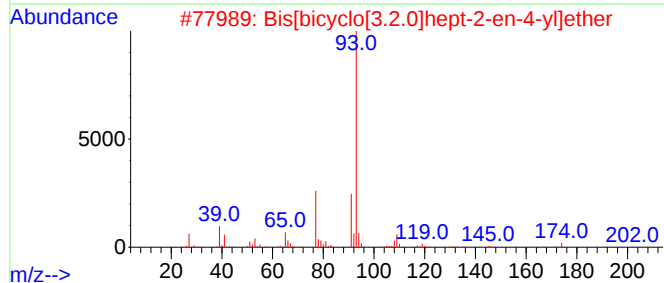
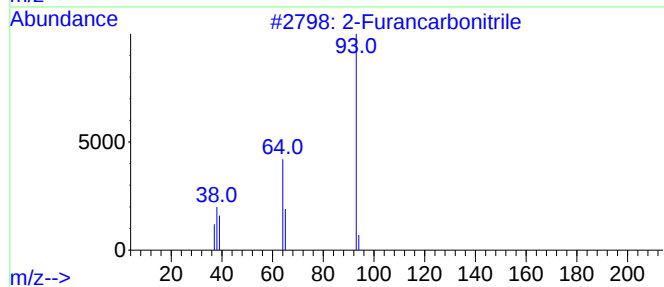
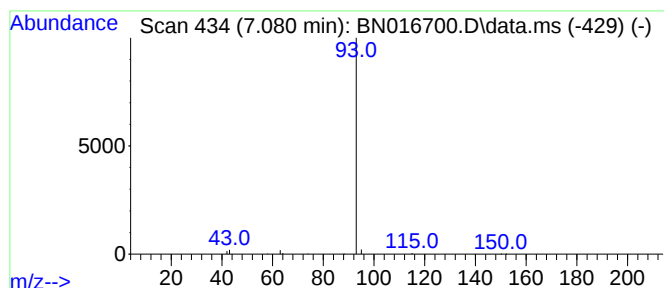
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Furancarbonitrile Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.080	7.57 ng	1830860	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\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

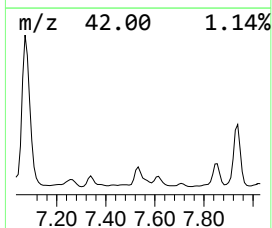
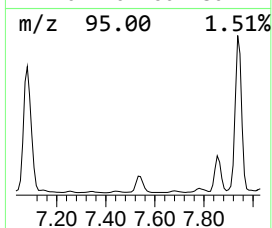
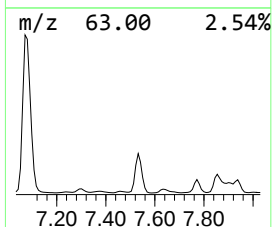
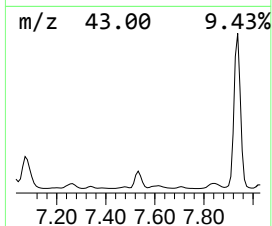
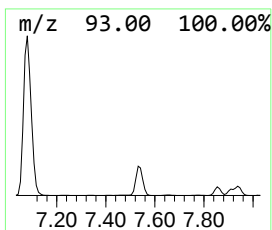
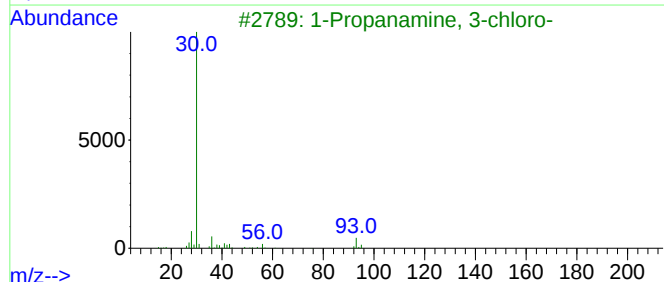
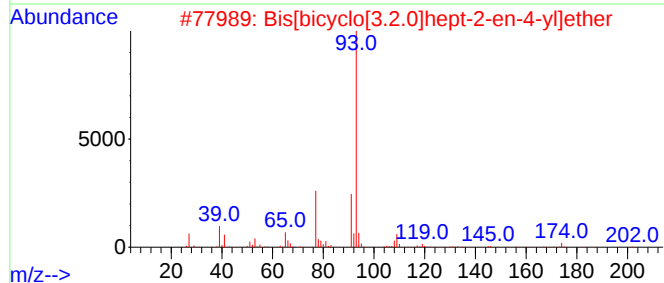
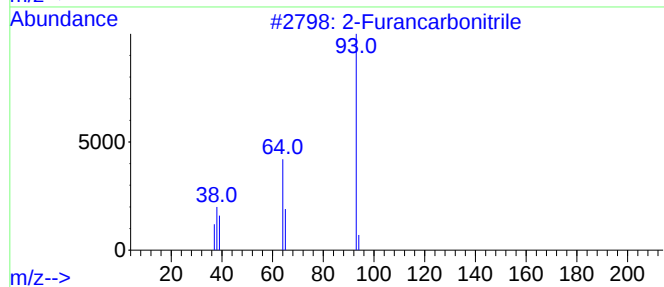
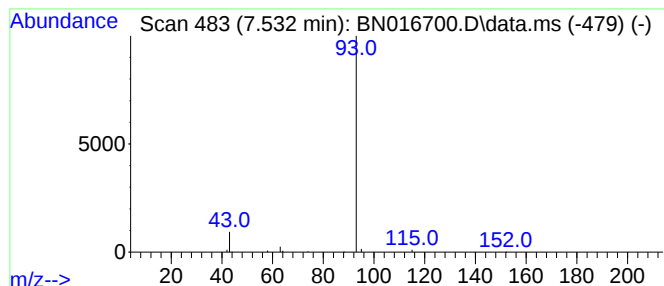
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Furancarbonitrile Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.532	1.27 ng	306302	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			4-(2-Aminoethyl)pyridine	122	C7H10N2	013258-63-4	1
5			Bromonitromethane	139	CH2BrNO2	000563-70-2	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

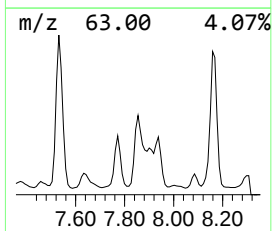
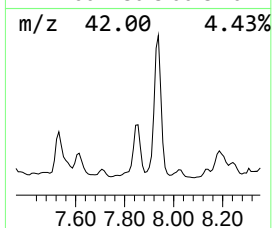
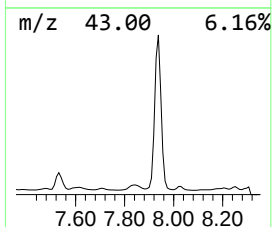
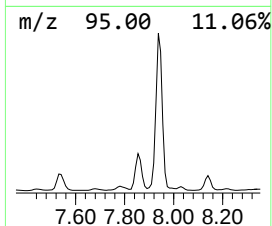
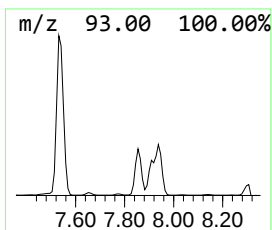
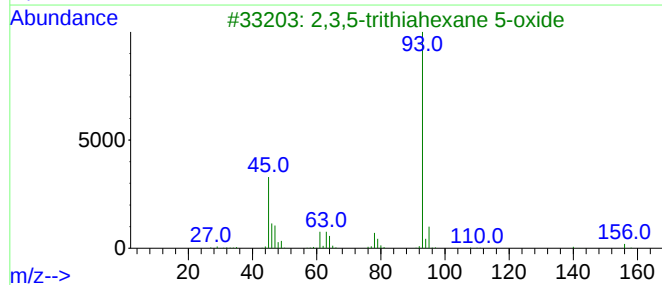
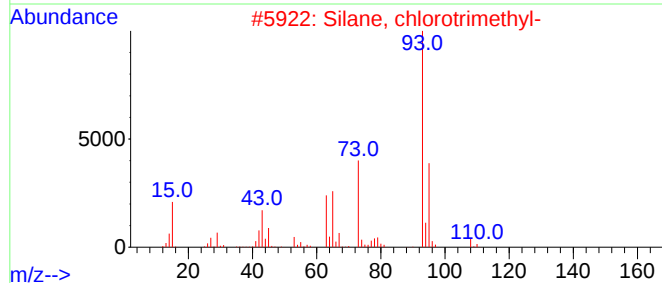
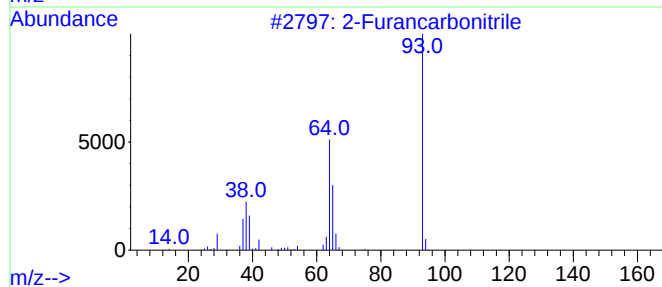
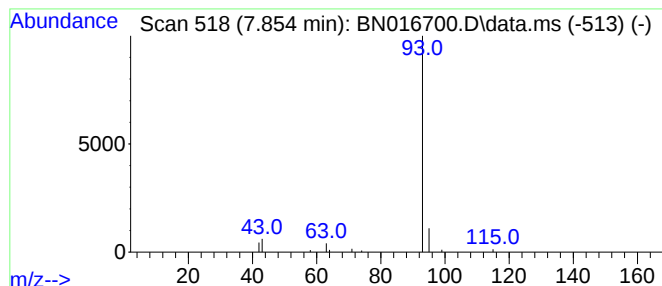
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Furancarbonitrile Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.854	0.41 ng	99301	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Furancarbonitrile	93	C5H3NO	000617-90-3	3
2			Silane, chlorotrimethyl-	108	C3H9ClSi	000075-77-4	2
3			2,3,5-trithiahexane 5-oxide	156	C3H8OS3	042474-27-1	1
4			Methylthio(methylthio-methyl)sul...	172	C3H8O2S3	058000-45-6	1
5			1,4-Methano-1H-Cyclopropa[d]pyri...	136	C8H12N2	109746-10-3	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

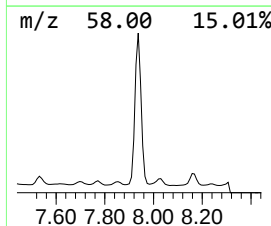
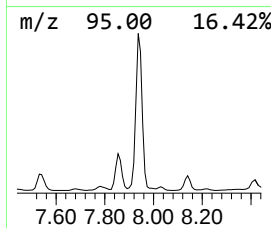
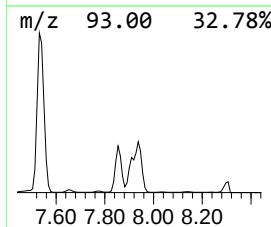
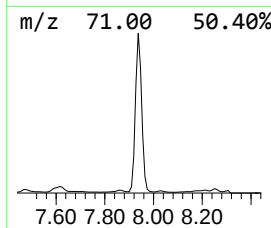
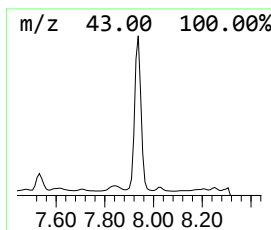
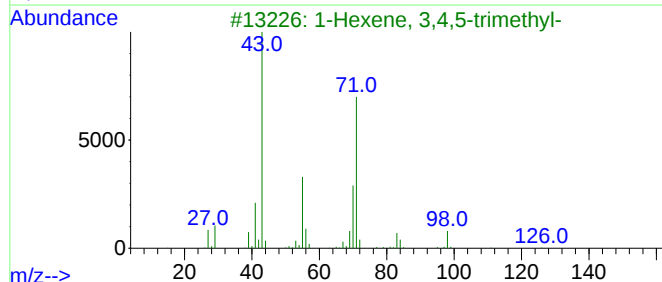
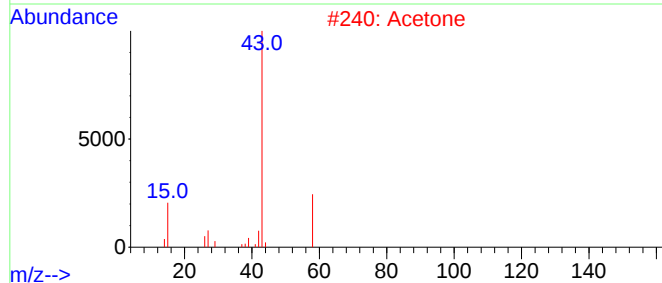
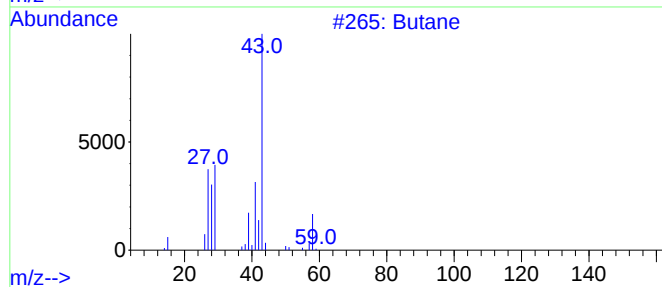
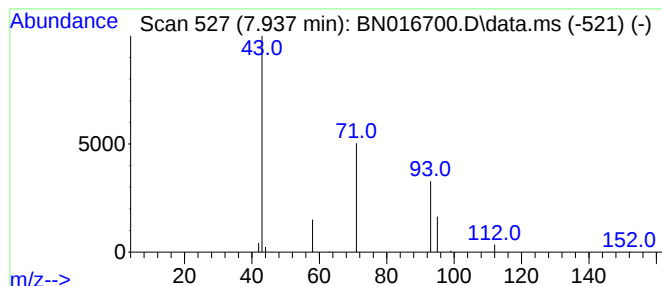
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.937	2.26 ng	547571	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			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	4
4			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3
5			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

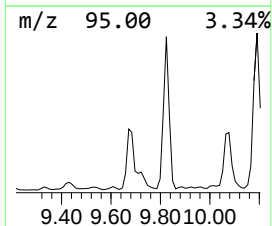
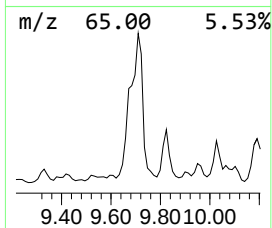
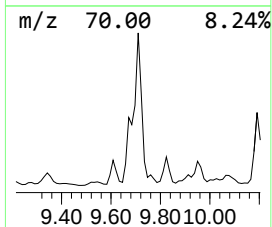
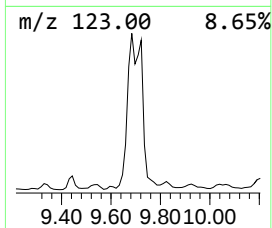
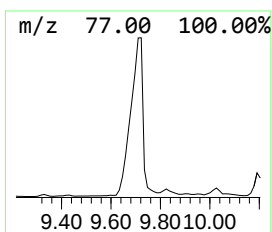
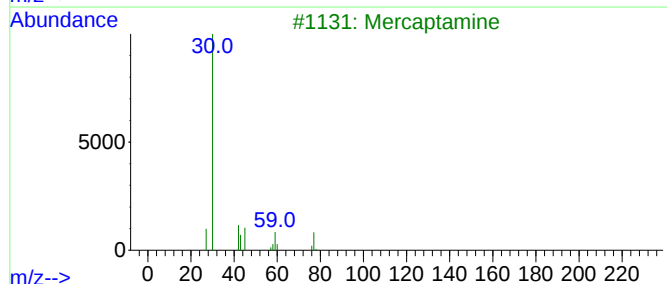
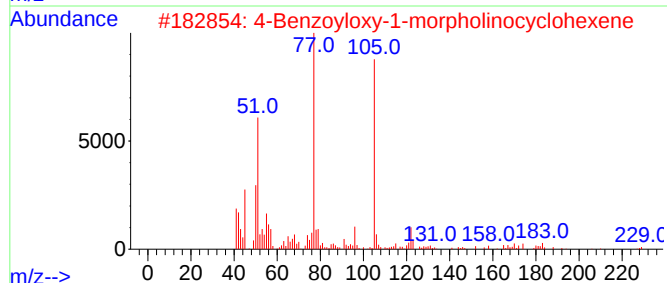
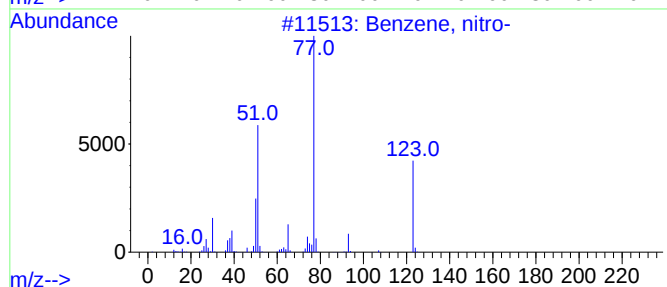
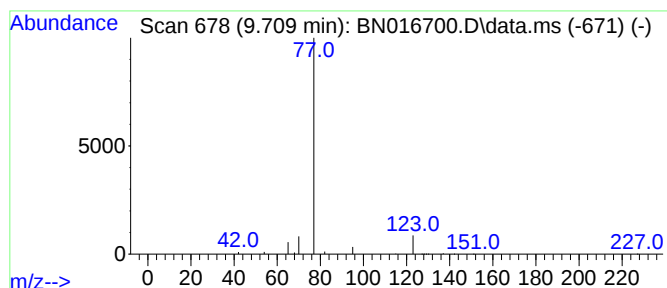
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, nitro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.709	0.99 ng	407694	Naphthalene-d8	10.406

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			Mercaptamine	77	C2H7NS	000060-23-1	1
4			Silanamine, N-silyl-	77	H7NSi2	005702-11-4	1
5			1,5-Hexadiene, 3,3,4,4-tetrafluoro-	154	C6H6F4	001763-21-9	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

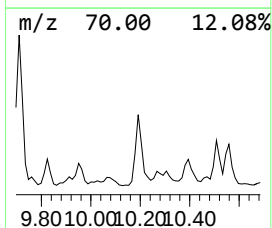
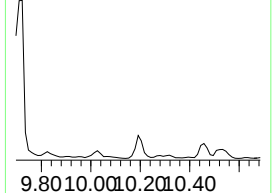
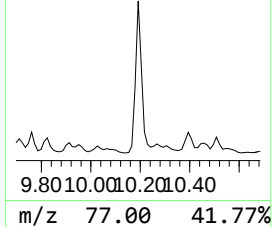
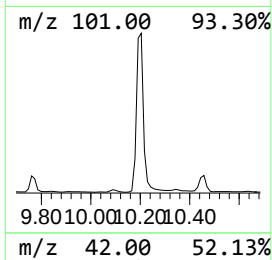
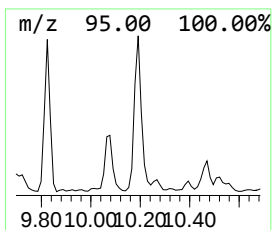
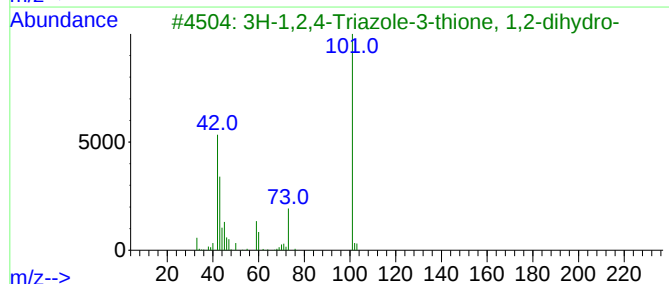
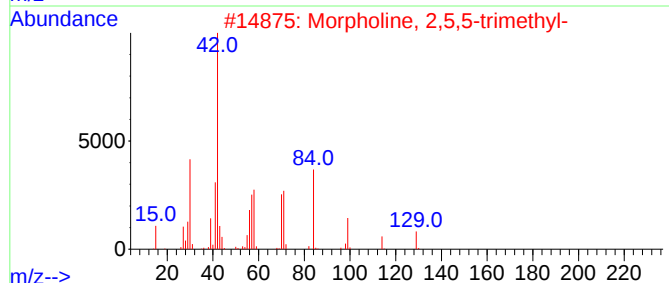
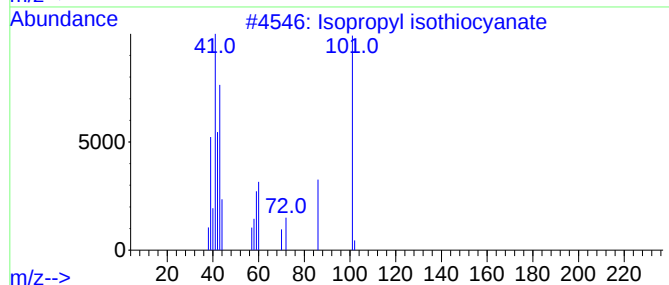
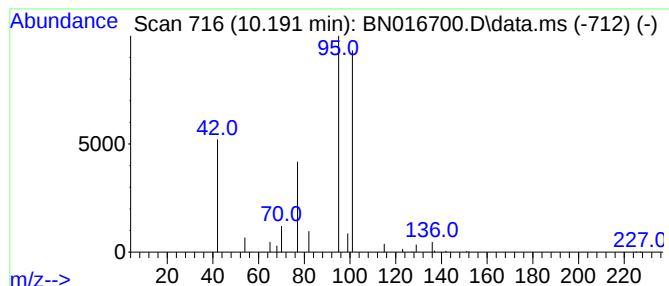
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Isopropyl isothiocyanate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.50 ng	208361	Naphthalene-d8	10.406

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9
2			Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	9
3			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4			2-Pyrimidinamine	95	C4H5N3	000109-12-6	5
5			Aminopyrazine	95	C4H5N3	005049-61-6	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

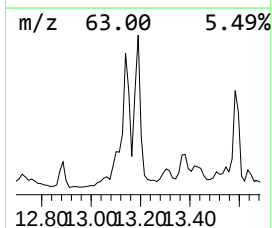
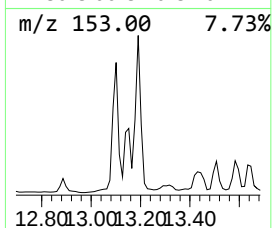
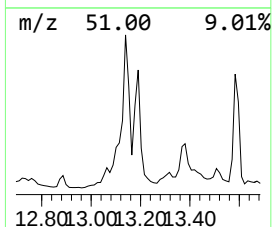
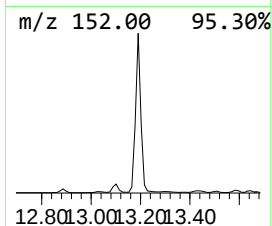
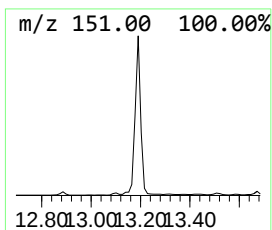
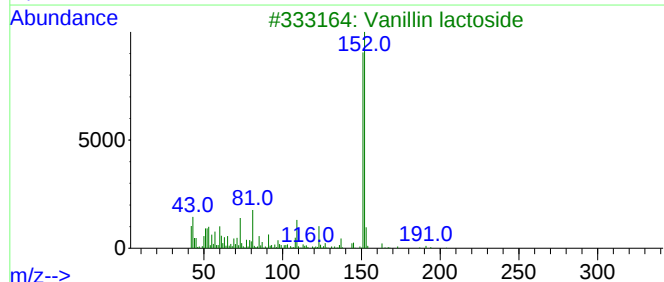
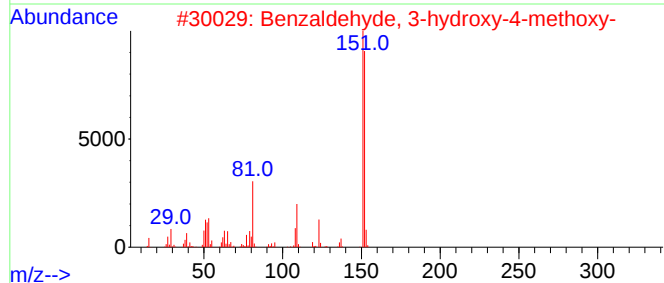
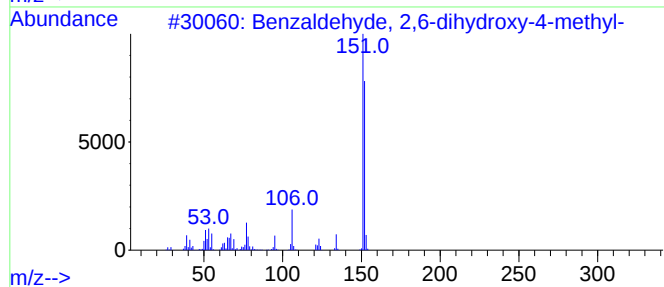
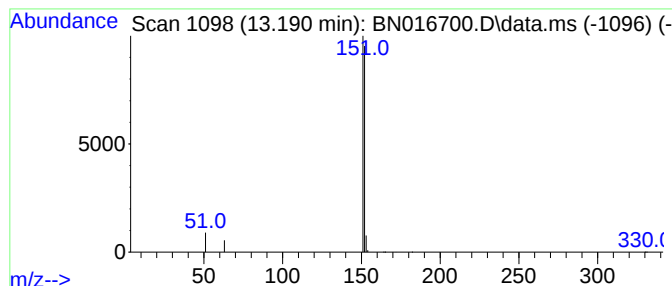
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzaldehyde, 2,6-dihydroxy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.190	0.73 ng	406953	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde, 2,6-dihydroxy-4-me...	152	C8H8O3	000526-37-4	74
2			Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	74
3			Vanillin lactoside	476	C20H28O13	1000129-94-7	64
4			Vanillin	152	C8H8O3	000121-33-5	9
5			Benzaldehyde, 2,4-dihydroxy-6-me...	152	C8H8O3	000487-69-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

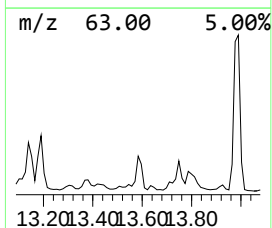
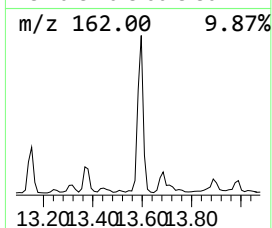
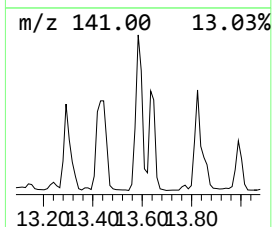
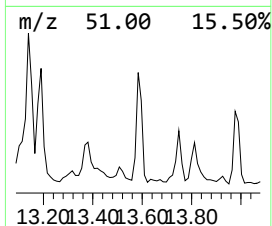
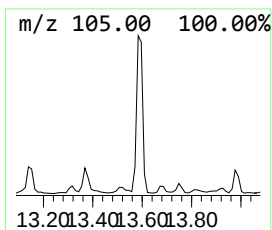
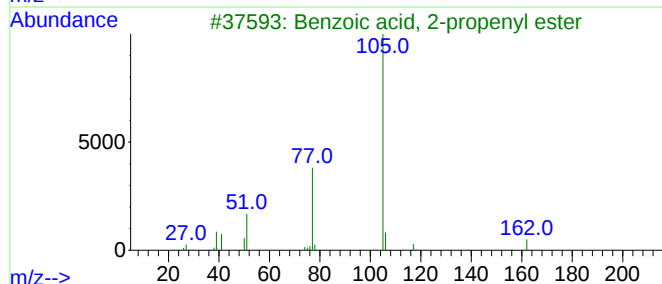
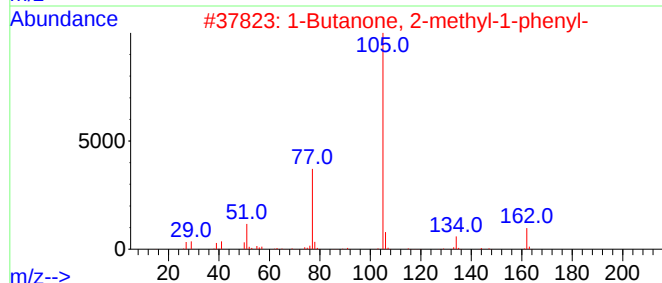
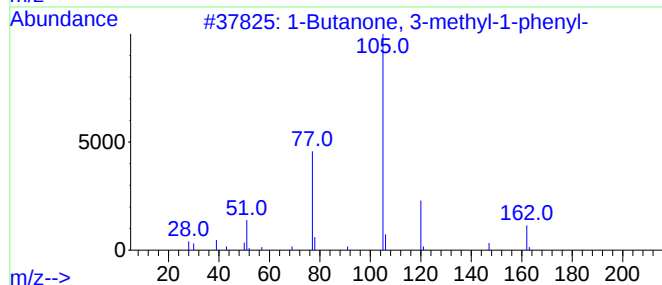
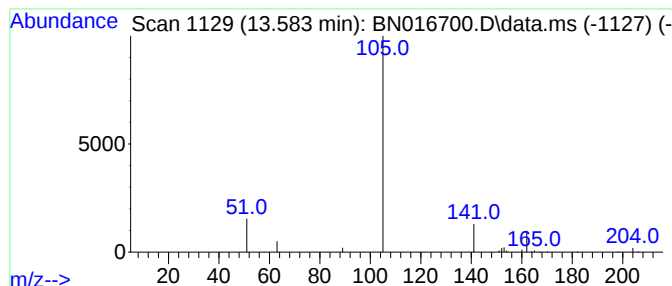
Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

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 10 1-Butanone, 3-methyl-1-phenyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.584	0.44 ng	244465	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Butanone, 3-methyl-1-phenyl-		162	C11H14O	000582-62-7	7
2	1-Butanone, 2-methyl-1-phenyl-		162	C11H14O	000938-87-4	7
3	Benzoic acid, 2-propenyl ester		162	C10H10O2	000583-04-0	5
4	Cyclobutyl phenyl ketone		160	C11H12O	005407-98-7	4
5	Phenol, 2,5-dichloro-, acetate		204	C8H6Cl2O2	030124-46-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

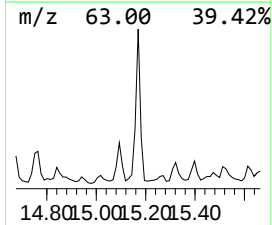
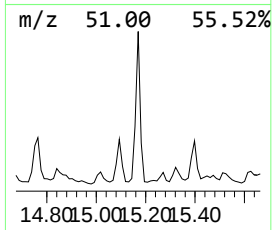
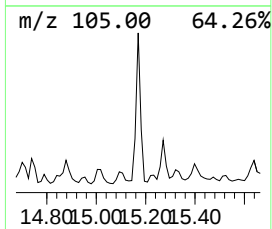
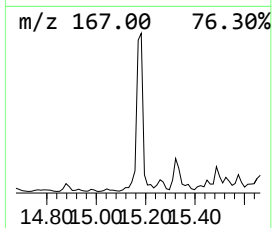
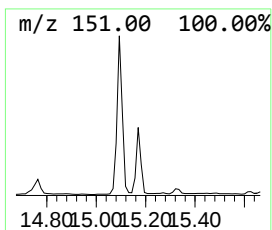
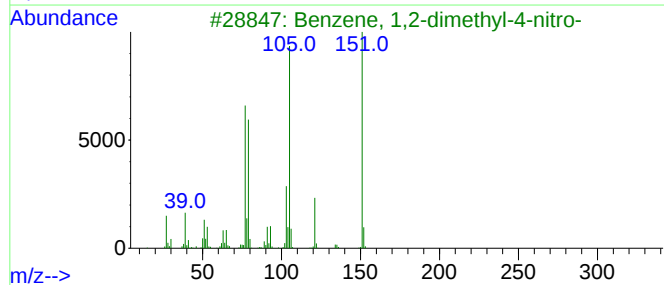
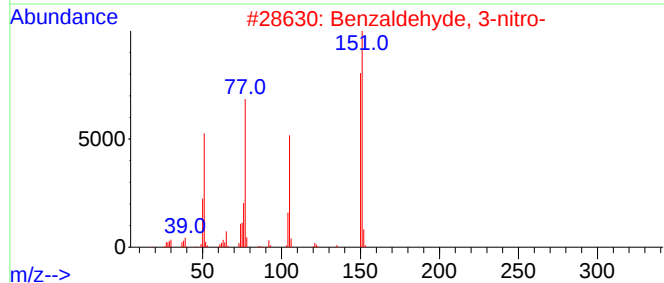
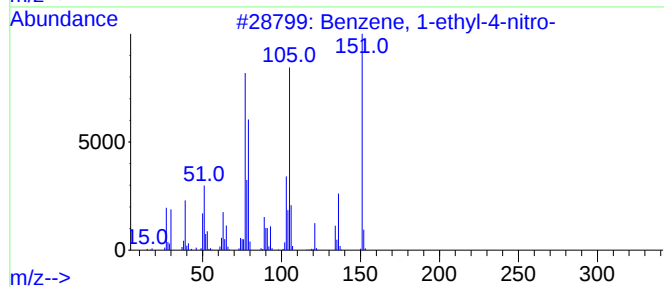
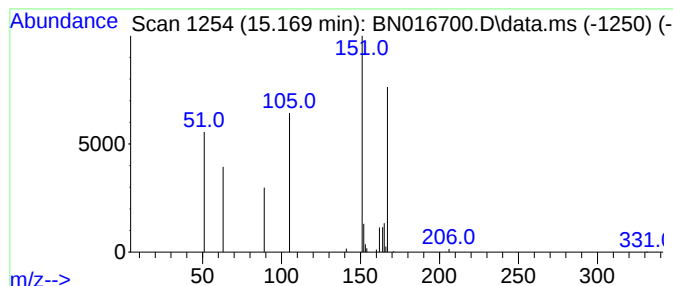
Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

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 11 Benzene, 1-ethyl-4-nitro- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.169	0.56 ng	312941	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-nitro-		151	C8H9NO2	000100-12-9	22
2	Benzaldehyde, 3-nitro-		151	C7H5NO3	000099-61-6	10
3	Benzene, 1,2-dimethyl-4-nitro-		151	C8H9NO2	000099-51-4	9
4	Benzaldehyde, 4-nitro-		151	C7H5NO3	000555-16-8	9
5	1H-Indole, 4-chloro-		151	C8H6ClN	025235-85-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

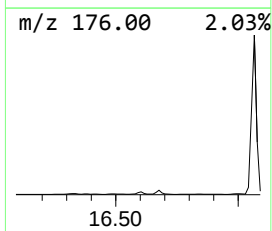
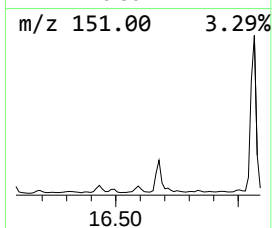
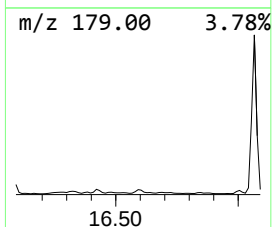
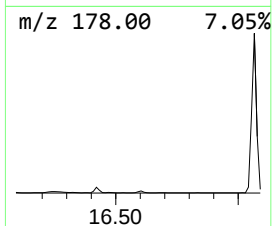
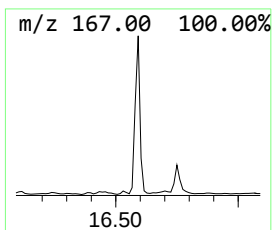
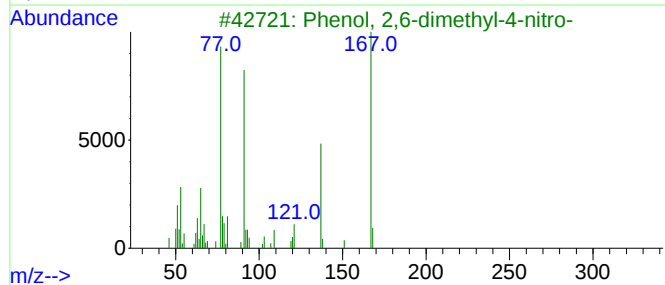
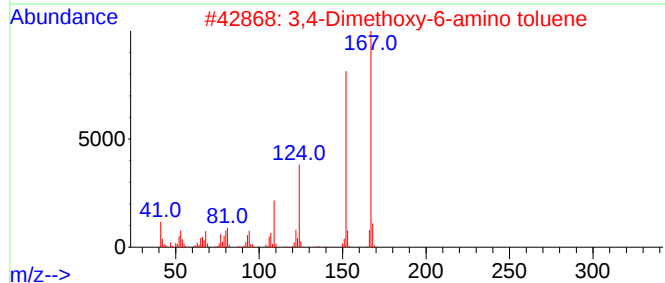
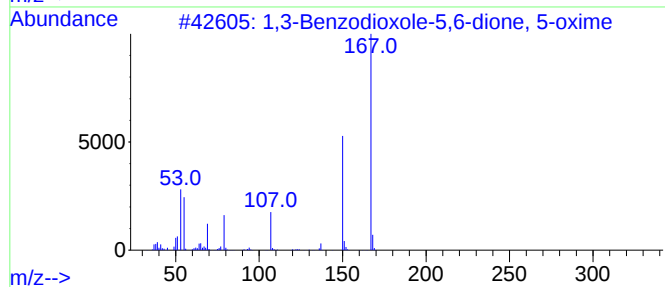
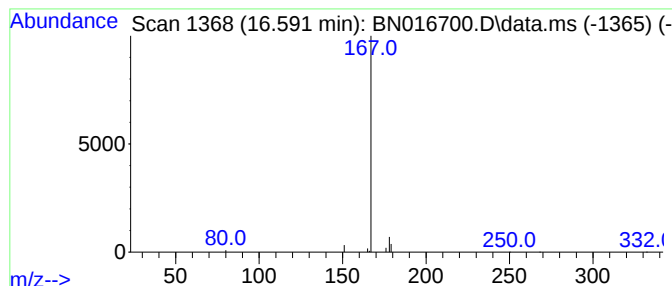
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1,3-Benzodioxole-5,6-dione,... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.592	0.36 ng	206103	Phenanthrene-d10	17.030

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzodioxole-5,6-dione, 5-oxime	167	C7H5NO4	1000337-44-2	5
2			3,4-Dimethoxy-6-amino toluene	167	C9H13NO2	041864-45-3	4
3			Phenol, 2,6-dimethyl-4-nitro-	167	C8H9NO3	002423-71-4	4
4			Benzoic acid, 4-nitro-	167	C7H5NO4	000062-23-7	4
5			Thioguanine	167	C5H5N5S	000154-42-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

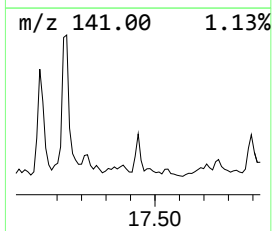
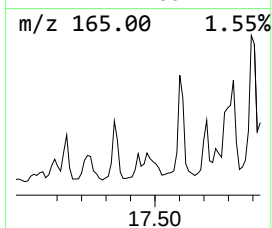
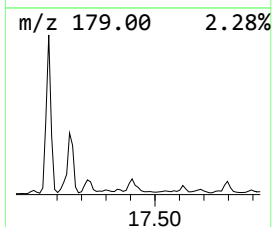
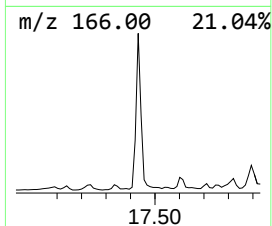
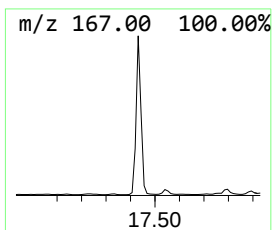
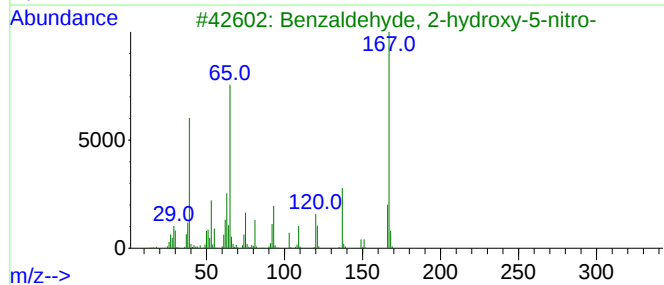
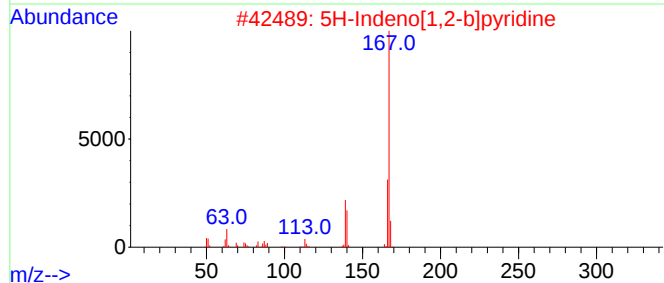
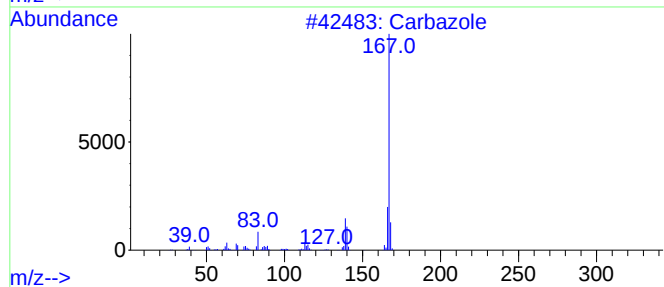
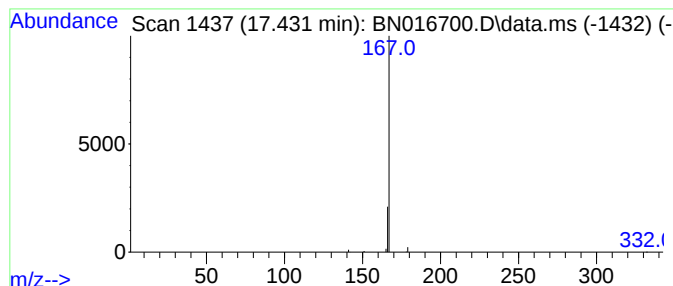
Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

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 13 Carbazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.431	0.70 ng	403096	Phenanthrene-d10		17.030	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Carbazole		167	C12H9N	000086-74-8	9
2	5H-Indeno[1,2-b]pyridine		167	C12H9N	000244-99-5	5
3	Benzaldehyde, 2-hydroxy-5-nitro-		167	C7H5NO4	000097-51-8	5
4	5-Fluoro-2-methyl-benzothiazole		167	C8H6FNS	000399-75-7	5
5	benzaldehyde, 2-hydroxy-4-nitro-		167	C7H5NO4	1000404-52-2	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

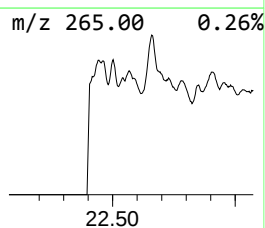
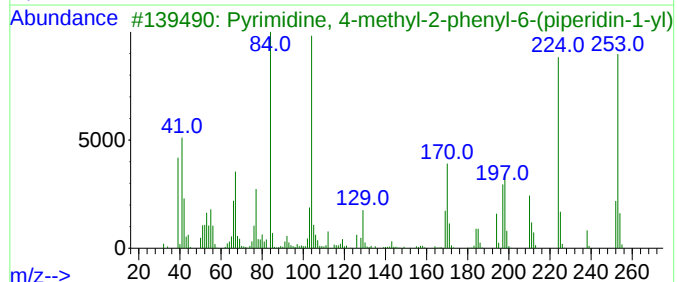
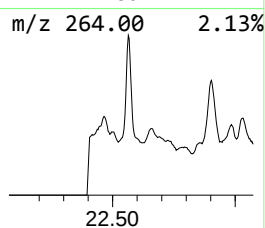
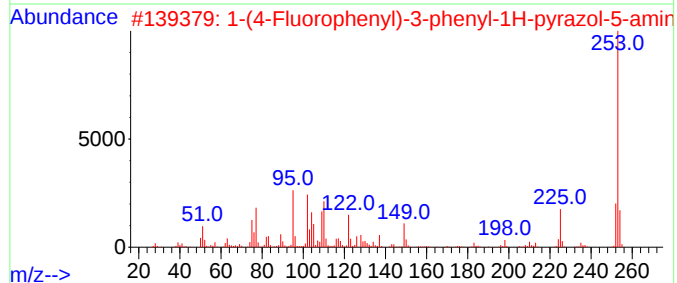
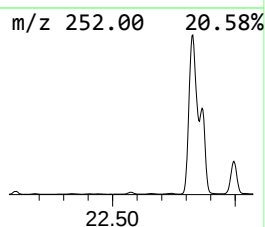
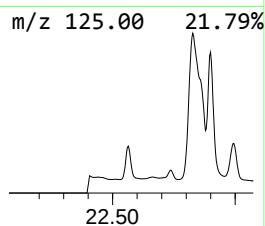
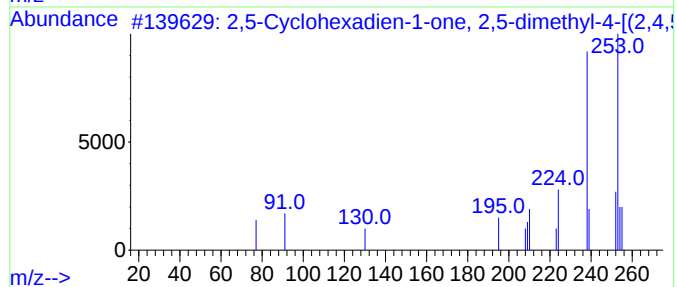
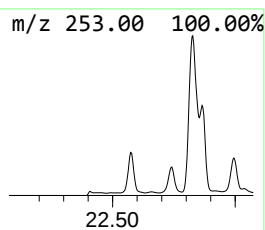
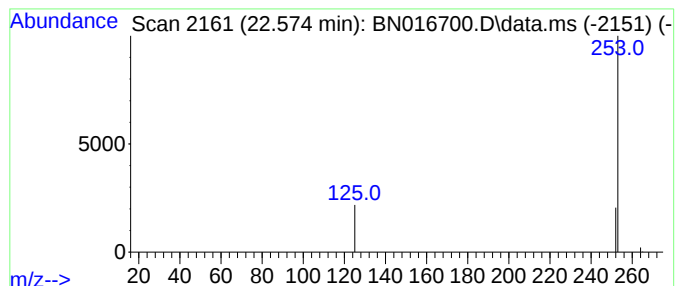
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2,5-Cyclohexadien-1-one, 2,... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.574	0.55 ng	202734	Perylene-d12	23.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,5-Cyclohexadien-1-one, 2,5-dim...	253	C17H19NO	054245-93-1	5
2		1-(4-Fluorophenyl)-3-phenyl-1H-p...	253	C15H12FN3	072411-51-9	5
3		Pyrimidine, 4-methyl-2-phenyl-6-...	253	C16H19N3	1000302-39-3	5
4		N-(4-Phenyl-1,3-thiazol-2-yl)-2-...	253	C14H11N3S	1000485-04-5	5
5		trans-3-Nitrochalcone	253	C15H11NO3	024721-24-2	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

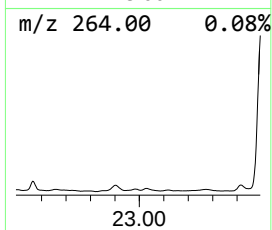
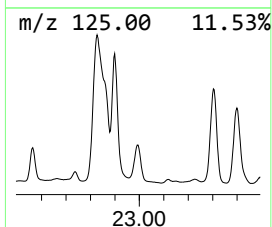
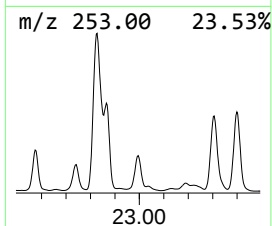
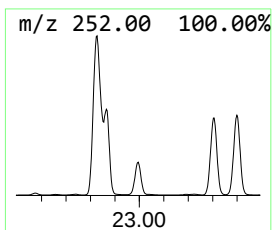
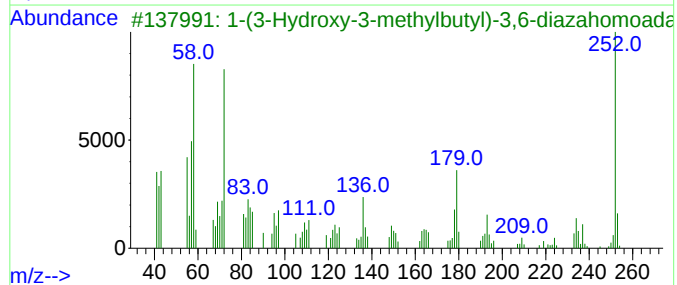
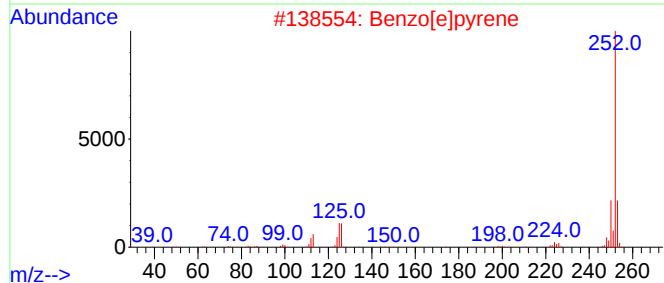
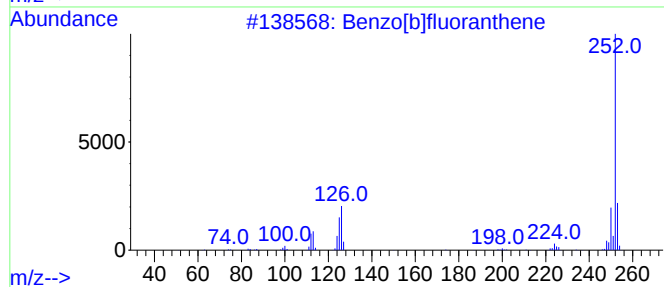
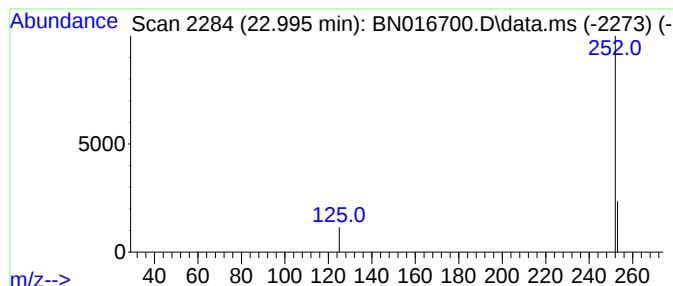
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzo[b]fluoranthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.995	1.97 ng	723146	Perylene-d12	23.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
2			Benzo[e]pyrene	252	C20H12	000192-97-2	9
3			1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	9
4			Perylene	252	C20H12	000198-55-0	9
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

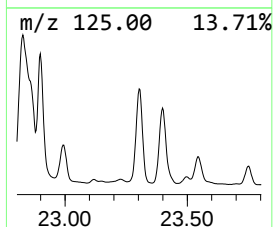
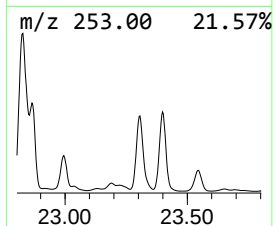
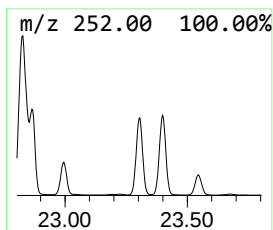
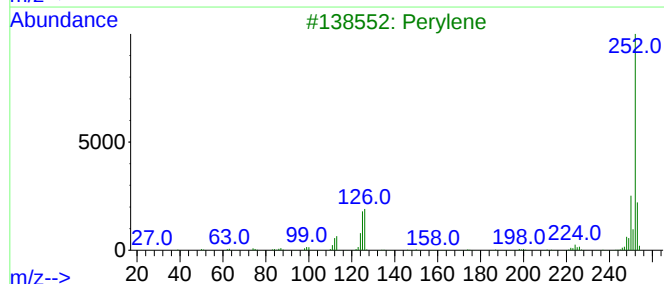
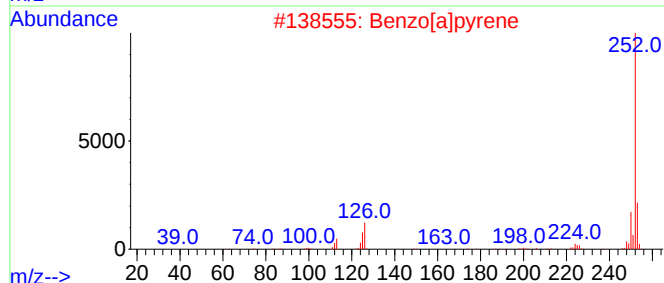
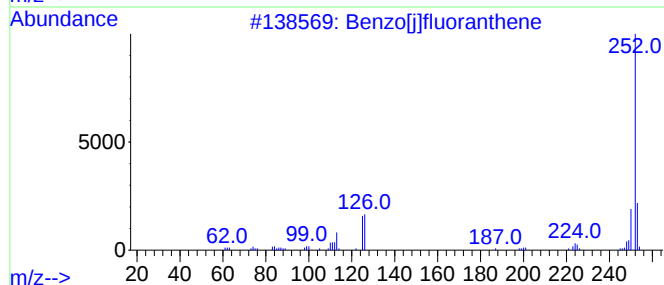
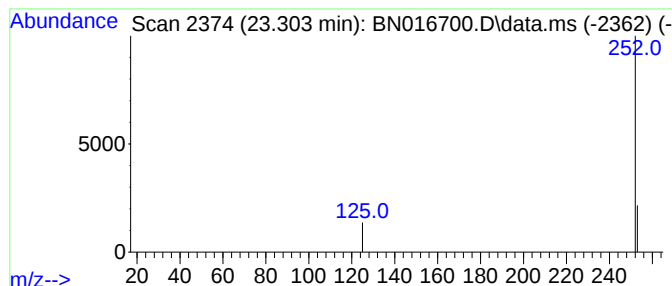
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Benzo[j]fluoranthene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.303	4.53 ng	1663760	Perylene-d12	23.498

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 : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

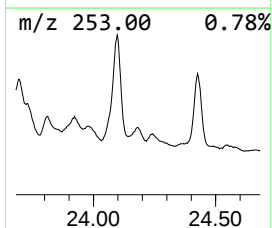
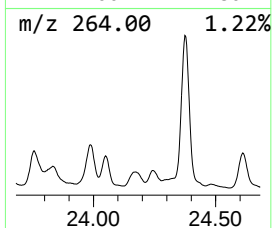
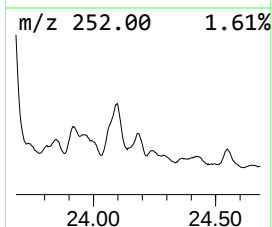
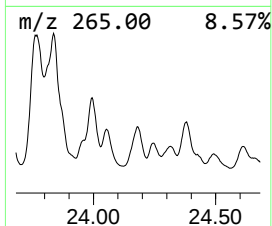
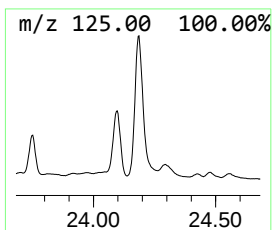
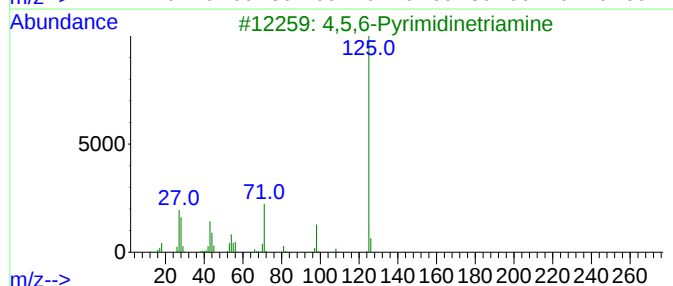
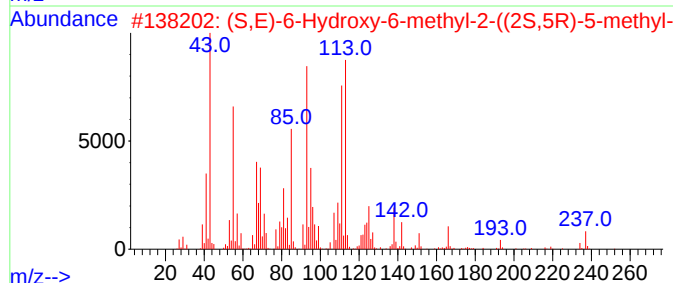
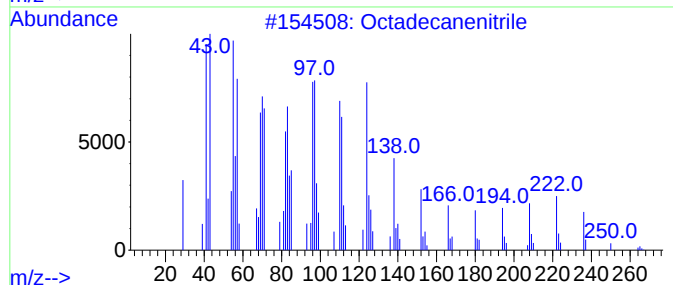
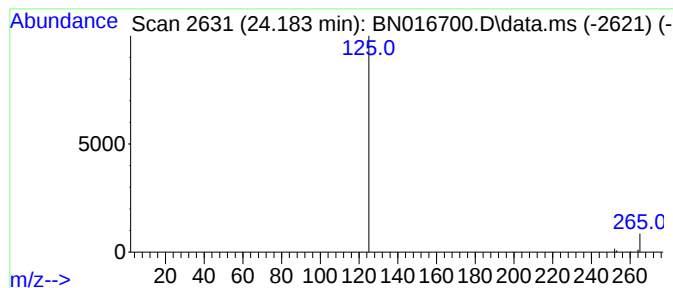
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Octadecanenitrile Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.183	0.42 ng	152883	Perylene-d12	23.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanenitrile	265	C18H35N	000638-65-3	3
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-Aminothiazole-5-carbonitrile	125	C4H3N3S	051640-52-9	2
5			2(1H)-Pyrimidinone, 4-amino-5-me...	125	C5H7N3O	000554-01-8	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

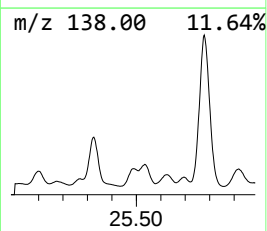
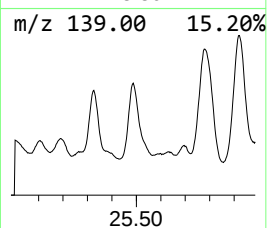
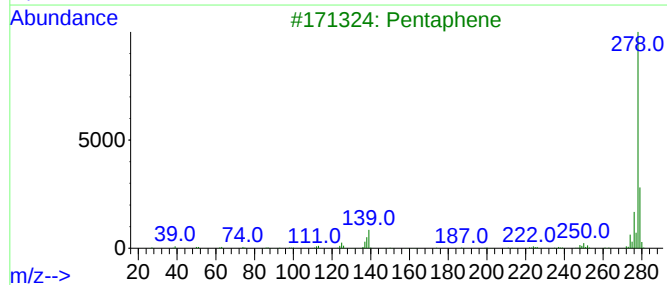
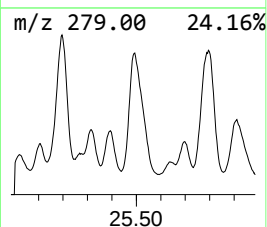
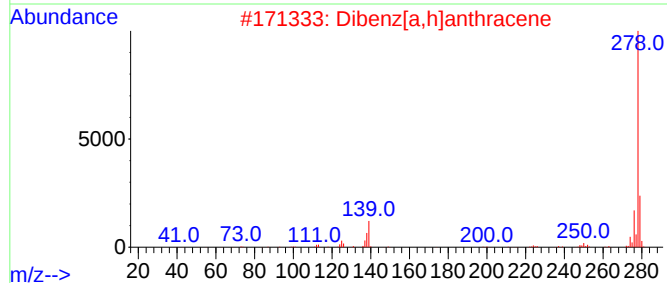
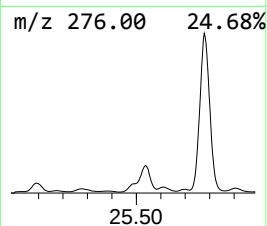
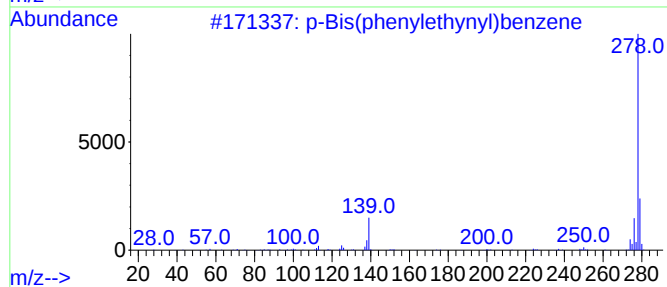
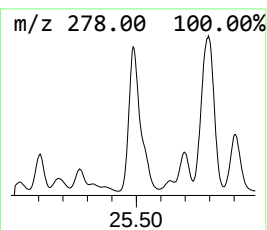
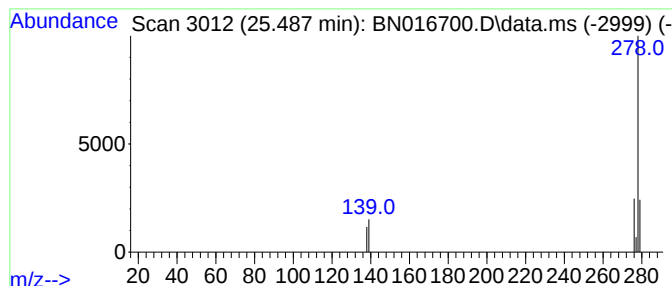
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 p-Bis(phenylethynyl)benzene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.487	0.59 ng	214938	Perylene-d12	23.498

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		Pentaphene	278	C22H14	000222-93-5	64
4		Picene	278	C22H14	000213-46-7	64
5		Benzo[b]triphenylene	278	C22H14	000215-58-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

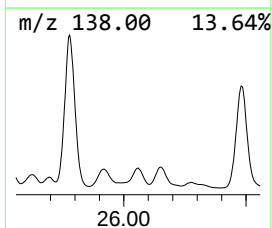
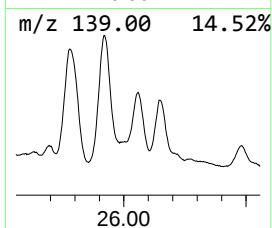
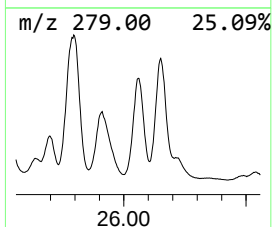
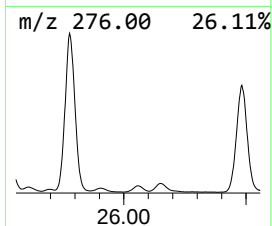
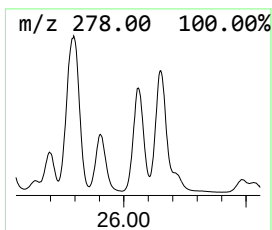
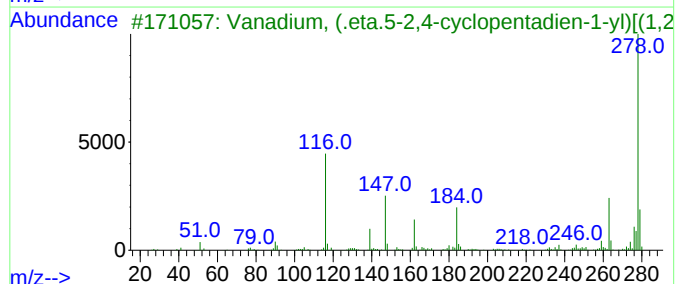
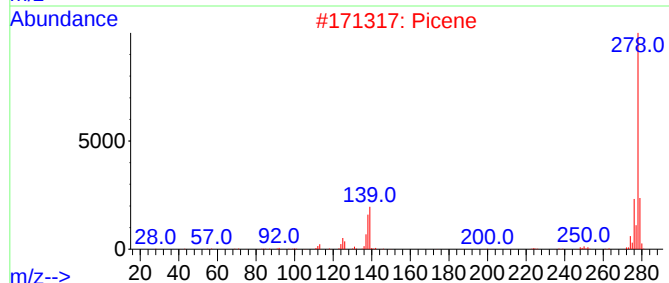
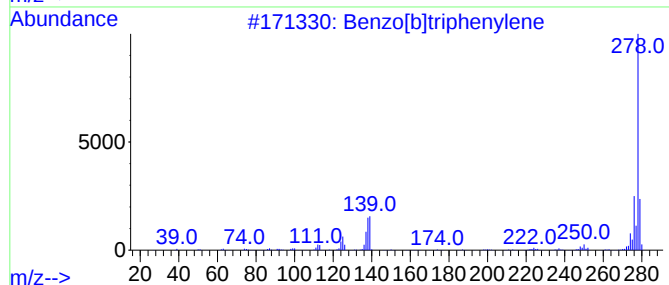
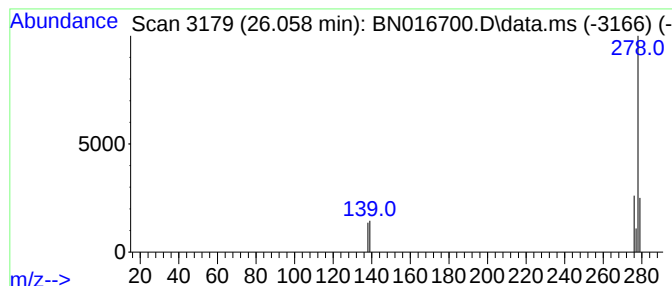
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzo[b]triphenylene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.058	0.44 ng	162669	Perylene-d12	23.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]triphenylene	278	C22H14	000215-58-7	80
2			Picene	278	C22H14	000213-46-7	80
3			Vanadium, (.eta.5-2,4-cyclopenta...	278	C17H23V	126948-97-8	78
4			Dibenz[a,h]anthracene	278	C22H14	000053-70-3	72
5			1-naphthalenol, 4-[2-(4-methoxyp...	278	C17H14N2O2	1000397-12-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016700.D
Acq On : 03 Oct 2021 10:00
Operator : CG/JU
Sample : M3892-11
Misc :
ALS Vial : 68 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-825-N-SO-0-0.5-092221

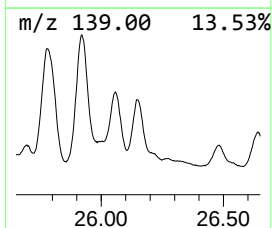
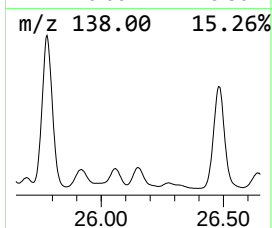
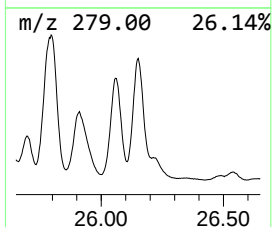
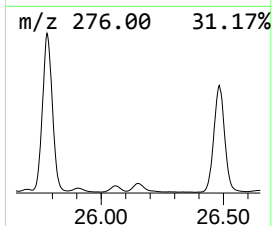
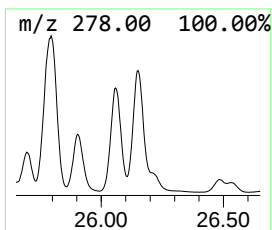
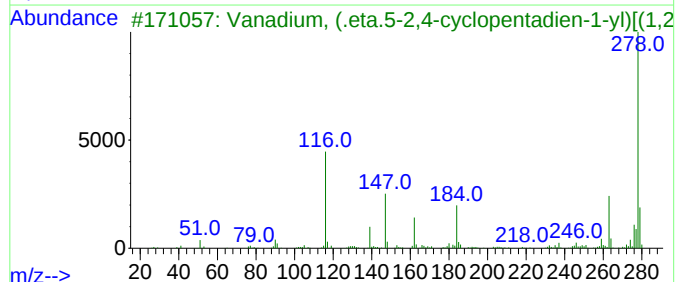
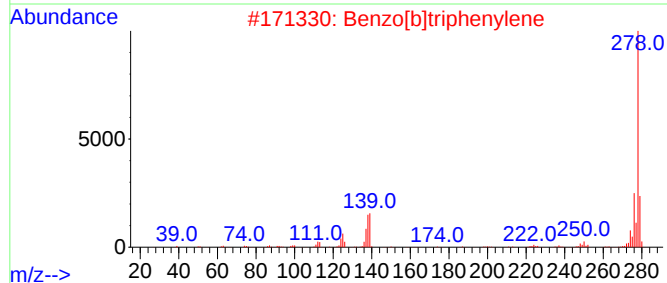
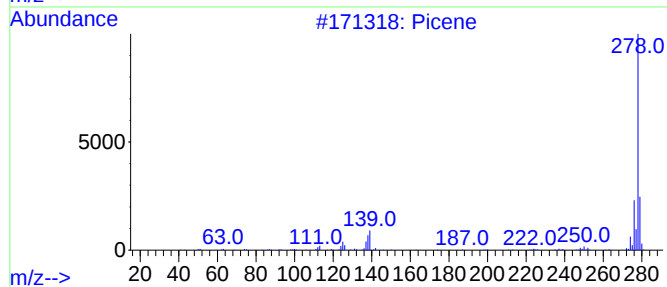
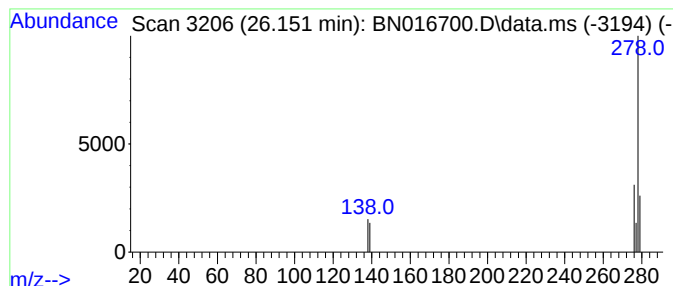
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Picene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.151	0.78 ng	285037	Perylene-d12	23.498

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			1-naphthalenol, 4-[2-(4-methoxyp...	278	C17H14N2O2	1000397-12-8	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 : BN016700.D
 Acq On : 03 Oct 2021 10:00
 Operator : CG/JU
 Sample : M3892-11
 Misc :
 ALS Vial : 68 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-825-N-SO-0-0.5-092221

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
2-Furancarboxit...	6.333	7.4	ng	1798680	1	7.642	96795	0.4
2-Furancarboxit...	6.628	0.6	ng	136135	1	7.642	96795	0.4
2-Furancarboxit...	7.080	7.6	ng	1830860	1	7.642	96795	0.4
2-Furancarboxit...	7.532	1.3	ng	306302	1	7.642	96795	0.4
2-Furancarboxit...	7.854	0.4	ng	99301	1	7.642	96795	0.4
Butane	7.937	2.3	ng	547571	1	7.642	96795	0.4
Benzene, nitro-	9.709	1.0	ng	407694	2	10.406	165531	0.4
Isopropyl isoth...	10.191	0.5	ng	208361	2	10.406	165531	0.4
Benzaldehyde, 2...	13.190	0.7	ng	406953	3	14.269	223298	0.4
1-Butanone, 3-m...	13.584	0.4	ng	244465	3	14.269	223298	0.4
Benzene, 1-ethy...	15.169	0.6	ng	312941	3	14.269	223298	0.4
1,3-Benzodioxol...	16.592	0.4	ng	206103	4	17.030	228802	0.4
Carbazole	17.431	0.7	ng	403096	4	17.030	228802	0.4
2,5-Cyclohexadi...	22.574	0.6	ng	202734	6	23.498	146942	0.4
Benzo[b]fluoran...	22.995	2.0	ng	723146	6	23.498	146942	0.4
Benzo[j]fluoran...	23.303	4.5	ng	1663760	6	23.498	146942	0.4
Octadecanenitrile	24.183	0.4	ng	152883	6	23.498	146942	0.4
p-Bis(phenyleth...	25.487	0.6	ng	214938	6	23.498	146942	0.4
Benzo[b]triphen...	26.058	0.4	ng	162669	6	23.498	146942	0.4
Picene	26.151	0.8	ng	285037	6	23.498	146942	0.4