

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016697.D
 Acq On : 03 Oct 2021 08:12
 Operator : CG/JU
 Sample : M3892-13
 Misc :
 ALS Vial : 65 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-826-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: BN016697.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	34423	73001	1.19%	0.124%
2	5.042	209	213	220	rBV	28534	72250	1.18%	0.122%
3	6.333	348	353	361	rVB	1657125	4256079	69.25%	7.215%
4	6.628	381	385	395	rBV	86947	226543	3.69%	0.384%
5	7.080	429	434	443	rVB	1921760	4540279	73.87%	7.697%
6	7.532	479	483	489	rVB	253818	494422	8.04%	0.838%
7	7.633	490	494	500	rVB	49311	103692	1.69%	0.176%
8	7.855	513	518	521	rBV	127601	231068	3.76%	0.392%
9	7.910	521	524	525	rBV	77887	121353	1.97%	0.206%
10	8.785	598	605	607	rBV2	30408	95194	1.55%	0.161%
11	9.697	671	677	680	rBV	90215	277887	4.52%	0.471%
12	9.824	684	687	691	rVB	47858	86644	1.41%	0.147%
13	10.191	712	716	720	rBV	80464	147336	2.40%	0.250%
14	10.407	729	733	735	rBV	105363	199768	3.25%	0.339%
15	10.457	735	737	740	rVB3	62229	121420	1.98%	0.206%
16	12.003	922	931	939	rBV	45129	72450	1.18%	0.123%
17	12.886	1071	1074	1077	rBV2	89391	142457	2.32%	0.242%
18	13.190	1095	1098	1101	rVB	188314	312068	5.08%	0.529%
19	13.584	1127	1129	1132	rBV	160156	261277	4.25%	0.443%
20	13.749	1137	1142	1145	rVB	61939	102173	1.66%	0.173%
21	13.990	1158	1161	1164	rVB	72926	130631	2.13%	0.221%
22	14.129	1168	1172	1176	rBV2	76775	136233	2.22%	0.231%
23	14.269	1179	1183	1185	rBV	151697	229457	3.73%	0.389%
24	14.332	1185	1188	1192	rVB2	212199	378727	6.16%	0.642%
25	14.751	1218	1221	1224	rVB	56883	87922	1.43%	0.149%
26	15.094	1244	1248	1251	rBV	102094	169081	2.75%	0.287%
27	15.322	1263	1266	1269	rBV	157255	225792	3.67%	0.383%
28	15.766	1295	1301	1305	rVB	87707	191389	3.11%	0.324%
29	16.007	1317	1320	1322	rVB2	87663	118019	1.92%	0.200%
30	17.018	1400	1403	1404	rBV	117651	174937	2.85%	0.297%
31	17.066	1404	1407	1410	rVV	1875888	2744515	44.65%	4.653%
32	17.152	1410	1414	1417	rVB	360088	536606	8.73%	0.910%
33	17.431	1432	1437	1440	rBV	241197	397786	6.47%	0.674%
34	17.894	1471	1475	1477	rBV2	45707	98660	1.61%	0.167%
35	17.955	1477	1480	1483	rVB2	58769	112151	1.82%	0.190%
36	18.418	1560	1566	1579	rVB2	88547	149778	2.44%	0.254%

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016697.D
 Acq On : 03 Oct 2021 08:12
 Operator : CG/JU
 Sample : M3892-13
 Misc :
 ALS Vial : 65 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-826-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	19.098	1686	1703	1712	rBV	4333873	6146269	100.00%	10.420%
38	19.202	1719	1724	1729	rVB2	74880	109968	1.79%	0.186%
39	19.247	1729	1733	1738	rBV2	57319	67475	1.10%	0.114%
40	19.460	1766	1776	1787	rBV	3783023	5684573	92.49%	9.637%
41	19.679	1815	1820	1822	rVV	111962	146836	2.39%	0.249%
42	19.708	1822	1826	1834	rVB	165288	236927	3.85%	0.402%
43	19.927	1862	1870	1875	rBV4	34455	75711	1.23%	0.128%
44	19.991	1878	1883	1885	rBV	74810	80294	1.31%	0.136%
45	20.155	1893	1900	1902	rBV3	72209	248234	4.04%	0.421%
46	20.304	1911	1914	1916	rBV	45586	88889	1.45%	0.151%
47	20.410	1923	1924	1926	rVB	94682	97538	1.59%	0.165%
48	20.463	1926	1929	1932	rBV	519579	860696	14.00%	1.459%
49	20.707	1947	1952	1957	rVB	121034	210902	3.43%	0.358%
50	20.824	1957	1963	1966	rBV	479362	1031439	16.78%	1.749%
51	20.866	1966	1967	1970	rVV2	135504	246206	4.01%	0.417%
52	20.920	1970	1972	1973	rVV	311411	395249	6.43%	0.670%
53	20.951	1973	1975	1979	rVV3	374165	827434	13.46%	1.403%
54	21.005	1979	1980	1983	rVB	108807	152972	2.49%	0.259%
55	21.217	1993	2000	2002	rBV3	2067568	3930761	63.95%	6.664%
56	21.270	2002	2005	2011	rVB	2181194	3746814	60.96%	6.352%
57	21.387	2014	2016	2020	rBV	291035	449461	7.31%	0.762%
58	21.610	2034	2037	2041	rVB2	120075	196306	3.19%	0.333%
59	21.790	2051	2054	2056	rVB	65718	107086	1.74%	0.182%
60	21.844	2056	2059	2061	rVV2	90156	175604	2.86%	0.298%
61	21.918	2064	2066	2070	rVV3	82414	219391	3.57%	0.372%
62	21.992	2070	2073	2074	rVV2	123500	199304	3.24%	0.338%
63	22.024	2074	2076	2079	rVV	217581	299533	4.87%	0.508%
64	22.098	2079	2083	2086	rVB	92754	157686	2.57%	0.267%
65	22.268	2096	2099	2102	rBV	66561	126309	2.06%	0.214%
66	22.396	2109	2111	2113	rVB2	74249	74985	1.22%	0.127%
67	22.567	2150	2159	2175	rVB2	118868	209889	3.41%	0.356%
68	22.735	2200	2208	2218	rBV	67158	103080	1.68%	0.175%
69	22.821	2220	2233	2241	rBV	1711049	3874554	63.04%	6.568%
70	22.988	2272	2282	2293	rVB2	258788	432314	7.03%	0.733%
71	23.300	2361	2373	2388	rVB	1061249	1930797	31.41%	3.273%
72	23.396	2388	2401	2418	rVB	1277696	2397909	39.01%	4.065%
73	23.495	2420	2430	2435	rBV2	109757	210126	3.42%	0.356%
74	23.539	2435	2443	2459	rVB	362916	720780	11.73%	1.222%
75	23.752	2496	2505	2516	rBV3	37651	104896	1.71%	0.178%
76	24.094	2598	2605	2616	rVB	47847	93404	1.52%	0.158%

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016697.D
 Acq On : 03 Oct 2021 08:12
 Operator : CG/JU
 Sample : M3892-13
 Misc :
 ALS Vial : 65 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-826-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	24.179	2618	2630	2644	rBV	125492	286124	4.66%	0.485%
78	24.371	2677	2686	2697	rBV2	47194	96821	1.58%	0.164%
79	25.097	2886	2898	2909	rBV3	35230	85877	1.40%	0.146%
80	25.179	2913	2922	2937	rVB3	27387	81540	1.33%	0.138%
81	25.484	2997	3011	3018	rBV2	101824	263516	4.29%	0.447%
82	25.692	3063	3072	3080	rBV2	38346	81912	1.33%	0.139%
83	25.774	3081	3096	3119	rVB2	536392	1630161	26.52%	2.764%
84	25.905	3121	3134	3159	rVB5	51376	168053	2.73%	0.285%
85	26.055	3164	3178	3191	rBV	88257	237868	3.87%	0.403%
86	26.148	3192	3205	3238	rVB	95400	323476	5.26%	0.548%
87	26.476	3281	3301	3333	rBV	368602	1223831	19.91%	2.075%
88	26.846	3394	3409	3436	rVB	66632	221307	3.60%	0.375%

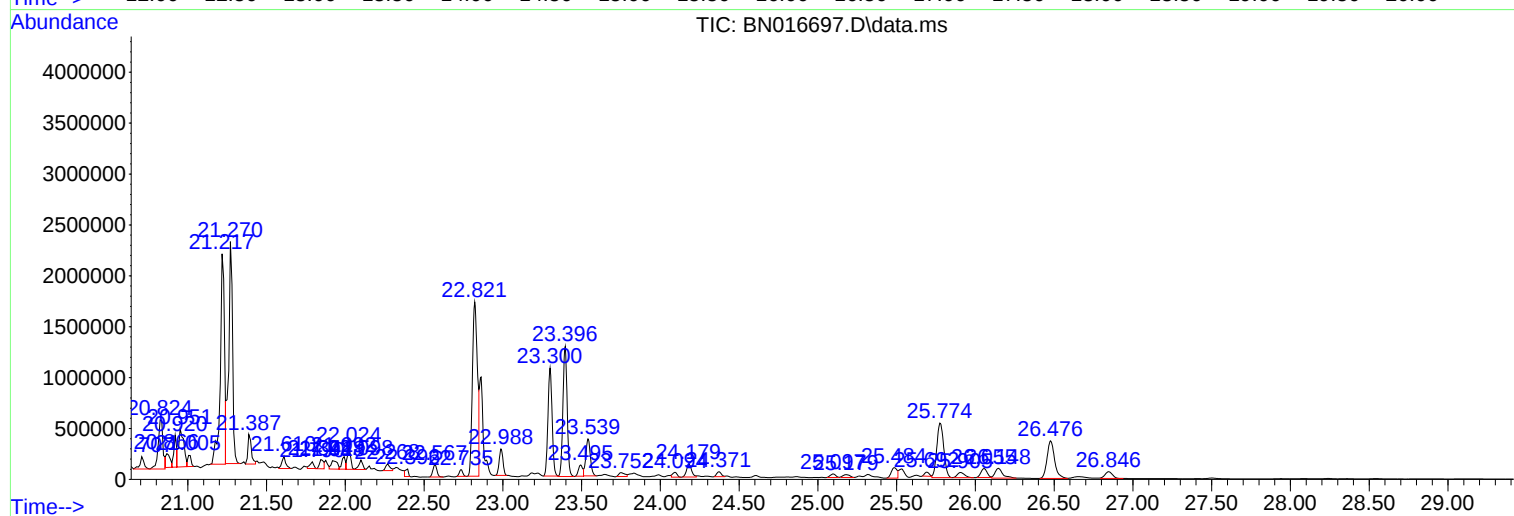
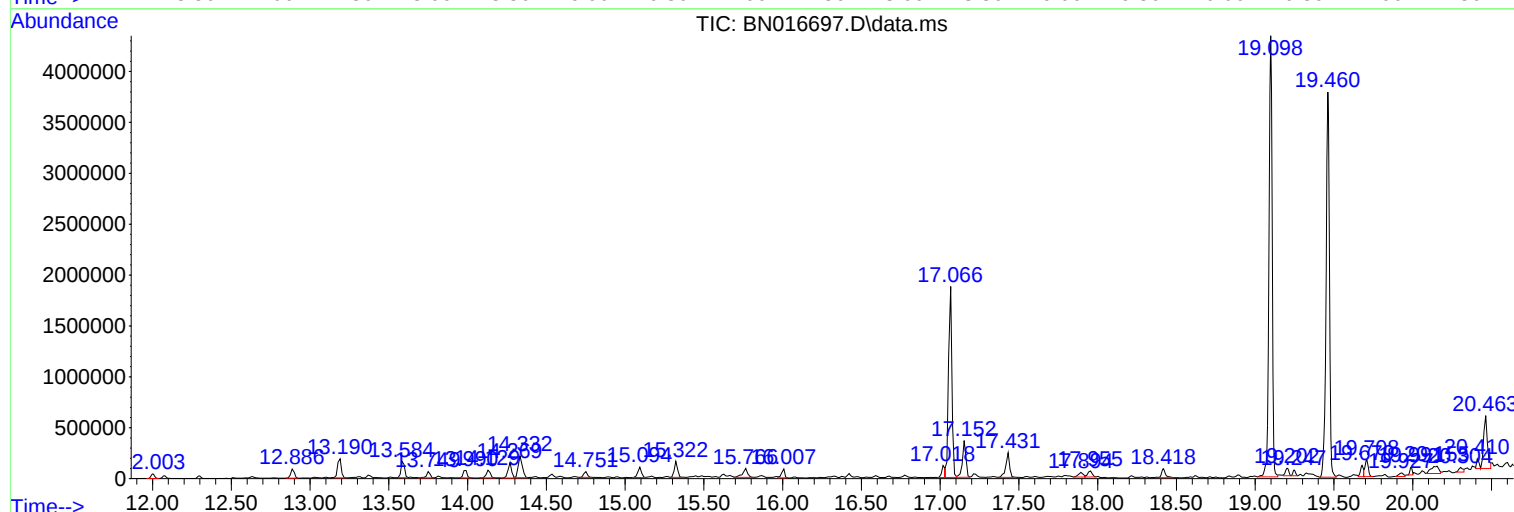
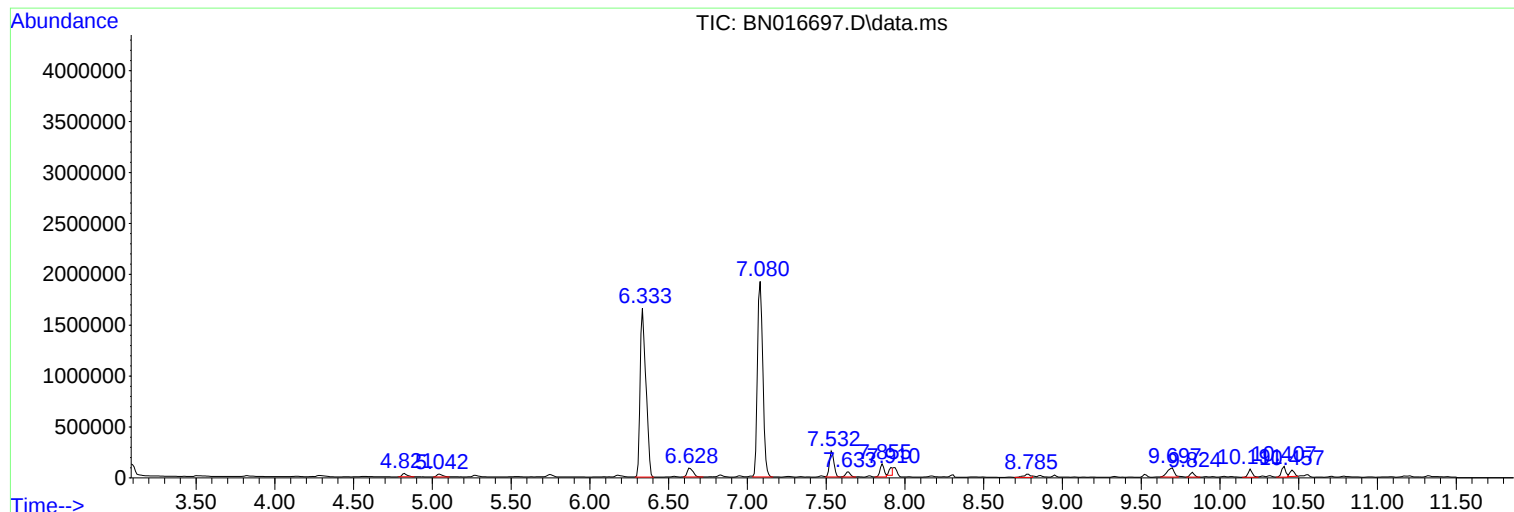
Sum of corrected areas: 58988132

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-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 : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

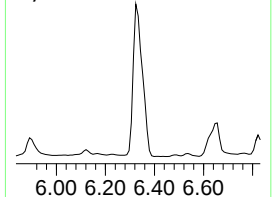
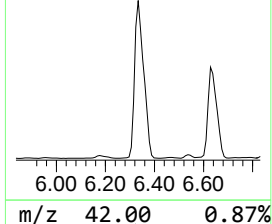
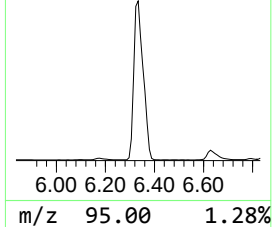
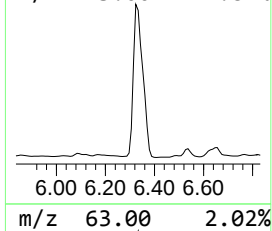
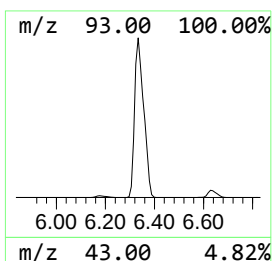
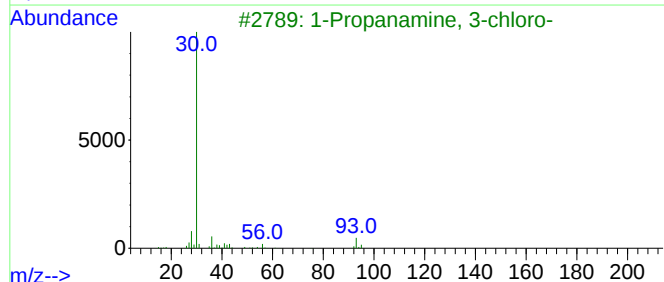
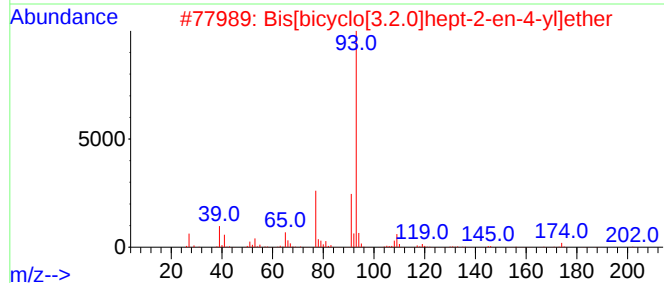
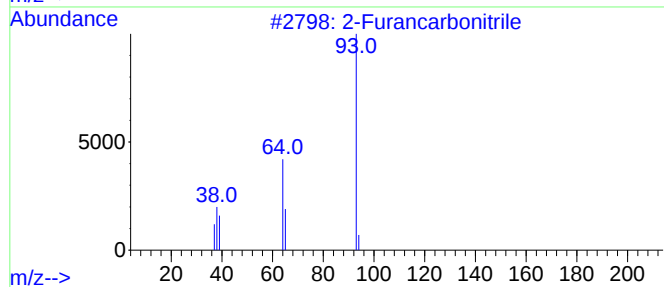
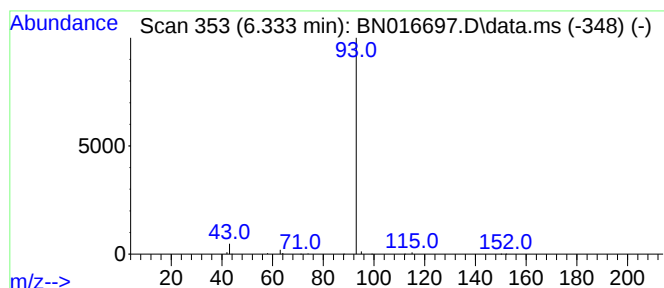
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	16.42 ng	4256080	1,4-Dichlorobenzene-d4	7.643

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 : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

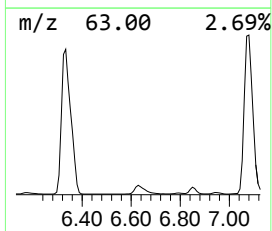
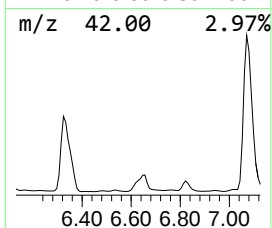
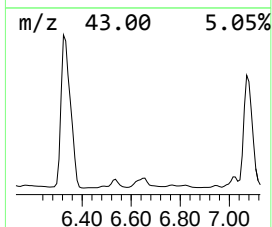
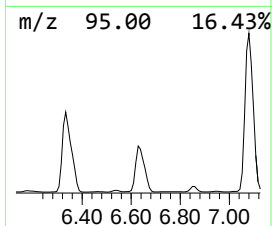
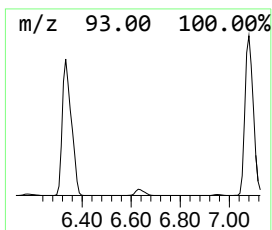
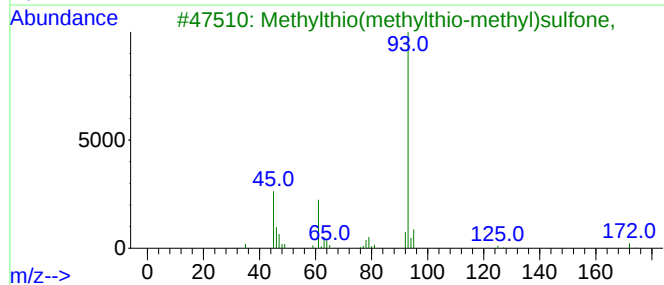
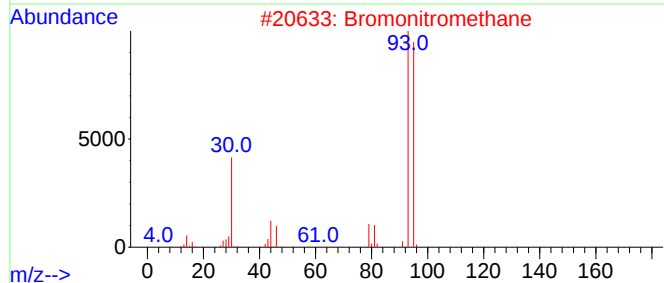
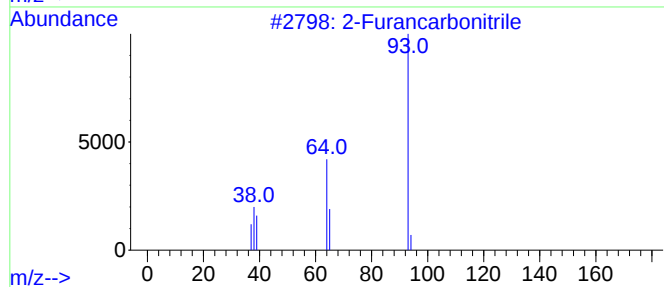
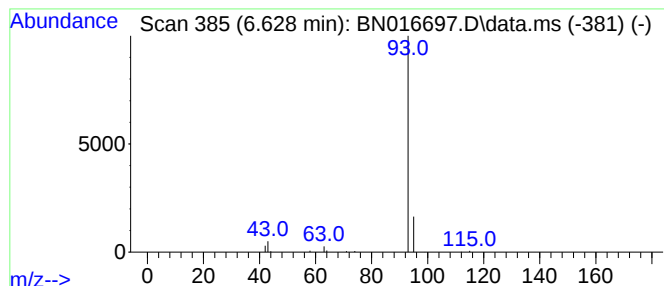
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Furancarbonitrile Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.628	0.87 ng	226543	1,4-Dichlorobenzene-d4	7.643

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 : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

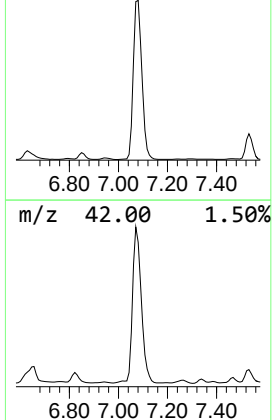
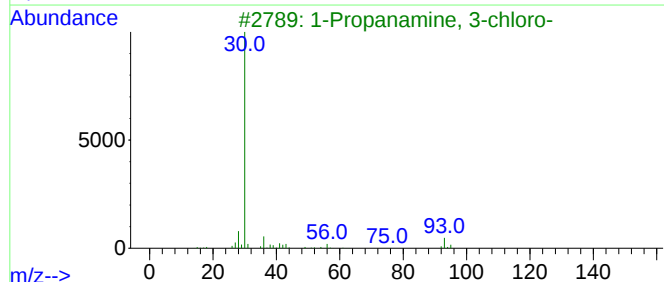
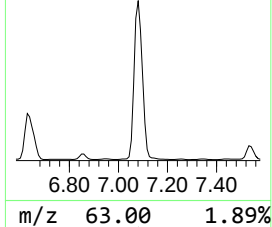
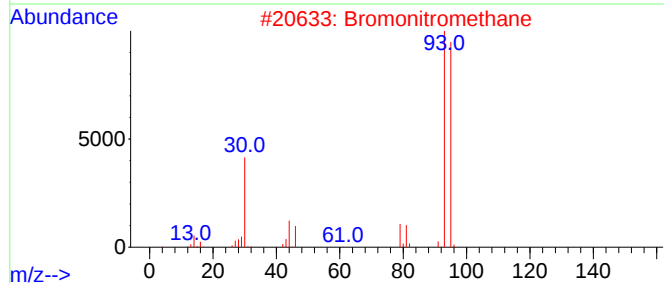
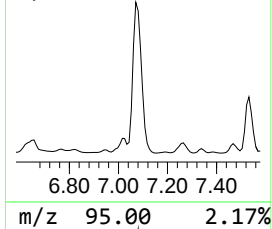
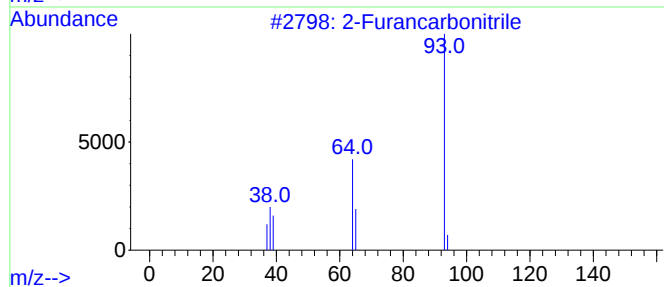
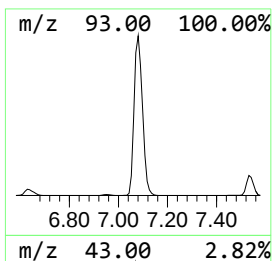
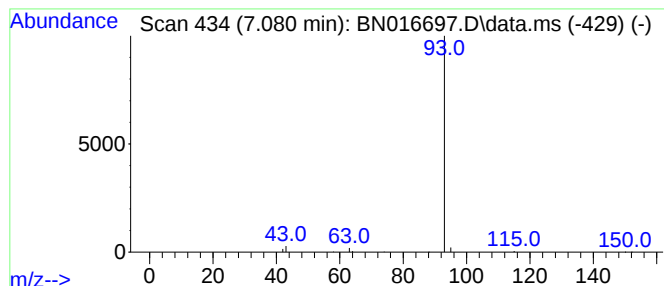
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	17.51 ng	4540280	1,4-Dichlorobenzene-d4	7.643

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			1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	1
4			Bis[bicyclo[3.2.0]hept-2-en-4-yl...]	202	C14H18O	1000153-89-5	1
5			4-(2-Aminoethyl)pyridine	122	C7H10N2	013258-63-4	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

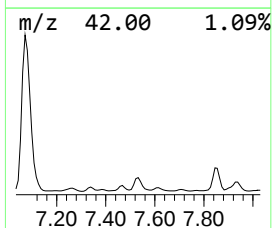
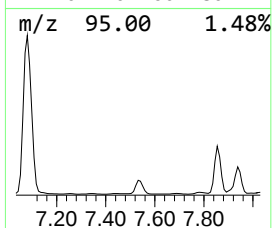
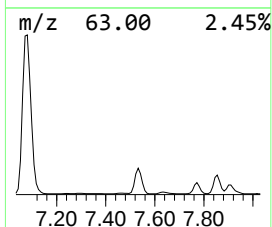
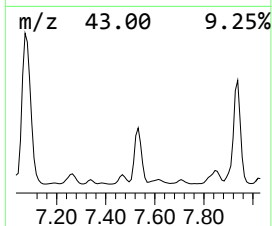
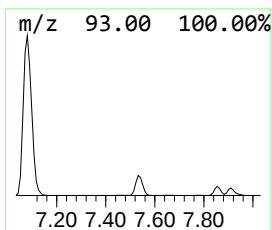
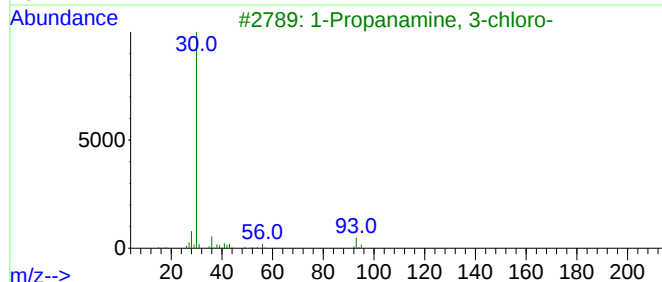
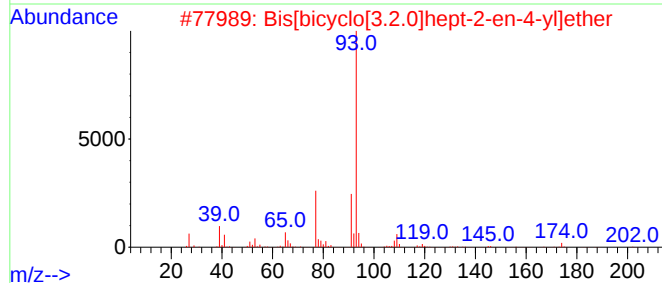
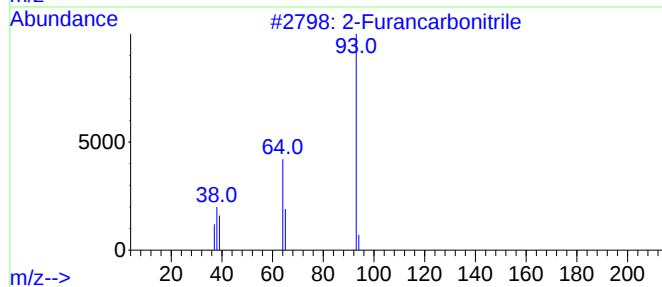
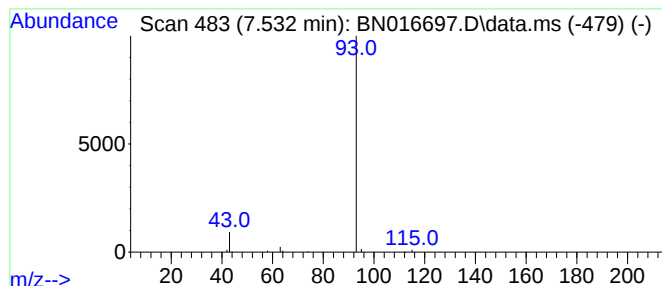
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2-Furancarbonitrile Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.532	1.91 ng	494422	1,4-Dichlorobenzene-d4	7.643

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 : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

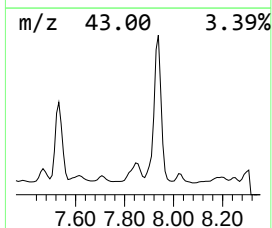
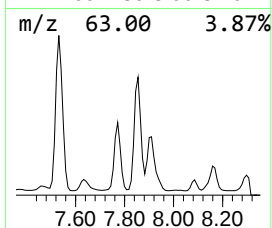
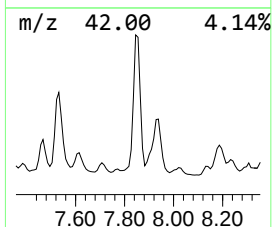
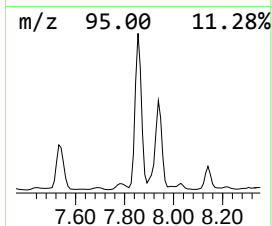
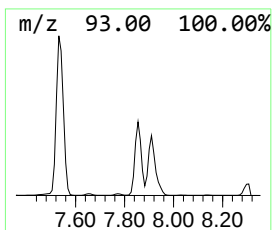
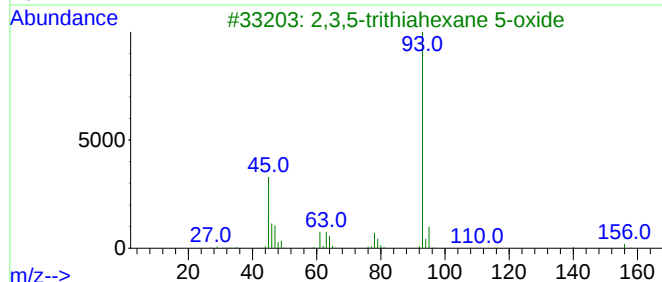
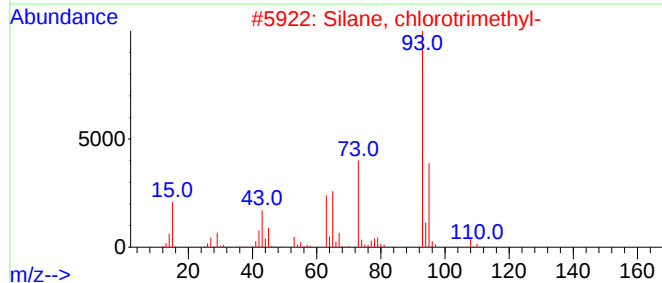
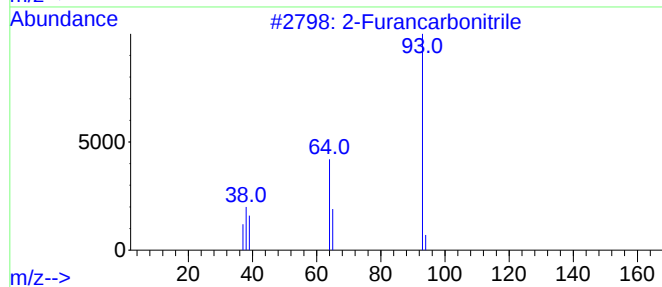
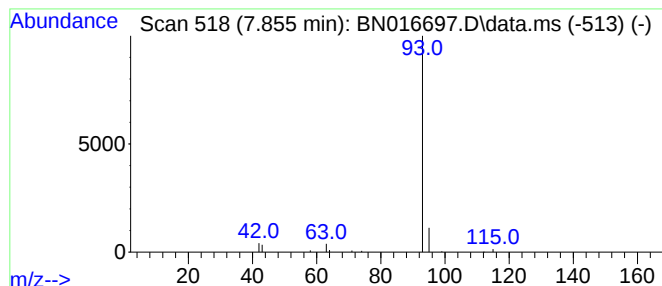
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 2-Furancarbonitrile Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.855	0.89 ng	231068	1,4-Dichlorobenzene-d4	7.643

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Furancarbonitrile	93	C5H3NO	000617-90-3	2
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 : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

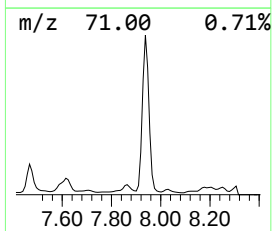
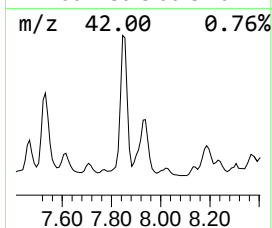
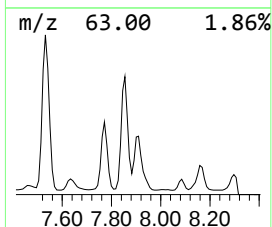
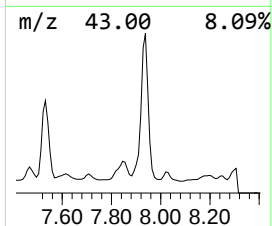
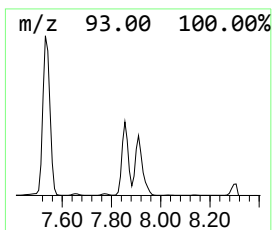
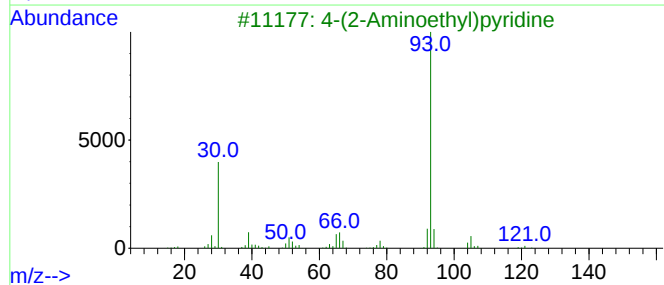
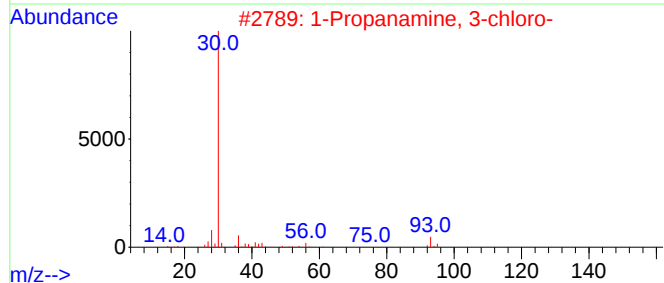
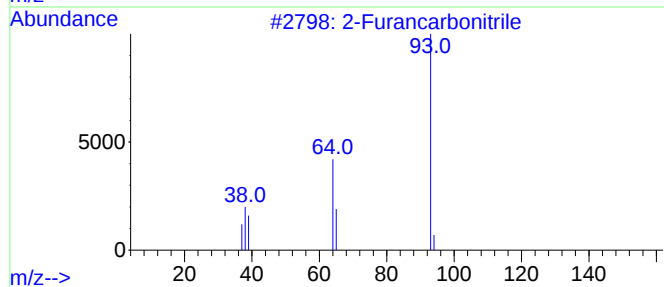
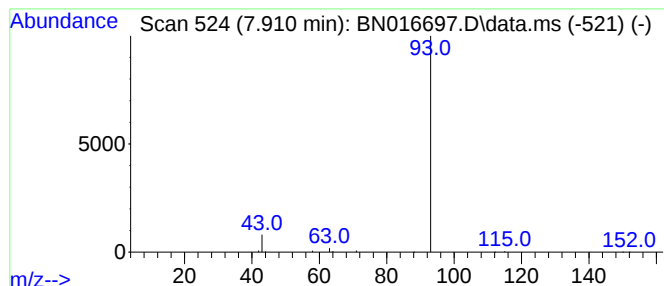
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Furancarbonitrile Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.910	0.47 ng	121353	1,4-Dichlorobenzene-d4	7.643

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			4-(2-Aminoethyl)pyridine	122	C7H10N2	013258-63-4	1
4			Ethanone, 1-cyclopropyl-2-(4-pyr...	161	C10H11NO	006580-95-6	1
5			2-Pyridinemethanamine, N-methyl-	122	C7H10N2	021035-59-6	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

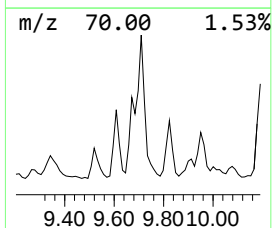
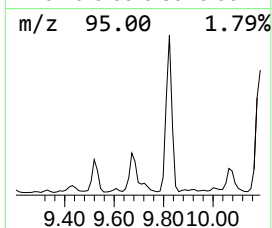
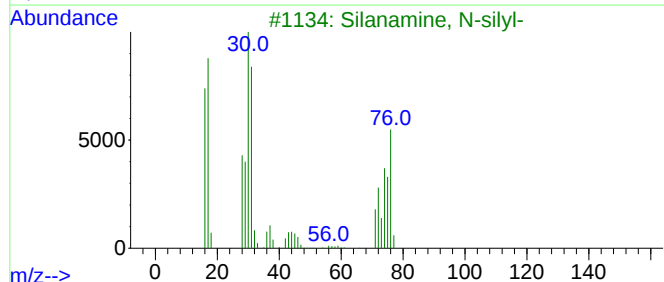
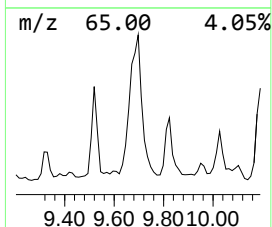
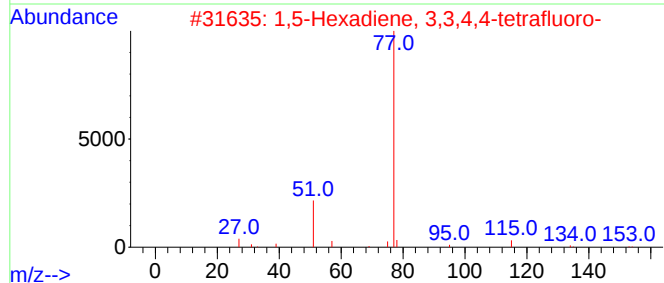
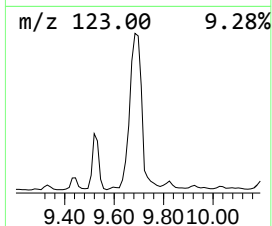
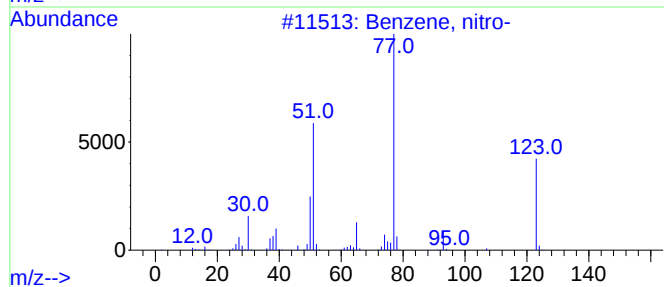
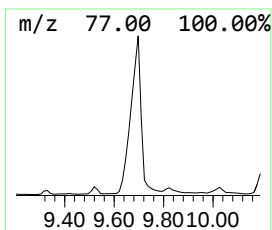
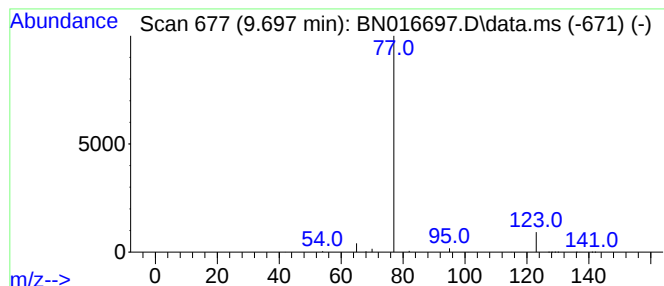
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, nitro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.697	0.56 ng	277887	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, nitro-	123	C6H5NO2	000098-95-3	3
2			1,5-Hexadiene, 3,3,4,4-tetrafluoro-	154	C6H6F4	001763-21-9	1
3			Silanamine, N-silyl-	77	H7NSi2	005702-11-4	1
4			Mercaptamine	77	C2H7NS	000060-23-1	1
5			Silanediol, dimethyl-	92	C2H8O2Si	001066-42-8	1



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

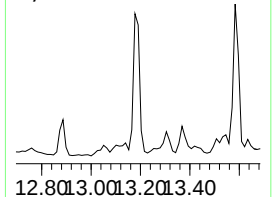
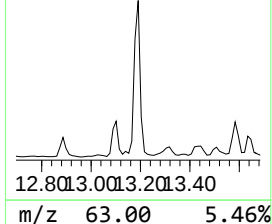
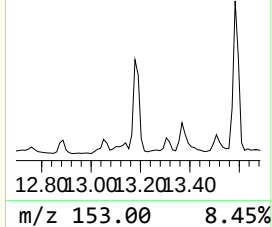
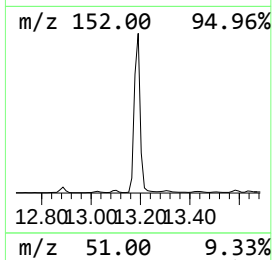
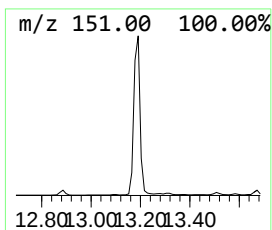
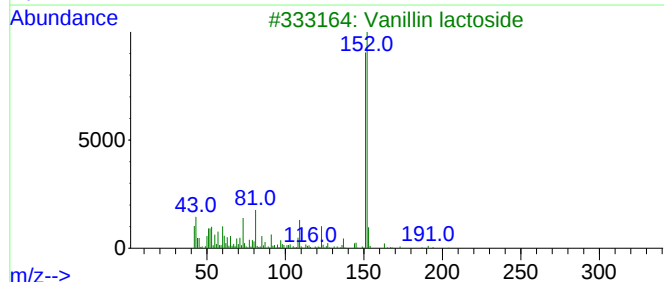
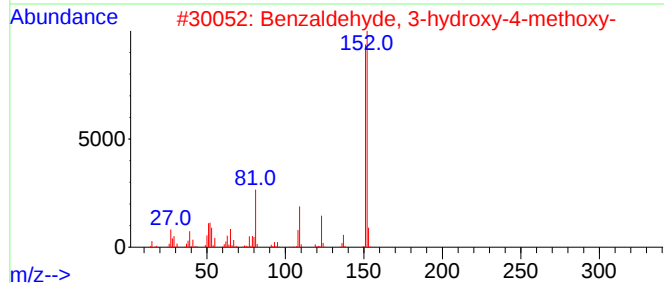
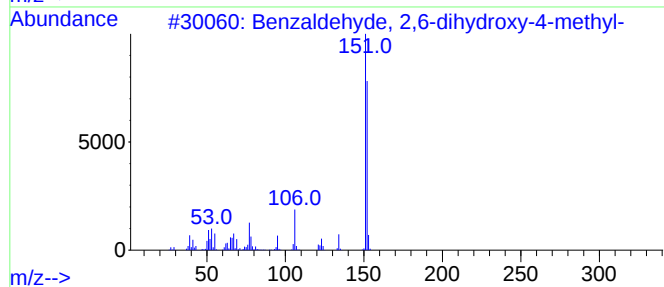
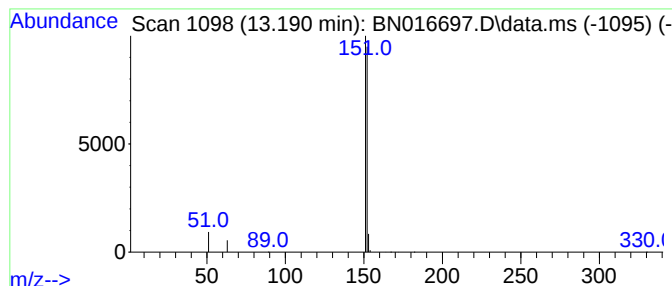
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzaldehyde, 2,6-dihydroxy... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.190	0.54 ng	312068	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			3-Pyridinol, 4-amino-2-ethyl-6-m...	152	C8H12N2O	1010351-35-8	9
5			Vanillin	152	C8H8O3	000121-33-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

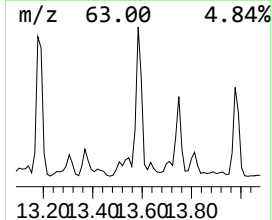
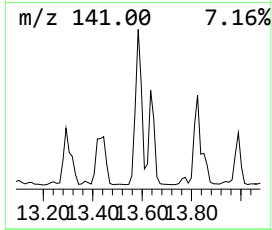
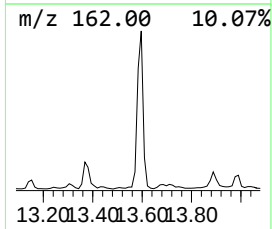
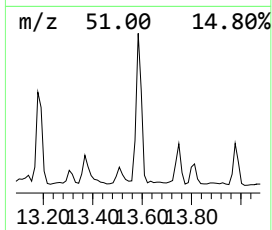
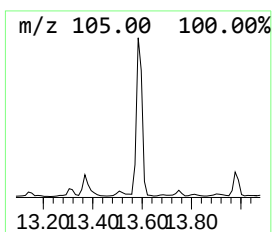
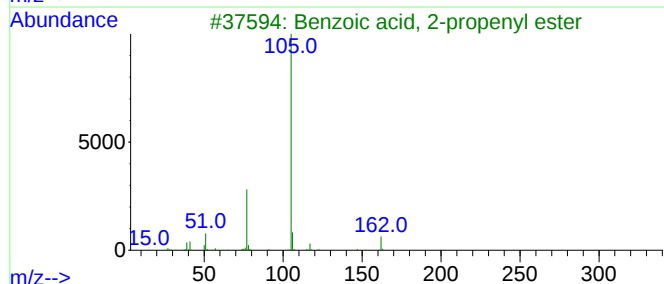
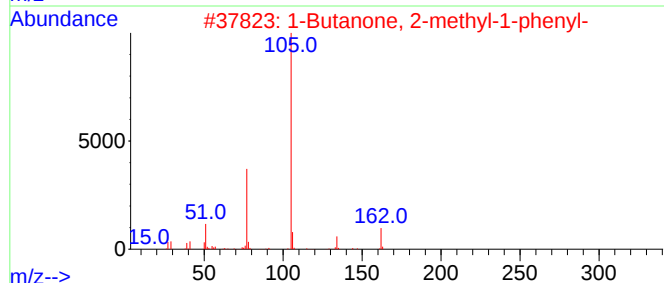
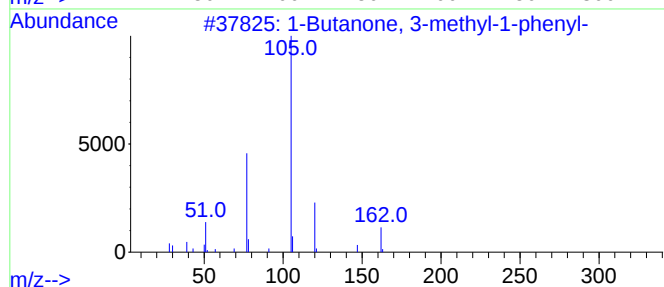
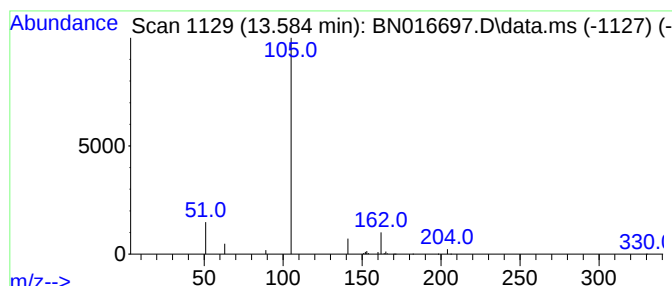
Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

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 1-Butanone, 3-methyl-1-phenyl- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.584	0.46 ng	261277	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	4
4	Cyclobutyl phenyl ketone	160	C11H12O	005407-98-7	4
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

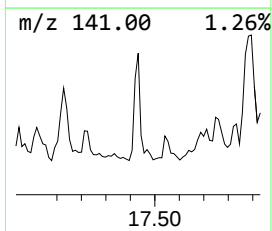
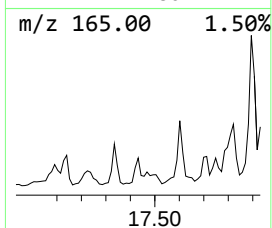
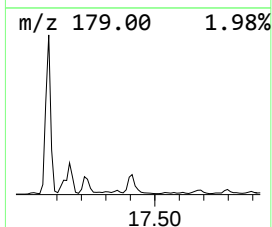
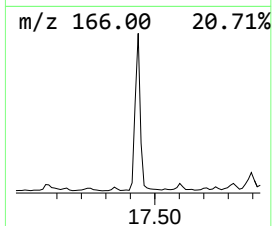
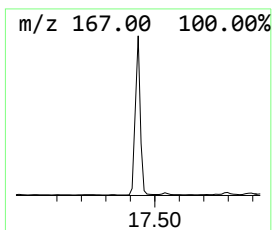
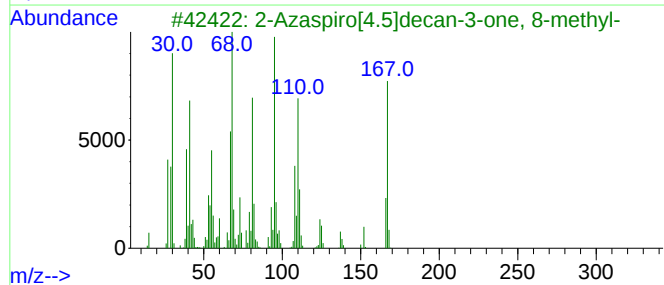
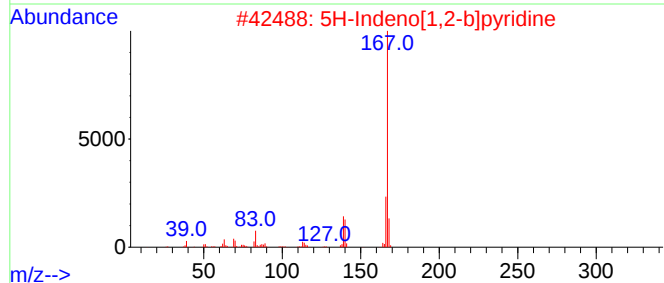
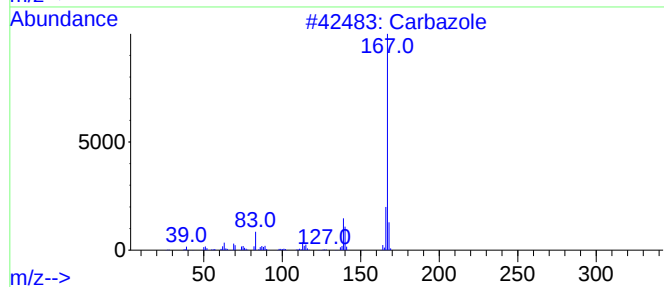
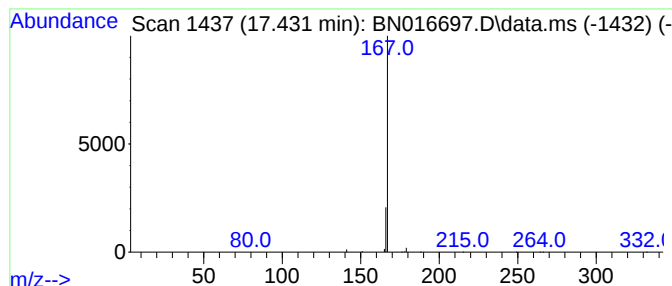
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Carbazole Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.432	0.91 ng	397786	Phenanthrene-d10	17.018

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	9
3			2-Azaspiro[4.5]decan-3-one, 8-me...	167	C10H17NO	196608-77-2	5
4			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
5			benzaldehyde, 2-hydroxy-4-nitro-	167	C7H5NO4	1000404-52-2	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

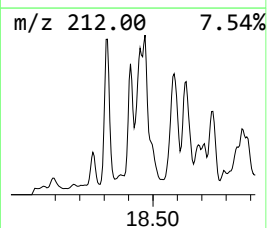
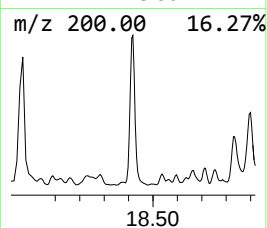
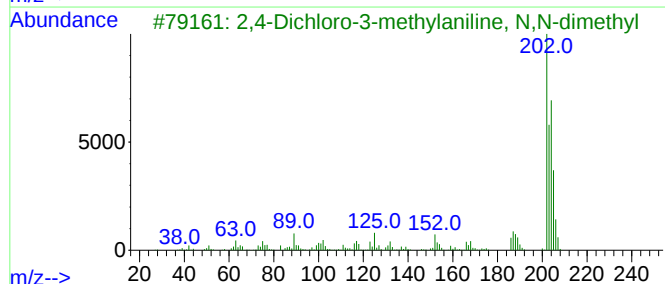
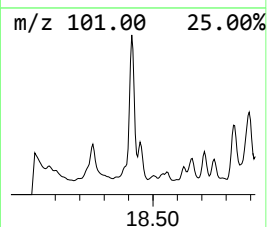
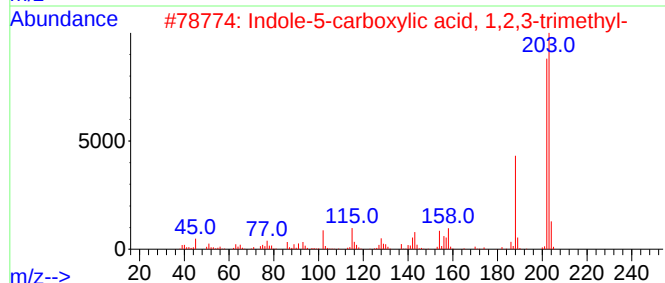
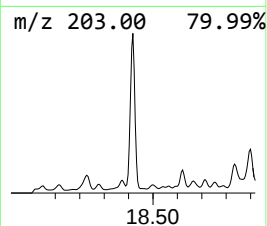
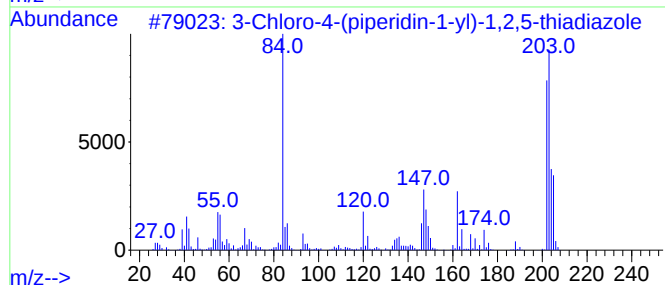
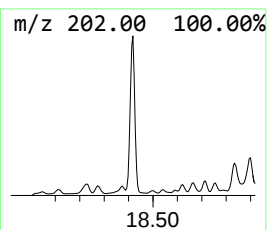
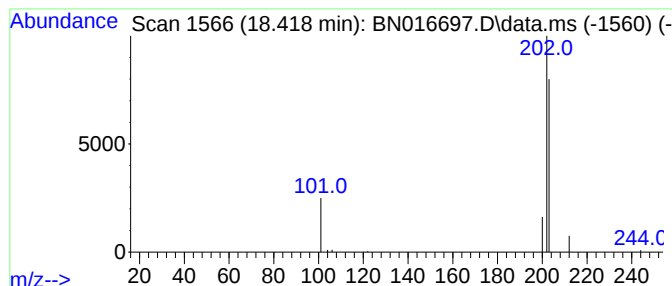
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 3-Chloro-4-(piperidin-1-yl)... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.418	0.34 ng	149778	Phenanthrene-d10	17.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-4-(piperidin-1-yl)-1,2,...	203	C7H10ClN3S	173053-54-8	5
2			Indole-5-carboxylic acid, 1,2,3-...	203	C12H13NO2	1000272-88-4	5
3			2,4-Dichloro-3-methylaniline, N,...	203	C9H11Cl2N	1000511-94-6	5
4			2-Chloro-6-cyclopropylpyridine-3...	203	C10H6ClN3	1000435-40-9	5
5			Pyrene	202	C16H10	000129-00-0	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

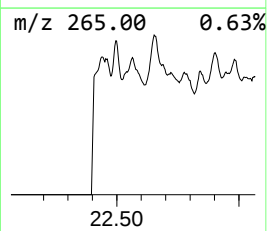
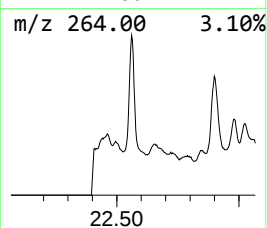
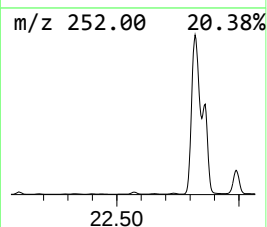
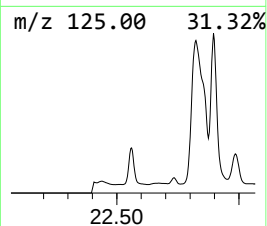
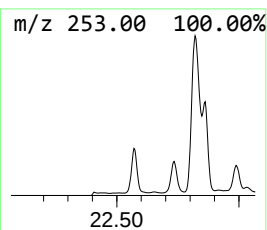
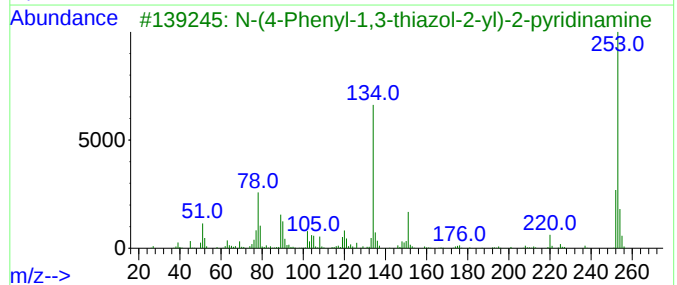
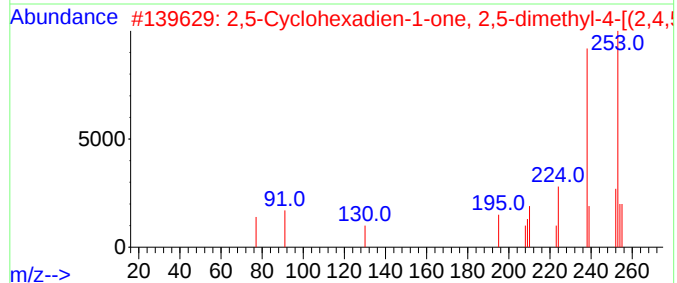
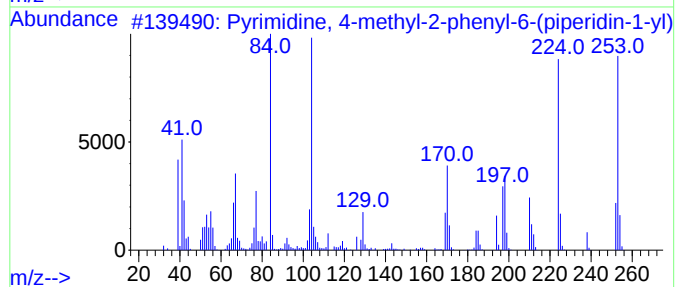
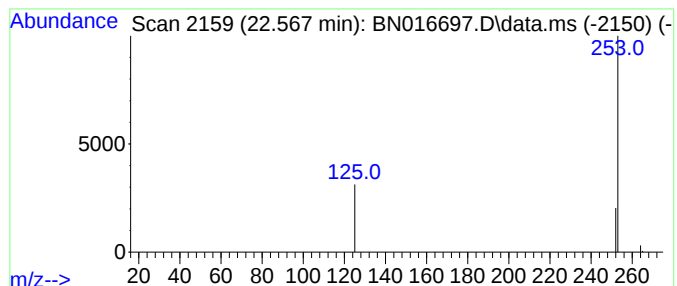
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pyrimidine, 4-methyl-2-phen... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.567	0.40 ng	209889	Perylene-d12	23.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrimidine, 4-methyl-2-phenyl-6-...	253	C16H19N3	1000302-39-3	5
2			2,5-Cyclohexadien-1-one, 2,5-dim...	253	C17H19NO	054245-93-1	5
3			N-(4-Phenyl-1,3-thiazol-2-yl)-2-...	253	C14H11N3S	1000485-04-5	5
4			Chalcone, 4-nitro-, (E)-	253	C15H11NO3	002960-55-6	5
5			1-(4-Fluorophenyl)-3-phenyl-1H-p...	253	C15H12FN3	072411-51-9	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

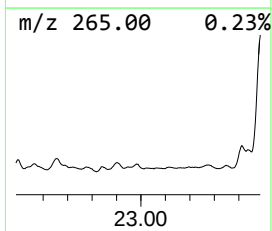
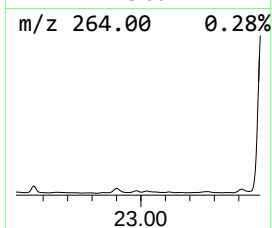
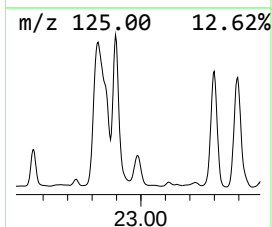
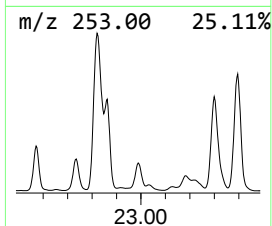
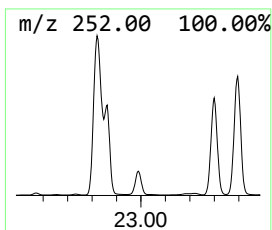
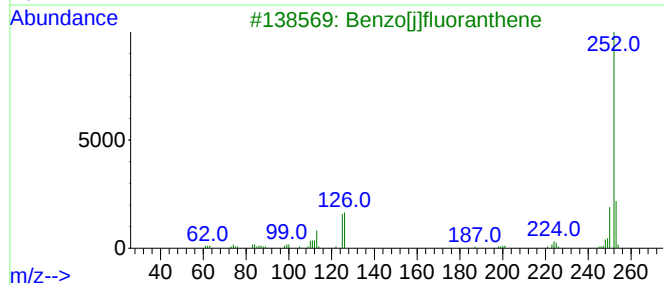
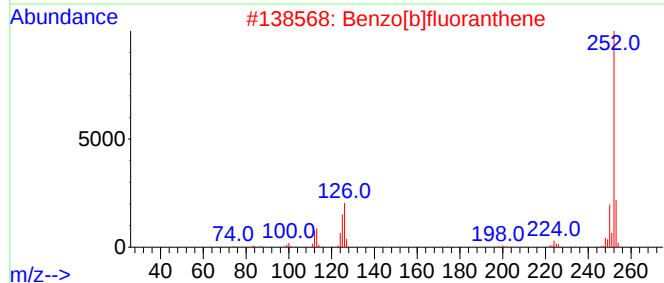
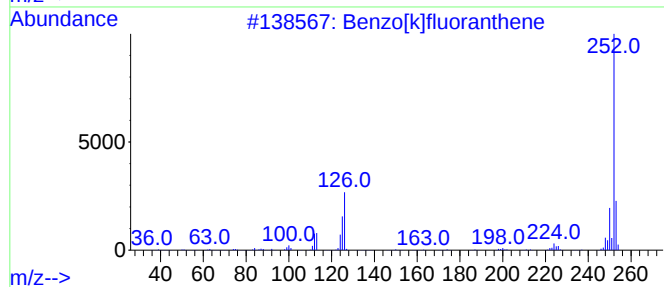
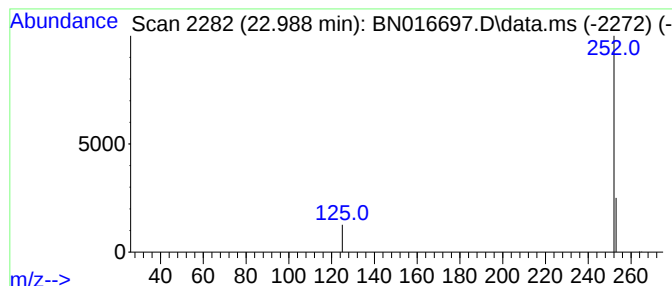
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzo[k]fluoranthene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.988	0.82 ng	432314	Perylene-d12	23.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	9
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
3			Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
4			Benzo[a]pyrene	252	C20H12	000050-32-8	9
5			Perylene	252	C20H12	000198-55-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

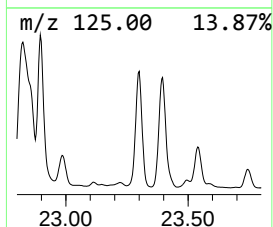
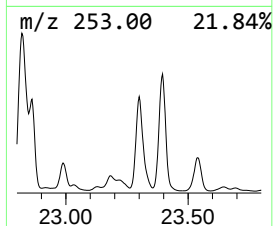
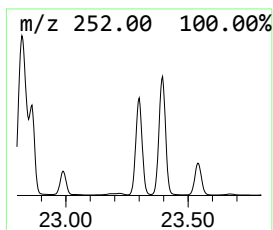
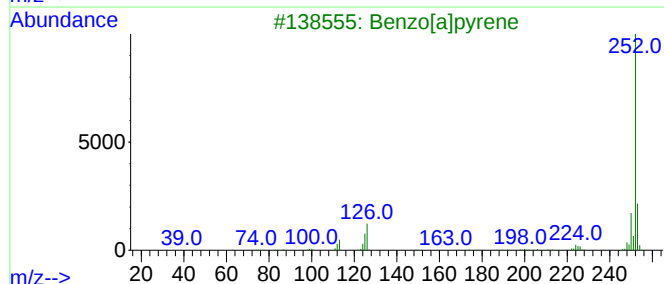
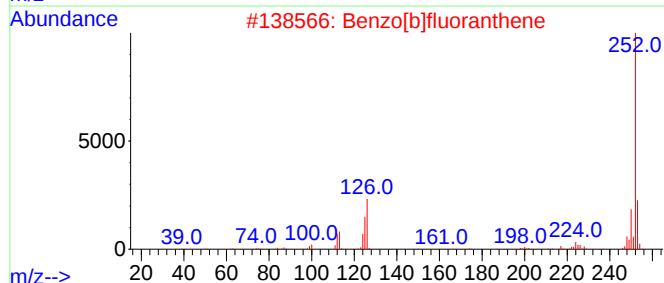
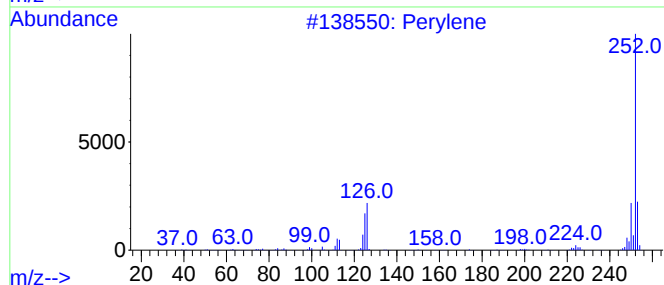
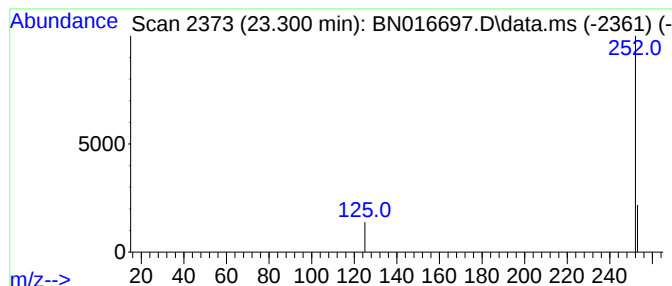
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.300	3.68 ng	1930800	Perylene-d12	23.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	9
2			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
3			Benzo[a]pyrene	252	C20H12	000050-32-8	9
4			Benzo[e]pyrene	252	C20H12	000192-97-2	9
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

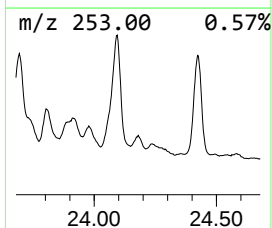
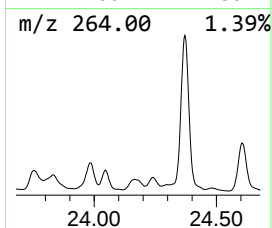
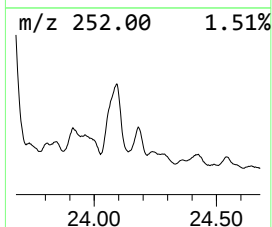
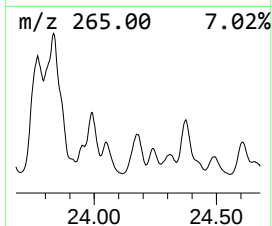
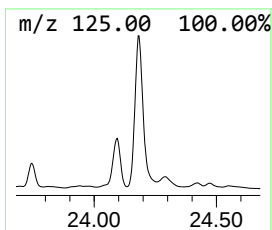
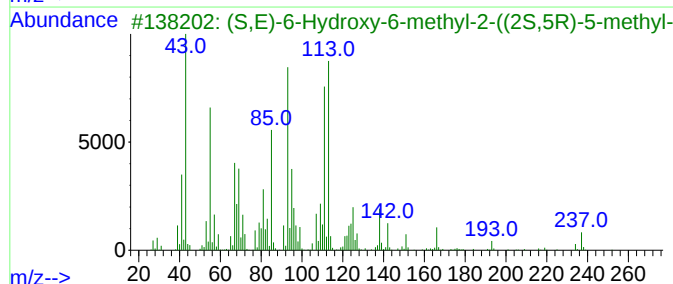
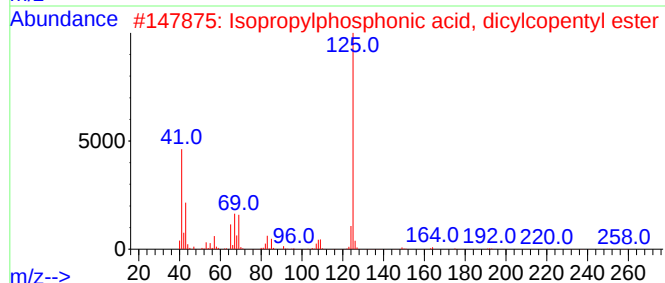
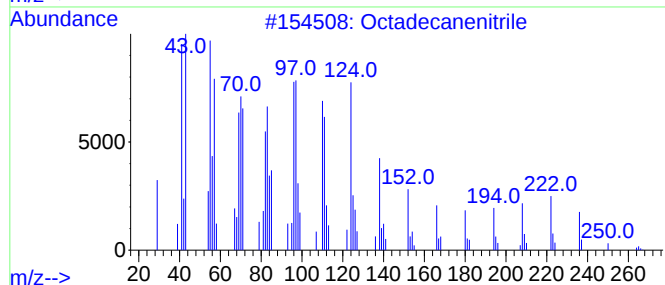
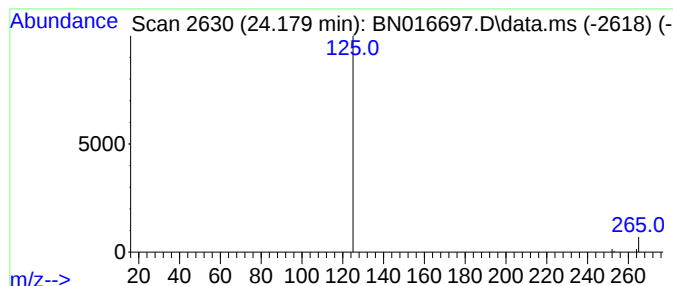
Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

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 Octadecanenitrile Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.179	0.54 ng	286124	Perylene-d12	23.495
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		Octadecanenitrile	265 C18H35N	000638-65-3 3
2		Isopropylphosphonic acid, dicylc...	260 C13H25O3P	1000273-18-4 3
3		(S,E)-6-Hydroxy-6-methyl-2-((2S,...	252 C15H24O3	088243-64-5 3
4		4,5,6-Pyrimidinetriamine	125 C4H7N5	000118-70-7 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 : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

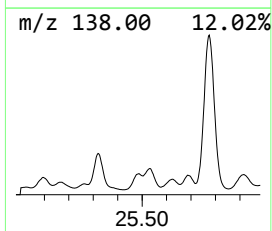
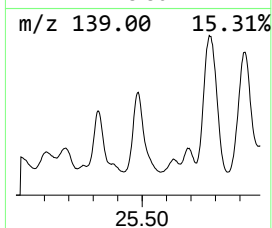
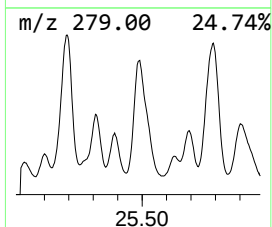
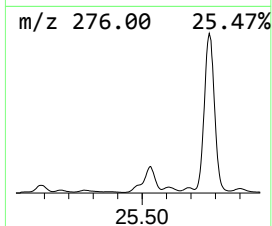
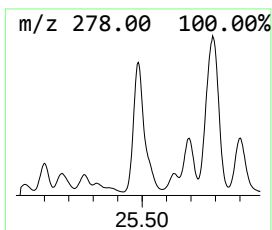
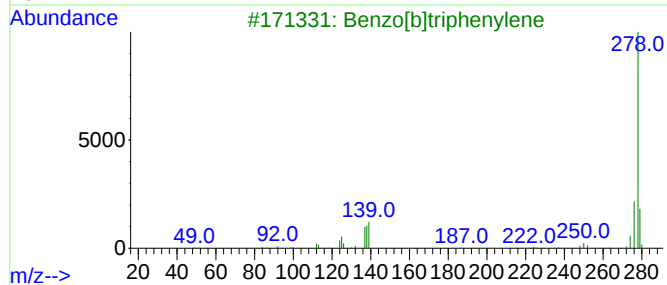
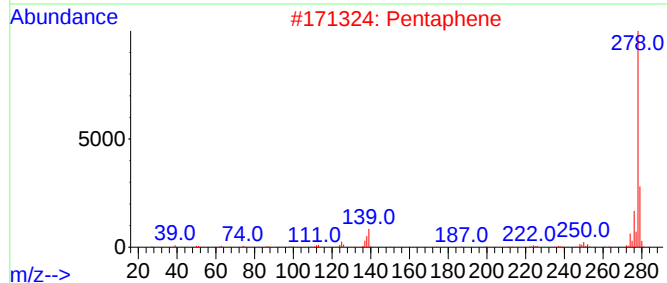
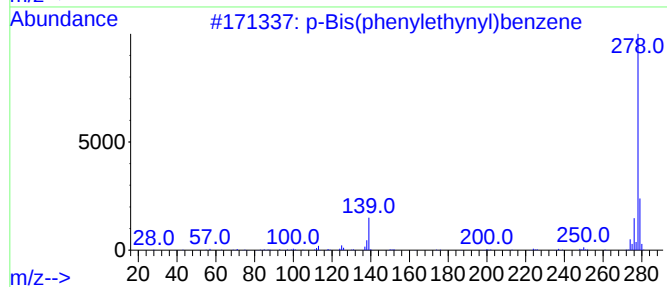
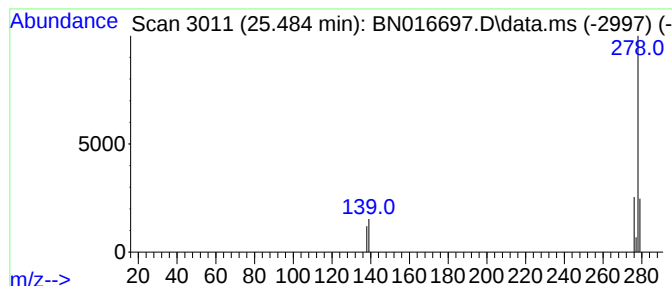
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 p-Bis(phenylethynyl)benzene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.483	0.50 ng	263516	Perylene-d12	23.495

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

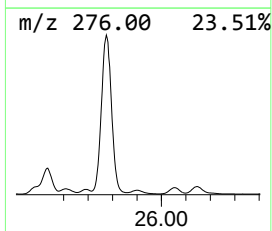
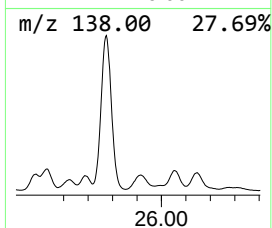
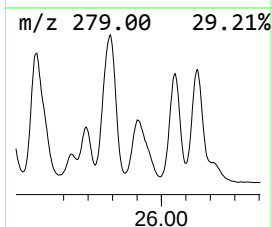
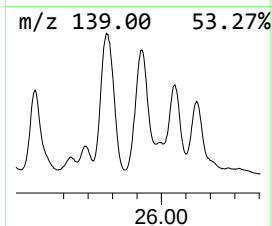
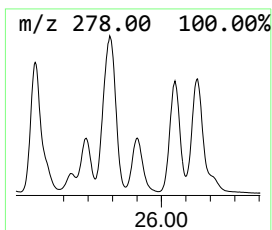
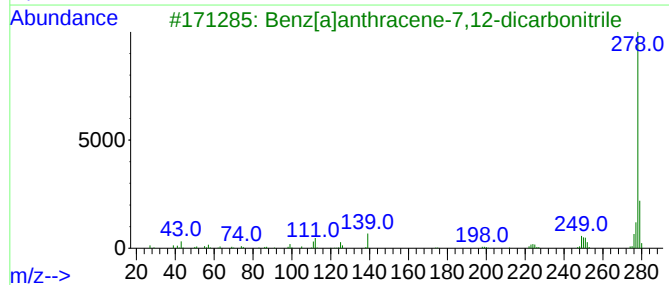
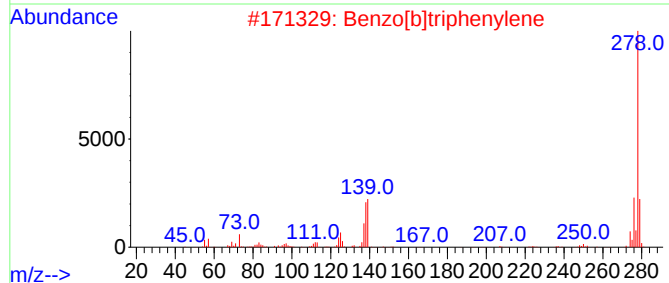
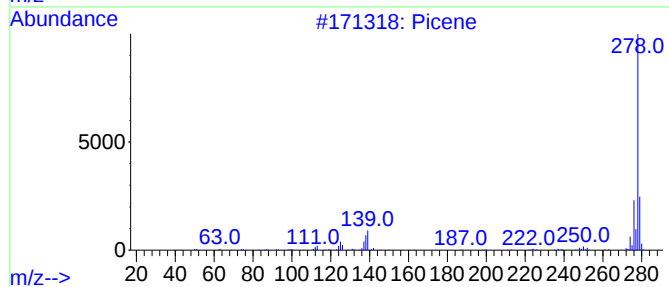
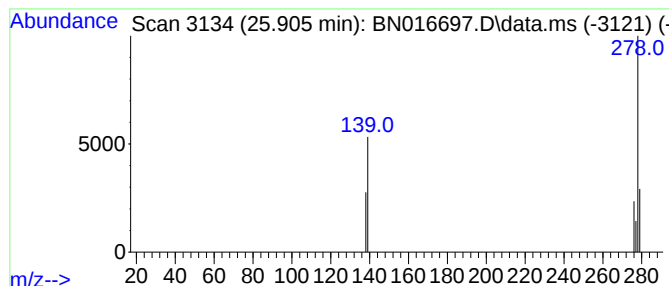
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Picene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.905	0.32 ng	168053	Perylene-d12	23.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Picene	278	C22H14	000213-46-7	72
2			Benzo[b]triphenylene	278	C22H14	000215-58-7	59
3			Benz[a]anthracene-7,12-dicarboni...	278	C20H10N2	035215-32-8	40
4			1H-1,4-Benzodiazepine-2,5-dione,...	278	C17H14N2O2	031965-37-4	38
5			1-naphthalenol, 4-[2-(4-methoxy...	278	C17H14N2O2	1000397-12-8	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

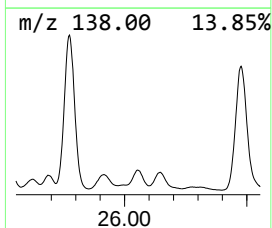
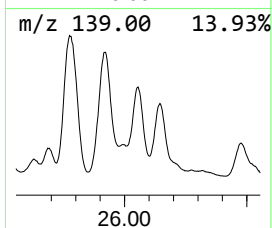
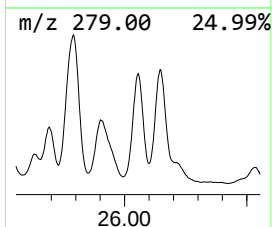
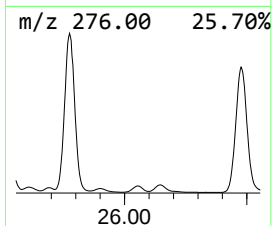
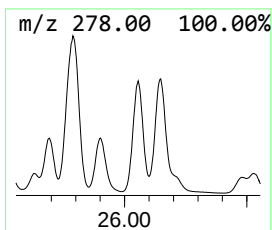
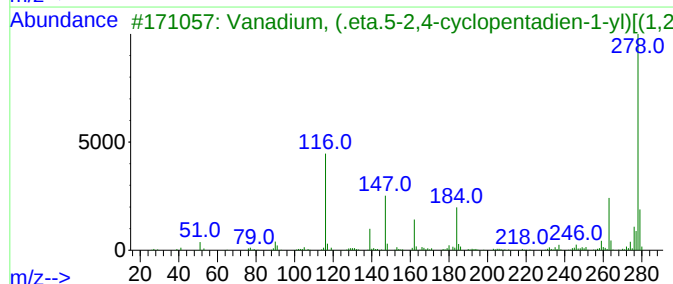
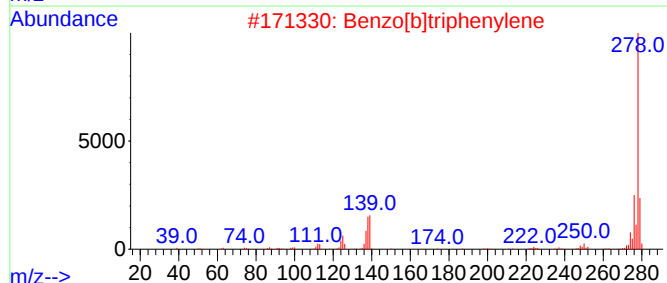
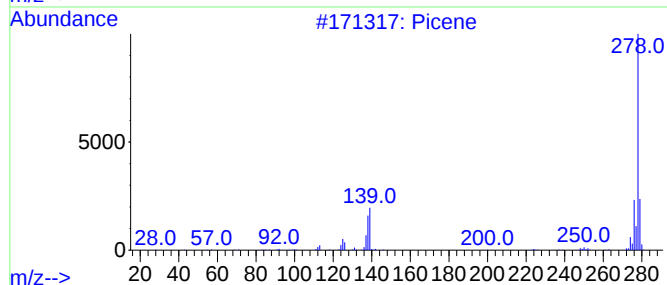
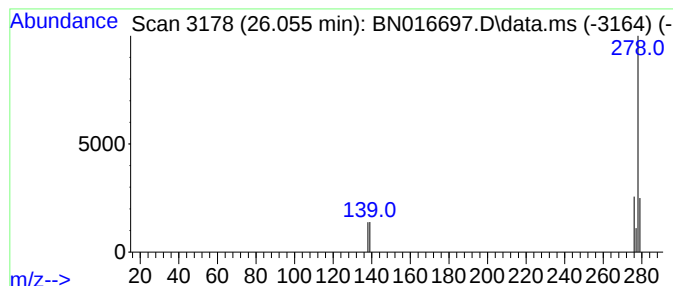
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Picene Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.055	0.45 ng	237868	Perylene-d12	23.495

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			Dibenz[a,h]anthracene	278	C22H14	000053-70-3	72
5			Benzo[b]chrysene	278	C22H14	000214-17-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

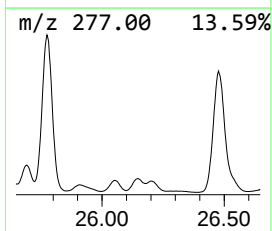
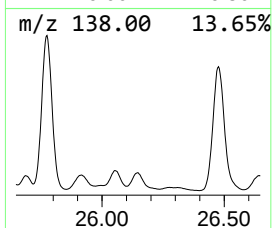
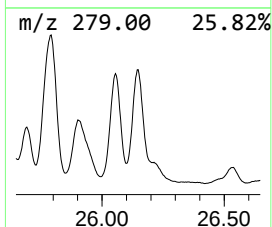
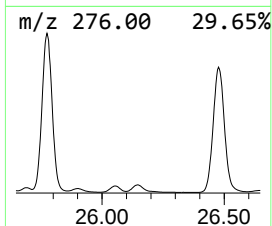
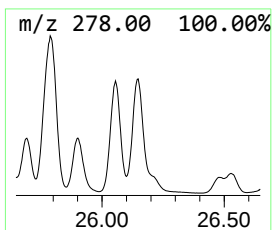
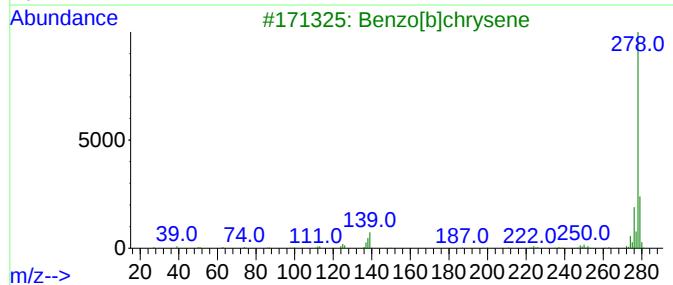
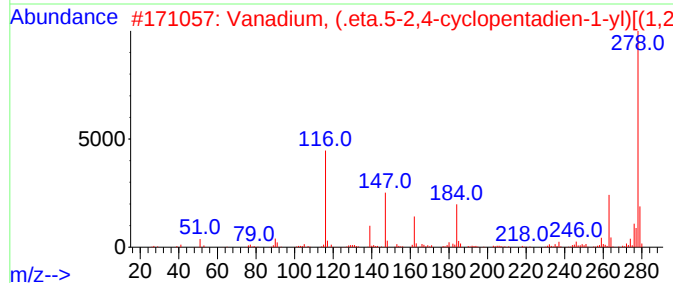
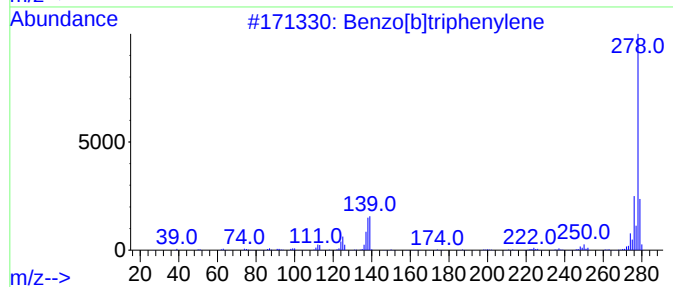
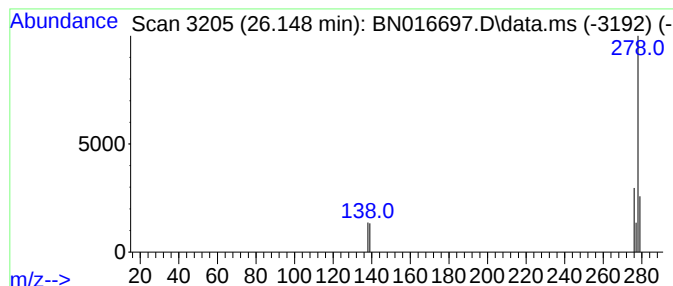
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Benzo[b]triphenylene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.148	0.62 ng	323476	Perylene-d12	23.495

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[b]triphenylene	278	C22H14	000215-58-7	80
2		Vanadium, (.eta.5-2,4-cyclopenta...	278	C17H23V	126948-97-8	78
3		Benzo[b]chrysene	278	C22H14	000214-17-5	72
4		1-naphthalenol, 4-[2-(4-methoxyp...	278	C17H14N2O2	1000397-12-8	72
5		Dibenz[a,h]anthracene	278	C22H14	000053-70-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016697.D
Acq On : 03 Oct 2021 08:12
Operator : CG/JU
Sample : M3892-13
Misc :
ALS Vial : 65 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-826-N-SO-0-0.5-092221

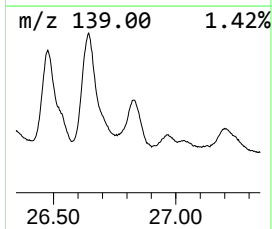
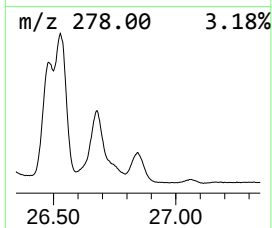
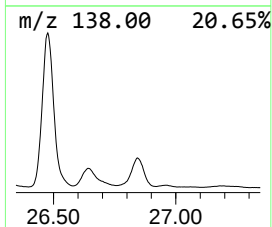
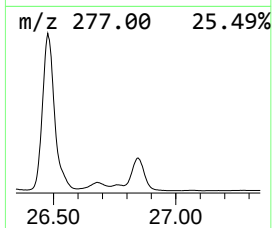
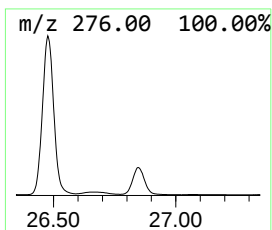
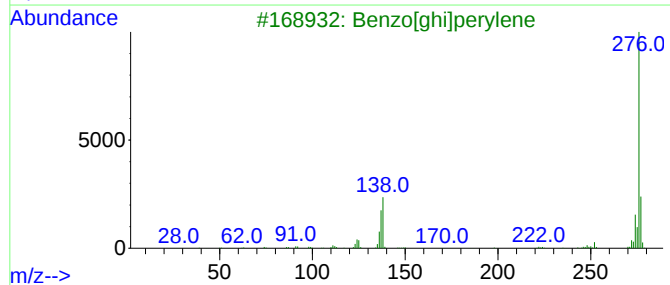
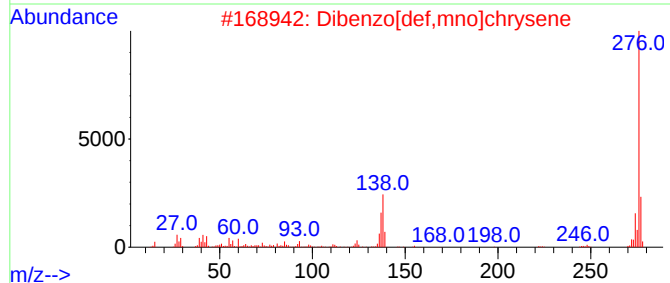
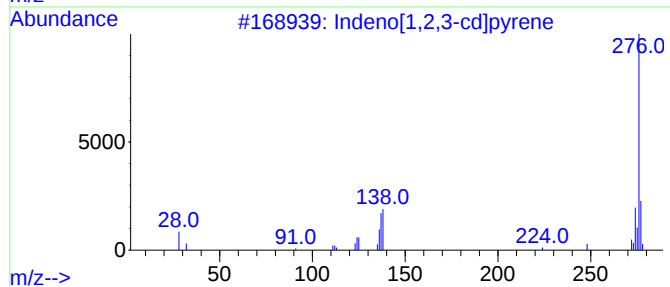
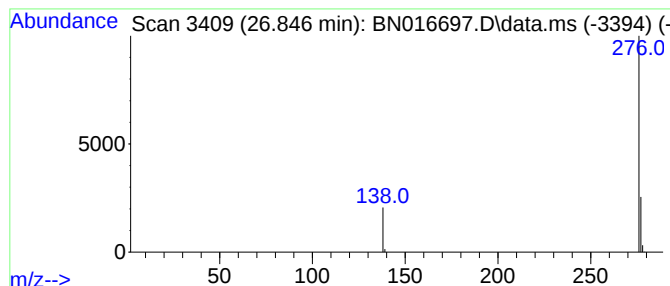
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Indeno[1,2,3-cd]pyrene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.846	0.42 ng	221307	Perylene-d12	23.495

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	83
2			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	83
3			Benzo[ghi]perylene	276	C22H12	000191-24-2	83
4			1H-benzimidazole, 2,2'-methylene...	276	C17H16N4	1000401-82-9	83
5			2-Benzyloxazolo[4,5-c]quinolin-4...	276	C17H12N2O2	211874-80-5	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016697.D
 Acq On : 03 Oct 2021 08:12
 Operator : CG/JU
 Sample : M3892-13
 Misc :
 ALS Vial : 65 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-826-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	16.4	ng	4256080	1	7.643	103692	0.4
2-Furancarboxit...	6.628	0.9	ng	226543	1	7.643	103692	0.4
2-Furancarboxit...	7.080	17.5	ng	4540280	1	7.643	103692	0.4
2-Furancarboxit...	7.532	1.9	ng	494422	1	7.643	103692	0.4
2-Furancarboxit...	7.855	0.9	ng	231068	1	7.643	103692	0.4
2-Furancarboxit...	7.910	0.5	ng	121353	1	7.643	103692	0.4
Benzene, nitro-	9.697	0.6	ng	277887	2	10.407	199768	0.4
Benzaldehyde, 2...	13.190	0.5	ng	312068	3	14.269	229457	0.4
1-Butanone, 3-m...	13.584	0.5	ng	261277	3	14.269	229457	0.4
Carbazole	17.432	0.9	ng	397786	4	17.018	174937	0.4
3-Chloro-4-(pip...	18.418	0.3	ng	149778	4	17.018	174937	0.4
Pyrimidine, 4-m...	22.567	0.4	ng	209889	6	23.495	210126	0.4
Benzo[k]fluoran...	22.988	0.8	ng	432314	6	23.495	210126	0.4
Perylene	23.300	3.7	ng	1930800	6	23.495	210126	0.4
Octadecanenitrile	24.179	0.5	ng	286124	6	23.495	210126	0.4
p-Bis(phenyleth...	25.483	0.5	ng	263516	6	23.495	210126	0.4
Picene	25.905	0.3	ng	168053	6	23.495	210126	0.4
Picene	26.055	0.5	ng	237868	6	23.495	210126	0.4
Benzo[b]triphen...	26.148	0.6	ng	323476	6	23.495	210126	0.4
Indeno[1,2,3-cd...	26.846	0.4	ng	221307	6	23.495	210126	0.4