

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016698.D
 Acq On : 03 Oct 2021 08:48
 Operator : CG/JU
 Sample : M3892-18
 Misc :
 ALS Vial : 66 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-832-J-SO-2-2.5-092221

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: BN016698.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.633	490	494	500	rVB	49307	102180	1.03%	0.151%
2	7.937	522	527	532	rVB	135312	241499	2.44%	0.357%
3	10.204	713	717	720	rBV	231070	408746	4.12%	0.604%
4	10.406	729	733	735	rBV	106378	183843	1.85%	0.272%
5	12.886	1071	1074	1078	rVB2	75949	125945	1.27%	0.186%
6	13.177	1094	1097	1101	rBV	176882	282092	2.85%	0.417%
7	14.269	1180	1183	1185	rBV	153006	224861	2.27%	0.332%
8	14.332	1185	1188	1192	rVB	235044	345616	3.49%	0.510%
9	15.322	1263	1266	1269	rBV	216207	313297	3.16%	0.463%
10	17.017	1400	1403	1404	rBV2	106171	172433	1.74%	0.255%
11	17.066	1404	1407	1410	rVV	2075638	2913964	29.39%	4.304%
12	17.151	1410	1414	1417	rVB	650281	1006136	10.15%	1.486%
13	17.212	1417	1419	1423	rBV	65166	140094	1.41%	0.207%
14	17.431	1431	1437	1440	rBV	225957	364518	3.68%	0.538%
15	17.954	1477	1480	1483	rVB2	78867	150988	1.52%	0.223%
16	18.417	1560	1566	1571	rBV2	158459	217368	2.19%	0.321%
17	18.904	1657	1664	1673	rVB2	66448	124872	1.26%	0.184%
18	19.102	1694	1704	1713	rVB	6562802	9527941	96.11%	14.072%
19	19.197	1719	1723	1729	rVB	106220	138690	1.40%	0.205%
20	19.465	1766	1777	1788	rBV	6213217	9913529	100.00%	14.641%
21	19.544	1788	1793	1800	rVV2	64711	133908	1.35%	0.198%
22	19.678	1815	1820	1822	rVV2	108949	148707	1.50%	0.220%
23	19.708	1822	1826	1833	rVB	317985	454932	4.59%	0.672%
24	20.016	1884	1887	1888	rBV2	109553	143664	1.45%	0.212%
25	20.112	1894	1896	1898	rBV2	103087	165131	1.67%	0.244%
26	20.155	1898	1900	1903	rVB	118247	183845	1.85%	0.272%
27	20.494	1930	1932	1934	rBV	65238	111270	1.12%	0.164%
28	20.601	1940	1942	1944	rVB	121797	168484	1.70%	0.249%
29	20.675	1947	1949	1951	rBV	109128	192642	1.94%	0.285%
30	20.717	1951	1953	1957	rVB2	111198	206773	2.09%	0.305%
31	20.887	1964	1969	1970	rBV2	153791	369950	3.73%	0.546%
32	20.919	1970	1972	1974	rVV	600197	835862	8.43%	1.234%
33	20.972	1974	1977	1979	rVV2	515688	1092613	11.02%	1.614%
34	21.015	1979	1981	1984	rVB2	70751	115092	1.16%	0.170%
35	21.174	1987	1996	1997	rBV	508489	922794	9.31%	1.363%
36	21.227	1997	2001	2003	rVV	4671475	7330201	73.94%	10.826%

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.280	2003	2006	2011	rVV	3900628	6244213	62.99%	9.222%
38	21.397	2014	2017	2022	rVV	604577	1012936	10.22%	1.496%
39	21.737	2047	2049	2051	rBV2	86643	163209	1.65%	0.241%
40	21.790	2051	2054	2057	rVV	177059	339798	3.43%	0.502%
41	21.843	2057	2059	2061	rVV2	103393	150994	1.52%	0.223%
42	21.949	2064	2069	2071	rVV3	248350	613464	6.19%	0.906%
43	21.992	2071	2073	2074	rVV2	229153	317595	3.20%	0.469%
44	22.024	2074	2076	2079	rVB	405798	551942	5.57%	0.815%
45	22.098	2079	2083	2086	rBV2	179156	366348	3.70%	0.541%
46	22.183	2089	2091	2094	rVB	94844	128186	1.29%	0.189%
47	22.289	2097	2101	2103	rBV3	70157	209941	2.12%	0.310%
48	22.395	2109	2111	2113	rVB2	252515	252175	2.54%	0.372%
49	22.574	2153	2161	2177	rVB	163555	263130	2.65%	0.389%
50	22.683	2183	2193	2200	rVB	212534	386568	3.90%	0.571%
51	22.738	2202	2209	2219	rVB	93501	146311	1.48%	0.216%
52	22.827	2222	2235	2243	rBV	2329793	5496186	55.44%	8.117%
53	22.995	2275	2284	2296	rVB	497359	814100	8.21%	1.202%
54	23.306	2364	2375	2391	rBV	1265274	2457393	24.79%	3.629%
55	23.406	2392	2404	2421	rVB	1812711	3453351	34.83%	5.100%
56	23.553	2438	2447	2459	rVB	484812	944690	9.53%	1.395%
57	25.493	3003	3014	3023	rBV3	116954	306947	3.10%	0.453%
58	25.788	3085	3100	3122	rVB2	556418	1698278	17.13%	2.508%
59	26.062	3169	3180	3195	rBV2	118012	302736	3.05%	0.447%
60	26.157	3197	3208	3220	rBV	88785	224615	2.27%	0.332%
61	26.490	3288	3305	3336	rVB	334128	1089447	10.99%	1.609%
62	26.856	3399	3412	3436	rVB	93246	299761	3.02%	0.443%

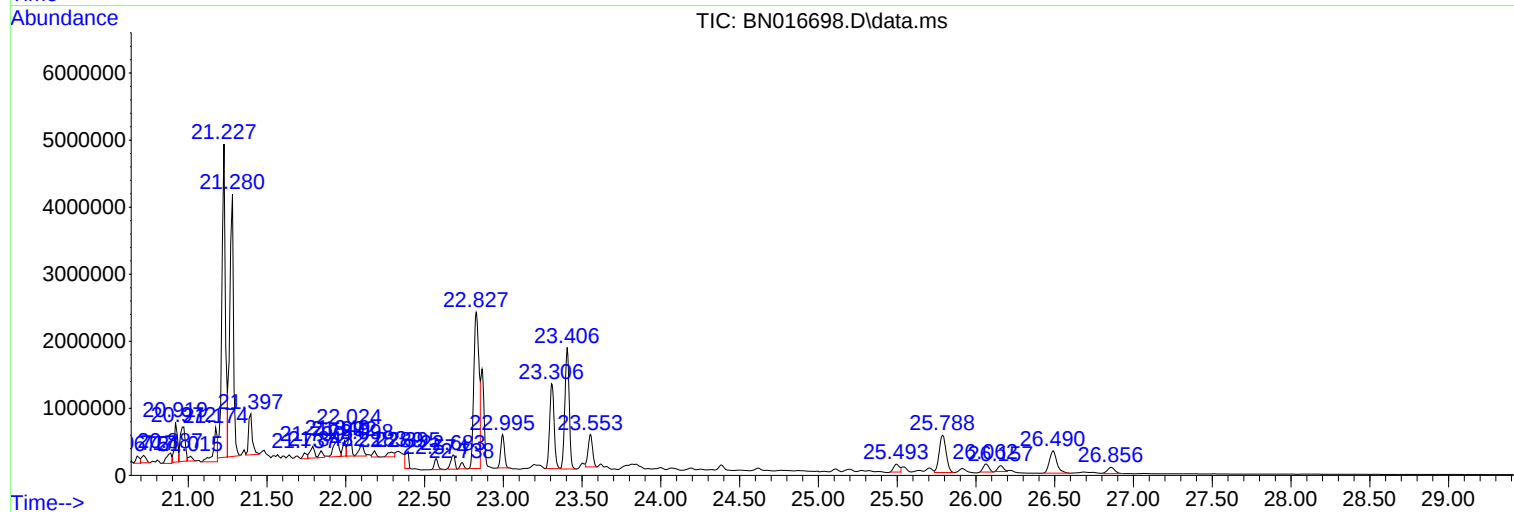
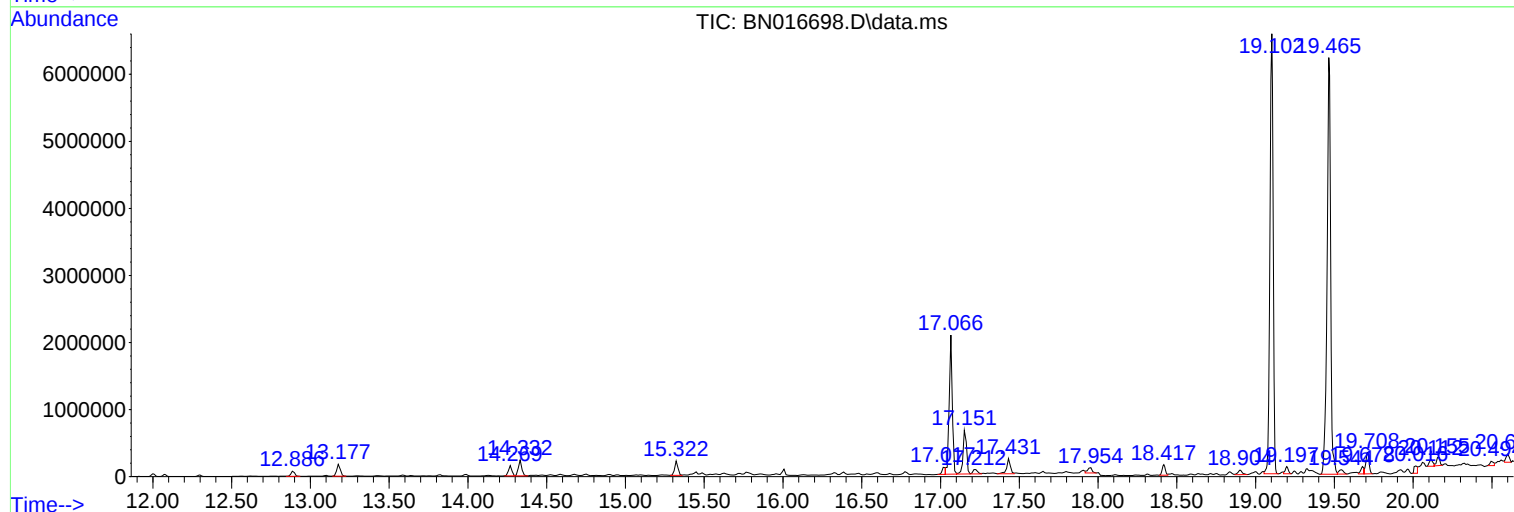
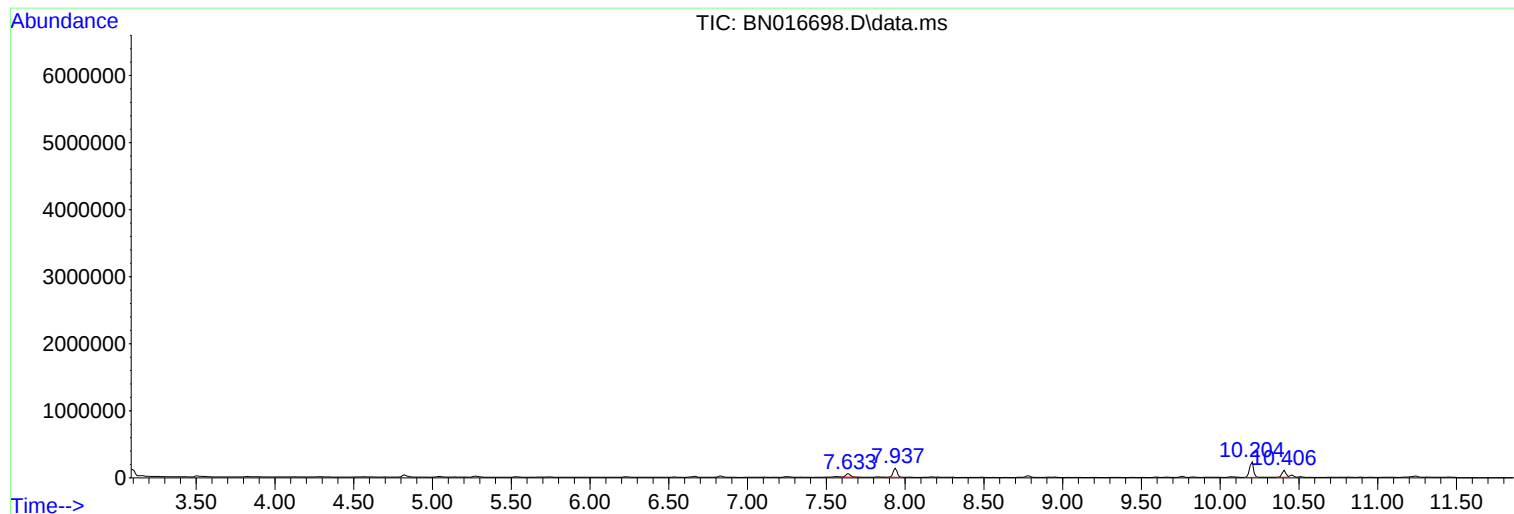
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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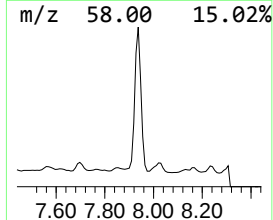
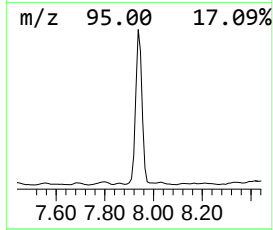
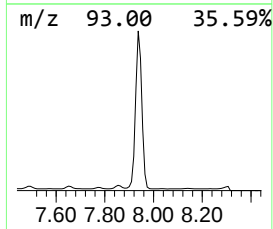
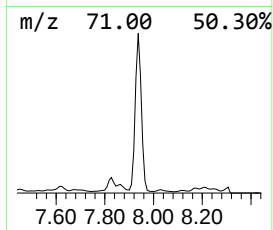
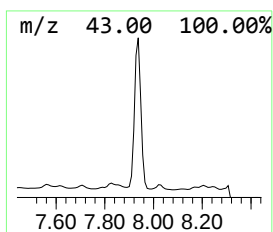
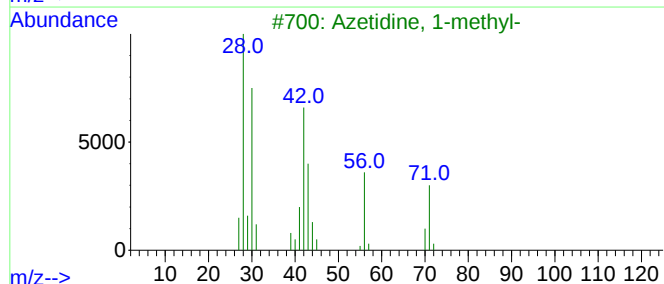
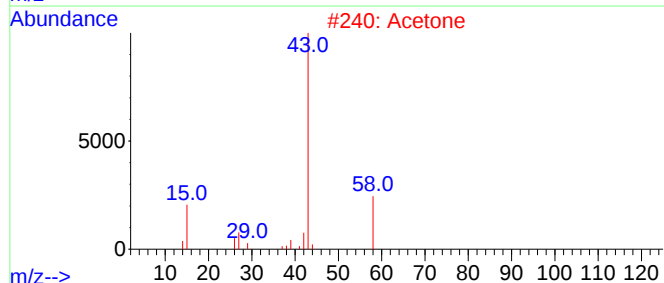
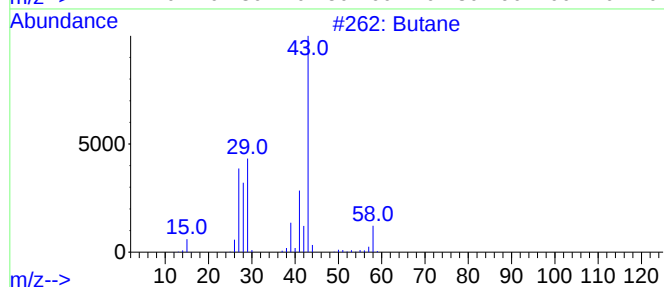
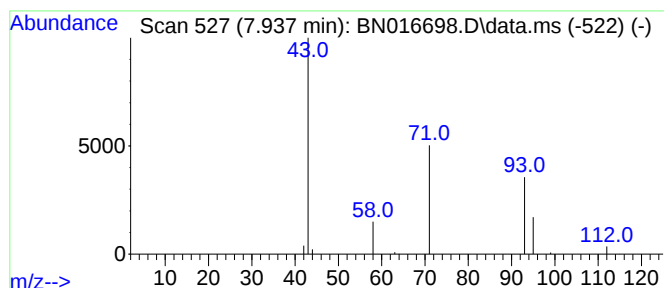
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.937	0.95 ng	241499	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			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3
4			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3
5			2-Propenamide	71	C3H5NO	000079-06-1	3



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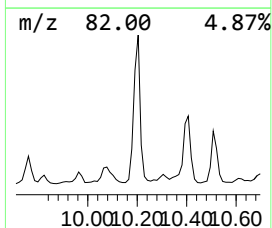
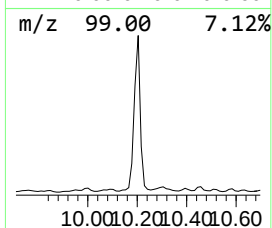
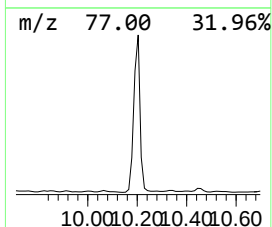
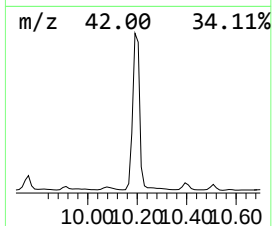
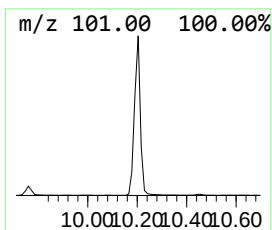
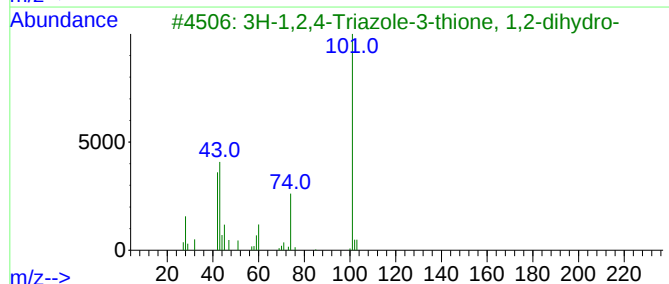
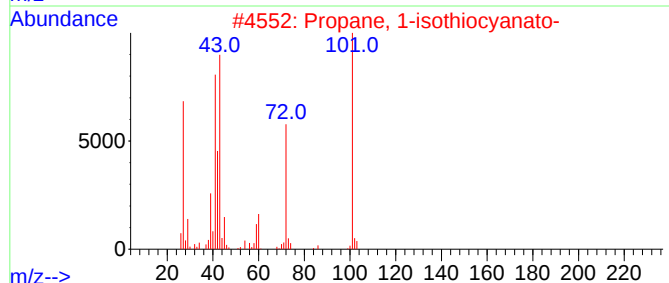
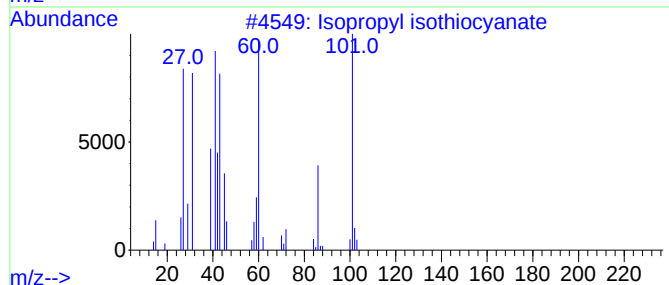
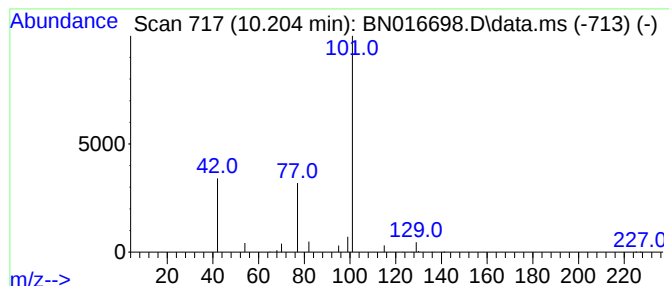
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl isothiocyanate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.204	0.89 ng	408746	Naphthalene-d8	10.406

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
2			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
3			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	4
4			2-Pyrrolidinethione	101	C4H7NS	002295-35-4	4
5			3-Aminopropionitrile	70	C3H6N2	000151-18-8	4



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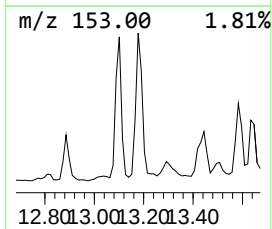
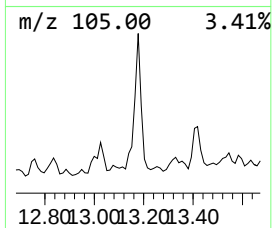
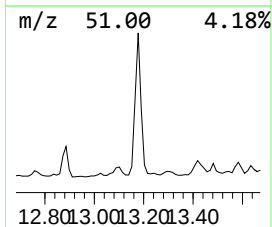
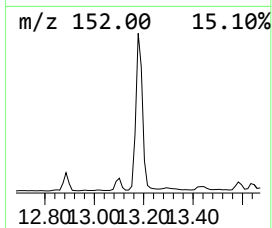
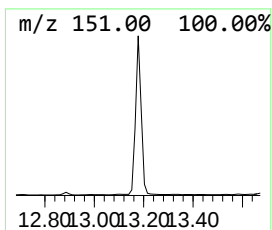
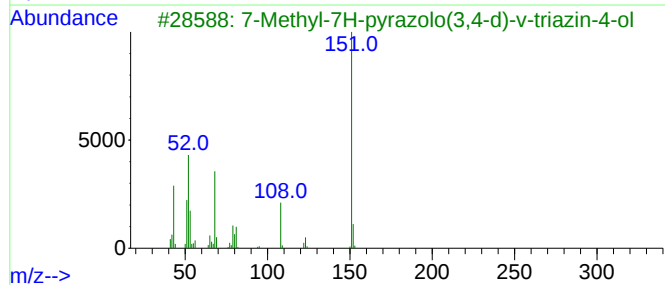
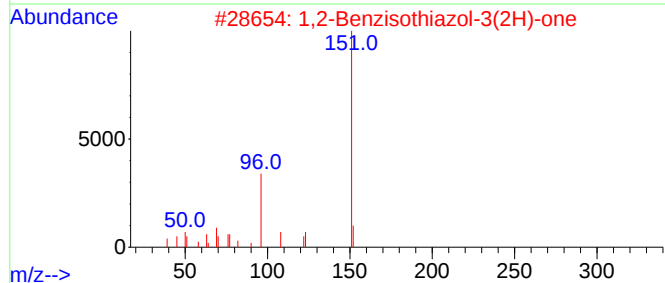
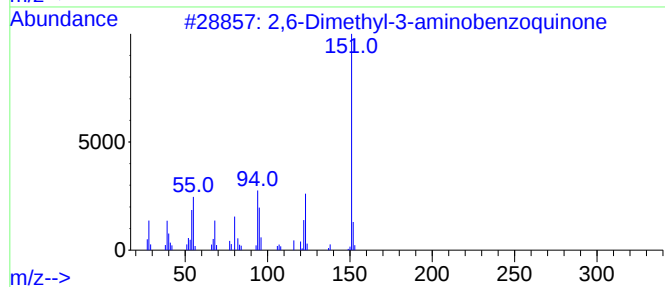
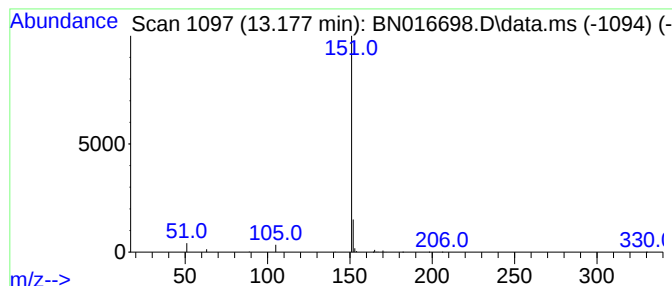
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.177	0.50 ng	282092	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	7
2			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
3			7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
4			Vanillin	152	C8H8O3	000121-33-5	5
5			Butane-1,3-dione, 1-(pyrrol-2-yl)-	151	C8H9NO2	022441-25-4	5



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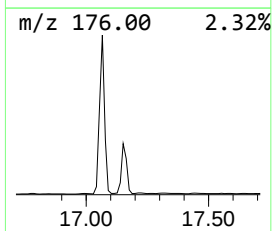
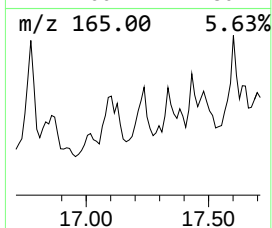
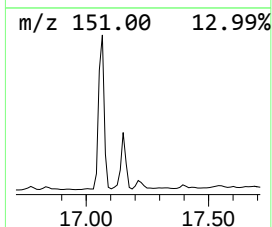
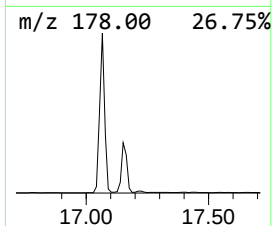
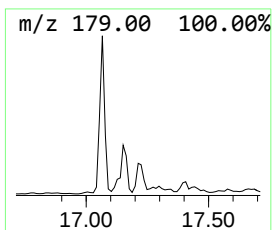
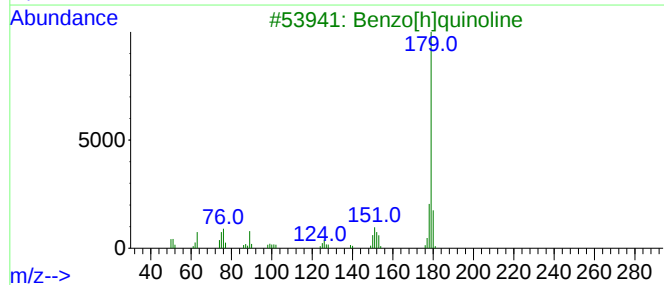
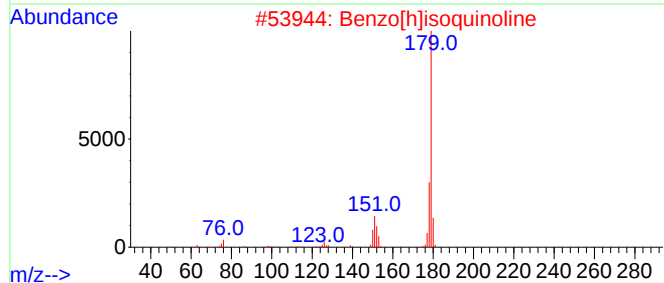
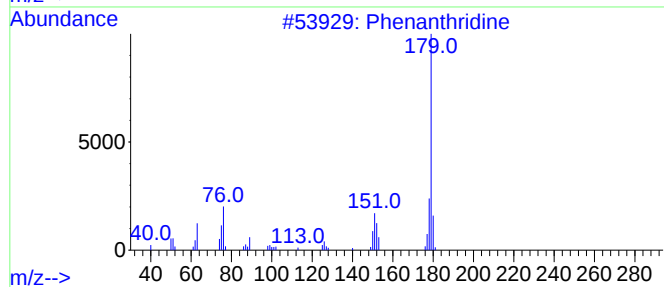
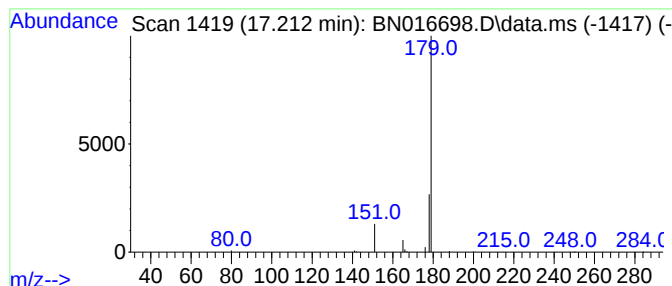
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Peak Number 4 Phenanthridine Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.212	0.32 ng	140094	Phenanthrene-d10	17.029

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthridine	179	C13H9N	000229-87-8	56
2			Benzo[h]isoquinoline	179	C13H9N	000229-71-0	56
3			Benzo[h]quinoline	179	C13H9N	000230-27-3	56
4			Acridine	179	C13H9N	000260-94-6	56
5			p-Phenylbenzonitrile	179	C13H9N	002920-38-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-2-2.5-092221

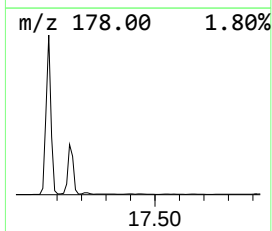
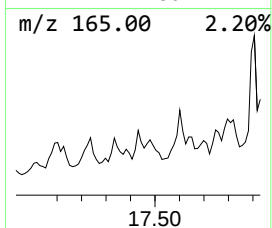
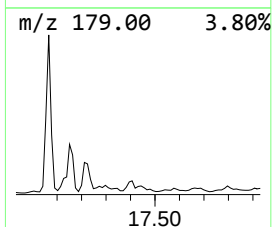
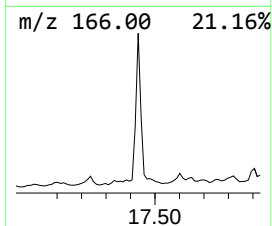
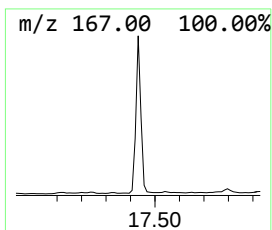
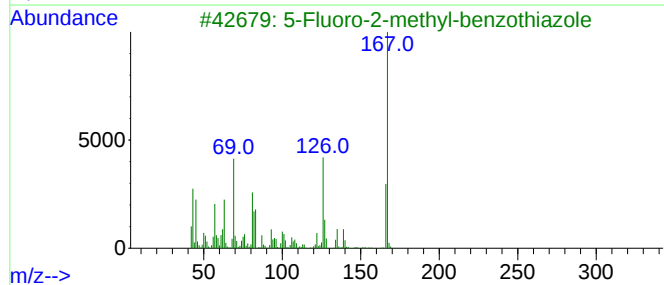
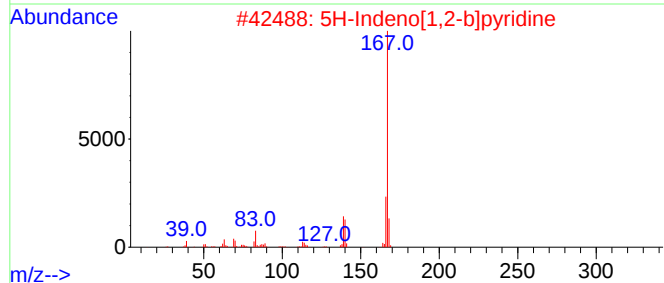
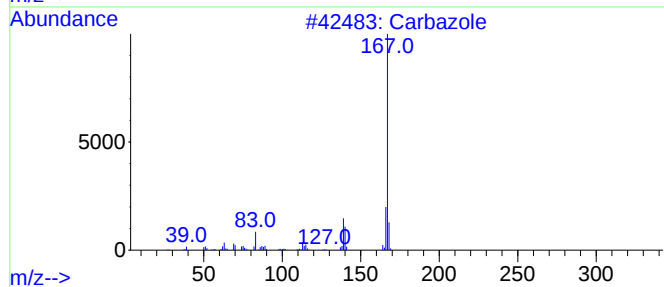
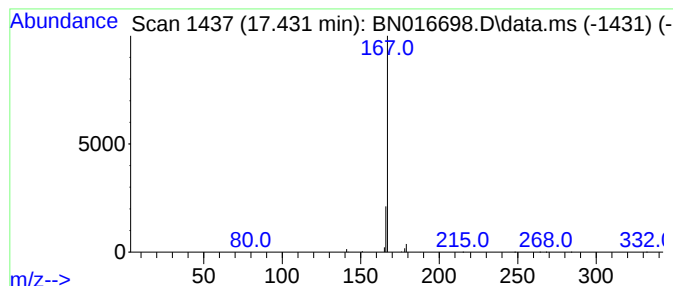
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Carbazole Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.85 ng	364518	Phenanthrene-d10	17.029

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			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
4			benzaldehyde, 2-hydroxy-4-nitro-	167	C7H5NO4	1000404-52-2	5
5			2-Azaspiro[4.5]decan-3-one, 8-me...	167	C10H17NO	196608-77-2	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
ALS Vial : 66 Sample Multiplier: 1

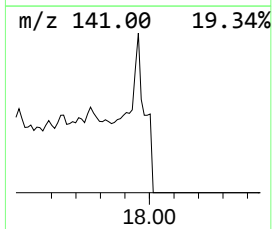
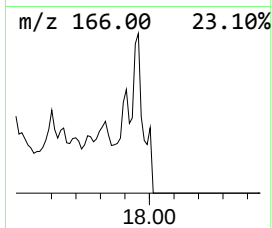
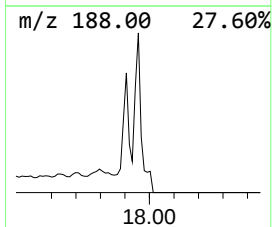
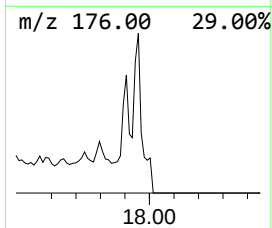
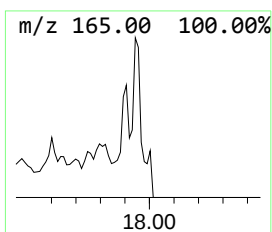
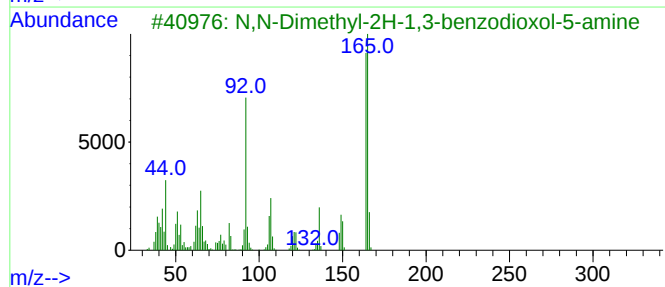
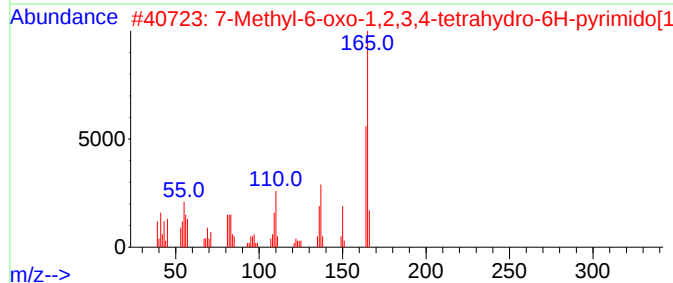
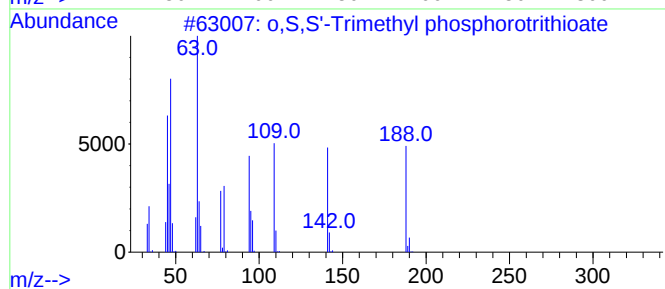
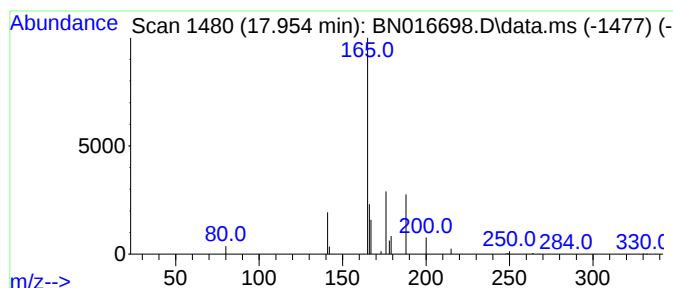
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ClientSampleId :
S-832-J-SO-2-2.5-092221

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 o,S,S'-Trimethyl phosphorot... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.954	0.35 ng	150988	Phenanthrene-d10		17.029	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	o,S,S'-Trimethyl phosphorotrithi...		188	C3H9OPS3	1000306-06-4	7
2	7-Methyl-6-oxo-1,2,3,4-tetrahydr...		165	C8H11N3O	026955-14-6	4
3	N,N-Dimethyl-2H-1,3-benzodioxol-...		165	C9H11NO2	1000388-48-7	4
4	2-Chloro-6-fluorocinnamic acid		200	C9H6ClFO2	000392-22-3	4
5	5-Amino-2-Mercaptobenzimidazole		165	C7H7N3S	002818-66-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
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Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-832-J-SO-2-2.5-092221

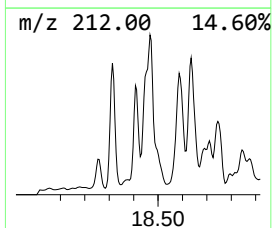
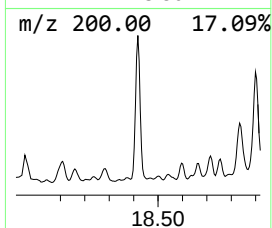
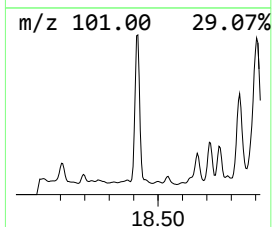
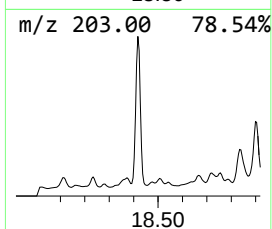
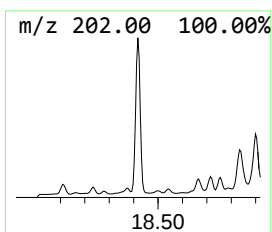
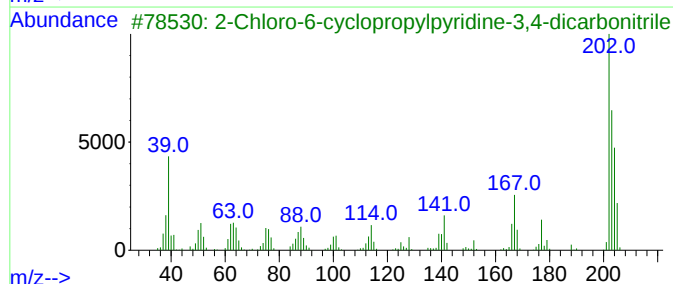
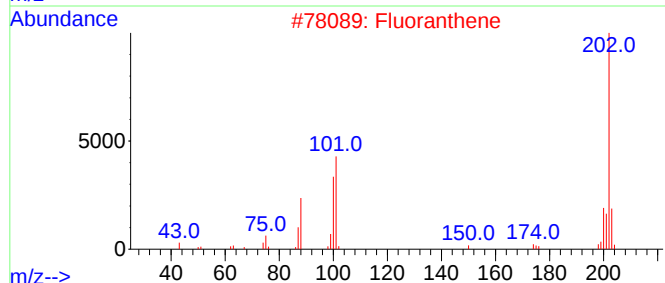
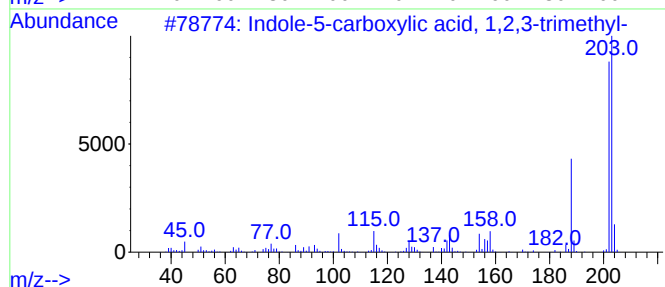
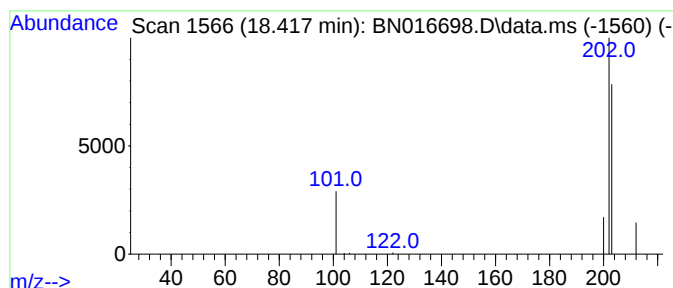
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Indole-5-carboxylic acid, 1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.417	0.50 ng	217368	Phenanthrene-d10	17.029

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole-5-carboxylic acid, 1,2,3-...	203	C12H13NO2	1000272-88-4	5
2			Fluoranthene	202	C16H10	000206-44-0	5
3			2-Chloro-6-cyclopropylpyridine-3...	203	C10H6ClN3	1000435-40-9	5
4			2,4-Dichloro-3-methylaniline, N...	203	C9H11Cl2N	1000511-94-6	5
5			Pyrene	202	C16H10	000129-00-0	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
ALS Vial : 66 Sample Multiplier: 1

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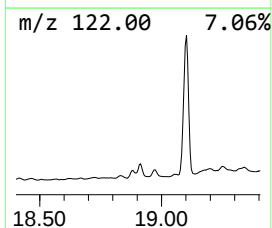
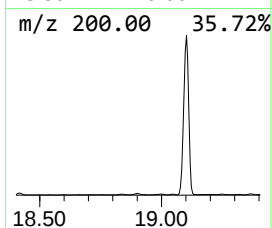
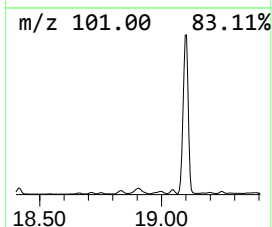
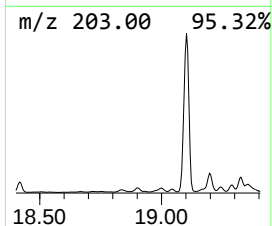
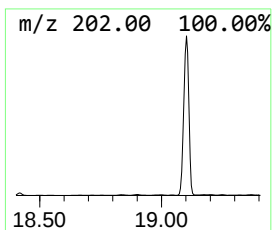
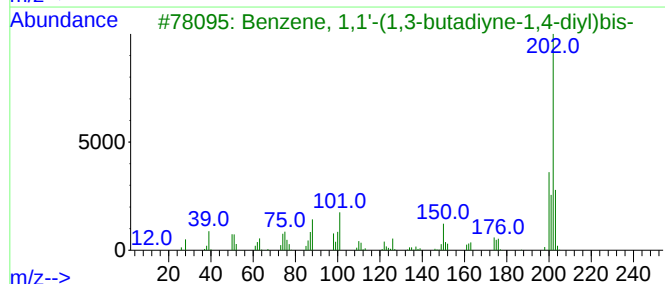
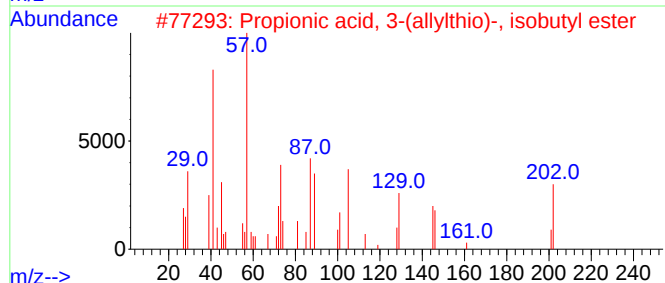
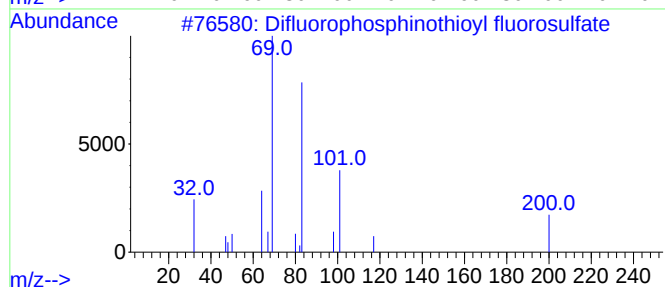
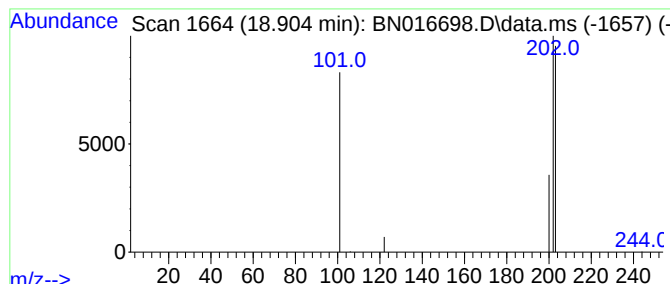
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Difluorophosphinothioyl flu... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.904	0.29 ng	124872	Phenanthrene-d10	17.029

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Difluorophosphinothioyl fluorosu...	200	F303PS2	018643-33-9	4
2			Propionic acid, 3-(allylthio)-, ...	202	C10H18O2S	024382-60-3	4
3			Benzene, 1,1'-(1,3-butadiene-1,4...	202	C16H10	000886-66-8	4
4			2,2,4,6,8-Pentamethyl-1,3-dioxa...	203	C9H21NO2Si	1000322-48-0	4
5			2,5-Dimethyl-1,4-diacetyl-1,2,4...	200	C8H16N4O2	021599-69-9	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
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ALS Vial : 66 Sample Multiplier: 1

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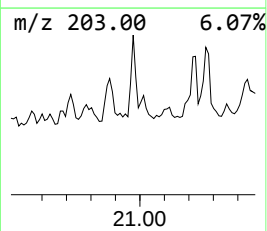
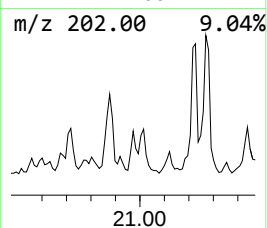
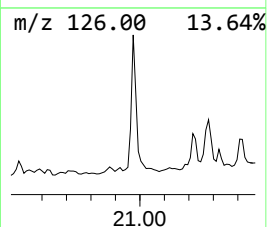
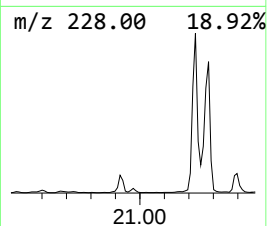
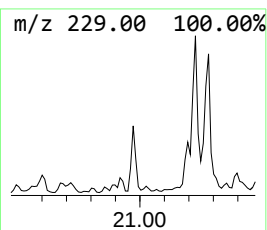
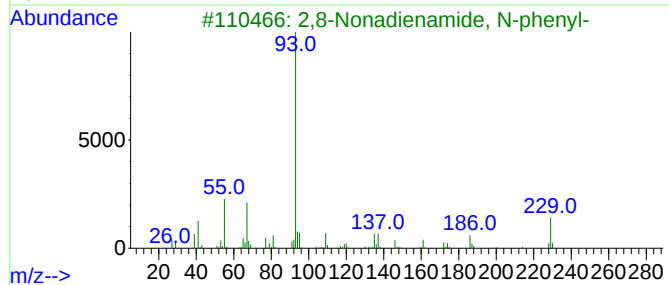
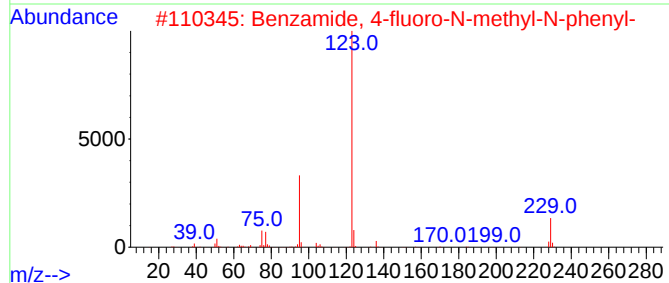
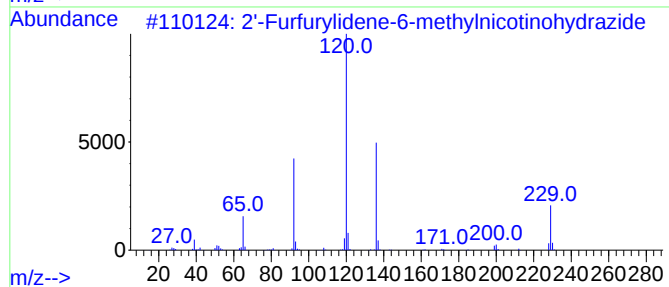
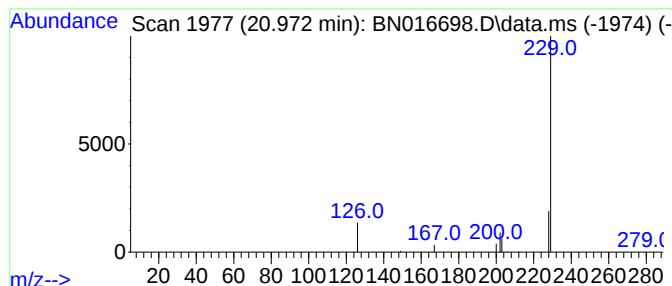
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2'-Furfurylidene-6-methylni... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.972	0.06 ng	1092610	Chrysene-d12	21.238

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2'-Furfurylidene-6-methylnicotin...	229	C12H11N3O2	328542-13-8	3
2			Benzamide, 4-fluoro-N-methyl-N-p...	229	C14H12FNO	037950-87-1	3
3			2,8-Nonadienamide, N-phenyl-	229	C15H19NO	128039-94-1	3
4			Benzonitrile, 4-iodo-	229	C7H4IN	003058-39-7	2
5			3-Formyl-6-phenyl-thiazolo(3,2-b...	229	C11H7N3OS	074829-44-0	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
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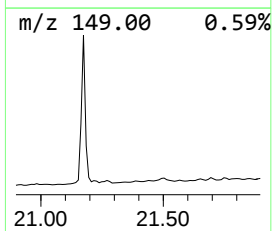
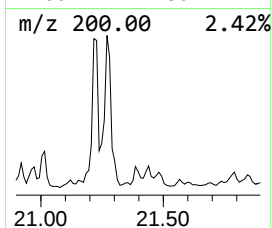
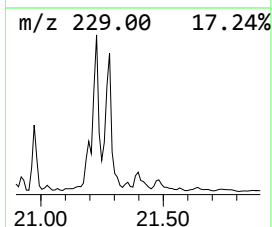
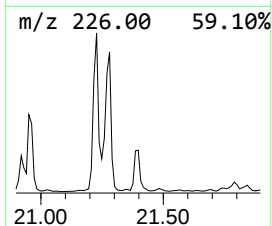
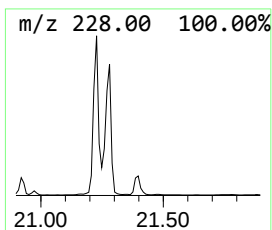
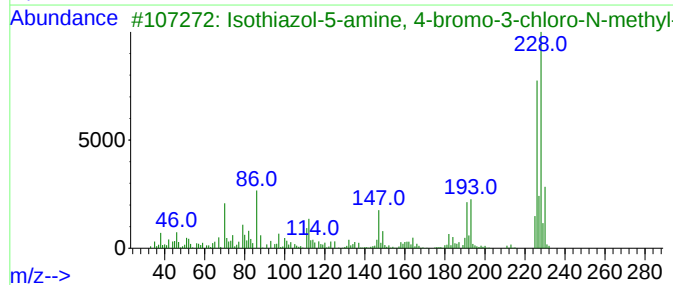
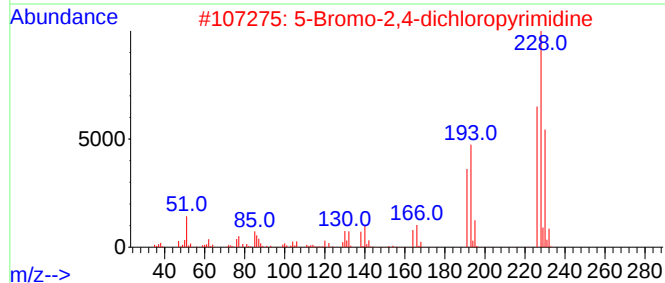
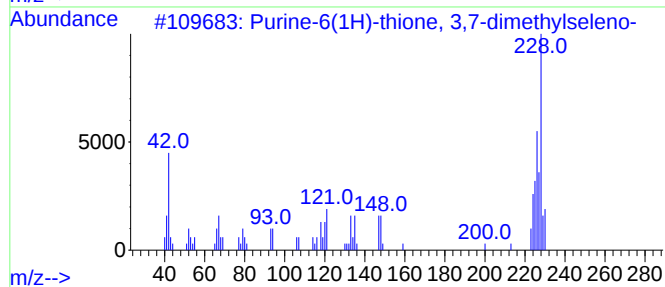
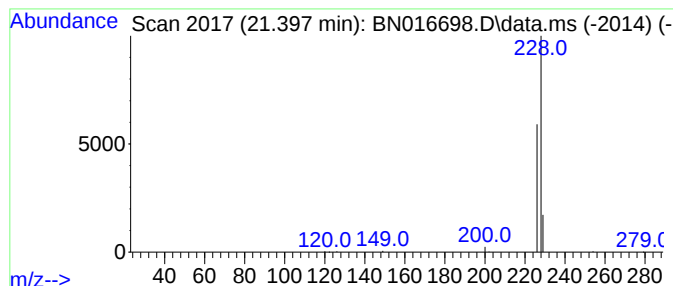
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Purine-6(1H)-thione, 3,7-di... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.397	0.06 ng	1012940	Chrysene-d12	21.238

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Purine-6(1H)-thione, 3,7-dimethy...	228	C7H8N4Se	023663-58-3	74
2			5-Bromo-2,4-dichloropyrimidine	226	C4HBrCl2N2	036082-50-5	9
3			Isothiazol-5-amine, 4-bromo-3-ch...	226	C4H4BrClN2S	1000272-59-9	9
4			Naphthacene	228	C18H12	000092-24-0	7
5			Triphenylene	228	C18H12	000217-59-4	7



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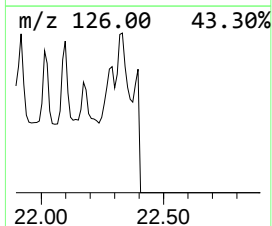
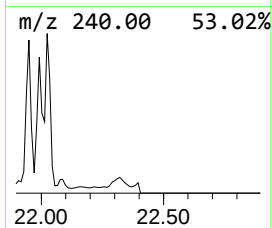
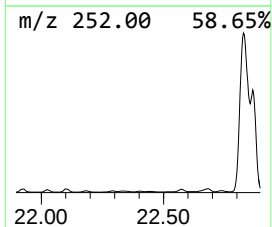
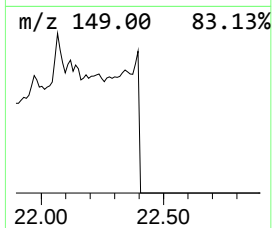
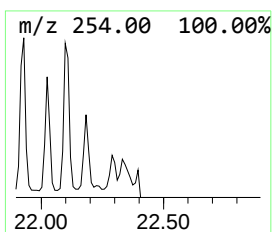
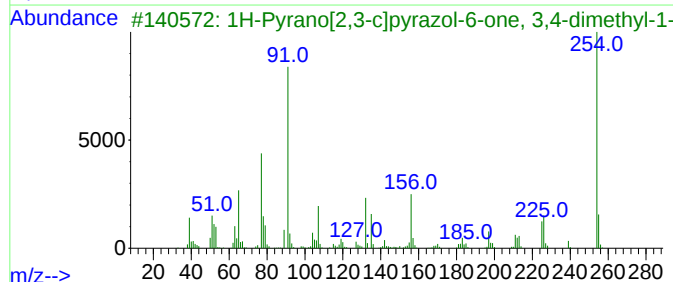
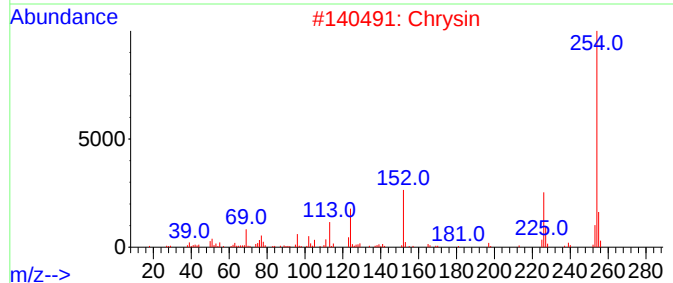
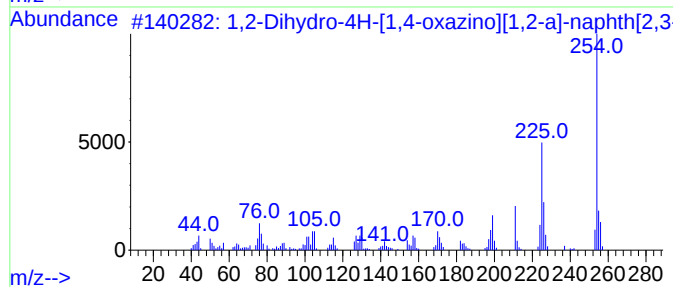
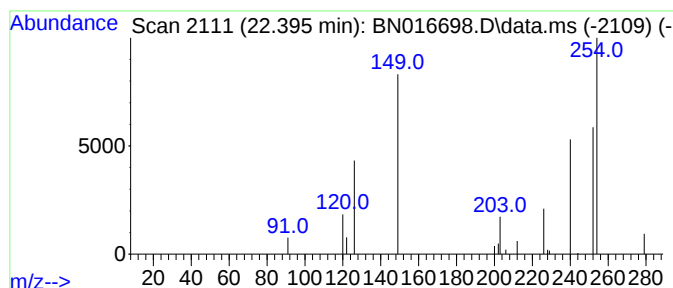
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1,2-Dihydro-4H-[1,4-oxazino... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.395	0.11 ng	252175	Perylene-d12	23.505	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dihydro-4H-[1,4-oxazino][1,2...	254	C14H10N2O3	038066-84-1	10
2	Chrysin	254	C15H10O4	000480-40-0	9
3	1H-Pyrano[2,3-c]pyrazol-6-one, 3...	254	C15H14N2O2	1010316-21-1	9
4	2,6-(Etheno[1,4]benzenoetheno)na...	254	C20H14	117054-70-3	9
5	9-Aza-bicyclo[4.2.1]nona-2,4-die...	149	C9H11NO	034668-54-7	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-2-2.5-092221

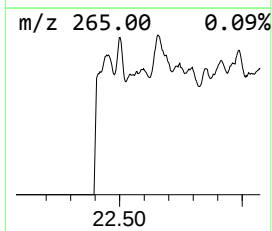
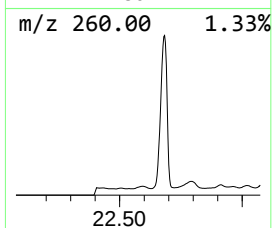
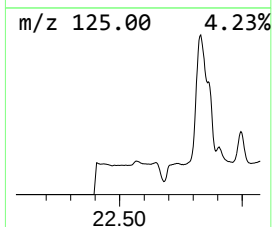
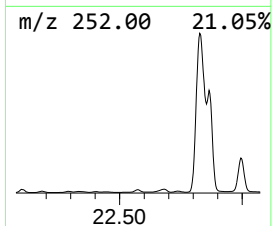
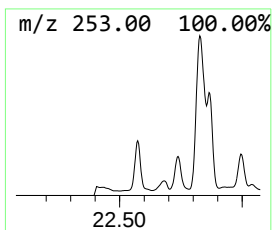
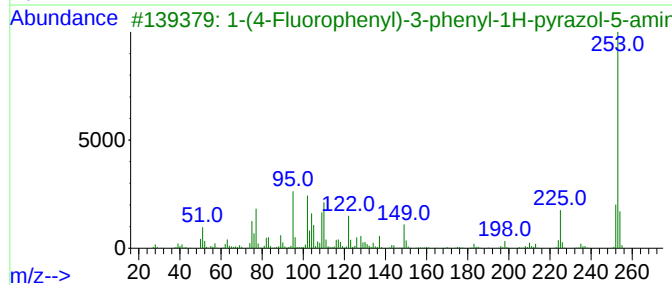
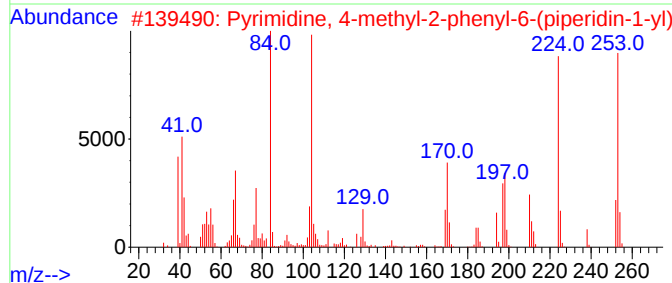
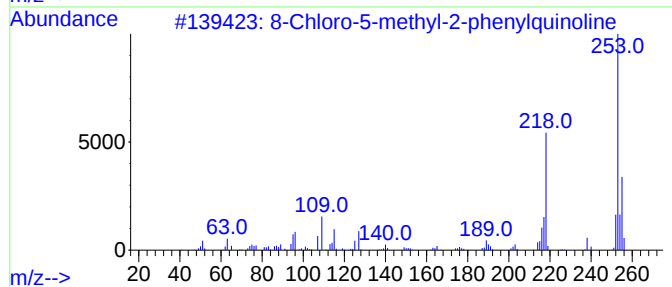
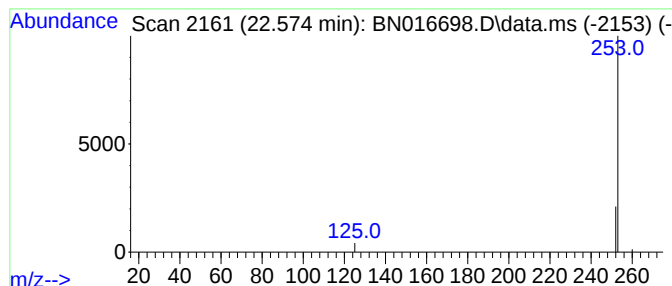
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 8-Chloro-5-methyl-2-phenylq... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.574	0.11 ng	263130	Perylene-d12	23.505

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		8-Chloro-5-methyl-2-phenylquinoline	253	C16H12ClN	025413-16-5	9
2		Pyrimidine, 4-methyl-2-phenyl-6-...	253	C16H19N3	1000302-39-3	5
3		1-(4-Fluorophenyl)-3-phenyl-1H-p...	253	C15H12FN3	072411-51-9	5
4		trans-3-Nitrochalcone	253	C15H11NO3	024721-24-2	5
5		N-(4-Phenyl-1,3-thiazol-2-yl)-2-...	253	C14H11N3S	1000485-04-5	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
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Instrument :
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ClientSampleId :
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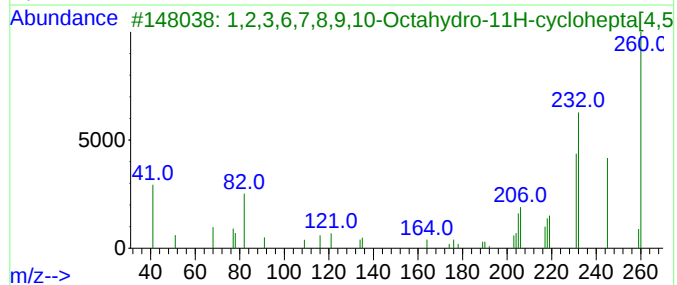
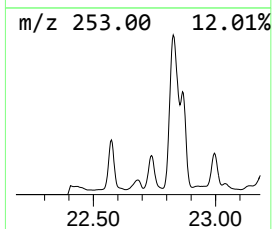
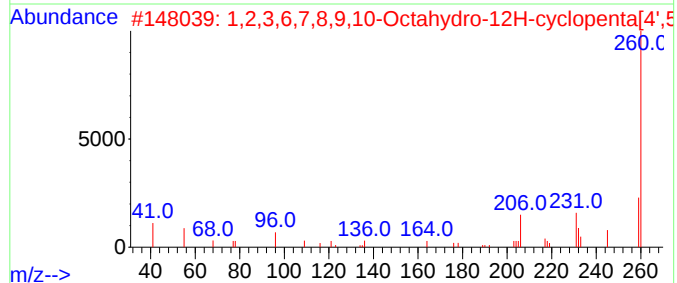
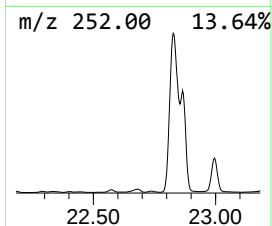
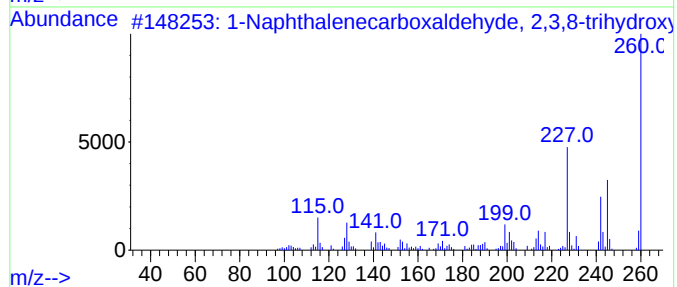
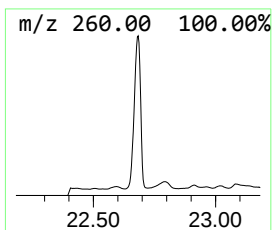
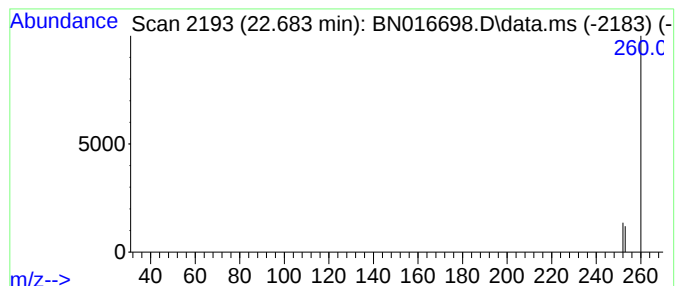
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Naphthalenecarboxaldehyde... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.683	0.16 ng	386568	Perylene-d12	23.505

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Naphthalenecarboxaldehyde, 2,3...	260	C15H16O4	040817-07-0	3
2			1,2,3,6,7,8,9,10-Octahydro-12H-c...	260	C14H16N2OS	057394-70-4	3
3			1,2,3,6,7,8,9,10-Octahydro-11H-c...	260	C14H16N2OS	102254-55-7	3
4			4-Biphenylol, 3,3'-dinitro-	260	C12H8N2O5	097851-14-4	3
5			1H,1H-Pentafluoropropyl iodide	260	C3H2F5I	000354-69-8	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
ALS Vial : 66 Sample Multiplier: 1

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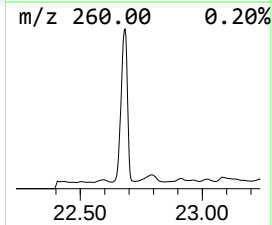
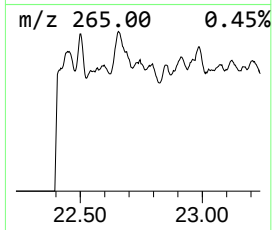
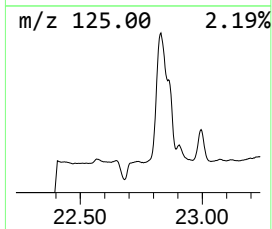
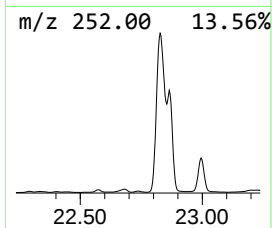
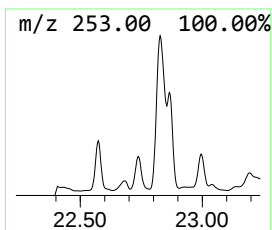
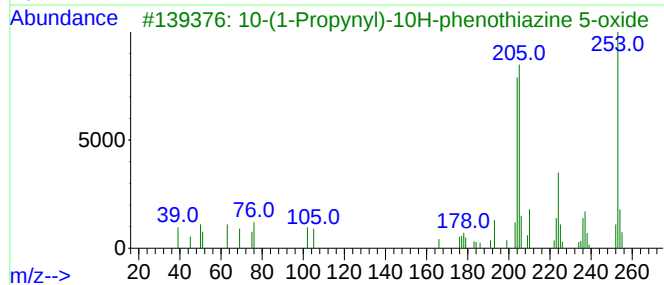
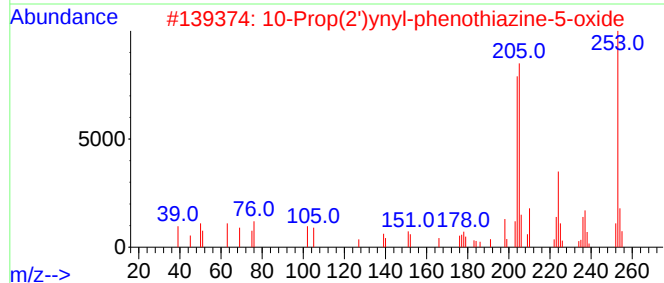
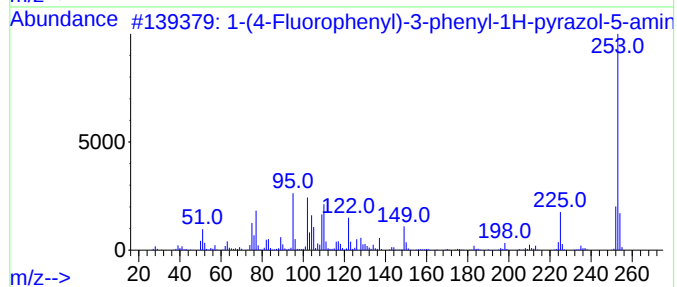
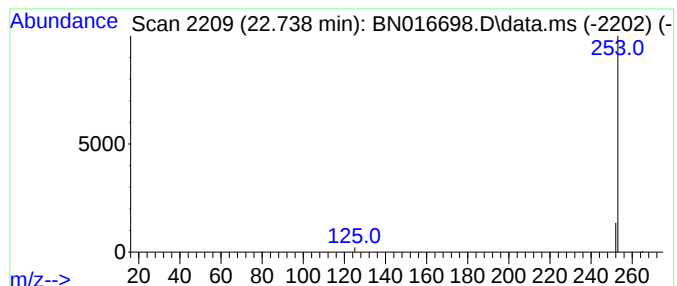
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-(4-Fluorophenyl)-3-phenyl... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.738	0.06 ng	146311	Perylene-d12	23.505

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Fluorophenyl)-3-phenyl-1H-p...	253	C15H12FN3	072411-51-9	5	
2	10-Prop(2')ynyl-phenothiazine-5-...	253	C15H11NOS	025206-52-4	5	
3	10-(1-Propynyl)-10H-phenothiazin...	253	C15H11NOS	145770-04-3	5	
4	2-Phenoxy-5-(trifluoromethyl)ben...	253	C13H10F3NO	050594-29-1	5	
5	9H-carbazole-3,6-diamine, N3,N3,...	253	C16H19N3	1010396-68-8	5	



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
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Instrument :
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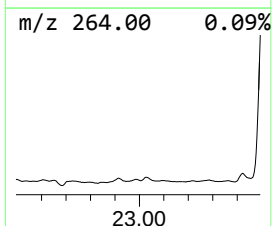
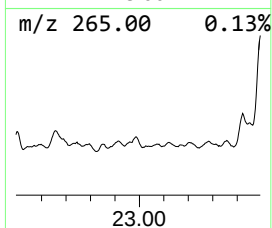
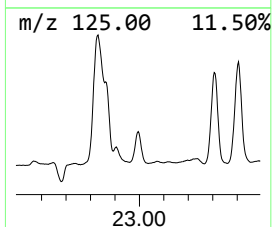
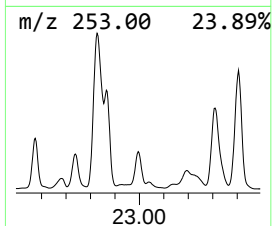
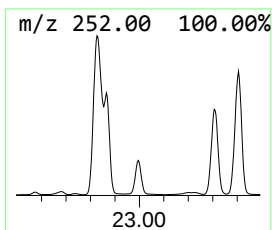
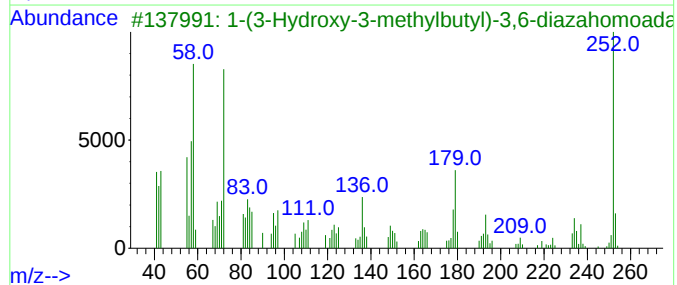
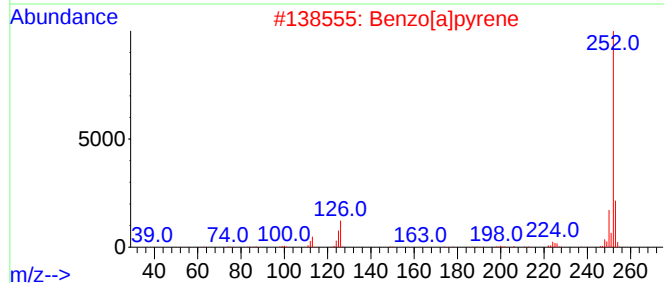
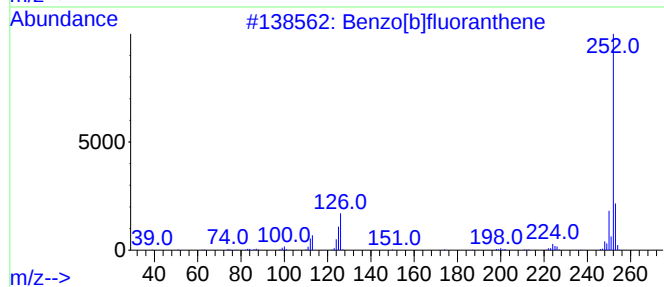
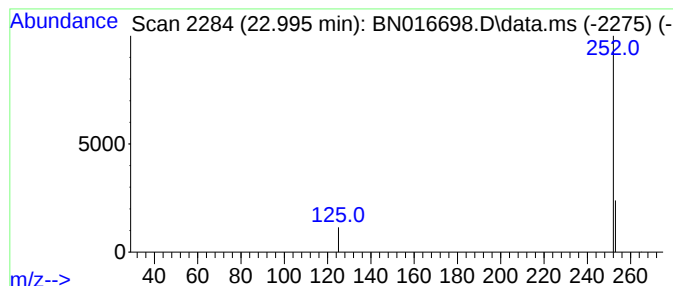
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Benzo[b]fluoranthene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.995	0.34 ng	814100	Perylene-d12	23.505

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
2			Benzo[a]pyrene	252	C20H12	000050-32-8	9
3			1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	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 : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
ALS Vial : 66 Sample Multiplier: 1

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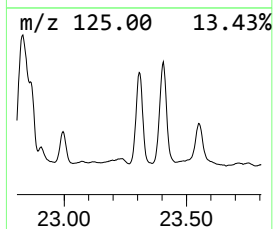
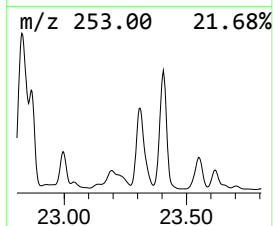
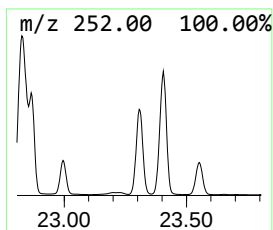
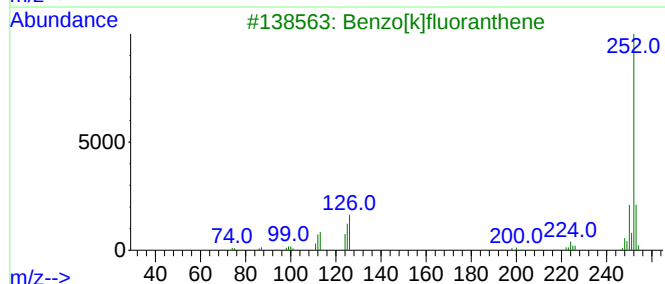
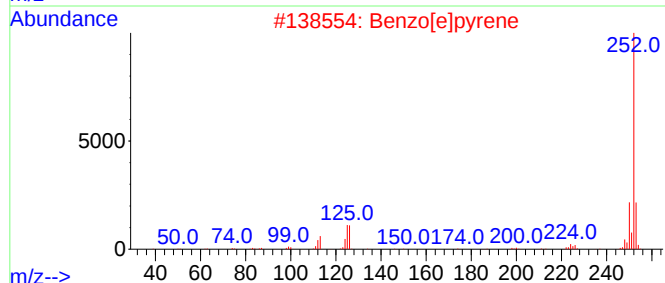
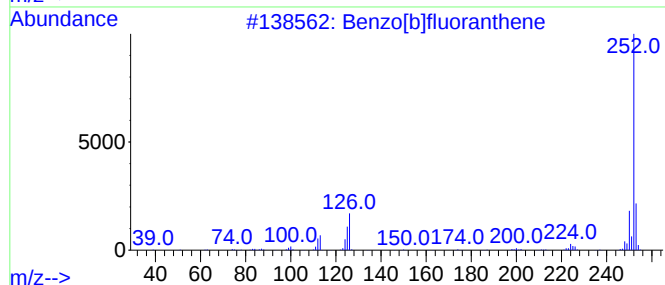
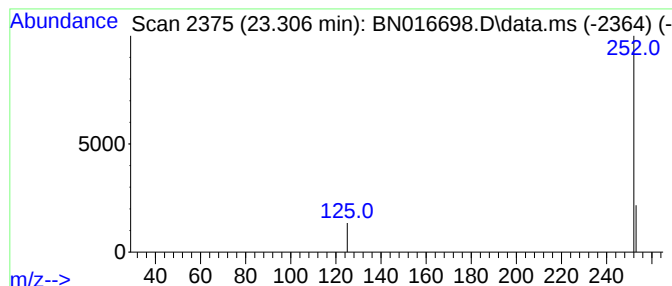
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Benzo[b]fluoranthene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.306	1.04 ng	2457390	Perylene-d12	23.505

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		Benzo[k]fluoranthene	252	C20H12	000207-08-9	9
4		Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
5		Perylene	252	C20H12	000198-55-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
ALS Vial : 66 Sample Multiplier: 1

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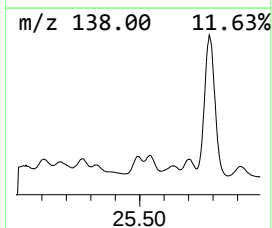
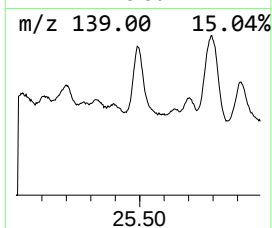
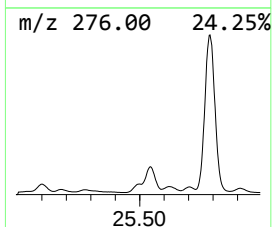
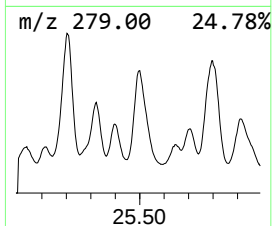
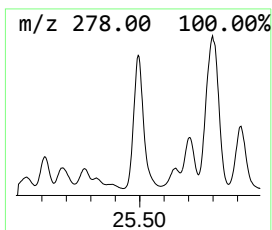
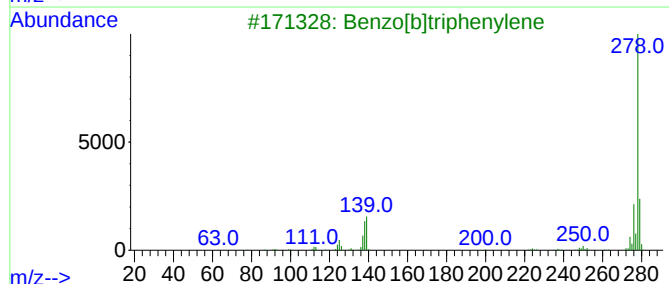
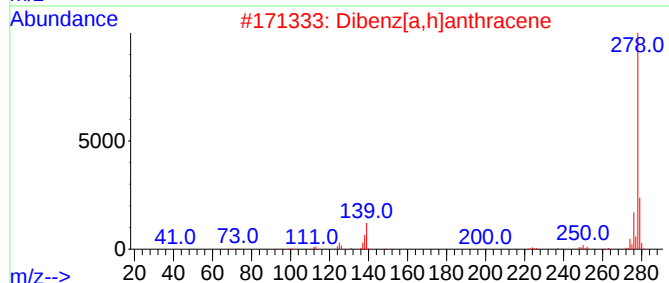
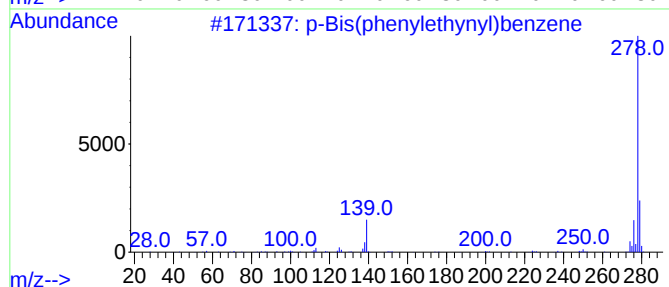
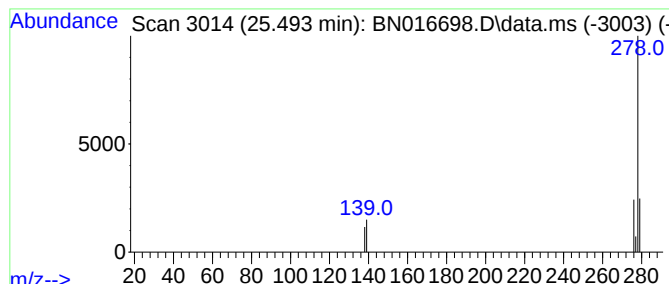
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 p-Bis(phenylethynyl)benzene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.494	0.13 ng	306947	Perylene-d12	23.505

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		p-Bis(phenylethynyl)benzene	278	C22H14	001849-27-0	72
2		Dibenz[a,h]anthracene	278	C22H14	000053-70-3	64
3		Benzo[b]triphenylene	278	C22H14	000215-58-7	64
4		Pentaphene	278	C22H14	000222-93-5	64
5		2-Naphthalenol, 1-[(4-methoxyph...	278	C17H14N2O2	013411-91-1	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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ClientSampleId :
S-832-J-SO-2-2.5-092221

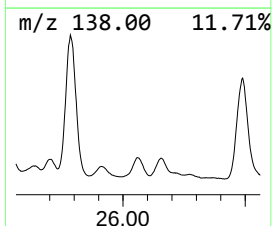
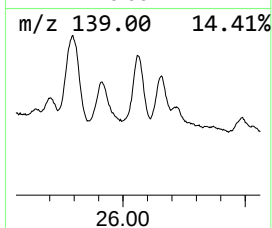
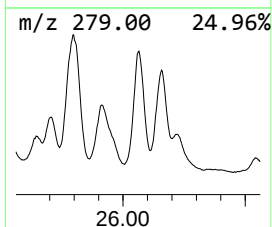
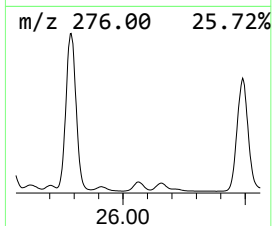
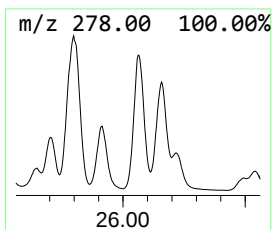
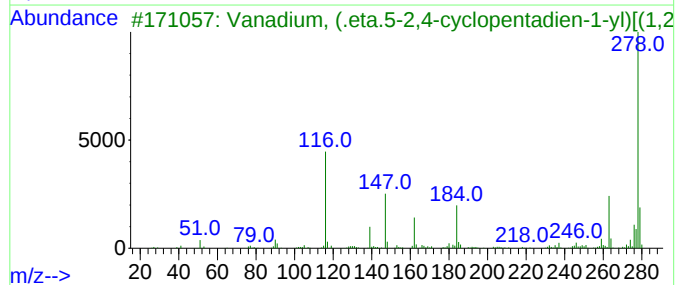
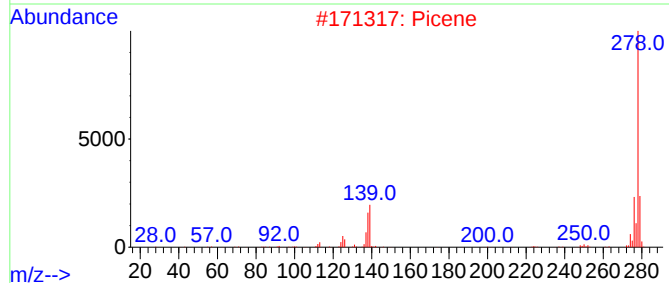
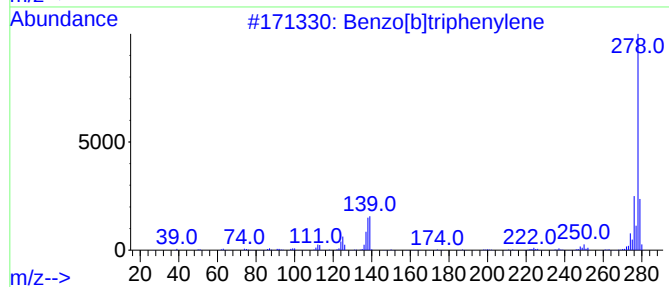
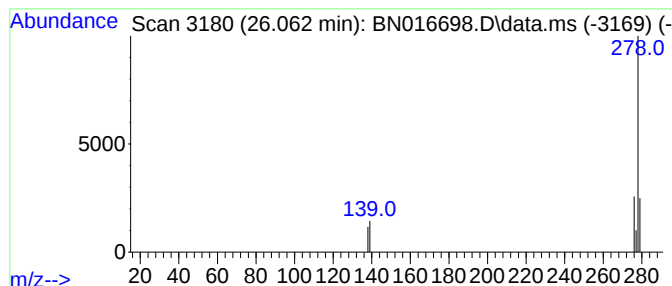
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Benzo[b]triphenylene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.062	0.13 ng	302736	Perylene-d12	23.505

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			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 : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
ALS Vial : 66 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-2-2.5-092221

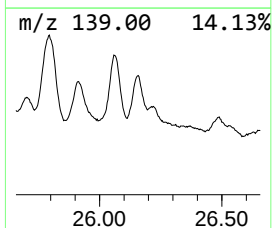
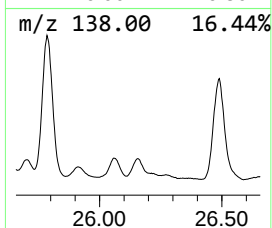
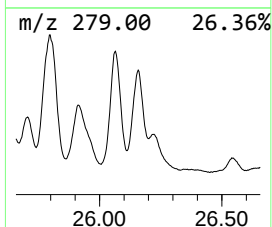
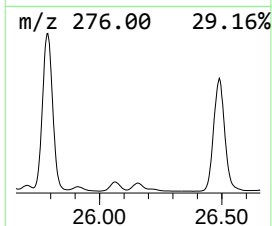
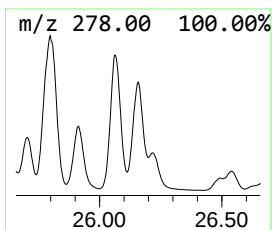
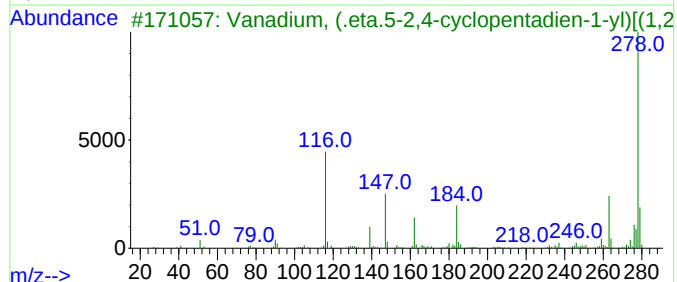
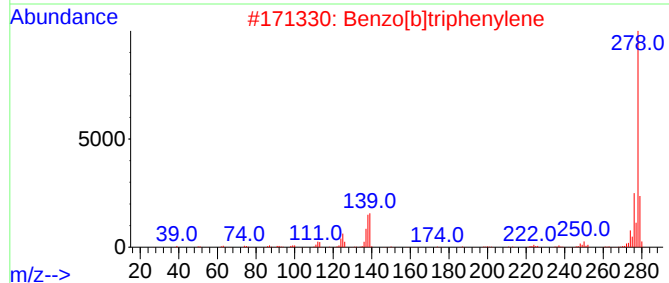
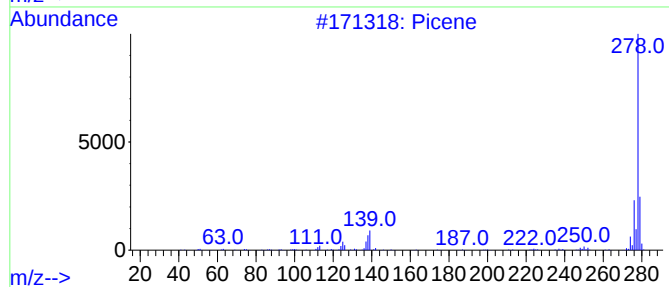
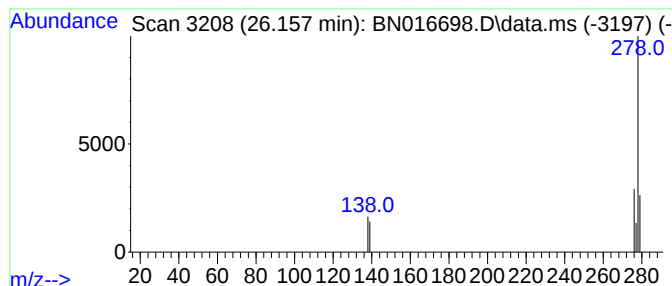
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Picene Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.157	0.10 ng	224615	Perylene-d12	23.505

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			Benz[a]anthracene-7,12-dicarboni...	278	C20H10N2	035215-32-8	72
5			1-naphthalenol, 4-[2-(4-methoxy...	278	C17H14N2O2	1000397-12-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016698.D
Acq On : 03 Oct 2021 08:48
Operator : CG/JU
Sample : M3892-18
Misc :
ALS Vial : 66 Sample Multiplier: 1

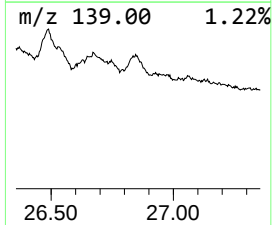
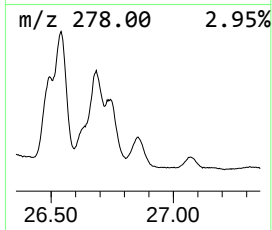
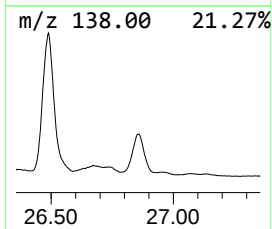
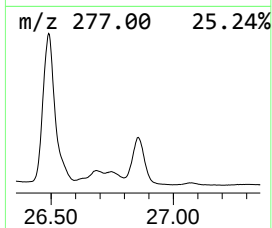
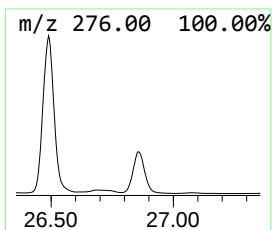
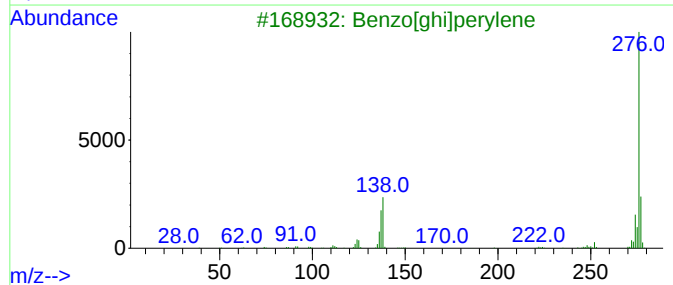
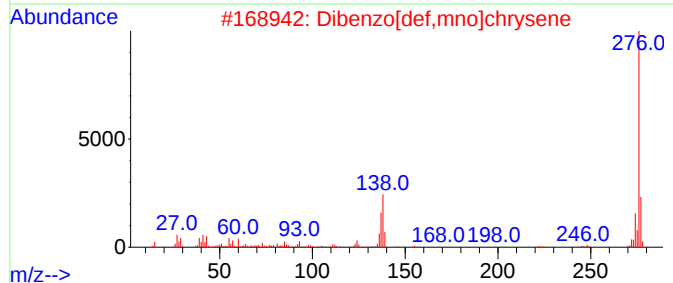
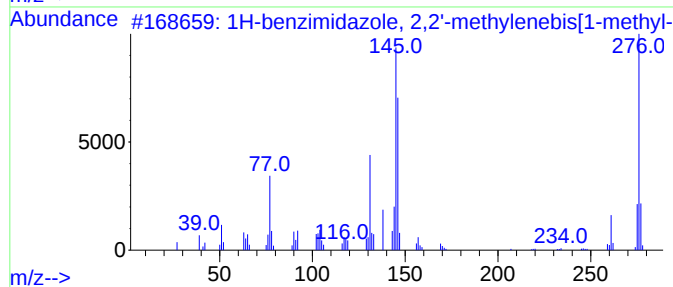
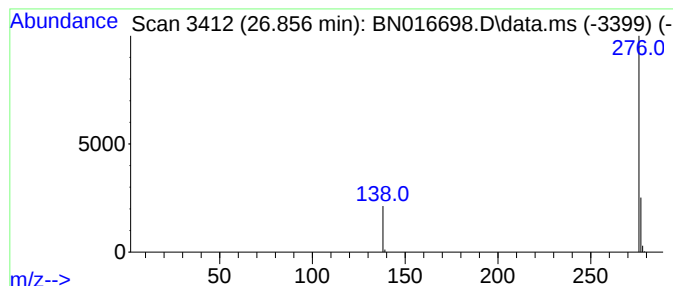
Instrument :
BNA_N
ClientSampleId :
S-832-J-SO-2-2.5-092221

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 1H-benzimidazole, 2,2'-meth... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.856	0.13 ng	299761	Perylene-d12	23.505	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-benzimidazole, 2,2'-methylene...	276	C17H16N4	1000401-82-9	83
2	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	83
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	83
4	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	83
5	1-(4-Hydroxy-3-methoxyphenyl)dec...	276	C17H24O3	000555-66-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016698.D
 Acq On : 03 Oct 2021 08:48
 Operator : CG/JU
 Sample : M3892-18
 Misc :
 ALS Vial : 66 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-832-J-SO-2-2.5-092221

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
Butane	7.937	0.9	ng	241499	1	7.642	102180	0.4
Isopropyl isoth...	10.204	0.9	ng	408746	2	10.406	183843	0.4
2,6-Dimethyl-3-...	13.177	0.5	ng	282092	3	14.269	224861	0.4
Phenanthridine	17.212	0.3	ng	140094	4	17.029	172433	0.4
Carbazole	17.431	0.8	ng	364518	4	17.029	172433	0.4
o,S,S'-Trimethy...	17.954	0.4	ng	150988	4	17.029	172433	0.4
Indole-5-carbox...	18.417	0.5	ng	217368	4	17.029	172433	0.4
Difluorophosphi...	18.904	0.3	ng	124872	4	17.029	172433	0.4
2'-Furfuryliden...	20.972	0.1	ng	1092610	5	21.238	7330200	0.4
Purine-6(1H)-th...	21.397	0.1	ng	1012940	5	21.238	7330200	0.4
1,2-Dihydro-4H-...	22.395	0.1	ng	252175	6	23.505	944690	0.4
8-Chloro-5-meth...	22.574	0.1	ng	263130	6	23.505	944690	0.4
1-Naphthaleneca...	22.683	0.2	ng	386568	6	23.505	944690	0.4
1-(4-Fluorophen...	22.738	0.1	ng	146311	6	23.505	944690	0.4
Benzo[b]fluoran...	22.995	0.3	ng	814100	6	23.505	944690	0.4
Benzo[b]fluoran...	23.306	1.0	ng	2457390	6	23.505	944690	0.4
p-Bis(phenyleth...	25.494	0.1	ng	306947	6	23.505	944690	0.4
Benzo[b]triphen...	26.062	0.1	ng	302736	6	23.505	944690	0.4
Picene	26.157	0.1	ng	224615	6	23.505	944690	0.4
1H-benzimidazol...	26.856	0.1	ng	299761	6	23.505	944690	0.4