

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016695.D
 Acq On : 03 Oct 2021 07:00
 Operator : CG/JU
 Sample : M3892-07
 Misc :
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-823-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: BN016695.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	36518	75006	1.29%	0.154%
2	7.633	490	494	499	rBV	52709	107734	1.86%	0.222%
3	7.937	523	527	532	rVB	60708	111078	1.91%	0.229%
4	9.671	668	675	678	rBV	48096	110564	1.91%	0.228%
5	10.191	713	716	721	rBV	60266	100609	1.73%	0.207%
6	10.407	729	733	735	rBV	112124	195685	3.37%	0.403%
7	12.003	922	931	939	rBV	45256	71868	1.24%	0.148%
8	12.886	1071	1074	1077	rBV	87619	141160	2.43%	0.291%
9	13.190	1094	1098	1101	rBV	49655	87731	1.51%	0.181%
10	14.269	1180	1183	1185	rBV	153615	228067	3.93%	0.470%
11	14.332	1185	1188	1191	rVB	160888	240101	4.14%	0.494%
12	15.322	1263	1266	1269	rBV	122617	176128	3.04%	0.363%
13	17.017	1400	1403	1404	rBV	127741	187056	3.22%	0.385%
14	17.066	1404	1407	1410	rVV	1575150	2341748	40.36%	4.822%
15	17.151	1410	1414	1417	rVB	314177	475898	8.20%	0.980%
16	17.431	1432	1437	1440	rBV2	214198	357197	6.16%	0.736%
17	17.894	1472	1475	1477	rBV2	71221	116896	2.01%	0.241%
18	17.955	1477	1480	1483	rVB2	55416	116885	2.01%	0.241%
19	18.417	1560	1566	1571	rBV	76340	103848	1.79%	0.214%
20	19.098	1687	1703	1711	rBV	4111711	5801605	100.00%	11.947%
21	19.197	1711	1723	1728	rVV	49914	99289	1.71%	0.204%
22	19.246	1728	1733	1737	rVV2	49484	63908	1.10%	0.132%
23	19.460	1766	1776	1787	rBV	3555935	5258737	90.64%	10.829%
24	19.678	1815	1820	1822	rBV	97865	122239	2.11%	0.252%
25	19.708	1822	1826	1833	rVB	173474	246164	4.24%	0.507%
26	20.112	1893	1896	1898	rBV2	40703	70428	1.21%	0.145%
27	20.707	1947	1952	1956	rBV3	110826	230655	3.98%	0.475%
28	20.866	1963	1967	1970	rBV3	87041	237999	4.10%	0.490%
29	20.919	1970	1972	1974	rVV	290830	416987	7.19%	0.859%
30	20.962	1974	1976	1979	rVV2	272210	563175	9.71%	1.160%
31	21.004	1979	1980	1983	rVV2	121770	154155	2.66%	0.317%
32	21.057	1983	1985	1987	rVV2	81963	112269	1.94%	0.231%
33	21.164	1991	1995	1998	rVV3	226342	677303	11.67%	1.395%
34	21.217	1998	2000	2002	rVV	2297007	3267420	56.32%	6.728%
35	21.270	2002	2005	2011	rVV	2289738	3610580	62.23%	7.435%
36	21.387	2014	2016	2022	rVV	371163	626940	10.81%	1.291%

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37	21.472	2022	2024	2027	rVV2	52878	114732	1.98%	0.236%
38	21.567	2031	2033	2037	rVV2	89569	174610	3.01%	0.360%
39	21.620	2037	2038	2041	rVB2	74669	105962	1.83%	0.218%
40	21.790	2050	2054	2056	rVB	61237	120936	2.08%	0.249%
41	21.843	2056	2059	2061	rBV2	194486	367691	6.34%	0.757%
42	21.886	2061	2063	2067	rVV2	1215413	2005385	34.57%	4.129%
43	21.981	2070	2072	2074	rVV	102699	170713	2.94%	0.352%
44	22.024	2074	2076	2078	rVV	135819	192840	3.32%	0.397%
45	22.119	2078	2085	2089	rVV	582847	1040860	17.94%	2.143%
46	22.257	2093	2098	2100	rBV2	125856	279754	4.82%	0.576%
47	22.311	2100	2103	2108	rVB2	567293	1010220	17.41%	2.080%
48	22.564	2149	2158	2176	rBV2	129597	223960	3.86%	0.461%
49	22.731	2198	2207	2218	rBV	70424	115417	1.99%	0.238%
50	22.817	2219	2232	2240	rBV	1746033	3915820	67.50%	8.063%
51	22.985	2272	2281	2292	rVB	272965	446131	7.69%	0.919%
52	23.180	2331	2338	2344	rBV2	30753	58056	1.00%	0.120%
53	23.296	2360	2372	2387	rBV	1096271	2022377	34.86%	4.164%
54	23.392	2387	2400	2418	rVB	1309009	2512334	43.30%	5.173%
55	23.491	2418	2429	2434	rBV	134569	256223	4.42%	0.528%
56	23.539	2434	2443	2459	rVB	390764	793970	13.69%	1.635%
57	23.748	2495	2504	2515	rBV3	42807	119479	2.06%	0.246%
58	24.094	2597	2605	2615	rVB	55173	111527	1.92%	0.230%
59	24.183	2620	2631	2643	rBV	87111	187927	3.24%	0.387%
60	24.371	2676	2686	2697	rBV	51991	103891	1.79%	0.214%
61	24.600	2745	2753	2781	rVB	26107	72996	1.26%	0.150%
62	25.097	2886	2898	2908	rVV3	34404	80946	1.40%	0.167%
63	25.179	2911	2922	2936	rVB5	32564	94518	1.63%	0.195%
64	25.480	2996	3010	3017	rBV2	117703	306328	5.28%	0.631%
65	25.689	3062	3071	3080	rBV	49925	105665	1.82%	0.218%
66	25.771	3080	3095	3119	rVB2	618563	1900854	32.76%	3.914%
67	25.904	3121	3134	3159	rVB4	60086	189310	3.26%	0.390%
68	26.048	3162	3176	3190	rBV2	103844	291806	5.03%	0.601%
69	26.141	3191	3203	3251	rVB	113691	401214	6.92%	0.826%
70	26.473	3280	3300	3333	rBV	432944	1466151	25.27%	3.019%
71	26.842	3392	3408	3436	rVB2	89657	297351	5.13%	0.612%

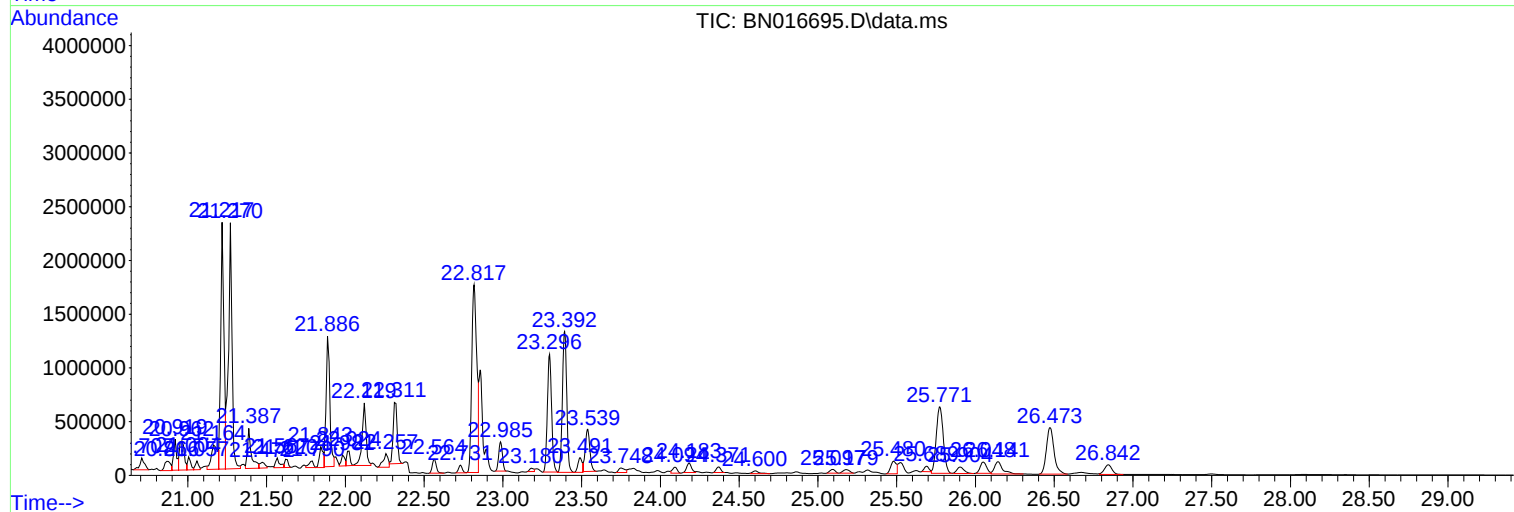
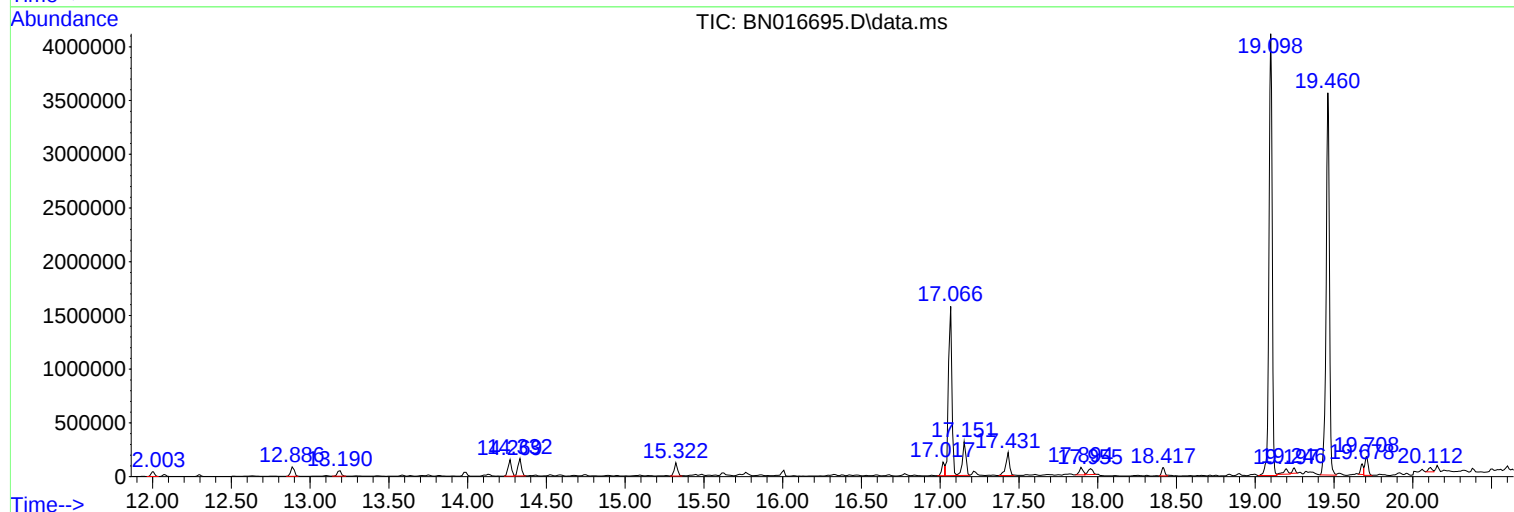
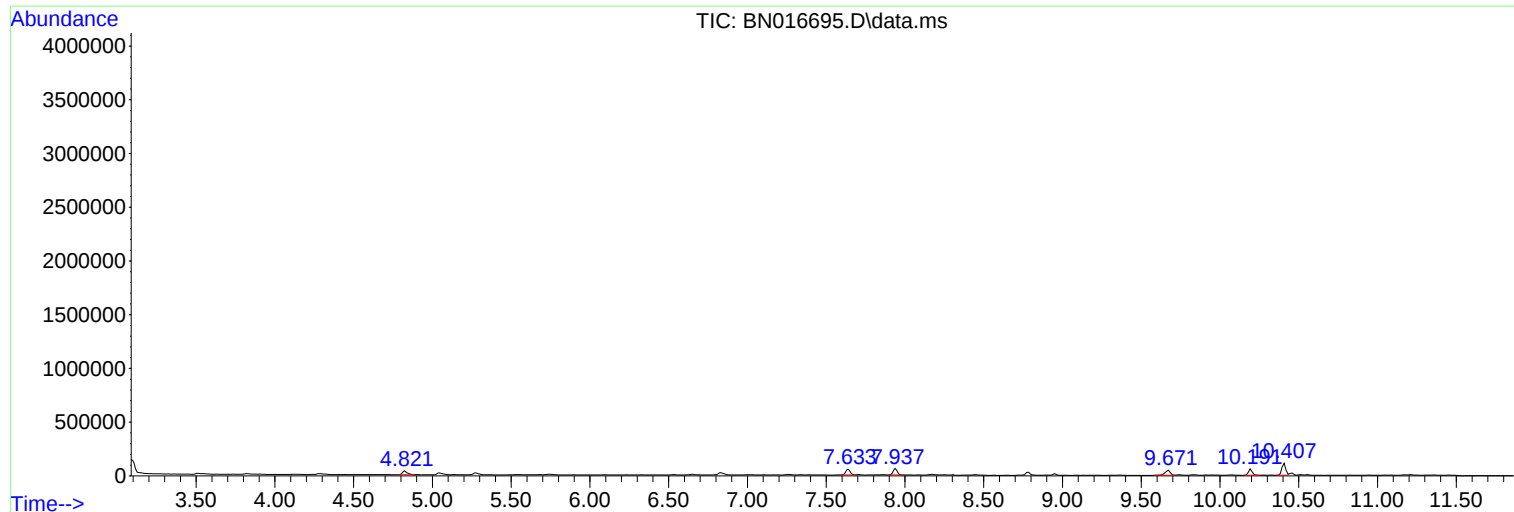
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-823-N-SO-0-0.5-092221

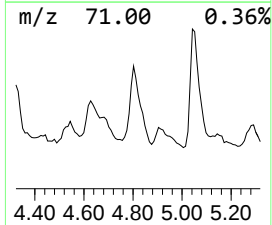
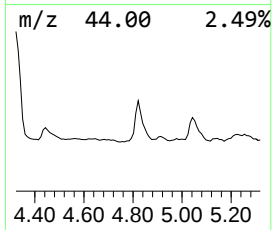
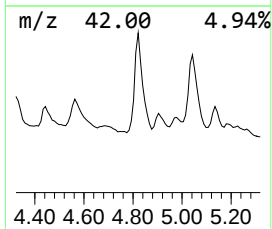
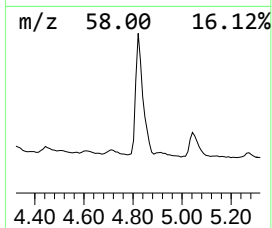
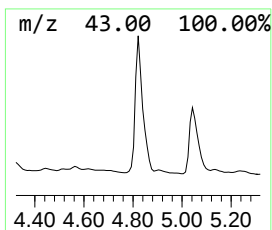
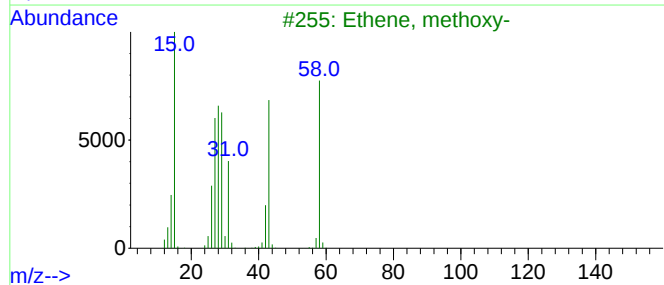
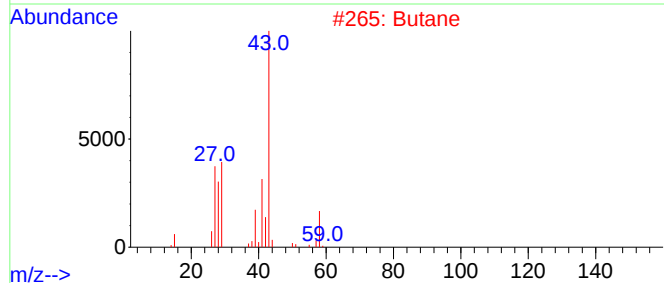
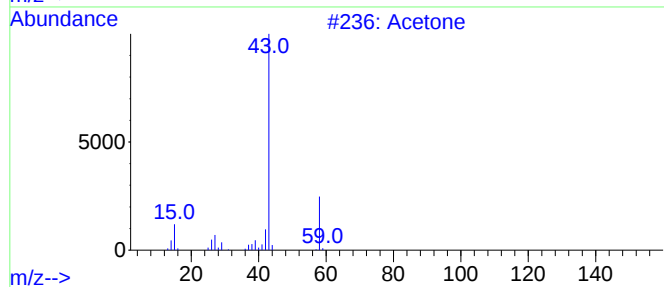
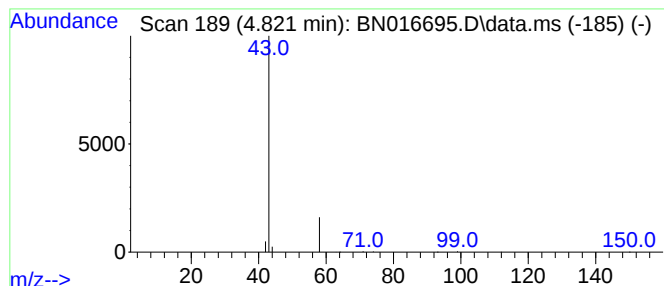
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.28 ng	75006	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetone	58	C3H6O	000067-64-1	4
2			Butane	58	C4H10	000106-97-8	4
3			Ethene, methoxy-	58	C3H6O	000107-25-5	3
4			Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5			Hydrogen isocyanate	43	CHNO	000075-13-8	2



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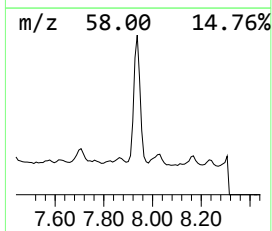
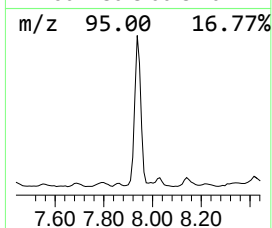
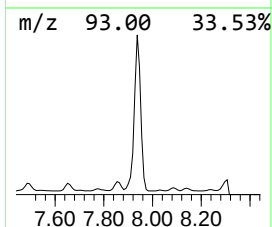
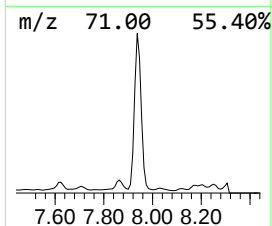
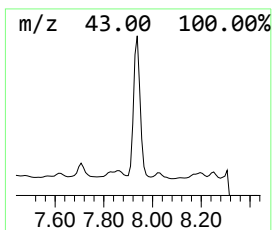
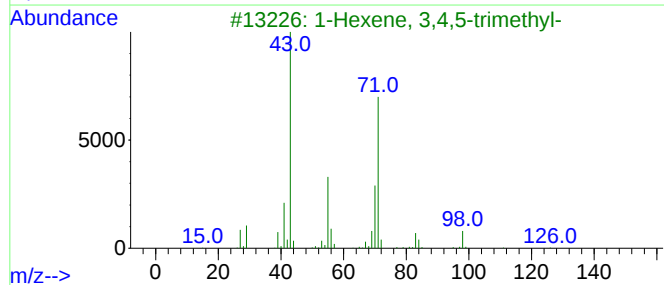
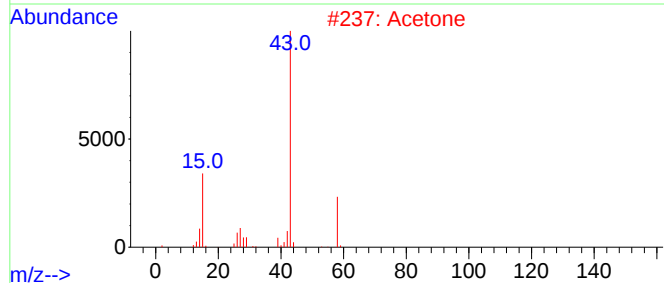
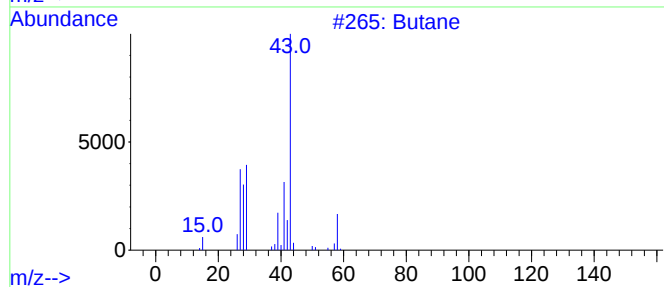
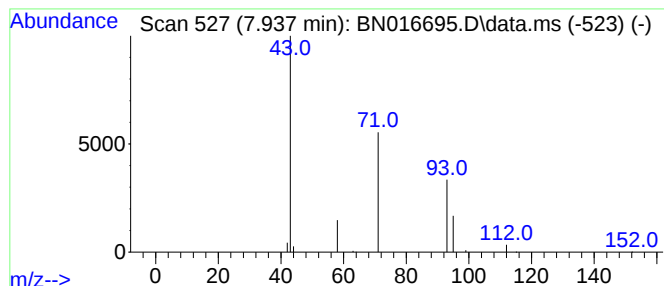
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.937	0.41 ng	111078	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane	58	C4H10	000106-97-8	4
2			Acetone	58	C3H6O	000067-64-1	4
3			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	4
4			Butanoic acid, 2-(2-cyanoethyl)-...	297	C15H23NO5	1010460-88-7	4
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	4



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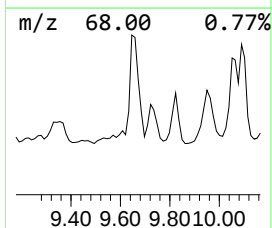
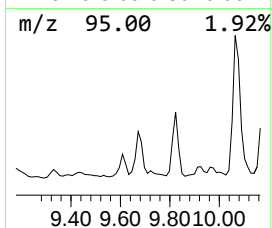
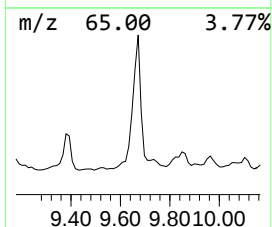
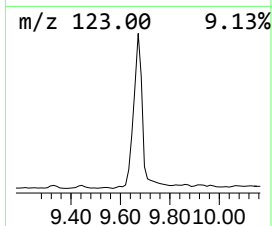
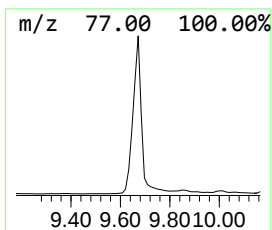
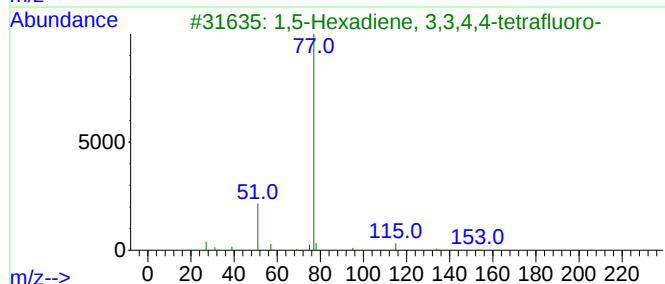
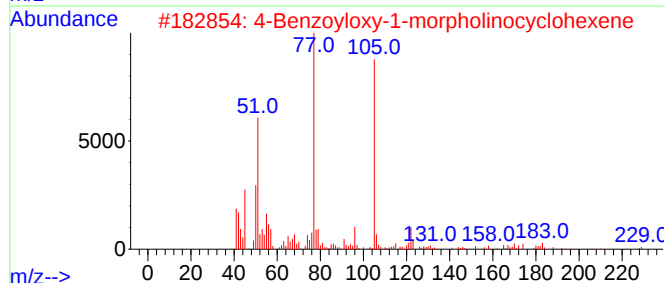
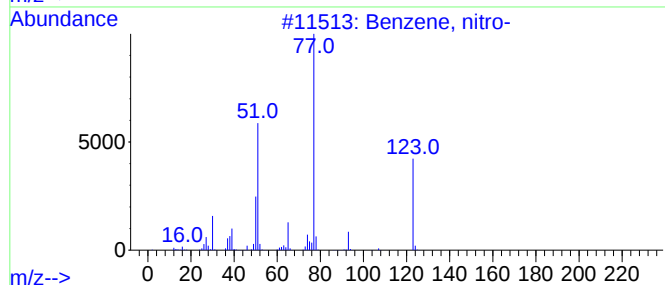
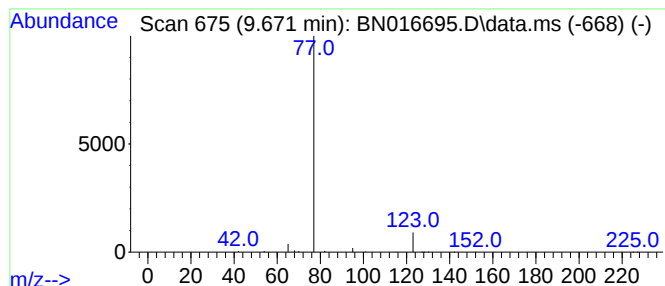
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzene, nitro- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.671	0.23 ng	110564	Naphthalene-d8	10.406

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, nitro-	123	C6H5NO2	000098-95-3	3
2			4-Benzoyloxy-1-morpholinocyclohe...	287	C17H21NO3	037138-56-0	1
3			1,5-Hexadiene, 3,3,4,4-tetrafluoro-	154	C6H6F4	001763-21-9	1
4			Silanamine, N-silyl-	77	H7NSi2	005702-11-4	1
5			Mercaptamine	77	C2H7NS	000060-23-1	1



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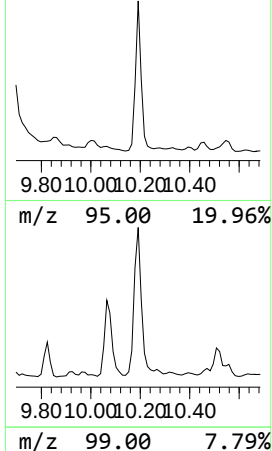
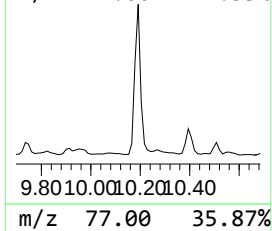
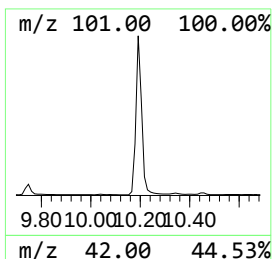
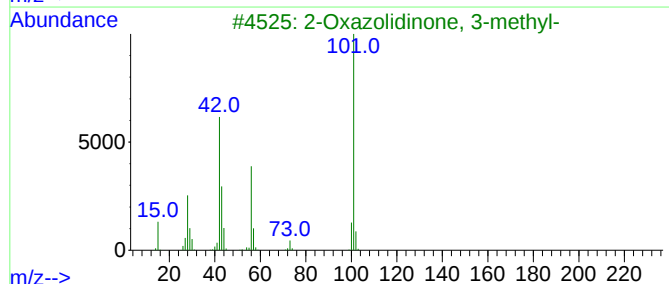
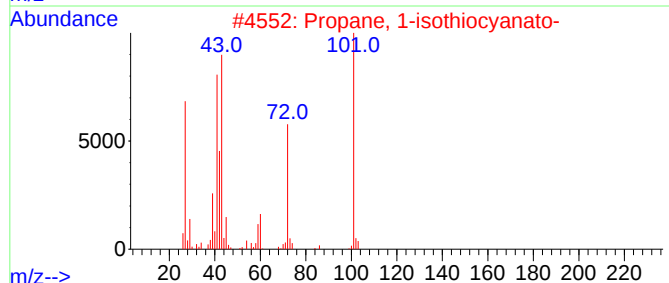
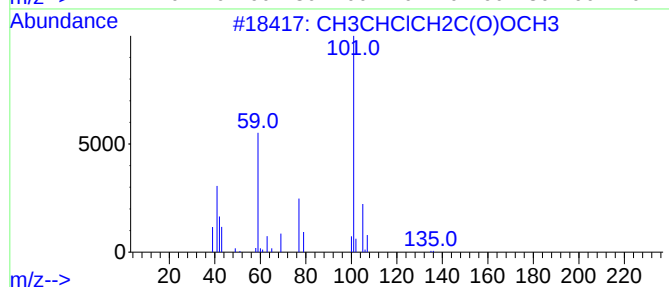
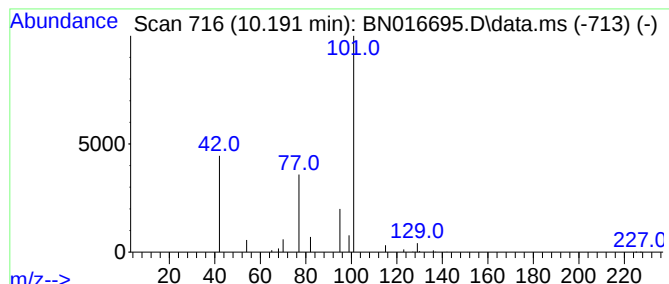
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 CH3CHClCH2C(O)OCH3 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.21 ng	100609	Naphthalene-d8	10.406

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			CH3CHClCH2C(O)OCH3	136	C5H9ClO2	000817-76-5	7
2			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
3			2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
4			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
5			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5



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Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-823-N-SO-0-0.5-092221

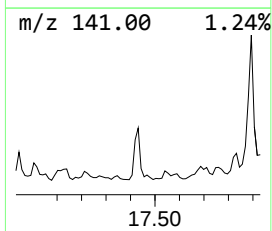
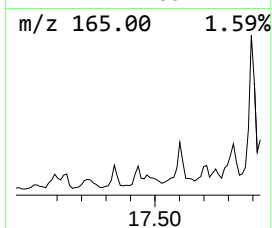
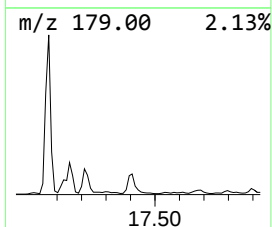
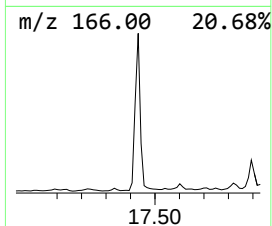
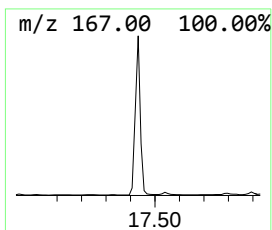
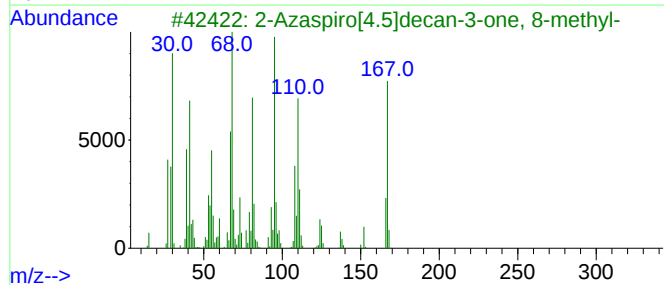
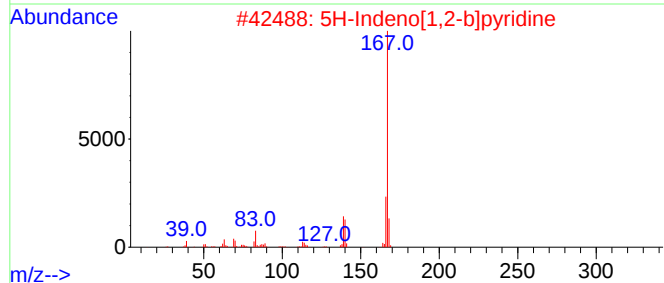
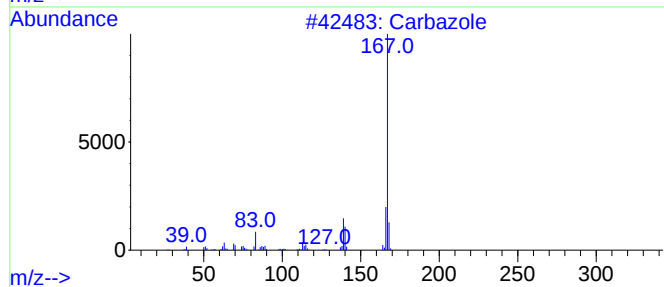
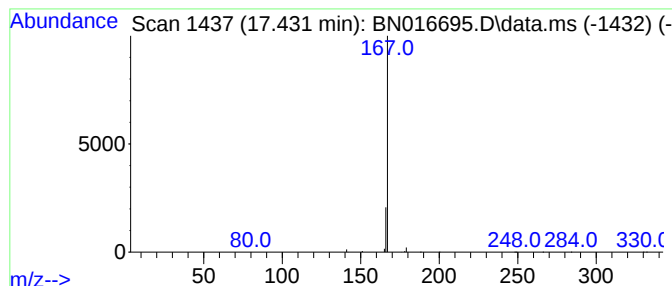
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Carbazole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.431	0.76 ng	357197	Phenanthrene-d10	17.017

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 : BN016695.D
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ClientSampleId :
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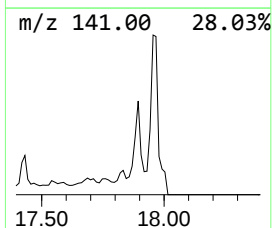
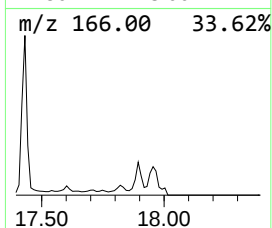
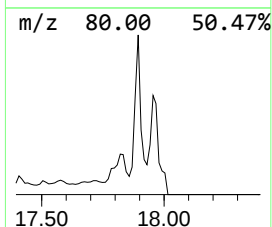
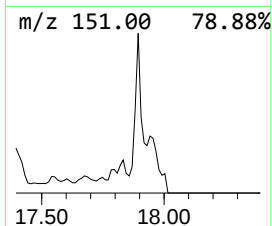
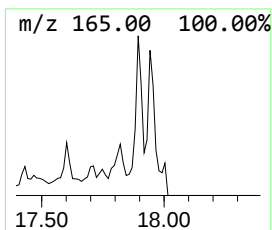
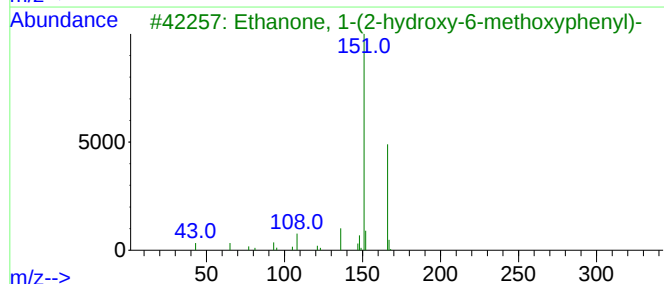
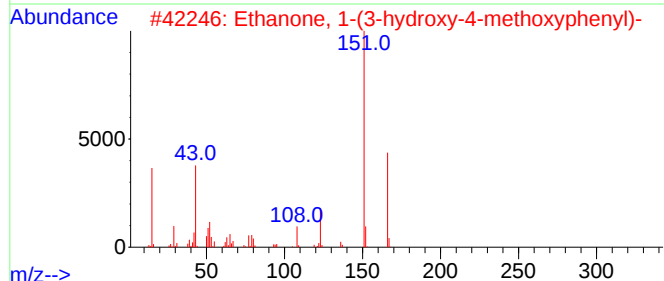
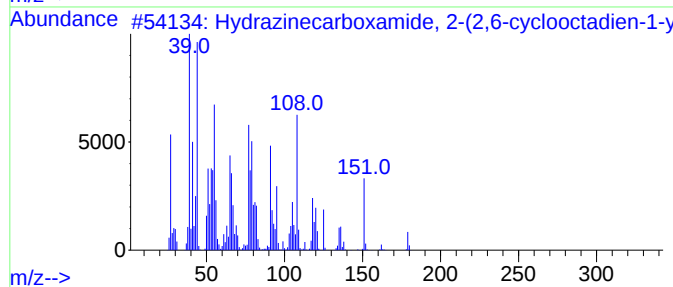
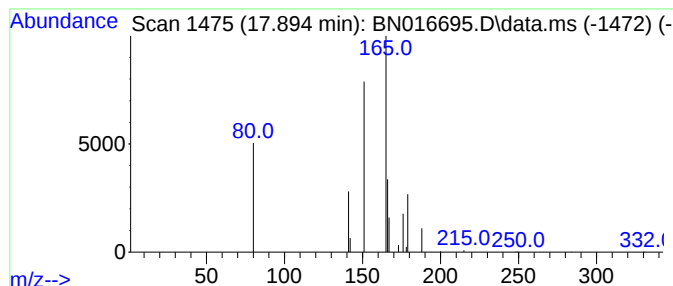
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hydrazinecarboxamide, 2-(2,... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.894	0.25 ng	116896	Phenanthrene-d10	17.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazinecarboxamide, 2-(2,6-cyc...	179	C9H13N3O	068344-44-5	7
2			Ethanone, 1-(3-hydroxy-4-methoxy...	166	C9H10O3	006100-74-9	5
3			Ethanone, 1-(2-hydroxy-6-methoxy...	166	C9H10O3	000703-23-1	5
4			1H-Isoindole-1,3(2H)-dione, 3a,4...	151	C8H9NO2	001469-48-3	5
5			Cyromazine	166	C6H10N6	066215-27-8	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
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Sample : M3892-07
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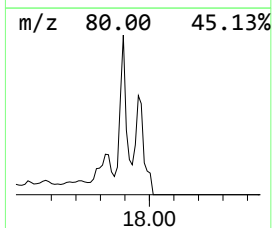
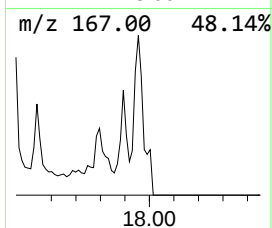
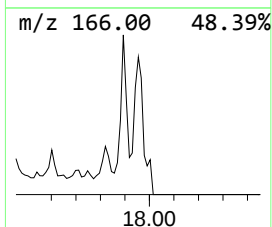
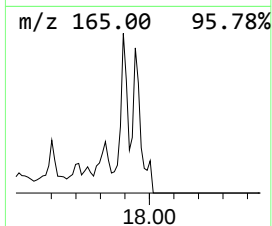
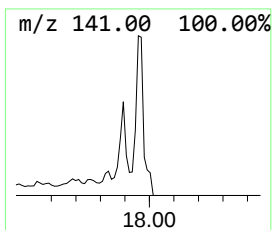
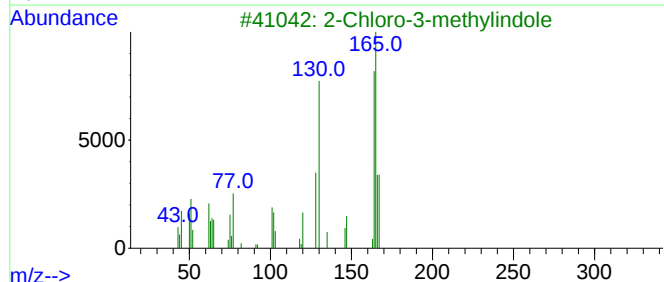
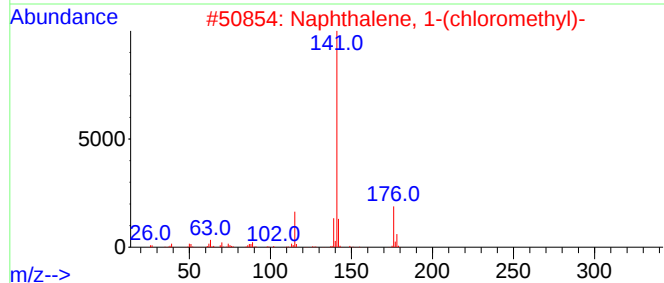
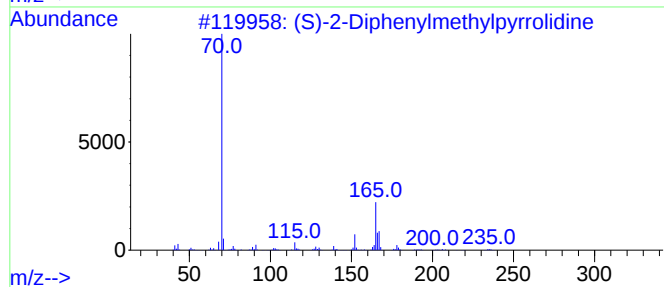
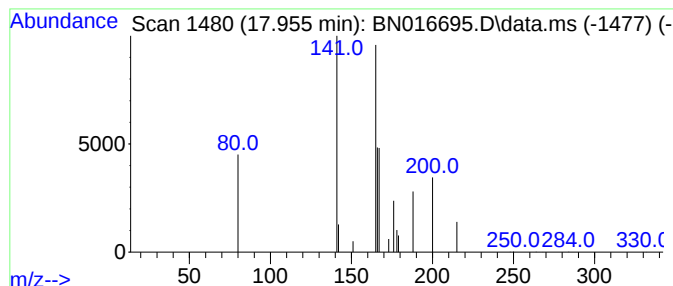
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 (S)-2-Diphenylmethylpyrroli... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.954	0.25 ng	116885	Phenanthrene-d10	17.017

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-2-Diphenylmethylpyrrolidine	237	C17H19N	188398-87-0	17
2		Naphthalene, 1-(chloromethyl)-	176	C11H9Cl	000086-52-2	10
3		2-Chloro-3-methylindole	165	C9H8ClN	051206-73-6	9
4		2-Methoxycarbonylmethylenethiour...	200	C7H8N2O3S	079361-42-5	9
5		Benzenesulfonyl chloride	176	C6H5ClO2S	000098-09-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

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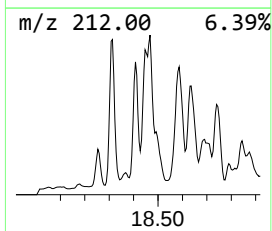
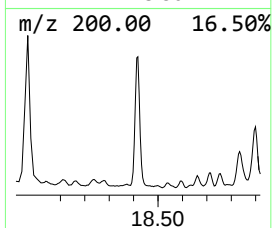
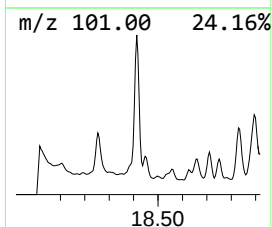
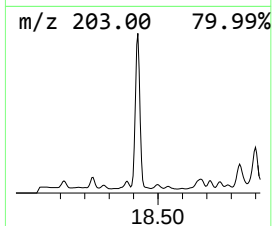
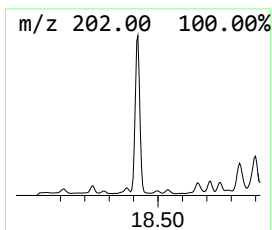
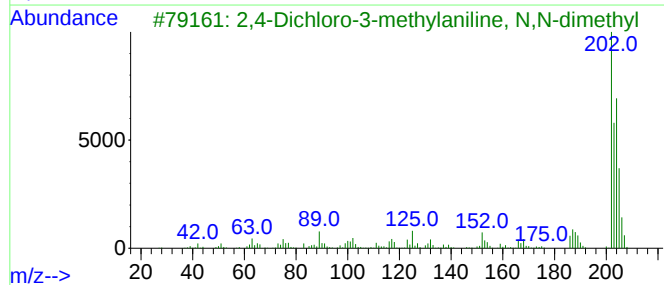
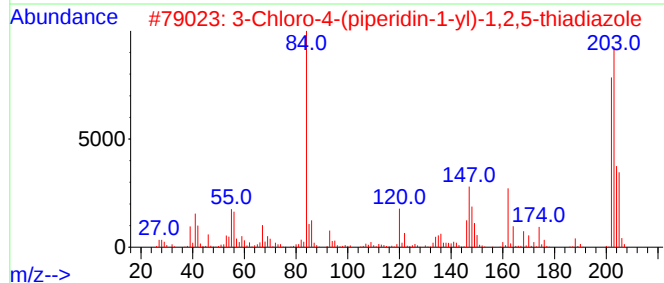
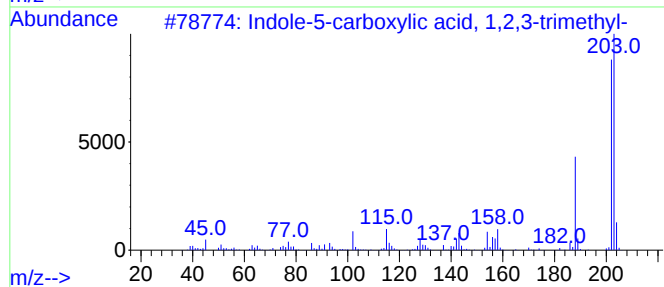
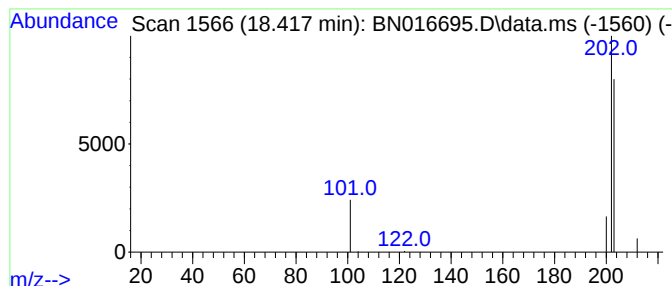
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Indole-5-carboxylic acid, 1... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.418	0.22 ng	103848	Phenanthrene-d10	17.017

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole-5-carboxylic acid, 1,2,3-...	203	C12H13NO2	1000272-88-4	5
2			3-Chloro-4-(piperidin-1-yl)-1,2-...	203	C7H10ClN3S	173053-54-8	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\
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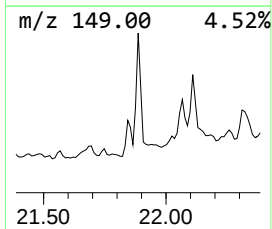
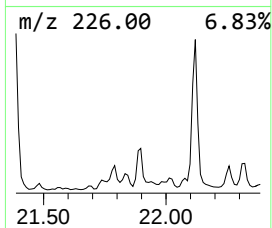
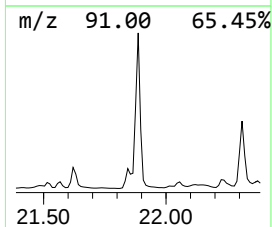
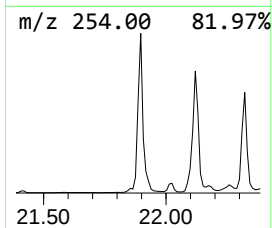
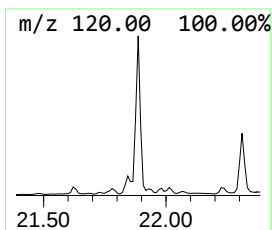
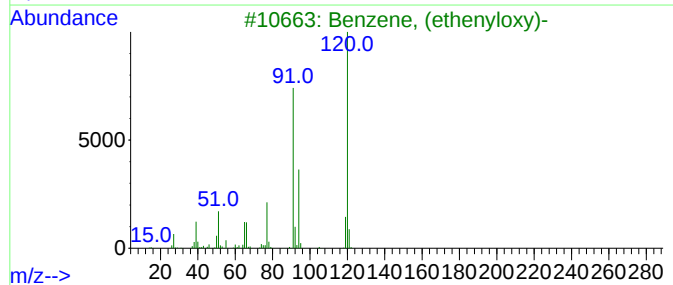
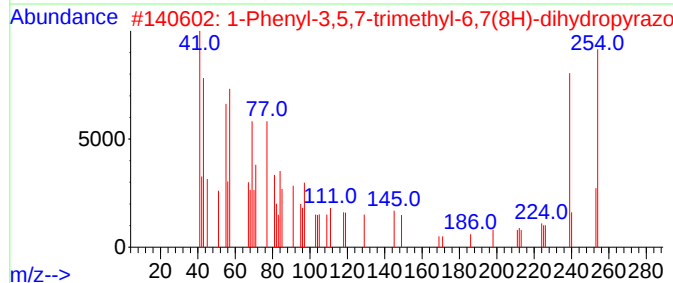
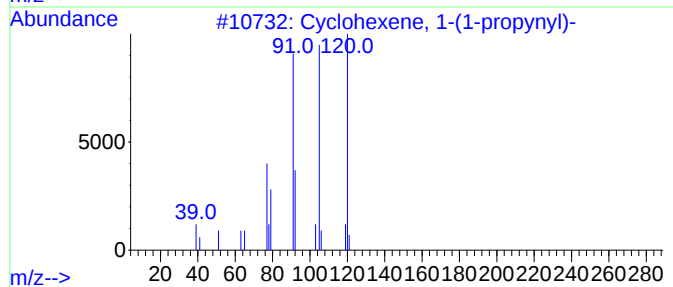
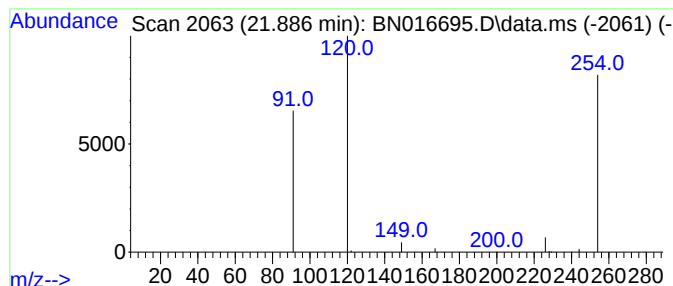
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexene, 1-(1-propynyl)- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.886	0.25 ng	2005390	Chrysene-d12	21.238	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-(1-propynyl)-	120	C9H12	001655-05-6	4
2	1-Phenyl-3,5,7-trimethyl-6,7(8H)...	254	C15H18N4	064899-23-6	4
3	Benzene, (ethenyloxy)-	120	C8H8O	000766-94-9	4
4	Benzofuran, 2,3-dihydro-	120	C8H8O	000496-16-2	4
5	4-Vinylphenol	120	C8H8O	002628-17-3	4



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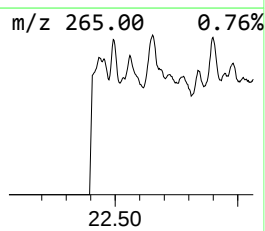
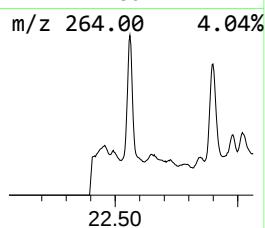
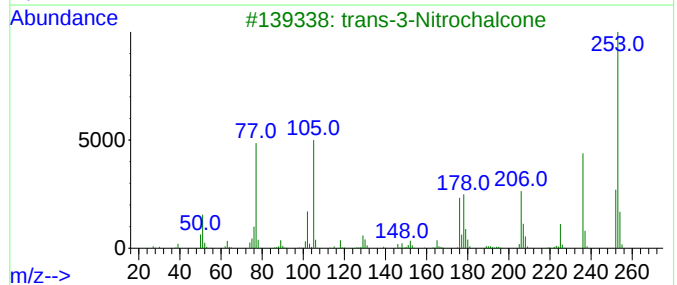
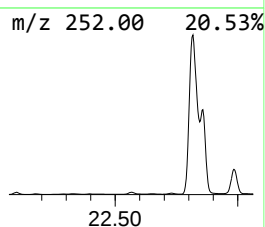
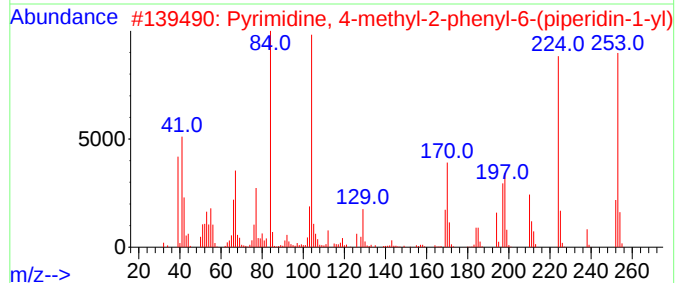
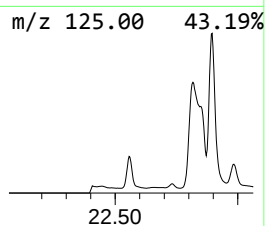
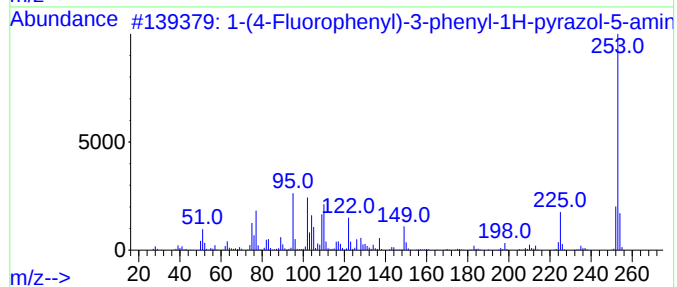
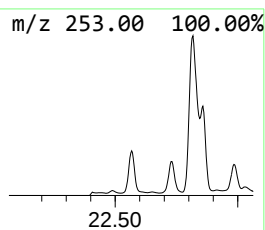
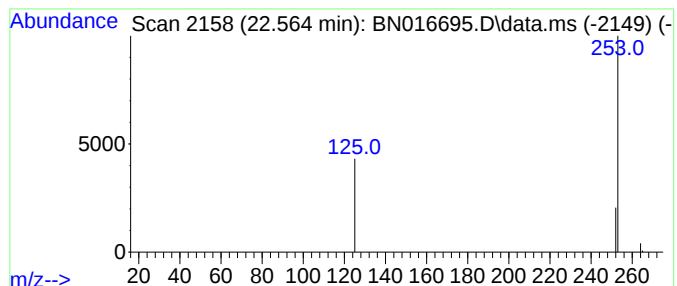
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-(4-Fluorophenyl)-3-phenyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.564	0.35 ng	223960	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(4-Fluorophenyl)-3-phenyl-1H-p...	253	C15H12FN3	072411-51-9	5		
2	Pyrimidine, 4-methyl-2-phenyl-6-...	253	C16H19N3	1000302-39-3	5		
3	trans-3-Nitrochalcone	253	C15H11NO3	024721-24-2	5		
4	2,5-Cyclohexadien-1-one, 2,5-dim...	253	C17H19NO	054245-93-1	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\
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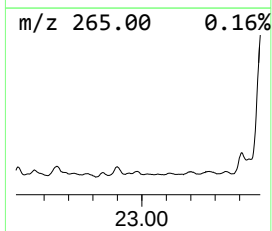
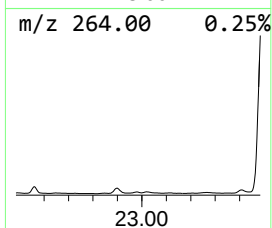
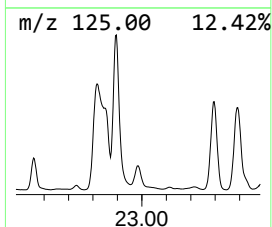
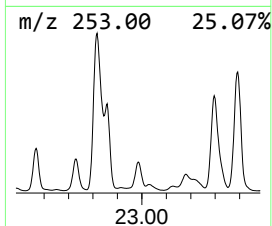
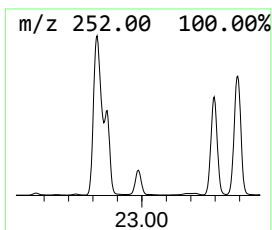
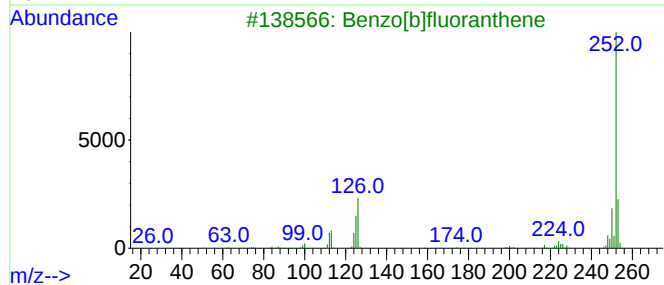
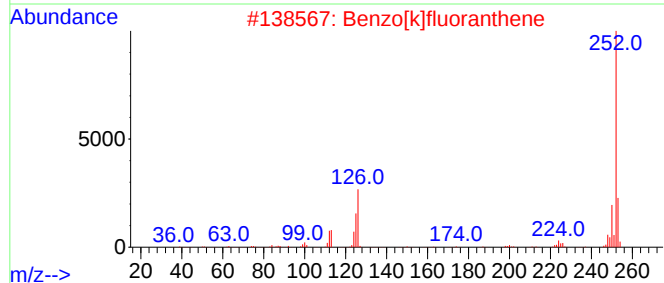
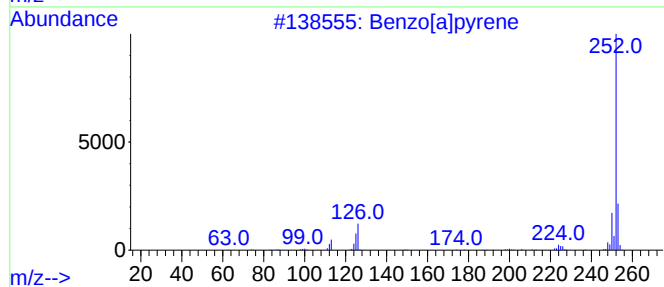
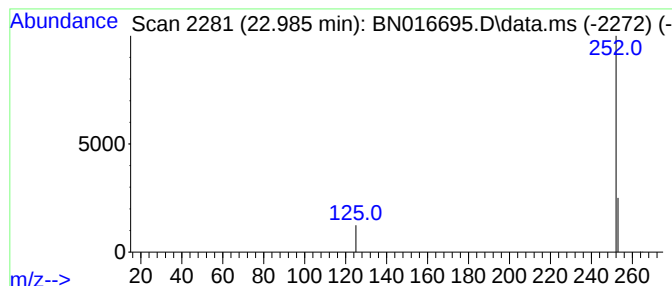
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzo[a]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.985	0.70 ng	446131	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[a]pyrene	252	C20H12	000050-32-8	9
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	9
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
4			1,2-Dichloro-4-(2,4,6-cyclohepta...	252	C12H6Cl2O2	033548-00-4	9
5			Benzo[e]pyrene	252	C20H12	000192-97-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-823-N-SO-0-0.5-092221

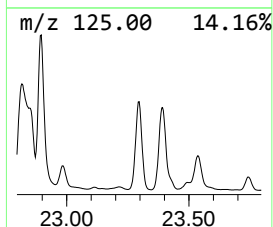
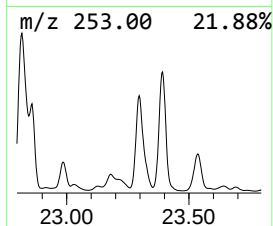
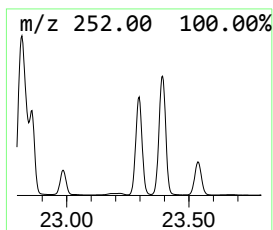
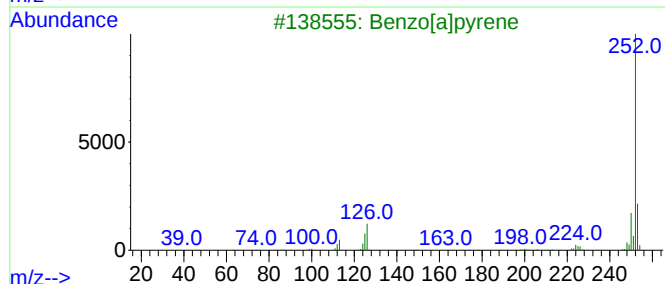
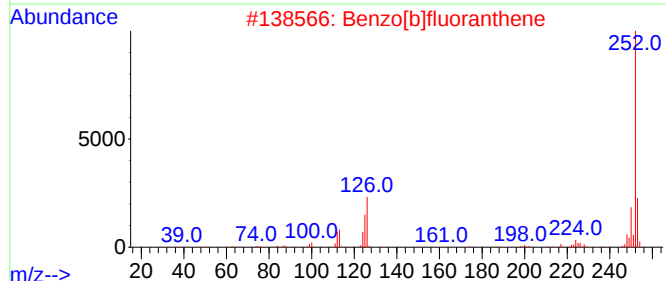
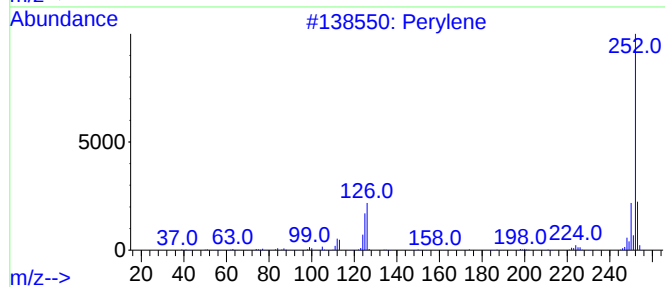
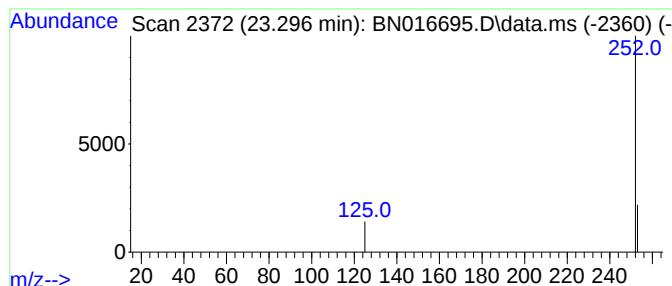
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.296	3.16 ng	2022380	Perylene-d12	23.488

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 : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-823-N-SO-0-0.5-092221

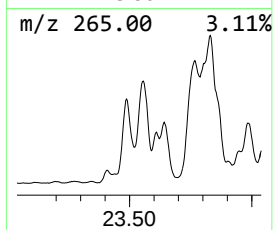
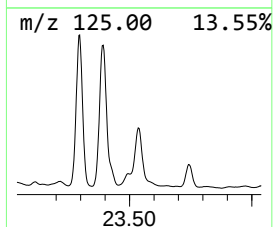
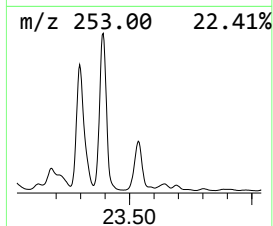
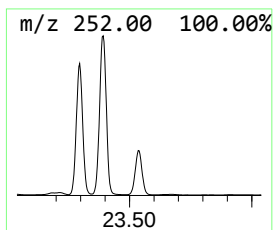
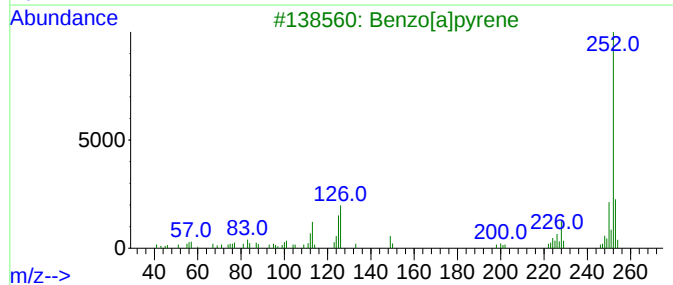
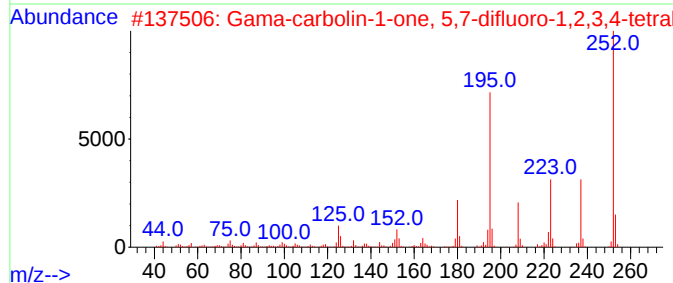
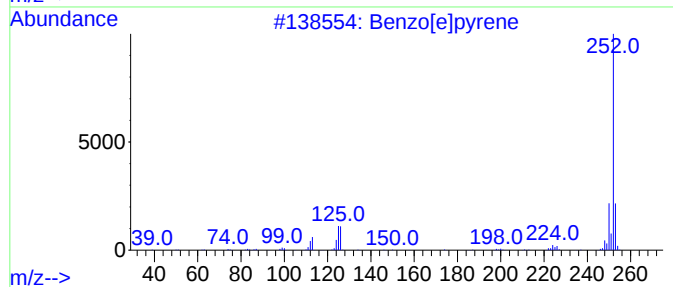
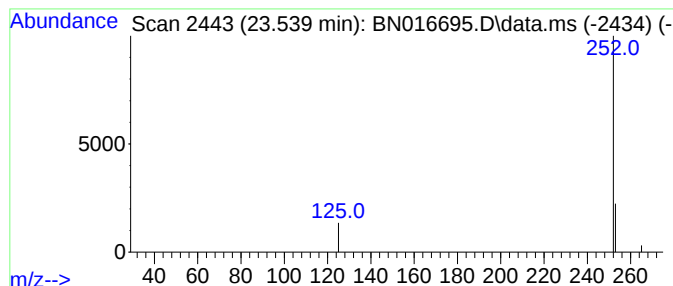
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.539	1.24 ng	793970	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	9
2			Gama-carbolin-1-one, 5,7-difluor...	252	C12H10F2N2O2	062223-53-4	9
3			Benzo[a]pyrene	252	C20H12	000050-32-8	9
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
5			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

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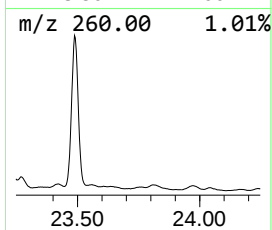
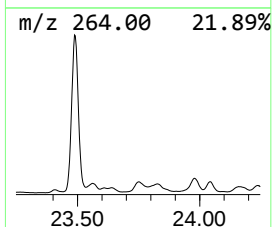
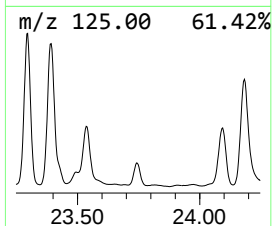
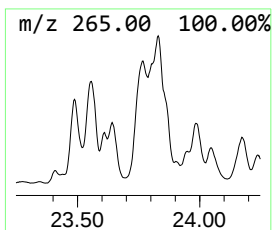
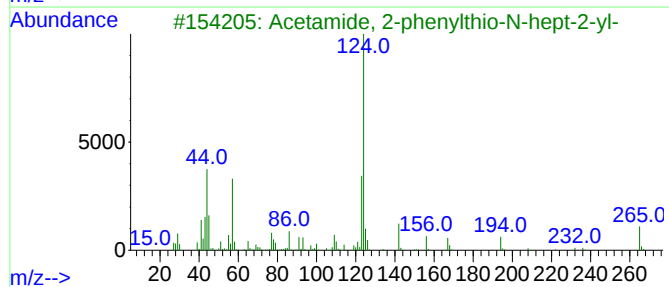
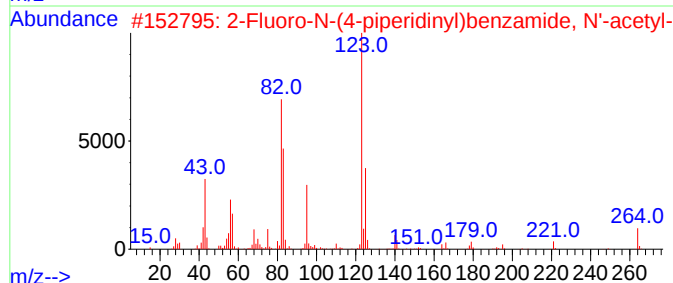
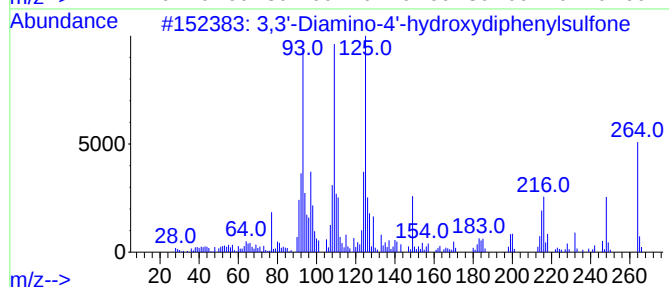
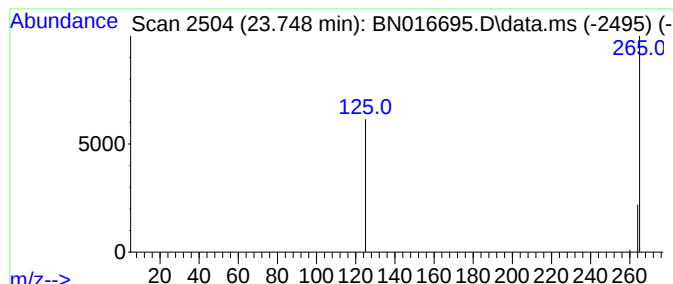
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 3,3'-Diamino-4'-hydroxydiph... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.748	0.19 ng	119479	Perylene-d12	23.488

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3,3'-Diamino-4'-hydroxydiphenyls...	264	C12H12N2O3S	014571-19-8	5
2		2-Fluoro-N-(4-piperidiny)benzam...	264	C14H17FN2O2	1178224-41-3	4
3		Acetamide, 2-phenylthio-N-hept-2...	265	C15H23NOS	1000419-83-0	4
4		Imidazol-5(4H)-one, 2,4-dibenzyl-	264	C17H16N2O	097978-58-0	4
5		Benzamide, 3-fluoro-N-nonyl-	265	C16H24FNO	1000407-28-6	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

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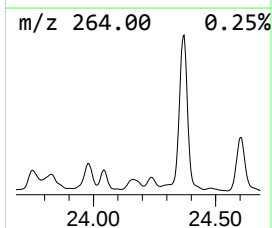
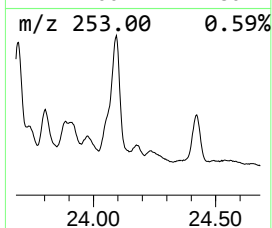
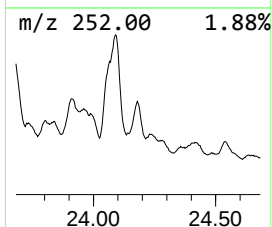
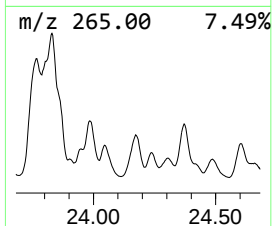
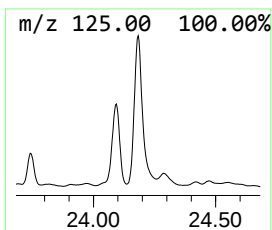
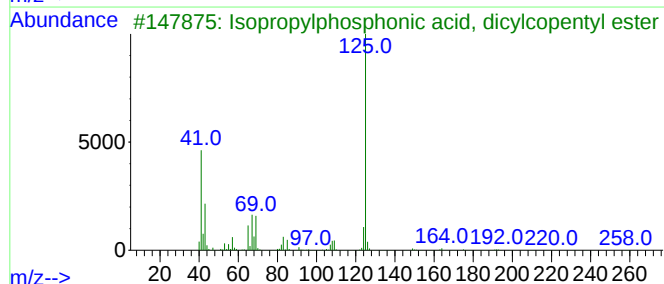
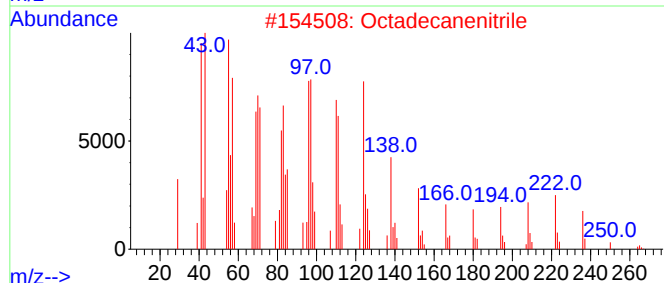
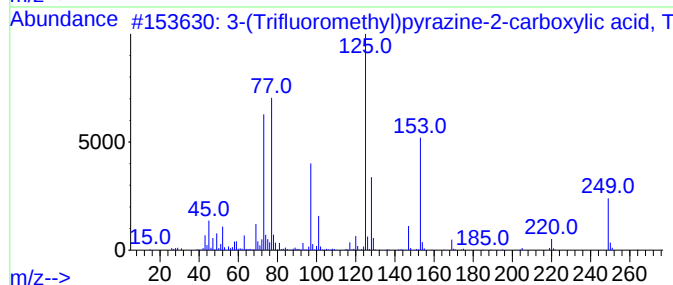
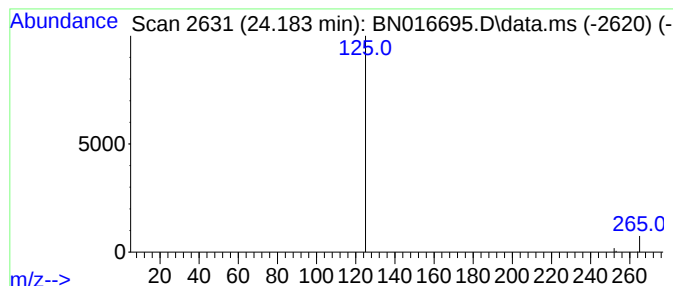
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 3-(Trifluoromethyl)pyrazine... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.183	0.29 ng	187927	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(Trifluoromethyl)pyrazine-2-ca...	264	C9H11F3N2O2Si	1000499-33-5	4		
2	Octadecanenitrile	265	C18H35N	000638-65-3	3		
3	Isopropylphosphonic acid, dicylc...	260	C13H25O3P	1000273-18-4	3		
4	(S,E)-6-Hydroxy-6-methyl-2-((2S,...	252	C15H24O3	088243-64-5	3		
5	4,5,6-Pyrimidinetriamine	125	C4H7N5	000118-70-7	2		



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-823-N-SO-0-0.5-092221

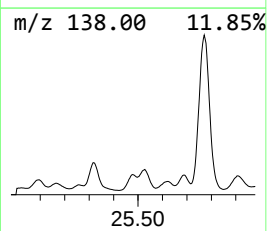
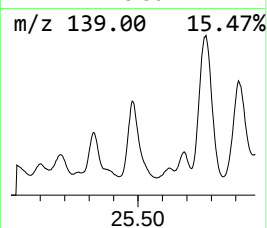
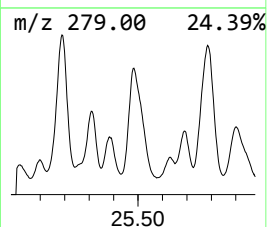
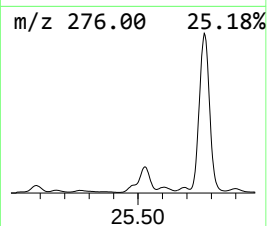
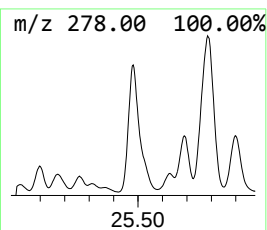
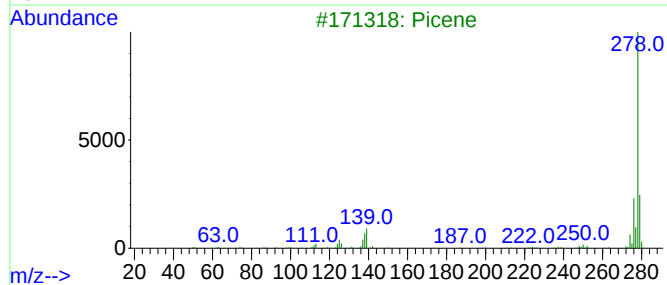
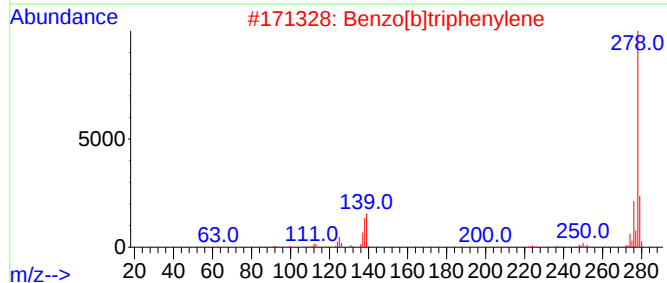
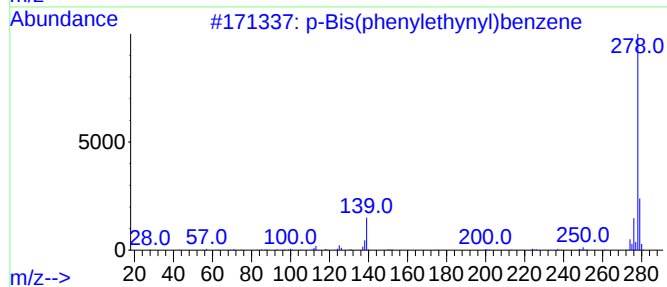
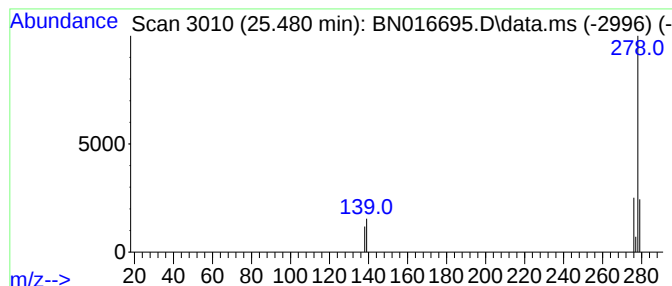
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 p-Bis(phenylethynyl)benzene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.480	0.48 ng	306328	Perylene-d12	23.488

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		p-Bis(phenylethynyl)benzene	278	C22H14	001849-27-0	72
2		Benzo[b]triphenylene	278	C22H14	000215-58-7	64
3		Picene	278	C22H14	000213-46-7	64
4		Pentaphene	278	C22H14	000222-93-5	64
5		Dibenz[a,h]anthracene	278	C22H14	000053-70-3	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

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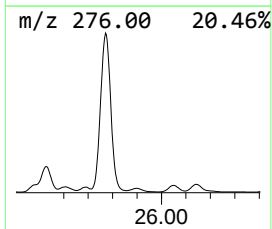
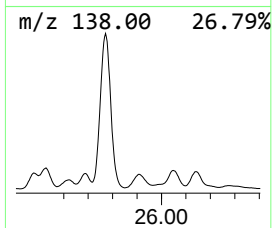
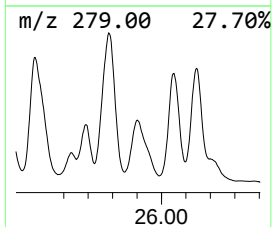
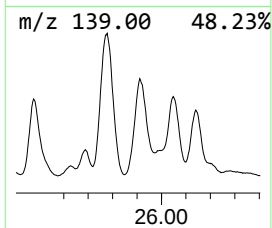
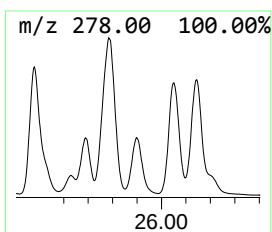
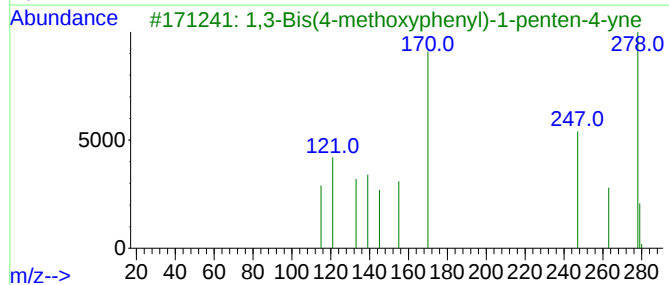
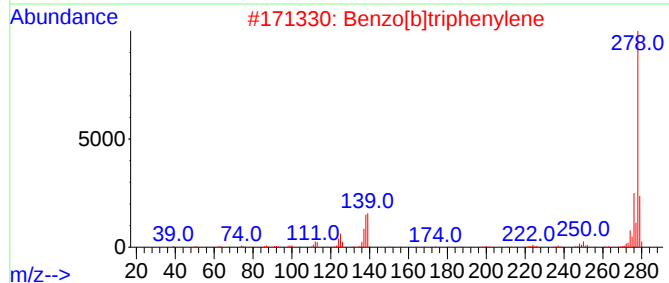
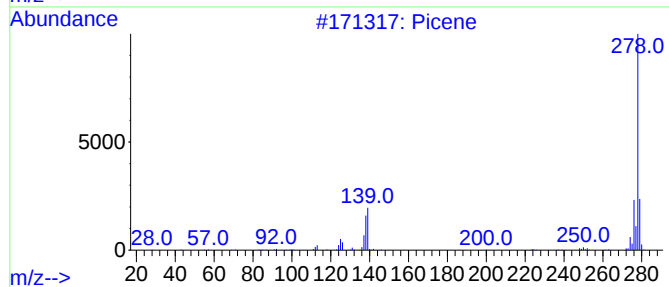
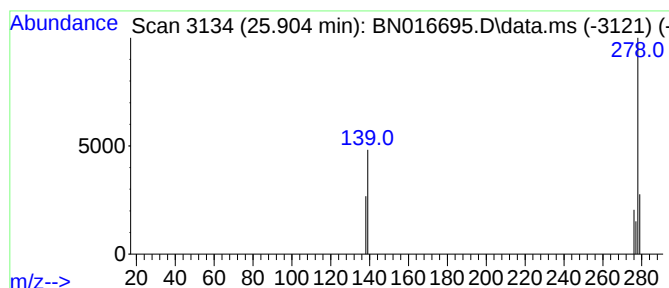
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Picene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.904	0.30 ng	189310	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Picene	278	C22H14	000213-46-7	64
2			Benzo[b]triphenylene	278	C22H14	000215-58-7	64
3			1,3-Bis(4-methoxyphenyl)-1-pente...	278	C19H18O2	117295-79-1	56
4			Benz[a]anthracene-7,12-dicarboni...	278	C20H10N2	035215-32-8	40
5			1-(Diethylamino)-3-methylpyrido[...	278	C17H18N4	1000331-84-4	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-823-N-SO-0-0.5-092221

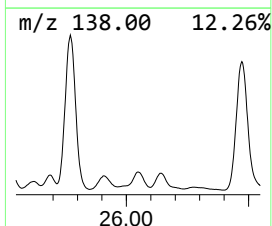
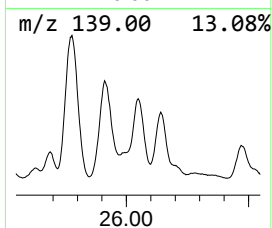
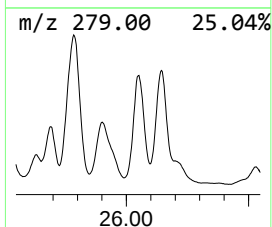
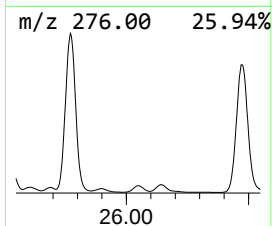
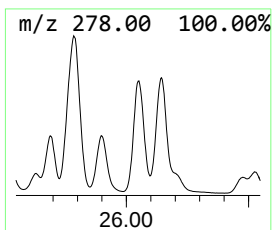
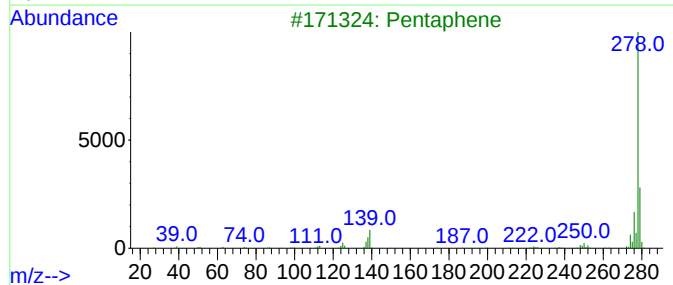
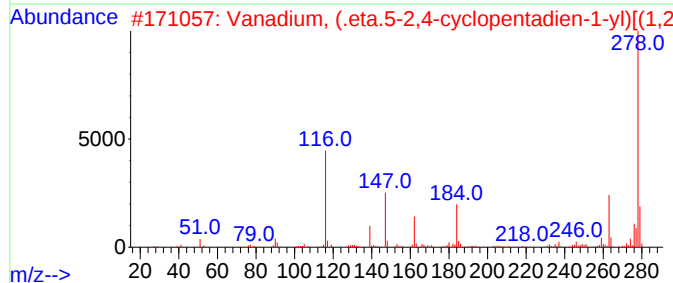
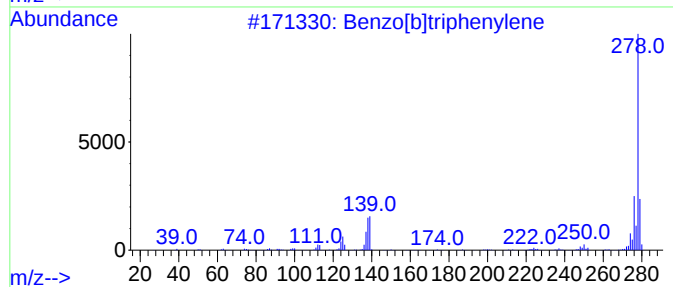
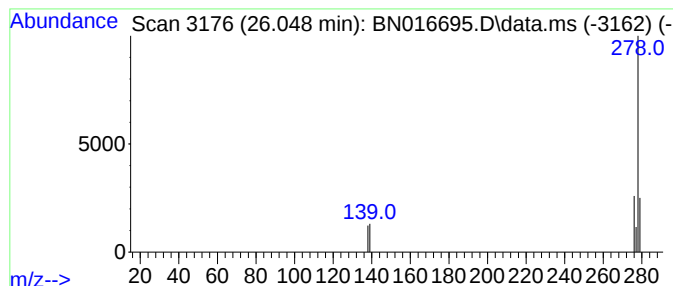
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Benzo[b]triphenylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.048	0.46 ng	291806	Perylene-d12	23.488

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			Pentaphene	278	C22H14	000222-93-5	72
4			Picene	278	C22H14	000213-46-7	72
5			1-naphthalenol, 4-[2-(4-methoxyp...	278	C17H14N2O2	1000397-12-8	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-823-N-SO-0-0.5-092221

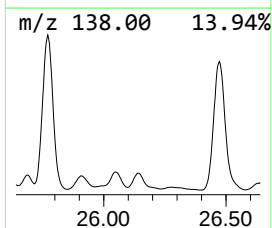
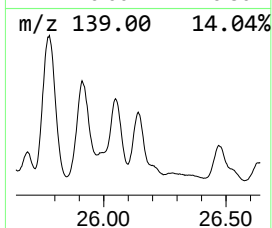
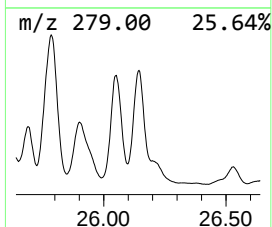
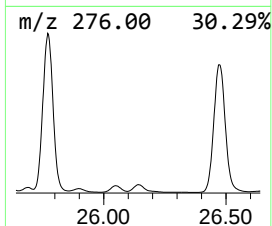
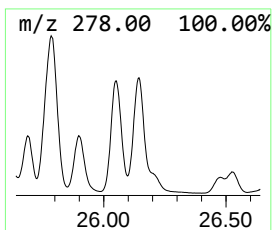
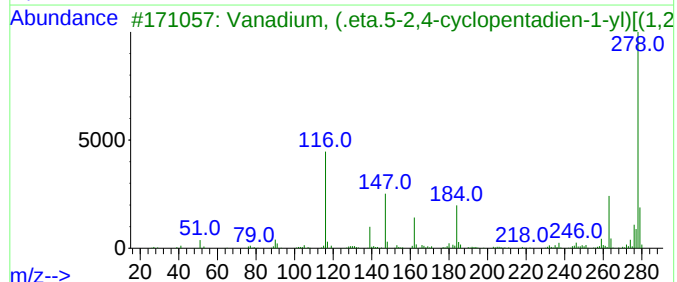
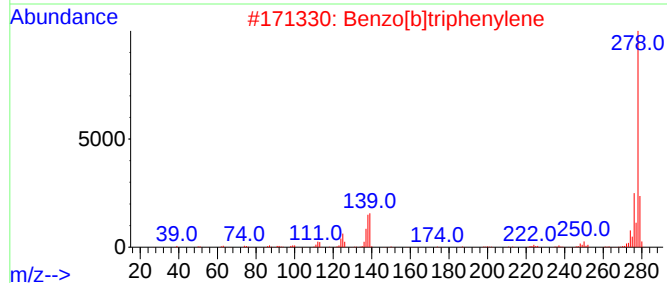
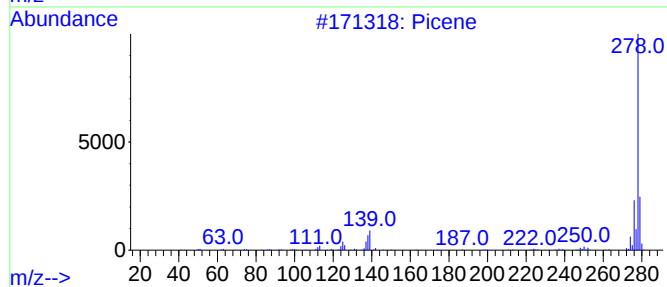
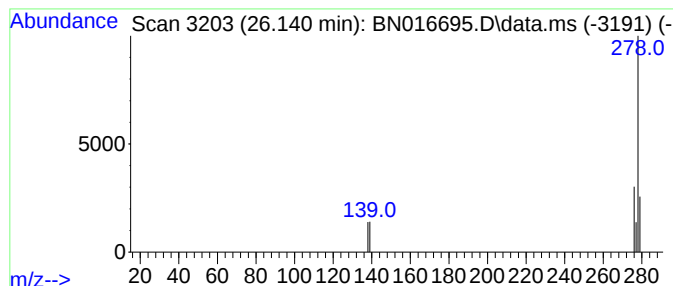
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Picene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.140	0.63 ng	401214	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Picene	278	C22H14	000213-46-7	80
2			Benzo[b]triphenylene	278	C22H14	000215-58-7	80
3			Vanadium, (.eta.5-2,4-cyclopenta...	278	C17H23V	126948-97-8	78
4			Pentaphene	278	C22H14	000222-93-5	72
5			Dibenz[a,h]anthracene	278	C22H14	000053-70-3	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016695.D
Acq On : 03 Oct 2021 07:00
Operator : CG/JU
Sample : M3892-07
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
S-823-N-SO-0-0.5-092221

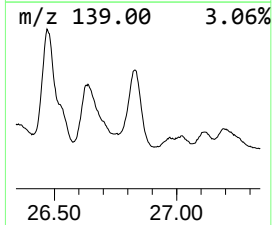
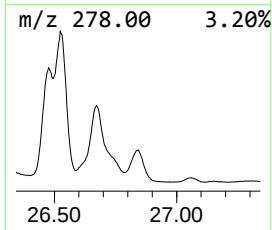
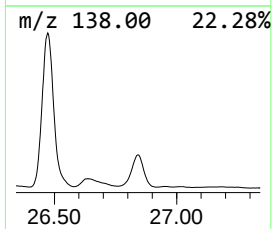
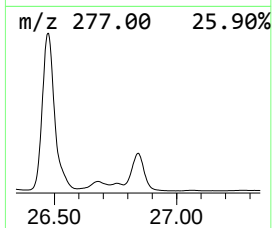
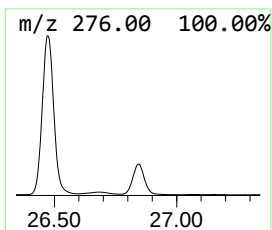
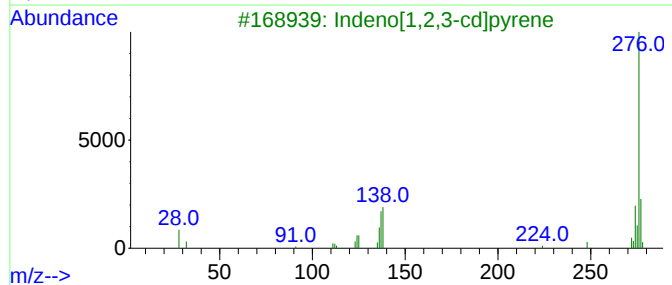
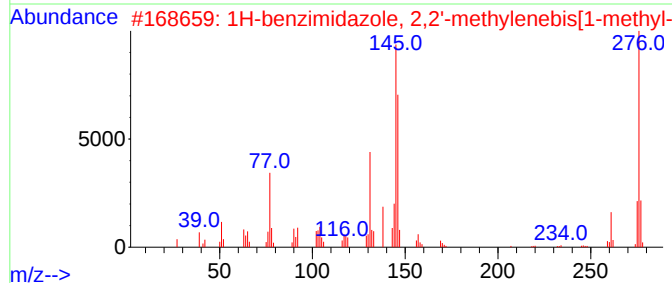
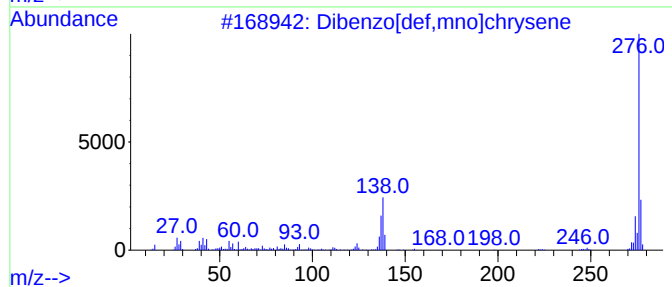
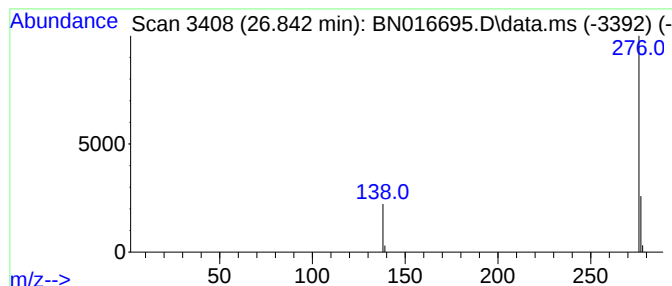
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Dibenzo[def,mno]chrysene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.842	0.46 ng	297351	Perylene-d12	23.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	83
2			1H-benzimidazole, 2,2'-methylene...	276	C17H16N4	1000401-82-9	83
3			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	83
4			Benzo[ghi]perylene	276	C22H12	000191-24-2	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 : BN016695.D
 Acq On : 03 Oct 2021 07:00
 Operator : CG/JU
 Sample : M3892-07
 Misc :
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 S-823-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
Acetone	4.821	0.3	ng	75006	1	7.642	107734	0.4
Butane	7.937	0.4	ng	111078	1	7.642	107734	0.4
Benzene, nitro-	9.671	0.2	ng	110564	2	10.406	195685	0.4
CH3CHClCH2C(O)OCH3	10.191	0.2	ng	100609	2	10.406	195685	0.4
Carbazole	17.431	0.8	ng	357197	4	17.017	187056	0.4
Hydrazinecarbox...	17.894	0.2	ng	116896	4	17.017	187056	0.4
(S)-2-Diphenylm...	17.954	0.2	ng	116885	4	17.017	187056	0.4
Indole-5-carbox...	18.418	0.2	ng	103848	4	17.017	187056	0.4
Cyclohexene, 1-...	21.886	0.2	ng	2005390	5	21.238	3267420	0.4
1-(4-Fluorophen...	22.564	0.3	ng	223960	6	23.488	256223	0.4
Benzo[a]pyrene	22.985	0.7	ng	446131	6	23.488	256223	0.4
Perylene	23.296	3.2	ng	2022380	6	23.488	256223	0.4
Benzo[e]pyrene	23.539	1.2	ng	793970	6	23.488	256223	0.4
3,3'-Diamino-4'...	23.748	0.2	ng	119479	6	23.488	256223	0.4
3-(Trifluoromet...	24.183	0.3	ng	187927	6	23.488	256223	0.4
p-Bis(phenyleth...	25.480	0.5	ng	306328	6	23.488	256223	0.4
Picene	25.904	0.3	ng	189310	6	23.488	256223	0.4
Benzo[b]triphen...	26.048	0.5	ng	291806	6	23.488	256223	0.4
Picene	26.140	0.6	ng	401214	6	23.488	256223	0.4
Dibenzo[def,mno...	26.842	0.5	ng	297351	6	23.488	256223	0.4