

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016617.D
 Acq On : 01 Oct 2021 03:00
 Operator : CG/JU
 Sample : PB139443BL
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139443BL

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: BN016617.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.240	124	126	136	rVB	5579	11287	5.69%	0.518%
2	4.821	186	189	205	rVB	63714	114603	57.72%	5.259%
3	5.282	235	239	256	rVB	31509	59548	29.99%	2.733%
4	6.831	403	407	422	rVB	23687	45798	23.07%	2.102%
5	7.642	491	495	515	rVB	52184	97760	49.24%	4.486%
6	8.306	565	567	569	rVB	6048	6250	3.15%	0.287%
7	8.784	601	605	616	rBV	28434	59932	30.19%	2.750%
8	10.406	729	733	752	rBV	94295	173810	87.54%	7.977%
9	12.007	919	932	970	rBV	58415	104890	52.83%	4.814%
10	12.505	1043	1044	1049	rBV3	1060	4268	2.15%	0.196%
11	12.898	1071	1075	1090	rBV	105600	198540	100.00%	9.112%
12	14.269	1180	1183	1186	rBV	119237	174947	88.12%	8.029%
13	15.766	1298	1301	1317	rBV2	6330	14225	7.16%	0.653%
14	17.017	1400	1403	1412	rBV	73663	138865	69.94%	6.373%
15	17.151	1412	1414	1425	rVB	2069	5611	2.83%	0.258%
16	19.063	1688	1696	1733	rBV	121589	196168	98.81%	9.003%
17	19.460	1767	1776	1793	rVB	8270	11736	5.91%	0.539%
18	19.678	1813	1820	1853	rBV	110202	150241	75.67%	6.895%
19	21.025	1980	1982	1989	rBV	1008	2044	1.03%	0.094%
20	21.164	1993	1995	1997	rBV	2048	2426	1.22%	0.111%
21	21.227	1997	2001	2003	rBV2	113719	176973	89.14%	8.122%
22	21.270	2003	2005	2016	rVB	26899	43383	21.85%	1.991%
23	22.321	2101	2104	2107	rBV	1346	2193	1.10%	0.101%
24	22.803	2218	2228	2234	rBV	16302	27799	14.00%	1.276%
25	22.848	2234	2241	2268	rVB2	19227	37332	18.80%	1.713%
26	23.382	2386	2397	2404	rBV	10600	21409	10.78%	0.983%
27	23.481	2414	2426	2468	rVB	84380	172923	87.10%	7.936%
28	24.083	2593	2602	2617	rBV2	3906	7337	3.70%	0.337%
29	24.853	2817	2827	2842	rVB	4063	8975	4.52%	0.412%
30	25.767	3070	3094	3142	rBV4	17373	71773	36.15%	3.294%
31	26.452	3273	3294	3329	rBV	8742	29916	15.07%	1.373%
32	26.818	3383	3401	3423	rBV	1065	3726	1.88%	0.171%
33	28.081	3747	3770	3792	rBV	606	2301	1.16%	0.106%

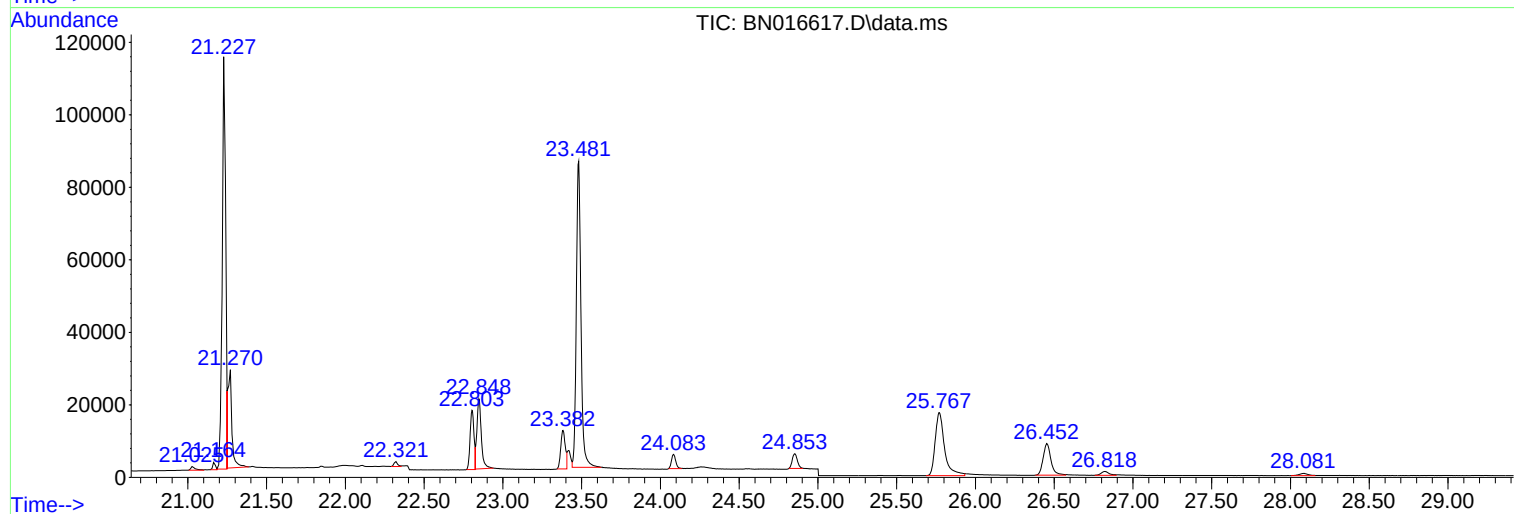
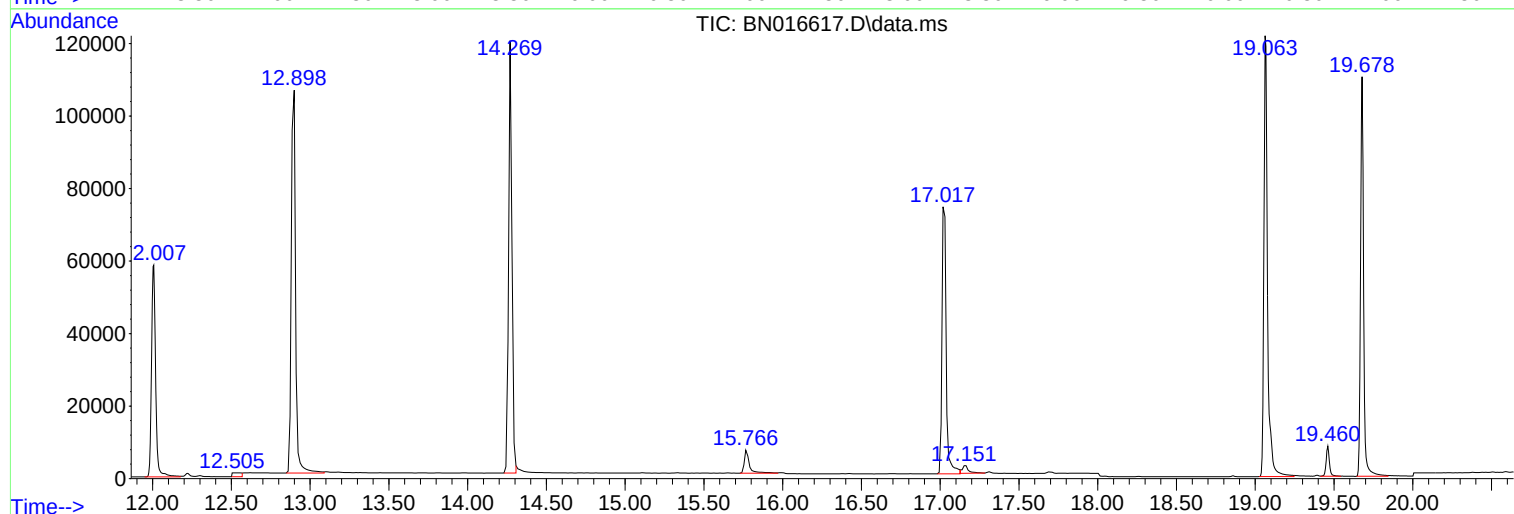
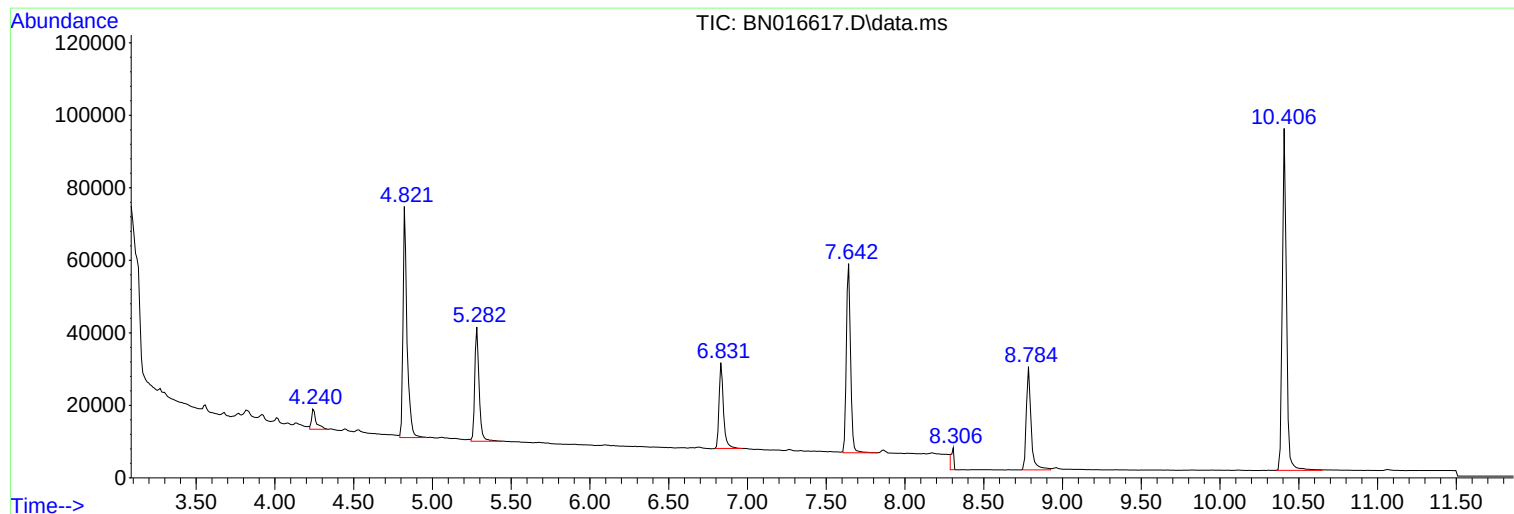
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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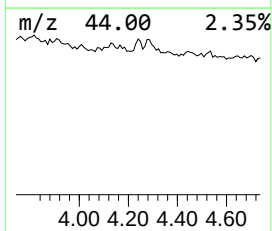
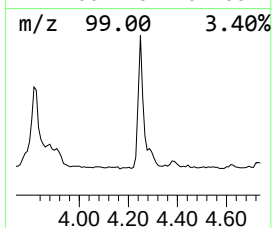
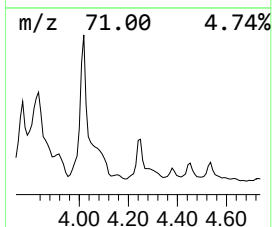
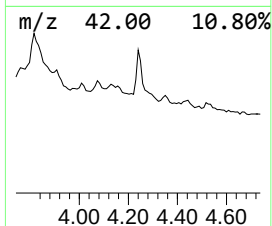
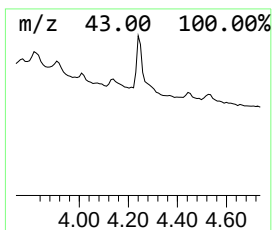
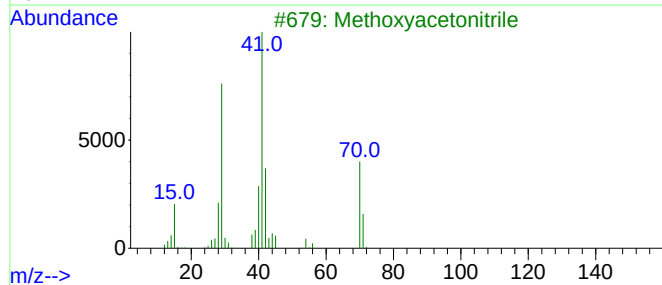
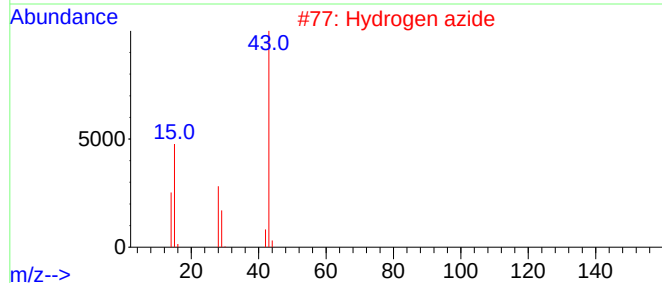
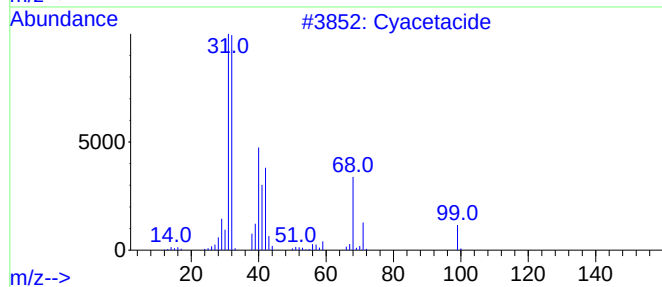
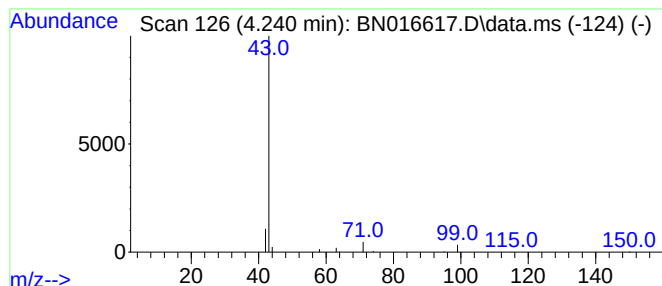
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyacetacide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.240	0.05 ng	11287	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyacetacide	99	C3H5N3O	000140-87-4	4
2			Hydrogen azide	43	HN3	007782-79-8	4
3			Methoxyacetoneitrile	71	C3H5NO	001738-36-9	4
4			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3
5			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	3



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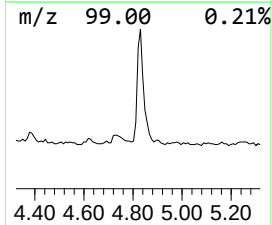
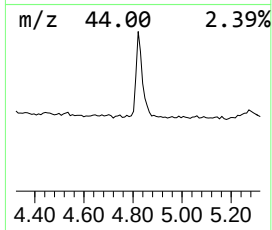
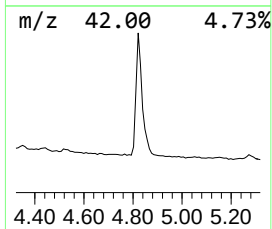
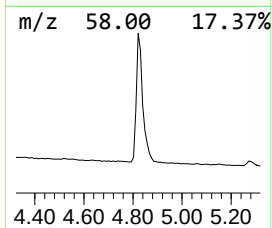
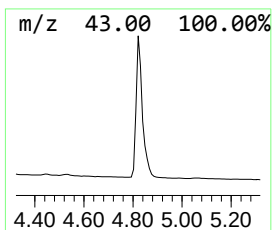
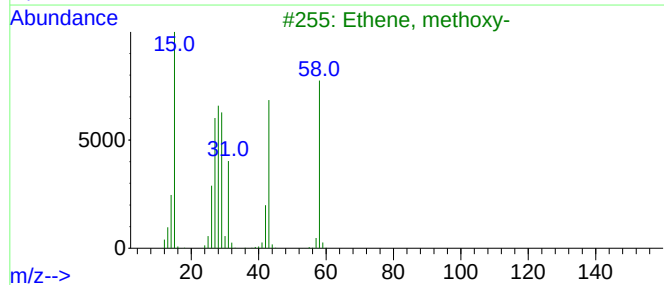
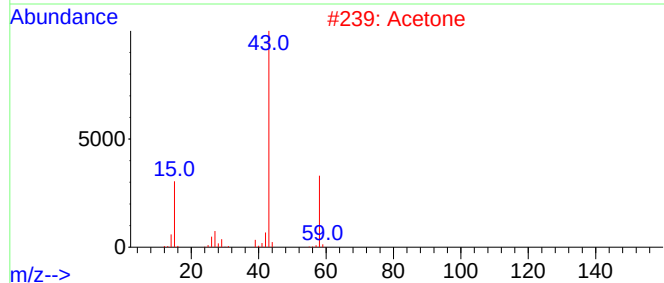
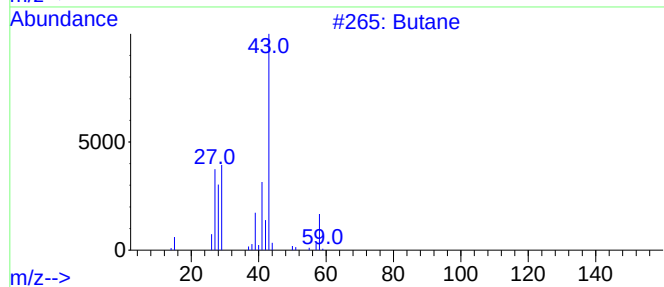
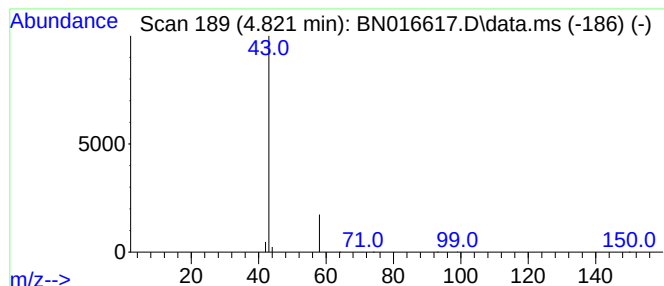
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.47 ng	114603	1,4-Dichlorobenzene-d4	7.642

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



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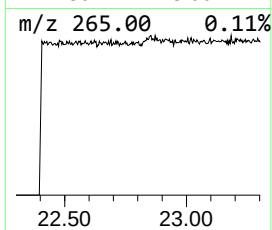
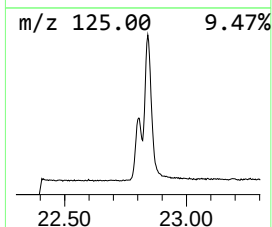
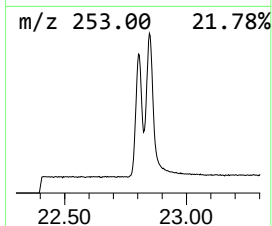
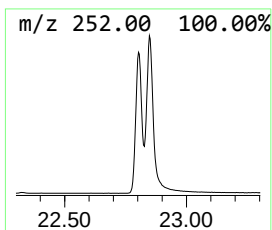
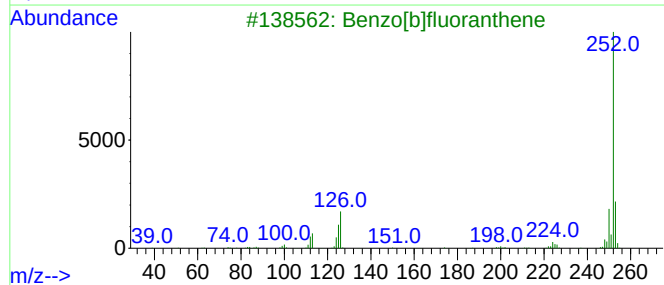
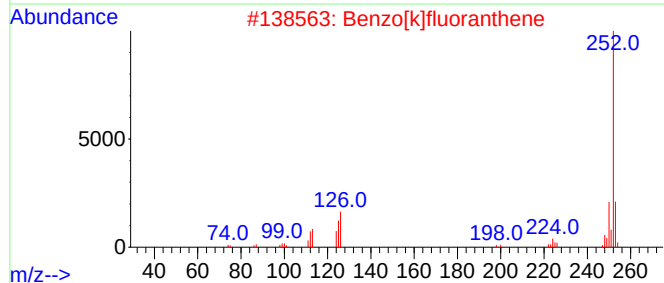
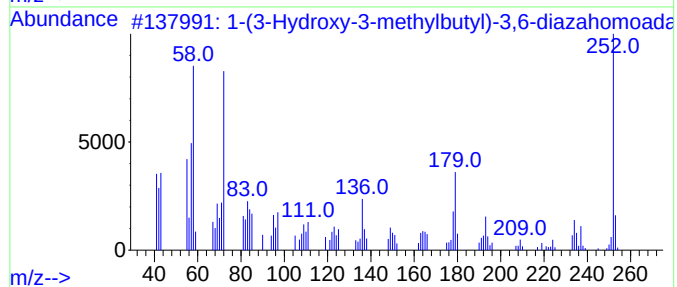
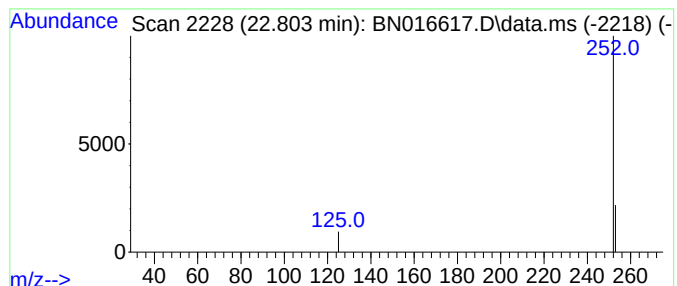
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-(3-Hydroxy-3-methylbutyl)... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.803	0.06 ng	27799	Perylene-d12	23.481

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	9		
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	9		
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	9		
4	Benzo[a]pyrene	252	C20H12	000050-32-8	9		
5	Benzo[e]pyrene	252	C20H12	000192-97-2	9		



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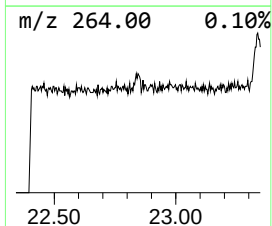
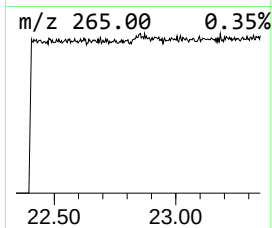
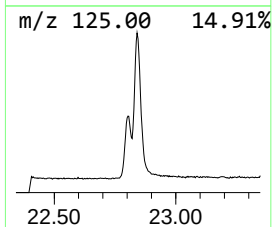
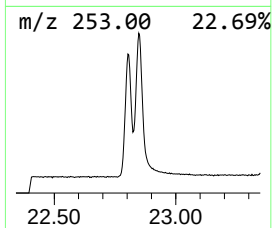
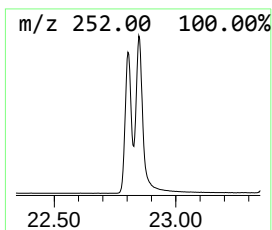
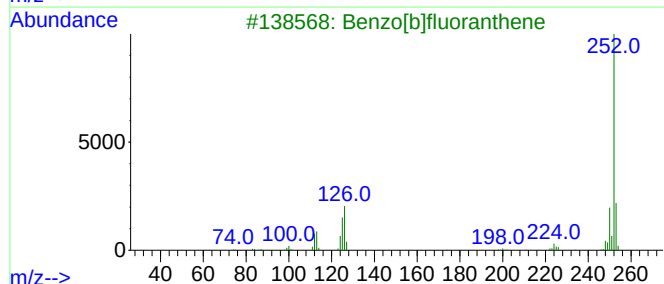
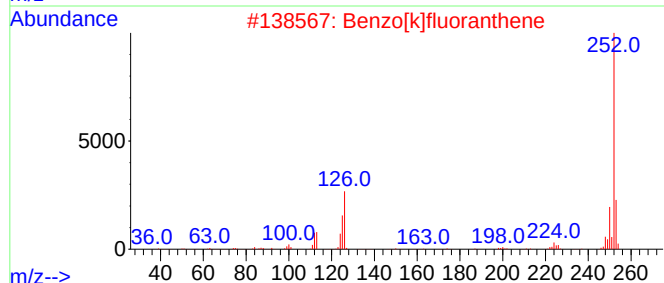
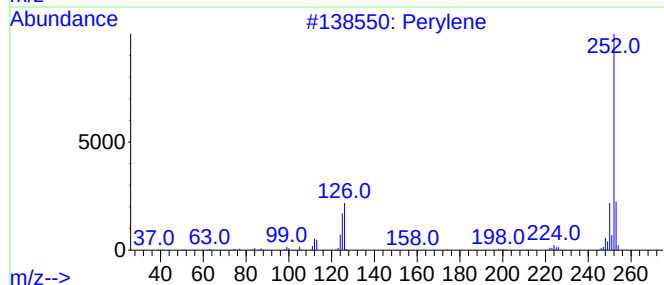
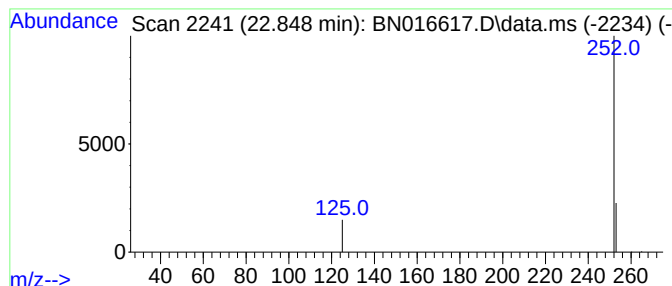
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Perylene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.848	0.09 ng	37332	Perylene-d12	23.481

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Perylene	252	C20H12	000198-55-0	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[j]fluoranthene	252	C20H12	000205-82-3	9



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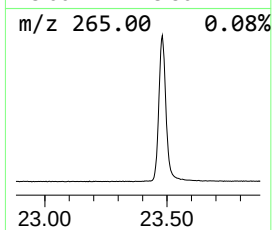
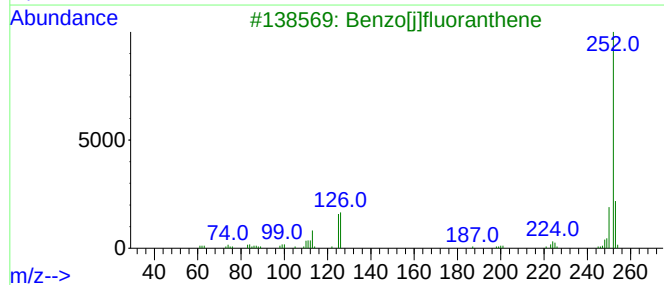
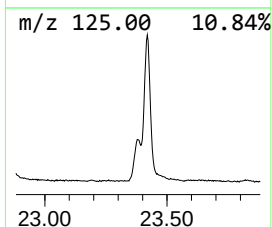
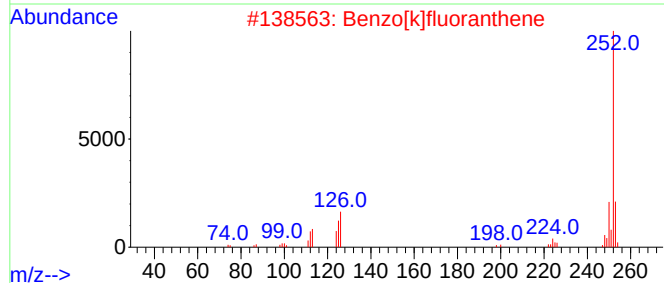
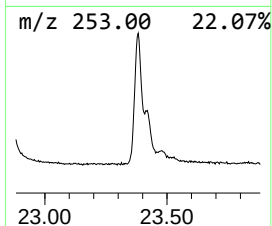
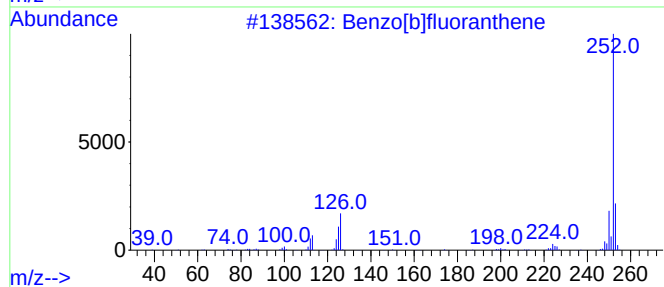
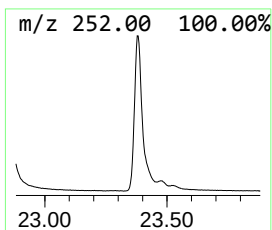
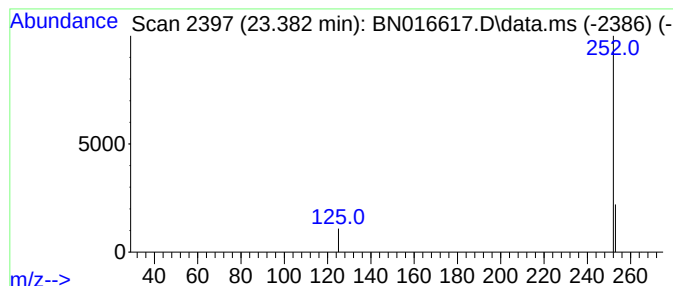
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzo[b]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.382	0.05 ng	21409	Perylene-d12	23.481

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



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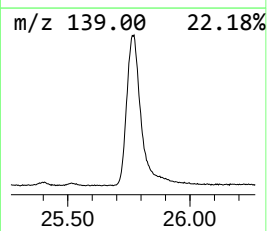
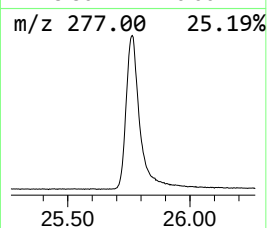
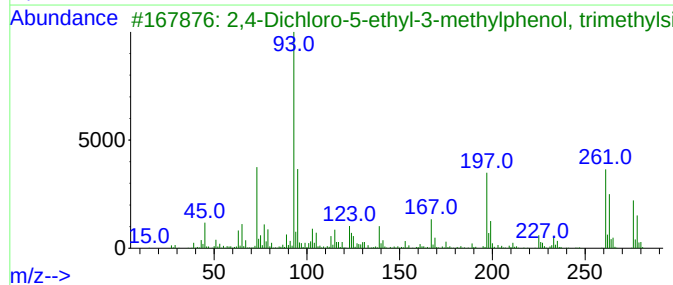
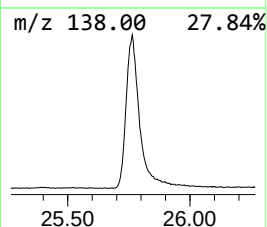
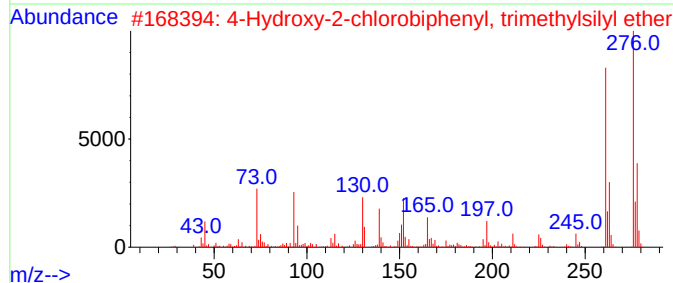
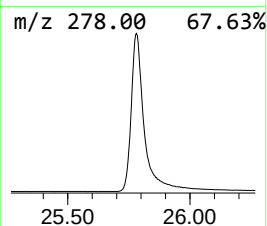
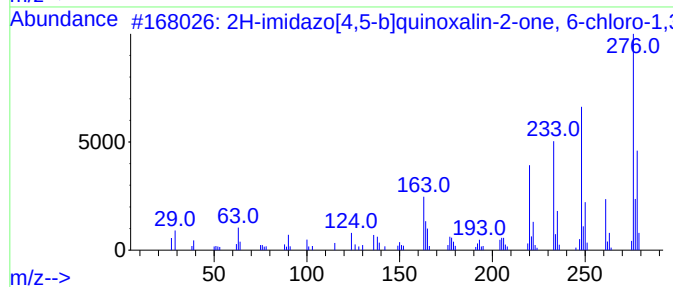
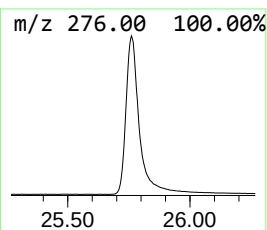
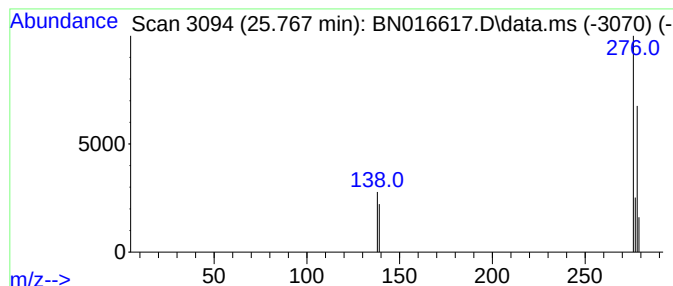
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2H-imidazo[4,5-b]quinoxalin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.767	0.17 ng	71773	Perylene-d12	23.481

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2H-imidazo[4,5-b]quinoxalin-2-on...	276	C13H13ClN4O	1010397-08-9	90
2			4-Hydroxy-2-chlorobiphenyl, trim...	276	C15H17ClOSi	1000447-61-8	83
3			2,4-Dichloro-5-ethyl-3-methylphe...	276	C12H18Cl2OSi	1010467-47-9	83
4			2-Hydroxy-5-bromobenzophenone	276	C13H9BrO2	055082-33-2	56
5			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	42



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016617.D
Acq On : 01 Oct 2021 03:00
Operator : CG/JU
Sample : PB139443BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139443BL

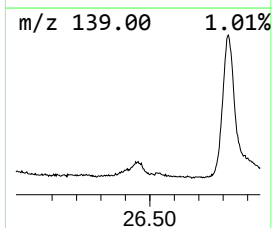
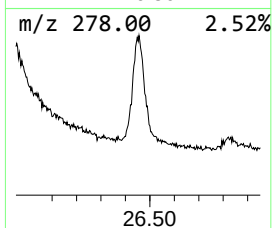
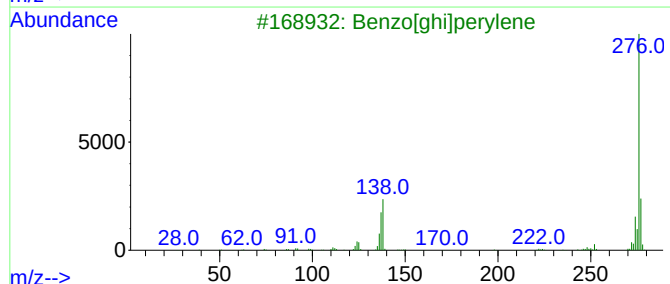
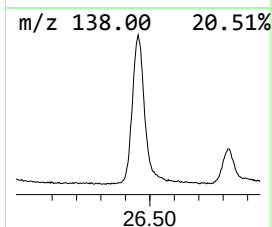
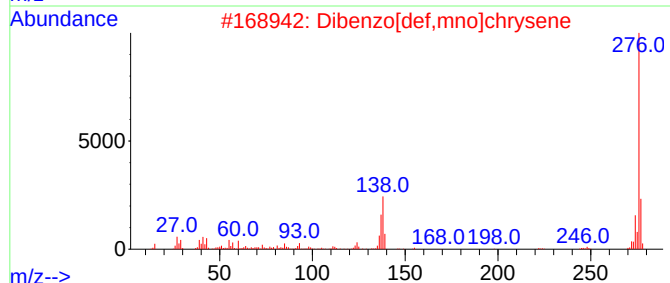
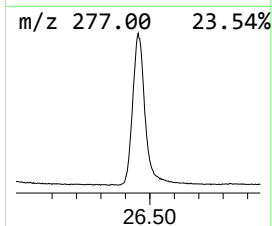
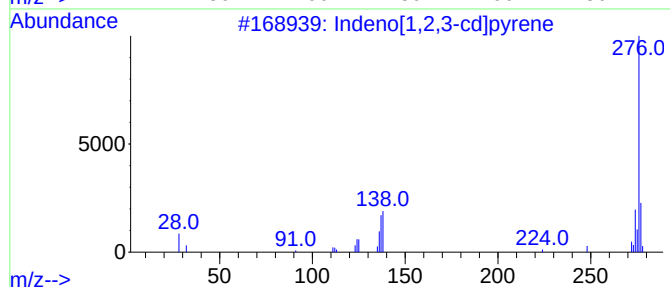
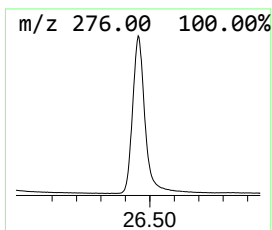
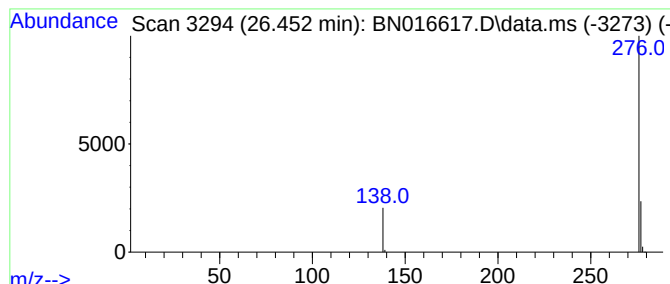
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Indeno[1,2,3-cd]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.452	0.07 ng	29916	Perylene-d12	23.481

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	83
2			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	83
3			Benzo[ghi]perylene	276	C22H12	000191-24-2	83
4			1H-benzimidazole, 2,2'-methylene...	276	C17H16N4	1000401-82-9	83
5			1-(4-Hydroxy-3-methoxyphenyl)dec...	276	C17H24O3	000555-66-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016617.D
Acq On : 01 Oct 2021 03:00
Operator : CG/JU
Sample : PB139443BL
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139443BL

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
Cyacetacide	4.240	0.0	ng	11287	1	7.642	97760	0.4
Butane	4.821	0.5	ng	114603	1	7.642	97760	0.4
1-(3-Hydroxy-3-...	22.803	0.1	ng	27799	6	23.481	172923	0.4
Perylene	22.848	0.1	ng	37332	6	23.481	172923	0.4
Benzo[b]fluoran...	23.382	0.0	ng	21409	6	23.481	172923	0.4
2H-imidazo[4,5-...	25.767	0.2	ng	71773	6	23.481	172923	0.4
Indeno[1,2,3-cd...	26.452	0.1	ng	29916	6	23.481	172923	0.4