

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016606.D
 Acq On : 30 Sep 2021 19:09
 Operator : CG/JU
 Sample : PB139306BL
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139306BL

Integration Parameters: rteint.p

Integrator: RTE

Smoother: OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 1 % of largest Peak

Max Peaks: 100

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: BN016606.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.249	124	127	137	rVB	4724	9729	5.22%	0.471%
2	4.830	186	190	211	rVB	54983	109394	58.67%	5.291%
3	5.282	235	239	251	rVB	30036	55052	29.52%	2.662%
4	6.831	403	407	421	rBV	22129	44221	23.71%	2.139%
5	7.642	491	495	506	rVB	48586	89240	47.86%	4.316%
6	8.306	565	567	569	rVB	6502	6740	3.61%	0.326%
7	8.784	602	605	616	rBV	28055	57377	30.77%	2.775%
8	10.407	730	733	754	rVB	87116	161472	86.59%	7.809%
9	12.007	921	932	945	rBV	56051	95726	51.34%	4.629%
10	12.505	1043	1044	1047	rBV3	1099	2774	1.49%	0.134%
11	12.899	1071	1075	1089	rBV	103966	186470	100.00%	9.018%
12	14.269	1180	1183	1187	rBV	109513	166540	89.31%	8.054%
13	15.766	1298	1301	1316	rBV2	6341	14150	7.59%	0.684%
14	17.030	1400	1404	1412	rBV	69891	131944	70.76%	6.381%
15	17.151	1412	1414	1425	rVB	2045	5294	2.84%	0.256%
16	19.068	1688	1697	1743	rBV	114465	185408	99.43%	8.967%
17	19.460	1767	1776	1796	rVB	7630	11370	6.10%	0.550%
18	19.679	1813	1820	1859	rBV	107327	142435	76.38%	6.888%
19	20.017	1885	1887	1889	rBV2	960	2089	1.12%	0.101%
20	21.026	1979	1982	1993	rBV	4671	10403	5.58%	0.503%
21	21.174	1993	1996	1997	rBV	1832	2410	1.29%	0.117%
22	21.238	1997	2002	2004	rVV3	101294	177985	95.45%	8.608%
23	21.270	2004	2005	2017	rVB	26600	31887	17.10%	1.542%
24	22.321	2102	2104	2108	rBV	1402	2112	1.13%	0.102%
25	22.810	2220	2230	2236	rBV	15895	27431	14.71%	1.327%
26	22.855	2236	2243	2272	rVB2	18441	35399	18.98%	1.712%
27	23.385	2388	2398	2406	rBV	10450	21670	11.62%	1.048%
28	23.485	2416	2427	2467	rVB	81299	162666	87.23%	7.867%
29	24.087	2595	2603	2619	rVB	3621	6963	3.73%	0.337%
30	24.857	2820	2828	2846	rVB2	3779	8402	4.51%	0.406%
31	25.774	3072	3096	3152	rBV3	16248	68996	37.00%	3.337%
32	26.459	3273	3296	3340	rBV3	8367	29252	15.69%	1.415%
33	26.825	3388	3403	3419	rBV2	861	2795	1.50%	0.135%
34	28.092	3751	3773	3793	rBV2	494	1947	1.04%	0.094%

Sum of corrected areas: 2067743

Instrument :

BNA_N

ClientSampleId :

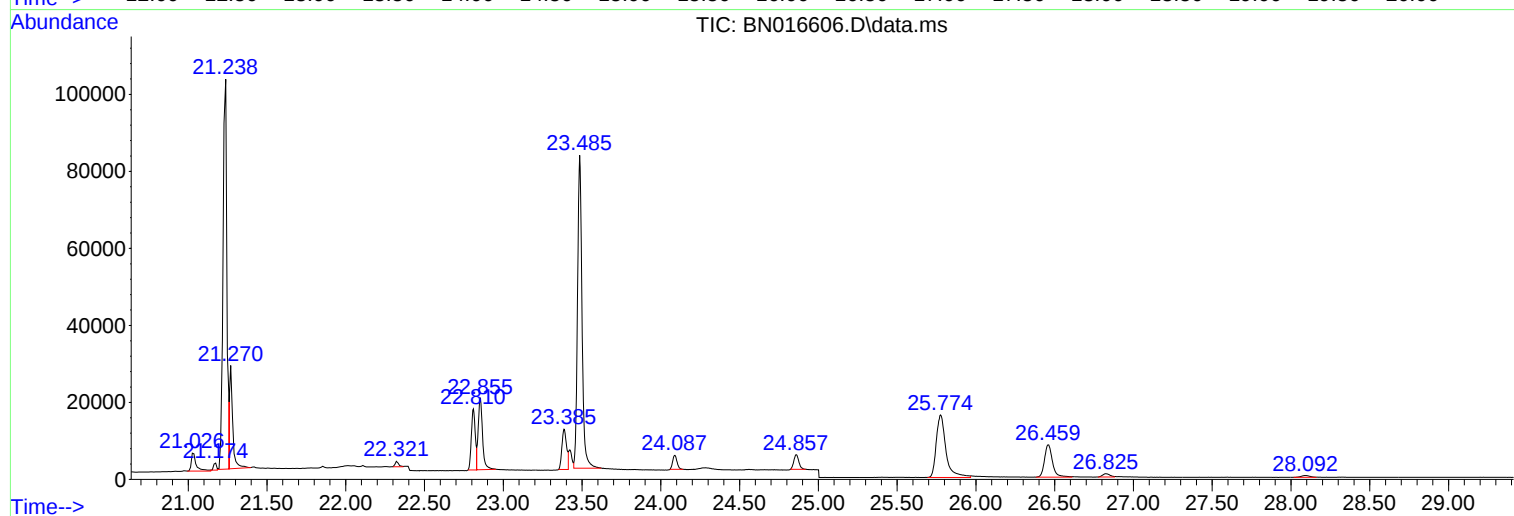
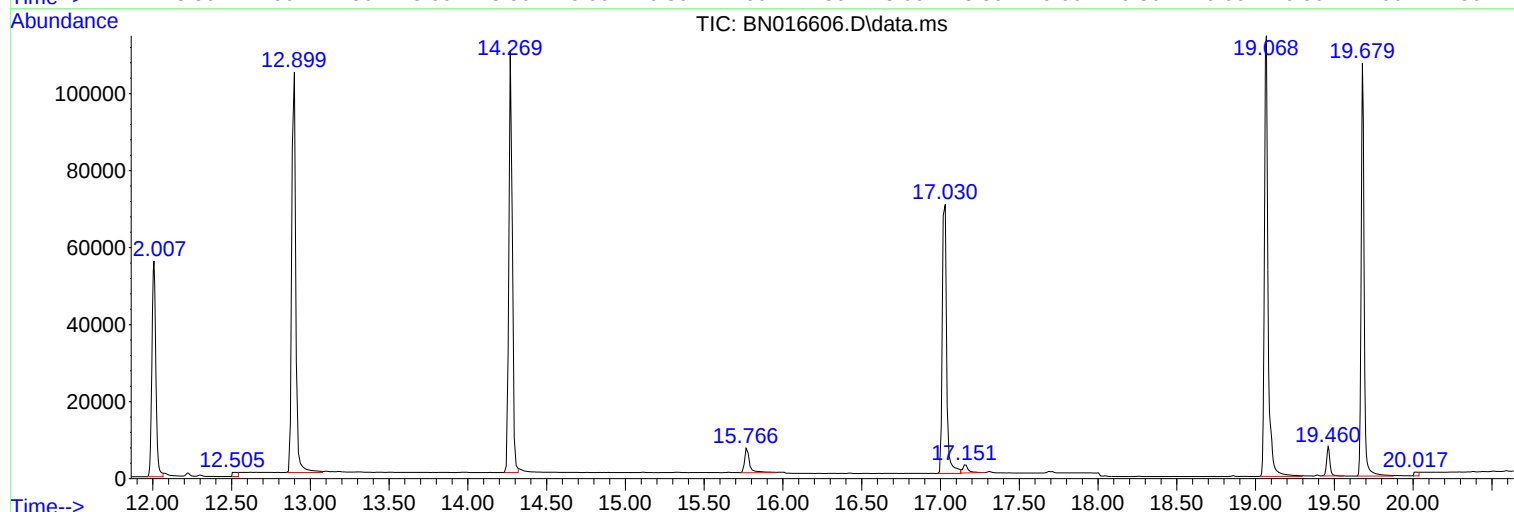
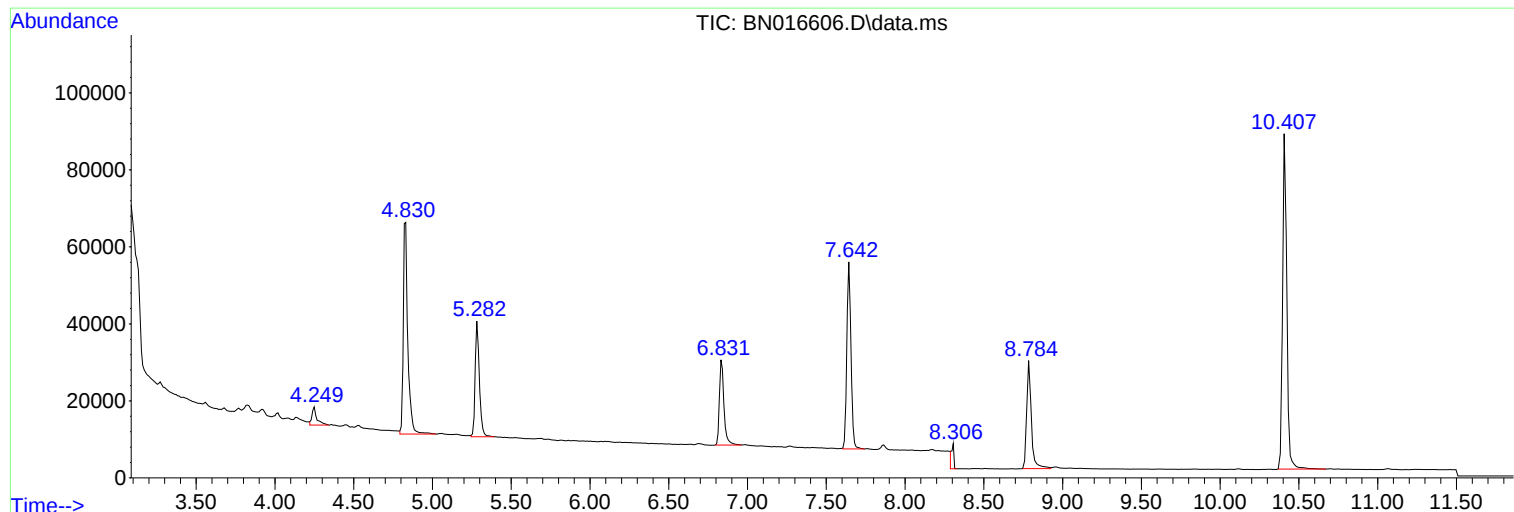
PB139306BL

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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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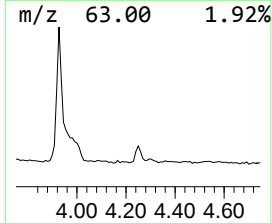
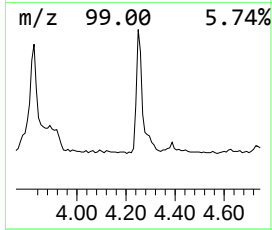
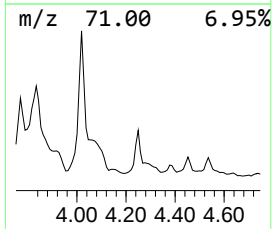
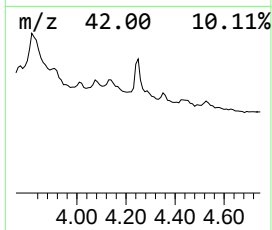
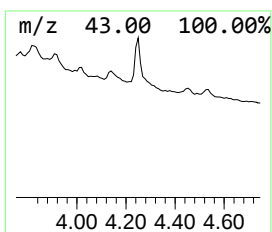
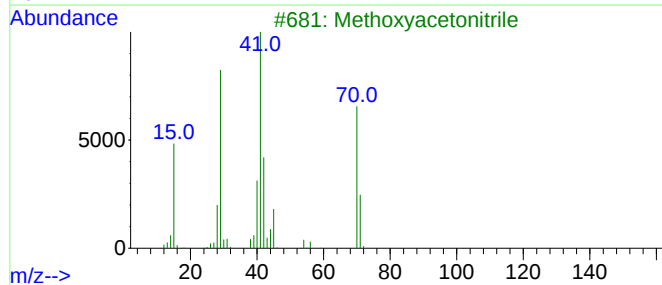
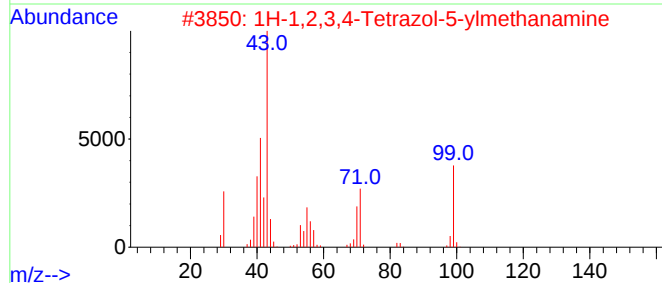
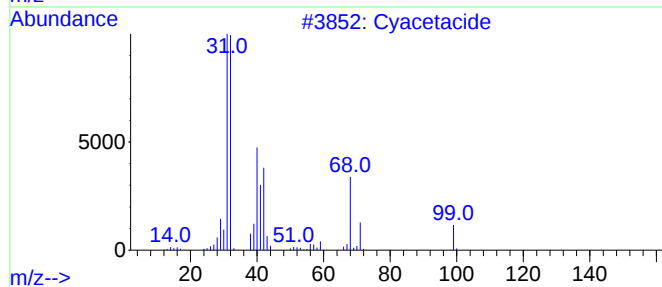
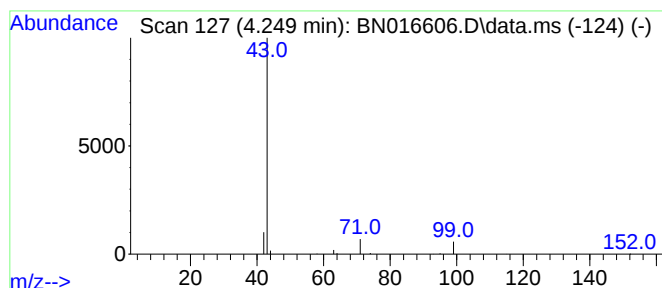
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.249	0.04 ng	9729	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyacetacide	99	C3H5N3O	000140-87-4	4
2		1H-1,2,3,4-Tetrazol-5-ylmethanamine	99	C2H5N5	031602-63-8	3
3		Methoxyacetoneitrile	71	C3H5NO	001738-36-9	3
4		Azetidine, 1-methyl-	71	C4H9N	004923-79-9	3
5		Hydrogen azide	43	HN3	007782-79-8	3



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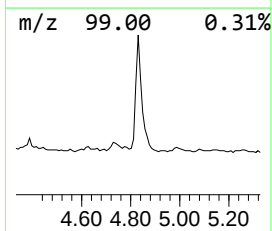
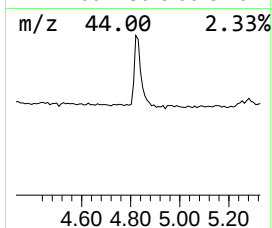
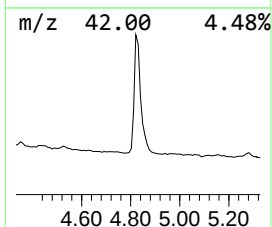
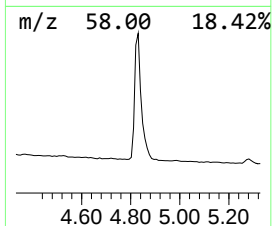
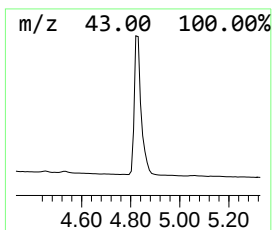
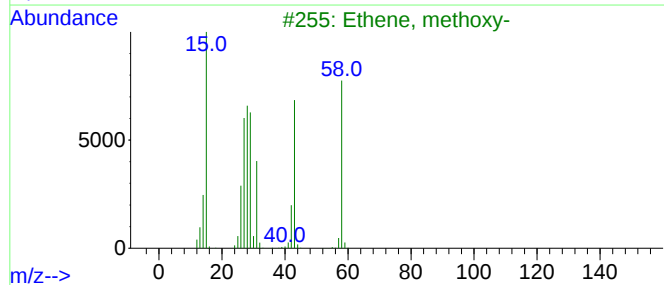
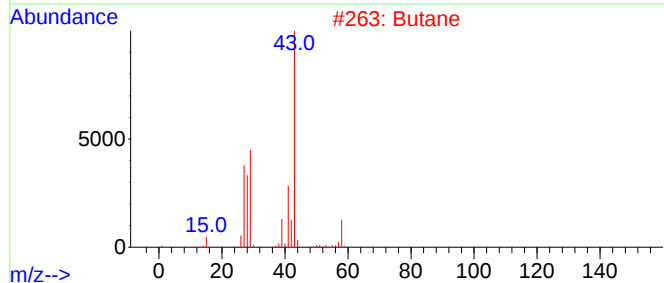
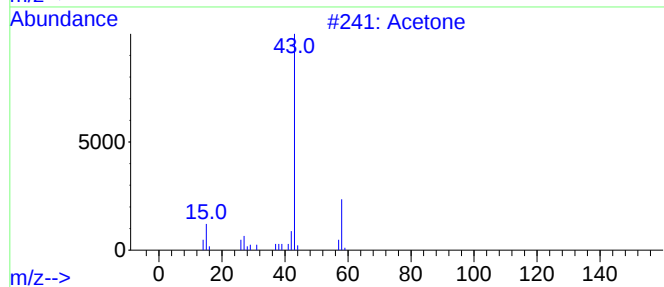
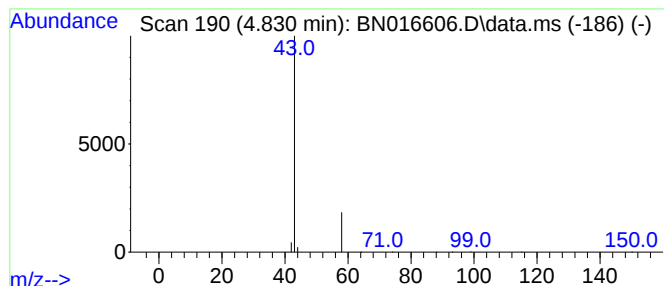
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Acetone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.830	0.49 ng	109394	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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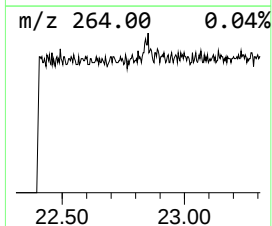
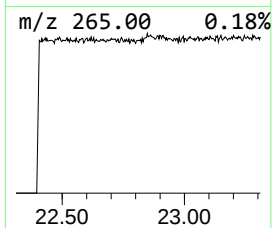
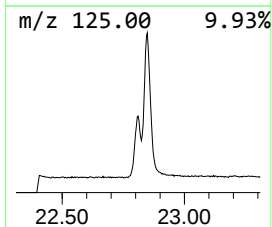
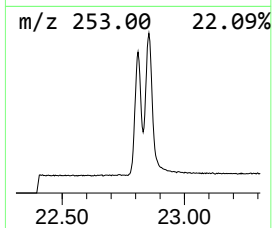
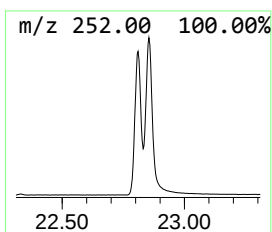
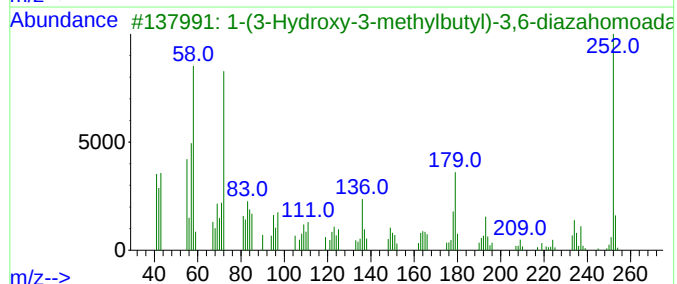
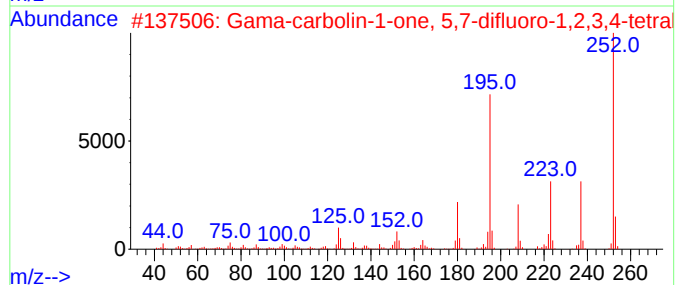
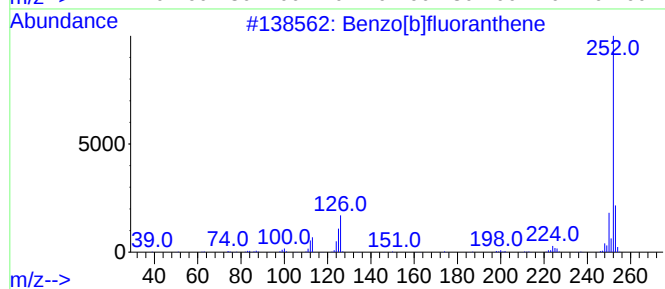
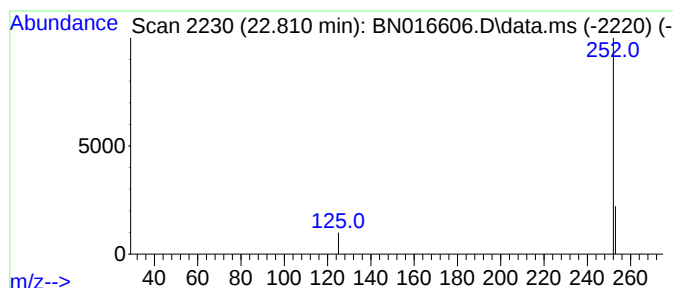
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzo[b]fluoranthene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.810	0.07 ng	27431	Perylene-d12	23.485

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
2			Gama-carbolin-1-one, 5,7-difluor...	252	C12H10F2N2O2	062223-53-4	9
3			1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	9
4			Perylene	252	C20H12	000198-55-0	9
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	9



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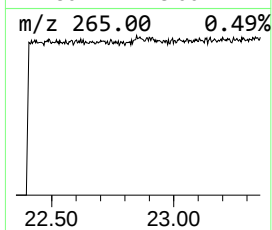
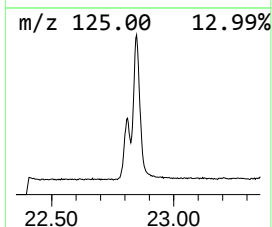
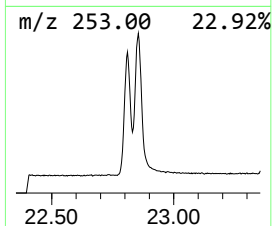
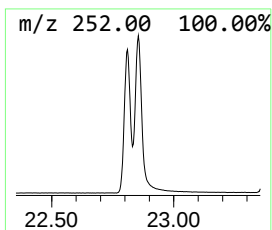
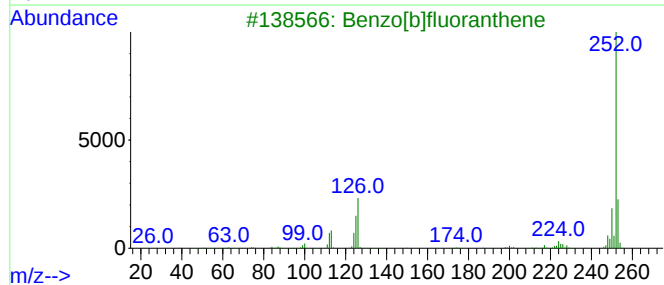
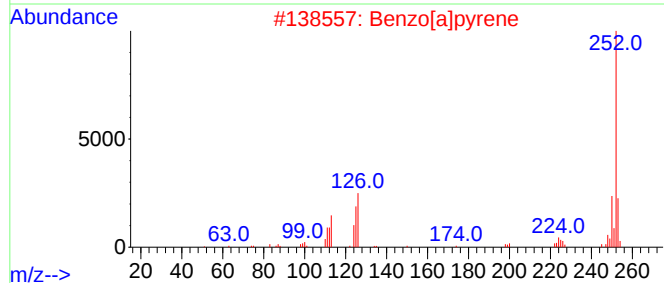
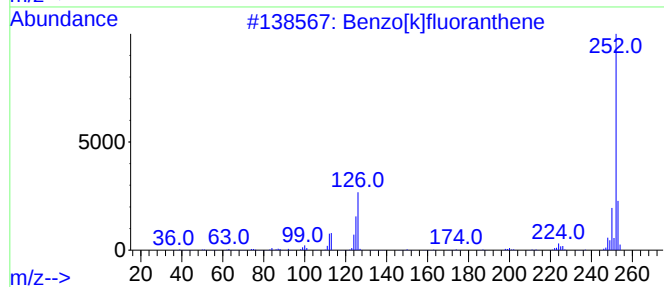
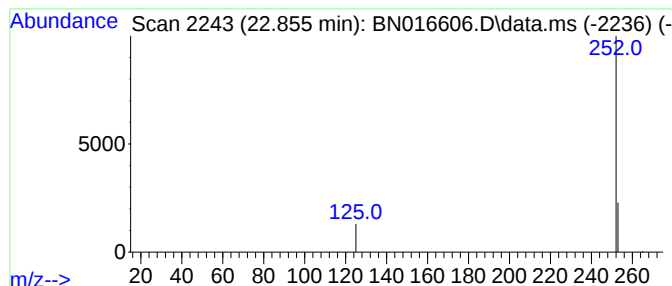
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzo[k]fluoranthene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.855	0.09 ng	35399	Perylene-d12	23.485

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[k]fluoranthene	252	C20H12	000207-08-9	9
2			Benzo[a]pyrene	252	C20H12	000050-32-8	9
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	9
4			Perylene	252	C20H12	000198-55-0	9
5			1-Amino-4-(phenylthio)isoquinoline	252	C15H12N2S	019653-19-1	9



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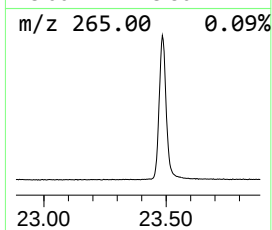
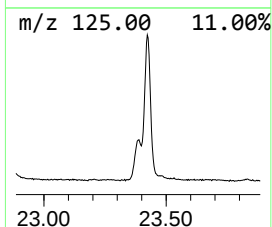
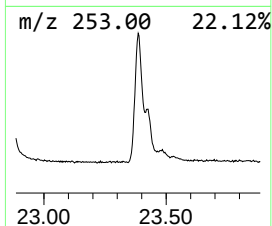
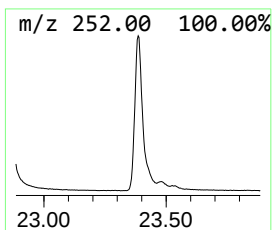
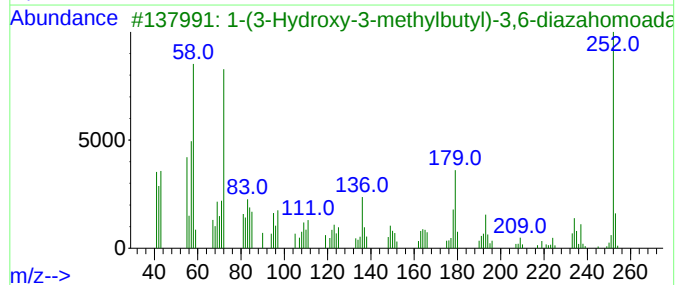
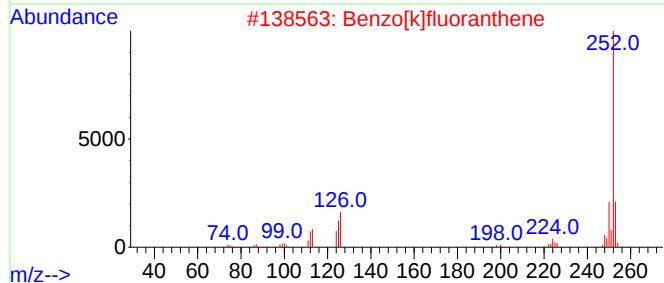
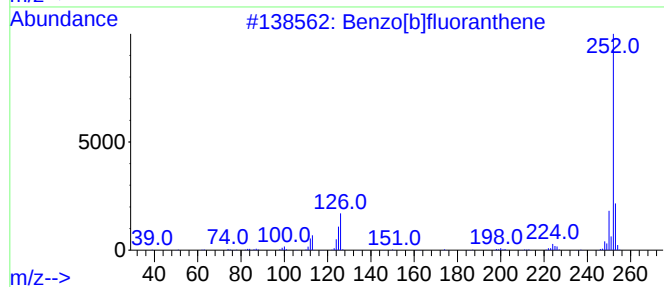
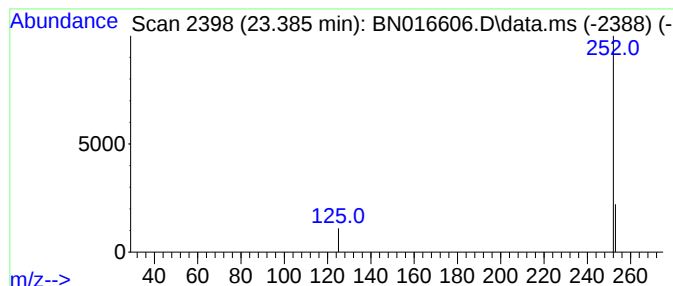
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzo[b]fluoranthene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.385	0.05 ng	21670	Perylene-d12	23.485

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			1-(3-Hydroxy-3-methylbutyl)-3,6-...	252	C14H24N2O2	1000216-02-0	9
4			Benzo[j]fluoranthene	252	C20H12	000205-82-3	9
5			Perylene	252	C20H12	000198-55-0	9



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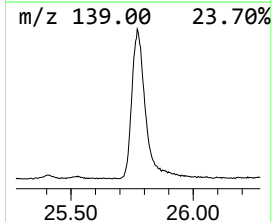
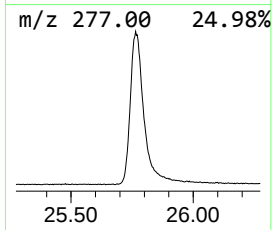
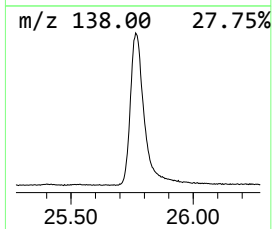
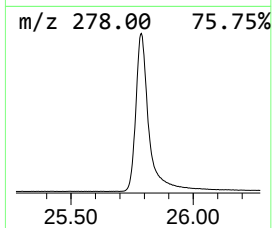
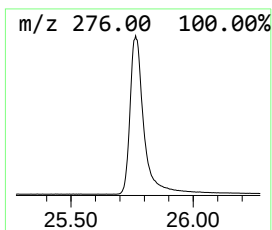
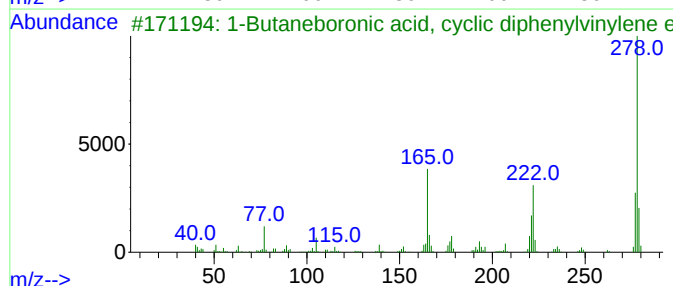
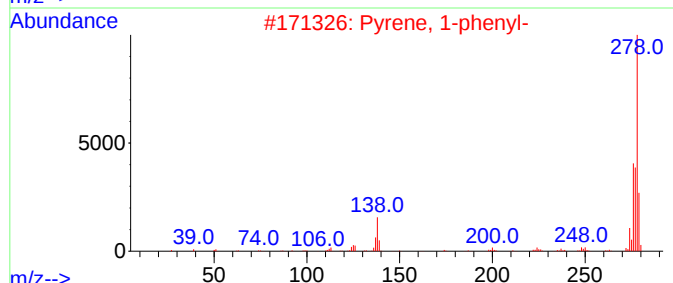
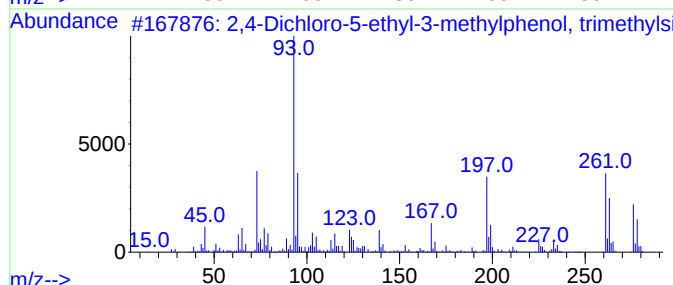
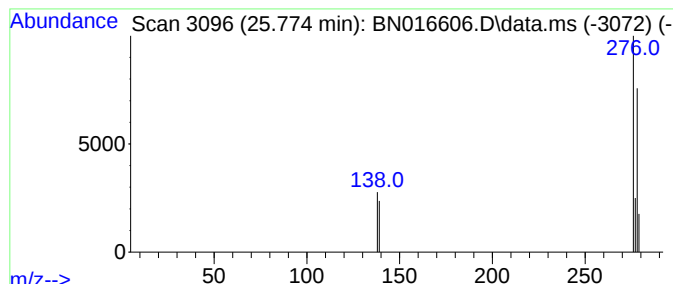
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2,4-Dichloro-5-ethyl-3-meth... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.774	0.17 ng	68996	Perylene-d12	23.485

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4-Dichloro-5-ethyl-3-methylphe...	276	C12H18Cl2OSi	1010467-47-9	83
2		Pyrene, 1-phenyl-	278	C22H14	005101-27-9	43
3		1-Butaneboronic acid, cyclic dip...	278	C18H19B02	024371-99-1	38
4		Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	37
5		Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	37



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016606.D
Acq On : 30 Sep 2021 19:09
Operator : CG/JU
Sample : PB139306BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139306BL

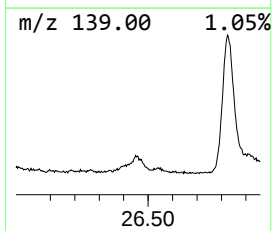
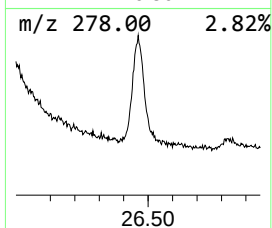
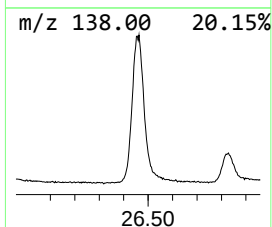
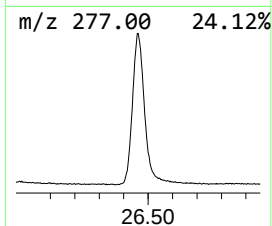
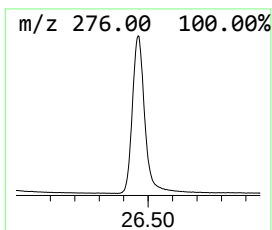
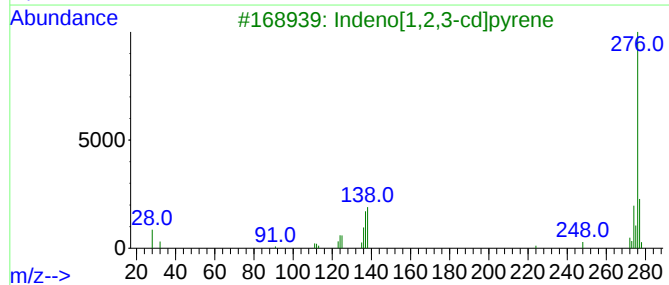
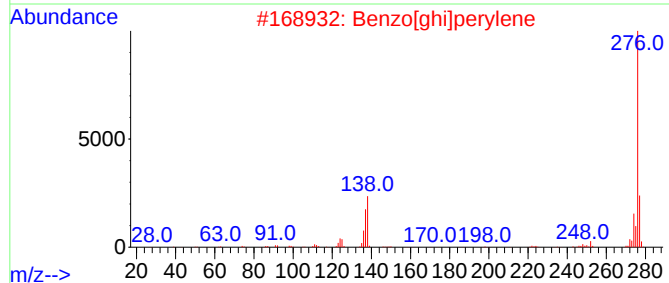
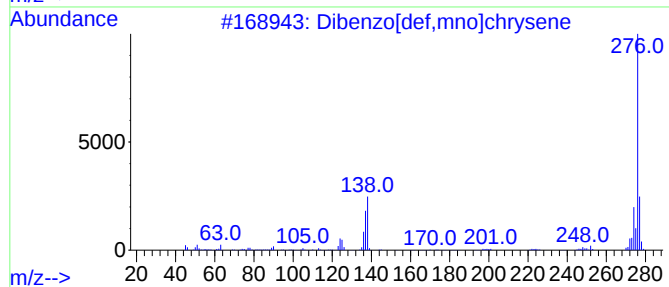
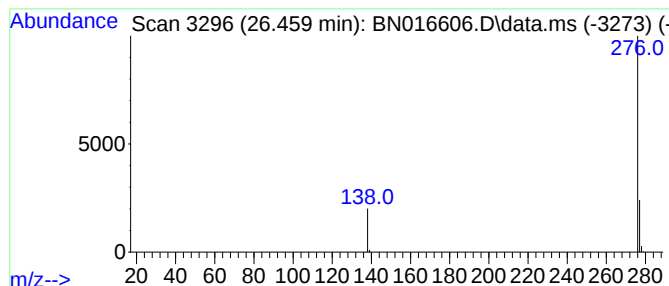
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Dibenzo[def,mno]chrysene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.459	0.07 ng	29252	Perylene-d12	23.485

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	83
2			Benzo[ghi]perylene	276	C22H12	000191-24-2	83
3			Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	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 : BN016606.D
Acq On : 30 Sep 2021 19:09
Operator : CG/JU
Sample : PB139306BL
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139306BL

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	4.249	0.0	ng	9729	1	7.642	89240	0.4
Acetone	4.830	0.5	ng	109394	1	7.642	89240	0.4
Benzo[b]fluoran...	22.810	0.1	ng	27431	6	23.485	162666	0.4
Benzo[k]fluoran...	22.855	0.1	ng	35399	6	23.485	162666	0.4
Benzo[b]fluoran...	23.385	0.1	ng	21670	6	23.485	162666	0.4
2,4-Dichloro-5-...	25.774	0.2	ng	68996	6	23.485	162666	0.4
Dibenzo[def,mno...	26.459	0.1	ng	29252	6	23.485	162666	0.4