

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016680.D
 Acq On : 02 Oct 2021 20:45
 Operator : CG/JU
 Sample : M3829-20
 Misc :
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 MW203D2-20210918

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: BN016680.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.253	16	19	28	rBV	12067	33612	17.69%	1.370%
2	3.364	28	31	47	rVB	40594	132388	69.66%	5.394%
3	3.816	76	80	96	rVB	11170	46449	24.44%	1.893%
4	4.821	185	189	206	rVB	44527	105182	55.35%	4.286%
5	5.273	234	238	245	rVB	6586	17391	9.15%	0.709%
6	5.678	279	282	297	rVB2	2097	8320	4.38%	0.339%
7	6.296	346	349	355	rVB	3696	8109	4.27%	0.330%
8	6.647	383	387	397	rVB	4205	10494	5.52%	0.428%
9	6.822	403	406	420	rVB2	4835	14216	7.48%	0.579%
10	7.264	450	454	460	rBV2	7473	17084	8.99%	0.696%
11	7.633	490	494	500	rVB	47910	99835	52.53%	4.068%
12	7.864	515	519	525	rBV	9966	20341	10.70%	0.829%
13	8.168	549	552	560	rVV	5904	17733	9.33%	0.723%
14	8.306	564	567	569	rVB	9472	11849	6.23%	0.483%
15	8.784	601	605	610	rBV	23900	48506	25.52%	1.976%
16	10.191	713	716	729	rBV	91076	157769	83.02%	6.428%
17	10.407	729	733	739	rVB	101911	177501	93.40%	7.232%
18	12.003	918	931	943	rBV	46786	74950	39.44%	3.054%
19	12.886	1071	1074	1078	rBV	93849	154055	81.06%	6.277%
20	13.178	1094	1097	1100	rBV	77562	120132	63.21%	4.895%
21	13.812	1144	1147	1155	rBV	2923	6612	3.48%	0.269%
22	14.269	1180	1183	1186	rBV	129827	188691	99.29%	7.688%
23	14.434	1193	1196	1201	rBV	3075	7594	4.00%	0.309%
24	15.715	1294	1297	1299	rBV	5732	8506	4.48%	0.347%
25	15.766	1299	1301	1305	rVB2	9885	16015	8.43%	0.653%
26	17.018	1400	1403	1406	rBV	100415	152569	80.28%	6.216%
27	19.063	1687	1696	1720	rBV	128734	182854	96.22%	7.450%
28	19.673	1813	1819	1841	rBV	113468	144369	75.97%	5.882%
29	21.164	1992	1995	1998	rBV	21414	25808	13.58%	1.052%
30	21.227	1998	2001	2009	rVV	126274	183383	96.49%	7.472%
31	22.321	2100	2104	2108	rBV	3120	5988	3.15%	0.244%
32	22.837	2231	2238	2258	rVB	4738	7482	3.94%	0.305%
33	23.419	2399	2408	2415	rBV	7402	12408	6.53%	0.506%
34	23.481	2415	2426	2462	rVB	91547	190046	100.00%	7.744%
35	24.083	2592	2602	2622	rBV	7646	15296	8.05%	0.623%
36	24.850	2816	2826	2851	rVB2	6741	16087	8.46%	0.655%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	25.757	3073	3091	3114	rBV	2141	6207	3.27%	0.253%
38	26.815	3382	3400	3419	rBV	1569	5347	2.81%	0.218%
39	28.078	3750	3769	3794	rBV	785	3084	1.62%	0.126%

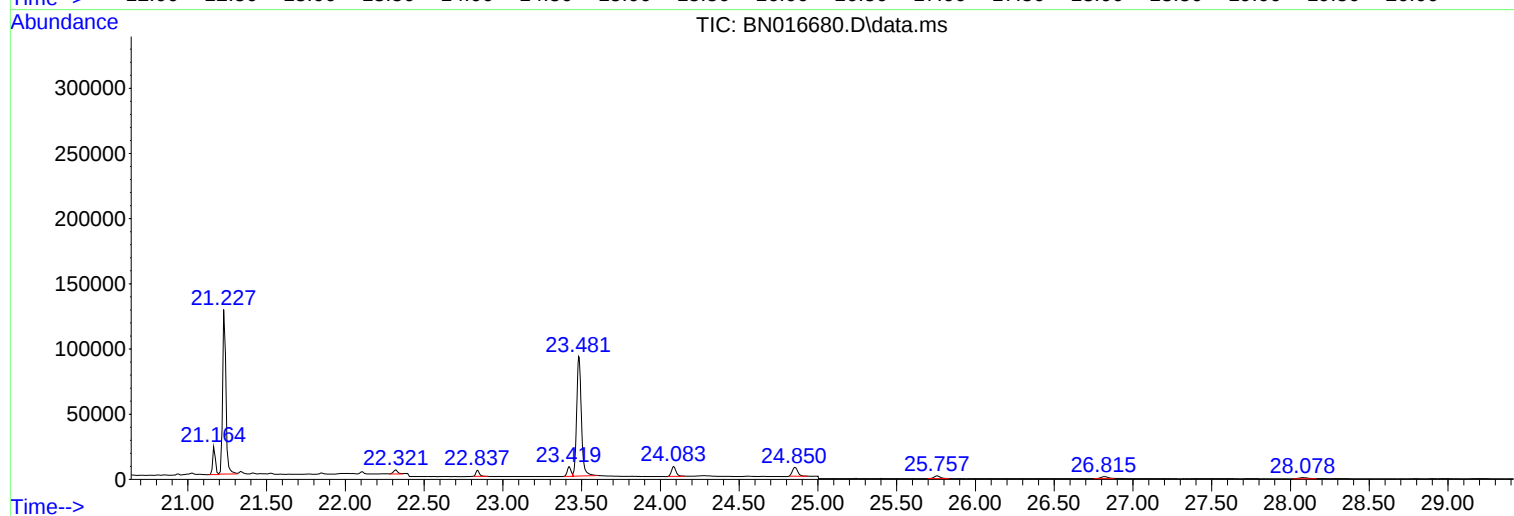
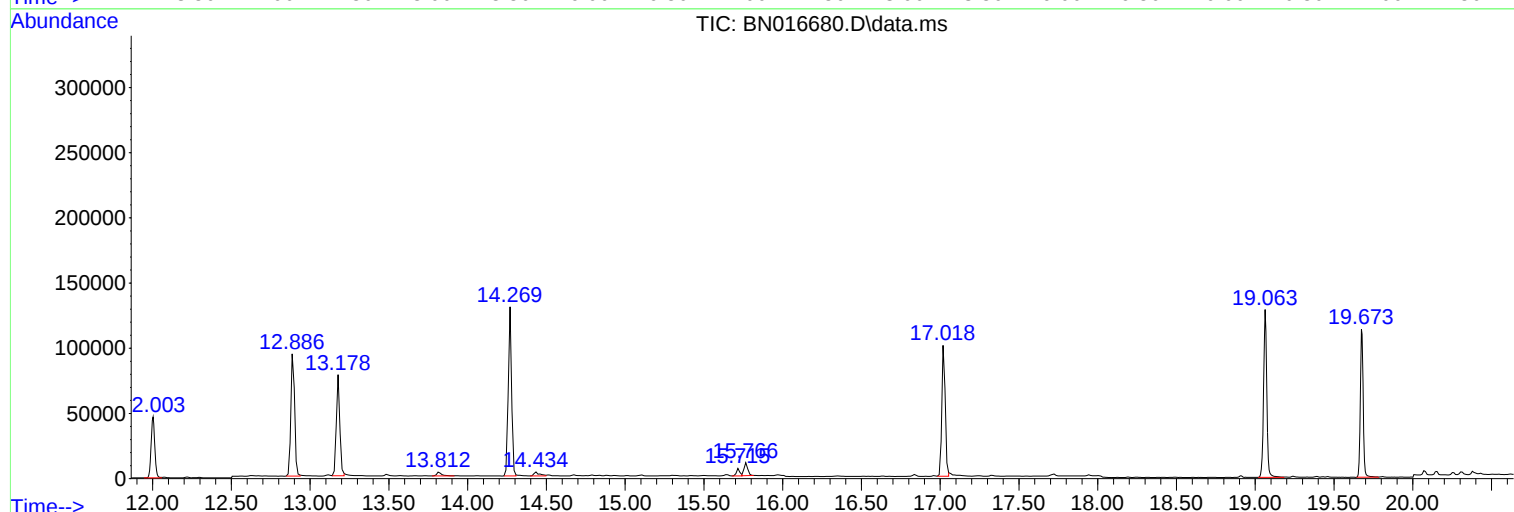
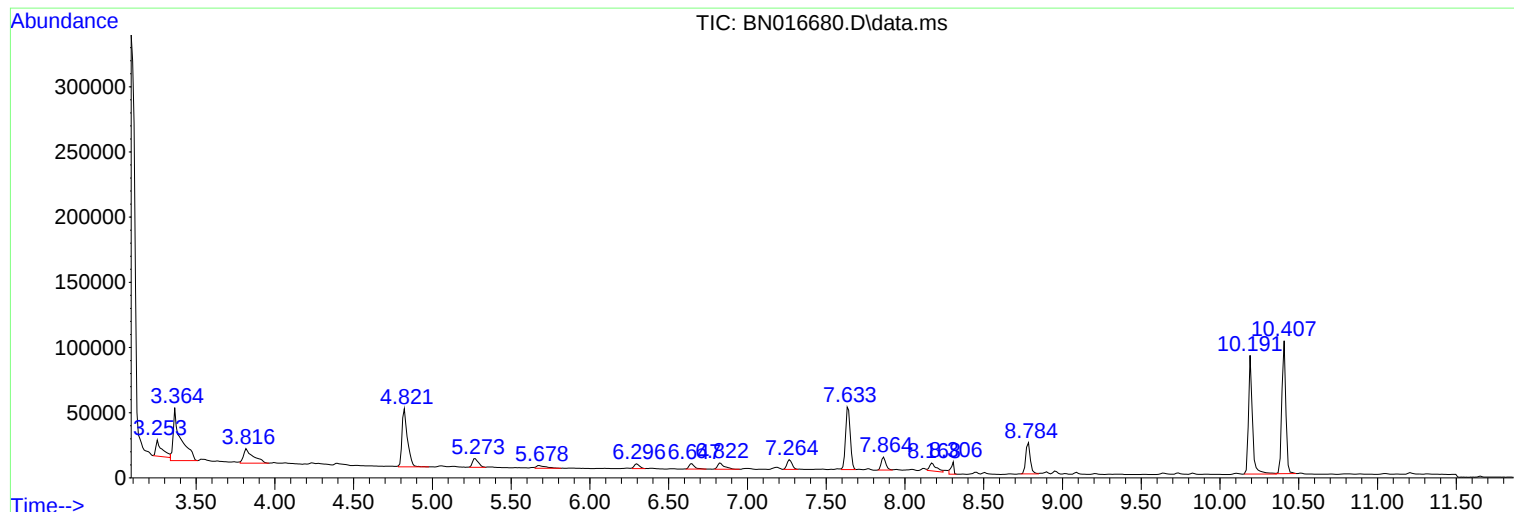
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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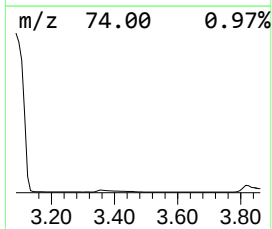
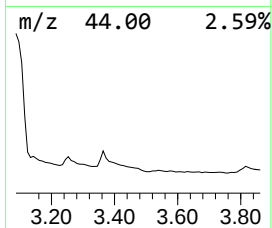
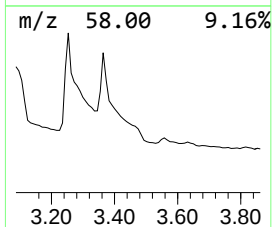
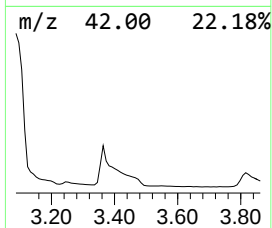
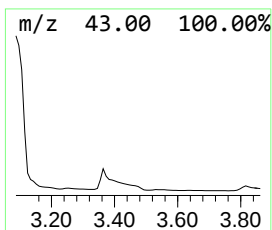
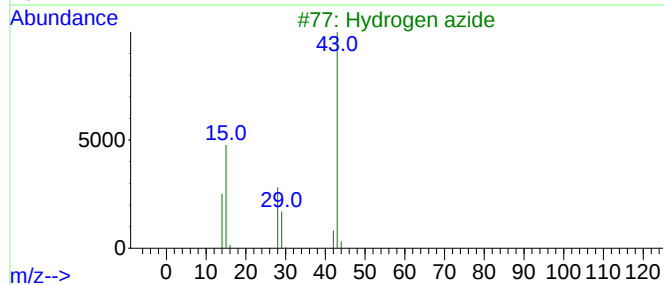
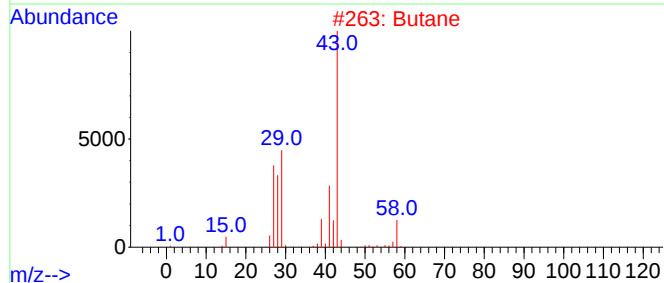
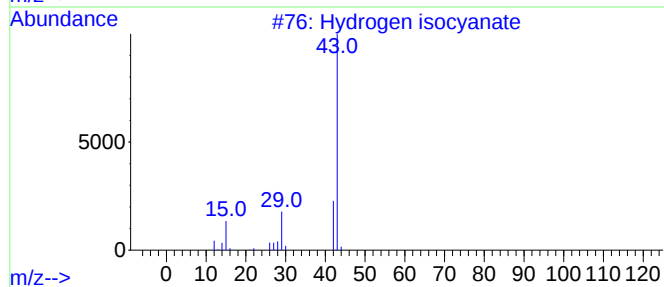
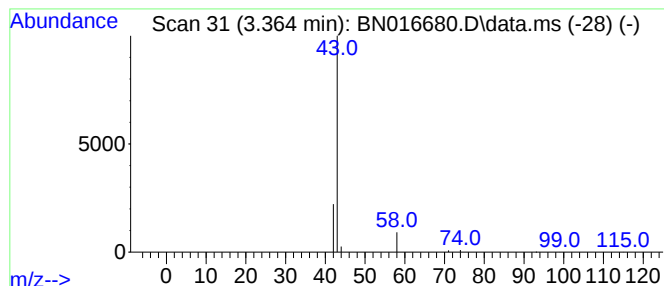
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hydrogen isocyanate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.53 ng	132388	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrogen isocyanate	43	CHNO	000075-13-8	4
2			Butane	58	C4H10	000106-97-8	4
3			Hydrogen azide	43	HN3	007782-79-8	2
4			1-Tetrazol-2-ylethanone	112	C3H4N4O	051410-11-8	2
5			O-Methylisourea	74	C2H6N2O	002440-60-0	2



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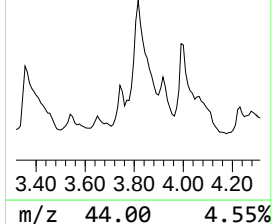
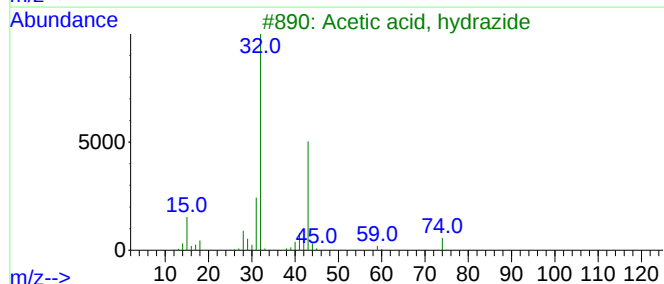
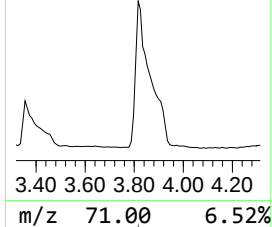
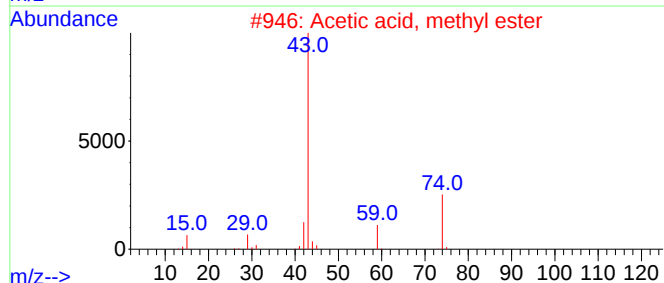
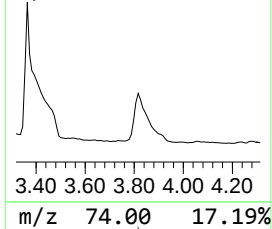
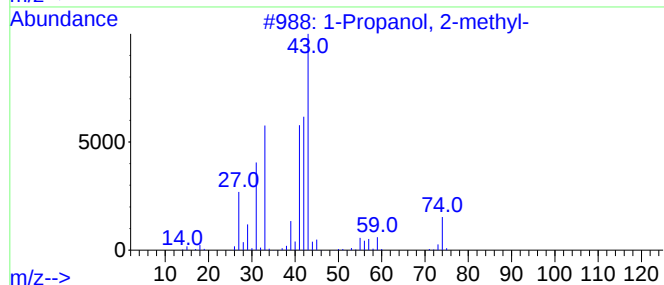
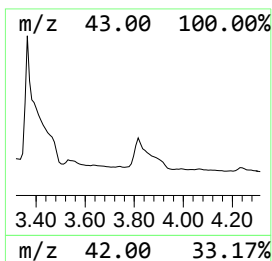
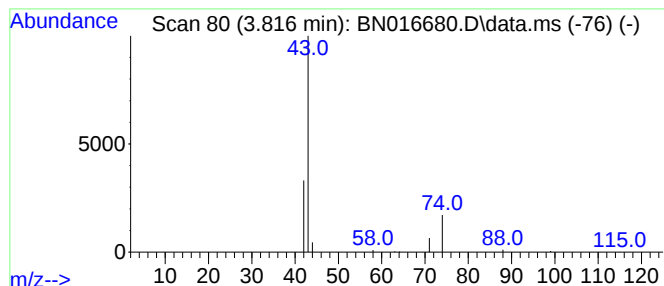
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.19 ng	46449	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	5
2		Acetic acid, methyl ester	74	C3H6O2	000079-20-9	5
3		Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	4
4		2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
5		1,4-Butanediamine	88	C4H12N2	000110-60-1	4



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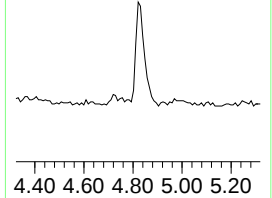
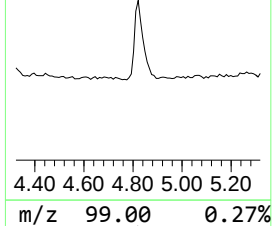
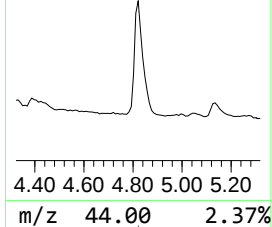
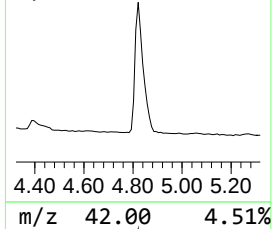
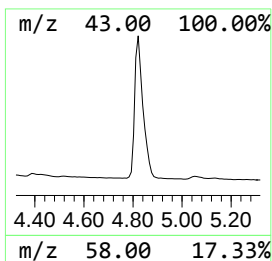
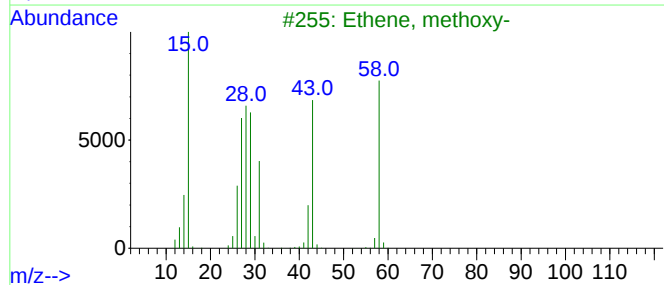
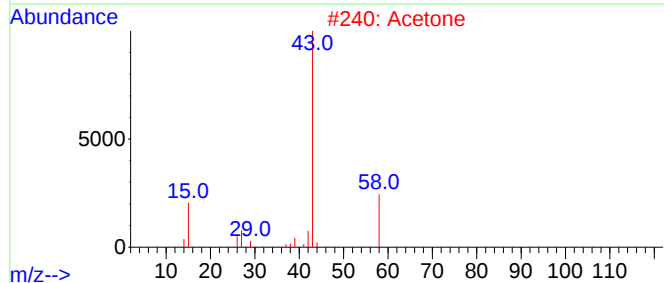
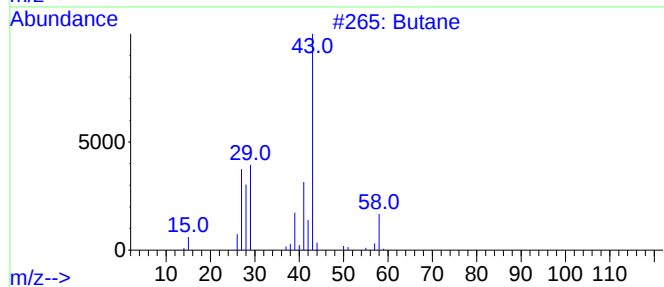
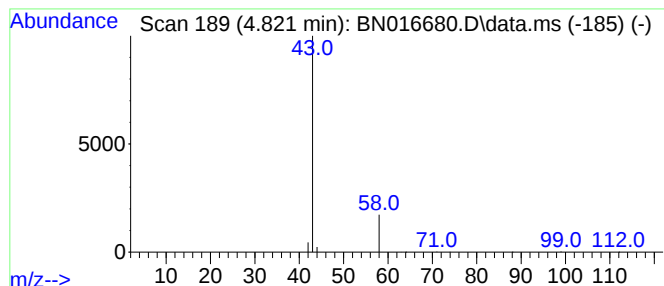
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.42 ng	105182	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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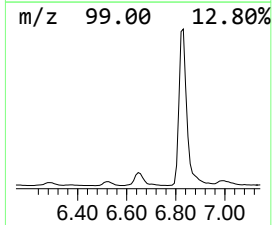
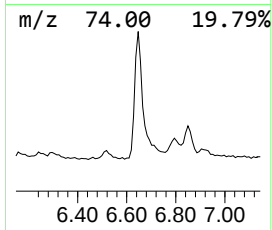
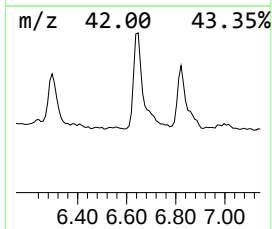
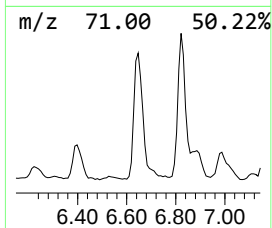
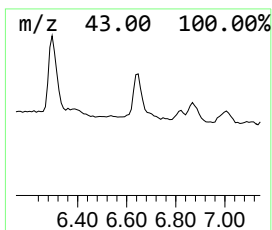
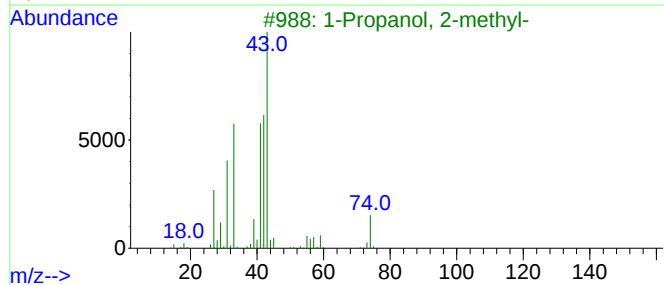
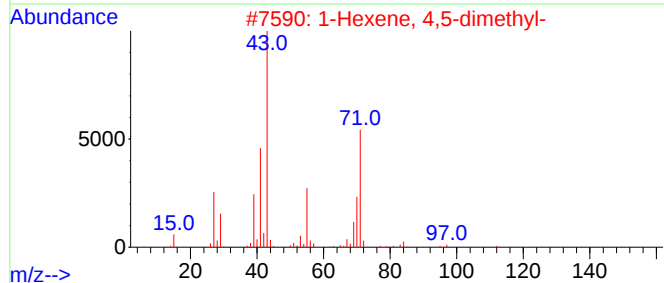
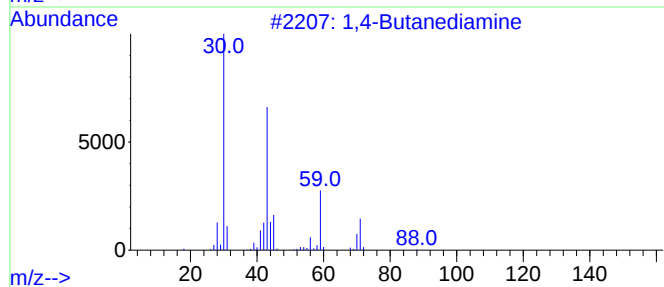
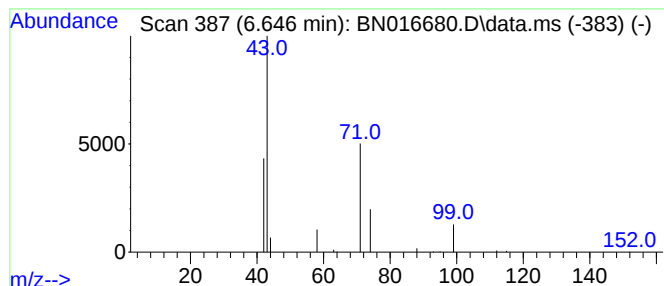
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,4-Butanediamine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.646	0.04 ng	10494	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Butanediamine	88	C4H12N2	000110-60-1	5
2			1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	5
3			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	4
4			Isobutane	58	C4H10	000075-28-5	4
5			Cyacetacide	99	C3H5N3O	000140-87-4	4



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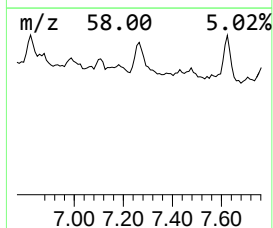
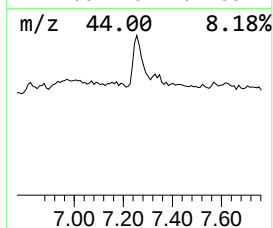
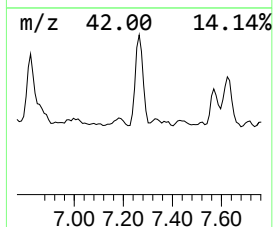
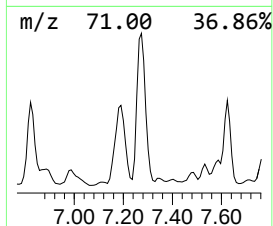
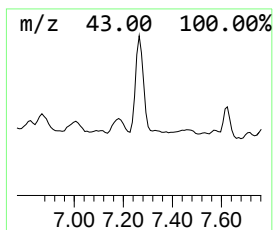
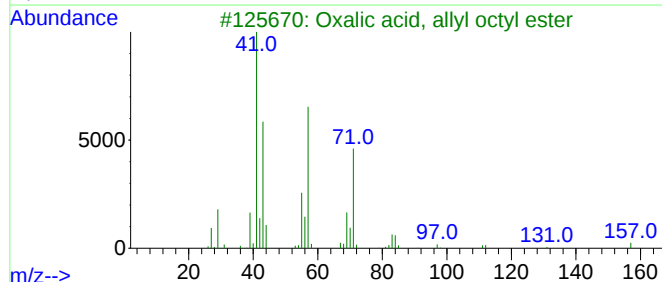
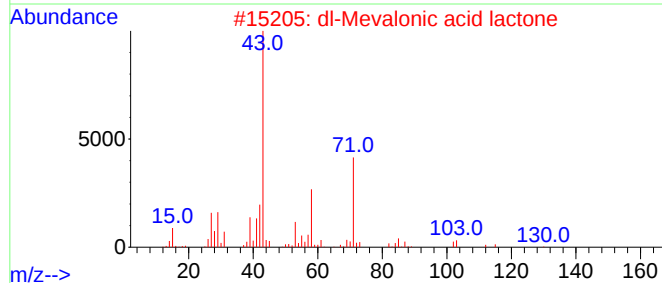
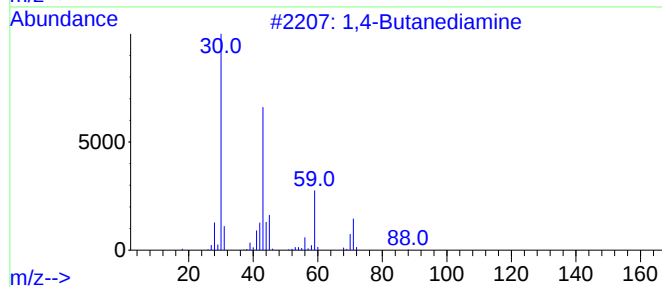
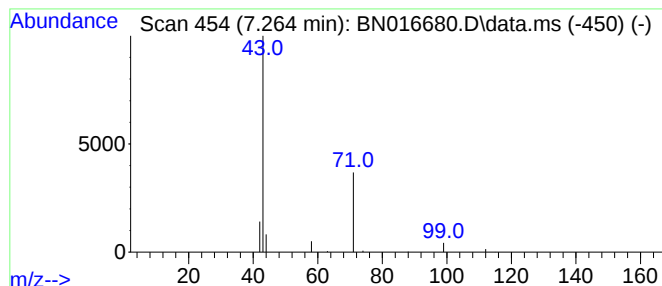
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1,4-Butanediamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.07 ng	17084	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Butanediamine	88	C4H12N2	000110-60-1	4
2			dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
3			Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4
4			Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	001487-49-6	4
5			1-Butanol	74	C4H10O	000071-36-3	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016680.D
Acq On : 02 Oct 2021 20:45
Operator : CG/JU
Sample : M3829-20
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D2-20210918

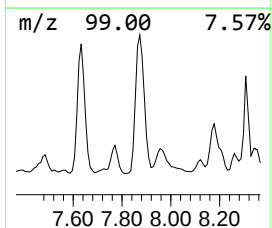
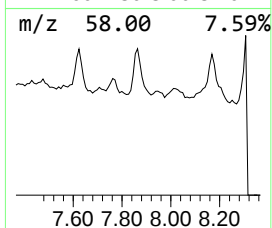
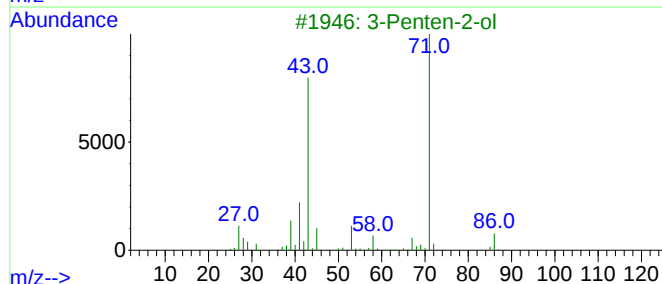
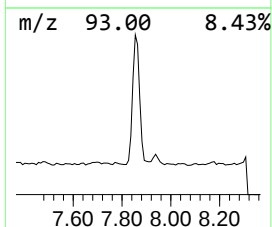
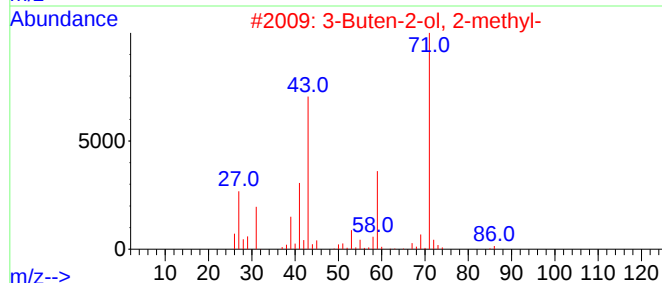
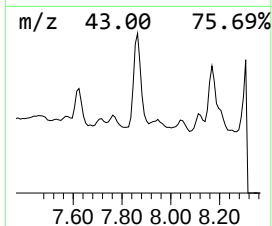
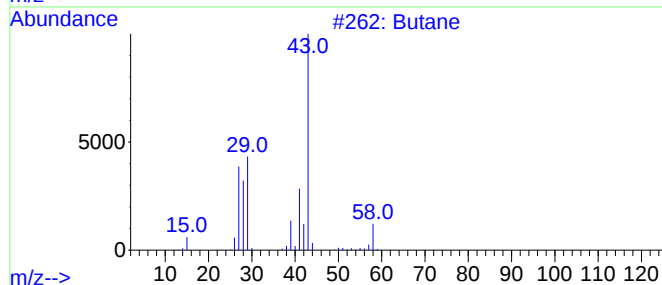
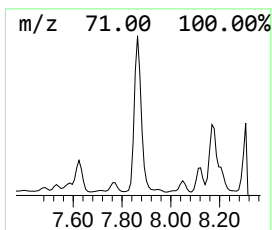
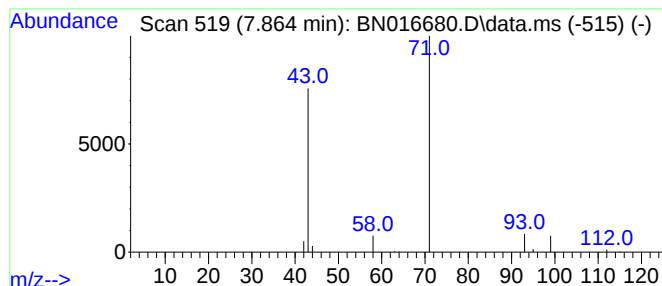
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.08 ng	20341	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane	58	C4H10	000106-97-8	4
2		3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
3		3-Penten-2-ol	86	C5H10O	001569-50-2	4
4		Hydrogen azide	43	HN3	007782-79-8	4
5		Methallyl butyrate	142	C8H14O2	1000428-83-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016680.D
Acq On : 02 Oct 2021 20:45
Operator : CG/JU
Sample : M3829-20
Misc :
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Instrument :
BNA_N
ClientSampleId :
MW203D2-20210918

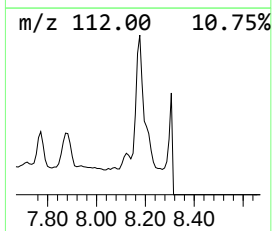
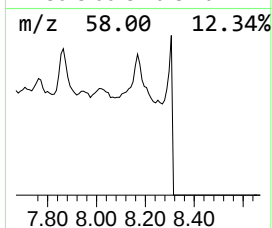
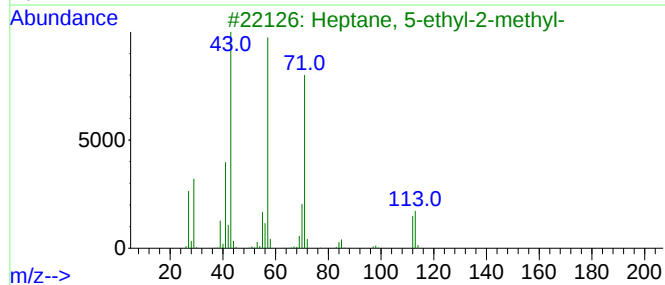
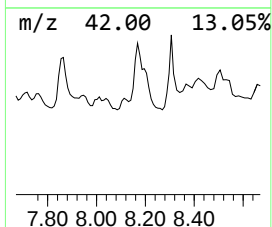
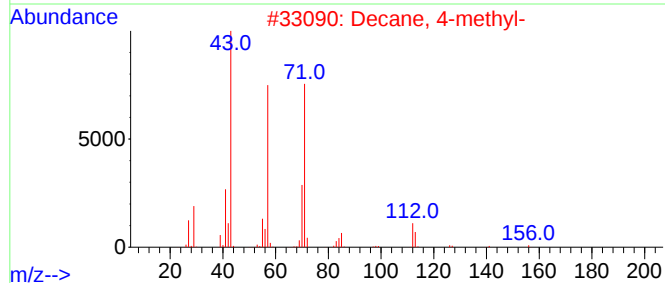
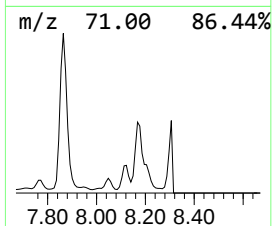
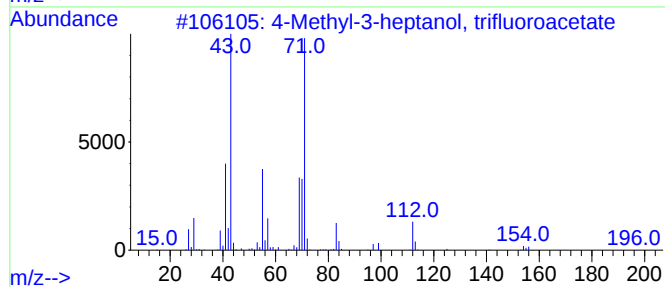
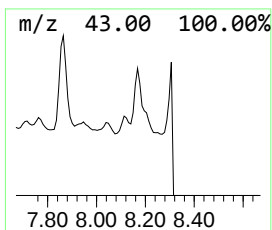
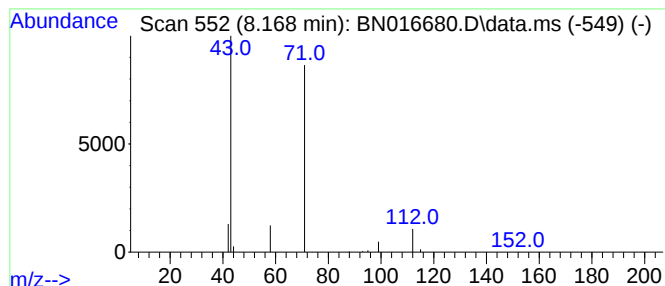
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4-Methyl-3-heptanol, triflu... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.07 ng	17733	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	43
2			Decane, 4-methyl-	156	C11H24	002847-72-5	9
3			Heptane, 5-ethyl-2-methyl-	142	C10H22	013475-78-0	9
4			Octane, 3-ethyl-	142	C10H22	005881-17-4	9
5			Butane	58	C4H10	000106-97-8	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016680.D
Acq On : 02 Oct 2021 20:45
Operator : CG/JU
Sample : M3829-20
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW203D2-20210918

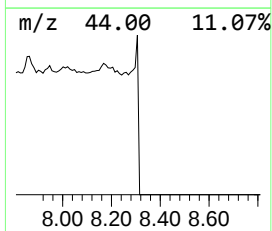
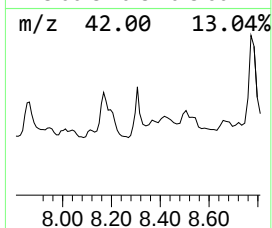
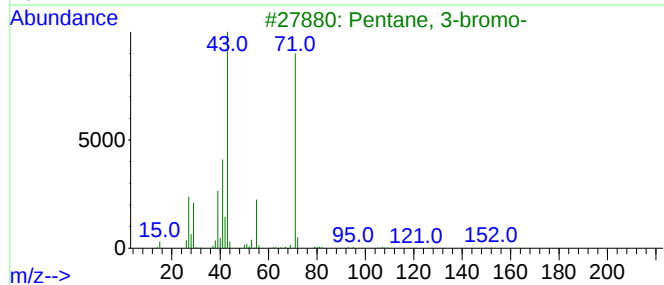
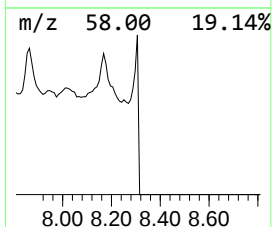
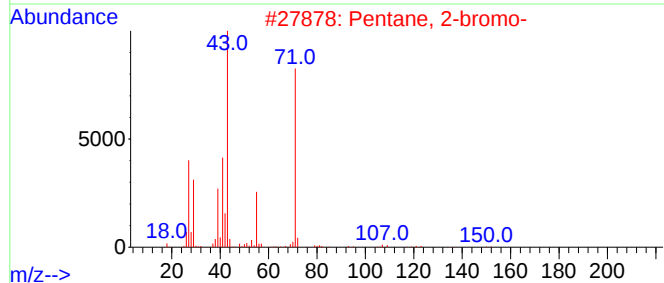
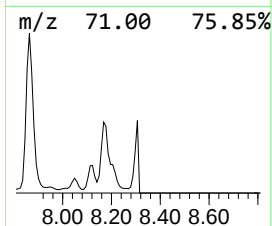
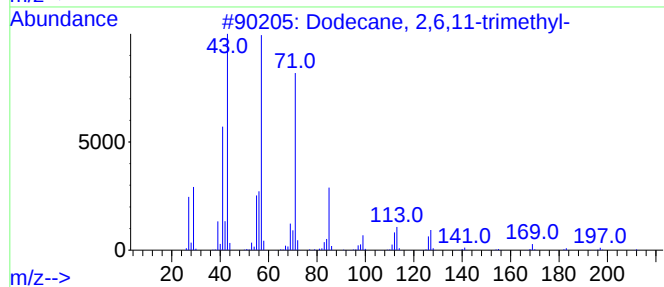
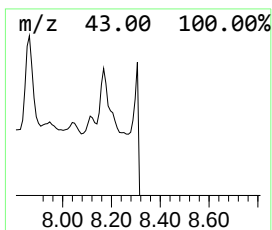
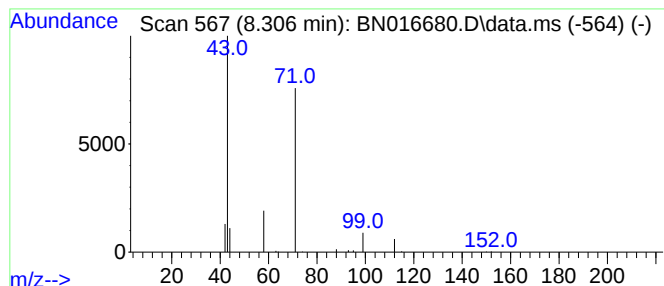
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Dodecane, 2,6,11-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.05 ng	11849	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	38
2			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	9
3			Pentane, 3-bromo-	150	C5H11Br	001809-10-5	9
4			Carbamic acid, methylnitroso-, e...	132	C4H8N2O3	000615-53-2	9
5			Acetone	58	C3H6O	000067-64-1	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016680.D
Acq On : 02 Oct 2021 20:45
Operator : CG/JU
Sample : M3829-20
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
MW203D2-20210918

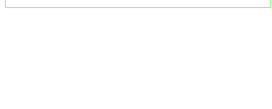
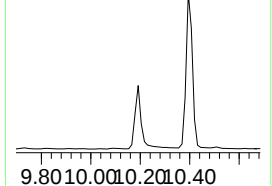
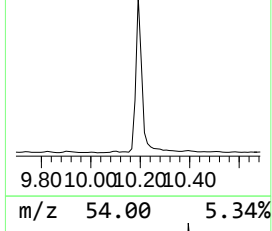
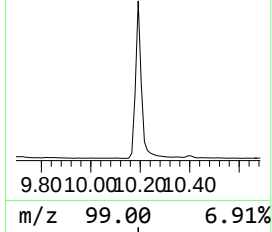
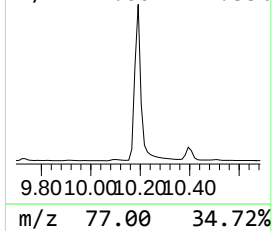
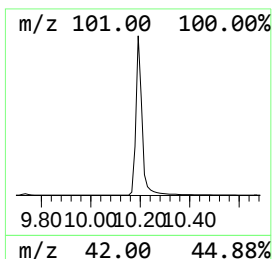
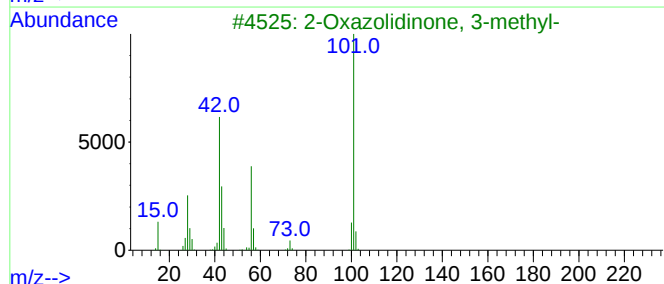
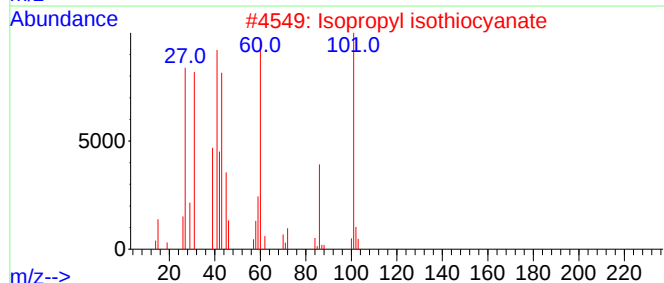
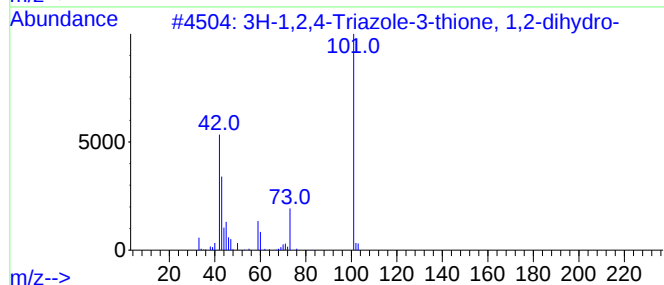
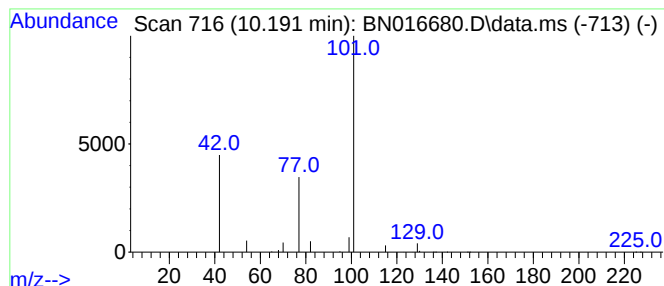
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 3H-1,2,4-Triazole-3-thione,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.36 ng	157769	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
2			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
3			2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
4			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
5			3-Aminopropionitrile	70	C3H6N2	000151-18-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016680.D
Acq On : 02 Oct 2021 20:45
Operator : CG/JU
Sample : M3829-20
Misc :
ALS Vial : 48 Sample Multiplier: 1

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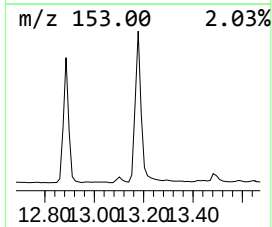
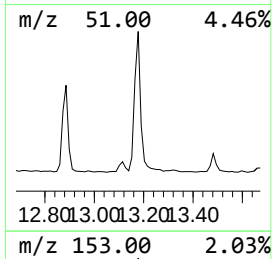
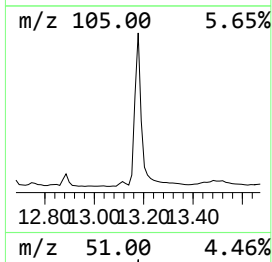
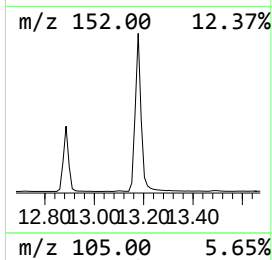
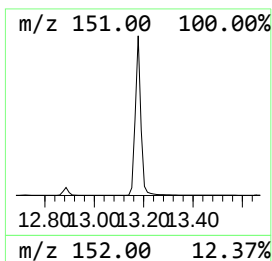
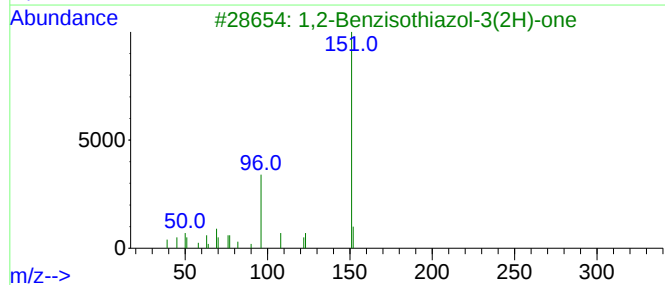
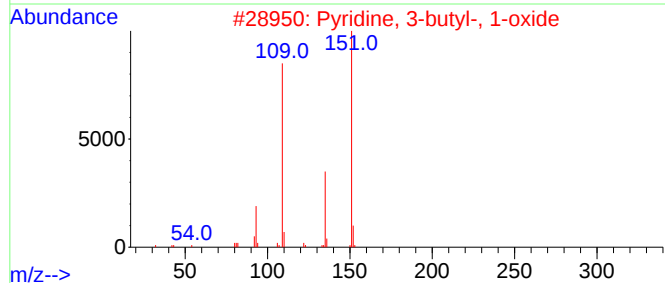
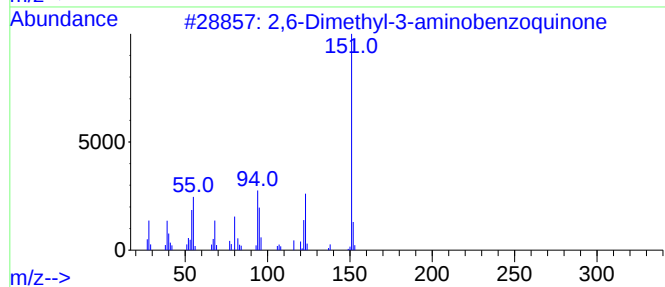
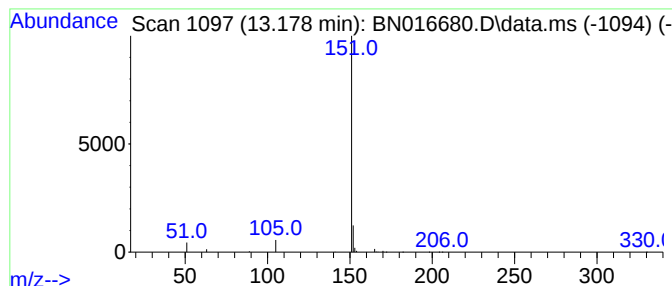
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.178	0.25 ng	120132	Acenaphthene-d10	14.269

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,6-Dimethyl-3-aminobenzoquinone	151	C8H9NO2	090005-56-4	7
2		Pyridine, 3-butyl-, 1-oxide	151	C9H13NO	031396-33-5	7
3		1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	7
4		7-Methyl-7H-pyrazolo(3,4-d)-v-tr...	151	C5H5N5O	018213-76-8	7
5		Carbamic acid, phenyl-, methyl e...	151	C8H9NO2	002603-10-3	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016680.D
Acq On : 02 Oct 2021 20:45
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Sample : M3829-20
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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
Hydrogen isocya...	3.364	0.5	ng	132388	1	7.642	99835	0.4
1-Propanol, 2-m...	3.816	0.2	ng	46449	1	7.642	99835	0.4
Butane	4.821	0.4	ng	105182	1	7.642	99835	0.4
1,4-Butanediamine	6.646	0.0	ng	10494	1	7.642	99835	0.4
1,4-Butanediamine	7.264	0.1	ng	17084	1	7.642	99835	0.4
Butane	7.864	0.1	ng	20341	1	7.642	99835	0.4
4-Methyl-3-hept...	8.168	0.1	ng	17733	1	7.642	99835	0.4
Dodecane, 2,6,1...	8.306	0.0	ng	11849	1	7.642	99835	0.4
3H-1,2,4-Triazo...	10.191	0.4	ng	157769	2	10.407	177501	0.4
2,6-Dimethyl-3-...	13.178	0.3	ng	120132	3	14.269	188691	0.4