

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016609.D
 Acq On : 30 Sep 2021 20:58
 Operator : CG/JU
 Sample : M3782-03DL 2X
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE132D2-20210914DL

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: BN016609.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	21	rBV	45997	69333	37.42%	3.974%
2	3.364	29	31	47	rVB	31761	95611	51.61%	5.480%
3	3.816	78	80	97	rVB	4469	20426	11.03%	1.171%
4	4.396	140	143	154	rVB	1959	7832	4.23%	0.449%
5	4.821	185	189	202	rVB	35126	88280	47.65%	5.060%
6	5.263	234	237	245	rVB	2986	8752	4.72%	0.502%
7	6.296	345	349	354	rBV	25601	52986	28.60%	3.037%
8	6.821	404	406	410	rBV	1514	3388	1.83%	0.194%
9	7.264	451	454	460	rBV	3358	7543	4.07%	0.432%
10	7.642	490	495	500	rBV	46522	96749	52.22%	5.545%
11	7.863	515	519	527	rVB2	3536	7741	4.18%	0.444%
12	8.177	550	553	562	rVV2	1850	9439	5.09%	0.541%
13	8.306	565	567	569	rVB	5646	5571	3.01%	0.319%
14	8.784	602	605	610	rBV	10305	20354	10.99%	1.167%
15	10.191	713	716	728	rBV	33077	60218	32.50%	3.451%
16	10.406	730	733	737	rBV	99151	173020	93.39%	9.917%
17	12.007	922	932	943	rBV	20605	33850	18.27%	1.940%
18	12.898	1071	1075	1078	rBV	38594	70219	37.90%	4.025%
19	14.268	1180	1183	1186	rBV	126345	185264	100.00%	10.619%
20	15.766	1299	1301	1305	rVB2	4280	6966	3.76%	0.399%
21	17.017	1400	1403	1407	rBV	82989	148285	80.04%	8.499%
22	19.068	1689	1697	1716	rBV	50973	74280	40.09%	4.257%
23	19.678	1813	1820	1842	rBV	51834	66530	35.91%	3.813%
24	21.025	1980	1982	1993	rVB	8076	12483	6.74%	0.715%
25	21.163	1993	1995	1998	rBV	27148	38857	20.97%	2.227%
26	21.227	1998	2001	2011	rVB	110728	177804	95.97%	10.191%
27	22.109	2081	2084	2089	rBV2	7412	9960	5.38%	0.571%
28	22.841	2235	2239	2252	rVB2	1674	2432	1.31%	0.139%
29	23.423	2403	2409	2414	rBV	1858	2547	1.37%	0.146%
30	23.484	2415	2427	2458	rVB	93111	181649	98.05%	10.411%
31	24.087	2596	2603	2615	rVB	2237	3967	2.14%	0.227%
32	25.760	3072	3092	3109	rBV	755	2382	1.29%	0.137%

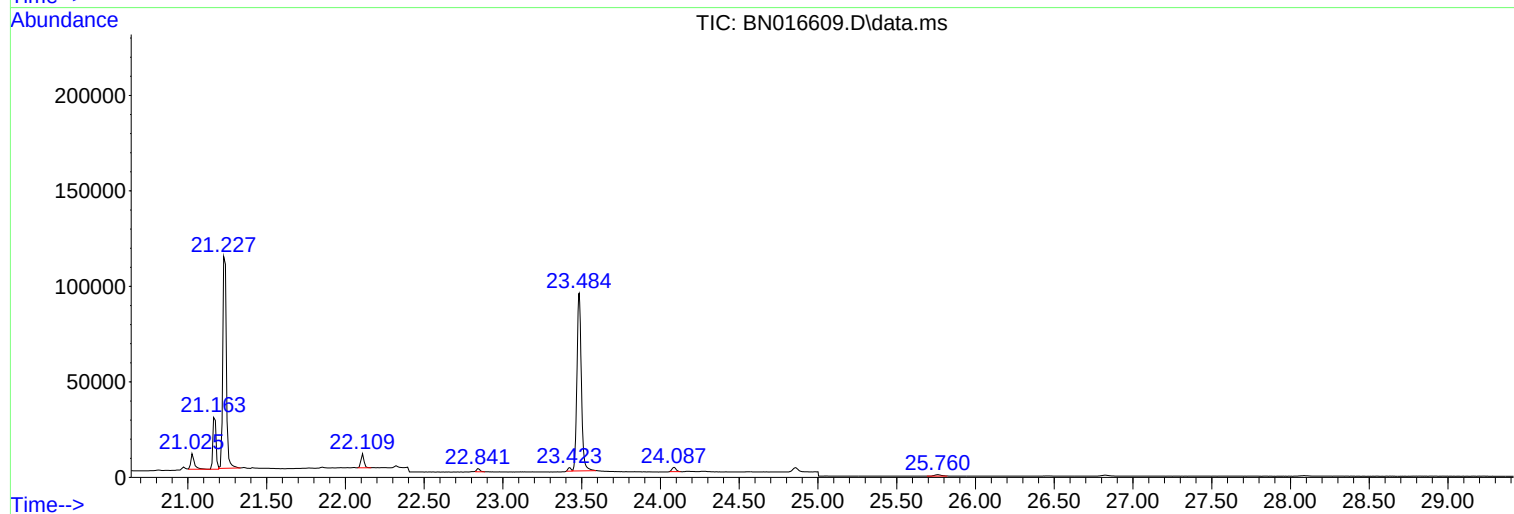
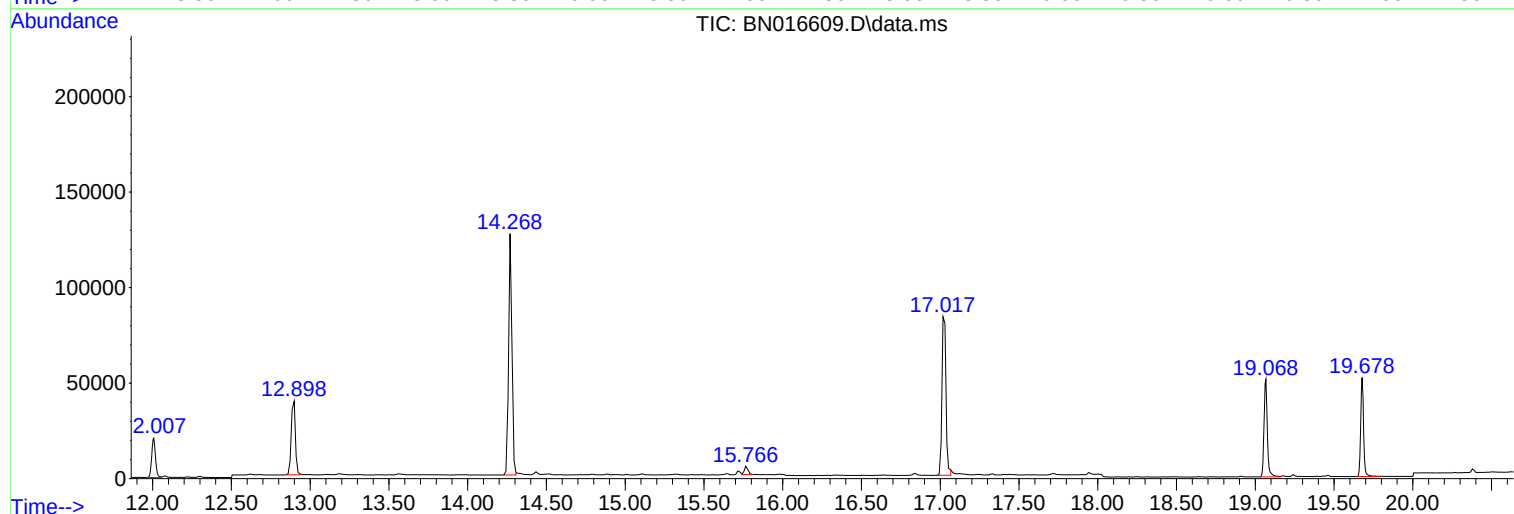
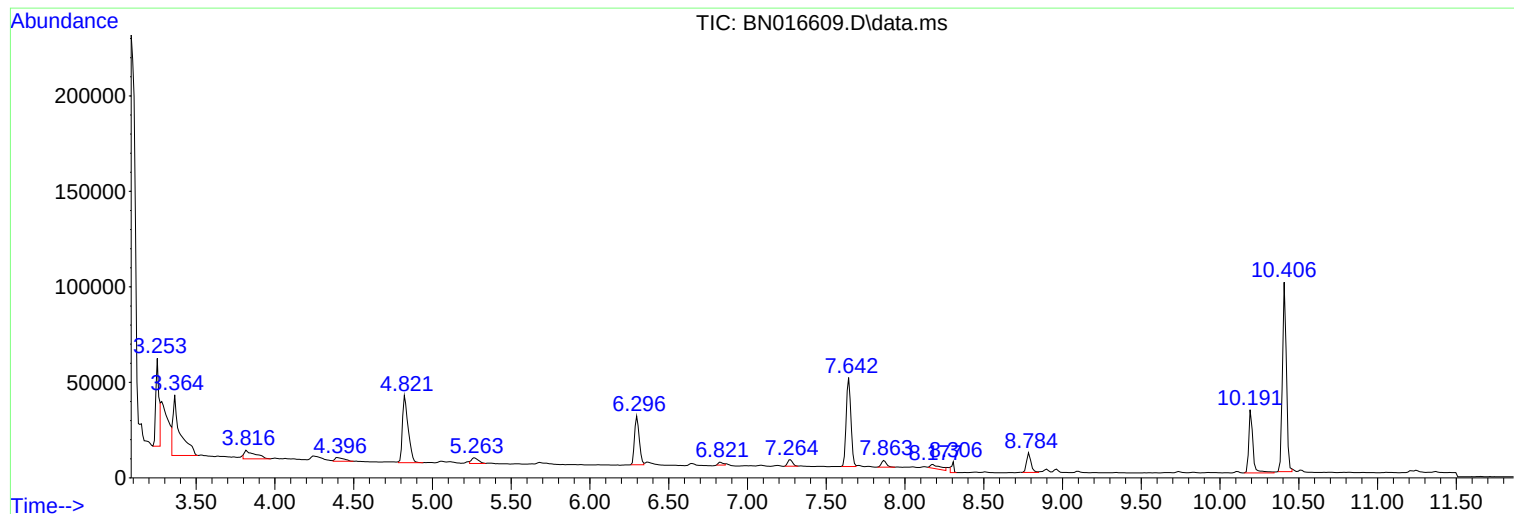
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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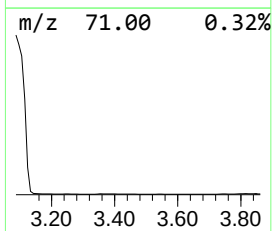
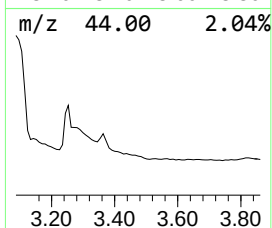
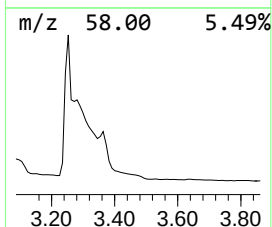
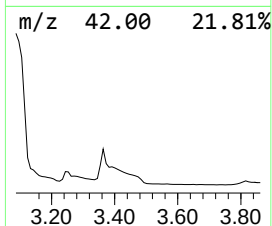
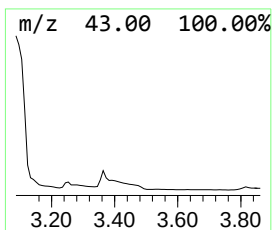
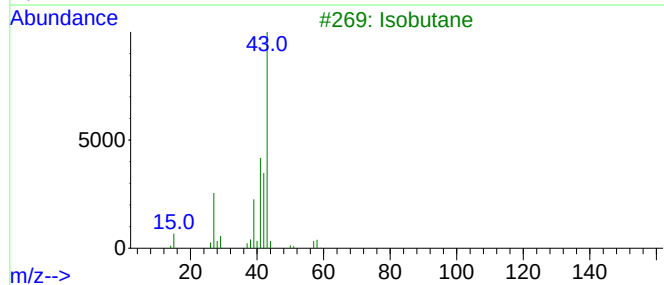
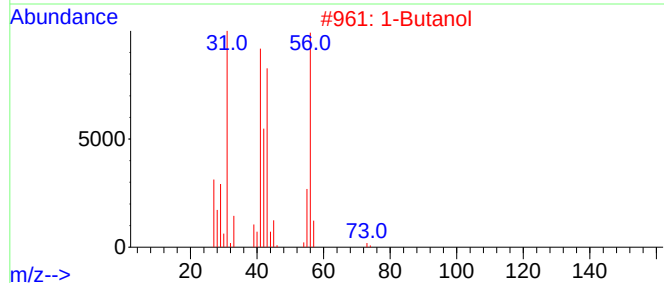
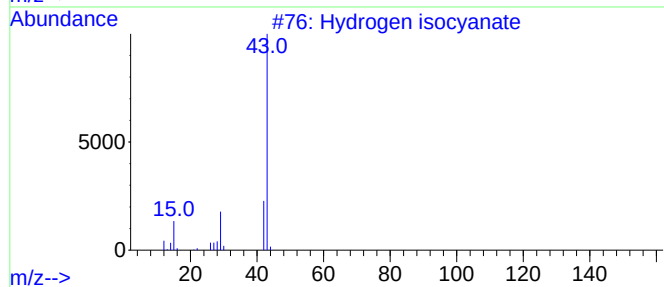
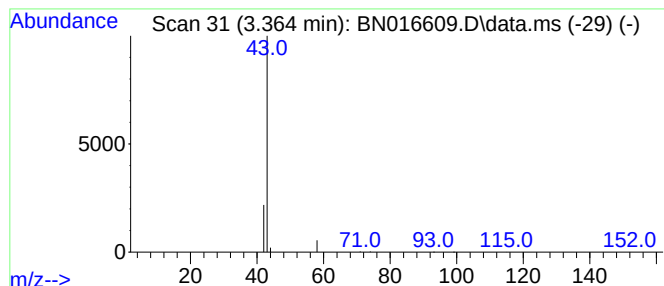
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 Hydrogen isocyanate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.364	0.40 ng	95611	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			1-Butanol	74	C4H10O	000071-36-3	3
3			Isobutane	58	C4H10	000075-28-5	3
4			Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	2
5			Methane, diazo-	42	CH2N2	000334-88-3	2



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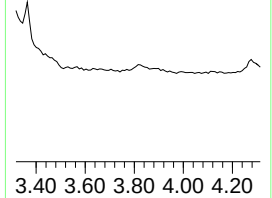
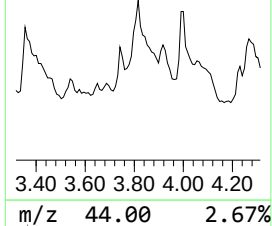
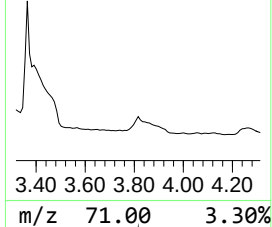
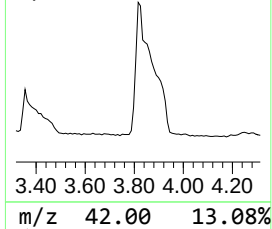
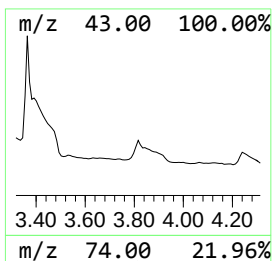
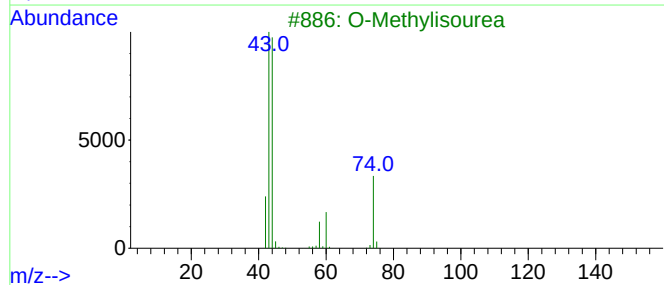
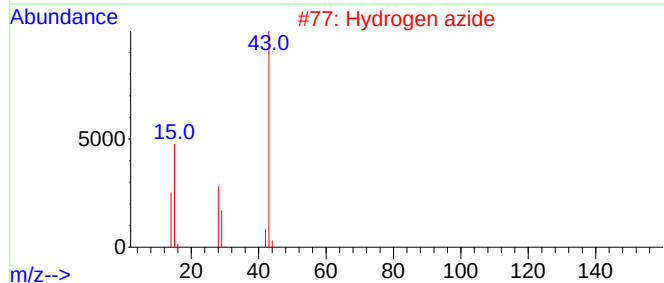
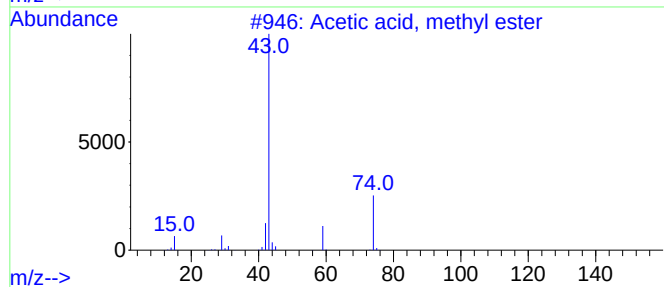
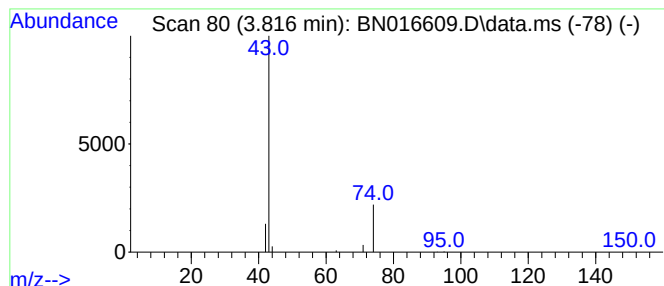
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Acetic acid, methyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.08 ng	20426	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, methyl ester	74	C3H6O2	000079-20-9	9
2			Hydrogen azide	43	HN3	007782-79-8	4
3			O-Methylisourea	74	C2H6N2O	002440-60-0	4
4			1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	3
5			Urea, methyl-	74	C2H6N2O	000598-50-5	3



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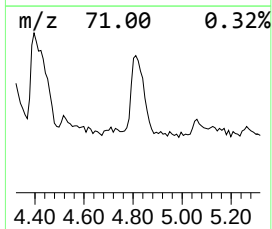
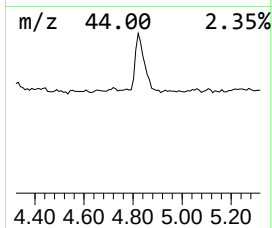
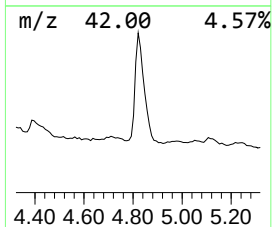
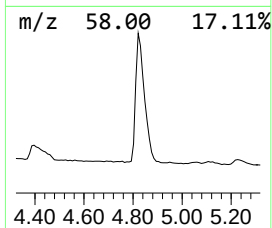
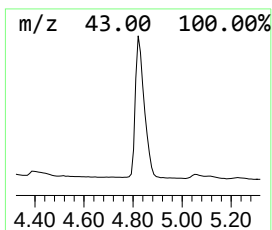
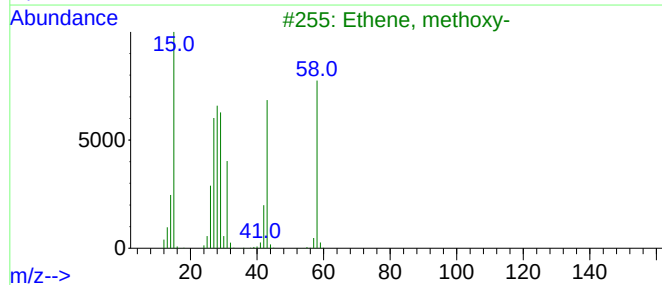
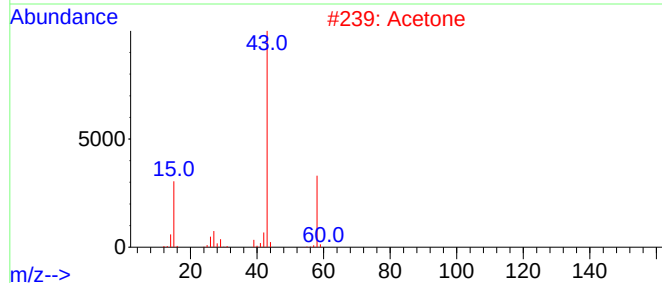
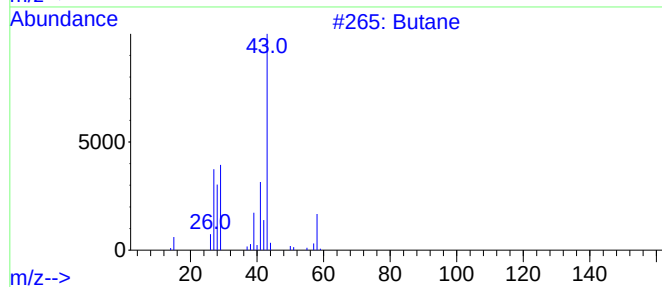
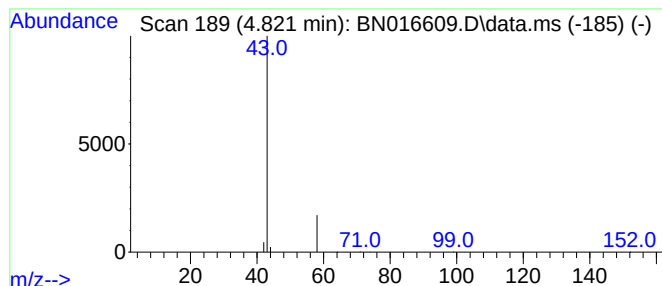
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.36 ng	88280	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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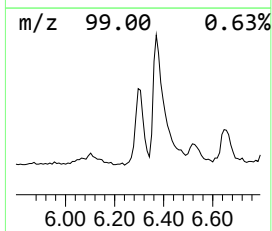
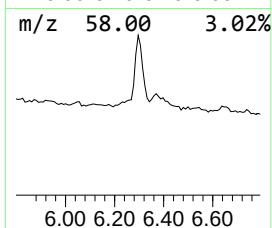
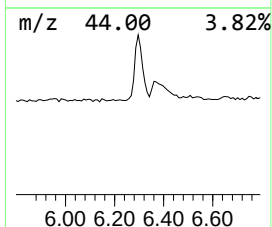
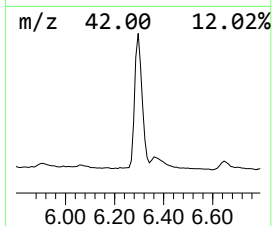
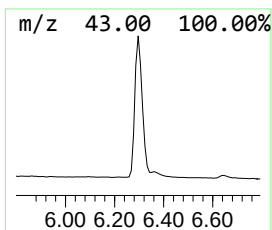
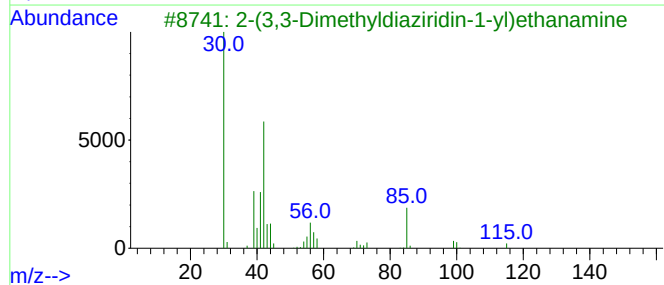
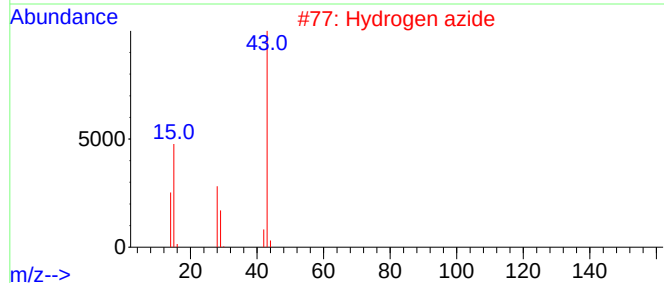
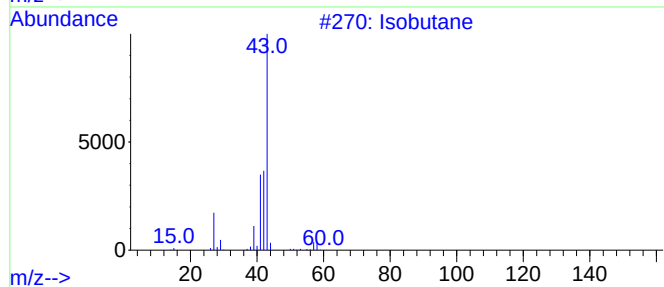
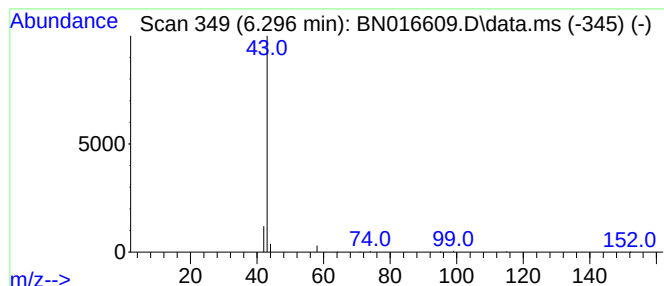
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Isobutane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.296	0.22 ng	52986	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	4
2			Hydrogen azide	43	HN3	007782-79-8	4
3			2-(3,3-Dimethyldiaziridin-1-yl)e...	115	C5H13N3	139223-40-8	2
4			2,3-Octanedione	142	C8H14O2	000585-25-1	2
5			Hydrogen isocyanate	43	CHNO	000075-13-8	2



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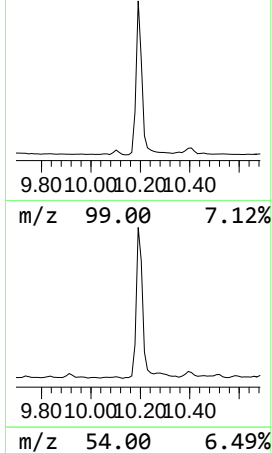
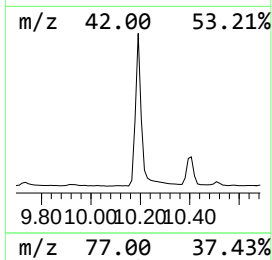
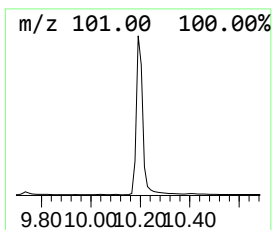
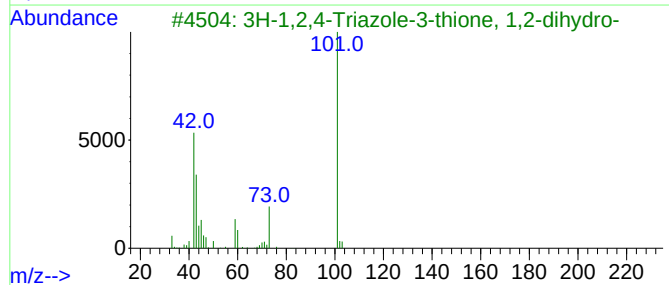
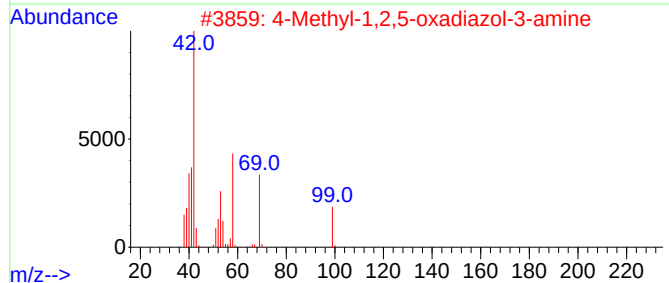
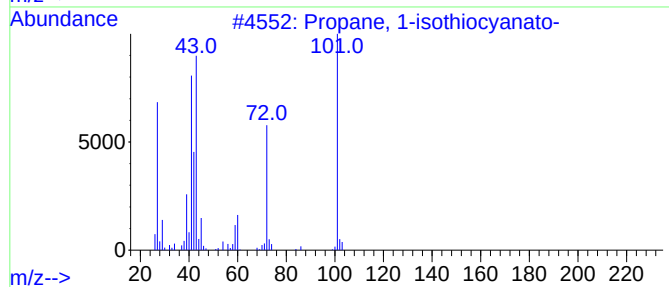
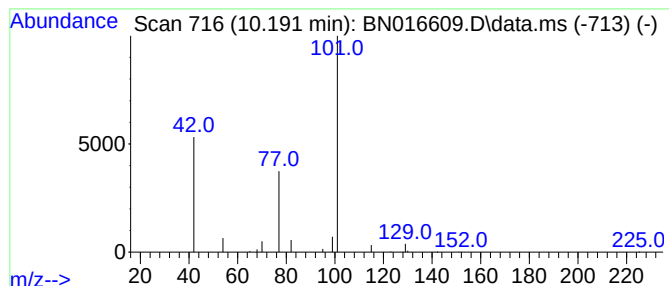
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Propane, 1-isothiocyanato- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.14 ng	60218	Naphthalene-d8	10.406

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
2			4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	5
3			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4			Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	5
5			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hydrogen isocya...	3.364	0.4	ng	95611	1	7.642	96749	0.4
Acetic acid, me...	3.816	0.1	ng	20426	1	7.642	96749	0.4
Butane	4.821	0.4	ng	88280	1	7.642	96749	0.4
Isobutane	6.296	0.2	ng	52986	1	7.642	96749	0.4
Propane, 1-isot...	10.191	0.1	ng	60218	2	10.406	173020	0.4