

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016692.D
 Acq On : 03 Oct 2021 05:12
 Operator : CG/JU
 Sample : M3915-02
 Misc :
 ALS Vial : 60 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 TT101D-20210921

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: BN016692.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.161	5	9	12	rBV	358487	529396	70.65%	16.420%
2	3.253	17	19	44	rVB	206950	749356	100.00%	23.242%
3	3.816	77	80	88	rBV	8534	25254	3.37%	0.783%
4	4.821	185	189	202	rVB	40973	88131	11.76%	2.734%
5	5.263	234	237	244	rVB	7465	18723	2.50%	0.581%
6	6.822	403	406	416	rVB2	4995	15005	2.00%	0.465%
7	7.080	430	434	440	rVB	4427	9017	1.20%	0.280%
8	7.264	450	454	459	rBV	8046	15863	2.12%	0.492%
9	7.633	490	494	500	rBV	52851	108127	14.43%	3.354%
10	7.864	515	519	527	rVB	3752	7603	1.01%	0.236%
11	8.784	601	605	611	rBV	23554	47200	6.30%	1.464%
12	10.191	713	716	726	rBV	11431	26510	3.54%	0.822%
13	10.407	729	733	737	rBV	106630	186539	24.89%	5.786%
14	12.003	920	931	943	rBV	48537	78081	10.42%	2.422%
15	12.886	1071	1074	1078	rBV	91472	152963	20.41%	4.744%
16	14.269	1180	1183	1186	rBV	140002	199507	26.62%	6.188%
17	15.766	1299	1301	1308	rVB2	11066	17779	2.37%	0.551%
18	17.017	1400	1403	1409	rBV	100657	164355	21.93%	5.098%
19	19.063	1688	1696	1720	rBV	139754	197705	26.38%	6.132%
20	19.678	1813	1820	1843	rBV	124261	156939	20.94%	4.868%
21	21.164	1992	1995	1998	rBV	27325	33829	4.51%	1.049%
22	21.227	1998	2001	2011	rVB	124841	184780	24.66%	5.731%
23	23.419	2400	2408	2414	rBV	4679	7582	1.01%	0.235%
24	23.481	2415	2426	2471	rVB	90775	184760	24.66%	5.731%
25	24.087	2593	2603	2622	rVB	4628	9467	1.26%	0.294%
26	24.857	2817	2828	2845	rVB	4359	9626	1.28%	0.299%

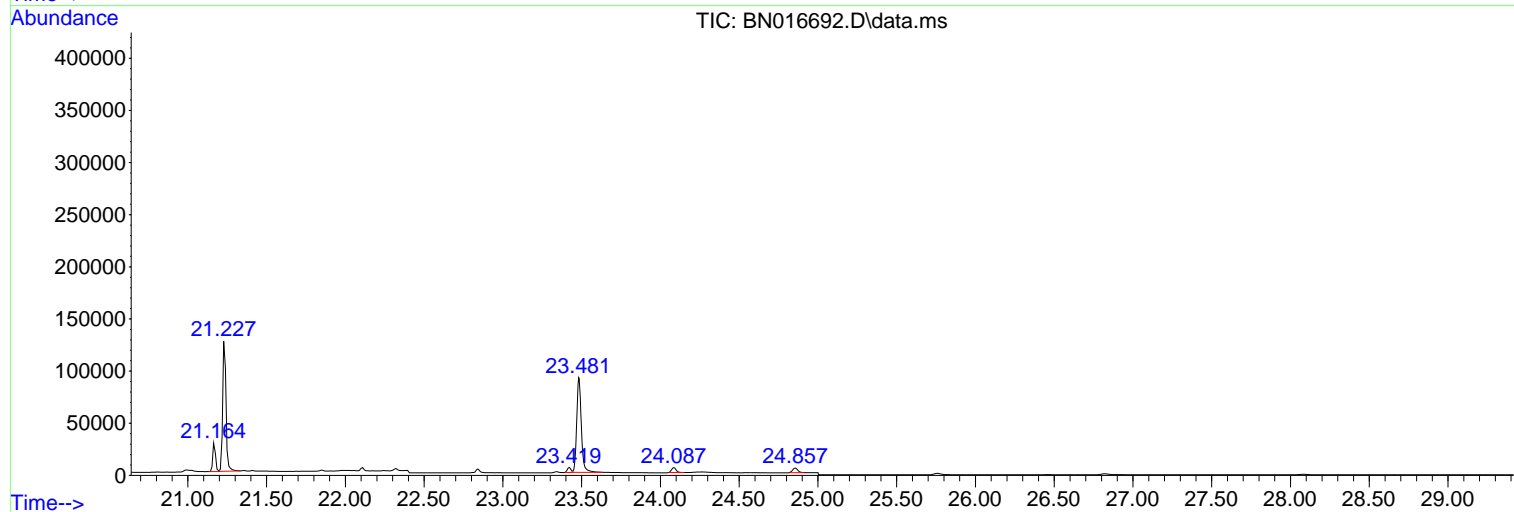
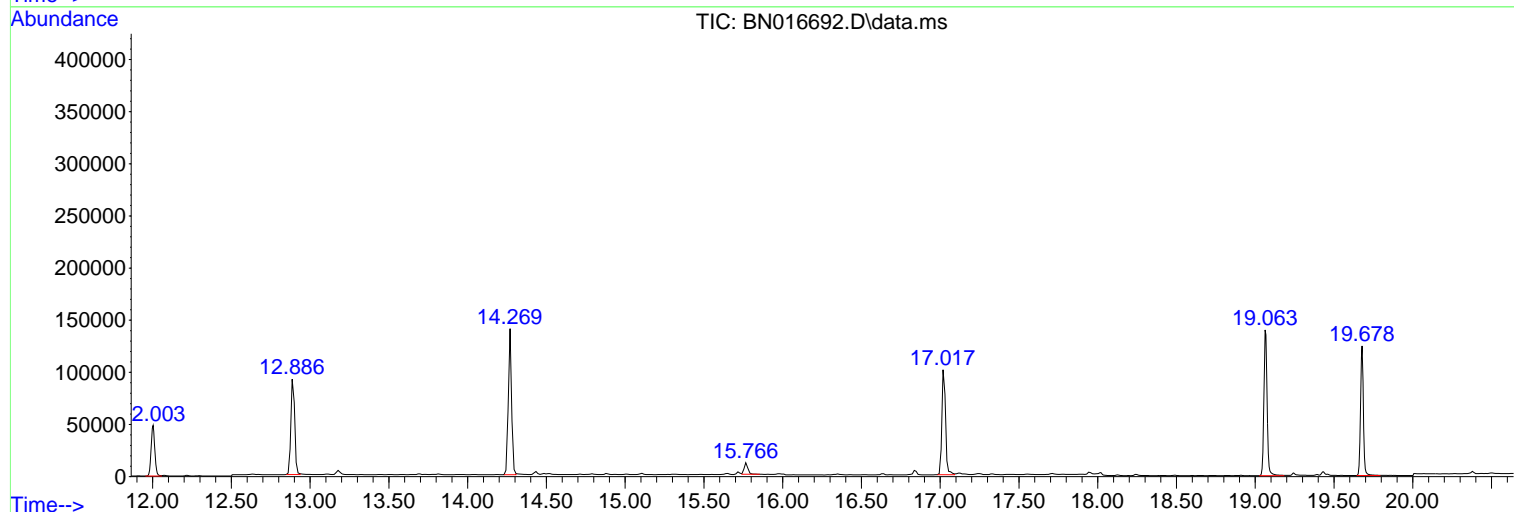
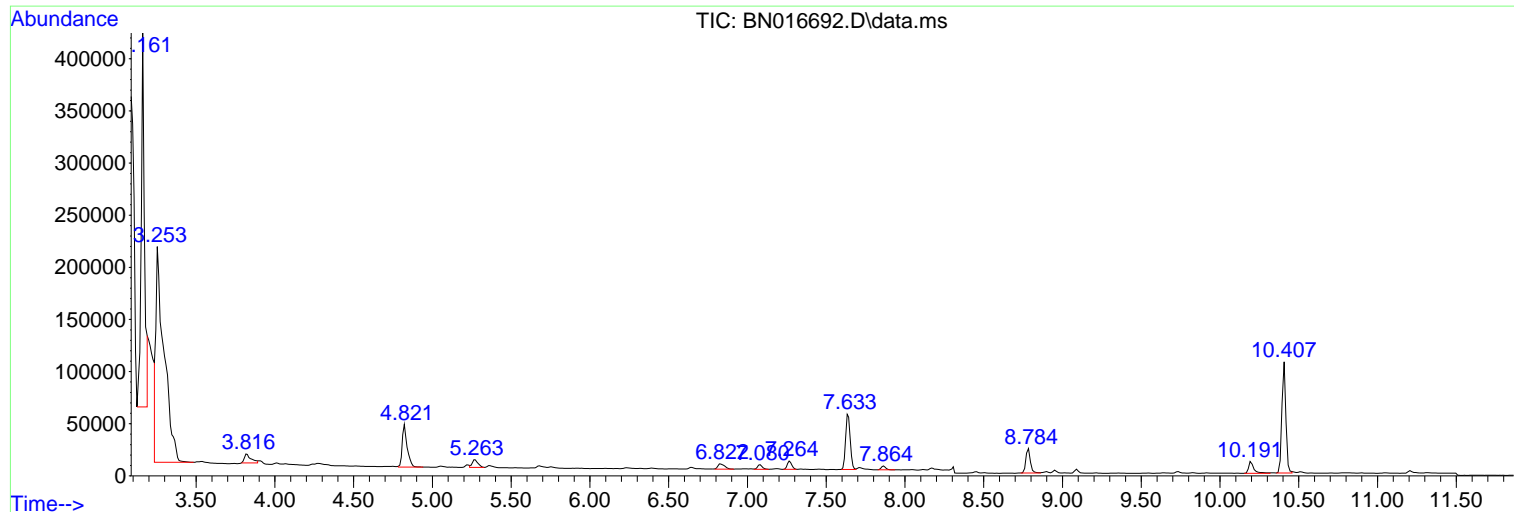
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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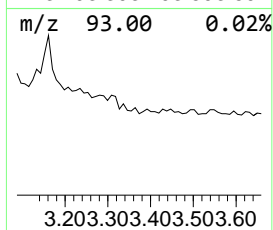
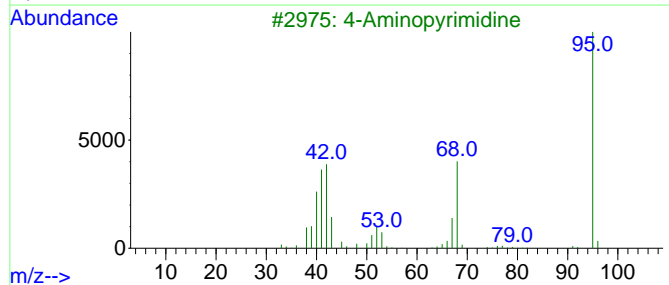
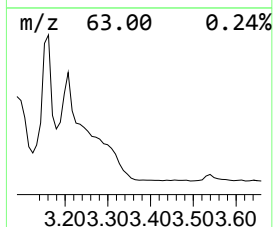
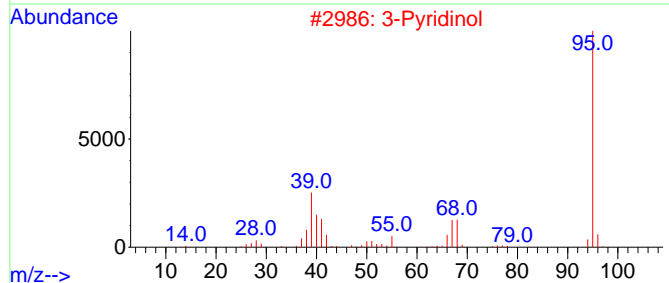
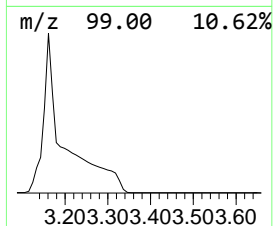
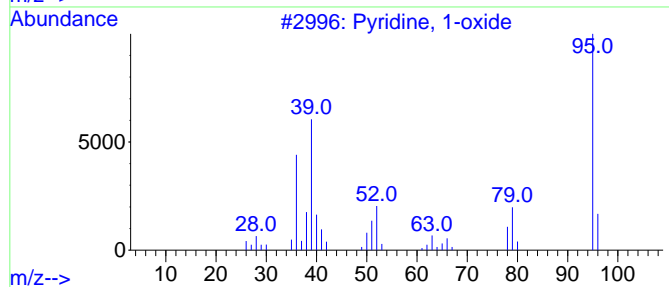
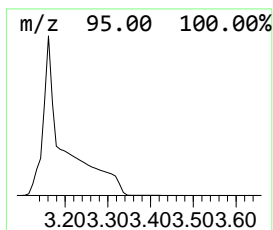
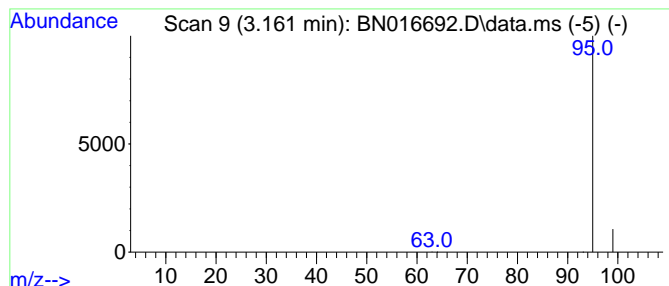
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 1 Pyridine, 1-oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.161	1.96 ng	529396	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2
2			3-Pyridinol	95	C5H5NO	000109-00-2	2
3			4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
4			4-Pyridinol	95	C5H5NO	000626-64-2	2
5			2-(Aminomethylene)aminoacrylontrile	95	C4H5N3	167320-31-2	2



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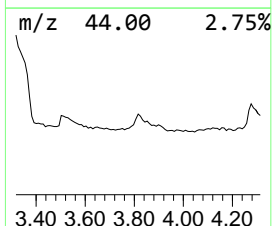
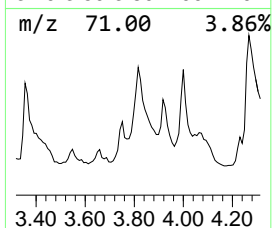
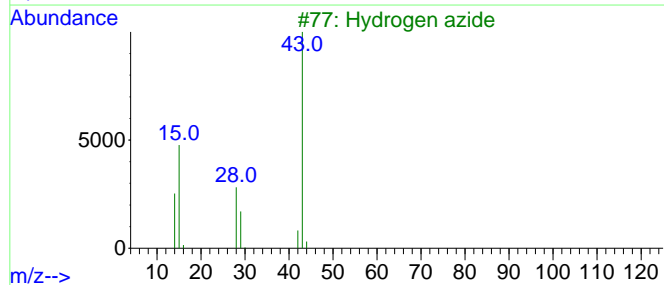
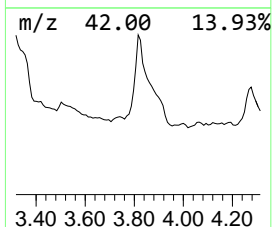
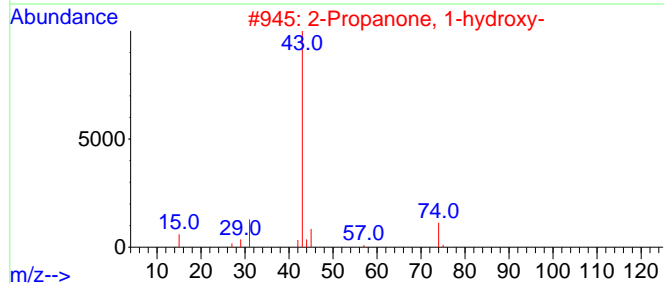
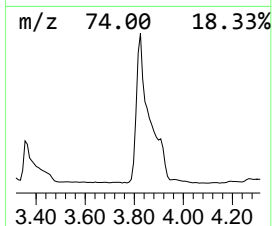
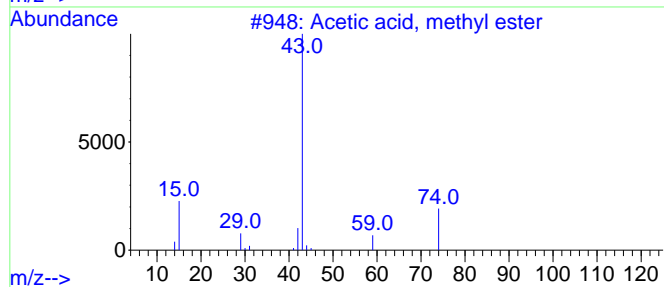
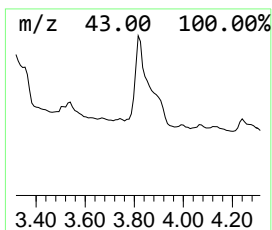
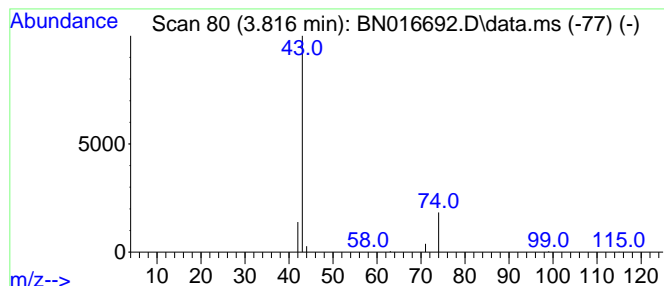
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TIC Library : C:\Database\NIST20.L
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 Peak Number 2 Acetic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.09 ng	25254	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		2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
3		Hydrogen azide	43	HN3	007782-79-8	4
4		O-Methylisourea	74	C2H6N2O	002440-60-0	4
5		1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	3



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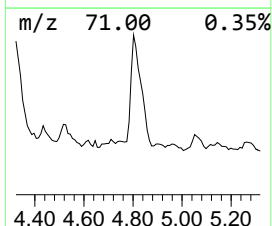
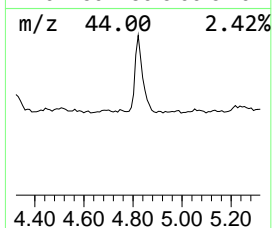
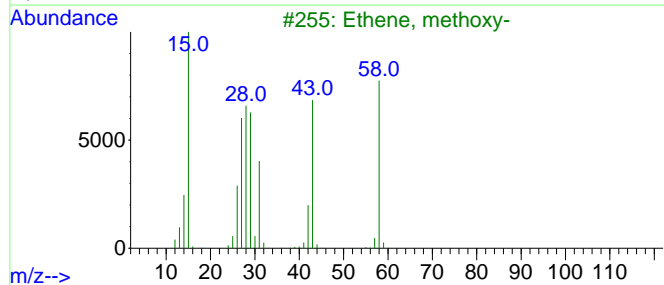
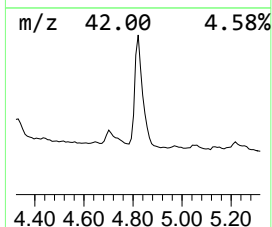
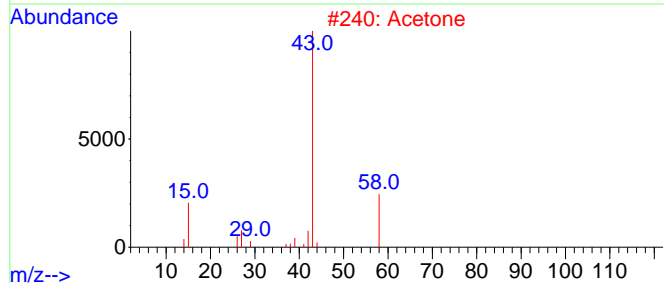
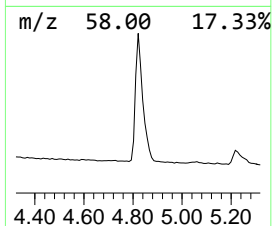
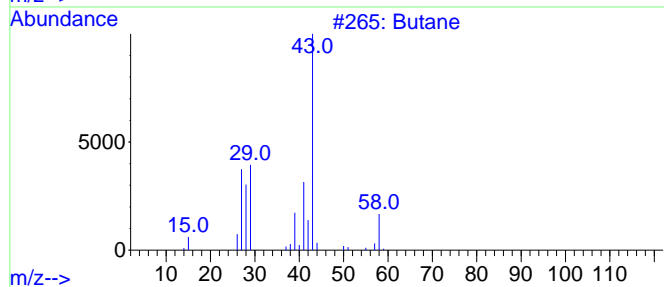
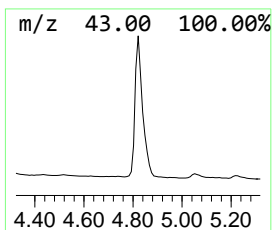
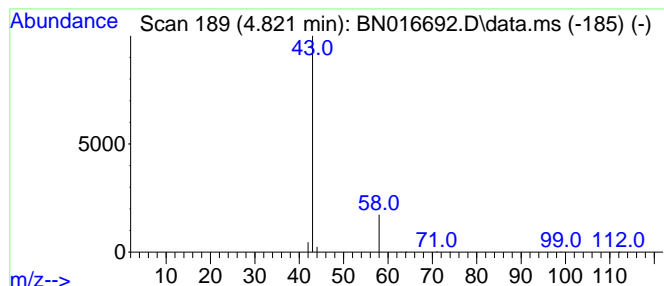
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TIC Library : C:\Database\NIST20.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.33 ng	88131	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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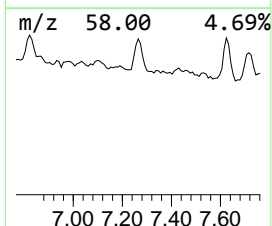
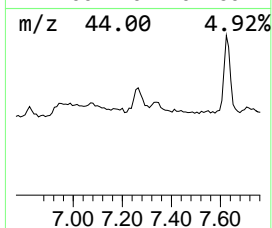
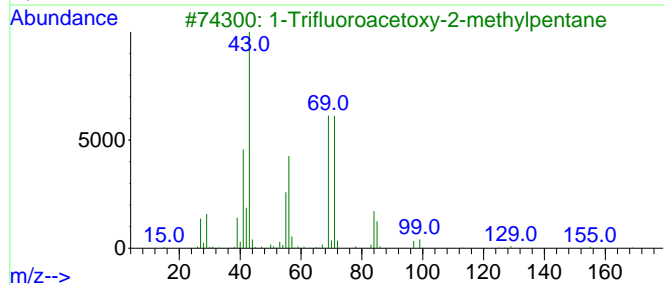
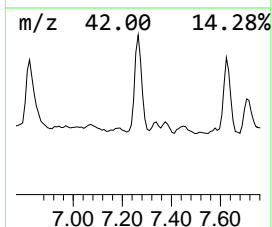
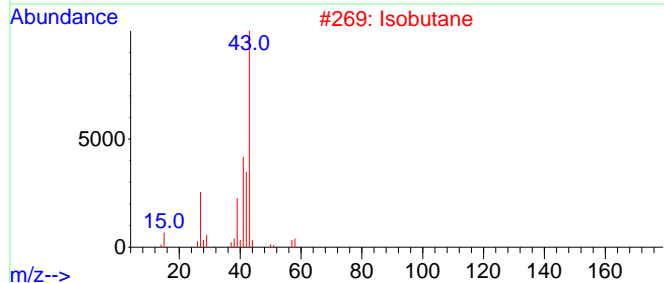
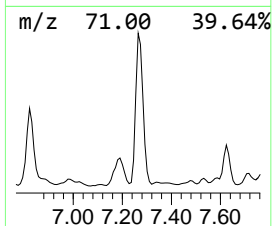
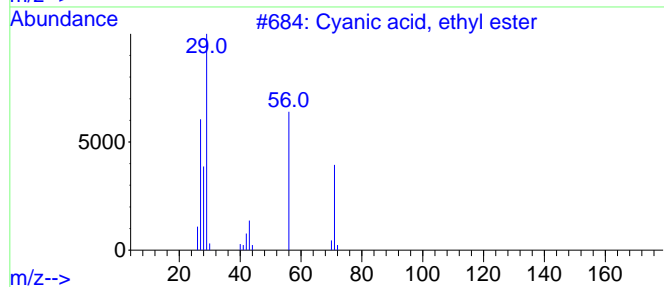
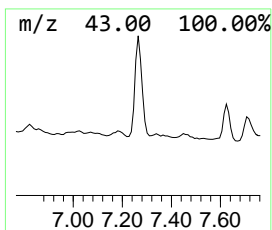
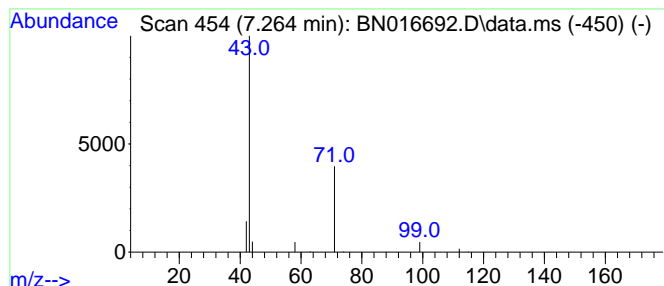
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 Peak Number 4 Cyanic acid, ethyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	15863	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	4
2			Isobutane	58	C4H10	000075-28-5	4
3			1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	4
4			dL-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
5			Hydrogen azide	43	HN3	007782-79-8	4



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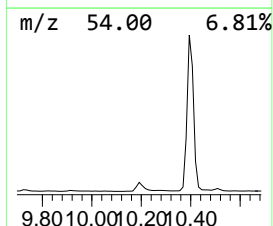
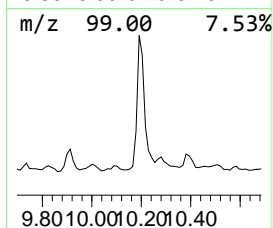
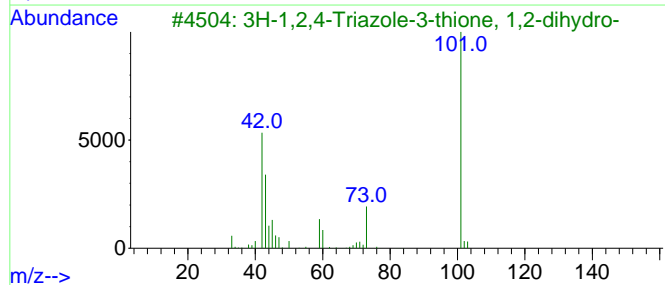
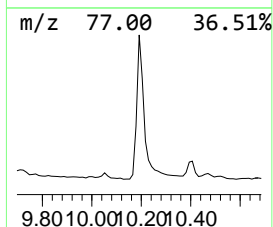
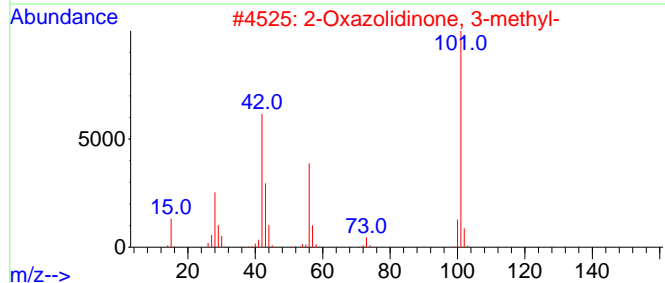
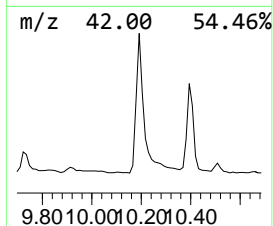
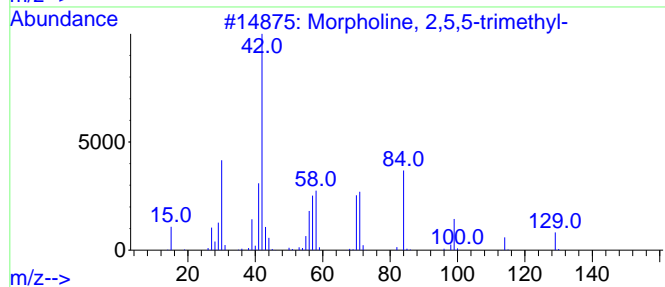
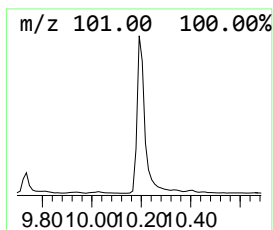
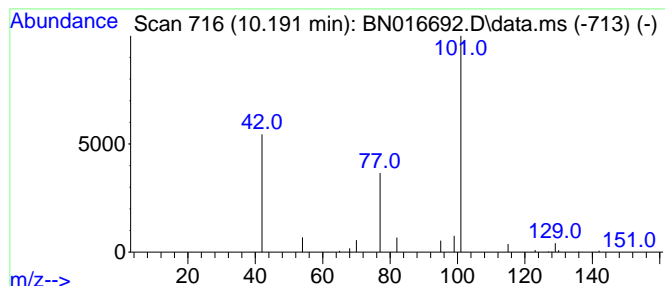
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 Peak Number 5 Morpholine, 2,5,5-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.06 ng	26510	Naphthalene-d8	10.406

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Morpholine, 2,5,5-trimethyl-	129	C7H15NO	1000460-73-8	7
2		2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
3		3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
4		4-Methyl-1,2,5-oxadiazol-3-amine	99	C3H5N3O	1000411-31-0	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
Pyridine, 1-oxide	3.161	2.0	ng	529396	1	7.642	108127	0.4
Acetic acid, me...	3.816	0.1	ng	25254	1	7.642	108127	0.4
Butane	4.821	0.3	ng	88131	1	7.642	108127	0.4
Cyanic acid, et...	7.264	0.1	ng	15863	1	7.642	108127	0.4
Morpholine, 2,5...	10.191	0.1	ng	26510	2	10.406	186539	0.4