

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052324\
 Data File : BM045755.D
 Acq On : 23 May 2024 16:08
 Operator : MA/JU
 Sample : PB160904BL
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB160904BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % 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_M\Methods\8270-BM052224.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM045755.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.775	282	287	303	rBV	2598806	4281433	24.33%	5.264%
2	5.251	361	368	380	rBV	4231035	6277391	35.67%	7.718%
3	5.546	412	418	432	rBV4	152418	342858	1.95%	0.422%
4	6.263	534	540	550	rBV	254040	493746	2.81%	0.607%
5	6.834	630	637	650	rBV	4103075	6743856	38.32%	8.291%
6	7.569	755	762	769	rVB	1190529	1822613	10.36%	2.241%
7	7.910	814	820	830	rBV	281398	538752	3.06%	0.662%
8	8.734	951	960	975	rBV	3757815	6475563	36.79%	7.961%
9	10.339	1223	1233	1242	rBV	1499332	2547447	14.47%	3.132%
10	12.822	1648	1655	1665	rBV	8489053	12807160	72.76%	15.746%
11	14.198	1881	1889	1900	rBV	2284140	3248042	18.45%	3.993%
12	15.698	2134	2144	2165	rBV	4342185	6251090	35.52%	7.685%
13	16.945	2349	2356	2367	rBV	2836854	3854819	21.90%	4.739%
14	19.580	2799	2804	2810	rBV	13517404	17600802	100.00%	21.639%
15	21.156	3067	3072	3080	rBV2	2936013	3927457	22.31%	4.829%
16	23.950	3539	3547	3558	rVB	1778480	4124474	23.43%	5.071%

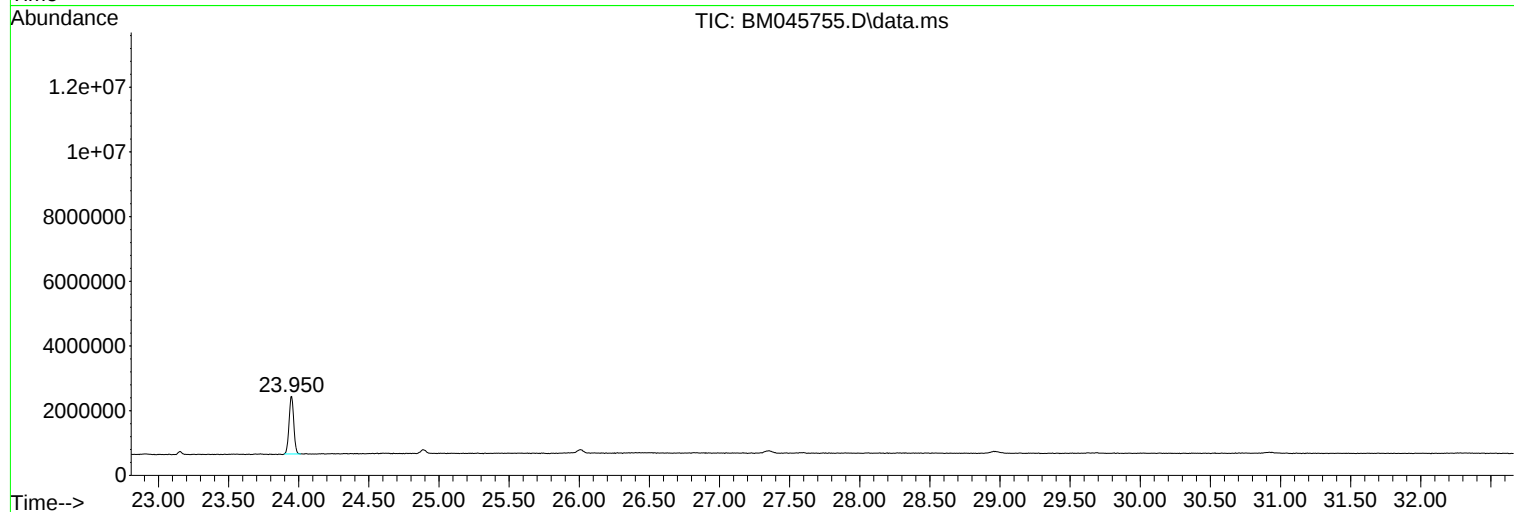
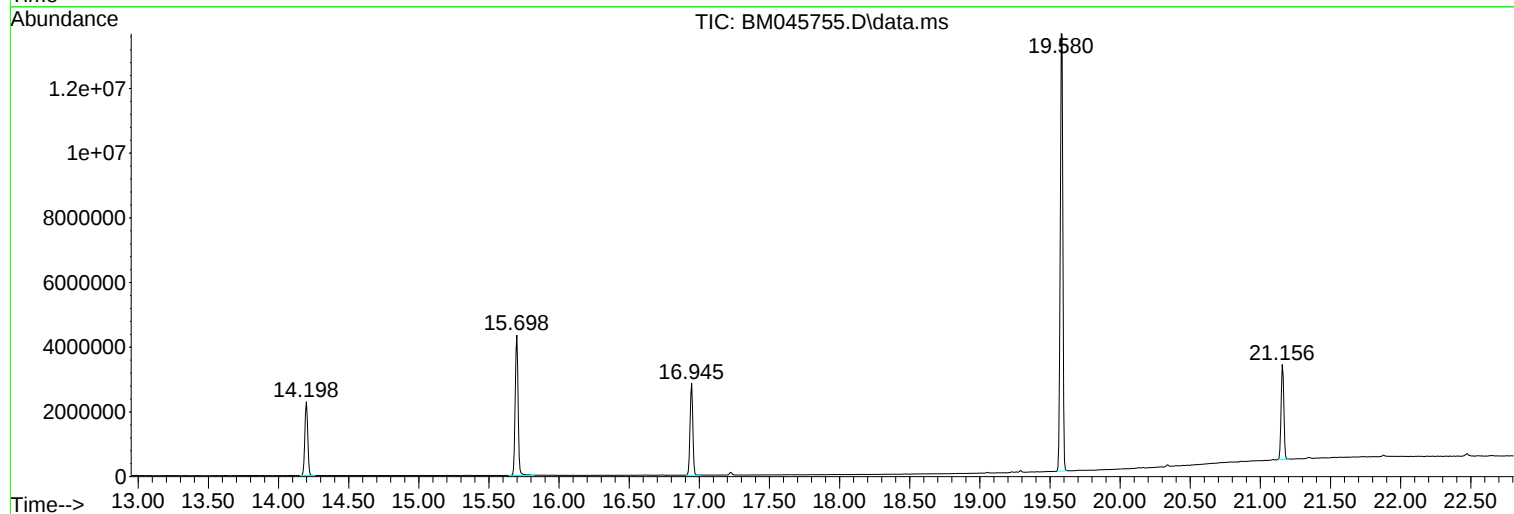
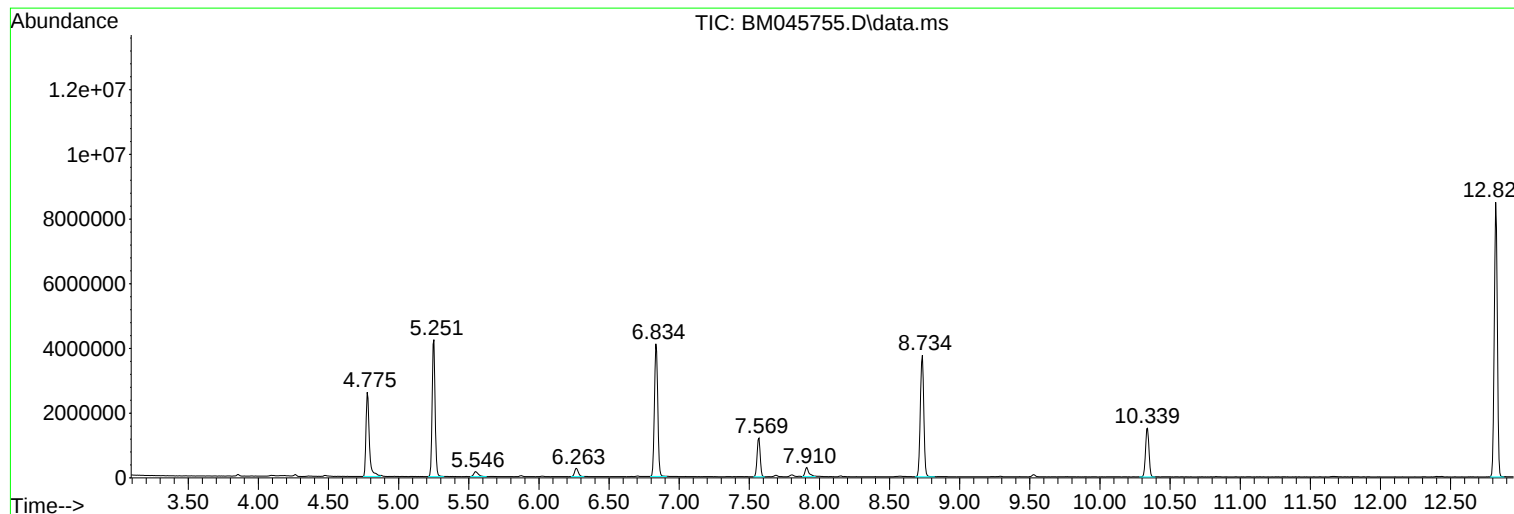
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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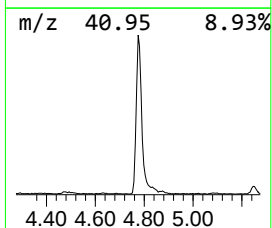
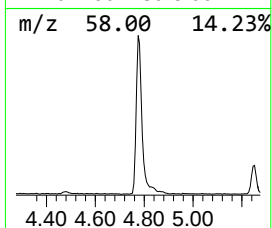
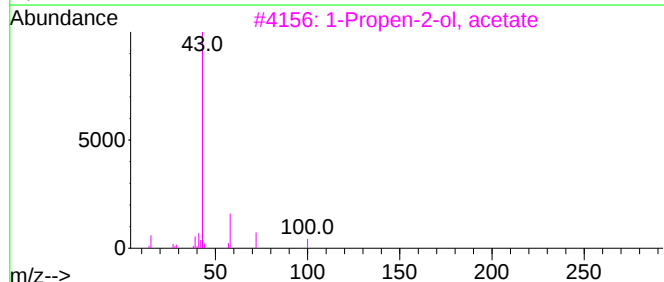
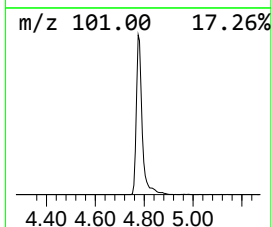
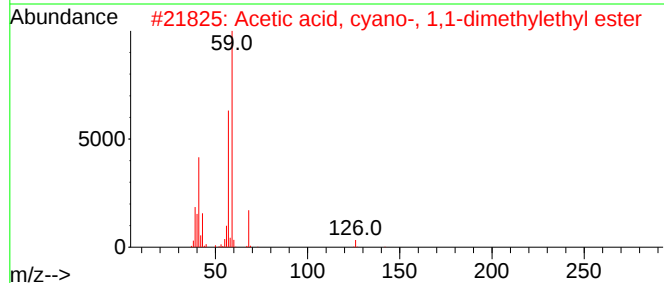
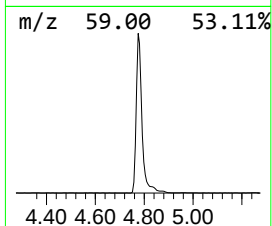
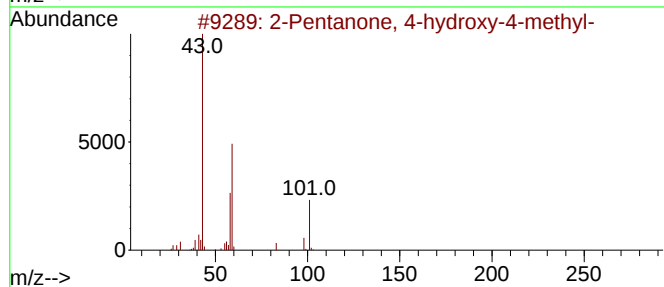
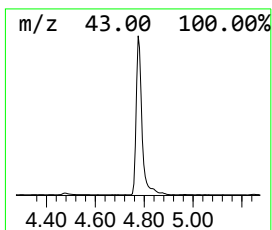
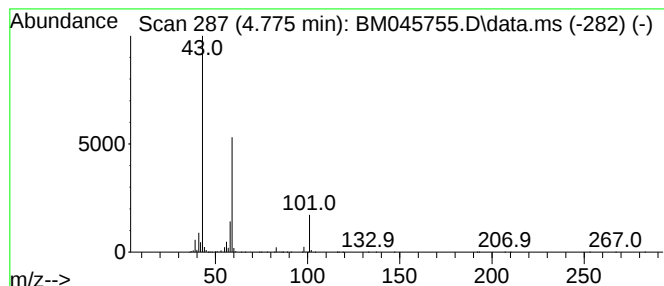
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM052224.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.775	46.98 ng	4281430	1,4-Dichlorobenzene-d4	7.569	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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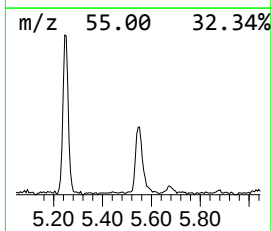
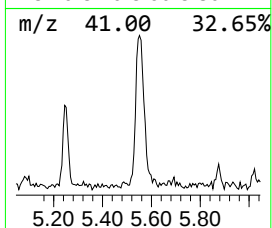
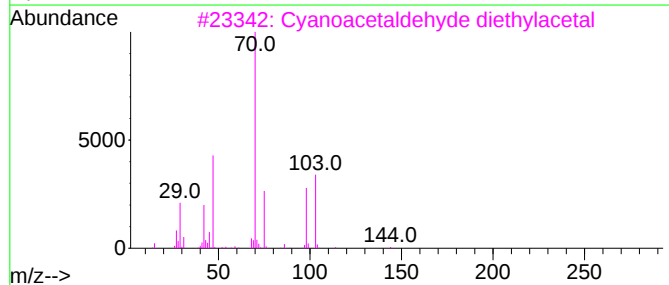
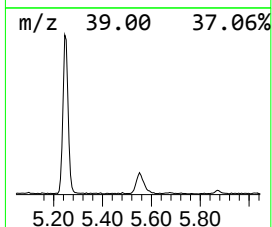
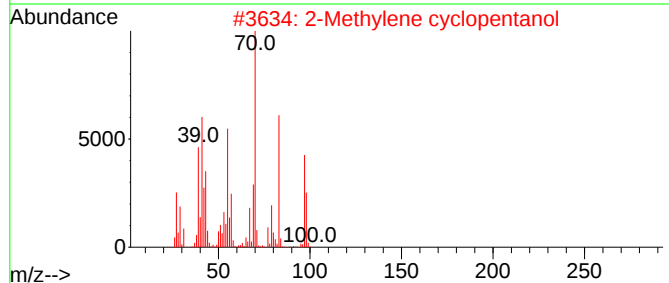
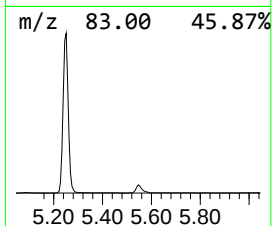
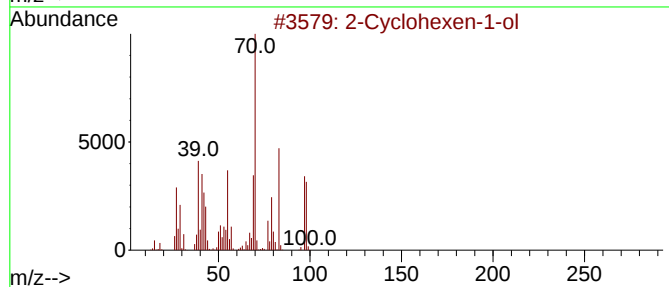
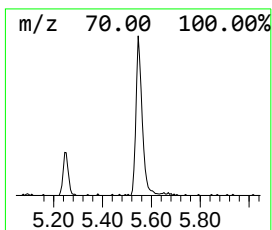
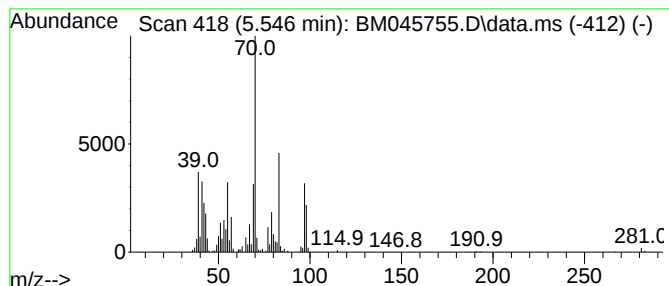
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Cyclohexen-1-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.546	3.76 ng	342858	1,4-Dichlorobenzene-d4	7.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	96
2			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	93
3			Cyanoacetaldehyde diethylacetal	143	C7H13NO2	002032-34-0	43
4			1,2-Cyclohexanediol	116	C6H12O2	000931-17-9	42
5			1-butoxycyclohexene	154	C10H18O	024159-57-7	42



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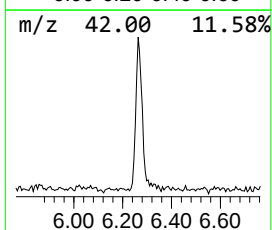
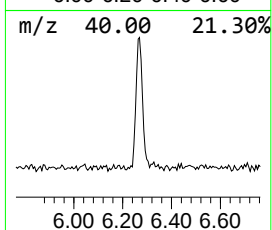
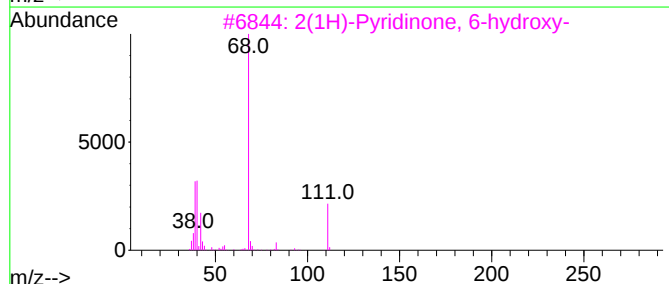
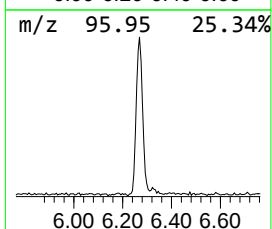
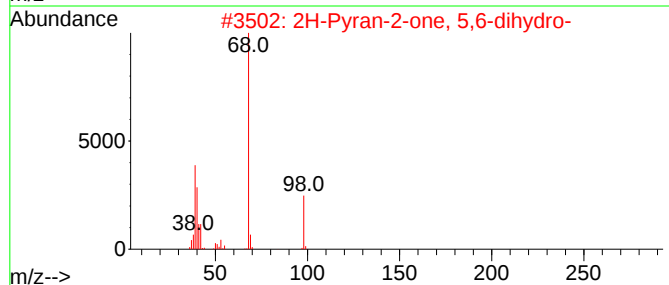
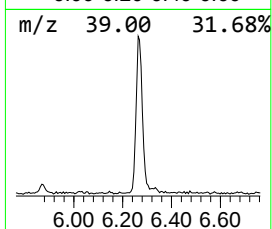
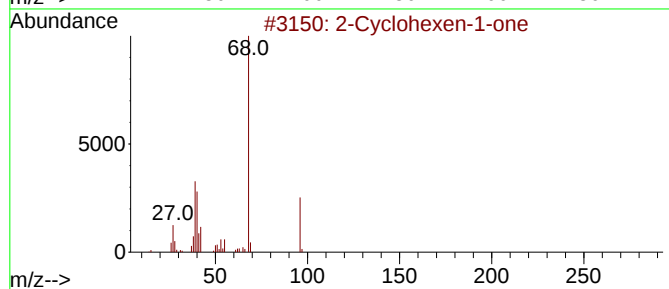
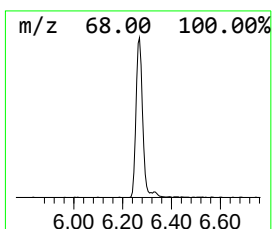
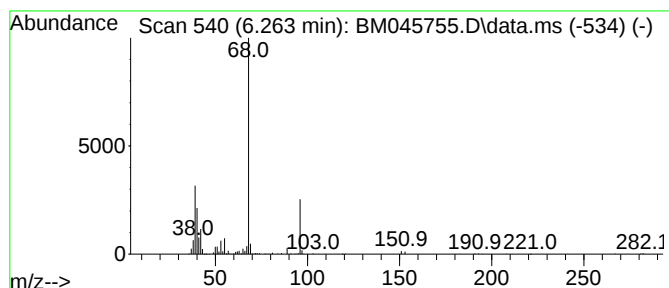
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Peak Number 3 2-Cyclohexen-1-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.263	5.42 ng	493746	1,4-Dichlorobenzene-d4	7.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	93
2			2H-Pyran-2-one, 5,6-dihydro-	98	C5H6O2	003393-45-1	58
3			2(1H)-Pyridinone, 6-hydroxy-	111	C5H5NO2	000626-06-2	53
4			5,6-Dihydro-2(1H)-pyridinone	97	C5H7NO	006052-73-9	42
5			7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	42



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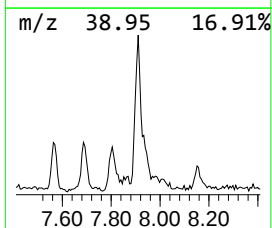
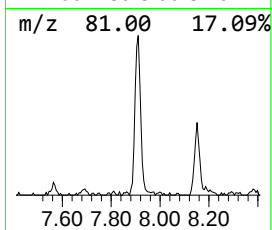
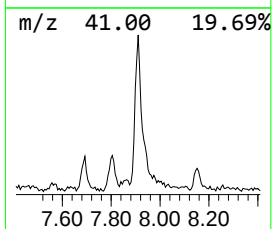
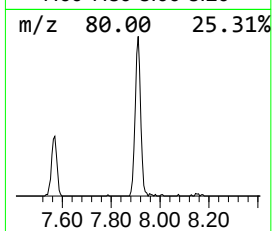
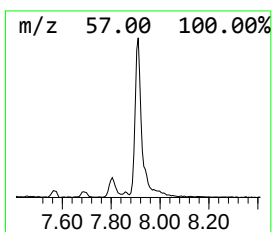
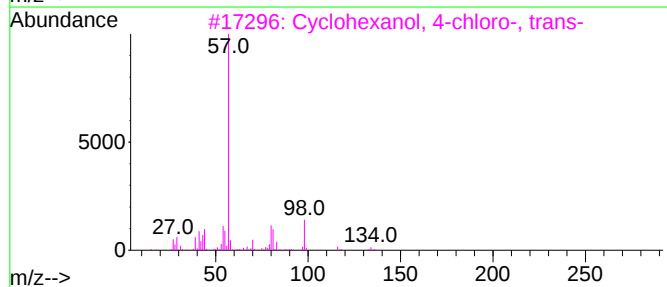
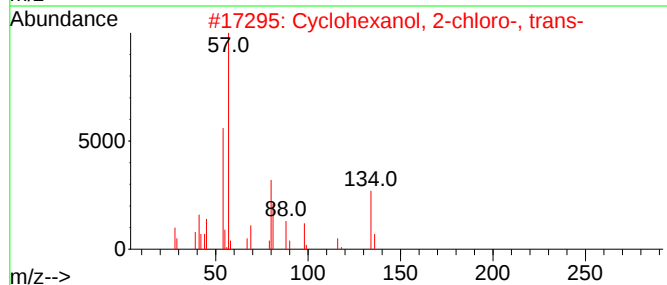
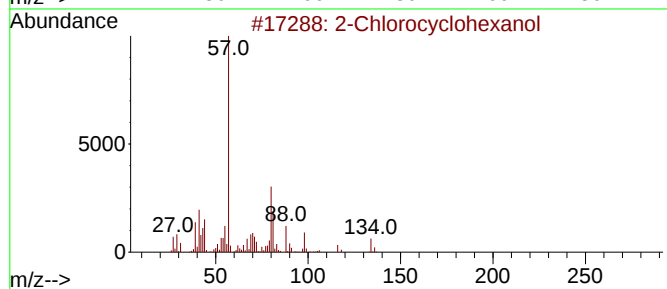
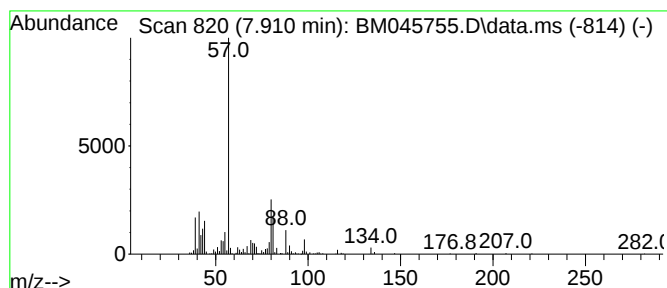
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Peak Number 4 2-Chlorocyclohexanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.910	5.91 ng	538752	1,4-Dichlorobenzene-d4	7.569

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	95
2			Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	43
3			Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	17
4			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	14
5			4-Chlorocyclohexanol	134	C6H11ClO	030485-71-3	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.775	47.0	ng	4281430	1	7.569	1822610	20.0
2-Cyclohexen-1-ol	5.546	3.8	ng	342858	1	7.569	1822610	20.0
2-Cyclohexen-1-one	6.263	5.4	ng	493746	1	7.569	1822610	20.0
2-Chlorocyclohe...	7.910	5.9	ng	538752	1	7.569	1822610	20.0