

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103023\
 Data File : BM042500.D
 Acq On : 30 Oct 2023 18:49
 Operator : MA/JU
 Sample : PB156526BL
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB156526BL

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-BM103023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042500.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.228	174	177	186	rBV	20680	41376	1.03%	0.196%
2	5.022	306	312	325	rBV	1058970	1439002	35.68%	6.834%
3	5.469	381	388	402	rBV	1412328	2083378	51.66%	9.894%
4	5.816	442	447	453	rBV2	52475	87427	2.17%	0.415%
5	6.587	572	578	584	rBV	64325	120753	2.99%	0.573%
6	7.093	658	664	683	rBV	1310707	2097882	52.02%	9.963%
7	7.928	800	806	815	rBV	359004	554699	13.76%	2.634%
8	8.269	855	864	874	rVB2	86015	174305	4.32%	0.828%
9	9.128	1002	1010	1022	rBV	1151250	1891303	46.90%	8.982%
10	10.745	1279	1285	1296	rBV	389752	670859	16.64%	3.186%
11	13.198	1695	1702	1717	rBV	2563929	3630633	90.03%	17.242%
12	14.575	1930	1936	1949	rBV	512525	756408	18.76%	3.592%
13	16.069	2184	2190	2206	rBV	1137101	1573109	39.01%	7.471%
14	17.327	2398	2404	2417	rBV	510719	752716	18.67%	3.575%
15	19.939	2843	2848	2863	rBV	3276761	4032519	100.00%	19.150%
16	21.509	3111	3115	3122	rBV	396356	556718	13.81%	2.644%
17	23.927	3521	3526	3538	rVB	281931	594309	14.74%	2.822%

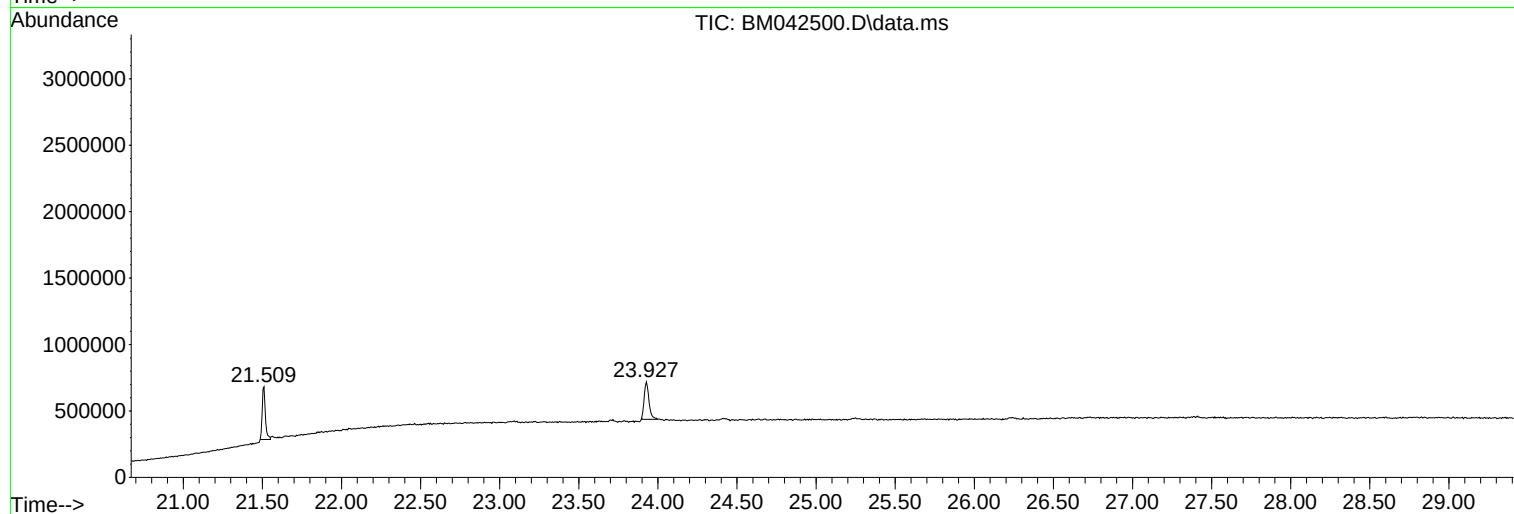
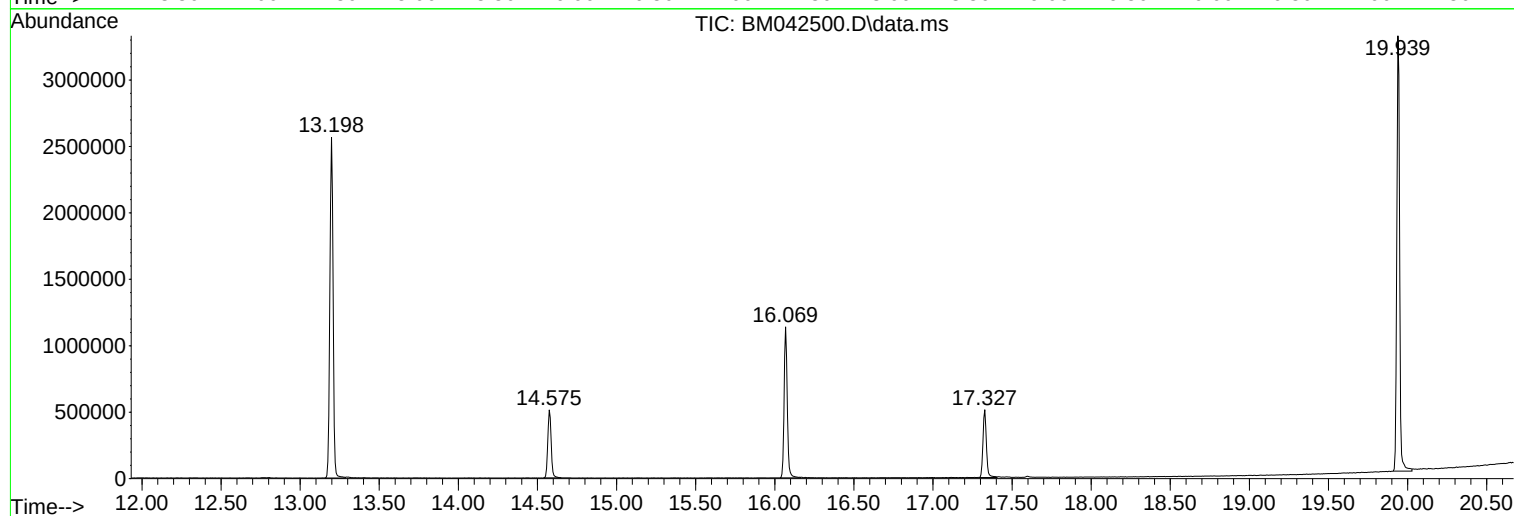
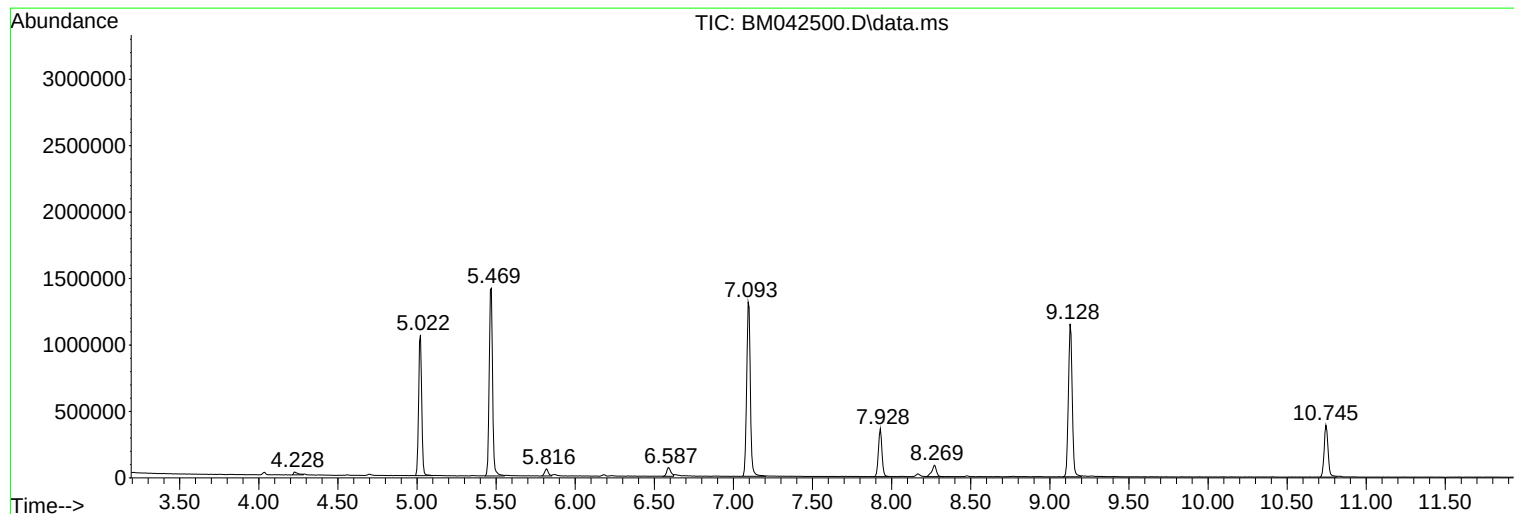
Sum of corrected areas: 21057396

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.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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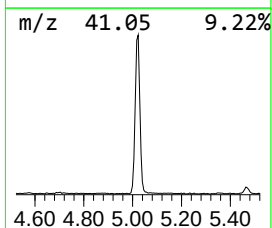
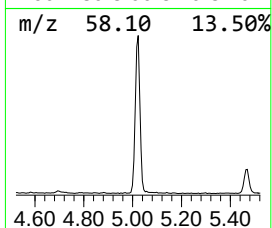
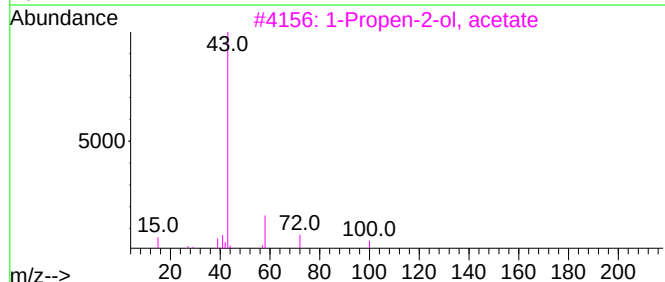
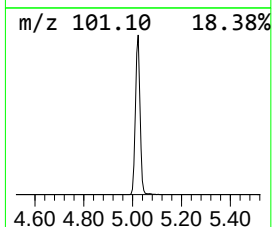
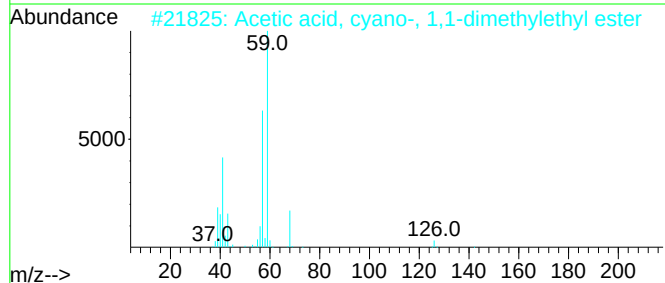
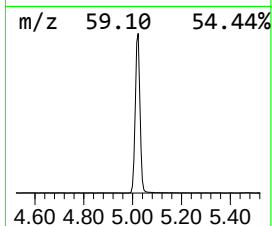
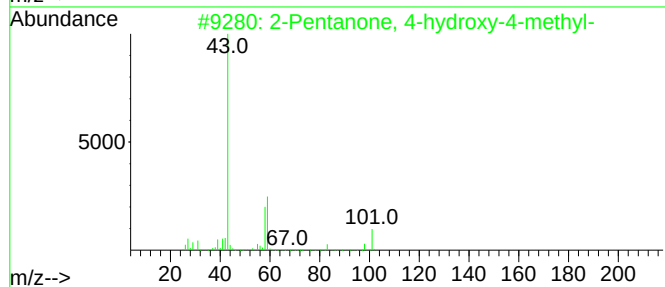
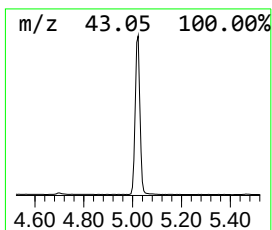
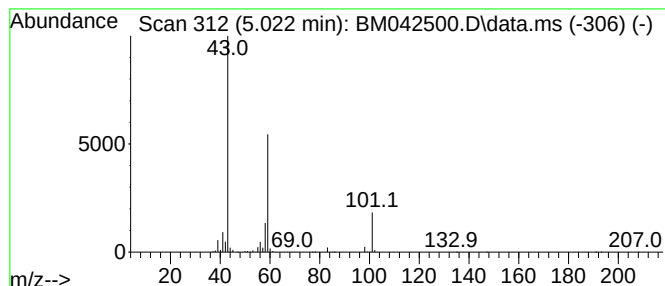
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	51.88 ng	1439000	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
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			1,2-Butanediol	90	C4H10O2	000584-03-2	9



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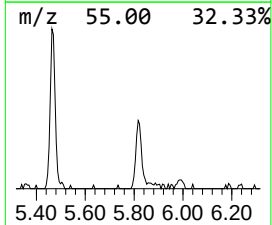
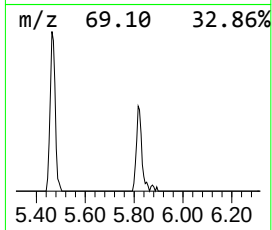
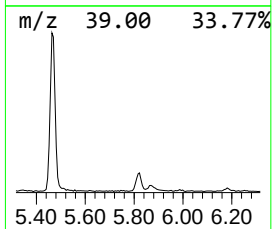
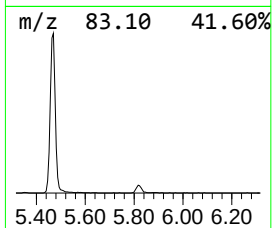
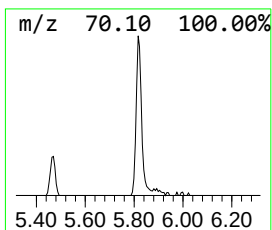
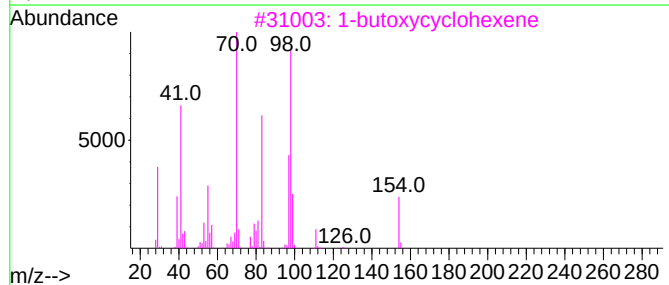
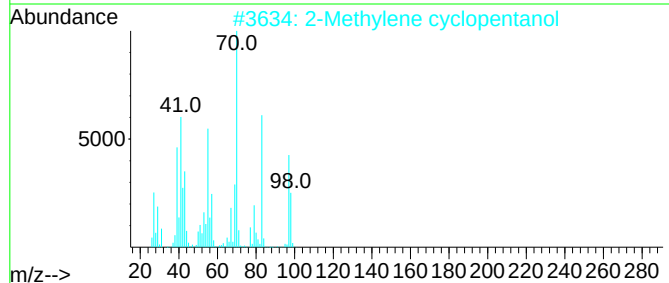
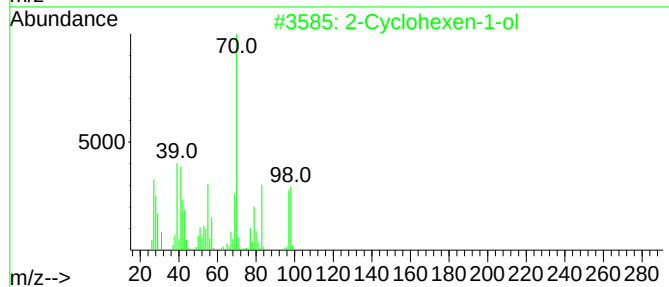
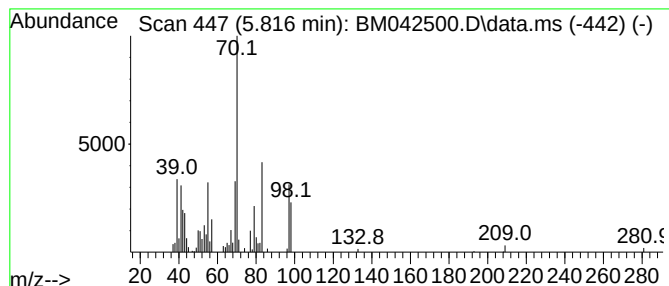
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.816	3.15 ng	87427	1,4-Dichlorobenzene-d4	7.928

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	95
2		2-Methylene cyclopentanol	98	C6H10O	020461-31-8	58
3		1-butoxycyclohexene	154	C10H18O	024159-57-7	40
4		1-propoxycyclohexene	140	C9H16O	061382-76-1	40
5		Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	38



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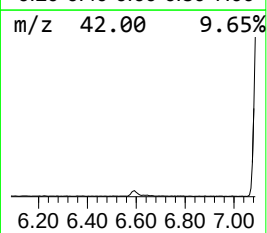
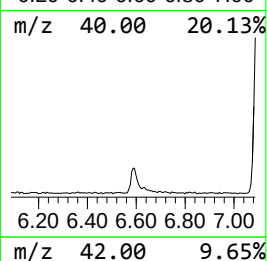
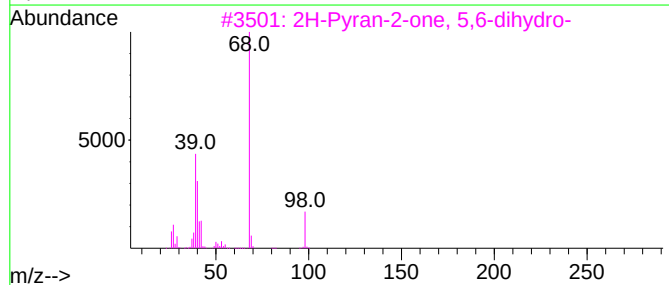
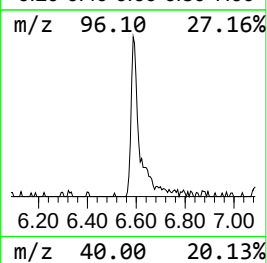
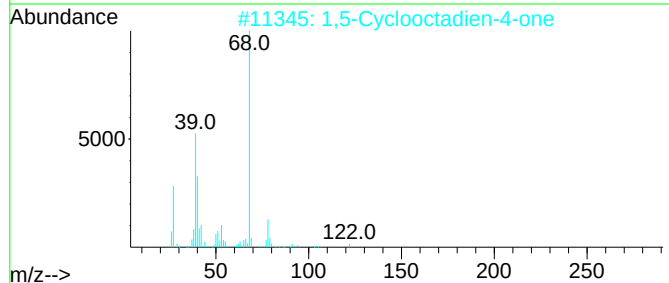
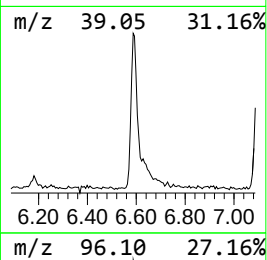
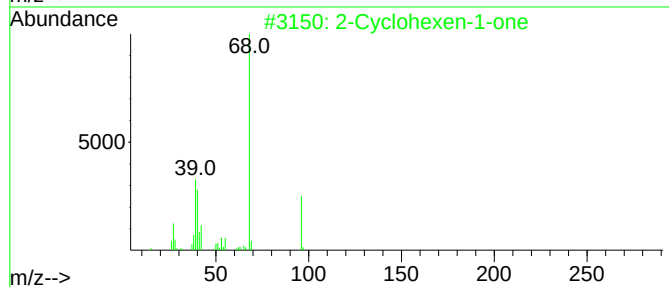
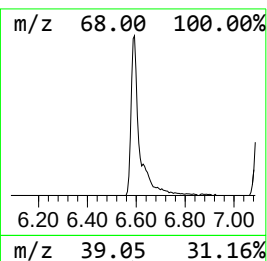
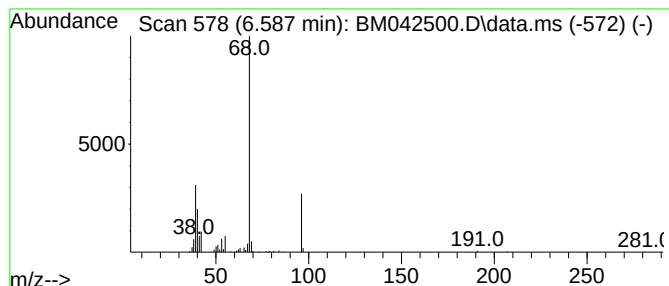
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Peak Number 3 2-Cyclohexen-1-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.587	4.35 ng	120753	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	93
2			1,5-Cyclooctadien-4-one	122	C8H10O	001460-21-5	53
3			2H-Pyran-2-one, 5,6-dihydro-	98	C5H6O2	003393-45-1	53
4			5,6-Dihydro-2(1H)-pyridinone	97	C5H7NO	006052-73-9	45
5			3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	45



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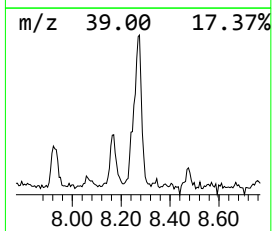
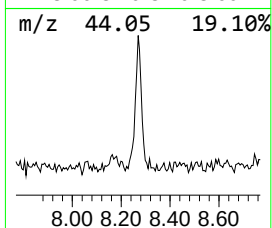
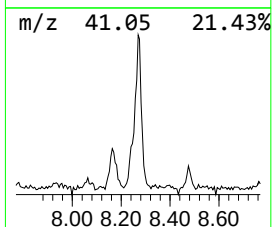
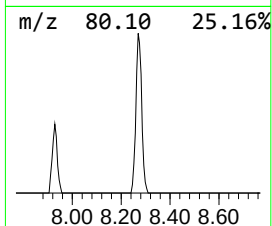
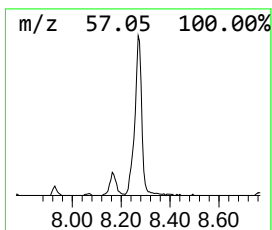
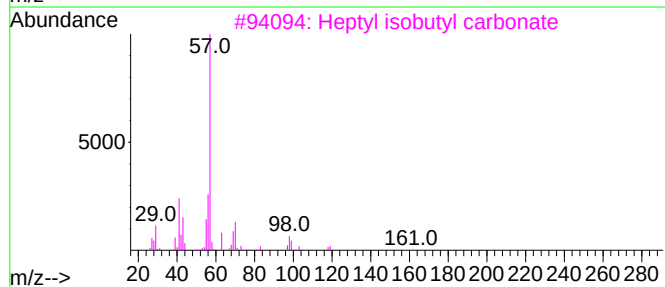
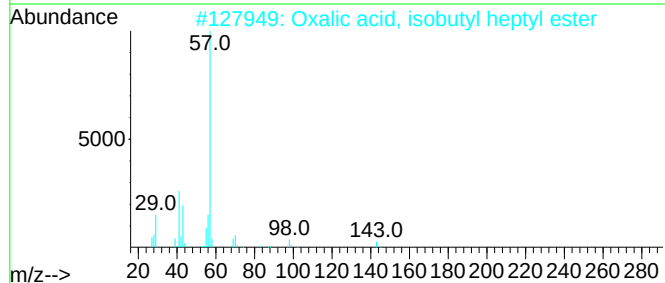
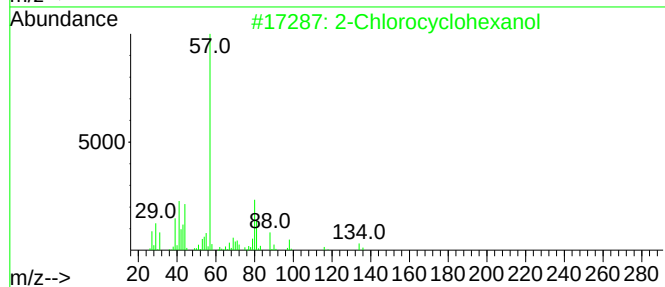
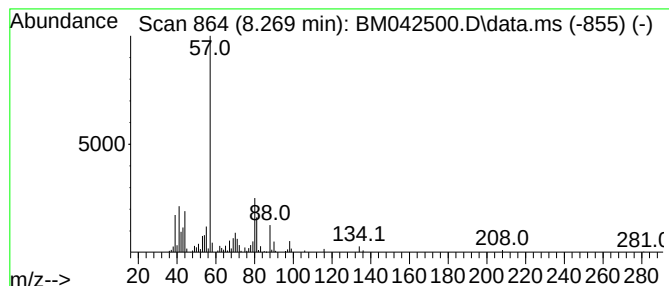
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 2-Chlorocyclohexanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.269	6.28 ng	174305	1,4-Dichlorobenzene-d4	7.928

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	93
2			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	22
3			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	22
4			Oxalic acid, heptyl propyl ester	230	C12H22O4	1000309-26-0	22
5			Butanoic acid, 2-hydroxy-3,3-dim...	132	C6H12O3	004026-20-4	17



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	51.9	ng	1439000	1	7.928	554699	20.0
2-Cyclohexen-1-ol	5.816	3.1	ng	87427	1	7.928	554699	20.0
2-Cyclohexen-1-one	6.587	4.3	ng	120753	1	7.928	554699	20.0
2-Chlorocyclohe...	8.269	6.3	ng	174305	1	7.928	554699	20.0