

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032324\
 Data File : BM044735.D
 Acq On : 22 Mar 2024 15:24
 Operator : MA/JU
 Sample : PB159652BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB159652BL

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-BM031324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044735.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.869	297	303	316	rBV	1704472	2518438	29.17%	5.591%
2	5.310	371	378	390	rBV	2876340	4303769	49.85%	9.554%
3	5.634	425	433	438	rBV	118285	204923	2.37%	0.455%
4	6.351	548	555	566	rBV	181346	319505	3.70%	0.709%
5	6.869	636	643	659	rBV	2580696	4244906	49.17%	9.424%
6	7.687	775	782	790	rBV	782358	1239316	14.36%	2.751%
7	7.963	823	829	832	rVV2	54596	90065	1.04%	0.200%
8	8.004	832	836	844	rVB	165679	276253	3.20%	0.613%
9	8.851	971	980	993	rBV	2361093	4024977	46.62%	8.935%
10	10.463	1246	1254	1265	rBV	913385	1560117	18.07%	3.463%
11	12.945	1669	1676	1696	rBV	4991336	7543048	87.37%	16.745%
12	14.327	1904	1911	1921	rBV	1103541	1697952	19.67%	3.769%
13	15.827	2159	2166	2180	rBV	2076997	3019323	34.97%	6.703%
14	17.086	2373	2380	2394	rBV	1190686	1757042	20.35%	3.901%
15	17.992	2529	2534	2545	rBV2	54950	107227	1.24%	0.238%
16	19.733	2823	2830	2841	rBV	6516990	8633281	100.00%	19.166%
17	21.286	3089	3094	3101	rBV	1317220	1705784	19.76%	3.787%
18	23.527	3468	3475	3488	rVB	920968	1799673	20.85%	3.995%

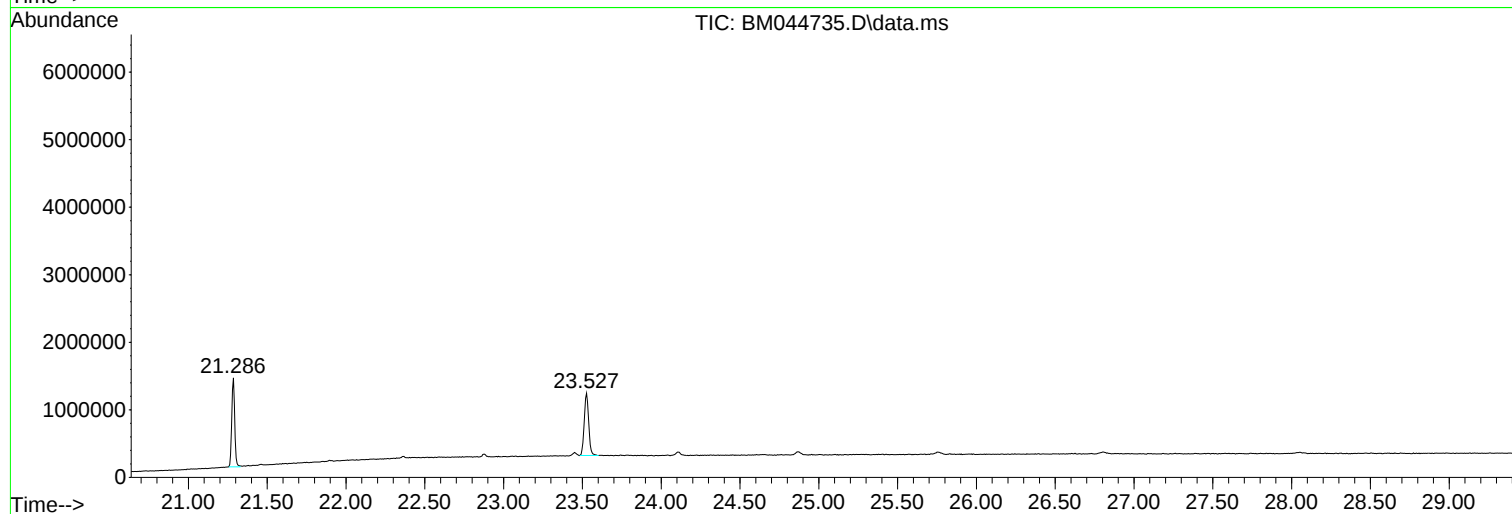
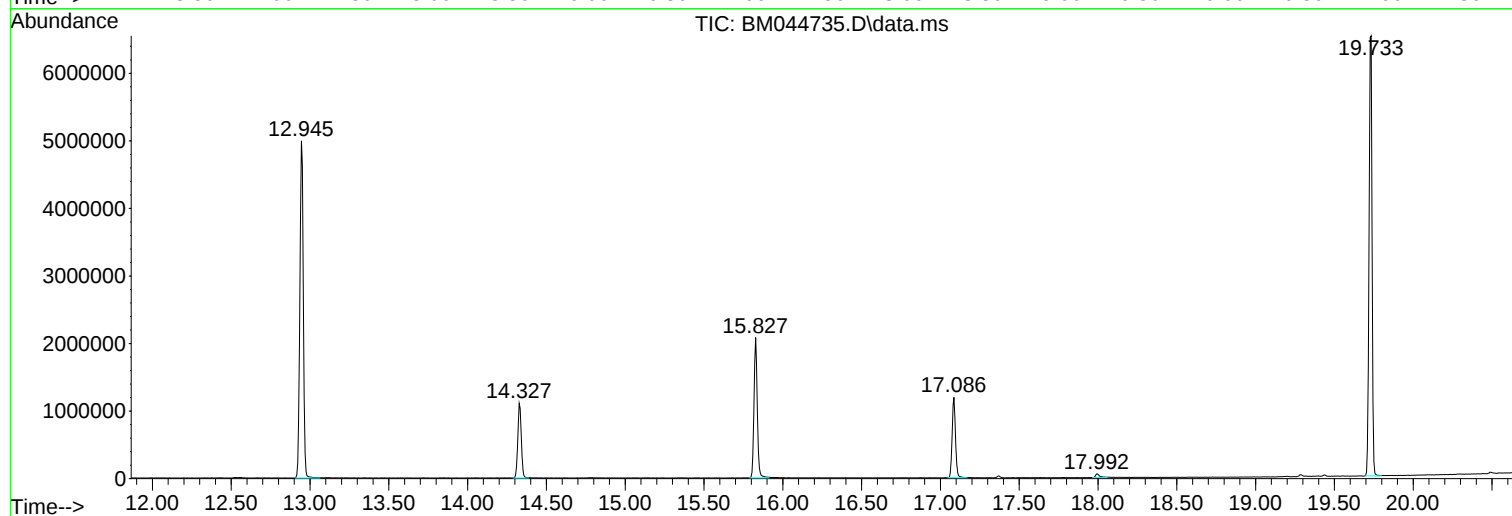
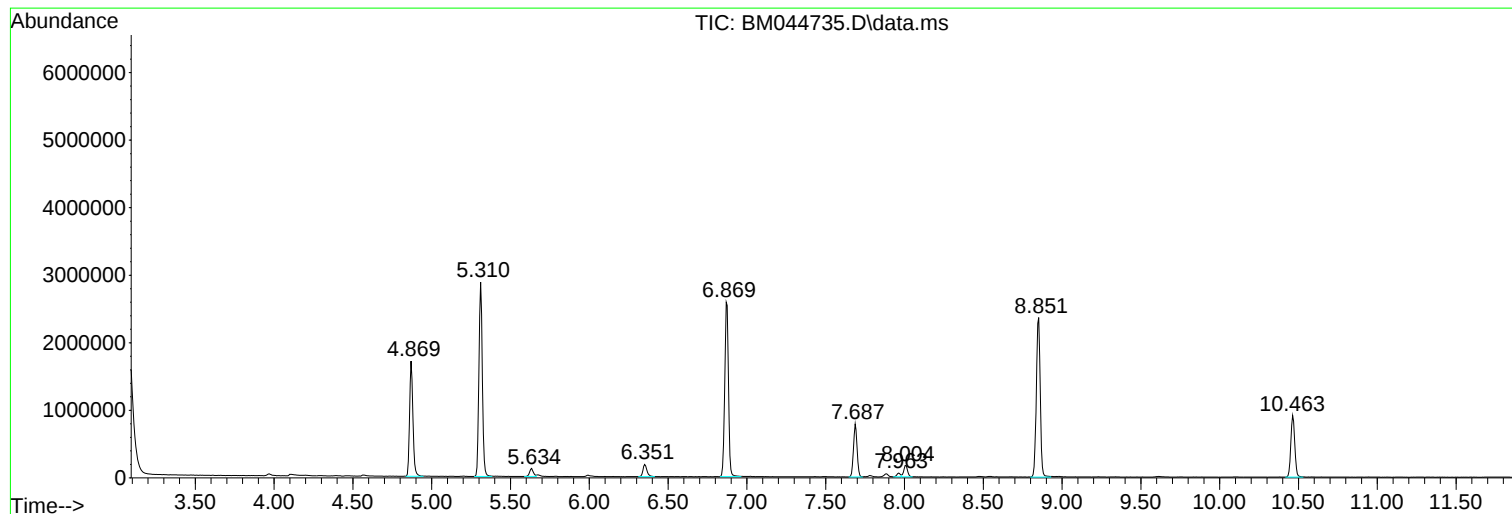
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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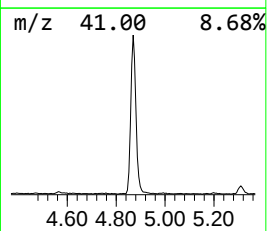
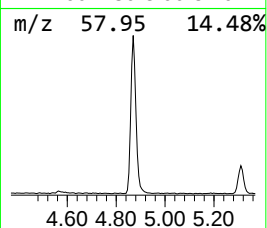
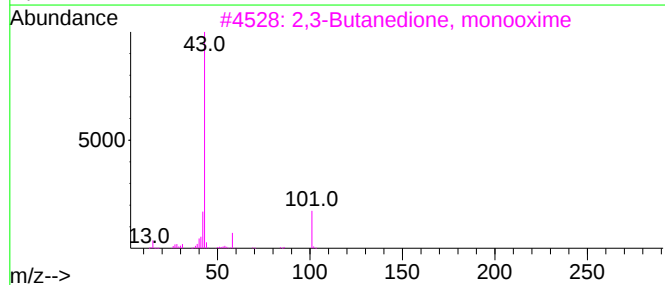
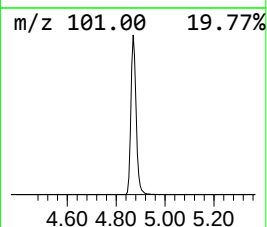
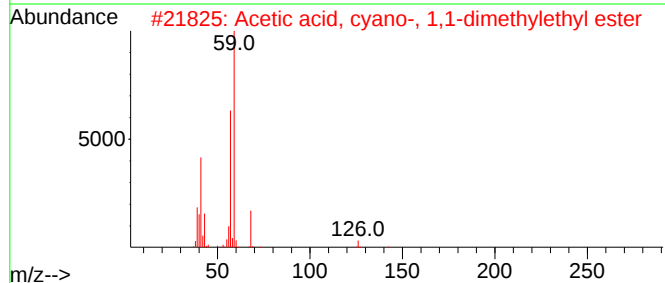
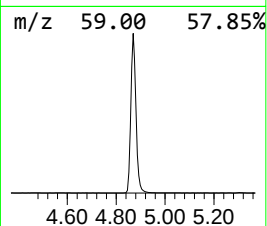
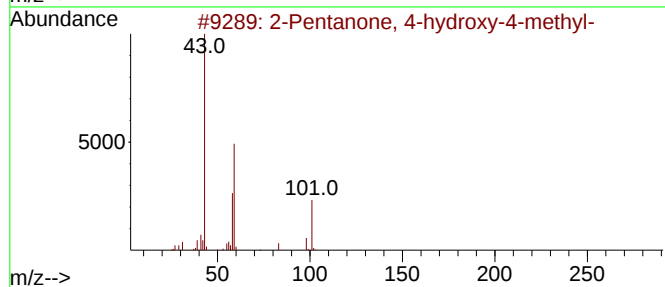
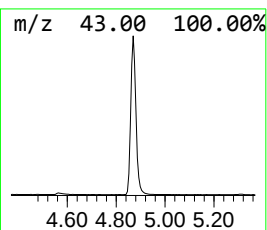
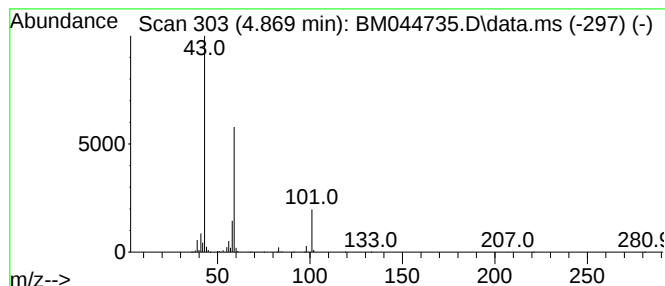
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.869	40.64 ng	2518440	1,4-Dichlorobenzene-d4	7.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	9		



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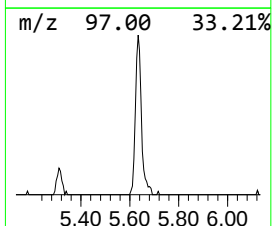
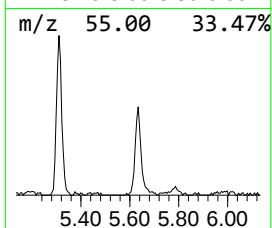
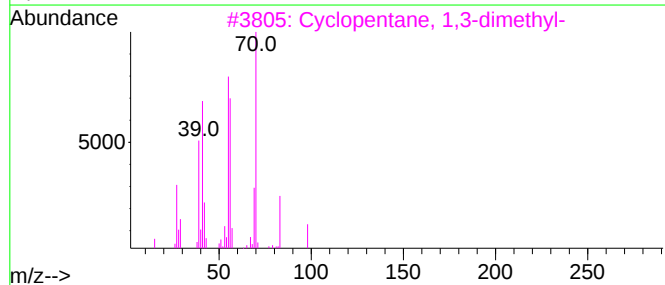
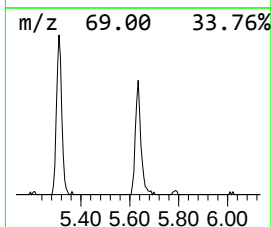
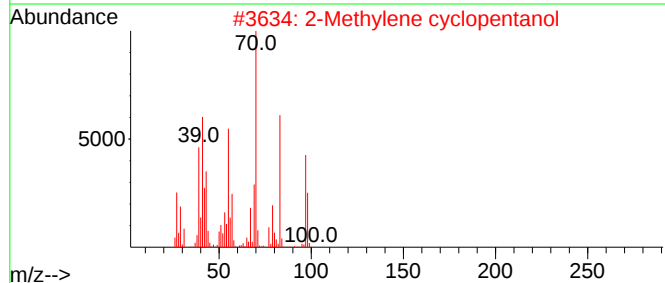
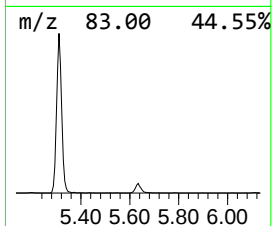
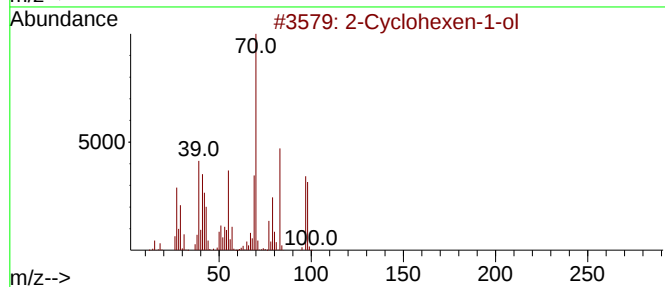
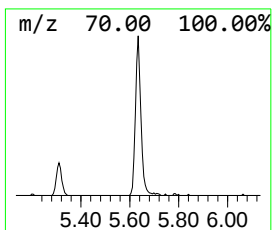
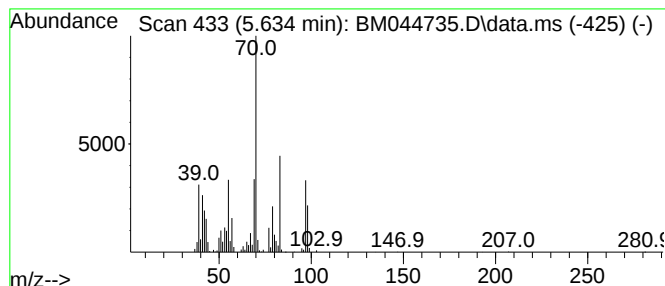
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Cyclohexen-1-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.634	3.31 ng	204923	1,4-Dichlorobenzene-d4	7.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	94
2			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	87
3			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	43
4			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	37
5			2,6-Cyclooctadien-1-ol	124	C8H12O	010017-18-2	32



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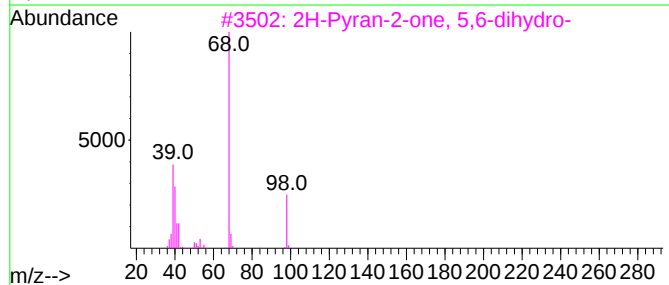
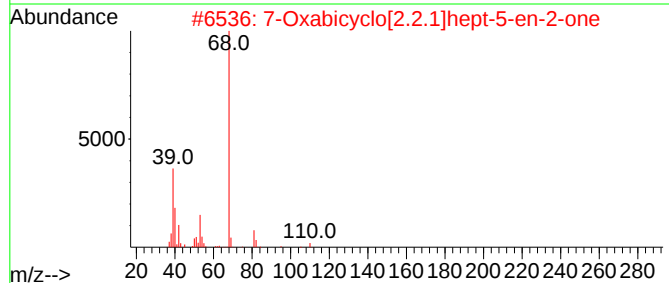
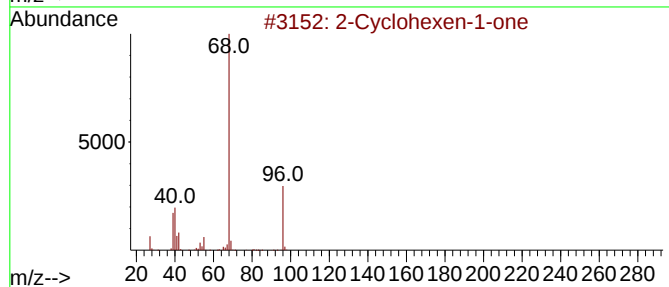
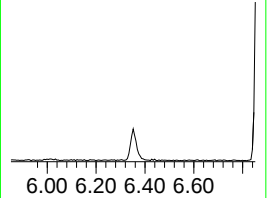
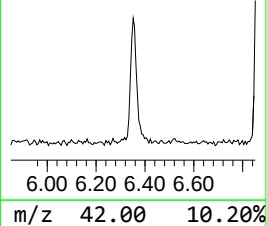
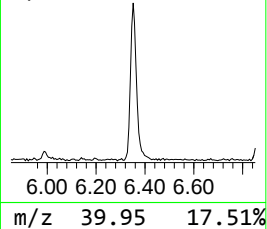
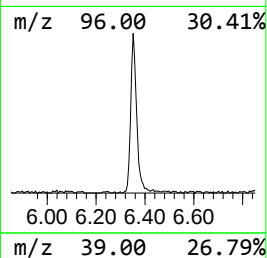
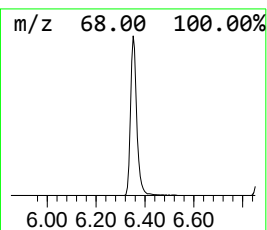
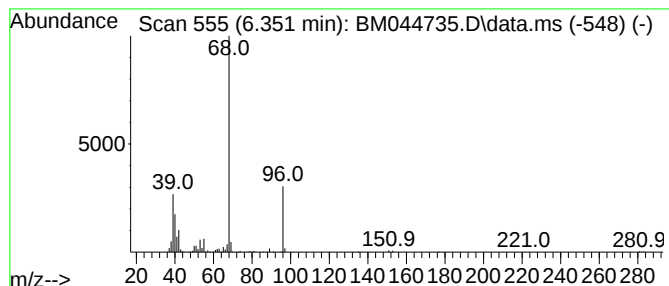
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Peak Number 3 2-Cyclohexen-1-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.351	5.16 ng	319505	1,4-Dichlorobenzene-d4	7.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2			7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	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	42
5			2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	36



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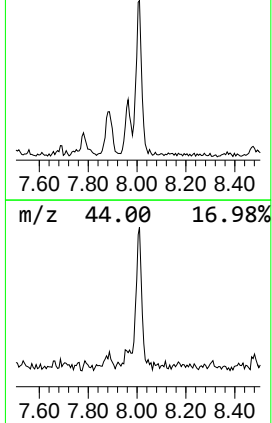
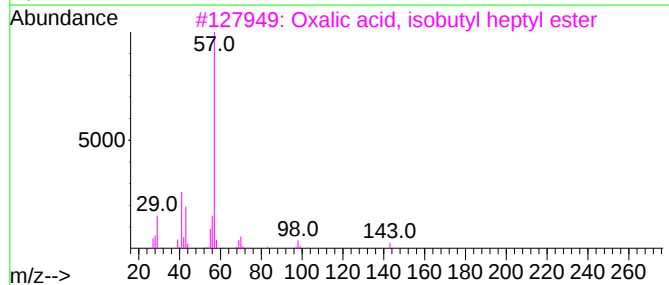
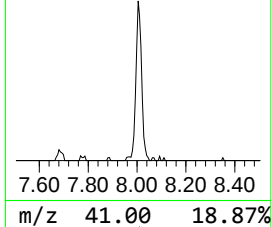
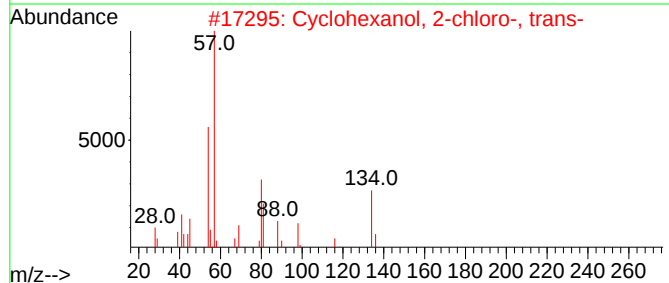
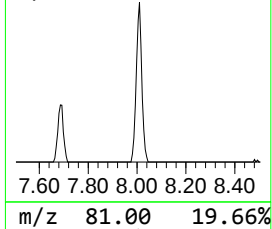
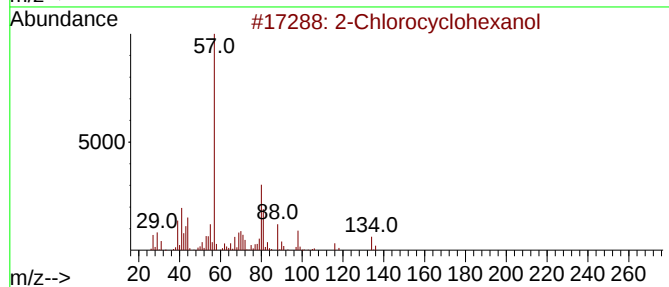
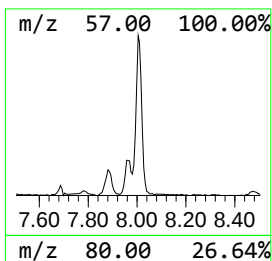
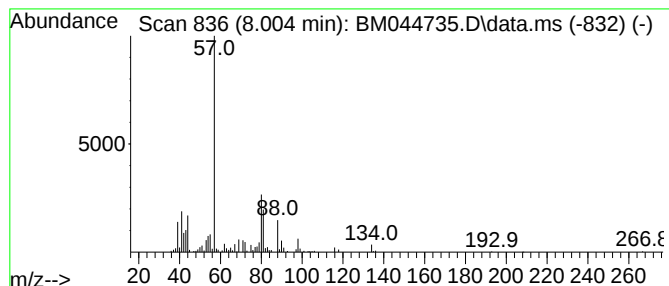
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Peak Number 4 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	4.46 ng	276253	1,4-Dichlorobenzene-d4	7.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	93
2			Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	28
3			Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	14
4			Butanoic acid, 2-hydroxy-3,3-dim...	132	C6H12O3	004026-20-4	10
5			(S)-(+)-3-Hydroxytetrahydrofuran	88	C4H8O2	086087-23-2	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.869	40.6	ng	2518440	1	7.687	1239320	20.0
2-Cyclohexen-1-ol	5.634	3.3	ng	204923	1	7.687	1239320	20.0
2-Cyclohexen-1-one	6.351	5.2	ng	319505	1	7.687	1239320	20.0
2-Chlorocyclohe...	8.004	4.5	ng	276253	1	7.687	1239320	20.0