

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092324\
 Data File : BM047600.D
 Acq On : 23 Sep 2024 11:04
 Operator : RC/JU
 Sample : PB163344BL
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB163344BL

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-BM092024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047600.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.104	169	173	179	rBV	105583	163081	1.27%	0.243%
2	4.952	311	317	328	rBV	3048054	4069375	31.58%	6.059%
3	5.416	388	396	409	rBV	4891170	6696921	51.97%	9.971%
4	5.746	444	452	456	rBV	172161	285501	2.22%	0.425%
5	6.463	568	574	582	rBV	295570	482435	3.74%	0.718%
6	7.004	658	666	675	rBV	4459618	6899886	53.54%	10.273%
7	7.840	802	808	815	rBV	1186703	1880169	14.59%	2.799%
8	8.004	830	836	844	rBV	77440	131092	1.02%	0.195%
9	8.081	844	849	855	rVV	79648	134773	1.05%	0.201%
10	8.157	855	862	869	rVB	233533	390744	3.03%	0.582%
11	8.992	996	1004	1014	rBV	3990292	6307114	48.94%	9.390%
12	10.634	1275	1283	1291	rBV	1430584	2404082	18.65%	3.579%
13	13.098	1694	1702	1717	rBV	8965059	12376375	96.04%	18.427%
14	14.469	1926	1935	1946	rBV	1658769	2463556	19.12%	3.668%
15	15.951	2180	2187	2204	rBV	2648139	3688983	28.63%	5.492%
16	17.204	2393	2400	2410	rBV	1697632	2376388	18.44%	3.538%
17	19.821	2839	2845	2851	rBV	11823929	12887172	100.00%	19.187%
18	21.427	3113	3118	3124	rBV2	1333540	1925766	14.94%	2.867%
19	24.450	3625	3632	3640	rBV	670334	1602114	12.43%	2.385%

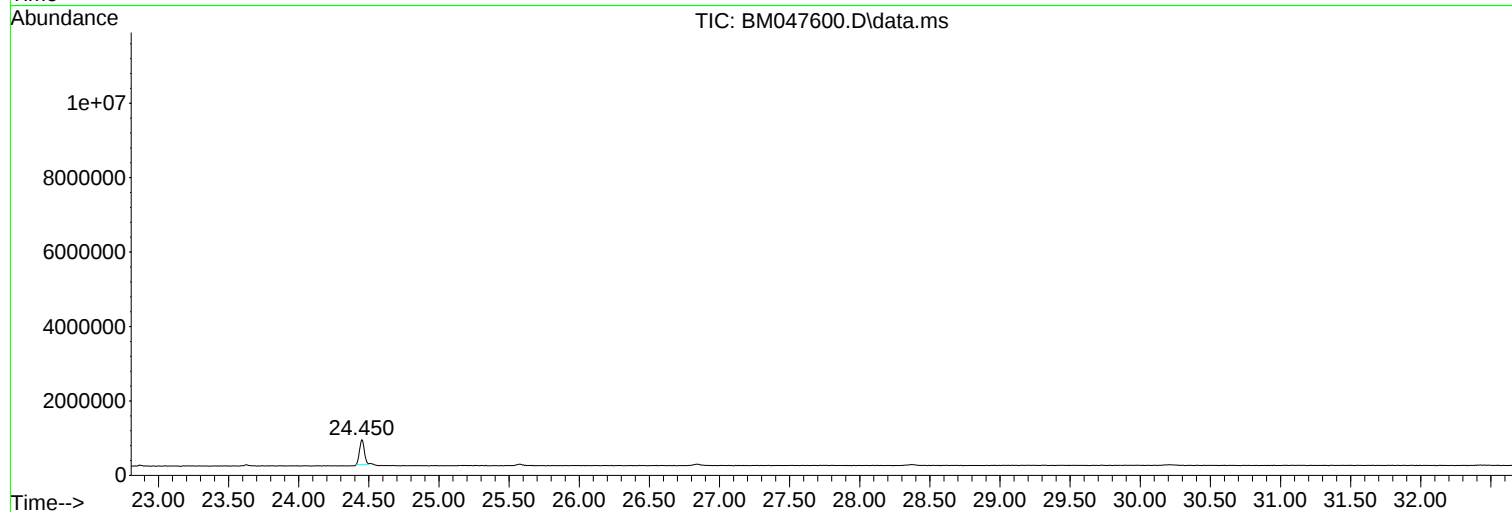
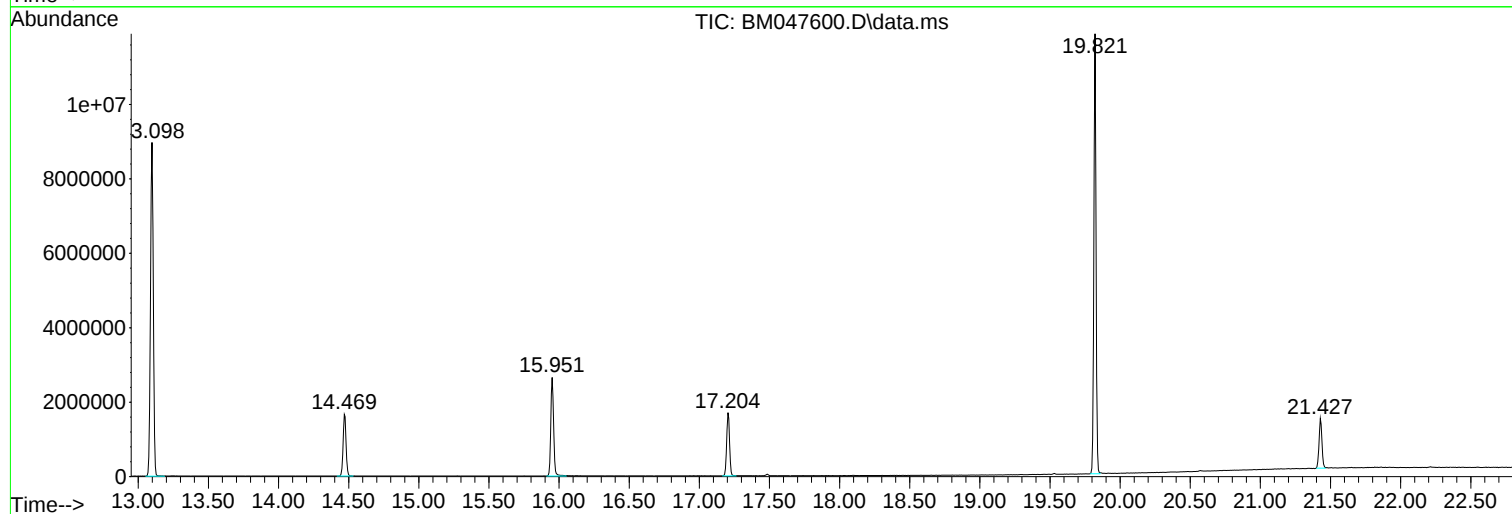
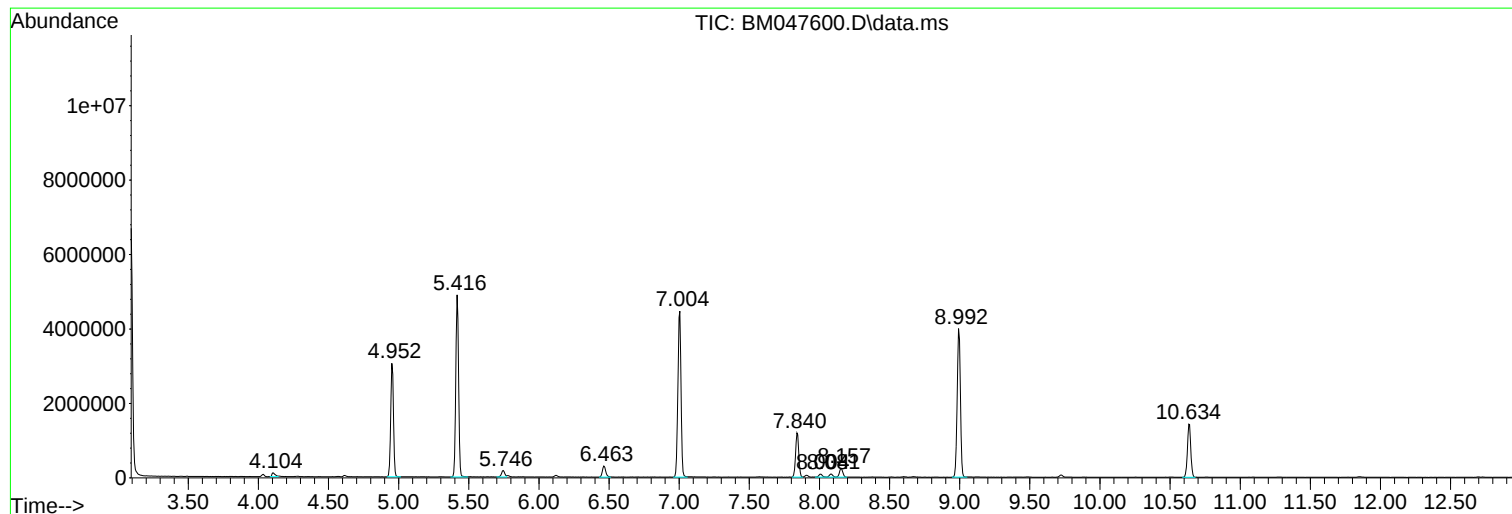
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 4 Sample Multiplier: 1

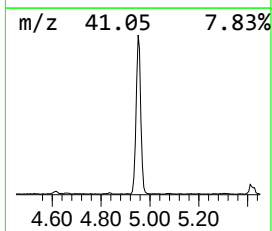
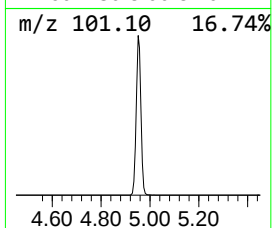
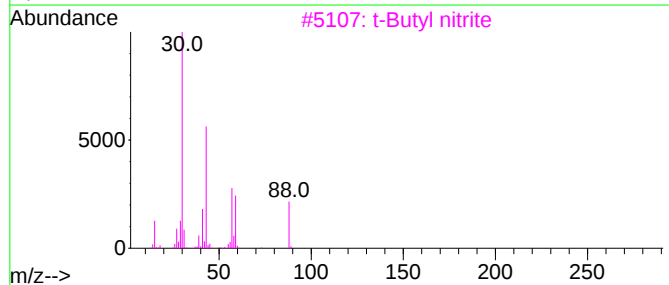
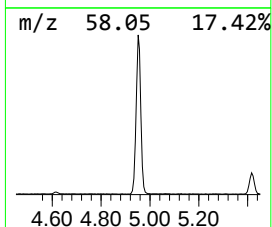
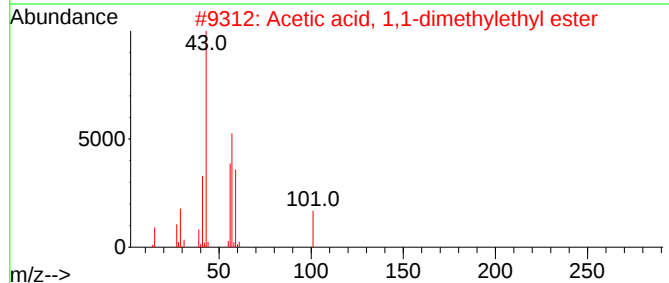
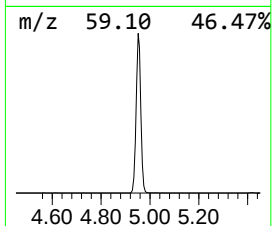
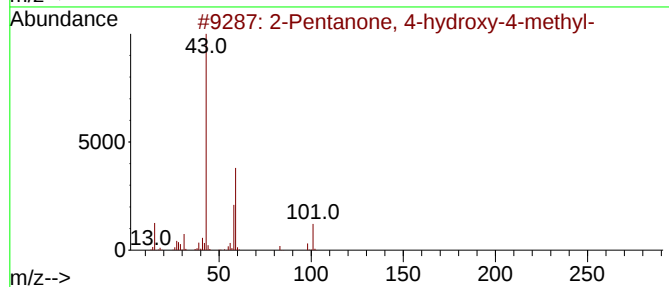
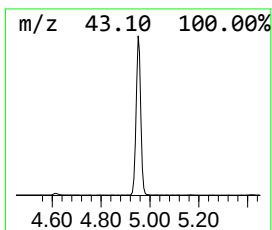
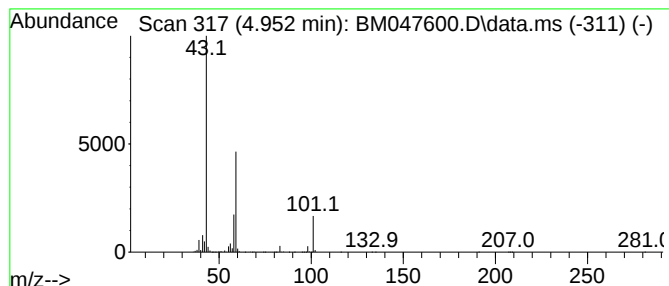
Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM092024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
4.952	43.29 ng	4069380	1,4-Dichlorobenzene-d4	7.845	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	t-Butyl nitrite	103	C4H9NO2	000540-80-7	38
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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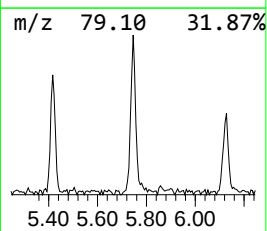
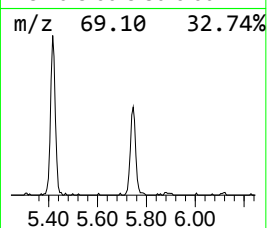
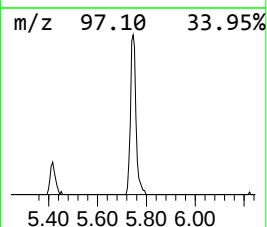
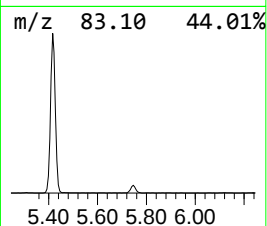
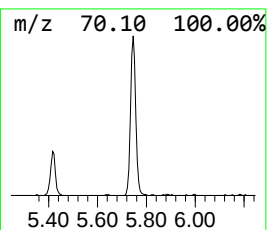
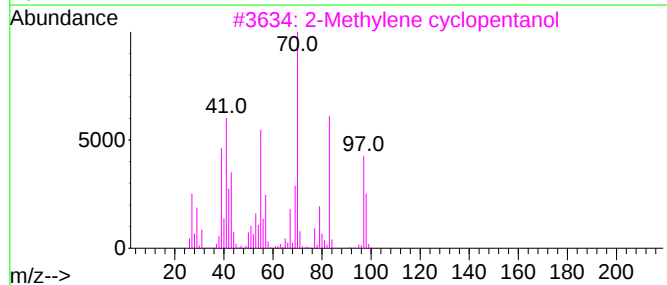
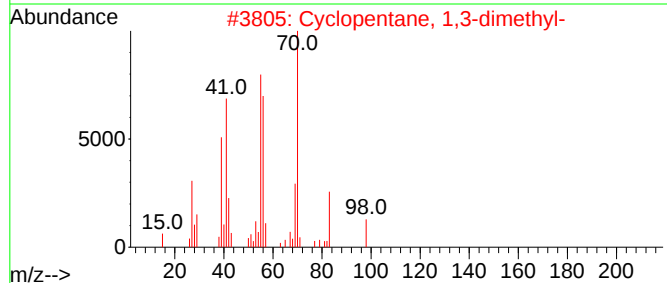
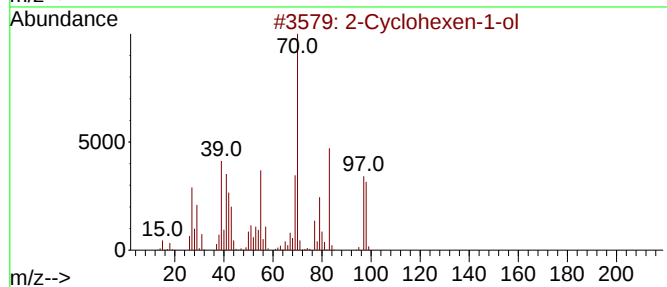
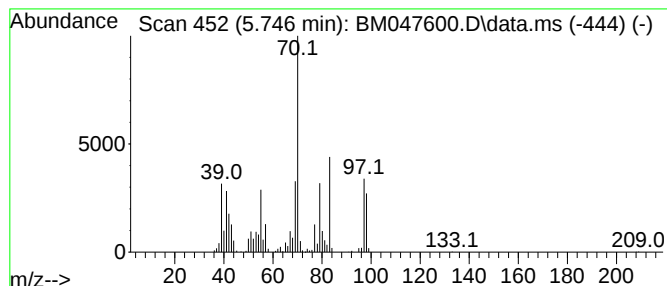
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.746	3.04 ng	285501	1,4-Dichlorobenzene-d4	7.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	93
2			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	50
3			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	47
4			2,6-Cyclooctadien-1-ol	124	C8H12O	010017-18-2	38
5			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	32



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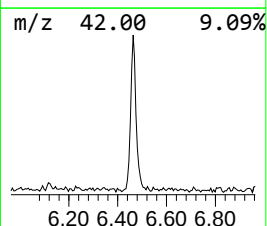
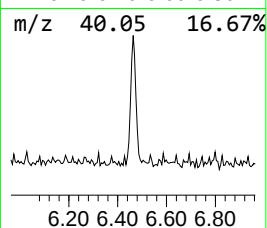
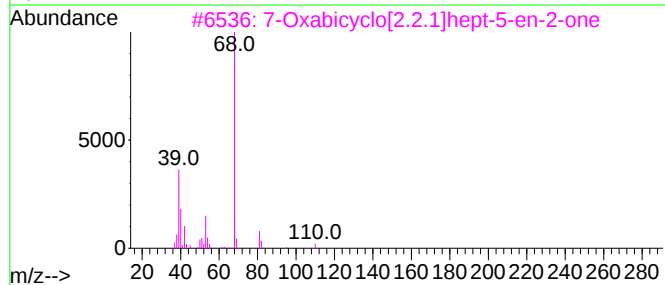
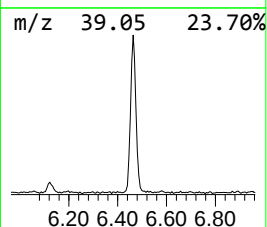
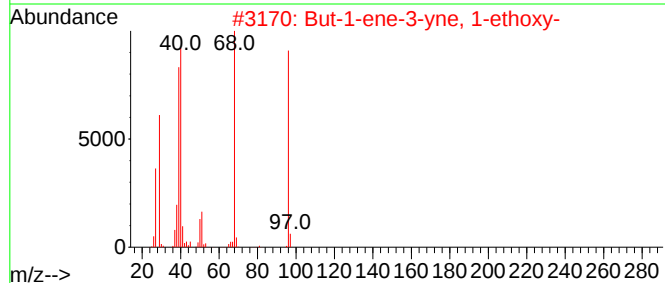
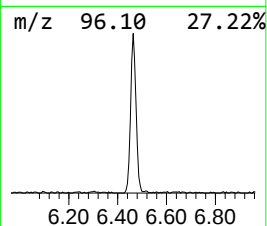
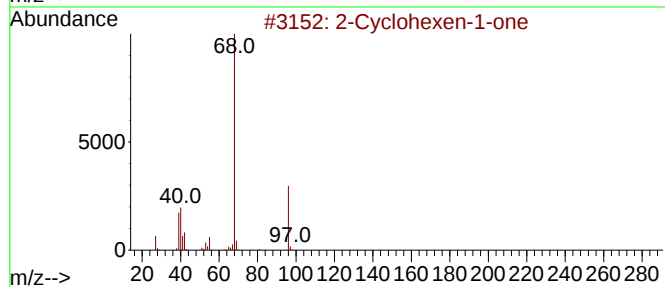
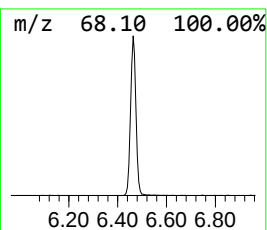
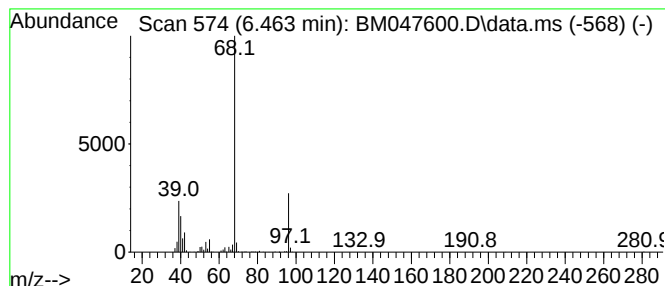
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.463	5.13 ng	482435	1,4-Dichlorobenzene-d4	7.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2			But-1-ene-3-yne, 1-ethoxy-	96	C6H8O	002806-41-9	38
3			7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	12
4			1H-Pyrazole	68	C3H4N2	000288-13-1	9
5			Furan	68	C4H4O	000110-00-9	9



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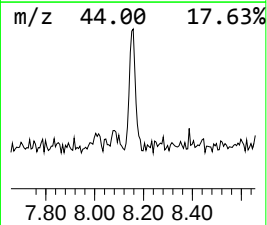
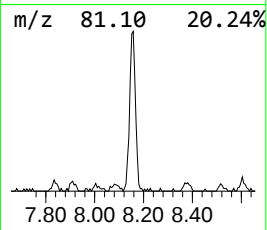
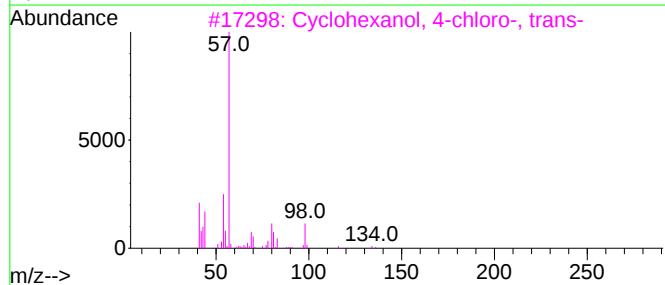
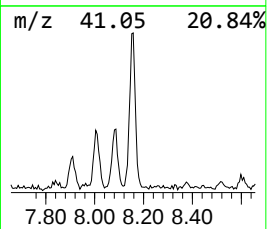
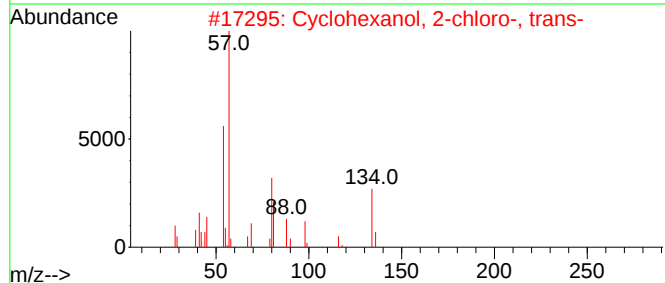
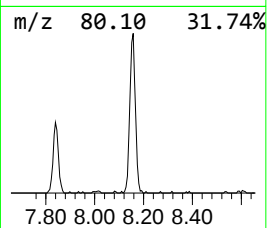
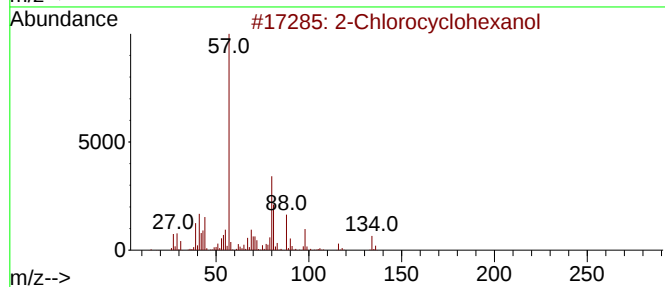
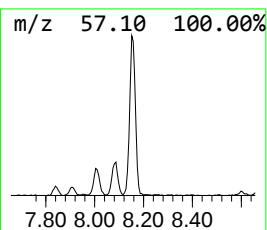
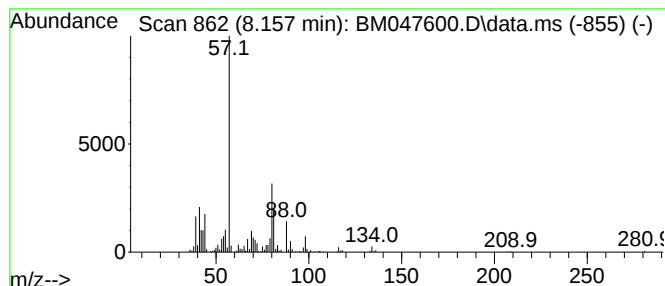
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.157	4.16 ng	390744	1,4-Dichlorobenzene-d4	7.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	94
2			Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	45
3			Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	25
4			(t-Butylthio)carbonylacetic acid...	204	C9H16O3S	1000192-52-7	17
5			4-Chlorocyclohexanol	134	C6H11ClO	030485-71-3	16



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.952	43.3	ng	4069380	1	7.845	1880170	20.0
2-Cyclohexen-1-ol	5.746	3.0	ng	285501	1	7.845	1880170	20.0
2-Cyclohexen-1-one	6.463	5.1	ng	482435	1	7.845	1880170	20.0
2-Chlorocyclohe...	8.157	4.2	ng	390744	1	7.845	1880170	20.0