

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121423\
 Data File : BF136570.D
 Acq On : 14 Dec 2023 16:07
 Operator : CG\JU
 Sample : PB157641BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB157641BL

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_F\Methods\8270-BF120523.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136570.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	9	16	23	rVB	864224	1915668	42.31%	7.772%
2	5.034	495	501	508	rBV	968408	1258428	27.79%	5.106%
3	5.434	564	569	572	rBV	2321247	2000565	44.18%	8.117%
4	5.598	594	597	607	rBV2	105593	107885	2.38%	0.438%
5	6.040	669	672	677	rBV	158290	125102	2.76%	0.508%
6	6.428	733	738	741	rBV	1991028	1975013	43.62%	8.013%
7	6.781	795	798	802	rBV	695386	617506	13.64%	2.505%
8	6.940	821	825	836	rBV	151381	154442	3.41%	0.627%
9	7.345	888	894	897	rBV	1688955	1916112	42.32%	7.774%
10	8.063	1011	1016	1019	rBV	943695	863943	19.08%	3.505%
11	9.145	1193	1200	1203	rBV	4205929	4006412	88.48%	16.255%
12	9.822	1309	1315	1318	rBV	1074800	1024393	22.62%	4.156%
13	10.610	1445	1449	1453	rBV	1824299	1619128	35.76%	6.569%
14	11.310	1564	1568	1571	rBV	1399915	1102549	24.35%	4.473%
15	12.910	1835	1840	1843	rBV	4432739	4527804	100.00%	18.370%
16	13.963	2014	2019	2022	rBV	839123	804865	17.78%	3.265%
17	15.439	2264	2270	2275	rBV	518395	627835	13.87%	2.547%

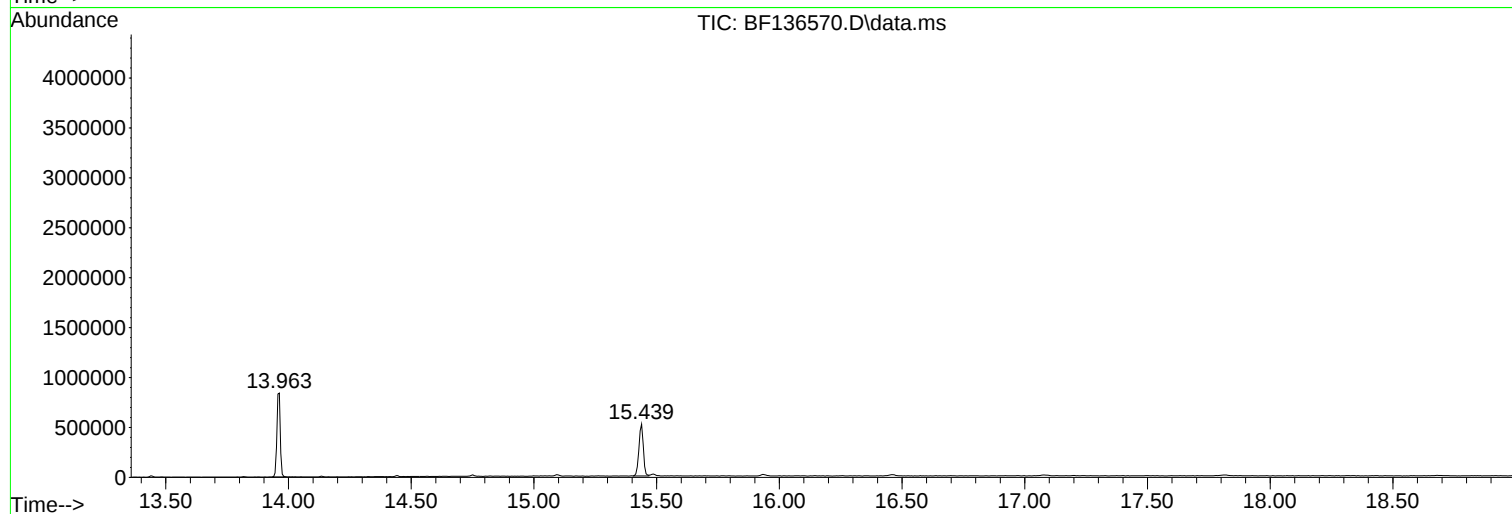
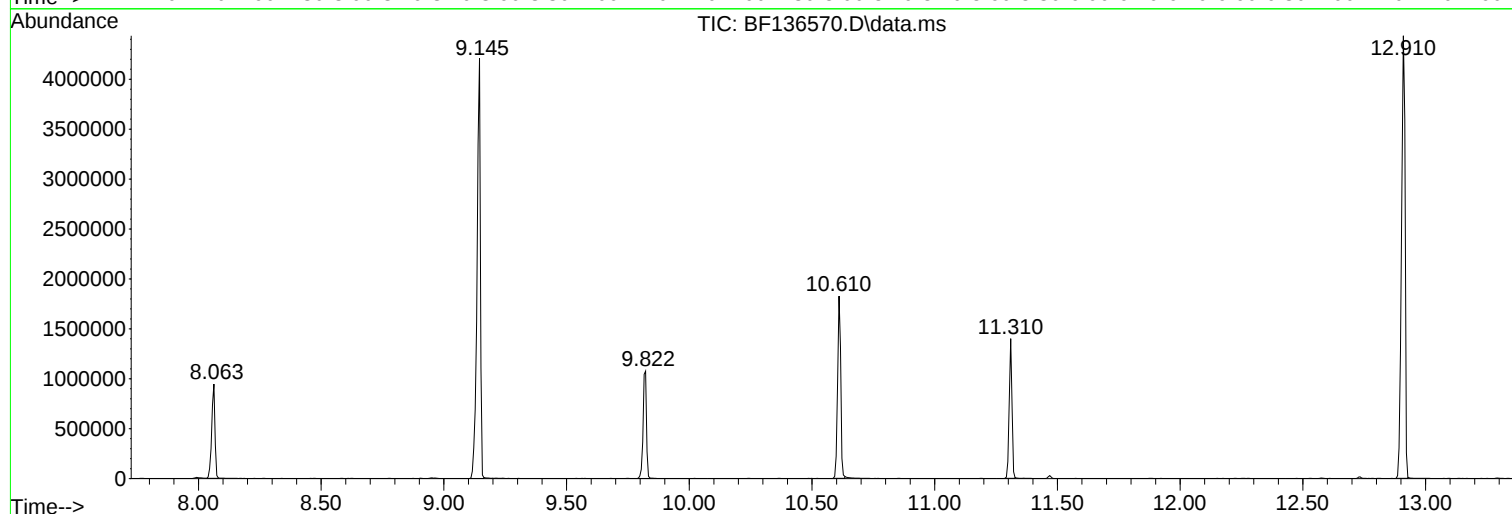
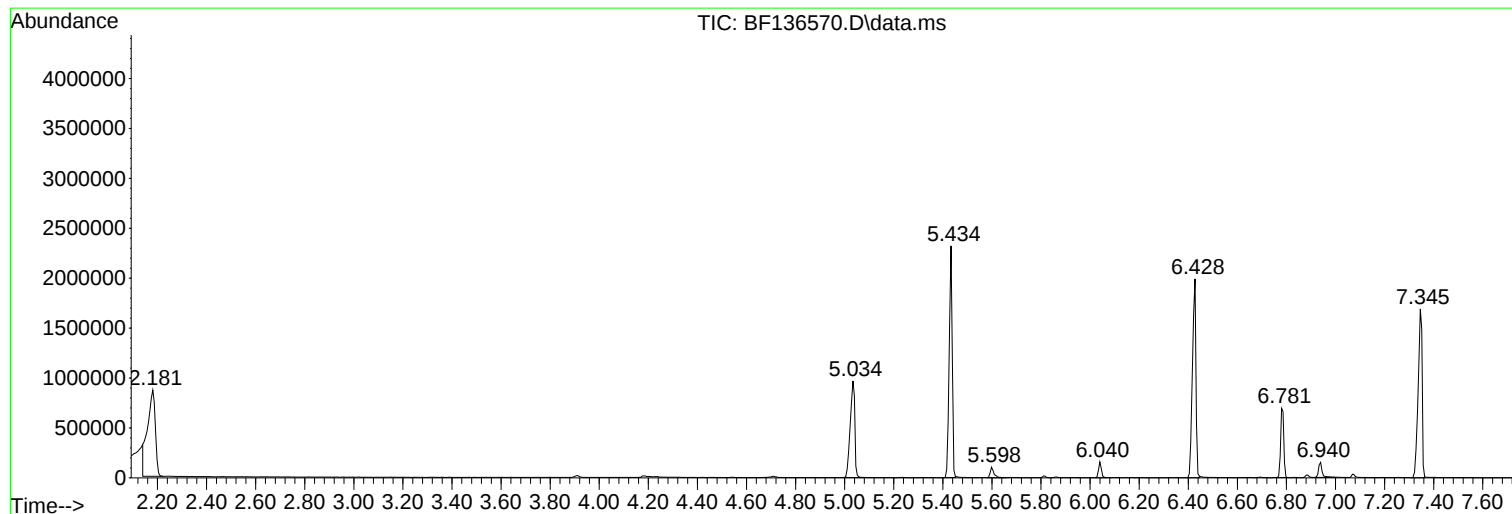
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF120523.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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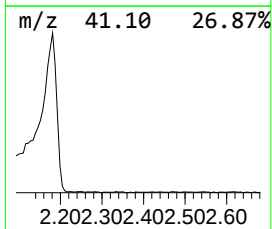
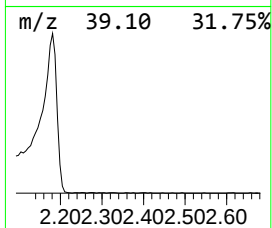
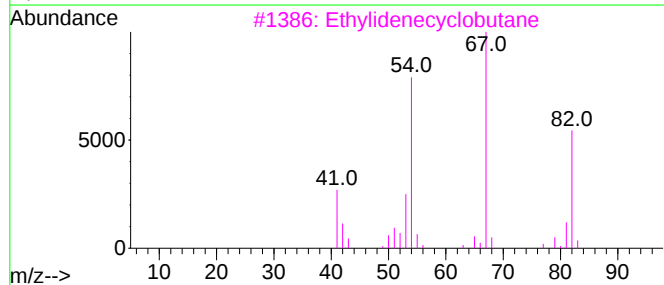
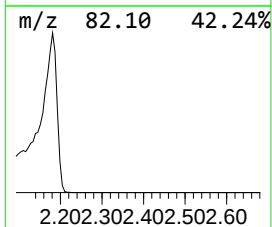
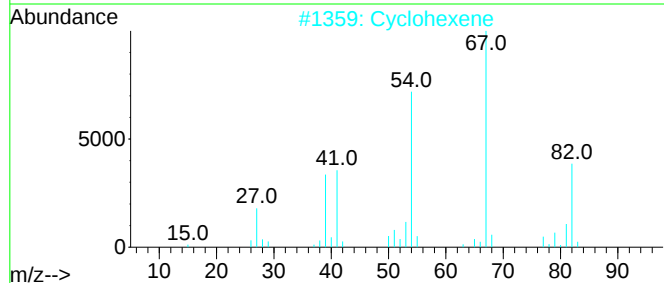
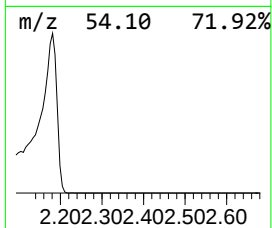
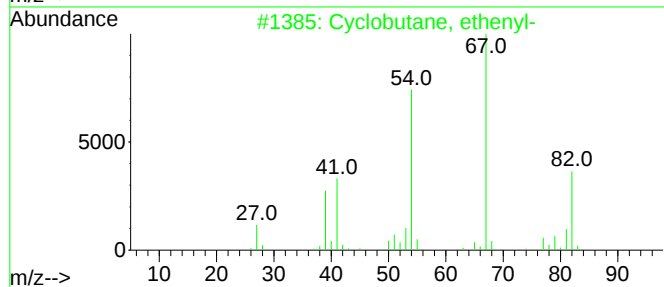
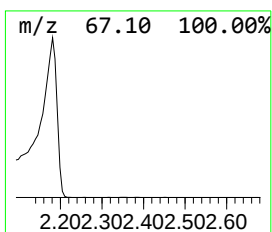
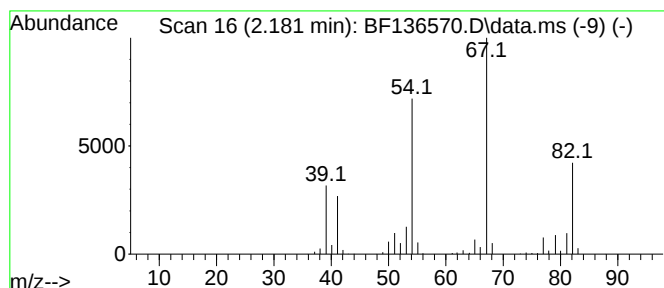
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclobutane, ethenyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.181	62.05 ng	1915670	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, ethenyl-	82	C6H10	002597-49-1	94
2			Cyclohexene	82	C6H10	000110-83-8	94
3			Ethylidenecyclobutane	82	C6H10	001528-21-8	87
4			(Z),(Z)-2,4-Hexadiene	82	C6H10	006108-61-8	81
5			C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	81



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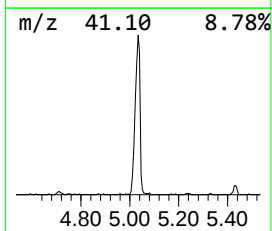
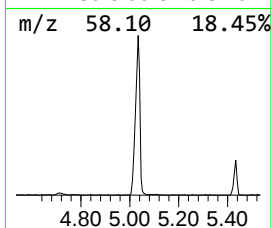
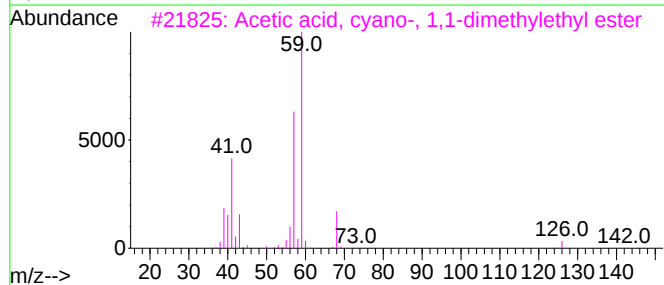
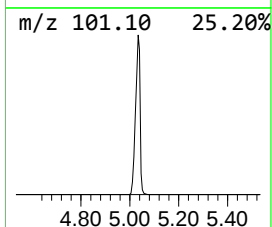
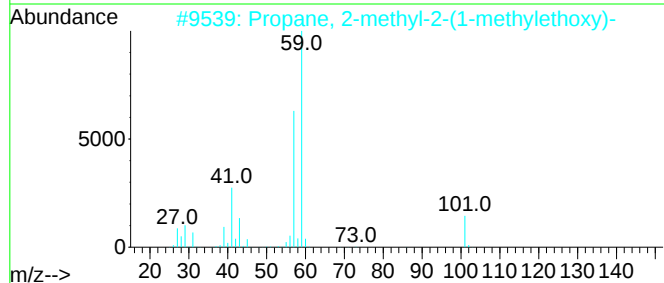
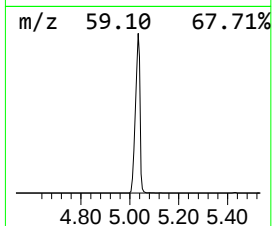
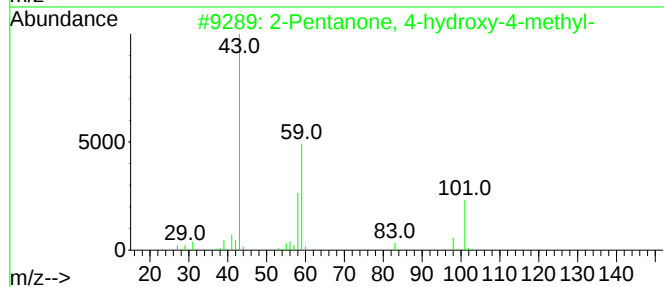
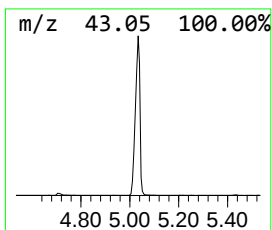
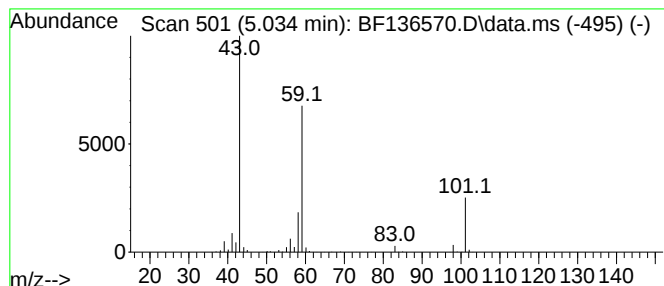
Instrument :
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ClientSampleId :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.034	40.76 ng	1258430	1,4-Dichlorobenzene-d4	6.787	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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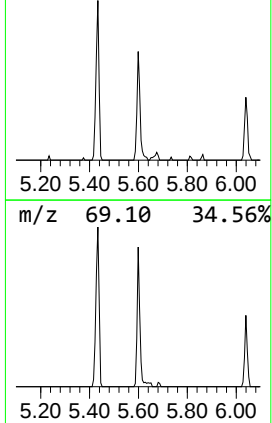
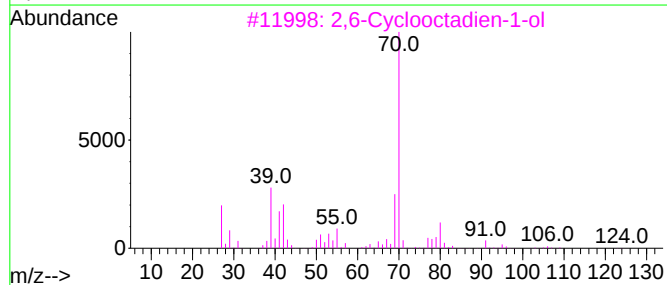
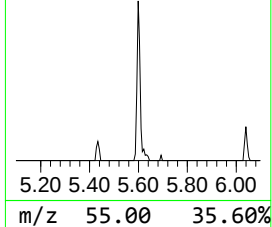
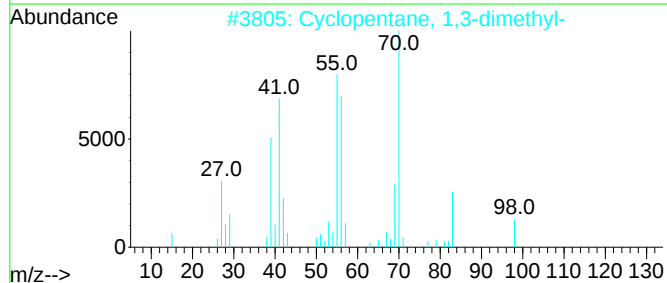
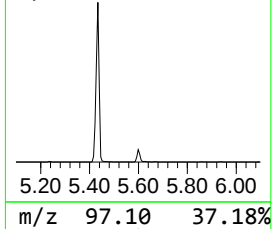
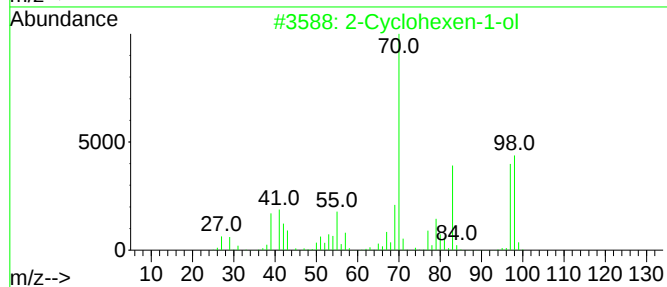
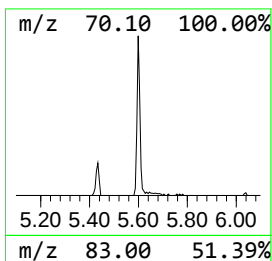
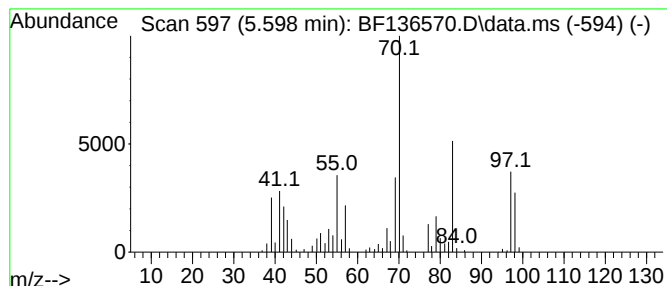
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Cyclohexen-1-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.598	3.49 ng	107885	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol			98	C6H10O	000822-67-3	64
2	Cyclopentane, 1,3-dimethyl-			98	C7H14	002453-00-1	38
3	2,6-Cyclooctadien-1-ol			124	C8H12O	010017-18-2	37
4	1-Cyclopropylpropan-1-amine			99	C6H13N	1000436-93-8	37
5	Cyclopentane, 1,3-dimethyl-, cis-			98	C7H14	002532-58-3	33



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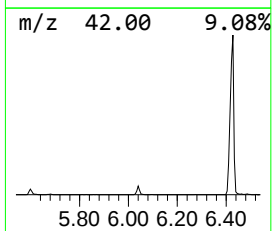
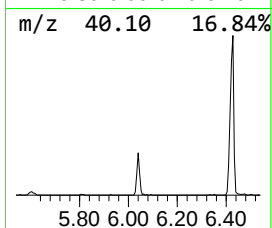
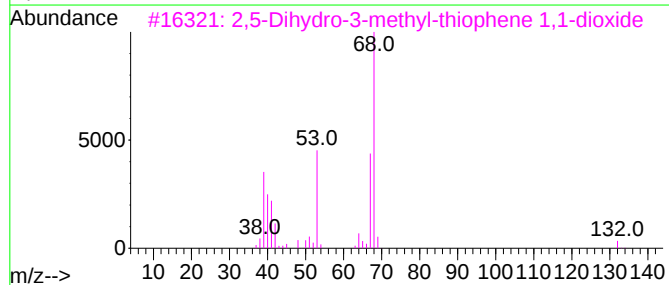
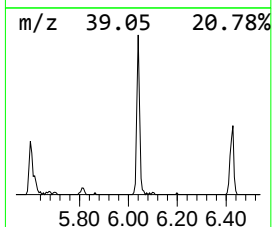
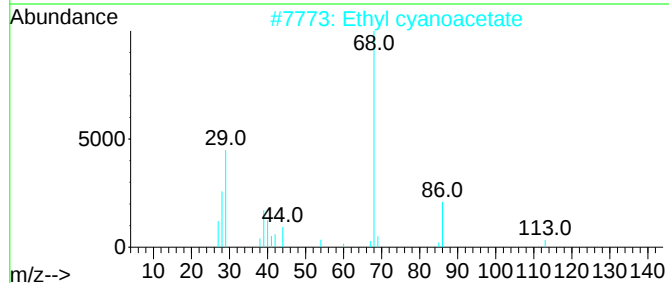
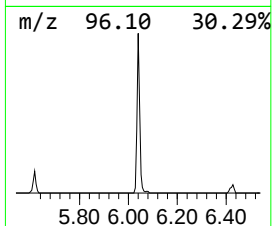
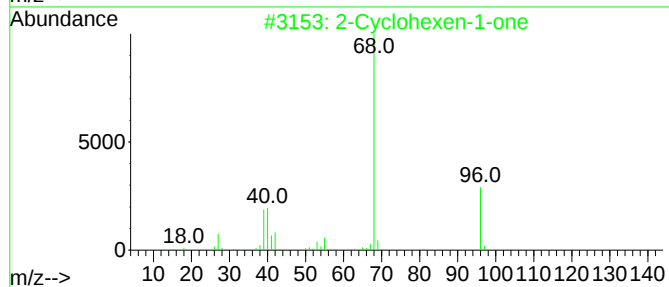
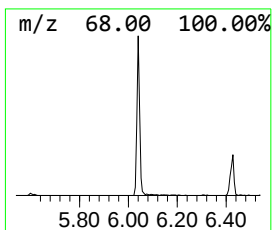
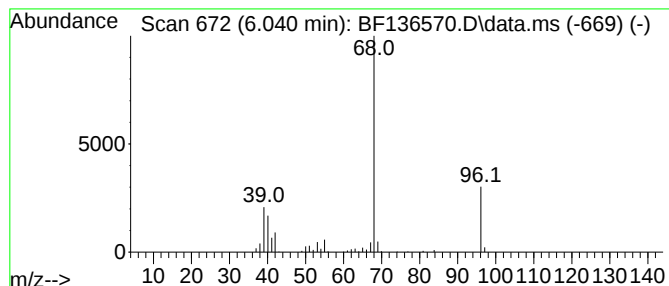
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.040	4.05 ng	125102	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2			Ethyl cyanoacetate	113	C5H7NO2	000105-56-6	36
3			2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	16
4			7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	12
5			1H-Pyrazole	68	C3H4N2	000288-13-1	9



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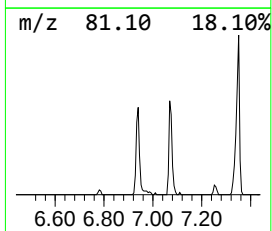
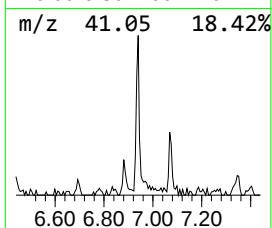
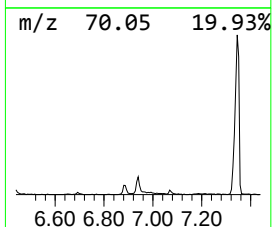
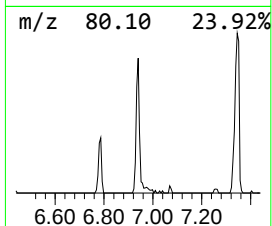
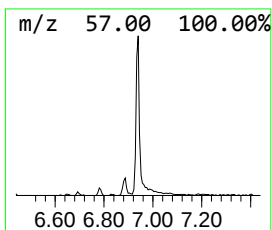
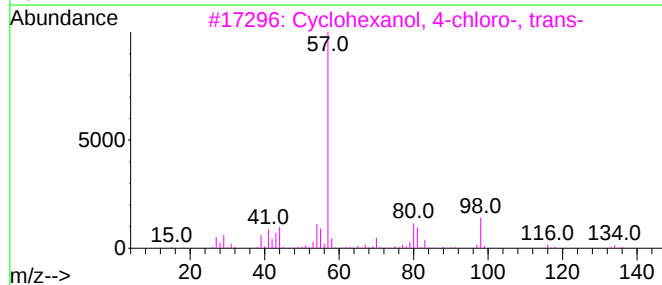
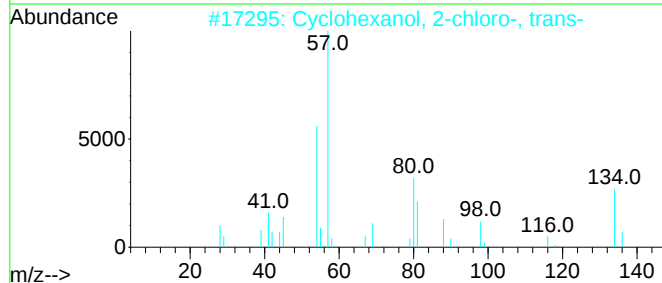
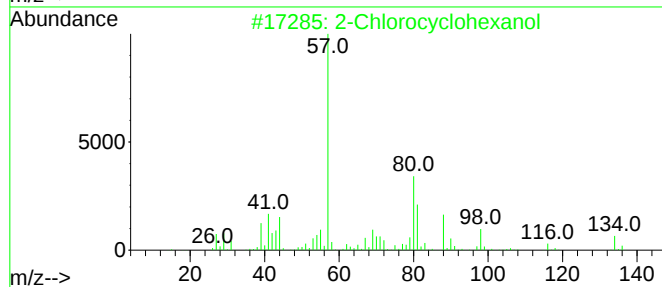
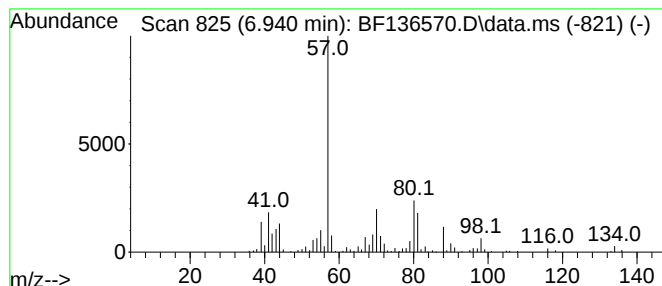
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.940	5.00 ng	154442	1,4-Dichlorobenzene-d4	6.787

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	38
3			Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	38
4			(S)-(+)-3-Hydroxytetrahydrofuran	88	C4H8O2	086087-23-2	37
5			3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	37



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclobutane, et...	2.181	62.0	ng	1915670	1	6.787	617506	20.0
2-Pentanone, 4-...	5.034	40.8	ng	1258430	1	6.787	617506	20.0
2-Cyclohexen-1-ol	5.598	3.5	ng	107885	1	6.787	617506	20.0
2-Cyclohexen-1-one	6.040	4.0	ng	125102	1	6.787	617506	20.0
2-Chlorocyclohe...	6.940	5.0	ng	154442	1	6.787	617506	20.0