

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022624\
 Data File : BF137381.D
 Acq On : 26 Feb 2024 12:48
 Operator : CG\JU
 Sample : PB159110BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB159110BL

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-BF022324.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137381.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	31	rVB	2389286	5324825	63.69%	10.488%
2	5.045	497	503	510	rBV	2513546	3033136	36.28%	5.974%
3	5.440	566	570	587	rBV	4460939	4316163	51.62%	8.501%
4	5.610	596	599	611	rBV2	203630	238785	2.86%	0.470%
5	6.051	671	674	687	rBV	308461	345446	4.13%	0.680%
6	6.434	734	739	762	rBV	4233855	4505540	53.89%	8.874%
7	6.798	798	801	808	rBV	1367423	1197931	14.33%	2.359%
8	6.951	823	827	845	rVB	440481	458781	5.49%	0.904%
9	7.357	892	896	926	rBV	3535693	4033832	48.25%	7.945%
10	8.075	1014	1018	1041	rBV	1764603	1726379	20.65%	3.400%
11	9.157	1196	1202	1205	rBV	7221091	7049743	84.32%	13.885%
12	9.828	1313	1316	1334	rVB	2180308	2061403	24.66%	4.060%
13	10.622	1447	1451	1470	rBV	3115555	2914707	34.86%	5.741%
14	11.322	1566	1570	1586	rBV	2555093	2249889	26.91%	4.431%
15	12.927	1837	1843	1846	rBV	7821323	8360954	100.00%	16.468%
16	13.974	2017	2021	2034	rBV	1916226	1770311	21.17%	3.487%
17	15.457	2268	2273	2281	rBV	923014	1183302	14.15%	2.331%

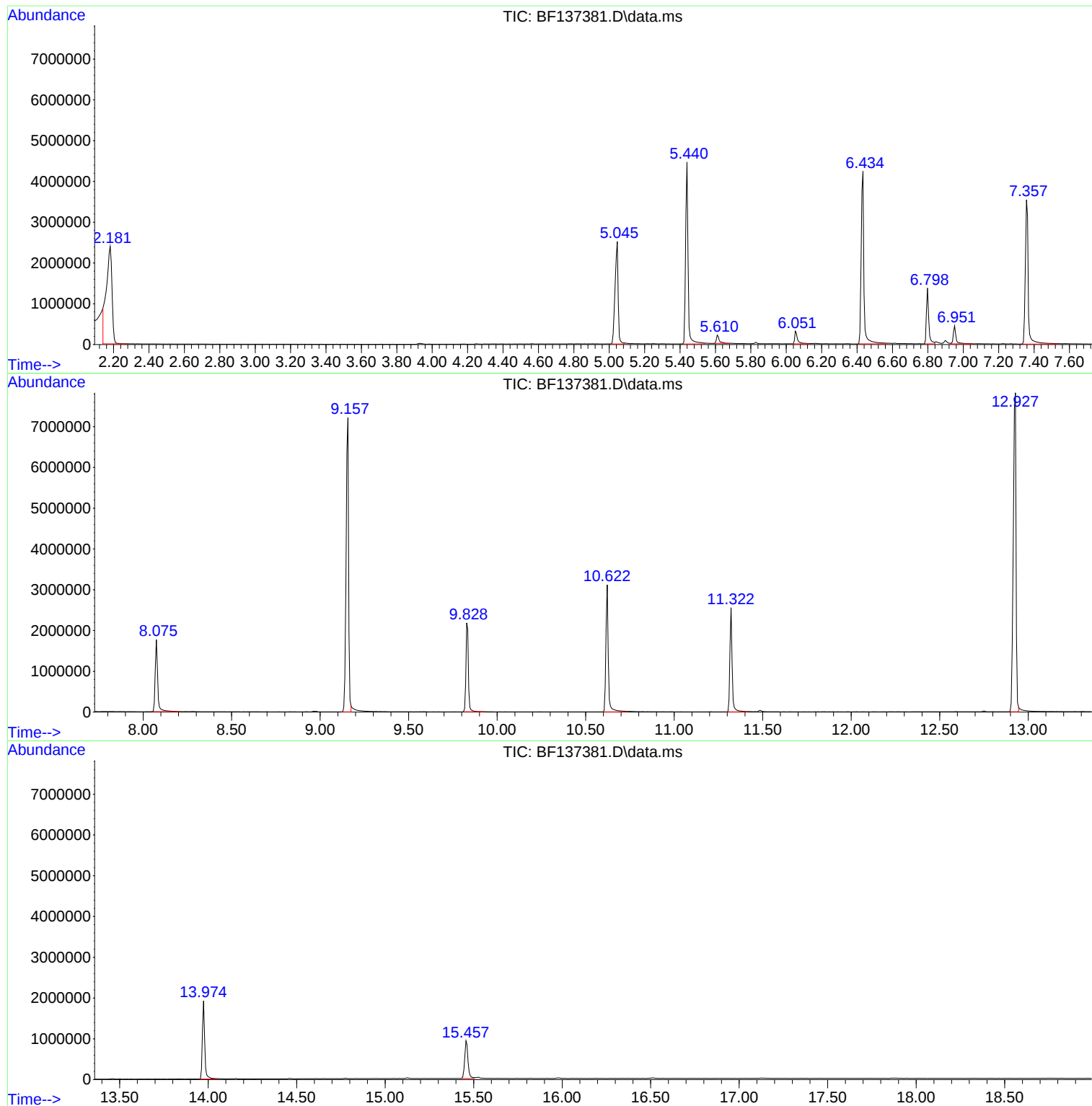
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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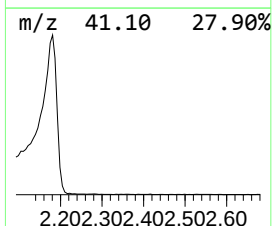
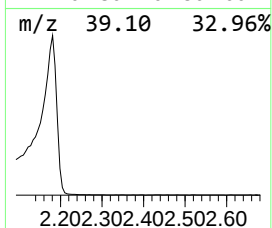
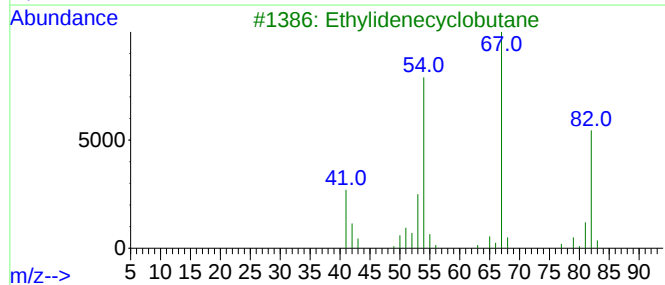
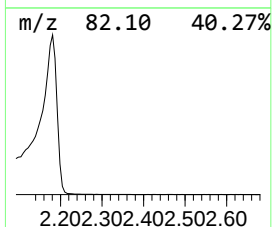
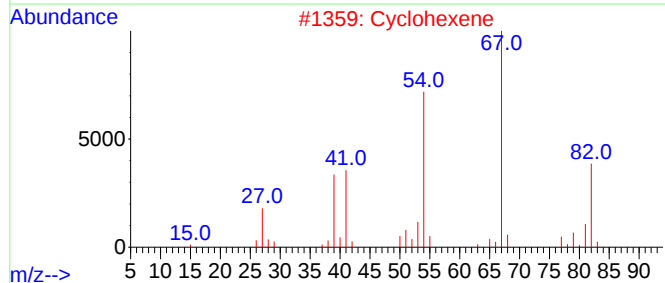
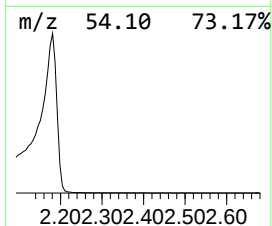
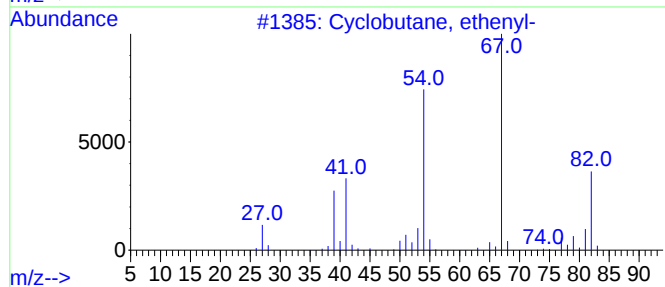
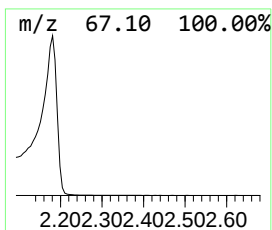
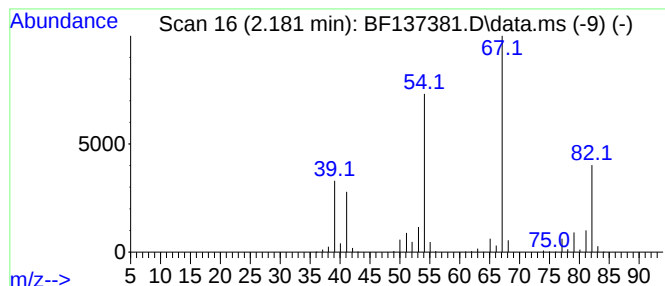
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	88.90 ng	5324830	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclobutane, ethenyl-	82	C6H10	002597-49-1	95
2			Cyclohexene	82	C6H10	000110-83-8	95
3			Ethylidenecyclobutane	82	C6H10	001528-21-8	91
4			Cyclopentane, methylene-	82	C6H10	001528-30-9	35
5			C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	35



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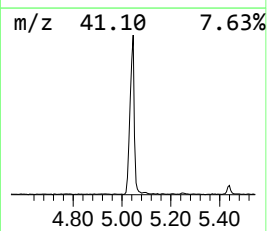
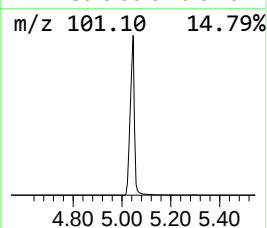
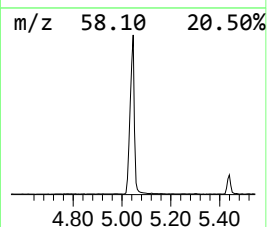
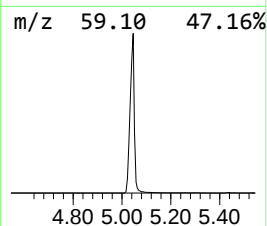
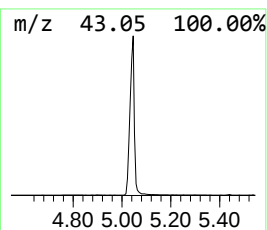
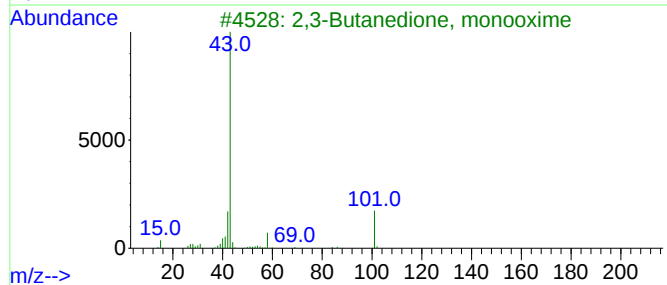
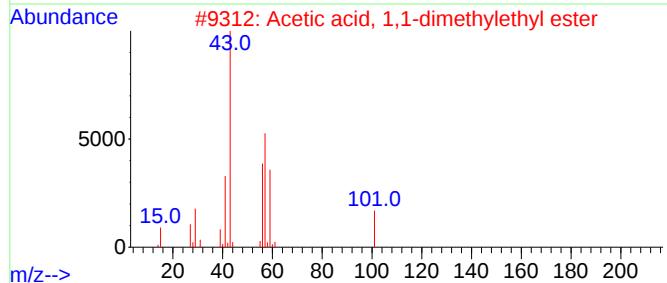
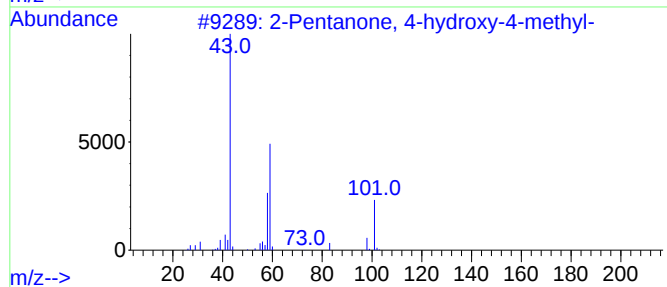
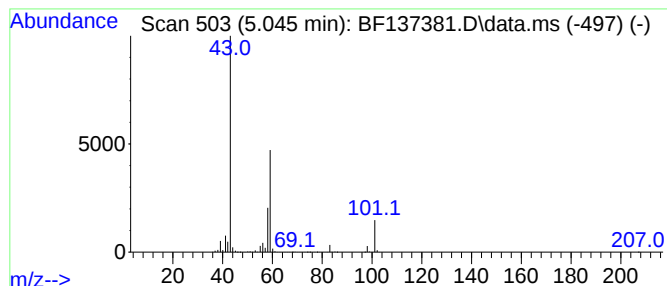
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	50.64 ng	3033140	1,4-Dichlorobenzene-d4	6.798

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	36
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			Acetone	58	C3H6O	000067-64-1	9



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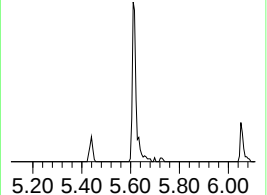
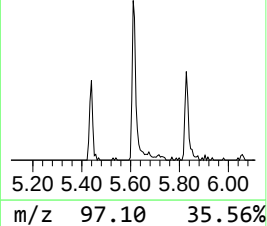
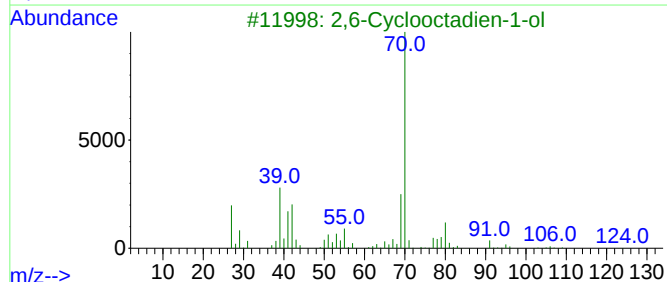
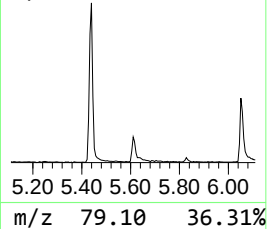
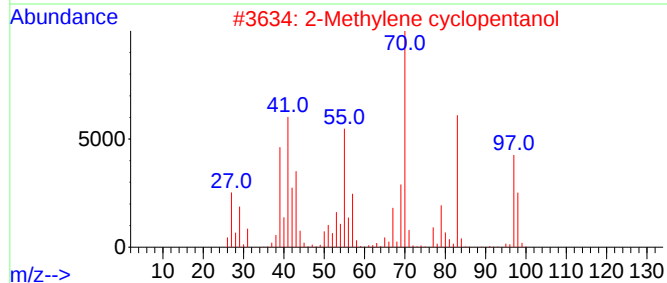
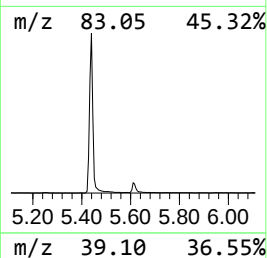
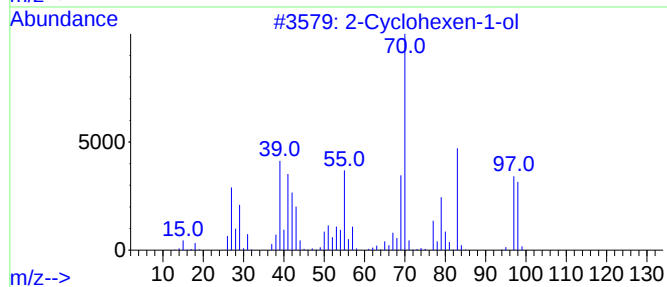
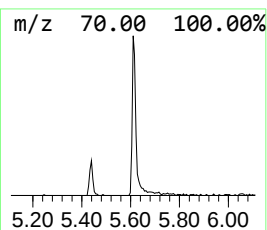
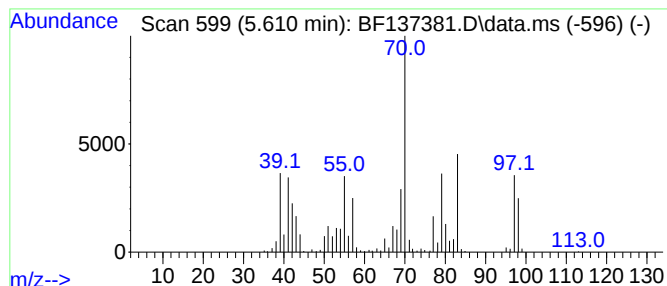
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Peak Number 3 2-Cyclohexen-1-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.610	3.99 ng	238785	1,4-Dichlorobenzene-d4	6.798

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	40
3			2,6-Cyclooctadien-1-ol	124	C8H12O	010017-18-2	38
4			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	37
5			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	32



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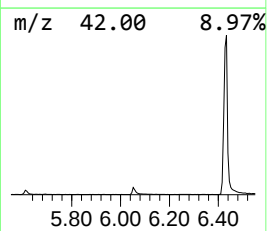
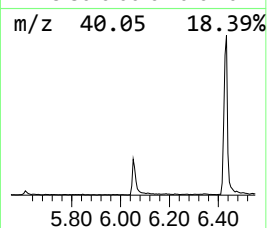
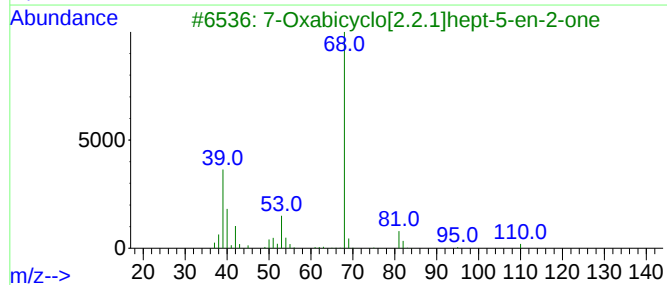
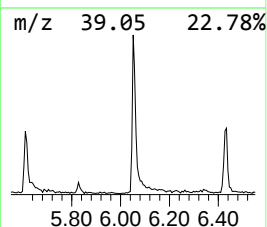
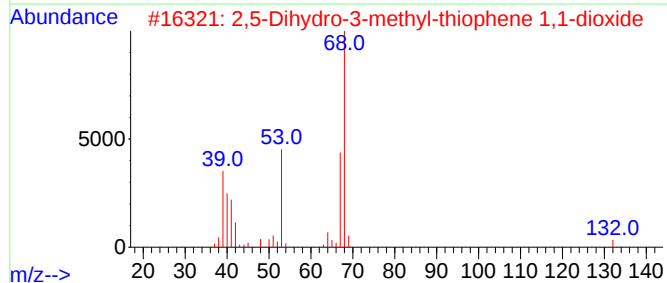
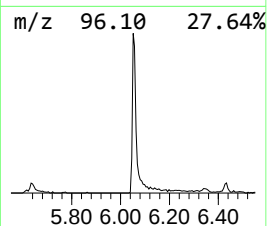
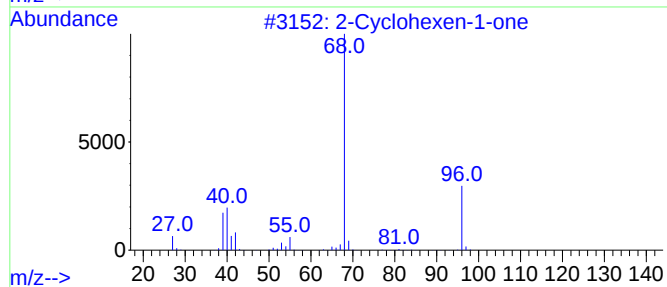
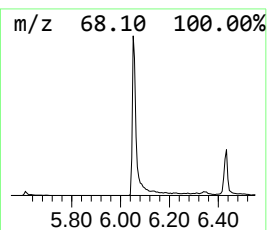
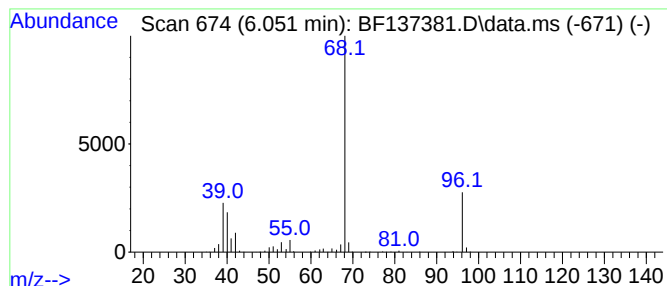
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Peak Number 4 2-Cyclohexen-1-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.051	5.77 ng	345446	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2			2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	33
3			7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	10
4			1H-Imidazole	68	C3H4N2	000288-32-4	9
5			1H-Pyrazole	68	C3H4N2	000288-13-1	9



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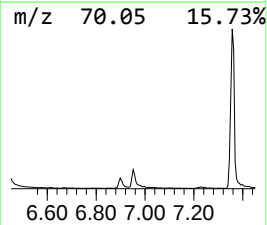
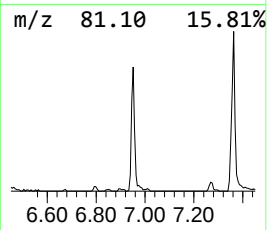
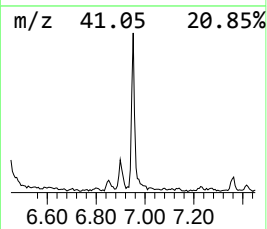
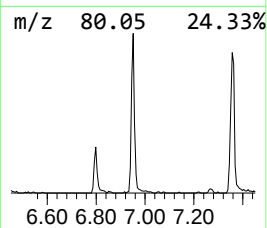
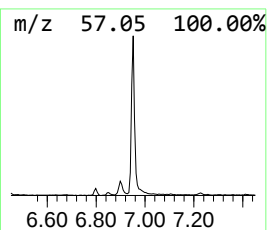
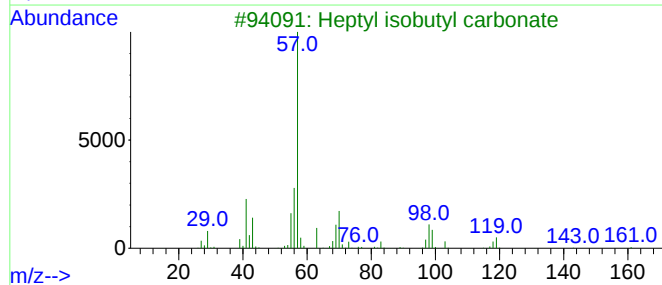
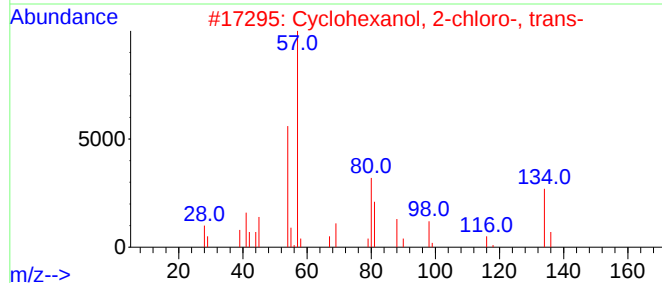
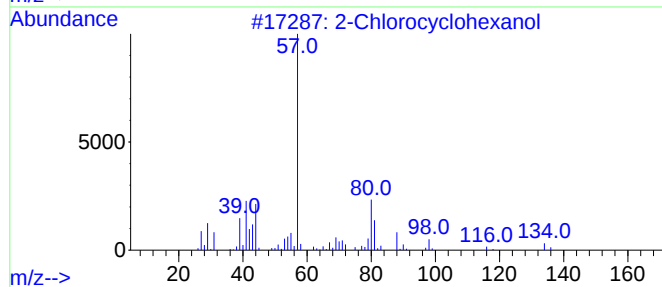
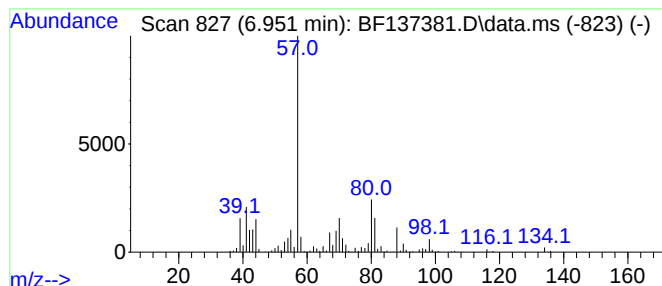
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Peak Number 5 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.951	7.66 ng	458781	1,4-Dichlorobenzene-d4	6.798

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	70
2			Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	45
3			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	27
4			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	27
5			(S)-(+)-3-Hydroxytetrahydrofuran	88	C4H8O2	086087-23-2	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclobutane, et...	2.181	88.9	ng	5324830	1	6.798	1197930	20.0
2-Pentanone, 4-...	5.045	50.6	ng	3033140	1	6.798	1197930	20.0
2-Cyclohexen-1-ol	5.610	4.0	ng	238785	1	6.798	1197930	20.0
2-Cyclohexen-1-one	6.051	5.8	ng	345446	1	6.798	1197930	20.0
2-Chlorocyclohe...	6.951	7.7	ng	458781	1	6.798	1197930	20.0