

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM091924\
 Data File : BM047573.D
 Acq On : 19 Sep 2024 16:33
 Operator : RC/JU
 Sample : PB163344BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB163344BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BM091424.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047573.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	185	rBV	111397	199764	1.32%	0.269%
2	4.951	311	317	326	rBV	3174127	4261120	28.13%	5.742%
3	5.416	389	396	407	rBV	5074185	7055489	46.57%	9.508%
4	5.745	444	452	456	rBV2	191577	318529	2.10%	0.429%
5	6.463	568	574	583	rBV	329498	545220	3.60%	0.735%
6	7.004	658	666	679	rBV	4808764	7364653	48.61%	9.924%
7	7.839	802	808	815	rBV	1299576	1998050	13.19%	2.693%
8	8.081	843	849	855	rBV2	95085	153727	1.01%	0.207%
9	8.157	855	862	868	rVB	255587	424111	2.80%	0.572%
10	8.992	997	1004	1015	rBV	4185478	6805312	44.92%	9.171%
11	10.633	1275	1283	1293	rBV	1514265	2568735	16.96%	3.462%
12	13.098	1695	1702	1708	rBV	9561408	13221374	87.27%	17.817%
13	14.468	1926	1935	1943	rBV	1874938	2709509	17.88%	3.651%
14	15.951	2180	2187	2201	rBV	3254068	4395646	29.01%	5.923%
15	17.204	2394	2400	2408	rBV	1993846	2746988	18.13%	3.702%
16	19.821	2839	2845	2854	rBV	12945632	15149881	100.00%	20.416%
17	21.433	3113	3119	3127	rBV	1573293	2271460	14.99%	3.061%
18	24.450	3625	3632	3641	rBV	796465	2017753	13.32%	2.719%

Sum of corrected areas: 74207321

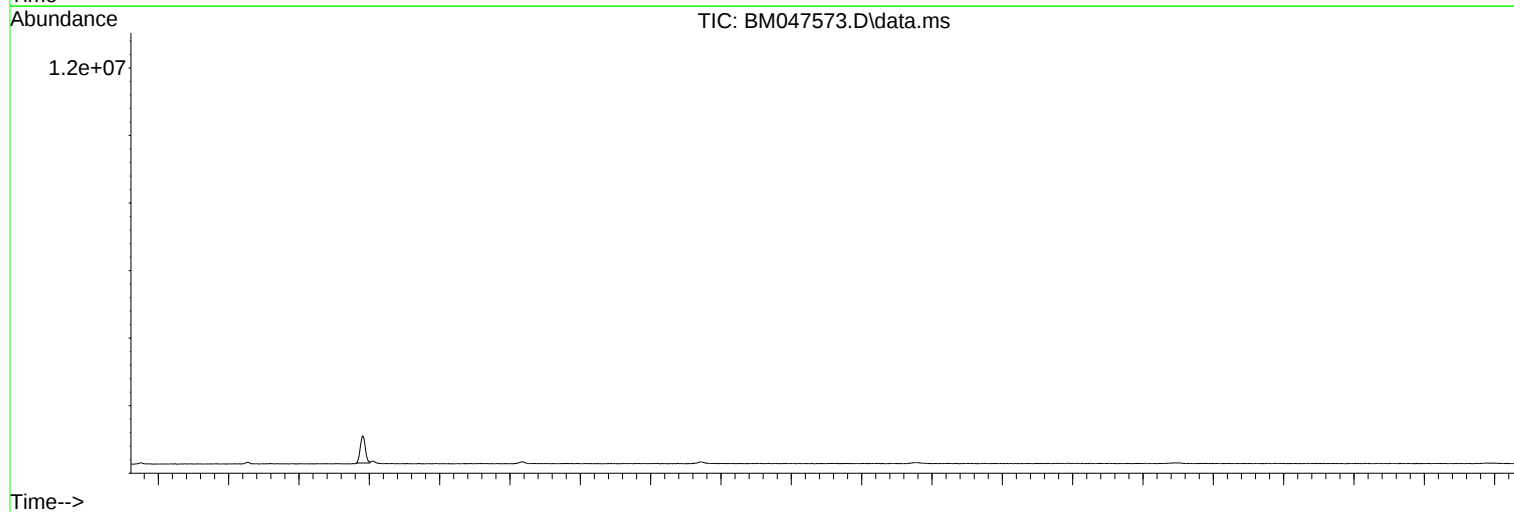
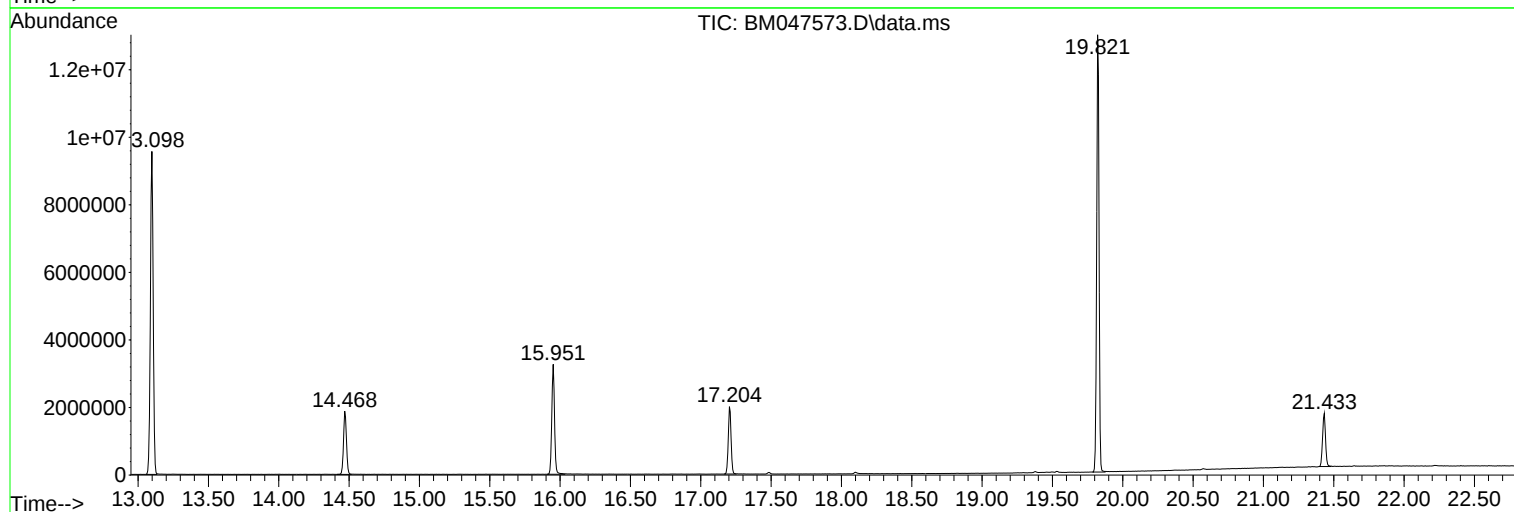
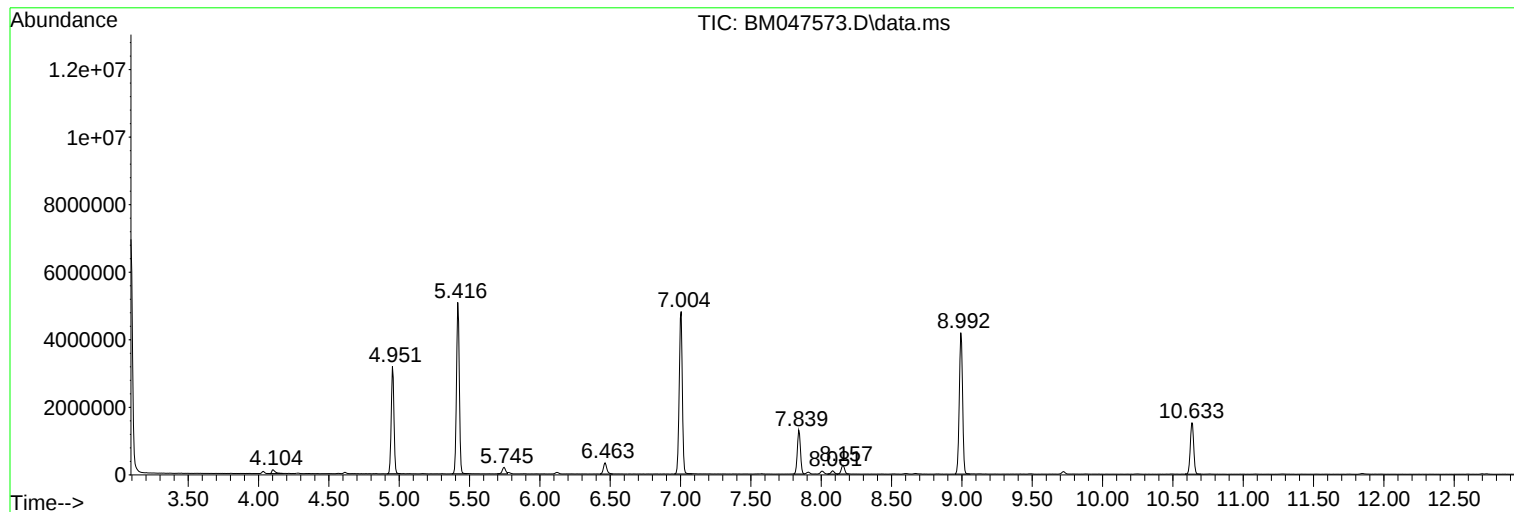
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TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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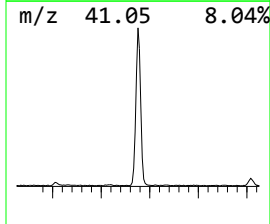
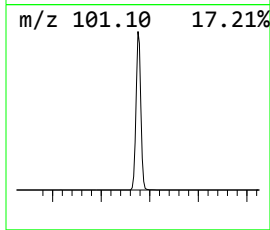
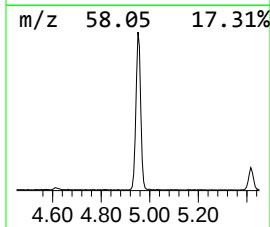
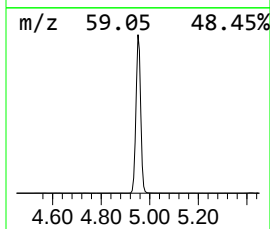
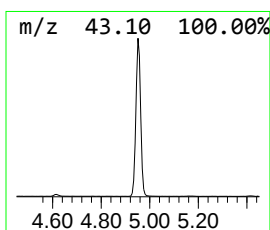
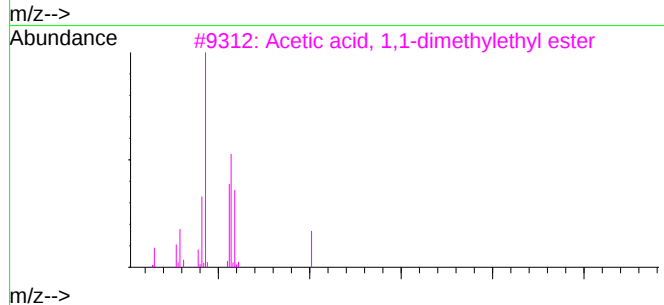
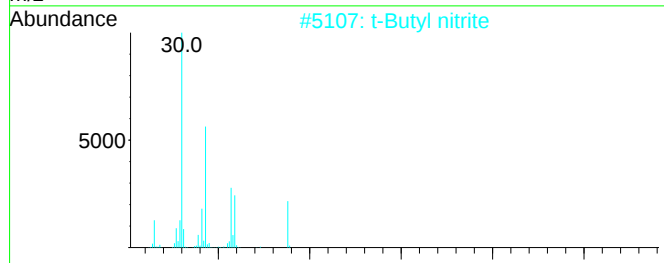
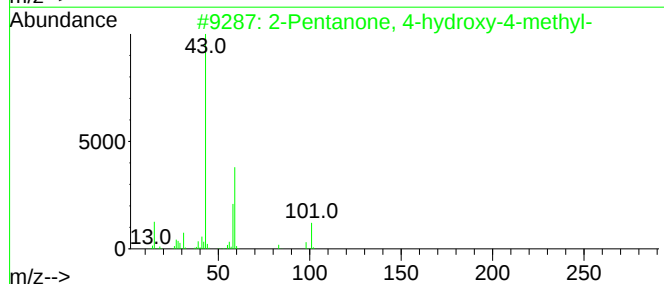
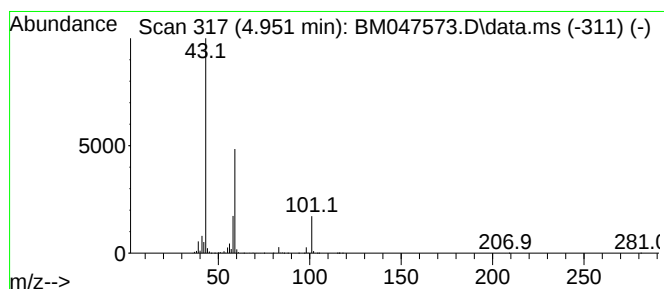
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091424.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
4.951	42.65 ng	4261120	1,4-Dichlorobenzene-d4	7.839	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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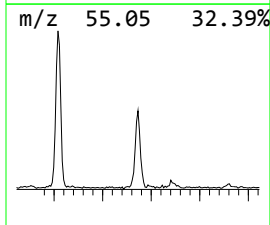
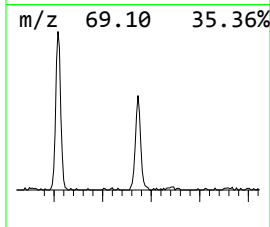
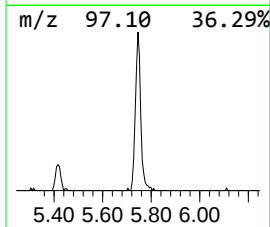
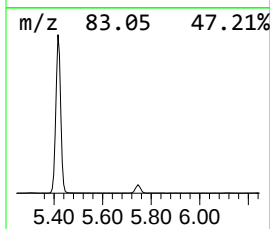
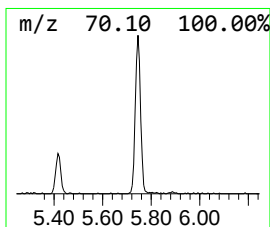
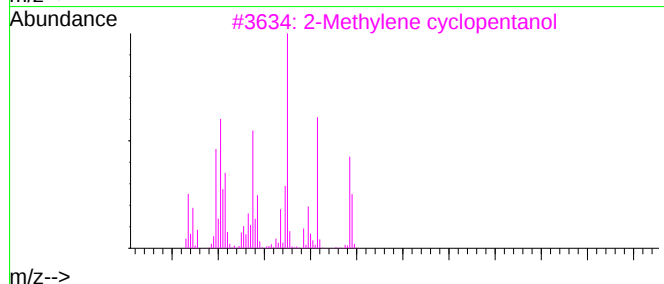
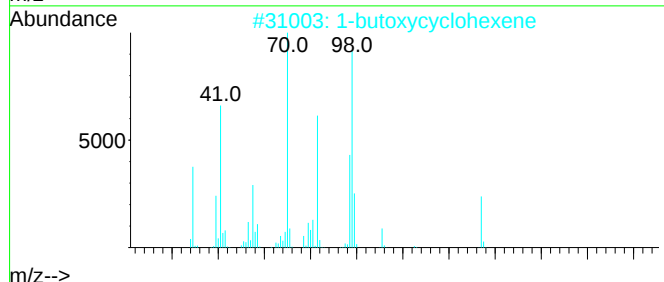
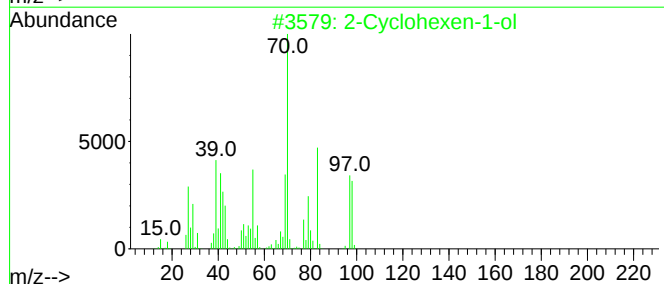
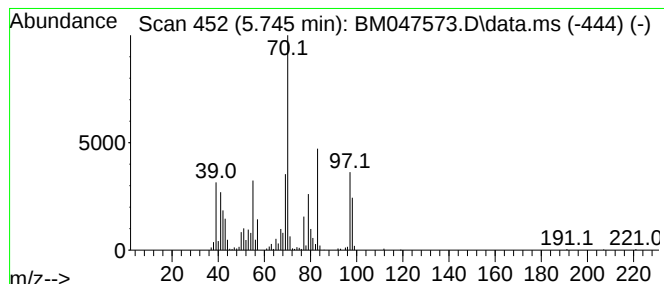
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.745	3.19 ng	318529	1,4-Dichlorobenzene-d4	7.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	93
2	1-butoxycyclohexene	154	C10H18O	024159-57-7	45
3	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	40
4	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	37
5	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	37



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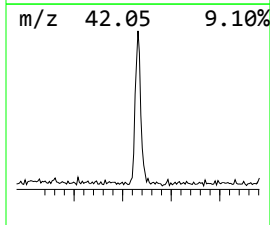
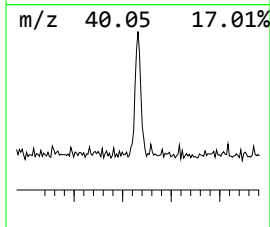
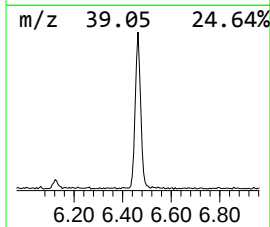
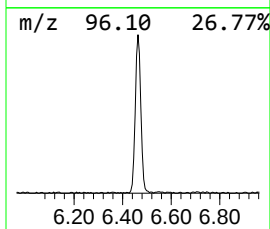
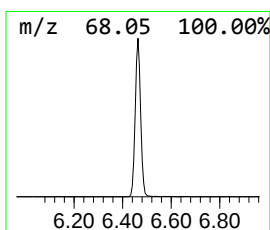
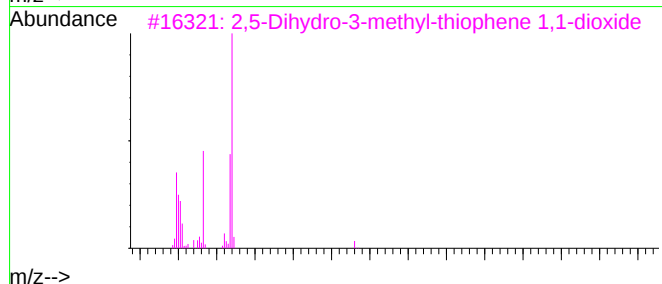
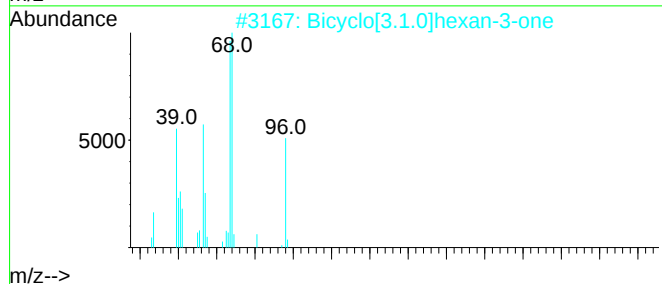
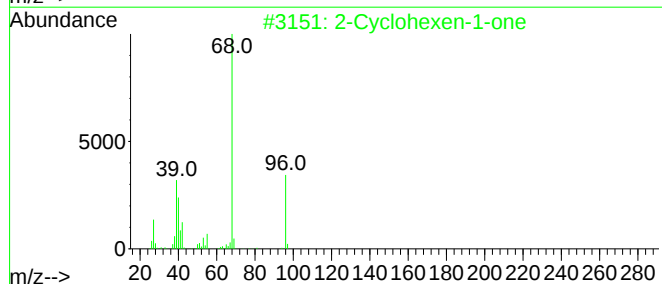
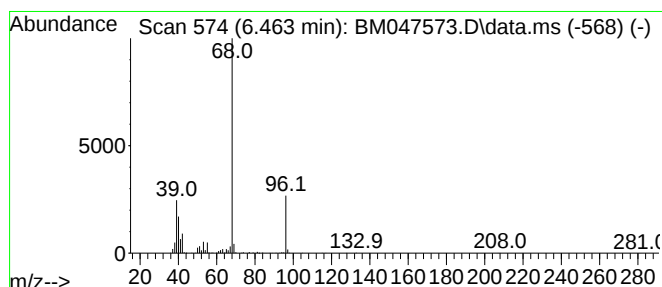
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.463	5.46 ng	545220	1,4-Dichlorobenzene-d4	7.839

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	Bicyclo[3.1.0]hexan-3-one	96	C6H8O	001755-04-0	25
3	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	17
4	1H-Imidazole	68	C3H4N2	000288-32-4	9
5	1H-Pyrazole	68	C3H4N2	000288-13-1	9



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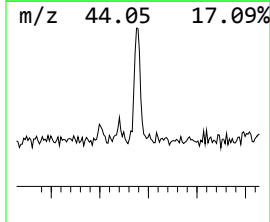
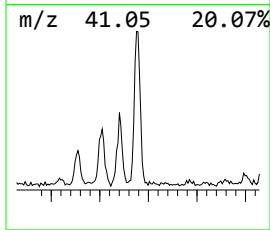
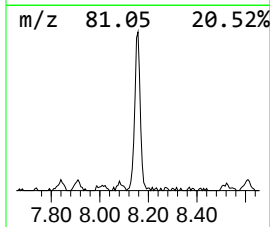
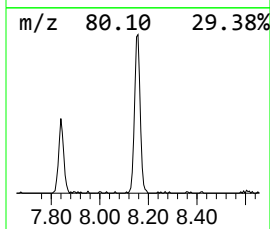
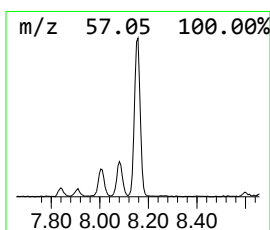
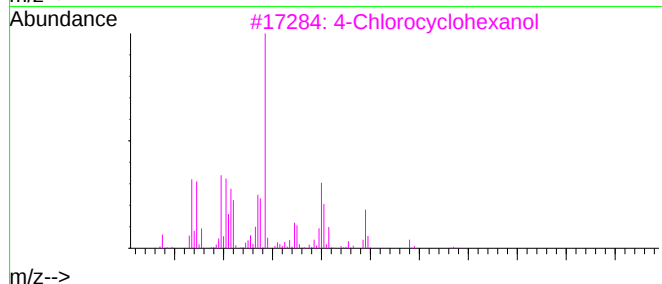
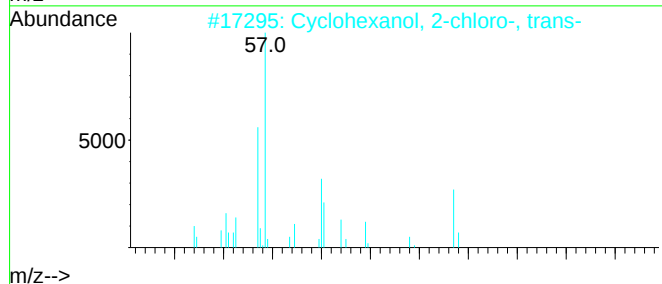
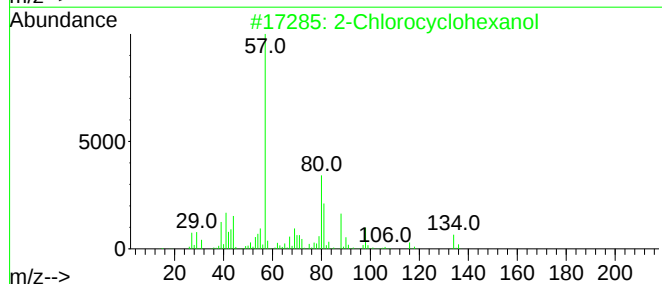
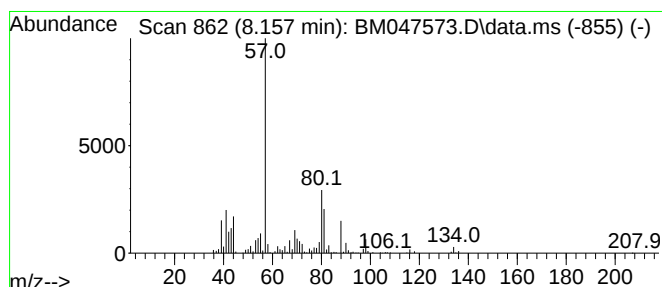
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TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Chlorocyclohexanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.157	4.25 ng	424111	1,4-Dichlorobenzene-d4	7.839

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	37
3	4-Chlorocyclohexanol	134	C6H11ClO	030485-71-3	33
4	Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	25
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.951	42.6	ng	4261120	1	7.839	1998050	20.0
2-Cyclohexen-1-ol	5.745	3.2	ng	318529	1	7.839	1998050	20.0
2-Cyclohexen-1-one	6.463	5.5	ng	545220	1	7.839	1998050	20.0
2-Chlorocyclohe...	8.157	4.3	ng	424111	1	7.839	1998050	20.0