Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

for

Inducing Chirality on ZnS Nanoparticles for Asymmetric Aldol Condensation Reaction

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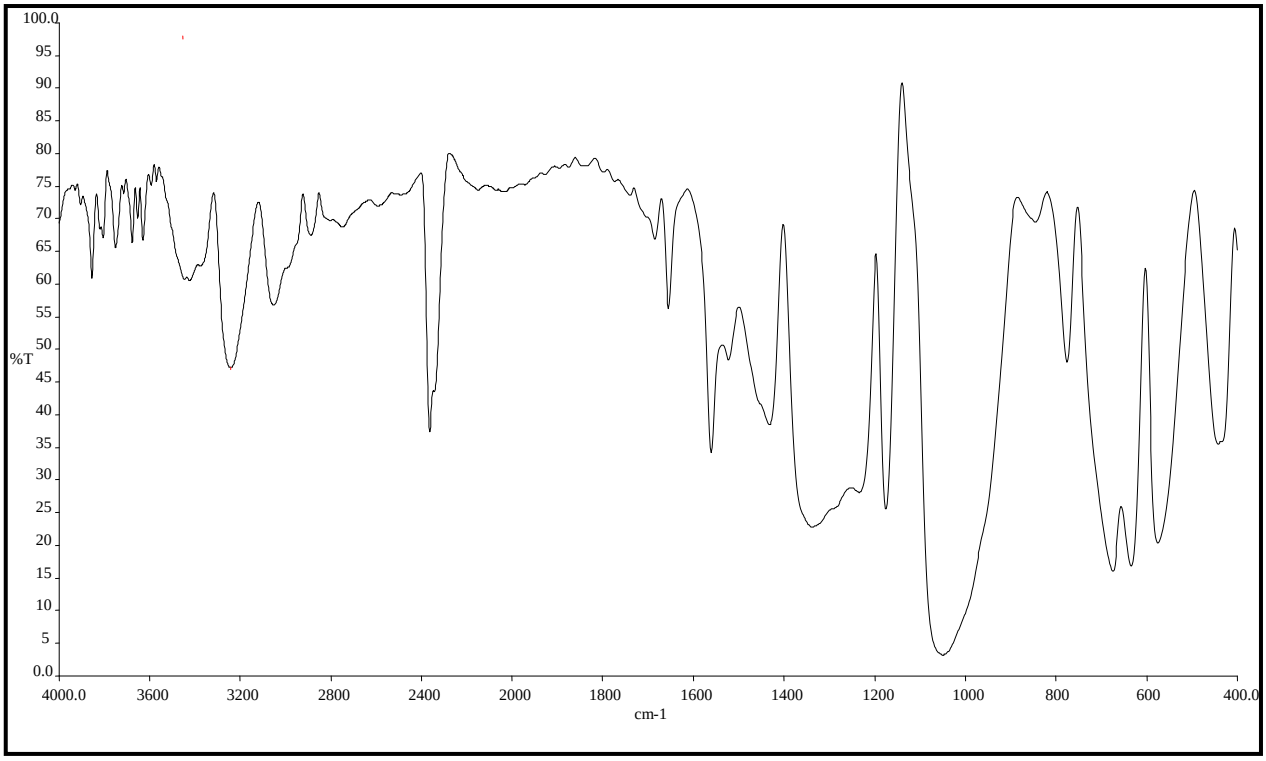


Figure 1(a). FTIR of L-Proline.

Band Assignment

Sl. No.	Wave numbers cm^{-1}	Band assignments	Sl. No.	Wave numbers cm^{-1}	Band assignments
1	3012	u_{as}CH2	12	1242	uC-O
2	2978	u_{as}CH2	13	1189	τCH2
3	2969	uCH	14	1090	Γring
4	2956	usCH2	15	1025	Γring
5	2938	usCH2	16	950	γOH
6	1645	uC=O	17	907	Γring
7	1544	δNH	18	866	Γring
8	1446	δCH2	19	850	ρCH2
9	1375	δOH	20	799	ρCH2
10	1320	τCH2	21	721	δC=O
11	1292	δCH	22	630	Δring

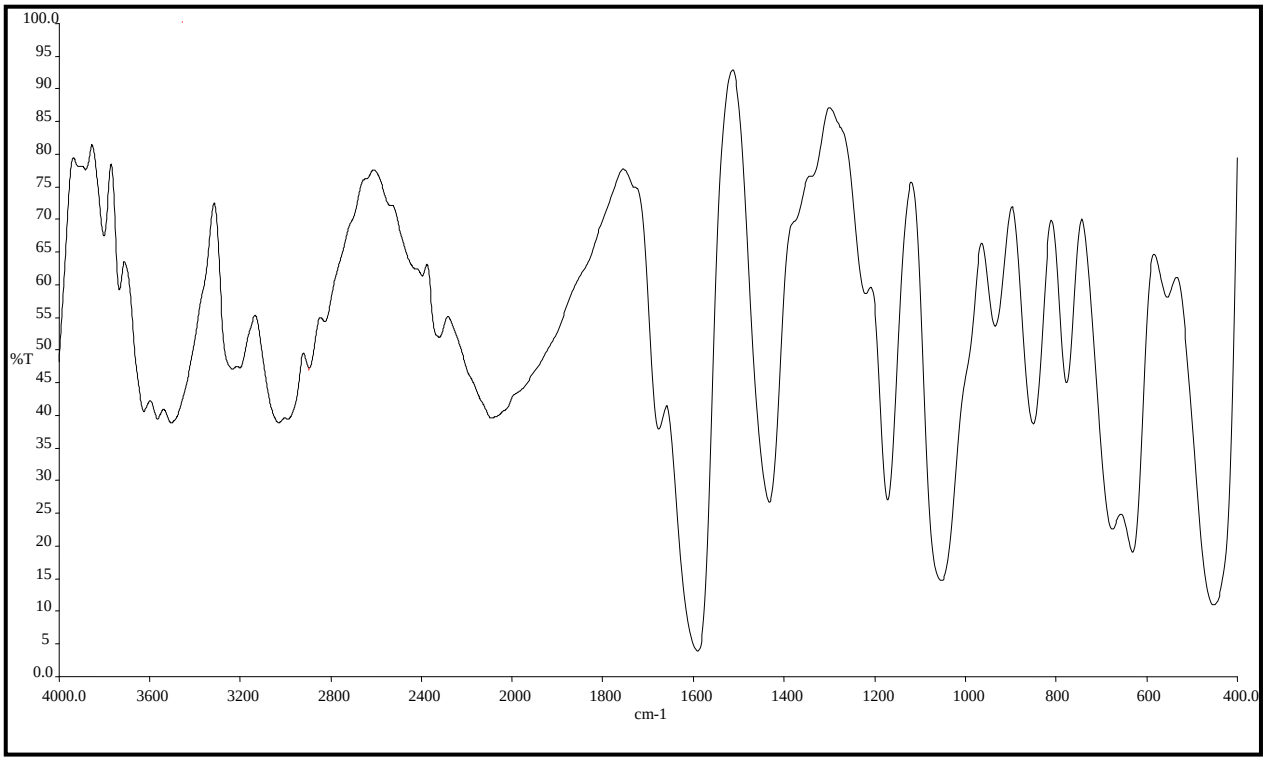


Figure 1(b). FTIR of L-proline/ZnS.

Band Assignment

Sl. No.	**Wave numbers cm^{-1}**	**Band assignments**	
1	3015	Asymmetric stretching	CH_2
2	2943	Asymmetric stretching	CH_2
3	2903	Symmetric stretching	CH_2
4	1661	Stretching	C=O
5	1552	In-place bending	NH
6	1392	In-place bending	OH
7	1331	Twisting	CH_2
8	1281	In-plane bending	CH
9	1153	Twisting	CH_2

10	1038	Stretching	Ring
11	946	Out of plane bending	OH
12	844	Rocking	CH_2
13	671	Stretching	Zn-S
14	636	In-plane bending	Ring
15	551	Stretching	Zn-S

CD spectra were recorded on a Jasco, J-815 CD spectrometer.

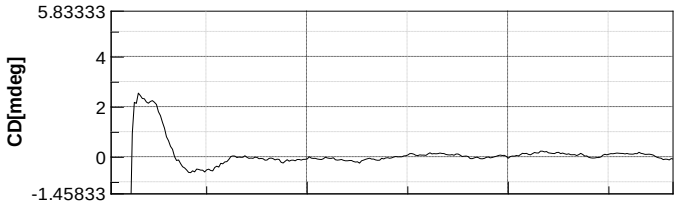


Figure 2(a). CD Spectra of undoped L-Proline adsorbed ZnS nanoparticles.

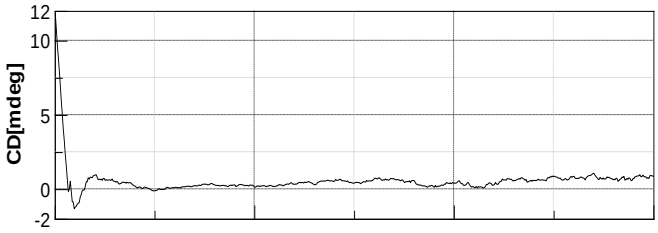


Figure 2(b). CD Spectra of undoped D-Proline adsorbed ZnS nanoparticles.

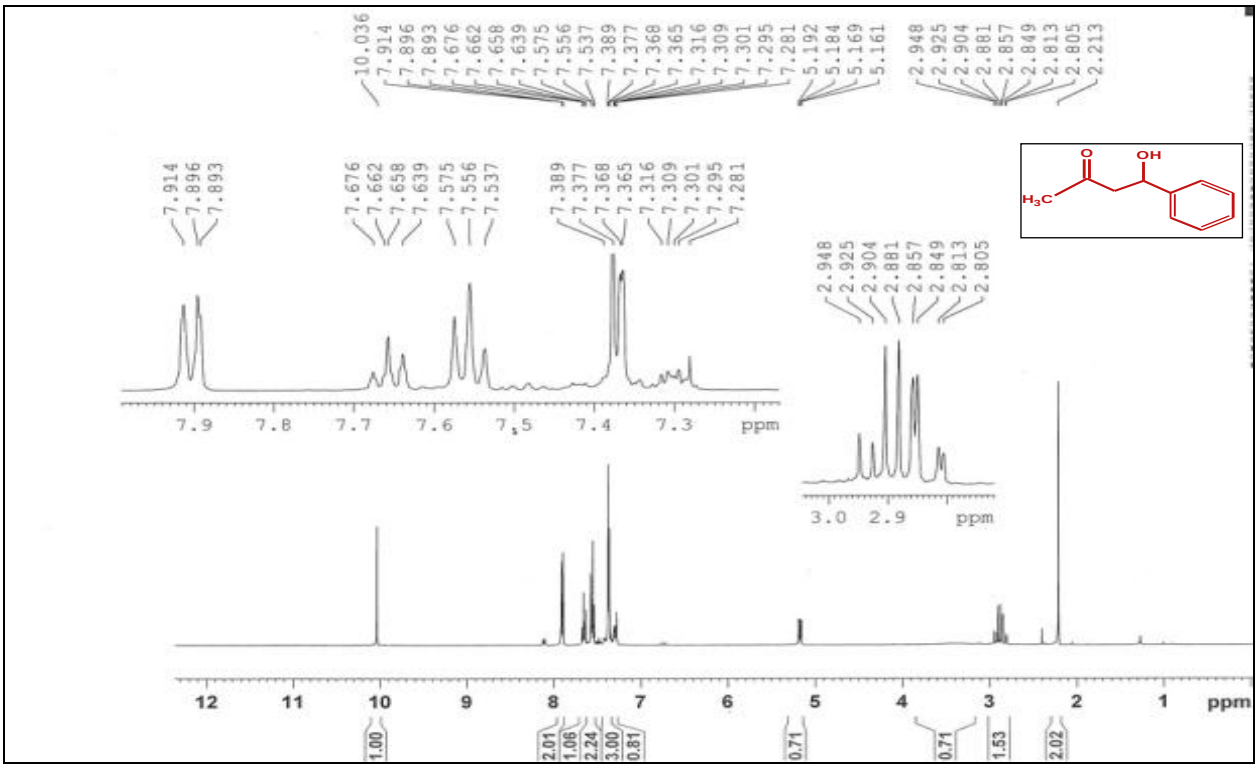


Figure 3(a): NMR of 4-Hydroxy-4phenylbutan-2-one after one recycle.

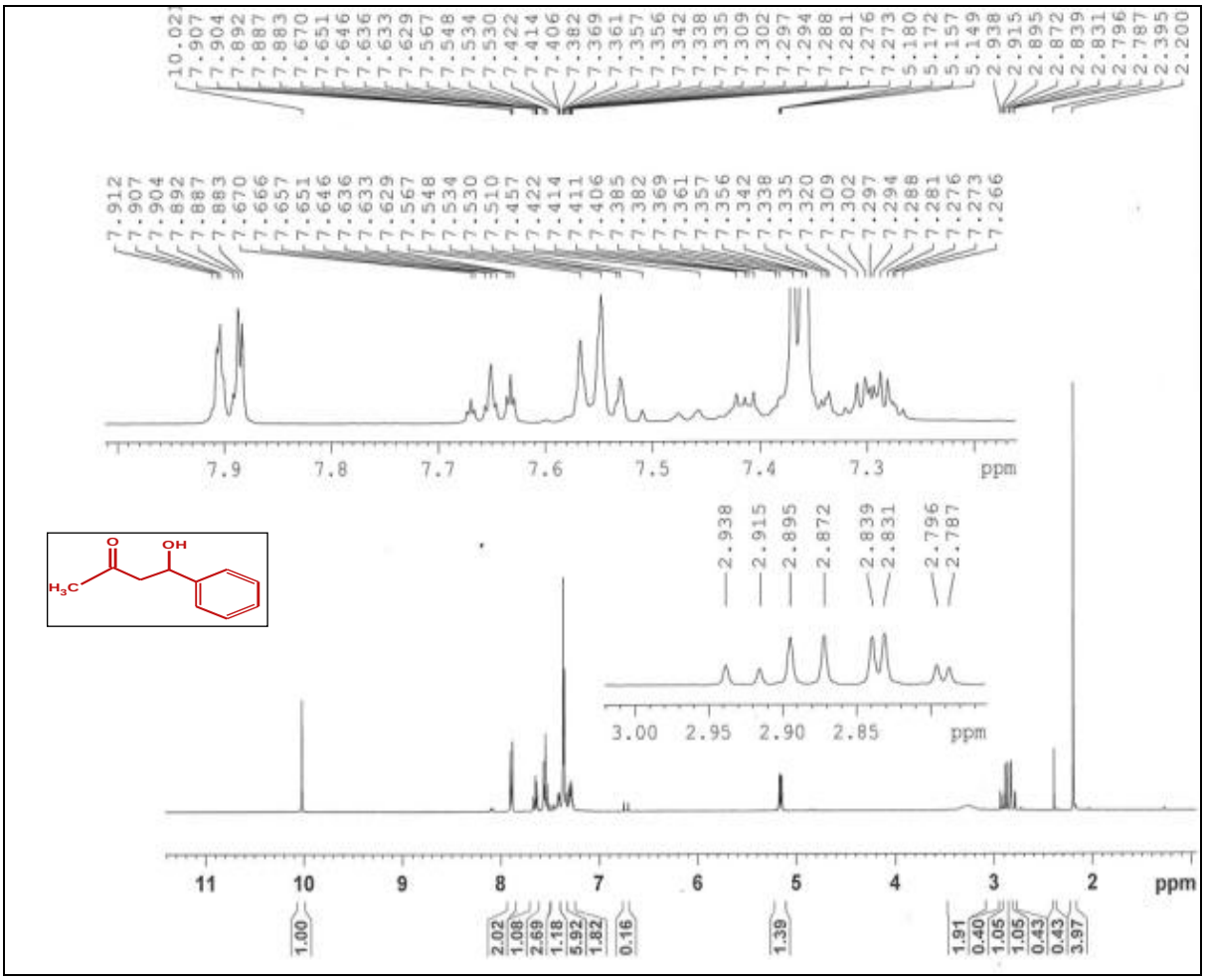


Figure 3(b). NMR of 4-Hydroxy-4phenylbutan-2-one after third cycle.

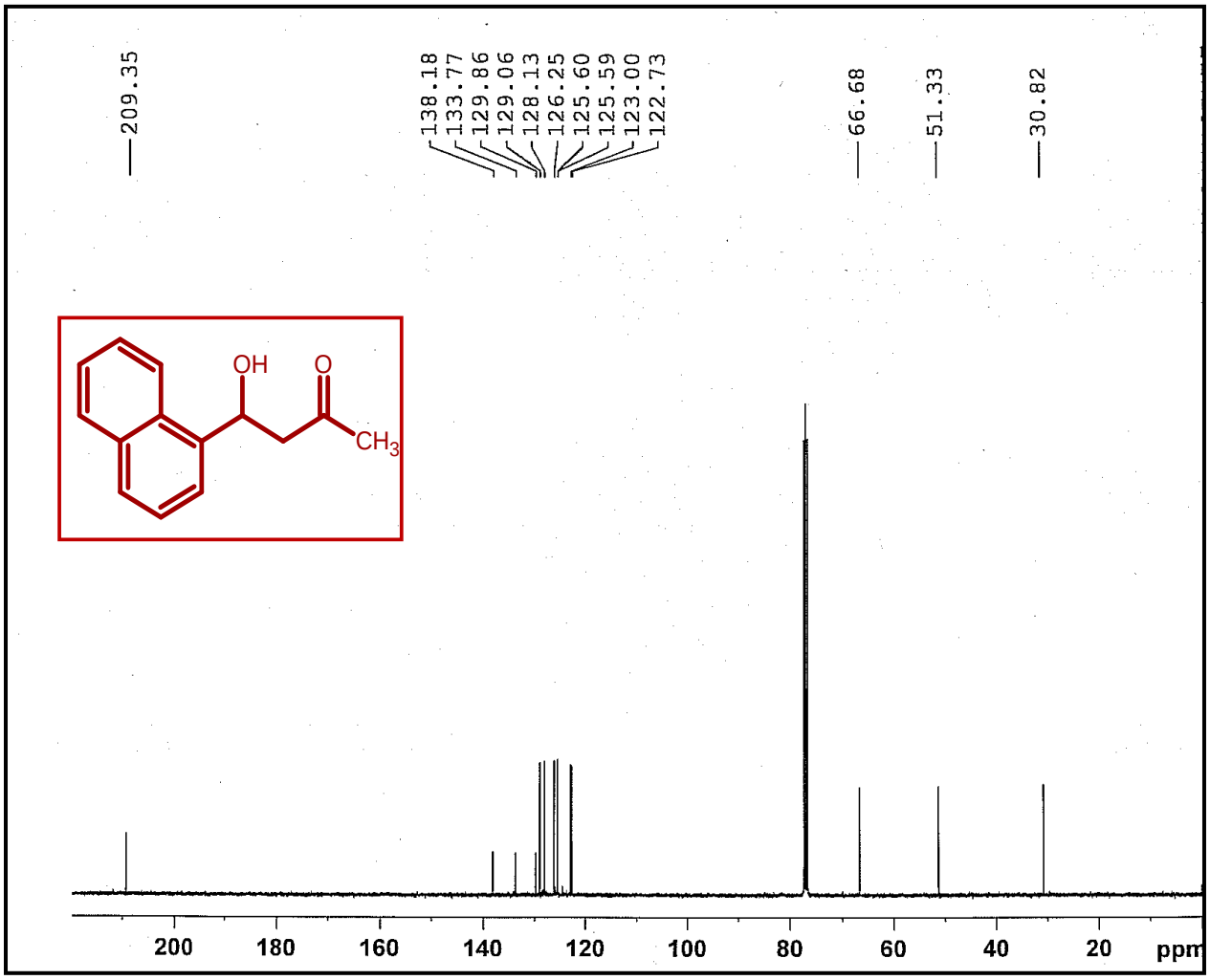
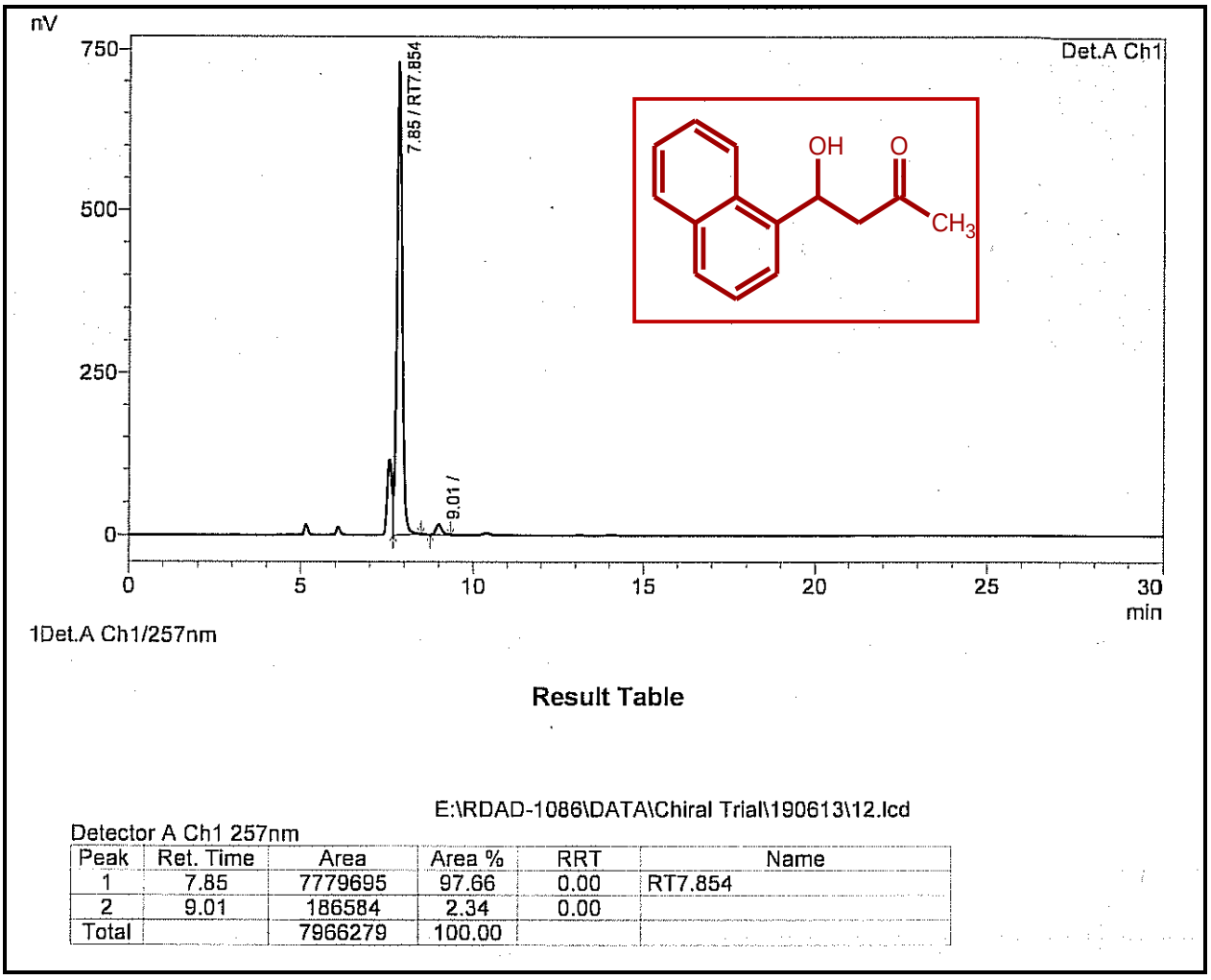


Figure 4. ^{13}C of 4-(1-Naphthyl)-4-hydroxybutan-2-one.



Result Table

E:\RDAD-1086\DATA\Chiral Trial\190613\12.lcd

Detector A Ch1 257nm

Peak	Ret. Time	Area	Area %	RRT	Name
1	7.85	7779695	97.66	0.00	RT7.854
2	9.01	186584	2.34	0.00	
Total		7966279	100.00		

Figure 5. Chiral HPLC of 4-(1-Naphthyl)-4-hydroxybutan-2-one.

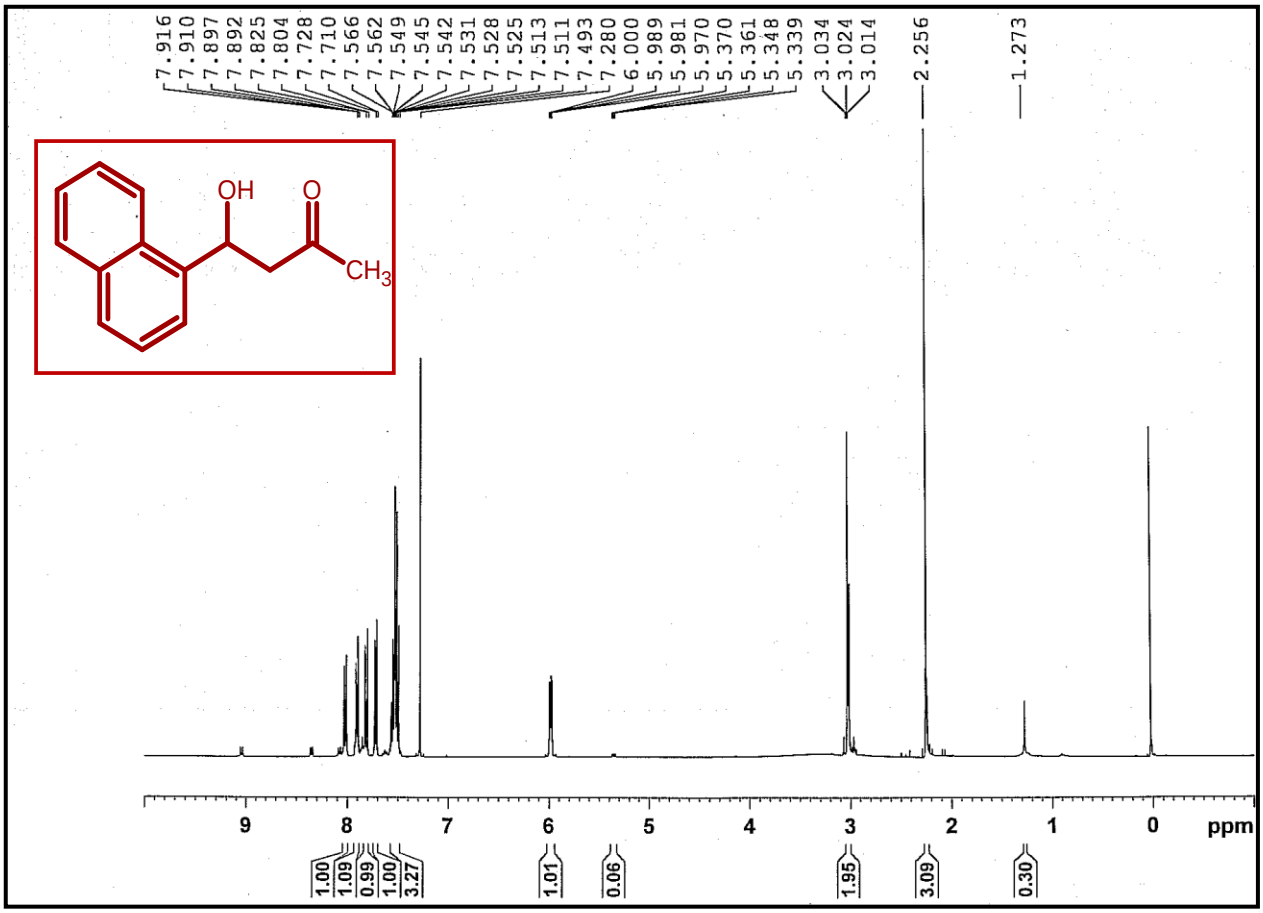
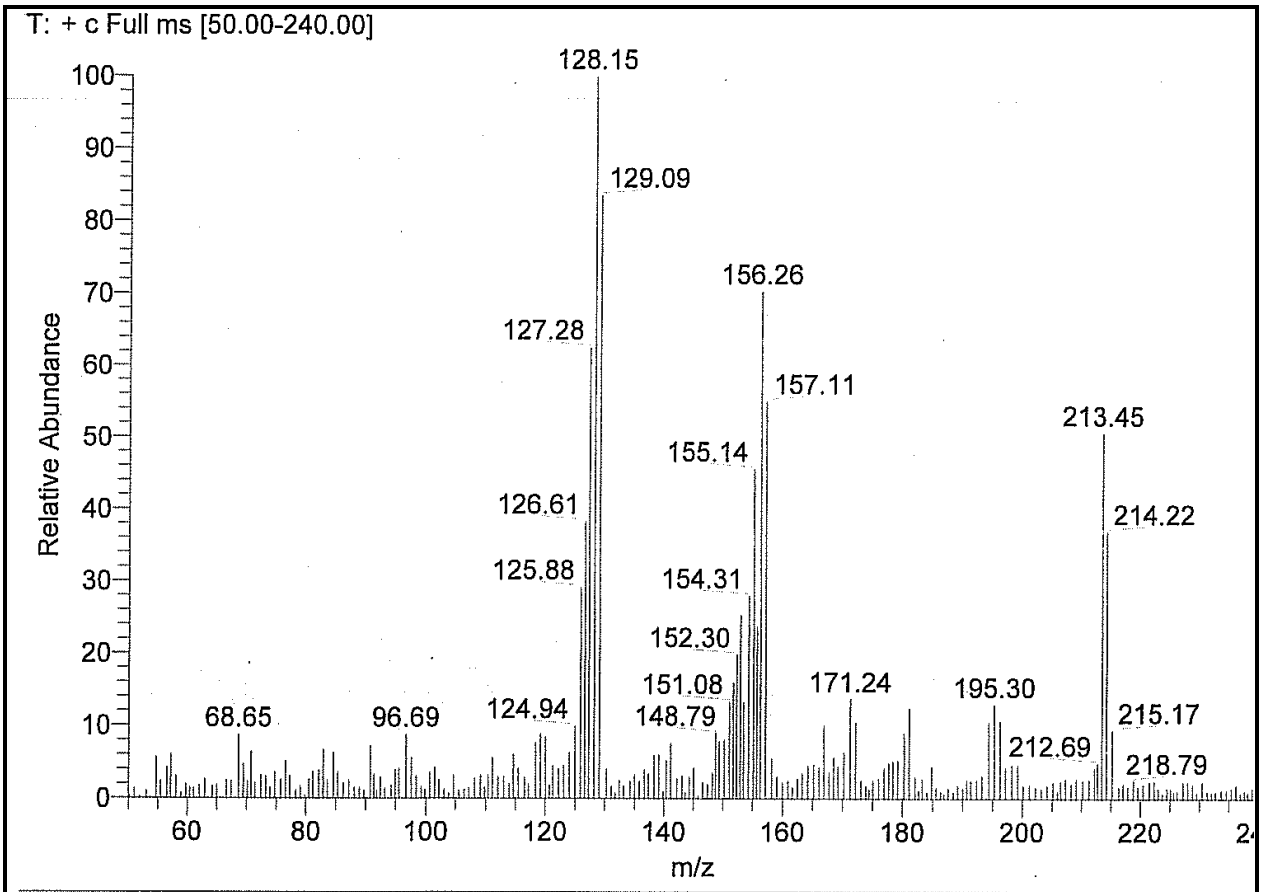


Figure 6. ^{1}**H NMR of 4-(1-Naphthyl)-4-hydroxybutan-2-one.**



EVS-P1NA#183 RT: 1.26
T: + c Full ms [50.00-240.00]

m/z	Intensity	Relative
125.88	130786.0	29.19
126.61	171884.0	38.37
127.28	280375.0	62.58
128.15	448010.0	100.00
129.09	374773.0	83.65
151.08	59717.0	13.33
151.73	71411.0	15.94
152.30	88910.0	19.85
152.90	113528.0	25.34
153.43	59388.0	13.26
154.31	125612.0	28.04
155.14	204769.0	45.71
155.66	106315.0	23.73
156.26	315242.0	70.36
157.11	246771.0	55.08
171.24	61252.0	13.67
181.08	55300.0	12.34
195.30	57862.0	12.92
213.45	227376.0	50.75
214.22	165951.0	37.04

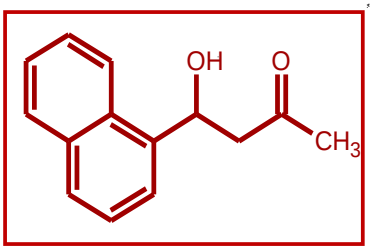


Figure 7. Mass spectrum of 4-(1-Naphthyl)-4-hydroxy2-butanone.

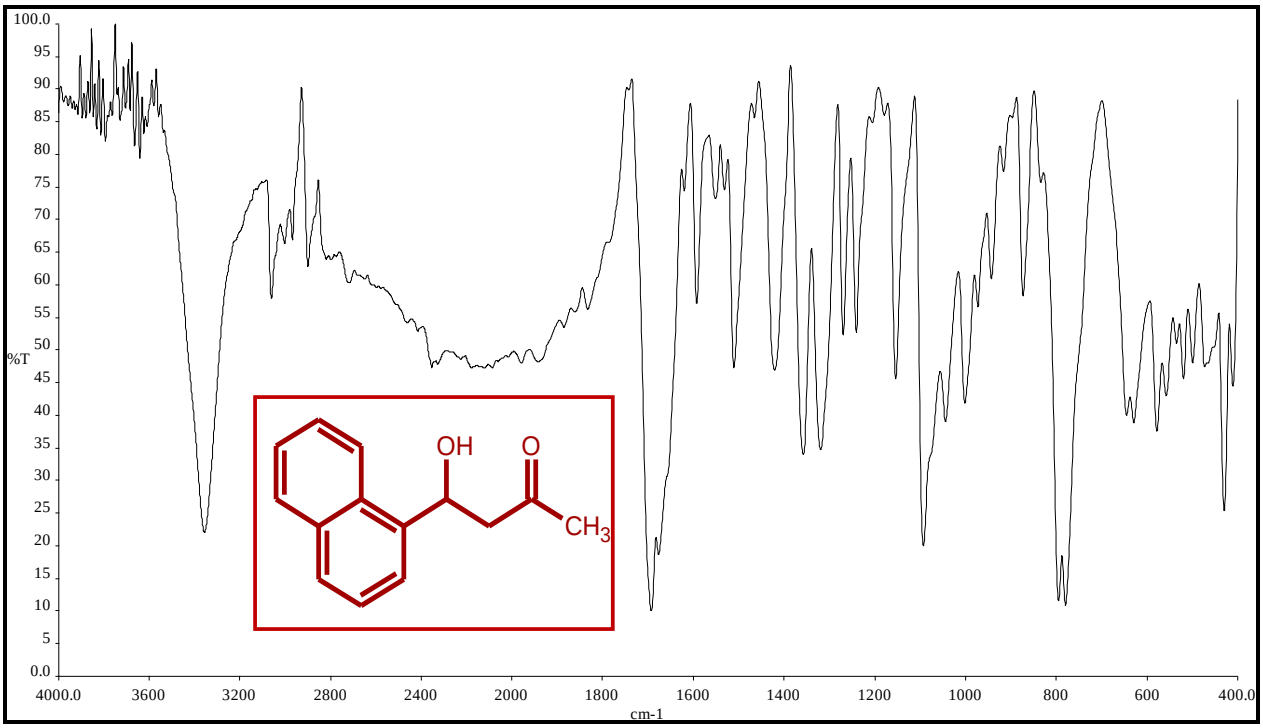


Figure 8. FTIR spectrum of 4-(1-Naphthyl)-4-hydroxybutan-2-one.

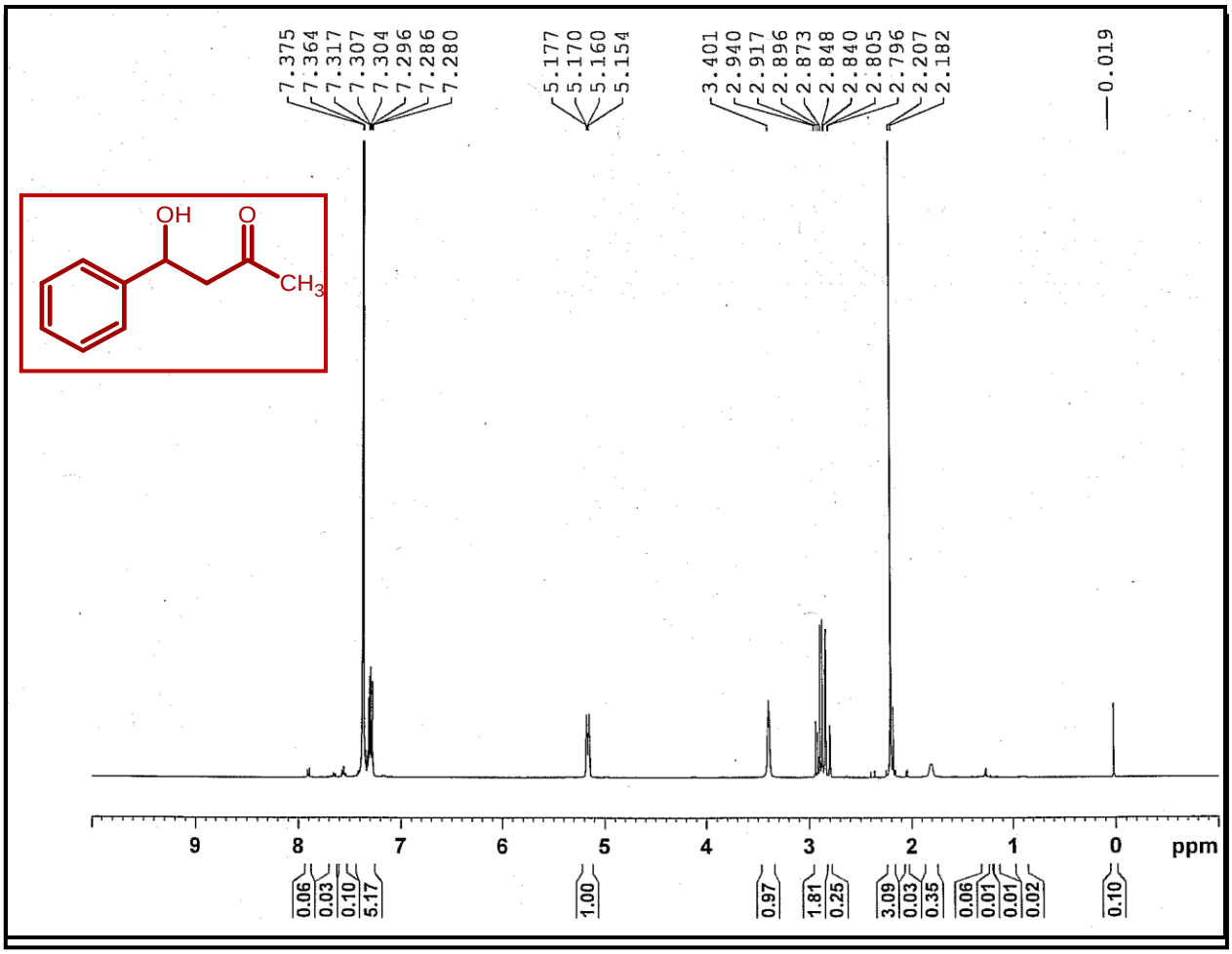


Figure 9. ^{1}H NMR of 4-Hydroxy-4-phenylbutan-2-one.

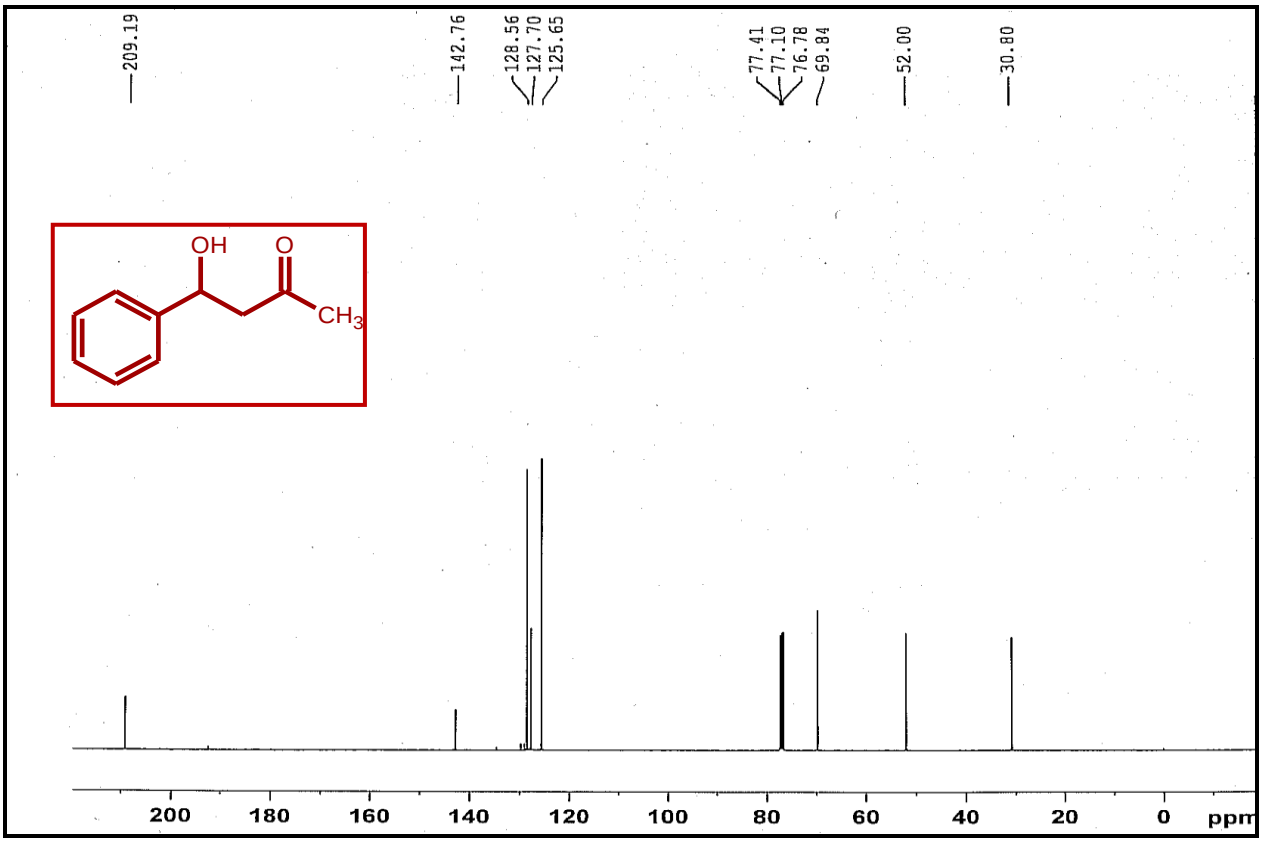
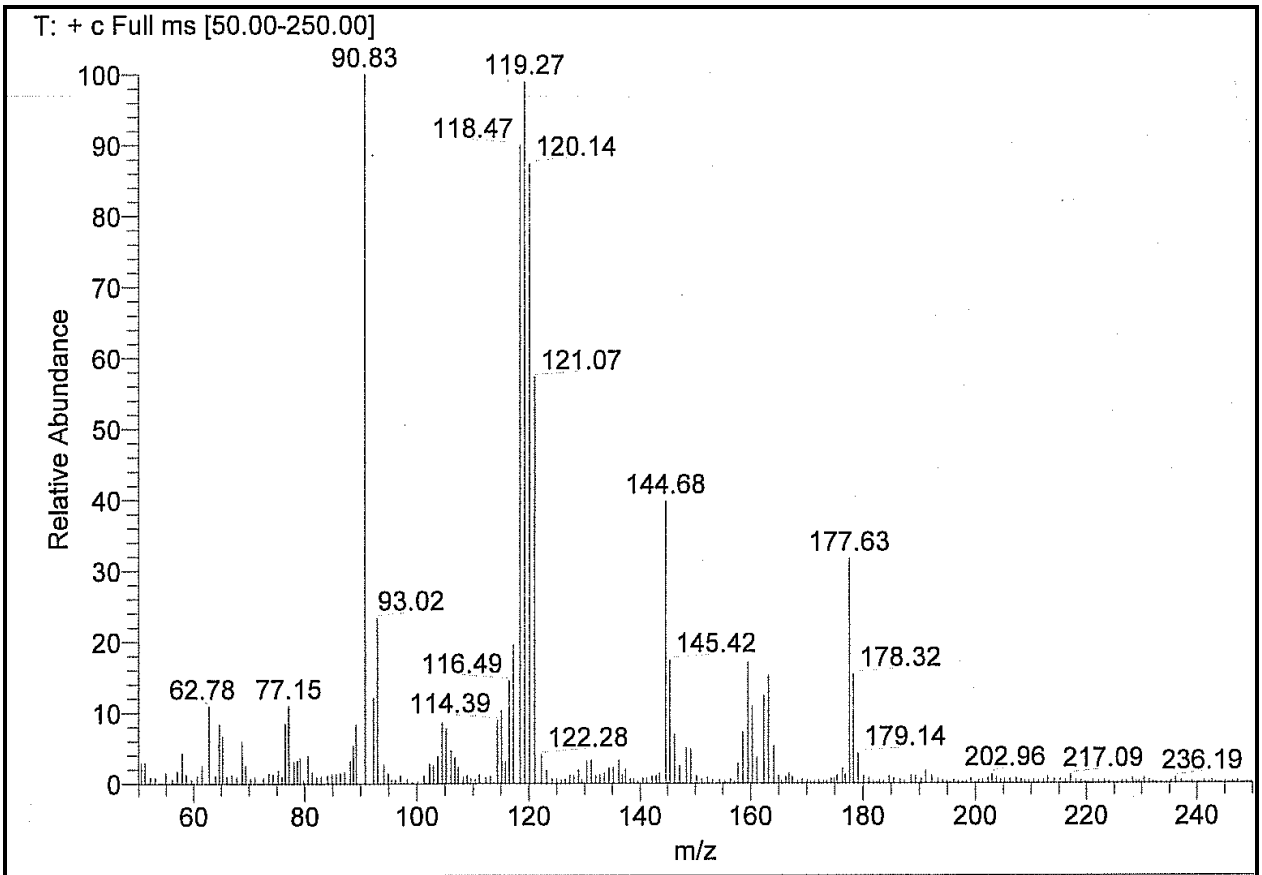


Figure 10. ^{13}C **of 4-Hydroxy-4-phenylbutan-2-one.**



EVS-PA#159 RT: 1.16
T: + c Full ms [50.00-250.00]

m/z	Intensity	Relative
62.78	205510.0	10.90
77.15	206230.0	10.94
90.83	1885695.0	100.00
92.31	228017.0	12.09
93.02	441280.0	23.40
115.13	193888.0	10.28
116.49	273707.0	14.51
117.24	371364.0	19.69
118.47	1696450.0	89.96
119.27	1865894.0	98.95
120.14	1649320.0	87.46
121.07	1081420.0	57.35
144.68	751518.0	39.85
145.42	327748.0	17.38
159.49	322316.0	17.09
160.26	204836.0	10.86
162.36	233544.0	12.39
163.15	286019.0	15.17
177.63	598386.0	31.73
178.32	290373.0	15.40

Figure 11. Mass spectrum of 4-Hydroxy-4-phenylbutan-2-one.

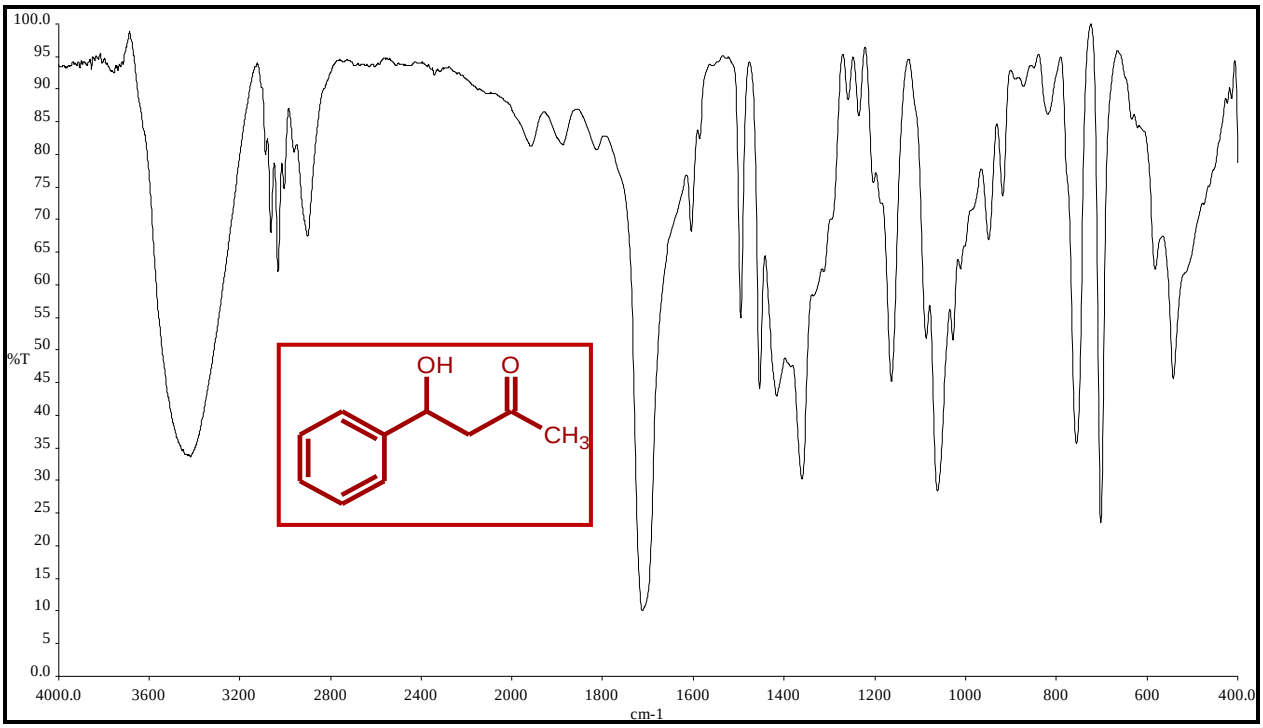
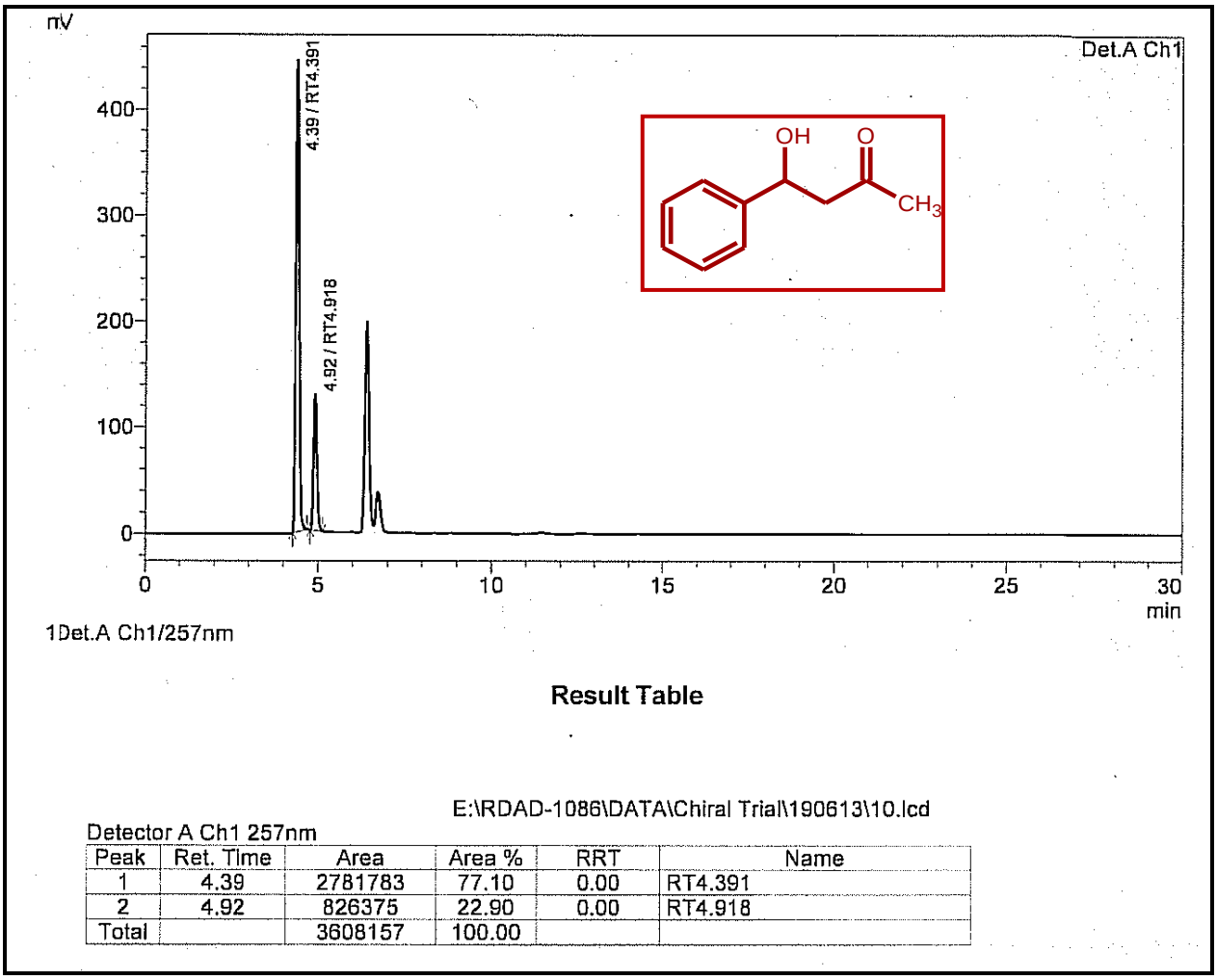


Figure 12. FTIR spectrum of 4-Hydroxy-4-phenylbutan-2-one.



Result Table

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Detector A Ch1 257nm

Peak	Ret. Time	Area	Area %	RRT	Name
1	4.39	2781783	77.10	0.00	RT4.391
2	4.92	826375	22.90	0.00	RT4.918
Total		3608157	100.00		

Figure 13. Chiral HPLC of 4-Hydroxy-4-phenylbutan-2-one.

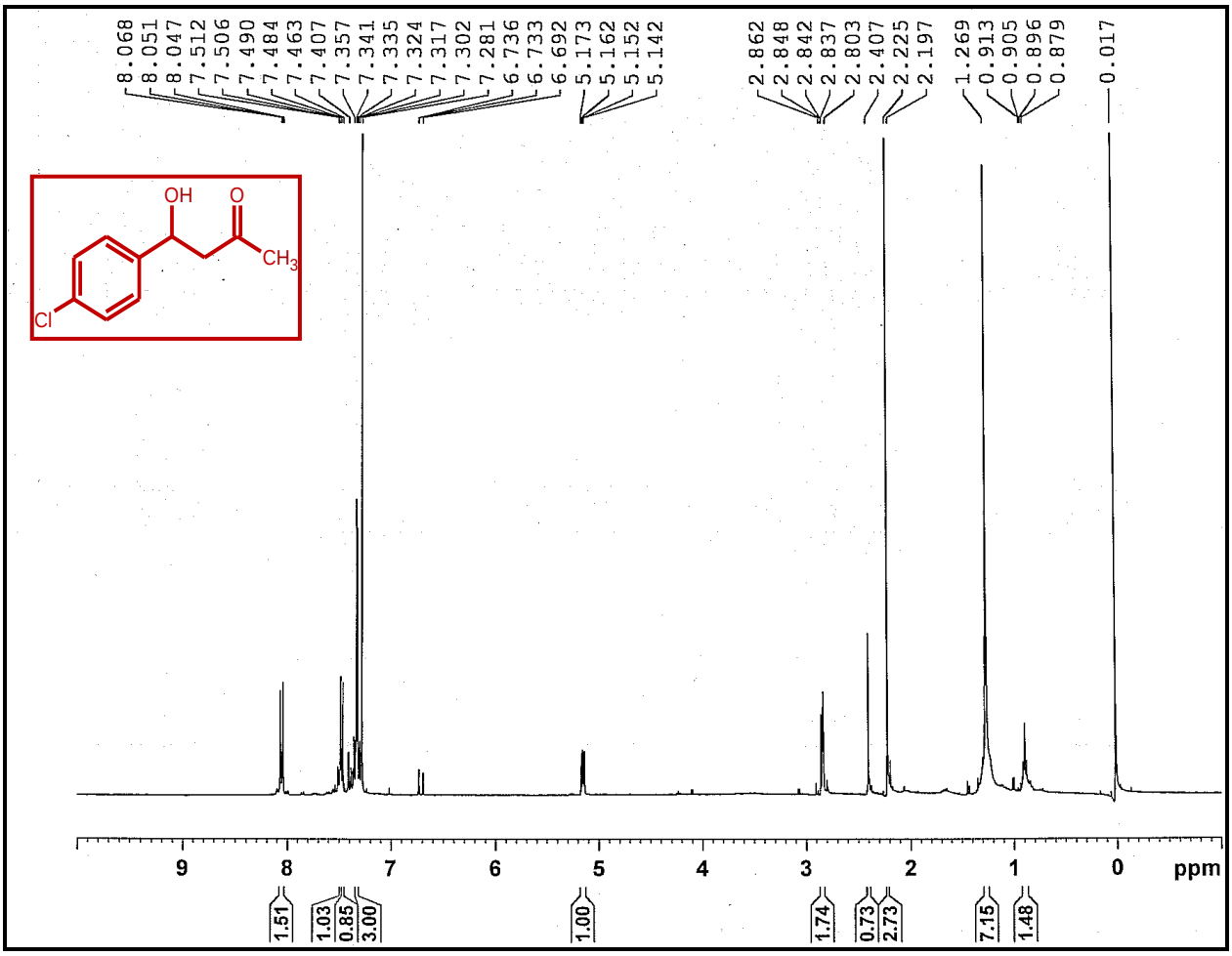


Figure 14. ^{1}H NMR of 4-Hydroxy-4-(4'-Chlorophenyl)butan-2-one.

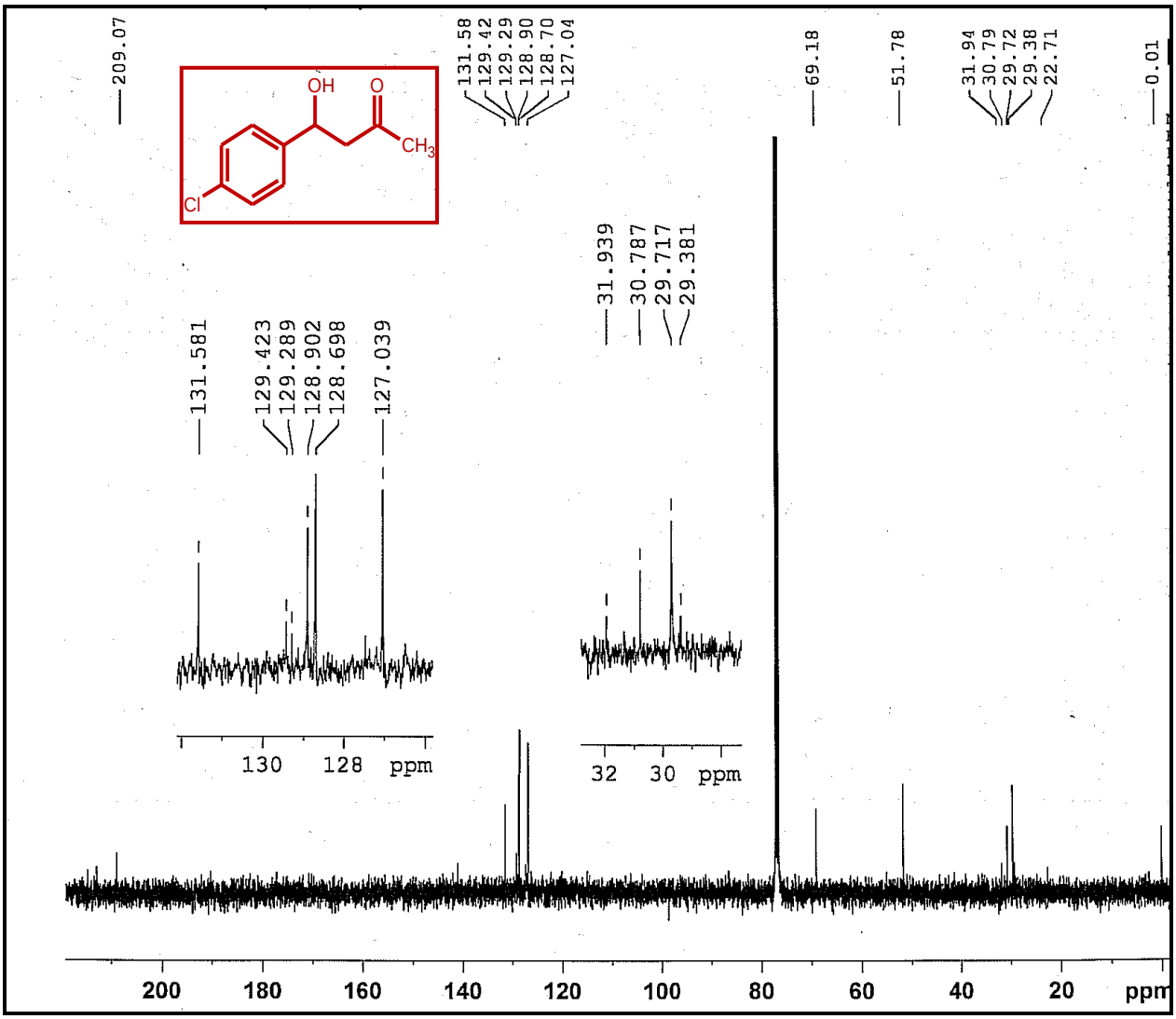


Figure 15. ^{13}**C of 4-Hydroxy-4-(4'-Chlorophenyl)butan-2-one.**

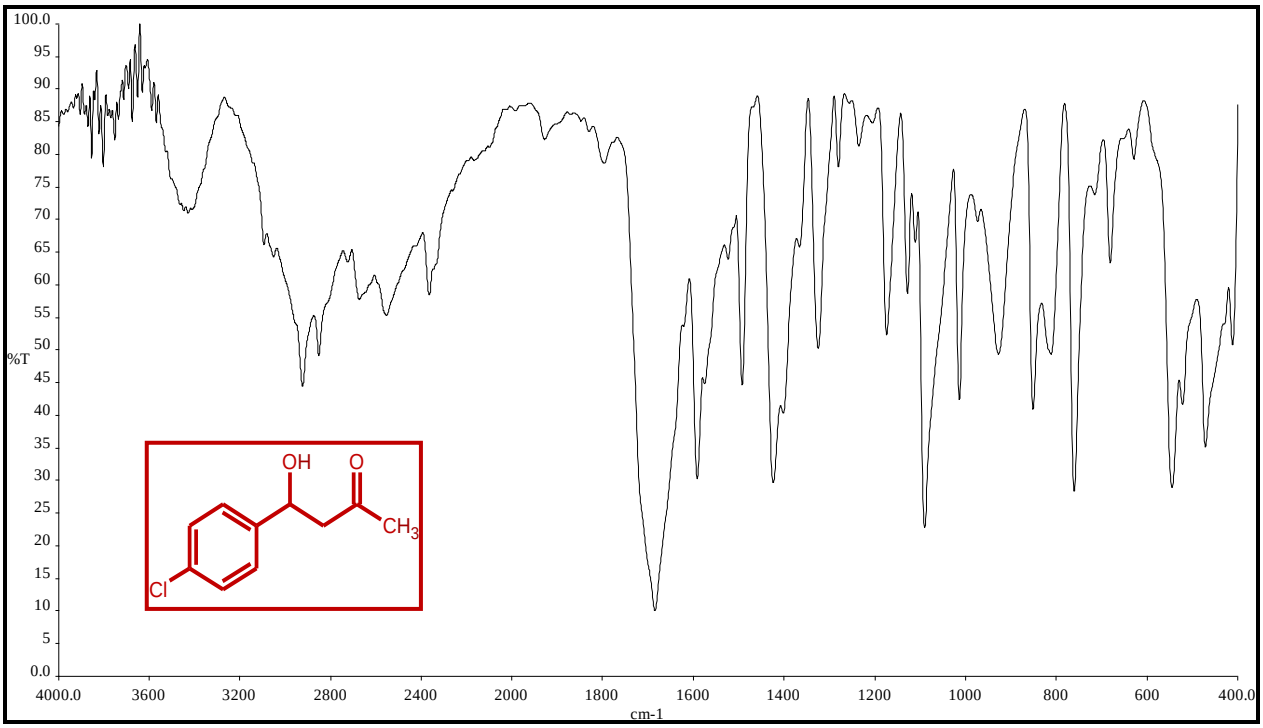
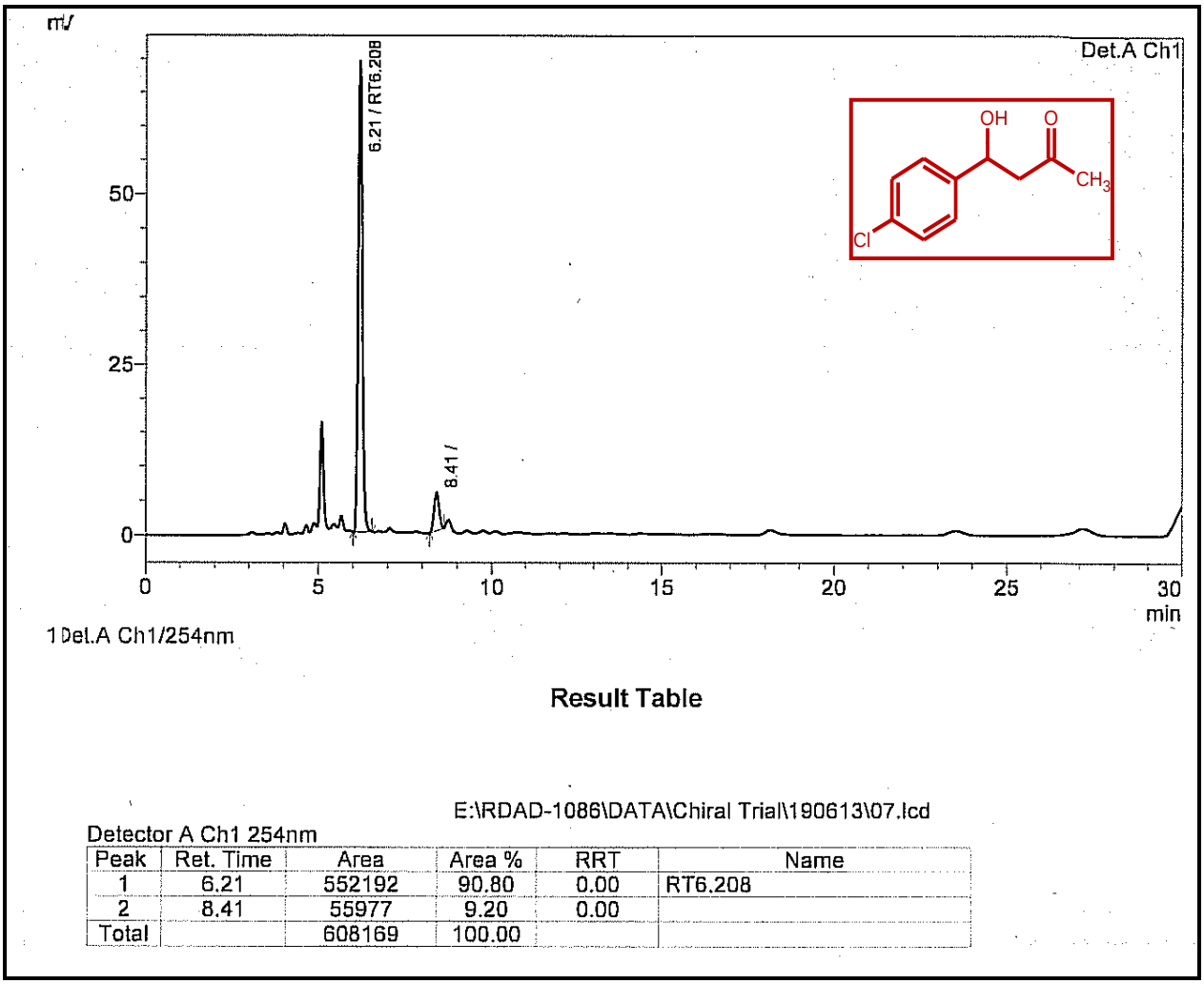


Figure 16. FTIR spectrum of 4-Hydroxy-4-(4'-Chlorophenyl)butan-2-one.



Result Table

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Detector A Ch1 254nm

Peak	Ret. Time	Area	Area %	RRT	Name
1	6.21	552192	90.80	0.00	RT6.208
2	8.41	55977	9.20	0.00	
Total		608169	100.00		

Figure 17. Chiral HPLC of 4-Hydroxy-4-(4'-Chlorophenyl)butan-2-one.

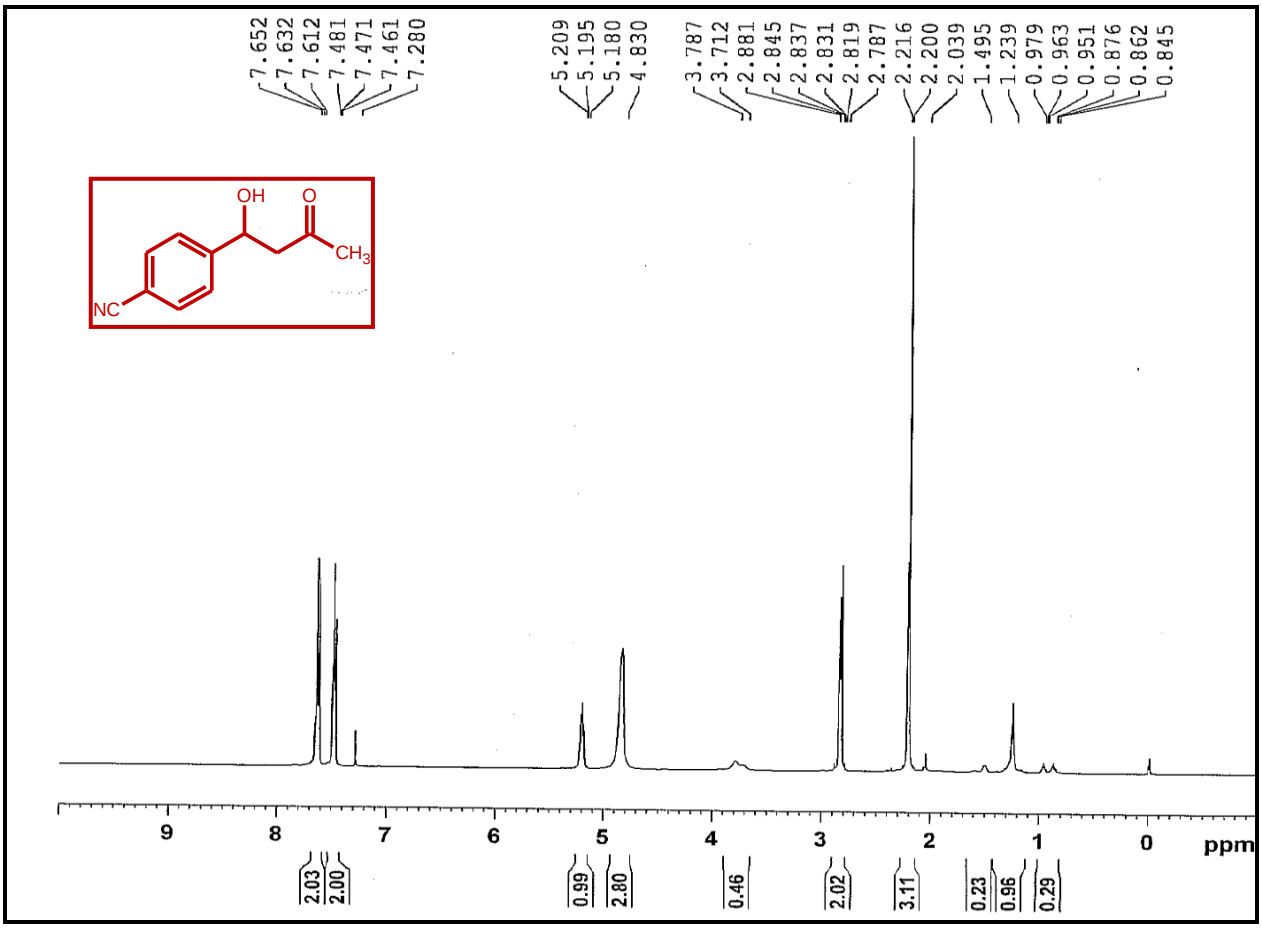


Figure 18. ^{1}H NMR of 4-Hydroxy-4-(4'-cyanophenyl)butan-2-one.

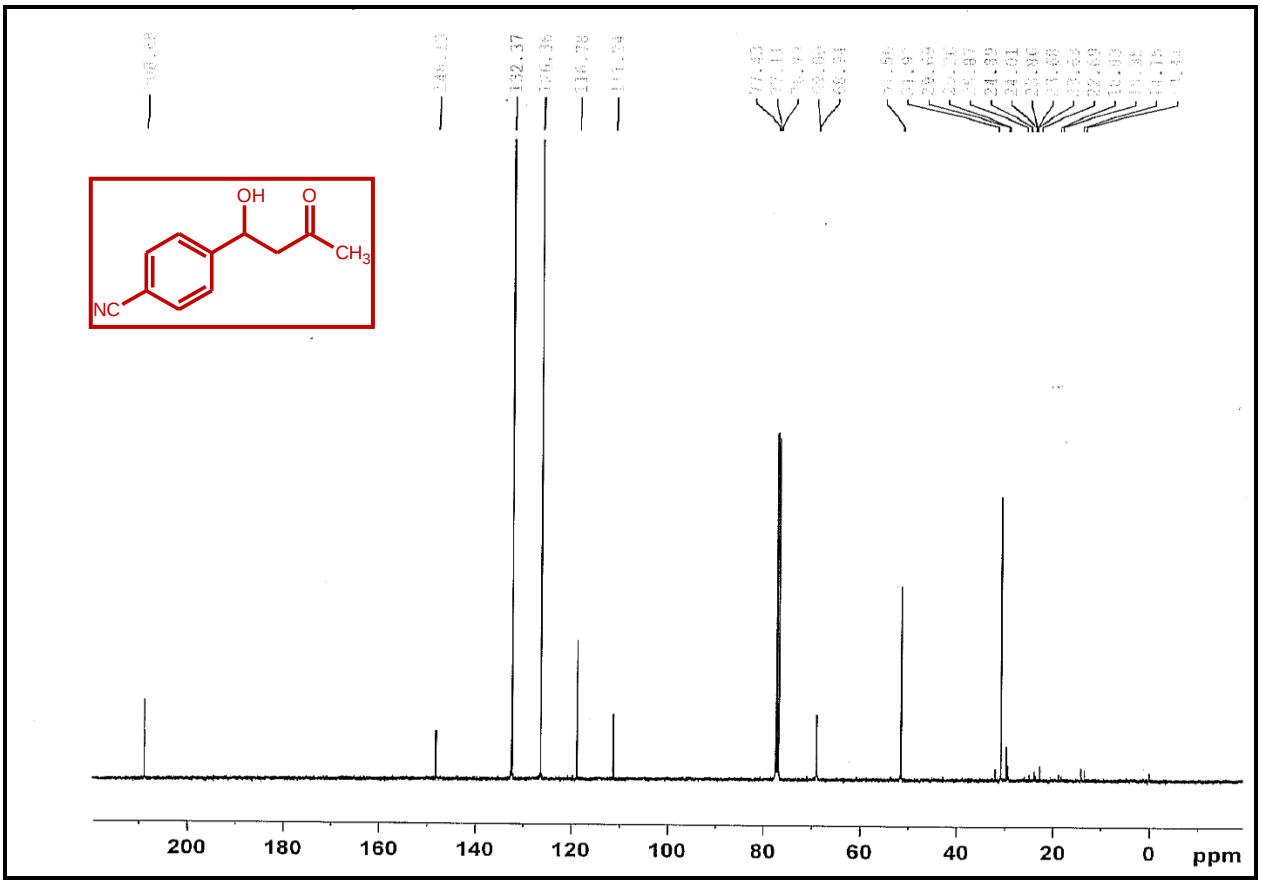
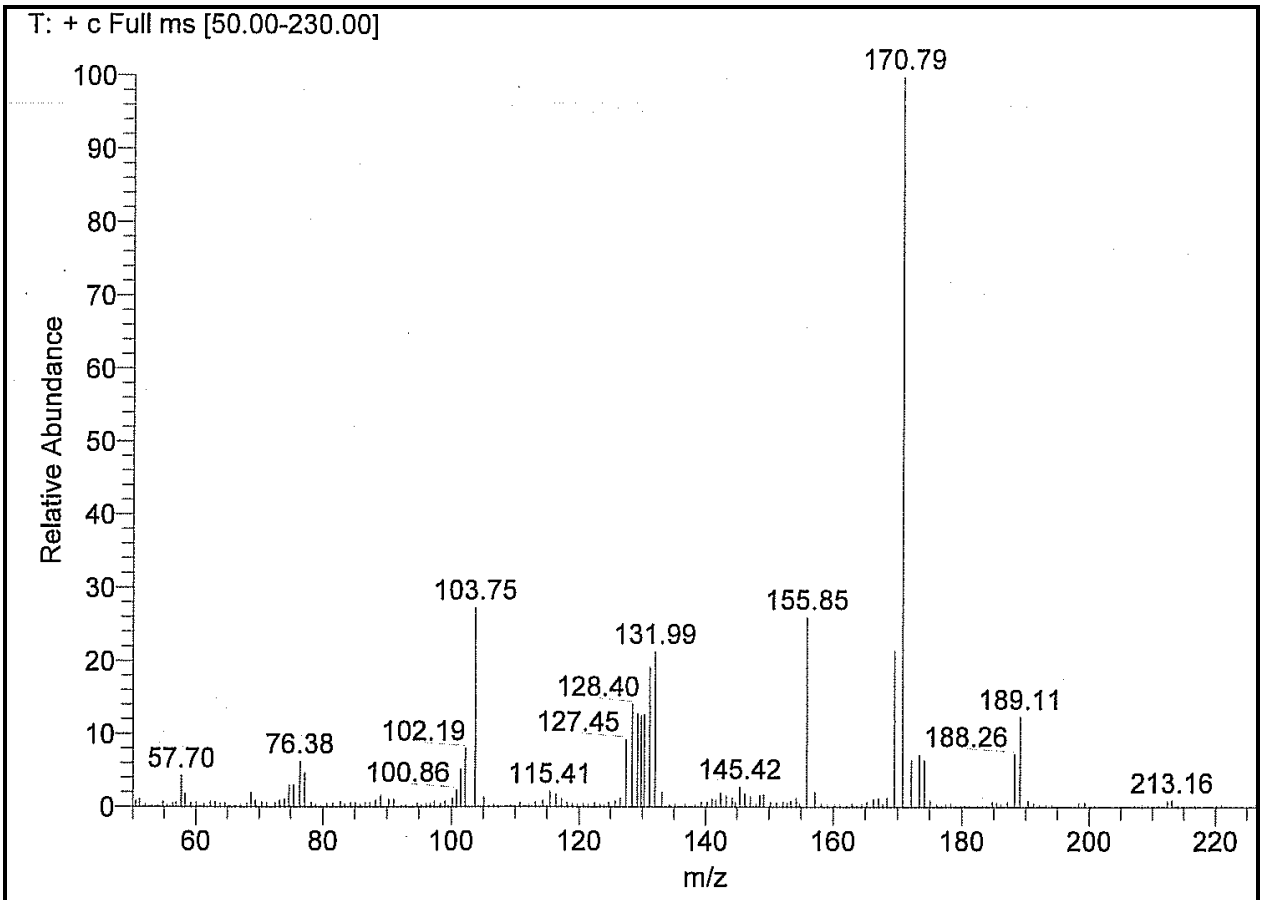


Figure 19. ^{13}**C of 4-Hydroxy-4-(4'-cyanophenyl)butan-2-one.**



EVS-PCYB#201 RT: 1.32
T: + c Full ms [50.00-230.00]

m/z	Intensity	Relative
76.38	196706.0	6.21
77.16	146267.0	4.62
101.49	162307.0	5.13
102.19	253360.0	8.00
103.75	864674.0	27.31
127.45	293140.0	9.26
128.40	446275.0	14.10
129.22	405305.0	12.80
129.76	394361.0	12.46
130.29	399611.0	12.62
131.15	608434.0	19.22
131.99	673921.0	21.29
155.85	823228.0	26.00
169.55	678087.0	21.42
170.79	3166173.0	100.00
172.18	204422.0	6.46
173.41	224854.0	7.10
174.18	202446.0	6.39
188.26	228656.0	7.22
189.11	390149.0	12.32

Figure 20. Mass spectrum of 4-Hydroxy-4-(4'-cyanophenyl)butan-2-one.

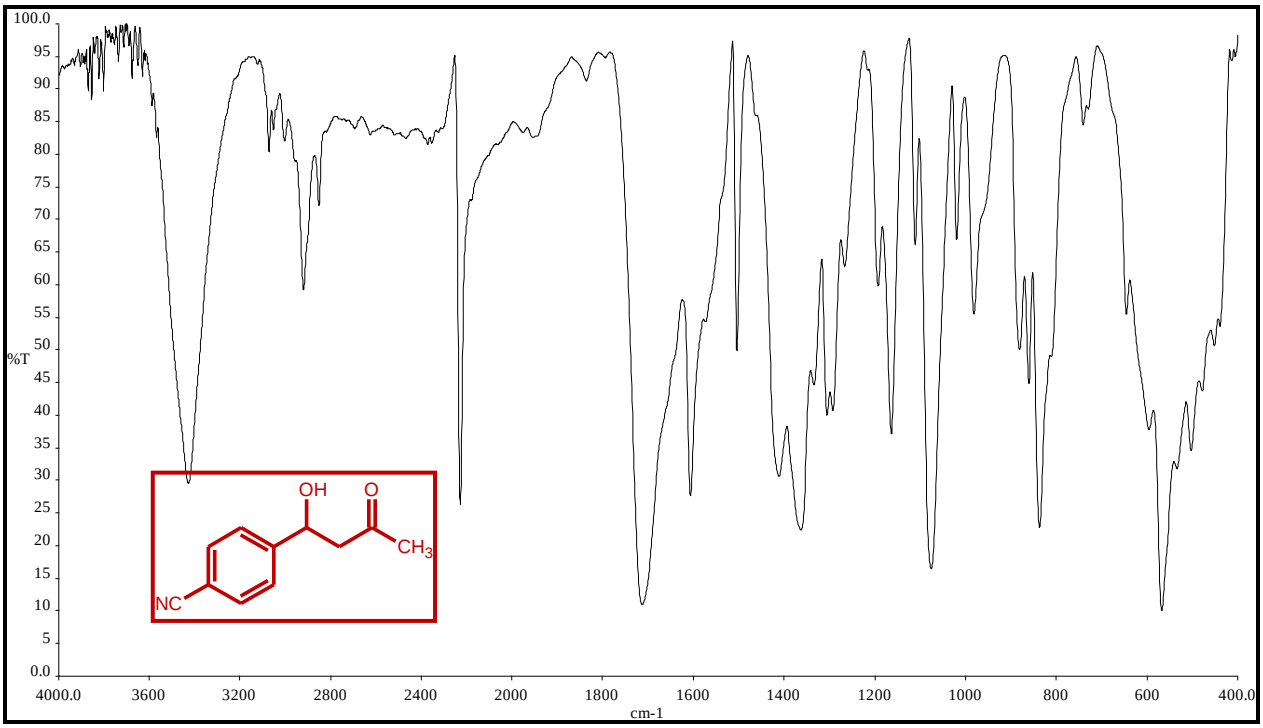
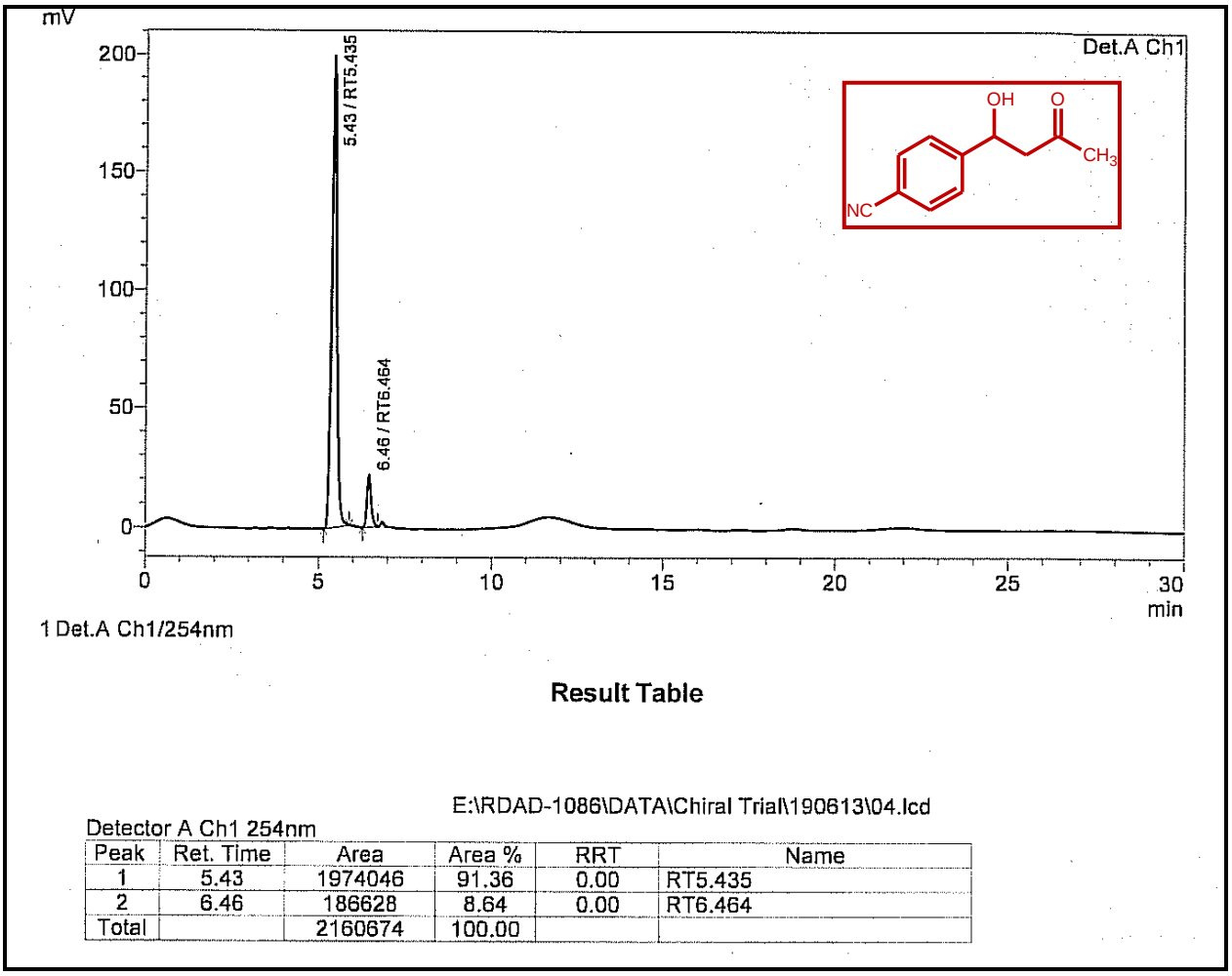


Figure 21. FTIR spectrum of 4-Hydroxy-4-(4'-cyanophenyl)butan-2-one.



Result Table

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Detector A Ch1 254nm

Peak	Ret. Time	Area	Area %	RRT	Name
1	5.43	1974046	91.36	0.00	RT5.435
2	6.46	186628	8.64	0.00	RT6.464
Total		2160674	100.00		

Figure 22. Chiral HPLC of 4-Hydroxy-4-(4'-cyanophenyl)butan-2-one.

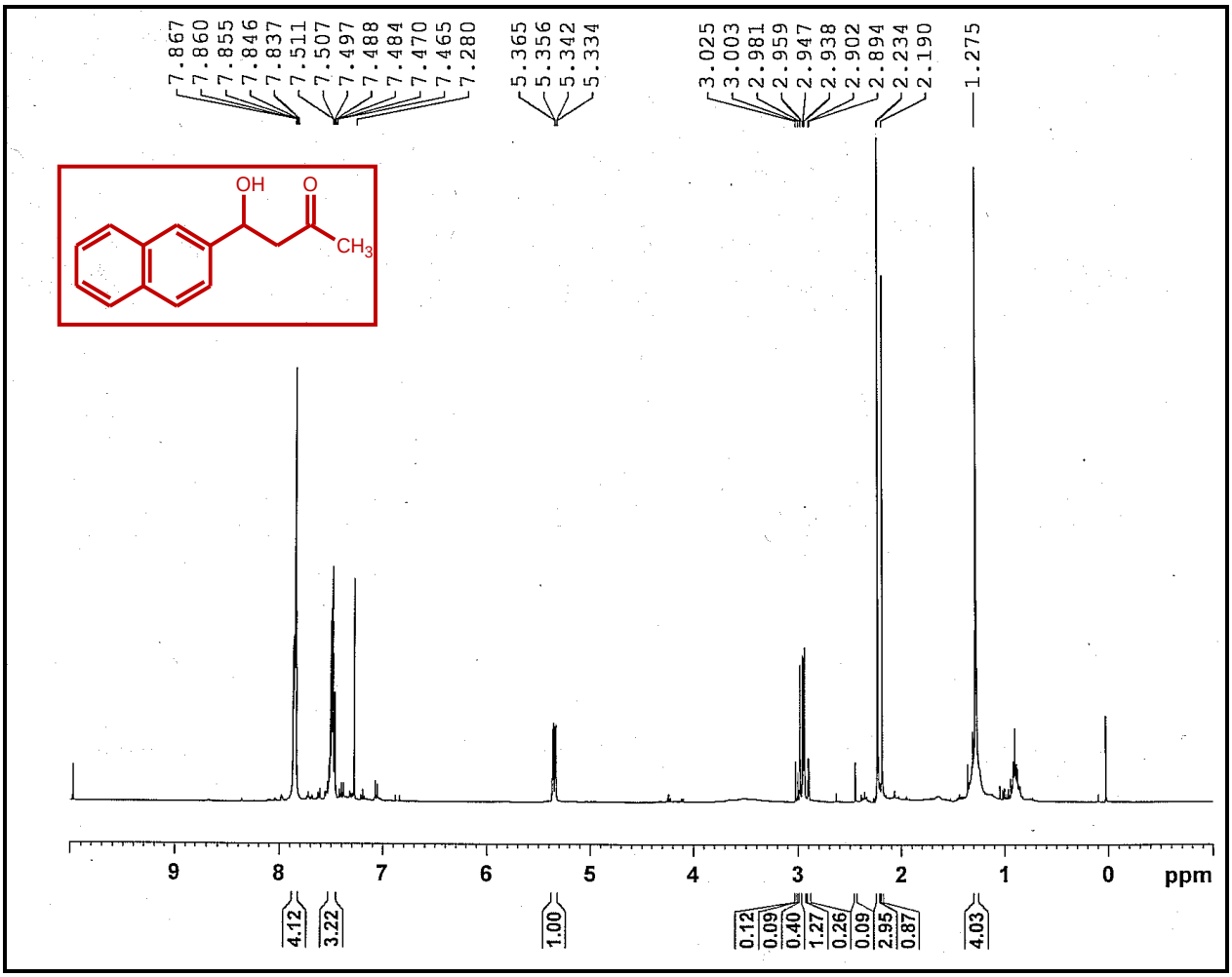


Figure 23. ^{1}H NMR of 4-(2-Naphthyl)-4-hydroxybutan-2-one.

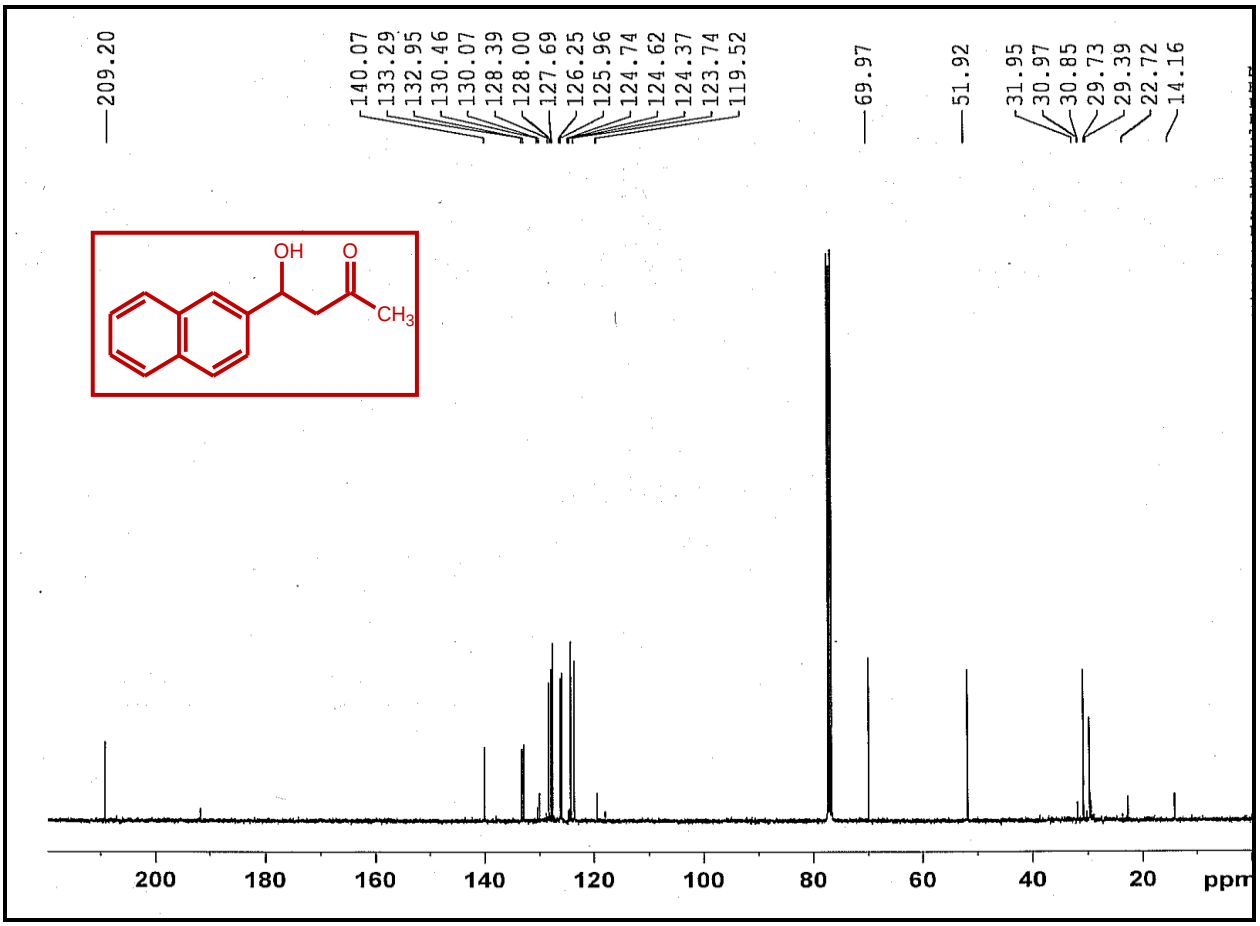
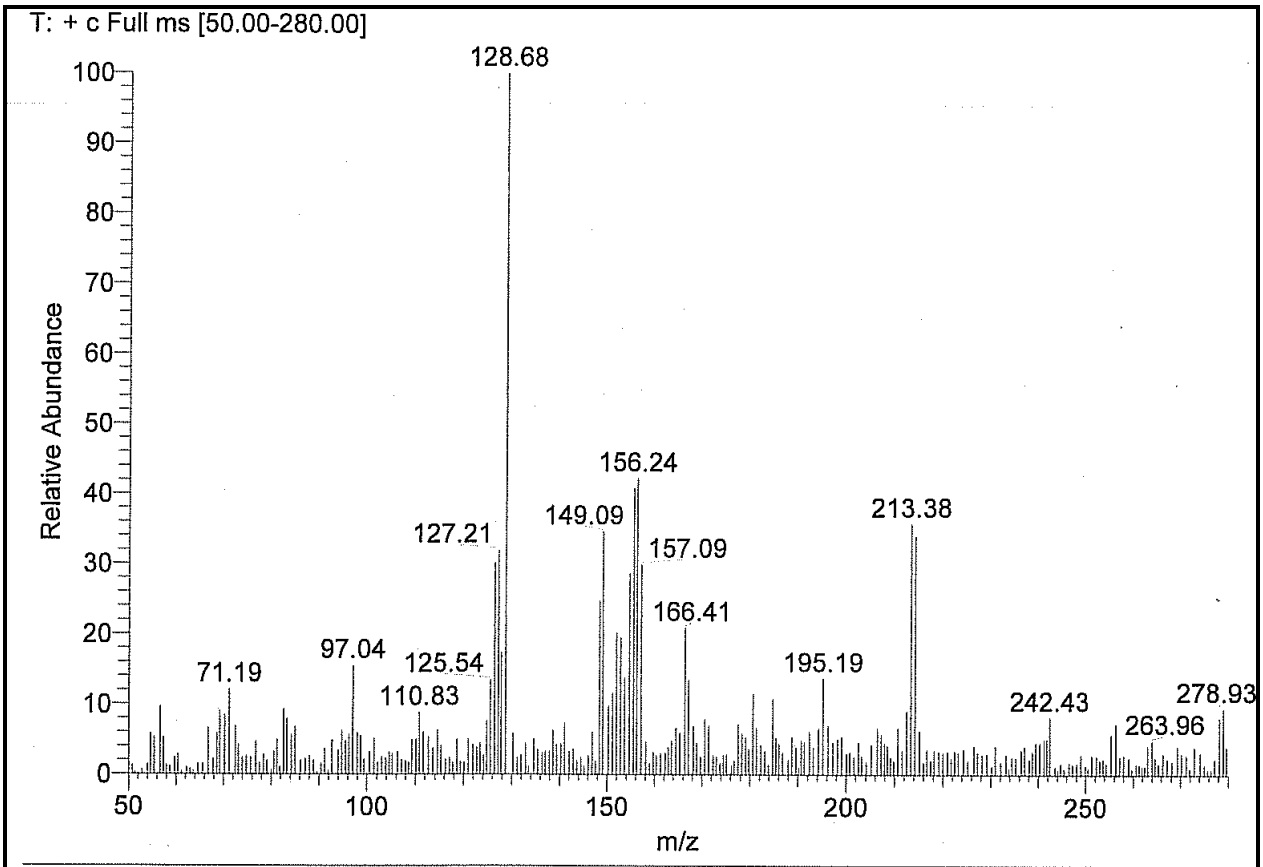


Figure 24. ^{13}**C spectrum of 4-(2-Naphthyl)-4-hydroxybutan-2-one.**



EVS-PNA_130618152849#179 RT: 1.48
T: + c Full ms [50.00-280.00]

m/z	Intensity	Relative
97.04	24405.0	15.41
125.54	21272.0	13.43
126.44	47761.0	30.16
127.21	50564.0	31.93
127.76	27394.0	17.30
128.68	158335.0	100.00
148.36	39200.0	24.76
149.09	54855.0	34.64
151.91	31947.0	20.18
152.83	30863.0	19.49
153.61	21715.0	13.71
154.62	45419.0	28.69
155.52	64754.0	40.90
156.24	66890.0	42.25
157.09	47362.0	29.91
166.41	33027.0	20.86
167.18	21189.0	13.38
195.19	21579.0	13.63
213.38	56651.0	35.78
214.20	53880.0	34.03

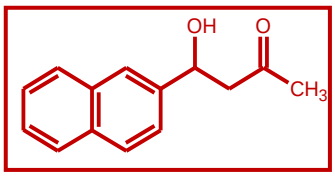


Figure 25. Mass spectrum of 4-(2-Naphthyl)-4-hydroxybutan-2-one.

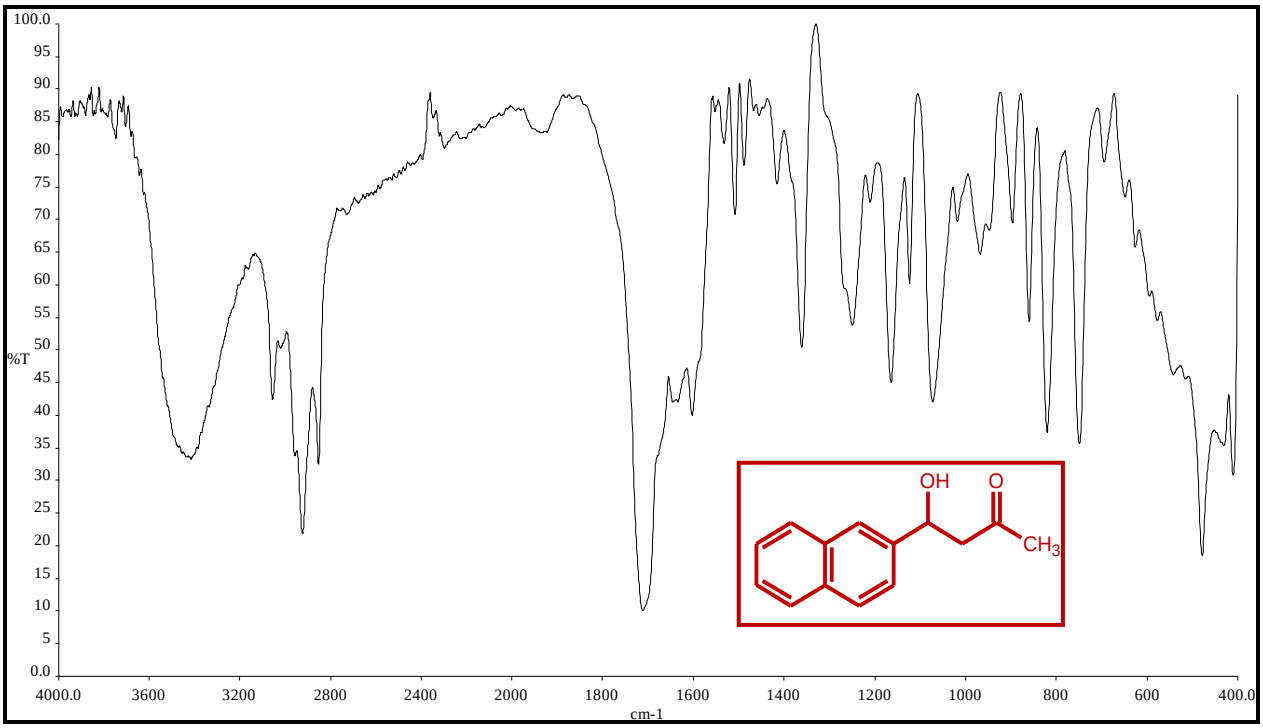
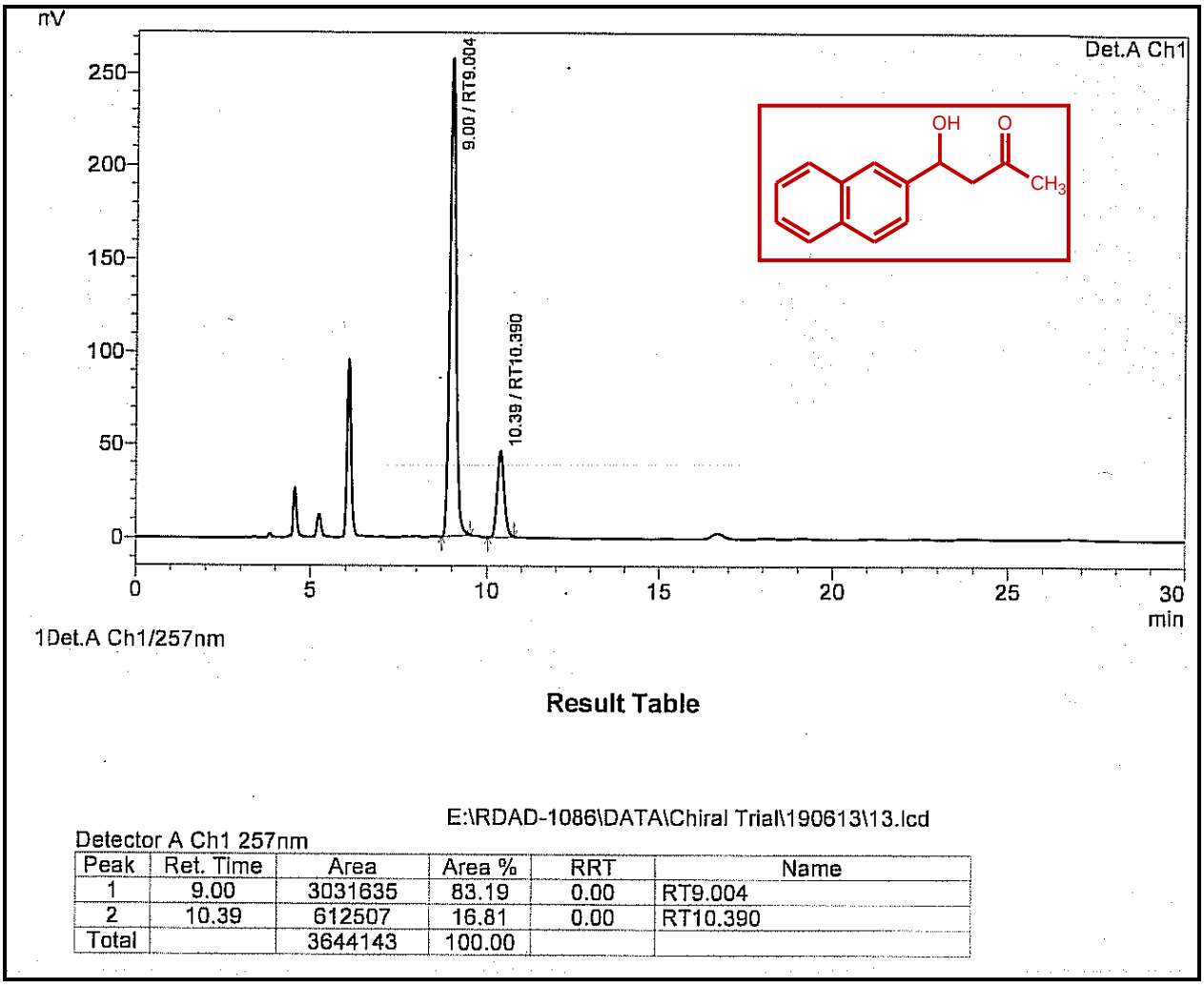


Figure 26. FTIR spectrum of 4-(2-Naphthyl)-4-hydroxybutan-2-one.



Result Table

E:\RDAD-1086\DATA\Chiral Trial\190613\13.lcd

Detector A Ch1 257nm

Peak	Ret. Time	Area	Area %	RRT	Name
1	9.00	3031635	83.19	0.00	RT9.004
2	10.39	612507	16.81	0.00	RT10.390
Total		3644143	100.00		

Figure 27. Chiral HPLC of 4-(2-Naphthyl)-4-hydroxybutan-2-one.

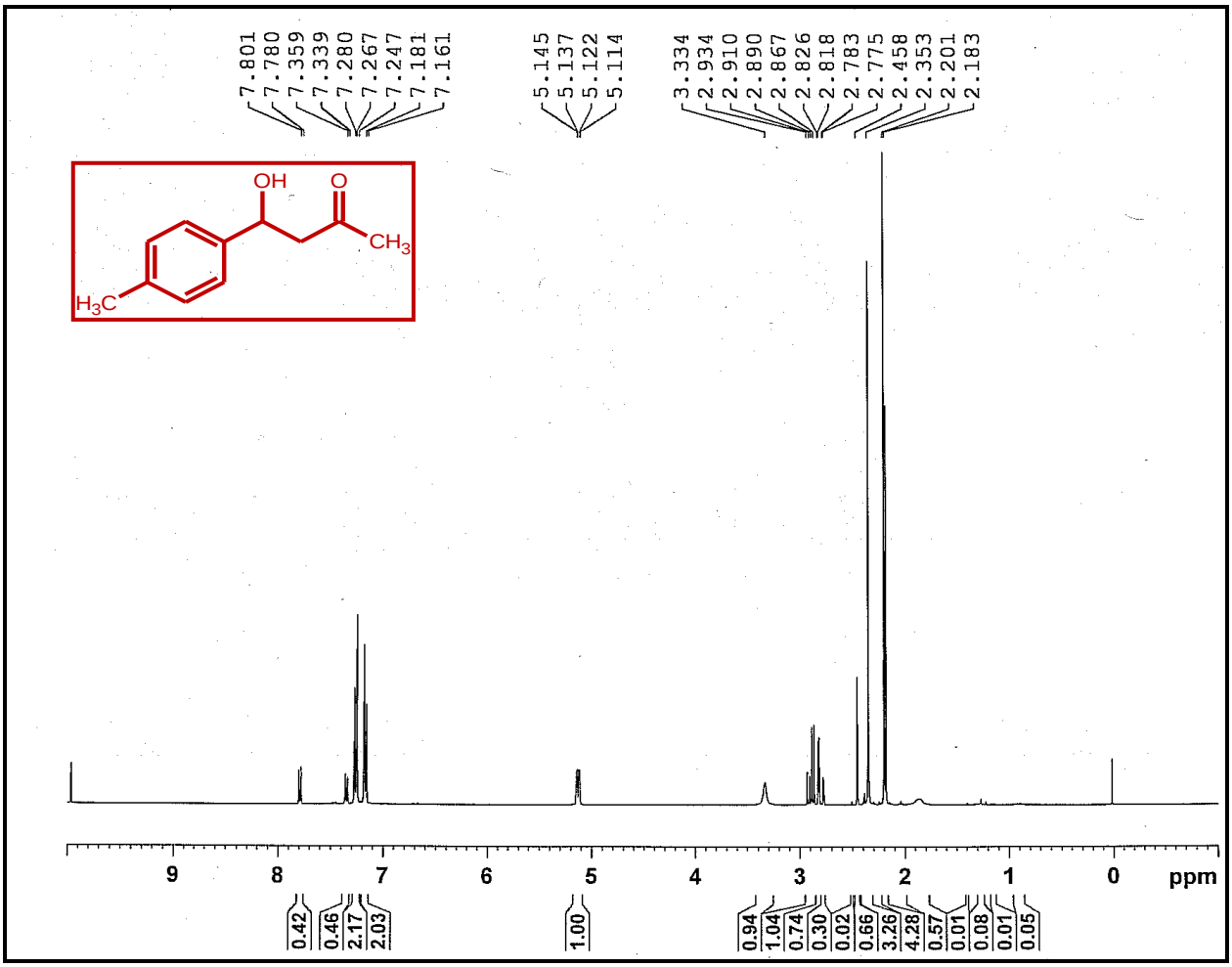


Figure 28. ^{1}H NMR of 4-Hydroxy-4-(4-methylphenyl)butan-2-one.

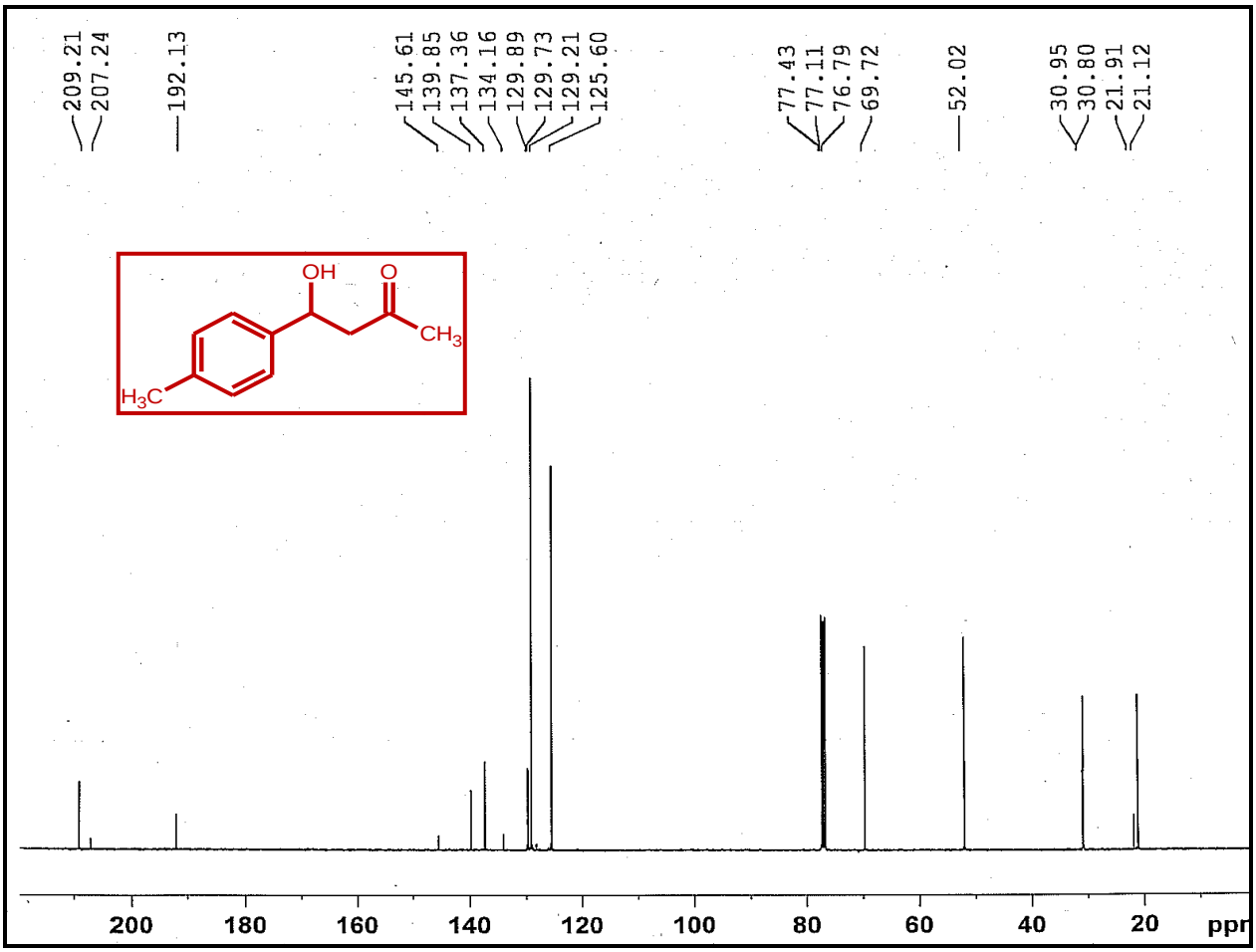
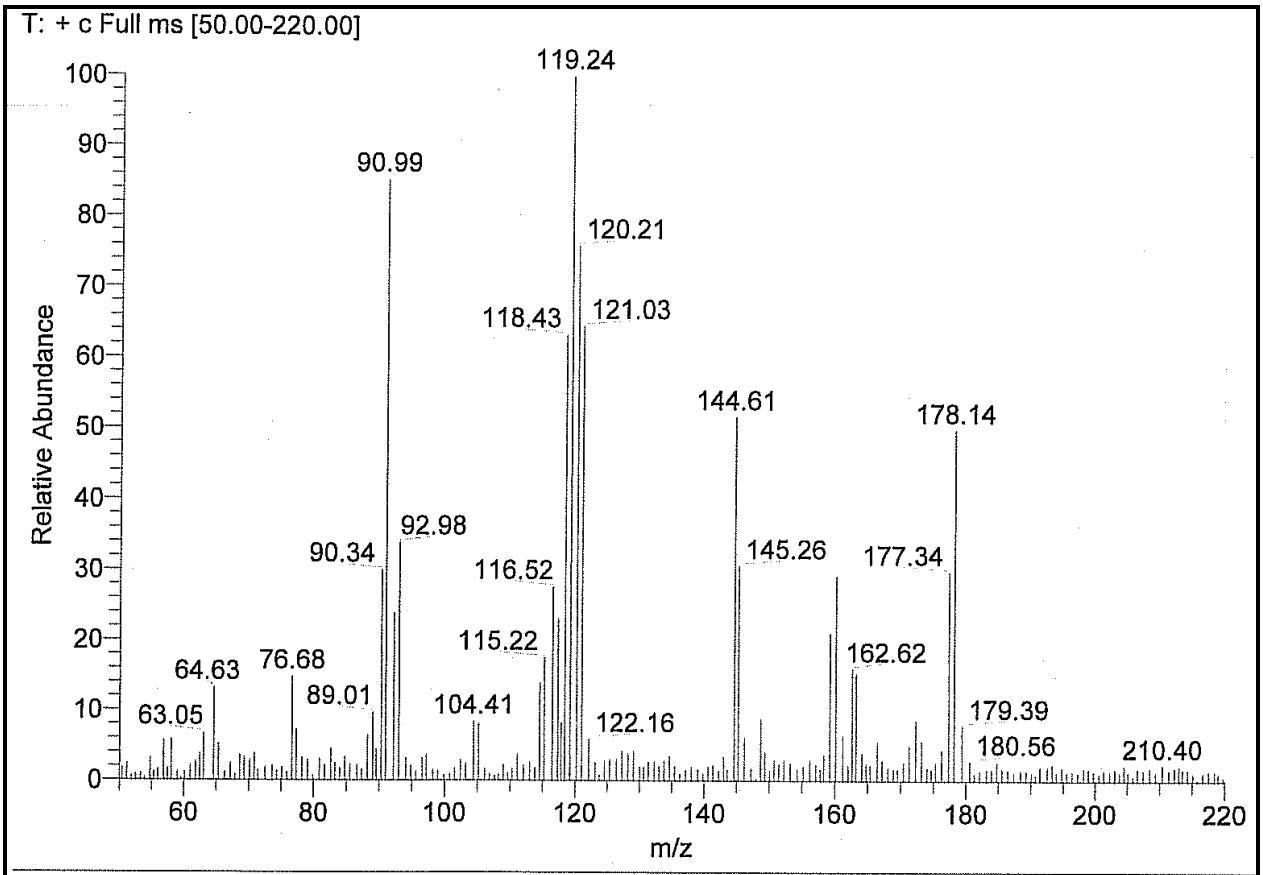


Figure 29. ^{13}**C spectrum of 4-Hydroxy-4-(4-methylphenyl)butan-2-one.**



EVS-PPA#197 RT: 1.23
T: + c Full ms [50.00-220.00]

m/z	Intensity	Relative
76.94	97736.0	18.30
90.46	256721.0	48.08
91.10	352028.0	65.93
92.82	276093.0	51.71
115.13	89589.0	16.78
116.18	80261.0	15.03
116.74	77808.0	14.57
117.31	139412.0	26.11
118.36	413913.0	77.52
119.21	533952.0	100.00
119.89	190995.0	35.77
120.51	442365.0	82.85
121.22	217588.0	40.75
144.39	143798.0	26.93
145.10	283884.0	53.17
159.19	93630.0	17.54
160.05	161129.0	30.18
163.10	105927.0	19.84
177.56	216884.0	40.62
178.27	172168.0	32.24

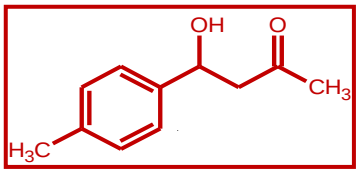


Figure 30. Mass spectrum of 4-Hydroxy-4-(4-methylphenyl)butan-2-one.

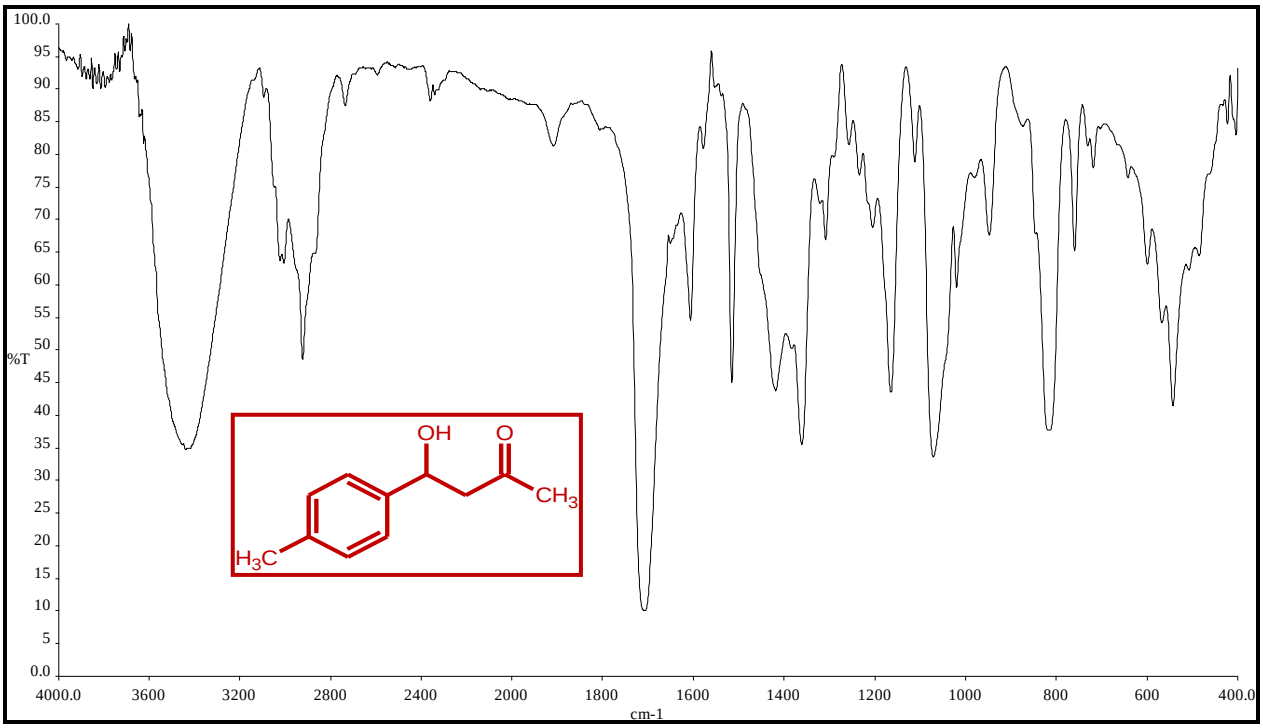
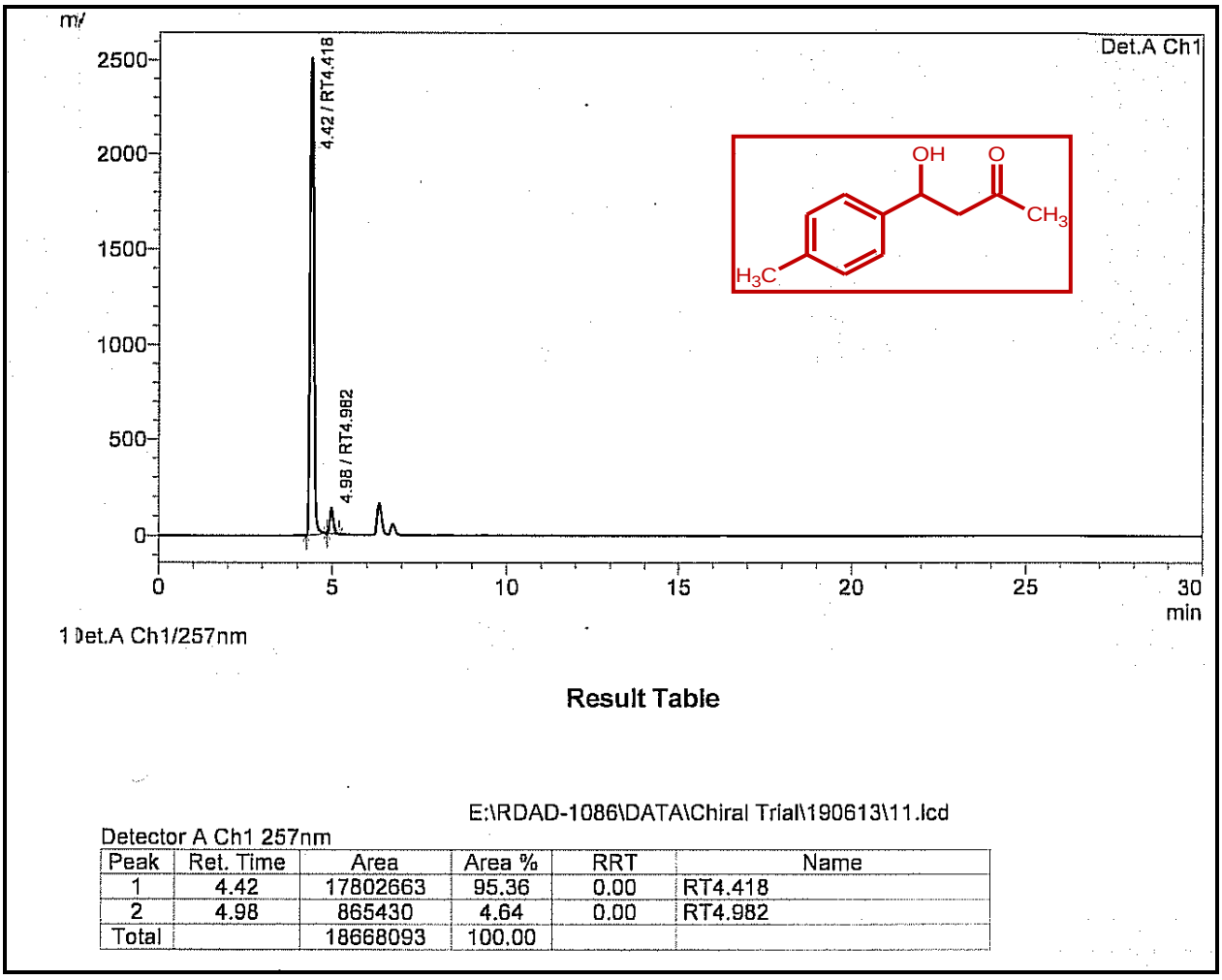


Figure 31. FTIR spectrum of 4-Hydroxy-4-(4-methylphenyl)butan-2-one.



Result Table

E:\RDAD-1086\DATA\Chiral Trial\190613\11.lcd

Detector A Ch1 257nm

Peak	Ret. Time	Area	Area %	RRT	Name
1	4.42	17802663	95.36	0.00	RT4.418
2	4.98	865430	4.64	0.00	RT4.982
Total		18668093	100.00		

Figure: HPLC of 4-Hydroxy-4-(4-methylphenyl)-butan-2-one

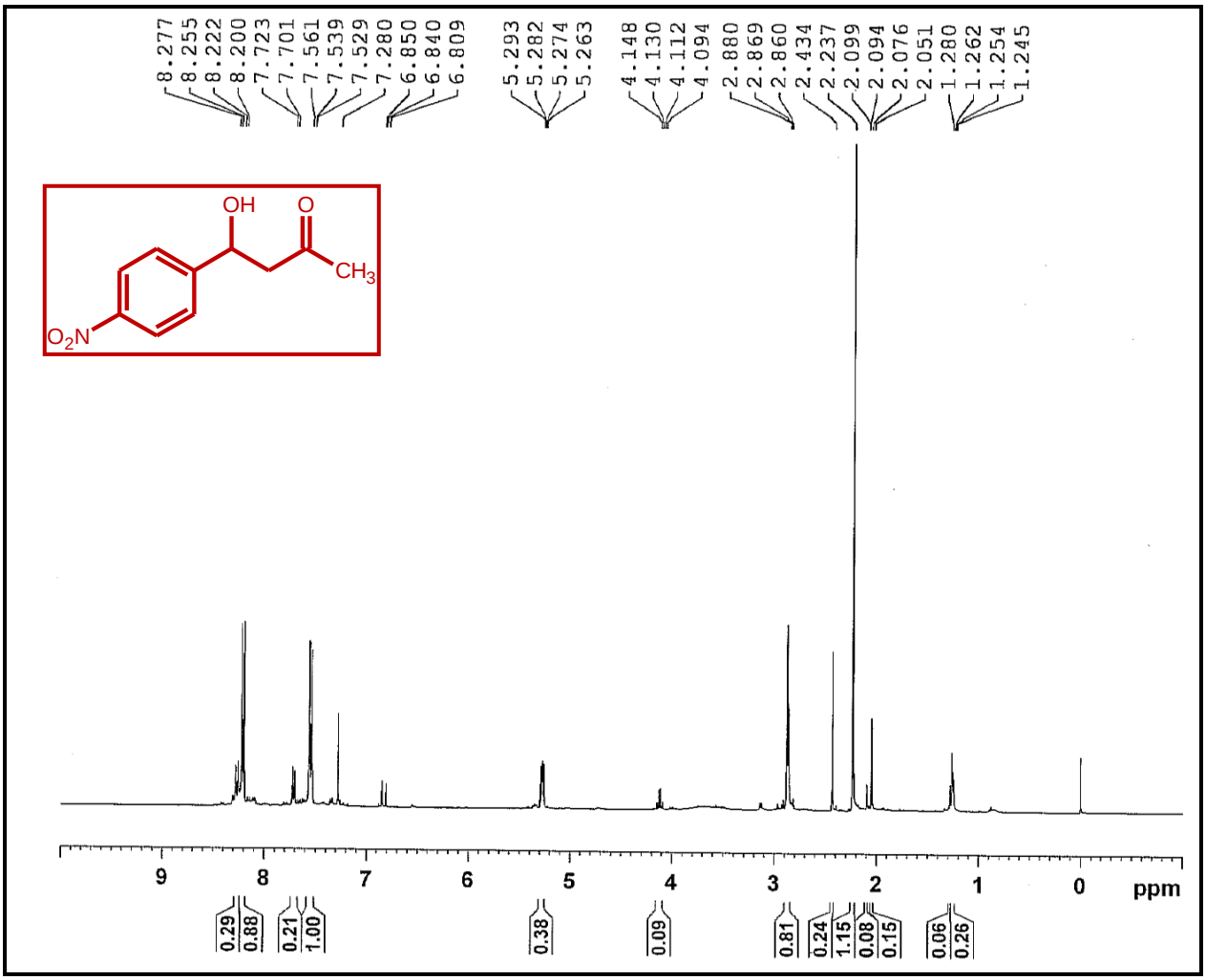


Figure : ^{1}H NMR of 4-Hydroxy-4-(4’-nitrophenyl)butan-2-one

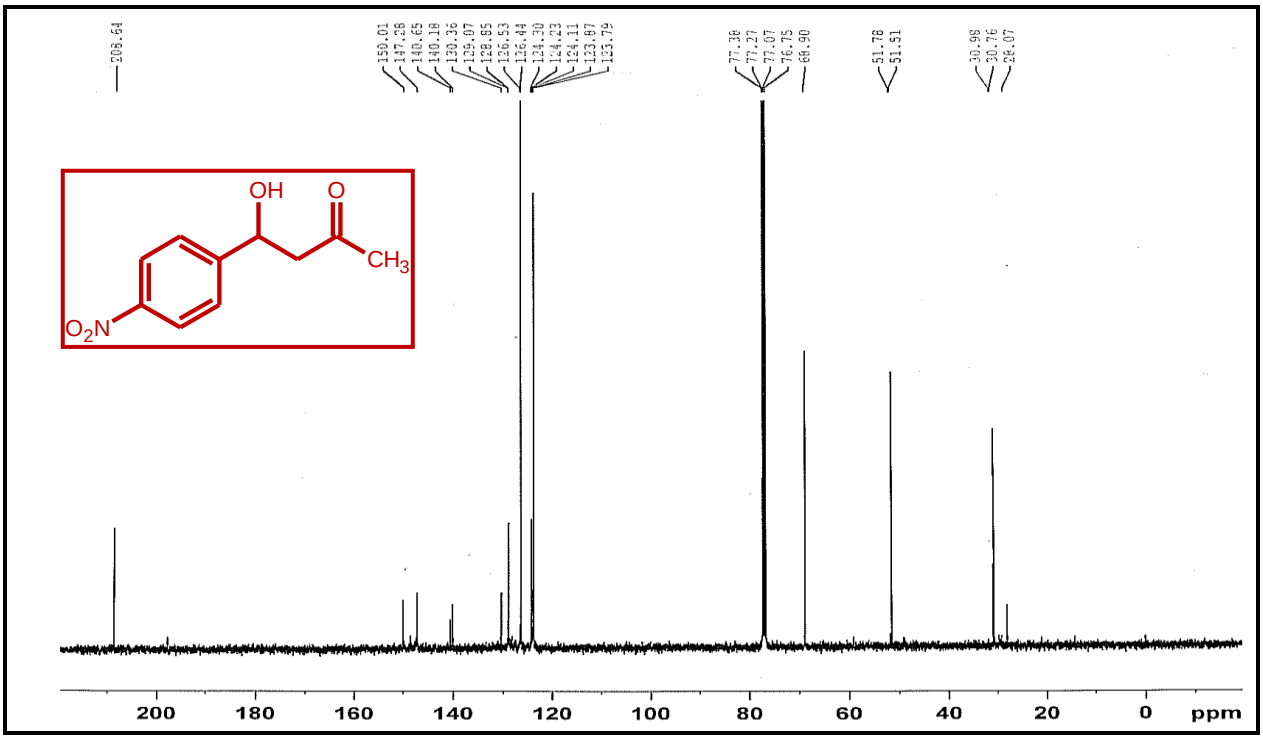
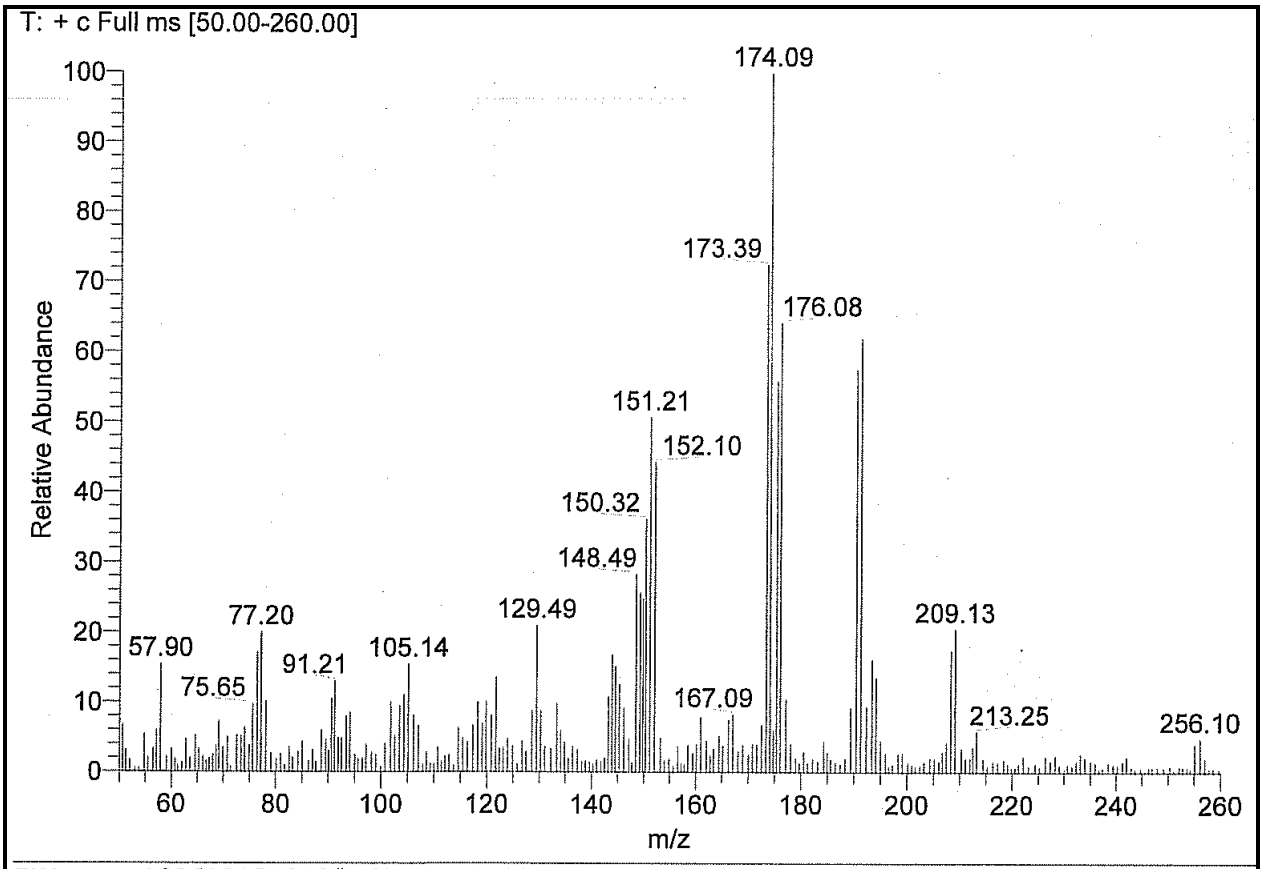


Figure : C13 of 4-Hydroxy-4-(4’-nitrophenyl)butan-2-one



EVS-PNB_130618154348#168 RT: 1.28
T: + c Full ms [50.00-260.00]

m/z	Intensity	Relative
76.49	59149.0	17.16
77.20	68916.0	20.00
105.14	53170.0	15.43
129.49	72478.0	21.03
143.90	58214.0	16.89
148.49	97832.0	28.38
149.28	88981.0	25.82
149.81	85900.0	24.92
150.32	125222.0	36.33
151.21	174968.0	50.77
152.10	153195.0	44.45
173.39	250274.0	72.61
174.09	344662.0	100.00
175.35	192980.0	55.99
176.08	221649.0	64.31
190.42	198633.0	57.63
191.29	213961.0	62.08
193.39	55747.0	16.17
208.32	60334.0	17.51
209.13	70872.0	20.56

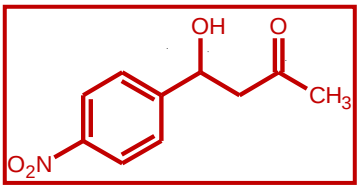


Figure : Mass of 4-Hydroxy-4-(4'-nitrophenyl)butan-2-one

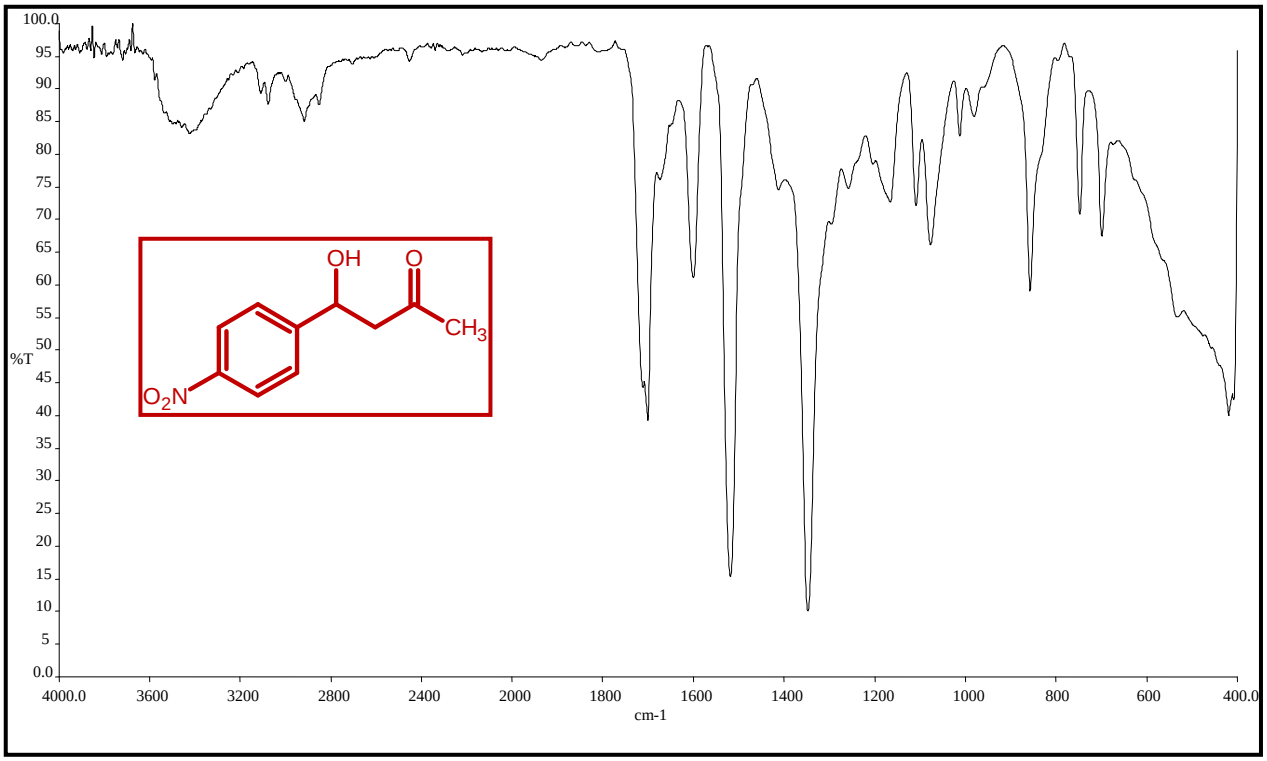
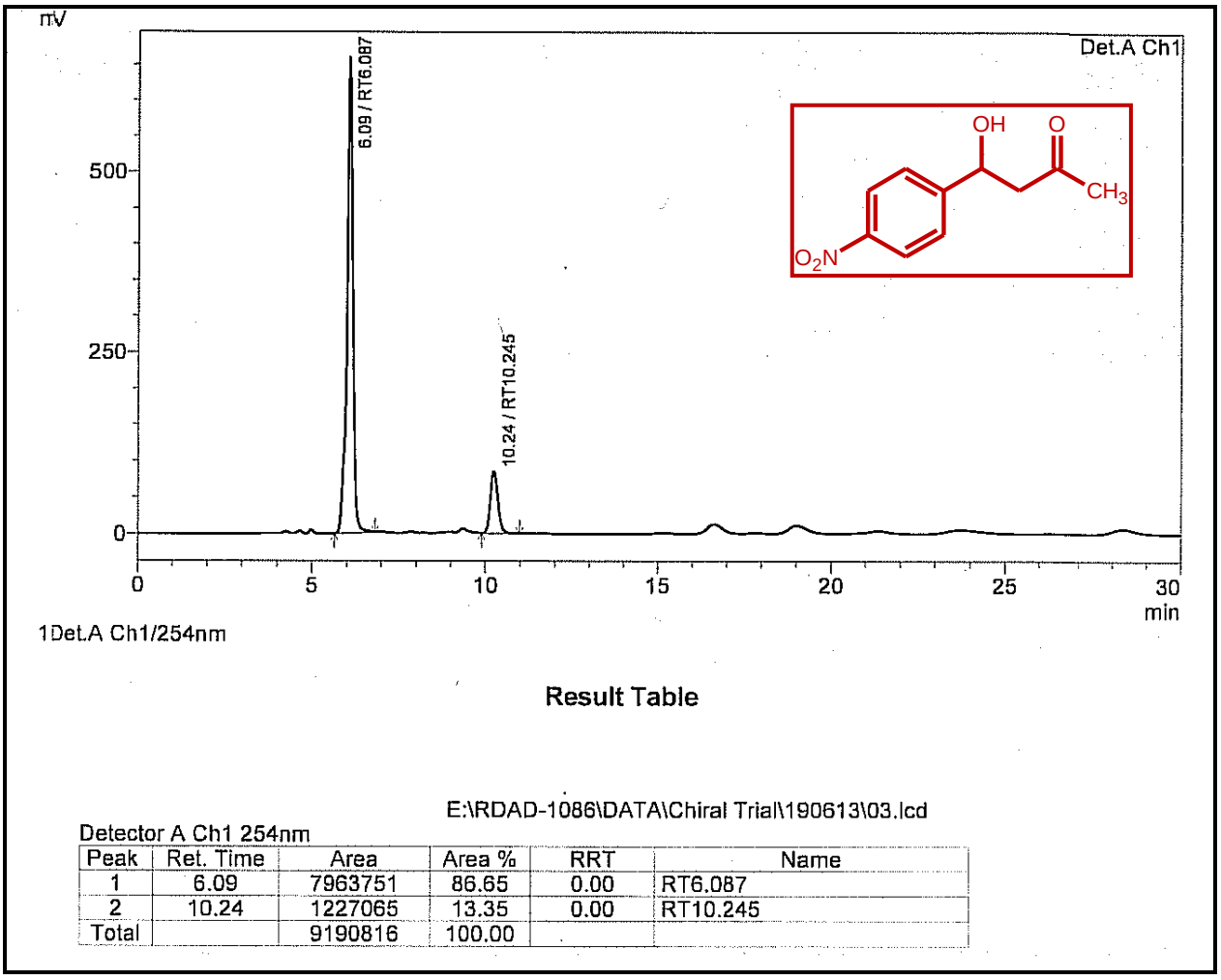


Figure: IR of 4-Hydroxy-4-(4’-nitrophenyl)butan-2-one



Result Table

E:\RDAD-1086\DATA\Chiral Trial\190613\03.lcd

Detector A Ch1 254nm

Peak	Ret. Time	Area	Area %	RRT	Name
1	6.09	7963751	86.65	0.00	RT6.087
2	10.24	1227065	13.35	0.00	RT10.245
Total		9190816	100.00		

Figure: HPLC of 4-Hydroxy-4-(4’-nitrophenyl)butan-2-one