Design, synthesis and biological evaluation of novel aryldiketo acids with enhanced antibacterial activity against multidrug resistant bacterial strains

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† Authors regret to inform that Branko Drakulić has passed away since completion of the research for this paper.

NMR spectra

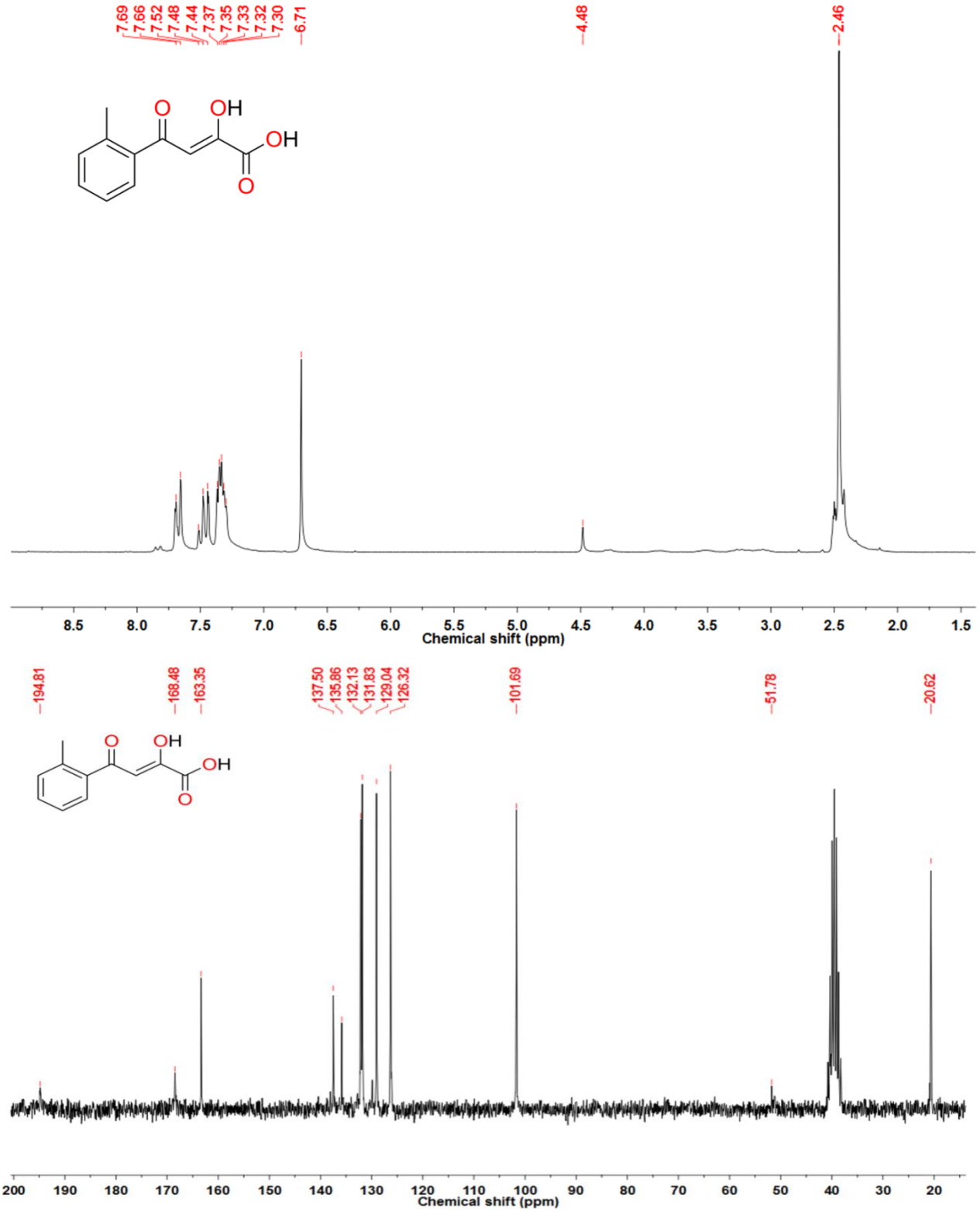
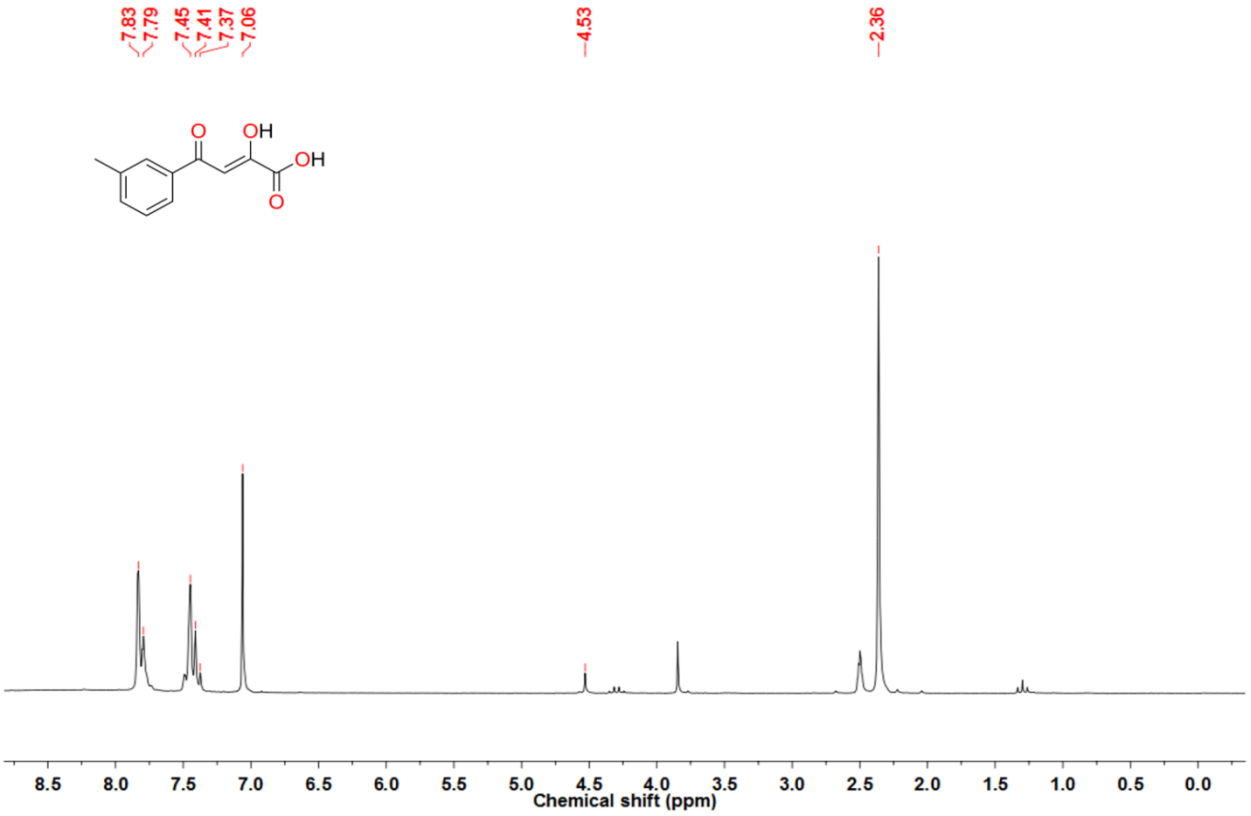


Figure S1. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-oxo-4-(*o*-tolyl)but-2-enoic acid **(2).**


7.83
7.79
7.45
7.41
7.37
7.06
4.53
2.36
O
OH
OH
O
8.5
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Chemical shift (ppm)

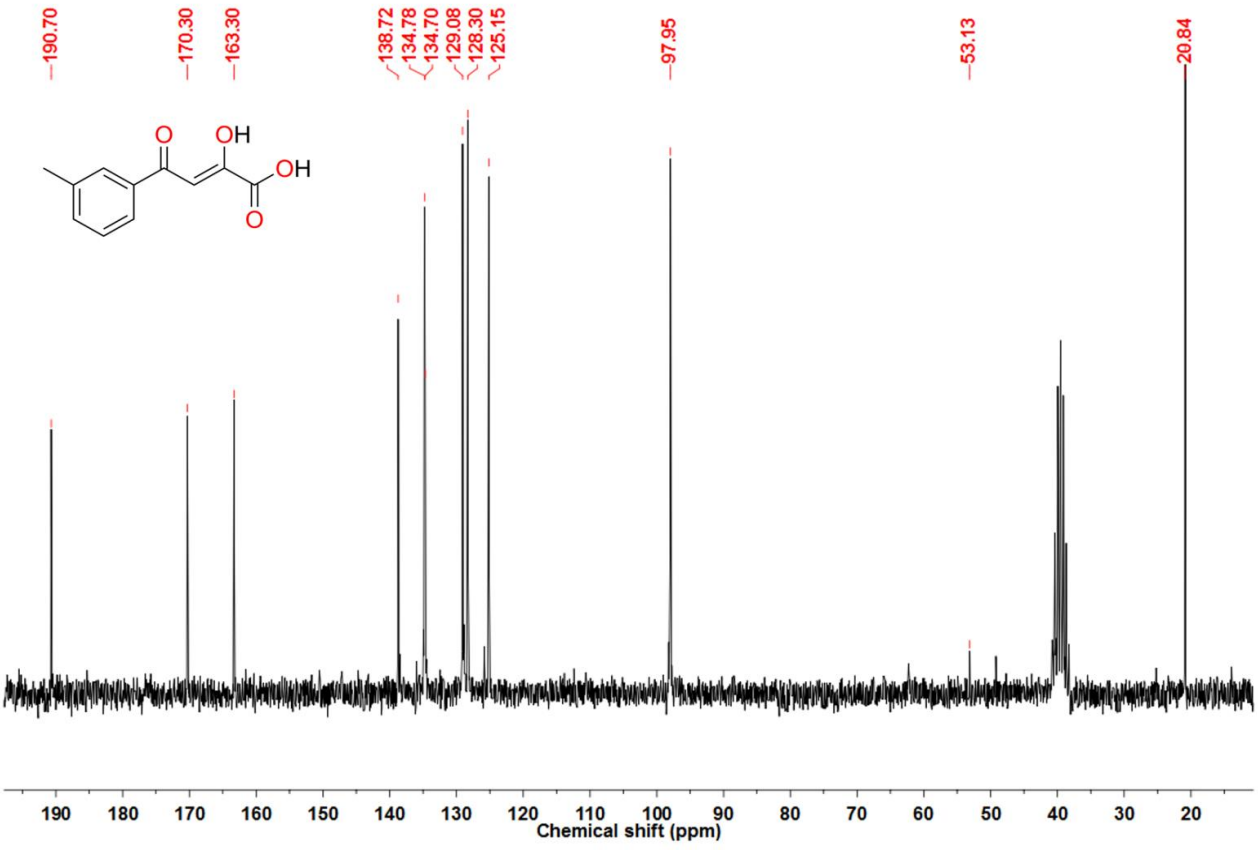
190.70
170.30
163.30
138.72
134.78
134.70
129.08
128.30
125.15
97.95
53.13
20.84
O
OH
OH
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
Chemical shift (ppm)

Figure S2. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-oxo-4-(*m*-tolyl)but-2-enoic acid **(3).**

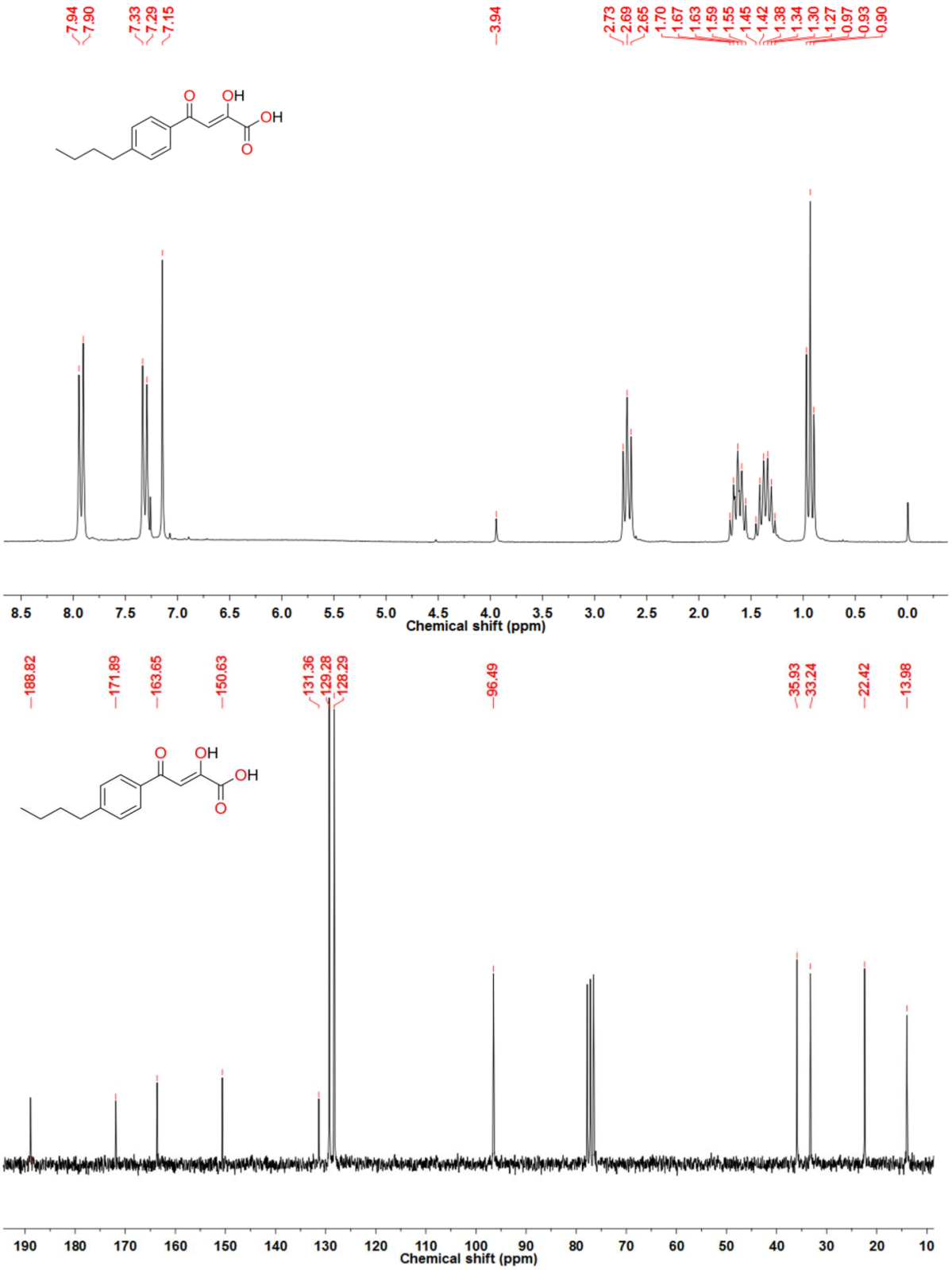

Figure S3. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-4-(4-butylphenyl)-2-hydroxy-4-oxobut-2-enoic acid **(4).**

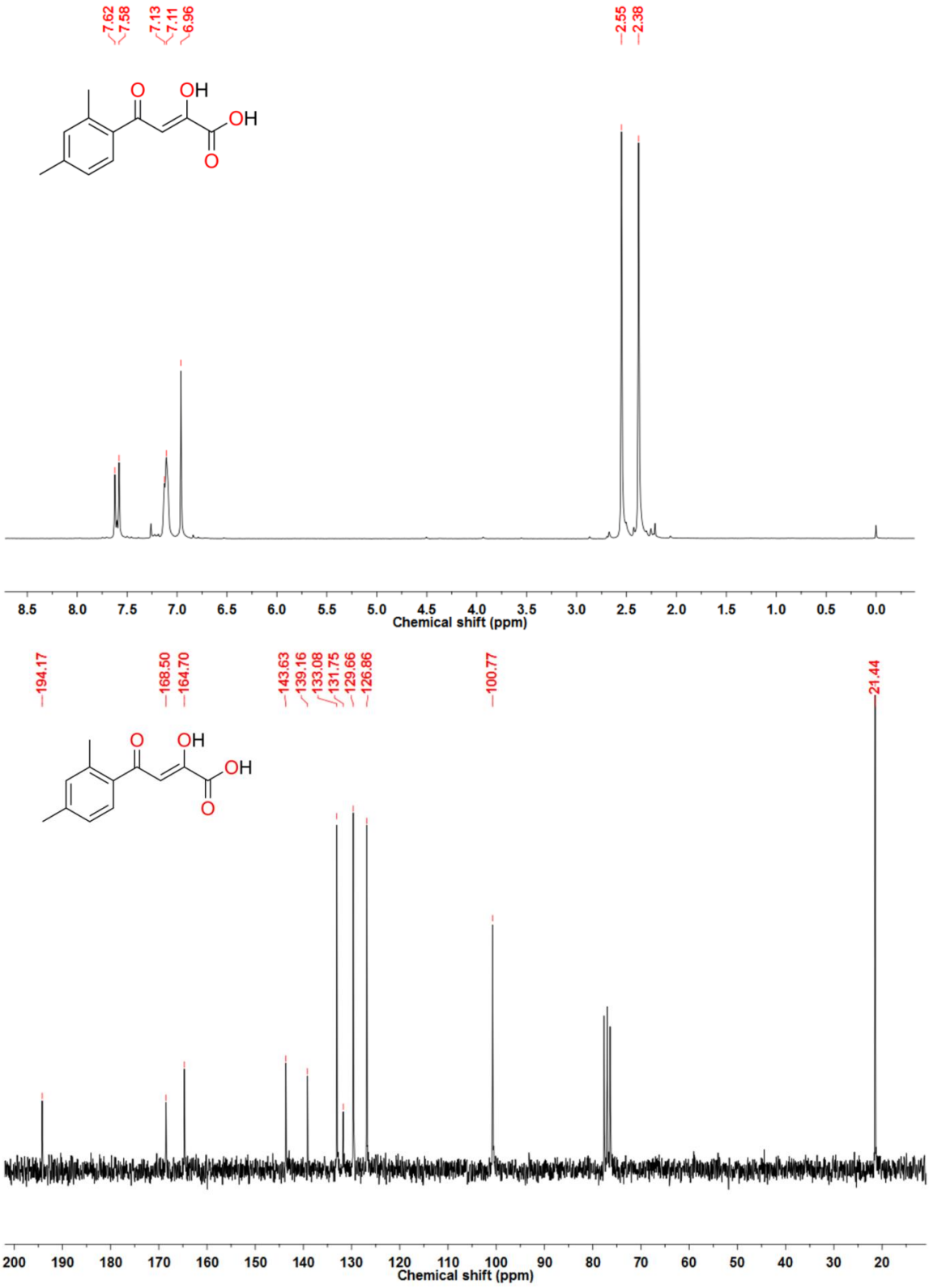

Figure S4. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-4-(2,4-dimethylphenyl)-2-hydroxy-4-oxobut-2-enoic acid **(5).**

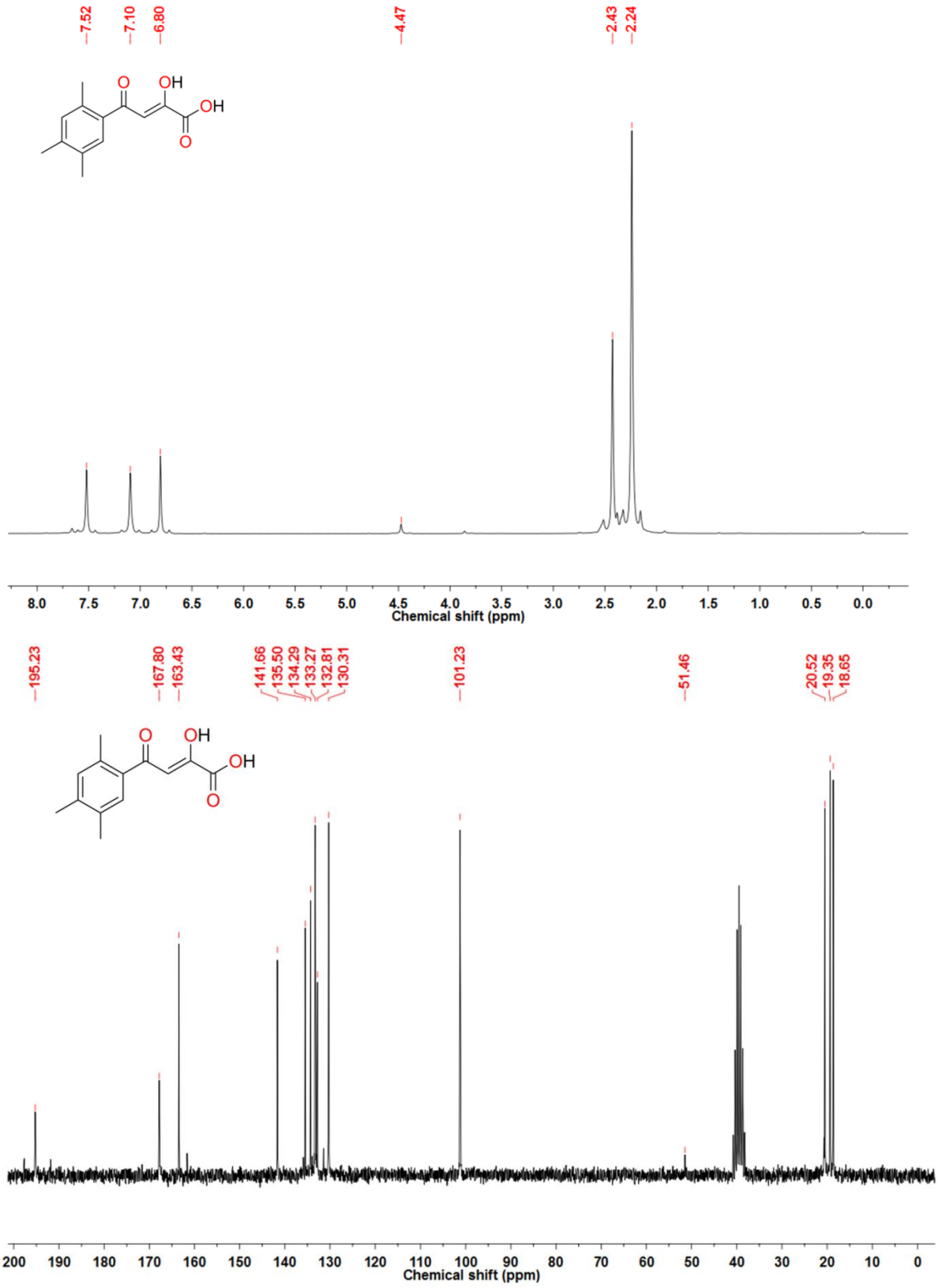

Figure S5. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-oxo-4-(2,4,5-trimethylphenyl)but-2-enoic acid **(6).**

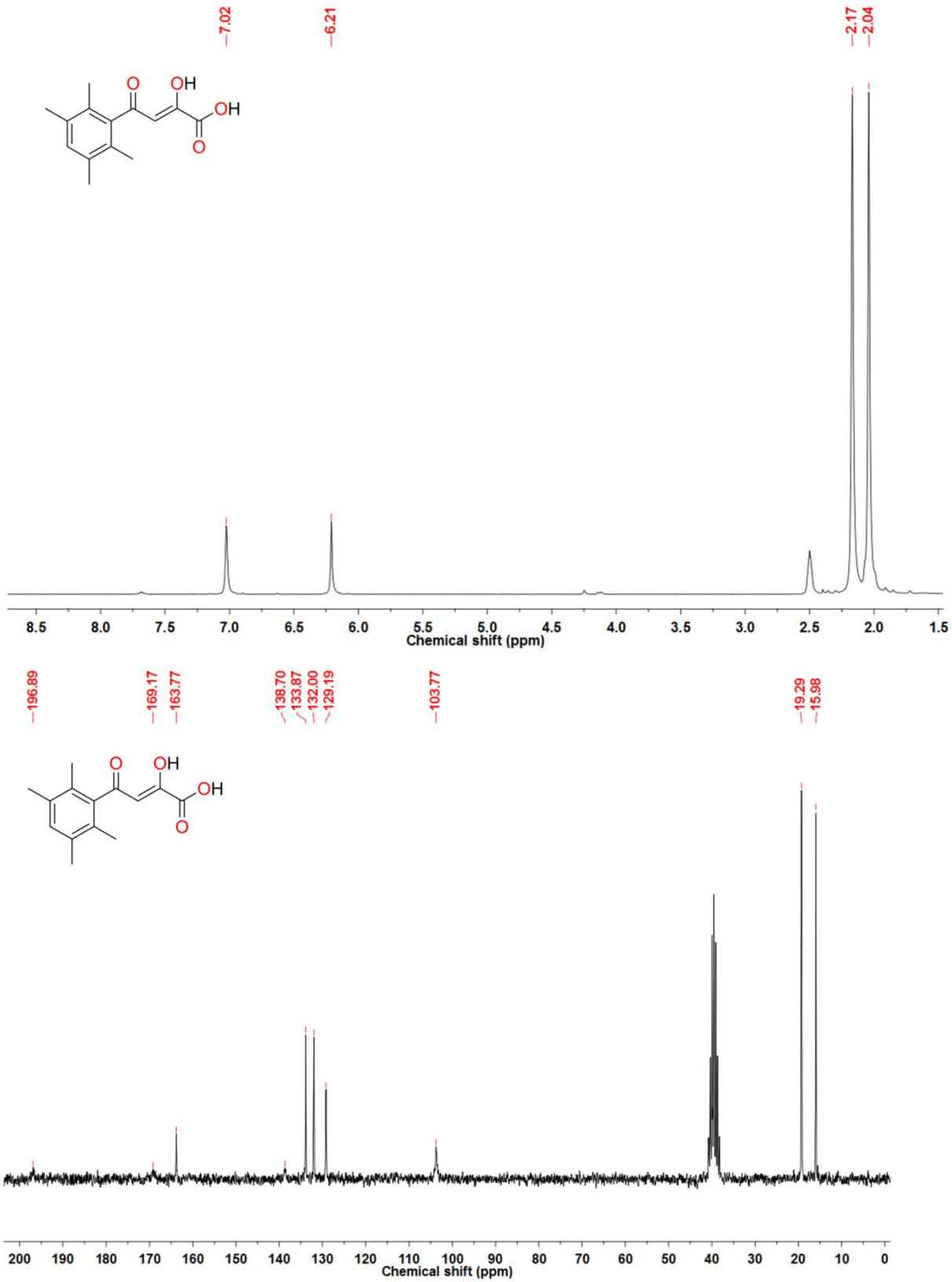

Figure S6. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-oxo-4-(2,3,5,6-tetramethylphenyl)but-2-enoic acid **(7).**

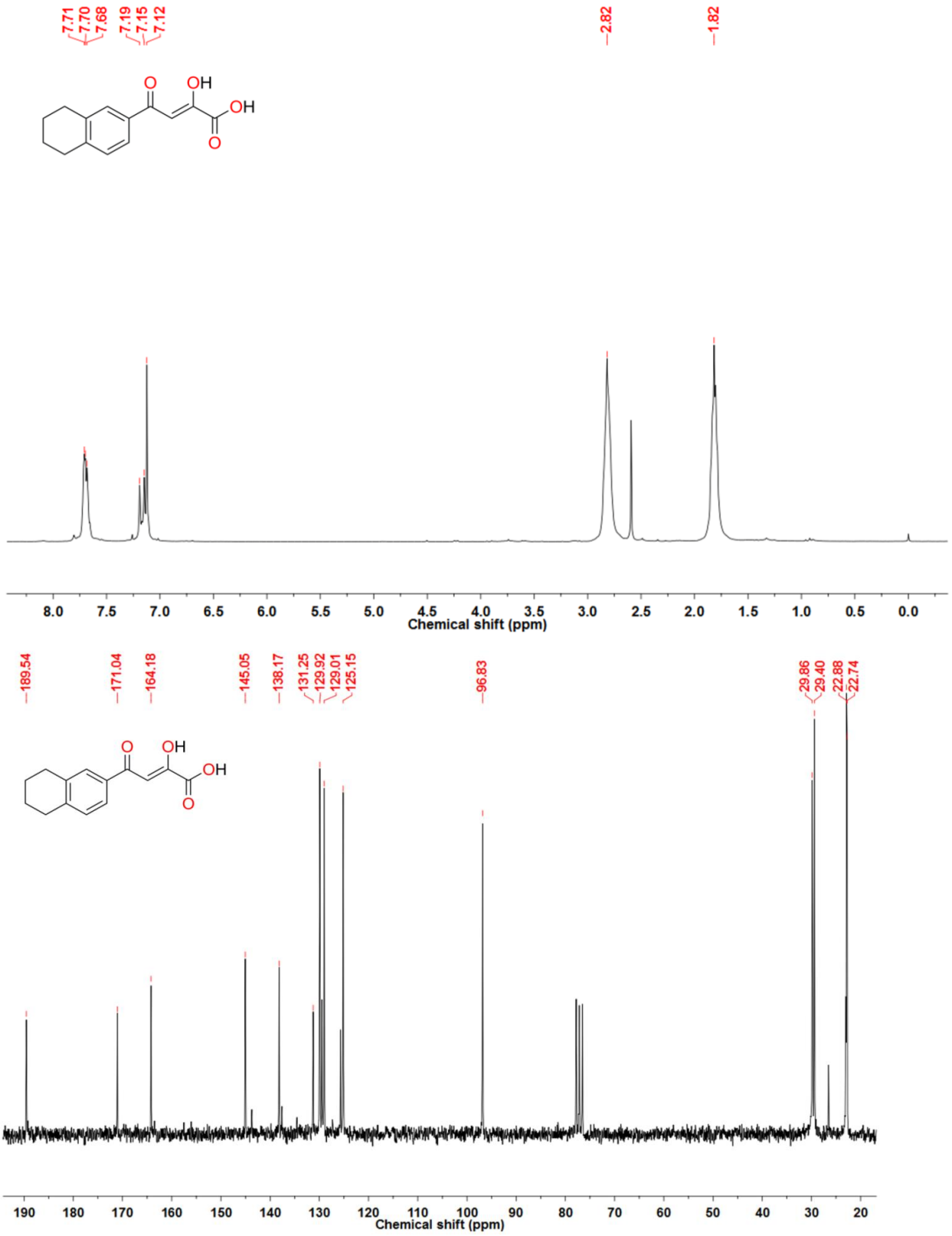

Figure S7. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-oxo-4-(5,6,7,8-tetrahydronaphthalen-2-yl)but-2-enoic acid **(8).**

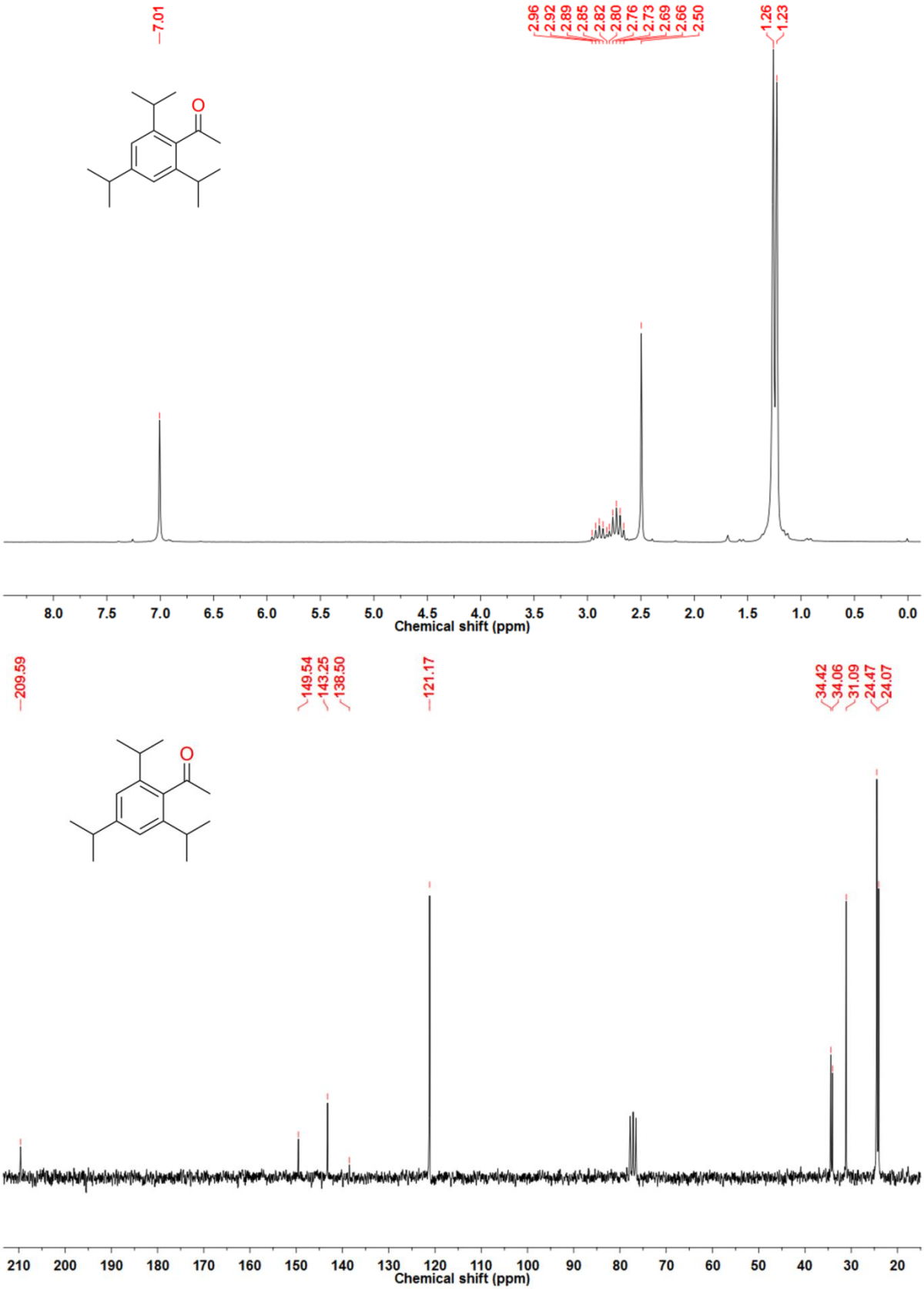

Figure S8. 1D ^{1}H and 1D ^{13}C NMR spectra of 1-(4-ethyl-2,6-diisopropylphenyl)ethanone **(5a).**

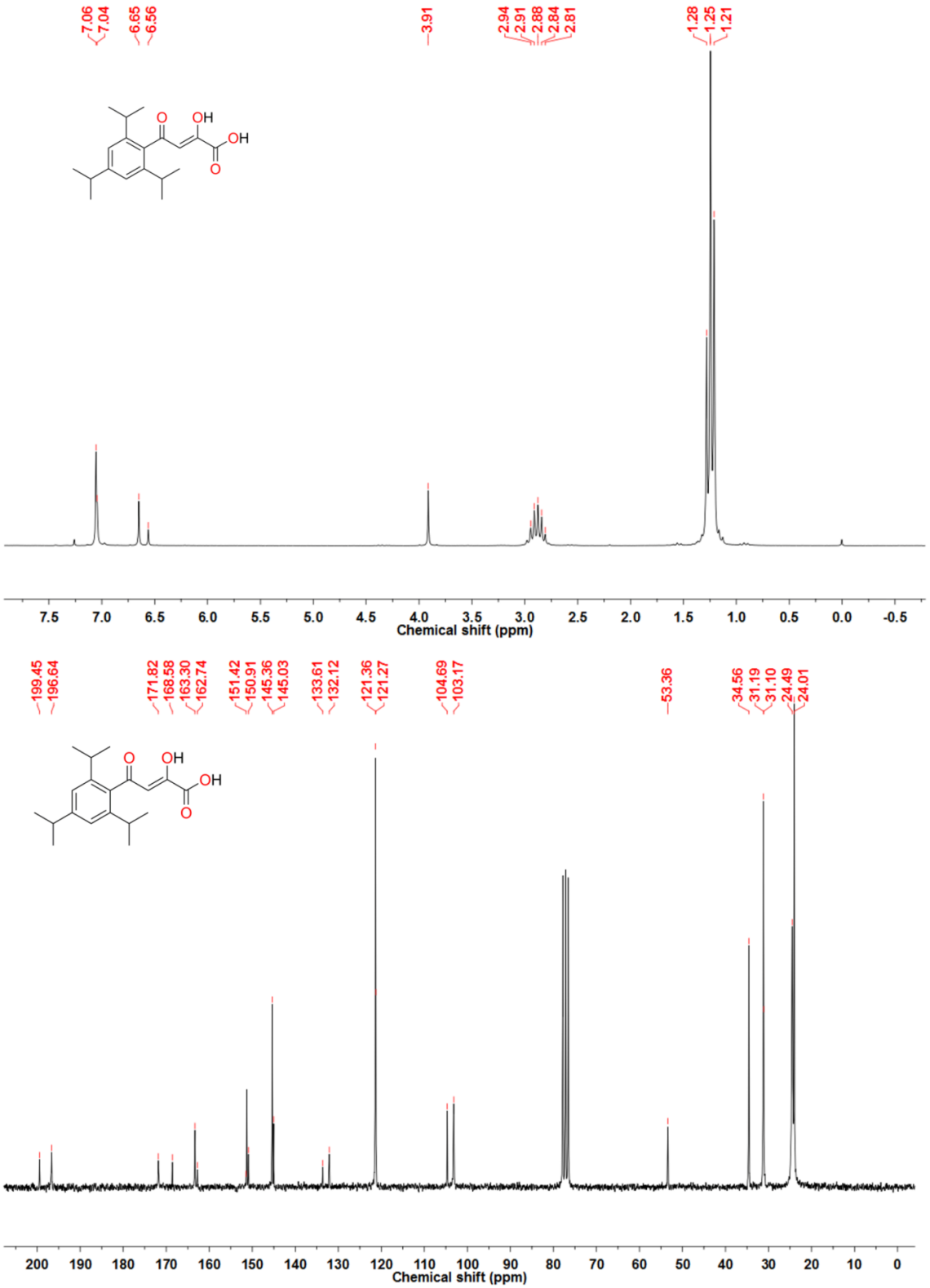

Figure S9. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-oxo-4-(2,4,6-triisopropylphenyl)but-2-enoic acid **(9).**

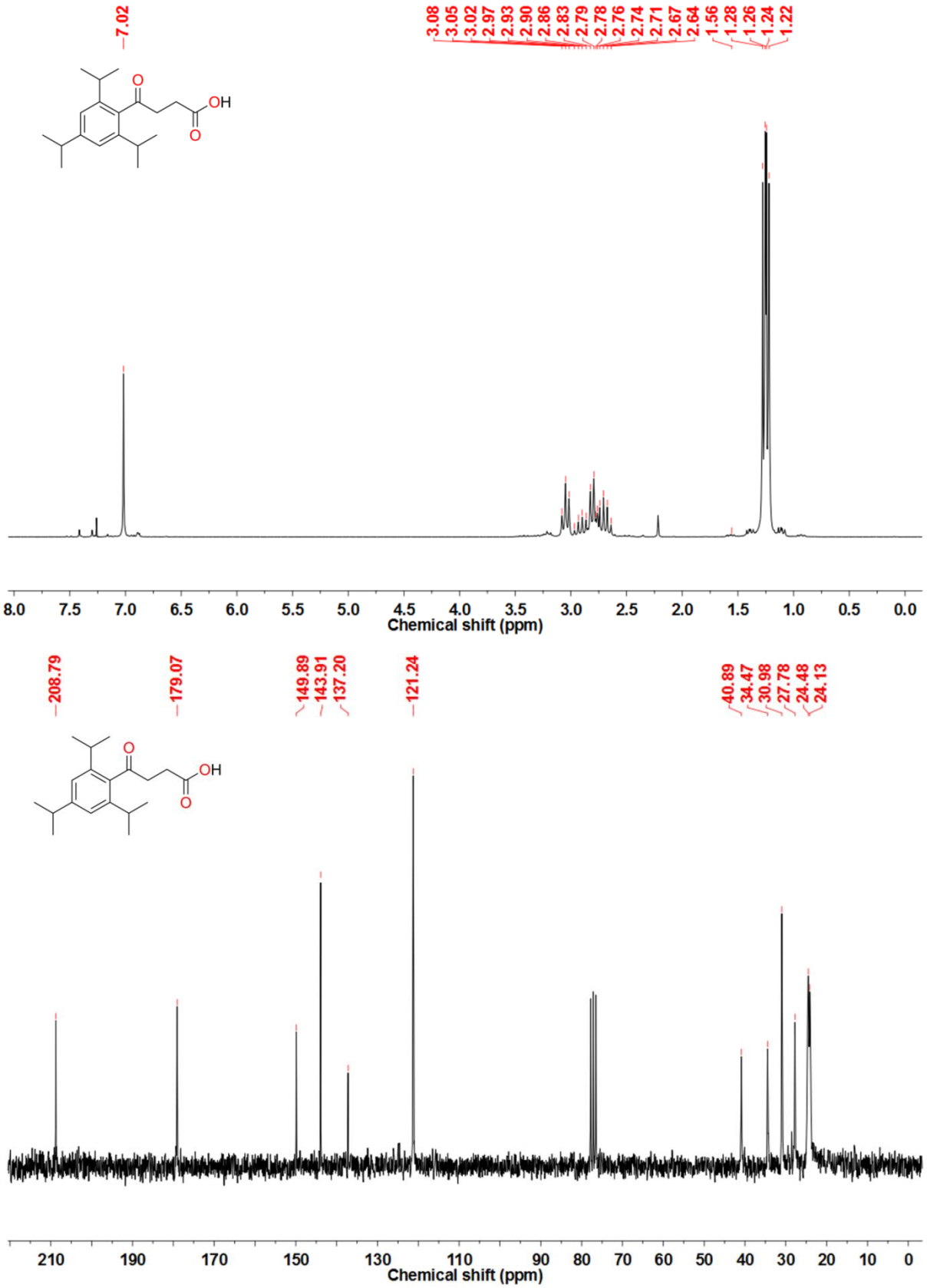

Figure S10. 1D ^{1}H and 1D ^{13}C NMR spectra of 4-oxo-4-(2,4,6-triisopropylphenyl)butanoic acid **(2a).**

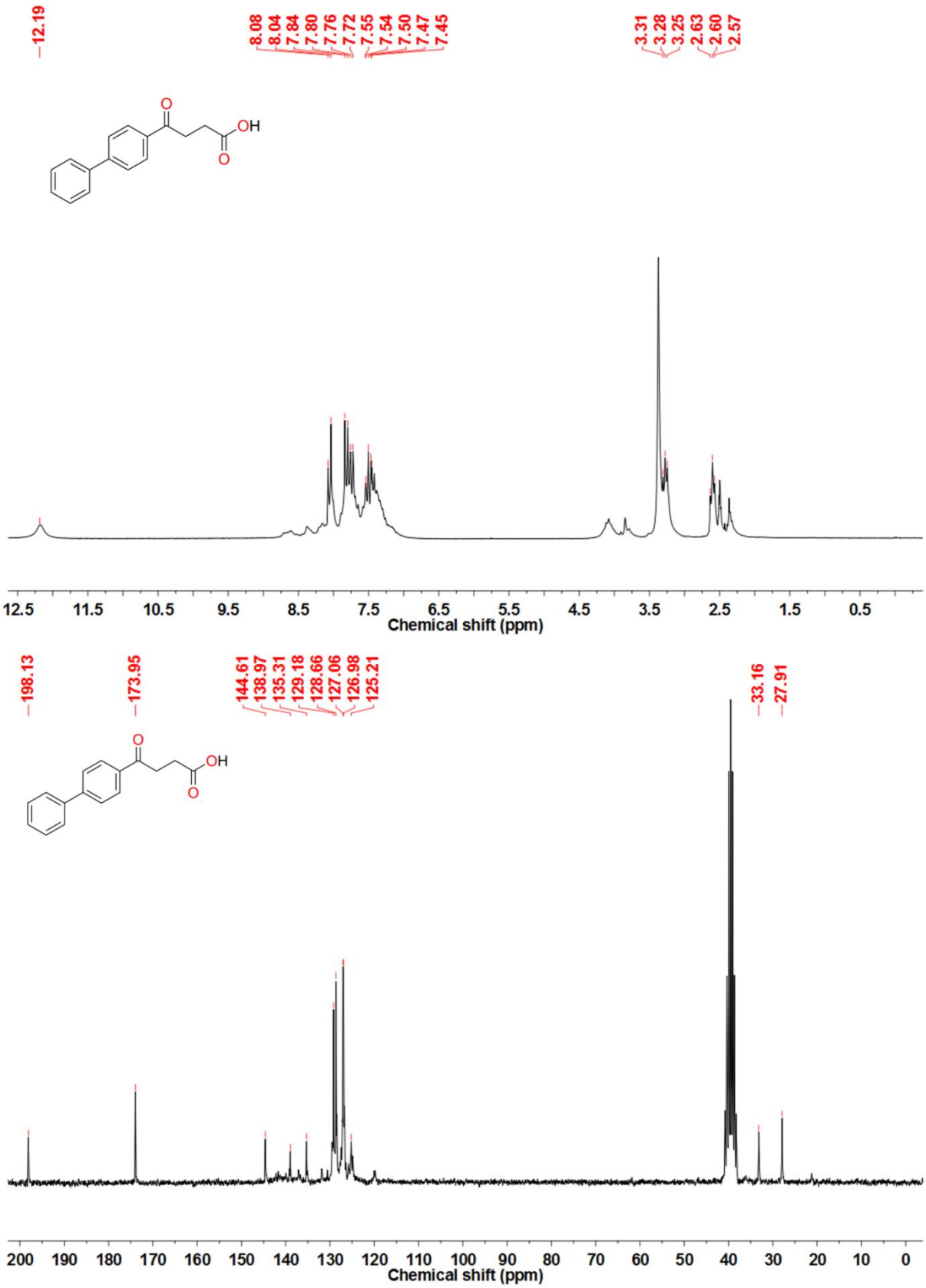

Figure S11. 1D ^{1}H and 1D ^{13}C NMR spectra of 4-([1,1'-biphenyl]-4-yl)-4-oxobutanoic acid **(3a).**

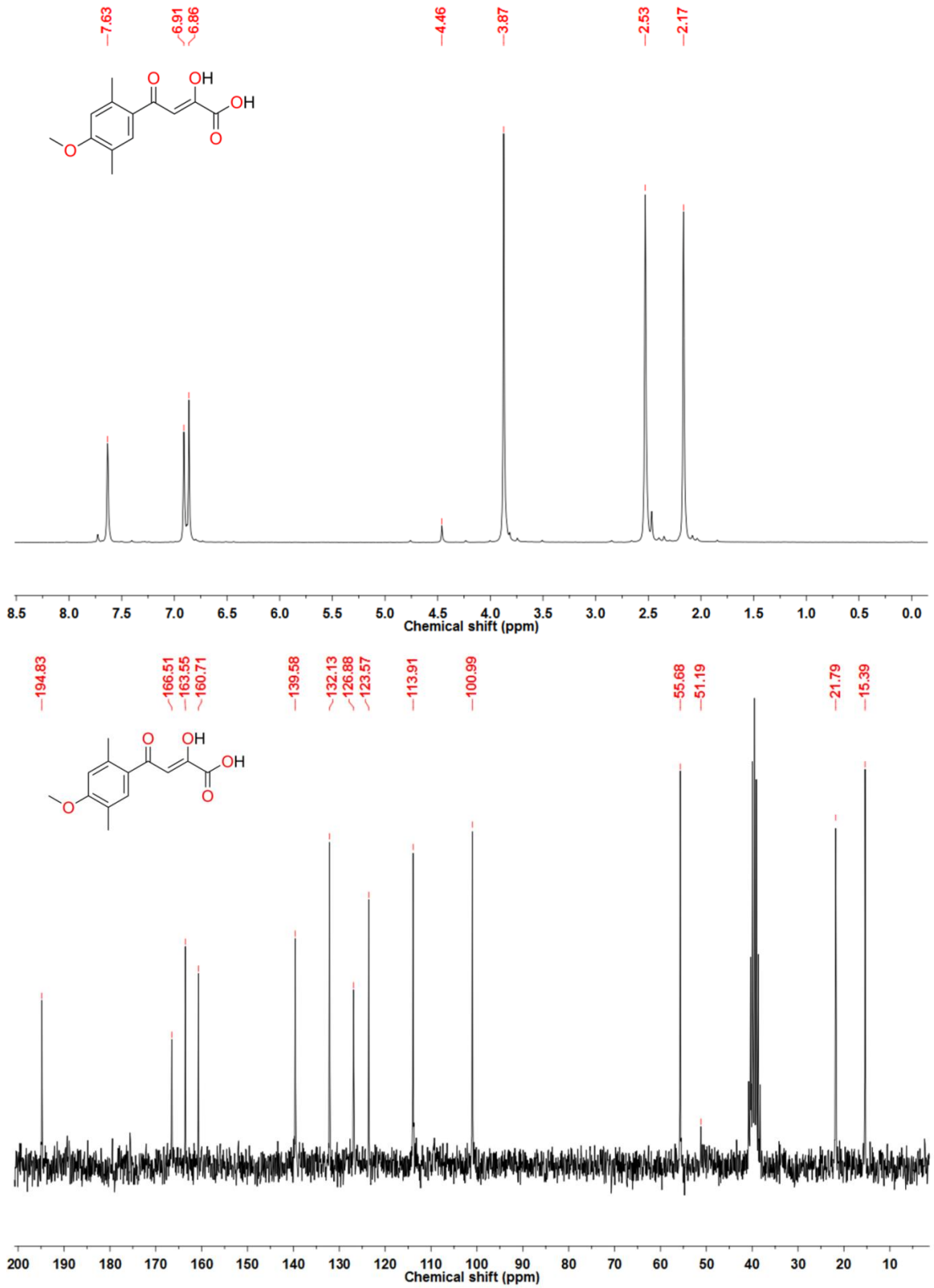

Figure S12. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-(4-methoxy-2,5-dimethylphenyl)-4-oxobut-2-enoic acid **(10).**

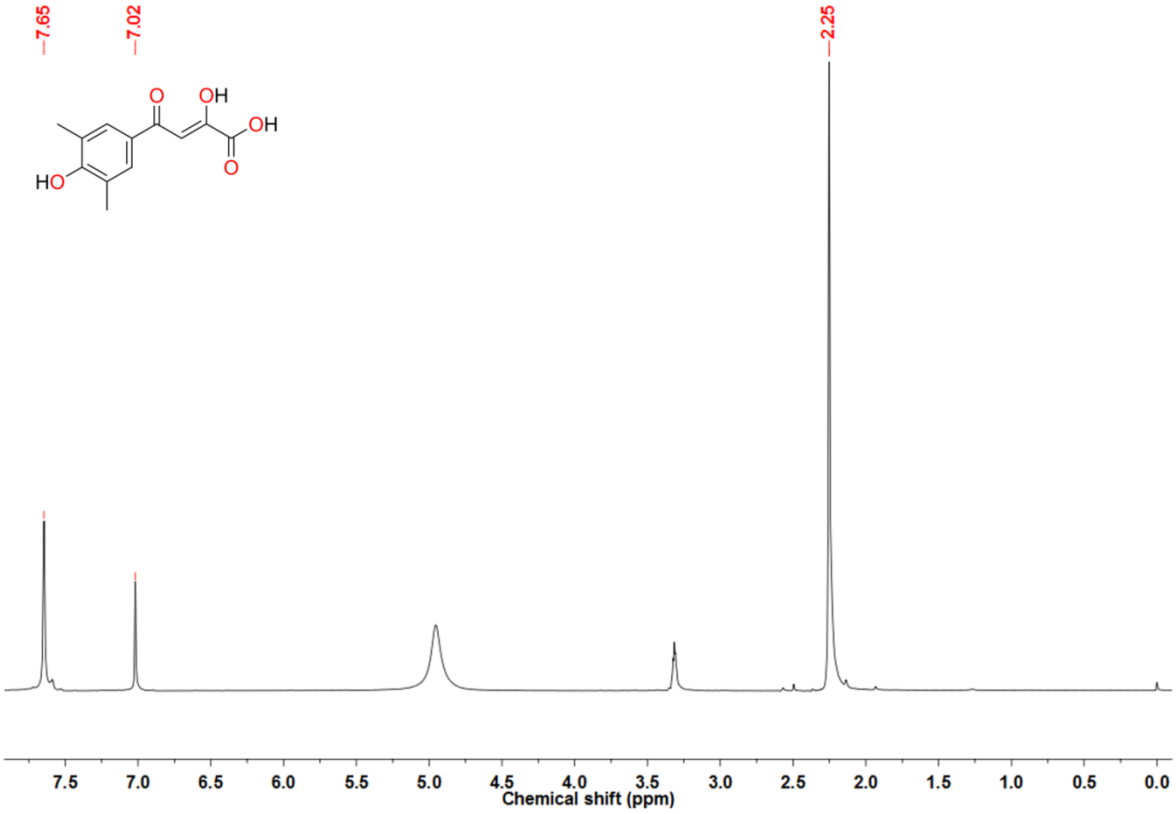

Figure S13. 1D ^{1}H NMR spectrum of (*Z*)-2-hydroxy-4-(4-hydroxy-3,5-dimethylphenyl)-4-oxobut-2-enoic acid **(11).**

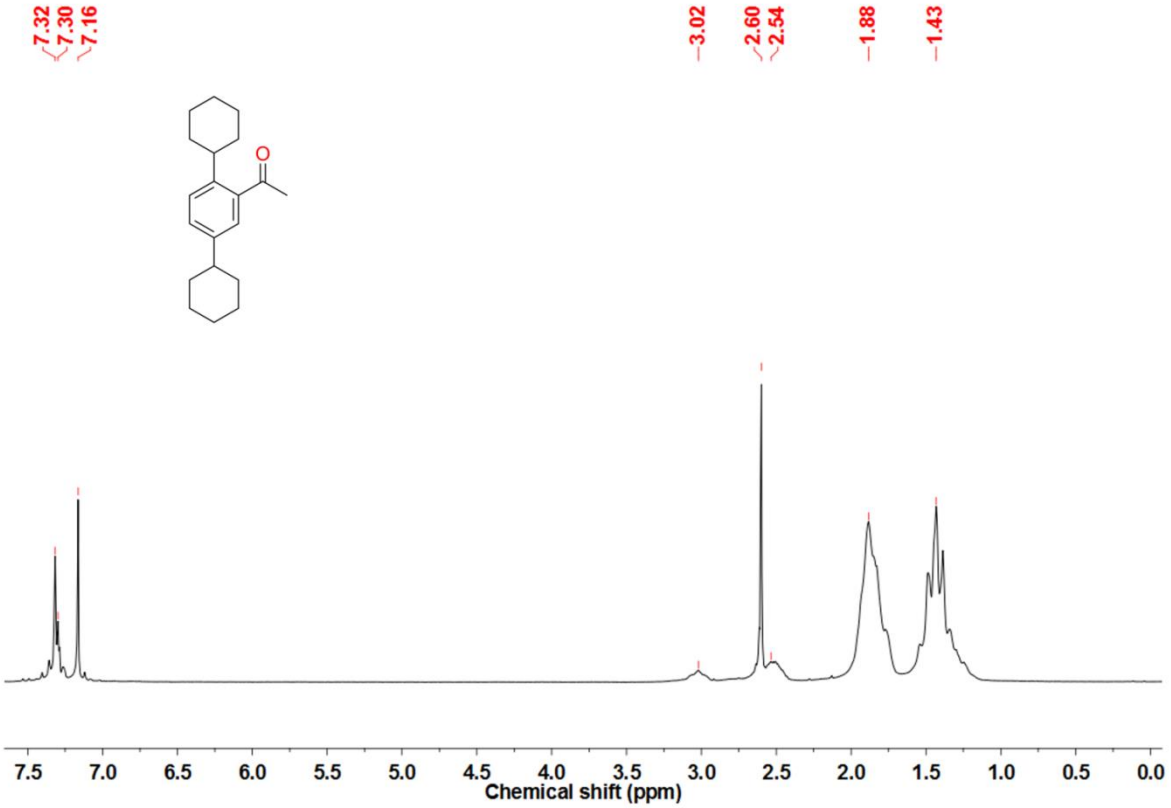

Figure S14. 1D ^{1}H spectrum of 1-(2,5-dicyclohexylphenyl)ethanone **(4a).**

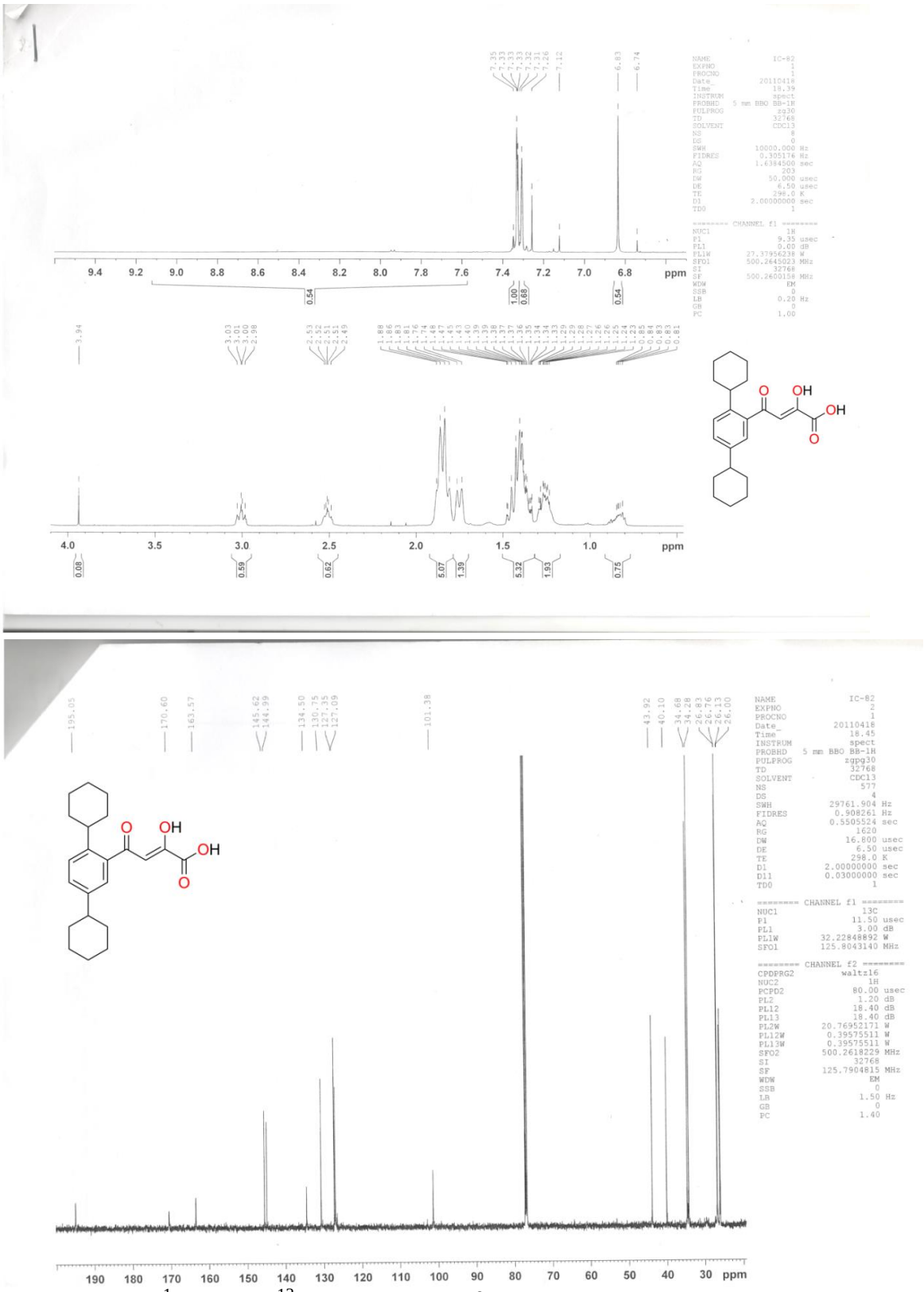

Figure S15. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-4-(2,5-dicyclohexylphenyl)-2-hydroxy-4-oxobut-2-enoic acid **(12).**

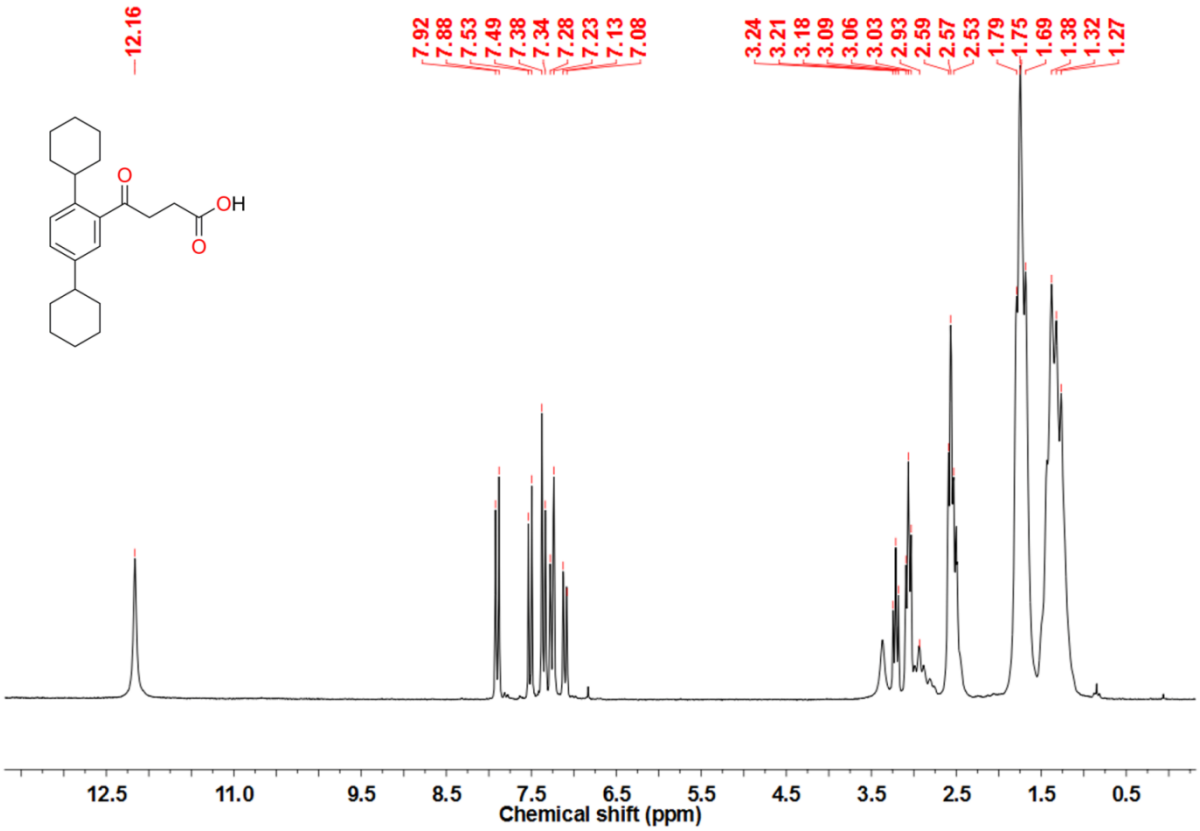

Figure S16. 1D ^{1}H NMR spectrum of 4-(2,5-dicyclohexylphenyl)-4-oxobutanoic acid **(1a).**

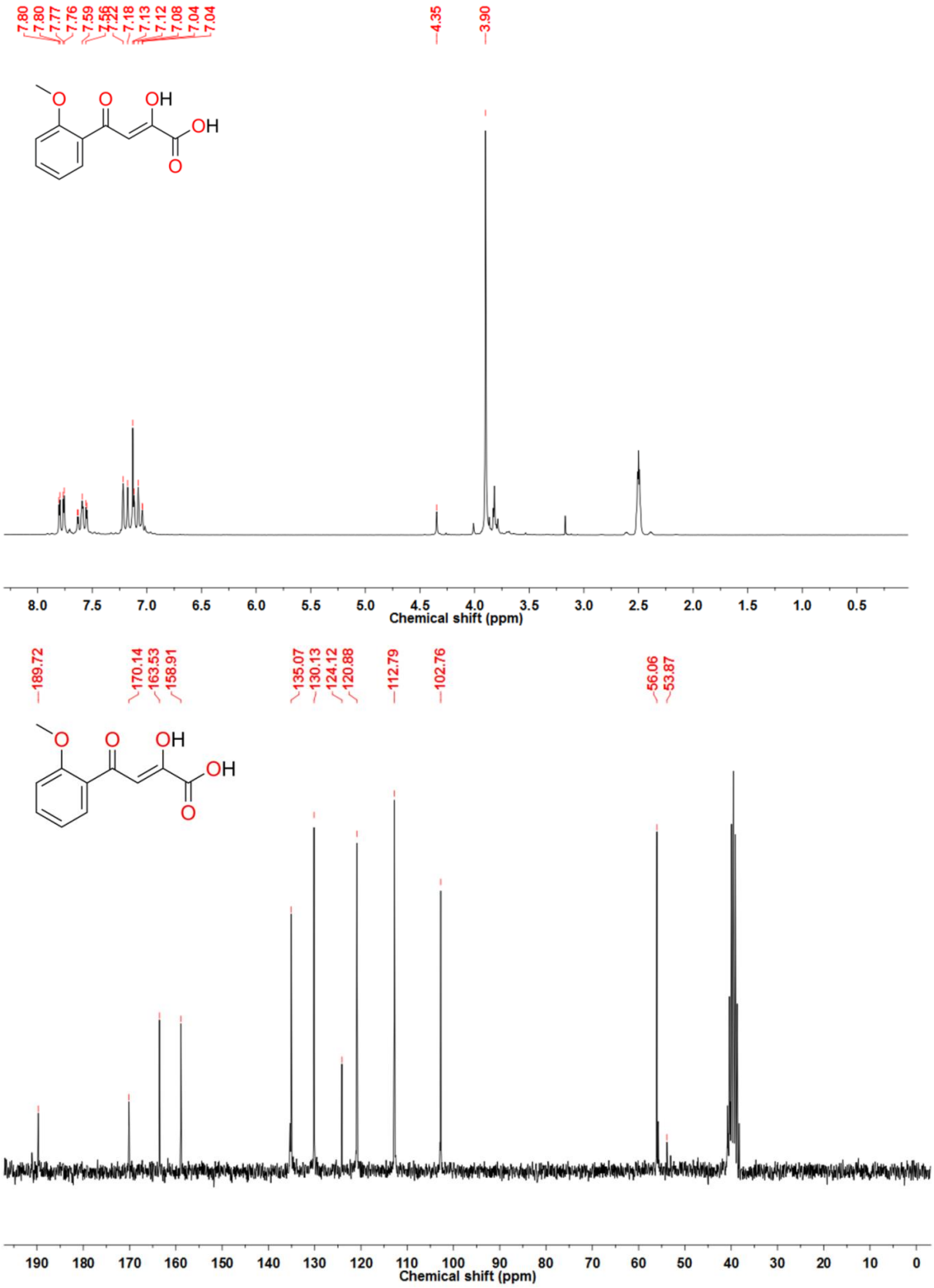

Figure S17. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-(2-methoxyphenyl)-4-oxobut-2-enoic acid **(13).**

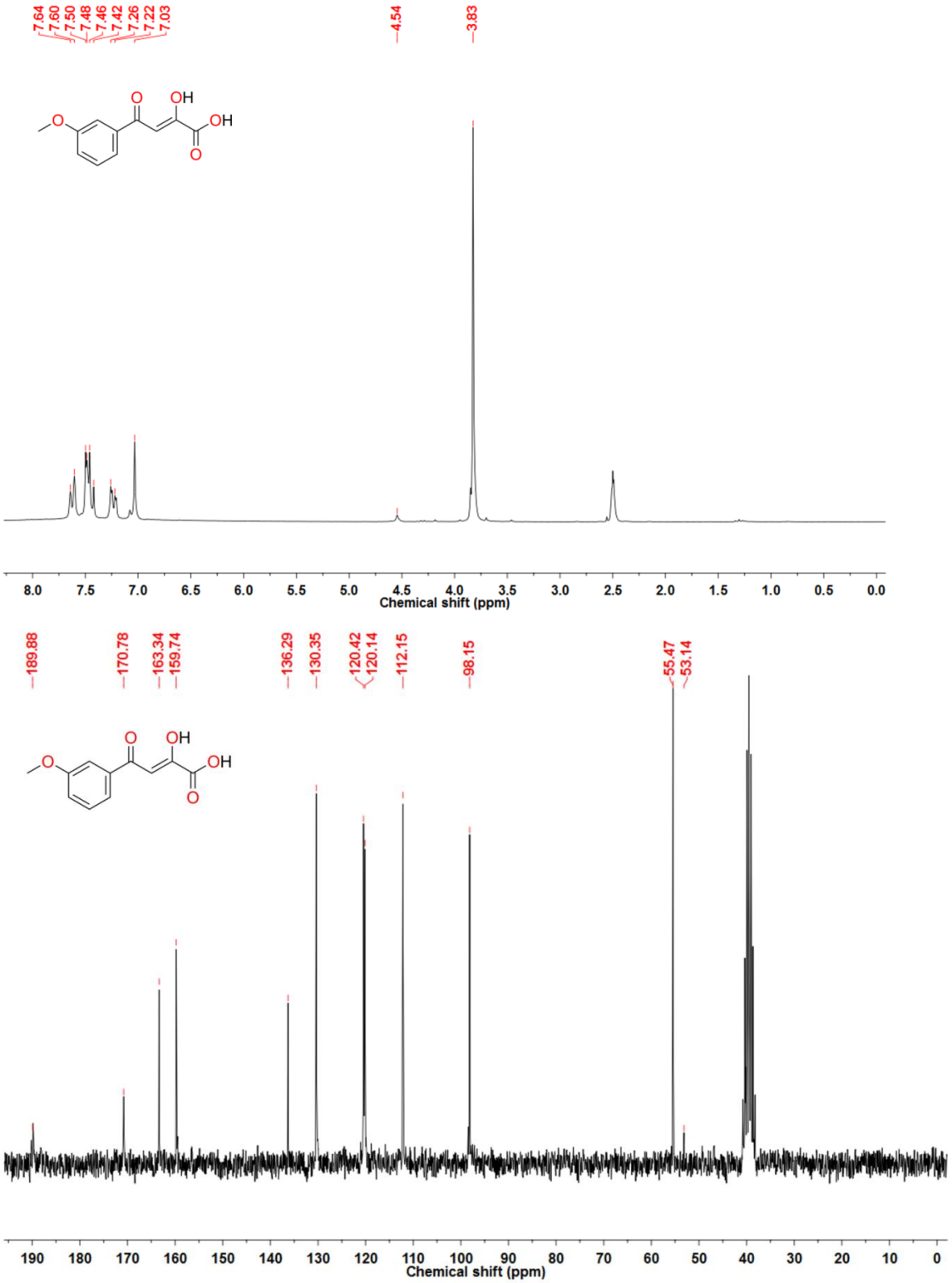

Figure S18. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-(3-methoxyphenyl)-4-oxobut-2-enoic acid **(14).**

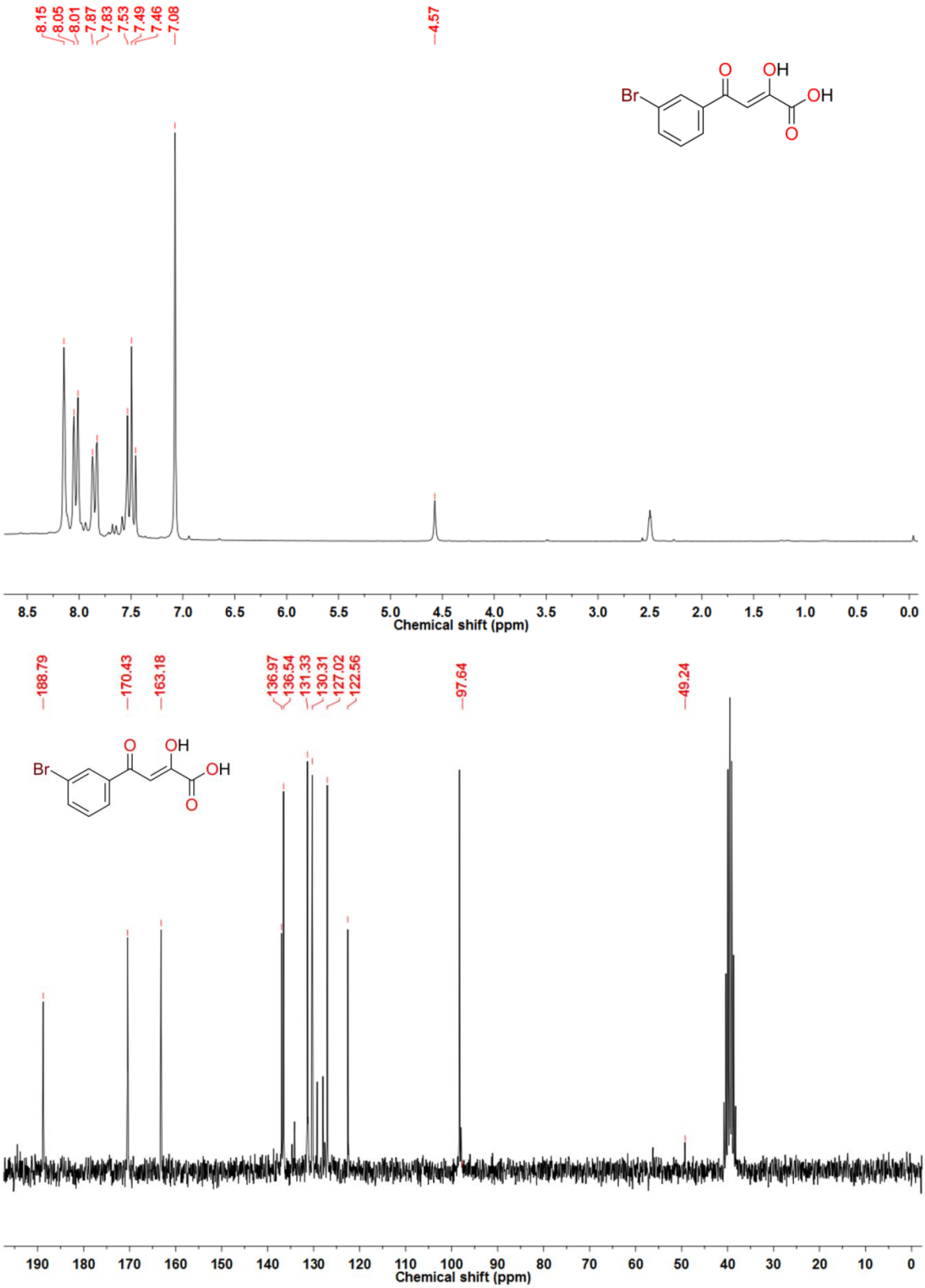

Figure S19. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-4-(3-bromophenyl)-2-hydroxy-4-oxobut-2-enoic acid **(15).**

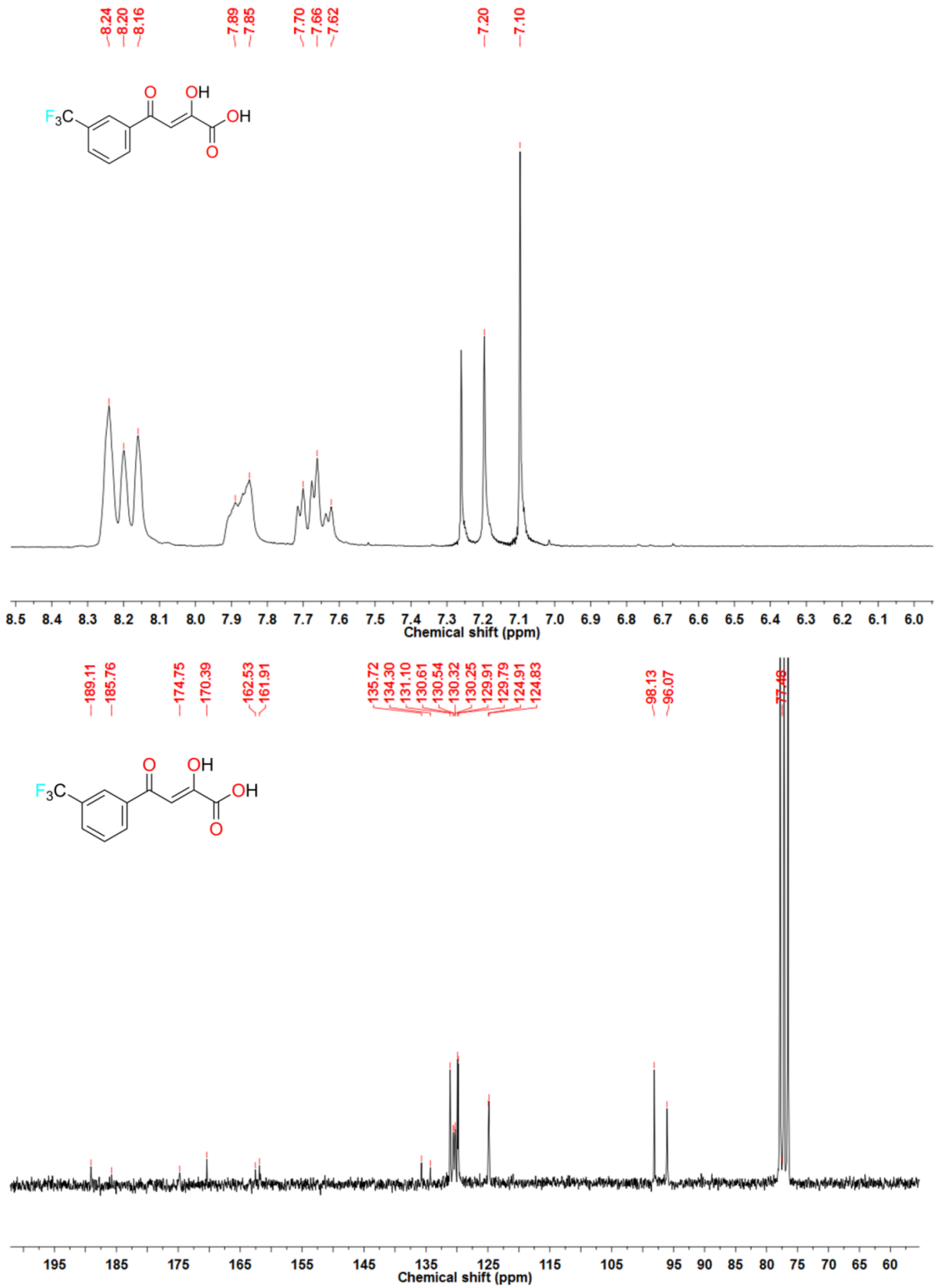

Figure S20. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-oxo-4-(3-(trifluoromethyl)phenyl)but-2-enoic acid **(16).**

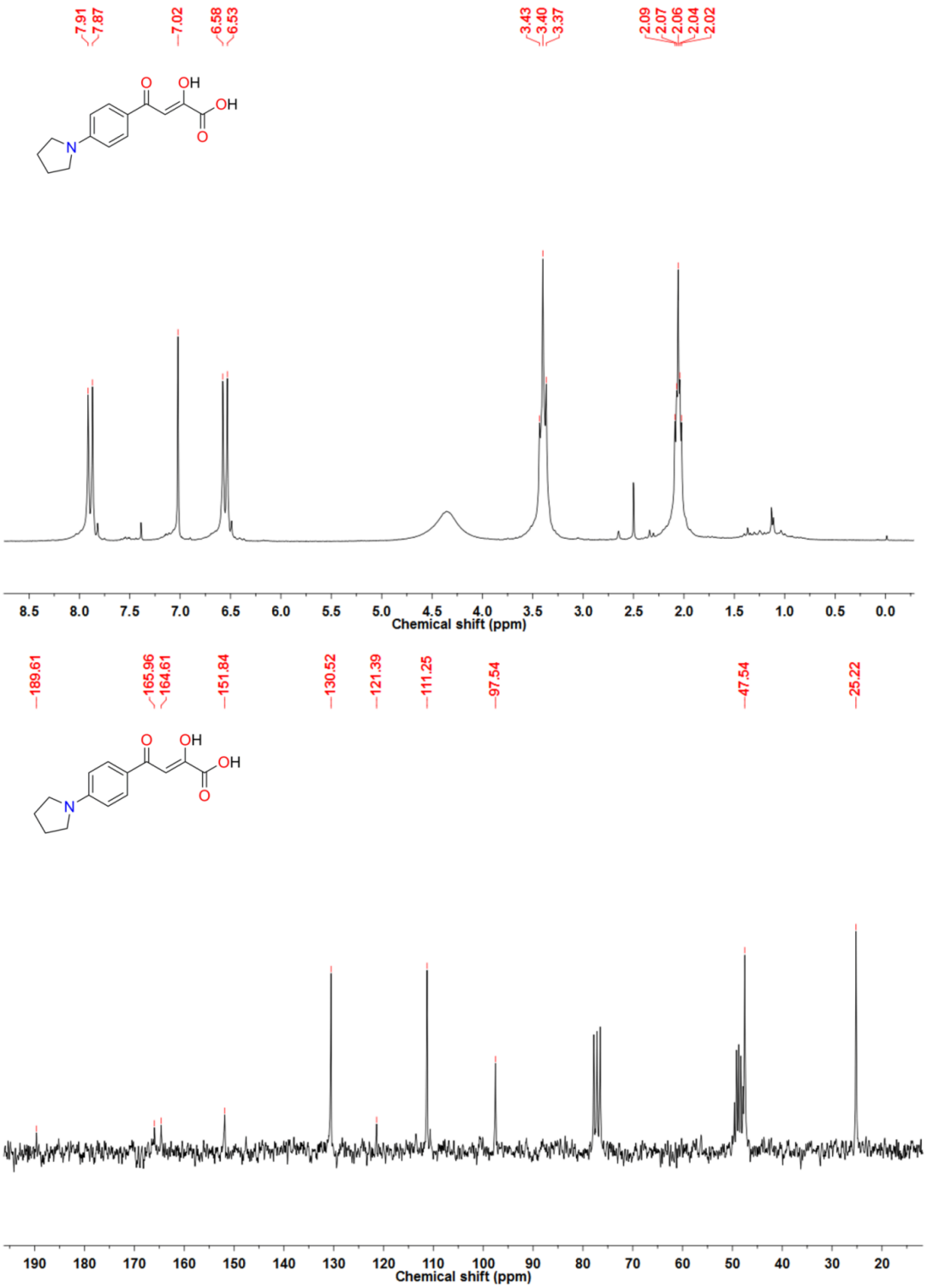

Figure S21. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-oxo-4-(4-(pyrrolidin-1-yl)phenyl)but-2-enoic acid **(17).**

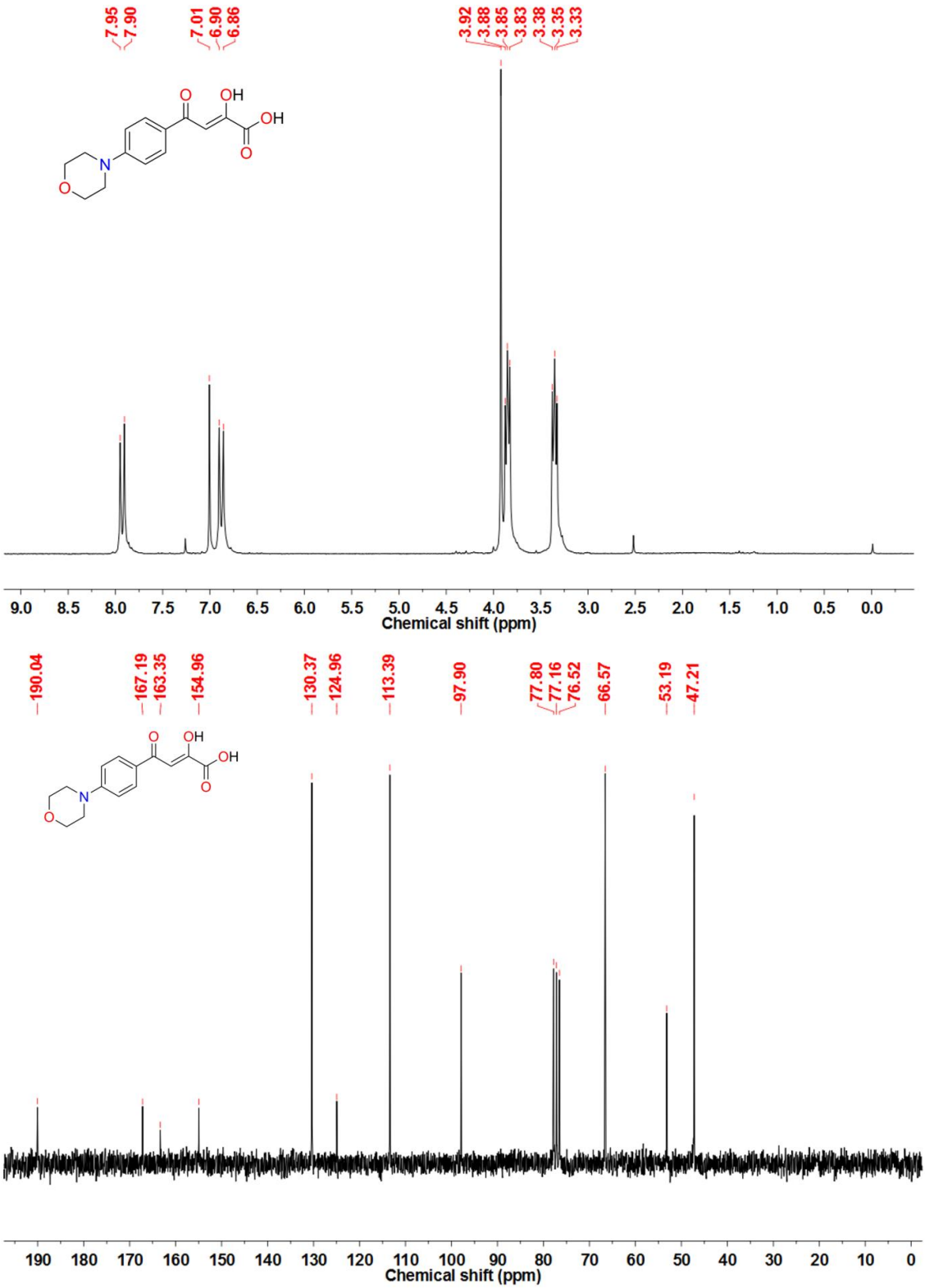

Figure S22. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-(4-morpholinophenyl)-4-oxobut-2-enoic acid **(18).**

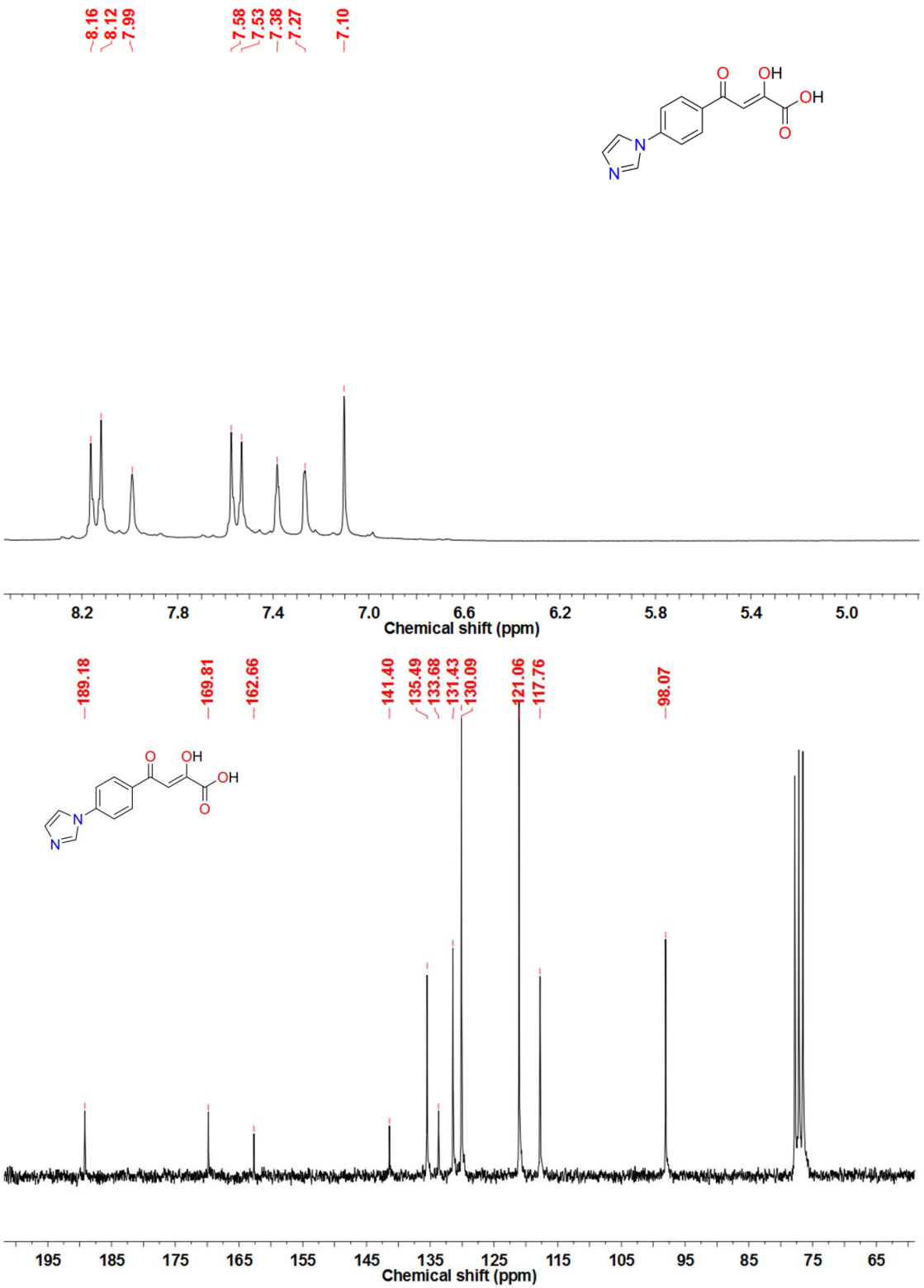

Figure S23. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-4-(4-(1*H*-imidazol-1-yl)phenyl)-2-hydroxy-4-oxobut-2-enoic acid **(19).**

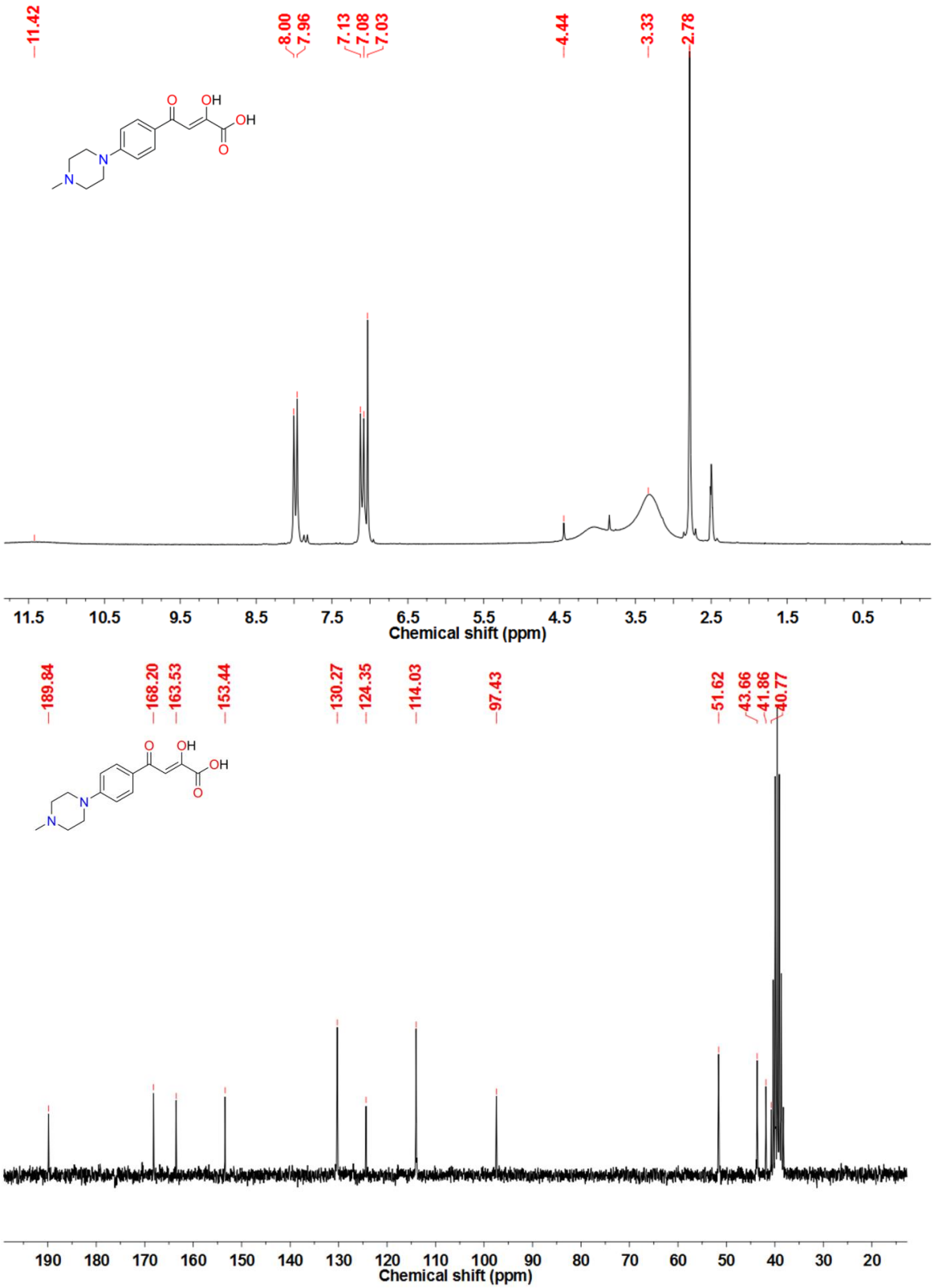

Figure S24. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-2-hydroxy-4-(4-(4-methylpiperazin-1-yl)phenyl)-4-oxobut-2-enoic acid **(20).**

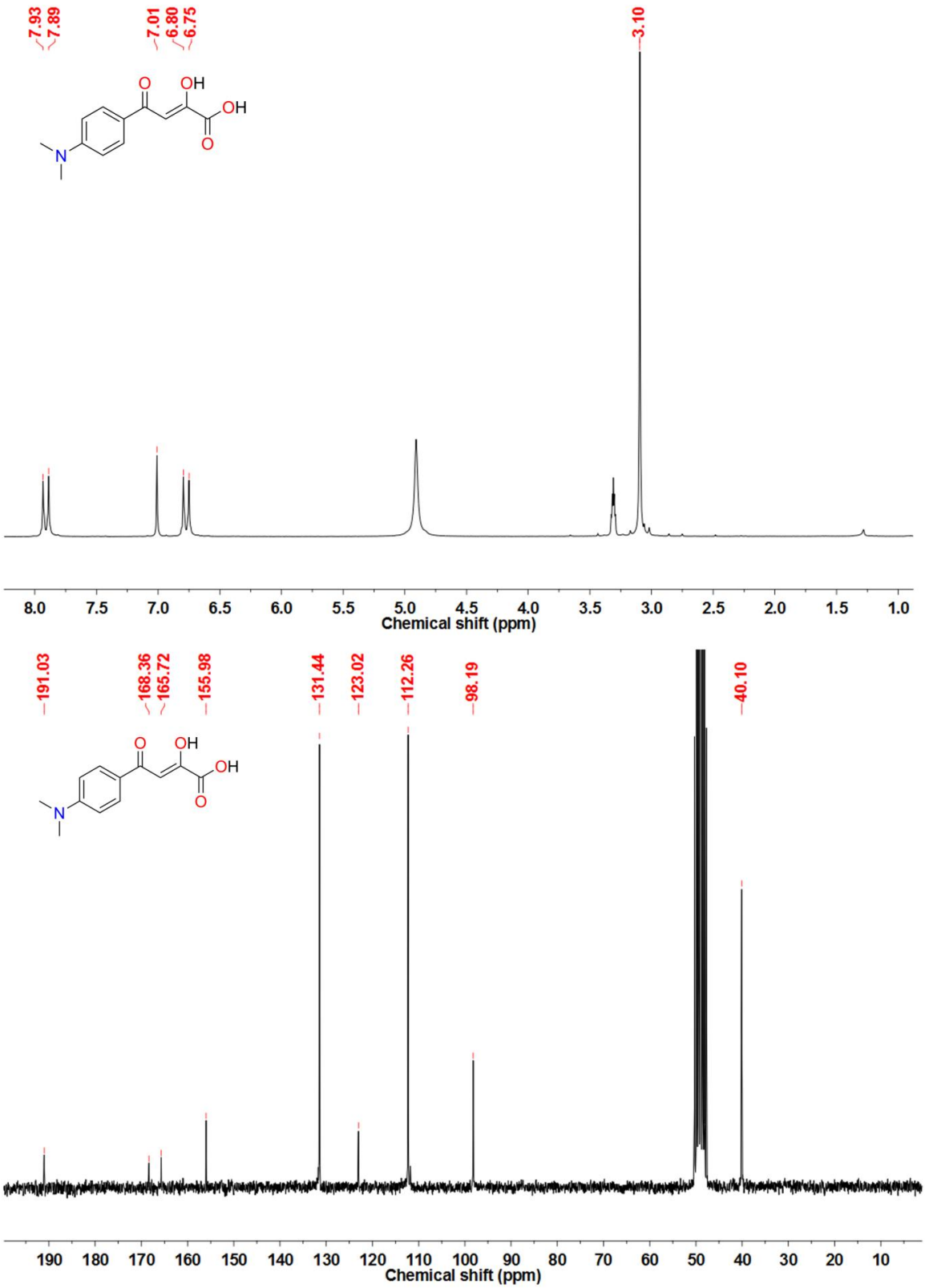

Figure S25. 1D ^{1}H and 1D ^{13}C NMR spectra of (*Z*)-4-(4-(dimethylamino)phenyl)-2-hydroxy-4-oxobut-2-enoic acid **(21).**

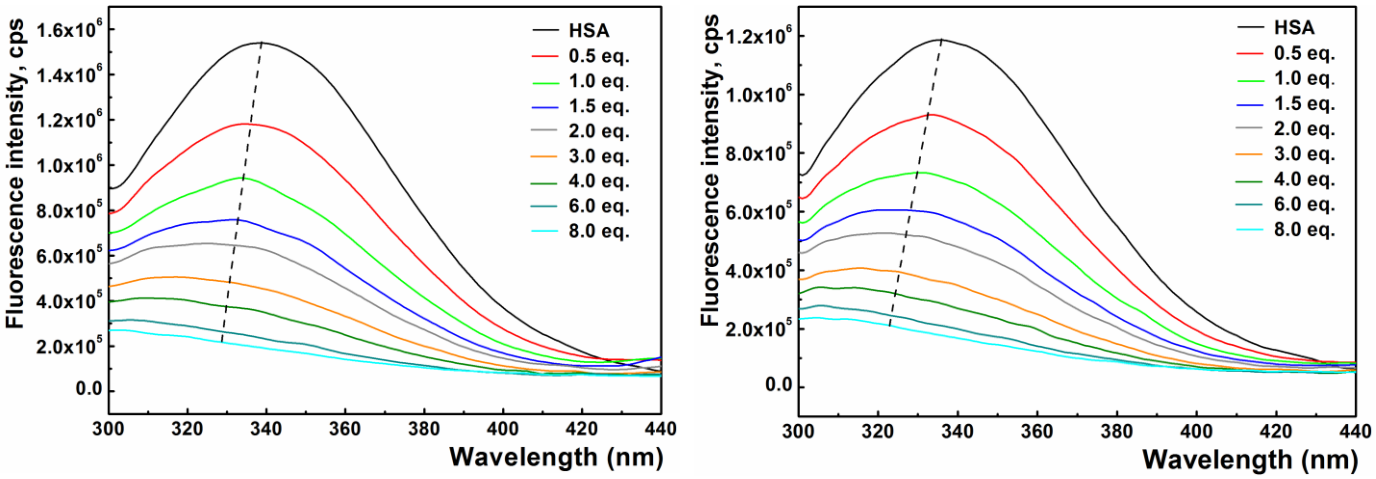

Figure S26. Changes in fluorescence emission spectra of HSA (c = 0.5 μM) upon addition of comp. **12** (c_{12} = 0.0; 0.25; 0.5; 0.75; 1; 1.5; 2.0; 3.0; 4.0 μM); T = 293 K, left; T = 313 K, right; 30 mM PBS, pH = 7.38.