

Supplementary material for the article:

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**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

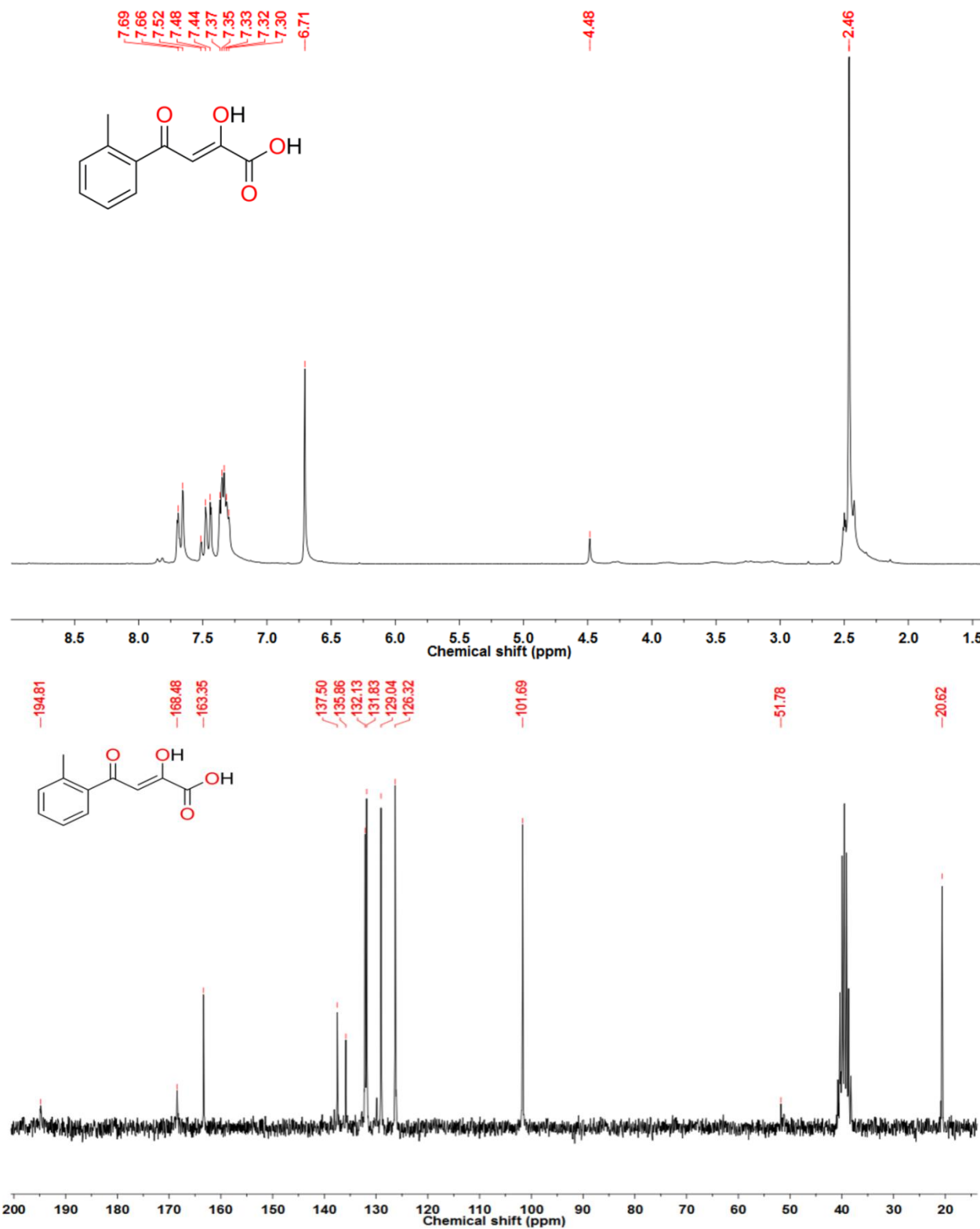
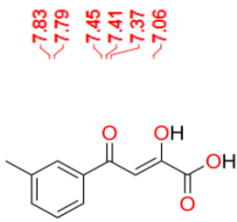
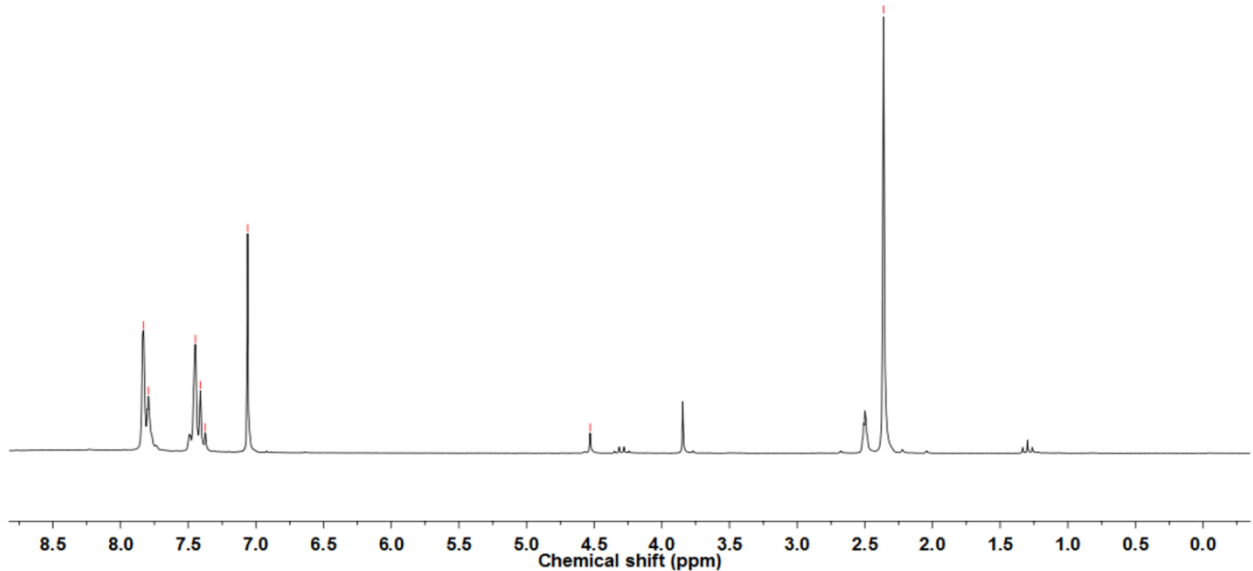


Figure S1. 1D <sup>1</sup>H and 1D <sup>13</sup>C NMR spectra of (Z)-2-hydroxy-4-oxo-4-(o-tolyl)but-2-enoic acid (2).



-4.53

-2.36



-190.70

-170.30

-163.30

-138.72

-134.78

-134.70

-129.08

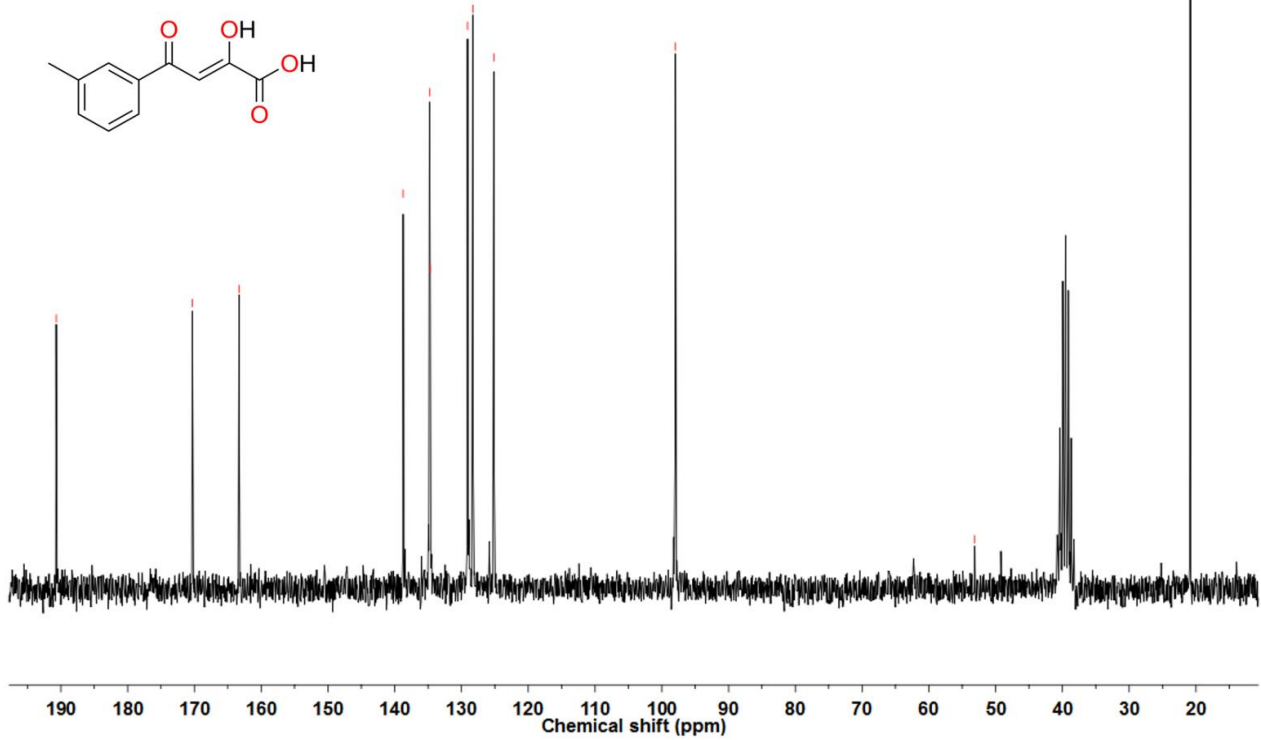
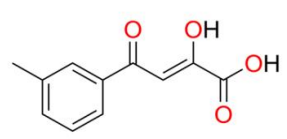
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-125.15

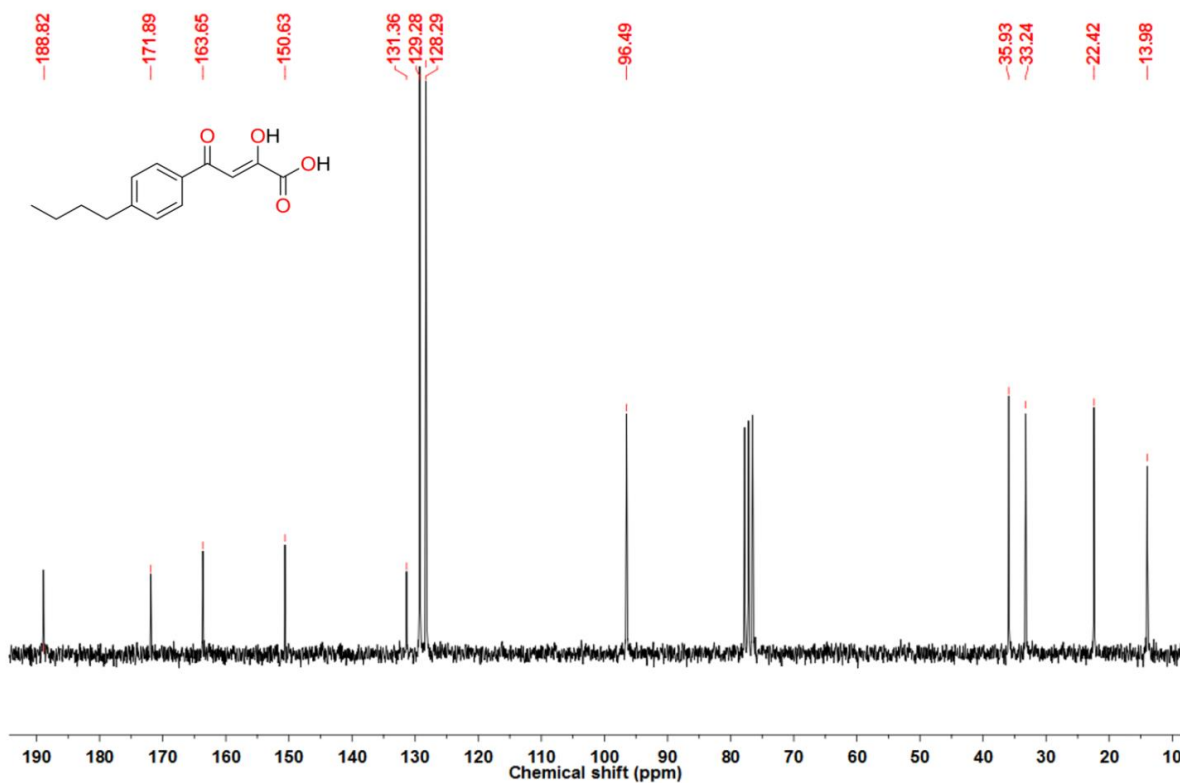
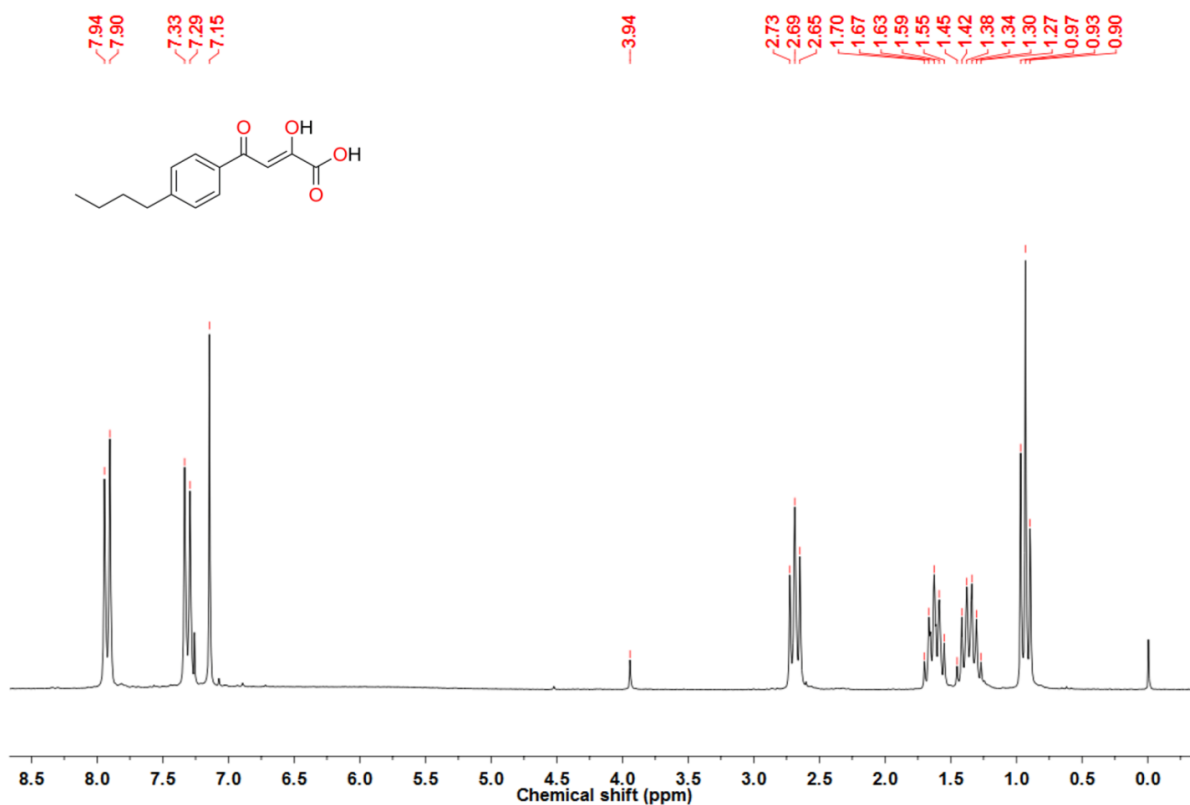
-97.95

-53.13

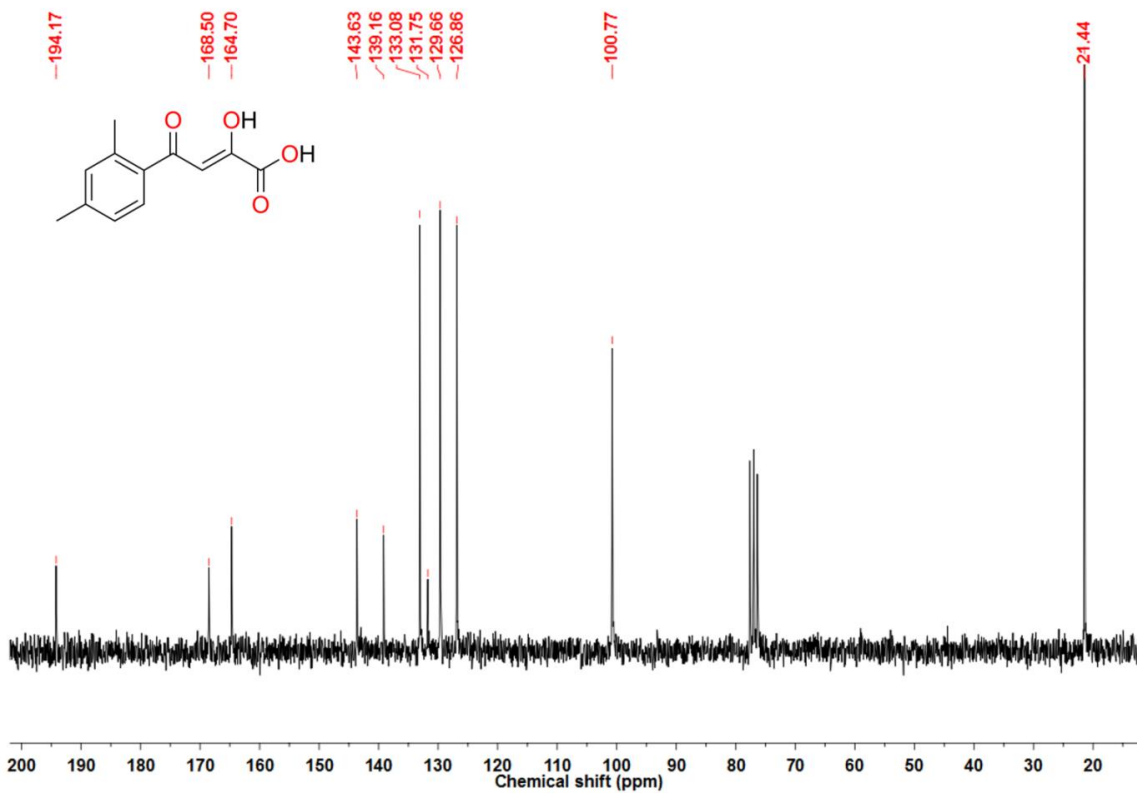
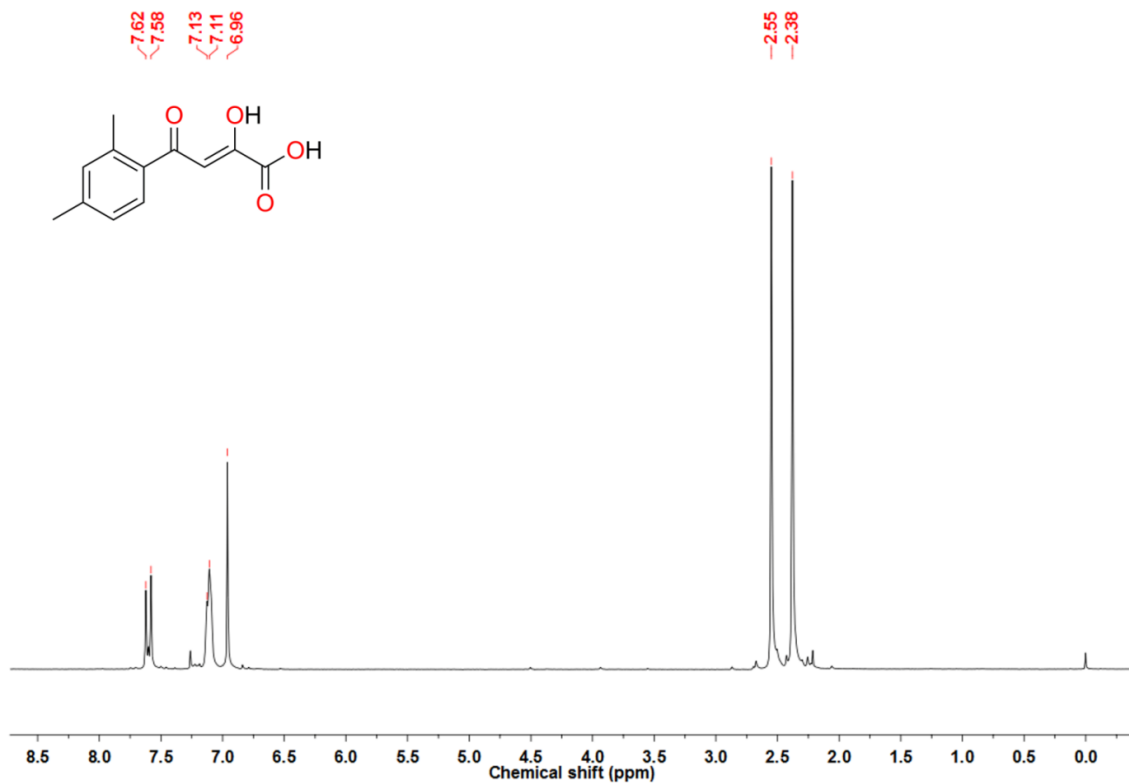
-20.84



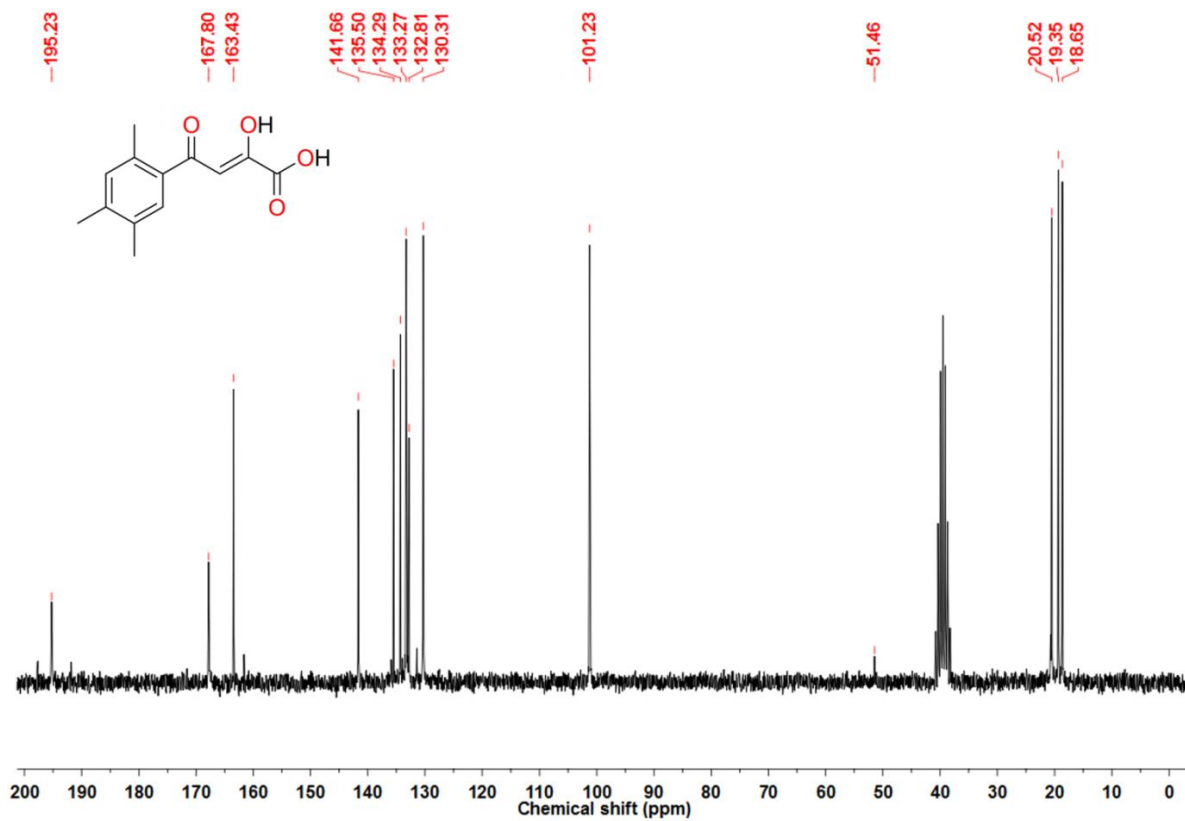
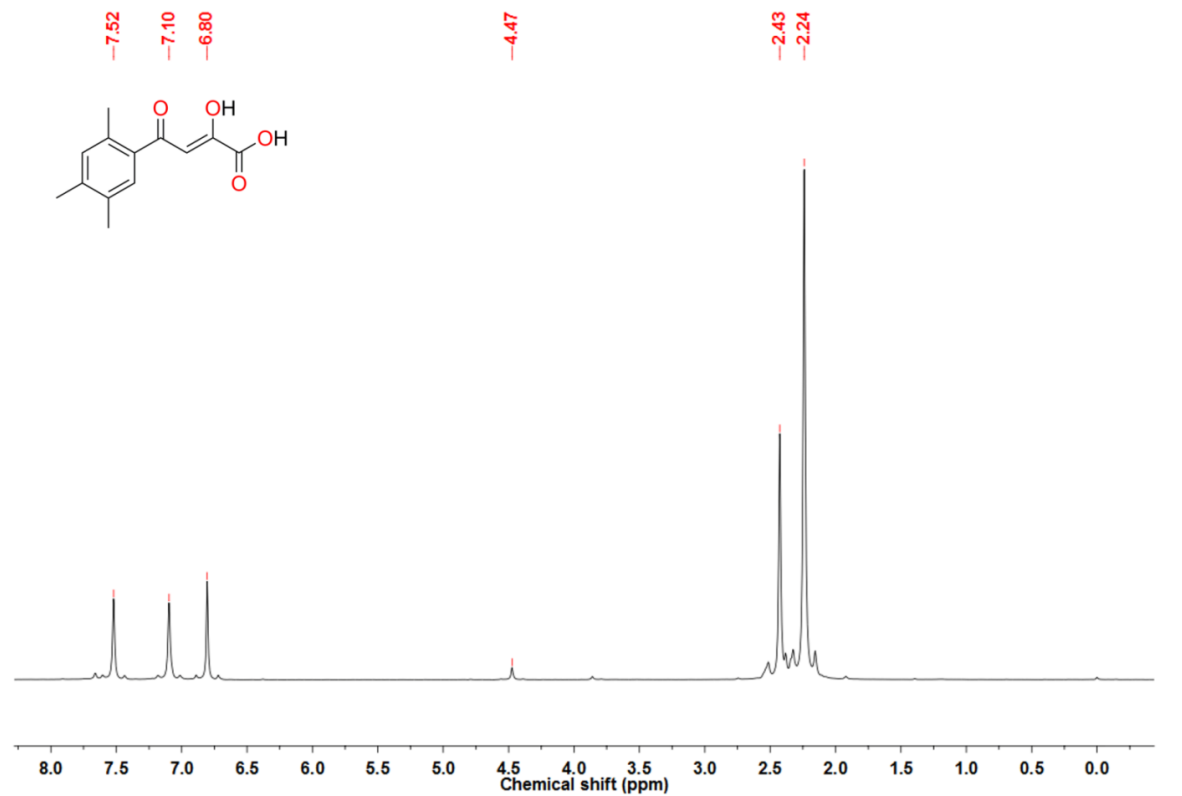
**Figure S2.** 1D  $^1\text{H}$  and 1D  $^{13}\text{C}$  NMR spectra of (Z)-2-hydroxy-4-oxo-4-(*m*-tolyl)but-2-enoic acid (**3**).



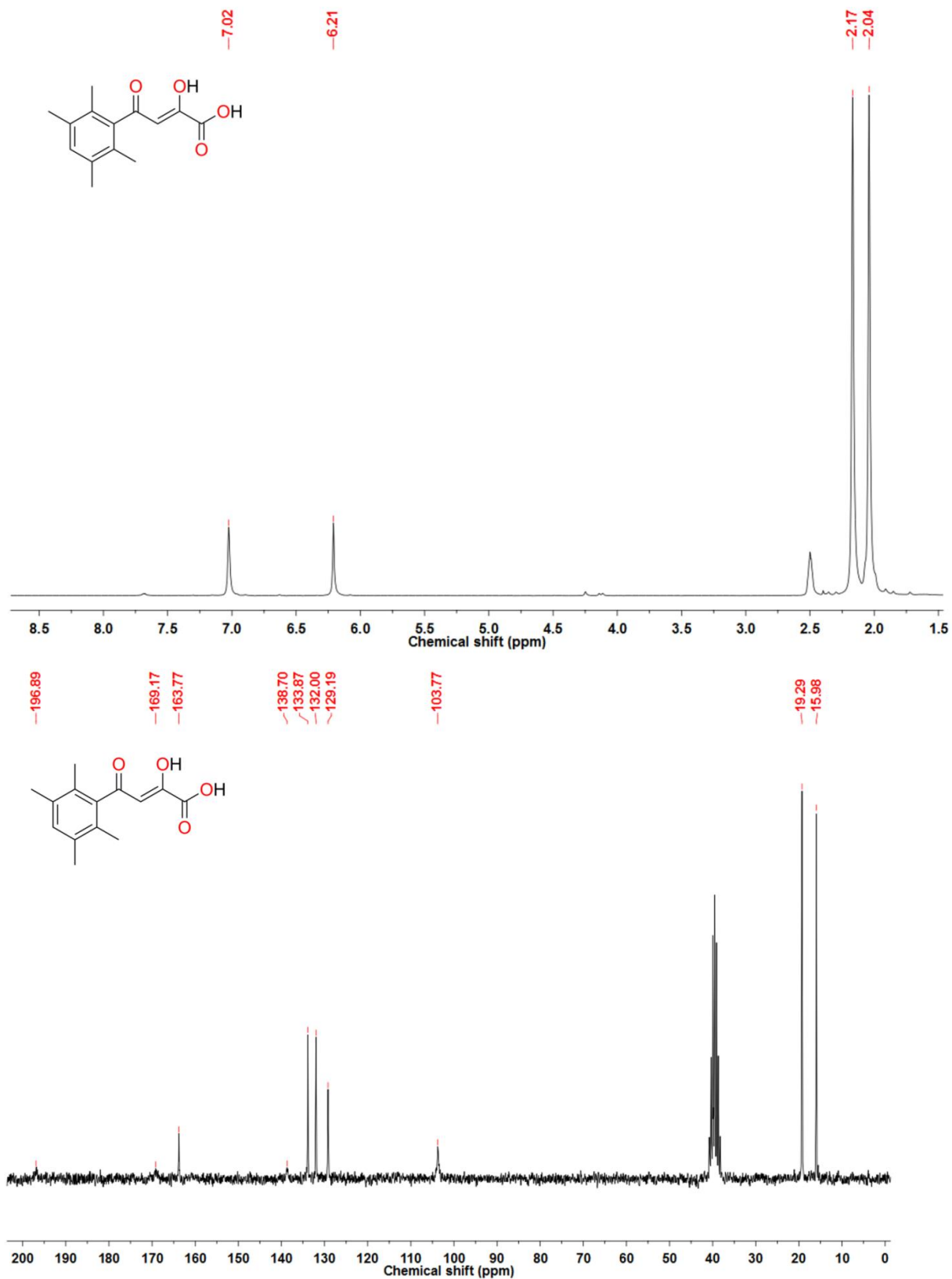
**Figure S3.** 1D  $^1\text{H}$  and 1D  $^{13}\text{C}$  NMR spectra of (Z)-4-(4-butylphenyl)-2-hydroxy-4-oxobut-2-enoic acid (**4**).



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

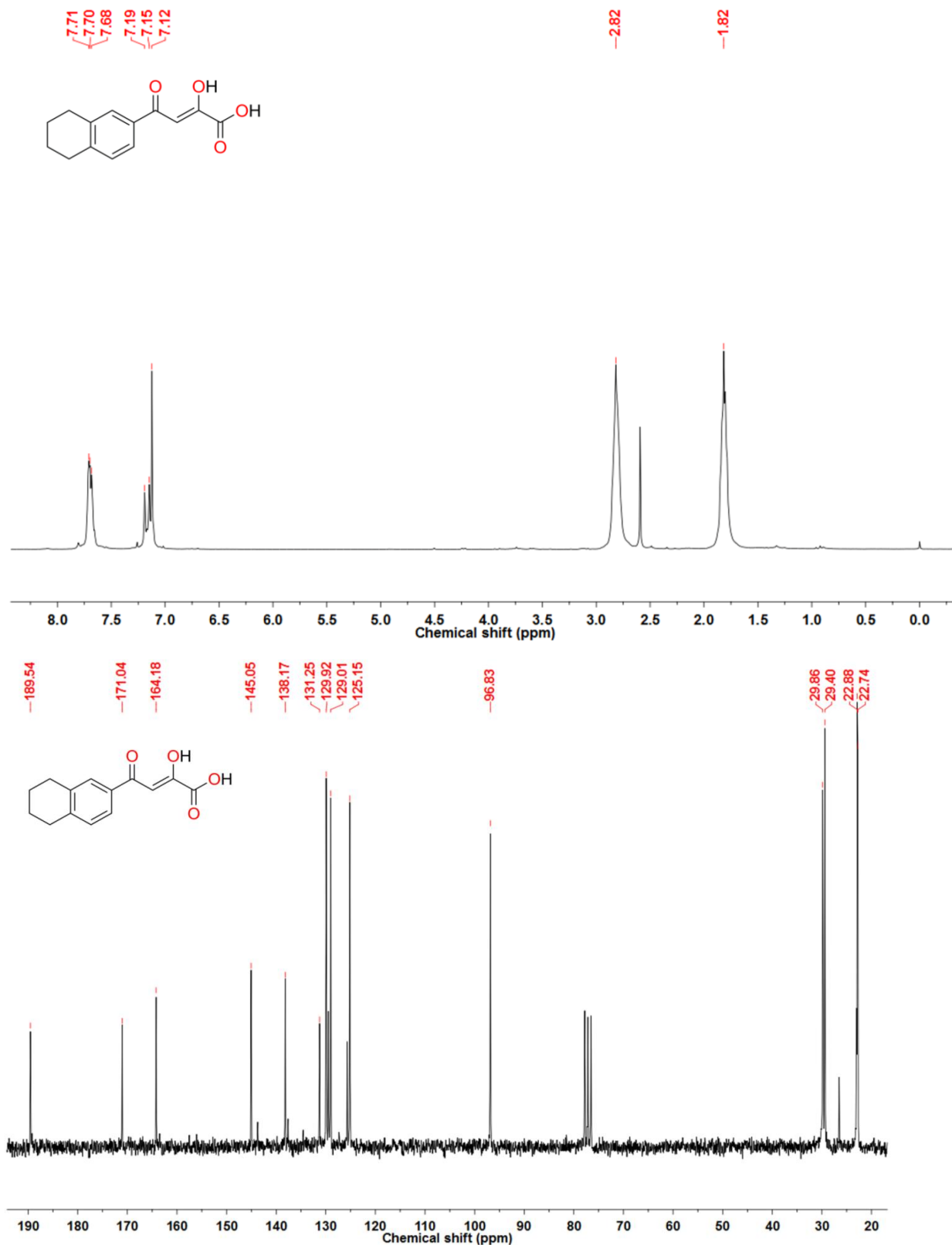


**Figure S5.** 1D <sup>1</sup>H and 1D <sup>13</sup>C NMR spectra of (Z)-2-hydroxy-4-oxo-4-(2,4,5-trimethylphenyl)but-2-enoic acid (**6**).

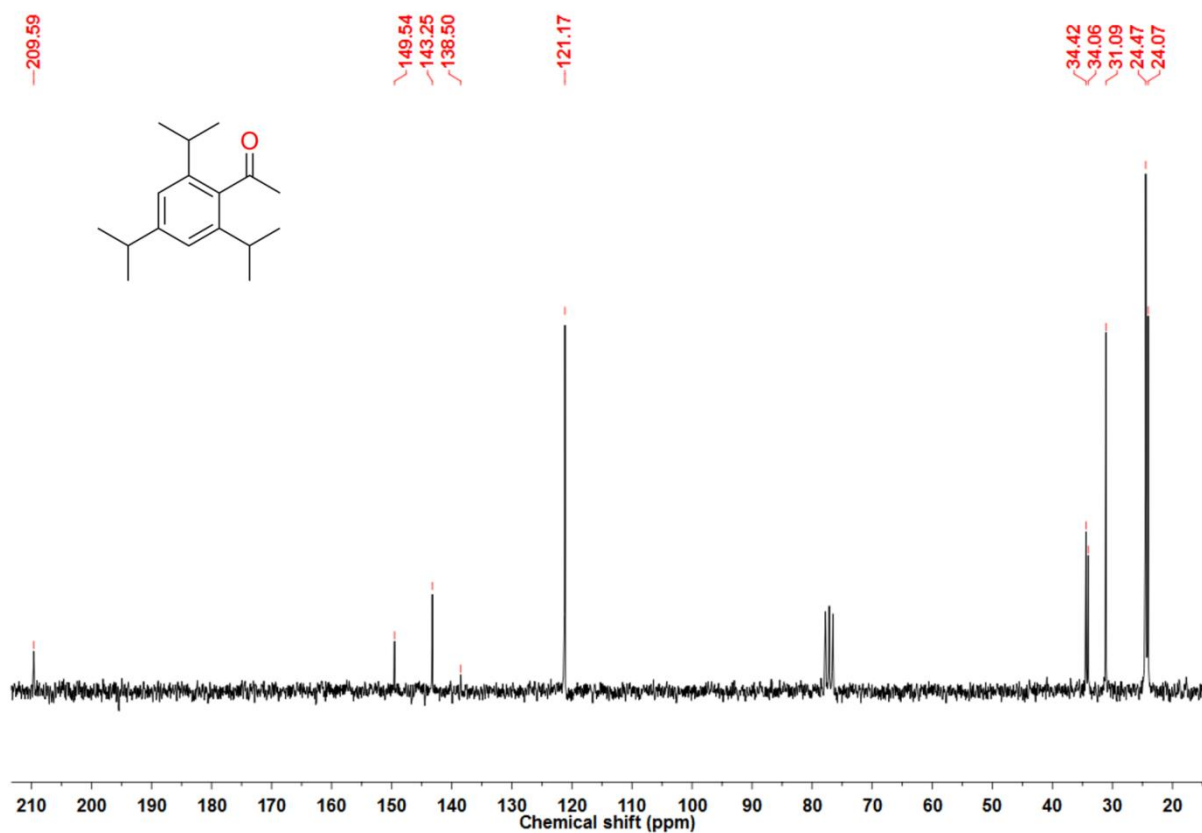
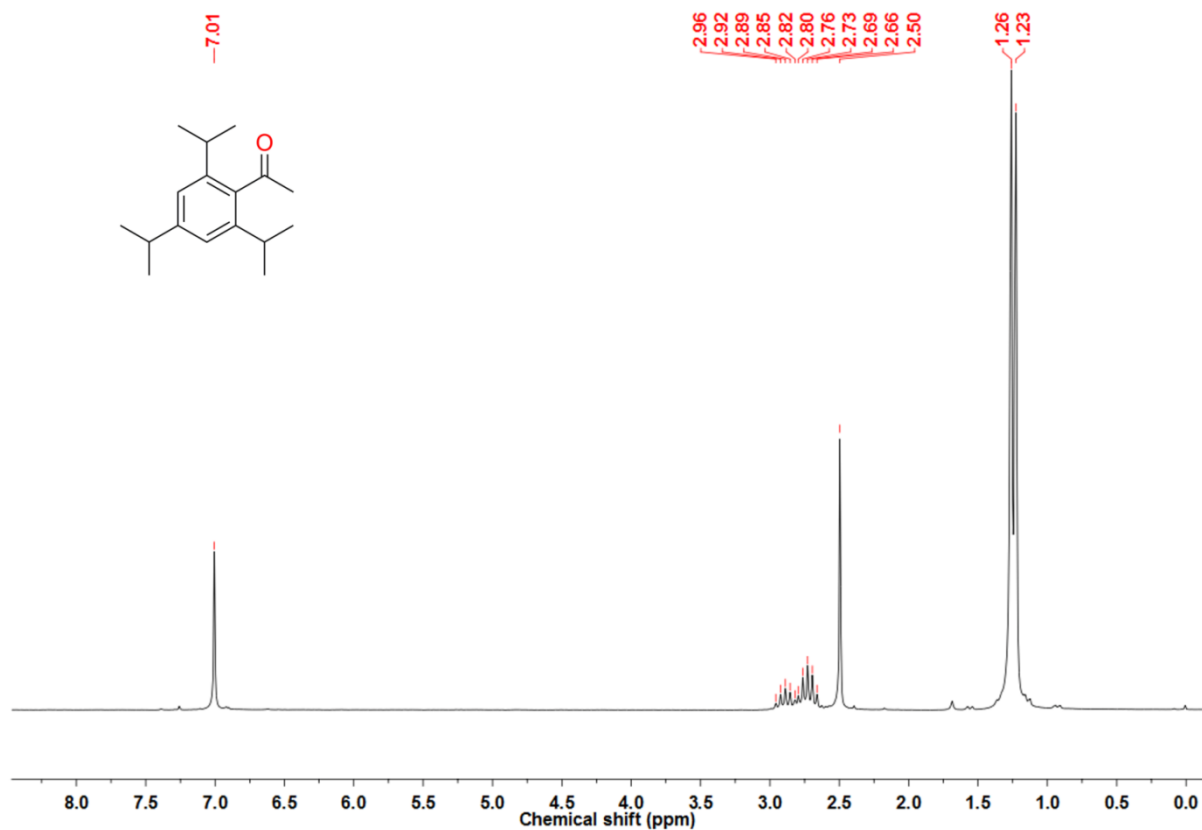


**Figure S6.** 1D  $^1\text{H}$  and 1D  $^{13}\text{C}$  NMR spectra of (Z)-2-hydroxy-4-oxo-4-(2,3,5,6-tetramethylphenyl)but-2-enoic acid (7).

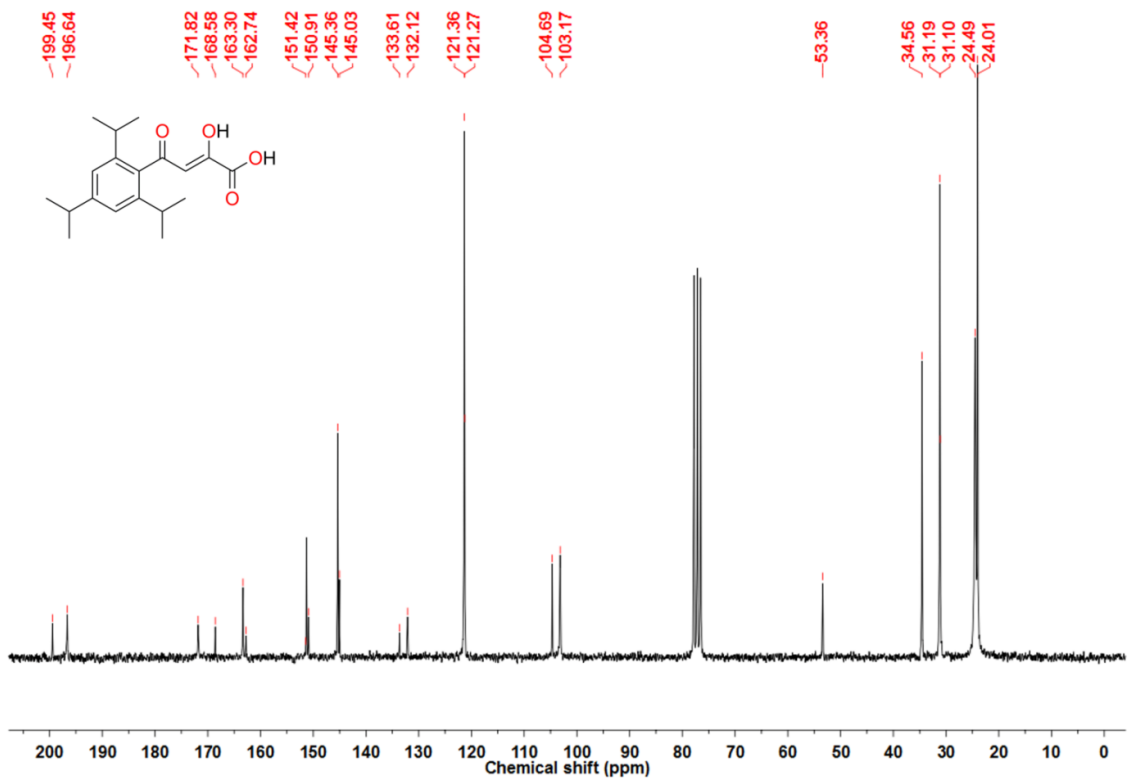
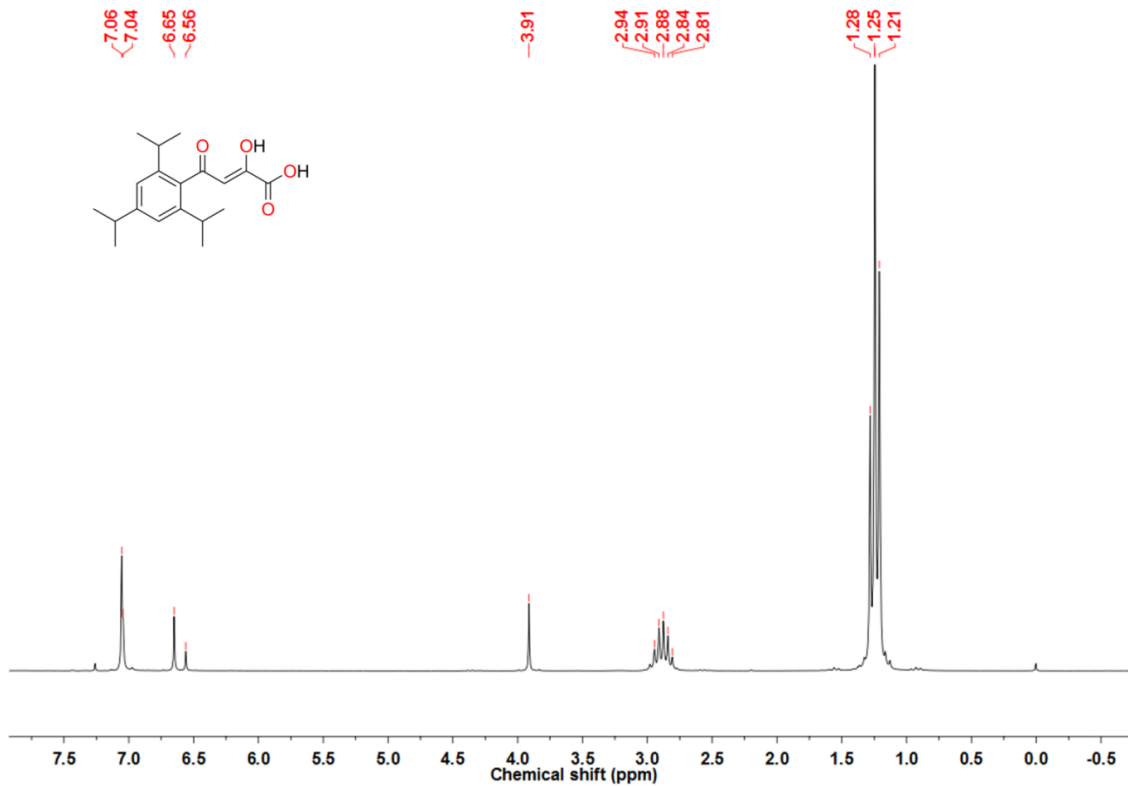




**Figure S7.** 1D <sup>1</sup>H and 1D <sup>13</sup>C NMR spectra of (Z)-2-hydroxy-4-oxo-4-(5,6,7,8-tetrahydronaphthalen-2-yl)but-2-enoic acid (**8**).



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



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

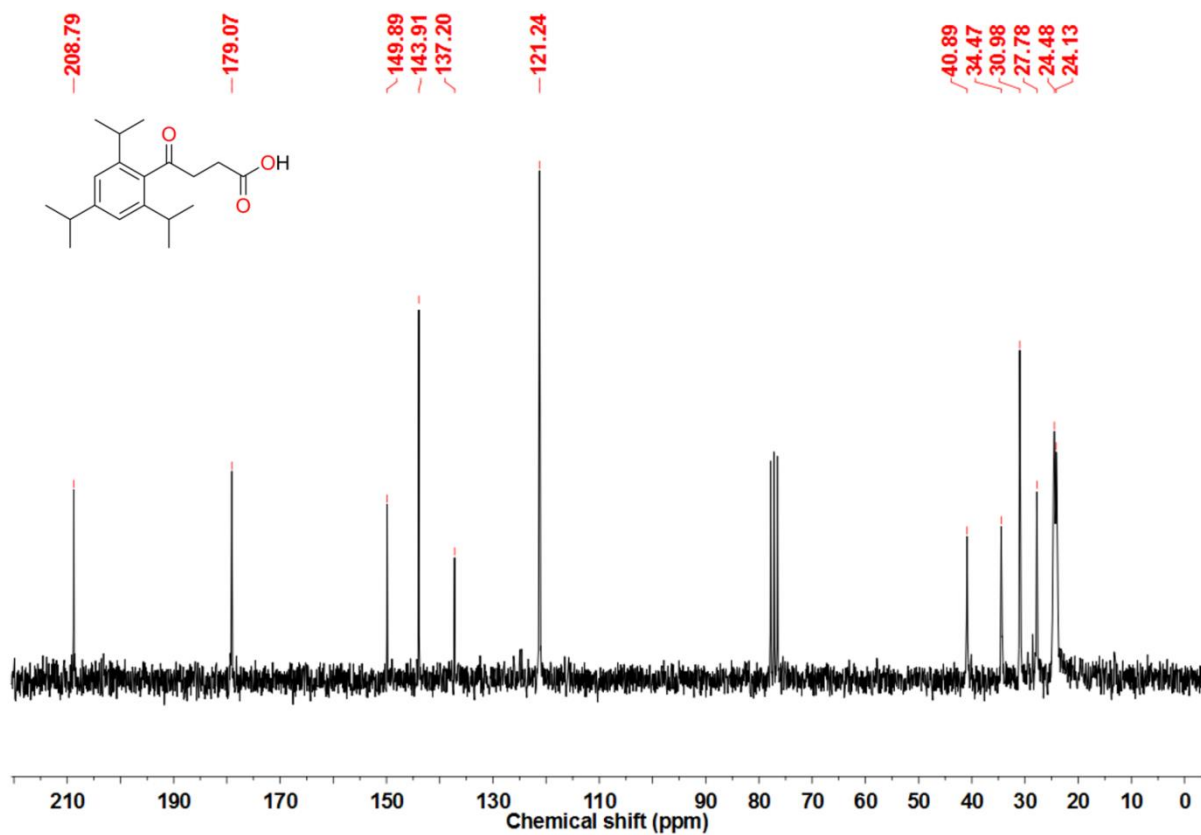
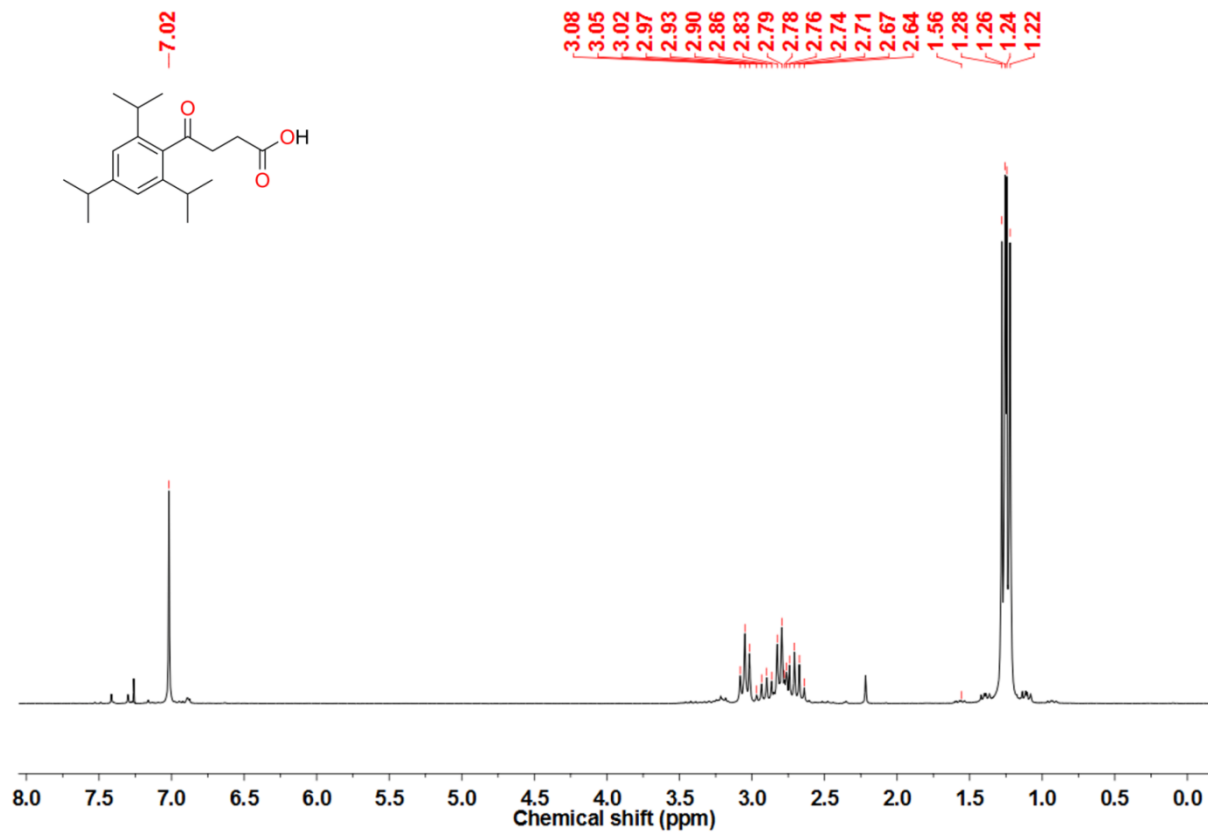


Figure S10. 1D  $^1\text{H}$  and 1D  $^{13}\text{C}$  NMR spectra of 4-oxo-4-(2,4,6-triisopropylphenyl)butanoic acid (2a).

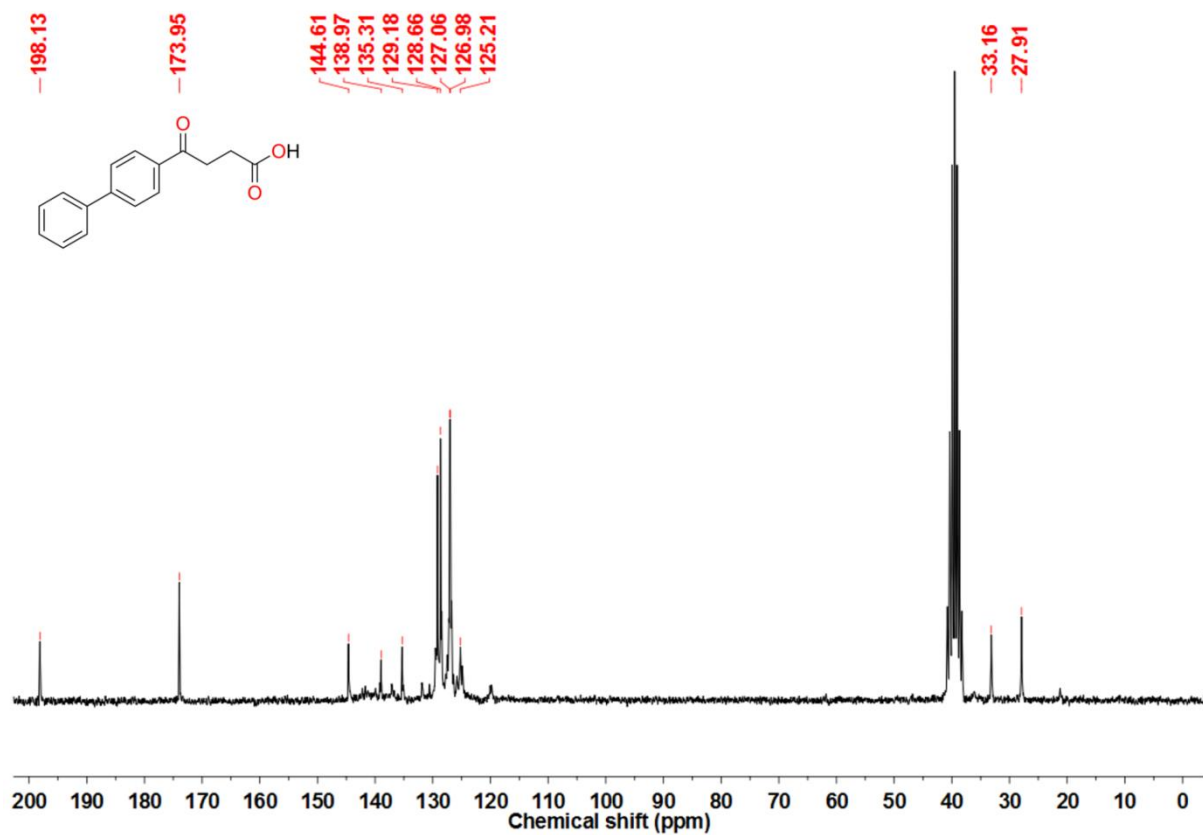
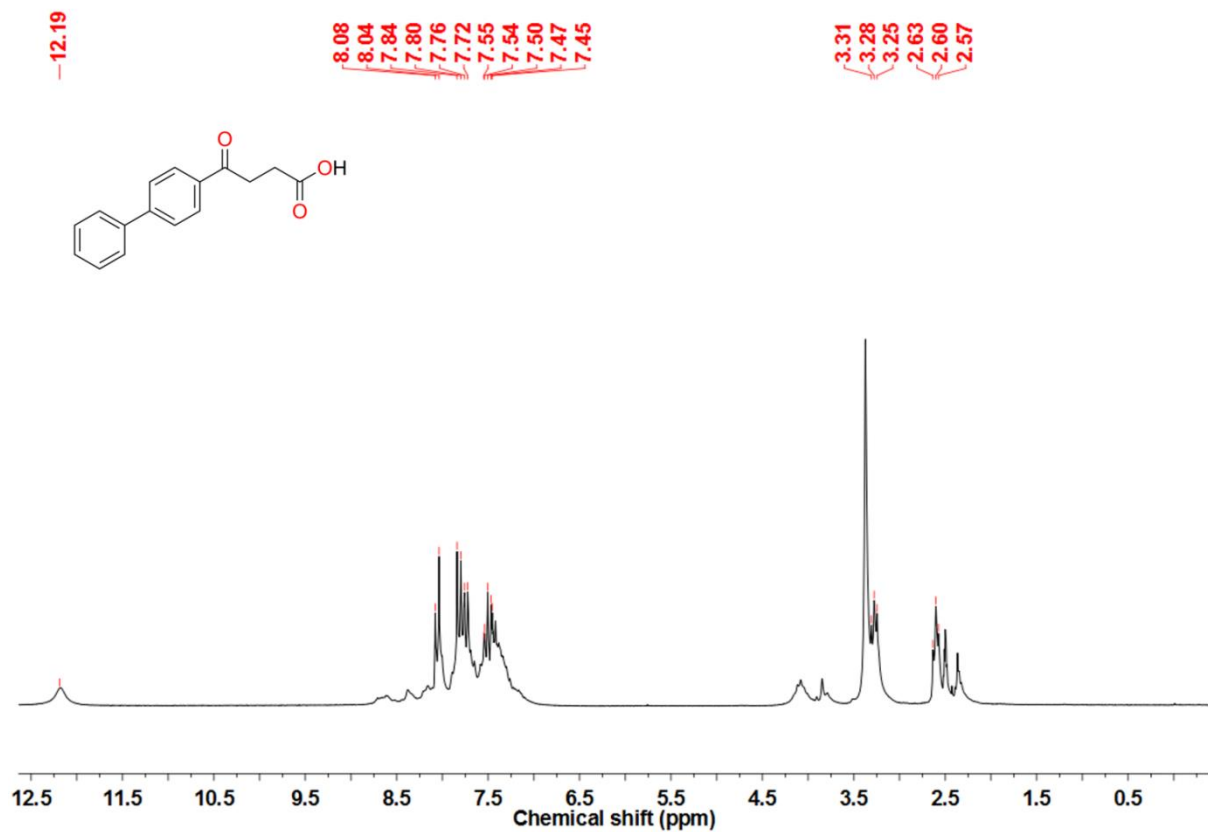
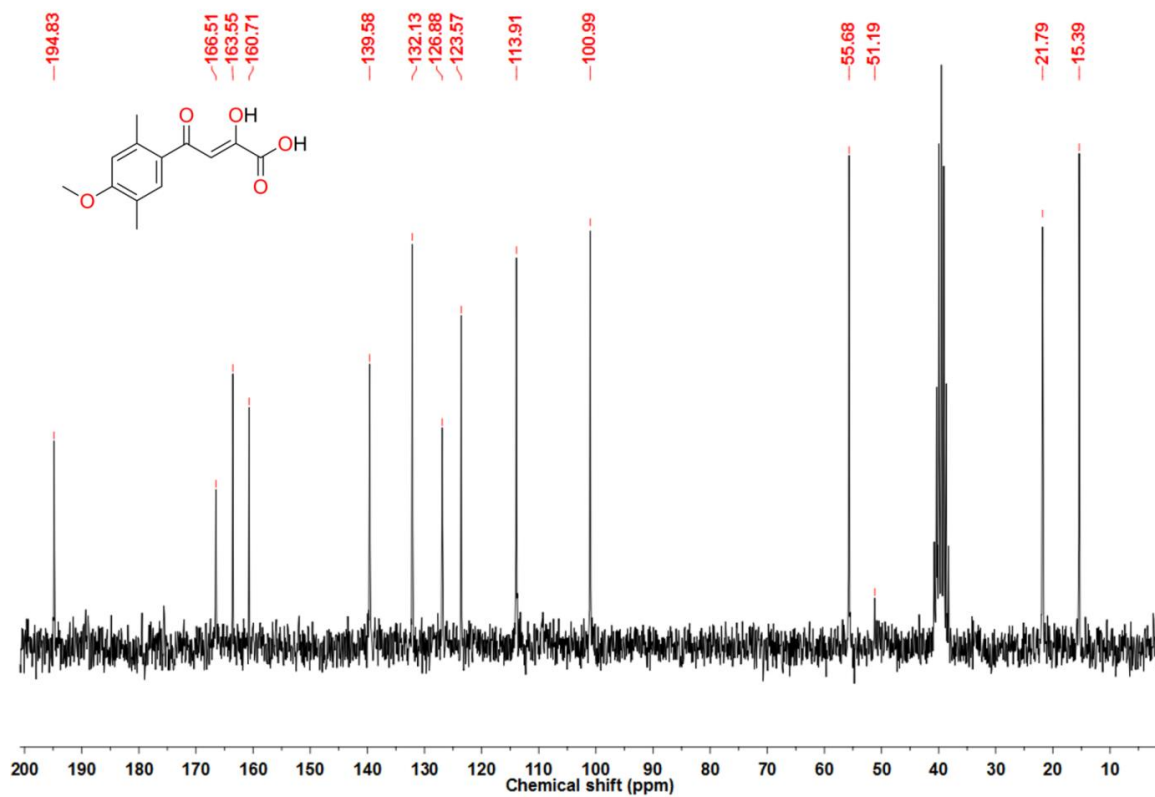
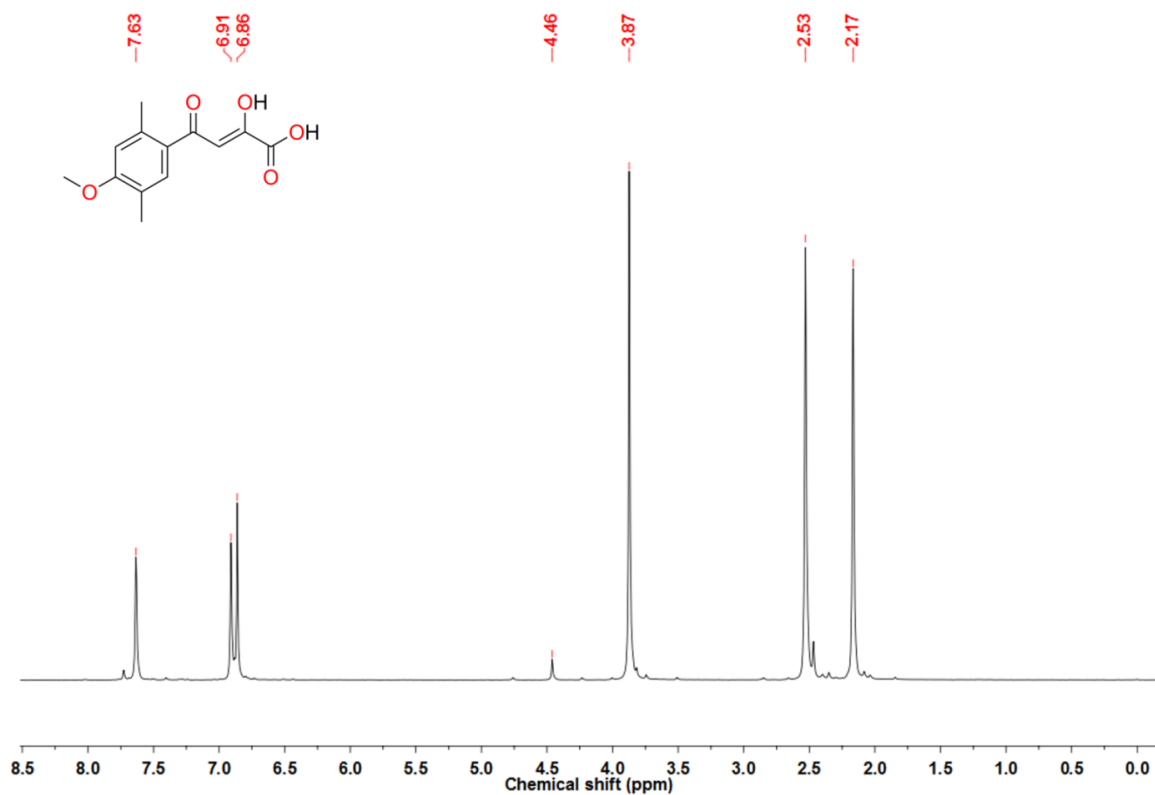
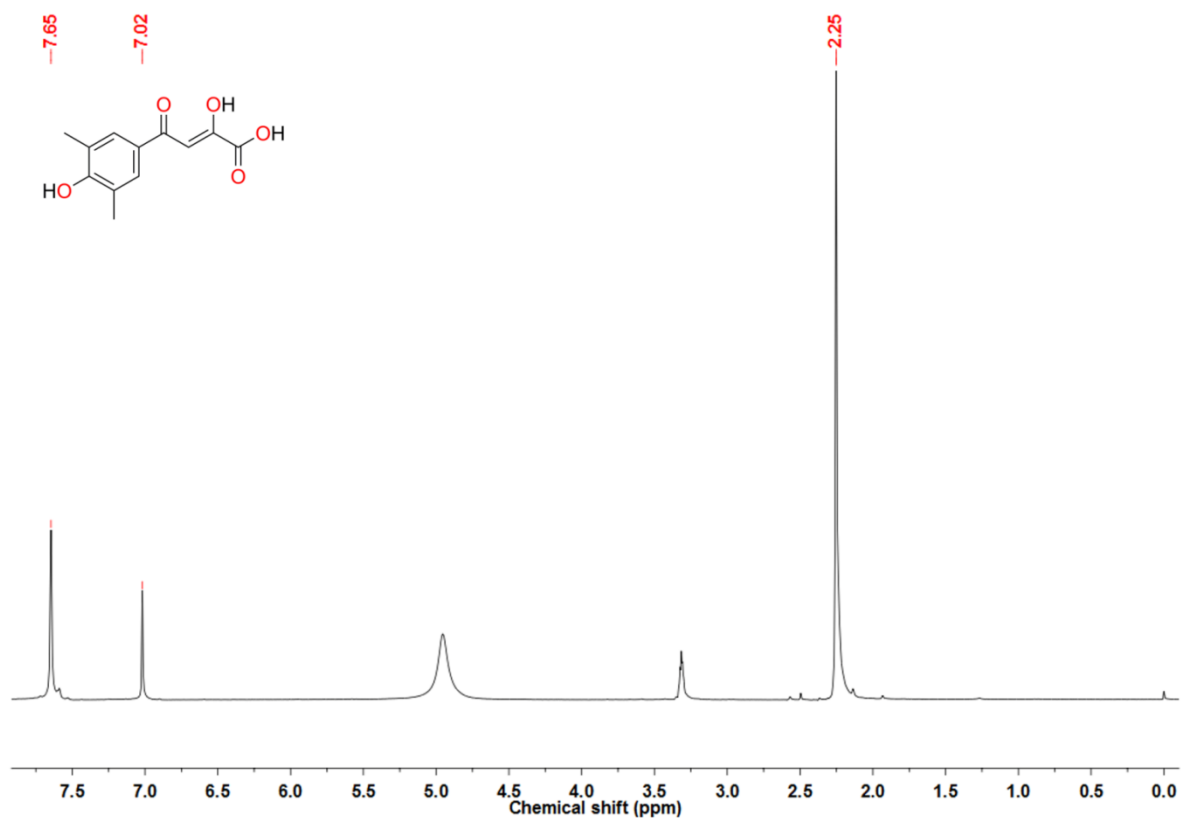


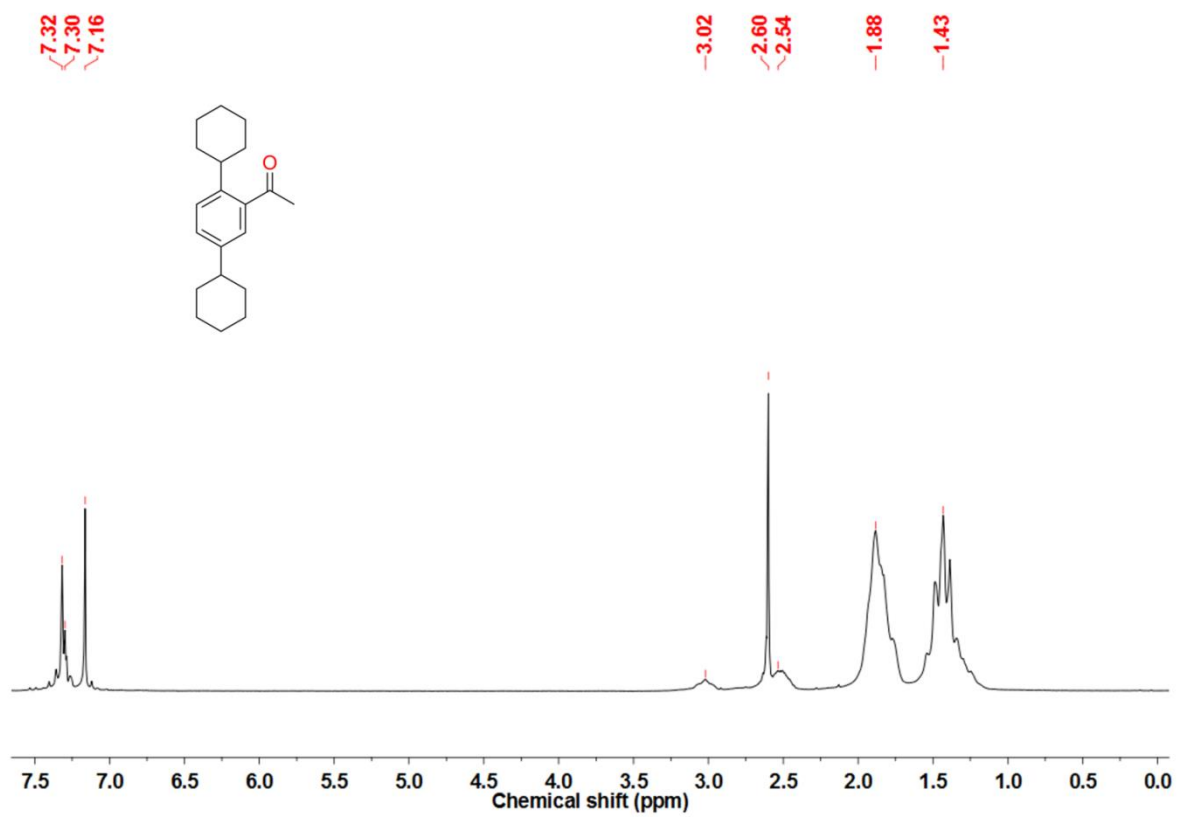
Figure S11. 1D <sup>1</sup>H and 1D <sup>13</sup>C NMR spectra of 4-([1,1'-biphenyl]-4-yl)-4-oxobutanoic acid (3a).



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



**Figure S13.** 1D <sup>1</sup>H NMR spectrum of (Z)-2-hydroxy-4-(4-hydroxy-3,5-dimethylphenyl)-4-oxobut-2-enoic acid (11).



**Figure S14.** 1D <sup>1</sup>H spectrum of 1-(2,5-dicyclohexylphenyl)ethanone (**4a**).



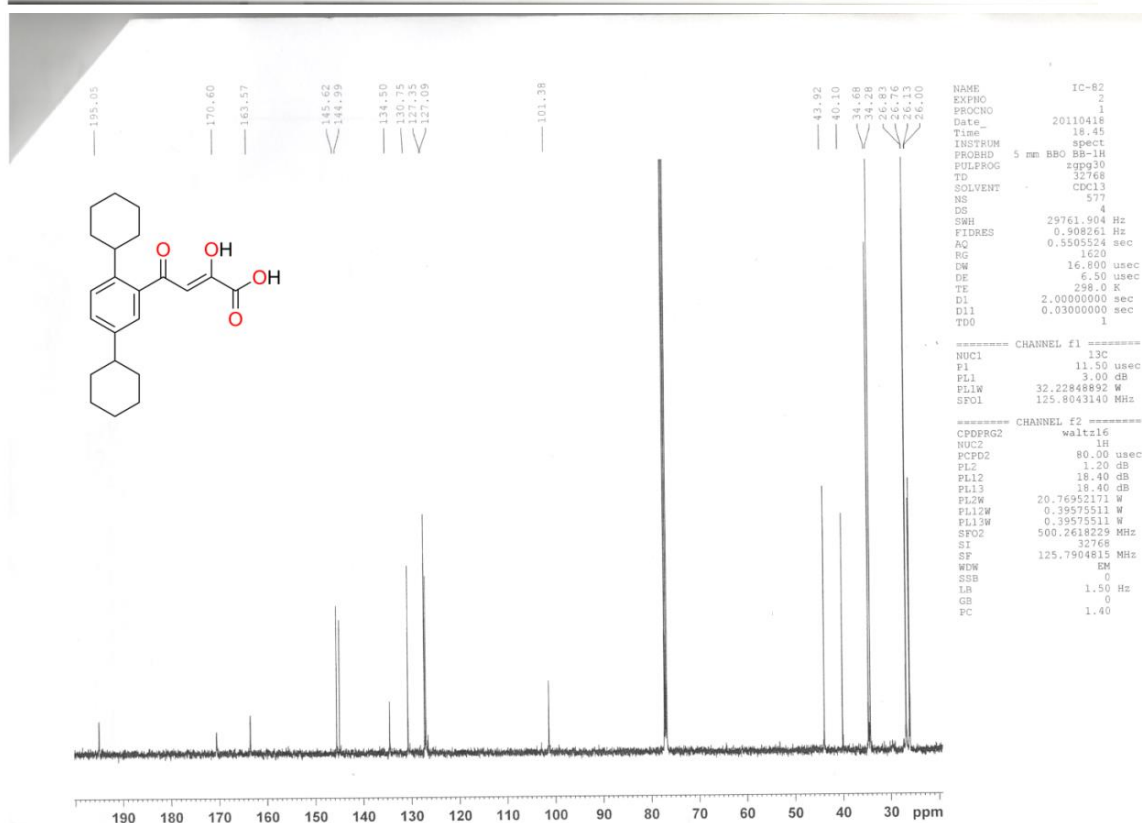
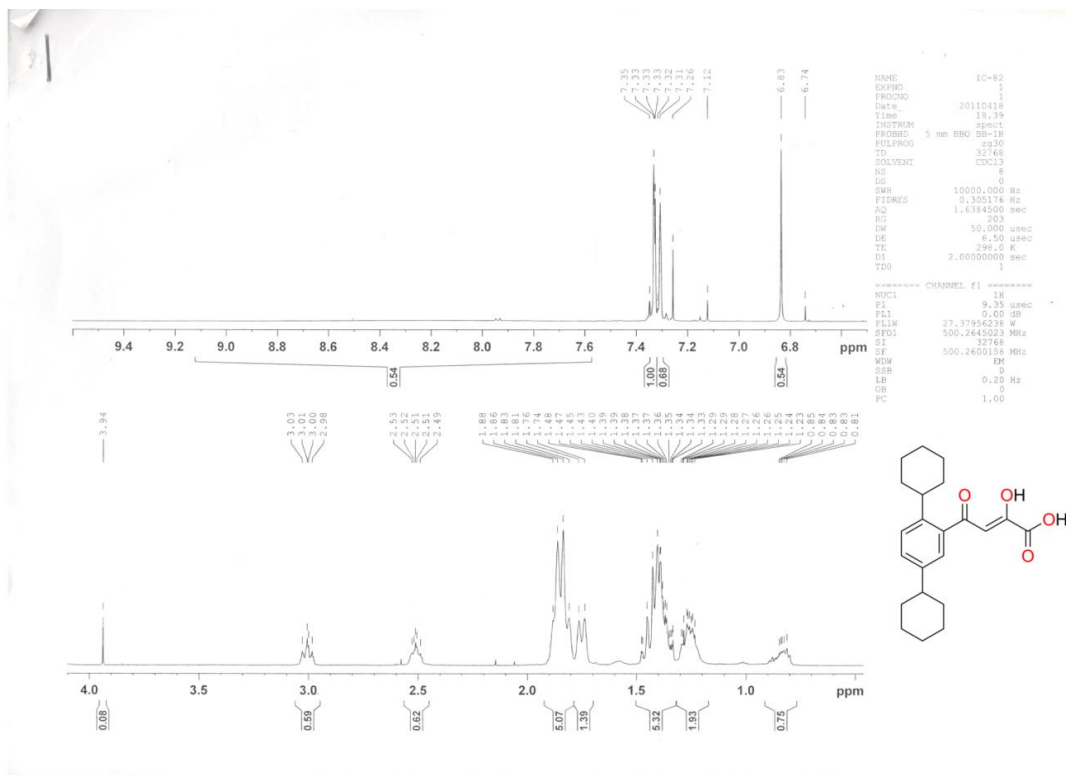
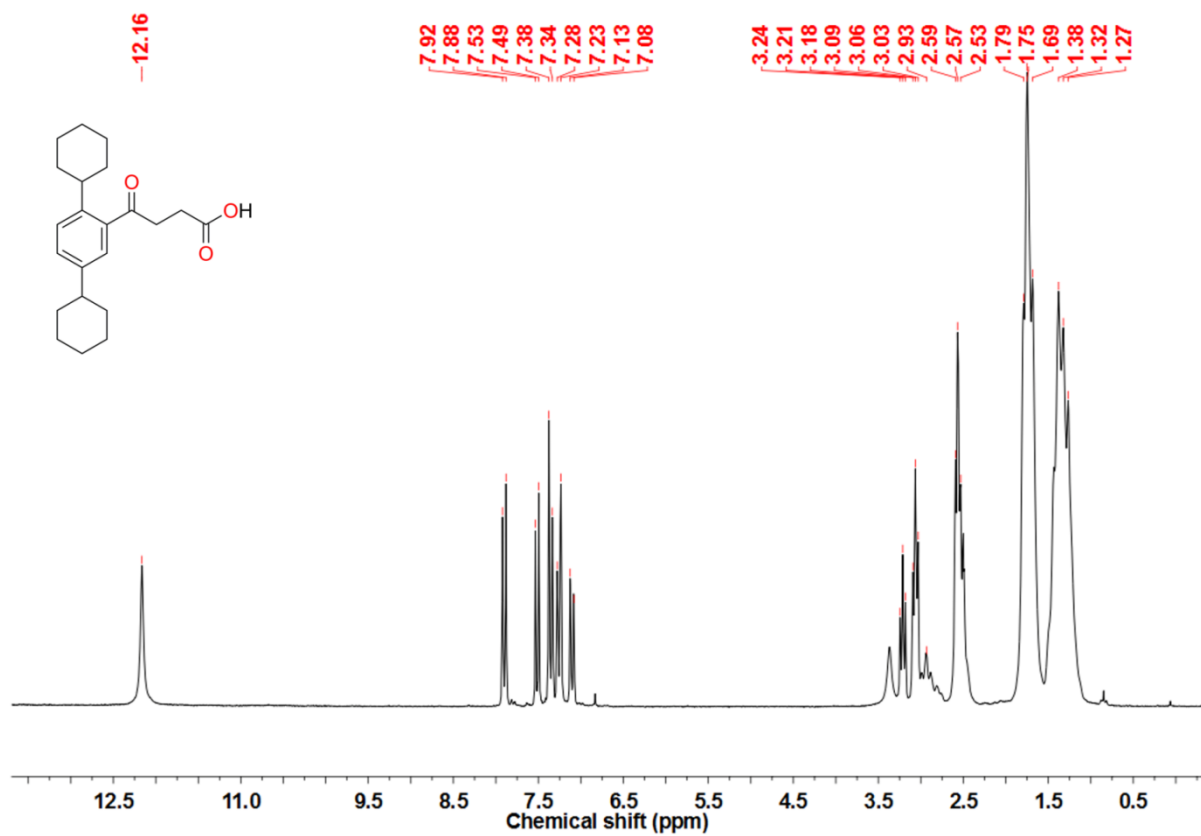
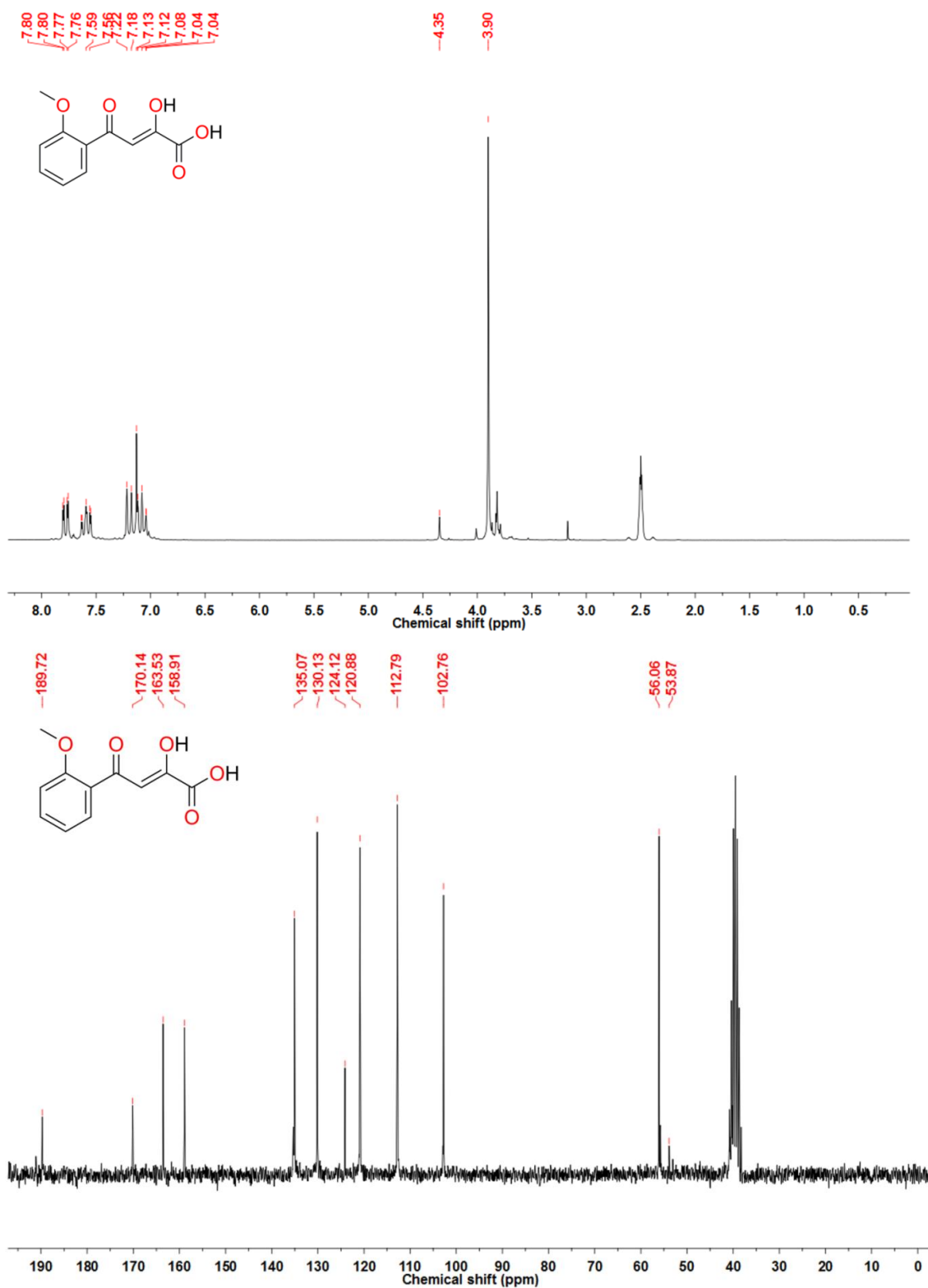


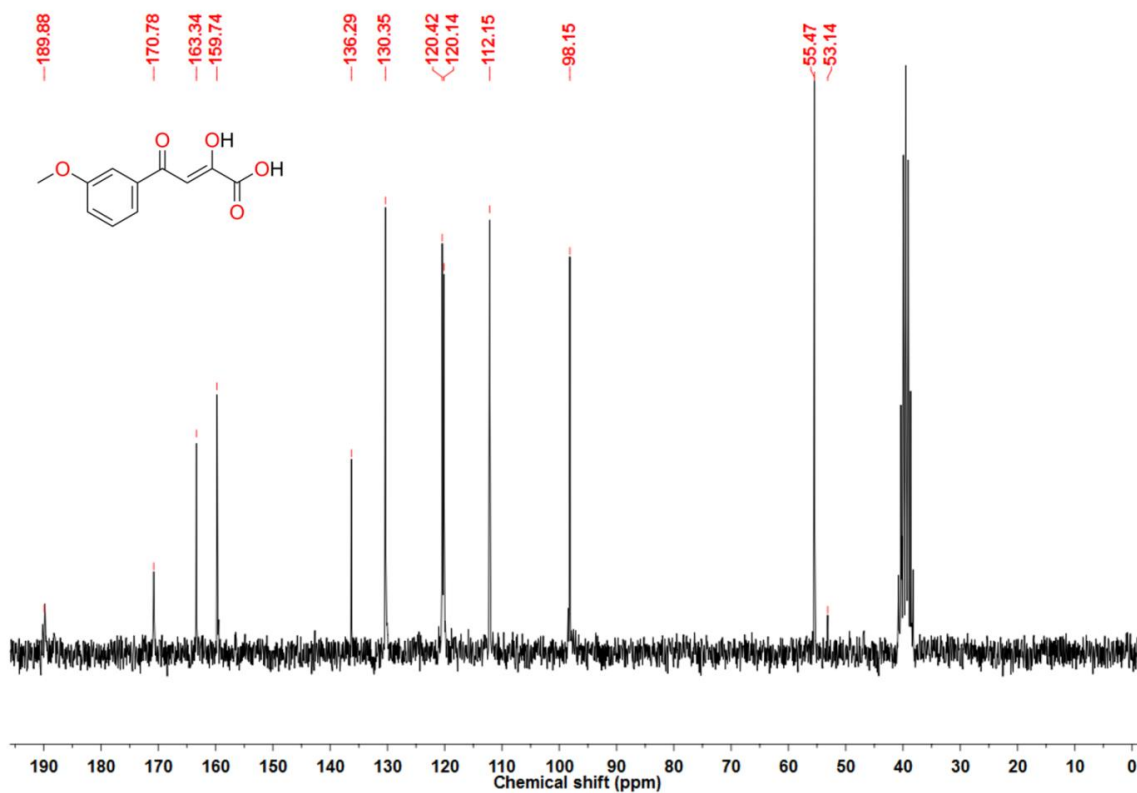
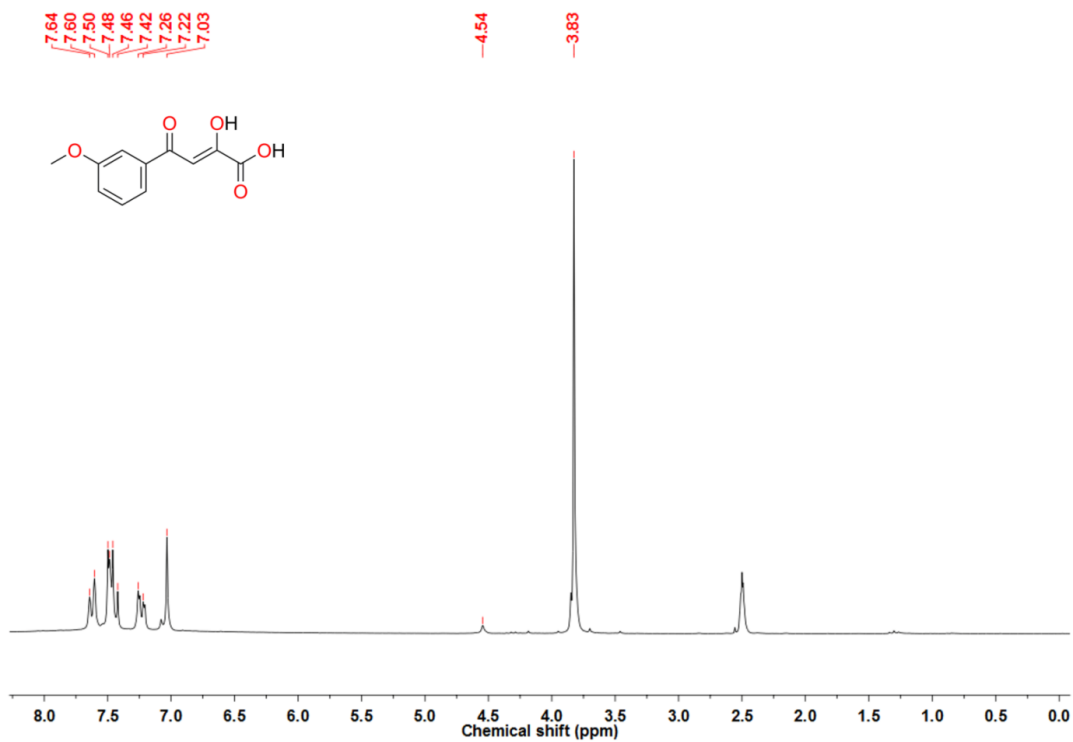
Figure S15. 1D <sup>1</sup>H and 1D <sup>13</sup>C NMR spectra of (Z)-4-(2,5-dicyclohexylphenyl)-2-hydroxy-4-oxobut-2-enoic acid (12).



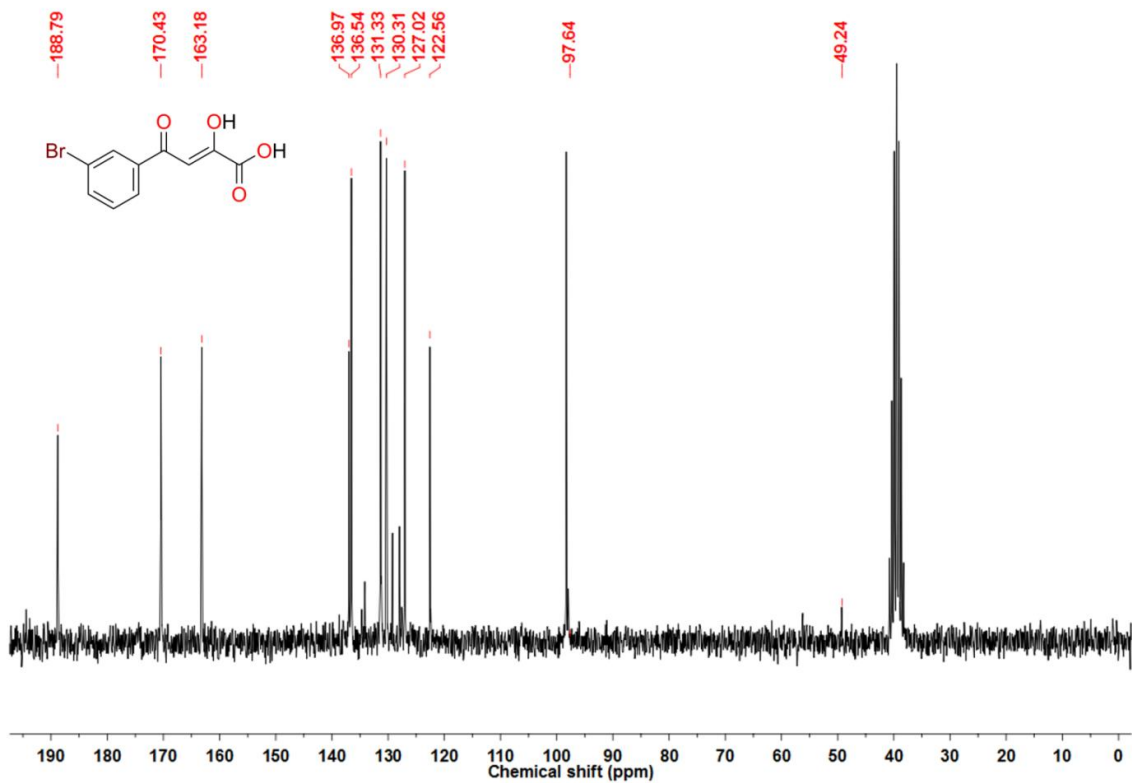
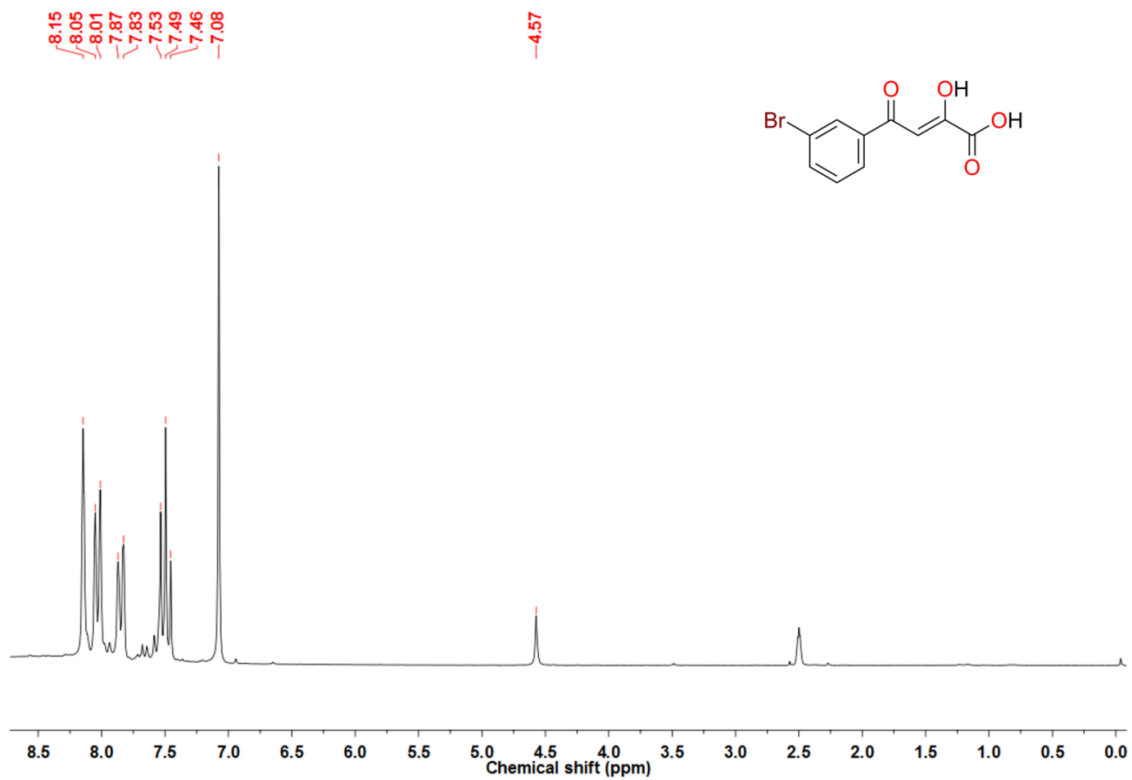
**Figure S16.** 1D  $^1\text{H}$  NMR spectrum of 4-(2,5-dicyclohexylphenyl)-4-oxobutanoic acid (**1a**).



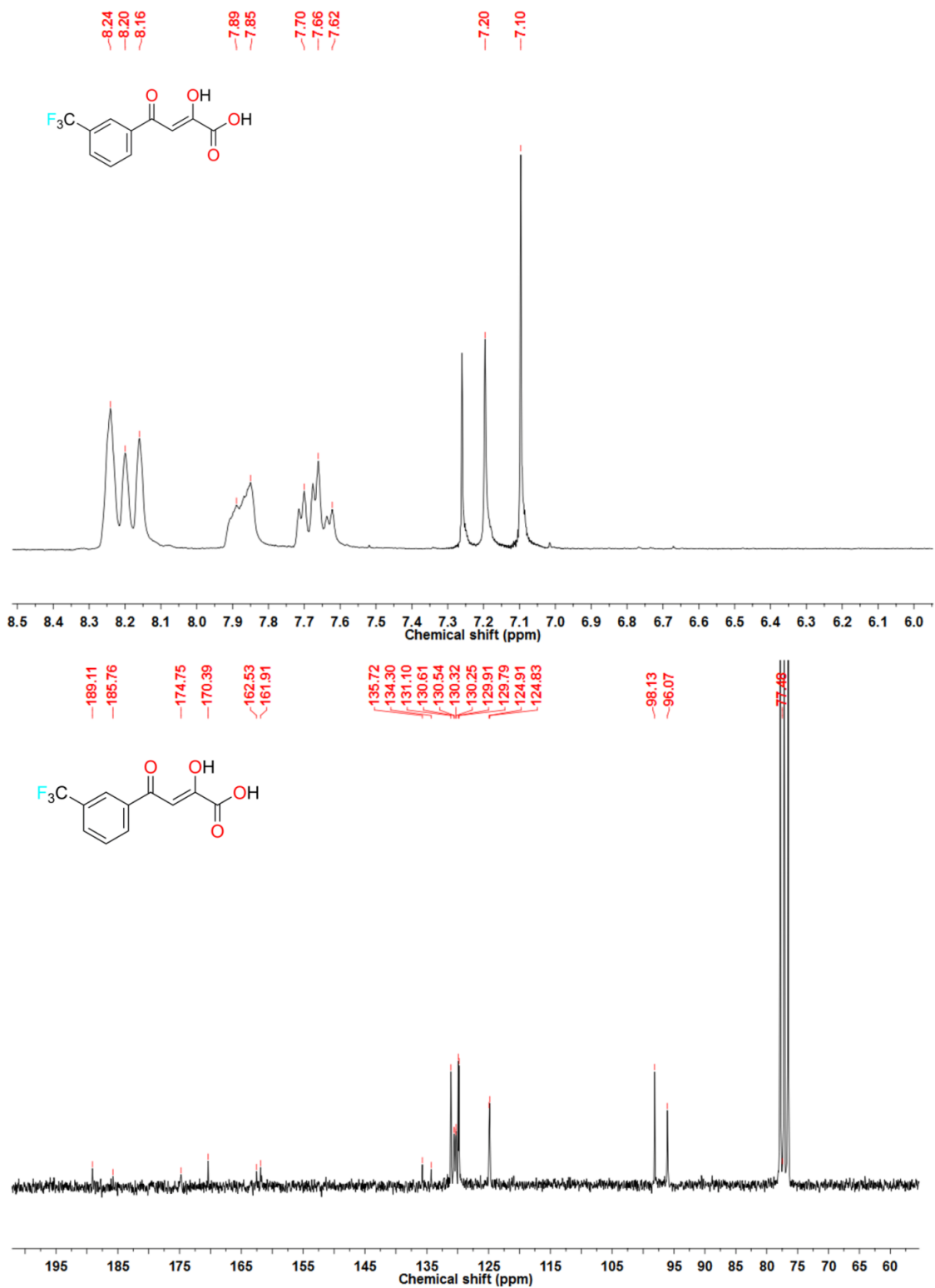
**Figure S17.** 1D <sup>1</sup>H and 1D <sup>13</sup>C NMR spectra of (Z)-2-hydroxy-4-(2-methoxyphenyl)-4-oxobut-2-enoic acid (13).



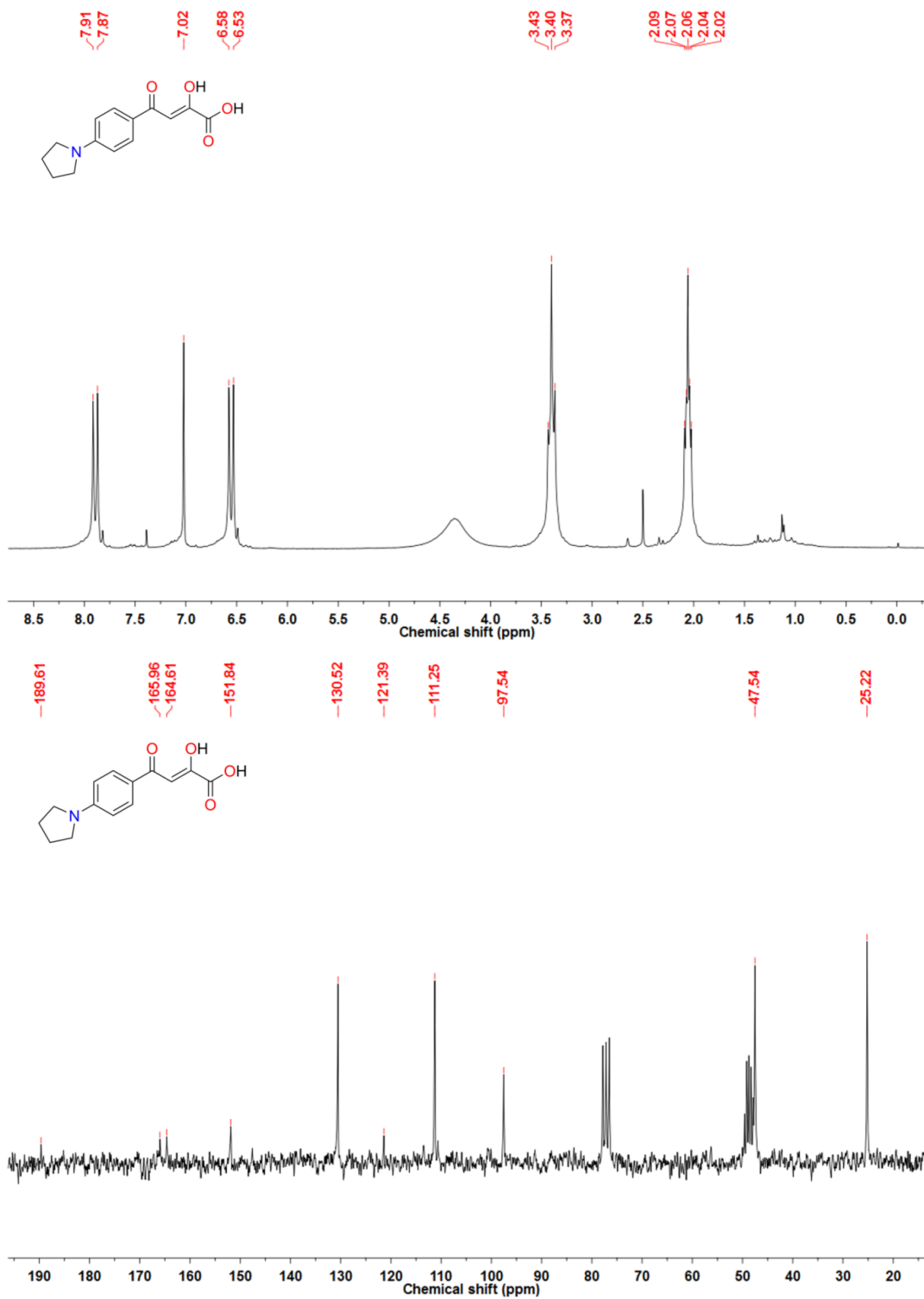
**Figure S18.** 1D  $^1\text{H}$  and 1D  $^{13}\text{C}$  NMR spectra of (Z)-2-hydroxy-4-(3-methoxyphenyl)-4-oxobut-2-enoic acid (**14**).



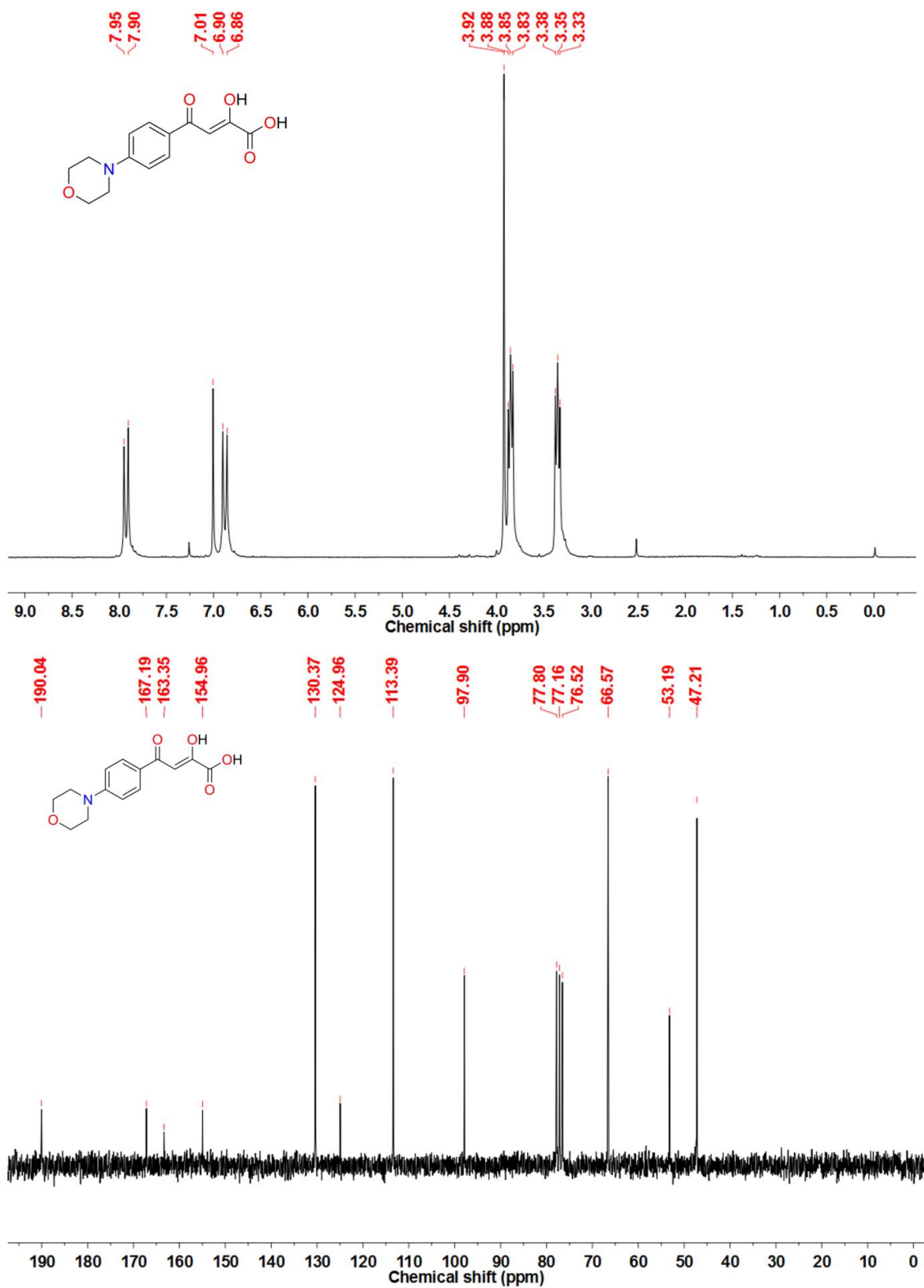
**Figure S19.** 1D <sup>1</sup>H and 1D <sup>13</sup>C NMR spectra of (Z)-4-(3-bromophenyl)-2-hydroxy-4-oxobut-2-enoic acid (15).



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

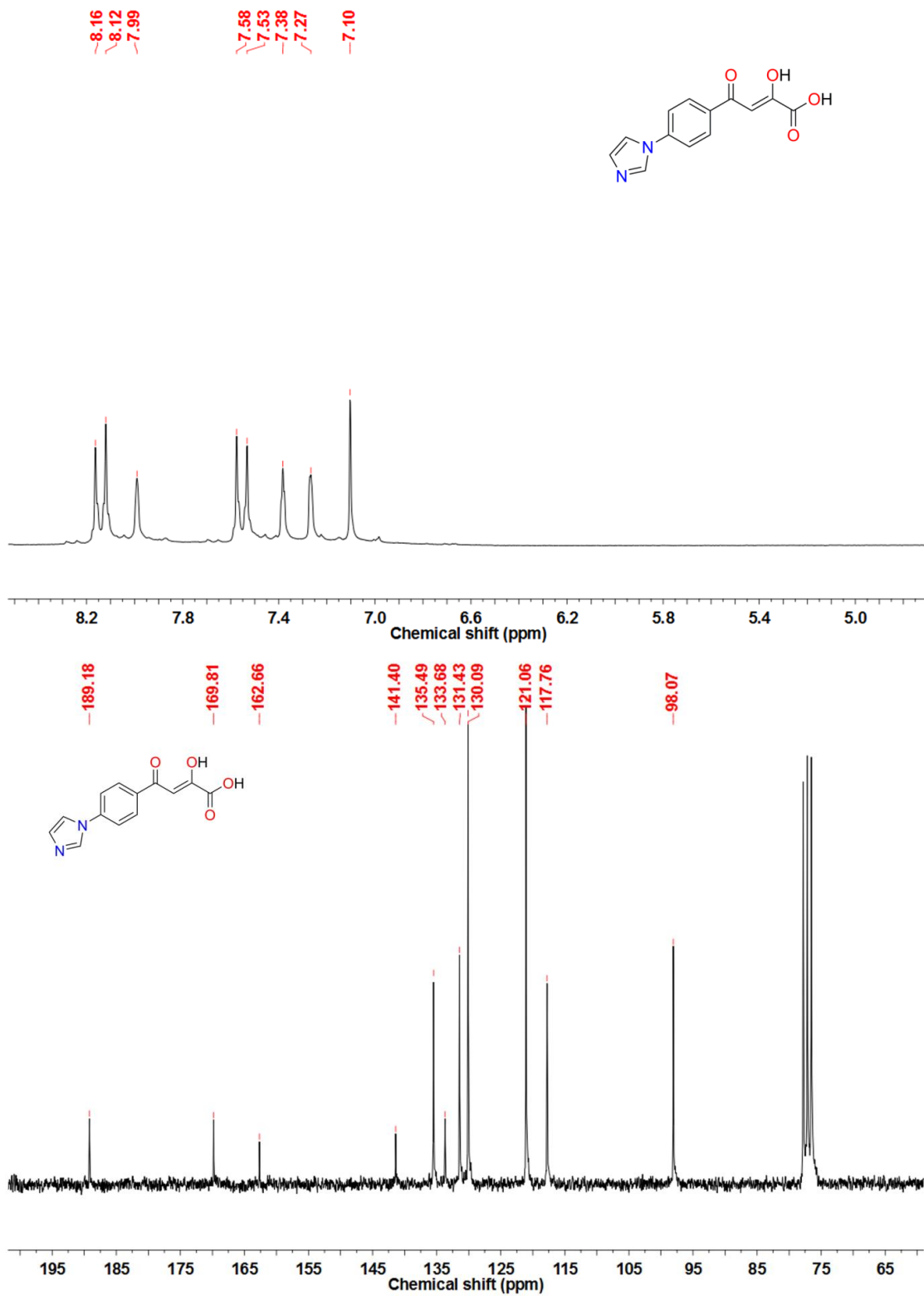


**Figure S21.** 1D  $^1\text{H}$  and 1D  $^{13}\text{C}$  NMR spectra of (Z)-2-hydroxy-4-oxo-4-(4-(pyrrolidin-1-yl)phenyl)but-2-enoic acid (**17**).

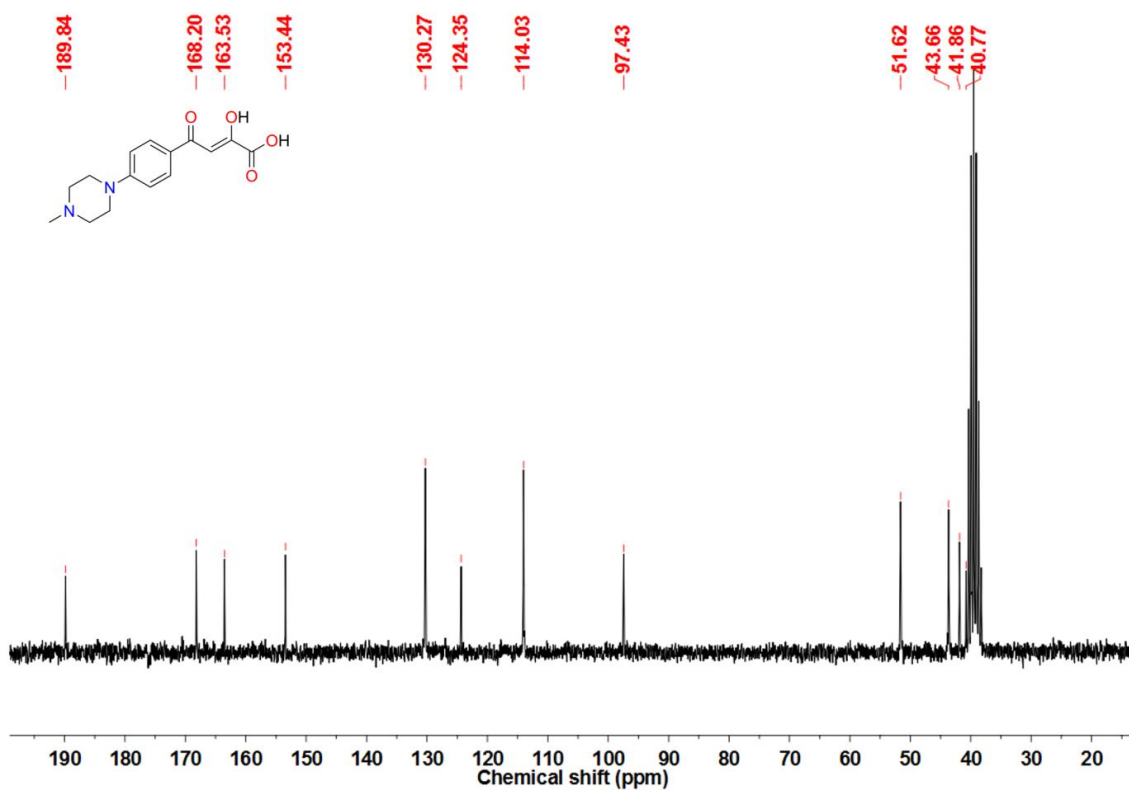
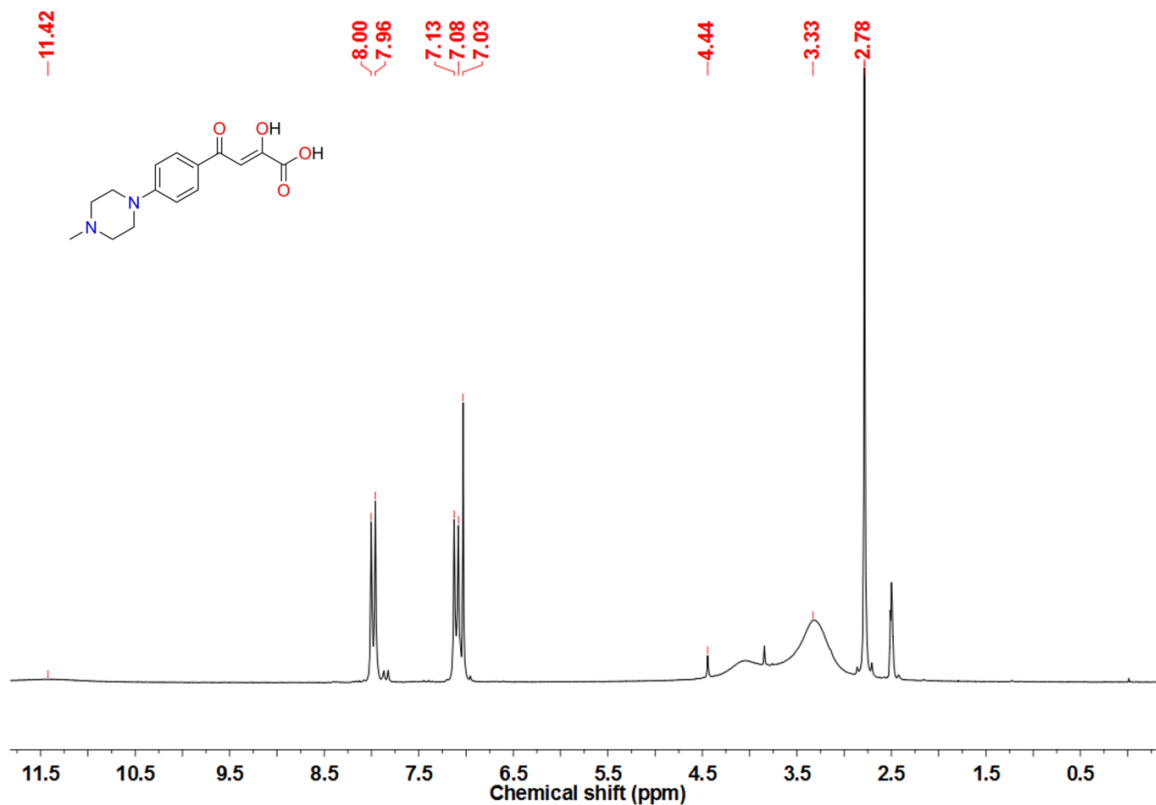


**Figure S22.** 1D <sup>1</sup>H and 1D <sup>13</sup>C NMR spectra of (Z)-2-hydroxy-4-(4-morpholinophenyl)-4-oxobut-2-enoic acid (18).

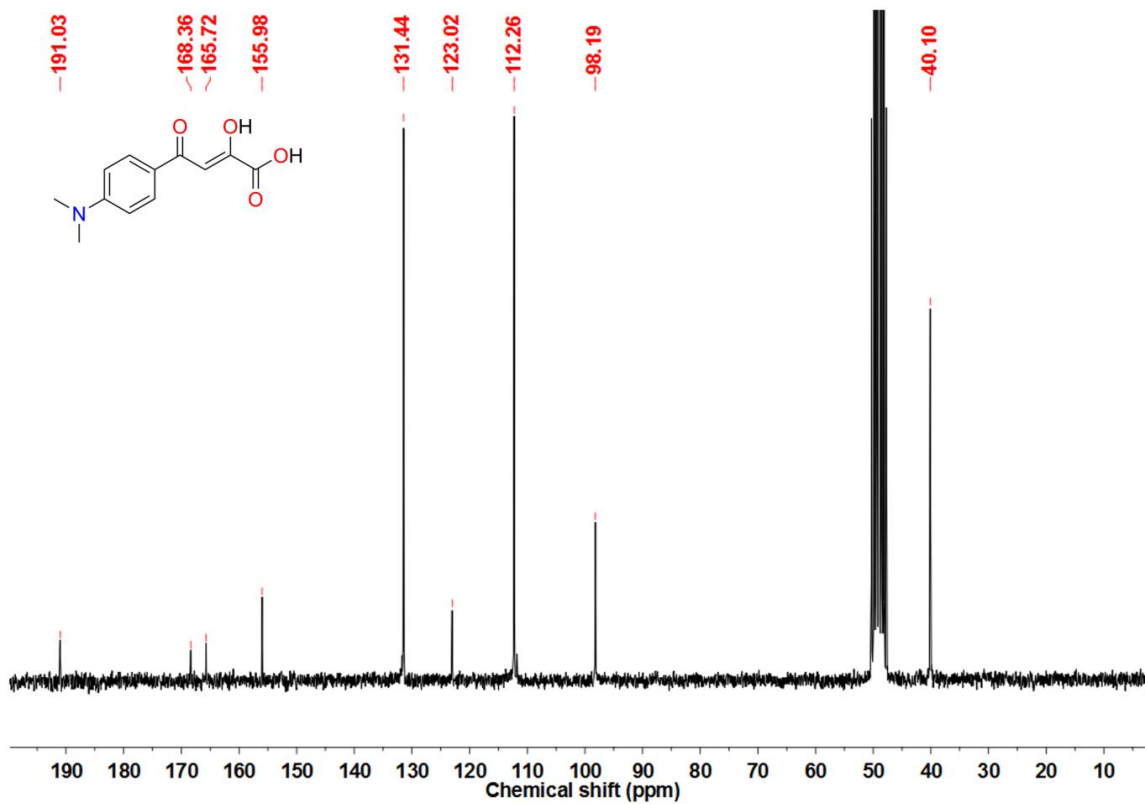
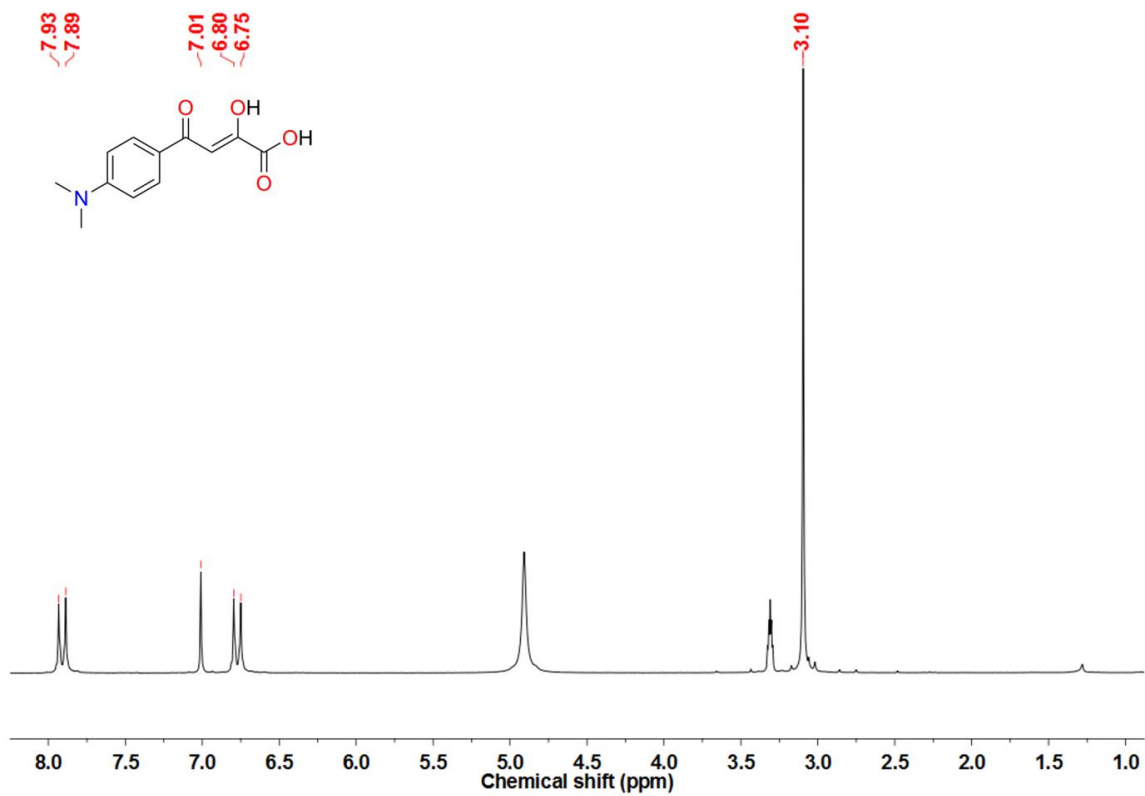




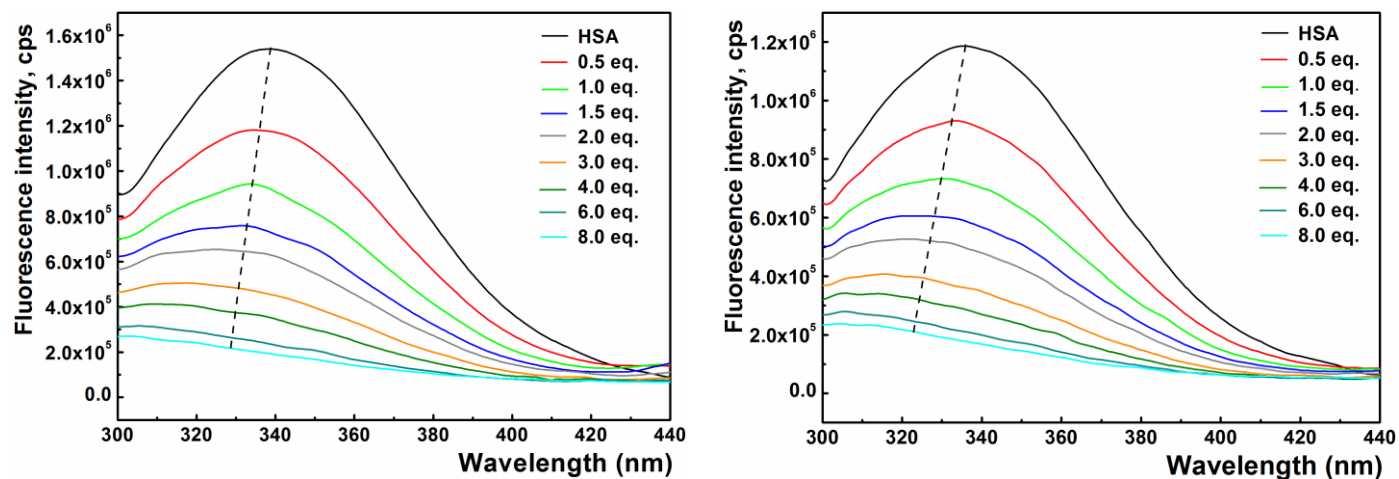
**Figure S23.** 1D <sup>1</sup>H and 1D <sup>13</sup>C NMR spectra of (Z)-4-(4-(1H-imidazol-1-yl)phenyl)-2-hydroxy-4-oxobut-2-enoic acid (**19**).



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



**Figure S25.** 1D  $^1\text{H}$  and 1D  $^{13}\text{C}$  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 ( $c = 0.5 \mu\text{M}$ ) upon addition of comp. **12** ( $c_{12} = 0.0; 0.25; 0.5; 0.75; 1; 1.5; 2.0; 3.0; 4.0 \mu\text{M}$ );  $T = 293$  K, left;  $T = 313$  K, right; 30 mM PBS, pH = 7.38.