

SUPPORTING INFORMATION

Rabenchromenone and Rabenzophenone, Phytotoxic Tetrasubstituted Chromenone and Hexasubstituted Benzophenone Constituents Produced by the Oak Decline Associated Fungus *Fimetariella rabenhorstii*

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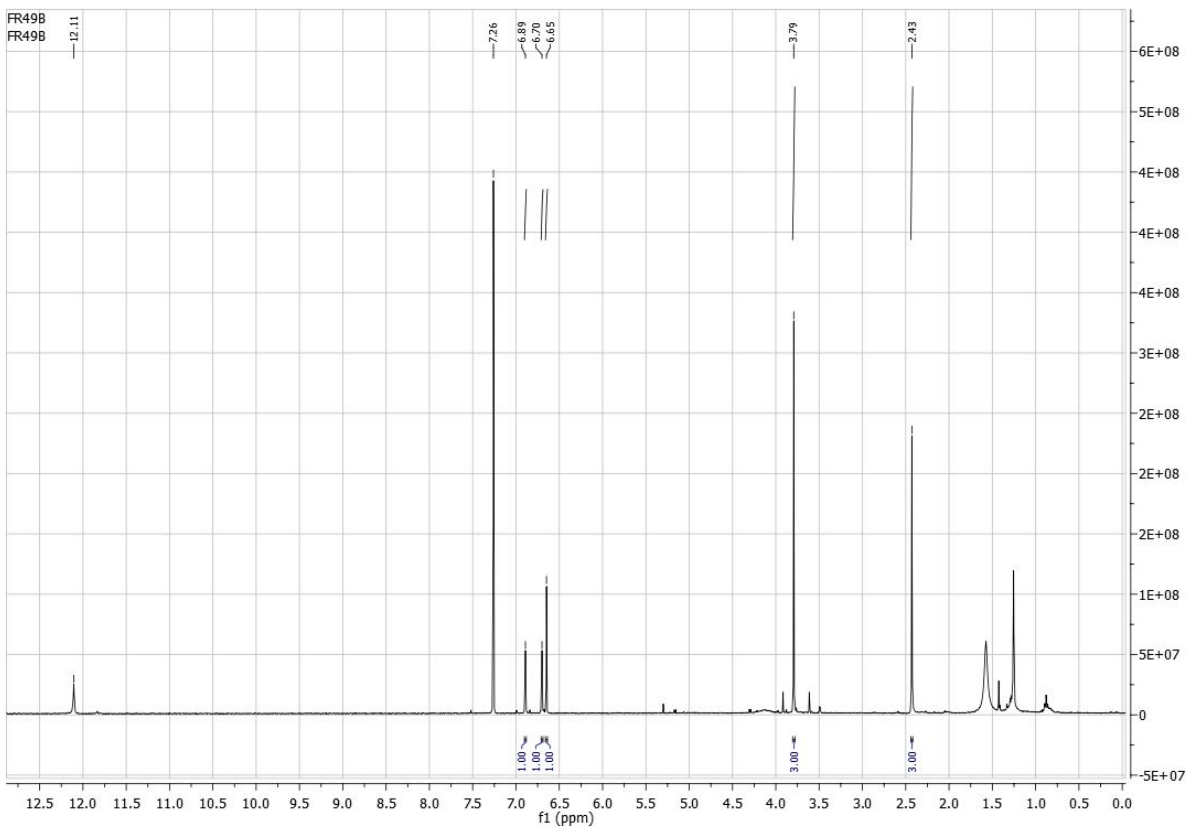
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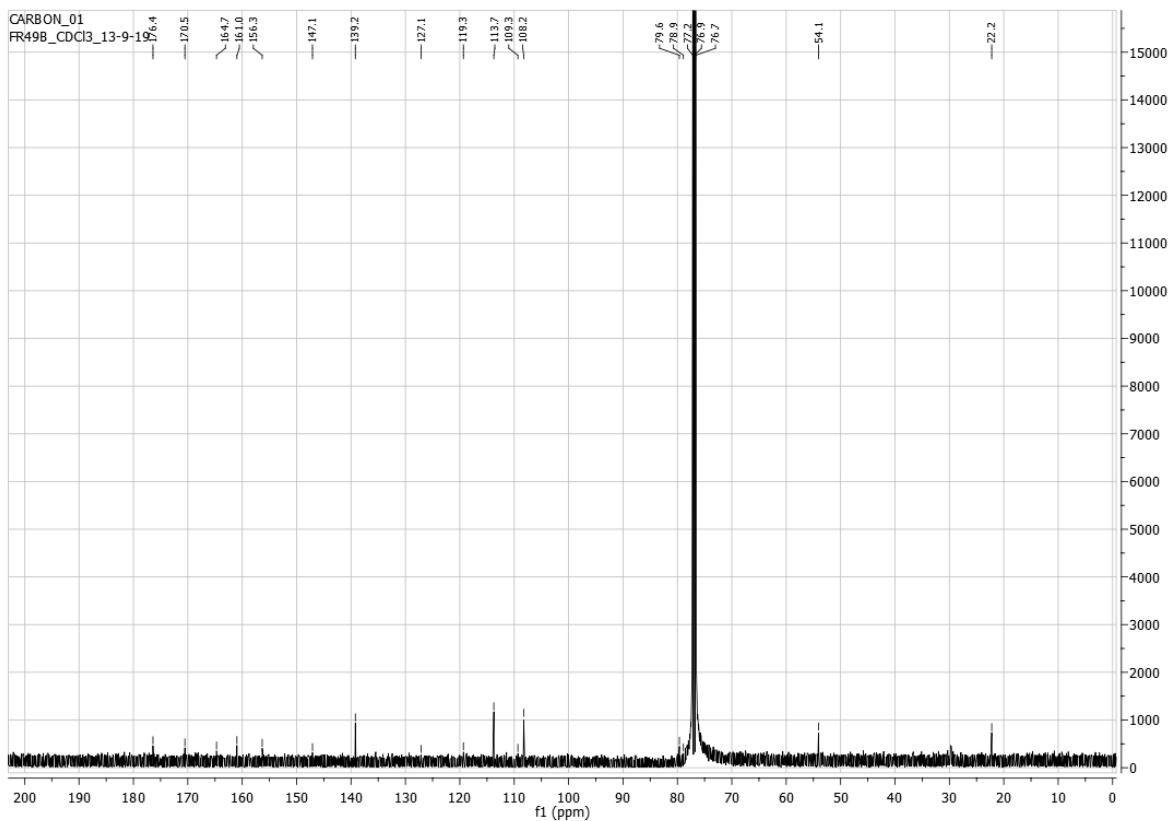
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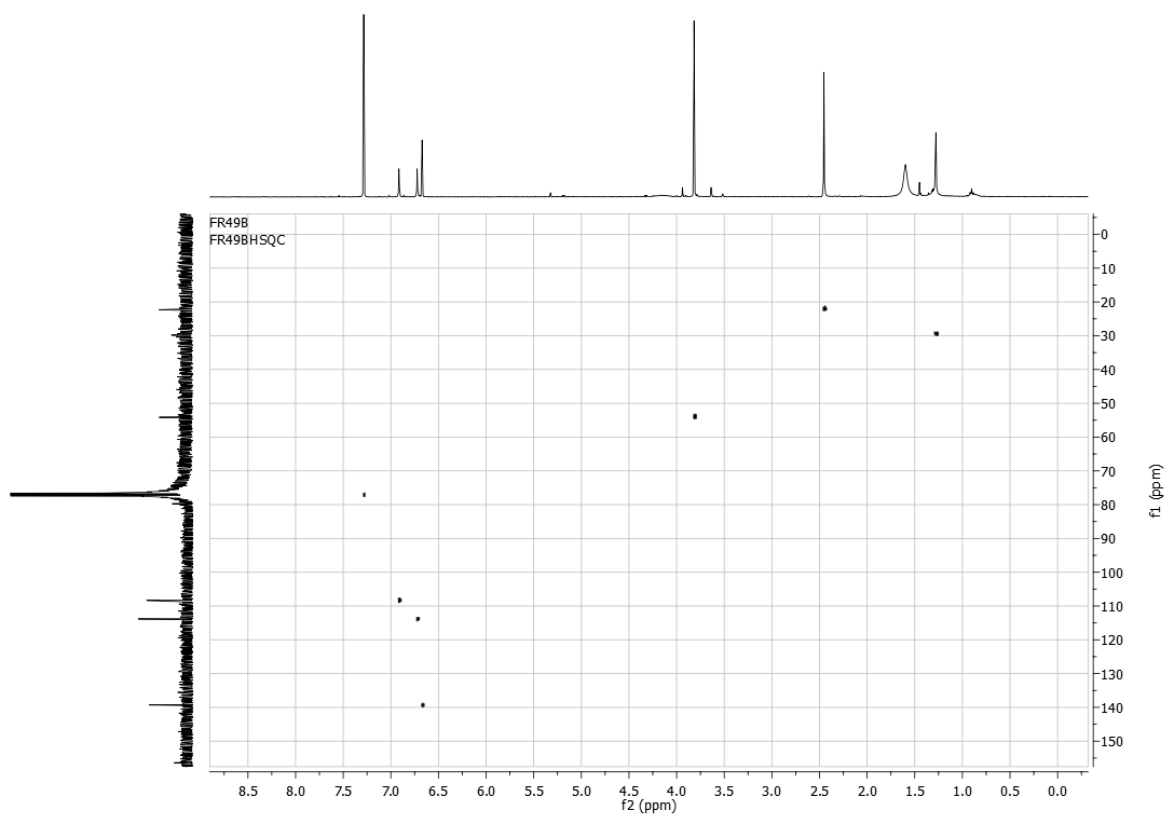
Page 8: **Figure S1.** ECD spectrum of (*R*)-**1** calculated with four different functionals and def2-TZVP basis set including PCM solvent model for acetonitrile, using input structures optimized at $\omega\text{B97X-D/6-311+G(d,p)/SMD}$ level, Boltzmann averaged over 2 conformers at 300 K. Calculated spectra were obtained as sums of Gaussian bands with 0.3 eV exponential half-width; BH&HLYP spectrum was red-shifted by 5 nm. The ECD spectra are not scaled.



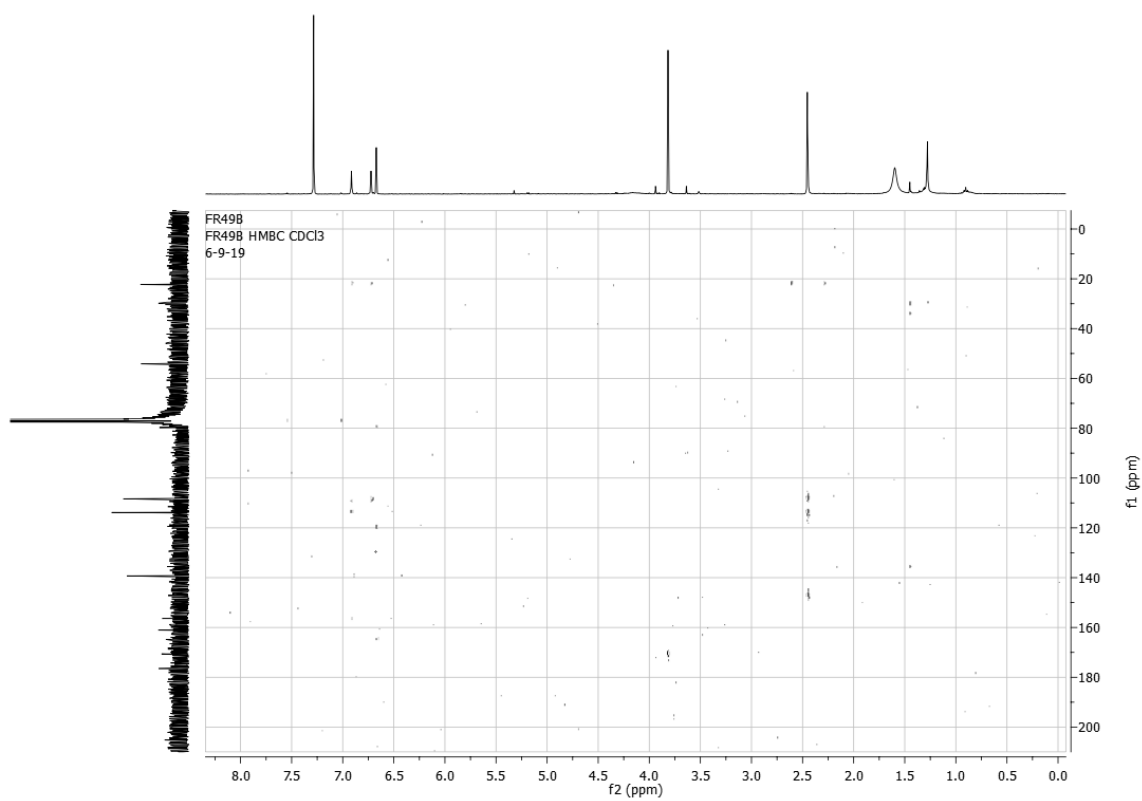
Spectra 1. ^1H NMR spectrum of Rabenchromenone (**1**) (CDCl_3 , 400 MHz).



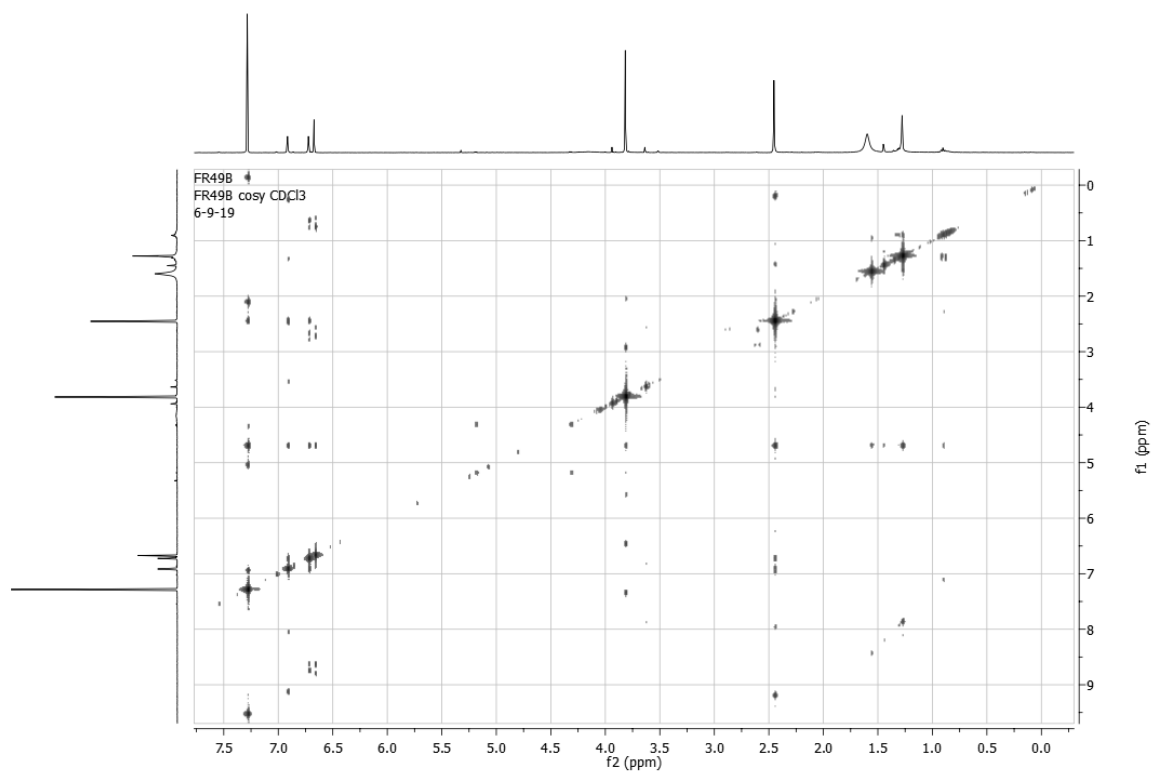
Spectra 2. ^{13}C NMR spectrum of Rabenchromenone (**1**) (CDCl_3 , 100 MHz).



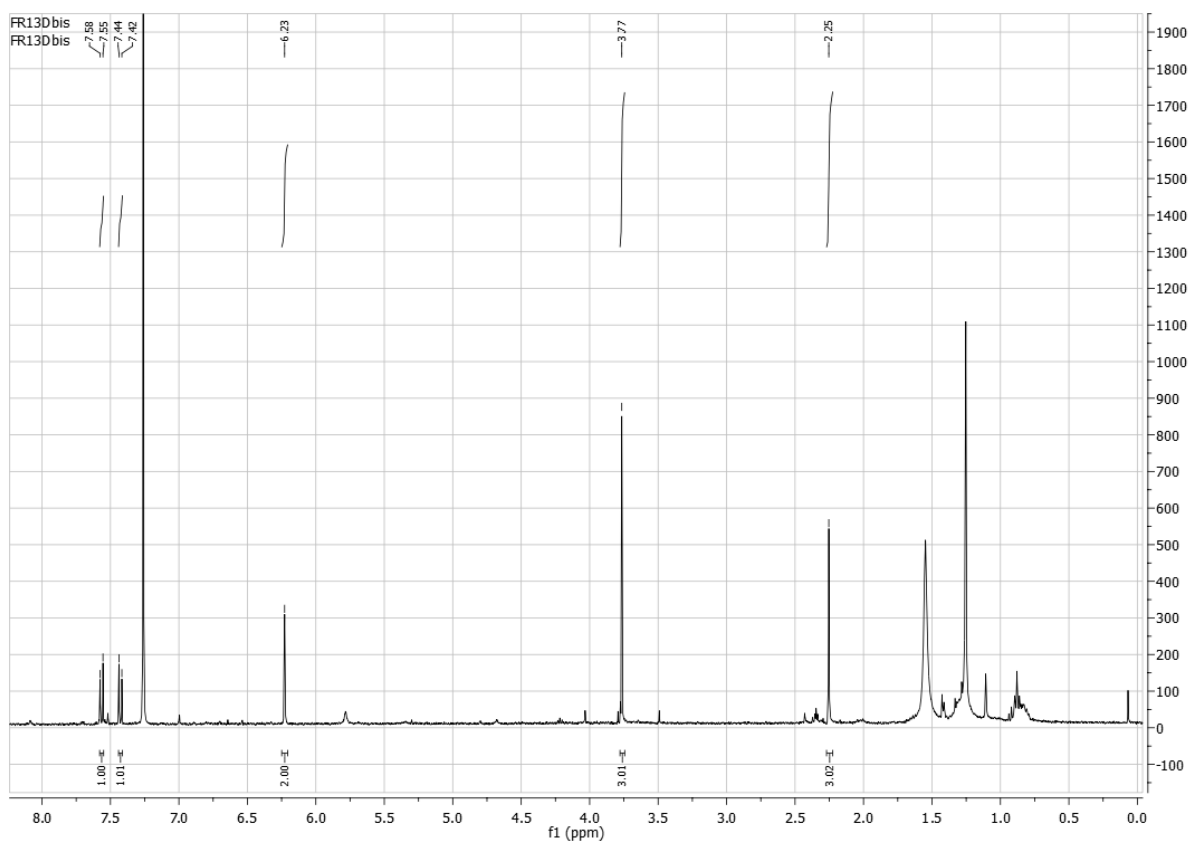
Spectra 3. HSQC spectrum of Rabenchromenone (**1**) (CDCl_3 , 400/100 MHz).



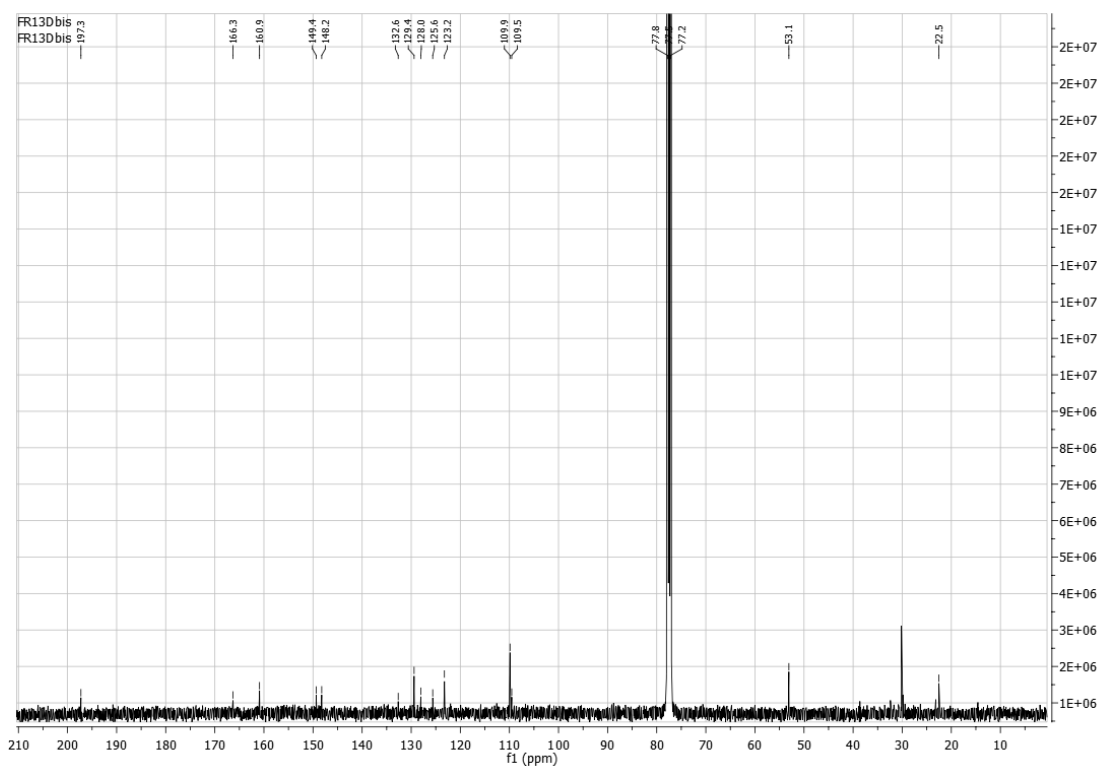
Spectra 4. HMBC spectrum of Rabenchromenone (**1**) (CDCl_3 , 400/100 MHz).



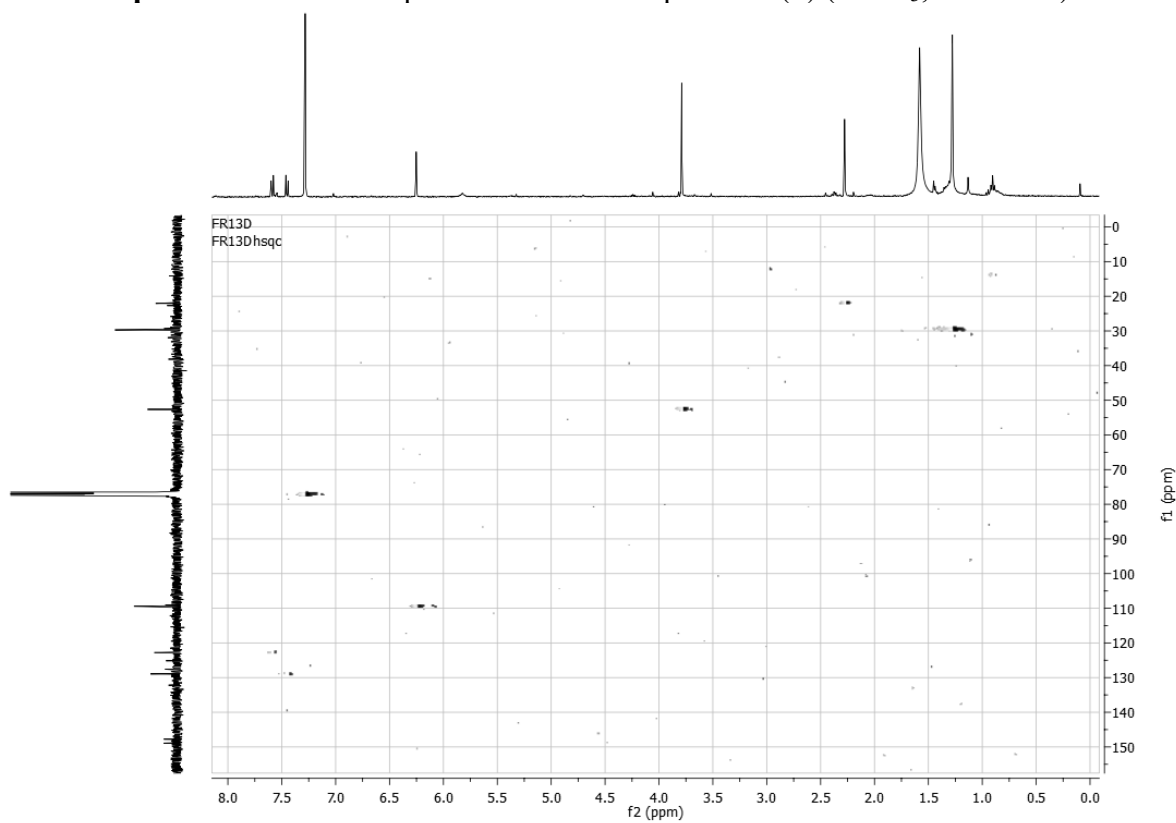
Spectra 5. COSY spectrum of Rabenchromenone (**1**) (CDCl₃, 400 MHz).



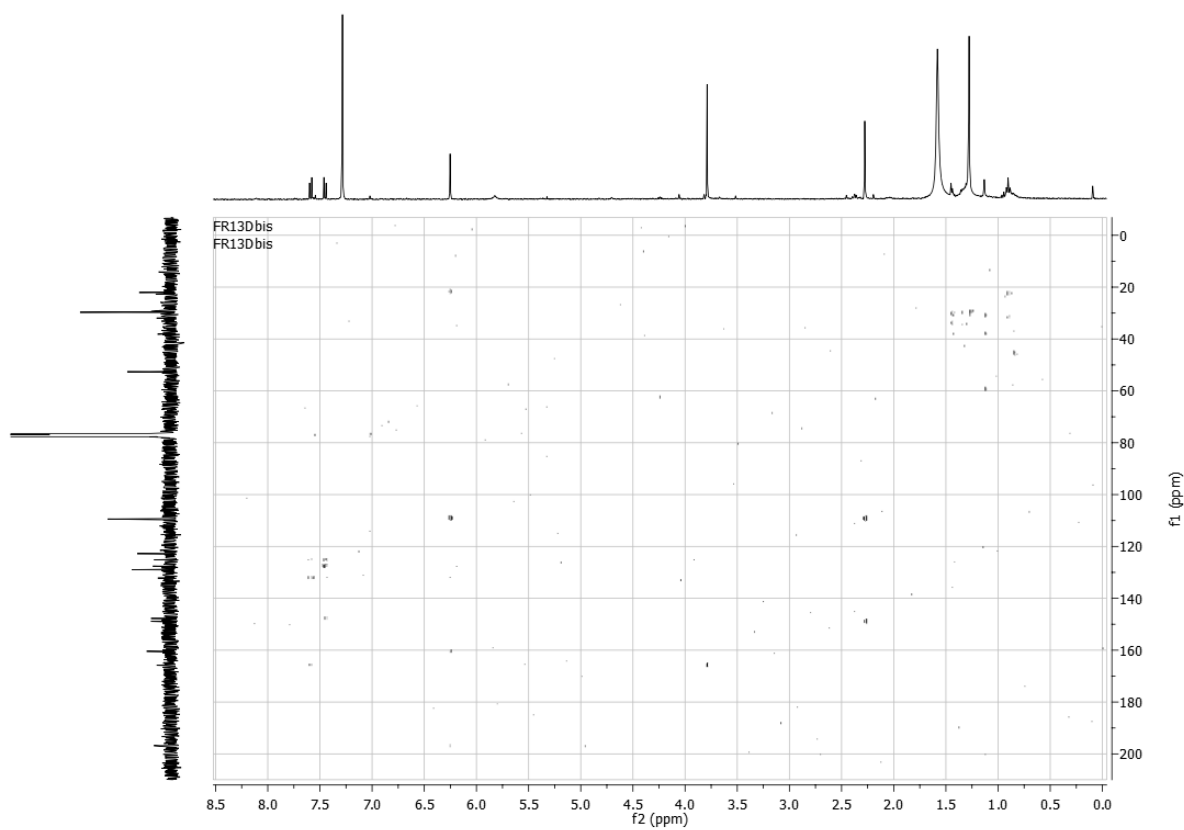
Spectra 6. ¹H NMR spectrum of Rabenzophenone (**2**) (CDCl₃, 400 MHz).



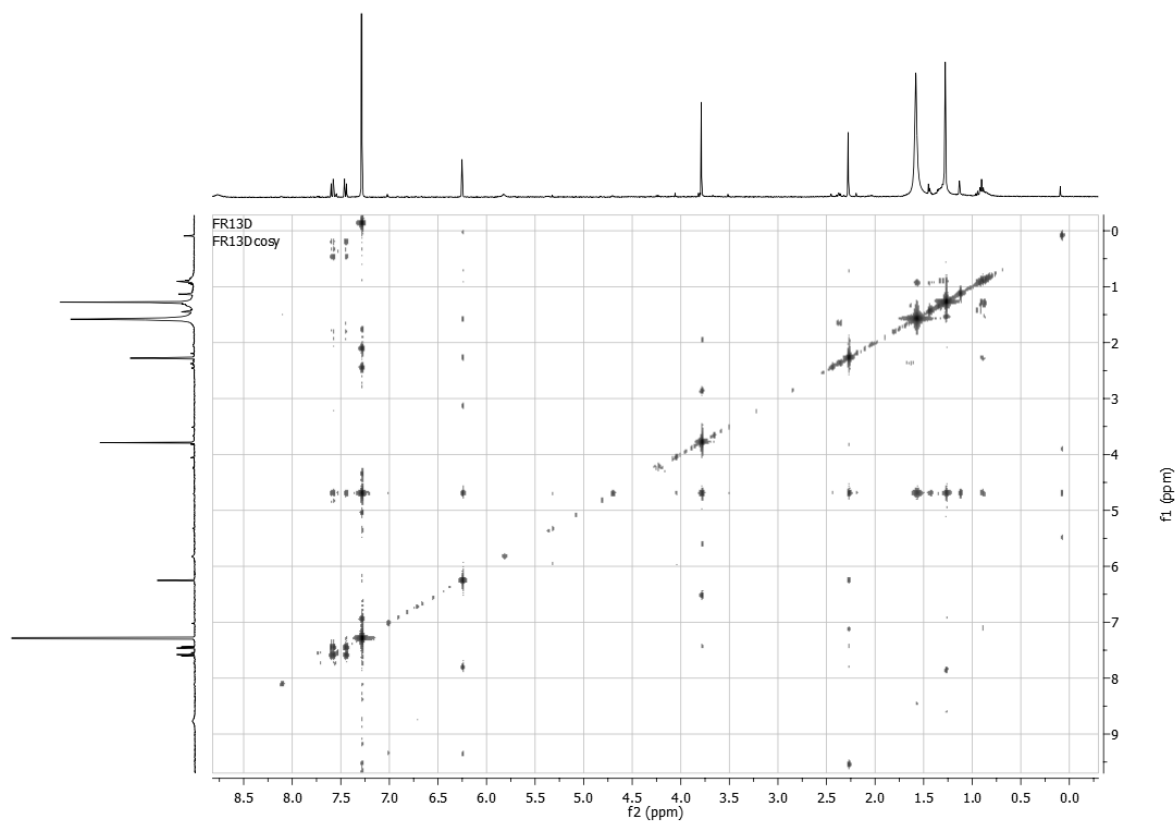
Spectra 7. ^{13}C NMR spectrum of Rabenzophenone (**2**) (CDCl_3 , 100 MHz).



Spectra 8. HSQC spectrum of Rabenzophenone (**2**) (CDCl_3 , 400/100 MHz).



Spectra 9. HMBC spectrum of Rabenzophenone (**2**) (CDCl_3 , 400/100 MHz).



Spectra 10. COSY spectrum of Rabenzophenone (**2**) (CDCl_3 , 400 MHz).

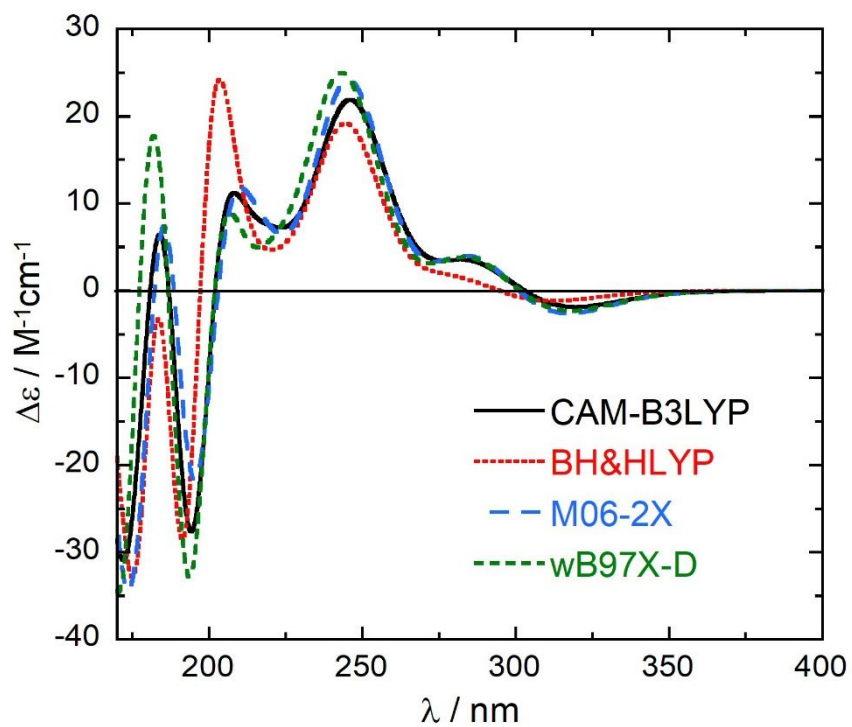


Figure S1. ECD spectrum of (*R*)-**1** calculated with four different functionals and def2-TZVP basis set including PCM solvent model for acetonitrile, using input structures optimized at ω B97X-D/6-311+G(d,p)/SMD level, Boltzmann averaged over 2 conformers at 300 K. Calculated spectra were obtained as sums of Gaussian bands with 0.3 eV exponential half-width; BH&HLYP spectrum was red-shifted by 5 nm. The ECD spectra are not scaled.