



Article

Inhibition of MurA enzyme from *Escherichia coli* and *Staphylococcus aureus* by diterpenes from *Lepechinia meyenii* and their synthetic analogs

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Supplementary Materials

NMR spectra

¹H NMR spectra were obtained at 600.13 MHz and ¹³C NMR spectra at 150.90 MHz on a Bruker AVANCEIII HD spectrometer.

ESI-ITMS spectra

ESI-ITMS spectra were obtained on a Bruker AmaZon SL spectrometer at negative ion mode.

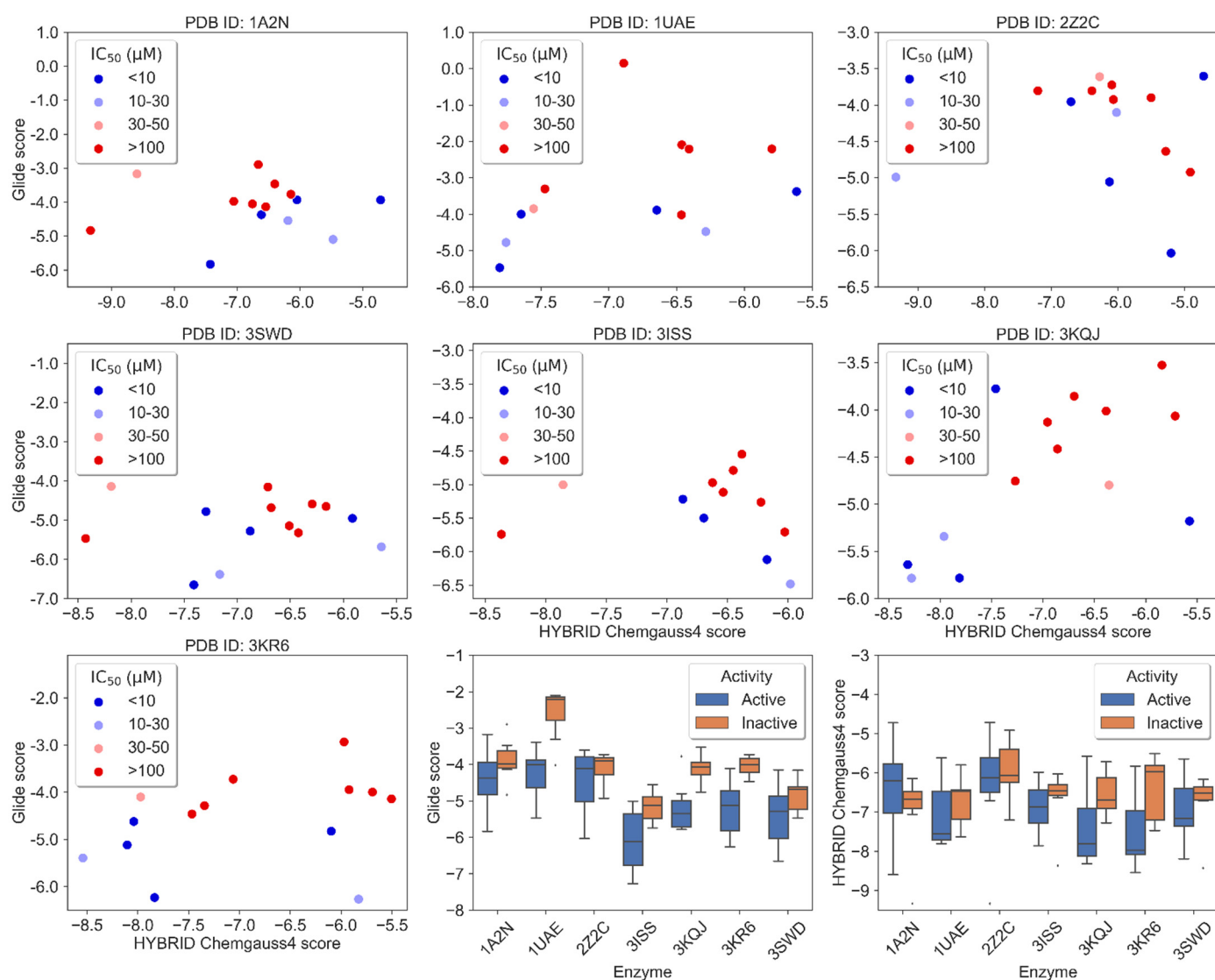


Figure S1. Docking results. Scatterplots of Glide and Hybrid scores for each compound and each enzyme used; boxplots of Hybrid and Glide docking scores of active and inactive compounds calculated for each enzyme separately.

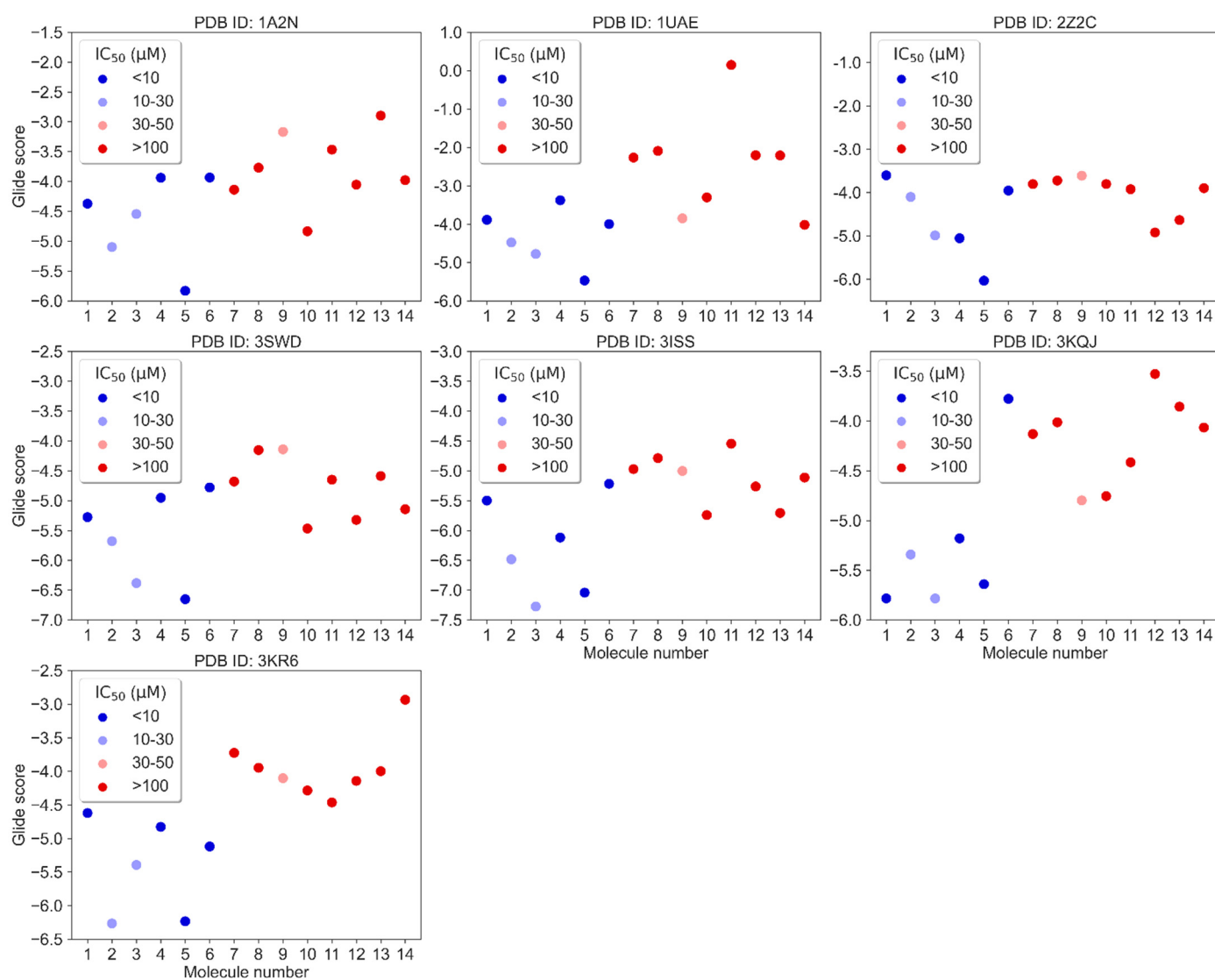
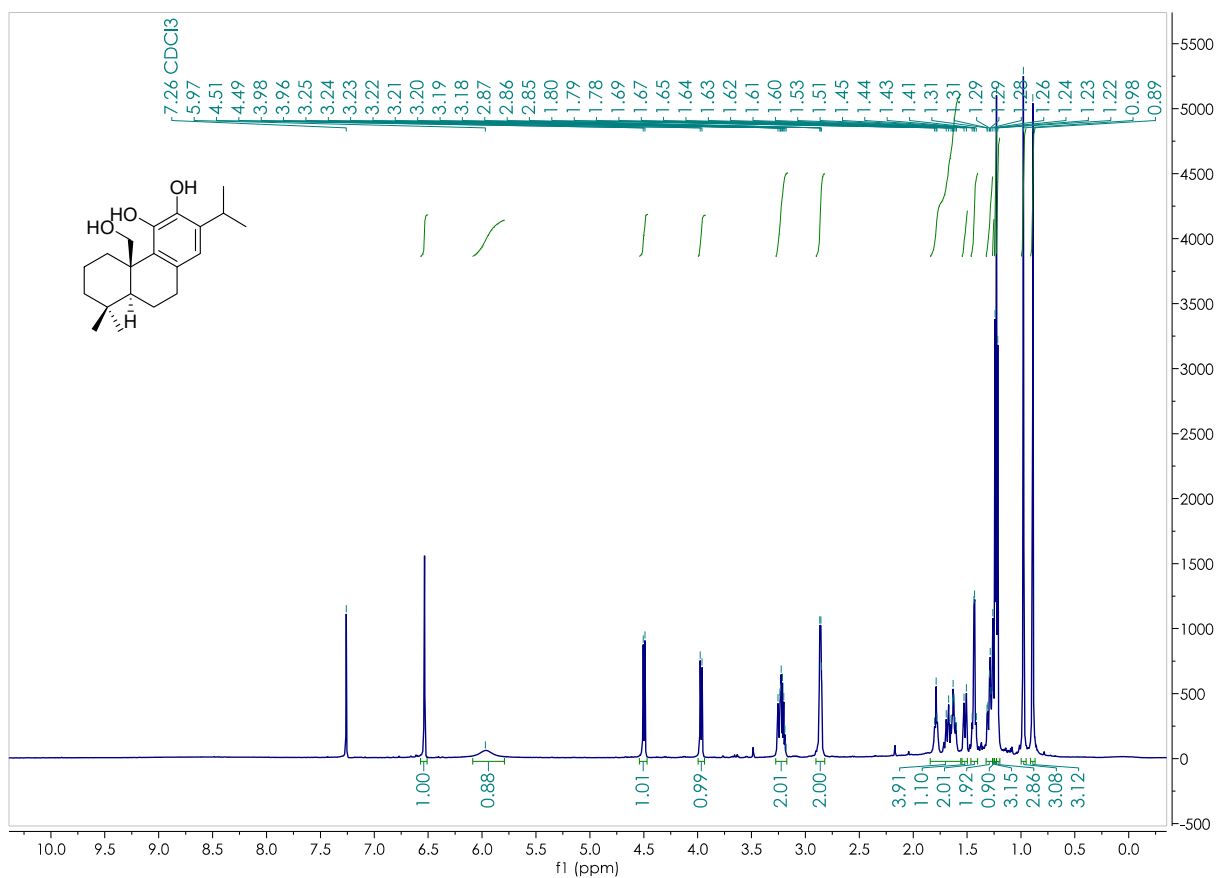
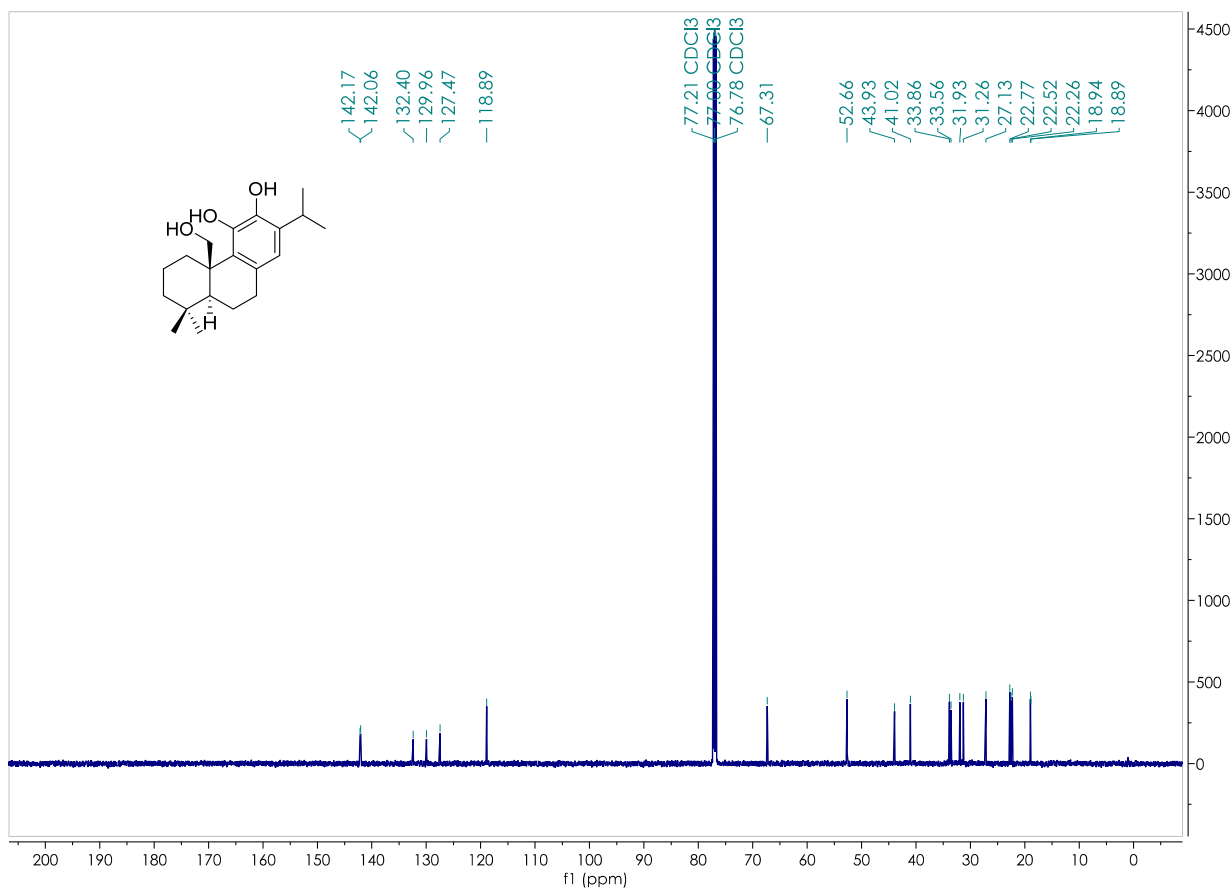
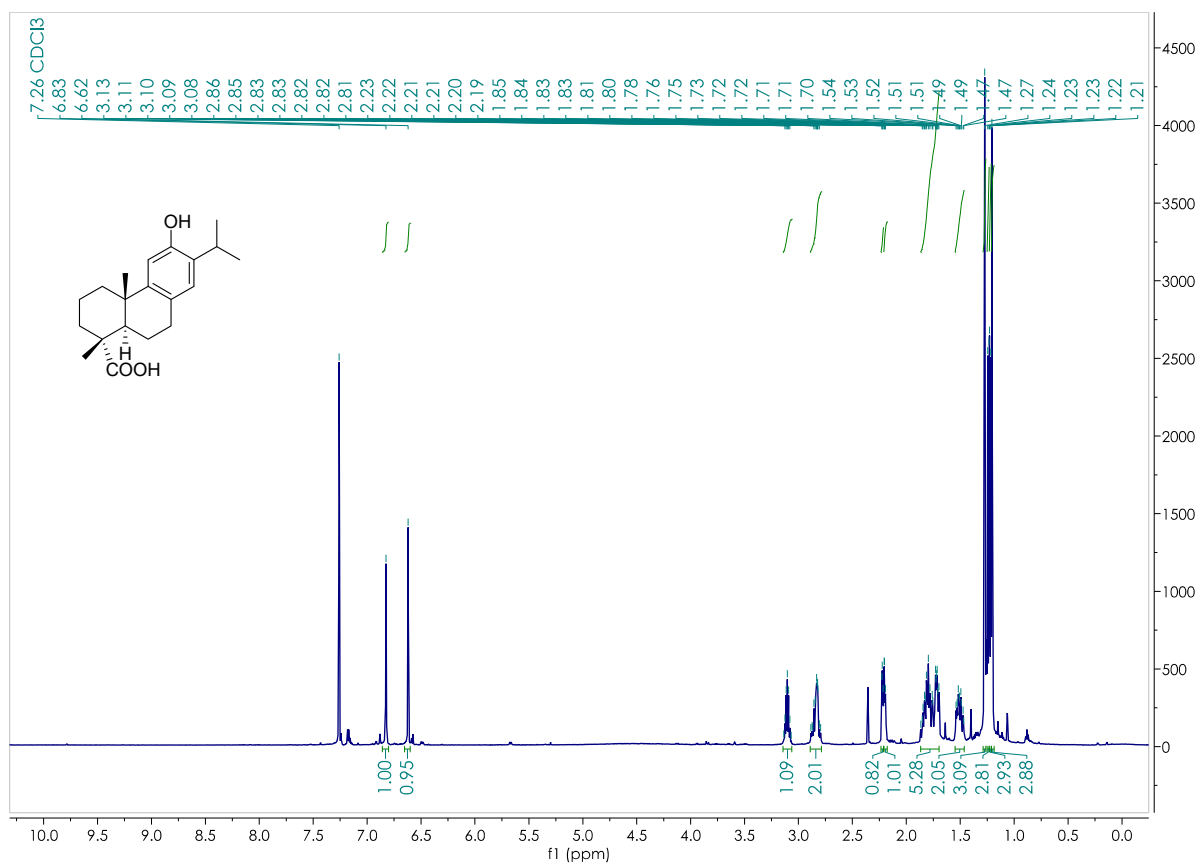
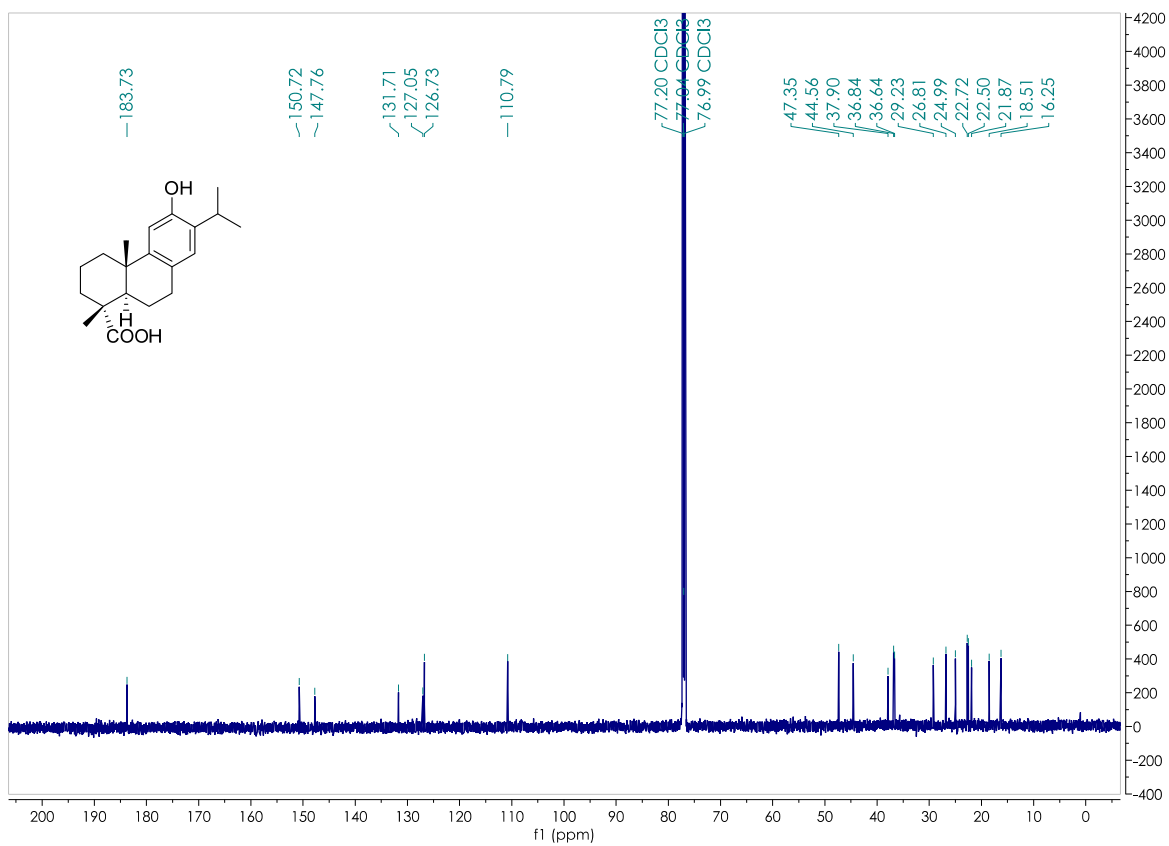
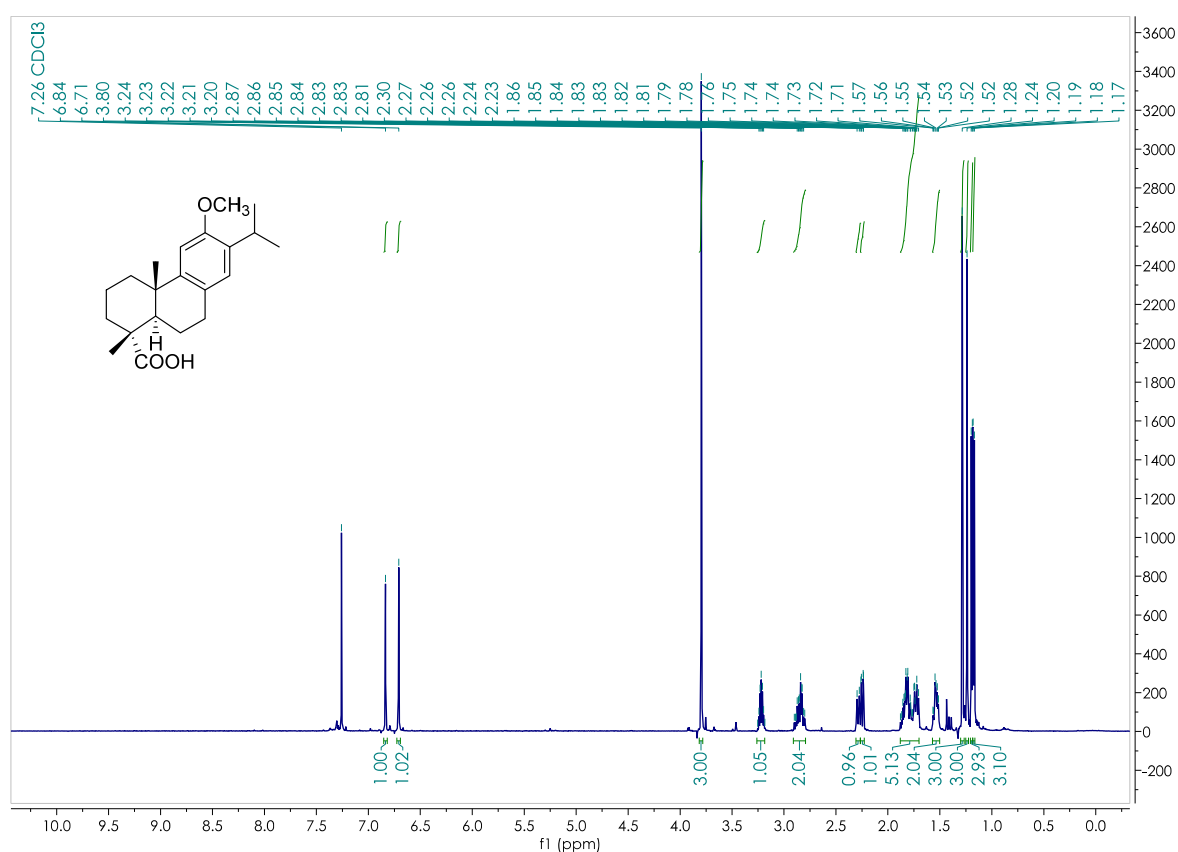
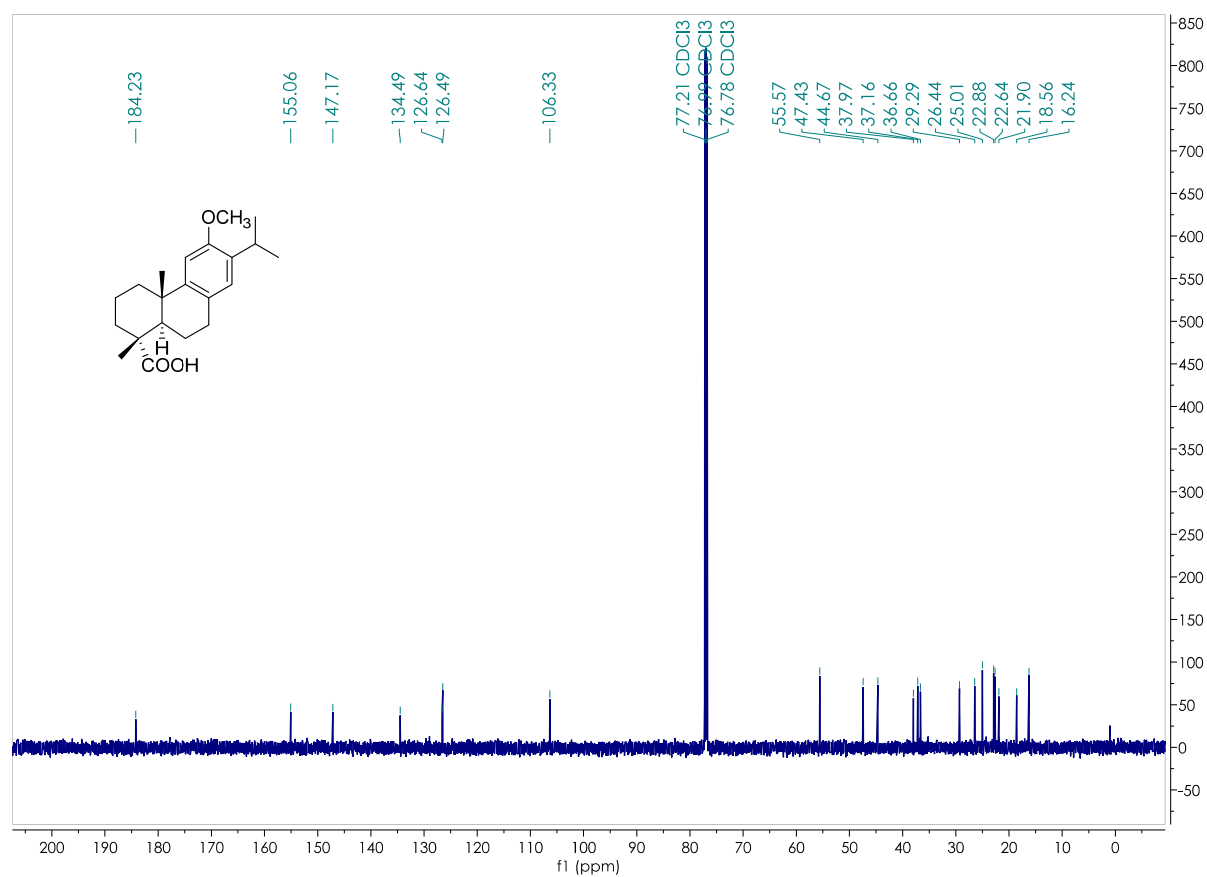


Figure S2. Glide scores per compound and each enzyme analyzed.

NMR spectra data

Figure S3. ¹H-NMR spectrum of compound 5Figure S4. ¹³C-NMR spectrum of compound 5

Figure S5. ¹H-NMR spectrum of compound 9Figure S6. ¹³C-NMR spectrum of compound 9

Figure S7. ¹H-NMR spectrum of compound 10Figure S8. ¹³C-NMR spectrum of compound 10

MS spectra data

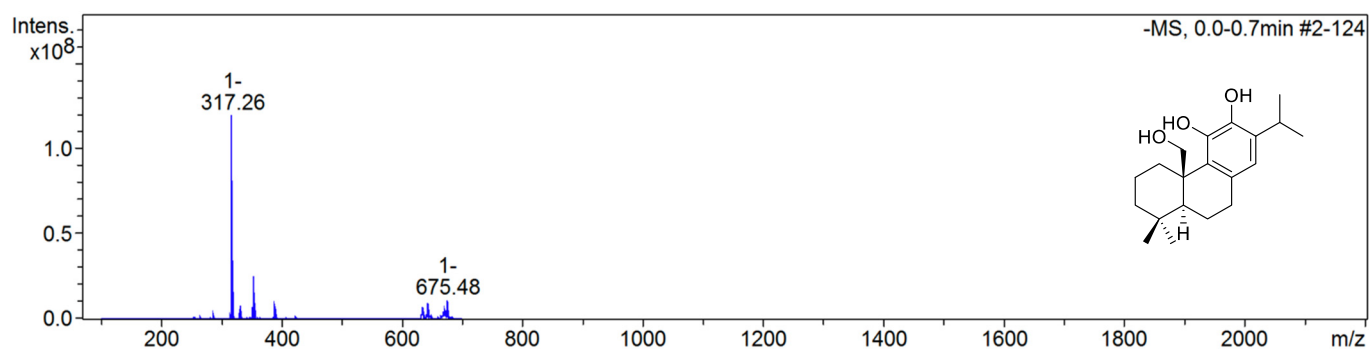


Figure S9. ESI-ITMS spectrum of compound 5

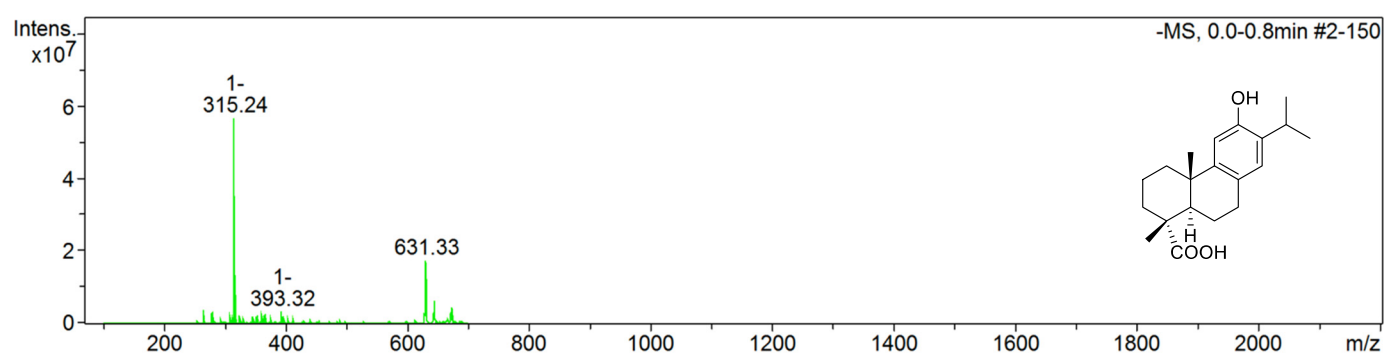


Figure S10. ESI-ITMS spectrum of compound 9

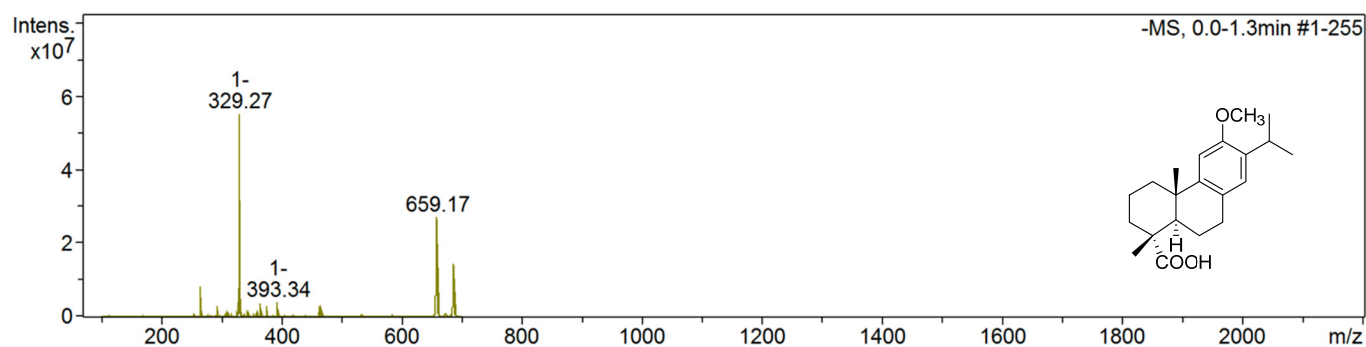


Figure S11. ESI-ITMS spectrum of compound 10