

Supporting Information

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Design, preparation and application of a Pirkle-type chiral stationary phase for enantioseparation of some racemic organic acids and molecular dynamics studies

**Reşit Çakmak, Selami Ercan, Murat Sünkür, Hayrullah Yılmaz,
and Giray Topal**

*Department of Chemistry, Faculty of science and Art, Batman University,
72100, Batman, Türkiye,*

*Department of Nursing, School of Health Science, Batman University,
72060, Batman, Türkiye*

*Department of Chemistry, Faculty of Education, Dicle University,
21280, Diyarbakır, Türkiye*

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Table S1. Chromatographic conditions on the separation column.

Flow rate	0.5 mLmin ⁻¹
Temperature	25 °C
Detection wavelength	220 nm
Mobil phase	0.2 M PBS for each pH
Volume of all test solutions	10 mL
Concentrations of all test solutions	3.0 mgmL ⁻¹ and 5.0 mgmL ⁻¹ 0.2 M PBS
pH of test solutions	6.0, 7.0 and 8.0
Number of fractions	12
Volume of fractions	3.0 mL

Table S2. Chromatographic conditions in the study

Total flow rate	0.8 mLmin ⁻¹
Injection volume	3.0 µL
Temperature	25 °C
Detection wavelength	220 nm
Backpressure	150 bar
Mobil phases composition for MA and 2-PPA	n-Hexane/2-PrOH/TFA ^a (80:18:2 v/v/v)
Analytical column for MA	Chiralpak AD-H
Analytical column for 2-PPA	Chiralpak AD-H
Retention time for MA	15 minutes
Retention time for 2-PPA	12 minutes

^a 5 % TFA solution in 2-propanol

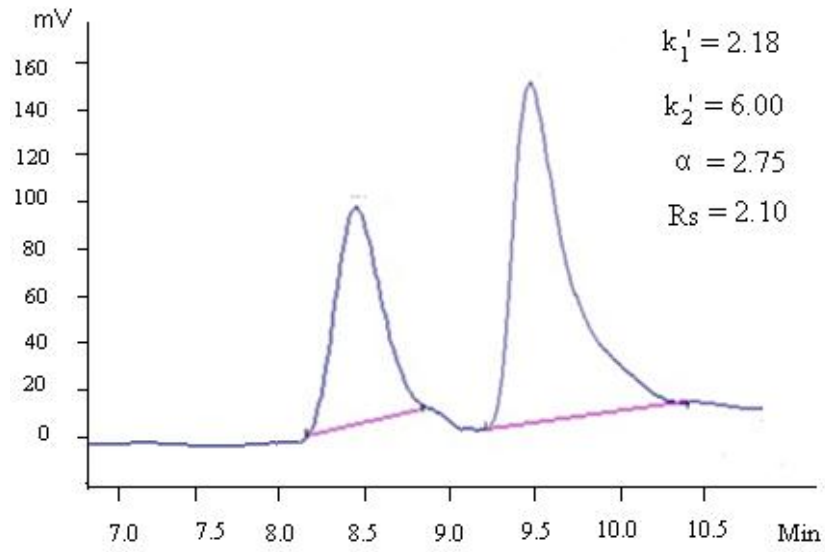


Figure S1. The chromatogram for 9th fraction at pH 6

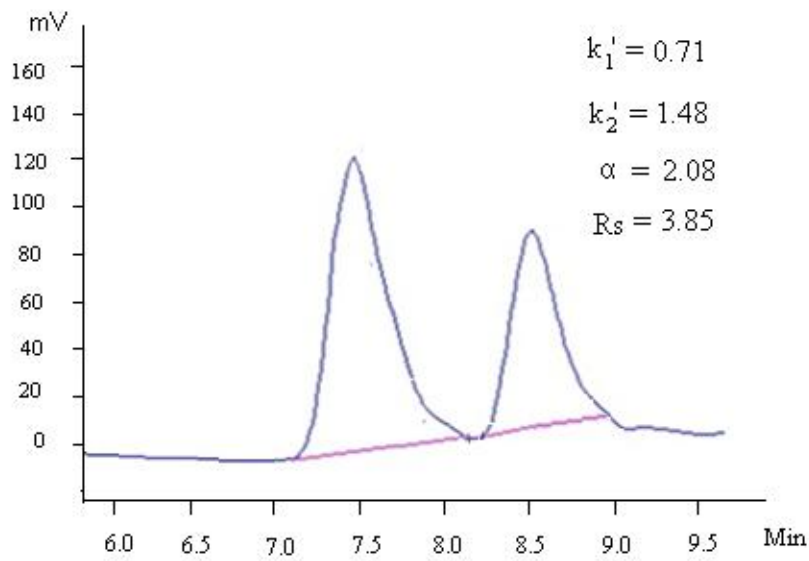


Figure S2. The chromatogram for 10th fraction at different pH 8

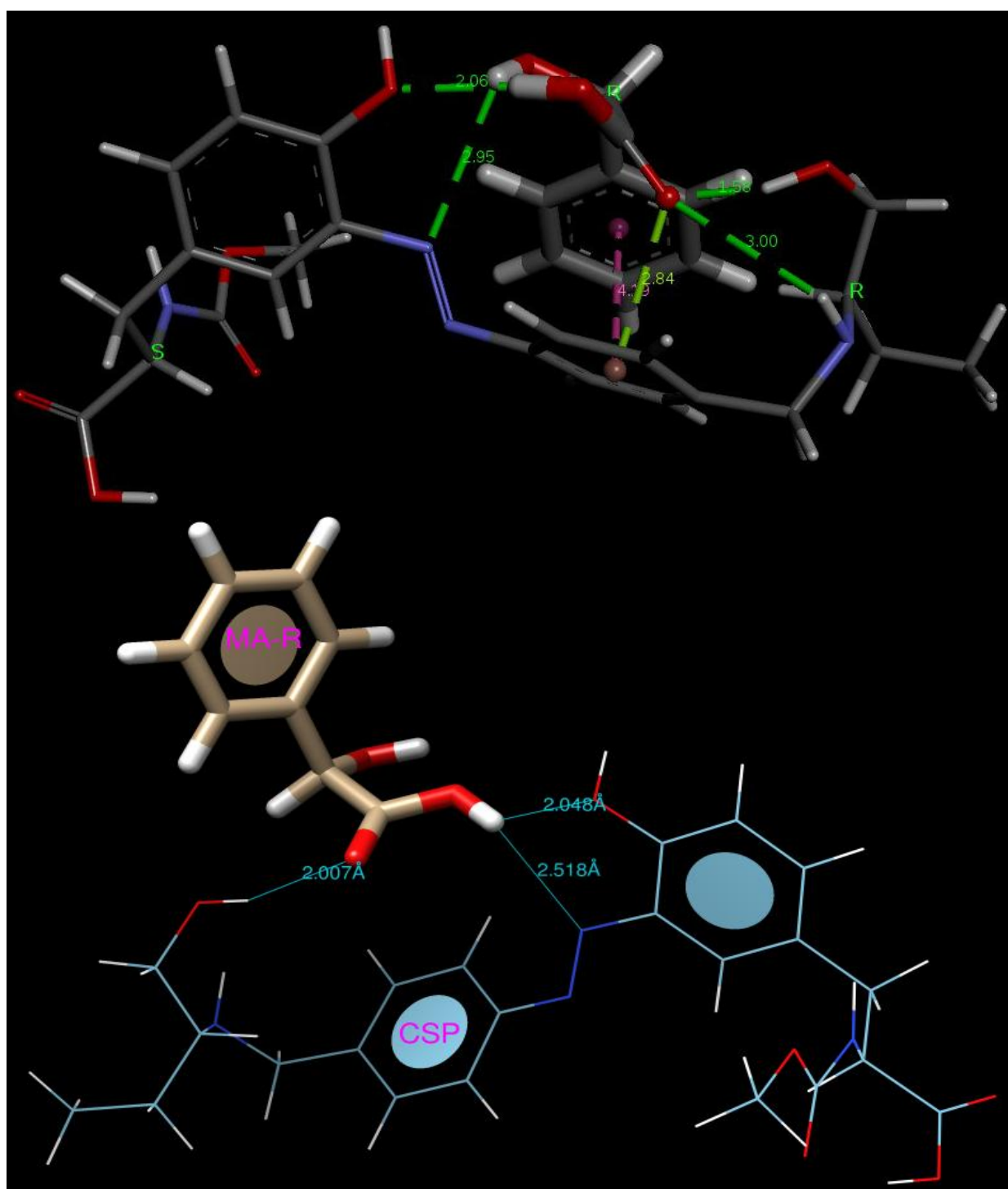


Figure S3. Integration of MA-R with CSP from docking (upper) and from quantum mechanical calculations (lower), ($E(\text{RB3LYP})=-2060,965432$ Hartree)

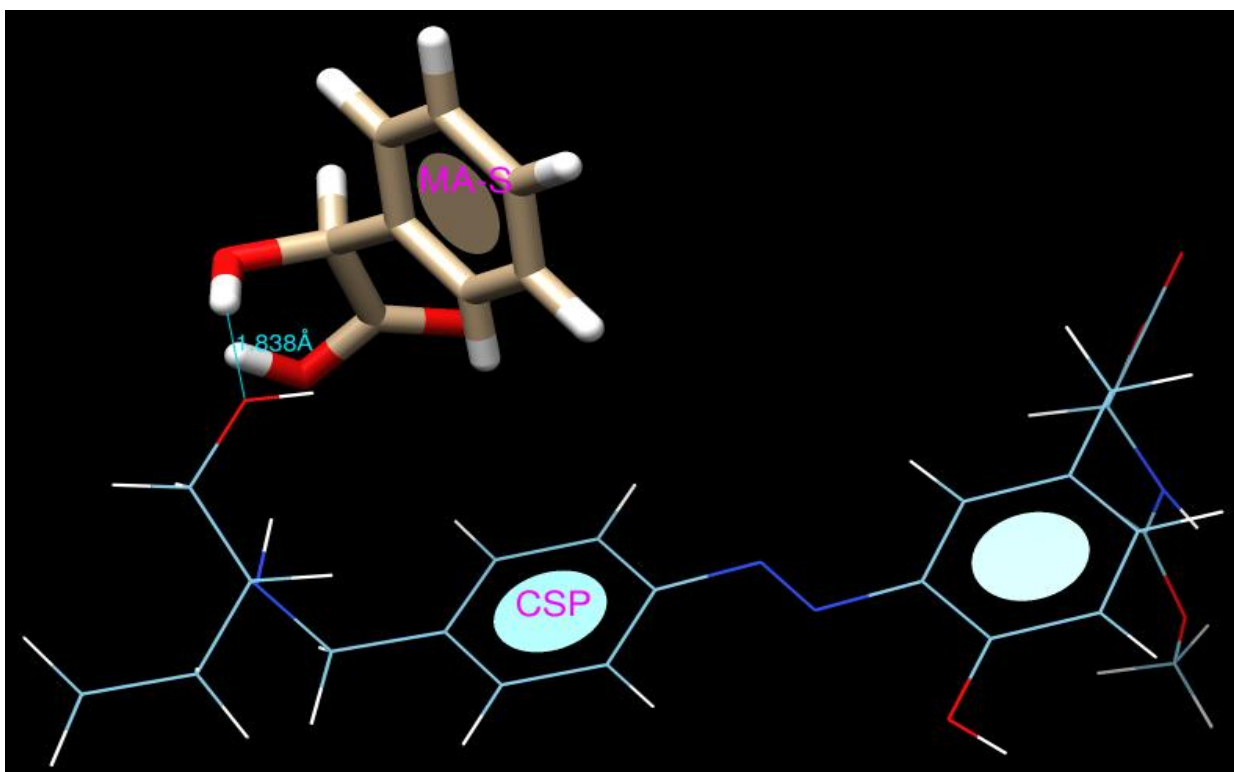
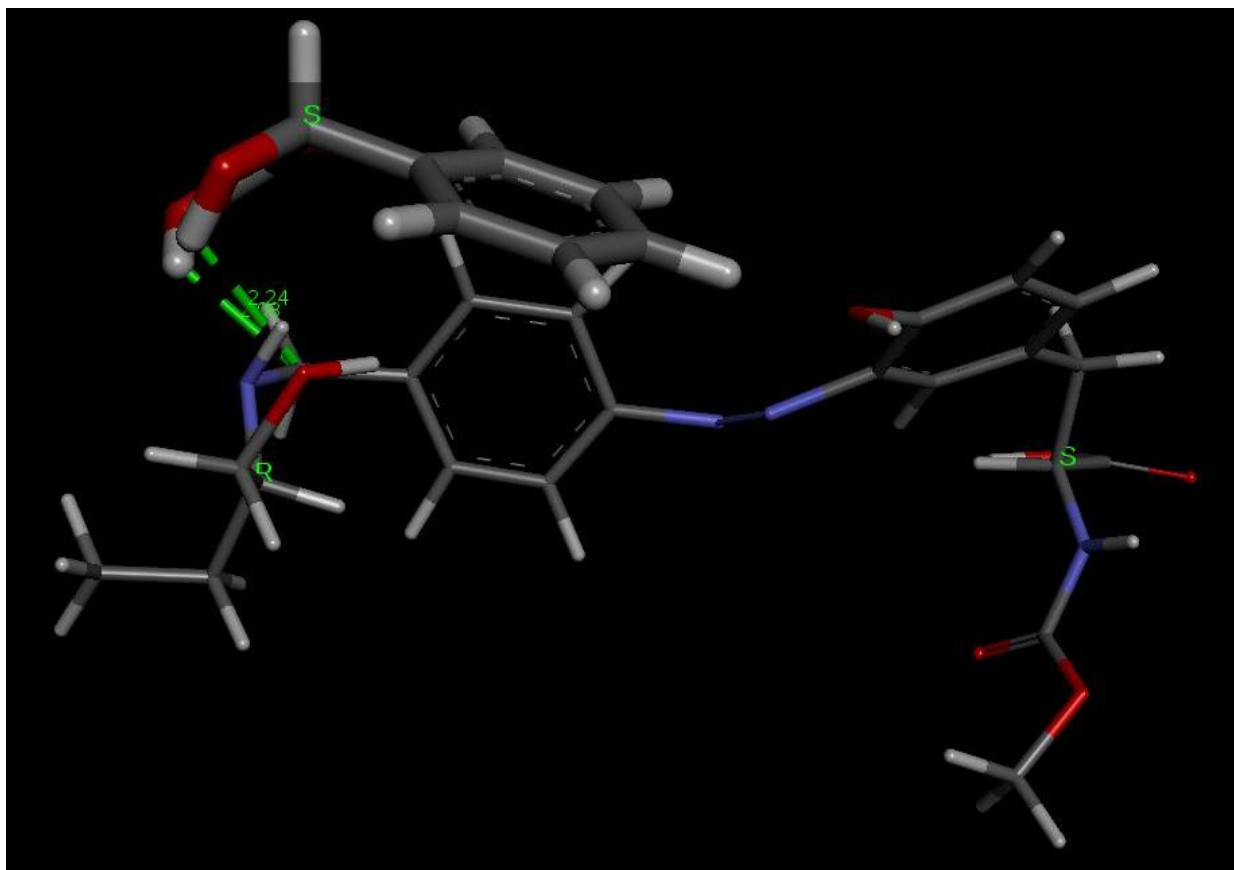


Figure S4. Integration of MA-S with CSP from docking (upper) and from quantum mechanical calculations (lower), ($E(\text{RB3LYP}) = -2060,9615805$ Hartree)

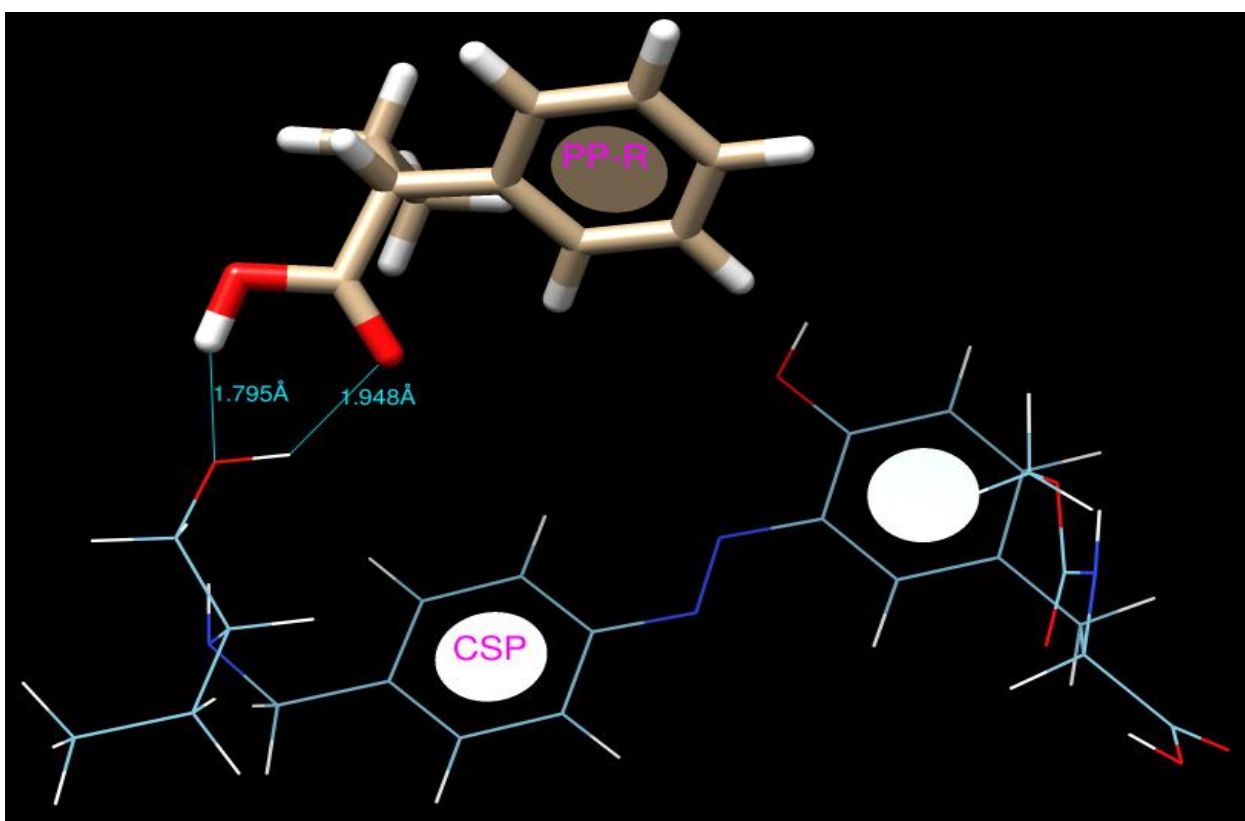
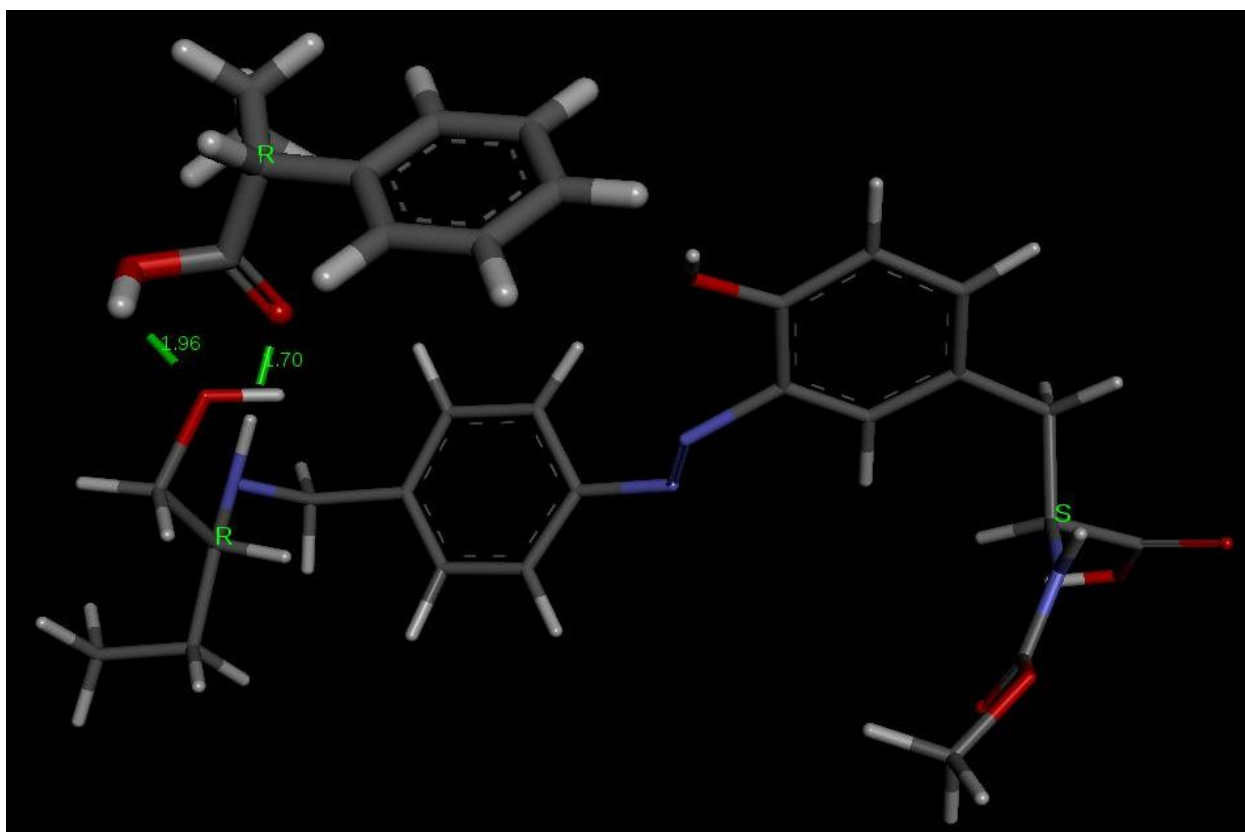


Figure S5. Integration of PP-R with CSP from docking (upper) and from quantum mechanical calculations (lower), ($E(\text{RB3LYP}) = -2064,3802923$ Hartree)

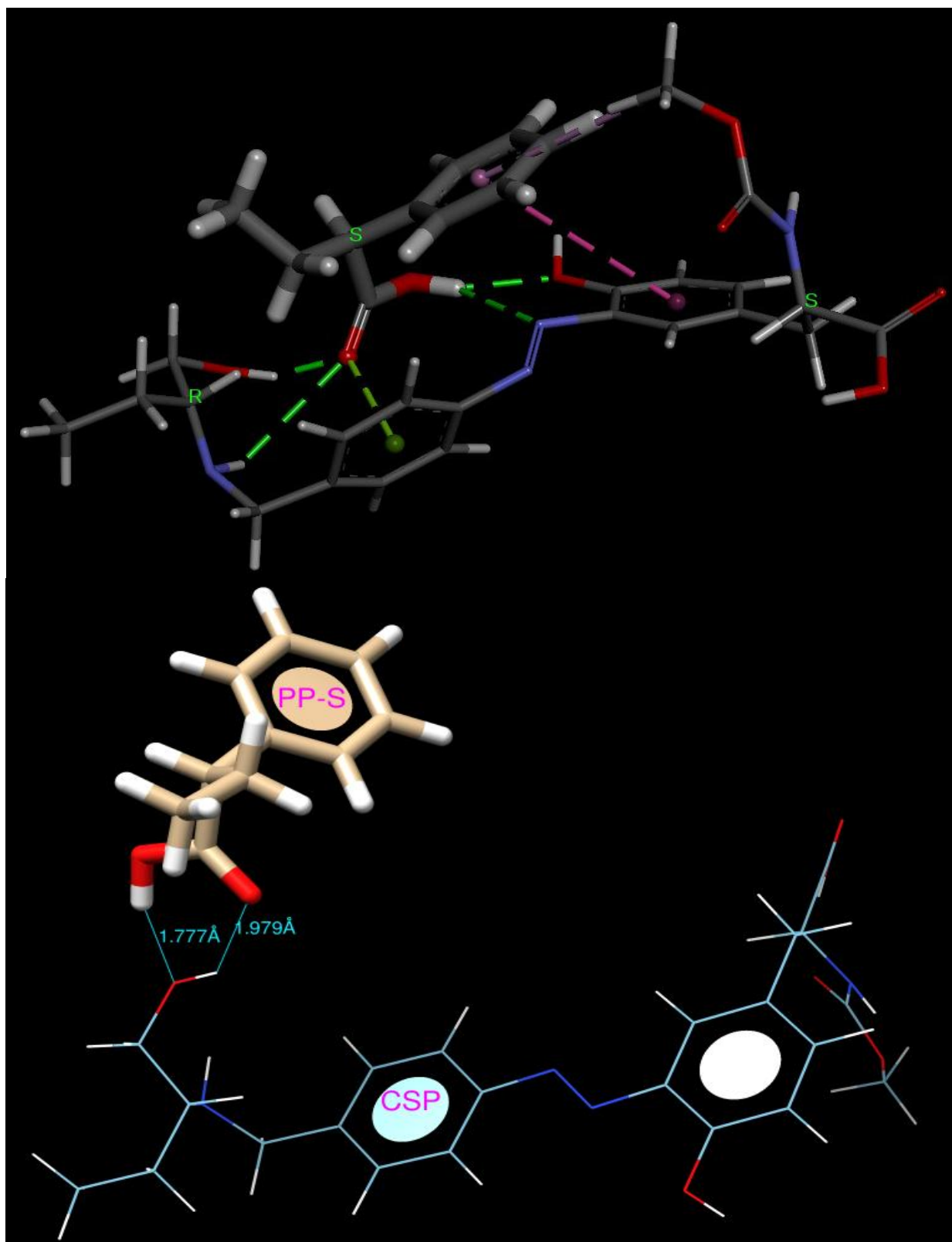


Figure S6. Integration of PP-S with CSP from docking (upper) and from quantum mechanical calculations (lower), ($E(\text{RB3LYP}) = -2064,3845521$ Hartree)

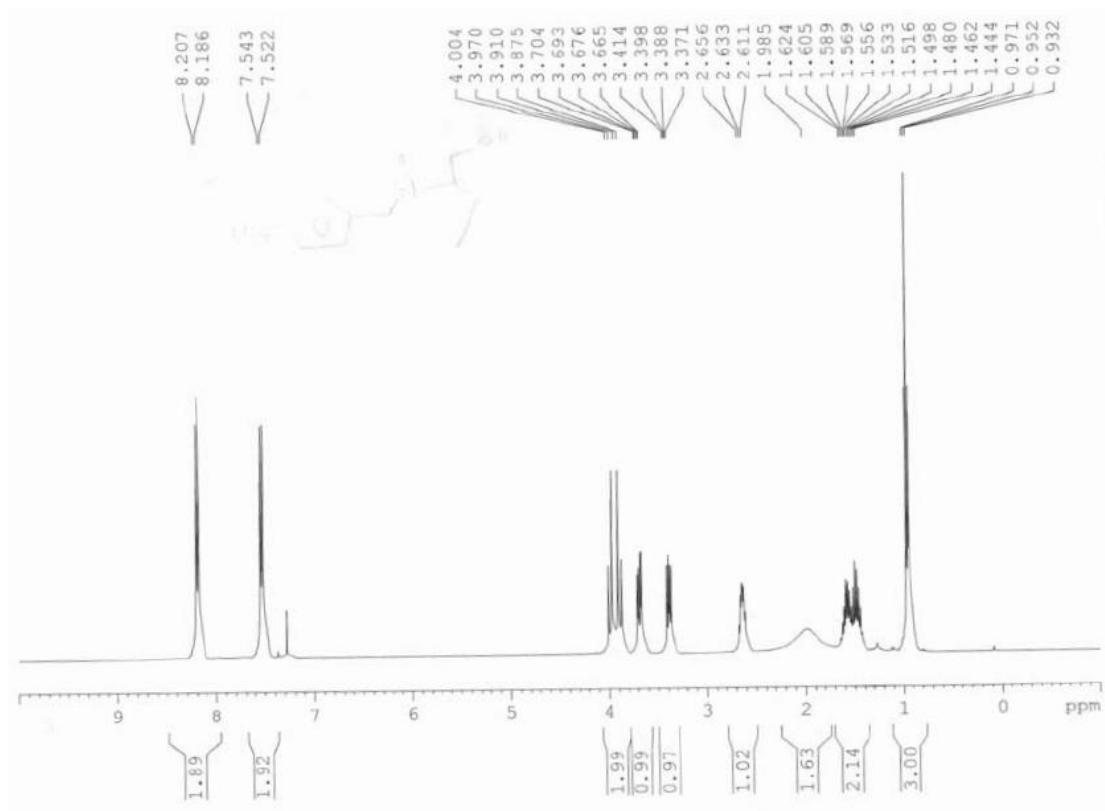


Figure 7a. NMR spectrum (CDCl₃; 400MHz) of compound (3)

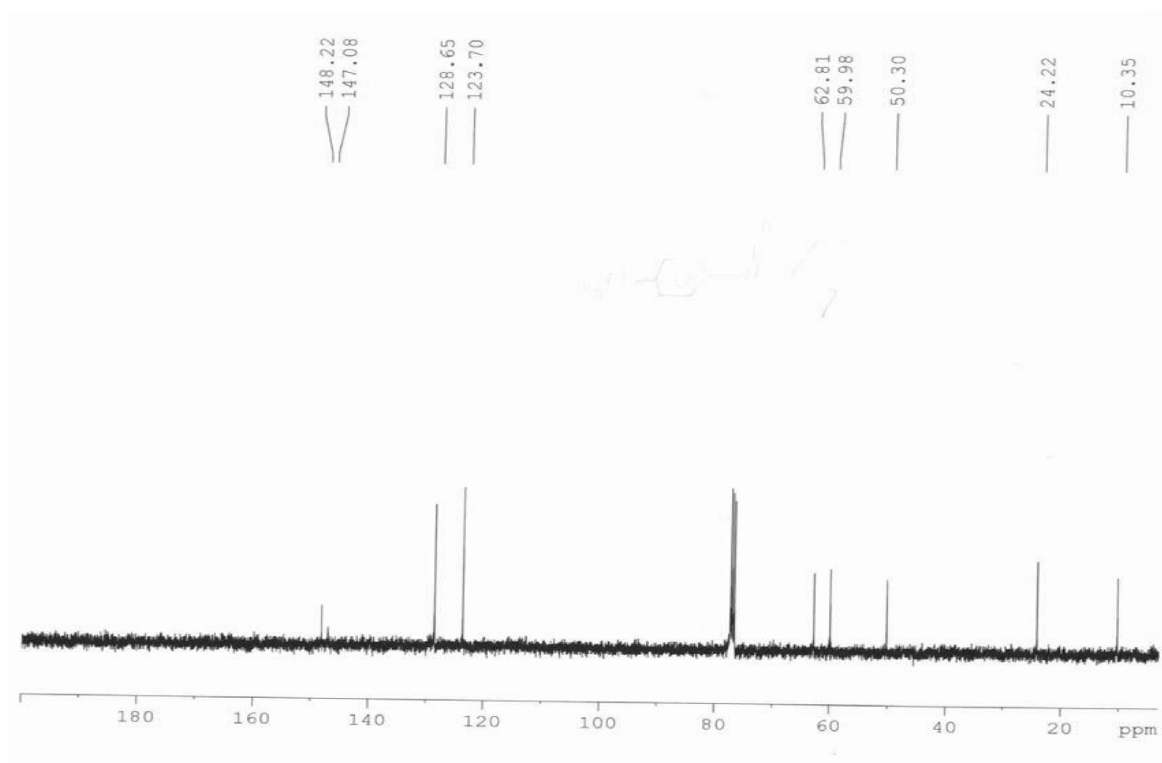


Figure 7b. ¹³C NMR spectrum (CDCl₃; 100MHz) of compound (3)

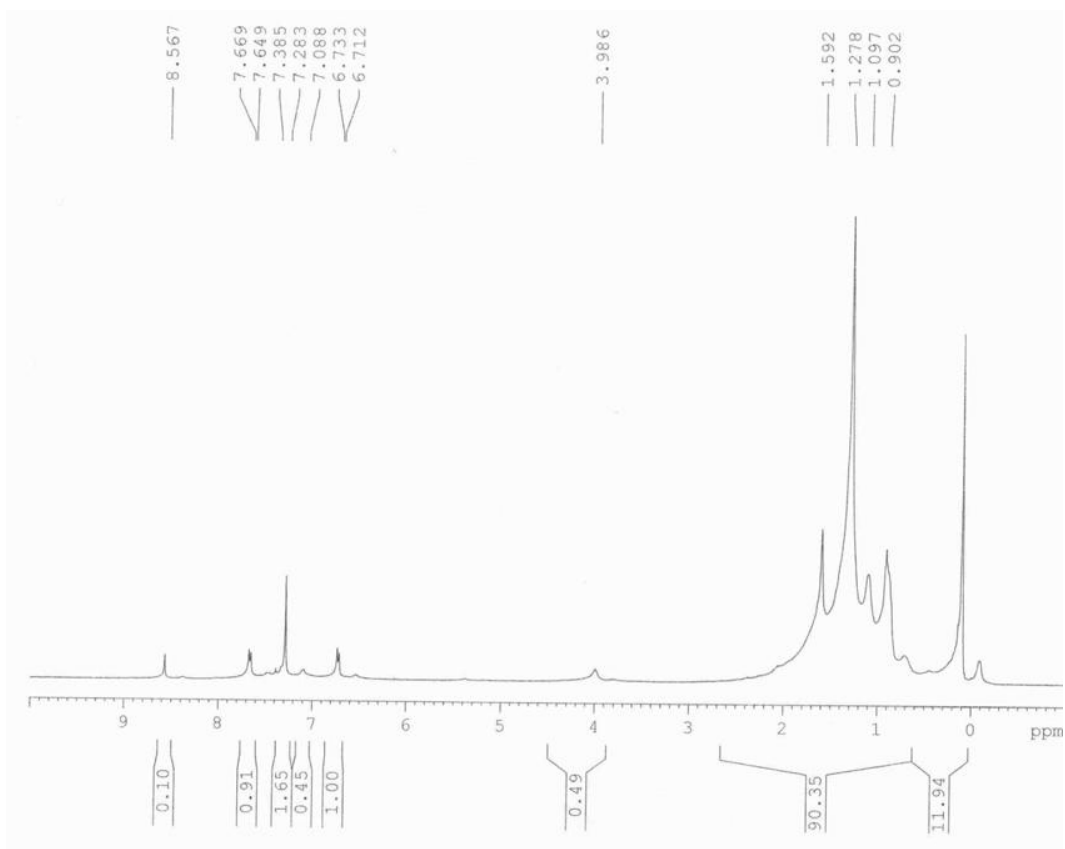


Figure 8a. ^1H NMR spectrum (CDCl_3 ; 400MHz) of compound (4)

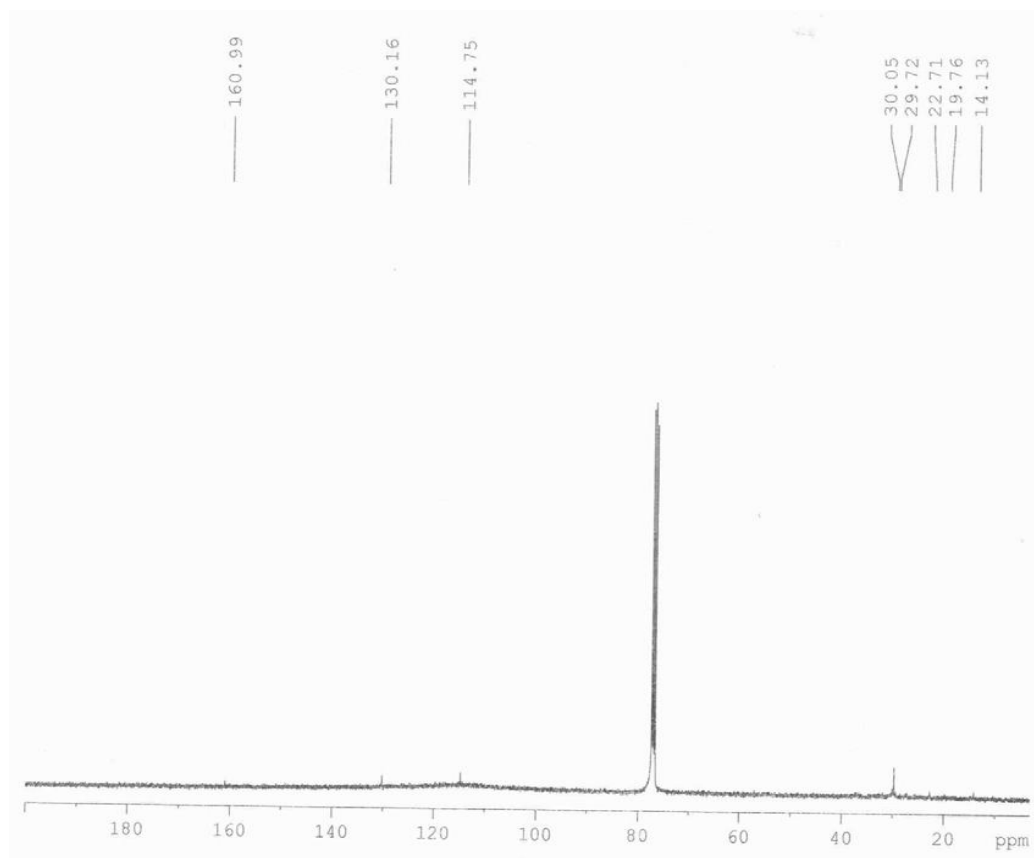


Figure 8b. ^{13}C NMR spectrum (CDCl_3 ; 100MHz) of compound (4)