

Fig. S1 ^1H -NMR spectrum of 14-6-14, 2Br^- in D_2O at 298.2K.

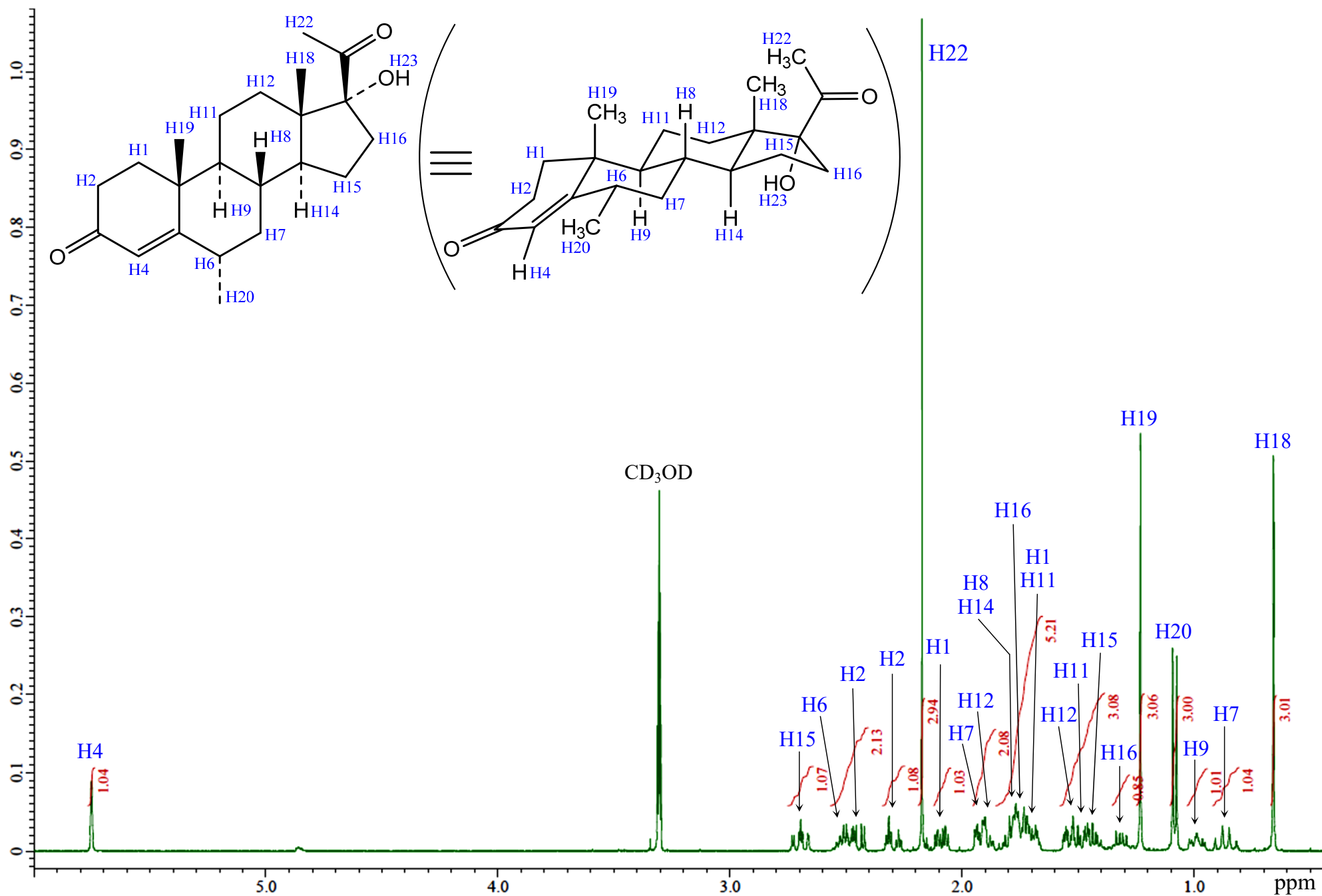


Fig. S2 ^1H -NMR spectrum of MP in CD_3OD at 298.2K.

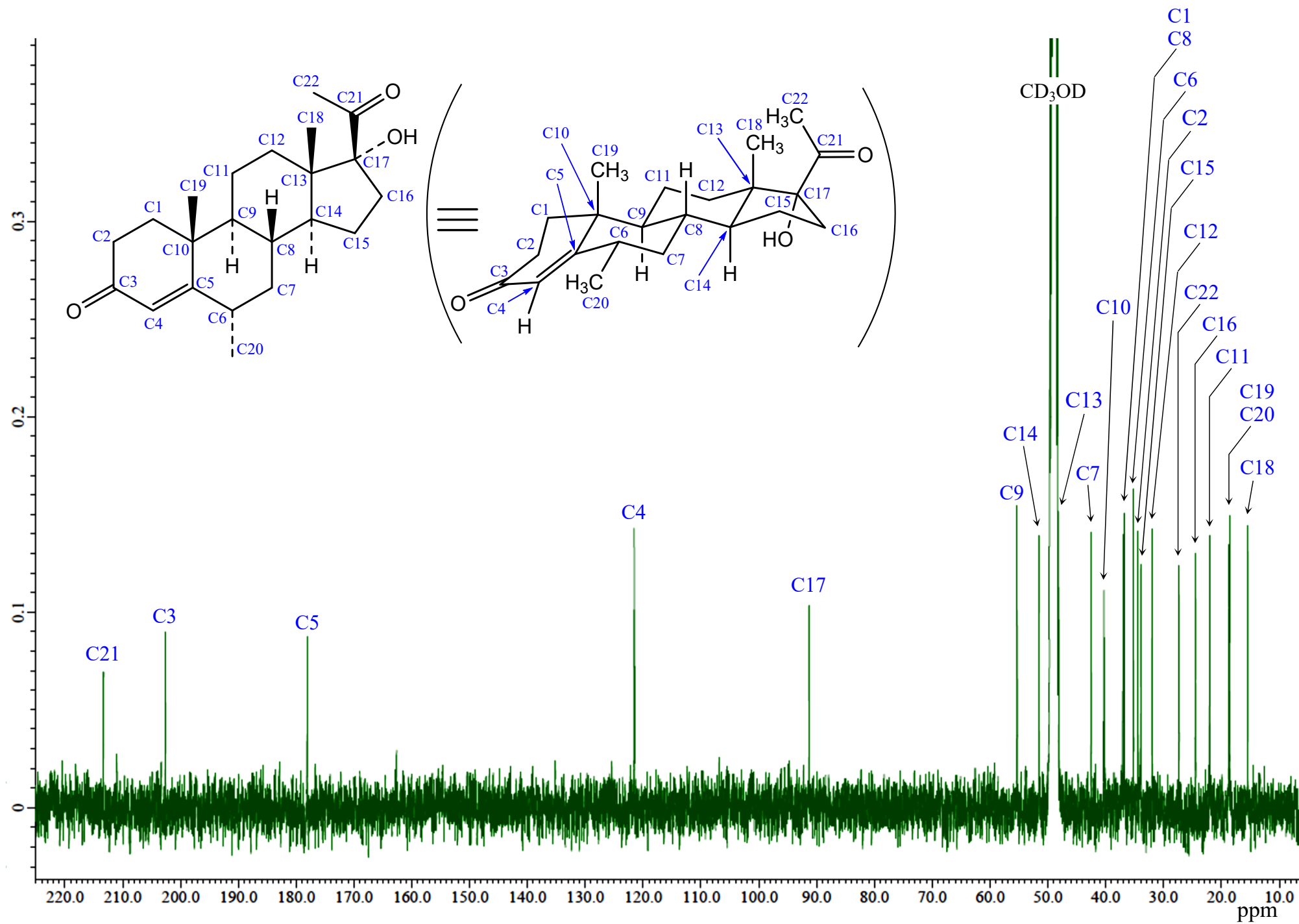


Fig. S3 ^{13}C -NMR spectrum of MP in CD_3OD at 298.2K.

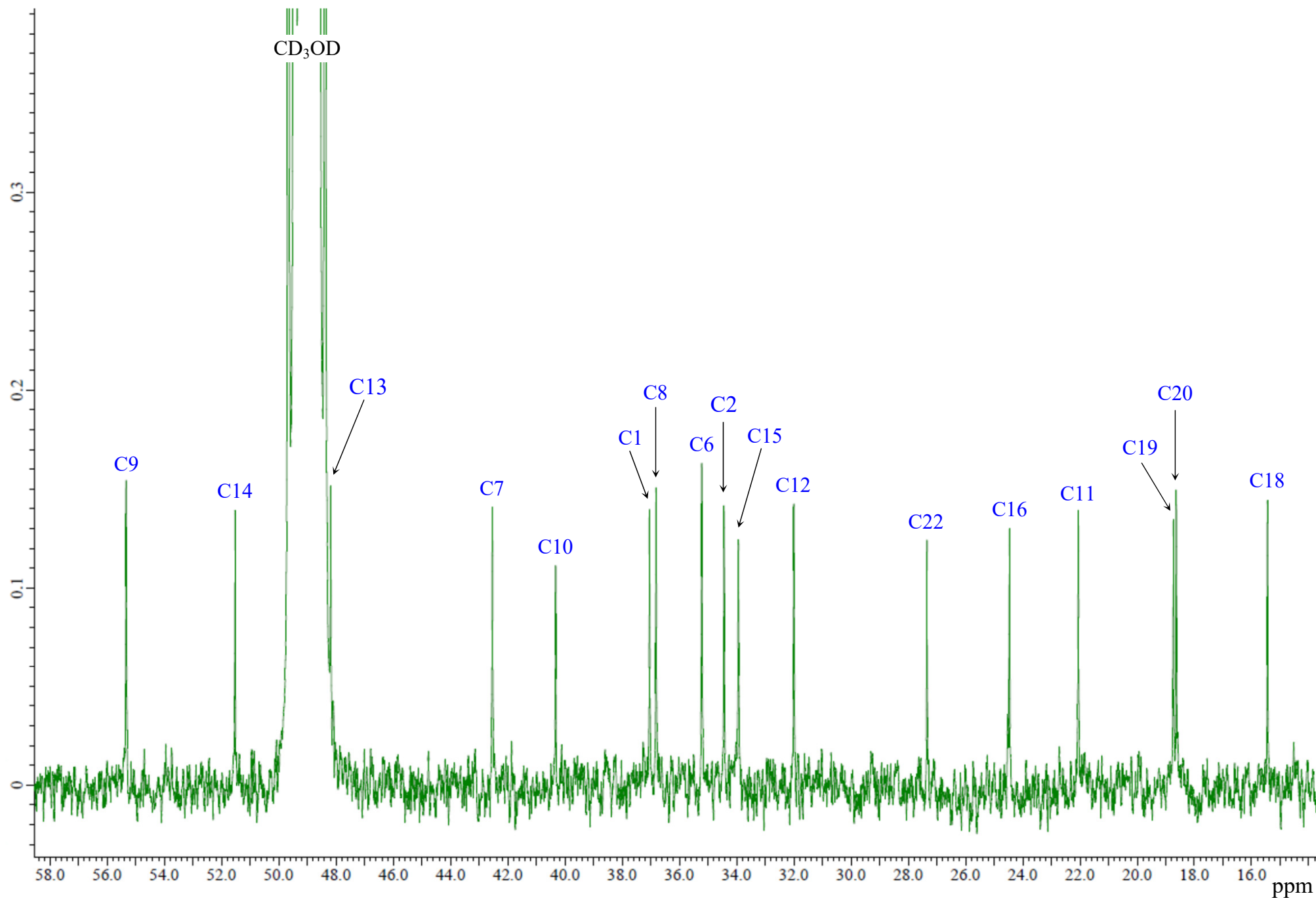


Fig. S4 ^{13}C -NMR spectrum of MP in CD_3OD at 298.2K, ranging from 14.8 to 58.6 ppm.

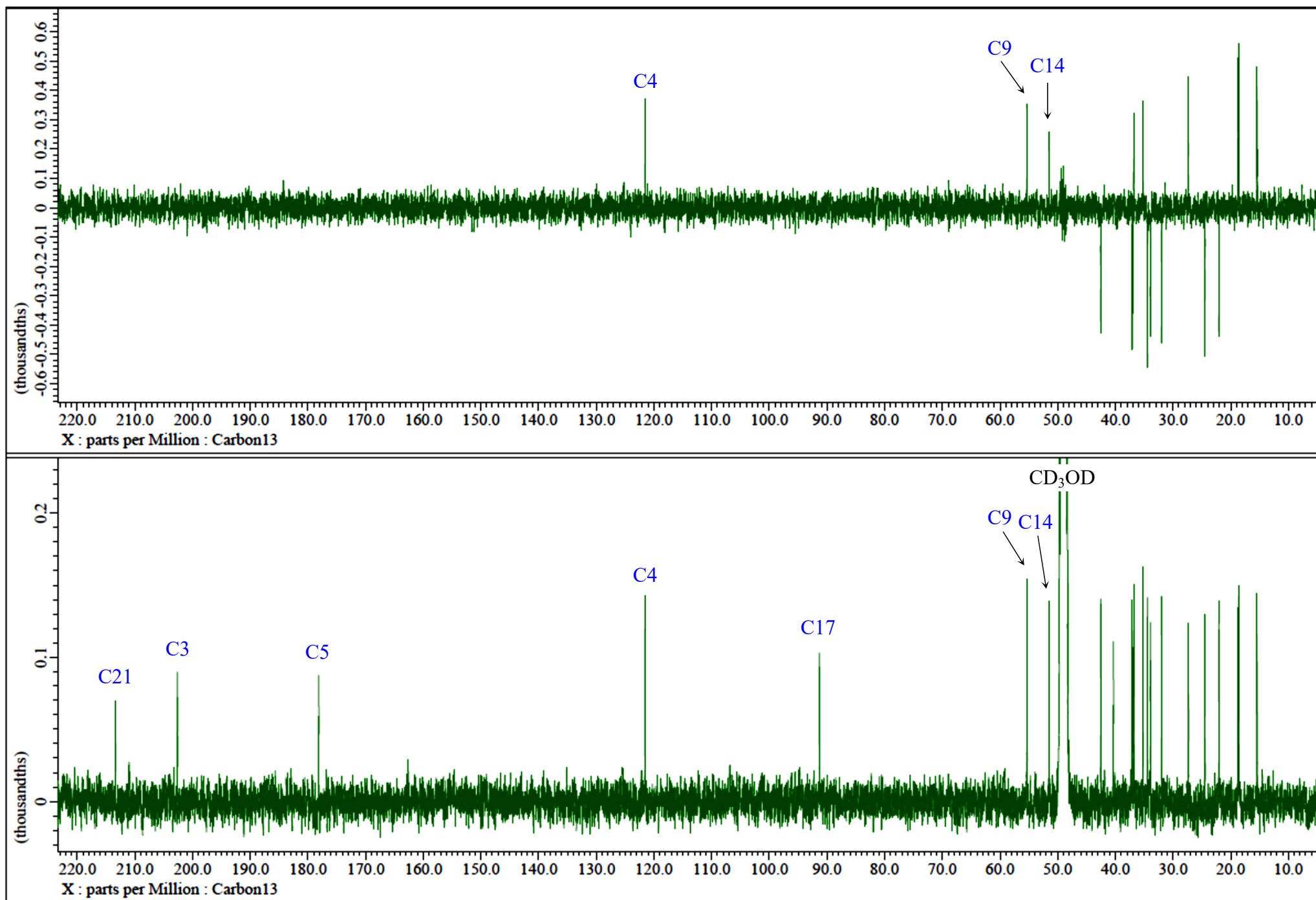


Fig. S5 DEPT135 (top) and ¹³C-NMR (bottom) spectra of MP in CD₃OD at 298.2K, ranging from 4 to 224 ppm, highlighting the differentiation of CH, CH₂, and CH₃ carbon types.

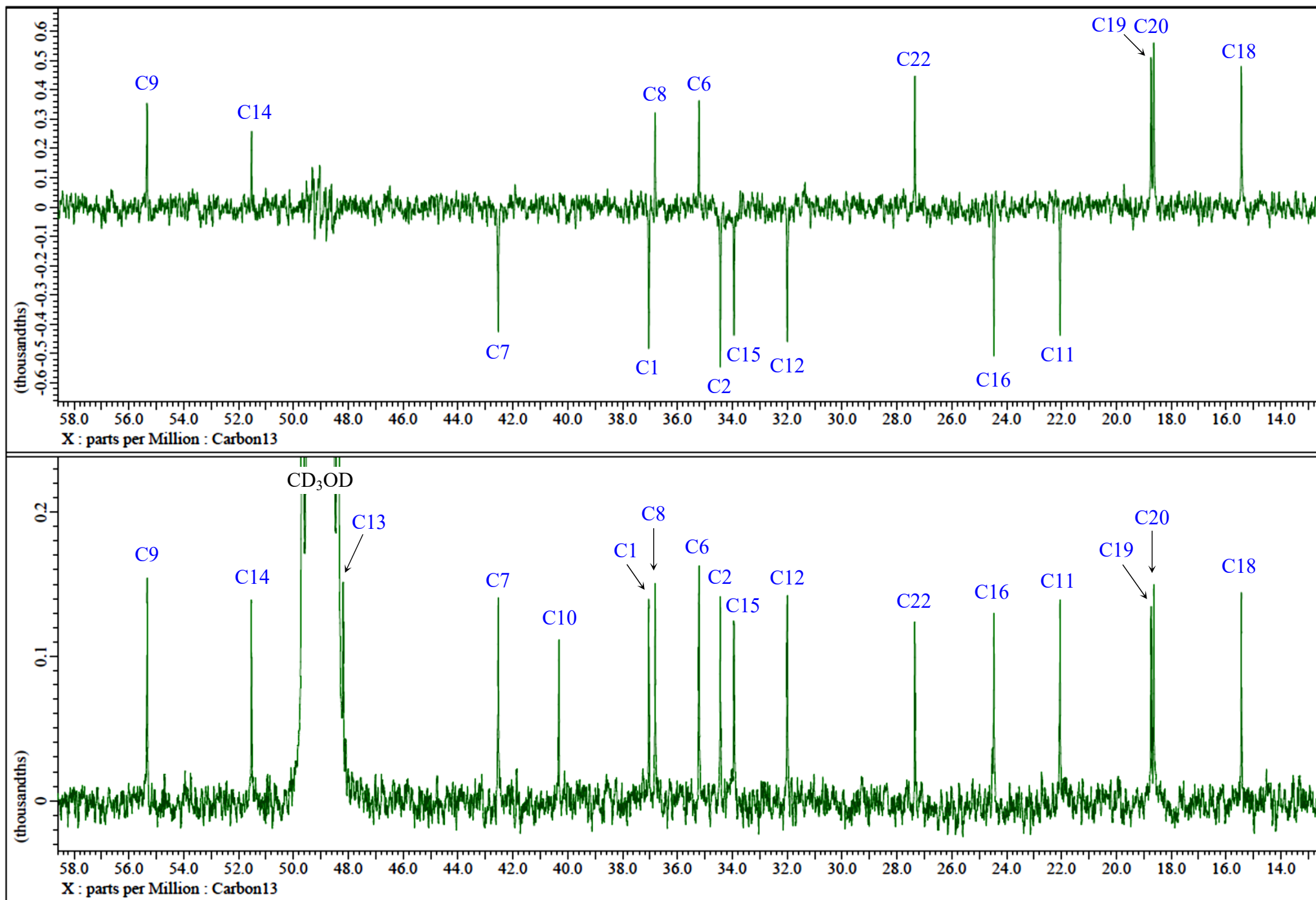


Fig. S6 DEPT135 (top) and ¹³C-NMR (bottom) spectra of MP in CD₃OD at 298.2K, ranging from 12.6 to 58.6 ppm, highlighting the differentiation of CH, CH₂, and CH₃ carbon types.

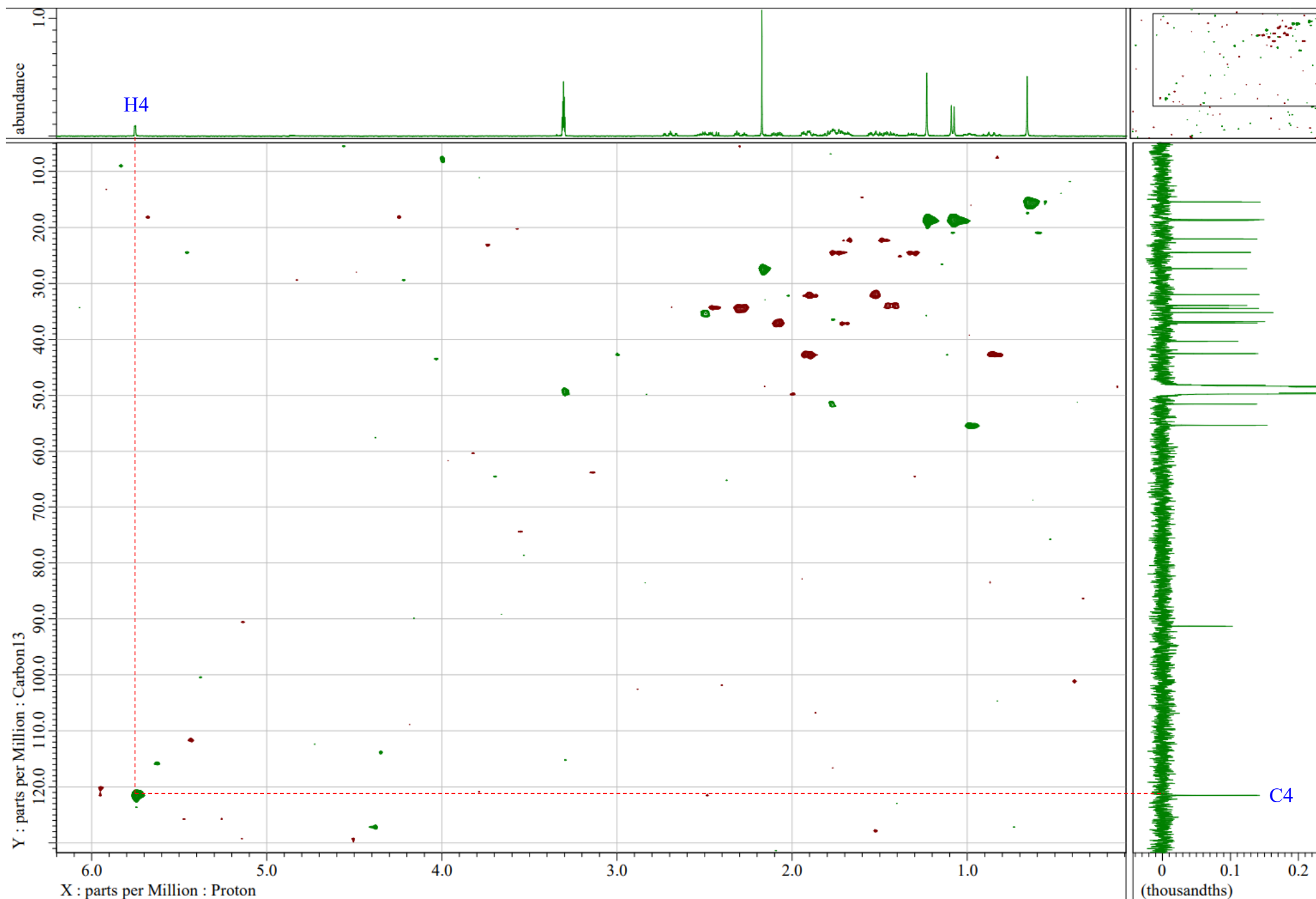


Fig. S7 Correlation signals between ^1H (0.1 to 6.2 ppm) and ^{13}C (5 to 132 ppm) in ^1H - ^{13}C HSQC spectrum of MP in CD_3OD at 298.2K.

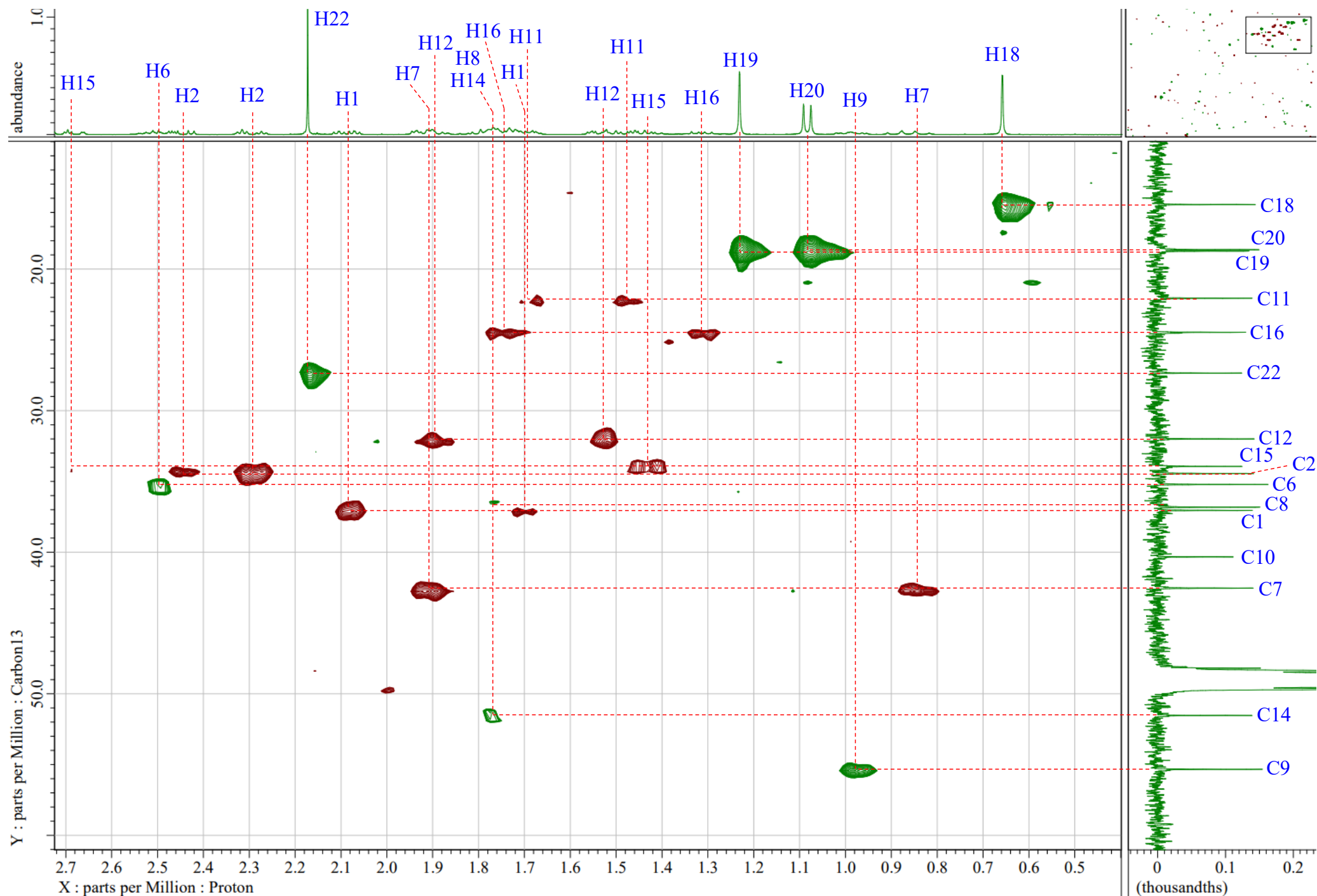


Fig. S8 Correlation signals between ^1H (0.4 to 2.72 ppm) and ^{13}C (11 to 61 ppm) in ^1H - ^{13}C HSQC spectrum of MP in CD_3OD at 298.2K.

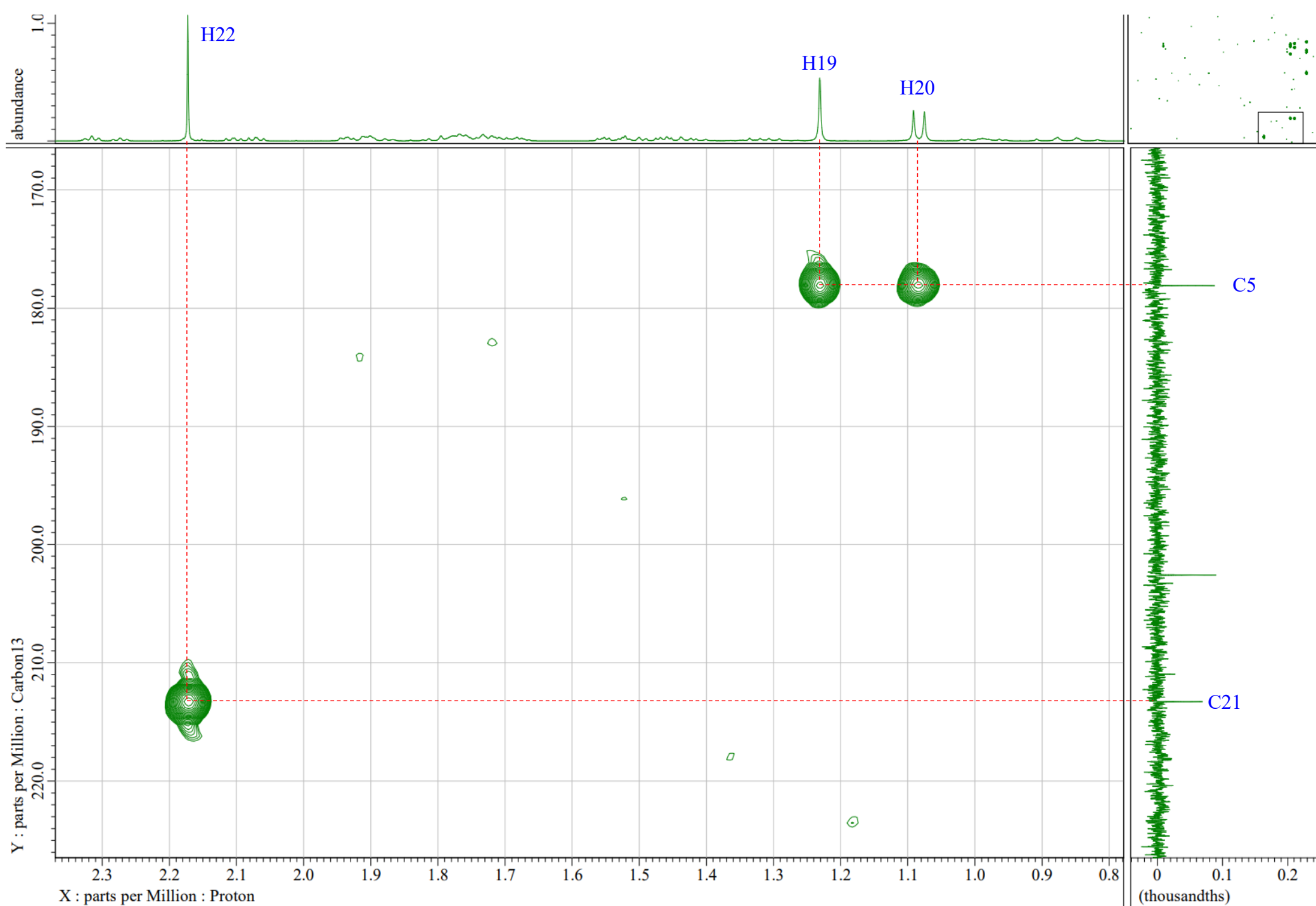


Fig. S9 Correlation signals between ^1H (0.78 to 2.37 ppm) and ^{13}C (167 to 226 ppm) in ^1H - ^{13}C HMBC spectrum of MP in CD_3OD at 298.2K.

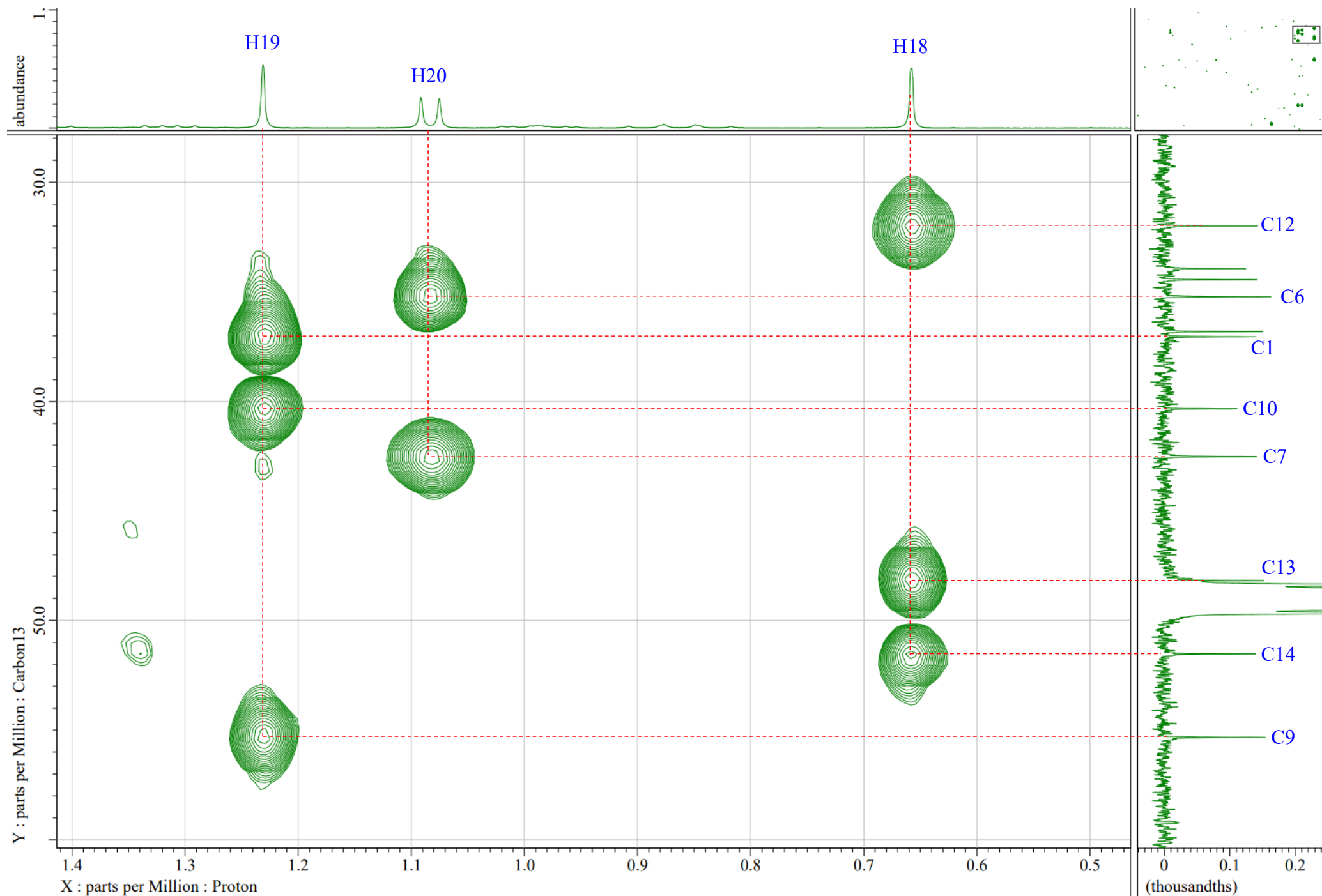


Fig. S10 Correlation signals between ^1H (0.46 to 1.41 ppm) and ^{13}C (28 to 60 ppm) in ^1H - ^{13}C HMBC spectrum of MP in CD_3OD at 298.2K.

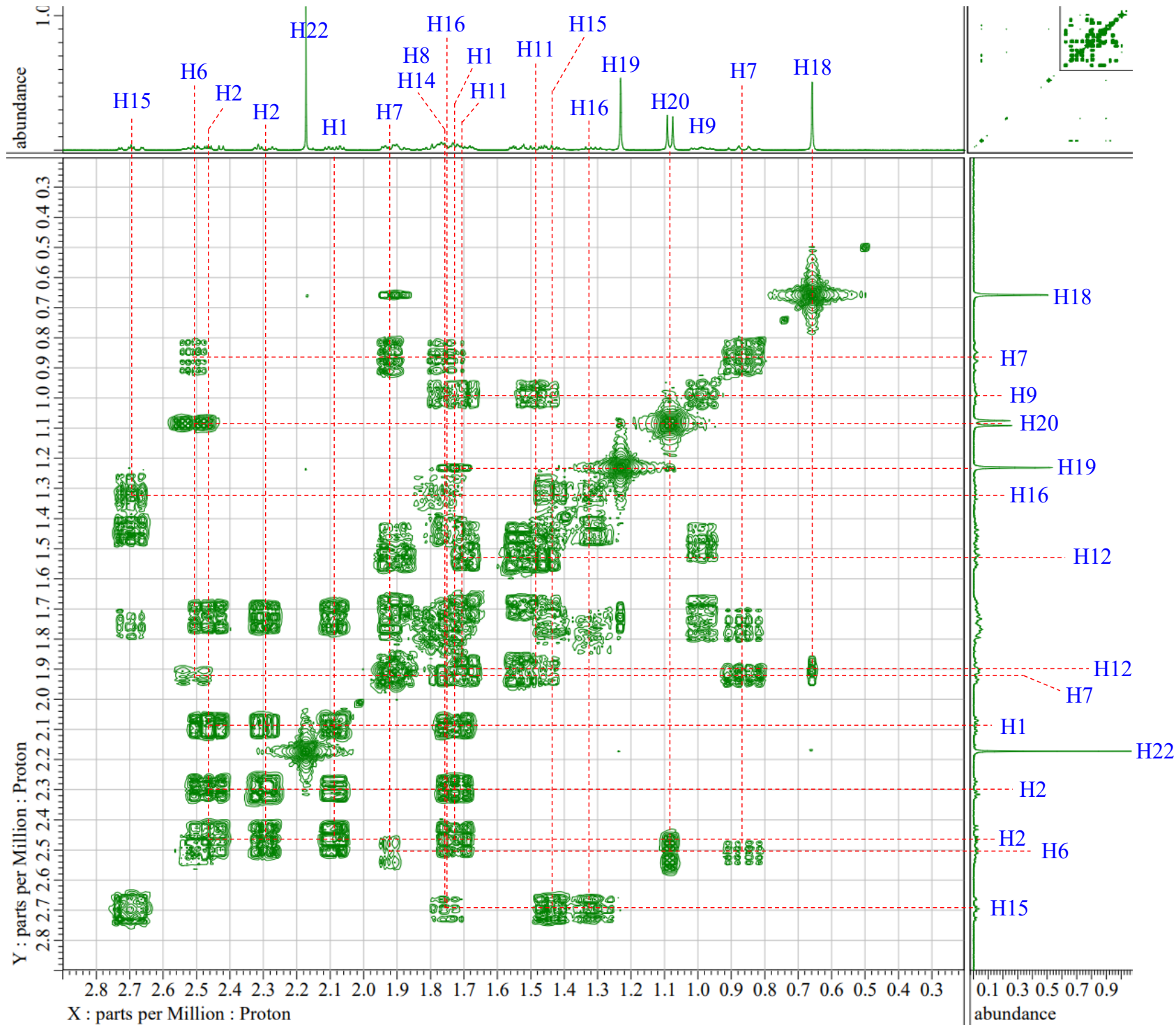


Fig. S11 Correlation signals between ^1H (0.2 to 2.9 ppm) and ^1H (0.2 to 2.9 ppm) in ^1H - ^1H COSY spectrum of MP in CD_3OD at 298.2K.

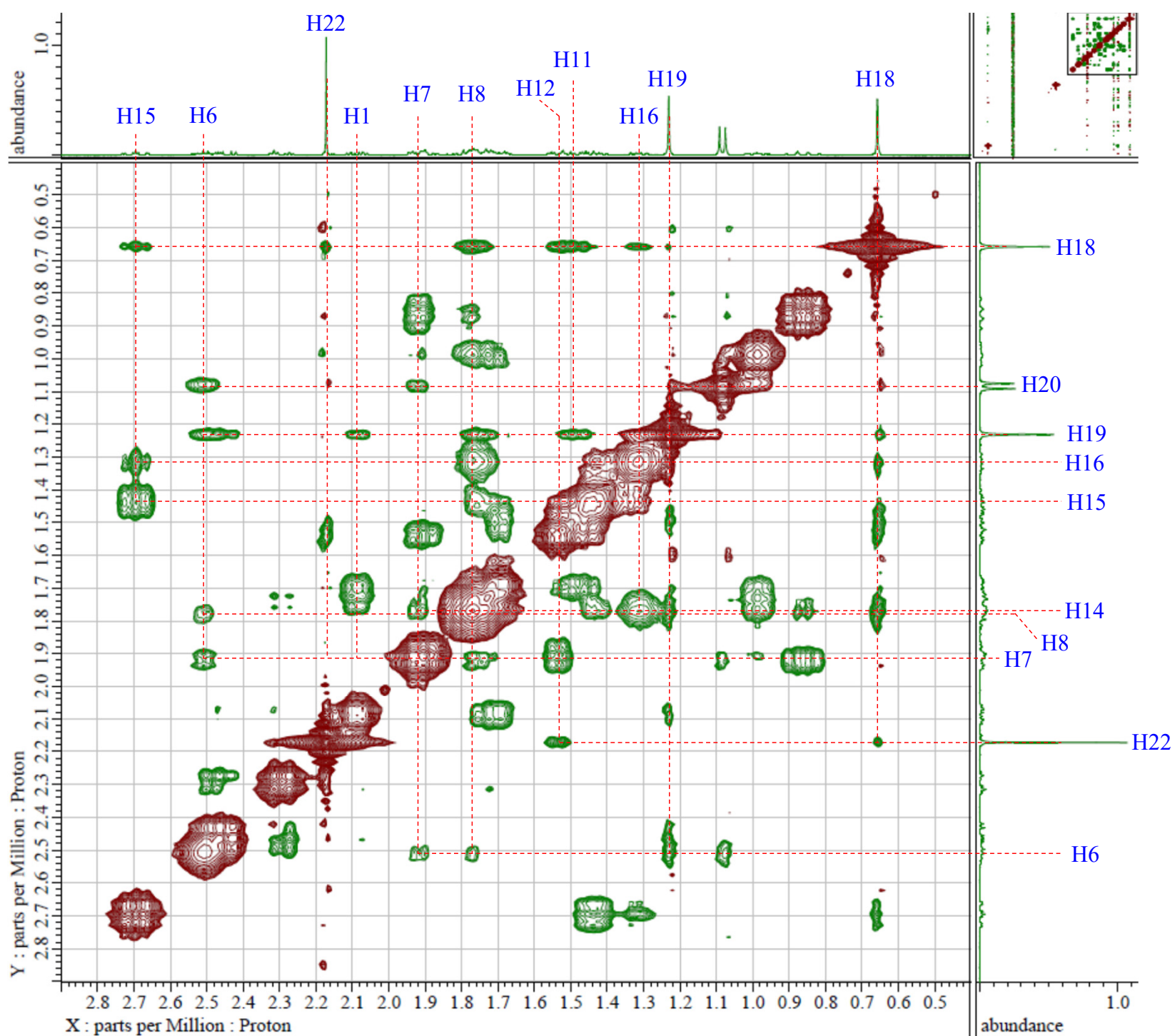


Fig. S12 Correlation signals between ^1H (0.4 to 2.9 ppm) and ^1H (0.4 to 2.9 ppm) in NOESY spectrum of MP in CD_3OD at 298.2K.

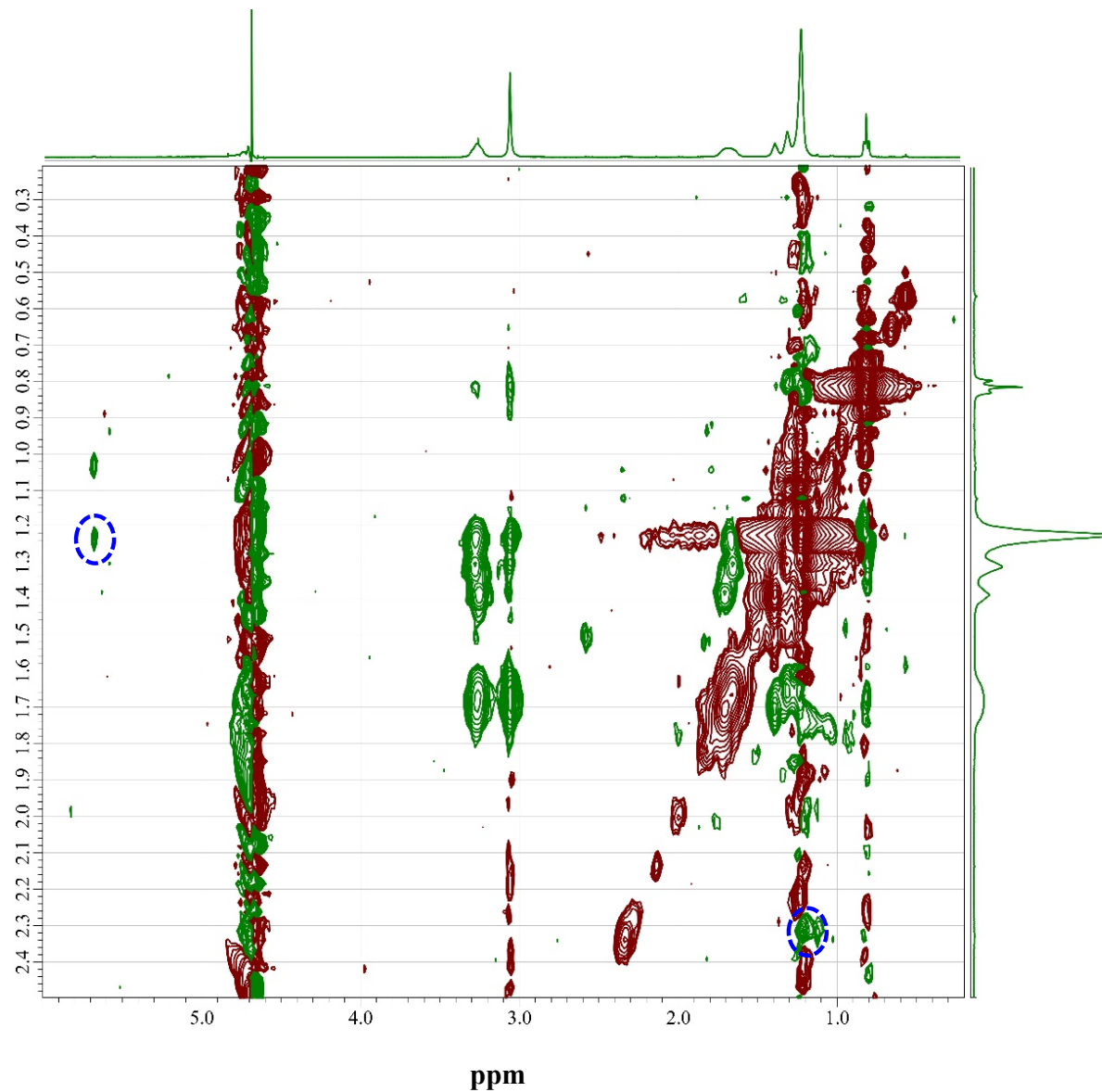


Fig. S13 ROESY spectrum of 2 mM 14-6-14,2Br⁻ solution with MP maximally solubilized in D₂O at 298.2 K.

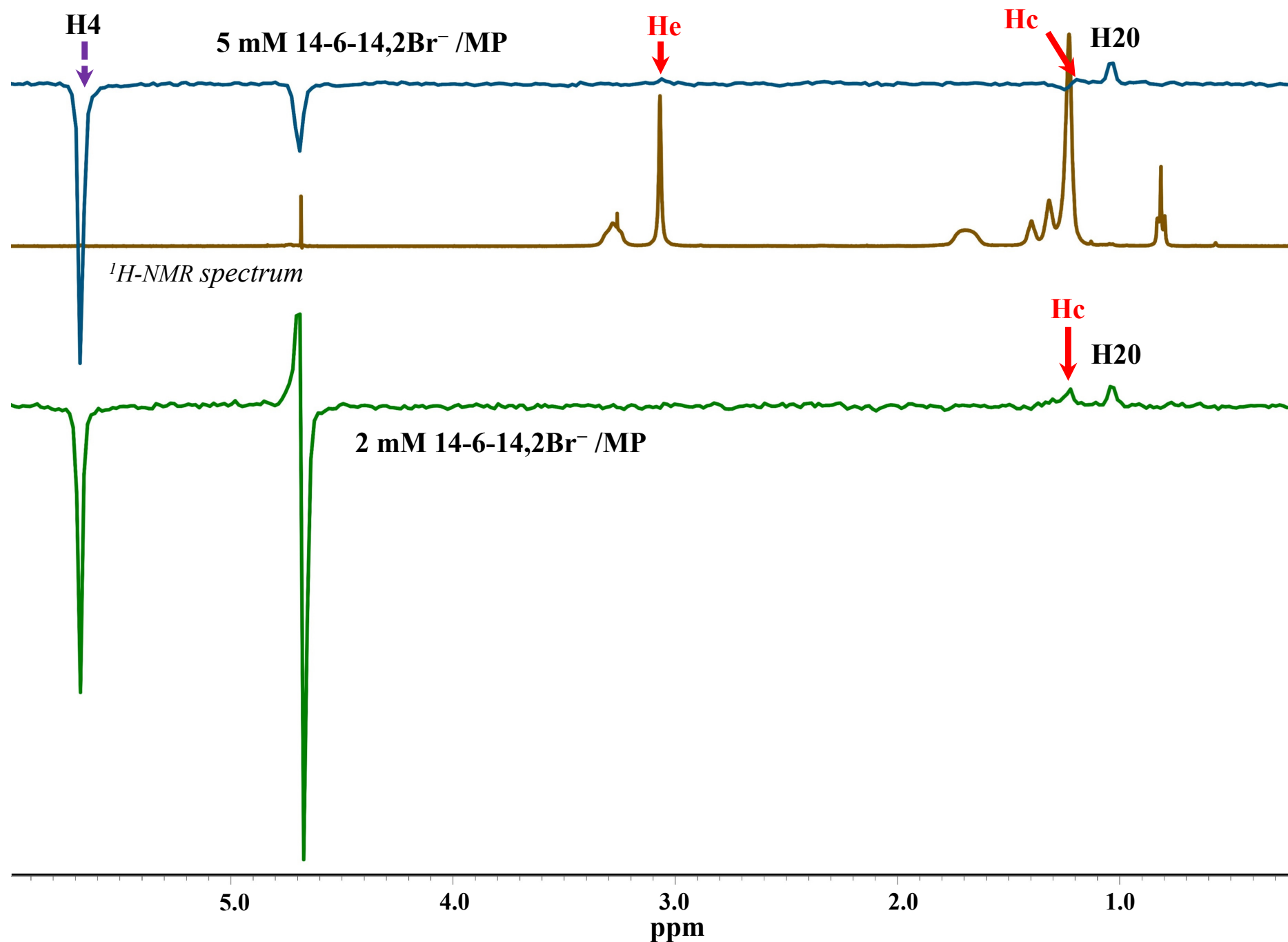


Fig. S14 The ROE spectra of 2 mM (bottom) and 5 mM 14-6-14,2Br⁻/MP (top) of obtained sliced data by one-dimensional processed at diagonal peak H4, diagonal peaks of 2D ROESY that mean irradiation positions for observing ROE correlations. For comparison, the ^1H -NMR spectrum of 5 mM 14-6-14,2Br⁻/MP is shown in the middle.

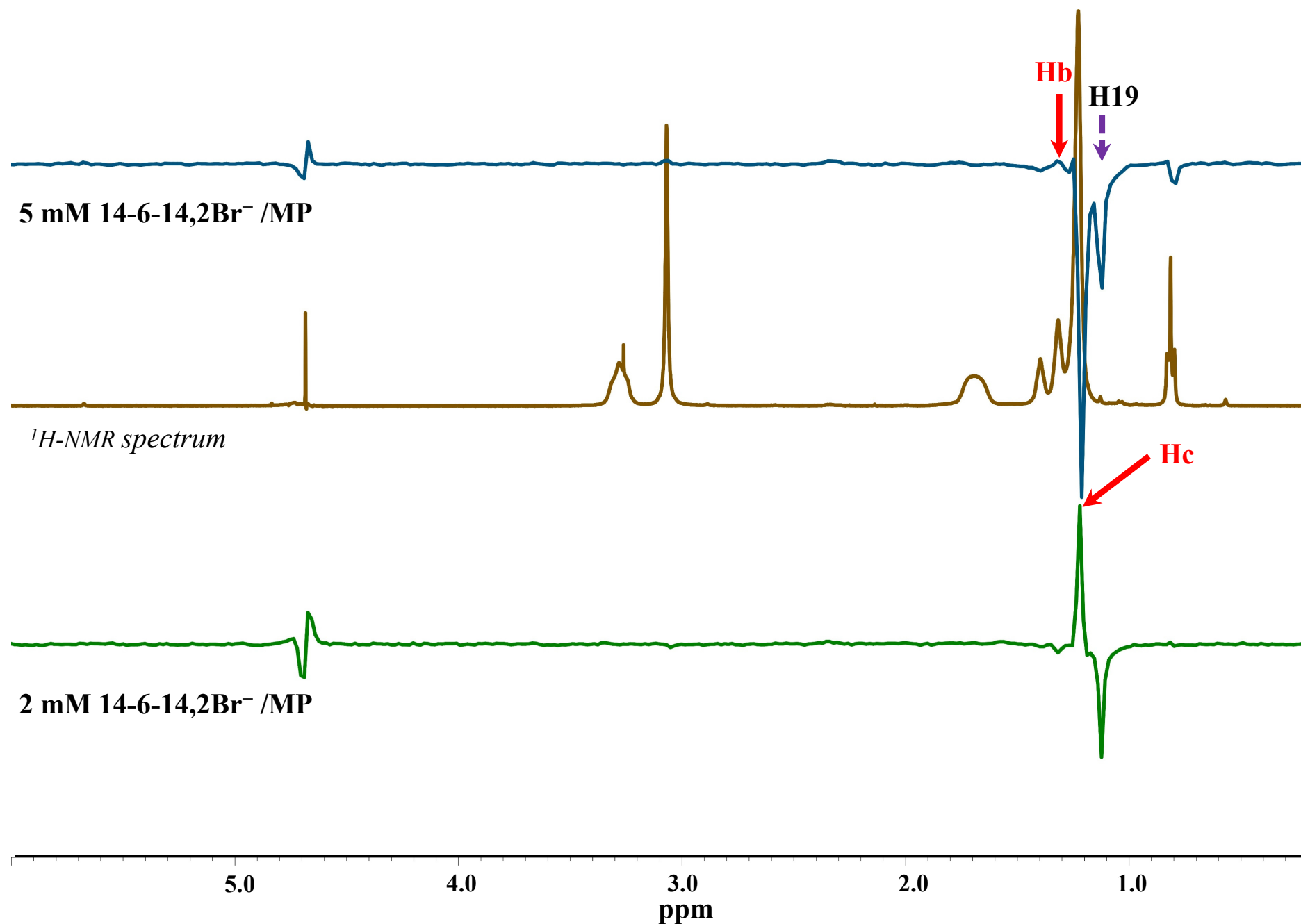


Fig. S15 The ROE spectra of 2 mM (bottom) and 5 mM 14-6-14,2Br⁻/MP (top) of obtained sliced data by one-dimensional processed at diagonal peak H19, diagonal peaks of 2D ROESY that mean irradiation positions for observing ROE correlations. For comparison, the ¹H-NMR spectrum of 5 mM 14-6-14,2Br⁻/MP is shown in the middle.

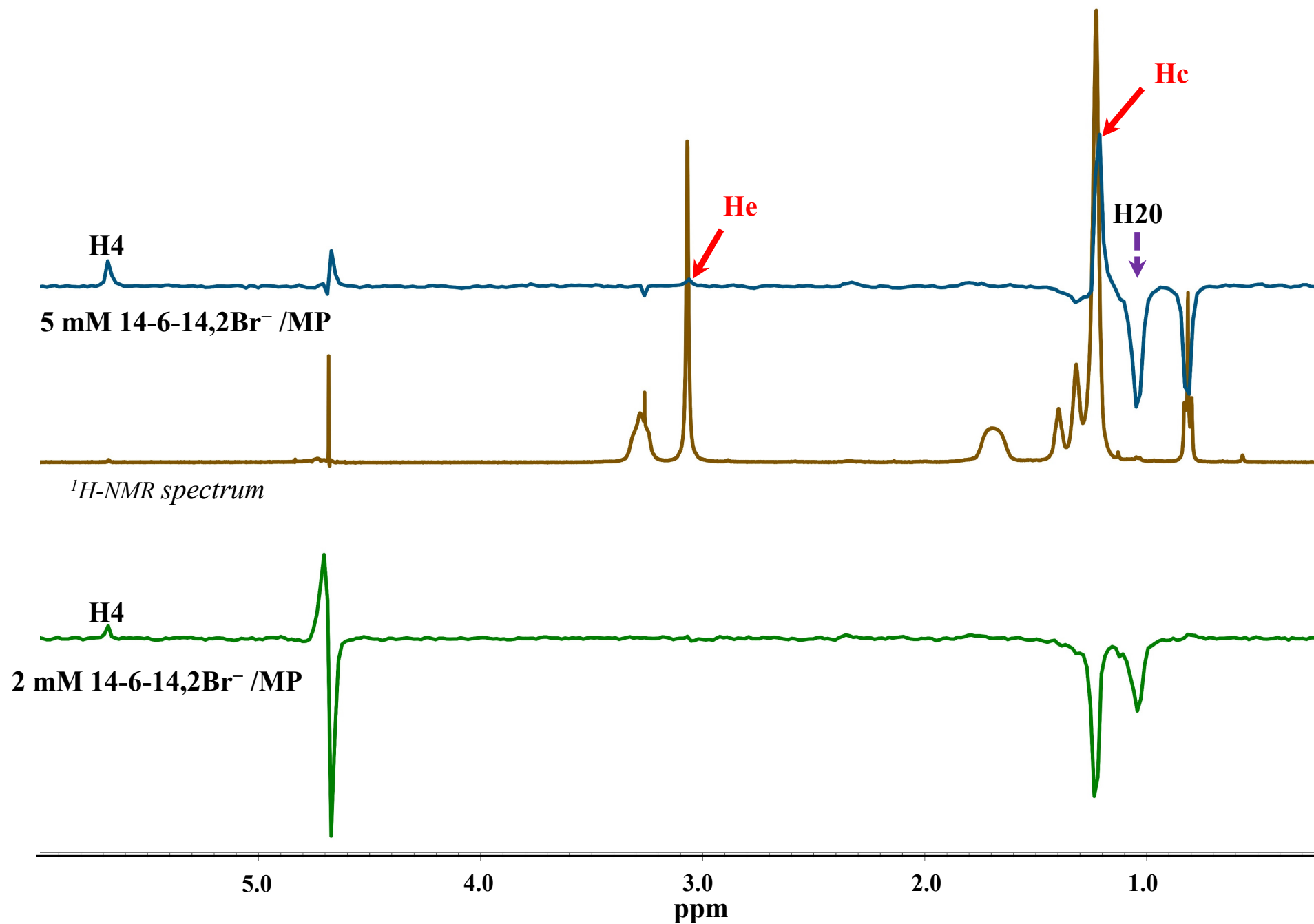


Fig. S16 The ROE spectra of 2 (bottom) and 5 mM 14-6-14,2Br⁻/MP (top) of obtained sliced data by one-dimensional processed at diagonal peak H20, diagonal peaks of 2D ROESY that mean irradiation positions for observing ROE correlations. For comparison, the ^1H -NMR spectrum of 5 mM 14-6-14,2Br⁻/MP is shown in the middle.

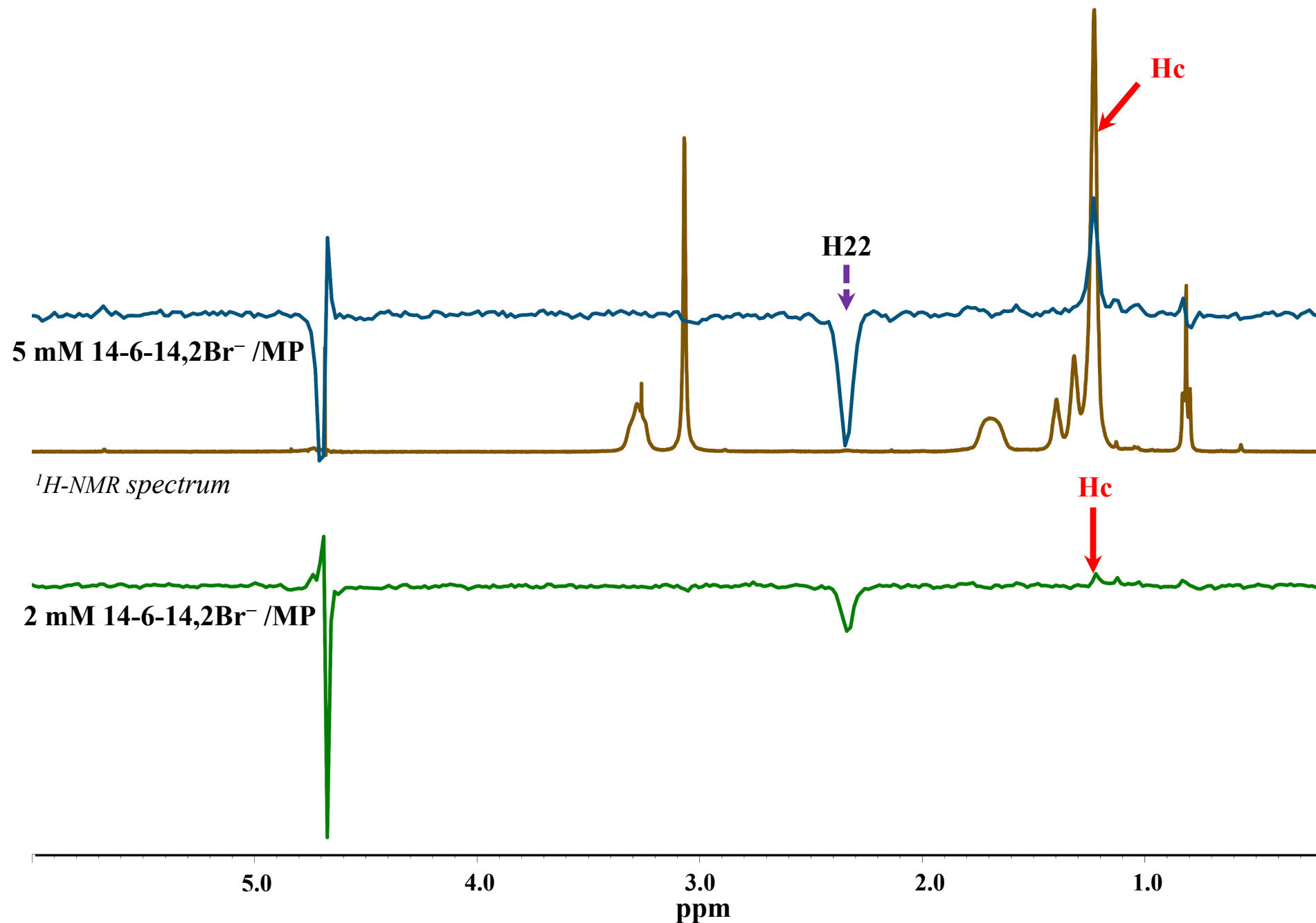


Fig. S17 The ROE spectra of 2 (bottom) and 5 mM 14-6-14,2Br⁻/MP (top) of obtained sliced data by one-dimensional processed at diagonal peak H22, diagonal peaks of 2D ROESY that mean irradiation positions for observing ROE correlations. For comparison, the ¹H-NMR spectrum of 5 mM 14-6-14,2Br⁻/MP is shown in the middle.

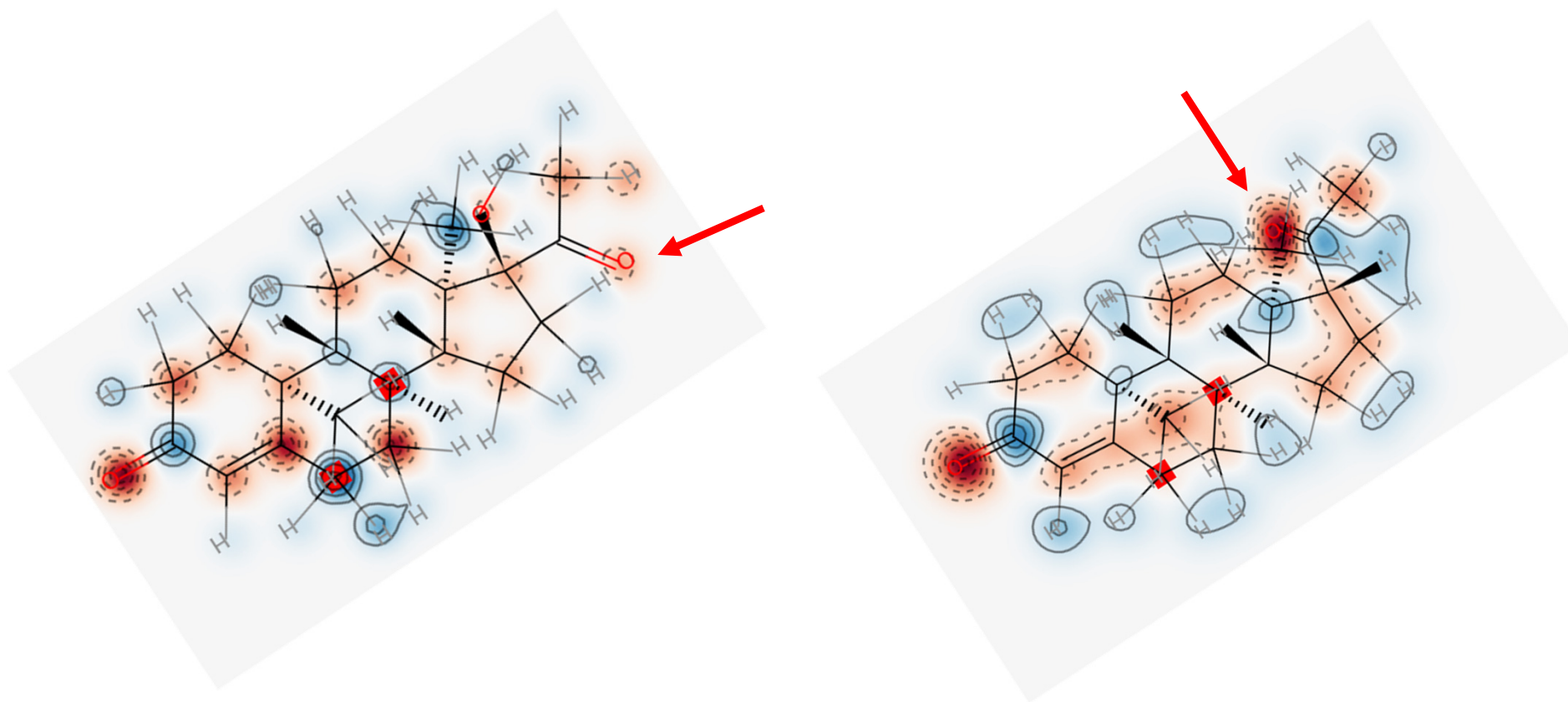


Fig. S18 Electron density map of MP (left) and progesterone (right) calculated using Psi4 with the Mulliken charge scheme and the STO-3G basis set. The map visually represents the electron density of each atom in the progesterone molecule. Regions of high electron density are indicated in red, while regions of low electron density are shown in blue.