Supporting information for:

Insights into the terahertz response of L-Glutamic acid and its receptor

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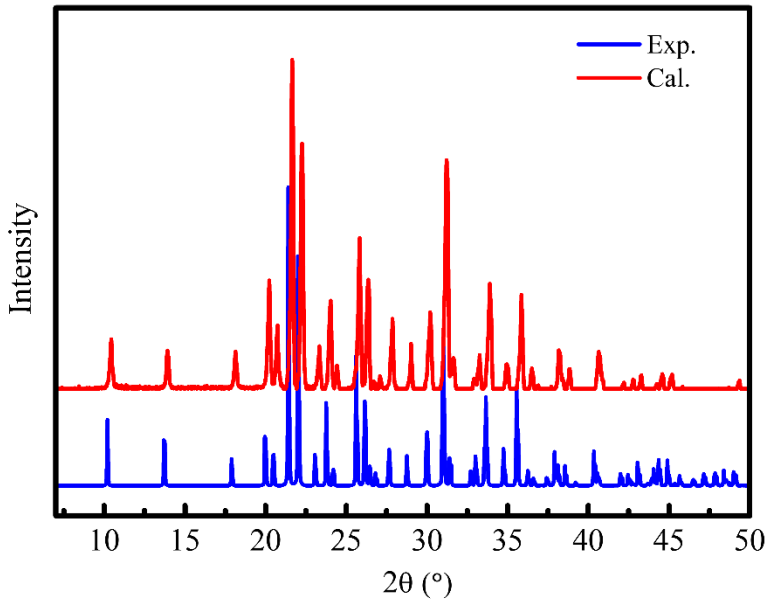

Fig. S1 The PXRD experimental (blue line) and calculated (red line) spectra of L-Glu.

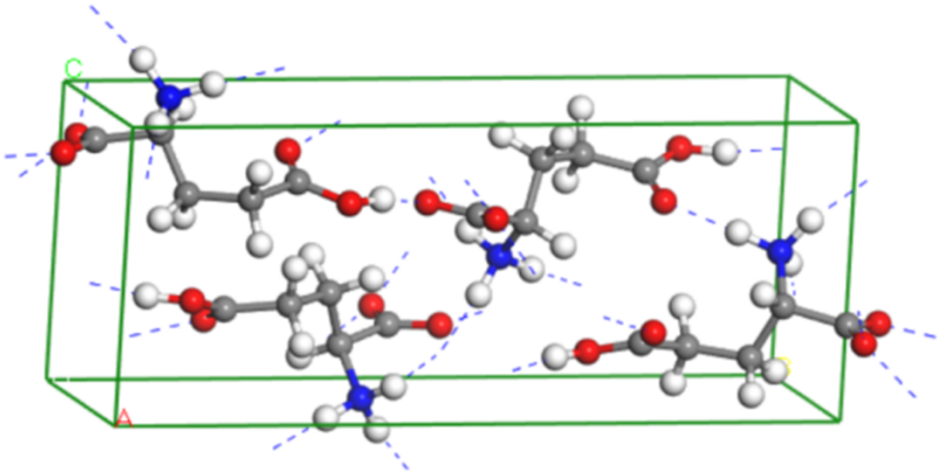

Fig. S2 Schematic diagram of unit cell structure of L-Glu.

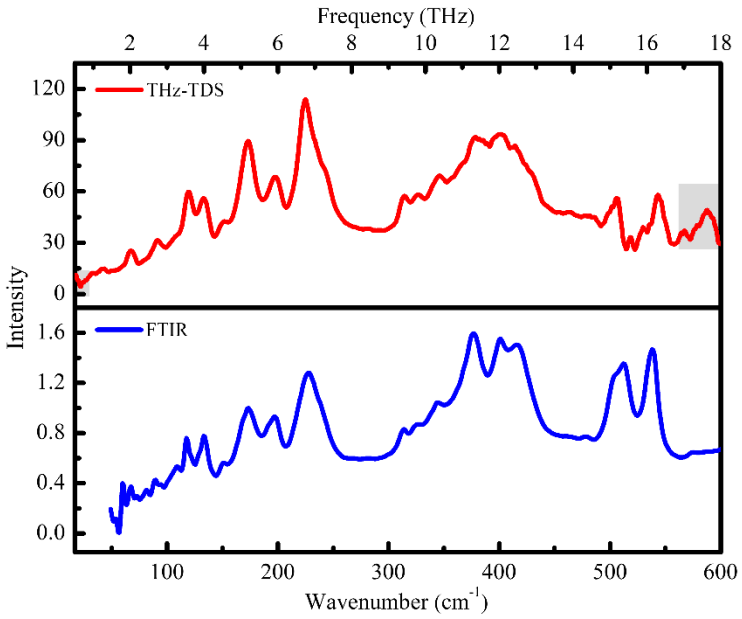

Fig. S3 THz absorption spectra of L-Glu obtained by THz-TDS (red line) and FTIR (blue line). The absorption in the grey area is for reference only.

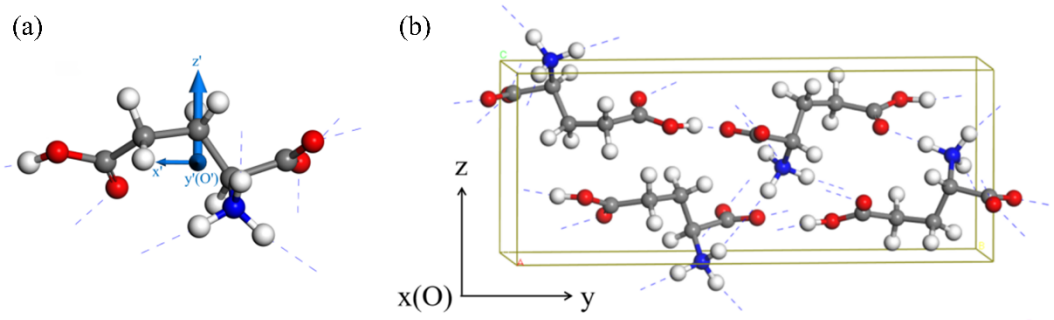

Fig. S4 (a) The coordinate system determined by the three principal axes of a single L-Glu molecule, and (b) the coordinate system of L-Glu unit cell.

Table S1 List of surrounding molecules that were included in molecular models used in ONIOM calculation.

GLU A 14 MM	HIS A 88 MM	SER A 114 MM
LEU A 115 MM	THR A 116 MM	ARG A 121 MM
VAL A 169 MM	SER A 173 MM	THR A 174 MM
GLU A 175 MM	TYR A 214 MM	ASP A 215 MM
TYR A 245 MM	HOH A 316 MM	HOH A 320 MM
HOH A 321 MM	HOH A 338 MM	HOH A 365 MM
GLU A1001 QM		

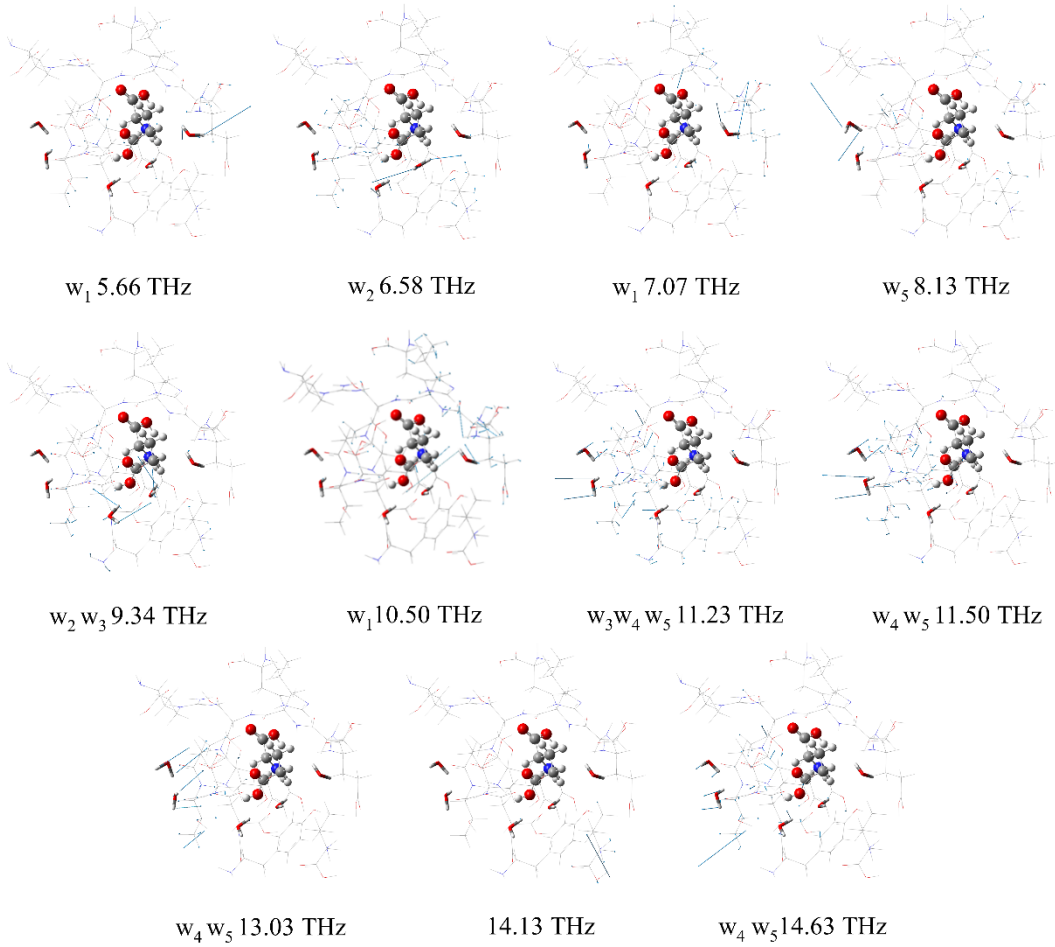

Fig. S5 Schematic diagram of normal modes of different water molecules in the NMDAR-L-Glu complex at specific frequencies.

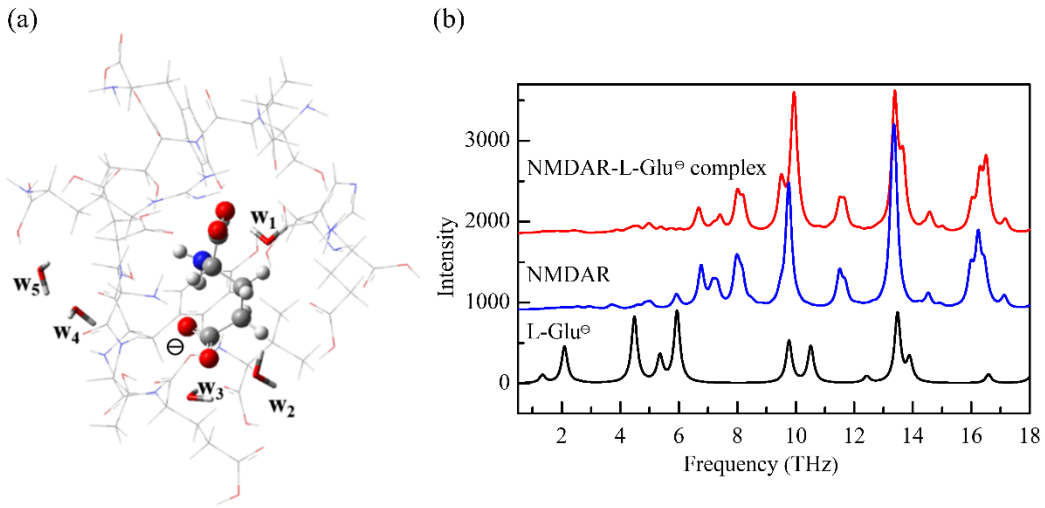

Fig. S6 (a) Structure diagram of the NMDAR-L-Glu⊖ complex, where L-Glu⊖ stands for HOOC-CH(NH_2)-(CH_2)$_2$-COO⊖. (b) THz spectra of NMDAR-L-Glu⊖ complex and NMDAR and L-Glu⊖

in the range of 0.5~18 THz obtained by theoretical calculation, the spectral intensity of L-Glu⊖ is amplified to 12 times to facilitate comparison.

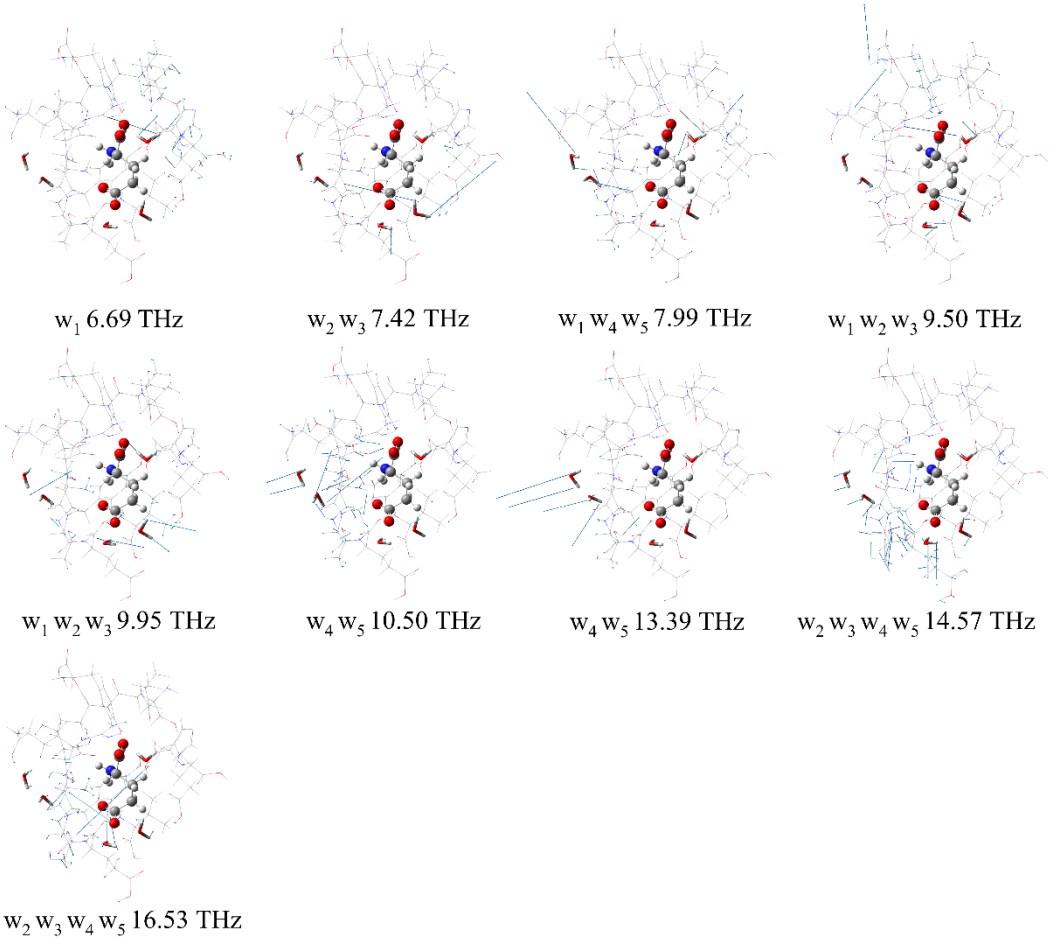

Fig. S7 Schematic diagram of normal modes of different water molecules in the NMDAR-L-Glu⊖ complex at specific frequencies.

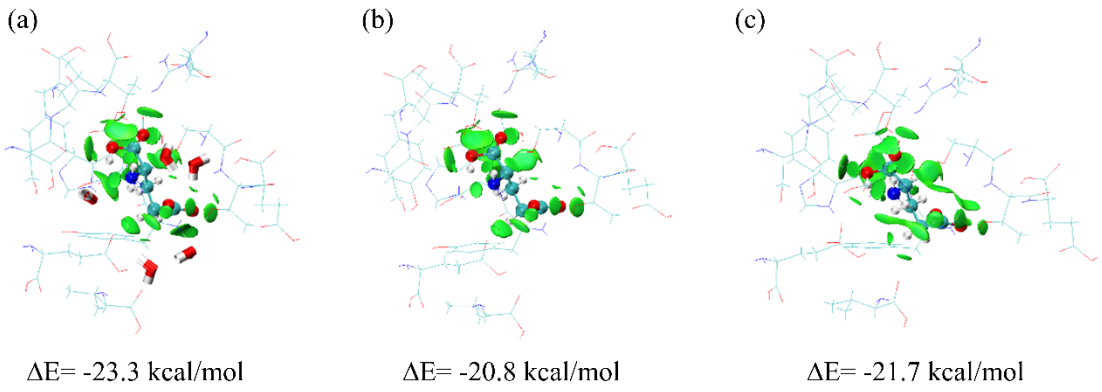

Fig. S8 Influence of water molecules on the conformation and binding energy of NMDAR-L-Glu⊖ complex.

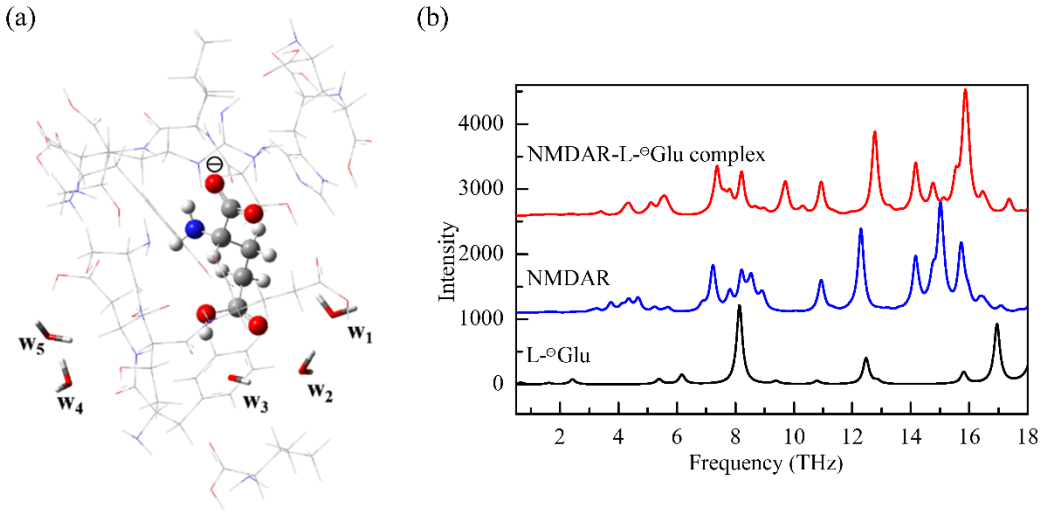

Fig. S9 (a) Structure diagram of the NMDAR-L-⊖Glu complex, where L-⊖Glu stands for ⊖OOC-$CH(NH_2)$-$(CH_2)_2$-COOH). (b) THz spectra of NMDAR-L-⊖Glu complex and NMDAR and L-⊖Glu in the range of 0.5~18 THz obtained by theoretical calculation, the spectral intensity of L-⊖Glu is amplified to 7 times to facilitate comparison.

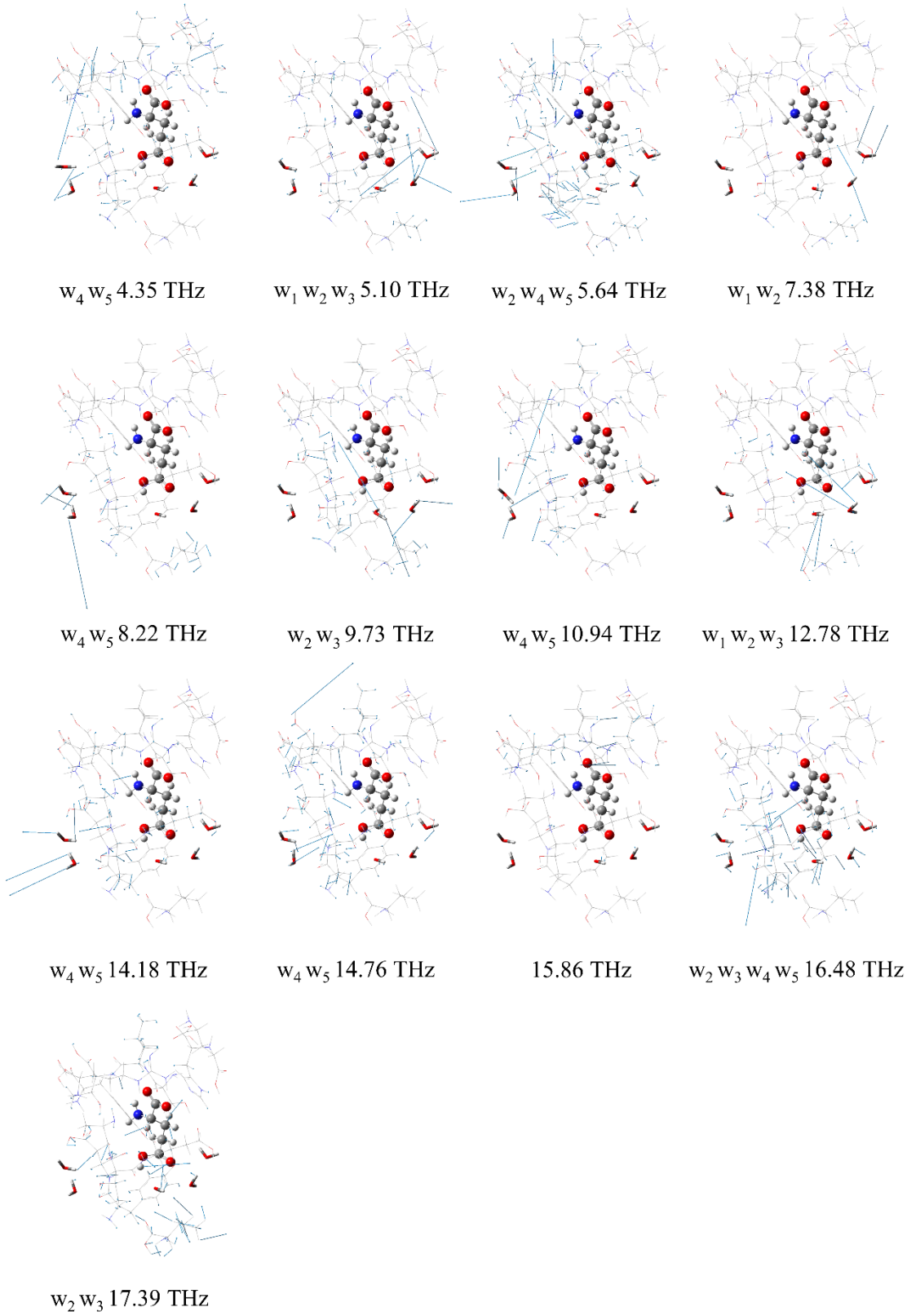

Fig. S10 Schematic diagram of normal modes of different water molecules in the NMDAR-L-⊖Glu complex at specific frequencies.

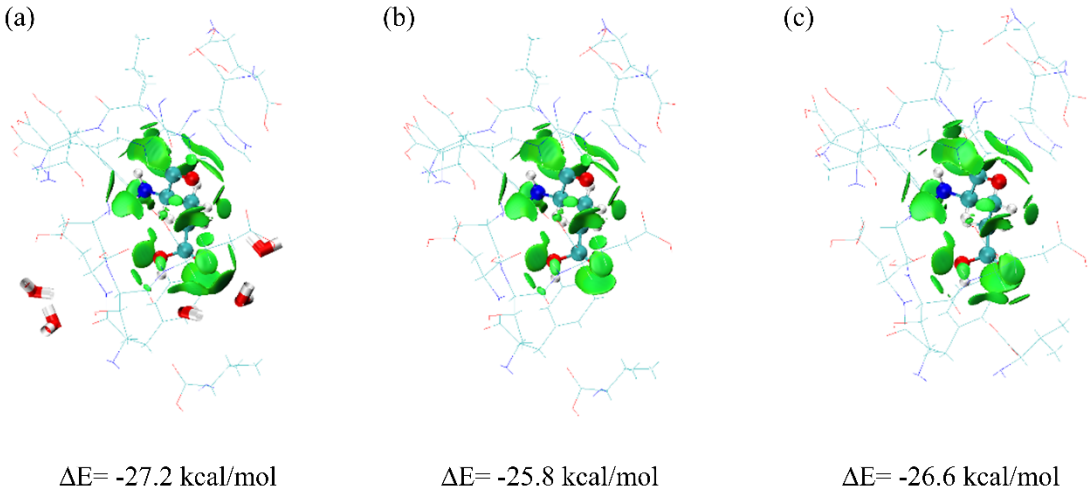

Fig. S11 Influence of water molecules on the conformation and binding energy of NMDAR-L-⊖Glu complex.