Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Effect of terahertz waves on the aggregation behavior of neurotransmitters

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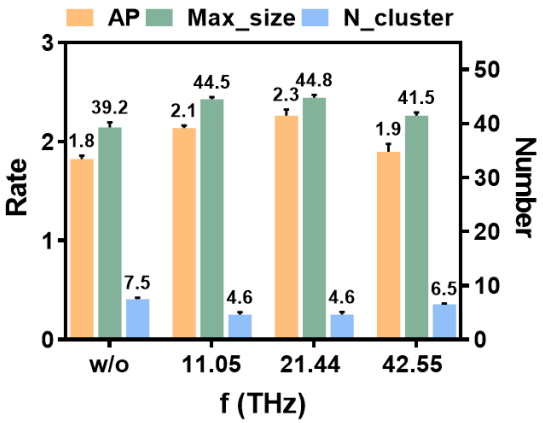

Figure S1. Comparison of the aggregation of nicotine molecules between the case without THz waves and with the 11.05, 21.44, and 42.55 THz waves at the strength of 0.5 V/nm in the x-direction.

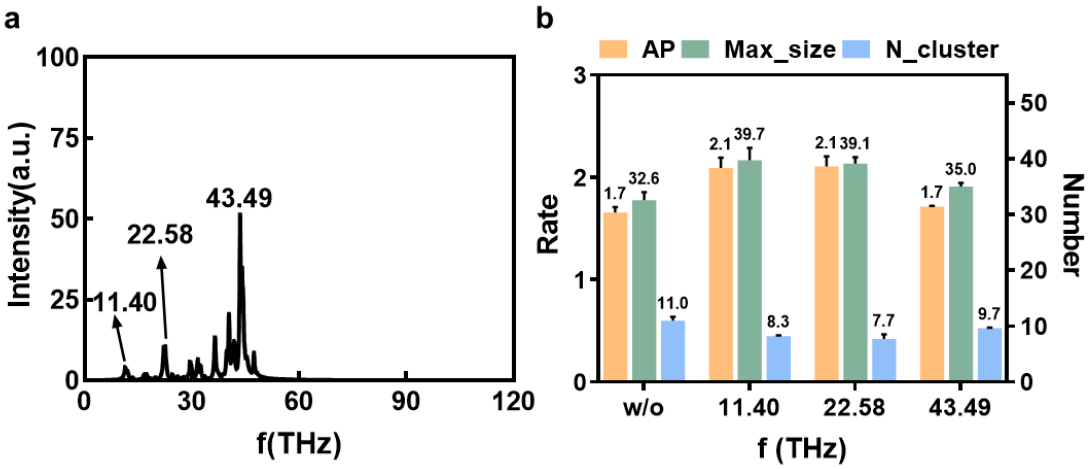

Figure S2. (a) The absorption spectra of NCT in solution using the CGenFF. (b) Comparison of the aggregation of nicotine molecules between the case without THz waves and with the 11.40, 22.58, and 43.49 THz waves at the strength of 0.5 V/nm.

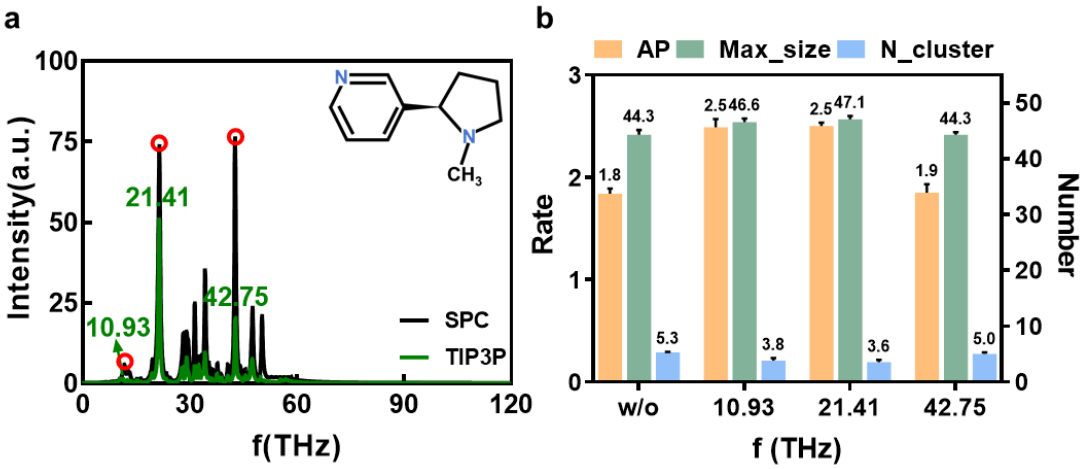

Figure S3. (a) The absorption spectra of the NCT in solution using different water models. Black line: SPC water model, green line: TIP3P water model. (b) Comparison of the aggregation of nicotine molecules between the case without THz waves and with the 10.93, 21.41, and 42.75 THz waves at the strength of 0.5 V/nm.

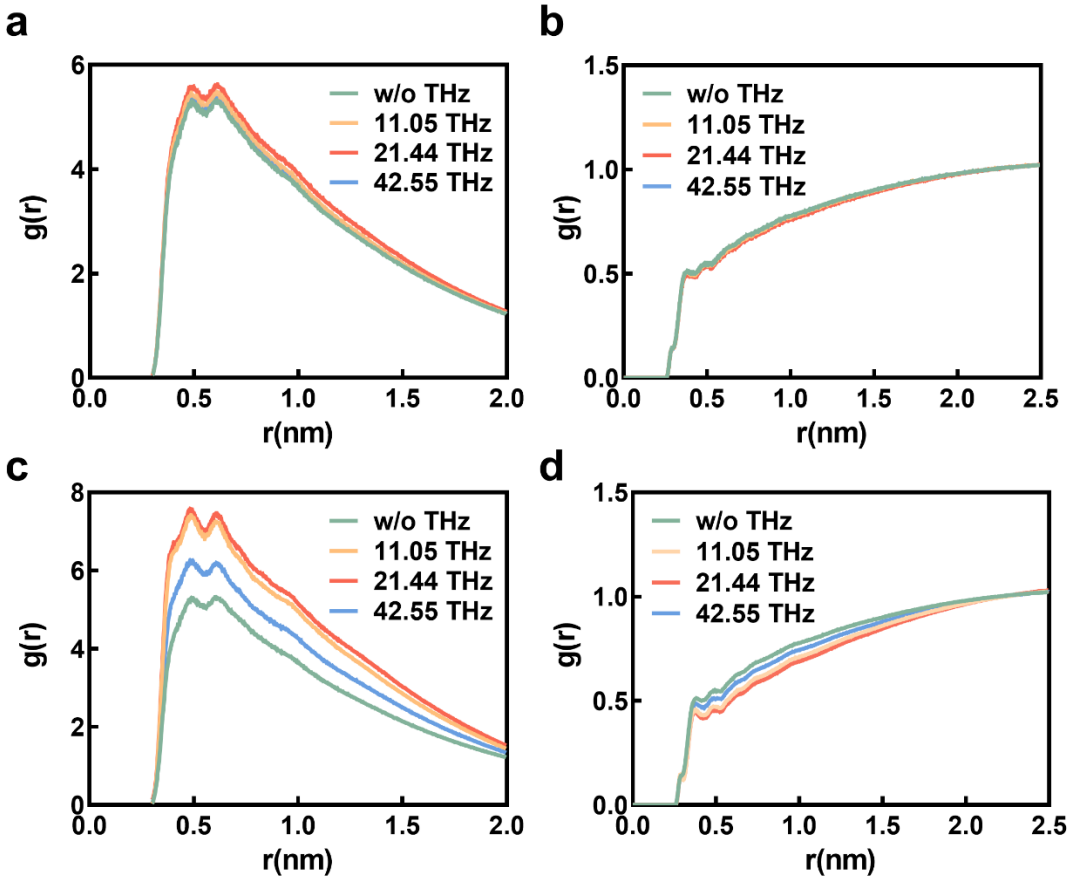

Figure S4. The w/o THz system and at *f* of 11.05, 21.44, and 42.55 THz, RDFs at an 0.25 V/nm were characterized as follows: (a) RDFs between pyridine rings (hydrogen atoms excluded) of nicotine molecules, and (b) RDFs between pyridine rings (hydrogen atoms excluded) of nicotine molecules and oxygen atoms of water. At a higher electric field strength of 1.0 V/nm, the RDFs are depicted with (c) shows the distribution between pyridine rings (hydrogen atoms excluded) of nicotine molecules; (d) illustrates the distribution between pyridine rings (hydrogen atoms excluded) of nicotine molecules and oxygen atoms of water molecules.

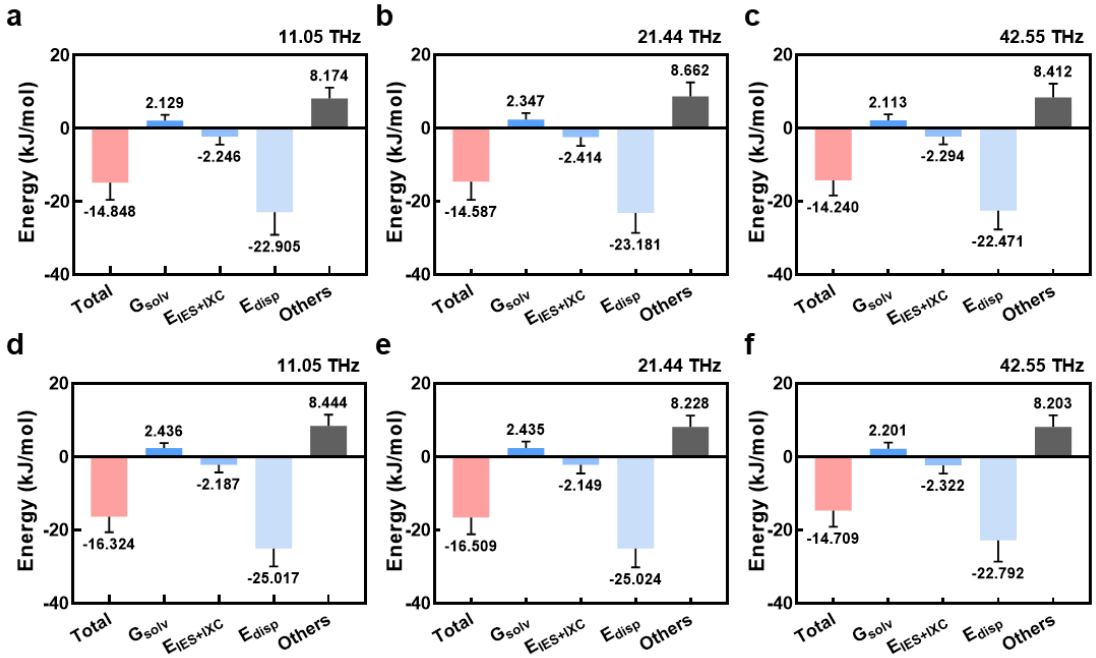

Figure S5. The determination of the system's binding energy was performed across various conditions, with a specific focus on the effects of electromagnetic fields. At an electric field strength of 0.25 V/nm, the nicotine molecule's energy profile was examined at *f* of (a) 11.05 THz, (b) 21.44 THz, and (c) 42.55 THz. A parallel analysis was carried out at an elevated electric field strength of 1.0 V/nm, with the NCT's energy profiles similarly assessed at frequencies of (a) 11.05 THz, (b) 21.44 THz, and (c) 42.55 THz. Sequentially, the presented values delineate the system's binding energy, solvation energy (G_{solv}), electrostatic energy ($E_{IES+IXC}$), density-dependent dispersion energy (E_{disp}), and other energies.

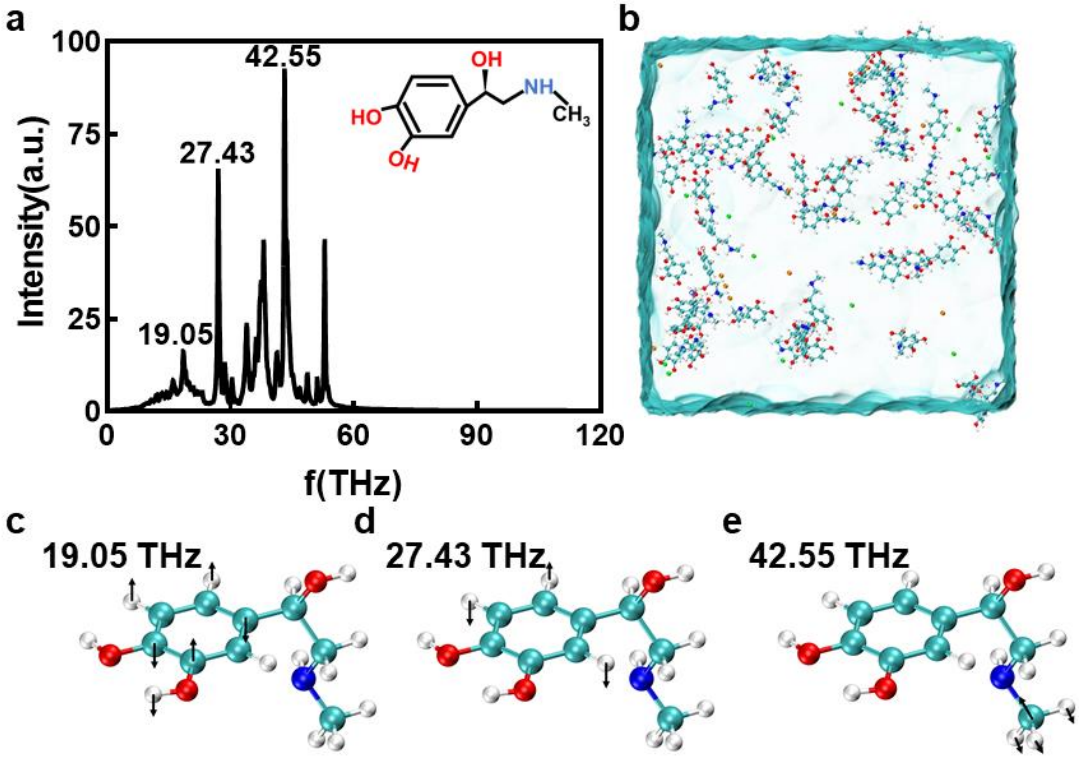

Figure S6. (a) Vibrational/absorption spectra of epinephrine (EPI) in a 0.15 mol/L NaCl solution, with an inset showing the molecule of epinephrine. (b) A model of the system with adrenaline concentration at 0.5 mol/L. the green bead stands for Na^+, the orange bead stands for Cl^-, and the water molecules are implicitly shown for clarity. (c) Vibrational modes of adrenaline at f of 19.05, 27.43, and 42.55 THz, with black arrows indicating the directions of atomic vibrations. Blue-N, red-O, cyan-C, and grey-H.

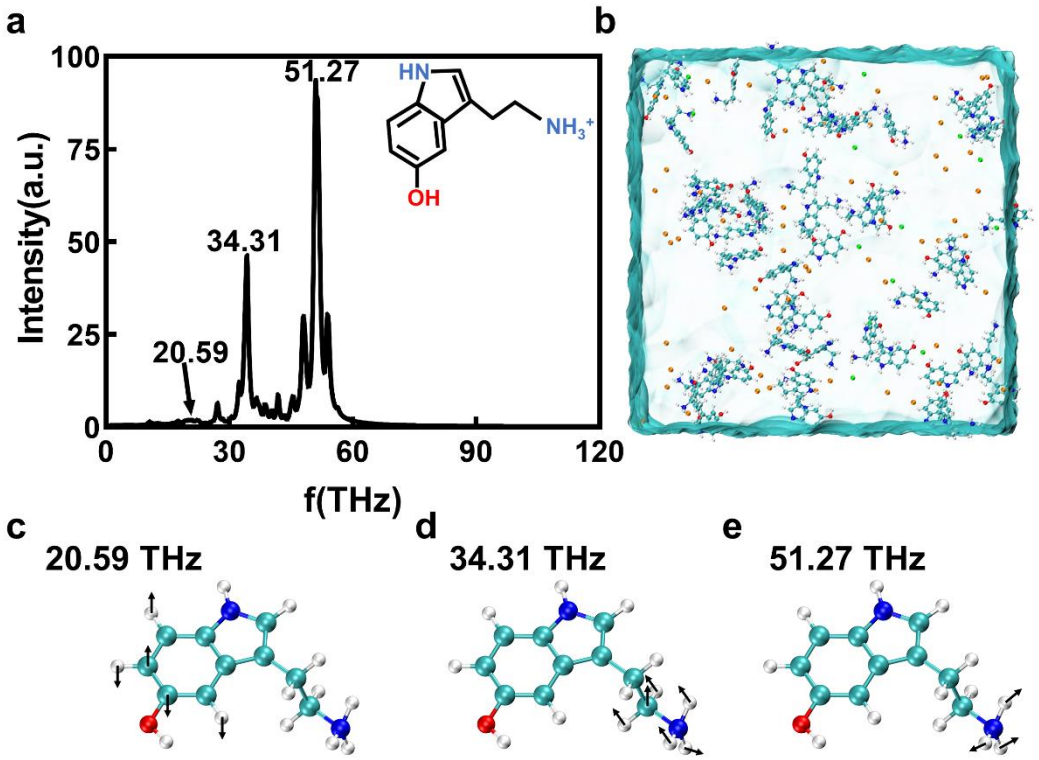

Figure S7. (a) Vibrational/absorption spectra of 5-hydroxytryptamine (5-HT) in a 0.15 mol/L NaCl solution, the inset shows the molecule of 5-HT. (b) A model of the system with 5-HT concentration at 0.5 mol/L. the green bead stands for Na^+, the orange bead stands for Cl^-, and the water molecules are implicitly shown for clarity. (c) Vibrational modes of 5-HT at f of 20.59, 34.31, and 51.27 THz, with black arrows indicating the directions of vibrations. Blue-N, red-O, cyan-C, and grey-H.

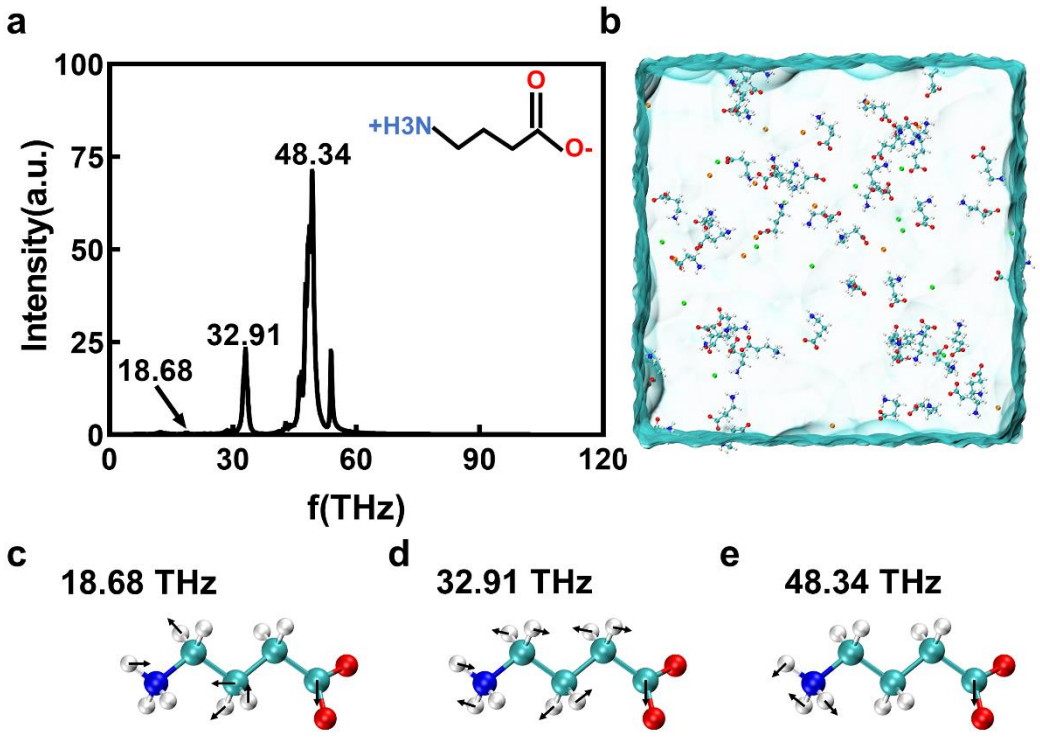

Figure S8. (a) Vibrational/absorption spectra of GABA in a 0.15 mol/L NaCl solution. The inset shows the molecule of GABA. (b) A model of the system with GABA concentration at 0.5 mol/L. the green bead stands for Na^+, the orange bead stands for Cl^-, and the water molecules are implicitly shown for clarity. (c) Vibrational modes of GABA at *f* of 18.68, 32.91, and 48.34 THz, with black arrows indicating the directions of vibrations. Blue-N, red-O, cyan-C, and grey-H.

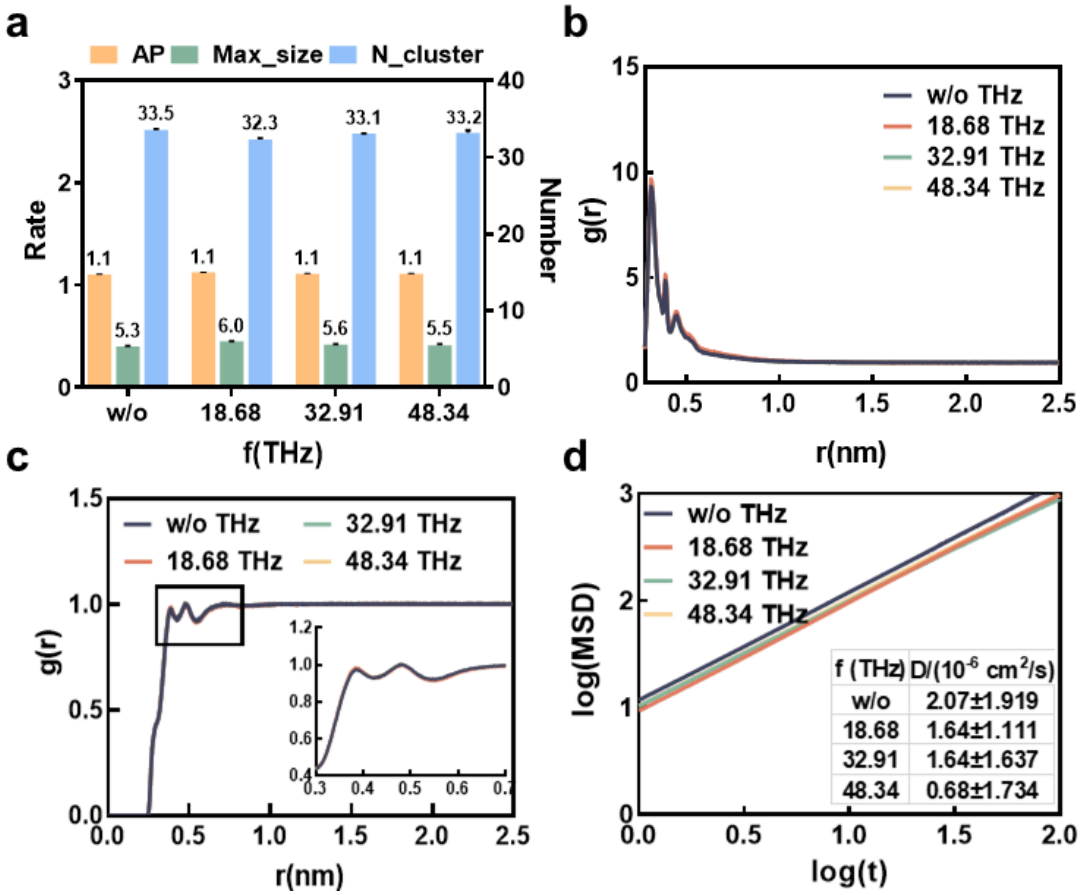

Figure S9. Analysis of the structural and dynamical properties of the GABA system. At E_0=0.5 V/nm, w/o THz and at frequencies of 18.68, 32.91, and 48.34 THz: (a) Analysis of the clustering within the system. (b) RDFs between heavy atoms within the molecules. (c) RDFs between heavy atoms of the GABA molecules and oxygen atoms of water molecules. (d) The relationship between the mean square displacement of molecules in the system and time, represented as a double logarithmic plot of log(MSD) versus log(t).