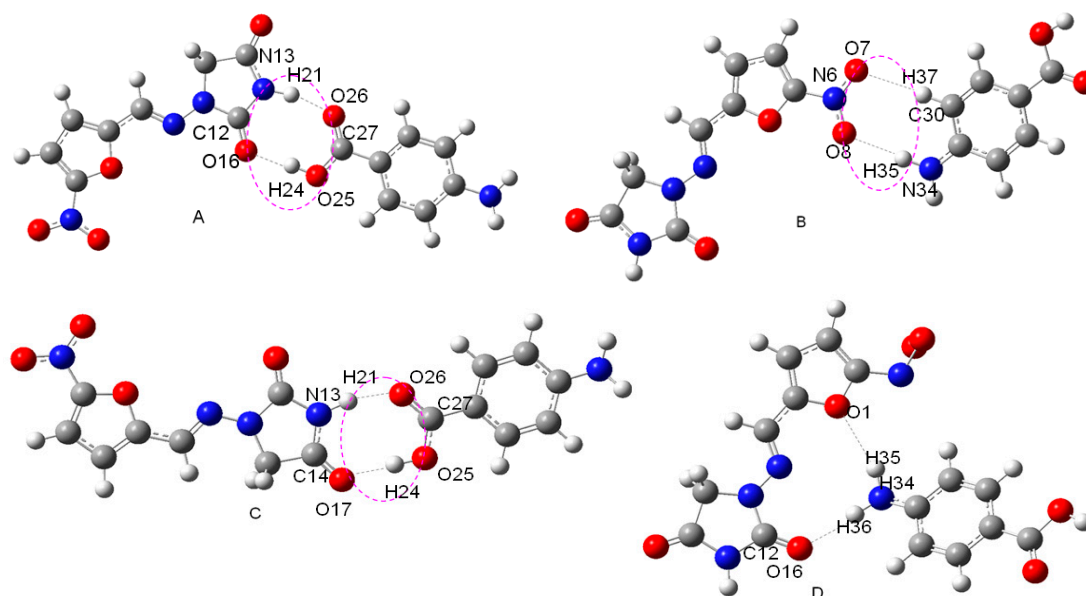


# Supplementary Materials: Raman and Terahertz Spectroscopic Investigation of Cocrystal Formation Involving Antibiotic Nitrofurantoin Drug and Coformer 4-aminobenzoic Acid

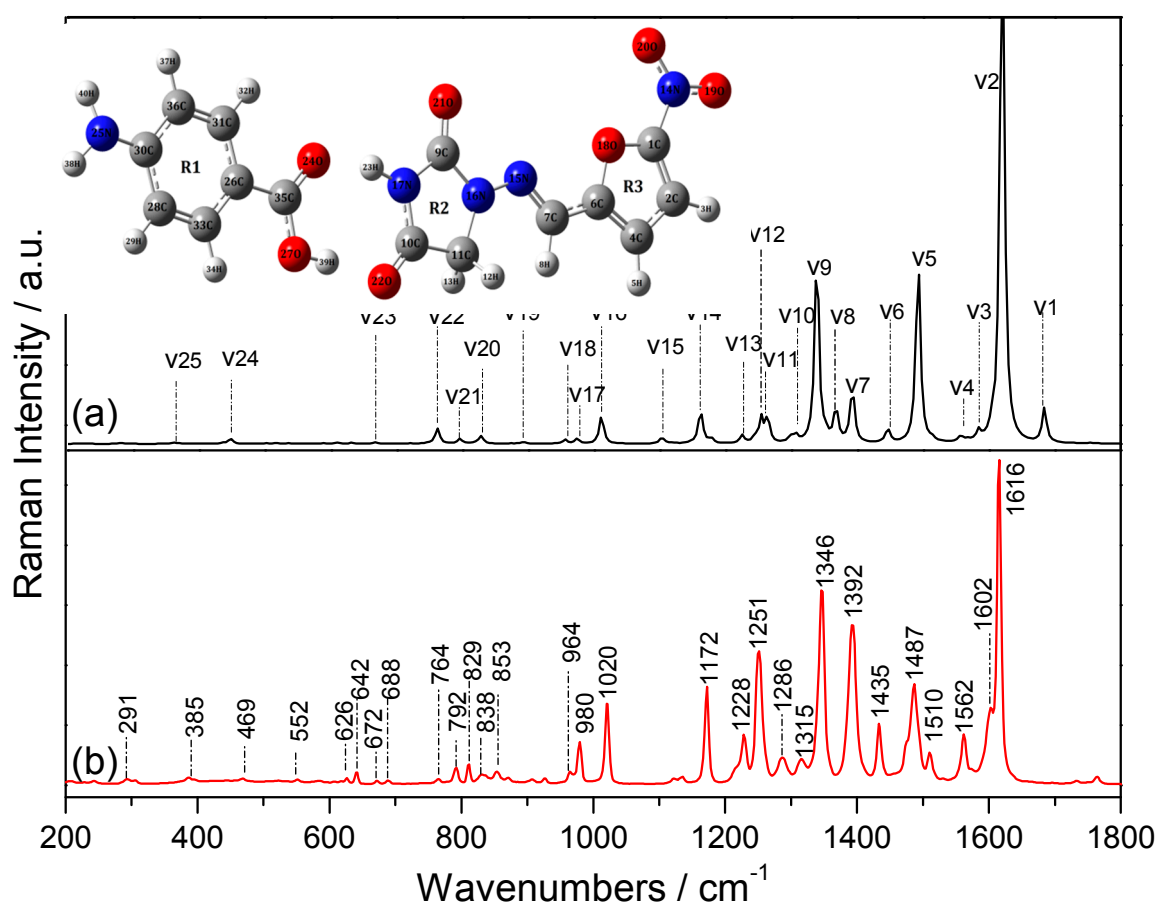
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**Table S1.** Vibrational modes assignment for Raman characteristic peaks of the cocrystal between NF and 4ABA.

Mode	Theoretical	Experimental	Mode Assignment
	Wavenumber /cm <sup>-1</sup>	Wavenumber /cm <sup>-1</sup>	
V1	1684		$\theta(\text{C7}=\text{N15}), \rho(\text{C7-H8}), \text{Def}(\text{R3})$
V2	1620	1616	$\theta(\text{C35}=\text{O24}), \rho(\text{O27-H39}, \text{N17-H23})$
V3	1584	1602	$\theta(\text{C1}=\text{C2}, \text{O19-N14-O20}), \rho(\text{C2-H3}, \text{C4-H5})$
V4	1556	1562	$\text{Def}(\text{R3}), \theta(\text{C7}=\text{N15}, \text{O19-N14-O20})$
V5	1492	1487	$\text{Def}(\text{R3}), \theta(\text{C7}=\text{N15}, \text{C7-H8})$
V6	1446	1435	$\delta(\text{H12-C11-H13})$
V7	1392	1392	$\theta(\text{O19-N14-O20}), \theta(\text{C26-C35-O27}), \rho(\text{N17-H23}, \text{C7-H8})$
V8	1368		$\text{Def}(\text{R3}), \theta(\text{C7-H8})$
V9	1337	1346	$\text{Def}(\text{R1}), \rho(\text{H38-N25-H40})$
V10	1306	1315	$\rho(\text{C7-H8}), \omega(\text{H12-C11-H13})$
V11	1263	1286	$\text{Def}(\text{R3}), \theta(\text{O19-N14-O20}), \rho(\text{C2-H3}, \text{C4-H5}, \text{C7-H8}), \omega(\text{H12-C11-H13})$
V12	1254	1251	$\theta(\text{C26-C35-O27}), \rho(\text{O27-H39})$
V13	1225	1228	$\text{Def}(\text{R3}), \theta(\text{C11-N16-N15}), \omega(\text{H12-C11-H13})$
V14	1161	1172	$\rho(\text{C2-H3}, \text{C4-H5}, \text{C7-H8})$
V15	1103		$\text{Def}(\text{R3}, \text{R2}), \rho(\text{C4-H5}, \text{C7-H8})$
V16	1011	1020	$\rho(\text{C2-H3}, \text{C4-H5})$
V17	974	980	$\text{Def}(\text{R3}), \rho(\text{C7-H8})$
V18	956	964	$\text{Def}(\text{R3}), \rho(\text{C7-H8}), \theta(\text{O19-N14-O20})$
V19	892	871	$\text{Def}(\text{R1})$
V20	827	829/838	$\omega(\text{C2-H3}, \text{C4-H5}, \text{C7-H8}, \text{N17-H23})$
V21	795	792	$\text{Def}(\text{R2}, \text{R3}), \theta(\text{O19-N14-O20})$
V22	761	764	$\text{Def}(\text{R2}, \text{R3}), \rho(\text{C7-H8})$
V23	665	642	$\text{Def}(\text{R2}), \rho(\text{C7-H8})$
V24	447	469	$\omega(\text{H38-N25-H40})$
V25	361	385	$\text{Def}(\text{R1})$



**Figure S1.** Molecular structure of the cocrystal between nitrofurantoin (NF) and 4-aminobenzoic acid(4ABA).



**Figure S2.** Raman vibrational modes of the cocrystal between NF and 4ABA. (a) theoretical calculation based on form C shown in Figure S1; (b) experimental spectrum.