† Electronic Supplementary Information

Molecular structure and hydrogen bond interactions ~~and chemical reactivity analysis~~ of Paracetamol– ~~4,4′–bipyridine~~ Paracetamol-4,4′–bipyridine cocrystal studied using vibrational spectroscopic and quantum chemical approach

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Crystal structure of paracetamol (PRA), 4,4′–bipyridine(BPY) and PRA-BPY cocrystal are shown in Fig.S1, Fig.S2 and Fig.S3. Experimental details of PXRD and DSC of prepared cocrystal are given below and PXRD plot of cocrystal is shown in Fig.S4. DSC plot of paracetamol, 4, 4′–bipyridine and paracetamol-4,4′–bipyridine cocrystal are shown in Fig.S5. Optimized structure of paracetamol (monomer) and 4, 4′–bipyridine (monomer) are shown in Fig. S6, S7. Experimental and calculated IR and Raman spectra of paracetamol (monomer) and 4, 4′–bipyridine (monomer) are shown in Fig.S8, S9, S10, S11. The molecular graph of a monomer of paracetamol-4,4′–bipyridine cocrystal(PRA-BPY) using AIM program is given in Fig.S12.~~HOMO and LUMO of PRA3-BPY2 (dimer+PRA) its energy band gap is shown in Fig.S13.The molecular electrostatic potential (MEPS) surface of paracetamol (monomer), 4,4′–bipyridine(monomer) and PRA-BPY(monomer) of cocrystal are given in Fig.S14, S15 and S16.~~The experimental and calculated geometric parameters of monomer and dimer+PRA of cocrystal are given in Table S1. Theoretical and experimental vibrational wavenumber of paracetamol (monomer) and 4, 4′–bipyridine (monomer) are listed in Table S2, S3. The experimental and theoretical wave number of the cocrystal using monomer and dimer+PRA model is given in Table S4.Geometrical parameters for hydrogen bonds in dimer+PRA of cocrystal are given in Table S5. Second-order perturbation theory analyses of the Fock Matrix, in the NBO basis for intra-molecular interactions in PRA-BPY (monomer) within PRA3-BPY2 (dimer+PRA) of cocrystal, is given in Table S6. ~~Reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softnesses (s_k^+, s_k^-), local electrophilicity indices (ωk^+, ωk^-) for paracetamol (monomer), PRA-BPY (monomer) and PRA3-BPY2 (dimer+PRA) using Hirshfeld atomic charges are given in Table S7, S8 and S9.~~

Part I. FIGURES

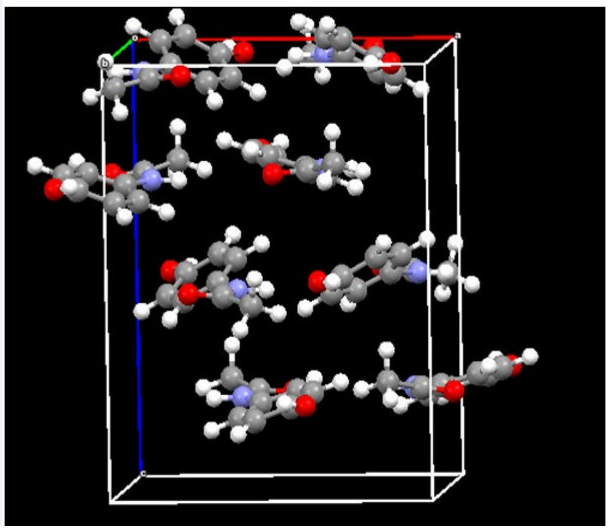

Fig. S1 Packing and orientation of paracetamol molecules in the crystal lattice. Cambridge Crystallographic Database (CSD) reference code is HXACAN01.

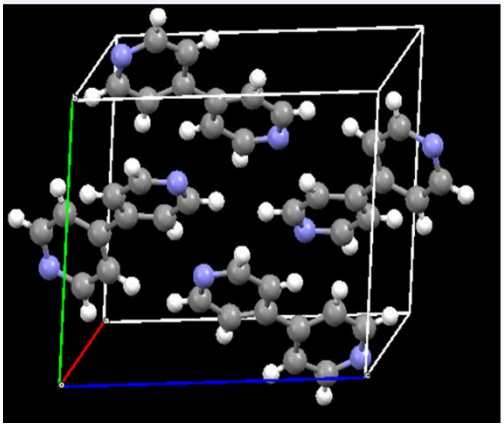

Fig. S2 Perspective view of the unit cell of 4, 4′–bipyridine (Cambridge Crystallographic Database (CSD) reference code:- HIQWEJ02) along *a*-axis

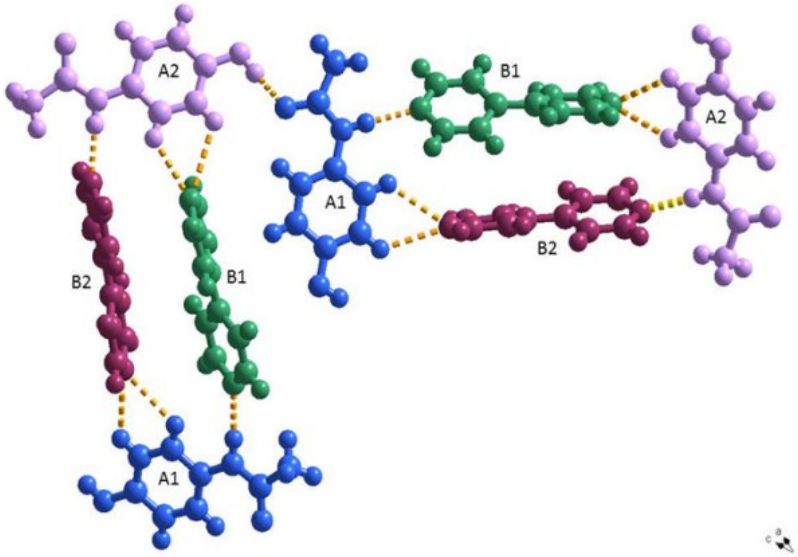

Fig. S3 Interactions between the molecules that are held together through hydrogen bonds in the crystal lattice of cocrystal (Cambridge Crystallographic Database (CSD) reference code is MUPQAP).

Powder X-ray Diffraction (PXRD)

PXRD patterns for the samples were collected using an Empyrean X-ray diffractometer (PANalytical, The Netherlands) equipped with a PIXel3D detector and a monochromatic Cu Kα radiation X-Ray tube (1.54056Å). The tube voltage and amperage were set at 45 kV and 40 mA, respectively. Sample was prepared for analysis by pressing a thin layer of the sample onto a metal sample holder. Instrument calibration was performed using a silicon reference standard. Each sample was scanned 2θ range of 5^{o} to 40^{o}, increasing at a step size of 0.02^{o} 2θ. The data were processed using High Score Plus Version 3.0 software (PANalytical, The Netherlands).

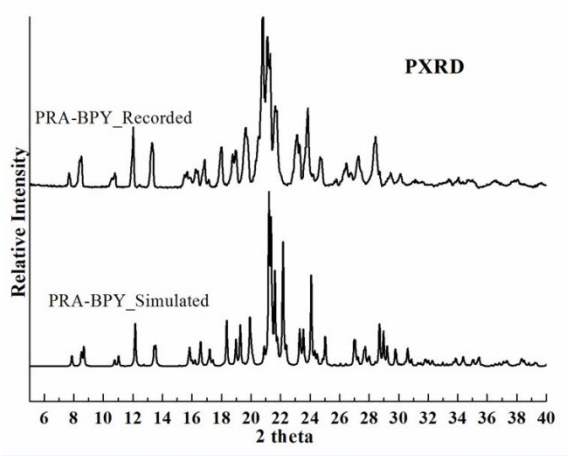

Fig. S4 PXRD overlapped of prepared PRA-BPY cocrystal with its simulated pattern.

Differential scanning calorimetry (DSC)

The DSC profiles of the solid samples were generated in the range of (30–200 °C) using a TA Q1000 DSC instrument with a refrigerated cooling unit. Temperature calibration was performed using an indium metal standard at the respective heating rate. Samples (1–2 mg) were crimped in non-hermetic aluminum pans and scanned at a heating rate of 10 °C/min under a continuously purged dry nitrogen atmosphere (flow rate 50 mL/min) using a similar empty pan as a reference. The data were collected in triplicate for each sample and analyzed using a TA Instruments Universal Analysis 2000 version 4.5A software.

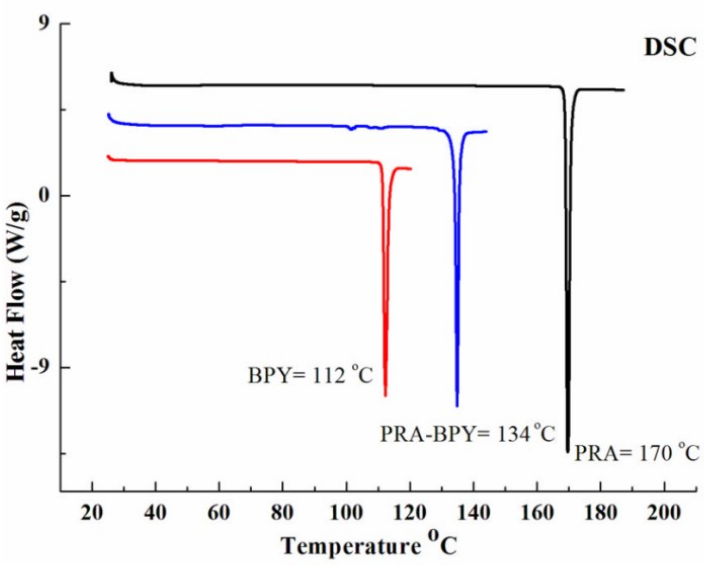

Fig. S5 DSC plot of PRA (melting point 170°C), 4,4′–bipyridine(melting point 112°C) and PRA-BPY cocrystal (melting point 134°C)

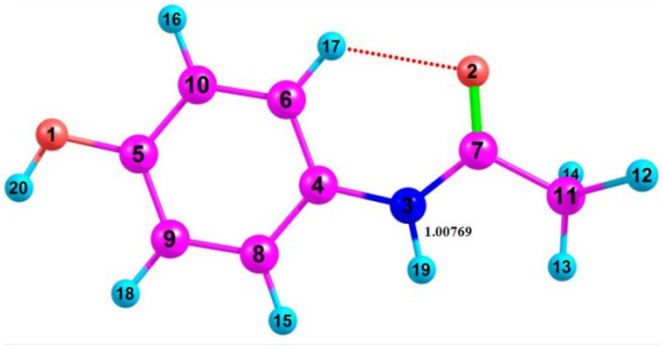

Fig. S6 Optimized structure of paracetamol

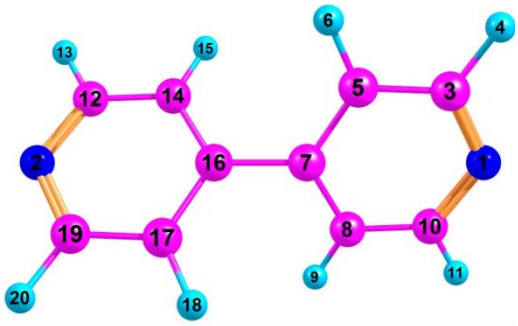

Fig. S7 Optimized structure of 4,4′–bipyridine

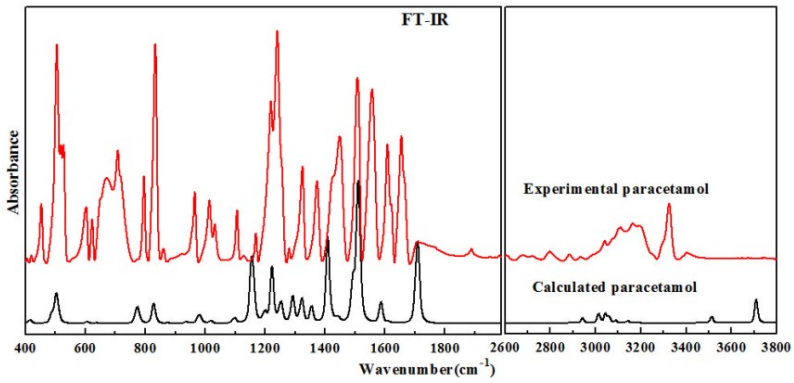

Fig. S8 Experimental and calculated (scaled) IR absorbance spectra of paracetamol in the region 400-1900cm^{-1} and 2600-3800cm^{-1}.

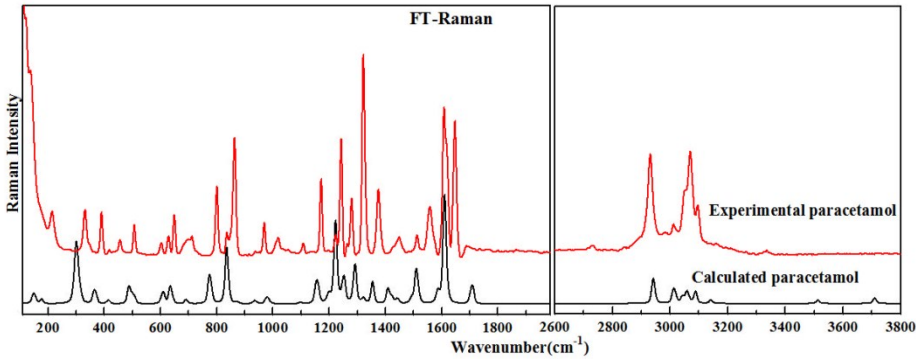

Fig. S9 Experimental and calculated (scaled) Raman scattering spectra of paracetamol in the region 100-1900cm^{-1} and 2600-3800cm^{-1}

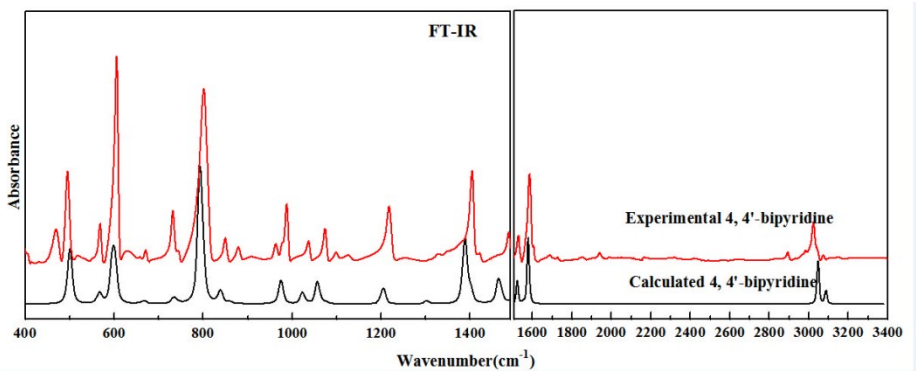

Fig. S10 Experimental and calculated (scaled) IR absorbance spectra of 4, 4′–bipyridine in the region 400-1500cm^{-1} and 1600-3400cm^{-1}.

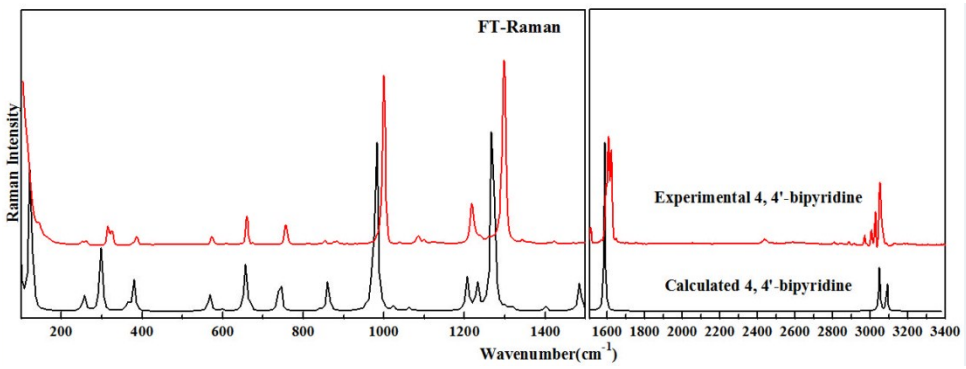

Fig. S11 Experimental and calculated (scaled) Raman scattering spectra of 4, 4′–bipyridine in the region 100-1500cm^{-1} and 1600-3400cm^{-1}

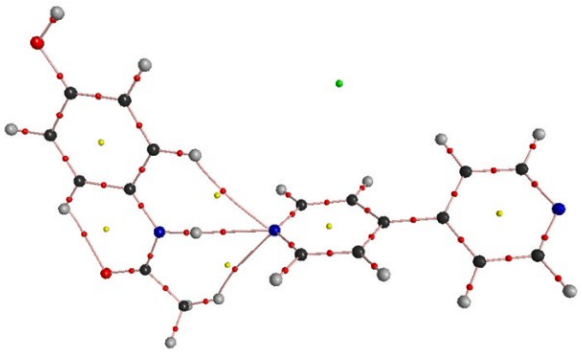

Fig. S12 Molecular graph of PRA-BPY (monomer) of cocrystal: bond critical points (small red spheres), ring critical points (small yellow sphere), bond paths (pink lines).

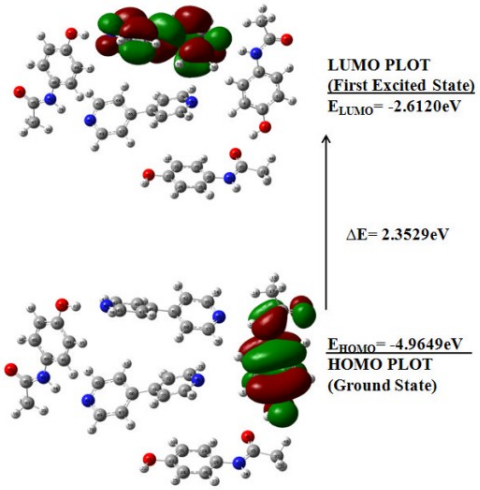

Fig. S13 HOMO-LUMO plot of PRA3-BPY2 (dimer +PRA) with orbitals involved in electronic transitions.

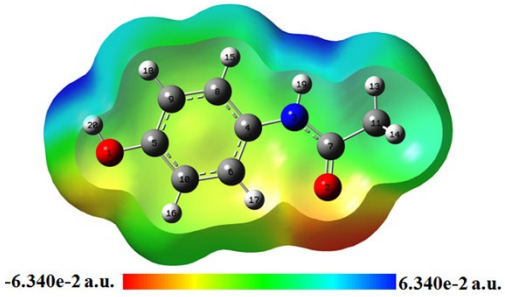

Fig. S14 Molecular electrostatic potential (MEP) formed by mapping of total density over electrostatic potential in the gas phase for the monomer of paracetamol.

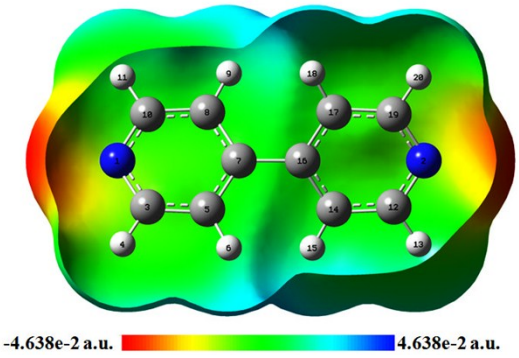

Fig. S15 Molecular electrostatic potential (MEP) formed by mapping of total density over electrostatic potential in the gas phase for the monomer of 4,4′–bipyridine.

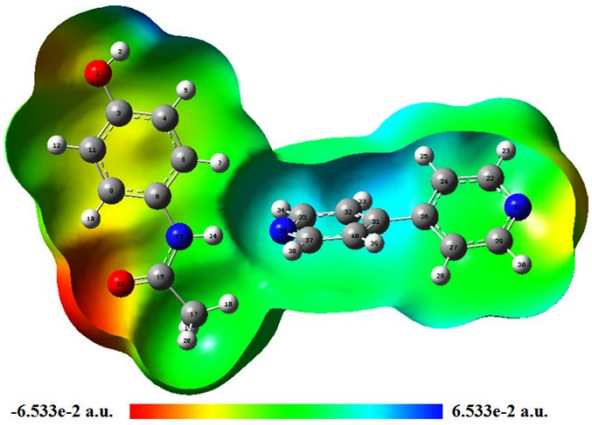

Fig. S16 Molecular electrostatic potential (MEP) formed by mapping of total density over electrostatic potential in the gas phase for the monomer of cocrystal (PRA-BPY).

Part II. TABLES

Table S1 The experimental and calculated geometric parameters of PRA-BPY cocrystal and calculated geometric parameters of, monomer and dimer+PRA of cocrystal using DFT/6-311g (d, p), bond lengths in angstrom (Å) and bond angles in degrees (°).

Geometrical parameters	Experimental	Computational optimized parameter at B3LYP/6-311g(d,p)	
		Monomer	Dimer+PRA
Bond length(Å)			
R(O1-H2)	0.90699	0.9623	0.9756
R(O1-C3)	1.35752	1.3710	1.3658
R(C3-C4)	1.39579	1.3946	1.3976
R(C3-C11)	1.38936	1.3940	1.3958
R(C4-H5)	0.95010	1.0865	1.0843
R(C4-C6)	1.38087	1.3908	1.3907
R(C6-H7)	0.94944	1.0843	1.0846
R(C6-C8)	1.39645	1.4004	1.4006
R(C8-C9)	1.39435	1.4034	1.4024
R(C8-N13)	1.41896	1.4134	1.4168
R(C9-H10)	0.95023	1.0786	1.0787
R(C9-C11)	1.38176	1.3897	1.3905
R(C11-H12)	0.95020	1.0835	1.0839
R(N13-H14)	0.88353	1.0191	1.0174
R(N13-C15)	1.34583	1.3717	1.3695
R(H14-N36)	2.04744	2.1068	2.1612
R(C15=O16)	1.23531	1.2201	1.2209
R(C15-C17)	1.50413	1.5226	1.5238
R(C17-H18)	0.98037	1.0907	1.0908
R(C17-H19)	0.97924	1.0921	1.0931
R(C17-H20)	0.98014	1.0924	1.0917
R(N21-C22)	1.33606	1.3359	1.3379
R(N21-C29)	1.33227	1.3359	1.3371
R(C22-H23)	0.94993	1.0863	1.0852
R(C22-C24)	1.38491	1.3917	1.3893
R(C24-H25)	0.94885	1.0835	1.0829
R(C24-C26)	1.38888	1.3993	1.3997
R(C26-C27)	1.39156	1.3992	1.4001
R(C26-C31)	1.48638	1.4827	1.4830
R(C27-H28)	0.95045	1.0835	1.0830
R(C27-C29)	1.38619	1.3917	1.3900
R(C29-H30)	0.94927	1.0863	1.0854
R(C31-C32)	1.39294	1.3999	1.3998
R(C31-C40)	1.38388	1.4000	1.3994
R(C32-H33)	0.95029	1.0830	1.0831
R(C32-C35)	1.37931	1.3896	1.3901

R(H34-C35)	0.94788	1.0858	1.0857
R(C35-N36)	1.33131	1.3383	1.3374
R(N36-C37)	1.33620	1.3382	1.3369
R(C37-H38)	0.95011	1.0857	1.0854
R(C37-C40)	1.37866	1.3896	1.3901
R(H39-C40)	0.94803	1.0830	1.0829
Bond Angle (°)			
A(H2-O1-C3)	109.15655	109.0016	110.4978
A(O1-C3-C4)	123.60911	122.9563	123.0604
A(O1-C3-C11)	117.83893	117.8813	118.0543
A(C4-C3-C11)	118.54728	119.1624	118.8852
A(C3-C4-H5)	119.95204	120.1987	120.5526
A(C3-C4-C6)	120.05989	120.1361	120.0731
A(H5-C4-C6)	119.98807	119.6651	119.3731
A(C4-C6-H7)	119.30241	119.4896	118.4396
A(C4-C6-C8)	121.35736	121.0107	121.2078
A(H7-C6-C8)	119.34022	119.4996	120.3523
A(C6-C8-C9)	118.44428	118.5495	118.5399
A(C6-C8-N13)	117.12806	117.6303	117.752
A(C9-C8-N13)	124.38023	123.8201	123.7079
A(C8-C9-H10)	119.95984	119.1507	119.2479
A(C8-C9-C11)	120.04522	120.2130	120.0858
A(H10-C9-C11)	119.99493	120.6361	120.6660
A(C3-C11-C9)	121.53742	120.928	121.2067
A(C3-C11-H12)	119.23542	118.7301	118.6122
A(C9-C11-H12)	119.22716	120.3419	120.1810
A(C8-N13-H14)	113.67730	115.2737	115.3662
A(C8-N13-C15)	128.22651	127.9256	128.0949
A(H14-N13-C15)	117.97706	116.8006	116.5354
A(N13-C15=O16)	123.40463	124.8105	124.9982
A(N13-C15-C17)	115.49467	114.3675	114.3459
A(O16=C15-C17)	121.09201	120.8219	120.6552
A(C15-C17-H18)	109.48015	113.9832	113.8604
A(C15-C17-H19)	109.43937	108.3334	108.5758
A(C15-C17-H20)	109.48058	108.3462	108.1736
A(H18-C17-H19)	109.50264	109.3974	109.3642
A(H18-C17-H20)	109.40821	109.3537	109.4456
A(H19-C17-H20)	109.51638	107.2050	107.2057
A(C22-N21-C29)	116.19520	116.8965	117.5614
A(N21-C22-H23)	117.98103	116.1090	115.9574
A(N21-C22-C24)	123.91516	123.8291	123.2834
A(H23-C22-C24)	118.10381	120.0615	120.7524
A(C22-C24-H25)	120.22754	119.8974	119.6661
A(C22-C24-C26)	119.52001	119.1686	119.4003
A(H25-C24-C26)	120.25244	120.9150	120.8999
A(C24-C26-C27)	116.94167	117.1087	117.0789
A(C24-C26-C31)	121.43154	121.4248	121.2946
A(C27-C26-C31)	121.62317	121.4665	121.6187
A(C26-C27-H28)	120.36249	120.9158	120.9292
A(C26-C27-C29)	119.19822	119.1651	119.3685
A(H28-C27-C29)	120.43927	119.9002	119.6958
A(N21-C29-C27)	124.21708	123.8308	123.2914
A(N21-C29-H30)	117.93340	116.1108	116.2597
A(C27-C29-H30)	117.84950	120.0580	120.4486
A(C26-C31-C32)	121.69957	121.4829	121.6396
A(C26-C31-C40)	121.53464	121.4959	121.2844
A(C32-C31-C40)	116.76575	117.0212	117.0685
A(C31-C32-H33)	120.37808	120.8329	120.9874
A(C31-C32-C35)	119.24558	119.3841	119.2858
A(H33-C32-C35)	120.37630	119.7665	119.7163
A(C32-C35-H34)	117.60059	120.3678	120.2843
A(C32-C35-N36)	124.22751	123.4599	123.5122
A(H34-C35-N36)	118.17185	116.1718	116.2033
A(H14-N36-C35)	108.23330	118.2907	122.4445
A(H14-N36-C37)	132.40810	124.4086	119.8167
A(C35-N36-C37)	116.16888	117.2925	117.3136
A(N36-C37-H38)	118.11777	116.1974	116.2061
A(N36-C37-C40)	123.77504	123.4549	123.4394
A(H38-C37-C40)	118.10718	120.3469	120.3504
A(C31-C40-C37)	119.81521	119.3870	119.3792
A(C31-C40-H39)	120.34107	120.8174	120.9096

A(C37-C40-H39)	119.84371	119.7786	119.6821
Dihedral angle(°)			
D(H2-O1-C3-C4)	-3.29151	-0.1377	-2.3896
D(H2-O1-C3-C11)	175.90832	179.8353	177.7164
D(O1-C3-C4-H5)	-0.25107	0.0871	0.28658
D(O1-C3-C4-C6)	179.72687	-179.995	179.8797
D(C11-C3-C4-H5)	-179.44558	-179.886	-179.8203
D(C11-C3-C4-C6)	0.53236	0.032	-0.2271
D(O1-C3-C11-C9)	-179.09162	179.9617	-179.7292
D(O1-C3-C11-H12)	0.92003	-0.0547	0.1606
D(C4-C3-C11-C9)	0.14973	-0.0642	0.37238
D(C4-C3-C11-H12)	-179.83861	179.9194	-179.7378
D(C3-C4-C6-H7)	179.57548	-179.878	179.7073
D(C3-C4-C6-C8)	-0.46365	0.0491	-0.12823
D(H5-C4-C6-H7)	-0.44659	0.0405	-0.69478
D(H5-C4-C6-C8)	179.51428	179.9672	179.4697
D(C4-C6-C8-C9)	-0.28711	-0.0968	0.3389
D(C4-C6-C8-N13)	177.31887	179.8099	-179.4949
D(H7-C6-C8-C9)	179.67374	179.8298	-179.4934
D(H7-C6-C8-N13)	-2.72027	-0.2634	0.67262
D(C6-C8-C9-H10)	-179.04645	-179.838	-180.0000
D(C6-C8-C9-C11)	0.96192	0.0644	-0.19435
D(N13-C8-C9-H10)	3.53532	0.262	-0.17653
D(N13-C8-C9-C11)	-176.45632	-179.836	179.62897
D(C6-C8-N13-H14)	-11.79471	-1.3411	-2.56881
D(C6-C8-N13-C15)	172.29849	178.5899	176.71926
D(C9-C8-N13-H14)	165.65462	178.5603	177.60657
D(C9-C8-N13-C15)	-10.25219	-1.5087	-3.10536
D(C8-C9-C11-C3)	-0.90819	0.0154	-0.16057
D(C8-C9-C11-H12)	179.08016	-179.968	179.95134
D(H10-C9-C11-C3)	179.10019	179.9158	179.64214
D(H10-C9-C11-H12)	-0.91147	-0.0674	-0.24596
D(C8-N13-N36-C35)	-89.00455	-83.5266	-111.42993
D(C8-N13-N36-C37)	68.51244	95.0264	61.07241
D(C15-N13-N36-C35)	83.45138	94.0808	68.24209
D(C15-N13-N36-C37)	-119.03162	-87.3662	-119.25557
D(C8-N13-C15=O16)	-5.57130	0.2929	1.10497
D(C8-N13-C15-C17)	173.36507	-179.608	-179.19769
D(H14-N13-C15=O16)	178.67366	-179.777	-179.61407
D(H14-N13-C15-C17)	-2.38997	0.3222	0.08327
D(N13-C15-C17-H18)	13.95709	-1.5295	6.69420
D(N13-C15-C17-H19)	-106.06734	-123.559	-115.38770
D(N13-C15-C17-H20)	133.89113	120.4533	128.58720
D(O16=C15-C17-H18)	-167.07978	178.5653	-173.59401
D(O16-C15-C17-H19)	72.89578	56.5359	64.32410
D(O16-C15-C17-H20)	-47.14575	-59.4519	-51.70100
D(C29-N21-C22-H23)	179.30124	179.604	179.96469
D(C29-N21-C22-C24)	-0.73022	-0.1682	0.90697
D(C22-N21-C29-C27)	0.46556	-0.1662	-1.0138
D(C22-N21-C29-H30)	-179.48855	179.5989	179.1512
D(N21-C22-C24-H25)	-179.93230	178.7478	178.0738
D(N21-C22-C24-C26)	0.01463	0.3203	0.1644
D(H23-C22-C24-H25)	0.03620	-1.0159	-0.9404
D(H23-C22-C24-C26)	179.98313	-179.443	-178.85
D(C22-C24-C26-C27)	0.95517	-0.1344	-1.1157
D(C22-C24-C26-C31)	-178.36300	179.8623	177.8849
D(H25-C24-C26-C27)	-179.09792	-178.545	-178.999
D(H25-C24-C26-C31)	1.58391	1.4513	0.002
D(C24-C26-C27-H28)	178.76785	-178.589	-178.054
D(C24-C26-C27-C29)	-1.19390	-0.169	1.0172
D(C31-C26-C27-H28)	-1.91539	1.4146	2.949
D(C31-C26-C27-C29)	178.12286	179.8343	-177.98
D(C24-C26-C31-C32)	20.21308	38.7268	36.5488
D(C24-C26-C31-C40)	-159.86246	-141.248	-142.428
D(C27-C26-C31-C32)	-159.07309	-141.277	-144.496
D(C27-C26-C31-C40)	20.85137	38.7487	36.5275
D(C26-C27-C29-N21)	0.50684	0.3373	0.0467
D(C26-C27-C29-H30)	-179.53902	-179.419	179.8751
D(H28-C27-C29-N21)	-179.45488	178.7733	179.1295
D(H28-C27-C29-H30)	0.49927	-0.983	-1.0422
D(C26-C31-C32-H33)	0.17561	1.4251	2.4824

D(C26-C31-C32-C35)	-179.89307	179.9414	-178.699
D(C40-C31-C32-H33)	-179.75228	-178.599	-178.5
D(C40-C31-C32-C35)	0.17905	-0.0829	0.3189
D(C26-C31-C40-C37)	-179.71988	179.894	178.6195
D(C26-C31-C40-H39)	0.32803	1.3941	0.5887
D(C32-C31-C40-C37)	0.20813	-0.0817	-0.4017
D(C32-C31-C40-H39)	-179.74395	-178.582	-178.433
D(C31-C32-C35-H34)	179.57828	-179.574	-179.874
D(C31-C32-C35-N36)	-0.33665	0.1572	-0.0349
D(H33-C32-C35-H34)	-0.49039	-1.0419	-1.0394
D(H33-C32-C35-N36)	179.59467	178.6895	178.7993
D(C32-C35-N36-H14)	162.44077	178.9594	172.3252
D(C32-C35-N36-C37)	0.07126	-0.0511	-0.1688
D(H34-C35-N36-H14)	-17.47372	-1.2988	-7.8301
D(H34-C35-N36-C37)	-179.84322	179.6907	179.6759
D(H14-N36-C37-H38)	23.26936	0.6118	6.6467
D(H14-N36-C37-C40)	-156.71769	-179.072	-172.622
D(C35-N36-C37-H38)	-179.66065	179.5557	179.347
D(C35-N36-C37-C40)	0.35230	-0.1286	0.0787
D(N36-C37-C40-C31)	-0.50081	0.197	0.2127
D(N36-C37-C40-H39)	179.45152	178.7127	178.268
D(H38-C37-C40-C31)	179.51215	-179.475	-179.027
D(H38-C37-C40-H39)	-0.53553	-0.9591	-0.9712

Table S2 Theoretical and experimental vibrational wavenumbers (cm^{-1}) of paracetamol

Unscaled	Scaled	IR	RAMAN	Assignment(% PED)
3835	3711	3325		[ν(O1H20)](100)
3630	3513	3294		[ν(N3H19)](100)
3246	3141	3163		R1[ν(CH)](98)
3191	3089	3113	3096	R1[ν(CH)](98)
3163	3061		3071	R1[ν(CH)](99)
3146	3045	3042	3052	R1[ν(CH)](99)
3116	3016		3013	[ν_s(C11H_3)](59)+[ν_a(C11H_3)](39)
3115	3015			[ν_s(C11H_3)](54)+[ν_a(C11H_3)](46)
3041	2944	2937	2932	[ν_s(C11H_3)](100)
1765	1708	1655	1648	[ν(C7=O2)](76)+[ν(C7N3)](5)
1665	1612	1608	1610	R1[ν(CC)(61)+δ_a(11)+δ_{in}(CH)(12)]
1639	1586	1558	1559	R1[ν(CC)(60) +δ_a'(7)]+[ρ(N3H19)](7)
1562	1512	1508	1513	[ρ(N3H19)](38)+[ν(C7N3)](14)+R1[ν(C4N3)(10)+δ_{in}(CH)(8)+ν(CC)(7)]
1542	1493			R1[δ_{in}(CH)(46)+ν(CC)(29)+ν(C5O1)(8)]+[ρ(N3H19)](6)
1492	1444	1450	1449	δ_a'(CH_3)(62)+δ_a(CH_3)(20)+δ_{sym}(CH_3)(5)+ρ'(CH_3)(5)
1469	1422	1423		δ_a(CH_3)(68)+δ_a'(CH_3)(23)+ρ(CH_3)(7)
1456	1410			R1[ν(CC)(32)+δ_{in}(CH)(23)+δ(C5H20O1)(7)]+[ρ(N3H19)](8)+[ν(C7N3)](5)
1400	1355	1373	1374	δ_{sym}(CH_3)(85)+[ν(C7C11)](7)
1366	1322	1325	1322	R1[ν(CC)(54)+ δ_{in}(CH)(25)+δ(C5H20O1)(16)]
1335	1292	1280	1280	R1[δ_{in}(CH)(37)+ν(CC)(30)+ν(C4N3)(8)]+[ν(C7N3)](7)
1293	1252	1240	1243	R1[ν(C5O1)(41)+ν(CC)(30)+δ_{tri}(5)+δ_{in}(CH)(5)]
1264	1223	1219	1224	R1[ν(C4N3)(18)+δ_{in}(CH)(16)+δ_{tri}(11)+ν(C5O1)(6)+ν(CC)(8)]+[ρ(N3H19)](14)+[ν(C7N3)](9)
1237	1198	1171	1172	R1[ν(C4N3)(17)+δ_{tri}(6)]+[ν(C7N3)](17)+[ν(C7C11)](13)+[δ_{sci}(C7C11)](7)+ [ρ(C7C11)](6)+ρ'(CH_3)(5)
1196	1157			R1[δ_{in}(CH)(62)+ν(CC)(9)+ν(C5O1)(5)+δ(C5H20O1)(11)]
1195	1157			R1[δ(C5H20O1)(39)+δ_{in}(CH)(15)+ν(CC)(25)]
1133	1097	1107	1108	R1[δ_{in}(CH)(60)+ν(CC)(23)]
1052	1018	1032	1019	ρ(CH_3)(55)+ρ'(CH_3)(19)+[ω(C7C11)](16)+δ_a(CH_3)(7)
1027	994	1014		R1[δ_{tri}(40)+ν(CC)(39)+δ_{in}(CH)(5)]
1012	980			ρ'(CH_3)(45)+ρ(CH_3)(15)+[ν(C7C11)](8)+[ν(C7N3)](7)+R1[δ_{tri}](7)
986	954	966	969	R1[δ_{out}(CH)(86)+puck(6)]
966	935		937	[ν(C7C11)](29)+[δ_{sci}(C7C11)](18)+[δ_{sci}(N3H19)](17)+[ν(C7N3)](15)+R1[ν(CC)](6)
904	875	862	863	R1[δ_{out}(CH)(80)+puck(12)]
865	837	833	836	R1[ν(CC)(46)+ν(C5O1)(8)+δ_a(15)+ν(C4N3)(10)]+δ_{sci}(N3H19)](6)
855	828			R1[δ_{out}(CH)(72)+δ_{ou}t(C5O1)(9)+τ_a(8)]
803	777	796	802	R1[δ_{tri}(25)+ν(C5O1)(17)+ν(CC)(6)+ν(C4N3)(6)]+[δ_{sci}(N3H19)](12)+[ν(C7C11)](9)+[δ_{sci}(C7C11)](5)
797	771			R1[δ_{out}(CH)(81)+τ_a(6)+δ_{out}(C5O1)(5)]
715	692	710	713	R1[puck(65)+δ_{out}(C5O1)(15)+δ_{out}(C4N3)(14)]
658	637	623	630	R1[δ_a'(64)+δ_{in}(C5O1)(6)+δ_{in}(C4N3)(5)]

630	609	604	603	[ν(C7C11)](19)+[δ_{sci}(C7C11)](18)+R1[δ_a'(14)+δ_a(14)+ν(C4N3)(5)]+[δ_{sci}(N3H19)](8)
626	606			[ω(C7C11)](59)+ [τ(C7N3)](14)+ρ(CH_3)(12)
526	509	519	508	R1[δ_{out}(C4N3)(30)+τ_a(28)+δ_{out}(C5O1)(27)]+[ω(N3H19)](6)
522	506	505		[ω(N3H19)](39)+[τ(C7N3)](22)+[ω(C7C11)](17)+R1[δ_{out}(C5O1)(6) +τ_a(5)]
507	490	455	456	[ρ(C7C11)](38)+R1[δ_a](33)+[δ_{sci}(C7C11)](8)+ρ'(CH_3)(6)
430	416	420	418	R1[δ_{in}(C5O1)(51)+δ_a'(18)+δ_{in}(C4N3)(16)]+[δ_{sci}(C7C11)](7)
423	409			R1[τ_a'(81)+δ_{out}(CH)(11)]
380	367	-	390	R1[puck(36)+δ_{out}(C5O1)(18)+δ_{out}(C4N3)(18)+δ_{out}(CH)(5)]+[τ(C7N3)](7)
327	316	-	333	[ρ(C7C11)](29)+[δ_{sci}(C7C11)](14)+[δ_{sci}(N3H19)](5)+R1[δ_{in}(C4N3)(14)+δ_a(12)+δ_{in}(C5O1)(9)+ν(C4N3)(6)]
315	304	-		R1[δ_{in}(C4N3)(23)+δ_{in}(C5O1)(9)+δ_a(9)+ν(C4N3)(5)+ν(C8C9)(5)]+[δ_{sci}(N3H19)](19)+[δ_{sci}(C7C11)](10)+[ν(C7N3)](9)+[ρ(C7C11)](5)
308	299	-		R1[τ(C5O1)](93)
185	179	-	215	R1[τ_a(55)+δ_{out}(C10H16)(6)]+[τ(C7N3)](15)+[ω(N3H19)](9)
156	151	-	138	[δ_{sci}(N3H19)](44)+R1[δ_{in}(C4N3)](33)+[ρ(C7C11)](10)
78.2	75.7	-	-	R1[τ_a(25)+δ_{out}(C4N3)(13)]+[τ(C7C11)](20)+[τ(C7N3)](17)+ [ω(N3H19)](13)
49.6	48	-	-	R1[τ(C4N3)](47)+[τ(C7C11)](26)+[ω(C7C11)](10)+[τ(C7N3)](9)
42.8	41.4	-	-	[τ(C7C11)](51)+[ω(C7C11)](12)+[τ(C7N3)](12)+[ω(N3H19)](9)+R1[τ(C4N3)](9)

Table S3 Theoretical and experimental vibrational wavenumbers (cm^{-1}) of 4,4'–bipyridine

Unscaled	Scaled	IR	Raman	Assignment(%PED)
3191	3089	3074	3088	R2[ν(CH)](49)+R1[ν(CH)](44)
3190	3088			R2[ν(CH)](51)+ R1[ν(CH)](45)
3186	3084			R2[ν(CH)](44)+R1[ν(CH)](48)
3185	3083			R1[ν(CH)](50)+R2[ν(CH)](44)
3151	3049	3024	3052	R1[ν(CH)](69)+ R2[ν(CH)](24)
3150	3049			R2[ν(CH)](69)+R1[ν(CH)](24)
3148	3047			R1[ν(CH)](89)+ R2[ν(CH)](5)
3147	3046			R2[ν(CH)](89)
1638	1585	1606	1606	R1[ν(CC)](28)+ ν(C7C16)(8)+δ_a(5)]+ R2[ν(CC)(28)+δ_a(5)]
1632	1580	1585	1596	R2[ν(CC)(22)+δ_a(5)]+ R1[ν(CC)(22)+δ_a(5)]
1606	1554	1529		R1[ν(CC)(22)+ν(C3N1)(6)+ν(C10N1)(6)+δ_a'(5)]+R2[ν(CC)(22)+ν(C19N2)(6)+ν(C12N2)(6)+δ_a'(5)]
1575	1524		1511	R2[ν(CC)(20)+ν(C19N2)(8)+ν(C12N2)(8)+δ_a'(6)]+R1[ν(CC)(20)+ν(C3N1)(8)+ ν(C10N1)](8)+δ_a'(6)]
1535	1486	1487		R2[δ_{in}(CH)(20)+ν(C19N2)(5)+ν(C12N2)(5)]+R1[δ_{in}(CH)(20)+ν(C7C16)(8)+ν(C10N1)(5) +ν(C3N1)(5)]
1514	1466			R1[δ_{in}(CH)(34)+ν(C10N1)(5)+ν(C3N1)(5)]+R2[δ_{in}(CH)(34)+ν(C19N2)(5)+ν(C12N2)(5)]
1448	1401	1404	1423	R2[δ_{in}(CH)(28)+ν(CC)](16)]+ R1[δ_{in}(CH)(28)+ ν(CC)(16)]
1435	1389			R1[δ_{in}(CH)(30)+ν(CC)(16)]+R2[δ_{in}(CH)(30)+ν(CC)(16)]
1362	1319			R1[δ_{in}(CH)](42) +R2[δ_{in}(CH)](42)
1347	1303			R2[δ_{in}(CH)](24)+ R1[δ_{in}(CH)](24)
1312	1270		1297	R1[ν(C7C16)(43)+δ_{tri}(8)]+R2[δ_{tri}](8)
1272	1231		1239	R1[ν(C10N1)(11)+ν(C3N1)(11)+ν(C7C8)(24)]+R2[ν(C19N2)(11)+ν(C12N2)(11)+ν(CC)(24)]
1256	1216	1219	1218	R2[ν(CC)(20)+ν(C19N2)(10)+ν(C12N2)(10)]+R1[ν(C3N1)(10)+ν(C10N1)(10)+ν(CC)(20)]
1247	1207			R2[δ_{in}(CH)](34)+ν(C12N2)(5)+ν(C19N2)(5)]+R1[δ_{in}(CH)](34)
1245	1205			R1[δ_{in}(CH)(34)+ν(C10N1)(5)+ν(C3N1)(5)]+R2[δ_{in}(CH)(34)+ν(C12N2)(5)+ν(C19N2)(5)]
1113	1078	1099	1101	R1[ν(CC)(20)+δ_{in}(CH)(14)]+ R2[ν(CC)(19)+δ_{in}(CH)(14)]
1112	1076	1074	1087	R2[δ_{in}(CH)(20)+ν(CC)(20)]+R1[δ_{in}(CH)(20)+ν(CC)(20)]
1097	1062		1040	R1[δ_{tri}(10)+δ_{in}(CH)(16)+ν(C10N1)(7)+ν(C3N1)(7)]+R2[δ_{tri}(10)+δ_{in}(CH)(14)+ν(C19N2)(7)+ ν(C12N2)(7)]
1093	1058			R2[δ_{in}(CH)(20)+ν(CC)(12)+ν(C12N2)(6)+ν(C19N2)(6)]+R1[δ_{in}(CH)(20)+ν(CC)(12)+ ν(C10N1)(6)+ν(C3N1)(6)]
1058	1024	1038	1039	R2[δ_{tri}(27)+ν(CC)(12)]+ R1[δ_{tri}(27)+ν(CC)(12)]
1014	982	987	1000	R1[δ_{tri}(22)+ν(C10N1)(5)+ν(C3N1)(5)]+R2[δ_{tri}(21)+ν(C19N2)(5)+ν(C12N2)(5)]
1008	976	977		R2[δ_{tri}(22)+ν(C12N2)(6)+ν(C19N2)(6)]+R1[δ_{tri}(22)+ν(C10N1)(6)+ν(C3N1)(6)]
1006	973			R2[δ_{out}(CH)(54)+τ_a'(5)]+ R1[δ_{out}(CH)](38)
1005	973			R1[δ_{out}(CH)](51)+ R2[δ_{out}(CH)](25)
989	957	964		R2[δ_{out}(CH)(40)+puck(9)]+ R1[δ_{out}(CH)(39)+puck(9)]
986	954			R1[δ_{out}(CH)](43)+puck(8)]+ R2[δ_{out}(CH)(40)+puck(8)]
890	862	879	884	R1[δ_{out}(CH)](54) + R2[δ_{out}(CH)](45)
890	861		854	R2[δ_{out}(CH)](54)+ R1[δ_{out}(C3H4)](44)
867	839	850		R2[δ_{out}(C16C7)(10) +δ_{out}(CH)(32)] +R1[δ_{out}(CH)(32) +δ_{out}(C7C16)(10)]

821	795	802		R1[δ_{out}(CH)](46)+ R2[δ_{out}(C17H18)](46)
768	743	744	757	R1[puck(34) +δ_{out}(C7C16)(7)]+ R2[puck(34)+δ_{out}(C16C7)(7)]
767	742			R2[δ_a(24)+ν(CC)(10)+δ_{tri}(5)]+R1[δ_a(24)+ν(C7C16)(17)+ν(CC)(10)+δ_{tri}(5)]
759	735	733		R2[puck](40)+R1[puck](40)
690	668	671	674	R1[δ_a'](44) +R2[δ_a'](43)
678	656		661	R2[δ_a'](45)+R1[δ_a'](45)
619	600	606	609	R1[δ_a](45)+R2[δ_a](45)
586	567	569	574	R2[δ_{out}(C16C7)(19)+τ_a(16)+puck(7)]+ R1[δ_{out}(C7C16)(19)+τ_a(16)+puck(7)]
518	501	496		R1[τ_a(21)+δ_{out}(C7C16)(13)+δ_{in}(C7C16)(9)+R2[τ_a(21)+δ_{out}(C16C7)(13)+δ_{in}(C16C7)(9)]
392	380	-	387	R2[τ_a'](42)+ R1[τ_a'](42)
387	375	-		R1[τ_a'](43)+R2[τ_a'](42)
376	364	-	325	R1[τ_a(21)+δ_{in}(C7C16)(17)+δ_{out}(C7C16)(5)]+R2[τ_a(21)+δ_{in}(C16C7)(17)+δ_{out}(C16C7)(5)]
308	298	-		R1[ν(C7C16)(27)+δ_a(25)]+R2[δ_a](25)
264	256	-	262	R1[τ_a(29)+δ_{in}(C7C16)(7)]+ R2[τ_a(29)+δ_{in}(C16C7)(7)]
128	124	-	144	R1[δ_{in}(C7C16)(31)+τ_a(8)]+ R2[δ_{in}(C16C7)(31)+τ_a(8)]
94.1	91.1	-	-	R1[δ_{out}(C7C16)(26)+τ_a(8)]+R2[δ_{out}(C16C7)(26)+τ_a(8)]+[τ(C7C16)](7)
63	61	-	-	[τ(C7C16)](89)

Table S4 Experimental and theoretical vibrational wavenumbers (cm^{-1}) of cocrystal with potential energy distribution (PED).

Unscaled	Scaled	IR	Raman	Assignment(%PED)	Calculated scaled freq	Simplified description of modes of PRA3-BPY2(dimer+PRA)
3836	3713	3224	-	[ν(O1H2)](100)	3709,3464,3403	OH stretch
3429	3319	3142	-	[ν(N13H14)](95)	3508,3381,3351	NH stretch
3245	3141			R1[ν(CH)](98)	3145,3138,3135	Ring CH stretch
3196	3093	3100		R2[ν(CH)](84)+R3[ν(CH)](5)	3095,3094,3092,3091	Ring CH stretch
3195	3092			R2[ν(CH)](88)+R3[ν(CH)](5)	3090,3089,3086,3085	Ring CH stretch
3188	3086			R3[ν(CH)](89)+R2[ν(CH)](6)	3069,3064,3064,3063	Ring CH stretch
3188	3085			R1[ν(CH)](97)	3095,3083,3082	Ring CH stretch
3187	3084			R3[ν(CH)](87)+R2[ν(CH)](6)	3064,3064,3063	Ring CH stretch
3178	3076			R1[ν(CH)](99)	3081,3079,3068	Ring CH stretch
3162	3061		3063	R2[ν(CH)](96)	3060	Ring CH stretch
3160	3058			R2[ν(CH)](95)	3057	Ring CH stretch
3154	3052			R3[ν(CH)](92)	3056	Ring CH stretch
3151	3050			R3[ν(CH)](95)	3052	Ring CH stretch
3145	3044	3036	3044	R1[ν(CH)](99)	3066,3065,3049	Ring CH stretch
3125	3025	3028	3013	[ν_a($C17H_3$)](100)	3036,3026,3024	CH_3asym stretch
3108	3008		2992	[ν_a($C17H_3$)](99)	3007,3006,3004	CH_3asym stretch
3043	2945	2924	2925	[ν_s($C17H_3$)](100)	2944,2942,2942	CH_3sym stretch
1758	1701	1645	1650	[ν(C15=O16)](60)+[ρ(N13H14)](16)+[τ(N13H14)](6)	1704,1698,1668	C=O stretch
1665	1612	1620	1621	R1[ν(CC)(54)+δ_a(9)+δ_{in}(CH)(10)]+[ρ(N13H14)](7)	1611,1610,1609	Ring CC stretch
1649	1596	1598	1609	[ρ(N13H14)](37)+[τ(N13H14)](17)+R1[ν(CC)](17)	1591,1588,1588	NH rocking
1643	1590		1600	R2[ν(CC)(48)+δ_a'(7)+δ_{in}(CH)(12)]+R3[ν(C26C31)](6)	1592,1589	Ring CC stretch
1633	1581	1574	1567	R3[ν(CC)(50)+δ_a(8)+δ_{in}(CH)(13)]	1586,1582	Ring CC stretch
1606	1554		1550	R3[ν(CC)(24)+ν(C22N21)(7)+ν(C29N21)(7)+δ_a'(6)]+R2[ν(CC)(21)+ν(C35N36)](6)+ν(C37N36)(6)]	1556,1554	Ring CC stretch
1598	1547	1533	1536	[ρ(N13H14)](44)+[τ(N13H14)](23)+R1[ν(CC)](5)+[ν(C15N13)](5)	1545,1538	NH rocking
1575	1525	1504	1513	R2[ν(CC)(22)+ν(C37N36)(9)+ν(C35N36)(9)]+R3[ν(CC)(18)+ν(C22N21)(8)+ν(C29N21)(8)+δ_a'(5)]	1525,1524	Ring CC stretch
1544	1495			R1[δ_{in}(CH)(46)+ν(C3O1)(7)+ν(CC)(33) +ν(C8N13)(7)]	1494,1493,1490	Ring in plane CH deformation
1538	1488	1488	1488	R2[δ_{in}(CH)(32)+ν(C35N36)(5)+ν(C37N36)(5)]+R3[ν(CC)](16)	1491,1489	Ring in plane CH deformation
1516	1468	1471	1465	R3[δ_{in}(CH)(40)+ν(C29N21)(6)+ν(C22N21)(6)]+ R2[δ_{in}(CH)](27)	1470,1469	Ring in plane CH deformation
1490	1443	1448	1457	δ_a'(CH_3)(56)+δ_a(CH_3)(25)+ρ(CH_3)(7)+ δ_{sym}(CH_3)(5)	1450,1445,1444	Asym CH_3def
1479	1432		1430	δ_a(CH_3)(64)+δ_a'(CH_3)(28)+ρ'(CH_3)(8)	1433,1430,1424	Asym CH_3def
1461	1414	1404	1424	R1[ν(CC)(31)+δ_{in}(CH)(21)+δ(C3H2O1)(6)]+[ρ(N13H14)](10)+[τ(N13H14)](7)	1423,1421,1409	Ring CC stretch
1450	1404			R2[δ_{in}(CH)](38)+ν(C37C40)(22)]+R3[δ_{in}(CH)(12)+ν(CC)(10)]	1406,1404	Ring in plane CH deformation
1437	1391	1376	1380	R3[δ_{in}(CH)(36)+ν(CC)(20)]+R2[δ_{in}(CH)(22)+ν(CC)(12)]	1394,1391	Ring in plane CH

						deformation
1398	1353			$\delta_{sym}(CH_3)(82)+[\nu(C15C17)](8)$	1364,1355,1353	Sym CH_3 stretch
1365	1321	1329	1332	$R1[\delta(C3H2O1)(16)+\nu(CC)(51)+\delta_{in}(CH)(24)]$	1351,1345,1322	CHO def + Ring CC stretch
1364	1320	1322		$R2[\delta_{in}(CH)](42)+R3[\delta_{in}(CH)](42)$	1323,1321	Ring in plane CH deformation
1347	1304			$R3[\delta_{in}(CH)](26)+R2[\delta_{in}(CH)](24)$	1306,1304	Ring in plane CH deformation
1336	1293		1295	$R1[\nu(C8N13)(12)+\delta_{in}(CH)(34)+\nu(CC)](18)]+[\nu(C15N13)](10)$	1297,1291,1291	Ring (CN stretch+ in plane CH deformation)
1312	1270	1271	1264	$R3[\nu(C26C31)(43)+\delta_{tri}(8)]+R2[\delta_{tri}](8)$	1270,1269	C26C31 stretch
1298	1257	1261		$[\tau(N13H14)](13)+[\rho(N13H14)](11)+R1[\nu(C3O1)(12)+\nu(CC)(31)+\nu(C8N13)(5)]+[\delta(C8N13N36)](6)+[\nu(C15N13)](5)$	1258,1255,1246	N13H14 torsion + N13H14 rocking
1275	1234	1234	1232	$R2[\nu(C35N36)(12)+\nu(C37N36)(12)+\nu(CC)(26)]+R3[\nu(C29N21)(8)+\nu(C22N21)(8)]$	1236,1233	Ring CN stretch
1275	1234			$R1[\nu(C3O1)(17)+\delta_{tri}(7)+\delta_{in}(CH)(7)]+[\tau(N13H14)](8)+[\rho(N13H14)](7)+ [\nu(C15N13)](7)$	1245,1241,1229	CO stretch
1258	1218	1216	1222	$R3[\nu(C22N21)(13)+\nu(C29N21)(13)+\nu(CC)(34)]+R2[\nu(CC)](16)+\nu(C37N36)(7)+\nu(C35N36)(6)]$	1221,1219	Ring CN stretch
1248	1208			$R3[\delta_{in}(CH)](34)+R2[\delta_{in}(CH)](28)$	1211,1208	Ring in plane CH deformation
1246	1206			$R3[\delta_{in}(CH)](28)+R1[\nu(C8N13)](9)+R2[\delta_{in}(CH)](12)$	1206,1205	Ring in plane CH deformation
1243	1203			$R1[\nu(C8N13)(23)+\delta_{tri}(7)]+[\nu(C15N13)](7)+[\nu(C15C17)](7)+[\delta(C8N13N36)](5)$	1200,1200,1210	Ring C8N13 stretch
1196	1157	1165	1168	$R1[\delta(C3H2O1)(47)+\nu(CC)(24)+\nu(C3O1)(7)+\delta_{in}(CH)(8)]$	1214,1204,1159,	Ring CHO deformation
1193	1155	1132	1137	$R1[\delta_{in}(CH)(77)+\nu(CC)(5)]$	1158,1153,1148	Ring in plane CH deformation
1131	1094	1106	1104	$R1[\delta_{in}(CH)(57)+\nu(CC)(22)]$	1100,1094,1093	Ring in plane CH deformation
1119	1083	1091	1091	$R2[\nu(CC)(36)+\delta_{in}(CH)(50)]$	1088,1085	Ring CC stretch
1113	1077	1064	1079	$R3[\nu(CC)(39)+\delta_{in}(CH)(49)]$	1083,1079	Ring CC stretch
1096	1061		1064	$R3[\delta_{in}(CH)](22)+\delta_{tri}(12)+\nu(C29N21)(10)+\nu(C22N21)(9)+\nu(CC)(10)]+R2[\delta_{tri}(7)+\nu(C35N36)(5)+\nu(C37N36)(5)$	1063,1061	Ring in plane CH deformation
1093	1058	1040	1042	$R2[\delta_{in}(CH)(25)+\nu(C35N36)(10)+\nu(C37N36)(9)+\nu(CC)(16)+\delta_{tri}(5)]+R3[\delta_{in}(CH)(13)+\nu(CC)(10)]$	1059, 1058	Ring in plane CH deformation
1059	1025	1018		$R2[\delta_{tri}(32)+\nu(CC)](10)]+R3[\delta_{tri}(26)+\nu(CC)(12)]$	1025,1025	Ring tri deformation
1056	1022	1004	1004	$\rho'(CH_3)(74)+[\omega(C15C17)](17)+ \delta_a(CH_3)(6)$	1025,1022,999	CH_3 rocking
1029	996	991	993	$R1[\delta_{tri}(32)+\nu(CC)(36)+\delta_{in}(CH)(5)]+\rho(CH_3)(12)$	995,993,992	Ring tri deformation
1020	988			$\rho(CH_3)(28)+R2[\delta_{tri}](17)+R1[\delta_{tri}](8)$	990,987	CH_3 rocking
1019	986			$\rho(CH_3)(24)+R2[\delta_{tri}(18)+\nu(C35N36)(5)+\nu(C37N36)(5)]+R1[\delta_{tri}](5)$	986,985	CH_3 rocking
1011	978	960	962	$R3[\delta_{tri}(29)+\nu(C29N21)(8)+\nu(C22N21)(8)+\nu(CC)(10)]+R2[\delta_{out}(CH)(11)+\delta_{tri}(5)]$	983,977	Ring tri deformation
1007	975			$R2[\delta_{out}(CH)](55)+R3[\delta_{out}(CH)](30)$	979,978	Ring out of plane CH deformation
1007	974			$R3[\delta_{out}(CH)](53)+\delta_{tri}(6)]+R2[\delta_{out}(CH)](20)$	976,975	Ring out of plane CH deformation
991	959		946	$R2[\delta_{out}(CH)](61)+puck(13)]+R3[\delta_{out}(CH)(15)+puck(5)]$	964,960	Ring out of plane CH deformation
987	956			$R3[\delta_{out}(CH)(62)+puck(13)]+R2[\delta_{out}(CH)](12)$	957,956	Ring out of plane CH deformation
987	955			$R1[\delta_{out}(CH)(86)+puck(6)]$	951,949,947	Ring out of plane CH deformation
964	933		929	$[\nu(C15C17)](27)+[\delta_{sci}(N13H14)](21)+[\delta_{sci}(C15C17)](17)+[\nu(C15N13)](12) +R1[\nu(CC)](5)$	941,935,933	C15C17 stretch+ NH scissoring
917	888	870	890	$R1[\delta_{out}(CH)(80)+puck(12)]$	923,901,881	Ring out of plane CH deformation
892	864	856	859	$R2[\delta_{out}(CH)](98)$	874,861	Ring out of plane CH deformation
890	861			$R3[\delta_{out}(CH)](99)$	860,859	Ring out of plane CH deformation
869	841	843	842	$R2[\delta_{out}(CH)(37)+\delta_{out}(C31C26)(10)]+R3[\delta_{out}(C26C31)(9)+ \delta_{out}(CH)(28)]$	843,843	Ring out of plane CH deformation
865	837			$R1[\nu(CC)(38)+\nu(C3O1)(7)+\delta_a(13)+\nu(C8N13)(11)]+[\delta_{sci}(N13H14)](8)$	838,838,837	Ring CC stretching

856	828	800		R1[δ_{out}(CH)(72)+δ_{out}(C3O1)(9)+τ_a(8)]	832,831,825	Ring out of plane CH deformation
824	797		797	R3[δ_{out}(CH)](48)+R2[δ_{out}(CH)](40)	800,797	Ring out of plane CH deformation
816	790			[τ(N13H14)](33)+R1[δ_{out}(CH)](22)+[ω(N13H14)](14)+[τ(C15N13)](11)	795	NH torsion+ Ring out of plane CH deformation
802	776		779	R1[δ_{tri}(22)+ν(C3O1)(15)+ν(C8N13)(6)+ν(C3C4)(5)]+[δ_{sci}(N13H14)](15)+[ν(C15C17)](8)+[δ_{sci}(C15C17)](5)	782,779,777	Ring tri deformation
797	772	756	761	R1[δ_{out}(CH)](68)+[τ(N13H14)](9)+[τ(C15N13)](6)	773	Ring out of plane CH deformation
770	745	742	736	R3[δ_a(22)+ν(C26C31)(16)+ν(CC)(10)+δ_{tri}(5)]+R2[δ_a'(19)+δ_a(6)+ν(CC)(10)]	748,745	Asym ring deformation
768	743			R2[puck(36)+δ_{out}(C31C26)(8)]+R3[puck(31)+δ_{out}(C26C31)(7)]	744,742	Ring puckering
759	734	733		R3[puck](43)+R2[puck](37)	734,732	Ring puckering
717	694		715	R1[puck(63)+δ_{out}(C8N13)(14)+δ_{out}(C3O1)(14)]	696,695,691	Ring puckering
689	667	673	661	R3[δ_a'](52)+R2[δ_a(26)+δ_a'(8)]	666,665	Ring asym deformation
676	655	650	651	R2[δ_a(40)+δ_a'(13)]+R3[δ_a'](37)	654,653	Ring asym deformation
659	638	629	632	R1[δ_a'(65)+δ_{in}(C3O1)(6)+δ_{in}(C8N13)(5)]	639,638,638	Ring asym deformation
629	609	609	612	[δ_{sci}(C15C17)](17)+[ν(C15C17)](17)+[δ_{sci}(N13H14)](10)+R1[δ_a'(12)+δ_a(12)+ν(C8N13)(6)]+[δ(C8N13N36)](6)	619,612,610	CC scissoring + CC stretch
624	604			R3[δ_a](44)+R2[δ_a'(32)+δ_a(11)]	608,603	Ring asym deformation
611	591			[ω(C15C17)](60)+ρ'(CH_3)(17)+[ω(N13H14)](8)+[τ(N13H14)](6)	603,590,584	CC wagging
587	568	573	574	R2[δ_{out}(C31C26)(19)+τ_a'(12)+puck(8)]+R3[δ_{out}(C26C31)(17)+τ_a(15)+puck(7)]	570,568	Ring out of plane CC deformation
529	512	530	531	R1[δ_{out}(C3O1)(30)+τ_a(30)+δ_{out}(C8N13)(26)]	523,517,508	Ring out of plane CO deformation + ring torsion
519	503	509	510	R3[τ_a(22)+δ_{out}(C26C31)(13)+δ_{in}(C26C31)(9)]+R2[τ_a'(16)+δ_{in}(C31C26)(10)+δ_{out}(C31C26)(12)+τ_a(5)]	501,500	Ring torsion
507	490	496	491	[ρ(C15C17)](35)+R1[δ_a](30)+ρ(CH_3)(8)+[δ_{sci}(C15C17)](7)	499,491,491	CC rocking
430	416	422	419	R1[δ_{in}(C3O1)(45)+δ_a'(16)+δ_{in}(N13C8)(15)]+[δ_{sci}(C15C17)](7) +[δ(C8N13N36)](5)	439,438,421	In plane CO deformation
425	411			R1[τ_a'(81)+δ_{out}(C9H10)(10)]	414,411,408	Ring torsion
395	383	-	393	R2[τ_a(53)+τ_a'(18)]+R3[τ_a'](10)	385,384	Ring torsion
387	375	-		R3[τ_a'](73)+R2[τ_a](9)	379,377	Ring torsion
385	373	-		R1[puck(32)+δ_{out}(C3O1)(17)+δ_{out}(C8N13)(14)]+[τ(N13H14)](7)+[τ(N13N36)](6)	376,373,368	Ring puckering
377	365	-		R3[τ_a(20)+δ_{in}(C26C31)(16)+δ_{out}(C26C31)(5)]+R2[δ_{out}(C31C26)(5)+δ_{in}(C31C26)](16)+τ_a'(15) +τ_a(5)]	368,367	Ring torsion + in plane CC deformation
330	319	-	327	[ρ(C15C17)](26)+R1[δ_{in}(C8N13)(12)+δ_a(10)+δ_{in}(C3O1)(8)+ν(C8N13)(6)]+[δ_{sci}(C15C17)](11)+ [τ(N13H14)](7) + [δ_{sci}(N13H14)](6)	326,322,314	CC rocking
317	307	-	298	[δ_{sci}(N13H14)](18)+[δ(C8N13N36)](18)+R1[δ_{in}(C8N13)(15)+δ_a(6)+δ_{in}(C3O1)(6)+ν(C8N13)(5)]+[δ_{sci}(C15C17)](6)+[ν(N13C15)](6)+[τ(N13H14)](5)	311,309,308	NH Scissoring + C8N13N36 deformation
313	303	-		R1[τ(C3O1)](25)+R3[ν(C26C31)(15)+δ_a(14)]+[δ(C8N13N36)](10)+R2[δ_a'](9)	308,303	Ring CO torsion
313	303	-		R1[τ(C3O1)](69)		Ring CO torsion
268	259	-	256	R3[τ_a(26)+δ_{in}(C26C31)(6)]+R2[τ_a'(19)+δ_{in}(C31C26)(7)+τ_a(6)]	264,258	Ring torsion
194	188	-	202	R1[τ_a](39)+[ω(N13H14)](16)+[τ(N13N36)](12)+[τ(N13H14)](12)	196,195,191	Ring torsion + NH wagging
165	160	-	156	[δ_{sci}(N13H14)](30)+R1[δ_{in}(C8N13)](18)+[δ(C8N13N36)](17)+[τ(N13H14)](15)+[ν(N36H14)](7) + [ρ(C15C17)](5)	172,163,157	NH scissoring
134	130	-	131	R3[δ_{in}(C26C31)](25)+R2[δ_{in}(C31C26)(20)+δ_{out}(C31C26)(5)]+[δ(C8N13N36)](14)	138,135	In plane ring CC deformation
107	104	-	111	[δ(C8N13N36)](24)+[τ(N13N36)](17)+[τ(C15C17)](11)+R3[δ_{out}(C26C31)](10)+R2[δ_{out}(C31C26)](10)+[τ(C35N36)](5)	119,116	C8N13N36 deformation
101	97.7	-		[τ(C15C17)](36)+[δ(C8N13N36)](13)+R3[δ_{out}(C26C31	105,103,93.2	CC torsion

				)](8)+R1[τ_a](6)		
76.7	74.3	-	-	[ω(N13H14)](31)+[τ(C15N13)](14)+R1[τ(C8N13)(9)+τ_a(9)]+[τ(C15C17)](7)+[τ(N13N36)](6)+[δ(C35N36N13)](5)	87.5,73.6,71.8	NH wagging
64.3	62.2	-	-	[ν(N36H14)](41)+[τ(C26C31)](28)+[τ(N13N36)](19)	71.2,70.8,69.7	N36H14 stretch
62	60	-	-	[τ(N13H14)](39)+[ν(N36H14)](33)+[τ(C26C31)](13)+[τ(N13N36)](7)	63.2,58.8,55.7	NH torsion
61.3	59.3	-	-	[τ(C15C17)](38)+[τ(C15N13)](31)+[ω(C15C17)](8)	57.4,51.4,46.5	CC torsion
46.5	45	-	-	[δ(C8N13N36)](70)+[τ(N13H14)](22)	37.3,37,32	C8N13N36 deformation
41.6	40.2	-	-	R1[τ(C8N13)](66)+[τ(C15N13)](9)+[τ(C15C17)](9)	28.6,28.2,23.3	Ring C8N13 torsion
13.8	13.4	-	-	[τ(N13H14)](57)+[τ(N13N36)](38)	21.1,20.2,18.6	N13H14 torsion
11.5	11.1	-	-	[τ(N13H14)](60)+[τ(N13N36)](18)+[τ(C35N36)](10)+[δ(C8N13N36)](9)	17.1,12.3,10.9	N13H14 torsion
8.3	8.03	-	-	[τ(N13N36)](56)+[τ(N13H14)](27)+[δ(C35N36N13)](12)	7.62,7.02,5.22	NN torsion+N13H14 torsion

Table S5 Geometrical parameters for intra and intermolecular hydrogen bonds in PRA3-BPY2 (dimer+PRA)of cocrystal: bond length (Å), bond angle (◦) and the sum of van der Waal radii of interacting atoms ($r_H + r_A$) in Å.

Interactions(D-H···A)	**d_{D-H}(Å)**	**$d_{H\cdots A}$(Å)**	**d_{D-A} (Å)**	**D-H···A(◦)**	**(r_H+r_A)(Å)**
C67-H68···O21	1.0838	2.5719	3.6375	167.4594	2.72
C29-H30···O36	1.0784	2.2363	2.8938	117.2749	2.72
O1-H2··· O36	0.9756	1.8484	2.7941	162.4254	2.72
C37-H40···O1	1.0900	2.5415	3.3613	131.2164	2.72
C4-H5···N76	1.0843	2.9706	3.7097	125.7336	2.75
C6-H7···N76	1.0846	2.9580	3.7112	126.8300	2.75
N13-H14···N56	1.0174	2.1612	3.1782	178.1101	2.75
C17-H18···N56	1.0908	2.7429	3.6848	144.3745	2.75
C9-H10···O16	1.0787	2.2002	2.8948	120.0294	2.72
O81-H82···N41	0.9783	1.9300	2.8684	159.8854	2.75
C84-H85···N41	1.0838	2.8306	3.498	119.7924	2.75
C86-H87···N61	1.0842	2.8765	3.6112	125.1534	2.75
N93-H94···N61	1.0156	2.2006	3.1564	156.1752	2.75
C89-H90···O96	1.0791	2.2368	2.9135	118.7293	2.72

Table S6 Second-order perturbation theory analyses of the Fock Matrix, in the NBO basis for intra-molecular interactions in PRA-BPY (monomer) within PRA3-BPY2 (dimer+PRA) of cocrystal

Donor NBO (i)	**ED(i)/e**	**Acceptor NBO (j)**	**ED(j)/e**	**E(2)[a] (kcal/mol)**	**E(j)-E(i)[b] (a.u.)**	**F(i,j)[c] (a.u.)**
Paracetamol						
πC3-C4	1.64691	π* C6-C8	0.41087	21.96	0.28	0.072
πC3-C4	1.64691	π*C9-C11	0.34164	18.25	0.29	0.065
πC6-C8	1.66584	π*C3-C4	0.39975	18.58	0.28	0.066
πC6-C8	1.66584	π* C9-C11	0.34164	20.16	0.29	0.069
πC9-C11	1.70490	π* C3-C4	0.39975	21.53	0.28	0.071
π C9-C11	1.70490	π* C6-C8	0.41087	19.07	0.28	0.067
LP(1) O1	1.97681	σ *C3-C4	0.02908	6.60	1.14	0.078
LP(2) O1	1.87041	π* C3-C4	0.39975	28.46	0.34	0.095
LP(1) N13	1.65539	π* C6-C8	0.41087	31.04	0.29	0.086
LP(1) N13	1.65539	π* C15-O16	0.30080	63.04	0.28	0.119
LP(2) O16	1.86580	σ *N13-C15	0.07427	24.08	0.71	0.119
LP(2) O16	1.86580	σ *C15-C17	0.05757	19.53	0.62	0.100
4,4′–bipyridine						
π N41-C49	1.72324	π* C42-C44	0.28159	26.01	0.33	0.083
π N41-C49	1.72324	π* C46- C47	0.34629	12.58	0.33	0.058
σ C42-H43	1.97973	σ *N41-C49	0.01818	5.43	1.05	0.068
πC42-C44	1.62822	π* N41-C49	0.39414	16.91	0.26	0.060
πC42-C44	1.62822	π* C46-C47	0.34629	23.90	0.29	0.070
πC46-C47	1.62038	π* N41-C49	0.39414	30.68	0.26	0.080
πC46-C47	1.62038	π* C42-C44	0.28159	16.31	0.29	0.062
πC46-C47	1.62038	π* C51-C60	0.34558	9.53	0.29	0.047
σ C49-H50	1.98012	σ *N41-C42	0.01735	5.33	1.06	0.067
πC51-C60	1.62319	π* C46-C47	0.34629	10.09	0.28	0.048
πC51-C60	1.62319	π* C52-C55	0.28596	16.61	0.28	0.063
πC51-C60	1.62319	π* N56-C57	0.38453	30.01	0.26	0.080
πC52-C55	1.63390	π* C51-C60	0.34558	23.57	0.29	0.074

πC52-C55	1.63390	π* N56-C57	0.38453	16.77	0.27	0.060
πN56-C57	1.71657	π* C51-C60	0.34558	12.91	0.33	0.059
πN56-C57	1.71657	π* C52-C55	0.28596	26.41	0.33	0.083
σ C57-H58	1.97987	σ *C55-N56	0.01722	5.35	1.05	0.067
LP(1) N56	1.90782	σ *C52-C55	0.02430	8.77	0.91	0.081
LP(1) N56	1.90782	σ *C57-C60	0.02433	8.76	0.91	0.081

[a]E(2) means energy of hyper conjugative interaction(stabilization energy),
[b]Energy difference between donor (i) and acceptor (j) NBO orbital.
[c]F(i,j) is theFock matrix element between i and j NBO orbitals

Table S7 Reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softness (s_k^+, s_k^-), local electrophilicity indices (ω_k^+, ω_k^-) for PRA (monomer) using Hirshfeld atomic charges.

Sites	f_k^+	s_k^+	ω_k^+	**Sites**	f_k^-	s_k^-	ω_k^-
1 O	0.1055	0.0199	0.187	1 O	0.0407	0.0077	0.0721
2 O	0.0796	0.015	0.1411	2 O	0.0335	0.0063	0.0594
3 N	0.0747	0.0141	0.1325	3 N	0.0015	0.0003	0.0026
4 C	0.0783	0.0147	0.1388	4 C	0.049	0.0092	0.0868
5 C	0.0836	0.0158	0.1483	5 C	0.0461	0.0087	0.0817
6 C	0.0554	0.0104	0.0983	6 C	0.1119	0.0211	0.1983
7 C	0.0348	0.0065	0.0616	7 C	0.0255	0.0048	0.0453
8 C	0.0656	0.0123	0.1162	8 C	0.1177	0.0222	0.2087
9 C	0.064	0.012	0.1134	9 C	0.1195	0.0225	0.2118
10 C	0.0652	0.0123	0.1157	10 C	0.1217	0.0229	0.2158
11 C	0.0183	0.0034	0.0324	11 C	0.0151	0.0028	0.0268
12 H	0.0229	0.0043	0.0407	12 H	0.019	0.0036	0.0337
13 H	0.0151	0.0028	0.0267	13 H	0.0118	0.0022	0.0209
14 H	0.0229	0.0043	0.0407	14 H	0.019	0.0036	0.0337
15 H	0.0371	0.007	0.0658	15 H	0.0588	0.0111	0.1043
16 H	0.0381	0.0072	0.0676	16 H	0.0592	0.0112	0.105
17 H	0.0287	0.0054	0.0509	17 H	0.0471	0.0089	0.0835
18 H	0.0383	0.0072	0.068	18 H	0.0591	0.0111	0.1048
19 H	0.0327	0.0062	0.058	19 H	0.0167	0.0031	0.0296
20 H	0.0391	0.0074	0.0693	20 H	0.0273	0.0051	0.0484

Table S8 Reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softness (s_k^+, s_k^-), local electrophilicity indices (ω_k^+, ω_k^-) for PRA-BPY (monomer) using Hirshfeld atomic charges.

Sites	f_k^+	s_k^+	ω_k^+	**Sites**	f_k^-	s_k^-	ω_k^-
1 O	0.09692	0.0325	0.488	1 O	0.011	0.0037	0.0555
2 H	0.03662	0.0123	0.1844	2 H	0.0044	0.0015	0.0222
3 C	0.08056	0.027	0.4056	3 C	0.0089	0.003	0.0449
4 C	0.05868	0.0197	0.2955	4 C	0.0018	0.0006	0.0089

5 H	0.03632	0.0122	0.1829	5 H	0.0018	0.0006	0.0089
6 C	0.06582	0.0221	0.3314	6 C	-0.01	-0.0034	-0.051
7 H	0.03369	0.0113	0.1697	7 H	-0.012	-0.0039	-0.058
8 C	0.07329	0.0246	0.3691	8 C	-0.005	-0.0017	-0.025
9 C	0.05438	0.0182	0.2738	9 C	0.0067	0.0022	0.0337
10 H	0.02733	0.0092	0.1376	10 H	0.0052	0.0018	0.0264
11 C	0.06099	0.0205	0.3071	11 C	0.0118	0.004	0.0595
12 H	0.0363	0.0122	0.1828	12 H	0.0092	0.0031	0.0461
13 N	0.08115	0.0272	0.4086	13 N	-0.005	-0.0016	-0.024
14 H	0.02208	0.0074	0.1112	14 H	-0.002	-0.0008	-0.012
15 C	0.03626	0.0122	0.1826	15 C	0.0007	0.0002	0.0033
16 O	0.08171	0.0274	0.4114	16 O	0.0184	0.0062	0.0925
17 C	0.01739	0.0058	0.0876	17 C	0.0017	0.0006	0.0086
18 H	0.01407	0.0047	0.0708	18 H	-0.01	-0.0032	-0.048
19 H	0.02211	0.0074	0.1113	19 H	0.0066	0.0022	0.0332
20 H	0.02196	0.0074	0.1106	20 H	0.0072	0.0024	0.0362
21 N	0.01479	0.005	0.0745	21 N	0.084	0.0282	0.4228
22 C	0.00796	0.0027	0.0401	22 C	0.052	0.0174	0.2617
23 H	0.0062	0.0021	0.0312	23 H	0.0334	0.0112	0.1683
24 C	0.0019	0.0006	0.0096	24 C	0.0453	0.0152	0.2281
25 H	0.0000	0.0000	0.0002	25 H	0.0251	0.0084	0.1263
26 C	-0.0039	-0.001	-0.019	26 C	0.0462	0.0155	0.2324
27 C	0.00342	0.0011	0.0172	27 C	0.0453	0.0152	0.2282
28 H	0.00176	0.0006	0.0089	28 H	0.0251	0.0084	0.1264
29 C	0.00889	0.003	0.0448	29 C	0.052	0.0174	0.2618
30 H	0.00692	0.0023	0.0348	30 H	0.0334	0.0112	0.1684
31 C	0.01123	0.0038	0.0566	31 C	0.067	0.0225	0.3372
32 C	0.00698	0.0023	0.0351	32 C	0.0505	0.0169	0.2541
33 H	0.00723	0.0024	0.0364	33 H	0.0281	0.0094	0.1415
34 H	-0.0051	-0.002	-0.026	34 H	0.0363	0.0122	0.1827
35 C	-0.0083	-0.003	-0.042	35 C	0.0616	0.0207	0.3102
36 N	-0.026	-0.009	-0.131	36 N	0.086	0.0289	0.4333
37 C	-0.0054	-0.002	-0.027	37 C	0.0618	0.0207	0.311
38 H	-0.0022	-0.0007	-0.011	38 H	0.0365	0.0123	0.1839
39 H	0.00785	0.0026	0.0395	39 H	0.0281	0.0094	0.1415
40 C	0.00815	0.0027	0.041	40 C	0.0504	0.0169	0.2536

Table S9 Reactivity descriptors as Fukui functions (f_k^+, f_k^-), local softness (s_k^+, s_k^-), local electrophilicity indices (ω_k^+, ω_k^-) for PRA3-BPY2 (dimer+PRA) using Hirshfeld atomic charges.

Sites	f_k^+	s_k^+	ω_k^+	**Sites**	f_k^-	s_k^-	ω_k^-
1 O	0.0574	0.0244	0.3503	1 O	0.0070	0.0030	0.0424
2 H	0.0142	0.0060	0.0866	2 H	0.0010	0.0004	0.0060
3 C	0.0455	0.0194	0.2778	3 C	0.0050	0.0021	0.0305
4 C	0.0337	0.0143	0.2054	4 C	-0.0029	-0.0012	-0.0174
5 H	0.0177	0.0075	0.1081	5 H	-0.0028	-0.0012	-0.0171
6 C	0.0320	0.0136	0.1953	6 C	-0.0090	-0.0038	-0.0548
7 H	0.0161	0.0068	0.0980	7 H	-0.0098	-0.0042	-0.0600
8 C	0.0436	0.0186	0.2662	8 C	-0.0017	-0.0007	-0.0103
9 C	0.0302	0.0128	0.1843	9 C	0.0066	0.0028	0.0401
10 H	0.0160	0.0068	0.0974	10 H	0.0050	0.0021	0.0303
11 C	0.0367	0.0156	0.2239	11 C	0.0094	0.0040	0.0574
12 H	0.0217	0.0092	0.1325	12 H	0.0076	0.0032	0.0462
13 N	0.0356	0.0152	0.2174	13 N	-0.0032	-0.0014	-0.0197
14 H	0.0113	0.0048	0.0686	14 H	-0.0026	-0.0011	-0.016
15 C	0.0198	0.0084	0.1207	15 C	0.0015	0.0006	0.0091
16 O	0.0425	0.0180	0.2590	16 O	0.0138	0.0059	0.0841
17 C	0.0093	0.0040	0.0570	17 C	0.0016	0.0007	0.0098
18 H	0.0063	0.0027	0.0383	18 H	-0.0060	-0.0025	-0.0363
19 H	0.0122	0.0052	0.0744	19 H	0.0042	0.0018	0.0257
20 H	0.0125	0.0053	0.0765	20 H	0.0062	0.0027	0.0380
21 O	0.0009	0.0004	0.0057	21 O	-0.0053	-0.0022	-0.0321
22 H	0.0027	0.0011	0.0163	22 H	0.0027	0.0011	0.0162
23 C	0.0024	0.0010	0.0148	23 C	-0.0031	-0.0013	-0.0186
24 C	0.0048	0.0021	0.0295	24 C	0.0041	0.0018	0.0252
25 H	0.0043	0.0018	0.0261	25 H	0.0043	0.0018	0.0265
26 C	0.0045	0.0019	0.0274	26 C	0.0063	0.0027	0.0381
27 H	0.0038	0.0016	0.0232	27 H	0.0056	0.0024	0.0340
28 C	-0.0010	-0.0004	-0.0063	28 C	0.0030	0.0013	0.0181
29 C	-0.0019	-0.0008	-0.0113	29 C	-0.0022	-0.0009	-0.0133
30 H	-0.0020	-0.0009	-0.0122	30 H	-0.0009	-0.0004	-0.0056
31 C	-0.0007	-0.0003	-0.0042	31 C	-0.0070	-0.0030	-0.0425
32 H	-0.0006	-0.0003	-0.0037	32 H	-0.0059	-0.0025	-0.0358
33 N	0.0045	0.0019	0.0273	33 N	0.0015	0.0007	0.0093
34 H	0.0044	0.0019	0.0267	34 H	0.0036	0.0015	0.0222
35 C	-0.0004	-0.0002	-0.0026	35 C	0.0020	0.0008	0.0121

36 O	-0.0100	-0.0040	-0.0610	36 O	-0.0034	-0.0015	-0.0209
37 C	0.0020	0.0008	0.0120	37 C	0.0023	0.0010	0.0142
38 H	0.0053	0.0022	0.0322	38 H	0.0046	0.0020	0.0281
39 H	0.0059	0.0025	0.0358	39 H	0.0033	0.0014	0.0201
40 H	-0.0047	-0.0020	-0.0289	40 H	0.0008	0.0003	0.0048
41 N	-0.0041	-0.0020	-0.0251	41 N	0.0479	0.0204	0.2923
42 C	-0.0020	-0.0009	-0.0122	42 C	0.0318	0.0135	0.1938
43 H	-0.0016	-0.0007	-0.0096	43 H	0.0184	0.0078	0.1125
44 C	0.0023	0.0010	0.0142	44 C	0.0260	0.0110	0.1583
45 H	0.0021	0.0009	0.0128	45 H	0.0139	0.0059	0.0845
46 C	0.0023	0.0010	0.0143	46 C	0.0328	0.0139	0.1999
47 C	0.0055	0.0023	0.0337	47 C	0.0288	0.0123	0.1759
48 H	0.0045	0.0019	0.0273	48 H	0.0167	0.0071	0.1016
49 C	0.0042	0.0018	0.0258	49 C	0.0346	0.0147	0.2109
50 H	0.0045	0.0019	0.0272	50 H	0.0218	0.0093	0.1331
51 C	0.0035	0.0015	0.0214	51 C	0.0306	0.0130	0.1865
52 C	0.0051	0.0021	0.0308	52 C	0.0289	0.0123	0.1761
53 H	0.0044	0.0019	0.0270	53 H	0.0164	0.0070	0.0998
54 H	0.0013	0.0006	0.0081	54 H	0.0209	0.0089	0.1275
55 C	0.0006	0.0003	0.0039	55 C	0.0326	0.0139	0.1988
56 N	-0.0088	-0.004	-0.0539	56 N	0.0486	0.0207	0.2964
57 C	-0.0015	-0.0006	-0.0091	57 C	0.0313	0.0133	0.1908
58 H	-0.0008	-0.0004	-0.0051	58 H	0.0194	0.0082	0.1182
59 H	0.0031	0.0013	0.0187	59 H	0.0132	0.0056	0.0804
60 C	0.0035	0.0015	0.0214	60 C	0.0239	0.0102	0.1458
61 N	-0.0031	-0.0010	-0.0190	61 N	0.0385	0.0164	0.2349
62 C	-0.0031	-0.0010	-0.0187	62 C	0.0237	0.0101	0.1447
63 H	-0.0018	-0.0008	-0.0108	63 H	0.0138	0.0059	0.0842
64 C	0.0006	0.0002	0.0035	64 C	0.0165	0.0070	0.1007
65 H	0.0011	0.0005	0.0068	65 H	0.0075	0.0032	0.0460
66 C	0.0017	0.0007	0.0104	66 C	0.0234	0.0099	0.1425
67 C	0.0048	0.0020	0.0292	67 C	0.0223	0.0095	0.1361
68 H	0.0034	0.0015	0.0209	68 H	0.0116	0.0049	0.0710
69 C	0.0039	0.0017	0.0238	69 C	0.0272	0.0116	0.1658
70 H	0.0045	0.0019	0.0271	70 H	0.0176	0.0075	0.1071
71 C	0.0021	0.0009	0.0128	71 C	0.0206	0.0088	0.1256
72 C	0.0030	0.0013	0.0182	72 C	0.0177	0.0075	0.1081

73 H	0.0031	0.0013	0.0189	73 H	0.0116	0.0049	0.0705
74 C	-0.0019	-0.0008	-0.0117	74 C	0.0186	0.0079	0.1136
75 H	-0.0016	-0.0007	-0.0098	75 H	0.0129	0.0055	0.0784
76 N	-0.0085	-0.0040	-0.0515	76 N	0.0280	0.0119	0.1710
77 C	0.0032	0.0013	0.0193	77 C	0.0182	0.0077	0.1111
78 H	0.0028	0.0012	0.0168	78 H	0.0110	0.0047	0.0668
79 C	0.0006	0.0003	0.0039	79 C	0.0169	0.0072	0.1028
80 H	0.0014	0.0006	0.0088	80 H	0.0122	0.0052	0.0742
81 O	0.0474	0.0201	0.2892	81 O	0.0053	0.0023	0.0324
82 H	0.0112	0.0048	0.0685	82 H	0.0016	0.0007	0.0098
83 C	0.0352	0.0149	0.2144	83 C	-0.0015	-0.0006	-0.0091
84 C	0.0263	0.0112	0.1607	84 C	-0.0069	-0.0029	-0.0421
85 H	0.0141	0.0060	0.0859	85 H	-0.0064	-0.0027	-0.0390
86 C	0.0256	0.0109	0.1559	86 C	-0.0049	-0.0021	-0.0296
87 H	0.0136	0.0058	0.0830	87 H	-0.0040	-0.0017	-0.0245
88 C	0.0350	0.0149	0.2136	88 C	0.0032	0.0014	0.0197
89 C	0.0245	0.0104	0.1492	89 C	0.0084	0.0036	0.0510
90 H	0.0134	0.0057	0.0815	90 H	0.0064	0.0027	0.0389
91 C	0.0296	0.0126	0.1803	91 C	0.0085	0.0036	0.0517
92 H	0.0177	0.0075	0.1081	92 H	0.0074	0.0032	0.0453
93 N	0.0289	0.0123	0.1765	93 N	-0.0019	-0.0008	-0.0118
94 H	0.0098	0.0042	0.0599	94 H	-0.0005	-0.0002	-0.0030
95 C	0.0158	0.0067	0.0967	95 C	0.0039	0.0017	0.0240
96 O	0.0349	0.0148	0.2131	96 O	0.0133	0.0057	0.0814
97 C	0.0079	0.0034	0.0482	97 C	0.0029	0.0012	0.0177
98 H	0.0105	0.0045	0.0640	98 H	0.0064	0.0027	0.0390
99 H	0.0052	0.0022	0.0320	99 H	-0.0020	-0.0009	-0.0122
100 H	0.0105	0.0045	0.0640	100 H	0.0056	0.0024	0.0341