Supplementary Information

Table S1. Conformers energies and dipole moment values of (2*E*)-HIPC.

Method			Gas	DMSO	Acetonitrile
AM1	Conformer I	Energy (Hartree)	0.186267	0.169524	0.169722
	SCAN 1	Dipole moment (Debye)	5.6746	7.1921	7.1752
	Conformer II	Energy (Hartree)	0.186506	0.17810	0.17831
	SCAN 2	Dipole moment (Debye)	5.5681	6.7998	6.7870
B3LYP	Conformer I	Energy (Hartree)	−1084.498	−1084.705	−1084.462
	SCAN 1	Dipole moment (Debye)	5. 7362	7.4136	7.2739
	Conformer II	Energy (Hartree)	−1084.665	−1084.6857	−1084.685
	SCAN 2	Dipole moment (Debye)	5.2643	6.4760	6.4640

Table S2. Optimized parameters of (2*E*)-HIPC.

Bond Length	B3LYP	HF	Experimental	Dihedral Angle	B3LYP	HF	Experimental *
N18–H39	1.020	0.999	0.950	C1–C2–C6–C5	−180.0	−180.1	−1.1
C1–H26	1.084	1.072	0.930	C3–C4–C2–C1	−179.9	−179.6	–0.7
C2–H27	1.083	1.072	0.930	C24–C23–C25–C20	−180.0	−180.4	
C3–H28	1.084	1.072	0.930	C23–C22–C21	120.3	119.0	120.3
C4–H29	1.082	1.071	0.930	H38–N16–N15–C7	2.7	3.6	
C6–H30	1.082	1.070	0.930	H39–N18–C20–C21	0.2	0.2	
C11–H35	1.076	1.064	0.930	H26–C1–C2–C3	−179.6	−179.9	
C12–H36	1.075	1.063	0.930	H27–C2–C3–C4	−179.7	−179.6	
C14–H37	1.077	1.065	0.930	H28–C3–C4–C5	−180.4	−180.6	
C21–H40	1.085	1.072	0.930	H29–C4–C5–C6	−181.4	−181.7	
C22–H41	1.084	1.071	0.930	H30–C6–C5–C7	−1.0	−1.0	
C23–H42	1.083	1.065	0.930	H35–C11–C12–N13	−179.0	−179.2	
C24–H43	1.084	1.082	0.930	H36–C12–N13–C14	−179.6	−179.6	
C25–H44	1.078	1.078	0.930	H37–C14–N13–C12	−180.8	−180.6	
C8–H31	1.096	1.081	0.970	H40–C21–C22–C23	−179.9	−179.9	
C8–H32	1.090	1.081	0.970	H41–C22–C23–C24	−179.9	−180.0	
C9–H33	1.093	1.073	0.970	H42–C23–C24–C25	−180.0	−180.2	
C9–H34	1.094	1.072	0.970	H43–C24–C25–C20	−180.0	−211.5	
O19–C17	1.240	1.221	1.227	H44–C25–C24–C23	−180.2	29.1	
N15–C7	1.300	1.266	1.296	H31–C8–C7–C5	−211.9	38.8	
C12–C11	1.374	1.353	1.350	H32–C8–C7–C5	29.3	−203.7	
N13–C14	1.327	1.300	1.311	H33–C9–N10–C11	42.1	−179.9	
C6–C1	1.390	1.380	1.385	C2–C3–C1–C6	−180.1	−180.0	1.6
C2–C3	1.395	1.385	1.368	H34–C9–N10–C11	−200.4	−180.0	
C22–C21	1.392	1.383	1.373	C1–C2–C6–C5	−180.0	−180.1	−1.1
C25–C24	1.394	1.384	1.384	C3–C4–C2–C1	−179.9	−179.6	−0.7
C1–C2	1.399	1.381	1.384	C24–C23–C25–C20	−180.0	−180.4	
C3–C4	1.396	1.384	1.388	H34–C9–N10–C11	−200.4	−180.0	
C23–C22	1.397	1.383	1.376	C1–C2–C6–C5	−180.0	−180.1	−1.1
C24–C23	1.396	1.383	1.383	C3–C4–C2–C1	−179.9	−179.6	−0.7
C4–C5	1.405	1.389	1.390	C24–C23–C25–C20	−180.0	−180.4	
C5–C6	1.409	1.391	1.385	C2–C3–C1–C6	−180.1	−180.0	1.6
C20–C25	1.405	1.390	1.380	C22–C21–C23–C24	−180.0	−180.0	0.8

Table S2. *Cont.*

Bond Length	B3LYP	HF	Experimental	Dihedral Angle	B3LYP	HF	Experimental *
C21–C20	1.405	1.391	1.393	C23–C22–C24–C25	−180.0	−180.0	−1.4
N18–C17	1.369	1.353	1.356	C8–C–7–C5–C4	−21.7	−39.3	−49.3
N10–C14	1.388	1.369	1.347	C17–N18–C20–C25	−0.4	−0.7	−43.5
N10–C11	1.398	1.386	1.362	N18–C17–N16–N15	1.0	0.9	−0.1
N13–C12	1.402	1.383	1.368	C12–C14–C11–N10	−180.3	−180.0	
N18–C20	1.408	1.393	1.418	C12–C11–N13–C14	−180.1	−182.1	0.7
N16–C17	1.412	1.406	1.365	C20–N18–C17–N16	−180.9	−180.0	−179.9
C5–C7	1.486	1.490	1.480	C17–N16–N15–C7	−183.5	−180.8	158.5
N16–N15	1.387	1.386	1.384	C5–C7–C8–C9	−91.0	−90.0	−95.6
C7–C8	1.515	1.514	1.499	N16–N15–C7–C8	1.4	2.0	0.4
N10–C9	1.468	1.456	1.450	C7–C8–C9–N10	−179.1	−182.2	50.1
C8–C9	1.557	1.550	1.534)	C8–C9–N10–C11	−79.2	−82.1	65.3
Bond angle				O19–N16–N18–C17	0.2	0.2	
C6–C1–C2	120.3	119.7	120.4	N18–C20–C25–C21	0.0	0.1	
C2–C3–C4	120.4	120.2	121.5	N15–C8–C5–C7	4.5	4.7	
C25–C24–C23	121.1	120.1	121.2	C7–C5–C4–C6	0.1	0.5	
C1–C2–C3	119.4	120.3	118.8	C9–C11–C14–N10	3.0	1.8	
H38–N16–N15	123.8	123.1	128.0	C17–N18–C20–C25	−0.4	−0.7	−43.5
H39–N18–C20	118.7	117.3	119.0	N18–C17–N16–N15	1.0	0.9	−0.1
H26–C1–C2	120.0	120.1	120.6				
H27–C2–C3	120.3	120.2	119.2				
H28–C3–C4	119.5	119.7	120.1				
H29–C4–C5	120.7	120.5	120.1				
H30–C6–C5	118.6	119.1	119.6				
H35–C11–C12	132.0	131.7	126.8				
H36–C12–N13	121.4	121.7	124.7				
H37–C14–N13	126.3	126.1	123.4				
H40–C21–C22	119.9	120.2	119.8				
H41–C22–C23	120.2	120.6	120.4				
H42–C23–C24	120.5	121.2	119.4				
H43–C24–C25	119.0	109.4	120.3				
H44–C25–C24	121.8	107.0	119.4				
H31–C8–C9	109.0	109.0	109.1				
H32–C8–H31	106.6	108.1	107.9				
H33–C9–N10	109.2	119.8	109.1				
H34–C9–H33	108.2	118.8	107.8				
O19–C17–N18	127.9	126.8	124.1				
N15–C7–C8	123.3	124.6	125.8				
C24–C23–C22	119.2	121.2	119.2				
C4–C5–C7	122.3	121.8	120.4				
C25–C20–N18	123.0	123.6	122.1				
N18–C17–N16	112.4	113.9	115.9				
C11–N10–C14	106.6	106.4	105.7				
C11–C12–N13	110.3	120.2	110.7				
C20–N18–C17	126.8	109.6	124.0				

Table S2. *Cont.*

Bond Length	B3LYP	HF	Experimental	Dihedral Angle	B3LYP	HF	Experimental *
C17–N16–N15	120.3	127.2	118.7				
C5–C7–C8	119.6	118.2	119.7				
N16–N15–C7	120.4	121.1	118.9				
C7–C8–C9	109.8	109.3	112.2				
C9–N10–C14	126.7	126.8	126.3				
C8–C9–N10	111.8	111.4	112.4				

***** Reference [14].

Table S3. Geometrical parameters of hydrogen bond in (2*E*)-HIPC.

D–H···A	D–H	H···A	*D*···A	D–H···A
N1–H39···N15	0.95	2.19	2.622	106
N1–H39···N13	0.95	2.23	3.121	156
N1–H38···O19	0.93	1.96	2.893	176
C–H31···O19	0.97	2.51	3.198	128
C–H34···O19	0.97	2.56	3.132	118
C2–H44···O19	0.93	2.54	2.944	106

Table S4. Computed energy values of (2*E*)-HIPC in solvents (DMSO and acetonitrile) and in gas phase.

Parameters	Acetonitrile	DMSO	Gas
Electro negativity (χ)	−3.9125	−3.6693	−4.0133
Chemical hardness (η)	2.1886	2.1997	2.0310
Softness (S)	1.0943	1.0998	1.0155
Electrophilicity index (ω)	5.2418	5.3221	4.1895
HOMO−1	−6.4780	−6.2426	−6.5198
HOMO	−6.1011	−5.8690	−6.0444
LUMO	−1.7239	−1.4695	−1.9822
LUMO+1	−0.5704	−0.2348	−0.8801
HOMO-LUMO	4.3772	4.3994	4.0621
HOMO−1-LUMO+1	5.9075	6.0078	5.6396
Dipole moment	8.6364	8.4925	6.6951

Table S5. Experimental and theoretical UV electronic absorption spectra of (2*E*)-HIPC (absorption wavelength λ (nm), transition energies E (eV) and oscillator strengths (*f*) using TD-DFT/B3LYP/6-311++G(d.p) method in acetonitrile, DMSO and gas phase.

Theoretical				Experimental	
Transition Energy E (eV)	*f*	λ (nm)	Major Contribution	λ (nm)	E (eV)
Acetonitrile					
3.8756	0.3188	319.907	HOMO- > LUMO (0.98)		
4.3128	0.0239	287.477	H-1- > LUMO (0.69)	283.1	4.4082
4.4316	0.4339	279.771	H-2- > LUMO (0.68)		
4.6786	0.0013	265.000	H-4- > LUMO (0.62)	234.9	5.1379

Table S5. *Cont*.

Theoretical				Experimental	
Transition Energy E (eV)	***f***	**λ (nm)**	**Major Contribution**	**λ (nm)**	**E (eV)**
4.8801	0.0097	254.059	H-3- > LUMO (0.46)	199.4	5.6754
DMSO					
3.8939	0.3164	318.404	HOMO- > LUMO (0.98)		
4.3324	0.0232	286.177	H-1- > LUMO (0.67)		
4.4585	0.4700	278.083	H-2- > LUMO (0.65)		
4.7218	0.0049	262.576	H-4- > LUMO (0.68)		
4.9173	0.0042	252.137	H-3- > LUMO (0.70)		
Gas					
3.5716	0.0974	347.136	HOMO- > LUMO (0.99)		
4.0738	0.0082	304.343	H-1- > LUMO (0.93)		
4.3669	0.5114	283.916	H-2- > LUMO (0.89)		
4.5195	0.0120	274.329	H-3- > LUMO (0.98)		
4.6340	0.0041	267.551	HOMO- > L+1 (0.42)		

Table S6. Detailed assignments of theoretical (DFT/B3LYP) and experimental FT-IR and FT-Raman wavenumbers of (2*E*)-HIPC.

Serial	**Experimental [a]**		**B3LYP/6-311++G(d,p)**				**Mode**
Number	**FT-IR**	**FT-Raman**	**Unscaled**	**Scaled**	$\mathbf{I_{IR}}$	$\mathbf{S_{Raman}}$	**Description [b]**
1.	3590 vw		3757	3599	40.2	100.0	νNH
2.	3433 vw		3583	3432	132.5	92.2	νNH
3.	3048 w		3175	3042	4.1	116.7	νCH
4.		3023 vw	3150	3018	7.2	41.9	νCH
5.		2980 vw	3110	2979	0.9	51.8	νCH
6.	2930 vw	2930 vw	3051	2923	1.1	30.7	νCH
7.			3051	2922	2.7	151.1	νCH
8.			3042	2914	14.8	122.3	νCH
9.	2908 vw		3036	2908	19.3	224.4	νCH
10.			3035	2907	21.4	57.5	νCH
11.			3032	2904	26.3	56.1	νCH
12.		2880 vw	3026	2899	4.0	102.7	νCH
13.			3021	2894	1.2	78.5	νCH
14.			3019	2893	0.8	52.2	νCH
15.			3015	2888	11.2	38.1	νCH
16.			2825	2707	9.3	16.1	νCH
17.			2788	2671	3.4	43.3	νCH
18.			2780	2663	18.5	18.9	νCH
19.			2745	2629	4.6	86.9	νCH
20.	1630 vw		1650	1622	514.3	42.2	νCN
21.		1611 s	1646	1618	2.4	409.5	νCC
22.			1624	1596	2.7	68.0	νCC
23.		1585 m	1618	1590	7.4	137.3	νCN
24.		1579 vw	1610	1583	278.2	34.4	νCC
25.		1540 vw	1572	1545	2.2	13.6	νCC

Table S6. *Cont*.

Serial Number	Experimental [a]		B3LYP/6-311++G(d,p)				Mode Description [b]
	FT-IR	FT-Raman	Unscaled	Scaled	I_{IR}	S_{Raman}	
26.		1516 vw	1541	1515	648.5	30.9	νCC
27.			1539	1513	16.4	8.1	νCC
28.			1536	1510	104.0	2.5	νCC
29.			1524	1498	18.9	4.7	νCC
30.		1495 vw	1523	1497	8.9	14.4	νCC
31.			1487	1462	8.5	3.8	νCC
32.			1471	1446	57.8	11.2	νCC
33.			1464	1439	4.4	4.8	νCC
34.			1461	1437	201.6	3.7	νCC
35.	1425 s		1454	1429	88.9	5.0	νCC
36.		1406 vw	1434	1409	31.1	17.8	νCO
37.			1407	1383	13.0	12.8	νCN
38.		1365 vw	1385	1362	104.2	5.7	νCN
39.		1350 vw	1376	1353	4.3	2.8	νCN
40.	1345 vw		1370	1347	6.6	24.1	νCC
41.	1315 w		1336	1313	33.2	16.5	νNN
42.		1301 vw	1321	1299	164.4	17.1	νCC
43.			1321	1298	26.1	6.9	νCC
44.			1309	1287	183.1	19.6	νCC
45.		1275 w	1300	1278	80.3	15.9	νCN
46.			1296	1274	81.6	36.8	νCC
47.		1245 vw	1262	1240	1.4	1.1	βHNN
48.	1230 s		1249	1228	165.0	5.5	βHCC
49.	1210 m		1228	1207	20.6	2.4	βHCC
50.	1198 vw	1198 vw	1221	1200	2.9	9.0	βHCC
51.			1209	1188	16.2	5.6	βHCC
52.			1207	1187	2.8	30.6	βHCC
53.		1180 vw	1204	1184	7.6	13.3	βHCC
54.		1165 vw	1185	1165	5.7	7.0	βHCC
55.	1152 m		1170	1150	18.1	11.3	βHCC
56.		1108 w	1129	1110	66.1	2.6	βHCN
57.		1095 vw	1116	1097	16.5	1.7	βHCC
58.		1080 vw	1101	1082	22.0	0.3	βHCC
59.	1063 vw		1081	1063	0.6	1.0	βHCC
60.		1051 vw	1069	1051	120.3	5.2	βHCC
61.		1045 vw	1060	1042	23.0	3.6	βHCC
62.			1059	1041	0.0	0.3	βHCC
63.		1040 vw	1058	1040	0.5	0.4	βHCH
64.			1054	1036	3.3	1.2	βHCC
65.	1018 vw		1033	1016	15.5	15.5	βHCH
66.		1012 s	1031	1014	3.8	0.9	βCCN
67.			1027	1010	18.9	9.7	βCCC
68.		1000 vw	1017	1000	8.5	50.9	βNCO

Table S6. *Cont*.

Serial Number	Experimental [a]		B3LYP/6-311++G(d,p)				Mode Description [b]
	FT-IR	FT-Raman	Unscaled	Scaled	I_{IR}	S_{Raman}	
69.		995 vw	1011	994	54.3	4.4	βCCC
70.	980 vw		1005	988	44.3	24.3	βCNC
71.		980 vw	997	980	5.6	4.3	βCCC
72.		965 vw	985	968	1.5	13.0	βCCC
73.			975	958	6.1	4.3	βCCC
74.	936 vw		948	932	13.4	20.1	βCCC
75.		910 vw	921	905	26.3	12.6	βCCC
76.	895 vw		915	899	15.2	1.2	βCNN
77.	885 vw		905	890	15.5	4.2	βCNC
78.			893	878	10.1	5.3	βCCN
79.		865 vw	883	868	0.9	5.5	βNCN
80.	858 vw		870	855	3.7	13.4	βCNC
81.		835 vw	846	832	259.8	0.6	βCCN
82.	820 vw		842	827	33.0	4.2	βCNN
83.			826	812	23.1	3.4	βCCC
84.		805 vw	825	811	58.3	6.0	βCNC
85.		761 vw	772	759	1.6	0.9	βCCC
86.		745 vw	761	748	16.8	1.6	γHNNC
87.		740 vw	756	743	43.9	1.5	γHCCC
88.	730 vw		739	727	38.5	3.4	γHCCC
89.	713 vw		725	712	24.5	1.8	γHCCC
90.		700 vw	718	706	3.9	1.7	γHCCC
91.		682 vw	698	686	2.0	0.5	γHCCC
92.	655 vw		668	656	45.4	1.3	γHCCC
93.		644 vw	652	641	3.8	3.3	γHCNC
94.		630 w	640	629	15.1	2.8	γHCCN
95.		620 vw	635	624	2.6	7.6	γHCNC
96.		612 vw	625	615	33.5	2.1	γHCCC
97.		598 vw	610	600	4.1	9.4	γHCCC
98.	535 vw		547	537	24.7	3.4	γHNCC
99.			539	530	26.0	0.8	γHCCC
100.		515 vw	528	519	39.4	1.3	γHCCC
101.	460 vw		468	460	101.7	1.4	γHCNC
102.		425 w	431	423	50.1	1.3	γHCNC
103.	420 vw		428	420	0.2	0.1	γHCCC
104.		412 w	419	412	0.4	1.0	γHCCC
105.		405 m	408	401	2.7	1.0	γCCCC
106.		396 w	400	393	0.9	1.1	γCCCC
107.	373 m		378	371	2.3	2.9	γHCCC
108.		345 w	356	350	4.0	0.1	γCCCC
109.		322 w	331	325	8.6	2.2	γCCCC
110.	310 m		320	315	2.9	2.6	γCNNC
111.		285 w	277	272	2.8	1.0	γCCCC

Table S6. *Cont*.

Serial Number	Experimental [a]		B3LYP/6-311++G(d,p)				Mode Description [b]
	FT-IR	FT-Raman	Unscaled	Scaled	I_{IR}	S_{Raman}	
112.		260 vw	270	265	1.8	2.8	γCNCC
113.		203 w	207	203	11.2	2.7	γCNCC
114.		198 w	199	195	2.6	4.6	γCCCN
115.		176 w	178	175	1.0	2.1	γCCNC
116.		160 w	169	166	1.0	0.8	γCCCC
117.		155 s	162	159	1.5	1.5	γCCCC
118.		145 s	159	156	0.1	4.7	γNNCN
119.		121 s	131	129	4.9	1.8	γCCNN
120.		115 s	114	112	2.5	3.2	γCCCC
121.			94	93	0.2	5.5	γCCCN
122.		82 s	84	83	0.1	6.9	γHNCC
123.			82	81	0.0	7.2	γCNCN
124.		58 m	54	53	1.0	2.0	γCCCN
125.			50	49	0.5	3.0	γCCCC
126.			39	39	0.3	0.7	γCCCN

[a] s: strong; vs: very strong; m: medium; w: weak; vw: very weak; [b] ν: stretching; β: in-plane bending; γ: out-of-plane bending; I_{IR}: IR intensity; S_{Raman}: Raman scattering activity.

Table S7. Theoretical (B3LYP) and experimental ^{1}H and ^{13}C NMR values of (2*E*)-HIPC in DMSO and acetonitrile.

Atom	^{13}C NMR			Atom	^{1}H NMR		
	Experimental	Theoretical (B3LYP)			Experimental	Theoretical (B3LYP)	
	DMSO	DMSO	Acetonitrile		DMSO	DMSO	Acetonitrile
C7 (in chain)	153.6	152.3	152.3	H44 (in ring)	7.41	9.1	9.10
C17 (in chain)	145.1	157.6	157.6	H39 (in chain NH)	8.88	8.81	8.80
C14 (in imidazole)	138.9	144.6	144.6	H37 (in imidazole)	7.43	8.46	8.45
C20 (in ring)	137.3	145.8	145.8	H30 (in ring)	7.85	7.97	7.96
C5 (in ring)	136.8	140.7	140.7	H29 (in ring)	7.85	7.70	7.69
C2 (in ring)	128.9	135.2	135.2	H28 (in ring)	7.65	7.72	7.72
C4 (in ring)	128.5	130.3	130.3	H26 (in chain)	7.65	7.72	7.72
C6 (in ring)	128.5	130.9	130.9	H27 (in ring)	7.65	7.79	7.78
C24 (in ring)	128.4	133.2	133.2	H38(in chain NH)	10.27	7.74	7.74
C22 (in ring)	128.4	133.2	133.2	H35 (in ring)	6.87	7.54	7.53
C1 (in ring)	128.3	133.5	133.5	H41 (in ring)	7.32	7.52	7.52
C3 (in ring)	128.3	133.5	133.5	H43 (in ring)	7.32	7.28	7.27
C12 (in imidazole)	126.4	126.3	126.3	H42 (in imidazole)	7.05	7.23	7.23
C23 (in ring)	122.6	126.3	126.1	H40 (in ring)	7.41	7.18	7.17
C25 (in ring)	119.9	120.0	120.0	H36 (in imidazole)	7.29	7.08	7.08
C21 (in ring)	119.9	120.1	120.1	H34 (in chain)	4.13	4.1	4.09
C11 (in imidazole)	119.4	119.4	119.9	H33 (in chain)	4.13	3.73	3.73
C9 (in chain)	42.1	45.6	45.6	H32 (in chain)	3.33	3.51	3.50
C8 (in chain)	28.3	33	32.9	H31 (in chain)	3.33	2.69	2.68