Supplementary Information for

Preferential solvation of *meso*–methyl BODIPYs with pyridine via *pseudo*-hydrogen bonds

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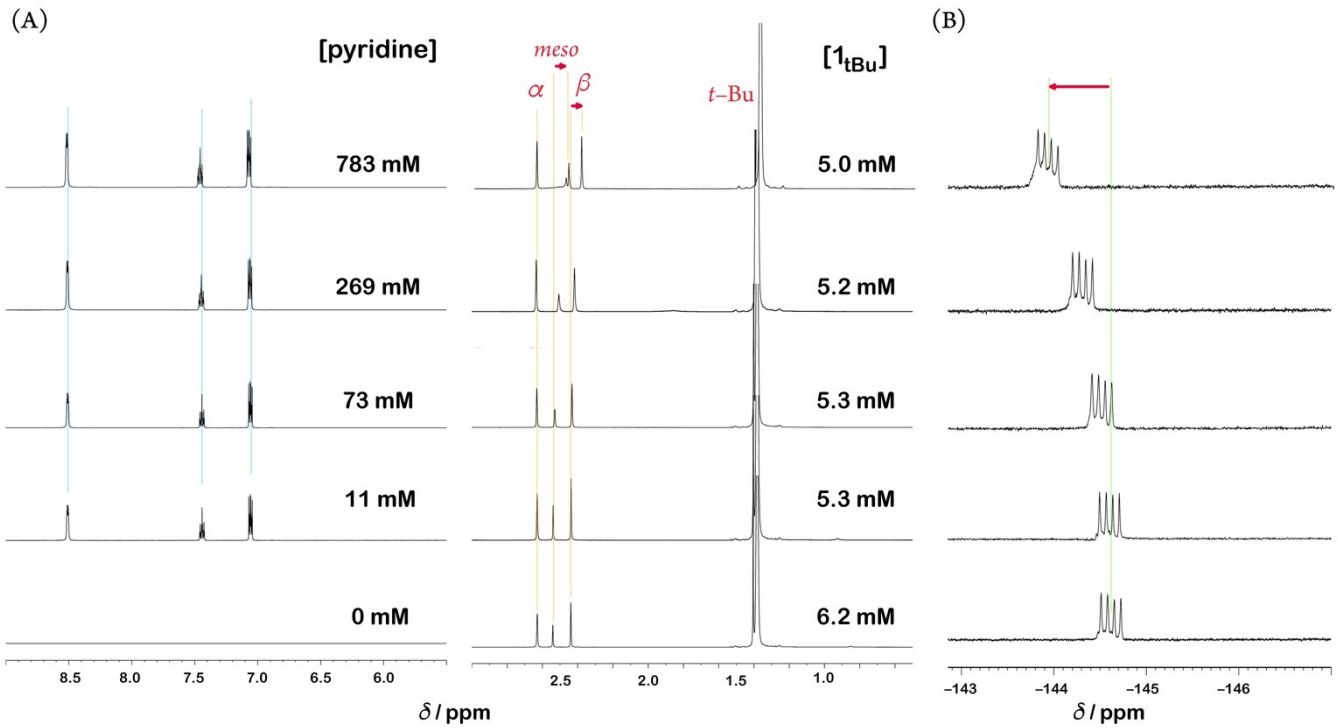


Fig S1. ^{1}H (500 MHz, A) and ^{19}F NMR spectra (470 MHz, B) of $\mathbf{1}_{t\mathbf{Bu}}$ (from 6.2×10^{-3} M diluted to 5.0×10^{-3} M, bottom to top) in the presence of added pyridine (up to 7.83×10^{-1} M, bottom to top) at 298 K in cyclohexane–d_{12}. The peak height in the aromatic region was normalised to that in the aliphatic region. In the absence of pyridine, the *meso*-proton is deshielded by the self-complementary C–H···F nonconhentional hydrogen bond formation in a dimer (Fig 7). The addition of excess amount of pyridine relieved the downfield shift, instead the more acidic pyridyl proton lead to downfield shift of the fluorine.

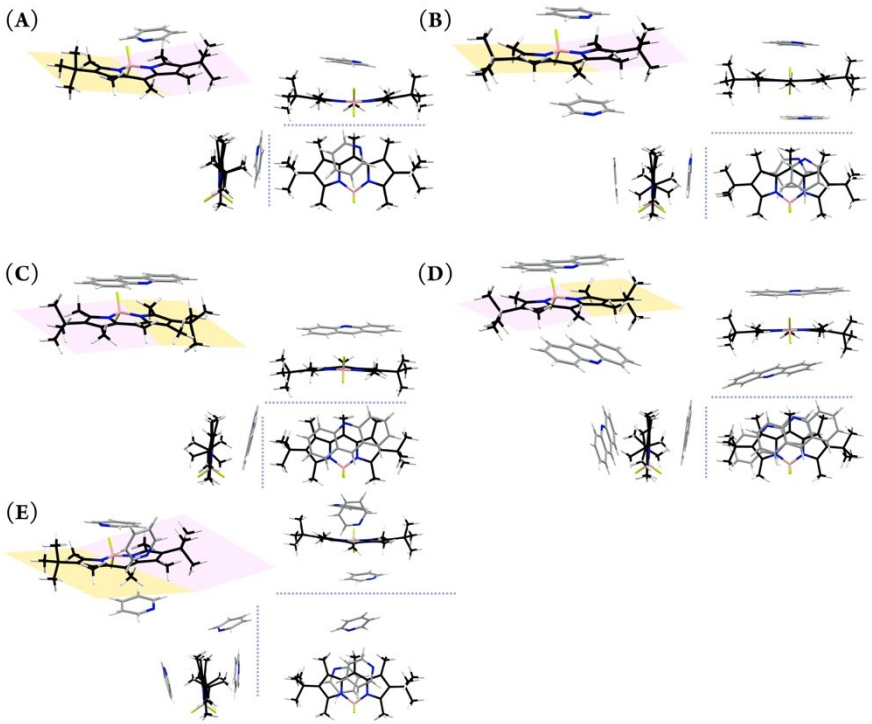


Fig S2. Geometry–optimised structures of $\mathbf{1}_{t\mathbf{Bu}}$·pyridine (A), $\mathbf{1}_{t\mathbf{Bu}}$·(pyridine)$_2$ (B), $\mathbf{1}_{t\mathbf{Bu}}$ ·acridine (C), $\mathbf{1}_{t\mathbf{Bu}}$ ·(acridine)$_2$ (D), and $\mathbf{1}_{t\mathbf{Bu}}$·(pyridine)$_3$ (E) generated by the dispersion-corrected DFT calculations at the B3LYP-D3(BJ)/6–31G(d,p) level of theory.

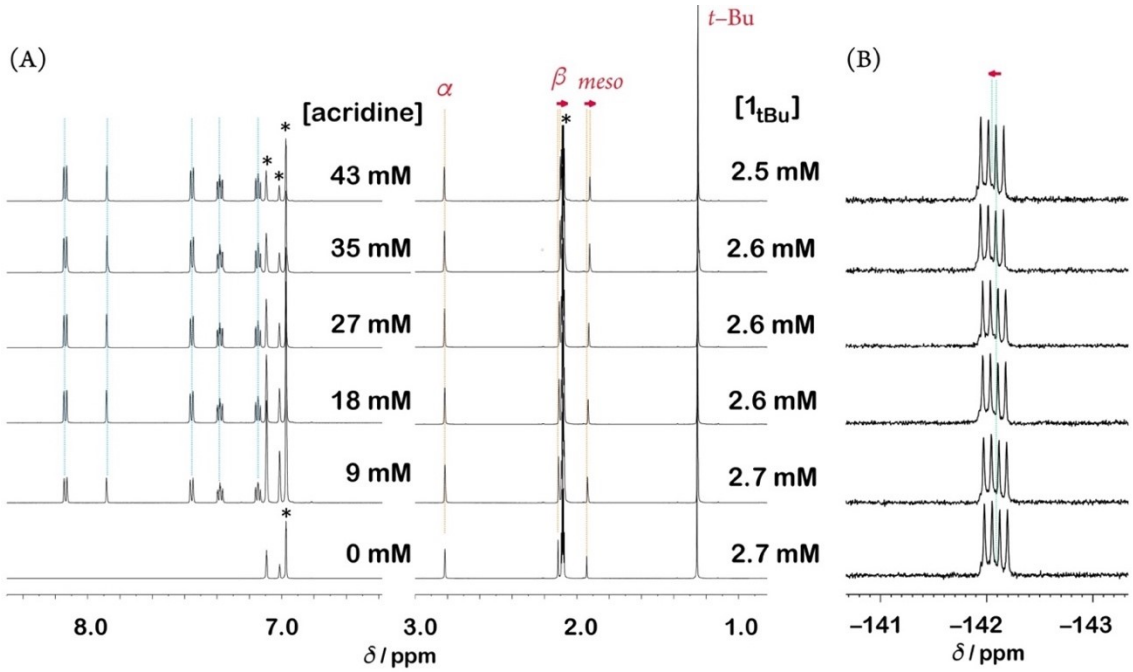


Fig S3. ^{1}H (500 MHz, A) and ^{19}F NMR spectra (470 MHz, B) of $\mathbf{1}_{t\mathbf{Bu}}$ (from 2.7 × 10^{-3} diluted up to 2.6 × 10^{-3} M, bottom to top) in the presence of added acridine (up to 4.3 × 10^{-2} M, bottom to top) at 298 K in toluene–d_8. The peak height in the aromatic region was normalised to that in the aliphatic region. An asterisk indicates a peak ascribed to residual solvent. A small upfield shift of *β*– and *meso*–methyl protons suggested shielding by the acridine plane. The proton of 9–acridine showed a downfield shift in the presence of $\mathbf{1}_{t\mathbf{Bu}}$, suggesting C–H···N *pseudo*-hydrogen-bond formation, as supported by the downfield shift of fluorine.

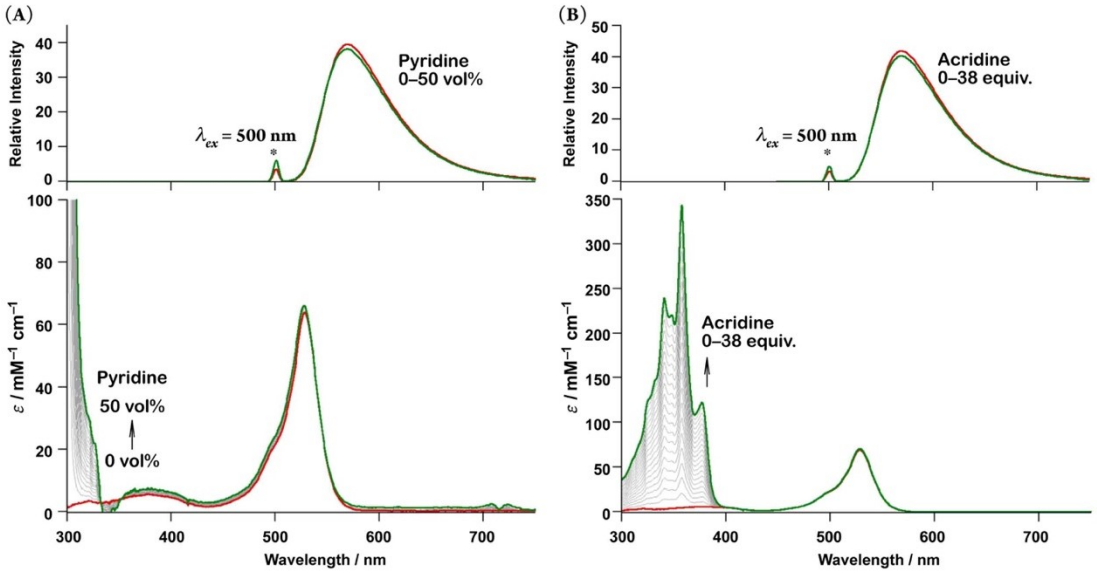


Fig S4. Spectrometric titration of $\mathbf{1}_{t\mathbf{Bu}}$ ($[\mathbf{1}_{t\mathbf{Bu}}]_0 = 1.4 \times 10^{-6}$ M, red line, diluted up to 6.9×10^{-7} M, green line via grey lines) with pyridine (up to 50 vol%, green line) (A, shown as constant $[\mathbf{1}_{t\mathbf{Bu}}]$) and $\mathbf{1}_{t\mathbf{Bu}}$ ($[\mathbf{1}_{t\mathbf{Bu}}]_0 = 1.37 \times 10^{-6}$ M, red line, diluted up to 9.1×10^{-5} M, green line via grey lines) with acridine (up to 3.5×10^{-5} M, green line) (B, shown as constant $[\mathbf{1}_{t\mathbf{Bu}}]$) at 298 K in toluene. Fluorescence spectra were obtained by the excitation at 480 and 500 nm for pyridine and acridine titration, respectively. Absorption spectra are shown as constant $[\mathbf{1}_{t\mathbf{Bu}}]$ in (A) and (B), and fluorescence spectra are normalised by the absorbance at the excitation wavelength (480 nm in (A) and 500 nm in (B)).

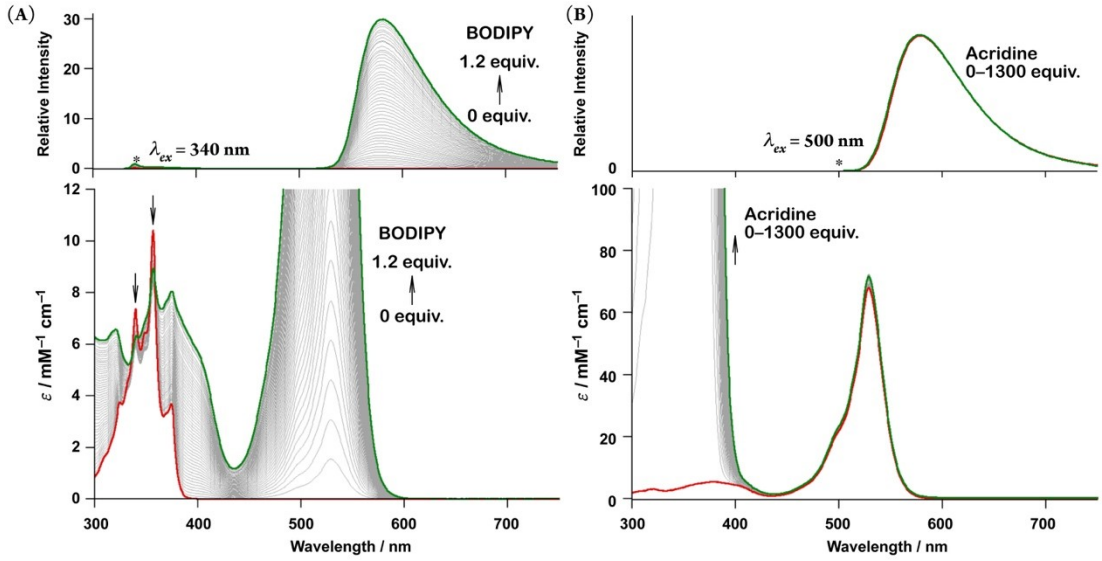


Fig S5. Spectrometric titration of acridine ($[\text{acridine}]_0 = 5.2 \times 10^{-5}$ M, red line, diluted up to 2.3×10^{-5} M, green line via grey lines) with $\mathbf{1}_{t\mathbf{Bu}}$ (up to 2.6×10^{-5} M, green line) (A) and $\mathbf{1}_{t\mathbf{Bu}}$ ($[\mathbf{1}_{t\mathbf{Bu}}]_0 = 3.8 \times 10^{-6}$ M, red line, diluted up to 2.0×10^{-6} M, green line via grey lines) with acridine (up to 2.6×10^{-3} M, green line) (B) at 298 K in cyclohexane. Fluorescence spectra (upper panels) were obtained by the excitation of acridine at 340 and $\mathbf{1}_{t\mathbf{Bu}}$ at 500 nm in (A) and (B). Absorption spectra are shown as constant [acridine] in (A) and constant $[\mathbf{1}_{t\mathbf{Bu}}]$ in (B). Fluorescence spectra are normalised by the absorbance at the excitation wavelength (340 nm in (A) and 500 nm in (B)). The spectral shape in (A) becomes distorted as increasing the inner filter effect of the intense absorption band of $\mathbf{1}_{t\mathbf{Bu}}$ at higher concentration.

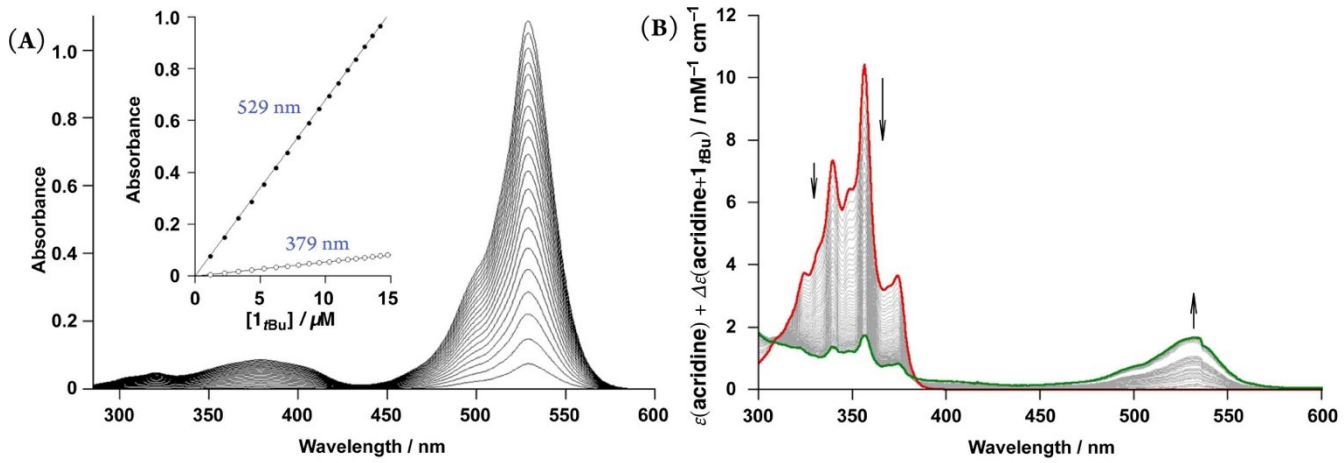


Fig S6. Absorption spectra of $\mathbf{1}_{t\mathbf{Bu}}$ at various concentration at 298 K in cyclohexane and the Beer's plot (ε_{529} = 68.0 and ε_{379} = 5.5 $mM^{-1}\,cm^{-1}$) (A). Mathematical subtraction of $\mathbf{1}_{t\mathbf{Bu}}$ from the observed spectral change in Fig S6A, and therefore the spectra are shown as constant [acridine] together with change of absorption of $\mathbf{1}_{t\mathbf{Bu}}$ and acridine (B). The spectral change was plotted as the titration isotherms in Fig 6B. We carefully confirmed the reproducibility of the titration experiment to minimise the experimental and mathematical error arising from the small molar absorptivity of acridine, which is approximately quarter of that of $\mathbf{1}_{t\mathbf{Bu}}$.

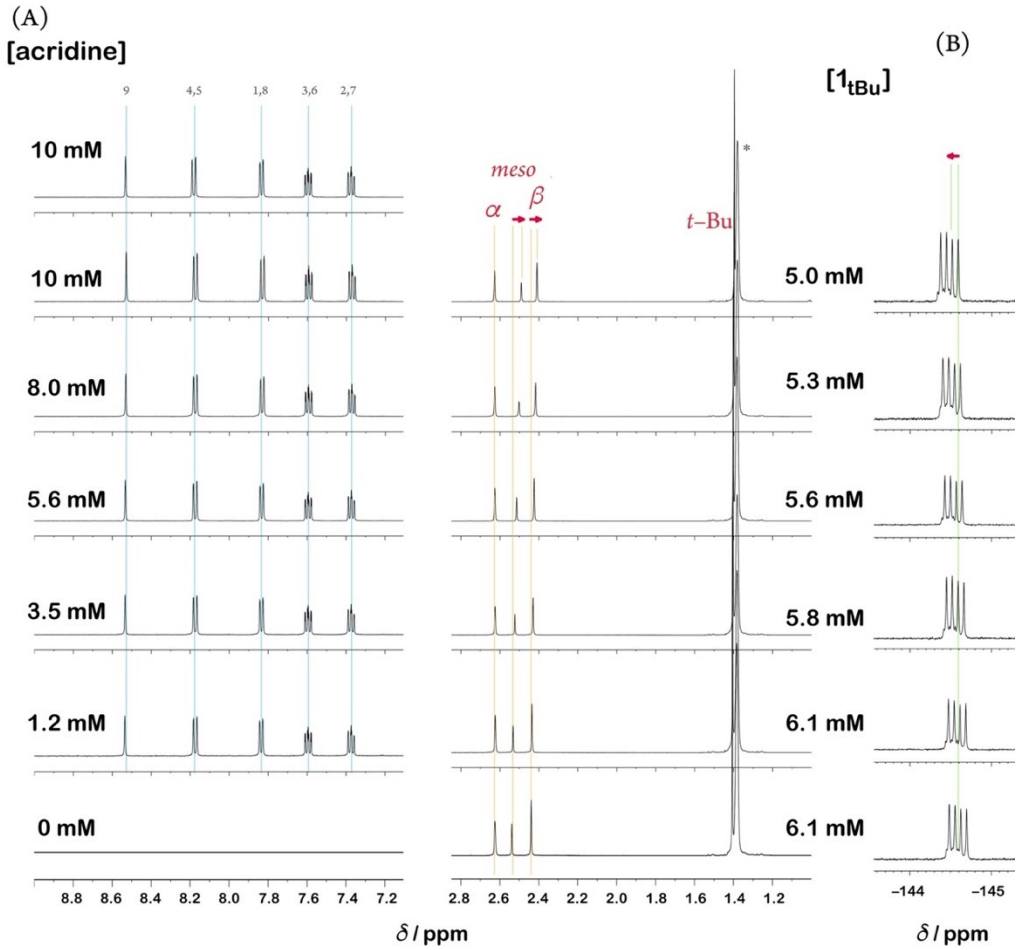


Fig S7. ^{1}H (500 MHz, A) and ^{19}F NMR spectra (470 MHz, B) of$\mathbf{1}_{t\mathbf{Bu}}$ (from 6.1 × 10^{-3} diluted up to 5.0 × 10^{-3} M, bottom to top) in the presence of added acridine (up to 10.0 × 10^{-2} M, bottom to top) at 298 K in cyclohexane–d_{12}. The peak height in the aromatic region was normalised to that in the aliphatic region. An asterisk indicates a peak ascribed to residual solvent. A small selective upfield shift of *β*– and *meso*–methyl protons suggested a shielding by the acridine plane.

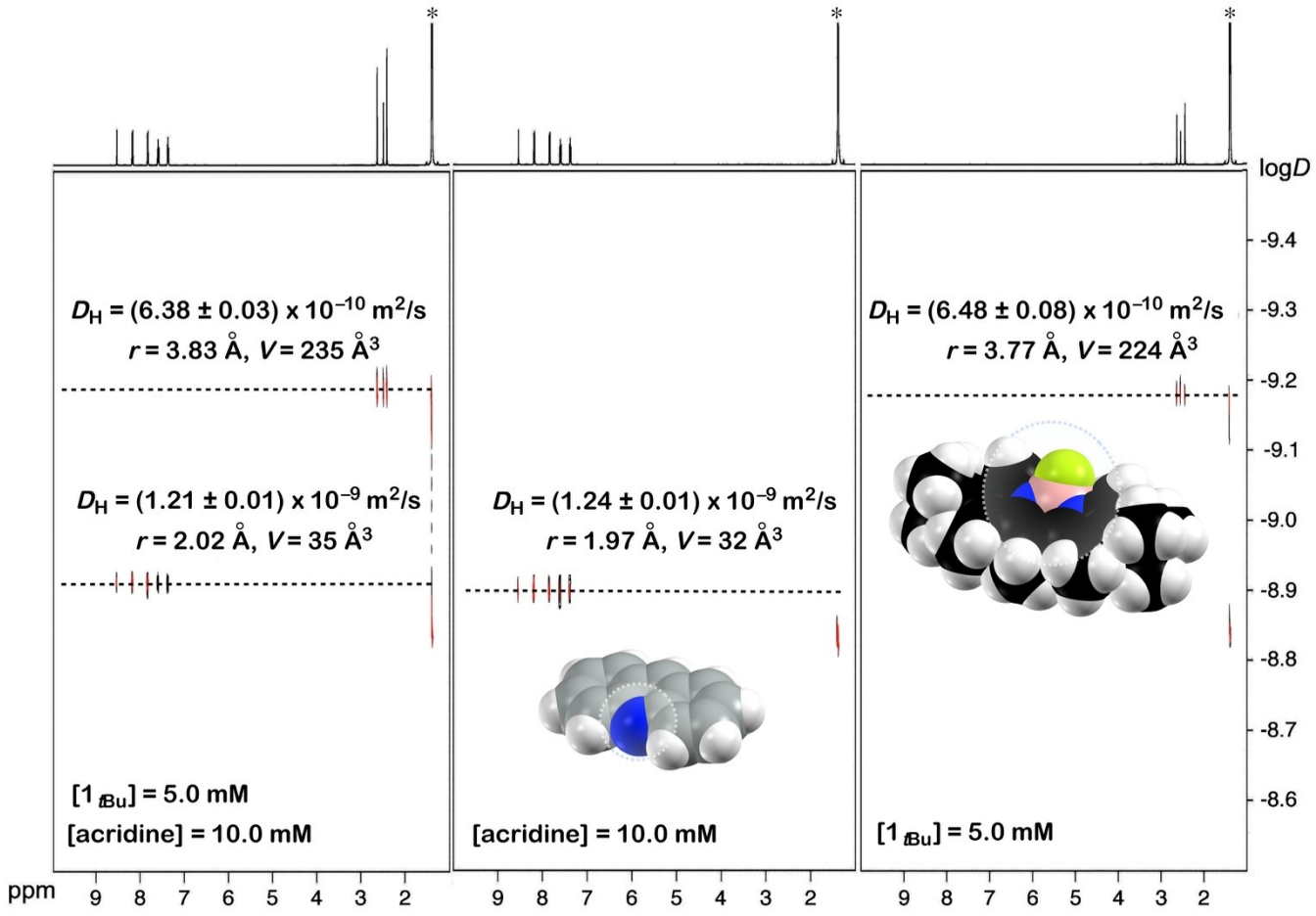


Fig S8. ^{1}H DOSY spectra (500 MHz) of a mixture of $\mathbf{1}_{\mathbf{tBu}}$ (5.0 mM) and acridine (10.0 mM) (left), acridine (5.0 mM) (middle), and $\mathbf{1}_{\mathbf{tBu}}$ (5.0 mM) (right) in cyclohexane-d_{12}. The geometry optimized structures of acridine and $\mathbf{1}_{\mathbf{tBu}}$ (B3LYP-D3(BJ)/6-31G(d,p)) with circles with radius (r) = 1.97 and 3.77 Å, respectively, are shown. The diffusion coefficients (D_H) became smaller than the corresponding components by mixing, suggesting interaction $\mathbf{1}_{\mathbf{tBu}}$ with acridine. Although $\mathbf{1}_{\mathbf{tBu}}$ is assumed to involve self-aggregated species, the diffusion coefficient of $\mathbf{1}_{\mathbf{tBu}}$ is larger than that of mixture of $\mathbf{1}_{\mathbf{tBu}}$ and acridine, in line with the fact that the binding constant for the $\mathbf{1}_{\mathbf{tBu}}$···acridine interaction is greater than the self-aggregation of $\mathbf{1}_{\mathbf{tBu}}$ (Fig 5).

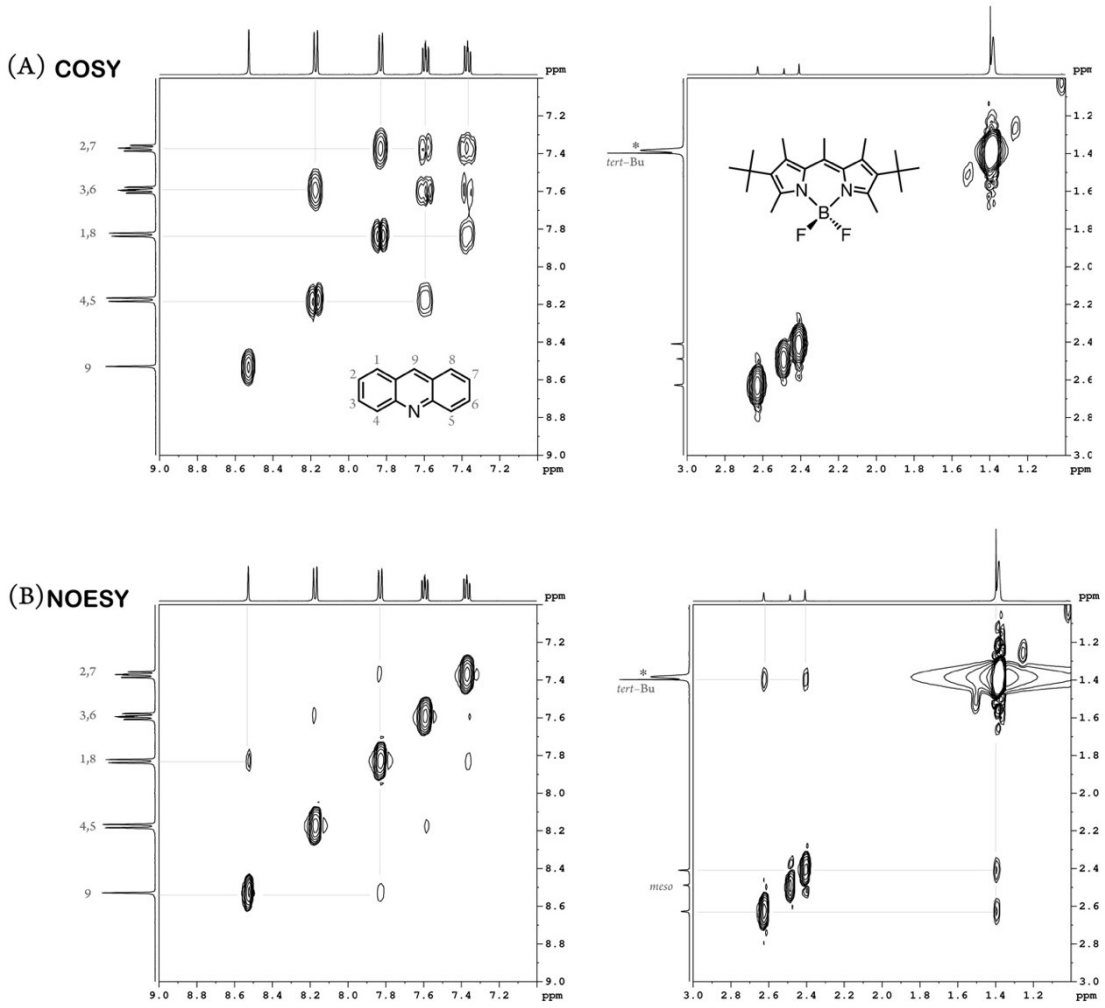


Fig S9. ^{1}H–^{1}H COSY (A) and NOESY (B) spectra (500 MHz) of a mixture of $\mathbf{1}_{\mathbf{tBu}}$ (5.0 mM) and acridine (10.0 mM) in cyclohexane-d_{12}. Aromatic (left) and aliphatic region (right) are shown separately. No intermolecular correlations between aromatic and aliphatic signals were found in COSY and NOESY spectra.

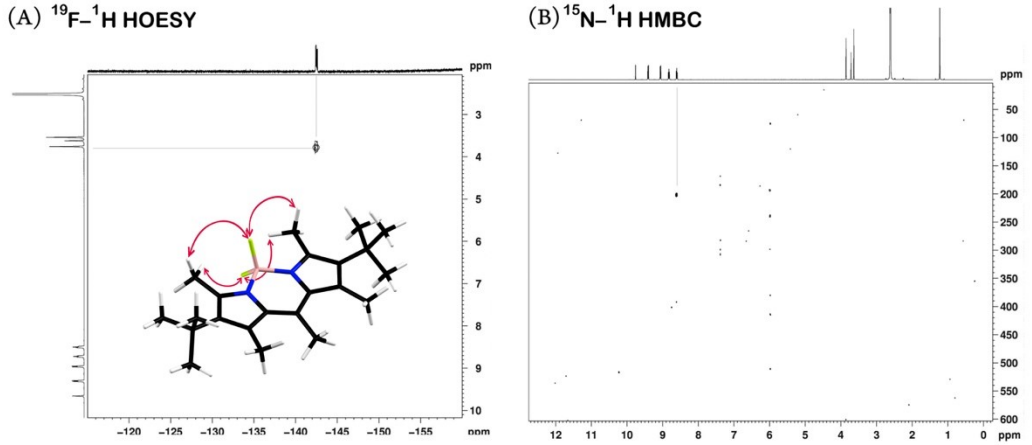


Fig S10. ^{19}F–^{1}H HOESY (A) and ^{15}N–^{1}H HMBC (B) spectra of the mixture of $\mathbf{1}_{\mathbf{tBu}}$ (5.0 mM) and acridine (10.0 mM) in cyclohexane-d_{12}. Only intramolecular correlations were found.

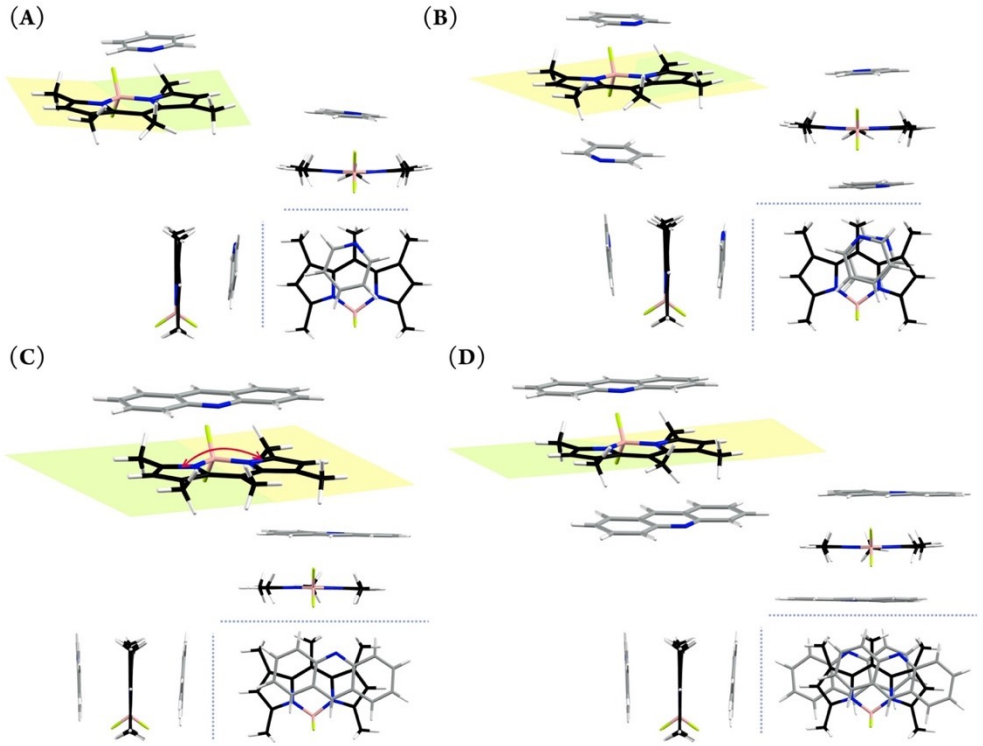


Fig S11. Geometry–optimised structures of $\mathbf{1_H}$·pyridine (A), $\mathbf{1_H}$·(pyridine)$_2$ (B), $\mathbf{1_H}$·acridine (C) and $\mathbf{1_H}$·(acridine)$_2$ (D) generated by the dispersion-corrected DFT calculations at the B3LYP-D3(BJ)/6–31G(d,p) level of theory.

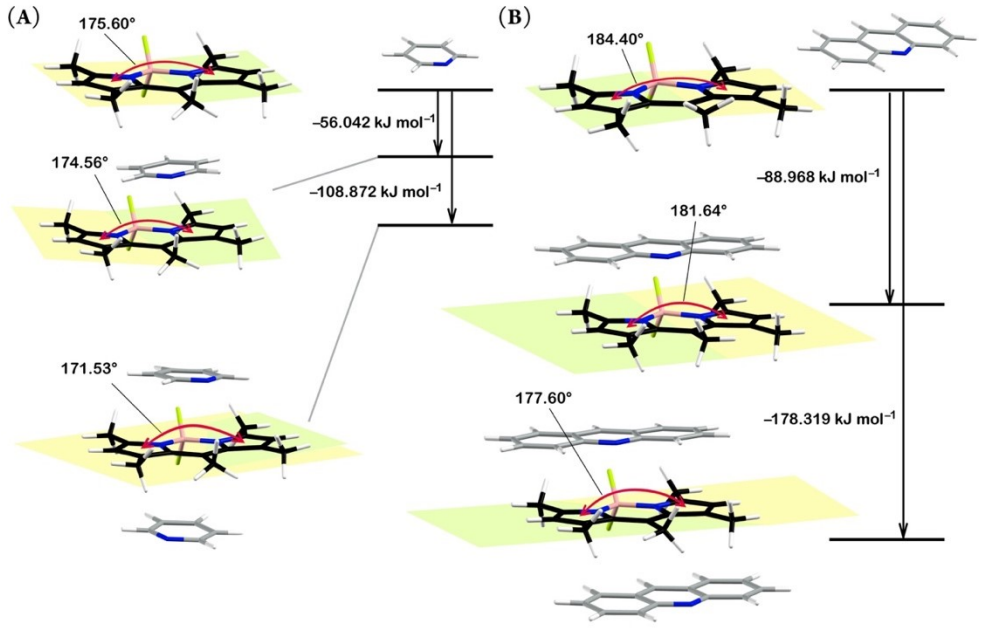


Fig S12. Geometry-optimised structures of $\mathbf{1_H}$, $\mathbf{1_H}$·pyridine, and $\mathbf{1_H}$·(pyridine)$_2$ (upper to lower in A), and $\mathbf{1_H}$, $\mathbf{1_H}$·acridine, and $\mathbf{1_H}$·(acridine)$_2$ (upper to lower in B) produced using DFT calculations at the B3LYP-D3(BJ)/6-31G(d,p) level, where dihedral angle between two pyrrole rings of $\mathbf{1_H}$ (yellow and pink planes), and close C–H···N, C–H···π and C–H···F separations are indicated. Vertical axes show relative stabilisation from the dissociation limit of two or three isolated components assuming toluene based on IEF-PCM DFT/B3LYP-D3(BJ) calculations at 6-31G(d,p) level.

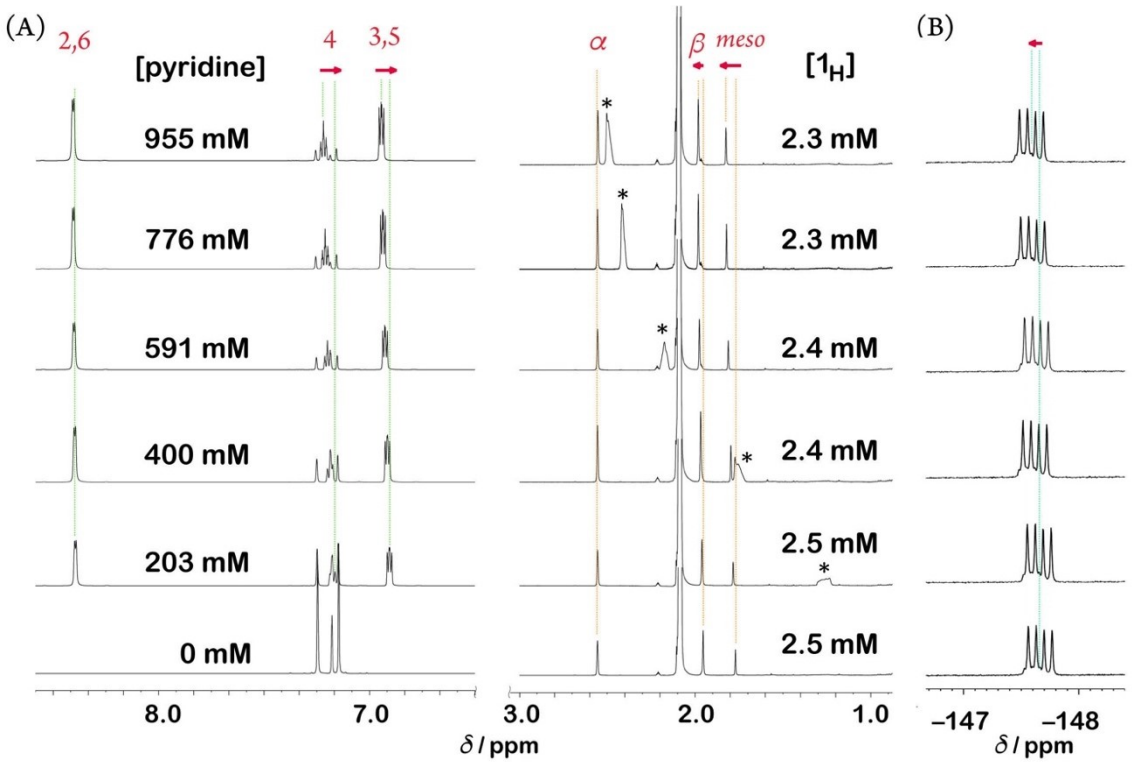


Fig S13. ^{1}H (500 MHz, A) and ^{19}F NMR spectra (470 MHz, B) of $\mathbf{1_H}$ (from 2.5×10^{-3} diluted up to 2.3×10^{-3} M) in the presence of added pyridine (up to 9.6×10^{-1} M, bottom to top) at 298 K in toluene–d_8. The peak height in the aromatic region was normalised to that in the aliphatic region. An asterisk indicates a peak ascribed to residual water.

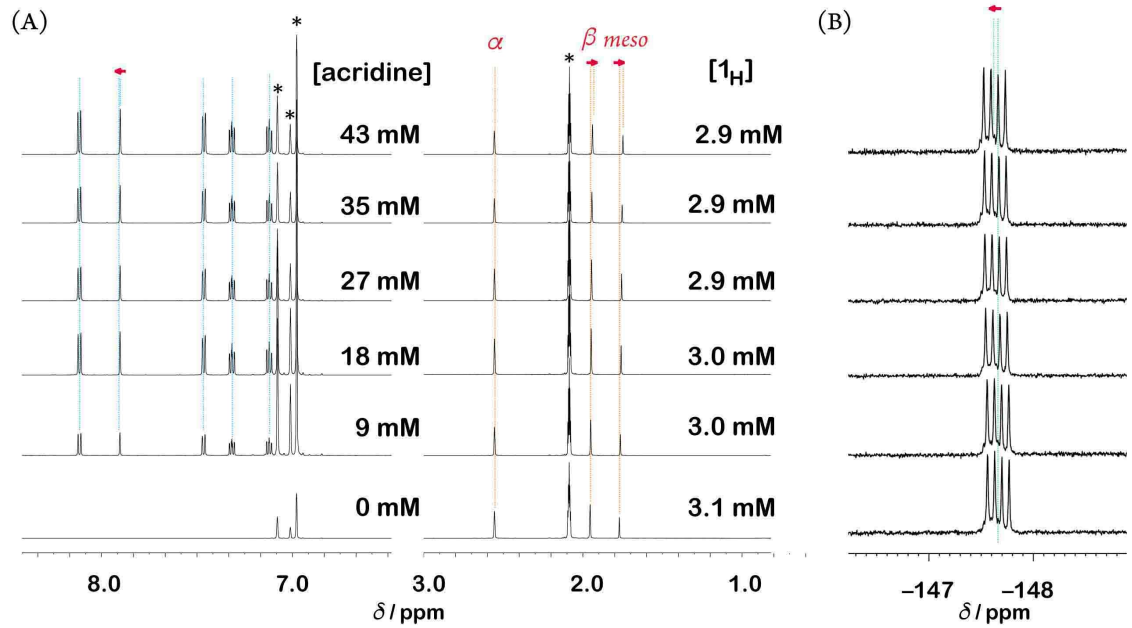


Fig S14. ^{1}H (500 MHz, A) and ^{19}F NMR spectra (470 MHz, B) of $\mathbf{1_H}$ (from 3.1×10^{-3} diluted up to 2.9×10^{-3} M, bottom to top) in the presence of acridine (up to 4.3×10^{-2} M, bottom to top) at 298 K in toluene–d_8. The peak height in the aromatic region are normalised to that in the aliphatic region. An asterisk indicates a peak ascribed to residual solvent.

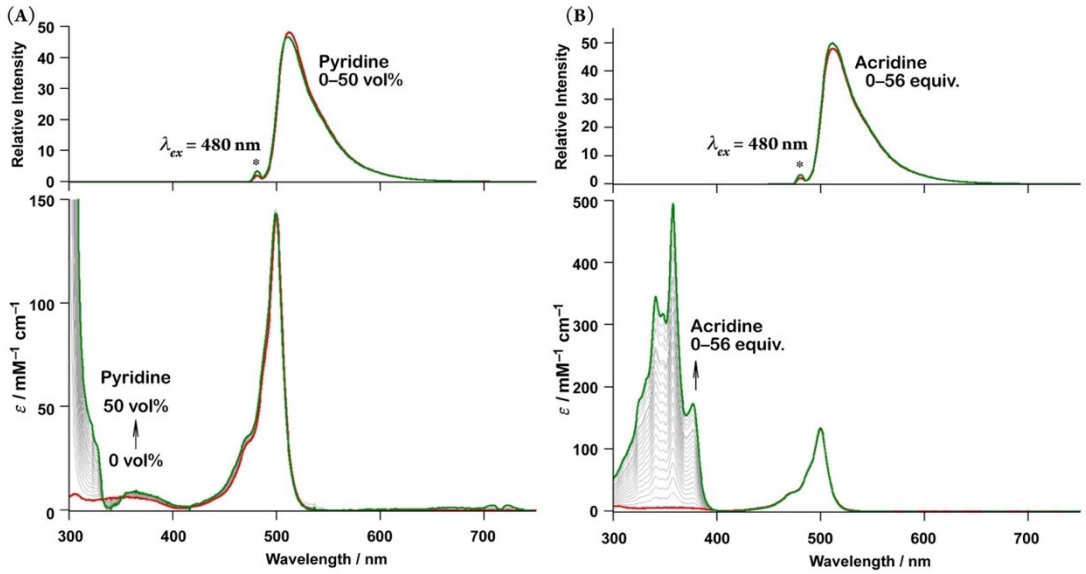


Fig S15. Spectrometric titration of $\mathbf{1_H}$ ($[\mathbf{1_H}]_0 = 9.5 \times 10^{-7}$ M, red line, diluted up to 4.3×10^{-7} M, green line via grey lines) with pyridine (up to 50 vol%, green line) (A) and $\mathbf{1_H}$ ($[\mathbf{1_H}]_0 = 9.5 \times 10^{-7}$ M, red line, diluted up to 6.3×10^{-7} M, green line via grey lines) with acridine (up to 3.5×10^{-5} M, green line) (B) at 298 K in toluene. Fluorescence spectra were obtained by the excitation at 480 and 500 nm for pyridine and acridine titration, respectively. Absorption spectra are shown as constant [$\mathbf{1_H}$] in (A) and (B), and fluorescence spectra are normalised by the absorbance at the excitation wavelength (480 nm in (A) and 500 nm in (B)).

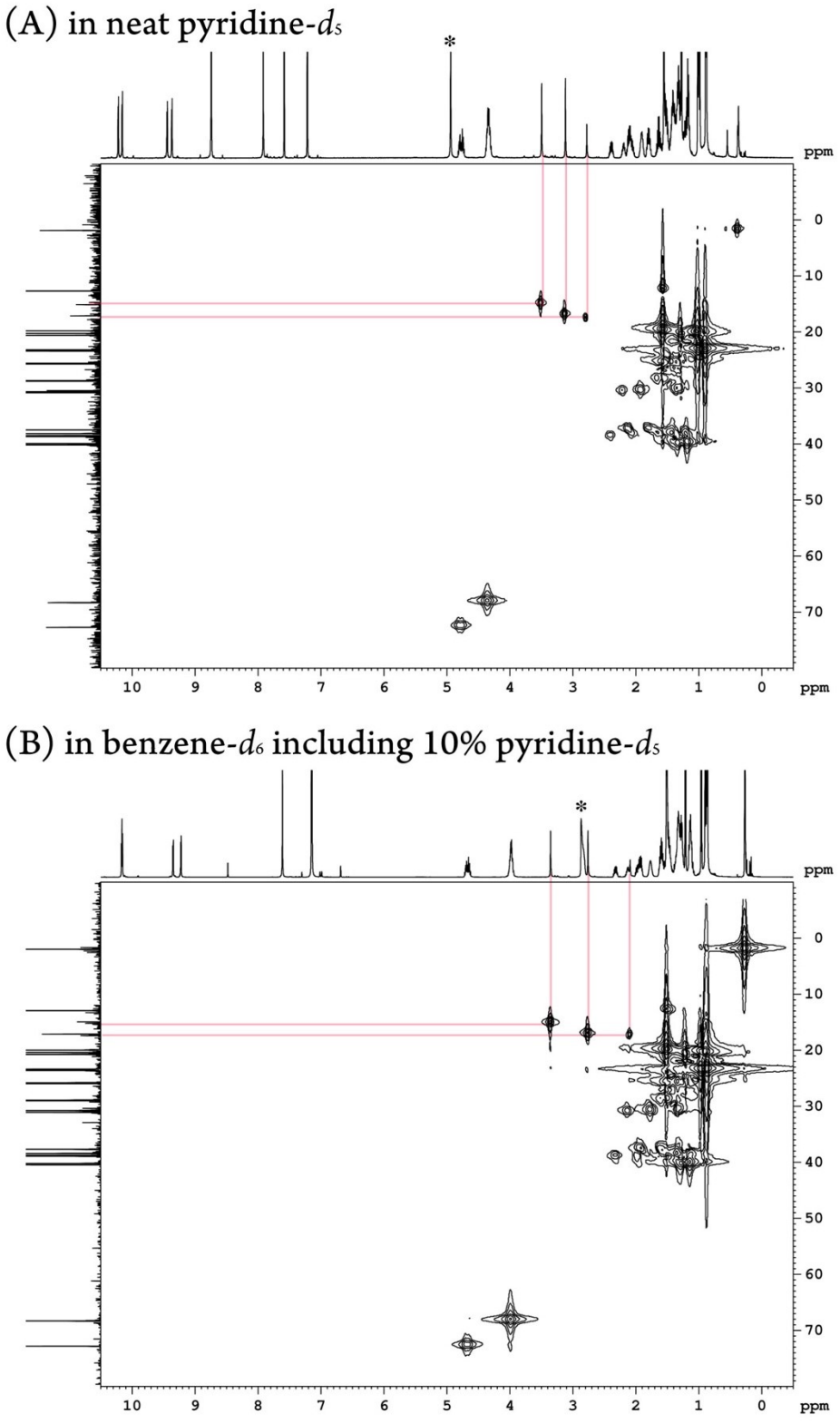
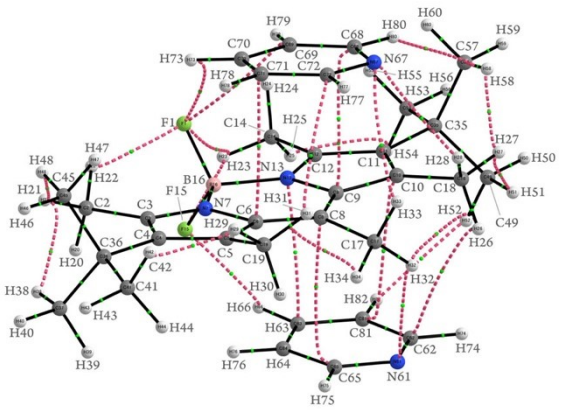
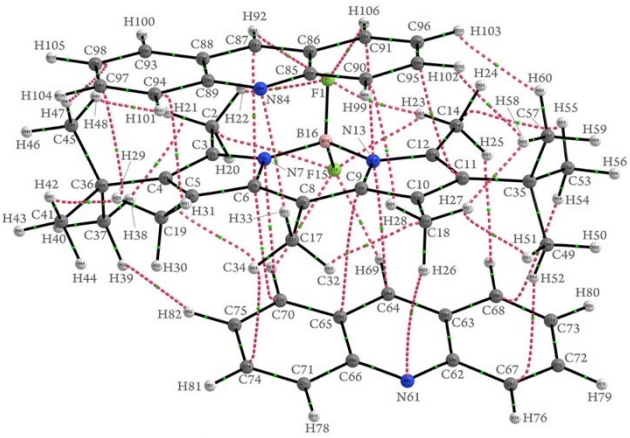


Fig S16. ^{13}C–^{1}H HMBC spectra of $\mathbf{1_{por}}$ in pyridine-d_5 (A) and in benzene-d_6 including 10% pyridine-d_5 (B).

Table S1. Summary of topological descriptors at the bond critical points of $\mathbf{1}_{t\mathbf{Bu}}\cdot(\text{pyridine})_2$ and $\mathbf{1}_{t\mathbf{Bu}}\cdot(\text{pyridine})_2$ complexes based on the QTAIM analyses of the optimised geometries at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.



$\mathbf{1}_{tBu}\cdot(\text{pyridine})_2$ complex



$\mathbf{1}_{tBu}\cdot(\text{acridine})_2$ complex

BCP #	Atoms	Electro density (ρ_{BCP}) in e au^{-3}	Laplacian ($\nabla^2\rho_{BCP}$) in e au^{-5}	Ellipticity ($\varepsilon = \lambda_1/\lambda_2 - 1$)	Kinetic energy density ($K_{BCP} = -H_{BCP}$) in Hartree	BPL – GBL_I
1	N7 - B16	0.155939	0.287201	0.003474	0.128096	0.00003
2	F1 - H22	0.014863	0.057292	0.157325	-0.00091	0.028904
3	C2 - C3	0.259199	-0.631336	0.047418	0.2195	0.000034
4	C6 - N7	0.303532	-0.872798	0.163843	0.455481	0.000206
5	C3 - N7	0.329283	-0.824439	0.157556	0.537453	0.000132
6	C3 - C4	0.296454	-0.754025	0.236515	0.283652	0.000965
7	C4 - C36	0.243373	-0.548864	0.03799	0.19253	0.000162
8	C4 - C5	0.302336	-0.762196	0.263624	0.293908	0.001144
9	C5 - C6	0.293986	-0.747793	0.217926	0.276693	0.000907
10	C2 - H21	0.281818	-0.984171	0.011533	0.292417	0.000242
11	C6 - C8	0.307326	-0.828773	0.219013	0.300908	0.000088
12	N13 - B16	0.15652	0.282984	0.000808	0.129073	0.000047
13	C8 - C9	0.307351	-0.829893	0.216141	0.300932	0.000125
14	C9 - N13	0.304434	-0.876828	0.164108	0.45739	0.000215
15	C9 - C10	0.296124	-0.759663	0.212558	0.280569	0.001025
16	C10 - C18	0.255866	-0.608924	0.031078	0.212561	0.000063
17	C10 - C11	0.302737	-0.767053	0.256147	0.294501	0.000924
18	C11 - C12	0.29648	-0.750585	0.245442	0.283722	0.001112
19	C11 - C35	0.24357	-0.549545	0.038789	0.192716	0.000147
20	F1 - H23	0.010743	0.052266	5.174968	-0.002415	0.269414
21	C12 - N13	0.327	-0.839064	0.161554	0.530605	0.000114
22	C12 - C14	0.258245	-0.62768	0.040799	0.21798	0.000032
23	C14 - H25	0.280266	-0.973658	0.011479	0.289716	0.000256

BCP #	Atoms	Electro density (ρ_{BCP}) in e au^{-3}	Laplacian ($\nabla^2\rho_{BCP}$) in e au^{-5}	Ellipticity ($\varepsilon = \lambda_1/\lambda_2 - 1$)	Kinetic energy density ($K_{BCP} = -H_{BCP}$) in Hartree	BPL – GBL_I
1	N7 - B16	0.158407	0.292778	0.004271	0.130759	0.000017
2	F1 - H22	0.012399	0.050366	0.236849	-0.001311	0.04094
3	C6 - N7	0.302808	-0.864488	0.162988	0.454889	0.00017
4	C2 - C3	0.25913	-0.630925	0.048643	0.21928	0.000038
5	C3 - N7	0.328307	-0.826906	0.156102	0.534699	0.000123
6	C3 - C4	0.297881	-0.76116	0.239498	0.286582	0.000958
7	C4 - C36	0.242277	-0.543969	0.03821	0.190935	0.000301
8	C4 - C5	0.301425	-0.758199	0.259659	0.292035	0.001121
9	C5 - C6	0.294522	-0.750751	0.21674	0.277559	0.000871
10	C2 - H21	0.282374	-0.988605	0.011301	0.293462	0.000231
11	C6 - C8	0.306051	-0.821262	0.219943	0.298559	0.000114
12	N13 - B16	0.157864	0.282861	0.003444	0.130644	0.000011
13	C8 - C9	0.306532	-0.823487	0.221554	0.299493	0.000133
14	C9 - C10	0.294146	-0.750075	0.210686	0.276951	0.001024
15	C10 - C11	0.304462	-0.776566	0.256989	0.297711	0.000869
16	C9 - N13	0.301994	-0.878267	0.16011	0.448687	0.000186
17	C11 - C12	0.296445	-0.75282	0.238254	0.283786	0.0011
18	C11 - C35	0.241917	-0.542864	0.03639	0.190516	0.000114
19	F1 - H23	0.011662	0.052152	0.598625	-0.00193	0.08979
20	C12 - N13	0.327196	-0.836018	0.158241	0.531254	0.000113
21	C12 - C14	0.259248	-0.632499	0.04144	0.219415	0.000049
22	C14 - H55	0.010863	0.045972	3.034071	-0.002653	0.403837
23	C14 - H24	0.275627	-0.939316	0.011855	0.281133	0.000196

24	F1 - B16	0.160233	0.877447	0.032861	0.086404	0.000001
25	F15 - H23	0.014109	0.056451	0.257158	-0.001186	0.031694
26	F15 - B16	0.161407	0.889319	0.031951	0.086751	0.000002
27	C8 - C17	0.25539	-0.610394	0.021349	0.213265	0.000179
28	C18 - H27	0.283522	-0.993802	0.009351	0.295566	0.00026
29	H27 - H51	0.013232	0.05093	0.133182	-0.002297	0.139206
30	H26 - H32	0.012072	0.050482	1.55591	-0.002778	0.805504
31	H29 - H42	0.015019	0.05654	0.445887	-0.002287	0.168505
32	C5 - C19	0.253746	-0.599953	0.02828	0.209211	0.000325
33	C19 - H29	0.283313	-0.994971	0.008919	0.295269	0.000272
34	C19 - H34	0.013401	0.058961	1.54509	-0.003237	0.807658
35	C2 - H20	0.27478	-0.937521	0.011691	0.279661	0.000135
36	C2 - H22	0.282143	-1.00161	0.007924	0.293622	0.000196
37	H21 - H48	0.011166	0.039538	0.090195	-0.001659	0.049154
38	H25 - H54	0.011755	0.048435	1.232112	-0.002678	0.457554
39	C14 - H23	0.285472	-1.025817	0.007212	0.299645	0.000319
40	C14 - H24	0.274603	-0.933116	0.012744	0.279255	0.000164
41	C18 - H26	0.274668	-0.931888	0.011215	0.279035	0.000119
42	C18 - H28	0.278721	-0.965734	0.009026	0.286346	0.000233
43	H27 - H58	0.013074	0.046687	0.051321	-0.001762	0.058555
44	C19 - H30	0.273507	-0.922397	0.01319	0.276778	0.000092
45	C19 - H31	0.281403	-0.979501	0.00921	0.29111	0.000328
46	C17 - H34	0.284273	-1.002433	0.010229	0.296839	0.000393
47	C17 - H32	0.283827	-1.008575	0.009114	0.296448	0.000386
48	C17 - H33	0.274543	-0.936739	0.012071	0.279302	0.000076
49	C35 - C49	0.239348	-0.532484	0.007531	0.187183	0.000174
50	C35 - C53	0.2424	-0.545759	0.001146	0.191388	0.000296
51	C36 - C41	0.241416	-0.541964	0.003393	0.189918	0.000325
52	H21 - H38	0.012364	0.049773	0.534996	-0.002522	0.503642
53	C36 - C37	0.238543	-0.528716	0.007161	0.186178	0.000183
54	C37 - H38	0.281415	-0.976326	0.006719	0.291192	0.000264
55	C37 - H39	0.276888	-0.945335	0.006826	0.282512	0.000222
56	C37 - H40	0.276326	-0.939654	0.006173	0.281437	0.000352
57	C41 - H42	0.279103	-0.95624	0.006308	0.286586	0.000228
58	C41 - H44	0.277936	-0.952465	0.005446	0.284332	0.000162

24	F15 - B16	0.158402	0.862524	0.036467	0.085358	0.000003
25	C2 - F15	0.009483	0.045768	2.315415	-0.00206	0.199363
26	F15 - H23	0.012842	0.055524	0.293242	-0.001719	0.06027
27	F1 - B16	0.158798	0.864672	0.034711	0.085616	0.000002
28	H31 - H34	0.013515	0.059634	1.560114	-0.003301	0.936366
29	C8 - C17	0.254987	-0.608675	0.020243	0.212547	0.000136
30	C17 - H33	0.274027	-0.934039	0.011626	0.278228	0.000072
31	C10 - C18	0.255612	-0.608735	0.028332	0.212049	0.000106
32	C18 - H27	0.282611	-0.987967	0.00819	0.293792	0.00025
33	H27 - H51	0.013169	0.052627	0.309989	-0.002562	0.256747
34	C18 - H32	0.013478	0.057572	1.696624	-0.002834	0.146224
35	H29 - H42	0.014302	0.055381	0.529361	-0.002449	0.198606
36	C5 - C19	0.255446	-0.608073	0.026854	0.21209	0.000192
37	C19 - H29	0.284462	-1.005385	0.008496	0.297443	0.000274
38	C19 - H31	0.283312	-0.994668	0.009014	0.294774	0.000335
39	C2 - H20	0.275682	-0.944969	0.011148	0.281309	0.000138
40	C2 - H22	0.280747	-0.988197	0.008562	0.290755	0.000194
41	H21 - H48	0.012655	0.043548	0.081312	-0.001548	0.042221
42	C14 - H23	0.285999	-1.029224	0.006856	0.300558	0.00032
43	C14 - H25	0.278266	-0.95967	0.010959	0.285923	0.000197
44	C18 - H26	0.273831	-0.925891	0.01088	0.277413	0.000087
45	C18 - H28	0.281056	-0.980163	0.007813	0.290588	0.000264
46	H27 - H58	0.011953	0.042081	0.084468	-0.001628	0.046578
47	C19 - H30	0.272622	-0.913833	0.012738	0.275195	0.000099
48	C17 - H34	0.284705	-1.008925	0.009242	0.297864	0.000384
49	C17 - H32	0.284787	-1.008702	0.009539	0.297974	0.000388
50	C35 - C53	0.241954	-0.54368	0.001221	0.190807	0.0003
51	C36 - C45	0.240172	-0.535893	0.007274	0.18843	0.000119
52	C36 - C41	0.242103	-0.544913	0.0024	0.19091	0.000295
53	H21 - H38	0.011318	0.045924	0.597848	-0.002419	0.863882
54	C36 - C37	0.2385	-0.528483	0.008042	0.186132	0.000147
55	C37 - H38	0.28075	-0.971733	0.006226	0.289884	0.000258
56	C37 - H39	0.276541	-0.940864	0.0068	0.281761	0.000237
57	C37 - H40	0.27629	-0.939902	0.005761	0.281386	0.00034
58	C41 - H42	0.279445	-0.960115	0.005416	0.287126	0.000192

59	C41 - H43	0.277416	-0.947234	0.004697	0.283432	0.000364
60	C36 - C45	0.240132	-0.535808	0.00727	0.188371	0.000075
61	C45 - H46	0.276033	-0.939006	0.00478	0.280853	0.000252
62	C45 - H47	0.276626	-0.942937	0.005085	0.282012	0.000229
63	C45 - H48	0.278569	-0.955186	0.0054	0.285726	0.000221
64	C49 - H50	0.276229	-0.939359	0.005865	0.28129	0.000295
65	C49 - H51	0.28087	-0.972466	0.006276	0.29016	0.000239
66	C49 - H52	0.276672	-0.941227	0.006302	0.282046	0.000233
67	C53 - H54	0.277857	-0.948545	0.005455	0.284212	0.000182
68	C53 - H55	0.279392	-0.961526	0.005034	0.287025	0.000186
69	C53 - H56	0.277238	-0.946091	0.003409	0.283133	0.000346
70	C35 - C57	0.238885	-0.530372	0.008744	0.186708	0.000119
71	C57 - H58	0.279447	-0.961473	0.006468	0.287387	0.000236
72	C57 - H59	0.276042	-0.938762	0.005535	0.28092	0.000284
73	C57 - H60	0.27662	-0.942634	0.00598	0.281997	0.00023
74	H32 - N61	0.007768	0.024733	0.357182	-0.000948	0.045929
75	H26 - C62	0.003553	0.012513	0.845676	-0.000723	0.117211
76	C8 - C65	0.006528	0.018837	1.036884	-0.000876	0.627898
77	C10 - C81	0.005855	0.015731	0.941454	-0.000652	0.377166
78	N61 - C62	0.343488	-1.029682	0.125107	0.562145	0.002424
79	N13 - C63	0.007615	0.022731	0.254922	-0.000713	0.013916
80	F15 - H66	0.009387	0.042432	0.356915	-0.001783	0.106455
81	C63 - C64	0.314263	-0.866705	0.194257	0.31624	0.000036
82	N61 - C65	0.342047	-1.029389	0.12449	0.557888	0.00239
83	C64 - C65	0.316516	-0.87562	0.226852	0.319847	0.000109
84	C63 - C81	0.31502	-0.869318	0.198609	0.317785	0.000063
85	C63 - H66	0.289565	-1.075023	0.006711	0.307129	0.000051
86	H33 - N67	0.004813	0.016075	0.643121	-0.000779	0.063319
87	H28 - N67	0.004501	0.014647	0.43269	-0.000684	0.033141
88	C9 - C68	0.007664	0.022604	1.935927	-0.001026	0.236542
89	C57 - H80	0.002998	0.009785	1.109758	-0.000591	0.453942
90	N67 - C68	0.342555	-1.020797	0.121035	0.560434	0.002438
91	F1 - C69	0.005935	0.028631	4.849692	-0.001638	0.34229
92	F1 - H73	0.006551	0.032051	1.17263	-0.001814	0.378438
93	C68 - C69	0.315861	-0.873403	0.220778	0.318404	0.000118

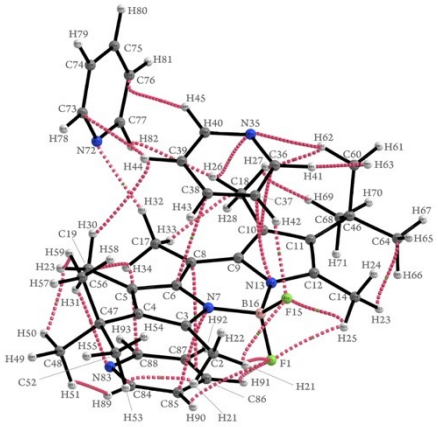
59	C41 - H43	0.2772	-0.945495	0.003988	0.283052	0.000353
60	C41 - H44	0.277908	-0.950865	0.004966	0.284269	0.000164
61	C45 - H46	0.275951	-0.937266	0.005285	0.280807	0.000279
62	C45 - H47	0.279473	-0.962987	0.004754	0.287267	0.000183
63	C45 - H48	0.278513	-0.953001	0.006491	0.285767	0.000228
64	C35 - C49	0.239894	-0.534703	0.007937	0.188019	0.000214
65	C49 - H50	0.275547	-0.930927	0.008353	0.280172	0.00037
66	C49 - H51	0.280692	-0.968248	0.008746	0.289994	0.000291
67	H54 - C68	0.006283	0.017468	0.838917	-0.000858	0.610812
68	C49 - H52	0.282002	-0.986545	0.006816	0.29209	0.000192
69	C53 - H54	0.279641	-0.964734	0.005181	0.287362	0.000143
70	C53 - H55	0.279421	-0.958999	0.005283	0.287237	0.000212
71	C53 - H56	0.276854	-0.941678	0.004487	0.28253	0.000365
72	C35 - C57	0.240076	-0.535458	0.008215	0.188404	0.000083
73	C57 - H58	0.279098	-0.957577	0.004784	0.286708	0.000183
74	C57 - H59	0.276061	-0.9383	0.00387	0.28102	0.000277
75	C57 - H60	0.277163	-0.944074	0.004534	0.282977	0.000195
76	H26 - N61	0.000744	0.003397	0.434806	-0.000249	0.088858
77	C9 - C65	0.004452	0.013078	2.995101	-0.000612	0.04964
78	H52 - C67	0.009	0.027823	1.50958	-0.001246	0.526439
79	N61 - C62	0.342056	-1.092131	0.114091	0.546007	0.002352
80	N13 - C64	0.005276	0.016447	0.419789	-0.000591	0.030862
81	C62 - C63	0.290458	-0.749721	0.14325	0.268202	0.000143
82	H25 - H83	0.003688	0.012561	0.352997	-0.000826	0.159539
83	F15 - H69	0.012686	0.047662	0.053647	-0.000782	0.016217
84	C63 - C64	0.313653	-0.861764	0.180499	0.31341	0.000042
85	C6 - C70	0.007935	0.023862	1.611981	-0.00104	0.253242
86	C64 - C65	0.313095	-0.859382	0.178804	0.312327	0.000016
87	N61 - C66	0.341154	-1.089148	0.11174	0.543637	0.00236
88	C65 - C66	0.290317	-0.749378	0.141985	0.267952	0.00015
89	C62 - C67	0.298677	-0.803161	0.165058	0.283507	0.000071
90	C63 - C68	0.295681	-0.778293	0.142566	0.278829	0.000083
91	F15 - H77	0.005702	0.026595	0.107696	-0.001472	0.04132
92	C64 - H69	0.289011	-1.075537	0.008234	0.306752	0.000046
93	N7 - H77	0.007183	0.024871	3.164298	-0.001082	0.602109

94	C6 - C71	0.006786	0.019463	1.231208	-0.000842	0.148456
95	C69 - C70	0.315079	-0.870334	0.197482	0.317929	0.000031
96	C70 - C71	0.314086	-0.864783	0.196939	0.315864	0.00007
97	H31 - C72	0.004133	0.013206	0.941904	-0.00075	0.056233
98	N67 - C72	0.342377	-1.036835	0.126618	0.558005	0.002388
99	C71 - C72	0.315582	-0.870049	0.228488	0.318034	0.000111
100	C70 - H73	0.288547	-1.064487	0.007143	0.304891	0.000036
101	C62 - H74	0.28796	-1.055617	0.032358	0.302332	0.000018
102	C62 - C81	0.315464	-0.871188	0.223109	0.317645	0.000112
103	C65 - H75	0.287933	-1.05471	0.032797	0.302243	0.00002
104	C64 - H76	0.286221	-1.039542	0.015076	0.300647	0.000019
105	C72 - H77	0.287398	-1.050148	0.033906	0.301291	0.000019
106	C71 - H78	0.28515	-1.027827	0.015622	0.298498	0.000009
107	C69 - H79	0.287351	-1.049654	0.014366	0.302857	0.000033
108	C68 - H80	0.289316	-1.067217	0.031319	0.30488	0.000023
109	H52 - H82	0.004179	0.014451	0.198821	-0.000946	0.068501
110	C81 - H82	0.28536	-1.028625	0.015232	0.298889	0.000007

94	H39 - H82	0.00508	0.017475	0.073026	-0.001056	0.015871
95	C65 - C70	0.296245	-0.780909	0.142402	0.280027	0.000078
96	C66 - C71	0.29925	-0.805806	0.167636	0.284677	0.000068
97	C67 - C72	0.326824	-0.918709	0.266591	0.342853	0.000014
98	C68 - C73	0.326953	-0.918991	0.269385	0.343093	0.000005
99	C72 - C73	0.295795	-0.780559	0.154625	0.280181	0.000019
100	H34 - C74	0.004704	0.014361	0.436282	-0.00078	0.109616
101	C71 - C74	0.326319	-0.916557	0.264958	0.341803	0.00001
102	C70 - C75	0.327569	-0.92285	0.265455	0.344266	0.000017
103	C74 - C75	0.296359	-0.783303	0.155501	0.281309	0.000024
104	C67 - H76	0.285855	-1.038205	0.017226	0.300173	0.000048
105	C70 - H77	0.287368	-1.048468	0.016425	0.302733	0.000064
106	C71 - H78	0.285511	-1.034297	0.018361	0.299533	0.000047
107	C72 - H79	0.285341	-1.029308	0.015025	0.298642	0.000031
108	C73 - H80	0.285114	-1.026369	0.017826	0.298355	0.000028
109	C74 - H81	0.2847	-1.022783	0.014968	0.297354	0.000028
110	C75 - H82	0.286488	-1.035244	0.017494	0.300833	0.000047
111	C68 - H83	0.284241	-1.019078	0.018025	0.296585	0.000059
112	H33 - N84	0.004889	0.015682	0.181987	-0.000706	0.024662
113	H31 - C94	0.006021	0.019476	1.841593	-0.001058	0.396218
114	H28 - C90	0.005481	0.016651	0.589159	-0.000885	0.121741
115	N84 - C85	0.341205	-1.084438	0.111237	0.544787	0.002358
116	C85 - C86	0.290419	-0.749927	0.142037	0.268177	0.000161
117	F1 - H92	0.005319	0.025275	0.128265	-0.001478	0.078714
118	C6 - C87	0.007024	0.021429	0.789673	-0.00094	0.025793
119	C86 - C87	0.314007	-0.863346	0.184305	0.314211	0.000038
120	C94 - C97	0.326846	-0.919108	0.266719	0.342916	0.000011
121	C87 - C88	0.312943	-0.858085	0.181576	0.312011	0.000049
122	N84 - C89	0.341298	-1.09069	0.113306	0.543773	0.002336
123	C88 - C89	0.290622	-0.750235	0.14465	0.268556	0.000144
124	C85 - C90	0.299374	-0.806726	0.167276	0.284971	0.000087
125	F1 - H106	0.010856	0.044835	0.118697	-0.001344	0.037653
126	N13 - C91	0.006905	0.020559	0.286618	-0.000622	0.008071
127	C11 - C96	0.005452	0.015047	2.635596	-0.000618	0.163298
128	H60 - H103	0.006481	0.02337	0.258808	-0.001407	0.083313

129	C86 - C91	0.295918	-0.780346	0.138985	0.279498	0.000061
130	C87 - H92	0.286915	-1.050742	0.008556	0.301738	0.000029
131	H47 - C98	0.006564	0.022413	18.343615	-0.001203	0.368171
132	C88 - C93	0.296742	-0.783772	0.143264	0.280827	0.000072
133	C89 - C94	0.299085	-0.804824	0.167393	0.284372	0.000066
134	H58 - H102	0.005659	0.020583	0.202212	-0.00132	0.194627
135	C90 - C95	0.327312	-0.921972	0.266451	0.343931	0.000012
136	C91 - C96	0.328583	-0.928663	0.266696	0.346426	0.000025
137	C95 - C96	0.296452	-0.785119	0.151608	0.281417	0.000026
138	H29 - C97	0.004931	0.015747	1.939951	-0.000829	0.09918
139	C93 - C98	0.326763	-0.917855	0.268365	0.34272	0.000004
140	C97 - C98	0.296011	-0.781385	0.156153	0.280654	0.000023
141	C90 - H99	0.285245	-1.030865	0.019622	0.299015	0.000051
142	C93 - H100	0.285417	-1.029034	0.016457	0.298863	0.000056
143	C94 - H101	0.285574	-1.034994	0.018275	0.299647	0.000049
144	C95 - H102	0.285906	-1.032392	0.013614	0.299631	0.000028
145	C96 - H103	0.285892	-1.029722	0.01754	0.299773	0.000041
146	C97 - H104	0.285123	-1.02723	0.015126	0.298237	0.000031
147	C98 - H105	0.284782	-1.021876	0.019076	0.297717	0.000028
148	C91 - H106	0.288483	-1.061782	0.015487	0.305349	0.000098

Table S2. Summary of topological descriptors at the bond critical points of $\mathbf{1}_{t\mathbf{Bu}}\cdot(\text{pyridine})_3$ complex based on the QTAIM analyses of the optimised geometries at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.



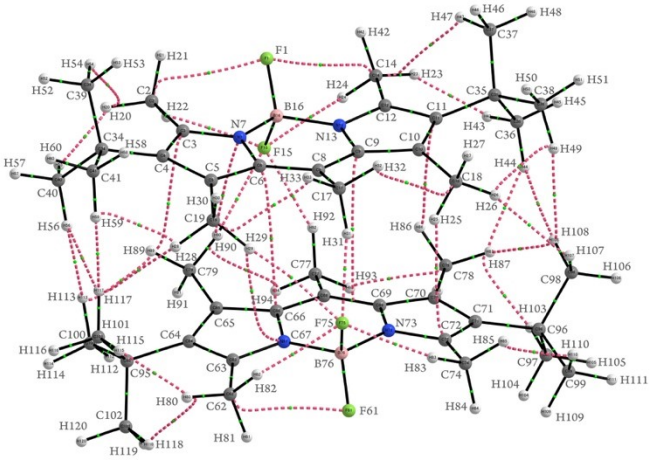
$\mathbf{1}_{t\mathbf{Bu}}\cdot(\text{pyridine})_3$ complex

BCP #	Atoms	Electro density (ρ_{BCP}) in e au^{-3}	Laplacian ($\nabla^2\rho_{BCP}$) in e au^{-5}	Ellipticity ($\varepsilon = \lambda_1/\lambda_2 - 1$)	Kinetic energy density ($K_{BCP} = -H_{BCP}$) in Hartree	BPL – GBL_I	BCP #	Atoms	Electro density (ρ_{BCP}) in e au^{-3}	Laplacian ($\nabla^2\rho_{BCP}$) in e au^{-5}	Ellipticity ($\varepsilon = \lambda_1/\lambda_2 - 1$)	Kinetic energy density ($K_{BCP} = -H_{BCP}$) in Hartree	BPL – GBL_I
1	F1 - H21	0.012365	0.051655	0.408852	-0.001491	0.044694	66	C39 - H44	0.285723	-1.03026	0.016568	0.29962	0.000004
2	N7 - B16	0.155663	0.279276	0.007649	0.128264	0.00001	67	C40 - H45	0.289735	-1.070032	0.032669	0.305875	0.000017
3	C6 - N7	0.304083	-0.874964	0.163887	0.456532	0.000199	68	C11 - C46	0.243658	-0.550023	0.038628	0.192925	0.000173
4	C2 - H20	0.281396	-0.982193	0.011392	0.291813	0.000262	69	C46 - C68	0.239335	-0.53246	0.007416	0.187127	0.000188
5	C2 - C3	0.257979	-0.626534	0.04138	0.217635	0.000035	70	C46 - C64	0.242414	-0.545828	0.001185	0.1914	0.000279
6	C3 - C4	0.296037	-0.747811	0.246781	0.282865	0.001085	71	C64 - H67	0.277053	-0.944533	0.003281	0.28281	0.000337
7	C6 - C38	0.007514	0.023431	0.411031	-0.001088	0.024281	72	H23 - C64	0.011509	0.050322	8.606085	-0.002899	0.134824
8	C4 - C5	0.301383	-0.760108	0.254178	0.291913	0.000947	73	C47 - C52	0.242355	-0.545557	0.001414	0.19131	0.000308
9	C3 - N7	0.326707	-0.842033	0.16157	0.529657	0.000109	74	C4 - C47	0.243403	-0.548757	0.039106	0.192491	0.000179
10	C6 - C8	0.30791	-0.833831	0.213169	0.30198	0.000143	75	C47 - C48	0.239539	-0.53336	0.007723	0.18747	0.00016
11	C5 - C6	0.296934	-0.762801	0.216141	0.282157	0.001064	76	C48 - H49	0.27597	-0.937466	0.006047	0.280839	0.000291
12	C8 - C9	0.308344	-0.83565	0.215632	0.302873	0.000119	77	C48 - H50	0.280903	-0.973707	0.006378	0.290143	0.000239
13	C9 - N13	0.303444	-0.879508	0.160766	0.453516	0.00028	78	C48 - H51	0.276487	-0.9402	0.006518	0.281713	0.000238
14	C9 - C10	0.296497	-0.760671	0.216963	0.281484	0.001052	79	C52 - H53	0.27827	-0.951556	0.005498	0.284971	0.000188
15	C10 - C11	0.303212	-0.769676	0.256839	0.295367	0.000957	80	C52 - H55	0.27714	-0.945202	0.003447	0.28295	0.000345
16	N13 - B16	0.155722	0.280824	0.005096	0.128211	0.000109	81	C52 - H54	0.278986	-0.958775	0.005005	0.286249	0.00018
17	C11 - C12	0.295764	-0.747242	0.243524	0.282393	0.001095	82	C47 - C56	0.238595	-0.529055	0.008968	0.18629	0.00014
18	F1 - H25	0.012537	0.051473	0.370936	-0.001392	0.038434	83	H29 - H59	0.01364	0.048342	0.044942	-0.001741	0.05909
19	F1 - B16	0.159603	0.871998	0.028102	0.085905	0.000001	84	C56 - H57	0.276049	-0.938257	0.005444	0.280866	0.000292
20	C12 - N13	0.327008	-0.834361	0.162004	0.530899	0.000129	85	C56 - H58	0.276633	-0.942842	0.005843	0.282038	0.000233
21	C12 - C14	0.258392	-0.628478	0.041436	0.21826	0.000031	86	C56 - H59	0.279764	-0.963571	0.006352	0.28806	0.000234
22	C14 - H23	0.281098	-0.980884	0.010999	0.291276	0.000251	87	C46 - C60	0.238528	-0.528818	0.009296	0.186243	0.000096
23	F15 - B16	0.161978	0.895389	0.032568	0.087092	0.000002	88	H27 - H62	0.012097	0.043682	0.072611	-0.001772	0.058778
24	F15 - H21	0.011812	0.054899	0.176086	-0.002243	0.177723	89	C60 - H61	0.275537	-0.934139	0.00611	0.280074	0.000292

25	F15 - H25	0.01107	0.052712	0.317383	-0.002339	0.234968
26	C14 - H25	0.284779	-1.019617	0.007117	0.298198	0.00031
27	C19 - H34	0.011787	0.050941	3.295435	-0.002809	0.172057
28	C8 - C17	0.256596	-0.616104	0.025284	0.215534	0.000202
29	C18 - H33	0.012422	0.052927	1.759006	-0.002719	0.149345
30	C10 - C18	0.254722	-0.604373	0.027319	0.21067	0.000175
31	H27 - H69	0.012904	0.051597	0.324083	-0.002549	0.281226
32	C5 - C19	0.255137	-0.605536	0.033183	0.211568	0.000017
33	H29 - H50	0.012669	0.049026	0.132196	-0.002293	0.141961
34	H20 - H53	0.012477	0.050396	0.890703	-0.002629	0.341183
35	C2 - H21	0.284932	-1.020849	0.007385	0.298562	0.000321
36	C2 - H22	0.274436	-0.932426	0.012658	0.278967	0.000148
37	C14 - H24	0.27424	-0.93091	0.0124	0.278576	0.000148
38	C18 - H27	0.283031	-0.992896	0.008116	0.294594	0.00026
39	C18 - H26	0.28111	-0.980805	0.007835	0.290544	0.000281
40	C68 - H69	0.281081	-0.973276	0.006285	0.290603	0.000239
41	C18 - H28	0.272963	-0.91614	0.011906	0.27584	0.000099
42	C19 - H29	0.283003	-0.988991	0.010377	0.294634	0.000259
43	C19 - H30	0.27904	-0.966682	0.010603	0.286859	0.000237
44	C19 - H31	0.274569	-0.935849	0.010855	0.278906	0.00011
45	C17 - H32	0.277011	-0.964936	0.011488	0.284606	0.000112
46	H26 - H82	0.003602	0.012217	0.380221	-0.0008	0.327662
47	C17 - H33	0.28321	-0.992044	0.011652	0.294814	0.000358
48	C17 - H34	0.283076	-0.996925	0.012071	0.294988	0.000321
49	N35 - H62	0.003582	0.012116	0.198338	-0.000616	0.037036
50	C10 - C36	0.005789	0.017314	2.060164	-0.000764	0.114481
51	H26 - N35	0.005159	0.017309	1.68704	-0.000833	0.105694
52	H41 - H63	0.005365	0.018684	0.257594	-0.001139	0.092105
53	N13 - C37	0.00653	0.01964	2.841017	-0.000662	0.095482
54	N35 - C36	0.343034	-1.02427	0.118166	0.561553	0.002426
55	F15 - H42	0.013362	0.04972	0.085752	-0.000754	0.019092
56	C36 - C37	0.315657	-0.872359	0.21767	0.318071	0.000122
57	H30 - H44	0.001938	0.006606	0.269466	-0.000419	0.276848
58	C37 - C38	0.314541	-0.867013	0.195946	0.317085	0.000037
59	C38 - C39	0.3142	-0.864924	0.198901	0.316138	0.00008
90	C60 - H62	0.280284	-0.972053	0.007294	0.288665	0.000255
91	C60 - H63	0.276482	-0.939323	0.006822	0.281742	0.000251
92	C64 - H65	0.279739	-0.963554	0.004867	0.287658	0.000198
93	C64 - H66	0.277309	-0.945403	0.005414	0.283155	0.000164
94	C68 - H70	0.276259	-0.938678	0.005975	0.281306	0.000321
95	C68 - H71	0.276683	-0.943136	0.006493	0.282141	0.000221
96	H32 - N72	0.013278	0.037562	0.075977	-0.000602	0.020999
97	C74 - C75	0.313792	-0.863335	0.197226	0.315322	0.000055
98	N72 - C73	0.343335	-1.021477	0.120274	0.562932	0.002378
99	H44 - C73	0.005532	0.0191	0.485423	-0.001121	0.043431
100	C73 - C74	0.31557	-0.87164	0.222389	0.317788	0.000111
101	C76 - C77	0.315678	-0.8726	0.221502	0.318043	0.000116
102	C75 - C76	0.313939	-0.864083	0.19754	0.31562	0.000057
103	N72 - C77	0.343086	-1.018905	0.118332	0.56243	0.002413
104	C73 - H78	0.288761	-1.065627	0.032018	0.304092	0.000018
105	C74 - H79	0.285785	-1.037819	0.014845	0.299934	0.000001
106	C75 - H80	0.286836	-1.050309	0.007346	0.301539	0
107	C76 - H81	0.285893	-1.03893	0.01475	0.300147	0.000002
108	C77 - H82	0.289081	-1.068117	0.031558	0.304675	0.000017
109	N83 - C88	0.343113	-1.035696	0.126491	0.56032	0.00241
110	H34 - C88	0.006965	0.023751	0.567604	-0.001294	0.06101
111	H31 - N83	0.005652	0.017595	0.088941	-0.000737	0.033727
112	H51 - H89	0.004469	0.014991	0.137527	-0.000942	0.054239
113	C84 - H89	0.289297	-1.066747	0.031193	0.304871	0.000025
114	N83 - C84	0.34209	-1.026048	0.118418	0.558696	0.002424
115	N7 - C85	0.007542	0.023464	1.756833	-0.000762	0.034715
116	F1 - H91	0.008733	0.040589	0.478165	-0.001884	0.144228
117	F1 - H90	0.006505	0.032227	2.551382	-0.001816	0.629287
118	C84 - C85	0.316211	-0.875102	0.221813	0.31917	0.000117
119	C85 - C86	0.315002	-0.870326	0.195517	0.317742	0.000024
120	C86 - C87	0.31423	-0.865246	0.197396	0.316162	0.00007
121	C8 - C87	0.005137	0.014692	2.02897	-0.000664	1.160864
122	C87 - C88	0.315245	-0.868436	0.227589	0.317336	0.00011
123	C88 - H93	0.287687	-1.052965	0.032876	0.30181	0.000017
124	C85 - H90	0.287567	-1.051373	0.014531	0.3033	0.000034

60	H45 - C76	0.005692	0.018882	6.002452	-0.000929	0.46253	125	C86 - H91	0.289127	-1.071579	0.007163	0.306251	0.000045
61	N35 - C40	0.342445	-1.036489	0.121812	0.558288	0.002395	126	C87 - H92	0.2847	-1.024293	0.016222	0.297731	0.000006
62	C39 - C40	0.315143	-0.867833	0.225578	0.317096	0.000128							
63	C36 - H41	0.289498	-1.067577	0.031084	0.305251	0.000025							
64	C37 - H42	0.289468	-1.074484	0.014332	0.307863	0.000055							
65	C38 - H43	0.286843	-1.047093	0.007402	0.301253	0.000012							

Table S3. Summary of topological descriptors at the bond critical points of $(\mathbf{1}_{t\mathbf{Bu}})_2$ based on the QTAIM analysis of the optimised geometries at the B3LYP-D3(BJ)/6-31G(d,p) level of theory.



BCP #	Atoms	Electro density (ρ_{BCP}) in e au^{-3}	Laplacian ($\nabla^2\rho_{BCP}$) in e au^{-5}	Ellipticity ($\varepsilon = \lambda_1/\lambda_2 - 1$)	Kinetic energy density ($K_{BCP} = -H_{BCP}$) in Hartree	BPL – GBL_I	BCP #	Atoms	Electro density (ρ_{BCP}) in e au^{-3}	Laplacian ($\nabla^2\rho_{BCP}$) in e au^{-5}	Ellipticity ($\varepsilon = \lambda_1/\lambda_2 - 1$)	Kinetic energy density ($K_{BCP} = -H_{BCP}$) in Hartree	BPL – GBL_I
1	F1 - C2	0.010026	0.047702	1.710864	-0.002107	0.395258	134	C100 - H113	0.280203	-0.964951	0.005602	0.288654	0.000196
2	N7 - B16	0.157362	0.292206	0.002625	0.129524	0.000016	135	C79 - H89	0.281065	-0.977132	0.010774	0.290881	0.000313
3	C2 - C3	0.259536	-0.633299	0.049156	0.220009	0.000045	136	C79 - H90	0.284776	-1.013882	0.009715	0.297572	0.000374
4	C3 - C4	0.296806	-0.756415	0.236447	0.28452	0.000959	137	C79 - H91	0.273332	-0.91981	0.014483	0.276623	0.000114
5	H20 - H54	0.011059	0.044803	0.521918	-0.002407	0.545692	138	C77 - H93	0.283176	-0.993403	0.013389	0.295206	0.000399
6	C6 - C66	0.004063	0.01101	2.003623	-0.000493	0.029617	139	C77 - H92	0.277865	-0.974441	0.011982	0.28643	0.000121
7	C4 - C5	0.301545	-0.7586	0.260796	0.292382	0.001183	140	C77 - H94	0.282838	-0.991845	0.013533	0.294266	0.000378
8	C3 - N7	0.329838	-0.819543	0.153478	0.539187	0.000135	141	C95 - C102	0.238585	-0.528869	0.007089	0.186299	0.00016
9	C5 - C6	0.293972	-0.748905	0.21492	0.276546	0.000827	142	C64 - C95	0.243382	-0.54875	0.037868	0.192593	0.000326
10	C6 - N7	0.302188	-0.873661	0.16222	0.450565	0.00019	143	C100 - H114	0.277106	-0.94445	0.004473	0.282873	0.000358
11	C6 - C8	0.305781	-0.819108	0.22077	0.298169	0.000166	144	C98 - H107	0.276849	-0.942757	0.004547	0.282346	0.000188
12	N13 - B16	0.156548	0.289541	0.002496	0.128703	0.000018	145	C96 - C99	0.241367	-0.541308	0.002823	0.189923	0.000282
13	C8 - C9	0.304978	-0.815367	0.218723	0.296556	0.000138	146	C71 - C96	0.24239	-0.544347	0.036902	0.191045	0.000226

14	C9 - C10	0.29425	-0.749714	0.216511	0.277097	0.000846
15	C9 - C69	0.003706	0.010345	3.57772	-0.000484	1.107329
16	C10 - C11	0.301713	-0.759612	0.260656	0.292651	0.001144
17	F1 - C14	0.009663	0.046702	2.158521	-0.002063	0.125921
18	C9 - N13	0.3023	-0.872023	0.163182	0.451125	0.000176
19	C11 - C12	0.297033	-0.757124	0.237652	0.284938	0.000977
20	C12 - N13	0.328883	-0.825851	0.154484	0.536336	0.000124
21	C12 - C14	0.259394	-0.632558	0.048376	0.219758	0.000045
22	C14 - H47	0.011375	0.046238	0.625244	-0.002423	0.598983
23	F15 - B16	0.15513	0.835944	0.029985	0.083468	0.000002
24	F1 - B16	0.166862	0.943154	0.037969	0.089218	0.000006
25	C8 - C17	0.253709	-0.602535	0.025121	0.211108	0.000345
26	C10 - C18	0.254347	-0.60331	0.026428	0.210489	0.000326
27	C38 - H50	0.278002	-0.952684	0.005406	0.284507	0.000164
28	C18 - H32	0.012627	0.055732	2.155495	-0.003083	0.52416
29	C41 - H58	0.278194	-0.954057	0.0052	0.284872	0.000169
30	C5 - C19	0.253289	-0.598453	0.026336	0.208854	0.000389
31	C19 - H33	0.012438	0.055007	1.913896	-0.003104	0.625042
32	C2 - H20	0.282812	-0.991879	0.011062	0.294289	0.000221
33	C2 - H21	0.276444	-0.952962	0.010409	0.282822	0.000126
34	C2 - H22	0.27954	-0.977535	0.00883	0.288359	0.000193
35	N7 - H90	0.005547	0.018888	0.468316	-0.000802	0.043175
36	F15 - H22	0.010022	0.043394	0.391984	-0.0016	0.059406
37	C14 - H23	0.281946	-0.985673	0.011034	0.2926	0.000221
38	C14 - H42	0.276083	-0.949873	0.010351	0.282107	0.000122
39	C14 - H24	0.28035	-0.983971	0.008512	0.289832	0.000201
40	F15 - H24	0.010627	0.045037	0.343136	-0.001517	0.048232
41	C18 - H25	0.28249	-0.990192	0.008955	0.29302	0.000322
42	C35 - C38	0.241858	-0.543778	0.003158	0.190553	0.000291
43	C18 - H26	0.284614	-1.004314	0.008555	0.297653	0.000261
44	C18 - H27	0.273081	-0.918081	0.012997	0.276074	0.000107
45	C34 - C41	0.242039	-0.544484	0.002859	0.190779	0.000275
147	C99 - H110	0.280048	-0.964275	0.005934	0.288401	0.000227
148	C97 - H103	0.281146	-0.973518	0.006778	0.290685	0.000259
149	H26 - H107	0.007145	0.025714	0.349861	-0.001459	0.149986
150	C96 - C98	0.240668	-0.53818	0.007542	0.189227	0.000058
151	C99 - H111	0.277229	-0.945643	0.004882	0.283121	0.00037
152	H89 - H113	0.012881	0.050543	0.509734	-0.002471	0.181145
153	H59 - H117	0.007845	0.027108	0.078319	-0.001349	0.012453
154	H80 - H115	0.012641	0.043554	0.083716	-0.001549	0.042262
155	C95 - C101	0.24083	-0.539005	0.007544	0.189402	0.000082
156	C102 - H120	0.2761	-0.938115	0.005982	0.281014	0.000338
157	C97 - H104	0.277252	-0.948812	0.0068	0.283188	0.000215
158	C97 - H105	0.276417	-0.939766	0.006418	0.281586	0.000355
159	C98 - H106	0.276122	-0.939898	0.004071	0.281091	0.000248
160	C98 - H108	0.278432	-0.951268	0.005011	0.28538	0.00018
161	C100 - H112	0.278179	-0.953981	0.005207	0.284879	0.000167
162	C101 - H115	0.278553	-0.953501	0.005741	0.285805	0.000227
163	C101 - H116	0.275995	-0.938229	0.004969	0.280845	0.000256
164	C101 - H117	0.279129	-0.956689	0.005138	0.286711	0.000176
165	C102 - H118	0.280536	-0.969888	0.006486	0.289468	0.000266
166	C102 - H119	0.27726	-0.948856	0.00639	0.283172	0.000224
134	C100 - H113	0.280203	-0.964951	0.005602	0.288654	0.000196
135	C79 - H89	0.281065	-0.977132	0.010774	0.290881	0.000313
136	C79 - H90	0.284776	-1.013882	0.009715	0.297572	0.000374
137	C79 - H91	0.273332	-0.91981	0.014483	0.276623	0.000114
138	C77 - H93	0.283176	-0.993403	0.013389	0.295206	0.000399
139	C77 - H92	0.277865	-0.974441	0.011982	0.28643	0.000121
140	C77 - H94	0.282838	-0.991845	0.013533	0.294266	0.000378
141	C95 - C102	0.238585	-0.528869	0.007089	0.186299	0.00016
142	C64 - C95	0.243382	-0.54875	0.037868	0.192593	0.000326
143	C100 - H114	0.277106	-0.94445	0.004473	0.282873	0.000358
144	C98 - H107	0.276849	-0.942757	0.004547	0.282346	0.000188
145	C96 - C99	0.241367	-0.541308	0.002823	0.189923	0.000282

46	C19 - H28	0.282246	-0.986527	0.009632	0.293122	0.000284
47	C19 - H29	0.282782	-0.994859	0.009397	0.293454	0.000338
48	C19 - H30	0.273377	-0.92063	0.013585	0.276617	0.000103
49	C17 - H31	0.278542	-0.982286	0.011908	0.287949	0.000106
50	C17 - H32	0.282296	-0.987036	0.014112	0.29336	0.000402
51	C17 - H33	0.282506	-0.98867	0.01424	0.293642	0.000396
52	C34 - C39	0.238316	-0.527649	0.007484	0.18595	0.000151
53	C4 - C34	0.242777	-0.54591	0.038713	0.191738	0.000398
54	C41 - H60	0.277137	-0.944919	0.004455	0.282954	0.000351
55	C11 - C35	0.242262	-0.543746	0.038184	0.191004	0.000382
56	C35 - C37	0.238341	-0.527784	0.007831	0.185958	0.000167
57	C37 - H47	0.280806	-0.971793	0.006607	0.289974	0.000264
58	C38 - H51	0.277118	-0.944508	0.004693	0.28291	0.00036
59	C35 - C36	0.240669	-0.538143	0.007163	0.189071	0.000081
60	H23 - H43	0.011742	0.040787	0.087477	-0.001579	0.042353
61	C37 - H48	0.27623	-0.938831	0.006098	0.281239	0.000361
62	H26 - H49	0.013763	0.053486	0.492152	-0.002425	0.172729
63	C39 - H52	0.27612	-0.93824	0.005963	0.281025	0.000345
64	H20 - H55	0.012986	0.044375	0.081236	-0.001506	0.040478
65	C34 - C40	0.240403	-0.536992	0.007385	0.188688	0.000082
66	H28 - H59	0.012666	0.049821	0.540963	-0.002446	0.185598
67	C11 - H86	0.004881	0.014531	0.651585	-0.000746	0.037593
68	C36 - H43	0.278457	-0.953739	0.005673	0.285614	0.000213
69	H49 - H108	0.005744	0.020136	0.471807	-0.001197	0.112763
70	C36 - H44	0.278179	-0.950915	0.005067	0.284903	0.000208
71	C36 - H45	0.276139	-0.93928	0.004666	0.281106	0.000262
72	C37 - H46	0.27726	-0.948869	0.006767	0.283169	0.000222
73	C38 - H49	0.280239	-0.964866	0.005854	0.288642	0.000212
74	C39 - H53	0.277304	-0.949223	0.006477	0.283247	0.000225
75	C39 - H54	0.280411	-0.969082	0.006495	0.289207	0.000266
76	C40 - H55	0.278716	-0.954609	0.006077	0.286123	0.000235
77	C40 - H56	0.278853	-0.955899	0.005617	0.286196	0.000208
146	C71 - C96	0.24239	-0.544347	0.036902	0.191045	0.000226
147	C99 - H110	0.280048	-0.964275	0.005934	0.288401	0.000227
148	C97 - H103	0.281146	-0.973518	0.006778	0.290685	0.000259
149	H26 - H107	0.007145	0.025714	0.349861	-0.001459	0.149986
150	C96 - C98	0.240668	-0.53818	0.007542	0.189227	0.000058
151	C99 - H111	0.277229	-0.945643	0.004882	0.283121	0.00037
152	H89 - H113	0.012881	0.050543	0.509734	-0.002471	0.181145
153	H59 - H117	0.007845	0.027108	0.078319	-0.001349	0.012453
154	H80 - H115	0.012641	0.043554	0.083716	-0.001549	0.042262
155	C95 - C101	0.24083	-0.539005	0.007544	0.189402	0.000082
156	C102 - H120	0.2761	-0.938115	0.005982	0.281014	0.000338
157	C97 - H104	0.277252	-0.948812	0.0068	0.283188	0.000215
158	C97 - H105	0.276417	-0.939766	0.006418	0.281586	0.000355
159	C98 - H106	0.276122	-0.939898	0.004071	0.281091	0.000248
160	C98 - H108	0.278432	-0.951268	0.005011	0.28538	0.00018
161	C100 - H112	0.278179	-0.953981	0.005207	0.284879	0.000167
162	C101 - H115	0.278553	-0.953501	0.005741	0.285805	0.000227
163	C101 - H116	0.275995	-0.938229	0.004969	0.280845	0.000256
164	C101 - H117	0.279129	-0.956689	0.005138	0.286711	0.000176
165	C102 - H118	0.280536	-0.969888	0.006486	0.289468	0.000266
166	C102 - H119	0.27726	-0.948856	0.00639	0.283172	0.000224
134	C100 - H113	0.280203	-0.964951	0.005602	0.288654	0.000196
135	C79 - H89	0.281065	-0.977132	0.010774	0.290881	0.000313
136	C79 - H90	0.284776	-1.013882	0.009715	0.297572	0.000374
137	C79 - H91	0.273332	-0.91981	0.014483	0.276623	0.000114
138	C77 - H93	0.283176	-0.993403	0.013389	0.295206	0.000399
139	C77 - H92	0.277865	-0.974441	0.011982	0.28643	0.000121
140	C77 - H94	0.282838	-0.991845	0.013533	0.294266	0.000378
141	C95 - C102	0.238585	-0.528869	0.007089	0.186299	0.00016
142	C64 - C95	0.243382	-0.54875	0.037868	0.192593	0.000326
143	C100 - H114	0.277106	-0.94445	0.004473	0.282873	0.000358
144	C98 - H107	0.276849	-0.942757	0.004547	0.282346	0.000188

78	C40 - H57	0.276009	-0.938285	0.005417	0.280939	0.000262
79	C41 - H59	0.279893	-0.962383	0.005781	0.288126	0.000202
80	F75 - B76	0.154812	0.833199	0.028819	0.083244	0.000003
81	H29 - N67	0.004424	0.015187	2.414624	-0.000752	0.381765
82	F61 - C62	0.009851	0.047092	1.90911	-0.002095	0.30437
83	N67 - B76	0.157291	0.294936	0.00216	0.129262	0.000027
84	C62 - C63	0.259622	-0.633859	0.048619	0.22022	0.000043
85	H28 - H117	0.005779	0.020693	0.40147	-0.001219	0.054968
86	C63 - C64	0.296695	-0.756761	0.233386	0.284373	0.000967
87	C3 - H89	0.004327	0.013605	2.37207	-0.000718	0.349932
88	H56 - H113	0.007031	0.024124	0.122316	-0.001279	0.012642
89	H80 - H118	0.011342	0.045826	0.489633	-0.002437	0.470295
90	C64 - C65	0.302864	-0.765316	0.262057	0.294813	0.001106
91	C63 - N67	0.33064	-0.820056	0.151489	0.541274	0.000139
92	C65 - C66	0.292641	-0.743016	0.210514	0.27415	0.000861
93	H29 - F75	0.003922	0.017952	1.090551	-0.001175	0.016093
94	C66 - N67	0.301765	-0.874917	0.159642	0.449068	0.000186
95	F15 - H92	0.014736	0.050592	0.050783	-0.000189	0.004
96	C66 - C68	0.306858	-0.823627	0.22536	0.300307	0.000178
97	N73 - B76	0.156149	0.284637	0.005897	0.12849	0.000082
98	C68 - C69	0.303547	-0.809097	0.214572	0.293747	0.000131
99	H87 - H108	0.011087	0.039546	0.140386	-0.001638	0.042019
100	C69 - C70	0.295414	-0.75414	0.219422	0.279371	0.001058
101	C72 - N73	0.326431	-0.838728	0.157608	0.529124	0.000135
102	C96 - C97	0.238948	-0.530652	0.007845	0.186649	0.000204
103	C70 - C71	0.302226	-0.764647	0.25705	0.293476	0.000957
104	H25 - C72	0.005061	0.01795	3.00889	-0.000916	0.067845
105	C69 - N73	0.302529	-0.878139	0.165031	0.450212	0.000184
106	C71 - C72	0.297955	-0.758351	0.246735	0.286448	0.001113
107	C99 - H109	0.277946	-0.952461	0.005881	0.284379	0.000169
108	C72 - C74	0.258452	-0.628851	0.040808	0.218417	0.00011
109	H31 - F75	0.017449	0.05522	0.026882	0.000529	0.001507
145	C96 - C99	0.241367	-0.541308	0.002823	0.189923	0.000282
146	C71 - C96	0.24239	-0.544347	0.036902	0.191045	0.000226
147	C99 - H110	0.280048	-0.964275	0.005934	0.288401	0.000227
148	C97 - H103	0.281146	-0.973518	0.006778	0.290685	0.000259
149	H26 - H107	0.007145	0.025714	0.349861	-0.001459	0.149986
150	C96 - C98	0.240668	-0.53818	0.007542	0.189227	0.000058
151	C99 - H111	0.277229	-0.945643	0.004882	0.283121	0.00037
152	H89 - H113	0.012881	0.050543	0.509734	-0.002471	0.181145
153	H59 - H117	0.007845	0.027108	0.078319	-0.001349	0.012453
154	H80 - H115	0.012641	0.043554	0.083716	-0.001549	0.042262
155	C95 - C101	0.24083	-0.539005	0.007544	0.189402	0.000082
156	C102 - H120	0.2761	-0.938115	0.005982	0.281014	0.000338
157	C97 - H104	0.277252	-0.948812	0.0068	0.283188	0.000215
158	C97 - H105	0.276417	-0.939766	0.006418	0.281586	0.000355
159	C98 - H106	0.276122	-0.939898	0.004071	0.281091	0.000248
160	C98 - H108	0.278432	-0.951268	0.005011	0.28538	0.00018
161	C100 - H112	0.278179	-0.953981	0.005207	0.284879	0.000167
162	C101 - H115	0.278553	-0.953501	0.005741	0.285805	0.000227
163	C101 - H116	0.275995	-0.938229	0.004969	0.280845	0.000256
164	C101 - H117	0.279129	-0.956689	0.005138	0.286711	0.000176
165	C102 - H118	0.280536	-0.969888	0.006486	0.289468	0.000266
166	C102 - H119	0.27726	-0.948856	0.00639	0.283172	0.000224
134	C100 - H113	0.280203	-0.964951	0.005602	0.288654	0.000196
135	C79 - H89	0.281065	-0.977132	0.010774	0.290881	0.000313
136	C79 - H90	0.284776	-1.013882	0.009715	0.297572	0.000374
137	C79 - H91	0.273332	-0.91981	0.014483	0.276623	0.000114
138	C77 - H93	0.283176	-0.993403	0.013389	0.295206	0.000399
139	C77 - H92	0.277865	-0.974441	0.011982	0.28643	0.000121
140	C77 - H94	0.282838	-0.991845	0.013533	0.294266	0.000378
141	C95 - C102	0.238585	-0.528869	0.007089	0.186299	0.00016
142	C64 - C95	0.243382	-0.54875	0.037868	0.192593	0.000326
143	C100 - H114	0.277106	-0.94445	0.004473	0.282873	0.000358

110	F75 - H83	0.013767	0.054205	0.254946	-0.001082	0.026392
111	F75 - H82	0.01076	0.045669	0.326387	-0.001527	0.052995
112	F61 - B76	0.167412	0.946989	0.037333	0.089681	0.000006
113	C68 - C77	0.25452	-0.606447	0.024763	0.212231	0.00019
114	H44 - H87	0.008134	0.028327	0.150687	-0.001412	0.02672
115	C70 - C78	0.255141	-0.606103	0.02953	0.211267	0.000214
116	H87 - H103	0.012815	0.05189	0.40759	-0.002607	0.346695
117	C78 - H93	0.013528	0.055822	1.499668	-0.002626	0.177808
118	F15 - H90	0.008614	0.033677	0.074253	-0.00107	0.001151
119	C65 - C79	0.253385	-0.599085	0.025014	0.209247	0.00042
120	H90 - H94	0.012773	0.05639	1.357411	-0.003219	0.833733
121	C62 - H80	0.282798	-0.991708	0.01114	0.294261	0.000226
122	C62 - H81	0.276289	-0.95192	0.010563	0.282569	0.000125
123	C62 - H82	0.279861	-0.980673	0.008799	0.289038	0.000194
124	C74 - H84	0.275862	-0.945487	0.011591	0.281547	0.000142
125	C74 - H83	0.284542	-1.017868	0.007028	0.297764	0.000295
126	H85 - H110	0.012706	0.049854	0.516964	-0.002486	0.19228
127	C74 - H85	0.279291	-0.965246	0.011473	0.287782	0.000253
128	H44 - H108	0.005908	0.020031	0.366665	-0.001126	0.004408
129	C78 - H86	0.280522	-0.978054	0.008063	0.28938	0.000229
130	C78 - H87	0.282861	-0.987602	0.008646	0.294181	0.000225
131	C78 - H88	0.273635	-0.922401	0.011325	0.277088	0.000112
132	H56 - H117	0.009823	0.032895	0.100884	-0.001351	0.012525
133	C95 - C100	0.242088	-0.544792	0.002619	0.190869	0.000272
134	C98 - H107	0.276849	-0.942757	0.004547	0.282346	0.000188
145	C96 - C99	0.241367	-0.541308	0.002823	0.189923	0.000282
146	C71 - C96	0.24239	-0.544347	0.036902	0.191045	0.000226
147	C99 - H110	0.280048	-0.964275	0.005934	0.288401	0.000227
148	C97 - H103	0.281146	-0.973518	0.006778	0.290685	0.000259
149	H26 - H107	0.007145	0.025714	0.349861	-0.001459	0.149986
150	C96 - C98	0.240668	-0.53818	0.007542	0.189227	0.000058
151	C99 - H111	0.277229	-0.945643	0.004882	0.283121	0.00037
152	H89 - H113	0.012881	0.050543	0.509734	-0.002471	0.181145
153	H59 - H117	0.007845	0.027108	0.078319	-0.001349	0.012453
154	H80 - H115	0.012641	0.043554	0.083716	-0.001549	0.042262
155	C95 - C101	0.24083	-0.539005	0.007544	0.189402	0.000082
156	C102 - H120	0.2761	-0.938115	0.005982	0.281014	0.000338
157	C97 - H104	0.277252	-0.948812	0.0068	0.283188	0.000215
158	C97 - H105	0.276417	-0.939766	0.006418	0.281586	0.000355
159	C98 - H106	0.276122	-0.939898	0.004071	0.281091	0.000248
160	C98 - H108	0.278432	-0.951268	0.005011	0.28538	0.00018
161	C100 - H112	0.278179	-0.953981	0.005207	0.284879	0.000167
162	C101 - H115	0.278553	-0.953501	0.005741	0.285805	0.000227
163	C101 - H116	0.275995	-0.938229	0.004969	0.280845	0.000256
164	C101 - H117	0.279129	-0.956689	0.005138	0.286711	0.000176
165	C102 - H118	0.280536	-0.969888	0.006486	0.289468	0.000266
166	C102 - H119	0.27726	-0.948856	0.00639	0.283172	0.000224
134	C100 - H113	0.280203	-0.964951	0.005602	0.288654	0.000196