

## Supplementary Information

### Experimental and DFT mechanistic insights on one-pot synthesis of 1*H*-pyrazolo[1,2-*b*]phthalazine-5,10-diones under catalysis of DBU-based ionic liquids

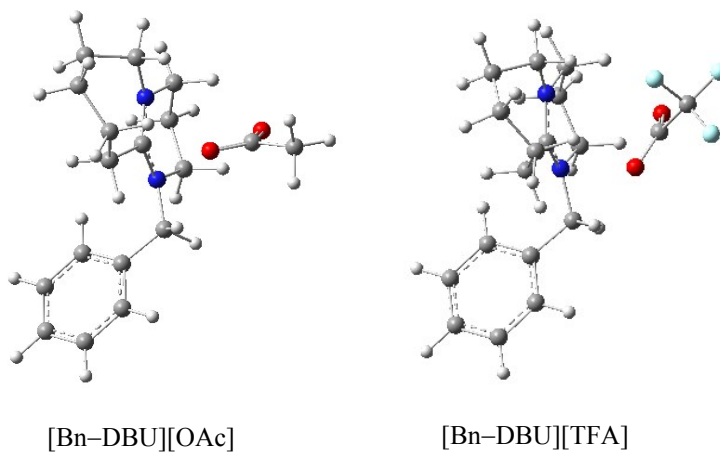
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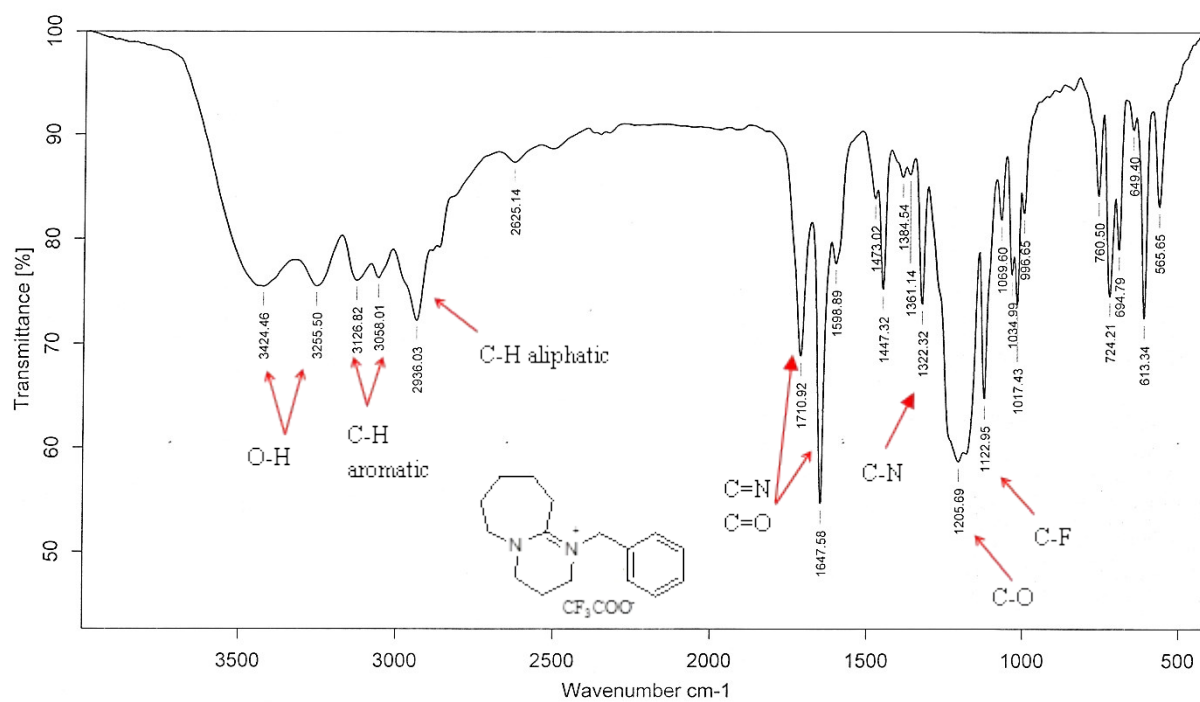
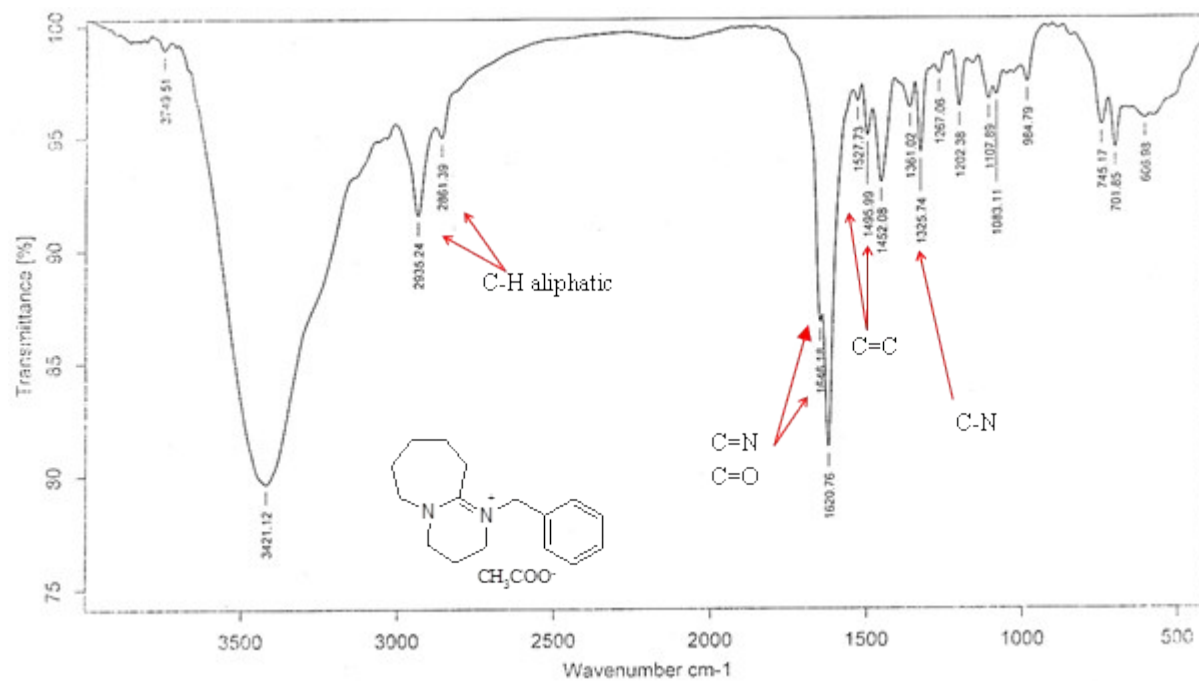
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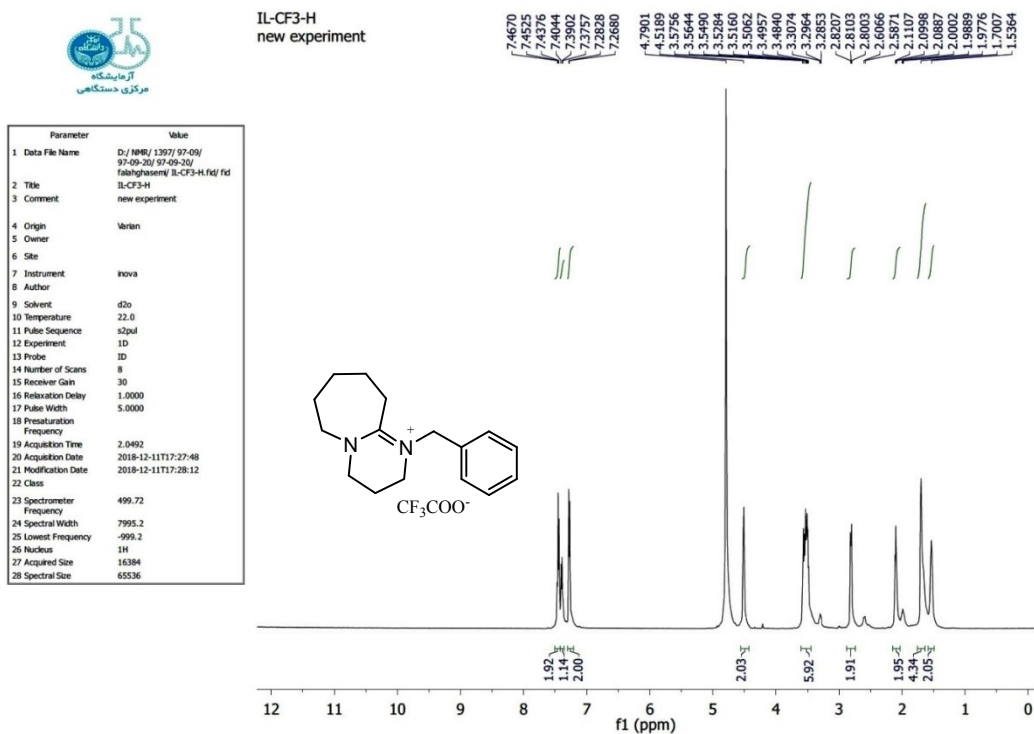
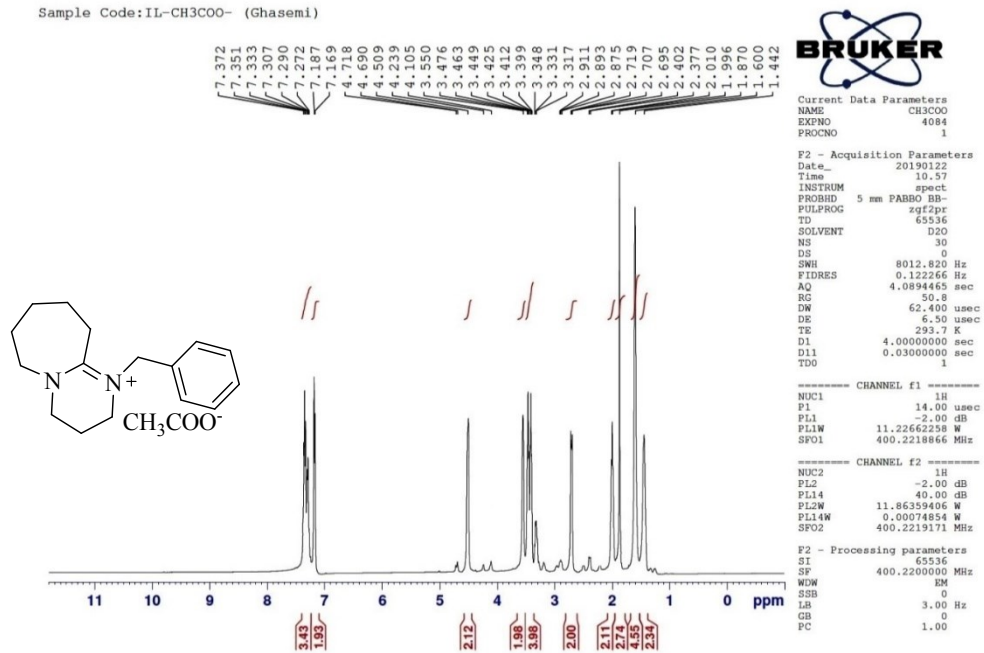
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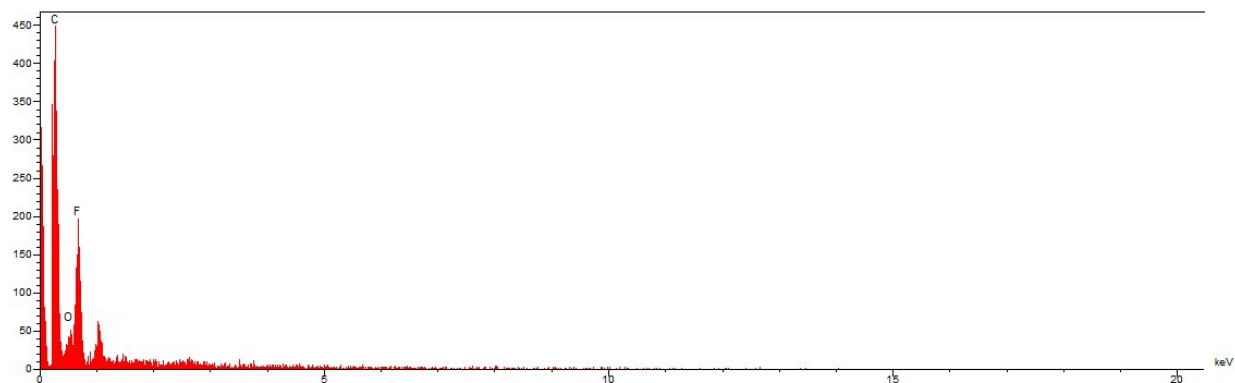
**Fig. S1** The optimized structures of [Bn-DBU][OAc] and [Bn-DBU][TFA] at B3LYP/SVP level of theory in gas phase.



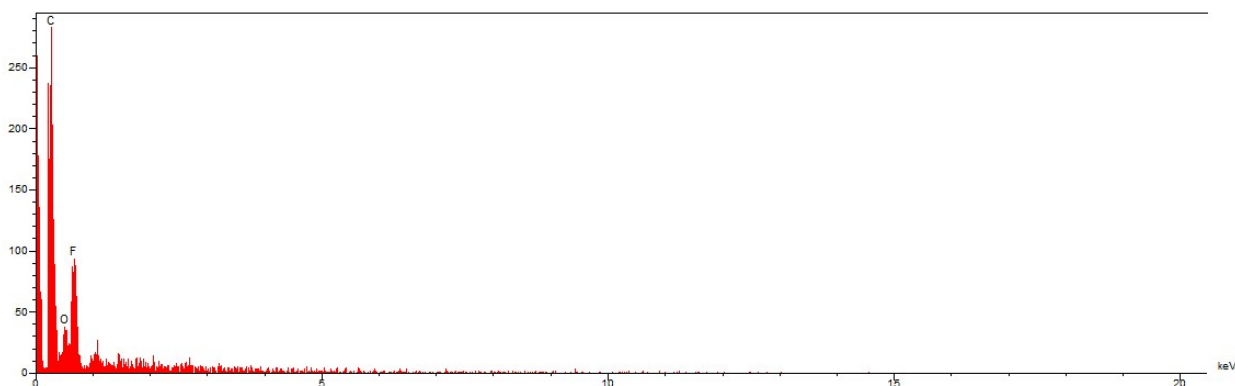
**Fig. S2** The FT-IR spectra of the two synthesized DBU-based ILs, [Bn-DBU][CH<sub>3</sub>CO<sub>2</sub>] (up) [Bn-DBU][CF<sub>3</sub>CO<sub>2</sub>] (below).



**Fig. S3** The <sup>1</sup>H NMR spectra of the two synthesized DBU-based ILs, (up) [Bn-DBU][CH<sub>3</sub>CO<sub>2</sub>], (below) [Bn-DBU][CF<sub>3</sub>CO<sub>2</sub>]



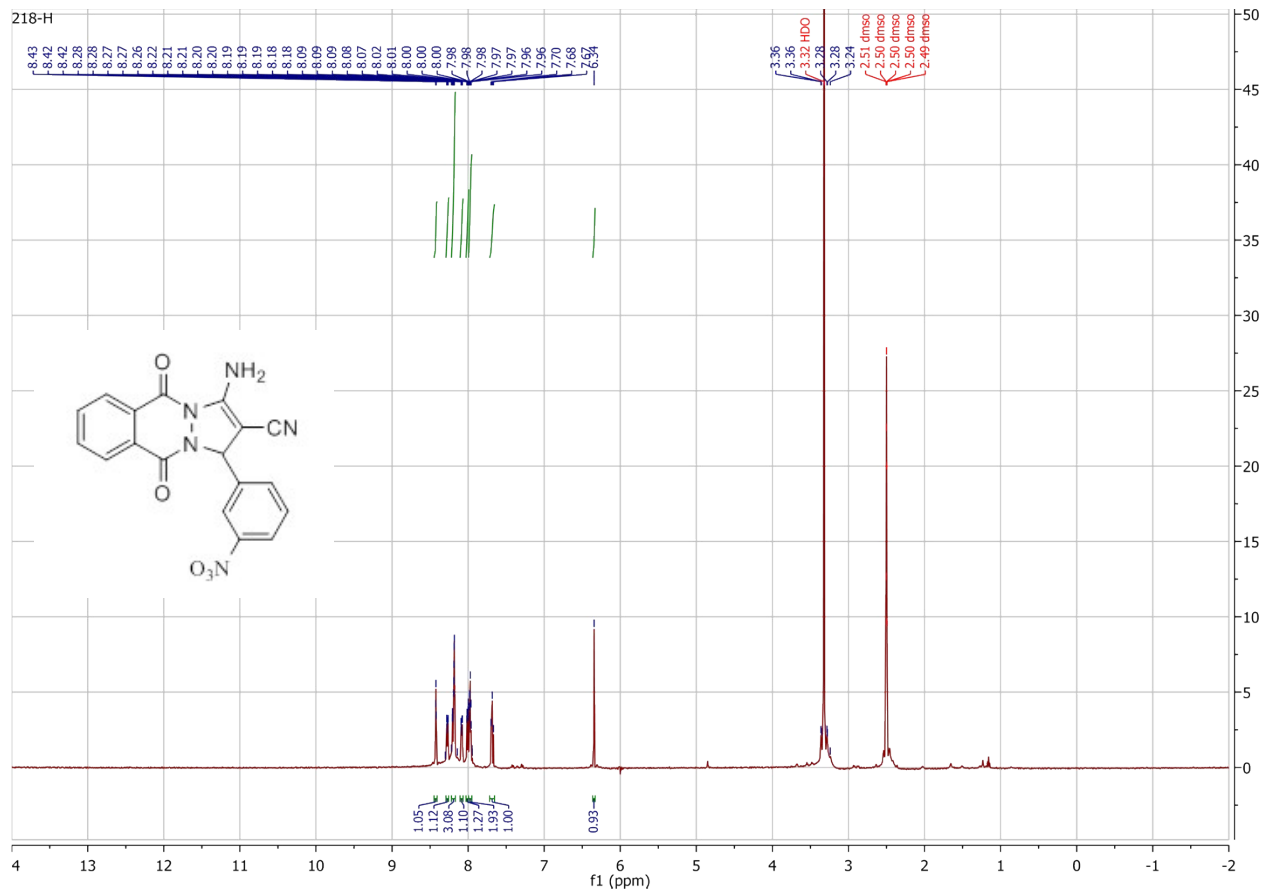
Elt	Line	Int	Error	K	Kr	W%	A%	ZAF	Formula	Ox%	Pk/Bg	Class	LConf	HConf	Cat#
C	Ka	212.8	37.4548	0.8124	0.3900	64.16	72.74	0.6077		0.00	127.02	A	61.74	66.58	0.00
O	Ka	26.2	37.4548	0.0498	0.0239	11.73	9.98	0.2039		0.00	21.70	A	10.47	12.99	0.00
F	Ka	104.0	37.4548	0.1378	0.0661	24.11	17.28	0.2743		0.00	47.11	A	22.81	25.41	0.00
				1.0000	0.4800	100.00	100.00			0.00					0.00



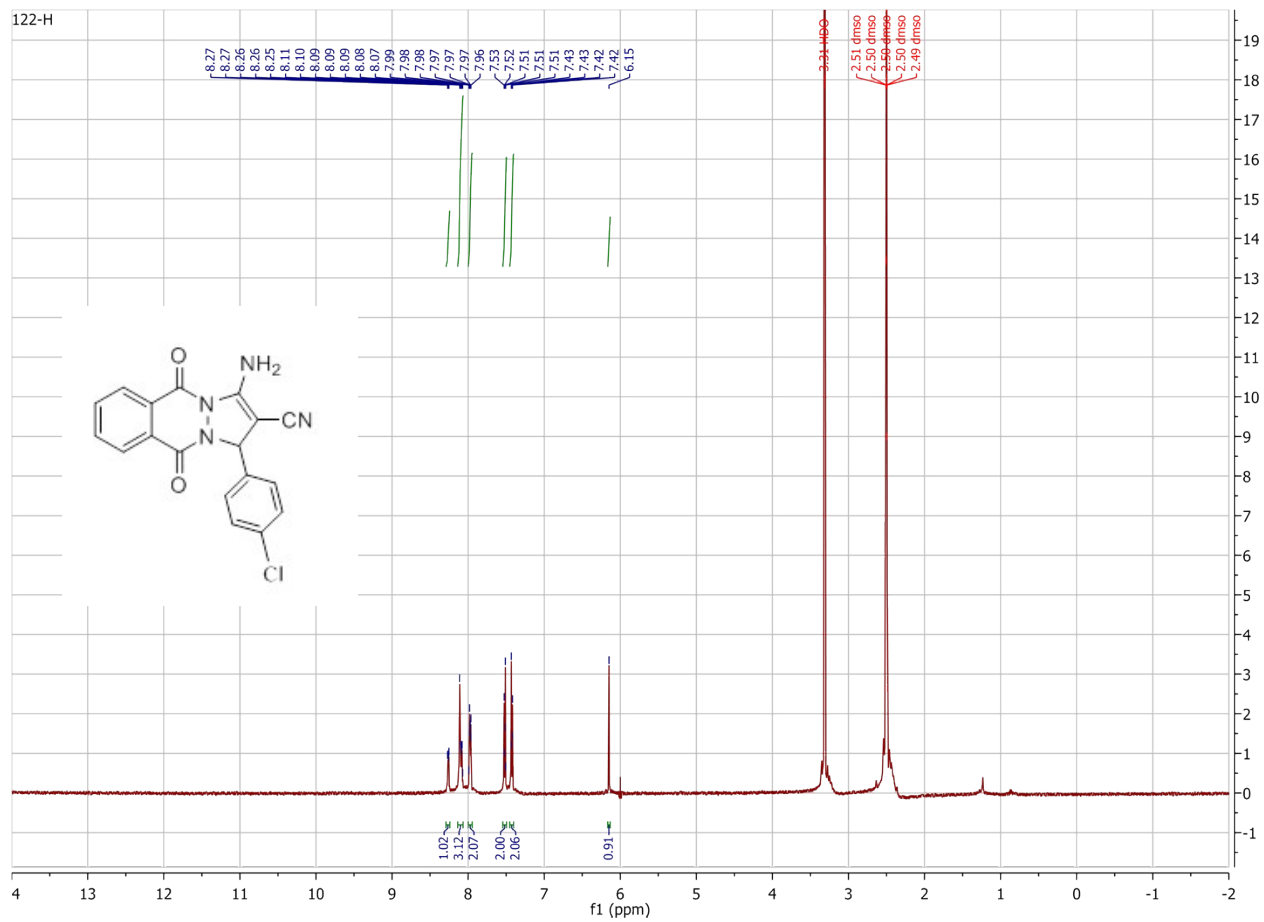
Elt	Line	Int	Error	K	Kr	W%	A%	ZAF	Formula	Ox%	Pk/Bg	Class	LConf	HConf	Cat#
C	Ka	188.9	16.0765	0.8502	0.4328	67.56	75.46	0.6404		0.00	466.40	A	64.58	70.55	0.00
O	Ka	21.1	16.0765	0.0472	0.0240	12.41	10.40	0.1937		0.00	16.81	A	10.76	14.05	0.00
F	Ka	65.7	16.0765	0.1026	0.0522	20.03	14.14	0.2608		0.00	30.55	A	18.52	21.53	0.00
				1.0000	0.5091	100.00	100.00			0.00					0.00

**Fig. S4** The EDX spectra of fresh [Bn-DBU][TFA] (up) and [Bn-DBU][TFA] after 4<sup>th</sup> recycling (below)

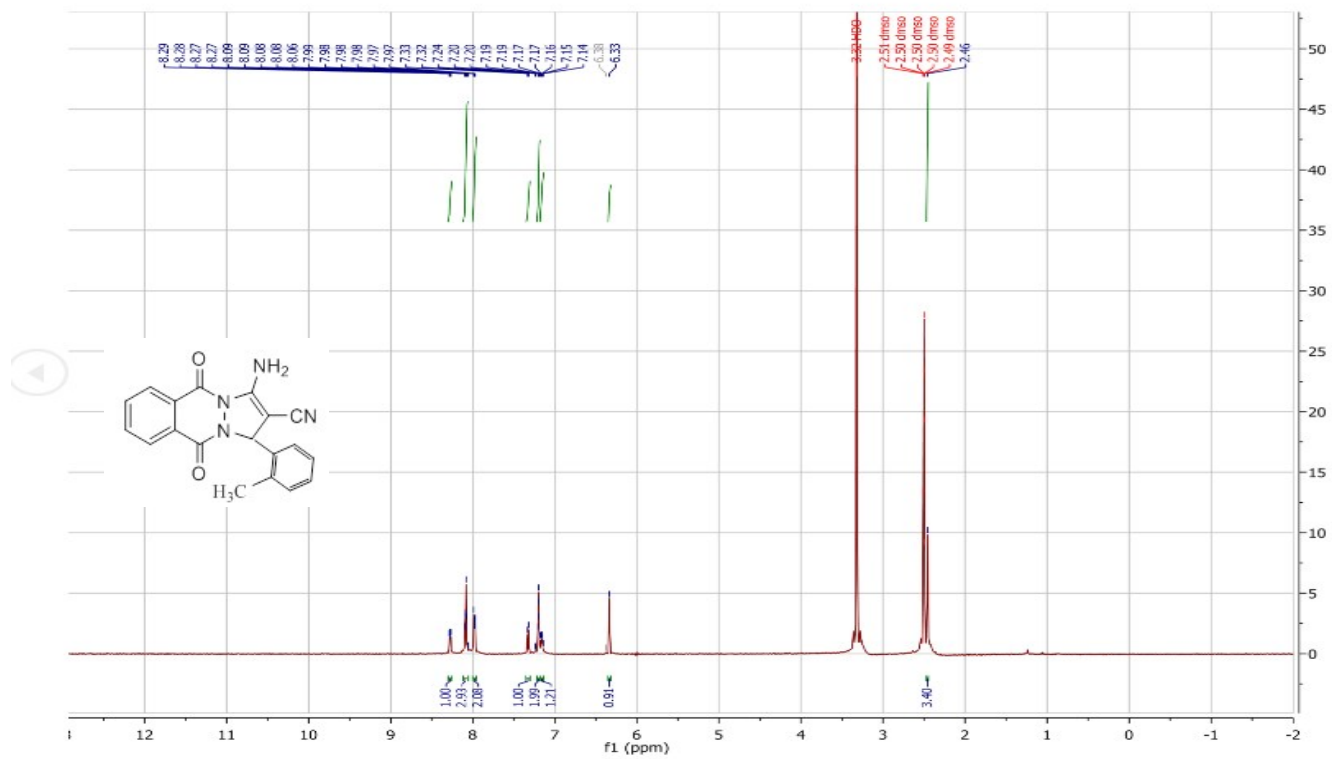
218-H



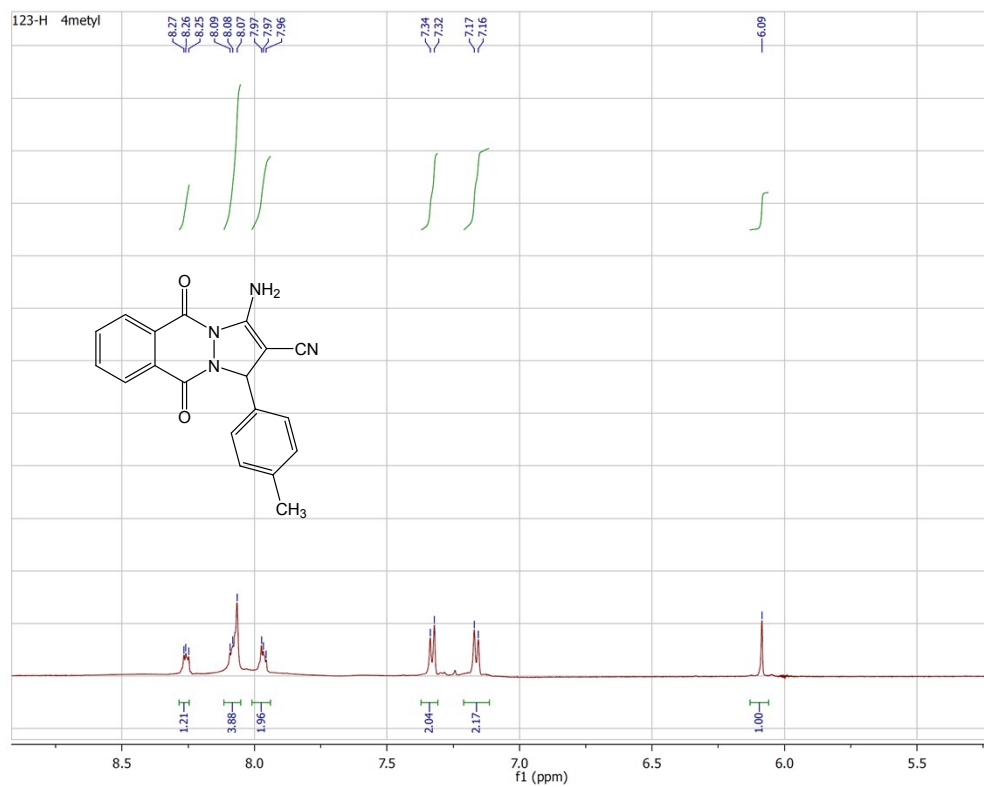
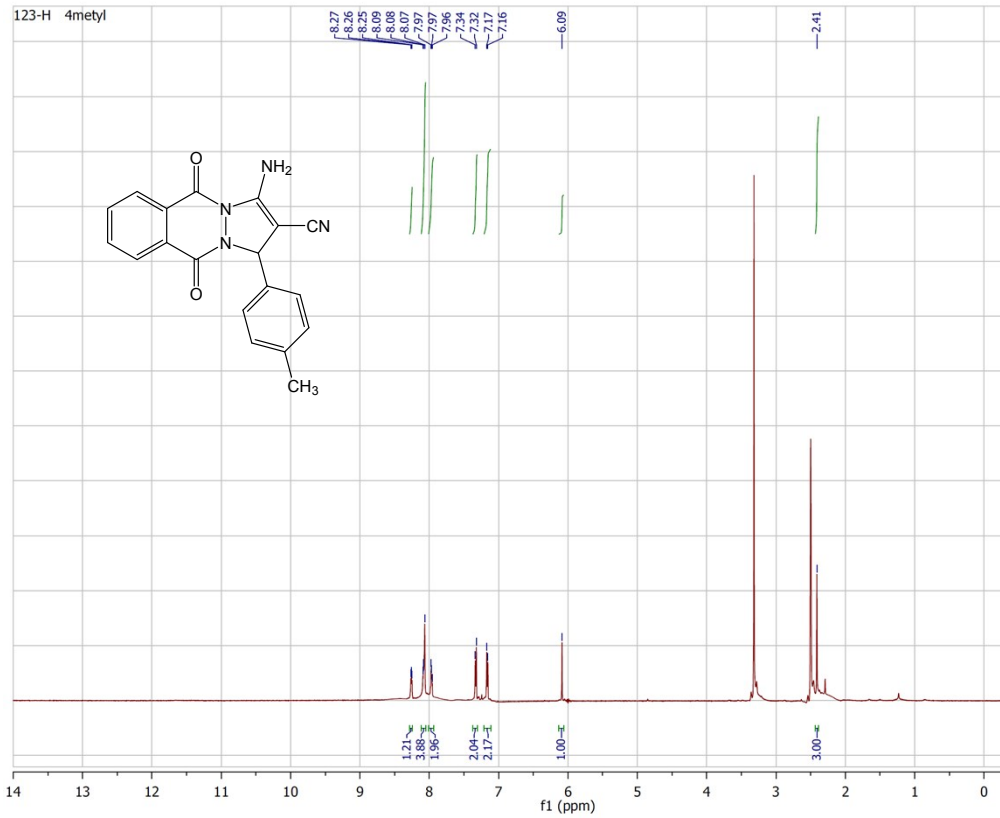
122-H



f1 (ppm)







f1 (ppm)

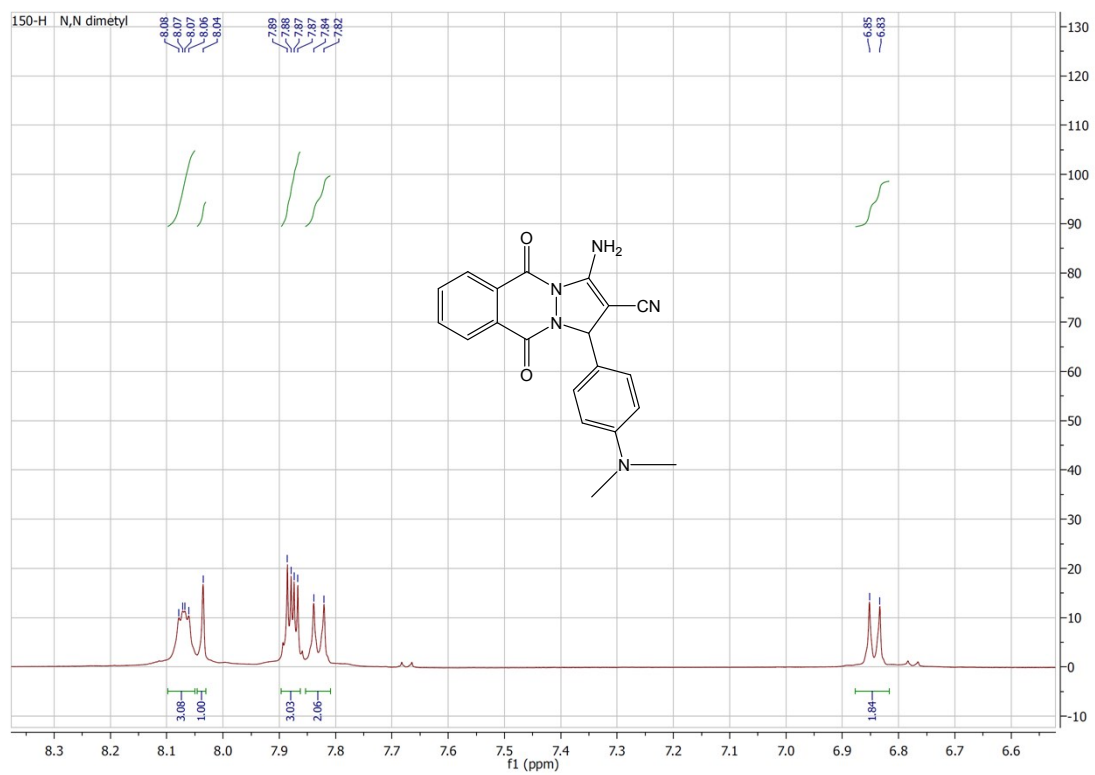
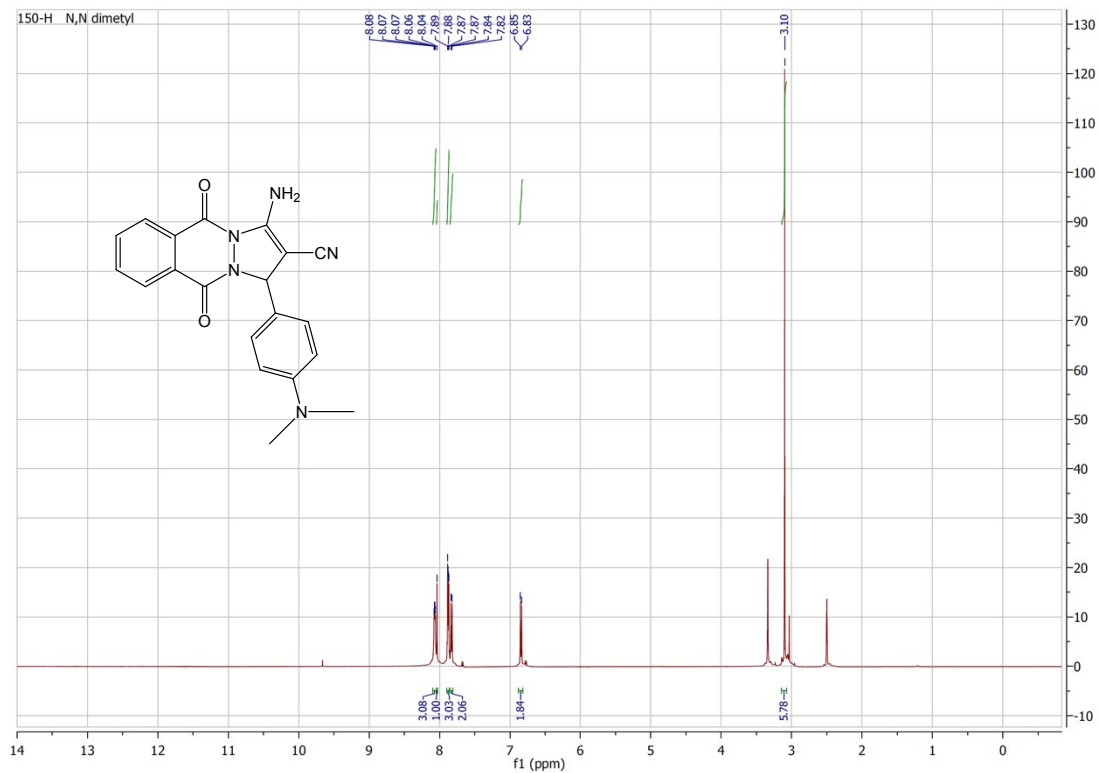
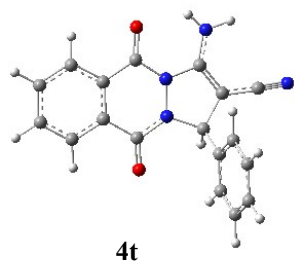
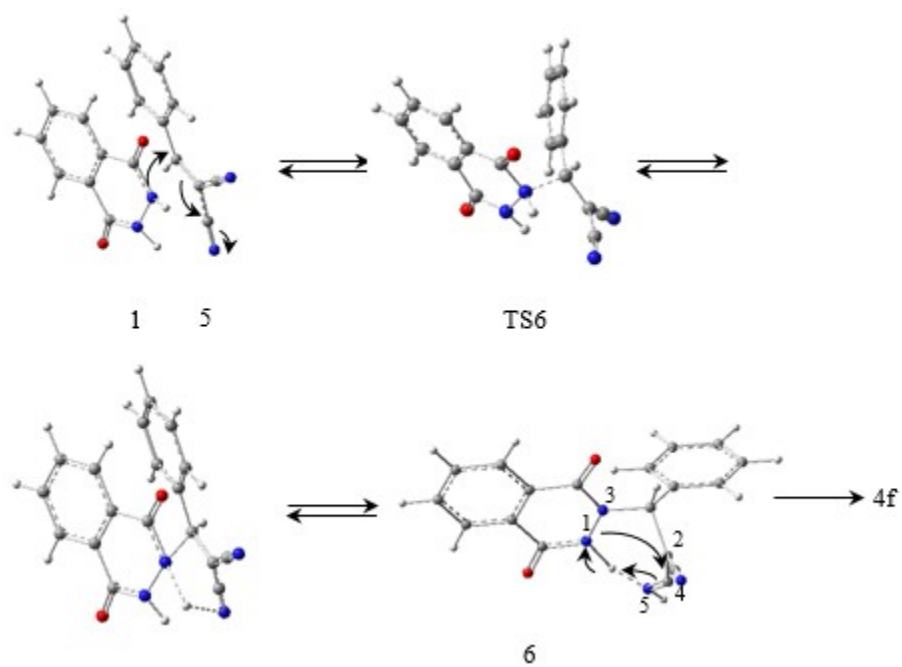


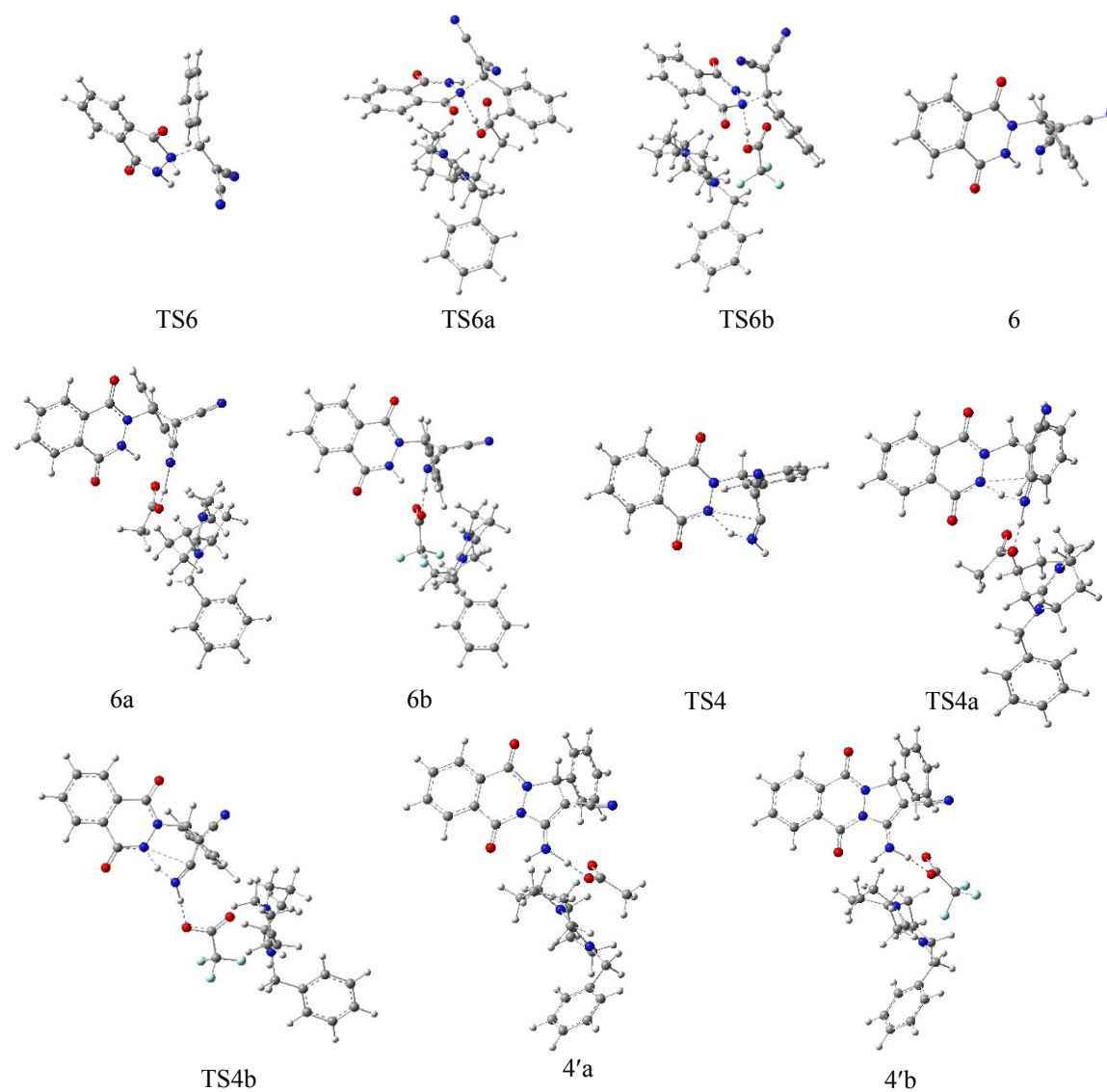
Fig. S5  $^1\text{H}$  NMR spectra of the synthesized 1H-pyrazolo[1,2-*b*]phthalazine-5,10-diones



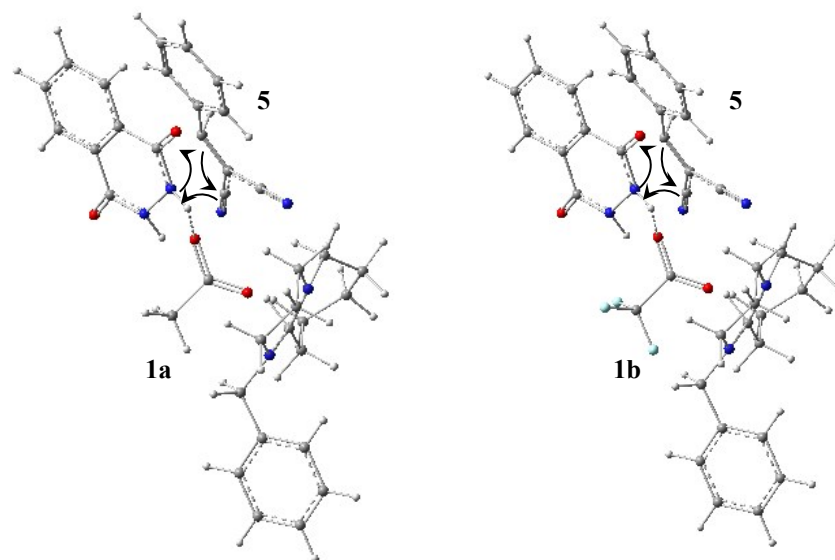
**Fig. S6** The optimized structures of **4t** using DFT at B3LYP/SVP level of theory in gas phase



**Fig. S7** The optimized structures of mechanistic proposal for the synthesis of **4t** at B3LYP/SVP level theory in gas phase.



**Fig. S8** The optimized structures for synthesis of **4t** with mechanism proposed at B3LYP/SVP level of theory in gas phase.



**Fig. S9** The approach of **5** to phthalhydrazide in its complexes with [Bn-DBU][AcO] and [Bn-DBU][TFA] ILs at B3LYP/SVP level of theory in gas phase.