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Supporting information for article:

Why are reactions of 2- and 8-thioquinoline derivatives with iodine different?

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S1. Synthesis of 1,4-Bis(quinolin-2-ylthio)but-2-yne (2TQB)

Melting point 172-175°C.

H1-NMR: (DMSO-d6, 400 MHz) δ 4.195 (s, 4H, 2 CH_2), 7.365- 8.148, (m, 12H, Ap-H).

Mass spectra of 2TQB are characterized by IE: m/z, I_r (%): 212.05 (100.0), 128.05 (29.9), 210.05 (23.5) 213.05 (16.8), 161.05 (10.7), 116.05 (6.7)

Table S1 The Mulliken's atomic charges of the dication in **2b** and **2a** crystals calculated at the level of HSE06/6-31G**(for H, C, N, O, S atoms)/DZVP(for I atoms) in CRYSTAL14

Atom	Atomic charges in **2a**	Atomic charges in **2b**	Difference of charges, Δq
S1	0.48	0.50	-0.03
S2	0.35	0.38	-0.03
N1	-0.62	-0.60	-0.02
N2	-0.55	-0.53	-0.01
C1	0.12	0.07	0.05
C2	-0.12	-0.13	0.01
H2	0.18	0.20	-0.01
C3	-0.06	-0.06	0.00
H3	0.18	0.19	-0.02
C4	0.02	0.04	-0.02
C5	-0.18	-0.13	-0.05
H5	0.17	0.18	-0.02
C6	-0.11	-0.11	0.00
H6	0.16	0.18	-0.02
C7	-0.15	-0.14	0.00
H7	0.18	0.20	-0.02
C8	-0.06	-0.08	0.02
H8	0.16	0.14	0.02
C9	0.35	0.28	0.07

C10	0.41	0.40	0.01
C11	-0.39	-0.39	0.00
H11A	0.22	0.22	0.01
C12	-0.09	-0.08	-0.01
H12A	0.23	0.22	0.00
C13	-0.47	-0.46	0.00
H131	0.24	0.22	0.01
H132	0.23	0.24	0.00
C14	0.11	0.08	0.03
C15	-0.14	-0.14	0.00
H15	0.18	0.20	-0.03
C16	-0.01	-0.04	0.03
H16	0.19	0.20	-0.01
C17	0.03	0.01	0.02
C18	-0.17	-0.15	-0.02
H18	0.19	0.19	0.00
C19	-0.15	-0.10	-0.05
H19	0.17	0.16	0.01
C20	-0.14	-0.14	0.00
H20	0.16	0.18	-0.02
C21	-0.10	-0.11	0.01
H21	0.20	0.17	0.03
C22	0.31	0.29	0.02

Sum of dication atoms charges	1.70	1.75
Sum of anion atoms charges	-1.72	-1.75
Sum of 0.5•H_2O atom charges	0.02	
Total charge	0.00	0.00

Figure S1 Experimental (top) and calculated (bottom) powder X-Ray diffractogram (293 K) for bulk product of the reaction of $I_2$with 2TQB isolated from the reaction mixture before crystallization procedure

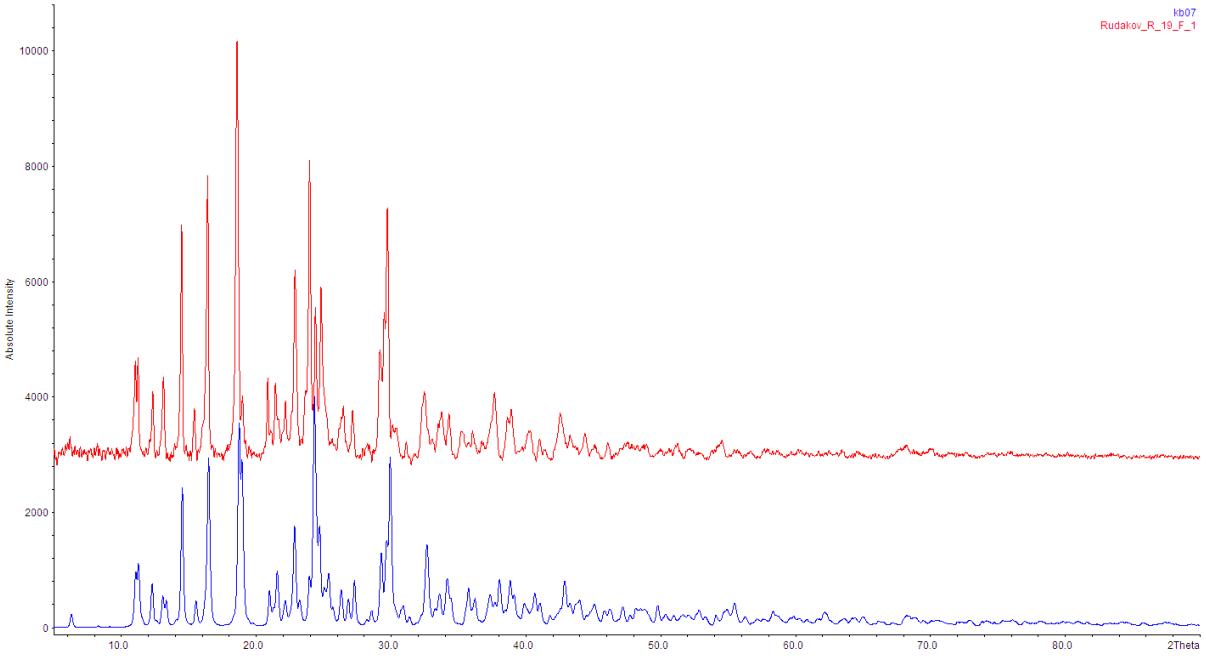

Figure S2 The rotation barriers performed by method GAFF versus torsion angles for 2TQB and 8TQB derivatives