Supporting Information

Molecular Engineering and Structure-Related Properties of Squaraine Dyes based on the Core and Wings Concept

G Hanumantha Rao,[†,‡] Prem Jyoti Singh Rana,[†] Ramesh Kumar Chitumalla,[§] Joonkyung Jang,[*,§] Surya Prakash Singh[*,†,‡]

[†]Polymers and Functional Materials Division, CSIR-Indian Institute of Chemical Technology, Uppal Road, Tarnaka, Hyderabad-500007, India.

[‡]Academy of Scientific and Innovative Research (AcSIR), CSIR- Human Resource Development Centre, (CSIR-HRDC) Campus, Kamla Nehru Nagar, Ghaziabad, Uttar Pradesh- 201002, India.

[§]Department of Nanoenergy Engineering, Pusan National University, Busan 46241, Republic of Korea.

E-Mail: Corresponding authors: spsingh@iict.res.in and jkjang@pusan.ac.kr

CONTENTS

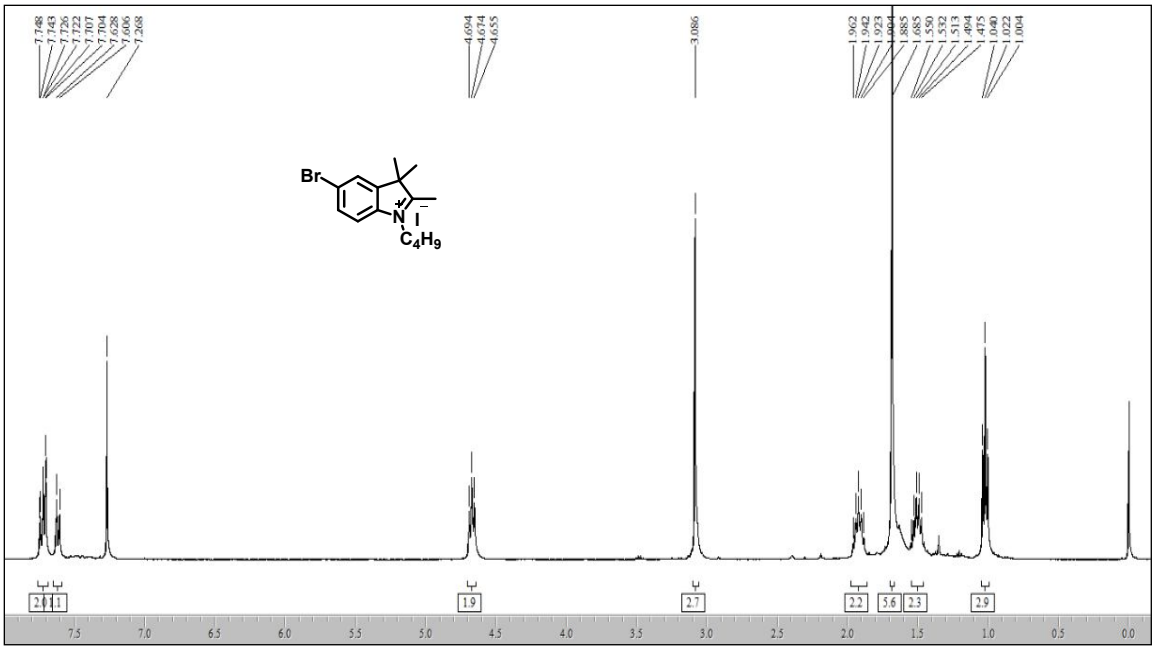


Figure S1. ^{1}H NMR spectra of 5-bromo-1-butyl-2,3,3-trimethyl-3*H*-indol-1-ium iodide in $CDCl_3$.

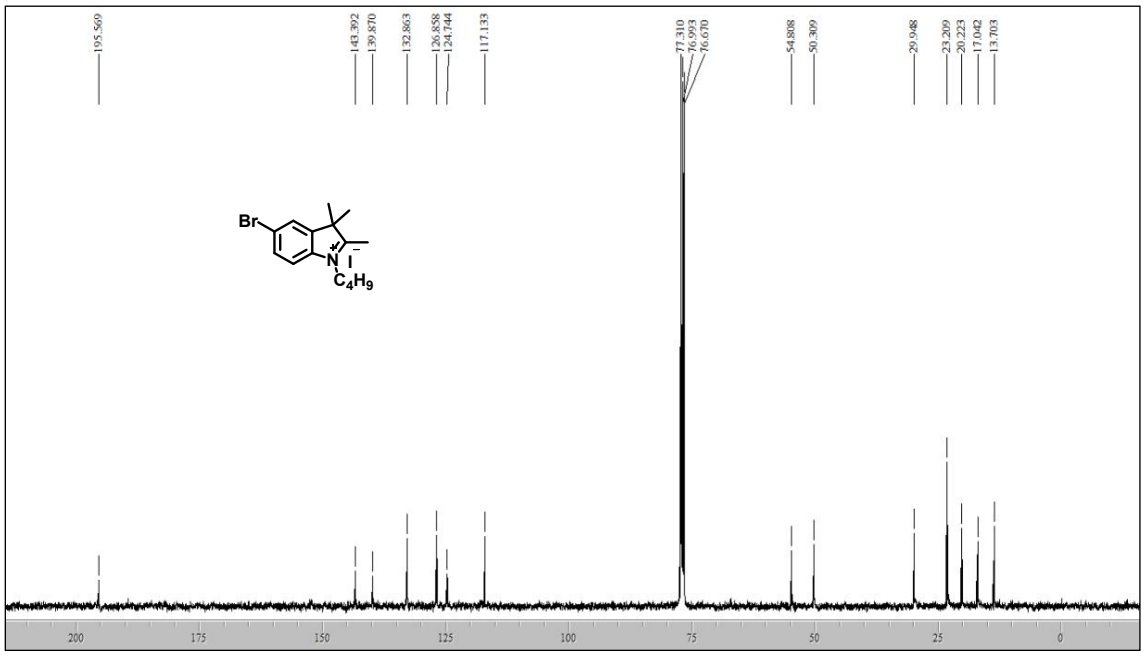


Figure S2. ^{13}C NMR spectra of 5-bromo-1-butyl-2,3,3-trimethyl-3*H*-indol-1-ium iodide in $CDCl_3$.

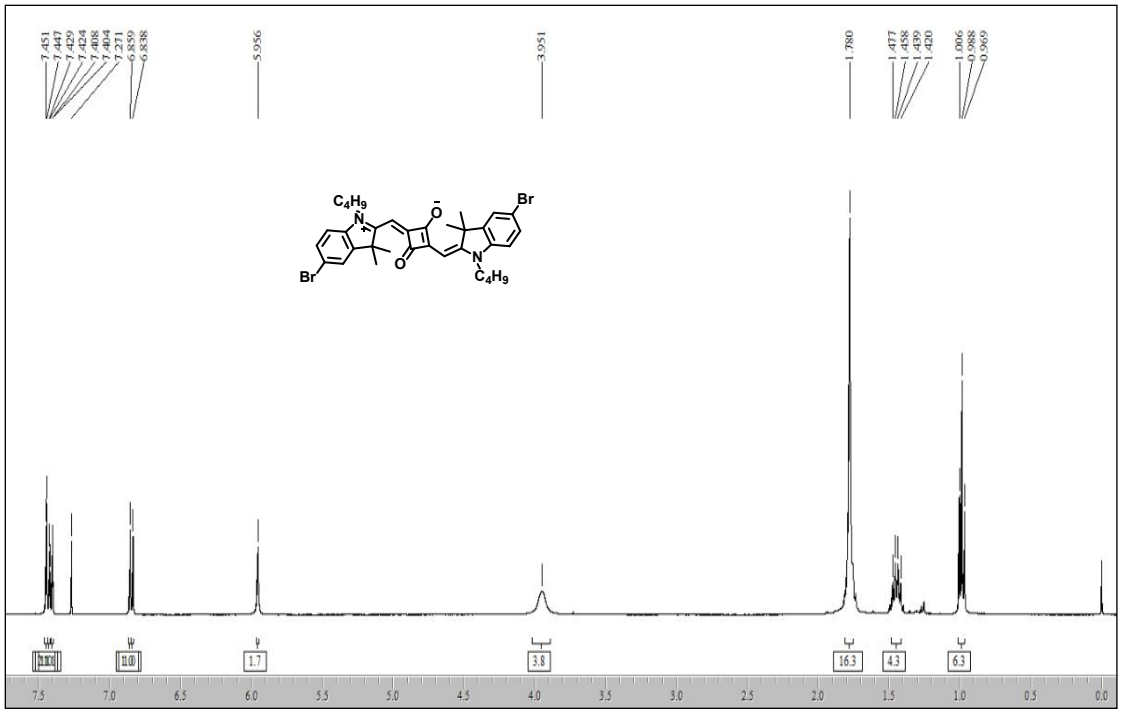


Figure S3. ^{1}H NMR spectra of **SQ-2Br** in $CDCl_3$.

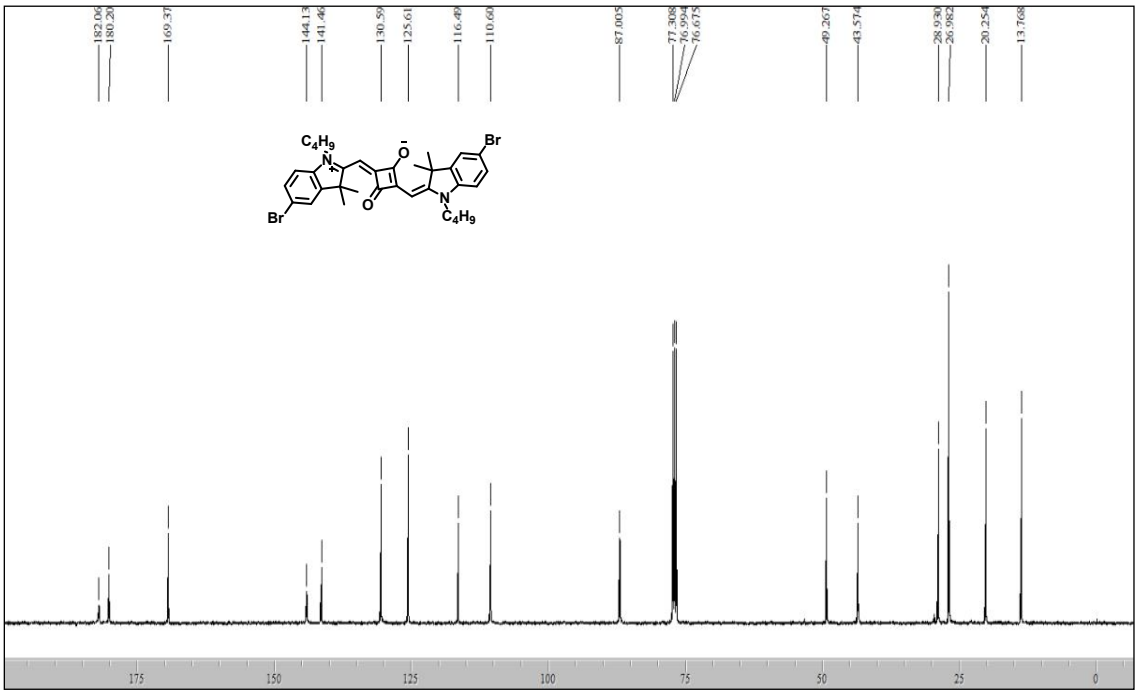


Figure S4. ^{13}C NMR spectra of **SQ-2Br** in $CDCl_3$.

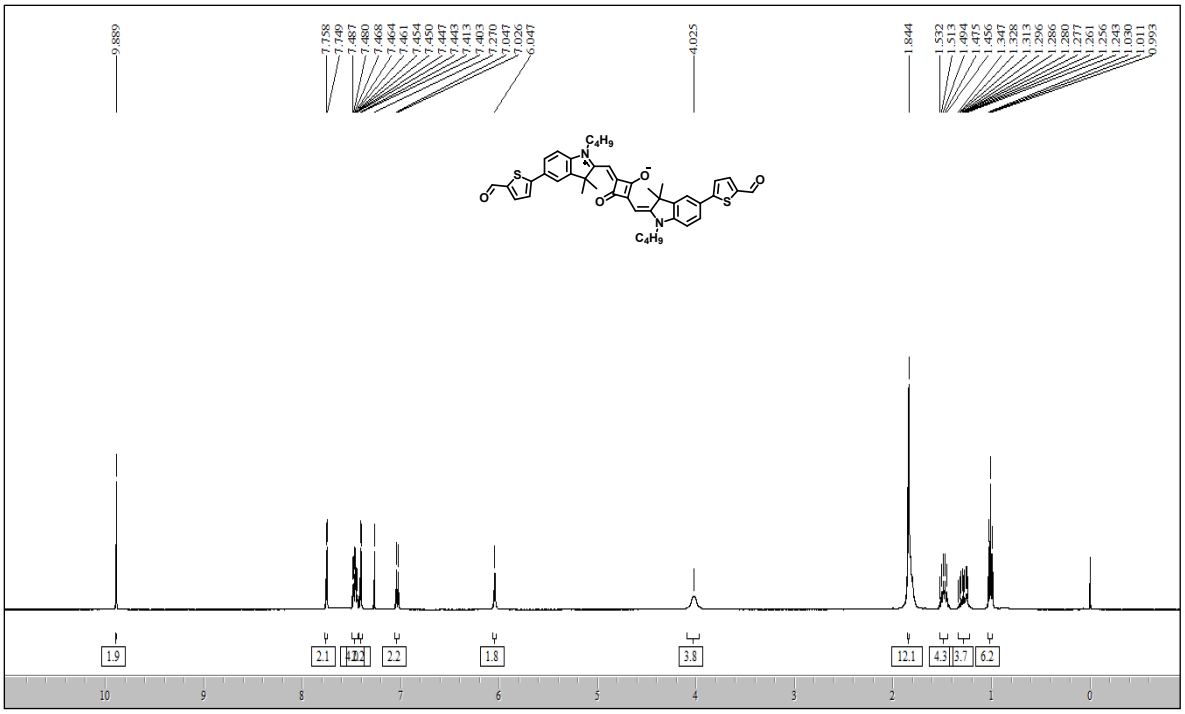


Figure S5. ^{1}H NMR spectra of **SQ-2CHO** in $CDCl_3$.

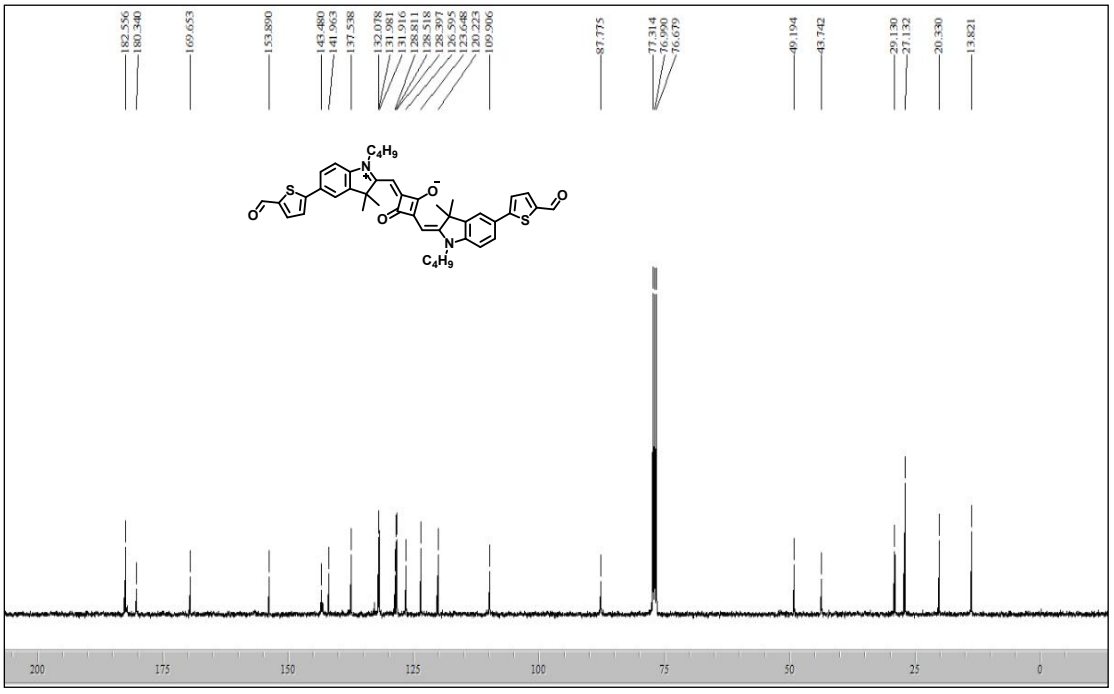


Figure S6. ^{13}C NMR spectra of **SQ-2CHO** in $CDCl_3$.

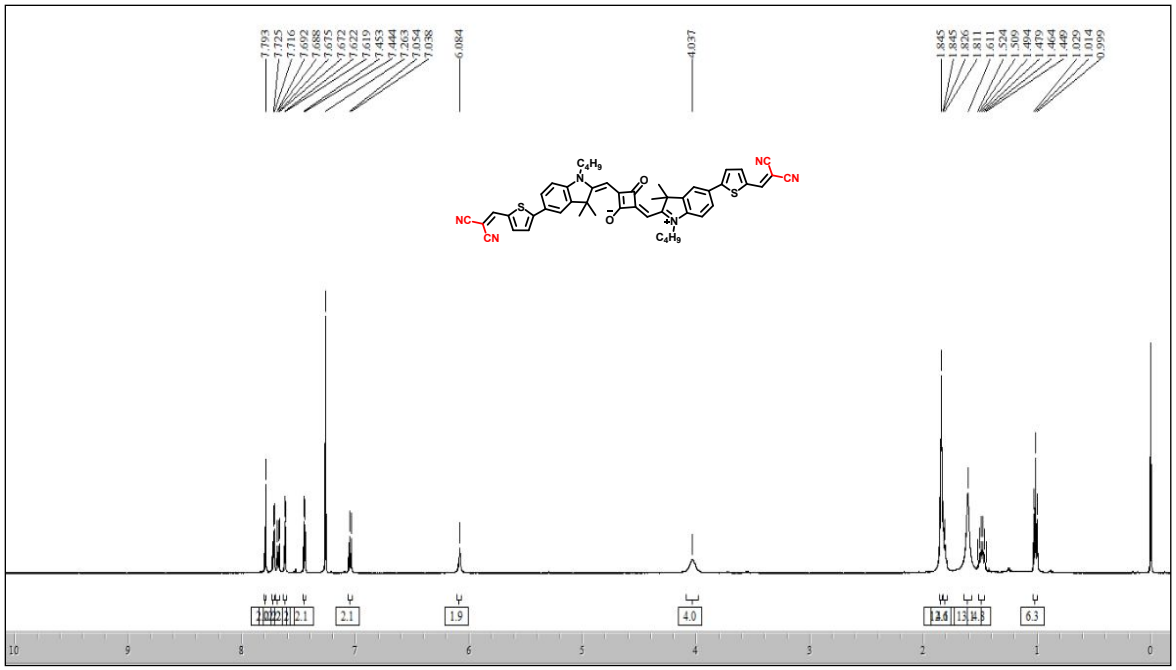


Figure S7. ^{1}H NMR spectra of **SQ-DICN** in $CDCl_3$.

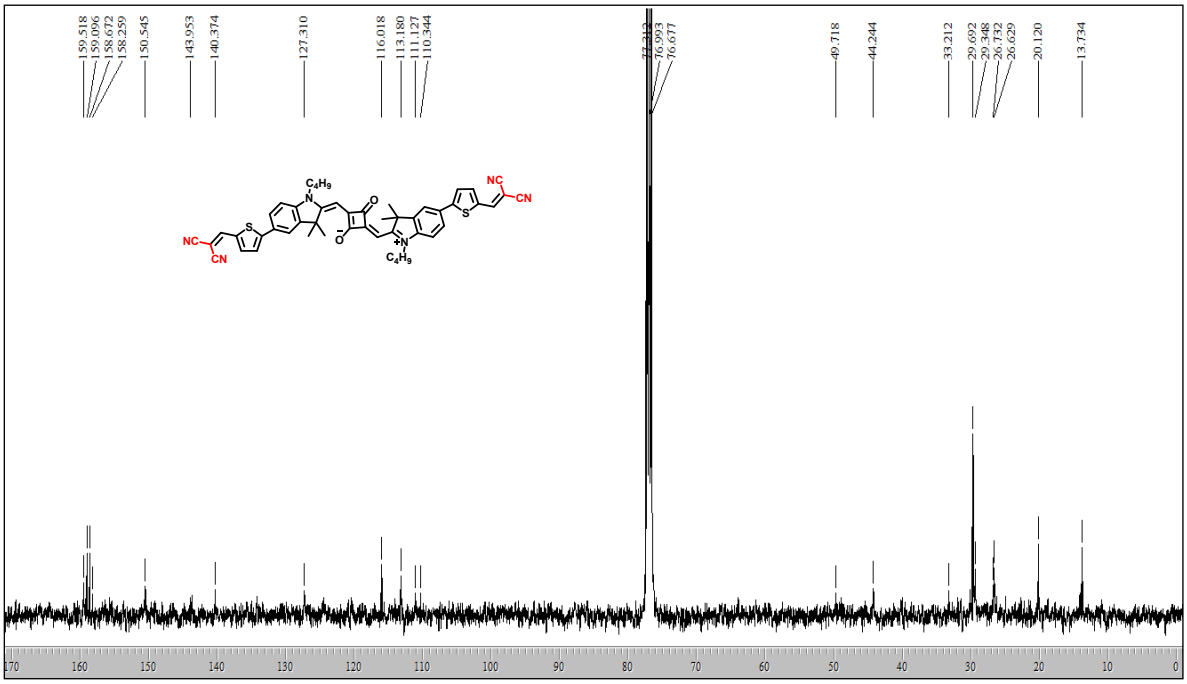


Figure S8. ^{13}C NMR spectra of **SQ-DICN** in $CDCl_3$.

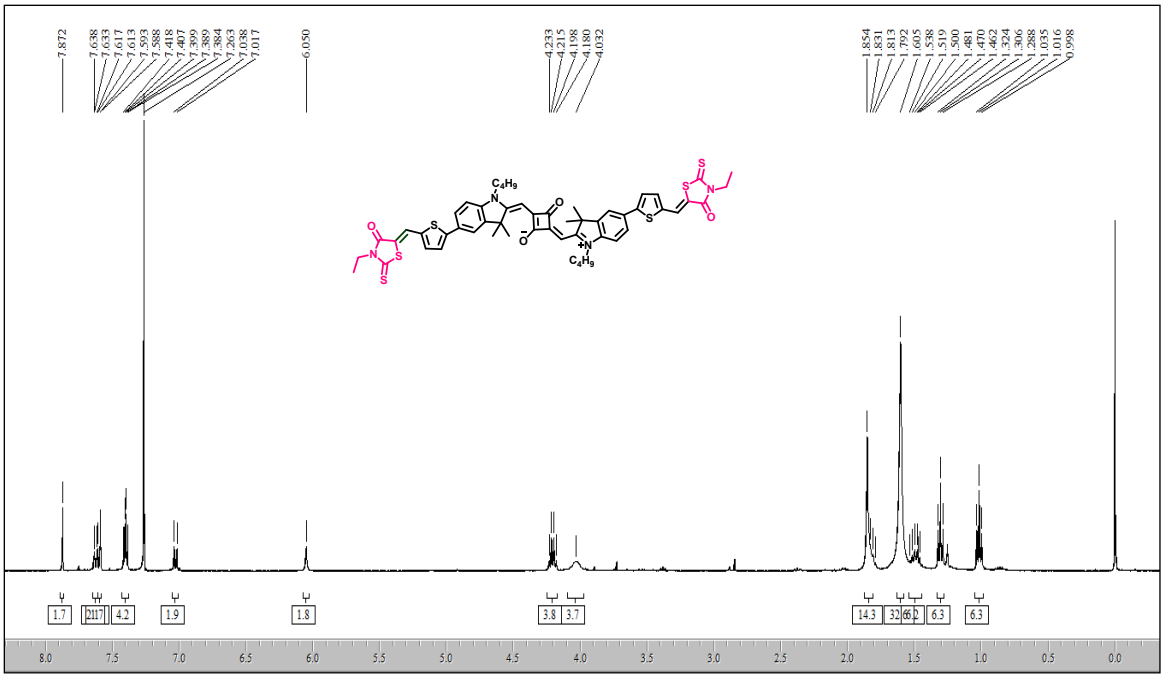


Figure S9. ^{1}H NMR spectra of **SQ-DIEt-RH** in $CDCl_3$.

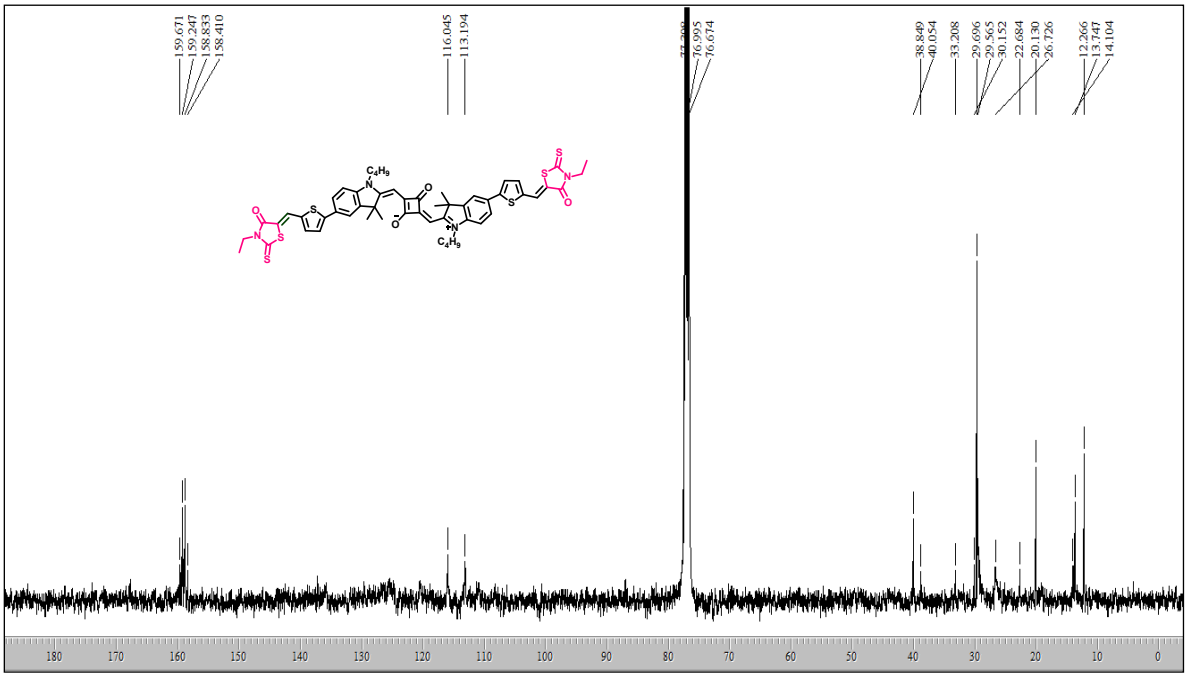


Figure S10. ^{13}C NMR spectra of **SQ-DIEt-RH** in $CDCl_3$.

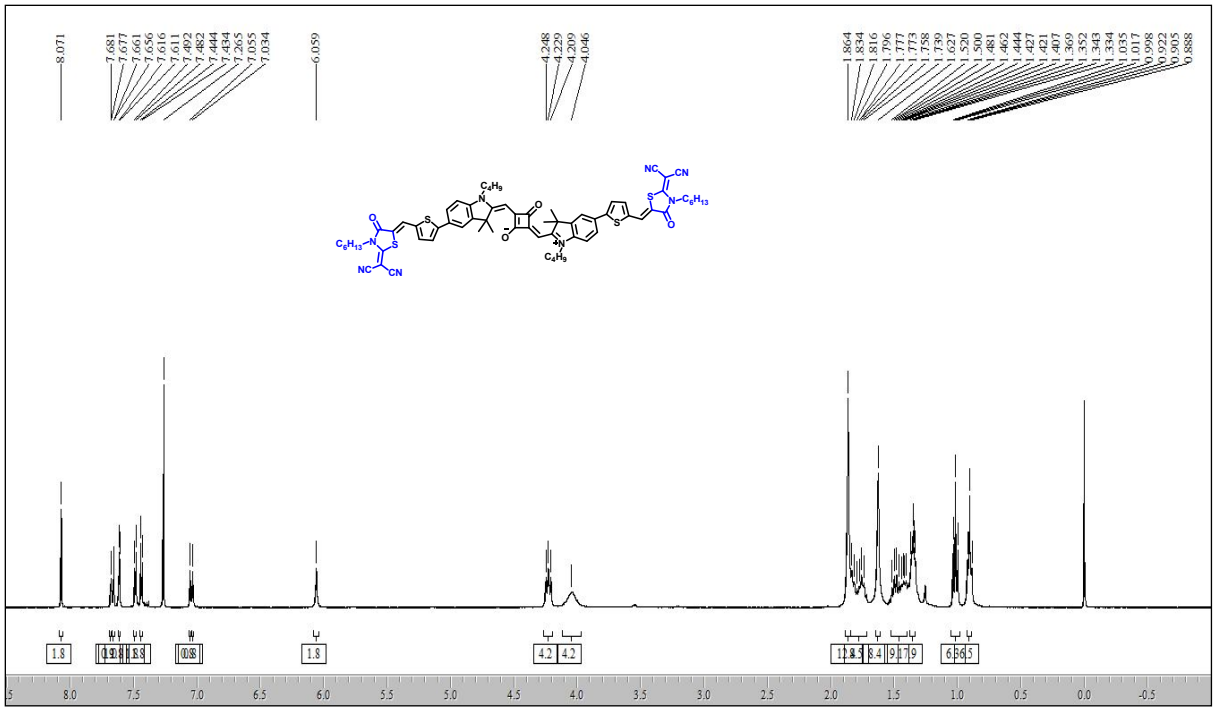


Figure S11. ^{1}H NMR spectra of **SQ-DICN-RH** in $CDCl_3$.

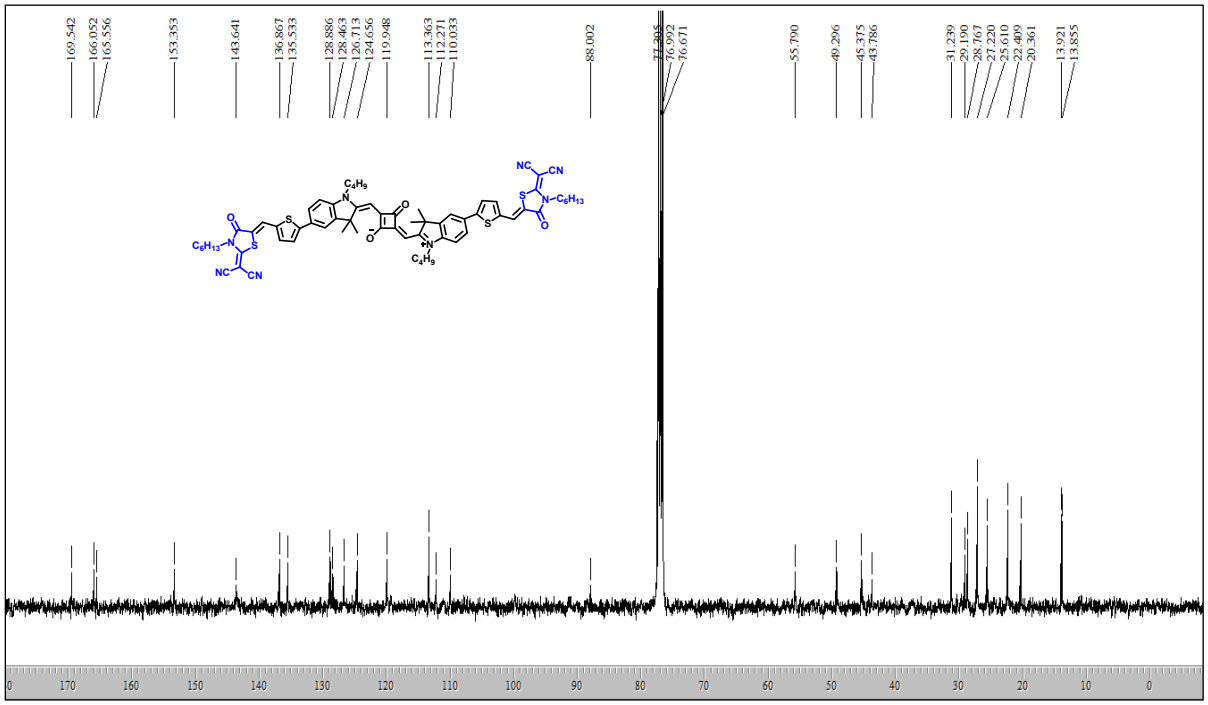


Figure S12. ^{13}C NMR spectra of **SQ-DICN-RH** in $CDCl_3$.

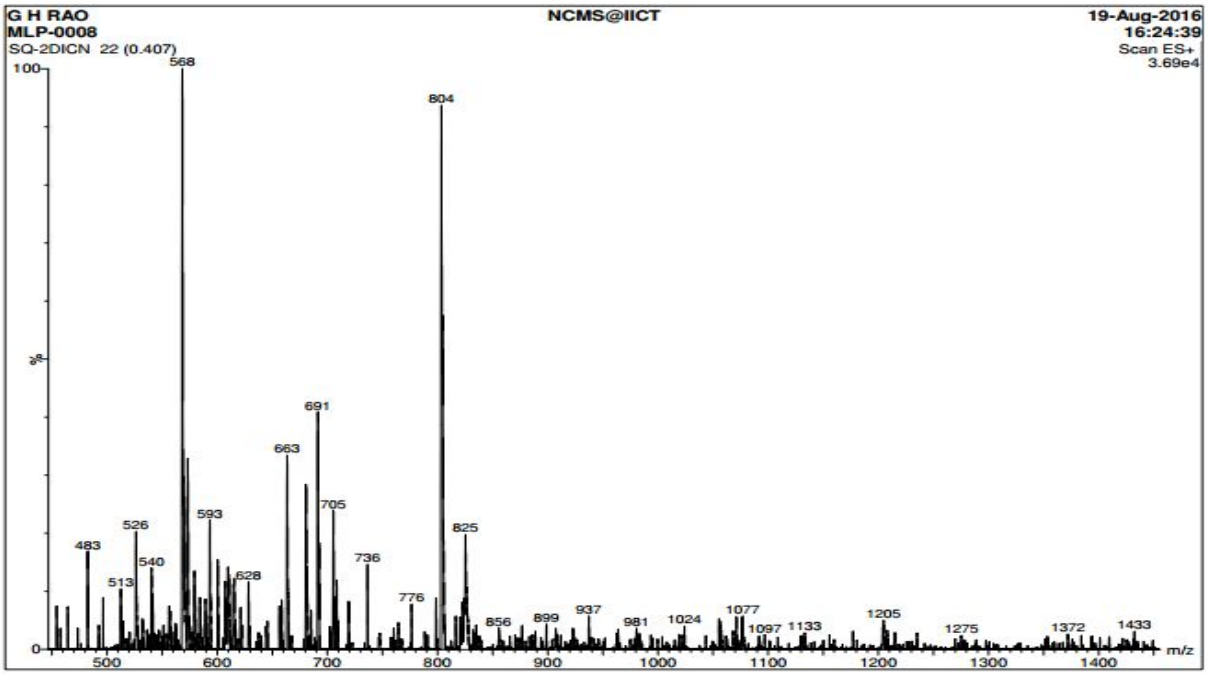


Figure S13. ESI-Mass spectrum of **SQ-DICN**.

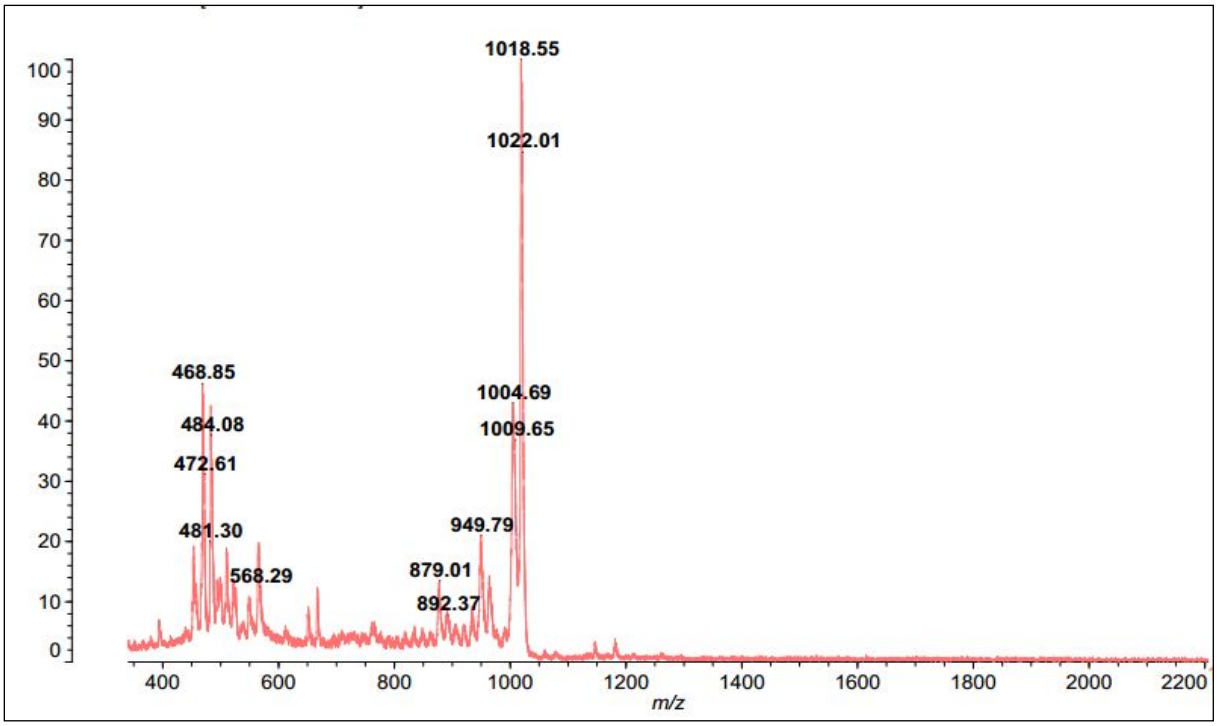


Figure S14. MALDI-TOF of **SQ-DIEt-RH**.

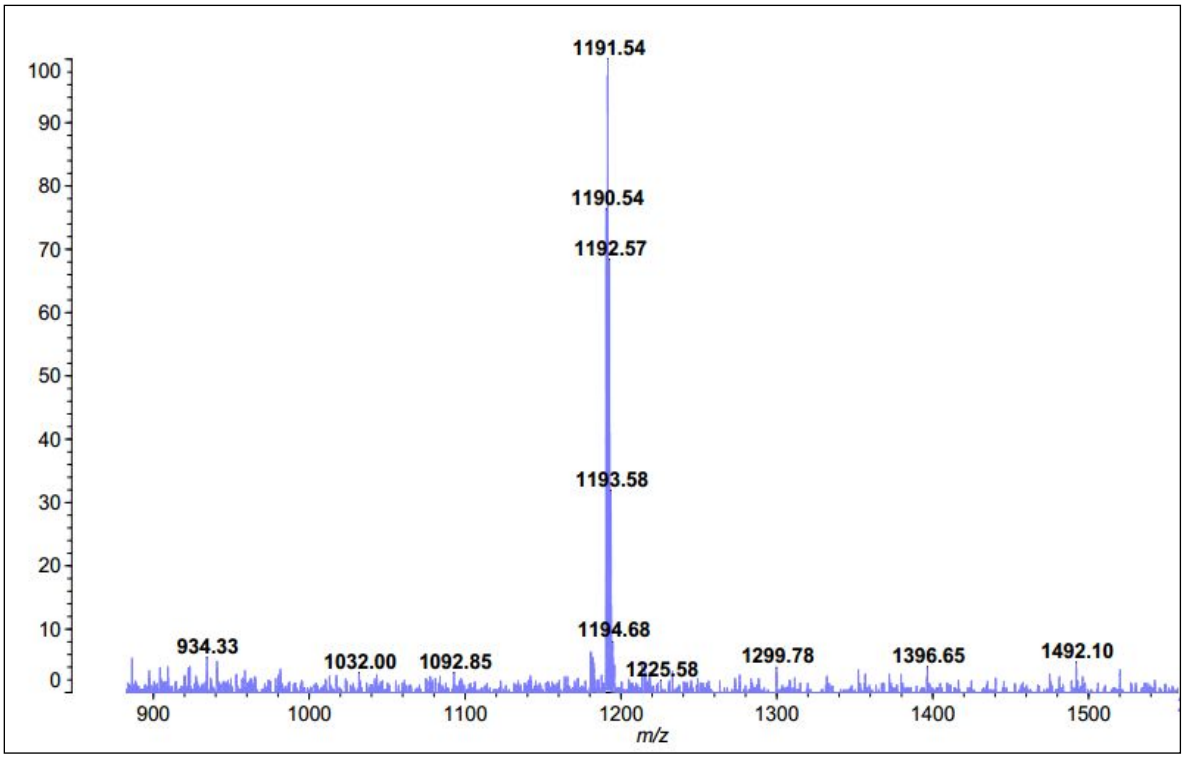


Figure S15. MALDI-TOF of **SQ-DICN-RH**.

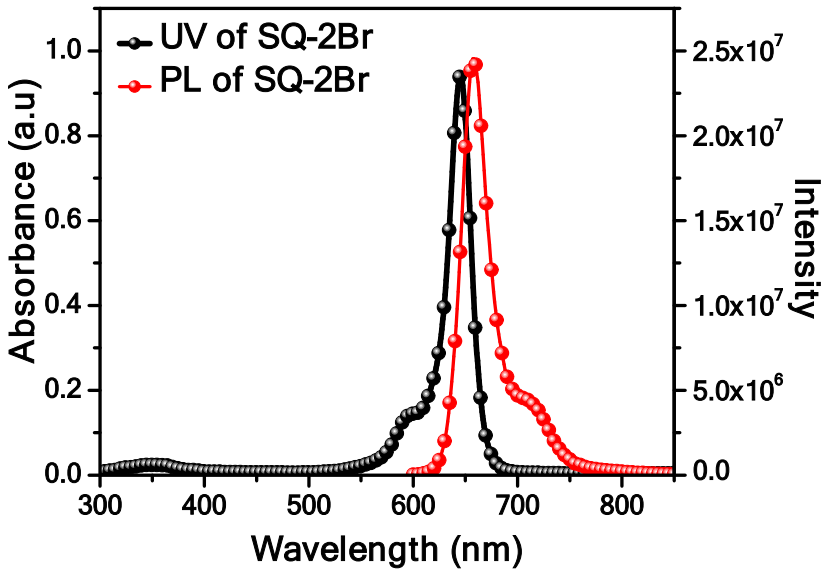


Figure S16. Absorption and photoluminescence of **SQ-2Br**.

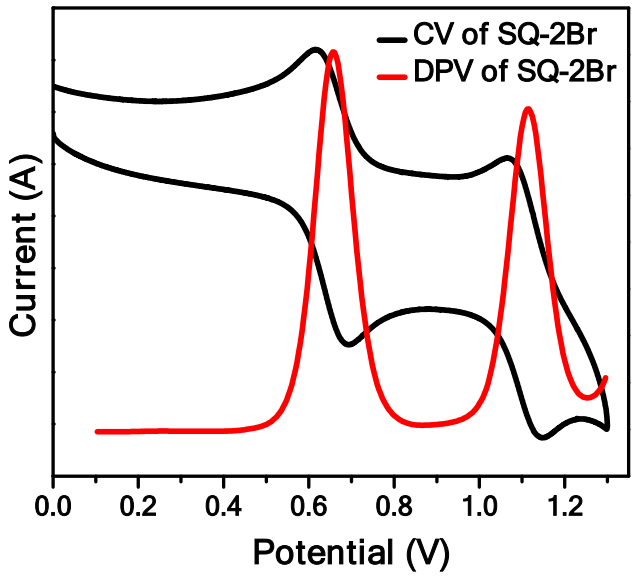
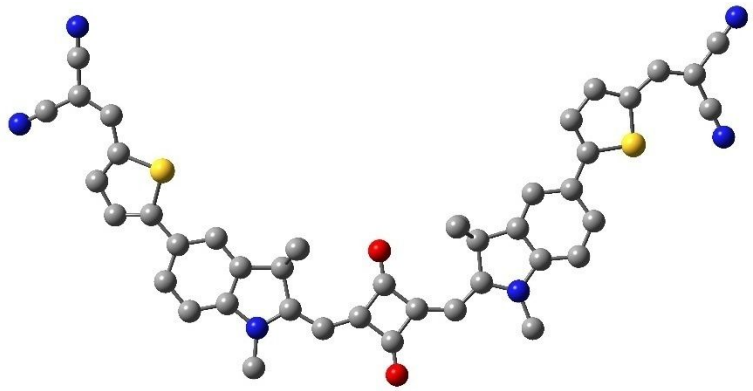
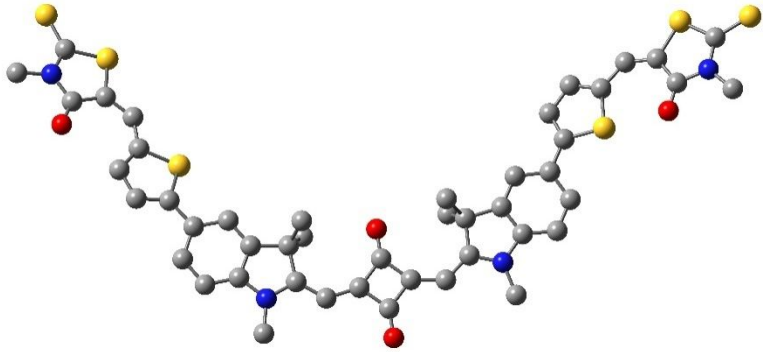


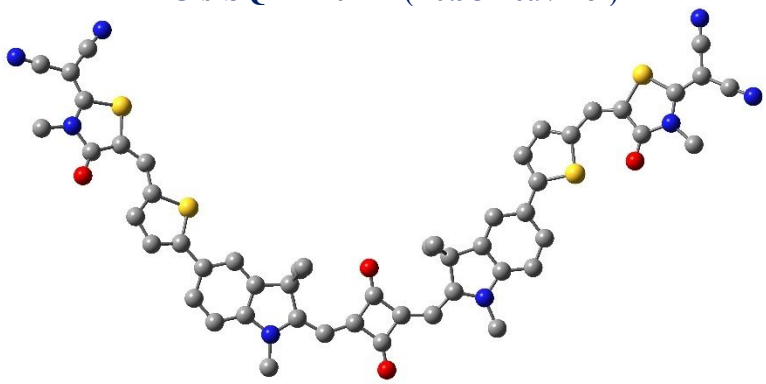
Figure S17. CV and DPV of **SQ-2Br**.



Cis-SQ-DICN(+0.95 kcal/mol)



Cis-SQ-DIEt-RH(+0.93 kcal/mol)



Cis-SQ-DICN-RH(+0.96 kcal/mol)

Figure S18. Ground state optimized structures of the SQ dyes (*cis* isomers) obtained at B3LYP/6-31G(d) level of theory. Hydrogen atoms are omitted for clarity.

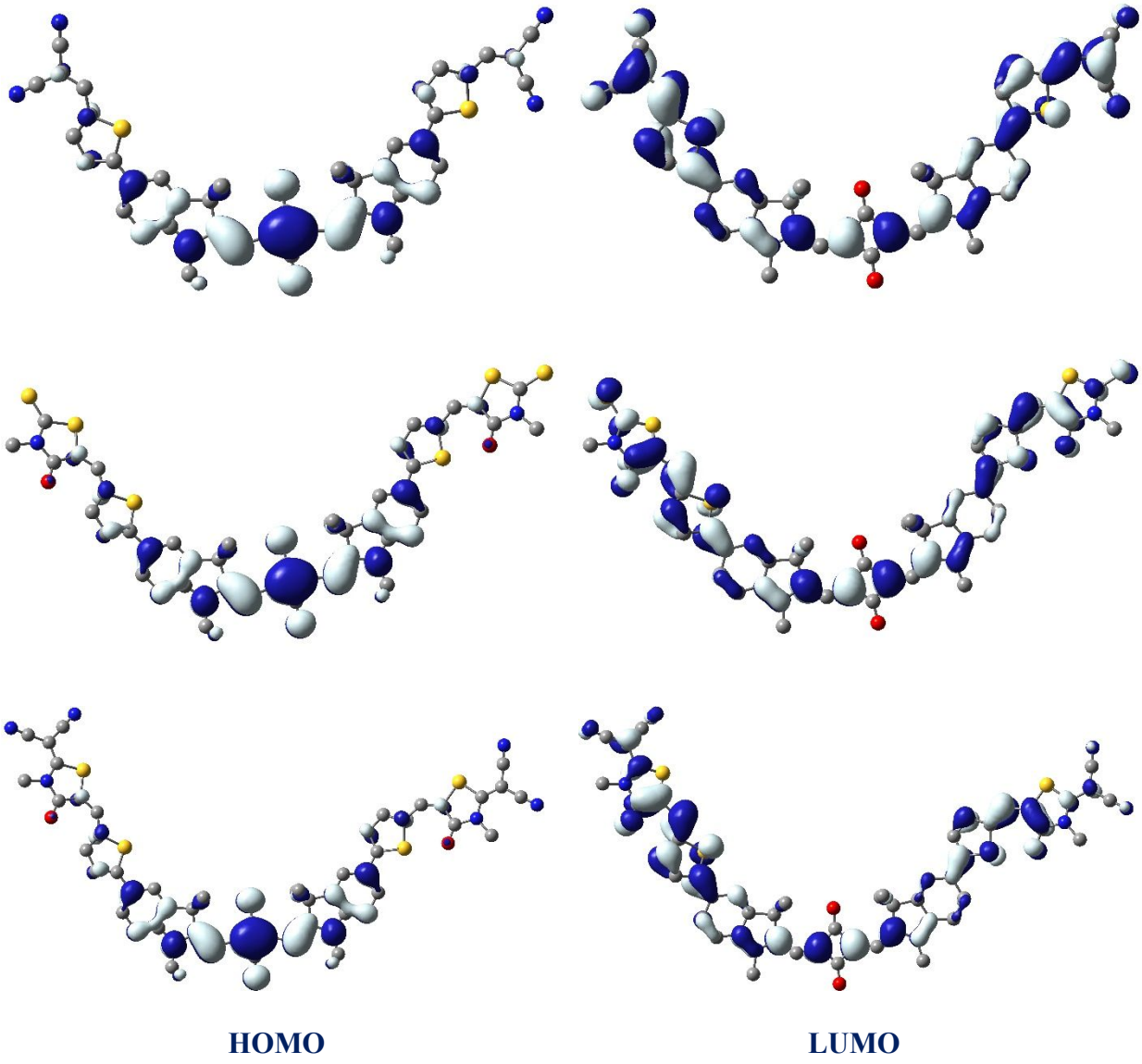


Figure S19. Isodensity plots (isosurface = 0.02 e Å^{-3}) of the frontier molecular orbitals of *cis*-SQ-DICN (top), *cis*-SQ-DIEt-RH (middle), and *cis*-SQ-DICN-RH (bottom).