

Electronic Supplementary Information

Halogen Functionalized D-A-D Type Unsymmetrical Squaraine Dyes for Dye-Sensitized Solar Cells

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General methods. All the chemicals and reagents required for the synthesis of **ISQ** dyes were purchased from commercial sources, and standard procedures are used for drying of solvents. ^1H - and ^{13}C - NMR spectra were recorded on Bruker NMR spectrometers AV 200 MHz, AV 400 MHz and AV-500 MHz frequency, in CDCl_3 . MALDI-TOF-MS was recorded on ABSciex 5800 MALDI TOF mass spectrometer. 4-hydroxy-3-5-dimethoxycinnamic acid (Sinapic acid) has been used for matrix preparation. Bruker FTIR spectrometer has been used to measure the IR-spectrum for **ISQ** dyes. Absorption spectra of **ISQ** dyes were recorded on SPECORD[®] 210/ PLUS, Analytikjena UV–Visible spectrophotometer at room temperature. For the light-harvesting efficiency (LHE) calculations, 6 μm thin film of TiO_2 coated on the transparent glass slide was dipped in 0.1 mM **ISQ** dye solution for 12 h at room temperature, then absorption spectra were recorded on SPECORD[®] 210/ PLUS, Analytikjena UV-visible spectrophotometer at room temperature and converted into light-harvesting efficiency ($\text{LHE} = 1-10^{-A}$). Fluorescence and lifetime of **ISQ** dyes were recorded on Edinburgh spectrofluorometer FS5 at room temperature. Cyclic voltammetry (CV) of **ISQ** dyes were performed on Biologic SP300 potentiostat in anhydrous CH_2Cl_2 solvent at 25 °C under an inert atmosphere, where platinum wire as a working electrode, platinum foil as a counter electrode, non-aqueous Ag/AgNO_3 (0.01M) as reference electrode, TBAClO_4 (0.1 M) as supporting electrolyte and Ferrocene/Ferrocene⁺ as an external reference, scan rate was 50 mVs^{-1} . Potential measured vs Fc/Fc^+ (eV) were converted to NHE (V) by addition of 0.7 V. $E_{0.0}$ optical band gap have been calculated from $1240/\lambda$, where λ is intersection point of absorption and fluorescence spectra of the **ISQ** dyes. Electrochemical impedance measurements (EIS) were performed using a BioLogic SP300 potentiostat equipped with a frequency response analyzer. EIS studies were carried out in dark with various applied potential and frequency ranges from 3 MHz to 10 mHz with sinus amplitude of 10 mV. For I - V characteristics of the cells were measured by using PHOTO EMISSION TECH (PET,

CT200AAA, USA) solar-simulator, and IPCE measurements were carried out with a Newport QE measurement kit. All the quantum mechanical calculations were conducted by using the Gaussian 09 software. The optimization of the ground-state geometry was carried out at the Density Functional Theory (DFT) level, using the B3LYP/6-311G** and B3LYP/LANL2DZ atomic basis sets.

DSSC fabrication. Fluorine-doped SnO₂ glass (8- 10 Ω /sq; Pilkington TEC 7) was washed with mucasol (2 % in water), de-ionized water, and isopropanol by using ultrasonic-bath to make cleaned. To grow a thin film TiO₂, FTO was treated with 40 mM aqueous TiCl₄ solution at 70 °C for 30 min, washed with the de-ionized water then EtOH, and dried at 110 °C for 10 min. A paste of TiO₂ nanocrystal (< 20 nm, Ti-Nanoxide T/SP, Solaronix) was coated on FTO conducting side by using doctor-blade technique and kept for 15 min in the air then heated at 120 °C in the air for 20 min, then coated with scattering layer TiO₂ paste (WER2-O, Dyesol) and heated at 120 °C for 10 min in the air, then sintered at 325 °C for 10 min, 375 °C for 10 min, 450 °C for 10 min and 500 °C for 15 min where the heating rate was 5 °C per min in the air. After completion of sintering, films were treated with 40 mM aqueous TiCl₄ solution at 70 °C for 30 min, washed with the de-ionized water then with EtOH and sintered at 500 °C for 20 min. Then cells (area of TiO₂ is 0.23 cm²) were immersed in 0.1 mM of **ISQ** dyes solution for 12 h. Platinum foil used as a cathode, 25 μm spacer, iodolyte Z-50 and Z-150 (Solaronix) were used as electrolytes, and area of black mask was 0.36 cm². The device performance of **ISQ** dyes were measured under standard simulator condition (AM 1.5 G, 100 mW/cm²).

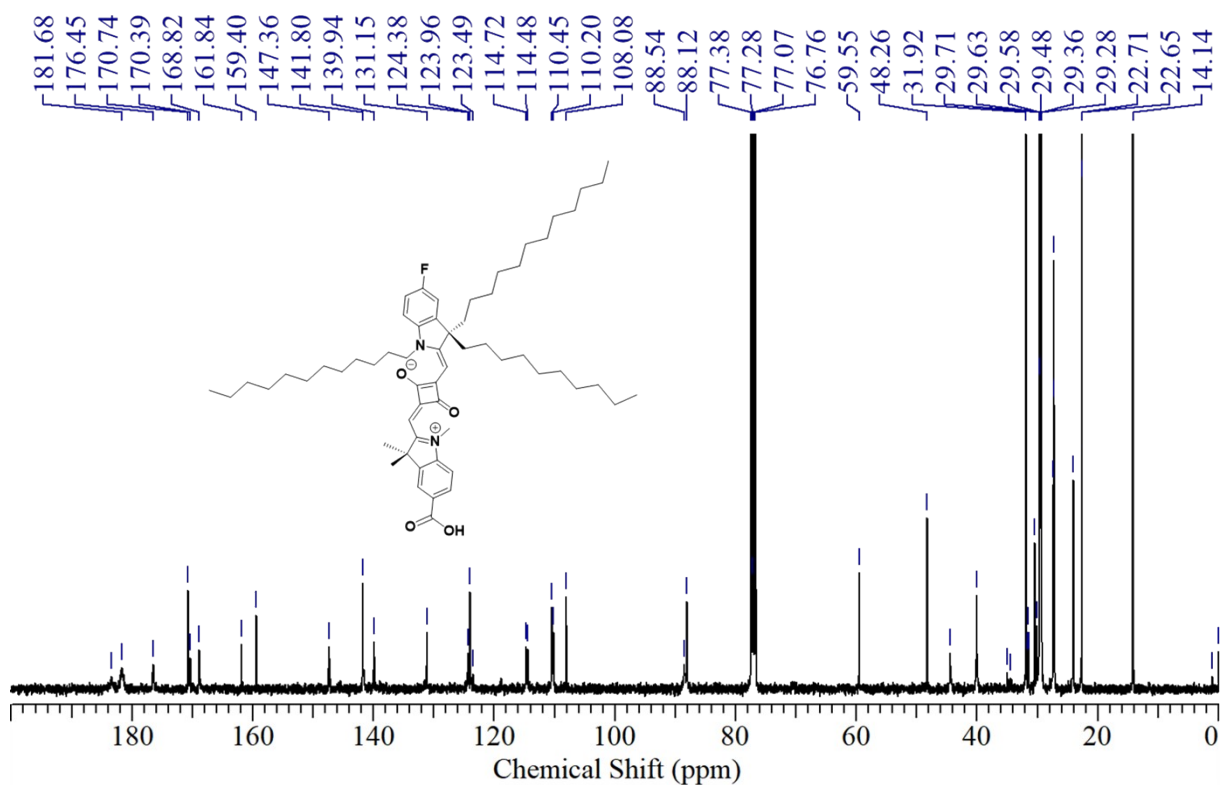
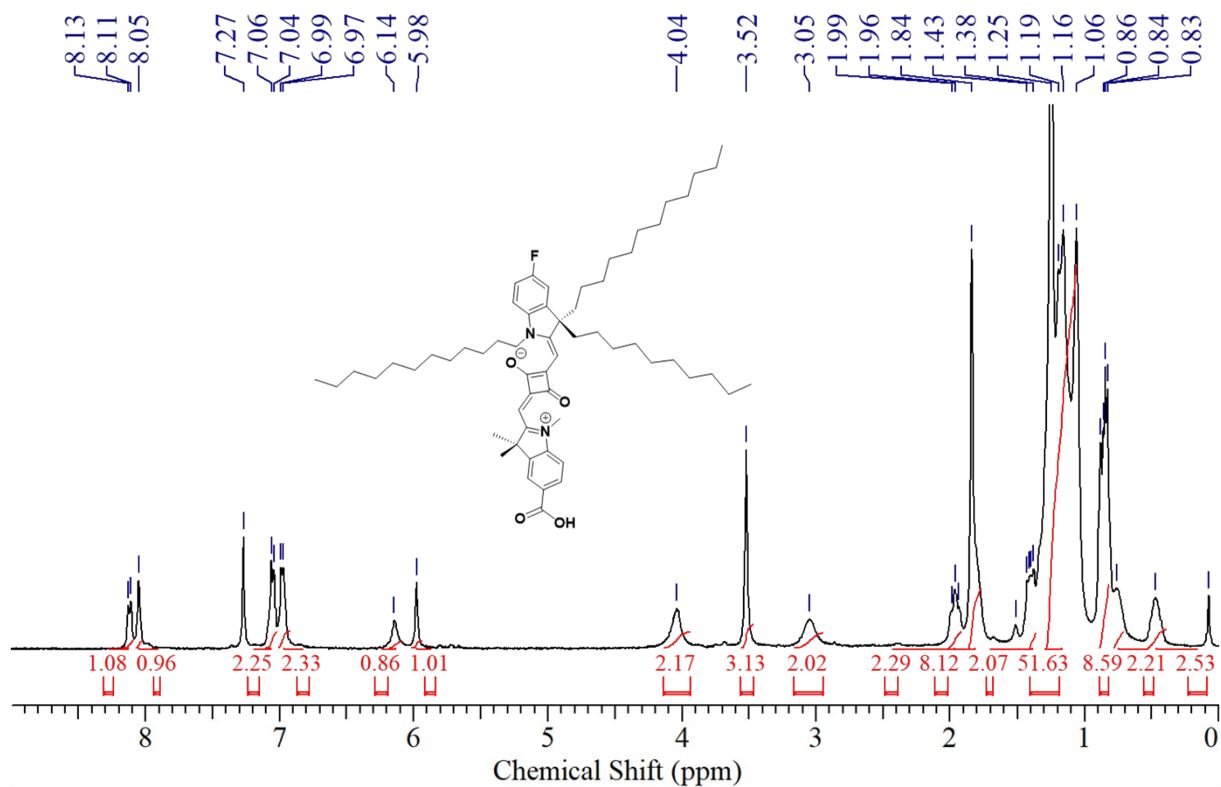


Figure S1. ¹H-NMR and ¹³C NMR spectra of ISQF dye in CDCl₃.

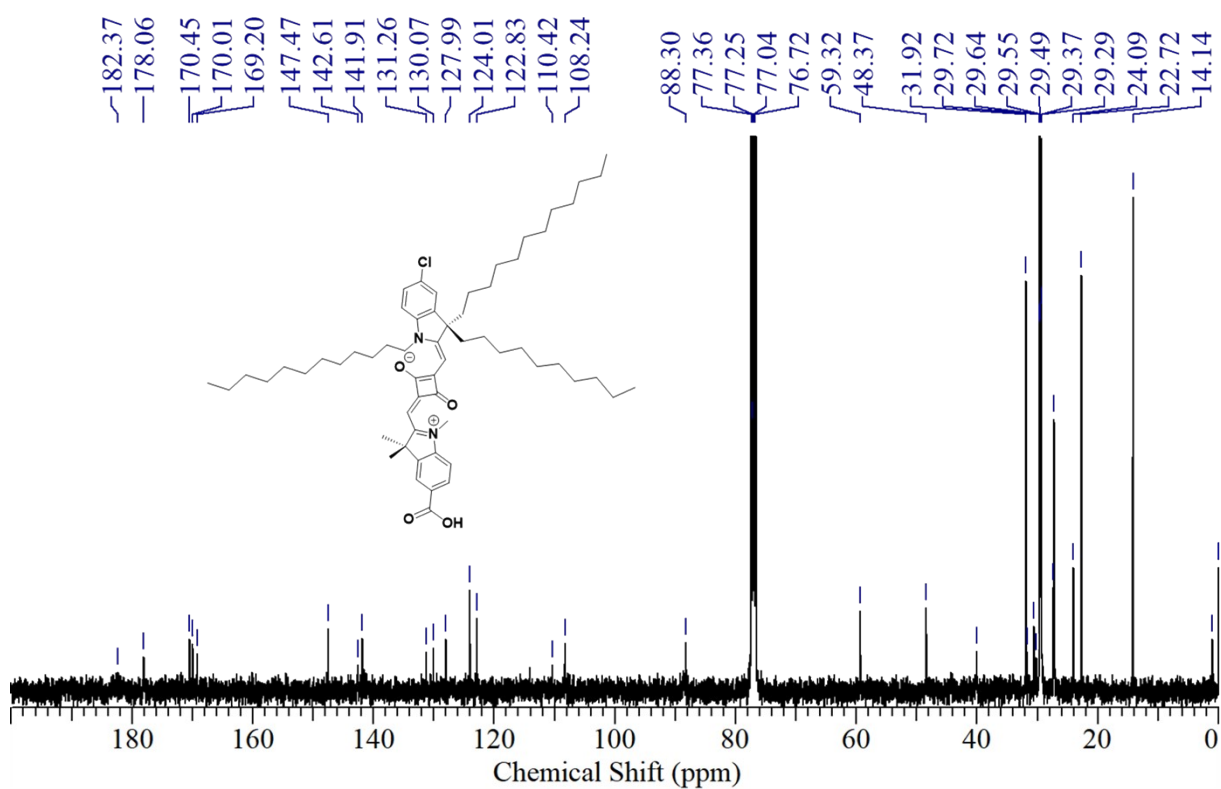
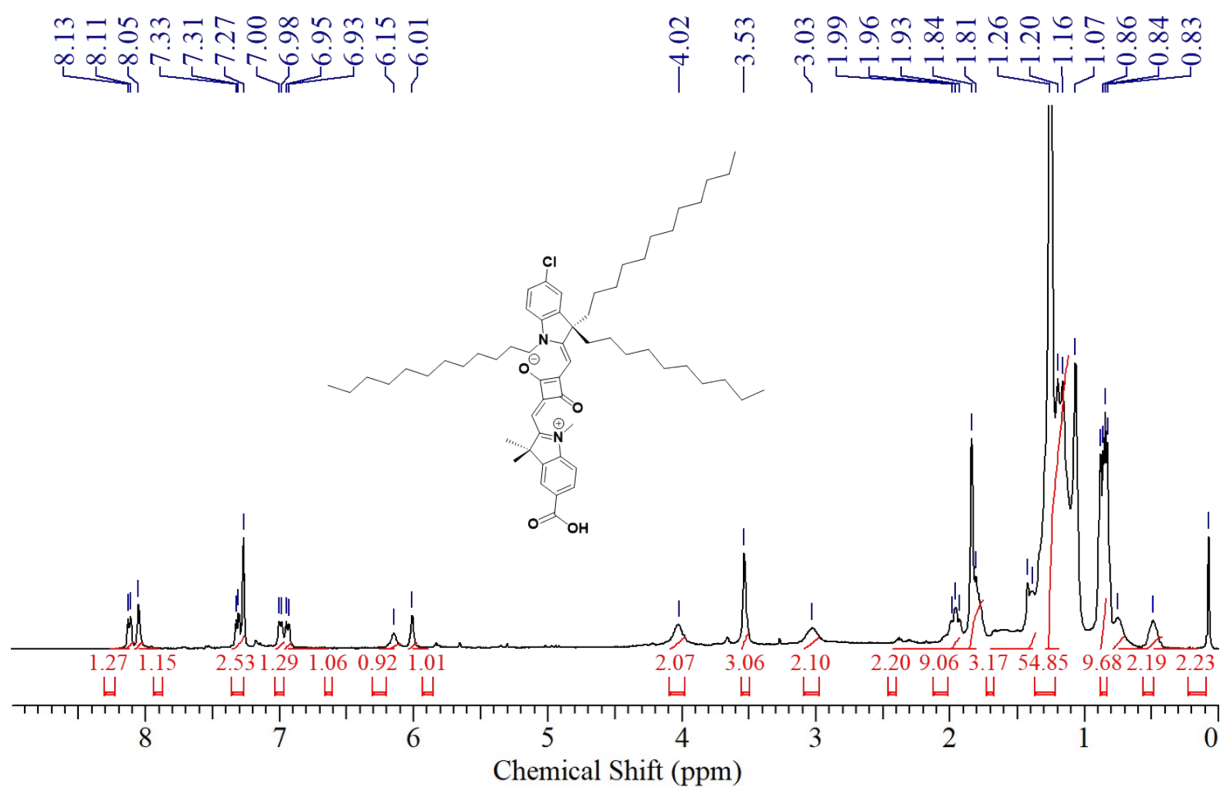


Figure S2. ^1H -NMR and ^{13}C NMR spectra of ISQCl dye in CDCl_3 .

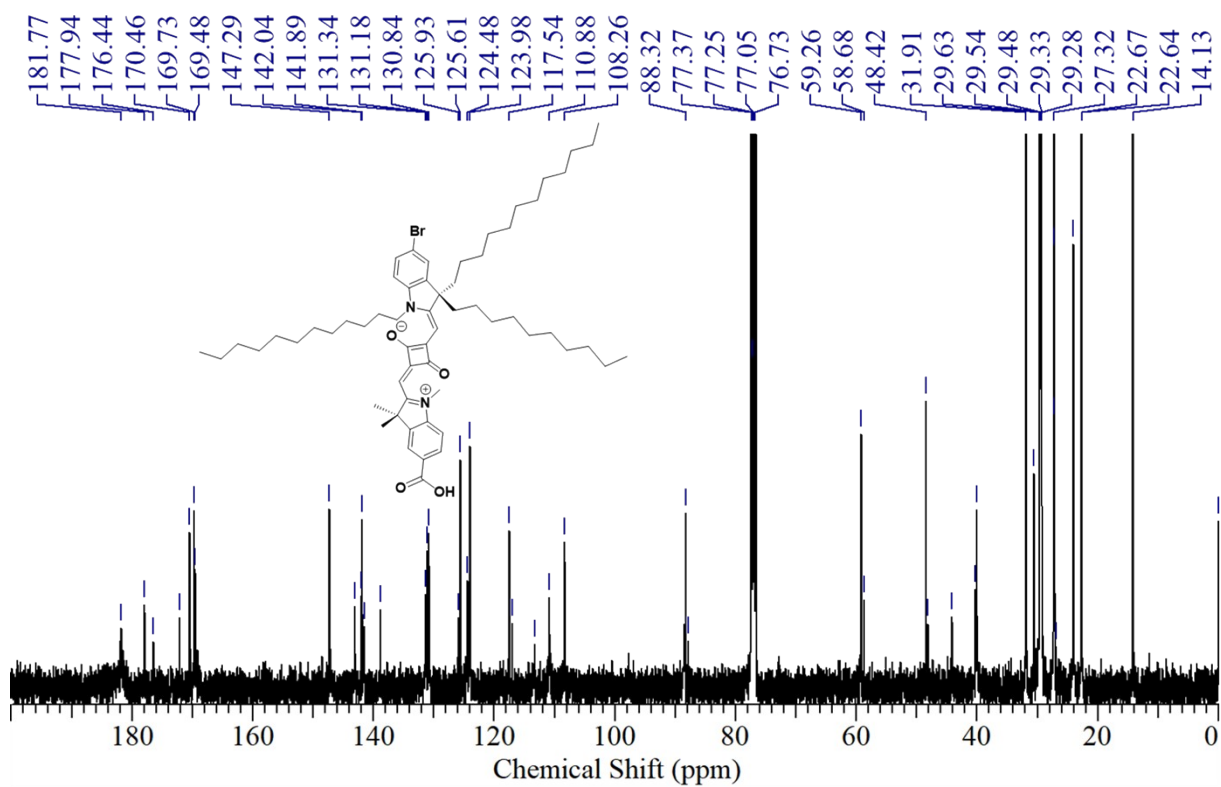
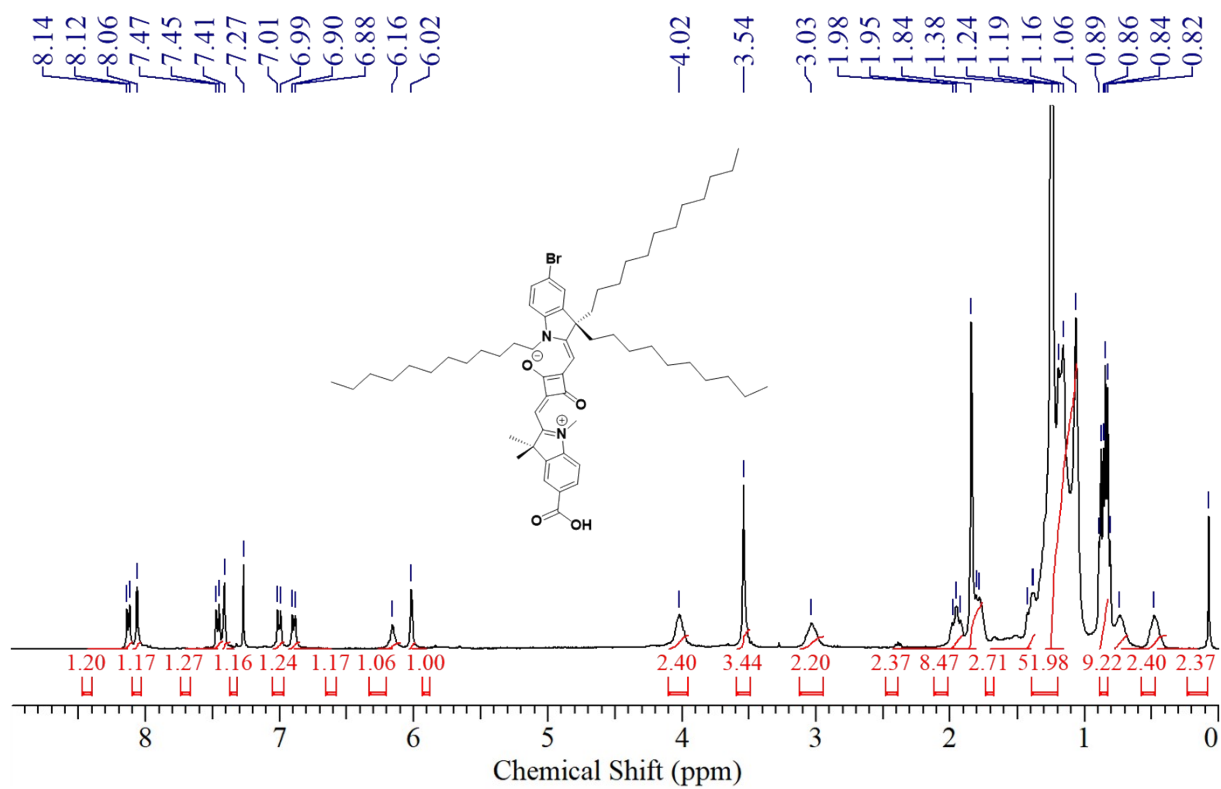


Figure S3. ¹H-NMR and ¹³C NMR spectra of ISQBr dye in CDCl₃.

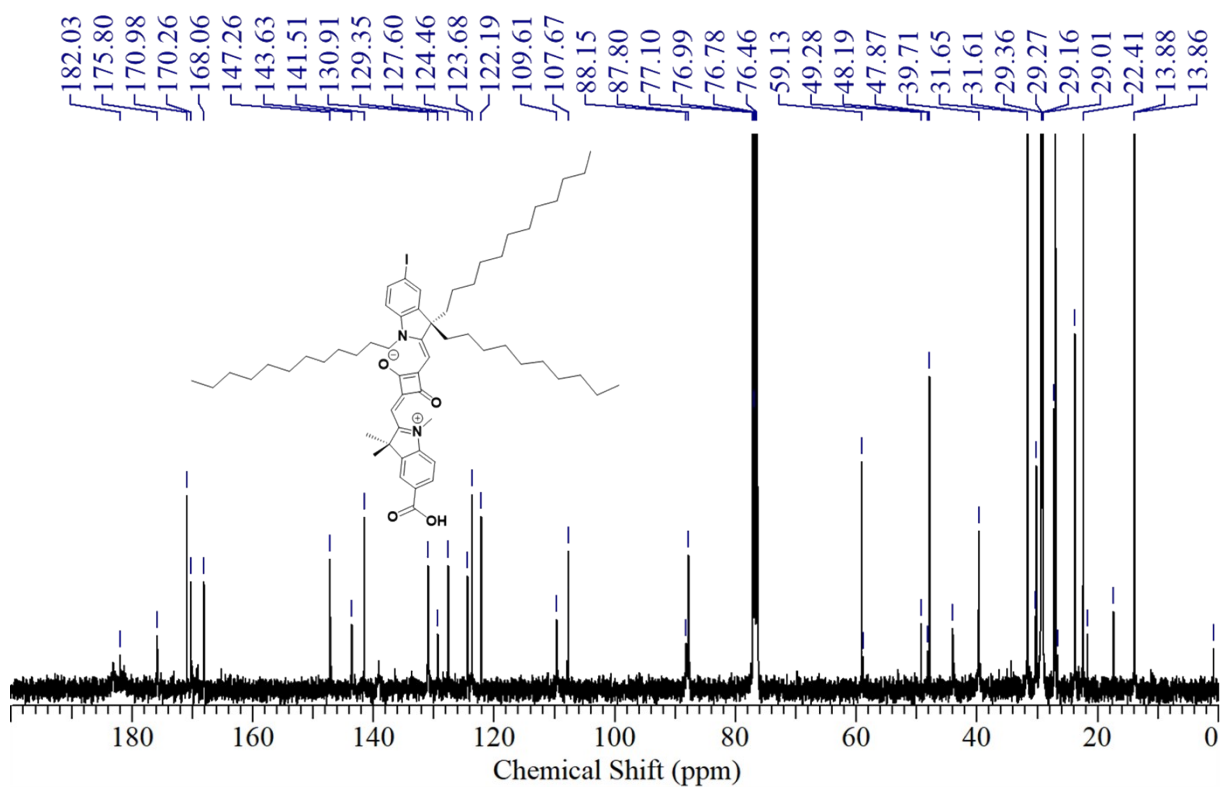
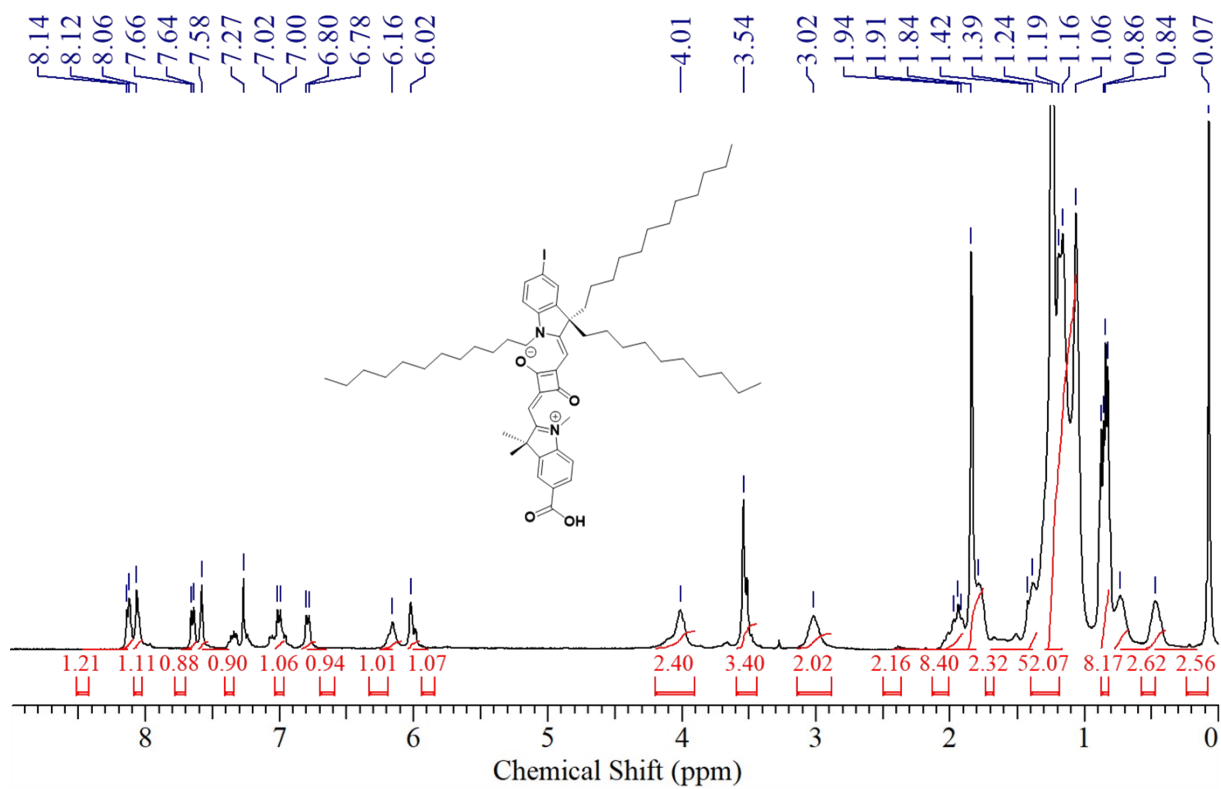


Figure S4. $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectra of ISQI dye in CDCl_3 .

^1H NMR Spectra of the final dye molecules showed two singlet peaks for the vinylene protons between 5.98-6.16 ppm which is the indication of unsymmetrical nature of squaraine dyes. Further, the IR-spectra for ISQF, ISQCl, ISQBr, and ISQI dyes were given in **figure S5**. The stretching frequency for carboxylic acid group appeared at 1699 cm^{-1} and squaric acid carbonyl peaks were appeared at 1598 cm^{-1} , 1567 cm^{-1} with the difference of few wave numbers for all the dyes.

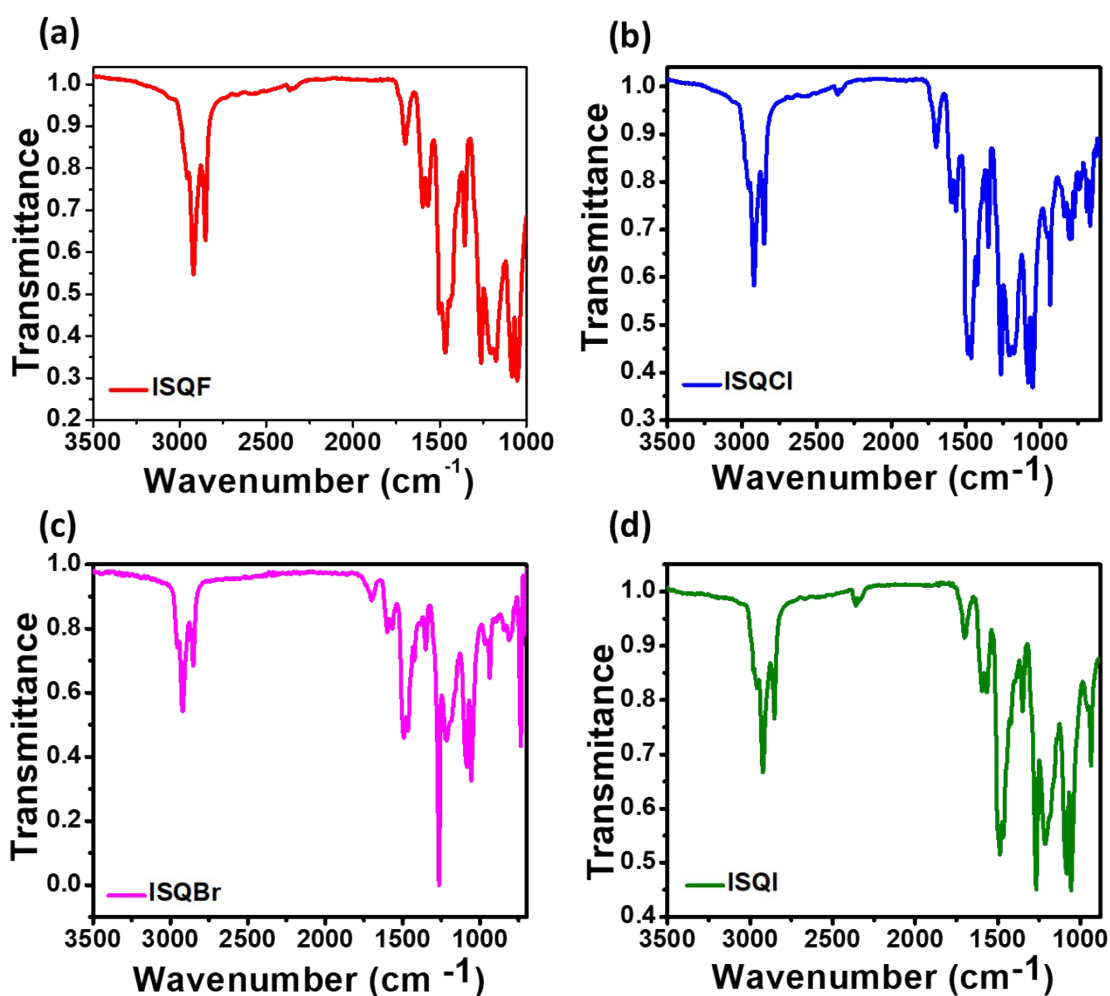


Figure S5. IR spectra of ISQ dyes.

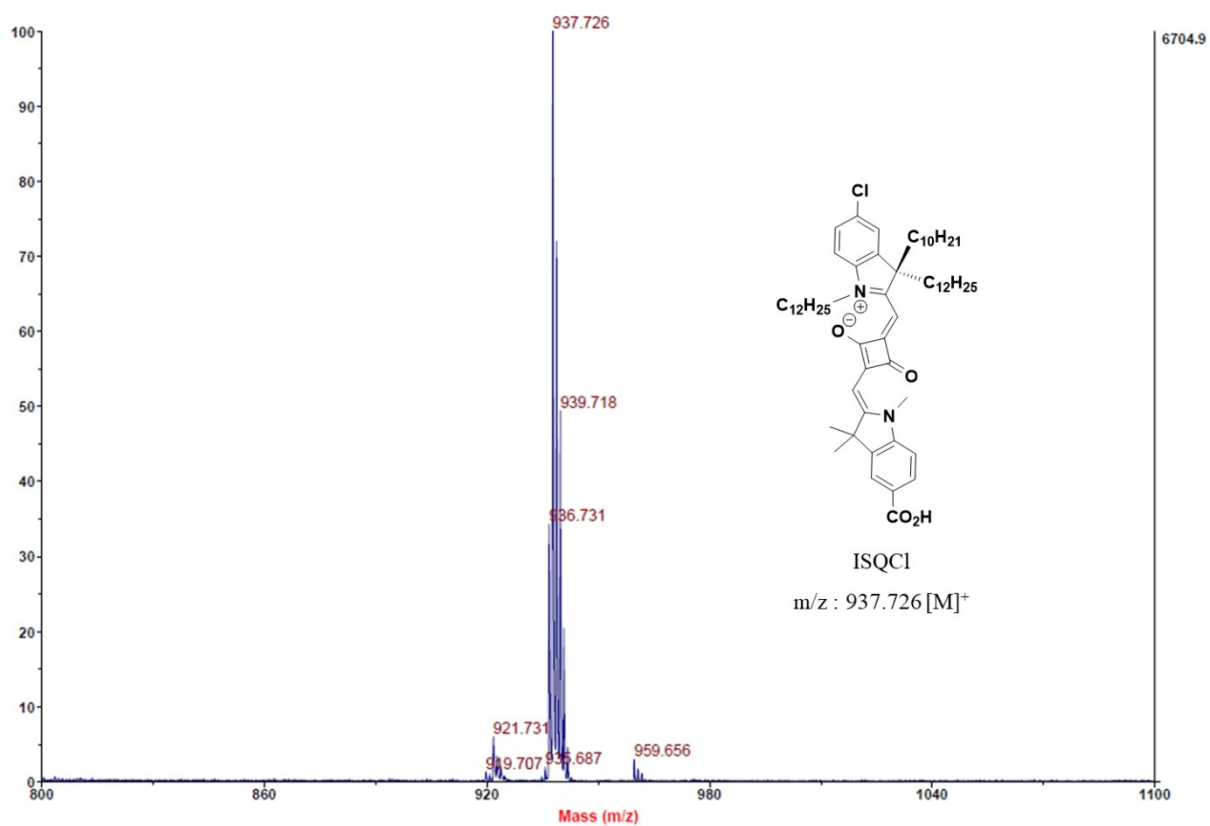
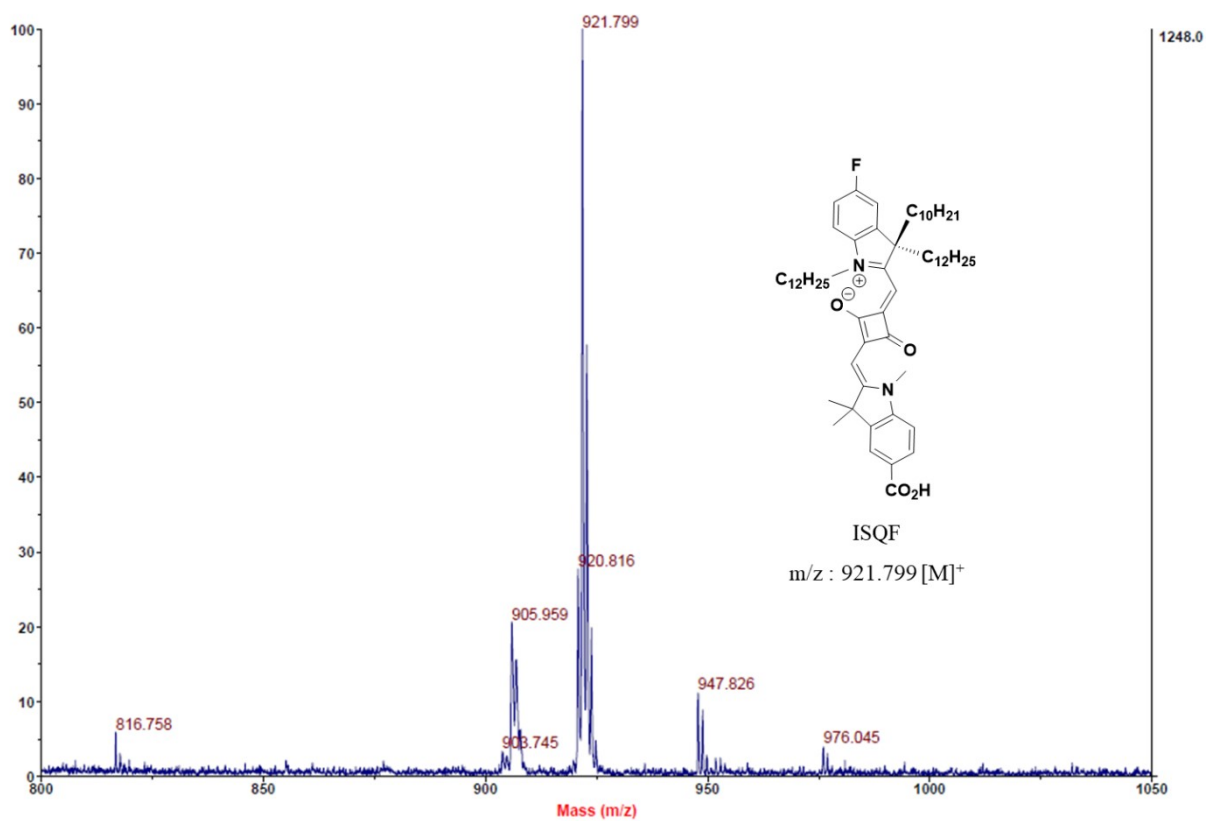


Figure S6. MALDI-TOF-MS spectra of ISQF and ISQCl dyes.

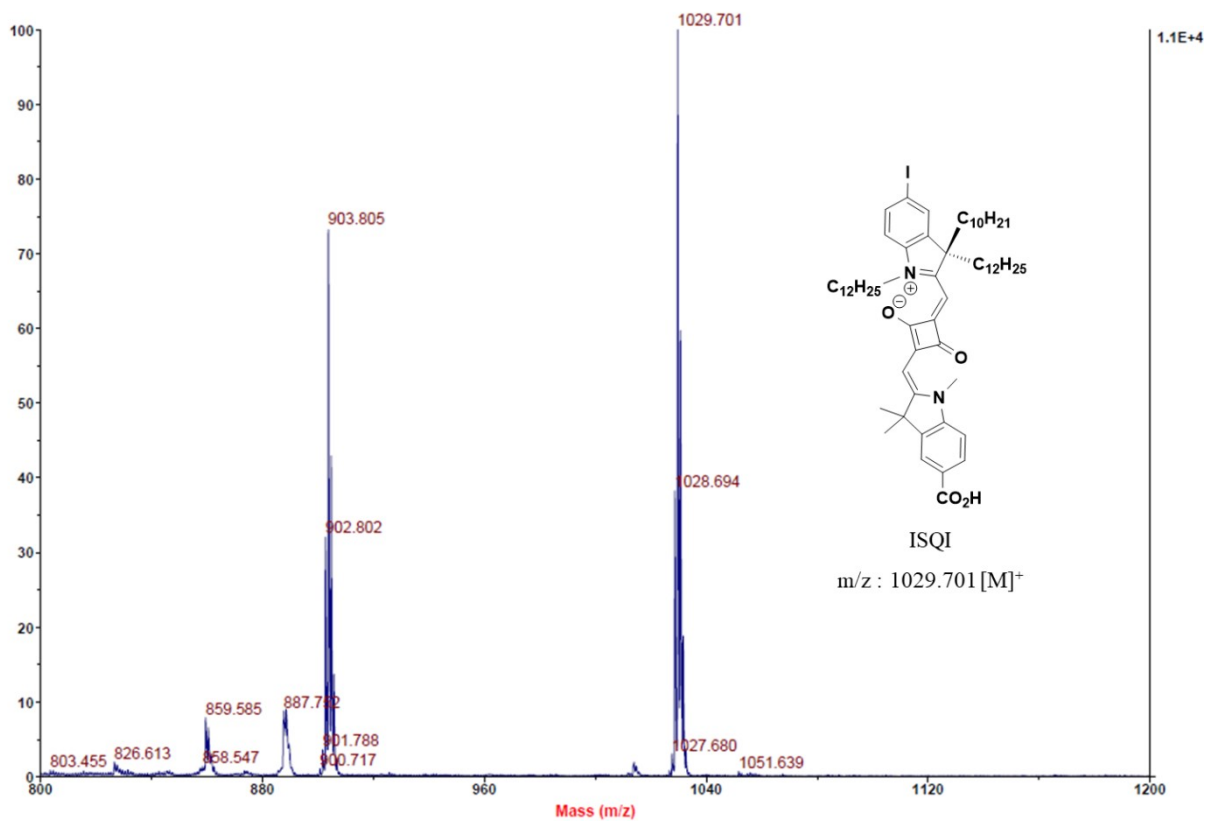
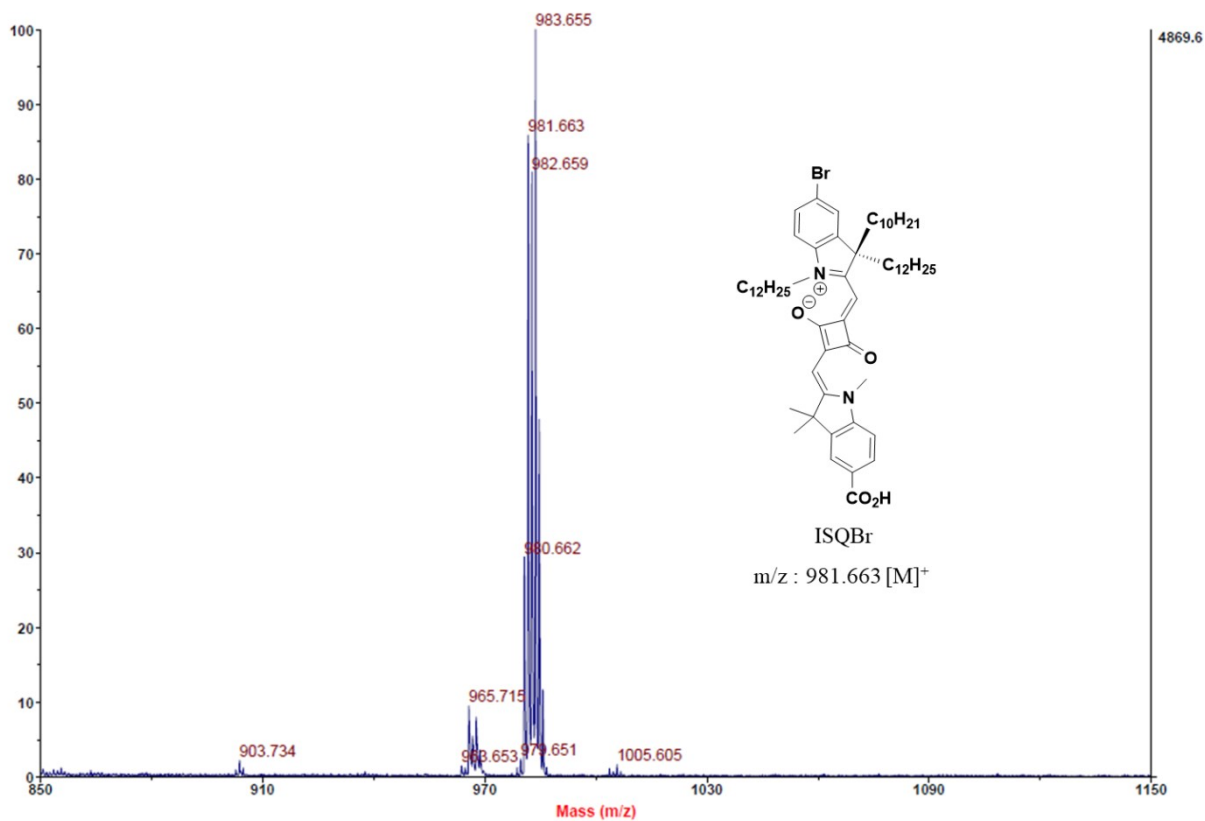


Figure S7. MALDI-TOF-MS spectra of ISQBr and ISQI dyes.

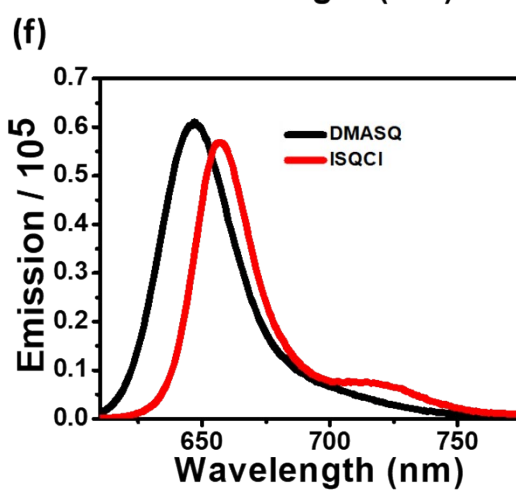
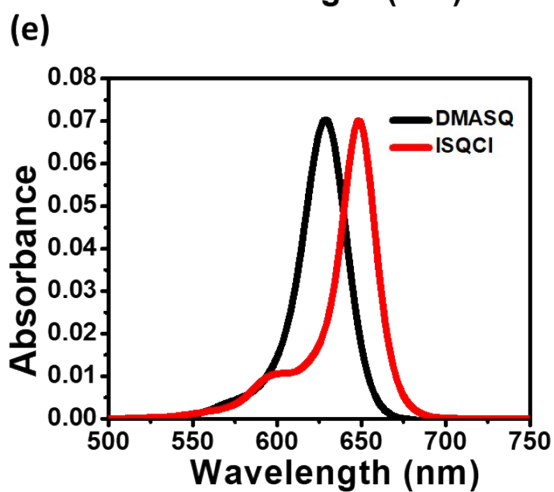
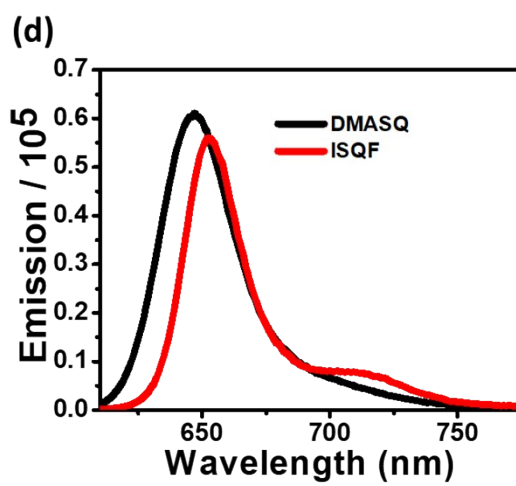
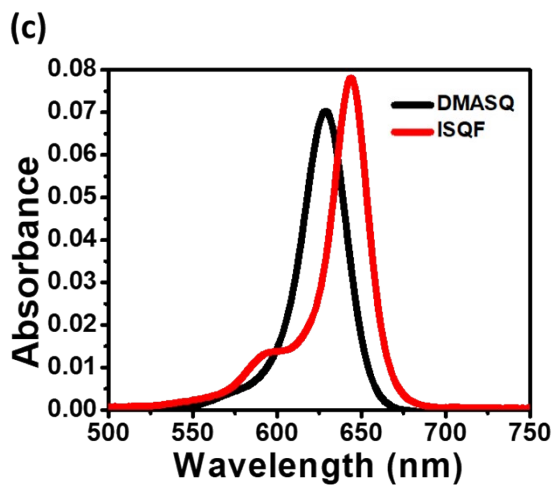
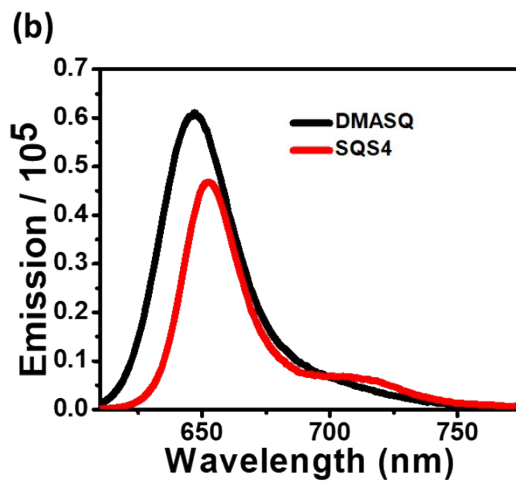
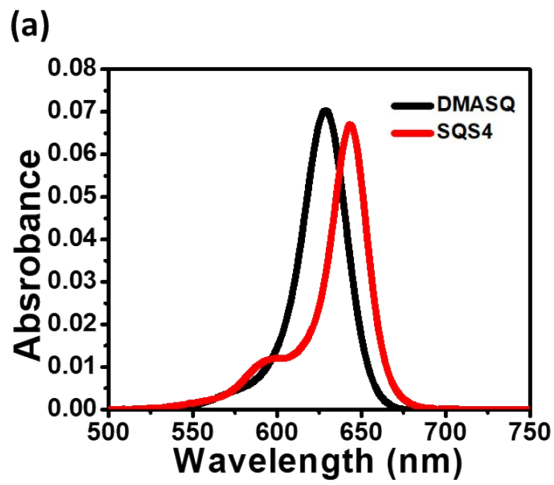
Fluorescence quantum yield of ISQ dyes. Fluorescence quantum yield is calculated relative method, according to the formula.

$$\phi_u = \frac{A_s \times F_u \times n_u^2}{A_u \times F_s \times n_s^2} \times \phi_s$$

Where ϕ_s and ϕ_u is quantum yield of the unknown sample and of the reference compound, A_s and A_u are the absorbance of the standard and unknown sample respectively, F_s and F_u are the integrated area under the fluorescence curve of the standard and the sample respectively, n_s^2 and n_u^2 are the refractive indexes of the solvent in which the reference and the unknown sample is dissolved respectively. **DMASQ**¹ was used as a reference dye which has quantum yield $\phi_s = 0.42$ in dichloromethane. $F_s = 256719$ for standard dye, and emission recorded from 610 to 800 nm.

Table S1. Fluorescence quantum yield of **ISQ** dyes.

Dyes	$\lambda_{ex}(nm)$	A_s	A_u	$A_{s/u}$	F_u	$F_{u/s}$	ϕ_u	Reference dye ¹ DMASQ
SQS4	596	0.0114	0.0118	0.96	176656	0.68	0.279	$F_s = 256719,$ $\phi_s = 0.42$ $\lambda_{em} = 610 - 800 \text{ nm}$ Solvent = CH_2Cl_2
ISQF	599	0.0137	0.0138	0.99	210790	0.82	0.342	
ISQCl	593	0.0095	0.0096	0.98	215960	0.84	0.349	
ISQBr	593	0.0095	0.0096	0.98	201371	0.78	0.325	
ISQI	590	0.0081	0.0076	1.0	179255	0.69	0.312	



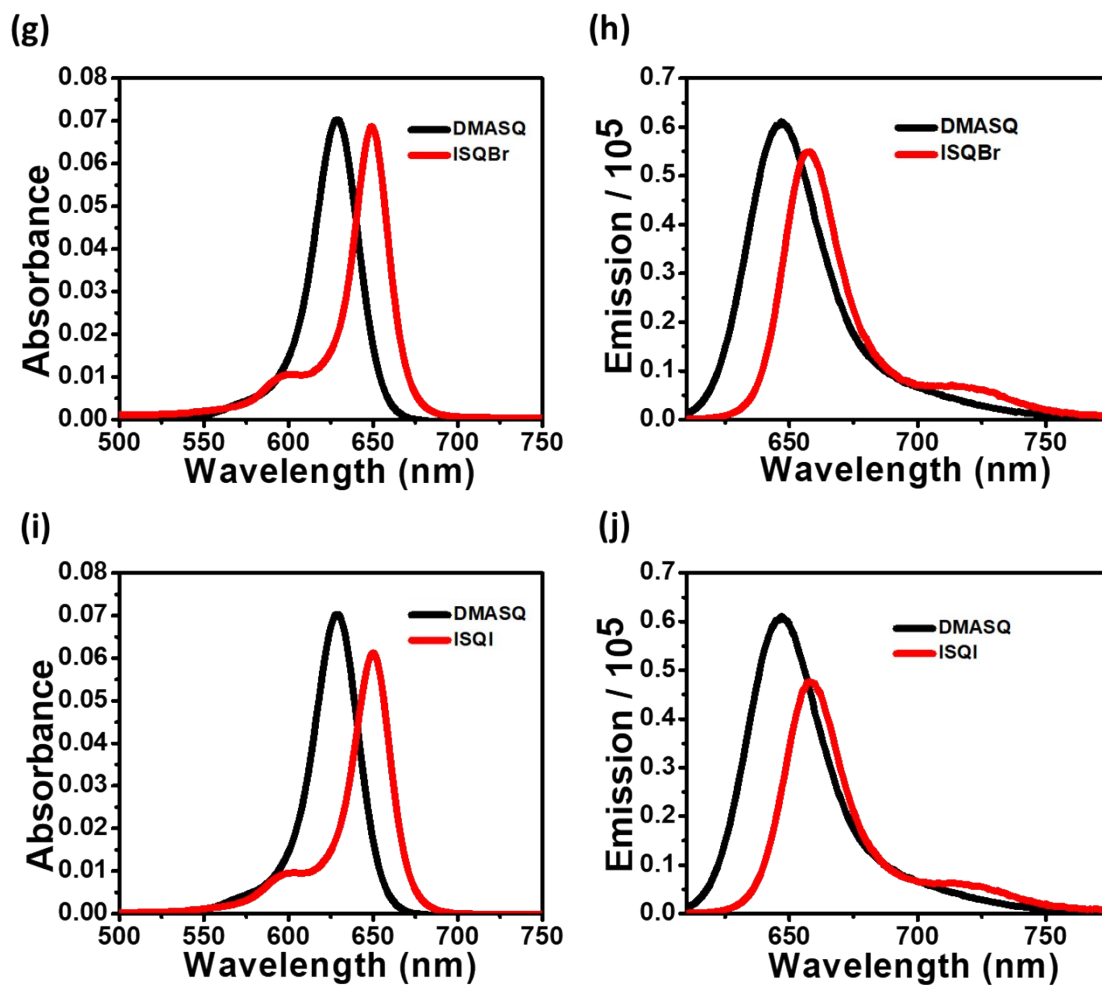
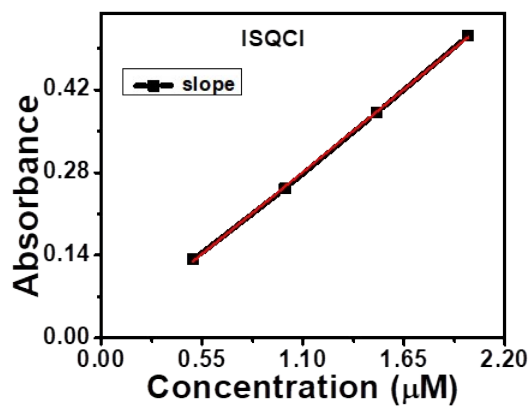
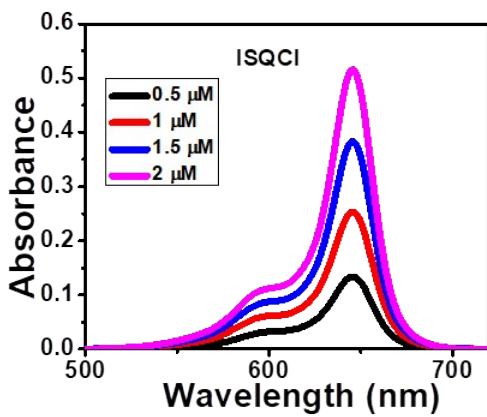
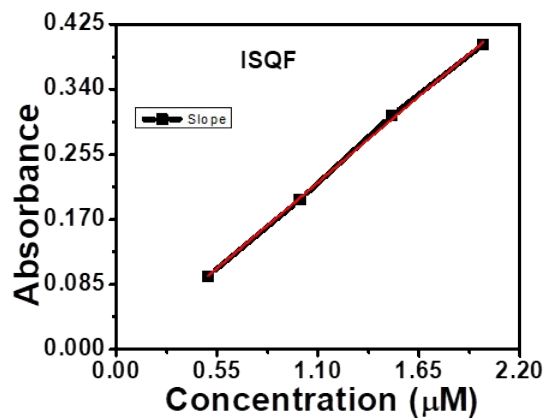
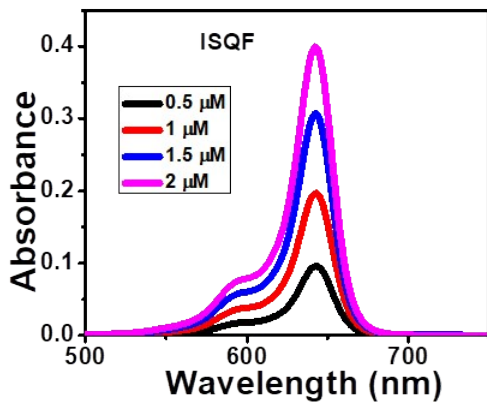
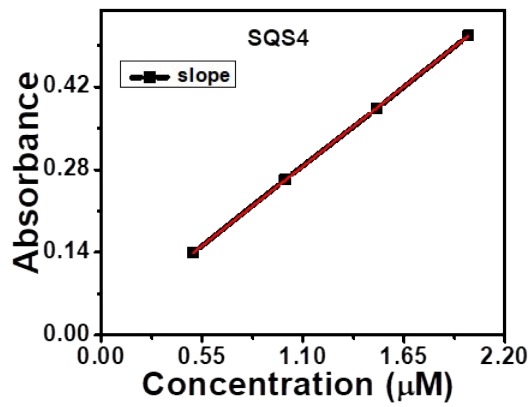
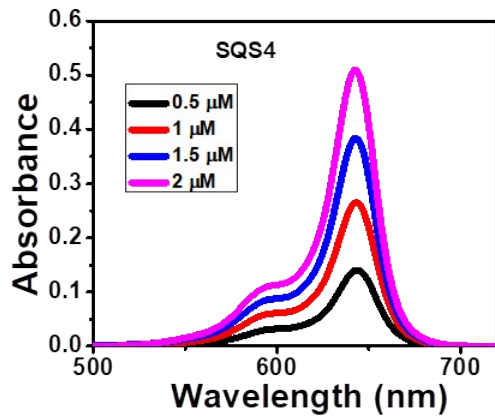


Figure S8. Absorption and Emission spectra (a - j) of ISQ dye in dichloromethane solution.



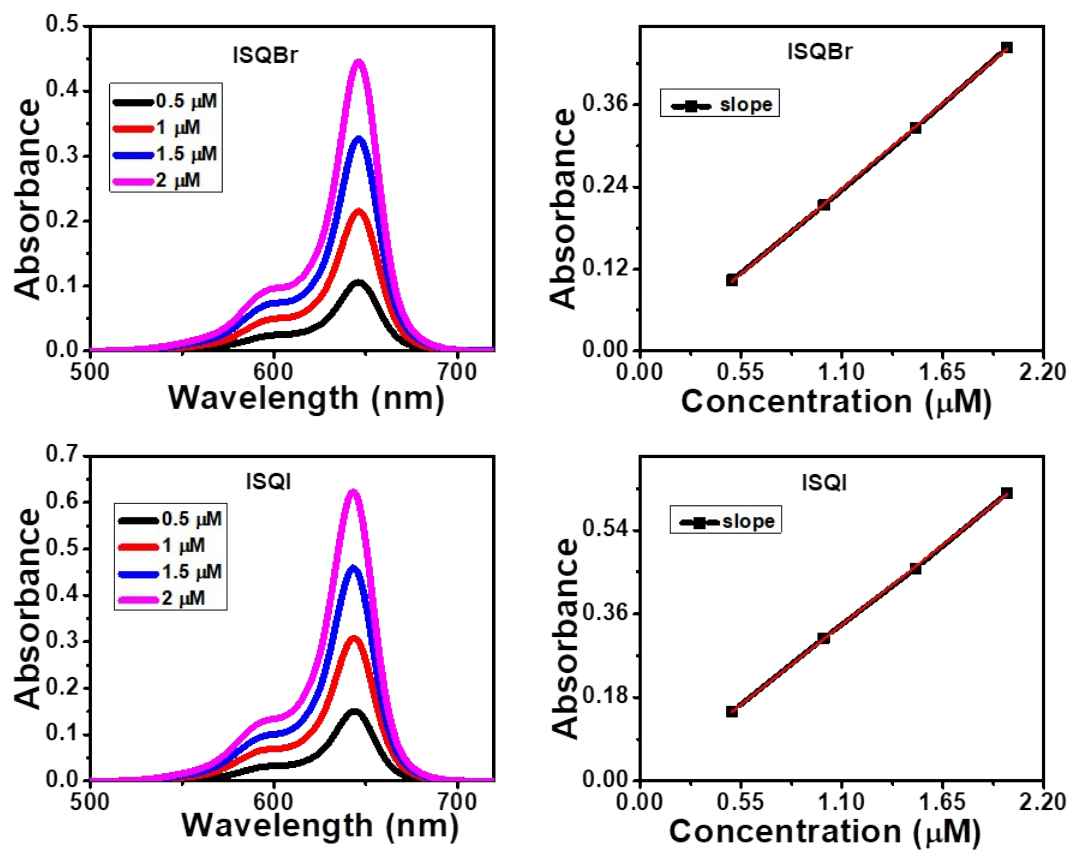


Figure S9. UV-Vis absorption spectra dyes at various concentrations (left), Beer-Lambert plots (right) of **ISQ** and **SQS4** dyes in $\text{CH}_3\text{CN}:\text{CHCl}_3$ (95% : 5%) solution (used quartz cuvette of 1.0 cm path length)

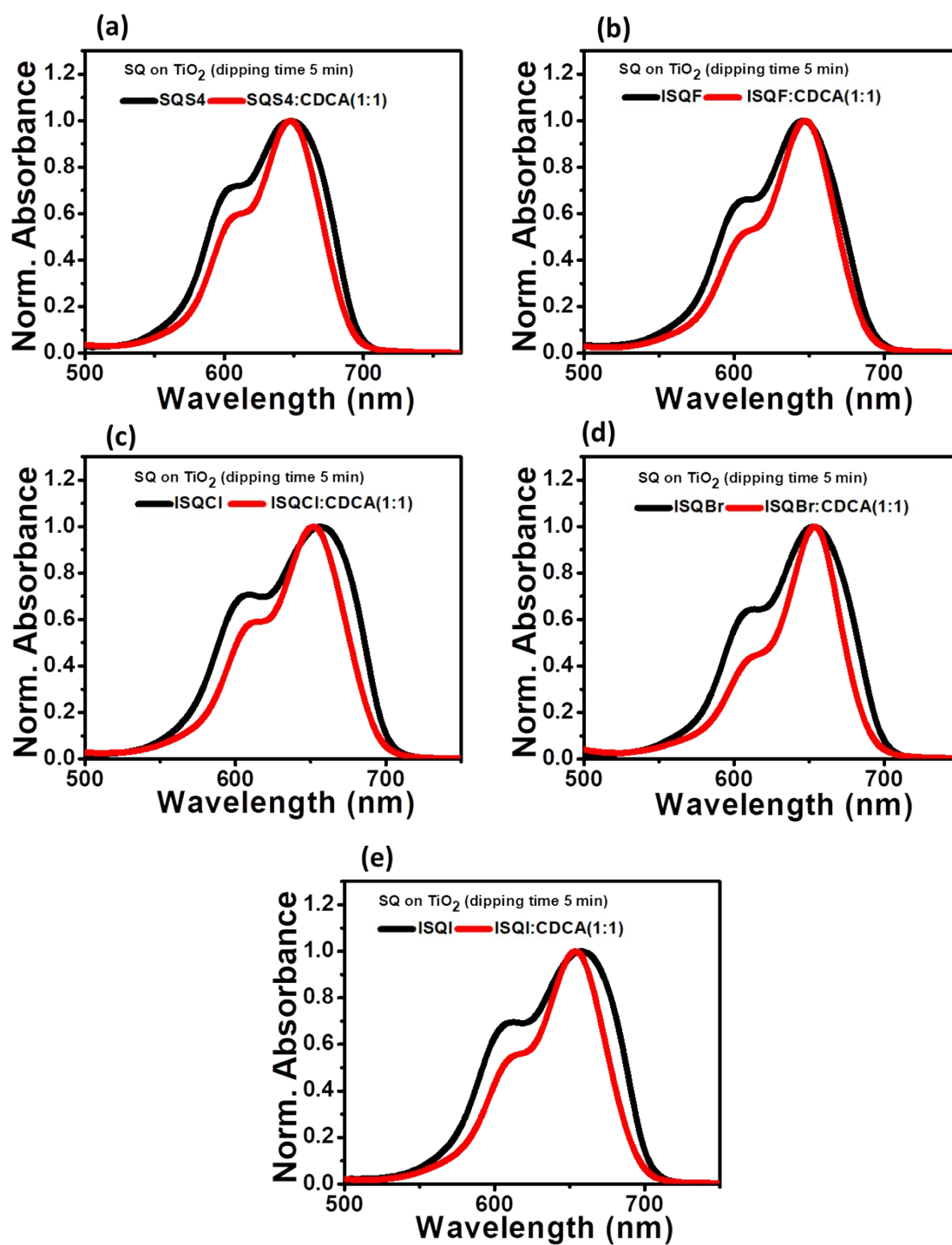


Figure S10. (a – e) Normalized absorption spectra of ISQ and SQS4 dyes on TiO₂ film with and without CDCA (TiO₂ film, thickness = 6 μm, dipping time = 5 min)

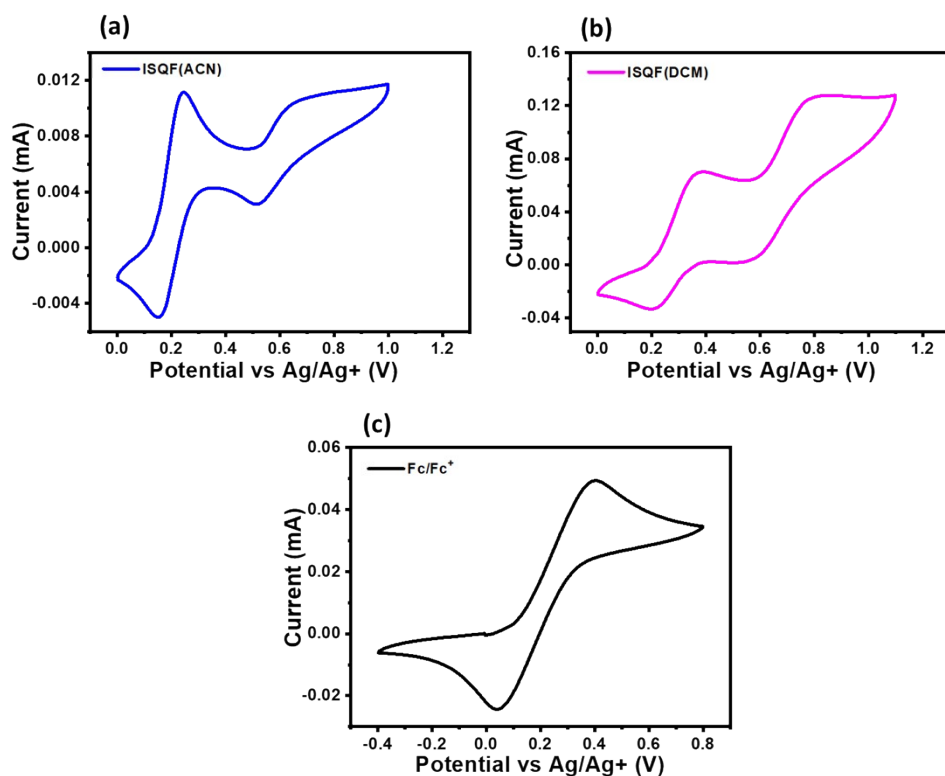


Figure S11. (a) Cyclic voltammograms of ISQF dye in CH₃CN, (b) Cyclic voltammograms of ISQF dye in CH₂Cl₂, (c) Cyclic voltammograms of Fc/Fc⁺ dye in CH₂Cl₂.

E_{ox} of the sensitizers have been measured by using the reference electrode of Ag/AgNO₃ and converted the potentials vs NHE by calibrating with Ferrocene/ Ferrocenium (Fc/Fc⁺) potential. Further, ferrocene was used as an external reference.²

$$E_{ox} = E_{onset} - E_{Fc/Fc^+} + 0.7$$

Where, E_{Fc/Fc^+} is onset potential of Fc/Fc⁺ in dichloromethane solutions (0.132 V, CV of ferrocene was provided in Figure S11(c) under the similar experimental conditions.

Calculation of E_{ox} and E_{ox^*} for the ISQF sensitizer is provided below,

$$E_{ox} = 0.218 - 0.132 + 0.7 = 0.786 \text{ V}$$

$$E_{ox^*} = E_{ox} - E_{0-0}$$

$$E_{ox^*} = 0.786 \text{ V} - 1.91 \text{ V}$$

$$E_{ox^*} = -1.12 \text{ V}$$

Table S2. Electrochemical characterizations of **ISQF** dye in two different solvents at room temperature.

Dyes	${}^c E_{\text{oxi/onset}}$ (V vs Ag/Ag ⁺)	E_{ox} (V vs NHE)	E_{ox^*} (V vs NHE)	${}^d E_{0-0}$ (eV)
ISQF^a	0.218	0.786	-1.12	1.91
ISQF^b	0.172	0.740	-1.17	1.91

^aCH₂Cl₂, ^bCH₃CN

DFT study of ISQ dyes.

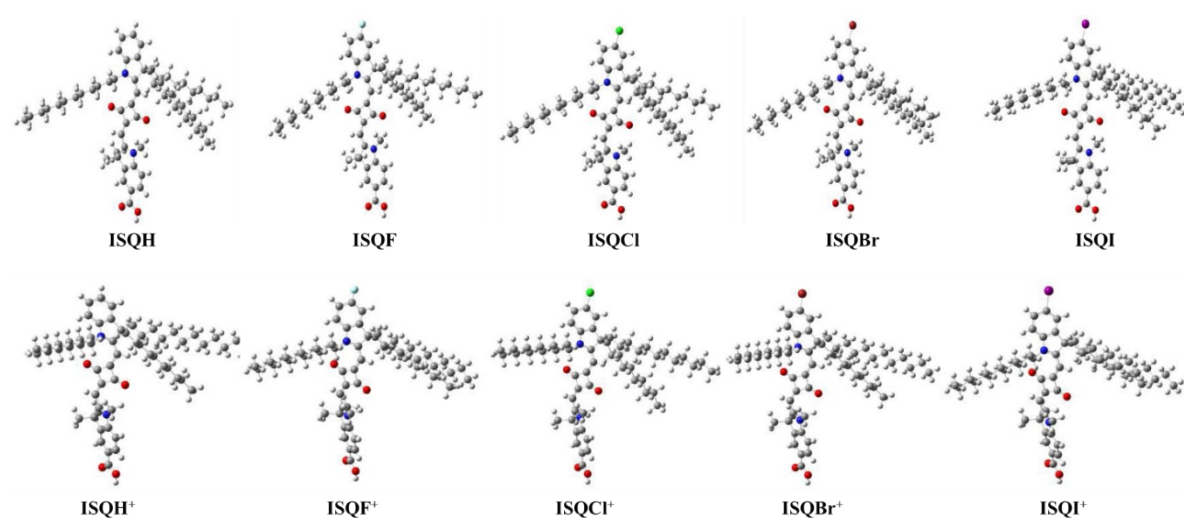


Figure S12. Optimized structures of ISQ dyes.

Table S3. Dipole moment and dihedral angles of ISQ dyes.

Dye	Dipole moment, D (D_x , D_y , D_z) D_{tot}		Dihedral N-O angles D1 , D2	
	Neutral	Charged	Neutral	Charged
ISQH (SQS4)	(-1.38, -0.16, 4.46) 4.67	(0.41, -3.82, 6.49) 7.54	4.50, 20.99	32.62, 30.46
ISQF	(-0.83, -1.15, 1.48) 2.05	(1.03, -0.80, 8.16) 8.27	11.79, 20.61	32.39, 30.29
ISQCl	(-0.59, -0.94, 1.97) 2.26	(-0.15, -0.70, 7.73) 7.76	2.76, 20.78	32.80, 30.05
ISQBr	(-0.71, 1.09, 2.04) 2.42	(2.28, -0.88, 8.21) 8.56	6.09, 20.85	31.50, 30.29
ISQI	(-1.19, -1.23, 2.01) 2.64	(2.34, -0.92, 8.06) 8.44	6.39, 20.87	32.36, 29.77

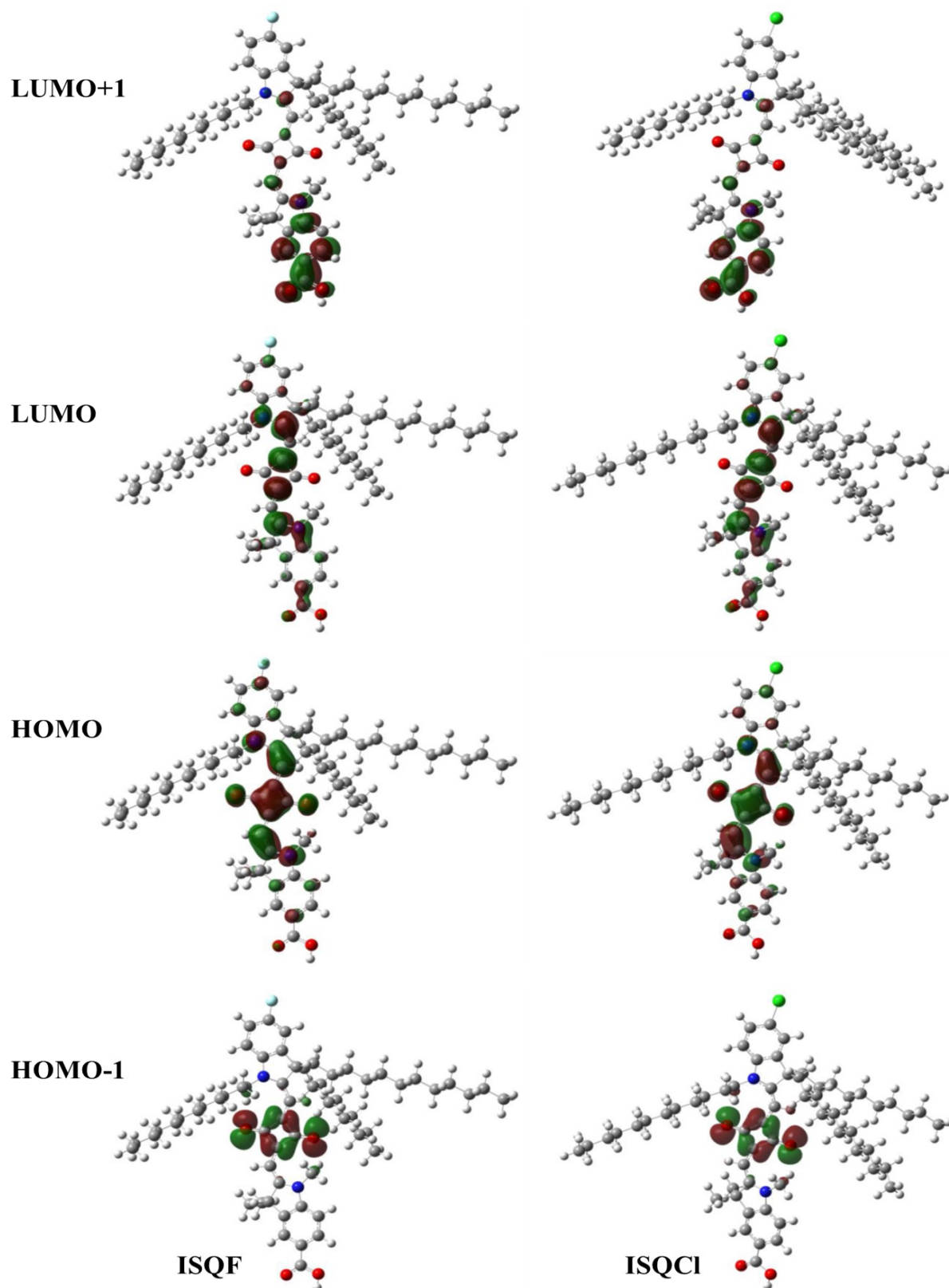
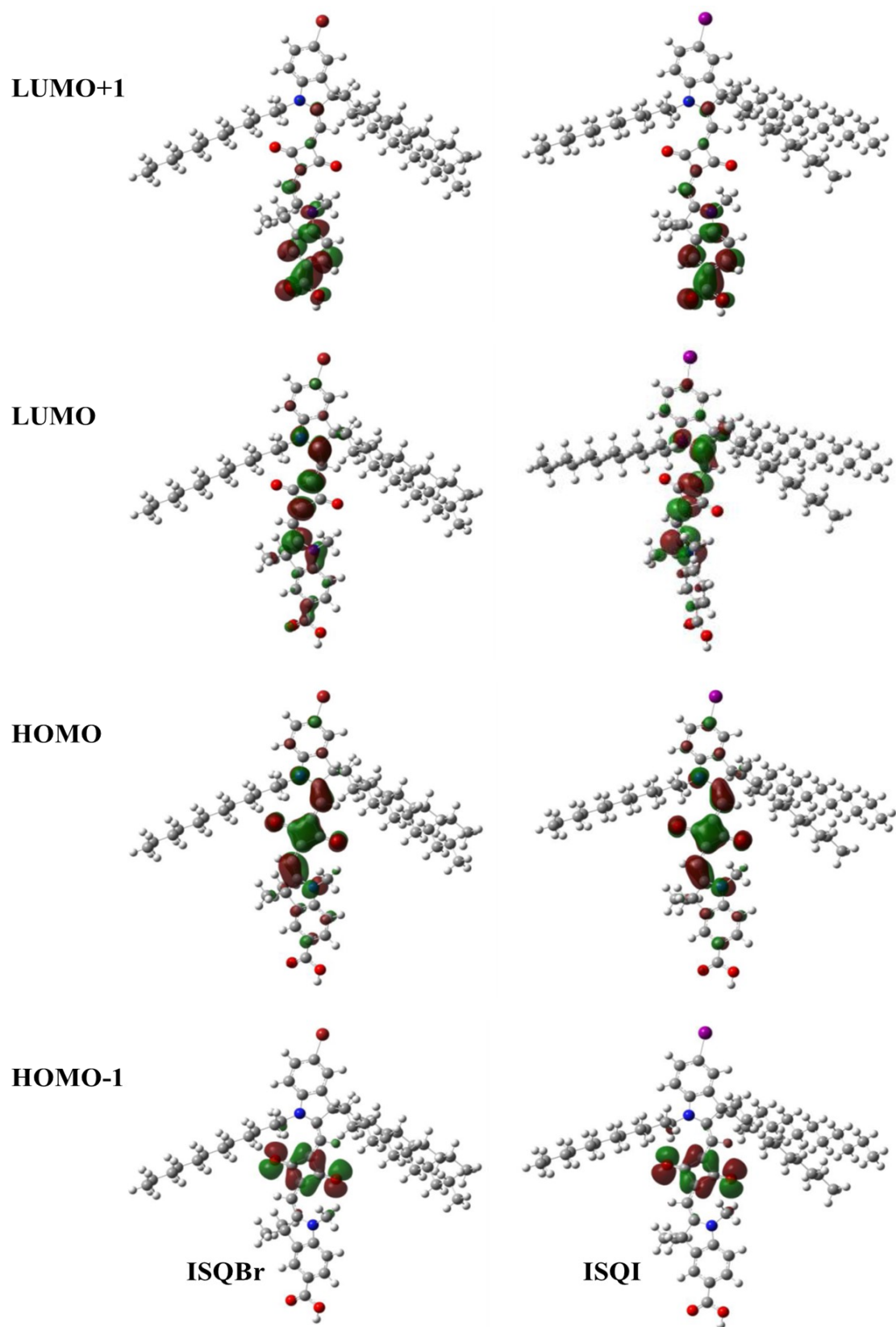


Figure S13. The calculated energy levels (HOMO, HOMO-1, LUMO, LUMO+1) of **ISQF** and **ISQCl** dyes.



Figure

re S14. The calculated energy levels (HOMO, HOMO-1, LUMO, LUMO+1) of **ISQBr** and **ISQI** dyes.

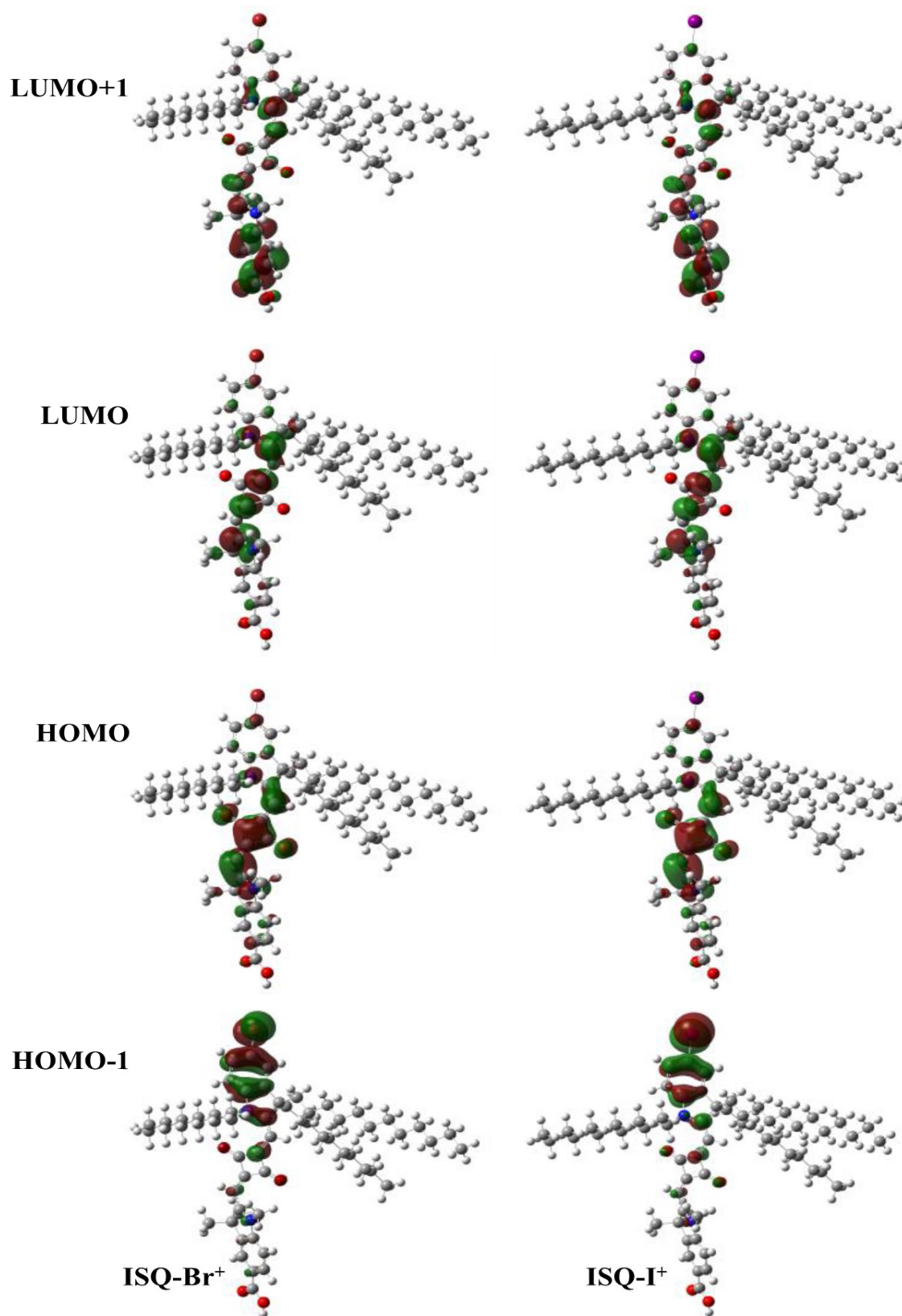


Figure S15. The calculated energy levels (HOMO, HOMO-1, LUMO, LUMO+1) oxidized dyes of **ISQ-Br⁺** and **ISQ-I⁺** dyes.

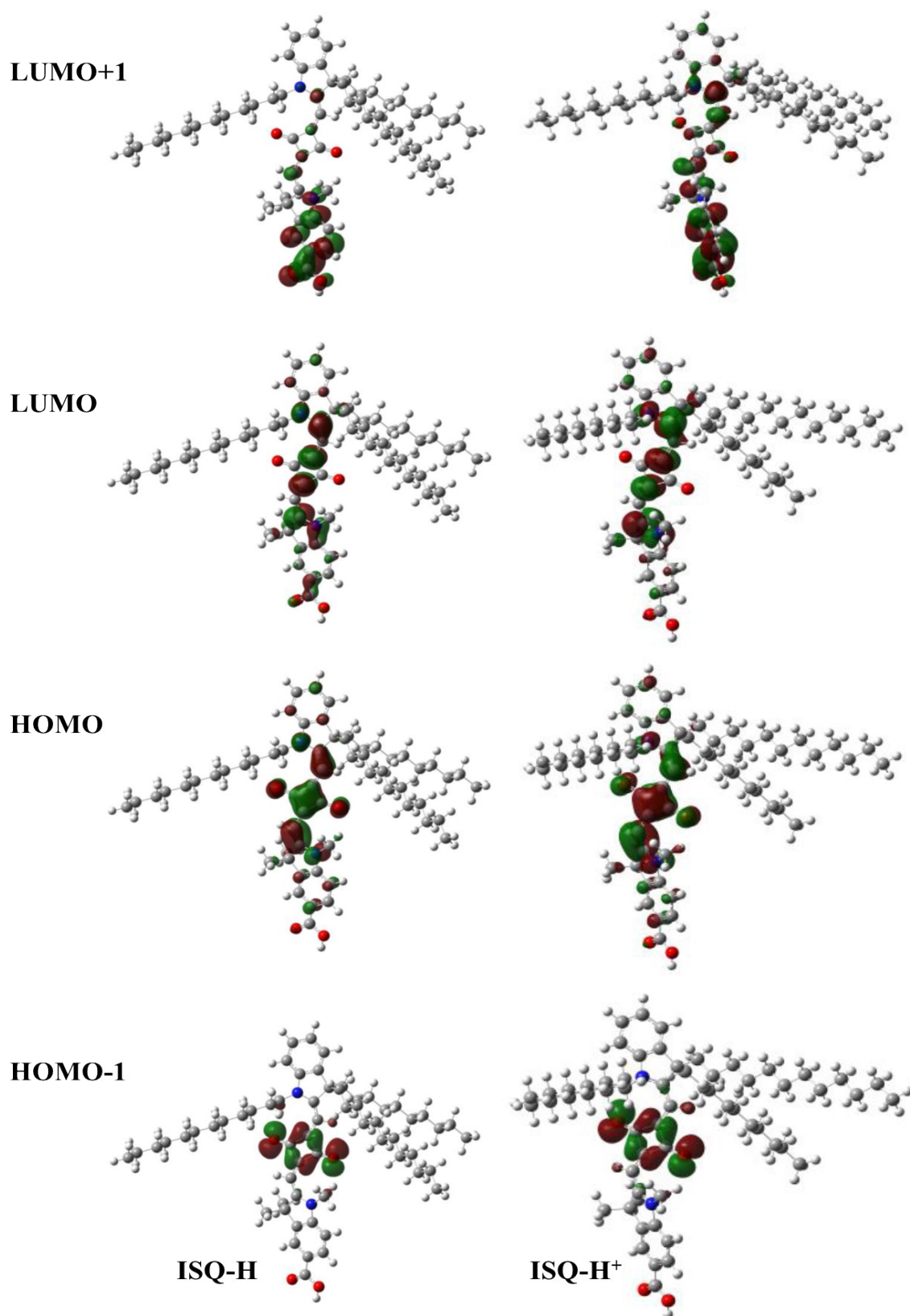


Figure S16. The calculated energy levels (HOMO, HOMO-1, LUMO, LUMO+1) neutral and oxidized of SQS4 or ISQ-H dyes.

Table S4. Computed frontier molecular orbital energies, energy gap and partial charges of ISQ dyes with SQS4 dye for neutral and positively charged species.

Dye	HOMO (eV)		LUMO (eV)		HOMO - LUMO (eV)	
	Neutral	Charged	Neutral	Charged	Neutral	Charged
ISQH (SQS4)	-4.99	-8.03	-2.27	-5.71	2.72	2.32
ISQF	-5.09	-8.12	-2.37	-5.81	2.72	2.31
ISQCl	-5.11	-8.12	-2.39	-5.82	2.72	2.30
ISQBr	-5.09	-8.09	-2.37	-5.79	2.72	2.30
ISQI	-5.08	-8.06	-2.36	-5.76	2.72	2.30

Table S5. Computed frontier molecular orbital energy levels (HOMO-1, LUMO+1) of neutral and positively charged of ISQ dyes with SQS4 dye.

Dye	HOMO-1 (eV)		HOMO (eV)		LUMO (eV)		LUMO+1 (eV)	
	Neutral	Charged	Neutral	Charged	Neutral	Charged	Neutral	Charged
ISQH (SQS4)	-6.17	-9.36	-4.99	-8.03	-2.27	-5.71	-1.11	-4.26
ISQF	-6.27	-9.43	-5.09	-8.12	-2.37	-5.81	-1.18	-4.34
ISQCl	-6.28	-9.41	-5.11	-8.12	-2.39	-5.82	-1.19	-4.33
ISQBr	-6.26	-9.25	-5.09	-8.09	-2.37	-5.79	-1.18	-4.32
ISQI	-6.25	-8.95	-5.08	-8.06	-2.36	-5.76	-1.17	-4.30

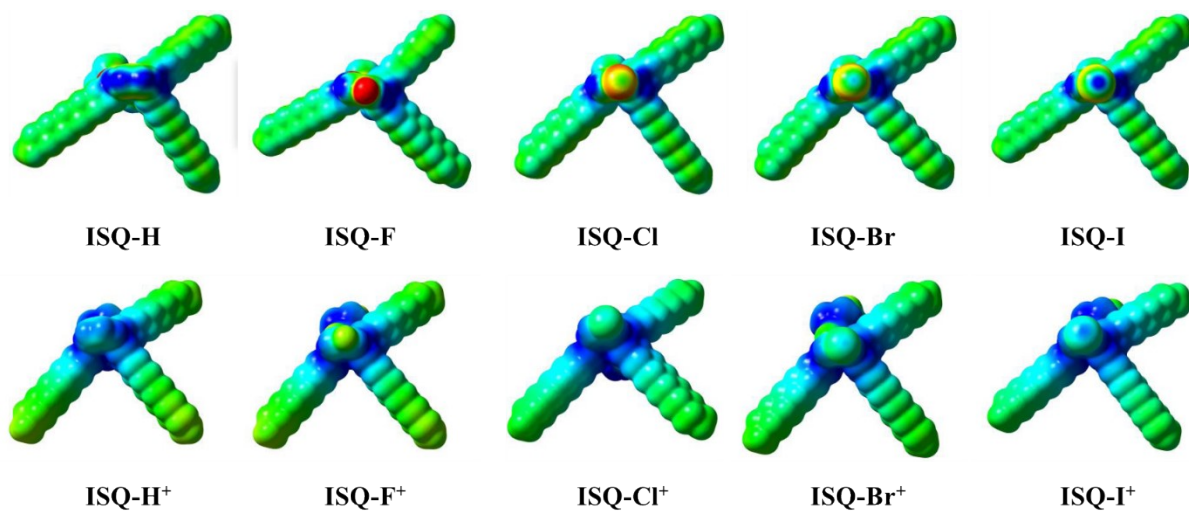
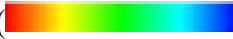


Figure S17. Molecular Electrostatic potential (MEP) mapped onto the van der waals surface top view of **ISQ-X** and **ISQ-X⁺** dyes. Color coding () red to blue is (-0.02 to +0.02) kcal/mol.

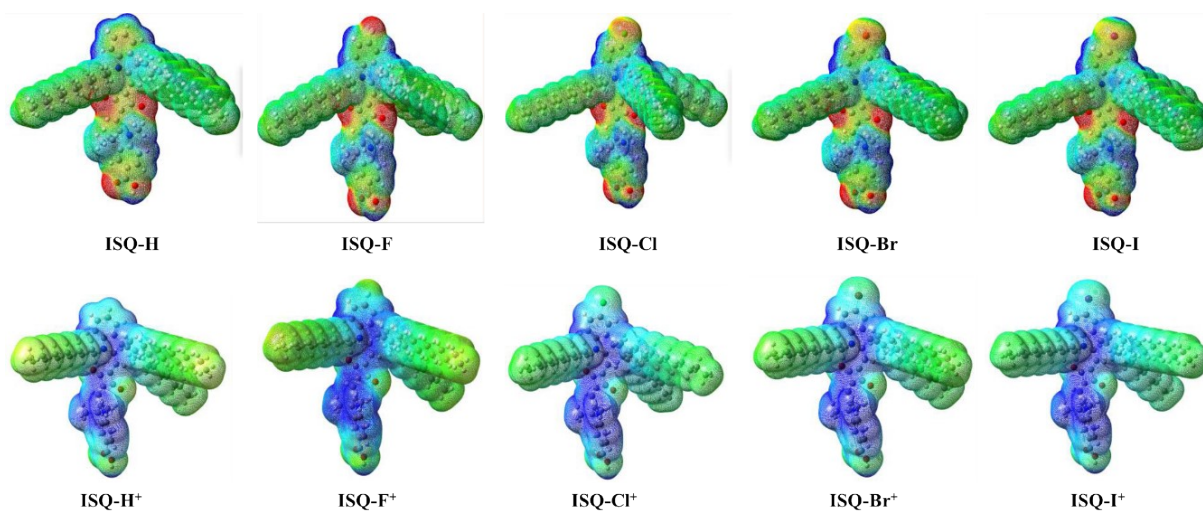



Figure S18. Molecular Electrostatic potential (MEP) mapped onto the van der waals surface side view of **ISQ-X** and **ISQ-X⁺** dyes. Color coding () red to blue is (-0.02 to +0.02) kcal/mol.

DSSC device performance.

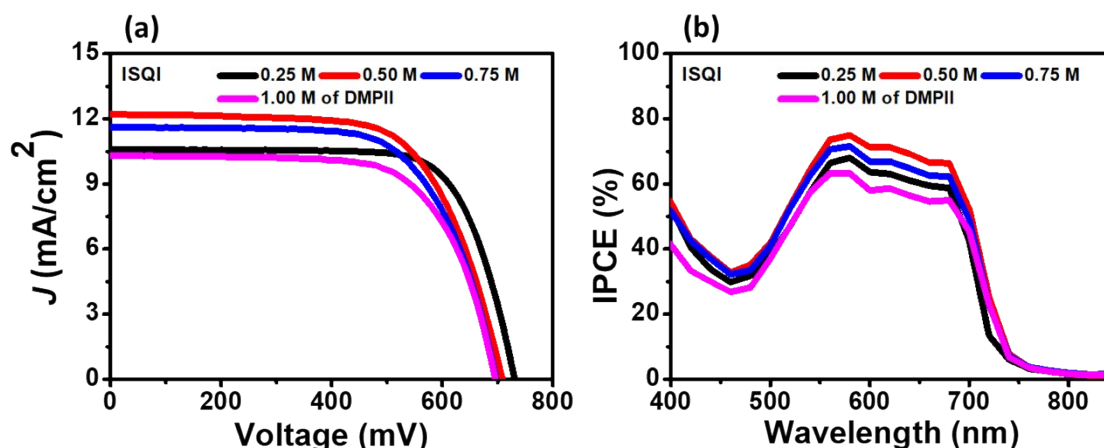


Figure S19. (a) and (b) I - V and IPCE curves of ISQI dye with different concentration of electrolytes.

Table S6. DSSC device performance of ISQI dye with different concentration of electrolytes.

I/I_3^-	CDCA (mM)	V_{oc} (mV)	J_{sc} (mA/cm ²)	ff (%)	η (%)
A	0.3	733 ± 1	10.61 ± 0.10	73 ± 0.88	5.67 ± 0.12
B	0.3	709 ± 2	12.21 ± 0.07	68 ± 0.50	5.81 ± 0.10
C	0.3	698 ± 1	11.62 ± 0.09	68 ± 1.00	5.51 ± 0.11
D	0.3	697 ± 1	10.31 ± 0.12	69 ± 0.77	4.96 ± 0.14

A = 0.25 M DMPII, 15 mM I₂, 0.125 M NaI, 0.5 M TBP, 0.1 M GuSCN,

B = 0.50 M DMPII, 30 mM I₂, 0.250 M NaI, 0.5 M TBP, 0.1 M GuSCN,

C = 0.75 M DMPII, 45 mM I₂, 0.375 M NaI, 0.5 M TBP, 0.1 M GuSCN, and

D = 1.00 M DMPII, 60 mM I₂, 0.500 M NaI, 0.5 M TBP, 0.1 M GuSCN in acetonitrile and valeronitrile (85:15, v/v).

Where, DMPII = 1,2-dimethyl-3-propylimidazolium iodide, TBP = 4-*tert*-Butylpyridine, and

GuSCN = guanidinium thiocyanate.

Dye desorption studies of ISQ dyes. ISQ dyes were desorbed from the TiO₂ surface by using 1 M of HCl in EtOH solution 2 mL (Table S7). The cuvette's path length was 0.1 cm², area of the photoanode was 0.23 cm² and 6 μm thick (Conditions for sensitization: sensitization time 12 h, [dye] = 0.1 mM in MeCN:CHCl₃ (95%:5%).

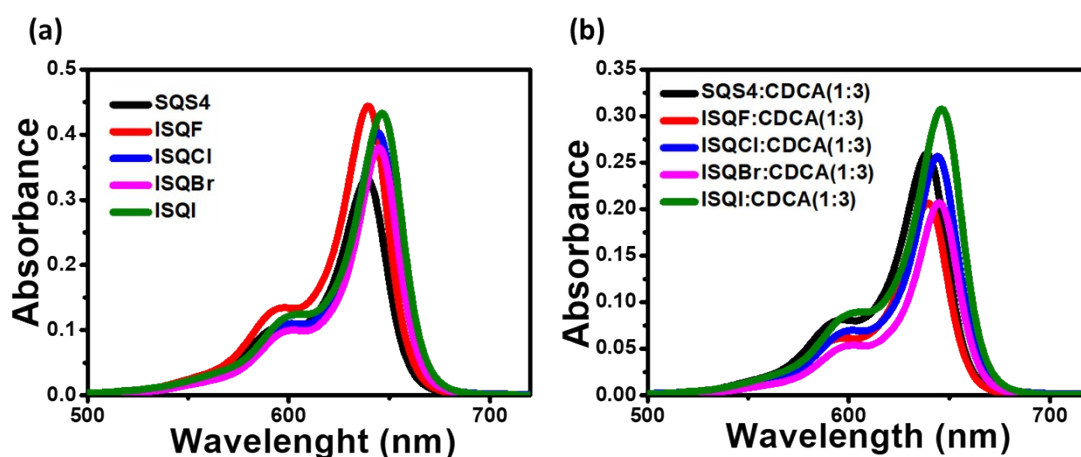
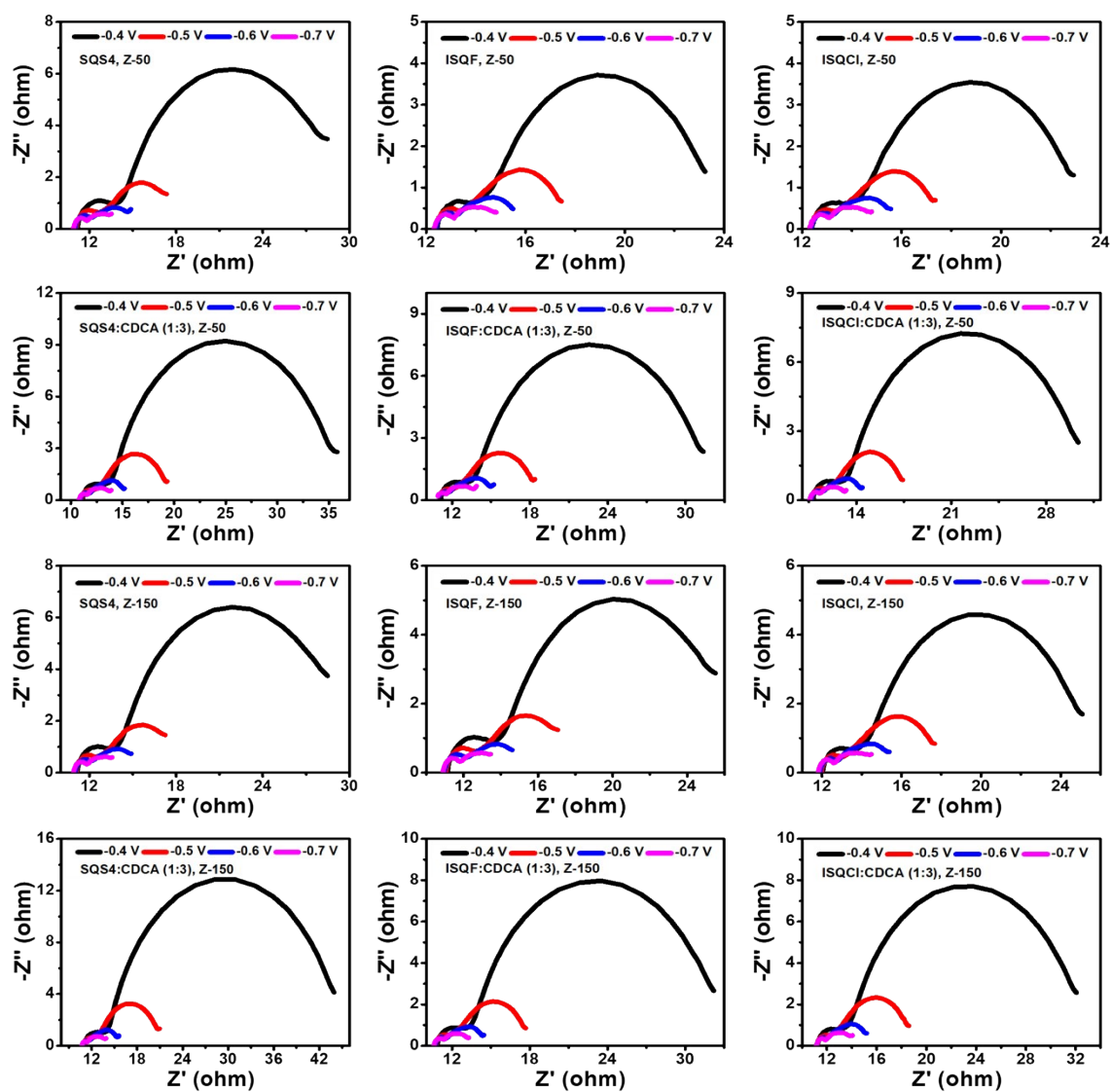


Figure S20. UV-vis absorption spectra of desorbed dyes with and without CDCA (ISQ and SQS4).

Table S7. Dye loading studies (ISQ and SQS4).

Dyes	CDCA	ϵ (M ⁻¹ cm ⁻¹)	Dye Loading on TiO ₂ (mol/cm ²)
SQS4	0	2.4×10^5	$1.13 \pm 0.25 \times 10^{-8}$
	3	2.4×10^5	$9.04 \pm 0.2 \times 10^{-9}$
ISQF	0	2.1×10^5	$1.35 \pm 0.4 \times 10^{-8}$
	3	2.1×10^5	$8.1 \pm 0.1 \times 10^{-9}$
ISQCl	0	2.5×10^5	$1.1 \pm 0.2 \times 10^{-8}$
	3	2.5×10^5	$8.6 \pm 0.2 \times 10^{-9}$
ISQBr	0	2.2×10^5	$1.3 \pm 0.2 \times 10^{-8}$
	3	2.2×10^5	$8.0 \pm 0.1 \times 10^{-9}$
ISQI	0	3.1×10^5	$1.2 \pm 0.1 \times 10^{-8}$
	3	3.1×10^5	$8.31 \pm 0.3 \times 10^{-9}$

Electrochemical Impedance Spectroscopy (EIS).



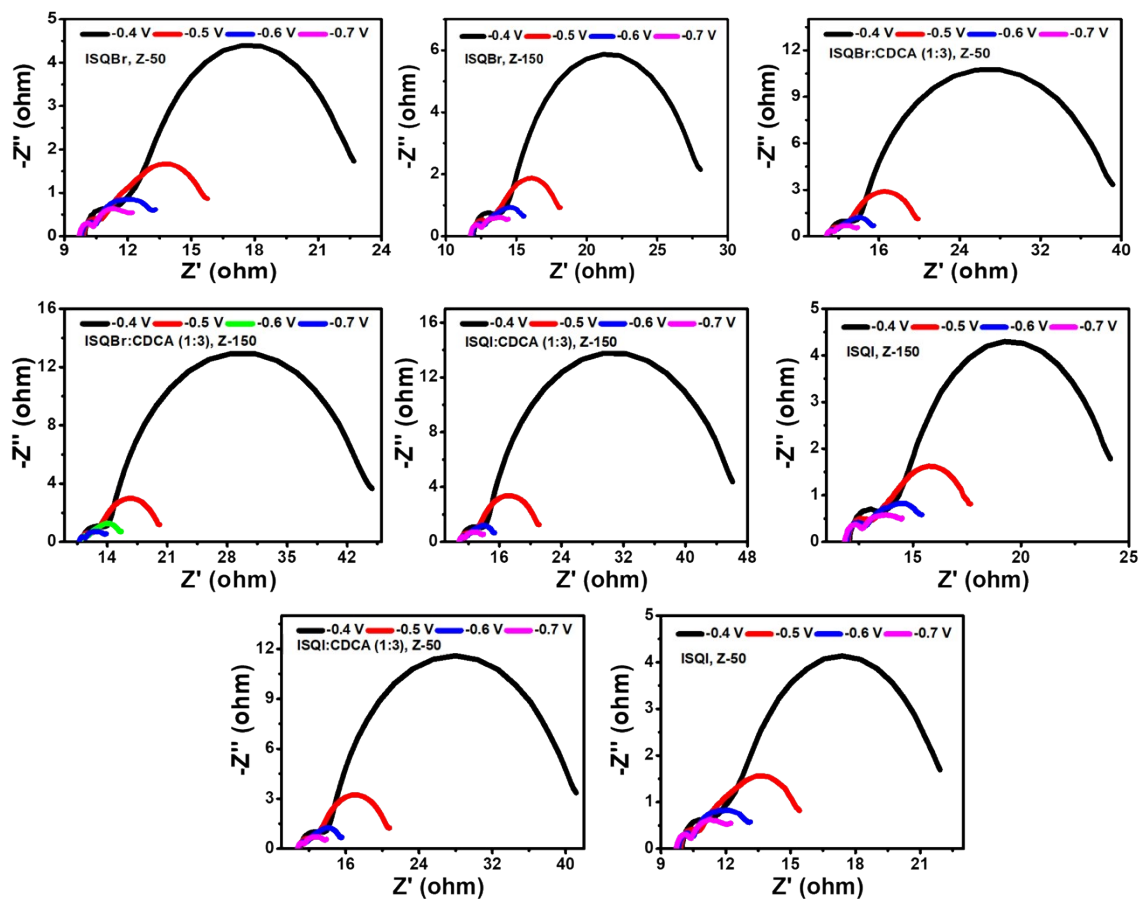


Figure S21. Nyquist plots of SQS4 and ISQ dyes.

Coordinates of optimized neutral ISQ-X dyes

ISQF

C 0.500000 -4.642000 -2.796000
C -0.843000 -4.878000 -2.482000
C -1.416000 -6.115000 -2.746000
C -0.597000 -7.083000 -3.321000
C 0.737000 -6.875000 -3.634000
C 1.310000 -5.624000 -3.367000
H -2.449000 -6.343000 -2.527000
H 1.317000 -7.673000 -4.074000
H 2.349000 -5.446000 -3.599000
C -0.233000 -2.660000 -1.882000
C -0.308000 -1.389000 -1.317000
H -1.271000 -1.195000 -0.865000
C 0.517000 -0.275000 -1.169000
C 1.784000 0.399000 -1.551000
O 2.795000 0.129000 -2.247000
C 1.397000 1.601000 -0.794000
C 0.117000 0.950000 -0.439000
C 2.092000 2.819000 -0.795000
C 1.928000 4.037000 -0.164000
H 2.920000 2.802000 -1.499000
O -0.931000 1.240000 0.189000
C 2.137000 6.348000 0.348000
C 1.227000 5.731000 1.224000
C 0.558000 6.453000 2.216000

H	-0.156000	5.988000	2.880000
C	1.738000	8.449000	1.456000
C	2.031000	9.883000	1.552000
O	2.819000	10.509000	0.829000
N	1.139000	4.359000	0.921000
C	2.358000	5.655000	-2.085000
H	1.284000	5.780000	-2.224000
H	2.852000	6.587000	-2.367000
H	2.703000	4.867000	-2.755000
C	0.407000	3.393000	1.743000
H	0.139000	3.861000	2.686000
H	-0.481000	3.020000	1.238000
H	1.053000	2.539000	1.950000
C	0.825000	7.819000	2.321000
H	0.324000	8.409000	3.073000
C	2.400000	7.698000	0.459000
H	3.098000	8.203000	-0.194000
C	2.690000	5.305000	-0.613000
C	4.221000	5.130000	-0.433000
H	4.468000	4.877000	0.599000
H	4.599000	4.338000	-1.083000
H	4.733000	6.058000	-0.692000
C	-4.235000	-1.470000	-3.875000
H	-3.906000	-1.777000	-4.875000
H	-5.074000	-2.126000	-3.613000
C	-4.727000	-0.013000	-3.929000

H -5.066000 0.291000 -2.932000
H -3.884000 0.642000 -4.177000
C -5.860000 0.213000 -4.944000
H -5.517000 -0.089000 -5.941000
H -6.704000 -0.444000 -4.698000
C -6.351000 1.670000 -4.998000
H -6.707000 1.968000 -4.004000
H -5.504000 2.327000 -5.228000
C -7.468000 1.905000 -6.029000
H -7.110000 1.608000 -7.022000
H -8.316000 1.248000 -5.800000
O 1.329000 10.524000 2.561000
H 1.562000 11.472000 2.579000
C -1.460000 -3.611000 -1.895000
C -1.988000 -3.953000 -0.452000
H -2.488000 -4.923000 -0.535000
H -1.113000 -4.122000 0.184000
C -2.592000 -3.141000 -2.888000
H -3.443000 -3.810000 -2.719000
H -2.239000 -3.359000 -3.901000
C -3.083000 -1.682000 -2.873000
H -2.260000 -1.013000 -3.135000
H -3.418000 -1.381000 -1.880000
C -2.960000 -3.003000 0.271000
H -2.535000 -2.004000 0.389000
H -3.877000 -2.891000 -0.314000

C	-3.330000	-3.540000	1.668000
H	-2.418000	-3.636000	2.270000
H	-3.744000	-4.551000	1.573000
C	-4.336000	-2.646000	2.412000
H	-3.925000	-1.633000	2.496000
H	-5.251000	-2.556000	1.813000
C	-4.698000	-3.166000	3.813000
H	-3.784000	-3.250000	4.414000
H	-5.103000	-4.182000	3.729000
C	-5.711000	-2.277000	4.555000
H	-5.306000	-1.261000	4.638000
H	-6.625000	-2.193000	3.954000
C	-6.073000	-2.795000	5.957000
H	-5.159000	-2.876000	6.559000
H	-6.475000	-3.811000	5.874000
C	-7.088000	-1.907000	6.697000
H	-6.686000	-0.891000	6.781000
H	-8.002000	-1.826000	6.095000
C	-7.451000	-2.425000	8.099000
H	-7.852000	-3.442000	8.016000
H	-6.537000	-2.505000	8.702000
C	-8.468000	-1.539000	8.839000
H	-8.067000	-0.521000	8.923000
H	-9.382000	-1.459000	8.238000
C	-8.830000	-2.056000	10.242000
H	-7.916000	-2.135000	10.843000

H -9.229000 -3.074000 10.158000
C -9.847000 -1.167000 10.973000
H -10.082000 -1.560000 11.964000
H -9.462000 -0.151000 11.101000
H -10.783000 -1.097000 10.412000
C -7.957000 3.362000 -6.082000
H -8.324000 3.658000 -5.092000
H -7.108000 4.021000 -6.303000
C -9.065000 3.603000 -7.122000
H -8.699000 3.308000 -8.112000
H -9.913000 2.944000 -6.903000
N 0.837000 -3.310000 -2.444000
C 2.213000 -2.812000 -2.596000
H 2.620000 -3.267000 -3.502000
H 2.206000 -1.738000 -2.763000
C 3.104000 -3.142000 -1.384000
H 2.725000 -2.602000 -0.511000
H 3.037000 -4.210000 -1.151000
C 4.570000 -2.749000 -1.634000
H 4.970000 -3.345000 -2.464000
H 4.603000 -1.703000 -1.952000
C 5.463000 -2.938000 -0.396000
H 5.073000 -2.322000 0.422000
H 5.404000 -3.979000 -0.053000
C 6.936000 -2.570000 -0.647000
H 6.988000 -1.543000 -1.026000

H	7.339000	-3.211000	-1.441000
C	7.821000	-2.694000	0.605000
H	7.419000	-2.047000	1.394000
H	7.764000	-3.719000	0.991000
C	9.294000	-2.328000	0.354000
H	9.348000	-1.310000	-0.051000
H	9.704000	-2.988000	-0.421000
C	10.174000	-2.418000	1.613000
H	9.764000	-1.757000	2.386000
H	10.119000	-3.435000	2.020000
C	11.646000	-2.051000	1.362000
H	11.699000	-1.038000	0.945000
H	12.060000	-2.719000	0.597000
C	12.522000	-2.124000	2.624000
H	12.110000	-1.456000	3.390000
H	12.471000	-3.137000	3.043000
C	13.995000	-1.756000	2.374000
H	14.046000	-0.746000	1.952000
H	14.409000	-2.426000	1.612000
C	14.861000	-1.826000	3.641000
H	15.900000	-1.559000	3.430000
H	14.491000	-1.140000	4.409000
H	14.856000	-2.833000	4.067000
C	-9.548000	5.060000	-7.168000
H	-10.332000	5.198000	-7.916000
H	-9.951000	5.372000	-6.201000

H -8.727000 5.739000 -7.418000

F -1.158000 -8.346000 -3.595000

ISQCI

C 0.365000 -4.149000 -3.294000

C -0.931000 -4.492000 -2.896000

C -1.455000 -5.738000 -3.214000

C -0.646000 -6.616000 -3.939000

C 0.645000 -6.288000 -4.338000

C 1.172000 -5.031000 -4.012000

H -2.451000 -6.032000 -2.918000

H 1.238000 -6.999000 -4.895000

H 2.176000 -4.774000 -4.315000

C -0.407000 -2.282000 -2.191000

C -0.576000 -1.002000 -1.671000

H -1.530000 -0.882000 -1.176000

C 0.133000 0.198000 -1.619000

C 1.352000 0.951000 -2.010000

O 2.410000 0.722000 -2.647000

C 0.838000 2.164000 -1.353000

C -0.393000 1.429000 -0.985000

C 1.430000 3.434000 -1.417000

C 1.142000 4.671000 -0.873000

H 2.280000 3.442000 -2.094000

O -1.481000 1.669000 -0.407000

C 1.134000 7.019000 -0.511000

C	0.252000	6.381000	0.380000
C	-0.508000	7.103000	1.303000
H	-1.201000	6.620000	1.976000
C	0.520000	9.142000	0.446000
C	0.688000	10.600000	0.455000
O	1.442000	11.245000	-0.286000
N	0.295000	4.990000	0.167000
C	1.496000	6.194000	-2.886000
H	0.420000	6.214000	-3.064000
H	1.917000	7.146000	-3.215000
H	1.930000	5.398000	-3.492000
C	-0.371000	4.019000	1.038000
H	-0.676000	4.516000	1.955000
H	-1.226000	3.556000	0.552000
H	0.334000	3.226000	1.290000
C	-0.362000	8.491000	1.325000
H	-0.937000	9.081000	2.023000
C	1.276000	8.391000	-0.482000
H	1.949000	8.913000	-1.148000
C	1.806000	5.970000	-1.385000
C	3.339000	5.942000	-1.151000
H	3.573000	5.782000	-0.098000
H	3.805000	5.145000	-1.733000
H	3.778000	6.892000	-1.460000
C	-5.103000	-1.693000	-2.927000
H	-4.772000	-1.144000	-3.816000

H -5.542000 -2.631000 -3.291000
C -6.185000 -0.877000 -2.200000
H -6.533000 -1.439000 -1.324000
H -5.742000 0.048000 -1.814000
C -7.391000 -0.532000 -3.091000
H -7.046000 0.053000 -3.952000
H -7.815000 -1.457000 -3.499000
C -8.494000 0.248000 -2.357000
H -8.848000 -0.343000 -1.504000
H -8.069000 1.167000 -1.936000
C -9.691000 0.608000 -3.253000
H -9.340000 1.213000 -4.098000
H -10.107000 -0.310000 -3.687000
O -0.097000 11.240000 1.402000
H 0.053000 12.204000 1.364000
C -1.535000 -3.345000 -2.089000
C -1.748000 -3.884000 -0.620000
H -2.646000 -4.511000 -0.655000
H -0.918000 -4.564000 -0.405000
C -2.868000 -2.894000 -2.791000
H -3.390000 -3.814000 -3.072000
H -2.593000 -2.408000 -3.733000
C -3.881000 -2.009000 -2.043000
H -3.434000 -1.066000 -1.725000
H -4.224000 -2.520000 -1.139000
C -1.858000 -2.905000 0.564000

H	-0.920000	-2.358000	0.679000
H	-2.632000	-2.155000	0.396000
C	-2.166000	-3.651000	1.877000
H	-1.409000	-4.428000	2.041000
H	-3.126000	-4.175000	1.782000
C	-2.214000	-2.722000	3.102000
H	-1.251000	-2.209000	3.202000
H	-2.961000	-1.938000	2.932000
C	-2.536000	-3.457000	4.415000
H	-1.792000	-4.245000	4.580000
H	-3.504000	-3.964000	4.317000
C	-2.572000	-2.530000	5.642000
H	-1.604000	-2.023000	5.740000
H	-3.315000	-1.740000	5.476000
C	-2.895000	-3.262000	6.956000
H	-2.153000	-4.053000	7.119000
H	-3.864000	-3.766000	6.860000
C	-2.925000	-2.336000	8.184000
H	-1.956000	-1.831000	8.279000
H	-3.667000	-1.545000	8.021000
C	-3.245000	-3.068000	9.498000
H	-4.214000	-3.572000	9.404000
H	-2.503000	-3.860000	9.660000
C	-3.272000	-2.144000	10.727000
H	-2.304000	-1.638000	10.822000
H	-4.015000	-1.352000	10.568000

C -3.589000 -2.876000 12.042000
H -2.846000 -3.667000 12.201000
H -4.557000 -3.381000 11.948000
C -3.613000 -1.945000 13.264000
H -3.841000 -2.495000 14.180000
H -2.647000 -1.453000 13.403000
H -4.370000 -1.164000 13.148000
C -10.807000 1.367000 -2.515000
H -11.162000 0.760000 -1.674000
H -10.393000 2.284000 -2.078000
C -12.002000 1.732000 -3.413000
H -11.649000 2.344000 -4.251000
H -12.412000 0.817000 -3.855000
N 0.658000 -2.832000 -2.864000
C 1.980000 -2.233000 -3.105000
H 2.325000 -2.590000 -4.077000
H 1.896000 -1.153000 -3.180000
C 2.995000 -2.596000 -2.005000
H 2.647000 -2.177000 -1.056000
H 3.032000 -3.683000 -1.877000
C 4.400000 -2.055000 -2.318000
H 4.759000 -2.492000 -3.259000
H 4.332000 -0.976000 -2.478000
C 5.417000 -2.354000 -1.203000
H 5.050000 -1.927000 -0.261000
H 5.481000 -3.437000 -1.044000

C	6.822000	-1.800000	-1.492000
H	6.755000	-0.717000	-1.647000
H	7.192000	-2.222000	-2.434000
C	7.837000	-2.091000	-0.373000
H	7.457000	-1.682000	0.572000
H	7.913000	-3.176000	-0.227000
C	9.237000	-1.517000	-0.645000
H	9.160000	-0.432000	-0.786000
H	9.617000	-1.921000	-1.591000
C	10.250000	-1.811000	0.475000
H	9.865000	-1.416000	1.422000
H	10.336000	-2.896000	0.609000
C	11.647000	-1.222000	0.212000
H	11.561000	-0.137000	0.080000
H	12.033000	-1.616000	-0.736000
C	12.660000	-1.516000	1.332000
H	12.273000	-1.125000	2.281000
H	12.750000	-2.601000	1.463000
C	14.055000	-0.922000	1.073000
H	13.965000	0.162000	0.941000
H	14.442000	-1.314000	0.126000
C	15.059000	-1.218000	2.197000
H	16.038000	-0.784000	1.982000
H	14.715000	-0.808000	3.151000
H	15.196000	-2.295000	2.331000
C	-13.115000	2.482000	-2.665000

H -13.949000 2.724000 -3.328000
H -13.509000 1.880000 -1.841000
H -12.743000 3.419000 -2.242000
Cl -1.314000 -8.263000 -4.375000

ISQBr

C 0.237000 -4.372000 -2.535000
C -1.085000 -4.559000 -2.118000
C -1.697000 -5.796000 -2.265000
C -0.952000 -6.833000 -2.839000
C 0.365000 -6.656000 -3.253000
C 0.982000 -5.406000 -3.100000
H -2.716000 -5.966000 -1.950000
H 0.914000 -7.477000 -3.689000
H 2.006000 -5.272000 -3.417000
C -0.402000 -2.317000 -1.717000
C -0.465000 -0.971000 -1.365000
H -1.394000 -0.715000 -0.873000
C 0.330000 0.168000 -1.490000
C 1.570000 0.774000 -2.040000
O 2.574000 0.388000 -2.690000
C 1.172000 2.097000 -1.535000
C -0.079000 1.508000 -1.008000
C 1.832000 3.303000 -1.813000
C 1.648000 4.622000 -1.444000
H 2.640000 3.157000 -2.526000

O	-1.114000	1.902000	-0.418000
C	1.789000	6.993000	-1.439000
C	0.932000	6.549000	-0.416000
C	0.273000	7.445000	0.430000
H	-0.398000	7.110000	1.206000
C	1.350000	9.268000	-0.781000
C	1.592000	10.698000	-1.003000
O	2.330000	11.179000	-1.875000
N	0.886000	5.143000	-0.420000
C	1.961000	5.807000	-3.679000
H	0.879000	5.865000	-3.802000
H	2.411000	6.673000	-4.169000
H	2.316000	4.905000	-4.180000
C	0.221000	4.353000	0.620000
H	0.005000	4.996000	1.469000
H	-0.690000	3.884000	0.254000
H	0.892000	3.558000	0.946000
C	0.493000	8.809000	0.234000
H	-0.003000	9.530000	0.867000
C	2.004000	8.343000	-1.626000
H	2.659000	8.719000	-2.400000
C	2.349000	5.787000	-2.179000
C	3.890000	5.699000	-2.023000
H	4.176000	5.676000	-0.971000
H	4.277000	4.801000	-2.507000
H	4.360000	6.567000	-2.488000

C -4.972000 -1.417000 -2.732000
H -4.565000 -1.067000 -3.688000
H -5.522000 -2.341000 -2.950000
C -5.944000 -0.364000 -2.174000
H -6.361000 -0.726000 -1.227000
H -5.385000 0.548000 -1.932000
C -7.095000 -0.013000 -3.131000
H -6.680000 0.365000 -4.073000
H -7.649000 -0.925000 -3.384000
C -8.069000 1.027000 -2.552000
H -8.491000 0.643000 -1.616000
H -7.512000 1.933000 -2.287000
C -9.216000 1.400000 -3.508000
H -8.795000 1.793000 -4.441000
H -9.771000 0.494000 -3.779000
O 0.904000 11.518000 -0.122000
H 1.101000 12.455000 -0.314000
C -1.613000 -3.266000 -1.503000
C -1.911000 -3.573000 0.017000
H -2.843000 -4.150000 0.028000
H -1.132000 -4.259000 0.364000
C -2.884000 -2.822000 -2.317000
H -3.491000 -3.724000 -2.448000
H -2.546000 -2.541000 -3.319000
C -3.809000 -1.723000 -1.767000
H -3.262000 -0.796000 -1.587000

H	-4.227000	-2.037000	-0.806000
C	-2.014000	-2.432000	1.046000
H	-1.049000	-1.928000	1.139000
H	-2.729000	-1.671000	0.731000
C	-2.434000	-2.965000	2.429000
H	-1.719000	-3.728000	2.760000
H	-3.404000	-3.472000	2.344000
C	-2.534000	-1.862000	3.497000
H	-1.563000	-1.360000	3.590000
H	-3.241000	-1.096000	3.158000
C	-2.972000	-2.382000	4.876000
H	-2.256000	-3.137000	5.224000
H	-3.936000	-2.898000	4.778000
C	-3.098000	-1.275000	5.936000
H	-2.135000	-0.760000	6.037000
H	-3.813000	-0.521000	5.585000
C	-3.545000	-1.791000	7.315000
H	-2.825000	-2.537000	7.672000
H	-4.503000	-2.315000	7.211000
C	-3.689000	-0.680000	8.369000
H	-2.731000	-0.155000	8.474000
H	-4.408000	0.066000	8.010000
C	-4.138000	-1.193000	9.748000
H	-5.092000	-1.723000	9.641000
H	-3.416000	-1.934000	10.110000
C	-4.293000	-0.080000	10.798000

H	-3.340000	0.451000	10.905000
H	-5.017000	0.660000	10.436000
C	-4.743000	-0.593000	12.177000
H	-4.017000	-1.329000	12.541000
H	-5.693000	-1.128000	12.069000
C	-4.901000	0.527000	13.217000
H	-5.220000	0.131000	14.185000
H	-3.958000	1.059000	13.370000
H	-5.646000	1.260000	12.896000
C	-10.192000	2.433000	-2.919000
H	-10.617000	2.039000	-1.987000
H	-9.637000	3.338000	-2.642000
C	-11.337000	2.816000	-3.873000
H	-10.913000	3.213000	-4.802000
H	-11.890000	1.912000	-4.152000
N	0.622000	-3.031000	-2.291000
C	1.990000	-2.568000	-2.577000
H	2.343000	-3.127000	-3.445000
H	1.981000	-1.520000	-2.863000
C	2.939000	-2.774000	-1.382000
H	2.592000	-2.156000	-0.548000
H	2.891000	-3.816000	-1.045000
C	4.390000	-2.399000	-1.727000
H	4.753000	-3.048000	-2.534000
H	4.406000	-1.377000	-2.115000
C	5.336000	-2.513000	-0.520000

H	4.972000	-1.859000	0.282000
H	5.302000	-3.534000	-0.122000
C	6.794000	-2.144000	-0.844000
H	6.825000	-1.128000	-1.255000
H	7.169000	-2.806000	-1.634000
C	7.728000	-2.228000	0.375000
H	7.347000	-1.569000	1.164000
H	7.696000	-3.245000	0.785000
C	9.187000	-1.853000	0.065000
H	9.218000	-0.838000	-0.349000
H	9.573000	-2.516000	-0.719000
C	10.111000	-1.928000	1.293000
H	9.720000	-1.268000	2.078000
H	10.082000	-2.943000	1.705000
C	11.570000	-1.545000	0.993000
H	11.599000	-0.530000	0.579000
H	11.964000	-2.206000	0.212000
C	12.488000	-1.614000	2.226000
H	12.092000	-0.955000	3.008000
H	12.462000	-2.630000	2.640000
C	13.948000	-1.227000	1.932000
H	13.973000	-0.213000	1.516000
H	14.344000	-1.887000	1.152000
C	14.854000	-1.296000	3.170000
H	15.882000	-1.016000	2.929000
H	14.501000	-0.621000	3.955000

H 14.874000 -2.307000 3.588000
C -12.307000 3.844000 -3.272000
H -13.107000 4.095000 -3.973000
H -12.773000 3.460000 -2.360000
H -11.788000 4.771000 -3.014000
Br -1.801000 -8.601000 -3.063000

ISQI

C -0.244000 -4.391000 -1.569000
C -1.572000 -4.366000 -1.135000
C -2.306000 -5.542000 -1.056000
C -1.681000 -6.744000 -1.422000
C -0.353000 -6.768000 -1.854000
C 0.387000 -5.580000 -1.931000
H -3.334000 -5.539000 -0.722000
H 0.113000 -7.702000 -2.129000
H 1.415000 -5.609000 -2.260000
C -0.656000 -2.169000 -1.131000
C -0.562000 -0.786000 -0.993000
H -1.458000 -0.352000 -0.569000
C 0.369000 0.219000 -1.254000
C 1.684000 0.588000 -1.838000
O 2.638000 -0.002000 -2.406000
C 1.454000 2.005000 -1.515000
C 0.127000 1.652000 -0.964000
C 2.276000 3.070000 -1.909000

C	2.270000	4.437000	-1.702000
H	3.071000	2.733000	-2.570000
O	-0.860000	2.246000	-0.466000
C	2.746000	6.749000	-1.961000
C	1.808000	6.553000	-0.932000
C	1.259000	7.625000	-0.225000
H	0.526000	7.481000	0.554000
C	2.616000	9.126000	-1.588000
C	3.065000	10.471000	-1.961000
O	3.887000	10.740000	-2.849000
N	1.563000	5.176000	-0.778000
C	2.807000	5.295000	-4.042000
H	1.748000	5.487000	-4.217000
H	3.387000	6.027000	-4.607000
H	3.043000	4.300000	-4.422000
C	0.764000	4.615000	0.314000
H	0.601000	5.382000	1.066000
H	-0.186000	4.218000	-0.038000
H	1.315000	3.792000	0.771000
C	1.675000	8.913000	-0.565000
H	1.268000	9.766000	-0.043000
C	3.156000	8.025000	-2.291000
H	3.879000	8.212000	-3.073000
C	3.148000	5.398000	-2.535000
C	4.656000	5.116000	-2.304000
H	4.910000	5.181000	-1.246000

H	4.923000	4.121000	-2.664000
H	5.257000	5.849000	-2.847000
C	-4.988000	-1.029000	-2.645000
H	-4.523000	-1.077000	-3.637000
H	-5.686000	-1.874000	-2.593000
C	-5.775000	0.287000	-2.520000
H	-6.250000	0.334000	-1.533000
H	-5.076000	1.130000	-2.564000
C	-6.846000	0.456000	-3.610000
H	-6.369000	0.397000	-4.596000
H	-7.549000	-0.384000	-3.560000
C	-7.629000	1.777000	-3.509000
H	-8.113000	1.837000	-2.527000
H	-6.926000	2.617000	-3.556000
C	-8.691000	1.943000	-4.609000
H	-8.206000	1.876000	-5.591000
H	-9.396000	1.104000	-4.560000
O	2.477000	11.478000	-1.209000
H	2.811000	12.349000	-1.498000
C	-1.967000	-2.931000	-0.792000
C	-2.354000	-2.905000	0.736000
H	-3.345000	-3.369000	0.800000
H	-1.672000	-3.590000	1.250000
C	-3.151000	-2.532000	-1.749000
H	-3.888000	-3.339000	-1.665000
H	-2.766000	-2.585000	-2.773000

C	-3.897000	-1.199000	-1.569000
H	-3.214000	-0.351000	-1.633000
H	-4.366000	-1.158000	-0.582000
C	-2.366000	-1.587000	1.532000
H	-1.354000	-1.179000	1.590000
H	-2.977000	-0.826000	1.043000
C	-2.897000	-1.806000	2.962000
H	-2.307000	-2.590000	3.452000
H	-3.926000	-2.182000	2.914000
C	-2.860000	-0.531000	3.822000
H	-1.829000	-0.165000	3.879000
H	-3.437000	0.257000	3.325000
C	-3.405000	-0.738000	5.246000
H	-2.832000	-1.532000	5.741000
H	-4.439000	-1.098000	5.189000
C	-3.358000	0.533000	6.110000
H	-2.323000	0.891000	6.170000
H	-3.928000	1.328000	5.614000
C	-3.907000	0.330000	7.533000
H	-3.339000	-0.467000	8.029000
H	-4.943000	-0.025000	7.473000
C	-3.856000	1.600000	8.399000
H	-2.820000	1.954000	8.459000
H	-4.423000	2.398000	7.903000
C	-4.406000	1.398000	9.821000
H	-5.442000	1.045000	9.760000

H	-3.839000	0.600000	10.317000
C	-4.354000	2.668000	10.687000
H	-3.318000	3.022000	10.749000
H	-4.921000	3.466000	10.193000
C	-4.903000	2.466000	12.110000
H	-4.336000	1.669000	12.604000
H	-5.938000	2.112000	12.049000
C	-4.848000	3.740000	12.968000
H	-5.246000	3.563000	13.970000
H	-3.821000	4.098000	13.076000
H	-5.433000	4.545000	12.515000
C	-9.471000	3.265000	-4.521000
H	-9.959000	3.333000	-3.541000
H	-8.767000	4.105000	-4.571000
C	-10.530000	3.429000	-5.625000
H	-10.042000	3.359000	-6.604000
H	-11.235000	2.591000	-5.574000
N	0.279000	-3.076000	-1.569000
C	1.673000	-2.819000	-1.962000
H	1.915000	-3.523000	-2.761000
H	1.768000	-1.823000	-2.382000
C	2.661000	-2.981000	-0.791000
H	2.460000	-2.202000	-0.050000
H	2.497000	-3.943000	-0.293000
C	4.120000	-2.875000	-1.266000
H	4.333000	-3.692000	-1.968000

H	4.241000	-1.941000	-1.820000
C	5.136000	-2.924000	-0.112000
H	4.944000	-2.086000	0.568000
H	4.986000	-3.839000	0.475000
C	6.597000	-2.863000	-0.590000
H	6.729000	-1.975000	-1.221000
H	6.804000	-3.728000	-1.232000
C	7.621000	-2.824000	0.557000
H	7.425000	-1.946000	1.183000
H	7.478000	-3.699000	1.202000
C	9.080000	-2.784000	0.072000
H	9.210000	-1.932000	-0.606000
H	9.288000	-3.682000	-0.523000
C	10.108000	-2.682000	1.212000
H	9.905000	-1.778000	1.799000
H	9.976000	-3.528000	1.897000
C	11.566000	-2.650000	0.722000
H	11.691000	-1.818000	0.018000
H	11.775000	-3.564000	0.153000
C	12.596000	-2.512000	1.855000
H	12.388000	-1.595000	2.421000
H	12.472000	-3.342000	2.562000
C	14.053000	-2.481000	1.363000
H	14.174000	-1.656000	0.651000
H	14.263000	-3.399000	0.803000
C	15.075000	-2.328000	2.499000

H 16.098000 -2.309000 2.116000
H 14.910000 -1.401000 3.055000
H 15.002000 -3.156000 3.210000
C -11.303000 4.753000 -5.533000
H -12.047000 4.837000 -6.328000
H -11.827000 4.838000 -4.577000
H -10.629000 5.610000 -5.617000
I -2.784000 -8.580000 -1.309000

SQS4

C 0.744000 -3.674000 -4.104000
C -0.567000 -4.107000 -3.886000
C -1.018000 -5.276000 -4.485000
C -0.141000 -6.005000 -5.305000
C 1.168000 -5.560000 -5.511000
C 1.634000 -4.384000 -4.909000
H -2.029000 -5.629000 -4.327000
H 1.836000 -6.130000 -6.143000
H 2.649000 -4.052000 -5.071000
C -0.162000 -2.074000 -2.717000
C -0.395000 -0.934000 -1.948000
H -1.381000 -0.931000 -1.504000
C 0.281000 0.232000 -1.594000
C 1.498000 1.074000 -1.745000
O 2.590000 1.009000 -2.363000
C 0.920000 2.102000 -0.867000

C	-0.306000	1.288000	-0.735000
C	1.476000	3.368000	-0.623000
C	1.132000	4.450000	0.163000
H	2.354000	3.539000	-1.241000
O	-1.428000	1.378000	-0.178000
C	1.045000	6.661000	1.028000
C	0.142000	5.828000	1.714000
C	-0.674000	6.318000	2.737000
H	-1.381000	5.688000	3.256000
C	0.336000	8.512000	2.396000
C	0.464000	9.934000	2.731000
O	1.231000	10.740000	2.185000
N	0.229000	4.521000	1.205000
C	1.527000	6.383000	-1.450000
H	0.459000	6.422000	-1.669000
H	1.934000	7.392000	-1.545000
H	2.008000	5.747000	-2.194000
C	-0.452000	3.371000	1.805000
H	-0.829000	3.654000	2.784000
H	-1.260000	3.003000	1.177000
H	0.264000	2.558000	1.930000
C	-0.565000	7.669000	3.070000
H	-1.183000	8.082000	3.852000
C	1.150000	7.995000	1.363000
H	1.836000	8.662000	0.859000
C	1.781000	5.840000	-0.021000

C	3.304000	5.790000	0.271000
H	3.499000	5.401000	1.271000
H	3.816000	5.154000	-0.453000
H	3.728000	6.794000	0.205000
C	-4.739000	-1.320000	-3.842000
H	-4.321000	-0.672000	-4.621000
H	-5.160000	-2.191000	-4.359000
C	-5.866000	-0.571000	-3.111000
H	-6.284000	-1.219000	-2.330000
H	-5.446000	0.299000	-2.594000
C	-6.998000	-0.111000	-4.046000
H	-6.582000	0.540000	-4.823000
H	-7.413000	-0.983000	-4.567000
C	-8.133000	0.630000	-3.318000
H	-8.548000	-0.021000	-2.539000
H	-7.720000	1.503000	-2.799000
C	-9.267000	1.085000	-4.253000
H	-8.853000	1.739000	-5.031000
H	-9.677000	0.212000	-4.775000
O	-0.376000	10.338000	3.758000
H	-0.249000	11.289000	3.938000
C	-1.269000	-3.141000	-2.935000
C	-1.627000	-3.955000	-1.632000
H	-2.496000	-4.570000	-1.894000
H	-0.808000	-4.658000	-1.458000
C	-2.528000	-2.561000	-3.678000

H	-3.021000	-3.419000	-4.146000
H	-2.161000	-1.941000	-4.503000
C	-3.606000	-1.781000	-2.904000
H	-3.186000	-0.902000	-2.411000
H	-4.034000	-2.412000	-2.121000
C	-1.905000	-3.232000	-0.301000
H	-0.997000	-2.732000	0.045000
H	-2.659000	-2.452000	-0.415000
C	-2.376000	-4.218000	0.785000
H	-1.634000	-5.018000	0.899000
H	-3.303000	-4.705000	0.457000
C	-2.613000	-3.547000	2.149000
H	-1.681000	-3.078000	2.487000
H	-3.337000	-2.733000	2.029000
C	-3.115000	-4.517000	3.232000
H	-2.390000	-5.332000	3.354000
H	-4.047000	-4.986000	2.893000
C	-3.354000	-3.844000	4.594000
H	-2.421000	-3.381000	4.936000
H	-4.073000	-3.026000	4.470000
C	-3.867000	-4.809000	5.677000
H	-3.147000	-5.626000	5.803000
H	-4.799000	-5.273000	5.333000
C	-4.109000	-4.133000	7.037000
H	-3.177000	-3.669000	7.380000
H	-4.829000	-3.315000	6.910000

C	-4.624000	-5.096000	8.120000
H	-5.556000	-5.561000	7.776000
H	-3.904000	-5.913000	8.249000
C	-4.869000	-4.419000	9.480000
H	-3.938000	-3.952000	9.824000
H	-5.591000	-3.604000	9.353000
C	-5.380000	-5.382000	10.565000
H	-4.658000	-6.196000	10.693000
H	-6.310000	-5.850000	10.221000
C	-5.623000	-4.696000	11.918000
H	-5.981000	-5.407000	12.667000
H	-4.704000	-4.244000	12.301000
H	-6.370000	-3.903000	11.830000
C	-10.406000	1.821000	-3.527000
H	-10.820000	1.168000	-2.749000
H	-9.997000	2.695000	-3.006000
C	-11.540000	2.275000	-4.461000
H	-11.127000	2.928000	-5.238000
H	-11.948000	1.401000	-4.983000
N	0.961000	-2.459000	-3.402000
C	2.272000	-1.793000	-3.434000
H	2.689000	-1.952000	-4.430000
H	2.153000	-0.720000	-3.311000
C	3.235000	-2.330000	-2.358000
H	2.838000	-2.075000	-1.371000
H	3.279000	-3.423000	-2.412000

C	4.646000	-1.737000	-2.514000
H	5.051000	-2.018000	-3.494000
H	4.570000	-0.647000	-2.503000
C	5.619000	-2.202000	-1.417000
H	5.226000	-1.900000	-0.438000
H	5.664000	-3.298000	-1.406000
C	7.039000	-1.637000	-1.588000
H	6.991000	-0.543000	-1.606000
H	7.433000	-1.943000	-2.565000
C	8.017000	-2.085000	-0.488000
H	7.628000	-1.771000	0.489000
H	8.057000	-3.181000	-0.464000
C	9.440000	-1.530000	-0.669000
H	9.400000	-0.435000	-0.693000
H	9.827000	-1.843000	-1.646000
C	10.421000	-1.977000	0.429000
H	10.036000	-1.661000	1.406000
H	10.459000	-3.073000	0.455000
C	11.844000	-1.425000	0.242000
H	11.806000	-0.330000	0.216000
H	12.228000	-1.741000	-0.736000
C	12.827000	-1.872000	1.338000
H	12.447000	-1.554000	2.316000
H	12.865000	-2.968000	1.365000
C	14.252000	-1.323000	1.148000
H	14.214000	-0.228000	1.120000

H 14.632000 -1.640000 0.170000
C 15.227000 -1.773000 2.246000
H 16.229000 -1.370000 2.081000
H 14.893000 -1.438000 3.232000
H 15.308000 -2.863000 2.278000
H -0.481000 -6.916000 -5.779000
C -12.674000 3.007000 -3.727000
H -13.462000 3.318000 -4.417000
H -13.130000 2.365000 -2.968000
H -12.301000 3.902000 -3.222000

Coordinates of optimized oxidized ISQ-X⁺ dyes

ISQF⁺

C -1.866000 0.552000 -4.475000
C -0.982000 1.623000 -4.639000
C -1.008000 2.368000 -5.812000
C -1.930000 1.982000 -6.780000
C -2.806000 0.911000 -6.639000
C -2.780000 0.169000 -5.454000
H -0.355000 3.208000 -5.995000
H -3.484000 0.665000 -7.441000
H -3.444000 -0.673000 -5.328000
C -0.597000 0.557000 -2.573000
C 0.016000 0.117000 -1.360000
H 0.461000 0.891000 -0.750000
C 0.250000 -1.166000 -0.946000

C 0.200000 -2.558000 -1.483000
O -0.231000 -3.089000 -2.523000
C 0.927000 -3.069000 -0.290000
C 1.003000 -1.674000 0.236000
C 1.444000 -4.328000 -0.073000
C 2.160000 -4.873000 1.014000
H 1.350000 -4.996000 -0.925000
O 1.526000 -1.114000 1.217000
C 3.651000 -6.203000 2.274000
C 3.018000 -5.265000 3.099000
C 3.288000 -5.154000 4.461000
H 2.810000 -4.416000 5.088000
C 4.871000 -6.987000 4.189000
C 5.871000 -7.928000 4.740000
O 6.469000 -8.783000 4.080000
N 2.105000 -4.504000 2.312000
C 4.273000 -5.694000 -0.140000
H 4.801000 -4.793000 0.171000
H 4.990000 -6.514000 -0.183000
H 3.876000 -5.536000 -1.144000
C 1.159000 -3.553000 2.913000
H 0.933000 -3.881000 3.924000
H 1.570000 -2.547000 2.913000
H 0.242000 -3.552000 2.328000
C 4.231000 -6.034000 4.999000
H 4.478000 -5.985000 6.048000

C	4.581000	-7.074000	2.814000
H	5.093000	-7.818000	2.220000
C	3.135000	-6.051000	0.853000
C	2.385000	-7.328000	0.379000
H	1.573000	-7.589000	1.059000
H	1.974000	-7.192000	-0.622000
H	3.084000	-8.164000	0.345000
C	3.901000	1.697000	-3.397000
H	3.984000	0.682000	-3.804000
H	4.024000	2.379000	-4.246000
C	5.036000	1.933000	-2.386000
H	4.945000	2.943000	-1.968000
H	4.918000	1.241000	-1.543000
C	6.441000	1.762000	-2.989000
H	6.528000	0.759000	-3.425000
H	6.567000	2.468000	-3.818000
C	7.572000	1.970000	-1.968000
H	7.481000	2.970000	-1.526000
H	7.448000	1.259000	-1.142000
C	8.980000	1.809000	-2.567000
H	9.069000	0.814000	-3.020000
H	9.110000	2.530000	-3.383000
O	6.082000	-7.761000	6.089000
H	6.746000	-8.394000	6.425000
C	-0.114000	1.766000	-3.394000
C	-0.460000	3.158000	-2.722000

H	0.084000	3.904000	-3.309000
H	-1.521000	3.349000	-2.901000
C	1.394000	1.633000	-3.820000
H	1.533000	2.337000	-4.646000
H	1.528000	0.636000	-4.252000
C	2.500000	1.889000	-2.784000
H	2.398000	1.215000	-1.930000
H	2.426000	2.908000	-2.397000
C	-0.189000	3.394000	-1.224000
H	-0.858000	2.772000	-0.620000
H	0.832000	3.120000	-0.953000
C	-0.421000	4.871000	-0.850000
H	-1.431000	5.168000	-1.154000
H	0.269000	5.500000	-1.425000
C	-0.237000	5.160000	0.650000
H	-0.942000	4.550000	1.227000
H	0.767000	4.846000	0.960000
C	-0.436000	6.643000	1.008000
H	-1.437000	6.959000	0.690000
H	0.273000	7.250000	0.434000
C	-0.262000	6.944000	2.506000
H	-0.980000	6.347000	3.082000
H	0.734000	6.618000	2.827000
C	-0.446000	8.431000	2.854000
H	-1.440000	8.758000	2.528000
H	0.275000	9.026000	2.281000

C	-0.279000	8.738000	4.352000
H	-1.006000	8.150000	4.925000
H	0.713000	8.404000	4.681000
C	-0.450000	10.228000	4.694000
H	0.281000	10.815000	4.124000
H	-1.439000	10.564000	4.360000
C	-0.290000	10.538000	6.192000
H	-1.024000	9.956000	6.763000
H	0.698000	10.198000	6.529000
C	-0.453000	12.029000	6.532000
H	-1.438000	12.369000	6.195000
H	0.282000	12.610000	5.964000
C	-0.294000	12.330000	8.030000
H	-0.416000	13.395000	8.238000
H	-1.037000	11.789000	8.622000
H	0.695000	12.032000	8.389000
C	10.108000	1.999000	-1.540000
H	10.021000	2.993000	-1.085000
H	9.980000	1.277000	-0.723000
C	11.518000	1.840000	-2.136000
H	11.604000	0.848000	-2.595000
H	11.649000	2.564000	-2.947000
N	-1.624000	-0.043000	-3.199000
C	-2.546000	-1.066000	-2.645000
H	-2.643000	-1.860000	-3.383000
H	-2.078000	-1.505000	-1.774000

C -3.909000 -0.462000 -2.257000
H -3.750000 0.318000 -1.506000
H -4.378000 0.020000 -3.117000
C -4.851000 -1.542000 -1.693000
H -4.998000 -2.326000 -2.445000
H -4.376000 -2.027000 -0.832000
C -6.220000 -0.985000 -1.266000
H -6.075000 -0.201000 -0.514000
H -6.700000 -0.502000 -2.125000
C -7.159000 -2.064000 -0.701000
H -6.675000 -2.553000 0.154000
H -7.307000 -2.845000 -1.456000
C -8.528000 -1.519000 -0.261000
H -8.382000 -0.741000 0.498000
H -9.013000 -1.028000 -1.113000
C -9.465000 -2.604000 0.298000
H -8.978000 -3.099000 1.147000
H -9.614000 -3.378000 -0.464000
C -10.834000 -2.064000 0.746000
H -10.686000 -1.291000 1.510000
H -11.321000 -1.567000 -0.102000
C -11.769000 -3.152000 1.300000
H -11.280000 -3.652000 2.145000
H -11.919000 -3.923000 0.534000
C -13.138000 -2.616000 1.753000
H -12.990000 -1.846000 2.520000

H	-13.628000	-2.116000	0.909000
C	-14.072000	-3.705000	2.306000
H	-13.582000	-4.206000	3.149000
H	-14.221000	-4.474000	1.539000
C	-15.436000	-3.162000	2.757000
H	-16.073000	-3.960000	3.146000
H	-15.322000	-2.414000	3.546000
H	-15.967000	-2.689000	1.926000
C	12.637000	2.022000	-1.100000
H	13.623000	1.904000	-1.554000
H	12.597000	3.016000	-0.647000
H	12.552000	1.288000	-0.294000
F	-1.971000	2.711000	-7.970000

ISQCI⁺

C	-2.118000	1.111000	-4.211000
C	-1.197000	2.159000	-4.266000
C	-1.243000	3.068000	-5.315000
C	-2.228000	2.882000	-6.288000
C	-3.143000	1.829000	-6.241000
C	-3.096000	0.917000	-5.183000
H	-0.548000	3.891000	-5.395000
H	-3.880000	1.720000	-7.022000
H	-3.796000	0.096000	-5.147000
C	-0.761000	0.787000	-2.398000
C	-0.170000	0.210000	-1.237000

H	0.360000	0.905000	-0.599000
C	-0.044000	-1.107000	-0.880000
C	-0.193000	-2.470000	-1.469000
O	-0.664000	-2.932000	-2.523000
C	0.505000	-3.075000	-0.301000
C	0.676000	-1.709000	0.277000
C	0.941000	-4.371000	-0.139000
C	1.634000	-4.999000	0.920000
H	0.800000	-4.999000	-1.014000
O	1.234000	-1.223000	1.278000
C	3.059000	-6.457000	2.113000
C	2.485000	-5.517000	2.980000
C	2.771000	-5.474000	4.342000
H	2.340000	-4.736000	5.002000
C	4.248000	-7.379000	3.986000
C	5.198000	-8.395000	4.491000
O	5.741000	-9.257000	3.794000
N	1.609000	-4.678000	2.231000
C	3.690000	-5.886000	-0.285000
H	4.271000	-5.030000	0.058000
H	4.359000	-6.742000	-0.369000
H	3.294000	-5.664000	-1.277000
C	0.723000	-3.699000	2.876000
H	0.491000	-4.049000	3.878000
H	1.188000	-2.716000	2.906000
H	-0.199000	-3.628000	2.304000

C	3.667000	-6.425000	4.838000
H	3.925000	-6.430000	5.885000
C	3.943000	-7.397000	2.611000
H	4.409000	-8.146000	1.985000
C	2.542000	-6.221000	0.704000
C	1.719000	-7.435000	0.188000
H	0.900000	-7.679000	0.865000
H	1.309000	-7.237000	-0.803000
H	2.371000	-8.305000	0.114000
C	3.722000	1.524000	-3.409000
H	3.689000	1.101000	-4.420000
H	3.943000	2.590000	-3.530000
C	4.859000	0.856000	-2.618000
H	4.881000	1.262000	-1.599000
H	4.647000	-0.216000	-2.517000
C	6.241000	1.040000	-3.267000
H	6.214000	0.649000	-4.291000
H	6.459000	2.111000	-3.354000
C	7.379000	0.352000	-2.493000
H	7.405000	0.739000	-1.467000
H	7.165000	-0.720000	-2.412000
C	8.762000	0.543000	-3.141000
H	8.734000	0.165000	-4.170000
H	8.980000	1.615000	-3.215000
O	5.428000	-8.291000	5.843000
H	6.057000	-8.972000	6.149000

C	-0.246000	2.070000	-3.078000
C	-0.493000	3.349000	-2.177000
H	-0.447000	4.196000	-2.868000
H	-1.527000	3.311000	-1.822000
C	1.229000	1.966000	-3.622000
H	1.511000	2.984000	-3.910000
H	1.193000	1.391000	-4.552000
C	2.340000	1.363000	-2.744000
H	2.150000	0.298000	-2.585000
H	2.369000	1.826000	-1.756000
C	0.442000	3.658000	-0.996000
H	0.439000	2.852000	-0.258000
H	1.471000	3.764000	-1.347000
C	0.025000	4.962000	-0.283000
H	-1.013000	4.874000	0.057000
H	0.045000	5.790000	-1.001000
C	0.926000	5.304000	0.916000
H	0.903000	4.475000	1.633000
H	1.965000	5.388000	0.577000
C	0.520000	6.603000	1.633000
H	-0.524000	6.526000	1.959000
H	0.558000	7.437000	0.922000
C	1.406000	6.931000	2.847000
H	1.365000	6.098000	3.559000
H	2.451000	7.006000	2.522000
C	1.005000	8.231000	3.566000

H	-0.042000	8.160000	3.883000
H	1.056000	9.067000	2.858000
C	1.883000	8.549000	4.789000
H	1.832000	7.713000	5.497000
H	2.931000	8.618000	4.473000
C	1.485000	9.848000	5.510000
H	1.542000	10.685000	4.804000
H	0.436000	9.781000	5.822000
C	2.358000	10.160000	6.737000
H	2.301000	9.323000	7.444000
H	3.408000	10.228000	6.427000
C	1.961000	11.459000	7.461000
H	0.912000	11.392000	7.769000
H	2.019000	12.295000	6.755000
C	2.837000	11.761000	8.686000
H	2.529000	12.687000	9.176000
H	2.772000	10.957000	9.424000
H	3.887000	11.868000	8.403000
C	9.900000	-0.153000	-2.377000
H	9.929000	0.223000	-1.347000
H	9.685000	-1.227000	-2.305000
C	11.283000	0.041000	-3.023000
H	11.253000	-0.331000	-4.053000
H	11.500000	1.112000	-3.091000
N	-1.848000	0.328000	-3.048000
C	-2.820000	-0.690000	-2.577000

H	-3.030000	-1.357000	-3.411000
H	-2.344000	-1.287000	-1.815000
C	-4.100000	-0.040000	-2.020000
H	-3.829000	0.626000	-1.194000
H	-4.579000	0.582000	-2.781000
C	-5.097000	-1.103000	-1.522000
H	-5.348000	-1.784000	-2.342000
H	-4.620000	-1.716000	-0.748000
C	-6.390000	-0.490000	-0.957000
H	-6.139000	0.205000	-0.147000
H	-6.876000	0.110000	-1.736000
C	-7.383000	-1.542000	-0.433000
H	-6.897000	-2.138000	0.348000
H	-7.632000	-2.239000	-1.242000
C	-8.679000	-0.931000	0.127000
H	-8.429000	-0.228000	0.930000
H	-9.169000	-0.341000	-0.656000
C	-9.668000	-1.981000	0.664000
H	-9.178000	-2.570000	1.448000
H	-9.918000	-2.685000	-0.138000
C	-10.964000	-1.371000	1.223000
H	-10.714000	-0.663000	2.023000
H	-11.456000	-0.784000	0.438000
C	-11.952000	-2.419000	1.765000
H	-11.460000	-3.007000	2.549000
H	-12.203000	-3.125000	0.965000

C	-13.247000	-1.810000	2.327000
H	-12.997000	-1.104000	3.128000
H	-13.740000	-1.221000	1.544000
C	-14.236000	-2.858000	2.867000
H	-13.743000	-3.447000	3.648000
H	-14.487000	-3.561000	2.066000
C	-15.525000	-2.241000	3.429000
H	-16.205999	-3.011000	3.800000
H	-15.310000	-1.561000	4.257000
H	-16.056000	-1.671000	2.662000
C	12.413000	-0.662000	-2.256000
H	13.380000	-0.502000	-2.738000
H	12.487000	-0.288000	-1.232000
H	12.243000	-1.741000	-2.204000
Cl	-2.313000	4.051000	-7.674000

ISQBr⁺

C	-2.003000	0.689000	-3.942000
C	-1.229000	1.850000	-3.998000
C	-1.382000	2.735000	-5.059000
C	-2.316000	2.411000	-6.049000
C	-3.078000	1.240000	-5.998000
C	-2.929000	0.355000	-4.927000
H	-0.804000	3.644000	-5.130000
H	-3.781000	1.018000	-6.787000
H	-3.512000	-0.554000	-4.891000

C -0.645000 0.572000 -2.106000
C 0.066000 0.043000 -0.987000
H 0.480000 0.776000 -0.307000
C 0.427000 -1.254000 -0.741000
C 0.465000 -2.577000 -1.433000
O 0.020000 -3.027000 -2.504000
C 1.306000 -3.145000 -0.345000
C 1.289000 -1.818000 0.337000
C 1.955000 -4.360000 -0.301000
C 2.796000 -4.931000 0.679000
H 1.875000 -4.940000 -1.216000
O 1.817000 -1.325000 1.350000
C 4.518000 -6.185000 1.699000
C 3.833000 -5.427000 2.658000
C 4.180000 -5.422000 4.006000
H 3.659000 -4.822000 4.736000
C 5.957000 -6.993000 3.445000
C 7.103000 -7.846000 3.832000
O 7.754000 -8.544000 3.050000
N 2.782000 -4.712000 2.011000
C 4.904000 -5.362000 -0.679000
H 5.349000 -4.442000 -0.301000
H 5.704000 -6.081000 -0.857000
H 4.419000 -5.149000 -1.632000
C 1.770000 -3.959000 2.766000
H 1.643000 -4.429000 3.738000

H	2.063000	-2.918000	2.873000
H	0.827000	-4.001000	2.227000
C	5.260000	-6.222000	4.390000
H	5.572000	-6.249000	5.423000
C	5.584000	-6.977000	2.087000
H	6.143000	-7.582000	1.387000
C	3.890000	-5.955000	0.335000
C	3.261000	-7.261000	-0.229000
H	2.535000	-7.686000	0.465000
H	2.768000	-7.078000	-1.184000
H	4.048000	-7.998000	-0.392000
C	3.682000	2.260000	-2.942000
H	3.842000	1.325000	-3.491000
H	3.690000	3.061000	-3.690000
C	4.841000	2.476000	-1.954000
H	4.675000	3.406000	-1.397000
H	4.839000	1.669000	-1.212000
C	6.220000	2.536000	-2.635000
H	6.382000	1.614000	-3.206000
H	6.228000	3.354000	-3.364000
C	7.381000	2.729000	-1.644000
H	7.216000	3.647000	-1.068000
H	7.377000	1.907000	-0.918000
C	8.761000	2.799000	-2.322000
H	8.924000	1.885000	-2.906000
H	8.768000	3.626000	-3.041000

O	7.383000	-7.790000	5.178000
H	8.143000	-8.362000	5.405000
C	-0.316000	1.918000	-2.779000
C	-0.754000	3.170000	-1.913000
H	-0.301000	4.036000	-2.406000
H	-1.835000	3.286000	-2.032000
C	1.174000	1.993000	-3.273000
H	1.206000	2.811000	-3.999000
H	1.380000	1.080000	-3.842000
C	2.303000	2.219000	-2.254000
H	2.314000	1.427000	-1.501000
H	2.149000	3.162000	-1.723000
C	-0.442000	3.217000	-0.406000
H	-1.029000	2.456000	0.118000
H	0.609000	3.001000	-0.208000
C	-0.780000	4.597000	0.194000
H	-1.819000	4.853000	-0.040000
H	-0.159000	5.361000	-0.288000
C	-0.572000	4.656000	1.717000
H	-1.222000	3.917000	2.200000
H	0.458000	4.361000	1.954000
C	-0.849000	6.045000	2.319000
H	-1.872000	6.351000	2.068000
H	-0.185000	6.781000	1.850000
C	-0.665000	6.096000	3.845000
H	-1.342000	5.372000	4.315000

H	0.352000	5.772000	4.097000
C	-0.915000	7.489000	4.447000
H	-1.928000	7.819000	4.188000
H	-0.231000	8.210000	3.985000
C	-0.744000	7.535000	5.975000
H	-1.434000	6.819000	6.438000
H	0.266000	7.198000	6.236000
C	-0.984000	8.930000	6.578000
H	-0.290000	9.645000	6.121000
H	-1.993000	9.269000	6.313000
C	-0.822000	8.974000	8.107000
H	-1.517000	8.260000	8.566000
H	0.186000	8.634000	8.374000
C	-1.061000	10.369000	8.711000
H	-2.067000	10.709000	8.442000
H	-0.365000	11.082000	8.255000
C	-0.901000	10.404000	10.238000
H	-1.078000	11.406000	10.634000
H	-1.607000	9.725000	10.724000
H	0.107000	10.102000	10.537000
C	9.922000	2.979000	-1.330000
H	9.759000	3.892000	-0.744000
H	9.917000	2.150000	-0.611000
C	11.303000	3.053000	-2.005000
H	11.465000	2.142000	-2.592000
H	11.310000	3.883000	-2.720000

N -1.646000 -0.039000 -2.767000
C -2.454000 -1.197000 -2.310000
H -2.538000 -1.892000 -3.144000
H -1.906000 -1.707000 -1.531000
C -3.831000 -0.752000 -1.781000
H -3.681000 -0.075000 -0.934000
H -4.372000 -0.187000 -2.544000
C -4.678000 -1.958000 -1.335000
H -4.831000 -2.632000 -2.186000
H -4.128000 -2.533000 -0.581000
C -6.044000 -1.545000 -0.761000
H -5.889000 -0.875000 0.093000
H -6.592000 -0.964000 -1.511000
C -6.905000 -2.740000 -0.317000
H -6.352000 -3.329000 0.424000
H -7.073000 -3.403000 -1.174000
C -8.262000 -2.325000 0.277000
H -8.093000 -1.666000 1.137000
H -8.812000 -1.729000 -0.461000
C -9.131000 -3.516000 0.715000
H -8.578000 -4.117000 1.447000
H -9.309000 -4.170000 -0.148000
C -10.482000 -3.097000 1.320000
H -10.303000 -2.446000 2.184000
H -11.033000 -2.493000 0.590000
C -11.356000 -4.286000 1.755000

H	-10.803000	-4.894000	2.482000
H	-11.539000	-4.935000	0.890000
C	-12.702000	-3.865000	2.367000
H	-12.519000	-3.218000	3.233000
H	-13.255000	-3.256000	1.642000
C	-13.580000	-5.052000	2.802000
H	-13.027000	-5.662000	3.525000
H	-13.765000	-5.698000	1.936000
C	-14.920000	-4.620000	3.415000
H	-15.518000	-5.484000	3.713000
H	-14.766000	-4.000000	4.302000
H	-15.511000	-4.038000	2.702000
C	12.456000	3.229000	-1.005000
H	13.421000	3.275000	-1.515000
H	12.341000	4.150000	-0.428000
H	12.494000	2.396000	-0.297000
Br	-2.552000	3.635000	-7.562000

ISQI⁺

C	-2.209000	0.920000	-3.314000
C	-1.449000	2.092000	-3.338000
C	-1.692000	3.056000	-4.307000
C	-2.700000	2.810000	-5.251000
C	-3.445000	1.623000	-5.228000
C	-3.206000	0.655000	-4.248000
H	-1.122000	3.973000	-4.343000

H -4.208000 1.448000 -5.971000
H -3.778000 -0.261000 -4.241000
C -0.709000 0.672000 -1.607000
C 0.092000 0.060000 -0.594000
H 0.545000 0.735000 0.120000
C 0.485000 -1.247000 -0.505000
C 0.481000 -2.491000 -1.331000
O -0.040000 -2.834000 -2.408000
C 1.401000 -3.159000 -0.372000
C 1.430000 -1.908000 0.442000
C 2.044000 -4.371000 -0.507000
C 2.946000 -5.055000 0.334000
H 1.888000 -4.845000 -1.472000
O 2.031000 -1.513000 1.458000
C 4.702000 -6.454000 1.070000
C 4.122000 -5.787000 2.157000
C 4.576000 -5.940000 3.464000
H 4.137000 -5.410000 4.296000
C 6.243000 -7.490000 2.594000
C 7.383000 -8.413000 2.791000
O 7.946000 -9.036000 1.886000
N 3.049000 -4.979000 1.679000
C 4.926000 -5.384000 -1.228000
H 5.427000 -4.520000 -0.792000
H 5.689000 -6.096000 -1.546000
H 4.376000 -5.058000 -2.112000

C	2.127000	-4.284000	2.589000
H	2.083000	-4.834000	3.525000
H	2.446000	-3.258000	2.756000
H	1.136000	-4.268000	2.141000
C	5.652000	-6.807000	3.670000
H	6.042000	-6.957000	4.665000
C	5.765000	-7.314000	1.281000
H	6.243000	-7.854000	0.476000
C	3.976000	-6.061000	-0.206000
C	3.265000	-7.282000	-0.855000
H	2.580000	-7.763000	-0.157000
H	2.708000	-6.983000	-1.744000
H	4.013000	-8.015000	-1.158000
C	3.540000	2.351000	-2.697000
H	3.615000	1.454000	-3.324000
H	3.512000	3.204000	-3.384000
C	4.791000	2.454000	-1.808000
H	4.719000	3.351000	-1.182000
H	4.815000	1.601000	-1.119000
C	6.105000	2.498000	-2.606000
H	6.167000	1.611000	-3.249000
H	6.092000	3.363000	-3.279000
C	7.359000	2.566000	-1.717000
H	7.298000	3.452000	-1.073000
H	7.371000	1.699000	-1.044000
C	8.674000	2.607000	-2.513000

H	8.729000	1.728000	-3.167000
H	8.669000	3.481000	-3.175000
O	7.769000	-8.517000	4.107000
H	8.522000	-9.131000	4.207000
C	-0.436000	2.068000	-2.197000
C	-0.793000	3.249000	-1.206000
H	-0.400000	4.153000	-1.682000
H	-1.881000	3.357000	-1.210000
C	1.006000	2.179000	-2.816000
H	0.983000	3.059000	-3.465000
H	1.143000	1.320000	-3.482000
C	2.227000	2.299000	-1.890000
H	2.278000	1.454000	-1.199000
H	2.154000	3.204000	-1.282000
C	-0.333000	3.209000	0.263000
H	-0.851000	2.405000	0.796000
H	0.737000	3.008000	0.345000
C	-0.640000	4.543000	0.971000
H	-1.708000	4.768000	0.874000
H	-0.109000	5.353000	0.457000
C	-0.252000	4.550000	2.460000
H	-0.796000	3.754000	2.982000
H	0.813000	4.310000	2.558000
C	-0.534000	5.895000	3.150000
H	-1.600000	6.135000	3.053000
H	0.008000	6.690000	2.624000

C	-0.144000	5.919000	4.638000
H	-0.692000	5.131000	5.169000
H	0.920000	5.672000	4.736000
C	-0.415000	7.272000	5.317000
H	-1.479000	7.518000	5.219000
H	0.131000	8.059000	4.782000
C	-0.022000	7.306000	6.804000
H	-0.571000	6.524000	7.341000
H	1.041000	7.056000	6.902000
C	-0.287000	8.664000	7.475000
H	0.261000	9.446000	6.936000
H	-1.350000	8.914000	7.378000
C	0.107000	8.703000	8.962000
H	-0.443000	7.924000	9.503000
H	1.170000	8.453000	9.061000
C	-0.156000	10.063000	9.631000
H	-1.218000	10.314000	9.533000
H	0.393000	10.842000	9.090000
C	0.242000	10.095000	11.115000
H	0.045000	11.073000	11.559000
H	-0.317000	9.350000	11.689000
H	1.306000	9.880000	11.242000
C	9.928000	2.654000	-1.624000
H	9.875000	3.532000	-0.968000
H	9.936000	1.779000	-0.962000
C	11.245000	2.696000	-2.418000

H	11.296000	1.822000	-3.077000
H	11.241000	3.574000	-3.074000
N	-1.756000	0.106000	-2.232000
C	-2.507000	-1.106000	-1.821000
H	-2.615000	-1.742000	-2.698000
H	-1.902000	-1.652000	-1.110000
C	-3.866000	-0.756000	-1.187000
H	-3.696000	-0.147000	-0.293000
H	-4.467000	-0.151000	-1.869000
C	-4.642000	-2.031000	-0.809000
H	-4.791000	-2.645000	-1.705000
H	-4.039000	-2.635000	-0.120000
C	-6.008000	-1.740000	-0.163000
H	-5.862000	-1.134000	0.739000
H	-6.611000	-1.133000	-0.848000
C	-6.784000	-3.018000	0.200000
H	-6.182000	-3.623000	0.889000
H	-6.919000	-3.625000	-0.703000
C	-8.158000	-2.746000	0.835000
H	-8.026000	-2.146000	1.744000
H	-8.759000	-2.136000	0.150000
C	-8.931000	-4.030000	1.181000
H	-8.332000	-4.638000	1.870000
H	-9.055000	-4.631000	0.272000
C	-10.313000	-3.771000	1.805000
H	-10.192000	-3.176000	2.718000

H	-10.911000	-3.160000	1.118000
C	-11.083000	-5.060000	2.137000
H	-10.486000	-5.670000	2.826000
H	-11.199000	-5.656000	1.224000
C	-12.469000	-4.809000	2.755000
H	-12.356000	-4.219000	3.672000
H	-13.066000	-4.197000	2.069000
C	-13.239000	-6.101000	3.079000
H	-12.643000	-6.713000	3.765000
H	-13.351000	-6.692000	2.162000
C	-14.624000	-5.845000	3.693000
H	-15.144000	-6.781000	3.906000
H	-14.543000	-5.289000	4.631000
H	-15.254000	-5.262000	3.016000
C	12.492000	2.734000	-1.521000
H	13.408000	2.766000	-2.114000
H	12.485000	3.615000	-0.873000
H	12.542000	1.851000	-0.879000
I	-3.103000	4.269000	-6.755000

SQS4⁺

C	-1.842000	0.480000	-4.683000
C	-0.956000	1.545000	-4.860000
C	-0.972000	2.258000	-6.054000
C	-1.877000	1.874000	-7.055000
C	-2.749000	0.794000	-6.861000

C -2.746000 0.075000 -5.661000
H -0.302000 3.090000 -6.221000
H -3.431000 0.507000 -7.649000
H -3.413000 -0.763000 -5.520000
C -0.602000 0.530000 -2.762000
C -0.011000 0.122000 -1.525000
H 0.417000 0.914000 -0.924000
C 0.224000 -1.147000 -1.075000
C 0.191000 -2.556000 -1.572000
O -0.217000 -3.118000 -2.603000
C 0.895000 -3.026000 -0.349000
C 0.954000 -1.618000 0.138000
C 1.416000 -4.276000 -0.085000
C 2.109000 -4.783000 1.034000
H 1.350000 -4.967000 -0.920000
O 1.453000 -1.028000 1.113000
C 3.583000 -6.061000 2.368000
C 2.921000 -5.105000 3.150000
C 3.158000 -4.953000 4.514000
H 2.658000 -4.203000 5.108000
C 4.766000 -6.775000 4.333000
C 5.762000 -7.689000 4.934000
O 6.384000 -8.556000 4.313000
N 2.020000 -4.377000 2.320000
C 4.257000 -5.615000 -0.045000
H 4.769000 -4.700000 0.253000

H	4.983000	-6.429000	-0.047000
H	3.882000	-5.490000	-1.061000
C	1.051000	-3.419000	2.870000
H	0.801000	-3.720000	3.884000
H	1.453000	-2.408000	2.854000
H	0.150000	-3.442000	2.262000
C	4.095000	-5.807000	5.100000
H	4.317000	-5.725000	6.153000
C	4.509000	-6.905000	2.955000
H	5.043000	-7.660000	2.394000
C	3.099000	-5.955000	0.931000
C	2.373000	-7.253000	0.478000
H	1.548000	-7.502000	1.145000
H	1.985000	-7.150000	-0.537000
H	3.080000	-8.083000	0.485000
C	3.910000	1.629000	-3.543000
H	3.991000	0.607000	-3.932000
H	4.051000	2.296000	-4.401000
C	5.030000	1.874000	-2.517000
H	4.940000	2.891000	-2.118000
H	4.893000	1.197000	-1.665000
C	6.443000	1.681000	-3.095000
H	6.528000	0.672000	-3.515000
H	6.588000	2.374000	-3.932000
C	7.560000	1.895000	-2.060000
H	7.469000	2.902000	-1.633000

H	7.418000	1.196000	-1.226000
C	8.975000	1.716000	-2.635000
H	9.063000	0.714000	-3.073000
H	9.122000	2.423000	-3.459000
O	5.937000	-7.482000	6.283000
H	6.599000	-8.098000	6.652000
C	-0.106000	1.717000	-3.606000
C	-0.457000	3.125000	-2.971000
H	0.098000	3.856000	-3.567000
H	-1.515000	3.315000	-3.172000
C	1.408000	1.571000	-4.005000
H	1.561000	2.258000	-4.842000
H	1.544000	0.565000	-4.416000
C	2.500000	1.842000	-2.957000
H	2.380000	1.187000	-2.091000
H	2.425000	2.870000	-2.592000
C	-0.209000	3.395000	-1.476000
H	-0.889000	2.788000	-0.869000
H	0.807000	3.126000	-1.182000
C	-0.443000	4.881000	-1.136000
H	-1.449000	5.173000	-1.459000
H	0.256000	5.496000	-1.714000
C	-0.278000	5.197000	0.360000
H	-0.994000	4.599000	0.938000
H	0.720000	4.884000	0.689000
C	-0.476000	6.686000	0.691000

H	-1.471000	7.002000	0.356000
H	0.244000	7.281000	0.116000
C	-0.319000	7.009000	2.186000
H	-1.047000	6.424000	2.761000
H	0.672000	6.683000	2.524000
C	-0.499000	8.501000	2.511000
H	-1.488000	8.829000	2.171000
H	0.231000	9.086000	1.938000
C	-0.345000	8.828000	4.007000
H	-1.079000	8.249000	4.580000
H	0.643000	8.494000	4.349000
C	-0.513000	10.322000	4.329000
H	0.222000	10.900000	3.757000
H	-1.500000	10.657000	3.985000
C	-0.361000	10.649000	5.824000
H	-1.099000	10.075000	6.397000
H	0.624000	10.312000	6.170000
C	-0.524000	12.145000	6.147000
H	-1.508000	12.482000	5.802000
H	0.213000	12.718000	5.574000
C	-0.370000	12.462000	7.642000
H	-0.490000	13.530000	7.837000
H	-1.116000	11.930000	8.237000
H	0.618000	12.167000	8.008000
C	10.089000	1.913000	-1.594000
H	10.000000	2.913000	-1.153000

H	9.945000	1.202000	-0.771000
C	11.506000	1.739000	-2.167000
H	11.594000	0.742000	-2.613000
H	11.653000	2.453000	-2.985000
N	-1.618000	-0.085000	-3.388000
C	-2.547000	-1.096000	-2.823000
H	-2.645000	-1.899000	-3.553000
H	-2.087000	-1.526000	-1.945000
C	-3.908000	-0.479000	-2.453000
H	-3.748000	0.312000	-1.713000
H	-4.368000	-0.007000	-3.324000
C	-4.861000	-1.542000	-1.877000
H	-5.014000	-2.335000	-2.618000
H	-4.392000	-2.020000	-1.009000
C	-6.225000	-0.966000	-1.460000
H	-6.072000	-0.172000	-0.719000
H	-6.699000	-0.491000	-2.327000
C	-7.176000	-2.026000	-0.879000
H	-6.698000	-2.506000	-0.016000
H	-7.333000	-2.817000	-1.621000
C	-8.539000	-1.458000	-0.449000
H	-8.384000	-0.668000	0.296000
H	-9.019000	-0.977000	-1.310000
C	-9.488000	-2.521000	0.130000
H	-9.007000	-3.004000	0.990000
H	-9.645000	-3.309000	-0.615000

C	-10.852000	-1.957000	0.565000
H	-10.696000	-1.169000	1.313000
H	-11.333000	-1.473000	-0.293000
C	-11.799000	-3.023000	1.143000
H	-11.317000	-3.506000	2.002000
H	-11.954000	-3.810000	0.396000
C	-13.163000	-2.463000	1.579000
H	-13.010000	-1.676000	2.327000
H	-13.647000	-1.979000	0.721000
C	-14.109000	-3.530000	2.156000
H	-13.627000	-4.012000	3.014000
H	-14.261000	-4.317000	1.409000
C	-15.471000	-2.965000	2.586000
H	-16.117001	-3.747000	2.991000
H	-15.355000	-2.198000	3.357000
H	-15.993000	-2.508000	1.741000
H	-1.899000	2.415000	-7.990000
C	12.611000	1.929000	-1.117000
H	13.603000	1.800000	-1.555000
H	12.570000	2.929000	-0.677000
H	12.511000	1.205000	-0.304000

Coordinates of optimized neutral ISQI --- I⁻ species

C	2.844000	1.936000	-1.304000
C	3.500000	0.788000	-0.854000
C	4.881000	0.782000	-0.707000

C	5.590000	1.952000	-1.020000
C	4.932000	3.100000	-1.467000
C	3.539000	3.104000	-1.614000
H	5.403000	-0.098000	-0.360000
H	5.493000	3.992000	-1.702000
H	3.038000	3.999000	-1.954000
C	1.153000	0.410000	-0.972000
C	-0.076000	-0.241000	-0.905000
H	0.006000	-1.237000	-0.491000
C	-1.407000	0.025000	-1.228000
C	-2.384000	0.958000	-1.846000
O	-2.357000	2.088000	-2.396000
C	-3.481000	0.011000	-1.592000
C	-2.510000	-0.940000	-1.007000
C	-4.799000	0.155000	-2.049000
C	-5.965000	-0.573000	-1.912000
H	-4.898000	1.018000	-2.703000
O	-2.520000	-2.099000	-0.526000
C	-8.166000	-1.382000	-2.292000
C	-7.556000	-2.092000	-1.242000
C	-8.212000	-3.134000	-0.583000
H	-7.742000	-3.694000	0.212000
C	-10.133000	-2.749000	-2.037000
C	-11.493000	-3.071000	-2.482000
O	-12.109000	-2.500000	-3.393000
N	-6.266000	-1.577000	-1.016000

C -6.861000 -0.533000 -4.298000
H -6.458000 -1.531000 -4.469000
H -7.759000 -0.416000 -4.907000
H -6.122000 0.198000 -4.631000
C -5.423000 -1.978000 0.113000
H -6.025000 -2.532000 0.827000
H -4.569000 -2.571000 -0.207000
H -5.037000 -1.083000 0.603000
C -9.508000 -3.453000 -0.993000
H -10.042000 -4.256000 -0.508000
C -9.448000 -1.700000 -2.691000
H -9.949000 -1.172000 -3.491000
C -7.203000 -0.320000 -2.802000
C -7.769000 1.107000 -2.578000
H -8.010000 1.272000 -1.527000
H -7.048000 1.863000 -2.890000
H -8.680000 1.240000 -3.164000
C 2.542000 -3.850000 -2.485000
H 2.387000 -3.414000 -3.479000
H 3.624000 -3.999000 -2.382000
C 1.833000 -5.213000 -2.416000
H 1.995000 -5.658000 -1.427000
H 0.752000 -5.062000 -2.511000
C 2.308000 -6.196000 -3.500000
H 2.155000 -5.744000 -4.487000
H 3.389000 -6.352000 -3.399000

C 1.594000 -7.559000 -3.455000
H 1.749000 -8.017000 -2.471000
H 0.513000 -7.403000 -3.553000
C 2.067000 -8.532000 -4.548000
H 1.916000 -8.069000 -5.531000
H 3.148000 -8.690000 -4.447000
O -12.074000 -4.112000 -1.775000
H -12.975000 -4.282000 -2.111000
C 2.473000 -0.309000 -0.578000
C 2.580000 -0.675000 0.951000
H 3.492000 -1.274000 1.051000
H 2.777000 0.257000 1.490000
C 2.806000 -1.511000 -1.539000
H 3.874000 -1.713000 -1.405000
H 2.699000 -1.140000 -2.564000
C 2.058000 -2.850000 -1.417000
H 0.982000 -2.714000 -1.532000
H 2.222000 -3.285000 -0.427000
C 1.428000 -1.392000 1.680000
H 0.547000 -0.747000 1.704000
H 1.128000 -2.304000 1.162000
C 1.823000 -1.749000 3.126000
H 2.154000 -0.843000 3.648000
H 2.686000 -2.426000 3.110000
C 0.680000 -2.403000 3.921000
H -0.178000 -1.720000 3.946000

H	0.339000	-3.300000	3.392000
C	1.072000	-2.779000	5.360000
H	1.419000	-1.881000	5.887000
H	1.925000	-3.468000	5.334000
C	-0.075000	-3.422000	6.159000
H	-0.926000	-2.731000	6.188000
H	-0.425000	-4.317000	5.631000
C	0.317000	-3.803000	7.597000
H	0.669000	-2.908000	8.125000
H	1.166000	-4.496000	7.568000
C	-0.831000	-4.442000	8.397000
H	-1.680000	-3.749000	8.427000
H	-1.185000	-5.336000	7.869000
C	-0.440000	-4.825000	9.835000
H	0.408000	-5.519000	9.805000
H	-0.086000	-3.931000	10.363000
C	-1.588000	-5.463000	10.636000
H	-2.438000	-4.770000	10.666000
H	-1.943000	-6.358000	10.109000
C	-1.198000	-5.846000	12.074000
H	-0.845000	-4.951000	12.600000
H	-0.349000	-6.538000	12.044000
C	-2.350000	-6.483000	12.866000
H	-2.040000	-6.743000	13.880000
H	-3.200000	-5.799000	12.943000
H	-2.703000	-7.397000	12.380000

C 1.351000 -9.893000 -4.516000
H 1.502000 -10.358000 -3.534000
H 0.271000 -9.736000 -4.617000
C 1.825000 -10.862000 -5.613000
H 1.676000 -10.395000 -6.593000
H 2.904000 -11.020000 -5.511000
N 1.452000 1.688000 -1.376000
C 0.520000 2.745000 -1.799000
H 1.029000 3.332000 -2.565000
H -0.356000 2.307000 -2.270000
C 0.079000 3.651000 -0.635000
H -0.513000 3.059000 0.069000
H 0.957000 4.011000 -0.088000
C -0.756000 4.843000 -1.133000
H -0.141000 5.465000 -1.796000
H -1.585000 4.463000 -1.735000
C -1.306000 5.715000 0.009000
H -1.950000 5.100000 0.649000
H -0.480000 6.059000 0.643000
C -2.104000 6.931000 -0.491000
H -2.896000 6.587000 -1.167000
H -1.447000 7.573000 -1.091000
C -2.733000 7.764000 0.639000
H -3.406000 7.125000 1.224000
H -1.947000 8.093000 1.330000
C -3.511000 8.991000 0.134000

H	-4.270000	8.663000	-0.587000
H	-2.829000	9.649000	-0.418000
C	-4.196000	9.793000	1.254000
H	-4.885000	9.136000	1.798000
H	-3.442000	10.115000	1.983000
C	-4.966000	11.023000	0.744000
H	-5.703000	10.702000	-0.002000
H	-4.273000	11.691000	0.219000
C	-5.682000	11.808000	1.856000
H	-6.379000	11.140000	2.378000
H	-4.948000	12.129000	2.605000
C	-6.452000	13.038000	1.344000
H	-7.180000	12.717000	0.590000
H	-5.755000	13.709000	0.829000
C	-7.175000	13.809000	2.458000
H	-7.712000	14.674000	2.061000
H	-7.903000	13.172000	2.968000
H	-6.469000	14.171000	3.210000
C	1.103000	-12.218000	-5.577000
H	1.463000	-12.882000	-6.367000
H	1.260000	-12.723000	-4.620000
H	0.025000	-12.094000	-5.713000
I	7.779000	1.972000	-0.788000
I	11.202000	1.998000	-0.429000

Coordinates of optimized neutral SQS4 --- I species

C -0.469000 -4.303000 -1.872000
C -1.787000 -4.137000 -1.438000
C -2.656000 -5.221000 -1.433000
C -2.188000 -6.472000 -1.868000
C -0.865000 -6.623000 -2.296000
C 0.020000 -5.536000 -2.302000
H -3.680000 -5.113000 -1.100000
H -0.515000 -7.592000 -2.627000
H 1.041000 -5.665000 -2.630000
C -0.611000 -2.072000 -1.321000
C -0.364000 -0.711000 -1.138000
H -1.211000 -0.193000 -0.709000
C 0.670000 0.193000 -1.368000
C 2.030000 0.432000 -1.921000
O 2.928000 -0.246000 -2.480000
C 1.940000 1.860000 -1.579000
C 0.576000 1.639000 -1.055000
C 2.872000 2.843000 -1.948000
C 3.000000 4.199000 -1.720000
H 3.636000 2.437000 -2.606000
O -0.353000 2.324000 -0.560000
C 3.710000 6.456000 -1.937000
C 2.745000 6.340000 -0.920000
C 2.302000 7.451000 -0.199000
H 1.549000 7.371000 0.571000
C 3.822000 8.826000 -1.522000

C	4.412000	10.124000	-1.865000
O	5.267000	10.322000	-2.740000
N	2.359000	4.994000	-0.791000
C	3.638000	5.037000	-4.041000
H	2.605000	5.339000	-4.218000
H	4.294000	5.713000	-4.592000
H	3.773000	4.029000	-4.436000
C	1.496000	4.499000	0.284000
H	1.398000	5.269000	1.044000
H	0.517000	4.201000	-0.085000
H	1.958000	3.621000	0.736000
C	2.853000	8.695000	-0.512000
H	2.531000	9.576000	0.022000
C	4.253000	7.688000	-2.240000
H	5.000000	7.812000	-3.012000
C	3.978000	5.081000	-2.530000
C	5.449000	4.644000	-2.298000
H	5.700000	4.662000	-1.237000
H	5.617000	3.635000	-2.676000
H	6.124000	5.323000	-2.822000
C	-4.902000	-0.352000	-2.510000
H	-4.463000	-0.267000	-3.511000
H	-5.642000	-1.161000	-2.567000
C	-5.616000	0.963000	-2.155000
H	-6.054000	0.878000	-1.154000
H	-4.877000	1.771000	-2.098000

C	-6.717000	1.349000	-3.158000
H	-6.278000	1.439000	-4.159000
H	-7.451000	0.537000	-3.218000
C	-7.440000	2.659000	-2.803000
H	-7.877000	2.570000	-1.801000
H	-6.707000	3.472000	-2.745000
C	-8.544000	3.041000	-3.804000
H	-8.106000	3.134000	-4.806000
H	-9.275000	2.226000	-3.864000
O	3.922000	11.174000	-1.101000
H	4.348000	12.010000	-1.372000
C	-1.999000	-2.690000	-0.999000
C	-2.335000	-2.720000	0.542000
H	-3.376000	-3.056000	0.613000
H	-1.735000	-3.521000	0.985000
C	-3.150000	-2.081000	-1.881000
H	-3.945000	-2.834000	-1.897000
H	-2.775000	-2.021000	-2.908000
C	-3.800000	-0.738000	-1.504000
H	-3.064000	0.067000	-1.472000
H	-4.244000	-0.805000	-0.507000
C	-2.149000	-1.466000	1.415000
H	-1.089000	-1.207000	1.469000
H	-2.655000	-0.598000	0.989000
C	-2.681000	-1.694000	2.844000
H	-2.192000	-2.575000	3.279000

H	-3.751000	-1.928000	2.800000
C	-2.465000	-0.484000	3.768000
H	-1.393000	-0.262000	3.828000
H	-2.933000	0.400000	3.320000
C	-3.021000	-0.688000	5.187000
H	-2.552000	-1.572000	5.637000
H	-4.094000	-0.910000	5.126000
C	-2.807000	0.524000	6.110000
H	-1.735000	0.742000	6.176000
H	-3.271000	1.408000	5.656000
C	-3.373000	0.327000	7.527000
H	-2.907000	-0.555000	7.982000
H	-4.445000	0.108000	7.460000
C	-3.161000	1.542000	8.446000
H	-2.089000	1.762000	8.514000
H	-3.626000	2.425000	7.990000
C	-3.728000	1.348000	9.863000
H	-4.800000	1.127000	9.796000
H	-3.262000	0.467000	10.321000
C	-3.518000	2.564000	10.782000
H	-2.447000	2.787000	10.848000
H	-3.986000	3.446000	10.327000
C	-4.081000	2.370000	12.200000
H	-3.612000	1.490000	12.655000
H	-5.152000	2.146000	12.135000
C	-3.869000	3.590000	13.109000

H	-4.275000	3.418000	14.109000
H	-2.806000	3.820000	13.217000
H	-4.360000	4.477000	12.699000
C	-9.273000	4.348000	-3.448000
H	-9.710000	4.256000	-2.446000
H	-8.543000	5.165000	-3.389000
C	-10.378000	4.730000	-4.447000
H	-9.941000	4.822000	-5.448000
H	-11.106000	3.913000	-4.507000
N	0.211000	-3.060000	-1.797000
C	1.630000	-2.951000	-2.169000
H	1.797000	-3.638000	-3.001000
H	1.849000	-1.953000	-2.537000
C	2.575000	-3.287000	-1.000000
H	2.452000	-2.530000	-0.219000
H	2.293000	-4.249000	-0.558000
C	4.045000	-3.326000	-1.452000
H	4.168000	-4.105000	-2.215000
H	4.289000	-2.374000	-1.929000
C	5.024000	-3.595000	-0.297000
H	4.918000	-2.804000	0.455000
H	4.753000	-4.533000	0.204000
C	6.492000	-3.668000	-0.751000
H	6.758000	-2.733000	-1.257000
H	6.598000	-4.462000	-1.499000
C	7.480000	-3.922000	0.400000

H	7.381000	-3.123000	1.145000
H	7.207000	-4.853000	0.912000
C	8.946000	-4.008000	-0.059000
H	9.219000	-3.078000	-0.571000
H	9.044000	-4.807000	-0.804000
C	9.938000	-4.264000	1.089000
H	9.843000	-3.464000	1.833000
H	9.663000	-5.194000	1.603000
C	11.402000	-4.356000	0.627000
H	11.677000	-3.426000	0.113000
H	11.496000	-5.155000	-0.118000
C	12.396000	-4.613000	1.773000
H	12.305000	-3.812000	2.517000
H	12.121000	-5.542000	2.288000
C	13.859000	-4.708000	1.309000
H	14.134000	-3.780000	0.794000
H	13.949000	-5.508000	0.565000
C	14.845000	-4.965000	2.459000
H	15.873000	-5.031000	2.097000
H	14.804000	-4.162000	3.200000
H	14.613000	-5.902000	2.973000
H	-2.855000	-7.324000	-1.871000
C	-11.101000	6.035000	-4.082000
H	-11.877000	6.279000	-4.811000
H	-11.579000	5.959000	-3.101000
H	-10.403000	6.875000	-4.045000

I -5.864000 -7.011000 -1.585000

Coordinates of optimized oxidized ISQI⁺ --- I⁻ species

C 2.822000 1.849000 -2.144000
C 3.569000 0.741000 -1.733000
C 4.956000 0.770000 -1.795000
C 5.577000 1.932000 -2.276000
C 4.830000 3.039000 -2.684000
C 3.430000 3.009000 -2.620000
H 5.547000 -0.078000 -1.482000
H 5.325000 3.926000 -3.050000
H 2.860000 3.872000 -2.931000
C 1.241000 0.314000 -1.477000
C 0.054000 -0.355000 -1.190000
H 0.224000 -1.323000 -0.738000
C -1.317000 -0.134000 -1.324000
C -2.400000 0.743000 -1.841000
O -2.487000 1.838000 -2.451000
C -3.421000 -0.208000 -1.372000
C -2.349000 -1.103000 -0.887000
C -4.796000 -0.116000 -1.634000
C -5.908000 -0.856000 -1.282000
H -5.015000 0.705000 -2.313000
O -2.255000 -2.232000 -0.345000
C -8.118000 -1.726000 -1.283000
C -7.340000 -2.361000 -0.298000

C -7.862000 -3.374000 0.510000
H -7.264000 -3.876000 1.256000
C -9.987000 -3.112000 -0.659000
C -11.389000 -3.485000 -0.876000
O -12.149000 -2.982000 -1.716000
N -6.045000 -1.810000 -0.297000
C -7.149000 -0.974000 -3.506000
H -6.749000 -1.974000 -3.679000
H -8.131000 -0.911000 -3.979000
H -6.489000 -0.252000 -3.987000
C -5.033000 -2.127000 0.714000
H -5.508000 -2.649000 1.540000
H -4.220000 -2.722000 0.304000
H -4.603000 -1.197000 1.090000
C -9.195000 -3.741000 0.318000
H -9.630000 -4.523000 0.921000
C -9.436000 -2.092000 -1.466000
H -10.065000 -1.622000 -2.210000
C -7.271000 -0.679000 -1.990000
C -7.836000 0.748000 -1.764000
H -7.923000 0.971000 -0.700000
H -7.190000 1.497000 -2.223000
H -8.828000 0.829000 -2.213000
C 2.506000 -4.002000 -2.939000
H 2.192000 -3.630000 -3.922000
H 3.595000 -4.125000 -2.992000

C 1.852000 -5.372000 -2.688000
H 2.171000 -5.753000 -1.711000
H 0.765000 -5.247000 -2.629000
C 2.187000 -6.409000 -3.774000
H 1.877000 -6.019000 -4.751000
H 3.275000 -6.538000 -3.827000
C 1.526000 -7.779000 -3.546000
H 1.838000 -8.175000 -2.572000
H 0.438000 -7.649000 -3.489000
C 1.857000 -8.807000 -4.641000
H 1.550000 -8.407000 -5.615000
H 2.945000 -8.939000 -4.695000
O -11.830000 -4.493000 -0.032000
H -12.766000 -4.700000 -0.220000
C 2.624000 -0.356000 -1.246000
C 2.967000 -0.627000 0.269000
H 3.900000 -1.203000 0.264000
H 3.216000 0.338000 0.718000
C 2.843000 -1.606000 -2.177000
H 3.924000 -1.781000 -2.193000
H 2.575000 -1.299000 -3.193000
C 2.159000 -2.950000 -1.868000
H 1.074000 -2.841000 -1.828000
H 2.479000 -3.321000 -0.891000
C 1.956000 -1.321000 1.201000
H 1.071000 -0.692000 1.321000

H	1.608000	-2.268000	0.785000
C	2.571000	-1.584000	2.589000
H	2.951000	-0.642000	3.003000
H	3.441000	-2.244000	2.482000
C	1.577000	-2.210000	3.582000
H	0.714000	-1.543000	3.696000
H	1.186000	-3.144000	3.161000
C	2.188000	-2.492000	4.965000
H	2.585000	-1.558000	5.382000
H	3.046000	-3.165000	4.850000
C	1.191000	-3.108000	5.962000
H	0.335000	-2.432000	6.079000
H	0.791000	-4.039000	5.543000
C	1.802000	-3.395000	7.344000
H	2.205000	-2.464000	7.761000
H	2.657000	-4.072000	7.227000
C	0.804000	-4.006000	8.342000
H	-0.050000	-3.328000	8.459000
H	0.400000	-4.937000	7.924000
C	1.414000	-4.295000	9.724000
H	2.268000	-4.974000	9.606000
H	1.818000	-3.365000	10.141000
C	0.416000	-4.906000	10.722000
H	-0.438000	-4.228000	10.840000
H	0.012000	-5.836000	10.306000
C	1.026000	-5.194000	12.105000

H	1.429000	-4.264000	12.521000
H	1.879000	-5.871000	11.987000
C	0.022000	-5.804000	13.095000
H	0.486000	-5.998000	14.065000
H	-0.826000	-5.133000	13.260000
H	-0.374000	-6.752000	12.720000
C	1.192000	-10.177000	-4.425000
H	1.499000	-10.580000	-3.453000
H	0.104000	-10.046000	-4.372000
C	1.523000	-11.201000	-5.525000
H	1.218000	-10.796000	-6.496000
H	2.610000	-11.333000	-5.577000
N	1.442000	1.571000	-1.993000
C	0.428000	2.583000	-2.330000
H	0.802000	3.133000	-3.196000
H	-0.495000	2.102000	-2.639000
C	0.140000	3.549000	-1.166000
H	-0.324000	2.989000	-0.349000
H	1.080000	3.957000	-0.777000
C	-0.791000	4.693000	-1.599000
H	-0.298000	5.286000	-2.381000
H	-1.689000	4.262000	-2.048000
C	-1.189000	5.621000	-0.439000
H	-1.714000	5.033000	0.324000
H	-0.288000	6.018000	0.044000
C	-2.086000	6.790000	-0.881000

H	-2.959000	6.391000	-1.410000
H	-1.543000	7.407000	-1.608000
C	-2.562000	7.677000	0.282000
H	-3.123000	7.062000	0.996000
H	-1.691000	8.062000	0.827000
C	-3.440000	8.857000	-0.169000
H	-4.288000	8.473000	-0.749000
H	-2.865000	9.494000	-0.853000
C	-3.972000	9.712000	0.994000
H	-4.554000	9.076000	1.671000
H	-3.127000	10.091000	1.582000
C	-4.843000	10.895000	0.537000
H	-5.674000	10.516000	-0.070000
H	-4.253000	11.543000	-0.123000
C	-5.407000	11.731000	1.698000
H	-5.999000	11.083000	2.355000
H	-4.578000	12.110000	2.308000
C	-6.277000	12.914000	1.238000
H	-7.100000	12.535000	0.621000
H	-5.683000	13.565000	0.587000
C	-6.848000	13.736000	2.403000
H	-7.461000	14.566000	2.043000
H	-7.474000	13.117000	3.052000
H	-6.048000	14.156000	3.019000
C	0.852000	-12.565000	-5.305000
H	1.109000	-13.269000	-6.101000

H 1.164000 -13.009000 -4.356000
H -0.237000 -12.470000 -5.284000
I 7.707000 2.017000 -2.359000
I 8.368000 2.773000 1.094000

Coordinates of optimized oxidized SQS4⁺ --- I⁻ species

C 1.075000 -3.608000 -2.957000
C -0.190000 -4.115000 -2.645000
C -0.497000 -5.437000 -2.939000
C 0.476000 -6.245000 -3.548000
C 1.739000 -5.724000 -3.851000
C 2.060000 -4.392000 -3.557000
H -1.471000 -5.849000 -2.704000
H 2.482000 -6.356000 -4.319000
H 3.039000 -4.002000 -3.790000
C -0.037000 -1.826000 -2.014000
C -0.412000 -0.564000 -1.552000
H -1.407000 -0.560000 -1.127000
C 0.127000 0.719000 -1.494000
C 1.253000 1.626000 -1.842000
O 2.366000 1.531000 -2.419000
C 0.543000 2.769000 -1.249000
C -0.595000 1.883000 -0.926000
C 0.957000 4.109000 -1.322000
C 0.476000 5.306000 -0.831000
H 1.831000 4.218000 -1.959000

O	-1.737000	1.985000	-0.415000
C	0.132000	7.639000	-0.540000
C	-0.701000	6.907000	0.326000
C	-1.596000	7.541000	1.192000
H	-2.250000	6.984000	1.847000
C	-0.810000	9.681000	0.324000
C	-0.842000	11.147000	0.298000
O	-0.146000	11.873000	-0.427000
N	-0.462000	5.532000	0.157000
C	0.719000	6.816000	-2.870000
H	-0.339000	6.683000	-3.097000
H	1.021000	7.809000	-3.209000
H	1.287000	6.073000	-3.431000
C	-1.038000	4.498000	1.020000
H	-1.474000	4.969000	1.896000
H	-1.783000	3.901000	0.498000
H	-0.245000	3.824000	1.345000
C	-1.639000	8.936000	1.180000
H	-2.322000	9.458000	1.833000
C	0.086000	9.018000	-0.545000
H	0.715000	9.611000	-1.195000
C	0.983000	6.671000	-1.350000
C	2.492000	6.861000	-1.046000
H	2.694000	6.753000	0.020000
H	3.091000	6.127000	-1.587000
H	2.811000	7.858000	-1.356000

C -4.629000 -1.874000 -3.314000
H -4.256000 -1.396000 -4.227000
H -4.941000 -2.886000 -3.602000
C -5.852000 -1.096000 -2.797000
H -6.224000 -1.574000 -1.882000
H -5.541000 -0.085000 -2.509000
C -6.995000 -1.006000 -3.822000
H -6.624000 -0.524000 -4.734000
H -7.300000 -2.019000 -4.113000
C -8.224000 -0.238000 -3.306000
H -8.593000 -0.719000 -2.392000
H -7.920000 0.776000 -3.017000
C -9.368000 -0.152000 -4.331000
H -9.000000 0.332000 -5.243000
H -9.668000 -1.166000 -4.622000
O -1.752000 11.696000 1.188000
H -1.731000 12.671000 1.127000
C -1.019000 -3.027000 -1.967000
C -1.332000 -3.531000 -0.504000
H -2.123000 -4.282000 -0.610000
H -0.449000 -4.076000 -0.158000
C -2.307000 -2.788000 -2.837000
H -2.693000 -3.784000 -3.080000
H -1.981000 -2.354000 -3.788000
C -3.485000 -1.964000 -2.286000
H -3.175000 -0.951000 -2.023000

H	-3.869000	-2.427000	-1.373000
C	-1.726000	-2.538000	0.605000
H	-0.886000	-1.872000	0.821000
H	-2.553000	-1.897000	0.297000
C	-2.126000	-3.273000	1.899000
H	-1.308000	-3.935000	2.211000
H	-2.986000	-3.923000	1.696000
C	-2.475000	-2.318000	3.053000
H	-1.608000	-1.682000	3.269000
H	-3.276000	-1.642000	2.731000
C	-2.907000	-3.041000	4.339000
H	-2.106000	-3.717000	4.663000
H	-3.774000	-3.677000	4.122000
C	-3.258000	-2.085000	5.491000
H	-2.390000	-1.453000	5.713000
H	-4.055000	-1.405000	5.165000
C	-3.702000	-2.804000	6.776000
H	-2.905000	-3.482000	7.105000
H	-4.570000	-3.437000	6.554000
C	-4.057000	-1.846000	7.926000
H	-3.190000	-1.213000	8.149000
H	-4.854000	-1.168000	7.597000
C	-4.503000	-2.564000	9.211000
H	-5.370000	-3.198000	8.988000
H	-3.706000	-3.240000	9.542000
C	-4.860000	-1.605000	10.360000

H	-3.995000	-0.968000	10.582000
H	-5.660000	-0.929000	10.031000
C	-5.303000	-2.321000	11.647000
H	-4.504000	-2.995000	11.976000
H	-6.167000	-2.958000	11.425000
C	-5.659000	-1.356000	12.787000
H	-5.965000	-1.895000	13.687000
H	-4.805000	-0.726000	13.051000
H	-6.482000	-0.694000	12.501000
C	-10.600000	0.611000	-3.815000
H	-10.968000	0.128000	-2.902000
H	-10.301000	1.626000	-3.525000
C	-11.745000	0.695000	-4.838000
H	-11.378000	1.179000	-5.750000
H	-12.043000	-0.319000	-5.129000
N	1.142000	-2.242000	-2.576000
C	2.376000	-1.465000	-2.765000
H	2.839000	-1.818000	-3.689000
H	2.142000	-0.415000	-2.912000
C	3.355000	-1.614000	-1.585000
H	2.902000	-1.170000	-0.694000
H	3.515000	-2.675000	-1.366000
C	4.700000	-0.927000	-1.875000
H	5.164000	-1.394000	-2.754000
H	4.511000	0.118000	-2.135000
C	5.681000	-0.999000	-0.692000

H	5.228000	-0.511000	0.179000
H	5.840000	-2.047000	-0.410000
C	7.040000	-0.343000	-0.991000
H	6.878000	0.702000	-1.279000
H	7.494000	-0.834000	-1.860000
C	8.023000	-0.397000	0.191000
H	7.573000	0.102000	1.058000
H	8.177000	-1.443000	0.486000
C	9.386000	0.248000	-0.114000
H	9.232000	1.293000	-0.409000
H	9.834000	-0.252000	-0.982000
C	10.372000	0.194000	1.065000
H	9.926000	0.696000	1.932000
H	10.523000	-0.851000	1.361000
C	11.736000	0.834000	0.755000
H	11.584000	1.879000	0.458000
H	12.181000	0.332000	-0.113000
C	12.724000	0.781000	1.932000
H	12.282000	1.285000	2.799000
H	12.875000	-0.264000	2.230000
C	14.089000	1.418000	1.619000
H	13.938000	2.462000	1.321000
H	14.531000	0.914000	0.752000
C	15.070000	1.360000	2.800000
H	16.030001	1.816000	2.545000
H	14.671000	1.888000	3.670000

H 15.263000 0.326000 3.101000
H 0.249000 -7.276000 -3.784000
C -12.972000 1.457000 -4.313000
H -13.766000 1.501000 -5.063000
H -13.383000 0.975000 -3.422000
H -12.711000 2.484000 -4.044000
I 1.676000 -8.017000 -0.997000

Table S8. Description of orbital occupancy of the donors and acceptors described in **Table 3** along with their bond orbitals and coefficients.

ISQ-H	BD (1)C4- H152: 62.39% C4(30.20% s, 69.80% p); 37.61% H 152 (100.00% s)
	RY*(1) I157: 100% (0.00% s, 100.00% p)
	LP (2) I157: 100% (3.18% s, 96.82% p)
	BD*(1)C4-H152: 37.61% C4(30.20% s, 69.80% p); 62.39% H152 s(100.00%)
ISQ-H ⁺	BD (1)C4-H152: 61.54% C4 (29.37% s, 70.63% p); 38.46% H152 (100.00% s)
	RY*(1) I157: 100% (0.50% s, 99.50% p)
ISQ-I	BD (1)C4- I156: 60.47% C4(22.84% s, 77.16% p); 39.53% I156 (5.08% s, 94.92% p)
	RY*(2) I157: 100% (66.00% s, 34.00% p)
ISQ-I ⁺	BD (1) C4 - I156: 55.55% C4 (21.20% s, 78.80% p); 44.45% I156(9.92% s, 90.08% p)
	RY*(1) I157 :100% (14.43% s, 85.57% p)

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