

Supporting Information

Molecular Engineering of Ruthenium-based Photosensitizers with Superior Photovoltaic Performance in DSSC: Novel *N*-Alkyl 2-Phenylindole-based Ancillary Ligand

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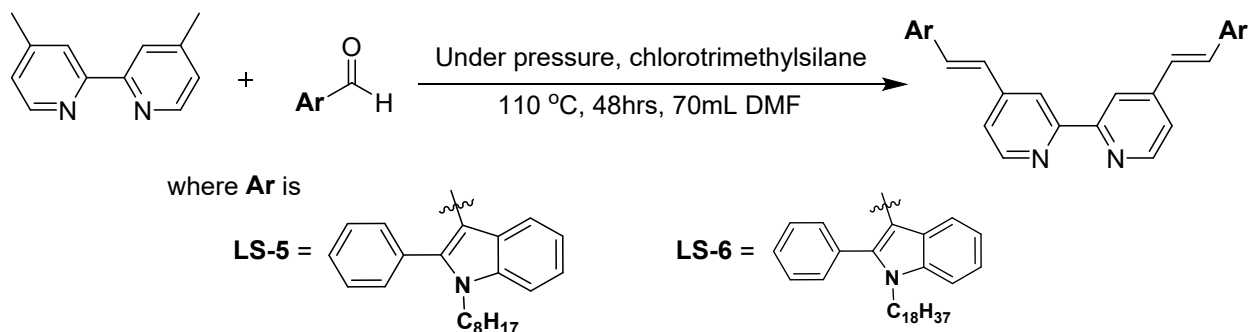
1. Materials

All chemicals were purchased from Sigma-Aldrich, Fisher Scientific or TCI-America and were used as received. Silica (230-400 mesh, Grade 60) for purification of dyes was purchased from Fischer Scientific. FT-IR (ATR) spectra were recorded on a Nicolet Nexus 470 FTIR spectrometer (Thermo Scientific, USA) and UV-Visible spectra were measured by using Cary 300 spectrophotometer. The Mass Spectrometry Analysis was carried out on a high-resolution mass spectrometer – the Thermo Fisher Scientific Executive Plus MS, a benchtop full-scan Orbitrap™ mass spectrometer using Heated Electrospray Ionization (HESI). ¹H-NMR spectra were recorded in a Bruker 500 MHz spectrometer. Fluorolog-3 spectrofluorometer (HORIBA Jobin Yvon Inc.) was used to measure fluorescence at room temperature.

2. Synthesis

2.1. Synthesis of Ligands

General procedure for the synthesis of ligands is given in Scheme 1S. The antenna ligand **LS-5** was synthesized in a pressure tube containing 4,4'-dimethyl-2,2'-bipyridine (5 mmol), 1-octyl-2-phenyl-1*H*-indole-3-carbaldehyde (10 mmol), 2.5 mL of chlorotrimethylsilane (30 mmol), and a magnetic stirrer bar in 70 mL of anhydrous DMF. Once the tube was closed with the cap, the reaction temperature was raised to 110 °C and allowed to run for 48 hours with continuous stirring. During the reaction, the color of the reaction mixture changed to dark red and then black. At the end of the reaction, the pressure was released after cooling the tube and the solvent was removed using rotary evaporator leaving dark red product; water was added into the flask and the mixture was filtered under vacuum to furnish the antenna ligand, which was thoroughly washed with water and *n*-hexane in sequence to obtain **LS-5**. It was then dried overnight under vacuum to obtain 84% yield. **LS-6** was also synthesized using the same procedure and used for next step without further purification.



Scheme 1S Synthetic route of electron-donating ancillary ligands **LS-5** and **LS-6**.

2.2. Synthesis of 2,2'-Bipyridinyl-4,4'-dicarboxylic Acid

2,2'-Bipyridinyl-4,4'-dicarboxylic acid was synthesized according to published procedure¹. In a three neck round bottom flask 4,4'-Dimethyl-2,2'-bipyridine (3g, 16.3mmol) was gradually added to a stirred solution of sodium dichromate ($\text{Na}_2\text{Cr}_2\text{O}_7$) (10.9g, 36.5mmol) in concentrated sulfuric acid (H_2SO_4) (93%, 45mL) and stirred for 30 min at 75 °C. After 30 min, the dark green reaction mixture was poured into cold water forming a light-yellow precipitate. The precipitate was then filtered under vacuum and dissolved in 10% aqueous sodium hydroxide. The product was crystallized by slowly acidifying the solution with 10 % aqueous hydrochloric acid at a pH of 2. The precipitation and acidification process was repeated three times to obtain white chromium free precipitates of 2,2'-Bipyridinyl-4,4'-dicarboxylic acid (2.50g, 88%).

2.3. Ru(2,2'-bipyridine-4,4'-dicarboxylic acid)-4,4'-bis((E)-2-(1-octyl-2-phenyl-1H-indol-3-yl)vinyl)-2,2'-bipyridine) (NCS)₂ (**SD-5**)

To a three-neck round-bottom flask, 0.12 mmol of dichloro-(*p*-cymene)-Ruthenium (II) dimer and 0.23 mmol of ancillary ligand were added into DMF under Argon protection. The mixture was reacted at 90 °C for 4 hours. Then, 0.23 mmol (0.06 g) of 2,2'-bipyridyl-4,4'-dicarboxylic acid was added and stirred for 5 hours at 140 °C. After that, excess of NH_4NCS (0.3 g) was sequentially added and the reaction mixture underwent another 4 hours stirring at 140 °C to complete the reaction. Upon completion, the mixture underwent rotary evaporation to get rid of most of the solvent. Ice was added to the residue to cool down the temperature and the unsolvable precipitate was filtered out under vacuum. The filtrate was

sequentially washed with deionized water (3 times) and diethyl ether (twice). The generated crude product was dried in the furnace (80 °C) and 0.4 g (80 %) of compound was collected.

The crude dyes were dissolved in methanol with small quantities of tetrabutylammonium hydroxide (TBAOH) and added into the column on the top of the silica gel (230-400mesh), and methanol was used as the mobile phase. The major dark red band was accumulated and dried over with rotary evaporation. The leftover was acidified by adding 0.1M HCl until the pH value reached 2.0, and the acidified mixture was maintained in a refrigerator for 2 days. Then, the precipitates were filtered out. To remove excess HCl, the solid was washed with plenty of de-ionized water for at least 5 times. After repeating the same purification technique three times, the dyes were obtained in the pure form. Product yield: 45 %. Color: dark red. FTIR-ATR ($\bar{\nu}/\text{cm}^{-1}$): 2102 (-N=C=S stretch); 1719 (C=O stretch in -COOH); ^1H NMR (500 MHz, DMSO- d_6) δ (ppm) 9.56 (s, 2H), 9.39 (s, 1H), 9.07 (d, J = 6.1 Hz, 1H), 8.91 (d, J = 5.0 Hz, 2H), 8.85 (s, 2H), 8.64 (d, J = 22.7 Hz, 1H), 8.49 (d, J = 14.6 Hz, 1H), 8.23 (d, J = 7.8 Hz, 2H), 7.91 (d, J = 4.9 Hz, 2H), 7.71 (d, J = 8.2 Hz, 2H), 7.67 – 7.46 (m, 12H), 7.35 (dt, J = 28.5, 7.2 Hz, 6H), 4.16 (t, J = 7.5 Hz, 4H), 1.58 (m, 12H), 1.32 (q, J = 7.3 Hz, 6H), 0.82 (t, J = 7.3 Hz, 12H).

2.4. Ru(2,2'-bipyridine-4,4'-dicarboxylic acid)-4,4'-bis((E)-2-(1-octadecyl-2-phenyl-1H-indol-3-yl)vinyl)-2,2'-bipyridine) (NCS)₂ (SD-6)

The aforementioned synthesizing and purifying procedures were also applied to generate **SD-6**. Product yield: 58 %. Color: dark red. FTIR-ATR ($\bar{\nu}/\text{cm}^{-1}$): 2102 (-N=C=S stretch); 1719 (C=O stretch in -COOH); ^1H NMR (500 MHz, DMSO- d_6) δ (ppm) 9.56 (s, 1H), 9.43 (d, J = 5.9 Hz, 2H), 9.11 (s, 1H), 9.09 – 9.05 (m, 4H), 8.94 (s, 2H), 8.91 (s, 2H), 8.67 (s, 2H), 8.51 (s, 2H), 8.29 (dd, J = 5.8, 1.8 Hz, 2H), 8.23 (d, J = 7.8 Hz, 1H), 7.84 (d, J = 5.9 Hz, 2H), 7.79 (d, J = 5.8 Hz, 2H), 7.71 (d, J = 8.1 Hz, 1H), 7.63 (ddt, J = 7.8, 5.8, 2.5 Hz, 6H), 7.34 – 7.30 (m, 2H), 7.08 (d, J = 5.9 Hz, 2H), 4.16 (t, J = 7.5 Hz, 2H), 3.16 (d, J = 9.9 Hz, 14H), 1.61 – 1.53 (m, 12H), 1.31 (hept, J = 6.9, 6.2 Hz, 22H), 1.08 – 1.03 (m, 6H), 0.95 (d, J = 7.3 Hz, 12H), 0.90 – 0.84 (m, 6H).

3. Analytical Measurements

3.1. UV-Visible and fluorescence spectra

UV-Visible spectra were recorded using a concentration of 2.0×10^{-5} M in dimethylformamide. The spectra were recorded at room temperature in a quartz cell (1.0 cm) on a Cary 3 Spectrophotometer. Molar absorptivity was calculated by using Beer-Lambert law:

$$A = c \epsilon l$$

Fluorescence spectra were measured in a 1 cm path length quartz cell using 2.0×10^{-5} M solutions of dimethylformamide on Fluorolog-311. The emitted light was detected in the steady state mode using a Hamamatsu R2658 detector. The emission was measured in the steady state mode by exciting at the λ_{max} for each dye with exit and entrance slits set at 5 nm at an integration time of 0.2 sec.

3.2. Fourier-Transform Infra-Red Spectroscopy

Attenuated Total Reflectance-Fourier Transform Infra-Red (ATR/FT-IR) spectra were recorded on a Thermo Nicolet, Nexus 470 FTIR Spectrophotometer with Omnic 7.2 software. The compound under investigation was placed in its powder form on a germanium crystal and a pressure probe was placed in position to apply consistent pressure to the sample. An average of 32 scans was used at a resolution of 4cm^{-1} . The complexes and intermediates were characterized using the same parameters. Figures 1S and 2S show the FT-IR of **SD-5** and **SD-6** in pure form, respectively.

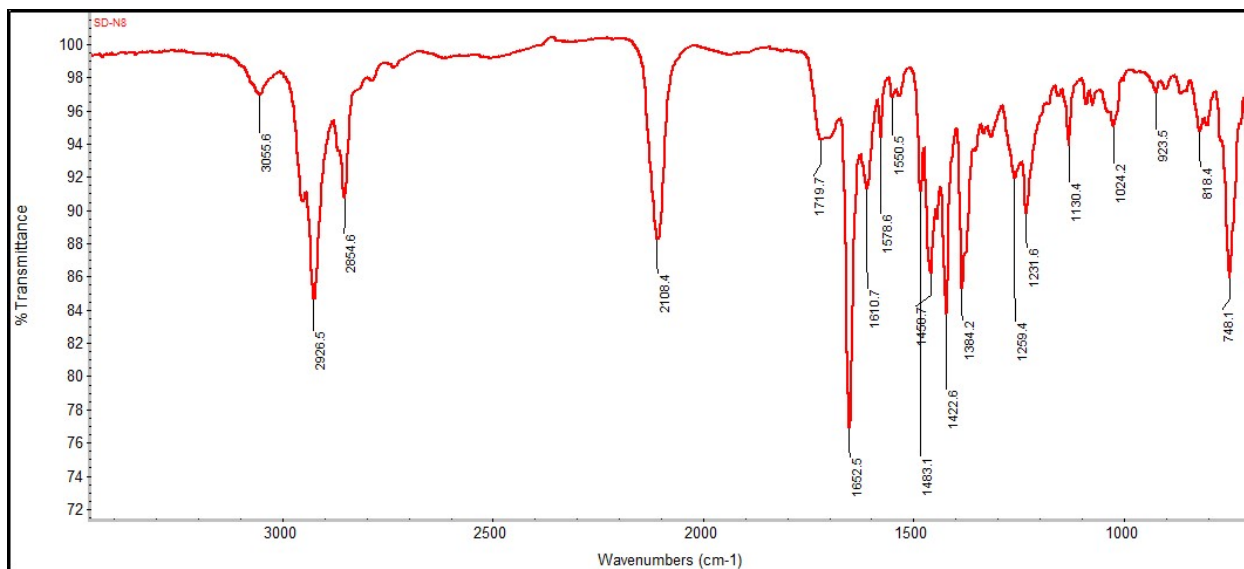


Figure 1S ATR/FT-IR spectrum of **SD-5**.

SD-5: 2108.4 cm⁻¹ (-NCS stretch, *N*-bonded isomer, very strong); 1719.7 cm⁻¹ (C=O stretch of –COOH).

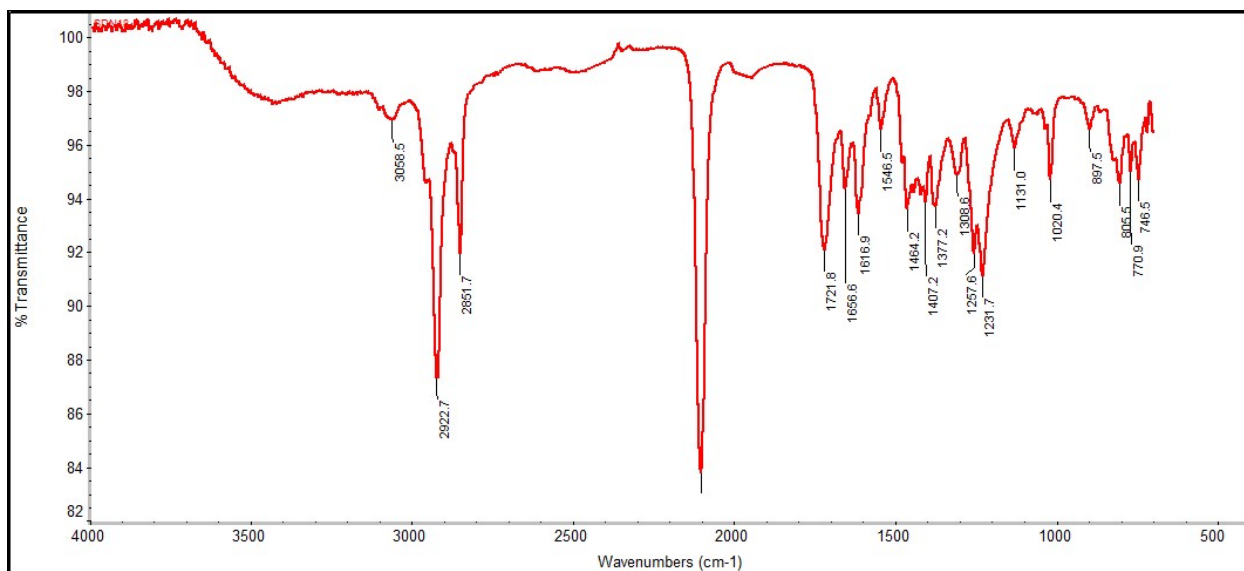


Figure 2S ATR/FT-IR spectrum of **SD-6**.

SD-6: 2102.8 cm⁻¹ (-NCS stretch, *N*-bonded isomer, very strong); 1721.8 cm⁻¹ (C=O stretch of –COOH).

3.3. Ground state oxidation potential (GSOP) and excited state oxidation potential (ESOP) measurements

The experimental HOMO and E_{0-0} energy values were calculated using a cyclic voltammetry (CV) and the UV-Vis absorption onset, respectively. The CV was carried in DMF with 0.1 M [TBA][PF₆] as an electrolyte at a scan rate of 50 mV s⁻¹. Glassy carbon was used as the working electrode (WE), Pt wire as counter electrode and Ag/Ag⁺ in acetonitrile was used as the reference electrode. Fc/Fc⁺ was used as internal reference, voltage measured was converted to NHE by addition of 0.63 V. Figures 3S and 4S show the CV plots of **SD-5** and **SD-6**, respectively.

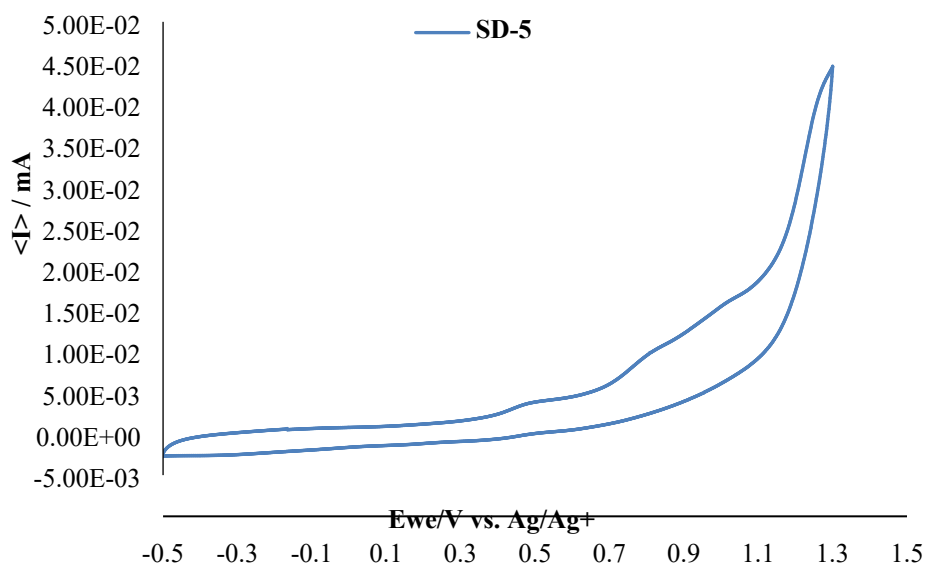


Figure 3S CV graph of **SD-5**.

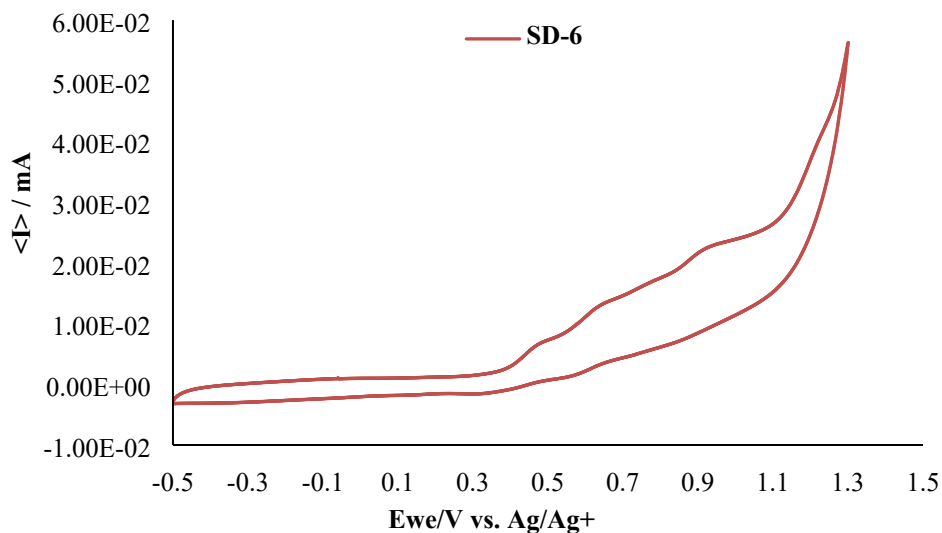


Figure 4S CV graph of **SD-6**.

3.4. Mass Spectroscopy

The Mass Spectrometry Analysis was carried out on a high-resolution mass spectrometer – the Thermo Fisher Scientific LTQ Orbitrap LX MS, a full-scan Orbitrap™ mass spectrometer – using Electrospray Ionization (ESI). Samples were dissolved in methanol and sonicated for 15 minutes. They were then diluted 1:1 with 50mM ammonium acetate and analyzed via syringe injection into the mass spectrometer at a flow rate of 10 $\mu\text{L}/\text{min}$. The mass spectrometer was operated in negative ion mode. The samples were analyzed via syringe injection. The Spray voltage was set at 3.5 kV and results were with the scan range of 400 – 3000 m/z.

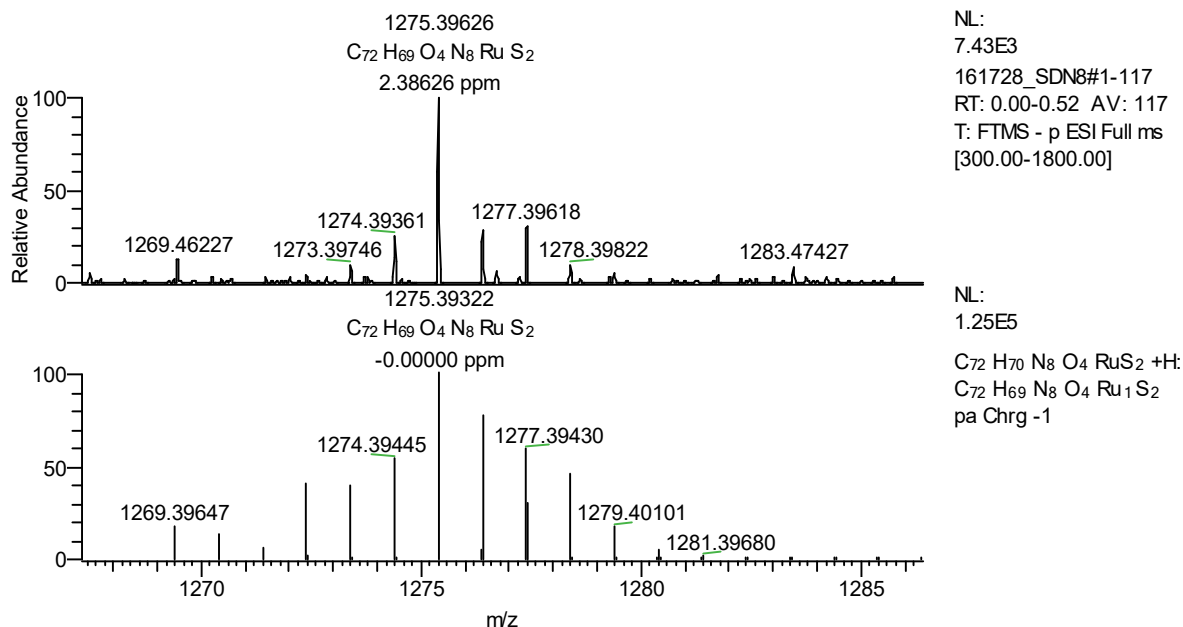


Figure 5S ESI mass spectrum of **SD-5**, $[M-H]^-$ Theo. $M/Z = 1275.39322$, Found. $M/Z = 1275.39626$, Error = 2.386 ppm.

3.5. 1H -NMR spectroscopy

1H -NMR spectra were recorded in a Bruker 500 MHz spectrometer. Splitting patterns reported here are: s (singlet), d (doublet), dd, (double-of-doublet), t (triplet) and m (multiplet). Chemical shifts (δ) and coupling constants (J) are reported in ppm and Hertz (Hz), respectively. Figure 6S and 7S display the 1H NMR spectra of **SD-5** and **SD-6**, respectively.

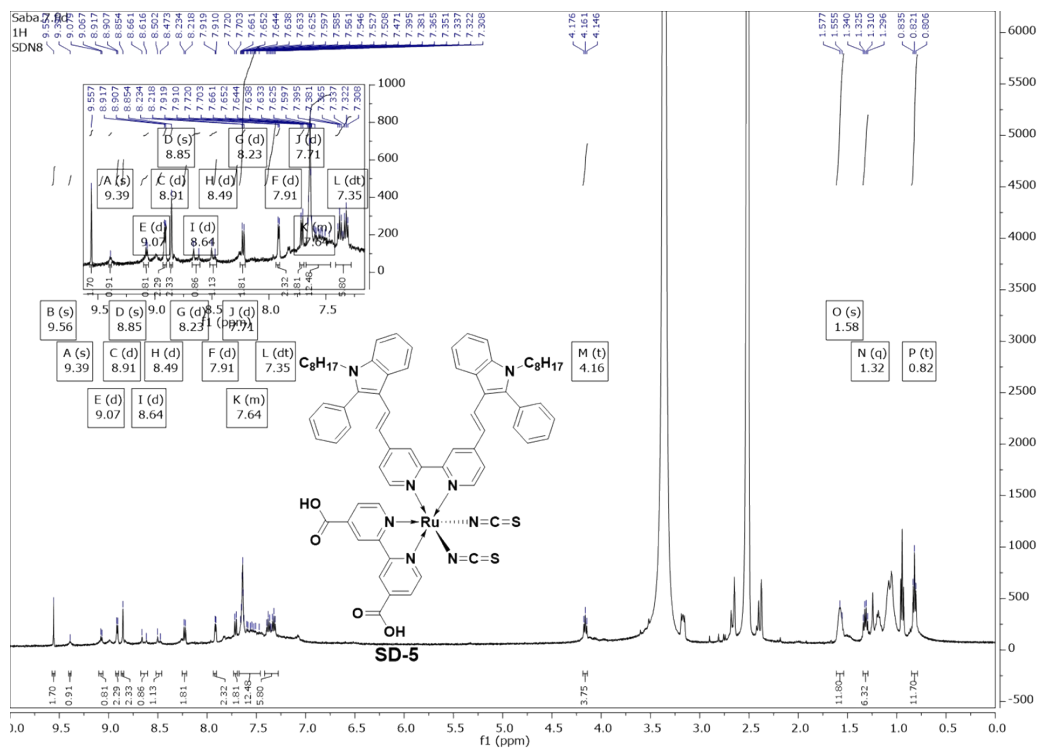


Figure 6S ^1H NMR spectra of SD-5.

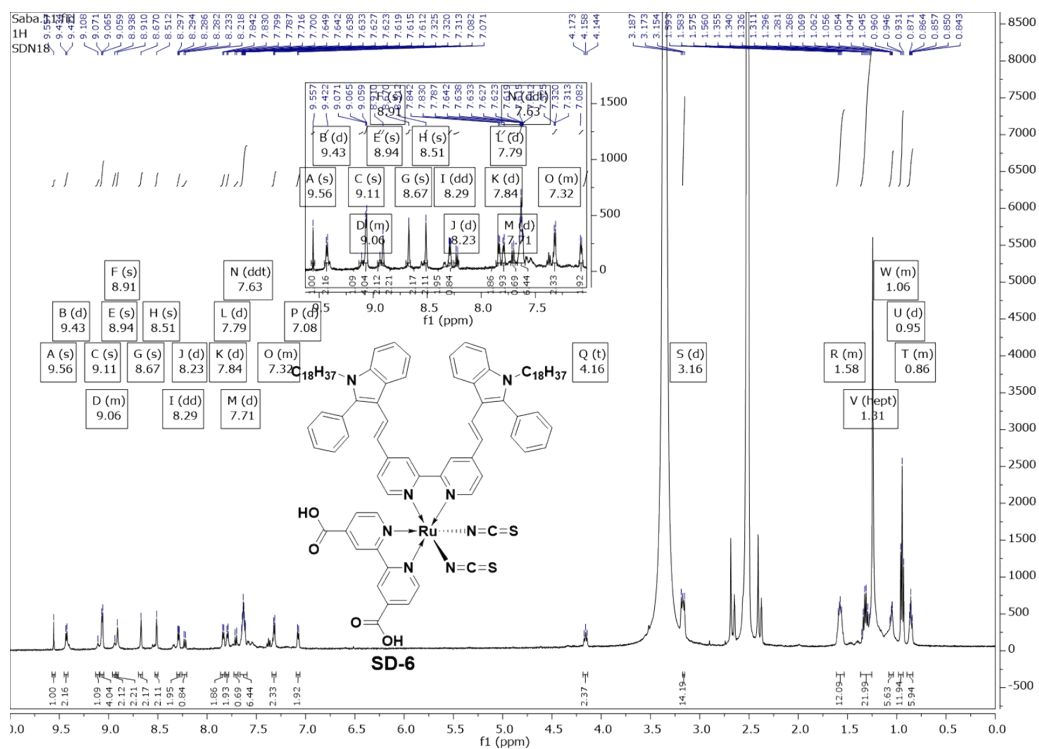


Figure 7S ^1H NMR spectra of SD-6.

4. Cell Preparations and Photovoltaic Characterizations

4.1. TiO_2 electrode preparation and device fabrication

The photo-anodes and counter electrodes were prepared using literature procedures². Fluorine-doped tin oxide (FTO) coated glasses (2.2 mm thickness, sheet resistance of $8 \Omega/\text{cm}^2$, TEC 8, Pilkington) were washed with detergent, water, acetone and ethanol, sequentially. After this FTO glass plates were immersed into a 40 mM aqueous TiCl_4 solution at 70°C for 30 min and washed with water and ethanol. Thin layer (8-12 nm thick) of TiO_2 (Solaronix, Ti-Nanoxide T/SP) was deposited (active area, 0.18 cm^2) on transparent conducting glass by squeegee printing. After drying the electrodes at 500°C for 30 min, scattering layer (5 nm thick) TiO_2 particles (Solaronix, Ti-Nanoxide T/SP) were printed. The TiO_2 electrodes were heated under an air flow at 350°C for 10 min, followed by heating at 500°C for 30 min. After cooling to room temperature, the TiO_2 electrodes were treated with 40 mM aqueous solution of TiCl_4 at 70°C for 30 min and then washed with water and ethanol. The electrodes were heated again at 500°C for 30 min and left to cool to 80°C before dipping into the dye solution. The dye solutions (0.3 mM) were prepared in 1:1:1 acetonitrile, tert-butyl alcohol and DMSO. Deoxycholic acid was added to the dye solution as a co-adsorbate at a concentration of 40 mM. The electrodes were immersed in the dye solutions with active area facing up and then kept at 25°C for 20 h to adsorb the dye onto the TiO_2 surface.

For preparing the counter electrode, pre-cut TCO glasses were washed with water followed by 0.1 M HCl in EtOH, and sonication in acetone bath for 10 min. These washed TCO were then dried at 400°C for 15 min. Thin layer of Pt-paste (Solaronix, Platisol T/SP) on TCO was printed and the printed electrodes were then cured at 450°C for 10 mins.

Photovoltaic and incident photon-to-current efficiency (IPCE) measurements were launched on sandwich cells, in which TiO_2 coated working electrodes and platinum coated counter electrodes were sealed using a $40 \mu\text{m}$ Surlyn spacer through heating of the polymer frame. The redox electrolyte consisted of a solution of 0.6 M DMPII, 0.05 M I_2 , 0.1 M LiI and 0.5 M TBP in acetonitrile (Solaronix, Iodolyte HI-30).

4.2. Photovoltaic measurements

Photovoltaic measurements of sealed cells were made by illuminating the cell through the conducting glass from the anode side with a solar simulator (SOL3A, Oriel) at AM 1.5 illuminations (light intensity: 100 mW cm⁻²).

4.3. Incident photon to current efficiency (IPCE) conversion

IPCE measurements were made on a Solar Cell Spectral Response Measurement System (Model QEX10). IPCE at each wavelength was calculated using Equation 1, where I_{SC} is the short-circuit photocurrent density (mA cm⁻²) under monochromatic irradiation, q is the elementary charge, λ is the wavelength of incident radiation in nm and P_0 is the incident radiative flux in W/m² ³.

$$IPCE(\lambda) = 1240 \left(\frac{I_{SC}}{q\lambda P_0} \right) \quad (1)$$

4.4. Electrochemical impedance spectroscopy (EIS)

The electrochemical impedance spectra were measured with an impedance analyzer potentiostat (Bio-Logic SP-150) under illumination using a solar simulator (SOL3A, Oriel) equipped with a 450 W xenon lamp (91160, Oriel). EIS spectra were recorded over a frequency range of 100 mHz to 200 kHz at room temperature. The applied bias voltage was set at the V_{oc} of the DSCs, with AC amplitude set at 10 mV. The electrical impedance spectra were fitted using Z-Fit software (Bio-Logic).

5. Molecular modeling

Equilibrium molecular geometries of new Ru(II) complexes were calculated using Adamo hybridized 1996 pure functional of Perdew, Burke and Ernzerhof (PBE1PBE) ⁴ and the full-electron basis set density Gauss double-zeta with polarization functions (DGDZVP) ^{5, 6}. The geometry optimization calculations were followed by energy calculations using time-dependent density functional theory (TD-DFT) utilizing the energy functional PBE1PBE and the basis set DGDZVP. The solvent (DMF) was accounted for by using the conductor-like polarizable continuum model (PCM), implemented in Gaussian 09, and the ground and excited state oxidation potentials were calculated. All DFT and TD-DFT jobs were submitted remotely at North Carolina State University's Supercomputer Jasta via HPC linkage.

Table 1S Cartesian coordinates for the optimized geometry of **SD-5**

Atoms	Cartesian coordinates		
0 1			
C	0.488993	0.982103	-0.31701
C	-0.93999	1.122084	0.023153
C	1.148196	-0.23921	-0.36442
C	2.509784	-0.32122	-0.69805
C	3.150475	0.901723	-0.97331
C	2.438438	2.081587	-0.90548
N	1.134682	2.144583	-0.58548
N	-1.40294	2.395837	0.032736
C	-2.69589	2.600232	0.337978
C	-3.57248	1.578836	0.643642
C	-3.12518	0.243776	0.635437
C	-1.77061	0.049098	0.319834
H	0.608141	-1.15361	-0.14402
H	4.199297	0.952539	-1.24414
H	-4.59602	1.83894	0.89037
H	-1.37711	-0.96123	0.304011
C	0.173824	3.769757	2.529489
C	0.652486	4.121509	3.78129
C	1.663552	5.077469	3.86413
H	0.238657	3.655031	4.667774
C	1.624975	5.243852	1.467074
C	2.152562	5.640961	2.691084
H	2.940527	6.382128	2.75472
C	2.080199	5.779481	0.174962
C	3.065511	6.753398	0.045529
C	1.821482	5.677393	-2.13567
C	3.430491	7.190993	-1.22269
H	3.555699	7.185334	0.910177

C	2.796922	6.64172	-2.33634
H	3.048261	6.954861	-3.3431
N	0.640763	4.310151	1.39369
N	1.468469	5.249919	-0.91427
C	-3.9583	-0.909	0.927671
H	-3.43544	-1.86029	0.945803
C	-5.29949	-0.86681	1.131639
H	-5.79689	0.09899	1.059027
C	3.152727	-1.62189	-0.74064
H	2.508187	-2.45905	-0.4923
C	4.455836	-1.83641	-1.05475
H	5.074379	-0.97035	-1.28445
C	2.243802	5.522251	5.162511
O	3.128774	6.349561	5.257371
O	1.683593	4.910788	6.211817
H	2.114065	5.251775	7.017847
C	4.487562	8.236055	-1.33586
O	4.742288	8.573842	-2.60438
H	5.437687	9.257607	-2.59498
O	5.054844	8.726966	-0.38006
Ru	-0.02846	3.869562	-0.51033
N	-0.55696	3.548681	-2.48088
N	-1.35892	5.446406	-0.39434
C	-0.87234	3.354921	-3.59703
C	-2.10989	6.349272	-0.3337
S	-1.30453	3.092698	-5.15818
S	-3.16581	7.602253	-0.2462
H	-3.01952	3.635735	0.334879
H	2.922851	3.028059	-1.11979
H	1.29376	5.220532	-2.96539
H	-0.61393	3.033252	2.421031

C	5.157041	-3.0868	-1.13333
C	4.693781	-4.45274	-1.02516
C	6.52511	-3.16088	-1.41567
C	5.821968	-5.27938	-1.24915
C	3.453937	-5.06694	-0.78309
N	6.917326	-4.47023	-1.49704
C	7.465076	-2.04519	-1.63212
C	5.753813	-6.67363	-1.21383
C	3.376673	-6.45404	-0.75294
H	2.5536	-4.48539	-0.61929
C	8.284296	-4.96078	-1.60316
C	8.057503	-1.8436	-2.88677
C	7.760449	-1.15799	-0.58895
C	4.515374	-7.25108	-0.96236
H	6.630744	-7.2931	-1.37745
H	2.41914	-6.93127	-0.56299
H	8.263442	-5.88128	-2.19377
H	8.864923	-4.23472	-2.17492
C	8.937165	-5.20357	-0.24552
C	8.931381	-0.77864	-3.09064
H	7.820032	-2.51399	-3.70895
C	8.634127	-0.09176	-0.79601
H	7.31	-1.31079	0.388228
H	4.427632	-8.33347	-0.92958
H	8.962541	-4.25778	0.309547
H	8.320336	-5.89736	0.338044
C	10.34894	-5.76152	-0.38785
C	9.222948	0.098866	-2.04545
H	9.379675	-0.63033	-4.06916
H	8.856864	0.587933	0.021854
H	10.31213	-6.70495	-0.94892

H	10.95632	-5.07057	-0.98765
C	11.03551	-6.00051	0.953562
H	9.904338	0.929869	-2.20576
H	10.42519	-6.6867	1.556085
H	11.07746	-5.05606	1.512828
C	12.44459	-6.56823	0.814389
H	12.40063	-7.51294	0.255184
H	13.05329	-5.88308	0.208565
C	13.13769	-6.80769	2.152076
H	12.52904	-7.49173	2.759574
H	13.18415	-5.86307	2.71168
C	14.54584	-7.37822	2.013295
H	15.15455	-6.69451	1.407464
H	14.49987	-8.32183	1.454136
C	15.23048	-7.61575	3.35461
H	14.66063	-8.32143	3.969327
H	16.23717	-8.02609	3.224299
H	15.32251	-6.68296	3.92219
C	-6.18629	-1.9582	1.423288
C	-5.92008	-3.33744	1.76622
C	-7.57585	-1.80629	1.468959
C	-7.17863	-3.94544	1.995639
C	-4.76186	-4.11501	1.930937
N	-8.16609	-2.99103	1.822198
C	-8.35768	-0.58467	1.205435
C	-7.31229	-5.29078	2.344854
C	-4.88668	-5.4525	2.286439
H	-3.7717	-3.69541	1.790697
C	-9.59021	-3.29331	1.775798
C	-9.12174	0.011144	2.219226
C	-8.32352	0.013306	-0.06116

C	-6.14918	-6.0376	2.486174
H	-8.28515	-5.74561	2.506178
H	-3.99275	-6.05742	2.411765
H	-9.80369	-4.02277	2.562342
H	-10.1414	-2.38671	2.031601
C	-10.0395	-3.816	0.414465
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H	-9.14011	-0.43148	3.212023
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H	-9.81634	-3.05808	-0.34643
H	-9.45557	-4.70718	0.154859
C	-11.5276	-4.14827	0.39325
C	-9.79846	1.767871	0.703377
H	-10.4206	1.634016	2.764015
H	-9.00497	1.635589	-1.29675
H	-11.7453	-4.89926	1.164425
H	-12.1052	-3.25394	0.662705
C	-12.0018	-4.66523	-0.96169
H	-10.3567	2.679645	0.509454
H	-11.4268	-5.56222	-1.22846
H	-11.7773	-3.91676	-1.73357
C	-13.4915	-4.99244	-0.99492
H	-13.7167	-5.73819	-0.22021
H	-14.0658	-4.09411	-0.73006
C	-13.9669	-5.51308	-2.34779
H	-13.395	-6.41348	-2.61177
H	-13.7388	-4.76935	-3.12388
C	-15.4574	-5.83673	-2.38583
H	-16.0293	-4.93643	-2.12616

H	-15.6862	-6.57767	-1.60881
C	-15.9216	-6.36083	-3.74024
H	-15.3911	-7.28064	-4.01061
H	-16.9935	-6.58366	-3.73846
H	-15.7356	-5.62728	-4.53264

Table 2S Cartesian coordinates for the optimized geometry of **SD-6**

Atoms	Cartesian coordinates		
0 1			
C	0.375714	2.858131	-0.35109
C	-0.94029	3.046415	0.289499
C	1.010051	1.626851	-0.45134
C	2.257227	1.497314	-1.08375
C	2.812773	2.684484	-1.59738
C	2.132989	3.877196	-1.46001
N	0.939126	3.98571	-0.85236
N	-1.39007	4.324969	0.305657
C	-2.58971	4.569794	0.86053
C	-3.38022	3.586323	1.42019
C	-2.94144	2.248606	1.420767
C	-1.68602	2.010925	0.838042
H	0.538822	0.741597	-0.03861
H	3.771287	2.698038	-2.10431
H	-4.32953	3.878546	1.855711
H	-1.30529	0.995881	0.812034
C	0.73406	5.788046	2.295231
C	1.495903	6.186839	3.381706
C	2.514103	7.116406	3.176641
H	1.291008	5.776787	4.363858
C	1.925457	7.163302	0.84723
C	2.727331	7.60682	1.893409

H	3.518954	8.329318	1.733456
C	2.079683	7.618017	-0.54309
C	3.030808	8.547586	-0.95206
C	1.286876	7.411754	-2.7216
C	3.099752	8.909284	-2.29275
H	3.722027	9.000488	-0.25093
C	2.209986	8.330477	-3.19644
H	2.226179	8.585129	-4.24984
N	0.934763	6.256932	1.054374
N	1.219901	7.056287	-1.42998
C	-3.68924	1.132896	1.972348
H	-3.1691	0.180076	1.958846
C	-4.95989	1.203676	2.44378
H	-5.47212	2.163305	2.394433
C	2.87673	0.187406	-1.16863
H	2.318144	-0.61404	-0.69587
C	4.058845	-0.07707	-1.78121
H	4.591182	0.753103	-2.24255
C	3.387148	7.607514	4.279808
O	4.281829	8.41474	4.123173
O	3.077528	7.062355	5.461164
H	3.687392	7.431522	6.126751
C	4.127326	9.906835	-2.70664
O	4.089333	10.16897	-4.01734
H	4.784384	10.82572	-4.20952
O	4.912762	10.42399	-1.93726
Ru	-0.16218	5.737801	-0.61716
N	-1.13514	5.331476	-2.39246
N	-1.41476	7.347863	-0.28679
C	-1.701	5.088697	-3.39426
C	-2.12204	8.271161	-0.11326

S	-2.48274	4.757236	-4.79853
S	-3.11591	9.553199	0.133616
H	-2.90813	5.606848	0.84844
H	2.553132	4.796804	-1.85269
H	0.570539	6.932897	-3.37975
H	-0.06962	5.070209	2.41152
C	4.725366	-1.34107	-1.91902
C	4.327193	-2.68007	-1.54293
C	5.961949	-1.46859	-2.56079
C	5.357258	-3.54538	-1.98616
C	3.215883	-3.24388	-0.8945
N	6.330504	-2.786	-2.61216
C	6.792747	-0.39802	-3.14333
C	5.319655	-4.92689	-1.78722
C	3.168354	-4.61875	-0.69791
H	2.393295	-2.63281	-0.54009
C	7.618547	-3.30918	-3.04555
C	7.003731	-0.32985	-4.52771
C	7.364906	0.578797	-2.31822
C	4.210404	-5.45348	-1.13725
H	6.1231	-5.57477	-2.12509
H	2.311047	-5.05631	-0.19367
H	7.443022	-4.27663	-3.5252
H	8.014916	-2.64474	-3.81534
C	8.620773	-3.44649	-1.90321
C	7.774796	0.693448	-5.07354
H	6.549332	-1.07196	-5.17931
C	8.134185	1.603487	-2.86719
H	7.211517	0.52913	-1.24346
H	4.149396	-6.52484	-0.96756
H	8.777094	-2.46121	-1.44718

H	8.201051	-4.09364	-1.12391
C	9.952316	-4.01332	-2.38403
C	8.342243	1.662123	-4.24465
H	7.926592	0.737908	-6.14844
H	8.573893	2.354046	-2.21617
H	9.78243	-4.98813	-2.8605
H	10.36745	-3.35876	-3.162
C	10.97318	-4.17287	-1.26151
H	8.942585	2.460705	-4.67174
H	10.56104	-4.83571	-0.48875
H	11.13526	-3.2006	-0.77691
C	12.3117	-4.72668	-1.74056
H	12.14773	-5.69464	-2.23365
H	12.72546	-4.05904	-2.50868
C	13.33276	-4.89892	-0.62008
H	12.92163	-5.57239	0.144468
H	13.49144	-3.93263	-0.12184
C	14.67466	-5.4428	-1.10149
H	15.08711	-4.7664	-1.8628
H	14.51545	-6.40659	-1.60447
C	15.69536	-5.62199	0.018317
H	15.285	-6.30243	0.777174
H	15.85117	-4.65937	0.524644
C	-5.7542	0.144074	3.000037
C	-5.39957	-1.19642	3.410432
C	-7.11225	0.296387	3.296501
C	-6.57918	-1.78336	3.930136
C	-4.2147	-1.95099	3.426014
N	-7.60116	-0.85248	3.860866
C	-7.95429	1.487387	3.082828
C	-6.61639	-3.08959	4.422192

C	-4.24232	-3.24896	3.921296
H	-3.27686	-1.543	3.065012
C	-9.00199	-1.1654	4.108511
C	-8.51512	2.170856	4.171427
C	-8.18376	1.967232	1.786728
C	-5.43222	-3.81623	4.409673
H	-7.53163	-3.52932	4.807329
H	-3.32809	-3.83616	3.931509
H	-9.05213	-1.80202	4.996669
H	-9.52132	-0.23841	4.35754
C	-9.67436	-1.84245	2.917635
C	-9.29178	3.308072	3.965023
H	-8.3268	1.820326	5.18308
C	-8.95991	3.107019	1.582939
H	-7.75923	1.439194	0.937023
H	-5.42697	-4.83504	4.786998
H	-9.61087	-1.17514	2.049351
H	-9.12306	-2.75385	2.657149
C	-11.1324	-2.18572	3.202763
C	-9.51704	3.778363	2.670497
H	-9.71577	3.831879	4.817284
H	-9.13144	3.467351	0.572393
H	-11.1882	-2.83747	4.084978
H	-11.6802	-1.26975	3.461382
C	-11.8209	-2.87112	2.026129
H	-10.1227	4.66627	2.511189
H	-11.2726	-3.78801	1.770905
H	-11.7599	-2.22193	1.142219
C	-13.2816	-3.21674	2.298235
H	-13.3426	-3.86008	3.186745
H	-13.8314	-2.29881	2.547495

C	-13.9664	-3.912	1.125276
H	-13.416	-4.83015	0.877735
H	-13.9029	-3.26975	0.236068
C	-15.428	-4.25839	1.392529
H	-15.9797	-3.3399	1.635868
H	-15.4918	-4.89739	2.284107
C	-16.1091	-4.95974	0.221051
H	-15.557	-5.87823	-0.02139
H	-16.0443	-4.32127	-0.67085
C	17.03928	-6.15892	-0.46532
H	16.8833	-7.12007	-0.97439
H	17.45038	-5.47671	-1.22221
C	18.05976	-6.342	0.654081
H	17.65017	-7.02692	1.409336
H	18.21352	-5.38165	1.165341
C	19.40497	-6.8742	0.168765
H	19.81495	-6.18819	-0.58529
H	19.25113	-7.83365	-0.34415
C	20.42541	-7.05957	1.28782
H	20.01649	-7.74737	2.040812
H	20.57782	-6.10065	1.802165
C	21.77141	-7.58862	0.801248
H	22.18061	-6.90011	0.049048
H	21.61896	-8.54695	0.285831
C	22.79188	-7.77551	1.920022
H	22.38345	-8.46519	2.671547
H	22.94354	-6.81758	2.43637
C	24.13833	-8.3026	1.432531
H	24.54718	-7.61242	0.681681
H	23.98673	-9.26012	0.915366
C	25.15866	-8.49082	2.550938

H	24.75127	-9.18191	3.301929
H	25.31082	-7.53386	3.069208
C	26.50577	-9.01688	2.064131
H	26.35398	-9.97247	1.54549
H	26.91404	-8.32557	1.315469
C	27.51755	-9.20343	3.189324
H	27.14967	-9.91471	3.937232
H	28.47292	-9.58234	2.811783
H	27.71524	-8.25632	3.703561
C	-17.571	-5.30702	0.485866
H	-17.6361	-5.94358	1.379121
H	-18.1242	-4.3884	0.72564
C	-18.2495	-6.01213	-0.68492
H	-17.696	-6.93065	-0.92423
H	-18.184	-5.37583	-1.57833
C	-19.7115	-6.36025	-0.42153
H	-19.7772	-6.99532	0.472747
H	-20.2657	-5.44168	-0.18398
C	-20.3881	-7.06783	-1.5919
H	-19.8336	-7.98635	-1.82912
H	-20.322	-6.43295	-2.48629
C	-21.8501	-7.41647	-1.32939
H	-21.9162	-8.05041	-0.43435
H	-22.405	-6.49791	-1.0935
C	-22.5253	-8.12589	-2.49939
H	-22.4589	-7.49225	-3.3946
H	-21.9705	-9.0446	-2.7349
C	-23.9875	-8.47452	-2.23753
H	-24.0543	-9.1073	-1.34172
H	-24.5428	-7.55577	-2.00334
C	-24.6618	-9.18555	-3.40685

H	-24.5952	-8.55383	-4.30358
H	-24.1077	-10.1052	-3.64111
C	-26.1243	-9.53401	-3.14687
H	-26.1915	-10.1649	-2.251
H	-26.6786	-8.61533	-2.91455
C	-26.7881	-10.2455	-4.32071
H	-27.8352	-10.4829	-4.10649
H	-26.7657	-9.62423	-5.22302
H	-26.275	-11.1851	-4.55405

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