

Supplementary Material for:

Enhancing the Photophysical Properties of NHC-Based Iron Sensitizers for Dye-Sensitized Solar Cells: A Computational Study

Wissam Helal,^{1,*} Ayat M. Siedat,^{1,2,*} Ahmad Musleh Alrub,³ Saleh Atiewi,^{4,5}
Ahmad S. Barham,¹ Mohammad I. Alkhatab,⁶ Basma Elzein^{7,8}

¹ *Department of Chemistry, The University of Jordan, Amman 11942, Jordan.*

² *Department of Chemistry, Al-Hussein Bin Talal University, Ma'an 71111, Jordan.*

³ *Department of Physics, Al-Hussein Bin Talal University, Ma'an 71111, Jordan.*

⁴ *Faculty of Information Technology, Al-Hussein Bin Talal University, Ma'an, Jordan 71110.*

⁵ *Faculty of Information Technology, Aqaba University of Technology, Aqaba, Jordan 77110.*

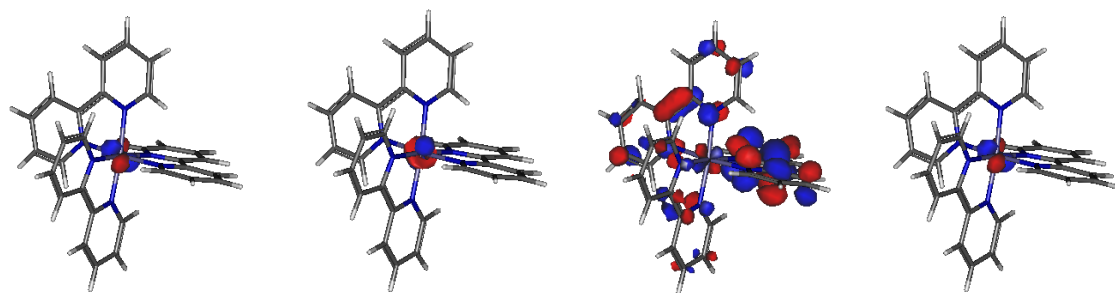
⁶ *ADNOC Technical Academy, Near Schlumberger - Al Shamkhah P.O.Box 898/13-
Abu Dhabi, United Arab Emirates.*

⁷ *Electrical Engineering Department, College of Engineerin, University of
Business and Technology, Jeddah, 21451, Saudi Arabia.*

⁸ *Sustainable Development Department, Global Council for Tolerance and Peace, 1605 Valetta,
Malta*

* Corresponding author.

E-mail: wissam.helal@ju.edu.jo (W.H.); ayat.saidat88@gmail.com (A.M.S.)

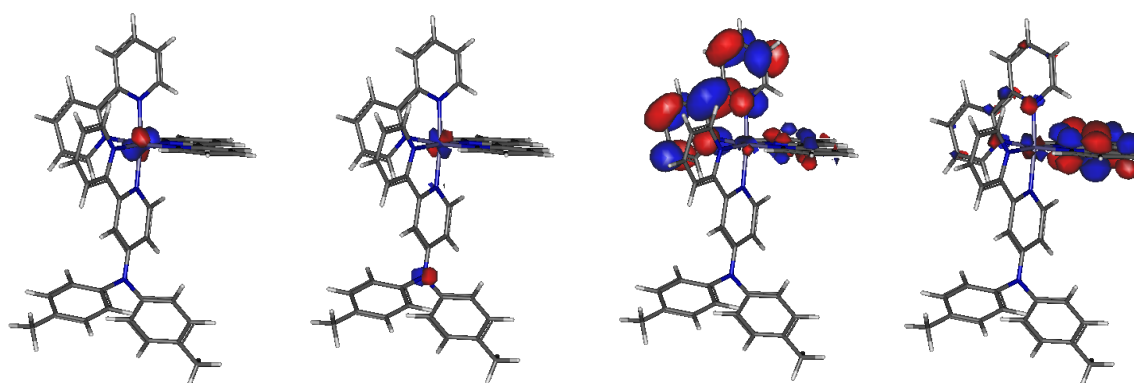


A1: HOMO-1

A1: HOMO

A1: LUMO

A1: LUMO+1

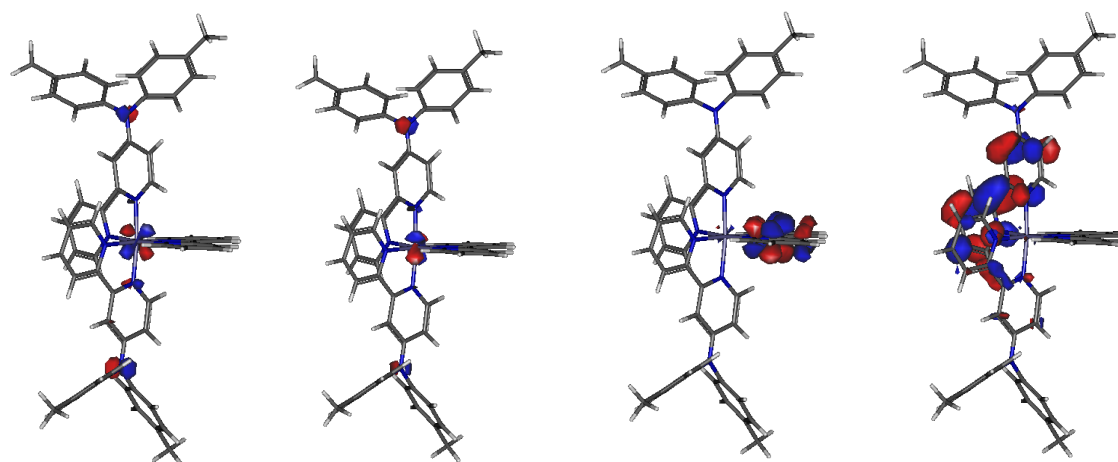


A2: HOMO-1

A2: HOMO

A2: LUMO

A2: LUMO+1



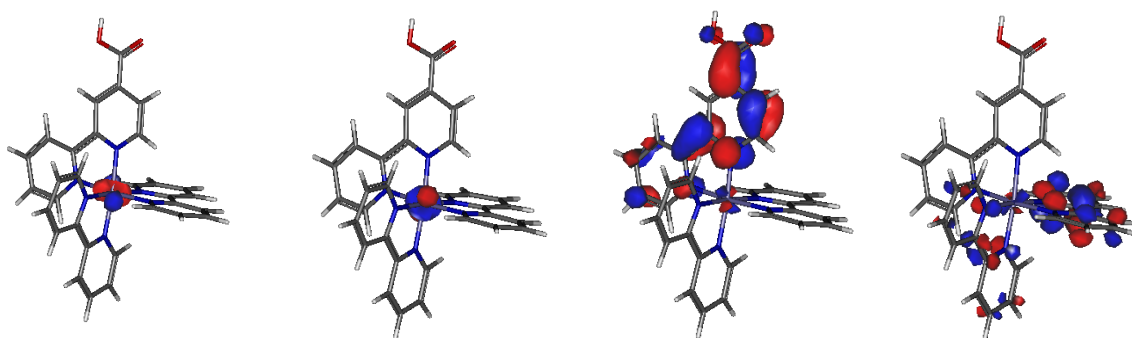
A3: HOMO-1

A3: HOMO

A3: LUMO

A3: LUMO+1

Figure S1: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **A1** – **A3**. Isosurface value 0.02.

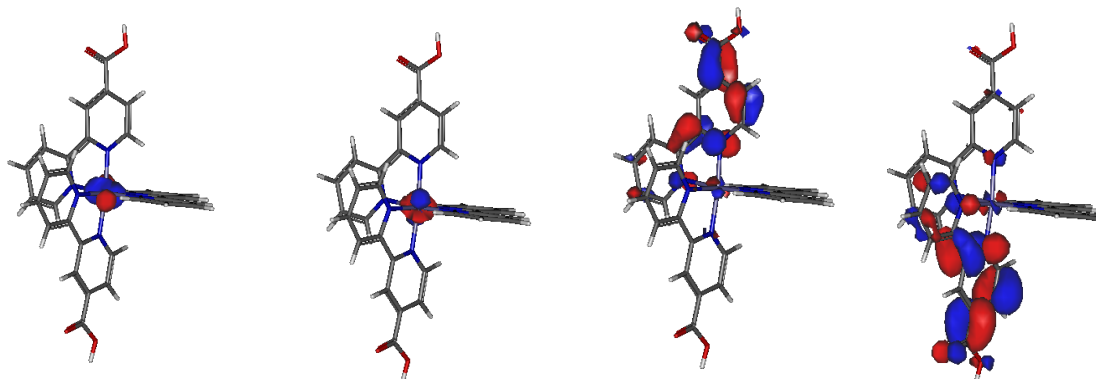


A4: HOMO-1

A4: HOMO

A4: LUMO

A4: LUMO+1

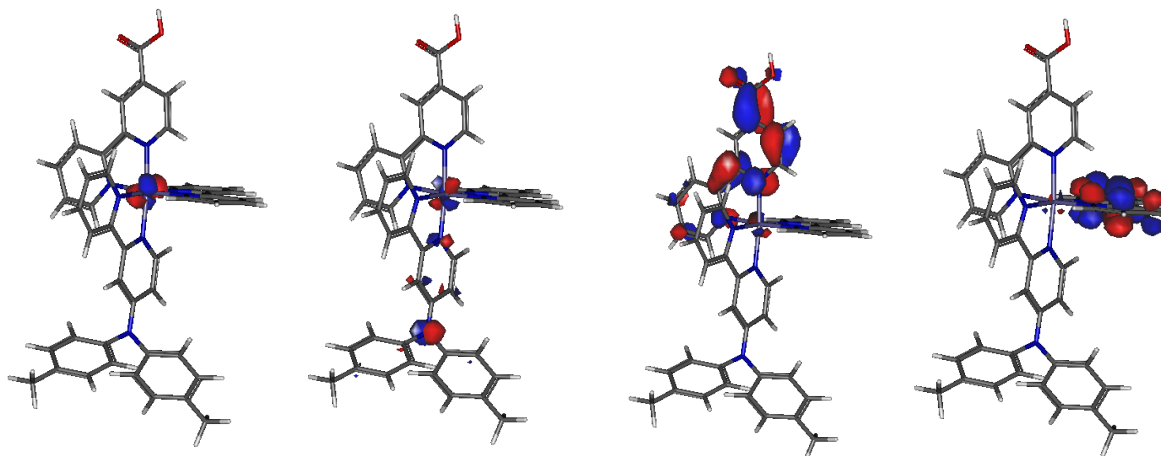


A5: HOMO-1

A5: HOMO

A5: LUMO

A5: LUMO+1



A6: HOMO-1

A6: HOMO

A6: LUMO

A6: LUMO+1

Figure S2: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **A4** – **A6**. Isosurface value 0.02.

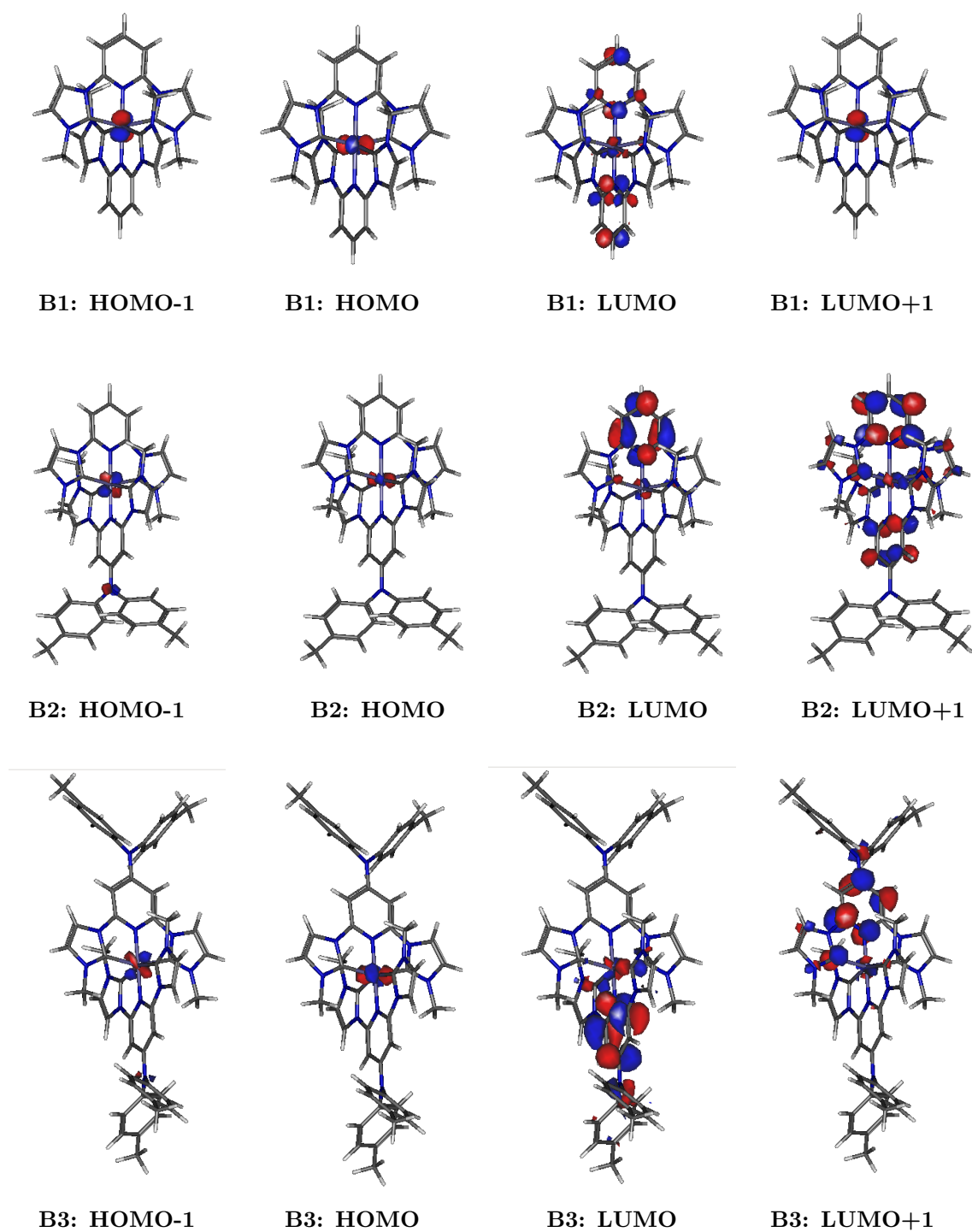


Figure S3: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **B1** – **B3**. Isosurface value 0.02.

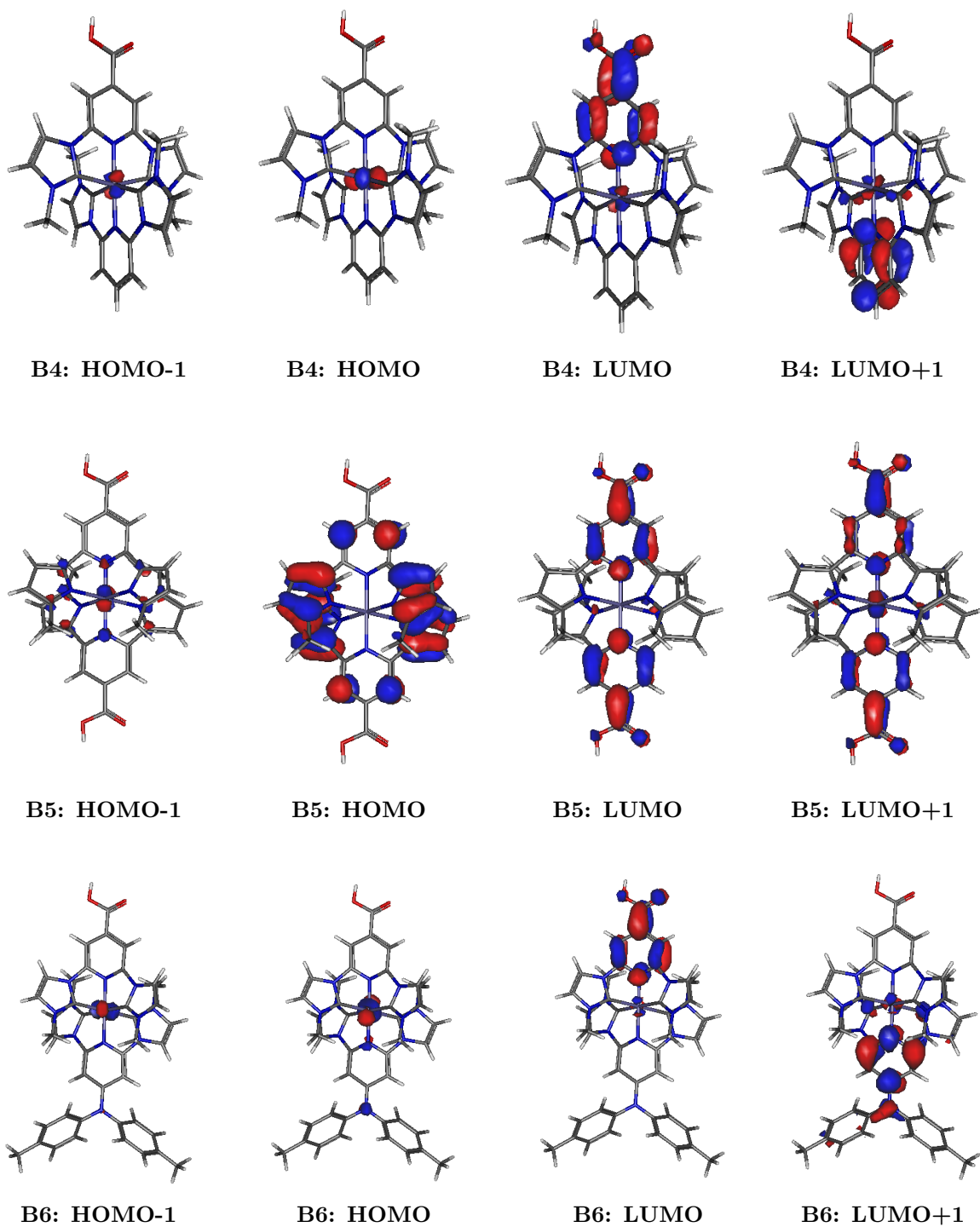


Figure S4: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **B4** – **B6**. Isosurface value 0.02.

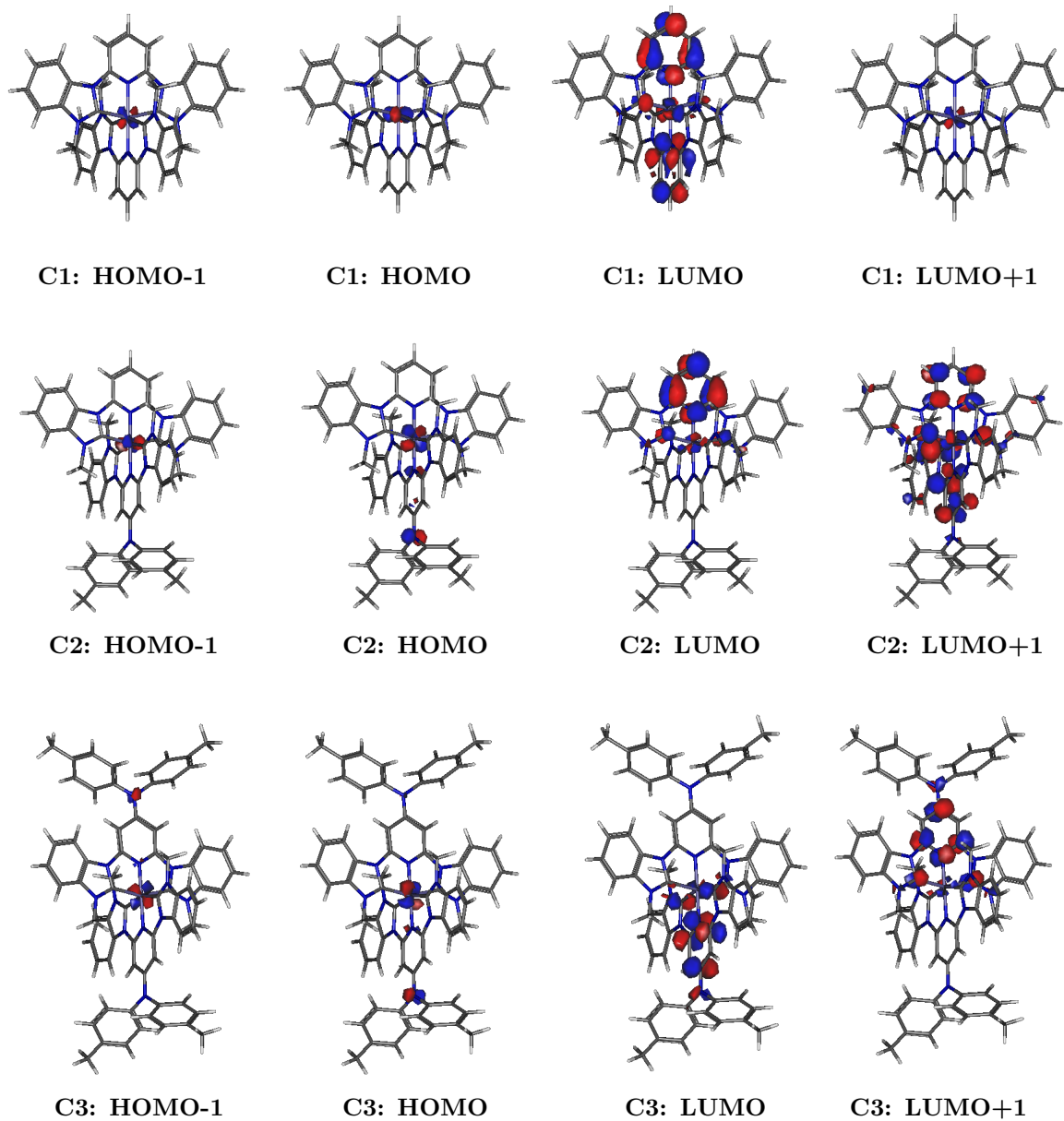


Figure S5: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **C1** – **C3**. Isosurface value 0.02.

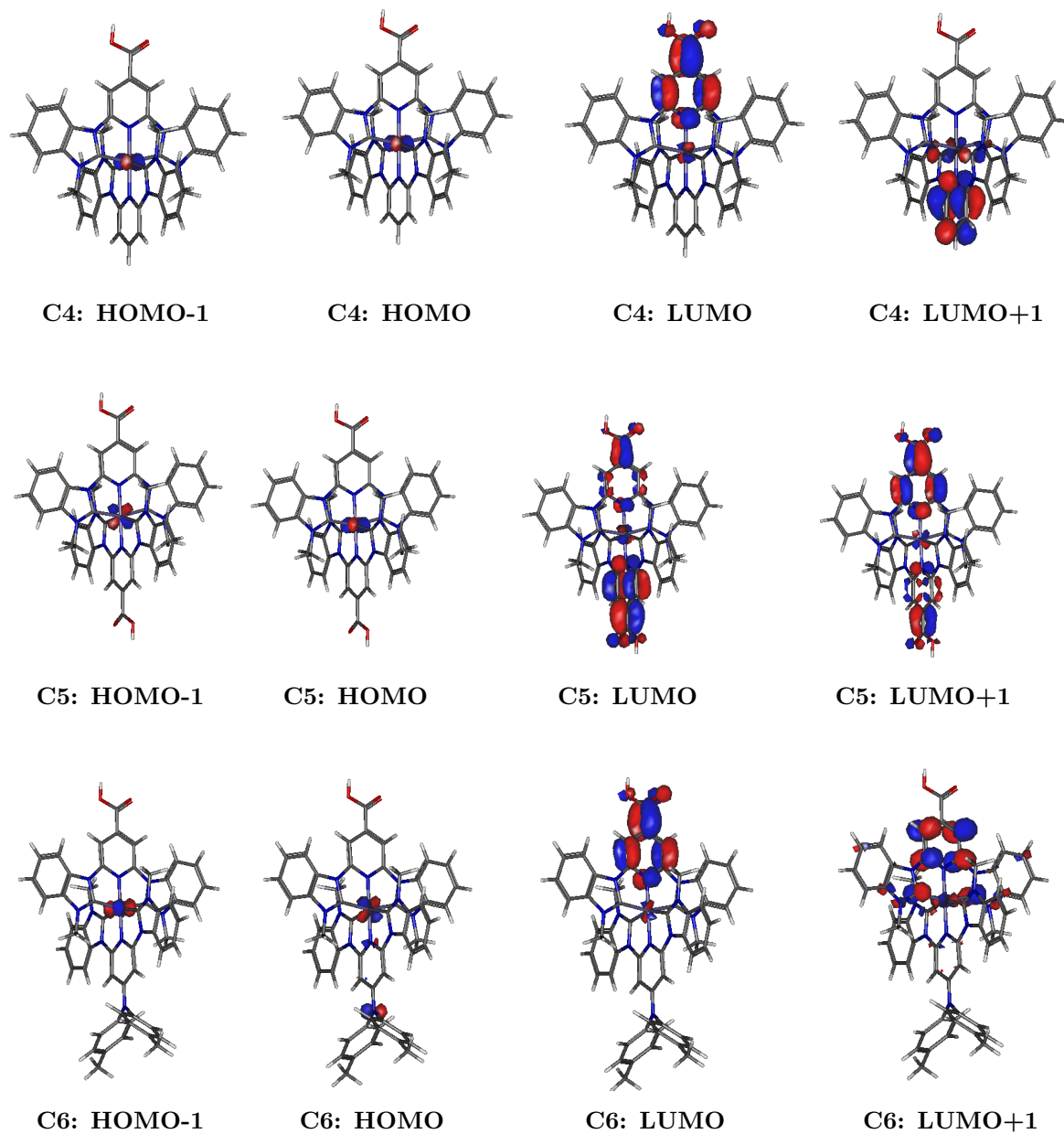


Figure S6: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **C4** – **C6**. Isosurface value 0.02.

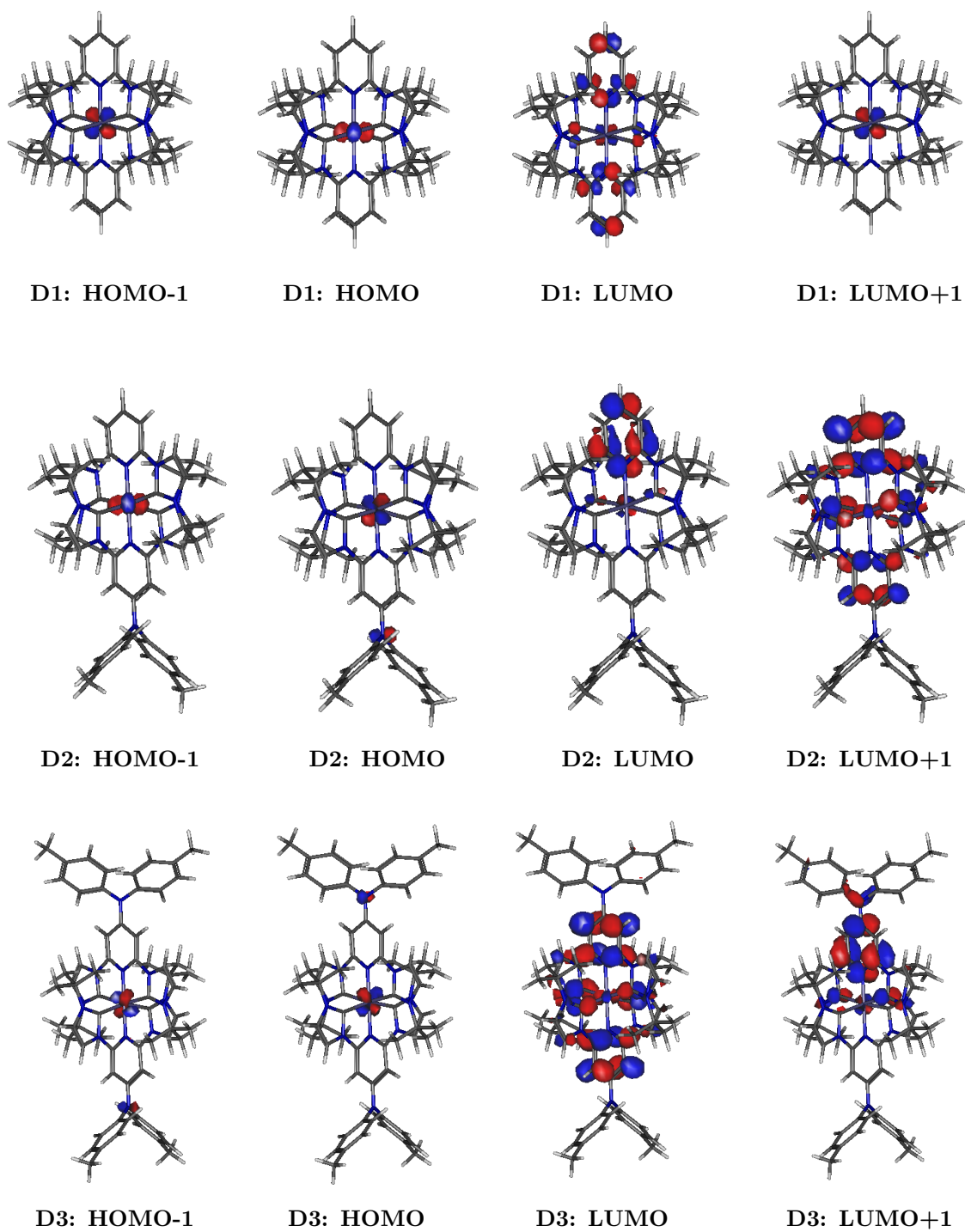
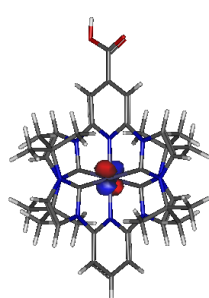
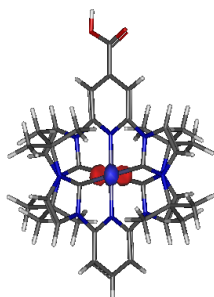


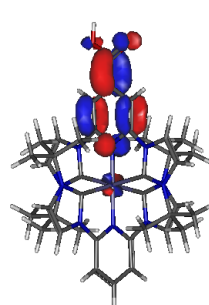
Figure S7: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **D1** – **D3**. Isosurface value 0.02.



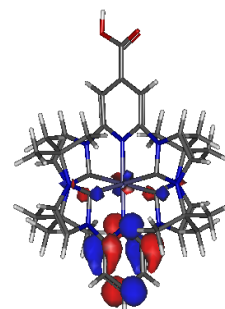
D4: HOMO-1



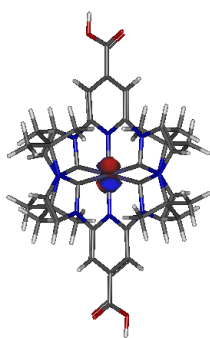
D4: HOMO



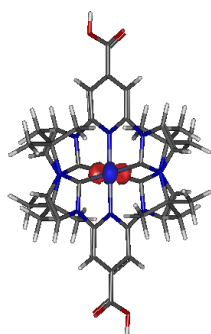
D4: LUMO



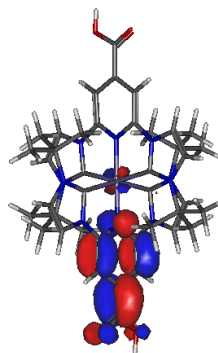
D4: LUMO+1



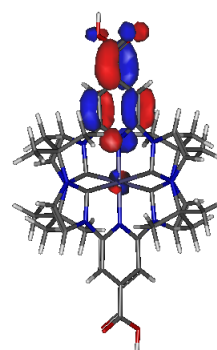
D5: HOMO-1



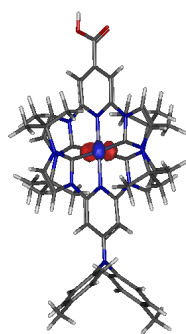
D5: HOMO



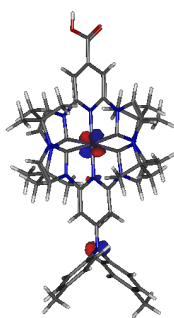
D5: LUMO



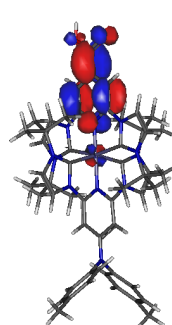
D5: LUMO+1



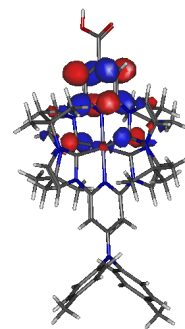
D6: HOMO-1



D6: HOMO



D6: LUMO



D6: LUMO+1

Figure S8: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **D4** – **D6**. Isosurface value 0.02.

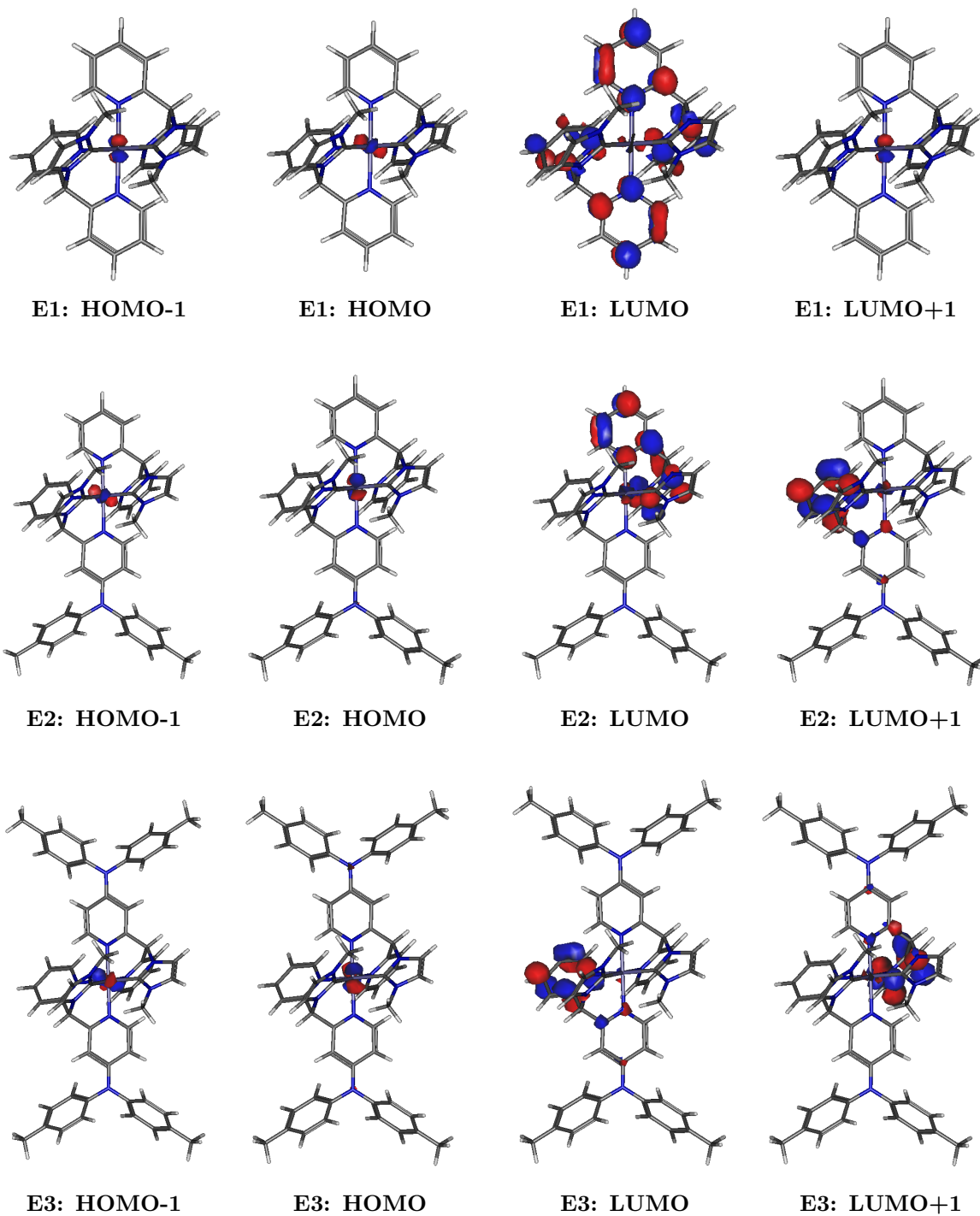


Figure S9: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **E1** – **E3**. Isosurface value 0.02.

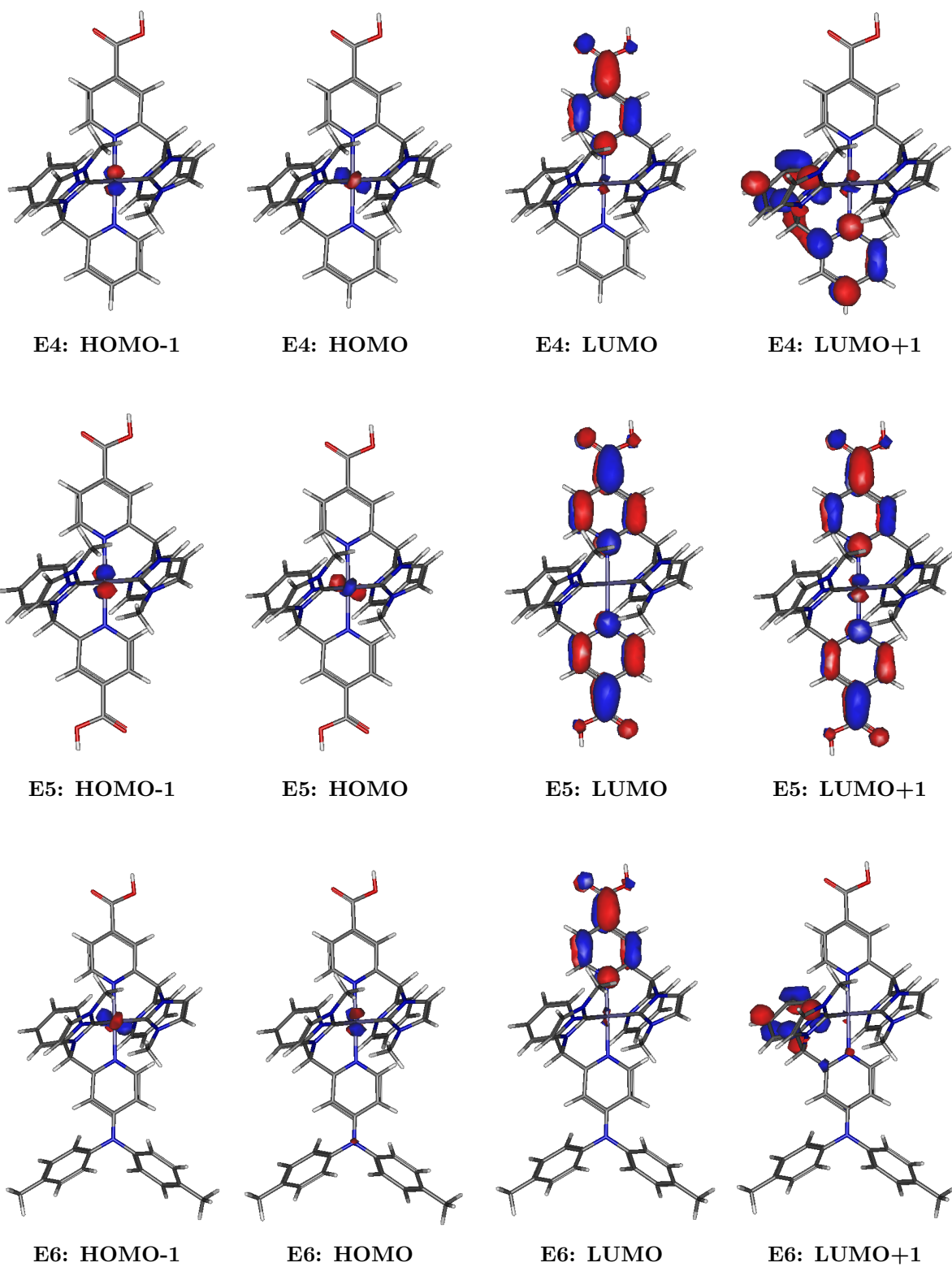


Figure S10: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **E4** – **E6**. Isosurface value 0.02.

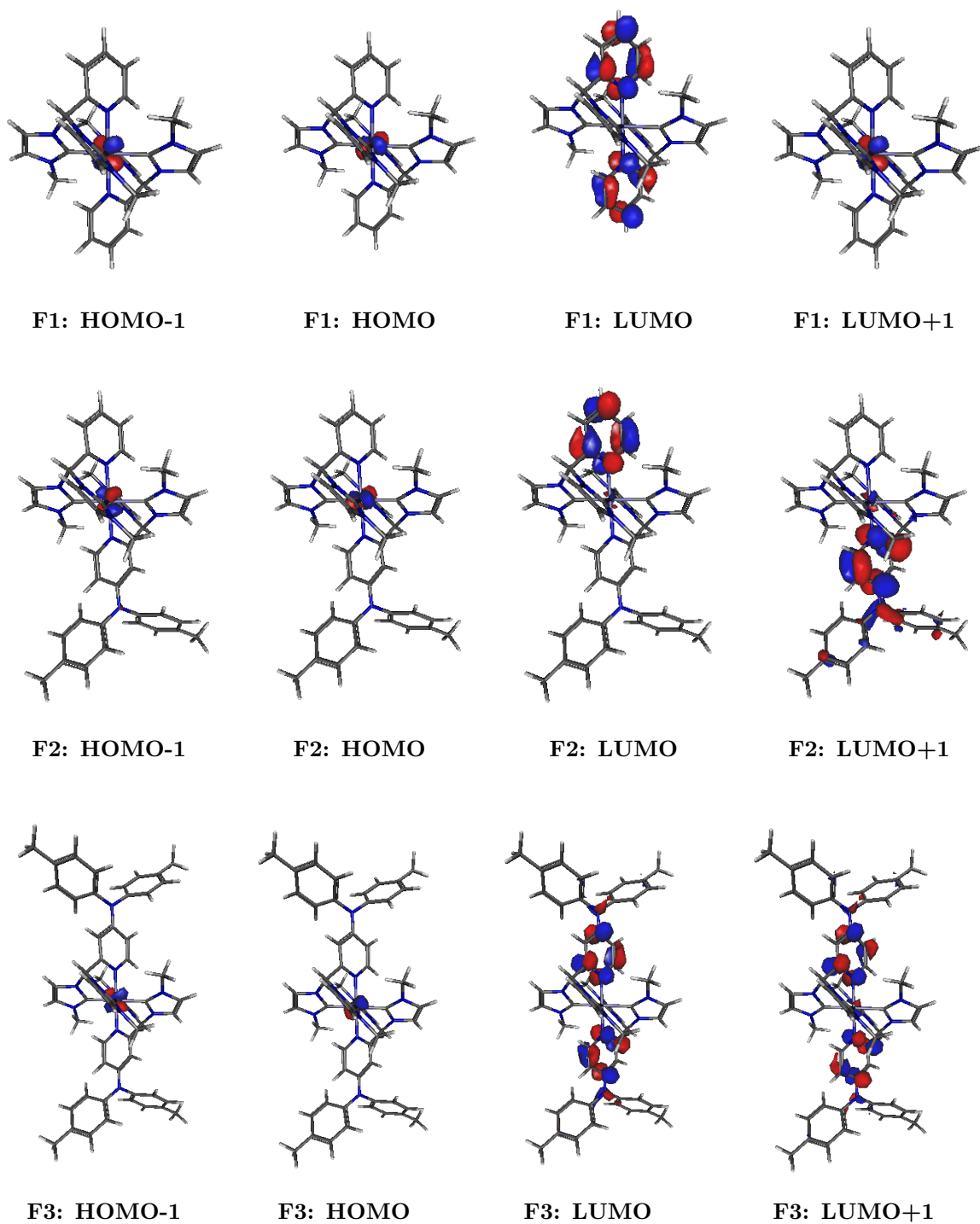


Figure S11: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **F1** – **F3**. Isosurface value 0.02.

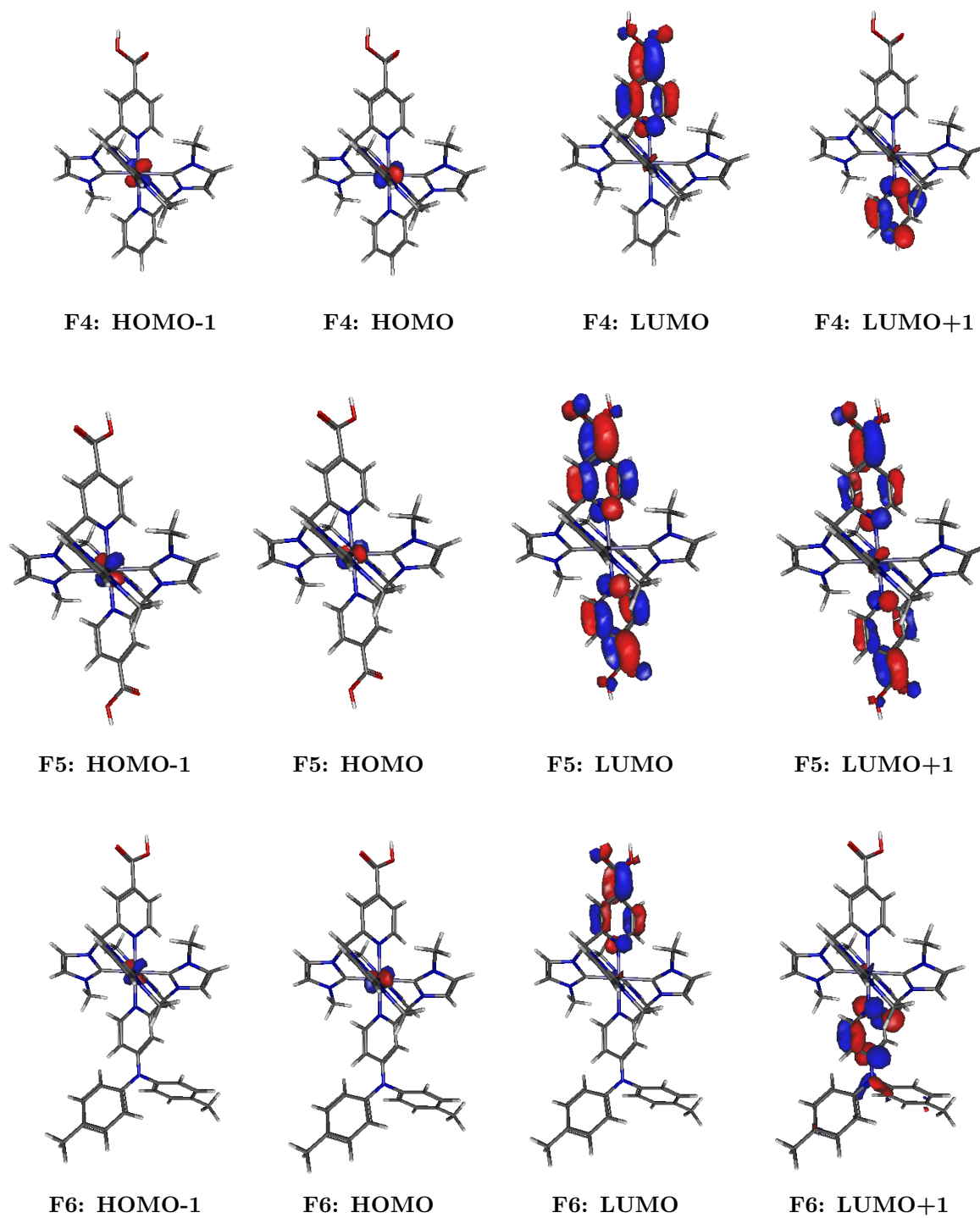


Figure S12: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **F4** – **F6**. Isosurface value 0.02.

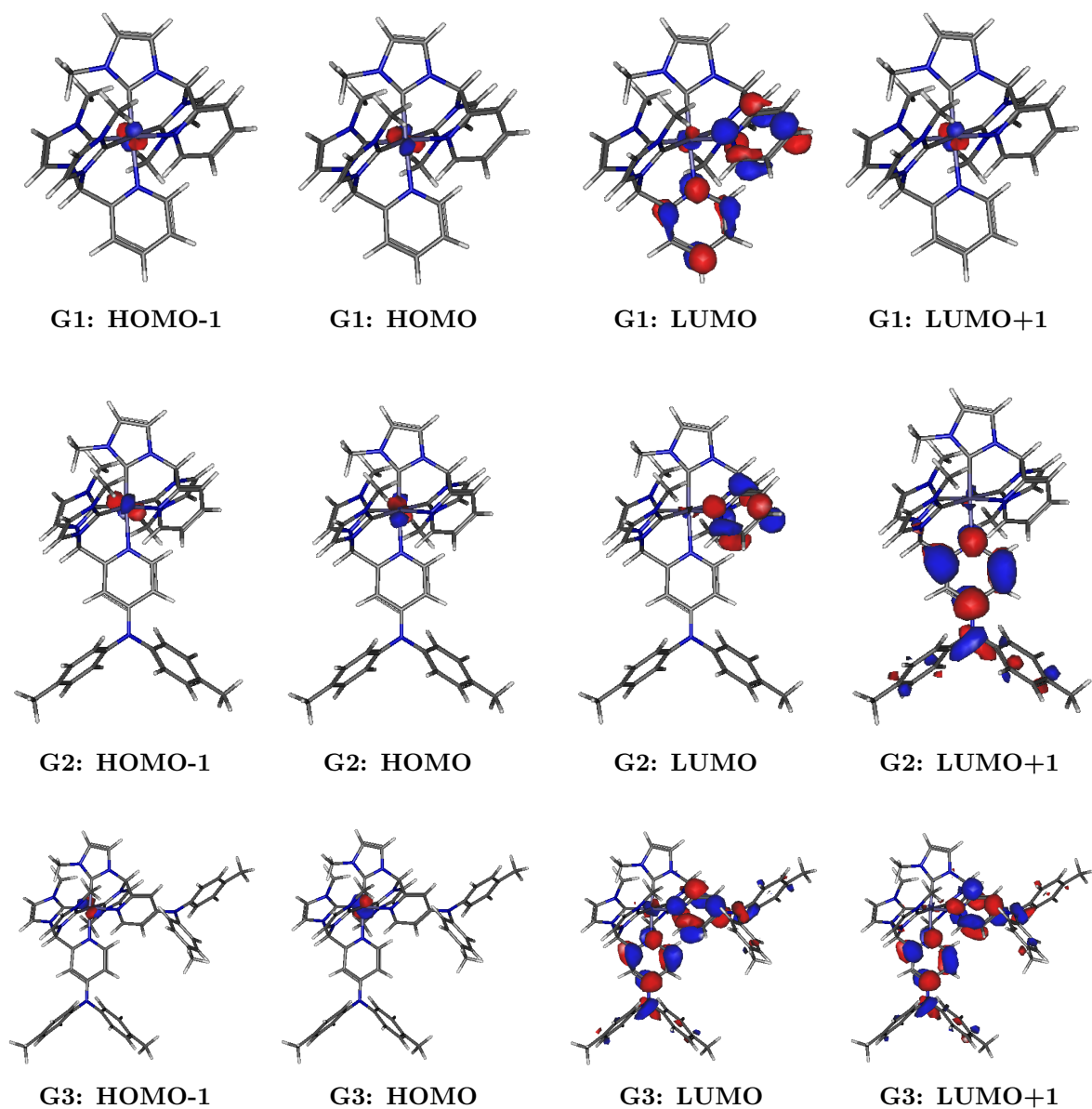


Figure S13: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **G1** – **G3**. Isosurface value 0.02.

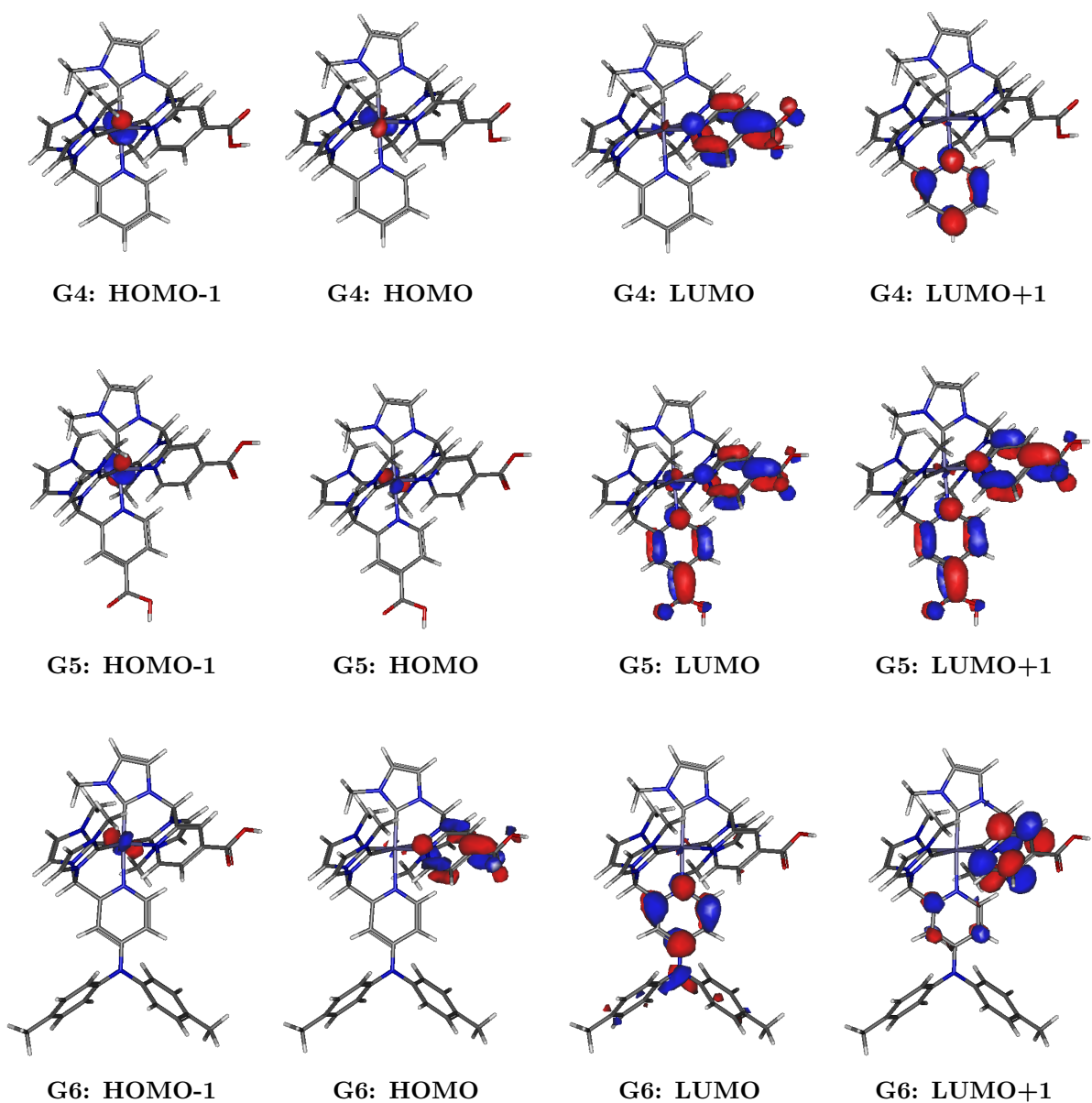


Figure S14: Frontier MOs (HOMO-1, HOMO, LUMO and LUMO+1) involved in the main transitions of iron dyes **G4** – **G6**. Isosurface value 0.02.

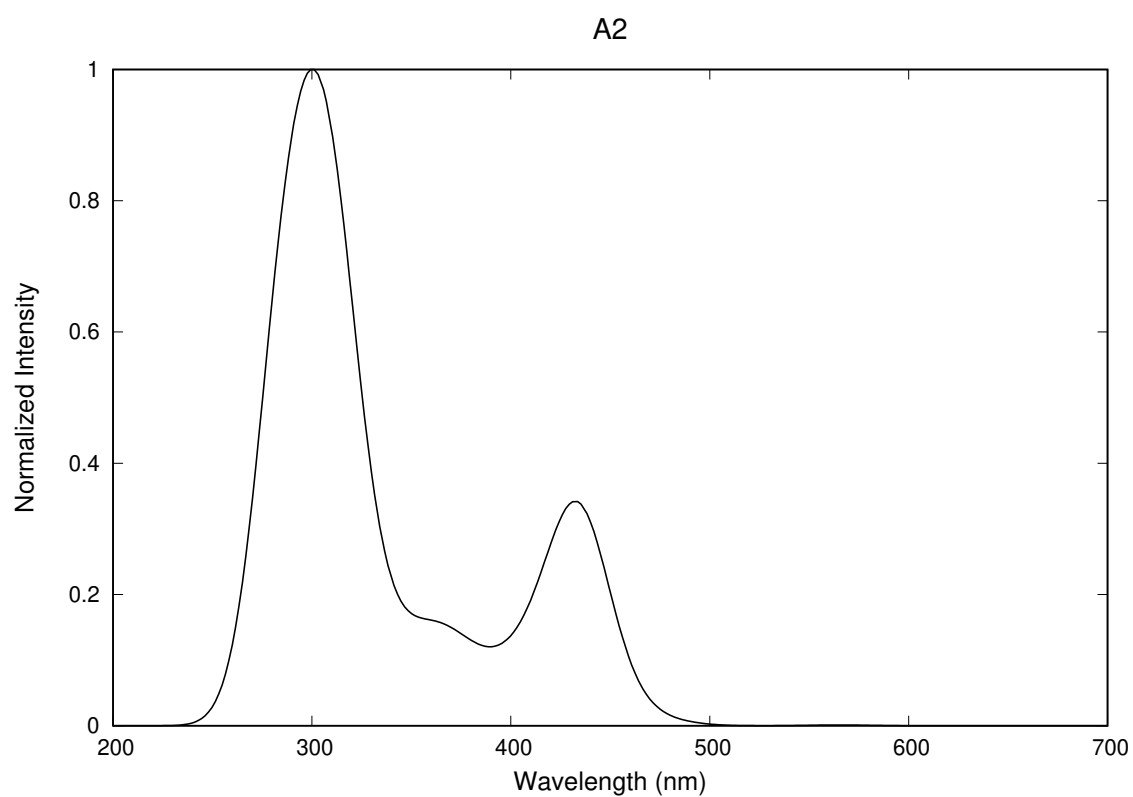
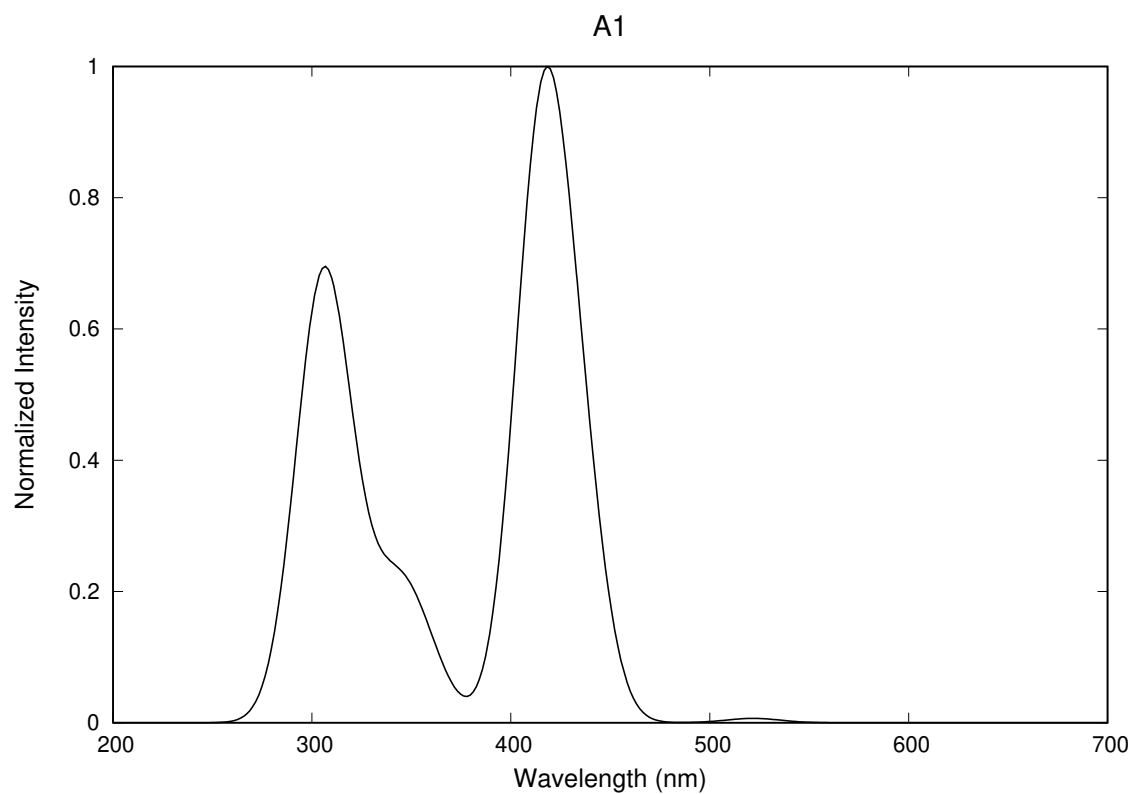


Figure S15: Calculated normalized absorption UV-vis spectra of iron dyes **A1** and **A2**.

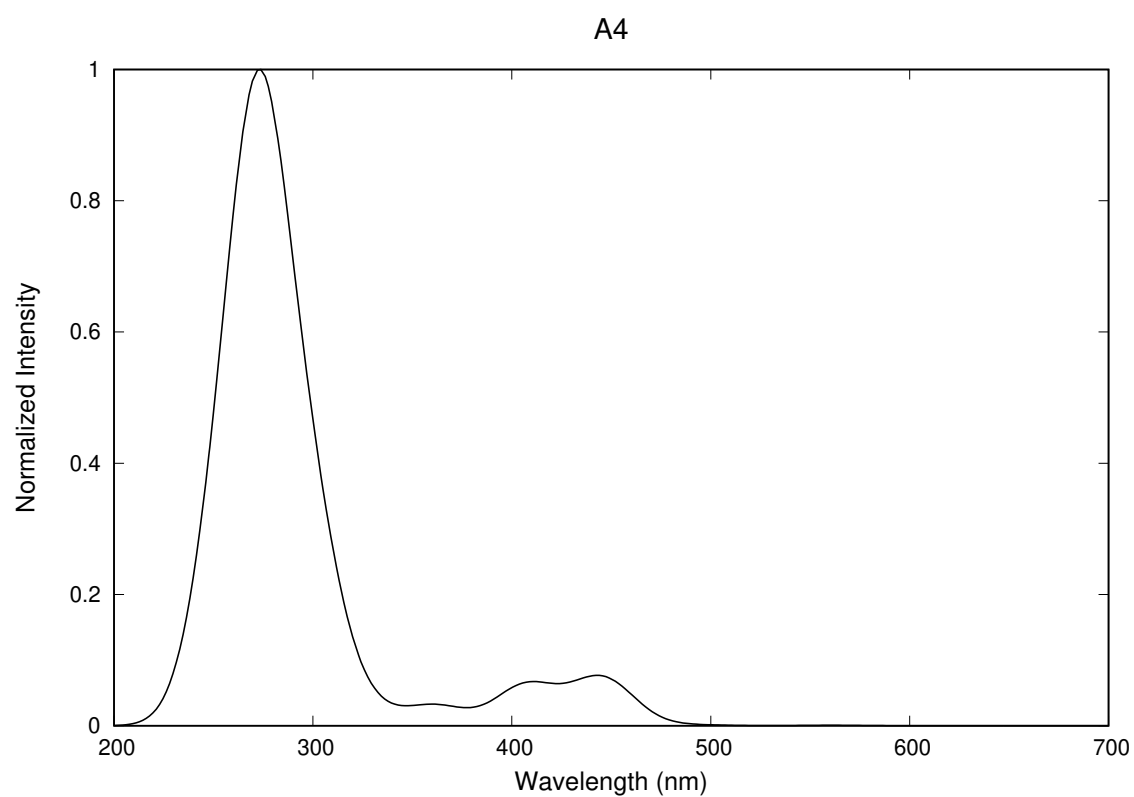
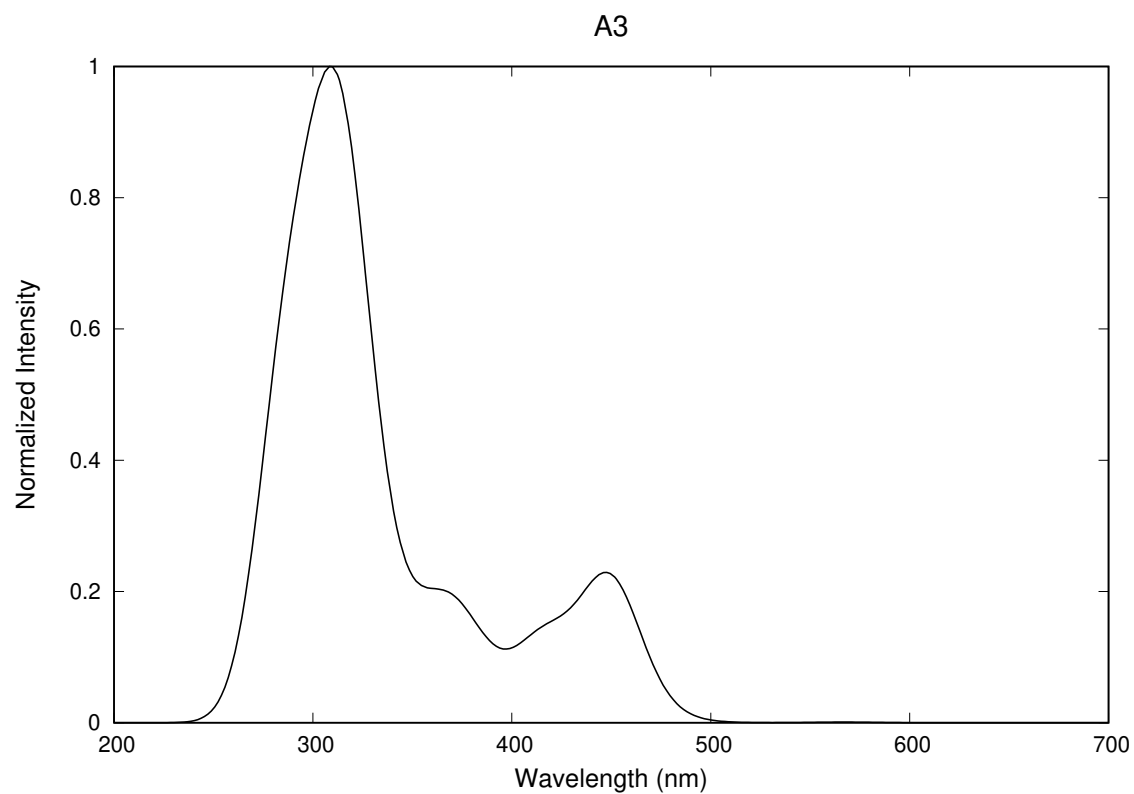


Figure S16: Calculated normalized absorption UV-vis spectra of iron dyes **A3** and **A4**.

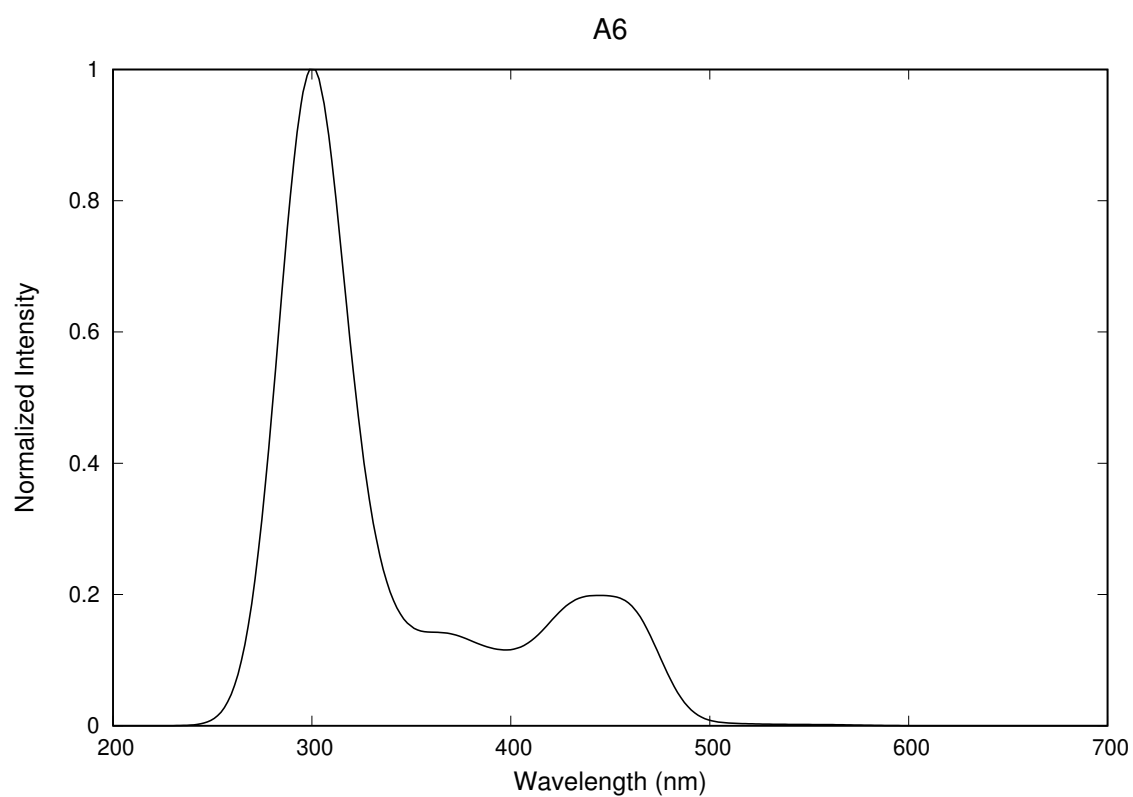
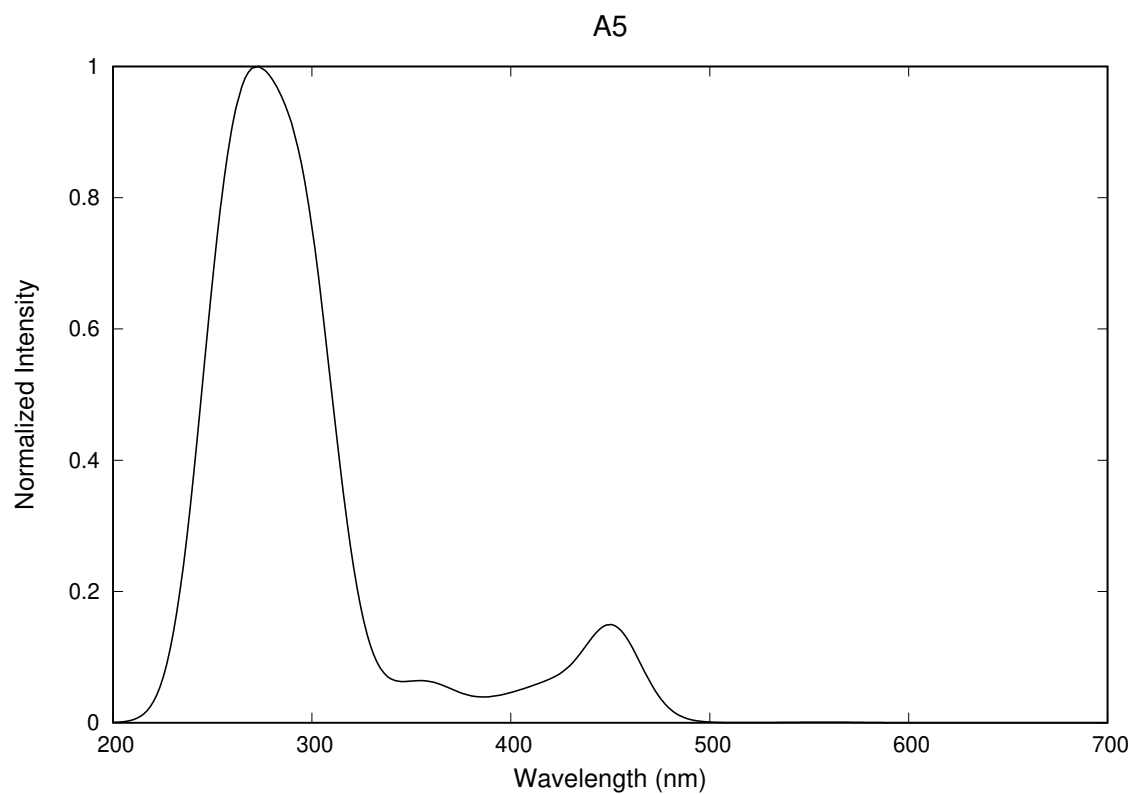


Figure S17: Calculated normalized absorption UV-vis spectra of iron dyes **A5** and **A6**.

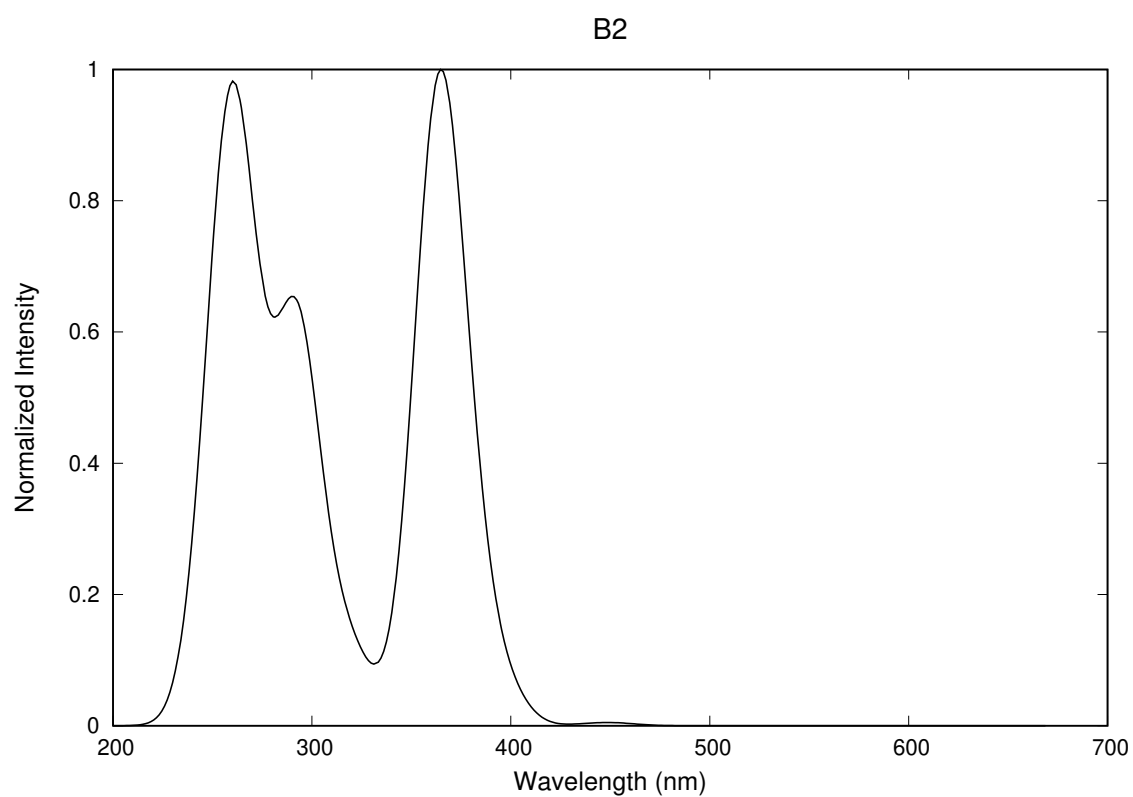
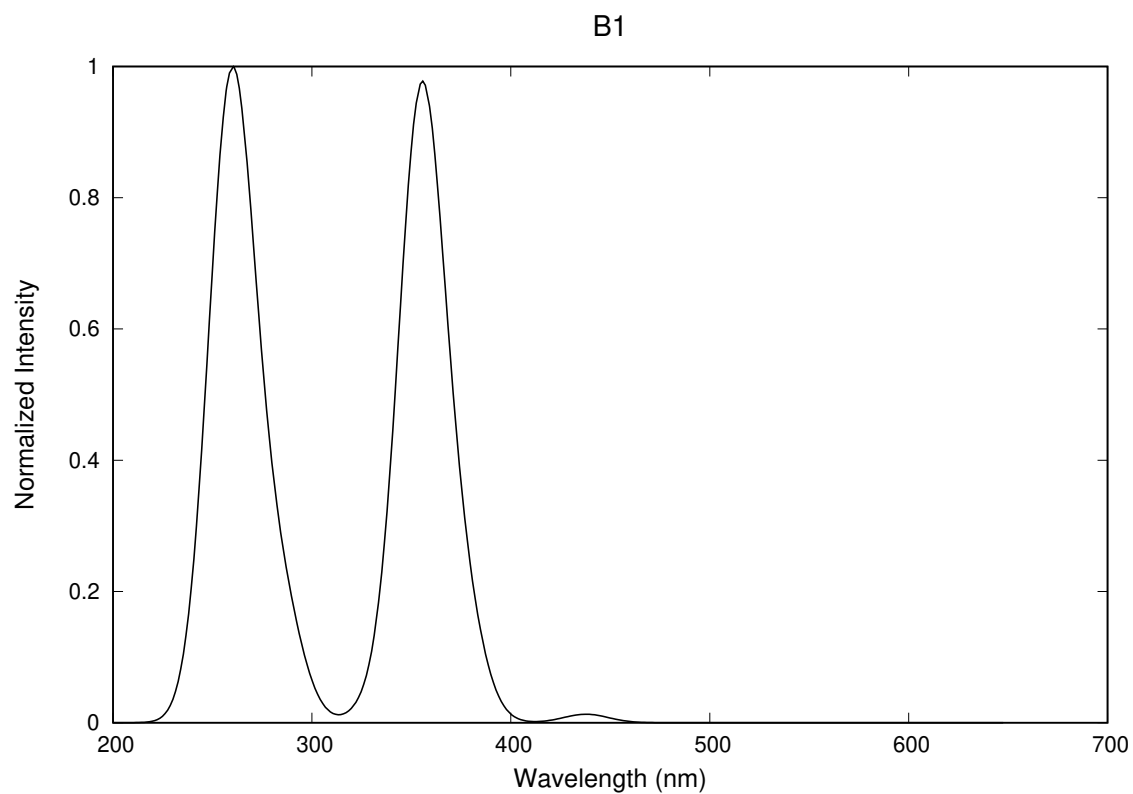


Figure S18: Calculated normalized absorption UV-vis spectra of iron dyes **B1** and **B2**.

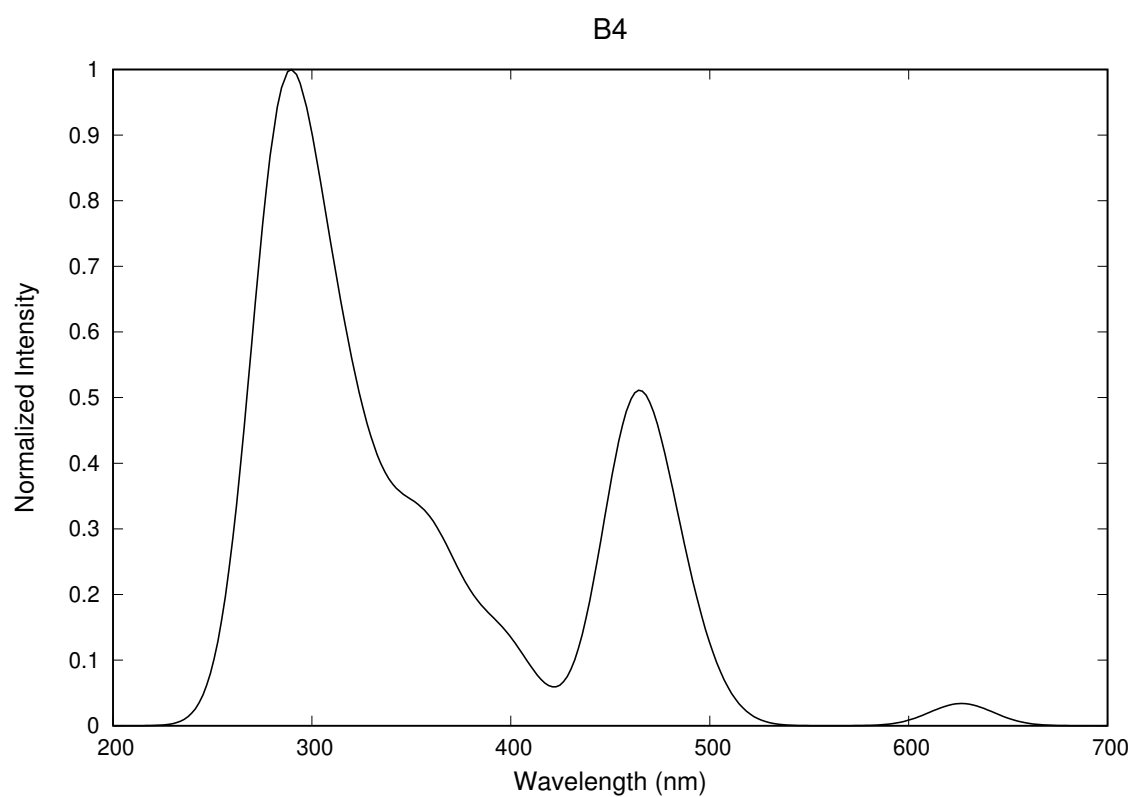
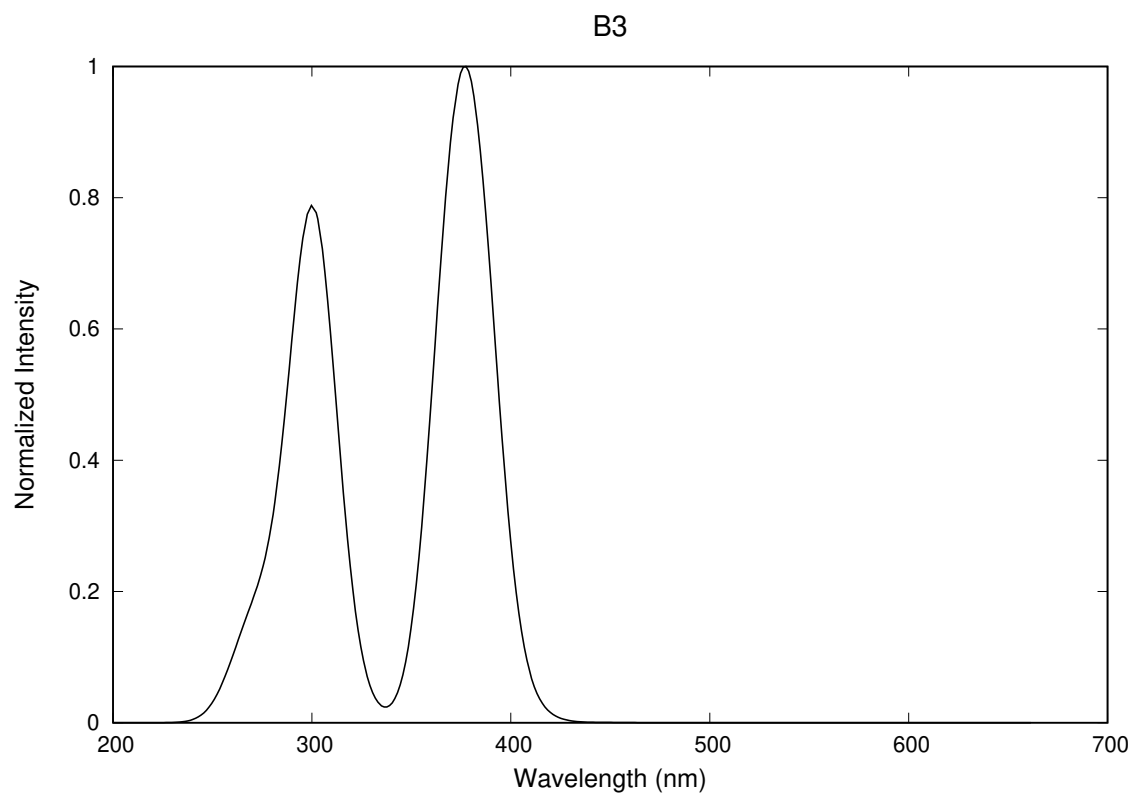


Figure S19: Calculated normalized absorption UV-vis spectra of iron dyes **B3** and **B4**.

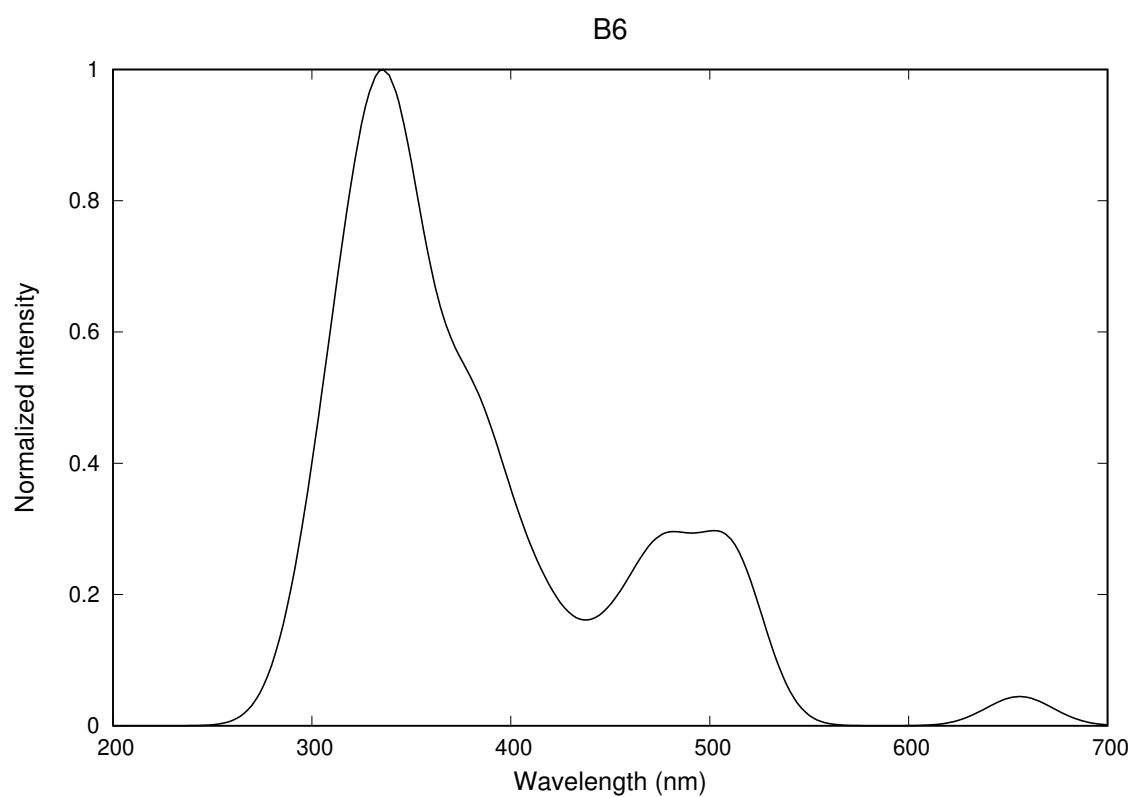
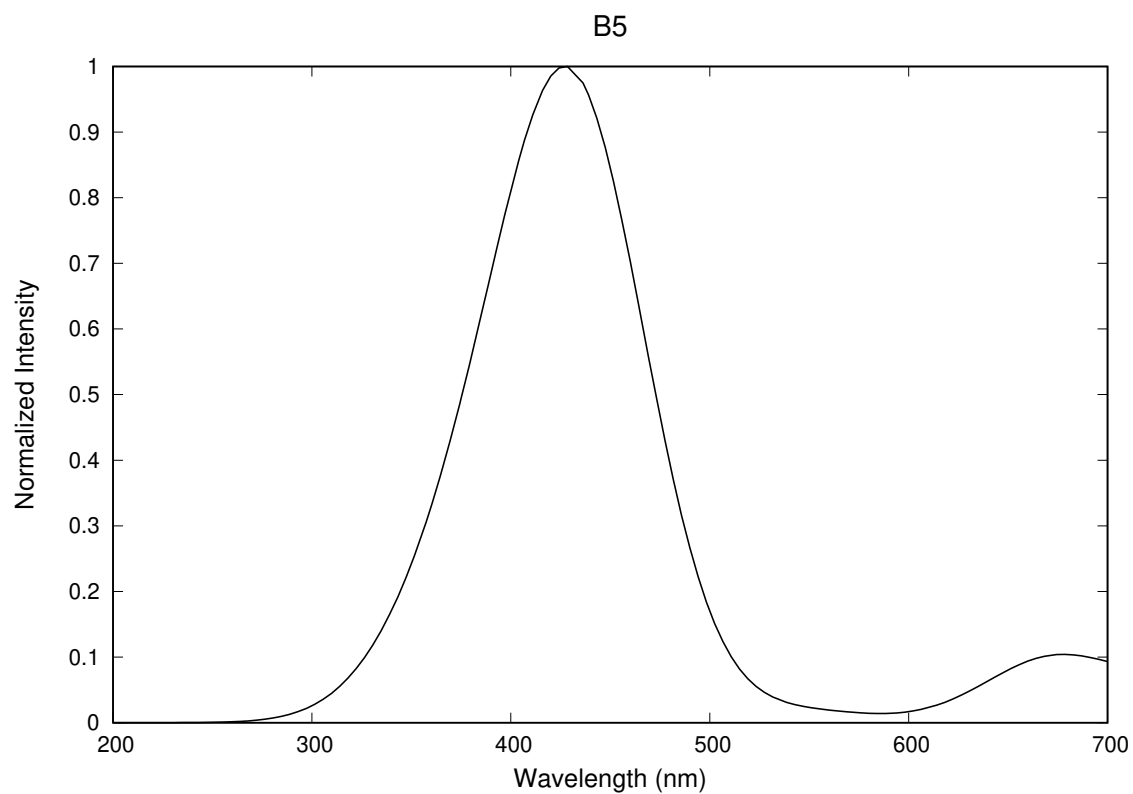


Figure S20: Calculated normalized absorption UV-vis spectra of iron dyes **B5** and **B6**.

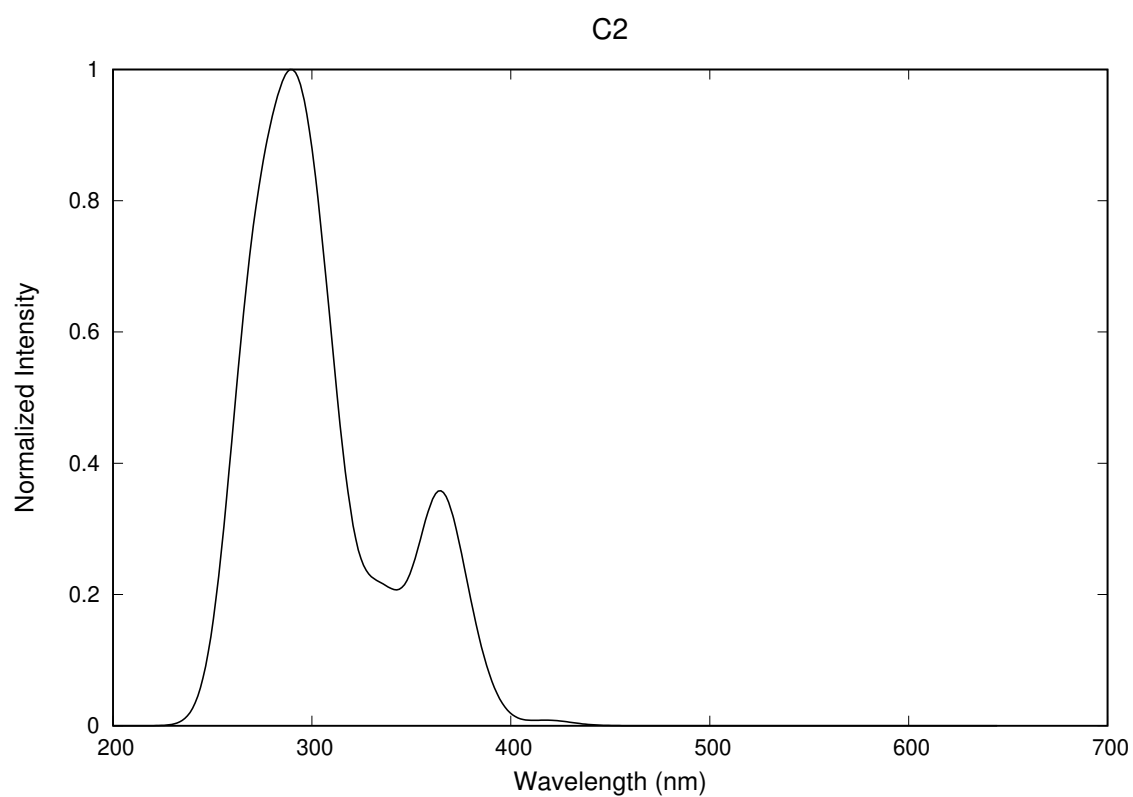
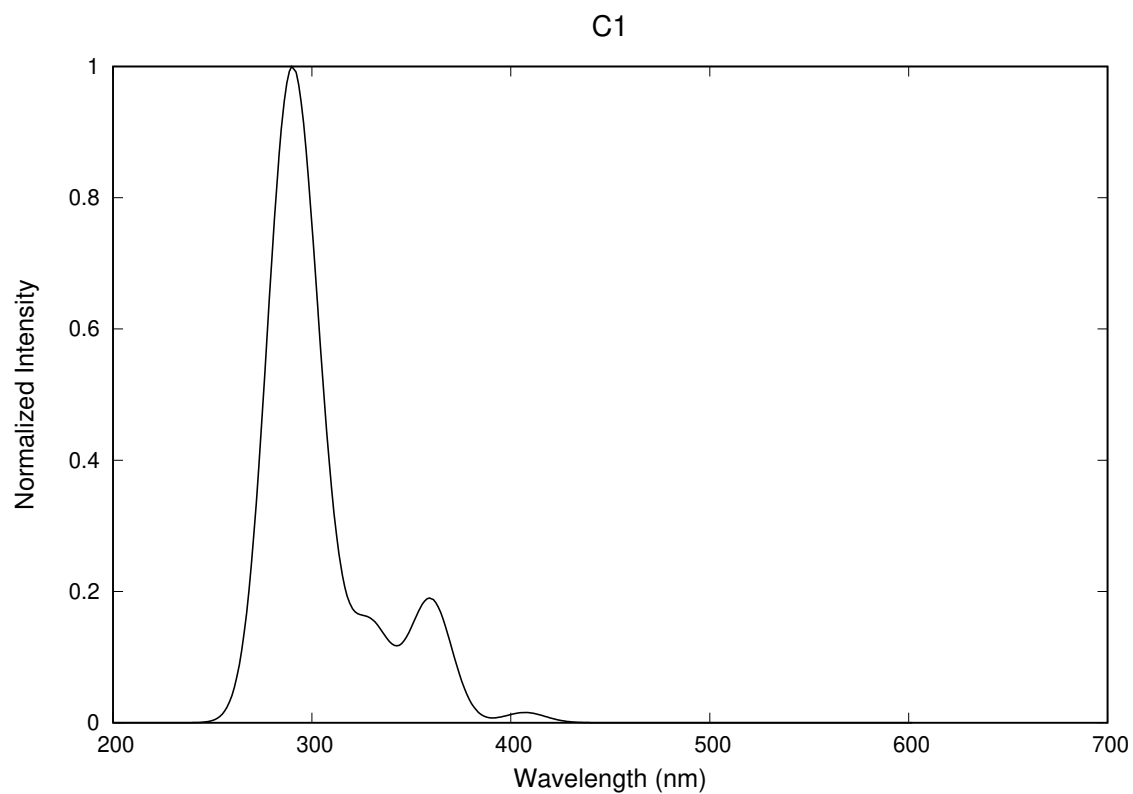


Figure S21: Calculated normalized absorption UV-vis spectra of iron dyes **C1** and **C2**.

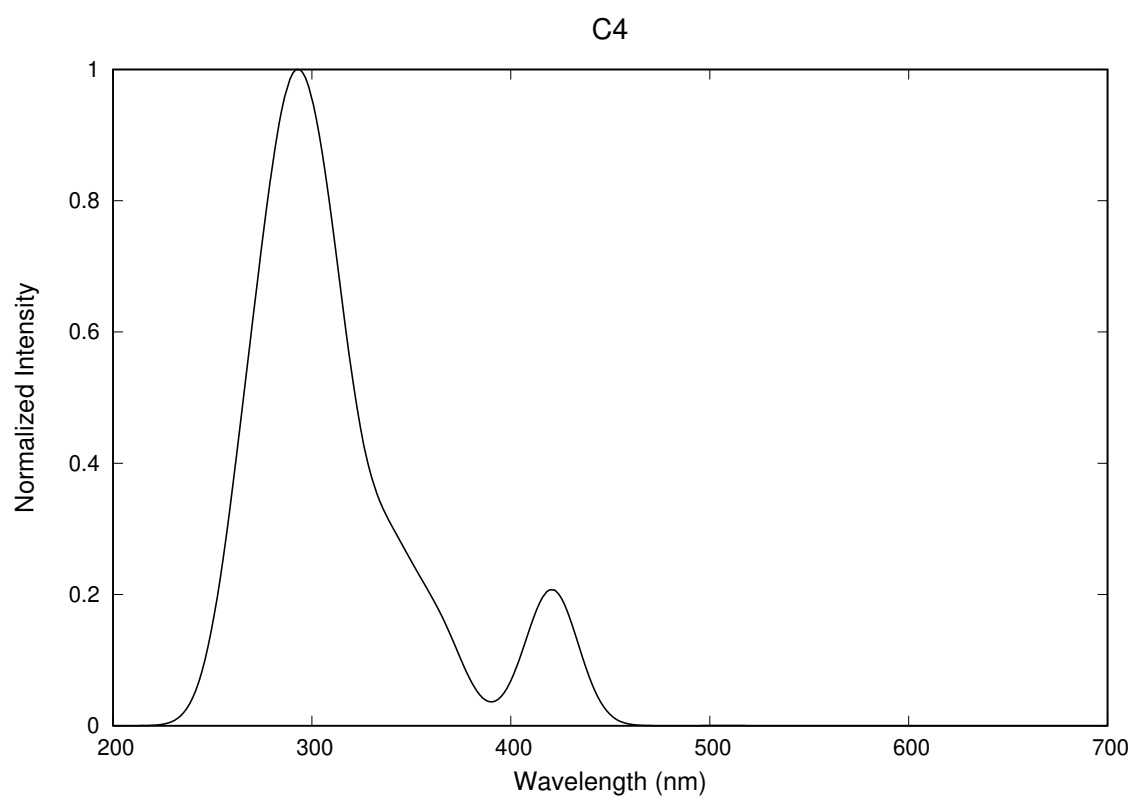
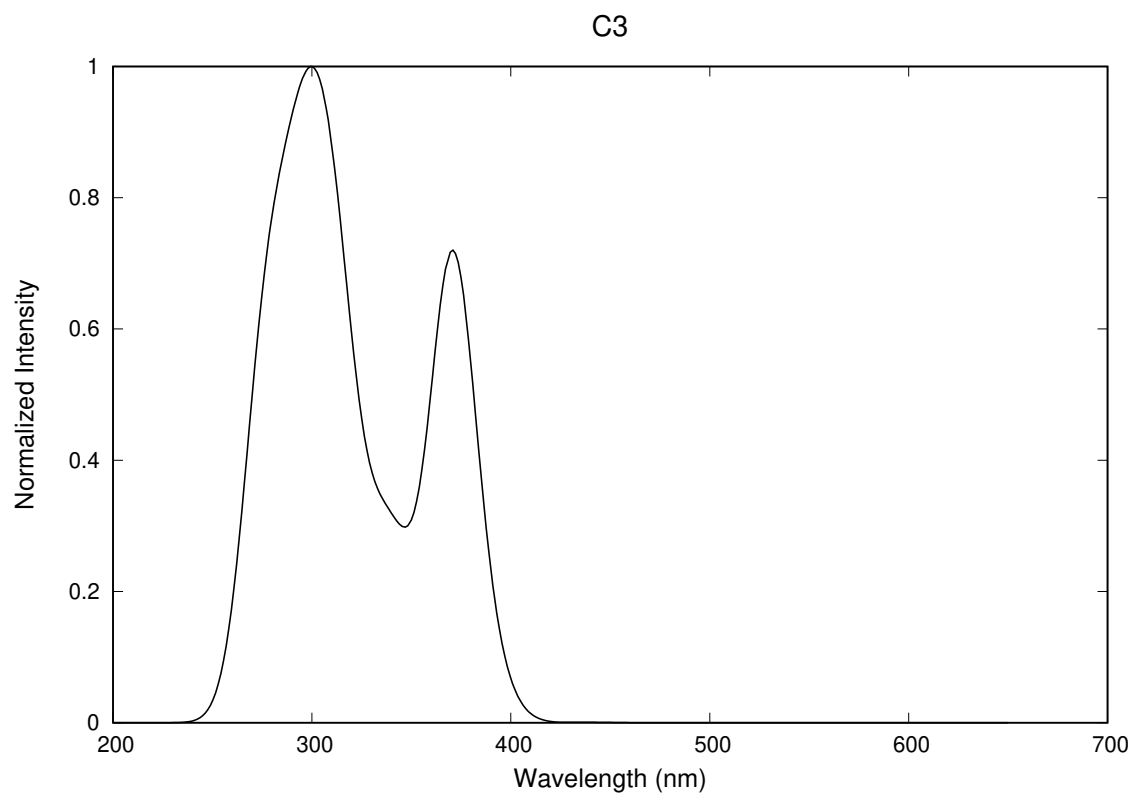


Figure S22: Calculated normalized absorption UV-vis spectra of iron dyes **C3** and **C4**.

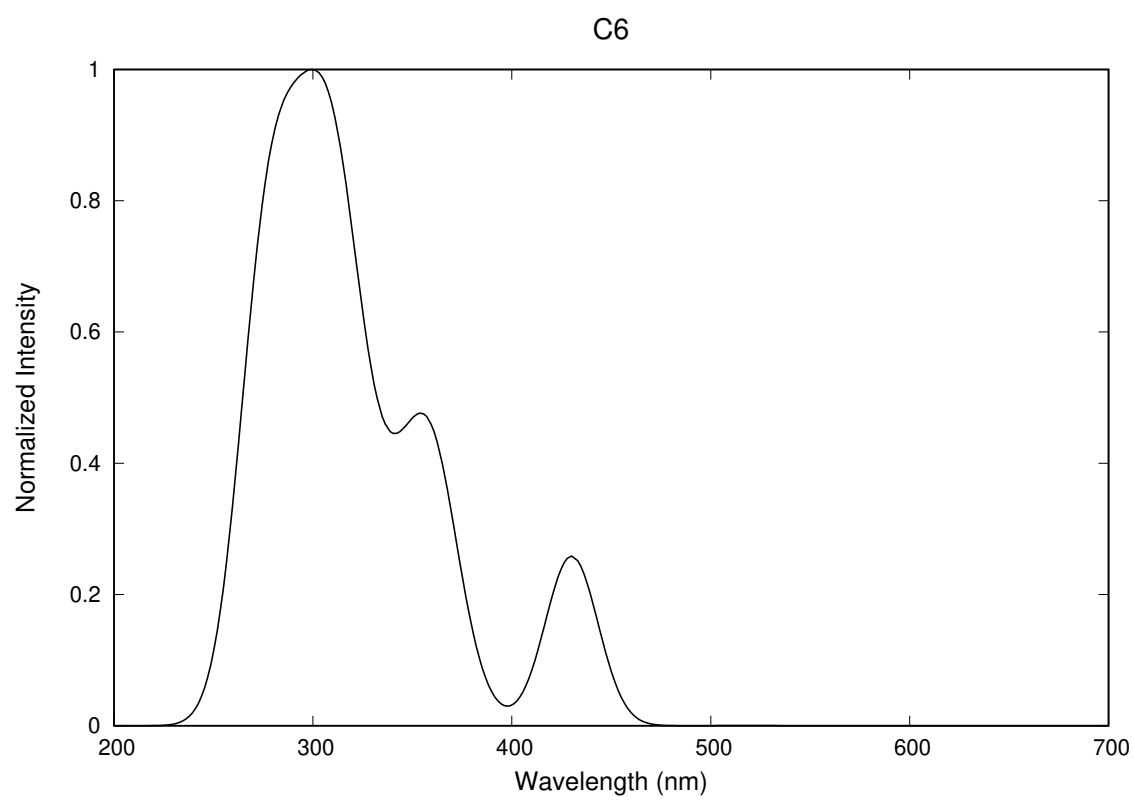
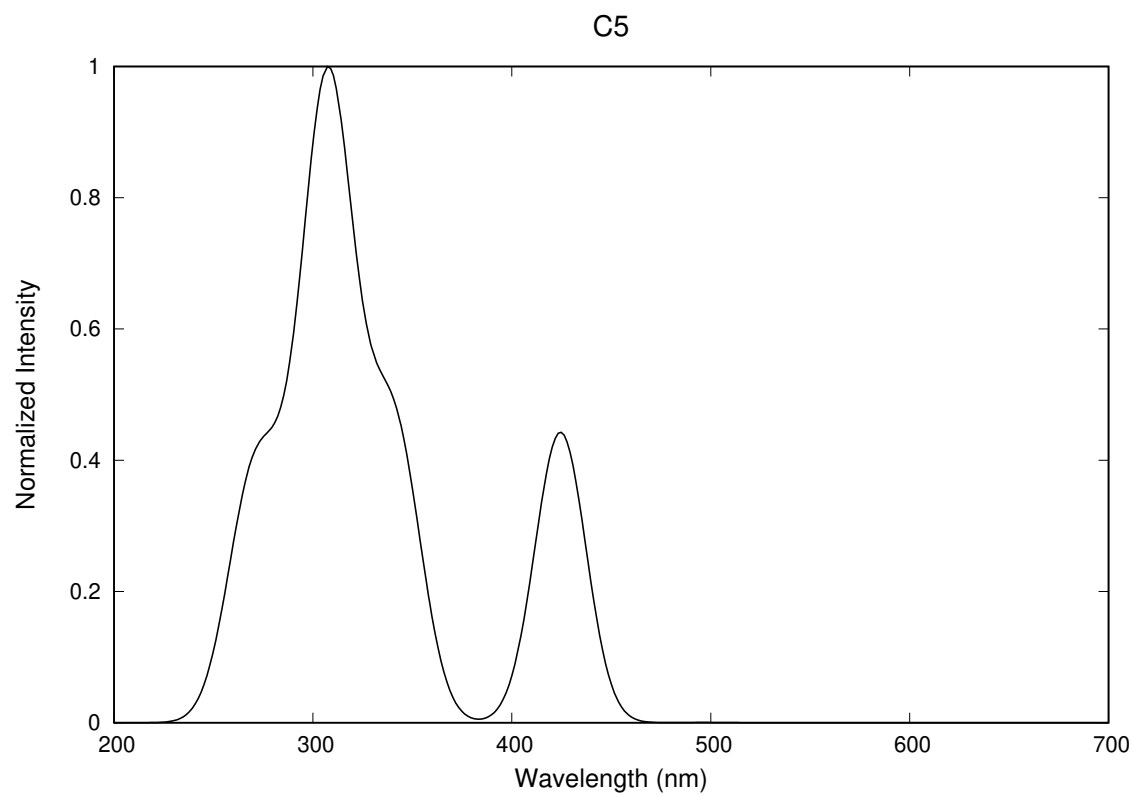


Figure S23: Calculated normalized absorption UV-vis spectra of iron dyes **C5** and **C6**.

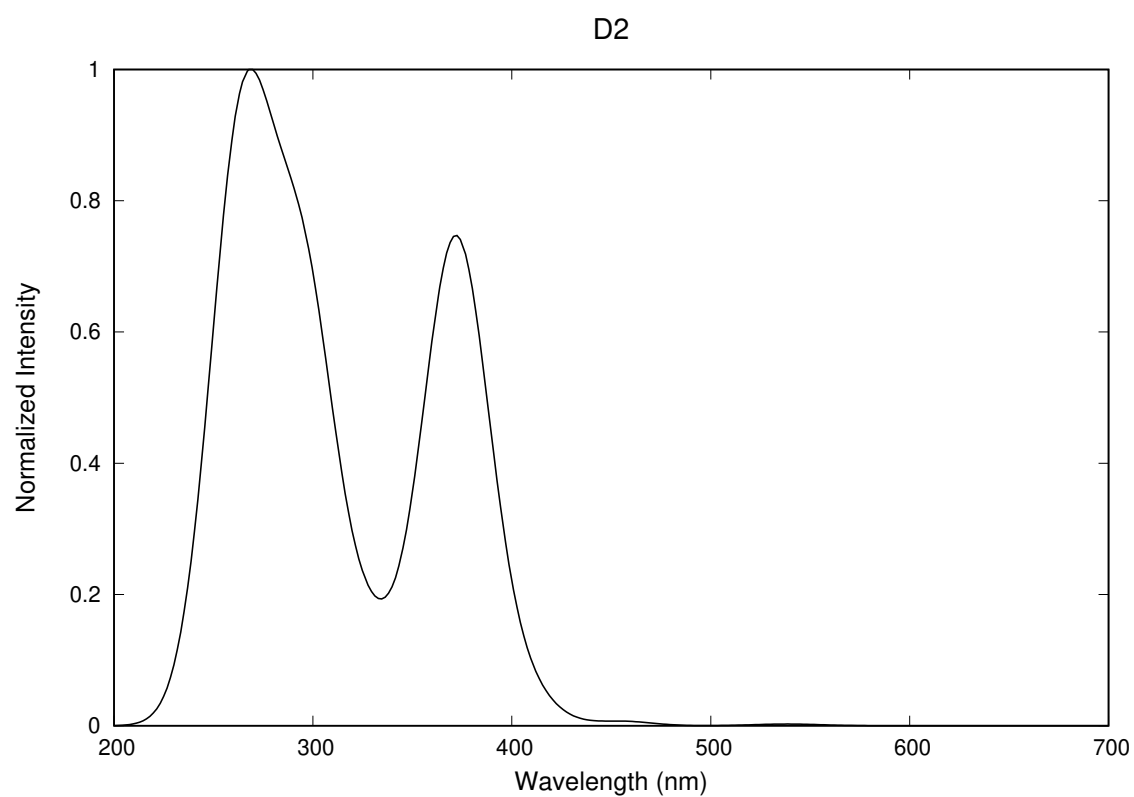
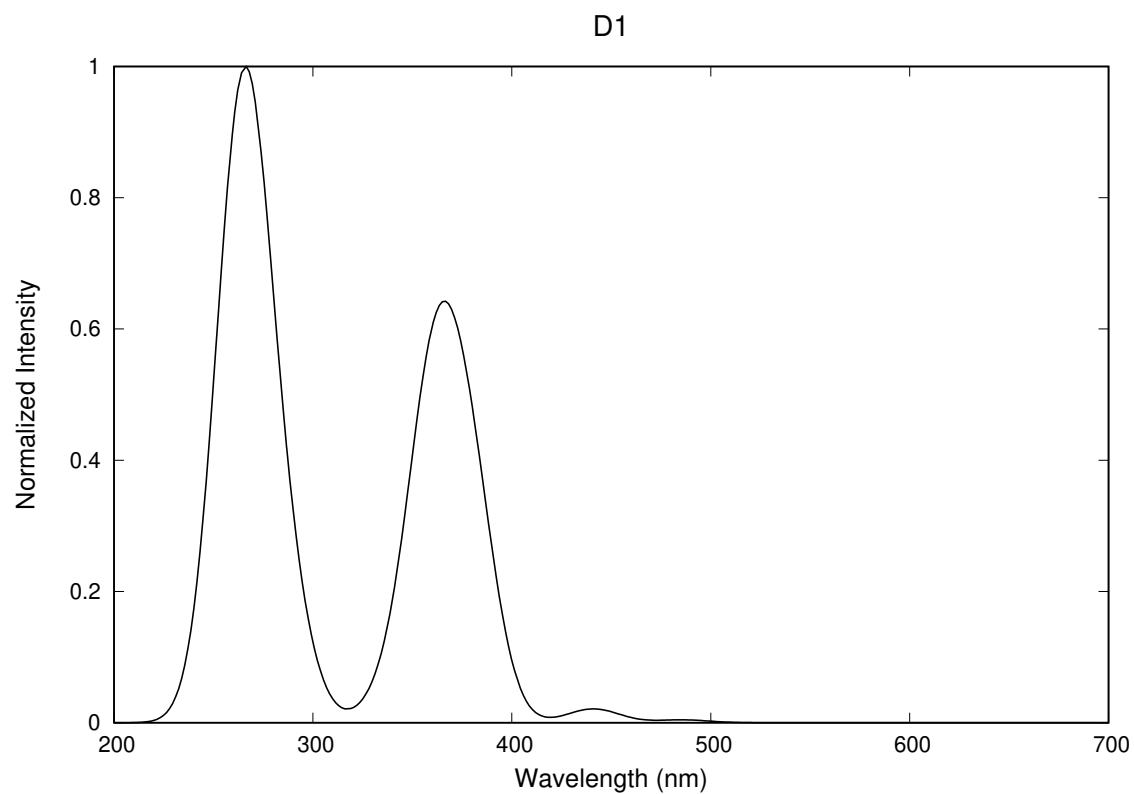


Figure S24: Calculated normalized absorption UV-vis spectra of iron dyes **D1** and **D2**.

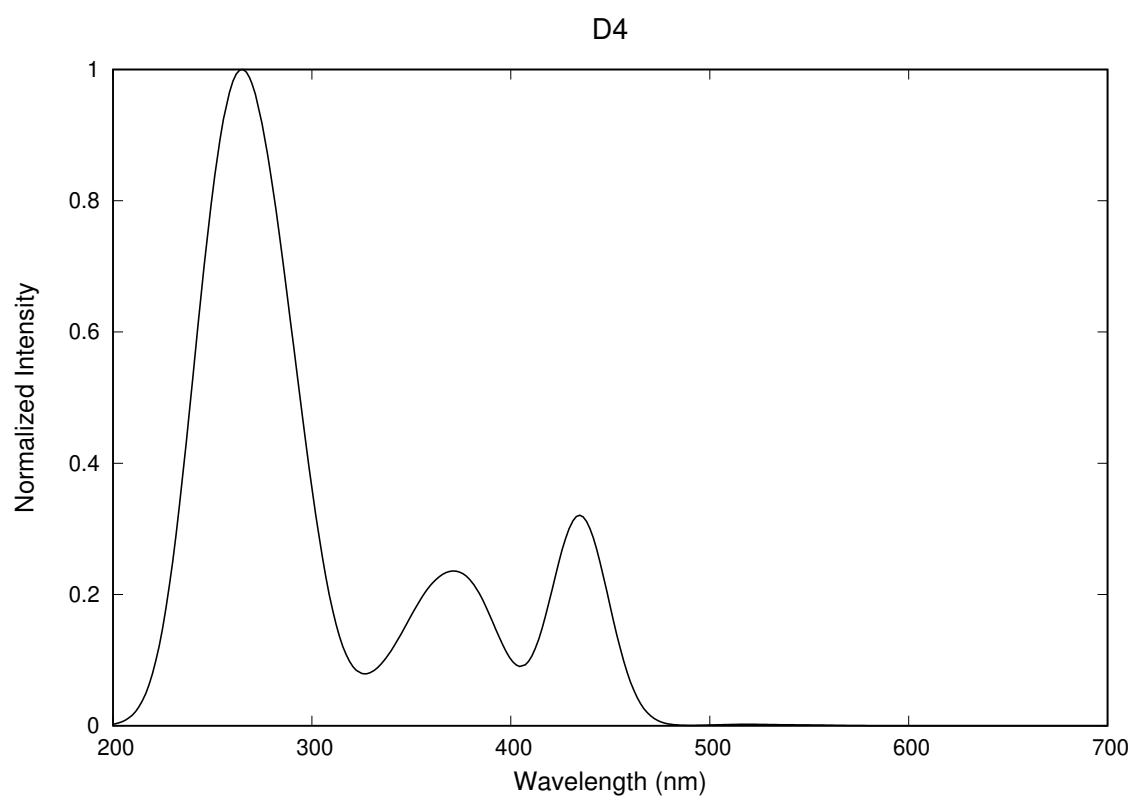
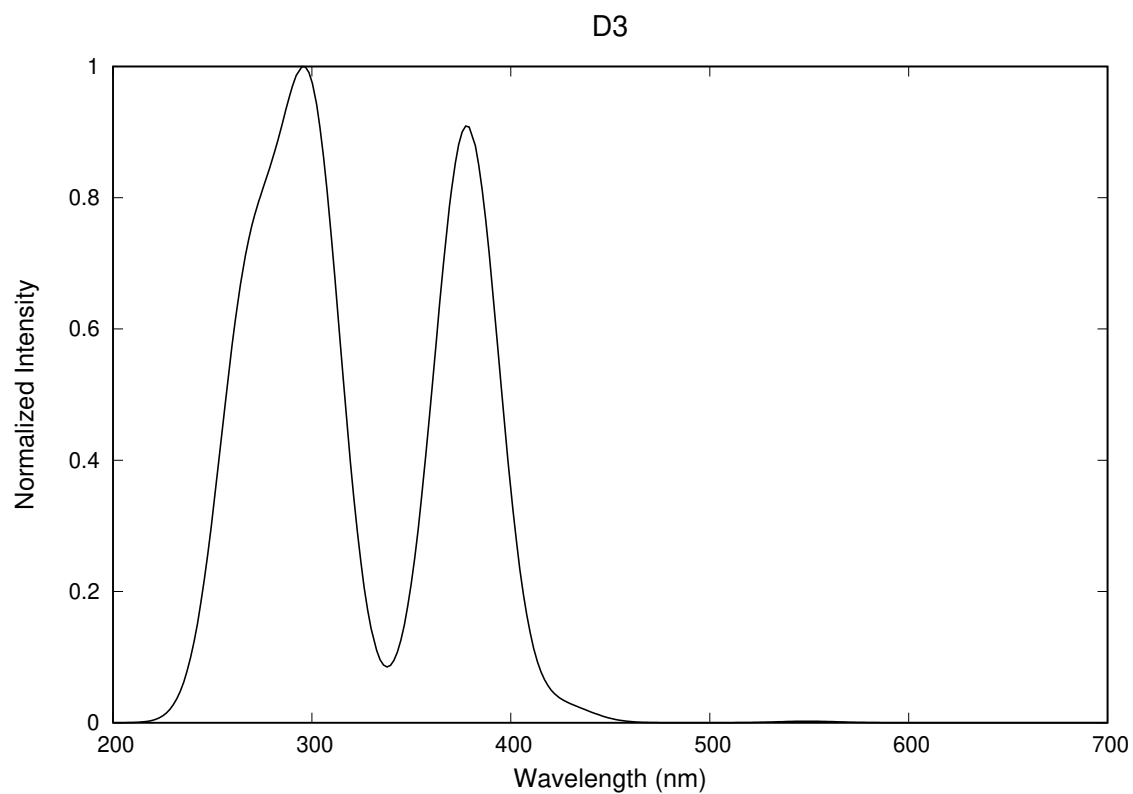


Figure S25: Calculated normalized absorption UV-vis spectra of iron dyes **D3** and **D4**.

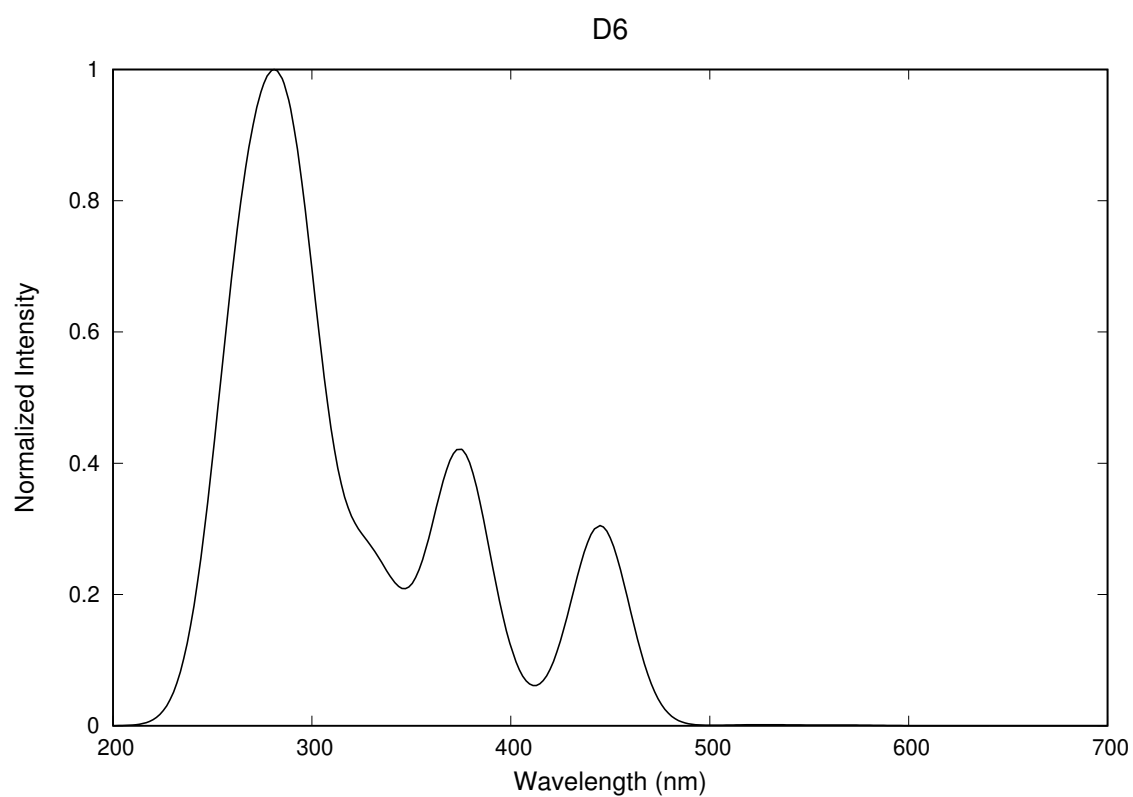
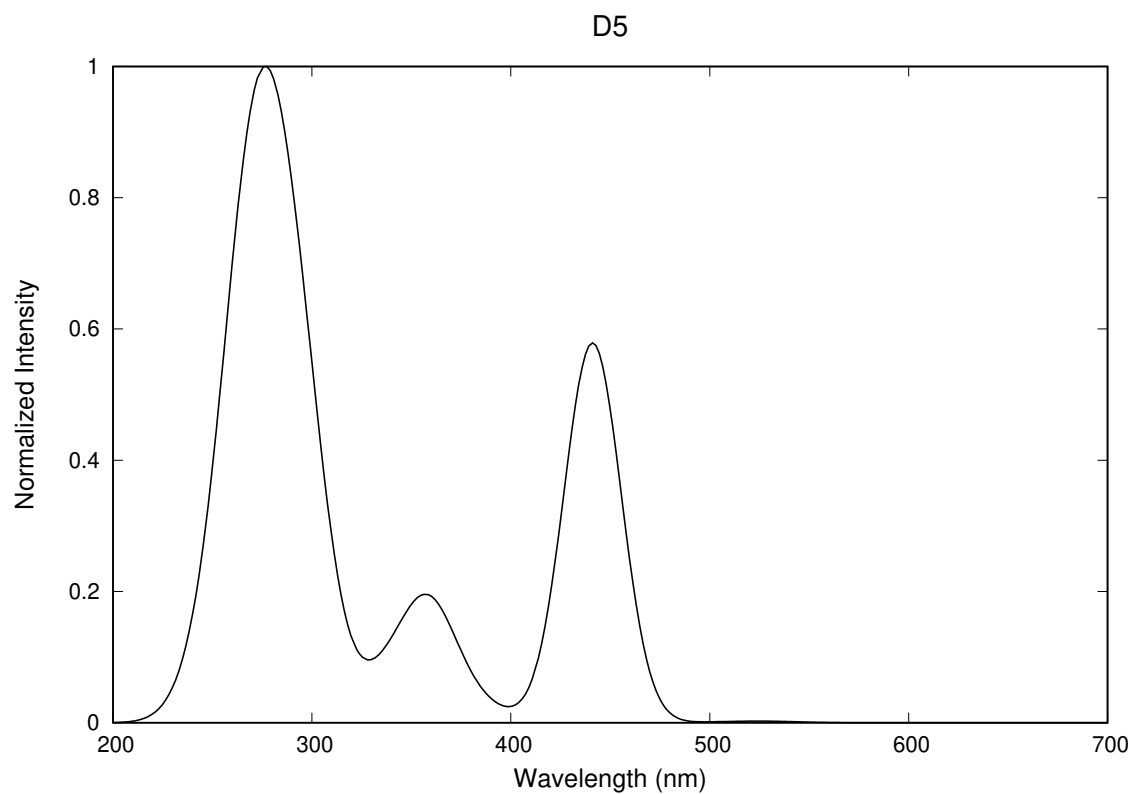


Figure S26: Calculated normalized absorption UV-vis spectra of iron dyes **D5** and **D6**.

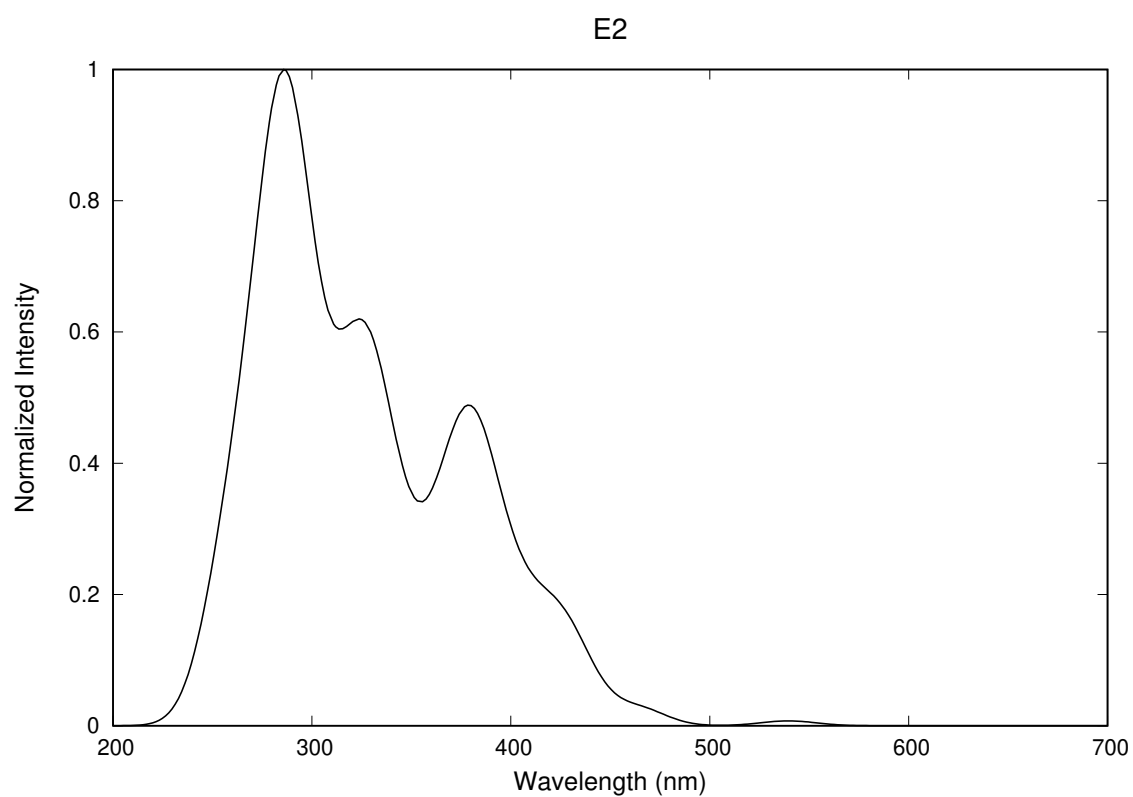
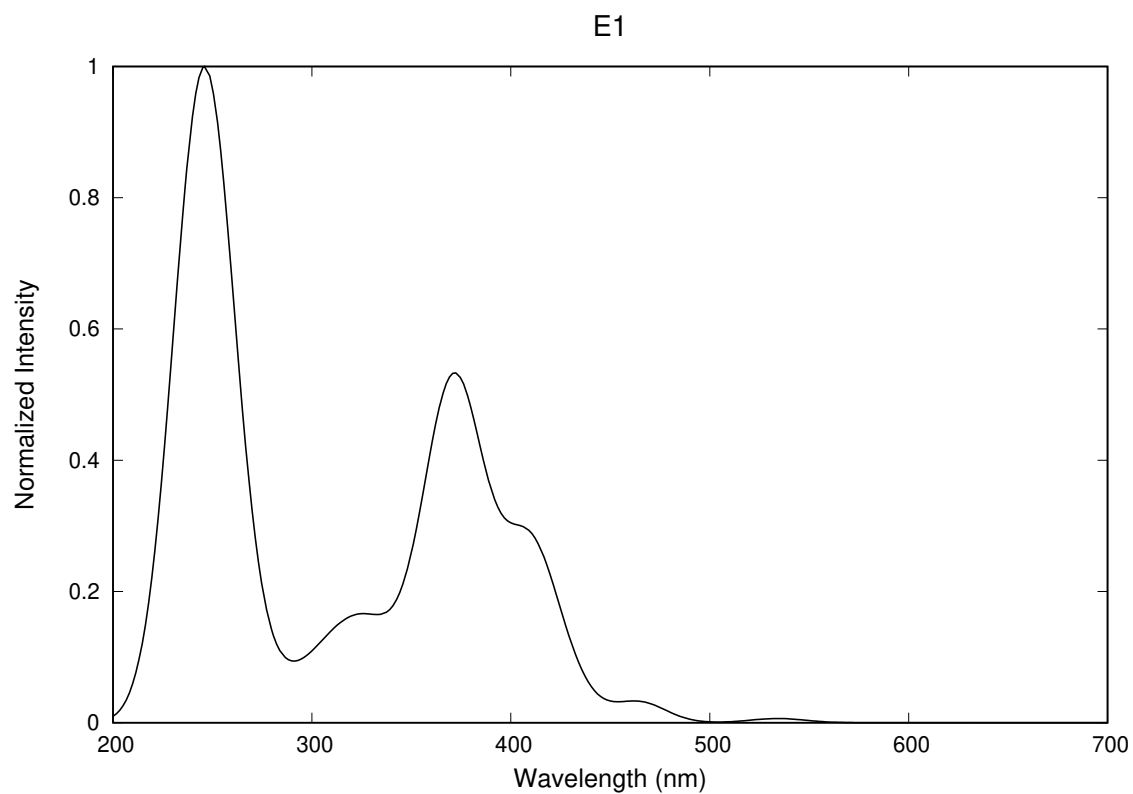


Figure S27: Calculated normalized absorption UV-vis spectra of iron dyes **E1** and **E2**.

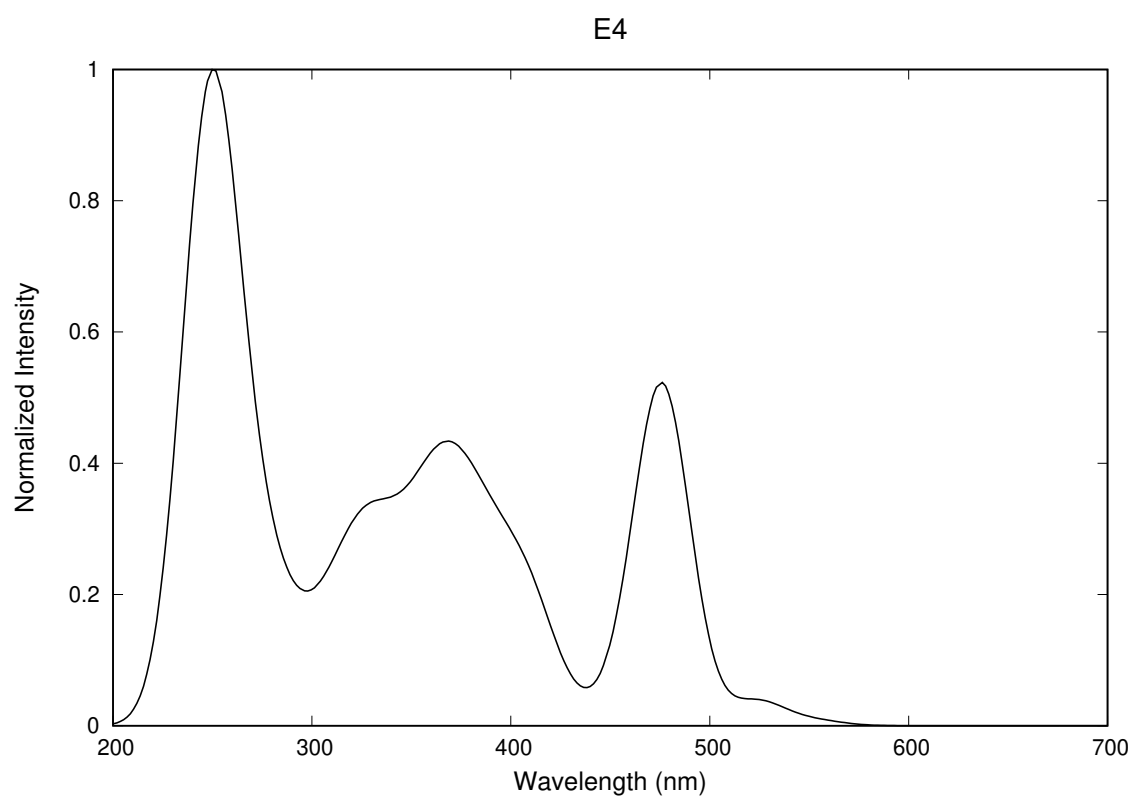
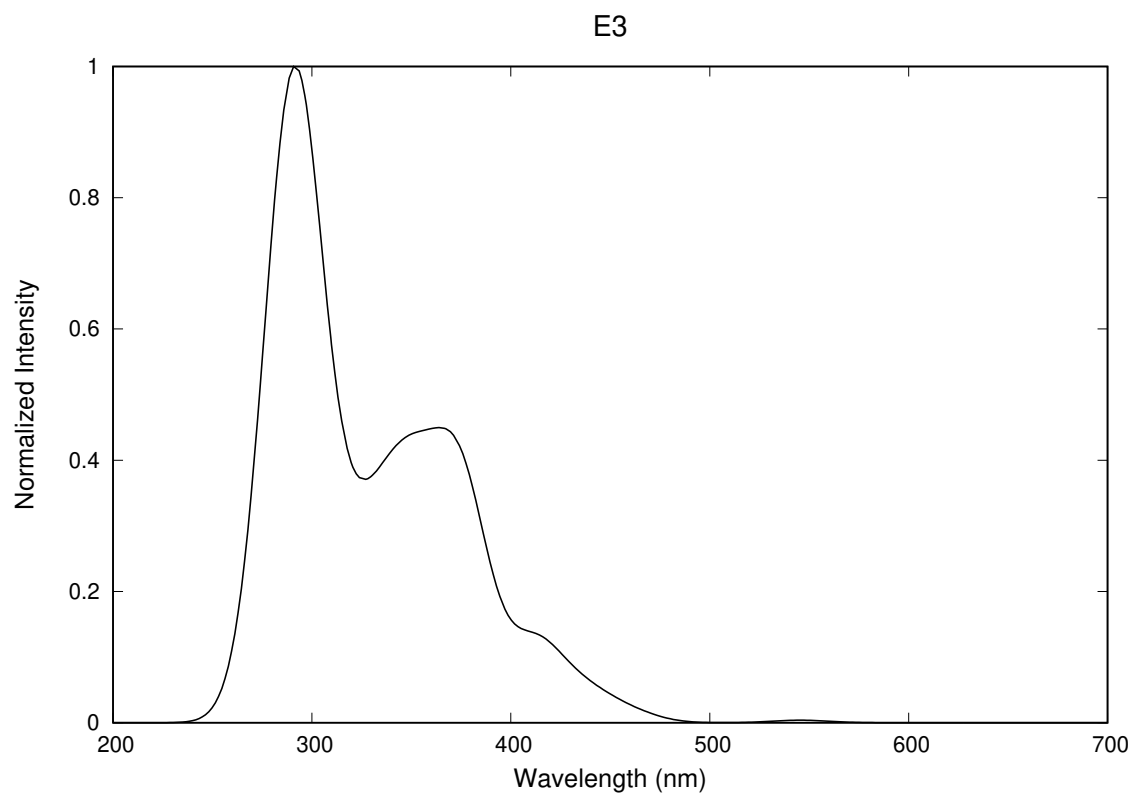


Figure S28: Calculated normalized absorption UV-vis spectra of iron dyes **E3** and **E4**.

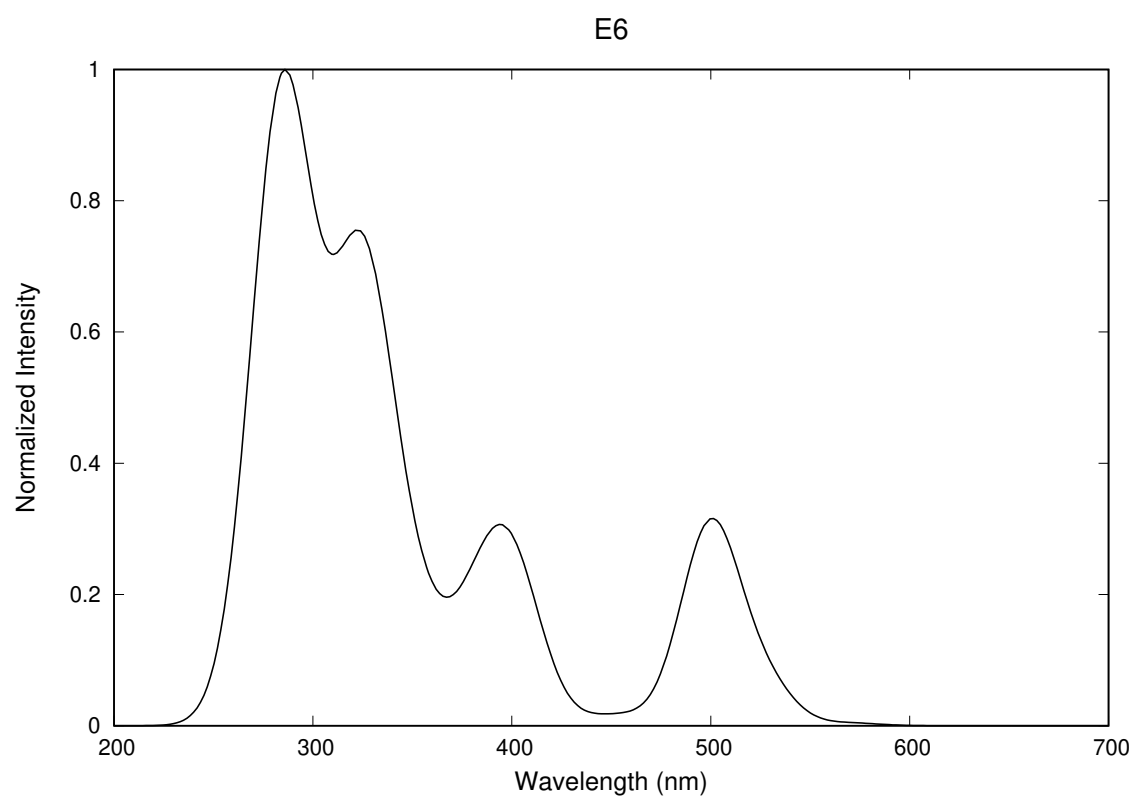
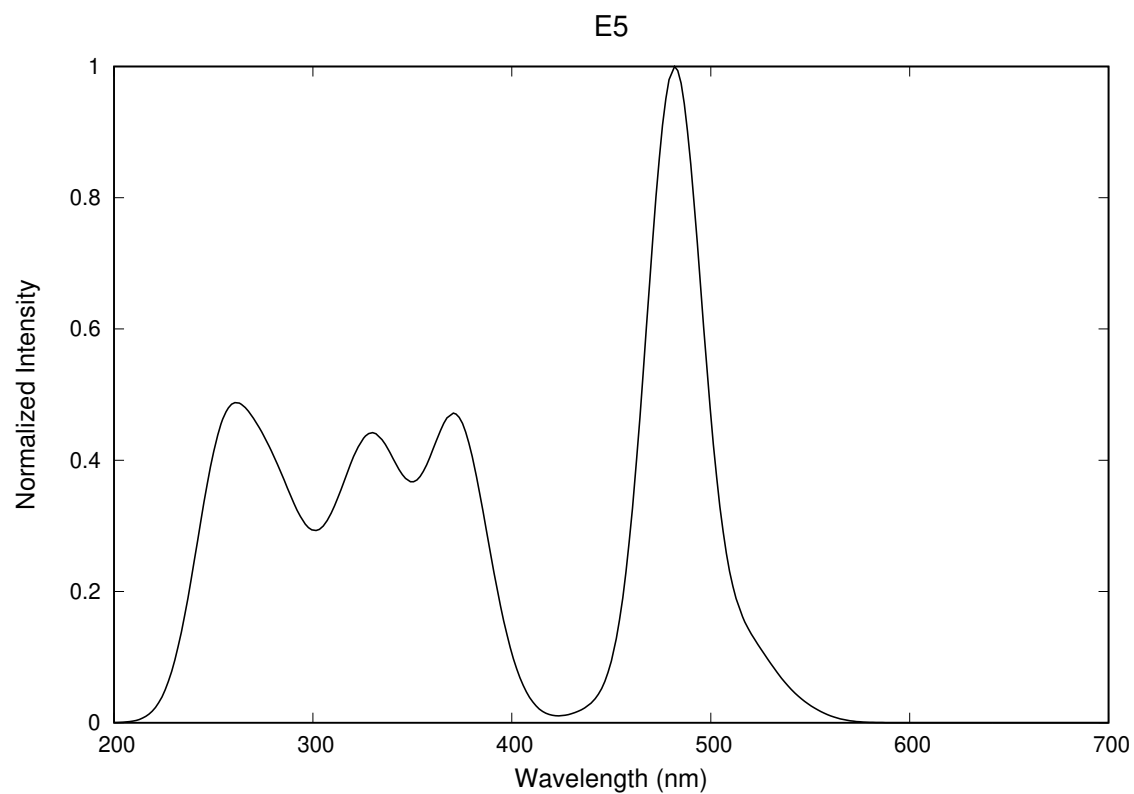


Figure S29: Calculated normalized absorption UV-vis spectra of iron dyes **E5** and **E6**.

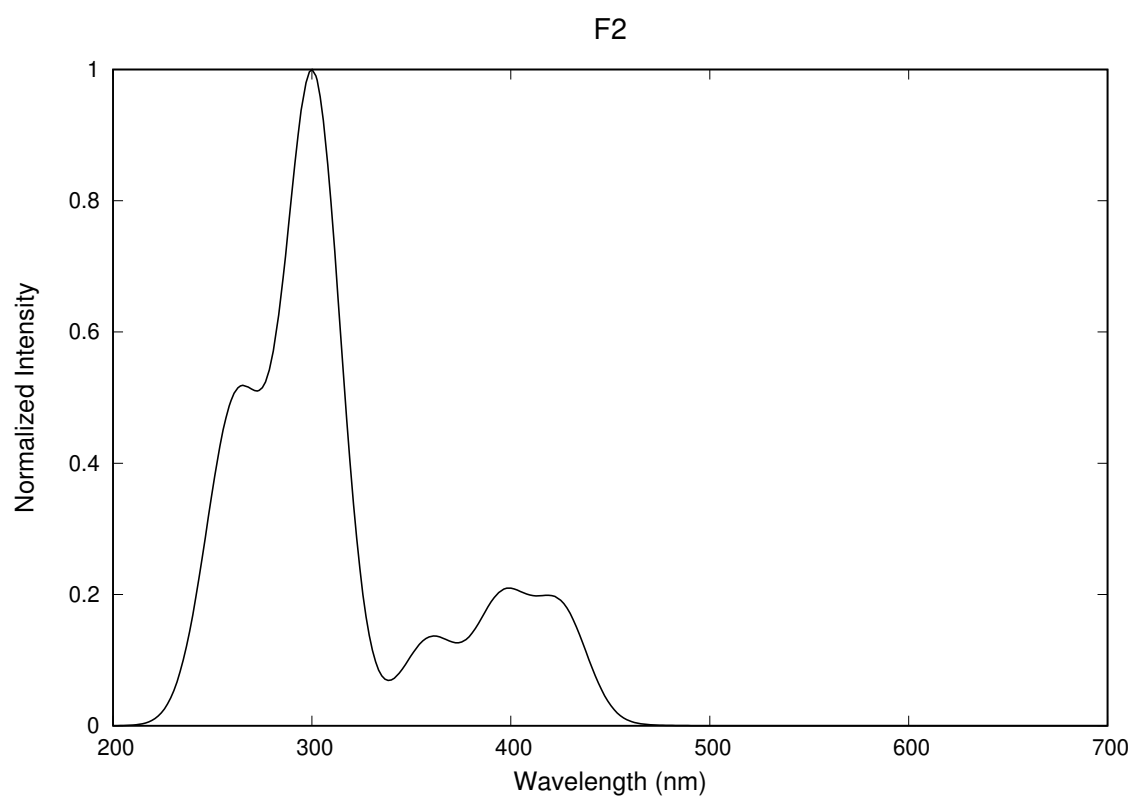
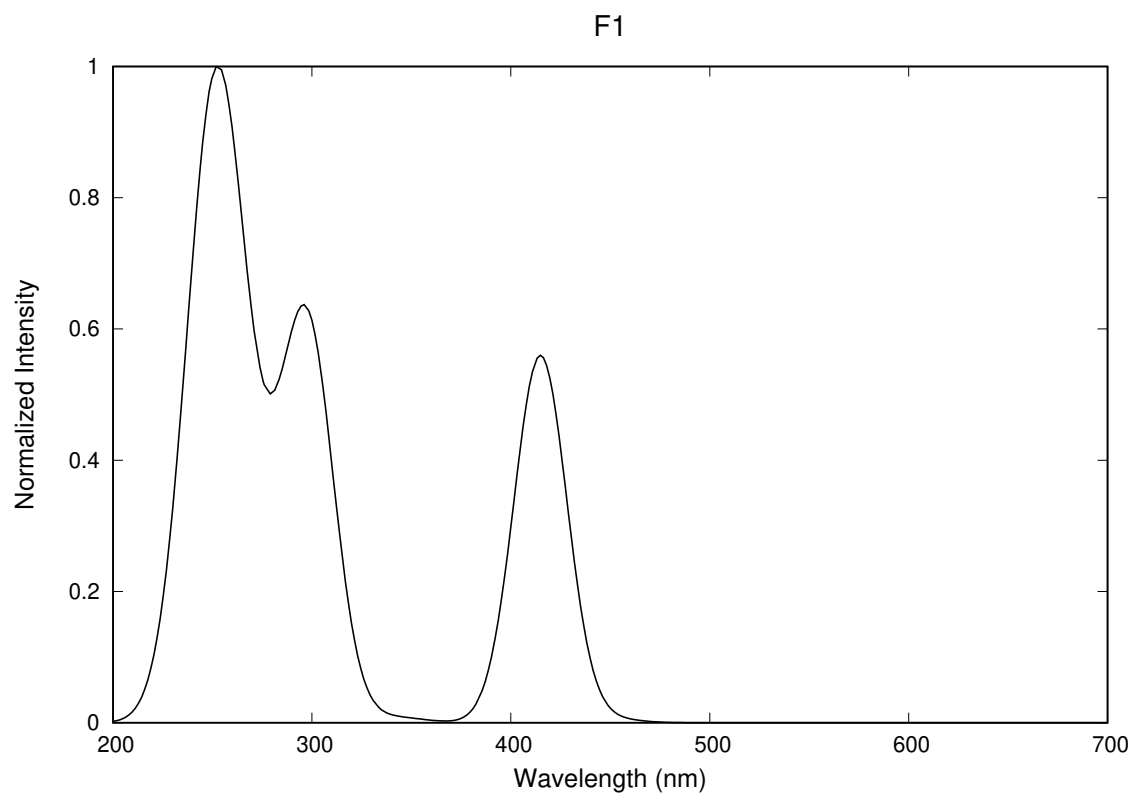


Figure S30: Calculated normalized absorption UV-vis spectra of iron dyes **F1** and **F2**.

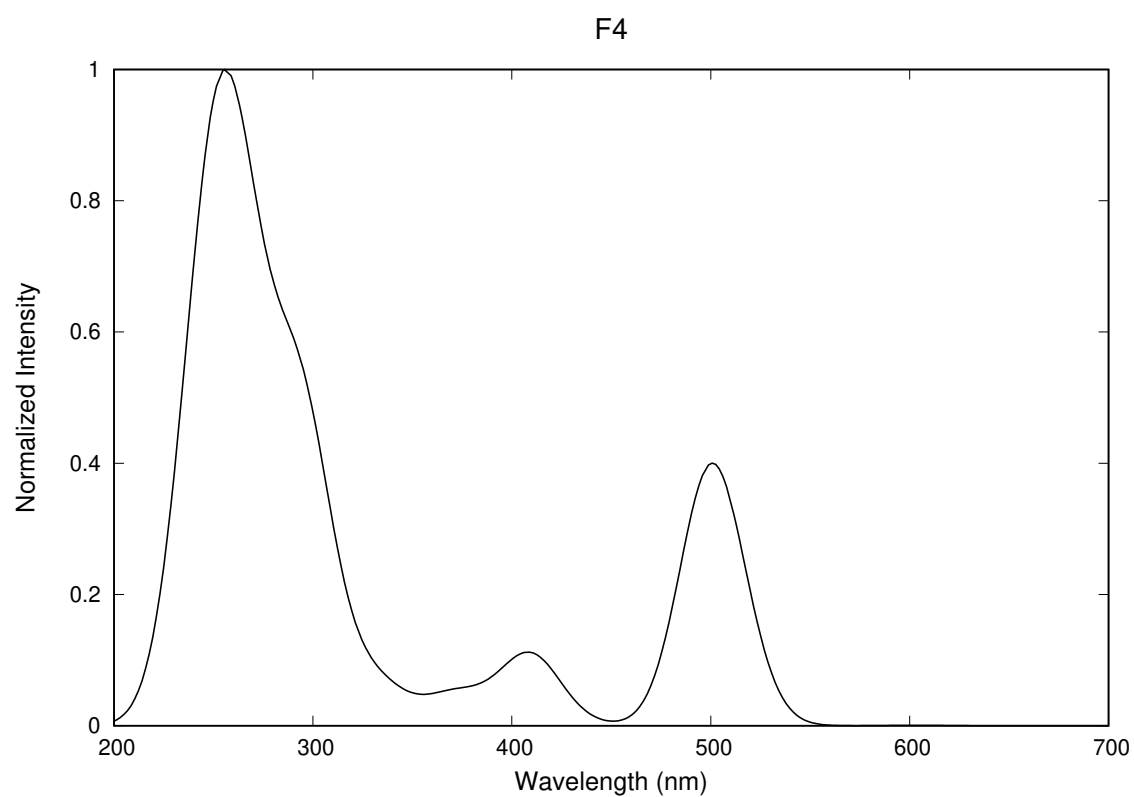
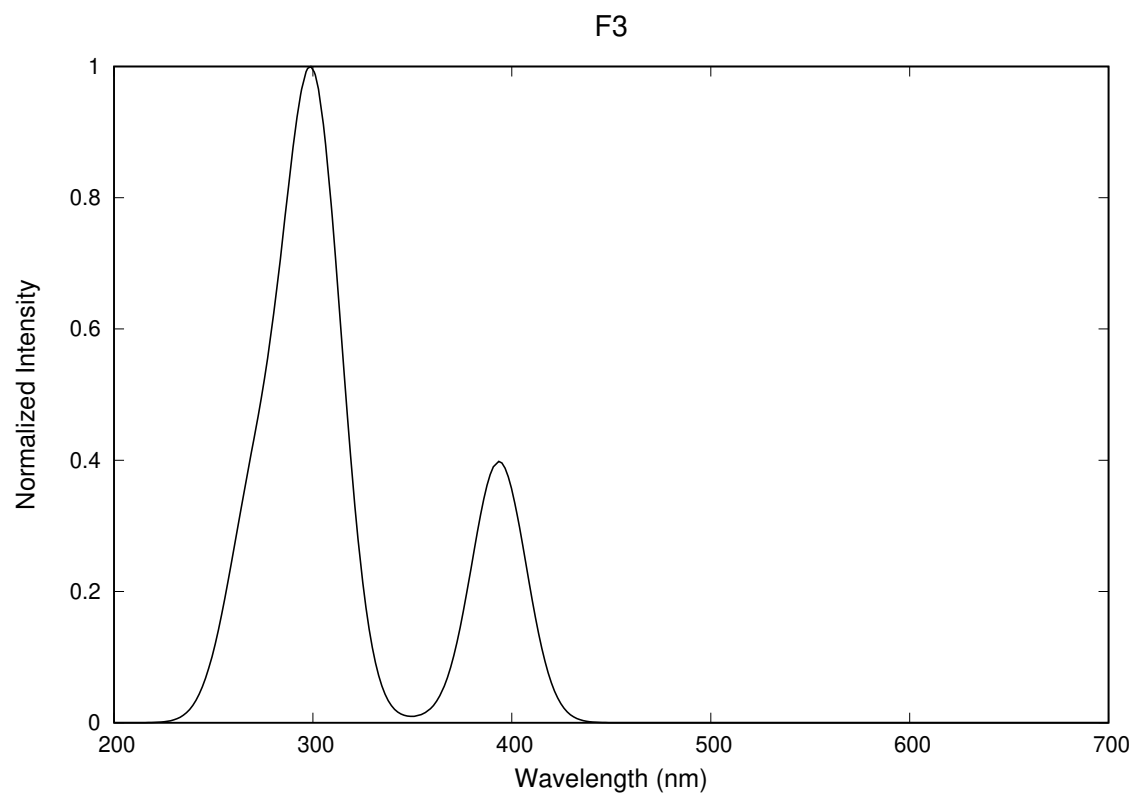


Figure S31: Calculated normalized absorption UV-vis spectra of iron dyes **F3** and **F4**.

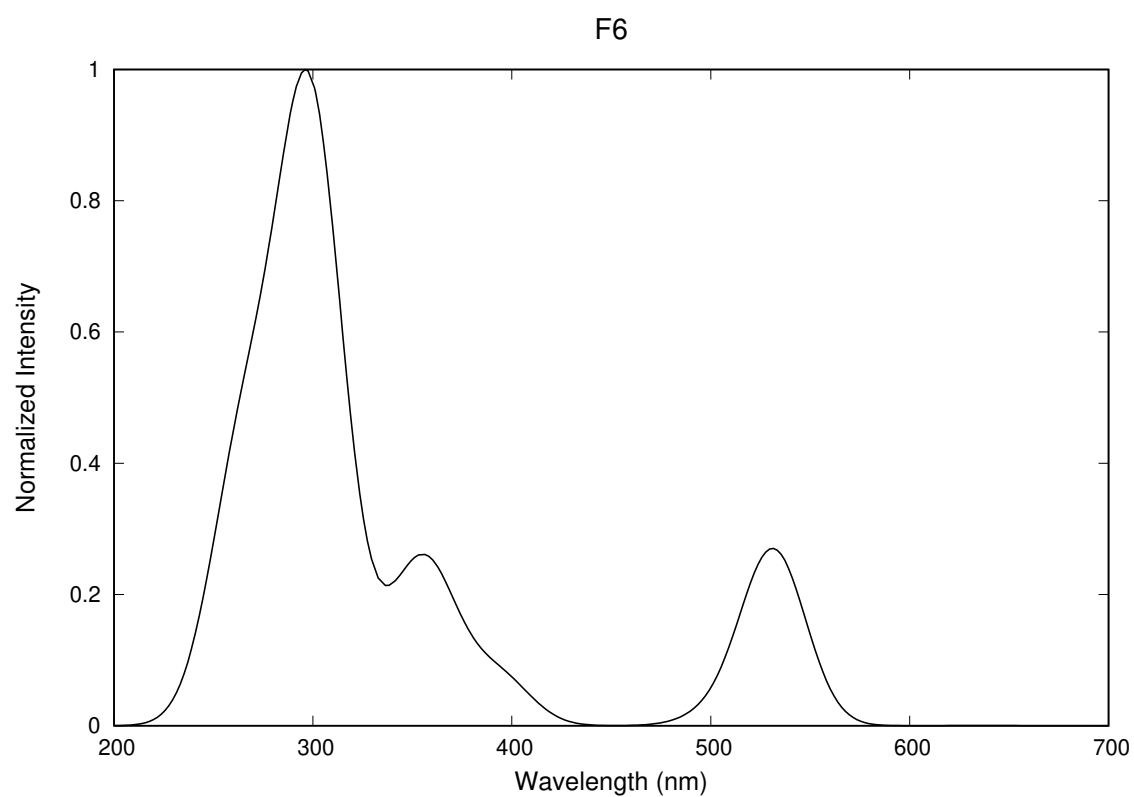
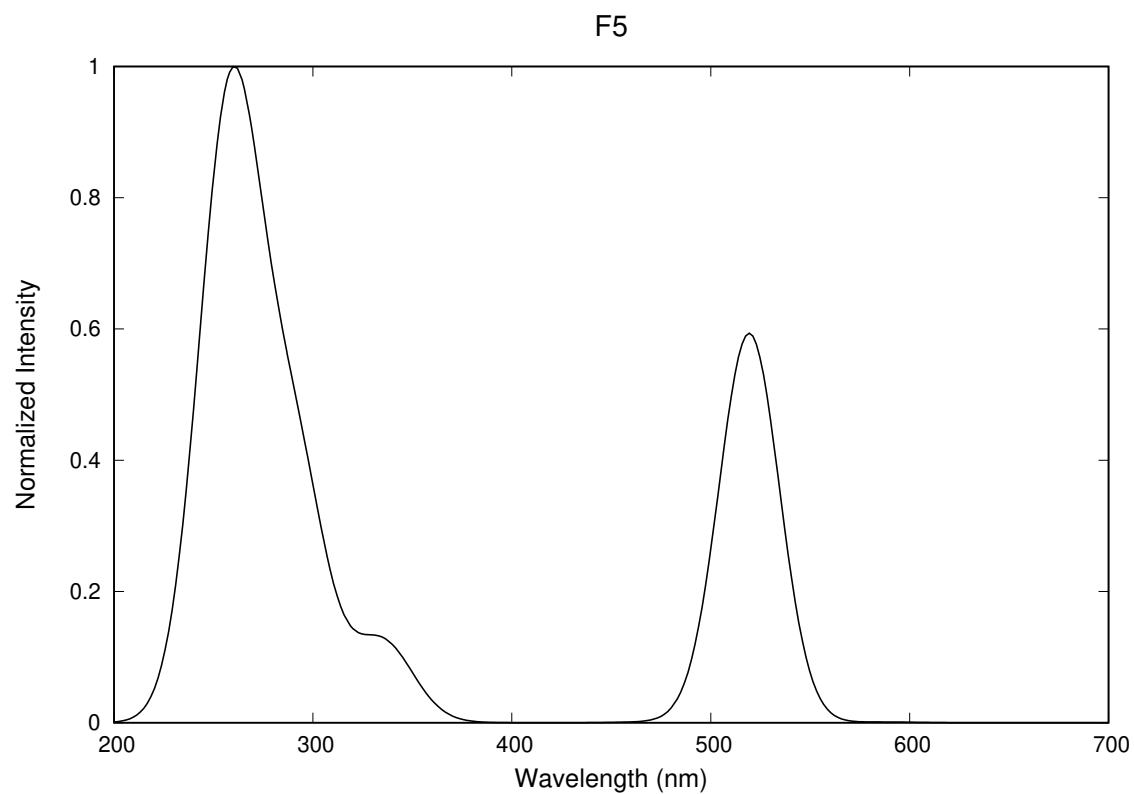


Figure S32: Calculated normalized absorption UV-vis spectra of iron dyes **F5** and **F6**.

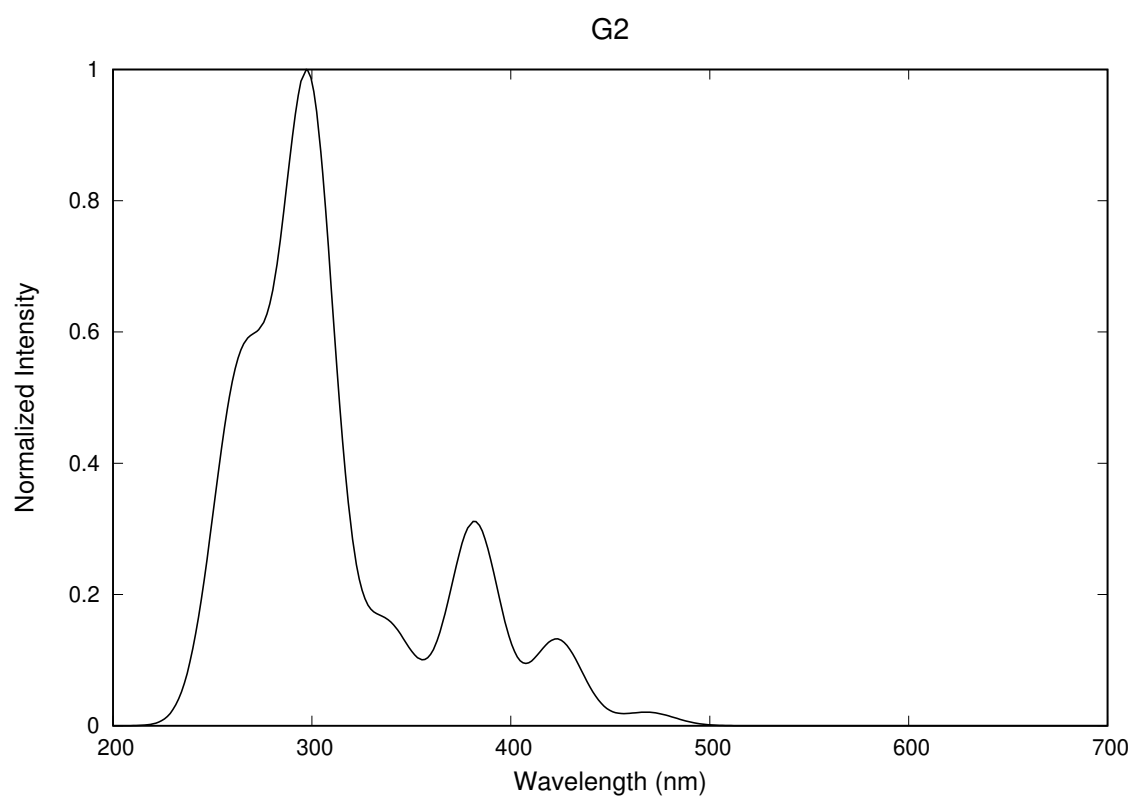
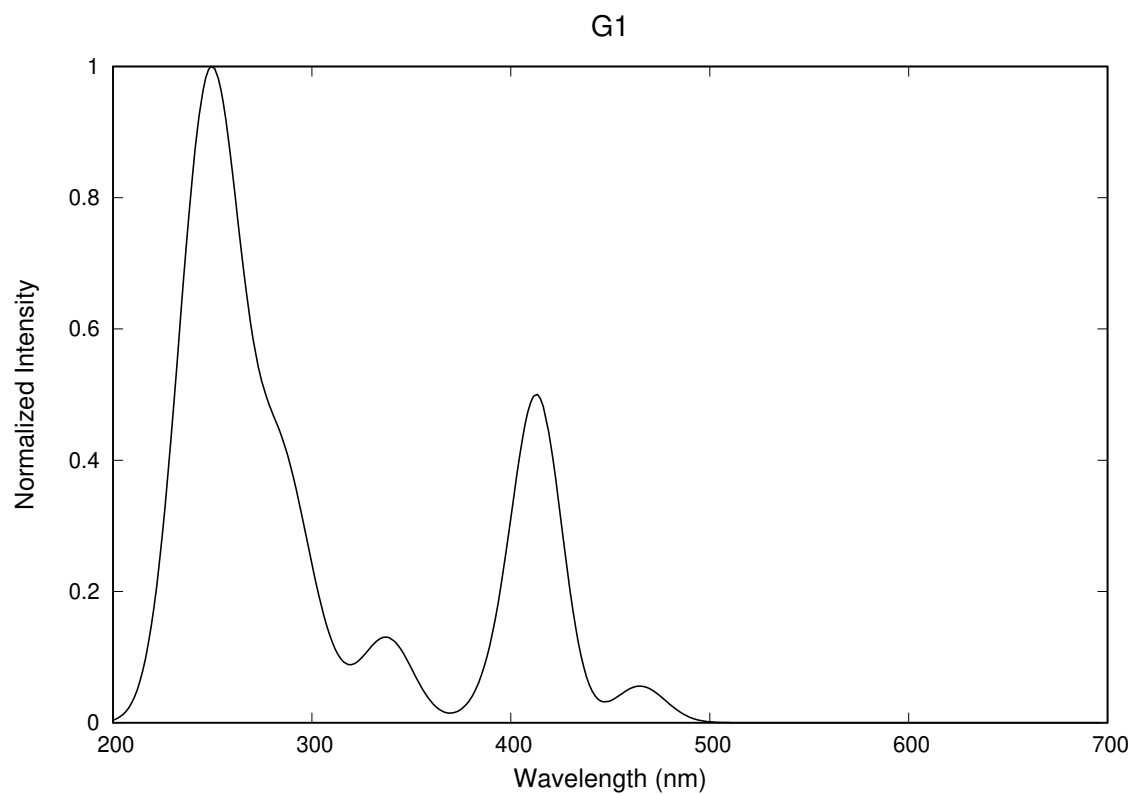


Figure S33: Calculated normalized absorption UV-vis spectra of iron dyes **G1** and **G2**.

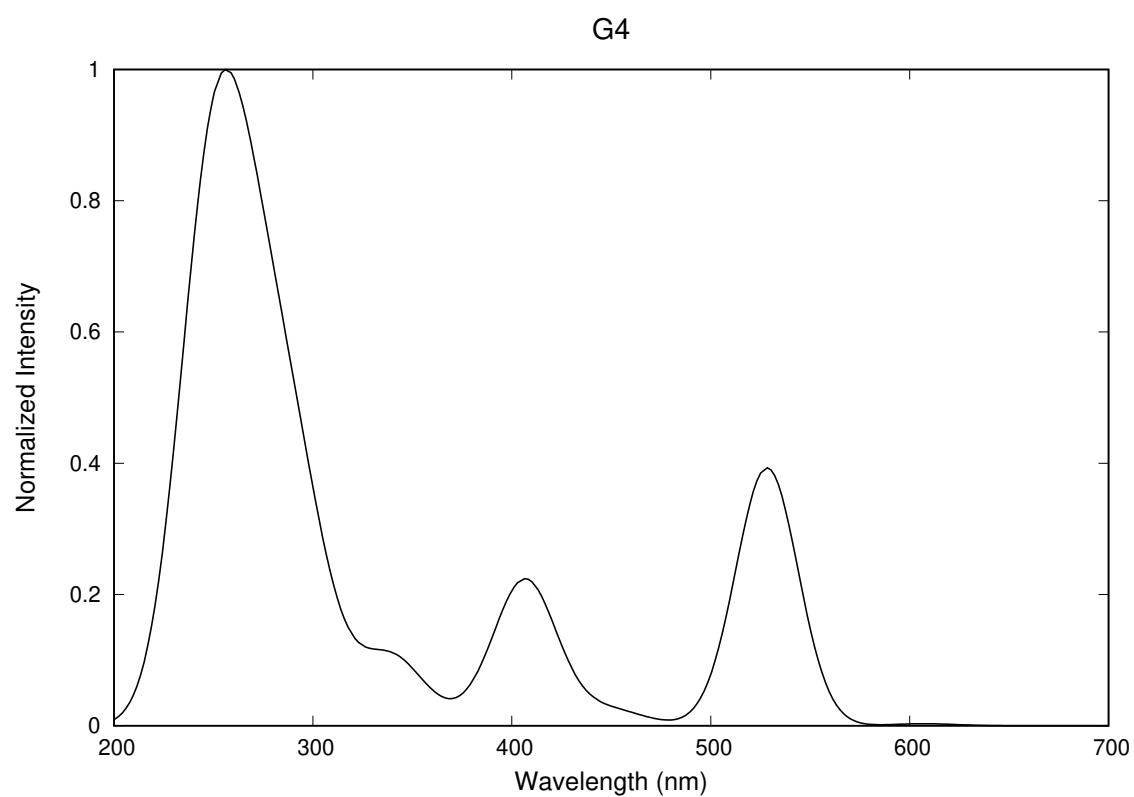
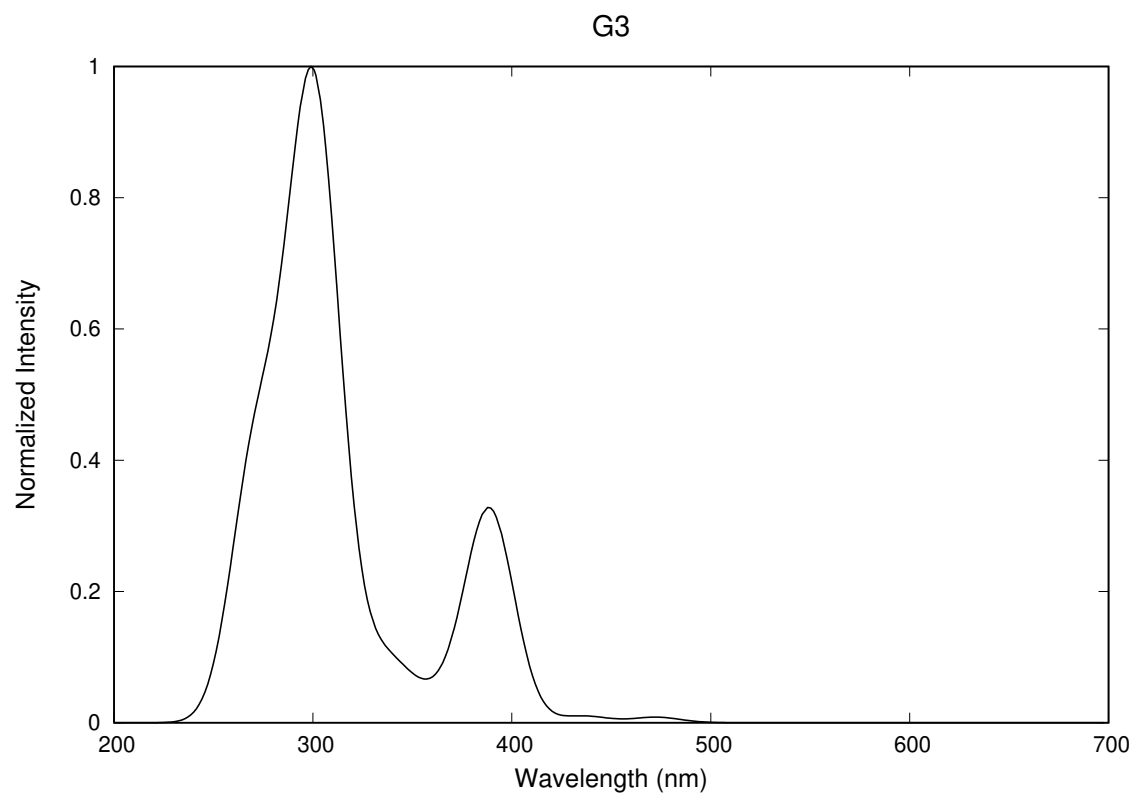


Figure S34: Calculated normalized absorption UV-vis spectra of iron dyes **G3** and **G4**.

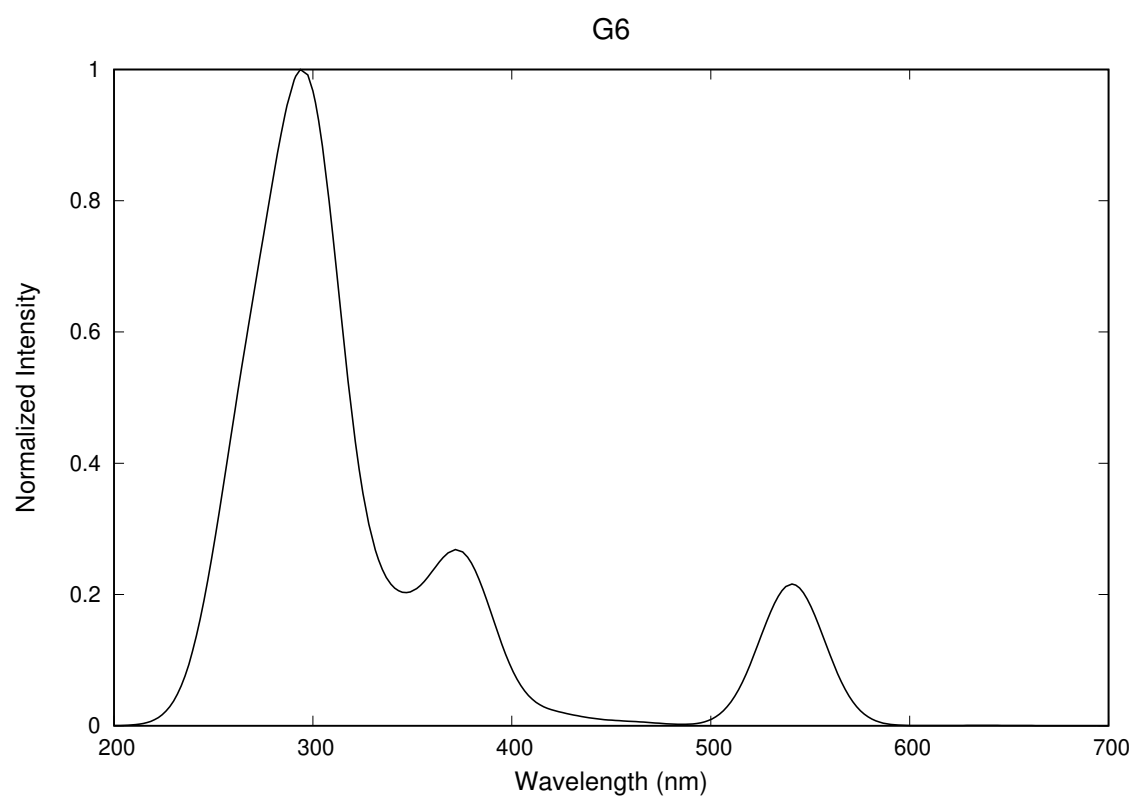
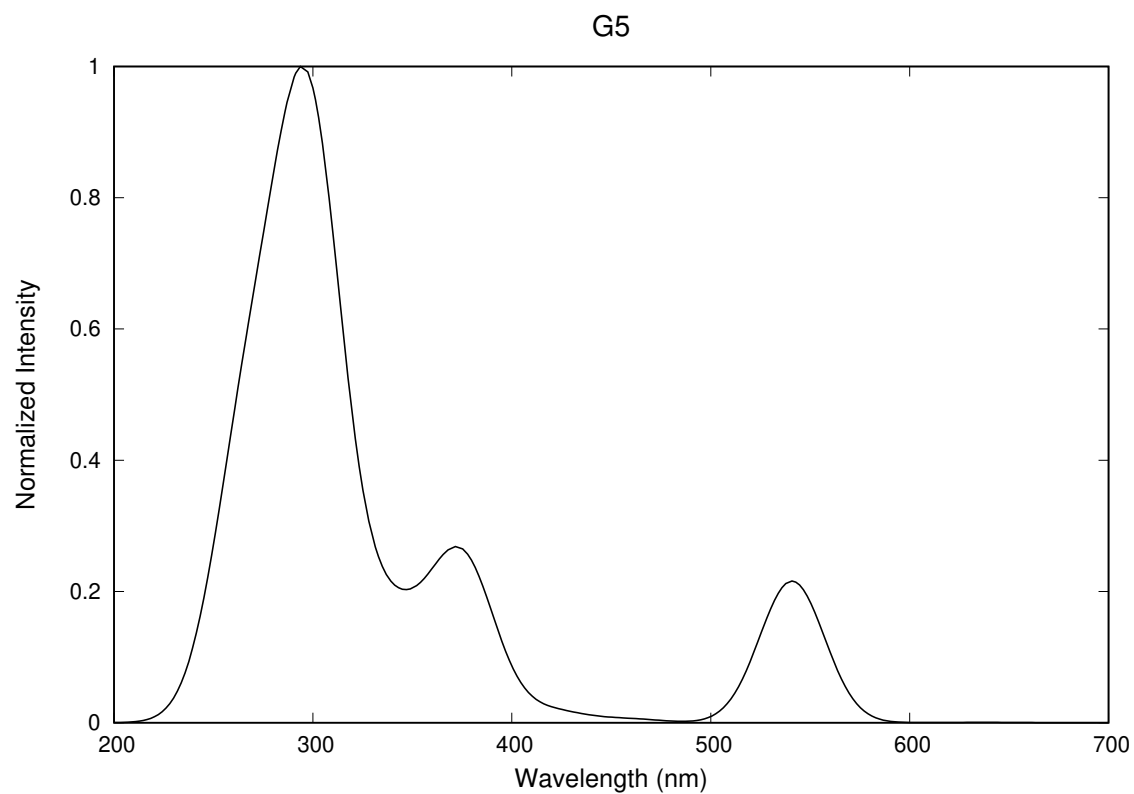


Figure S35: Calculated normalized absorption UV-vis spectra of iron dyes **G5** and **G6**.