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## **Electronic Supplementary Information**

### **Photophysical, electrochemical, and photoelectrochemical properties of new azulene-based dye molecules**

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Fig. 1S Optimized ground-state geometries and atom labels for Azu-1, Azu-2, Guai-1, and Guai-2.

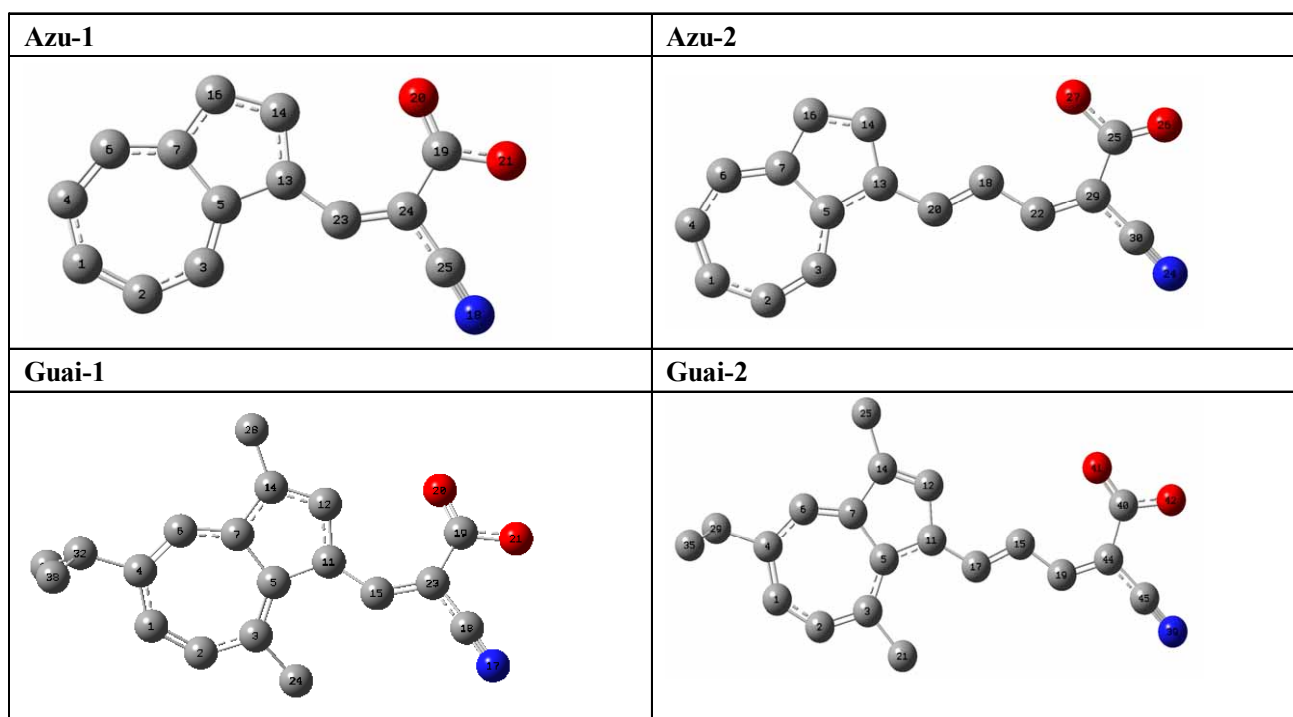


Table 1S Dihedral angles for the optimized structures of Azu-1, Azu-2, Guai-1, and Guai-2.

Azu-1	Azu-2	Guai-1	Guai-2
$ 4-6-7-16  = -180.0$	$ 4-6-7-16  = 180.0$	$ 4-5-7-14  = -178.6$	$ 4-6-7-14  = -180.0$
$ 2-3-5-13  = -180.0$	$ 2-3-5-13  = 180.0$	$ 2-3-5-11  = 176.4$	$ 2-3-5-11  = 180.0$
$ 14-13-24-24  = 0.0$	$ 14-13-20-18  = 0.0$	$ 14-12-11-15  = -169.6$	$ 12-11-17-15  = 0.0$
$ 5-13-23-24  = 180.0$	$ 5-13-20-18  = -180.0$	$ 3-5-11-15  = -16.8$	$ 5-11-17-15  = -180.0$
$ 13-23-24-19  = 0.0$	$ 18-22-29-25  = 0.0$	$ 11-15-23-19  = -7.5$	$ 15-19-44-40  = 0.0$
$ 13-23-24-25  = 180.0$	$ 18-22-29-30  = 180.0$	$ 11-15-23-18  = 175.7$	$ 15-19-44-45  = 180.0$

<sup>a</sup> The numbers within the two vertical lines denote the atoms involved in the corresponding dihedral angles (see Fig. 1S).