

# Supporting Information: Infrared spectroscopy from electrostatic embedding QM/MM: local normal mode analysis of blue-light-induced infrared spectra of arabidopsis thaliana plant cryptochrome<sup>†</sup>

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## 1 Theoretical Infrared spectrum of FAD embedded in cryptochrome

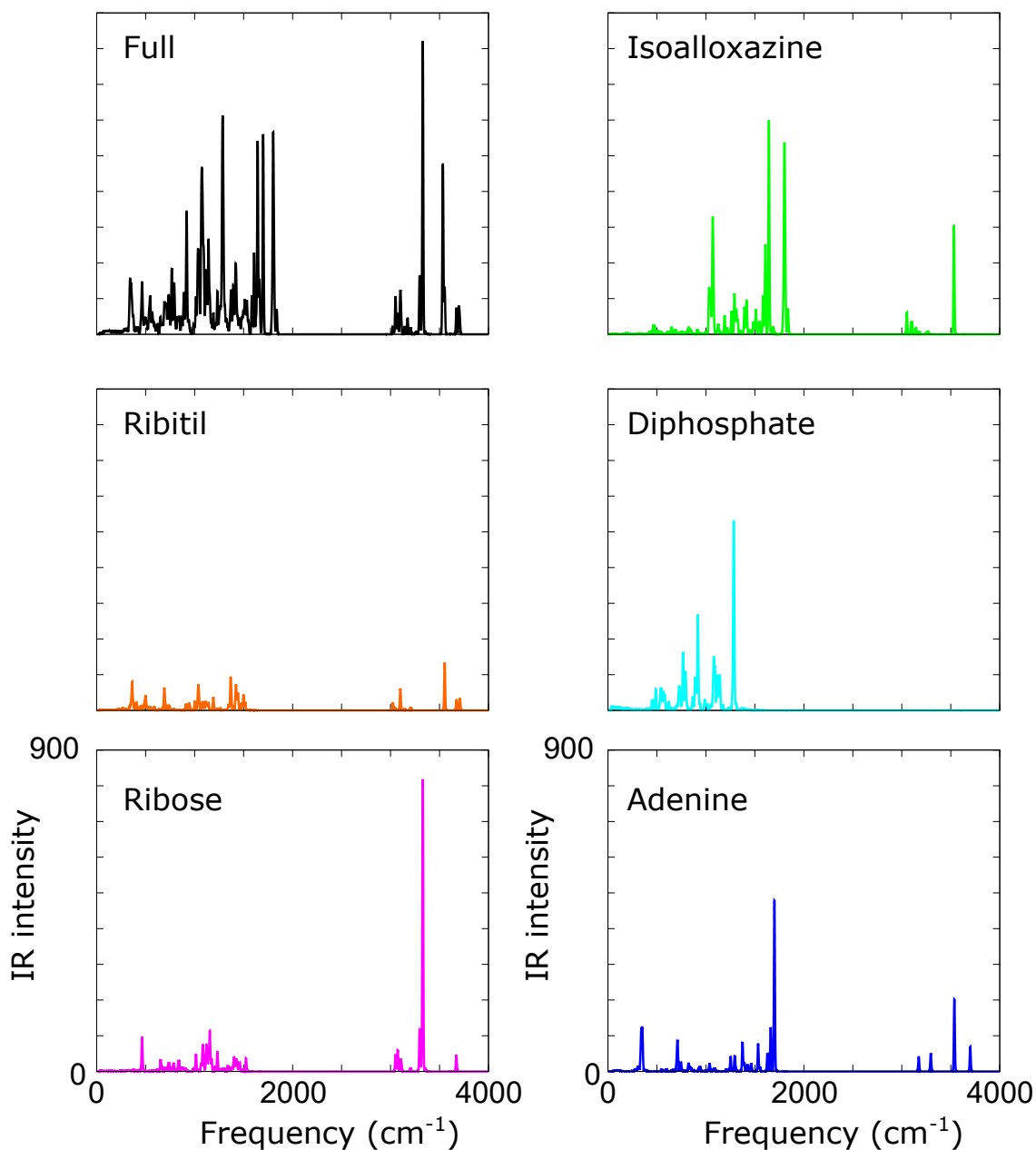


Fig. 1 Full range IR theoretical spectrum of FAD embedded in cryptochrome protein decomposed in fragments.

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## 2 Theoretical Infrared spectrum of FAD<sup>•-</sup> embedded in cryptochrome

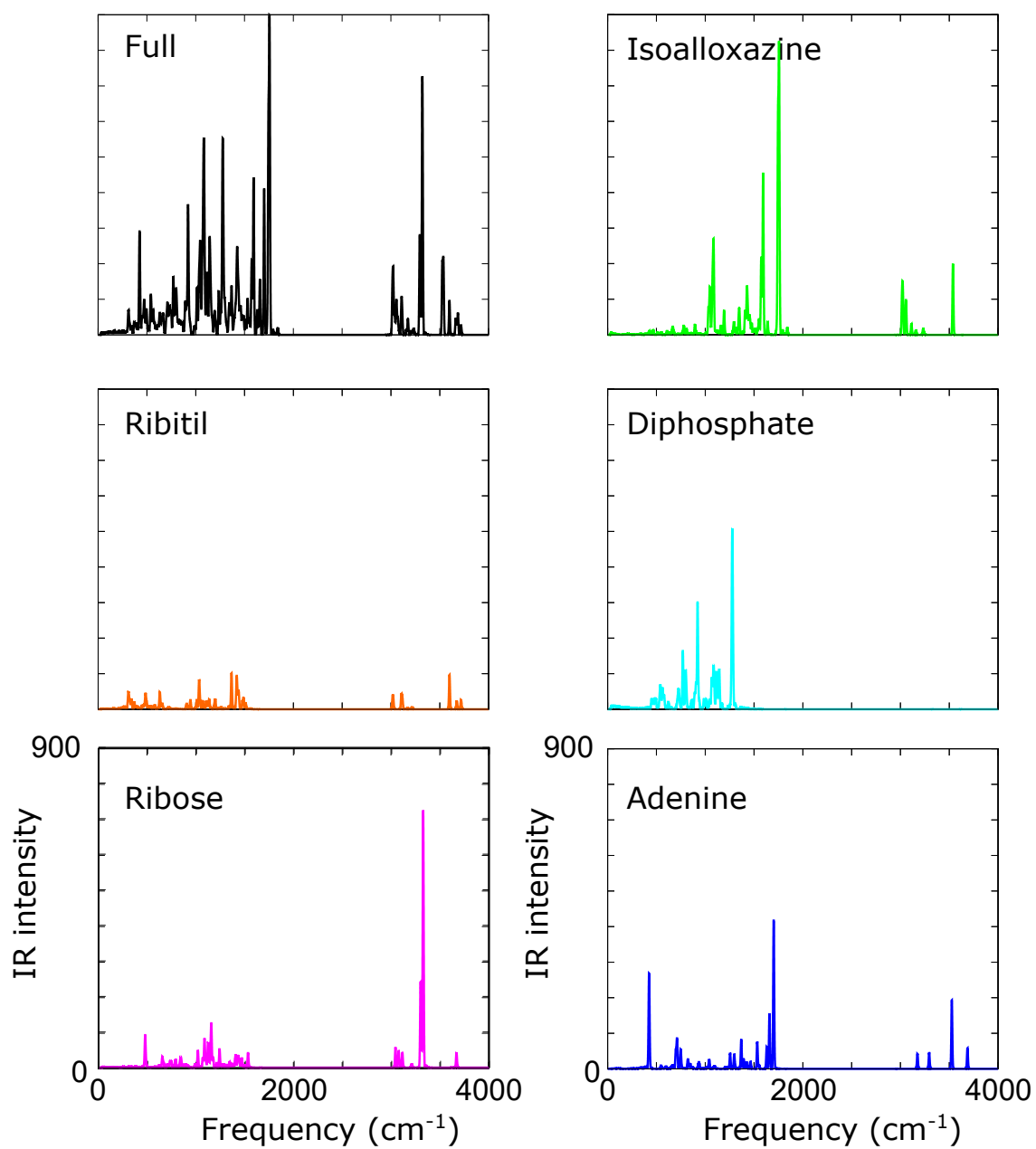


Fig. 2 Full range IR theoretical spectrum of FAD<sup>•-</sup> embedded in cryptochrome protein decomposed in fragments.

### 3 Theoretical Infrared spectrum of FADH<sup>•</sup> embedded in cryptochrome

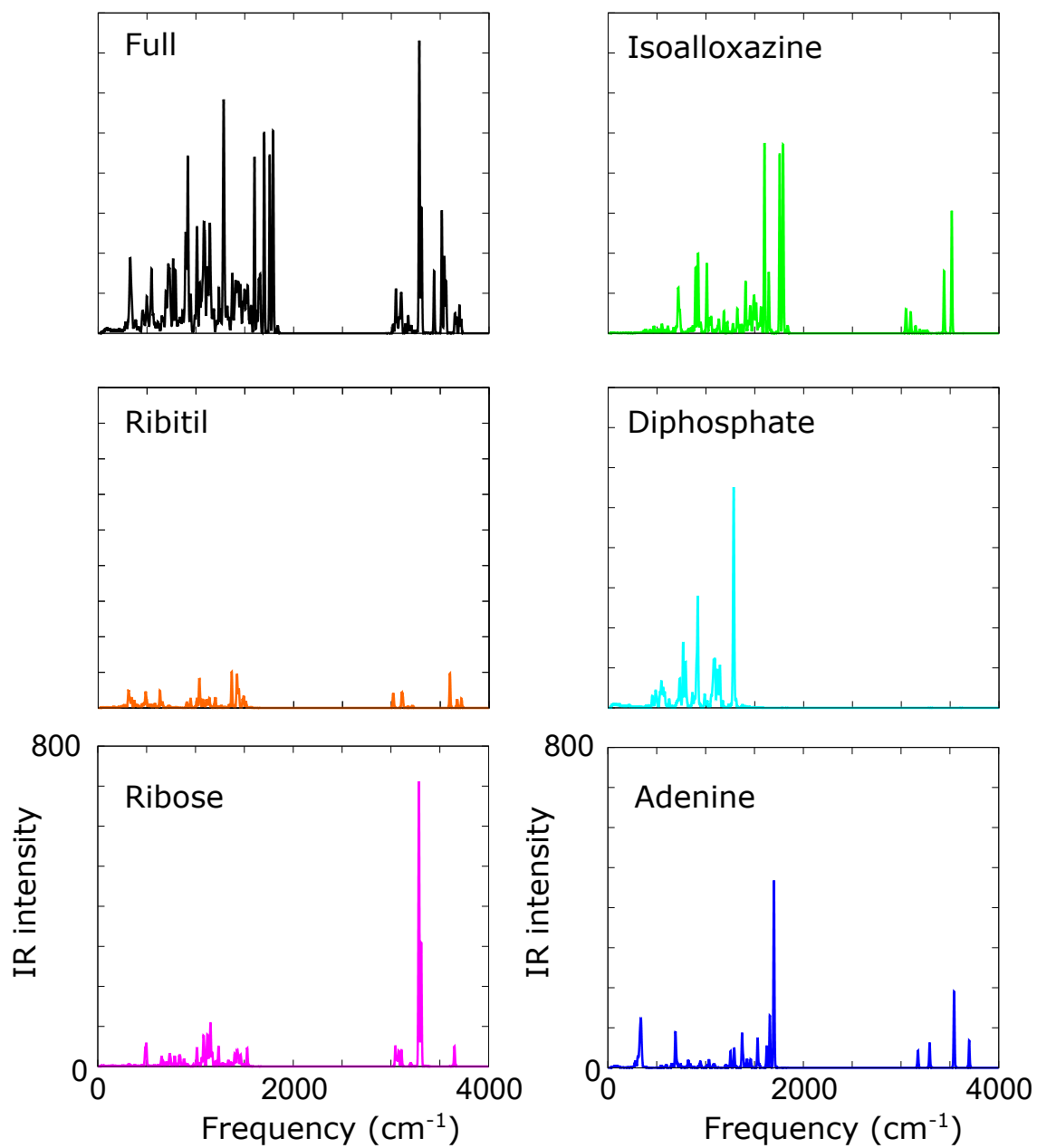


Fig. 3 Full range IR theoretical spectrum of FADH<sup>•</sup> embedded in cryptochrome protein decomposed in fragments.

#### 4 Theoretical Infrared spectrum of FADH<sup>-</sup> embedded in cryptochrome

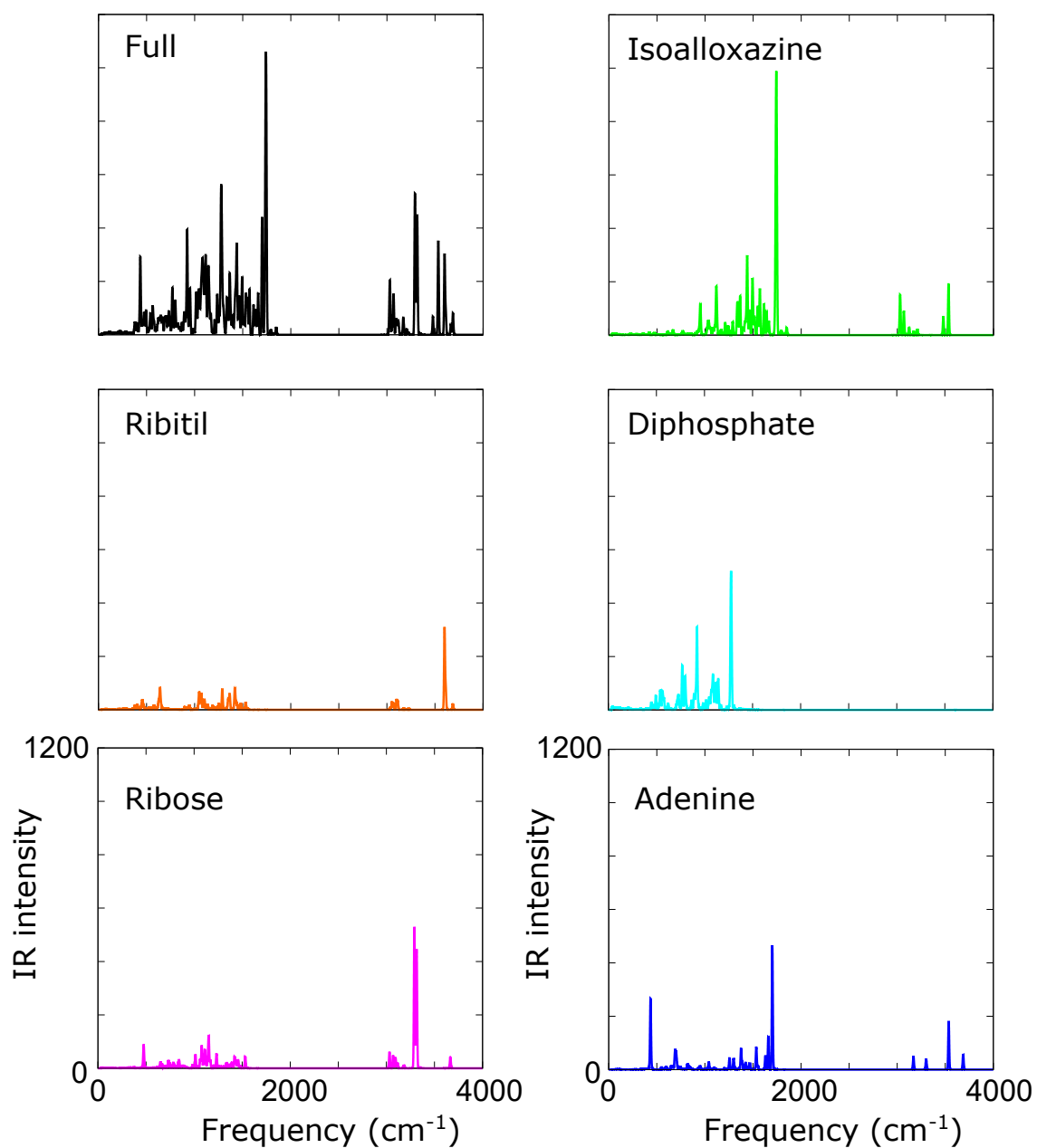


Fig. 4 Full range IR theoretical spectrum of FADH<sup>-</sup> embedded in cryptochrome protein decomposed in fragments.