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Supplementary Information for: Computational and photophysical characterization of a Laurdan malononitrile derivative†

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† Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/cXCP00000x/

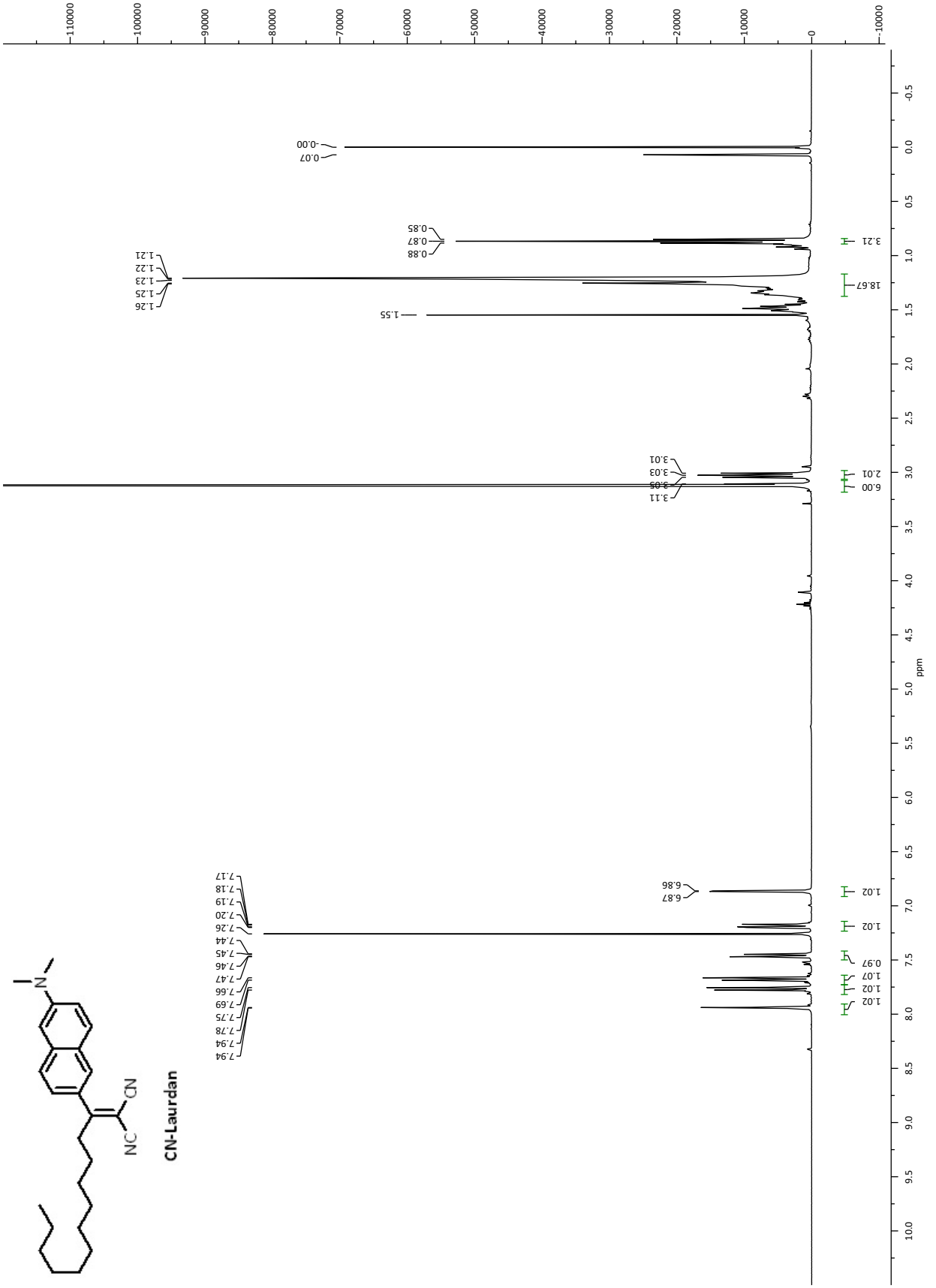

Fig. 1 400 MHz ^{1}H NMR spectrum of CN-Laurdan in $CDCl_3$.

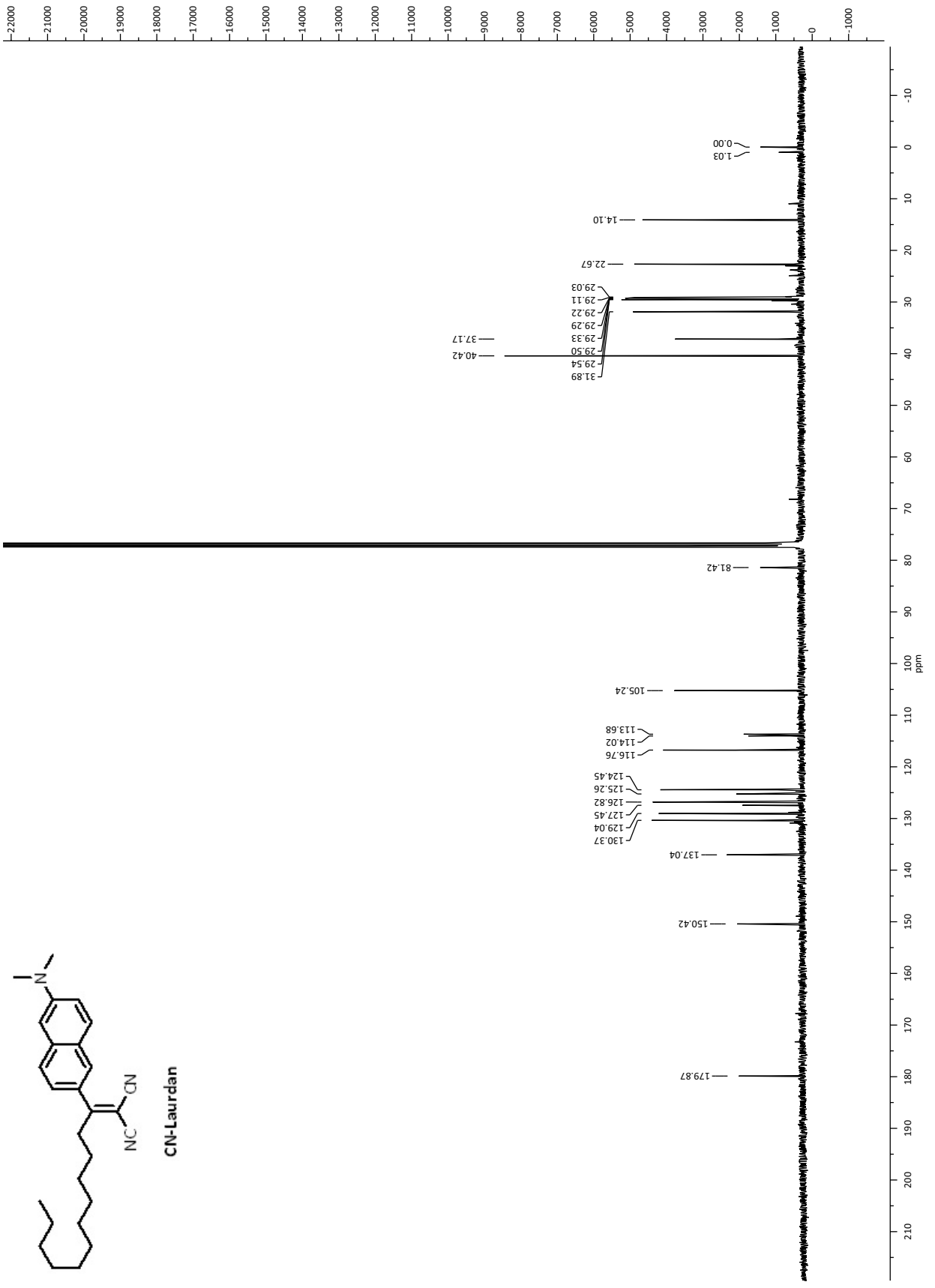

Fig. 2 101 MHz ^{13}C NMR spectrum of CN-Laurdan in $CDCl_3$.

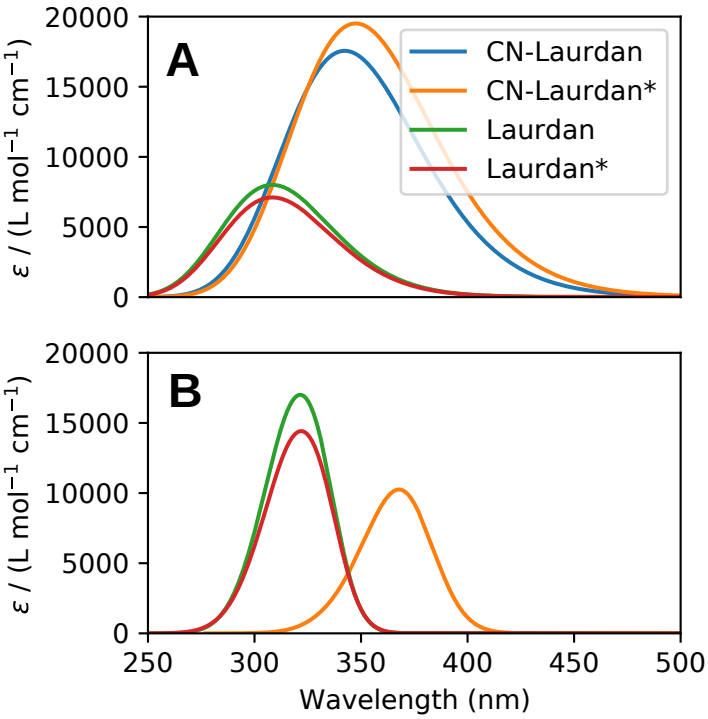

Fig. 3 Simulated absorption spectra of Laurdan and CN-Laurdan. The data is plotted on a wavelength scale, and is otherwise identical to Fig. 3 in the main text. Variants in which the alkyl chain is replaced by a methyl group are denoted with an asterisk (*). (A) Purely electronic spectra with only a phenomenological broadening applied, and (B) electronic spectra that include FCHT effects.

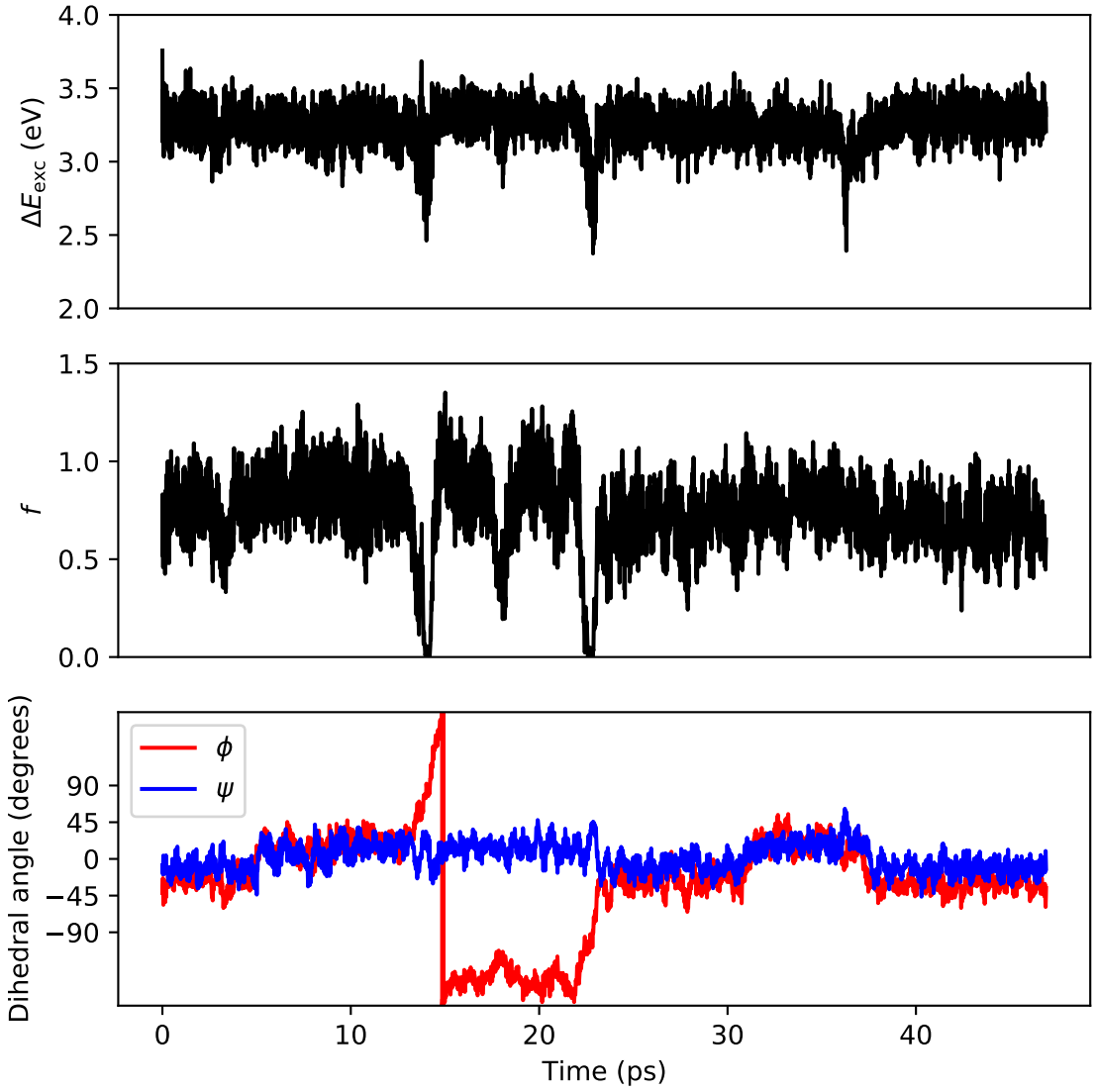

Fig. 4 The excitation energy (top), oscillator strength (middle), and selected dihedral angles (bottom) extracted from an excited-state MD run of CN-Laurdan in vacuum. A time-step of 0.5 fs is used; all other simulation details are identical to the ones described in the main text.