

Supplementary Materials

# Yellow-Green and Blue Fluorescent 1,8-Naphthalimide-Based Sensors for Metal Cations

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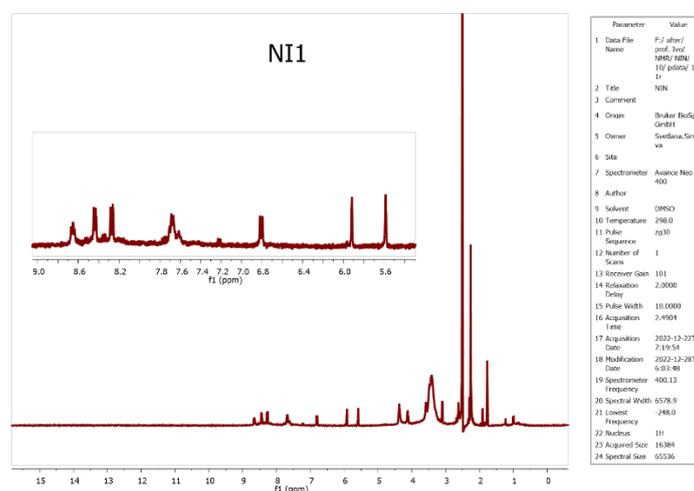


Figure S1. <sup>1</sup>H-NMR spectra of NI1

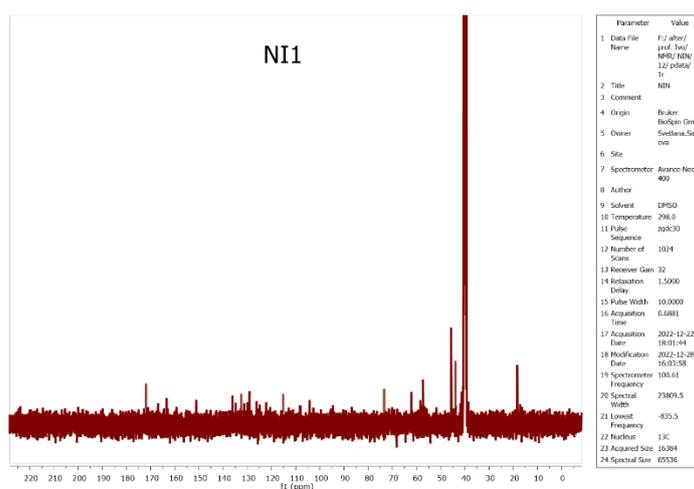
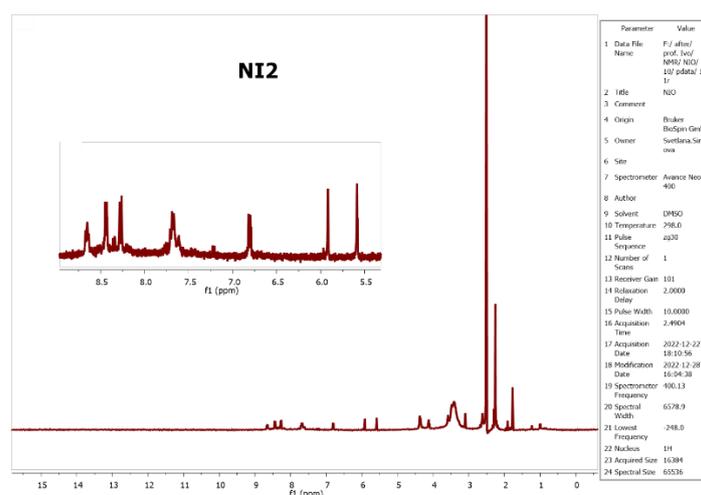
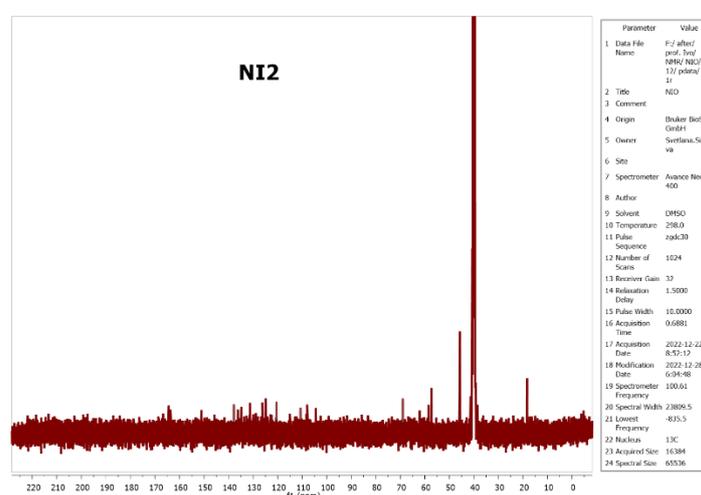


Figure S2. <sup>13</sup>C-NMR spectra of NI1

Figure S3.  $^1\text{H-NMR}$  spectra of NI2Figure S4.  $^{13}\text{C-NMR}$  spectra of NI2

### Computational Details

Default G09 optimization algorithm and convergence criteria were applied. C1 symmetry (i.e. no symmetry) was assumed for all systems. Local minima were verified by establishing that the Hessians had only positive eigenvalues. The optimized at B3LYP/6-31+G(d,p) level geometries in the gas phase were re-optimized in toluene, chloroform, methanol, *N,N*-dimethylformamide (DMF) and water by using IEFPCM (Integral Equation Formalism Polarizable Continuum Model [1]) method. The solvents are defined by the G09 default internal parameters including the dielectric constant  $\epsilon$  values [2].

Solvent	dielectric constant $\epsilon$
toluene	2.3741
chloroform	4.7113
methanol	32.613
DMF	37.219
water	78.3553

TDDFT excitation energies were computed at TDPBE0/6-311+G(2d,p)//B3LYP/6-31+G(d,p) level of theory; in each TDDFT calculation, the lowest 20 excited states were computed. Solvent effects were included in TDDFT calculations (via IEFPCM). The NI-

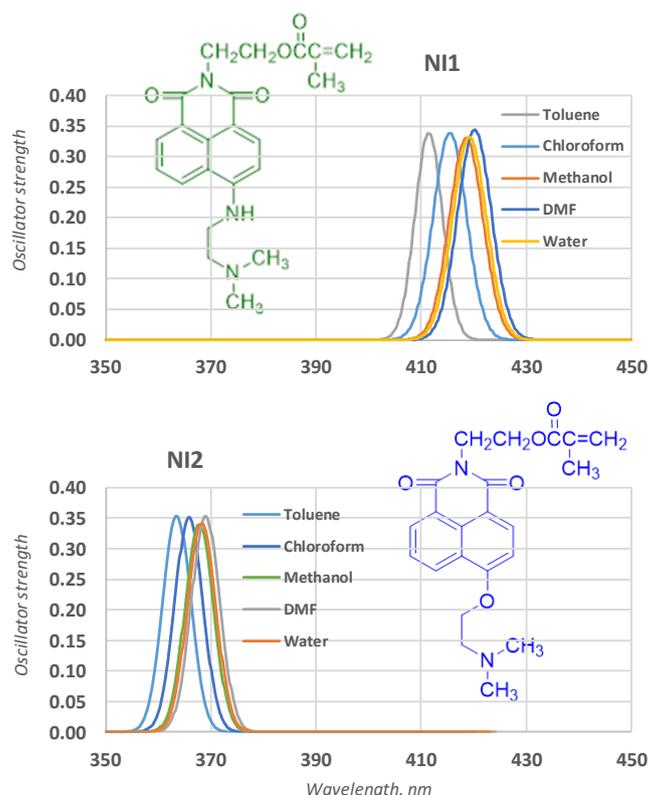
metal complexes were also optimized at B3LYP/6-31+G(d,p)-SDD level of theory. The differences  $\Delta E_{el}$ ,  $\Delta E_{th}$ ,  $P\Delta V$  (work term) and  $\Delta S$  between the products of the complex formation reactions (complexes) and reactants (NI ligands and metal cations) were used to evaluate the Gibbs energy of the complex formation in DMF,  $\Delta G^{37}$  ( $\epsilon^{DMF}=37$ ), at  $T=298.15$  K by the thermochemical values calculated in Gaussian based on the harmonic vibrational frequencies according to the equation:

$$\Delta G^{37} = \Delta E_{el} + \Delta E_{th} + P\Delta V - T\Delta S \quad (1),$$

where  $E_{el}$  is electronic energy,  $E_{th}$  – thermal energy,  $P$  – pressure (1.0 atm),  $V$  – volume,  $S$  – entropy.

A negative  $\Delta G$  implies a thermodynamically favorable complex formation, whereas a positive value implies an unfavorable one.

PyMOL graphical program was used to generate the molecular graphics images [3].



**Figure S5.** TDPBE0/6-311+G(2d,p) simulated spectra (Gaussian broadening, band width on  $\frac{1}{2}$  height: 0.1 eV).

## References

- [1] Cancès E, Mennucci B, Tomasi J. A new integral equation formalism for the polarizable continuum model: Theoretical background and applications to isotropic and anisotropic dielectrics. *J Chem Phys* 1997;107:3032–41. <https://doi.org/10.1063/1.474659>.
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- [3] Schrödinger, L.; DeLano, W. *PyMOL*. 2020. Available online: <http://www.pymol.org/pymol> (accessed on 5 October 2022).