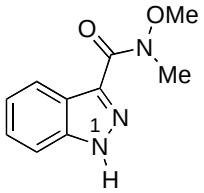
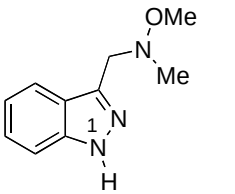
Electronic supplementary information (ESI)

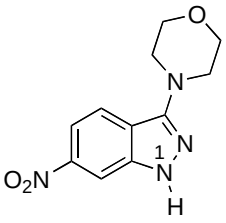
1*H*-indazoles (framed those cases where there is only N–H···N HBs)



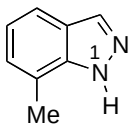
CEXYAG
N–H···O=C



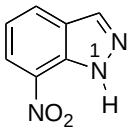
CEXYIO
Catemer N–H···N



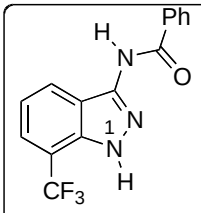
COFFUY No coord.



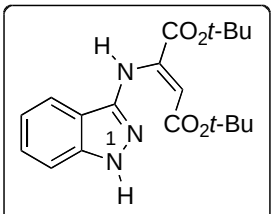
FETXUY
Catemer N–H···N



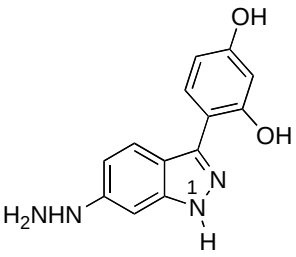
FULKUS
Dimer N–H···N



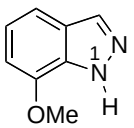
FUQYIA
Dimer N–H···N



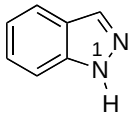
FUWPAO
Dimer N–H···N



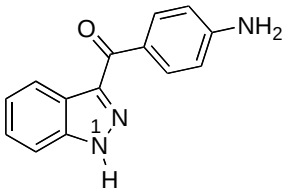
GEFBUO No coord.



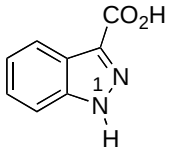
IHESIX
Trimer N–H···N



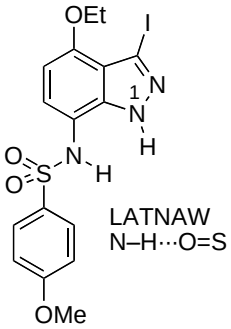
INDAZL
Catemer N–H···N



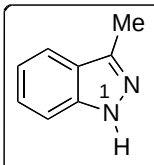
JOKVUB
N–H···O=C



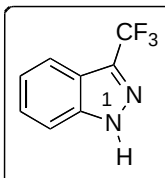
LABNIL N–H···O=C
O–H···N



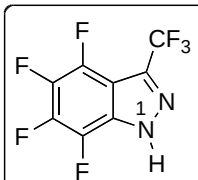
LATNAW
N–H···O=S



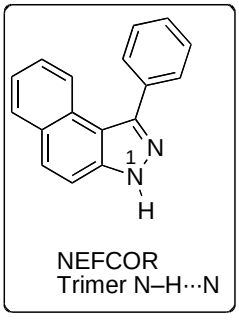
LIDFUA Dimer
N–H···N



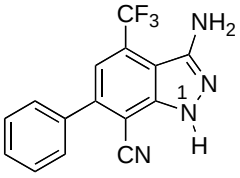
LIDGAH
Catemer N–H···N



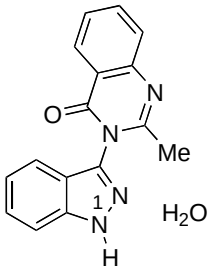
LIDGEL
Catemer N–H···N



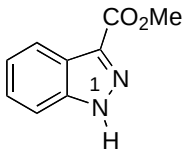
NEFCOR
Trimer N–H···N



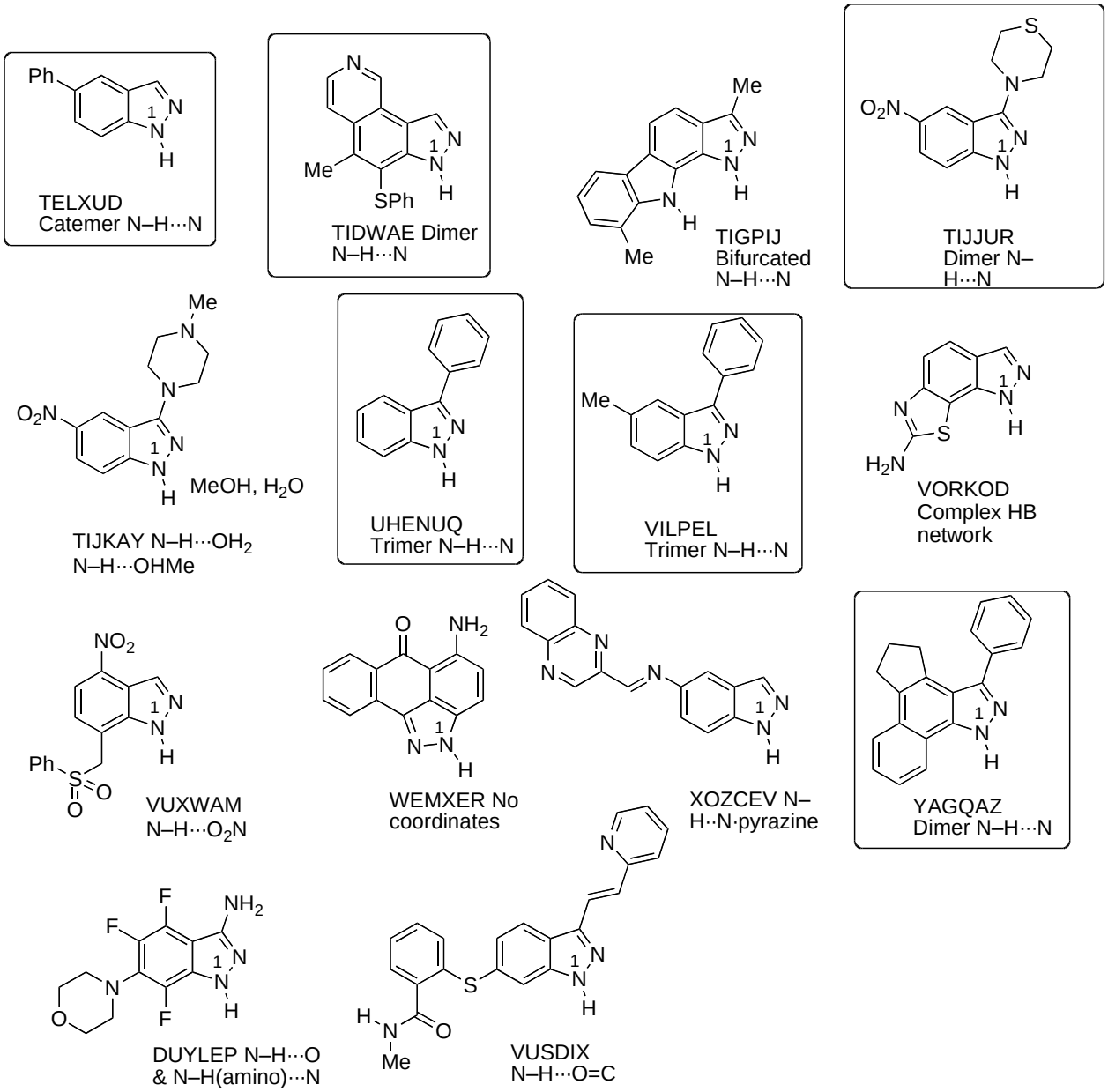
ODOTUX
N–H···NC



RECYIH N–
H···OH2



SUHVUM
N–H···O=C



Figs. 1S to 3S:

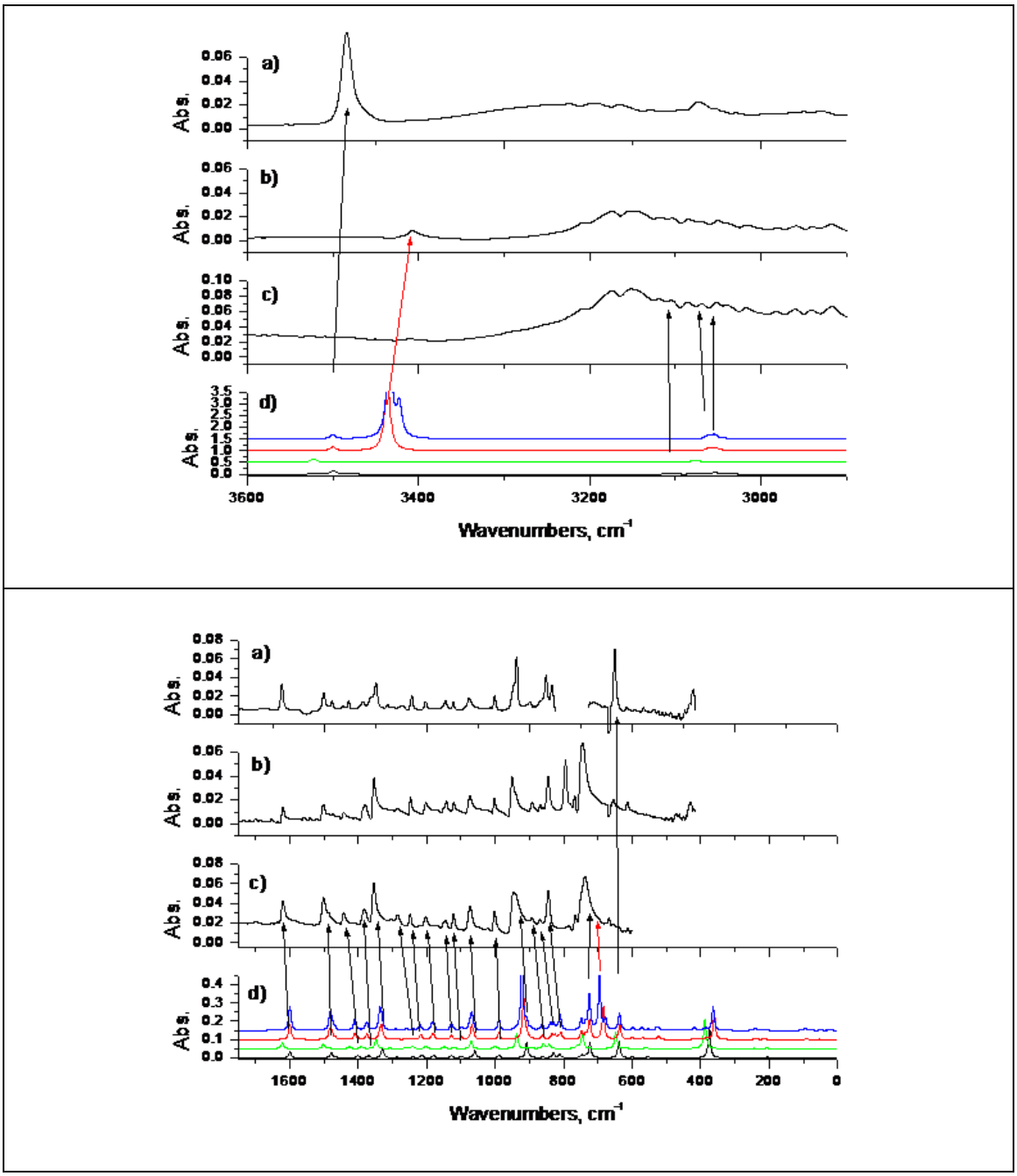


Fig. 1S Experimental and scaled predicted IR spectra of INDAZL: a) Experimental IR spectrum in CCl4 solution; b) Experimental IR spectrum in film conditions; c) Experimental IR spectrum from ATR technique; Exp. Cond.: 200 scans, 1 cm^{-1} of resolution; d) Scaled predicted IR spectra for the INDAZL monomer (freq. scaling factor of 0.953 in black, SQMFF methodology in green) , for the dimer (freq. scaling factor of 0.953 in red) and for the trimer (freq. scaling factor of 0.953 in blue); (Lorentzian function, Pitch = 1 cm^{-1}, FWHM = 8 cm^{-1}).

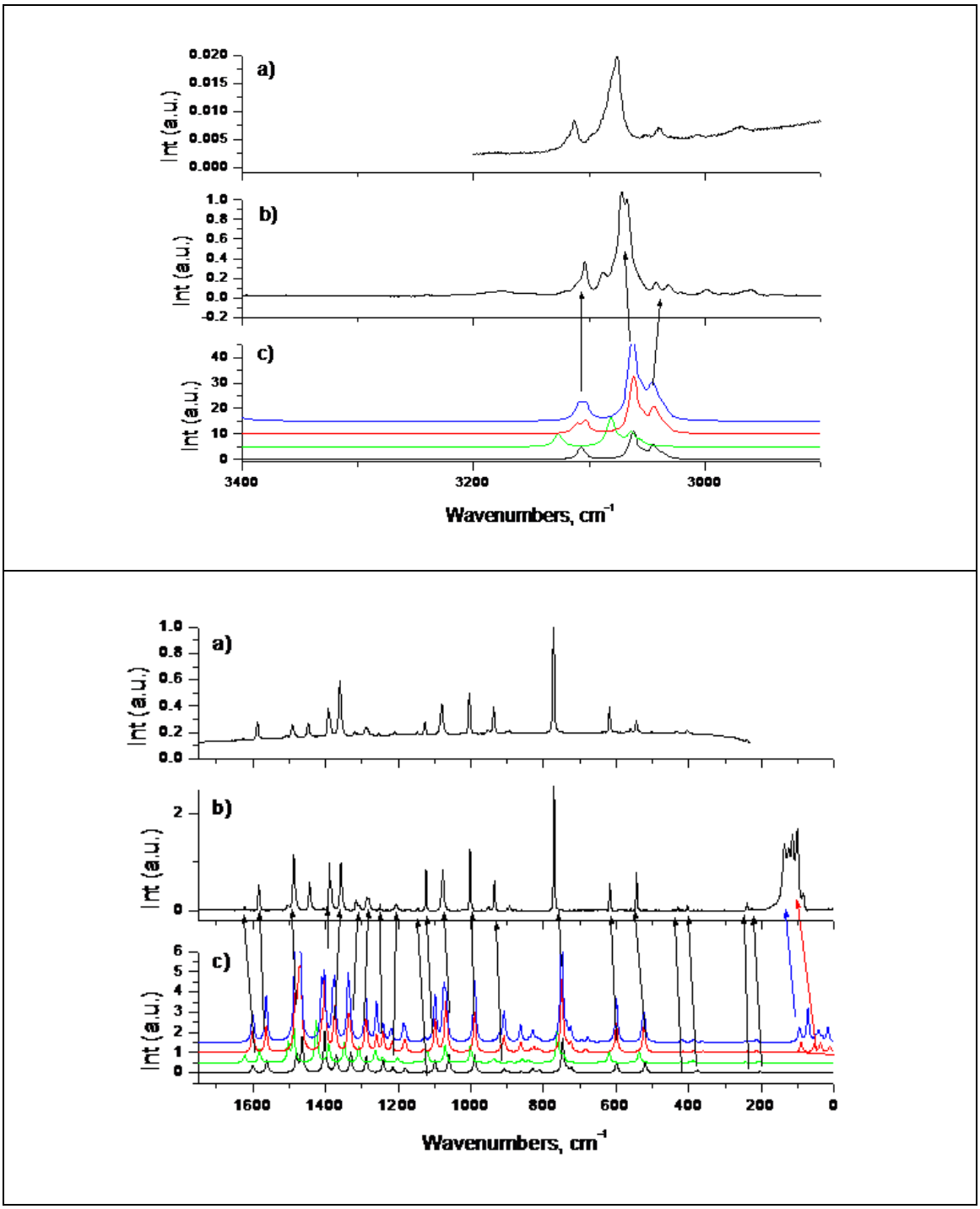


Fig. 2S Experimental and scaled predicted Raman spectra of INDAZL: a) Experimental Raman spectrum of the solid (Renishaw microscope, 785 nm); a) Experimental Raman spectrum of the solid (FT-Raman Bruker, 1064 nm); Exp. Cond.: 200 scans, 1 cm^{-1} of resolution; c) Scaled predicted IR spectra for the INDAZL monomer (freq. scaling factor of 0.953 in black, SQMFF methodology in green) , for the dimer (freq. scaling factor of 0.953 in red) and for the trimer (freq. scaling factor of 0.953 in blue); (Lorentzian function, Pitch = 1 cm^{-1}, FWHM = 8 cm^{-1}).

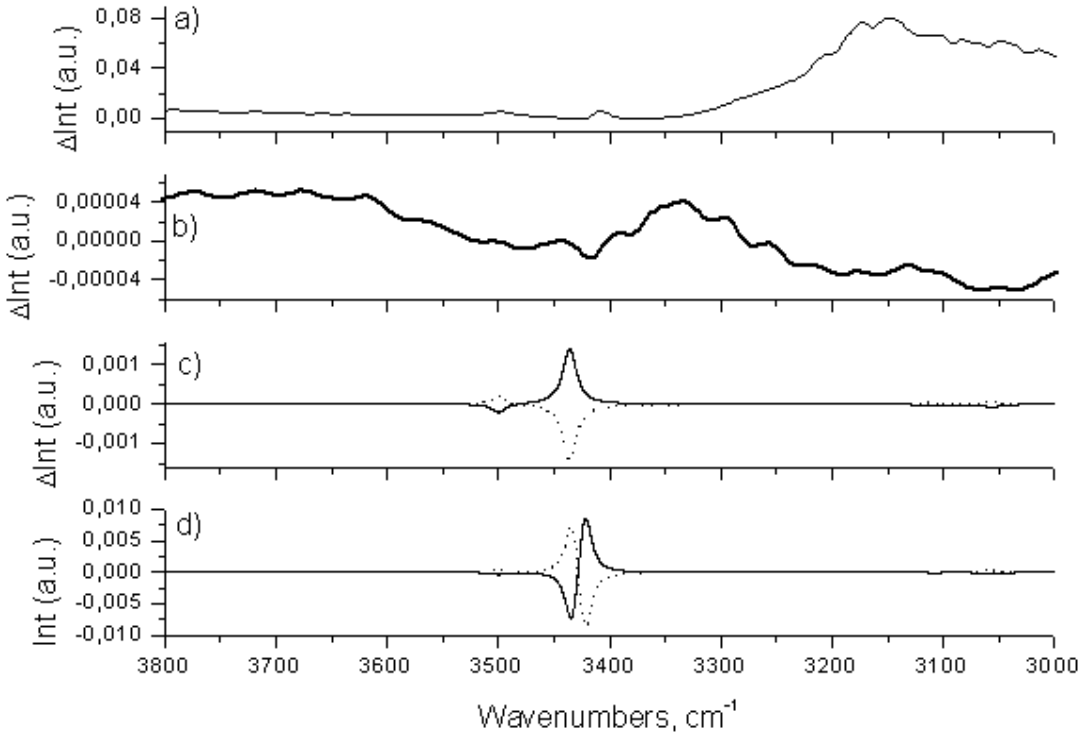


Fig. 3S Experimental and theoretical VCD spectra of INDAZL in the 3800 cm^{-1}- 3000 cm^{-1} spectral region: a) Experimental IR spectrum in fluorolube mull, 4000 scans, 8 cm^{-1} of resolution. b) Experimental VCD spectrum in fluorolube mull, 4000 scans, 8 cm^{-1} of resolution. c) and d) Predicted scaled VCD spectra for the INDAZL dimer (c) and trimer (d) (solid line for *S* configuration - *P* helix model, dotted line for *R* configuration - *M* helix model); Lorentzian function, Pitch = 1 cm^{-1}, FWHM = 8 cm^{-1}.