**Electronic Supplementary Information to Journal of New Chemistry**

# Conformational Insights and Vibrational Study of a Promising Anticancer Agent: The Role of the Ligand in Pd(II)-Amine Complexes

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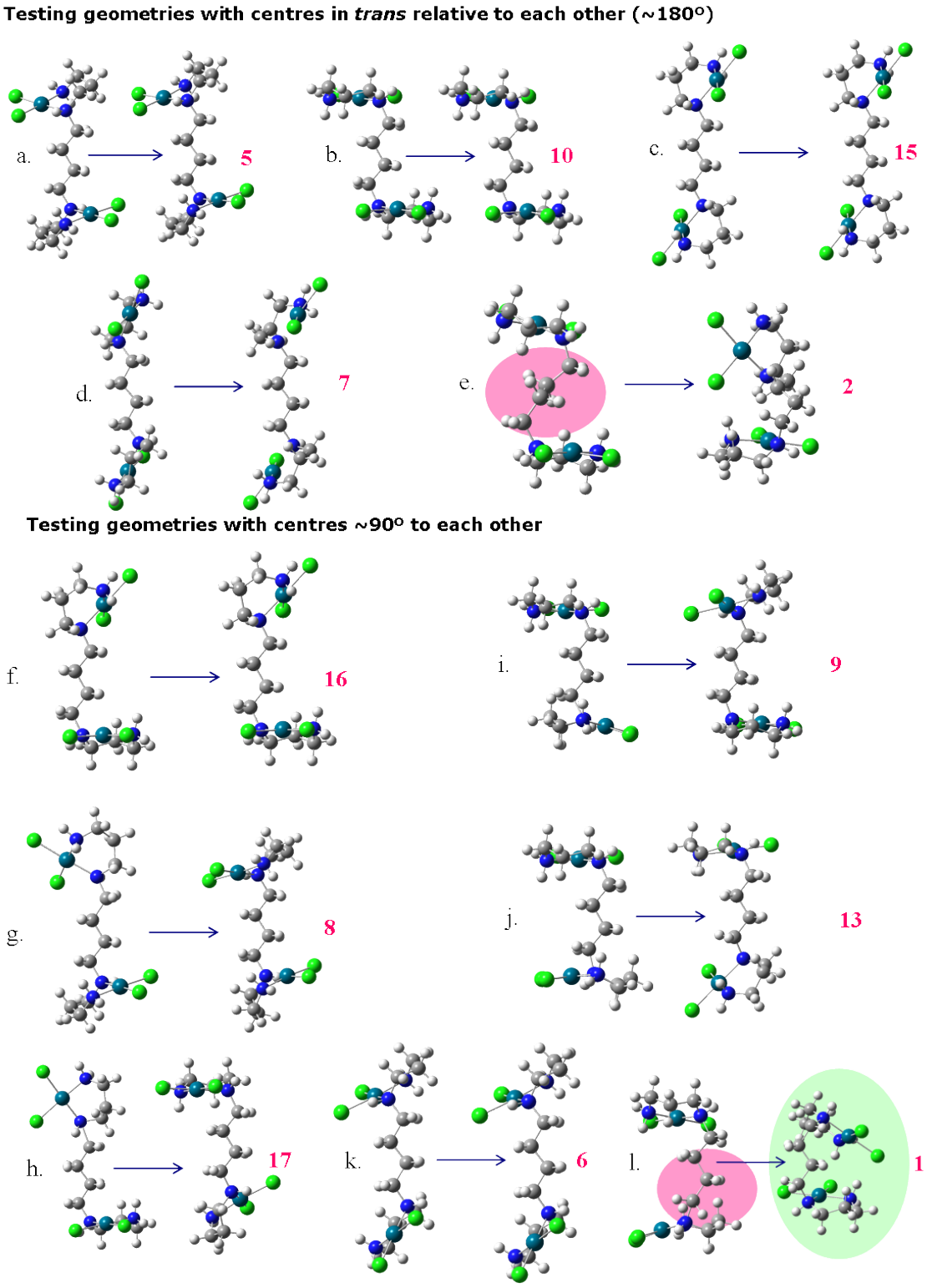
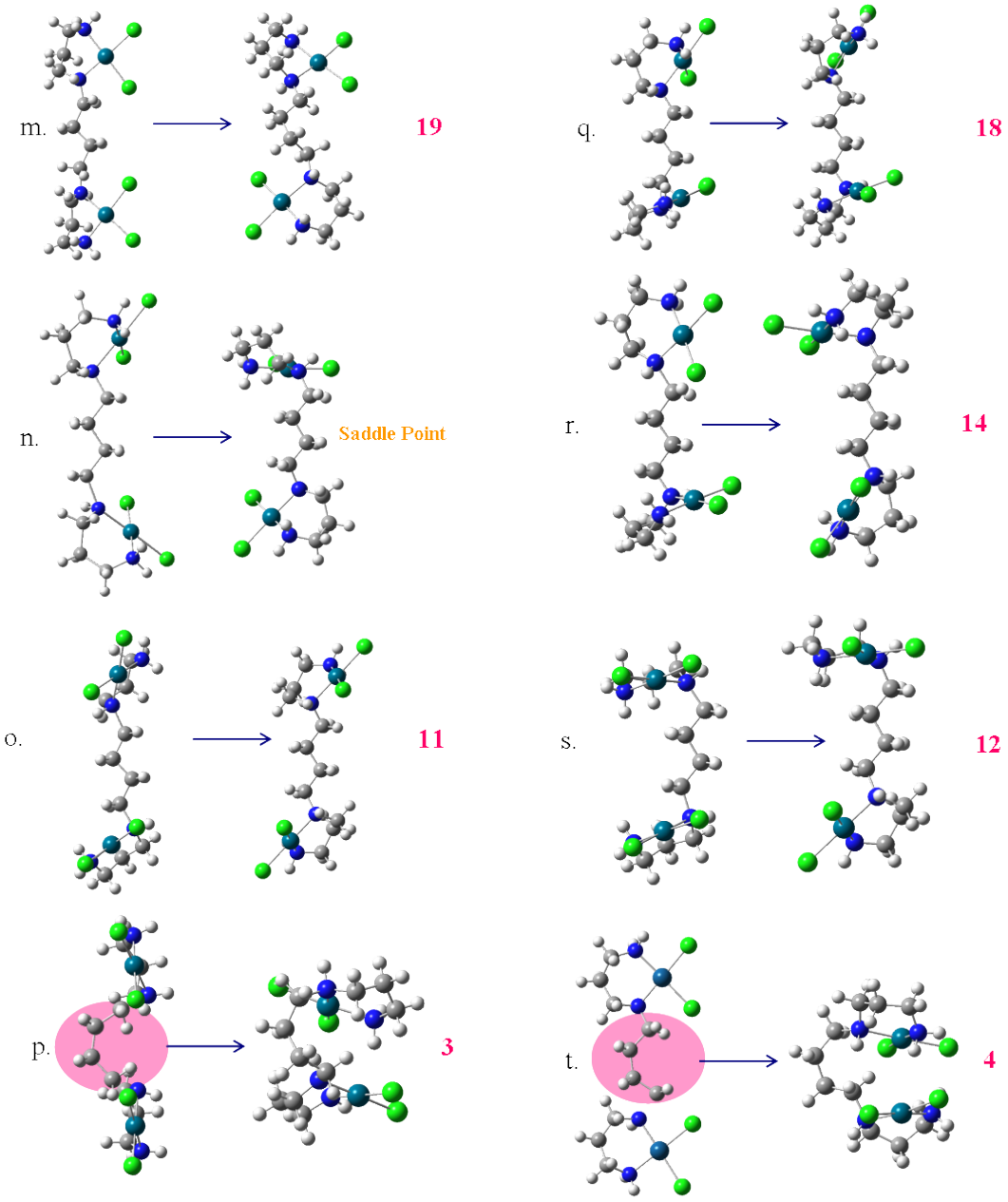
**Figure S1** – Conformational study of $Pd_2$-Spm. Input geometries are listed with letters and the obtained optimized conformers (mPW1PW/6-31G*) are listed in arabic numbers from 1 to 19 in order of increasing energy and thus from the most stable to the less stable one. Configurations are presented in groups, the pink area stands for a non-linear amine configuration and the yellow areas to a region of a fair degree of coplanarity between the metal centre and the central amine. A graphic with the relative energies is also presented.



**Testing geometries with centres in *cis* relative to each other – linear amine**



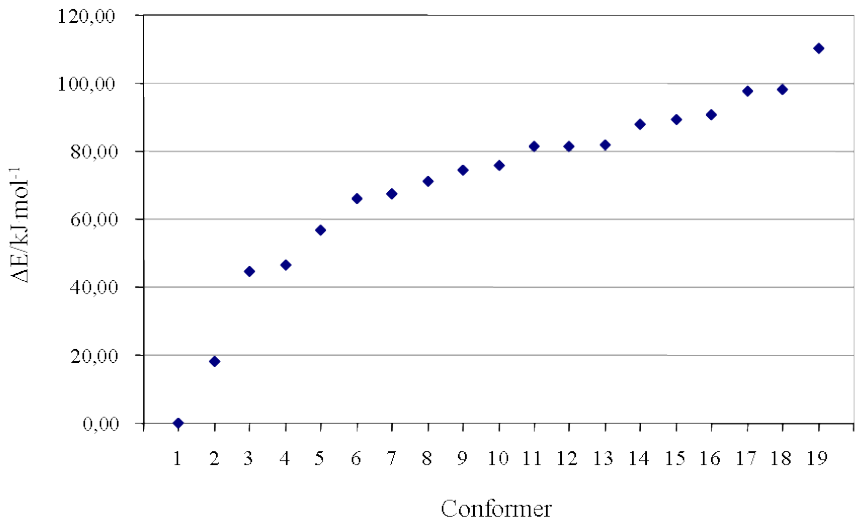



**Figure S2** – Calculated two molecule structure for $Pd_2$-Spm.
(The distance between atoms is in picometers).