Table S1. Electronic energies, interaction energies and the corresponding counterpoise-corrected interaction energies calculated at the (U)B3LYP/6-311++G(d,p) level of theory within the framework of IEFPCM in water.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Complex | RNA2- | Mg2+(H2O)6 | RNA2--Mg2+.•(H2O)4 | H2O | IE | IE(BSSE50%)) |
| RNA2- -Mg2+(H2O)4 | -1710.95695 | -658.78488 | -2216.86735 | -76.466467 | -36.6 | -33.4 |
| RNA2- -Fe2+(H2O)4 | -1710.95695 | -1722.29917 | -3280.38356 | -76.466467 | -37.9 | -34.7 |