

# Supramolecular theranostics to reach out the brain

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# Supramolecular theranostics to reach out the brain”

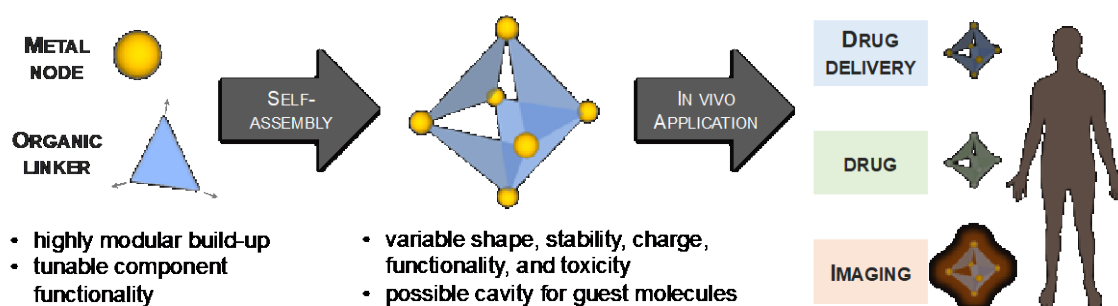
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The biomedical application of discrete supramolecular coordination complexes, specifically self-assembled 3D-metallacages, is an emergent field of study.<sup>[1]</sup> The robustness and modular composition of such metal-based supramolecular entities allow for the incorporation of different functionalities in the same scaffold to enable imaging in cells *via* different modalities, but also active tumor targeting and stimuli-responsiveness. Thus, metallacages may constitute ideal platforms to develop multimodal *theranostics*. Of note, the host-guest chemistry of metallacages can also be exploited to design novel targeted drug delivery systems for anticancer chemotherapeutics and radioactive imaging agents.<sup>[2,3]</sup>

In this lecture, I aim at summarizing the key concepts and challenges in this fascinating research area, starting with the main synthetic and design principles and illustrating representative examples from our group. In details, we have developed “lantern-shaped” cationic  $[Pd_2L_4]^{4+}$  cages (L = bitopic monodentate N-donor ligand) either as drug delivery systems for the anticancer drug cisplatin or tethered to a blood-brain-barrier (BBB)-translocating peptide while encapsulating  $[^{99m}Tc]TcO_4^-$ ,<sup>[3]</sup> and thus, enabling its brain penetrability in mouse models. Certainly, the myriad of possible metallacage-structures and their almost limitless modularity and tunability suggest that the biomedical applications of such complex chemical entities will continue along this already promising path.



## References

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[2] Han, J.; Räder, A.F.B.; Reichart, F.; Aikman, B.; Wenzel, M.N.; Woods, B.; Weinmüller, M.; Ludwig, S.B.; Stürup, S.; Groothuis, G.M.M.; Permentier, H.P.; Bischoff, R.; Kessler, K.; Horvatovich, P.; Casini, A., *Bioconjug. Chem.* **2018**, *29*, 3856-3865.

[3] Woods, B.; Silva R.D.M.; Schmidt, C.; Wragg, D.; Cavaco, M.; Neves, V.; Ferreira, V.F.C.; Gano, L.; Morais, T.S.; Mendes, F. Correia, J.D.G.; Casini, A., *Bioconjug. Chem.* **2021**, *32*, 1399-1408.

# CURRICULUM VITAE

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## SUMMARY OF EDUCATION AND CAREER

Angela Casini is Chair of Medicinal and Bioinorganic Chemistry and Liesel Beckmann Distinguished professor at the Technical University of Munich (TUM) since 2019. Since 2021, she is *ad interim* Chair of Pharmaceutical Radiochemistry, and is core member of the Munich Institute of Data Science (MDSI). She completed her PhD in Chemistry at the University of Florence (Italy) in 2004, and successively moved to the EPFL (Switzerland) as principal investigator funded by the Swiss National Science Foundation (*Ambizione* program). Between 2011-2015 she has been assistant professor at the University of Groningen (The Netherlands), holding a Rosalind Franklin Fellowship. Between 2015-2019, she was also Chair and Director of Postgraduate Taught Masters at the School of Chemistry of Cardiff University (UK), before taking up her current position at TUM. Her research interests are in Medicinal Inorganic and Bioinorganic Chemistry. Specifically, the study of the role of metal ions in biological systems and of the mechanisms of action of organometallic anticancer agents are active research topics in her group. Furthermore, novel applications for metal-based compounds and supramolecular coordination complexes are explored in various domains of chemical biology, drug delivery and medicine. In these fields, she has authored more than 270 publications (including 12 book chapters) and has a *H index* of 74. Since 2021, in the search for novel supramolecular inorganic materials, she coordinates the 4-year TUM Innovation Network (ca. 4 Million Euro investment) “*Artificial Intelligence Powered Multifunctional Materials Design*” (ARTEMIS). The network focuses on using machine learning to develop novel materials for energy research and regenerative medicine.

Her international recognition is demonstrated by the numerous invitations to hold (plenary) lectures in international conferences and training schools, as well as seminars at different institutions worldwide. To mention a few in different domains of chemistry, she has been plenary speaker at the 8<sup>th</sup> Latin American Symposium on Organometallic Chemistry (SiLQOM08, 2022, virtual), and at the 2<sup>nd</sup> International Conference on Noncovalent Interactions (ICNI 2022, Strasbourg), and she will be plenary at the 25<sup>th</sup> Conference on Organometallic Chemistry (EuCOMC 2023, Alcalá de Henares) as well as at the 16<sup>th</sup> International Symposium on Applied Bioinorganic Chemistry ([ISABC16](#), Ioannina). Noteworthy, she has been invited to present her work at the the prestigious Nobel Symposium #168: *Visions of bio-inorganic chemistry: Metals and the molecules of life*, Royal Swedish Academy of Sciences, Stockholm in May 2022.

Angela was also invited for named lectures, including the 36<sup>th</sup> H. Martin Friedman Lecture 2021 at Brooklyn College of The City University of New York, and the 2019 TGH Jones Memorial Lecture, University of Queensland. She has also been visiting professor at the University of Burgundy (2013), the University of Sassari (2013 & 2014), the Technical University of Munich (2013 & 2014 August-Wilhelm Scheer Visiting Professorship), as well as international visiting Scholar at Colorado State University (2016) and guest professor at the University of Groningen (2015). Between 2016-2019, she was also Hans Fischer Senior Fellow and “honorary fellow” of the prestigious Institute for Advanced Studies of the Technical University of Munich. In 2019, the British Council has selected her to represent UK at the Regional Meeting for the Brazilian Society of Chemistry of the State of Minas Gerais in the frame of the UK Brazil Year of Science and Innovation program. The latter is a joint initiative led by the UK and Brazilian governments that aims to foster projects in science and innovation between the two countries.

Concerning honours and awards, she has received the 2019 ACS Inorganic Lectureship award, the 2019 Burghausen Diamond of Chemistry Award - an acknowledgement of chemical and industrial innovation - the 2014 Early career investigator award at the GRC Metals in Medicine "New Frontiers" and the 2012 European Medal for Biological Inorganic Chemistry. In 2014 she has been listed by Thomson Reuters as one of the "World's most influential scientific minds" in the field of Pharmacology. She is also member of the Editorial Board of *Chemistry*

*Eur. J.* and of *J. Inorg. Biochem.*, and has served in the editorial advisory board of other journals (e.g. *ACS Bioconjugate Chemistry*, *Inorganic Chemistry*). She has also been Guest Editor of special issues for various journals, including *ChemMedChem*, *EurJIC*, *Dalton Trans*, *CurrOpinChemBiol*, and *Frontiers in Chemistry* among others. In 2019, she was Lead Editor of the RSC book entitled “*Anticancer Metal-based Drugs*” in the *Metallobiology* series.

In terms of organizational skills, she was co-Chair of the 2022 Gordon Research Conference “Metals in Medicine” (Andover, US). In 2015, she was Chair of the “1<sup>st</sup> International Symposium on Clinical and Experimental Metallo drugs in Medicine” (Honolulu, US) which received the NIH endorsement and financial support. Since 2019, she has also joined the international scientific committee of the “International symposium on Metallomics”, a conference dedicated to the advancements in the study of metal ions in biology and related spectroscopic and analytical methods. During the years, she participated in numerous EU COST Actions and bilateral networks related to the study of metal ions in biological systems. Presently, she is member of EU COST Action CA18202 “*Network for Equilibria and Chemical Thermodynamics Advanced Research*” (NECTAR). Between 2016-2019, she was UK responsible of the RSC Dalton UK-US-Canada collaborative network in Bioinorganic Chemistry “*Targeting zinc finger proteins with metal compounds: implications for therapy and toxicity*”, and member of the Inorganic Biochemistry Discussion Group (RSC, Dalton Division), as well as member of the Translational Research Committee of the Welsh Cancer Research centre. In 2016, she was also member of the Board of the Young Academy of Europe and Chair of the Selection Committee. Moreover, she is reviewer for several international funding agencies. Since 2022, she is permanent member of the advisory board of the Institute of Advanced Materials ([INAM](#)) in Spain.