RSEQ
Real Sociedad Española de Química

ugr Universidad de Granada

XXXVIII REUNIÓN BIENAL

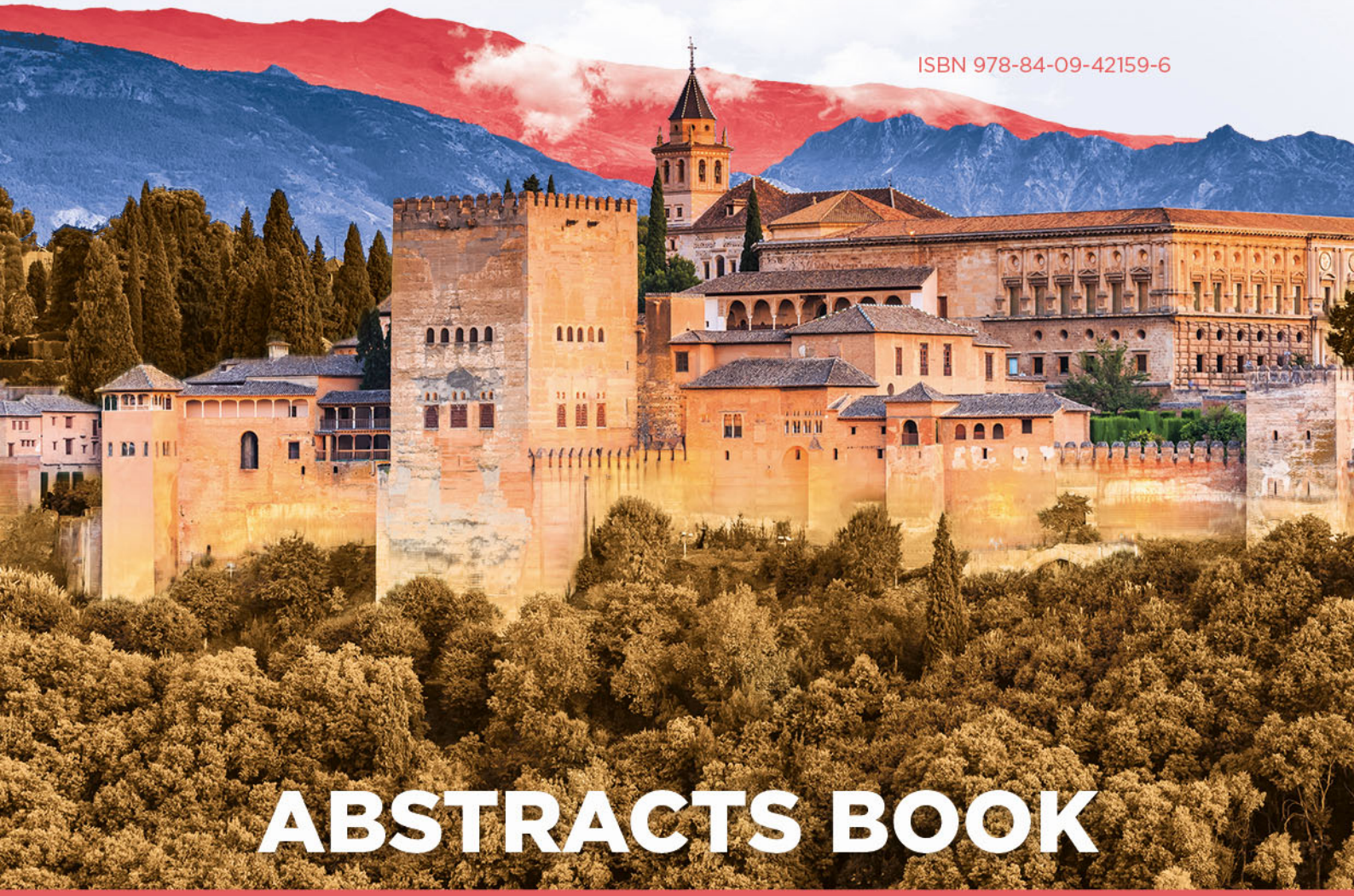
RSEQ

GRANADA 2021

27 - 30 DE JUNIO 2022

REAL SOCIEDAD ESPAÑOLA DE QUÍMICA

ISBN 978-84-09-42159-6



ABSTRACTS BOOK

www.bienal2022.com

PENTAFLUOROPHENYL-BIS(2-PHENYLBENZOTHIAZOLE) Pt^{IV} DERIVATIVES: OPTOELECTRONIC AND BIOLOGICAL STUDIES

D. Gómez de Segura,[a] N. Gimenez,[a] D. Rincón,[a] M. T. Moreno,[a] E. Lalinde,[a] I. P. López,[b] Igancio M. Larráyoz,[c] J. G. Pichel[b]

[a] *Departamento de Química-Centro de Investigación en Síntesis Química de La Rioja, (CISQ), Universidad de La Rioja, 26006, Logroño, España*

[b] *Unidad de Cáncer de Pulmón y Enfermedades Respiratorias (CIBIR), Fundación Rioja Salud, 26006, Logroño, España*

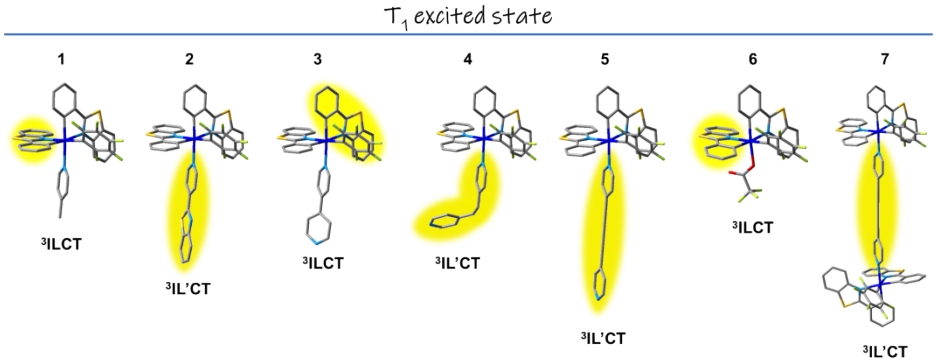
[c]*Unidad de Biomarcadores y Señalización Molecular (CIBIR), Fundación Rioja Salud, 26006, Logroño, España*

e-mail: daseguz@unirioja.es

Keywords: *luminescent, theoretical calculations, cytotoxicity, photoinduced activity, platinum.*

Luminescent complexes based on organic chromophores with late transition metals have attracted a great interest due to their interesting applications in fields such as photocatalysis, biosensing, photosensitizers and optoelectronic devices. In particular, numerous studies have been published on cyclometalated d^6 (Ru^{II}, Os^{II} or Ir^{III}) and d^8 (Pt^{II}) systems, whereas luminescent Pt^{IV} complexes have received less attention.[1] Our group has recently published two series of neutral pentafluorophenylbis(cyclometalated) Pt^{IV} with Cl^- or CN^- as auxiliary ligands.[2] In this field, 2-arylbenzothiazole chromophores have been employed as ligands to form yellow-orange phosphorescent metal complexes and recent studies have also demonstrated promising antiproliferative activity.[3]

In this communication, we present a series of luminescent mononuclear Pt^{IV} complexes, *fac*-$[Pt(pbt)_2(C_6F_5)L]^{n+}$ (pbt = 2-phenylbenzothiazole; L = 4-Mepy **1**, pybt **2**, 4,4'-bpy **3**, bpe **4**, bpyb **5**, n = 1; $OCOCF_3$, **6** n = 0), and a bimetallic complex *fac*-$[\{Pt(pbt)_2(C_6F_5)\}_2(\mu\text{-bpyb})](PF_6)_2$ (**7**), in which the *trans* ligand to the C(pbt) is varied to modify the optical properties and lipophilicity. All complexes have been fully characterized and their structure confirmed by X-ray diffraction studies on **1**, **4** and **6**. Optical properties have been investigated in detail and supported by DFT/TD-DFT theoretical calculations. **4** is not emissive due to a fast photoisomerization process *E/Z* on the bpe ligand. The *in-vitro* antiproliferative activity of selected compounds (**1**-**3** and **6**) against two human tumor cell lines (A549 and HeLa) and their selectivity index against the non-tumor cell line BEAS-2B were examined. Cationic complexes **1**-**3** exhibit IC_{50} values in the nanomolar range, revealing an encouraging antineoplastic activity, whereas the neutral complex **6** shows low cytotoxicity in the dark and high photocytotoxicity by short irradiation with blue light.



References

[1] A. Vivancos, A. Jiménez-García, D. Bautista, P. González-Herrero, *Inorg. Chem.* **2021**, 60, 7900-7913

[2] N. Giménez, R. Lara, M. T. Moreno, E. Lalinde, *Chem. Eur. J.* **2019**, 25, 5514-5526

[3] E. Lalinde, R. Lara, I. P. López, M. T. Moreno, E. Alfaro-Arnedo, J. G. Pichel, S. Piñeiro-Hermida, *Chem. Eur. J.* **2018**, 24, 2440-2456