XXXVI Reunión Bienal de la Real Sociedad Española de Química (RSEQ) - 2017

Apellidos presentador	Nombre presentador	Código	Nombre de la sesión	Título	Tema	Fecha de presentación
Follana Berná	Jorge	PP-127	POSTERS - SESIÓN B	Synthesis, Characterization and Photophysical Studies of Conjugated Phthalocyanine-Porphyrin Dimers Supramolecularly Connected with C_{60}	Materiales orgánicos optoelectrónicos para conversión de energía	27/06/2017
Fraga Timiraos	Ana	PP-267	POSTERS - SESIÓN B	PHOTOREPAIR OF PYRIMIDINE DIMERS BY 8-OXO-GUANOSINE AS A FLAVIN MIMIC	Química en la frontera con la Biología	27/06/2017
Francos	Javier	PP-157	POSTERS - SESIÓN B	FIRST PLATINUM COMPLEXES BEARING A PHOSPHINO-OXIME LIGAND: SYNTHESIS, STRUCTURE AND REACTIVITY	Diseño de ligandos para las reacción de formación y rotura de enlaces	27/06/2017
Frattini	Marcello	PP-187	POSTERS - SESIÓN B	TETRAMETHYLBENZIDINE: A PHOTOACOUSTIC PROBE FOR THE DETECTION OF REACTIVE OXYGEN SPECIES	Fotoquímica	27/06/2017
G. Rull	Silvia	PP-150	POSTERS - SESIÓN B	C-N BOND FORMATION REACTION CATALYZED BY A SINGLE COMPONENT NHC-Ni^0 PRECURSOR. MECHANISTIC STUDIES.	Diseño de ligandos para las reacción de formación y rotura de enlaces	27/06/2017
Galindo	Francisco	PP-009	POSTERS - SESIÓN A	A SPECTROSCOPIC STUDY TO ASSESS THE PHOTOCHEMICAL GENERATION OF SINGLET OXYGEN BY GRAPHENE OXIDE	Grafeno y otros materiales 2D	26/06/2017
Gallego Gómez	Iván	PP-240	POSTERS - SESIÓN B	GLYCOPEPTIDES FOR PROTEIN SELECTIVE RECOGNITION AND CELLULAR INTERNALIZATION	Química en la frontera con la Biología	27/06/2017
Gallet	Bertrand	PP-138	POSTERS - SESIÓN B	Lab Reactor-A modular flow reactor	Química en flujo continuo	27/06/2017
García Álvarez	Joaquín	PP-155	POSTERS - SESIÓN B	EXPLOITING *DEEP EUTECTIC SOLVENTS* AND RLi/RMgX REAGENT PARTNERSHIPS: CHEMOSELECTIVE ULTRAFAST ADDITION TO KETONES AND IMINES UNDER AEROBIC AMBIENT TEMPERATURE CONDITIONS	Diseño de ligandos para las reacción de formación y rotura de enlaces	27/06/2017
García Domínguez	Patricia	PP-025	POSTERS - SESIÓN A	A SYNTHETIC APPROACH TOWARDS THE PRENYLATED INDOLE DIKETOPIPERAZINE ALKALOIDS OKARAMINE S AND J	Productos Naturales, sondas moleculares con estructuras privilegiadas	26/06/2017
García García	Pablo Anselmo	PP-013	POSTERS - SESIÓN A	NEW CYTOTOXIC NEOLIGNANS FROM THE COBALT CRUST FUNGUS	Productos Naturales, sondas moleculares con estructuras privilegiadas	26/06/2017
García Herraiz	Ana	PP-332	POSTERS - SESIÓN C	VISIBLE LIGHT-DRIVEN CYCLOPROPANATION OF UNACTIVATED OLEFINS	Síntesis Orientada a Objetivos y Nuevos Métodos de Síntesis	28/06/2017
García Laureiro	José Ignacio	PP-190	POSTERS - SESIÓN B	SÍNTESIS Y PROPIEDADES DE NUEVOS DISOLVENTES VERDES DERIVADOS DE GLICEROL	Química Verde	27/06/2017
García Marquina	Guillermo	PP-096	POSTERS - SESIÓN A	COMPUTATIONAL ENGINEERING OF A NATURAL ACYLTRANSFERASE	Química Supramolecular	26/06/2017
Garcia Martos	Daniel	PP-103	POSTERS - SESIÓN A	Heck reaction: an aqueous biphasic approach.	Química Organometálica y Catálisis	26/06/2017
García Peña	Diego	PP-255	POSTERS - SESIÓN B	MITOCHONDRIA-TARGETTED REDOX MODULATORS	Química en la frontera con la Biología	27/06/2017
Garcia Roca	Alèria	PP-212	POSTERS - SESIÓN B	New Synthetic Approach for the Synthesis of N-Heterocycles by Cobalt-Catalyzed Annulation Reactions of Aryl Halides with Alkynes	Química Organometálica y Catálisis	27/06/2017
García-Antón	Jordi	PP-071	POSTERS - SESIÓN A	Novel Cobalt-based Nanoparticles as Water Oxidation Catalysts	Nanocatálisis	26/06/2017
García-Avello Méndez	Marta	PP-177	POSTERS - SESIÓN B	ENANTIOPURE CHIRAL-AT-METAL (M = Ir, Rh) HALF SANDWICH COMPLEXES USING CHIRAL SULFUR MESOIONIC CARBENE (MIC) LIGANDS	Diseño de ligandos para las reacción de formación y rotura de enlaces	27/06/2017
García-López	Diego	PP-169	POSTERS - SESIÓN B	A computational approach to the mechanism of two strategies for C-H activation: Ni-pincer and Ti_2-alkyl complexes	Diseño de ligandos para las reacción de formación y rotura de enlaces	27/06/2017

NEW CYTOTOXIC NEOLIGNANS FROM THE COBALT CRUST FUNGUS

P. A. García[1], M. Maisterra[1,2], M. Á. Castro[1], L. M. Muñoz-Centeno[1], R. C. Calhelha[2], I. C. F. R. Ferreira[2]

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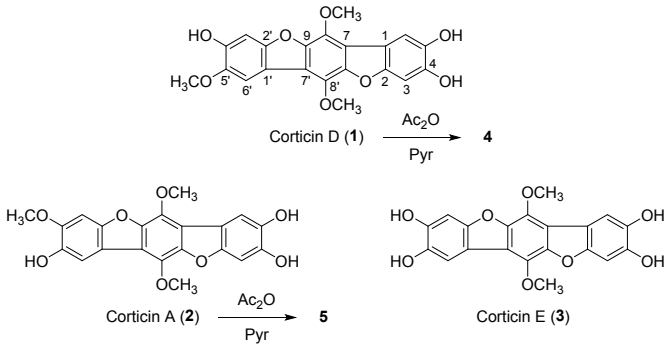
Palabras Clave: *Terana coerulea, Neolignans, Terphenyls, Corticin, Cytotoxicity*

Terana coerulea (Phanerochaetaceae family) is known as the cobalt crust fungus and it is used for its antibiotic properties at the Irati's Forest (Navarra, Spain). Previous mycochemical investigations reported the isolation of corticins A-C,[1] *p*-terphenyl neolignans related to the antitumoural telephoric acid.[2] In this job, from powdered dry fungi, six extracts of increasing polarity were obtained and tested for cytotoxicity against four human tumour cell lines and one non-tumour primary cell culture with the sulforhodamine B assay. From the most cytotoxic one, the EtOAc extract, we isolated and identified three *p*-terphenyl neolignans. One of them was previously described as corticin A by Briggs *et al.*,[1] whose earlier structure has been revised in this work using one- and two-dimensional NMR, HRMS, positive and negative MS/MS and its peracetyl derivative in comparison with 4''-deoxy and 4,5-dimethoxy candidusines A.[3] The other two neolignans are new natural products, named corticins D and E. These neolignans were less cytotoxic than the EtOAc extract itself, maybe due to an aerial oxidation and degradation produced when these neolignans, with catechol moieties, are definitively purified.



Referencias

[1] L. H. Briggs, R. C. Cambie, I. C. Dean, R. Hodges, W. B. Ingram, P. S. Rutledge. *Aust. J. Chem.* **1976**, 29, 179-190.

[2] K. Tateishi, H. Hoshi, K. Matsunaga. *PCT Int. App.* **2005**, WO 2005095413 A1 20051013.

[3] Z. K. Guo, T. Yan, Y. Guo, Y. C. Song, R. H. Jiao, R. X. Tan, H. M. Ge. *J. Nat. Prod.* **2012**, 75, 15-21.

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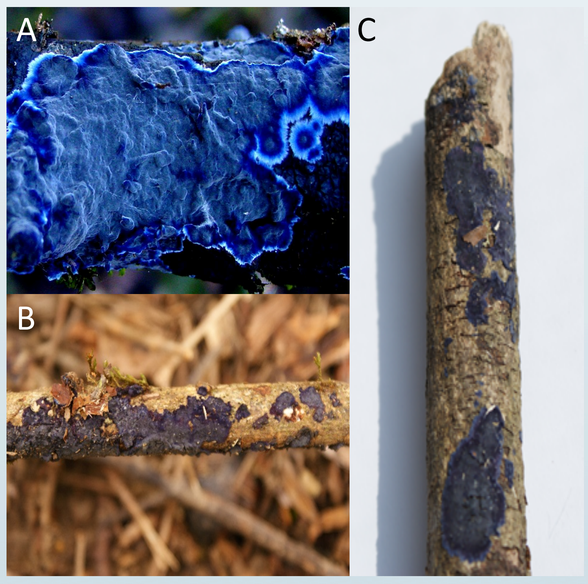

The cobalt crust fungus, *Terana coerulea* (Lam.) Kuntze (Phanerochaetaceae family), is a saprotrophic fungus that is easily recognized by the indigo-blue colour of its hymeneal surface (Pictures A,[1] B and C). It was selected for a bio-guided study after an ethnobotanical survey at the Irati's Forest (Navarra, Spain, Picture D), where it is used for its antibiotic properties. Previous mycochemical investigations reported the isolation of corticins A-C,[2] *p*-terphenyl neolignans related to the antitumoural telephoric acid (Figure 1).[3]

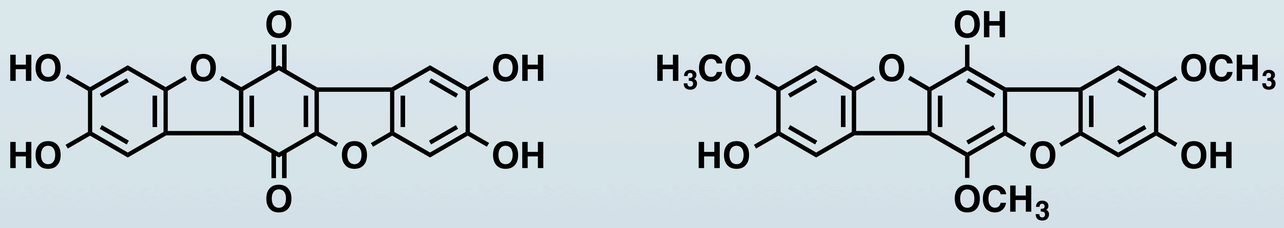

Figure 1: Thelephoric acid and corticin A inexactly identified by *Briggs et al.* and isolated from *T. coerulea* cultures (formerly named as *Corticium caeruleum*).[2]

In this job, from powdered dry fungi, six extracts of increasing polarity were obtained (hexane, CH_2Cl_2, EtOAc, *n*-BuOH soluble fraction from MeOH, H_2O soluble fraction from MeOH and final aqueous decoction) and tested for cytotoxicity against four human tumour cell lines and one non-tumour primary cell culture with the sulforhodamine B assay (Table 1).

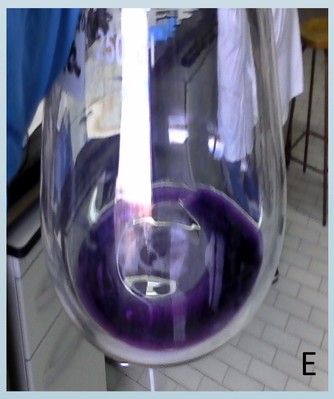

Table 1: Cytotoxicity of extracts and corticins from *Terana coerulea* (GI_{50} ± SD, in μg/mL).

Sample	HeLa	NCI-H460	HepG2	MCF-7	PLP2
Hexane ext	73 ± 3	71 ± 3	77 ± 6	75 ± 3	157 ± 5
CH_2Cl_2 ext	13 ± 2	20 ± 1	50 ± 4	15 ± 1	8.7 ± 0.8
EtOAc ext	5.7 ± 0.5	12 ± 1	175 ± 8	3.2 ± 0.2	31 ± 3
BuOH ext[a]	55 ± 6	100 ± 8	341 ± 13	77 ± 5	> 400
H_2O ext[a]	62 ± 2	215 ± 16	339 ± 25	93 ± 4	> 400
Decoction	224 ± 14	> 400	> 400	279 ± 17	> 400
1	20 ± 1	68.7 ± 0.6	43.4 ± 0.9	57 ± 4	128 ± 9
1+2 (9:1)	14 ± 1	15 ± 1	20 ± 2	12.5 ± 0.9	59 ± 5
1+2+3 (2:1:1)	19 ± 1	23.8 ± 0.1	35 ± 2	18.3 ± 0.6	84 ± 8
Ellipticine	0.91 ± 0.04	1.03 ± 0.09	1.91 ± 0.06	1.1 ± 0.2	3.2 ± 0.7

[a]BuOH and H_2O soluble fractions from the MeOH extract.

From the most cytotoxic one, the EtOAc extract (Picture E), we isolated and identified three *p*-terphenyl neolignans (**1**-**3**, Figure 2). One of them (**2**) was previously described as corticin A by Briggs *et al.* (Figure 1),[2] whose earlier structure has been revised in this work using one- and two-dimensional NMR (Table 2, Figure 3), HRMS, positive and negative MS/MS, with the preparation of the peracetyl derivatives (**4**-**5**) and comparing them with 4''-deoxy and 4,5-dimethoxy candidusines A.[4] The other two neolignans are new natural products, named corticins D (**1**) and E (**3**). These natural neolignans were less cytotoxic than the EtOAc extract itself, maybe due to an aerial oxidation and degradation produced when these compounds, with catechol moieties, are definitively purified.

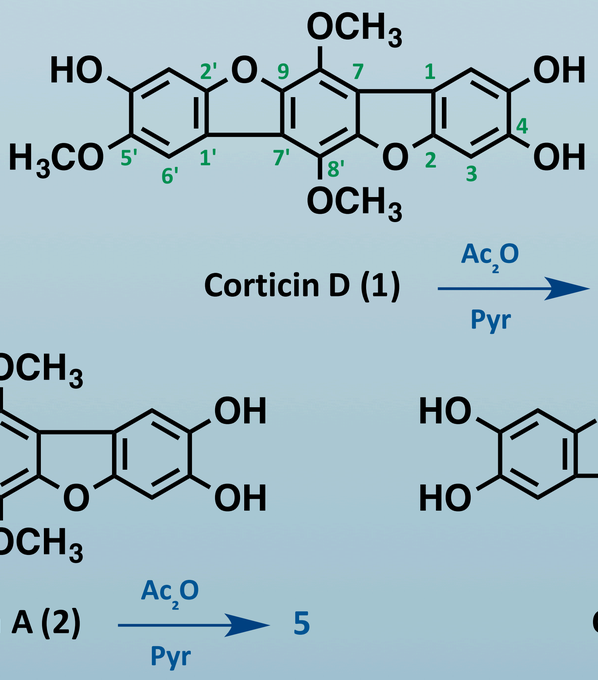

Figure 2: New terphenyl neolignans **1** and **3**, corrected structure for corticin A (**2**) and preparation of the triacetylderivatives **4**-**5**.

Table 2: ^{1}H NMR (400 MHz, δ in ppm, CD_3OD[a] or $CDCl_3$[b]) data of neolignans **1**-**5** and of corticin A triacetate from Briggs *et al.*[2].

Position	**1**[a]	**2**[a]	**3**[a]	**4**[b]	**5**[b]	Corticin A triacetate[b][2]
H-3	7.01 (1H, s)	6.99 (1H, s)	7.00 (2H, s)	7.29 (1H, s)	7.17 (1H, s)	7.16 (1H, s)
H-6	7.52 (1H, s)	7.51 (1H, s)	7.51 (2H, s)	7.73 (1H, s)	7.83 (1H, s)	7.83 (1H, s)
H-3'	7.04 (1H, s)	7.19 (1H, s)	7.00 (2H, s)	7.42 (1H, s)	7.41 (1H, s)	7.42 (1H, s)
H-6'	7.60 (1H, s)	7.51 (1H, s)	7.51 (2H, s)	7.96 (1H, s)	7.95 (1H, s)	7.96 (1H, s)
CH_3O-4'	-	3.96 (3H, s)	-	-	3.92 (3H, s)	3.92 (3H, s)
CH_3O-5'	3.98 (3H, s)	-	-	3.96 (3H, s)	-	-
CH_3O-8	4.31 (3H, s)	4.30 (3H, s)	4.30 (6H, s)	4.37 (3H, s)*	4.35 (3H, s)*	4.36 (3H, s)*
CH_3O-8'	4.34 (3H, s)	4.30 (3H, s)	4.30 (6H, s)	4.35 (3H, s)*	4.33 (3H, s)*	4.34 (3H, s)*
CH_3-COO-	-	-	-	2.34 (3H, s)	2.34 (3H, s)	2.35 (3H, s)
	-	-	-	2.37 (6H, s)	2.35 (6H, s)	2.36 (6H, s)
	-	-		2.37 (6H, s)	2.35 (6H, s)	2.36 (6H, s)

* Interchangeable signals.

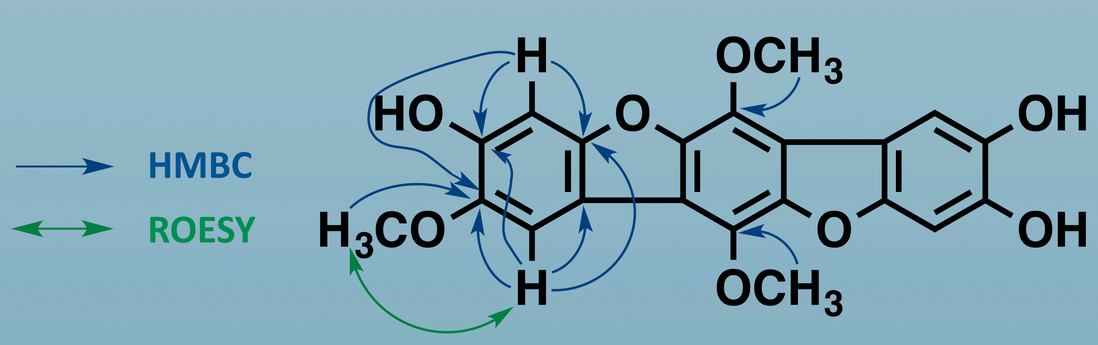

Figure 3: Key HMBC and ROESY correlations for the structure elucidation of compound **1**.

References:

[1] G. Martínez Fernández. Micología de Riberas [web]. June 15, 2017. Available on: http://setasdelpisuerga4.webnode.es/
[2] L. H. Briggs, R. C. Cambie, I. C. Dean, R. Hodges, W. B. Ingram, P. S. Rutledge. *Aust. J. Chem.* **1976**, 29, 179-190.
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Keywords: *Terana coerulea*, Neolignans, Terphenyls, Corticin, Cytotoxicity

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XXXVI REUNIÓN BIENAL
DE LA REAL SOCIEDAD ESPAÑOLA DE QUÍMICA
Sitges 25-29 junio 2017

CERTIFICADO DE PARTICIPACIÓN

Los Presidentes del Comité Organizador de la

XXXVI REUNIÓN BIENAL DE LA SOCIEDAD ESPAÑOLA DE QUÍMICA

celebrada en Sitges, del 25 al 29 de junio de 2017

CERTIFICAN QUE:

Pablo Anselmo García García, Maitane Maisterra Udi, María Ángeles Castro González, Luz María Muñoz Centeno, Ricardo C. Calhelha, Isabel C.F.R. Ferreira

han contribuido con su PÓSTER con título:

NEW CYTOTOXIC NEOLIGNANS FROM THE COBALT CRUST FUNGUS

Y para que conste se expide el presente certificado

en Sitges el 29 de junio de 2017.

DOCUMENTO FIRMADO DIGITALMENTE

Prof. Dr. Agustí Lledós
Co-Presidente del Comité Organizador

Prof. Dra. Mariona Sodupe
Co-Presidente del Comité Organizador

PP-013