PERSONAL INFORMATION

Family name, First name: Osuna Oliveras, Sílvia
Address: Travessera Can Casica 4, 17481 Sant Julià de Ramis (Girona)
Cell phone: 627823355
Email: silvia.osuna@udg.edu
Date of birth: July 1, 1983 (Nationality: Spanish)
Web site: https://www.osunalab.com
Researcher ID: www.researcherid.com/rid/B-6191-2009
Google Scholar: http://scholar.google.com/citations?user=rHtokY4AAAAJ
ORCID: 0000-0003-3657-6469

CV SUMMARY

Prof. Osuna is an ICREA research professor and part time Full Professor at the Universitat de Girona (UdG). Her research is based on the rational design of enzymes and is funded by **European Research Council (ERC) – Consolidator Grant** project, ERC- **Proof-of-Concept** grant, Spanish I+D research project, and three Marie Curie doctoral network ITN. Prof. Osuna has a long list of publications, including *Nature*, *Nature Catal.*, *Nature Chem. Biol.*, *Nature Commun.*, *PNAS*, *ACIE*, *JACS*, among others. She has published one review paper in *Nat. Rev. Methods Primers*, two in *Phys. Chem. Chem. Phys.*, eight in *Chem. Commun.*, one in *Chem. Soc. Rev.*, one in *Acc. Chem. Res.*, one in WIRES *Comput Mol Sci.*, and 5 book chapters. Her publications accumulate more than **5050 citations**, with an **h index of 40** (self-citations excluded).

Osuna has demonstrated the key role played by computational tools in biocatalysis (Chem. Comm. **2017**, most downloaded paper of 2017 in Physical Chemistry, *Nat. Rev. Methods Primers* ***2021***, most cited review in biocatalysis according to google academics), and especially the importance of conformational dynamics in enzyme design (*ChemComm* **2018**, *ACIE* **2019)**. Most importantly, she has developed new computational tools based on inter-residue correlations that allow, for the first time, the prediction of distal active site mutations that lead to enhanced enzymatic activity (ACS Catal. **2017**; *WIRESCompSci* ***2021***; *ACS Catal.* **2021;** *ACS Catal.* **2024**). Osuna has established many collaborations with experimental groups mainly located in Europe: with Prof. M. Reetz (*ACIE* **2020**; *NatComm* **2021**), Prof. B. Hauer (Univ. Mainz, *ACIE* **2023**, *ACIE* **2024**), Prof. Sterner (Univ. Regensburg, *ACS Catal.* **2021**, *ACS Catal.* **2023**, *ACS Catal.* **2024,** Prot. Sci. **2025**), PD Dr. Andrea Hupfeld (Univ. Regensburg, ACIE **2025**, ACS Catal. **2025**, ACIE **2025**), Prof. Schallmey (TU Braunschweig, *FEBS J.* **2021**, *ACS Catal.* **2024**, *ACS Catal.* **2025**), Prof. S. Flitsch and Prof. N. Turner (*Nat. Rev. Methods Primers* **2021**), and Prof. Schallmey (*FEBS J.* **2021**, *ACS Catal.* **2024**, *ACS Catal.* **2025**), Prof. Grogan (*ACIE* **2024**), Prof. D. Zhou (*Nat. Cat.* ***2019***), Prof. Kazlauskas (Univ of Minnesota, US, bioRxiv1), Prof. Tokuriki (Univ British Columbia, CAN, bioRxiv2), and Prof. Noji (Univ Tokyo, JP). She has also established collaborations with Dr. Sabio (CNIO) to unveil the key role exerted by p38gamma in liver cancer (*Nature* ***2019***), with Dr. S. Sanchez (IRB, Barcelona) to investigate the role of conformational dynamics in micro-motor self-propulsion (*NatComm* ***2019***, *ACIE* ***2020***), among others.

She has been awarded many prestigious awards: **Banco Sabadell Foundation Award for Sciences and Engineering** (2025; FundBancSab-video), BIOTRANS Junior Award (2025), Chemistry Europe Lecture Award (JIQ-RSEQ) (2024), Spanish **Young National Research Award 'María Teresa Toral'** (2023), Emerging Scientific Talent award of Societat Catalana de Química (2023), **EuChemS Lecture award** (2022), Marcial Moreno award by the Catalan division of the *Royal Spanish Society of Chemistry RSEQ-Cat* (2021), **Catalan National Research Award – Young Talent 2019** from Fundació Catalana de Recerca i Innovació (FCRi), Young Investigator Award by the company Lilly and *Royal Spanish Society of Chemistry RSEQ* (2019), the Young Investigator Award of EuCheMS Organic Division (2017), the **Young Researcher award by the *Royal Spanish Society of Chemistry*** (RSEQ 2016), and the **Research award by the *Fundación Princesa de Girona*** (FPdGi 2016- Science category; FPdGi-video). She was invited to

be part of the **committee** of the Premios nacionales de investigación – Ciencias y Tecnologías Químicas 2024 and 2025, *Premio Fundación Princesa de Girona FPdGi 2024*, *Catalan National Award* 2022, *Premios Rey Jaime I* 2017 awards, has acted as external reviewer in the 2018, 2021 ERC-StG call, and has been a panel member in the 2017, 2021 *Ramón y Cajal*, 2020, 2022 and 2023 Spanish I+D projects, among others. She has served as referee for more than 150 publications in international journals and she has been invited to be part of the horizon group selected by the Generalitat de Catalunya to advice and help in science policies (2023). She is member of the International Advisory Board of ACS Catalysis (2021), Physical Chemistry panel of the evaluation of Spanish I+D research projects (Excelencia y Retos) (2021), member of the Access Committee of the Partnership for Advanced Computing in Europe (PRACE) (2020), among others. She was the **conference chair and organizer of the Girona Seminar 2022** on Biocatalysis, was member of the Girona Seminar organizing committee 2016, 2018, 2024 and member of the local organizing committee of the 24th EuroQSAR 2024. She is also member of the scientific committee of the REQOMED 2026 conference.

EDUCATION

2010 PhD in Chemistry (Excellent *cum laude*), Department of Chemistry, University of Girona, Spain, March 2010 (**Special Award for PhD thesis, *Premi Extraordinari***)

2007 Diploma d'Estudis Avançats (DEA), MSc defense, University of Girona, Spain, June 2007

2005 BSc in Chemistry, University of Girona, Spain, July 2005

CURRENT POSITION

2024 - Part time **Full Professor** at the Universitat de Girona

2018 – **ICREA research position** (ICREA 2017 senior call, started on January 1st 2018)

2023 – 2028 **European Research Council – Consolidator Grant (ERC-CoG)** project (FASTEN, ERC-2022-CoG-101088032, 1.9M€/5 years) "Fast yet accurate routine rational design of novel enzymes".

2024 – 2026 **European Research Council – Proof of Concept Grant (ERC-POC)** project (KITZYME, ERC-2023-POC-101158166, 150k€/1.5 years) "Development of rationally designed enzyme kits".

PREVIOUS POSITIONS

2023 – 2025 **European Research Council – Proof of Concept Grant (ERC-POC)** project (GREENZYME, ERC-2022-POC-101112805, 150k€/1.5 years) "Computational design of industrial enzymes for green chemistry".

2020 – 2023 **Human Frontier Science Program – Program Grants** project (RGP0054/2020, 1.35M$/3 years, Osuna team: 337,500$).

2016 – 2022 **European Research Council – Starting Grant (ERC-StG)** project (ERC-2015-StG-679001-NETMODEZYME, 1.45M€/5 years)

2014 – 2018 Career Integration Grant (FP7-PEOPLE-2013-CIG) by the European Commission

2016 – 2018 **Ramón y Cajal position** (RYC-2014-16846), Institut de Química Computacional i Catàlisi (IQCC), University of Girona, Spain

2013 – 2015 Juan de la Cierva postdoctoral researcher (JCI-2012-14438), Institut de Química Computacional i Catàlisi (IQCC), University of Girona, Spain

2012 – 2013 Reintegration phase of '**Marie Curie International Outgoing Fellowship for Career Development (IOF)**', IQCC, University of Girona, Spain (PIOF-GA-2009-252856)

2010 – 2012 2-year '**Marie Curie International Outgoing Fellowship for Career Development (IOF)**' postdoctoral appointment, Houk Lab, University of California, Los Angeles (UCLA), US (PIOF-GA-2009-252856)

2005 – 2009 4-years PhD fellowship, 'Beca de Formación de Personal Universitario' (AP2005-2992, Spanish Ministry), IQC, University of Girona, Spain

FELLOWSHIPS AND GRANTS

2025 – 2028 3-year R&D Project "THERAZYME", Spanish Ministry, MINECO (PI: Osuna, 237.000€)
2026-2030 **MSCA-Doctoral Network (MSCA-DN)** project (ELEGANCE, HORIZON-MSCA-2024-DN-01-01, 4.5M€/4 years, Osuna team: 282.188€).
2026-2030 **MSCA-Doctoral Network (MSCA-DN)** project (HALOVERSE, HORIZON-MSCA-2024-DN-JD-101226357, 3.9M€/4 years, Osuna team: 376.250€).
2025-2029 **MSCA-Doctoral Network (MSCA-DN)** project (COMENZE, HORIZON-MSCA-2023-DN-101169327, 2.56M€/4 years, Osuna team: 251.971€).
2023 – 2025 1.5-year Proof of Concept Project "EVOCAT", Spanish Ministry, MINECO (PI: Osuna)
2023 – 2026 3-year R&D Project "COCOZYME", Spanish Ministry, MINECO (PI: Osuna)
2020 – 2023 **Human Frontier Science Program – Program Grants** project (RGP0054/2020, 1.35M$/3 years, Osuna team: 337,500$).
2019 – 2021 3-year R&D Project "EnzExplora", Spanish Ministry, MINECO (PI: Osuna)
2016 – 2020 **European Research Council – Starting Grant (ERC-StG)** project (ERC-2015-StG-679001-NETMODEZYME, 1.45M€/5 years, PI: Osuna)
2016 – 2020 5-year 'Ramón y Cajal' position by MINECO (Spain, score: **99.5/100**)
2015 – 2018 3-year R&D Project "*SpinEnzymeCat*", Spanish Ministry, MINECO, (PI: Osuna & Swart)
2014 – 2018 4-year Career Integration Grant (FP7-PEOPLE-2013-CIG) by the European Commission (score: 95.6/100)
2013 – 2016 3-year postdoctoral grant 'Juan de la Cierva (JdC)' (Spanish Ministry).
2010 – 2013 3-year postdoctoral fellowship, 'Marie Curie International Outgoing Fellowship for Career Development (IOF)' granted by the European Commission (score: **93.4/100**)
2010 – 2010 2-year postdoctoral fellowship, 'Beatriu de Pinós A' (Catalan Government) – declined in favor of IOF Marie Curie fellowship obtained the same year
2005 – 2009 4-years PhD fellowship, 'Beca de Formación de Personal Universitario' (Spanish Ministry)
2005 – 2005 4-years PhD fellowship, 'Beca de Formació d'Investigadors' (Catalan Government) –declined in favor of FPU awarded the same year.
2004 – 2005 Collaboration research fellowship for undergraduate students, "Beca de Colaboración" (Spanish Ministry)
2004 – 2005 Research fellowship for undergraduate students, *Beca de Colaboración* (Spanish Ministry)

AWARDS

2025 **Fundación Banco Sabadell Award – Science and Engineering**
2025 **BIOTRANS** Junior research award
2023 **Premio Nacional de Investigación Jóvenes** – María Teresa Toral
2023 Premi Talent Jove Emergent – Societat Catalana de Química (SCQ)
2022 **EuChemS Lecture award**
2021 Marcial Moreno award by the Catalan division of the Real Sociedad Española de Química (RSEQ)
2019 **Premi Nacional de Recerca – Talent Jove** (Catalan National Research Award – Young Talent) from **Fundació Catalana de Recerca i Innovació (FCRi).**
2019 **Lilly** and Real Sociedad Española de Química (RSEQ) Young Researcher Award
2017 Young Researcher Award of EuCheMS Organic Division
2016 **Real Sociedad Española de Química** (RSEQ) Young Researcher Award
2016 **Princess of Girona Foundation Research Award - FPdGi**
2016 Special mention at the European Young Chemist Award 2016 (EYCA)
2015 Nominated by the Institució Catalana de Recerca i Estudis Avançats (ICREA) and selected by Lindau committee to attend the Lindau Nobel Laureate meeting for young researchers (July 2015).

2011 Special Award for PhD thesis (*Premi Extraordinari*): Award for the best PhD thesis defended in 2010 within the Chemistry Department at the University of Girona (Spain), July 2011.

SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

Supervised Doctoral Thesis [Total: **11**]: Dr. Juan Pablo Martínez (PhD defense November 2016), Dr. Adrià Romero (FI fellowship, PhD defense December 2018), Dr. Miguel Ángel Maria-Solano (FPI fellowship, PhD defense March 2021), Dr. Lorenzo d'Amore (UdG fellowship, PhD defense December 2021), Dr. Eila Serrano-Hervás (FI, PhD defense July 2022), Dr. Christian Curado Carballada (ERC-StG, PhD defense March 2023), Dr. Carla Calvó Tusell (ERC-StG, PhD defense June 2023), Dr. Miquel Estévez (ERC-StG, PhD defense July 2023), Dr. Jordi Soler Parpal (FPU fellowship, defense September 2023), Dr. Guillem Casadevall (ERC-StG/ERC-POC, defense September 2024), Dr. Cristina Duran (FPI, PhD defense June 2025).

On-going supervision of Doctoral Thesis [Total: **6**]: Ms. Akram Doustmohammadi (HFSP, 2021-2024), Mr. Javier Moreno (2023-2026), Ms. Janet Sanchez (2023-2027), Ms. Jonnely Luizaga (2023-2026), Ms. Esther Pruna (ERC-CoG, 2023-2026), Ms. Rupal Sharma (UdG fellowship, 2025-2028).

Supervisor of master students [Total: **9**]: Ms. Berta Cortada (2025-2026), Mr. Mario Bonachea (2023-2024), Ms. Janet Sanchez (2022-2023), Mr. Guillem Casadevall (2017-2018), Ms. Carla Calvó (2017-2018), Ms. Leila Pujals (2017-2018), Mr. Miquel Estévez (2016-2017), Mr. Ferran Planas (2015-2016), Ms. Eila Serrano (2015-2016).

Supervisor of postdoctoral fellows [Total: **11**]: Dr. Cristina Duran (ERC-CoG, 2025-2027), Dr. Alexander Swoboda (Erwin Schrödinger fellowship 2024-2026), Dr. Guillem Casadevall (ERC-CoG, 2025-2027), Dr. Eila Serrano (Investigo fellowship at IdiBGi, 2023-2025), Dr. Eduard Masferrer (ERC-POC, 2023-2025 and Juan de la Cierva 2025-2027), Dr. Miquel Estévez (ERC-POC, 2023-2025), Dr. Christian Curado Carballada (industrial research contract, 2023-2024), Dr. Dhani Ram Mahato (HFSP, Sept. 2021- March 2024), Dr. Sergi Ruiz-Barragán (HFSP, Sept. 2021 – Sept. 2022), Dr. Ferran Feixas (ERC-StG, May 2017-May 2019), Dr. Javier Iglesias-Fernández (Nov 2016-April 2019, Marie Curie fellowship EnzVolNet H2020-MSCA-IF-2016-753045; Juan de la Cierva (May 2019-April 2021)), Dr. Marc Garcia-Borràs (May 2015-Jan 2016, Juan de la Cierva (Jan 2019-Feb 2020) and Beatriu de Pinós 2020-2022).

PUBLICATIONS AND SCIENTIFIC RESULTS

Osuna has a long list of publications, including *Nature*, *Nature Catal.*, *Nature Chem. Biol.*, *Nature Commun.*, *PNAS*, *ACIE*, *JACS*, among others. She has published **one** review paper in *Nat. Rev. Methods Primers*, **one** in *Phys. Chem. Chem. Phys.*, **two** in *Chem. Commun.*, **one** in *Chem. Soc. Rev.*, **one** in *Acc. Chem. Res.*, **one** in WIRES *Comput Mol Sci.*, and **5 book chapters**. Her publications accumulate more than **5050 citations**, with an **h index of 41** (self-citations excluded).

The whole updated list of publications can be found at: https://www.osunalab.com/publications/

Most cited publications: *[Self-citations excluded]*

1. Bell, E. L.; Finnigan, W.; France, S. P.; Green, A. P.; Hayes, M. A.; Hepworth, L. J.; Lovelock, S. L.; Niikura, H.; **Osuna, S.**; Romero, E., et al. Biocatalysis. *Nat. Rev. Methods Primers* **2021**, *1*, 46. [544 citations, most cited review in biocatalysis according to google academics]

2. García-Simón,C.; Garcia-Borràs, M.; Gómez, L.; Parella, T.; **Osuna, S.**; Juanhuix, J.; Imaz, I.; Maspoch, D.; Costas, M.; Ribas, X., Sponge-like molecular cage for purification of fullerenes, *Nature Commun.* **2014**, 5, 5557. [174 citations]

3. Jiménez-Osés, G.†; **Osuna, S.†**; Gao, X.†; Sawaya, M.R.; Gilson, L.; Collier, S. J.; Huisman, G.H.; Yeates, T.O.; Tang, Y.; Houk, K.N. **(†: The authors have contributed equally to the work)** "The

Role of Distant Mutations and Allosteric Regulation on Active Site Dynamics and Catalysis", *Nature Chem. Biol.* **2014**, *10, 431-436. [+cover]* [156 citations]
4. Arqué, X.; Romero-Rivera, A.; Feixas, F.; Patiño, T*.; **Osuna, S*.**, Sánchez, S*. Intrinsic enzymatic properties modulate the self-propulsion of micromotors, *Nature Commun.* **2019**, *10*, 2826. [139 citations]
5. Noey, E. L.; Tibrewal, N.; Jiménez-Osés, G.; **Osuna, S.**; Park, J.; Bond, C.; Cascio, D.; Liang, J.; Zhang, X.; Huisman, G.; Tang, Y.; Houk, K. N. Origins of Stereoselectivity in Evolved Ketoredutases, *Proc. Natl. Acad. Sci. USA* **2015**, *112*, E7065-E7072. [122 citations]
6. Bian, S.; Scott, A. M.; Cao, Y.; Liang, Y.; **Osuna, S.**; Houk, K. N.; Braunschweig, A. B. "Covalently Patterned Graphene Surfaces by a Force-Accelerated Diels-Alder Reaction", *J. Am. Chem. Soc.* **2013**, 135, 9240-9243. [121 citations]
7. **Osuna, S.**; Swart, M; Solà, M. "Dispersion Corrections Essential for the Study of Chemical Reactivity in Fullerenes", *J. Phys. Chem. A,* **2011**, 115, 3491-3496. [111 citations]
8. **Osuna, S.**; Swart, M.; Solà, M. "The Reactivity of Endohedral Fullerenes. What Can Be Learnt from Computational Studies?" *Phys. Chem. Chem. Phys.*, **2011**, 13, 3585-3603. [+cover] [109 citations]
9. Li, A., Acevedo-Rocha, C.G., D'Amore, L., Chen, J., Peng, Y., Garcia-Borràs, M., Gao, C., Zhu, J., Rickerby, H., **Osuna, S.***, Zhou, J.* and Reetz, M.T.* Regio- and Stereoselective Steroid Hydroxylation at C7 by Cytochrome P450 Monooxygenase Mutants. *Angew. Chem. Int. Ed.* **2020**, *59,* 12499-12505. [106 citations]
10. Maria-Solano, M. A.; Serrano-Hervás, E.; Romero-Rivera, A.; Iglesias-Fernández, J.; **Osuna, S.*** Role of conformational dynamics for the evolution of novel enzyme function, *Chem. Commun.* **2018**, 54, 6622-6634. [106 citations]

Most relevant publications in the 2018-2025 period: *[Self-citations excluded]*
1. Li, J.; Duran, C.; Pogrányi, B.; Cornish, K. A. S.; Cartwright, J.; **Osuna, S.***; Unsworth, W. P.*; Grogan, G.* Divergent Oxidation Reactions of E- and Z-Allylic Primary Alcohols by an Unspecific Peroxygenase, *Angew. Chem. Int. Ed.* **2025**, e20242241. [4 citations]
2. Staar, S.; Estévez-Gay, M.; Kaspar, F.; **Osuna, S.***; Schallmey, A.* Engineering of Conserved Sequence Motif 1 Residues in Halohydrin Dehalogenase HheC Simultaneously Enhances Activity, Stability, and Enantioselectivity, *ACS Catal.* **2025**, *15*, 5257-5272. [5 citation]
3. Duran, C.; Kinateder, T.; Hiefinger, C.; Sterner, R.*, **Osuna, S.***; **2024**, Altering Active Site Loop Dynamics Enhances Standalone Activity of Tryptophan Synthase alpha -Subunit, *ACS Catal.* ***2024****, 14, 15976-15987.* [8 citations]
4. Ludwig, J.; Curado-Carballada, C.; Hammer, S. C.; Schneider, A.; Diether, S.; Kress, N.; Ruiz-Barragán, S.; **Osuna, S.***; Hauer, B.* Controlling Monoterpene Isomerization by Guiding Challenging Carbocation Rearrangement Reactions in Engineered Squalene-Hopene Cyclases, *Angew. Chem. Int. Ed.* **2024**, e202318913. [3 citations]
5. Casadevall, G.; Duran, C.; **Osuna, S.*** AlphaFold2 and Deep Learning for Elucidating Enzyme Conformational Flexibility and Its Application for Design, *JACS Au* **2023**, *3*, 1554–1562. [46 citations]
6. Schneider, A., Curado, C., Lystbaek, T. B., **Osuna, S.***, Hauer, B.*, Harnessing the Structure and Dynamics of the Squalene-Hopene Cyclase for (−)-Ambroxide Production, *Angew. Chem. Int. Ed.* ***2023***, e202301607. [10 citations]
7. Palone, A.; Casadevall, G.; Ruiz-Barragan, S.; Call, A.; **Osuna, S.***; Bietti, M.*; Costas, M.* C-H Bonds as Functional Groups: Simultaneous Generation of Multiple Stereocenters by Enantioselective Hydroxylation at Unactivated Tertiary C-H Bonds, *J. Am. Chem. Soc.* **2023**, *145*, 15742–15753. [37 citations]
8. Casadevall, G.; Duran, C.; Estévez-Gay, M.; **Osuna, S.*** Estimating conformational heterogeneity of tryptophan synthase with a template-based AlphaFold2 approach, *Prot. Sci.* ***2022****, 31, e4426. [16 citations]*

9. Maria-Solano, M.A.*; Kinateder, T.; Iglesias-Fernández, J.; Sterner, R.*; **Osuna, S***. In Silico Identification and Experimental Validation of Distal Activity-Enhancing Mutations in Tryptophan Synthase. *ACS Catal.* **2021**, *11*, 13733-13743. [41 citations]
10. Acevedo-Rocha, C.; Li, A.; D'Amore, L.; Hoebenreich, S.; Sanchis, J.; Lubrano, P.; Ferla, M. P.; Garcia-Borràs, M.; **Osuna, S.***; Reetz, M.*; Pervasive cooperative mutational effects on multiple catalytic enzyme traits emerge via long-range conformational dynamics, *Nature Commun.* **2021**, 12, 1621. [93 citations]
11. **Osuna, S.*** The challenge of predicting distal active site mutations in computational enzyme design, *WIREs Comput Mol Sci.* **2021**, e1502 (doi: 10.1002/wcms.1502). [99 citations]
12. Li, A., Acevedo-Rocha, C.G., D'Amore, L., Chen, J., Peng, Y., Garcia-Borràs, M., Gao, C., Zhu, J., Rickerby, H., **Osuna, S.***, Zhou, J.* and Reetz, M.T.*, Regio- and Stereoselective Steroid Hydroxylation at C7 by Cytochrome P450 Monooxygenase Mutants. *Angew. Chem. Int. Ed.* **2020**, *59,* 12499-12505. [106 citations]
13. Chen, X.; Zhang, H.; Maria-Solano, M. A.; Liu, W.; Li, J.; Feng, J.; Liu, X.; **Osuna, S.***; Guo, R. T.; Wu, Q.*; Zhu, D.*, Ma, Y. Efficient reductive desymmetrization of bulky 1,3-cyclodiketones enabled by structure-guided directed evolution of a carbonyl reductase, *Nature Catal.* **2019**, *2*, 931-941. [92 citations]
14. Maria-Solano, M. A.; Iglesias-Fernández, J.*; **Osuna, S.*** Deciphering the Allosterically Driven Conformational Ensemble in Tryptophan Synthase Evolution, *J. Am. Chem. Soc.* **2019**, *141*, 33, 13049-13056. [52 citations]
15. Curado-Carvallada, C.; Feixas, F.; Iglesias-Fernández, J.; **Osuna, S***. Hidden conformations in Aspergillus niger Monoamine oxidase are key for catalytic efficiency, *Angew. Chem. Int. Ed.* **2019**, *58*, 3097-3101 [26 citations]
16. Tomás-Loba, A.; Manieri, E.; González-Terán, B.; Mora, A.; Leiva-Vega, L.; Santamans, A. M.; Romero-Becerra, R.; Rodríguez, E.; Pintor-Chocano, A.; Feixas, F.; López, J. A.; Caballero, B.; Trakala, M.; Blanco, O.; Torres, J. L.; Hernández-Cosido, L.; Montalvo-Romeral, V.; Matesanz, N.; Roche-Molina, M.; Bernal, J. A.; Mischo, H.; León, M.; Caballero, A.; Miranda-Saavedra, D.; Ruiz-Cabello, J.; Nevzorova, Y. A.; Cubero, F. J.; Bravo, J.; Vázquez, J.; Malumbres, M.; Marcos, M.; **Osuna, S.**; Sabio, G. p38 gamma is essential for cell cycle progression and liver tumourigenesis, *Nature* **2019**, *568*, 557-560. [86 citations]

PARTICIPATION IN INTERNATIONAL CONFERENCES

Dr. Osuna has contributed to **104 conferences** with **76 oral communications** (**45** of which as **Invited speaker or Plenary speaker**). She has been **invited as plenary speaker** at the **Gordon Research Conference on Biocatalysis** 2016 and 2024, **Gordon Research Conference on Protein Engineering** 2025, 2022 EuChemS conference, ESPA 2024 and TheoBio2017, as invited speaker at: BIOTRANS 2025, ECI conference on Enzyme Engineering 2025, **European Submit of Industrial Biotechnology** 2024, 2023 EuChemS Comp Chem, Electrochemical Society (ECS) meeting 2016 and 2017, 252nd ACS meeting (Washington), 256th ACS meeting (Boston), 262nd ACS meeting (Atlanta), Biotransformations 2017, AmineBioCat 2020, Biotrans 2021 (July 2021), **Solvay Conference** (2022), among others. She was invited to participate in the Bürgenstock and Lindau meetings in 2018, and 2014, respectively.

She was the **conference chair and organizer** of the Girona Seminar 2022 on Biocatalysis, was member of the organizing committee 2016, 2018, and 2024, member of the local organizing committee of EuroQSAR 2025, and member of the scientific committee of REQOMED 2026 and RSEQ BIENAL de química 2027.

Selected invited conference participations in the 2018-2025 period:

1. Osuna, S. Computational Design of efficient enzymes through coevolution and correlation-mediated allosteric networks. **Keynote lecture** at ECI conference on Enzyme Engineering, Denmark 2025.
2. Osuna, S. Computational Design of Enzymes Through Coevolution and Correlation-

Mediated Allosteric Networks. **Plenary lecture** at Gordon research conference on Protein Engineering, USA 2025.

3. Osuna, S. Beyond the active site: Designing efficient enzymes through correlation and evolutionary information, **Junior Award lecture** at BIOTRANS, Switzerland 2025.
4. Osuna, S. Beyond AlphaFold: How to computationally generate efficient enzymes?, **Invited lecture** at Elixir Conference, Barcelona 2025.
5. Osuna, S. Beyond AlphaFold: How to generate efficient enzymes?, **Invited lecture** at WetLab meets DryLab workshop, Switzerland 2025.
6. Osuna, S. Decoding Nature's catalysts for rational enzyme design: How evolution reshapes allosteric networks? **Invited lecture** at TRENCA meeting, Benicassim 2024.
7. Osuna, S. Beyond AlphaFold: Can we computationally generate efficient enzymes?, **Invited lecture** at **European Submit of Industrial Biotechnology** conference, Graz, Austria 2024.
8. Osuna, S. Computationally Designing Enzymes with Nature-Like Catalytic Efficiencies, **Plenary lecture**, at Gordon research conference on Biocatalysis, USA 2024.
9. Osuna, S. Catalysis in confined spaces: insights from enzymatic to synthetic catalysts, **Plenary lecture** at Electronic Structure Principles and Applications (ESPA), Tarragona, June 2024.
10. Osuna, S. Towards the development of fast yet accurate computational design protocols, **Invited keynote lecture** at TIS Forum 2023, Hoffmann-LaRoche, Basel, Switzerland, September 2023.
11. Osuna, S. Can we computationally design efficient enzymes?, **Invited lecture** at Beilstein symposium, Rüdesheim am Rhein, Germany, September 2023.
12. Osuna, S. Computational enzyme design: Towards the development of computational protocols for the design of efficient enzymes, **Invited lecture** at **EuChemS Comp Chem** 2023, Thessaloniki, Greece, August 2023.
13. Osuna, S. Computational enzyme design, **Plenary lecture** at the Solvay conference (Participation by invitation only), Brussels, Belgium, October 2022.
14. Osuna, S. Can we rationally design efficient enzymes?, **Plenary lecture** at 2022 EuChemS conference, Lisbon, PT, August 2022.
15. Osuna, S. Conformationally-driven computational enzyme design: Predicting distal activity-enhancing mutations in tryptophan synthase, **Invited lecture** at APFED conference: Advances in Protein Folding, Evolution, and Design, Bayreuth, Germany, April 6-8th 2022.
16. Osuna, S. Conformational regulation in enzyme design and evolution, **Invited lecture** at ACS fall meeting, Atlanta, USA, August 2021.
17. Osuna, S. Conformational regulation in enzyme design and evolution, **Invited lecture** at Biotrans conference, Graz, AU, July 2021.
18. Osuna, S. Computational exploration of enzyme conformational landscapes: Identifying key conformational states for chiral amine production, **Invited lecture** at AmineBioCat conference, Stuttgart, DE, February 2020.
19. Osuna, S. Computational tools for enzyme design, **Invited lecture** at **Protein Engineering Canada 2018**, Vancouver, Canada, June 2018.
20. Osuna, S. The role of Conformational Dynamics on the evolution of novel enzymatic activities, **Invited lecture** at **254th ACS meeting**, Boston, USA August 2018.
21. Osuna, S. The role of Conformational Dynamics on the evolution of novel enzymatic activities, **Invited lecture** at the European Young Chemist Network symposium at **7th EuChemS**, Liverpool, UK August 2018.

PARTICIPATION IN RESEARCH PROJECTS

The applicant has participated in **16 research projects**. She is currently managing a total of *ca.* 5.8 M€ from European and national funding agencies.

European Research Council (ERC) grants:

Consolidator Grant: "*Fast yet accurate routine rational design of novel enzymes*" (FASTEN, ERC-2022-COG-101088032), PI: Osuna. Total: 1,996,250€. Period: 2023-2028
Proof of Concept: "Computational design of industrial enzymes for green chemistry" (GREENZYME, ERC-2022-POC-101112805) PI: Osuna. Total: 150,000€. Period: 2023-2024
Proof of Concept: "Development of rationally designed enzyme kits" (KITZYME, ERC-2023-POC-101158166), PI: Osuna. Total: 150,000€. Period: 2024-2025

MINECO I+D research projects: (1) "Rational design of efficient therapeutic enzymes", (THERAZYMES, PID2024-155349NB-I00) PI: Osuna. Total: 237,500€ (+ 1 FPI fellowship associated) , (2) "Conformationally-driven computational enzyme design for enhanced stand-alone or in complex activity", (COCOZYME, PID2021-129034NB-I00), PI: Dr. Osuna. Total: 157,300€ (+ 1 FPI fellowship associated). Period: 2023-2025; (3) **Proof of Concept:** "Computational evolution of new (bio)catalysts", (EVOCAT, PDC2022-133950-I00), PI: Dr. Osuna. Total: 143,750€. Period: 2023-2025.

Generalitat de Catalunya:
SGR 2021– Generalitat de Catalunya: "Theoretical Chemistry of Biosystems (TCBioSys)" (SGR 2021 00487), PI: Dr. Osuna. Total: 60,000€. Period: 2023-2025
PRODUCTE project: "Rationally Engineering Enzyme Kits for Industrial Biocatalysis (BIOKIT)" (2025 PROD 00025), PI: Osuna. Total: 150,000€. Period: 2025-2027

Marie Curie Doctoral Networks: (1) ELEGANCE, (HORIZON-MSCA-2024-DN-01-01), 4.5M€/4 years, Osuna team: 282.188€. Period: 2026-2030. (2) HALOVERSE, HORIZON-MSCA-2024-DN-JD-101226357, 3.9M€/4 years, Osuna team: 376.250€. Period: 2026-2030, (3) COMENZE, (HORIZON-MSCA-2023-DN-101169327), 2.56M€/4 years. Total Osuna team: 251,971.20€ Period: 2025-2029.

INVITED PRESENTATIONS AT RESEARCH CENTERS AND UNIVERSITIES

She has been invited to give talks at: IBMB-CSIC (January 2025), IQAC-CSIC (February 2025), IQS (May 2025), CIGBioGune (October 2024), University of Geneva (February 2024), Regensburg University (August 2023), Institut de Recerca Biomèdica (IRB, February 2023), ICIQ (2023), Barcelona Supercomputer Center (BSC, June 23rd 2022), university of Basel (2022), TU Brawnschweig (virtual, Jan. 2021), Uppsala Univ (virtual, Dec. 2020), Univ Barcelona (virtual, Oct. 2020), DE Shaw research center (NYC, US, 2018), Biomagune (San Sebastián, 2018), CSIC Madrid (2018), CIQUS (Santiago de Compostela, 2018), Institut de Recerca Biomèdica (IRB, Barcelona, 2017), Marburg University (DE, 2016), University of Manchester (UK, 2016), Oxford University (UK, 2016), Institut Català d'Investigació Química (ICIQ, Tarragona, 2016), Barcelona Super Computing Center (BSC, Barcelona, 2015), Universidad de la Rioja (Spain, 2015), University of Texas El Paso (UTEP, US 2013).

KNOWLEDGE TRANSFER

Osuna has made contact and established collaborations with industrial partners. She has been invited to give talks at the following conferences organized by industrial partners: **Hoffmann-LaRoche** to give a talk at TIS Forum (Switzerland), **AstraZeneca** at ELRIG Therapeutic OLIGO and European Chemical Biology Symposium (Sweden **c-Lecta** at a mini-symposium organized by them at VAAM conference (Germany), **CODEXIS** at the Protein Engineering Forum (San Francisco, USA), **BRAIN Biotech** at the Biotransformations workshop (Germany). Since 2010, Osuna has collaborated with the company **CODEXIS** (US) and has published two publications (**one** *Nature Chem. Biol.*, and **one** *Proc. Nat. Acad. Sci. - USA*), as well as with Biosyntia (**one** *ACS Catal.*, **one** *ACIE*, **one** *Nat. Commun.*). She has additionally established: 2 collaboration projects with **BIOMAR** (31,515€, period: 7 months), a 2-year collaboration with **SEQENS** (116,000€, period:

24 months), one collaboration project with **CPTx** (8.000€, 1 month), one collaboration project with EVORALIS (13,800€, 3 months). Osuna has signed NDA agreements with BASF, Esteve, Dr. Reddy's, EVORALIS. She has also **2 patents** of rationally design EGF derivatives (ES Patent P202431076, ES Patent P202431079). Osuna lab has developed the **Shortest Path Map web** for enzyme design: https://spmosuna.com/

OUTREACH ACTIVITIES

Dr. Osuna has published **five papers** to promote science communication to the general public. In addition to that, she has participated in many TV programs at local and National channels: Espejo Público –Antena 3, TIPS –TVE2, Lab24 –Canal24h, 8 al dia – 8TV, and at the local TV Girona and La xarxa TV. Her research and awards received have also been highlighted in many newspapers: La Vanguardia, El Periódico, ABC, El Punt diari, Hora nova, L'Empordà, among others. She has also been invited to participate in debates about the presence of women in science, such as the EuChemS Global breakfast event (February 2025).

MEMBERSHIPS AND COMMISSIONS OF TRUST

- Membership in **editorial committees**: International Editorial Advisory Board of: ACS Catalysis (2023-present), Catal (2025-present), European Journal of Organic Chemistry (2021-2025), ChemPlusChem (2020-2027), ACS Catalysis Early Career Advisory Board (2020-2022)
- Member of **international boards**: Member the **Scientific Advisory Board** of Instituto de Materiales Avanzados de la Universitat Jaume I. Panel member of EuroHPC and PRACE.
- **Committee of the awards:** National Awards 2024 and 2025 – Chemistry category, Best PhD thesis of RSEQ Chemical Biology (2025), FPdGi– Science Category (2024), European award of Young Research group leaders (2024), Lilly and RSEQ PhD (2023), Catalan National Award (FCRi, 2022), Premios Rey Jaime I (2017).
- Committee of PhD thesis: Agata Raczynska (2025), Aitor Vega (2025), Artur Brotons (2024), Maria Bzowka (2023), Sergio González Granda (2022), José Emilio Sánchez Aparicio (2022), Antonio Moreno (2021), Busra Topal (2020), Albert Artigas Ruf (2020), Jaime Rodríguez-Guerra (2018), Marina Cañellas Fontanilles (2018), Lur Alonso Cotchico (2018).

IMPACT IN SOCIETY

- POLICY Member of the horizon group selected by the Generalitat de Catalunya to advice and help in science policies (2023)

- **GENDER-EQUALITY:** Participation in multiple round tables related to the participation of women in STEM, expositions and webpages focused on highlighting Spanish female researchers. Member of the gender action plan of IQCC.

ADDITIONAL MERITS

She has been on two maternity leaves: May - October 2019, June – November 2021.