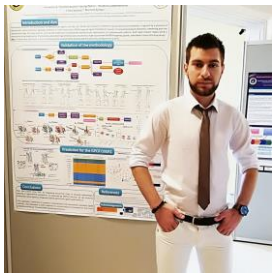
Curriculum vitae

PERSONAL INFORMATION

Athanasios A. Panagiotopoulos



Apollonos 2, 71305 Heraklion (Greece)

+30 694 941 3089, ID: AH 716090, TRN: 150266004

athpanagiotopoulos@hotmail.com

Skype Thanasis.Panagiotopoulos

Gender Male|Date of birth 13 Aug 1991|Nationality Greek|Father's Name Antonios A. Panagiotopoulos

PROFESSIONAL EXPERIENCE

(14/07/2021–Current)

Post-Doctoral Research

Laboratory of Experimental Endocrinology, Department of Experimental Medicine,

University of Crete, School of Medicine. Supervisor: Prof. Dr. Maria-Eleni Kampa.

Voutes Campus, 70013 Heraklion (Greece).

http://www.med.uoc.gr/

- Design of specific antagonists of the membrane androgen receptor, OXER1.

Company or industry Higher education

(30/11/2017–14/07/2021)

Doctoral Dissertation

Laboratory of Experimental Endocrinology, Department of Experimental Medicine,

University of Crete, School of Medicine. Supervisor: Prof. Dr. Maria-Eleni Kampa.

Voutes Campus, 70013 Heraklion (Greece).

http://www.med.uoc.gr/

- Identifications of new micromolecular ligands for the membrane receptor of androgens, OXER1 and study of their mechanism of action.

Company or industry Higher education

(01/09/2014–23/06/2017)

Assistant of Undergraduate Inorganic Chemistry Laboratories

Laboratory of Inorganic Chemistry, University of Crete, Department of Chemistry.

Supervisor: Prof. Dr. Athanassios G. Coutsolelos and Eleutheria Vardalachaki.

Voutes Campus, 70013 Heraklion (Greece).

http://eilotas.chemistry.uoc.gr/uocchem/

- Preparation and recycling of chemical reagents,
- Supervision of undergraduate students,
- Teaching inorganic chemistry subjects.

Company or industry Higher education

(22/06/2015–16/07/2015) **Participation in Experiments at the Nuclear Research Center-CEA**

Commissariat a l' Energie Atomique (CEA). Supervisor: Prof. Dr. Vincent Artero,
Cedex Grenoble, 38054 Grenoble (France).
http://www.cea.fr/Pages/le-cea/les-centres-cea/grenoble.aspx

- Study of new catalysts for photochemical and electrochemical production of hydrogen fuel.

Company or industry Higher education

(01/09/2014–27/01/2016) **Master Thesis**

Laboratory of Bioinorganic Chemistry, University of Crete, Department of Chemistry.
Supervisor: Prof. Dr. Athanassios G. Coutsolelos.
Voutes Campus, 70013 Heraklion (Greece).
http://eilotas.chemistry.uoc.gr/uocchem/

- Photocatalytic production of H_2 with metalloporphyrins.

Company or industry Higher education

(20/02/2014–03/07/2014) **Diplomatic Thesis**

Laboratory of Bioinorganic Chemistry, University of Crete, Department of Chemistry.
Supervisor: Prof. Dr. Athanassios G. Coutsolelos.
Voutes Campus, 70013 Heraklion (Greece).
http://eilotas.chemistry.uoc.gr/uocchem/

- Synthesis and characterization of new porphyrin derivatives.

Company or industry Higher education

(01/07/2013–30/09/2013) **Practical Exercise**

General Hospital of Amaliada, Department of Biochemistry – Microbiology.
Supervisor: Euthimia Sainatoudi, Evangelistrias 122, 27200 Amaliada (Greece).

- Chemical – Biochemical – Microbiological Analyses.

Company or industry Activities related to human health and social care

(01/11/2011–10/02/2012) **Assistant of Undergraduate General Chemistry Laboratories**

Laboratory of General Chemistry, University of Crete, Department of Chemistry.
Supervisor: Dr. Spiridon Kornilios. Voutes Campus, 70013 Heraklion (Greece).
http://eilotas.chemistry.uoc.gr/uocchem/

- Preparation of Chemical Reagents.

Company or industry Higher education

EDUCATION AND TRAINING

(2021–Current) **Post-Doctoral Researcher of Medical School** EPP State 10
University of Crete, Voutes Campus, 70013 Heraklion (Greece).

(2017–2021) **Doctor of Medical School** EPP State 10
University of Crete, Voutes Campus, 70013 Heraklion (Greece).

(2014–2016) **Holder of a Master's Degree in Chemistry (9.83/10)** EPP State 7
University of Crete, Voutes Campus, 70013 Heraklion (Greece).

(2010–2014) **Graduate of Chemistry Department (9.30/10)** EPP State 6
University of Crete, Voutes Campus, 70013 Heraklion (Greece).

(2006–2009) **High school graduate (19.1/20)** EPP State 4
Simopoulou General High School of Ilia, 27069 Efyra (Greece).

(2003–2006) **Midle school graduate (19.3/20)** EPP State 2
Simopoulou Midle School of Ilia, 27069 Efyra (Greece).

(1997–2003) **School graduate** EPP State 1
Primary School of Rodia Ilias, 27069 Efyra (Greece).

INDIVIDUAL SKILLS

Native language: Greek

Other languages

	COMPREHENSION		SPEAKING		WRITING
	Verbal	Written (reading)	Communication	Oral expression	
English	C2	C2	C2	C2	C2
French	C2	C2	C2	C2	C2

Levels: A1 and A2: Basic user - B1 and B2: Independent user - C1 and C2: Expert user
Common European Framework of Reference for Languages

Communication skills: Communication skills acquired during the thesis, internship, master's research work, doctoral research work as well as international conferences.

Organizational / management skills: Organizational and management skills acquired during thesis, internship, undergraduate assistantship, graduate assistantship, graduate thesis and doctoral research.

Professional skills

- Knowledge of the use and organization of laboratory conditions,
- Knowledge of using chemical synthesis methods,
- Knowledge of using qualitative analysis methods,
- Knowledge of using quantitative analysis methods,
- Knowledge of using a mass spectrometer (Maldi-TOF),
- Knowledge of using a UV-Vis spectrophotometer,
- Knowledge of using a cyclic voltammetry system,
- Knowledge of using an NMR spectrometer,
- Knowledge of using gas and liquid chromatography,
- Knowledge of using biochemical analyzers,
- Knowledge of using molecular modeling programs and methods,
- Knowledge of using QSAR programs (Quantitative Structure - Activity Relationship),
- Knowledge of using cell culture methods,
- Knowledge of using methods to measure and study intracellular metabolites,
- Knowledge of using microscopes,
- Knowledge of using *in vitro* and *in silico* methods.

Digital proficiency

SELF EVALUATION				
Data processing	Communication	Content Creation	Safety	Solving problems
Expert user	Expert user	Expert user	Expert user	Expert user

Digital Skills - Self-Assessment Table

Certificate from the Chemistry Department of the University of Crete

- Knowledge of using the tools Microsoft Office™,
- Knowledge of using the tools OpenOffice™,
- Knowledge of using the programs MATLAB,
- Knowledge of using the programs XRay,
- Knowledge of using the programs GC,
- Knowledge of using the programs Origin,
- Knowledge of using the programs BrukerNMR,
- Knowledge of using the programs ChemDraw,

- Knowledge of using the tools MicrosoftWorks™,
- Knowledge of using the programs LabView,
- Knowledge of using the programs QSAR,
- Knowledge of using the programs of molecular simulation,
- Knowledge of using the supercomputer system Aris-GRNET.

Military Service

Fulfillment of military obligations in the period from 11/15/2021 to 11/15/2022 in the 547th Airborne Infantry Battalion, the 545th Airborne Infantry Battalion and the Reserve Infantry Officer School (SEAP) with the specialty Nurse and Support Brigadier General.

ADDITIONAL INFORMATION

Honors and awards

1. Grant from the Federation of American Societies for Experimental Biology (FASEB) for the purpose of participating in the conference "The Steroid Hormones and Receptors in Health and Disease, FASEB-RRSH 2021".

2. Funding from the National Technology and Research Infrastructure Network for use of the Aris-GRNET supercomputer system, for experiments on: **Natural Products on OXER1: development of novel therapeutics for cancer and inflammatory diseases**.

3. Funding for access to the Joliot-Curie Rome supercomputer, GENCI at CEA, France, for experiments on: **Epitope vaccines based on the dynamics of mutated SARS-CoV-2 proteins at all atom resolution** from the Pan-European program: **PRACE Support to Mitigate Impact Of COVID-19 Pandemic.**

4. Research member of the research funded by the Hellenic Foundation for Research and Innovation (H.F.R.I.), titled: **Deciphering the actions and pharmacological selectivity of the novel lipid/steroid GPCR, OXER1 in inflammation and cancer.**

5. Scholarship of the Hellenic Society of Biochemistry & Molecular Biology for the purpose of participating in the 70th Panhellenic Congress of the HSBMB.

6. Scholarship from IKY (State Scholarships Foundation) for the preparation of the doctoral dissertation. Scholarship co-financed by Greece and the European Union (European Social Fund – ESF) through the Operational Program "Human Resources Development, Education and Lifelong Learning" in the context of the project “Strengthening Human Resources Research Potential via Doctorate Research – 2nd Cycle” (MIS-5000432), implemented by the State Scholarships Foundation (IKY).

7. Funding from the National Technology and Research Infrastructure Network for use of the Aris-GRNET supercomputer system, for experiments on: **Natural Products on OXER1**.

8. Accepted for a scholarship from the Hellenic Foundation for Research and Innovation (H.F.R.I.) for the preparation of the doctoral thesis.

9. Award of Excellence 2017 from the Rodia cultural association.

10. Medal of Excellence 2017 from the Simopoulo Expression cultural association.

11. 1st Prize from the Royal Society of Chemistry for the best research paper – Heraklion, Crete, Greece, 21 October 2016.

12. PERSPECT H2O COST Action CM 1202 grant to attend an international conference in Milazzo, Italy, September 2016.

13. PERSPECT H2O COST Action CM 1202 grant to attend an international conference in Tarragona, Spain, April 2016.

14. Maria Michael Manassaki Endowment Scholarship 2014 – 2015.

15. PERSPECT H2O COST Action CM 1202 grant to attend an international conference in Engelberg, Switzerland, November 2015.

16. PERSPECT H2O COST Action CM 1202 grant to attend an international conference in Gdansk, Poland, September 2015.

17. Grant PERSPECT H2O COST Action CM 1202 for participation in experiments at the Center for Nuclear Research-CEA – France.

18. 1st ranked graduate of the department since 1987 (1050 graduates).

19. 1st ranked graduate of the Chemistry department during the swearing in of the graduates (July 2014).

20. 1st ranked during the selection of postgraduate students in the Department of Chemistry (July 2014).

21. J. Latsis charity foundation scholarship for Ac. Year 2012 – 2013.

22. J. Latsis charity foundation scholarship for Ac. Year 2011 – 2012.

23. J. Latsis Public Benefit Institution Award "Aristoi" (Higher level of access to higher education - Municipality of Pineias), Simopoulo 2009.

24. 1st Eurobank EFG Award "The Great Moment for Education" (Higher degree of access for higher education) – Municipality of Pineias, Tripoli 2009.

25. Progress Award for the Year 2008 – 2009 "Expression Association", Municipality of Pineias, Efyra 2009.

26. Excellence and Progress Award Sch. Year 2008 – 2009 (grade 19.1).

27. Progress Award for the Year 2007-2008 "Expression Association", Municipality of Pineias, Efyra 2008.

28. Excellence and Progress Award Sch. Year 2007 – 2008 (grade 19.2).

29. 1st Prize of the GEITONA Schools Competition (Topic: Writing a Treatise on the reorganization of the Fire-stricken Ilia, participating students of the high schools of the Prefecture of Ilia), Pyrgos 2008.

30. 1st Prize for the best exhibition K.E.T.A. of Western Greece with the theme "A sustainable Business Idea" (Participating students from the high schools of Western Greece), Patras 2008.

31. Progress Award for the Year 2006 – 2007 "Expression Association", Municipality of Pineias, Efyra 2007.

32. Excellence and Progress Award Sch. Year 2006 – 2007 (grade 18.6).

33. Excellence and Progress Award Sch. Year 2005 – 2006 (grade 19.3).

34. Excellence and Progress Award Sch. Year 2004 – 2005 (grade 18.5).

35. Excellence and Progress Award Sch. Year 2003 – 2004 (grade 18.7).

36. 1st J. Alexandris Endowment Award (Best Design Exhibition of the Municipality of Pineias 2003), Rodia.

Conferences

1. 13th International Meeting on Rapid Responses to Steroid Hormones (RRSH) 2022, Paris (France), 20 – 23 September, 2022. Posted of research work.

- The role of the membrane androgen receptor OXER1 in androgen induced calcium changes.

Athanasios A. Panagiotopoulos, Konstantina Kalyvianaki, Evangelia Konstantinou, George Notas, Elias Castanas and Marilena Kampa.

2. The Steroid Hormones and Receptors in Health and Disease (12th RRSH), FASEB, 25 – 27 May, 2021. Posted of research work.

- Testosterone and natural polyphenols are antagonists of OXER1- An *in silico* and *in vitro* approach.

Athanasios A. Panagiotopoulos, Christina Papachristofi, Konstantina Kalyvianaki, Panagiotis Malamos, Panayiotis A. Theodoropoulos, George Notas, Theodora Calogeropoulou, Elias Castanas and Marilena Kampa.

3. EFMC-ISMC & EFMC-YMCS Virtual Poster Session, 09 September 2020. Posted of research work.

- A simple open source bio-informatic methodology for initial exploration of GPCR ligands' agonistic/antagonistic properties.

Athanasios A. Panagiotopoulos, Christina Papachristofi, Konstantina Kalyvianaki, Panagiotis Malamos, Panayiotis A. Theodoropoulos, George Notas, Theodora Calogeropoulou, Elias Castanas and Marilena Kampa.

4. 70th Panhellenic Conference of the Hellenic Society of Biochemistry & Molecular Biology, Athens (Greece), 29 November – 01 December, 2019. Posted of research work.

- Simulation of G_{α} proteins binding on GPCRs may predict ligands' agonistic/antagonistic properties.

Athanasios A. Panagiotopoulos, Christina Papachristofi, Konstantina Kalyvianaki, Panagiotis Malamos, Panayiotis A. Theodoropoulos, George Notas, Theodora Calogeropoulou, Elias Castanas & Marilena Kampa.

5. 7th Panhellenic Forum of Young Scientists of the Hellenic Society of Biochemistry & Molecular Biology, Athens (Greece), 28 November, 2019. Posted of research work.

- Simulation of G_{α} proteins binding on GPCRs may predict ligands' agonistic/antagonistic properties.

Athanasios A. Panagiotopoulos, Christina Papachristofi, Konstantina Kalyvianaki, Panagiotis Malamos, Panayiotis A. Theodoropoulos, George Notas, Theodora Calogeropoulou, Elias Castanas and Marilena Kampa.

6. Clinical & Translational Oncology Conference 2019, Heraklion (Greece), 14 – 15 November, 2019.

7. E.E.F.I.E. 2019 "Precision Medicine in the treatment of cancer & the Precision Medicine Unit of Crete", Heraklion (Greece), 13 March, 2019.

8. 69th Panhellenic Conference of the Hellenic Society of Biochemistry & Molecular Biology, Larissa (Greece), 23 – 25 November, 2018. Posted of research works.

- An *in silico* method for the identification of nuclear localization signal of cargo proteins.

Athanasios. A. Panagiotopoulos, Chara Polioudaki, Sotirios. G. Ntallis, Dimitris Dellis, George Notas, Chistos. A. Panagiotidis, Panagiotis. A. Theodoropoulos, Elias Castanas and Marilena Kampa.

- Evidence for nuclear translocation of the membrane androgen receptor, OXER1.

Panagiotis Malamos, Athanasios. A. Panagiotopoulos, Konstantina Kalyvianaki, Chara Polioudaki, Panagiotis. A. Theodoropoulos, George Notas, Elias Castanas and Marilena Kampa.

- A comparative study of the membrane androgen receptors OXER1, GPRC6A and ZIP9.

Konstantina Kalyvianaki, Athanasios A. Panagiotopoulos, Panagiotis Malamos, Eleni Moustou, Maria Tzardi, Efstathios N. Stathopoulos, Georgios S. Ioannidis, Kostas Marias, George Notas, Panayiotis A. Theodoropoulos, Elias Castanas and Marilena Kampa.

9. 11th International Meeting on Rapid Responses to Steroid Hormones (RRSH) 2018, Dublin (Ireland), 04 – 06 September 2018. Posted of research works.

- Evidence for nuclear translocation of the membrane androgen receptor, OXER1.

Athanasios. A. Panagiotopoulos, Panagiotis Malamos, Konstantina Kalyvianaki, Chara Polioudaki, Panagiotis. A. Theodoropoulos, George Notas, Elias Castanas and Marilena Kampa.

- A comparative study of the membrane androgen receptors OXER1, GPRC6A and ZIP9.

Konstantina Kalyvianaki, Athanasios A. Panagiotopoulos, Panagiotis Malamos, Eleni Moustou, Maria Tzardi, Efstathios N. Stathopoulos, Georgios S. Ioannidis, Kostas Marias, George Notas, Panayiotis A. Theodoropoulos, Elias Castanas and Marilena Kampa.

10. 19th Chemistry Department Graduate Student Conference, Heraklion, 02 – 04 May, 2017. Presentation of research work – Invited Speaker.

- Photocatalytic production H_2.

Athanasios A. Panagiotopoulos and Athanasios G. Coutsolelos.

11. EUROFILLERS POLYMER BLENDS 2017, Heraklion (Greece), 23 – 27 April, 2017.

12. 22nd Panhellenic Chemistry Conference, Thessaloniki (Greece), 02 – 04 December, 2016. Presentation of research work – Invited Speaker.

- Photocatalytic production H_2 with metalloporphyrins.

Athanasios A. Panagiotopoulos and Athanasios G. Coutsolelos.

13. Athens International Catalysis Symposium (AICS 2016), Athens (Greece), 03 – 04 November, 2016. Presentation of research work – Invited Speaker.

- Porphyrins and Cobaloximes: Molecular Photocatalytic Systems for Hydrogen Evolution.

Athanasios A. Panagiotopoulos, Kalliopi Ladomenou, Dongyue Sun, Vincent Artero and Athanassios G. Coutsolelos.

14. The 2nd Israel-Greece Joint Meeting on Nanotechnology and Bionanoscience, Heraklion (Greece), 25 – 27 October, 2016. Presentation of research work – Invited Speaker.

- Porphyrin Pt as catalyst and porphyrin Pd as photosensitizer: a novel catalytic system for hydrogen evolution.

Athanasios A. Panagiotopoulos and Athanasios G. Coutsolelos.

15. Organic & Perovsite Solar Cells Conference and MCWG Meetings of Cost Action MP1307, Heraklion (Greece), 19 – 21 October, 2016. Presentation of research work – Invited Speaker.

- Porphyrin Pt as catalyst and porphyrin Pd as photosensitizer: a novel catalytic system for hydrogen evolution.

Athanasios A. Panagiotopoulos and Athanasios G. Coutsolelos.

16. International Symposium: Chemistry at the Interface of Biology and Medicine, Heraklion (Greece), 23 – 26 September, 2016.

17. COST Action CM1202-Supramolecular Photocatalytic Water Splitting in connection with a meeting of Working Groups 3 and 4 on the theme: Photoinduced charge transfer, separation, and accumulation, Milazzo (Italy), 04 – 06 September, 2016. Presentation of research work – Invited Speaker.

- Photocatalytic H_2 production with metalloporphyrins and cobaloximes.

Athanasios A. Panagiotopoulos, Kalliopi Ladomenou, Dongyue Sun, Vincent Artero and Athanassios G. Coutsolelos.

- Photocatalytic hydrogen production based on a water-soluble porphyrin derivative as sensitizer and a series of Wilkinson type complexes as catalysts.

Athanasios A. Panagiotopoulos, Efthymios Fasoulakis, Eleutheria Vardalachaki and Athanassios G. Coutsolelos.

18. COST Action CM1202 Tarragona Training School and the Meeting of Working Groups 1 and 2, Tarragona (Spain), 11 – 14 April, 2016. Presentation of research work – Invited Speaker.

- Photocatalytic H_2 production with metalloporphyrins.

Athanasios A. Panagiotopoulos and Athanasios G. Coutsolelos.

19. 18th Chemistry Department Graduate Student Conference, Heraklion, 26 – 27 March, 2016. Presentation of research work – Invited Speaker.

- Photocatalytic H_2 production with metalloporphyrins.

Athanasios A. Panagiotopoulos and Athanasios G. Coutsolelos.

20. Joint Working Group Meeting of WGs 3 and 4: Novel experimental and theoretical tools to describe the photophysics and photochemistry of supramolecular water splitting, Engelberg (Switzerland), 27 – 29 November, 2015. Presentation of research work – Invited Speaker.

- Porphyrins and Cobaloximes: Molecular Photocatalytic Systems for Hydrogen Evolution.

Athanasios A. Panagiotopoulos, Kalliopi Ladomenou, Dongyue Sun, Vincent Artero and Athanassios G. Coutsolelos.

21. 2nd COST Action CM 1202 PERSPECT-H2O Meeting: Hydrogen Production, Gdansk University of Technology (Poland), 04 – 09 September, 2015. Presentation of research work – Invited Speaker.

- Porphyrin Pt as catalyst and porphyrin Pd as photosensitizer: a novel catalytic system for hydrogen evolution.

Athanasios A. Panagiotopoulos and Athanasios G. Coutsolelos.

- The influence of the pyridine ligand on the sixth position of various cobaloximes on the photochemical H_2 production.

Athanasios A. Panagiotopoulos, Kalliopi Ladomenou, Dongyue Sun, Vincent Artero and Athanassios G. Coutsolelos.

22. Solar Fuels: moving from materials to devices Early Career Researchers' Symposium, Imperial College, London (United Kingdom), 06 July, 2015. Presentation of research work – Invited Speaker.

- Porphyrin Pt as catalyst and porphyrin Pd as photosensitizer: a novel catalytic system for hydrogen evolution.

Athanasios A. Panagiotopoulos and Athanasios G. Coutsolelos.

- The influence of the pyridine ligand on the sixth position of various cobaloximes on the photochemical H_2 production.

Athanasios A. Panagiotopoulos, Kalliopi Ladomenou, Dongyue Sun, Vincent Artero and Athanassios G. Coutsolelos.

23. Solar Fuels: moving from materials to devices SFN International Discussion Meeting, Royal Society of Chemistry, London (United Kingdom), 07 – 08 July, 2015. Presentation of research work – Invited Speaker.

- Porphyrin Pt as catalyst and porphyrin Pd as photosensitizer: a novel catalytic system for hydrogen evolution.

Athanasios A. Panagiotopoulos and Athanasios G. Coutsolelos.

Memberships

- Member of Royal Society of Chemistry,
- Member of European Federation for Medicinal Chemistry and Chemical Biology (EFMC-YSN),
- Member of the Hellenic Society of Biochemistry and Molecular Biology,
- Reviewer in the international journal of chemistry *"Macromolecules",*
- PRACE Support to Mitigate Impact Of COVID-19 Pandemic.

Publications
Total Citations: 207
h-Index: 7
h-10-Index: 6

1. Recognition motifs for Importin 4 (LPPRS(G/P)P) and Importin 5 (KP(K/Y)LV) binding, by bio-informatic simulation and experimental in vitro validation, Athanasios A. Panagiotopoulos*, Konstantina Kalyvianaki*, Paraskevi K. Tsodoulou, Maria N. Darivianaki, Dimitris Dellis, George Notas, Panayiotis A. Theodoropoulos, Christos A. Panagiotidis, Elias Castanas, Marilena Kampa, ***Computational and Structural Biotechnology Journal***, 2022, **Accepted**. *Equal contribution. IF: 7.271.

2. Importins involved in the nuclear transportation of steroid hormone receptors: In silico and in vitro data, Konstantina Kalyvianaki*, Athanasios A. Panagiotopoulos*, Maria Patentalaki, Elias Castanas, Marilena Kampa, ***Frontiers in Endocrinology***, 2022, **13**, 954629.

doi: 10.3389/fendo.2022.954629. *Equal contribution. IF: 3.675.

3. From Traditional Ethnopharmacology to Modern Natural Drug Discovery: A Methodology Discussion and Specific Examples, Stergios Pirintsos, Athanasios A. Panagiotopoulos, Michalis Bariotakis, Vangelis Daskalakis, Christos Lionis, George Sourvinos, Ioannis Karakasiliotis, Marilena Kampa, Elias Castanas, ***Molecules***, 2022, **27** (13), 4060.

doi: 10.3390/molecules27134060. PMID: 35807306. IF: 4.927.

4. OXER1 mediates testosterone-induced calcium responses in prostate cancer cells, Athanasios A. Panagiotopoulos, Konstantina Kalyvianaki, Burcin Serifoglou, Evangelia Konstantinou, George Notas, Elias Castanas, Marilena Kampa, ***Molecular and Cellular Endocrinology***, 2022, **539**, 111487.

doi: 10.1016/j.mce.2021.111487. PMID: 34634385. IF: 4.102. Citations: 2.

5. Natural polyphenols inhibit the dimerization of the SARS-CoV-2 main protease: the case of fortunellin and its structural analogs, Athanasios A. Panagiotopoulos, Ioannis Karakasiliotis, Danai-Maria Kotzampasi, Marios Dimitriou, George Sourvinos, Marilena Kampa, Stergios. A. Pirintsos, Elias Castanas, Vangelis Daskalakis, ***Molecules***, 2021, **26** (19), 6068.

doi: 10.3390/molecules26196068. PMID: 34641612. IF: 4.411. Citations: 7.

6. New Antagonists of the Membrane Androgen Receptor OXER1 from the ZINC Natural Product Database, Athanasios A. Panagiotopoulos, Konstantina Kalyvianaki, Stergios A. Pirintsos, George Notas, Elias Castanas, Marilena Kampa, ***ACS Omega***, 2021, **6** (44), 29664–29674.

doi: 10.1021/acsomega.1c04027. PMID: 34778638. IF: 3.512. Citations: 5.

7. ERα36–GPER1 Collaboration Inhibits TLR4/NFκB-Induced Pro-Inflammatory Activity in Breast Cancer Cells, George Notas, Athanasios A. Panagiotopoulos, Rodanthi Vamvoukaki, Konstantina Kalyvianaki, Foteini Kiagiadaki, Alexandra Deli, Marilena Kampa, Elias Castanas, ***International Journal of Molecular Sciences***, 2021, **22** (14), 7603.

doi: 10.3390/ijms22147603. PMID: 34299224. IF: 5.923. Citations: 3.

8. p-cymene impairs SARS-CoV-2 and Influenza A (H1N1) viral replication: *In silico* predicted interaction with SARS-CoV-2 nucleocapsid protein and H1N1 nucleoprotein, Athanasios A. Panagiotopoulos, Melpomeni Tseliou, Ioannis Karakasiliotis, Danai-Maria Kotzampasi, Vangelis Daskalakis, Nikolaos Kesesidis, George Notas, Christos Lionis, Marilena Kampa, Stergios Pirintsos, George Sourvinos, Elias Castanas, ***Pharmacology Research & Perspectives***, 2021, **9**:e00798, 1-12. doi: 10.1002/prp2.798. PMID: 34128351. IF: 2.590. Citations: 8.

9. The sequence [EKRKI(E/R)(K/L/R/S/T)] is a nuclear localization signal for importin 7 binding (NLS7), Athanasios A. Panagiotopoulos, Chara Polioudaki, Sotirios G. Ntallis, Dimitrios Dellis, George Notas, Christos A. Panagiotidis, Panagiotis A. Theodoropoulos, Elias Castanas, Marilena Kampa, ***Biochimica et Biophysica Acta (BBA) - General Subjects***, 2021, **1865**, 5, 129851.

doi: 10.1016/j.bbagen.2021.129851. PMID: 33482249. IF: 3.670. Citations: 5.

10. The natural polyphenol fortunellin is a dimerization inhibitor of the SARS-CoV-2 3C-like proteinase, revealed by molecular simulations, Athanasios A. Panagiotopoulos, Danai-Maria Kotzampasi, George Sourvinos, Marilena Kampa, Stergios. A. Pirintsos, Elias Castanas, Vangelis. Daskalakis, ***ARXIV***, 2020, (ARXIV: https://arxiv.org/abs/2007.07736). Citations: 2.

11. A simple open source bio-informatic methodology for initial exploration of GPCR ligands' agonistic/antagonistic properties, Athanasios A. Panagiotopoulos, Christina Papachristofi, Konstantina Kalyvianaki, Panagiotis Malamos, Panayiotis A. Theodoropoulos, George Notas, Theodora Calogeropoulou, Elias Castanas, Marilena Kampa, ***Pharmacology Research & Perspectives***, 2020, **8**:e00600, 1-12. doi: 10.1002/prp2.600. PMID: 32662237. IF: 2.590. Citations: 5.

12. Membrane androgen receptors (OXER1, GPRC6A AND ZIP9) in prostate and breast cancer: A comparative study of their expression, Konstantina Kalyvianaki, Athanasios A. Panagiotopoulos, Panagiotis Malamos, Eleni Moustou, Maria Tzardi, Efstathios N. Stathopoulos, Georgios S. Ioannidis, Kostas Marias, George Notas, Panayiotis A. Theodoropoulos, Elias Castanas, Marilena Kampa, ***Steroids***, 2019, **142**, 100-108.

doi: 10.1016/j.steroids.2019.01.006. PMID: 30707908. IF: 2.500. Citations: 22.

13. Eicosanoids in prostate cancer, Athanasios A. Panagiotopoulos, Konstantina Kalyvianaki, Elias Castanas, Marilena Kampa, ***Cancer Metastasis Rev***., 2018, **37**, 237-243.

doi: 10.1007/s10555-018-9750-0. PMID: 30078159. IF: 9.260. Citations: 14.

14. Photochemical hydrogen production and cobaloximes: influence of cobalt axial N-ligand on the system stability, Athanasios A. Panagiotopoulos, Kalliopi Ladomenou, Dongyue Sun, Vincent Artero, Athanassios G. Coutsolelos, ***Dalton Trans***., 2016, **45**, 6732-6738.

doi: 10.1039/C5DT04502A. PMID: 26978600. IF: 4.390. Citations: 75.

15. Photochemical hydrogen evolution using Sn-porphyrin as photosensitizer and a series of Cobaloximes as catalysts, Georgios Landrou, Athanasios A. Panagiotopoulos, Kalliopi Ladomenou, Athanassios G. Coutsolelos, ***J. Porphyrins Phthalocyanines***, 2016, **20**, 534-541.

doi: 10.1142/S1088424616500243. IF: 1.816. Citations: 16.

16. Photocatalytic hydrogen production based on a water-soluble porphyrin derivative as sensitizer and a series of Wilkinson type complexes as catalysts, Athanasios A. Panagiotopoulos, Efthymios Fasoulakis, Eleutheria Vardalachaki, Athanassios G. Coutsolelos, ***J. Porphyrins Phthalocyanines***, 2016, **20**, 1-7. doi: 10.1142/S1088424616500905. IF: 1.816. Citations: 11.

17. Porphyrin Sensitized Evolution of Hydrogen using Dawson and Keplerate Polyoxometalate Photocatalysts, Athanasios A. Panagiotopoulos, Antonios Douvas, Panagiotis Argitis, Athanassios G. Coutsolelos, ***ChemSusChem***, 2016, **22**, 3213-3219.

doi: 10.1002/cssc.201600995. PMID: 27775226. IF: 8.470. Citations: 28.

Certifications

- Google Digital Skills Certificate, 18/07/2017.
- Certification by the National Technology and Research Infrastructure Network for use of the supercomputer system Aris-GRNET.

Books

In Greek Language:

1. Principles of Design and Development of New Drugs, Athanasios A. Panagiotopoulos, Evangelia K. Konstantinou and Efthimios G. Fasoulakis, *Litsa Medical Publications*, **2021**, number of pages: 176, University textbook. ISBN: 978-960-372-230-4. Book code in Eudoxus: 112698855.

2. Chemistry of Natural Products, Athanasios A. Panagiotopoulos and Andreas N. Athanasakis, *Papazisi Publications*, **2019**, number of pages: 272, University textbook. ISBN: 978-960-456-495-8, Book code in Eudoxus: 86192610.

3. Analyses of Clinical Chemistry, Athanasios A. Panagiotopoulos, *Ziti Publications*, **2017**, number of pages: 320, University textbook. ISBN: 978-960-456-495-8, Book code in Eudoxus: 68402021.

4. Laboratory Exercises in Biochemistry, Athanasios A. Panagiotopoulos and Georgia N. Nikolakakou, *Ziti Publications*, **2017**, number of pages: 296, University textbook. ISBN: 978-960-456-496-5, Book code in Eudoxus: 68406178.

In English Language:

1. Introduction to enzymes and biotechnology, Athanasios A. Panagiotopoulos and Efthymios G. Fasoulakis, *Lambert Academic Publishing*, **2017**, number of pages: 68, University textbook. ISBN: 978-620-2-02486-0, EAN: 9786202024860.

2. Exercises For Biochemistry Laboratory I, Athanasios A. Panagiotopoulos, Georgia N. Nikolakakou and Efthymios G. Fasoulakis, *Lambert Academic Publishing*, **2017**, number of pages: 141, University textbook. ISBN: 978-3-659-63944-9, EAN: 9783659639449.

3. Exercises For Biochemistry Laboratory II, Athanasios A. Panagiotopoulos, Georgia N. Nikolakakou and Efthymios G. Fasoulakis, *Lambert Academic Publishing*, **2017**, number of pages: 145, University textbook. ISBN: 978-620-2-06036-3, EAN: 978620206036-3.

4. Exercises For Biochemistry Laboratory III, Athanasios A. Panagiotopoulos, Georgia N. Nikolakakou and Efthymios G. Fasoulakis, *Lambert Academic Publishing*, **2017**, number of pages: 156, University textbook. ISBN: 978-3-8454-3997-6, EAN: 9783845439976.

Patents

- Para-cymene analogues as anti-virals, GR-22-0002175198, UK-2002141.6, RF: 93.84.142364/01.
- Compounds useful as anti-viral agents, US-17/799,055, PCT/EP2021/053389.

Virtual Workshops and Webinars

1. Ligand-Based Drug Design and SAR Analysis, 22 June, 2020.

- MOEsaic / R-Group Profiles and Analysis / MMP Analysis / Similarity and Substructure Searching / Descriptor Calculations / Conformational Searching / Molecular Alignments / Pharmacophore Modeling and Searching.

2. Developability Assessment and Property Prediction by pH-Dependent Conformational Sampling, 23 June, 2020.

- Antibody Modeling / Developability Assessment / Solubility and Aggregation Prediction / Titration, pI, and pKa Calculation.

3. Organizing Protein Structural Families and Data Mining, 24 June, 2020.

- Moe Project / Specialized Protein Families / Project Search / Organizing and Centralizing Project Data / Protein Family Modeling.

4. Small Molecule Virtual Screening, 24 June, 2020.

- MOE Databases / Descriptors / Fingerprints / QSPR Modeling / Pharmacophore Modeling / Template-Forced Docking / Scaffold Replacement / MedChem Transformations.

5. Computational Modeling of PROTAC-Mediated Ternary Complexes: Applications and Insight, 25 June, 2020.

- PROTAC / Targeted Protein Degradation / Ternary Complexes / Protein-Protein Docking.

6. Cheminformatics and QSAR, 25 June, 2020.

- MOE databases / Calculated Descriptors / Fingerprints / QSAR Modeling / Binary QSAR / Similarity Searching / Consensus Modeling.

7. Biologics: Protein Alignments, Modeling and Docking, 26 June, 2020.

- Protein Alignments and Superposition / Loop and Linker Modeling / Homology Modeling / Protein-Protein Docking / Protein Solubility Analysis / 2D Hot Spot Mapping / PLIF / Biologics QSAR Modeling.

8. Developability Assessment and Property Prediction by pH-Dependent Conformational Sampling, 07 July, 2020.

- Antibody Modeling / Developability Assessment / Solubility and Aggregation Prediction / Titration, pI, and pKa Calculation.

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10. Peptide Modeling, Conformational Searching and Docking, 09 July, 2020.

- Structure preparation / Non-natural amino acids / Conformational searching / Distance restraints / Peptide-protein docking / Protein-ligand interaction fingerprints.

11. Antibody Modeling and Protein Engineering, 05 August, 2020.

- Protein Engineering / Protein Properties / Developability / Hot Spot Analysis / Antibody Modeling / Humanization / Molecular Surfaces.

12. Organizing Protein Structural Families and Data Mining, 06 August, 2020.

- Moe Project / Specialized Protein Families / Project Search / Organizing and Centralizing Project Data / Protein Family Modeling.

13. Peptide Modeling, Conformational Searching and Docking, 07 August, 2020.

- Structure preparation / Non-natural amino acids / Conformational searching / Distance restraints / Peptide-protein docking / Protein-ligand interaction fingerprints.

14. Drug Development Complemented: COSMO-RS Applications to Solubility & Cocrystals Confirmation, 03 September, 2020.

- Recent COSMO-RS applications in the context of rational drug development.

15. 31th Panhellenic Neurology e-Conference, 03 – 06 September, 2020.

16. EFMC-ISMC First Time Disclosures & Late Breaking News, 07 – 08 September, 2020.

17. EFMC-ISMC & EFMC-YMCS Virtual Poster Session, 09 September, 2020.

- A simple open source bio-informatic methodology for initial exploration of GPCR ligands' agonistic/antagonistic properties.

Athanasios A. Panagiotopoulos, Christina Papachristofi, Konstantina Kalyvianaki, Panagiotis Malamos, Panayiotis A. Theodoropoulos, George Notas, Theodora Calogeropoulou, Elias Castanas and Marilena Kampa.

18. Virtual 7th EFMC Young Medicinal Chemists' Symposium, 10 – 11 September, 2020.

19. 15th Meeting of the European Association of Neuro-Oncology (EANO), 09 – 13 September, 2020.

20. Cryo-EM for Drug Discovery: Recent scientific results and practical considerations, Thermo Fisher Scientific, 29 September, 2020.

21. 4th EFMC-YSN MedChemBioOnline, 29 September, 2020.

22. 1st MercachemSyncom Digital Conference, 07 – 08 October, 2020.

23. Exploring New Modality Space by Precision Chemistry, 07 – 08 October, 2020.

- Recent advances in the new modality space, including targeted delivery, conjugates and molecular glues.

24. Solvent Analysis for Lead Optimization, 13 October, 2020.

- Solvent Analysis / 3D-RISM / Lead Optimization / Water Placement.

25. Protein Alignments and Homology Modeling, 14 October, 2020.

- Homology Modeling / Loop Modeling / Loop Conformational Searching / Sequence Alignments / Structure Superposition / Multimer Alignments and Superpositions.

26. Combinatorial Library Enumeration for Structure-Based Drug Design, 15 October, 2020.

- Fragment Libraries / Reaction Databases / Library Enumeration / Pharmacophore Filters / Structure-Based Drug Design.

27. Protein-Protein Docking and Epitope Analysis, 20 October, 2020.

- Protein-Protein Docking / Molecular Surfaces / Protein Patches / Interaction Fingerprints / Clustering / Epitope Analysis.

28. In Silico Fragment-Based Drug Design: Approaches and Applications, 21 October, 2020.

- Scaffold Replacement / Fragment Linking / R-Group Screening / Medicinal Chemistry Transformations / Fragment Libraries / Pharmacophore Models.

29. Applications of Pharmacophores in Drug Design, 22 October, 2020.

- Pharmacophore Modeling / Pharmacophore Consensus / Flexible Alignments / Pharmacophore Searching / Protein-Ligand Interaction Fingerprints (PLIF).

30. Structure-Based Drug Design and Ligand Modification, 27 October, 2020.

- Molecular Surfaces and Maps / Ligand Interactions / Docking / Ligand Optimization / Ligand Selectivity / Protein Alignments and Superposition.

31. Creating and Analyzing Focused Mutant Libraries for Protein Engineering, 28 October, 2020.

- Inputting Multiple Sequence Data / Mutation Frequencies / Targeted Mutant Libraries / Protein Engineering.

32. Revealing Conformational Behavior in Solution through NMR Data Analysis, 29 October, 2020.

- Conformer Generation / LowModeMD / QM Refinement / Solution Conformer Distribution.

33. Mining of Biomolecular Data Through an Intuitive Web-Based Platform, 04 November, 2020.

- PSILO / Macromolecular repository / 3D query searching / Pocket similarity / Display electron density / Central repository / Specialized protein databases.

34. Reverse Fingerprints (I): Application to Structural Motif Detection and Atomic Activity Contributions, 05 November, 2020.

- Molecular Fingerprints / Structural Motif Detection / Pharmacophores / Toxicology / Fingerprint Bit Score Visualization.

35. Reverse Fingerprints (II): Fingerprints to Pharmacophore Queries, 11 November, 2020.

- Molecular Fingerprints / Consensus Models / Pharmacophore Elucidation / 3D Query Generation.

36. Mining Activity Data to Guide a Medicinal Chemistry Campaign, 12 November, 2020.

- MOEsaic / Activity Data Mining / SAR / Matched Molecular Pairs / R-group Analysis / R-group Profiling / Free-Wilson Analysis / Compound Suggestions.

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37. Protein-Protein Docking and Epitope Analysis, 17 November, 2020.

- Protein-Protein Docking / Molecular Surfaces / Protein Patches / Interaction Fingerprints / Clustering / Epitope Analysis.

38. Protein Engineering and Affinity Modeling, 18 November, 2020.

- Protein Engineering / Protein Properties / Developability / Hot Spot Analysis.

39. Antibody Modeling and Developability, 19 November, 2020.

- Protein Annotation / Protein Patches / Virtual Mutagenesis / Antibody Homology Modeling / Protein Properties / Developability.

40. Applications of Pharmacophores in Drug Design, 23 November, 2020.

-Pharmacophore Modeling / Pharmacophore Consensus / Flexible Alignments / Pharmacophore Searching / Protein-Ligand Interaction Fingerprints (PLIF).

41. Biologics: Protein Alignments, Modeling and Docking, 24 November, 2020.

- Protein Alignments and Superposition / Loop and Linker Modeling / Homology Modeling / Protein-Protein Docking.

42. 5th EFMC-YSN MedChemBioOnline, Artificial Intelligence applied to Medicinal Chemistry, 25 November, 2020.

43. Application of Docking and Fragment Replacement to Structure-Based Drug Design, 25 November, 2020.

- Docking / Pharmacophore Modeling / Fragment-Based Design / Scaffold Replacement / Protein-Ligand Interaction Fingerprints (PLIF).

44. Creating and Analyzing Focused Mutant Libraries for Protein Engineering, 08 December, 2020.

- Inputting Multiple Sequence Data / Mutation Frequencies / Targeted Mutant Libraries / Protein Engineering.

45. From Structure to Dynamics Simulation: Workflow for Preparing, Running and Visualizing MD Trajectories, 09 December, 2020.

- Structure Preparation / Force Field / Solvation / AMBER / NAMD / Visualization / Player.

46. Advanced Small Molecule Docking, 10 December, 2020.

-Structure Preparation / Protein Binding Site Visualization / Template-Based Docking / Covalent Docking / Pharmacophores / Protein-Ligand Interaction Fingerprints (PLIF) / Multiple Processor Calculations.

47. EFMC-Trends in Medicinal Chemistry Online Symposia (TIMCOS), 10 December, 2020.

48. 7th Panhellenic Conference of the Hellenic Academy of Neuroimmunology, 10 – 13 December, 2020.

49. In Silico Fragment-Based Drug Design: Approaches and Applications, 16 December, 2020.

- Scaffold Replacement / Fragment Linking / R-Group Screening / Medicinal Chemistry Transformations / Fragment Libraries / Pharmacophore Models.

50. **Biologics by Design (CCG – MOE), 28 January, 2021.**

51. Remote Control of G Protein-Coupled Receptor Function from the Extracellular Vestibule, BioSolveIT, 15 April, 2021.

51. Practical Guide: Set Up MOE High-Performance Computing on AWS Cloud, 20 April, 2021.

- Webinar / Cloud / AWS / HPC / High-Throughput Screening / Large Scale Calculations / SLURM / Amazon Cluster.

52. **DrugSpace Symposium — Last Call and Speaker Line-Up, BioSolveIT, 21 – 22 April, 2021.**

53. Solvent Analysis for Lead Optimization, 21 April, 2021.

- Webinar / Solvent Analysis / 3D-RISM / Lead Optimization / Water Placement.

54. **Quantitative Predictions of Protein Solubility Using a QSPR Approach, 22 April, 2021.**

- Virtual Workshop / Homology Modeling / Protein Properties Calculations / QSAR/QSPR Modeling / Protein Patch Analysis.

55. **UGM & Conference 2021, 19 – 20 May, 2021.**

- MOE / Biological Therapeutics / Protein Modelling / Protein Engineering / Small Molecule / SBDD / LBDD / FBDD / Computational Chemistry / Medicinal Chemistry / Cheminformatics / Drug Discovery.

56. Influencing Gαi/s protein Activity by Peptidic Guanine Nucleotide Exchange Modulators, BioSolveIT, 15 April, 2021.

57. 7th EFMC-YSN MedChemBioOnline, 25 May, 2021.

- Epigenetics: The Road Towards a Polypharmacological Approach.

58. **1st Edelris Symposium on Affinity Selection-Mass Spectrometry in Drug Discovery, 02 – 03 June, 2021.**

- High throughput approach technology for successful Hit generation in drug discovery.

59. **Biologics: Protein Alignments, Modeling and Docking, 15 June, 2021.**

- Virtual Workshop / Protein Alignments and Superposition / Loop and Linker Modeling / Homology Modeling / Protein- Protein Docking.

60. **The Application of Docking and Fragment Replacement to Structure-Based Drug Design, 16 June, 2021.**

- Webinar / Docking / Pharmacophore Modeling / Fragment-Based Design / Scaffold Replacement / Protein-Ligand Interaction Fingerprints (PLIF).

61. **In Silico Fragment-Based Drug Design: Approaches and Applications, 17 June, 2021.**

- Webinar / Scaffold Replacement / Fragment Linking / Ligand Growing / R-Group Screening / Medicinal Chemistry Transformations / Combinatorial Fragment Libraries / Pharmacophore Models / Fragment Databases.

62. **European Symposium on Organic Chemistry (ESOC 2021), Virtual Mini Symposium, 05 – 06 July, 2021.**

63. **Predicting CYP Selectivity, Reactivity, and Sites of Metabolism, 17 August, 2021.**

- Cytochrome P450 (CYP) / Oxidative Metabolism / Small Molecule Liabilities / Pharmacophore Modeling.

64. **Protein Engineering and Affinity Modeling, 18 August, 2021.**

- Protein Engineering / Protein Properties / Developability / Hot Spot Analysis.

65. **Kinase Protein Family Searching and Molecular Docking, 19 August, 2021.**

- Protein Family Databases / Database Mining / Protein Annotations / Pharmacophore Modeling / Docking / Protein-Ligand Interaction Fingerprints (PLIF) / MOE Project / Kinase Proteins.

66. **Structure Refinement Using Electron Density and Solvent Analysis, 31 August, 2021.**

- Structure Preparation / Sidechain Rotamer Exploration / Electron Density Maps / X-Ray / CryoEM / Solvent Analysis with 3D-RISM.

67. **Ligand-Based Drug Design and SAR Analysis, 01 September, 2021.**

- MOEsaic / R-Group Profiles and Analysis / MMP Analysis / Similarity and Substructure Searching / Descriptor Calculations / Conformational Searching / Molecular Alignments / Pharmacophore Modeling and Searching.

68. **Protein Alignments and Homology Modeling for Biologics, 02 September, 2021.**

- Alignments and Superposition / Loop and Linker Modeling / Homology Modeling.

69. **Receptor Pocket Similarity, 09 September, 2021.**

- Pocket Similarity / Pocket Search / Protein Families / Alpha Carbons / PLB score / Druggable Sites.

70. **High-Throughput Screening with MOE, 16 September, 2021.**

- Cloud / HPC / High-Throughput Screening / Large Scale Calculations / Protein Alignments and Superposition / Loop and Linker Modeling / Homology Modeling / Protein-Protein Docking / Small molecule Docking / Pharmacophore Modeling / Fragment-Based.

71. **EuroQSAR 2021 ‘’European Symposium on Quantitative Structure-Activity Relationship”, 22 September, 2021.**

- Virtual Screening Compound Libraries / Descriptors / QSAR / Drug Discovery.

72. **UGM & Conference 2021, 22 – 23 September, 2021.**

- MOE / Biological Therapeutics / Protein Modelling / Protein Engineering / Small Molecule / SBDD / LBDD / FBDD / Computational Chemistry / Medicinal Chemistry / Cheminformatics / Drug Discovery.

73. **Small Molecule Virtual Screening, 05 October, 2021.**

- Virtual Screening Compound Libraries / Descriptors, Fingerprints and QSPR Modeling / Pharmacophore Modeling / Template-based Docking / Compound Design.

74. **Antibody Modeling and Developability, 06 October, 2021.**

- Protein Annotation / Protein Patches / Virtual Mutagenesis / Antibody Homology Modeling / Protein Properties / Developability.

75. **PSILO, 07 October, 2021.**

- Macromolecular Repository / 3D Query Searching / Pocket Similarity / Display Electron Density / Central Repository / Specialized Protein Databases.

76. **2nd Symeres Precision Chemistry Conference '' Tools for Molecular Recognition and Diagnostics", 12 – 13 October, 2021.**

- Macromolecular Repository / Pocket Similarity / Display Electron Density / Central Repository / Virtual Mutagenesis.

77. **SPICA 2021 "The Importance of Chromatography in the Development of Vaccines", 14 October, 2021.**

- MOE databases / Virtual Mutagenesis / Antibody Homology Modeling / Protein Properties / Developability.

78. **Cheminformatics and QSAR, 19 October, 2021.**

- MOE databases / Calculated Descriptors / Fingerprints / QSAR Modeling / Binary QSAR / Similarity Searching / Consensus Modeling.

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82. **Protein-Protein Docking and Epitope Analysis, 03 November, 2021.**

- Protein-Protein Docking / Molecular Surfaces / Protein Patches / Interaction Fingerprints / Clustering / Epitope Analysis.

83. **Reverse Fingerprints IV: Application to Motif Detection and Pharmacophore Query Generation, 04 November, 2021.**

- Molecular Fingerprints / Structural Motif Detection / Pharmacophore Queries / Fingerprint Bit Visualization.

84. **Free Energy Calculations with Thermodynamic Integration in MOE using AMBER, 16 November, 2021.**

- Thermodynamic Integration / Free Energy Calculation / FEP / AMBER / Binding Affinity.

85. **Developability Assessment and Property Prediction by pH-Dependent Conformational Sampling, 17 November, 2021.**

- Antibody Modeling / Developability Assessment / Solubility and Aggregation Prediction / Titration, pI, and pKa Calculation.

86. **Modeling PROTAC-Mediated Targeted Protein Degradation: Case Studies and Recent Developments, 18 November, 2021.**

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87. **From Structure to Dynamics Simulation: Workflow for Preparing, Running and Visualizing MD Trajectories, 30 November, 2021.**

- Structure Preparation / Force Field / Solvation / AMBER / NAMD / Visualization / Player.

88. **MOEsaic: Mining Activity Data to Guide a Medicinal Chemistry Campaign, 01 December, 2021.**

- Activity Data Mining / SAR / Matched Molecular Pairs / R-group Analysis / R-group Profiling / Free-Wilson Analysis / Compound Suggestions.

89. **Protein Surface Charge and Hydrophobic Patch Analysis, 02 December, 2021.**

- Protein Patch Analysis / Protein Interaction Hot Spots / Antibodies and Related Derivatives / Interaction Sites / 2D Patch Depiction / Comparative Analysis / Key Active Regions.

90. **Structure-Based Molecular Transformations, 09 December, 2021.**

- Medicinal Chemistry Transformations / Bioisosteres / Lead Optimization / Ligand Ranking and Scoring / Structure-Based Design / Ligand Synthetic Accessibility.

91. **Introduction to PSILO, 25 January, 2022.**

- Macromolecular Repository / 3D Query Searching / Pocket Similarity / Display Electron Density / Central Repository / Specialized Protein Databases.

92. **Protein Alignments and Homology Modeling for Biologics, 26 January, 2022.**

- Alignments and Superposition / Loop and Linker Modeling / Homology Modeling.

93. **Fragment-Based Drug Design: Scaffold Replacement, Fragment Linking, R-Group Exploration and Bioisosteric Replacements, 27 January, 2022.**

- Scaffold Hopping / Fragment Linking / Ligand Growing / R-Group Screening / Medicinal Chemistry Transformations / Pharmacophores / Fragment Databases.

94. **Using Structures from Cryo Electron Microscopy for Drug Design, 03 February, 2022.**

- MOE / Cryo Electron Microscopy / Structure Preparation / Protonate3D / Electron Density / Protein Geometry.

95. **Structure-Based Molecular Transformations, 09 February, 2022.**

- Medicinal Chemistry Transformations / Bioisosteres / Lead Optimization / Ligand Ranking and Scoring / Structure-Based Design / Ligand Synthetic Accessibility.

96. **Template-Guided Docking of Small Molecules to Explore R-Group Substitutions, 10 February, 2022.**

- Docking / Template Setup / Sketcher Integration / SMARTS Matches / Wildcards / SAR Analysis / Kinase Database Mining / Structure Preparation / Pharmacophores.

97. **Modeling PROTAC-Mediated Targeted Protein Degradation: Case Studies and Recent Developments, 22 February, 2022.**

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99. **Protein Surface Charge and Hydrophobic Patch Analysis, 15 March, 2022.**

- Protein Patch Analysis / Protein Interaction Hot Spots / Antibodies and Related Derivatives / Interaction Sites / 2D Patch Depiction / Comparative Analysis / Key Active Regions.

100. Molecular Modeling in the Cloud: A Turnkey Solution for Scalable Simulations, 16 March, 2022.

- MOE / Molecular modeling / Cloud / PROTACs / Protein Degradation / Virtual Screening.

101. **MOEsaic: Mining Activity Data to Guide a Medicinal Chemistry Campaign, 17 March, 2022.**

- Activity Data Mining / SAR / Matched Molecular Pairs / R-group Analysis / R-group Profiling / Free-Wilson Analysis / Compound Suggestions.

102. **Antibody Modeling and Developability Assessment, 24 March, 2022.**

- Antibody Modeling / Developability / Liability / Aggregation.

103. **Kinase Protein Family Searching and Molecular Docking, 05 April, 2022.**

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104. **Reverse Fingerprints (IV): Application to Motif Detection and Pharmacophore Query Generation, 06 April, 2022.**

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105. **Easily Access, Analyze, and Manage AlphaFold Structures in PSILO, 07 April, 2022.**

- PSILO / AlphaFold Structures / Macromolecular Repository / Visualization / Pocket Similarity / Specialized Protein Databases.

106. **Fragment-Based Drug Design: Scaffold Replacement, Fragment Linking, R-Group Exploration and Bioisosteric Replacements, 19 April, 2022.**

- Scaffold Hopping / Fragment Linking / Ligand Growing / R-Group Screening / Medicinal Chemistry Transformations / Pharmacophores / Fragment Databases.

107. **Peptide Modeling and Docking, 20 April, 2022.**

- Structure Preparation / Protein-Peptide Interaction Analysis / Conformational Searching / Protein-Peptide Docking / Protein-Ligand Interaction Fingerprints.

108. **Molecular Visualization and Publication-Quality Graphics in MOE, 21 April, 2022.**

- Molecular Graphics / Visual Effects / Publication-Quality Images.

109. **Easily Access, Analyze, and Manage AlphaFold Structures in PSILO, 05 May, 2022.**

- PSILO / AlphaFold Structures / Macromolecular Repository / Visualization / Pocket Similarity / Specialized Protein Databases.

110. **Molecular Visualization and Publication-Quality Graphics in MOE, 18 August, 2022.**

- Molecular Graphics / Visual Effects / Publication-Quality Images.

111. **Database AutoPH4: Pharmacophore Analysis of Multiple Protein Structures, 31 August, 2022.**

- Automated Pharmacophore Generation / Binding Site Analysis / Protein Ensembles.

112. **New and Enhanced Features in MOE 2022.02, 14 September, 2022.**

- Combinatorial Library Enumeration / MOEsaic Docking Calculations / scFv and Custom Antibody Homology Models / GPU-Acceleration / Hydrogen Mass Repartitioning / Molecular Dynamics / Thermodynamic Integration / Database Viewer Enhancements.

113. **Antibody Modeling and Developability Assessment, 15 September, 2022.**

- Antibody Modeling / Developability / Liability / Aggregation.

114. **New and Enhanced Features in Biologics in MOE 2022.02, 29 September, 2022.**

- scFv and Custom Antibody Homology Models / GPU-Acceleration / Hydrogen Mass Repartitioning / Database Viewer Enhancements.

115. **Easily Access, Analyze, and Manage AlphaFold Structures in PSILO, 20 October, 2022.**

- PSILO / AlphaFold Structures / Macromolecular Repository / Pocket Similarity / Specialized Protein Databases / Visualization.

116. **MOE Database Viewer: Advanced Molecular and Data Visualization, 27 October, 2022.**

- Database Viewer / 2D, 3D, Carbohydrate and Sequence Displays / Plotting / Range and Rule-based Coloring / Images and Graphic Objects.

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