

Matthieu Montes, Professeur des Universités, CNAM

## Liste de publications

(en rouge : étudiants directement encadrés ou co-encadrés, \*contributions équivalentes)

### 1 Articles dans des revues et conférences internationales à comité de lecture

P48. Langenfeld F, Peng Y, Lai YK, Rosin PL, Aderinwale T, Terashi G, Christoffer C, Kihara D, Benhabiles H, Hammoudi K, Cabani A, Windal F, Melkemi M, Giachetti A, Mylonas S, Axenopoulos A, Daras P, Otu E, Zwiggelaar R, Hunter D, Liu H, Montes M. SHREC2020 track: Multi-domain protein shape retrieval challenge. *Computer & Graphics*, 2020, 91:189-198

P47. Bouchara T, Montes M. Immersive sonification of protein surfaces. 2020 IEEE Conference on Virtual Reality and 3D User Interfaces Abstracts and Workshops (VRW), 2020, 380-383

P46. Réau M, Lagarde N, Zagury JF, Montes M. Hits Discovery on the Androgen Receptor: In Silico Approaches to Identify Agonist Compounds. *Cells*. 2019 Nov 13;8(11) pii: E1431

P45. Dufies M, Grytsai O, Ronco C, Camara O, Ambrosetti D, Hagege A, Parola J, Mateo L, Ayrault M, Giuliano S, Grépin R, Lagarde N, Montes M, Auberger P, Demange L, Benhida R, Pagès G. New CXCR1/CXCR2 inhibitors represent an effective treatment for kidney or head and neck cancers sensitive or refractory to reference treatments. *Theranostics*, 2019, 9 (18):5332-5346

P44. Langenfeld F, Axenopoulos A, Benhabiles H, Daras P, Giachetti A, Han X, Hammoudi K, Kihara D, Lai T, Liu H, Melkemi M, Mylonas S, Terashi G, Wang Y, Windal F, Montes M. SHREC'19 Protein Shape Retrieval Contest. *Eurographics Workshop on 3D Objects Retrieval*, 2019; 25-31

P43. Réau M, Lagarde N, Zagury JF, Montes M. Nuclear Receptors DataBase Including Negative Data (NR-DBIND): A database dedicated to nuclear receptors binding data including negative data and pharmacological profile. *J Med Chem*, 2019, 62(6):2894-2904

P42. Langenfeld F, Axenopoulos A, Chtzifis A, Craciun D, Daras P, Du B, Giachetti A, Lai YK, Li H, Li Y, Masoumi M, Peng Y, Rosin PL, Sirugue J, Sun L, Thermos S, Toews M, Wei Y, Wu Y, Zhai Y, Zhao T, Zhen Y, Montes M. SHREC'18 – Protein Shape Retrieval. *Eurographics Workshop on 3D Objects Retrieval*, 2018; 53-61

P41. Rayar A, Lagarde N, Martin F, Blanchard F, Liagre B, Ferroud C, Zagury JF, Montes M, Sylla-Iyarreta Veitia M. New selective cyclooxygenase-2 inhibitors from cyclocoumarol: Synthesis, characterization, biological evaluation and molecular modeling. *Eur J Med Chem* 2018, 146:577-587

P40. Réau M, Langenfeld F, Zagury JF, Lagarde N, Montes M. Decoys Selection in Benchmarking Databases. *Frontiers in Pharmacol*, 2018; 9,11

P39. Liu WQ, Lepelletier Y, Montes M, Borriello L, Jarray R, Grepin R, Leforban B, Loukaci A, Benhida R, Hermine O, Dufour S, Pages G, Garbay C, Raynaud F, Hadj-Slimane R, Demange L. NRPa-308, a new neuropilin-1 antagonist, exerts in vitro anti-angiogenic and anti-proliferative effects and in vivo anti-cancer effects in a mouse xenograft model. *Cancer Lett*, 2018; 414, 88-98

P38. Réau M, Langenfeld F, Zagury JF, Montes M. Predicting the affinity of Farnesoid X Receptor ligands through a hierarchical ranking protocol: a D3R Grand Challenge 2 case study. *J Comput Aided Mol Des*, 2017, 1-8

P37. Rayar A, Lagarde N, Ferroud C, Zagury JF, Montes M, Sylla-Iyarreta Veitia M. Update on COX-2 selective inhibitors: chemical classification, side effects and their use in cancers and neuronal diseases. *Curr Top Med Chem*, 2017; 17(26), 2935-2956

P36. Craciun D, Sirugue J, Montes M, Global-to-Local Protein Shape Similarity System driven by Digital Elevation Models, *IEEE Biosmart*, 2017

P35. Lagarde N, Delahaye S, Jérémie A, Ben Nasr N, Guillemain H, Empereur-mot C, Laville V, Labib T, Réau M,

Matthieu Montes, Professeur des Universités, CNAM

Langenfeld F, Zagury JF, Montes M. Discriminating agonist from antagonist ligands of the nuclear receptors using different chemoinformatics approaches. *Mol Inf*, 2017; 36 (10)

P34. Mouhsine H, Guillemain H, Moreau G, Fourati N, Zerrouki C, Baron B, Desallais L, Gizzi P, Ben Nasr N, Perrier J, Ratsimandresy R, Spadoni JL, Do H, England P, Montes M\*, Zagury JF\*. Identification of an in vivo orally active dual-binding protein-protein interaction inhibitor targeting TNF $\alpha$  through combined in silico/in vitro/in vivo screening. *Sci Rep*, 2017; 7(1), 3424

P33. Craciun D, Levieux G, Montes M. Shape Similarity System driven by Digital Elevation Models for Non-Rigid Shape Retrieval. *Eurographics Workshop on 3D Object Retrieval*, 2017.

P32. Song N, Craciun D, Christoffer CW, Han X, Kihara D, Levieux G, Montes M, Qin H, Sahu P, Terashi T, Liu H. SHREC 2017 – Classification of Protein Shapes. *Eurographics Workshop on 3D Object Retrieval*, 2017

P31. Empereur-mot C, Zagury JF, Montes M. Screening Explorer – An interactive tool for the analysis of screening results. *J Chem Inf Model*. 2016; 56(12): 2281-2286

P30. Moreau G, Fourati N, Zerrouki C, Mouhsine H, Montes M, Port M, Sylla-Iyarreta M, Zagury JF, Yaakoubi N. Surface acoustic wave biosensors for the quantification of the TNF $\alpha$ /SPD-304 interaction. *30th Eurosensors Conference, Procedia Engineering* 2016; 168:432-435

P29. Lagarde N, Delahaye S, Zagury JF, Montes M. Discriminating agonist and antagonist ligands of the nuclear receptors using 3D-pharmacophores. *J. Cheminform* 2016, 8(1):43

P28. Desallais L, Bouchez C, Mouhsine H, Moreau G, Ratsimandresy R, Montes M, Do H, Quintin-Colonna F, Zagury JF. Immunization against an IL-6 peptide induces anti-L-6 antibodies and modulates the Delayed-Type Hypersensitivity reaction in cynomolgus monkeys. *Scientific Reports*. 2016, 6:19549

P27. Empereur-Mot C, Guillemain H, Latouche A, Zagury JF, Viallon V, Montes M. Predictiveness curves in virtual screening. *J Cheminform* 2015, 7:52

P26. Spadoni JL, Rucart P, Le Clerc S, van Manen D, Coulonges C, Ulveling D, Laville V, Labib T, Taing L, Delaneau, Montes M, Schuitemaker H, Noirel J, Zagury JF. Identification of Genes Whose Expression Profile Is Associated with Non-Progression towards AIDS Using eQTLs.. *Plos One* 2015; 10(9):e0136989.

P25. Lagarde N, Zagury JF, Montes M. Benchmarking datasets for the evaluation of virtual ligand screening methods: review and perspectives. *J Chem Inf Model*. 2015, 55 (7): 1297–1307

P24. Levieux, G.; Montes, M., "Towards real-time interactive visualization modes of molecular surfaces: examples with Udock," *Virtual and Augmented Reality for Molecular Science (VARMS@IEEEVR)*, 2015:19-23

P23. Lagarde N, Zagury JF, Montes M. Importance of the pharmacological profile of the bound-ligand in enrichment: Towards the use of decoy ligands. *J Chem Inf Model*. 2014, 54 (10): 2915–2944

P22. Liu WQ, Meggale V, Borriello L, Leforban B, Montes M, Goldwasser E, Gresh N, Piquemal JP, Hadj-Slimane R, Hermine O, Garbay C, Raynaud F, Lepelletier Y, Demange L. Synthesis and structure-activity relationship of non-peptidic antagonists of Neuropilin-1 receptor. *Bioorg Med Chem Lett* 2014, 24, 4254-4259

P21. Le Clerc S, Delaneau O, Coulonges C, Spadoni JL, Labib T, Laville V, Ulveling D, Noirel J, Montes M, Schächter F, Caillat-Zucman S, Zagury JF. Evidence for a Role of Mica Variants in non Progression and Elite Control in AIDS After Imputation. *J Infect Dis* 2014; 210(12):1946-1950

P20. Desallais L, Avouac J, Fréchet M, Elhai M, Ratsimandresy R, Montes M, Mouhsine H, Do H, Zagury JF, Allanore Y. Targeting IL-6 by both passive or active immunization strategies prevents bleomycin-induced skin fibrosis. *Arthritis Research & Therapy*. 2014; 16:R157.

Matthieu Montes, Professeur des Universités, CNAM

- P19. Borriello L, Montes M, Lepelletier Y, Leforban B, Liu WQ, Demange L, Delhomme B, Pavoni S, Jarray R, Boucher JL, Dufour S, Hermine O, Garbay C, Hadj-Slimane R, Raynaud F. Structure-Based Discovery of a Small non-peptidic Neuropilins antagonist exerting in vitro and in vivo Anti-Tumor Activity on breast cancer model. *Cancer Lett.* 2014; 349(2):120-127
- P18. Lagarde N, Ben Nasr N, Jeremie A, Guillemain H, Laville V, Labib T, Zagury JF, Montes M. NRLiSt BDB, the manually curated nuclear receptors Ligands and Structures benchmarking database. *J Med Chem* 2014, Mar 17; 57(7):3117-3125
- P17. Leveux G, Tiger G, Natkin S, Zagury JF, Montes M. FD169: UDock, the protein docking entertainment system. *Faraday Discuss.* 2014, 169 (1): 425-441
- P16. Maréchal X, Genin E, Qin L, Sperandio O, Montes M, Basse N, Richey N, Miteva MA, Reboud-Ravaux M, Vidal J, Villoutreix BO. 1,2,4-Oxadiazoles Identified by Virtual Screening and their Non-covalent inhibition of the Human 20S Proteasome. *Curr Med Chem* 2013; 20(18):2351-2362
- P15. Ben Nasr N\*, Guillemain H\*, Lagarde N\*, Zagury JF, Montes M. Multiple structures for Virtual Ligand Screening: defining binding site properties-based criteria to optimize the selection of the query. *J Chem Inf Model.* 2013 Feb 25; 53(2):293-311
- P14. Limou S, Delaneau O, van Manen D, An P, Sezgin E, Le Clerc S, Coulonges C, Troyer JL, Veldink JH, van den Berg LH, Spadoni JL, Taing L, Labib T, Montes M, Delfraissy JF, Schachter F, O'Brien SJ, Buchbinder S, van Natta ML, Jabs DA, Froguel P, Schuitemaker H, Winkler CA, Zagury JF. Multicohort genome-wide association study reveals a new signal of protection against HIV-1 acquisition. *J Infect Dis.* 2012 Apr 1; 205(7):1155-62.
- P13. Le Clerc S, Coulonges C, Delaneau O, Van Manen D, Herbeck JT, Limou S, An P, Martinson JJ, Spadoni JL, Therwath A, Veldink JH, van den Berg LH, Taing L, Labib T, Mellak S, Montes M, Delfraissy JF, Schächter F, Winkler C, Froguel P, Mullins JI, Schuitemaker H, Zagury JF. Screening Low Frequency SNPs From Genome Wide Association Study Reveals A New Risk Allele for Progression to Aids. *J Acquir Immune Defic Syndr.* 2011 Mar 1; 56(3):279-284.
- P12. Giganti D\*, Guillemain H\*, Spadoni JL, Nilges M, Zagury JF, Montes M. Comparative evaluation of 3D-virtual screening methods: impact of molecular alignment on enrichment. *J Chem Inf Model* 2010, Jun 28; 50(6):992-1004.
- P11. Limou S, Coulonges C, Herbeck J, Van Manen D, Ping An, Le Clerc S, Delaneau O, Diop G, Taing L, Montes M, Spadoni JL, Labib T, Therwath A, Rouzioux C, Delfraissy JF, Lelièvre JD, Lévy Y, Hercberg S, Dina C, Phair J, Donfield S, Goedert J, Schächter FS, Gut I, Froguel P, Mullins J, Winkler C, Zagury JF. Multi-cohort genetic association study reveals CXCR6 as a new chemokine receptor involved in AIDS long-term non-progression. *J Infect Dis* 2010, Sep 15; 202(6):908-15
- P10. Basse N, Montes M, Marechal X, Qin L, Bouvier-Durand M, Genin E, Vidal J, Villoutreix BO, Reboud-Ravaux M. Novel Organic Proteasome Inhibitors Identified by Virtual and in Vitro Screening. *J Med Chem* 2010, Jan 14; 53(1):509-13
- P9. Le Clerc S, Limou S, Coulonges C, Carpentier W, Dina C, Taing L, Delaneau O, Labib T, Sladek R, ANRS Genomic Group, Deveau C, Guillemain H, Ratsimandresy R, Montes M, Spadoni JL, Lelièvre JD, Lévy Y, Therwath A, Schächter F, Matsuda F, Gut I, Froguel P, Delfraissy JF, Hercberg S, Zagury JF, Genome-Wide Association Study Identifies New Susceptibility Alleles for AIDS Progression (ANRS Genomewide Association Study 03), *J Infect Dis* 2009, Oct 15; 200(8):1194-201
- P8. Limou S, Le Clerc S, Coulonges C, Carpentier W, Dina C, Delaneau O, Labib T, Taing L, Sladek R; ANRS Genomic Group, Deveau C, Ratsimandresy R, Montes M, Spadoni JL, Lelièvre JD, Lévy Y, Therwath A, Schächter F, Matsuda F, Gut I, Froguel P, Delfraissy JF, Hercberg S, Zagury JF. Genomewide Association Study of an AIDS-Nonprogression Cohort Emphasizes the Role Played by HLA Genes (ANRS Genomewide Association Study 02), *J Infect Dis* 2009, Feb 1; 199(3):419-26

Matthieu Montes, Professeur des Universités, CNAM

P7. Hennebert O, Montes M, Favre-Reguillon A, Chermette H, Ferroud C, Morfin R. Steroid substrate-induced epimerase mechanism in the active site of the human 11  $\beta$  Hydroxysteroid dehydrogenase type 1, *J Steroid Biochem Mol Biol* 2009, Mar; 114(1-2):57-63

P6. Montes M\*, Braud E\*, Miteva M, Goddard ML, Mondesert O, Kolb S, Brun MP, Ducommun B, Garbay C, Villoutreix BO. Receptor-based virtual ligand screening for the identification of novel CDC25 phosphatase inhibitors, *J Chem Inf Model* 2008, Jan; 48(1):157-65

P5. Villoutreix BO, Renault N, Lagorce D, Sperandio O, Montes M, Miteva MA. Free Resources to assist Structure-Based virtual ligand screening experiments, *Curr Prot Pept Sci* 2007, Aug; 8(4):381-411

P4. Montes M, Miteva MA, Villoutreix BO. Structure-Based virtual ligand screening with LigandFit, pose prediction and enrichment of compound collections, *Proteins* 2007, 68:712-25

P3. Miteva MA, Violas S, Montes M, Gomez D, Tuffery P, Villoutreix BO. FAF-Drugs : Free ADME-Tox Filtering of compound collections. *Nucleic Acids Res* 2006, 34:738-44

P2. Miteva MA\*, Lee WH\*, Montes MO, Villoutreix BO. Fast Structure-Based virtual ligand screening combining FRED, DOCK and Surflex. *J Med Chem* 2005, 48:6012-22

P1. Brun MP, Braud E, Angotti D, Mondesert O, Quaranta M, Montes M, Miteva MA, Gresh N, Ducommun B, Garbay C. Design, synthesis and biological evaluation of novel naphthoquinone derivatives with CDC25 phosphatase inhibitory activity. *Bioorg Med Chem* 2005, Aug 15; 13(16):4871-79

## 2 Chapitres d'ouvrages collectifs

C3. Montes M, Zagury JF. *La bioinformatique, Panorama de la virologie* (2013), Belin Sup Sciences, ISBN 978-2-7011-5884-6

C2. Montes M. *Designing Protein-Protein Interaction Inhibitors, Computational Protein-Protein Interactions* (2009), Taylor&Francis, CRC Press, ISBN:978-1-4200-7005-7

C1. Autin L\*, Montes M\*, Miteva MA, Villoutreix BO. Computer tools to study intermolecular interactions, *Recent Research Developments in Protein Engineering, Vol2* (2007) Part I, ISBN:978-81-308-0208-4

## 3 Brevets

B7. Rignault R, Montes M, Raynaud F, Demange L, Hermine O, Lepelletier Y. A Neupilin antagonist in combination with a P38-alpha kinase inhibitor for the treatment of cancer. EP19305719.7

B6. Belaid-Choukair Z, Montes M, Hermine O. Agents capable of inhibiting the binding between leptin and VEGF165. EP15306490

B5. Belaid-Choukair Z, Montes M, Hermine O. Agents capable of inhibiting the binding between leptin and neupilin-1. EP15306471

B4. Montes M, Desallais L, Zagury JF. Traitement de pathologies liées à un effet excessif de l'IL-6 par immunisation active WO2013021284A2

B3. Montes M, Mouhsine H, Guillemain H, Zagury JF. Traitement d'une pathologie liée à un effet excessif du TNF par un composé de benzene-sulfonamide, FR1055867 ; WO2012017166

B2. Montes M, Basse N, Marechal X, Vidal J, Reboud-Ravaux M, Villoutreix BO. Piperazine derivatives as proteasome modulators, EP08305378.5, WO2010001365A1

Matthieu Montes, Professeur des Universités, CNAM

B1. Montes M, Basse N, Marechal X, Vidal J, Reboud-Ravaux M, Villoutreix BO. Nitrogen heterocycle derivatives as proteasome modulators, EP08305377.7, WO2010001366A1

#### 4. Banques et logiciels

BL1. UDock, voir publication P17. <http://udock.fr>

BL2. NRLiSt BDB, voir publication P18. <http://nrlist.drugdesign.fr>

BL3. Screening Explorer, voir publication P31. <http://stats.drugdesign.fr>

BL4. NR-DBIND, voir publication P43. <http://nr-dbind.drugdesign.fr>

BL5. VTX. <http://vtx.drugdesign.fr>