

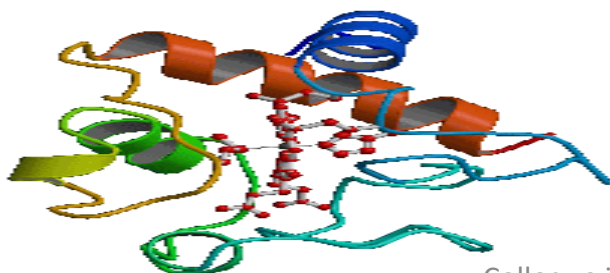
Colloque international #ComoresTice 4. L'Afrique francophone : la recherche comme levier d'un développement effectif des secteurs de l'éducation, de la santé et de l'économie verte

Les NTIC pilotées par l'intelligence artificielle au service de la santé : de l'innovation pédagogique à la découverte de médicaments candidats contre les maladies chroniques

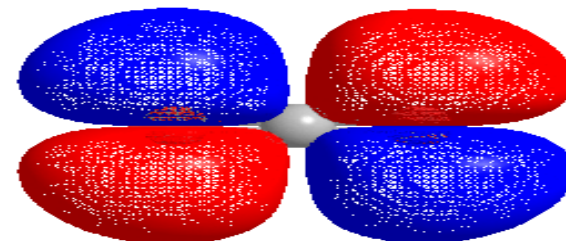
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Présentée par : Pr Said El Rhabori





- **Introduction et Problématique**

- **Matériels & Méthodes**

- **Résultats & Discussion**

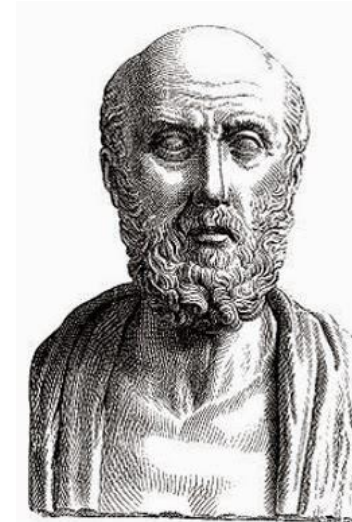
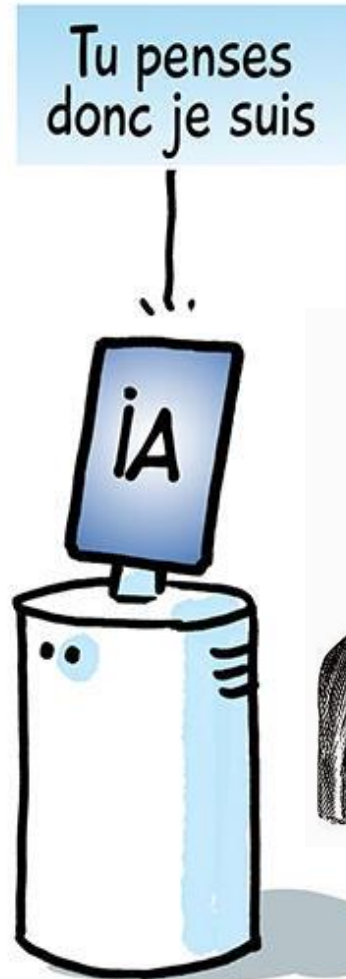
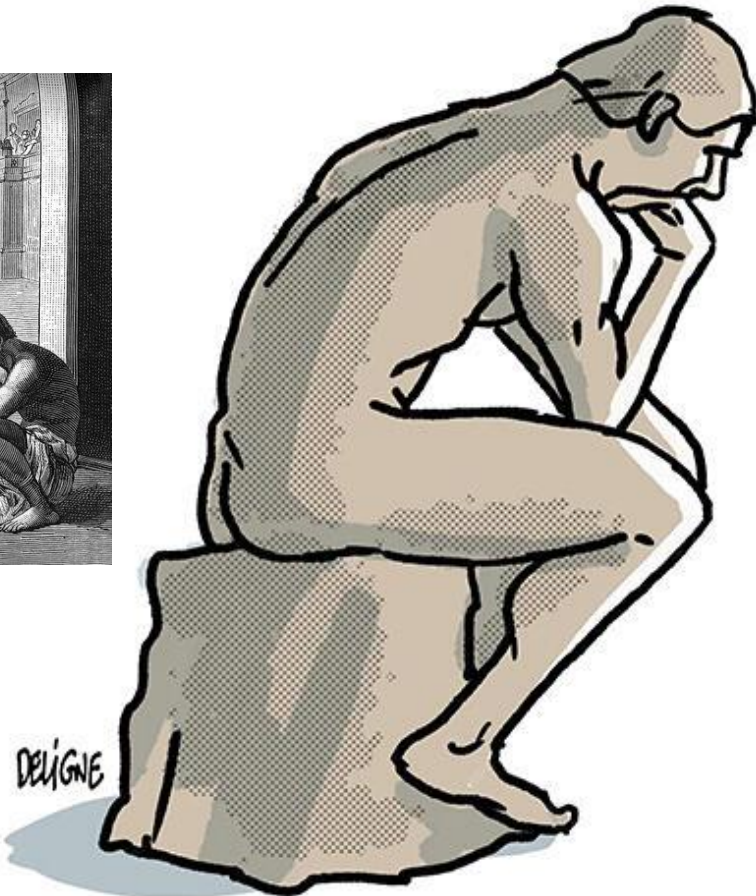
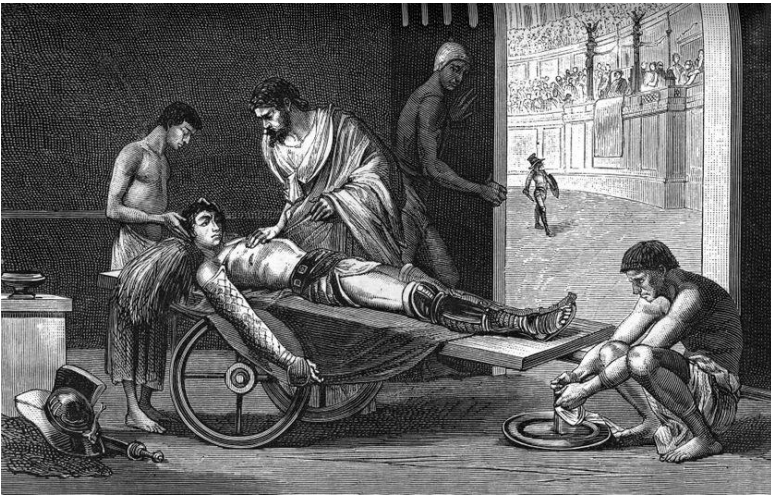
- **Conclusion générale &
Perspectives**



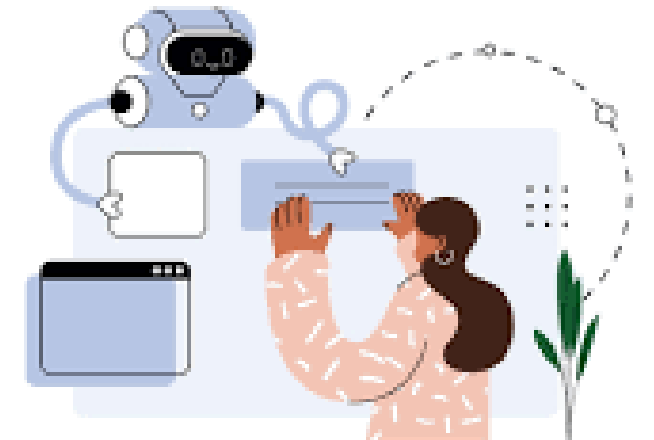
Introduction & Problématique

Introduction & problématique

□ Souffrance cognitive : La recherche pré-IA



❑ De l'Innovation Pédagogique à l'Impact Sanitaire (Découverte Thérapeutique)

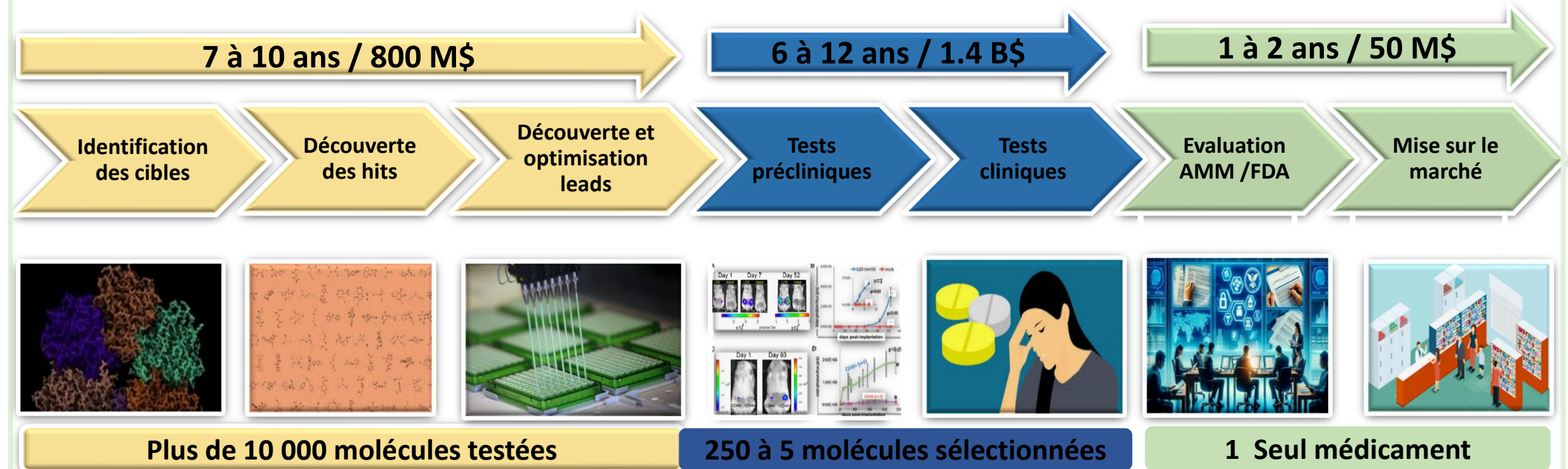


Colloque international #ComoresTice 4/16 et 17 octobre 2026/Université Sorbonne

Introduction et problématique

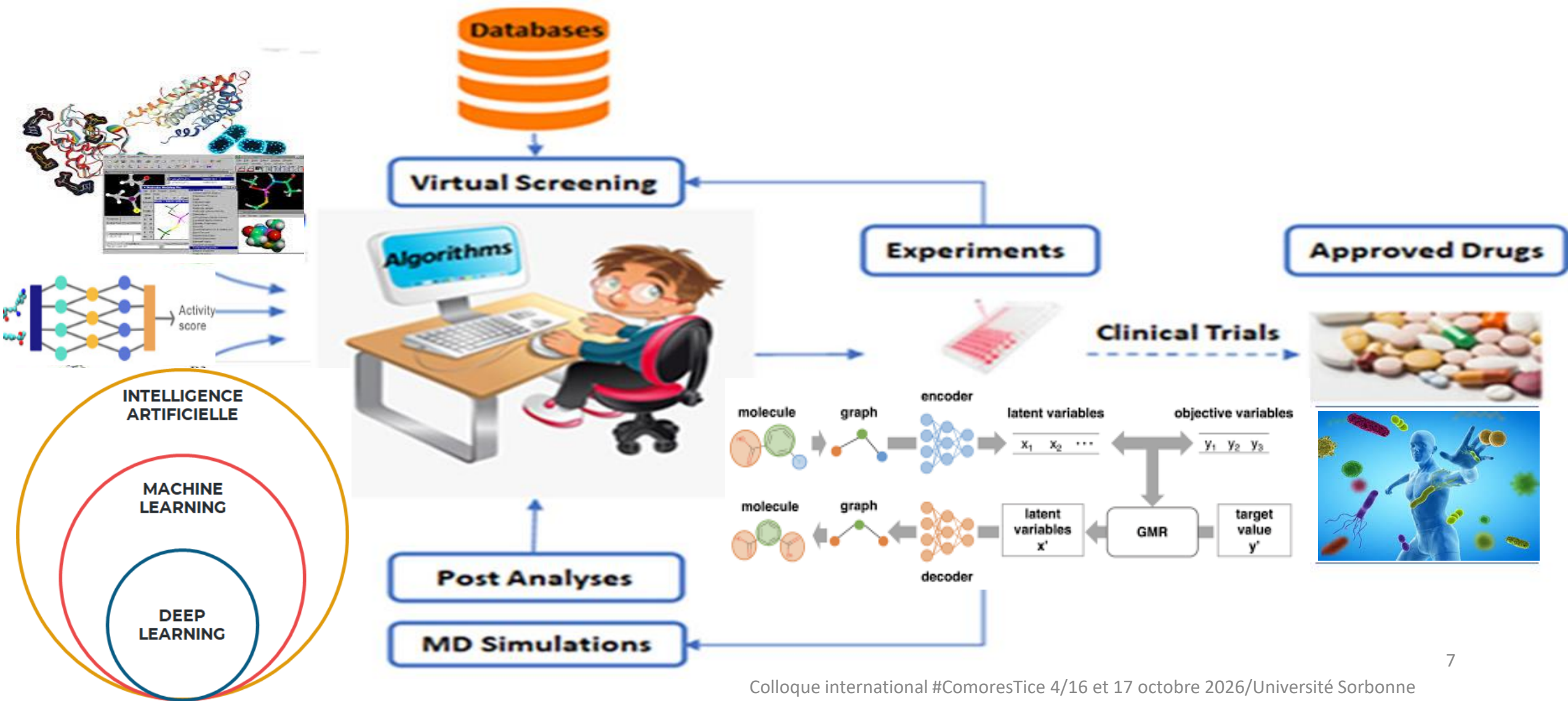
❑ Développement de nouveaux médicaments

❖ Coût du processus



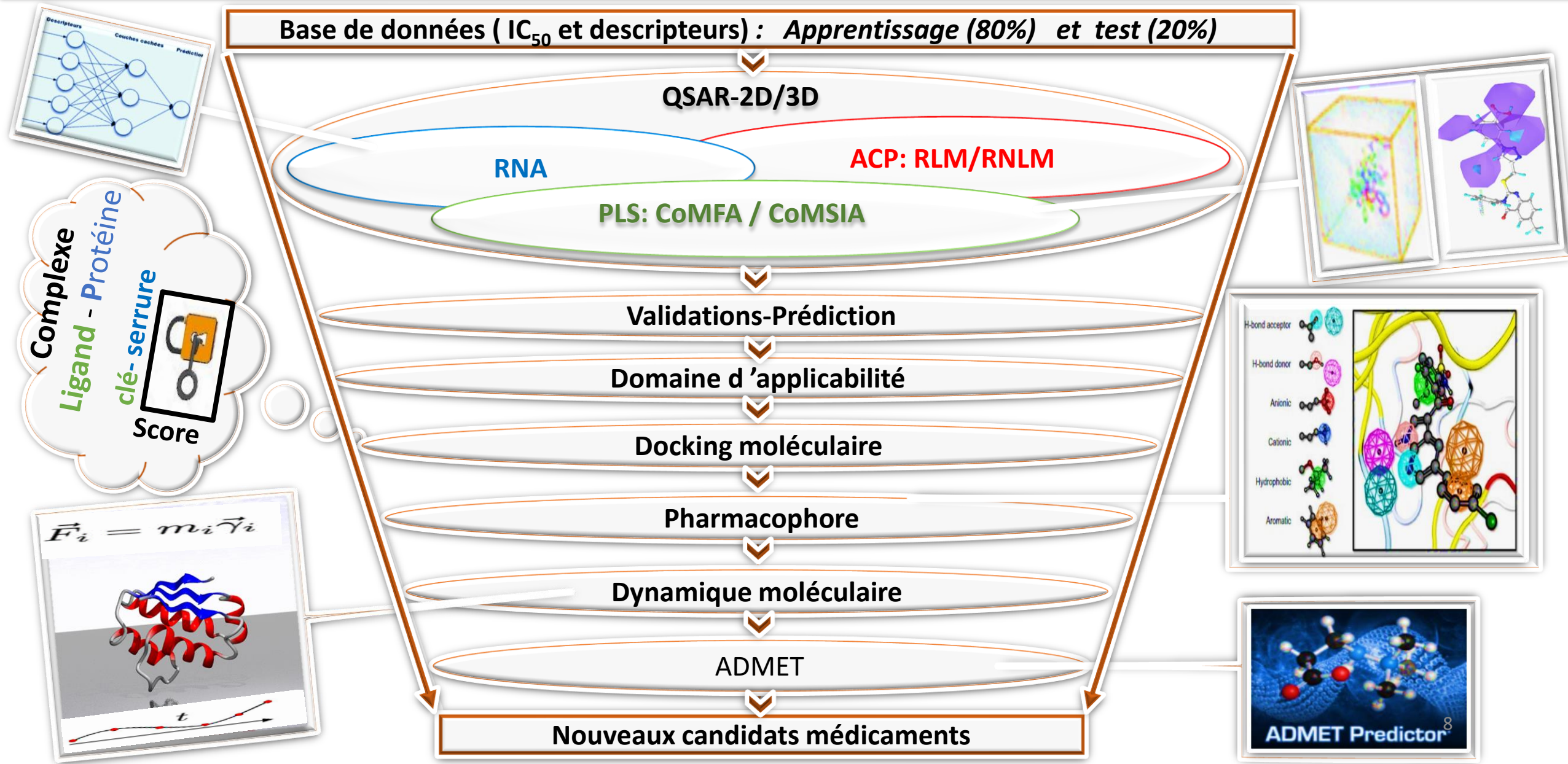
Introduction & problématique

IA - Découverte de médicaments (in silico)



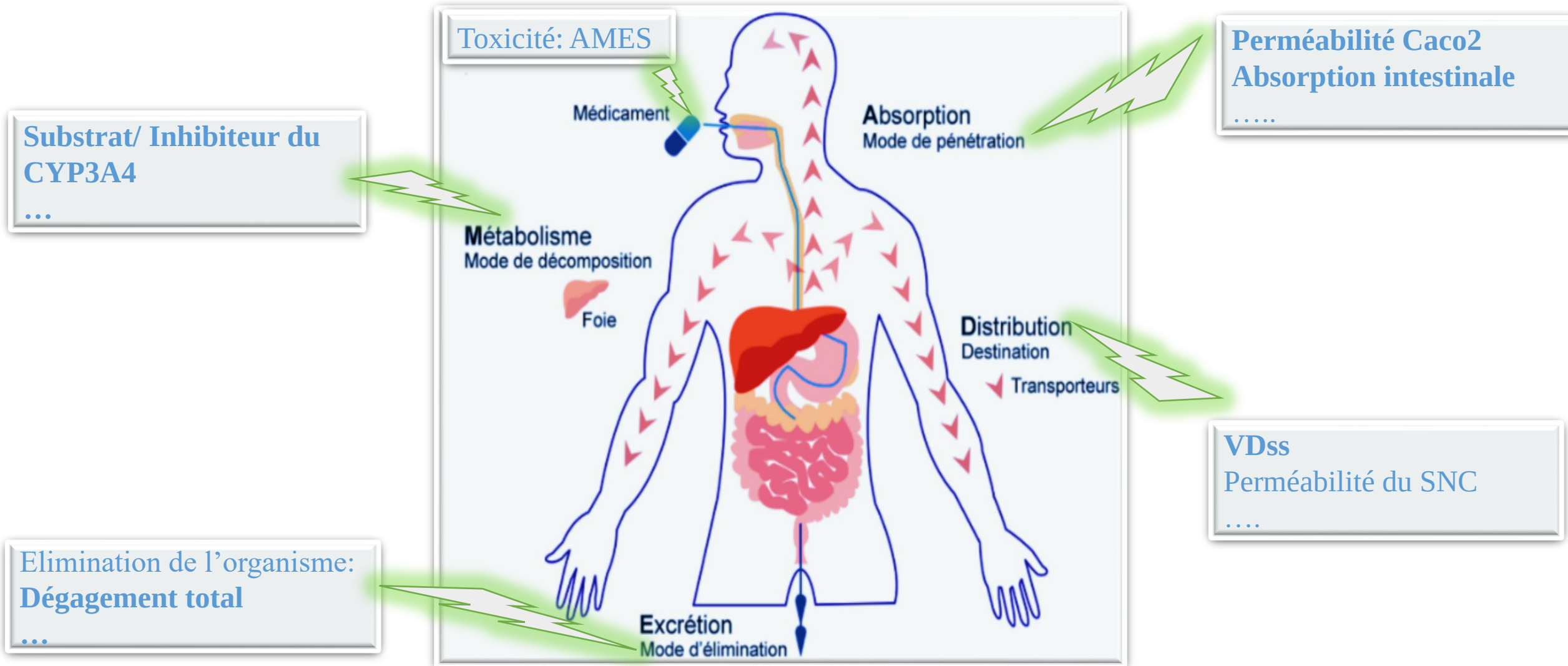
Méthodologie

❑ Combinaison de la LBDD et la SBDD :



Méthodologie

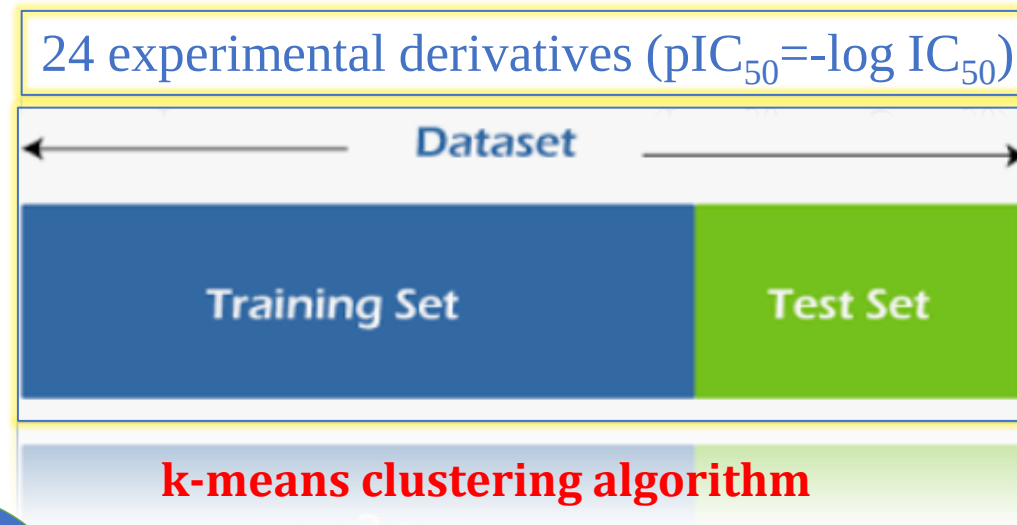
❑ Propriétés pharmacocinétiques d'un médicament :



Résultats et discussion

Résultats & Discussion

Collecte/division de l'ensemble de données



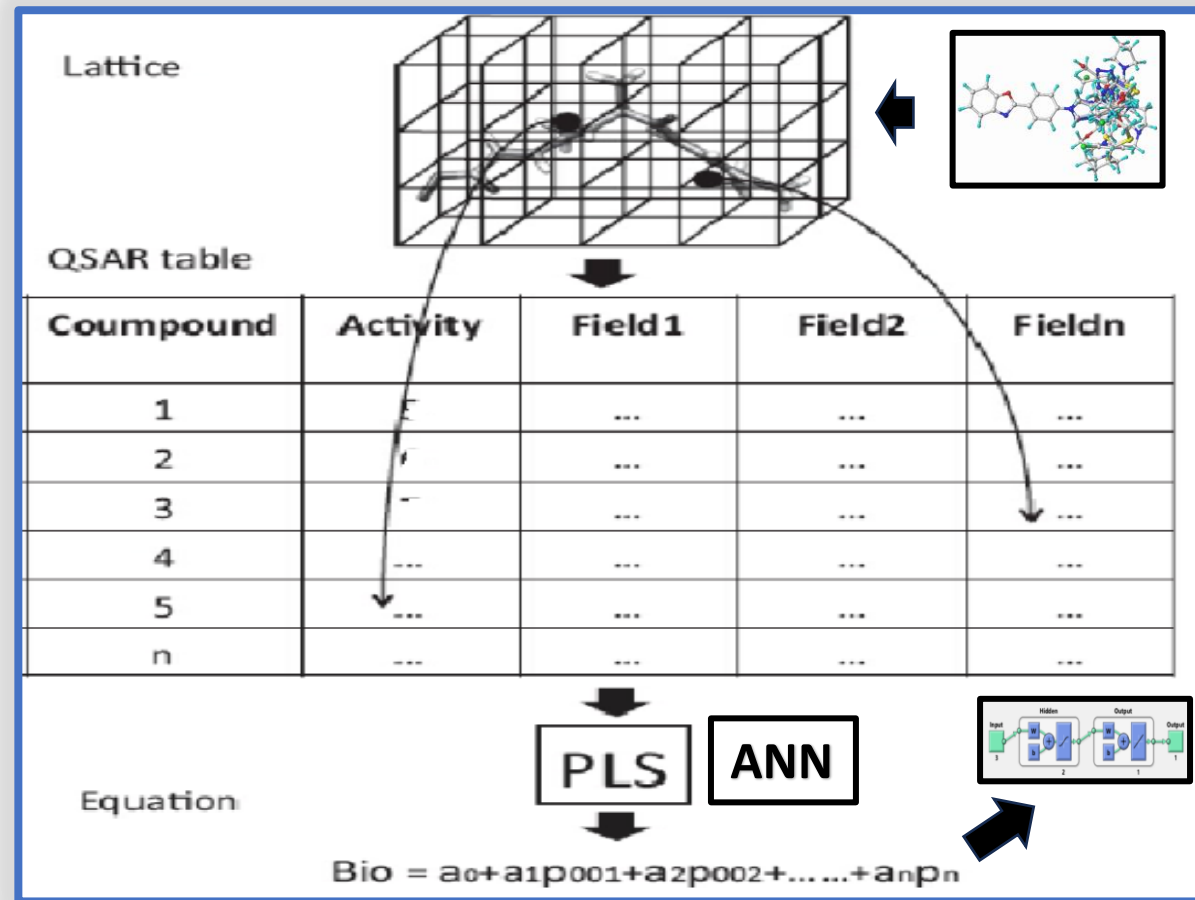
17 compounds
(Predictive Model)

7 compounds
(Validation)

Résultats & Discussion

Modèles basés sur l'apprentissage automatique / Profond

Alignement des molécules – PLS



Validation du modèle CoMSIA / SEA

Fields (SEA)	Fraction
Steric	0.072
Electrostatic	0.410
HB Acceptor	0.519

Statistical parameters :

- $Q^2 = 0.71$; $R^2 = 0.95$;
- $N = 3$; $SEE = 0.19$;
- $F\text{-test} = 36.08$; $p\text{-value} < 0.05$
- $R^2_{pred} = 0.92$.

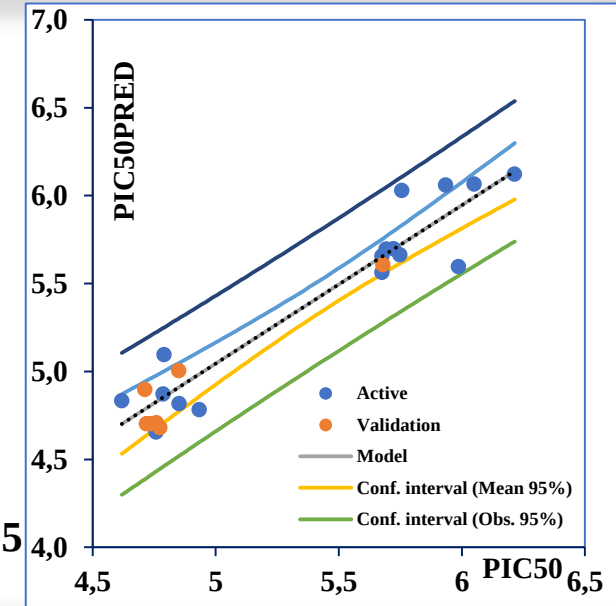


Figure 1. Alignment of compounds, PLS and ANN for Comparative Molecular Similarity Index Analysis (CoMSIA) Models

Résultats & Discussion

Domaine d'applicabilité utilisant "Open Genetic Algorithm Toolbox"

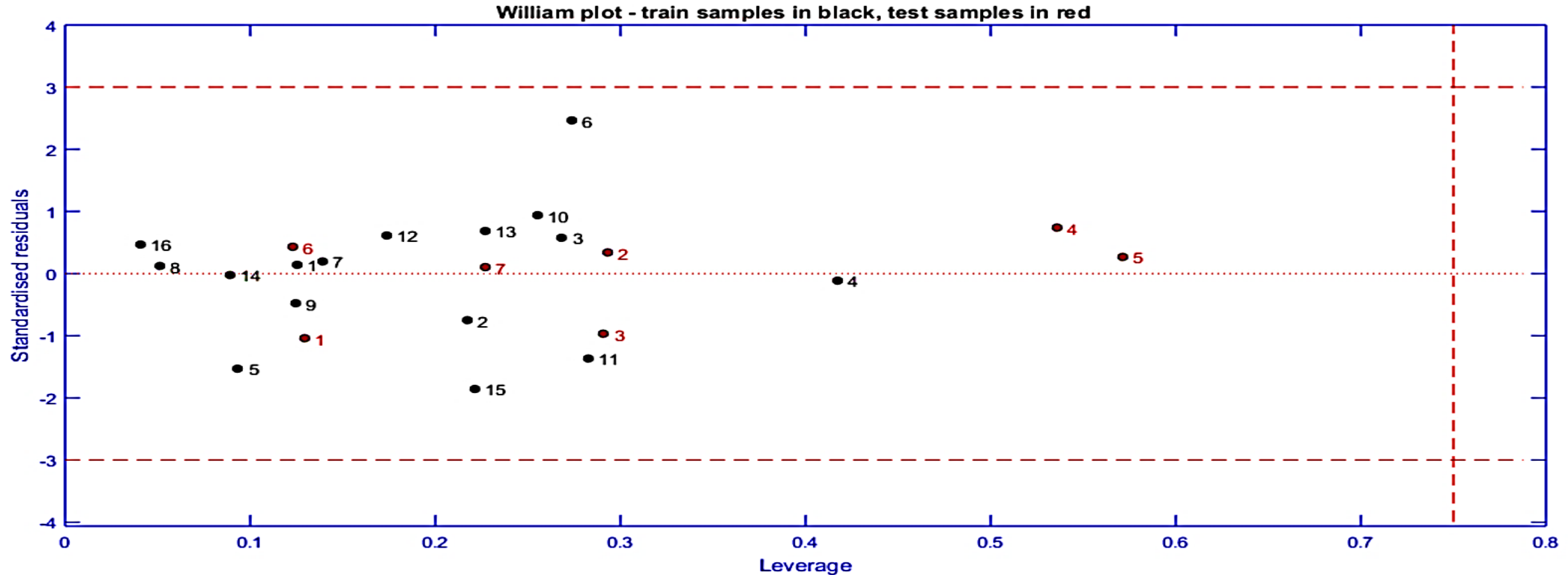


Figure.2: William's plot the CoMSIA (SEA) model ($h^* = 0.750$)

Résultats & Discussion

Prédiction de champs à l'aide d'un algorithme d'isocontours :

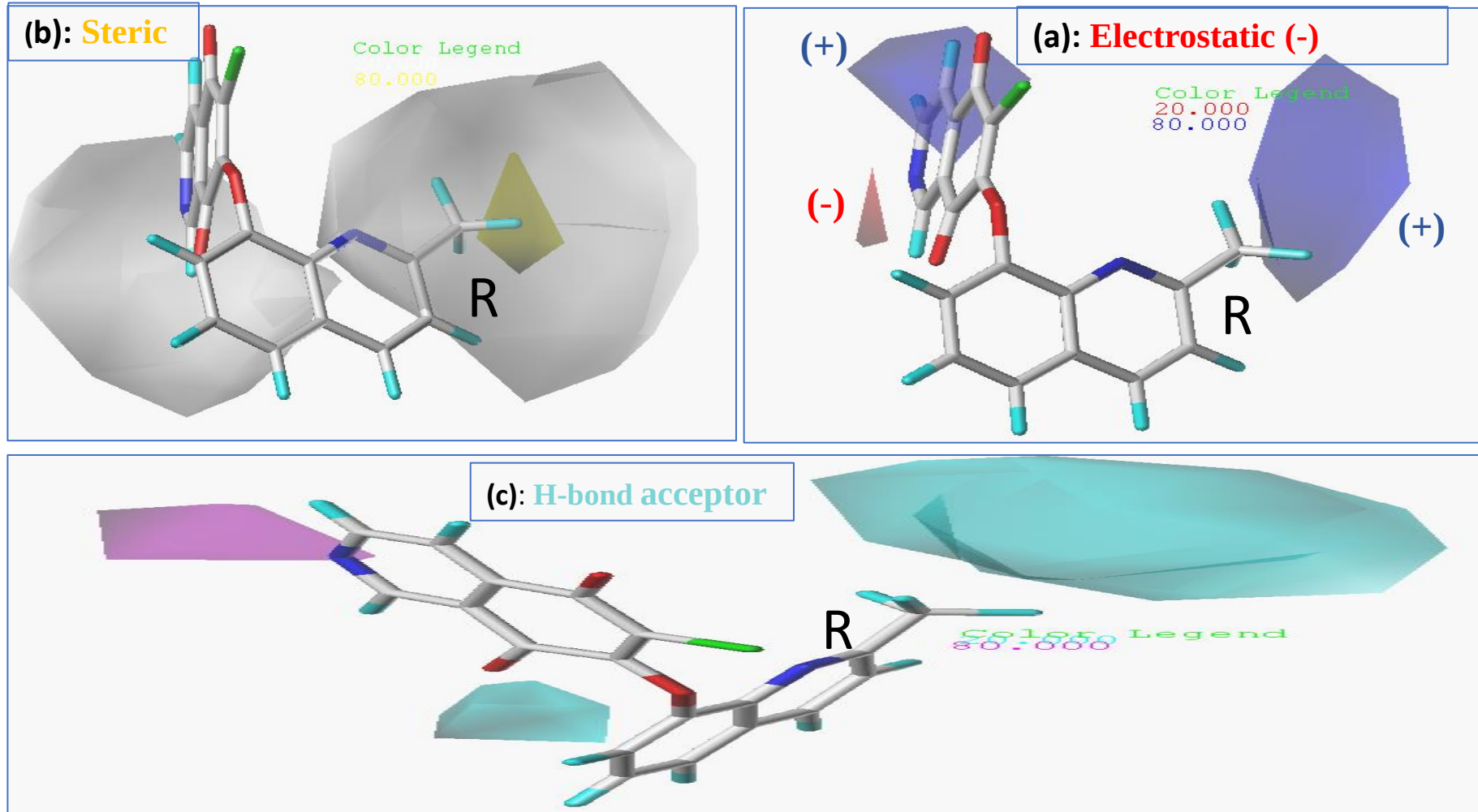
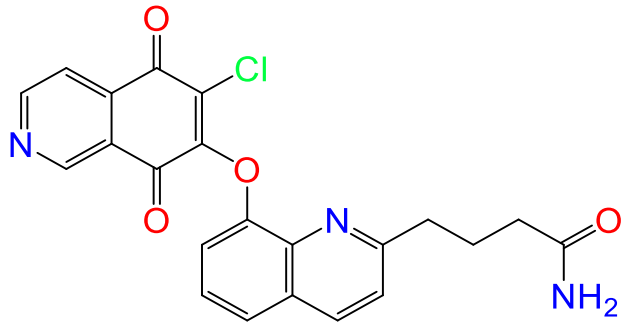


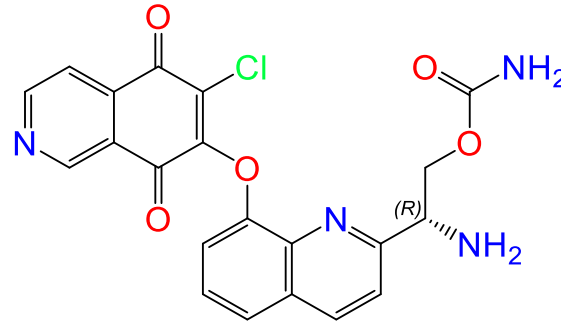
Figure 3. Contour maps of CoMSIA analysis of the most active molecule

Résultats & Discussion

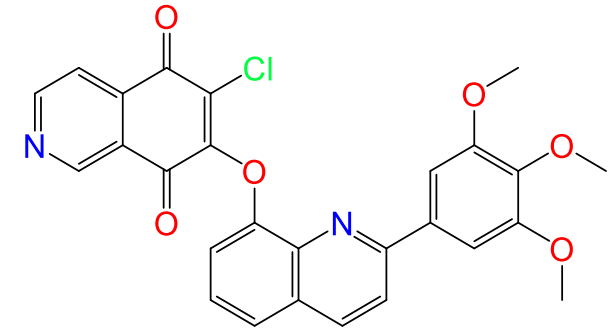
Prédiction de nouveaux candidats médicaments



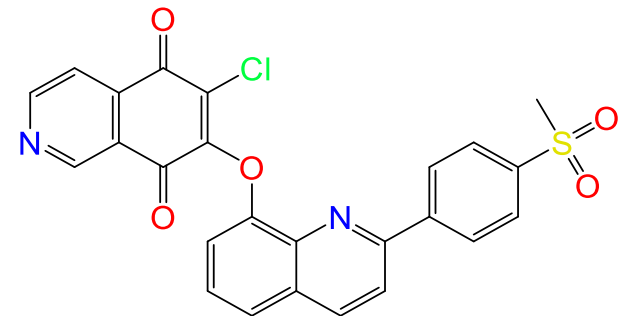
Ligand 1 (pIC_{50} = 6.231) / No toxic



Ligand 2 (pIC_{50} = 6.245) / No toxic

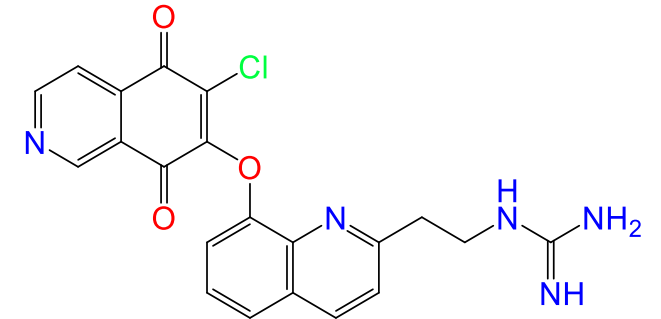


Ligand 3 (pIC_{50} = 6.111) / No toxic



Ligand 4 (pIC_{50} = 6.092) / No toxic

Name	h_i	Comments on the AD	Lipinski validation	SA
Ligand1	0.138	Inside (h_1 less than h^*)	Yes	3.380
Ligand2	0.116	Inside (h_2 less than h^*)	Yes	3.960
Ligand3	2.065	Outside (h_3 more than h^*)	Yes	3.840
Ligand4	1.054	Outside (h_4 more than h^*)	Yes	3.580
Ligand5	0.415	Inside (h_5 less than h^*)	Yes	3.440

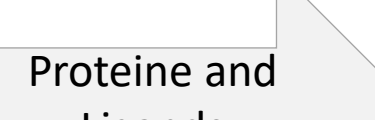


Ligand 5 (pIC_{50} = 6.700) / No toxic

Figure 4. Chemical structures of novel designed molecules and their best pIC_{50} values

Prédiction d'interactions par des algorithmes d'amarrage moléculaire

Figure 5. 3D interactions of complex 3S7S- exemestane (co-ligand)



Proteine and
Ligands
preparation

Figure 6. Re-docking results With RMSD=0.26 A°(co- ligand =green and docked ligand=red)

Step 3 : Docking of the most and least active molecules

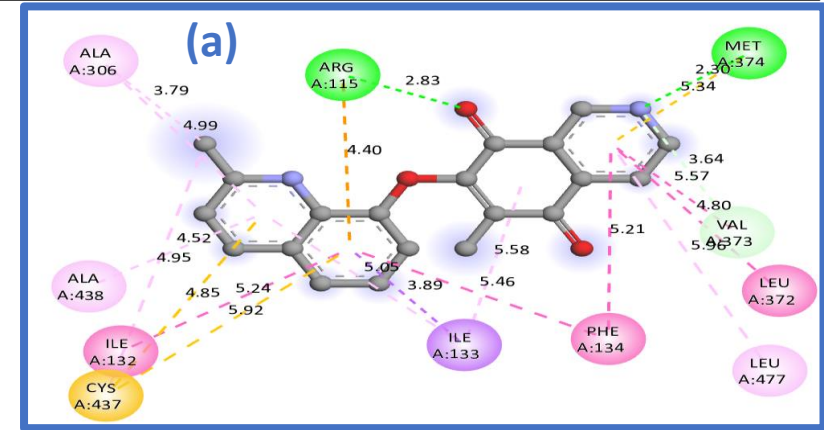
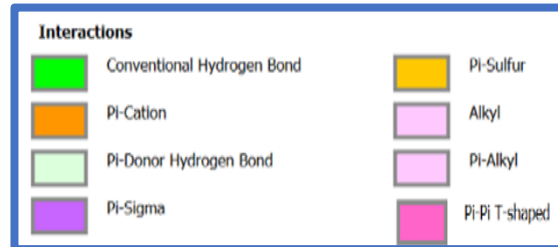
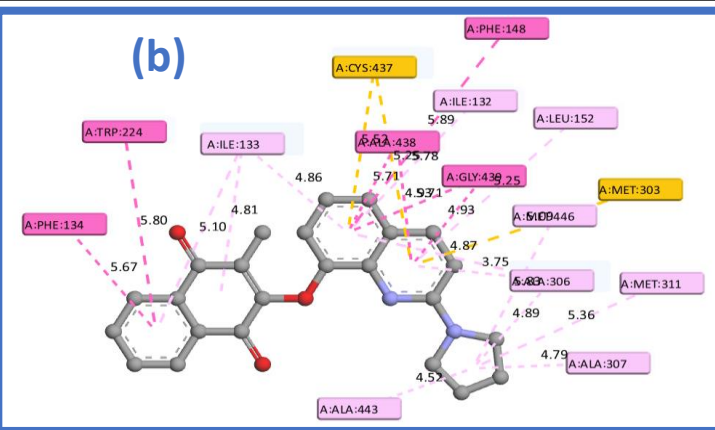
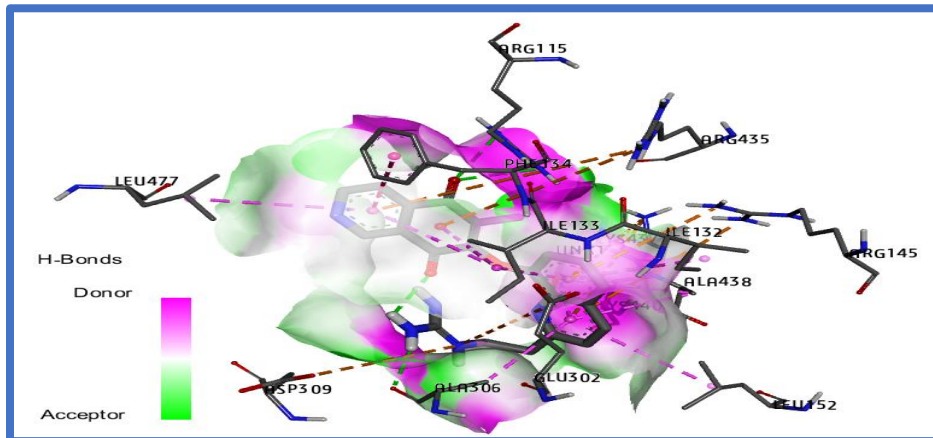


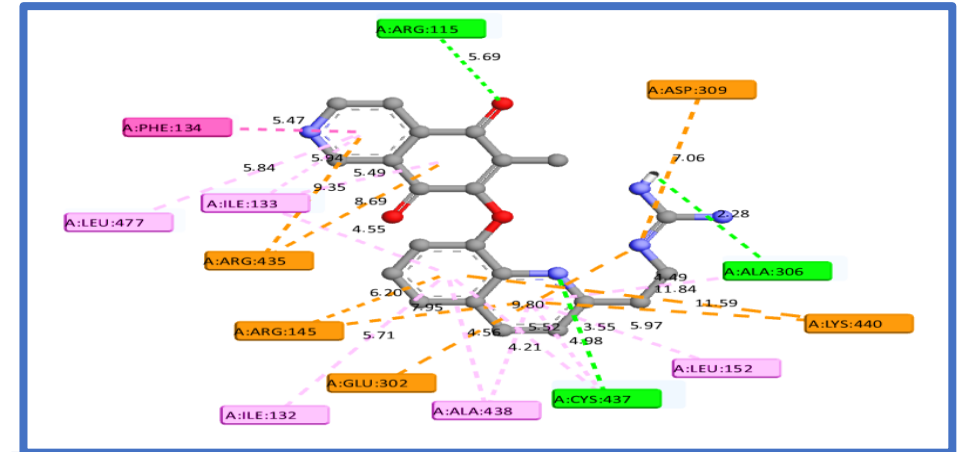
Figure 7. 2D interactions of most active molecule (a) and least active (b) molecule with aromatase enzyme.

Résultats & Discussion

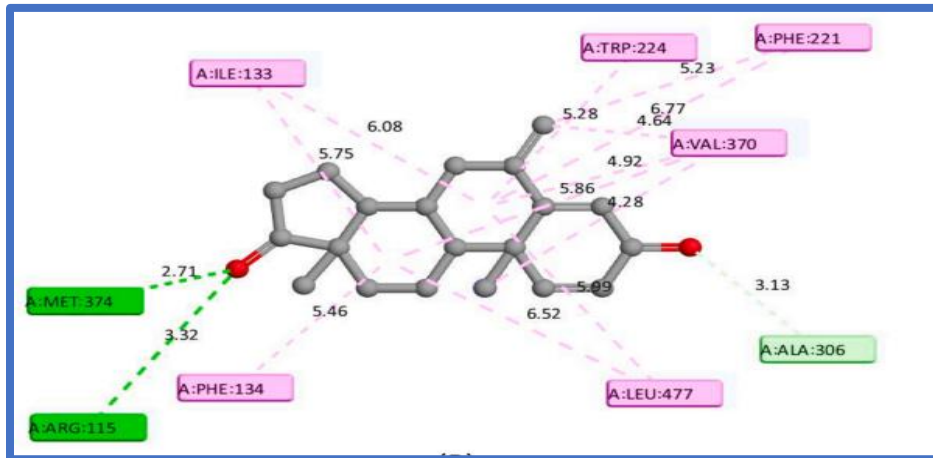
Validation des interactions de nouveaux candidats-médicaments



3D interactions of best candidate (Ligand 5) - Aromatase

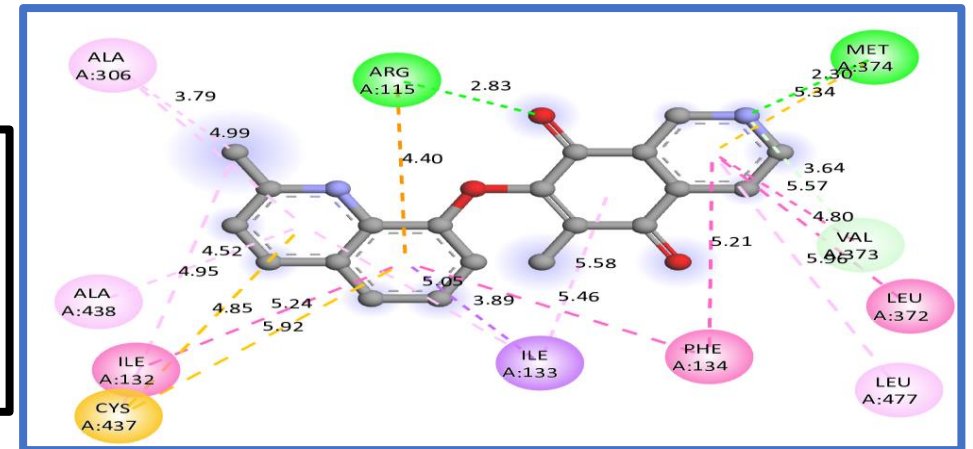


2D interactions of best candidate (Ligand 5) - Aromatase



2D interactions of Exemestane (reference) - Aromatase

Interactions			
	Conventional Hydrogen Bond		Pi-Sulfur
	Pi-Cation		Alkyl
	Pi-Donor Hydrogen Bond		Pi-Alkyl
	Pi-Sigma		Pi-Pi T-shaped
	Carbon Hydrogen Bond		



2D interactions of most active molecule - Aromatase

Figure 8. 2D / 3D interactions of the new designed drug-candidate compared with the most active molecule and the reference drug

Résultats & Discussion

Stabilité via des algorithmes de dynamique moléculaire (stochastiques)

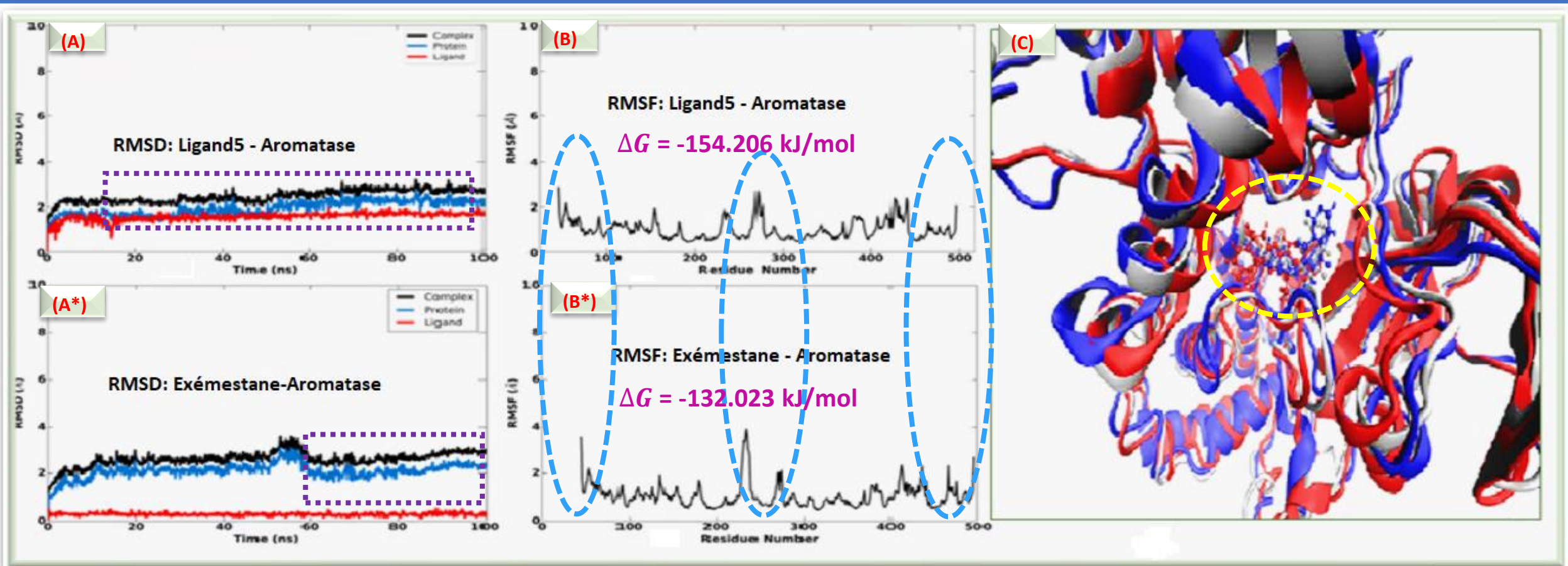
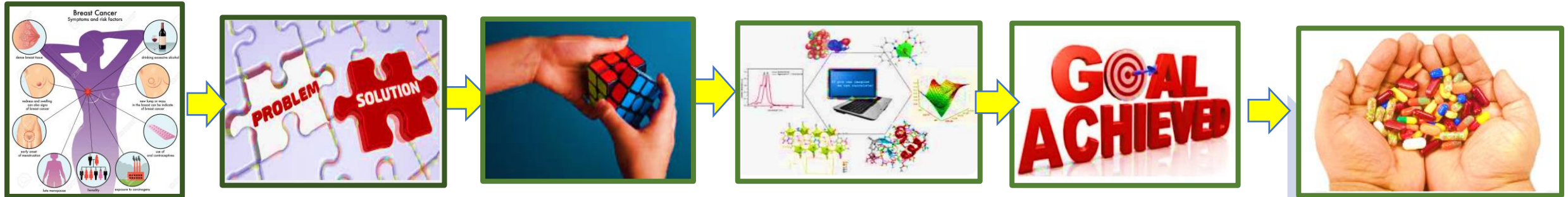


Figure 9. RMSD (A, A*) , RMSF (B, B*) and the aligned structures of Ligand5-3S7S during molecular dynamic simulation; red 0 ns, white 50 ns, blue 100 ns (C) (* : Exémestane)

Conclusion



**NTIC pilotés par IA
(CADD-AI)**

**Forte performance
prédictive des
modèles**

**Nouveau candidats
médicaments contre le
cancer du sein**

Publications / Découverte de candidats-médicaments par IA

- **S. El Rhabori**, M. Alaqarbeh, Y. El Allouche, L. Naanaai, A. El Aissouq, M. Bouachrine, S. Chtita, F. Khalil, **Exploring innovative strategies for identifying anti-breast cancer compounds by integrating 2D/3D-QSAR, molecular docking analyses, ADMET predictions, molecular dynamics simulations, and MM-PBSA approaches**, Journal of Molecular Structure. 1320 (2025) 139500. <https://doi.org/10.1016/J.MOLSTRUC.2024.139500>.
- **S. El Rhabori**, M. Alaqarbeh, A. El Aissouq, M. Bouachrine, S. Chtita, F. Khalil, **Design, 3D-QSAR, molecular docking, ADMET, molecular dynamics and MM-PBSA simulations for new anti-breast cancer agents**, Chemical Physics Impact. 8 (2024) 100455. <https://doi.org/10.1016/J.CHPHI.2023.100455>.
- **S. El Rhabori**, A. El Aissouq, O. Daoui, S. Elkhatabi, S. Chtita, F. Khalil, **Design of new molecules against cervical cancer using DFT, theoretical spectroscopy, 2D/3D-QSAR, molecular docking, pharmacophore and ADMET investigations**, Heliyon. 10 (2024) e24551. <https://doi.org/10.1016/J.HELİYON.2024.E24551>.
- **S. El Rhabori**, A. El Aissouq, S. Chtita, F. Khalil, **QSAR, molecular docking and ADMET studies of quinoline, isoquinoline and quinazoline derivatives against Plasmodium falciparum malaria**, Structural Chemistry. 34 (2023) 585–603. <https://doi.org/10.1007/S11224-022-01988-Y>.
- **S. El Rhabori**, A. El Aissouq, S. Chtita, F. Khalil, **Design of novel quinoline derivatives as antibreast cancer using 3D-QSAR, molecular docking and pharmacokinetic investigation**, Anti-Cancer Drugs. 33 (2022) 789–802. <https://doi.org/10.1097/CAD.0000000000001318>.
- **S. El Rhabori**, A. El Aissouq, S. Chtita, F. Khalil, **3D-QSAR, molecular docking and ADMET studies of thioquinazolinone derivatives against breast cancer**, Journal of the Indian Chemical Society. 99 (2022) 100675. <https://doi.org/10.1016/J.JICS.2022.100675>.





Merci

pour votre attention

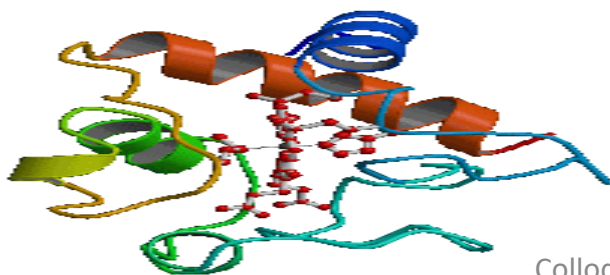
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