Virtual screening of different subclasses of lignans with anticancer potential and based on genetic profile

Mayara dos Santos Maia[1], Francisco Jaime Bezerra Mendonça-Junior [2,5] *, Gabriela Cristina Soares Rodrigues[3], Adriano Soares da Silva[4], Niara Isis Pereira de Oliveira[4], Pablo Rayff da Silva[5], Cícero Francisco Bezerra Felipe[5], Ana Pavla Almeida Diniz Gurgel[6], Anuraj

[1] Department of Molecular Biology, Federal University of Paraíba, João Pessoa-PB, Brazil; mayarasm@ltf.ufpb.br.

[2] Laboratory of Synthesis and Drug Delivery, State Universtiy of Paraiba, João Pessoa-PB, Brazil; franciscojaime@servidor.uepb.edu.br

[3] Miriri Foods and Bioenergy S/A; gaby.ecologia@gmail.com.

[4] Program in Ecology and Environmental Monitoring, Federal University of Paraíba, João Pessoa-PB, Brazil; Adriano.soares05071997@gmail.com; naira.isis.ni@gmail.com.

[5] Postgraduate Program in Natural Synthetic and Bioactive Products, Federal University of Paraíba, João Pessoa-PB, Brazil; pablo-rayff@hotmail.com; cicero@dbm.ufpb.br.

[6] Program in Cellular and Molecular Biology, Federal University of Paraíba, João Pessoa-PB, Brazil; ana.pavla@academico.ufpb.br.

[7] In Silico Research Laboratory, Eminent Bioscience, Indore, Madhya Pradesh, India; anuraj@eminentbio.com

[8] Laboratory of Cheminformatics, Program of Natural and Synthetic Bioactive Products (PgPNSB), Health Sciences Center, Federal University of Paraíba, João Pessoa-PB, Brazil; luciana.scotti@gmail.com; mtscotti@gmail.com.
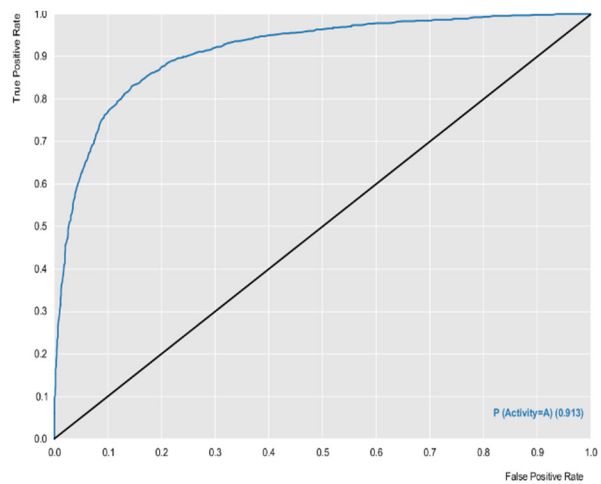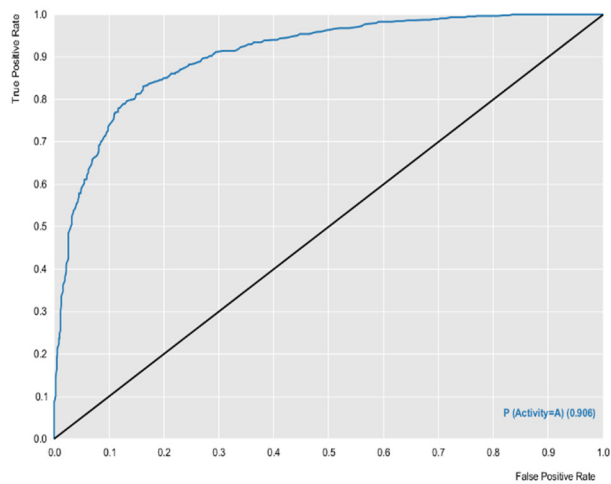
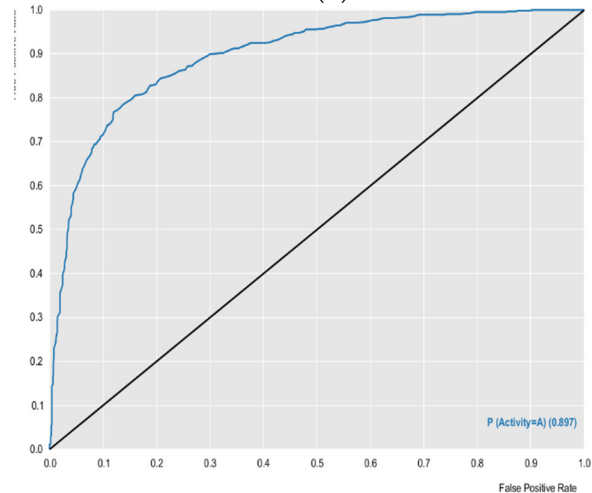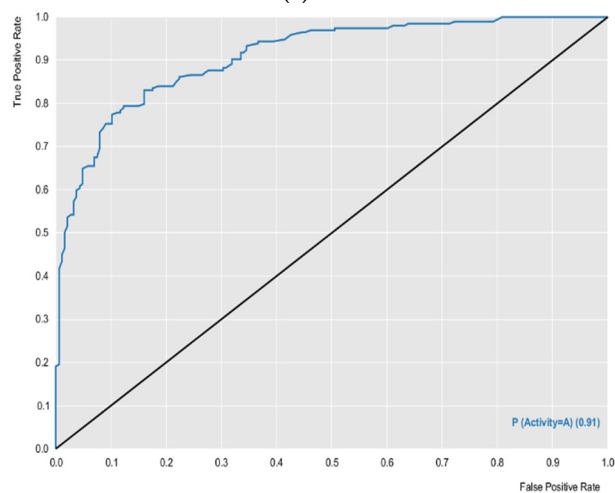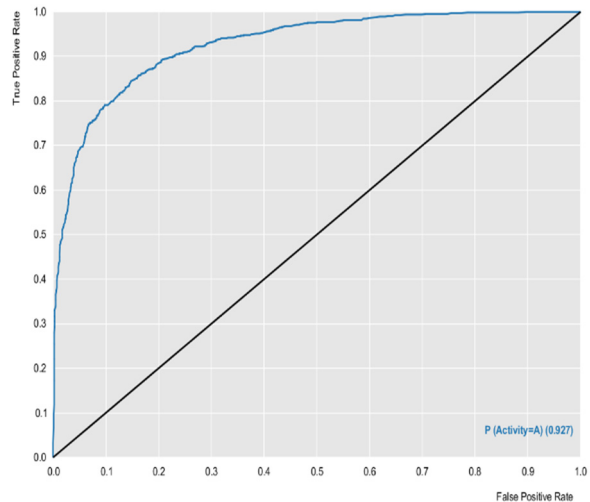* Correspondence: franciscojaime@servidor.uepb.edu.br
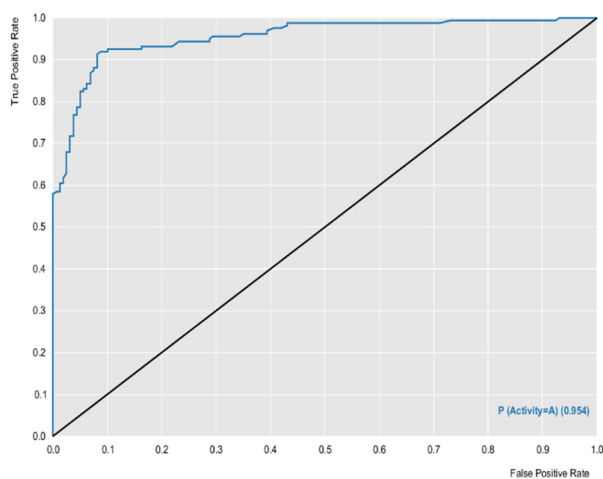
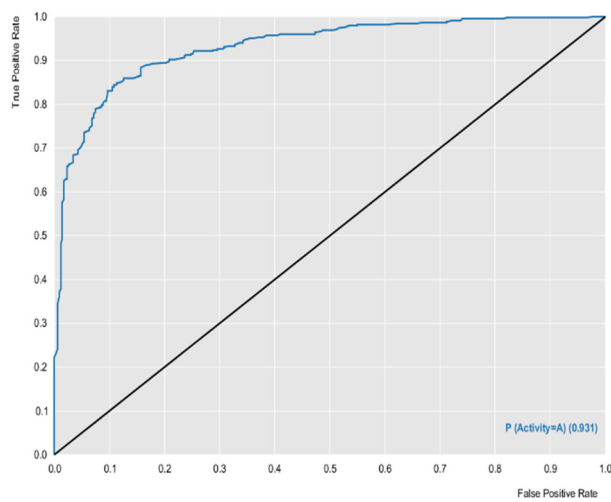(a)
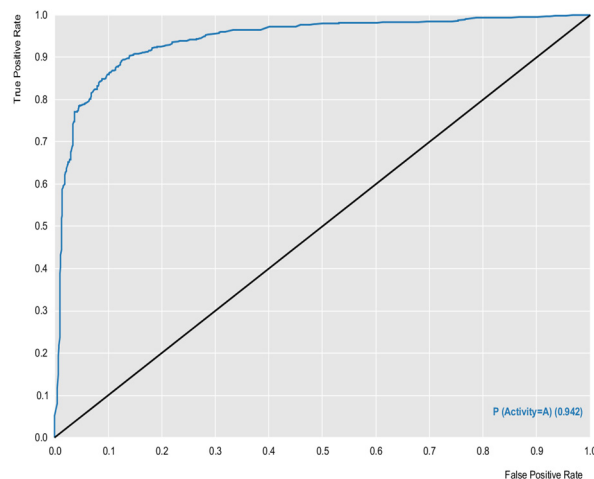
(b)

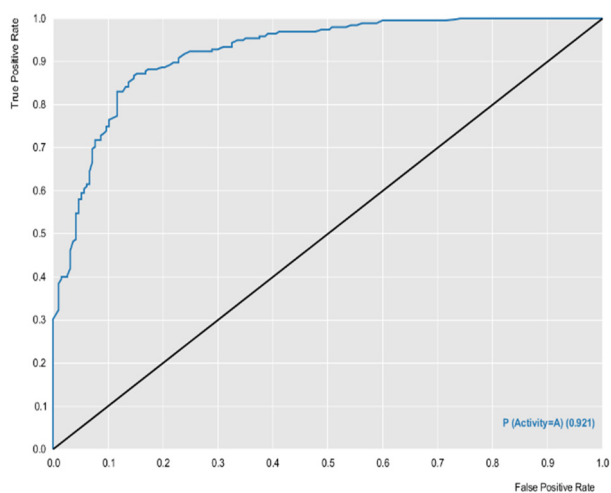(**c**)

(**d**)

(**e**)

(**f**)

(**g**)

(**h**)

(**i**) (**j**)
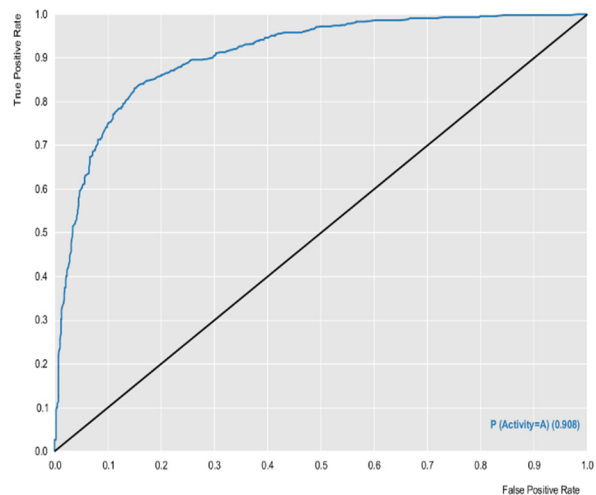
Figure 1. ROC (Receiver Operating Characteristic) curve generated for the five selected protein models. (**a**) ABL test; (**b**) ABL cross; (**c**) EFGR test; (**d**) EFGR cross; (**e**) HDAC test; (**f**) HDAC cross; (**g**) mTOR test; (**h**) mTOR cross; (**i**) PARP test; and (**j**) PARP cross.