Prof De Simone got her master degree in Chemistry and Pharmaceutical Technology in 2006 at the University of Bologna and in 2010 she defended her PhD thesis titled "A multi-methodological approach for bio-recognition study".

She was Post Doc Junior at Italian Institute of Technology (IIT) Genova (Italy) in 2012 to 2013.

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In 2015-16 she spent 6 months at the Department of Medicinal Chemistry of Ludwing Maximilians University of Munich, Germany, as visiting scientist carrying out a research project aimed at the development of an analytical method for the simultaneous characterization of selective ligands towards hDAT, hNET and hSERT transporters.

Since September 2019 she works as associate professor at the Department of Drug Science and Technology, University of Turin (Italy).

Her work is mainly focused on: (1) development of fast automated analytical techniques to screen and characterize new ligands for the key target enzymes BACE-1 and GSK-3 involved in Alzheimer's Disease, (2) application of multi-methodological approach applied to monitoring beta-amyloid aggregation and to the investigation of ligand-target interaction (3) characterization of Multi Target Direct Ligands (MTDLs);

During her career, international scientific collaborations have been established with many research groups.

Since 2020 she is member of the scientific committee of the international congress "Recent Development of on Pharmaceutical Analysis" (RDPA) and member of the editorial board of the journal "Pharmaceuticals".

Prof De Simone is the author of 60 papers on international journals, 2 chapters in books, and several oral communications at international congresses.