Information to be requested from all CA17104 participants:

	
Indicate your Working Group(s) in COST Action17104:	**WG2**
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biography:	
Link to webpage with group description:	

Orcid ID or Scopus ID	**ORCID: 0000-0003-2398-1254** **SCOPUS: 24577345000**
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Expertise relevant for this COST Action:	**Medicinal chemistry, with a focus on the use of computational tools in:** **i) design and optimization of pharmacological agents** **ii) structural conformational studies on target proteins (i.e. finalized to plan mutagenesis, understand PPI, protein-DNA interaction, …)**
Available facilities to conduct work, relevant for this COST Action:	GPU-equipped workstations, CPU own cluster, access to the department supercomputer equipped with several CPU and GPU cores (V100 Nvidia), software such as OpenEye, LigandScout, Schrodinger, CCDC, Gaussian, Amber, …
Matherials/Methods that could be shared with other members of this COST Action:	Computer simulations including virtual screening, molecular docking, molecular dynamics, pharmacophore modeling; hit-to-lead optimization, rational design of bioactive ligands, rationalization of existing data, chemoinformatics analyses on bioactive compounds or chemical libraries. Thanks to a long-term collaboration with the Univerity of Rome La Sapienza, I have access to a unique library of more than 1,000 natual compounds for screening purposes.

NOTE: By submitting this form to the Grant Manager of CA17104, I agree that this information can be used within the scope of this COST Action (e.g. may be included on the webpage of CA17104).