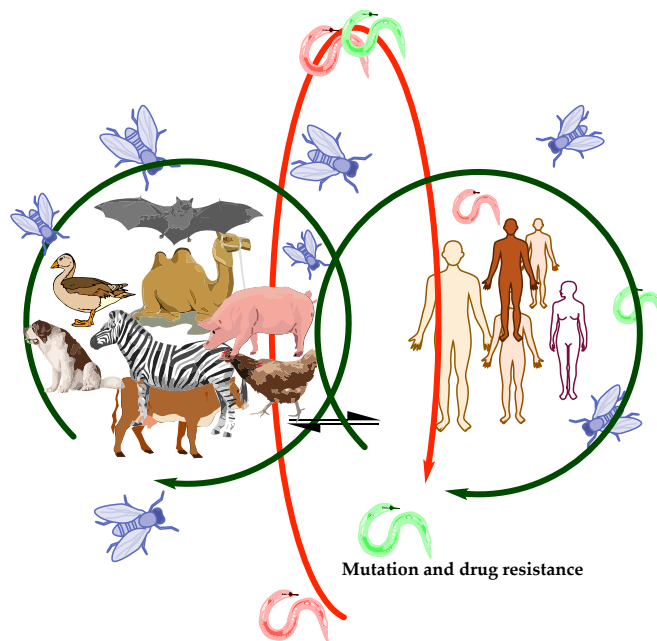




Available technologies within the COST Action OneHealthdrugs





IN-SILICO TECHNOLOGIES

AI methods for prediction of activity	AI methods for prediction of toxicity	AI methods for prediction of metabolic fate
Essia Sebai (TN)	Guy Caljon (BE)	Mehmet Salih Yıldırım (TR)
Maria Paola Costi (IT)	Melek Gul (TR)	
Biljana Otašević (RS)	Rita Guedes (PT)	
Mehmet Salih Yıldırım (TR)		
Melek Gul (TR)		
Ana Mikelić (HR)		
Rita Guedes (PT)		
Karen Angeliki Krogfelt (DK)		

In silico drug design	In silico drug target interactions	In silico off target effects
Thomas J. Schmidt (DE)	Thomas J. Schmidt (DE)	Guy Caljon (BE)
Huseyin Istanbulu (TR)	Andrea Ilari (IT)	Rita Guedes (PT)
Bahne Stechmann (DE)	Huseyin Istanbulu (TR)	Sinan Ince (TR)
Maria Paola Costi (IT)	Maria Paola Costi (IT)	Florence McCarthy (IE)
Outi Salo-Ahen (FI)	Narimantas Čėnas (LT)	
Melek Gul (TR)	Ana Domingos (PT)	
Elisa Uliassi (IT)	Melek Gul (TR)	
Trond Vidar Hansen (NO)	Harry de Koning (UK)	
Rita Guedes (PT)	Ana Mikelić (HR)	
Christophe Dardonville (ES)	Christophe Dardonville (ES)	
Karen Angeliki Krogfelt (DK)	Rita Guedes (PT)	
Brindusa Dragoi (RO)	John Igoli (NG)	
Claudia Federo (PT)	Claudia Federo (PT)	
Lori Doko (AL)	Suranga Kodithuwakku (EE)	
Florence McCarthy (IE)	Daniele Aiello (IT)	
Suranga Kodithuwakku (EE)		
Daniele Aiello (IT)		



Prediction of ecotoxicity (degradability and others)	Bioinformatics
Guy Caljon (BE)	Outi Salo-Ahen (FI)
Essia Sebai (TN)	José Gonçalves (PT)
Mehmet Salih Yıldırım (TR)	Ana Domingos (PT)
Melek Gul (TR)	Mehmet Salih Yıldırım (TR)
Claudia Federo (PT)	Harry de Koning (UK)
Dijana Blazhekovikj - Dimovska (MK)	Håvard Jenssen (DK)
Daniele Aiello (IT)	Gad Baneth (IL)
	Rita Guedes (PT)
	Karen Angeliki Krogfelt (DK)
	Claudia Federo (PT)
	Suranga Kodithuwakku (EE)
	Nuno Pedro Moreira Santarém (PT)
	Margarida Duarte (PT)

AI in prediction of analytical response	AlphaFold AI predictions of protein structure	parasites, platforms for in vivo testing
Biljana Otašević (RS)	Harry de Koning (UK)	Daniel Sojka (CZ)



STRUCTURAL BIOLOGY

Crystallisation of proteins with ligands	Crystallisation of proteins without ligands	CryoEM
Andrea Ilari (IT)	Andrea Ilari (IT)	Andrea Ilari (IT)
Daniel Sojka (CZ)	Daniel Sojka (CZ)	Harry de Koning (UK)
Maria Paola Costi (IT)	Harry de Koning (UK)	Lori Doko (AL)
Harry de Koning (UK)	Karen Angeliki Krogfelt (DK)	
Sinan Ince (TR)	Nuno Pedro Moreira Santarém (PT)	
Nuno Pedro Moreira Santarém (PT)		

In silico structural prediction and analysis	NMR technologies
Guy Caljon (BE)	Huseyin Istanbulu (TR)
Andrea Ilari (IT)	Theodora Calogeropoulou (GR)
Daniel Sojka (CZ)	Bahne Stechmann (DE)
Maria Paola Costi (IT)	Mehmet Salih Yildirim (TR)
Outi Salo-Ahen (FI)	Melek Gul (TR)
Ana Domingos (PT)	Harry de Koning (UK)
Biljana Otašević (RS)	David Magri (MT)
Melek Gul (TR)	Christophe Dardonville (ES)
Harry de Koning (UK)	John Igoli (NG)
Elisa Uliassi (IT)	Karen Angeliki Krogfelt (DK)
Sébastien Pomel (FR)	Sandra Gemma (IT)
Rita Guedes (PT)	Chiara Borsari (IT)
Karen Angeliki Krogfelt (DK)	Ioannis Papanastasiou (GR)
Claudia Federo (PT)	Claudia Federo (PT)
Florence McCarthy (IE)	Florence McCarthy (IE)
Maria João Queiroz (PT)	Dijana Blazhekovikj - Dimovska (MK)
Daniele Aiello (IT)	Daniele Aiello (IT)
Thomas J. Schmidt (DE)	Thomas J. Schmidt (DE)
	Maria Paola Costi (IT)

Nanoscale resolution infrared spectroscopic imaging	Transcriptomics and Proteomics including bioinformatics
Daniela Täuber (DE)	Suranga Kodithuwakku (EE)
	Maria Paola Costi (IT)



MEDICINAL CHEMISTRY

Green methods	Capacity for scale-up synthesis	Parallel synthesis
George Magoulas (GR)	Theodora Calogeropoulou (GR)	Theodora Calogeropoulou (GR)
Theodora Calogeropoulou (GR)	Annette Ives (CH)	Davioud-Charvet Elisabeth (FR)
Davioud-Charvet Elisabeth (FR)	Davioud-Charvet Elisabeth (FR)	Bahne Stechmann (DE)
Essia Sebai (TN)	Bahne Stechmann (DE)	Maria Paola Costi (IT)
Maria Paola Costi (IT)	Narimantas Čėnas (LT)	Melek Gul (TR)
Biljana Otašević (RS)	Mehmet Salih Yıldırım (TR)	Elisa Uliassi (IT)
Mehmet Salih Yıldırım (TR)	Lucia Tamborini (IT)	Håvard Jenssen (DK)
Melek Gul (TR)	Christophe Dardonville (ES)	Christophe Dardonville (ES)
Elisa Uliassi (IT)	Chiara Borsari (IT)	Karen Angeliki Krogfelt (DK)
Trond Vidar Hansen (NO)	Ioannis Papanastasiou (GR)	Sandra Gemma (IT)
Lucia Tamborini (IT)	Florence McCarthy (IE)	Claudia Federo (PT)
David Magri (MT)	Maria Alice Carvalho (PT)	Florence McCarthy (IE)
Sinan Ince (TR)	Maria João Queiroz (PT)	Maria Alice Carvalho (PT)
Sandra Gemma (IT)	Daniele Aiello (IT)	Maria João Queiroz (PT)
Chiara Borsari (IT)		Daniele Aiello (IT)
Claudia Federo (PT)		
Lori Doko (AL)		
Dijana Blazhekovikj - Dimovska (MK)		
Maria Alice Carvalho (PT)		
Maria João Queiroz (PT)		
Daniele Aiello (IT)		

PROTACS	Multitarget compounds	
Andrea Ilari (IT)	Huseyin Istanbulu (TR)	Karen Angeliki Krogfelt (DK)
Bahne Stechmann (DE)	George Magoulas (GR)	Jovana Ajdukovic (RS)
Melek Gul (TR)	Theodora Calogeropoulou (GR)	Sandra Gemma (IT)
Elisa Uliassi (IT)	Annette Ives (CH)	Chiara Borsari (IT)
Sandra Gemma (IT)	Davioud-Charvet Elisabeth (FR)	Claudia Federo (PT)
	Essia Sebai (TN)	Florence McCarthy (IE)
	Bahne Stechmann (DE)	Maria Alice Carvalho (PT)
	Maria Paola Costi (IT)	Suranga Kodithuwakku (EE)



	Mehmet Salih Yıldırım (TR)	Maria João Queiroz (PT)
	Melek Gul (TR)	Daniele Aiello (IT)
	Elisa Uliassi (IT)	
	Lucia Tamborini (IT)	
	Rita Guedes (PT)	
	David Magri (MT)	

Multicomponent reactions	flow chemistry facilities	Physical organic chemistry & structure-activity relationships
Maria Paola Costi	Maria Paola Costi	Maria Paola Costi
Theodora Calogeropoulou (GR)	Lucia Tamborini (IT)	David Magri (MT)

Physicochemical properties (pKa, logP, solubility)	Metal-catalyzed synthesis, C-H activation reactions	Partial synthetic modifications of natural products
Maria Paola Costi		
Christophe Dardonville (ES)	Maria João Queiroz (PT)	Thomas J. Schmidt (DE)



FORMULATION PROPERTIES

Targeted	Inexpensive (standard)
Dijana Blazhekovikj - Dimovska (MK)	Guy Caljon (BE)
Essia Sebai (TN)	Huseyin Istanbulu (TR)
Maria Paola Costi (IT)	Annette Ives (CH)
Mehmet Salih Yıldırım (TR)	Davioud-Charvet Elisabeth (FR)
Melek Gul (TR)	Essia Sebai (TN)
Jovana Ajdukovic (RS)	Mehmet Salih Yıldırım (TR)
Sinan Ince (TR)	Harry de Koning (UK)
Claudia Federo (PT)	John Igoli (NG)
Suranga Kodithuwakku (EE)	Karen Angeliki Krogfelt (DK)
Maria João Queiroz (PT)	Ioannis Papanastasiou (GR)
Socorro Espuelas (ES)	Claudia Federo (PT)
	Florence McCarthy (IE)

Decrease toxicity	For oral administration
Annette Ives (CH)	Guy Caljon (BE)
Davioud-Charvet Elisabeth (FR)	Annette Ives (CH)
Essia Sebai (TN)	Davioud-Charvet Elisabeth (FR)
Dijana Blazhekovikj - Dimovska (MK)	Essia Sebai (TN)
Mehmet Salih Yıldırım (TR)	Mehmet Salih Yıldırım (TR)
Melek Gul (TR)	Claudia Federo (PT)
Harry de Koning (UK)	Anabela Cordeiro da Silva (PT)
Håvard Jenssen (DK)	Gabriela Hřčková (SK)
Karen Angeliki Krogfelt (DK)	Suranga Kodithuwakku (EE)
Jovana Ajdukovic (RS)	Socorro Espuelas (ES)
Claudia Federo (PT)	Katarzyna Gořdzik (PL)
Lori Doko (AL)	



ENVIRONMENTAL IMPACT

Compound degradability in water (including the metabolites)	Metabolites toxicity (Metabolites identity is derived from pharmacokinetic in human and animal bodies)	Ecotox profiling
Davioud-Charvet Elisabeth (FR)	Davioud-Charvet Elisabeth (FR)	Eli Thoré (SE)
Essia Sebai (TN)	Mehmet Salih Yıldırım (TR)	Davioud-Charvet Elisabeth (FR)
Christophe Dardonville (ES)	Melek Gul (TR)	Maria Paola Costi (IT)
Karen Angeliki Krogfelt (DK)	Karen Angeliki Krogfelt (DK)	Mehmet Salih Yıldırım (TR)
Florence McCarthy (IE)	Sinan Ince (TR)	Melek Gul (TR)
Socorro Espuelas (ES)	Claudia Federo (PT)	Sinan Ince (TR)
Katarzyna Goździk (PL)		Daniele Aiello (IT)

Use of waste material as source of starting materials	Use of waste material as source of bioactive compounds
Theodora Calogeropoulou (GR)	Thomas J. Schmidt (DE)
José Gonçalves (PT)	José Gonçalves (PT)
Elisa Uliassi (IT)	Harry de Koning (UK)
Claudia Federo (PT)	John Igoli (NG)
Lori Doko (IT)	Dijana Blazhekovikj - Dimovska (MK)
Suranga Kodithuwakku (EE)	Suranga Kodithuwakku (EE)
Thomas J. Schmidt (DE)	



PARASITOLOGY

HTS screening	Target identification	Target validation
Guy Caljon (BE)	Guy Caljon (BE)	Guy Caljon (BE)
Sarah Hendrickx (BE)	Sarah Hendrickx (BE)	Sarah Hendrickx (BE)
Annette Ives (CH)	Anabela Cordeiro da Silva (PT)	Anabela Cordeiro da Silva (PT)
Bahne Stechmann (DE)	Annette Ives (CH)	Annette Ives (CH)
Maria Paola Costi (IT)	Dijana Blazhekovikj - Dimovska	Daniel Sojka (CZ)
Giulia Saporito (IT)	Daniel Sojka (CZ)	Davioud-Charvet Elisabeth (FR)
Mehmet Salih Yildirim (TR)	Davioud-Charvet Elisabeth (FR)	Ana Tomás (PT)
Melek Gul (TR)	Ana Tomás (PT)	Mehmet Salih Yildirim (TR)
Harry de Koning (UK)	Maria Paola Costi (IT)	Melek Gul (TR)
Donatella Taramelli (IT)	Roland Hellinger (AT)	Harry de Koning (UK)
Rita Guedes (PT)	Mehmet Salih Yildirim (TR)	Sébastien Pomel (FR)
Joana Tavares (PT)	Melek Gul (TR)	Rita Guedes (PT)
Kayhan Ilbeigi (BE)	Harry de Koning (UK)	Joana Tavares (PT)
John Igoli (NG)	Sébastien Pomel (FR)	Claudia Federo (PT)
Anabela Cordeiro da Silva (PT)	Rita Guedes (PT)	Nuno Pedro Moreira Santarém (PT)
Florence McCarthy (IE)	Kayhan Ilbeigi (BE)	Margarida Duarte (PT)
Nuno Pedro Moreira Santarém (PT)	Claudia Federo (PT)	
	Florence McCarthy (IE)	
	Suranga Kodithuwakku (EE)	
	Daniele Aiello (IT)	
	Nuno Pedro Moreira Santarém (PT)	
	Margarida Duarte (PT)	



OMIC approaches	In vitro phenotypic screening	In vitro cellular toxicity
Guy Caljon (BE)	Guy Caljon (BE)	Guy Caljon (BE)
Annette Ives (CH)	Sarah Hendrickx (BE)	Sarah Hendrickx (BE)
Katarzyna Goździk (PL)	Huseyin Istanbulu (TR)	Anabela Cordeiro da Silva (PT)
Daniel Sojka (CZ)	Anabela Cordeiro da Silva (PT)	Annette Ives (CH)
Davioud-Charvet Elisabeth (FR)	Annette Ives (CH)	Daniel Sojka (CZ)
Maria Paola Costi (IT)	Daniel Sojka (CZ)	Ana Tomás (PT)
Roland Hellinger (AT)	Essia Sebai (TN)	Bahne Stechmann (DE)
Ana Domingos (PT)	Ana Tomás (PT)	Maria Paola Costi (IT)
Harry de Koning (UK)	Bahne Stechmann (DE)	Roland Hellinger (AT)
Sébastien Pomel (FR)	Roland Hellinger (AT)	Harry de Koning (UK)
Gad Baneth (IL)	Harry de Koning (UK)	Donatella Taramelli (IT)
Karen Angeliki Krogfelt (DK)	Donatella Taramelli (IT)	Sébastien Pomel (FR)
Suranga Kodithuwakku (EE)	Sébastien Pomel (FR)	Joana Tavares (PT)
Daniele Aiello (IT)	Joana Tavares (PT)	David Magri (MT)
Nuno Pedro Moreira Santarém (PT)	Kayhan Ilbeigi (BE)	Kayhan Ilbeigi (BE)
	John Igoli (NG)	John Igoli (NG)
	Sarah D'Alessandro (IT)	Sarah D'Alessandro (IT)
	Karen Angeliki Krogfelt (DK)	Karen Angeliki Krogfelt (DK)
	Claudia Federo (PT)	Brindusa Dragoi (RO)
	Lori Doko (AL)	Claudia Federo (PT)
	Florence McCarthy (IE)	Florence McCarthy (IE)
	Suranga Kodithuwakku (EE)	Gabriela Hřčková (SK)
	Nuno Pedro Moreira Santarém (PT)	Suranga Kodithuwakku (EE)
	Margarida Duarte (PT)	Nuno Pedro Moreira Santarém (PT)
	Katarzyna Goździk (PL)	Socorro Espuelas (ES)
		Katarzyna Goździk (PL)

In vitro ADMET	In vitro safety pharmacology panels	PK/PD simulation systems
Guy Caljon (BE)	Annette Ives (CH)	Guy Caljon (BE)
Theodora Calogeropoulou (GR)	Maria Paola Costi (IT)	Annette Ives (CH)
Annette Ives (CH)	Daniel Sojka (CZ)	Daniel Sojka (CZ)
Davioud-Charvet Elisabeth (FR)	Claudia Federo (PT)	Rita Guedes (PT)
Maria Paola Costi (IT)	Katarzyna Goździk (PL)	Sarah Hendrickx (BE)
Melek Gul (TR)		Kayhan Ilbeigi (BE)
David Magri (MT)		Anabela Cordeiro da Silva (PT)
Kayhan Ilbeigi (BE)		
Socorro Espuelas (ES)		



In vivo study for activity	In vivo study for toxicity
Guy Caljon (BE)	Guy Caljon (BE)
Sarah Hendrickx (BE)	Sarah Hendrickx (BE)
Huseyin Istanbulu (TR)	Anabela Cordeiro da Silva (PT)
Anabela Cordeiro da Silva (PT)	Annette Ives (CH)
Annette Ives (CH)	Daniel Sojka (CZ)
Daniel Sojka (CZ)	Essia Sebai (TN)
Essia Sebai (TN)	Ana Domingos (PT)
Ana Tomás (PT)	Sébastien Pomel (FR)
Maria Paola Costi (IT)	Joana Tavares (PT)
Ana Domingos (PT)	Kayhan Ilbeigi (BE)
Sébastien Pomel (FR)	Dijana Blazhekovikj - Dimovska (MK)
Joana Tavares (PT)	Gabriela Hřčková (SK)
Kayhan Ilbeigi (BE)	Nuno Pedro Moreira Santarém (PT)
Sinan Ince (TR)	Socorro Espuelas (ES)
Gabriela Hřčková (SK)	
Nuno Pedro Moreira Santarém (PT)	
Socorro Espuelas (ES)	
Katarzyna Goździk (PL)	

In vivo PK	Immune profiling
Guy Caljon (BE)	Annette Ives (CH)
Sarah Hendrickx (BE)	
Anabela Cordeiro da Silva (PT)	
Annette Ives (CH)	
Davioud-Charvet Elisabeth (FR)	
Mehmet Salih Yıldırım (TR)	
Daniel Sojka (CZ)	
Sébastien Pomel (FR)	
Joana Tavares (PT)	
Kayhan Ilbeigi (BE)	
Socorro Espuelas (ES)	
Nuno Pedro Moreira Santarém (PT)	