VIRTUAL SCREENING & PHYTOCHEMICAL PROFILING

for cosmetics efficacy prediction

in silico testing

Biological activity prediction of **pure molecules**
based on their chemical structure

You have	*or*	▪ a molecule with a known chemical structure ▪ a biological target (enzyme, receptor, etc.)
You want to	*or*	▪ identify targets that may interact with your molecule ▪ find the active molecules that act on your biological target
We supply	*or*	▪ a list of potential biological targets ▪ a list of potential active molecules ▪ a list of possible dermocosmetics applications & related *in vitro* assays
How ?		1. similarity searching by chemoinformatics *structural comparison of 1,500,000 active ligands* 2. virtual screening by *in silico* technology (SELNERGY™) *docking/binding on 10,000 protein structures*

phytochemical profiling

Biological activity prediction of **natural extracts**
based on their phytochemical composition

You have	▪ an extract
You want to	▪ identify the bioactive molecules present in your extract ▪ find targets that bind to your extract's molecules
We supply	▪ a list of potential molecules present in your extract ▪ a list of possible dermocosmetics applications & related *in vitro* assays
How ?	1. UHPLC/HRMS profiling method (GAINS™) to discover and identify potentiel molecules in the extract 2. data mining (GPDB) and similarity searching on molecules identified from mass fragmentation 3. virtual screening by *in silico* technology (SELNERGY™)

A new era for biological activity substantiation

In the era of artificial intelligence, the use of digital data has become an essential analysis tool in the field of biology.

This is why QIMA Life Sciences has signed an exclusive distribution agreement with Greenpharma to expand its expertise to *in silico* virtual screening.

This technology is offered prior to the *in vitro* and *ex vivo* assays historically provided by Bioalternatives for cosmetic claim substantiation.

Reducing the attrition rate of *in vitro* assays and targeting the most appropriate efficacy studies more efficiently are QIMA Life Sciences' main concerns in order to help you with your R&D projects.

In addition, this new approach allows a substantiation of the ingredient activity at molecular level and paves the way for intellectual property rights.

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QIMA Life Sciences

+500 online assays
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