

Company Name **SoftMining**
Field of Activity Drug design and Data Mining
Contact Person Stefano Piotto
Phone +39 320 423 0068
E-mail piotto@unisa.it stefano@softmining.it

EXECUTIVE SUMMARY

1. Company profile

SoftMining Srl will be established in June 2018. More info at (www.softmining.it). The founders are:

Stefano Piotto	CEO - Chemist/Bioinformatician – Professor of Chemistry and Biomaterials at the University of Salerno	www.softmatter.unisa.it http://docenti.unisa.it/005870/en/curriculum
Luigi Di Biasi	Bioinformatician	www.softmining.it
Lucia Sessa	Drug designer- PhD Pharmaceutical Sciences	www.softmining.it

SoftMining is supported by an international Scientific Board made up of researchers and entrepreneurs from various European universities and biotech companies. The board has counseling and address function. Refer to <http://www.softmining.it/index.php/pubs/> for an updated list of their scientific publications.

2. Business idea

SoftMining wants to change the way to do pharmaceutical research by using sophisticated computing techniques. Over the last ten years, our group has developed **new methods for the design of drugs and to check their potential toxicity without the use of animal models**. Some of these methods and the main results are shown at <http://www.softmining.it/>. The results obtained are extraordinary from a **scientific** and **social point** of view (because it greatly reduces animal experimentation). SoftMining has also developed new techniques of data mining currently applied to analysis of biomedical data.

3. Company assets

SoftMining has more accurate and more efficient algorithms for molecular docking than those currently available. SoftMining offers these products and its expertise to pharma companies for developing new drugs. The techniques developed by the SoftMining team permitted to optimize the design process and to reduce time, costs and risks in designing new antibiotics (Piotto, Concilio et al. 2013, Piotta, Concilio et al. 2013, Concilio, Iannelli et al. 2015, Sessa, Concilio et al. 2016, Piotta, Sessa et al. 2017, Sessa, Petrone et al. 2017), and to develop new anticancer drug (Piotto, Concilio et al. 2014, Piotta, Trapani et al. 2014, Török, Crul et al. 2014). We have recently received a CLINGLIO Project (GA No: 755179) funded by the European Commission H2020-SC1-2017-Two-Stage-RTD for more than 6M€.

A limited list of software and methods developed are:

1) Drug design

- a) **FLOCKING** offers unprecedented ability to design novel protein inhibitors, exploiting all atoms molecular dynamics. It permits to design or optimize small molecules as well as peptides for protein interaction. Flocking is currently under patenting process.

- b) **YADA** is a new tool for molecular docking that is capable to distribute efficiently calculations onto general purposes computer grid and that combines biological and structural information of the receptor. www.yada.unisa.it
- c) **GRIMD** Biologists and chemists are facing problems of high computational complexity that require the use of several computers organized in clusters or in specialized grids. Regrettably, the diffusion of Grid Computing is strongly limited because two main limitations: it is confined to scientists with strong Computer Science background and the analyses of a large amount of data produced can be cumbersome. GRIMD is very flexible because it shields the typical computational biologist from the need to write specific code for tasks such as molecular dynamics or docking calculations. Furthermore, it permits an efficient use of GPU cards whenever is possible. GRIMD calculations scale almost linearly and, therefore, permits to exploit efficiently each machine in the network.

2) Computational toxicology

- a) **eTox** Toxicity prediction suite of a wide array of molecules. eTox is an in silico tool for predicting ADME properties and the toxic potential (endocrine and metabolic disruption, some aspects of carcinogenicity and cardiotoxicity) of small molecules (<500 Dalton). The toxicity potential is evaluated via a fully flexible docking (flexible receptor/flexible ligand) protocol. Currently, eTox permits the investigation of 19 proteins known to trigger adverse effects.

3) Data Mining

- a) **PROTCOMP** is a data mining tool based on compression algorithms. Originally written to perform genomic and proteome analysis and to design new antimicrobial peptides, the algorithm is powerful, flexible, scalable, and applicable in different contexts. ProtComp permits to perform genomic and big data analysis in a tiny fraction of the normal time
- b) **SM_SEARCH** A new generation search engine. SM_search is not a Google-like engine. It is an alternative to the traditional search. It is the ProtComp algorithm applied to file search. Rather than using keywords or tags, consider the whole content of a file to find "similar" objects.
- c) **SM_HEALTH** is an application of the ProtComp algorithm to automatically detect similarity in electrocardiograms and electroencephalograms. The process is real-time and takes place on the biomedical device. The main difference with existing software is that instead of searching for a pattern in an electroXgram, it analyses the whole dataset in real time. No privacy problem, no cloud-based app, no connection problem.
- d) **AI-HISTO** is an artificial neural network trained for the categorization of histological samples photos. AI-HISTO is part of a platform (in collaboration with Pharma Bullet Srl) that combines blood test data with biomarker results to achieve an early prostate cancer detection accuracy close to 100%. AI-HISTO will be made freely available on the softmining web server.

4. Market opportunity

Pharma market: The pharmaceutical market, considering the international dimension of major pharmaceutical companies, is the world market, starting with Big Pharma (such as Pfizer, Merck, GSK, Bayer, AstraZeneca). SoftMining offers Big Pharma new tools for drug design.

Data mining: SoftMining applies the new methods developed for data and knowledge mining for process optimization. SoftMining is already collaborating with 3 companies for process optimization and AI projects.

5. Investment needed

The strength of SoftMining is mainly the expertise of staff employed in the company.

Economic, capital and cash flow analyses are extraordinary since the third year of activity. The company cost analysis for the first two years costs around 300 k€/year. This is mainly due to job contracts. The analysis of revenues indicates a positive break-even already in the second year and from the third year revenues higher than 2M €.

The present value of the company is based on the value of the software platform above € 400k and the projection of revenues from similar companies.

SoftMining needs investments to complete the development of products and to protect the intellectual property. The funding of the company will be realized by means of scientific grants and by selling, in the next years, the 30% of the company.