6 Conclusion

We shortly reviewed the area of computational chemistry, and in particular QSAR. A major event in the area has been the activation of the new REACH legislation, which foresees the exploitation of such mathematical tools for the risk assessment of produced chemicals.

This is further enhancing the importance of these techniques, but also generating a number of issues, that we stated as a “non-free/non-accessible knowledge” problem. We illustrated this phenomenon in Section 4, and we pointed out that it involves both the research world and the chemical companies.

Going back to a scientific point of view, it remains a scientific challenge to evaluate the biological effects of compounds using only in silico tools, and more research is needed. No public model under REACH still exists; we also hope to be an impulse in this direction.