Link, Merge, Grow

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Executive Summary

Fragment-based drug discovery (FBDD) is a recently mainstream approach in the pharmaceutical sciences used to generate the starting chemical matter in the early stages of drug discovery. While it received high expectations on its potential to transform the lead discovery process, it also received skepticism on its utility and reliability. In this research, we explore how various actors contributed to the emergence and development of the field. At the same time, we also look at how these actors seized opportunities from the field's progress. This research uses publications, patents, interviews and archival analysis in order to trace the co-evolution of the field with its participants.

We find that the various proponents of FBDD from academic groups, new ventures and big pharmaceutical firms played important roles in the development of the field. FBDD's theoretical foundations were laid by academia, but the application of this basic knowledge by industry practitioners was crucial for its further growth. The major development in the field was first published by researchers in the large pharmaceutical firm Abbott but it was the small firms that were important in evangelizing and demonstrating the practical value of FBDD in drug discovery. These new ventures deployed processes of differentiation and legitimation to claim their niches within the field and also, advocate for the field's wider acceptance. With the success stories of these firms, proponents within large pharmaceutical firms were able to find further motivation in establishing the approach within their research groups. Currently, as a routine approach in the pharmaceutical sciences, FBDD is now applied by both small and big firms in the industry and academic groups to kickstart their drug discovery process.

In Chapter 2, we begin this research by situating FBDD in the wider context of the pharmaceutical industry. We did this through a bibliometric analysis of the publications in the innovation literature about the pharmaceutical industry. We find that there is a need for better-engaged research between innovation scholars and industry practitioners. By peeking into the black box of the innovation process in the pharmaceutical industry, new insights can be gotten on innovative ways of bringing drugs into the market.

In Chapter 3, we traced how FBDD developed over time through a bibliometric analysis of its publications. We find that while academia was crucial in laying down the foundations of the field, it was the industry that played a crucial role in applying the technique to their various projects that the field further developed and became widely used within the industry. We also find that interdisciplinary research was important for the crucial pieces of the puzzle to come together to what will become FBDD.

In Chapter 4, we then looked at the role of various actors in taking opportunities from the field's development and in turn, contributing to the field to gain wider recognition. We looked at how smaller companies commercialized their technologies. We surveyed 67 small firms

practicing the field, showing their technological areas and data on their founding and current state. From this set of companies, we conducted a case study of four selected companies working on different areas of FBDD. We tracked the various processes that the firms used in their paths towards commercialization. We show that they mobilized resources in order to create opportunities for themselves while also enabling the field's wider acceptance.

In Chapter 5, we also looked at the adoption of FBDD in large pharmaceutical companies. We surveyed the publications in the field to explore the various paths taken by firms to adopt FBDD. From these large companies, we interviewed practitioners in two large pharmaceutical firms that either played a crucial role by serving as proponents of the approach within the company or by applying the approach to their projects. Contributing to the absorptive capacity theory, we show that individuals play a crucial role in every step of the absorption process. Moreover, we show that maintaining constant contact with the field at large is crucial as it informs these proponents of strategies to further the knowledge absorption of this new approach.

Finally, in Chapter 6, we explored the role of individual researchers in the development of the field and explored some policy recommendations for future researchers. Looking at the publications in FBDD, we find that scientists are highly collaborative and highly mobile. They moved across institutions in order to gain knowledge and also help the field diffuse. We then explored how researchers can be trained to be more collaborative and mobile. We show the potential of the ITN initiative of the European Union to train such researchers.

From this exploration of the development of FBDD, we then put forward various recommendations to various stakeholders in the pharmaceutical sciences including universities, research institutes, startups, large pharmaceutical firms and policymakers. From these insights on how FBDD was adopted and commercialized, we hope to guide how actors involved with any emerging technology could effectively engage with such innovations.

Keywords: Fragment-based Drug Discovery, Pharmaceutical Sciences, Drug Discovery, Drug Development, Innovation Studies, Field Development, Absorptive Capacity, Optimal Distinctiveness