## Contents

1 Introduction .............................................. 1

2 Target-based analysis of ionization states of bioactive compounds .......... 23

3 Formation of activity cliffs is accompanied by systematic increases in ligand efficiency from lowly to highly potent compounds ................................. 29

4 Matched molecular pairs derived by retrosynthetic fragmentation ............. 41

5 Systematic identification of matching molecular series and mapping of screening hits ................................................................. 49

6 Prediction of compound potency changes in matched molecular pairs using support vector regression .......................................................... 61

7 Compound optimization through data set-dependent chemical transformations ......................................................... 75

8 Visualization of multi-property landscapes for compound selection and optimization .............................................................. 89

9 Chemical space visualization: transforming multi-dimensional chemical spaces into similarity-based molecular networks .......................... 105

10 Conclusion .............................................. 117

Bibliography ............................................. 119