Annexure D
Supplementary Data for Chapter 9

D.1 SPICERX STATISTICS

D.1.1 Statistics of Research Articles for Spices/Herbs

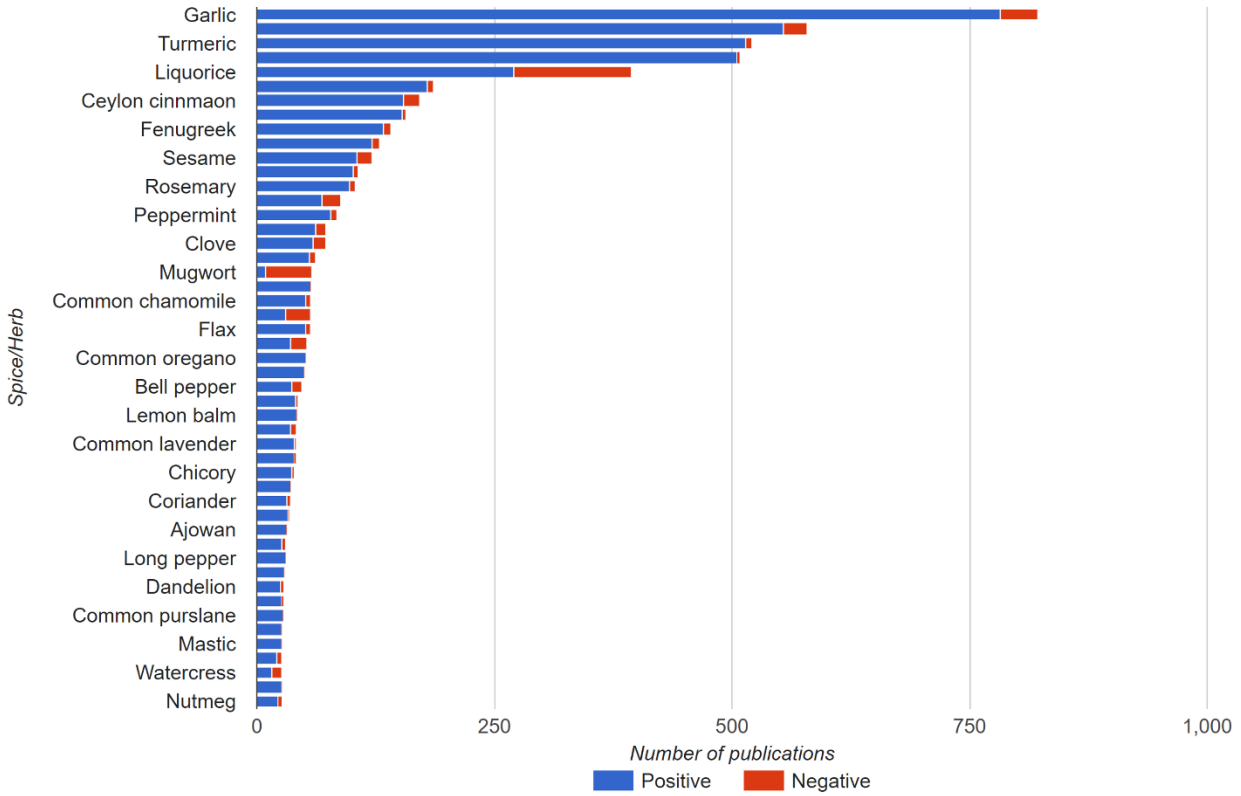

Figure D.1.1. Statistics of research articles reporting positive and negative disease associations for spices/herbs with 10 or more publications. Statistics of research articles reporting positive and negative disease associations for Top 50 spices (with 10 or more publications). Among the spices/herbs with the largest number of disease associations were Garlic (782+40), Ginkgo (554+25), Turmeric (515+6) and Ginger (505+3) with more than 500 research articles reported for each. Liquorice (123) and Mugwort (49) had the largest number of negative disease associations. For more details, please refer to the interactive graphics on the SpiceRx webpage: http://cosylab.iiitd.edu.in/spicerx/#stats

D 1.2 Statistics of research articles for MeSH disease categories

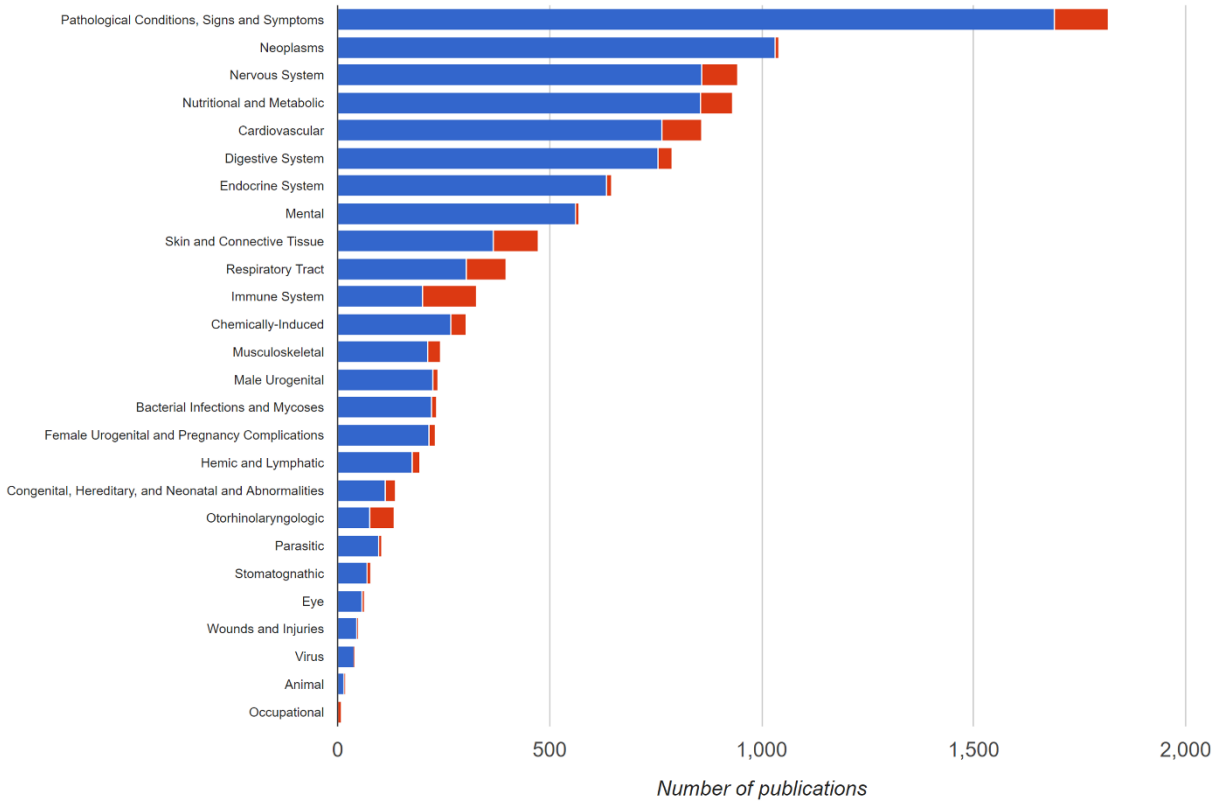

Figure D.1.2. Statistics of research articles with reports of positive and negative associations of spices/herbs corresponding to MeSH disease categories. A total of 25 MeSH disease categories were reported with therapeutic and/or adverse effects for culinary spices and herbs. Among major disease categories that are influenced by spices/herbs were 'Pathological Conditions, Signs and Symptoms' (1690+127), 'Neoplasms' (1033+9), 'Nervous System Diseases' (859+84), 'Nutritional and Metabolic Diseases' (857+74), 'Cardiovascular Disease' (765+95), 'Digestive Systems Disease' (755+35), 'Endocrine Systems Diseases' (635+10) and 'Mental Disorders' (561+7), with more than 500 research articles reported for each. Together, these MeSH categories cover a large number of diseases for which diet has been reported to have major role in pathological development and progression such as diabetes mellitus type 2, obesity, coronary artery disease, hypertension, and prostate cancer, among others. For more details, please refer to the interactive graphics on the SpiceRx webpage: http://cosylab.iiitd.edu.in/spicerx/#stats

D.1.3 Statistics of research articles for therapeutic effects of phytochemicals

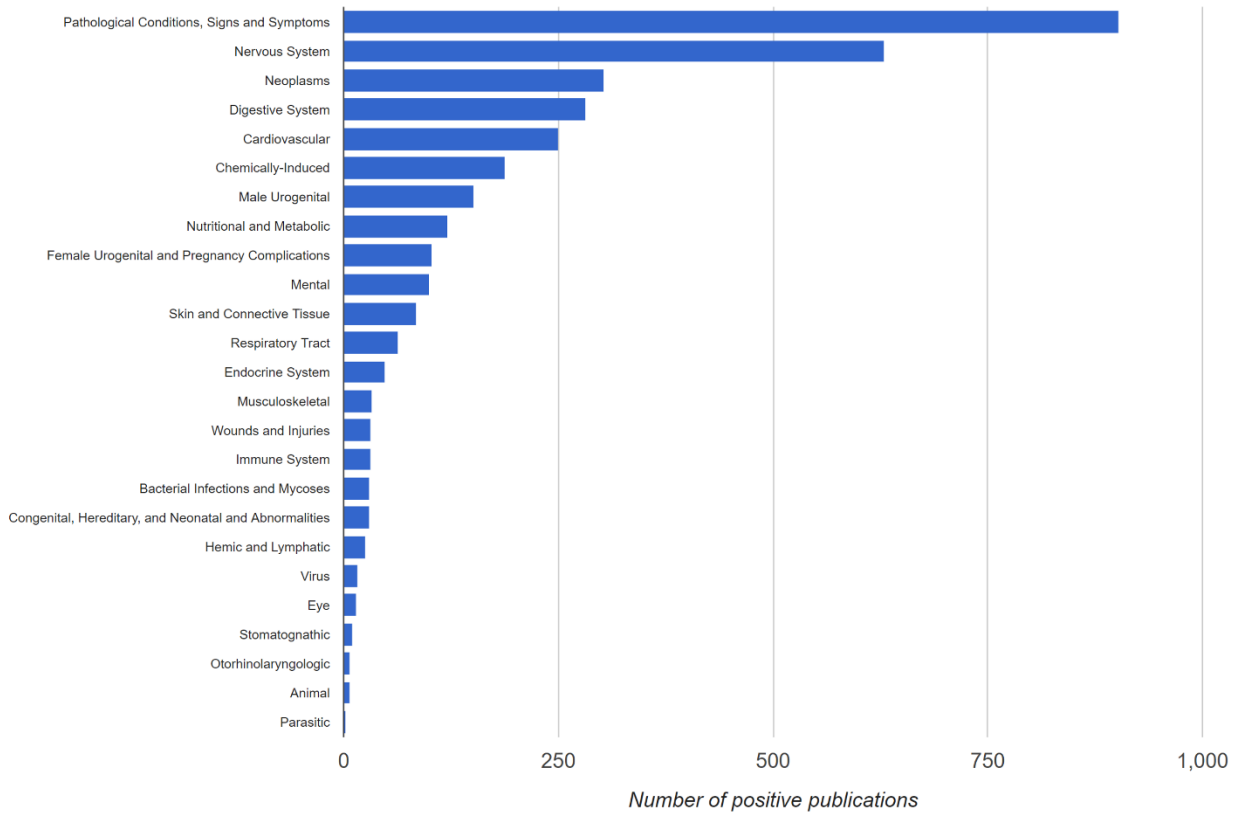

Figure D.1.3: Statistics of research articles reporting positive associations for phytochemicals against MeSH disease categories. These data were obtained from the Comparative Toxicogenomics Database. Amongst the top disease categories that phytochemicals were beneficial against were 'Pathological conditions, signs and symptoms' (903), 'Nervous system disorders (629)', 'Neoplasms' (303) 'Digestive system disorders' (283) and 'Cardiovascular disorders' (250). To explore further, please refer to the interactive graphics on the SpiceRx webpage: http://cosylab.iiitd.edu.in/spicerx/#stats

D.1.4 Molecular weight distribution of phytochemicals

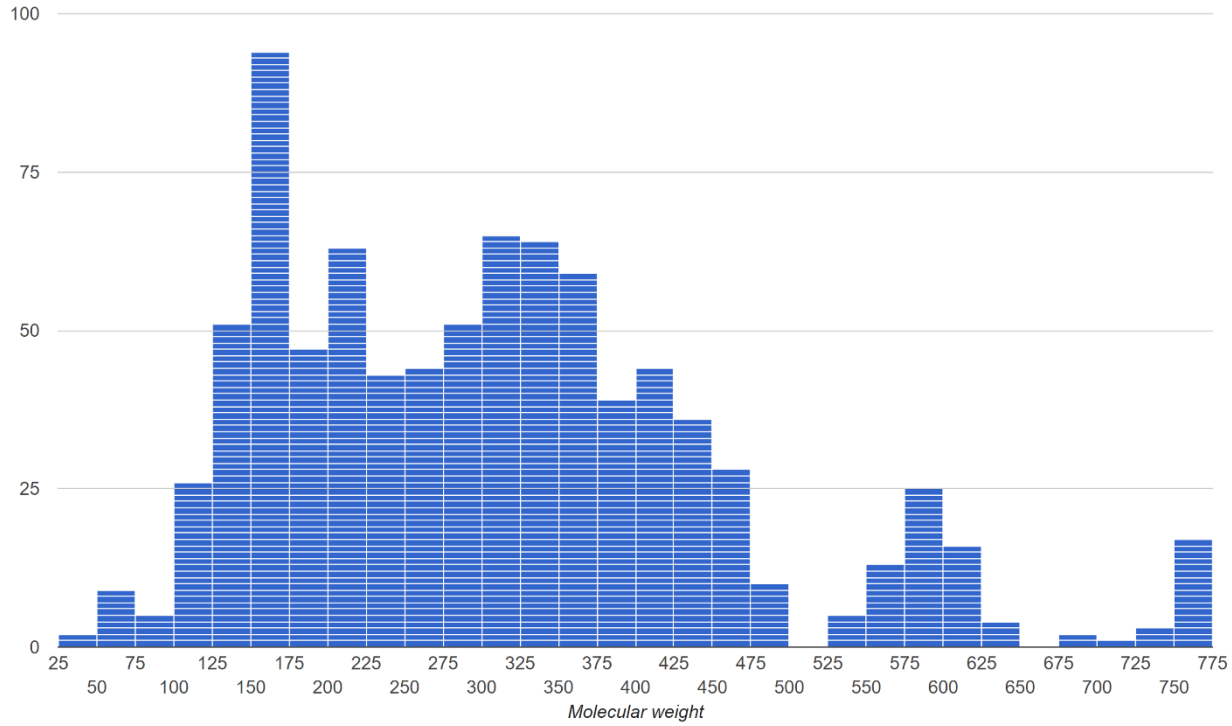

Figure D.1.4: Distribution of molecular weights of phytochemicals from spices/herbs. The majority of the compounds had weight below 500 g/mol. To explore these data, please refer to the interactive graphics on the SpiceRx webpage: http://cosylab.iiitd.edu.in/spicerx/#stats

D.1. 5 Partition coefficient distribution of phytochemicals

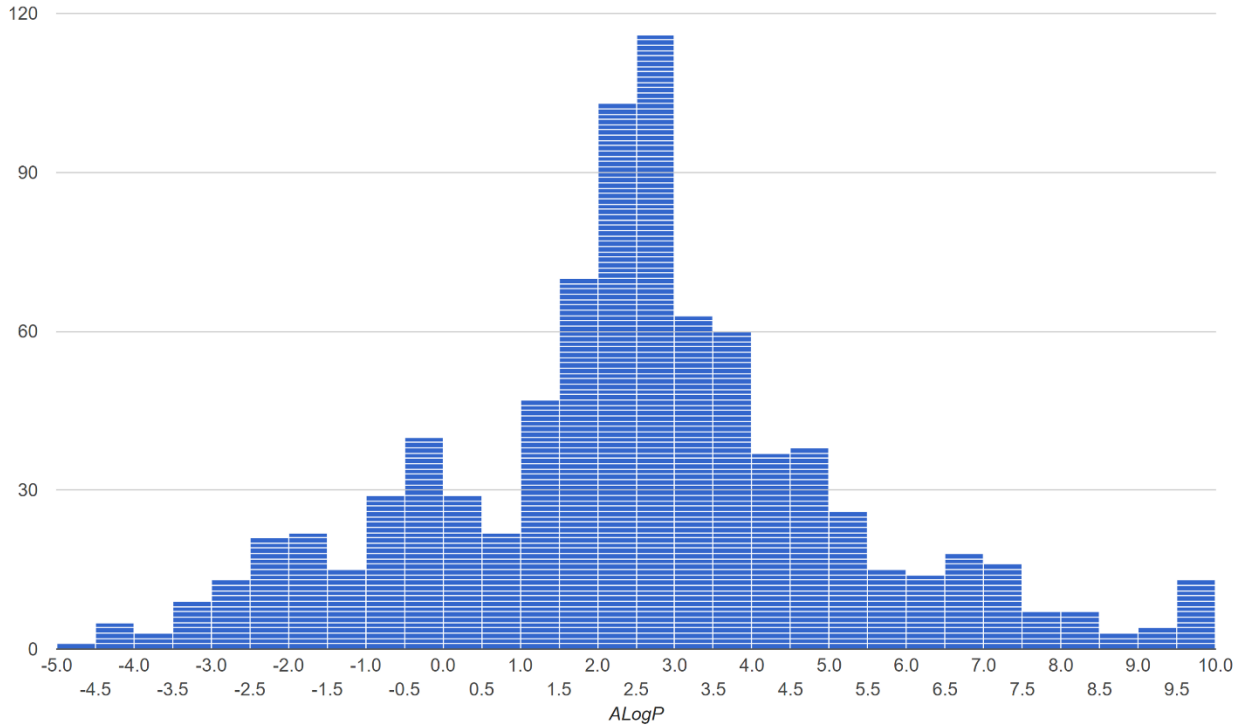

Figure D.1.5: Distribution of partition coefficients (ALogP) of phytochemicals from spices/herbs. The majority of the molecules compounds had the partition coefficient below 5, thus fulfilling one of the criteria for drug-likeness. To explore these data, please refer to the interactive graphics on the SpiceRx webpage: http://cosylab.iiitd.edu.in/spicerx/#stats