LIST OF TABLES

Table	Caption	Page
Table 1.1.	Classes of terpenoid with their isoprene units and molecular formula	4
Table 1.2.	Terpenoids approved for therapeutic use	12 -13
Table 3.1.	Molar refraction (R_M) at 589 nm, (cm^3mol^{-1})	89
Table 4.1.	Structures and activity of 47 compounds of 23-hydroxybetulinic acid derivatives	114 - 118
Table 4.2.	Correlation matrix of 15 training RMGPa inhibitors	120
Table 4.3.	SIC_1, CIC_1, quantum chemical descriptors, molar refractivity and molar volume of 15 training RMGPa inhibitors	121
Table 4.4.	List of experimental and predicted logIC_{50} of 15 training RMGPa inhibitors	123
Table 4.5.	Quantum chemical descriptors, SIC_1 and CIC_1 of 5 test RMGPa inhibitors	124
Table 4.6.	List of experimental and predicted logIC_{50} of 5 test RMGPa inhibitors	124
Table 4.7.	Correlation matrix of 20 training antiproliferative compounds against HeLa cells with quantum chemical, molar refractivity and molar volume parameters	126
Table 4.8.	Correlation matrix of 20 training antiproliferative compounds against HeLa cells with different topological indices	126
Table 4.9.	Quantum chemical descriptors, molar refractivity and molar volume of 20 training antiproliferative compounds against HeLa cells	127 - 128

Table 4.10.	Topological indices of 20 training antiproliferative compounds against HeLa cells	128 - 129
Table 4.11.	List of experimental and predicted $logIC_{50}$ of 20 training antiproliferative compounds against HeLa cells	130 - 131
Table 4.12.	Quantum chemical descriptors, SIC_1 and CIC_1 of 8 test antiproliferative compounds against HeLa cells	131 - 132
Table 4.13.	List of experimental and predicted $logIC_{50}$ of 8 test antiproliferative inhibitors against HeLa cells	132
Table 4.14.	Predicted Antiproliferative activity/ RMGPa inhibitory activity of studied compounds	134 - 135
Table 4.15.	The binding energies of 47 docked compounds	135 - 136
Table 5.1.	The Gibbs free energy of P and PH_2 in gas phase and solution, together with solvation free energies of species calculated at 6-31G* and 6-311G** basis set	157
Table 5.2.	Difference in the interaction energies (ΔE_{diff}), difference in solvation free energy (ΔG_{diff}), ΔG^0 (total) and absolute E^0 of puupehedienone (P) and puupehenone (PH_2) complexes with different water molecules	159
Table 6.1.	Minimal inhibitory concentration (MIC) and selected molecular electronic properties of the studied compounds	164
Table 6.2.	Correlation matrix of $MIC_{(SW480)}$ and the electronic descriptors for the studied compounds	168
Table 7.1.	Structural feature of oleanolic acid and its derivatives having PTP1B inhibitory activity	173 - 178
Table 7.2.	Binding energy (EB), Solvent accessible surface area (SASA), Molar refractivity (MR), Molar volume (MV), Partition coefficient (logP), HOMO energy (EH), LUMO energy (EL) and Dipole moment (μ) of 41 PTP1B inhibitors	184 - 185

Table 7.3.	List of experimental and predicted pIC_{50} of 28 training compounds	186 - 187
Table 7.4.	List of experimental and predicted pIC_{50} of 7 test compounds	188
Table 8.1.	DFT calculated energies of the various conformers of halomon and the relative energies with respect to the most stable conformation	196
Table 8.2.	Optimized structural parameters of most stable conformer of halomon with experimental data	197 - 199
Table 9.1.	Structural feature of sesquiterpene lactones from Inula falconeri with anti-inflammatory activity	203 - 205
Table 9.2.	SIC_1, CIC_1, quantum chemical descriptors, entropy at 298 K and electronegativity of 20 inhibitors	207 - 208
Table 9.3.	List of experimental and predicted $logIC_{50}$ of 16 training compounds	209
Table 9.4.	List of experimental and predicted $logIC_{50}$ of 4 test compounds	210