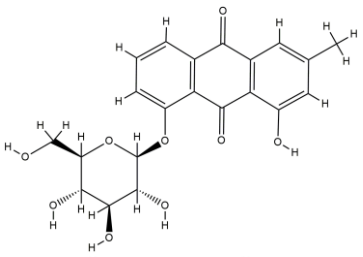
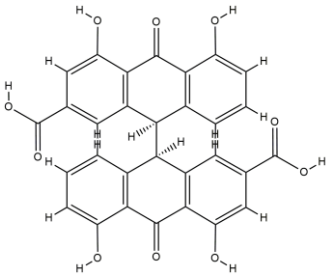
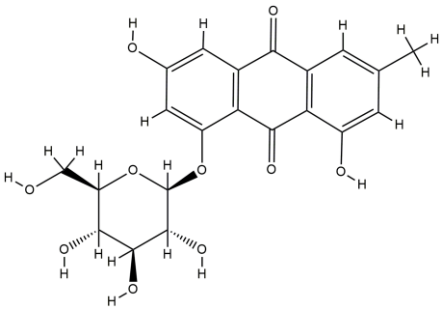
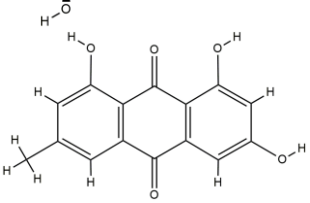
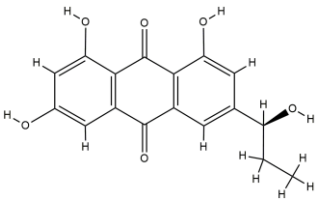
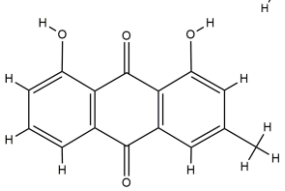
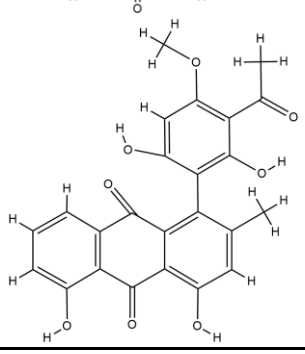
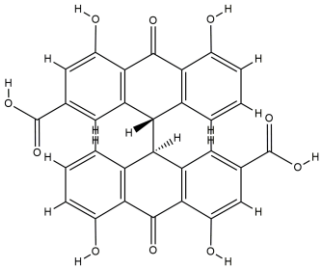
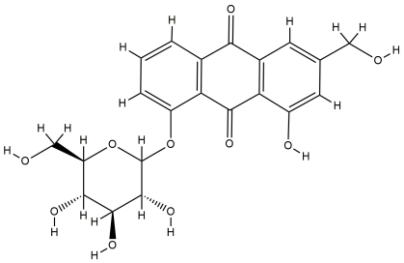
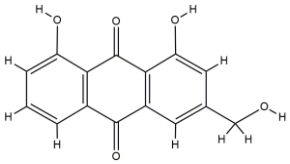
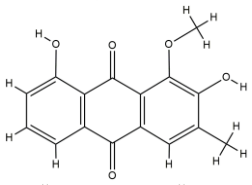
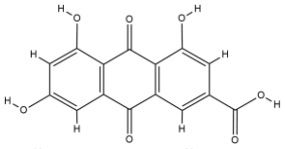
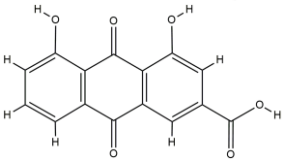
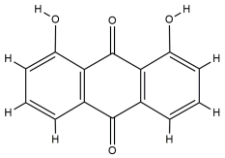
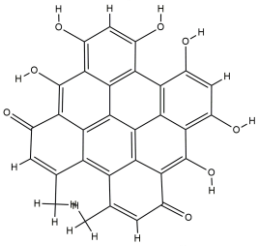
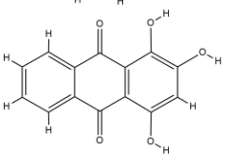
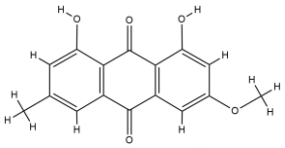
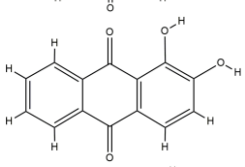
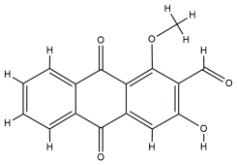
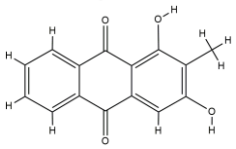
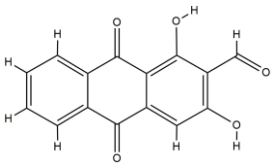
Supplementary Table 1. Chemical structures of a total of 21 anthraquinones considered as small molecules in this study for possible matrix metalloproteinase inhibition achieved by ChemDraw version 12.0.2.1076 software

PubChem ID	Ligand name	Chemical structure	Molecular weight (g/mol)
442731	Pulmatin (Chrysophanol 8-O-glucoside)		416.4
92826	Sennidin A		538.5
99649	Emodin-8-glucoside		432.4
3220	Emodin		270.24
101286218	Rhodoptilometrin		314.29
10208	Chrysophanol		254.24
442753	Knipholone		434.4

PubChem ID	Ligand name	Chemical structure	Molecular weight (g/mol)
10459879	Sennidin B		538.5
126456371	Aloe Emodin 8-Glucoside		432.4
10207	Aloe-emodin		270.24
3083575	Obtusifolin		284.26
361510	Emodic acid		300.22
10168	Rhein		284.22
2950	Danthron		240.21
3663	Hypericin		504.40
6683	Purpurin		256.21

PubChem ID	Ligand name	Chemical structure	Molecular weight (g/mol)
10639	Physcion		284.26
6293	Alizarin		240.21
2948	Damnacanthal		282.25
124062	Rubiadin		254.24
160712	Nordamnacanthal		268.22