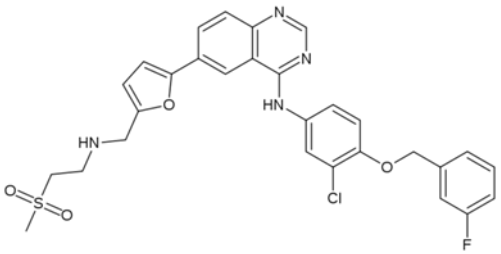
Table 2: Docking scores of different 2-methylindoline compounds in the EGF receptor active sites

Molecule (Kcal/mol)	Autodock Score
	-13.8
AZ2	-7.9
AZ3	-8.1
AZ4	-8.3
AZ5	-7.6
AZ6	-8.0
AZ7	-7.9

The Aminoacetylenic 2-methylindoline derivatives also have favorable binding energies to COX-1 and COX-2 enzymes so they seem to have good fitting to these active sites (Table 3).

AZ5 was predicted to have best binding (-8.0 kcal/mol) with the COX-1 active site . As shown in (Figure 62) , AZ5 has a good fitting and makes many van der Waals contacts with the surrounding hydrophobic residues (i.e. Val349, Tyr355, Leu359, Trp387, Phe518, Met522, Ile523 and Leu531). Moreover, it makes a strong hydrogen bond with the backbone amide of Met522 .

AZ5 was also the best binder with the COX-2 active site (Figure 63) where it has a similar binding mode to that adopted in the COX-1 pocket. In addition to the extensive hydrophobic interactions made by AZ5, an electrostatic interaction with the Leu352 backbone amide was made by its protonated nitrogen atom.