**SUPPLEMENTARY FILE**

*In Silico* Analysis for Exploring the Potential Inhibitors Against Breast Cancer (MCF7) Using Curcumin Analogue Compounds

Neni Frimayanti 1,\*, Adel Zamri 2, Yum Eryanti 2

1 Sekolah Tinggi Ilmu Farmasi (STIFAR), Pekanbaru, Riau, Indonesia

2 Department of Chemistry, Faculty of Mathematics and Natural of Mathematics and Natural Sciences, Universitas Riau, Riau, 28293, Indonesia

\* Corresponding author: nenifrimayanti@gmail.com

**Table S.1**. Molecular structure of curcumin analogue with their biological activity

|  |  |  |
| --- | --- | --- |
| **14.25** | **10.17** | **55.16** |
| **Cpd 1** | **Cpd 2** | **Cpd 33** |
| **55.55** | **2.31** | **19.49** |
| **Cpd 4** | **Cpd 5** | **Cpd 6** |
| **27.54** | **54.96** | **3.67** |
| **Cpd 7** | **Cpd 8** | **Cpd 9** |
| **9.59** | **18.46** | **21.30** |
| **Cpd 10** | **Cpd 11** | **Cpd 12** |
| **8.97** | **7.43** | **229.34** |
| **Cpd 13** | **Cpd 14** | **Cpd 15** |
| **16.62** | **3.97** | **2.82** |
| **Cpd 16** | **Cpd 17** | **Cpd 18** |
| **7.40** | **44.69** | **65.20** |
| **Cpd 19** | **Cpd 20** | **Cpd 21** |
| **3.81** | **14.26** | **38.84** |
| **Cpd 22** | **Cpd 23** | **Cpd 24** |
| **1.64** | **13.34** | **63.0** |
| **Cpd 25** | **Cpd 26** | **Cpd 27** |
| **3.81** | **17.03** | **32.32** |
| **Cpd 28** | **Cpd 29** | **Cpd 30** |
| **25.25** | **5.20** | **5.94** |
| **Cpd 31** | **Cpd 32** | **Cpd 33** |
| **6.07** | **131.49** | **9.69** |
| **Cpd 34** | **Cpd 35** | **Cpd 36** |
| **69.00** | **22.85** | **23.70** |
| **Cpd 37** | **Cpd 38** | **Cpd 39** |
| **19.64** | **23.78** | **56.11** |
| **Cpd 40** | **Cpd 41** | **Cpd 42** |
| **60.63** | **54.18** | **4.99** |
| **Cpd 43** | **Cpd 44** | **Cpd 45** |



**Figure S.1**. RMSD graph for active compounds