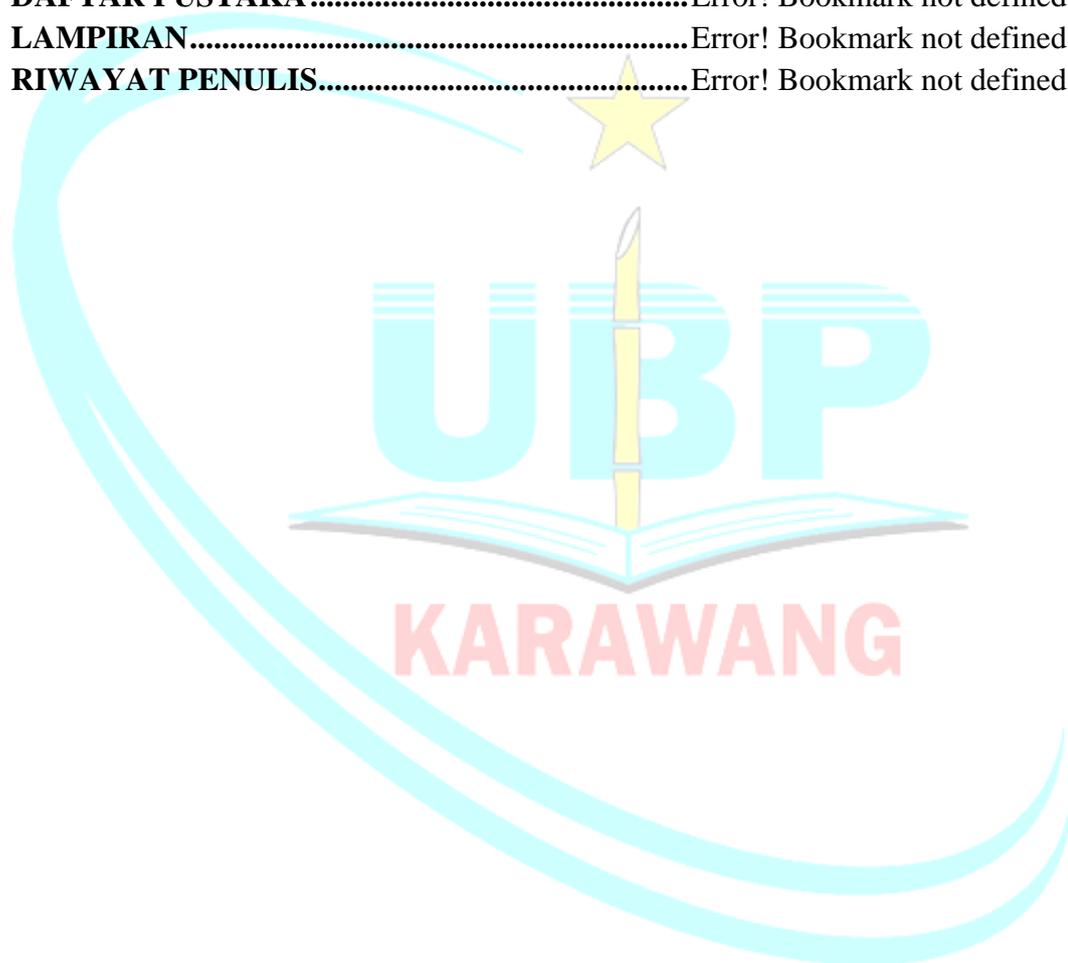


DAFTAR ISI

COVER.....	i
LEMBAR PERSETUJUAN.....	ii
LEMBAR	
PENGESAHAN.....	Error!
Bookmark not defined.	
LEMBAR PERNYATAAN	Error! Bookmark not defined.
KATA PENGANTAR.....	Error! Bookmark not defined.
ABSTRAK	Error! Bookmark not defined.
ABSTRACT	Error! Bookmark not defined.
DAFTAR ISI.....	Error! Bookmark not defined.
DAFTAR TABEL	xii
DAFTAR GAMBAR.....	xiii
DAFTAR SINGKATAN.....	xiv
DAFTAR LAMPIRAN	xv
BAB I PENDAHULUAN.....	Error! Bookmark not defined.
1.1 Latar belakang	Error! Bookmark not defined.
1.2 Rumusan Masalah	Error! Bookmark not defined.
1.3 Tujuan Penelitian.....	Error! Bookmark not defined.
1.4 Manfaat.....	Error! Bookmark not defined.
1.4.1 Peneliti	Error! Bookmark not defined.
1.4.2 Institusi	Error! Bookmark not defined.
1.4.3 Masyarakat.....	Error! Bookmark not defined.
BAB II TINJUAN PUSTAKA	Error! Bookmark not defined.
2.1 Daun Sambung Nyawa	Error! Bookmark not defined.
2.1.1 Klasifikasi Tanaman Sambung Nyawa..	Error! Bookmark not defined.
2.1.2 Morfologi Tanaman Sambung Nyawa..	Error! Bookmark not defined.
2.1.3 Manfaat Tanaman	Error! Bookmark not defined.
2.1.4 Penggunaan Tradisional.....	Error! Bookmark not defined.
2.1.5 Kandungan Kimia.....	Error! Bookmark not defined.
2.2 Inflamasi	Error! Bookmark not defined.
2.3 Jalur Induksi Inflamasi	Error! Bookmark not defined.
2.4 Anti-Inflamasi.....	Error! Bookmark not defined.
2.5 <i>Cyclooxygenase-1</i>	Error! Bookmark not defined.
2.6 Inhibitor <i>Cyclooxygenase-1</i>	Error! Bookmark not defined.
2.6.1 Ibuprofen.....	Error! Bookmark not defined.
2.7 <i>Cyclooxygenase-2</i>	Error! Bookmark not defined.
2.8 Inhibitor <i>Cyclooxygenase-2</i>	Error! Bookmark not defined.
2.8.1 Celecoxib	Error! Bookmark not defined.
2.9 Flavonoid.....	Error! Bookmark not defined.
2.10 <i>Rational Drug Design</i>	Error! Bookmark not defined.

2.11 Penambatan Molekuler (<i>Molecular Docking</i>).....	Error! Bookmark not defined.
2.12 Protein Data Bank (Pdb).....	Error! Bookmark not defined.
2.13 <i>Molecular Dynamic</i>	Error! Bookmark not defined.
2.14 Farmakokinetika Dan Toksisitas	Error! Bookmark not defined.
2.15 Hasil Penelitian Yang Relevan.....	Error! Bookmark not defined.
BAB III METODE PENELITIAN	Error! Bookmark not defined.
3.1 Jenis dan Rancangan Penelitian.....	Error! Bookmark not defined.
3.2 Sampel	Error! Bookmark not defined.
3.3 Bahan Penelitian.....	Error! Bookmark not defined.
3.3.1 Senyawa Uji.....	Error! Bookmark not defined.
3.3.2 Reseptor	Error! Bookmark not defined.
3.4 Alat Penelitian	Error! Bookmark not defined.
3.4.1 Perangkat Keras Komputer.....	Error! Bookmark not defined.
3.4.2 Perangkat Lunak Komputer	Error! Bookmark not defined.
3.5 Variabel Penelitian	Error! Bookmark not defined.
3.5.1 Variabel Bebas	Error! Bookmark not defined.
3.5.2 Variabel Terikat	Error! Bookmark not defined.
3.5.3 Definisi Operasional Variabel	Error! Bookmark not defined.
3.6 Lokasi Penelitian dan Waktu Penelitian.....	Error! Bookmark not defined.
3.7 Prosedur Penelitian.....	Error! Bookmark not defined.
3.7.1 Preparasi Struktur Ligan	Error! Bookmark not defined.
3.7.2 Identifikasi Reseptor Target.....	Error! Bookmark not defined.
3.7.3 Preparasi Reseptor dengan Ligan Alami.....	Error! Bookmark not defined.
3.7.4 Validasi Reseptor	Error! Bookmark not defined.
3.7.5 <i>Virtual Screening</i> dan <i>docking</i> Terhadap Reseptor Target.....	Error! Bookmark not defined.
Bookmark not defined.	
3.7.6 Visualisasi Hasil <i>Docking</i>	Error! Bookmark not defined.
3.7.7 Simulasi Molekuler Dinamik.....	Error! Bookmark not defined.
3.7.8 <i>Lipinski's rule of Five</i>	Error! Bookmark not defined.
3.7.9 Prediksi Farmakokinetik dan Toksisitas	Error! Bookmark not defined.
3.7 Diagram Penelitian	Error! Bookmark not defined.
3.8 Analisis Data	Error! Bookmark not defined.
BAB IV HASIL DAN PEMBAHASAN	Error! Bookmark not defined.
4.1 Preparasi Senyawa Flavonoid	Error! Bookmark not defined.
4.2 Identifikasi Reseptor Target	Error! Bookmark not defined.
4.3 Preparasi Reseptor Dengan Ligan Alami	Error! Bookmark not defined.
4.4 Validasi Reseptor Metode <i>Docking</i>	Error! Bookmark not defined.
4.5 <i>Virtual Screening</i> dan <i>Docking Ligan Uji</i> Terhadap Reseptor Target .	Error! Bookmark not defined.
Bookmark not defined.	
4.6 Visualisasi Hasil <i>Docking</i>	Error! Bookmark not defined.
4.7 Simulasi Dinamika Molekular.....	Error! Bookmark not defined.

4.7.1 Analisis Simulasi Dinamika Molekular Reseptor 1EQG	Error!
Bookmark not defined.	
4.7.2 Analisis Simulasi Dinamika Molekular Reseptor 3LN1	Error!
Bookmark not defined.	
4.8 <i>Lipinski's Rule Of Five</i>	Error! Bookmark not defined.
4.9 Prediksi Farmakokinetika dan Toksisitas	Error! Bookmark not defined.
BAB V KESIMPULAN DAN SARAN	Error! Bookmark not defined.
5.1 Kesimpulan	Error! Bookmark not defined.
5.2 Saran	Error! Bookmark not defined.
DAFTAR PUSTAKA	Error! Bookmark not defined.
LAMPIRAN	Error! Bookmark not defined.
RIWAYAT PENULIS	Error! Bookmark not defined.





DAFTAR TABEL

Tabel 2.1 Hasil Penelitian Yang Relevan	16
Tabel 3.1 Definisi Operasional Variabel	22
Tabel 4.1 Hasil Preparasi Senyawa Flavonoid	30
Tabel 4.2 Jumlah Residu Pada RMSD	35
Tabel 4.3 Pengaturan <i>Grid Box</i> dan Hasil Validasi <i>Docking</i>	38
Tabel 4.4 Hasil <i>Virtual Screening</i> Reseptor 1EQG dan 3LN1	40
Tabel 4.5 Perbandingan Visualisasi Hasil <i>Docking</i> Reseptor Target	42
Tabel 4.6 Nilai Rata-rata, Minimum dan Maksimum RMSD Kompleks 1EQG..	49
Tabel 4.7 Nilai Rata-rata, Minimum dan Maksimum RMSF Reseptor 1EQG....	51
Tabel 4.8 Nilai Rata-rata, Minimum dan Maksimum RMSD Kompleks 3LN1...54	
Tabel 4.9 Nilai Rata-rata, Minimum dan Maksimum RMSF Reseptor 3LN1....	56

Tabel 4.10 Hasil Pengujian <i>Drug Scan</i> Pada Senyawa Flavonoid	58
Tabel 4.11 Hasil Pengujian Farmakonetika Pada Senyawa Flavonoid	61
Tabel 4.12 Hasil Pengujian Toksisitas Pada Senyawa Flavonoid	64



DAFTAR GAMBAR

Gambar 2.1 Daun Sambung Nyawa	6
Gambar 2.2 Struktur Celecoxib	12
Gambar 2.3 Struktur Flavonoid	13
Gambar 3.1 Senyawa Turunan Flavonoid	20
Gambar 3.2 Alur Penelitian	28
Gambar 4.1 Hasil Plot Ramachandran (a) 1EQG (b) 3LN1.....	34
Gambar 4.2 Hasil Overall quality factor ERRAT (a) 1EQG (b) 3LN1.....	36
Gambar 4.3 Overlay Struktur Ligan Alami (a) 1EQG, (b) 3LN1.....	39
Gambar 4.4 Hasil Visualisasi 2D dan 3D 1EQG.....	45
Gambar 4.5 Hasil Visualisasi 2D dan 3D 3LN1.....	46
Gambar 4.6 Hasil RMSD Dinamika Molekul 1EQG	49

Gambar 4.7 Hasil RMSF Dinamika Molekul 1EQG.....	50
Gambar 4.8 Grafik Protein RMSF dan Kontak Residu.....	52
Gambar 4.9 Interkasi Residu Kontak Dengan Senyawa Homoorinetin.....	52
Gambar 4.10 Hasil RMSD Dinamika Molekul 3LN1.....	54
Gambar 4.11 Hasil RMSF Dinamika Molekul 3LN1.....	55
Gambar 4.12 Grafik Protein RMSF dan Kontak Residu.....	57
Gambar 4.13 Interaksi Residu Dengan Senyawa Apigenin.....	57



DAFTAR SINGKATAN

COX	: <i>Cyclooxygenase</i>
COX-1	: <i>Cyclooxygenase 1 (Siklooksigenase 1)</i>
COX-2	: <i>Cyclooxygenase 2 (Siklooksigenase 2)</i>
PDB	: <i>Protein Datan Bank</i>
2D	: 2 Dimensi
3D	: 3 Dimensi
CaCO2	: <i>Human Epithelial Colorectal Adenocarcinoma Cells</i>
%VDSS	: <i>Volume Distribution</i>
%BBB	: <i>Persentase Blood Brain Barrier</i>

OCT2	: <i>Organic Cation Transpoter 2</i>
ADMET	: Absorpsi, Distribusi, Metabolisme, Ekresi dan Toksisitas
LD50	: <i>Lethal Dose</i>
<i>G.procumbens</i>	: <i>Gynura procumbens</i>
AINS	: <i>Anti Inflammation Non Steroid</i>
MD	: <i>Molekular Dynamic</i>
SAVES	: <i>Structure Analysis and Verification Server</i>
ΔG	: Energi bebas gibbs
RMSD	: <i>Root Mean Standar Deviation</i>
RMSF	: <i>Root Mean Standar Fluctuation</i>
PGE	: <i>Prostaglandin Gyceryl Ester</i>
NO	: <i>Nitrit Oxide</i>
%HIA	: <i>Persentase Human Intestinal Absorbtion</i>
LGA	: <i>Lamarcian Genetic Algoritm</i>
Ns	: <i>Nanosecond</i>
kcal	: Kilokalori

DAFTAR LAMPIRAN

Lampiran 1. 2 Preparasi Ligan Senyawa Flavonoid	73
Lampiran 2. 1 Reseptor 1EQG	74
Lampiran 2. 2 Reseptor 3LN1	74
Lampiran 3. 1 Prose MD	75
Lampiran 4. 1 <i>Drug Scan</i> Homoorientin	76
Lampiran 4. 2 <i>Drug Scan</i> Apigenin	76
Lampiran 4. 3 <i>Drug Scan</i> Negletein	77
Lampiran 4. 4 <i>Drug Scan</i> Luteolin	77
Lampiran 4. 5 <i>Drug Scan</i> Kaemferol	78
Lampiran 5. 1 Pkcsn Homoorientin	79

Lampiran 5. 2 Pkcsm Apigenin	81
Lampiran 5. 3 Pkcsm Negletein	82
Lampiran 5. 4 Pkcsm Luteolin	83
Lampiran 5. 1 pKCSM Kaemferol	84

