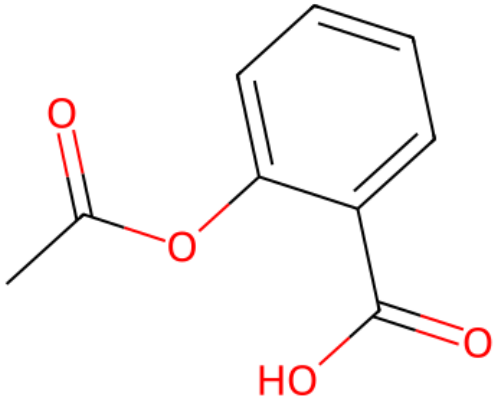
■ PharmaClaw Drug Discovery Report

SAMPLE REPORT — Aspirin (Acetylsalicylic Acid)

SMILES: `CC(=O)Oc1ccccc1C(=O)O`
Molecular Formula: C■H■O■
Disease Target: Pain / Inflammation / Cardiovascular
Report Type: Full Pipeline (9 Agents)



1. Molecular Properties

Property	Value	Status
Molecular Weight	180.04 g/mol	■ < 500
LogP	1.31	■ < 5
TPSA	63.6 Å²	■ < 140
H-Bond Donors	1	■ < 5
H-Bond Acceptors	3	■ < 10
Rotatable Bonds	2	■ ≤ 10
Aromatic Rings	1	—
Heavy Atoms	13	—

2. Drug-Likeness Assessment

Rule	Result	Details

Lipinski Rule of Five	■ PASS	0 violations
Veber Rules	■ PASS	TPSA=63.6, RotB=2
QED Score	0.550	0 = unfavorable, 1 = favorable

3. ADME Predictions

Property	Prediction	Confidence
Bbb	moderate	medium
Solubility	{'logS_estimate': -2.39, 'class': 'moderate', 'rationale': 'ESOL-approximation from descriptors'}	
Gi Absorption	high	
Cyp3A4 Inhibition	{'risk': 'low', 'rationale': 'Below risk thresholds'}	
Pgp Substrate	unlikely	
Plasma Protein Binding	moderate-low	

4. Toxicology & Safety Profile

Overall Risk: **LOW**

Check	Result
Lipinski Violations	0 — ■ PASS
Veber Violations	0 — ■ PASS
QED Score	0.55
PAINS Alerts	0 — ■ Clean

5. Intellectual Property Analysis

Overall IP Risk: **LOW**
Max Tanimoto Similarity: **0.2041** (threshold: 0.85)

Bioisostere Suggestions:

6. Consensus Assessment

Category	Assessment
Drug-likeness	■ Excellent — All rules pass, well-known drug
Safety	■ Low risk — No PAINS, no structural alerts
ADME	■ High GI absorption, moderate BBB, good solubility
IP Status	■ LOW risk — Well off-patent
Overall Score	8.5 / 10 — Established drug with excellent profile