5. Kesimpulan

Berdasarkan hasil penelitian, dengan menggunakan algoritma *firefly* untuk seleksi fitur dan *support vector machine*, dapat digunakan untuk pembangunan model prediksi *larvicidal phytocompound* sebagai anti-*Ae. aegypti*. Fitur yang telah diseleksi sebelumnya menggunakan standar deviasi < 0.5, diseleksi kembali menggunakan algoritma *firefly* untuk mendapatkan kombinasi fitur dari setiap kernel berdasarkan nilai error terkecil, sehingga terpilih 9 fitur untuk kernel linear, 8 fitur untuk kernel poly, dan 7 fitur untuk kernel rbf. *Hyperparameter tuning* dilakukan untuk mendapatkan parameter yang memiliki performa lebih baik, sehingga didapatkan kernel linear dengan skor R^2 data latih 0.710 dan data uji 0.866, beserta skor Q^2 0.965. Skor tersebut memenuhi *threshold* yang telah disepakati sehingga model dianggap valid untuk memprediksi aktifitas senyawa yang tidak diketahui nilainya sebagai anti *Ae. aegypti*.

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Lampiran

Dataset

No.	Name	SMILES	pLC50
1	(-)-Camphene	CC1(C)[C@H]2CC[C@H](C2)C1=C	2.79
2	(±)-camphor	CC1(C)[C@@H]2CC[C@@]1(C)C(=O)C2	2.36
3	1,4-cineole	CC(C)C12CCC(C)(CC1)O2	2.31
4	1,8-cineole	CCC1CCC(C)(C)OC1(C)C	2.04
5	carvacrol	CC(C)c1ccc(C)c(O)c1	3.47
6	carvacryl acetate	CC(C)c1ccc(C)c(OC(=O)C)c1	3.32
7	carvacryl chloroacetate	CC(C)c1ccc(C)c(OC(=O)CCl)c1	3.64
8	carvacryl trichloroacetate	CC(C)c1ccc(C)c(OC(=O)C(Cl)(Cl)Cl)c1	3.59
9	carvacryl propionate	CCC(=O)Oc1cc(ccc1C)C(C)C	3.49
10	carvacryl benzoate	CC(C)c1ccc(C)c(OC(=O)c2ccccc2)c1	3.66
11	2-Hydroxy-3-methyl-6-(1-methylethyl)-benzaldehyde	CC(C)c1ccc(C)c(O)c1C=O	3.43
12	carvacrylglycolic acid	CC(C)c1ccc(C)c(OCC(=O)O)c1	3.09
13	thymyl acetate	CC(C)c1ccc(C)cc1OC(=O)C	3.32
14	thymyl chloroacetate	CC(C)c1ccc(C)cc1OC(=O)CCl	3.66
15	thymyl trichloroacetate	CC(C)c1ccc(C)cc1OC(=O)C(Cl)(Cl)Cl	3.85
16	thymyl propionate	CCC(=O)Oc1cc(C)ccc1C(C)C	3.49