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Supplementary Material: A New Cytotoxic Dimeric Sesquiterpene Isolated from *Inula racemosa* Hook. f. (Root): *In Vitro* and *In Silico* Analyses

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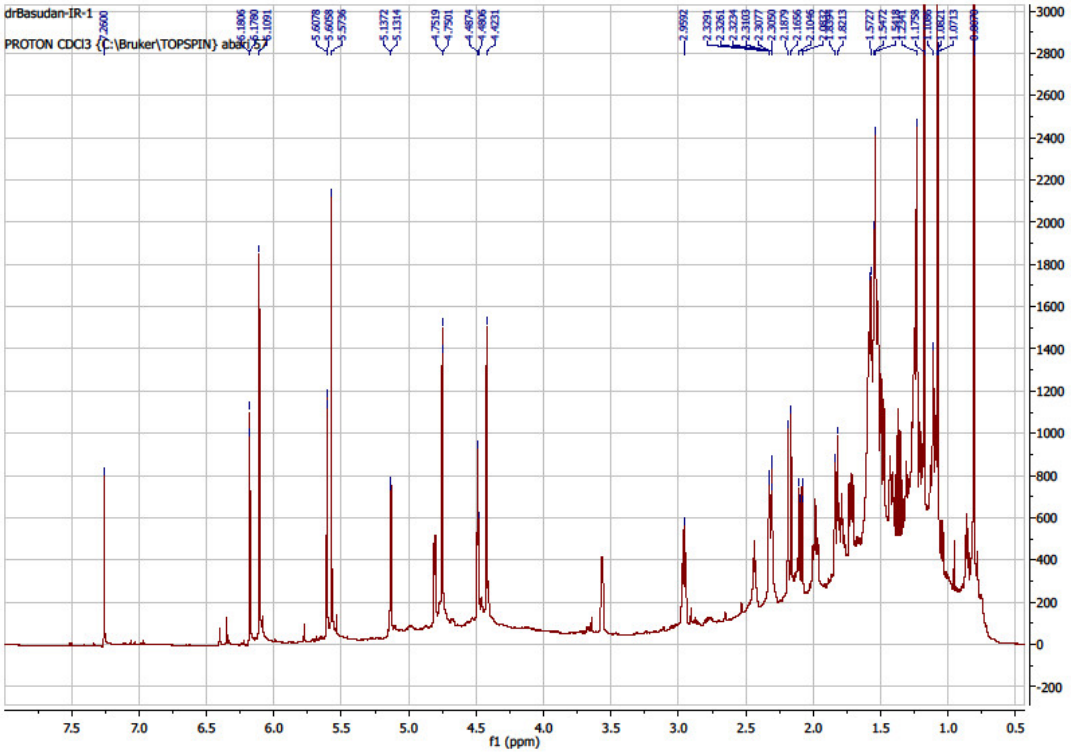

Figure S1. [1]H NMR spectrum of compound **1** (Disesquicin).

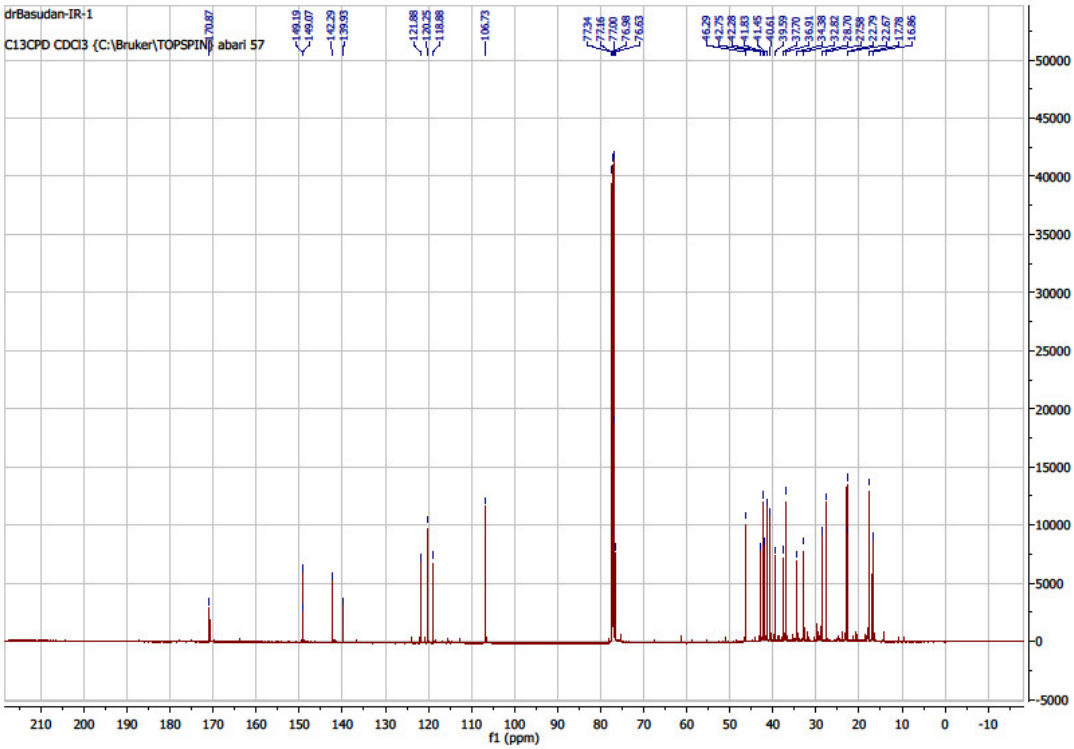

Figure S2. [13]C NMR spectrum of compound **1** (Disesquicin).

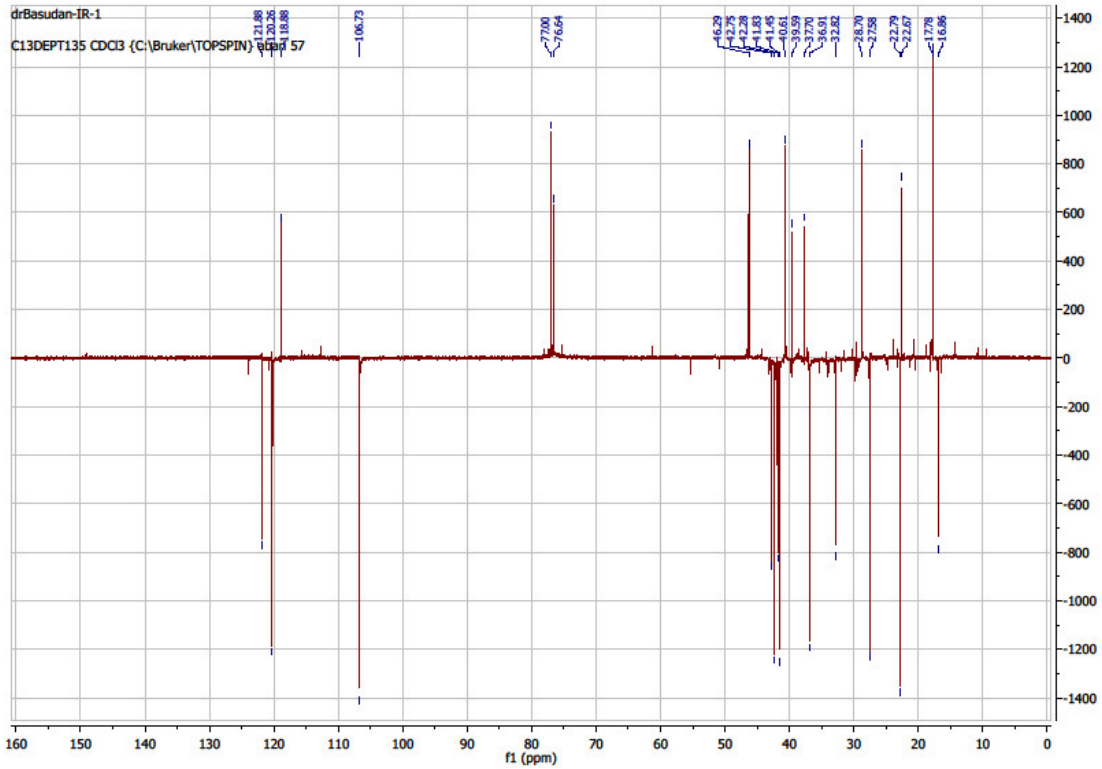

Figure S3. DEPT spectrum of compound **1** (Disesquicin).

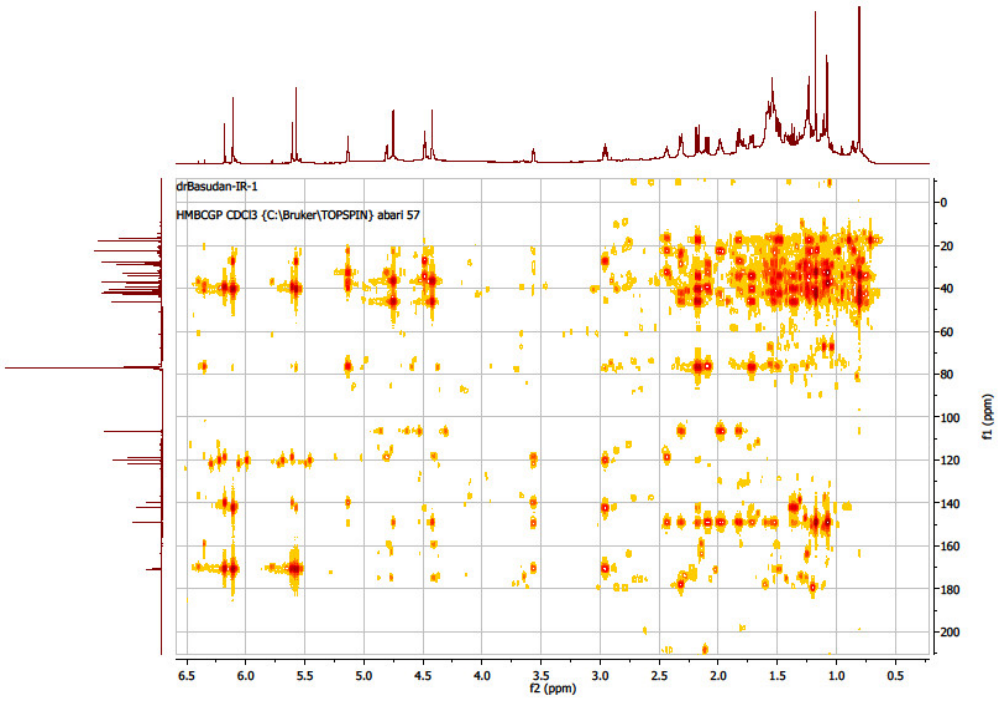

Figure S4. HMBC spectrum of compound **1** (Disesquicin).

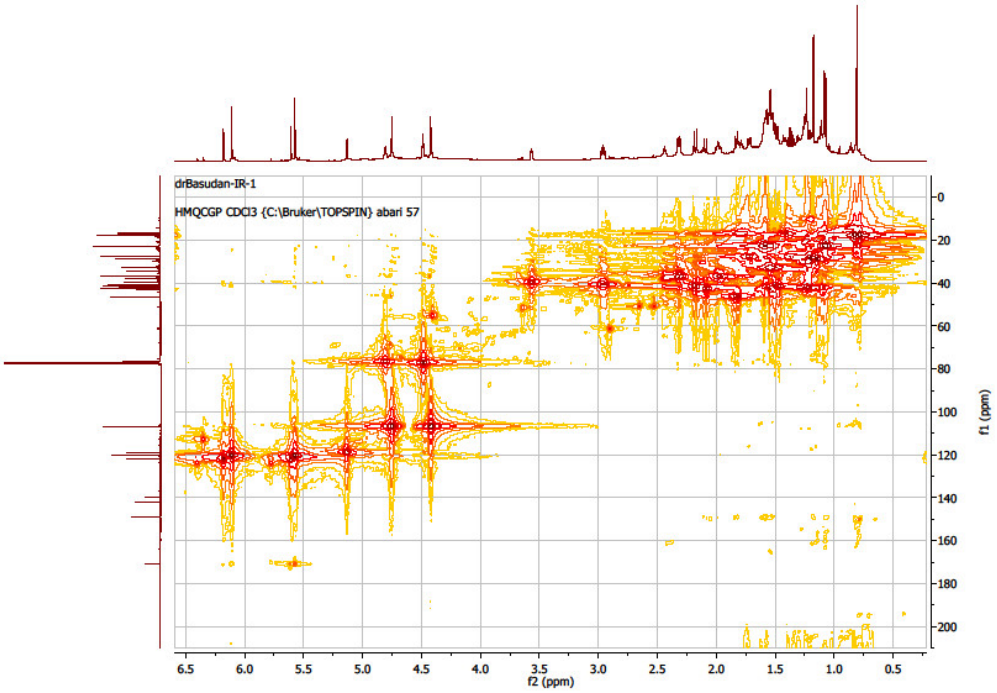

Figure S5. HMQC spectrum of compound **1** (Disesquicin).

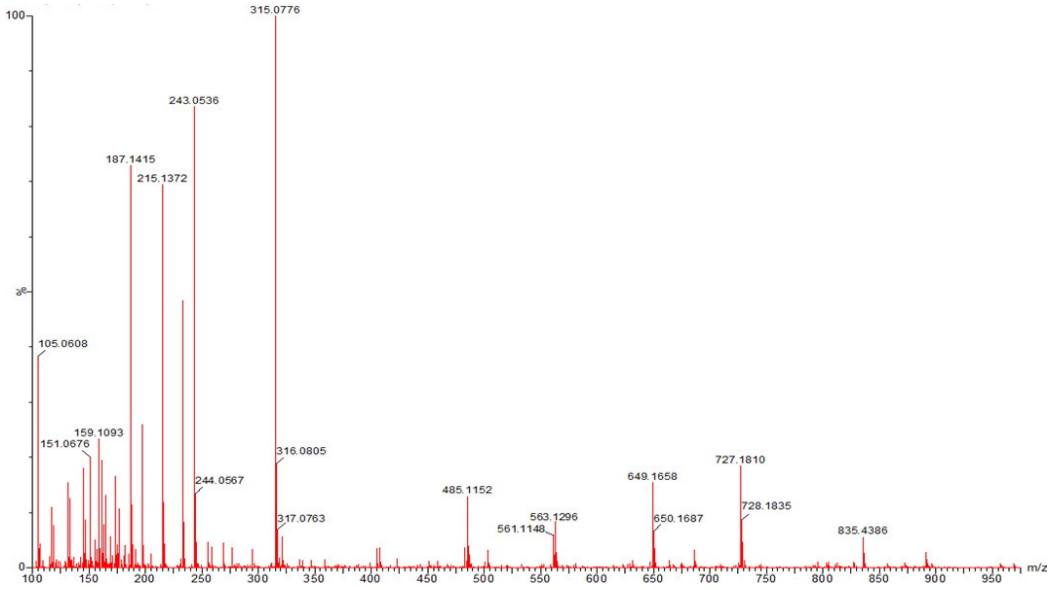

Figure S6. Mass spectrum of compound **1** (Disesquicin).

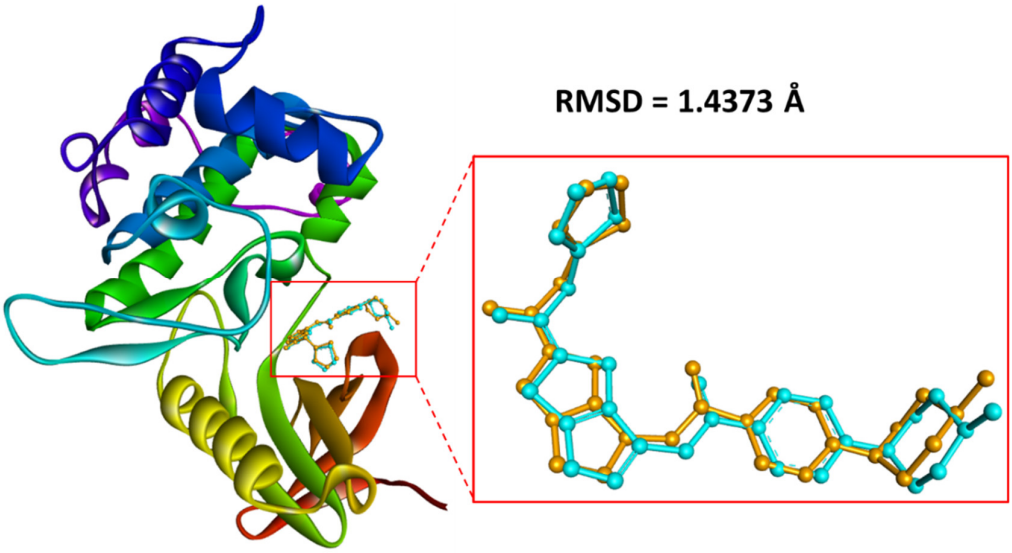

Figure S7. Re-docking of PHA-680626 with PLK-1 and comparison of the docking pose (golden color) with the X-ray crystal structure pose (teal color). The RMSD (root mean square deviation) between the two poses was 1.4373 Å.

Table 1. Molecular docking parameters of compound **1** with different kinases.

Target	PDB Id and Resolution	Grid Dimensions (Å)	Grid Position (Å)	Binding Energy (kcal mol^{-1})	
				Cognate Ligand	Compound 1
MEK1	1S9J; 2.4 Å	31.5 × 24.7 × 26.7	34.3 × 36.5 × 42.2	−8.4	−8.0
ERK2	1WZY; 2.5 Å	28.7 × 25.2 × 27.1	7.5 × 7.8 × 44.0	−8.3	−7.9
JNK	2P33; 2.4 Å	24.4 × 26.5 × 26.9	20.5 × 9.2 × 30.4	−9.0	−8.1
JAK	4OLI; 2.8 Å	27.1 × 26.4 × 26.6	−30.3 × 23.8 × 39.5	−8.8	−7.5
PKA	6E99; 1.9 Å	33.3 × 28.1 × 26.1	−7.4 × 7.5 × −13.2	−9.4	−8.0
PLK−1	2OWB; 2.1 Å	27.7 × 32.7 × 33.0	2.06 × 25.2 × 66.8	−10.0	−8.9
CDK2	6GUE; 2.0 Å	25.7 × 29.9 × 24.4	−6.5 × −22.2 × 20.7	−8.8	−8.1