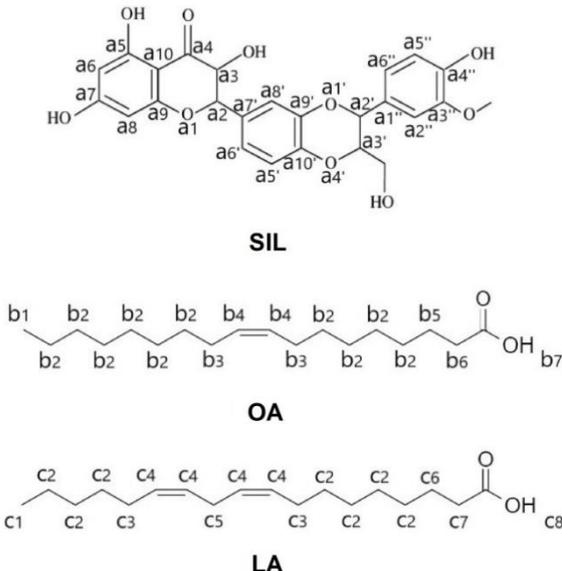


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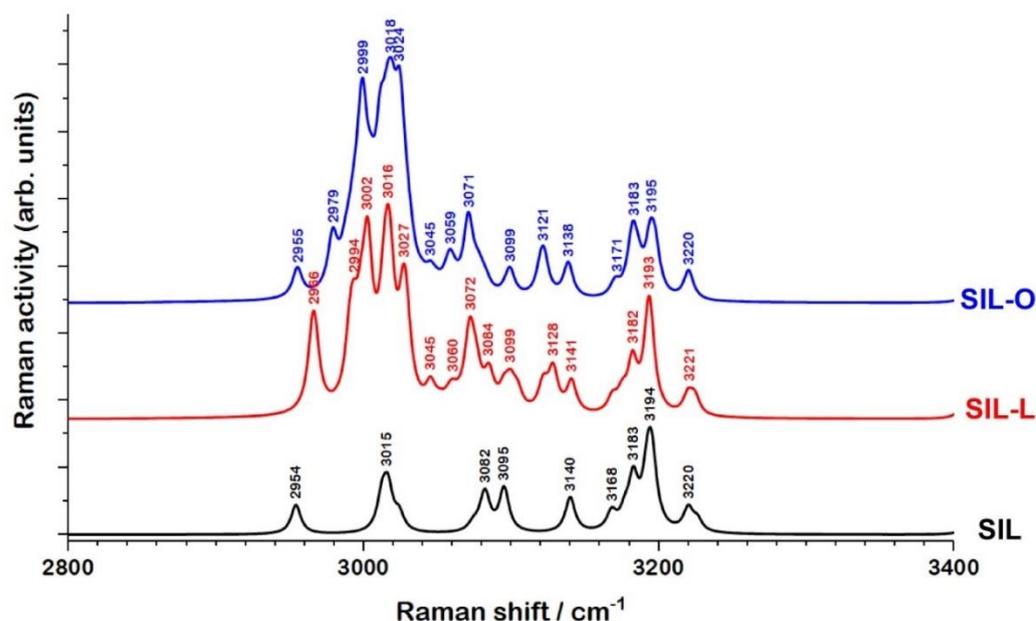
## SUPPLEMENTAL DATA

# **Synthesis, characterization, and in vitro-in ovo toxicological screening of silibinin fatty acids conjugates as prodrugs with potential biomedical applications**

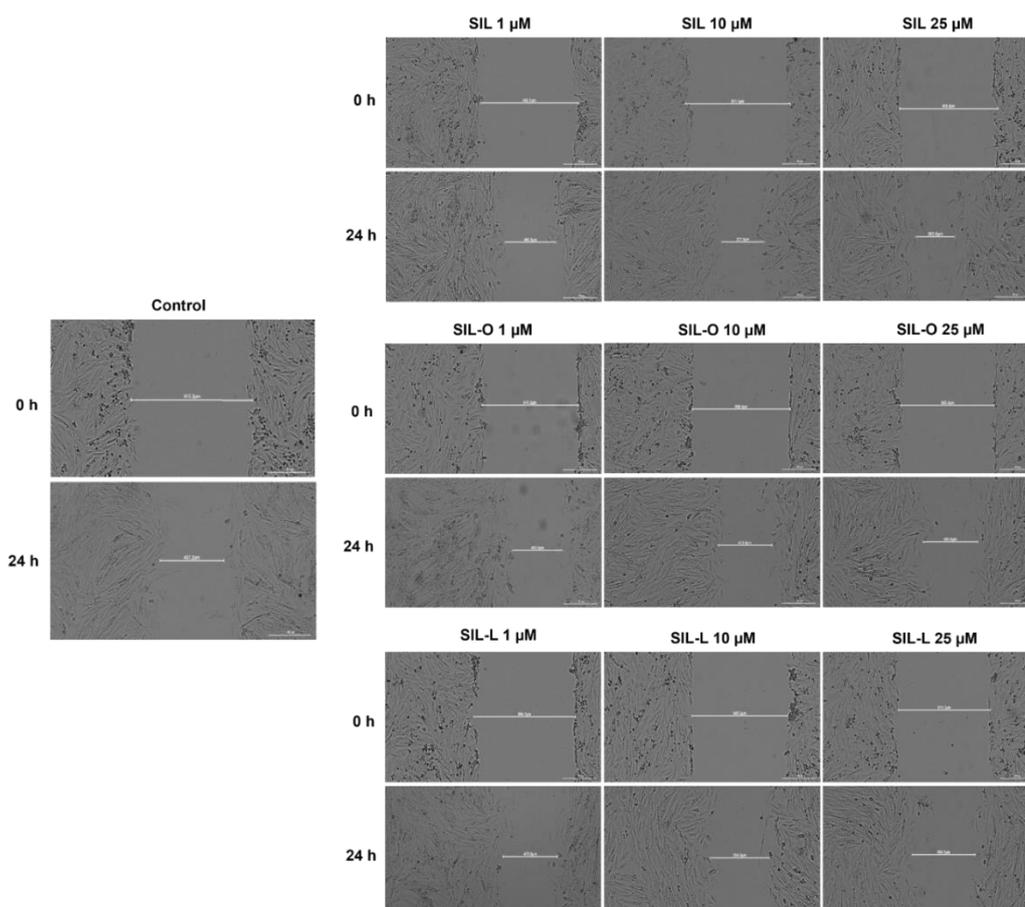
**Table S1.** <sup>1</sup>H NMR chemical shifts and structures of SIL, OA, and LA.

SIL $\delta(^1\text{H})$ (ppm)	SIL-O $\delta(^1\text{H})$ (ppm)	SIL-L $\delta(^1\text{H})$ (ppm)	Chemical structures of SIL, OA, and LA
-	12.40 (b7)	(c8) - missing	 <p><b>SIL</b></p> <p><b>OA</b></p> <p><b>LA</b></p>
11.89 (a5-OH)	11.88	11.88	
10.85 (a7-OH)	10.82	10.83	
-	9.61	-	
9.14 (a4''-OH)	9.22	9.16	
-	7.80	-	
-	7.48	-	
-	7.14	7.11	
7.09 (a8')	7.12	7.08	
7.02 (a6')	7.02	7.02	
6.98 (a2'')	6.99	6.98	
6.97 (a5')	6.97	6.96	
6.87 (a5''')	6.87	6.87	
6.81 (a6''')	6.81	6.80	
-	6.46	-	
-	6.20	-	
5.92 (a6)	5.92	5.92	
5.88 (a8)	5.87	5.87	
5.81 (a3-OH)	5.81	5.81	
-	-	5.33 (c4)	
-	5.3 (b4)	-	
5.09 (a2, a3)	5.09	5.09	
4.95	4.99	4.93	
4.91 (a2', a3')	4.93	4.90	
4.61 (a2, a3)	4.61	4.61	
-	4.51 (water)	4.51 (water)	
4.17 (a2', a3')	4.16	4.04	
-	3.94	-	

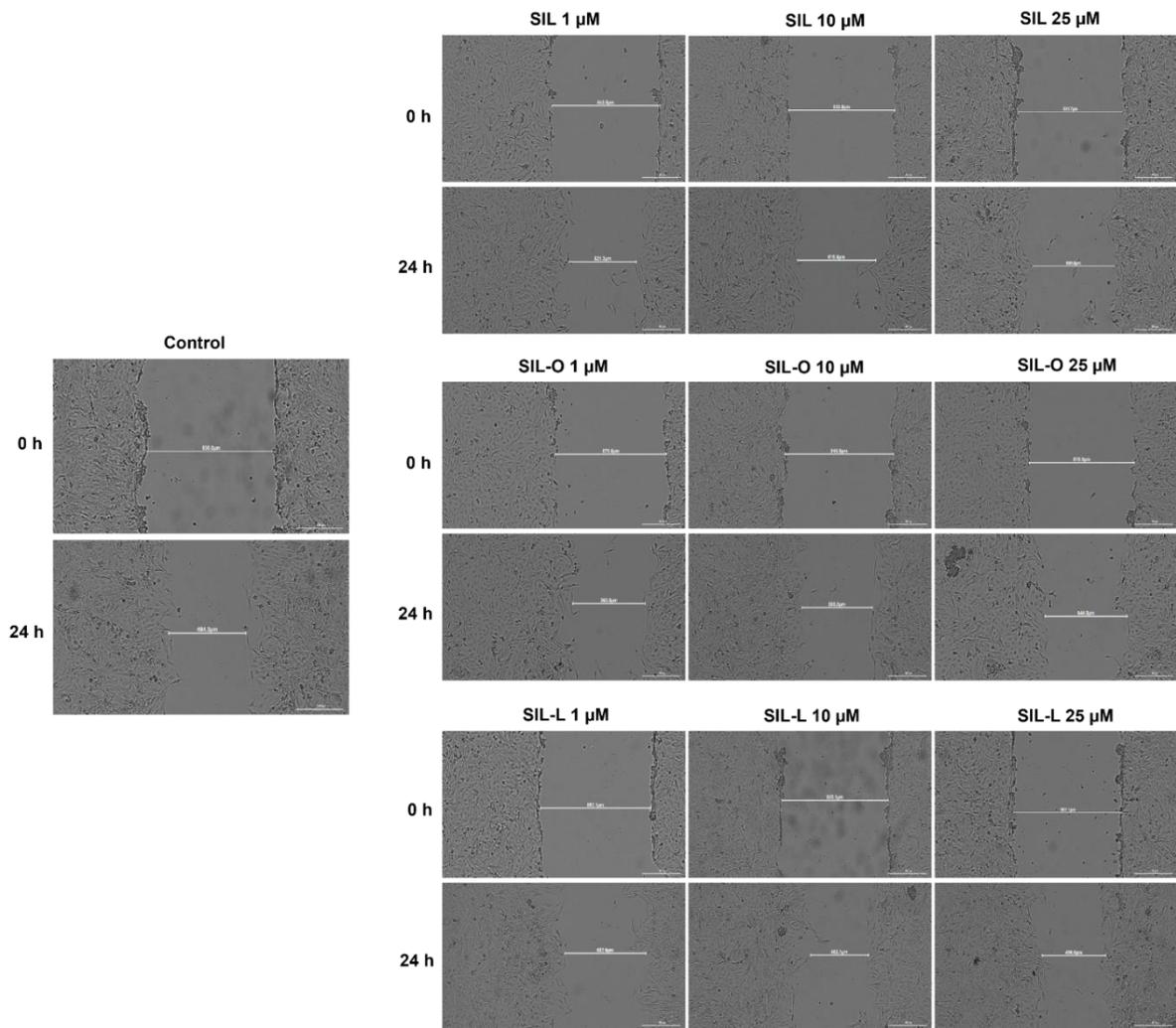




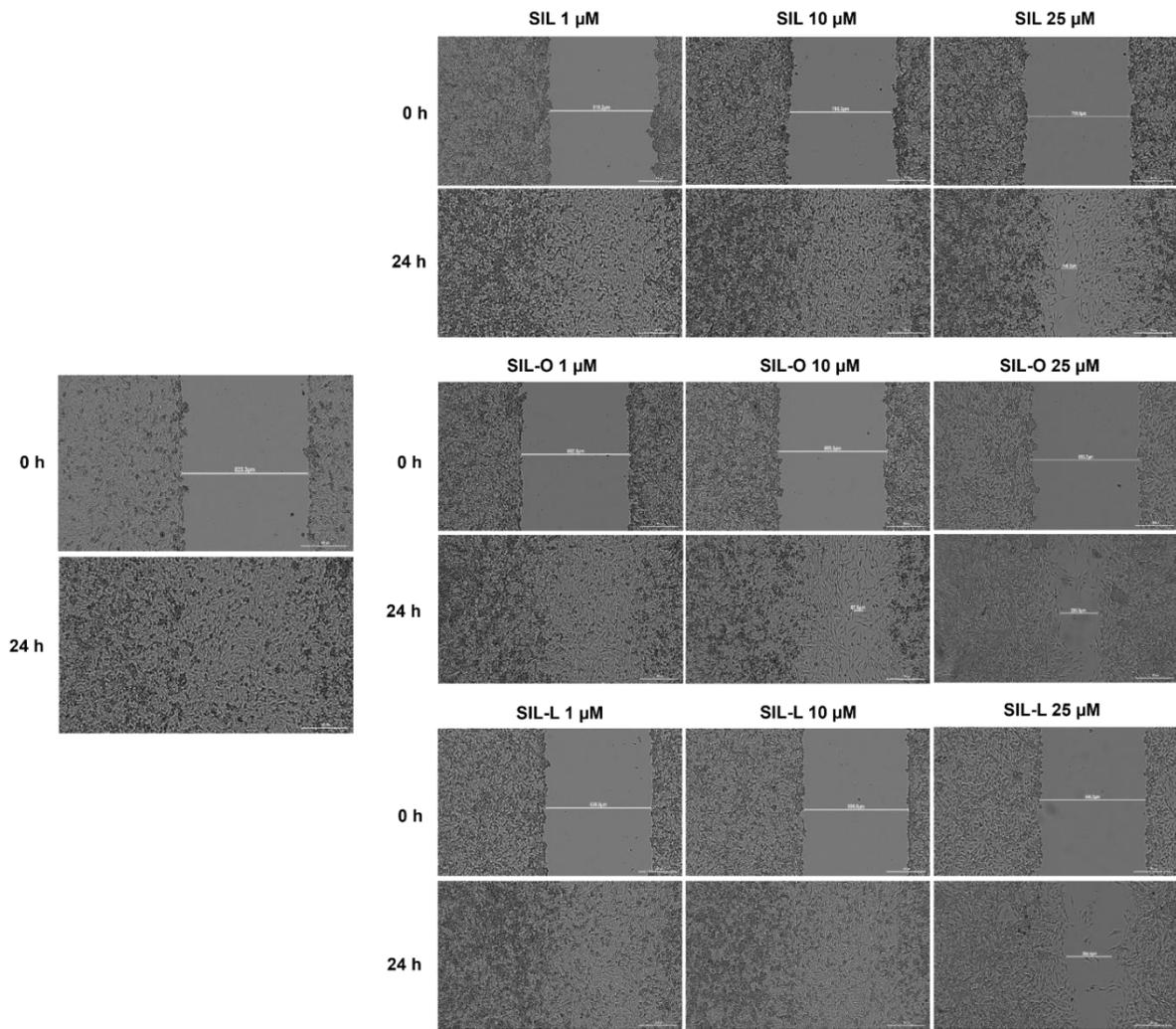
**Figure S2. Theoretical Raman spectra of SIL, SIL-O, and SIL-L obtained by density functional theory calculations, in the high wavenumber region. SIL: Silibinin; SIL-O: Silibinin oleate; SIL-L: Silibinin linoleate.**



**Figure S3. Representative images illustrating the impact of SIL, SIL-O, and SIL-L at 1, 10, and 25  $\mu\text{M}$  on the migration rate in H9c2(2-1) cells following a 24 h treatment. The scale bars indicate 300  $\mu\text{m}$ . SIL: Silibinin; SIL-O: Silibinin oleate; SIL-L: Silibinin linoleate**



**Figure S4. Representative images illustrating the impact of SIL, SIL-O, and SIL-L at 1, 10, and 25  $\mu\text{M}$  on the migration rate in HepaRG cells following a 24 h treatment. The scale bars indicate 300  $\mu\text{m}$ . SIL: Silibinin; SIL-O: Silibinin oleate; SIL-L: Silibinin linoleate**



**Figure S5. Representative images illustrating the impact of SIL, SIL-O, and SIL-L at 1, 10, and 25 μM on the migration rate in HaCaT cells following a 24 h treatment. The scale bars indicate 300 μm. SIL: Silibinin; SIL-O: Silibinin oleate; SIL-L: Silibinin linoleate**