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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

SIL $\boldsymbol{\delta}(^{1}H)$ (ppm)	δ ⁽¹ H) (ppm)	SIL-L $\boldsymbol{\delta}(^{1}\mathrm{H})$ (ppm)	Chemical structures of SIL, OA, and LA
-	12.40 (b7)	(c8) - missing	
11.89 (a5-	11.88	11.88	
OH)	11.00	11.00	
10.85 (a7-	10.82	10.83	
OH)	10.02	10.05	
-	9.61	-	
9.14 (a4"-	9.22	9.16	
OH)			
-	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	ОН О
6.97 (a5')	6.97	6.96	$\begin{array}{c} 0H & 0 \\ a_{3} \\ a_{7} \\ H0 \\ a_{8} \\ a_{9} \\ a_{1} \\ a_{1} \\ a_{1} \\ a_{2} \\ a_{1} \\ a_{2} \\ a_{3} \\ a_{1} \\ a_{2} \\ a_{3} \\ a_{1} \\ a_{2} \\ a_{2} \\ a_{3} \\ a_{2} \\ a_{2} \\ a_{2} \\ a_{3} \\ a_{2} \\ a_{2} \\ a_{3} \\ a_{2} \\ a_{2} \\ a_{3} \\ a$
6.87 (a5'')	6.87	6.87	
6.81 (a6'')	6.81	6.80	a6' a10' 04'
-	6.46	-	HO
-	6.20	-	SIL
5.92 (a6)	5.92	5.92	b1 b2 b2 b2 b4 b4 b2 b2 b5
5.88 (a8)	5.87	5.87	b2 b2 b2 b3 b3 b2 b2 b6 OH b7
5.81 (a3-OH)	5.81	5.81	OA
-	-	5.33 (c4)	
-	5.3 (b4)	-	
5.09 (a2, a3)	5.09	5.09	
4.95	4.99	4.93	
4.91 (a2',	4.93	4.90	
a3')			
4.61 (a2, a3)	4.61	4.61	
-	4.51 (water)	4.51 (water)	
4.17 (a2', a3')	4.16	4.04	
-	3.94	-	

 Table S1. ¹H NMR chemical shifts and structures of SIL, OA, and LA.

https://doi.org/10.17305/bb.2024.10600

3.78 (a3'')	3.78	3.78
3.55 (a3'- OH)	3.55	3.55
3.33 (a3'- OH)	3.32	3.32
2.51 (DMSO)	2.51	2.51
-	-	2.80 (c5)
-	2.31 (b6)	2.27 (c7)
-	2.18	-
-	-	2.02 (c3)
-	1.98 (b3)	-
-	1.49 (b5)	-
	-	1.54 (c6)
-	1.25 (b2)	1.14-1.20 (c2)
-	0.84 (b1)	0.89 (c1)

SIL: Silibinin; SIL-O: Silibinin oleate; SIL-L: Silibinin linoleate; OA: Oleic acid; LA: Linoleic acid



Figure S1. Theoretical Raman spectra of SIL, SIL-O, and SIL-L obtained by density functional theory calculations, in the low wavenumber region. SIL: Silibilin; SIL-O: Silibilin oleate; SIL-L: Silibilin linoleate.



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



Figure S3. Representative images illustrating the impact of SIL, SIL-O, and SIL-L at 1, 10, and 25 μ M on the migration rate in H9c2(2-1) cells following a 24 h treatment. The scale bars indicate 300 μ 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 µM on the migration rate in HepaRG cells following a 24 h treatment. The scale bars indicate 300 µm. 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 μ M on the migration rate in HaCaT cells following a 24 h treatment. The scale bars indicate 300 μ m. SIL: Silibinin; SIL-O: Silibinin oleate; SIL-L: Silibinin linoleate