Supplementary Material

Investigation of antimicrobial and anti-inflammatory efficacy of newly synthesized pyrogallol-coumarin hybrids: *in vitro* and *in silico* studies

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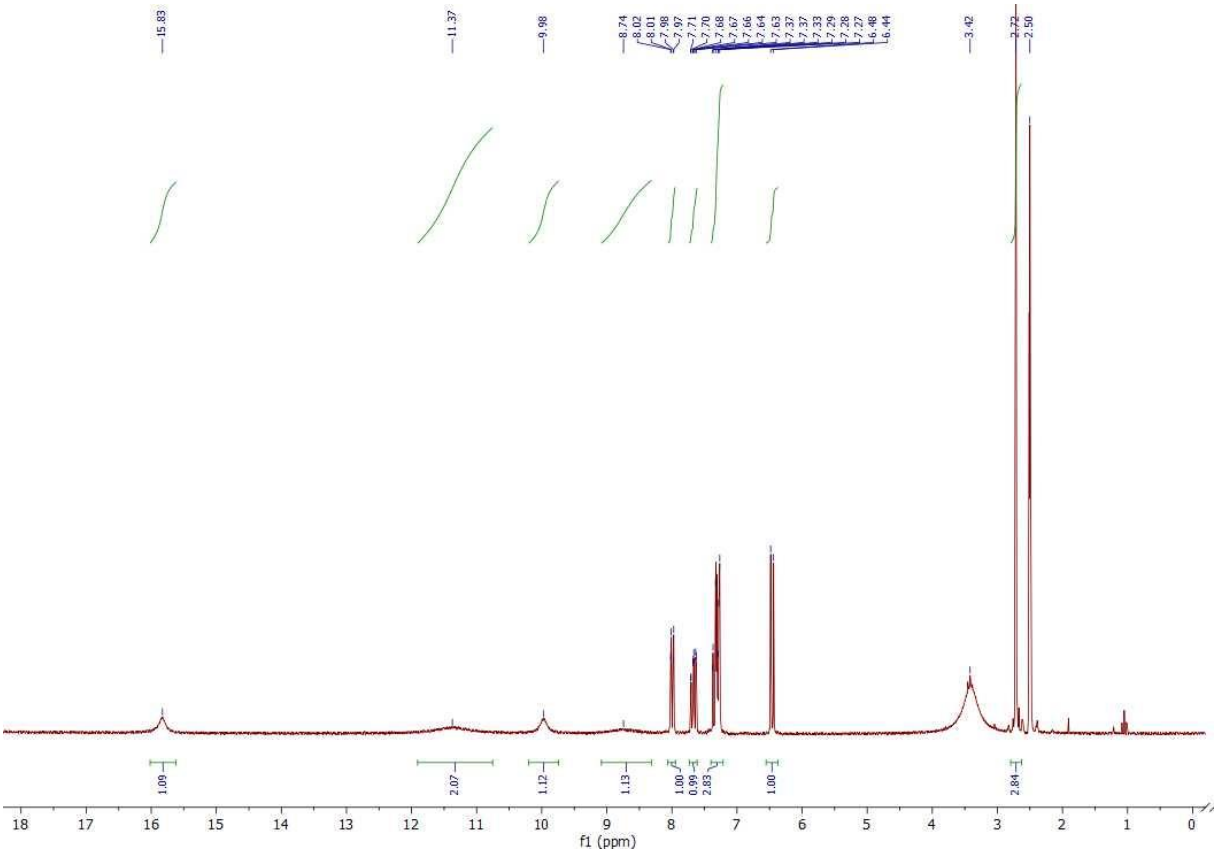

Figure S1. ^{1}H NMR (200 MHz) spectrum of **PCH-1** recorded in DMSO-d_6

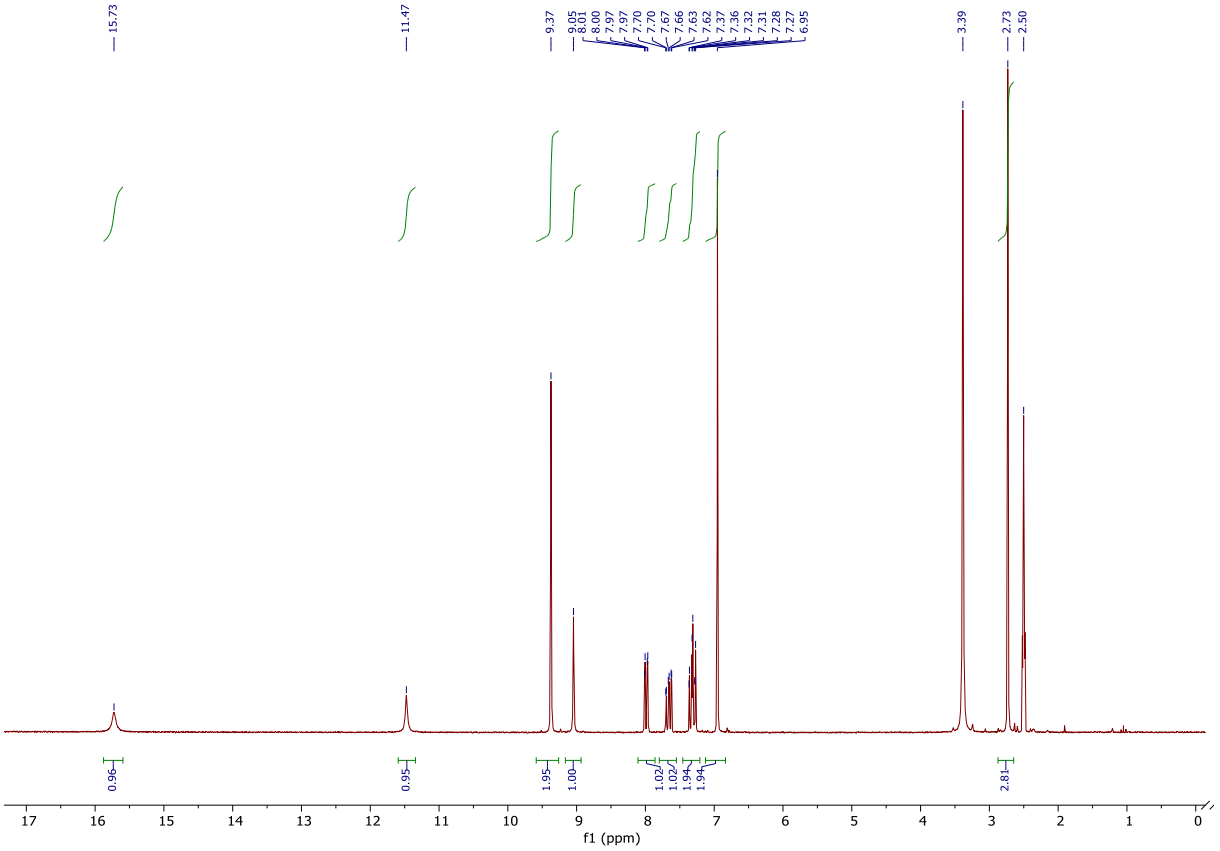

Figure S2. ^{1}H NMR (200 MHz) spectrum of **PCH-2** recorded in DMSO-d_6

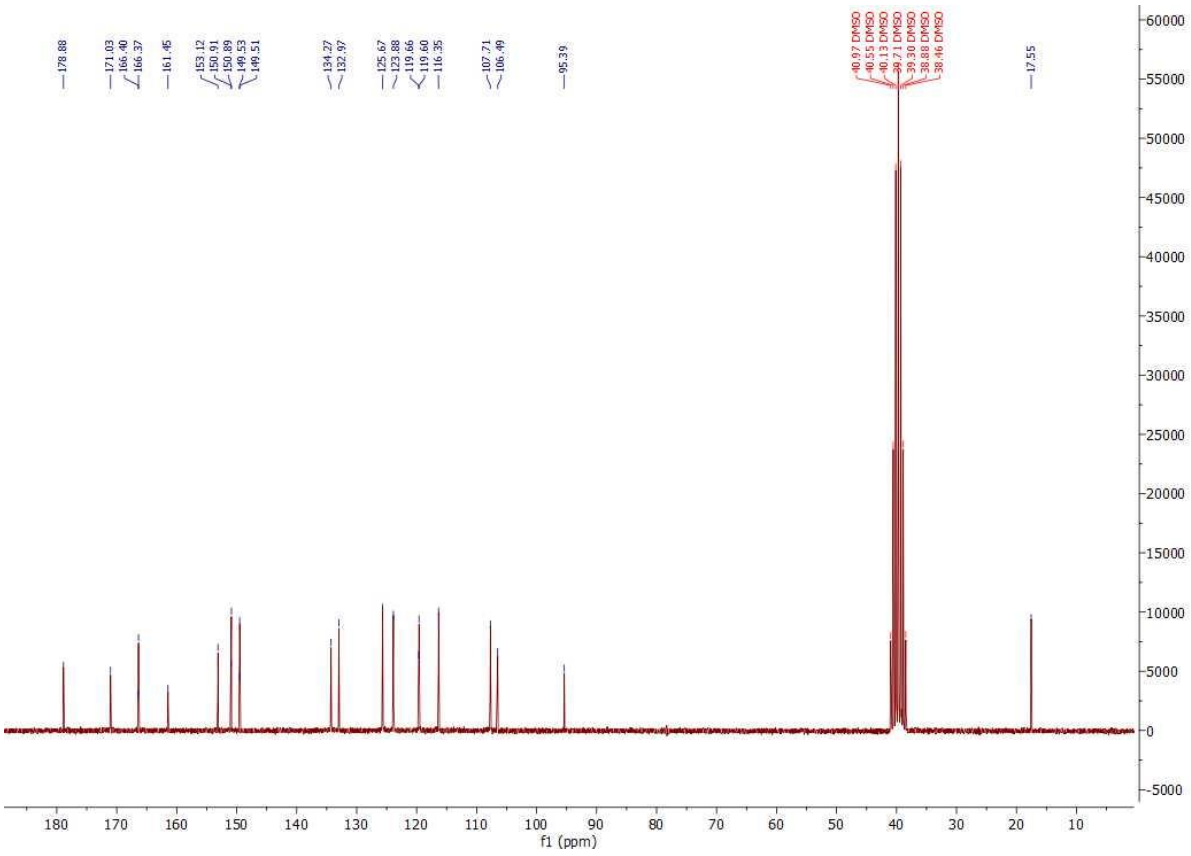

Figure S3. ^{13}C NMR (50 MHz) spectrum of **PCH-1** recorded in DMSO-d_6

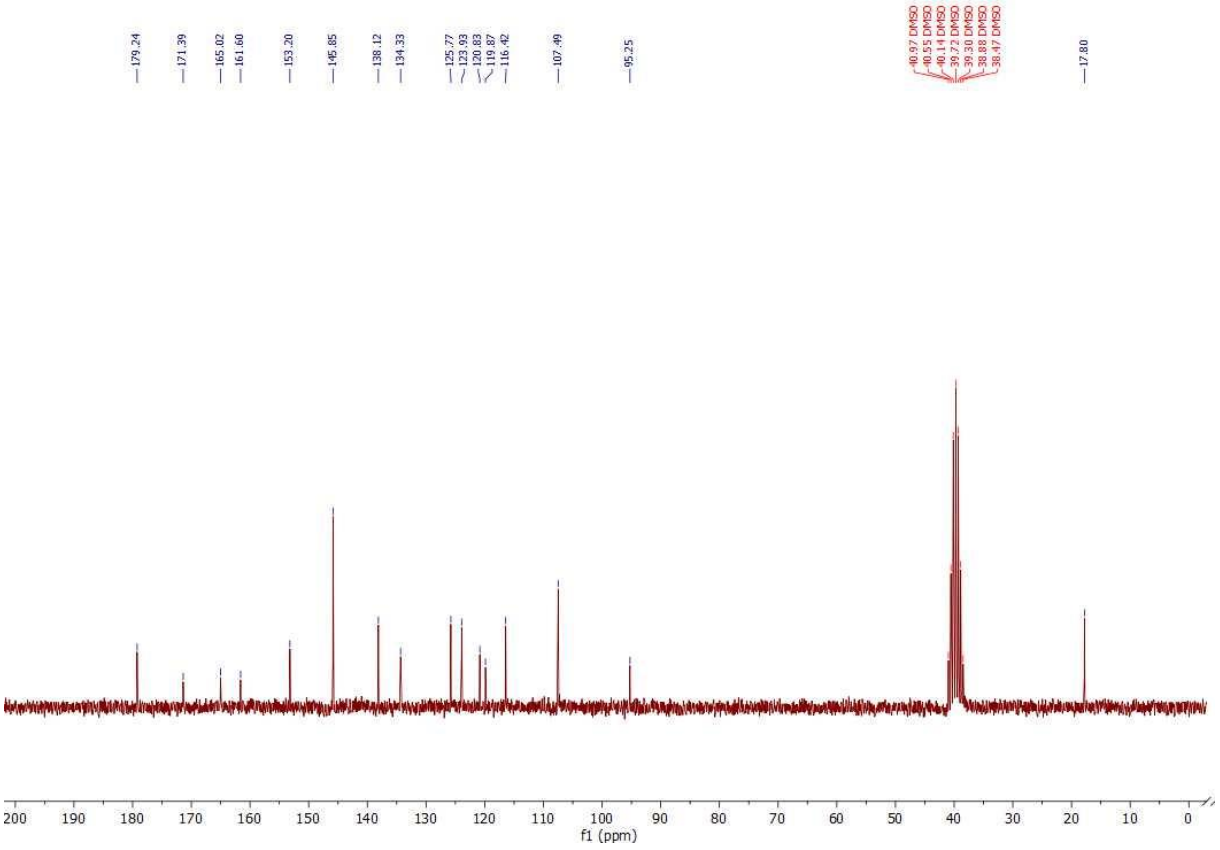

Figure S4. ^{13}C NMR (50 MHz) spectrum of **PCH-2** recorded in DMSO-d_6

Table S1. Experimental and theoretical values of chemical shifts for **PCH-1** and **PCH-2** in ^{1}H NMR spectra

^{1}H NMR , δ (ppm)				
Atoms	**PCH-1**		**PCH-2**	
	Experimental	Calculated	Experimental	Calculated
N1—H	15.83	15.05	15.72	15.04
N2—H	11.38	/	11.47	/
C2'—H	2.72	2.70	2.73	2.72
C5—H	8.00	8.49	7.99	8.52
C6—H	7.30	7.52	7.30	7.52
C7—H	7.67	7.96	7.66	7.92
C8—H	7.30	7.52	7.30	7.52
C2"—H/OH	11.38	/	6.95	7.19
C3"—H/OH	9.97	/	9.35	/
C4"—H/OH	8.80	/	9.46	/
C5"—H/OH	7.30	7.52	9.35	/
C6"—H	6.46	6.73	6.95	7.19
R/MAE	**0.999/0.19**		**0.999/0.20**	

Table S2. Experimental and theoretical values of chemical shifts for **PCH-1** and **PCH-2** in ^{13}C NMR spectra

^{13}C NMR , δ (ppm)				
Atoms	**PCH-1**		**PCH-2**	
	Experimental	Calculated	Experimental	Calculated
C2	17.6	14.1	17.6	13.9
C3	95.4	98.4	95.2	97.4
C4	171.0	182.7	171.4	182.1
C5	123.9	126.3	125.8	127.1
C6	119.7	120.0	124.0	123.2
C7	134.3	135.9	138.1	135.5
C8	116.4	115.9	119.9	116.3
C9	153.1	156.7	153.2	156.3
C10	119.6	120.0	120.8	119.7
C1'	178.9	185.1	179.4	183.4
C2'	17.6	14.1	17.8	13.9
C1''	106.5	102.1	134.4	123.0
C2''	150.9	150.6	107.5	104.7
C3''	125.7	131.6	145.8	142.0
C4''	179.5	150.4	145.8	142.0
C5''	107.7	111.8	145.8	142.0
C6''	107.7	111.8	116.4	105.1
R/MAE	**0.997/3.20**		**0.992/3.91**	

Table S3. Activity (%) and IC_{50} (μM) values of PCH-1 for *in vitro* LOX inhibition assay

Concentration (μM)	Activity (%)	IC_{50} (μM)
25	32.8 ± 2.4	
30	36.8 ± 2.4	
40	51.4 ± 1.8	38.1 ± 1.3
50	65.1 ± 2.0	
60	84.9 ± 0.1	

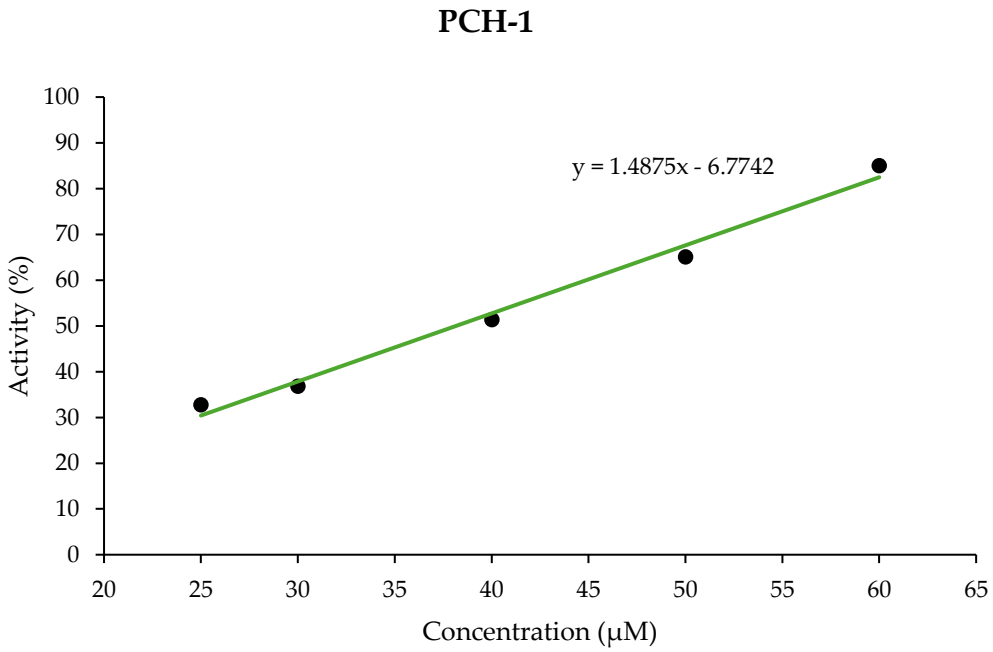

Figure S5. Inhibitory curve of PCH-1 for *in vitro* LOX inhibition assay

Table S4. Activity (%) and IC_{50} (μM) values of PCH-2 for *in vitro* LOX inhibition assay

Concentration (μM)	Activity (%)	IC_{50} (μM)
20	20.7 ± 2.7	
25	38.9 ± 3.1	
30	41.9 ± 1.4	34.1 ± 1.2
40	67.0 ± 0.9	
50	71.7 ± 2.2	

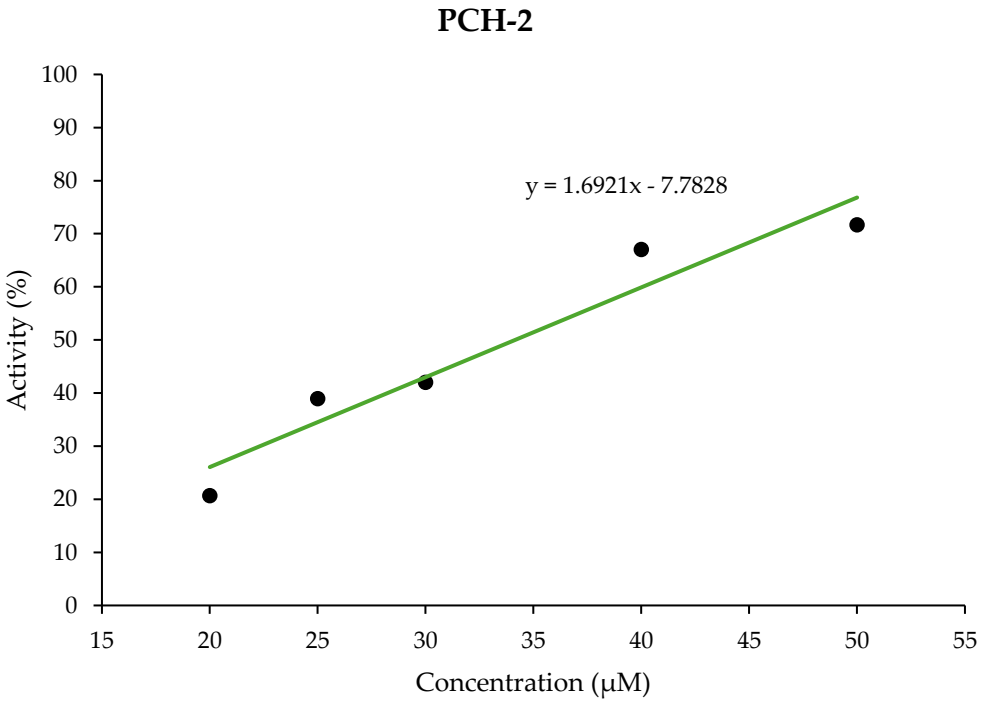

Figure S6. Inhibitory curve of PCH-2 for *in vitro* LOX inhibition assay

Table S5. Activity (%) and IC_{50} (μM) values of H-1 for *in vitro* LOX inhibition assay

Concentration (μM)	Activity (%)	IC_{50} (μM)
25	21.6 ± 1.4	
40	33.9 ± 0.8	
50	37.8 ± 1.0	65.4 ± 0.6
75	57.5 ± 1.1	
100	73.5 ± 0.6	

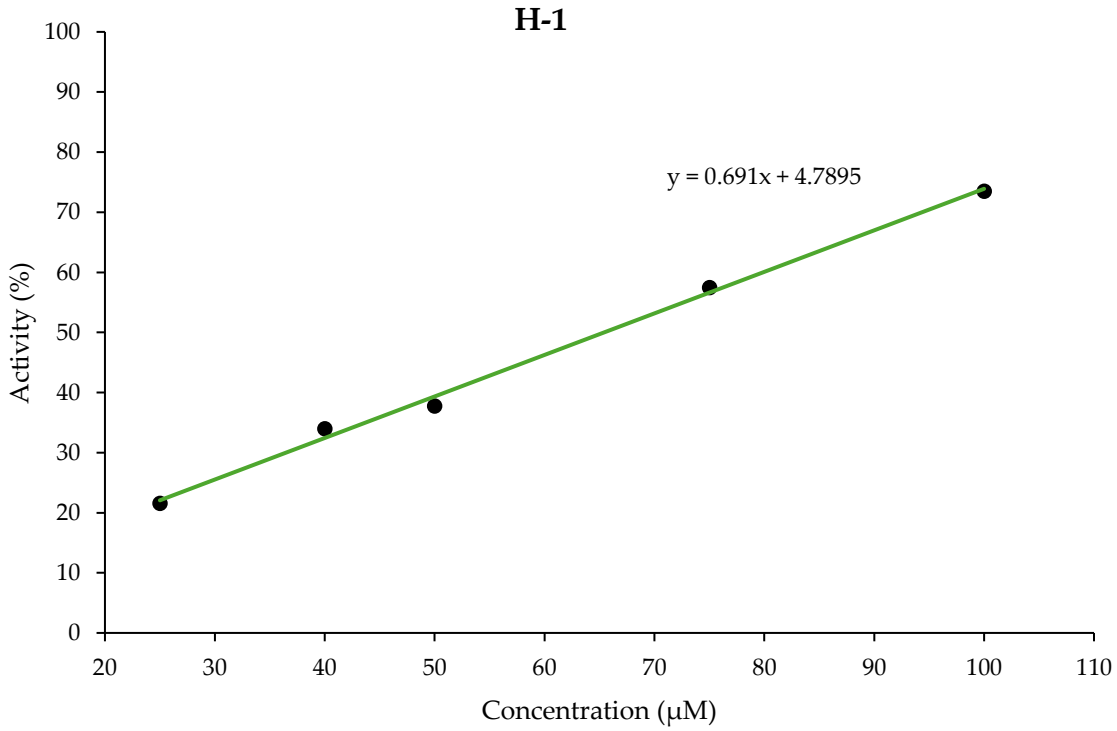

Figure S7. Inhibitory curve of H-1 for *in vitro* LOX inhibition assay

Table S6. Activity (%) and IC_{50} (μM) values H-2 for *in vitro* LOX inhibition assay

Concentration (μM)	Activity (%)	IC_{50} (μM)
25	32.0 ± 0.1	
40	44.4 ± 1.7	
50	56.0 ± 1.1	46.0 ± 0.9
75	73.4 ± 0.3	
100	91.9 ± 0.2	

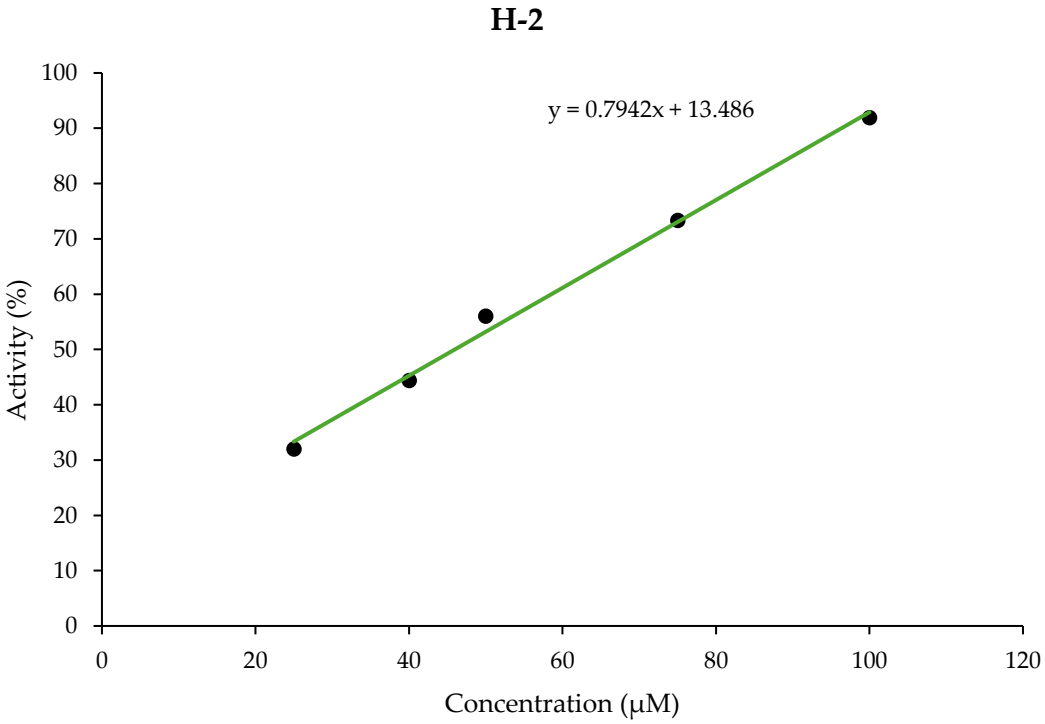

Figure S8. Inhibitory curve of H-2 for *in vitro* LOX inhibition assay

Table S7. Activity (%) and IC_{50} (μM) values of 3AcHyC for *in vitro* LOX inhibition assay

Concentration (μM)	Activity (%)	IC_{50} (μM)
25	26.4 ± 1.3	
40	35.8 ± 0.8	
50	43.5 ± 3.1	57.9 ± 1.6
75	63.4 ± 0.4	
100	81.2 ± 0.2	

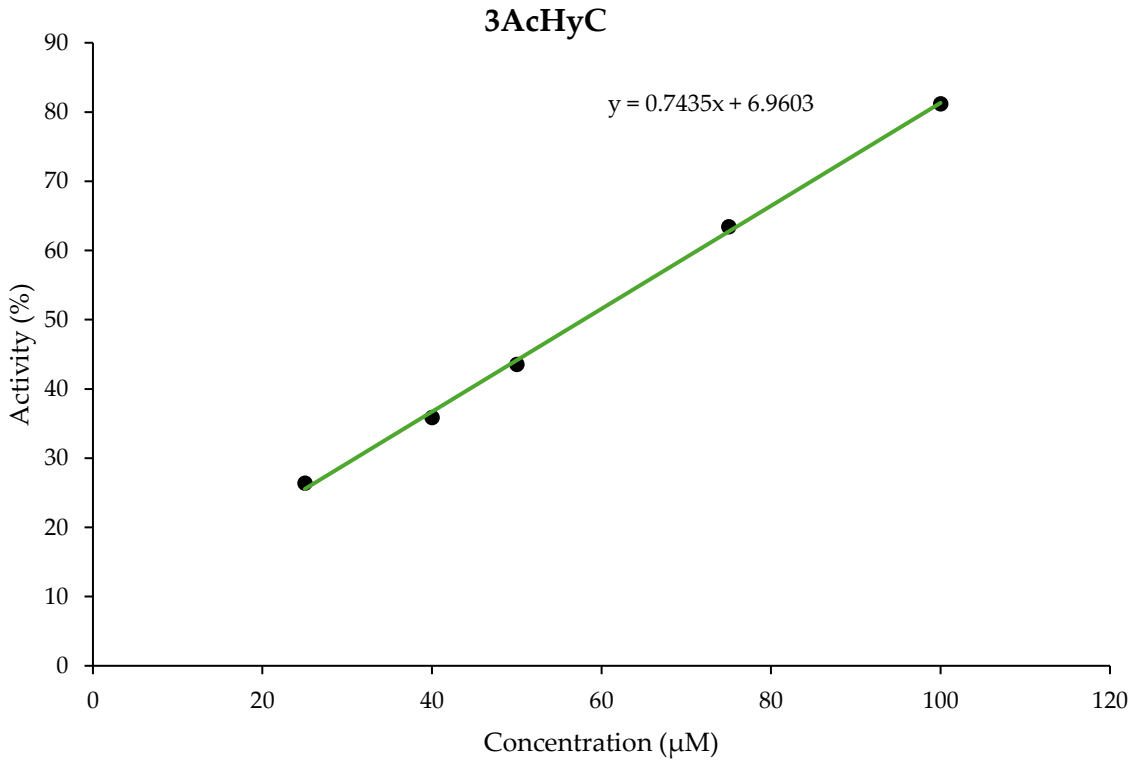

Figure S9. Inhibitory curve of 3AcHyC for *in vitro* LOX inhibition assay

Table S8. Activity (%) and IC_{50} (μM) values of reference compound nordihydroguaiaretic acid (NDGA)for *in vitro* LOX inhibition assay

Concentration (μM)	Activity (%)	IC_{50} (μM)
5	9.9 ± 0.7	
10	21.1 ± 1.6	
15	51.3 ± 1.8	17.3 ± 0.1
20	56.2 ± 0.9	
25	74.3 ± 0.4	

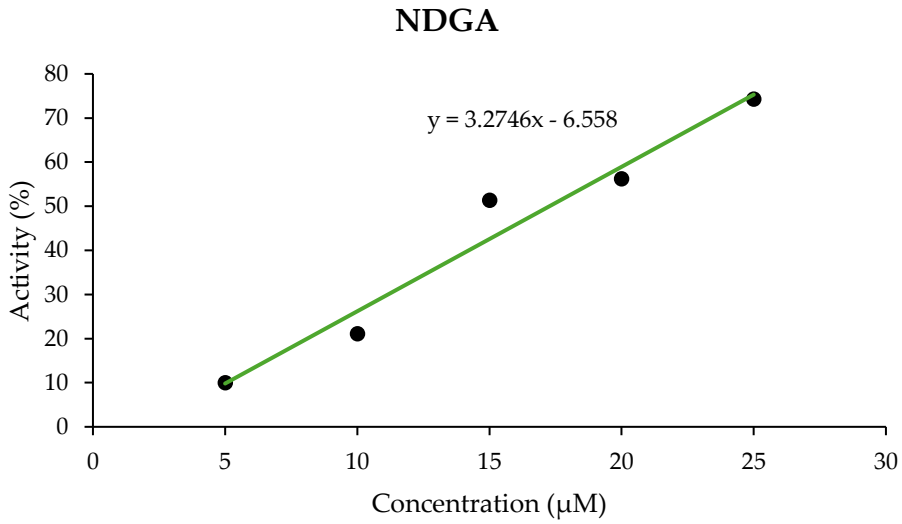

Figure S10. Inhibitory curve of NDGA for *in vitro* LOX inhibition assay

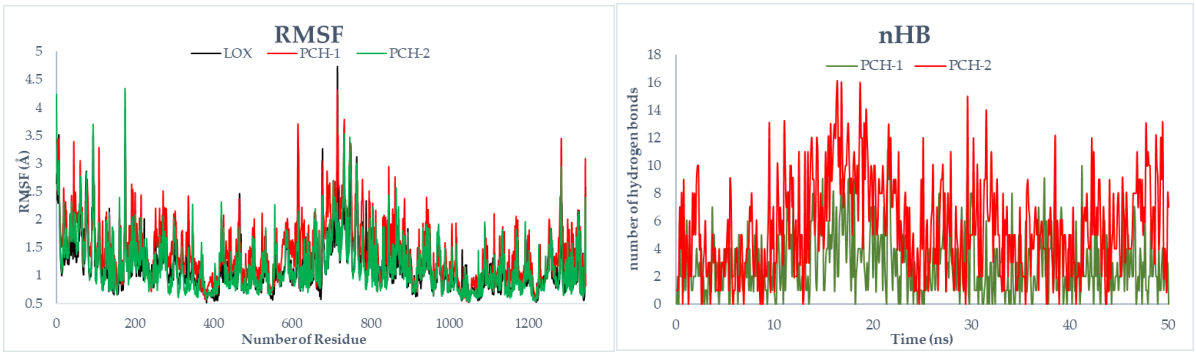

Figure S11. RMSF and nHB values describing the behaviour of LOX- **PCH-1** and LOX-**PCH-2** systems in 50 ns timeframe