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Supporting information

Bio-guided Isolation of Acetogenins from *Annona cherimola* deciduous leaves: Production of Nanocarriers to Boost the Bioavailability Properties.

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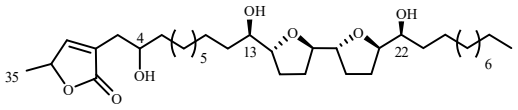
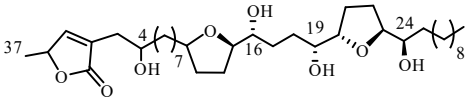
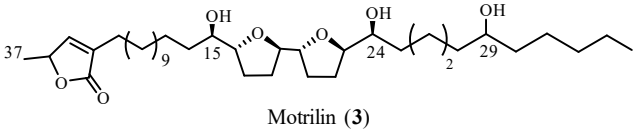
Physical data



Molvizarin (**1**)



Cherimolin-1 (**2**)



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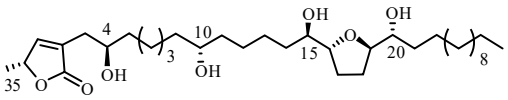
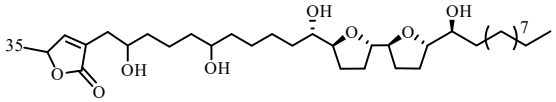


Annonacin (**4**)



Annonisin (**5**)

Molvizarin (**1**). This compound was obtained as a colourless oil in 0.001% yield; HRMS (ESI) calcd for $C_{35}H_{61}O_7$ $[M-H]^-$: 593.4417, found: 593.4460.

Cherimolin-1 (**2**). This compound was obtained as a colourless oil in 0.0002% yield; HRMS (ESI) calcd for $C_{37}H_{65}O_8$ $[M-H]^-$: 637.4679, found: 637.4723.

Motrilin (**3**). This compound was obtained as a colourless oil in 0.0002% yield;

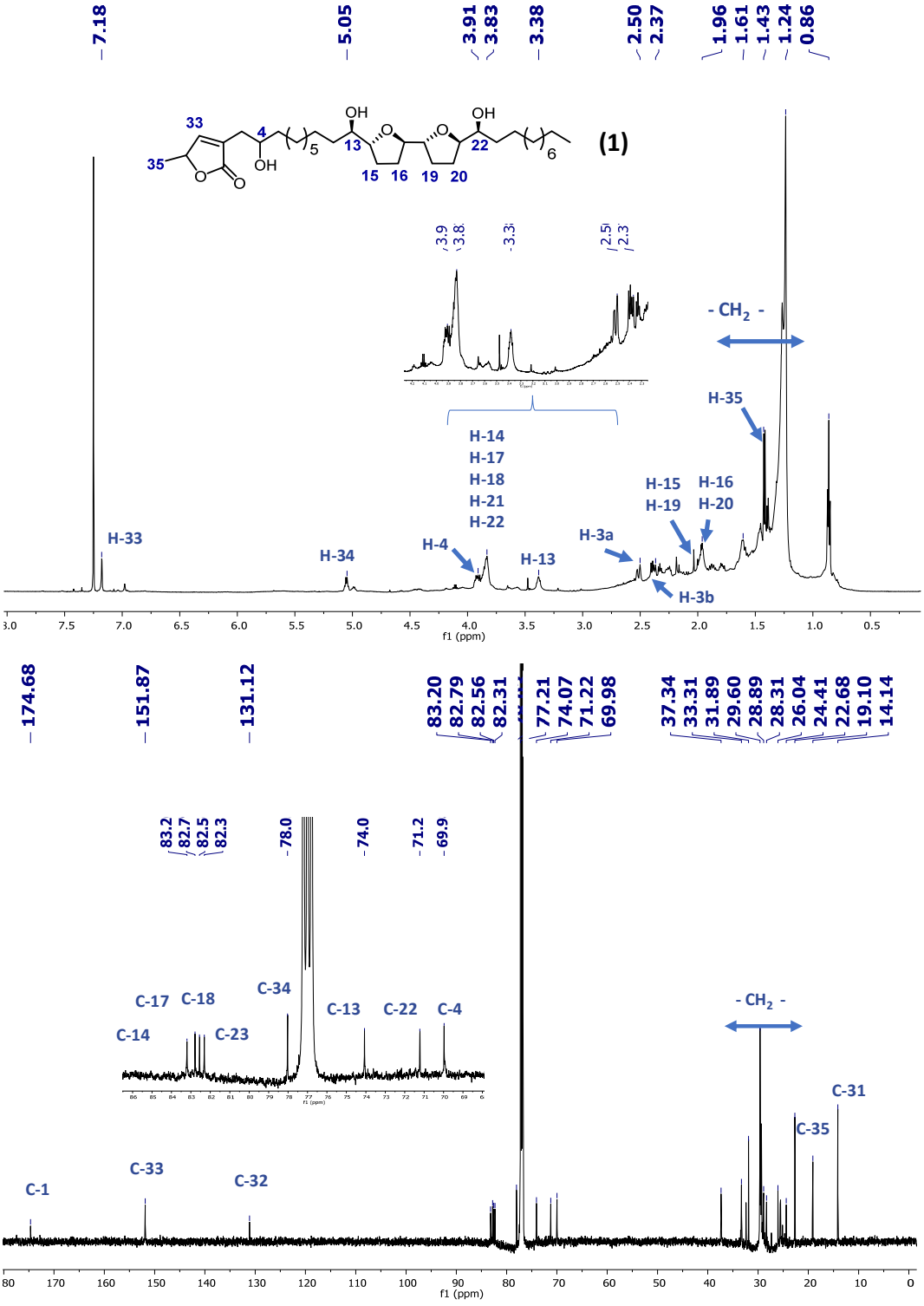
HRMS (ESI) calcd for $C_{37}H_{65}O_7$ $[M-H]^-$: 621.4679, found: 621.4717.

Annonacin (**4**). This compound was obtained as a yellow oil in 0.003% yield; HRMS (ESI) calcd for $C_{35}H_{64}O_7$ $[M+H]^+$: 597.4736, found: 597.4730.

Annonisin (**5**). This compound was obtained as a colourless oil in 0.001% yield; HRMS (ESI) calcd for $C_{36}H_{63}O_{10}$ $[M+HCOO]^-$: 655.4421, found: 655.4424.

^{1}H-NMR and ^{13}C-NMR Spectroscopy of ACGs 1–5 (^{1}H NMR 600 MHz, ^{13}C NMR 150 MHz, $CDCl_3$)

Molvizarin (**1**)



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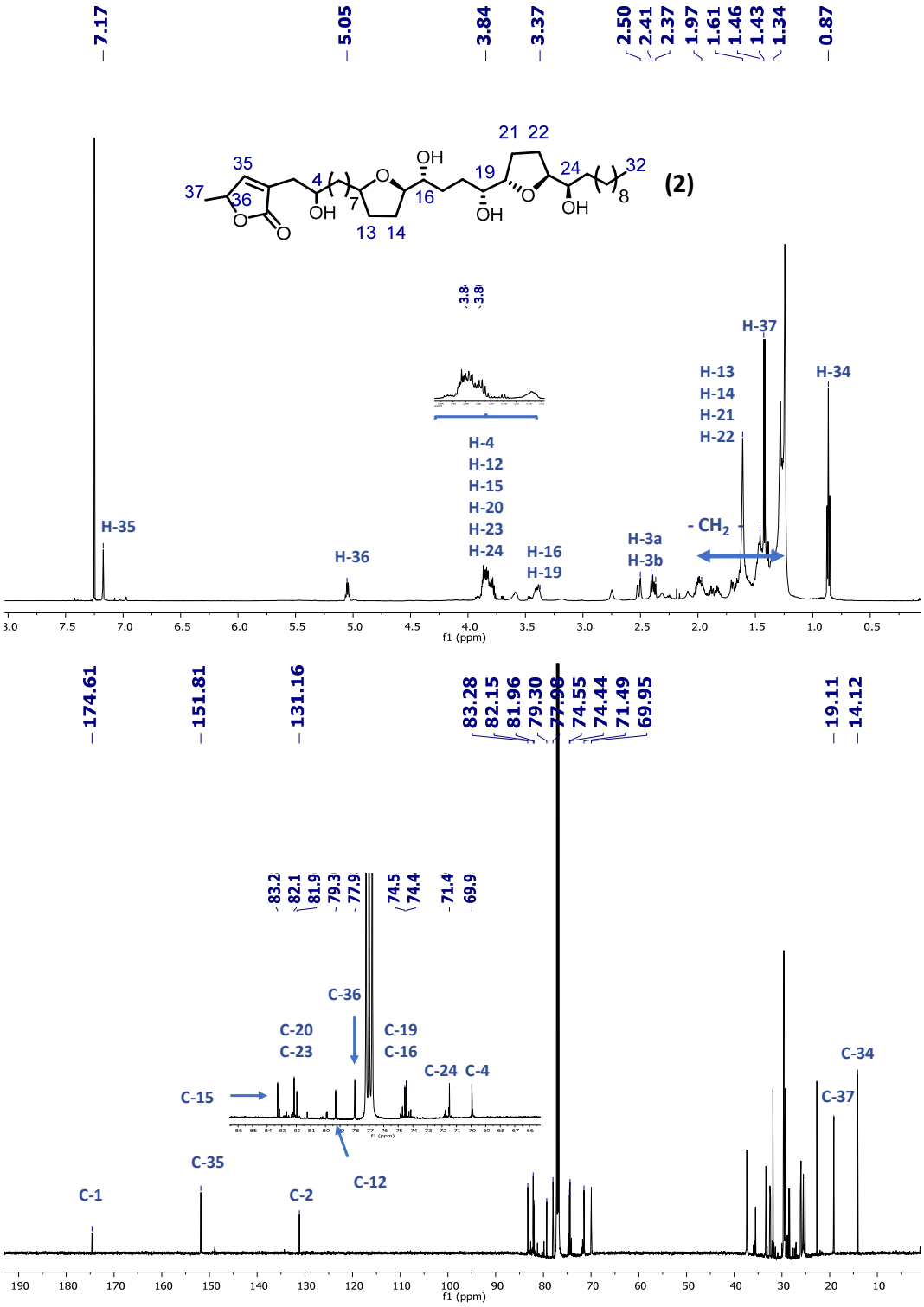

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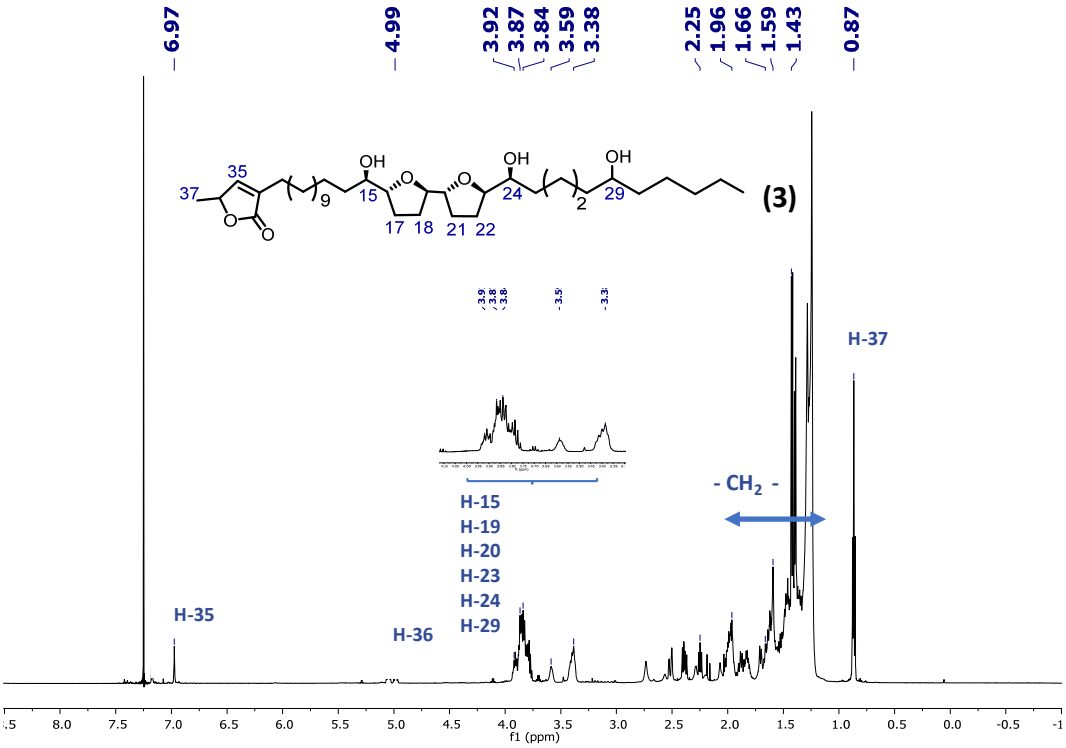
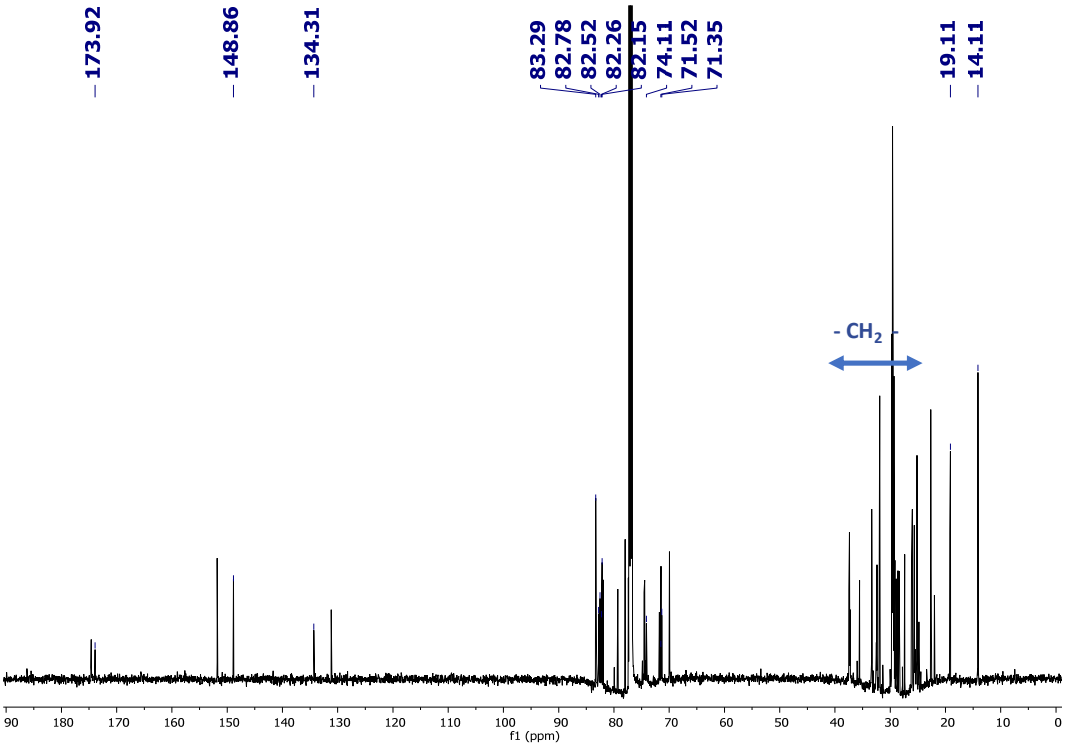
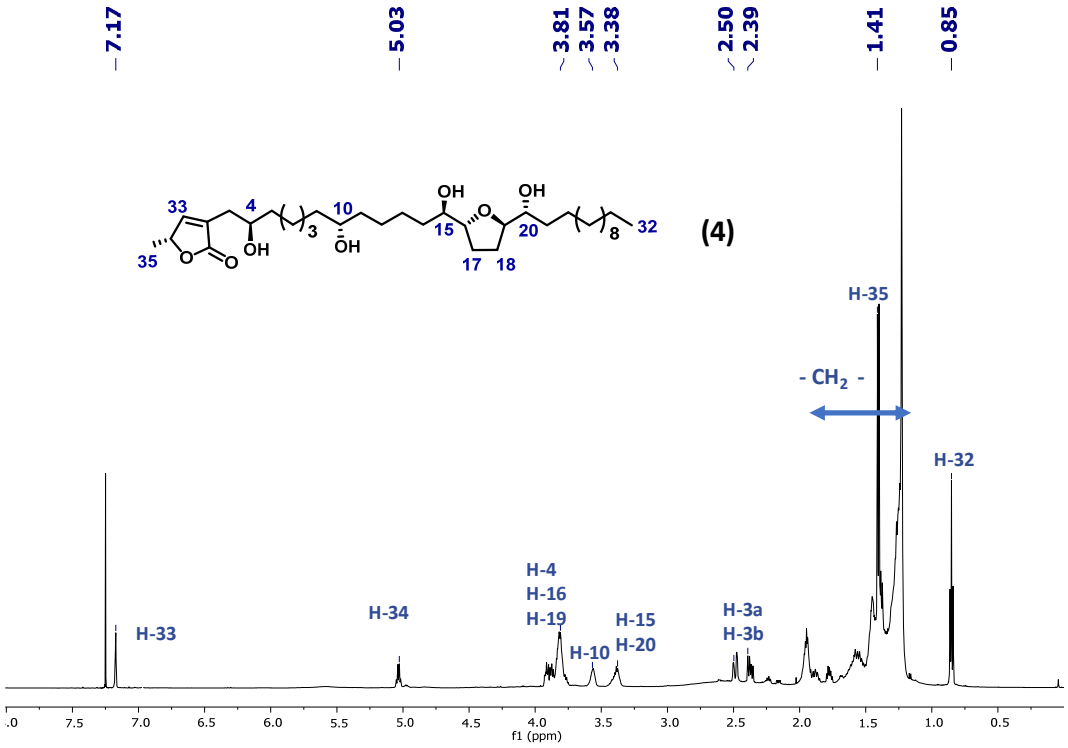
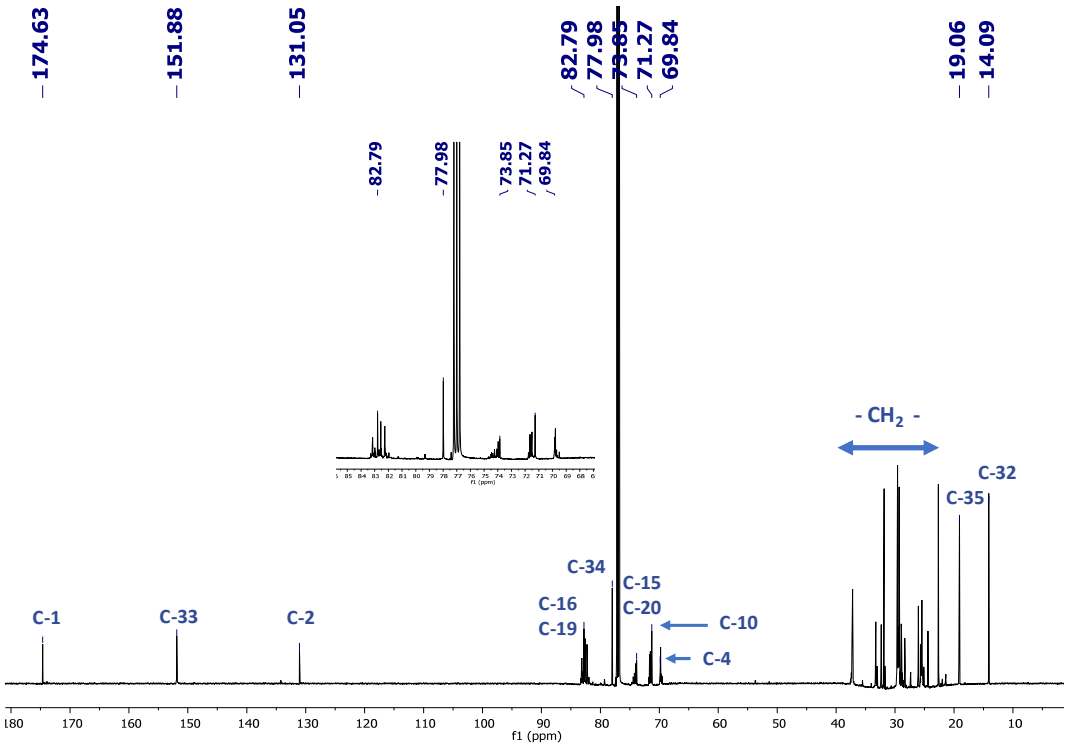

6.97
4.99
3.92
3.87
3.84
3.59
3.38
2.25
1.96
1.66
1.59
1.43
0.87
OH
OH
OH
35
37
9
15
17 18 21 22
24
2
29
(3)
H-37
- CH2 -
H-15
H-19
H-20
H-23
H-24
H-29
H-35
H-36
f1 (ppm)

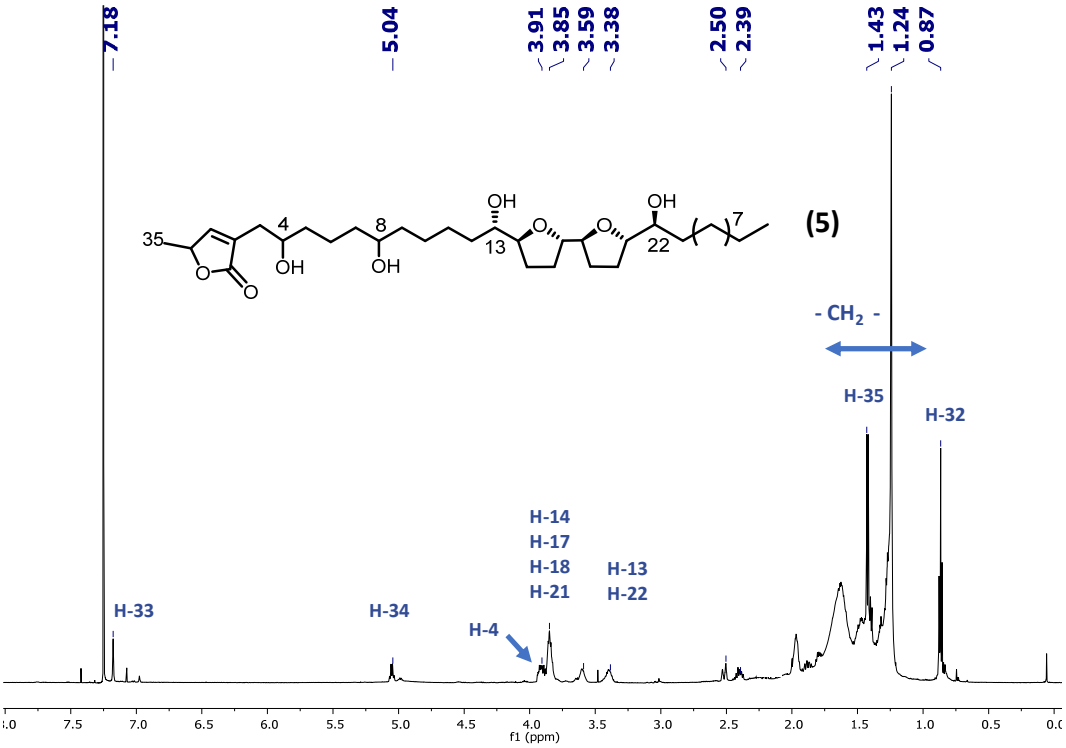

173.92
148.86
134.31
83.29
82.78
82.52
82.26
82.15
74.11
71.52
71.35
19.11
14.11
- CH2 -
f1 (ppm)

Annonacin (**4**)


7.17
5.03
3.81
3.57
3.38
2.50
2.39
1.41
0.85
(4)
H-35
- CH2 -
H-32
H-4
H-16
H-19
H-34
H-33
H-10
H-15
H-20
H-3a
H-3b
f1 (ppm)


174.63
151.88
131.05
82.79
77.98
73.85
71.27
69.84
19.06
14.09
- CH2 -
C-32
C-35
C-34
C-15
C-16
C-20
C-19
C-10
C-4
C-1
C-33
C-2
f1 (ppm)

Annonisin (**5**)


7.18
5.04
3.91
3.85
3.59
3.38
2.50
2.39
1.43
1.24
0.87
(5)
- CH2 -
H-35
H-32
H-14
H-17
H-18
H-21
H-13
H-22
H-33
H-34
H-4
f1 (ppm)

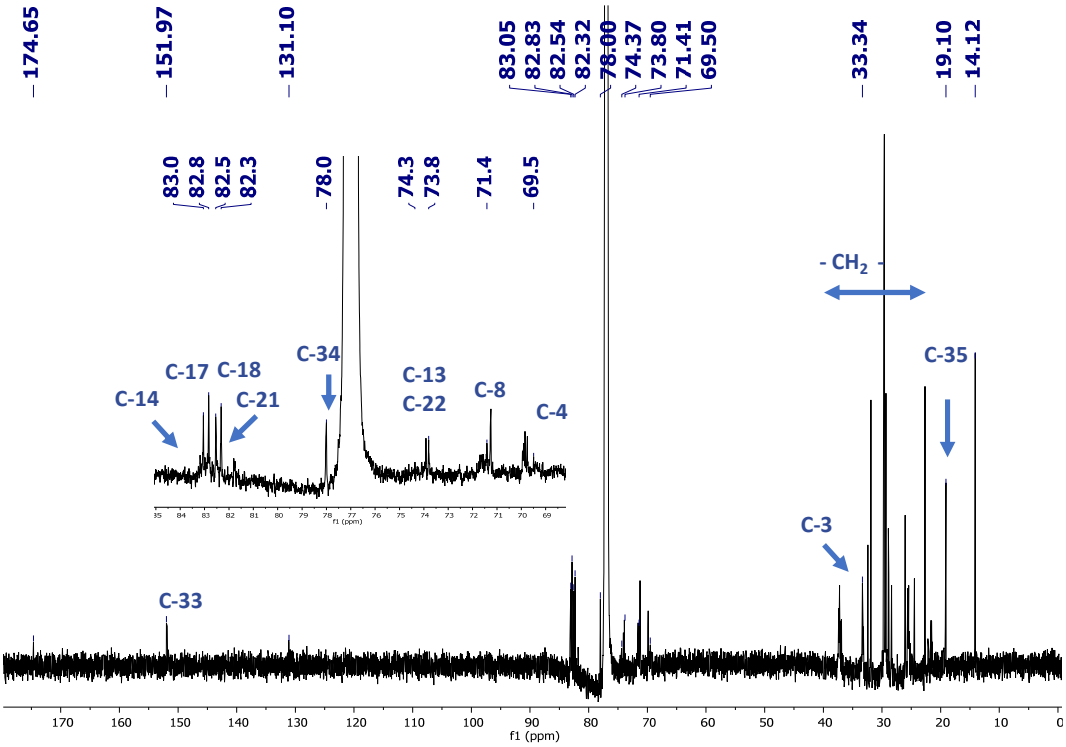

174.65
151.97
131.10
83.05
82.83
82.54
82.32
78.00
74.37
73.80
71.41
69.50
33.34
19.10
14.12
83.0
82.8
82.5
82.3
78.0
74.3
73.8
71.4
69.5
- CH2 -
C-17
C-18
C-14
C-21
C-34
C-13
C-22
C-8
C-4
C-35
C-3
C-33
f1 (ppm)

Figure S1. Cell viability by dye exclusion against ovarian carcinoma cells (IGROV-1) for the first (**A**), second (**B**) and third (**C**) fractionations of *A. cherimola* deciduous leaves. Extracts were evaluated at 100 ppm for 24 h. Experiments were performed in triplicate and data are expressed as mean ± SD, n = 3, * $p < 0.05$ vs untreated cells (DMSO 0.1%).

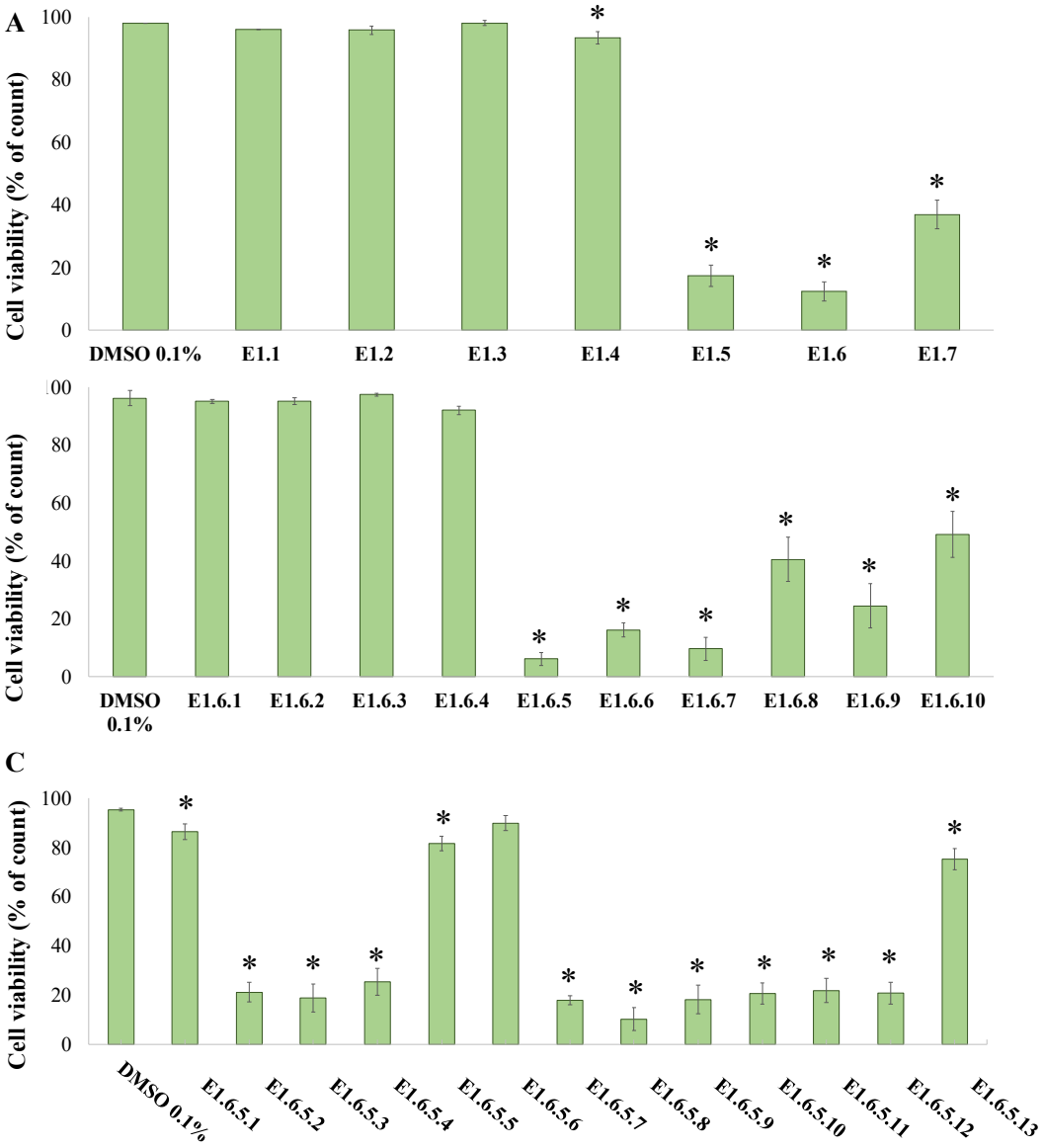


Figure S2. D_2O ^1H NMR comparison between α-CD, α-CD/urea polyrotaxane, SMPMs-ACGs and SMPMs-ACGs with phenol, from bottom to top.

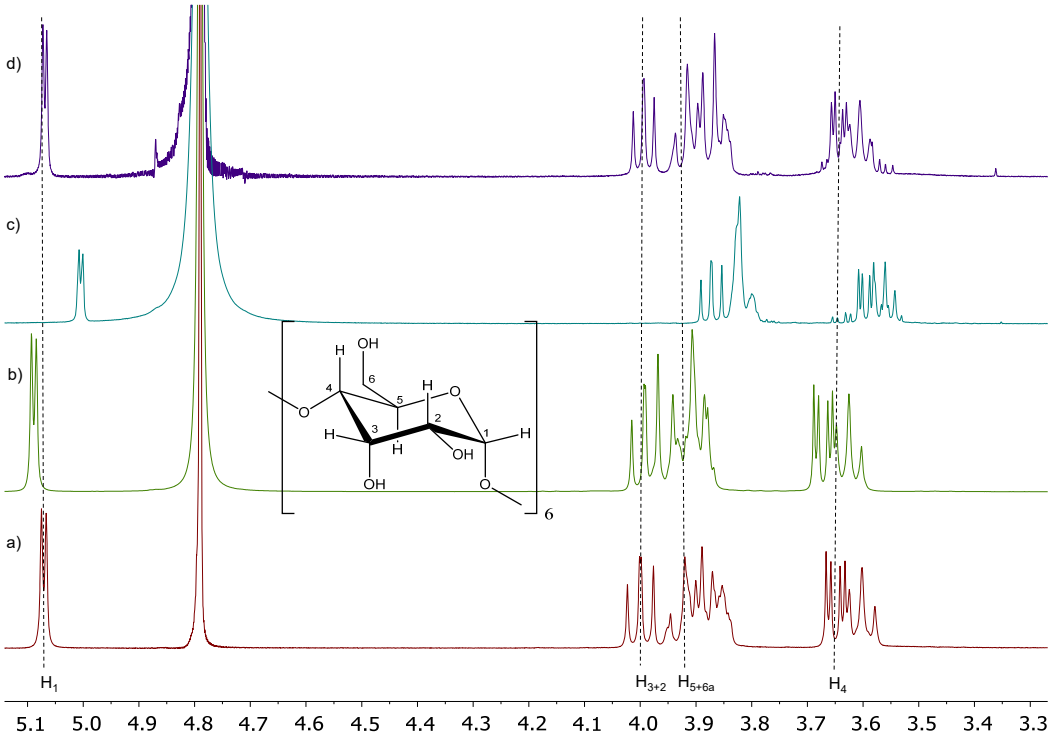


Figure S3. (Top) ^{1}H-NMR of SMPMs-ACGs/α-CD at different ppm to differenciate alpha-cyclodextrin signals and annonacin signals. (Bottom) ROESYAD 2D experiment of SMPMs-ACGs/α-CD.

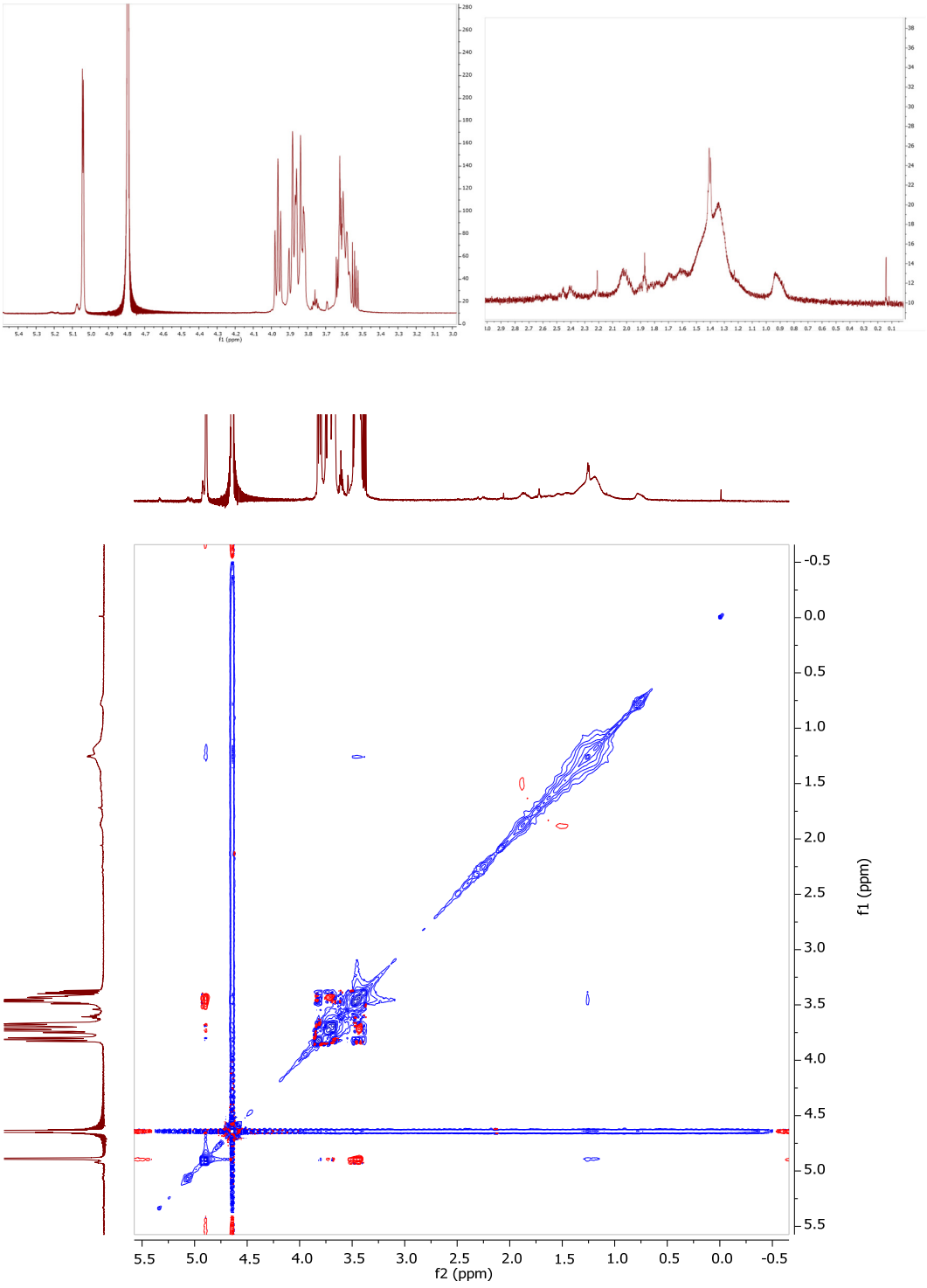


Figure S4. SMPMs wall thickness size distribution that are associated with *α*-CD/urea, with a mean size of 96.02 nm.

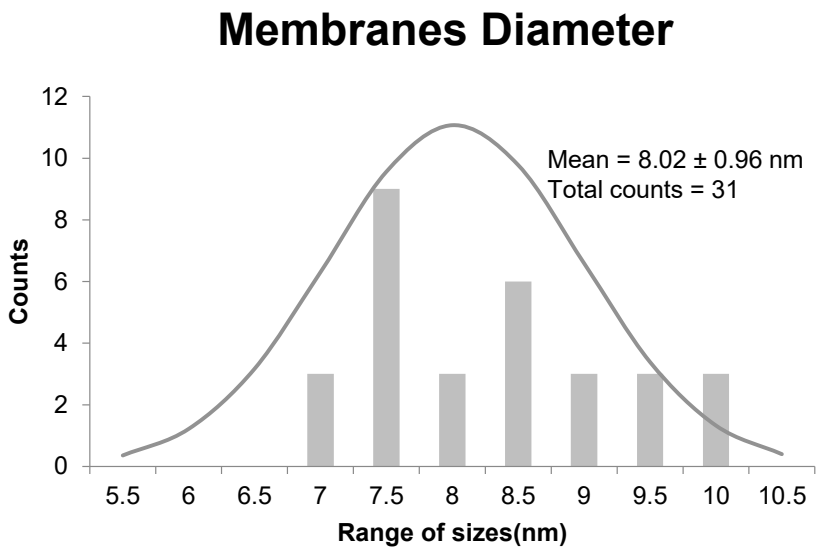


Figure S5. SMPMs size distribution that are associated with α-CD/urea, with a mean size of 96.02 nm. Two normal distributions can be observed at 60 and 140 nm of mean.

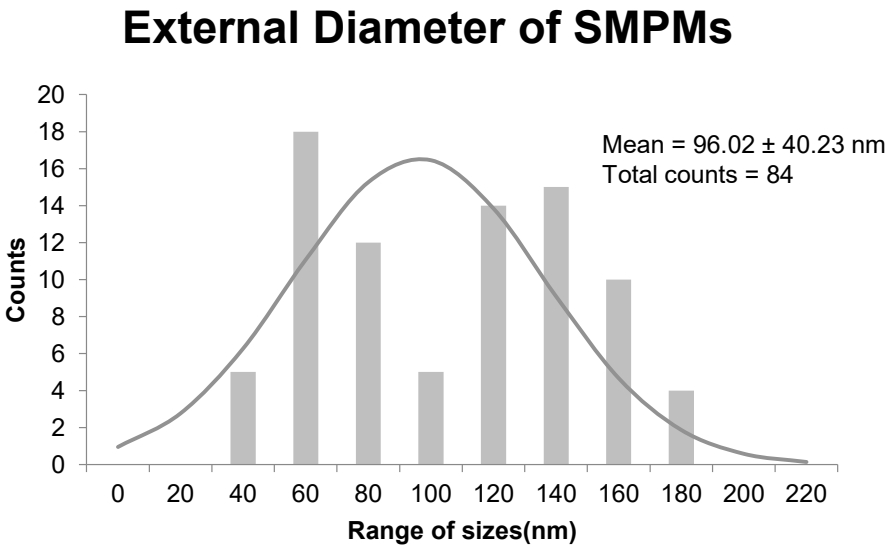


Figure S6. PM3 model of the SMPM shell in the case of two units of α-CD and thirty-two molecules of urea. (A) Biased geometry, with a distance of 26.46 Å between cyclodextrin molecules. (B) Truncated cone geometry, with a distance of 17.47 Å between cyclodextrin molecules (hydrogens are not represented).

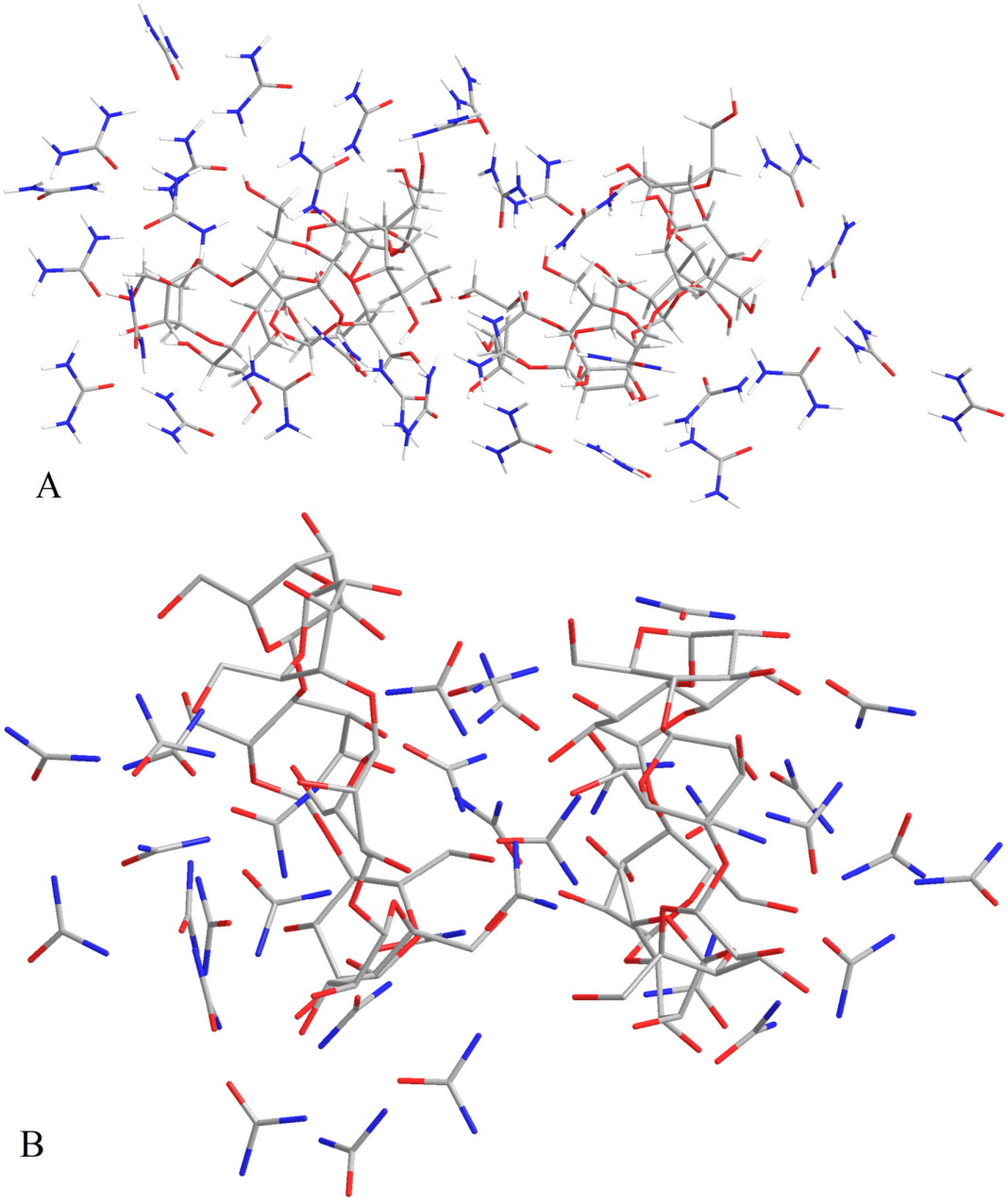


Figure S7. Calibration curve for annonacin in $CHCl_3$.

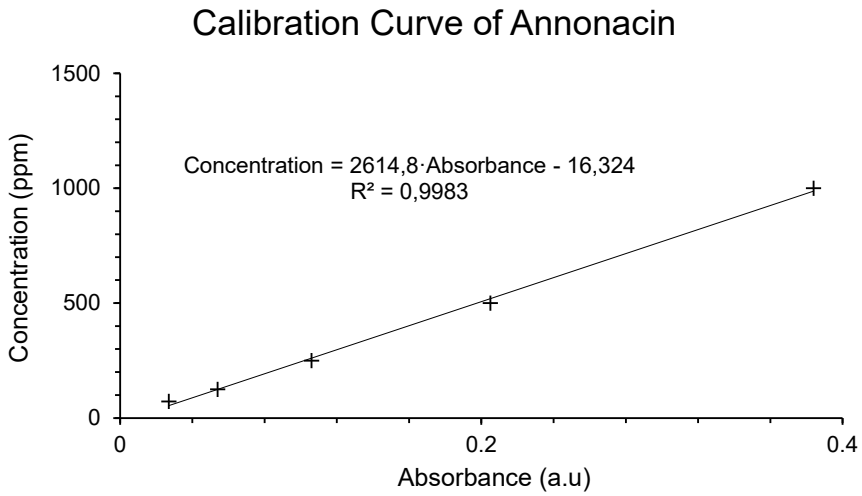


Figure S8. Critical micellar concentration experiment

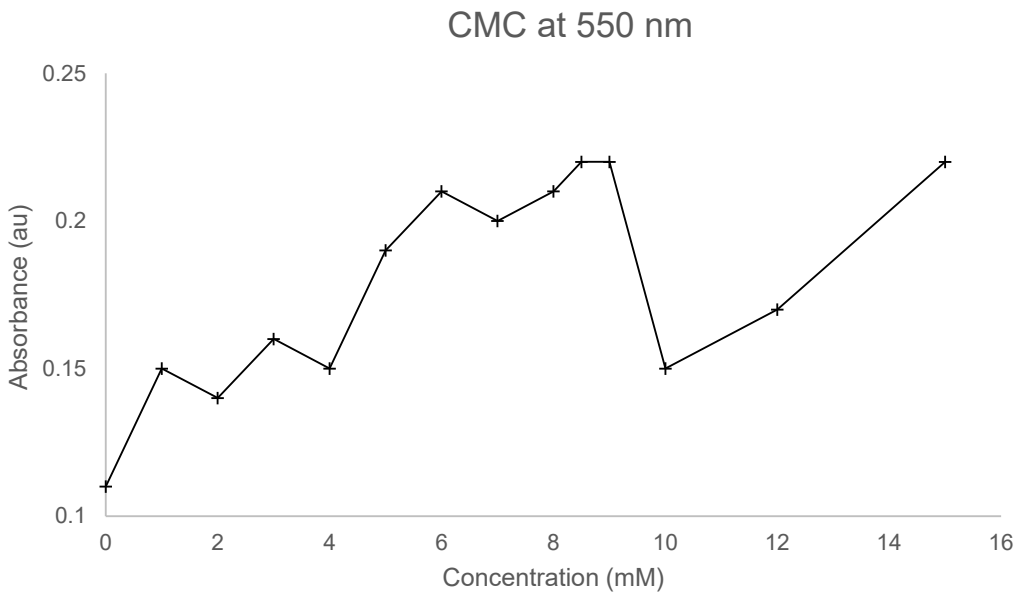


Figure S9. XRD experiment of (A) a-cyclodextrin and (B) SMPMs-ACGs