

## SUPPLEMENTARY INFORMATION

### **Direct Synthesis of Rhenium and Technetium-99m Metallosurfactants by a Transmetallation Reaction of Lipophilic groups. Potential applications in the radiolabeling of liposomes**

Jordi Borràs,<sup>†</sup> Verónica Mesa,<sup>†</sup> Joan Suades\*,<sup>†</sup> and Ramon Barnadas-Rodríguez\*,<sup>‡</sup>

Number of pages: 15

Number of figures: 22

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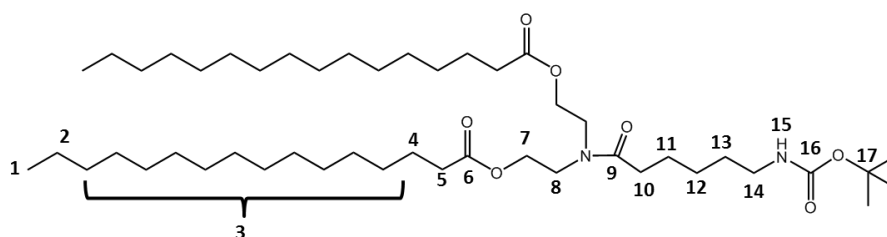
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\* E-mail for J.S: joan.suades@uab.cat

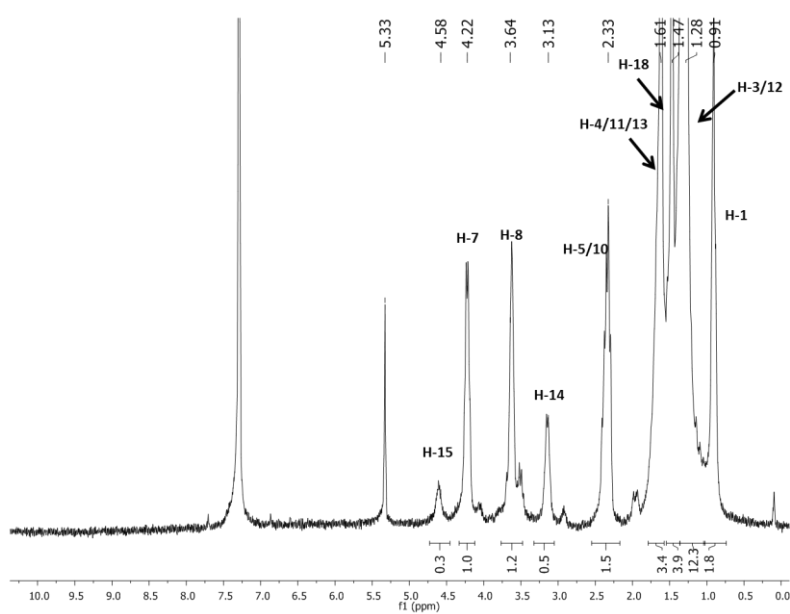
\* E-mail for R.B.-R.: ramon.barnadas@uab.cat

# Structural characterization

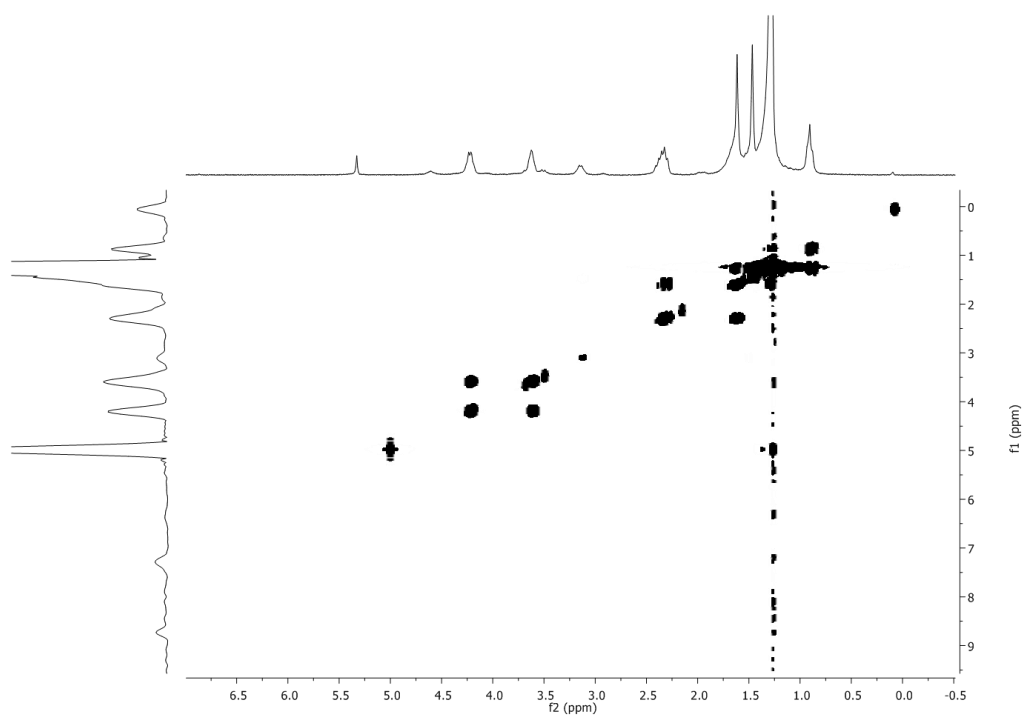
## (Spectroscopic and spectrometric data)



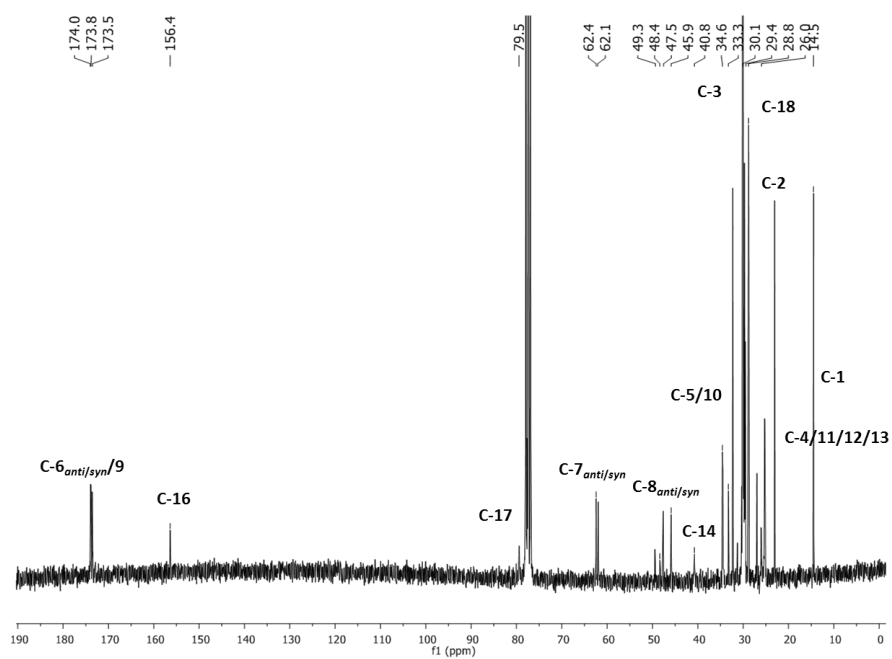
**Scheme 1:** PD Boc-protected.



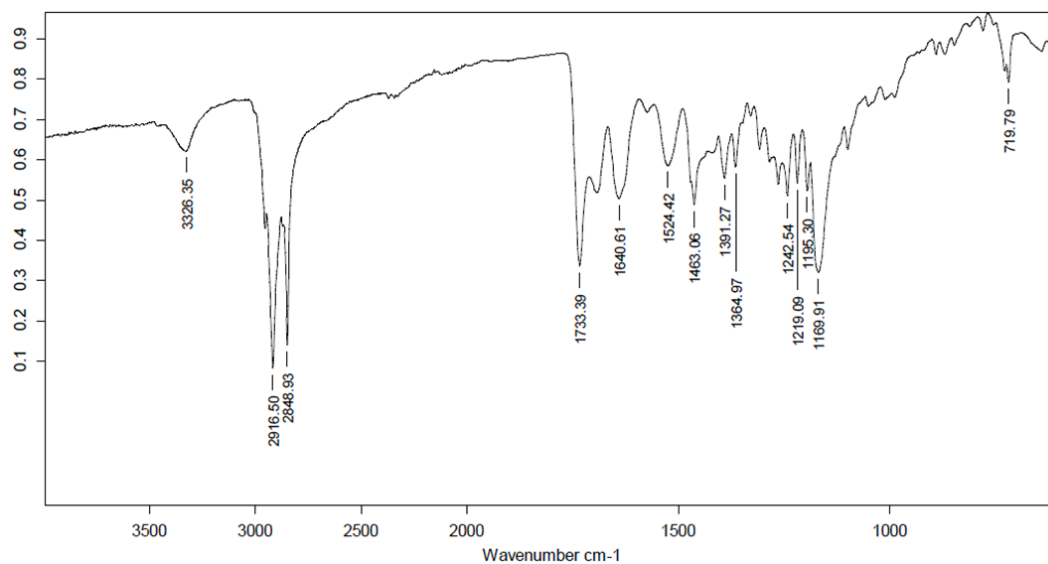
**Figure S1:** <sup>1</sup>H-RMN (CDCl<sub>3</sub>-250 MHz) of PD Boc-protected



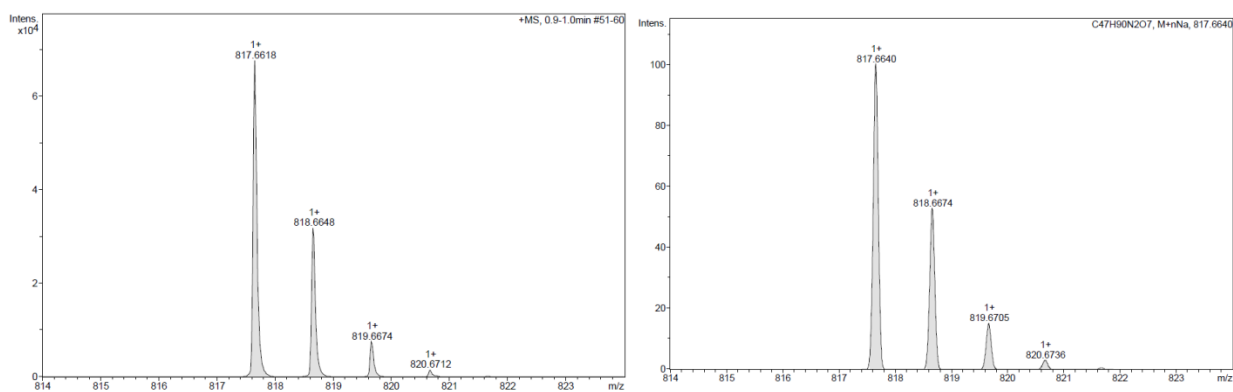
**Figure S2:**  $^1\text{H}$ -COSY-RMN ( $\text{CDCl}_3$ -250 MHz) of PD Boc-protected



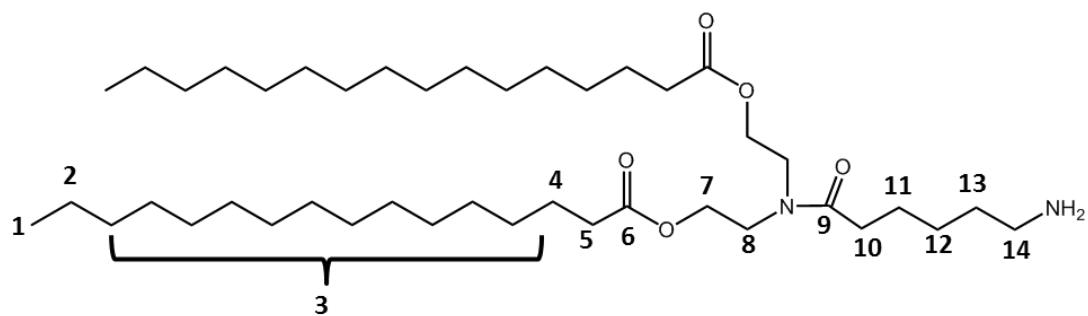
**Figure S3:**  $^{13}\text{C}$ -RMN ( $\text{CDCl}_3$ -250 MHz) of PD Boc-protected



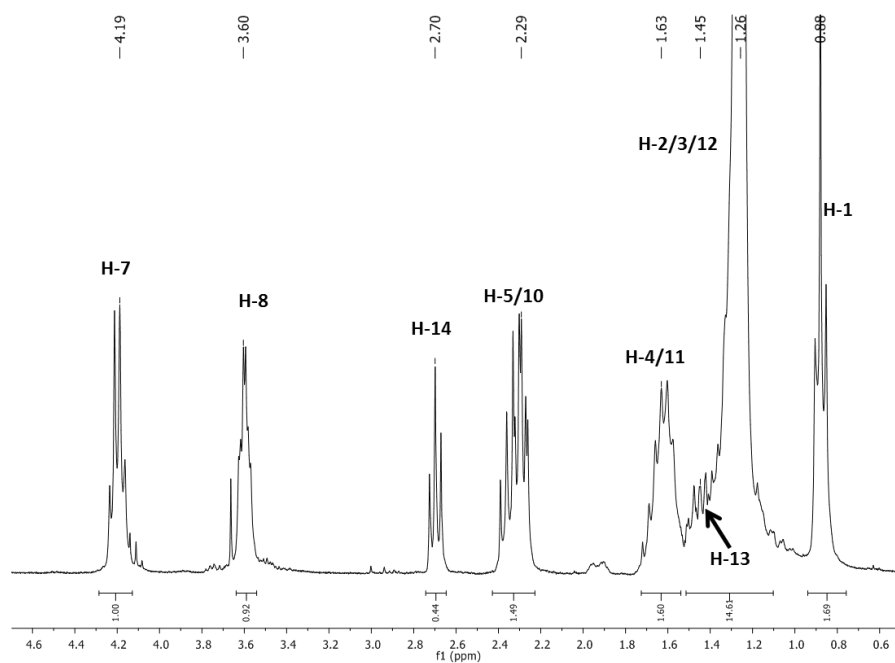
**Figure S4:** IR-ATR of PD Boc-protected



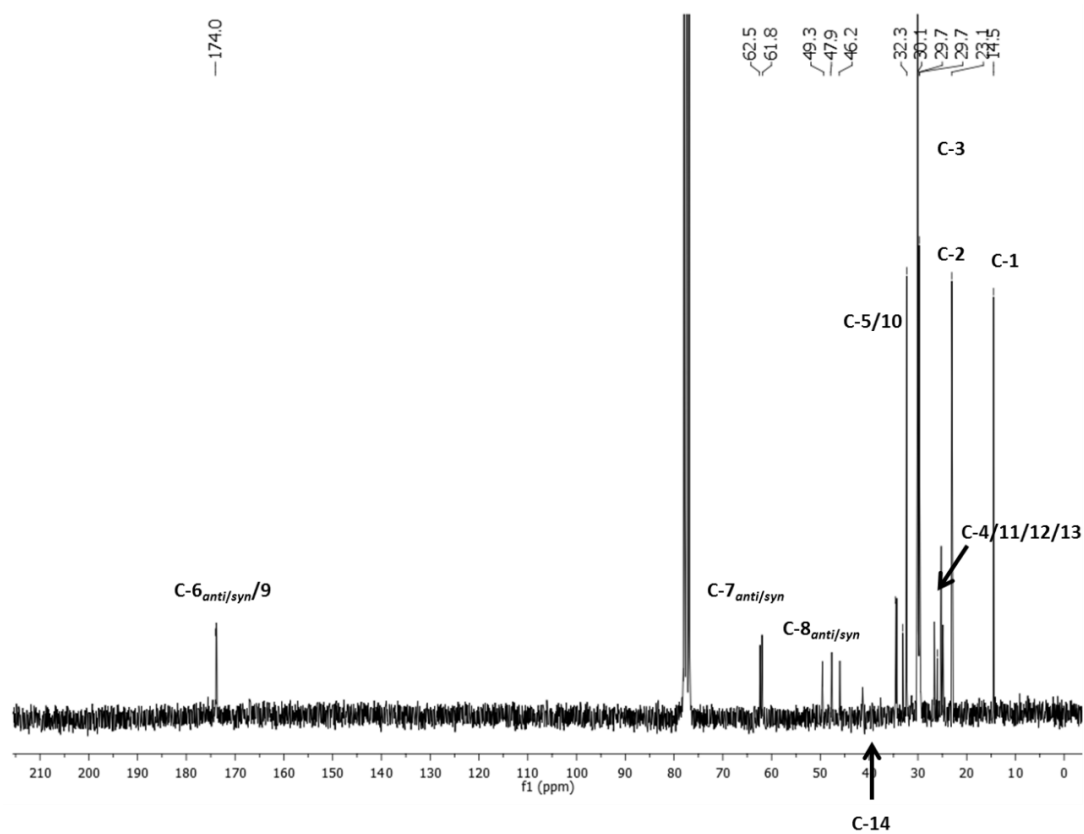
**Figure S5:** ESI-HRMS (positive mode) Recorded isotopic distribution of PD Boc-protected(left) and the corresponding theoretical distribution (right).



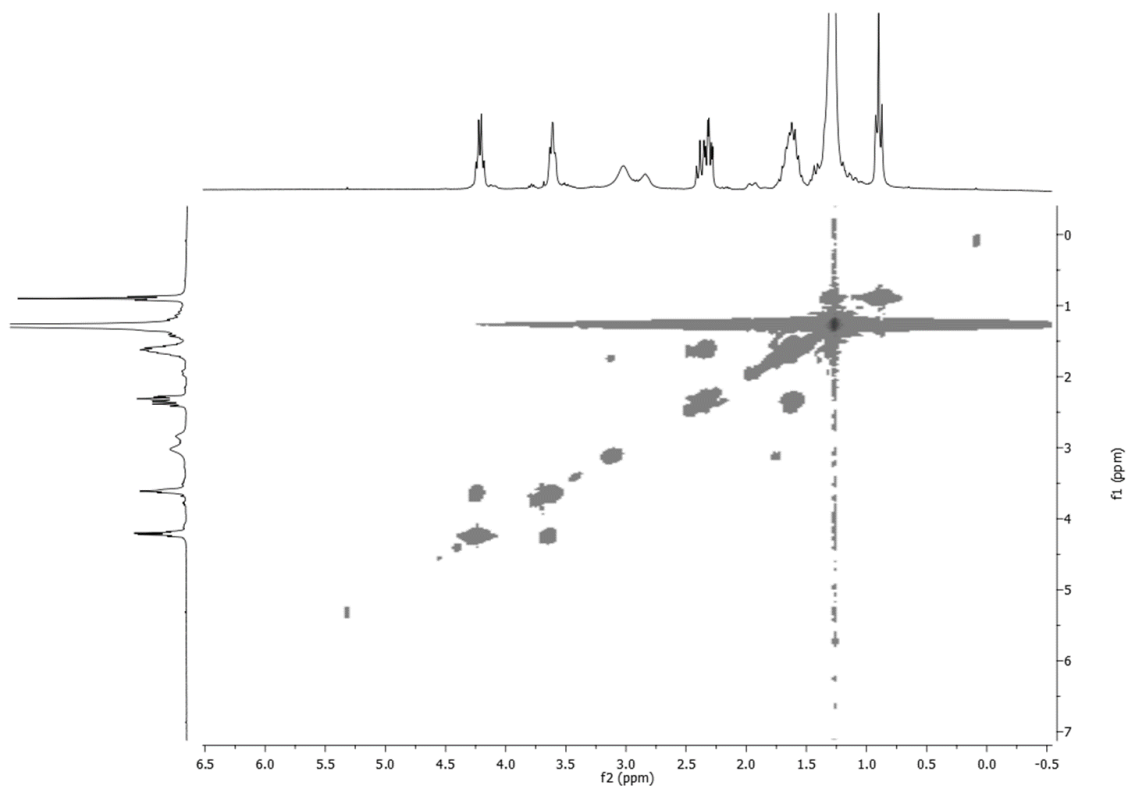
**Scheme 2:** PD amine deprotected.



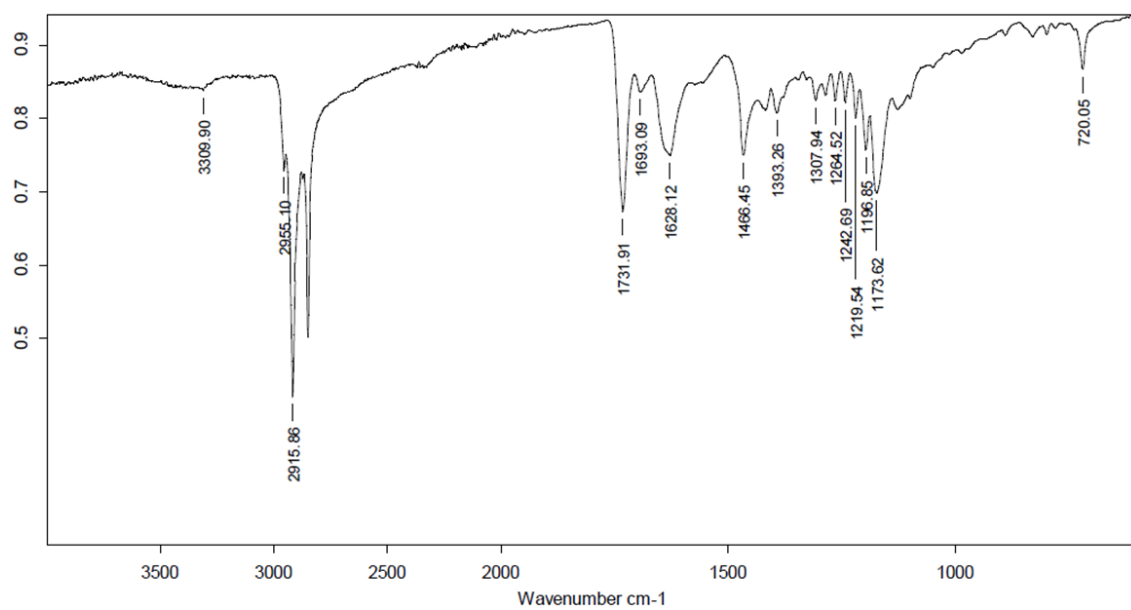
**Figure S6:**  $^1\text{H}$ -RMN ( $\text{CDCl}_3$  -250 MHz) of PD amine deprotected



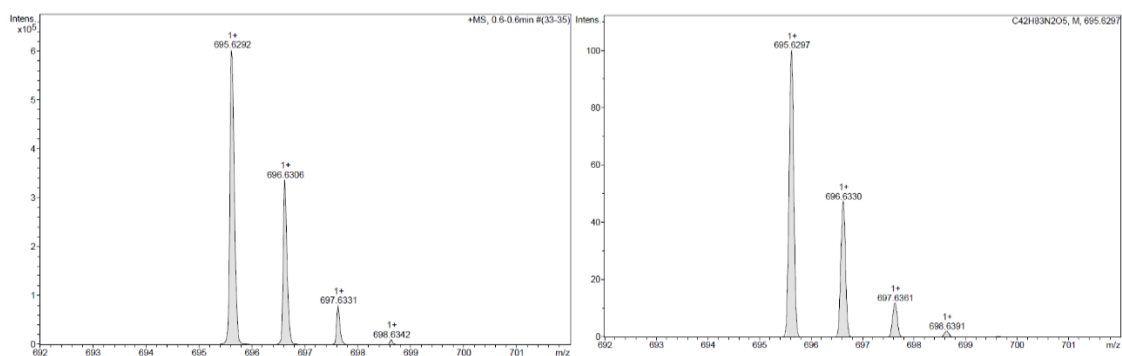
**Figure S7:**  $^{13}\text{C}$ -RMN ( $\text{CDCl}_3$ -250 MHz) of PD amine deprotected



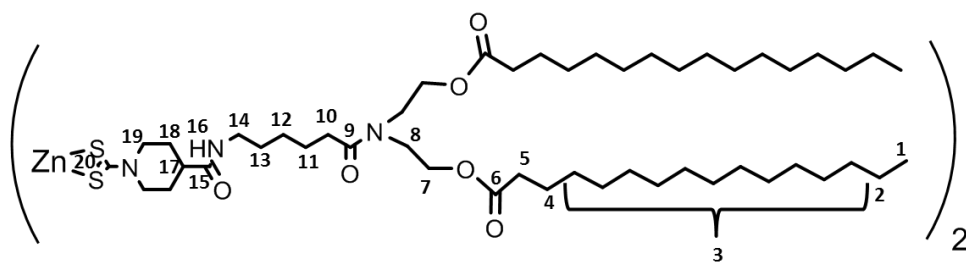
**Figure S8:**  $^1\text{H}$ -COSY-RMN ( $\text{CDCl}_3$ -250 MHz) of PD amine deprotected



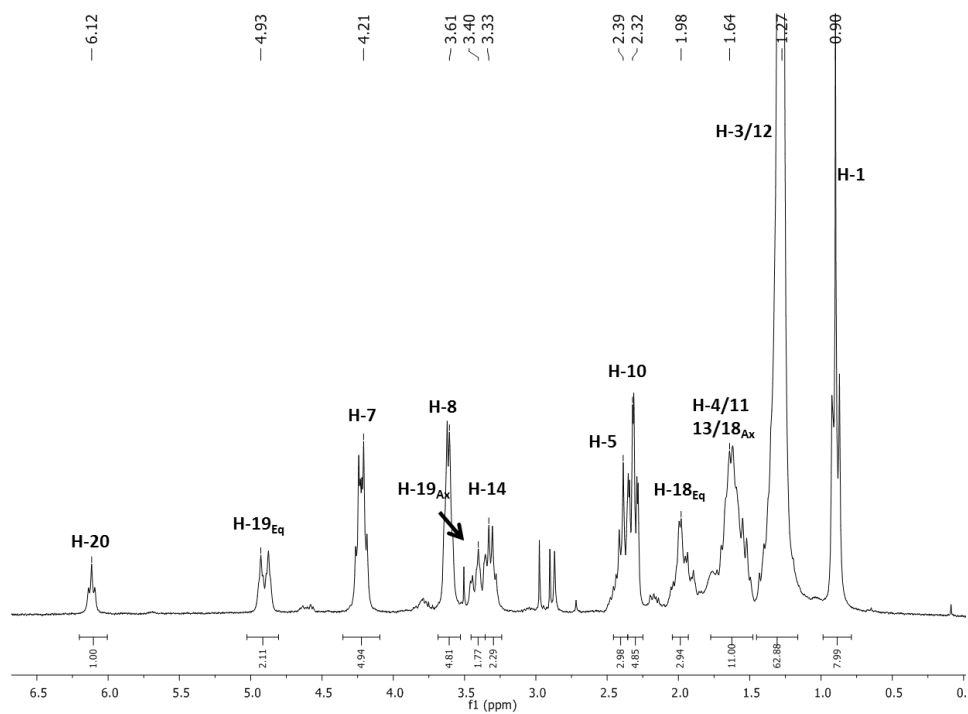
**Figure S9:** IR-ATR of PD amine deprotected



**Figure S10:** ESI-HRMS (positive mode) Recorded isotopic distribution of PD amine deprotected (left) and the corresponding theoretical distribution (right).



**Scheme 3: ZnC**



**Figure S11:**  $^1\text{H}$ -RMN ( $\text{CDCl}_3$ -250 MHz) of ZnC



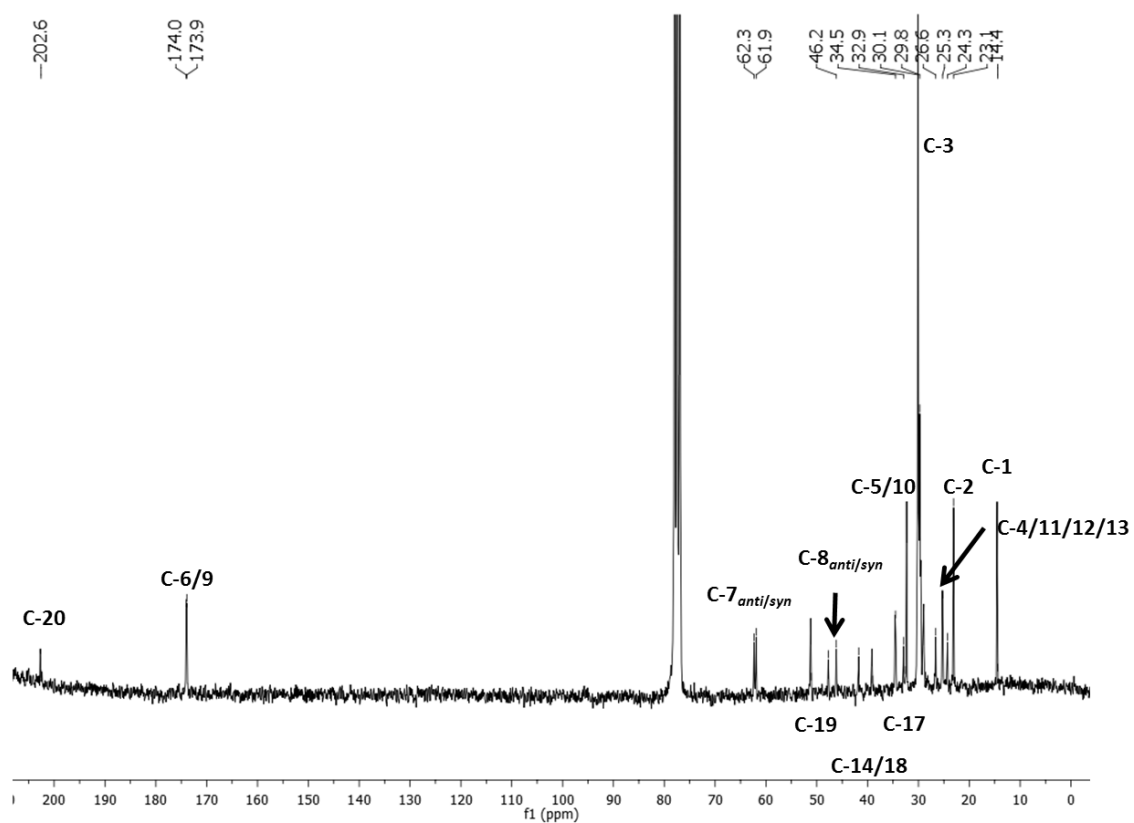


Figure S12:  $^{13}\text{C}$ -RMN ( $d\text{-CDCl}_3$ -250 MHz) of ZnC

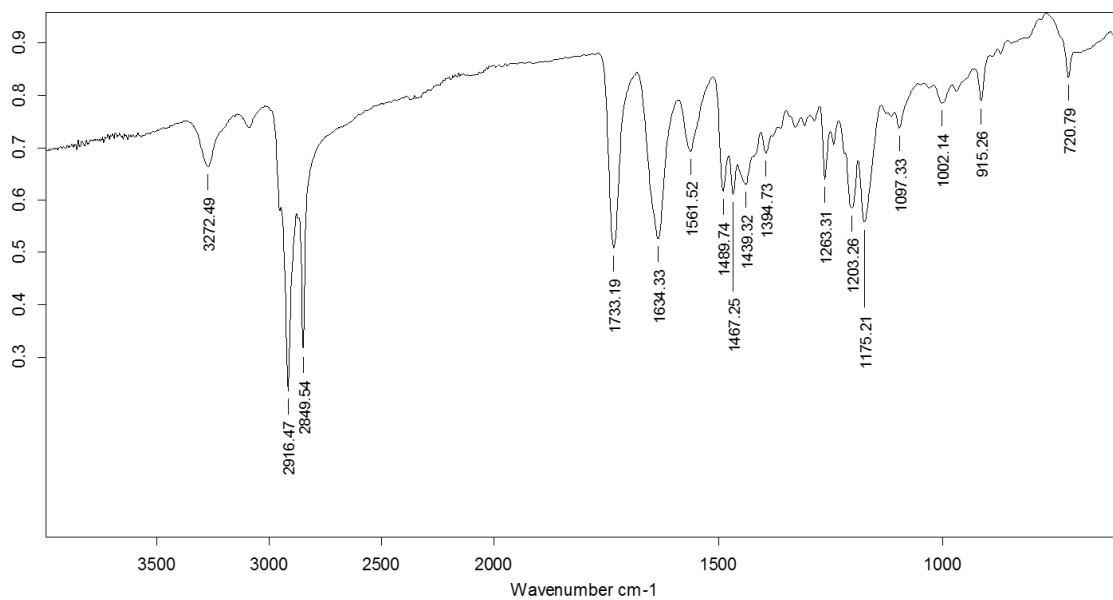
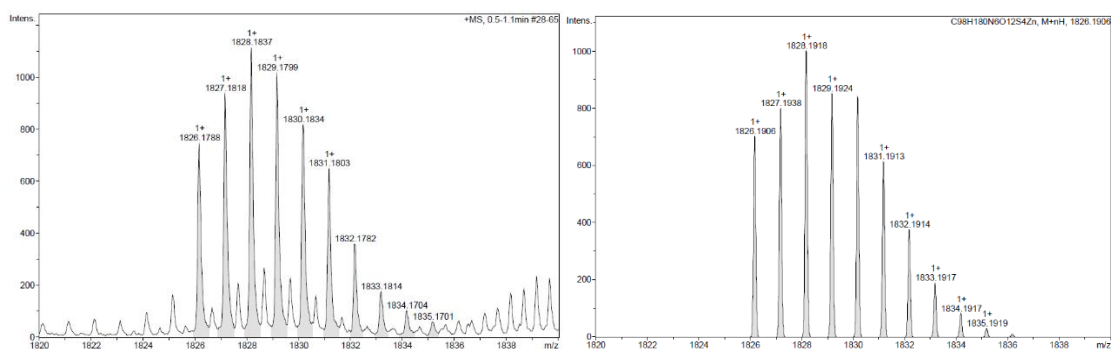
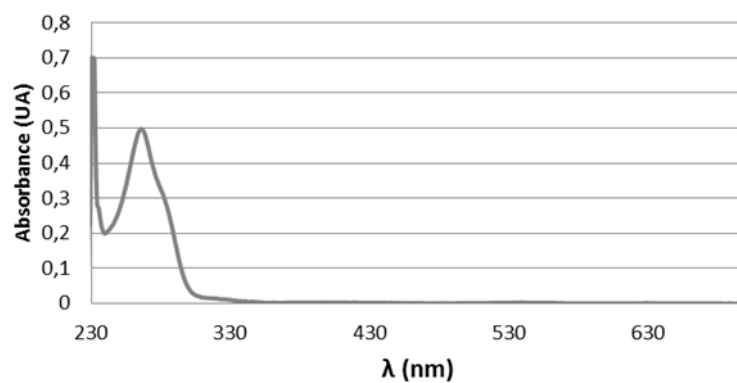


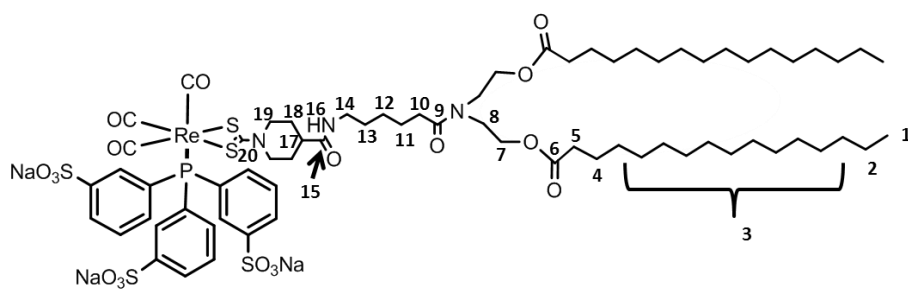
Figure S13: IR-ATR of ZnC



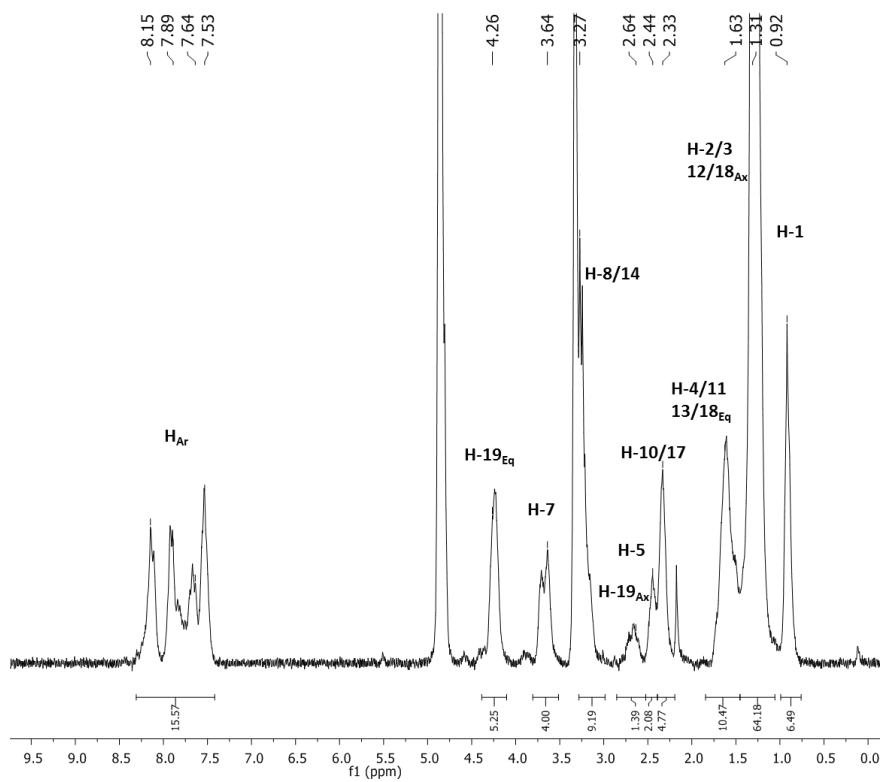
**Figure S14: ESI-HRMS (positive mode)** Recorded isotopic distribution of ZnC (left) and the corresponding theoretical distribution (right).



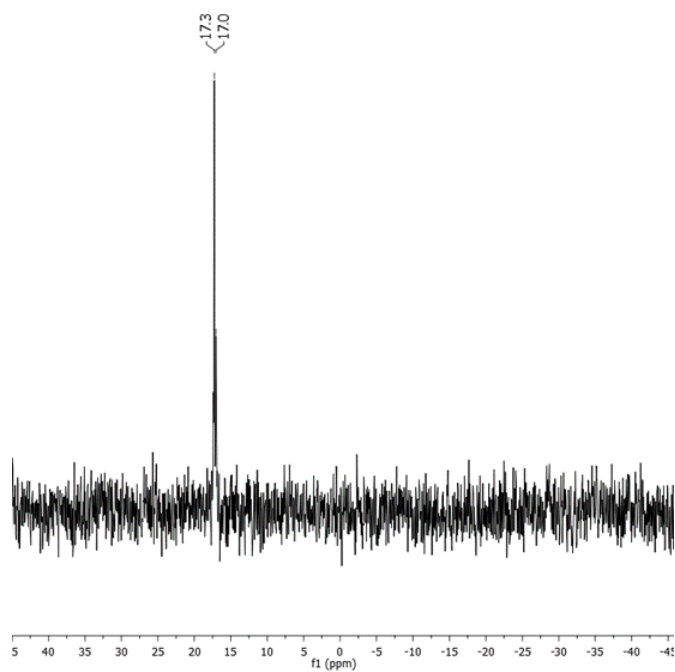
**Figure S15: UV-Vis concentration of ZnC 0.1 mM.**



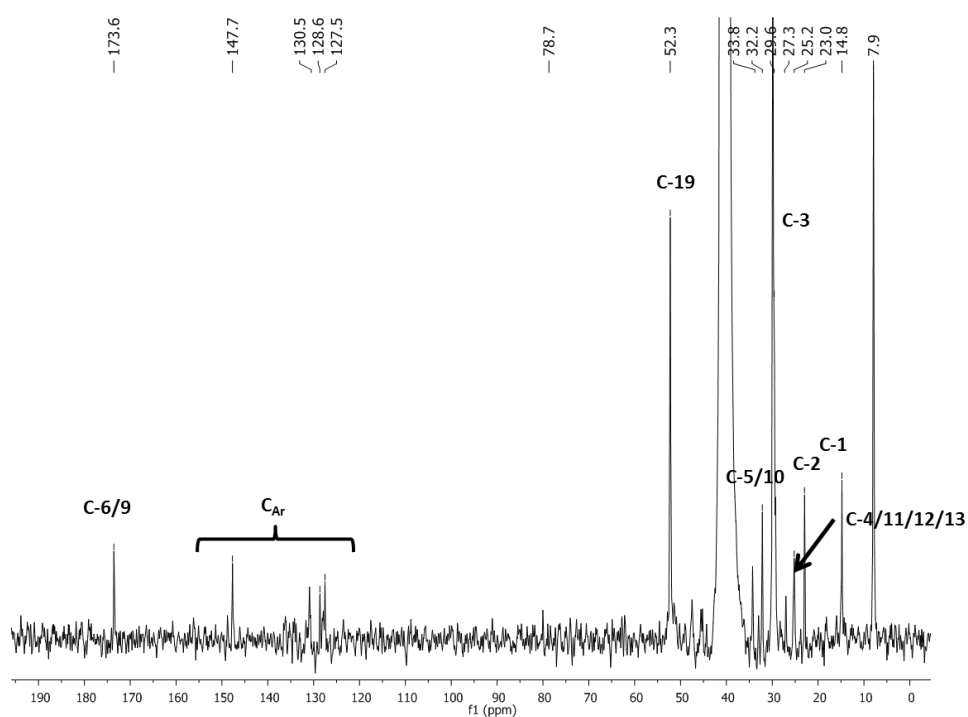
**Scheme 4: ReC**



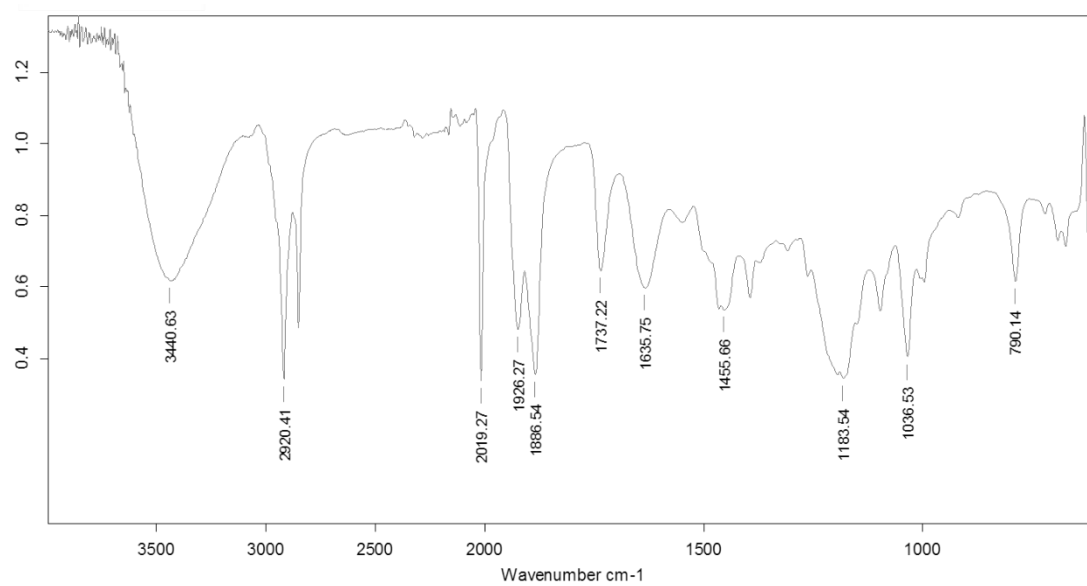
**Figure S16:**  $^1\text{H}$ -RMN ( $d_4$ -MeOD-250 MHz) of ReC



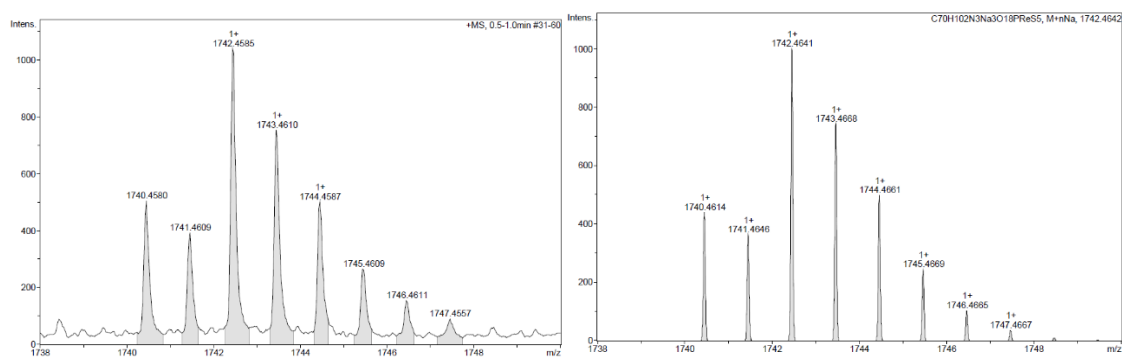
**Figure S17:**  $^{31}\text{P}$ -RMN ( $d_6$ -DMSO-250 MHz) of ReC



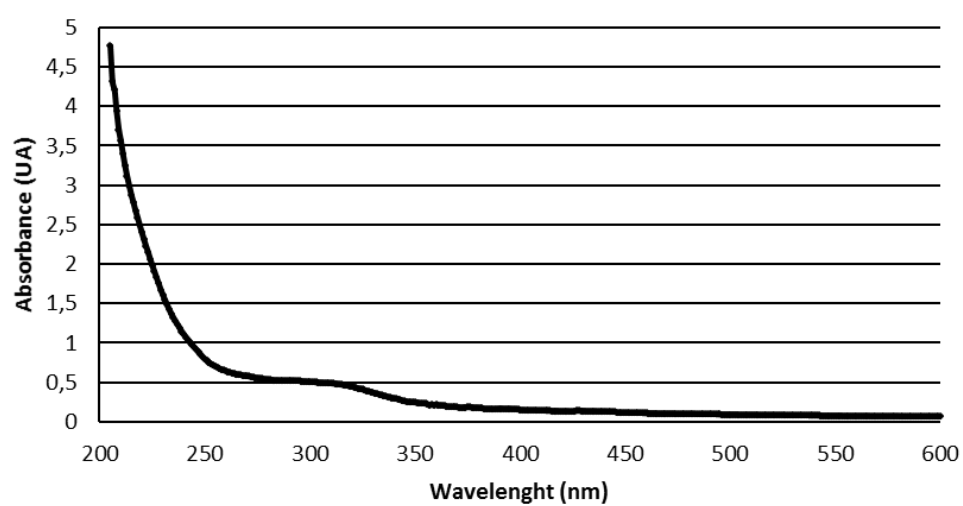
**Figure S18:**  $^{13}\text{C}$ -RMN ( $d_4$ -MeOD-250 MHz) of ReC



**Figure S19: IR-ATR of ReC**

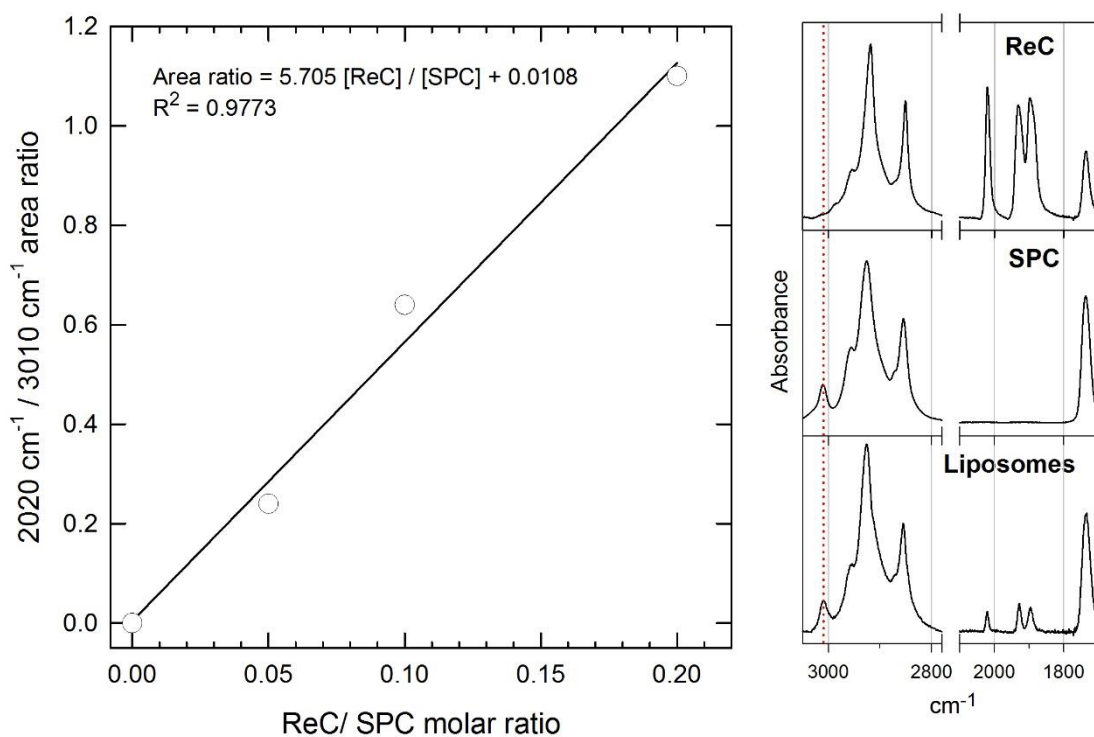


**Figure S20: ESI-HRMS (positive mode) Recorded isotopic distribution of ReC (left) and the corresponding theoretical distribution (right).**



**Figure S21:** UV-Vis concentration of ReC 50 μM.

## Aggregation studies



**Figure S22:** Infrared spectra (right) of the ReC (up), SPC (middle) and samples of ReC with liposomes (down), showing the peaks used (3010 cm<sup>-1</sup> and 2020 cm<sup>-1</sup>) for obtaining the calibration curve (left) that allows to obtain the relative amount of ReC in samples with liposomes.