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Supporting Information

Novel Polyhedral Silsesquioxanes [POSS(OH)$_{32}$] as Anthracycline Nanocarriers—Potential Anticancer Prodrugs

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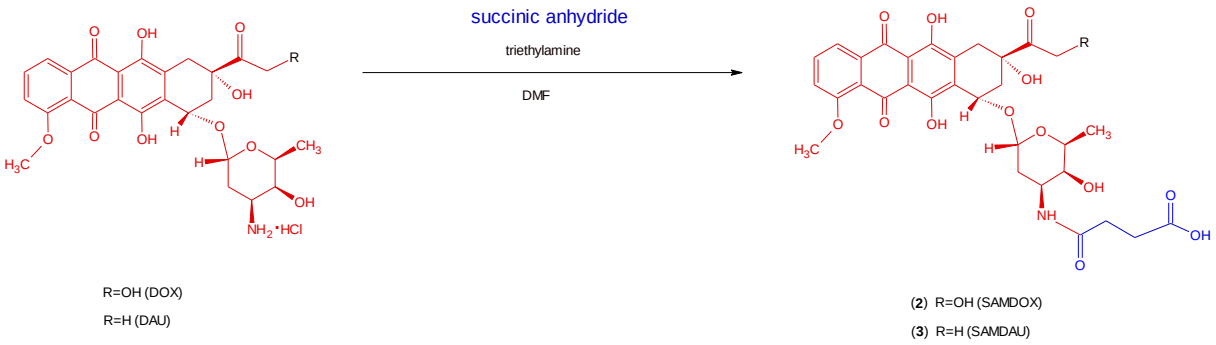

Fig. S1. Scheme for the synthesis of SAMDOX and SAMDAU.

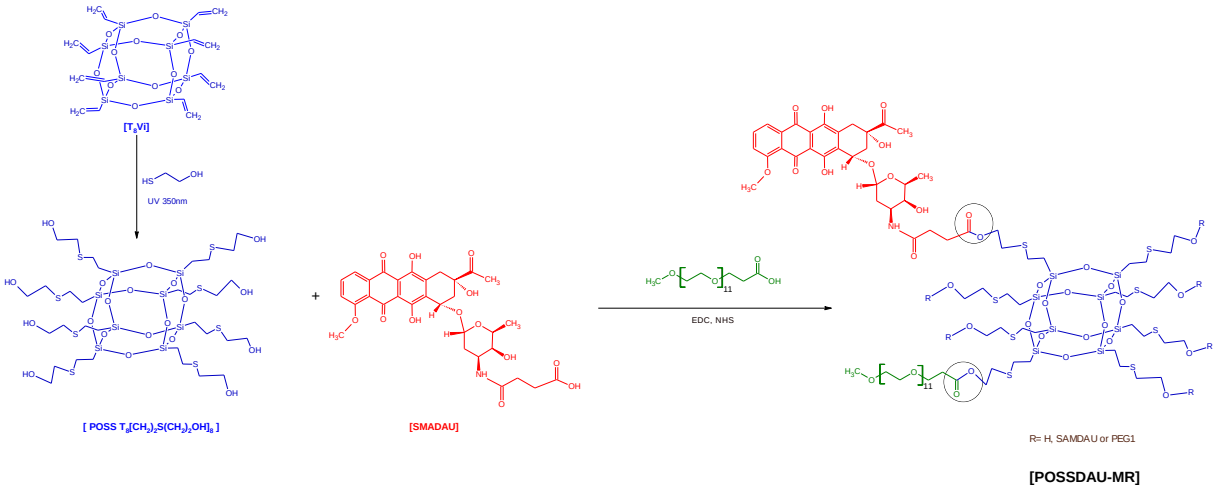

Fig. S2. Scheme for the synthesis of POSSDAU-MR.

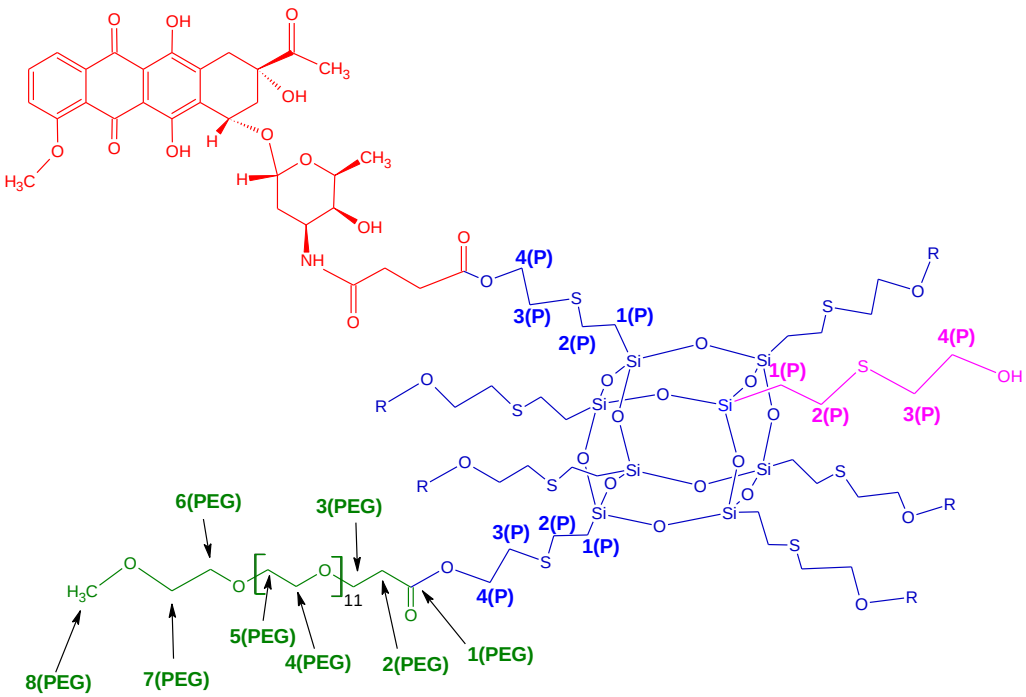

Fig. S3. Structure of POSSDAU-MR

Table S1. NMR results for POSSDAU-MR.

Type of Substitution	Signal	The Value of Chemical Shift [ppm] ^{1}H-NMR [DMSO-d6, 295K, 500MHz]	The Value of Chemical Shift [ppm] ^{13}C-NMR [DMSO-d6, 295K, 500MHz]
Unsubstituted POSS Corner	1(P)	1.02	13.1
	2(P)	2.63	25.7
	3(P)	2.56	33.9
	4(P)	3.53	61.4
Substituted POSS Corner	1(P)	1.02	13.1
	2(P)	2.63	25.7
	3(P)	2.75	29.8
	4(P)	4.14	63.4
Substituted and Unsubstituted PEG	1(PEG)	-	-
	2(PEG)	2.45/2.56	35.3/34.0
	3(PEG)	3.73/3.60	65.7/66.9
	4(PEG)	3.51/3.52	70.3/70.1
	5(PEG)		
	6(PEG)		

	7(PEG)	3.43	71.8
	8(PEG)	3.25	58.6

Table S2. Concentrations of the reagents used in conjugation reaction **4**–**9**.

Products	Reactants	m [g]	n [mol]	V [ml]
***PossDoxPEG1* (4)**	SAMDOX	0.1366	$2.1193 \cdot 10^{-4}$	-
	NHS_{SAMDOX}	0.0366	$3.1801 \cdot 10^{-4}$	-
	EDC_{SAMDOX}	0.0610	$3.1821 \cdot 10^{-4}$	-
	DMF_{SAMDOX}	-	-	9.0
	PEG1	0.1000	$1.6987 \cdot 10^{-4}$	-
	NHS_{PEG1}	0.0293	$2.5458 \cdot 10^{-4}$	-
	EDC_{PEG1}	0.0488	$2.5456 \cdot 10^{-4}$	-
	DMF_{PEG1}	-	-	9.0
	POSS	0.0438	$2.1193 \cdot 10^{-5}$	-
	DMF_{POSS}	-	-	9.0
***PossDoxPEG2* (5)**	SAMDOX	0.1366	$2.1224 \cdot 10^{-4}$	-
	NHS_{SAMDOX}	0.0366	$3.1801 \cdot 10^{-4}$	-
	EDC_{SAMDOX}	0.0610	$3.1821 \cdot 10^{-4}$	-
	DMF_{SAMDOX}	-	-	9.0
	PEG2	0.2229	$1.0614 \cdot 10^{-4}$	-
	NHS_{PEG2}	0.0183	$1.5900 \cdot 10^{-4}$	-
	EDC_{PEG2}	0.0305	$1.5910 \cdot 10^{-4}$	-
	DMF_{PEG2}	-	-	9.0
	POSS	0.0365	$1.7660 \cdot 10^{-5}$	-
	DMF_{POSS}	-	-	9.0
***PossDoxPEGB3* (6)**	SAMDOX	0.0343	$5.3294 \cdot 10^{-5}$	-
	NHS_{SAMDOX}	0.0092	$7.9937 \cdot 10^{-5}$	-
	EDC_{SAMDOX}	0.0153	$7.9812 \cdot 10^{-5}$	-
	DMF_{SAMDOX}	-	-	9.0
	PEGB3	0.0800	$2.6667 \cdot 10^{-5}$	-
	NHS_{PEGB3}	0.0046	$3.9969 \cdot 10^{-5}$	-
	EDC_{PEGB3}	0.0077	$4.0167 \cdot 10^{-5}$	-
	DMF_{PEGB3}	-	-	9.0
	POSS	0.0095	$4.5966 \cdot 10^{-6}$	-
	DMF_{POSS}	-	-	9.0
***PossDauPEG1* (7)**	SAMDAU	0.1333	$2.1239 \cdot 10^{-4}$	-
	NHS_{SAMDAU}	0.0367	$3.1888 \cdot 10^{-4}$	-
	EDC_{SAMDAU}	0.0612	$3.1925 \cdot 10^{-4}$	-
	DMF_{SAMDAU}	-	-	9.0
	PEG1	0.0675	$1.1466 \cdot 10^{-4}$	-

	NHS_{PEG1}	0.0293	$1.5284 \cdot 10^{-4}$	-
	EDC_{PEG1}	0.0488	$2.5456 \cdot 10^{-4}$	-
	DMF_{PEG1}	-	-	9.0
	POSS	0.0438	$2.1193 \cdot 10^{-5}$	-
	DMF_{POSS}	-	-	9.0
***PossDauPEG2* (8)**	SAMDAU	0.1332	$2.1224 \cdot 10^{-4}$	-
	NHS_{SAMDAU}	0.0367	$3.1888 \cdot 10^{-4}$	-
	EDC_{SAMDAU}	0.0611	$3.1873 \cdot 10^{-4}$	-
	DMF_{SAMDAU}	-	-	9.0
	PEG2	0.2229	$1.0614 \cdot 10^{-4}$	-
	NHS_{PEG2}	0.0183	$1.5901 \cdot 10^{-4}$	-
	EDC_{PEG2}	0.0305	$1.5910 \cdot 10^{-4}$	-
	DMF_{PEG2}	-	-	9.0
	POSS	0.0365	$1.7660 \cdot 10^{-5}$	-
	DMF_{POSS}	-	-	9.0
***PossDauPEGB3* (9)**	SAMDAU	0.0334	$5.3219 \cdot 10^{-5}$	-
	NHS_{SAMDAU}	0.0092	$7.9937 \cdot 10^{-5}$	-
	EDC_{SAMDAU}	0.0153	$7.9812 \cdot 10^{-5}$	-
	DMF_{SAMDAU}	-	-	2.5
	PEGB3	0.0800	$2.6667 \cdot 10^{-5}$	-
	NHS_{PEGB3}	0.0046	$3.9969 \cdot 10^{-5}$	-
	EDC_{PEGB3}	0.0077	$4.0167 \cdot 10^{-5}$	-
	DMF_{PEGB3}	-	-	2.5
	POSS	0.0095	$4.5966 \cdot 10^{-6}$	-
	DMF_{POSS}	-	-	2.5

Table S3. Concentrations of the conjugates **4**–**9** in drugs release study.

Type of Nanoconjugate	$M_{CONJUGATES}$	V_{BUFFER}	V_{DMF}	$C_{CONJUGATES}$
PossDoxPEG1 (4)	6.3 mg	80 mL	1 mL	0.07778 mg/mL
PossDoxPEG2 (**5**)	4.6 mg	50 mL	1 mL	0.09019 mg/mL
PossDoxPEGB3 (**6**)	5.2 mg	65 mL	1 mL	0.07879 mg/mL
PossDauPEG1 (**7**)	4.9 mg	50 mL	1 mL	0.09608 mg/mL
PossDauPEG2 (**8**)	6.7 mg	80 mL	1 mL	0.08272 mg/mL
PossDauPEGB3 (**9**)	1.4 mg	50 mL	1 mL	0.02745 mg/mL

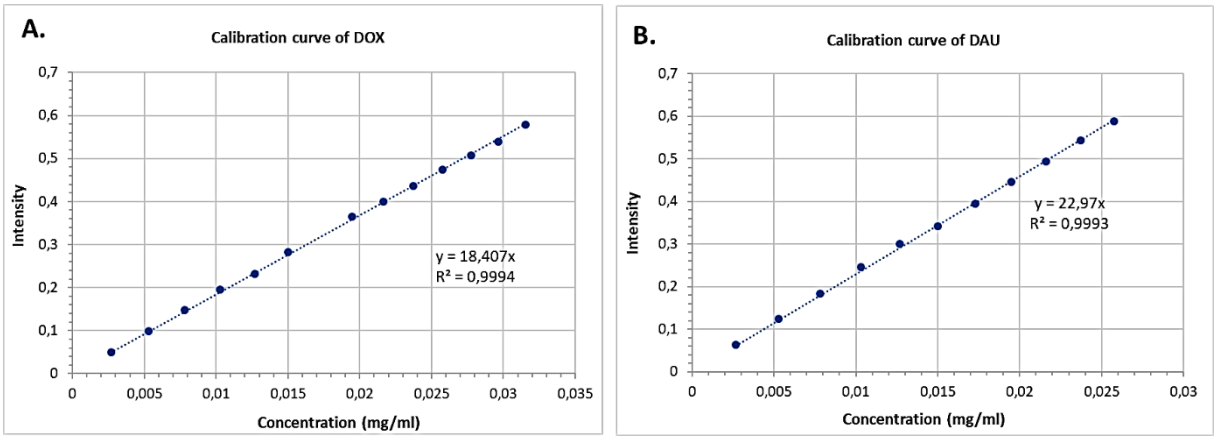

Fig. S4. Calibration curves (UV-VIS) for: (**A**) DOX in H_2O/DMF (5:1) (**B**) DAU in H_2O/DMF.

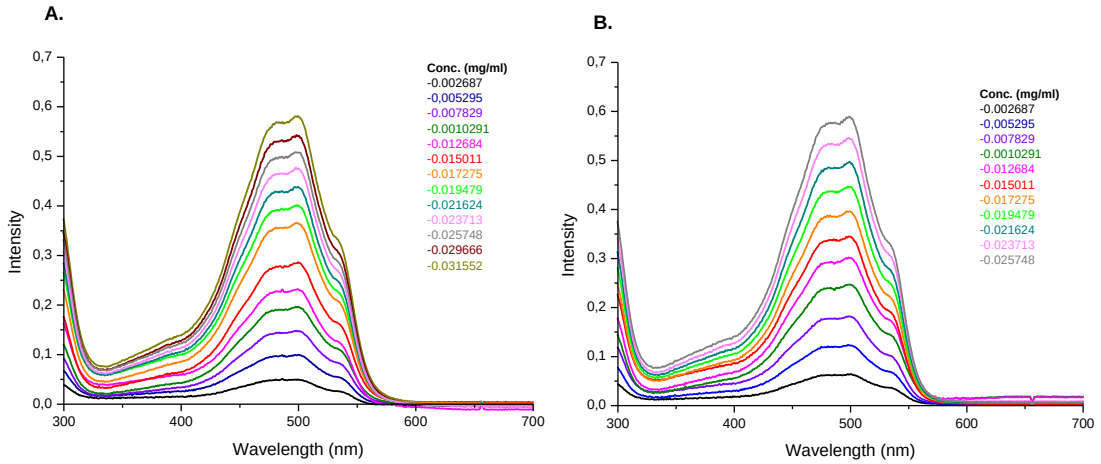

Fig. S5. Dependence of absorbance intensity on anthracycline concentration (**A**. DOX, **B**. DAU) (UV-Vis spectrum).

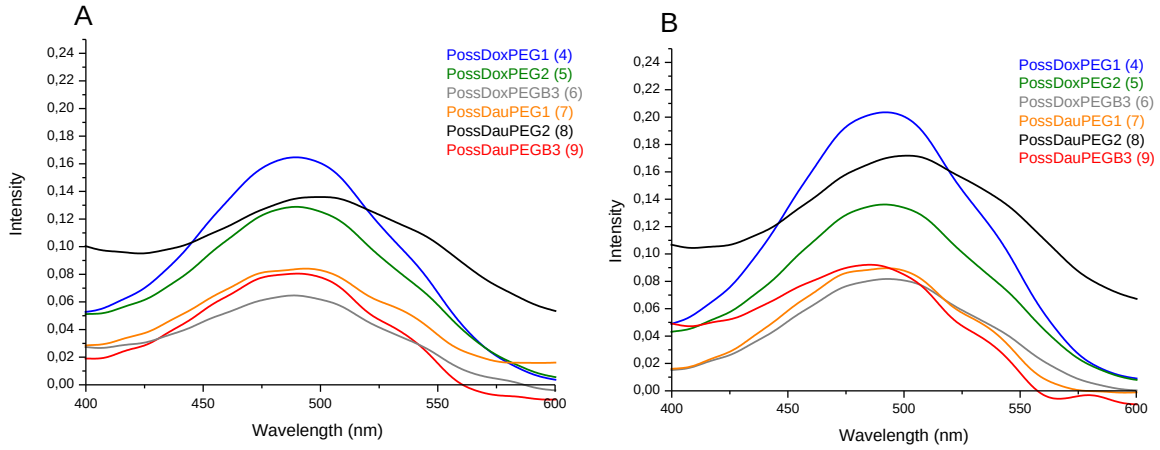

Fig. S6. A Study of DOX/DAU release from nanoconjugates at pH 5.5 at 310 K quantified by UV-Vis method after 21 h (**A**) and after 42 h (**B**).

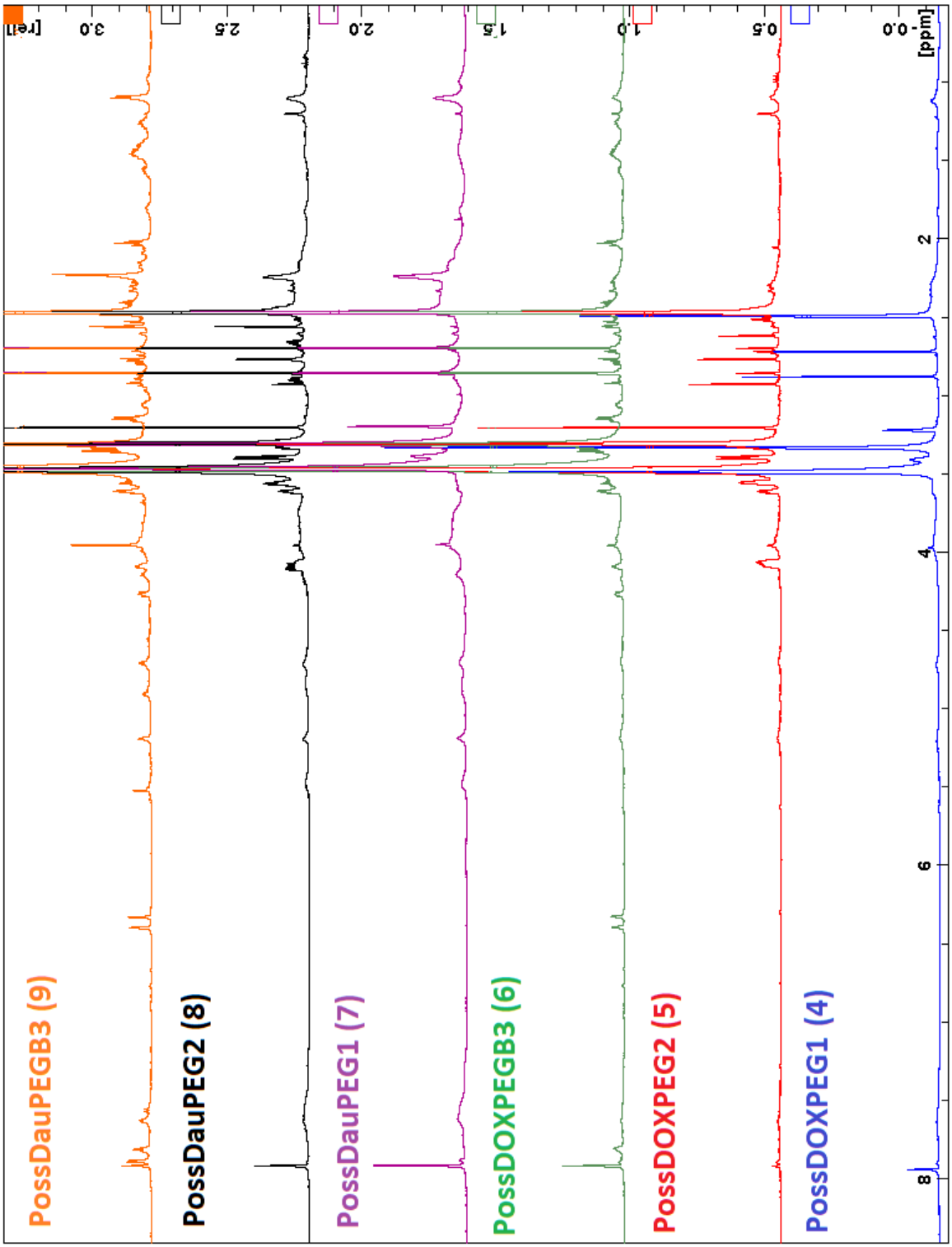

Fig. S7. ^{1}H-NMR spectra of **4–9** (500 MHz, 295 K, DMSO-d6).