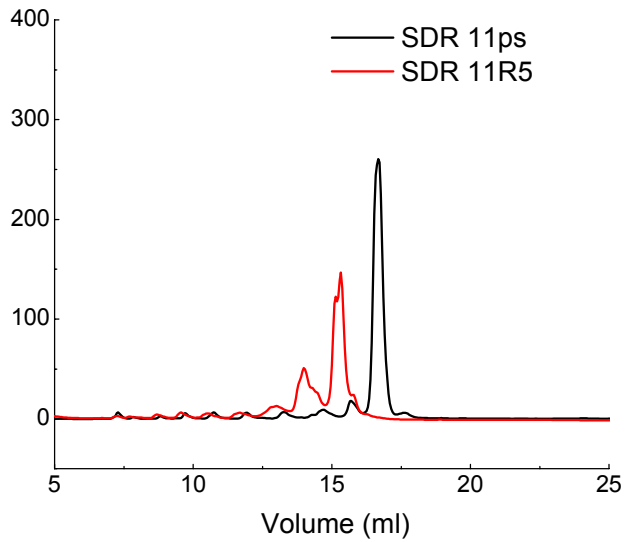


Supplemental Data

Figure S1

(A) Sample HPLC traces



(B) A sample mass spectrometry trace

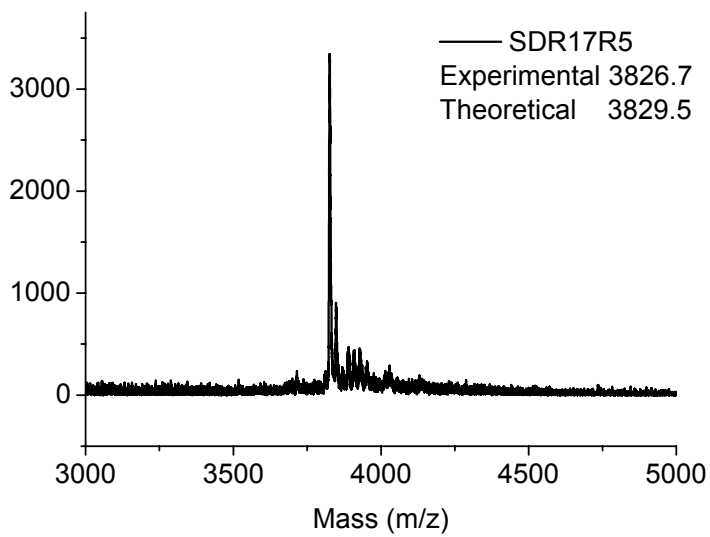


Table S1: Mean distances determined using measured $P(r)$ from 20 – 70 Å.

Nitroxide positions	$\langle r_{\text{DEER}} \rangle$ (Å)	$\langle r_{\text{model}} \rangle$ (Å)
(9;17)	29.3	24.5
(12;19)	29.6	31.1
(9;23)	32.6	34.7
(9;24)	35.3	38.8
(11;23)	38.9	42.4
(12;24)	44.8	46.6
R.M.S.D. (Å)	3.1	
R^2	0.89	

Table S2: Comparison between modeling with and without a fine search.

Nitroxide positions	$\langle r_{\text{DEER}} \rangle$ (Å)	NASNOX; + fine search ^(a)		NASNOX; - fine search ^(a)	
		$\langle r \rangle$ (Å)	Number of output distance	$\langle r \rangle$ (Å)	Number of output distance
(9;17)	25.2	24.5	18,315	25.6	4,702
(12;19)	28.1	31.1	19,879	32.2	5,409
(9;23)	32.7	34.7	19,503	36.3	5,766
(9;24)	37.9	38.8	20,493	40.4	5,026
(11;23)	40.5	42.4	20,607	43.7	5,292
(12;24)	47.2	46.6	21,321	47.6	4,899
R.M.S.D. ^(b)	-----	1.7	-----	2.8	-----

(a) NASNOX modeling was carried using the step sizes described in the text.

(b) Root mean square deviation between measured ($\langle r_{\text{DEER}} \rangle$) and modeled ($\langle r \rangle$) average distances.