

Synthesis and preliminary investigations into Norbornane-based amphiphiles and their self-assembly

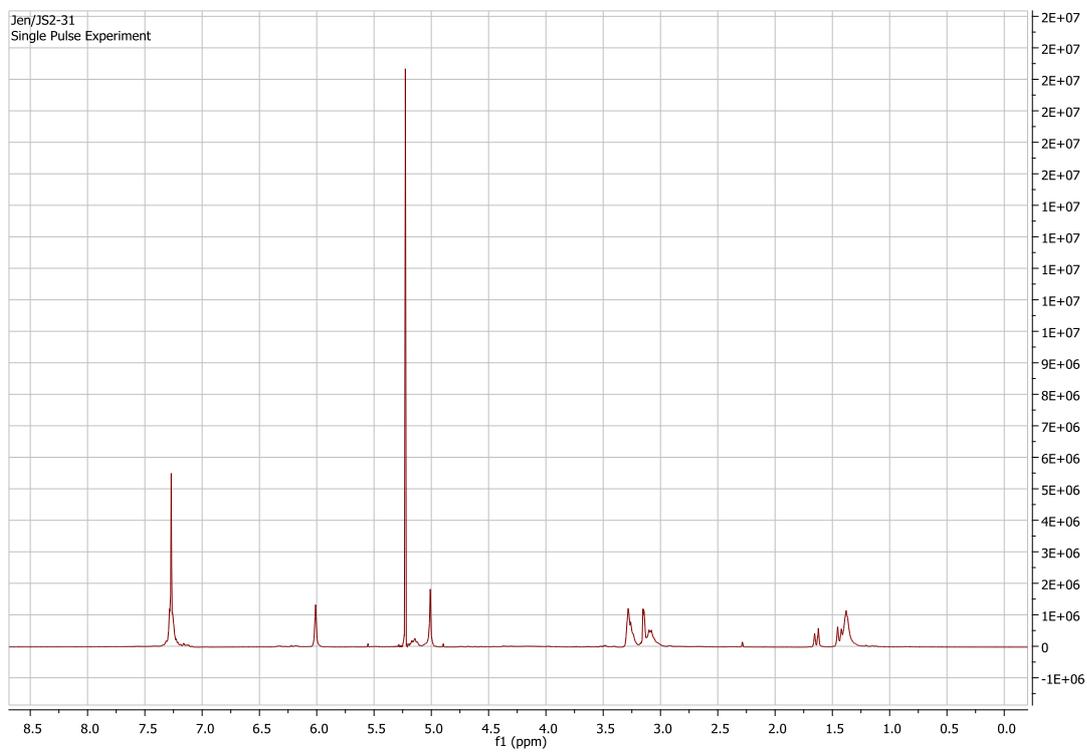
Jennifer S. Squire,^a Alessandra Sutti,^b Xavier A. Conlan,^a Grégory Durand,^{c,d}
and Luke C. Henderson.*^{a,b}

SUPPLEMENTARY INFORMATION

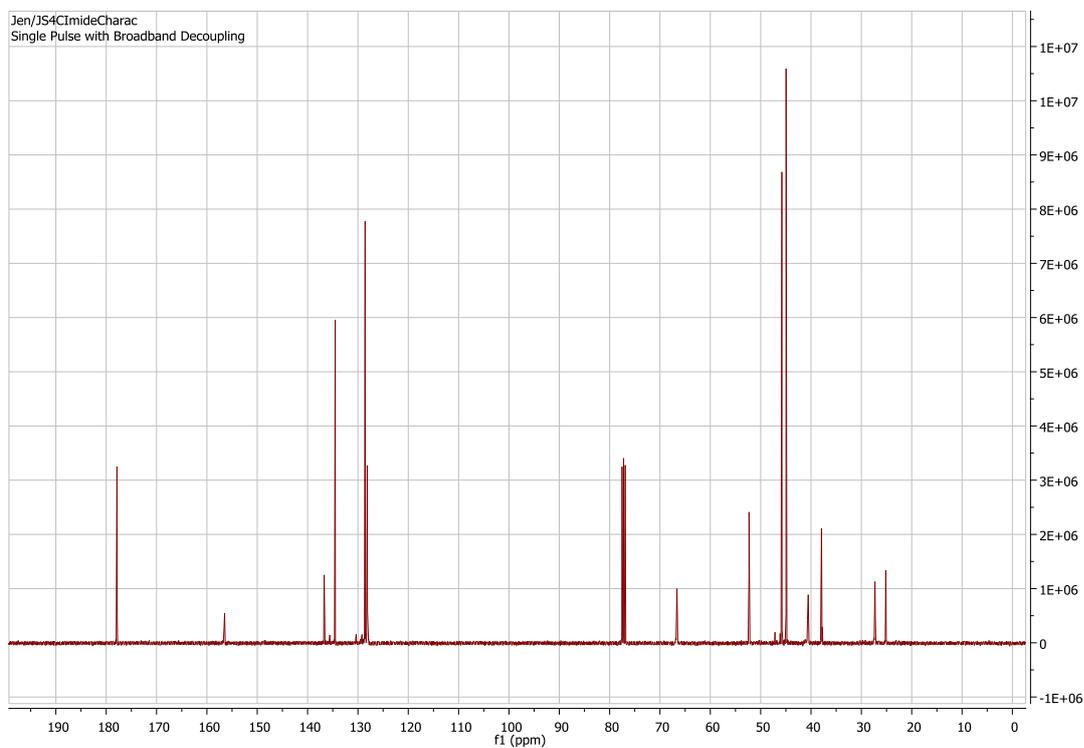
Page S2-17	¹H and ¹³C NMR for all novel compounds
Page S18	Representative Example of CMC calculation
Page S18	Representative DLS Output
Page S19	Optimisation Table for compounds 4 and 6
Page S20	Corralation of methylene units versus $\log P$ and $\log k'_w$

Benzyl (4-((3aR,4S,7R,7aS)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2H-4,7-methanoisindol-2-yl)butyl)carbamate 3

¹H NMR Spectrum:

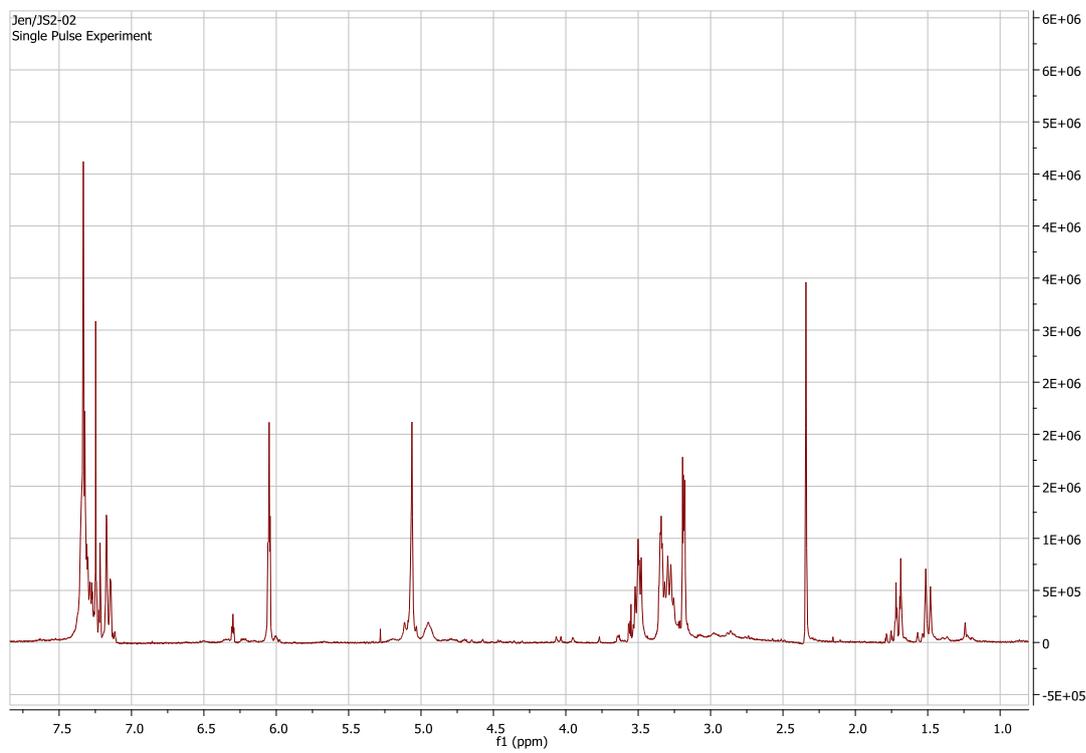


¹³C NMR Spectrum:

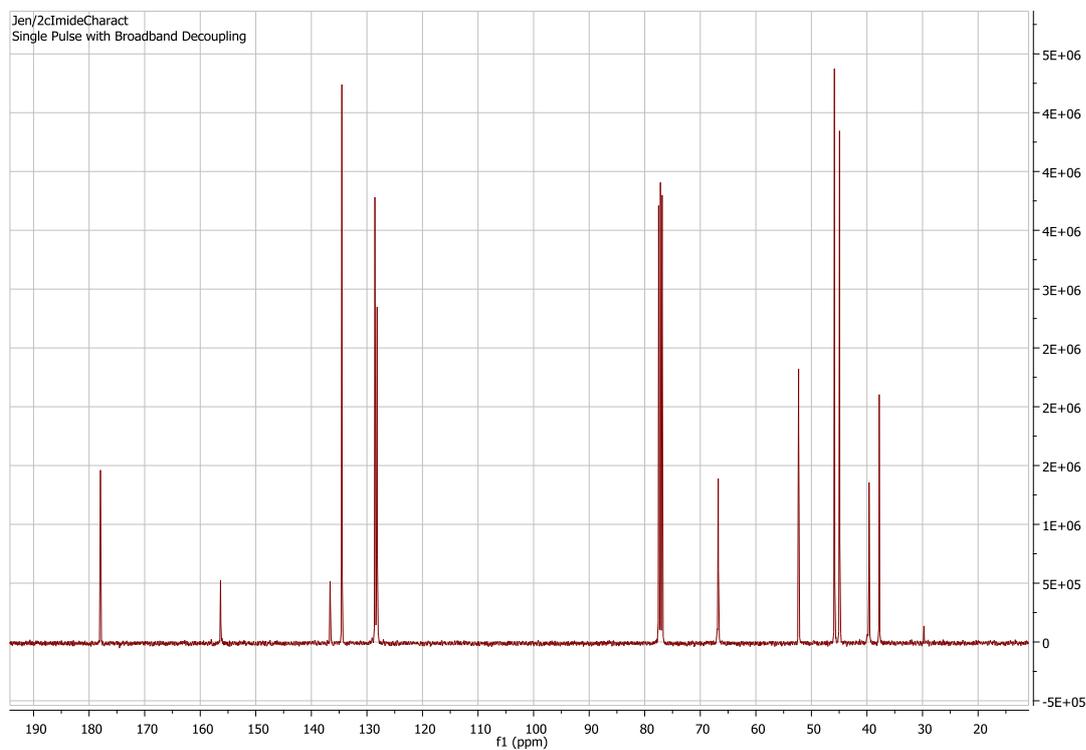


Benzyl (2-((3aR,4S,7R,7aS)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2H-4,7-methanoisindol-2-yl)ethyl)carbamate 2

¹H NMR Spectrum:

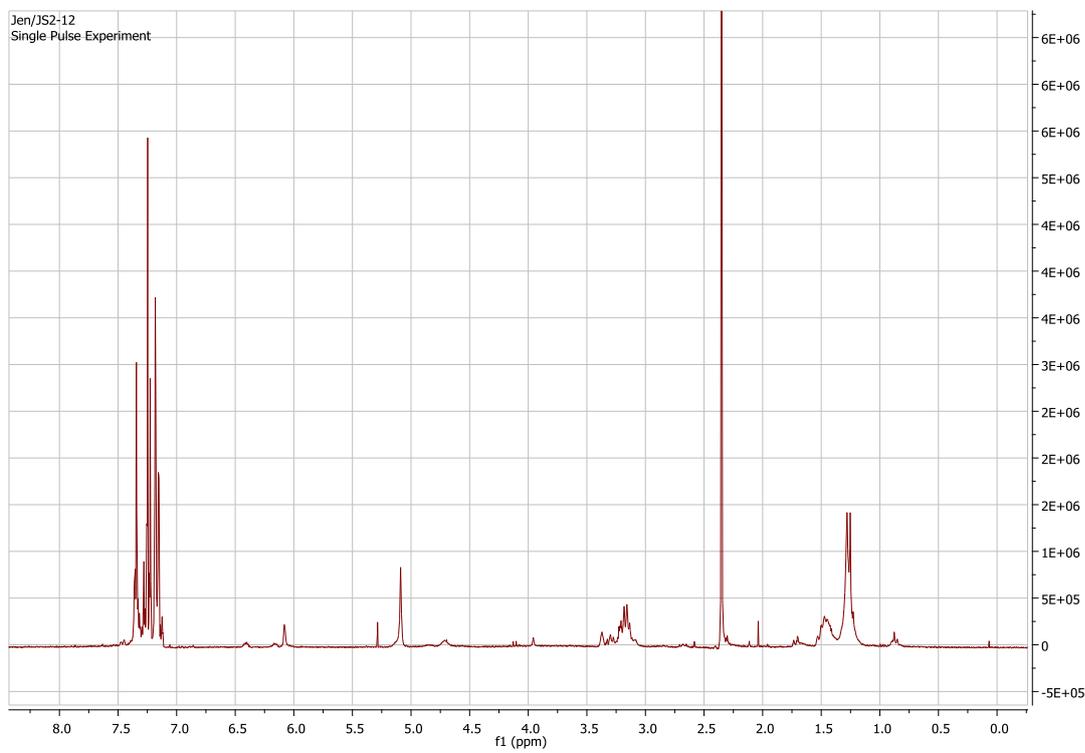


¹³C NMR Spectrum:

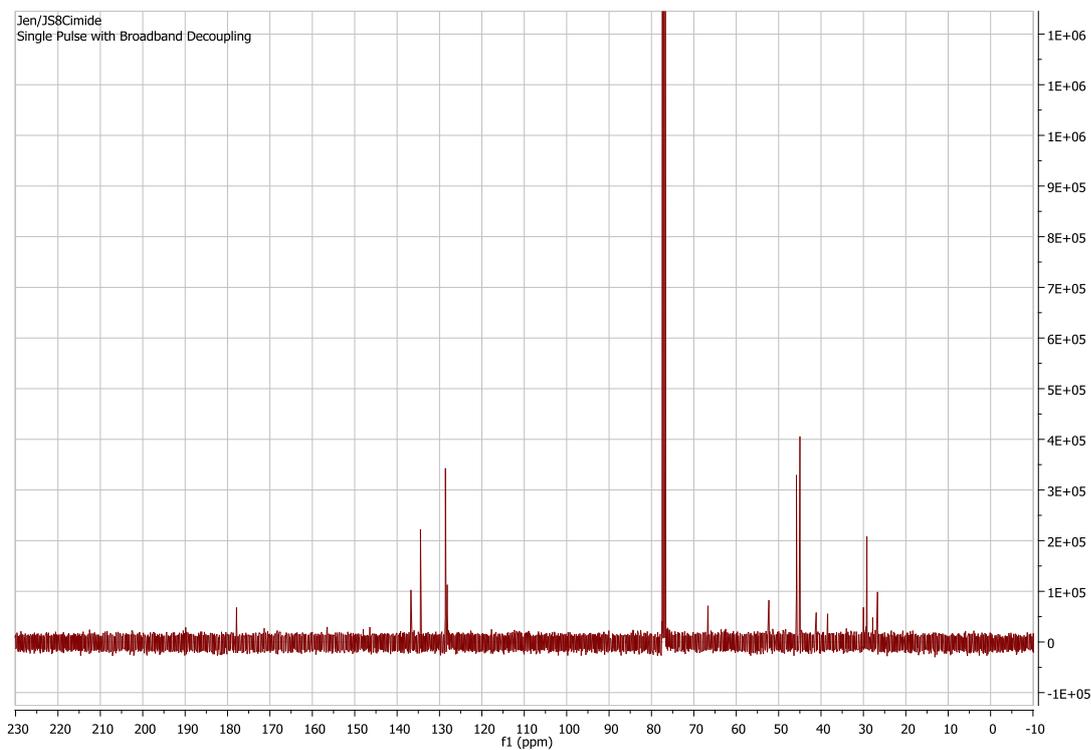


Benzyl (8-((3aR,4S,7R,7aS)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2H-4,7-methanoisoindol-2-yl)octyl)carbamate 4

¹H NMR Spectrum:

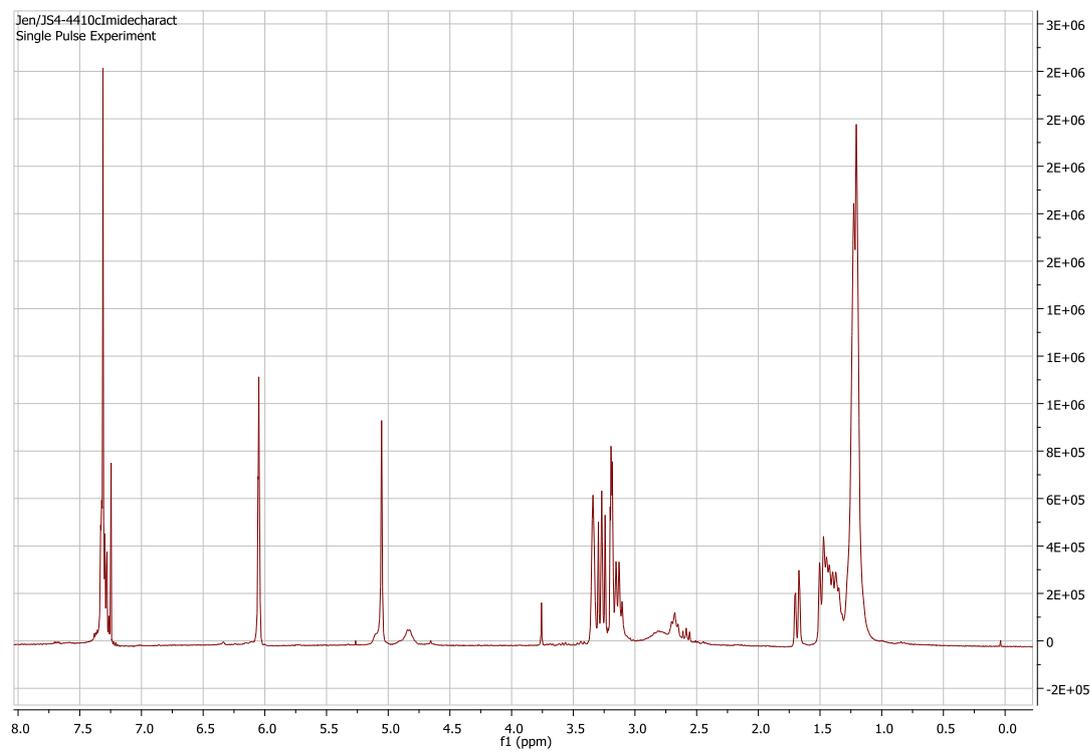


¹³C NMR Spectrum:

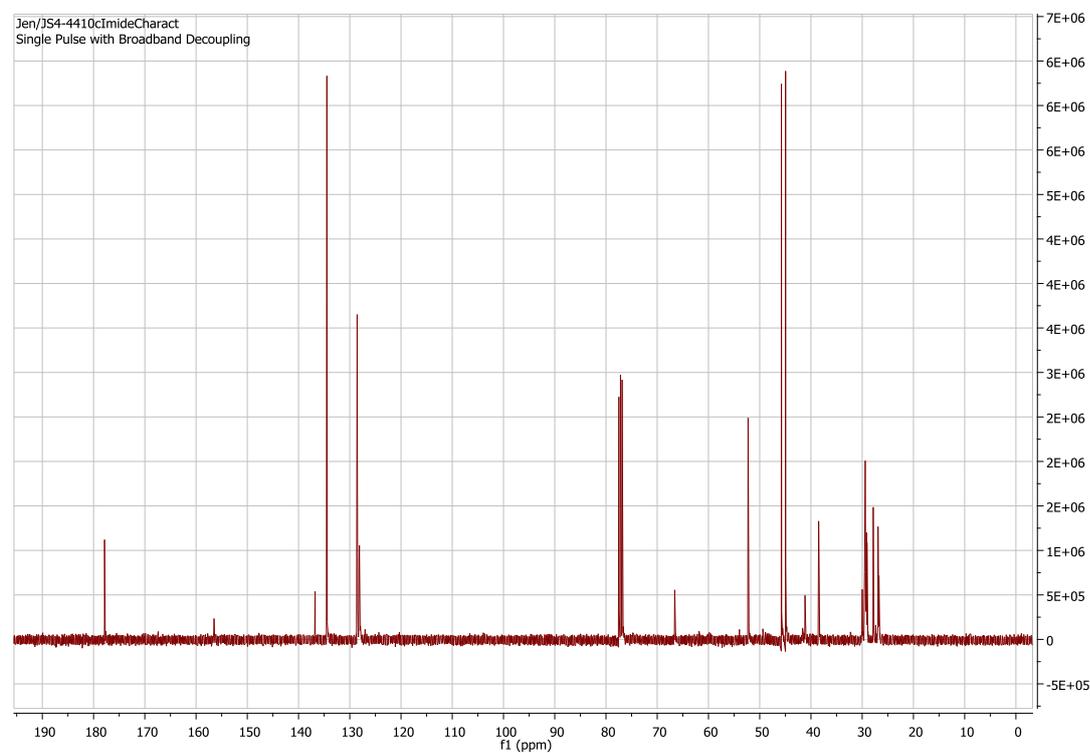


Benzyl (10-((3aR,4S,7R,7aS)-1,3-dioxo-1,3,3a,4,7,7a-hexahydro-2H-4,7-methanoisindol-2-yl)decyl)carbamate 5

^1H NMR Spectrum:

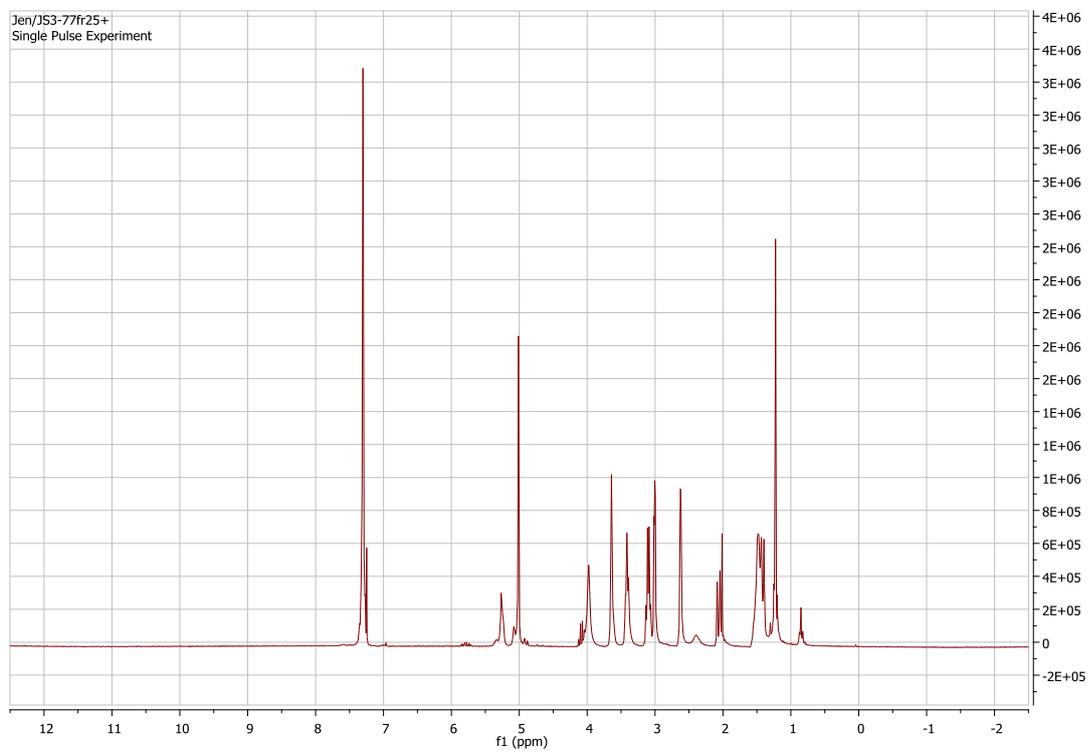


^{13}C NMR Spectrum:

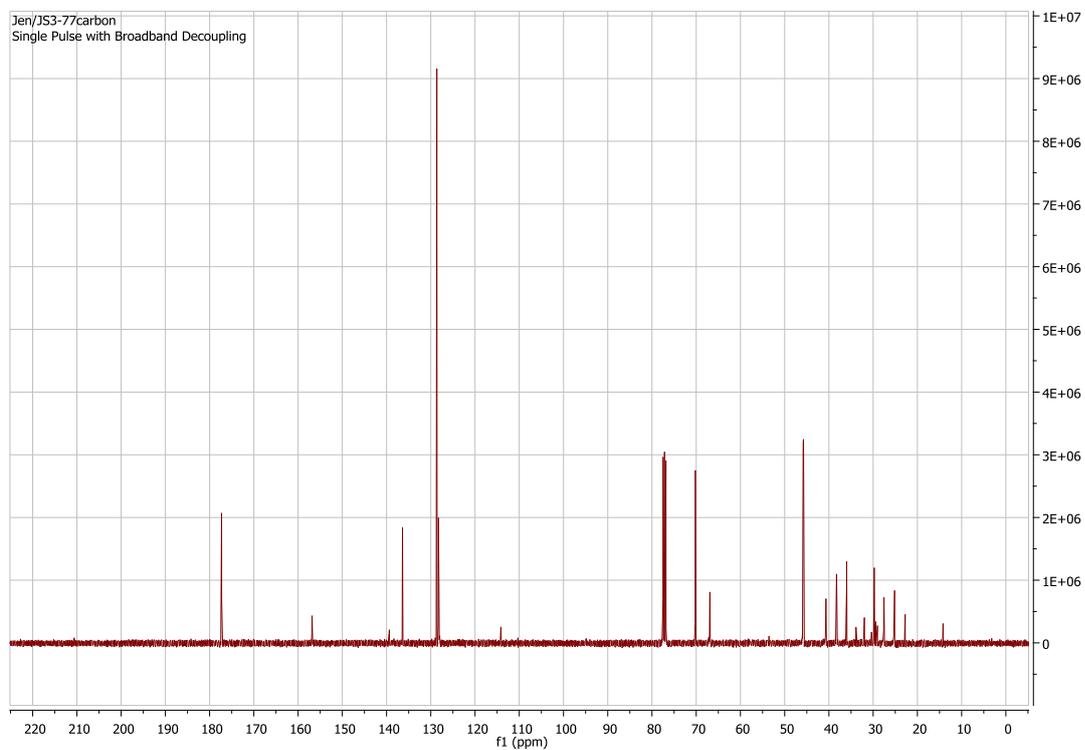


Benzyl (4-((3aR,4R,5R,6S,7S,7aS)-5,6-dihydroxy-1,3-dioxooctahydro-2H-4,7-methanoisindol-2-yl)butyl)carbamate 8

¹H NMR Spectrum:

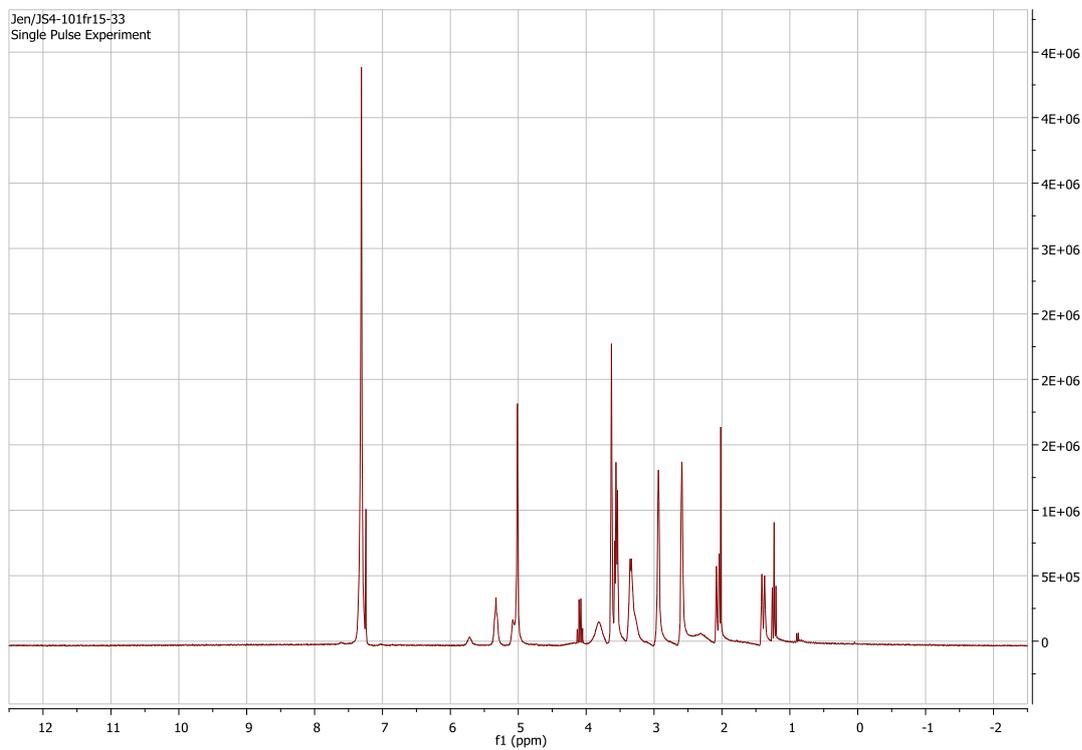


¹³C NMR Spectrum:

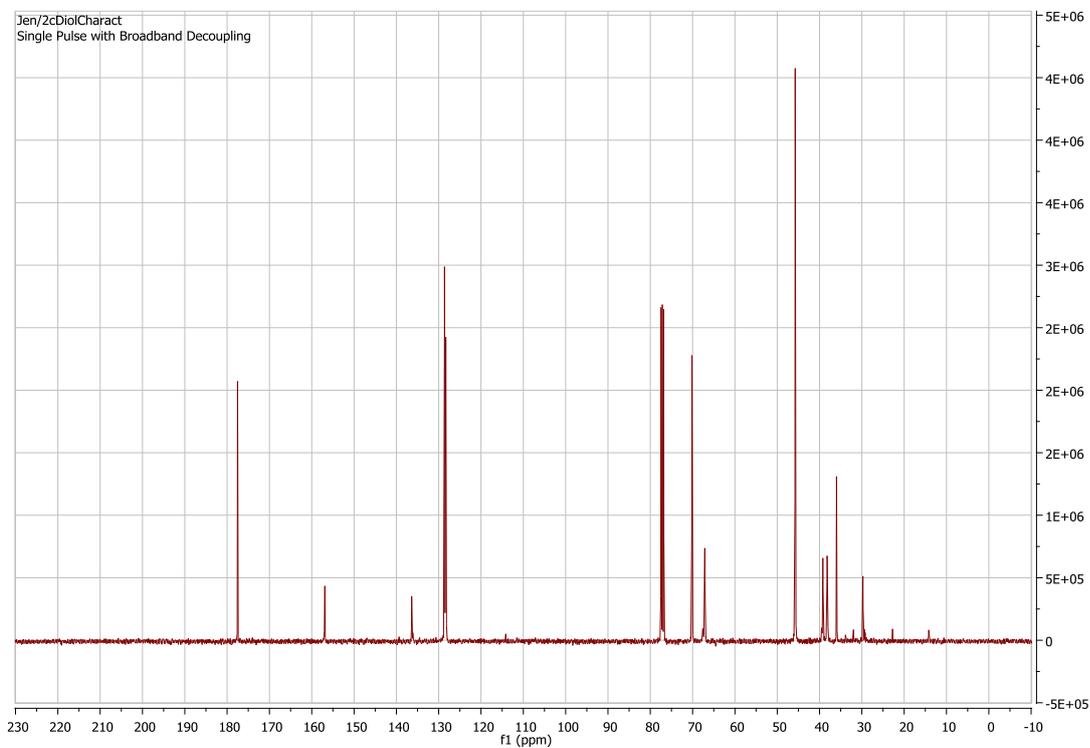


Benzyl [2-(5,6-dihydroxy-1,3-dioxooctahydro-2H-4,7-methanoisindol-2-yl)ethyl]carbamate 7

^1H NMR Spectrum:

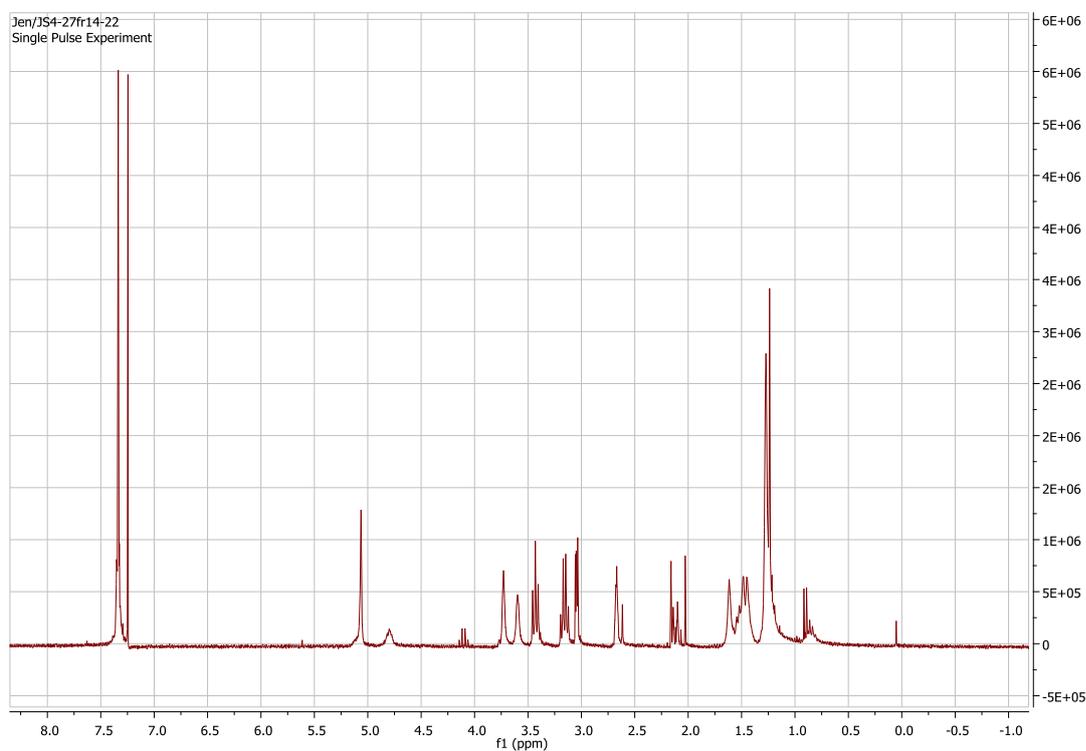


^{13}C NMR Spectrum:

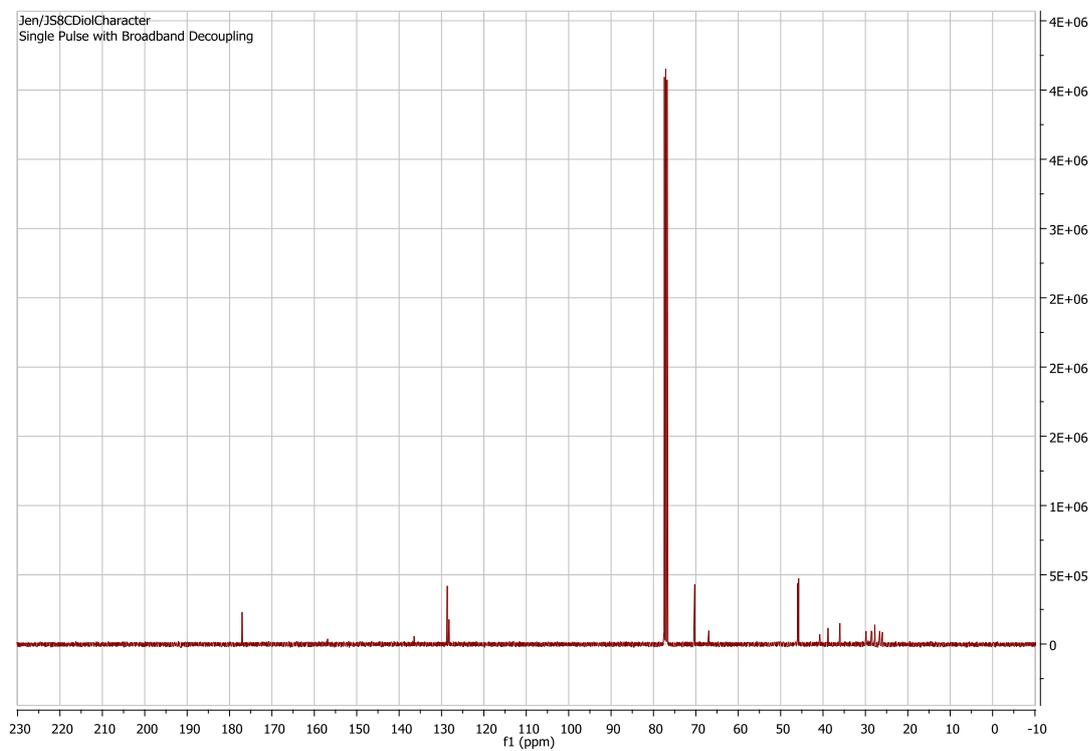


Benzyl [2-(5,6-dihydroxy-1,3-dioxooctahydro-2H-4,7-methanoisindol-2-yl)octyl]carbamate 9

^1H NMR Spectrum:

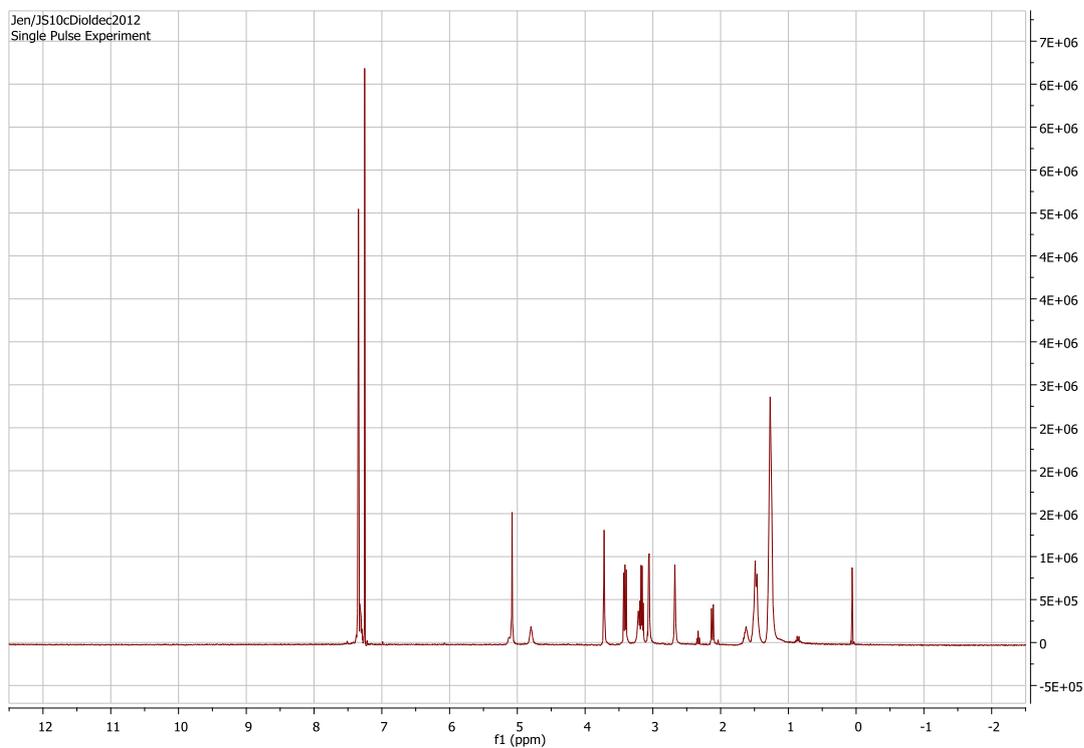


^{13}C NMR Spectrum:

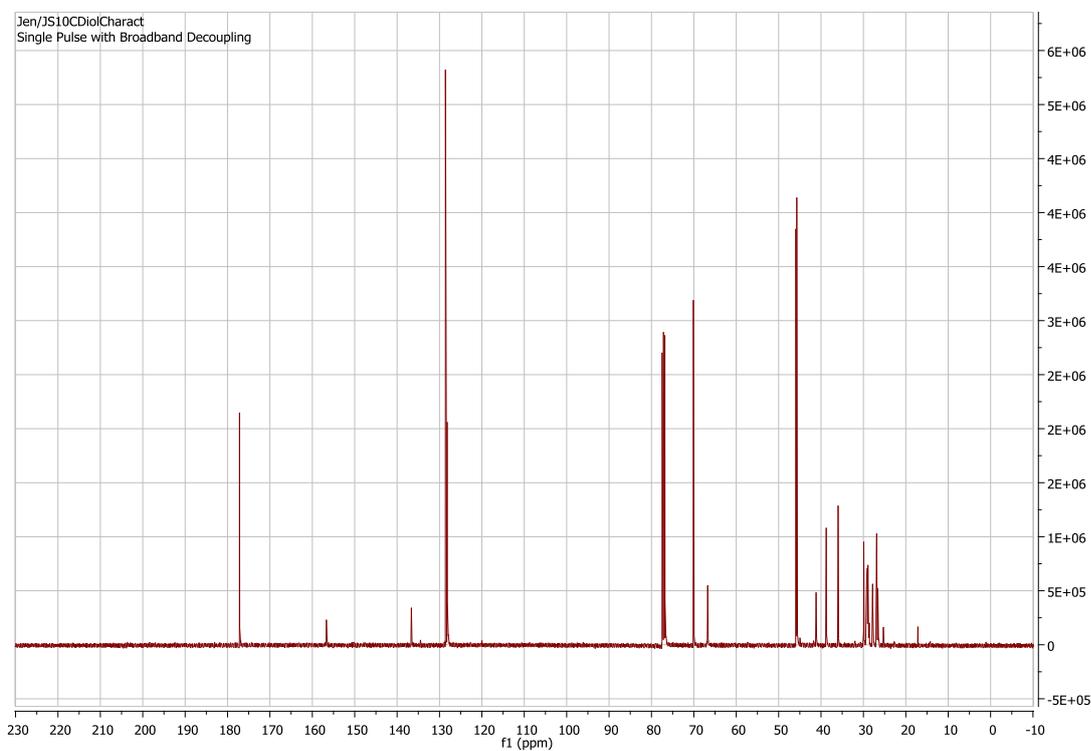


Benzyl [2-(5,6-dihydroxy-1,3-dioxooctahydro-2H-4,7-methanoisindol-2-yl)dodecanyl]carbamate 10

¹H NMR Spectrum:

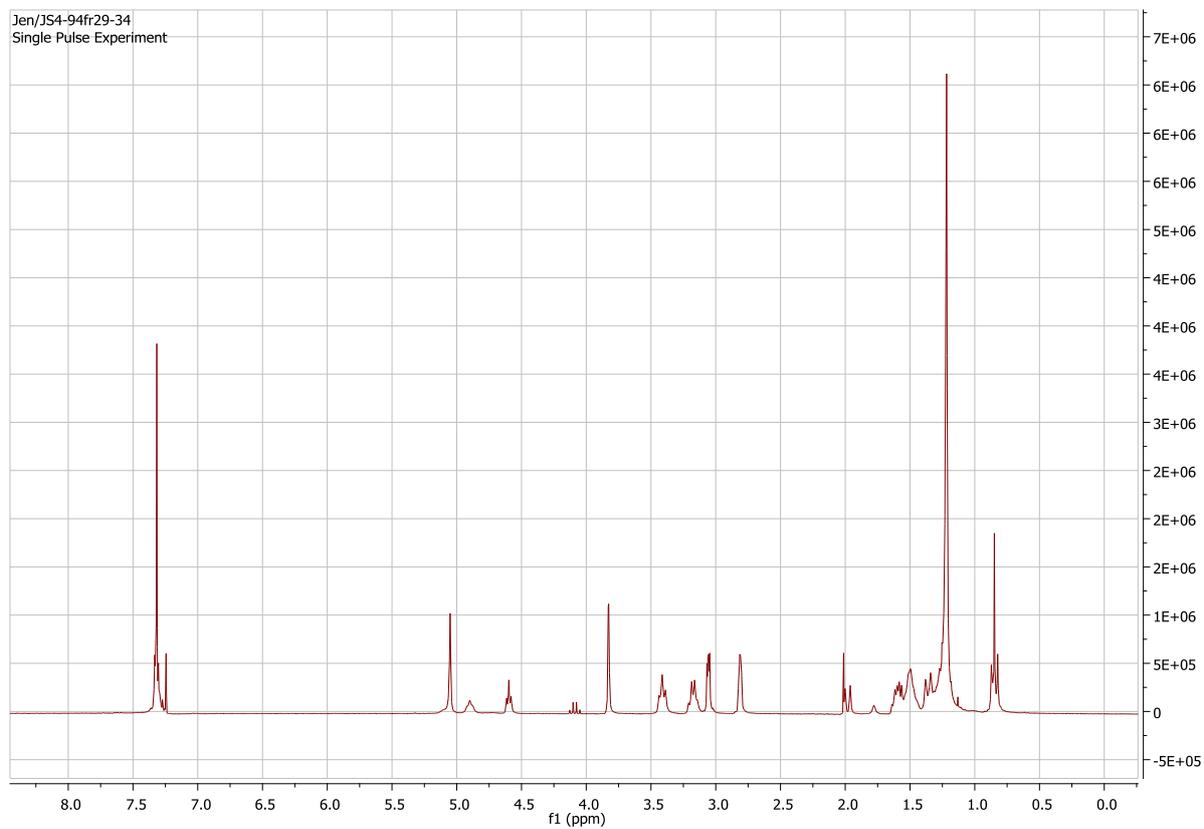


¹³C NMR Spectrum:

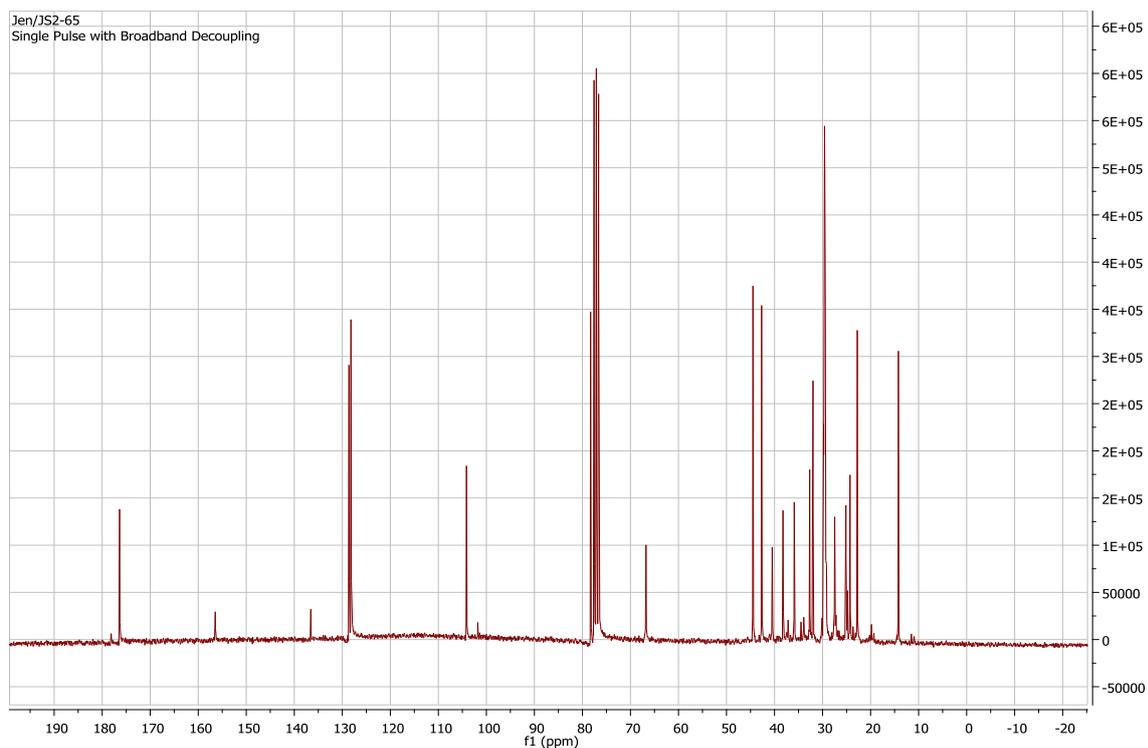


Benzyl [2-(2-dodecyl-5,7-dioxooctahydro-6H-4,8-methano[1,3]dioxolo[4,5-f]isoindol-6-yl)butyl]carbamate

^1H NMR Spectrum:

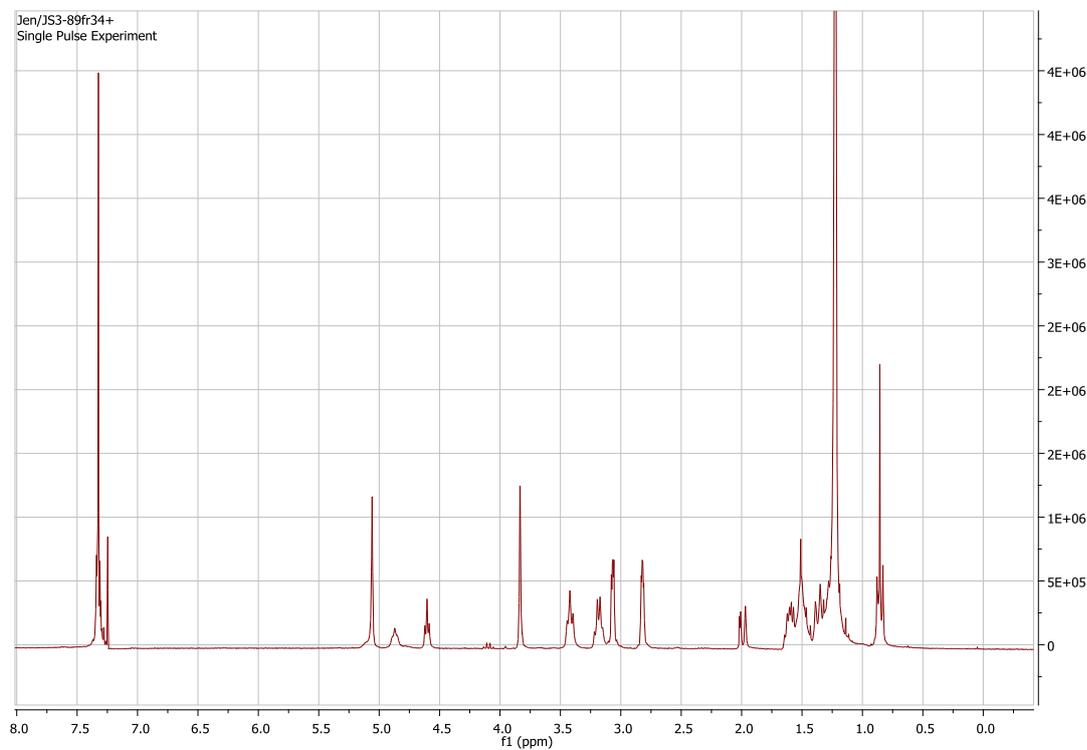


^{13}C NMR Spectrum:

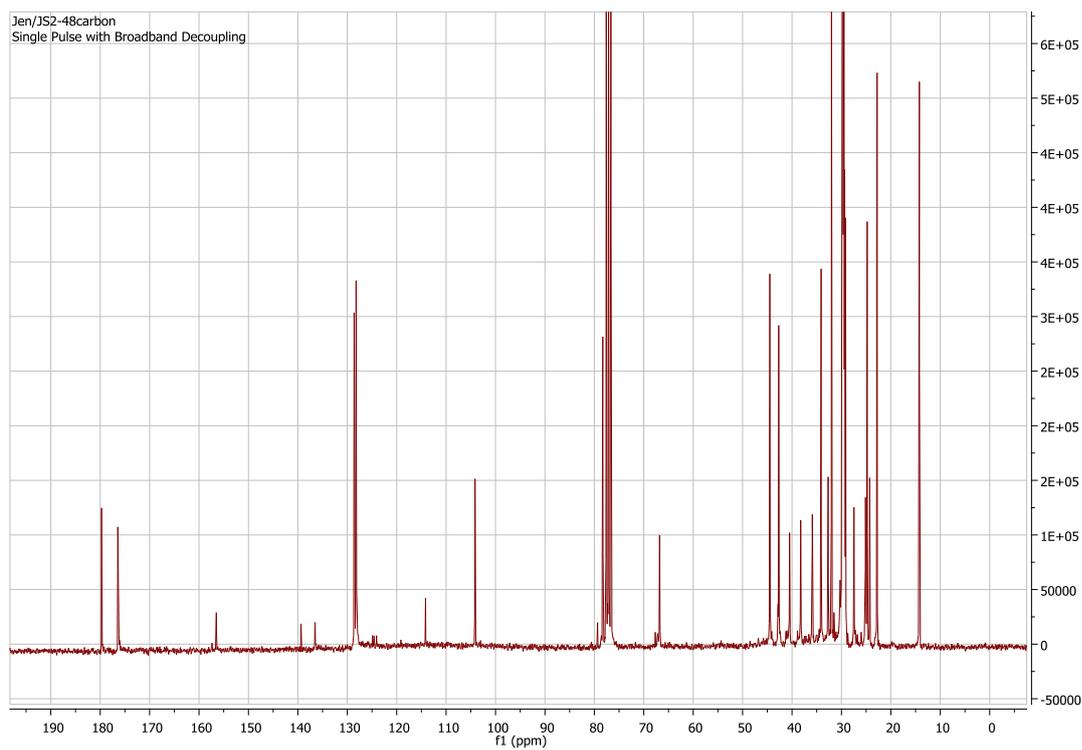


benzyl [2-(2hexaodecyl-5,7-dioxooctahydro-6H-4,8-methano[1,3]dioxolo[4,5-f]isoindol-6-yl)butyl]carbamate

¹H NMR Spectrum:

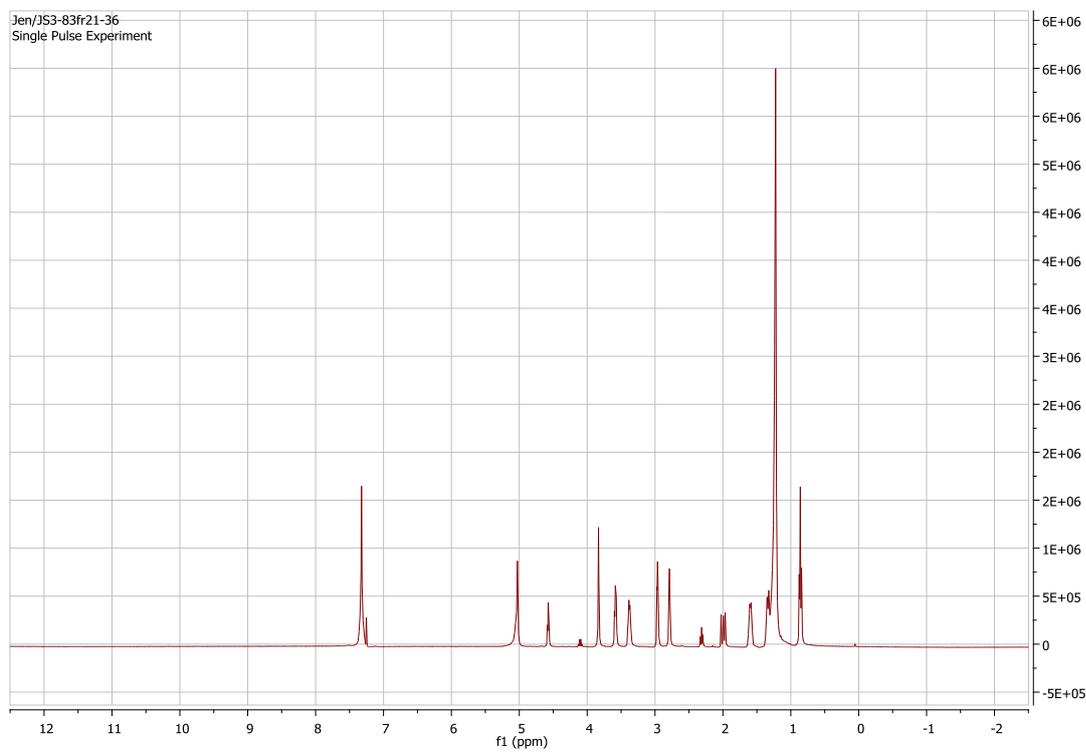


¹³C NMR Spectrum:

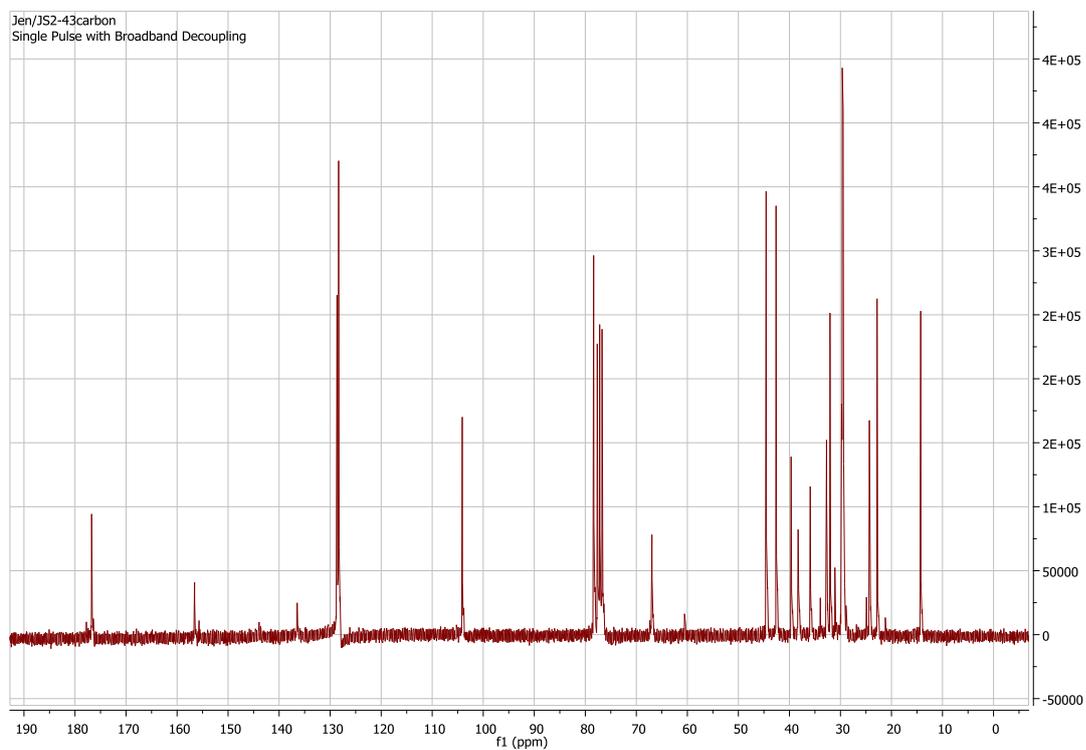


benzyl [2-(2-dodecyl-5,7-dioxooctahydro-6H-4,8-methano[1,3]dioxolo[4,5-f]isoindol-6-yl)ethyl]carbamate

¹H NMR Spectrum:

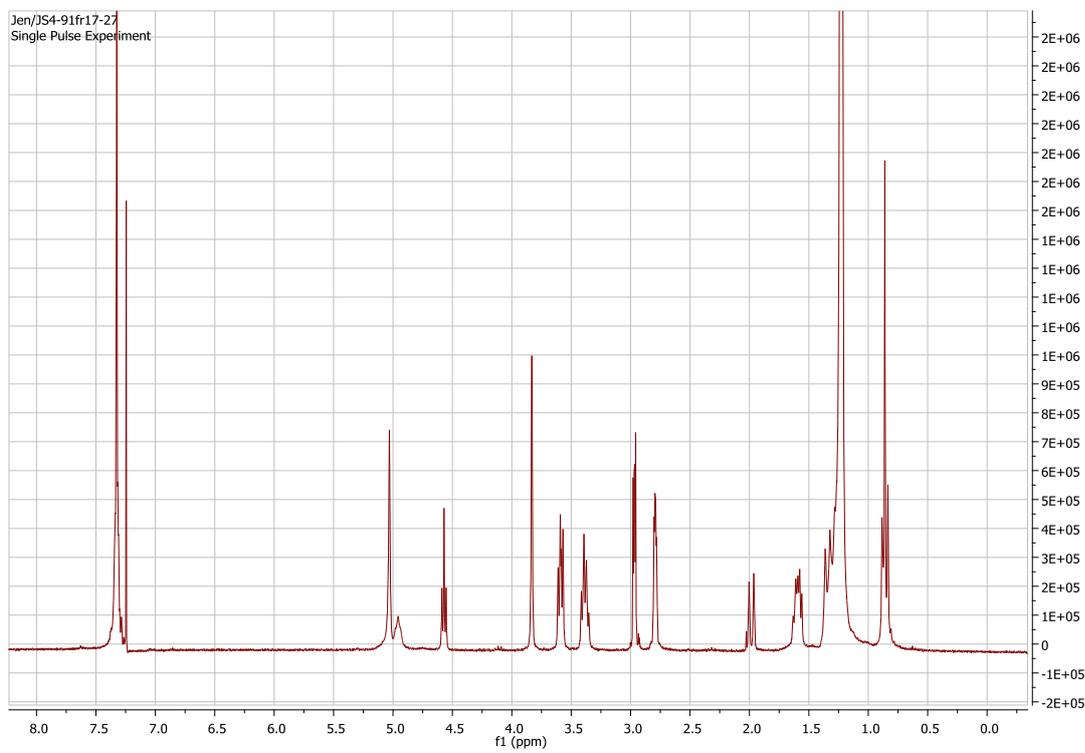


¹³C NMR Spectrum:

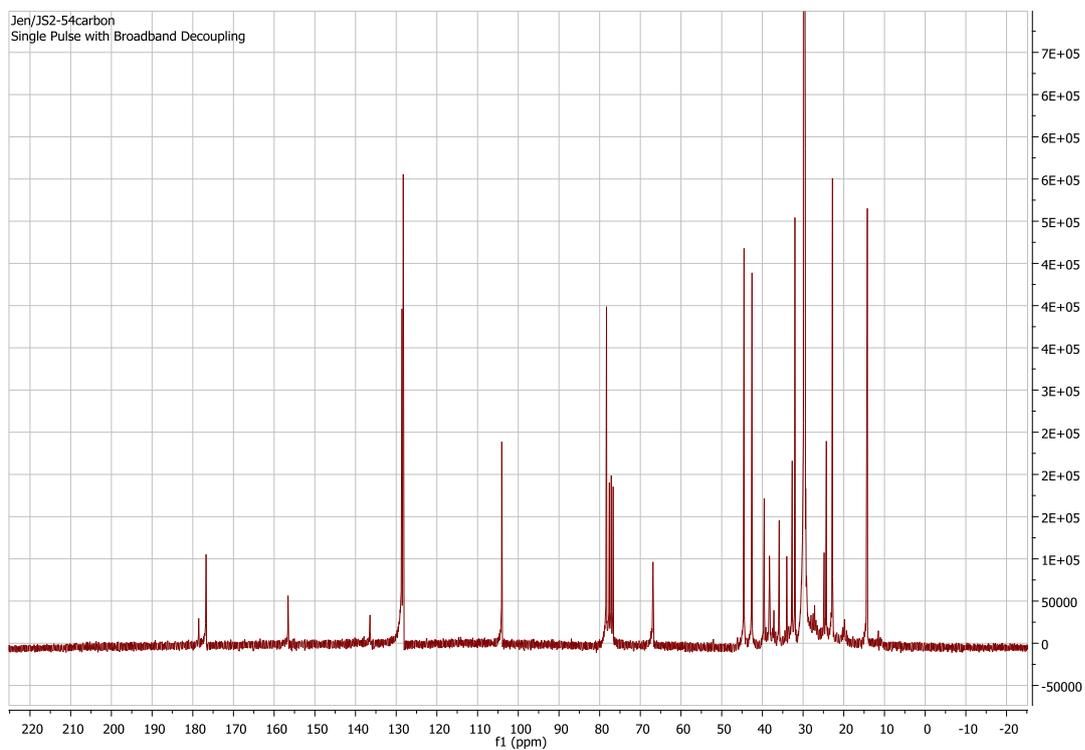


benzyl [2-(2-hexadecyl-5,7-dioxooctahydro-6*H*-4,8-methano[1,3]dioxolo[4,5-*f*]isoindol-6-yl)butyl]carbamate

¹H NMR Spectrum:

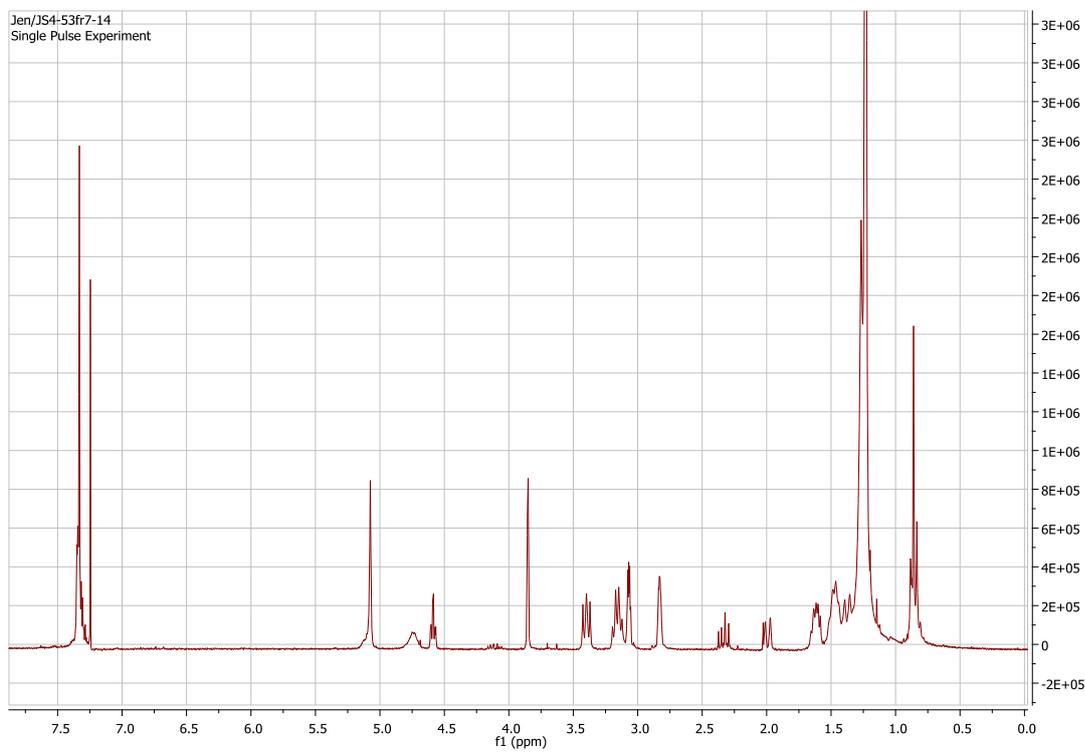


¹³C NMR Spectrum:

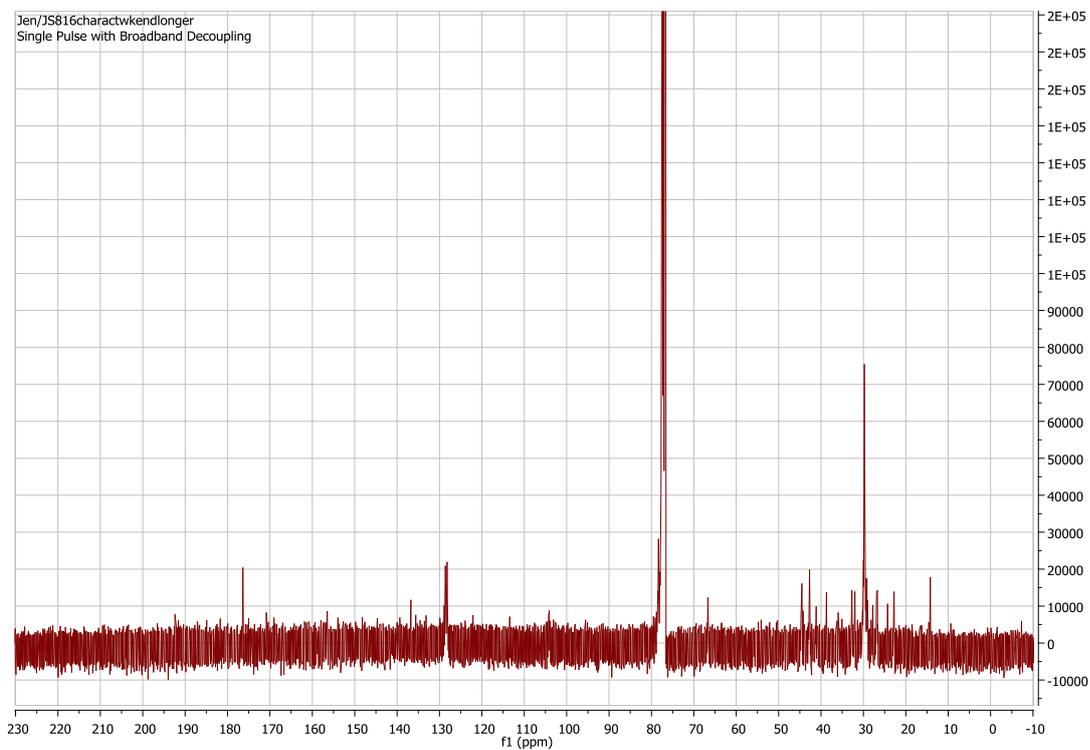


benzyl [2-(2hexadecyl-5,7-dioxooctahydro-6H-4,8-methano[1,3]dioxolo[4,5-f]isoindol-6-yl)octyl]carbamate

¹H NMR Spectrum:

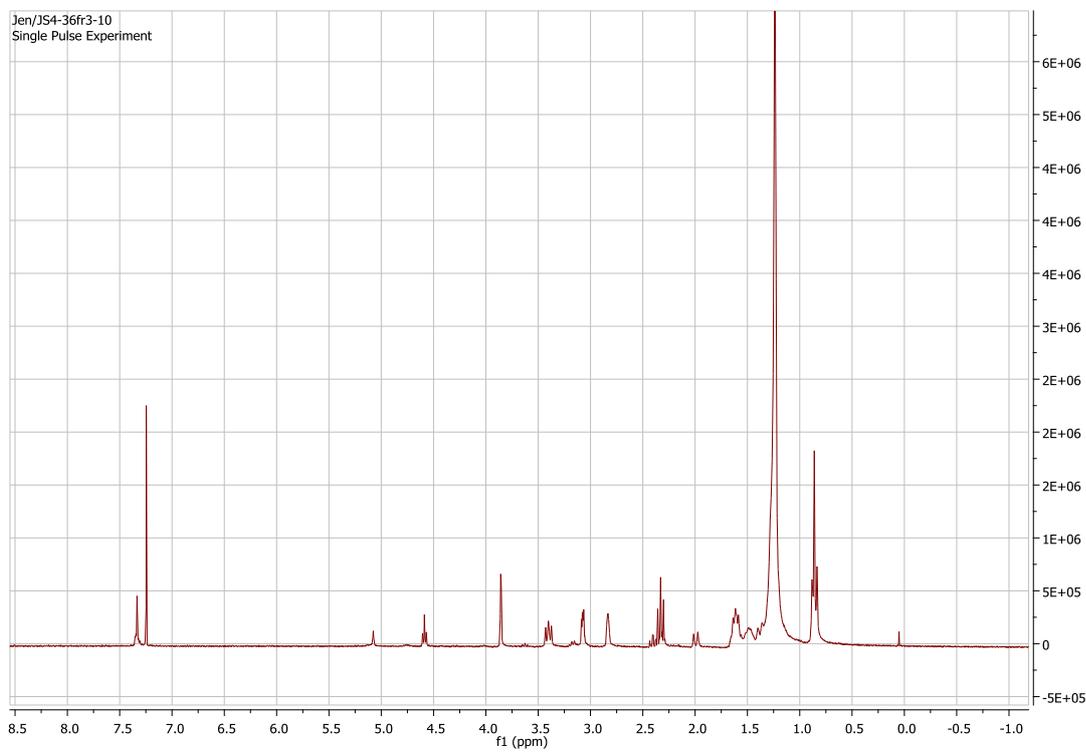


¹³C NMR Spectrum:

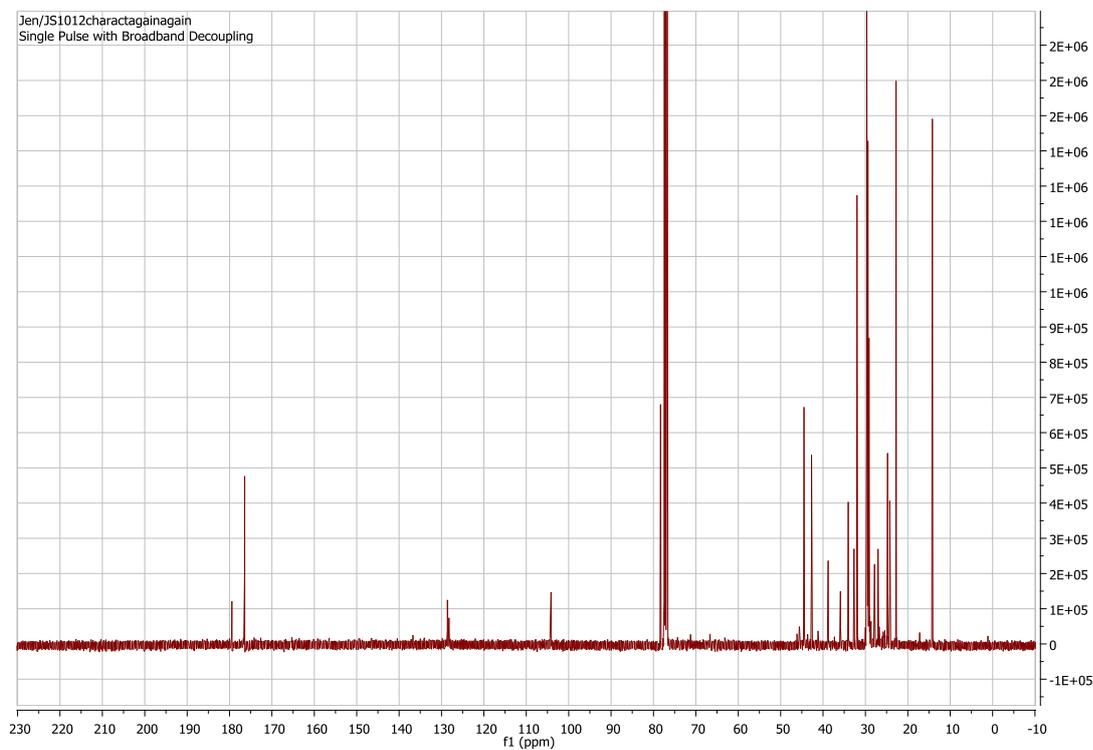


benzyl [2-(2-dodecyl-5,7-dioxooctahydro-6H-4,8-methano[1,3]dioxolo[4,5-f]isoindol-6-yl)decyl]carbamate

¹H NMR Spectrum:

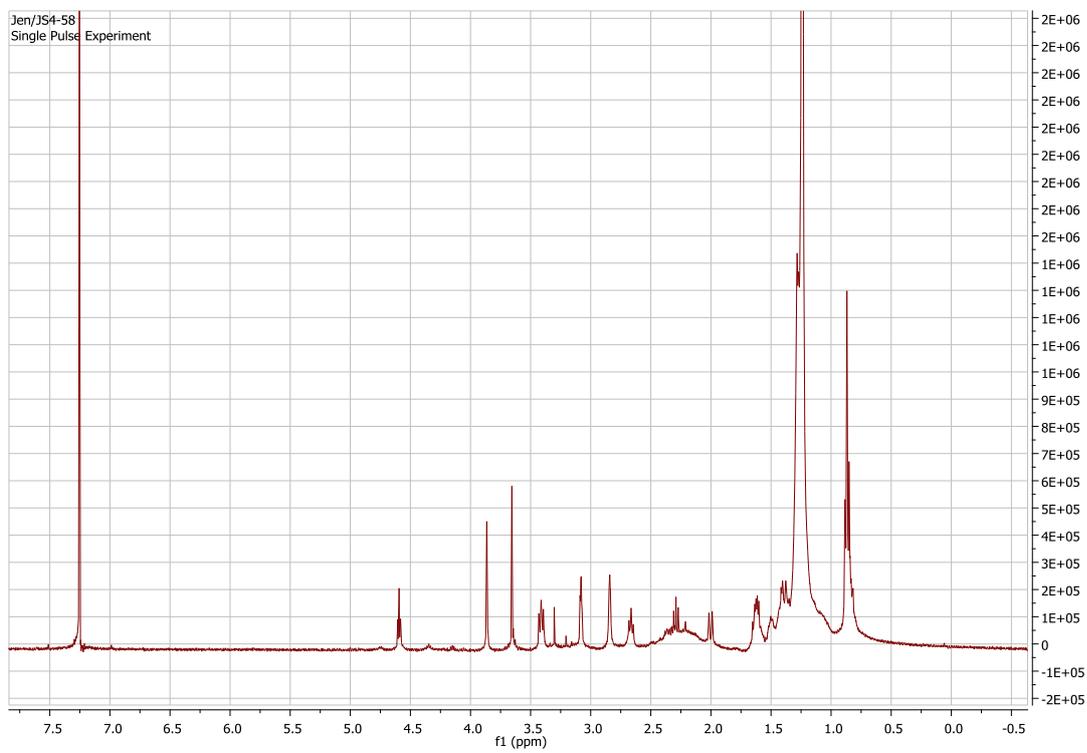


¹³C NMR Spectrum:

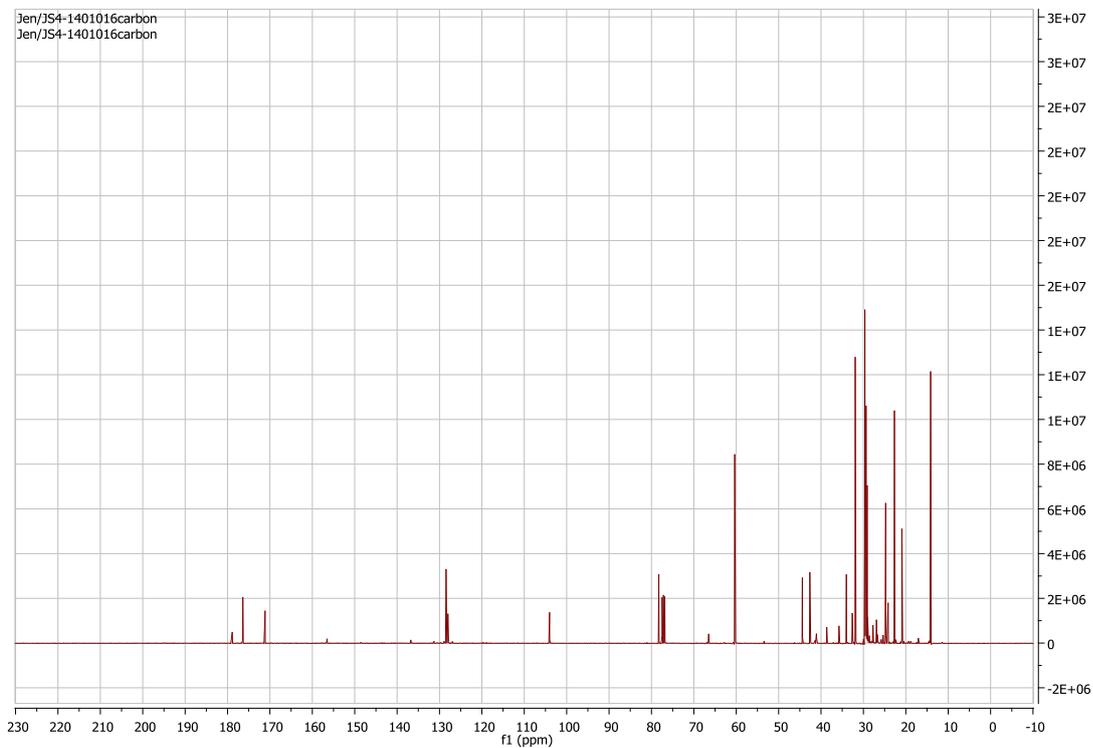


benzyl [2-(2-hexaacyl-5,7-dioxooctahydro-6*H*-4,8-methano[1,3]dioxolo[4,5-*f*]isoindol-6-yl)decyl]carbamate

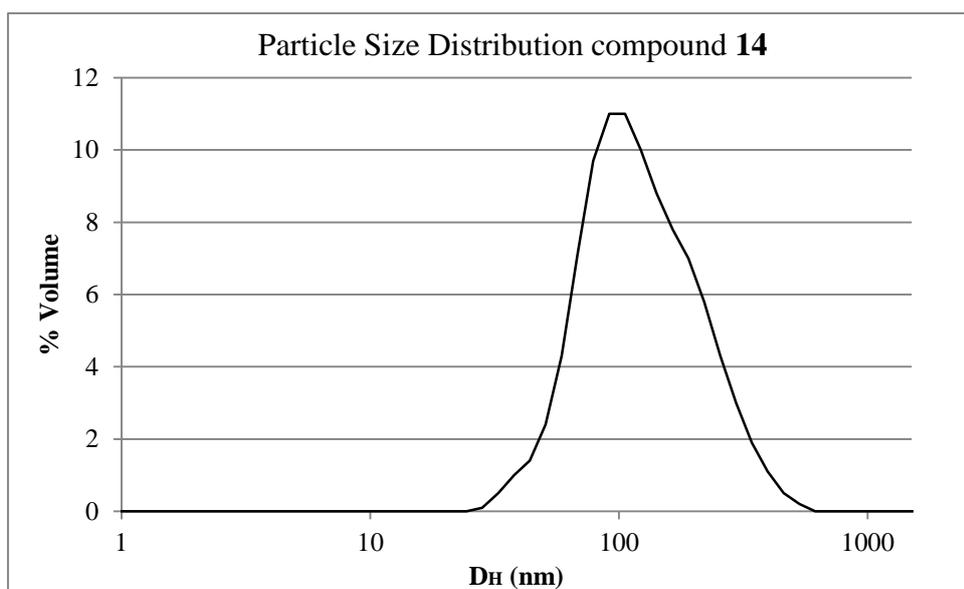
¹H NMR Spectrum:



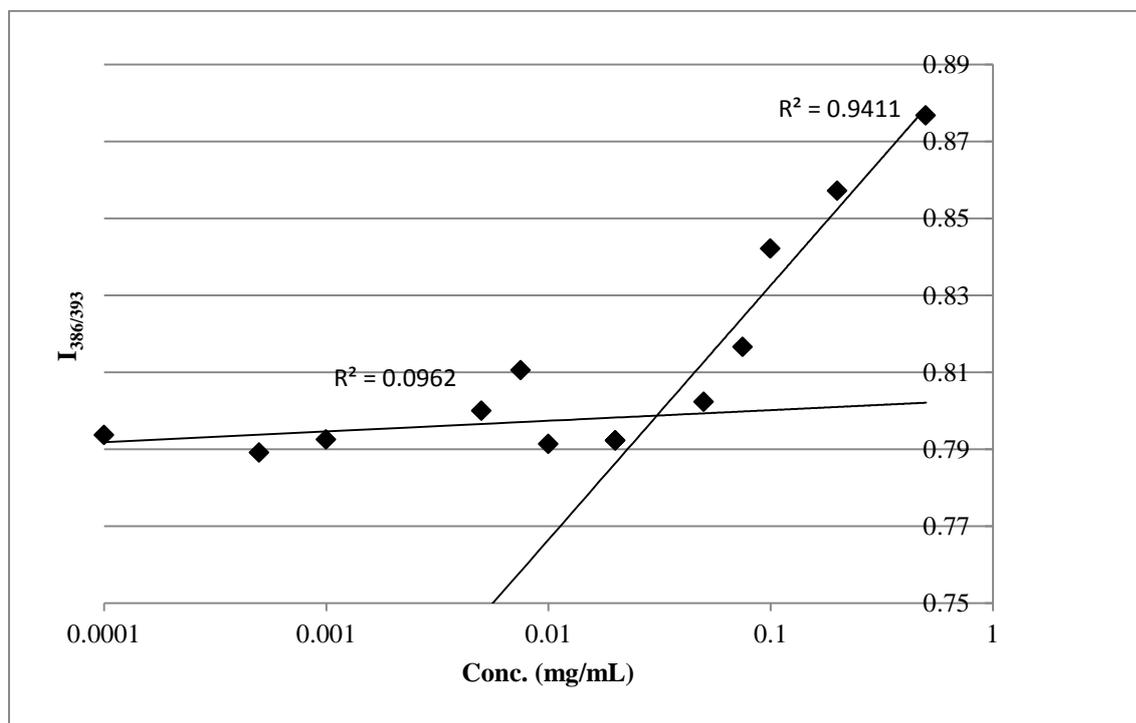
¹³C NMR Spectrum:



Representative DLS output



Representative procedure for determining CAC values (pyrene)



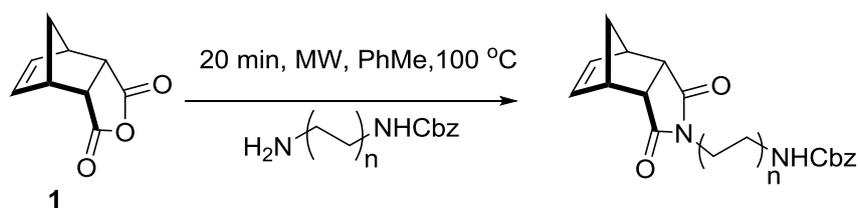


Table 1. Imide optimisation studies for compounds **4** and **6**^a

Entry	Product	Time (min)	Temp (°C)	Equiv.	Yield (%)
1	4	30	120	1.5	16
2	4	30	140	1.5	14
3	4	40	140	2	31
4	4	45	120	2	30
5	4	45	140	2	40
6	4	55	120	2	64
7	6	20	100	1.5	15
8	6	40	140	2	26
9	6	40	120	2	35
10	6	55	120	2	52

^a Reaction conditions: Anhydride **1**, PhMe, MW.

Correlation of methylene units versus $\log P$ and $\log k'_w$

