Highly Efficient Multigram Synthesis of Dibenzoazacyclooctyne (DBCO) Without Chromatography

Stuart A. McNelles, Julia L. Pantaleo, Alex Adronov

Department of Chemistry & Chemical Biology, McMaster University, 1280 Main Street West, Hamilton, Ontario, Canada, L8S 4M1

Supporting Information

¹H NMR spectra and HPLC traces for the products synthesized.

¹H NMR Spectra

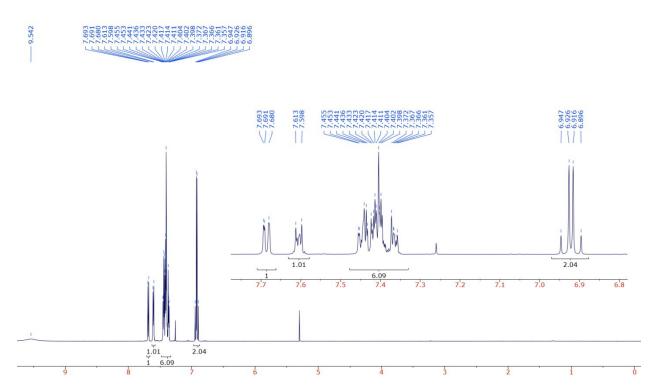


Figure S1. ¹H NMR spectrum of Compound 2 in CDCl₃



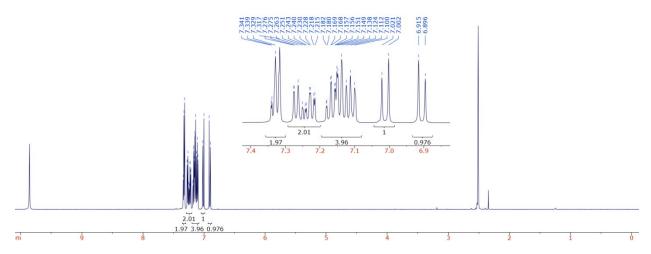


Figure S2. ¹H NMR spectrum of Compound 3 in CDCl₃

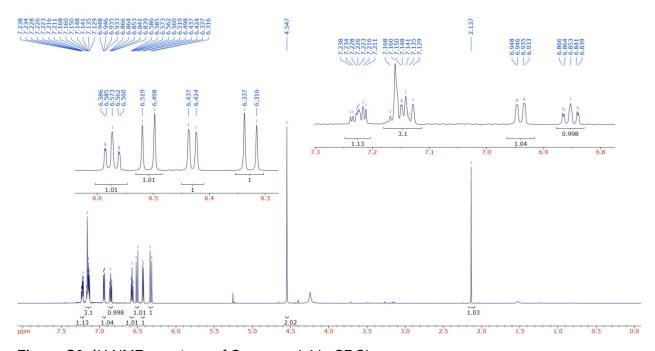


Figure S3. ¹H NMR spectrum of Compound 4 in CDCl₃

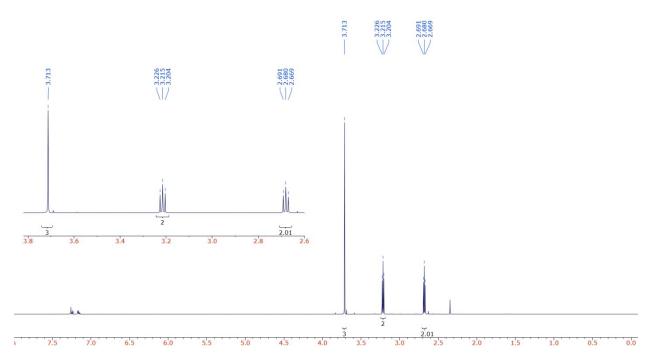


Figure S4. ¹H NMR spectrum of Compound 5 in CDCl₃

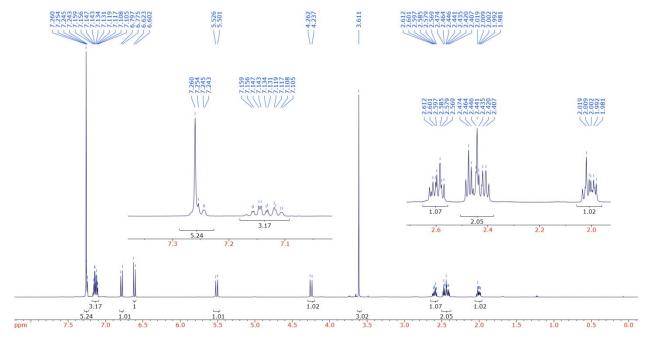


Figure S5. ¹H NMR spectrum of Compound 6 in CDCl₃

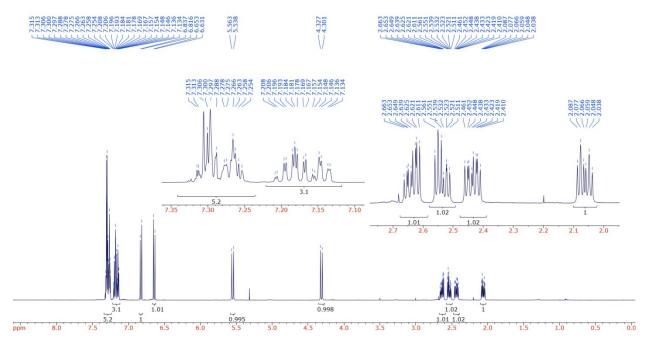


Figure S6. ¹H NMR spectrum of Compound 7 in CDCl₃

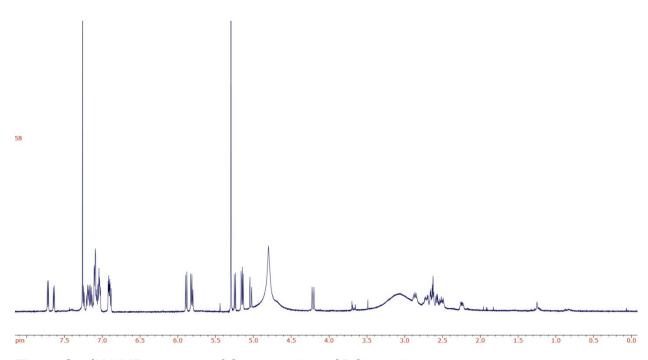


Figure S7. ^{1}H NMR spectrum of Compound 8 in CDCl $_{3}$ (crude)

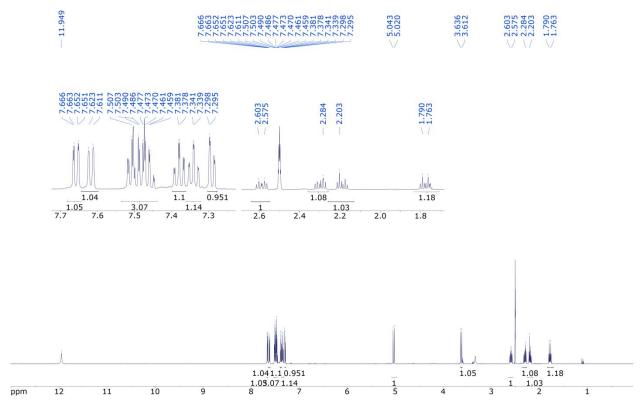


Figure S8. ¹H NMR spectrum of Compound 9 in DMSO-d₆

HPLC Traces

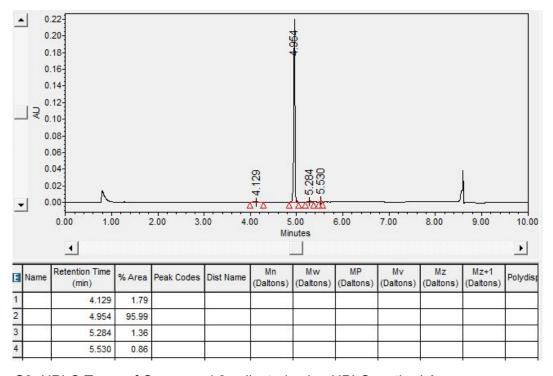


Figure S9. HPLC Trace of Compound 2 collected using HPLC method 1

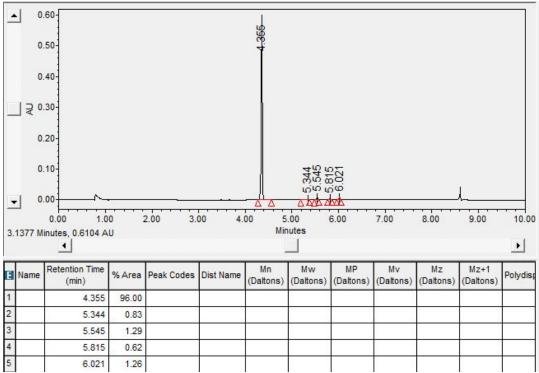


Figure S10. HPLC Trace of Compound 3 collected using HPLC method 1

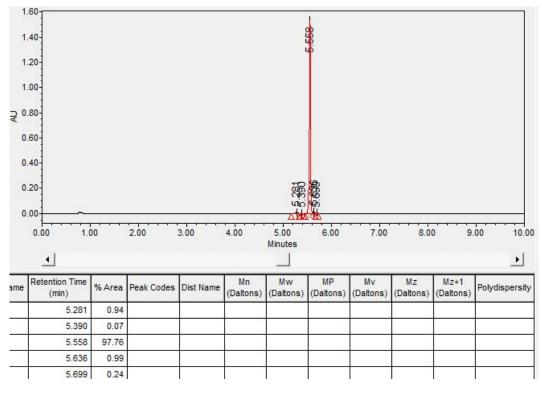


Figure S11. HPLC Trace of Compound 4 collected using HPLC method 1

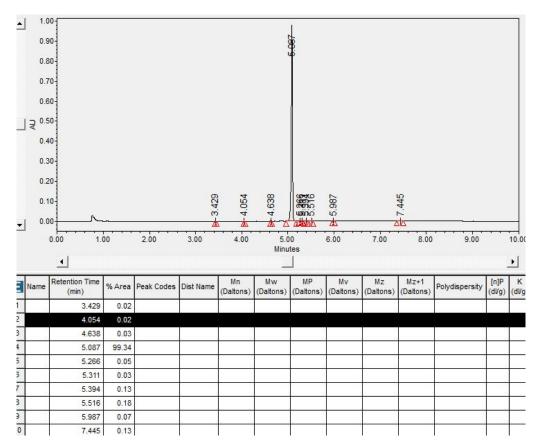


Figure S12. HPLC Trace of Compound 6 collected using HPLC method 1

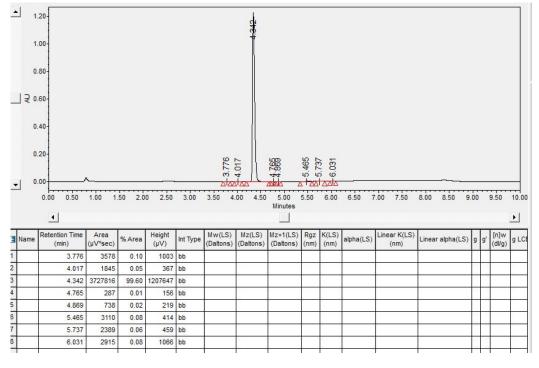


Figure S13. HPLC Trace of Compound 7 collected using HPLC method 1

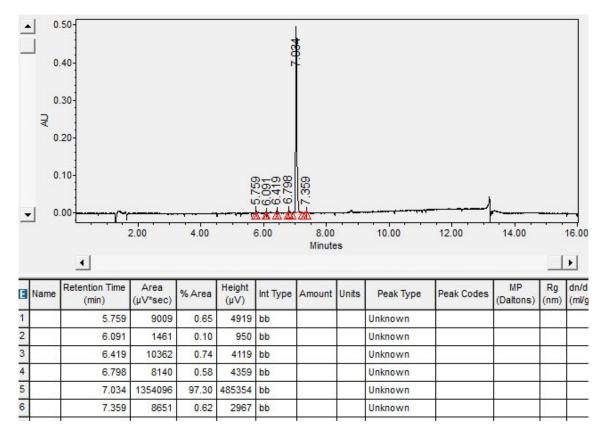


Figure S14. HPLC Trace of Compound 9 collected using HPLC method 2