

1. ABOUT THE DATASET

Title: Aminoxy-BCN glycoconjugates

Creators: Ryan McBerney, Jonathan P Dolan, Emma E Cawood, Michael E Webb, W Bruce Turnbull

Organisation: University of Leeds

Publication Year: 2022

Description: NMR spectroscopy data for aminoxybicyclononyne derivatives and glycan conjugates, and protein mass spectrometry data for protein ligation reactions

Cite as: Ryan McBerney, Jonathan P Dolan, Emma E Cawood, Michael E Webb, W Bruce Turnbull (2022): Aminoxy-BCN glycoconjugates. University of Leeds. [Dataset] <https://doi.org/10.5518/1195>

Related publication: Ryan McBerney, Jonathan P Dolan, Emma E Cawood, Michael E Webb, W Bruce Turnbull, A Bioorthogonal, Bifunctional Linker for Engineering Synthetic Glycoproteins. *JACS Au*. <https://doi=10.1021/jacsau.2c00312>.

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2. TERMS OF USE

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3. PROJECT AND FUNDING INFORMATION

Funding organisation: EPSRC, BBSRC, The Wellcome Trust, Icen Glycoscience

Grant no.:

EPSRC: 1799721

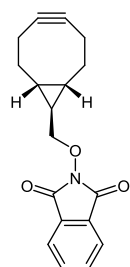
BBSRC: BB/M011151/1

Wellcome: 109154/Z/15/A; 097827/Z/11/A; WT094232MA; 094232/Z/10/Z

4. CONTENTS

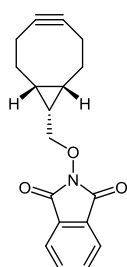
NMR spectroscopy.zip

FID data and associated files for the ¹H, ¹³C, COSY and HSQC spectra where available for compounds shown below. ¹H NMR of 10 and 13 recorded at 275K; water suppressed via presaturation.



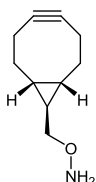
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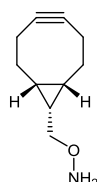
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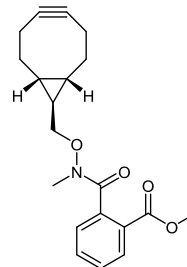
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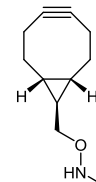
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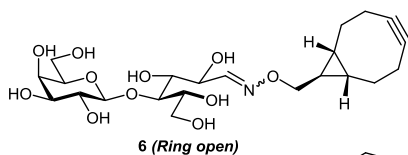
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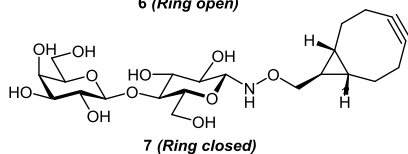


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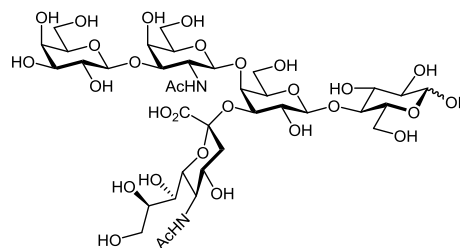


6 (Ring open)



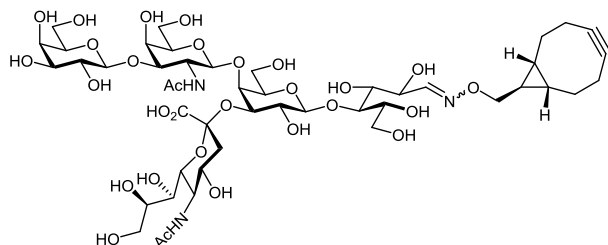
7 (Ring closed)

File Name: 6-7 Lac-BCN



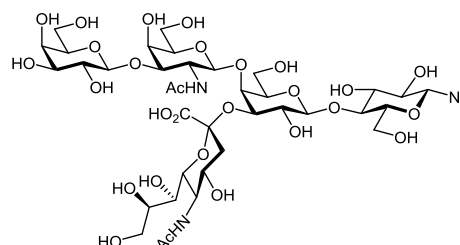
10

File Name: 10 GM1os



11

File Name: 11 GM1-BCN



13

File Name: 13 GM1-N3

Protein_ESMS_BAF.zip

Bruker electrospray mass spectrometry .baf files for derivatives of the CTB(W88E) protein

Folder Code	Description
W88E	CTB(W88E) following purification
Ox-W88E	Oxidised-CTB(W88E) prepared by treatment of CTB(W88E) with NaIO ₄ for 5 mins

BCN-W88E	Product of oxime ligation reaction between oxidised CTB(W88E) and aminoxybicyclononyne following purification by desalting column
(Lac)BCN-CTB(W88E)	product of SPAAC ligation of BCN-CTB(W88E) and lactosyl azide (9)
(GM1)BCN-CTB(W88E)	product of SPAAC ligation of BCN-CTB(W88E) and GM1 azide (13)
Met-W88E	CTB(M37L-M68L-M101L-K43M-W88E) - non-binding CTB mutant with native methionine residues mutated to leucine and K43 mutated to methionine
N3-W88E	Met-W88E expressed in defined growth media supplemented with azidohomoalanine in place of methionine
(Lac)N3-W88E-1hr (Lac)N3-W88E-2hr (Lac)N3-W88E-3hr (Lac)N3-W88E-4hr	product of SPAAC ligation of N3-W88E and lactose-BCN oxime (7) after 1 hr, 2 hr, 3 hr, 4 hr in the timecourse
(GM1)N3-W88E	product of SPAAC ligation of N3-W88E and GM1-BCN oxime (11)

CD.zip

CD measurements performed on a Jasco J715 spectropolarimeter at 20 °C, over a wavelength range of 260-180 nm. The measurements were made using a cuvette of 1 mm path length, with a bandwidth of 2.5, a step of 1 nm, at 1 sec per step.

PBS 00002.csv: phosphate-buffered saline

CTBwt00003.csv: wild type El Tor cholera toxin B-subunit 0.17 g/mL

CTBw88e00004.csv: W88E mutant of wild type El Tor cholera toxin B-subunit 0.16 g/mL

5. METHODS

Detailed information about methods is available in the related publication in Section 1 above.