**1. ABOUT THE DATASET**

**Title:** Cholera toxin B-subunit glycopeptide conjugates

**Creators:** Jonathan P Dolan, Michael E Webb, W Bruce Turnbull

**Organisation:** University of Leeds

**Publication Year**: 2022

**Description:** NMR spectroscopy data for galactosamine derivatives; polyacrylamide gel electrophoresis data for sortase-mediated protein ligation reactions; protein mass spectrometry data for oxime-mediated protein ligation reactions

**Cite as:** Jonathan P Dolan, Michael E Webb, W Bruce Turnbull (2022): Cholera toxin B-subunit glycopeptide conjugates. University of Leeds. [Dataset] https://doi.org/10.5518/1194

**Related publication:** Jonathan P. Dolan, Darren Machin, Simone Dedola, Robert A. Field, Michael E. Webb, W. Bruce Turnbull, Synthesis of cholera toxin B-subunit glycoconjugates using site-specific orthogonal oxime and sortase ligation reactions. *Front. Chem. – Chem. Biol*. 2022, 10, 958272.

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**2. TERMS OF USE**

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**3. PROJECT AND FUNDING INFORMATION**

**Funding organisation:** BBSRC, Iceni Glycoscience

**Grant no.:** BB/M011151/1

**4. CONTENTS**

**NMR\_spectroscopy.zip**

FID data and associated files for the 1H, 13C, COSY and HSQC spectra are available for compounds shown below. The files for each compound are contained in separate folders with sub-folders coded as follows: 1H (10), 13C (11), COSY (12), HSQC (13), DEPT-135 (14). The files were processed using MestReNova.



**Protein\_ESMS\_BAF.zip**

Bruker electrospray mass spectrometry .baf files for CTB-LPETGA, Oxidised CTB-LPETGA and biotinylated CTB-LPETGA proteins

|  |  |  |
| --- | --- | --- |
| **Protein** | **Description** | **Folder Code** |
| CTB-LPETGA | CTB-LPETGA following purification | CTB-LPETGA |
| Oxidised-CTB-LPETGA | Crude LC-MS following treatment of CTB-LPETGA with NaIO4 for 5 mins | Ox-LPETGA |
| Biotin-CTB-LPETGA | LC-MS following purification of BCN-CTB-LPETGA by desalting column following oxime ligation | Biotin-LPETGA |

**SDS-PAGE.zip**

ImageLab .scn files and corresponding .tif files used for densitometry measurements

|  |  |
| --- | --- |
| **Image Code** | **Description** |
| CTB-1 | Sortase 7M-His6 ligation of CTB-LPETGA and peptide **1** over 2 hours. |
| CTB-2 | Sortase 7M-His6 ligation of CTB-LPETGA and glycopeptide **2** over 2 hours. |
| CTB-1-DMSO | Sortase 7M-His6 ligation of CTB-LPETGA and peptide **1** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-2-DMSO | Sortase 7M-His6 ligation of CTB-LPETGA and glycopeptide **2** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-7 | Sortase 7M-His6 ligation of CTB-LPETGA and peptide **7** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-8 | Sortase 7M-His6 ligation of CTB-LPETGA and glycopeptide **8** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-9 | Sortase 7M-His6 ligation of CTB-LPETGA and glycopeptide **9** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-10 | Sortase 7M-His6 ligation of CTB-LPETGA and glycopeptide **10** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-11 | Sortase 7M-His6 ligation of CTB-LPETGA and glycopeptide **11** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-12 | Sortase 7M-His6 ligation of CTB-LPETGA and glycopeptide **12** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-10,13-18 | Sortase 7M-His6 ligation to CTB-LPETGA in the presence of 10% (v/v) DMSO after 2 hours. Lane 1: CTB-LPETGA (unlabelled); Lane 2: CTB-LPETGA (incubated with Sortase 7M); Lane 3: Glycopeptide **13**; Lane 4: Glycopeptide **14**; Lane 5: Glycopeptide **15**; Lane 6: Glycopeptide **16**; Lane 7: Glycopeptide **17**; Lane 8: Glycopeptide **18**; Lane 9: Glycopeptide **10**. |
| CTB-10-7M | Sortase 7M-His6 ligation of CTB-LPETGA and Glycopeptide **10** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-10-CBD7M | His6-CBD-Sortase 7M ligation of CTB-LPETGA and Glycopeptide **10** in the presence of 10% (v/v) DMSO over 2 hours. |
| CTB-10,13-18-CBD7M | His6-CBD-Sortase 7M ligation to CTB-LPETGA in the presence of 10% (v/v) DMSO after 2 hours (Pre-purification of CBD-Sortase 7M with chitin resin and size-exclusion chromatography). Lane 1: CTB-LPETGA (unlabelled); Lane 2: Glycopeptide **13**; Lane 3: Glycopeptide **14**; Lane 4: Glycopeptide **15**; Lane 5: Glycopeptide **16**; Lane 6: Glycopeptide **17**; Lane 7: Glycopeptide **18**; Lane 8: Glycopeptide **10**. |
| CTB-10,13-18-purified | His6-CBD-Sortase 7M ligation to CTB-LPETGA in the presence of 10% (v/v) DMSO after 2 hours (Post-purification of CBD-Sortase 7M with chitin resin and size-exclusion chromatography). Lane 1: CTB-LPETGA (unlabelled); Lane 2: Glycopeptide **13**; Lane 3: Glycopeptide **14**; Lane 4: Glycopeptide **15**; Lane 5: Glycopeptide **16**; Lane 6: Glycopeptide **17**; Lane 7: Glycopeptide **18**; Lane 8: Glycopeptide **10**. |
| Biotin-CTB-CBD7M | His6-CBD-Sortase 7M ligation to CTB-LPETGA in the presence of 10% (v/v) DMSO after 2 hours (Post-purification of CBD-Sortase 7M with chitin resin and size-exclusion chromatography). Lane 1: CTB-LPETGA (unlabelled); Lane 2: CTB-LPETGA (oxidised); Lane 3: Biotin-CTB-LPETGA; Lane 4: Biotin-CTB-**13**; Lane 5: Biotin-CTB-**14**; Lane 6: Biotin-CTB-**15**; Lane 7: Biotin-CTB-**16**; Lane 8: Biotin-CTB-**17**; Lane 9: Biotin-CTB-**18**; Lane 10: Biotin-CTB-**10**. |

**5. METHODS**

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