

# From Bench Scale to kilolab Production of Renewable Ferulic Acid-based Bisphenols: Optimisation and Evaluation of Different Purification Approaches Towards a Technical Feasibility and Process Environmental Sustainability<sup>†</sup>

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**Table S1** Regression coefficient of fitting ( $R^2$ ) to membrane permeability curves using acetone. The fitting can be linear ( $J_v = a \Delta P + b$ ,  $a = L_p$  by Eq.1) or a power ( $J_v = a \Delta P^b$ )

| Membrane    | Type of fitting | a    | b    | $R^2$ |
|-------------|-----------------|------|------|-------|
| Duramem 200 | Power           | 17.9 | 0.53 | 0.98  |
| Duramem 300 | Power           | 50.7 | 0.28 | 0.98  |
| Duramem 500 | Power           | 105  | 0.45 | 0.99  |
| GMT-oNF1    | Linear          | 1.8  | 1.4  | 0.99  |
| GMT-oNF2    | Linear          | 2.0  | 3.2  | 0.99  |
| Nano 450    | Linear          | 9.9  | 2.8  | 0.99  |

**Table S2** Regression coefficient of fitting ( $R^2$ ) to membrane permeability curves using an acetone-based solution at a concentration of 1 g/L, containing 80% (w/w) of **BDF** and 20% (w/w) of **EtDfE**. The fitting can be linear ( $J_v = a \Delta P + b$ ,  $a = L_p$  by Eq.1) or a power ( $J_v = a \Delta P^b$ )

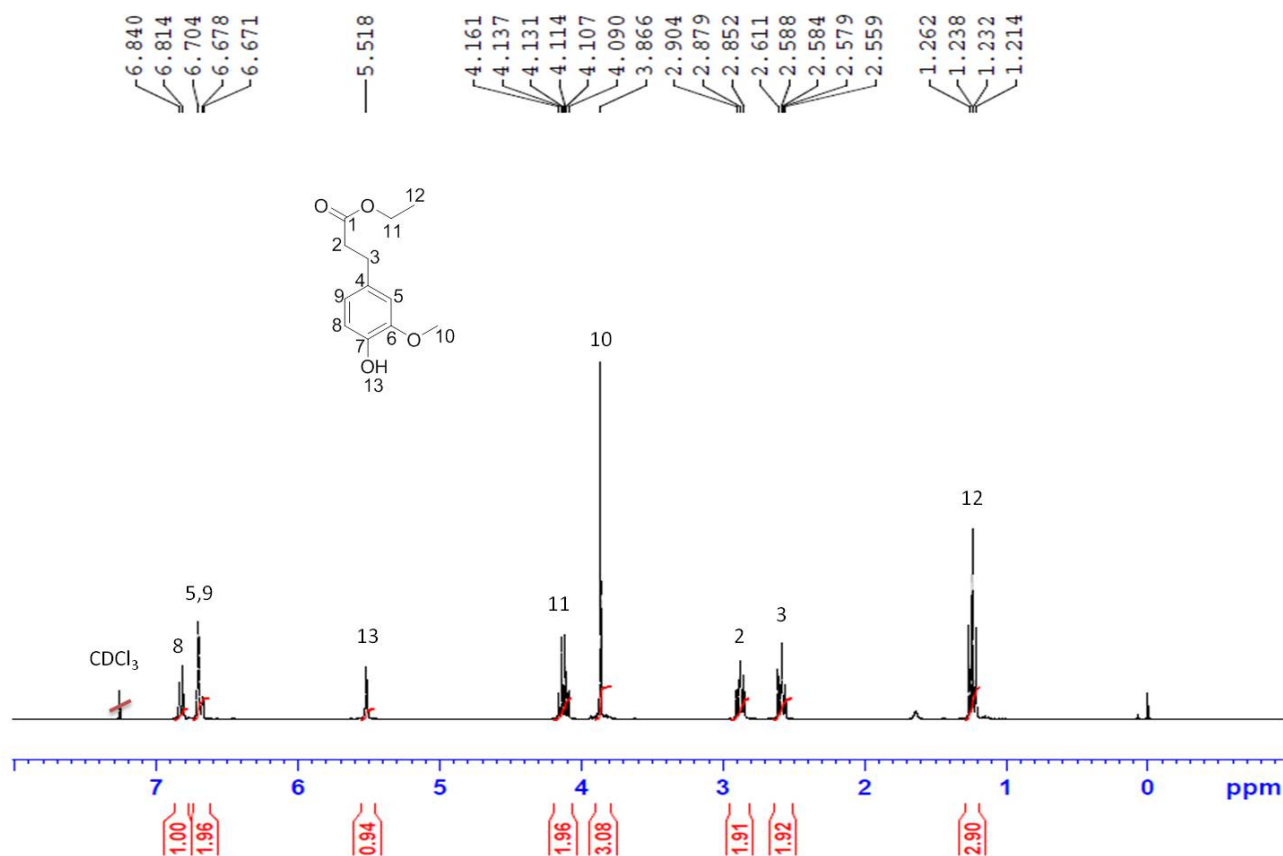
| Membrane    | Type of fitting | a    | b    | $R^2$ |
|-------------|-----------------|------|------|-------|
| Duramem 200 | Power           | 4.9  | 0.88 | 1.0   |
| Duramem 300 | Power           | 9.0  | 0.76 | 0.99  |
| Duramem 500 | Power           | 38.7 | 0.64 | 0.98  |
| GMT-oNF1    | Linear          | 1.6  | 4.5  | 0.96  |
| GMT-oNF2    | Linear          | 1.3  | 5.2  | 0.92  |
| Nano 450    | Linear          | 2.6  | -0.2 | 0.94  |

**Table S3** Regression coefficient of fitting ( $R^2$ ) to **BDF** rejection curves. The fitting can be linear ( $R = a \Delta P + b$ ) or a power ( $R = a \Delta P^b$ )

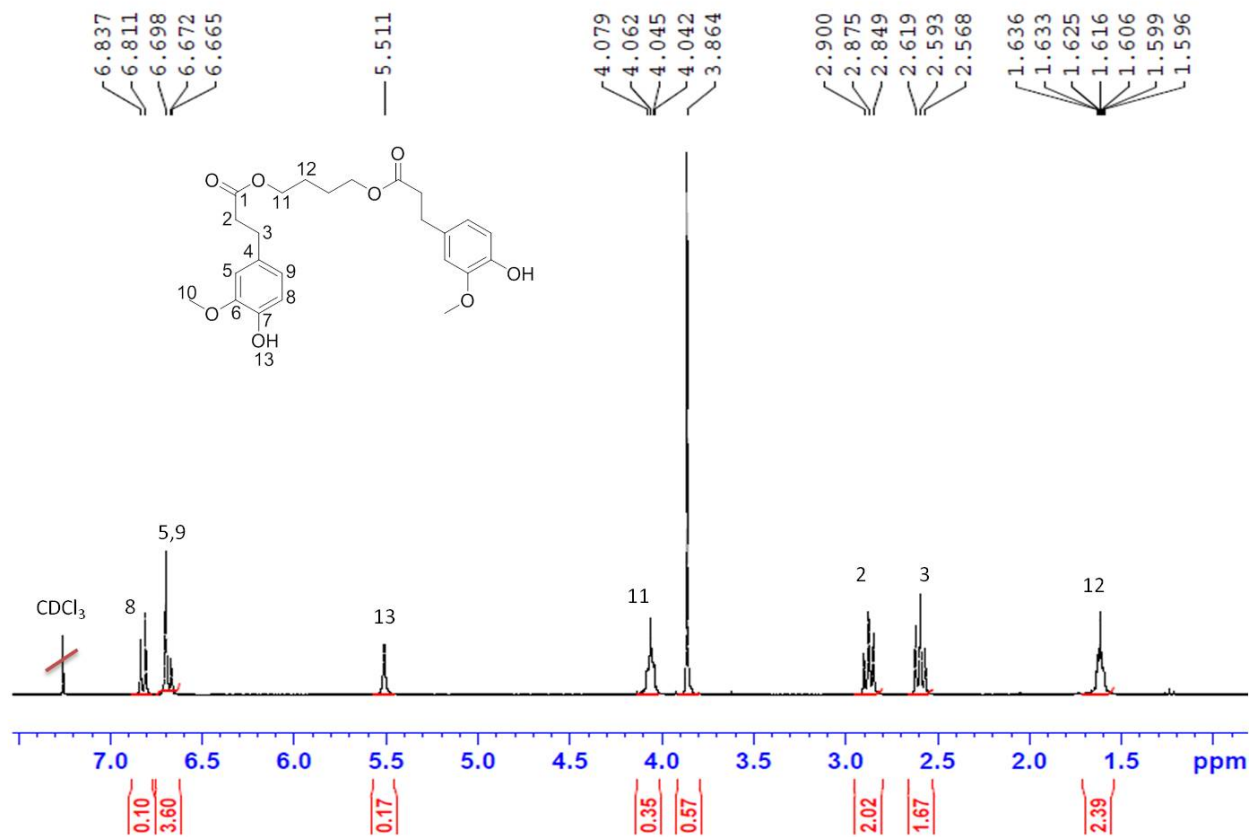
| Membrane    | Type of fitting | a    | b    | $R^2$ |
|-------------|-----------------|------|------|-------|
| Duramem 200 | Power           | 70.6 | 0.09 | 1.0   |
| Duramem 300 | Power           | 27.7 | 0.31 | 0.99  |
| Duramem 500 | Linear          | 2.7  | -2.0 | 0.98  |
| GMT-oNF1    | Power           | 75.9 | 0.07 | 1.0   |
| GMT-oNF2    | Power           | 59.5 | 0.14 | 1.0   |
| Nano 450    | Linear          | 30.3 | 0.23 | 0.99  |

**Table S4** Regression coefficient of fitting ( $R^2$ ) to **EtDfFe** rejection curves. The fitting can be linear ( $R=a \Delta P + b$ ) or a power ( $R=a \Delta P^b$ )

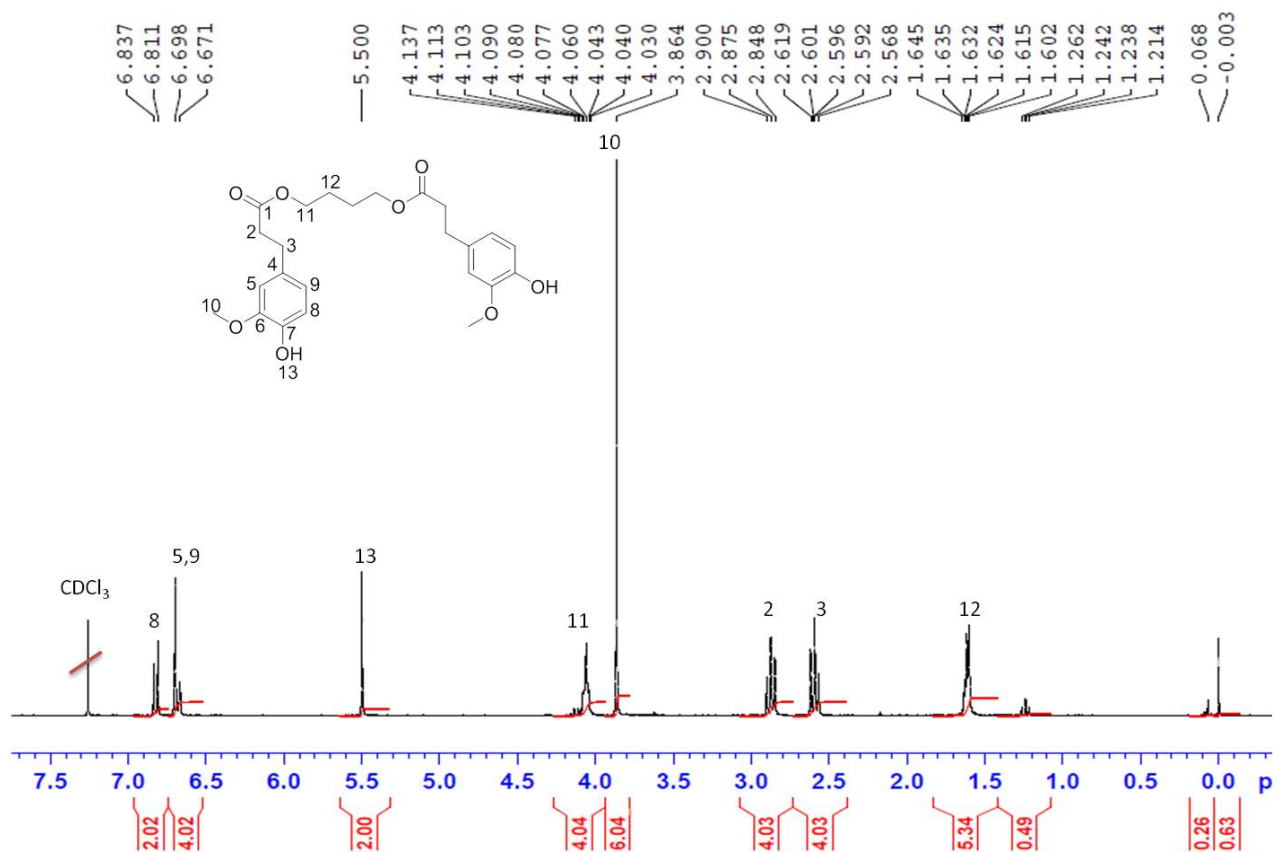
| Membrane    | Type of fitting | a    | b    | $R^2$ |
|-------------|-----------------|------|------|-------|
| Duramem 200 | Power           | 49.3 | 0.16 | 0.99  |
| Duramem 300 | Power           | 12.6 | 0.48 | 0.99  |
| Duramem 500 | Linear          | 1.8  | -2.4 | 0.95  |
| GMT-oNF1    | Power           | 27.8 | 0.25 | 0.99  |
| GMT-oNF2    | Power           | 13.3 | 0.47 | 1.0   |
| Nano 450    | Power           | 10.8 | 0.47 | 0.95  |



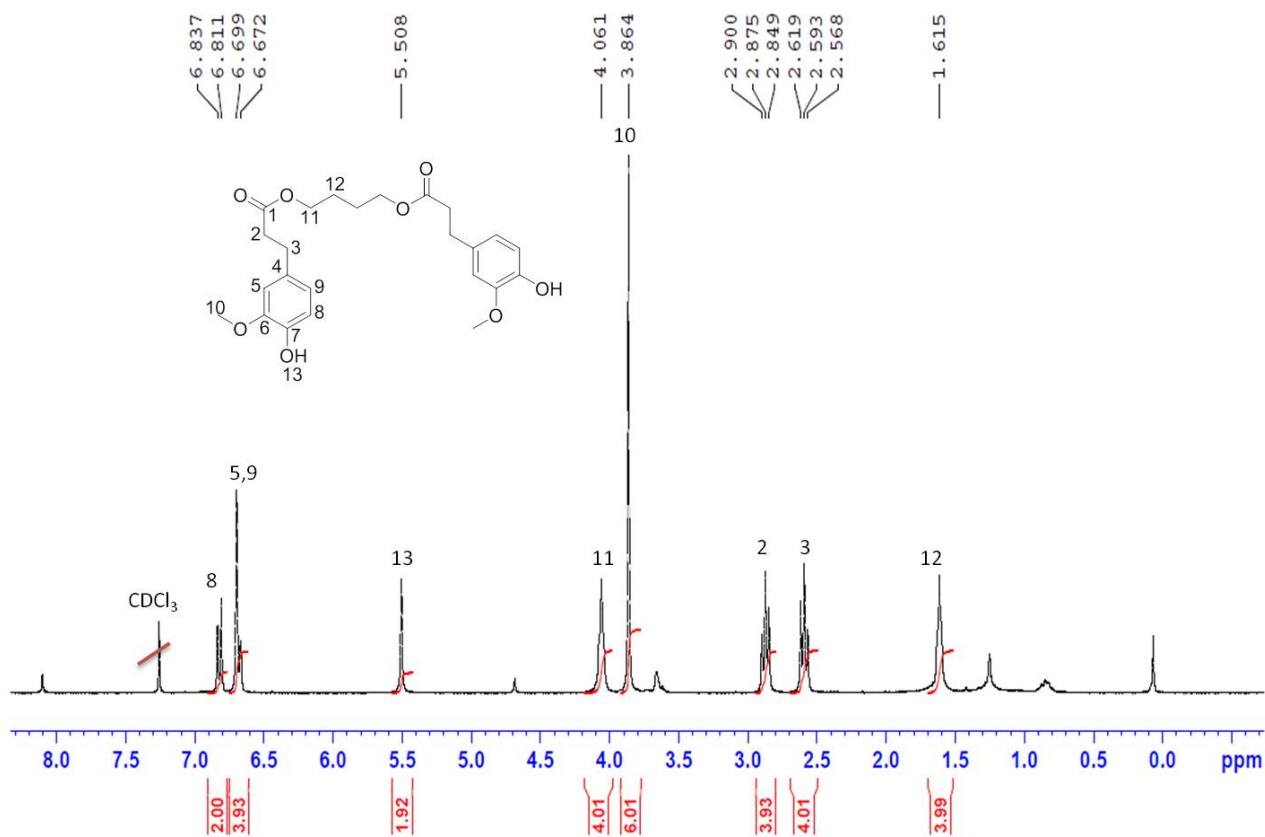
**Figure S1**  $^1\text{H}$  NMR spectrum of ethyl dihydroferulate (EtDfFe) produced at laboratory scale (CDCl<sub>3</sub>, 300 MHz)



**Figure S2** <sup>1</sup>H NMR spectrum of bis-*O*-dihydroferuloyl 1,4-butanediol (BDF) produced in the laboratory and purified by flash chromatography on silica gel (CDCl<sub>3</sub>, 300 MHz)

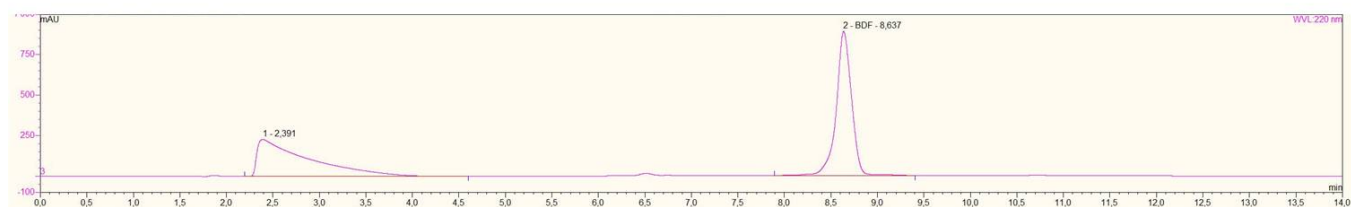


**Figure S3**  $^1\text{H}$  NMR spectrum of bis-*O*-dihydroferuloyl 1,4-butanediol (BDF) produced in kilolab scale and purified by recrystallisation ( $\text{CDCl}_3$ , 300 MHz)

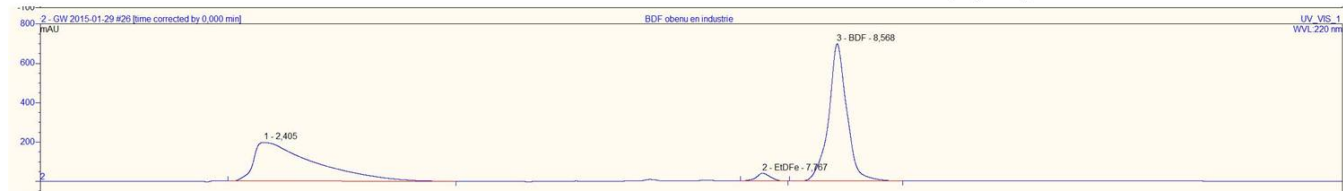


**Figure S4**  $^1\text{H}$  NMR spectrum of bis-*O*-dihydroferuloyl 1,4-butanediol (BDF) produced in laboratory scale and purified by diananofiltration ( $\text{CDCl}_3$ , 300 MHz)

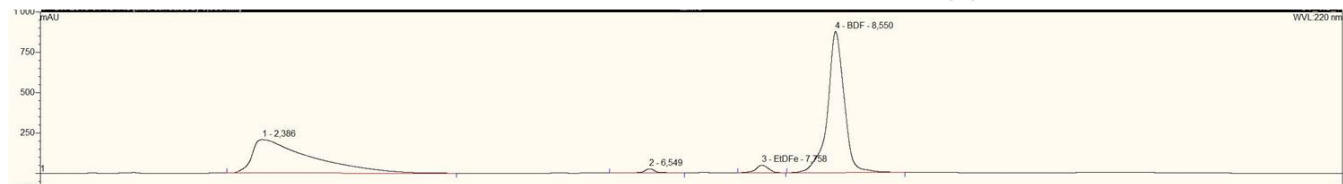
(a) Flash Chromatography



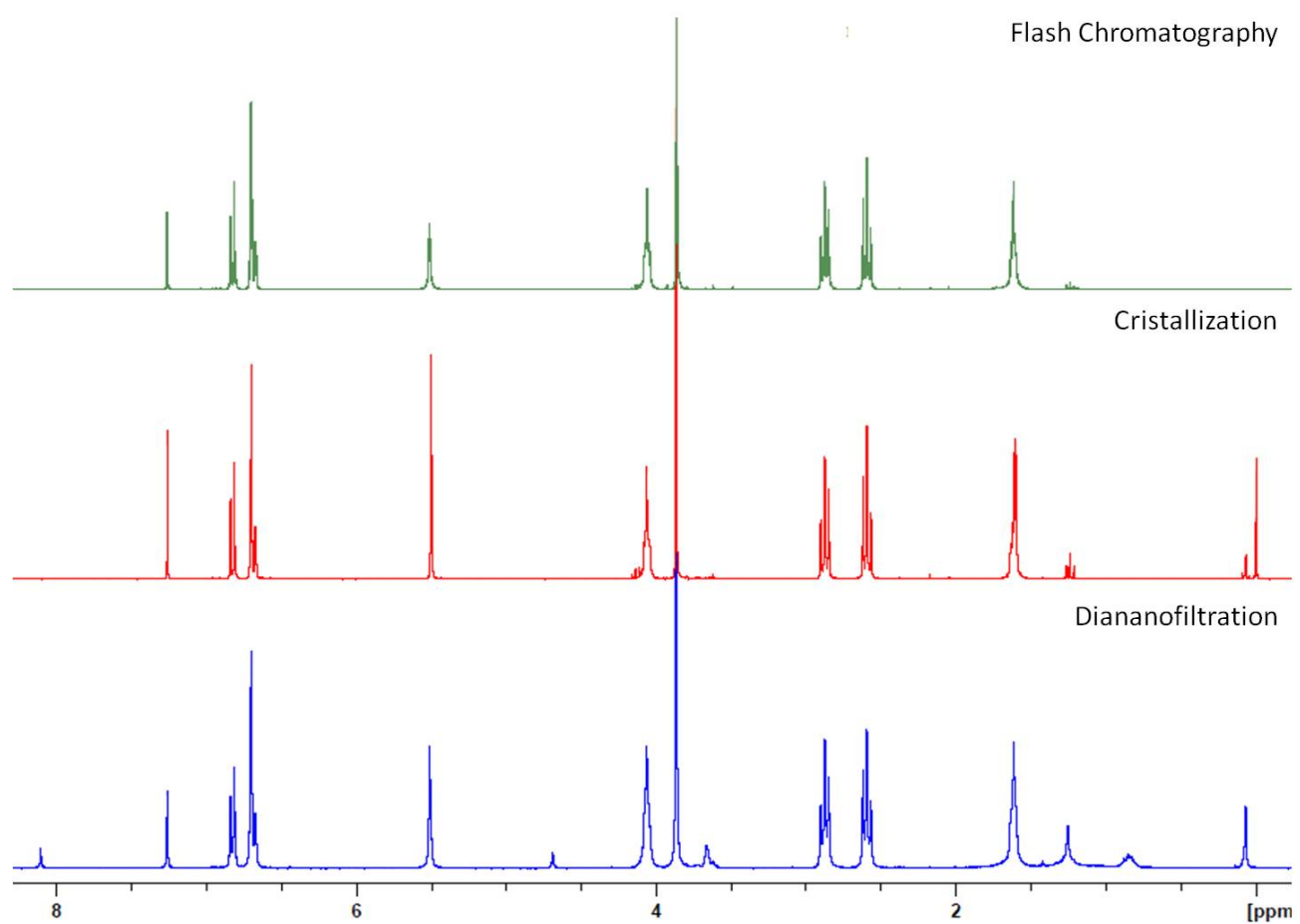
(b) Crystallization



(c) Diananofiltration



**Figure S5** HPLC spectra of bis-*O*-dihydroferuloyl 1,4-butanediol (BDF) purified by the different purification methods



**Figure S6**  $^1\text{H}$  NMR spectra of bis-*O*-dihydroferuloyl 1,4-butanediol (BDF) purified by the different purification methods ( $\text{CDCl}_3$ , 300 MHz)