Development and evaluation of a Raman flow cell for monitoring continuous flow reactions.

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Figure S1. Calibration of HPLC by measuring the weight of water at 20°C pumped through the pump every 30 seconds for 150 seconds at varying flow rates.
Figure S2. The effect of varying flow rate on a 0.1004 M solution of 4-cyanobiphenyl in 66.7% DMF. The spectral range observed was between Raman shifts 1291.08 and 1300.69 cm\(^{-1}\).

Figure S3. Raman spectra of the calibration solutions representing 0, 20, 40, 60, 80, 100% conversions of 4-cyanobiphenyl. The greatest variance in the spectra can be observed between 1530 cm\(^{-1}\) and 1640 cm\(^{-1}\).
Figure S4. GCMS calibration of conversion using reaction calibration standards of 0.0994, 0.0764, 0.0579, 0.0397, 0.0193, 0.000 M 4-bromobenzonitrile, 0.1156, 0.0957, 0.0802, 0.0677, 0.0413, 0.0205 M phenyl boronic acid, 0.2485, 0.2544, 0.2440, 0.2394, 0.2400, 0.2438 M potassium carbonate, and 0.0000, 0.0220, 0.0391, 0.0598, 0.0797, 0.0989 M 4-cyanobiphenyl in 66.7% DMF respectively. The chromatographic region of interest was between 5 to 20 minutes (Supplementary information 5). The data was subject to mean centring normalisation and auto scaling before PLSR analysis.

Figure S5. Chromatogram demonstrating the retention times of the internal standard (decane) at 6.44 mins, 4-bromobenzonitrile at 11.13 mins and 4-cyanobiphenyl at 15.35 mins.
Figure S6. Mass spectra of decane from 30 to 540 m/z.

Figure S7. Supporting information 5 Mass spectra of 4-bromobenzonitrile from 30 to 505 m/z.
Figure S8. Mass spectra of 4-cyanobiphenyl from 30 to 540 m/z.