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Supplementary Material

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

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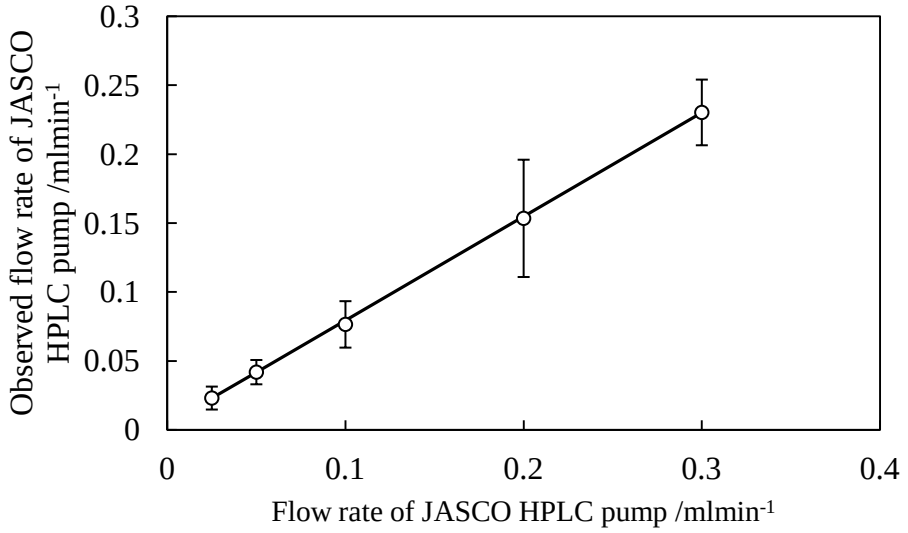

Figure S1. Calibration of HPLC by measuring the weight of water at 20˚C pumped through the pump every 30 seconds for 150 seconds at varying flow rates.

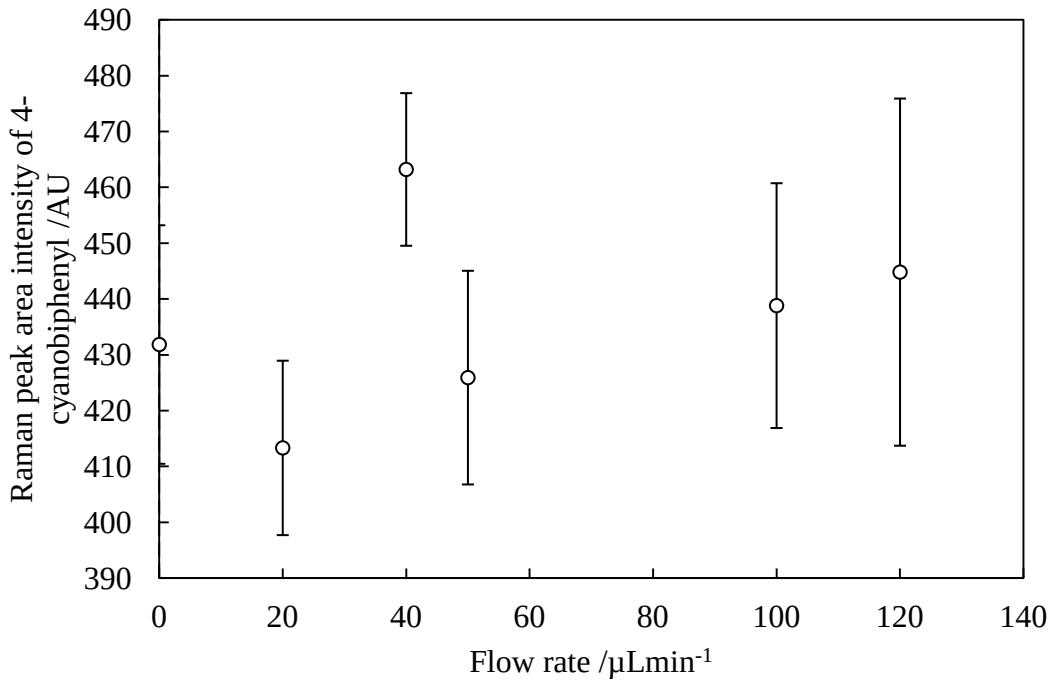

Figure S2. The effect of varying flow rate on a 0.1004 M solution of 4-cyanobiphenyl in 66.7% DMF. The spectral range observed was between Raman shifts1291.08 and 1300.69 cm^{-1}.

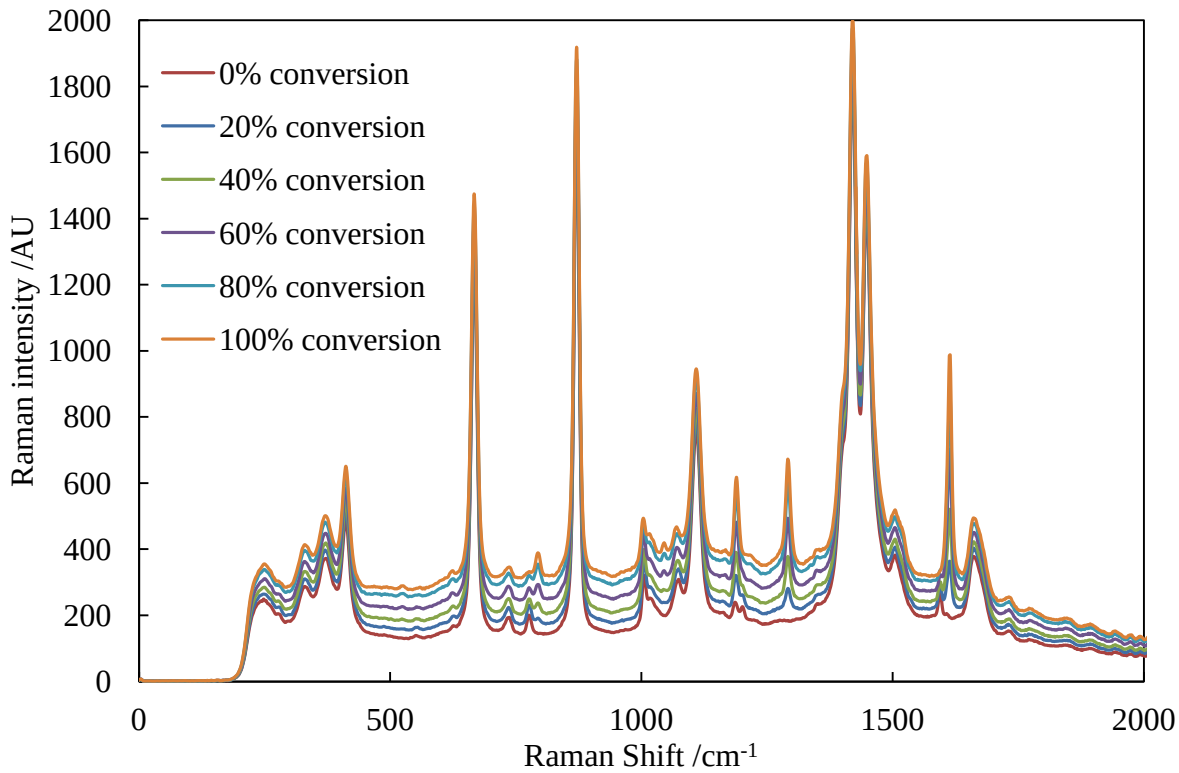

Figure S3. Raman spectra of the calibration solutions representing 0, 20, 40, 60, 80, 100% conversions of 4-cyanobiphenyl. The greatest variance in the spectra can be observed between 1530 cm^{-1} and 1640 cm^{-1}.

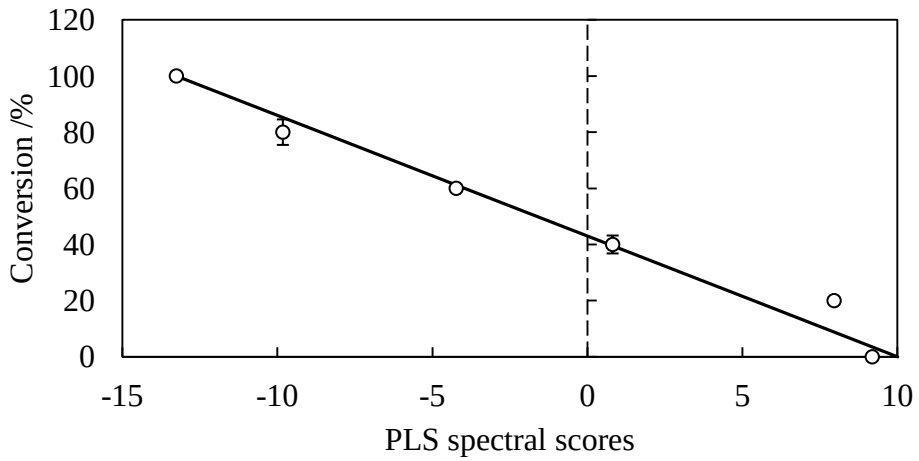

Figure S4. GCMS calibration of conversion using reaction calibration standards of 0.0994, 0.0764, 0.0579, 0.0397, 0.0193, 0.000 M 4-bromobenzonitrile, 0.1156, 0.0957, 0.0802, 0.0677, 0.0413, 0.0205 M phenyl boronic acid, 0.2485, 0.2544, 0.2440, 0.2394, 0.2400, 0.2438 M potassium carbonate, and 0.0000, 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.*

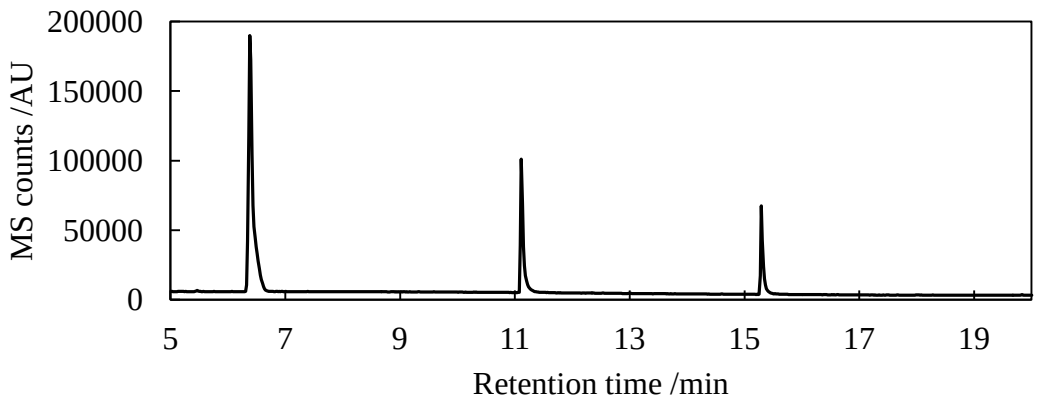

Figure S5. Chromatogram demonstrating the retention times of the internal standard (decane) at 6.44 mins, 4-bromobenzonitrile at 11.13 mins and 4-cyanobiphenyl at 15.35 mins.

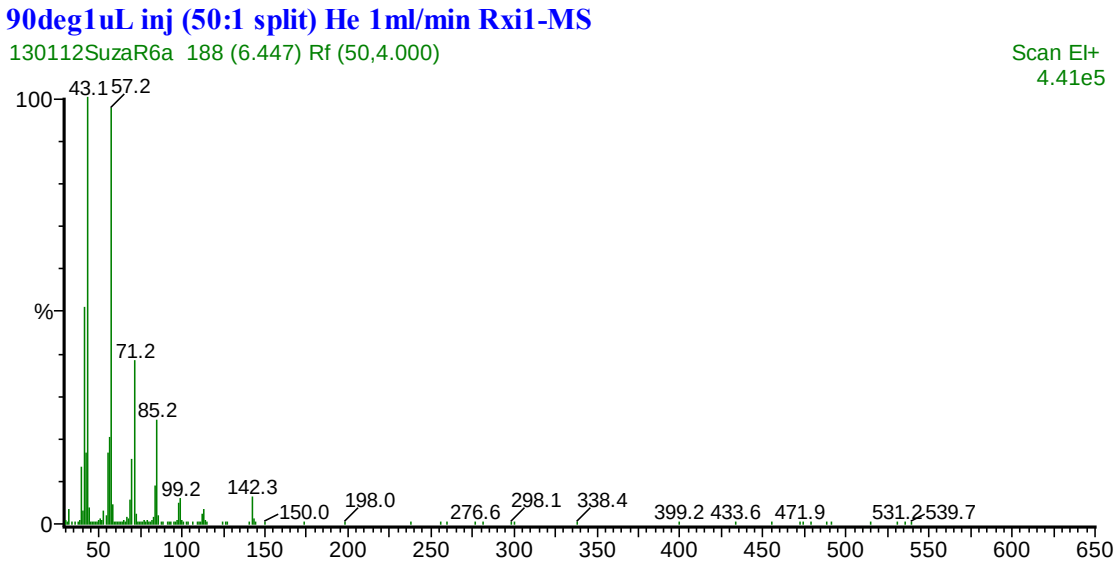

Figure S6. Mass spectra of decane from 30 to 540 m/z.

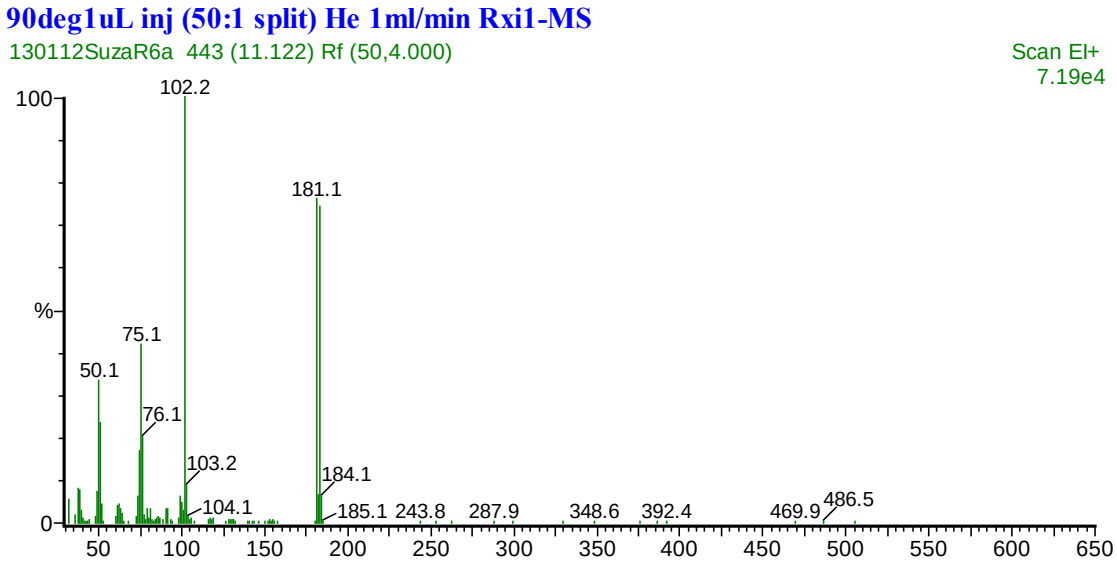

Figure S7. Supporting information 5 Mass spectra of 4-bromobenzonitrile from 30 to 505 m/z.

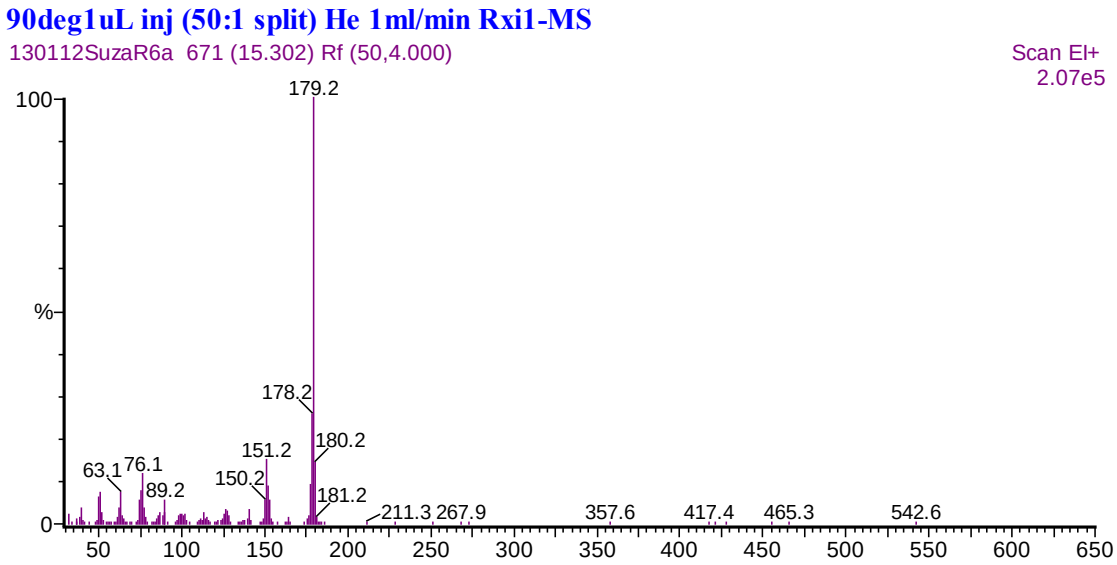

Figure S8. Mass spectra of 4-cyanobiphenyl from 30 to 540 m/z.