Electronic Supplementary Information

Pattern Recognition of Solid Materials by Multiple Probe Gases

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Supplementary Text

Selection of solid materials. In general, discrimination of chemically different targets by means of the pattern recognition approaches is rather easy, such as discrimination between hydrophobic and hydrophilic materials. Thus, as a proof-of-concept, we selected practically difficult sets of materials in terms of hydrophobic polymers as well as the different molecular weight of polymers in this present study.

Supplementary Figures

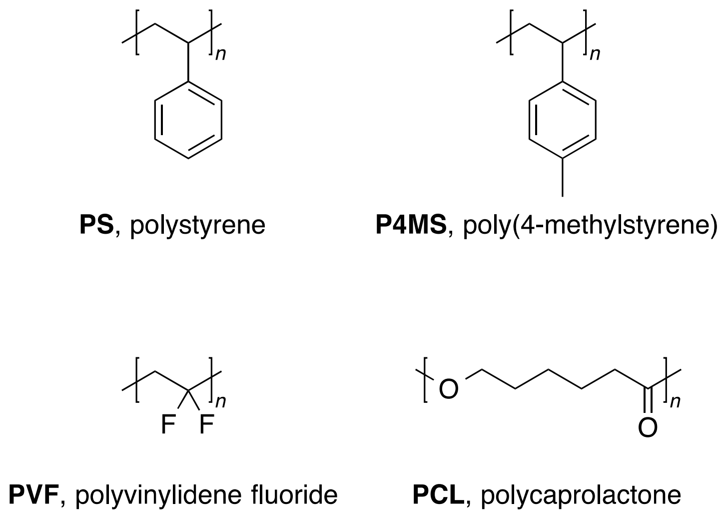

Fig. S1 Structures of polymer materials used in this study.

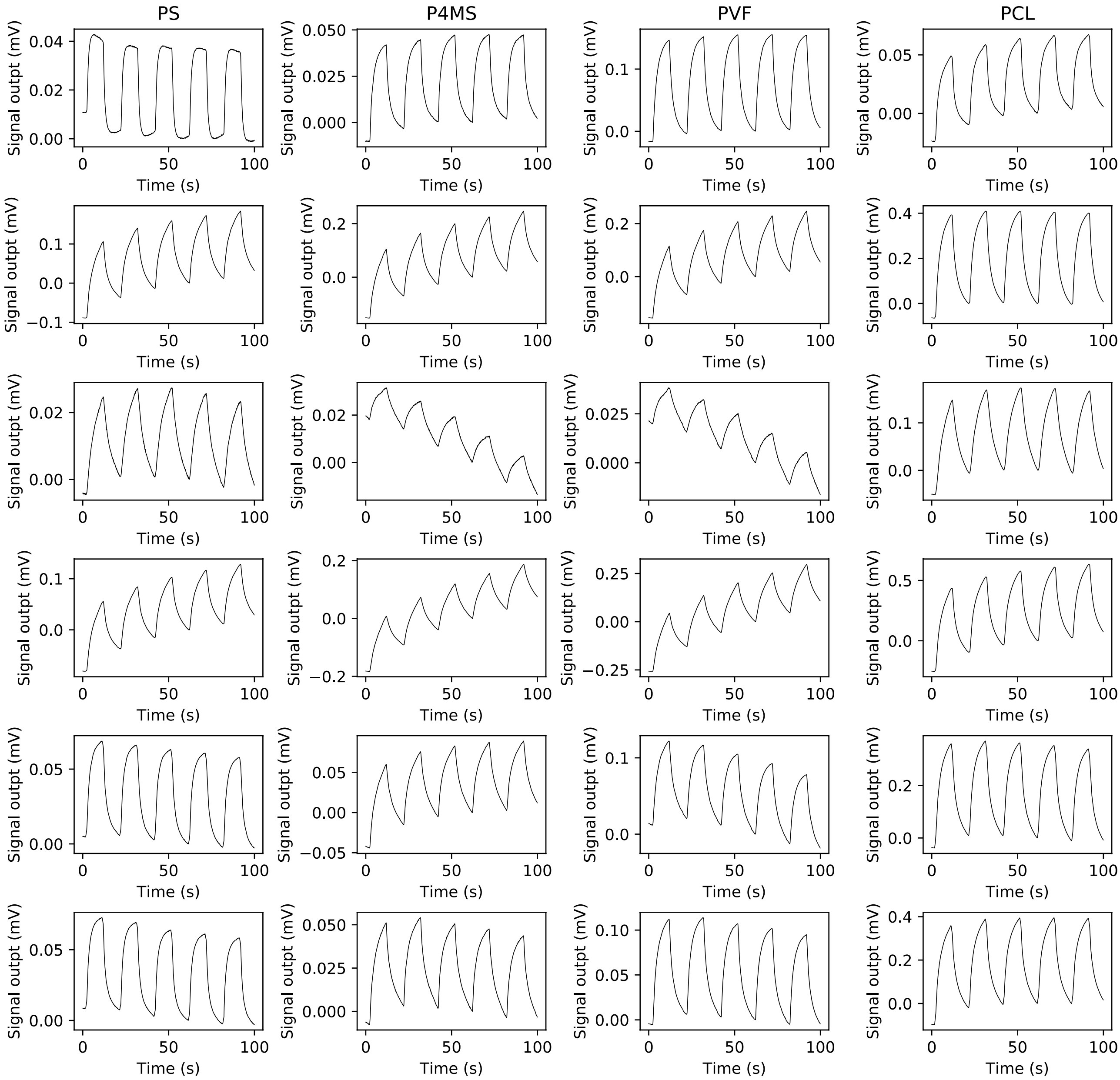

Fig. S2 Signal responses of each material measured with 12 different vapours. Top to bottom figures indicate the response to water, ethanol, 1-hexanol, hexanal, *n*-heptane, and methylcycloehxane, respectively.

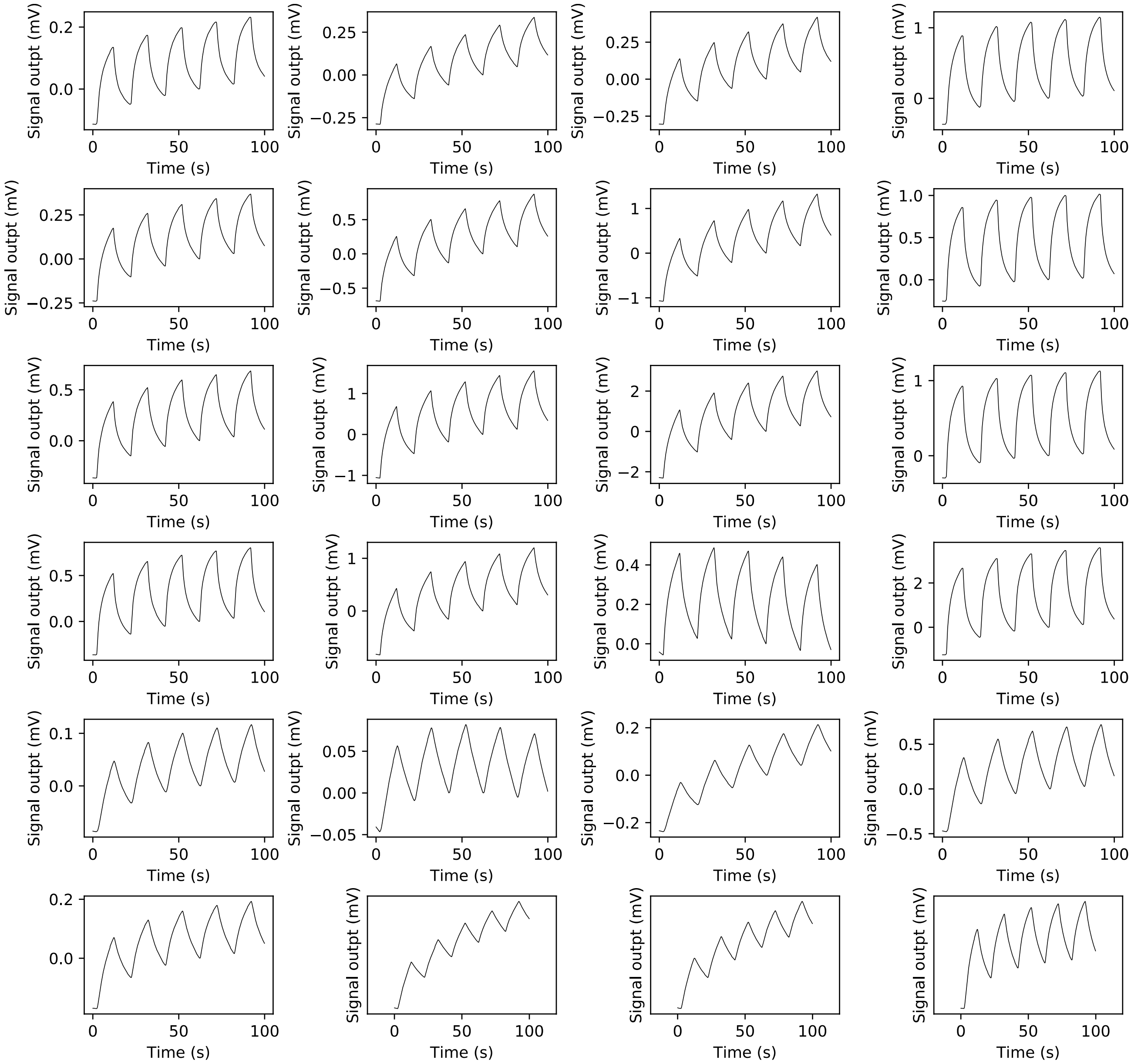

Fig. S2 (*Continued*) Signal responses of each material measured with 12 different vapours. Top to bottom figures indicate the response to toluene, ethyl acetate, acetone, chloroform, aniline and propionic acid, respectively.

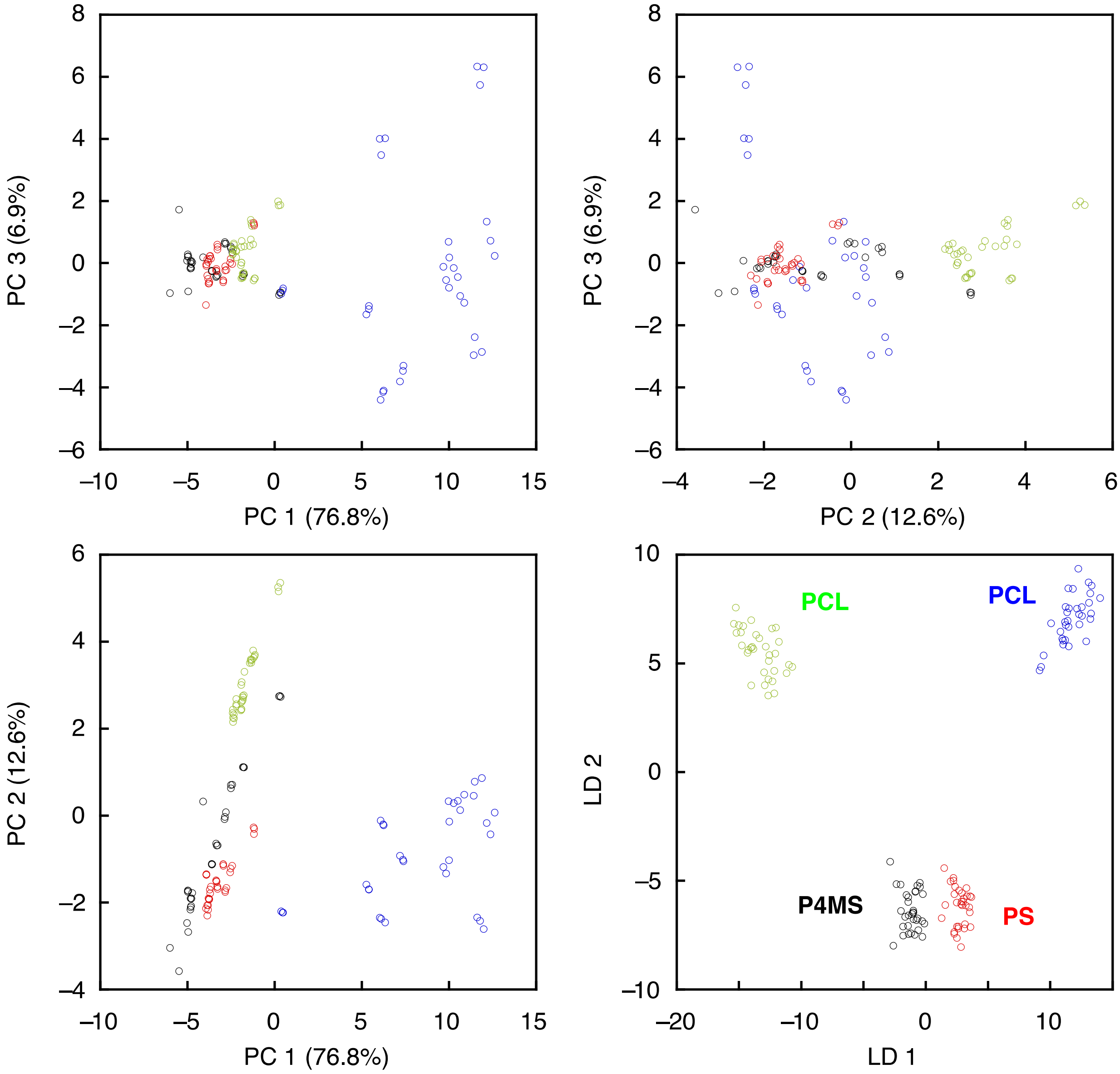

Fig. S3 Identification of polymers by pattern recognition. PCA (*Top left, Top right, Bottom left*) and LDA (*Bottom right*) score plots to identify 4 materials coated on MSS by measuring with 12 different vapours. **PS (350k)**, polystyrene (red); **P4MS**, poly(4-methylstyrene) (black); **PVF**, poly(vinylidene fluoride) (green); **PCL**, polycaprolactone (blue). $N = 11$.

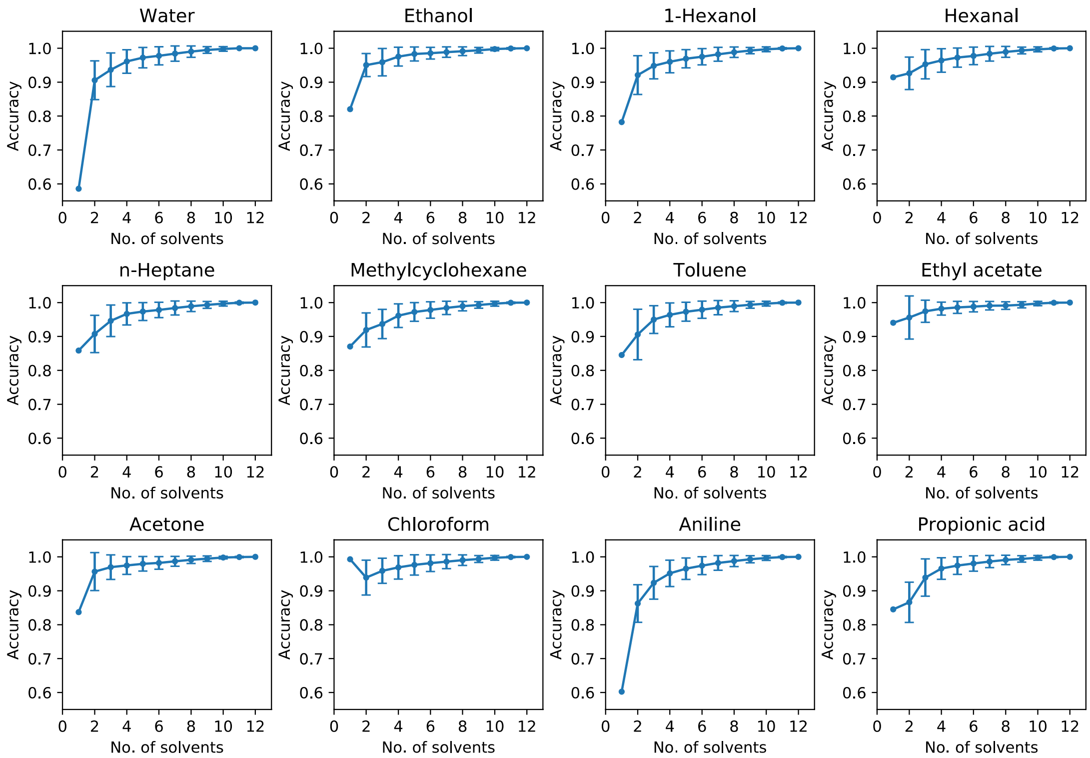

Fig. S4 Classification accuracy of polymer materials of selected combinations including selected solvents as a function of number of solvents (*n*). Average classification accuracies with standard deviations are shown.

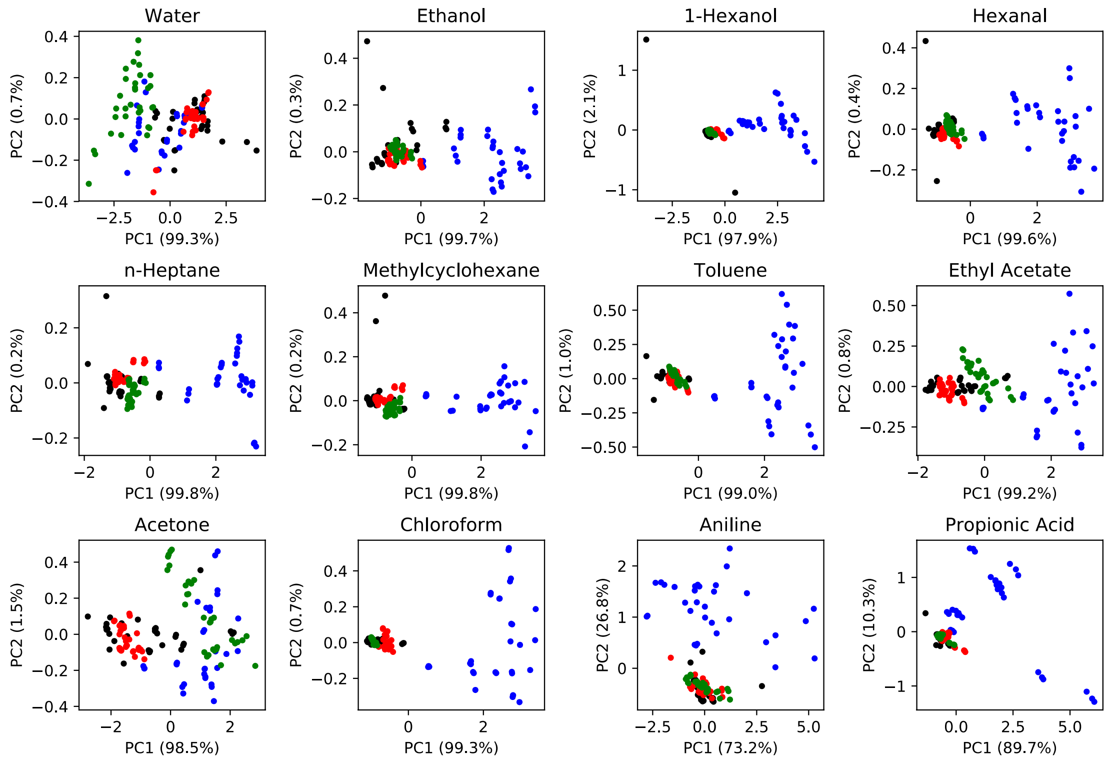

Fig. S5 PCA score plots of features from each solvent to discriminate 4 different polymer materials. **PS (350k)**, polystyrene (red); **P4MS**, poly(4-methylstyrene) (black); **PVF**, poly(vinylidene fluoride) (green); **PCL**, polycaprolactone (blue). $N = 11$.

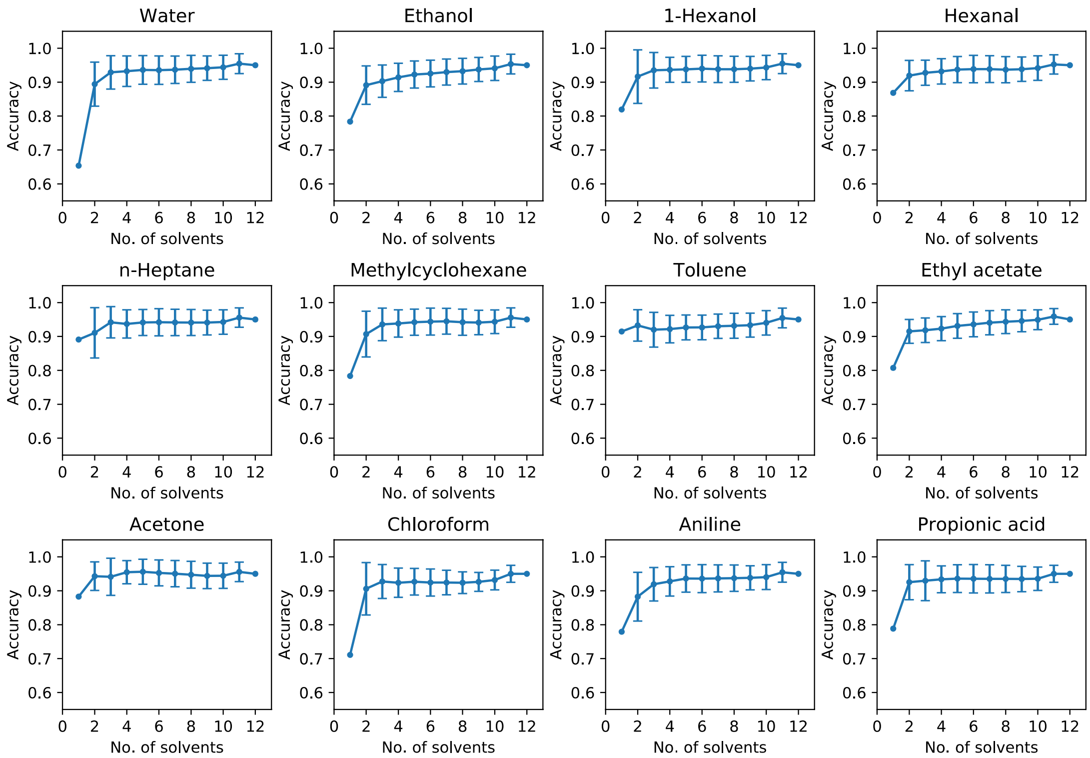

Fig. S6 Classification accuracy of different molecular weight of selected combinations including selected solvents as a function of number of solvents (n). Average classification accuracies with standard deviations are shown.

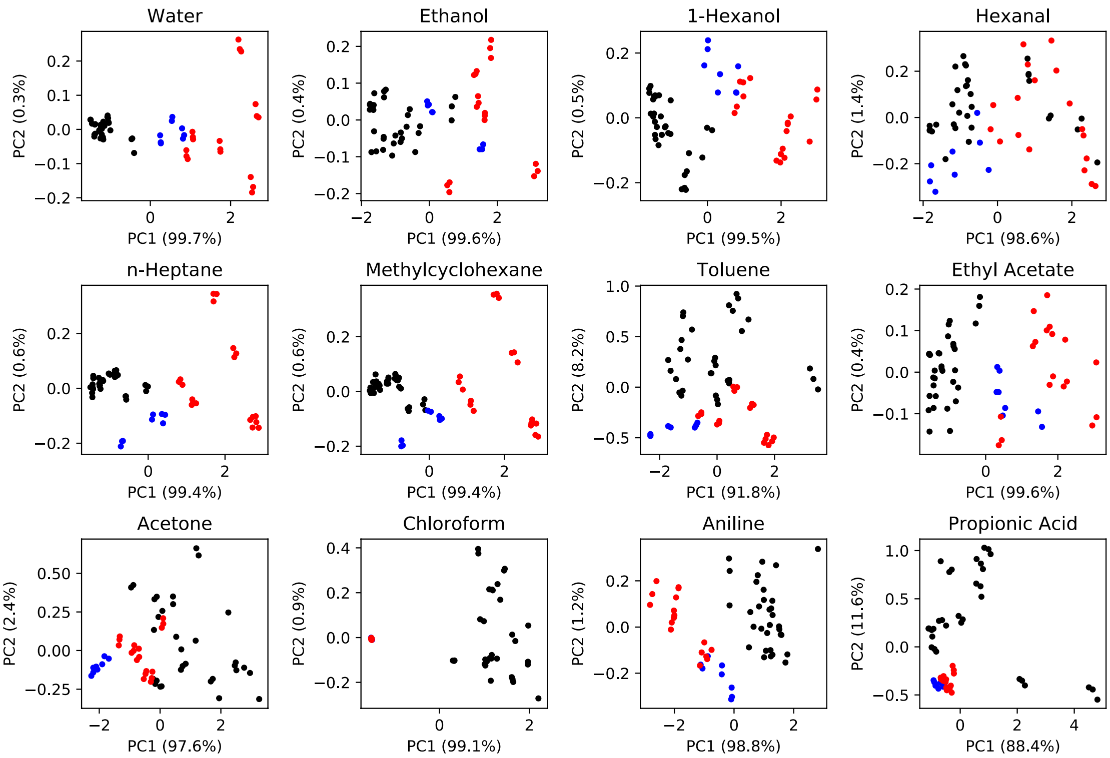

Fig. S7 PCA score plots of features from each solvent to discriminate 4 different polymer materials. **PS (350k)**, polystyrene, Mw = 350000 (blue); **P4MS**, poly(4-methylstyrene), Mw = 72000 (black); **PS (280k)**, polystyrene, Mw = 280000 (red); **PS (35k)**, polystyrene, Mw = 35000 (green).

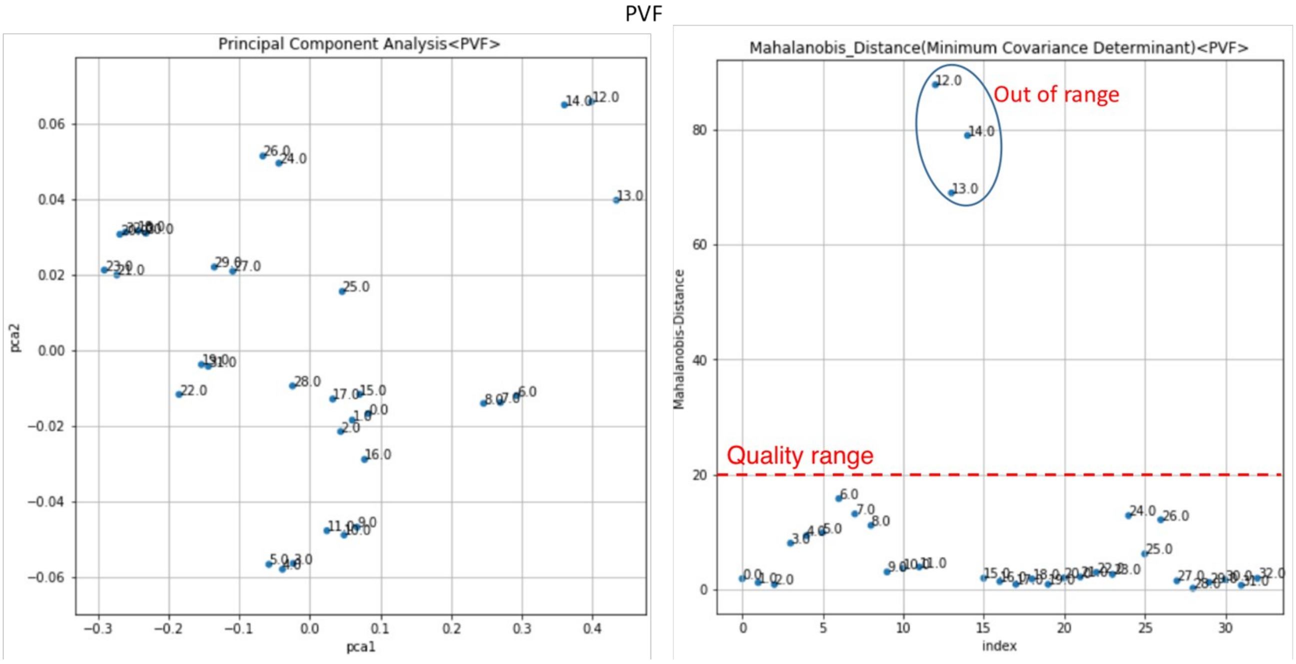

Fig. S8 PCA score plots of polyvinylfluoride (**PVF**) (*left*) and their Mahalanobis distances (*right*). Red dashed line is an example of the range for determination of quality.

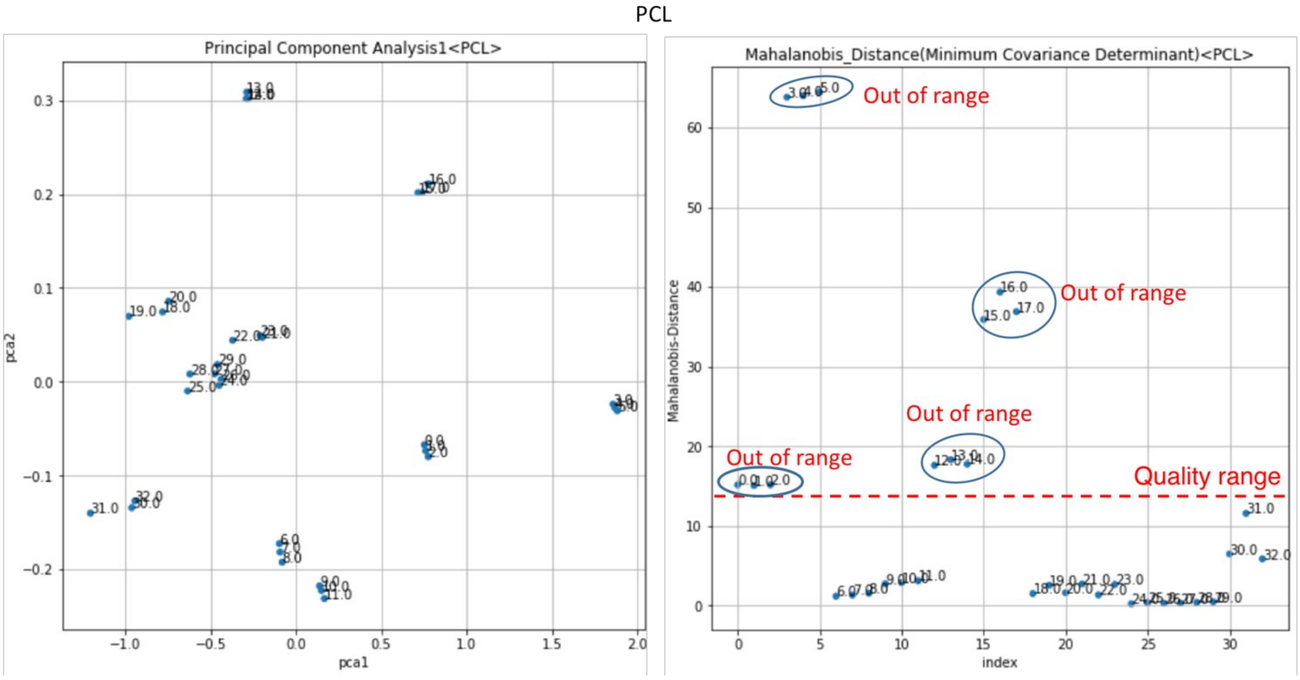

Fig. S9 PCA score plots of polycaprolactone (**PCL**) (*left*) and their Mahalanobis distances (*right*). Red dashed line is an example of the range for determination of quality.