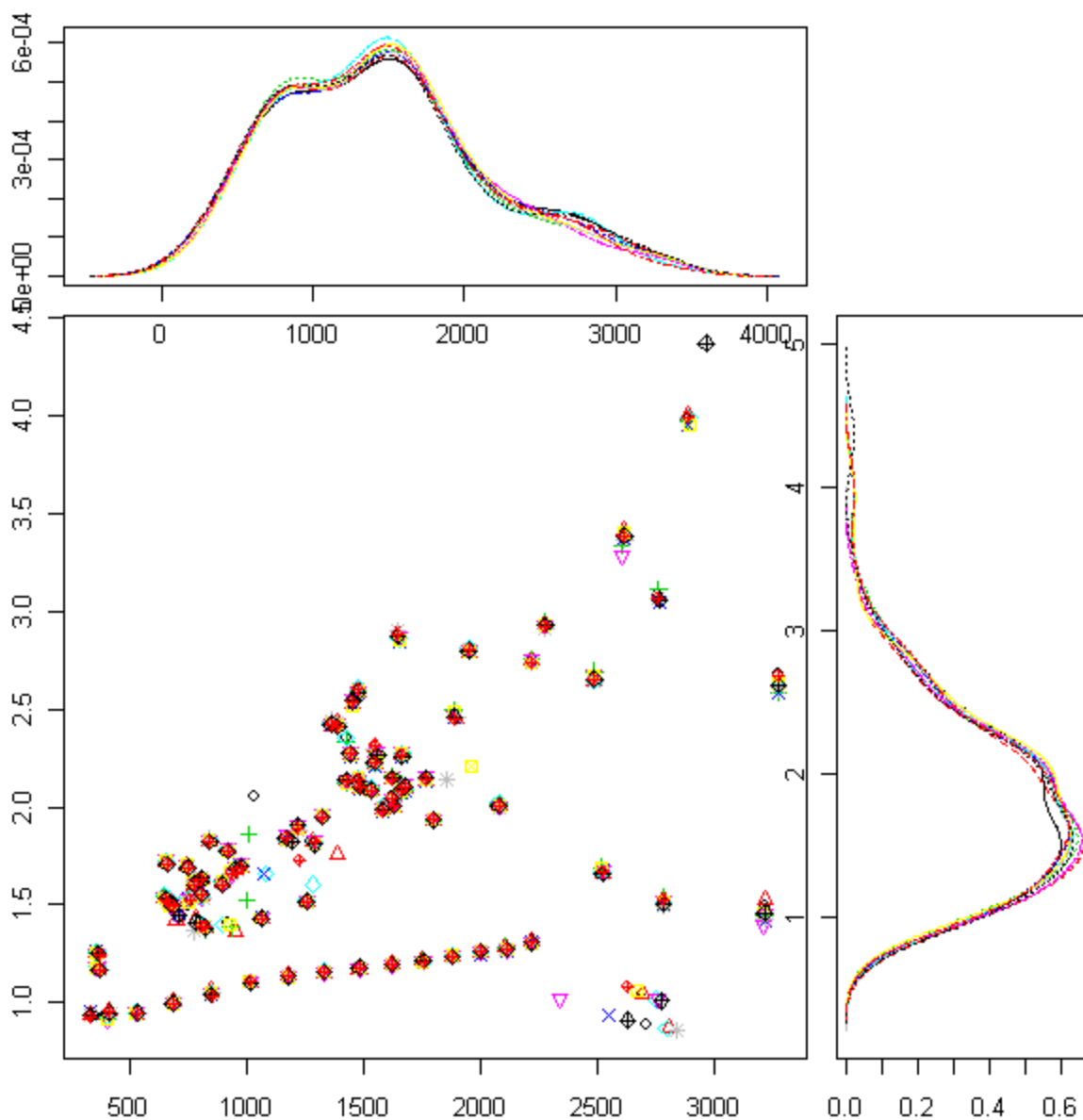
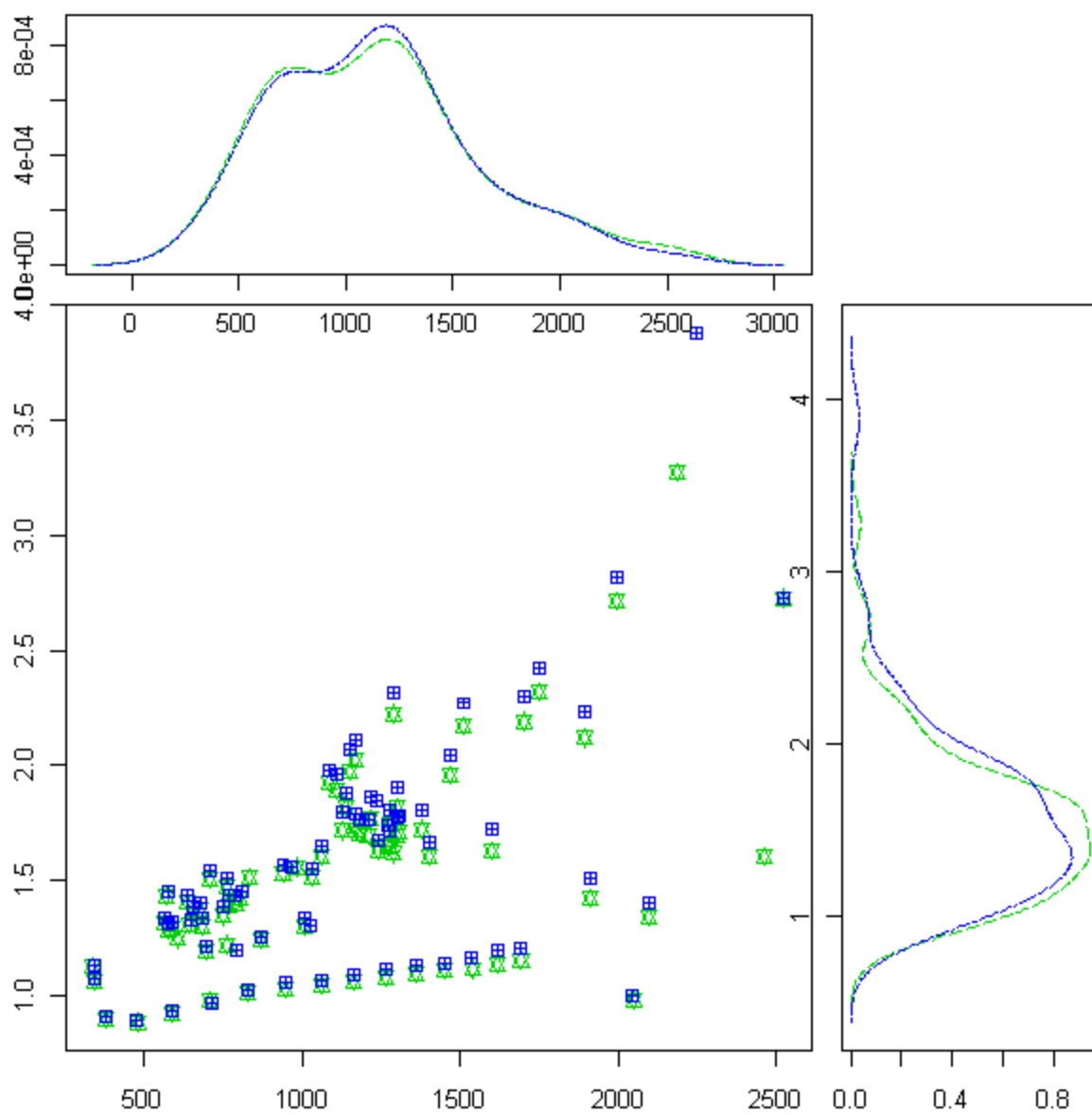


Figure S1. The scatter and density plots of the first and the second retention times of the peak list of each dataset. The scatter and density plots for two sets of data are depicted in (a) for compound standards with 5°C/min, (b) 7°C/min, (c) 10°C/min, and (d) for a spiked-in sample. The total number of GCxGC-MS experiments is 10, 2, 4, and 5 for compound standards with 5°C/min, 7°C/min, 10°C/min, and for a spiked-in sample, respectively.

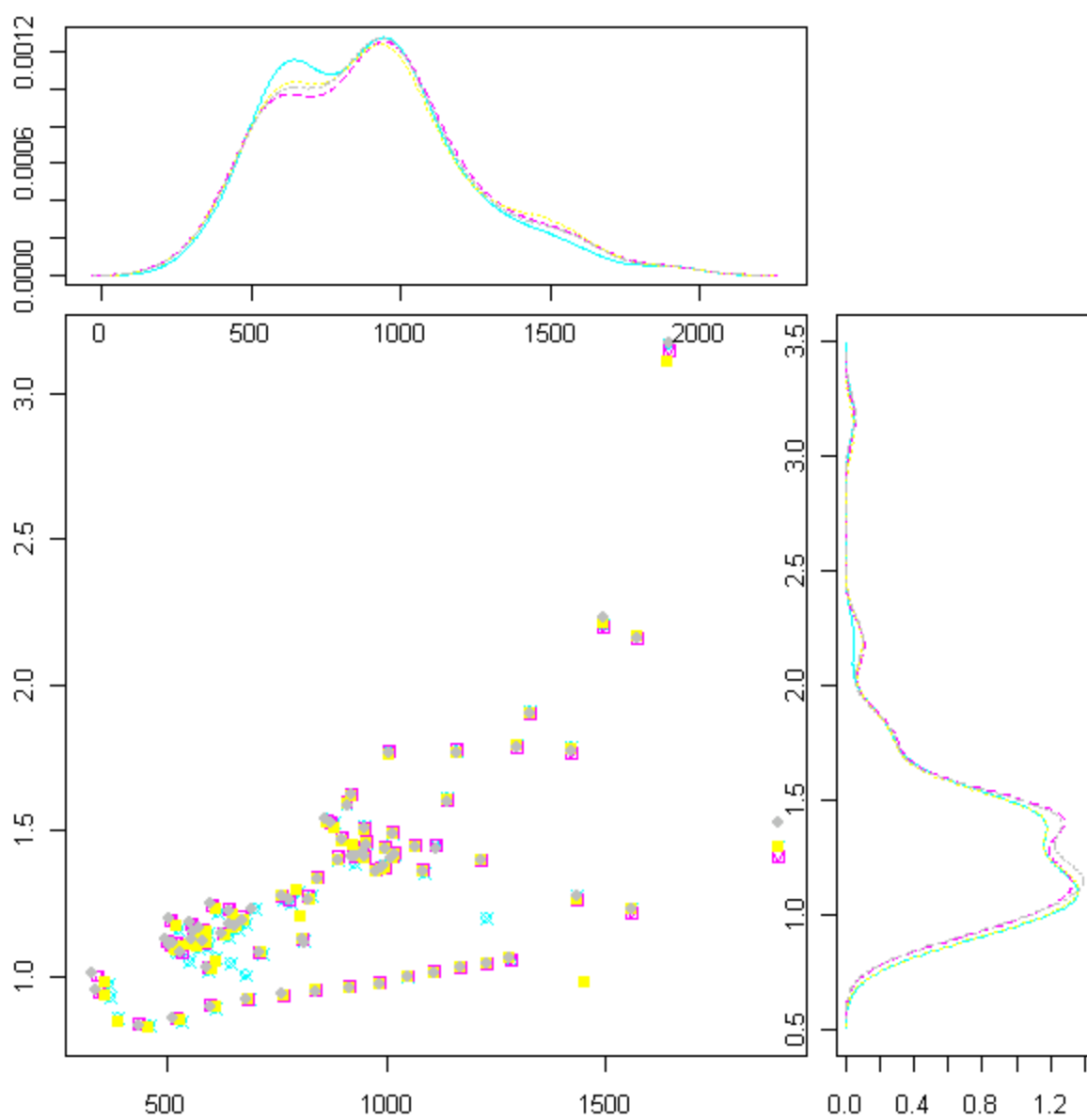
(a)



(b)



(c)



(d)

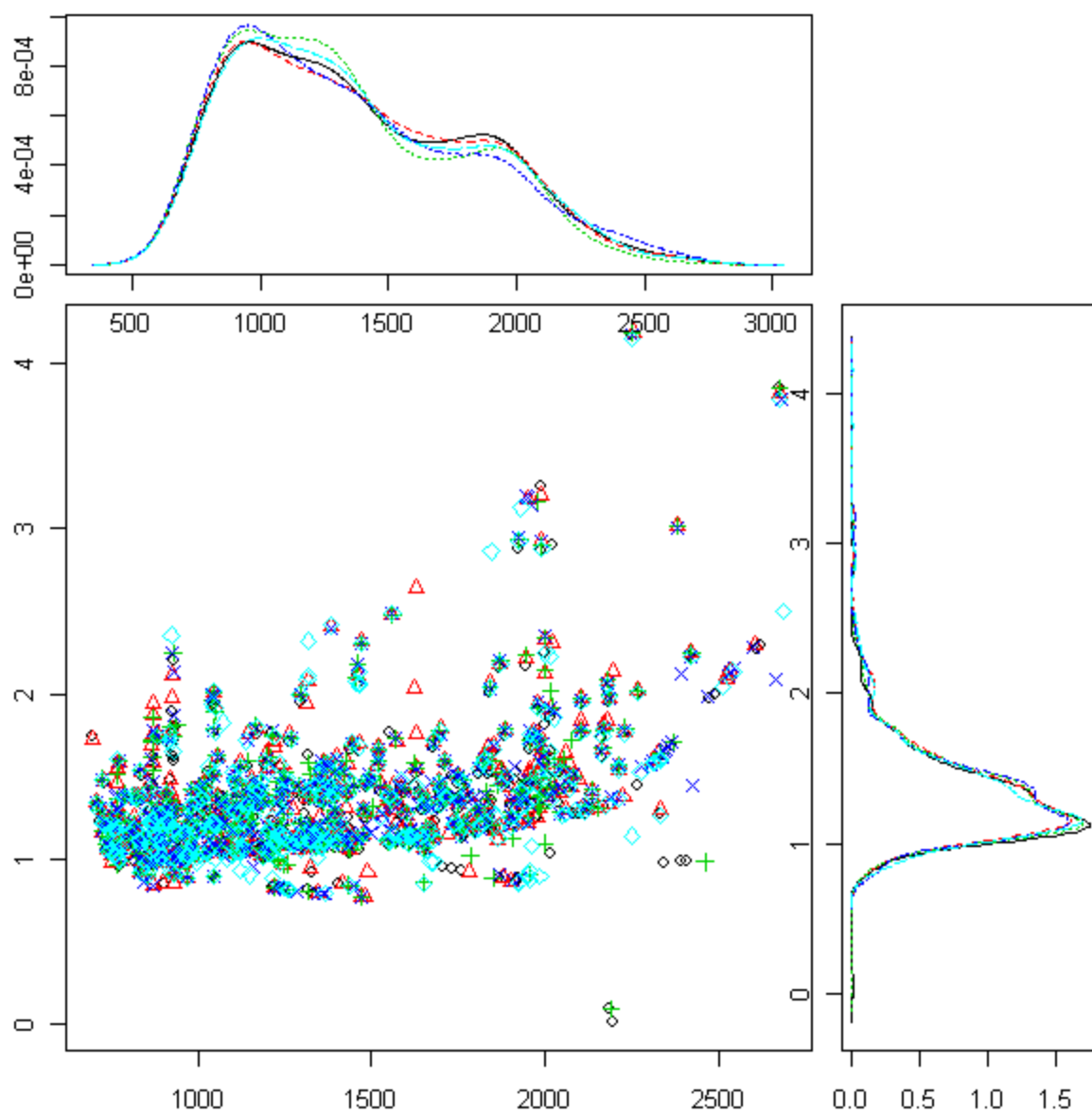
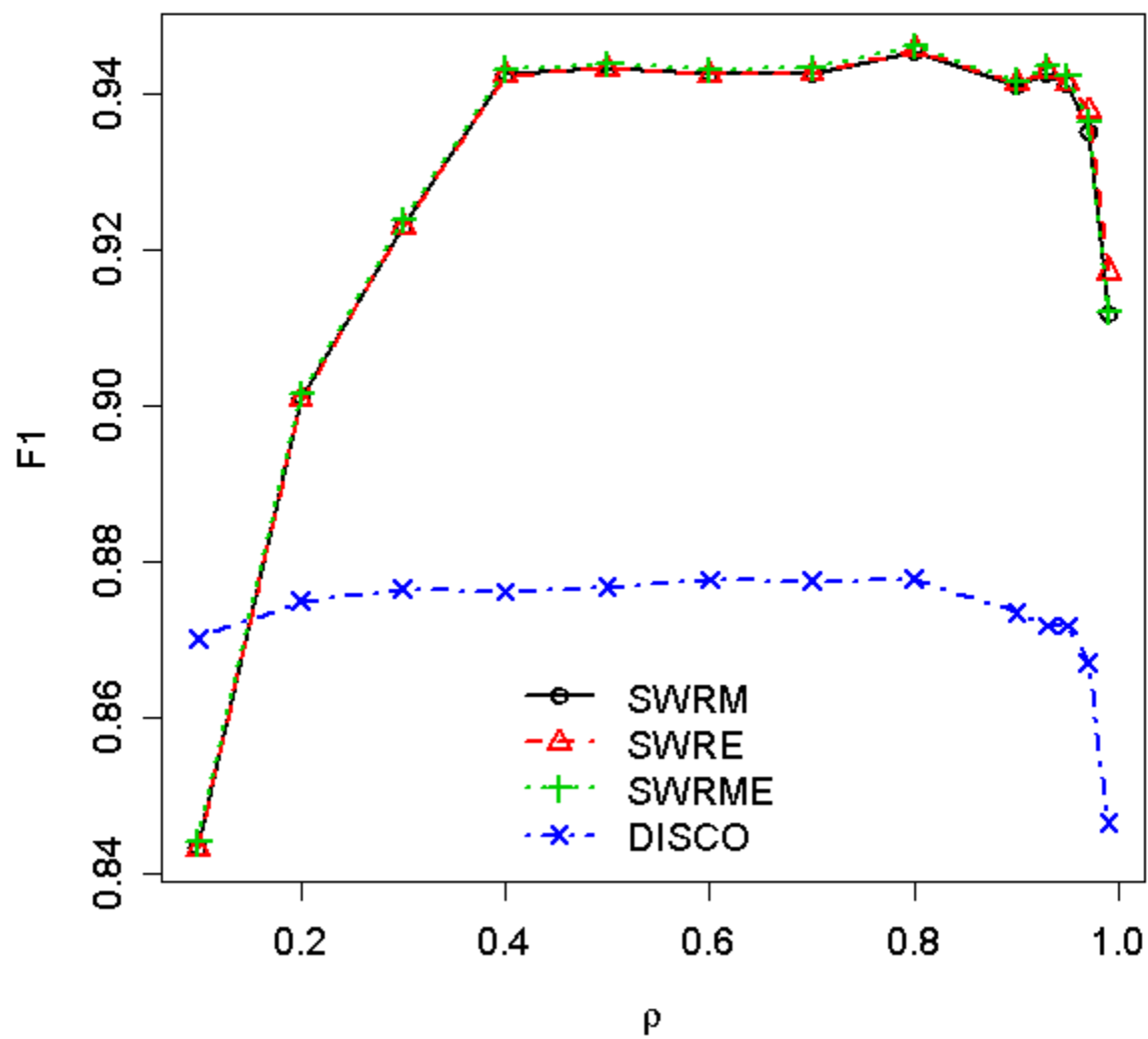
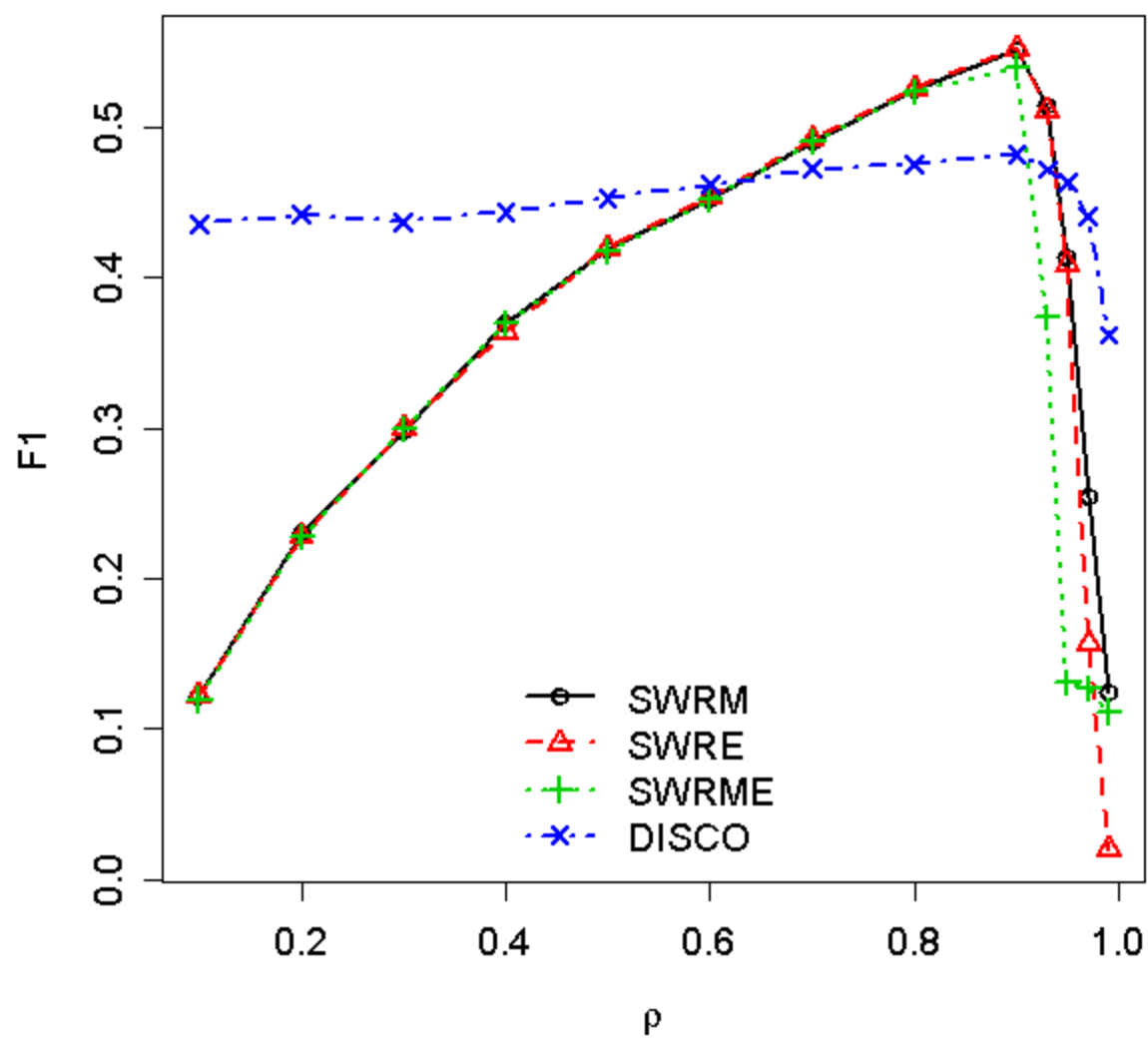


Figure S2. The F1 scores of pairwise alignments for homogeneous and heterogeneous chromatograms. (a) The homogeneous peak alignment of compound standards. (b) The homogeneous peak alignment of a spiked-in sample. (c) The heterogeneous peak alignment of compound standards.

(a)



(b)



(c)

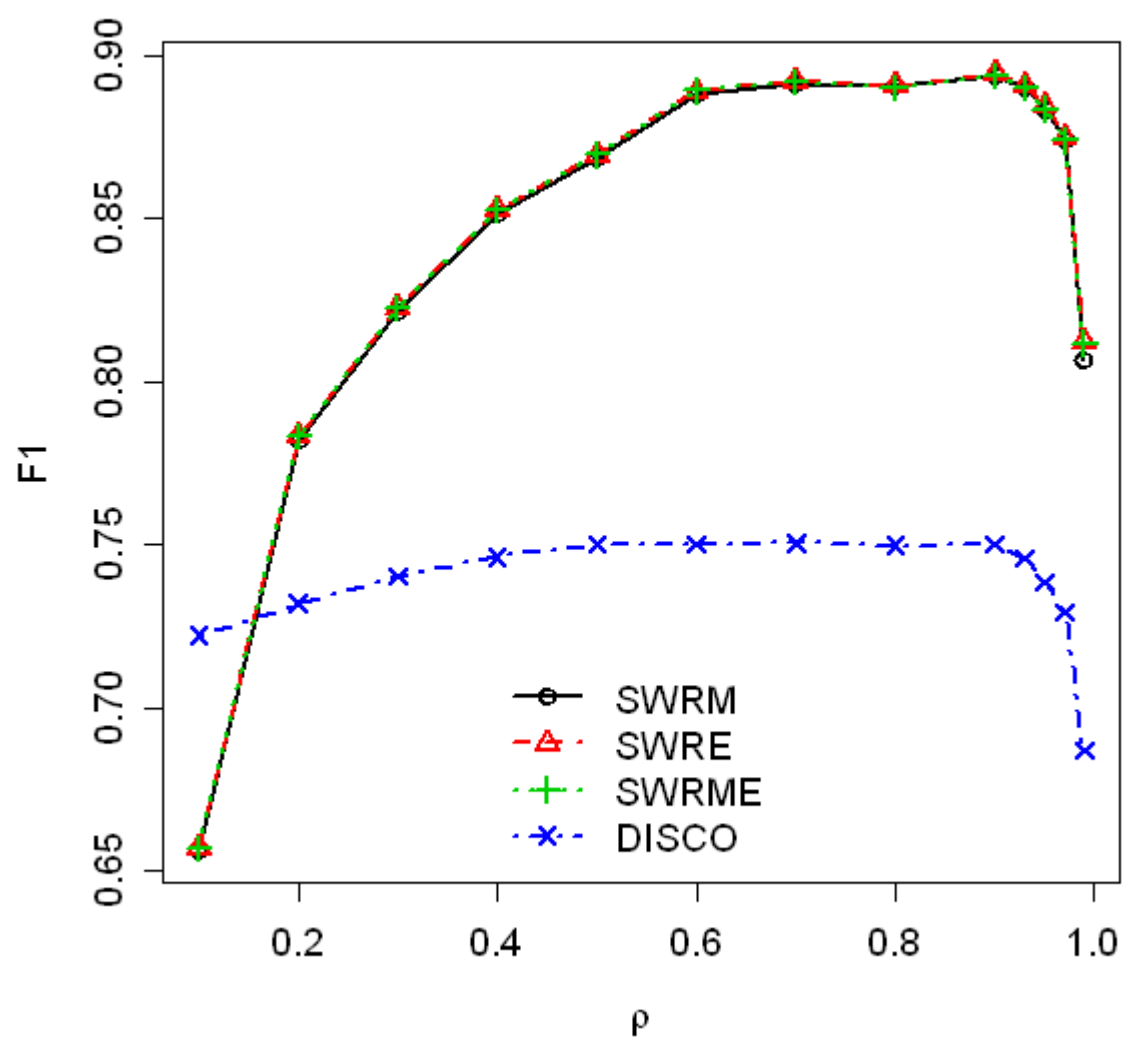


Figure S3. The pairwise alignments for homogeneous and heterogeneous chromatograms of compound standards data using SWRM. (a) The homogeneous peak alignment between S1 (5 °C/min) and S10 (5 °C/min). (b) The heterogeneous peak alignment between S1 (5 °C/min) and S11 (7 °C/min). (c) The heterogeneous peak alignment between S1 (5 °C/min) and S13 (10 °C/min). (d) The heterogeneous peak alignment between S11 (7 °C/min) and S13 (10 °C/min).

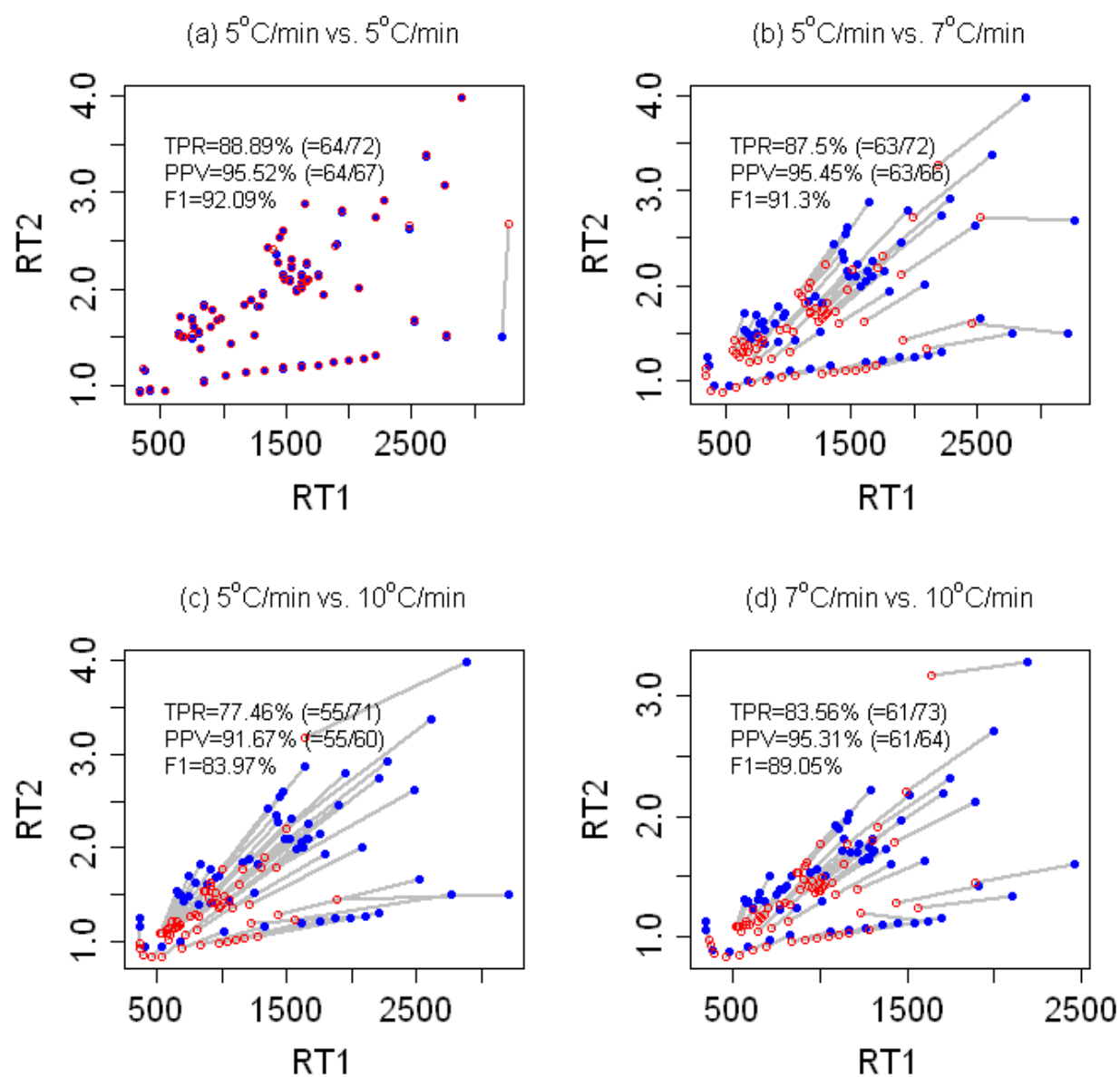


Figure S4. The pairwise alignments for homogeneous and heterogeneous chromatograms of compound standards data using SWRE. (a) The homogeneous peak alignment between S1 (5 °C/min) and S10 (5 °C/min). (b) The heterogeneous peak alignment between S1 (5 °C/min) and S11 (7 °C/min). (c) The heterogeneous peak alignment between S1 (5 °C/min) and S13 (10 °C/min). (d) The heterogeneous peak alignment between S11 (7 °C/min) and S13 (10 °C/min).

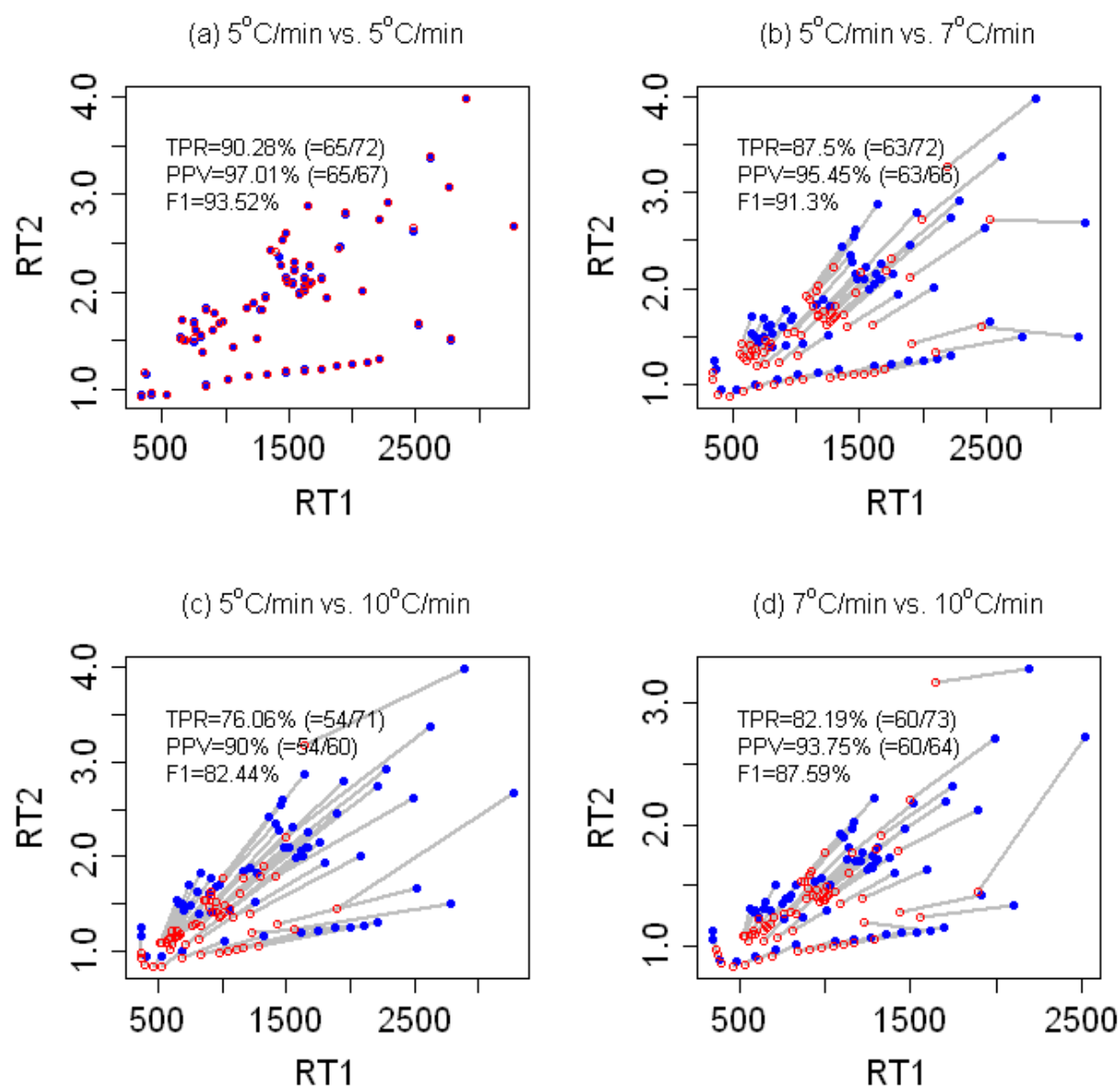


Figure S5. The pairwise alignments for homogeneous and heterogeneous chromatograms of compound standards data using SWRME. (a) The homogeneous peak alignment between S1 (5 °C/min) and S10 (5 °C/min). (b) The heterogeneous peak alignment between S1 (5 °C/min) and S11 (7 °C/min). (c) The heterogeneous peak alignment between S1 (5 °C/min) and S13 (10 °C/min). (d) The heterogeneous peak alignment between S11 (7 °C/min) and S13 (10 °C/min).

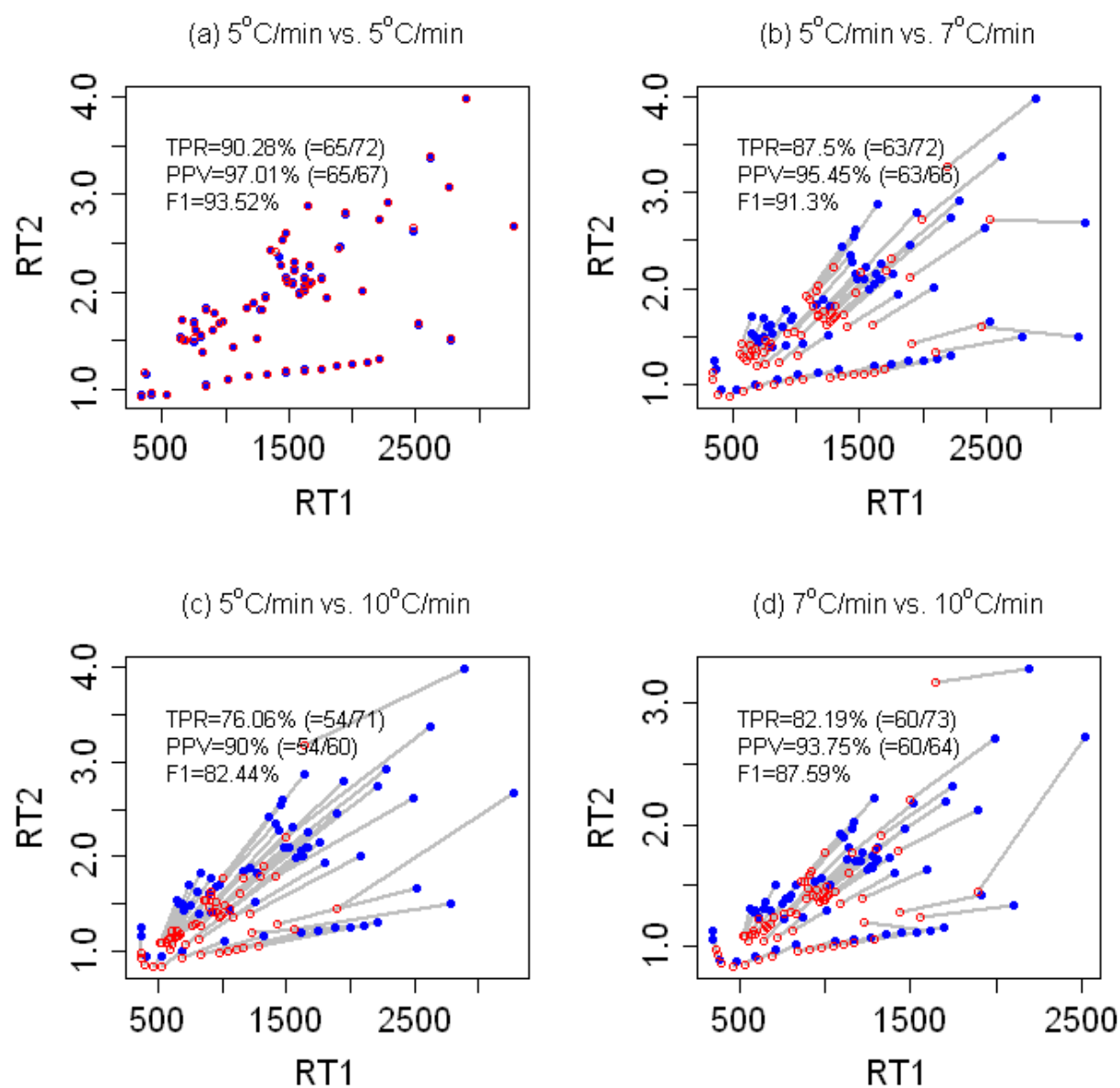


Figure S6. The pairwise alignments for homogeneous and heterogeneous chromatograms of compound standards data using DISCO. (a) The homogeneous peak alignment between S1 (5 °C/min) and S10 (5 °C/min). (b) The heterogeneous peak alignment between S1 (5 °C/min) and S11 (7 °C/min). (c) The heterogeneous peak alignment between S1 (5 °C/min) and S13 (10 °C/min). (d) The heterogeneous peak alignment between S11 (7 °C/min) and S13 (10 °C/min).

