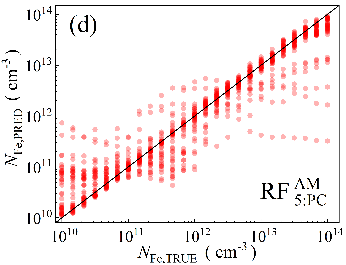
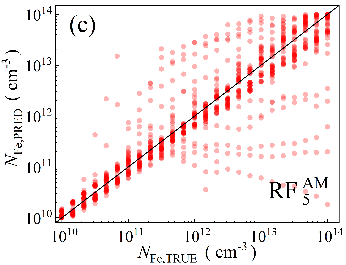
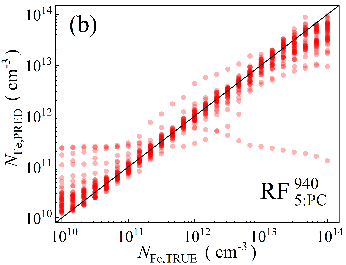
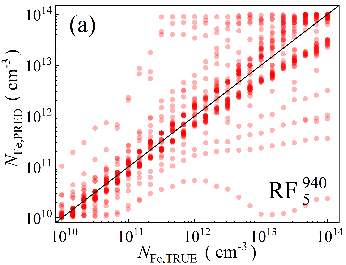
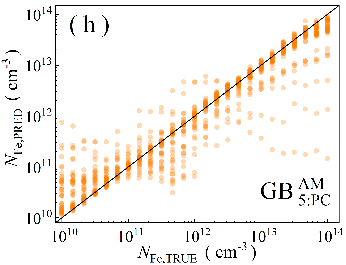
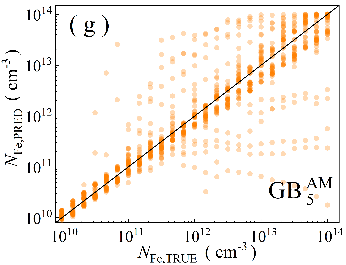
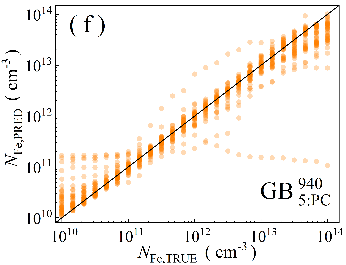
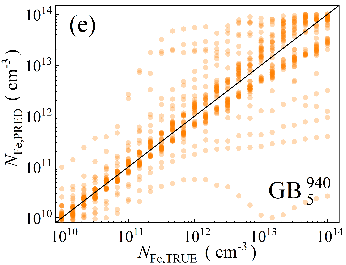
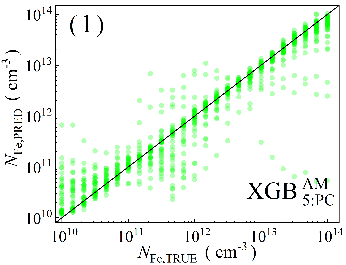
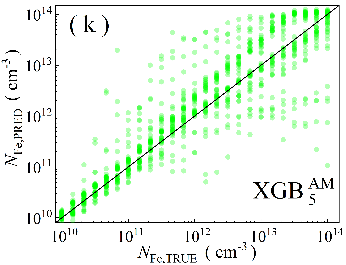
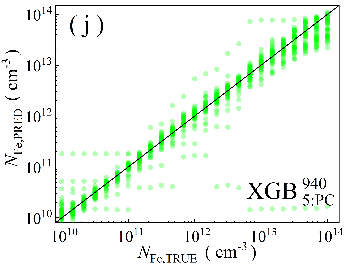
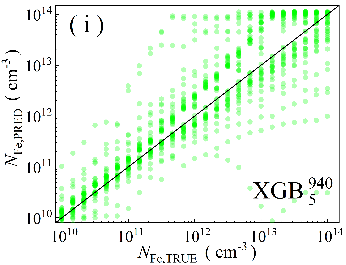
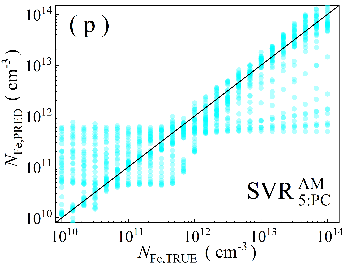
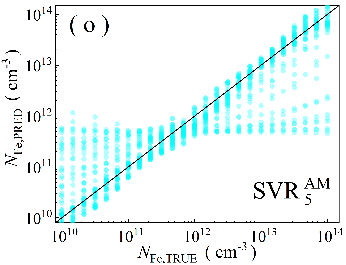
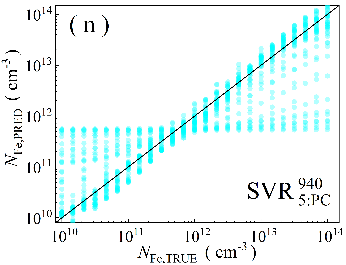
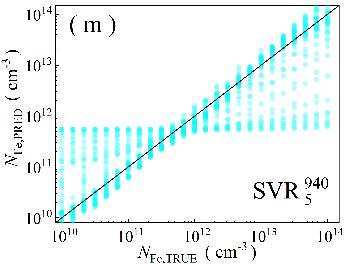


Fig.S12. Scatter plots of the iron concentrations between the reference values and ML predicted values for *N*B-altered test phase in the case of 4D features. ML algorithms: RF (a-d), GB (e-h), XGB (i-l), SVR (m-p), DNN (q-t). The data are obtained for monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 (c, d, g, h, k, l, o, p, s, t illuminations. PCA was used for the panels b, d, f, h, j, l, n, p, r, and t. The black lines are the identify lines servings as the references.









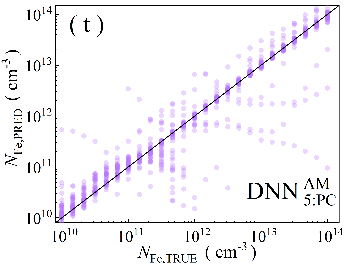
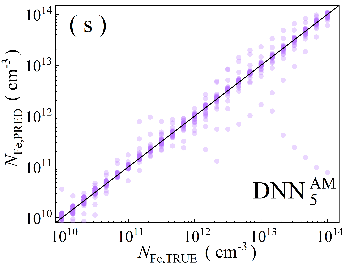
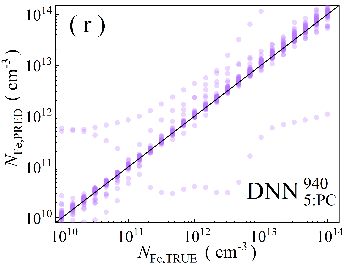
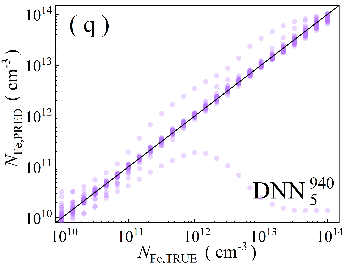
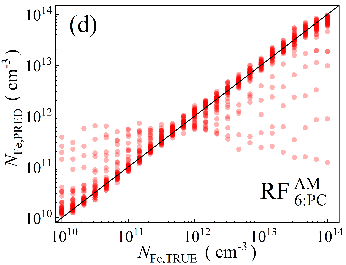
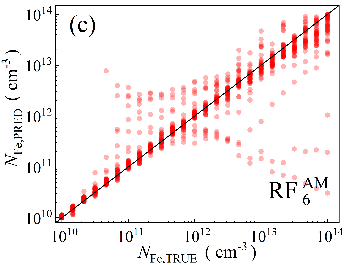
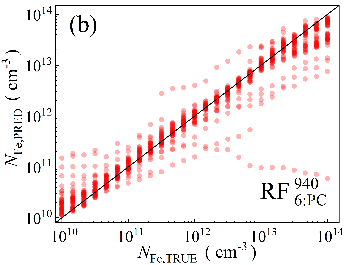
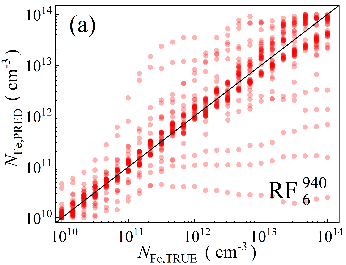
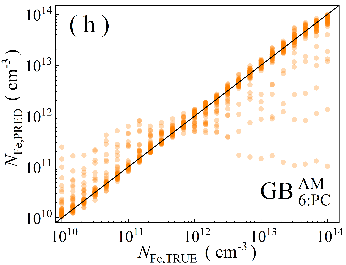
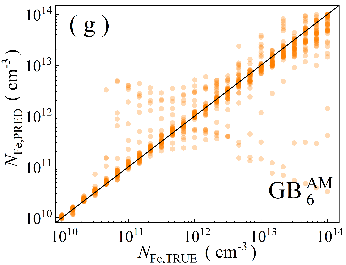
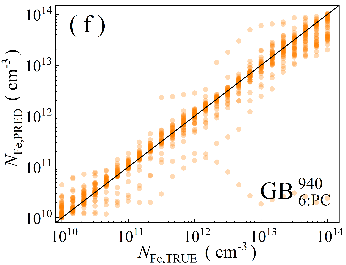
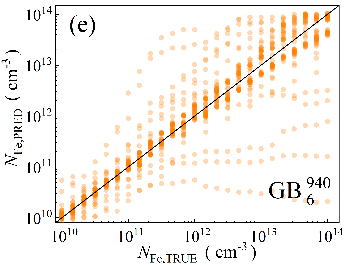
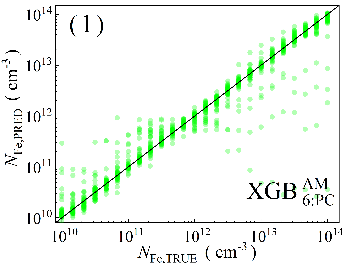
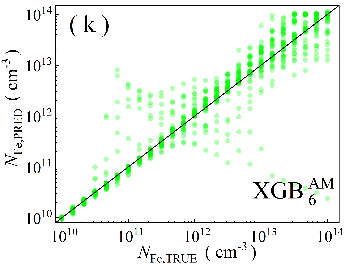
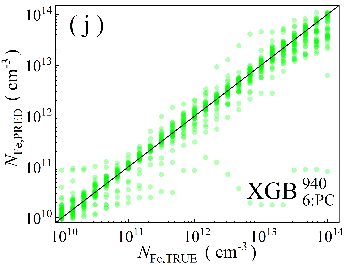
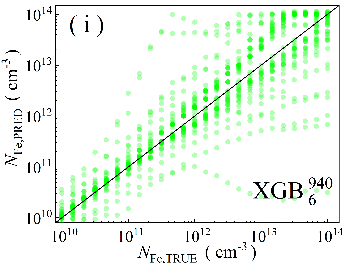
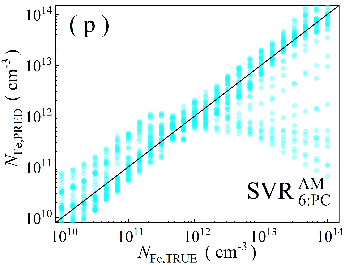
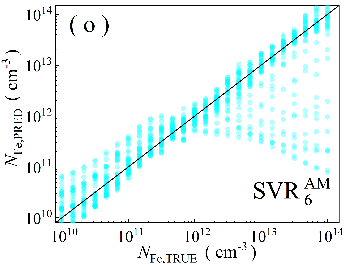
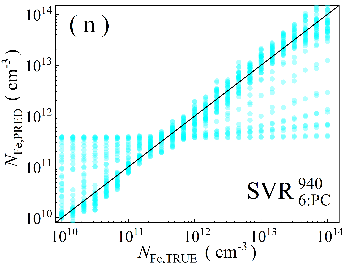
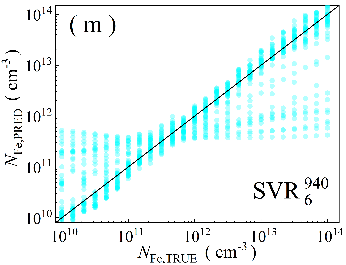


Fig.S13. Scatter plots of the iron concentrations between the reference values and ML predicted values for *N*B-altered test phase in the case of 5D features. ML algorithms: RF (a-d), GB (e-h), XGB (i-l), SVR (m-p), DNN (q-t). The data are obtained for monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 (c, d, g, h, k, l, o, p, s, t illuminations. PCA was used for the panels b, d, f, h, j, l, n, p, r, and t. The black lines are the identify lines servings as the references.









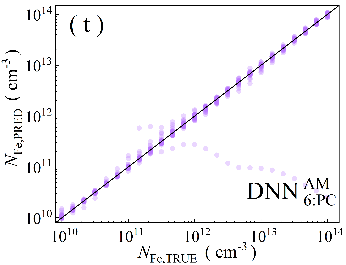
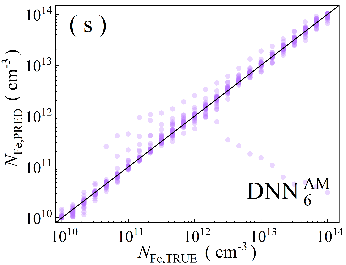
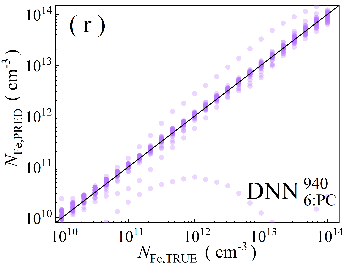
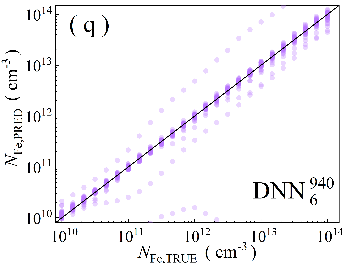
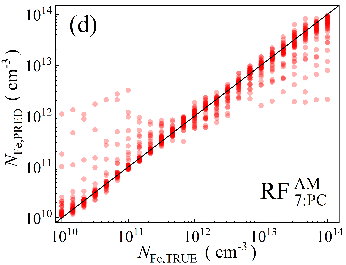
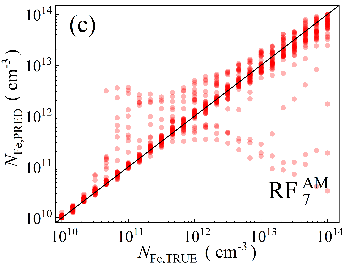
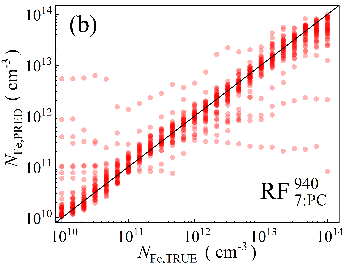
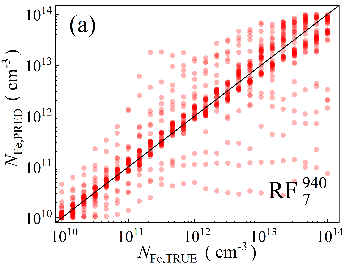
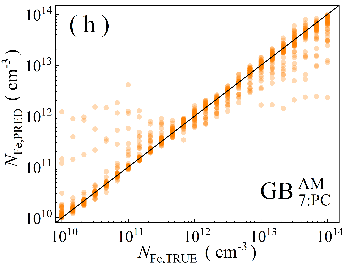
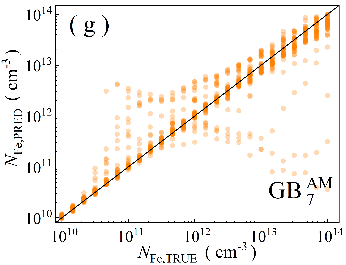
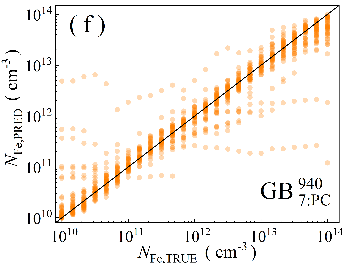
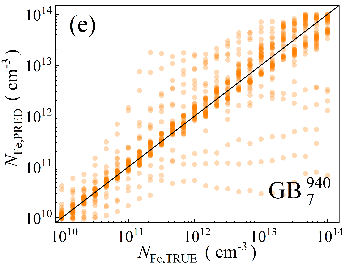
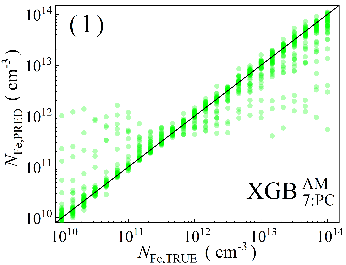
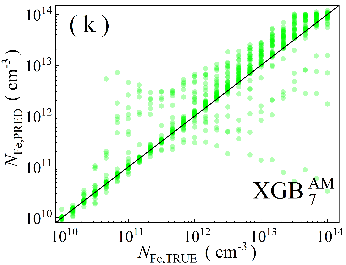
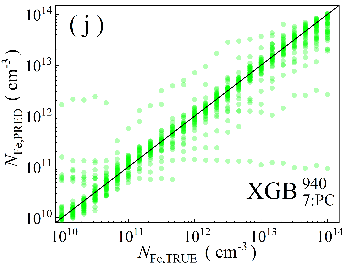
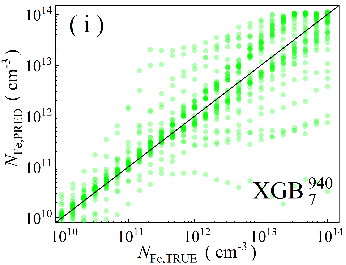
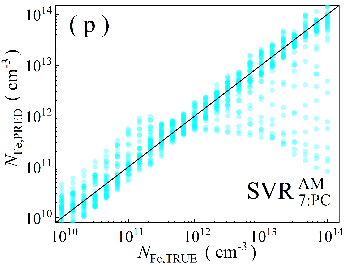
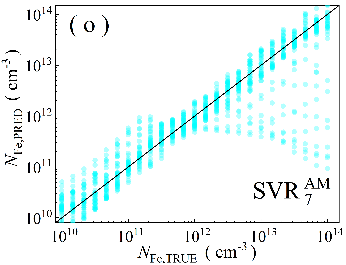
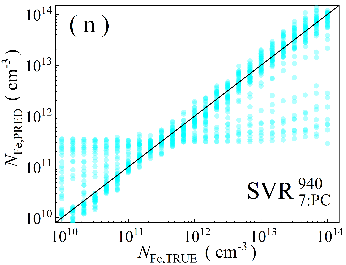
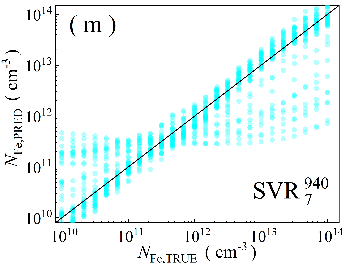


Fig.S14. Scatter plots of the iron concentrations between the reference values and ML predicted values for *N*B-altered test phase in the case of 6D features. ML algorithms: RF (a-d), GB (e-h), XGB (i-l), SVR (m-p), DNN (q-t). The data are obtained for monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 (c, d, g, h, k, l, o, p, s, t illuminations. PCA was used for the panels b, d, f, h, j, l, n, p, r, and t. The black lines are the identify lines servings as the references.









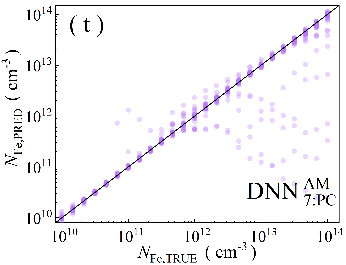
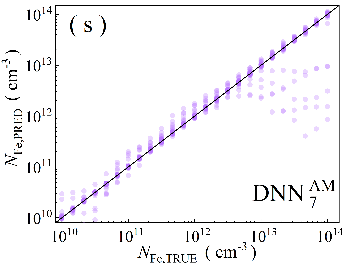
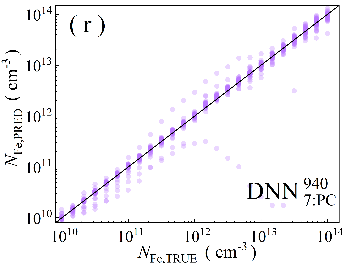
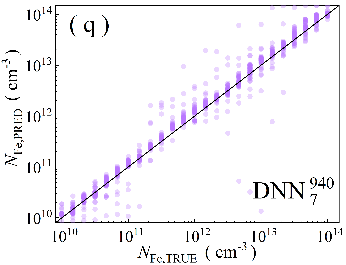
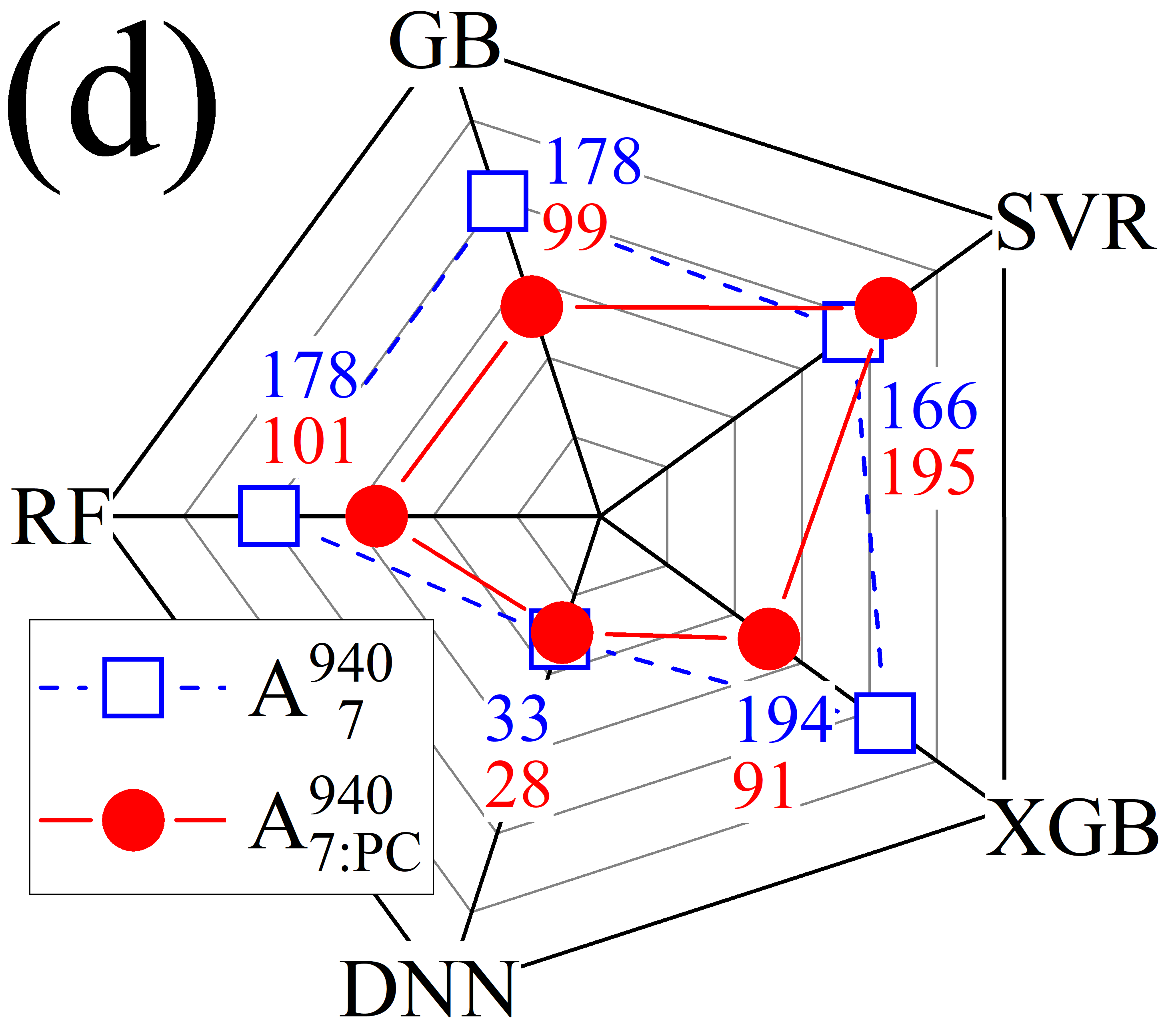
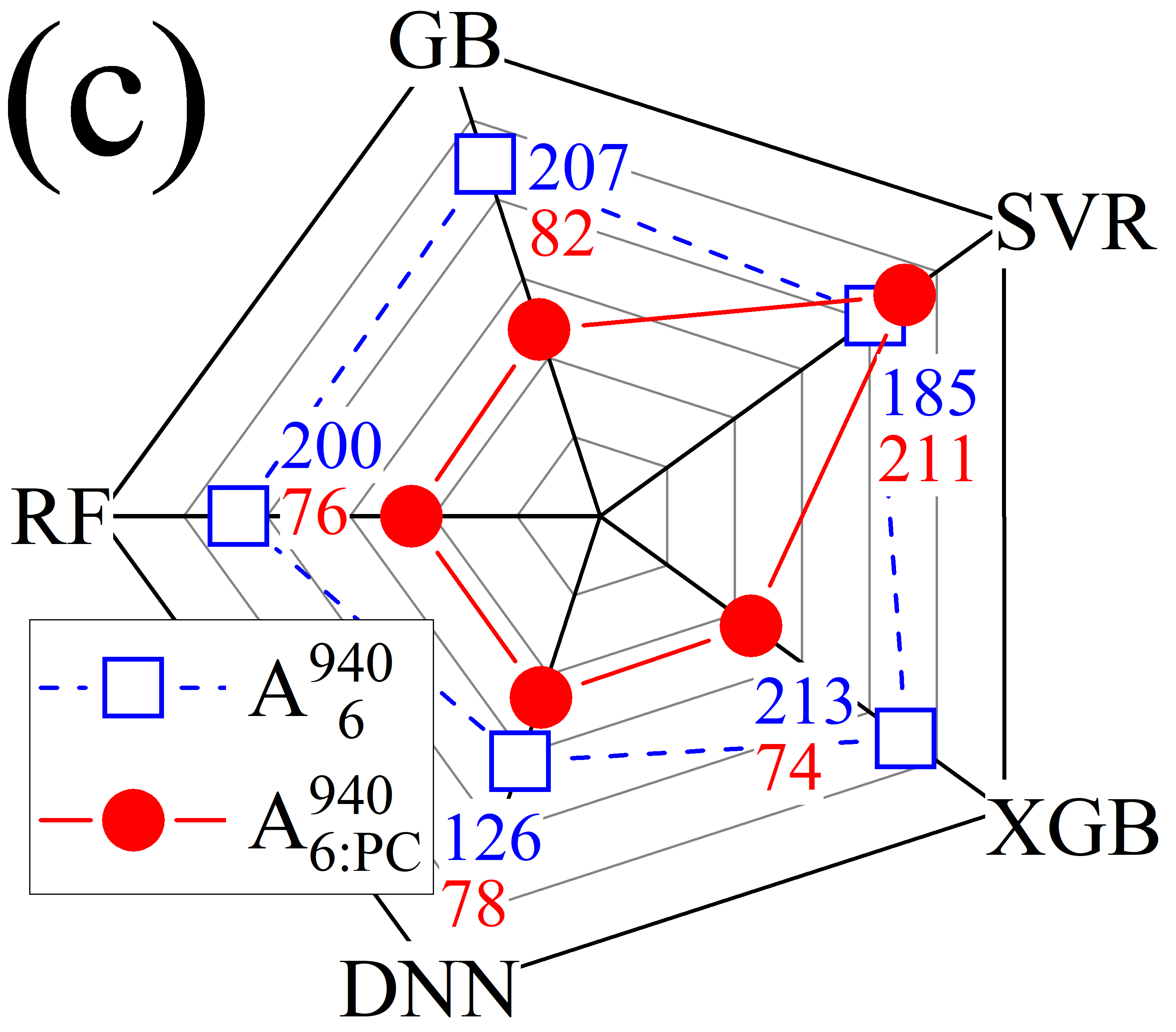
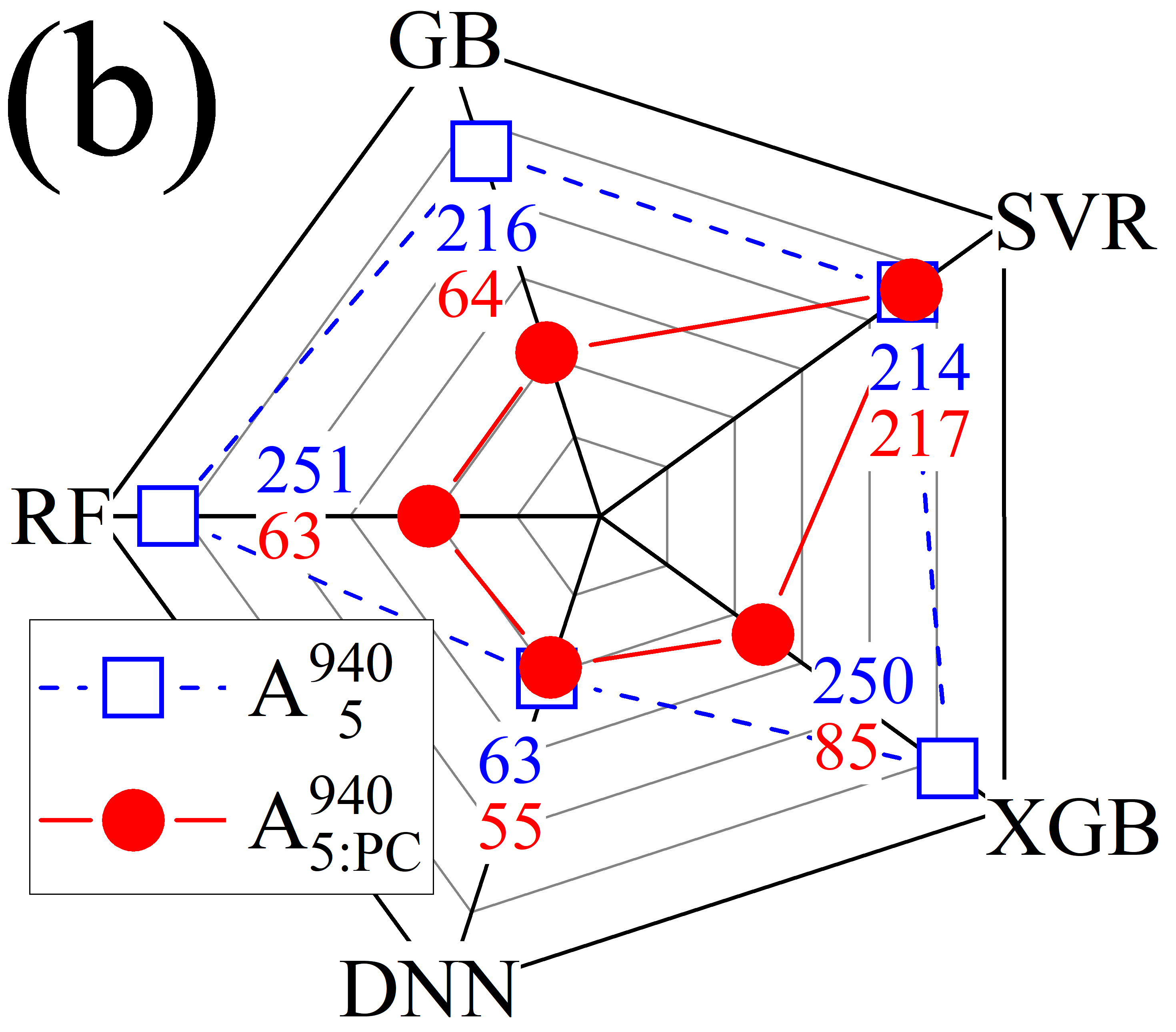
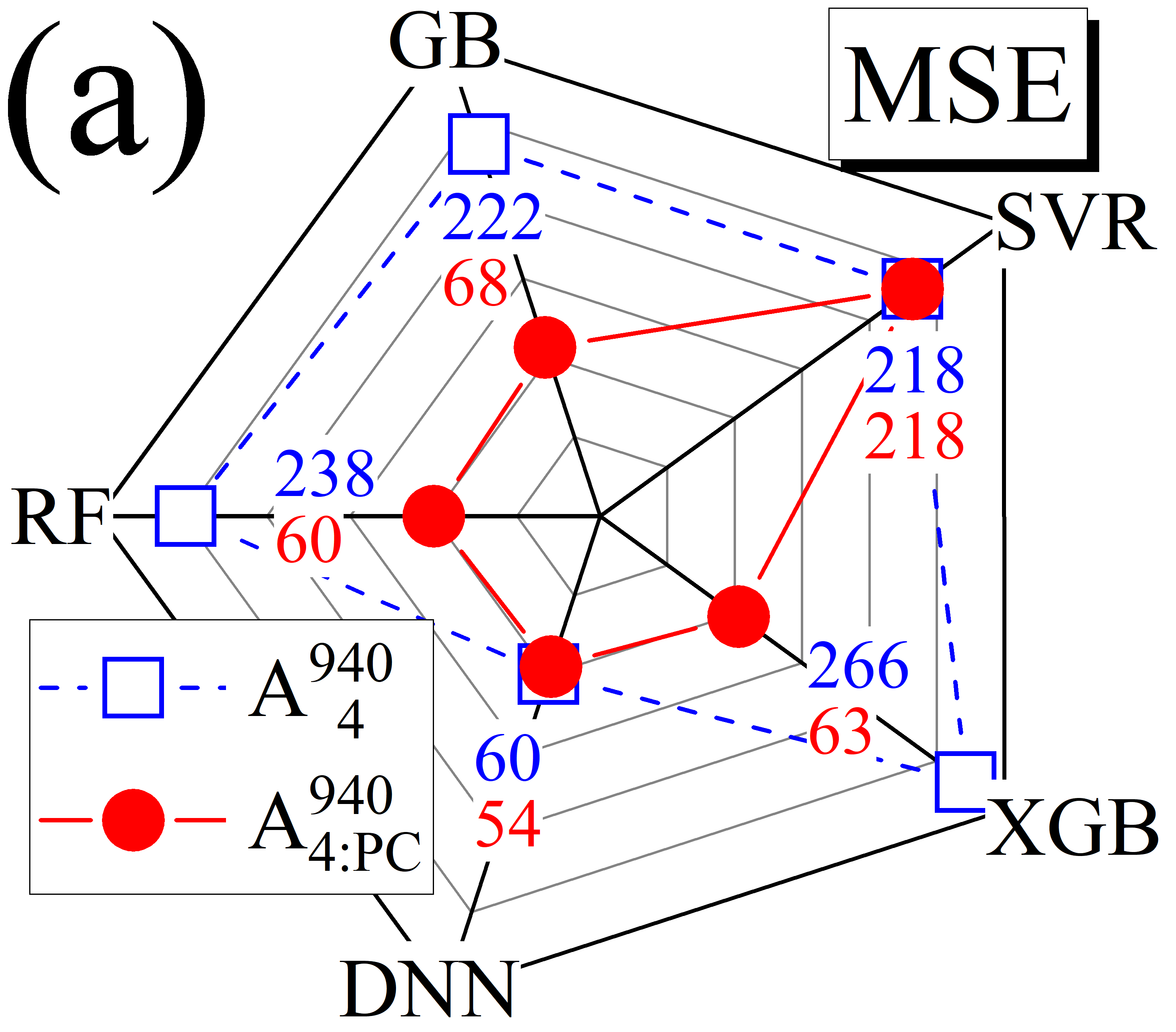
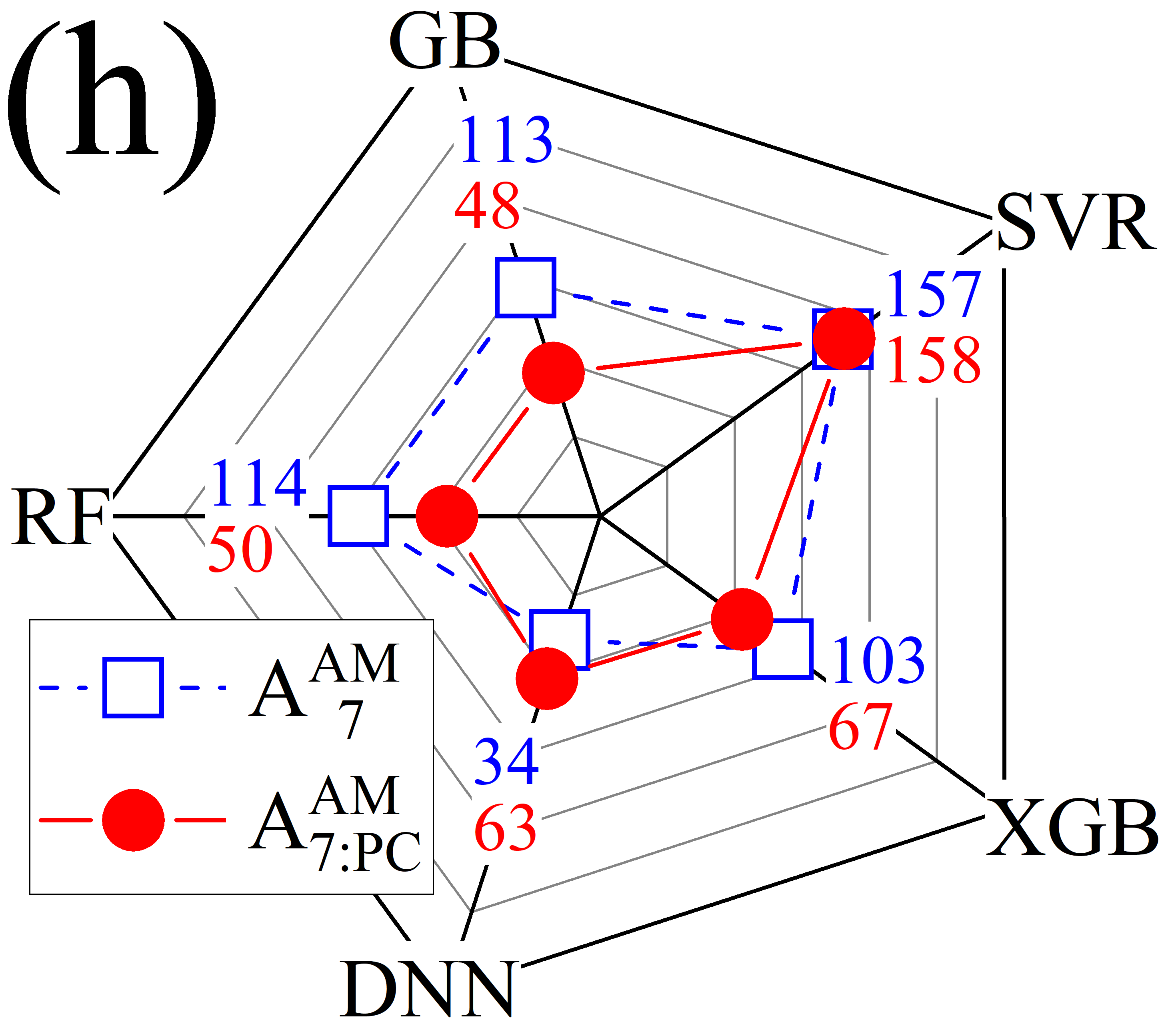
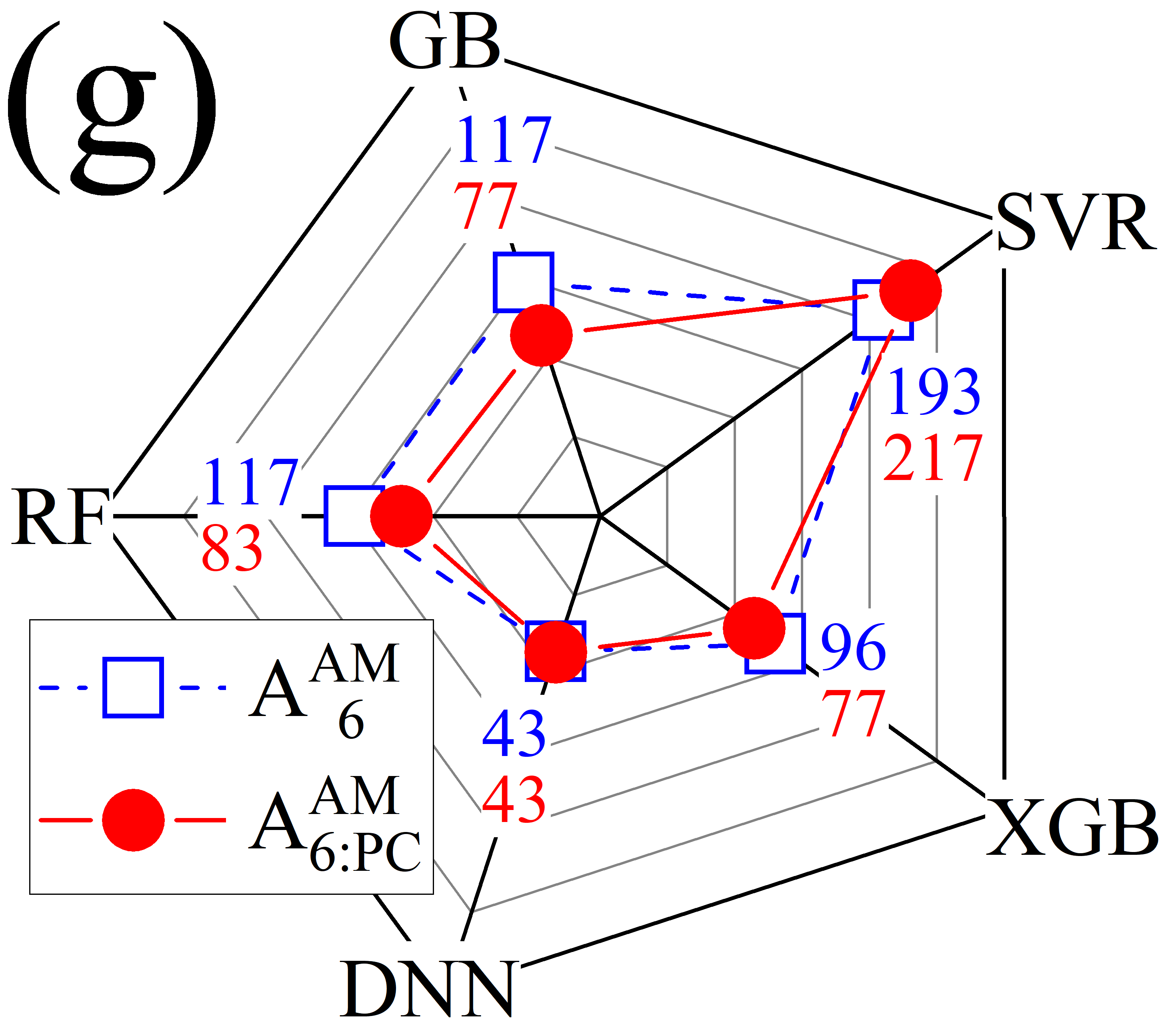
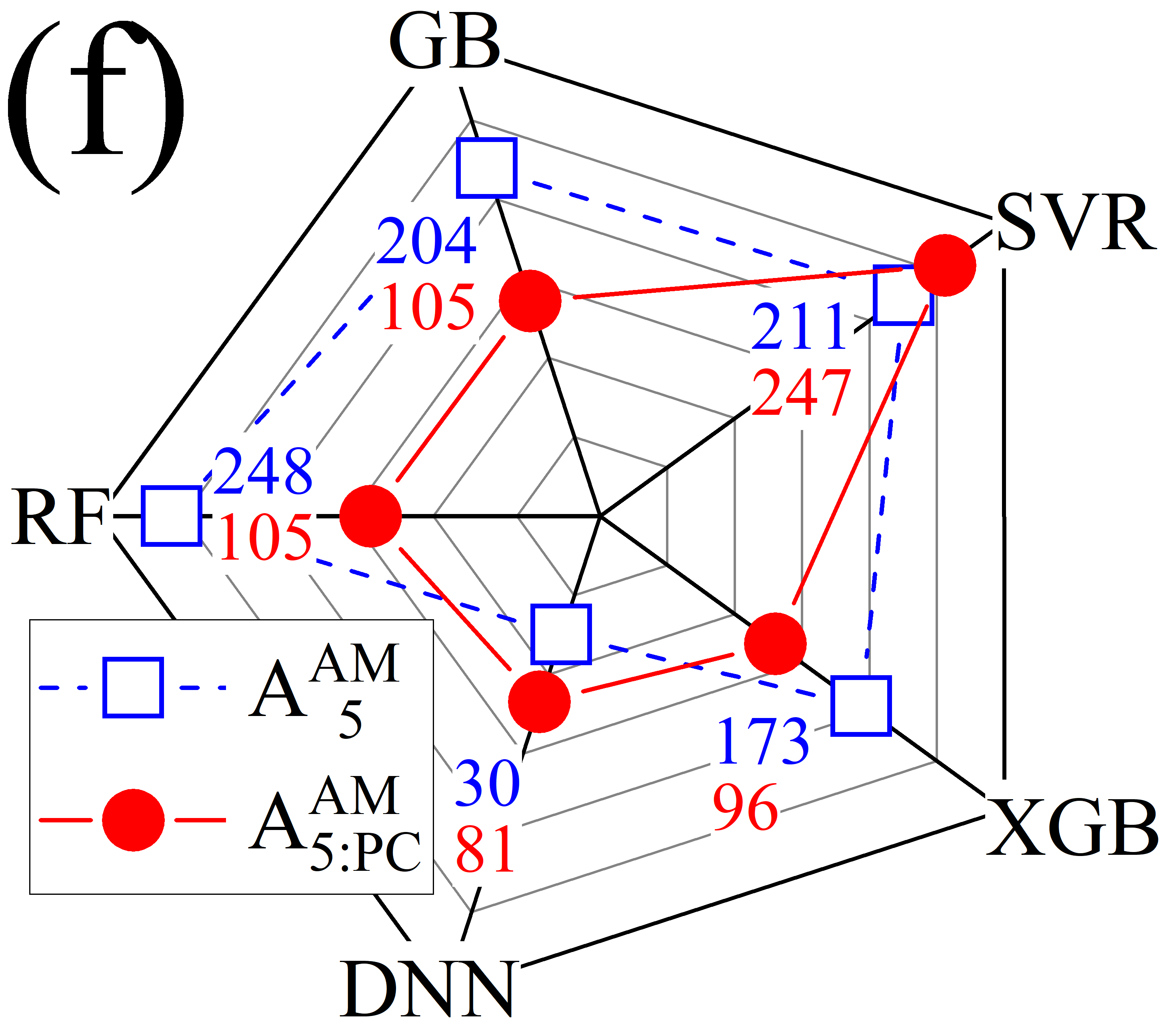
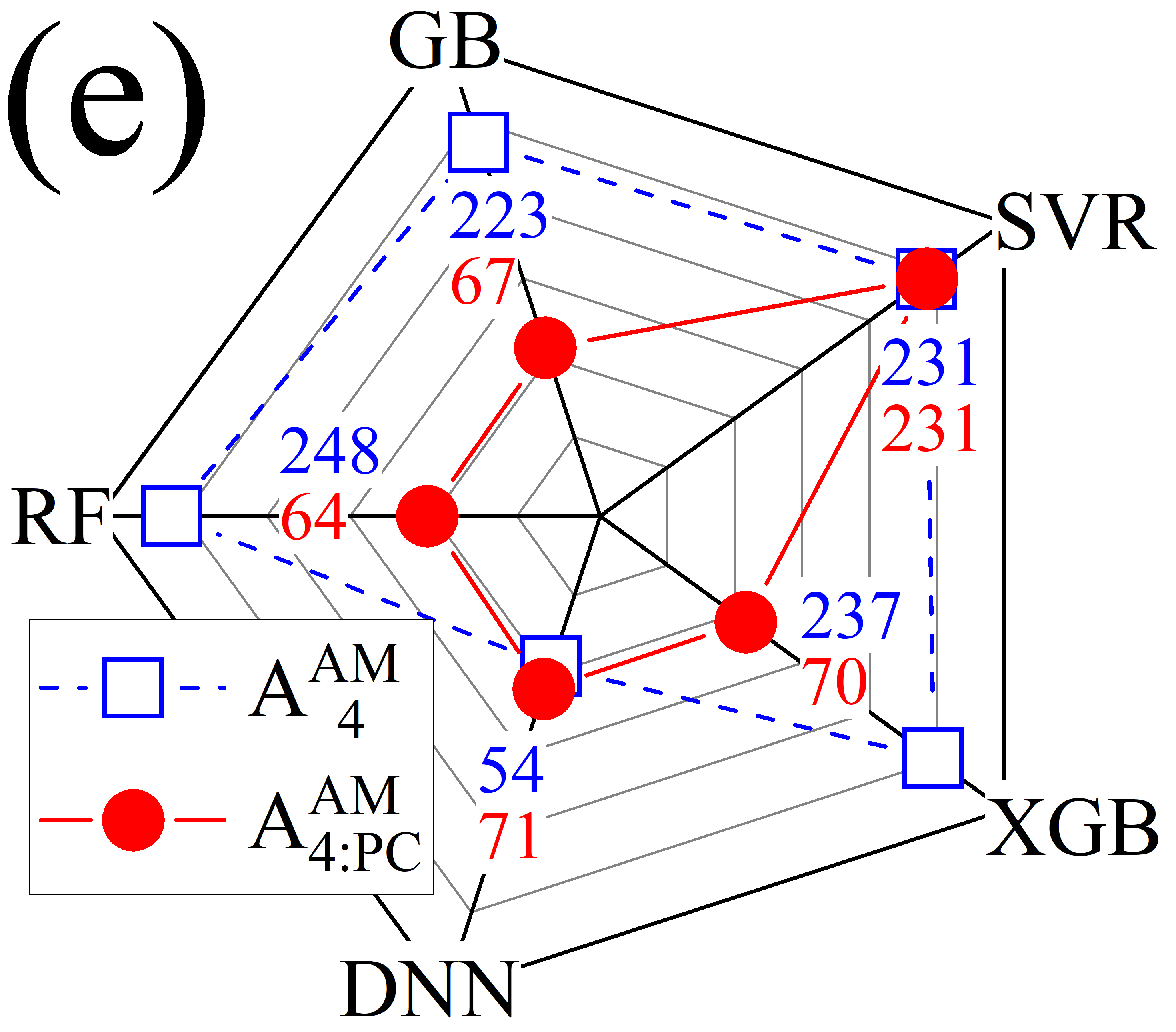
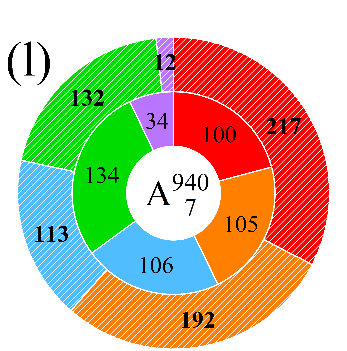
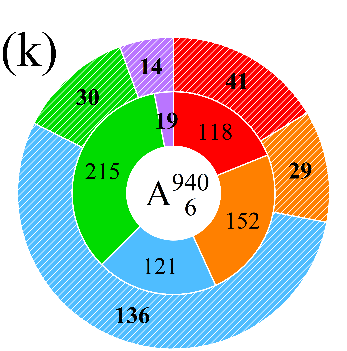
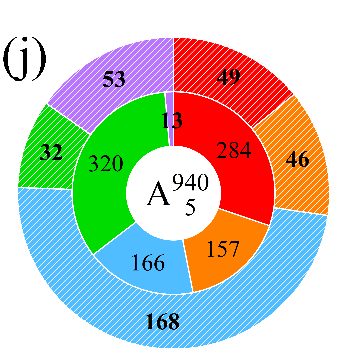
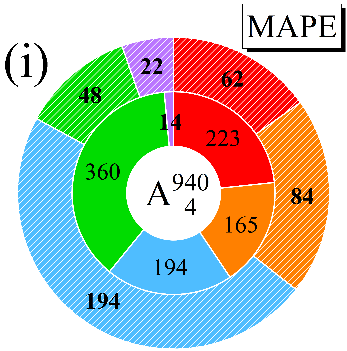
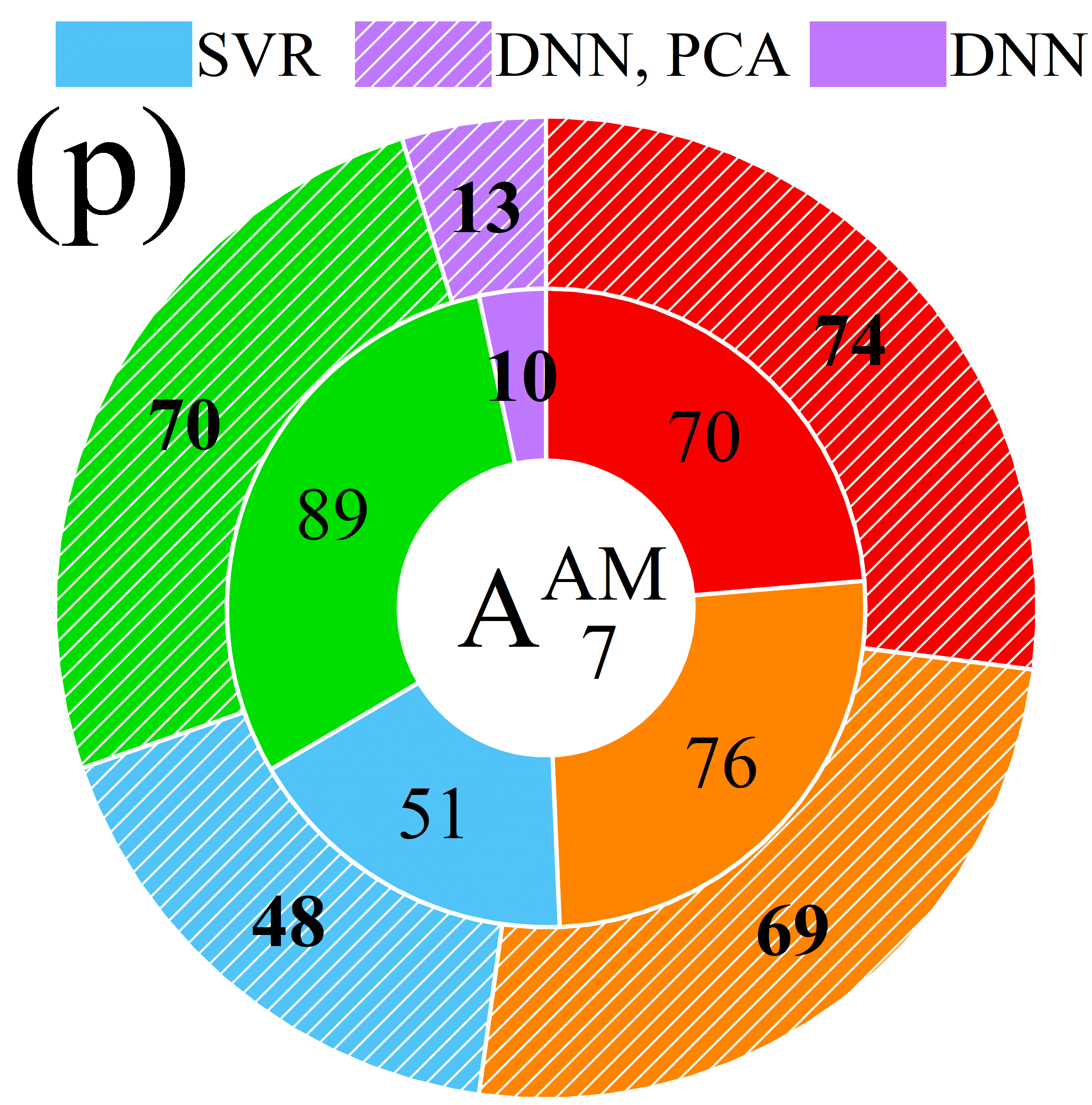
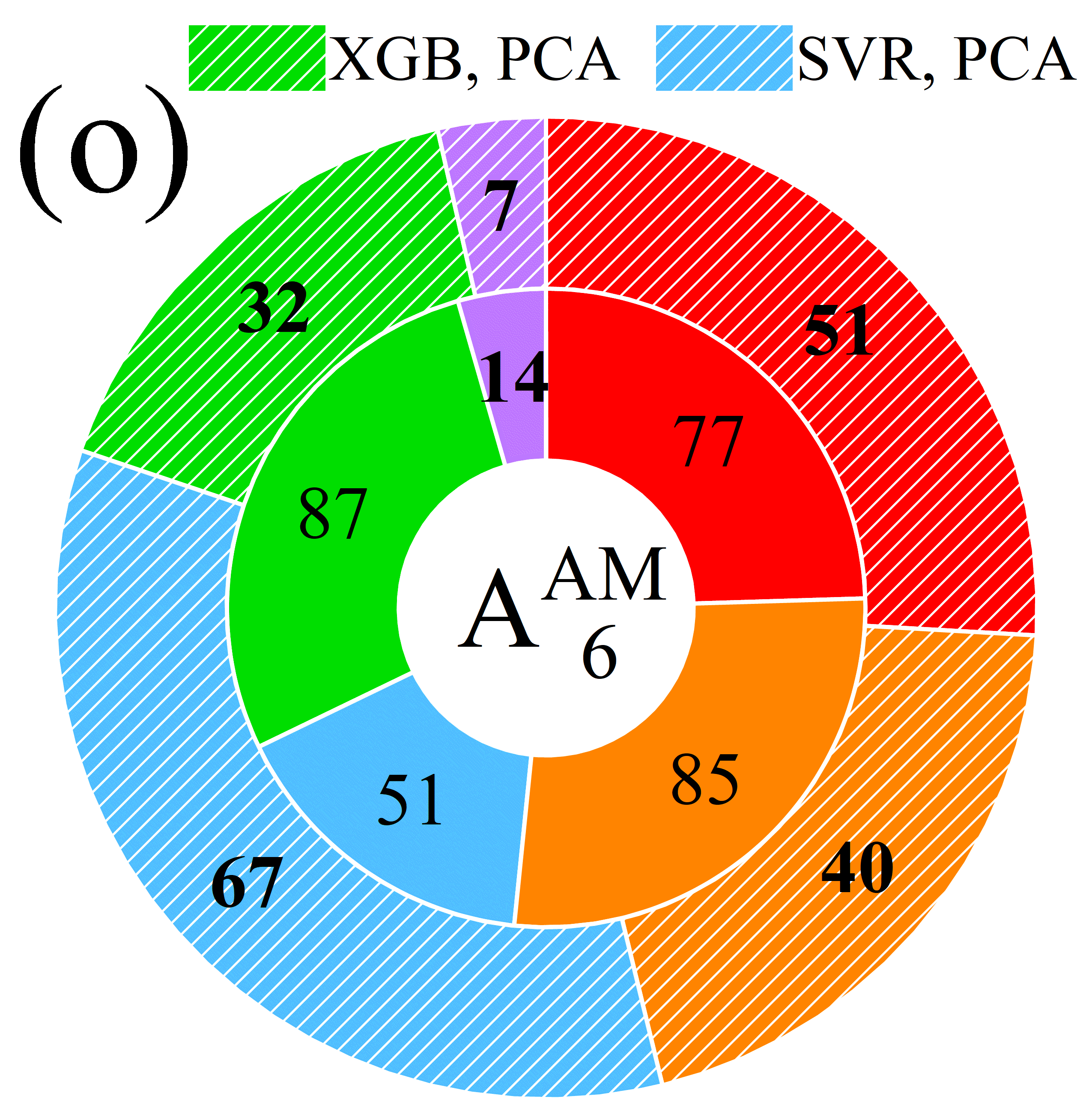
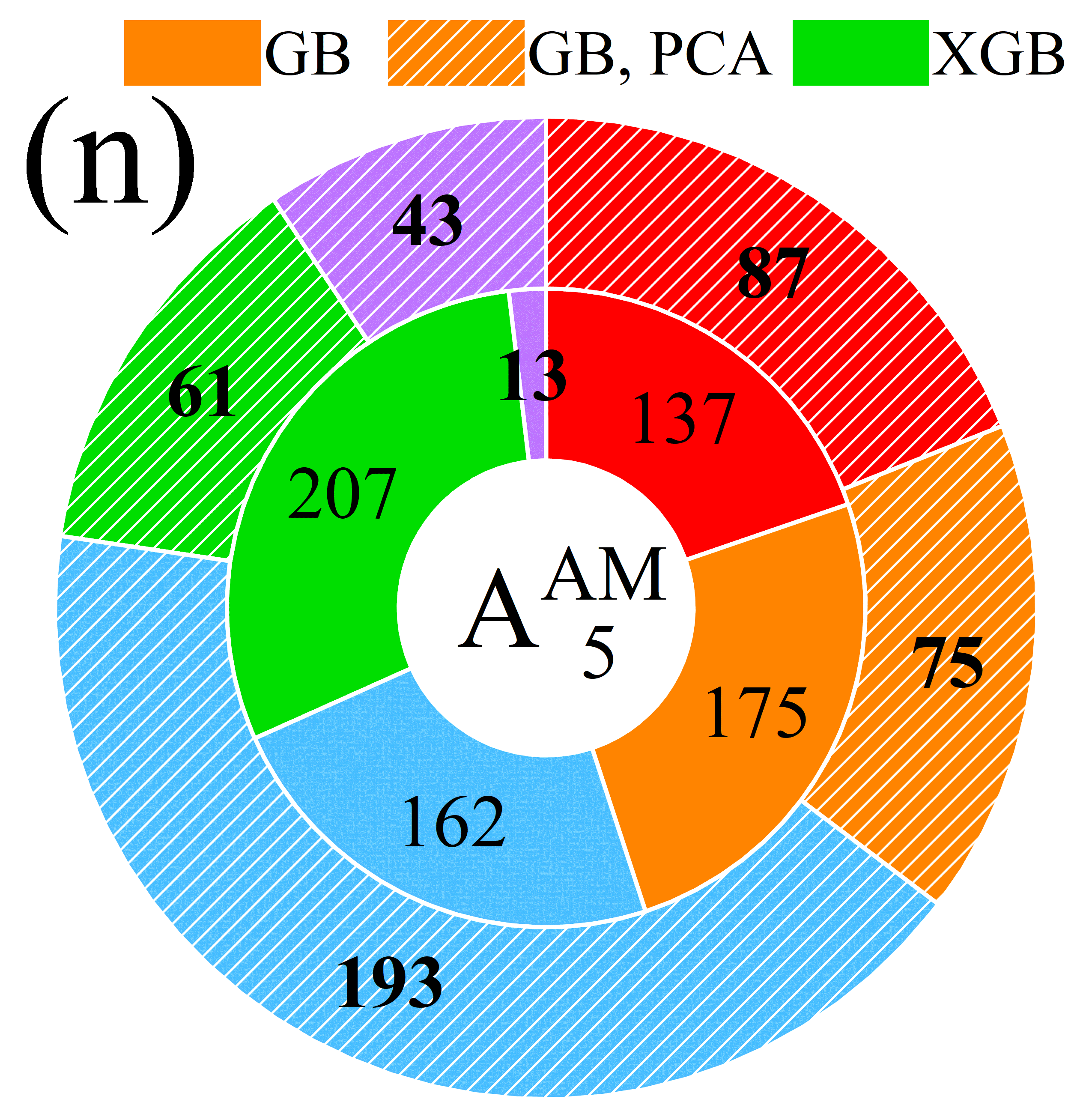
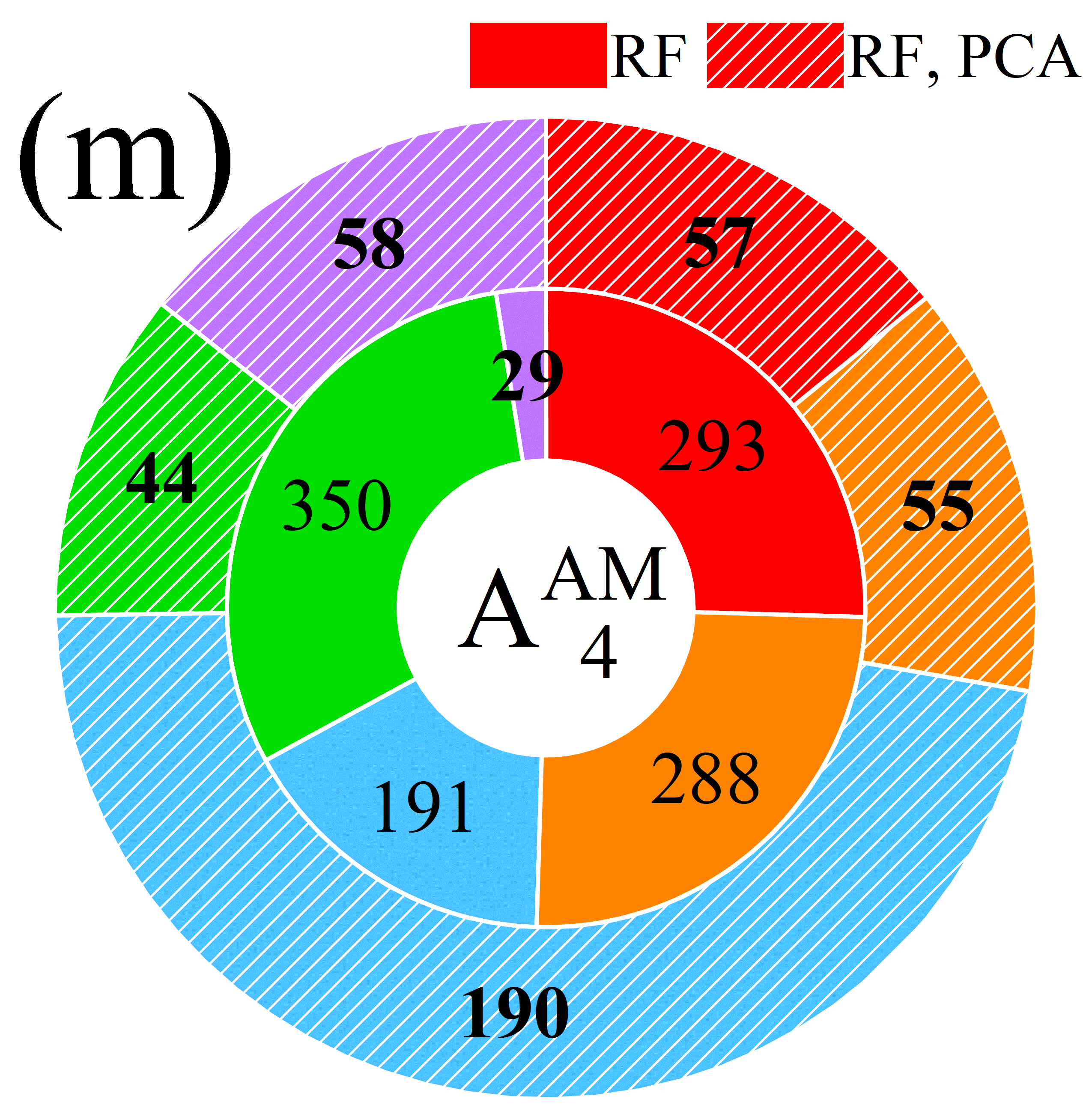


Fig.S15. Scatter plots of the iron concentrations between the reference values and ML predicted values for *N*B-altered test phase in the case of 7D features. ML algorithms: RF (a-d), GB (e-h), XGB (i-l), SVR (m-p), DNN (q-t). The data are obtained for monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 (c, d, g, h, k, l, o, p, s, t illuminations. PCA was used for the panels b, d, f, h, j, l, n, p, r, and t. The black lines are the identify lines servings as the references.









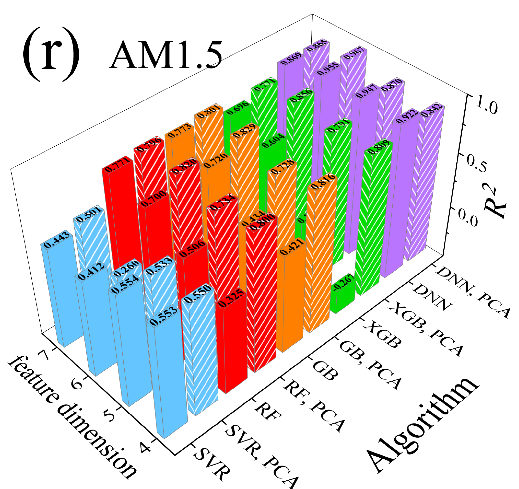
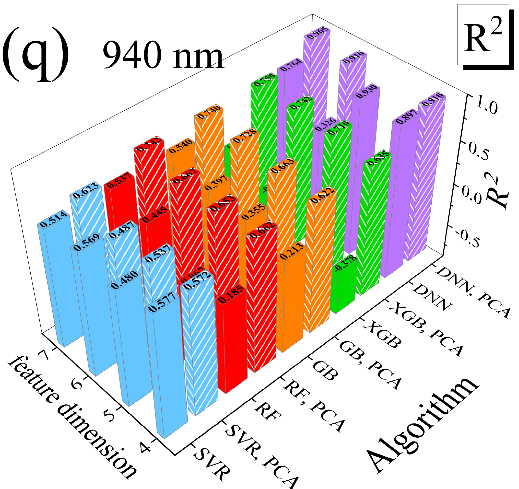


Fig.S24 MSE (a-h), MAPE (i-p), and R2 (q, r) scores obtained by various models, feature combinations, illumination conditions for *N*B-altered test dataset. Illumination: 940 nm (a-d, i-l, q), AM (e-h, m-p, r). Feature dimension: 4 (a, e, i, m), 5 (b, f, g, n), 6 (c, g, k, o), and 7 (d, h, l, p). Results obtained with (circles in (a-h) panels, shaded areas in (i-r) panels) and without (squares in (f-h) and solid areas in (i-r)) PCA applying. The numbers in panels (a–h) represent MSE values multiplied by 1000, while the numbers in panels (i–p) indicate MAPE values in percentage..