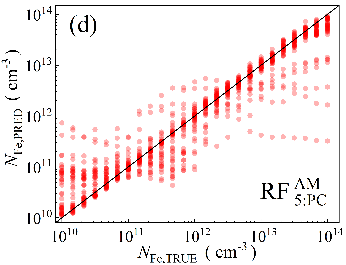
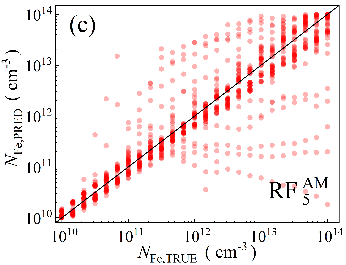
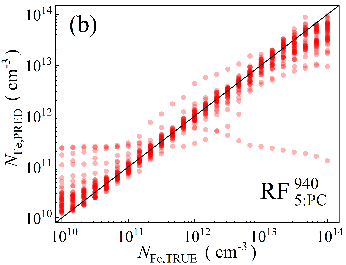
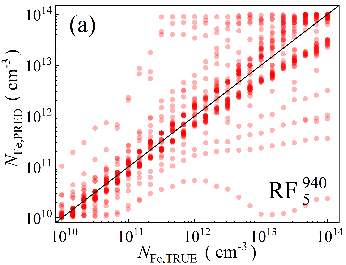
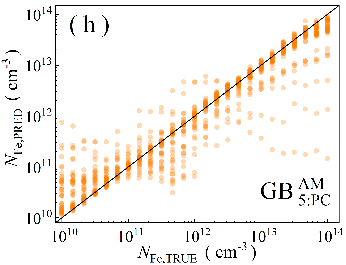
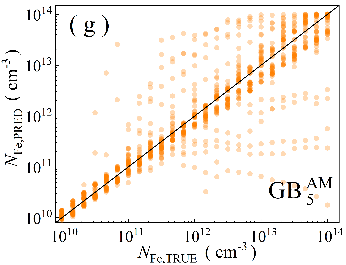
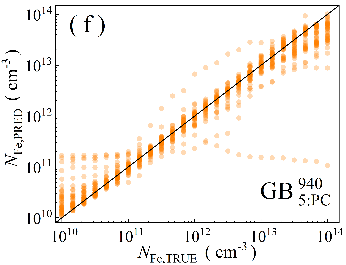
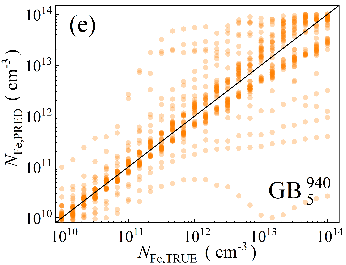
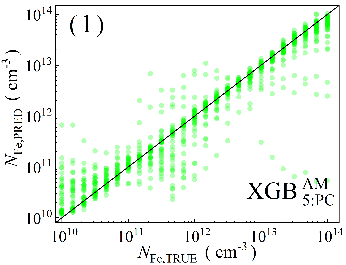
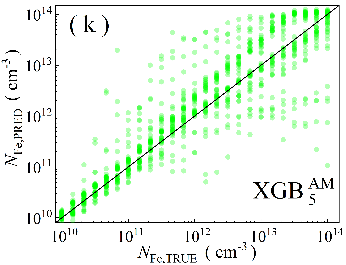
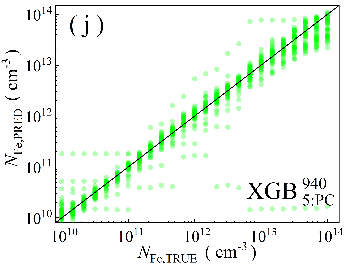
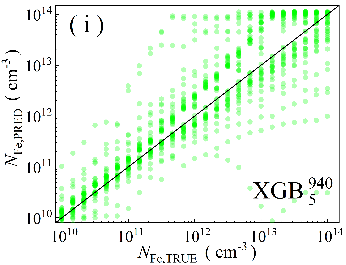
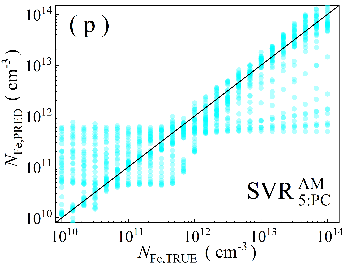
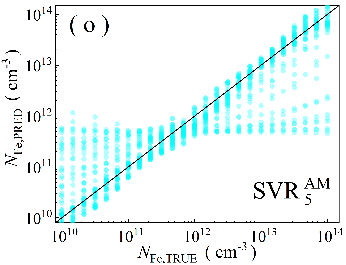
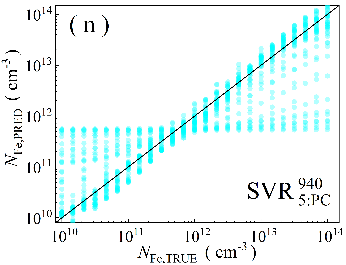
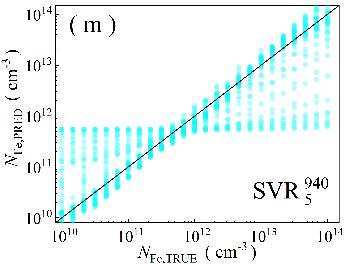


Fig.S12. Scatter plots of the iron concentrations between the reference values and ML predicted values for test phase B-altered in the case of 4D features. ML algorithms: RF (a-d), GB (e-h), XGB (i-l), SVR (m-p), DNN (q-t). The data are obtained for monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 (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.









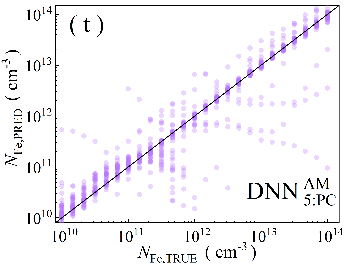
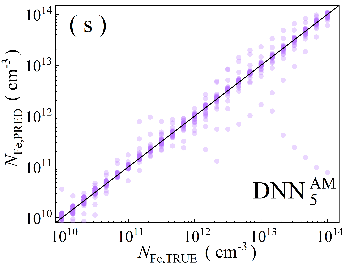
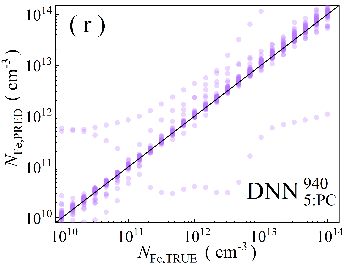
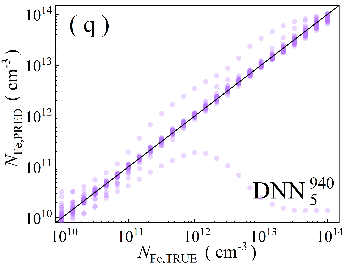
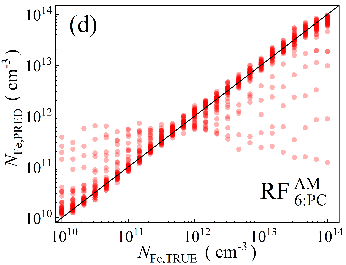
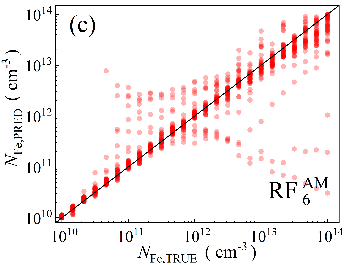
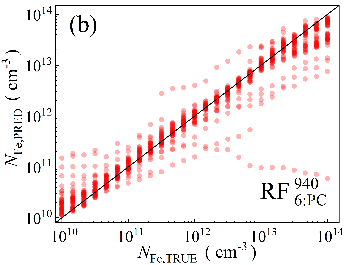
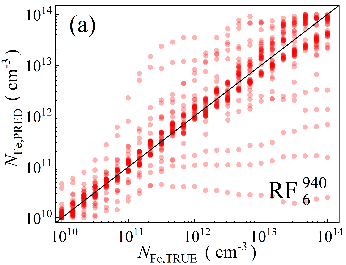
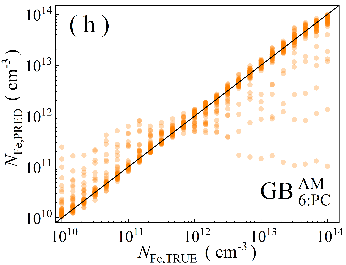
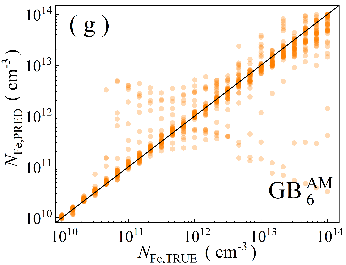
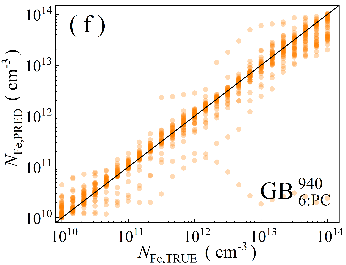
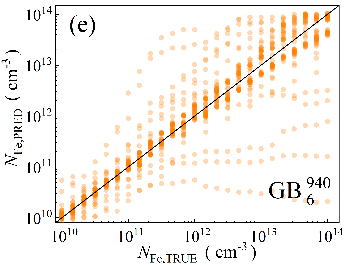
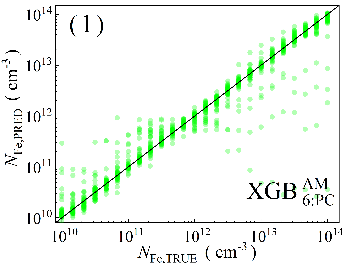
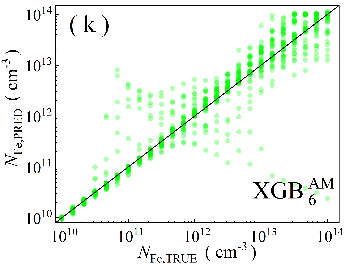
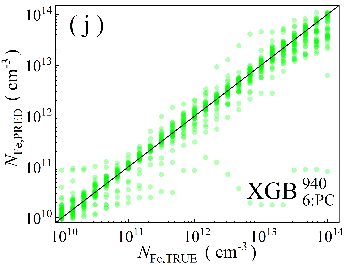
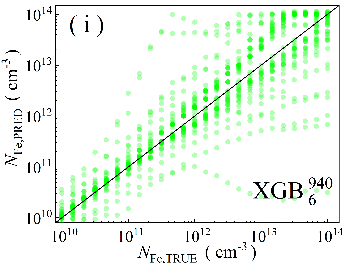
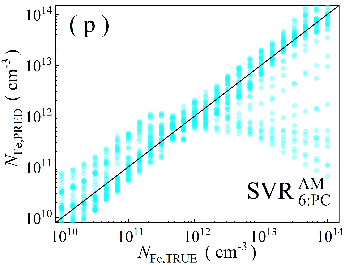
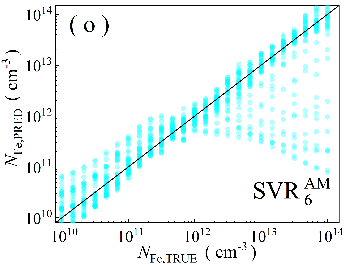
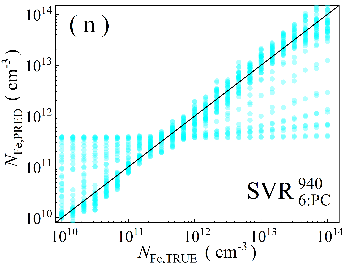
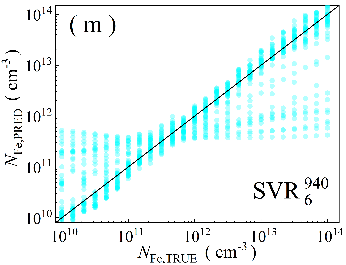


Fig.S13. Scatter plots of the iron concentrations between the reference values and ML predicted values for test phase B-altered in the case of 5D features. ML algorithms: RF (a-d), GB (e-h), XGB (i-l), SVR (m-p), DNN (q-t). The data are obtained for monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 (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.









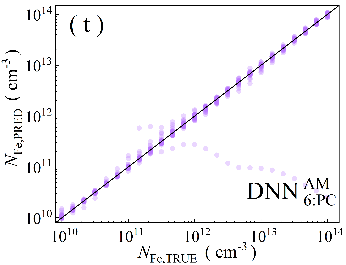
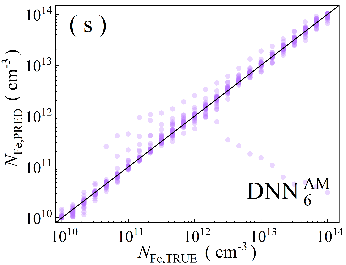
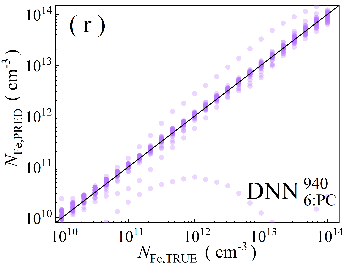
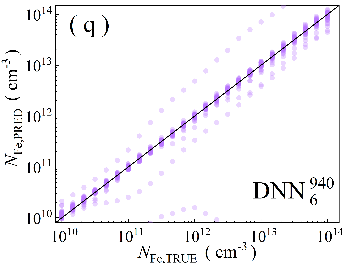
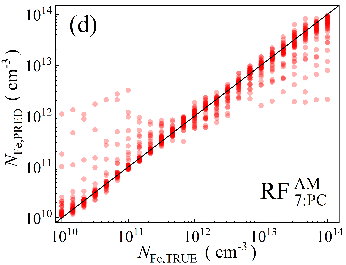
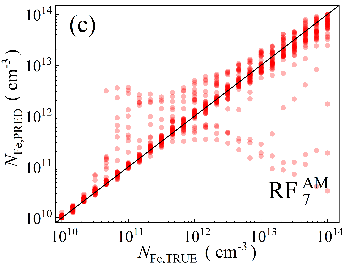
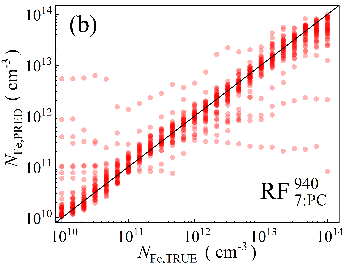
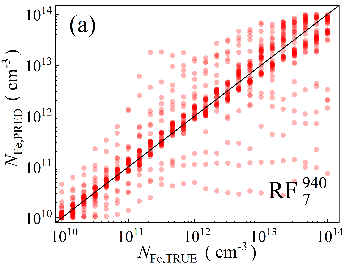
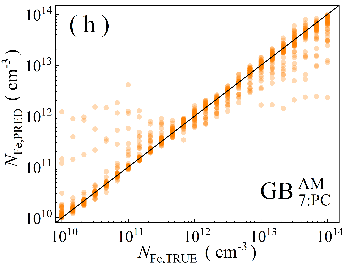
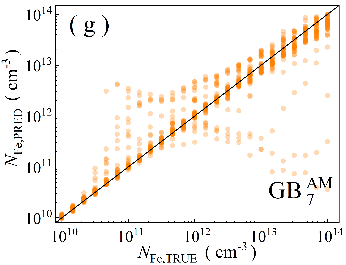
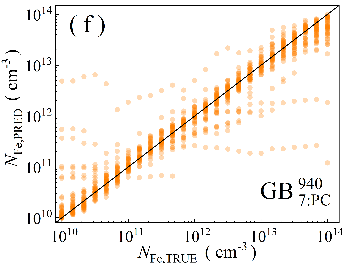
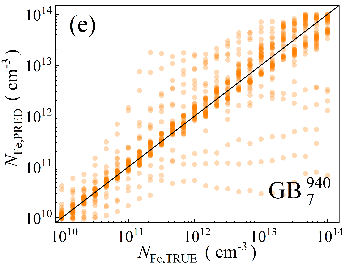
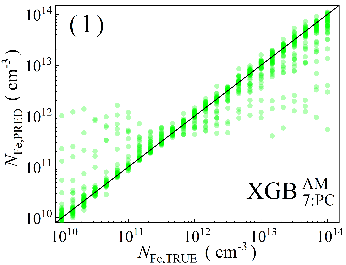
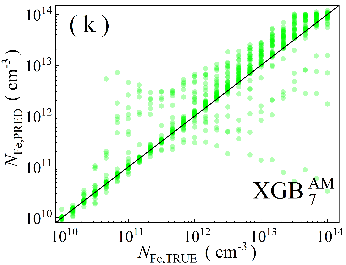
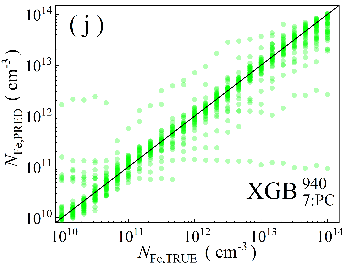
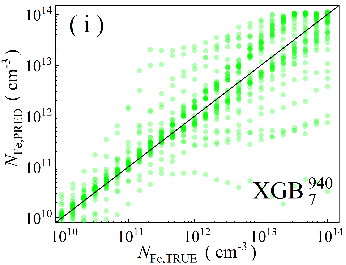
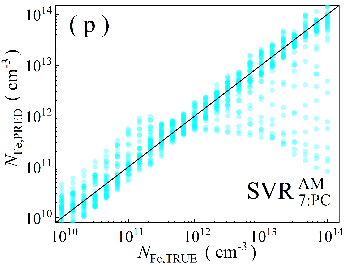
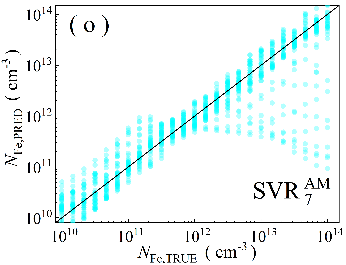
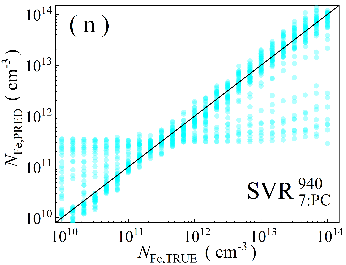
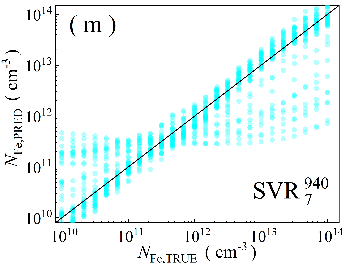


Fig.S14. Scatter plots of the iron concentrations between the reference values and ML predicted values for test phase B-altered in the case of 6D features. ML algorithms: RF (a-d), GB (e-h), XGB (i-l), SVR (m-p), DNN (q-t). The data are obtained for monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 (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.









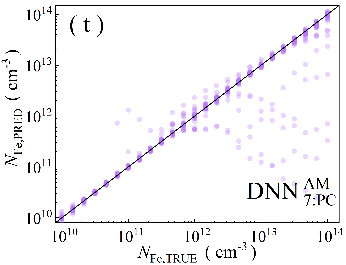
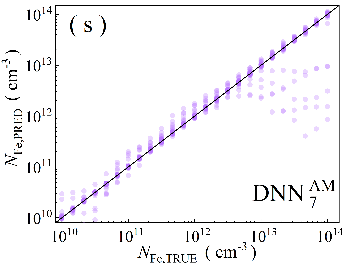
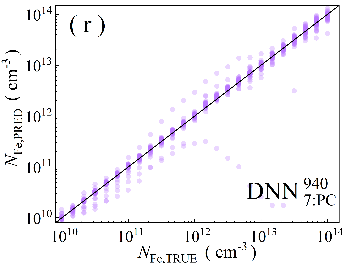
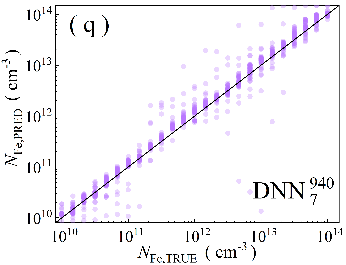
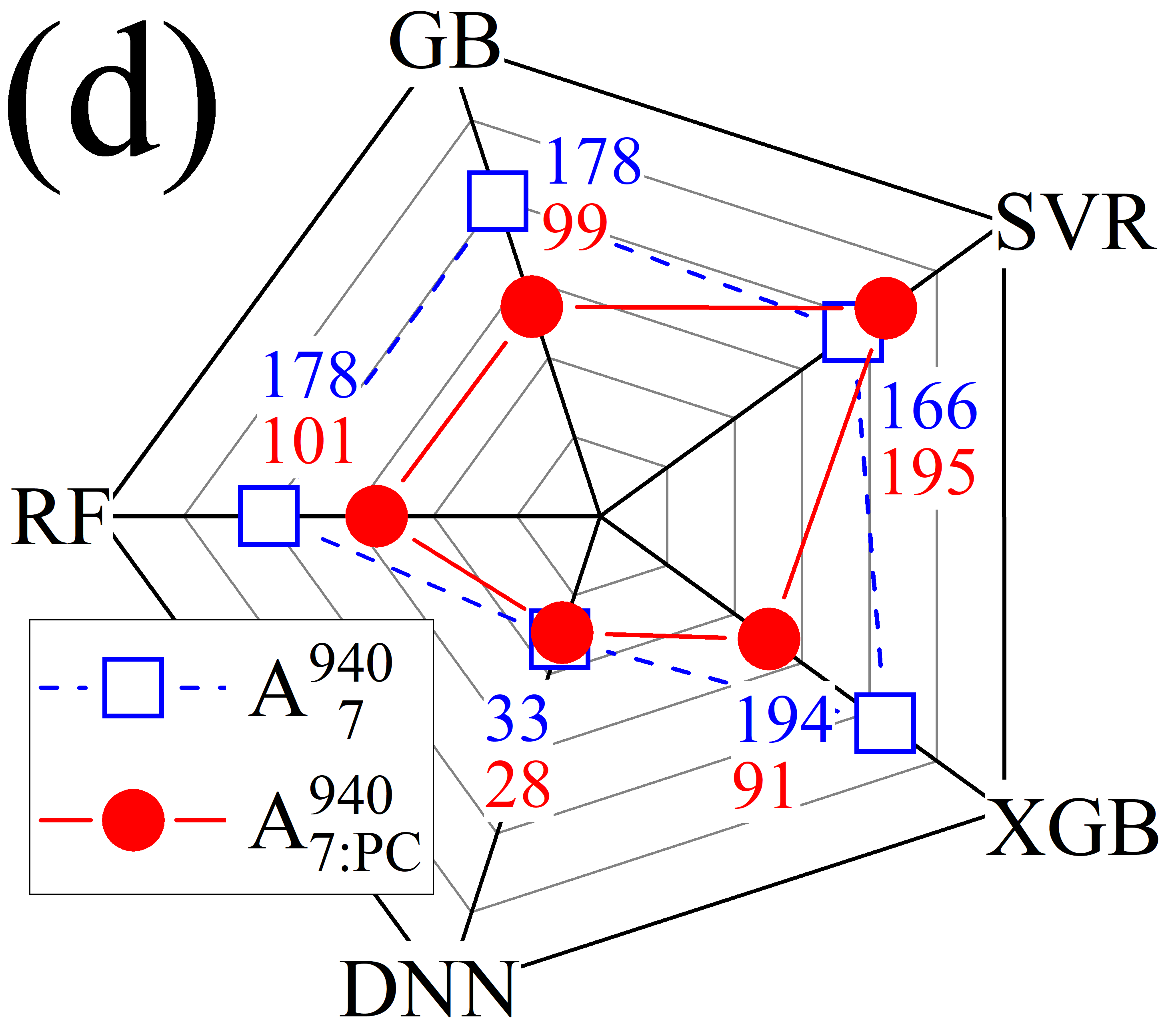
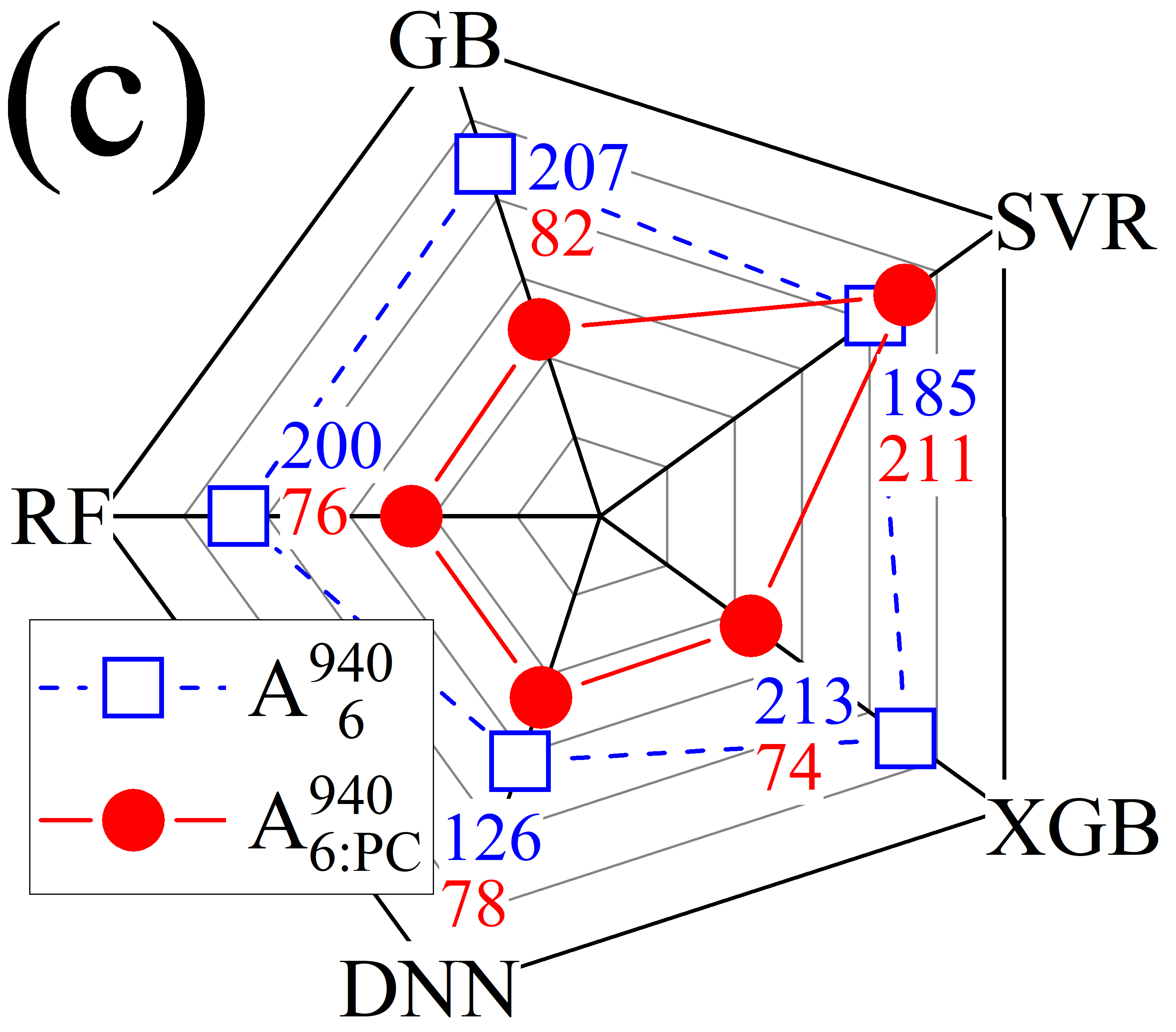
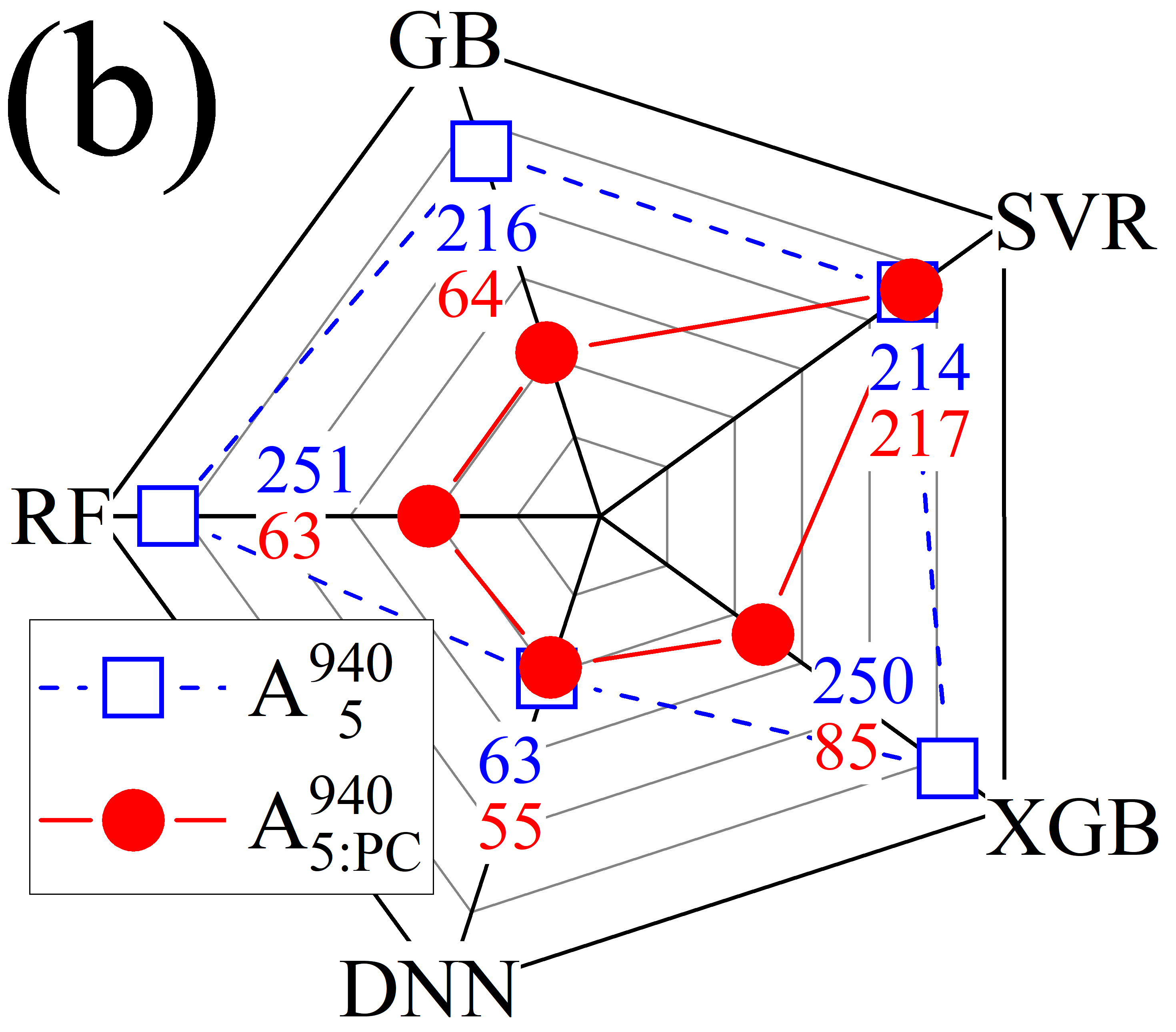
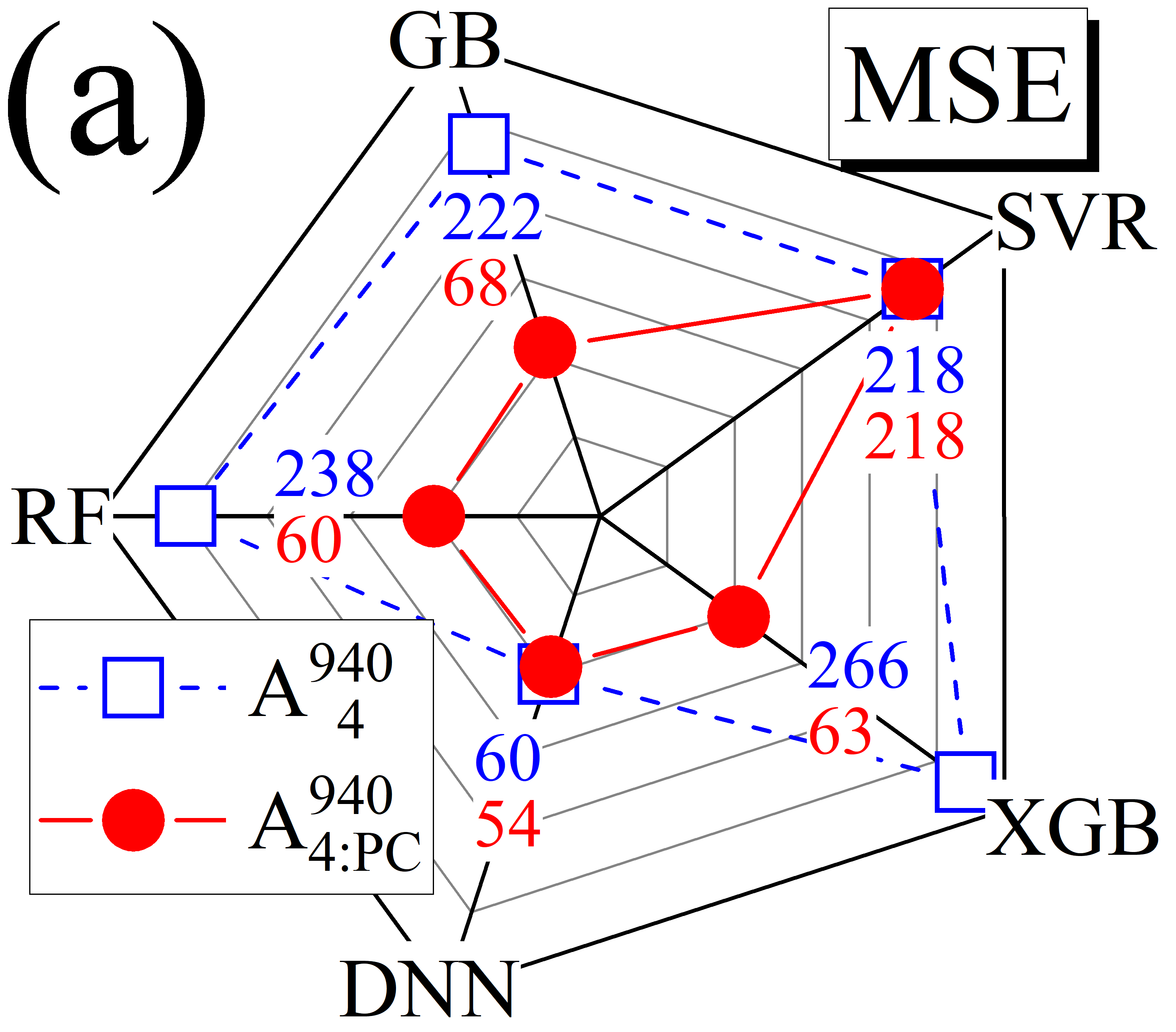
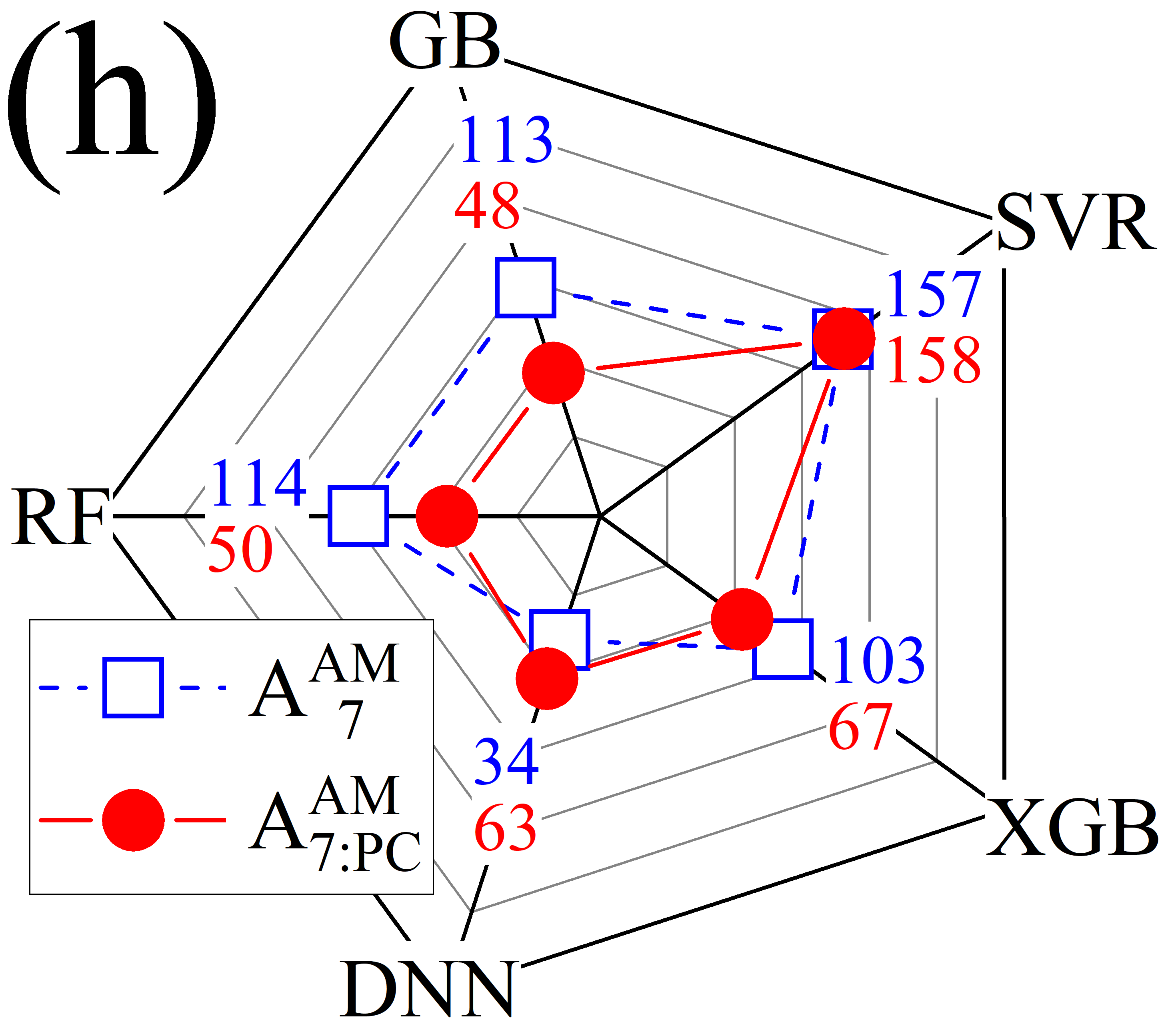
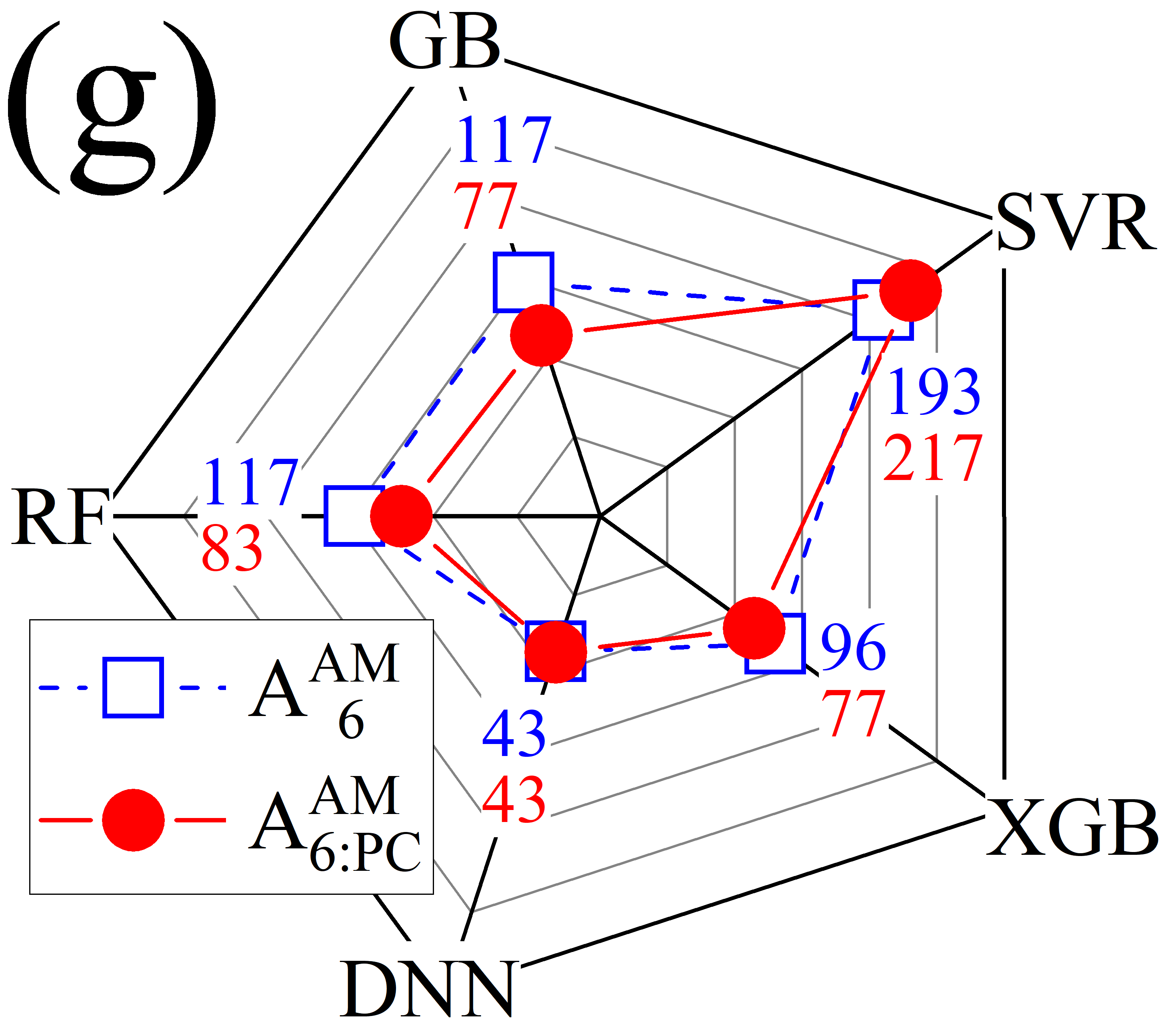
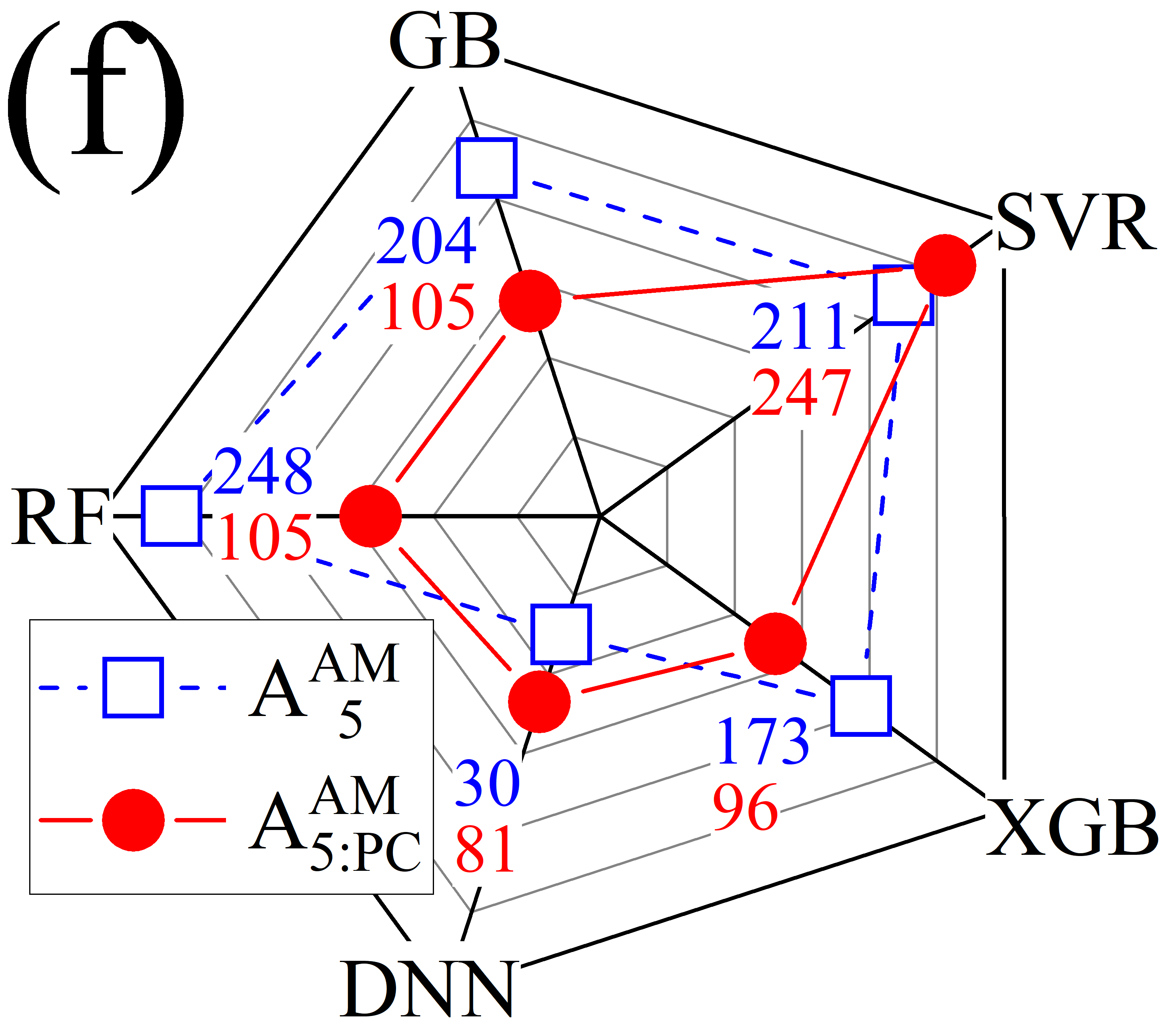
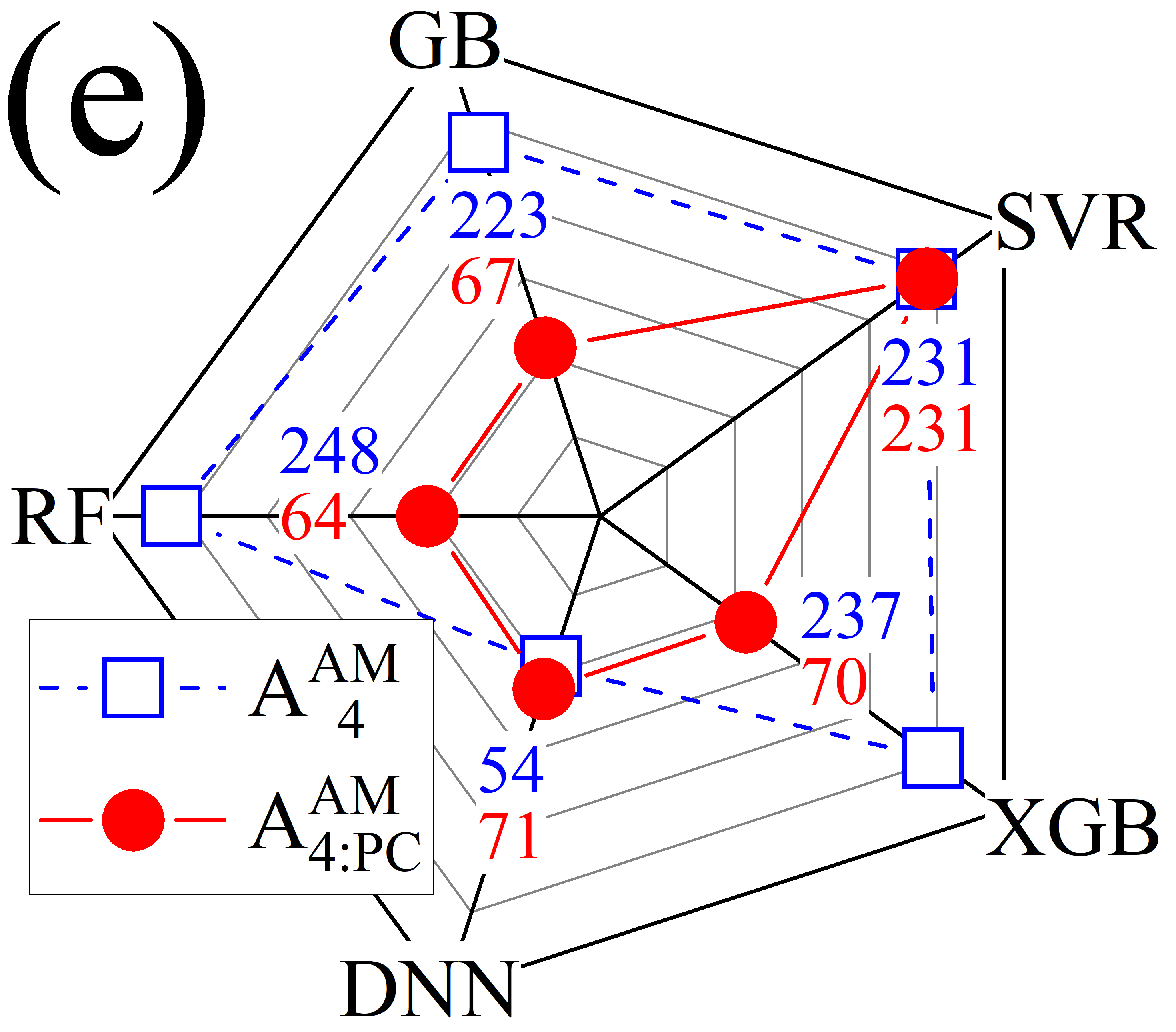
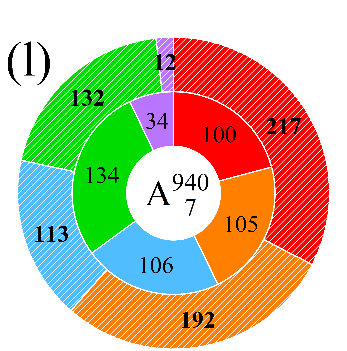
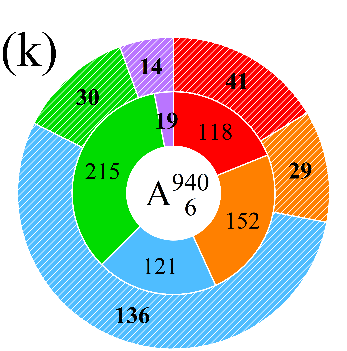
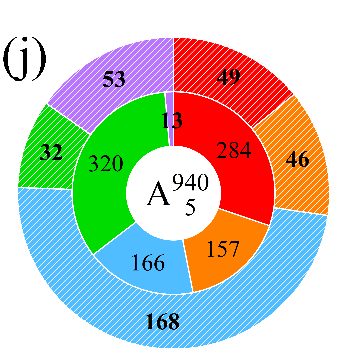
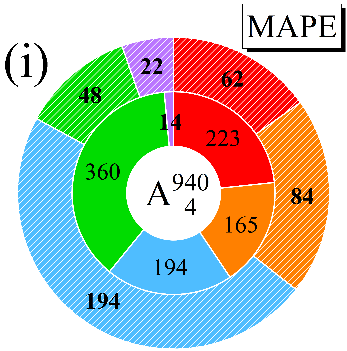
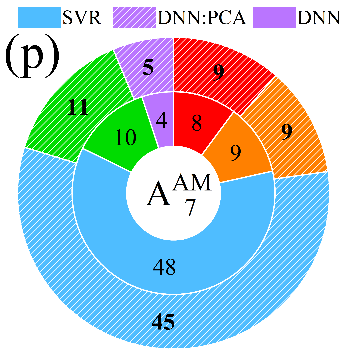
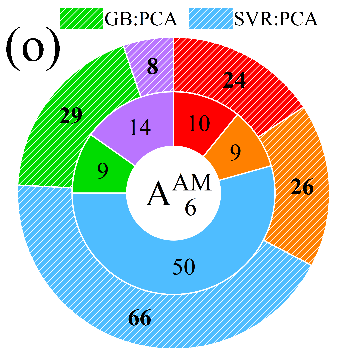
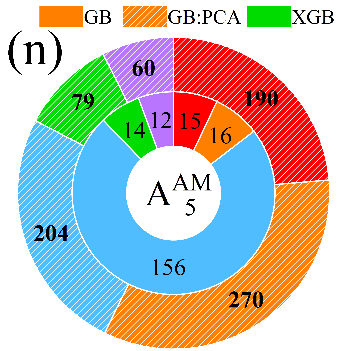
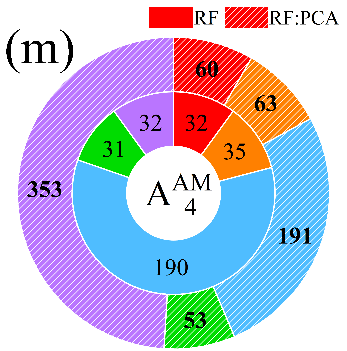


Fig.S15. Scatter plots of the iron concentrations between the reference values and ML predicted values for test phase B-altered in the case of 7D features. ML algorithms: RF (a-d), GB (e-h), XGB (i-l), SVR (m-p), DNN (q-t). The data are obtained for monochromatic (a, b, e, f, i, j, m, n, q, r) and AM1.5 (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.









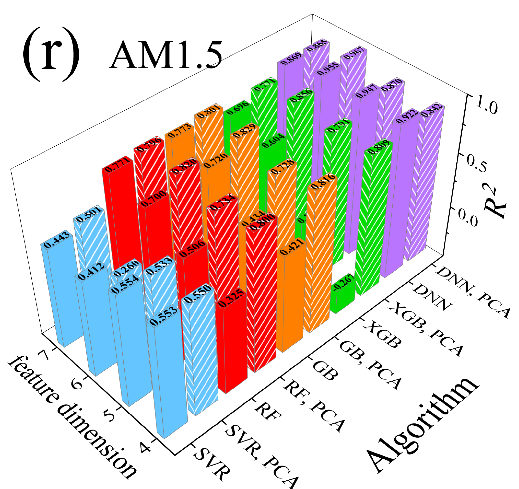
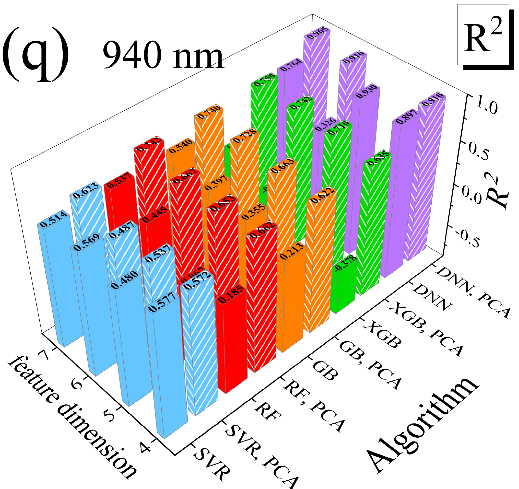


Fig.S24. MSE (a-h), MAPE (i-p), and R2 (q, r) scores obtained by various models, feature combinations, illumination conditions for B-altered test dataset. Illumination: 940 nm (a-d, i-l, q), AM (e-h, m-p, r). Feature dimension: 4 (a, e, i, m), 5 (b, f, g, n), 6 (c, g, k, o), and 7 (d, h, l, p). Results obtained with PCA applying