**All the following results are obtained for 40 epochs.**

**POM\_QM 5 fold**  
Consolidated Average Scores Across All Folds:

Train Score: 0.8676788

Validation Score: 0.8373375

Test Score: 0.8391313

**GCN\_QM 5 fold**

Cross-Validation Results:

Mean Train Score: 0.8910 ± 0.0030

Mean Valid Score: 0.8466 ± 0.0024

Mean Test Score: 0.8508 ± 0.0063

**DMPNN\_QM 5 fold**

Cross-Validation Results:

Mean Train Score: 0.8943 ± 0.0018

Mean Valid Score: 0.8555 ± 0.0011

Mean Test Score: 0.8547 ± 0.0033

**POM 5 fold**  
Consolidated Average Scores Across All Folds:

Train Score: 0.9308097

Validation Score: 0.8644711

Test Score: 0.8647679