Summary - Substrate, Group A, 𝚫𝚫G Version

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# *Substrate*

### Model

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_9 + NPA\_ConnectMetal + diff\_NBO\_4\_13 | 0.657 | 0.447 | 0.633 |
| ddg ~ NPA\_9 + NPA\_13 + diff\_NBO\_4\_ConnectMetal | 0.651 | 0.147 | 0.734 |

***3-Fold cross-validation***

| Rsquared |
| --- |
| 0.591 |