Summary - Substrate, Group C, 𝚫𝚫G Version

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# *Substrate*

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_10 + Total\_1 + Aniso.Polar | 0.698 | 0.569 | 0.262 |
| ddg ~ NPA\_ConnectMetal + Total\_1 + B5\_3\_9 | 0.687 | 0.561 | 0.262 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_13 + Total\_1 + Dist.3..9. + B5\_3\_9 | 0.781 | 0.626 | 0.245 |
| ddg ~ diff\_NBO\_4\_13 + Total\_1 + Dist.3..9. + B5\_3\_9 | 0.782 | 0.625 | 0.239 |