Summary - Int 1, Group B, 𝚫𝚫G Version

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# *Intermidiate 1*

## Water

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ diff\_NBO\_4\_10 + Dist.10..30. + B1\_3\_9 | 0.663 | 0.375 | 0.386 |

***RMSE on top model***

| RMSE |
| --- |
| 0.407 |

***Multicollinearity check***

|  | x |
| --- | --- |
| diff\_NBO\_4\_10 | 1.127 |
| Dist.10..30. | 1.289 |
| B1\_3\_9 | 1.194 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.072 | 14.132 | 0.0000000 |
| diff\_NBO\_4\_10 | 0.295 | 0.078 | 3.800 | 0.0006129 |
| Dist.10..30. | 0.350 | 0.083 | 4.225 | 0.0001855 |
| B1\_3\_9 | -0.531 | 0.080 | -6.657 | 0.0000002 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ diff\_NBO\_4\_10 + dip\_z\_1 + Dist.10..30. + B1\_3\_9 | 0.724 | 0.443 | 0.356 |
| ddg ~ diff\_NBO\_4\_10 + dip\_y\_1 + Dist.10..30. + B1\_3\_9 | 0.718 | 0.441 | 0.356 |

***Multicollinearity check***

|  | x |
| --- | --- |
| diff\_NBO\_4\_10 | 1.147 |
| dip\_z\_1 | 1.044 |
| Dist.10..30. | 1.289 |
| B1\_3\_9 | 1.212 |

***RMSE on top model***

| RMSE |
| --- |
| 0.369 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.066 | 15.365 | 0.0000000 |
| diff\_NBO\_4\_10 | 0.270 | 0.072 | 3.748 | 0.0007327 |
| dip\_z\_1 | -0.179 | 0.069 | -2.613 | 0.0137299 |
| Dist.10..30. | 0.349 | 0.076 | 4.571 | 0.0000731 |
| B1\_3\_9 | -0.508 | 0.074 | -6.867 | 0.0000001 |

## Methanol

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_3 + NPA\_4 + Dist.31..36. | 0.572 | 0.446 | 0.363 |
| ddg ~ NPA\_3 + diff\_NBO\_4\_31 + Dist.31..36. | 0.555 | 0.415 | 0.387 |

***RMSE on top model***

| RMSE |
| --- |
| 0.459 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_3 + diff\_NBO\_4\_10 + Dist.31..36. + B1\_9\_3 | 0.654 | 0.516 | 0.344 |
| ddg ~ NPA\_3 + NPA\_4 + Dist.31..36. + B1\_9\_3 | 0.654 | 0.501 | 0.372 |

***RMSE on top model***

| RMSE |
| --- |
| 0.413 |