Summary - Int 5, Group B, 𝚫𝚫G Version

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## Water

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ diff\_NBO\_4\_10 + X.32.30. + B1\_3\_9 | 0.568 | 0.340 | 0.373 |
| ddg ~ diff\_NBO\_4\_10 + Dist.33..30. + B1\_3\_9 | 0.564 | 0.323 | 0.382 |

***Multicollinearity check***

|  | x |
| --- | --- |
| diff\_NBO\_4\_10 | 1.149 |
| X.32.30. | 1.168 |
| B1\_3\_9 | 1.127 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.082 | 12.472 | 0.0000000 |
| diff\_NBO\_4\_10 | 0.244 | 0.089 | 2.755 | 0.0096078 |
| X.32.30. | 0.268 | 0.089 | 2.993 | 0.0052915 |
| B1\_3\_9 | -0.344 | 0.088 | -3.913 | 0.0004472 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_7 + NPA\_32 + Dist.10..7. + B1\_3\_9 | 0.651 | 0.427 | 0.386 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_7 | 2.982 |
| NPA\_32 | 2.681 |
| Dist.10..7. | 2.768 |
| B1\_3\_9 | 1.076 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.075 | 13.660 | 0.0000000 |
| NPA\_7 | 0.602 | 0.130 | 4.616 | 0.0000644 |
| NPA\_32 | 0.401 | 0.124 | 3.239 | 0.0028571 |
| Dist.10..7. | 0.509 | 0.126 | 4.052 | 0.0003164 |
| B1\_3\_9 | -0.426 | 0.078 | -5.439 | 0.0000061 |

## Methanol

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ diff\_NBO\_10\_7 + Dist.10..7. + B1\_3\_9 | 0.623 | 0.383 | 0.380 |
| ddg ~ NPA\_10 + Dist.10..7. + B1\_3\_9 | 0.603 | 0.357 | 0.382 |

***Multicollinearity check***

|  | x |
| --- | --- |
| diff\_NBO\_10\_7 | 1.224 |
| Dist.10..7. | 1.273 |
| B1\_3\_9 | 1.152 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.076 | 13.363 | 0.0000000 |
| diff\_NBO\_10\_7 | -0.260 | 0.085 | -3.037 | 0.0047251 |
| Dist.10..7. | 0.350 | 0.087 | 4.011 | 0.0003392 |
| B1\_3\_9 | -0.494 | 0.083 | -5.956 | 0.0000012 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_4 + diff\_NBO\_10\_7 + Dist.10..7. + B1\_3\_9 | 0.670 | 0.433 | 0.358 |
| ddg ~ diff\_NBO\_4\_10 + diff\_NBO\_10\_7 + Dist.10..7. + B1\_3\_9 | 0.665 | 0.427 | 0.361 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_4 | 1.262 |
| diff\_NBO\_10\_7 | 1.497 |
| Dist.10..7. | 1.274 |
| B1\_3\_9 | 1.181 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.072 | 14.061 | 0.0000000 |
| NPA\_4 | 0.174 | 0.082 | 2.104 | 0.0435534 |
| diff\_NBO\_10\_7 | -0.340 | 0.090 | -3.788 | 0.0006556 |
| Dist.10..7. | 0.346 | 0.083 | 4.174 | 0.0002245 |
| B1\_3\_9 | -0.468 | 0.080 | -5.861 | 0.0000018 |