Summary - Int 4, Group B, 𝚫𝚫G Version

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## Water

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_31 + B1\_3\_9 + B5\_3\_9 | 0.584 | 0.282 | 0.377 |
| ddg ~ diff\_NBO\_4\_10 + B1\_3\_9 + B5\_3\_9 | 0.572 | 0.274 | 0.409 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_31 | 1.309 |
| B1\_3\_9 | 1.298 |
| B5\_3\_9 | 1.482 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.080 | 12.718 | 0.0000000 |
| NPA\_31 | -0.284 | 0.093 | -3.054 | 0.0045254 |
| B1\_3\_9 | -0.503 | 0.092 | -5.434 | 0.0000056 |
| B5\_3\_9 | 0.320 | 0.099 | 3.236 | 0.0028173 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ diff\_NBO\_4\_10 + Dist.30..32. + B1\_3\_9 + B5\_3\_9 | 0.664 | 0.077 | 0.475 |
| ddg ~ Dist.30..32. + B1\_3\_9 + L\_3\_9 + loc.B5\_3\_9 | 0.668 | 0.004 | 0.557 |

***Multicollinearity check***

|  | x |
| --- | --- |
| diff\_NBO\_4\_10 | 1.097 |
| Dist.30..32. | 1.399 |
| B1\_3\_9 | 1.276 |
| B5\_3\_9 | 1.739 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.073 | 13.934 | 0.0000000 |
| diff\_NBO\_4\_10 | 0.235 | 0.078 | 3.035 | 0.0048423 |
| Dist.30..32. | -0.256 | 0.088 | -2.924 | 0.0064017 |
| B1\_3\_9 | -0.533 | 0.084 | -6.372 | 0.0000004 |
| B5\_3\_9 | 0.405 | 0.098 | 4.150 | 0.0002402 |

## Methanol

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_6 + dip\_x\_1 + Dist.30..31. | 0.580 | 0.459 | 0.371 |
| ddg ~ NPA\_31 + dip\_x\_1 + Dist.30..31. | 0.552 | 0.430 | 0.369 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_6 | 1.033 |
| dip\_x\_1 | 1.336 |
| Dist.30..31. | 1.304 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.080 | 12.662 | 0.0000000 |
| NPA\_6 | -0.271 | 0.083 | -3.271 | 0.0025714 |
| dip\_x\_1 | -0.550 | 0.094 | -5.835 | 0.0000018 |
| Dist.30..31. | 0.447 | 0.093 | 4.803 | 0.0000352 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_5 + NPA\_6 + dip\_x\_1 + Dist.30..31. | 0.668 | 0.529 | 0.348 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_5 | 1.177 |
| NPA\_6 | 1.083 |
| dip\_x\_1 | 1.430 |
| Dist.30..31. | 1.320 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.018 | 0.073 | 14.008 | 0.00e+00 |
| NPA\_5 | -0.228 | 0.080 | -2.857 | 7.57e-03 |
| NPA\_6 | -0.318 | 0.077 | -4.149 | 2.41e-04 |
| dip\_x\_1 | -0.614 | 0.088 | -6.972 | 1.00e-07 |
| Dist.30..31. | 0.420 | 0.085 | 4.964 | 2.38e-05 |