Summary - Int 4, Group A, 𝚫𝚫G Version

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## *Water*

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_32 + dip\_x\_1 + Dist.10..30. | 0.722 | 0.645 | 0.484 |
| ddg ~ NPA\_31 + dip\_x\_1 + Dist.10..30. | 0.716 | 0.599 | 0.559 |

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

| Q2 | MAE |
| --- | --- |
| 0.537 | 0.625 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_32 | 1.442 |
| dip\_x\_1 | 1.411 |
| Dist.10..30. | 1.072 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.122 | 0.143 | 7.822 | 0.0000018 |
| NPA\_32 | -0.483 | 0.177 | -2.724 | 0.0164776 |
| dip\_x\_1 | -0.727 | 0.175 | -4.144 | 0.0009931 |
| Dist.10..30. | -0.782 | 0.153 | -5.120 | 0.0001558 |

## *Methanol*

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ diff\_NBO\_10\_30 + Iso.Polar + B1\_3\_9 | 0.697 | 0.513 | 0.583 |
| ddg ~ Iso.Polar + B1\_3\_9 + L\_3\_9 | 0.681 | 0.474 | 0.623 |

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

| Q2 | MAE |
| --- | --- |
| 0.281 | 1.148 |

***Multicollinearity check***

|  | x |
| --- | --- |
| diff\_NBO\_10\_30 | 1.258 |
| Iso.Polar | 2.639 |
| B1\_3\_9 | 2.278 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.122 | 0.150 | 7.491 | 0.0000029 |
| diff\_NBO\_10\_30 | -0.754 | 0.173 | -4.360 | 0.0006530 |
| Iso.Polar | 1.074 | 0.250 | 4.287 | 0.0007521 |
| B1\_3\_9 | -0.961 | 0.233 | -4.131 | 0.0010189 |