Summary - Int 3, Group A, 𝚫𝚫G Version

Inbal Lorena Eshel

16/03/25

## *Water*

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ Iso.Polar + B1\_3\_9 + L\_3\_9 | 0.659 | 0.423 | 0.633 |

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

| Q2 | MAE |
| --- | --- |
| 0.298 | 1.121 |

***Multicollinearity check***

|  | x |
| --- | --- |
| Iso.Polar | 11.291 |
| B1\_3\_9 | 4.367 |
| L\_3\_9 | 5.543 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.122 | 0.159 | 7.062 | 0.0000057 |
| Iso.Polar | 2.583 | 0.549 | 4.702 | 0.0003399 |
| B1\_3\_9 | -1.767 | 0.342 | -5.172 | 0.0001417 |
| L\_3\_9 | -1.518 | 0.385 | -3.943 | 0.0014731 |

## *Methanol*

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_35 + dip\_x\_1 + Dist.10..35. | 0.641 | 0.475 | 0.568 |
| ddg ~ diff\_NBO\_10\_35 + Iso.Polar + B1\_3\_9 | 0.634 | 0.470 | 0.548 |
| ddg ~ NPA\_6 + NPA\_29 + Dist.10..35. | 0.631 | 0.452 | 0.632 |
| ddg ~ NPA\_29 + Dist.10..35. + L\_9\_3 | 0.633 | 0.444 | 0.613 |
| ddg ~ NPA\_29 + Dist.10..35. + loc.B5\_3\_9 | 0.618 | 0.429 | 0.645 |
| ddg ~ NPA\_29 + Dist.10..40. + Dist.10..35. | 0.594 | 0.398 | 0.617 |

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

| Q2 | MAE |
| --- | --- |
| 0.402 | 0.648 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_35 | 1.132 |
| dip\_x\_1 | 1.243 |
| Dist.10..35. | 1.139 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.122 | 0.163 | 6.884 | 0.0000075 |
| NPA\_35 | 0.822 | 0.178 | 4.606 | 0.0004075 |
| dip\_x\_1 | 0.471 | 0.187 | 2.520 | 0.0245178 |
| Dist.10..35. | -0.479 | 0.179 | -2.676 | 0.0180786 |