Summary - Int 1, Group A, 𝚫𝚫G Version

Inbal Lorena Eshel

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# *Intermidiate 1*

## Water

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_9 + diff\_NBO\_4\_10 + Aniso.Polar | 0.672 | 0.549 | 0.561 |
| ddg ~ diff\_NBO\_4\_10 + diff\_NBO\_3\_9 + Aniso.Polar | 0.659 | 0.470 | 0.626 |

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

| Q2 | MAE |
| --- | --- |
| 0.388 | 0.791 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_9 | 3.020 |
| diff\_NBO\_4\_10 | 2.451 |
| Aniso.Polar | 1.383 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.122 | 0.156 | 7.201 | 0.0000046 |
| NPA\_9 | -1.318 | 0.279 | -4.729 | 0.0003229 |
| diff\_NBO\_4\_10 | 1.199 | 0.251 | 4.778 | 0.0002946 |
| Aniso.Polar | 0.594 | 0.189 | 3.149 | 0.0071022 |

## Methanol

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_3 + NPA\_10 + NPA\_32 | 0.804 | 0.617 | 0.514 |
| ddg ~ NPA\_10 + NPA\_32 + diff\_NBO\_3\_9 | 0.757 | 0.587 | 0.594 |

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

| Q2 | MAE |
| --- | --- |
| 0.539 | 0.623 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_3 | 3.628 |
| NPA\_10 | 3.734 |
| NPA\_32 | 2.756 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 1.122 | 0.121 | 9.309 | 0.0000002 |
| NPA\_3 | 1.123 | 0.236 | 4.752 | 0.0003091 |
| NPA\_10 | 1.147 | 0.240 | 4.787 | 0.0002898 |
| NPA\_32 | -1.527 | 0.206 | -7.415 | 0.0000033 |