Summary - Int 4, Group C, 𝚫𝚫G Version

Inbal Lorena Eshel

03/02/25

## Water

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_10 + NPA\_31 + B5\_3\_9 | 0.697 | 0.502 | 0.288 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_10 | 2.587 |
| NPA\_31 | 2.583 |
| B5\_3\_9 | 1.013 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.067 | 2.184 | 0.0432916 |
| NPA\_10 | 0.412 | 0.110 | 3.730 | 0.0016661 |
| NPA\_31 | -0.377 | 0.110 | -3.417 | 0.0032860 |
| B5\_3\_9 | -0.371 | 0.069 | -5.364 | 0.0000516 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_31 + diff\_NBO\_10\_30 + Iso.Polar + loc.B5\_3\_9 | 0.771 | 0.561 | 0.284 |
| ddg ~ NPA\_10 + NPA\_31 + Dist.3..9. + Iso.Polar | 0.755 | 0.508 | 0.277 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_31 | 1.780 |
| diff\_NBO\_10\_30 | 1.777 |
| Iso.Polar | 2.134 |
| loc.B5\_3\_9 | 2.116 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.060 | 2.438 | 0.0268282 |
| NPA\_31 | -0.346 | 0.082 | -4.211 | 0.0006632 |
| diff\_NBO\_10\_30 | 0.499 | 0.082 | 6.081 | 0.0000159 |
| Iso.Polar | -0.560 | 0.090 | -6.233 | 0.0000120 |
| loc.B5\_3\_9 | 0.319 | 0.089 | 3.566 | 0.0025774 |

## Methanol

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ dip\_x\_1 + B5\_3\_9 + B5\_9\_3 | 0.696 | 0.580 | 0.267 |
| ddg ~ dip\_x\_1 + B5\_3\_9 + loc.B5\_9\_3 | 0.693 | 0.575 | 0.267 |

***Multicollinearity check***

|  | x |
| --- | --- |
| dip\_x\_1 | 3.316 |
| B5\_3\_9 | 1.067 |
| loc.B5\_9\_3 | 3.314 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.068 | 2.166 | 0.0447935 |
| dip\_x\_1 | 0.443 | 0.126 | 3.511 | 0.0026806 |
| B5\_3\_9 | -0.299 | 0.071 | -4.185 | 0.0006218 |
| loc.B5\_9\_3 | 0.271 | 0.126 | 2.152 | 0.0460659 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ diff\_NBO\_10\_30 + dip\_x\_1 + Iso.Polar + B5\_9\_3 | 0.757 | 0.586 | 0.288 |

***Multicollinearity check***

|  | x |
| --- | --- |
| diff\_NBO\_10\_30 | 1.813 |
| dip\_x\_1 | 3.714 |
| Iso.Polar | 1.118 |
| B5\_9\_3 | 4.975 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.062 | 2.365 | 0.0310225 |
| diff\_NBO\_10\_30 | 0.222 | 0.085 | 2.606 | 0.0191117 |
| dip\_x\_1 | 0.680 | 0.122 | 5.567 | 0.0000425 |
| Iso.Polar | -0.317 | 0.067 | -4.731 | 0.0002263 |
| B5\_9\_3 | -0.521 | 0.141 | -3.680 | 0.0020244 |