Summary - Int 3, Group C, 𝚫𝚫G Version

Inbal Lorena Eshel

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## Water

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ Dist.10..40. + Dist.31..32. + B5\_3\_9 | 0.657 | 0.515 | 0.268 |

***Multicollinearity check***

|  | x |
| --- | --- |
| Dist.10..40. | 4.162 |
| Dist.31..32. | 3.976 |
| B5\_3\_9 | 1.095 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.071 | 2.052 | 0.0559289 |
| Dist.10..40. | -0.428 | 0.149 | -2.872 | 0.0105815 |
| Dist.31..32. | 0.480 | 0.146 | 3.294 | 0.0042859 |
| B5\_3\_9 | -0.299 | 0.076 | -3.906 | 0.0011367 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_1 + Dist.10..40. + Dist.31..32. + B5\_3\_9 | 0.691 | 0.538 | 0.267 |
| ddg ~ Dist.10..40. + Dist.31..32. + B5\_3\_9 + loc.B5\_3\_9 | 0.692 | 0.536 | 0.265 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_1 | 1.213 |
| Dist.10..40. | 4.171 |
| Dist.31..32. | 4.262 |
| B5\_3\_9 | 1.096 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.070 | 2.097 | 0.0521990 |
| NPA\_1 | 0.105 | 0.079 | 1.329 | 0.2026113 |
| Dist.10..40. | -0.437 | 0.146 | -2.993 | 0.0086109 |
| Dist.31..32. | 0.531 | 0.148 | 3.597 | 0.0024168 |
| B5\_3\_9 | -0.296 | 0.075 | -3.958 | 0.0011272 |

## Methanol

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ dip\_x\_1 + Dist.29..31. + B5\_3\_9 | 0.553 | 0.384 | 0.304 |
| ddg ~ Total\_1 + Dist.29..31. + B5\_3\_9 | 0.576 | 0.381 | 0.303 |

***Multicollinearity check***

|  | x |
| --- | --- |
| dip\_x\_1 | 1.097 |
| Dist.29..31. | 1.098 |
| B5\_3\_9 | 1.011 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.081 | 1.796 | 0.0903483 |
| dip\_x\_1 | 0.141 | 0.087 | 1.615 | 0.1247381 |
| Dist.29..31. | -0.151 | 0.087 | -1.722 | 0.1032181 |
| B5\_3\_9 | -0.342 | 0.084 | -4.073 | 0.0007917 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_1 + NPA\_10 + dip\_x\_1 + B5\_3\_9 | 0.660 | 0.480 | 0.283 |
| ddg ~ diff\_NBO\_29\_31 + Total\_1 + Dist.29..31. + B5\_3\_9 | 0.656 | 0.462 | 0.278 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_1 | 5.023 |
| NPA\_10 | 2.536 |
| dip\_x\_1 | 6.467 |
| B5\_3\_9 | 1.015 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.073 | 1.998 | 0.0630360 |
| NPA\_1 | -0.426 | 0.168 | -2.533 | 0.0221698 |
| NPA\_10 | 0.341 | 0.120 | 2.857 | 0.0114184 |
| dip\_x\_1 | 0.591 | 0.191 | 3.096 | 0.0069335 |
| B5\_3\_9 | -0.325 | 0.076 | -4.301 | 0.0005491 |