Summary - Int 5, Group C, 𝚫𝚫G Version

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03/02/25

## Water

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_5 + Total\_1 + B5\_3\_9 | 0.785 | 0.681 | 0.238 |
| ddg ~ NPA\_6 + Total\_1 + B5\_3\_9 | 0.786 | 0.671 | 0.232 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_5 | 1.170 |
| Total\_1 | 1.478 |
| B5\_3\_9 | 1.289 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.056 | 2.593 | 0.0189410 |
| NPA\_5 | 0.180 | 0.063 | 2.880 | 0.0103935 |
| Total\_1 | -0.362 | 0.070 | -5.144 | 0.0000812 |
| B5\_3\_9 | -0.496 | 0.066 | -7.551 | 0.0000008 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ NPA\_6 + Total\_1 + Dist.10..35. + B5\_3\_9 | 0.822 | 0.712 | 0.202 |
| ddg ~ NPA\_6 + NPA\_9 + Total\_1 + B5\_3\_9 | 0.831 | 0.697 | 0.225 |

***Multicollinearity check***

|  | x |
| --- | --- |
| NPA\_6 | 1.205 |
| Total\_1 | 1.411 |
| Dist.10..35. | 1.682 |
| B5\_3\_9 | 1.577 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.053 | 2.763 | 0.0138688 |
| NPA\_6 | -0.207 | 0.060 | -3.480 | 0.0030905 |
| Total\_1 | -0.257 | 0.064 | -3.991 | 0.0010508 |
| Dist.10..35. | -0.127 | 0.070 | -1.809 | 0.0893567 |
| B5\_3\_9 | -0.417 | 0.068 | -6.126 | 0.0000146 |

## Methanol

### Model 3P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ dip\_z\_1 + Total\_1 + B5\_3\_9 | 0.787 | 0.662 | 0.219 |
| ddg ~ NPA\_10 + Total\_1 + B5\_3\_9 | 0.781 | 0.646 | 0.233 |

***Multicollinearity check***

|  | x |
| --- | --- |
| dip\_z\_1 | 1.045 |
| Total\_1 | 1.474 |
| B5\_3\_9 | 1.440 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.056 | 2.604 | 0.0185402 |
| dip\_z\_1 | 0.178 | 0.059 | 3.024 | 0.0076575 |
| Total\_1 | -0.252 | 0.070 | -3.611 | 0.0021566 |
| B5\_3\_9 | -0.471 | 0.069 | -6.819 | 0.0000030 |

### Model 4P

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| ddg ~ dip\_z\_1 + Total\_1 + B5\_3\_9 | 0.787 | 0.662 | 0.219 |
| ddg ~ NPA\_5 + dip\_z\_1 + Total\_1 + B5\_3\_9 | 0.794 | 0.658 | 0.230 |

***Multicollinearity check***

|  | x |
| --- | --- |
| dip\_z\_1 | 1.045 |
| Total\_1 | 1.474 |
| B5\_3\_9 | 1.440 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 0.146 | 0.056 | 2.604 | 0.0185402 |
| dip\_z\_1 | 0.178 | 0.059 | 3.024 | 0.0076575 |
| Total\_1 | -0.252 | 0.070 | -3.611 | 0.0021566 |
| B5\_3\_9 | -0.471 | 0.069 | -6.819 | 0.0000030 |