Summary - Int 1

# *Water*

### model

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| Yield ~ dip\_x + dip\_z + Pol.aniso + B5 | 0.8528257 | 0.7527432 | 5.47147 |

***Multicollinearity:***

|  | x |
| --- | --- |
| dip\_x | 4.065980 |
| dip\_z | 3.975966 |
| Pol.aniso | 1.172276 |
| B5 | 1.126356 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 56.285714 | 1.364122 | 41.261490 | 0.0000000 |
| dip\_x | 19.785712 | 2.818581 | 7.019742 | 0.0000029 |
| dip\_z | 11.417952 | 2.787207 | 4.096557 | 0.0008426 |
| Pol.aniso | -8.080628 | 1.513432 | -5.339274 | 0.0000665 |
| B5 | -5.293276 | 1.483494 | -3.568115 | 0.0025664 |

## *Methanol*

### model

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| Yield ~ NPA\_1 + NPA\_5 + NPA\_31 + B5 | 0.7684858 | 0.6444058 | 6.757291 |
| Yield ~ dip\_x + NPA\_2 + Dihedral.5\_4\_3\_9. + B5 | 0.7511360 | 0.5564078 | 7.773650 |

***Multicollinearity:***

|  | x |
| --- | --- |
| NPA\_1 | 2.702500 |
| NPA\_5 | 3.027356 |
| NPA\_31 | 1.057187 |
| B5 | 1.359285 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 56.285714 | 1.710906 | 32.898197 | 0.0000000 |
| NPA\_1 | 14.733590 | 2.882064 | 5.112166 | 0.0001044 |
| NPA\_5 | -16.416983 | 3.050369 | -5.381965 | 0.0000611 |
| NPA\_31 | -7.183322 | 1.802589 | -3.985004 | 0.0010651 |
| B5 | -11.539967 | 2.043977 | -5.645840 | 0.0000365 |