Summary - Int only water or only methanol

# *Intermidiate only Water*

### 2 parameters

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| Yield ~ dip\_z + NPA\_31 | 0.8287654 | 0.7514872 | 14.07249 |
| Yield ~ Dist.30..10. + Angle.3\_4\_10. | 0.8242487 | 0.7036654 | 12.93859 |
| Yield ~ Dist.30..10. + NPA\_31 | 0.7969529 | 0.6933426 | 14.14820 |
| Yield ~ Dist.30..10. + NPA\_9 | 0.8116513 | 0.6742453 | 16.12182 |
| Yield ~ Dist.30..10. + diff.3.9 | 0.8139908 | 0.6618175 | 17.18389 |
| Yield ~ diff.3.9 + diff.4.10 | 0.7594720 | 0.5956424 | 15.94967 |
| Yield ~ NPA\_9 + diff.4.10 | 0.7501299 | 0.5687645 | 16.21833 |
| Yield ~ Dist.30..10. + NPA\_3 | 0.7826620 | 0.5613893 | 21.35031 |
| Yield ~ Dist.30..10. + Dihedral.10\_4\_3\_9. | 0.7611129 | 0.0550213 | 30.25973 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 73.25000 | 3.993150 | 18.343912 | 0.0000000 |
| dip\_z | 21.12141 | 4.391684 | 4.809411 | 0.0005451 |
| NPA\_31 | 29.73265 | 4.391684 | 6.770216 | 0.0000307 |

### 1 parameter

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| Yield ~ Dist.30..10. | 0.597788 | 0.4471777 | 22.2533 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 73.25000 | 5.859400 | 12.501281 | 0.0000000 |
| Dist.30..10. | -25.67924 | 6.080586 | -4.223152 | 0.0011823 |

## *Methanol*

### 2 parameters

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| Yield ~ Dist.4..10. + Dist.30..10. | 0.8928803 | 0.7180993 | 11.84323 |
| Yield ~ Dist.30..10. + NPA\_9 | 0.8808131 | 0.6831164 | 13.43610 |
| Yield ~ Dist.30..10. + diff.3.9 | 0.8610470 | 0.6655881 | 13.99626 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 73.25000 | 3.158308 | 23.192797 | 0.00e+00 |
| Dist.4..10. | -13.49690 | 3.416344 | -3.950684 | 2.27e-03 |
| Dist.30..10. | -32.39633 | 3.416344 | -9.482748 | 1.30e-06 |

### 1 parameter

| formula | R.sq | Q.sq | MAE |
| --- | --- | --- | --- |
| Yield ~ Dist.30..10. | 0.7408882 | 0.6610895 | 12.86268 |

***Scaled Coefficients:***

|  | Estimate | Std. Error | t value | Pr(>|t|) |
| --- | --- | --- | --- | --- |
| (Intercept) | 73.25000 | 4.702938 | 15.575371 | 0.00e+00 |
| Dist.30..10. | -28.58807 | 4.880469 | -5.857649 | 7.75e-05 |