

predFerm() demonstrations

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Load functions.

```
source('readFormula.R')
source('predFerm.R')
```

Show arguments.

```
args(predFerm)
```

```
## function (donor, acceptor, biomassform = "C5H7O2N", fs = 0, elements = c("C",
##      "H", "O", "N"), order = "sort", dropzero = TRUE, dropsub = FALSE,
##      tol = 1e-10)
## NULL
```

Example calls.

1. Glucose to ethanol (section 5.6.1 in R & M)

```
predFerm(donor = 'C6H10O5', acceptor = 'CH3CH2OH')
```

```
##      H2O      C6H10O5      CO2      CH3CH2OH
## -0.04166667 -0.04166667  0.08333333  0.08333333
```

```
predFerm(donor = 'C6H10O5', acceptor = 'CH3CH2OH', fs = 0.22)
```

```
##      C6H10O5      NH3      H2O      CO2      CH3CH2OH      C5H7O2N
## -0.04166667 -0.01100000 -0.00866667  0.06500000  0.06500000  0.01100000
```

2. Glucose to lactic acid

```
predFerm(donor = 'C6H10O5', acceptor = 'C3H6O3', fs = 0.1)
```

```
##      C6H10O5      H2O      NH3      C3H6O3      C5H7O2N
## -0.04166667 -0.02666667 -0.00500000  0.07500000  0.00500000
```

3. Lipids to acetic acid

```
predFerm(donor = 'C57H104O6', acceptor = 'CH3COOH', fs = 0.1)
```

```
##      H2O      CO2      NH3 C57H104O6  CH3COOH  C5H7O2N
## -0.072500 -0.071875 -0.005000 -0.003125  0.112500  0.005000
```

4. Citrate to two products (Example 5.6 in R & M)

```
predFerm(donor = 'COOHCH2COHCOOHCH2COOH', acceptor = 'HCOOH(H3CCOOH)2')
```

```
##      H2O COOHCH2COHCOOHCH2COOH  HCOOH(H3CCOOH)2
##      -0.05555556      -0.05555556      0.05555556
##      CO2
##      0.05555556
```