

# cheg325 homework7 SIS 12.5-2

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starting with the definition of  $K_{OW}$  for solute partitioning

$$K_{OW,i} = \frac{C_i^O}{C_i^W}$$

now if we rearrange very very very slightly

$$C_i^O = K_{OW,i} C_i^W$$

now we can relate the concentration in the octanol (as our proxy for fatty tissue) to the concentration of solute in the whole fish if we define  $w_B$  to be the proportion of the fish that is fatty tissue. right below (12.5-9) homeboy sandler says  $w_B = 0.05$  or so for a fish. let phase  $F$  be the fish phase

$$C_i^F = w_B C_i^O = w_B K_{OW,i} C_i^W$$

another way sandler describes this is by making a  $K_{B,W}$  where phase B is biotia or some other nice sounding word. this is functionally the same

now we can do all this lovely math

```
import pandas as pd
import numpy as np
from IPython.display import display, HTML

data = {
    'name': ['Aldrin', 'Dieldrin', 'Lindane', 'Diazinon'],
    'solubility': [27, 140, 7000, 40000],
    'log Kow': [5.52, 4.32, 3.61, 3.31]
}

df = pd.DataFrame(data)
df
```

	name	solubility	log Kow
0	Aldrin	27	5.52
1	Dieldrin	140	4.32
2	Lindane	7000	3.61
3	Diazinon	40000	3.31

```
df['Kow'] = np.power(10.0, df['log Kow'], dtype=float)
df['fish concentration (g/L)'] = np.round(0.05 * df['solubility'] * df['Kow'] * 1e-6, 3)
display(HTML(df[['name', 'fish concentration (g/L)']].to_html(index=False)))
```

name	fish concentration (g/L)
Aldrin	0.447
Dieldrin	0.146
Lindane	1.426
Diazinon	4.083

```
# filler
```