Calculation of plasma levels of bioavailable 25-hydroxyvitamin D

Definitions:

$[D_{total}]$ = measured total 25-hydroxyvitamin D levels in nmol/L × 10^{-9} = total 25-hydroxyvitamin D levels in mol/L

[Alb] = measured albumin levels in g/dL ÷ 6,643g/mol = albumin levels in mol/L

$[VDBP_{total}]$ = measured vitamin D binding protein levels in mg/L × 10^{-3} ÷ 58,000g/mol = VDBP levels in mol/L

$[D_{Alb}]$ = albumin-bound 25-hydroxyvitamin D levels in mol/L

$[D_{VDBP}]$ = vitamin D binding protein-bound 25-hydroxyvitamin D levels in mol/L

$[D_{free}]$ = free (unbound) 25-hydroxyvitamin D levels in mol/L

$[D_{bioavailable}]$ = bioavailable 25-hydroxyvitamin D levels in mol/L = $[D_{free}] + [D_{Alb}]$

K_{Alb} = affinity constant between 25-hydroxyvitamin D and albumin = 6 × $10^{5}$$mol^{-1}$

K_{VDBP} = affinity constant between 25-hydroxyvitamin D and vitamin D binding protein = 7 × $10^{8}$$mol^{-1}$

Equations:

$[D_{VDBP}] = [D_{total}] - [D_{Alb}] - [D_{free}]$ *(1)*

$[D_{Alb}] = K_{Alb} \times [Alb] \times [D_{free}]$ *(2)*

$[D_{VDBP}] = K_{VDBP} \times [D_{free}] \times ([VDBP_{total}] - [D_{VDBP}])$ *(3)*

From equations *(1)* and *(2)*

$[D_{VDBP}] = [D_{total}] – (K_{Alb} \times [Alb] + 1) \times [D_{free}]$ *(4)*

From equations *(3)* and *(4)*

$[D_{free}] = \{[D_{total}] – (K_{Alb} \times [Alb] + 1) \times [D_{free}]\} \div K_{VDBP} \div ([VDBP_{total}] – \{[D_{total}] – (K_{Alb} \times [Alb] + 1) \times [D_{free}]\})$ *(5)*

This can be simplified to fit a second-degree polynomial ($ax^2 + bx + c = 0$) where $x=[D_{free}]$:

$a = K_{VDBP} \times K_{Alb} \times [Alb] + K_{VDBP}$

$b = K_{VDBP} \times [VDBP_{total}] - K_{VDBP} \times [D_{total}] + K_{Alb} \times [Alb] + 1$

$c = - [D_{total}]$

$$[D_{free}] = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$[D_{bioavailable}] = [D_{free}] + [D_{Alb}] = (K_{Alb} \times [Alb] + 1) \times [D_{free}]$