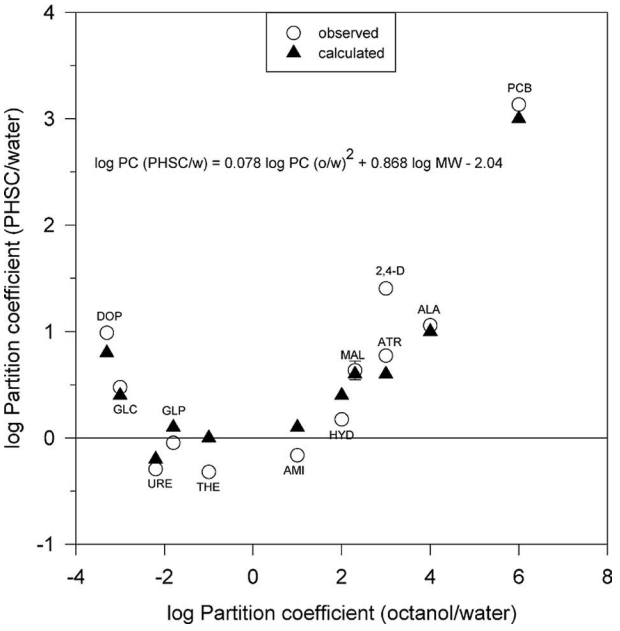

FIGURE 5.1 Correlation of the logarithm of stratum corneum/water partition coefficients (log PC sc/w) and logarithm of octanol/water partition coefficients of the 12 test chemicals. Open symbols express observed values, and each represents the mean of a test chemical ± SD (n = 5). Closed symbols express calculated values by Equation (5.3). *Abbreviations: DOP*, dopamine; *GLC*, glycine; *URE*, urea; *GLP*, glyphosate; *THE*, theophylline; *AMI*, aminopyrine; *HYD*, hydrocortisone; *MAL*, malathion; *ATR*, atrazine; *2,4-D*, 2,4-dichlorophenoxyacetic acid; *ALA*, alachlor; *PCB*, polychlorinated biphenyls.

However, the overall relationship of the PC PHSC/w of these chemicals to their PC o/w is nonlinear. This nonlinear relationship is adequately described by the following equation:

$$\log \text{PC PHCS/w} = 0.078 \log \text{PC o/w}^2 + 0.868 \log \text{MW} - 2.04$$

$$\text{Student} - \text{t values}: -8.29 \quad 2.04 \tag{5.3}$$

$$n = 12;\ r^2 = 0.90;\ S = 0.33;\ F = 42.59$$

The logarithm of MW gave a stronger correlation in this regression than MW (t = 1.55) itself. In Figure 5.1, the calculated log PC PHSC/w (Y estimate) values are compared to the corresponding observed values for these chemicals. As shown, the calculated values are acceptably close to the observed values. The correspondence with minimal scatter suggests that this equation would be useful in predicting in vitro partitioning in the PHSC for important environmental chemicals (16).

5.11 CONCLUSION

A new in vitro model employing PHSC (callus) to investigate the interaction between chemicals and human skin has been developed in our laboratory. The PHSC (callus) offers an experimentally easy in vitro model for the determination of chemical partitioning from water into the SC. Due to the heterogeneous nature of the SC, the number and affinity of the SC binding sites may vary from chemical to chemical, depending upon molecular structure. For most lipophilic compounds, the PC PHSC/w was governed by the lipid domain, whereas PCs of the more hydrophilic