



Figure 3.31. (Continued.)

Once these conditions are met, we can attempt to deal with the potency, or binding affinity. This belongs to the domain of **three-dimensional quantitative structure-activity relationships (3D-QSARs)** (400) and we illustrate the use of a particular variant, **CoMFA** (187, 401), on ACE inhibitors at the end of this chapter. Condition 3.3 allows us to utilize compounds capable of presenting the **pharma-**

cophoric pattern, but incapable of binding, to help **determine** the location of **receptor-occupied** space in relation to the pharmacophore (receptor-mapping) (402). This allows a crude, low resolution map of the position of the receptor relative to the pharmacophoric elements and indicates in which directions chemical modifications may be productive.

The number and diversity of compounds