

Supporting Information Figure S3:

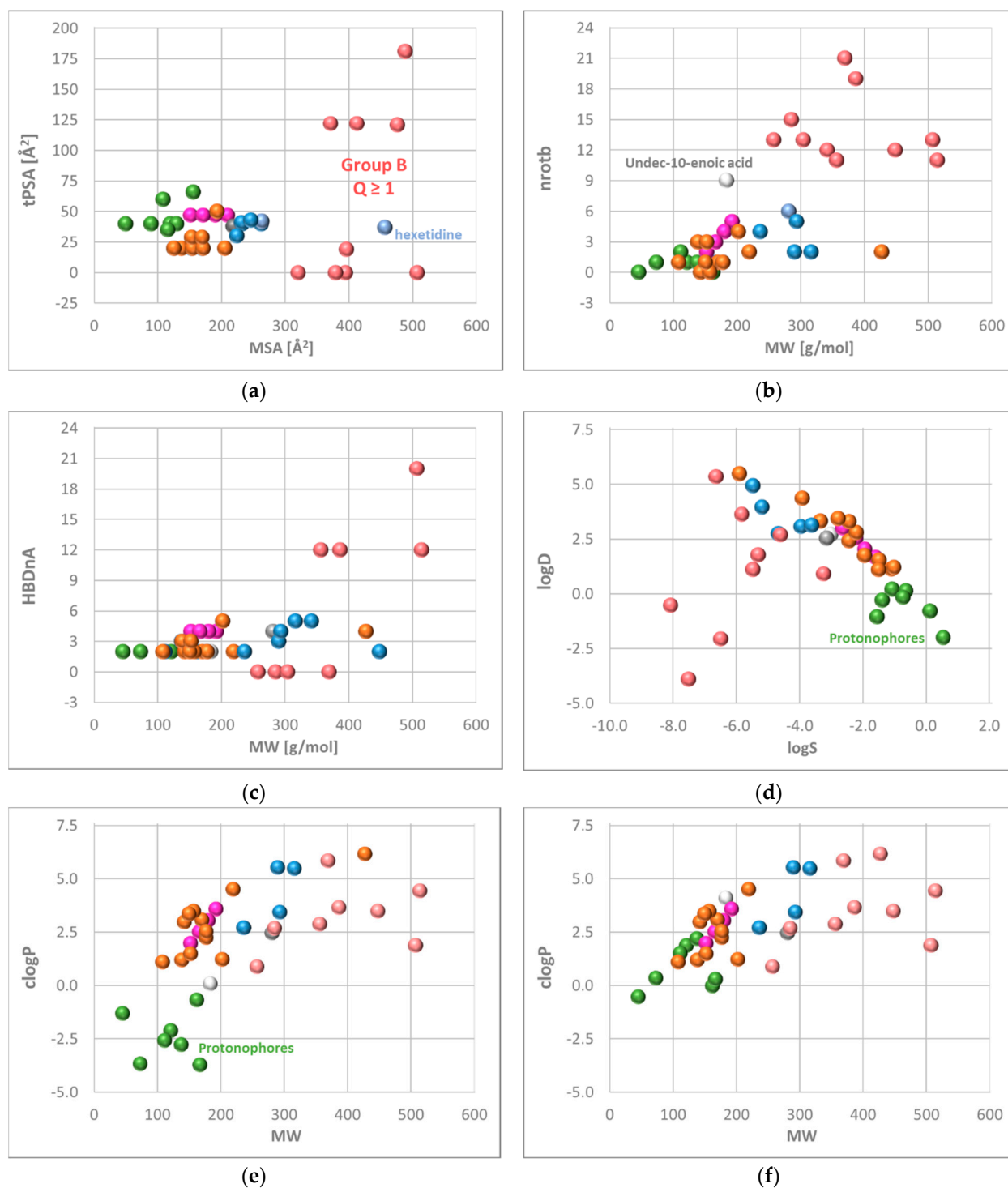


Figure S3. Two-dimensional plots for members of different mechanism-of-action categories:

(a) plot of topological polar surface area (tPSA) vs Connolly molecular surface area (MSA); (b) plot of number of rotatable bonds (nrotb) vs molecular weight (MW); (c) plot of hydrogen bonding capacity (HBDnA) vs molecular weight (MW); (d) plot of distribution coefficient (logD) vs aqueous solubility (logS); (e) plot of partition coefficient (clogP) of the predominant species vs molecular weight (MW); (f) plot of partition coefficient (clogP) of the active species vs molecular weight (MW).

Members of categories are colored as follows:

- **Protonophores**
- **Parabens (unclear mechanism)**
- **Solubilization of lipids and denaturing proteins**
- 3-Iodo-2-propynylbutylcarbamate
- **Intracellular enzyme inhibitors**
- **Interaction with mem-brane component destroying membrane integrity**