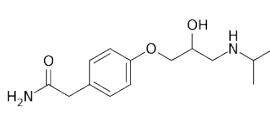
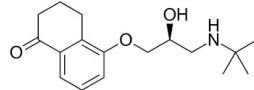
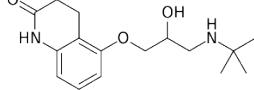
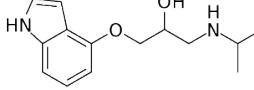
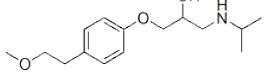
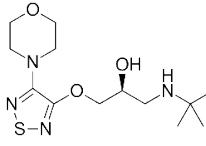
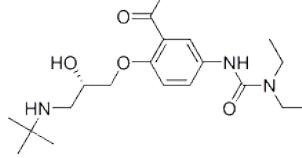
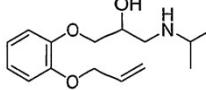
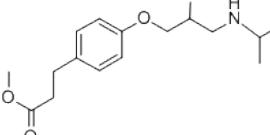


## Supplementary material

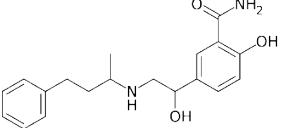
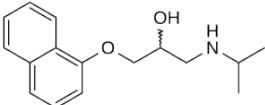
### Surfactant-mediated liquid chromatographic modes with sodium dodecyl sulphate for the analysis of basic drugs

N. Pankajkumar-Patel, E. Peris-García, M.J. Ruiz-Angel, M.C. García-Alvarez-Coque\*

**Table S1.** Structures, dissociation constants ( $pK_a$ ) in water, and octanol-water partition coefficients ( $\log P_{o/w}$ ) of the studied  $\beta$ -adrenoceptor antagonists.

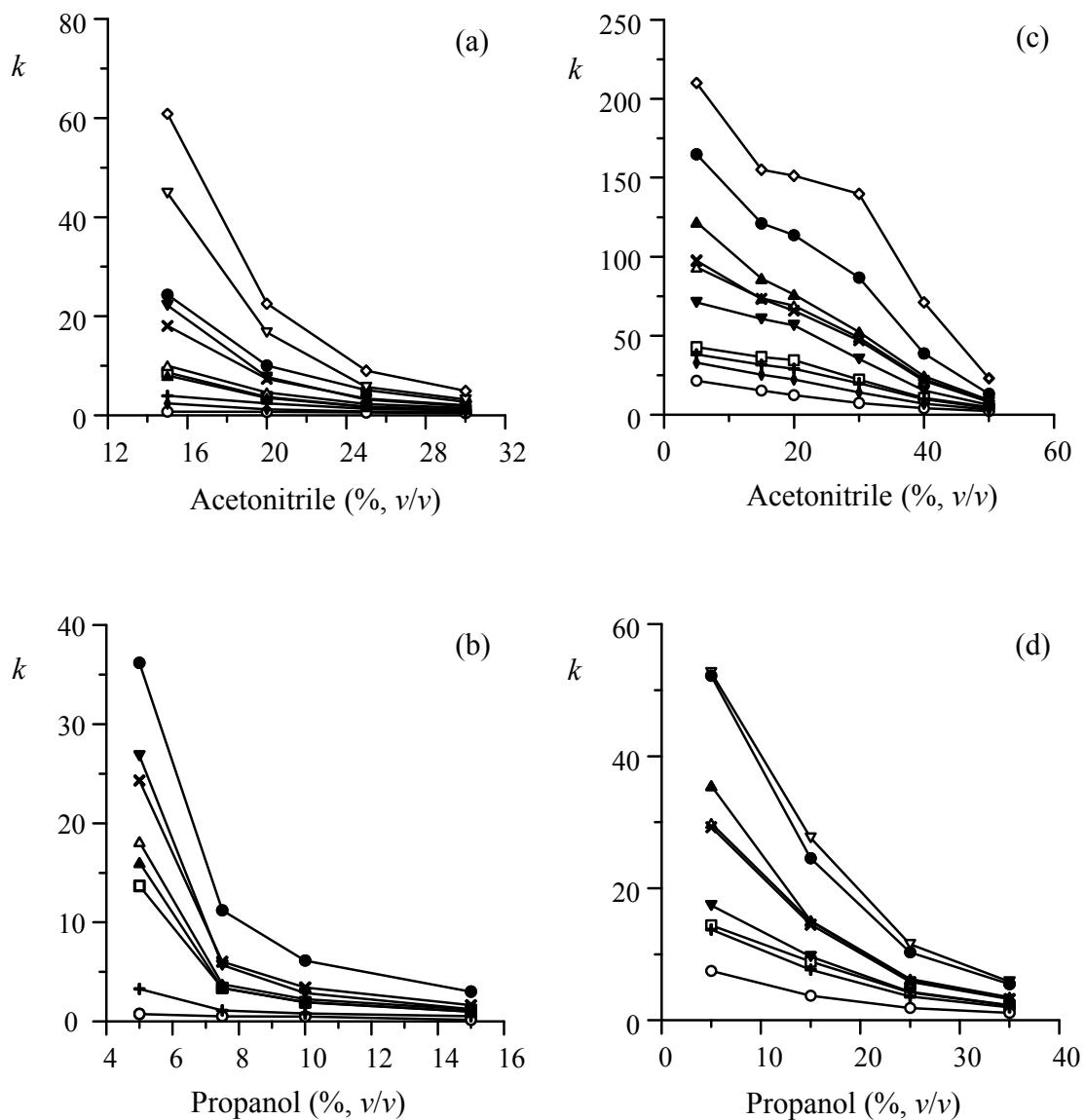
| Compound   | Code | Structure   | $pK_a$ <sup>a</sup> | $\log P_{o/w}$ <sup>b</sup> |
|------------|------|---|---------------------|-----------------------------|
| Atenolol   | 1    |    | 9.6                 | -0.026                      |
| Acebutolol | 2    |    | 9.2                 | 1.19                        |
| Carteolol  | 3    |  | NA                  | 1.42                        |
| Pindolol   | 4    |  | 8.8, 9.7            | 1.48                        |
| Metoprolol | 5    |  | 9.7                 | 1.69                        |
| Timolol    | 6    |  | 9.2                 | 1.75                        |
| Celiprolol | 7    |  | NA                  | 1.93                        |
| Oxprenolol | 8    |  | 9.5                 | 1.83                        |
| Esmolol    | 9    |  | NA                  | 2.00                        |

**Table S1** (continued).

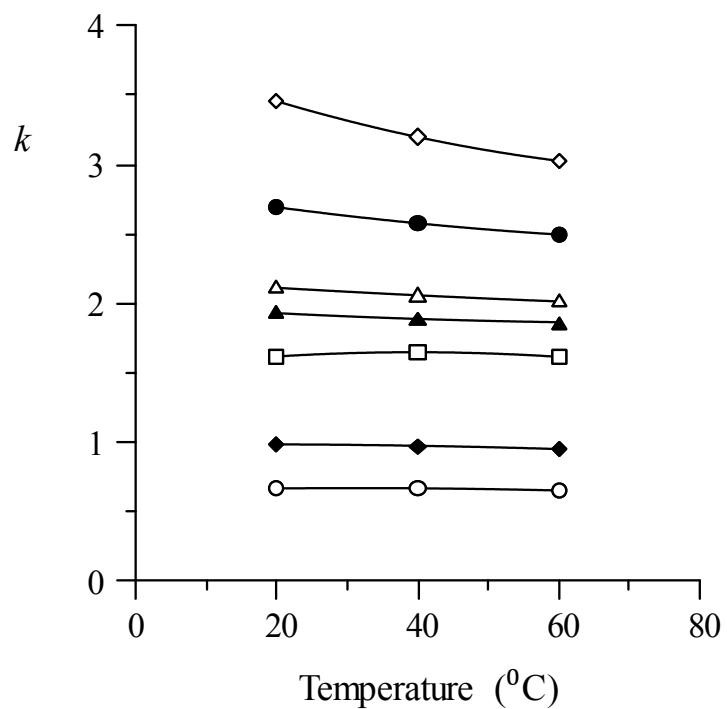
| Compound    | Code | Structure   | pK <sub>a</sub> <sup>a</sup> | log P <sub>o/w</sub> <sup>b</sup> |
|-------------|------|---|------------------------------|-----------------------------------|
| Labetalol   | 10   |  | 7.4, 8.7                     | 2.41                              |
| Propranolol | 11   |  | 9.5                          | 2.60                              |

<sup>a</sup> Ref. [30]. NA: not available

<sup>b</sup> Ref. [31]. Values calculated from the structure by applying the on-line interactive LOGKOW program of the Environmental Science Centre of Syracuse Research Corporation.



**Figure S1.** Variation of retention in RPLC (a,b) and MLC/HSLC with 0.075 M SDS (c,d), at increasing concentrations of acetonitrile (a,c), and 1-propanol (b,d). Solute identity: (□) acebutolol, (○) atenolol, (◆) carteolol, (▼) celiprolol, (x) esmolol, (▽) labetalol, (Δ) metoprolol, (●) oxprenolol, (+) pindolol, (◊) propranolol, and (▲) timolol.



**Figure S2.** Variation of retentions factors at increasing temperature, using the standard microemulsion mobile phase composition: 0.114 M SDS, 1.14% ( $v/v$ ) octane, 8.2% ( $v/v$ ) 1-butanol and 0.5% ( $v/v$ ) TFA. See Fig. S1 for solute identity.

**Table S2.** Efficiencies in RPLC, MLC and HSLC.<sup>a</sup>

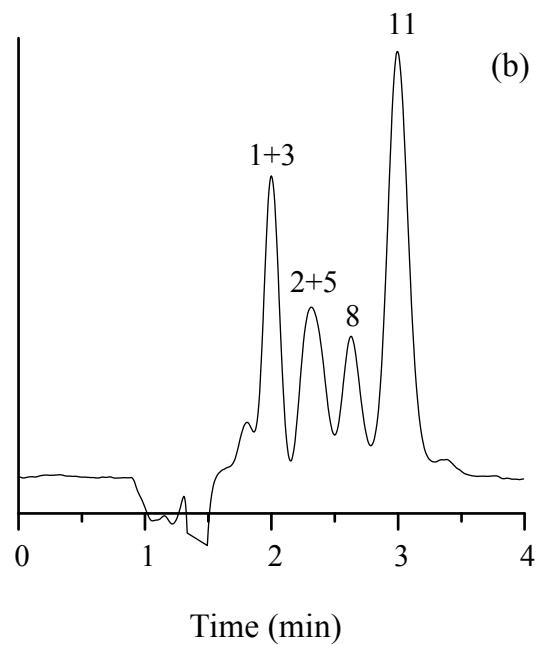
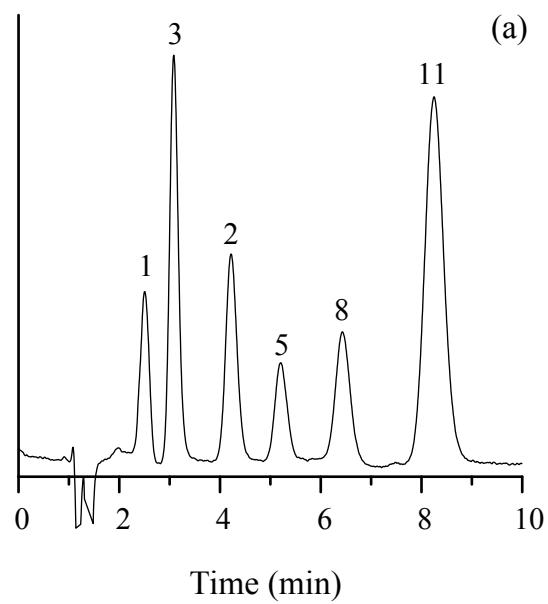
| Mobile phase | RPLC       |            | MLC                  |                       |                          | HSLC                  |                       |                        |                        |
|--------------|------------|------------|----------------------|-----------------------|--------------------------|-----------------------|-----------------------|------------------------|------------------------|
|              | 20% ACN    | 15% PrOH   | 0.15 M SDS<br>5% ACN | 0.15 M SDS<br>15% ACN | 0.1125 M SDS<br>10% PrOH | 0.15 M SDS<br>30% ACN | 0.15 M SDS<br>50% ACN | 0.15 M SDS<br>25% PrOH | 0.15 M SDS<br>35% PrOH |
| Acebutolol   | 1577       | 2202       | 1811                 | 2040                  | 2205                     | 3919                  | 2672                  | 1160                   | 770                    |
| Alprenolol   | 1328       |            | 1676                 | 2219                  |                          | 5664                  | 8486                  |                        |                        |
| Atenolol     | 997        | 1976       | 2588                 | 1552                  | 1711                     | 2598                  | 1711                  | 704                    | 338                    |
| Carteolol    | 943        |            | 2103                 | 1915                  |                          | 3525                  | 2196                  |                        |                        |
| Celiprolol   | 2139       | 2209       | 1879                 | 2184                  | 2171                     | 4377                  | 3221                  | 1147                   | 787                    |
| Esmolol      | 1848       | 2129       | 1577                 | 2384                  | 2868                     | 5209                  | 4692                  | 1459                   | 904                    |
| Labetalol    | 1604       | 1021       | 1711                 | 1839                  | 2160                     | 5075                  | 5907                  | 1696                   | 1092                   |
| Metoprolol   | 1797       | 1806       | 683                  | 2499                  | 2930                     | 5449                  | 5296                  | 1635                   | 1013                   |
| Nadolol      | 986        |            |                      | 1457                  |                          | 4024                  | 2612                  |                        |                        |
| Oxprenolol   | 1411       | 1069       | 2080                 | 2571                  | 3081                     | 6125                  | 6830                  | 2123                   | 1350                   |
| Pindolol     | 1670       | 4030       | 2068                 | 2157                  | 2337                     | 4187                  | 2719                  | 1110                   | 822                    |
| Propranolol  | 1228       |            | 974                  | 2023                  |                          | 5285                  | 7997                  |                        |                        |
| Timolol      | 1679       | 1995       | 2464                 | 2457                  | 3001                     | 5459                  | 6165                  | 1628                   | 1084                   |
| Mean         | 1500 ± 300 | 2000 ± 900 | 1800 ± 500           | 2100 ± 300            | 2500 ± 500               | 5000 ± 1000           | 4700 ± 2300           | 1400 ± 400             | 900 ± 300              |

<sup>a</sup> Ref. [43].

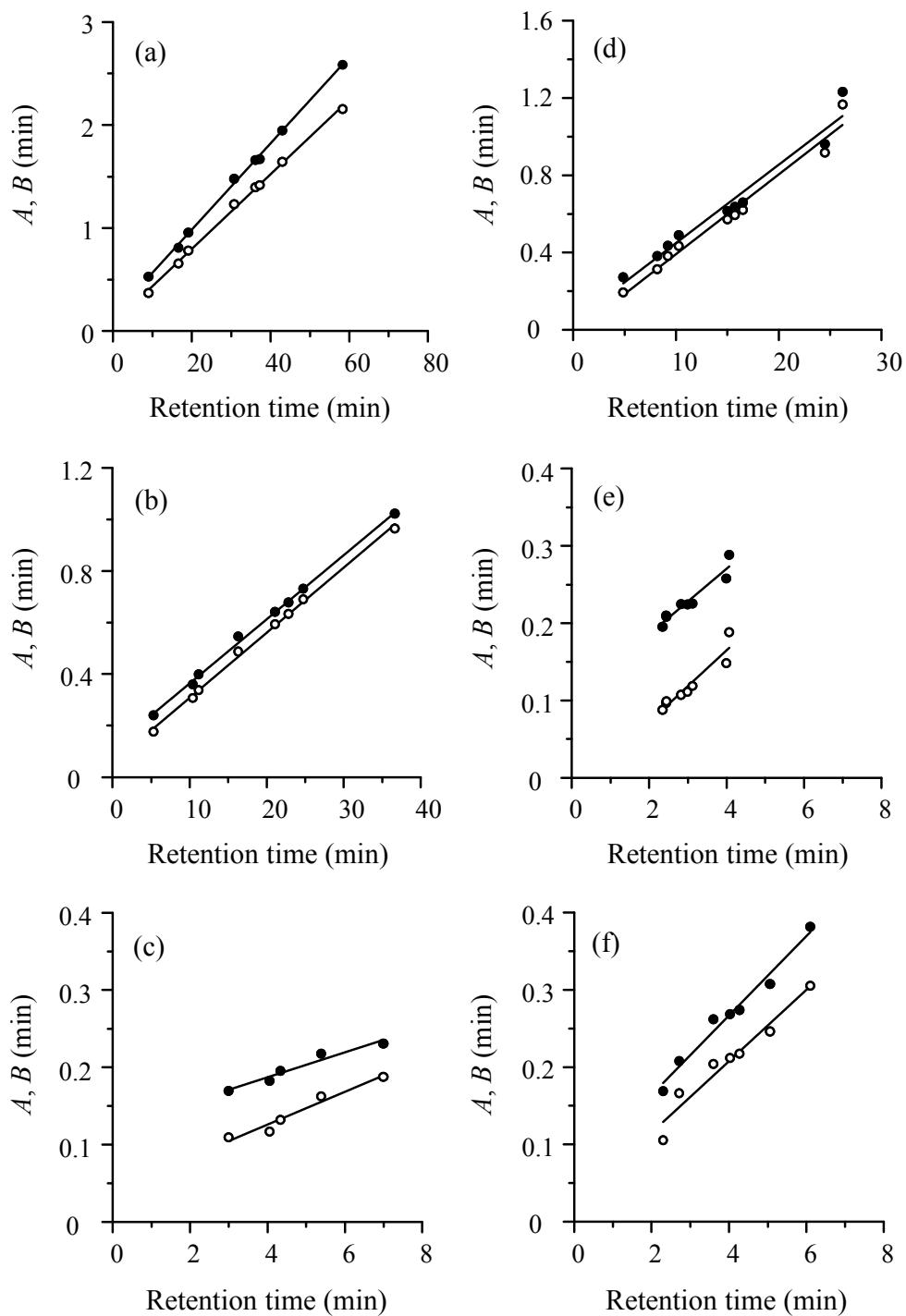
**Table S3.** Efficiencies in MELC.

| Mobile phase | MELC  |   |   |  |
|--------------|---|---|---|--|
|              | 0.114 M SDS / 1.14% octane / 8.2% 1-butanol | 0.173 M SDS / 1.14% octane / 8.2% 1-butanol | 0.114 M SDS / 0.28% octane / 8.2% 1-butanol | 0.114 M SDS / 1.14% octane / 17.3% 1-butanol |
| Acebutolol   | 977   | 973   | 1421  | 1328   |
| Atenolol     | 1022  | 1266  | 1107  | 2218   |
| Carteolol    | 874   | 831   | 1266  | 1061   |
| Metoprolol   | 1256  | 1271  | 1871  | 1366   |
| Oxprenolol   | 1393  | 1138  | 2053  | 1457   |
| Propranolol  | 1315  | 1279  | 1987  | 1403   |
| Timolol      | 1162  | 1145  | 1644  | 1446   |
| Mean         | 1100 ± 190                                  | 1130 ± 170                                  | 1600 ± 400                                  | 1500 ± 400                                   |

<sup>a</sup> Ref. [43].



**Figure S3.** Experimental chromatograms obtained for mixtures of  $\beta$ -adrenoceptor antagonists in MELC with: (a) 0.114 M SDS / 0.28% octane / 8.2% 1-butanol, and (b) 0.114 M SDS / 1.14% octane / 17.3% 1-butanol, using the XTerra column. See Section 2.1 for peak identity.



**Figure S4.** Half-width plots (left ( $\circ$ ) and right ( $\bullet$ )) for the  $\beta$ -adrenoceptor antagonists eluted with: (a) MLC (0.15 M SDS/15% acetonitrile), (b) HSLC (0.15 M SDS/30% acetonitrile), (c) HSLC (0.15 M SDS/50% acetonitrile), (d) MLC (0.1125 M SDS/10% 1-propanol), (e) HSLC (0.15 M SDS/35% 1-propanol), (f) MELC (0.114 M SDS/1.14% octane/8.2% 1-butanol).