Supplementary Information

Table SI summarized the relationship between the interaction energy difference (ΔΔE) and the resolution (Rs) for several chiral drugs separated by capillary electrophoresis using β-cyclodextrin derivatives as selectors. Combining the results of the experiments and theoretical calculations, we concluded that the chiral drugs can be separated when the interaction energy differences between each pair of enantiomers and chiral selectors were greater than or approximately equal to 6 kJ mol^{-1}. The corresponding electropherograms and chemical structures of the chiral drugs separated by CE can be seen in Figure 1-23.

Table SI. The interaction energy difference (ΔΔE) and resolution (Rs) for several chiral drugs separated by CE

Chiral drugs	β -CD derivatives	ΔΔE (kJ mol^{-1})	Rs
Tulobuterol	6-Sulfated-β-CD	15.41	6.17
Clorprenaline	6-Sulfated-β-CD	10.92	1.50
Glycopyrrolate	6-Sulfated-β-CD	13.33/7.15/11.09	8.8/2.2/10.09
Pheniramine	6-Sulfated-β-CD	14.27	6.11
Chlorpheniramine	6-Sulfated-β-CD	21.84	22.06
Brompheniramine	6-Sulfated-β-CD	37.68	30.22
Anisodamine	6-Sulfated-β-CD	13.04	5.8
Atropine	6-Sulfated-β-CD	18.30	11.65
Atropine Methyl bromide	6-Sulfated-β-CD	16.52	7.09
Homatropine	6-Sulfated-β-CD	20.74	20.02
Oxybutynin	6-Sulfated-β-CD	12.66	4.93
Salmeterol	6-Sulfated-β-CD	5.89	/
Tropicamide	6-Carboxymethyl-β-CD	12.60	5.13
Homatropine Hydrobromide	6-Carboxymethyl-β-CD	17.38	6.29
Homatropine Methyl bromide	6-Carboxymethyl-β-CD	10.27	4.67
Atropine	6-Carboxymethyl-β-CD	11.82	4.85
Atropine Methobromide	6-Carboxymethyl-β-CD	9.53	4.59
Anisodamine	6-Carboxymethyl-β-CD	6.05/18.97/9.22	1.13/6.92/2.58
Anisodamine	2,6- Glycine-β-CD	8.34	1.68
Gatifloxacin	2,6-Sulfamic acid-β-CD	5.83	/
Ofloxacin	2,6-Sulfamic acid-β-CD	5.96	/
Fleroxacin	2,6-Sulfamic acid-β-CD	5.72	/
Ciprofloxacin	2,6-Sulfamic acid-β-CD	4.99	/
Leucovorin Calcium	6- Cyclohexane-β-CD	2.21	/
Leucovorin Calcium	6- Butyl amine-β-CD	4.49	/

Electropherograms and chemical structures of the chiral compounds using β-cyclodextrin derivatives as selectors separated by capillary electrophoresis were summarized as following:

1. Tulobuterol separated by 6-Sulfated β-cyclodextrin

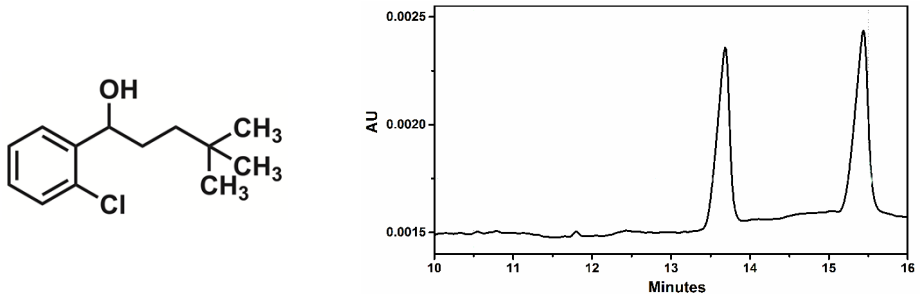

Figure 1. Electropherogram and chemical structure of Tulobuterol separated by 6-Sulfated β-cyclodextrin.

2. Clorprenaline separated by 6-Sulfated β-cyclodextrin

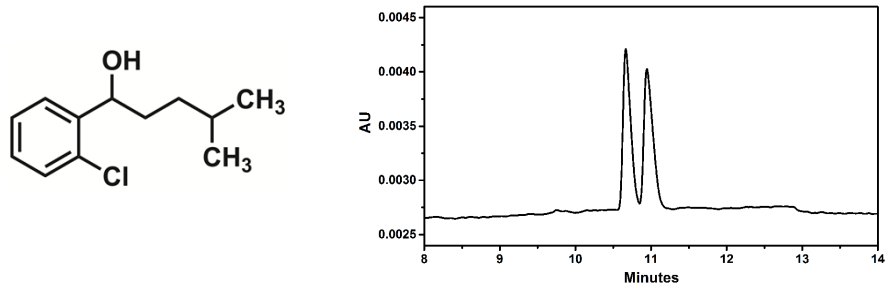

Figure 2. Electropherogram and chemical structure of Clorprenaline separated by 6-Sulfated β-cyclodextrin.

3. Glycopyrrolate separated by 6-Sulfated β-cyclodextrin

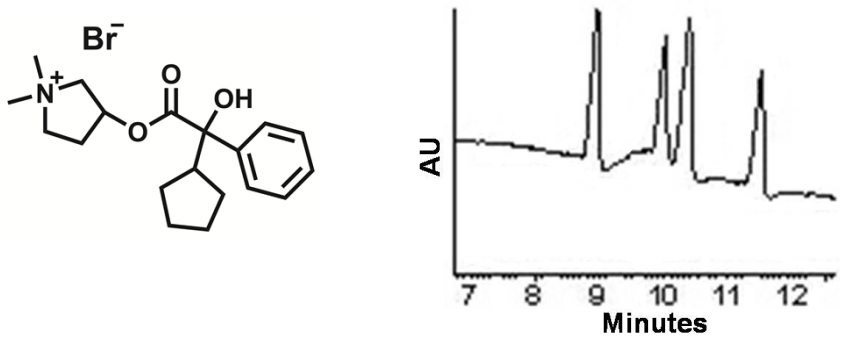

Figure 3. Electropherogram and chemical structure of Glycopyrrolate separated by 6-Sulfated β-cyclodextrin.

4. Anisodamine separated by 6-Sulfated β-cyclodextrin

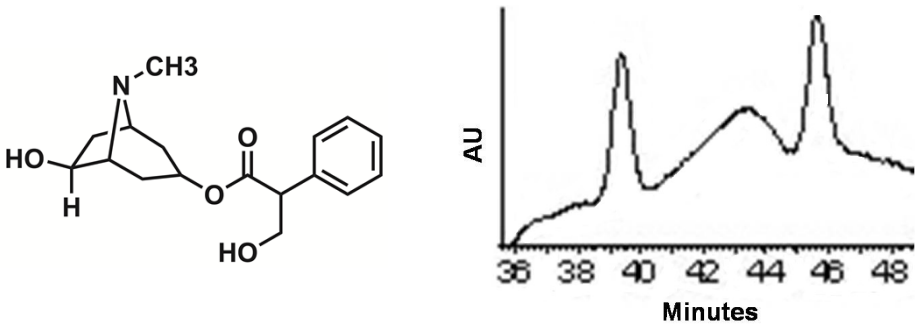

Figure 4. Electropherogram and chemical structure of Anisodamine separated by 6-Sulfated β-cyclodextrin.

5. Atropine separated by 6-Sulfated β-cyclodextrin

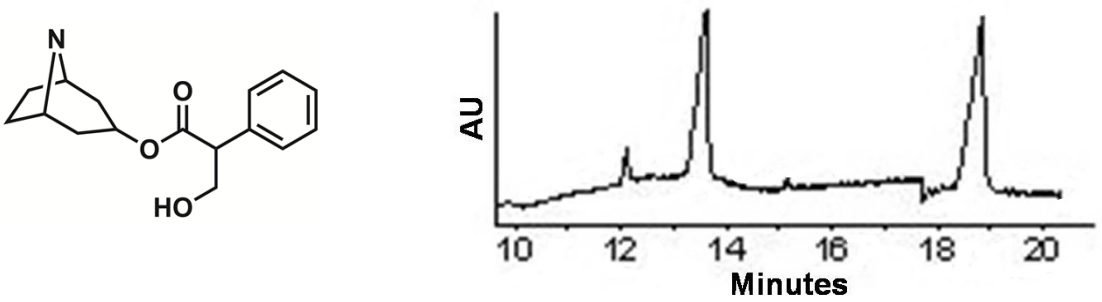

Figure 5. Electropherogram and chemical structure of Atropine separated by 6-Sulfated β-cyclodextrin.

6. Atropine Methyl bromide separated by 6-Sulfated β-cyclodextrin

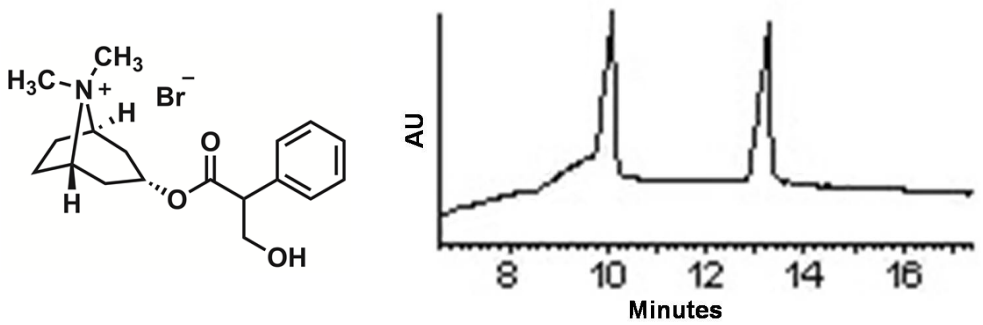

Figure 6. Electropherogram and chemical structure of Atropine Methyl bromide separated by 6-Sulfated β-cyclodextrin.

7. Homatropine separated by 6-Sulfated β-cyclodextrin

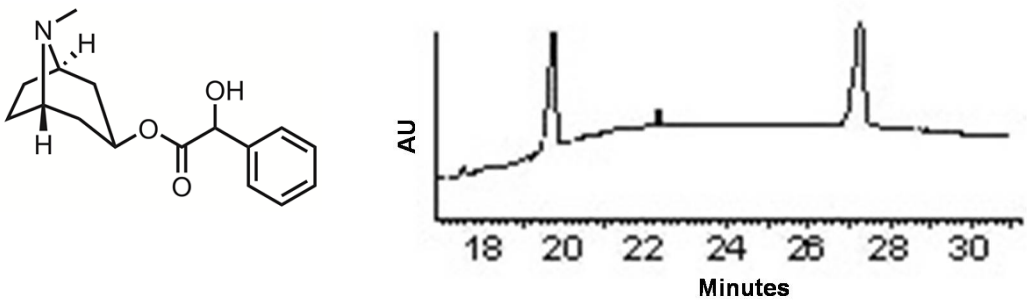

Figure 7. Electropherogram and chemical structure of Homatropine separated by 6-Sulfated β-cyclodextrin.

8. Oxybutynin separated by 6-Sulfated β-cyclodextrin

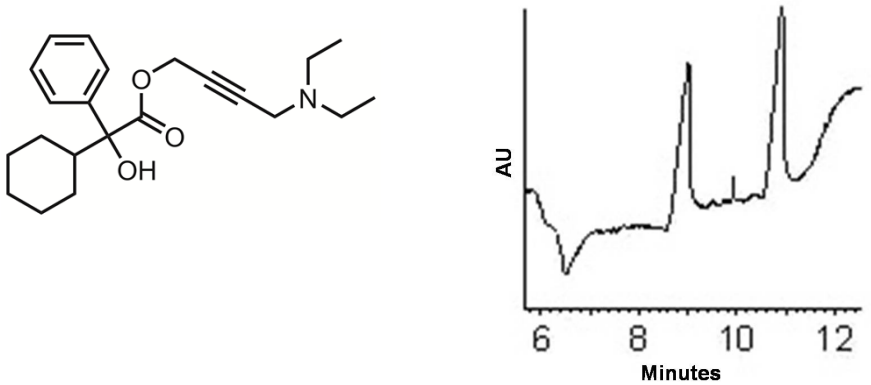

Figure 8. Electropherogram and chemical structure of Oxybutynin separated by 6-Sulfated β-cyclodextrin.

9. Salmeterol separated by 6-Sulfated β-cyclodextrin

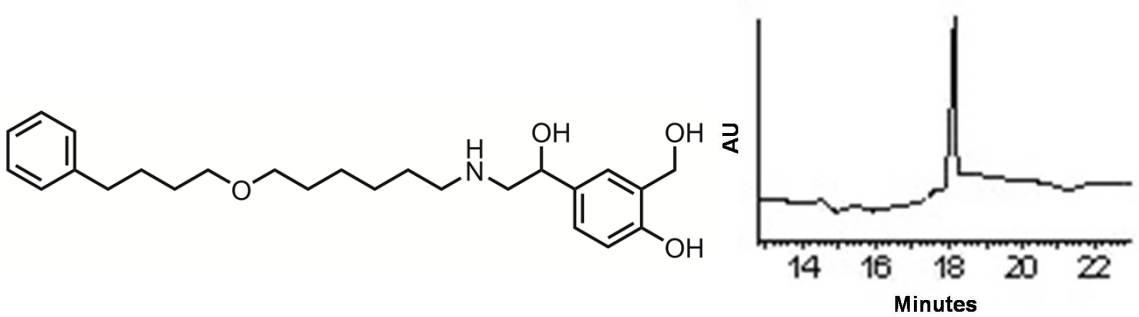

Figure 9. Electropherogram and chemical structure of Salmeterol separated by 6-Sulfated β-cyclodextrin.

10. Tropicamide separated by 6-Carboxymethyl β-cyclodextrin

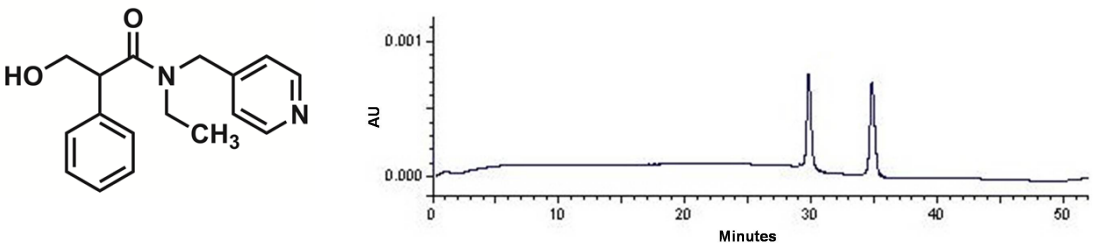

Figure 10. Electropherogram and chemical structure of Tropicamide separated by 6-Carboxymethyl β-cyclodextrin.

11. Homatropine Hydrobromide separated by 6-Carboxymethyl β-cyclodextrin

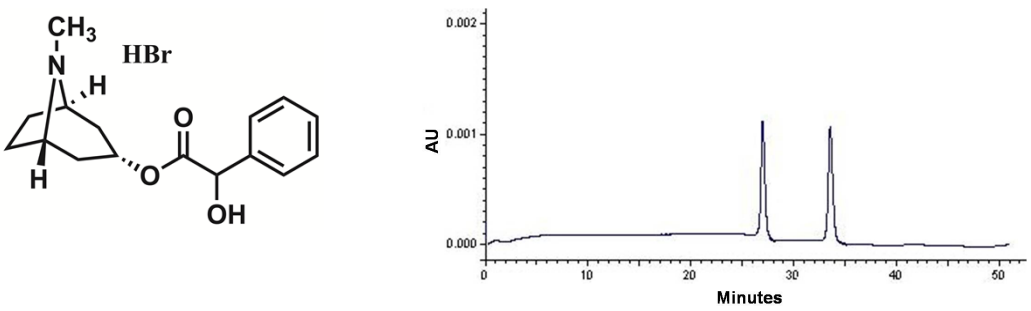

Figure 11. Electropherogram and chemical structure of Homatropine Hydrobromide separated by 6-Carboxymethyl β-cyclodextrin.

12. Homatropine Methyl bromide separated by 6-Carboxymethyl β-cyclodextrin

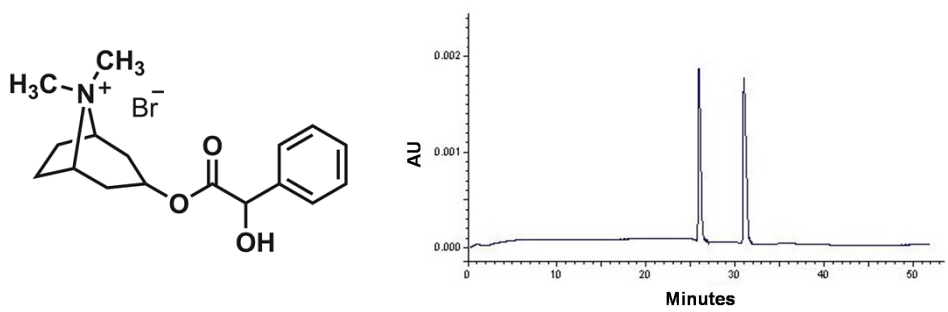

Figure 12. Electropherogram and chemical structure of Homatropine Methyl bromide separated by 6-Carboxymethyl β-cyclodextrin.

13. Atropine separated by 6-Carboxymethyl β-cyclodextrin

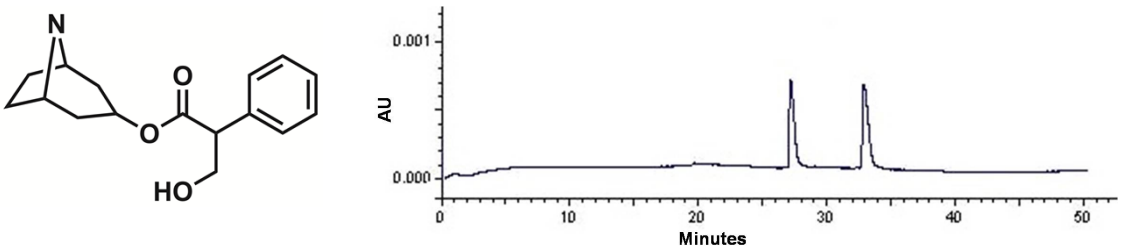

Figure 13. Electropherogram and chemical structure of Atropine separated by 6-Carboxymethyl β-cyclodextrin.

14. Atropine Methobromide separated by 6-Carboxymethyl β-cyclodextrin

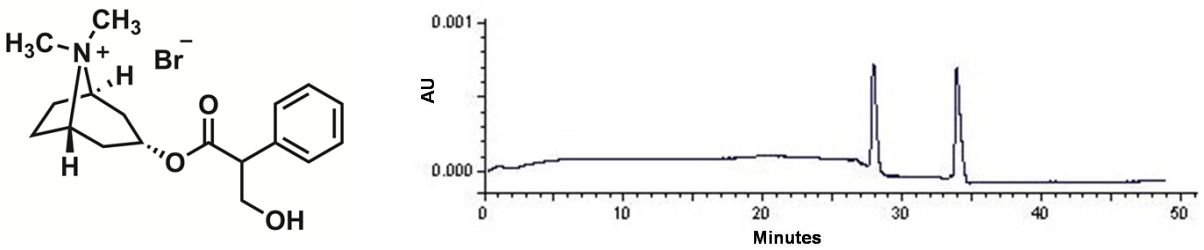

Figure 14. Electropherogram and chemical structure of Atropine Methobromide separated by 6-Carboxymethyl β-cyclodextrin.

15. Anisodamine separated by 6-Carboxymethyl β-cyclodextrin

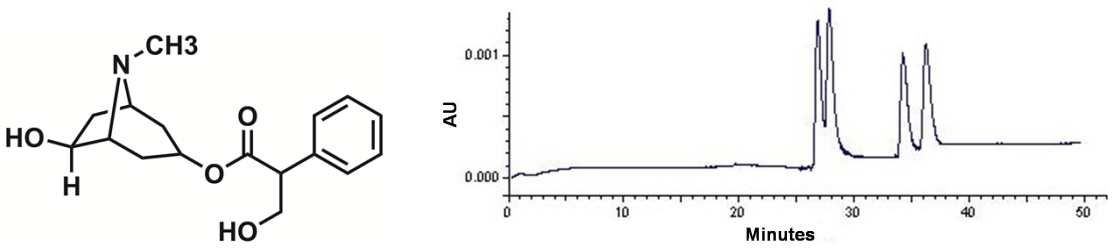

Figure 15. Electropherogram and chemical structure of Anisodamine separated by 6-Carboxymethyl β-cyclodextrin.

16. Anisodamine separated by 2,6- Glycine β-cyclodextrin

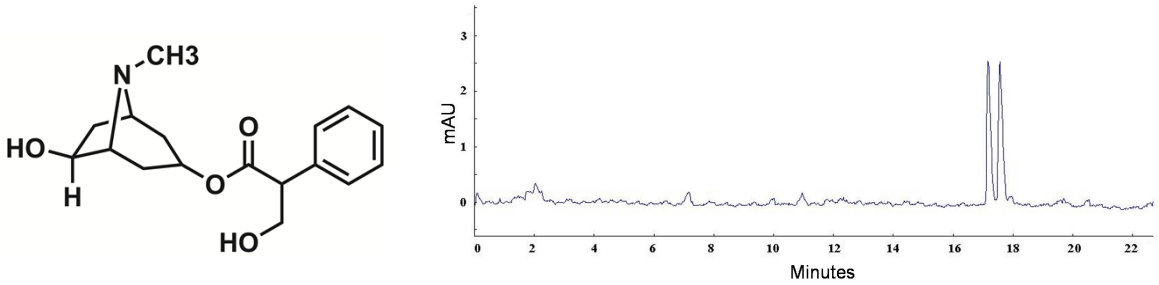

Figure 16. Electropherogram and chemical structure of Anisodamine separated by 2,6- Glycine β-cyclodextrin.

17. Gatifloxacin separated by 2,6-Sulfamic acid β-cyclodextrin

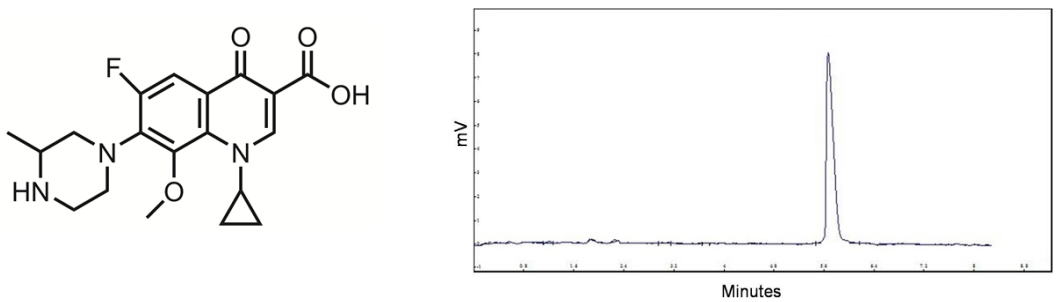

Figure 17. Electropherogram and chemical structure of Gatifloxacin separated by 2,6-Sulfamic acid β-cyclodextrin.

18. Ofloxacin separated by 2,6-Sulfamic acid β-cyclodextrin

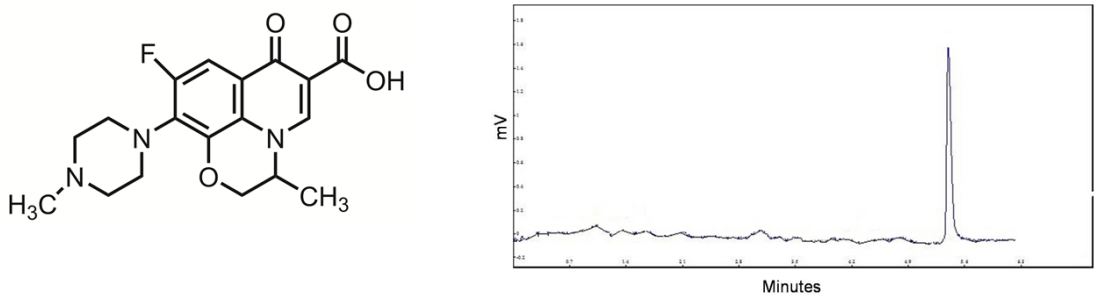

Figure 18. Electropherogram and chemical structure of Ofloxacin separated by 2,6-Sulfamic acid β-cyclodextrin.

19. Fleroxacin separated by 2,6-Sulfamic acid β-cyclodextrin

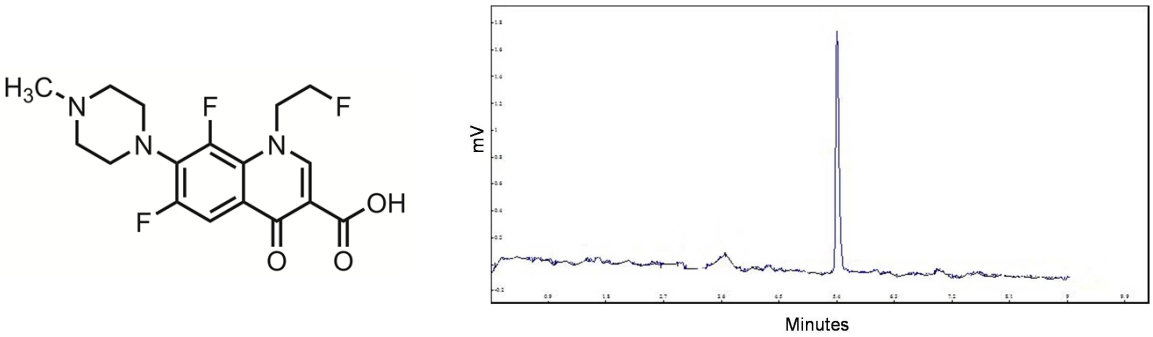

Figure 19. Electropherogram and chemical structure of Fleroxacin separated by 2,6-Sulfamic acid β-cyclodextrin.

20. Ciprofloxacin separated by 2,6-Sulfamic acid β-cyclodextrin

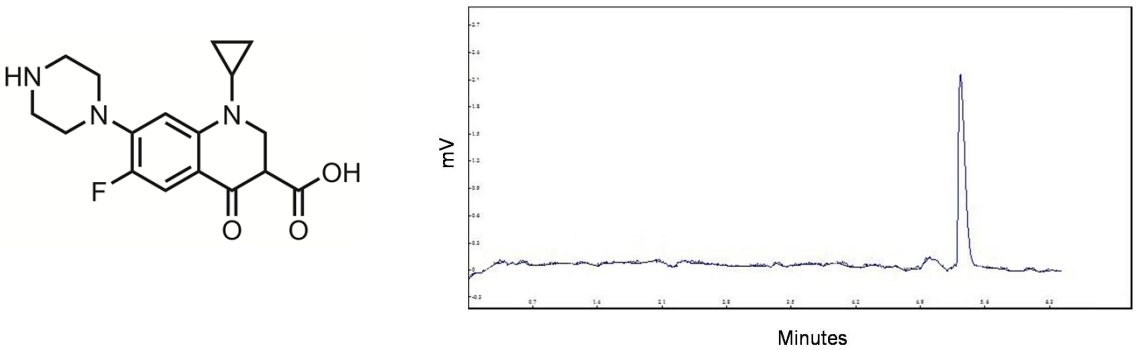

Figure 20. Electropherogram and chemical structure of Ciprofloxacin separated by 2,6-Sulfamic acid β-cyclodextrin.

21. Pheniramine separated by 6-Sulfated β-cyclodextrin

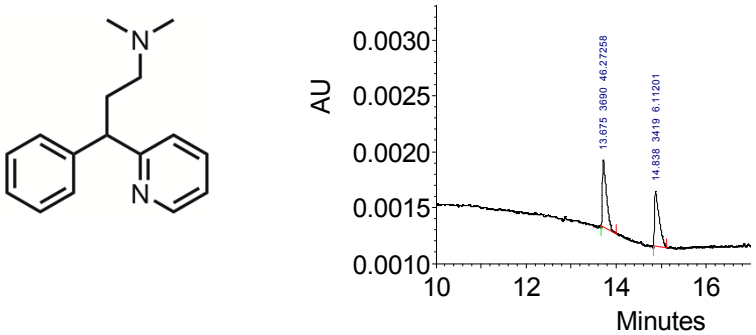

Figure 21. Electropherogram and chemical structure of Pheniramine separated by 6-Sulfated β-cyclodextrin.

22. Chlorpheniramine separated by 6-Sulfated β-cyclodextrin

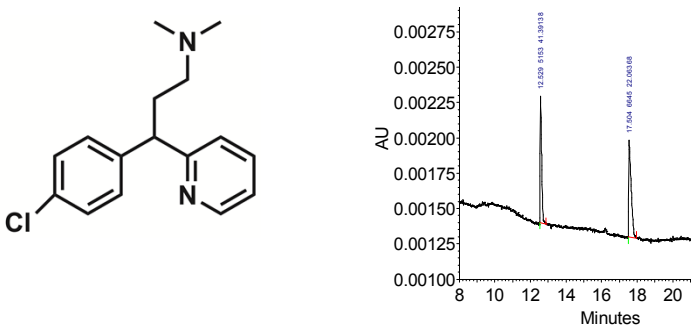

Figure 22. Electropherogram and chemical structure of Chlorpheniramine separated by 6-Sulfated β-cyclodextrin.

23. Brompheniramine separated by 6-Sulfated β-cyclodextrin

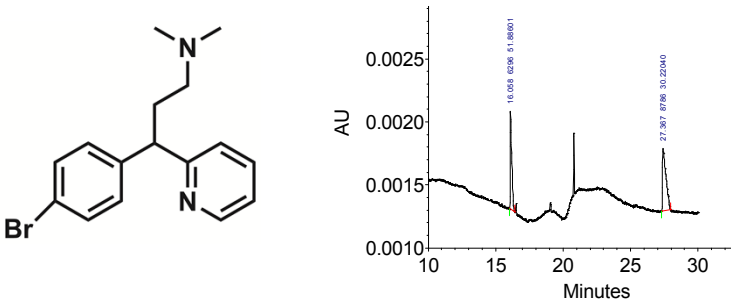

Figure 23. Electropherogram and chemical structure of Brompheniramine separated by 6-Sulfated β-cyclodextrin.