CD spectra of pharmaceutical substances - Steroids (8)

1. Spironolactone

Spironolactone, synthesized as a compound that inhibits the accumulation of sodium by androsterone and displays diuretic activity, is used orally as an antihypertensive drug.[1)]

Figure 1 shows the CD/UV spectra of spironolactone. The UV spectral absorption in the wavelength region from 350 to 300 nm is assigned to the n-π* transition (R-band) of α, β-unsaturated ketone (enone), and the corresponding CD shows a negative sign that agrees with that of testostelone.[2)] The UV absorption and positive CD in the wave length region from 300 to 270 nm can be assigned to the n-π* transition[3)] of the 7α-thioacetyl group. The UV absorption in the far-ultraviolet region less than 250 nm can be assigned to two transitions that overlap each other, the π-π* transition (K-band) of enone and the π-π* transition[3)] of the thioacetyl group. The corresponding negative CD (testosterone shows a positive CD) is considered to be due to the result of the interaction between both of the chromophores.

2. Potassium canrenoate

Potassium canrenoate, synthesized using an intermediate product in the synthesis of spironolactone, is used in intravenous injections as a potassium-sparing diuretic agent.[1)]

Figure 2 shows the CD/UV spectra of potassium canrenoate. The UV absorption in the wavelength region from 400 to 310 nm is assigned to the R-band of the $\Delta^{4,6}$-diene-3-one (linear dienone). The corresponding positive CD agrees with that of the chlormadinone acetate.[4)] In the shorter wave length region below 310 nm, the UV absorption due to the K-band of the linear dienone and the corresponding negative CD are observed.

References

1) The Manual of Japanese Pharmacopoeia, 12th Edition, Hirokawa Shoten, 1991

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1] Wavelength (nm)
2] Sample: Wako Pure Chemicals Industries, Biochemical reagent, Dioxane solution
400 - 256 nm: 5.0 mg / 10 ml (1.2 mM), 10 mm Cell
280 - 206 nm: 5.0 m g/ 20 ml (0.60 mM), 1 mm Cell
3] Measurement apparatus
CD: J-720W Circular Dichroism Spectrophotometer
UV: Ubest V-560 Ultraviolet and Visible Light Spectrophotometer
4] The structure of spironolactone
5] IR spectrum (KBr tablet method)
6] Measurement apparatus: FT/IR-350
7] Figure 1. The CD/UV and IR spectra of spironolactone
8] Sample: SIGMA D-7287, Ethanol solution
450 - 314 nm: 5.0 mg / 10 ml (1.3 mM), 10 mm Cell
320 - 192 nm: 5.0 mg / 20 ml (0.63 mM), 1 mm Cell
9] The structure of potassium canrenoate
10] Figure 2. The CD/UV and IR spectra of potassium canrenoate

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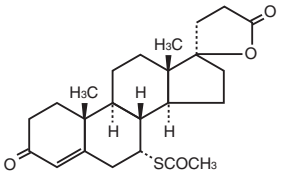
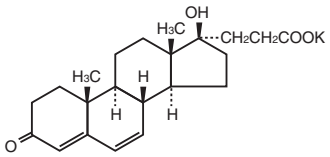
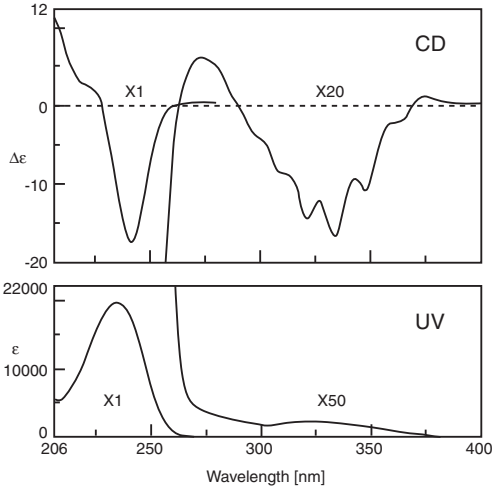
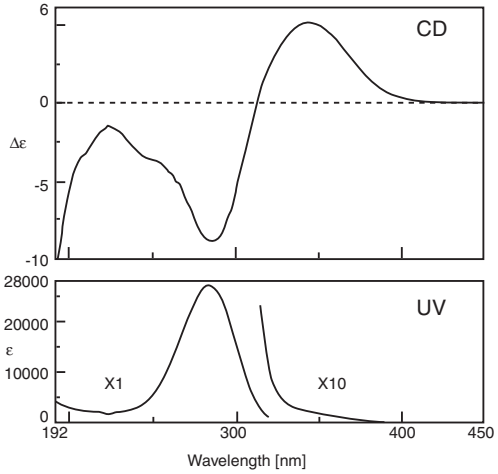


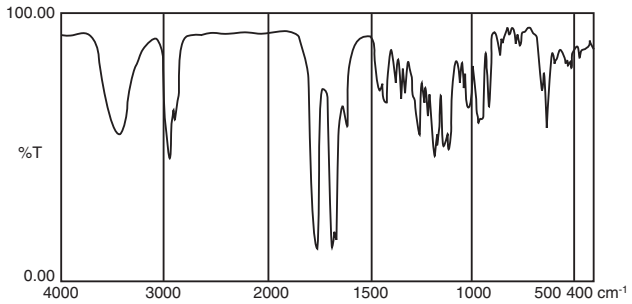
7a -Acetylthio-3-oxo-17a-pregn-4-ene-21, 17b-catbolactone (Spironolactone)
$C_{24}H_{32}O_4S$=416.58

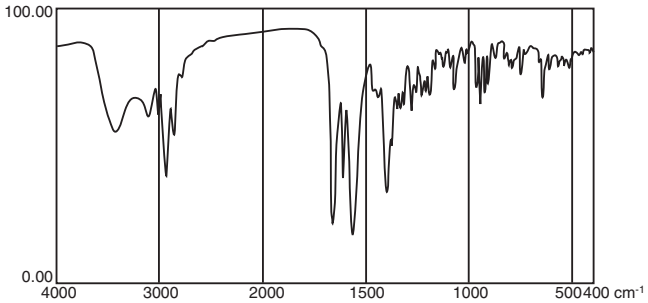


17-Hydroxy-3-oxo-17α-pregna-4, 6-diene-21-carboxylate potassium salt (Potassium canrenoate) $C_{22}H_{29}O_4K$=396.57









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