REACTIONS OF 1-(3,4-DIETHOXYBENZYLIDENE)-6,7-DIETHOXY-1,2,3,4-TETRAHYDROISOQUINOLINE WITH POLYFLUOROCARBONYL COMPOUNDS

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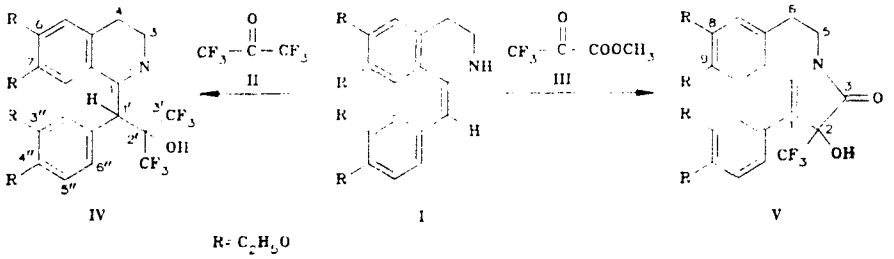
In our search for novel methods of modifying the biological activity of compounds containing fluorinated substituents we have studied the reaction of 1-(3,4-diethoxybenzylidene)-6,7-diethoxy-1,2,3,4-tetrahydroisoquinoline (I) with hexafluoroacetone (II) and with methyl trifluoropyruvate (III).

The starting I is hydroxyalkylated at 20°C by ketone II or ketoester III at the exocyclic β-C-atom. In the case of ketoester III this is accompanied by lactamization. Reaction of equimolecular amounts of the reagents in Freon-113 over 24 h leads to products IV and V in ≈95% yields.



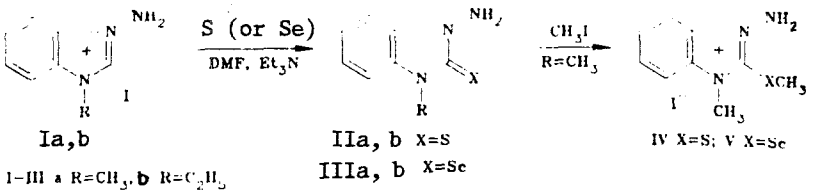
IV I V

R= C_2H_5O

1-[2-Hydroxy-1-(3,4-diethoxyphenyl)-2-trifluoromethyl-3,3,3-trifluoropropyl]-7,8-diethoxy-3,4-dihydroisoquinoline (IV). Mp 78-79°C (from aqueous acetone). PMR spectrum: [$(CD_3)_2CO$], δ: 1.20-1.41 (12H, m, $4CH_3$); 2.67 (2H, m, 3-H); 3.75 (2H, m, 4-H); 3.90-4.20 (8H, m, $4CH_2$); 4.81 (1H, s, CH); 6.85 (1H, s, 2"-H); 6.87 (1H, d, 5"-H); 7.22 (1H, d, 6"-H); 7.35 ppm (2H, s, 5- and 8-CH).

2-Hydroxy-1-(3,4-diethyoxyphenyl)-3-oxo-2-trifluoromethyl-8,9-diethoxy-2,3,5,6-tetrahydropyrrolo[2,1-*a*]isoquinoline (V). Mp 161-162°C (from pentane). PMR spectrum: [$(CD_3)_2CO$], δ: 1.22-1.42 (12H, m, $4CH_3$); 2.98 (2H, m, 5-H); 3.51 (2H, m, 6-H); 6.72-7.00 ppm (5H, H_{Ar}). ^{19}F NMR spectrum [$(CD_3)_2CO$], δ: 0.25 (s, CF_3).

Elemental analytical data for IV and V agreed with those calculated.



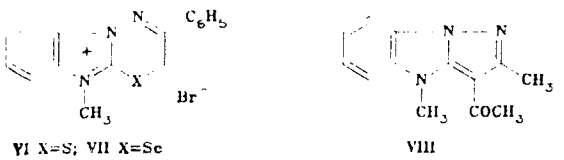
Ia,b

I–III a R=CH_3, b R=C_2H_5

IIa, b X=S

IIIa, b X=Se

IV X=S; V X=Se



VI X=S; VII X=Se

VIII

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