Part IV

Some 2-(2-Carboxyethyl)amino-1,4-naphthoquinone Derivatives

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1,4-Naphthoquinone has been treated with β-alanine and with its ethyl ester to yield 2-(2-carboxyethyl)amino-1,4-naphthoquinone (I) and its ethyl ester (II), respectively. The former has been cyclized to a quinoline derivative (IV) and the latter has been converted to the corresponding amide (III).

IN GENERAL, 1,4-benzoquinones undergo 1,4-addition reactions with amines to yield aminophenols. If excess quinone is used the resulting aminophenols are oxidized to aminoquinones.

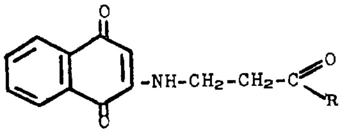
In the present study, a reaction between a β-amino acid (β-alanine) and two moles of 1,4-naphthoquinone in boiling 95% ethanol produced 2-(2-carboxyethyl)amino-1,4-naphthoquinone (I). Similarly, the ethyl ester of β-alanine, on treatment with 1,4-naphthoquinone in 95% ethanol at room temperature, has produced 2-(2-carbethoxyethyl)amino-1,4-naphthoquinone (II). The latter (II) has been converted to the corresponding amide (III) by means of methanolic ammonia. The acid (I) has been cyclized to 4,5,10-trioxo-1,2,3,4,5,10-hexahydrobenzo [g] quinoline (IV) by means of heating in polyphosphoric acid at 100° C. The product was isolated by addition of water to the reaction mixture, and filtering.

Physical properties, yields, analyses, and other data of I through IV are reported in Table I. All melting points are uncorrected and were taken in capillary tubes immersed in an oil bath except that of IV where the tube was placed in a metal block heated by a flame. Analytical samples were all obtained by recrystallization from 95% ethanol.

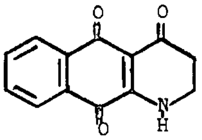
Table I. Data for Compounds I through IV

Compound	Yield, %	M.P., ° C.	Formula	Nitrogen, % Calcd.	Nitrogen, % Found	Color	Time Allowed for Reaction, Hours
I	82.7	204–206	$C_{13}H_{11}NO_4$	5.71	5.67	Dk. red	5
II	21.6	123.5–125	$C_{15}H_{15}NO_4$	5.03	5.12	Dk. red	44
III	56.5	238–241	$C_{13}H_{12}N_2O_3$	11.47	11.13	Orange	18
IV	33.7	220–315d.	$C_{13}H_9NO_3^a$	6.16	6.13	Dk. brown	1.7

[a] Calcd: C, 68.71; H, 3.99. Found: C, 68.84; H, 4.01.



I, R = OH   II, R = OC_2H_5
III, R = NH_2



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