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NOMENCLATURE OF BENZYLISOQUINOLINE AND RELATED ALKALOIDS

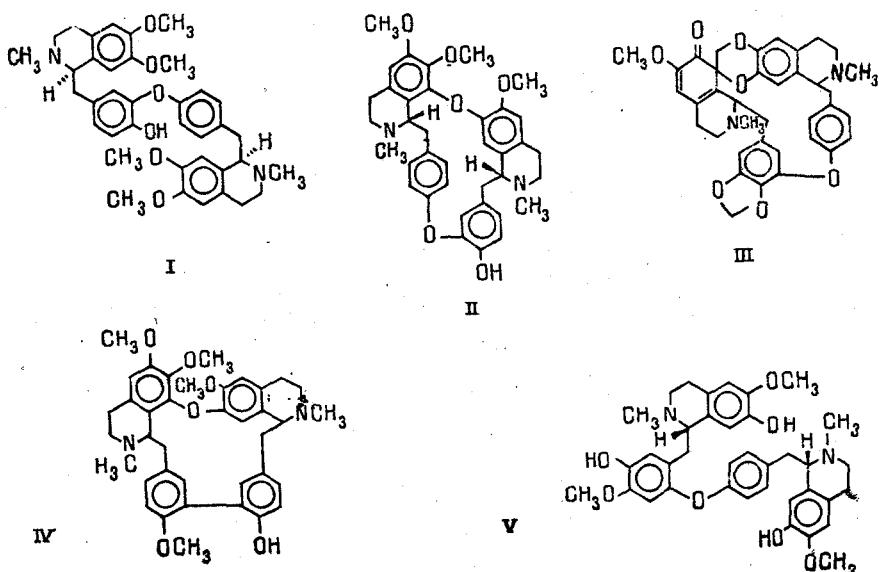
O. N. Tolkataev

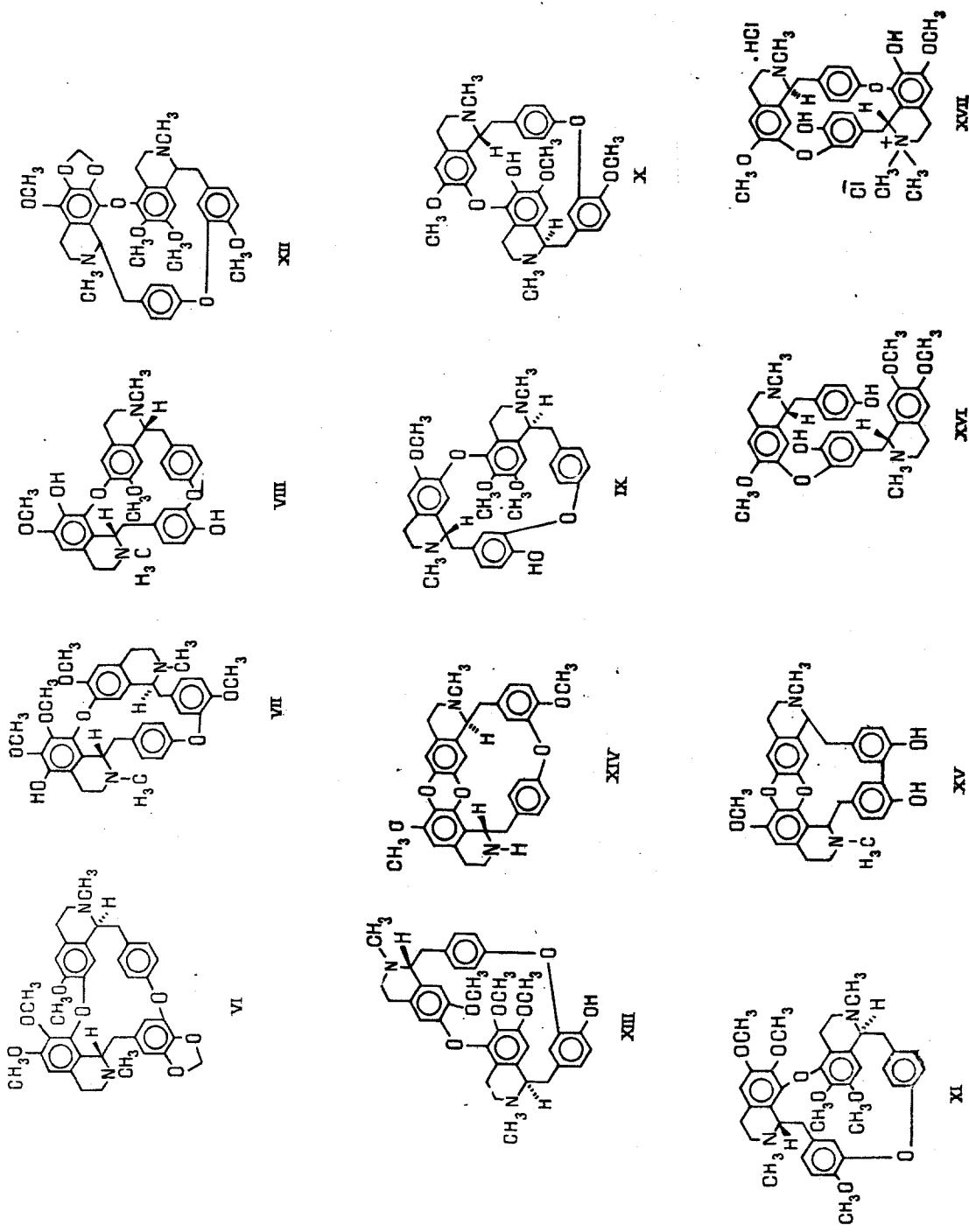
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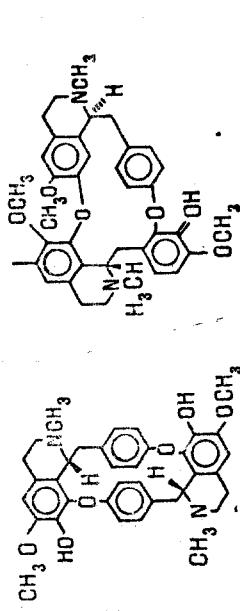
A classification of the bisbenzylisoquinoline, benzylisoquinoline, and related alkaloids is proposed which is based on the biogenetic characteristics of these alkaloids.

The bisbenzylisoquinoline alkaloids form a large — more than 160 — group of plant bases found in plants of twelve families [1]. Characteristic of them is a common pathway of biosynthesis through the oxidative coupling of benzylisoquinoline fragments. In accordance with the method of coupling of these fragments, the alkaloids can be divided into thirty subgroups, including benzylisoquinoline-aporphine, benzylisoquinoline-proaporphine, and other alkaloids genetically related to them. M. Shamma included this biogenetic principle in the basis of the broad classification that he has proposed of 26 subgroups of bisbenzylisoquinoline alkaloids [2]. However, when this classification is subjected to careful consideration, it can be seen to have several defects; for example, not all the alkaloids mentioned above can be classified on this principle.

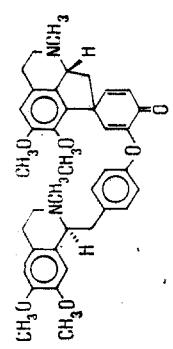
In order to broaden the possibility of numerical classification, we have introduced letter symbols for the type of substitution: o — OH, om — OCH₃, m — CH₃, omo — OCH₂O, d — dehydro, h — homo, : — additional bond, x — bond cleavage, R and S — symbols of absolute configuration. The figures relating to the right-hand half bear a prime. This permits intramolecular ether or carbon-carbon bonds in the aporphine, coumarin, and other alkaloids to be shown. The 1-benzyl-1,2,3,4-tetrahydroisoquinoline skeleton is taken as the basis in all cases. Let us give some examples.



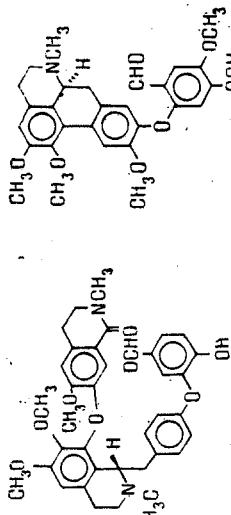


CH₃O

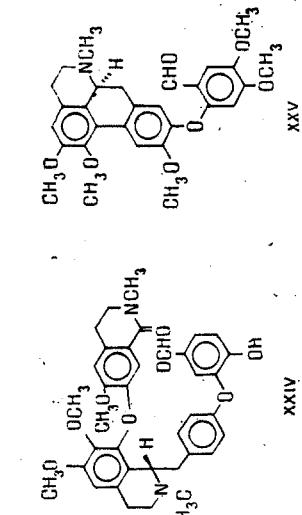
XVIII



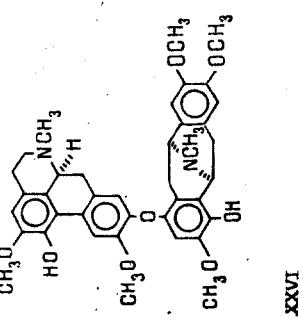
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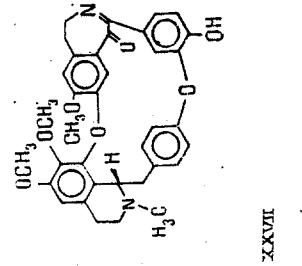
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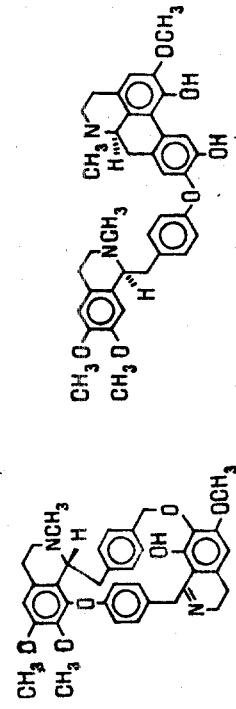
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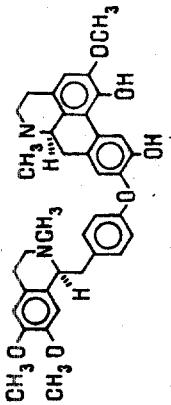
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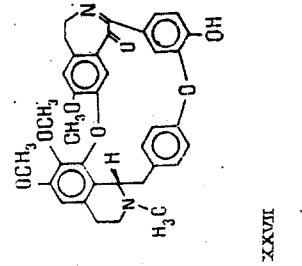
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XXXI

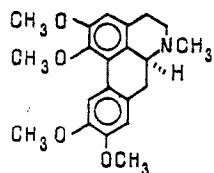


XXXII

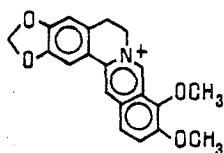


I. Dauricine — R, R, 2m, 2'm, 6om, 6'om, 7om, 7'om, 12o, 11o:12'; II. Hydroxyacanthine — S, R, 2m, 2'm, 6om, 6'om, 7om, 12o:11', 8o:7' III. Repanduline — 2m, 2'm, 6om, 7od, 12omo:13, 7'om:8, 7'o:8, 11o:12'; IV. Rodiasine — 2m, 2'm, 6om, 7om, 6'om, 8o:7', 12om, 12o:11', 11:11'; V. Magnolamine — S, S, 2m, 2'm, 6om, 6'om, 7o, 7'o, 12om, 13o, 10o:12'; VI. (+)-Tenuipine — S, S, 2m, 2'm, 6om, 6'om, 12omo:13, 8o:7', 12o:11'; VII. Thalisoridine — S, S, 2m, 2'm, 5o, 6om, 7om, 6'om, 12'om, 8o:7', 12o:11'; VIII. Thalicrine — S, R, 2m, 2'm, 60, 7om, 7'om, 12o, 8o:6', 11o:12'; IX. Thalictine — S, S, 2m, 2'm, 6om, 6'om, 7'om, 12o, 7o:5', 11o:12'; X. Panurensine — R, R, 2m, 2'm, 6o, 7om, 6'om, 12om, 5o:7', 11o:12'; XI. Thalidasine — S, S, 2m, 2'm, 6om, 7om, 6'om, 7'om, 12om, 8o:5', 11o:12'; XII. Thalifidine — 2m, 2'm, 5om, 6omo:7, 6'om, 7'om, 12'om, 8o:5', 12o:11'; XIII. Nemuarine — R, R, 2m, 2'm, 6om, 7om, 7'om, 12o:12'; XIV. Trilobine — S, S, 2'm, 6om, 12'om, 7o:6', 8o:7', 12o:11'; XV. Tiliacorinine — 2m, 2'm, 6om, 12o, 12'o, 7o:6', 8o:7', 11:11'; XVI. Liensinine — R, R, 2m, 2'm, 6om, 7'om, 12o, 12'o, 12'o:11'; XVII. Tubocurarine chloride — S, R, 2m, 2'm, 6om, 6'om, 7'om, 12'o, 7o:11', 12o:8'; XVIII. Isochondodendrine — R, R, 2m, 2'm, 6om, 6'om, 7o, 7'o, 8o:12'; XIX. Thalibrunine — S, S, 2m, 2'm, 6om, 7om, 8o:7', 10o:12'; XX. Insularine — R, R, 2m, 2'm, 6om, 6'om, 7om, 7'om:11, 8o:12', 12o:8'; XXI. Cissampareine — R, —, 2m, 6om, 7om, 6'om, 8'o, 1'd, 2'd, 7'om, 12, 8o:12', XXII. Pakistanine — S, R, 2m, 2'm, 6om, 7om, 6'om, 7'om, 12o:11', 12'o, 8':9'; XXIV. Baluchistanamine — S, —, 2m, 2'm, 6om, 7om, 6'om, 12'o, 8o:7', 12o; 11, 1' x 15', 1' od, 15' od; XXV. Hernandaline — S, 2m, 6om, 7om, 12om, 12'o, 13'om, 8:10, 13'o:10', 1' x 15', 15' od; XXVI. Pennsylpavine — S, S, 2m, 2'm, 6om, 7o, 6'om, 7'om, 12om, 12'o, 13'om, 8:10, 13:o:10', 3':14', 15':2', 15'd, 2'd, 1'x2'. Stepinonine — S, —, 2m, 6om, 7om, 6'om, 12'o, 13'o:11', 8o:7', 1'od, 15':2', 15'd, 2'd, 1'x2'.

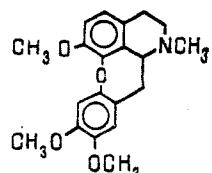
The last six alkaloids were not included in M. Shamma's classification. We give only a few bisbenzylisoquinoline alkaloids. Alkaloids of other types can be classified by an analogous method. Lists of the alkaloids of these types known at the present time are given in reviews [1, 2]. The monomeric benzylisoquinoline alkaloids can also be classified on this principle:



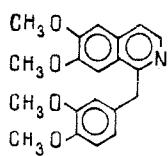
XXVIII



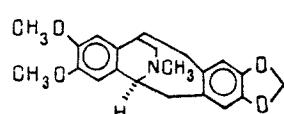
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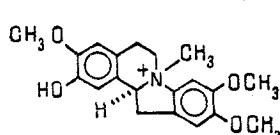
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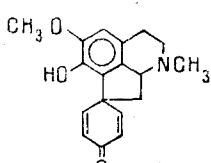
XXXI



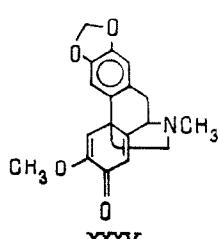
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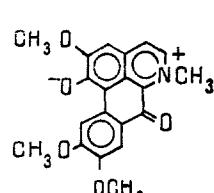
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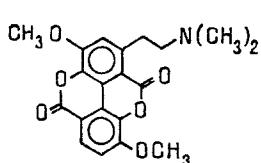
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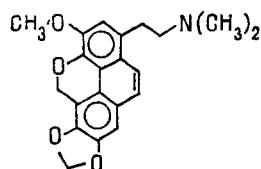
XXXV



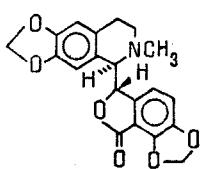
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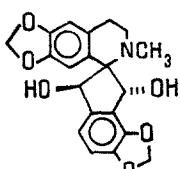
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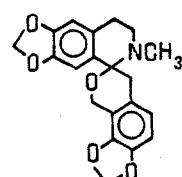
XXXVIII



XXXIX



XL



XLI

XXVIII. Glaucine — S, 6^{om}, 7^{om}, 12^{om}, 13^{om}, 2^m, 8:10; XXIX. Berberine — 6^{omo}:7, 11^{om}, 12^{om}, 2^{dm}:10, 1^d, 15^d, 2^d; XXX. Coularine — S, 2^m, 7^{om}, 12^{om}, 13^{om}, 8:10; XXXI. Papaverine — 1^d, 2^d, 3^d, 4^d, 6^{om}, 7^{om}, 11^{om}, 12^{om}; XXXII. Reframine — S, 2^m, 6^{om}, 7^{om}, 12^{omo}:13, 4:10; XXXIII. (-)-Crytaustolaine — S, 2^m, 6^{om}, 7^o, 12^{om}, 13^{om}, 2:10; XXXIV. Glasiovine — 2^m, 6^{om}, 7^o, 12^{od}, 8:9; XXXV. Amurine — 2^m, 6^{om}, 7^{od}, 12^{omo}:13, 4^d:10; XXXVI. Corunnine — 2^m, 6^{om}, 7^o, 12^{om}, 13^{om}, 8:10, 1^d, 2^d, 3^d, 4^d, 15^{od}; XXXVII. Thapsine — 2^{m₂}, 6^{om}, 7^o:15, 1^x:15, 15^{od}, 1^x:2, 1^{od}, 12^{om}, 11^o:1, 8:10; XXXVIII. Thaliglucine — 2^{m₂}, 1^x:2, 6^{om}, 1^d, 15^d, 12^{omo}:13, 7^{om}:11, 8:10; XXXIX. Bicuculline — 1^S, 15^R, 2^m, 6^{omo}:7, 12^{omo}:11, 15^{om}(od):10; XL. Ochrobirine — 2^m, 6^{omo}; 7, 11^{omo}:12, 15^o, 10^{m(o)}:1; XLI. Hypercorine — 2^m, 6^{omo}:7, 11^{omo}:12, 1^{om}:10.

The homobenzylisoquinoline, homoaporphine, and homoproaporphine alkaloids correspondingly have a 1h:15 bond. Thus, all the isoquinoline alkaloids can be classified according to a single principle. The figure-and-letter nomenclature is convenient for use in information machines.

SUMMARY

A classification of the bisbenzylisoquinoline, benzylisoquinoline, and related alkaloids is proposed which is based on their biogenetic characteristics. The figure-and-letter nomenclature is convenient for use in information machines.

LITERATURE CITED

1. O. N. Tolkataev, E. P. Nakova, and R. P. Evstigneeva, Khim. Prir. Soedin., 451 (1977).
2. M. Shamma and J. Moniot, Heterocycles, 4, 1817 (1976).