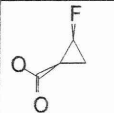
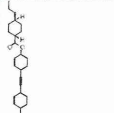
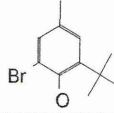
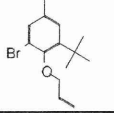
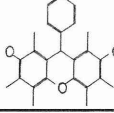
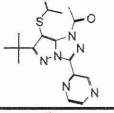
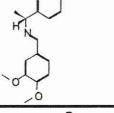
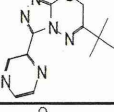
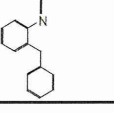
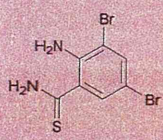

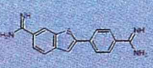
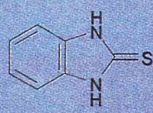
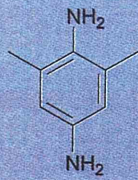


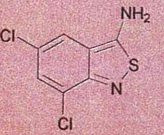
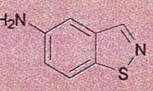

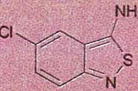
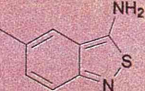
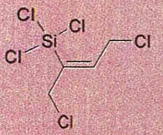
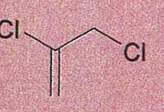
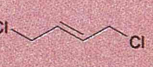
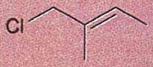
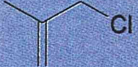
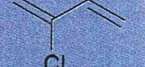
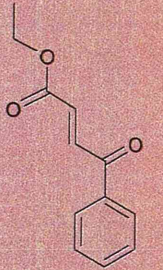
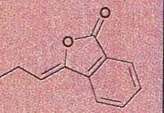
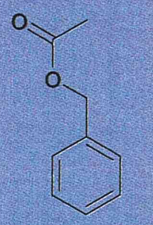
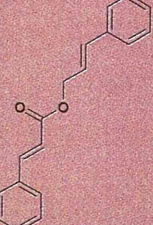
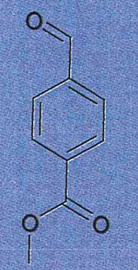
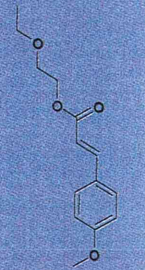
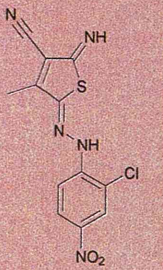

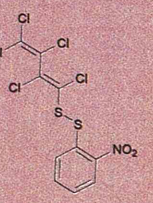
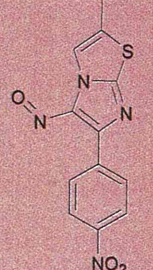
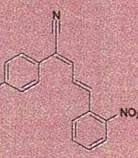
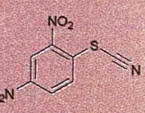
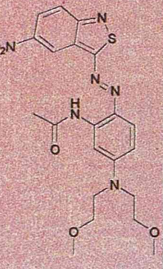
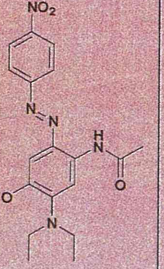


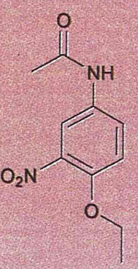
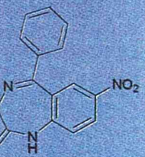



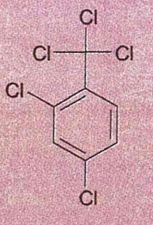
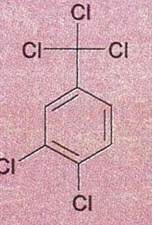
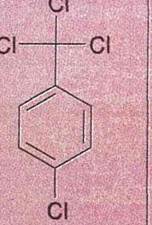
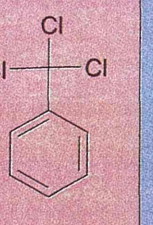
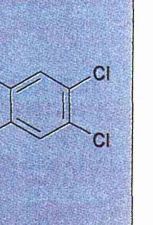
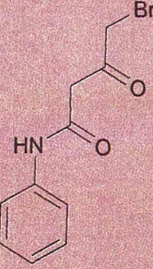
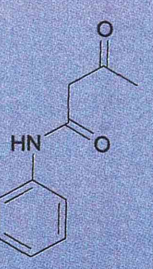
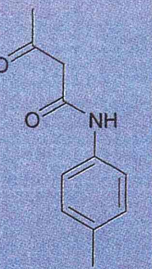
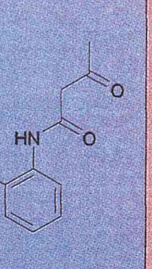
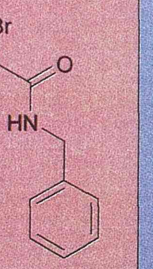
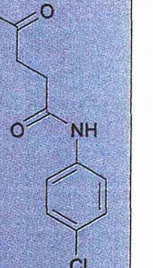
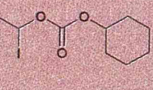
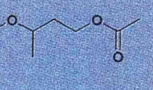
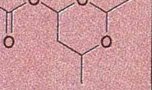
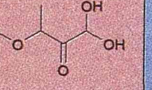
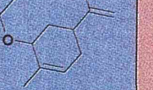
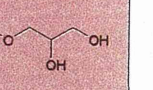
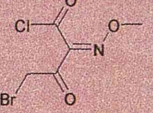
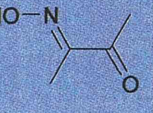
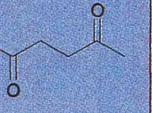
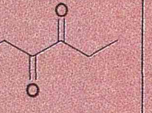
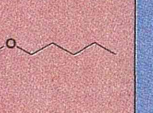
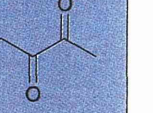
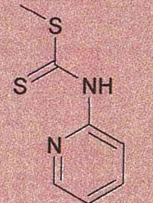
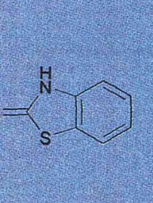
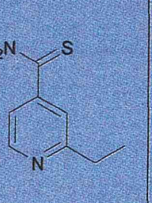
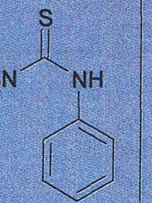
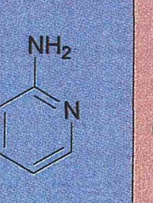
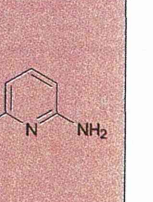
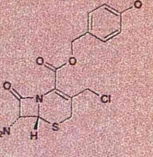
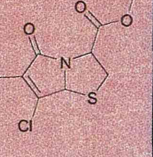
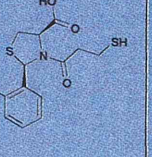
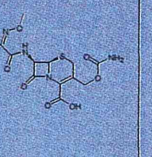

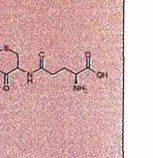
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995		264.0532	A	+	JP.188021-38-7	-	-	-
996		348.2657	C	-	JP.153164-65-9	+	+	+
997		340.2752	C	-	JP.110130-88-6	+	+	+
998		251.1953	C	-	JP.13156-95-1	+	+	+
999		260.2336	C	-	JP.110675-26-8	+	-	-
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別表2 (Aグループの結果)

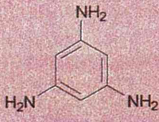
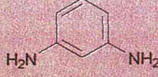
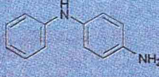
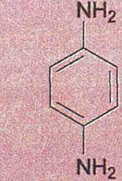
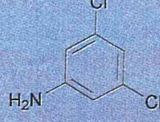
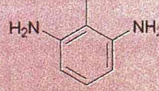
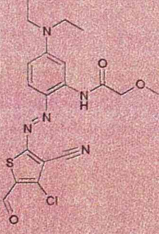


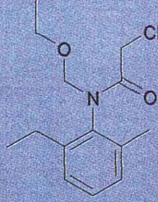
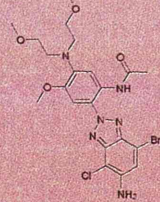
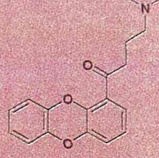
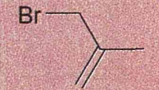
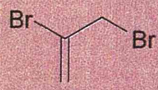
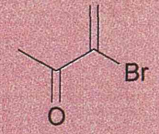


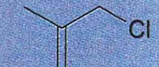
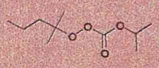

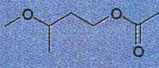
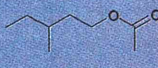
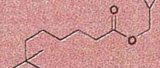

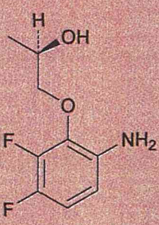
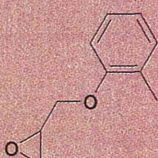
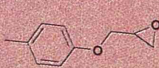
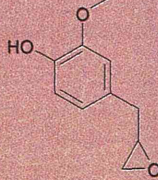
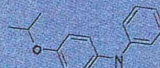
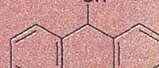
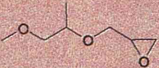
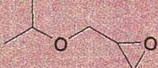
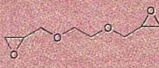
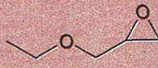
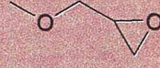
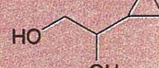
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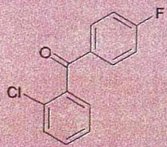
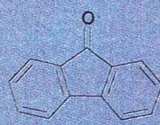

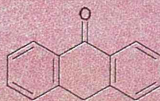
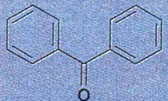
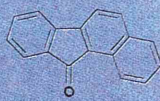


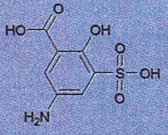
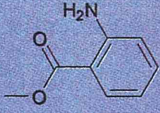

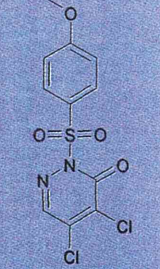
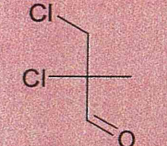
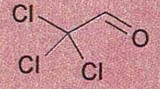
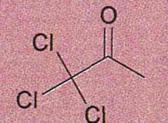

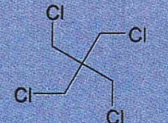

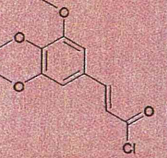
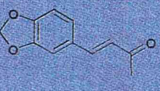
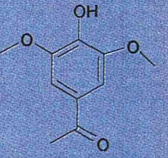

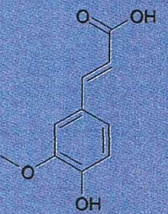
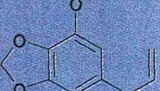
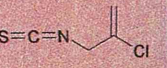
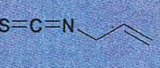
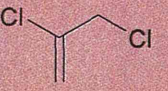

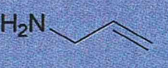
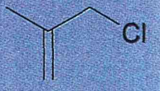

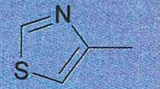
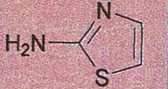
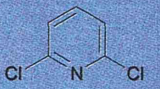
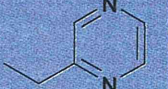
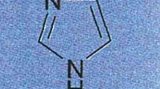
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厚生労働科学研究費補助金（化学物質リスク研究事業）
分担研究報告書

分担研究課題：化学物質の構造の精密化、高度化に関する研究

研究分担者：出水庸介 国立医薬品食品衛生研究所有機化学部 第二室長

研究要旨

本年度は構造類似性に基づいた予測法の開発を目的とした。国立医薬品食品衛生研究所変異遺伝部が行っている AMES/QSAR International Collaborative Study のデータ 4021 件中の任意の 1000 件を用いて予測法を適用した。この 1000 件のなかの A グループ（47 件）及び B グループ（79 件）の構造の精密化、高度化に対応するため、エネルギー安定構造である三次元構造を求めた。

A. 研究目的

構造活性相関をより高度化するためには、そのもととなる化学物質の構造を高度化する必要がある。そこで化学計算による化学物質の精密な構造データの取得を目的とした。分子力学法と配座探索法（コンフォメーションルサーチ）を用いて化学物質の精密な三次元構造を求めることとした。

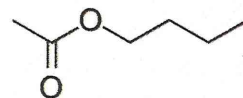
B. 研究方法

AMES/QSAR International Collaborative Study のデータ 4021 件中の任意の 1000 件のなかの A グループ（47 件）及び B グループ（79 件）の化合物について化学計算による化合物の精密な構造データの取得を行った。方法は昨年度と同じ方法で行った。分子力学計算（MMFF, OPLS2005 力場等）を用いたコンフォメーション探索により最安定構造を計算した。ソフトウェアはシ

ュレディンガー社の Macromodel を用いた。

【最安定構造を求める方法論】

(I) 初期座標の入力



(II) 配座探索により最安定構造（グローバルミニマム）を求める



(III) ファイルフォーマットの変換



(IV) 最安定構造の表示

