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Nihon Eiseigaku Zasshi
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METABOLISM OF PCB

By

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Purpose

Since it was confirmed by GC-MS-COM analysis of the PCB metabolites that there are the following bodies: SO_2CH_3 (I), SCH_3 (II), and OH (III), it was clearly established that PCB is metabolized by two pathways: a hydroxide system and a methyl sulfonation system. (Nihon Eiseigaku Zasshi, 29, 85 (1974), 30, 123 (1975), Nihon Kōshū Eisei Zasshi, 21, 331 (1974), 22, 465 (1975), Kankyō Osen Doku Shimpojiumu, 81 (1975), Yūki Masu Shimpojiumu, 135 (1975)) Here let us summarize these results and attempt an approach to the connections between the process of PCB metabolism and their influence. We also report here that new metabolites dihydroxin (IV), mercapto (V), and methyl sulfoxide (VI) were found in the feces of mice to which 2,5,2',5'-tetrachlorobiphenyl (TCB) had been administered.

Methodology

Administration: 2,5,2',5'-TCB was given to the mice either orally or abdominally. Extraction of the metabolites: Saponified by 1N-NaOH/Et OH, neutralized, and then concentrated, dissolved in benzene or directly extracted with benzene. Fractionation: Benzene elution in Merck silica gel 60. GC: 4% dexyl GC-300, 2 mmø x 1 m. MS-COM: As reported in previous reports.

Results and Discussion

Fig. 1 shows the mass spectrum (MS) of 2,5,2',5'-TCB metabolite IV. Its

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M^+ shows a 4-chlorine isotope peak at 322, which is 16 greater than that of the M^+ of metabolite III, 306. Its mode of fragmentation resembles that of 3-OH-2,5,2',5'-TCB, and the detachment of CO and CHO can be seen. The mass spectrum in Fig. 2 is supposed, on account of the behavior of the chromatography and because of the formation of thiacycloheptatriene ions, to be that of 4-SH-2,5,2',5'-TCB, the demethylated form (V) of metabolite II. The mass spectrum in Fig. 3 is supposed, since detachment of CH_3 and SH is seen, to be that of 4-CH_3SO-2,5,2',5'-TCB (VI). In Fig. 4 are shown the metabolic pathways of these metabolites, along with those of the ones whose structure has already been determined, using 2,5,2',5'-TCB as typical of the metabolic modes of PCB. It is believed that the onset of metabolism passes through arene oxide due to the addition of one oxygen. In the pathway for the formation of IV, by the addition of water in the same way as in the metabolism of naphthalene, transdihydrodiol is passed, and a diol body is then believed to be produced by dehydrogenation. With the discovery of VI, it became clear that the pathway of the formation of I is that VI and I are produced by the addition of one hydrogen gradually from II.

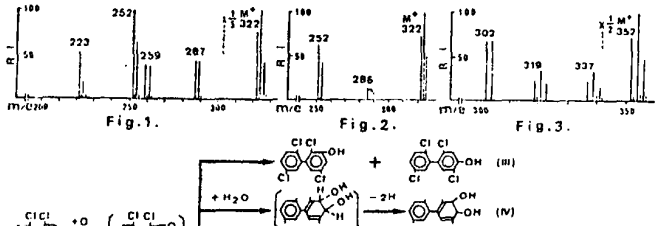

Fig.4. Metabolic scheme of PCB