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It has been reported that 2-bromopropane might be a causative agent for reproductive toxicity and have immunotoxic effects. 1-Bromopropane known as an alternative to ozone depleting solvents, which has structural similarity to 2-bromopropane, has been reported to be neurotoxic to rats in long-term inhalation exposure.
To elucidate mechanisms of 1- or 2-bromopropane-induced toxicities in the molecular level, formation of N7-guanine adducts by 1- or 2-bromopropane was investigated in vitro. N7-Guanine adducts of 1- and 2-bromopropane (N7-propyl guanine and N7-isopropyl guanine, respectively) were chemically synthesized in three steps in relatively high yields and structurally characterized by analyses of 1H NMR, 13C NMR, UV, HPLC and LC/MS/MS (ESI) to use as standard materials. N7-Propyl guanine and N7-isopropyl guanine were detected and identified by UV, HPLC and LC/MS/MS analyses after incubation of calf thymus DNA with 1- or 2-bromopropane at a physiological condition for 16 hr, followed by thermal hydrolysis. In addition, time response and dose response effect of DNA adduct formation were investigated. Furthermore in vivo treatment of 2-bromopropane resulted in detection of RNA adduct of 2-bromopropane after analyses of ESI LC/MS/MS. The present results suggest that 1- and 2-bromopropane may form a DNA adducts at N7-position of 2'-deoxyguanosine at a physiological condition, which may be responsible for certain toxicities.

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PPAR-γ ligands binding energy and bioactivity

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PPAR-γ(Peroxisome Proliferator-Activated Receptor γ) 리간드들은 논문 조사를 통해 이루어졌다. PPAR-γ의 45개 알려진 화합물들을 찾았고, 12 생물활성 화합물을 선택했다. 리간드(rosiglitazone)과 단백질의 결합된 구조는(1fm6)는 PDB로부터 획득했고, 단백질 coordinate를 가져와 PPAR 의 활성 영역 잔기들은 확인했다.(2TYR, 1SER, 1HIS). CoMFA와 Flexi Dock을 통해 단백질과 리간드 사이의 상호작용과 결합에너지에 대한 상호 관계를 밝혔다.

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3D-QSAR and docking studies of selective COX-2 inhibitors

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The three-dimensional quantitative structure-activity relationship (3D-QSAR) approach using comparative molecular field analysis (CoMFA) and comparative molecular similarity analysis (CoMSIA) was applied to 62 derivatives known as COX-2 selective inhibitors. Partial least square (PLS) analyses produced good predicted models with q2 value of 0.803 (s=0.285, F=215.401, r2=0.951) and 0.769 (s=0.192, F=245.364, r2=0.980) for CoMFA and CoMSIA, respectively. The