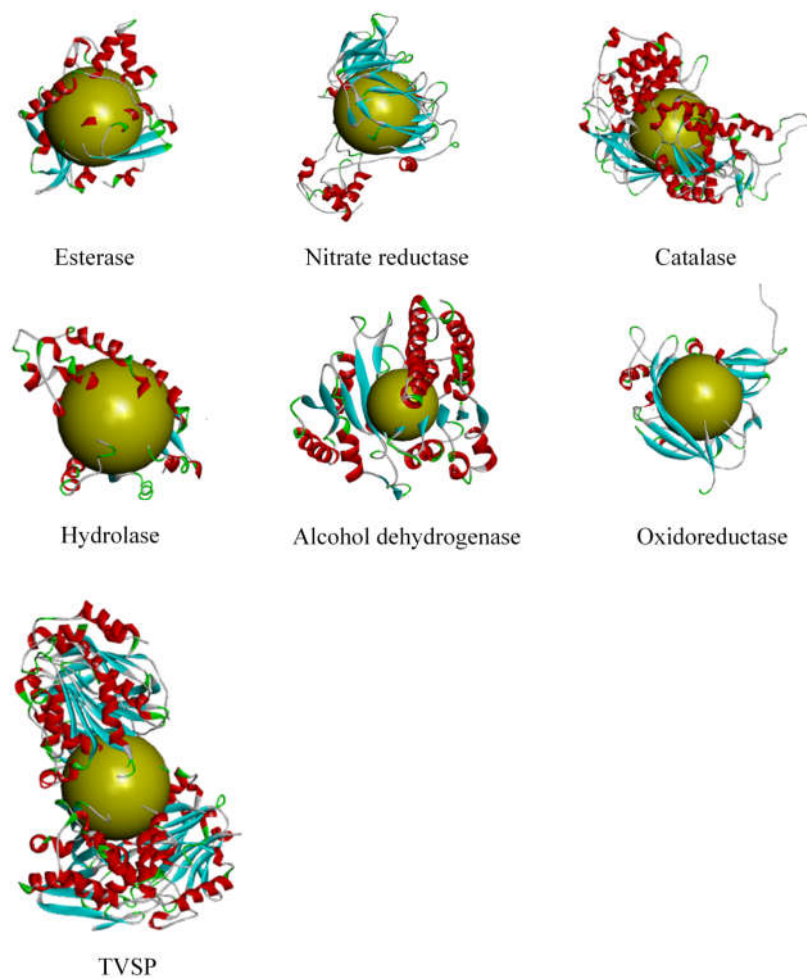
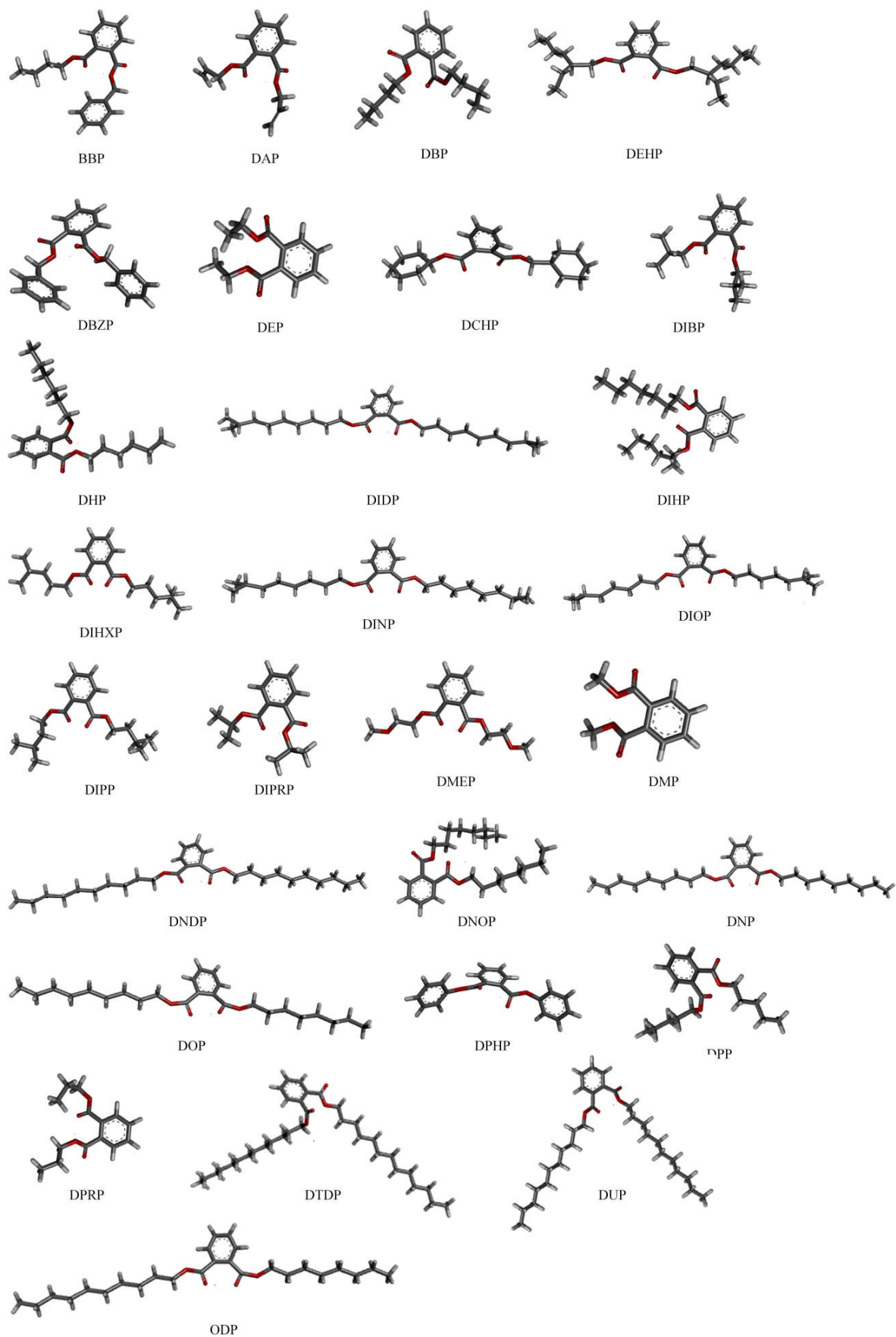


# Molecular design and Mechanism Analysis of Phthalic Acid Ester Substitutes: Improved Biodegradability in Processes of Sewage Treatment And Soil Remediation

Shuhai Sun<sup>1,†</sup>, Qilin Zuo<sup>1,†</sup>, Meijin Du<sup>2,†</sup>, Yu Li<sup>2,\*</sup>



**Figure S1.** The docking site of proteins.



**Figure S2.** Molecular structure diagram of PAEs.

### Aerobic Bacteria:



Esterase  
PDB ID: 7CUZ



Nitrate reductase  
PDB ID: 1HZV

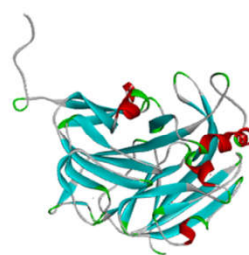


Catalase  
PDB ID: 1P80

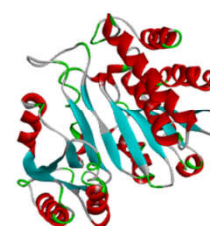
### Anaerobic Bacteria:



Hydrolase  
PDB ID: 2IOF

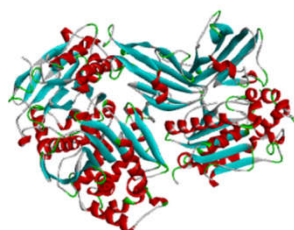


Oxidoreductase  
PDB ID: 1NIC



Alcohol dehydrogenase  
PDB ID: 3FMX

### Biodegradable Complex Proteins:



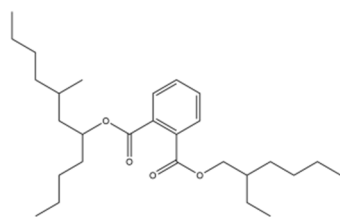
Soil composite degradation enzyme

**Figure S3.** The structure of proteins.

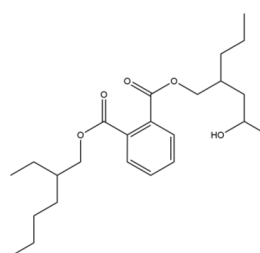
**Table S1.** Molecular structure of DBP and DEHP substitutes.

Molecular	Chemical structure diagram	Molecular	Chemical structure diagram
DBP-1		DEHP-1	

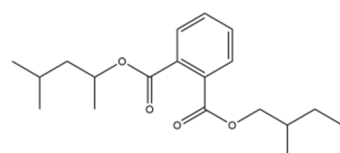
DBP-2



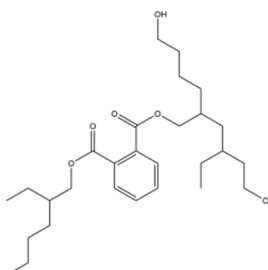
DEHP-2



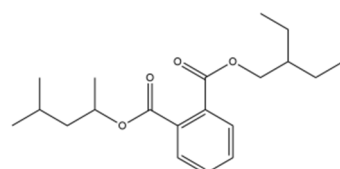
DBP-3



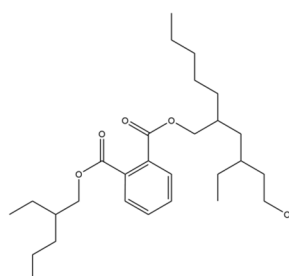
DEHP-3



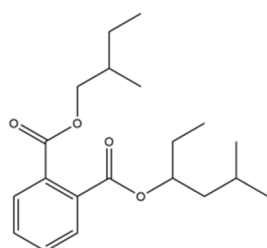
DBP-4



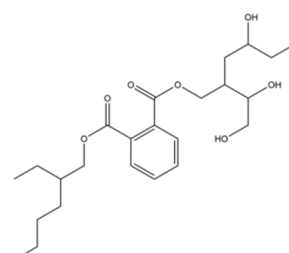
DEHP-4



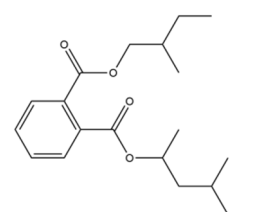
DBP-5



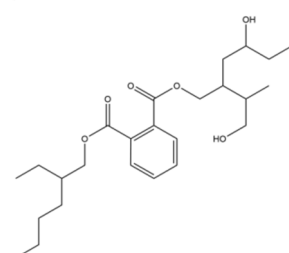
DEHP-5



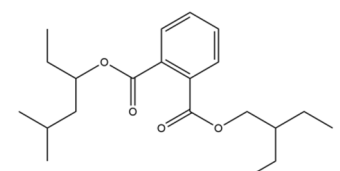
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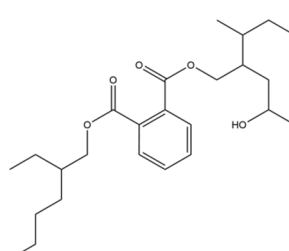
DEHP-6



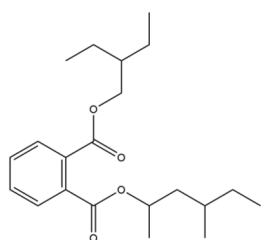
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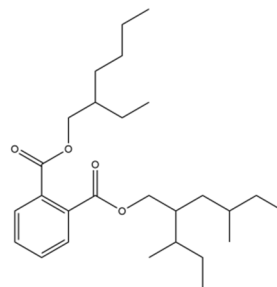
DEHP-7



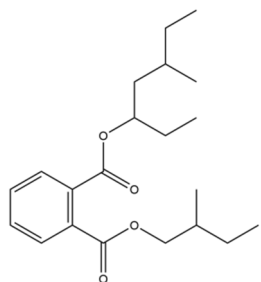
DBP-8



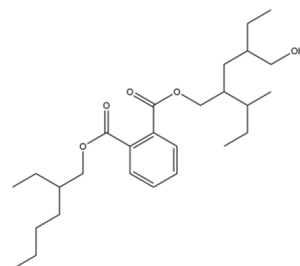
DEHP-8



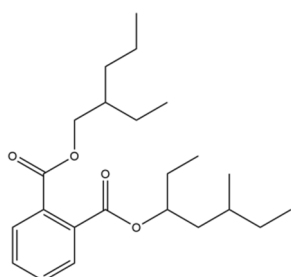
DBP-9



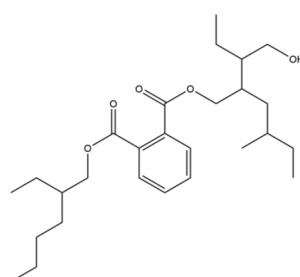
DEHP-9



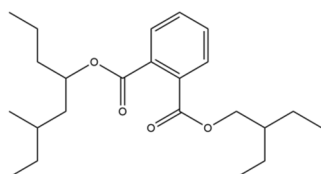
DBP-10



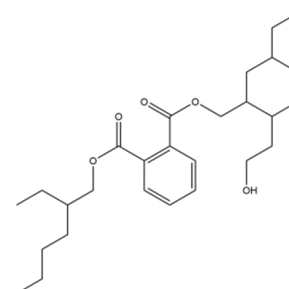
DEHP-10



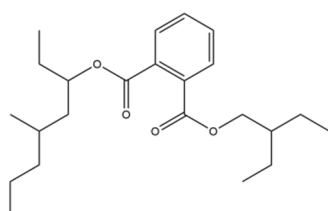
DBP-11



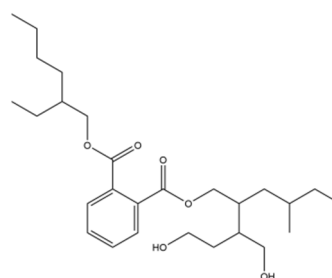
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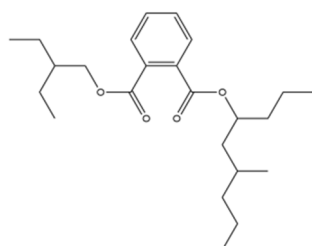
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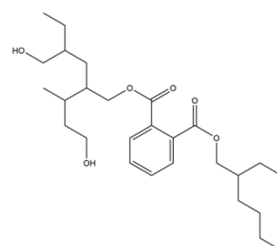
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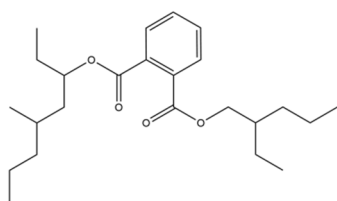
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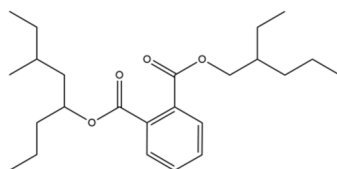
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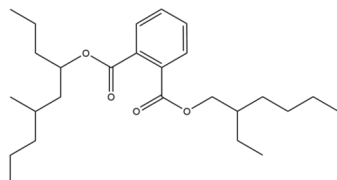
DBP-14



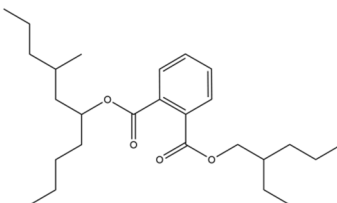
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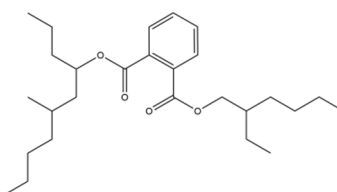
DBP-16



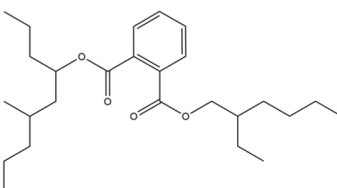
DBP-17



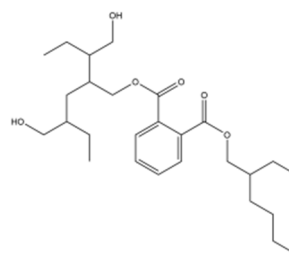
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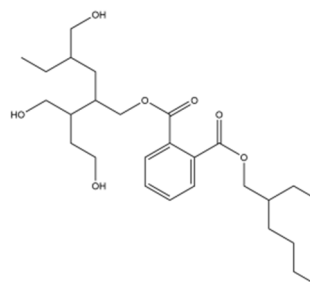
DBP-19



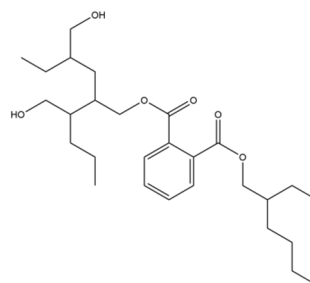
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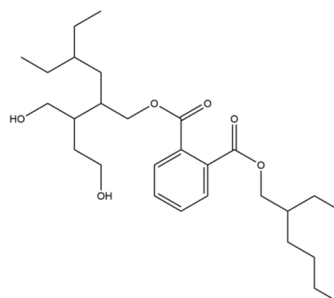
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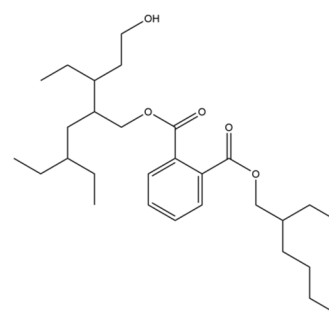
DEHP-16



DEHP-17



DEHP-18



DEHP-19

