Supplementary Material

Identification of New Dioxygenases Able to Recognize Polycyclic Aromatic Hydrocarbons with High Aromaticity

Content

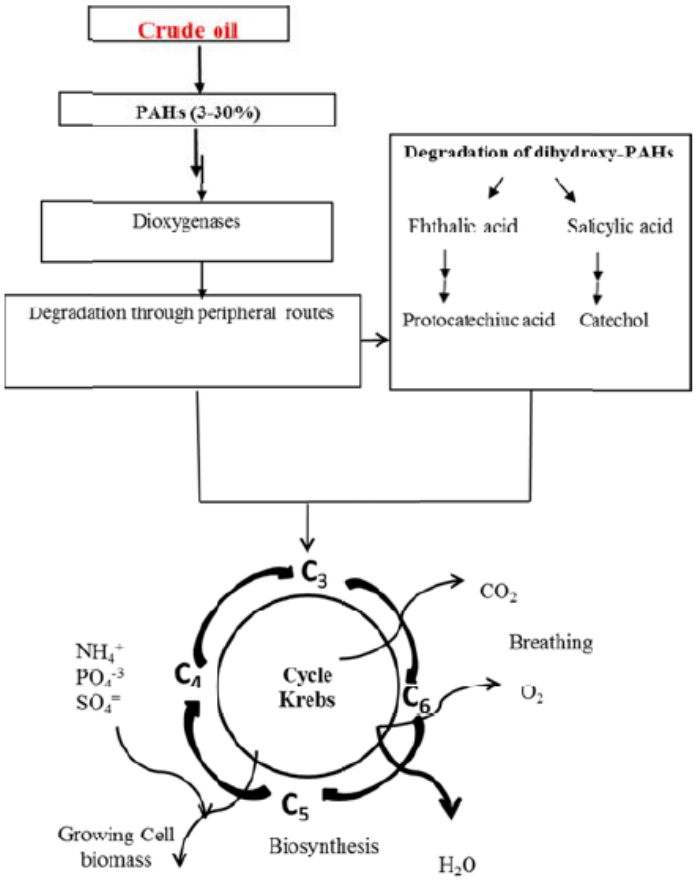


Figure S1: Main principle of aerobic degradatio of PAHs.

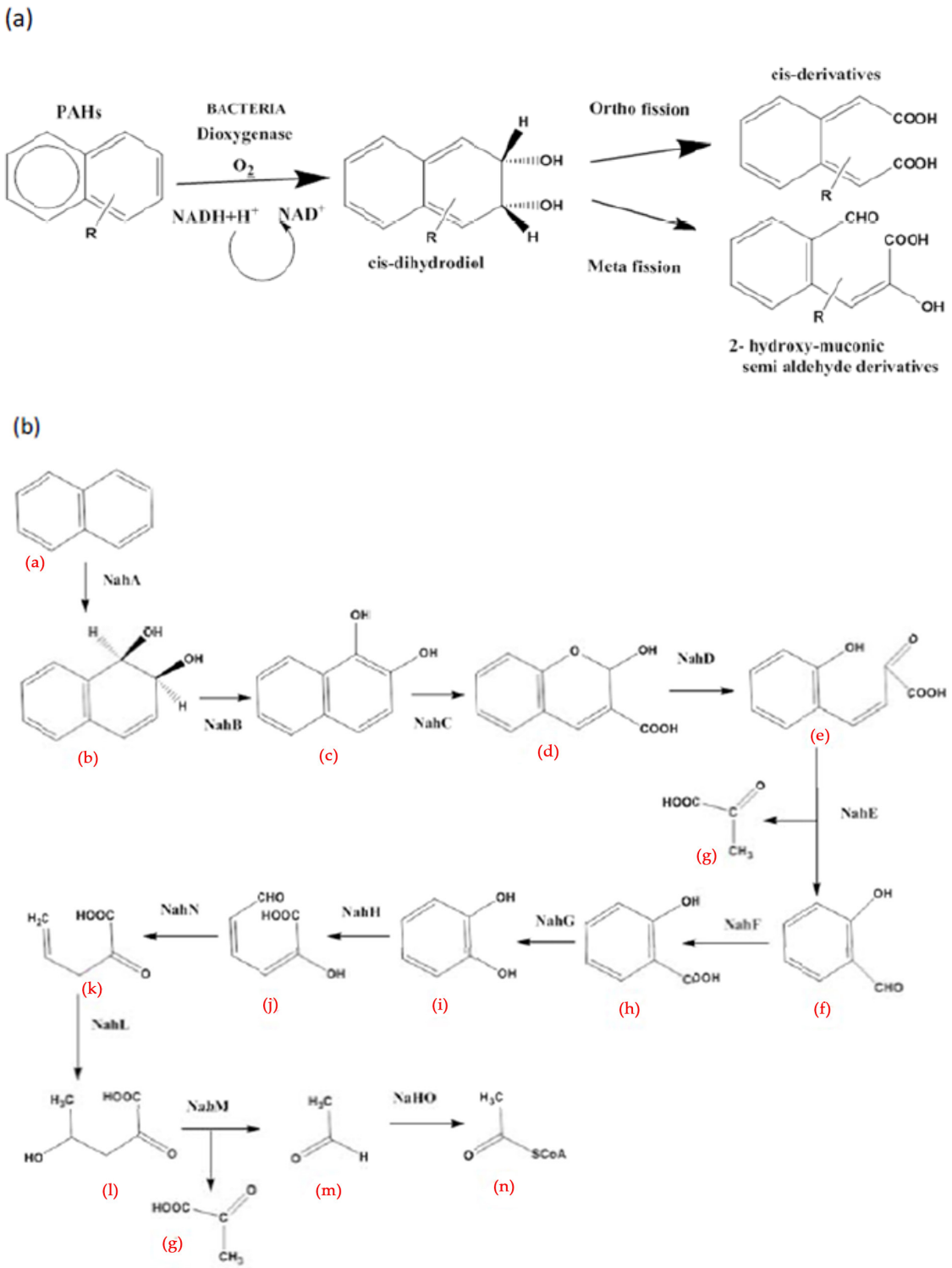


Figure S2: (**a**) Bioremediation of PAHs by organism and (**b**) Pathways for degradation of naphthalene by *Pseudomonas putida*.

NahA, naphthalene dioxygenase; *NahB*, cis-1,2-dihydro-1,2-dihydroxynaphthalene-1,2-dehydrogenase; *NahC*, 1,2-dihydroxynaphthalene dioxygenase; *NahD*, 2-hydroxychromene-2-carboxylate isomerase; *NahE*, trans-o-hydroxybenzylindene pyruvate hydratase-aldolase; *NahF*,

salicylaldehyde hydrogenase; *NahN,* 2-hydroxymuconic semialdehyde hydrolase; *NahL,* 2-oxopenta-4-dienoete hydratase; *NahM,* 4-hydroxy-2-oxovalerate aldolase; *NaHO,* acetaldehyde dehydrogenase.

Products: a) naphthalene; b) cis-1,2-dihydro-1,2-dihydroxynaphthalene; c) 1,2-dihydroxynaphthalene; d) 2-hydroxychromene-2-carboxylic acid; e) cis-o-hydroxybenzylpyruvate; f) salicylaldehyde; g) pyruvate; h) salicitate; i) catecol; j) 2-hydroxymuconic semialdehyde; k) 2-oxovalerate-4-dienoate; l) 4-hydroxy-2-oxovalerate; m) acetaldehyde; n) acetal-CoA

Table S1: PAHs biodegradation by different microorganism.

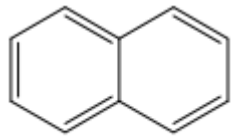
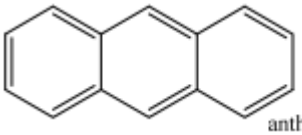
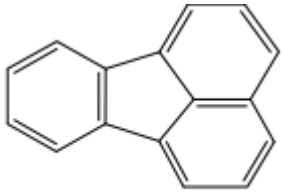
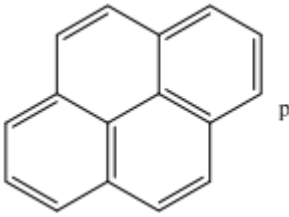
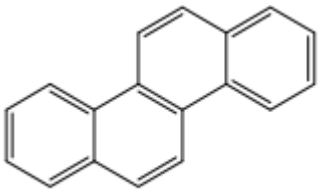
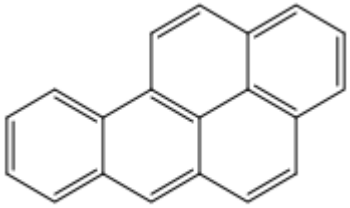
PAHs	Microorganism	Biodegradation (%)	Literature
Napthalene	*Sphingomonas paucimobilis* EPA 505	96.3%	[7]
	Sphingobium yanoikuyae B1	-	Benzo(hi)
	Sphingomonas paucimobilis NBRC 139345	-	[7]
	Actinobacteria	-	-
	Rhodococcus wratislaviensis IFP 2016 and *Rhodococcus aetherivorans* IFP 2017	90%	[27]
Anthracene	*Actinobacteria*	93.3%	[27]
	Sphingobium yanoikuyae B1	28.7%	[7]
	Sphingomonas paucimobilis EPA 505	-	[7]
	Sphingomonas sp. BA2	~26%	[6]
	Mycobacterium gilvum VF1	53%, 58%, 71%	[4]
	Dyadobacteria koreensis	75%	[7]
	Rhodococcus wratislaviensis IFP 2016 and *Rhodococcus aetherivorans* IFP 2017	>90%	[27]
	Norcardia, beijerinckia Paracoccus	-	-
Pyrene	*Micobacterium gilvum* VF1	53%, 58%, 71%	[4]
	Dyadobacteria koreensis	73%	[7]
	Sphingomonas paucimobilis EPA 505	95%	[7]

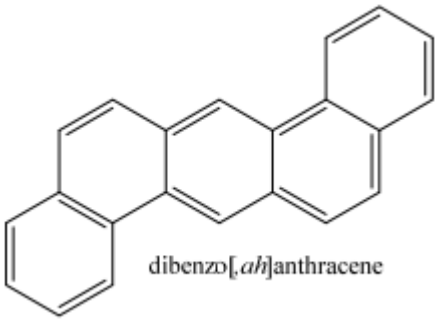
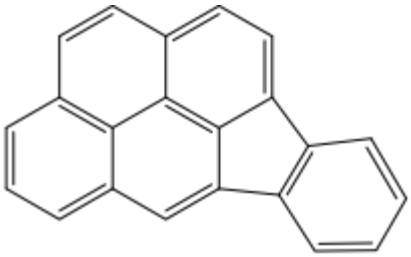
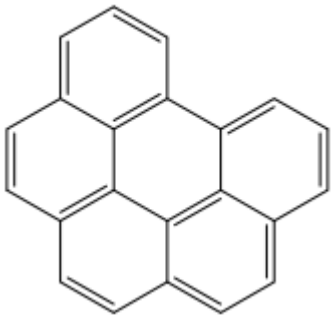
	Rhodococcus wratislaviensis IFP 2016 and *Rhodococcus aetherivorans* IFP 2017	>90%	[27]
Fluoranthene	*Sphingomonas paucimobilis* EPA 505	85-90%	[7]
	Sphingobium yanoikuyae B1	20-60%	[19]
	Sphingomonas paucimobilis NBRC 139345	82%	
	Mycobacterium sp. Strains KA5, BS5 AND KF4	-	-
Chrysene	*Pseudomonas aeroginosa*	65% 72%	[27]
	Dyadobacter koreensis	83%	[27]
dibenzo[a,h]anthracene	-	-	-
Indeno[1,2,3-cd]pyrene	*Pseudomonas aeroginosa*	-	[27]
Benzo[zhi]perylene	*Pseudomonas aeroginosa*	-	[27]
Benzo[a]pyrene	*Pseudomonas aeroginosa*	-	[27]

Table S2: Molecule surface area of dioxygenases and PAHs.

Protein			
Paraburkholderia **2xsh**	*Pseudomonas* **4hjl**	*Sphingobium* **2gbx**	*Phodococcus* **1ulj**
421.550 Å^2	2500.585 Å^2	361.44 Å^2	1360.404 Å^2
Ligands (surface area)			
Napthalene		148.537	
Anthracene		191.340	
Chrysene		229.453	
Fluoranthene		260.251	
Pryrene		201.585	
Benzo(a)pyrene		242.556	
Dibenzi(a,h)anthracene		-	
Indeno(1,2,3-cd)pyrene		258.116	
Benzoperylene		-	

Table S3: Docking scores of biodegrade PAHs by dioxygenases from different microorganisms.

Docking score (kcal/mol) No. ID PDB Microorganism				
PAHs	**2gbx** *Sphingomonas* Biphenyl	**4hjl** *Pseudomonas* Napthalene	**2xsh** *Paraburkholderia* Biphenyl	**1ulj** *Rodococcus* Biphenyl
 naphthalene	-5.1	-6.1	-5.9	-6.7
 anthracene	-7.6	-7.6	-8.3	**-7.3**
 fluoranthene	-6.9	-8.1	-6.5	---
 pyrene	-7.1	-8.1	-7.9	--
 chrysene	**-7.6**	**-8.9**	**-8.4**	--
 benzo[*a*]pyrene	--	**-9.9**	--	--

 dibenzo[,*ah*]anthracene	--	--	--	--
 indeno[1,2,3-*cd*]pyrene	--	**-9.0**	--	--
benzo[*ghi*]perylene 	--	--	--	--

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