Supplementary data for the article:

Lješević, M.; Gojgić-Cvijović, G.; Ieda, T.; Hashimoto, S.; Nakano, T.; Bulatović, S.; Ilić, M.; Beškoski, V. Biodegradation of the Aromatic Fraction from Petroleum Diesel Fuel by Oerskovia Sp. Followed by Comprehensive GC×GC-TOF MS. *Journal of Hazardous Materials* **2019**, *363*, 227–232. https://doi.org/10.1016/j.jhazmat.2018.10.005

Supplementary data

Biodegradation of the aromatic fraction from petroleum diesel fuel by Oerskovia sp. followed by comprehensive GC×GC-TOF MS

Marija Lješević, Gordana Gojgić-Cvijović, Teruyo Ieda, Shunji Hashimoto, Takeshi Nakano, Sandra Bulatović, Mila Ilić, Vladimir Beškoski

Table S1. Identification of bacterial strains according to the results of the 16s rRNA analysis

Figure S1. Phylogenetic tree showing the relatedness of *Oerskovia* sp. CHP-ZH25 to five other bacterial strains isolated from different oil contaminated soil.

Table S2. Selected PAHs analyzed using GC×GC-TOF MS

Table S3. Percentage of degradation of selected PAHs derivatives based on total peak volume value

Figure S2. Selected Ion Chromatograms of m/z 128.0626 after 30 days. (A) Abiotic control; (B) Degraded $C_{10}H_8$ compounds (naphthalene derivatives).

Figure S3. Selected Ion Chromatograms of *m/z* 142.0783, 156.0939, 170.1096, 184.1252, 198.1409, 212.1565, 226.1722, 240.1878 after 30 days. (A) Abiotic control; (B) Degraded alkyl naphthalenes.

Figure S4. Selected Ion Chromatograms of m/z 154.0783 after 30 days. (A) Abiotic control; (B) Degraded $C_{12}H_{10}$ compounds (acenaphthylene/biphenyl derivatives).

Figure S5. Selected Ion Chromatograms of m/z 168.0939, 182.1096, 196.1252, 210.1409, 224.1565, 238.1722, 252.1878, 266.2035, 280.2192, 294.2349 after 30 days. (A) Abiotic control; (B) Degraded alkyl acenaphthylene/alkyl biphenyl.

Figure S6. Selected Ion Chromatograms of m/z 154.0782 after 30 days. (A) Abiotic control; (B) Degraded $C_{12}H_{10}$ compounds (acenaphthene derivatives).

Figure S7. Selected Ion Chromatograms of m/z 154.0782, 168.0939, 182.1096, 196.1252, 210.1409, 224.1565, 238.1722, 252.1878, 266.2035, 280.2191, 294.2348 after 30 days. (A) Abiotic control; (B) Degraded alkyl acenaphthenes.

Figure S8. Selected Ion Chromatograms of m/z 166.0783 after 30 days. (A) Abiotic control; (B) Degraded $C_{13}H_{10}$ compounds (fluorene derivatives).

Figure S9. Selected Ion Chromatograms of m/z 180.0939, 194.1096, 208.1252, 222.1409, 236.1565, 250.1722, 264.1878, 278.2035, 292.2192, 306.2349 after 30 days. (A) Abiotic control; (B) Degraded alkyl fluorenes.

Figure S10. Selected Ion Chromatograms of m/z 178.0783 after 30 days. (A) Abiotic control; (B) Degraded $C_{14}H_{10}$ compounds (phenanthrenes/anthracenes derivatives).

Figure S11. Selected Ion Chromatograms of m/z 192.0939, 206.1096, 220.1252, 234.1409, 248.1565, 262.1722, 276.1878, 290.2035, 304.2191, 318.2349 after 30 days. (A) Abiotic control; (B) Degraded alkyl phenanthrenes/alkyl anthracenes.

Figure S12. Selected Ion Chromatograms of m/z 134.0190 after 30 days. (A) Abiotic control; (B) Degraded C₈H₆S compounds (benzo[b]thiophene derivatives).

Figure S13. Selected Ion Chromatograms of m/z 134.0190, 148.0347, 162.0503, 176.0660, 190.0816, 204.0973, 218.1129 after 30 days. (A) Abiotic control; (B) Degraded alkyl benzo[b]thiophenes.

Figure S14. Selected Ion Chromatograms of m/z 184.0347 after 30 days. (A) Abiotic control; (B) Degraded dibenzothiophene ($C_{12}H_8S$).

Figure S15. Selected Ion Chromatograms of *m/z* 198.0503, 212.066, 226.0816, 240.0973, 254.1129, 268.1286, 282.1442, 296.1599 after 30 days. (A) Abiotic control; (B) Degraded alkyl dibenzothiophenes.

Table S1. Identification of bacterial strains according to the results of the 16s rRNA analysis. The most similar strains were determined by the NCBI Blast tool.

Strain	Identification (GenBank accession number)	Number of nucleotides	Most similar type strain (GenBank accession number)	% of similarity	
ZH	Oerskovia sp. CHP-ZH25 (JX430000)	1382	Oerskovia enterophila DSM 43852 (NR_026239)	99	
NR	Rhodoccocus sp. CHP- NR31(JX965395) 1176 Rhodococcus cerastii C5 (NR_117103)		99		
315	Gordonia sp. CHP- 315(JX429999)	1388	Gordonia amicalis IEGM (NR_028735)	99	
A	Micrococcus sp. CHP-A35 (JX965396)	1372	Micrococcus yunnanensis YIM 65004 (NR_116578)	100	
Y	Sphingobacterium sp. CHP-Y37 (JX965397)	1389	Sphingobacterium detergens 6.2S (NR_118238)	98	
YG	Cupriavidus sp. CHP- YG38 (JX965398)	1398	Cupriavidus metallidurans CH34 (NR_074704)	99	

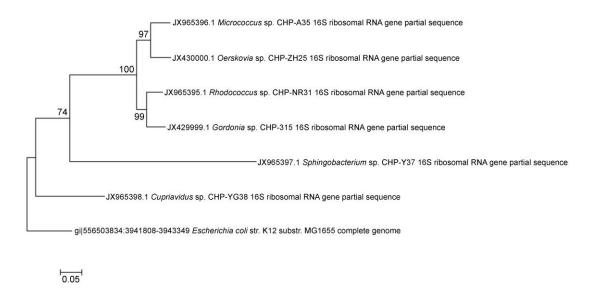


Figure S1. Phylogenetic tree showing the relatedness of *Oerskovia* sp. CHP-ZH25 to five other bacterial strains isolated from different oil contaminated soil.

The evolutionary history was inferred by using the Maximum Likelihood method based on the Tamura-Nei model. The percentages of replicate trees in which the associated taxa are clustered together in the bootstrap test (500 replicates) are shown next to the branches. The *E. coli* strain represents an outgroup.

Table. S2. Selected PAHs analyzed using GC×GC-TOF MS

Compound	Num. of Me-	Formula	Nominal mass	Exact mass	Compound	Num. of Me-	Formula	Nominal mass	Exact mass
	0	C10H8	128	128.0626		0	C12H8	152	152.0626
	1	C11H10	142	142.07825		1	C13H10	166	166.07825
	2	C12H12	156	156.0939		2	C14H12	180	180.0939
N1-411	3	C13H14	170	170.10955	Acenaphthylene	3	C15H14	194	194.10955
Naphthalene	4	C14H16	184	184.125201		4	C16H16	208	208.125201
	5	C15H18	198	198.140851	Biphenyl	5	C17H18	222	222.140851
	6	C16H20	212	212.156501		6	C18H20	236	236.156501
	7	C17H22	226	226.172151		7	C19H22	250	250.172151
	8	C18H24	240	240.187801		8	C20H24	264	264.187801
	0	C12H10	154	154.07825		0	C13H10	166	166.07825
	1	C13H12	168	168.0939		1	C14H12	180	180.0939
	2	C14H14	182	182.10955		2	C15H14	194	194.10955
	3	C15H16	196	196.125201	Fluorene	3	C16H16	208	208.125201
A comonhthana	4	C16H18	210	210.140851		4	C17H18	222	222.140851
Acenaphthene	5	C17H20	224	224.156501		5	C18H20	236	236.156501
	6	C18H22	238	238.172151		6	C19H22	250	250.172151
	7	C19H24	252	252.187801		7	C20H24	264	264.187801
	8	C20H26	266	266.203451		8	C21H26	278	278.203451
	9	C21H28	280	280.219101		9	C22H28	292	292.219101
	10	C22H30	294	294.234751		10	C23H30	306	306.234751
	0	C14H10	178	178.07825		0	C8H6S	134	134.019021
	1	C15H12	192	192.0939		1	C9H8S	148	148.034671
	2	C16H14	206	206.10955		2	C10H10S	162	162.050321
	3	C17H16	220	220.125201		3	C11H12S	176	176.065971
Phenanthrene	4	C18H18	234	234.140851	Benzo[b]thiophene	4	C12H14S	190	190.081621
Anthracene	5	C19H20	248	248.156501		5	C13H16S	204	204.097272
	6	C20H22	262	262.172151		6	C14H18S	218	218.112922
	7	C21H24	276	276.187801					
	8	C22H26	290	290.203451					
	9	C23H28	304	304.219101					
	10	C24H30	318	318.234751					

Compound	Num. of Me-	Formula	Nominal mass	Exact mass
	0	C12H8S	184	184.034671
	1	C13H10S	198	198.050321
	2	C14H12S	212	212.065971
Dibenzothiophene	3	C15H14S	226	226.081621
-	4	C16H16S	240	240.097272
	5	C17H18S	254	254.112922
	6	C18H20S	268	268.128572
	7	C19H22S	282	282.144222
	8	C20H24S	296	296.159872

Table S3. Percentage of degradation of selected PAHs derivatives based on total peak volume value

	Peak	Removal	
PAHs derivatives	Abiotic control	Test with microorganism	rate (%)
TIC	26826654956	13292252155	50.4
Naphthalene derivatives	347895815	108714773	68.8
Alkyl Naphthalenes	781660154	349919820	55.2
Acenaphthylene/biphenyl derivatives	281387830	119977763	57.4
Alkyl Acenaphthylenes/biphenyls	599884088	485650151	19.0
Acenaphthene derivatives	129873835	45544167	64.9
Alkyl Acenaphthenes	849874364	552383524	35.0
Fluorene derivatives	212986435	113697899	46.6
Alkyl Fluorenes	393500004	372191256	5.4
Phenanthrene, Anthracene derivatives	213028732	164704559	22.7
Alkyl Phenanthrenes/anthracenes	197588730	196675322	0.5
Benzo[b]thiophene derivatives	8201017	2242315	72.7
Alkyl Benzo[b]thiophenes	275631217	193953150	29.6
Dibenzothiophene derivatives	3825050	82068	97.9
Alkyl Dibenzothiophenes	71739479	55039479	23.3

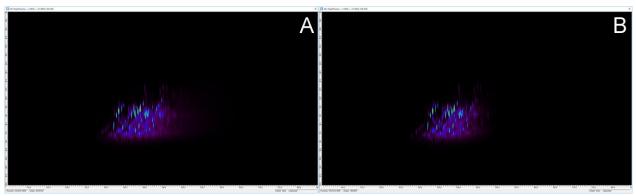


Figure S2. Selected Ion Chromatograms of m/z 128.0626 after 30 days. (A) Abiotic control; (B) Degraded $C_{10}H_8$ compounds (naphthalene derivatives).

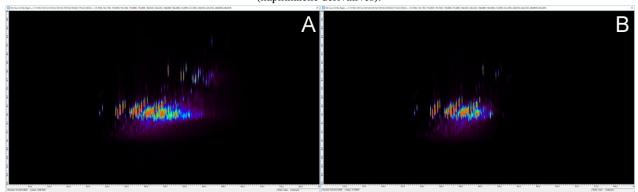


Figure S3. Selected Ion Chromatograms of *m/z* 142.0783, 156.0939, 170.1096, 184.1252, 198.1409, 212.1565, 226.1722, 240.1878 after 30 days. (A) Abiotic control; (B) Degraded alkyl naphthalenes.

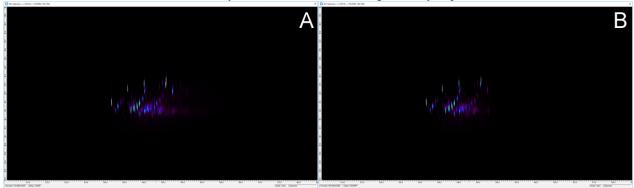


Figure S4. Selected Ion Chromatograms of m/z 154.0783 after 30 days. (A) Abiotic control; (B) Degraded $C_{12}H_{10}$ compounds (acenaphthylene/biphenyl derivatives).

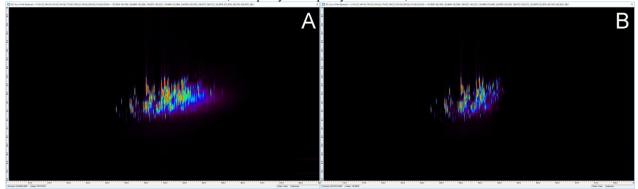


Figure S5. Selected Ion Chromatograms of *m/z* 168.0939, 182.1096, 196.1252, 210.1409, 224.1565, 238.1722, 252.1878, 266.2035, 280.2192, 294.2349 after 30 days. (A) Abiotic control; (B) Degraded alkyl acenaphthylene/alkyl biphenyl.

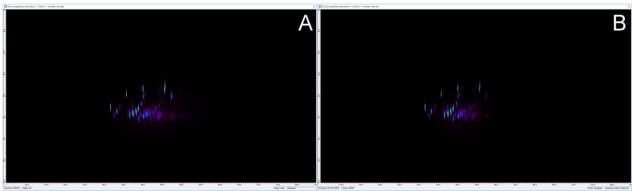


Figure S6. Selected Ion Chromatograms of m/z 154.0782 after 30 days. (A) Abiotic control; (B) Degraded $C_{12}H_{10}$ compounds (acenaphthene derivatives).

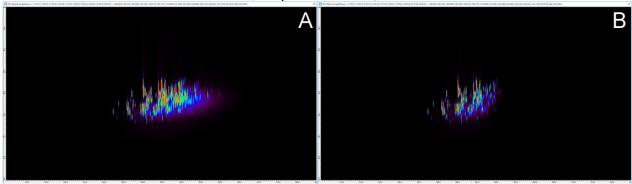


Figure S7. Selected Ion Chromatograms of *m/z* 154.0782, 168.0939, 182.1096, 196.1252, 210.1409, 224.1565, 238.1722, 252.1878, 266.2035, 280.2191, 294.2348 after 30 days. (A) Abiotic control; (B) Degraded alkyl acenaphthenes.

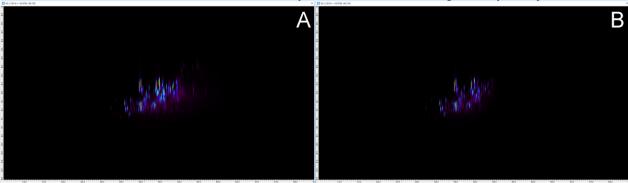


Figure S8. Selected Ion Chromatograms of m/z 166.0783 after 30 days. (A) Abiotic control; (B) Degraded $C_{13}H_{10}$ compounds (fluorene derivatives).

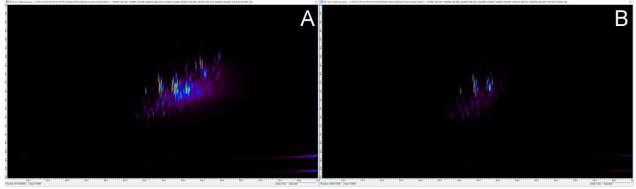


Figure S9. Selected Ion Chromatograms of *m/z* 180.0939, 194.1096, 208.1252, 222.1409, 236.1565, 250.1722, 264.1878, 278.2035, 292.2192, 306.2349 after 30 days. (A) Abiotic control; (B) Degraded alkyl fluorenes.

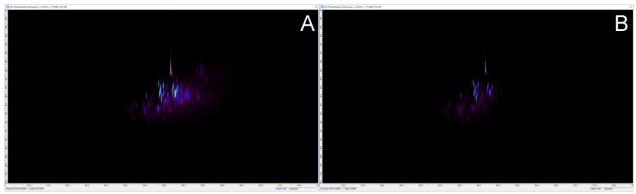


Figure S10. Selected Ion Chromatograms of m/z 178.0783 after 30 days. (A) Abiotic control; (B) Degraded $C_{14}H_{10}$ compounds (phenanthrenes/anthracenes derivatives).

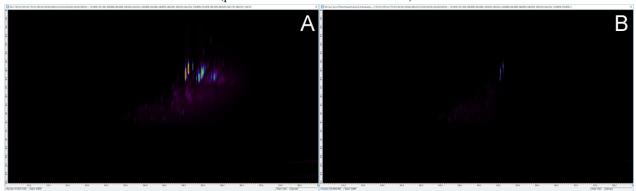


Figure S11. Selected Ion Chromatograms of *m/z* 192.0939, 206.1096, 220.1252, 234.1409, 248.1565, 262.1722, 276.1878, 290.2035, 304.2191, 318.2349 after 30 days. (A) Abiotic control; (B) Degraded alkyl phenanthrenes/alkyl anthracenes.

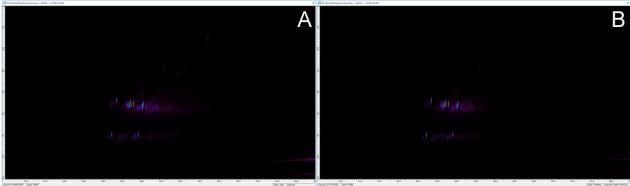


Figure S12. Selected Ion Chromatograms of m/z 134.0190 after 30 days. (A) Abiotic control; (B) Degraded C_8H_6S compounds (benzo[b]thiophene derivatives).

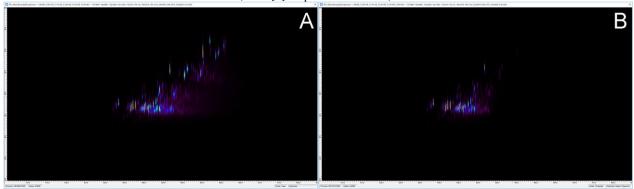


Figure S13. Selected Ion Chromatograms of *m/z* 134.0190, 148.0347, 162.0503, 176.0660, 190.0816, 204.0973, 218.1129 after 30 days. (A) Abiotic control; (B) Degraded alkyl benzo[b]thiophenes.

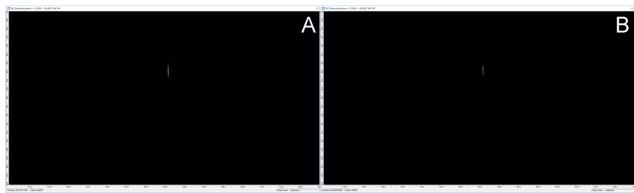


Figure S14. Selected Ion Chromatograms of m/z 184.0347 after 30 days. (A) Abiotic control; (B) Degraded dibenzothiophene $(C_{12}H_8S)$.

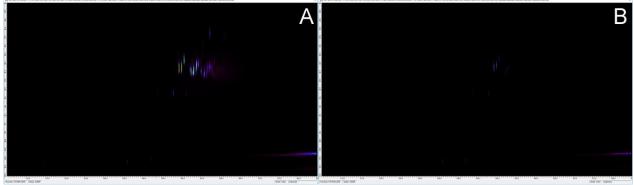


Figure S15. Selected Ion Chromatograms of *m/z* 198.0503, 212.066, 226.0816, 240.0973, 254.1129, 268.1286, 282.1442, 296.1599 after 30 days. (A) Abiotic control; (B) Degraded alkyl dibenzothiophenes.