Supporting Information for Reconstruction of Realistic Kerogen's Molecular Models in Shale Oil and Gas Reservoirs: The Physicochemical Inversion Method

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This Supporting Information document provides additional tables that support and extend the analysis presented in the main manuscript. It is organized into three parts: the detailed identification of pyrolysates obtained at different pyrolysis temperatures, the comparison of the computational time required for DFT calculations, and the complete set of molecular structures reconstructed by PIM.

Part 1. The detailed identification of pyrolysate with different pyrolysis temperatures.

Table S1. The detailed identification of pyrolysate with the pyrolysis temperature at 650°C.

R.T. (min)	Molecular fragment	Percent of peak area
1.64	Acetonitrile	2.28
1.74	Ethanolamine	0.82
11.13	4-Hydroxyimino-but-2-enoic acid, ethyl ester	0.89
31.44	Tetradecane	0.49
35.54	Pentadecane	0.53
39.42	Hexadecane	0.44
43.11	Heptadecane	0.59
45.29	Tetradecanoic acid	0.68
46.61	Eicosane	0.41
49.26	1-Hexadecanol	0.79
49.95	Heneicosane	0.78
52.10	n-Hexadecanoic acid	9.53
53.15	Eicosane	0.4
55.68	n-Heptadecanol-1	1.4
56.21	Heneicosane	0.42
58.30	Octadecanoic acid	20.11
59.14	Eicosane	0.44
59.32	4-Amino-9-fluorenone	0.56
61.95	Eicosane	1.35
62.30	Perylene	0.97
62.43	Benzo[k]fluoranthene	0.99
64.55	2-(2,4,6-Cycloheptatrienylidene)-1,3-indandione	1.27
64.66	Eicosane	0.94
65.31	2-(2,4,6-Cycloheptatrienylidene)-1,3-indandione	1.59
66.49	1-Hydroxypyrene	1.28
67.27	Heneicosane	1.14
67.39	l-(+)-Ascorbic acid 2,6-dihexadecanoate, Isopropyl palmitate	5.36
67.87	Benzo[b]naphtho[2,3-d]thiophene, 6-methyl-	1.05
68.08	Epibuphanamine	1.3
69.67	Benzo[c]phenanthrene, 5-methyl-	1.15
69.77	Heptadecane, 9-octyl-	2.21
69.98	Benz[a]anthracene, 9-methyl-	0.73
70.19	11H-Indeno[1,2-b]quinoline, 2,6-dimethyl-	0.74
70.92	Benzo[b]naphtho[2,3-d]thiophene, 6,8-dimethyl-	0.65

72.20	Eicosane	2.42
73.34	Benzo[j]fluoranthene	6.97
74.11	Benzo(a)pyren-7-ol	0.55
74.53	Tetratriacontane	2.15
74.86	Dinaphtho[1,2-b:1',2'-d]furan, Dinaphtho[2,1-b:1',2'-d]furan	1.64
75.03	Benzo[e]pyrene	1.87
75.19	Benzo(a)pyrene 4,5-oxide	0.7
75.33	Benzo[k]fluoranthene	2.25
86.80	Tetratriacontane	2.03

Table S2. The detailed identification of pyrolysate with the pyrolysis temperature at 800°C.

R.T. (min)	Molecular fragment	Percent of peak area
1.77	Ala-Gly	4.67
2.27	Cyclopropane, 1-ethyl-2-methyl-, cis-	2.55
2.75	Benzene	2.35
4.13	Toluene	3.29
7.14	o-Xylene	1.35
8.03	p-Xylene	1.63
12.5	Benzene, 1-ethyl-3-methyl-	1.19
26.56	Naphthalene, 2-methyl-	0.57
31.43	Tetradecane	0.82
35.52	Pentadecane	0.69
39.4	Hexadecane	0.59
43.08	Heptadecane	0.74
46.59	Eicosane	0.59
49.24	2-((2-Ethoxyethoxy)carbonyl)benzoic acid	0.66
49.93	Heneicosane	0.64
52.02	n-Hexadecanoic acid	9.96
53.12	Eicosane	0.55
56.18	Heneicosane	0.55
57.12	9,12-Octadecadienoic acid (Z,Z)-	0.82
57.29	trans-13-Octadecenoic acid	1.13
58.21	Octadecanoic acid	25.44
58.55	Hexadecanamide	1.66
59.12	Eicosane	0.81

61.93	Eicosane	0.71
63.5	9-Octadecenamide, (Z)-	2.75
64.63	Tetracosane	0.82
67.23	Eicosane	1.39
69.74	Heneicosane	1.85
72.16	Tetratriacontane	2.28
73.25	Benzo[k]fluoranthene	1.58
74.51	Tetratriacontane	2.29
76.77	2-methylhexacosane	0.85
81.07	Tetratetracontane	1.72

Table S3. The detailed identification of pyrolysate with the pyrolysis temperature at 950°C.

R.T. (min)	Molecular fragment	Percent of peak area
1.92	Methylenecyclopropane	5.47
2.18	Glycine	5.38
2.32	1-Hexene	1.6
2.63	1,4-Cyclohexadiene	0.92
2.80	Benzene	3.79
4.20	Toluene	3.82
7.18	Benzene, 1,3-dimethyl-	1.32
8.00	Styrene	0.98
8.08	o-Xylene	0.74
12.52	Mesitylene	1.02
21.50	Naphthalene	0.67
26.57	Naphthalene, 1-methyl-	0.64
43.08	Heptadecane	0.54
49.25	2-((2-Chloroethoxy)carbonyl)benzoic acid	0.63
52.05	n-Hexadecanoic acid	11.83
58.21	Octadecanoic acid	25.68
58.55	Hexadecanamide	3.31
61.94	Heneicosane	0.84
63.52	9-Octadecenamide, (Z)-	5.78
64.64	Tetracosane	0.92
67.25	Eicosane	1.88

69.76	Tetracosane	2.7
72.18	Tetratriacontane	3.21
73.27	Benzo[k]fluoranthene	1.52
74.52	Tetratriacontane	2.68
76.78	Tetratriacontane	1.02

Part 2. The comparison of the computational time required for DFT calculations

Table S4 Single point energy and time comparison for various methods and sites of Figure 3.

	B3LYP/6-31G(d)		B3LYP-D3/6-311+G(d, p)	
	BDE (a.u.)	Time	BDE (a.u.)	Time
1	0.1183	46min	0.1210	612min
2	0.1696	57min	0.1705	687min
3	0.1657	74min	0.1672	1263min

Part 3. The complete set of molecular structures reconstructed by PIM.

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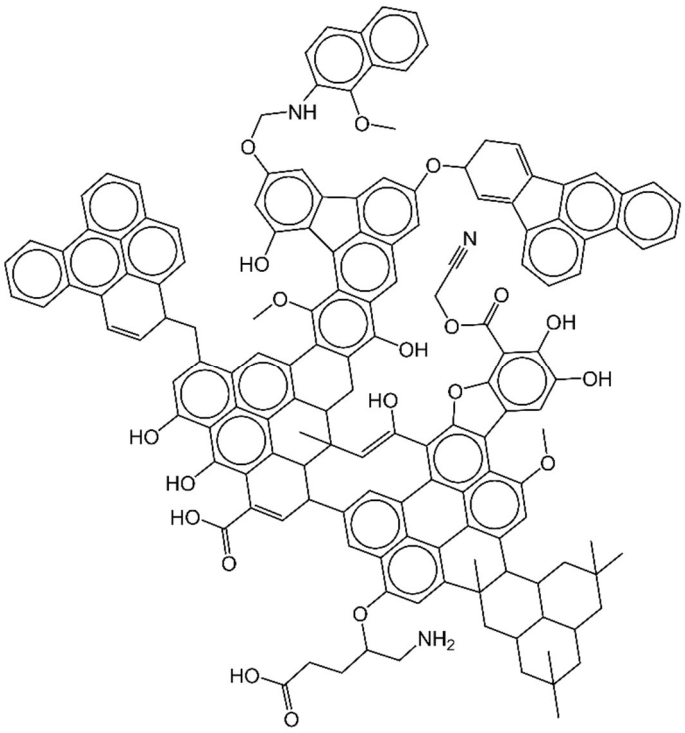

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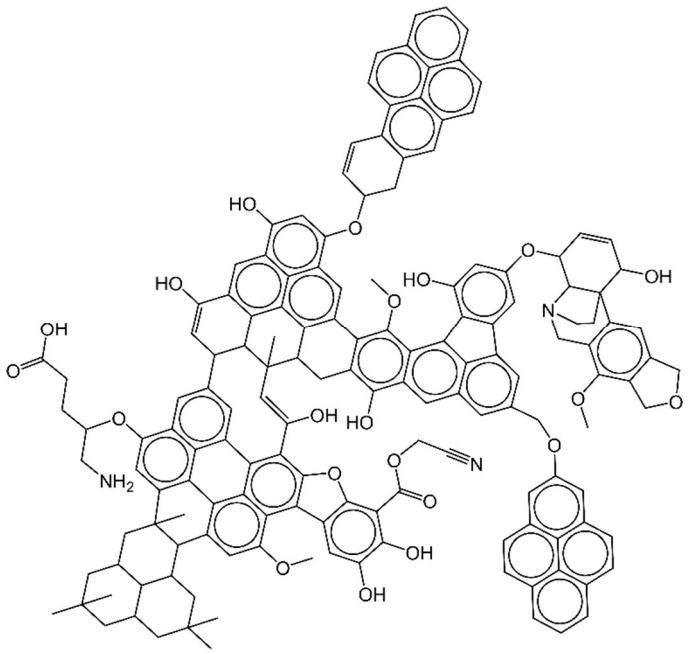

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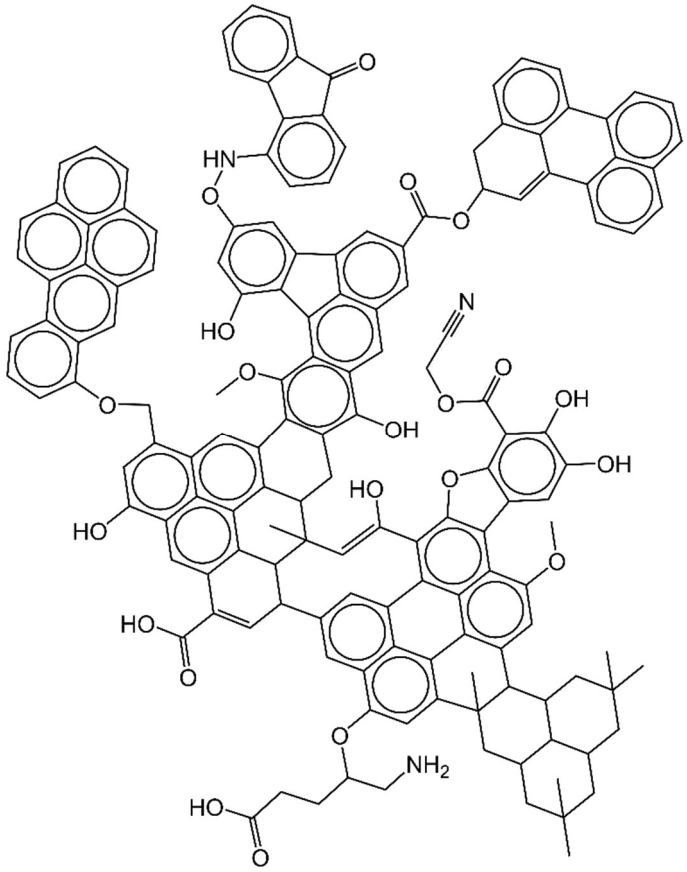

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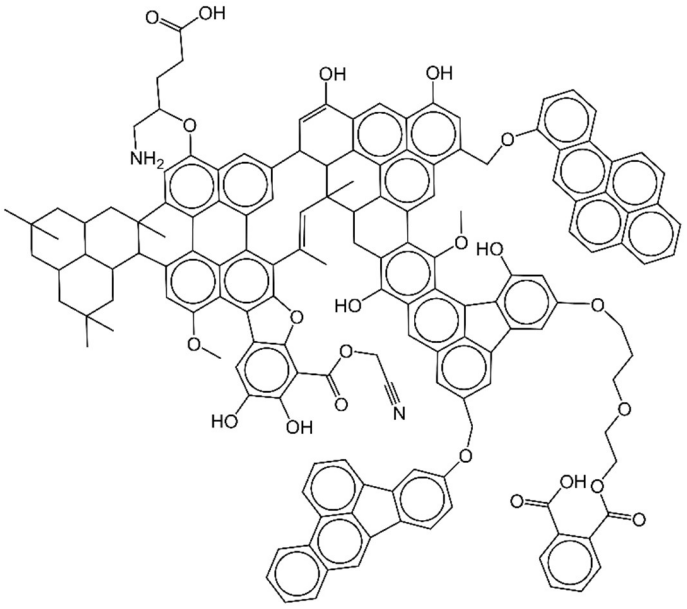

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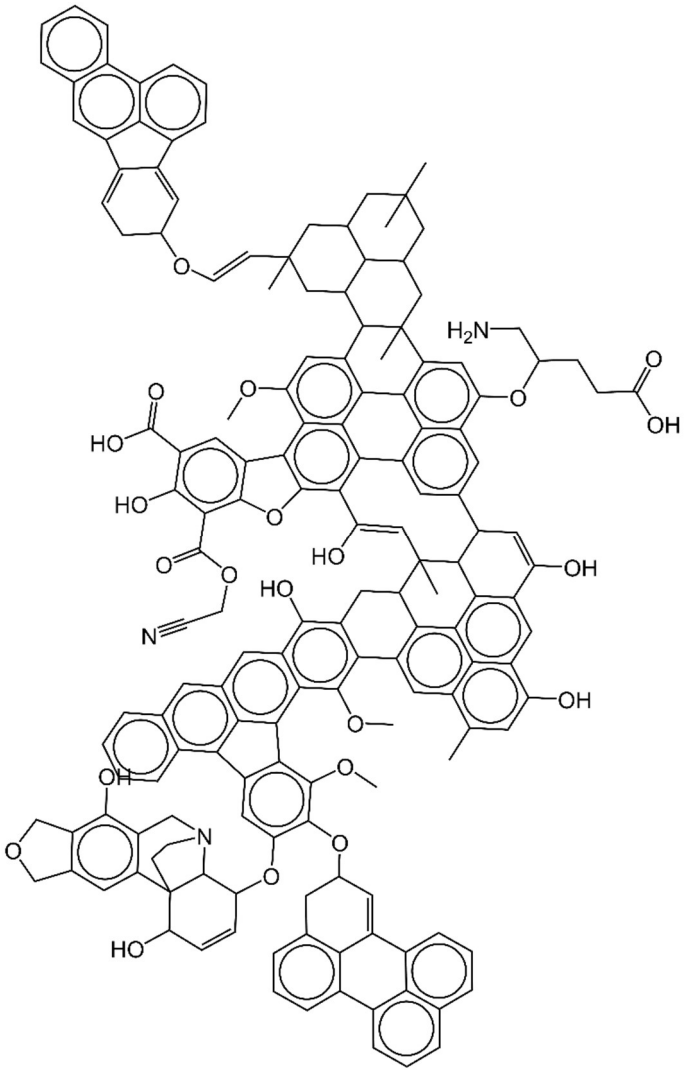

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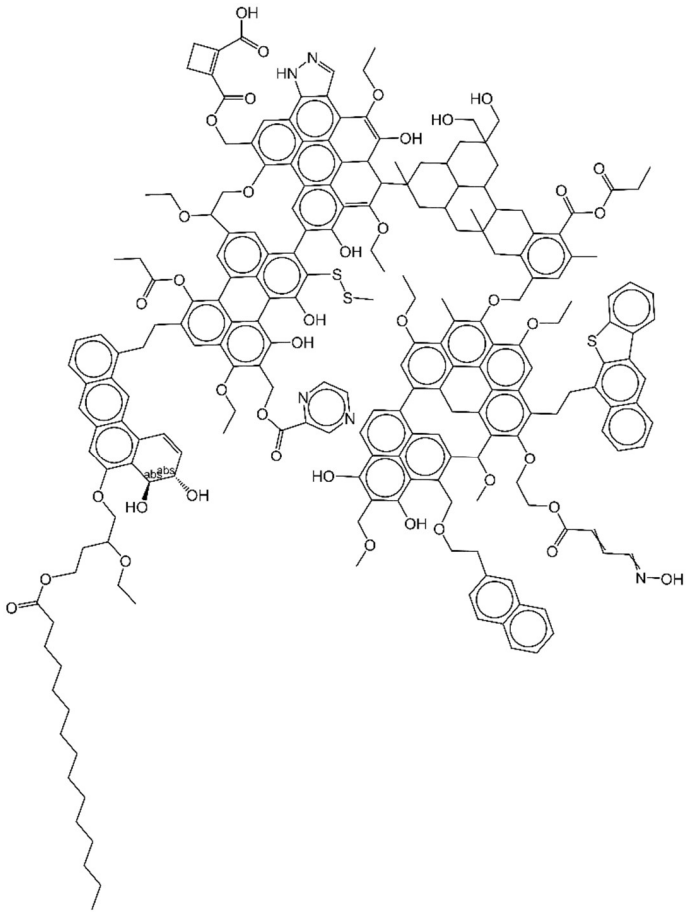

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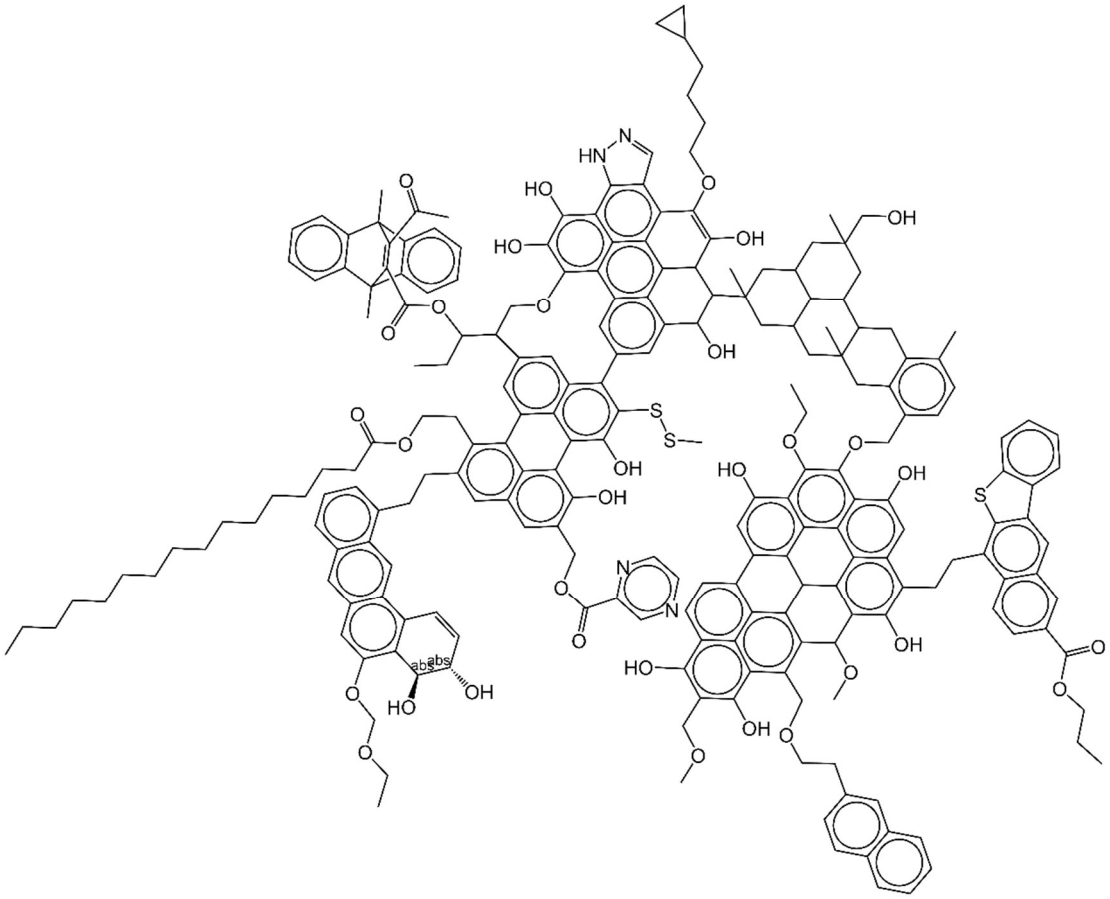

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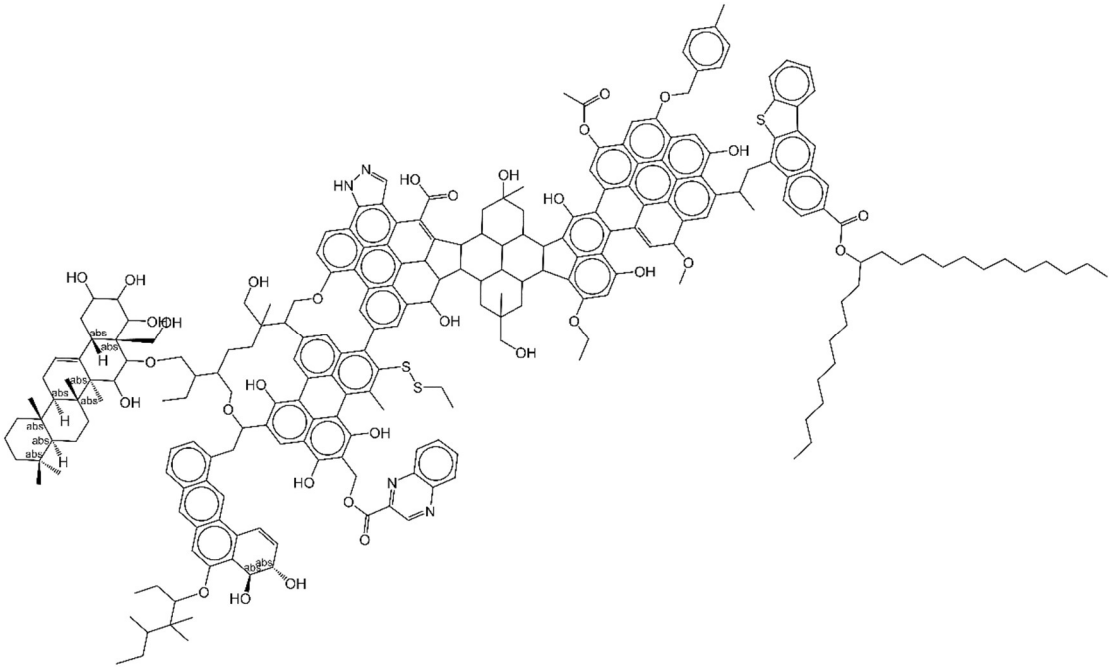

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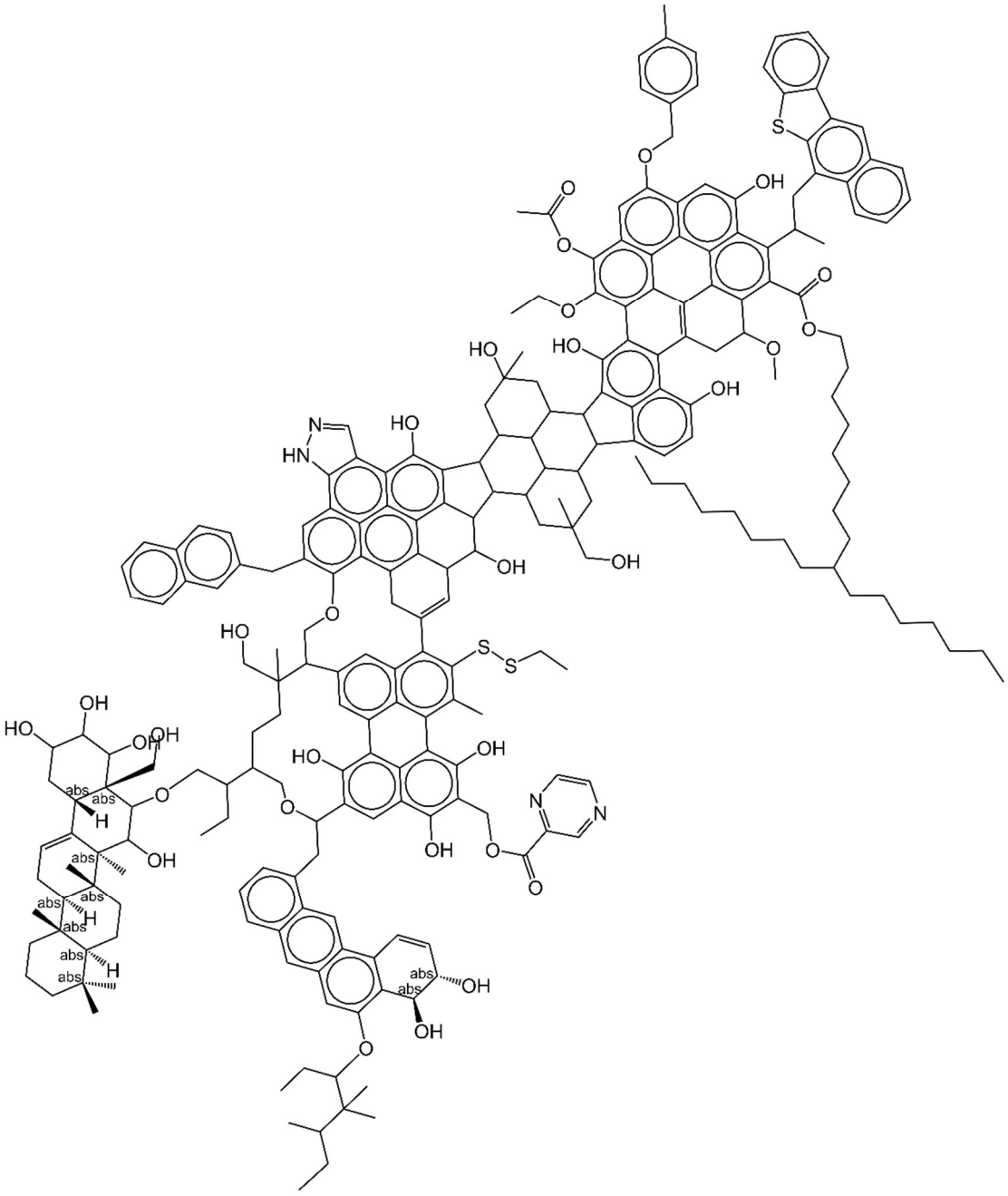

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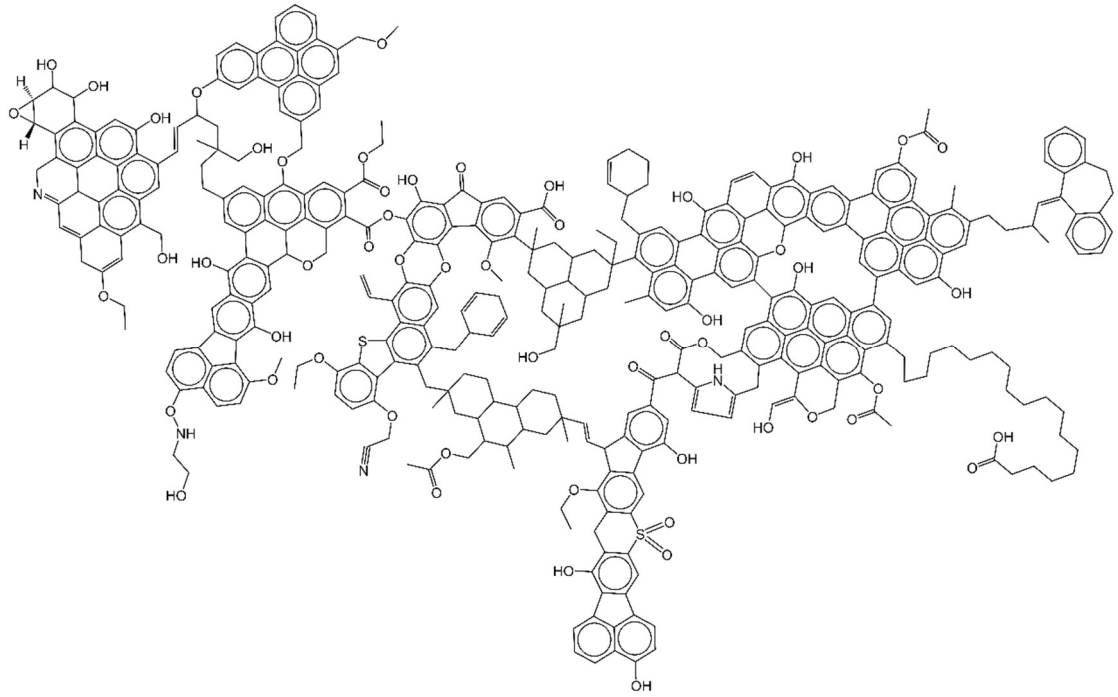

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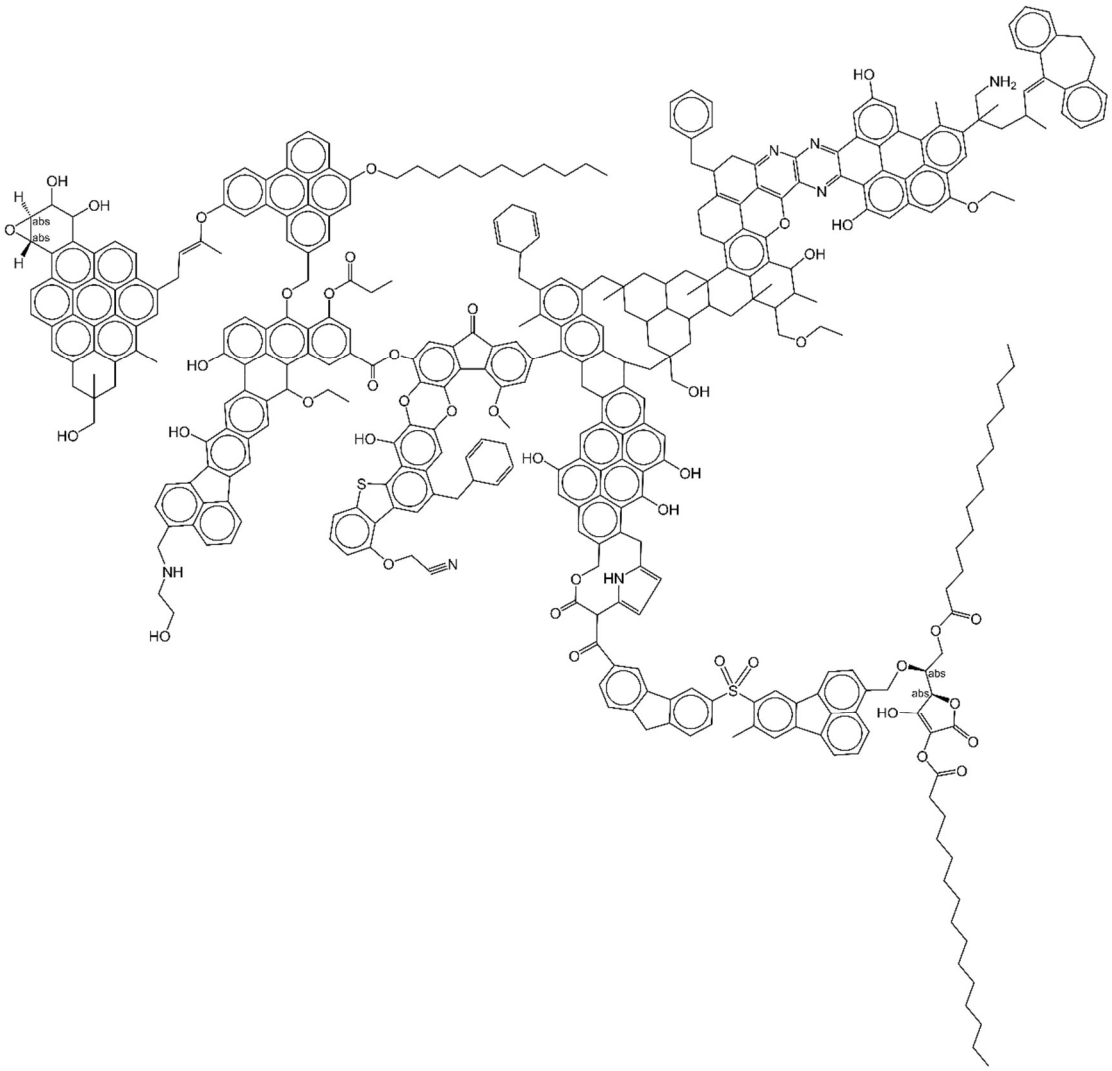

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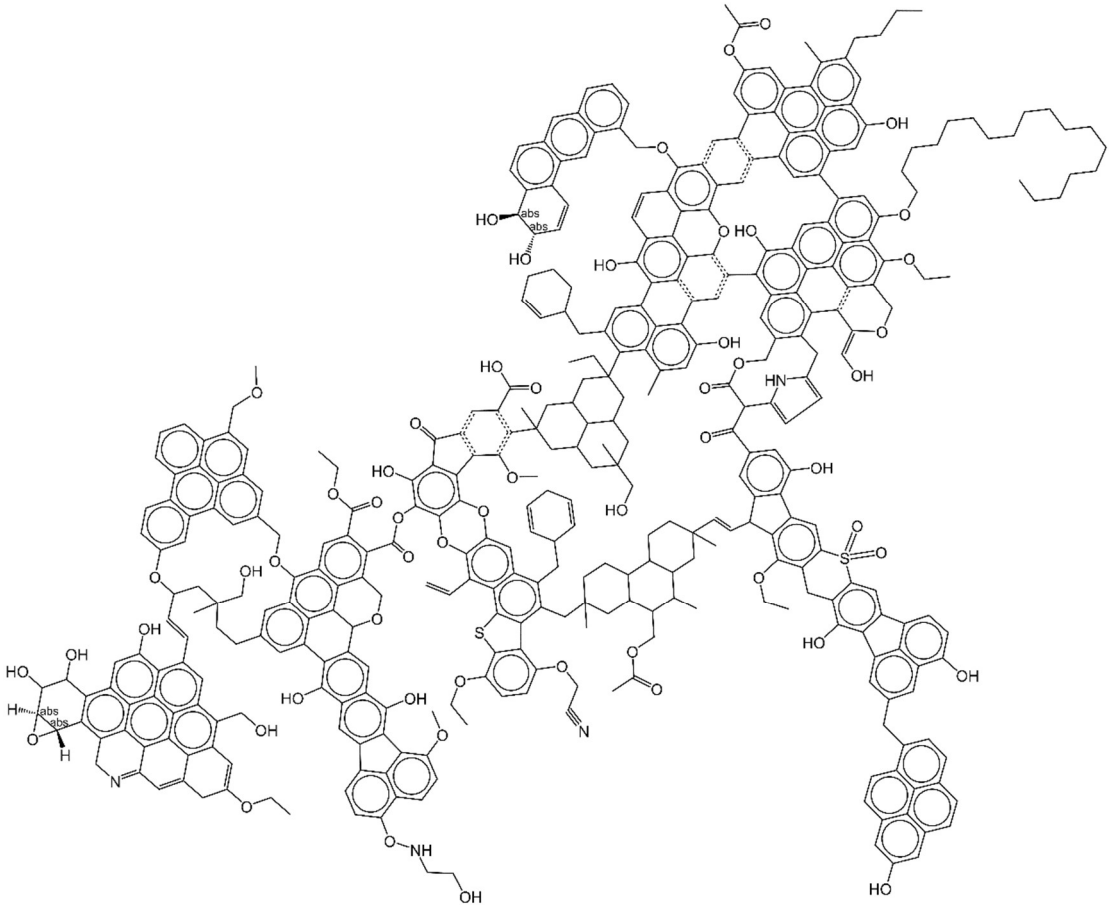

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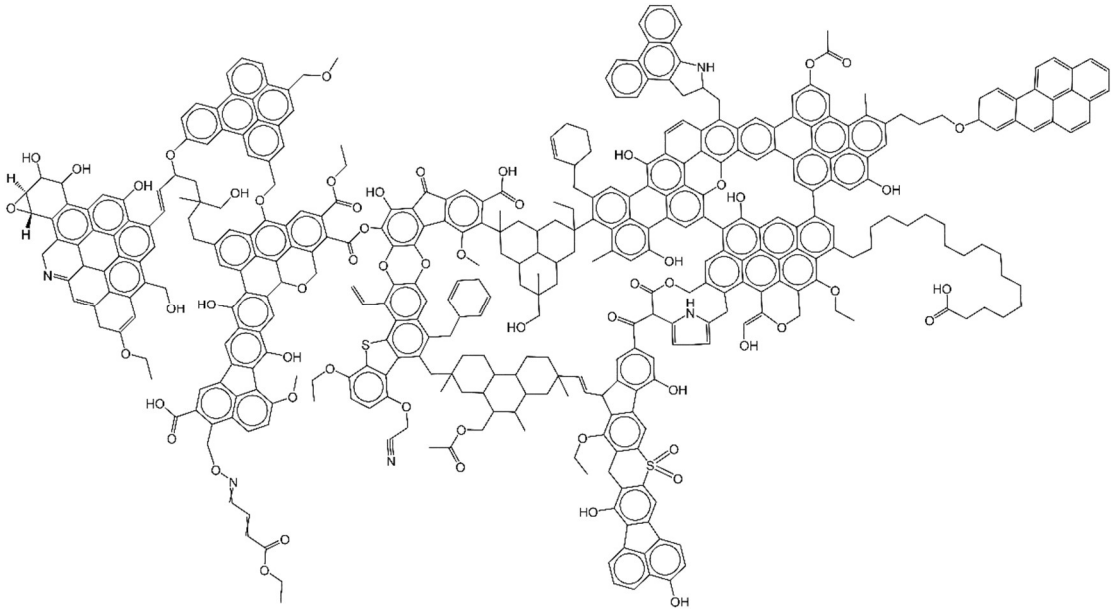

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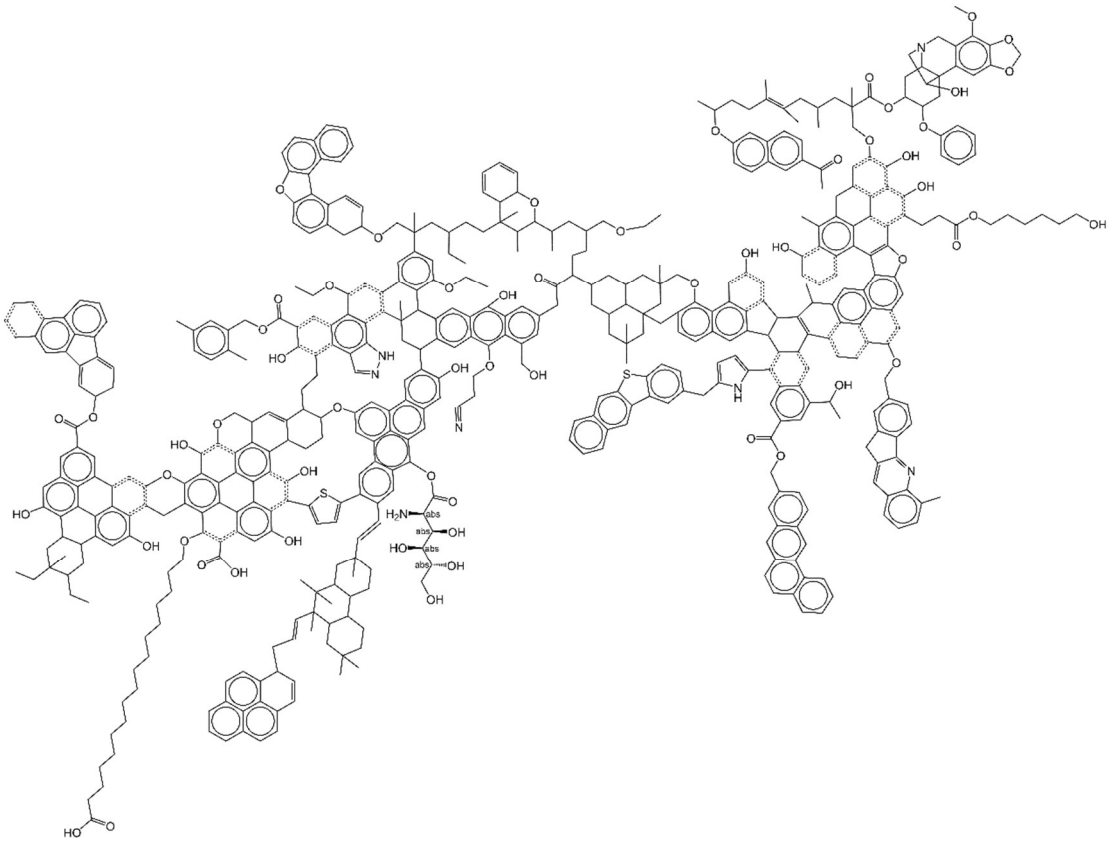

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