Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.
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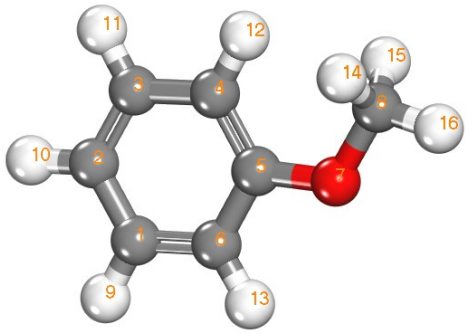
Supplementary Information

Table S1: Unique imaginary frequency identified for each transition state of the reactions for both non-catalytic and catalytic transmethylation

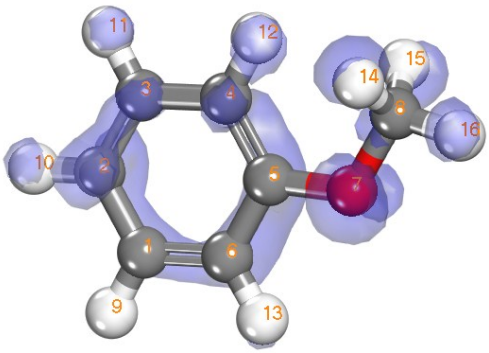
Reactant	Via	Product	Orientation	Imaginary frequency (Frequency(1/cm); Intensity(km/mol))		
				Non-catalytic (TS)	Catalytic	
					Cleavage (TS1)	Methyl cation transfer (TS2)
			Ortho	-15.49/0.03		-352.36/6.86
	phenol	Cresol	Meta	-11.96/0.14		-285.63/7.12
			Para	-10.15/0.11		-435.58/5.90
			Ortho	-304.25/658.68		-345.63/7.72
	o-cresol	Xylenol	Meta	-144.6/1.40		-311.78/158.17
			Para	-270.32/163.89		-343.56/192.81
	2,4-xylenol	2,4,6-phenol	Ortho	-237.38/453.09		-171.58/6.64
anisole	2,6-xylenol	2,3,6-phenol	Meta	-229.42/129.61	-331.54/99.74	-511.45/499.08
	benzene	Toluene	-	-686.39/37.85		-233.06/16.67
			Ortho	-244.71/129.42		-138.44/101.67
	toluene	Xylene	Meta	-240.01/87.44		-320.08/188.36
			Para	-36.49/27.64		-302.45/185.02
			Ortho	-283.22/185.03		-98.98/4.73
	anisole	methyl-anisole	Meta	-6823.26/7.10		-313.60/67.33
			Para	-267.68/159.39		-309.34/2.79

Fig S2. (a) Mulliken bond order of the anisole molecule for the transmethylation reaction; (b) Fukui indices of anisole atoms under electrophilic attack (Fukui (-)). Isovalue 0.035. Atoms are colored as follows: carbon atom (grey), hydrogen atom (white) and oxygen atom (red)



Bond ID	Mulliken Bond order
C8-O7	0.515
C5-O7	0.668
C8-H14	0.798
C8-H15	0.799
C6-H13	0.813
C4-H12	0.814
C3-H11	0.821
C1-H9	0.824
C2-H10	0.825
C8-H16	0.826
C4-C5	1.003
C3-C4	1.025
C5-C6	1.030
C1-C2	1.032
C1-C6	1.054
C2-C3	1.063

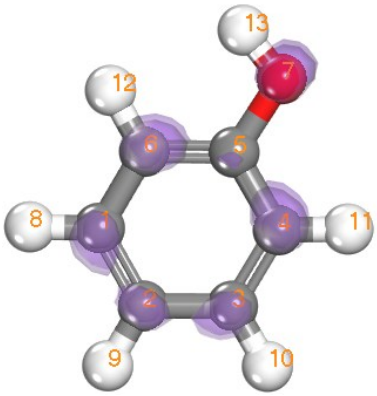
(a)



Atom	Fukui (-) index
O7	0.129
C2	0.125
C6	0.086
C5	0.075
C4	0.072
C3	0.071
C1	0.061
H10	0.057
H11	0.046
H13	0.046
H9	0.044
H12	0.040
H15	0.038
H14	0.037
H16	0.036
C8	0.035

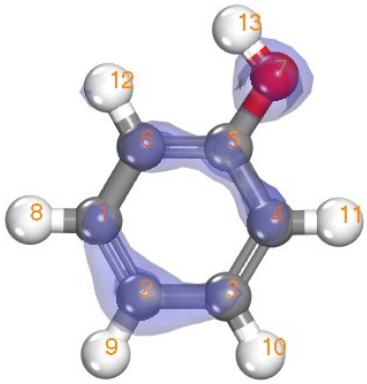
(b)

Fig S3. Fukui indices for (a) radical attack on phenol molecule (Fukui (0)), and (b) electrophilic attack on phenol molecule (Fukui (-)). Isovalue 0.035. Atoms are colored as follows: carbon atom (grey), and hydrogen atom (white) and oxygen atom (red)



Atom	Fukui (0) index
C4	0.105
O7	0.103
C2	0.102
C6	0.100
C1	0.099
C3	0.095
C5	0.073
H8	0.057
H10	0.056
H11	0.056
H9	0.055
H12	0.055
H13	0.044

(a)



Atom	Fukui (-) index
O7	0.152
C2	0.136
C4	0.089
C5	0.089
C6	0.083
C1	0.073
C3	0.068
H9	0.061
H13	0.055
H11	0.050
H8	0.049
H10	0.048
H12	0.048

(b)