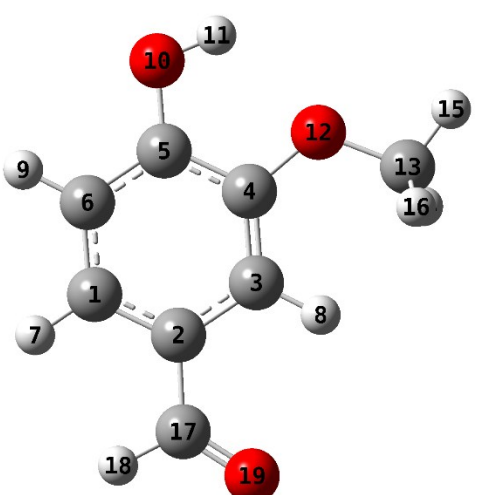
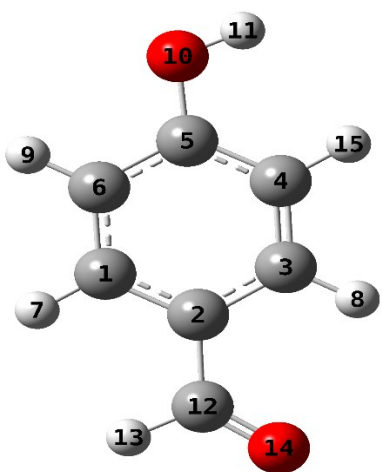


### Electronic Supplementary Information

**Table S1:** The Cartesian co-ordinates of few important structures/products under vanillin conversion process.

Structures	Tag	Symbol	X	Y	Z
<p>Vanillin</p> 	1	C	-1.13951	-1.67326	-2.7E-05
	2	C	-1.47317	-0.31746	-0.00002
	3	C	-0.45809	0.657554	-4.2E-05
	4	C	0.865263	0.263767	-0.00007
	5	C	1.197604	-1.11223	0.000009
	6	C	0.194096	-2.07286	-2E-06
	7	H	-1.92672	-2.41977	-0.00003
	8	H	-0.74942	1.699845	0.000036
	9	H	0.475389	-3.11869	0.000024
	10	O	2.497041	-1.49085	0.000071
	11	H	3.042058	-0.6908	-1.9E-05
	12	O	1.958248	1.088416	-5.7E-05
	13	C	1.743875	2.498861	0.000025
	14	H	1.19681	2.810193	0.894819
	15	H	2.733528	2.951429	-0.00014
	16	H	1.196334	2.810215	-0.89448
	17	C	-2.88669	0.09134	0.000017
	18	H	-3.60893	-0.75226	0.000028
	19	O	-3.28271	1.239377	0.000039
<p>p-hydroxybenzaldehyde</p> 	1	C	0.179776	1.339576	-6E-06
	2	C	1.008635	0.209615	-9E-06
	3	C	0.424081	-1.06463	0
	4	C	-0.9539	-1.20441	0.000012
	5	C	-1.76971	-0.06408	0.000015
	6	C	-1.20113	1.212589	0.000006
	7	H	0.626541	2.329003	-1.3E-05
	8	H	1.070308	-1.93457	-2E-06
	9	H	-1.85202	2.078038	0.000009
	10	O	-3.12854	-0.14082	0.000026
	11	H	-3.40923	-1.0625	0.000031
	12	C	2.473438	0.370378	-2.2E-05
	13	H	2.820419	1.425921	-2.8E-05
	14	O	3.276343	-0.53893	-2.6E-05
	15	H	-1.40557	-2.19215	0.000019
<p>Guaiacol</p>	1	C	-0.43936	-0.08047	-0.00009
	2	C	0.477492	0.98703	0.00002
	3	C	1.840317	0.725771	0.00014
	4	C	2.298133	-0.59356	0.000107
	5	C	1.392694	-1.6483	-5.7E-05
	6	C	0.016782	-1.39363	-0.00019
	7	H	2.528173	1.5629	0.000262
	8	H	3.363894	-0.78929	0.000214
	9	H	1.743868	-2.67323	-9.3E-05
	10	H	-0.68295	-2.2192	-0.00036
	11	O	-1.75494	0.317596	-0.00041

	12	O	0.029334	2.274592	0.000033
	13	H	-0.93705	2.250544	-0.00043
	14	C	-2.76768	-0.68096	0.000362
	15	H	-2.70186	-1.30856	0.895039
	16	H	-3.71653	-0.14722	0.000897
	17	H	-2.70301	-1.30879	-0.89424

Benzene					
	1	C	-0.69728	-1.20773	0
	2	C	-1.39458	-9E-06	0
	3	C	-0.6973	1.207725	0
	4	C	0.697279	1.207726	0
	5	C	1.394621	0.000009	0
	6	C	0.697294	-1.20772	0
	7	H	-1.23913	-2.14633	0
	8	H	-1.23915	2.146311	0
	9	H	1.239163	-2.1463	0
	10	H	1.239136	2.146315	0
	11	H	2.478383	0.000015	0
	12	H	-2.47867	-1.5E-05	0

Phenol					
	1	C	-0.93816	-0.02429	-0.00017
	2	C	-0.2631	1.197539	-5.3E-05
	3	C	1.130957	1.217371	-0.00008
	4	C	1.85509	0.02752	0.000088
	5	C	1.170095	-1.1887	0.00013
	6	C	-0.2206	-1.22157	-8.3E-05
	7	H	1.648459	2.170181	-0.00011
	8	H	2.938309	0.046256	0.000133
	9	H	1.722666	-2.12168	0.000137
	10	H	-0.76355	-2.159	-0.00037
	11	O	-2.30513	-0.11054	0.000005
	12	H	-0.82351	2.128104	0.000037
	13	H	-2.68704	0.773222	0.001164

o-quinonemethide					
	1	C	-1.86496	-0.56904	-5E-06
	2	C	-1.74904	0.876941	0.000003
	3	C	-0.5354	1.467799	0.000007
	4	C	0.686332	0.677361	0.000003
	5	C	0.578847	-0.83286	0.000003
	6	C	-0.7826	-1.37924	-7E-06
	7	H	-2.86054	-1.0019	-0.00001
	8	H	-0.44299	2.54915	0.000009
	9	H	-0.87065	-2.45918	-1.2E-05
	10	O	1.569577	-1.55229	0.000008
	11	C	1.907644	1.244388	-9E-06
	12	H	2.795448	0.623208	-1.6E-05

	13	H	2.031086	2.321754	-1.3E-05
	14	H	-2.6539	1.473198	0.000004

**Table S2:** The electronic energy added with zero point vibrational energies (ZPVEs), ZPVEs, and multiplicities of all structures involved in each reaction scheme under vanillin conversion.

S. No.	Structures	E	ZPVE	E <sub>corr</sub> = (E+ZPVE)	Multiplicities
1	VAN	-535.479129	0.146324	-535.332805	1
2	1_a	-495.531144	0.105442	-495.425702	2
3	1_b	-496.168451	0.117688	-496.050763	1
4	1_b*	-496.67007	0.118694	-496.551376	2
5	TS1_1	-496.662931	0.119898	-496.543033	2
6	1_c	-496.708131	0.127052	-496.581079	2
7	2_a	-420.229349	0.100617	-420.128732	2
8	2_b	-420.918827	0.113488	-420.805339	1
9	VAN^	-535.981212	0.146541	-535.834671	2
10	TS3_1	-535.974424	0.147908	-535.826516	2
11	3_a	-536.01123	0.155034	-535.856196	2
12	TS3_2	-535.992663	0.152612	-535.840051	2
13	3_b*	-536.009358	0.151515	-535.857843	2
14	3_b	-422.116911	0.136975	-421.979936	1
15	4_a	-459.534327	0.128689	-459.405638	2
16	4_b	-460.226679	0.141665	-460.085014	1
17	VAN*	-535.981218	0.146612	-535.834606	2
18	TS5_1	-535.974158	0.148387	-535.825771	2
19	5_a	-536.01825	0.155176	-535.863074	2
20	TS5_2	-536.00106	0.153144	-535.847916	2
21	5_b	-536.015226	0.151448	-535.863778	2
22	5_b*	-421.420894	0.113679	-421.307215	1
23	TS5_3	-421.413517	0.115036	-421.298481	2
24	5_c	-421.453153	0.121281	-421.331872	2
25	TS5_4	-421.432313	0.119628	-421.312685	2
26	5_d	-421.450919	0.117956	-421.332963	2
27	5_d*	-308.060843	0.104531	-307.956312	2
28	TS5_5	-308.051649	0.106128	-307.945521	2
29	5_e	-308.095531	0.11275	-307.982781	2
30	5_f	-232.311245	0.100168	-232.211077	1
31	5a_b*	-421.420899	0.11384	-421.307059	2
32	TS5a_3	-421.411952	0.115411	-421.296541	2
33	5a_c	-421.45709	0.122421	-421.334669	2
34	5a_d	-345.669074	0.109378	-345.559696	1
35	5a_d*	-346.171137	0.109574	-346.061563	2
36	TS5a_4	-346.16358	0.110777	-346.052803	2
37	5a_e	-346.205356	0.117199	-346.088157	2
38	TS5a_5	-346.185388	0.115262	-346.070126	2
39	VAN^	-535.460362	0.144939	-535.315423	1
40	TS6_1	-535.349531	0.139835	-535.209696	1
41	6_a	-535.425284	0.144296	-535.280988	1
42	6_b	-420.269625	0.100176	-420.169449	2
43	6_c	-420.918827	0.113486	-420.805341	1
44	6_c*	-421.420908	0.113877	-421.307031	2
45	TS6_2	-421.411951	0.115411	-421.29654	2

46	<b>6_d</b>	-421.459366	0.122592	-421.336774	2
47	<b>6_e</b>	-345.669073	0.109378	-345.559695	1
48	<b>TS6_3</b>	-345.52594	0.103699	-345.422241	1
49	<b>6_f</b>	-345.659808	0.105563	-345.554245	1
50	<b>7_a</b>	-534.812117	0.132082	-534.680035	2
51	<b>TS7_1</b>	-534.776626	0.130554	-534.646072	2
52	<b>7_b</b>	-534.788937	0.132075	-534.656862	2
53	<b>TS7_2</b>	-534.788502	0.1317	-534.656802	2
54	<b>7_c</b>	-534.8118	0.1337	-534.6781	2
55	<b>7_d</b>	-535.48892	0.147287	-535.341633	1
56	<b>TS7_3</b>	-535.433549	0.143003	-535.290546	1
57	<b>7_e</b>	-535.452335	0.142204	-535.310131	1
58	<b>7_e*</b>	-459.489405	0.117646	-459.371759	2
59	<b>TS7_4</b>	-459.486367	0.118394	-459.367973	2
60	<b>7_f</b>	-459.553769	0.125995	-459.427774	2
61	<b>TS7_5</b>	-459.519555	0.123219	-459.396336	2
62	<b>7_g</b>	-459.524014	0.122229	-459.401785	2
63	<b>7a_d</b>	-534.286515	0.123553	-534.162962	1
64	<b>TS7a_1</b>	-534.134931	0.11699	-534.017941	1
65	<b>7a_e</b>	-534.267085	0.118741	-534.148344	1
66	<b>TS7a_2</b>	-420.773476	0.107541	-420.665935	1
67	<b>7a_f</b>	-420.907319	0.109409	-420.79791	1
68	<b>TS7a1_1</b>	-534.143256	0.117838	-534.025418	1
69	<b>7a1_e</b>	-534.276899	0.119734	-534.157165	1
70	<b>TS7a1_2</b>	-420.773805	0.107608	-420.666197	1
71	<b>7b_f</b>	-459.593197	0.12702	-459.466177	2
72	<b>TS7b_1</b>	-459.544345	0.123336	-459.421009	2
73	<b>7b_g</b>	-459.60158	0.12744	-459.47414	2
74	<b>7b_h</b>	-460.246771	0.140859	-460.105912	1
75	<b>TS7b_2</b>	-460.100921	0.134906	-459.966015	1
76	<b>7b_i</b>	-460.234639	0.136904	-460.097735	1