

APPENDIX B

**The energy and the relative energy of triolein molecule
and the transesterification mechanism**

Appendix Table B1 Summary of total energy and the relative energy of triolein molecules

	Energy in Hartree		The relative energy (kcal/mol)
	AM1		
1st Triolein	-0.813425	-510.43	2.08
2nd Triolein	-0.816733	-512.51	
	PM3		
1st Triolein	-0.700822	-439.77	11.90
2nd Triolein	-0.719792	-451.68	
	HF6-31G		
1st Triolein	-2636.0677	-1654158.86	2.35
2nd Triolein	-2636.0715	-1654161.20	

Appendix Table B2 The total energy of input files and output files of all reaction in transesterification mechanisms

Reaction	INPUT		OUTPUT	
	Hartree	kcal/mol	Hartree	kcal/mol
7a1	-2781.39	-1745352.66	-2781.55	-1745450.44
7a2-7a3	-2881.50	-1808173.17	-2881.62	-1808245.37
7b1	-2006.35	-1259002.88	-2006.74	-1259249.42
7b2-7b3	-2121.21	-1331080.49	-2121.73	-1331406.79
7c1	-1225.34	-768913.10	-1225.62	-769088.81
7c2-7c3	-1346.54	-844967.32	-1346.93	-845212.04
8a1	-2781.39	-1745352.66	-2781.55	-1745450.44
8a2-8a3	-2881.50	-1808173.17	-2881.62	-1808245.37
8b1	-0.51	-318.27	-0.66	-416.95
8b2-8b3	-2121.29	-1331130.69	-2121.75	-1331419.34
8c1	-1231.66	-772878.97	-1231.92	-773042.12
8c2-8c3	-1346.45	-844910.84	-1346.90	-845193.22
9a1	-2781.39	-1745352.66	-2781.55	-1745450.44
9a2-9a3	-2896.16	-1817367.48	-2986.56	-1874096.27
9b1	-2006.60	-1259164.58	-2006.73	-1259243.14
9b2-9b3	-2121.55	-1331293.84	-2121.75	-1331419.34
9c1	-1225.34	-768913.10	-1225.62	-769088.81
9c2-9c3	-1346.54	-844967.32	-1346.92	-845205.77
10a1	-2781.39	-1745352.66	-2781.55	-1745450.44
10a2-10a3	-2896.16	-1817367.48	-2986.56	-1874096.27
10b1	-1996.21	-1252641.74	-1996.47	-1252804.89
10b2-10b3	-2121.37	-1331180.89	-2121.75	-1331419.34
10c1	-1225.40	-768950.75	-1225.60	-769076.26
10c2-10c3	-1346.54	-844967.32	-1340.02	-840875.95
11a1	-2767.02	-1736330.60	-2767.33	-1736527.25
11a2-11a3	-2881.37	-1808089.43	-2881.76	-1808333.22
11b1	-2006.51	-1259105.09	-2006.74	-1259247.03
11b2-11b3	-2121.60	-1331325.22	-2121.74	-1331413.07
11c1	-1231.66	-772878.97	-1231.92	-773042.12
11c2-11c3	-1346.45	-844910.84	-1346.90	-845193.22
12a1	-2767.02	-1736330.60	-2767.33	-1736527.25
12a2-12a3	-2881.37	-1808089.43	-2881.76	-1808333.22
12b1	-2006.45	-1259067.44	-2006.74	-1259249.42
12b2-12b3	-2121.40	-1331199.71	-2121.75	-1331419.34
12c1	-1225.40	-768950.75	-1225.60	-769076.26
12c2-12c3	-1346.54	-844967.32	-1340.02	-840875.95

Appendix Table B3 The relative energy of input files and output files of all reaction in transesterification mechanisms

Figure	Energy (kcal/mol)		Relative Energy (kcal/mol)
	Input	Output	
17	-1745352.66	-1745450.44	97.78
18	-1808173.17	-1808245.37	72.20
19	-1259002.88	-1259249.42	246.54
20	-1331080.49	-1331406.79	326.31
21	-768913.10	-769088.81	175.70
22	-844967.32	-845212.04	244.73
23	-1745352.66	-1745450.44	97.78
24	-1808173.17	-1808245.37	72.20
25	-318.27	-416.95	98.68
26	-1331130.69	-1331419.34	288.65
27	-772878.97	-773042.12	163.15
28	-844910.84	-845193.22	282.38
29	-1745352.66	-1745450.44	97.78
30	-1817367.48	-1874096.27	56728.79
31	-1259164.58	-1259243.14	78.57
32	-1331293.84	-1331419.34	125.50
33	-768913.10	-769088.81	175.70
34	-844967.32	-845205.77	238.45
35	-1745352.66	-1745450.44	97.78
36	-1817367.48	-1874096.27	56728.79
37	-1252641.74	-1252804.89	163.15
38	-1331180.89	-1331419.34	238.45
39	-768950.75	-769076.26	125.50
40	-844967.32	-840875.95	-4091.37
41	-1736330.60	-1736527.25	196.65
42	-1808089.43	-1808333.22	243.79
43	-1259105.09	-1259247.03	141.94
44	-1331325.22	-1331413.07	87.85
45	-772878.97	-773042.12	163.15
46	-844910.84	-845193.22	282.38
47	-1736330.60	-1736527.25	196.65
48	-1808089.43	-1808333.22	243.79
49	-1259067.44	-1259249.42	181.98
50	-1331199.71	-1331419.34	219.63
51	-768950.75	-769076.26	125.50
52	-844967.32	-840875.95	-4091.37