ONIOM2(B3LYP/6-31G*:PM3) optimized Cartesian coordinates for the transition states located for the acyl transfer reaction to cyclohexane-1,2-diol. Electronic energies (in a.u) at the ONIOM2(B3LYP/6-31G*:PM3) and single-point energies calculated at the B3LYP/6-31G*//ONIOM2(B3LYP/6-31G*:PM3) level of theory are given in parenthesis

Catalyst Moc-(π-Me)His-^{A}Gly-Cha-Phe-OMe

(1R,2R)e,e-α												
Et= -844.665214 (-2913.1550836)												
6	-1.661134	3.301105	-0.640261	6	-5.511126	2.614834	4.592775	1	-3.929120	6.456043	-1.308261
6	-3.006163	3.076363	-1.338270	6	-5.482490	1.734581	3.516088	1	-3.125461	5.621009	-2.630039
6	-3.932306	4.289593	-1.119819	6	-3.600354	-3.230638	-1.561398	1	-4.209076	4.340710	-0.056222
6	-3.271660	5.612501	-1.541531	8	-1.463973	-0.272128	-0.840560	1	-4.864088	4.141346	-1.674936
6	-1.911061	5.819083	-0.845138	8	7.710033	0.544706	0.370433	1	2.977910	6.916112	-0.782585
6	-1.040522	4.606383	-1.119210	6	-3.153255	-0.720565	2.581869	1	1.294531	7.367281	-0.421632
6	1.523587	5.493376	-1.327558	8	-1.908442	-0.570850	3.125443	1	2.113170	6.173634	0.612698
8	1.407648	5.372985	-2.485415	6	-1.513177	-1.409693	4.190991	1	-2.057950	-2.149214	-2.599839
6	2.021576	6.546835	-0.405154	8	-3.973050	-1.443166	3.104726	1	-4.093103	-3.237564	-0.562531
7	2.883818	3.853042	-0.659867	1	4.341452	-4.367577	0.626789	1	-3.379500	-4.295587	-1.783106
6	3.017385	2.650331	-1.321431	1	3.343040	-4.018637	-0.798221	1	-3.483682	2.171139	-0.922800
6	4.277091	2.136356	-1.119493	1	2.841077	-6.282989	0.090803	6	-4.978278	-2.322892	-5.062772
7	4.928010	3.073010	-0.320238	1	3.431729	-5.851522	2.486221	6	-4.011155	-2.865219	-4.023939
6	4.055120	4.074323	-0.075522	1	1.805014	-6.537258	2.353729	6	-4.570900	-2.685892	-2.611907
6	4.917601	0.875621	-1.634996	1	2.310636	-2.309225	3.072497	6	-5.923230	-3.389878	-2.498161
6	5.089562	-0.198679	-0.543476	1	3.727730	-3.367639	2.921489	6	-6.896589	-2.858885	-3.539326
7	6.320182	-1.019845	-0.726753	1	1.816101	-4.591509	3.927913	6	-6.333501	-3.003196	-4.944603
6	7.562774	-0.438425	-0.348285	1	-0.234804	-5.040886	2.572627	1	-3.808604	-3.937923	-4.217526
6	3.918243	-1.206409	-0.507887	1	-0.053267	-3.305796	2.881928	1	-3.025383	-2.353527	-4.095111
8	3.288623	-1.513067	-1.508409	1	1.267827	-2.456204	-0.557763	1	-5.092024	-1.227278	-4.940323
7	3.576700	-1.703559	0.774765	1	0.873168	-1.783786	1.042073	1	-4.564319	-2.472402	-6.078358
6	2.733475	-2.928479	1.006925	1	1.003557	-4.997798	-0.983178	1	-5.790131	-4.483380	-2.623638
6	3.300913	-4.175089	0.298071	1	0.365178	-6.026170	0.312929	1	-6.341333	-3.249997	-1.481977
6	2.424550	-5.388681	0.611619	1	4.328954	-1.644300	1.429193	1	-7.860873	-3.396807	-3.460485
6	0.999136	-5.139541	0.115635	1	5.174118	0.307736	0.453305	1	-7.126600	-1.794454	-3.332648
6	0.414630	-3.906568	0.824892	1	6.329792	-1.535053	-1.582625	1	-6.239342	-4.076599	-5.204178
6	1.292154	-2.675130	0.533230	1	5.896620	1.125036	-2.090852	1	-7.038896	-2.574401	-5.681937
6	2.408803	-5.639036	2.119365	1	4.291521	0.499029	-2.465317	1	-4.726978	-1.593269	-2.429111
6	1.831762	-4.412840	2.826862	1	2.201959	2.220689	-1.888733	1	-0.801139	4.513310	-2.183795
6	0.404217	-4.165831	2.339989	1	4.315979	4.936811	0.521187	8	0.258636	4.711051	-0.410071
6	2.704355	-3.192771	2.531381	1	-0.275265	-2.917122	-1.445810	1	0.584244	3.778705	-0.326469
6	-1.005693	-3.626400	0.310989	1	-4.020598	-1.654842	0.319956	1	-1.427418	6.730493	-1.215506
8	-2.013026	-3.730051	0.991637	1	-2.412847	0.745591	1.142435	8	8.600085	-1.166844	-0.834211
7	-1.143324	-3.247297	-1.064738	1	-0.641434	-0.886469	4.592848	6	9.909022	-0.823111	-0.418857
6	-2.295115	-2.425523	-1.530661	1	-2.277267	-1.526349	4.966864	1	10.026829	-0.916107	0.665632
6	-2.350998	-1.118403	-0.717833	1	-1.215046	-2.393679	3.796057	1	10.513935	-1.569692	-0.940066
7	-3.430259	-0.860299	0.144660	1	-4.563657	1.592803	0.367522	1	10.179932	0.188101	-0.739443
6	-3.312199	0.089416	1.288563	1	-5.482361	0.385357	1.300054	6	6.335146	3.088923	0.071601
6	-4.554382	0.993328	1.310524	1	-2.959750	3.160591	1.720820	1	6.696257	2.070962	0.323341
6	-4.565204	1.923408	2.480801	1	-3.016562	4.723991	3.650530	1	6.950453	3.488508	-0.740258
6	-3.682394	3.003353	2.535760	1	-4.651817	4.379348	5.492111	1	6.450415	3.725607	0.950465
6	-3.712729	3.880047	3.613094	1	-6.232652	2.460423	5.402680	1	-2.048597	5.932911	0.237483
6	-4.627424	3.687463	4.643465	1	-6.179433	0.887764	3.484482	1	-1.837092	3.369657	0.451410
				1	-2.831966	2.900788	-2.407320	8	-0.648925	2.332630	-0.906576
								1	-0.968825	1.427350	-0.690262