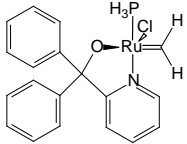
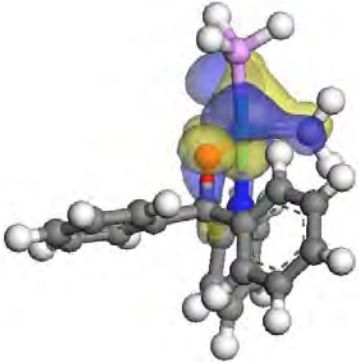
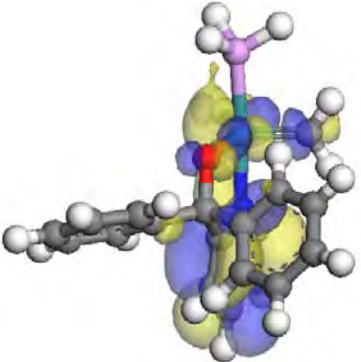
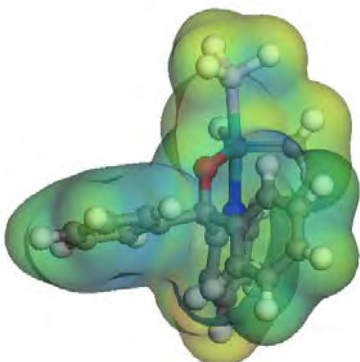
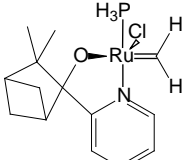
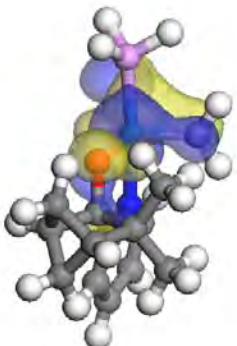
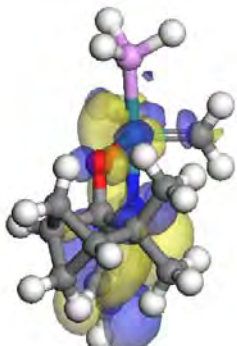
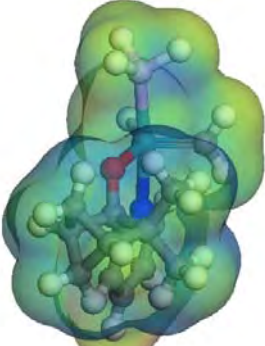
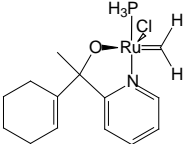
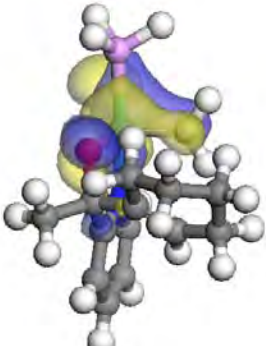
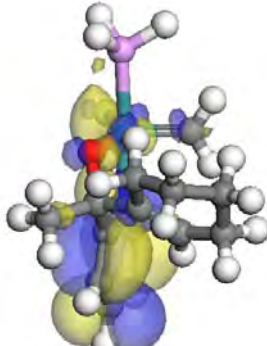
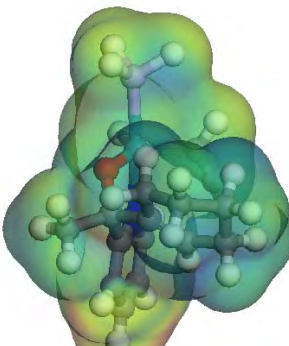
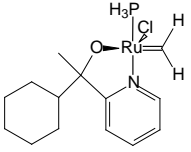
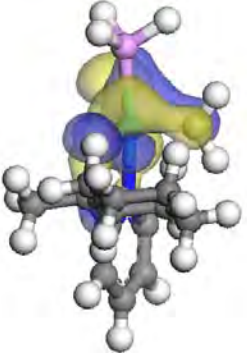
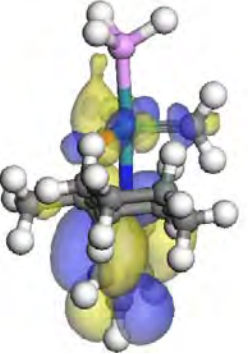
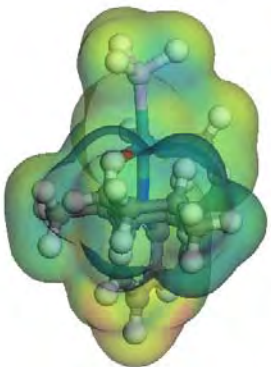
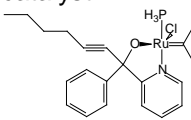
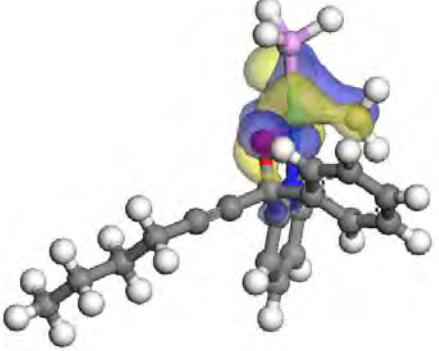
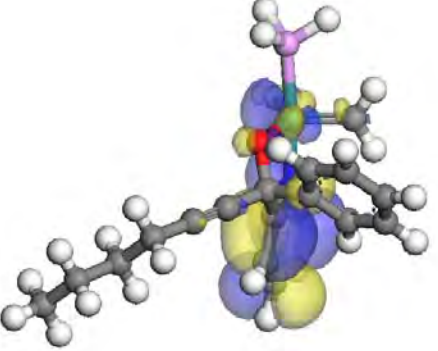
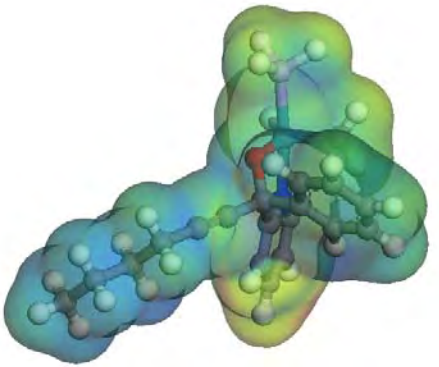
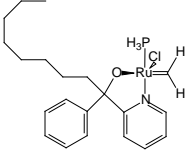
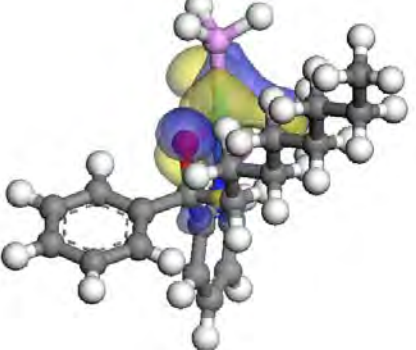
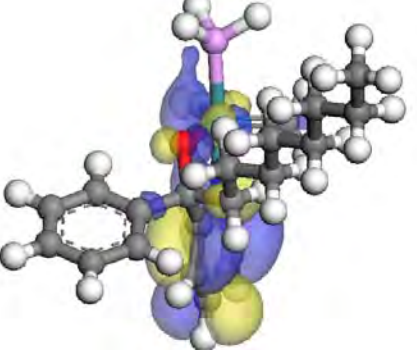
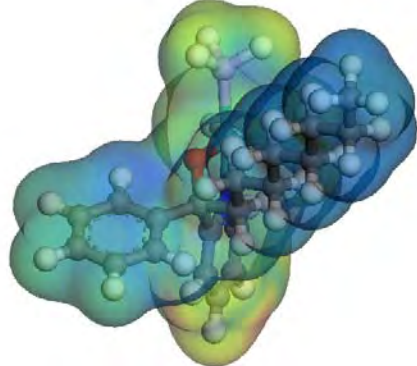
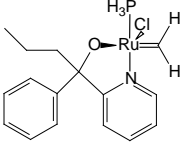
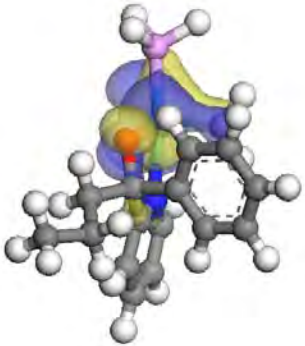
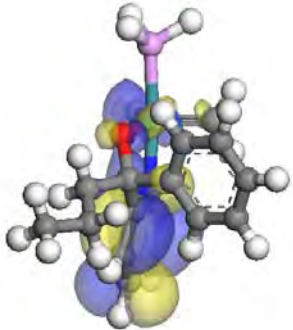
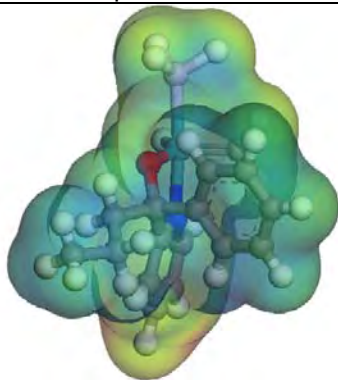
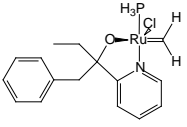
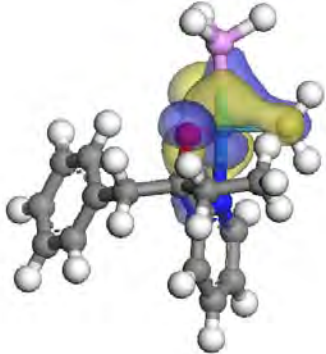
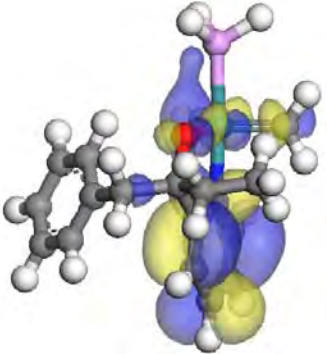
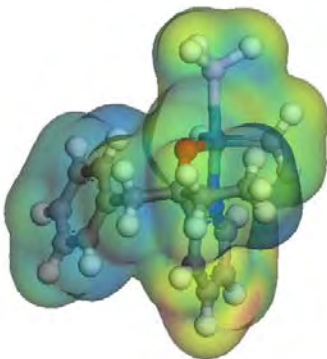
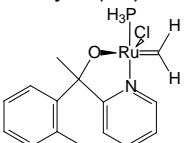
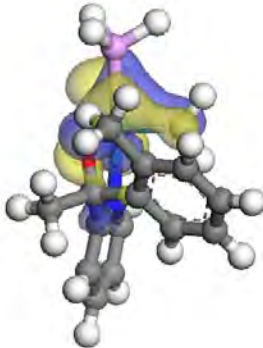
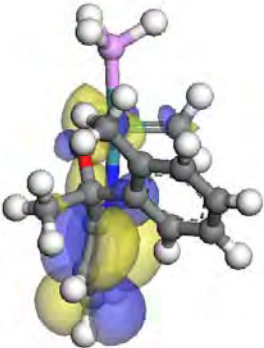
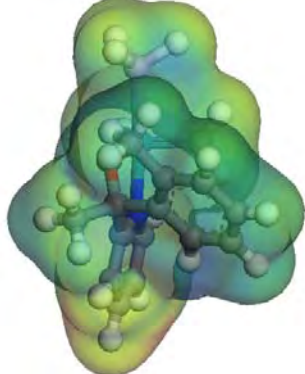


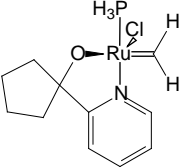
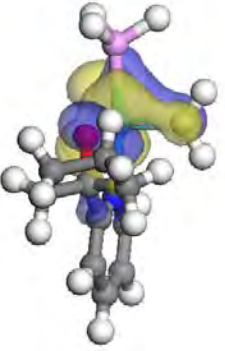
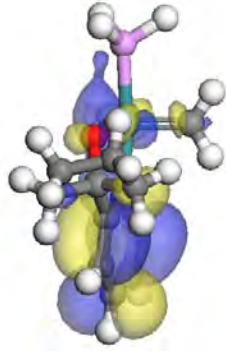
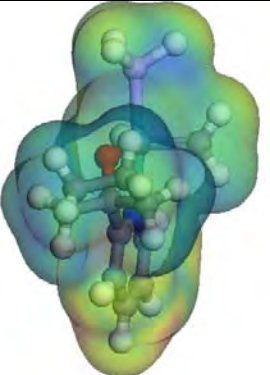
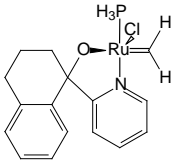
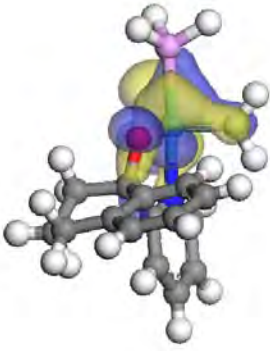
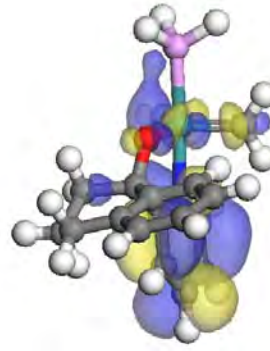
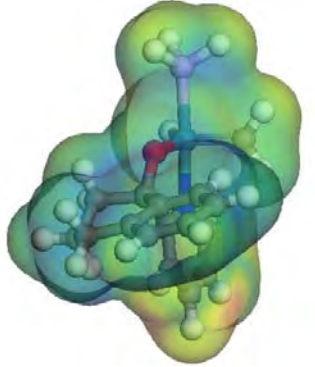
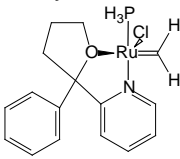
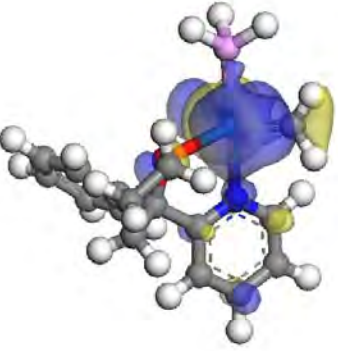
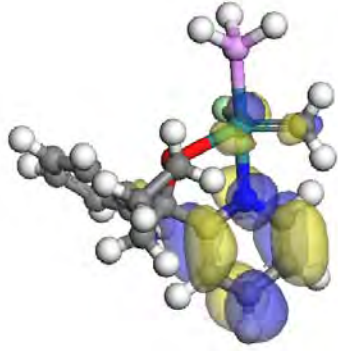
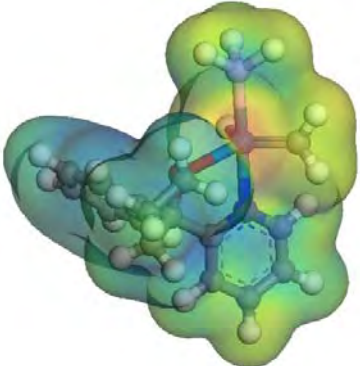
Appendix II

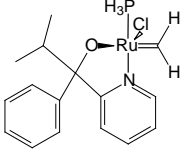
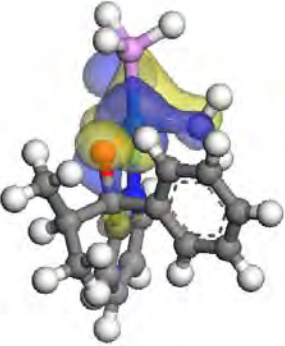
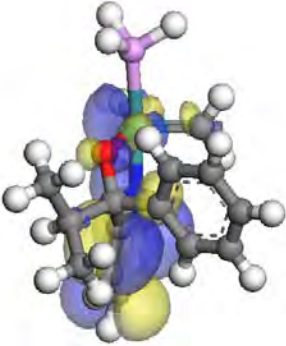
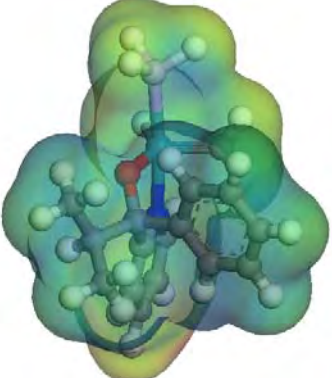
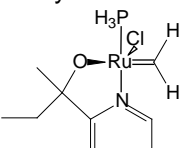
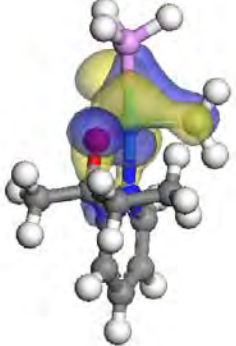
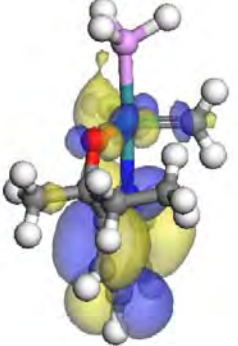
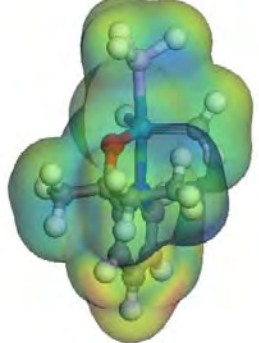
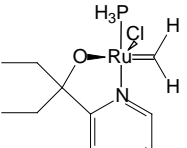
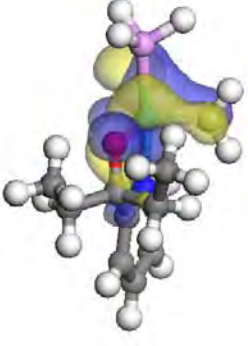
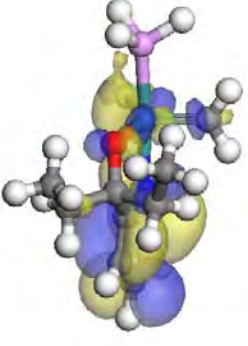
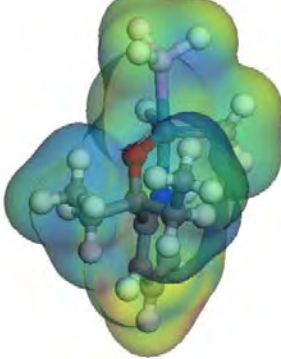
Modelling of 43 ligands when coordinated
to a simplified catalyst

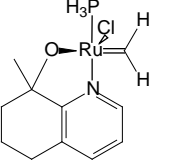
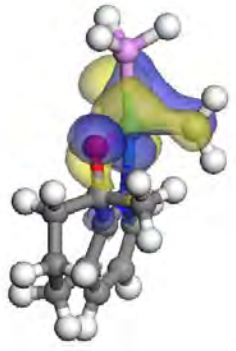
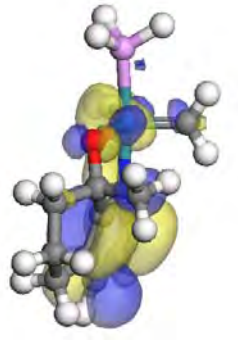
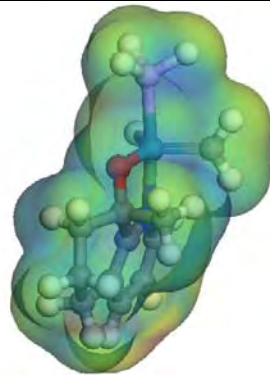
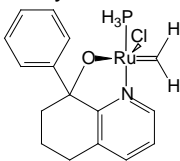
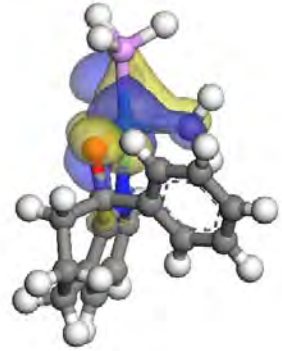
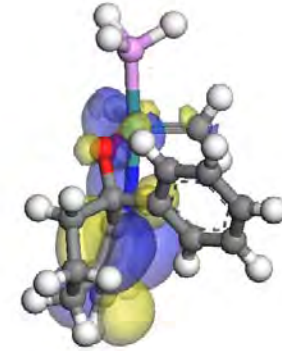
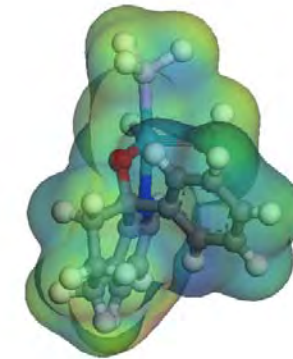
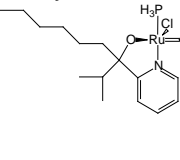
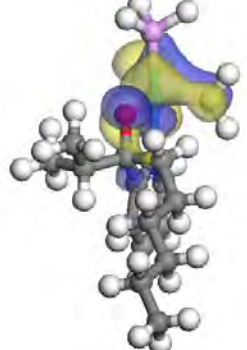
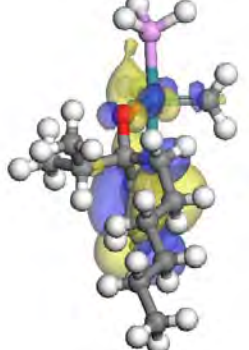

Name :	HOMO	LUMO	Nucleophilic Fukui
<p>Diphenylpyridin-2-yl methanol ligand attached to simplified catalyst (52)</p> 			
<p>1,3,3-trimethyl-2-[2]-pyridyl-norbornan-2-ol ligand attached to simplified catalyst</p> 			
<p>1-cyclohex-1-enyl-1-[2]-pyridyl ethanol ligand attached to simplified catalyst</p> 			

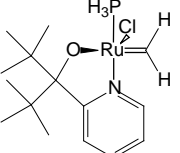
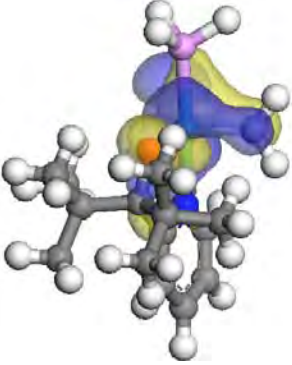
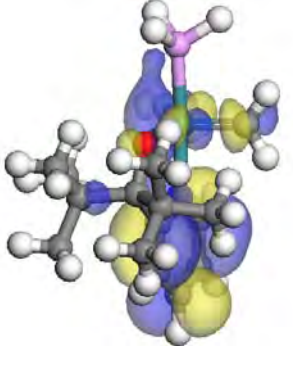
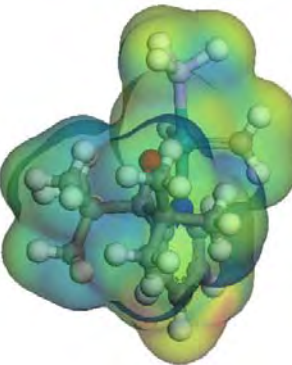
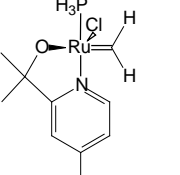
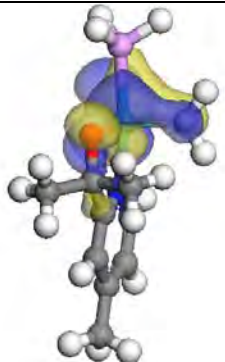
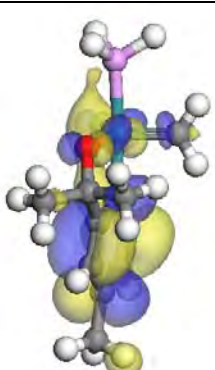
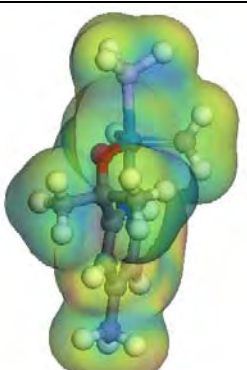
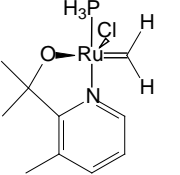
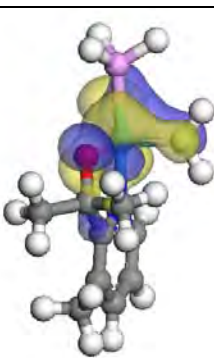
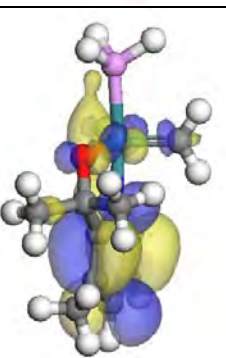

Name :	HOMO	LUMO	Nucleophilic Fukui
<p>1-cyclohexyl-1-[2]-pyridyl ethanol ligand attached to simplified catalyst (54)</p> 			
<p>1-phenyl-1-(pyridyl-3)-heptin(2)-ol(1) ligand attached to simplified catalyst</p> 			
<p>1-phenyl-1-pyridin-2-yl-nonan-1-ol ligand attached to simplified catalyst</p> 			

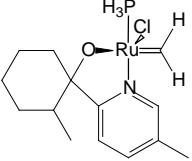
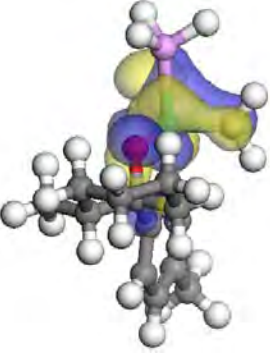
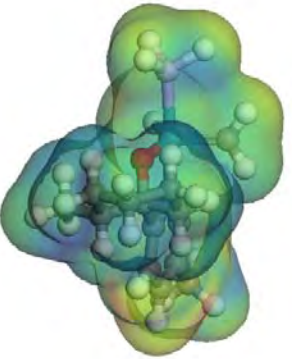
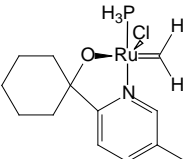
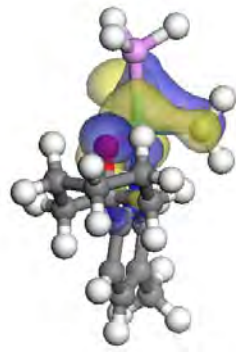
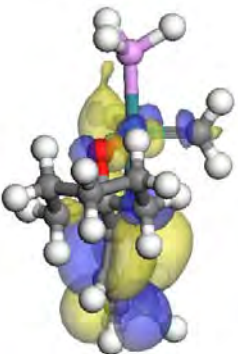
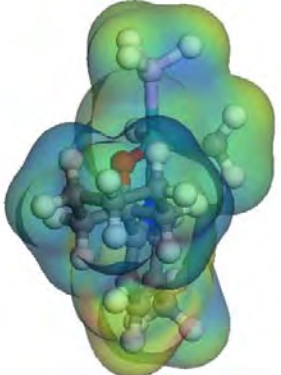
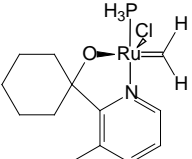
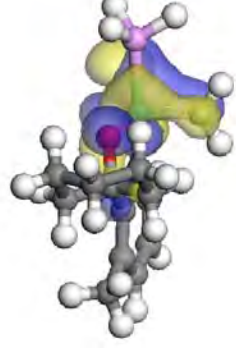
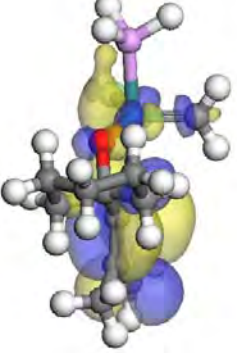
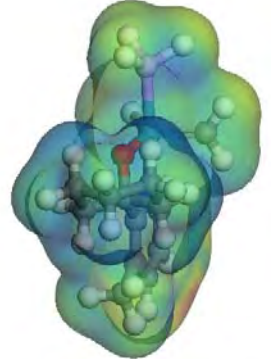
Name :	HOMO	LUMO	Nucleophilic Fukui
<p>1-phenyl-1-[2]-pyridyl-butan-1-ol ligand attached to simplified catalyst</p> 			
<p>1-phenyl-2-pyridin-2-yl-butan-2-ol ligand attached to simplified catalyst</p> 			
<p>1-[2]-pyridyl-1-o-tolyl ethanol ligand attached to simplified catalyst (63)</p> 			

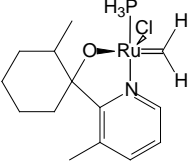
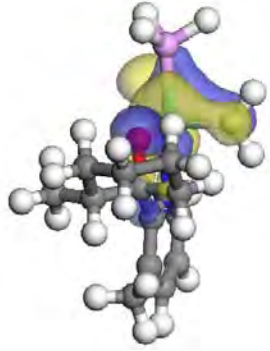
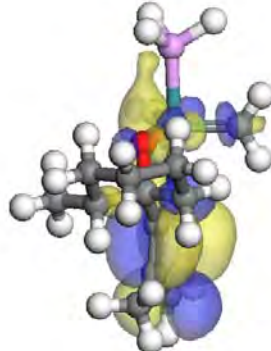
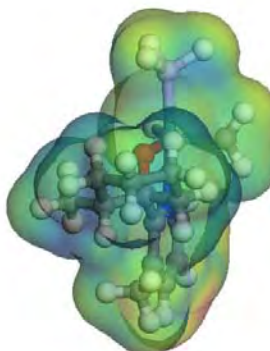
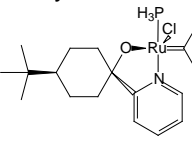

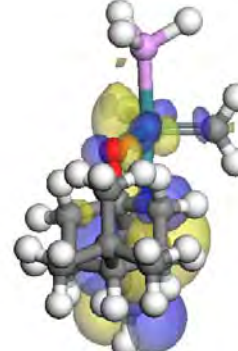
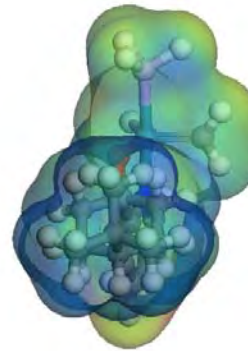
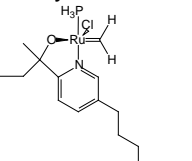
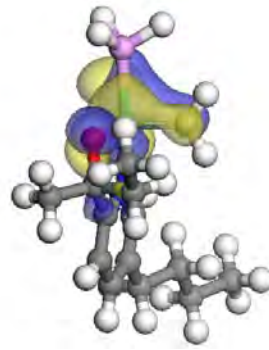
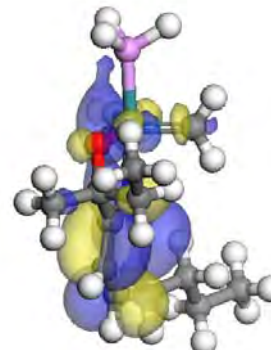
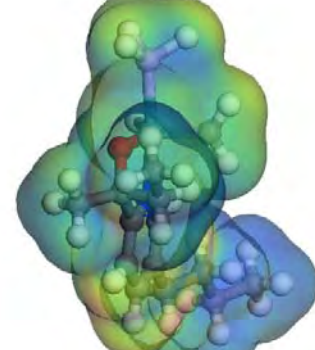
Name :	HOMO	LUMO	Nucleophilic Fukui
<p>1-[2]-pyridyl-cyclopentanol ligand attached to simplified catalyst</p> 			
<p>1-[2]-pyridyl-1,2,3,4-tetrahydro-[1]-naphthol ligand attached to simplified catalyst</p> 			
<p>2-(2-phenyl-tetrahydrofuran-2-yl) pyridine ligand attached to simplified catalyst</p> 			

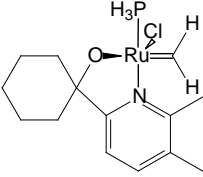
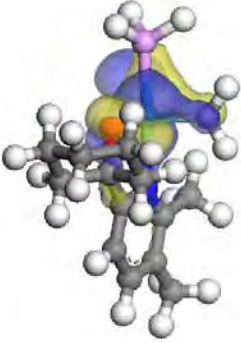
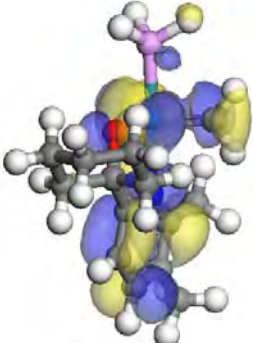
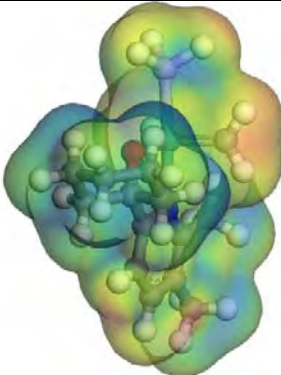
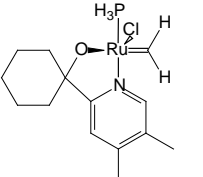
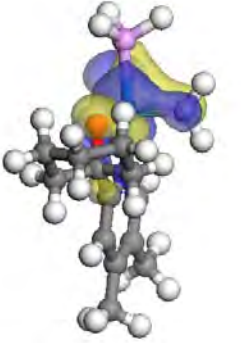
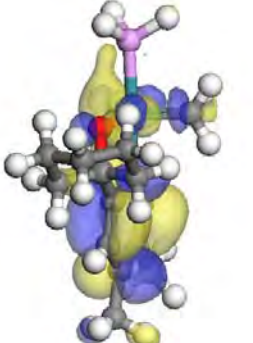
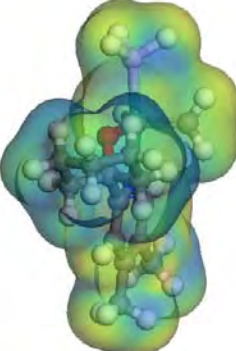
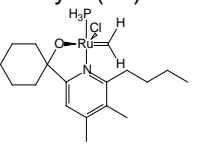
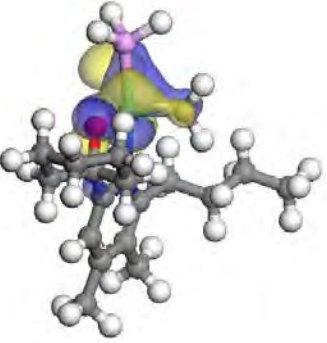
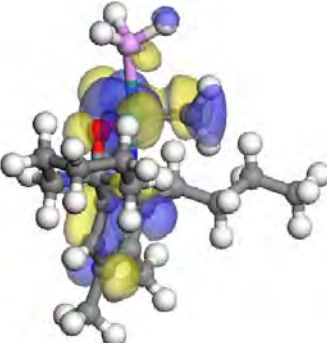
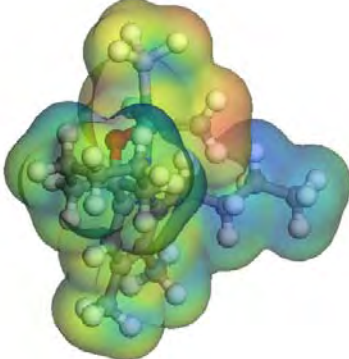
Name :	HOMO	LUMO	Nucleophilic Fukui
2-methyl-1-phenyl-1-pyridin-2-yl-propan-1-ol ligand attached to simplified catalyst (64) 			
2-[2]-pyridyl-butan-2-ol ligand attached to simplified catalyst 			
3-pyridin-2-yl-pentan-3-ol ligand attached to simplified catalyst 			

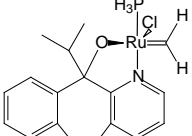
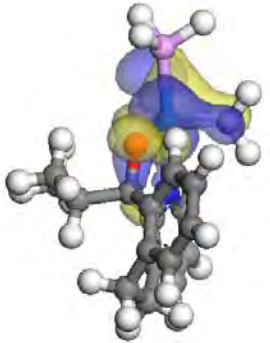
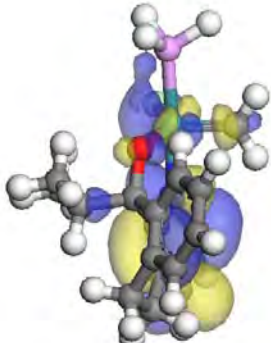
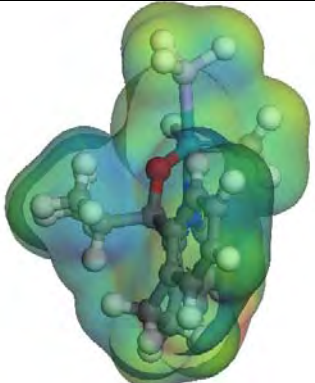
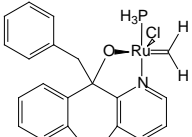
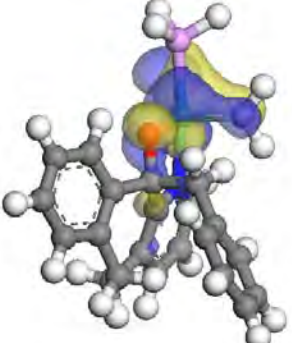
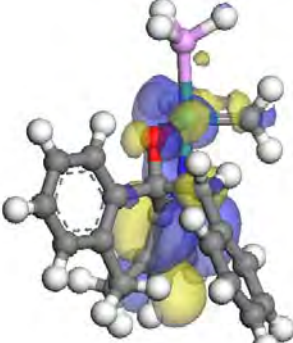
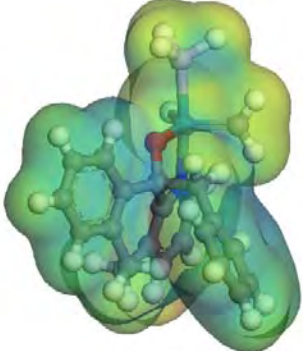
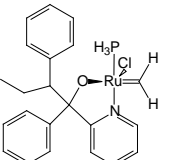
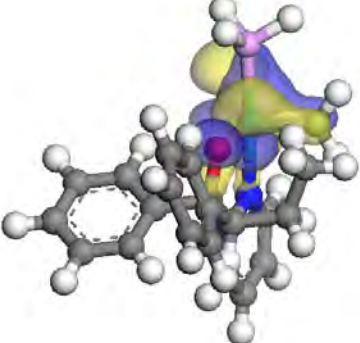
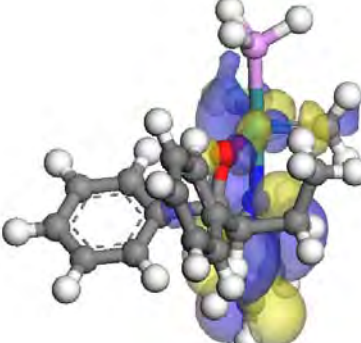
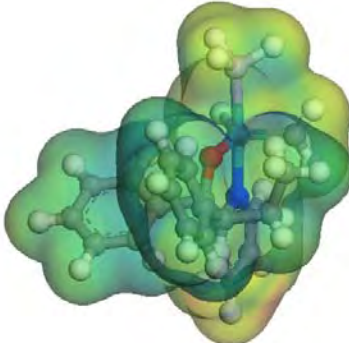
Name :	HOMO	LUMO	Nucleophilic Fukui
<p>8-methyl-5,6,7,8-tetrahydroquinolin-8-ol ligand attached to simplified catalyst (57)</p> 			
<p>8-phenyl-5,6,7,8-tetrahydroquinolin-8-ol ligand attached to simplified catalyst</p> 			
<p>α-(n-hexyl)-α-(iso-propyl)-2-pyridin methanol ligand attached to simplified catalyst</p> 			

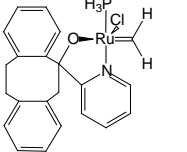
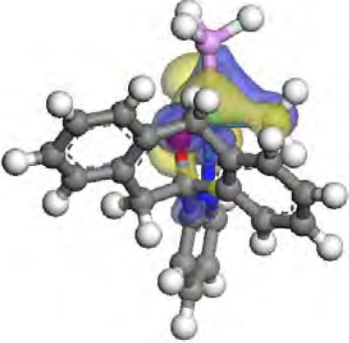
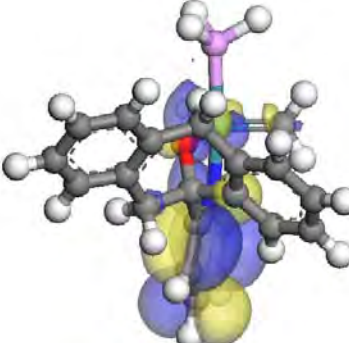
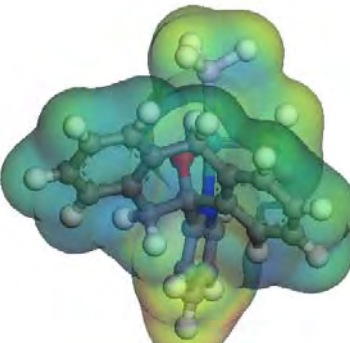
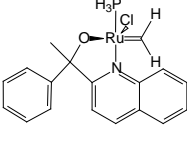
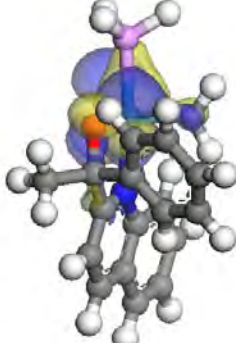


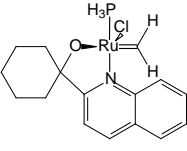


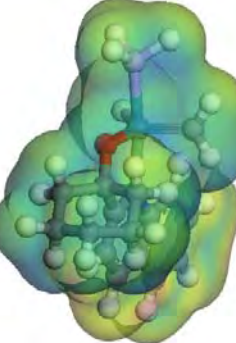
Name :	HOMO	LUMO	Nucleophilic Fukui
<p>2,2,4,4-tetramethyl-3-pyridin-2-yl-pentan-3-ol ligand attached to simplified catalyst</p> 			
<p>2-(4-methyl-pyridin-2-yl) propan-2-ol ligand attached to simplified catalyst</p> 			
<p>2-(3-methyl-[2]-pyridyl) propan-2-ol ligand attached to simplified catalyst</p> 			

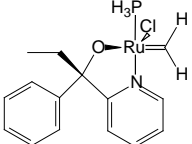
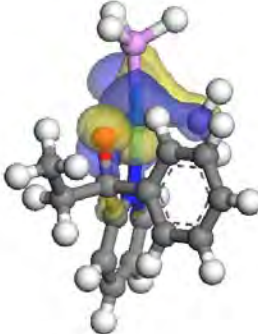
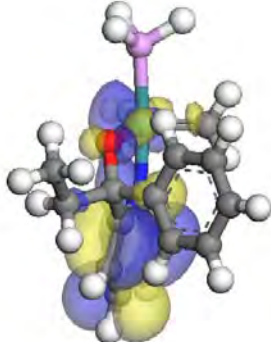
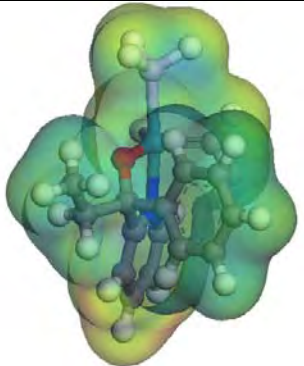
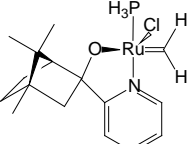
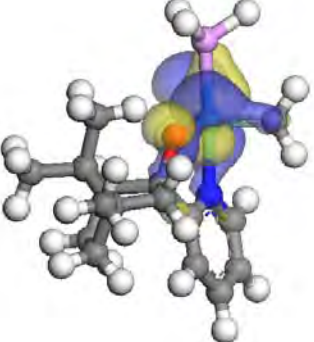
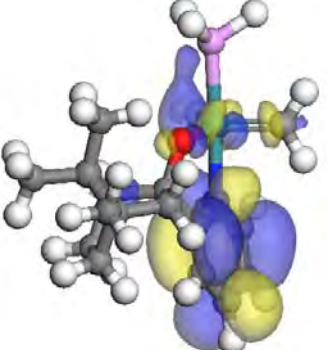
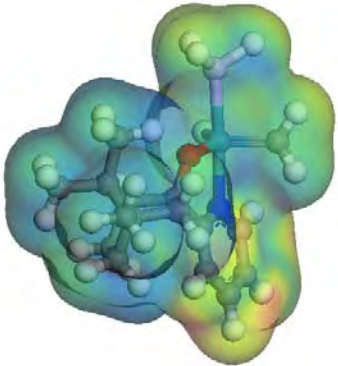
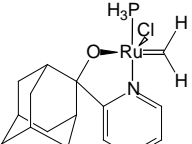
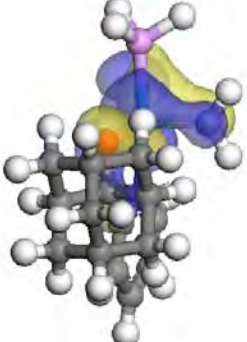
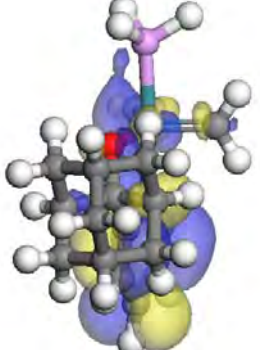
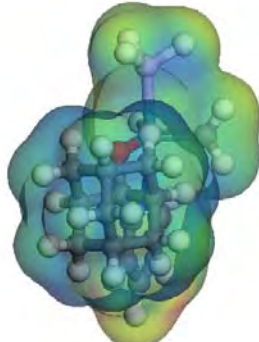
Name :	HOMO	LUMO	Nucleophilic Fukui
<p>2-methyl-1-(5-methyl-pyridin-2-yl) cyclohexanol ligand attached to simplified catalyst</p> 			
<p>1-(5-methyl-pyridin-2-yl) cyclohexanol ligand attached to simplified catalyst (58)</p> 			
<p>1-(3-methyl-pyridin-2-yl) cyclohexanol ligand attached to simplified catalyst</p> 			

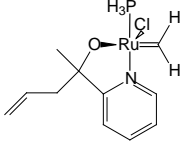
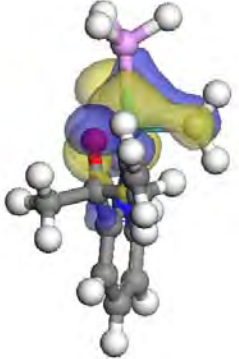
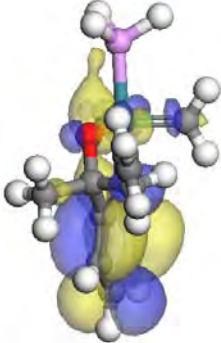
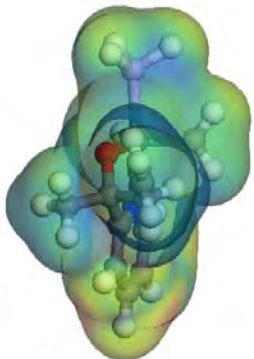
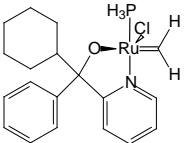
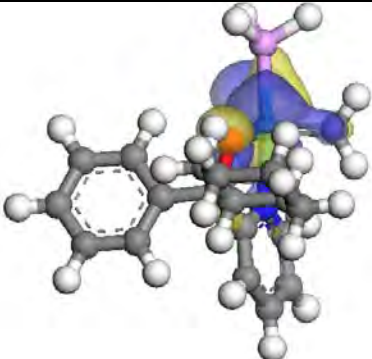
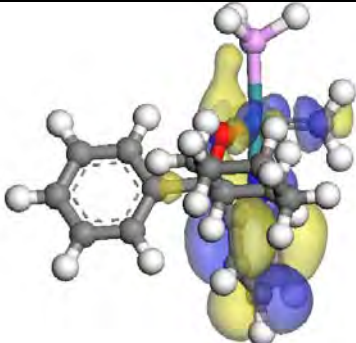
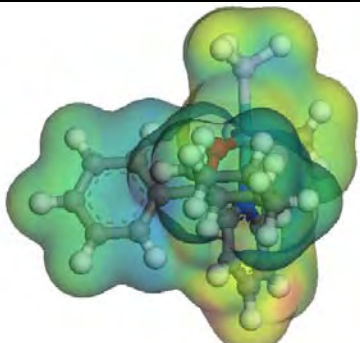
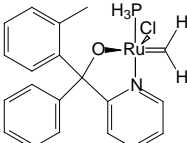
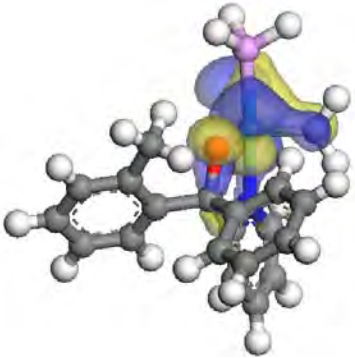
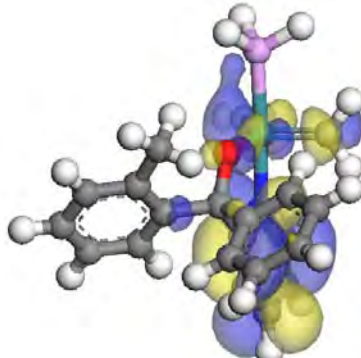
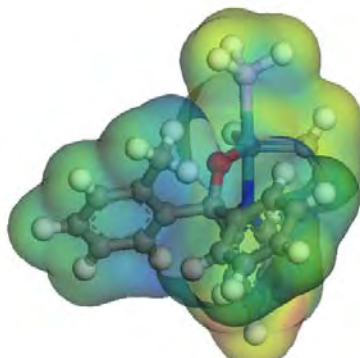
Name :	HOMO	LUMO	Nucleophilic Fukui
<p>2-methyl-1-(3-methyl-pyridin-2-yl) cyclohexanol ligand attached to simplified catalyst</p> 			
<p>1-[2]-pyridyl-cis-tert-butyl-cyclohexanol ligand attached to simplified catalyst</p> 			
<p>5-butyl-α-ethyl-α-methyl-2-pyridin methanol ligand attached to simplified catalyst</p> 			

Name :	HOMO	LUMO	Nucleophilic Fukui
<p>(dimethyl-2',3'-pyridyl-5')-1-cyclohexanol-1 ligand attached to simplified catalyst</p> 			
<p>(Dimethyl-3',4'-pyridyl-5')-1-cyclohexanol-1 ligand attached to simplified catalyst</p> 			
<p>1-(6-butyl-4,5-dimethyl-pyridin-2-yl) cyclohexanol ligand attached to simplified catalyst (59)</p> 			

Name :	HOMO	LUMO	Nucleophilic Fukui
<p>11-isopropyl-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridine-11-ol ligand attached to simplified catalyst (56)</p> 			
<p>11-benzyl-6,11-dihydro-5H-benzo[5,6]cyclohepta[1,2-b]pyridine-11-ol ligand attached to simplified catalyst</p> 			
<p>1,2-diphenyl-1-pyridin-2-ylbutan-1-ol ligand attached to simplified catalyst (55)</p> 			

Name :	HOMO	LUMO	Nucleophilic Fukui
5-pyridin-2-yl-5,6,11,12-tetrahydro-dibenzo[a,c]cycloocten-5-ol ligand attached to simplified catalyst 			
1-[2]-quinolyl-1-phenyl ethanol ligand attached to simplified catalyst (61) 			
1-[2]-quinolyl-cyclohexanol ligand attached to simplified catalyst (60) 			

Name :	HOMO	LUMO	Nucleophilic Fukui
(-)-1-phenyl-1-[2]-pyridyl-propan-1-ol ligand attached to simplified catalyst 			
(1R,2R,4R)-2-exo-hydroxy-2-endo-(pyridine-2-yl)-1,7,7-trimethyl bicyclo [2.2.1] heptane ligand attached to simplified catalyst (66) 			
2-pyridin-2-yl-adamantan-2-ol ligand attached to simplified catalyst (65) 			

Name :	HOMO	LUMO	Nucleophilic Fukui
<p>2-pyridin-2-yl-pent-4-en-2-ol ligand attached to simplified catalyst</p> 			
<p>cyclohexyl-phenyl-[2]-pyridyl methanol ligand attached to simplified catalyst</p> 			
<p>phenyl-[2]-pyridyl-o-tolyl methanol ligand attached to simplified catalyst (62)</p> 			

Name :	HOMO	LUMO	Nucleophilic Fukui
Cyclohexyl- pyridin-2-yl methanol ligand attached to simplified catalyst (53) 