SUPPLEMENTARY MATERIAL

CALCULATION of POSSIBLE REACTION PATHS of LYNCOMYCIN MOLECULE THROUGH DFT CALCULATION METHOD

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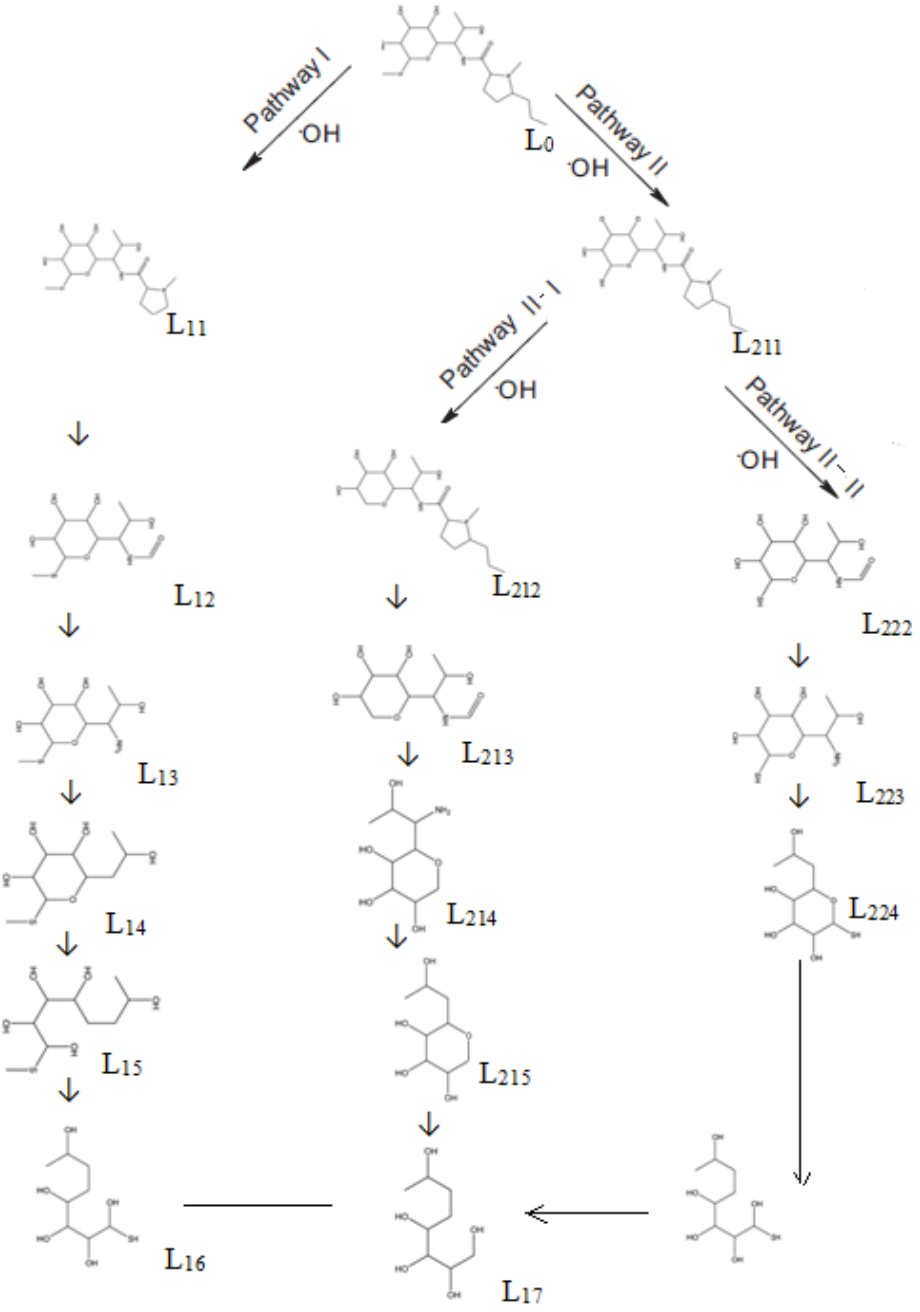
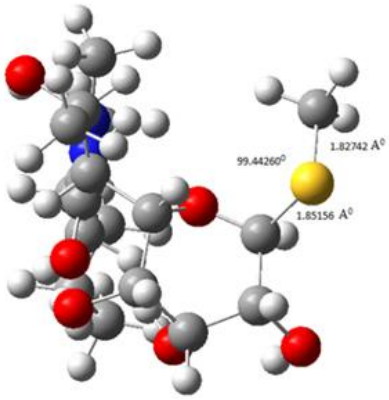
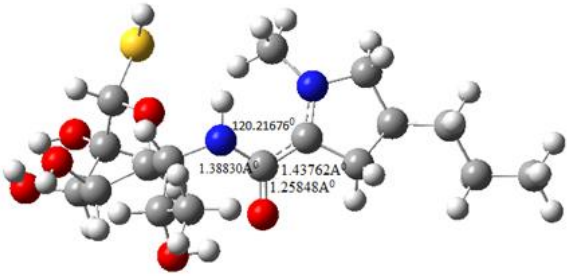
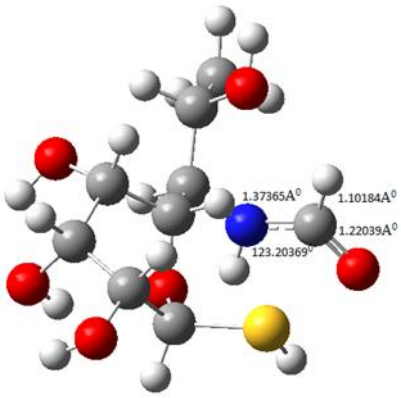


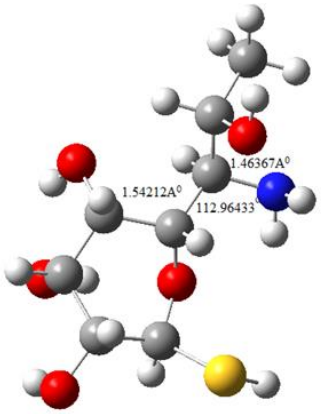
Fig.S1.

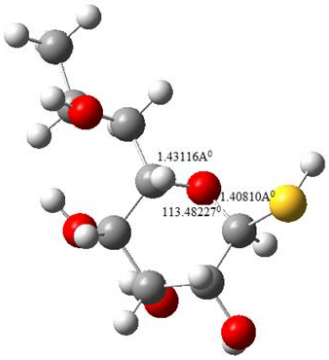




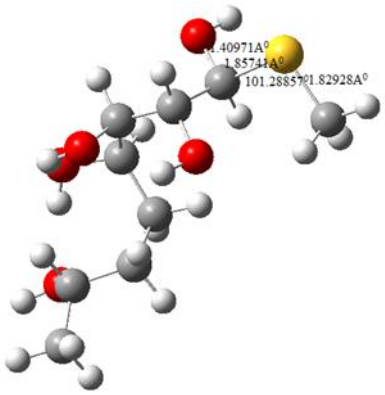
L_0 L_{211}

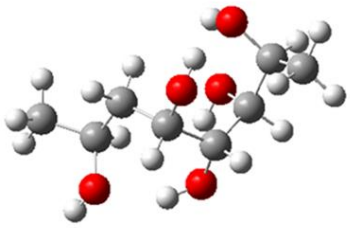






L_{222} L_{223} L_{224}





L_{16} L_{17}

Fig.S2.

Table 1: Energy, enthalpy, entropy, gibbs free energy values for the gaseous phase and aqueous phase of the degraded fragments of Lyncomycin molecule

1.(HF)	**L0**	**L11**	**L12**	**L13**	**L14**	**L15**	**L16**	**L17**
HF_G	-1664.7601891	-1546.7978	-1296.7405972	-1183.4006842	-1128.0491865	-1129.2631697	-1089.9475657	-691.7740044
ΔE	-1664.210914	-1546.338449	-1296.413543	-1183.085335	-1127.754258	-1128.943211	-1089.659078	-691.486256
ΔH	-1664.209970	-1546.337505	-1296.412598	-1183.084391	-1127.753314	-1128.942267	-1089.658134	-691.485312
ΔG	-1664.304025	-1546.421070	-1296.481294	-1183.149224	-1127.815591	-1129.007317	-1089.719628	-691.540662
HF_S	-1664.7481708	-1546.805752	-1296.7589023	-1183.4150197	-1128.0693039	-1129.2678652	-1089.9543748	-691.7684783
ΔE	-1664.200375	-1546.347134	-1296.432527	-1183.100498	-1127.773390	-1128.949412	-1089.667160	-691.482614
ΔH	-1664.199431	-1546.346190	-1296.431582	-1183.099554	-1127.772446	-1128.948467	-1089.666216	-691.481670
ΔG	-1664.294424	-1546.430426	-1296.502216	-1183.165530	-1127.835987	-1129.016403	-1089.729858	-691.540446
2.1.(HF)	**L0**	**L211**	**L212**	**L213**	**L214**	**L215**	**L17**	
HF_G	-1664.7601891	-1625.4413989	-1227.2616663	-859.2339033	-745.8969379	-690.5544502	-691.7740044	
ΔE	-1664.210914	-1624.923847	-1226.744615	-858.939482	-745.614220	-690.289698	-691.486256	
ΔH	-1664.209970	-1624.922903	-1226.743671	-858.938538	-745.613276	-690.288754	-691.485312	
ΔG	-1664.304025	-1625.014309	-1226.830082	-859.000051	-745.669921	-690.342874	-691.540662	
HF_S	-1664.7481708	-1625.4400089	-1227.2587022	-859.2588196	-745.9157689	-690.569952	-691.7684783	
ΔE	-1664.200375	-1624.923443	-1226.742842	-858.964651	-745.633264	-690.306194	-691.482614	
ΔH	-1664.199431	-1624.922498	-1226.741898	-858.963706	-745.632320	-690.305250	-691.481670	
ΔG	-1664.294424	-1625.012569	-1226.827430	-859.025967	-745.689053	-690.359970	-691.540446	
2.2.(HF)	**L0**	**L211**	**L222**	**L223**	**L224**	**L16**	**L17**	
HF_G	-1664.7601891	-1625.4413989	-1257.4228785	-1144.0846754	-1088.7336272	-1089.9475657	-691.7740044	
ΔE	-1664.210914	-1624.923847	-1257.127124	-1143.800751	-1088.469290	-1089.659078	-691.486256	
ΔH	-1664.209970	-1624.922903	-1257.126180	-1143.799807	-1088.468345	-1089.658134	-691.485312	
ΔG	-1664.304025	-1625.014309	-1257.191843	-1143.860548	-1088.528913	-1089.719628	-691.540662	
HF_S	-1664.7481708	-1625.4400089	-1257.4428949	-1144.0964429	-1088.7537095	-1089.9543748	-691.7684783	
ΔE	-1664.200375	-1624.923443	-1257.147986	-1143.813544	-1088.489232	-1089.667160	-691.482614	
ΔH	-1664.199431	-1624.922498	-1257.147042	-1143.812600	-1088.488288	-1089.666216	-691.481670	
ΔG	-1664.294424	-1625.012569	-1257.213839	-1143.874545	-1088.547882	-1089.729858	-691.540446	

Table 2. Mulliken loads of the heavy atoms of the studied molecules

APT L_0	L_{11}	L_{12}	L_{13}	L_{14}	L_{15}
O_{11} -0.806382	O_{11} -0.750864	O_{11} -0.526494	O_{11} -0.860038	O_{11} -0.828547	O_9 -0.228212
O_{12} -0.601210	O_{12} -0.294258	O_{12} -0.619427	O_{12} -0.316327	O_{12} -0.313591	O_{11} -0.258525
O_{14} -0.677656	O_{14} -0.310899	O_{14} -0.660659	O_{14} -0.320893	14 O -0.307825	O_{13} -0.268234
O_{16} -0.689424	O_{16} -0.340576	O_{16} -0.649637	O_{16} -0.319121	15 H 0.000000	S_{15} 0.064980
S_{18} -0.230684	S_{18} -0.175516	S_{18} 0.104437	S_{18} -0.201040	16 O -0.359063	O_{28} -0.239380
N_{25} -0.777974	N_{25} -0.436045	N_{25} -0.543784	N_{25} -0.184563	18 S -0.245104	O_{33} -0.203297
O_{33} -0.667325	O_{33} -0.298481	O_{33} -0.632524	O_{33} -0.363602	31 O -0.360373	
O_{36} -0.961545	O_{36} -0.815511	O_{36} -0.479355			
N_{46} -0.667944	N_{46} -0.531620				
L_{16}	L_{17}	L_{211}	L_{212}	L_{213}	L_{214}
O_{11} -0.375313	O_9 -0.646524	O_{11} -0.806102	O_{11} -0.494272	O_{11} -0.485495	O_{11} -0.487155
O_{13} -0.360245	O_{11} -0.672449	O_{12} -0.298240	O_{12} -0.237619	O_{12} -0.625464	O_{12} -0.626757
S_{15} -0.227613	O_{13} -0.692649	O_{14} -0.326231	O_{14} -0.246626	O_{14} -0.654873	O_{14} -0.658295
O_{28} -0.402836	O_{23} -0.639021	O_{16} -0.345171	O_{16} -0.232486	O_{16} -0.633652	O_{16} -0.637287
O_{33} -0.345292	O_{28} -0.659311	S_{18} -0.159014	N_{20} -0.298117	N_{20} -0.547955	N_{20} -0.728199
		N_{21} -0.635725	O_{28} -0.232444	O_{28} -0.622386	O_{28} -0.637626
		O_{29} -0.282741	O_{31} -0.605135	O_{31} -0.464787	
		O_{32} -0.879534	N_{41} -0.431394		
		N_{42} -0.647293			
L_{215}	L_{222}	L_{223}	L_{224}		
O_{11} -0.770529	O_{11} -0.847370	O_{11} -0.516818	O_{11} -0.836362		
O_{12} -0.323676	O_{12} -0.595180	O_{12} -0.619741	O_{12} -0.308736		
O_{14} -0.326129	O_{14} -0.625393	O_{14} -0.659983	O_{14} -0.304284		
O_{16} -0.315774	O_{16} -0.627928	O_{16} -0.643903	O_{16} -0.358326		
O_{26} -0.373021	S_{18} -0.189657	S_{18} -0.066985	S_{18} -0.247485		
	N_{21} -0.670077	N_{21} -0.727635	O_{27} -0.359047		
	O_{29} -0.587428	O_{29} -0.646215			
	O_{32} -0.749394				
