

## SUPPLEMENTARY INFORMATION

# Influence of $\gamma$ -Irradiation on the Electronic Structure and the Chemical and Mechanical Properties of Poly(hydroxybutyrate-valerate)/Poly(caprolactone) Blends: Insights from Experimental Data and Computational Approaches

Francisco Rosario <sup>1</sup>, João Paulo Almirão de Jesus <sup>2</sup>, Suzan Aline Casarin <sup>3</sup> and Felipe de Almeida La Porta <sup>2,4,\*</sup>

<sup>1</sup> Department of Materials Science and Engineering, Federal University of Technology—Paraná, Londrina 86036–370, Paraná, Brazil; rosario@utfpr.edu.br

<sup>2</sup> Post-Graduation Program in Chemistry, State University of Londrina, Rodovia Celso Garcia Cid, 445, km 380, Londrina 86057-970, Paraná, Brazil; joao.paulo.almirao@uel.br

<sup>3</sup> Department of Materials Science and Engineering, Federal University of São Carlos. Rod. Washington Luiz, s/n—Monjolinho, São Carlos 13565-905, São Paulo, Brazil; suzancasarin@ufscar.br

<sup>4</sup> Laboratory of Nanotechnology and Computational Chemistry, Department of Chemistry, Federal University of Technology—Paraná, Londrina 86036–370, Paraná, Brazil

\* Correspondence: felipelaporta@utfpr.edu.br

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## S.1 – CARTESIAN COORDINATES OF THE OPTIMIZED STRUCTURES

### S.1.1 COORDINATES - PHBV

0 1

C	-14.83952600	2.37604200	-1.63222800
H	-14.93929900	3.39918300	-2.05567000
C	-13.44120300	1.80887500	-1.69068200
H	-13.09045400	1.87400400	-2.73134300
H	-12.79562500	2.49780600	-1.12611800
C	-13.29212700	0.38995300	-1.14588800
H	-13.71100600	0.32566000	-0.13919800
C	-13.90520100	-0.68542300	-2.03420800
H	-13.74080400	-1.67528200	-1.60100600
H	-14.98330000	-0.52433900	-2.11705000
H	-13.46235900	-0.65906100	-3.03598200
C	-11.39663400	-0.64634300	-0.07516700
C	-9.88296300	-0.72514200	-0.10885700
H	-9.56015400	-0.95148100	-1.13154000
H	-9.50555400	0.27618600	0.12601100
C	-9.30452400	-1.73910700	0.88296100
H	-9.70163400	-1.53949300	1.88122100
C	-9.53554000	-3.19558000	0.48962800
H	-10.61291100	-3.32500800	0.34377400
H	-9.05023700	-3.37827400	-0.47823000
C	-9.03242900	-4.20106500	1.53078800
H	-9.53124300	-4.05152400	2.49519500
H	-9.23577300	-5.22681800	1.20704100
H	-7.95354000	-4.10633000	1.68714200
O	-11.84842800	0.17715500	-1.04768900
O	-7.85461600	-1.55070500	0.92905000
O	-15.80620600	1.81276100	-1.16146700
O	-12.11553700	-1.21908600	0.71879000
C	-7.36515400	-0.57229900	1.71865200

C	-5.85249700	-0.52212700	1.63142700
O	-8.05620900	0.17286800	2.38634000
H	-5.45166700	-1.53443200	1.75506700
H	-5.60243600	-0.20510600	0.61259300
C	-5.21958100	0.44111900	2.64026500
H	-5.66825200	1.43023000	2.52807400
C	-5.29735200	-0.02953400	4.08415200
O	-3.79479300	0.55433500	2.32956800
H	-4.79713300	0.68414900	4.74490200
H	-6.34375600	-0.10788400	4.38906100
H	-4.81558000	-1.00590200	4.20332600
C	-3.42565200	1.40789900	1.35155800
C	-1.92312800	1.37501800	1.15333200
O	-4.20532200	2.08677800	0.71110700
H	-1.42937400	1.43802500	2.12933900
H	-1.68102200	0.38880900	0.74098000
C	-1.41286200	2.46682200	0.20805900
H	-1.97808800	2.43314900	-0.72634600
C	-1.44359500	3.86921100	0.80952600
O	-0.01251400	2.17984800	-0.10205600
H	-2.46898200	4.05463700	1.14658100
H	-0.80083800	3.88361500	1.69957800
C	-1.01667300	4.96948600	-0.16768500
H	-1.66730600	4.98733900	-1.04956700
H	-1.07572900	5.95323000	0.30886100
H	0.01315600	4.82312300	-0.50739900
C	0.25052300	1.29094200	-1.08222900
C	1.74560300	1.10414000	-1.24931000
O	-0.60535500	0.70964600	-1.72133600
H	2.23175000	2.08574700	-1.27221800
H	2.10463000	0.59349000	-0.34841500
C	2.11500100	0.28235600	-2.48805400



H	1.58093300	-0.66958100	-2.46344800
C	1.87810500	1.00459500	-3.80526000
O	3.54850100	-0.00319700	-2.43731800
H	2.18996700	0.37780500	-4.64551500
H	0.81380300	1.22638500	-3.91635800
H	2.44481500	1.94098000	-3.84424400
C	3.96022300	-1.04438600	-1.68370900
C	5.46921200	-1.17907800	-1.73793700
O	3.21292100	-1.75472200	-1.03900700
H	5.79949100	-1.10858400	-2.78016600
H	5.88337100	-0.30850300	-1.21655100
C	5.98698800	-2.46336600	-1.08355100
H	5.58263900	-2.54547300	-0.07186400
C	5.69669100	-3.72836500	-1.88655200
O	7.44266200	-2.36324500	-0.98053300
H	4.61705000	-3.75652500	-2.06793800
H	6.18930400	-3.64429600	-2.86424300
C	6.13379700	-5.01790300	-1.18363800
H	5.62760000	-5.13065900	-0.21809300
H	5.88653000	-5.89310300	-1.79292100
H	7.21336800	-5.02787000	-1.00498400
C	7.95932700	-1.69491000	0.07189700
C	9.47351200	-1.67286200	0.00123400
O	7.28879300	-1.16806300	0.93865400
H	9.83922000	-2.68470300	-0.20649400
H	9.74138300	-1.05449200	-0.86302000
C	10.12843500	-1.10342600	1.26348800
H	9.70699900	-0.11896100	1.47623500
C	10.02725300	-2.01196600	2.47892500
O	11.55740200	-0.93512600	1.00408600
H	10.54145600	-1.56352000	3.33370900
H	8.97700300	-2.15592600	2.74437200

H	10.48187800	-2.98760200	2.27605200
C	11.95350800	0.17721900	0.34582600
C	13.45410300	0.18610900	0.13654600
O	11.18948000	1.03840000	-0.04648600
H	13.93716300	-0.33790700	0.96964600
H	13.65681900	-0.40418300	-0.76633800
C	14.04736000	1.59063100	-0.06195000
H	13.47785200	2.10040300	-0.84482800
C	14.01440200	2.43582100	1.21725000
O	15.37380600	1.48137600	-0.59525400
H	12.98825000	2.43986600	1.60409100
H	14.63370000	1.93902300	1.98099400
C	14.49154600	3.87725400	1.01088000
H	15.95437000	1.11280100	0.08550000
H	13.84185900	4.40395200	0.30285500
H	14.47753000	4.43276100	1.95432000
H	15.50977800	3.90461300	0.61202200

## S.1.2 COORDINATES - PCL

0 1

C	16.37681100	-0.48649400	0.00009700
H	17.34886300	0.05549100	0.00007100
C	15.15424200	0.39966200	-0.00001500
H	15.24455000	1.06749300	-0.87177500
H	15.24454000	1.06771900	0.87157100
C	13.81721800	-0.34230500	0.00006900
H	13.77307200	-1.00239800	-0.87450300
H	13.77310000	-1.00225000	0.87475500
C	12.61135900	0.60633000	0.00000600
H	12.66420500	1.26473800	-0.87907500
H	12.66422100	1.26486400	0.87899100
C	11.26867600	-0.13817300	0.00007000
H	11.20333000	-0.78963600	0.88056100
H	11.20329700	-0.78972700	-0.88035100
C	10.08730100	0.81924300	0.00004100
H	10.08482900	1.46517000	-0.88435500
H	10.08483800	1.46521900	0.88440300
O	16.35734400	-1.70027400	0.00020500
O	8.87379000	0.02773000	0.00007800
C	7.70713700	0.71272100	-0.00005800
C	6.52151200	-0.23170800	-0.00001400
O	7.64573400	1.92602600	-0.00018700
H	6.62079200	-0.88923900	0.87359200
H	6.62081200	-0.88933900	-0.87354300
C	5.17073000	0.48688100	-0.00007400
H	5.11147000	1.14500500	0.87488400
H	5.11149600	1.14491100	-0.87510300
C	3.98632400	-0.48801300	-0.00004000
H	4.05318700	-1.14522900	0.87897900
H	4.05320200	-1.14530500	-0.87900200

C	2.62855000	0.22845300	-0.00008000
H	2.54989000	0.87855700	-0.88052300
H	2.54986000	0.87860000	0.88032900
C	1.46606800	-0.75170000	-0.00007300
H	1.47559800	-1.39754400	0.88433100
H	1.47557900	-1.39753700	-0.88448100
O	0.23764900	0.01703400	-0.00005400
C	-0.91651300	-0.68833400	-0.00008600
C	-2.11809600	0.23577700	-0.00005100
O	-0.95715800	-1.90256900	-0.00012700
H	-2.02978500	0.89505900	-0.87351900
H	-2.02981400	0.89494700	0.87350600
C	-3.45726800	-0.50423400	-0.00011600
H	-3.50640900	-1.16300900	-0.87521300
H	-3.50642000	-1.16314500	0.87487900
C	-4.65604600	0.45295100	-0.00005000
H	-4.59856000	1.11124400	-0.87892900
H	-4.59856900	1.11111500	0.87892600
C	-6.00386700	-0.28206800	-0.00011300
H	-6.07380300	-0.93321900	0.88031900
H	-6.07377400	-0.93312100	-0.88061900
C	-7.17877300	0.68322500	-0.00007300
H	-7.17663100	1.32935900	-0.88433500
H	-7.17662900	1.32929900	0.88423000
O	-8.39779800	-0.09967300	-0.00010500
C	-9.55985900	0.59428800	0.00014000
C	-10.75240000	-0.34117300	0.00017800
O	-9.61105800	1.80800600	0.00032600
H	-10.65723600	-0.99945700	0.87380100
H	-10.65714500	-0.99970600	-0.87324200
C	-12.09931000	0.38474200	0.00002800
H	-12.15535800	1.04331600	0.87482300

H	-12.15530100	1.04306500	-0.87496000
C	-13.28922100	-0.58362200	0.00012100
H	-13.22373200	-1.24124100	0.87943500
H	-13.22368000	-1.24147600	-0.87901200
C	-14.64372100	0.13677900	-0.00001500
H	-14.72349700	0.78738700	-0.88011900
H	-14.72356900	0.78757800	0.87994000
C	-15.82504500	-0.82401200	0.00004000
H	-15.78326100	-1.47152400	0.88978600
H	-15.78321800	-1.47168300	-0.88958800
O	-17.02860400	-0.05050400	-0.00005600
H	-17.78838700	-0.64587300	-0.00011900

## S.1.3 COORDINATES - BA

0 1

C	-10.21590800	5.87610800	0.66479100
H	-9.74375300	6.87079800	0.51042100
C	-9.55208000	4.74571200	-0.08488100
H	-9.49683400	5.02788200	-1.14678400
H	-8.50741200	4.70783300	0.25762600
C	-10.20814900	3.37771100	0.08872200
H	-10.32436200	3.14618000	1.14987600
C	-11.54739700	3.23592800	-0.62436100
H	-11.94868600	2.22946600	-0.48204300
H	-12.26348600	3.95037600	-0.20967100
H	-11.43605900	3.42478300	-1.69784800
C	-9.22448700	1.17784000	0.03733200
C	-8.15759200	0.34434800	-0.64445000
H	-8.24890200	0.46420400	-1.72990600
H	-7.18960600	0.77086400	-0.35844400
C	-8.19849200	-1.13646000	-0.25349000
H	-8.16882300	-1.22539100	0.83533200
C	-9.39367700	-1.89467800	-0.82583900
H	-10.29737600	-1.35833100	-0.51816800
H	-9.34453800	-1.84993400	-1.92196000
C	-9.47760700	-3.35237700	-0.36096300
H	-9.55649200	-3.41333100	0.73049200
H	-10.35900300	-3.84344100	-0.78582300
H	-8.59488600	-3.92014100	-0.67047000
O	-9.24997800	2.42881800	-0.47716000
O	-7.00409600	-1.78169100	-0.79214100
O	-11.17674600	5.76308900	1.39779700
O	-9.94868300	0.79898300	0.93563300
C	-5.85490400	-1.68899300	-0.08270500
C	-4.73955200	-2.46006100	-0.76081500

O	-5.75188900	-1.06807500	0.95672500
H	-4.66329700	-2.09705900	-1.79398200
H	-5.06475100	-3.50580500	-0.84229900
C	-3.39537900	-2.35772900	-0.03706100
H	-3.10033700	-1.30400900	0.03275600
H	-3.51323800	-2.70650400	0.99554300
C	-2.29100000	-3.16090800	-0.73677200
H	-2.18168200	-2.80821800	-1.77227100
H	-2.59319800	-4.21655600	-0.80146700
C	-0.93750700	-3.05945300	-0.01949600
H	-1.03610200	-3.41384600	1.01453300
H	-0.61934900	-2.01132300	0.02472200
C	0.14362700	-3.87622600	-0.72016600
H	0.32051400	-3.51130300	-1.73536600
H	-0.12112600	-4.93642300	-0.75478700
O	1.39327500	-3.84245000	0.01443900
C	2.24790600	-2.82746900	-0.25770700
C	3.49423700	-2.92964100	0.59858300
O	2.02715100	-1.96337400	-1.08269300
H	3.94879200	-3.91066600	0.40795200
H	3.17241500	-2.95587900	1.64794400
C	4.49684900	-1.79959900	0.35666900
H	4.80229700	-1.80483800	-0.69618900
H	4.00103200	-0.83560600	0.52160200
C	5.73331400	-1.90945600	1.25849100
H	6.22574200	-2.87785300	1.09036300
H	5.41696500	-1.90398100	2.31200800
C	6.74312000	-0.77756200	1.02247600
H	6.25770900	0.19363900	1.18303000
H	7.08956100	-0.79994100	-0.01739500
C	7.94859600	-0.88602700	1.95072300
H	8.50370200	-1.81097200	1.77357700

H	7.64396600	-0.83888900	2.99980500
O	8.84830000	0.23888500	1.78679100
C	9.82758300	0.12505300	0.85698200
C	10.66490400	1.38690500	0.80424300
O	9.99356600	-0.86318200	0.17041700
H	10.98034300	1.62123800	1.82892200
H	9.99817300	2.20853100	0.50920900
C	11.86651900	1.29206000	-0.13851100
H	12.50373900	0.45447600	0.16970300
H	11.51728900	1.04834700	-1.14857200
C	12.68857100	2.58704000	-0.16755700
H	13.02671400	2.82542300	0.85161600
H	12.04231800	3.42122500	-0.47795800
C	13.90206800	2.50450700	-1.10276800
H	13.57466400	2.27933400	-2.12565300
H	14.55899200	1.68130600	-0.79460100
C	14.71733100	3.79035000	-1.12775800
H	15.07943100	4.02555800	-0.11475700
H	14.08714600	4.62885200	-1.46295100
O	15.81802900	3.60246400	-2.02210700
H	16.34499000	4.41066700	-2.05153100



## S.1.4 COORDINATES - BB

0 1

C	-12.96696400	5.01373600	-0.64218000
H	-13.82639400	5.56403600	-0.19804900
C	-11.97329900	4.47229400	0.35754500
H	-12.54026500	3.84330100	1.06244600
H	-11.63147700	5.32787400	0.96207700
C	-10.79488500	3.71011600	-0.24949800
H	-11.17751300	2.87136900	-0.84311900
H	-10.27120500	4.36378900	-0.95729500
C	-9.81186400	3.19343100	0.80965600
H	-10.34534600	2.54425600	1.51852100
H	-9.42890200	4.04123400	1.39640300
C	-8.63353200	2.42010900	0.20086000
H	-8.09358900	3.06013600	-0.50849600
H	-9.00827600	1.55620600	-0.36048600
C	-7.65949100	1.93543000	1.26974400
H	-8.14161700	1.23984900	1.96132700
H	-7.23756300	2.77375800	1.83020900
O	-12.88267700	4.88780000	-1.84662700
O	-6.50500200	1.28346700	0.67946300
C	-6.57877600	-0.04928100	0.47381500
C	-5.27489200	-0.57005200	-0.09628400
O	-7.55499900	-0.72426200	0.73645400
H	-4.99160800	0.04584400	-0.95757300
H	-4.50720700	-0.41377600	0.66965300
C	-5.32626200	-2.05164100	-0.48175600
H	-5.65351600	-2.63926700	0.37847700
C	-6.18465200	-2.34922900	-1.70121900
O	-3.97100300	-2.47764200	-0.82937900
H	-6.14797800	-3.41547800	-1.94207700
H	-7.22231600	-2.07642100	-1.49453200

H	-5.83308300	-1.78642800	-2.57265100
C	-3.13401500	-2.80915500	0.17742200
C	-1.77513400	-3.20241500	-0.36717900
O	-3.43941200	-2.77332300	1.35363500
H	-1.90978900	-3.95346900	-1.15417600
H	-1.35739500	-2.31192000	-0.84962900
C	-0.80853300	-3.70369800	0.71025400
H	-0.76880300	-2.97853000	1.52679000
C	-1.14031100	-5.09616200	1.24059000
O	0.52532500	-3.79120000	0.12077700
H	-2.18084100	-5.07494300	1.58128400
H	-1.08377600	-5.81049700	0.40850700
C	-0.23247900	-5.55007900	2.38854600
H	-0.30095900	-4.86264300	3.23942700
H	-0.52311100	-6.54499200	2.74099200
H	0.81439600	-5.59800900	2.07367600
C	1.26871900	-2.66155800	0.06408200
C	2.62685600	-2.93808200	-0.55046200
O	0.87915100	-1.57763600	0.45186900
H	2.45532800	-3.30517200	-1.57157500
H	3.07596300	-3.78017800	-0.00884300
C	3.55476800	-1.72152600	-0.55309400
H	3.06232200	-0.89172400	-1.07335600
H	3.70790100	-1.38187300	0.47814300
C	4.91024900	-2.01774800	-1.20832700
H	4.74973900	-2.34745000	-2.24544600
H	5.39296400	-2.85815900	-0.68948100
C	5.85205500	-0.80547000	-1.19643800
H	6.04182600	-0.49461400	-0.16256300
H	5.37719300	0.04088300	-1.70914500
C	7.18395900	-1.11046400	-1.87458800
H	7.04029600	-1.38498100	-2.92314500

H	7.71640100	-1.91312500	-1.35741800
O	8.03602900	0.06159300	-1.92409500
C	8.84740400	0.28549000	-0.86196700
C	9.67057200	1.54090900	-1.06937400
O	8.89770400	-0.43982300	0.11117900
H	8.97699500	2.35795900	-1.30645600
H	10.26975100	1.39405900	-1.97806600
C	10.55952000	1.89711800	0.12370500
H	9.93476500	2.02415500	1.01590300
H	11.22729100	1.05561500	0.34206000
C	11.38367000	3.16847800	-0.11879100
H	10.70486500	4.00447400	-0.34301300
H	12.00719500	3.03249700	-1.01471300
C	12.27488200	3.53913600	1.07342300
H	12.96721800	2.71732600	1.29585200
H	11.66096800	3.68463600	1.97128700
C	13.08727800	4.80453800	0.83283400
H	12.41270700	5.65223600	0.63531400
H	13.73236200	4.67511700	-0.05022200
O	13.87825000	5.05489000	1.99830000
H	14.39812000	5.85678900	1.86266100

## S.1.5 COORDINATES - BC

0 1

C	14.90871800	3.61760500	0.67850600
H	15.86566700	3.77194700	1.22555300
C	14.24806000	2.28113000	0.91756900
H	14.12085900	2.17773500	2.00705000
H	14.98751200	1.50907400	0.64997800
C	12.92654900	2.07040400	0.17780500
H	12.22168200	2.85737200	0.47149200
H	13.09193000	2.20286900	-0.89810400
C	12.30865600	0.69148900	0.44573000
H	12.15747900	0.56184200	1.52685900
H	13.01710400	-0.09155500	0.13765000
C	10.97192500	0.48729300	-0.28113300
H	11.11060800	0.61711300	-1.36203900
H	10.25273500	1.24622900	0.04818300
C	10.38713200	-0.89705600	-0.01941300
H	10.18403300	-1.04596900	1.04437300
H	11.05775900	-1.68353500	-0.37593800
O	14.47428300	4.49060400	-0.04451100
O	9.16071000	-1.10666400	-0.76375200
C	8.00191400	-0.72723300	-0.17365700
C	6.82132400	-0.99659700	-1.08491900
O	7.93953200	-0.23662300	0.93598400
H	6.90409200	-2.02855200	-1.44788700
H	6.94522900	-0.36238900	-1.97339500
C	5.46569400	-0.74692300	-0.42036400
H	5.37500900	-1.38465500	0.46713600
H	5.42600800	0.28579100	-0.05518100
C	4.29087500	-1.01248200	-1.37086400
H	4.34430200	-2.04728000	-1.73808800
H	4.38388400	-0.36637700	-2.25602900

C	2.92573400	-0.77878100	-0.70800300
H	2.85606700	0.25687200	-0.35175100
H	2.82253200	-1.43197300	0.16611700
C	1.77374700	-1.05029500	-1.66973000
H	1.76659100	-2.09355600	-1.99595200
H	1.82341000	-0.39533900	-2.54341900
O	0.49015500	-0.74049100	-1.06586200
C	-0.12039500	-1.72029100	-0.36589300
C	-1.46823900	-1.25034900	0.14312900
O	0.34889500	-2.82908400	-0.19788100
H	-1.35659800	-0.25646900	0.59054500
H	-2.11551000	-1.13277900	-0.73335300
C	-2.11498300	-2.22426800	1.13267700
H	-2.17729800	-3.21502200	0.67807300
C	-1.42015900	-2.28940700	2.48396000
O	-3.47667500	-1.76411300	1.40218100
H	-1.95061600	-2.97274700	3.15319900
H	-0.39892300	-2.65627600	2.35457400
H	-1.38819800	-1.30084500	2.95450400
C	-4.44275400	-2.09232300	0.51741300
C	-5.77818800	-1.51987100	0.94954200
O	-4.24697600	-2.74247700	-0.49110800
H	-5.96575000	-1.79955600	1.99268100
H	-5.67771900	-0.42923400	0.92879900
C	-6.94266900	-1.94558000	0.04968500
H	-6.68517900	-1.74550800	-0.99338300
C	-7.36535400	-3.40102300	0.23182200
O	-8.10529600	-1.12987800	0.39124000
H	-6.47282000	-4.01905500	0.08849300
H	-7.69727900	-3.54250600	1.26897800
C	-8.46281400	-3.84866000	-0.73937700
H	-8.13482700	-3.74111400	-1.77963200

H	-8.71663800	-4.90130700	-0.57790100
H	-9.37516600	-3.25896100	-0.60789100
C	-8.20019100	0.10117500	-0.16472100
C	-9.49331000	0.78080200	0.24010300
O	-7.35361800	0.57682400	-0.89547800
H	-9.60513000	0.67733200	1.32660300
H	-10.31609000	0.19751000	-0.19601400
C	-9.57592600	2.24602100	-0.19369100
H	-8.74610100	2.80434200	0.25677800
H	-9.42777300	2.31037000	-1.27761400
C	-10.90944500	2.89997600	0.19105800
H	-11.05384700	2.82320800	1.27879700
H	-11.73566100	2.33708400	-0.26765900
C	-10.99452600	4.37160500	-0.23361300
H	-10.86040200	4.45800000	-1.31930500
H	-10.18137900	4.94443600	0.22997100
C	-12.31941800	5.02075900	0.14351400
H	-12.46610800	4.97048400	1.23373900
H	-13.15196900	4.48034800	-0.33336700
O	-12.28918400	6.38207100	-0.29512100
H	-13.12387200	6.80852700	-0.06457700

## S.1.6 COORDINATES - BD

0 1

C	14.15557300	5.37689400	-0.08804100
H	15.02337100	5.92498300	-0.51858400
C	14.06480300	3.92155400	-0.47999000
H	15.01731200	3.45305700	-0.18387700
H	14.06870400	3.88633500	-1.58120800
C	12.86665000	3.16848100	0.09927100
H	12.88798400	3.24650400	1.19284800
H	11.94278100	3.66650400	-0.21823100
C	12.83250100	1.69240400	-0.31862500
H	13.75781800	1.19807200	0.01209700
H	12.82134600	1.62274800	-1.41572200
C	11.61962900	0.94215200	0.24984500
H	10.69522500	1.41421500	-0.10243900
H	11.62104300	1.00609900	1.34548000
C	11.61278500	-0.52719000	-0.15971900
H	12.50098000	-1.04583000	0.21113800
H	11.55477200	-0.63500900	-1.24608400
O	13.37159100	5.95355300	0.63750300
O	10.50336400	-1.24126200	0.44185500
C	9.32852800	-1.24704300	-0.23245700
C	8.27811400	-2.03484100	0.52450900
O	9.16310000	-0.69656100	-1.30271900
H	8.22301300	-1.62597700	1.54154400
H	8.65713300	-3.05899500	0.64140600
C	6.90488600	-2.02988200	-0.15010100
H	6.55478400	-0.99572500	-0.25126800
H	7.00197600	-2.41632100	-1.17138800
C	5.86863000	-2.85522200	0.62397000
H	5.78385200	-2.46850000	1.64949300
H	6.22312900	-3.89259100	0.71453800

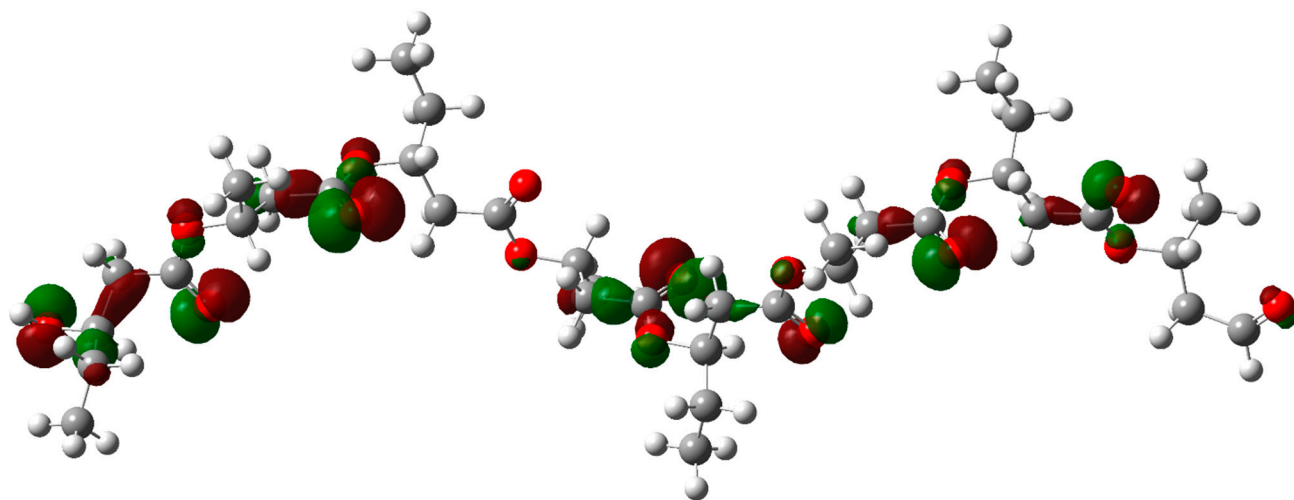
C	4.48439900	-2.84291800	-0.03979100
H	4.55923100	-3.22464500	-1.06606500
H	4.11319900	-1.81329300	-0.10207700
C	3.47381000	-3.68782300	0.72915100
H	3.32615000	-3.30476600	1.74231000
H	3.78711500	-4.73417000	0.77698300
O	2.19196500	-3.72747300	0.05180600
C	1.30319600	-2.74834700	0.34407500
C	0.03120000	-2.91855100	-0.46250100
O	1.51631700	-1.86109500	1.14612500
H	-0.33021800	-3.94301100	-0.30702800
H	0.30819200	-2.86399200	-1.52395500
C	-1.04980300	-1.89019800	-0.12355100
H	-1.30900000	-1.97365000	0.93860300
H	-0.64295400	-0.88090700	-0.25600500
C	-2.31064900	-2.06136800	-0.98091900
H	-2.70792000	-3.07805700	-0.85061500
H	-2.04322500	-1.96917800	-2.04382300
C	-3.40488400	-1.04041100	-0.63792900
H	-3.01681900	-0.02153700	-0.76330600
H	-3.69775100	-1.15041200	0.41266500
C	-4.63792700	-1.21193300	-1.51866500
H	-5.09534200	-2.19429100	-1.37562100
H	-4.39262500	-1.07397600	-2.57487000
O	-5.63299300	-0.18966300	-1.24781500
C	-6.54348200	-0.44822700	-0.28482300
C	-7.53576300	0.69177300	-0.17033500
O	-6.56475700	-1.46985200	0.37347200
H	-6.98729700	1.63866400	-0.10965700
H	-8.10411200	0.71357200	-1.10685800
C	-8.49705600	0.54089500	1.01251300
H	-8.98762300	-0.43301100	0.95708100



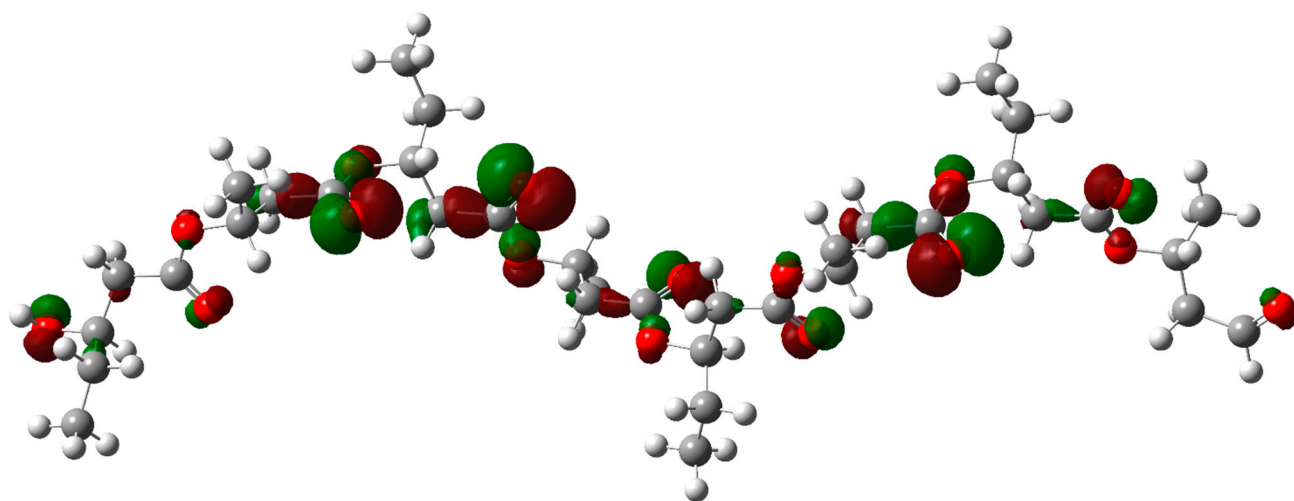
C	-7.84705800	0.74479900	2.37221600
O	-9.52836500	1.57164800	0.90057900
H	-8.59201400	0.65504800	3.16797800
H	-7.07909600	-0.01634800	2.53030100
H	-7.38724000	1.73660500	2.44059300
C	-10.57170600	1.33480400	0.07443300
C	-11.52805600	2.51029200	0.05394900
O	-10.69789400	0.31824900	-0.58099300
H	-11.58783400	2.93875500	1.06192800
H	-11.07814200	3.28116000	-0.58474500
C	-12.92293500	2.17573900	-0.49732500
H	-12.80301000	1.66287700	-1.45638100
C	-13.74208700	1.28958900	0.44864000
O	-13.61436700	3.38976900	-0.82221700
H	-13.14084400	0.40999500	0.70708200
H	-13.90876500	1.84152400	1.38747500
C	-15.08327000	0.84071700	-0.14096900
H	-13.82779000	3.85537300	-0.00127400
H	-14.92818700	0.23166000	-1.03865400
H	-15.64442100	0.23645300	0.57943400
H	-15.70073900	1.69865900	-0.42298800

## S.2 – MOLECULAR ORBITAL MAPS FROM HOMO-4 TO LUMO+4

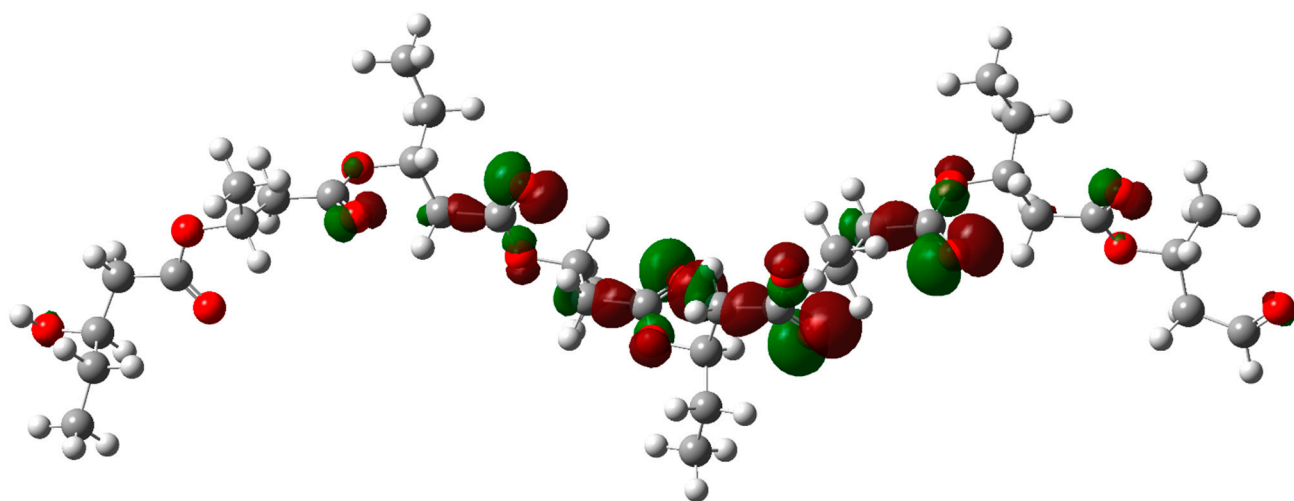
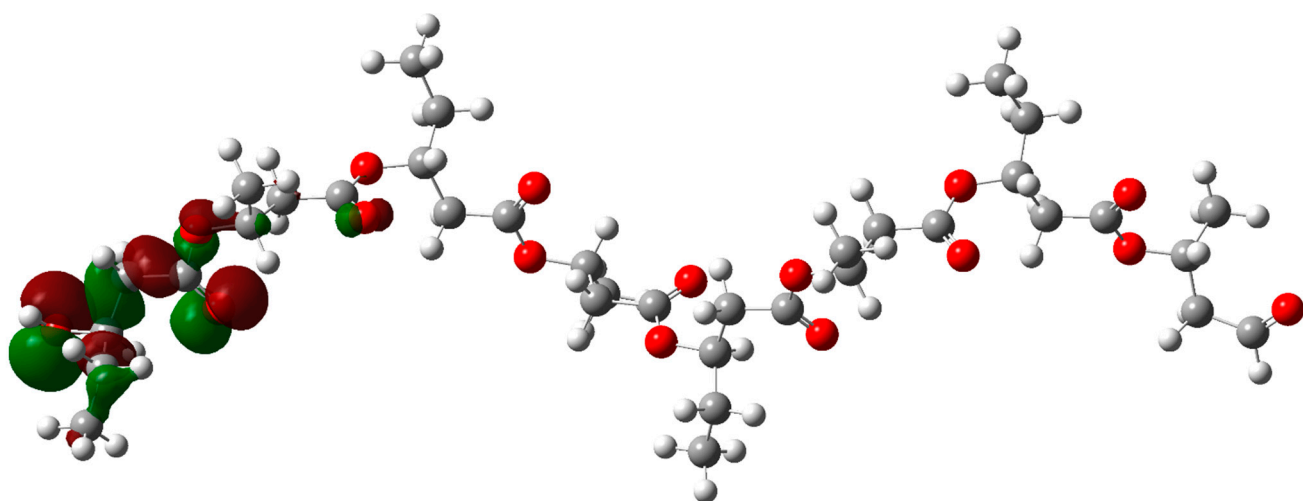
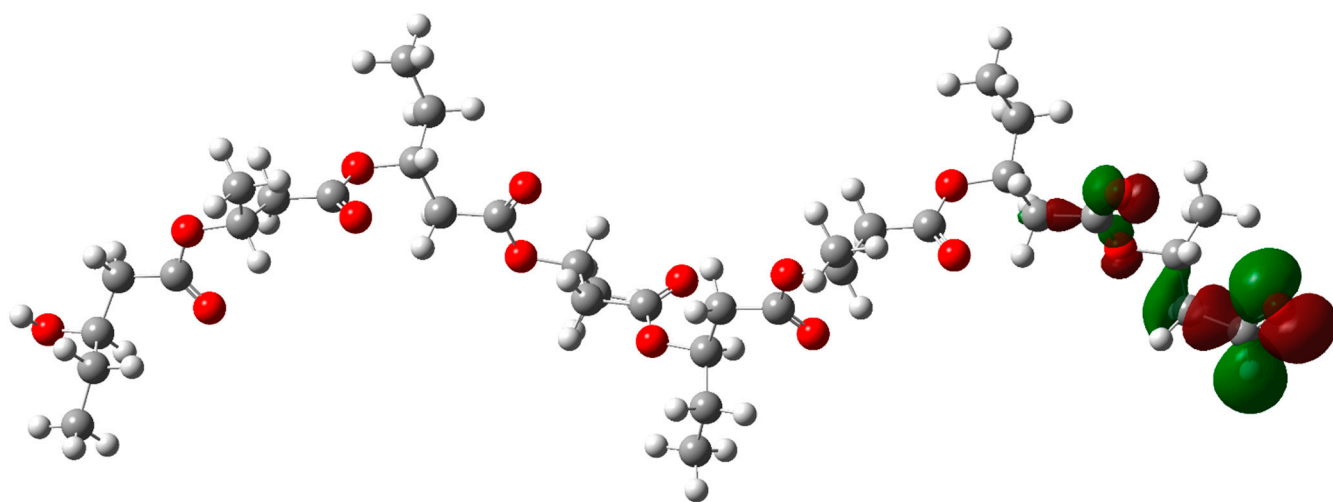
### S.2.1 MOLECULAR ORBITALS - PHBV

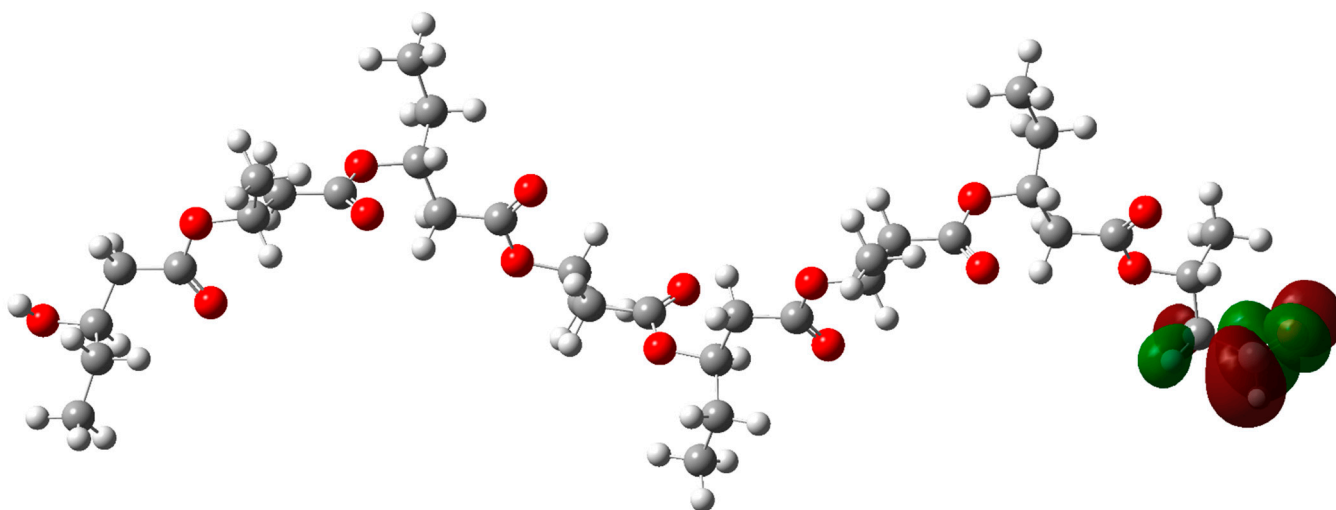
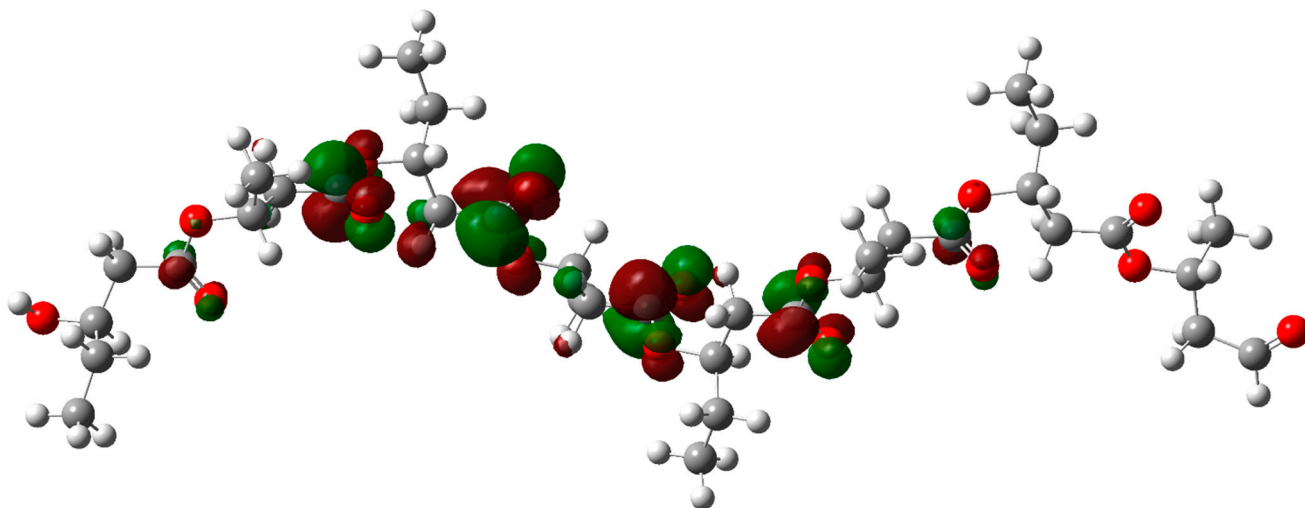
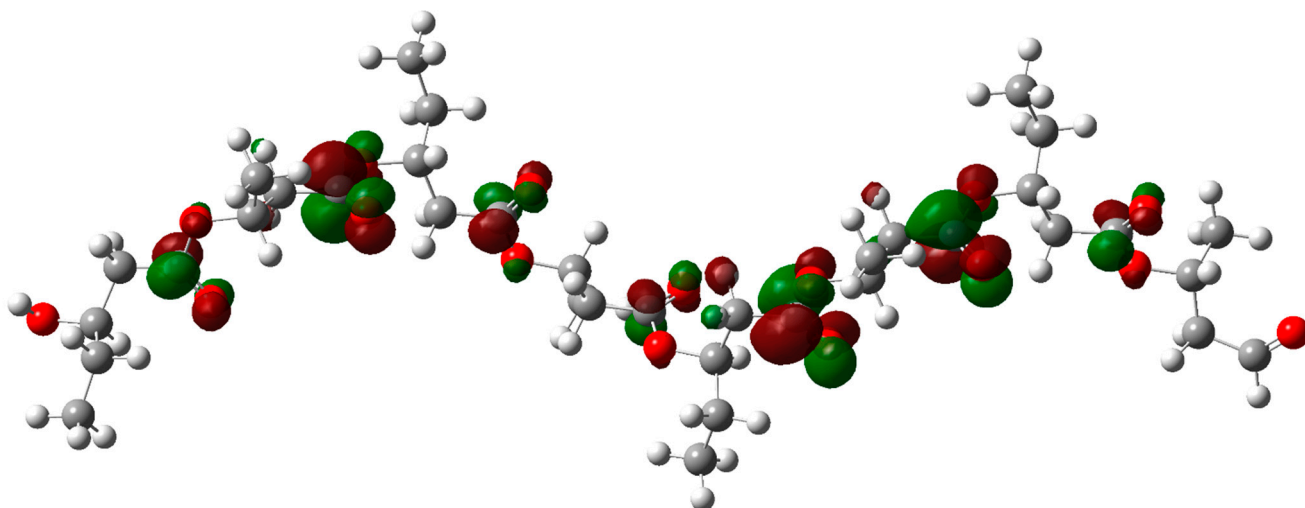


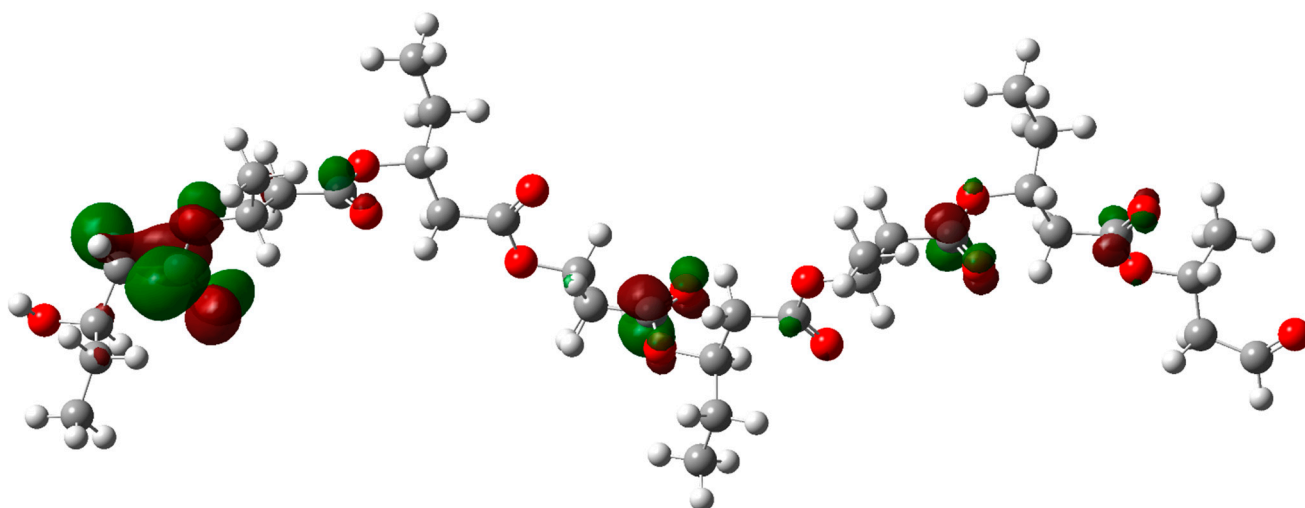
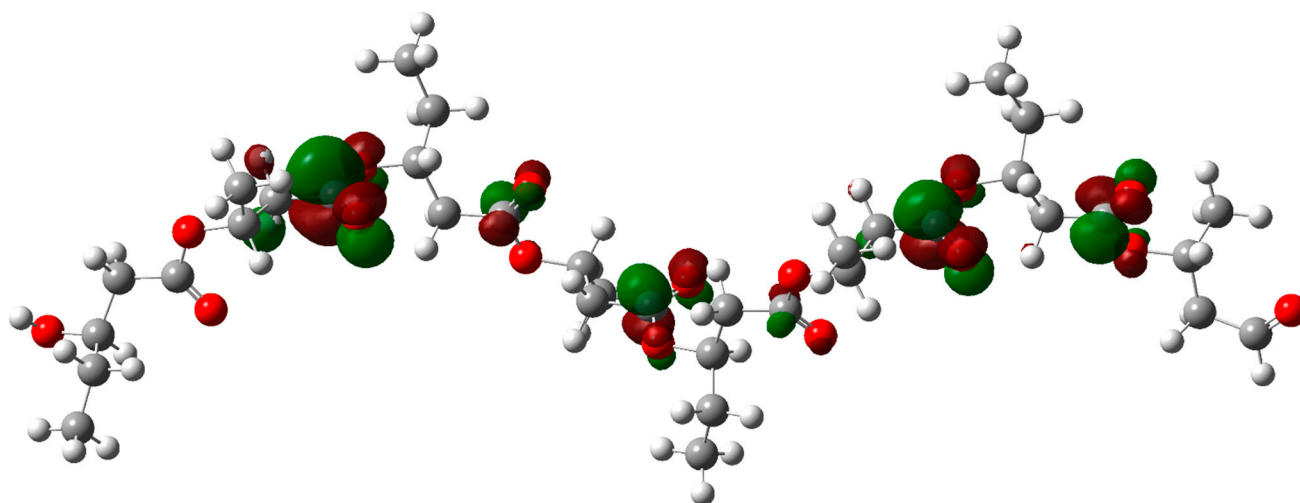
HOMO-4



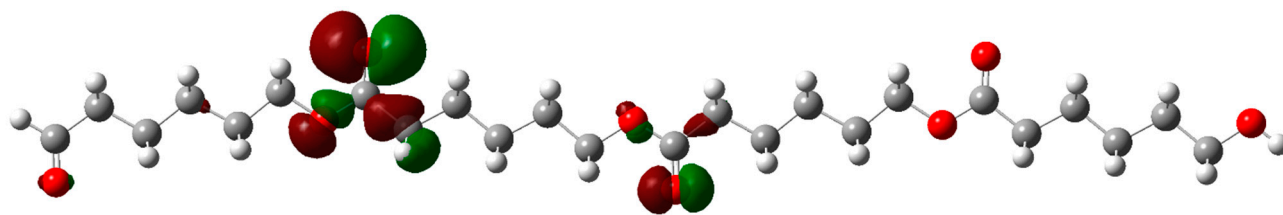
HOMO-3

**HOMO-2****HOMO-1****HOMO**

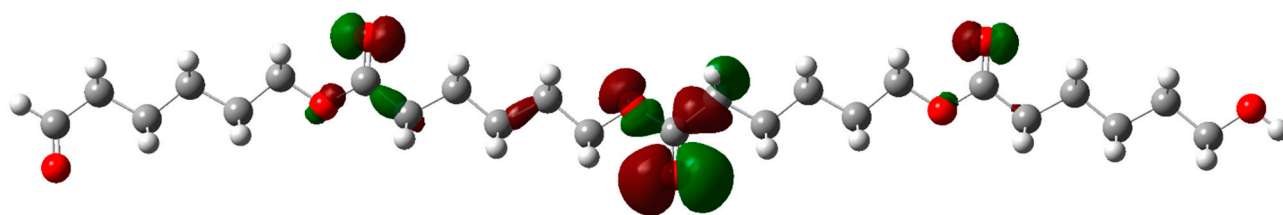
**LUMO****LUMO+1****LUMO+2**

**LUMO+3****LUMO+4**

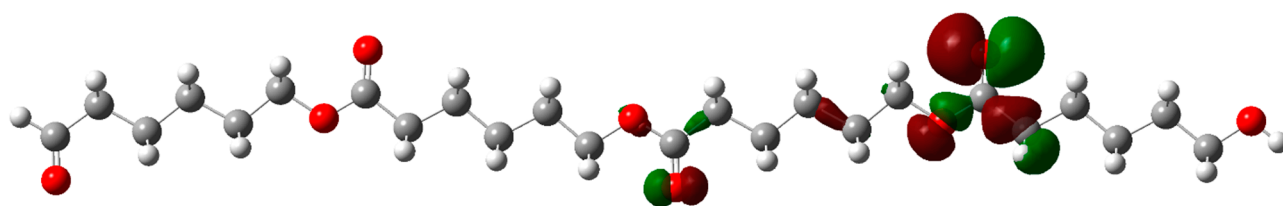
## S.2.2 MOLECULAR ORBITALS - PCL



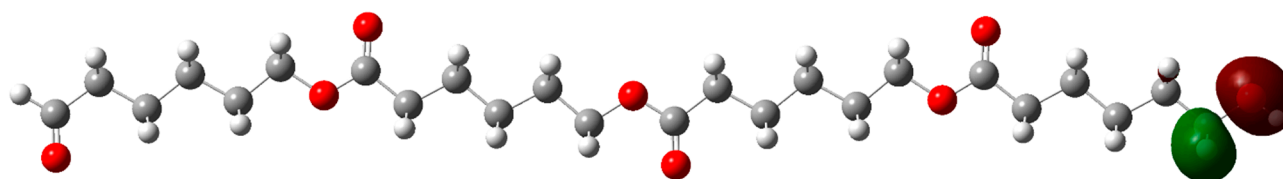
HOMO-4



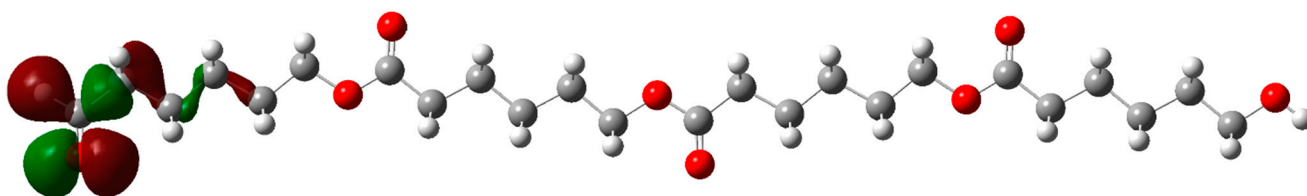
HOMO-3



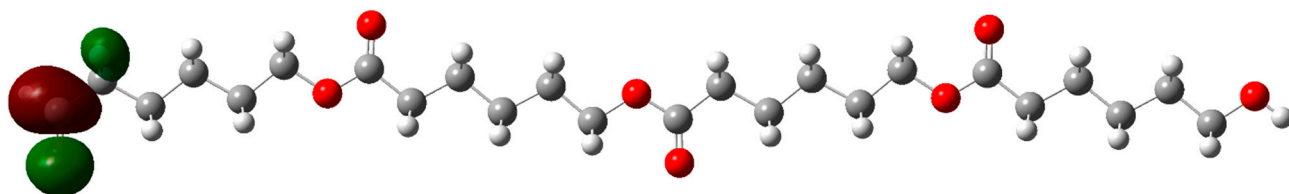
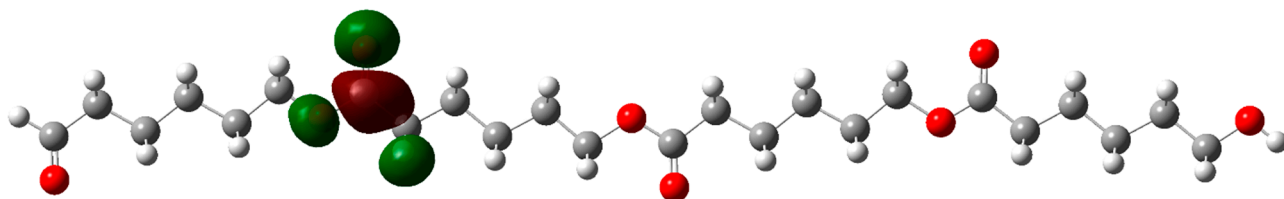
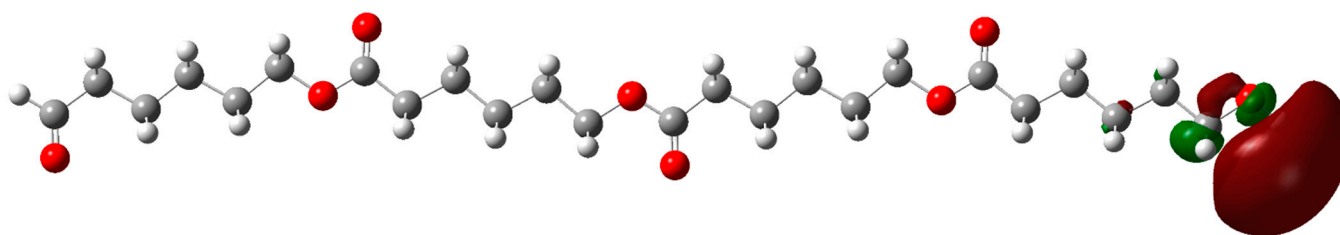
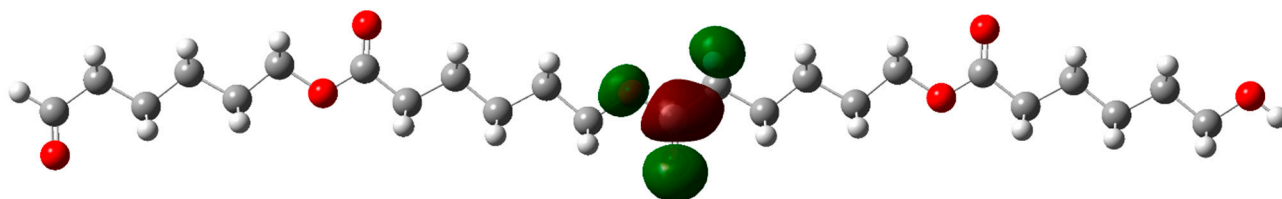
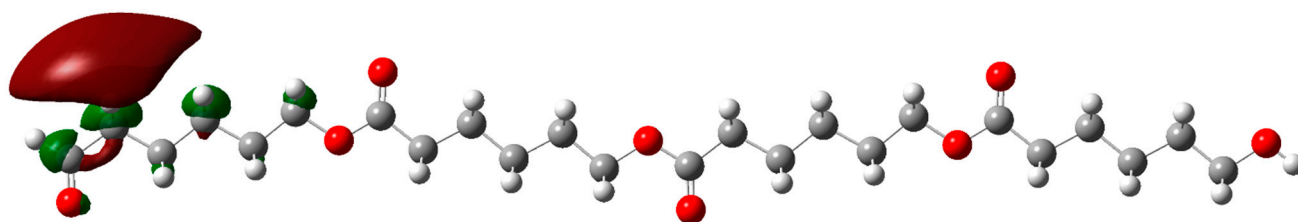
HOMO-2



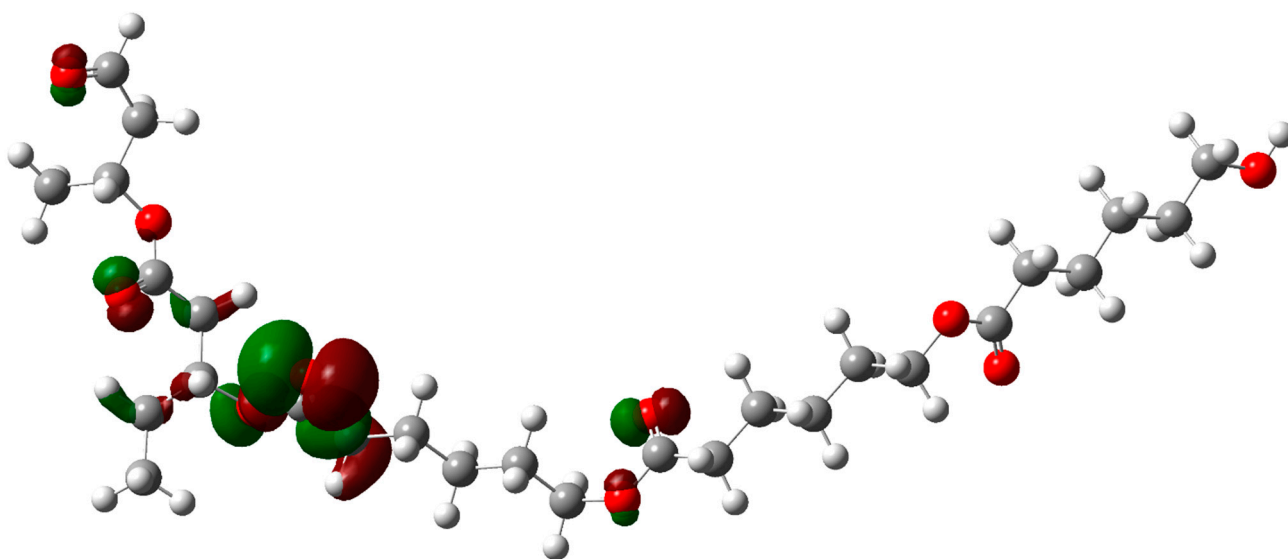
HOMO-1



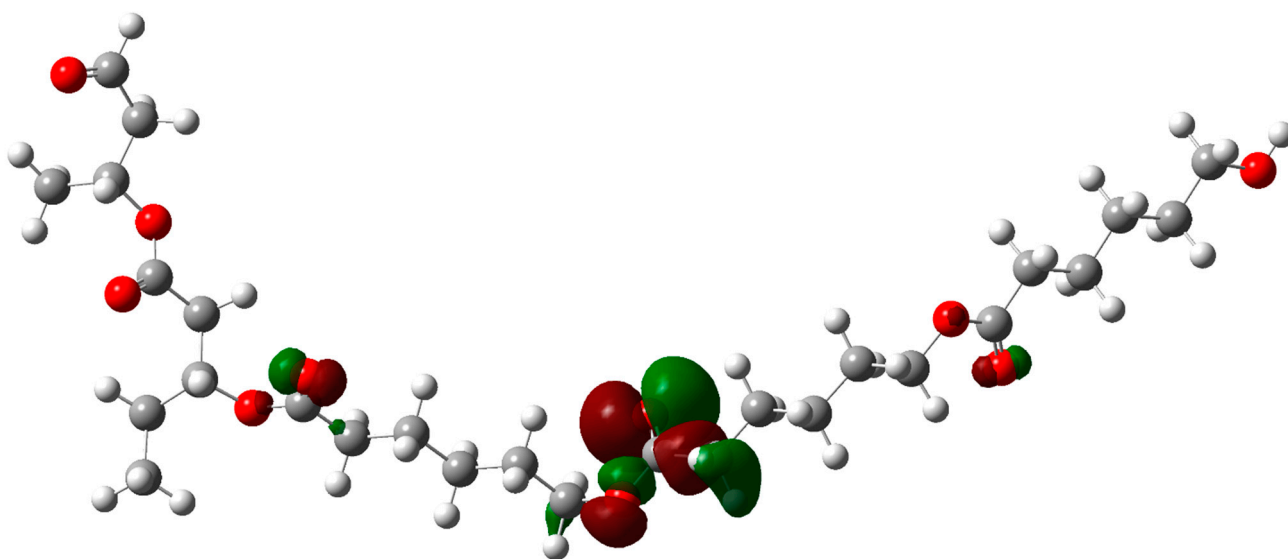
HOMO

**LUMO****LUMO+1****LUMO+2****LUMO+3****LUMO+4**

## S.2.3 MOLECULAR ORBITALS - BA

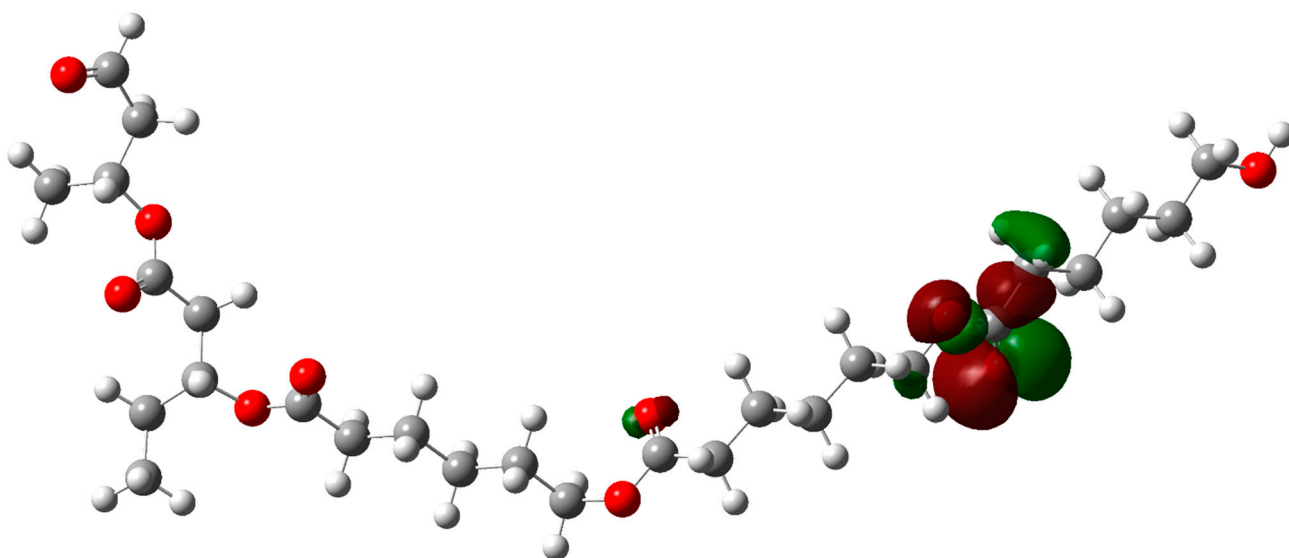
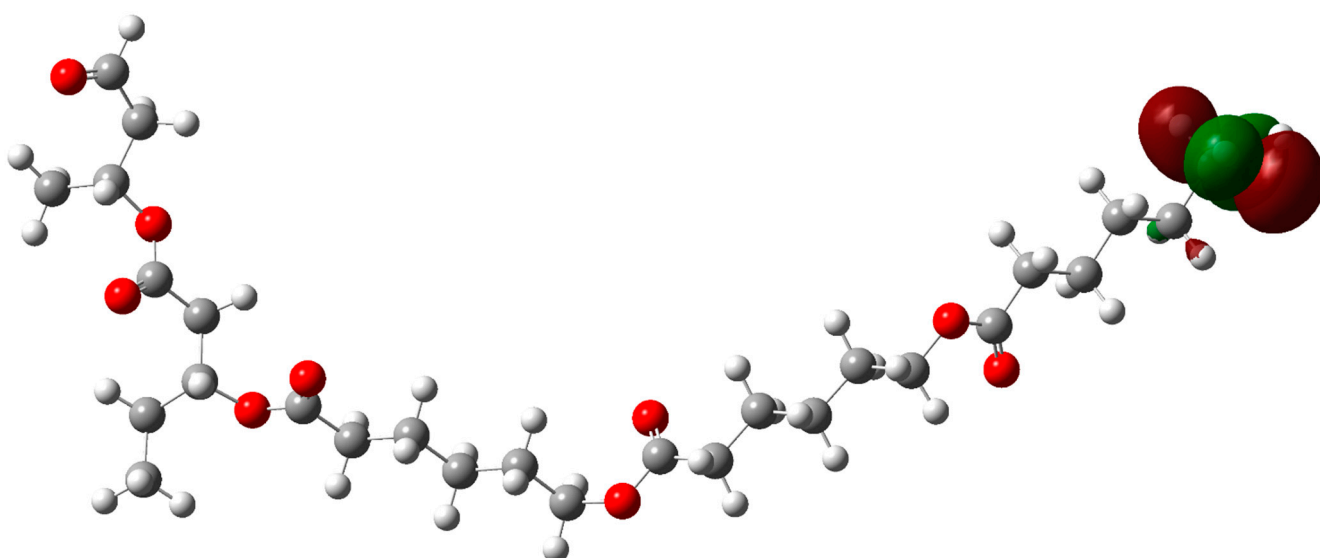


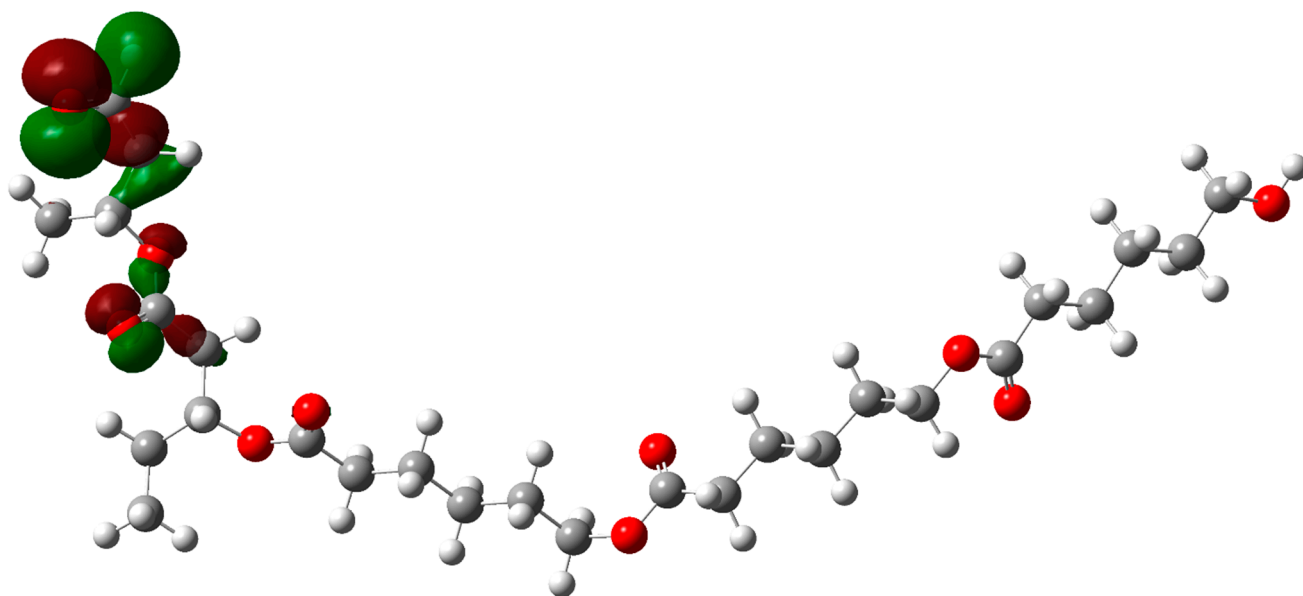
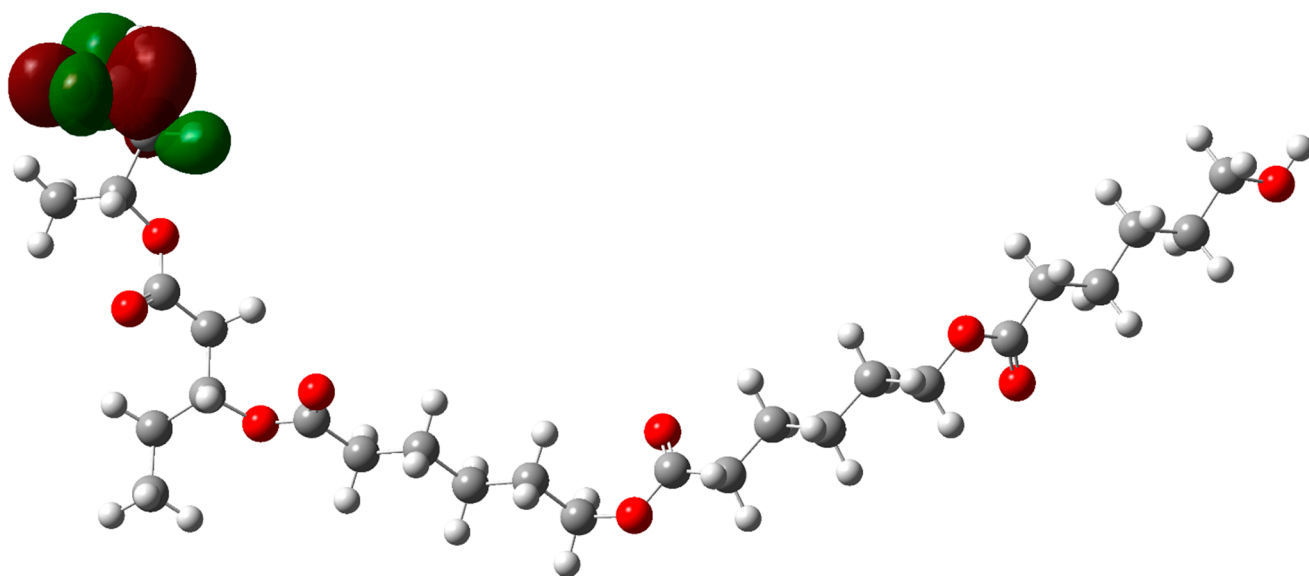
HOMO-4

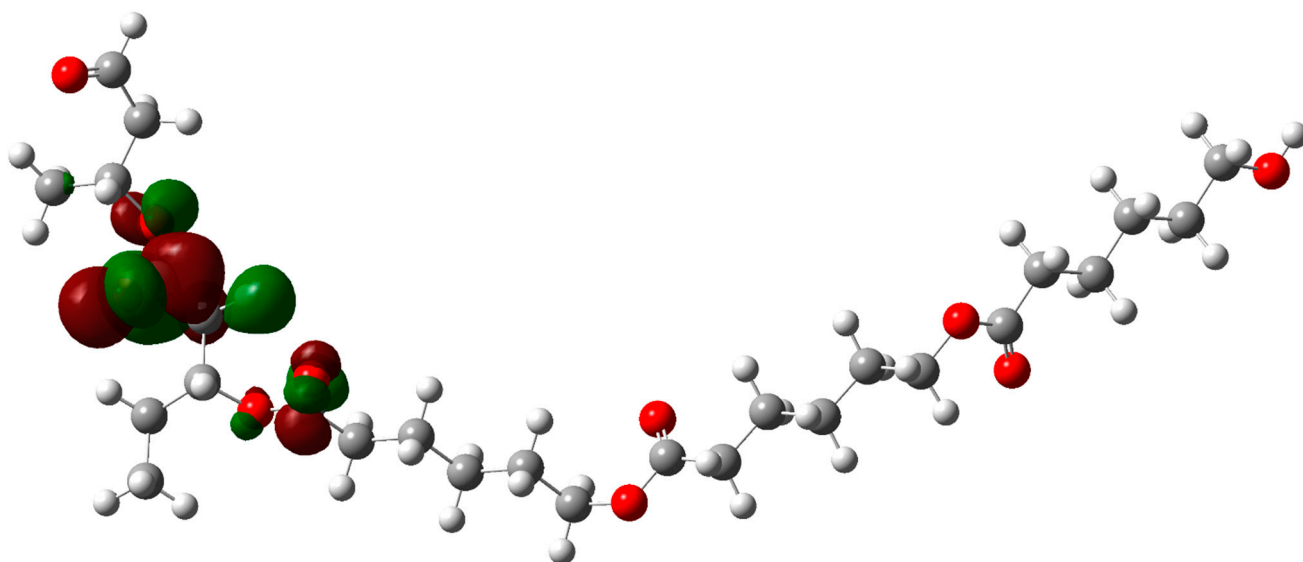
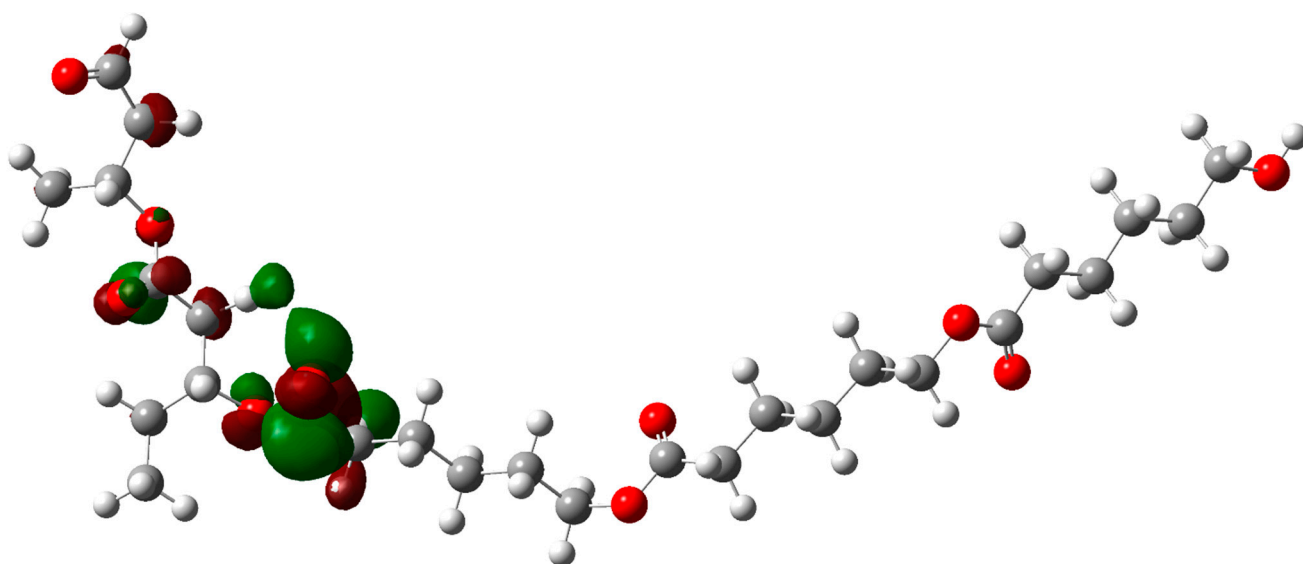


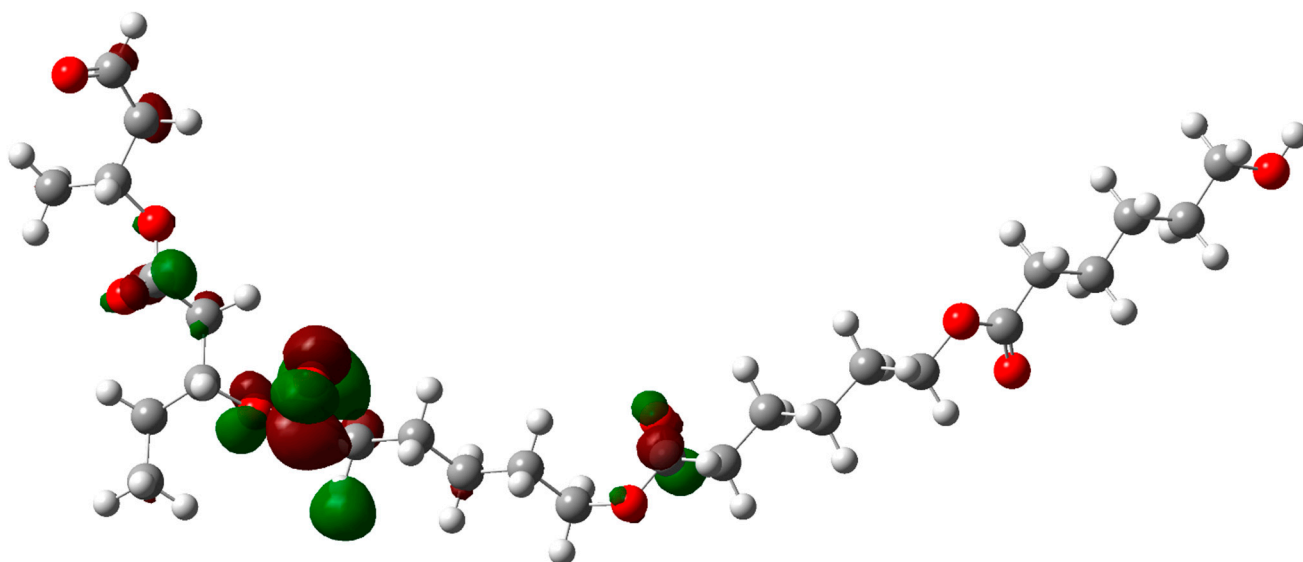
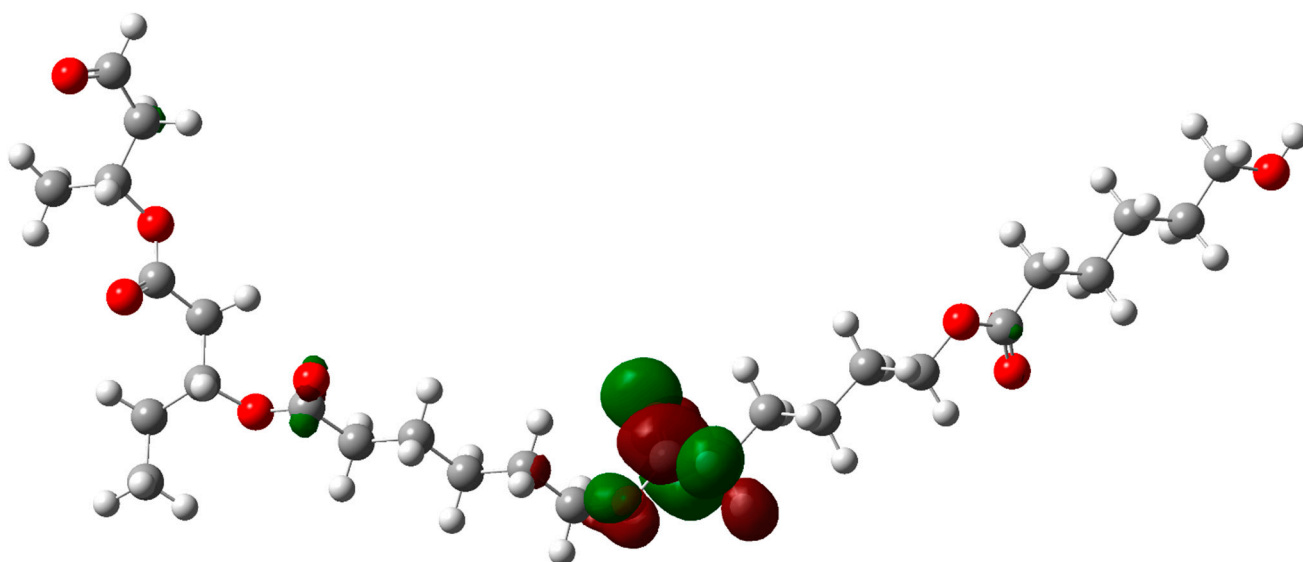
HOMO-3



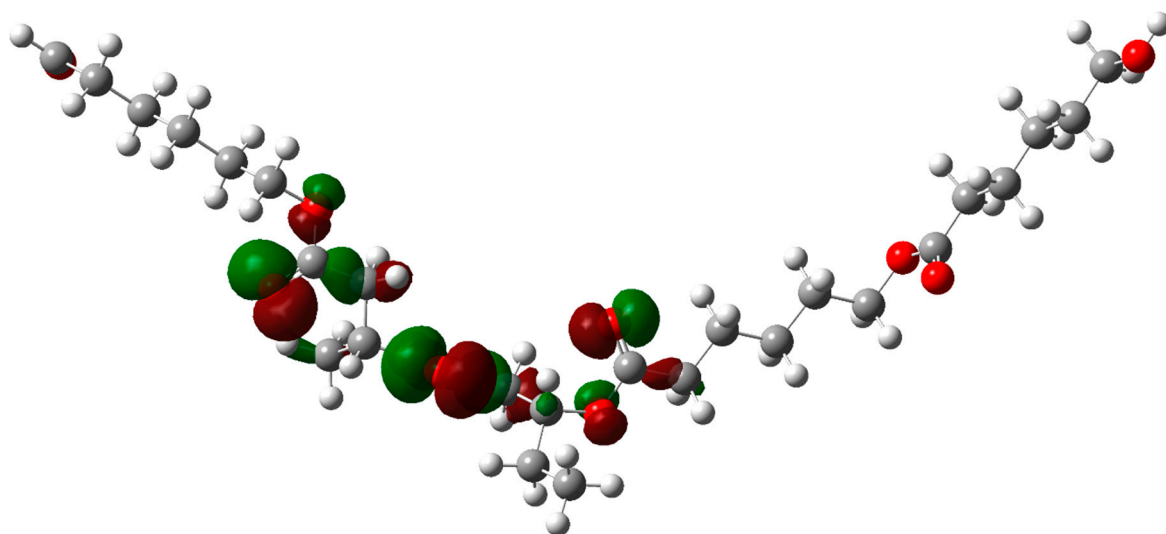
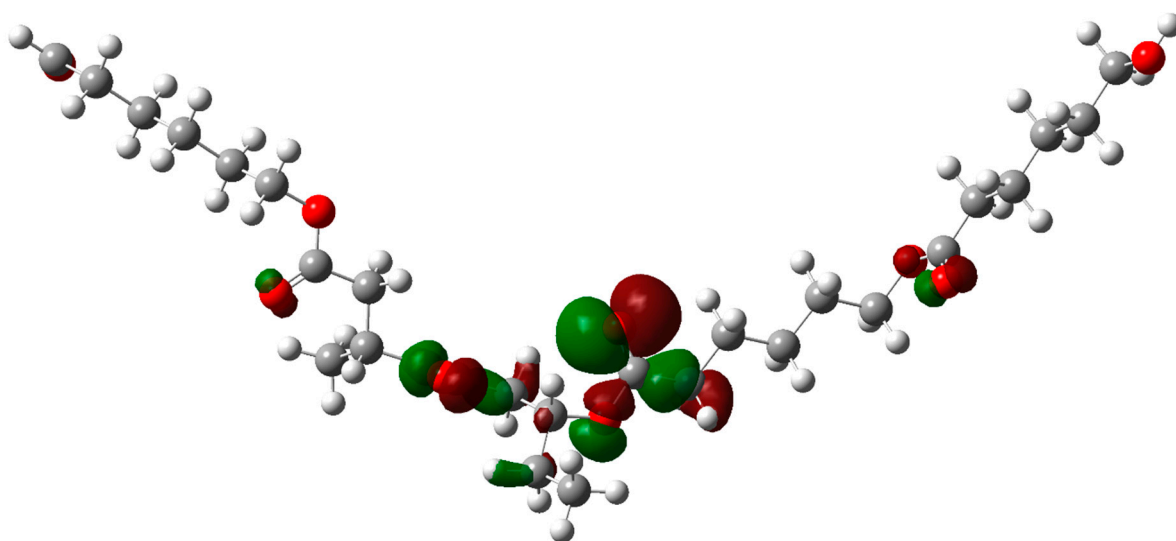
**HOMO-2****HOMO-1**

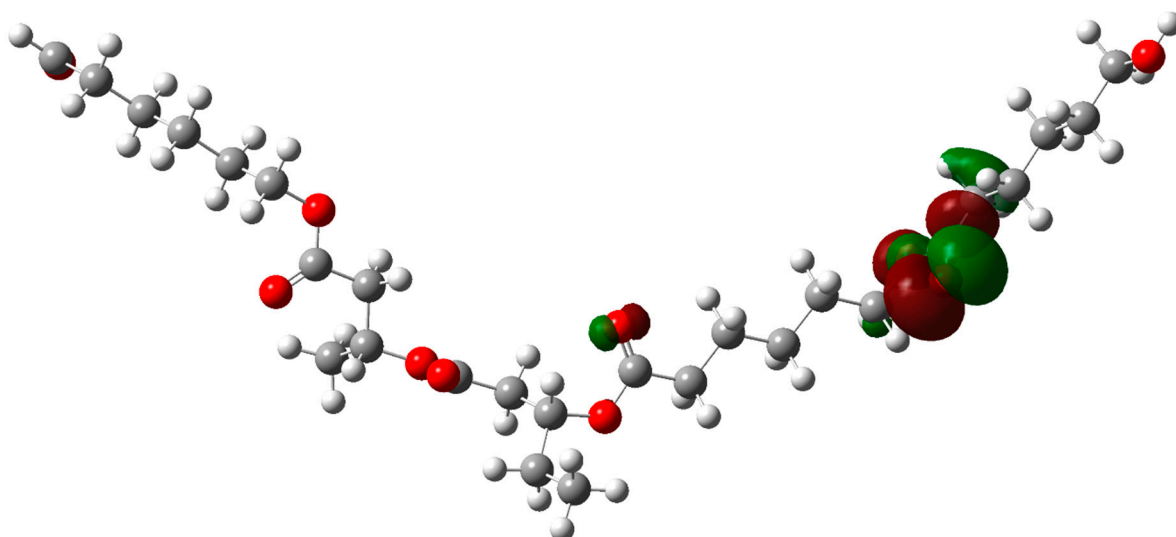
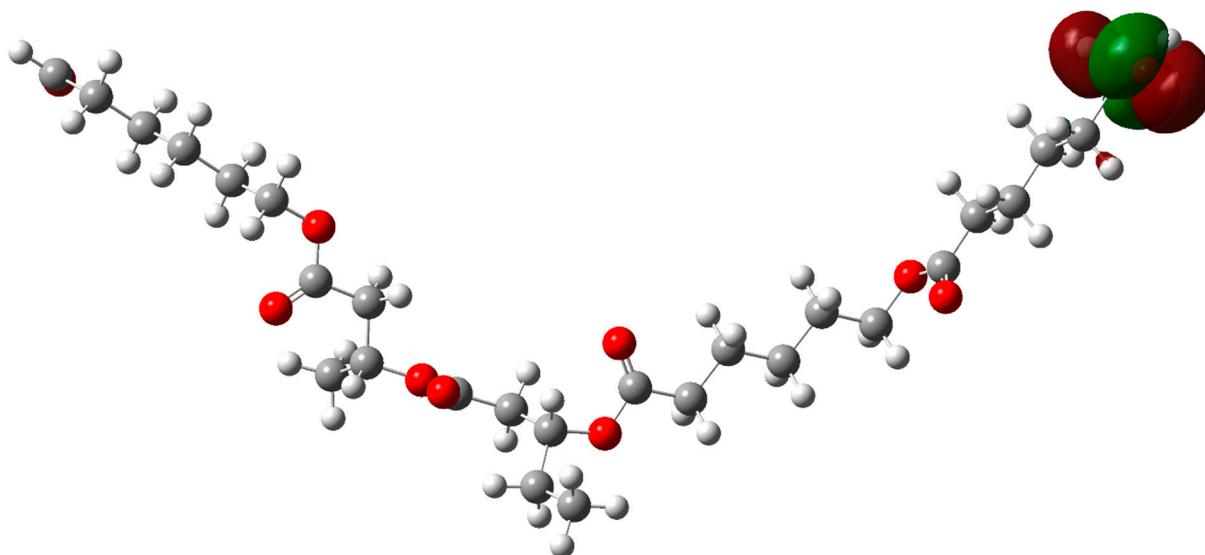
**HOMO****LUMO**

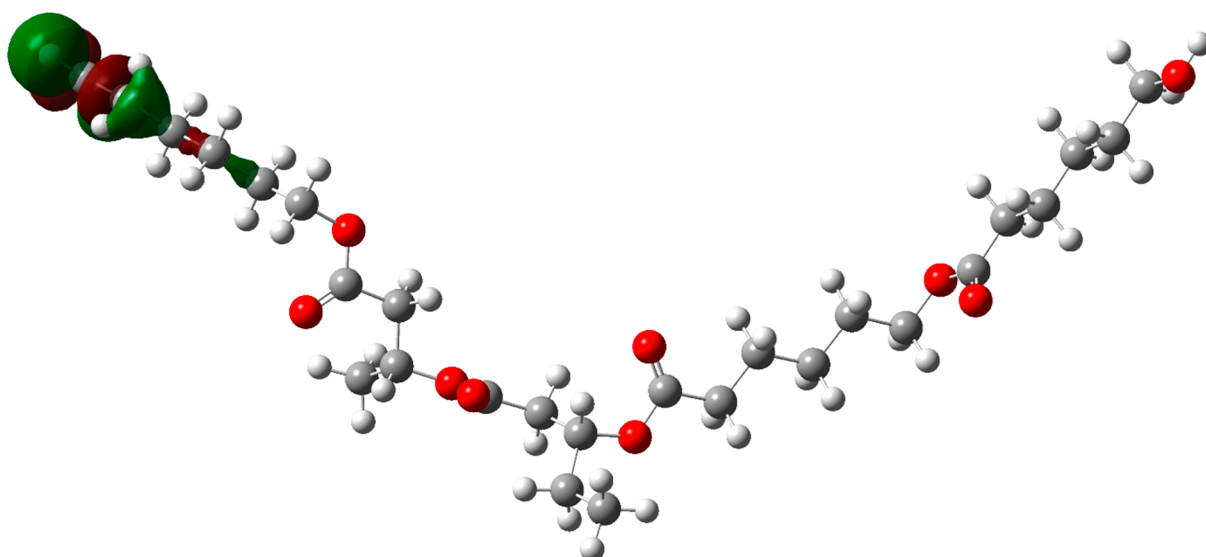
**LUMO+1****LUMO+2**

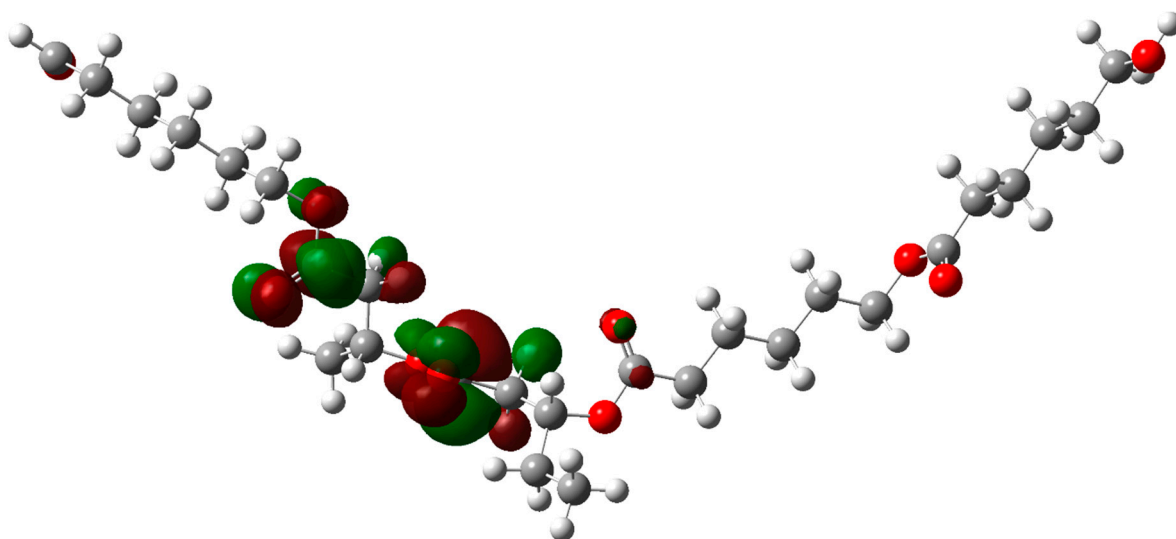
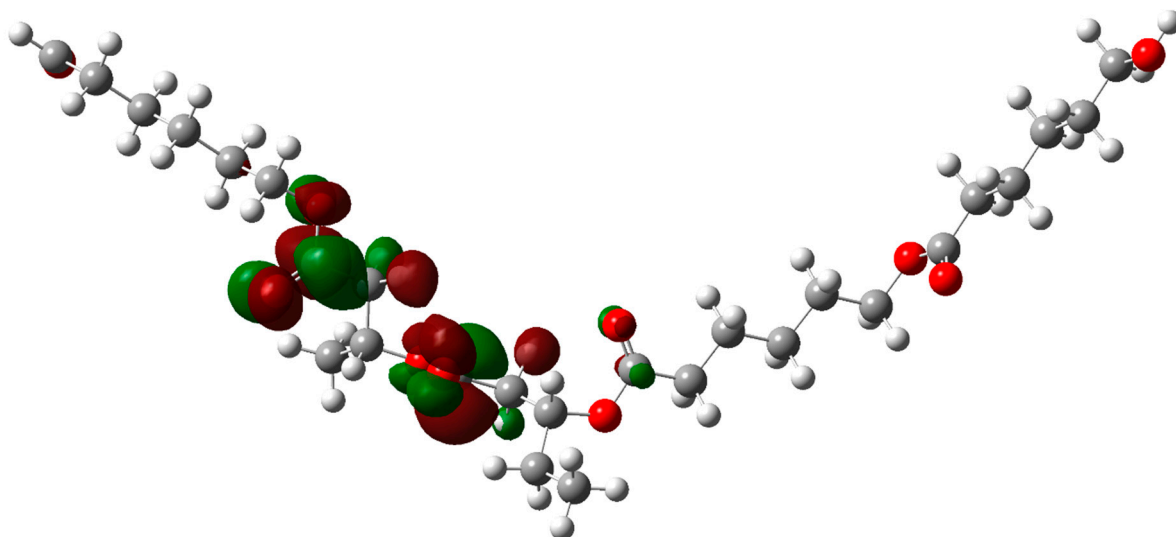
**LUMO+3****LUMO+4**

## S.2.4 MOLECULAR ORBITALS - BB

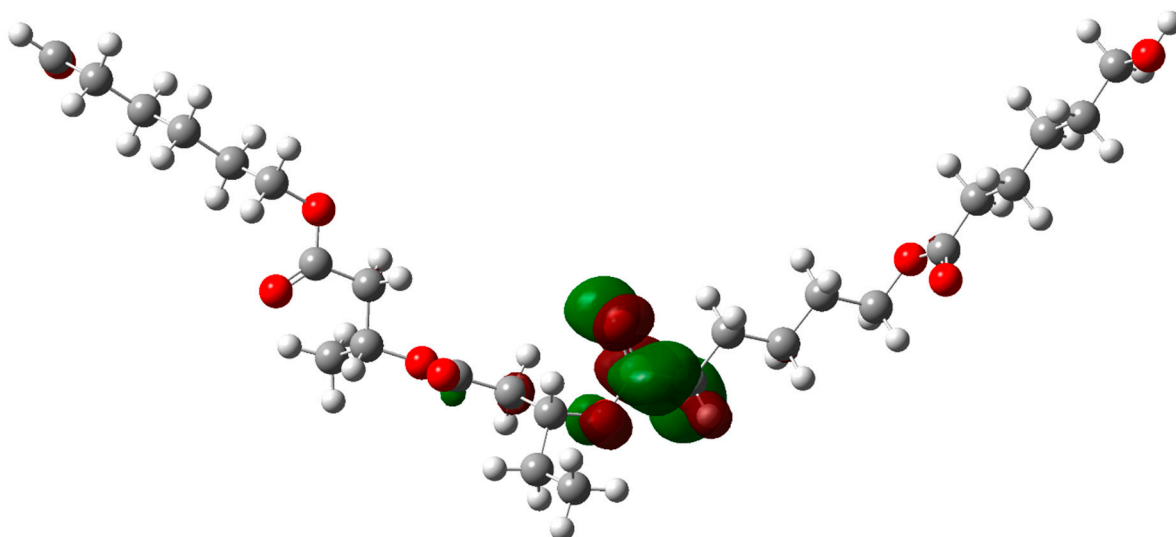
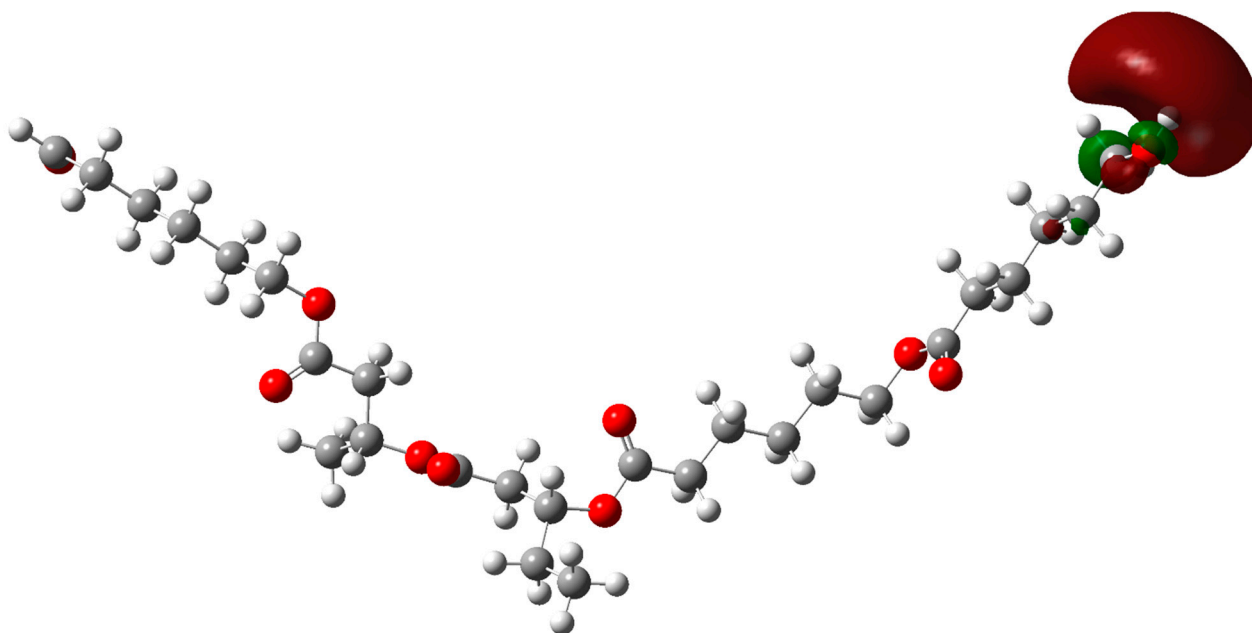
**HOMO-4****HOMO-3**

**HOMO-2****HOMO-1**

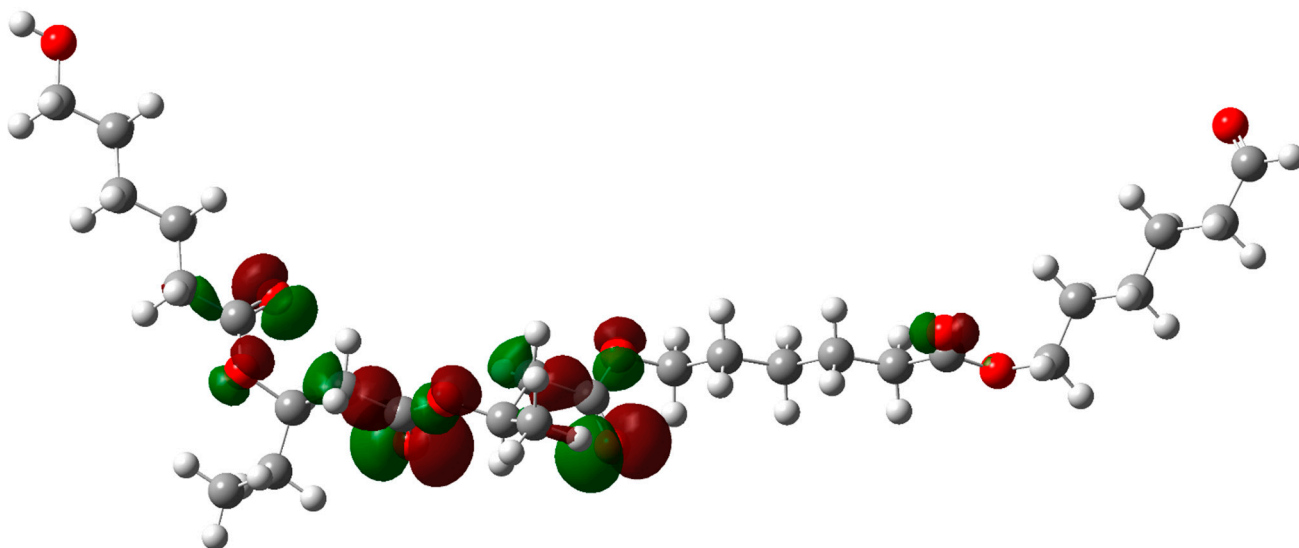
**HOMO****LUMO**

**LUMO+1****LUMO+2**

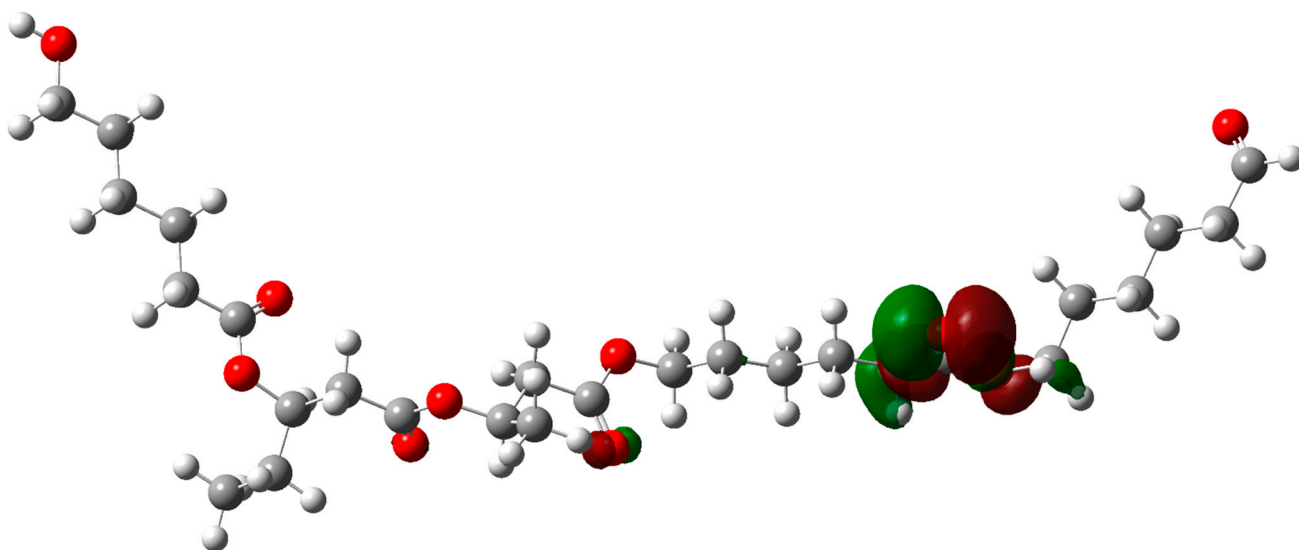


**LUMO+3****LUMO+4**

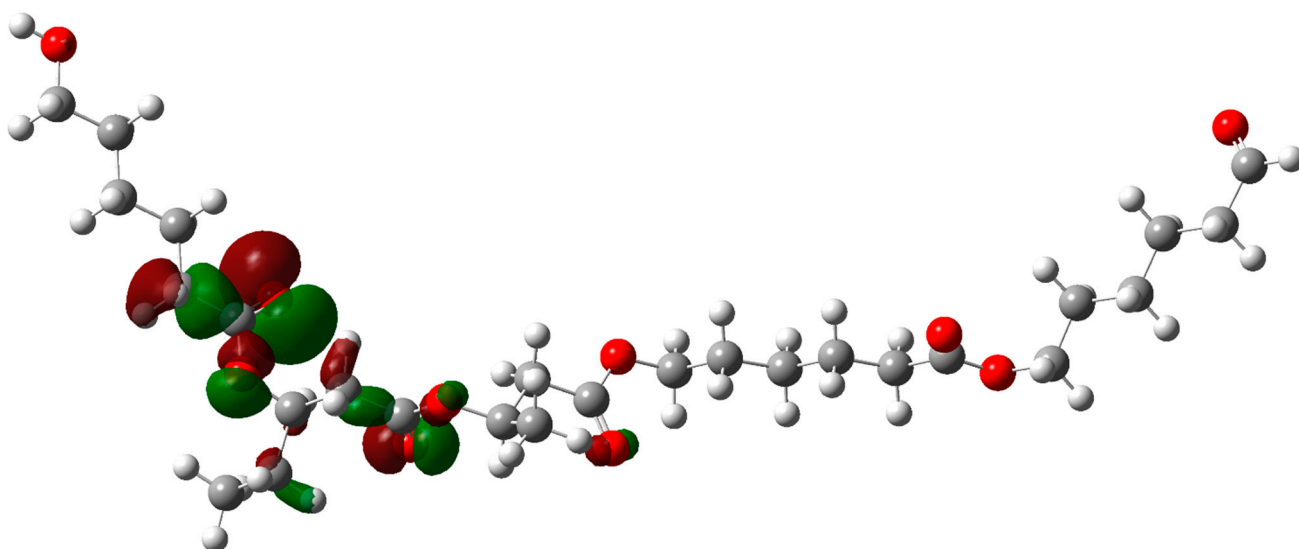
## S.2.5 MOLECULAR ORBITALS - BC

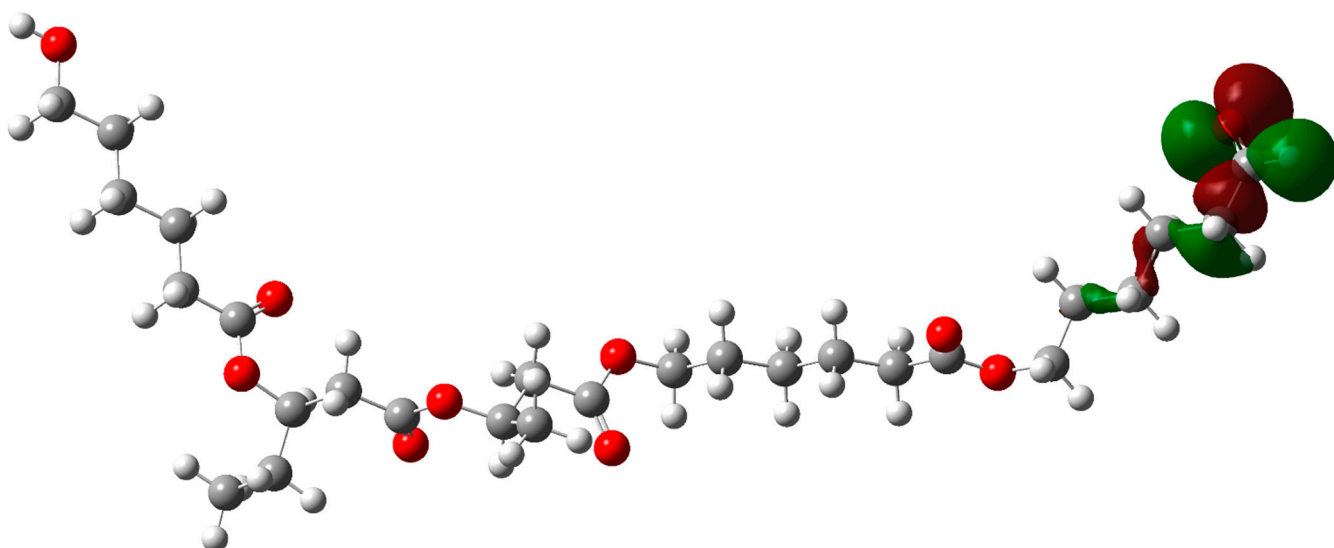
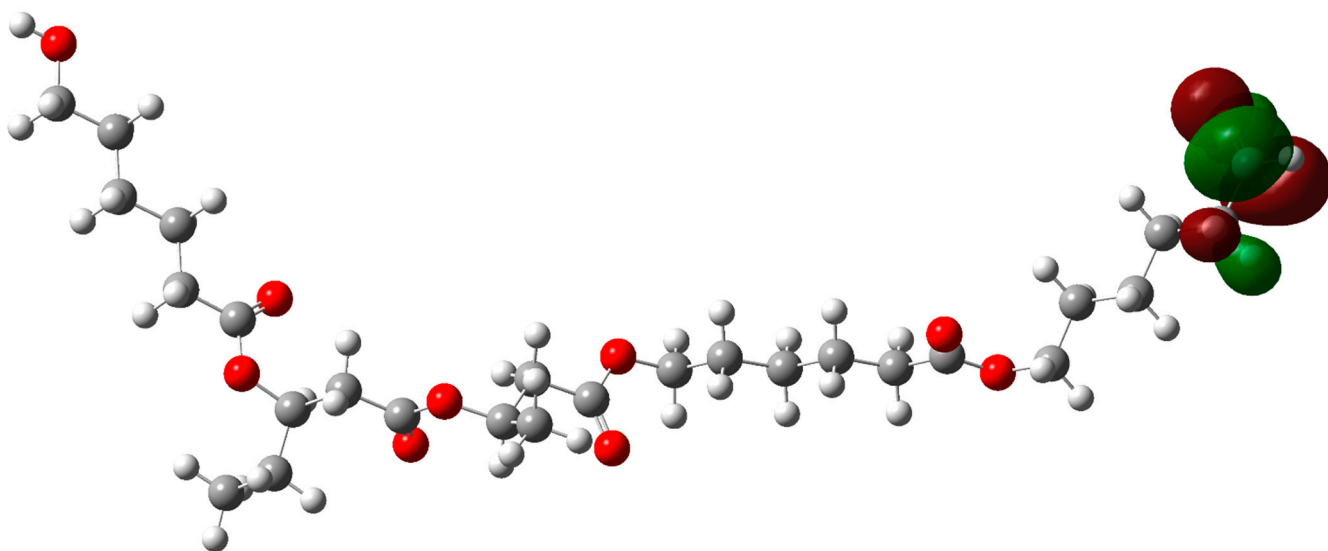


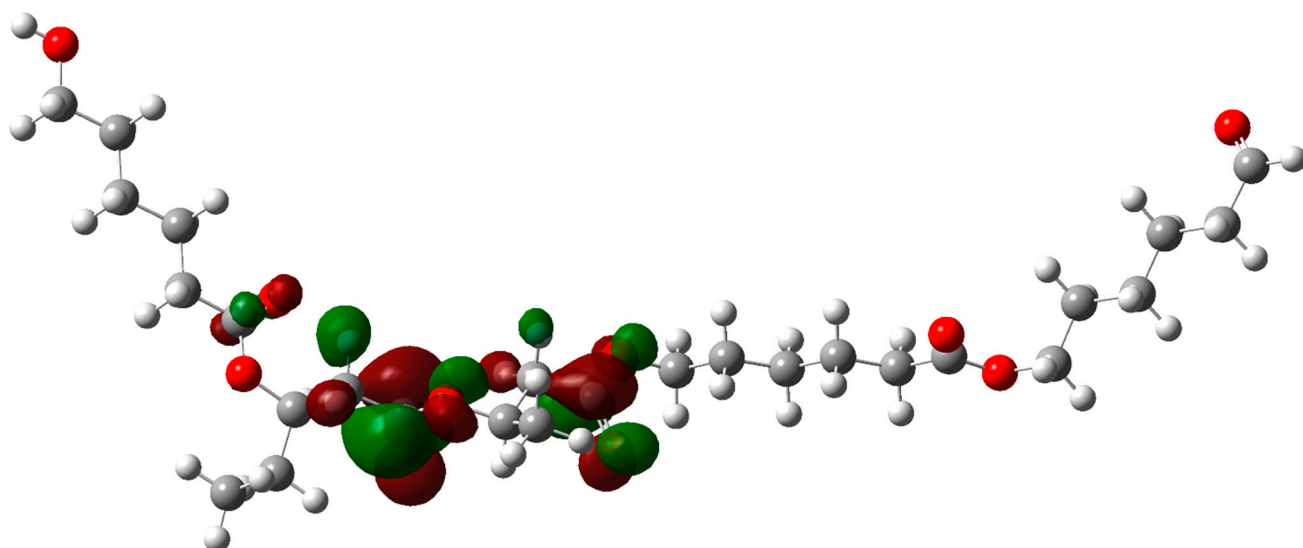
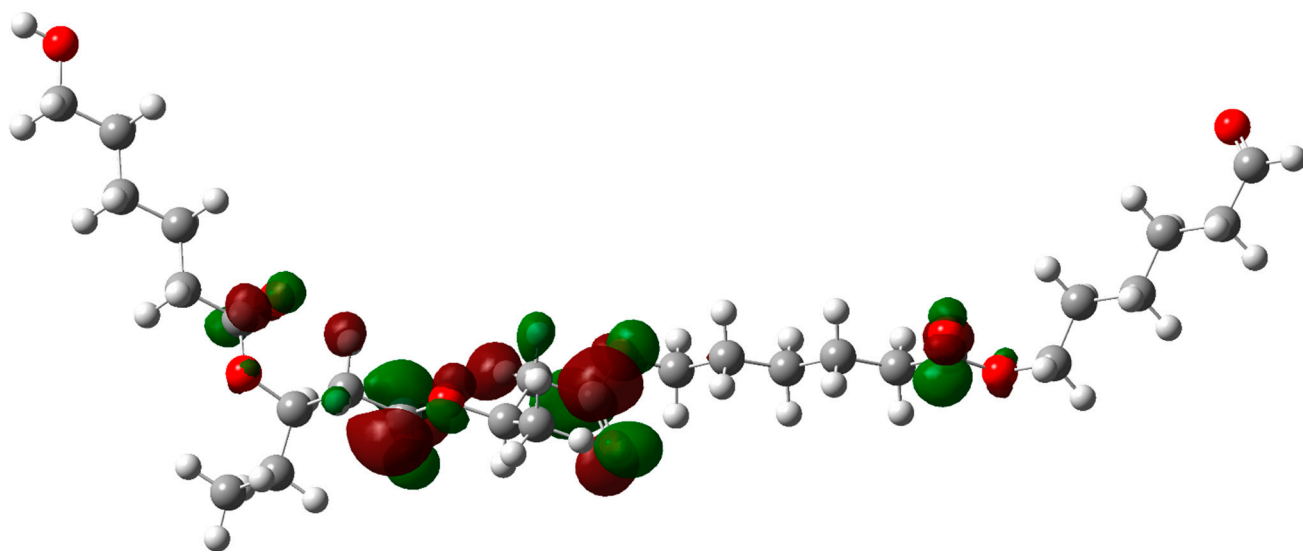
HOMO-4

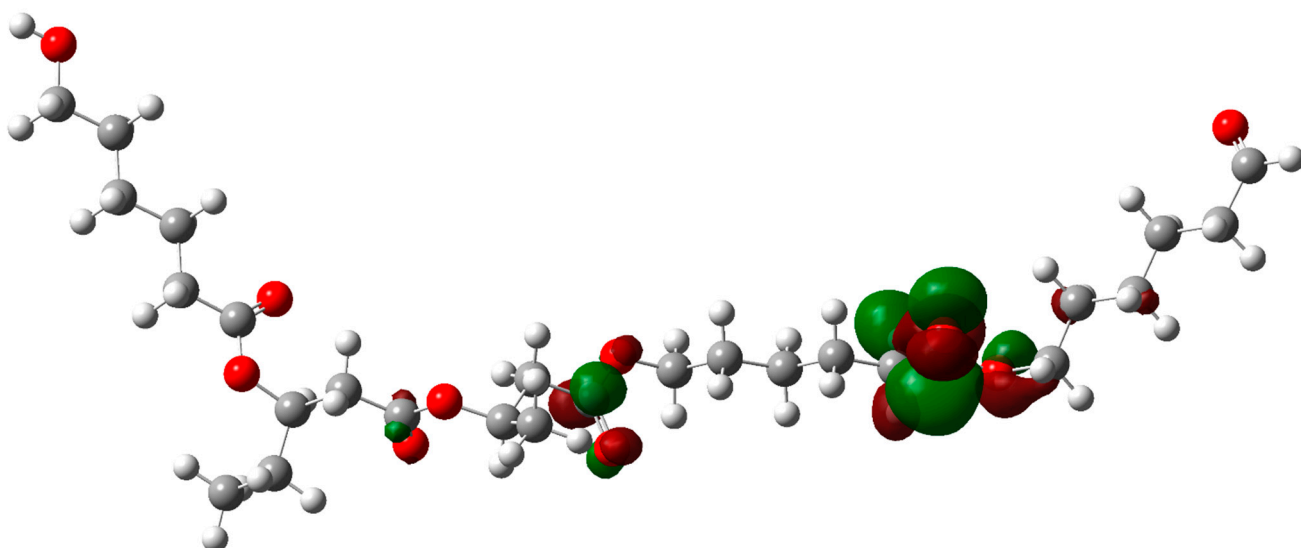
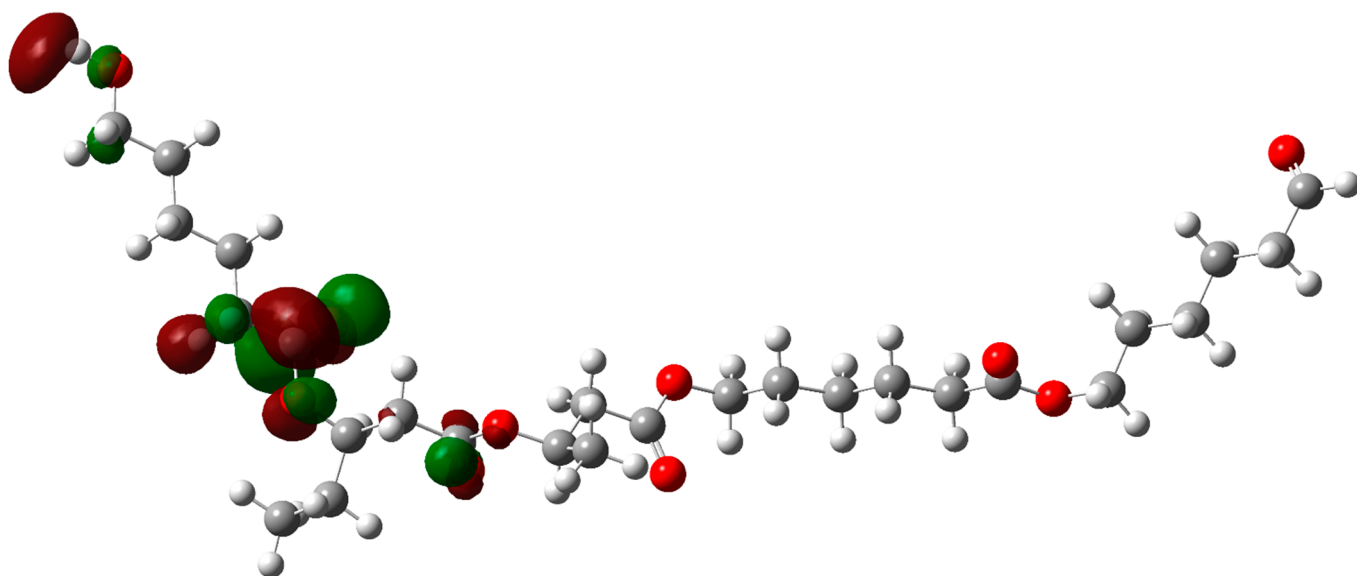


HOMO-3

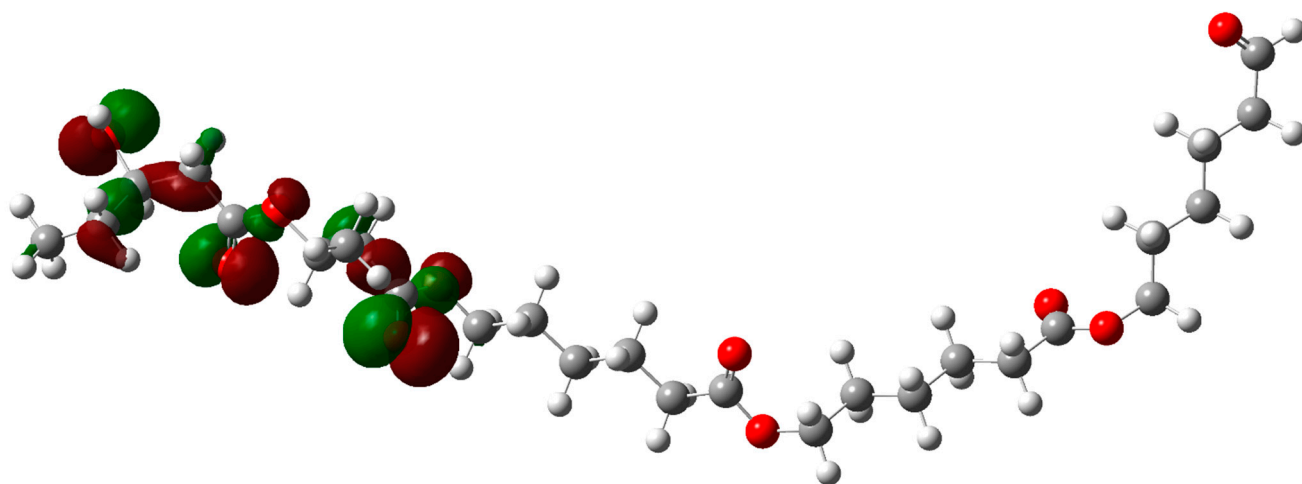
**HOMO-2****HOMO-1**

**HOMO****LUMO**

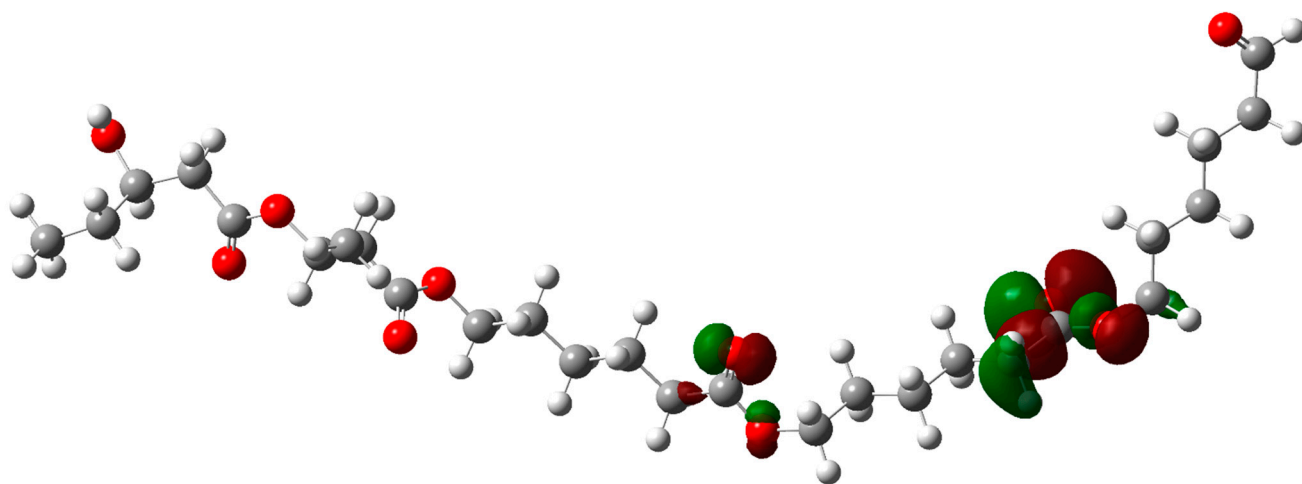
**LUMO+1****LUMO+2**

**LUMO+3****LUMO+4**

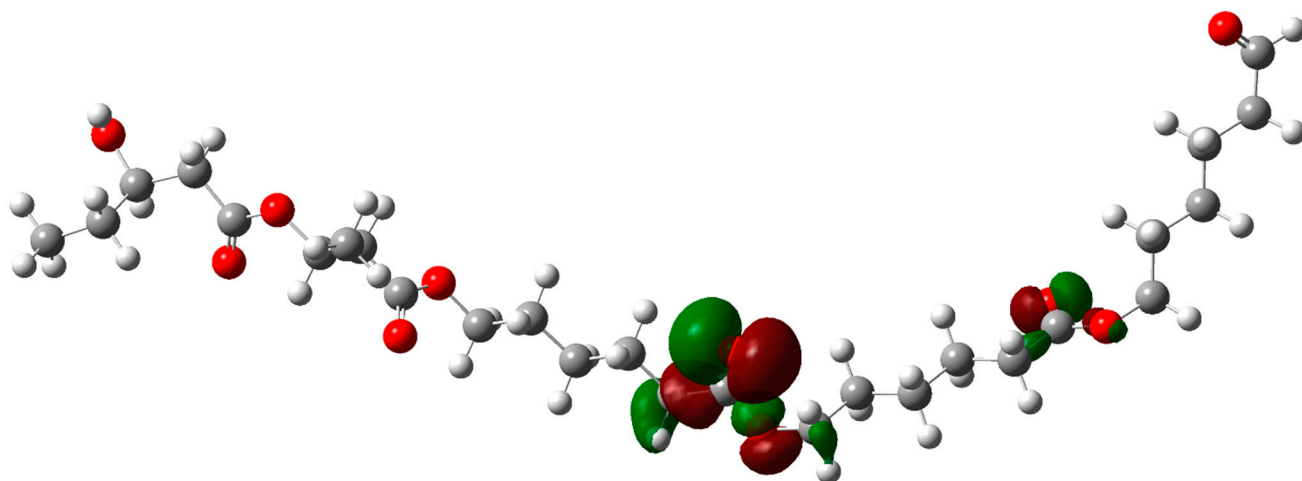
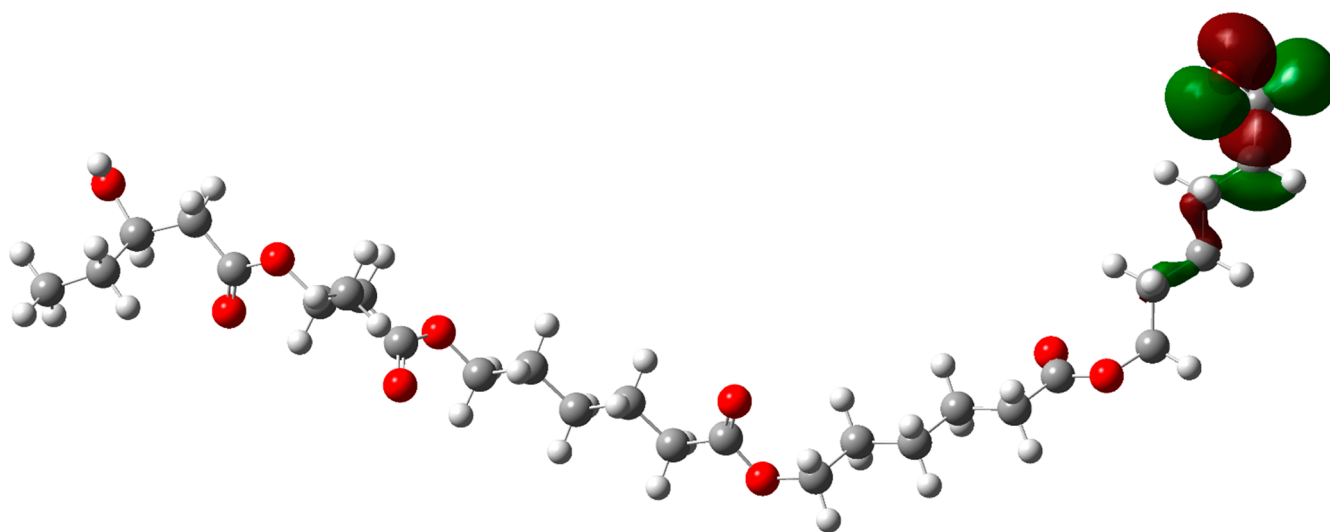
## S.2.6 MOLECULAR ORBITALS - BD



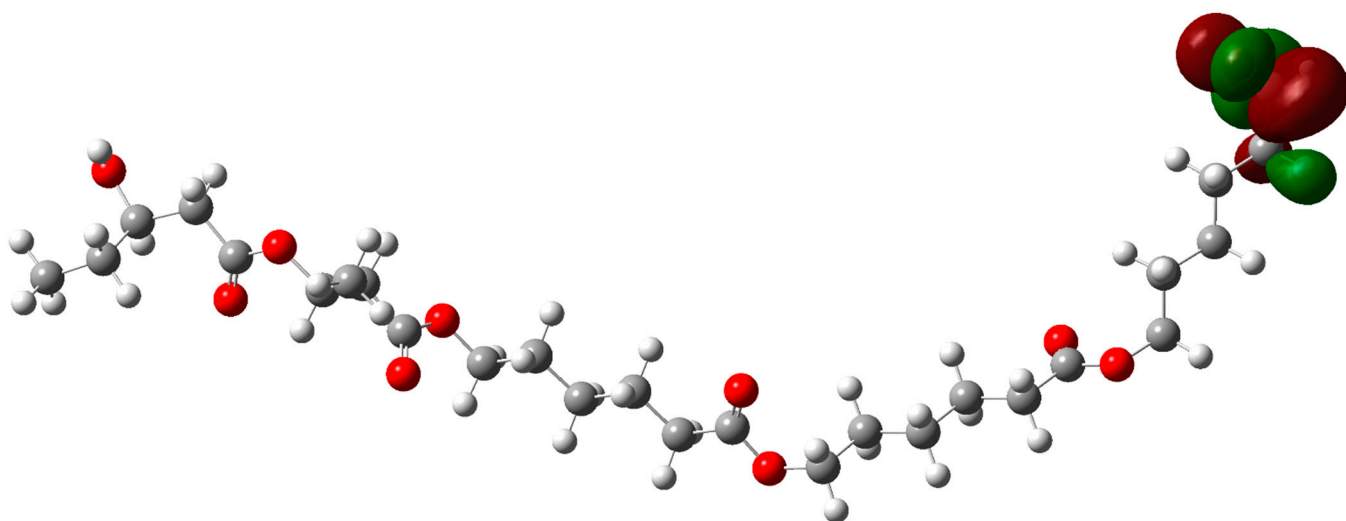
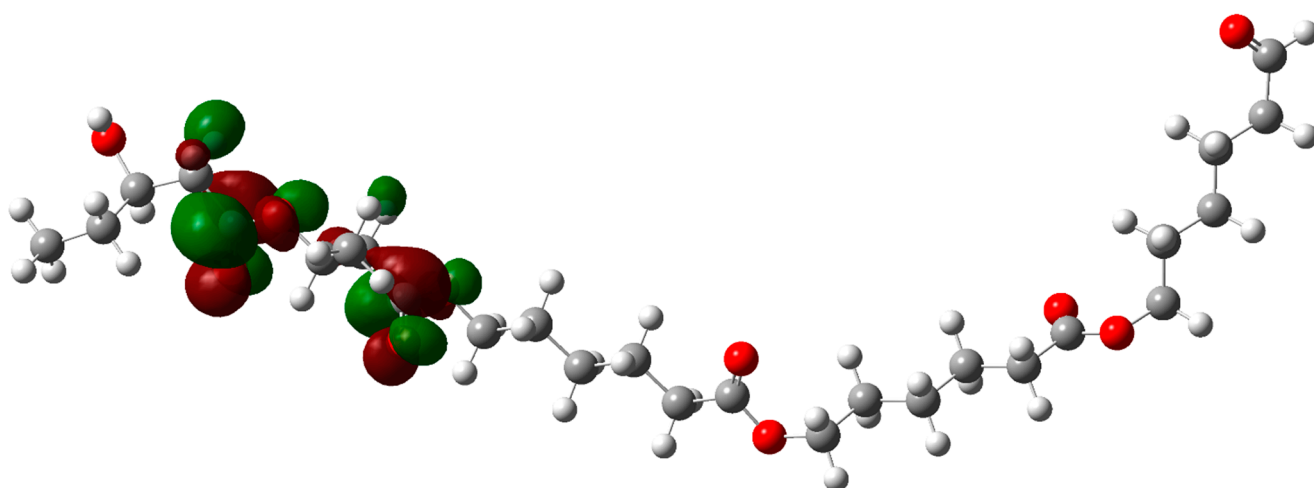
HOMO-4

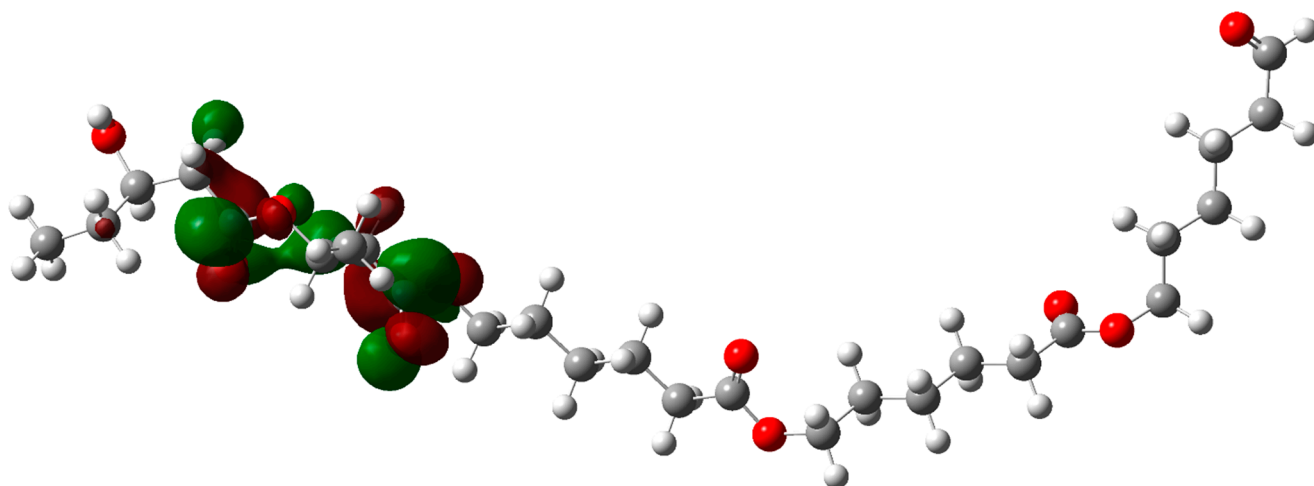
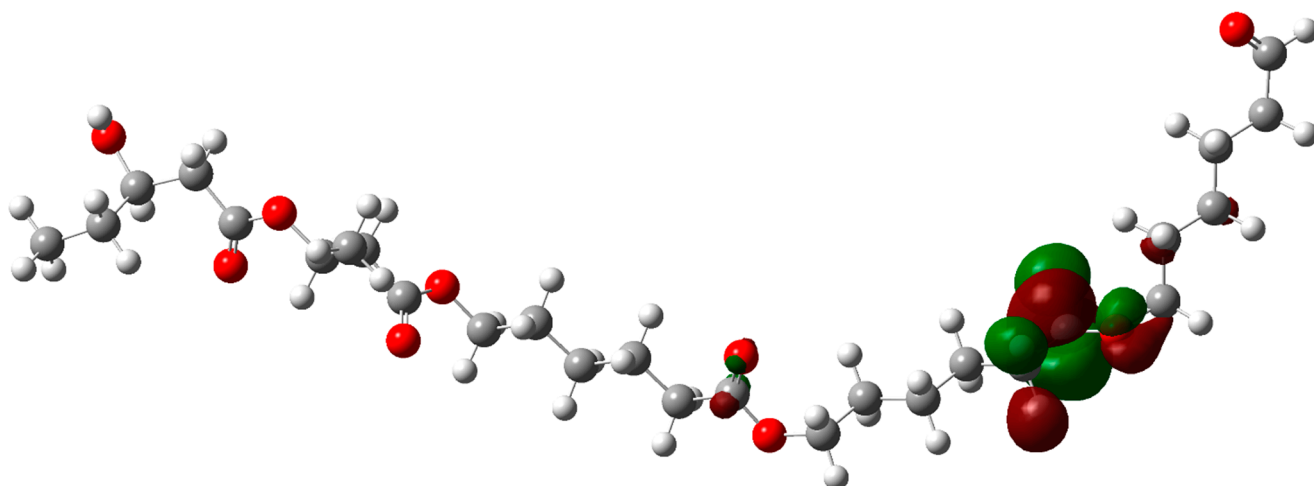
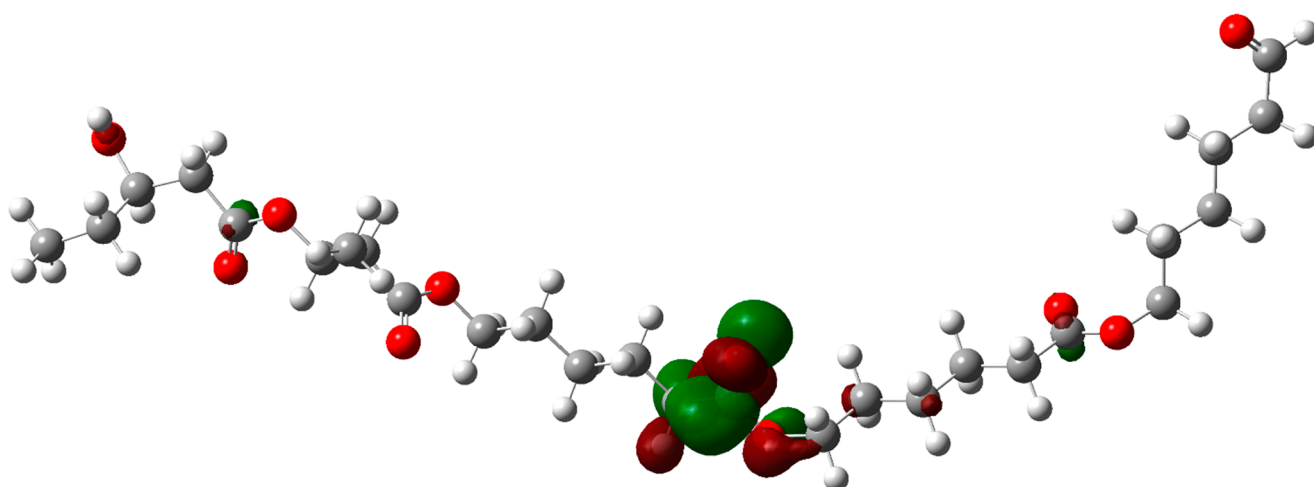


HOMO-3

**HOMO-2****HOMO-1****HOMO**



**LUMO****LUMO+1**

**LUMO+2****LUMO+3****LUMO+4**