Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Bismuth subsalicylate, a low-toxicity catalyst for the ring-opening polymerization (ROP) of L-lactide (L-LA) with aliphatic diols initiators: Synthesis, characterization, and mechanism of initiation

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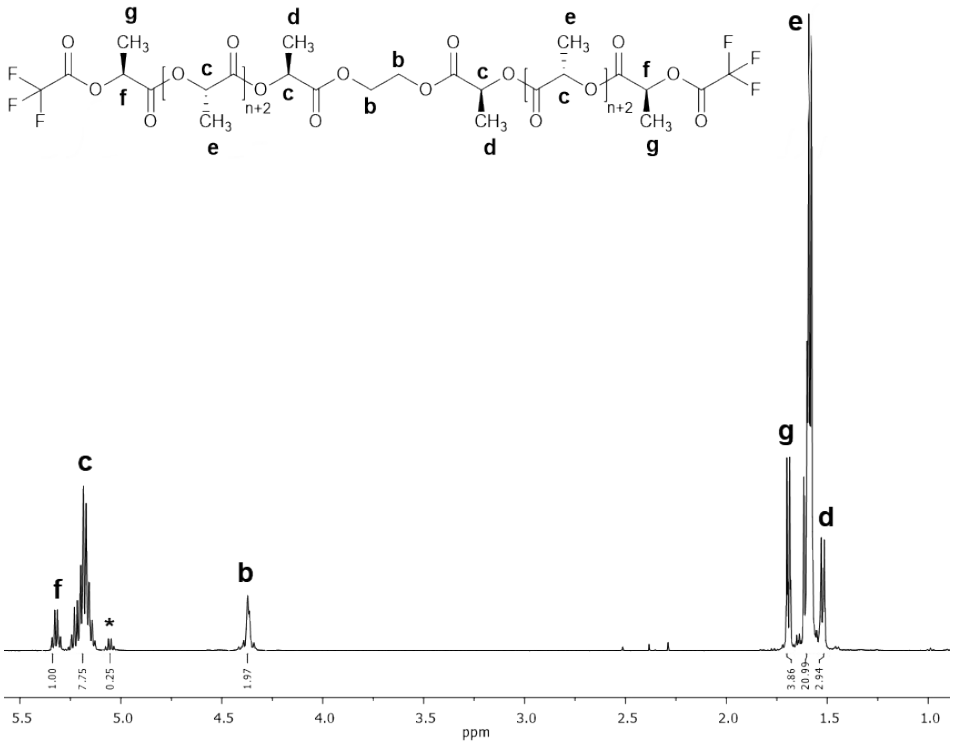

Figure S1. ^{1}H NMR spectrum of HOPLLA$_2$OH (500 MHz, $CDCl_3$) derivatized with TFAA.

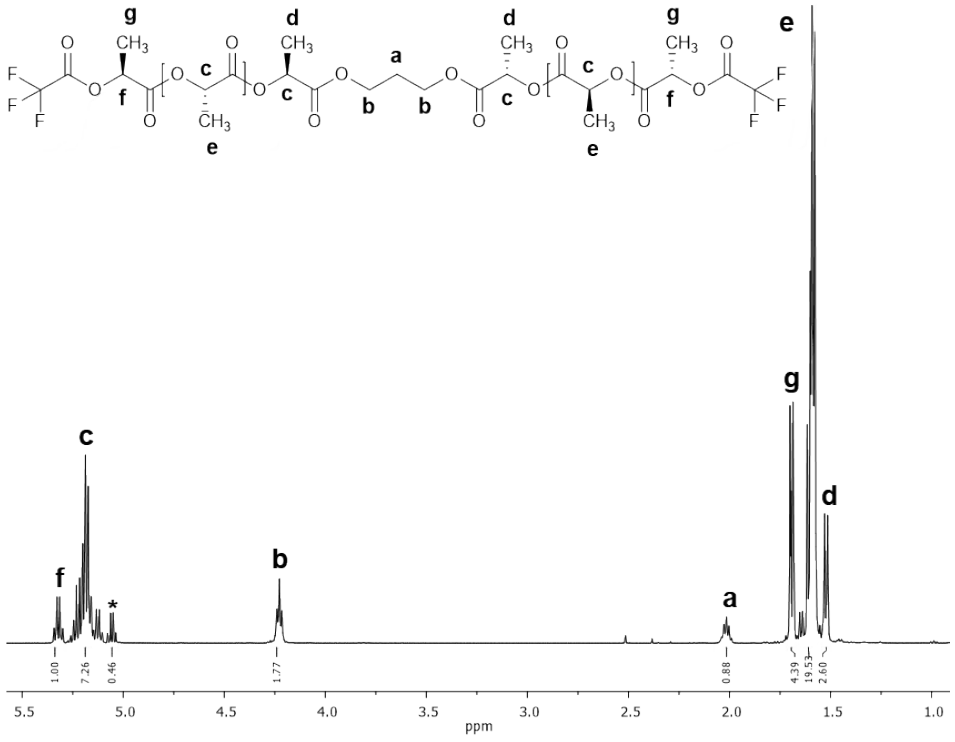

Figure S2. ^{1}H NMR spectrum of HOPLLA$_3$OH (500 MHz, $CDCl_3$) derivatized with TFAA.

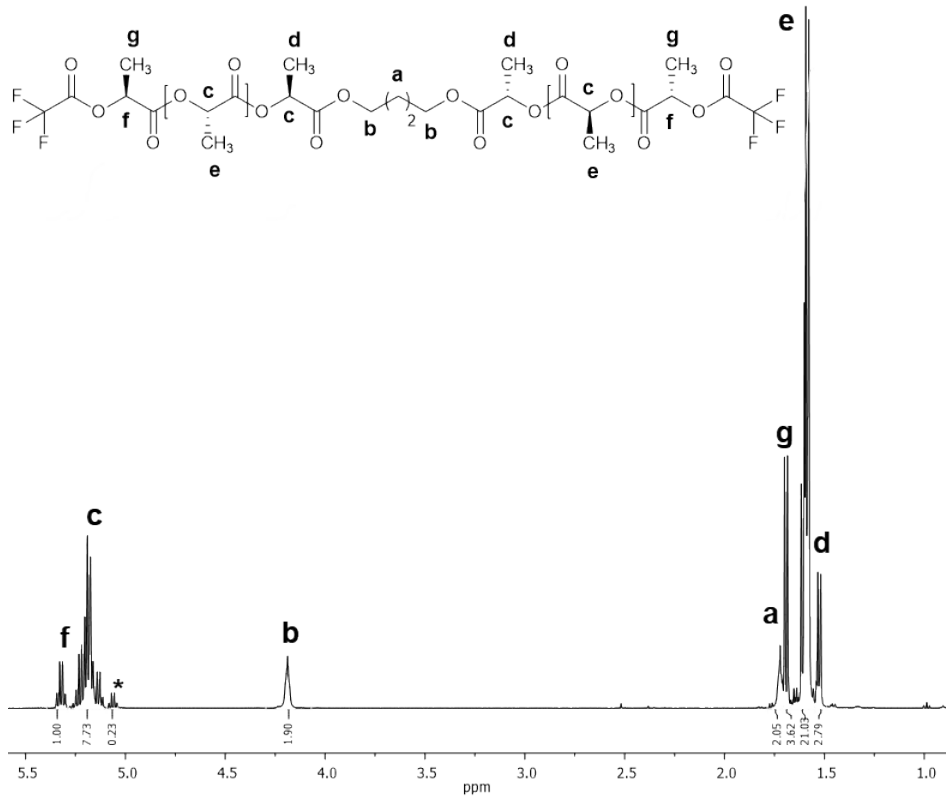

Figure S3. ^{1}H NMR spectrum of HOPLLA$_4$OH (500 MHz, $CDCl_3$) derivatized with TFAA.

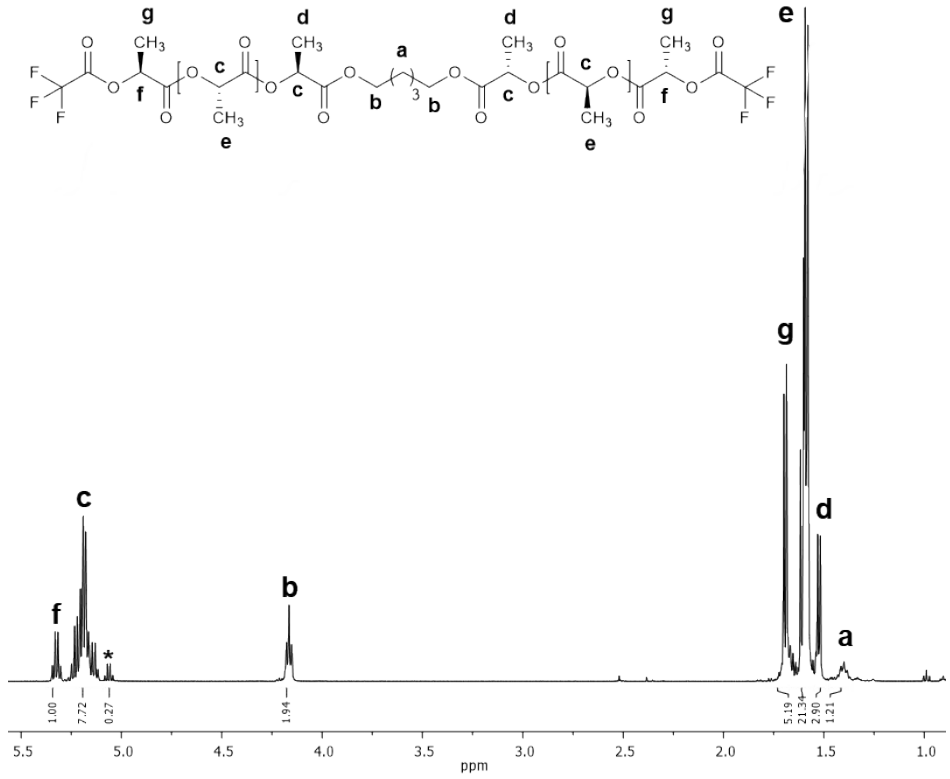

Figure S4. ^{1}H NMR spectrum of HOPLLA$_5$OH (500 MHz, $CDCl_3$) derivatized with TFAA.

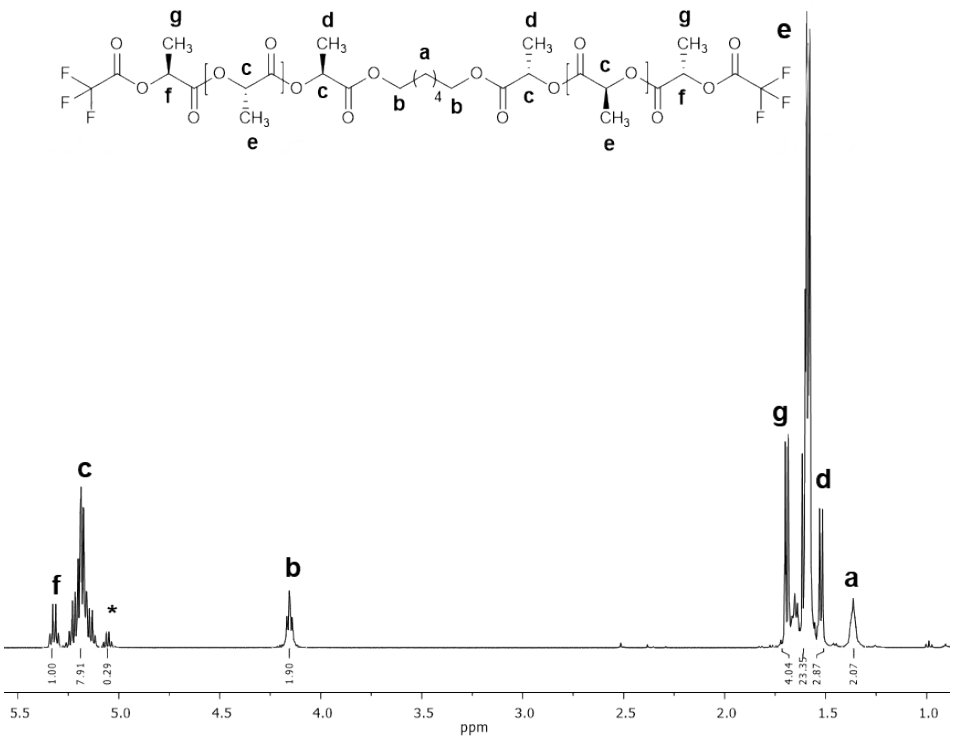

Figure S5. ^{1}H NMR spectrum of HOPLLA$_6$OH (500 MHz, $CDCl_3$) derivatized with TFAA.

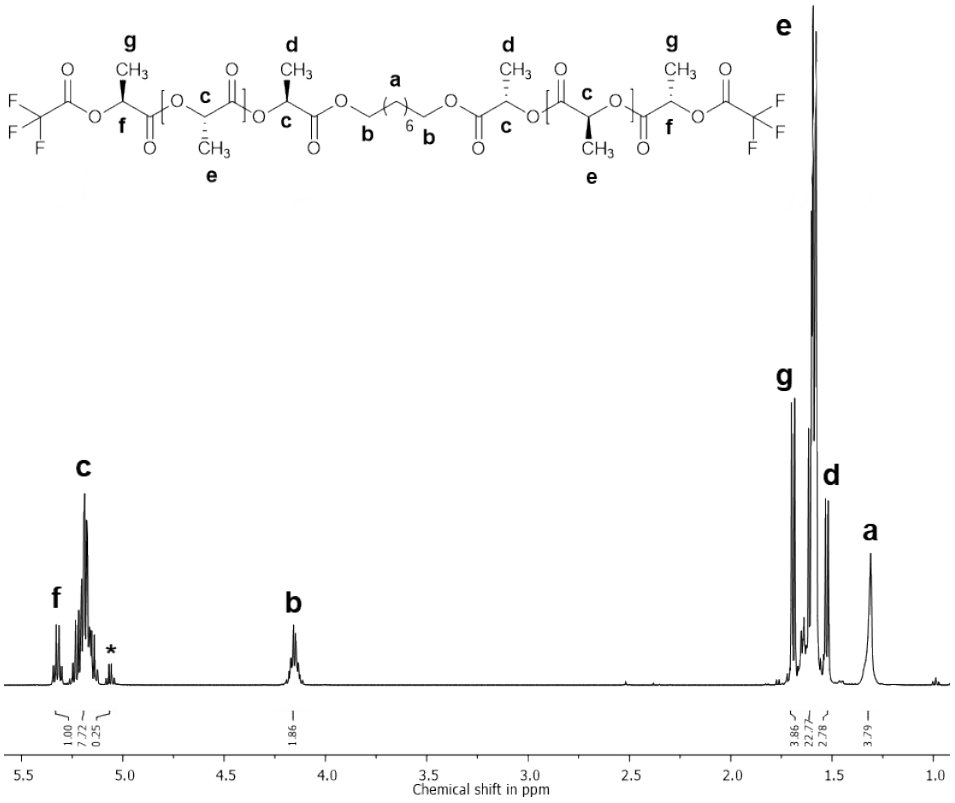

Figure S6. ^{1}H NMR spectrum of HOPLLA$_8$OH (500 MHz, $CDCl_3$) derivatized with TFAA.

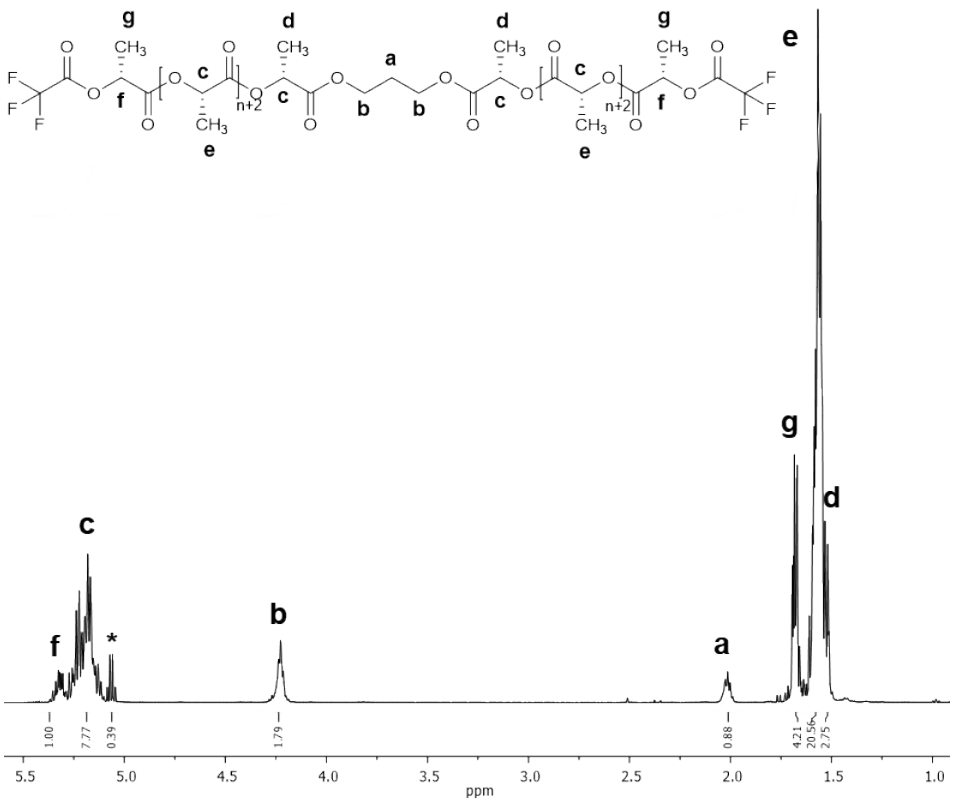

Figure S7. ^{1}H NMR spectrum of HOPDLLA$_3$OH (500 MHz, $CDCl_3$) derivatized with TFAA.

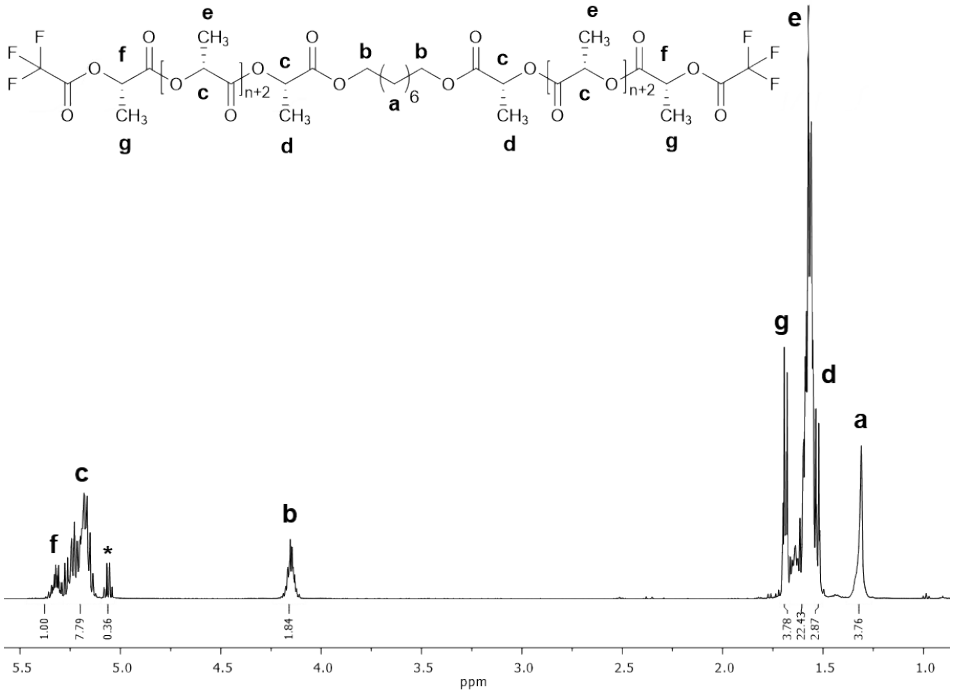

Figure S8. ^{1}H NMR spectrum of HOPDLLA$_8$OH (500 MHz, $CDCl_3$) derivatized with TFAA.

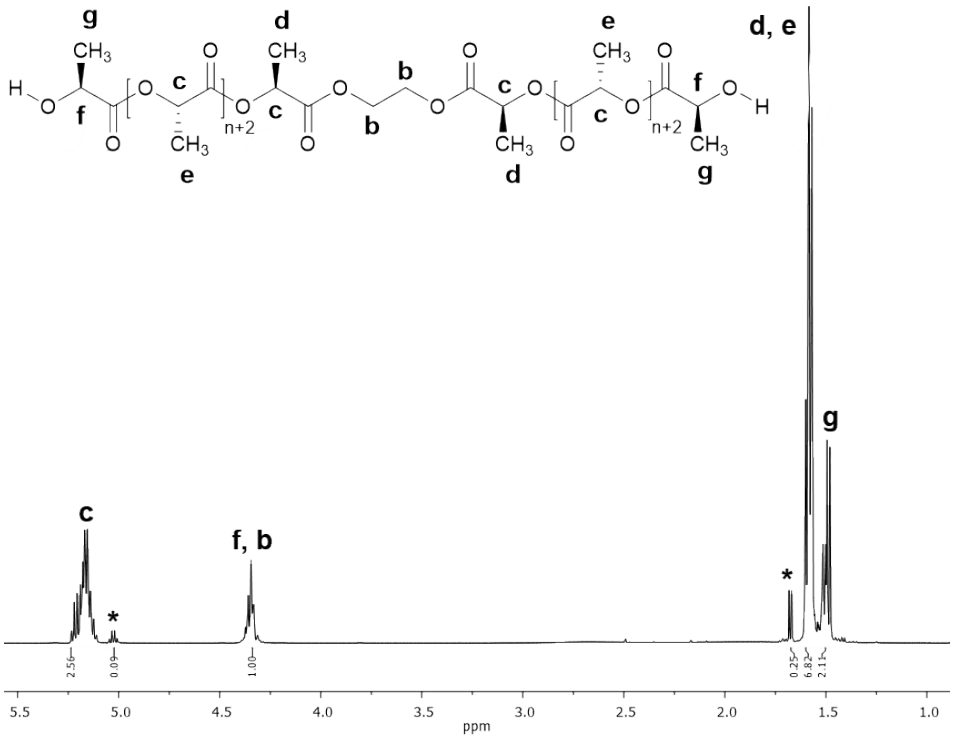

Figure S9. ^{1}H NMR spectrum of HOPLLA$_2$OH (500 MHz, CDCl$_3$).

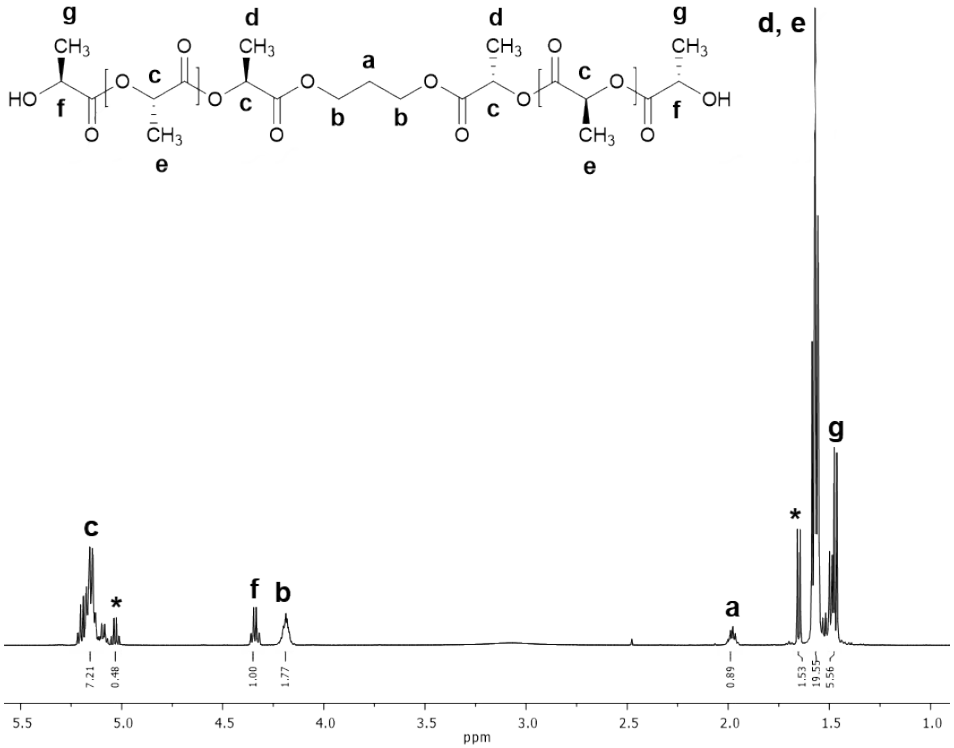

Figure S10. ^{1}H NMR spectrum of HOPLLA$_3$OH (500 MHz, CDCl$_3$).

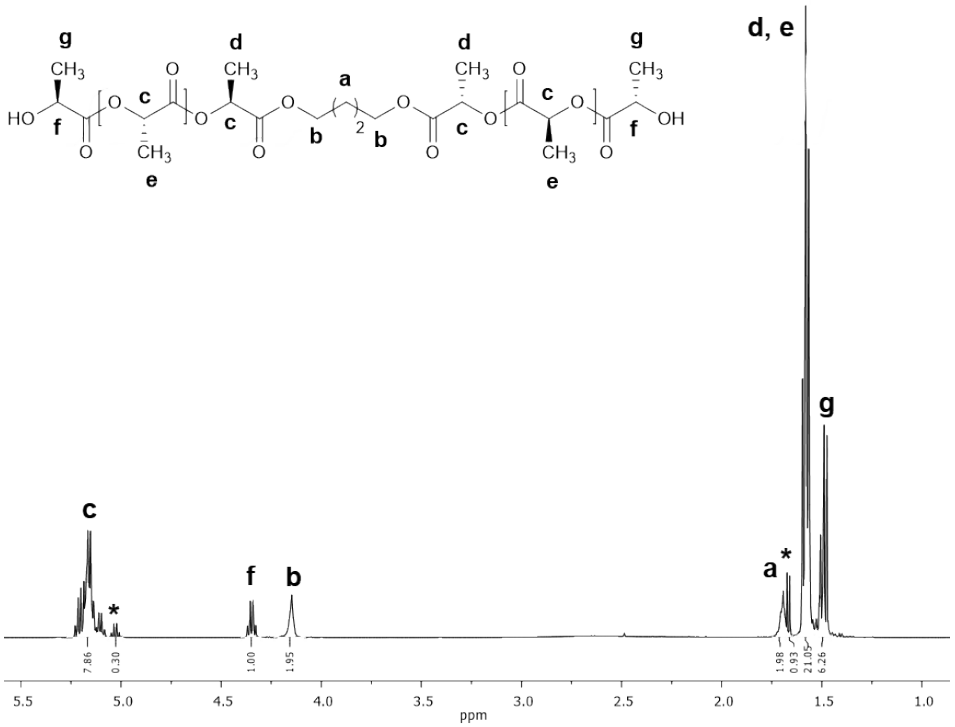

Figure S11. ^{1}H NMR spectrum of HOPLLA$_4$OH (500 MHz, $CDCl_3$).

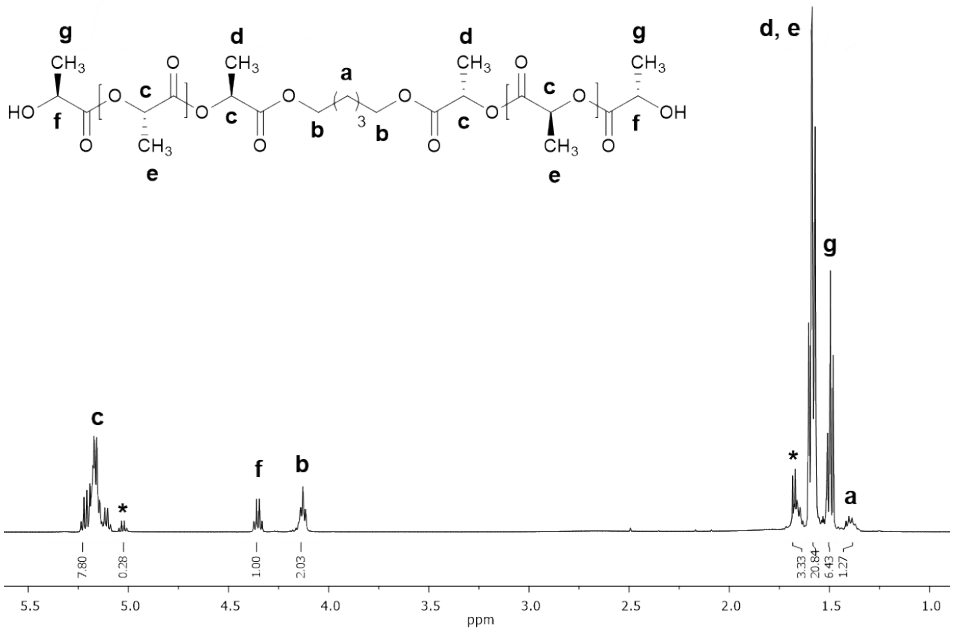

Figure S12. ^{1}H NMR spectrum of HOPLLA$_5$OH (500 MHz, $CDCl_3$).

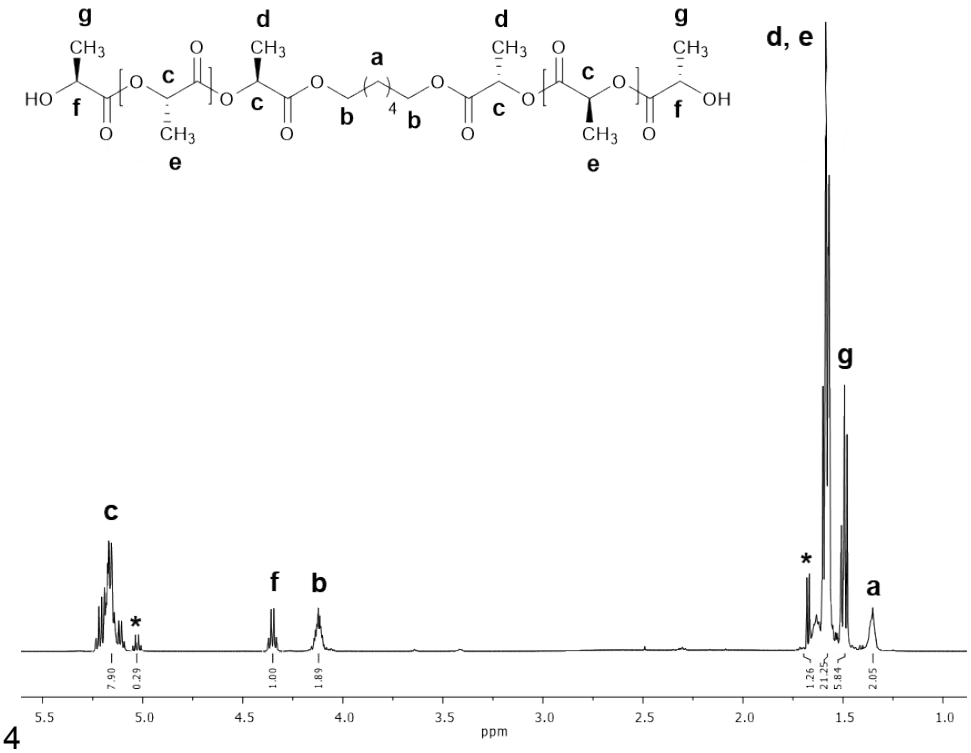

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Figure S13. ^{1}H NMR spectrum of HOPLLA$_6$OH (500 MHz, $CDCl_3$).

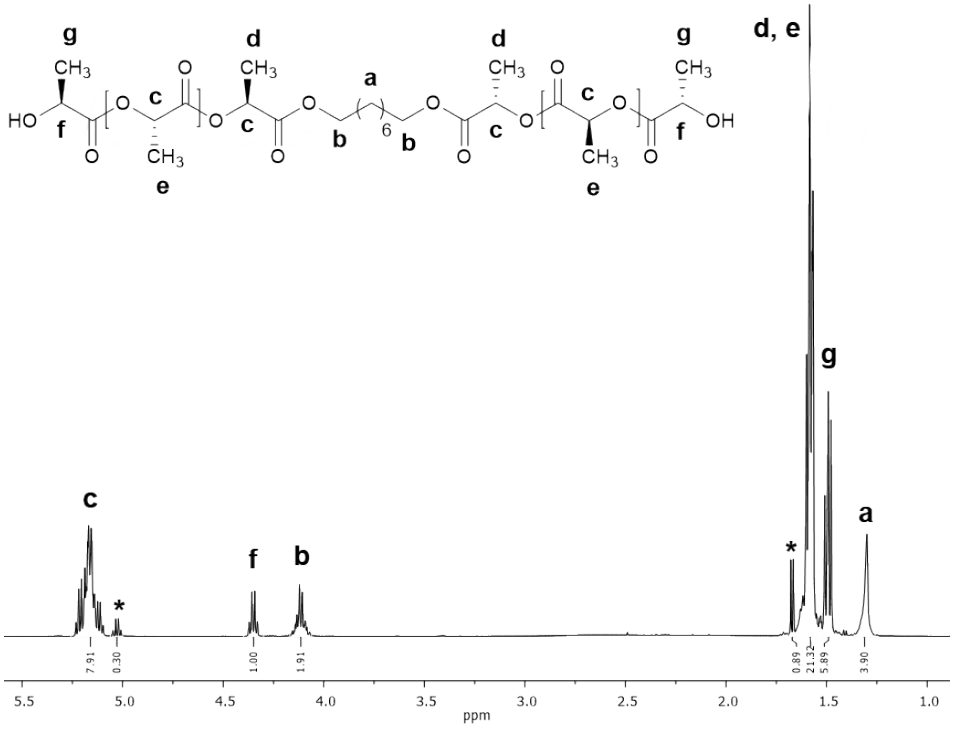


Figure S14. ^{1}H NMR spectrum of HOPLLA$_8$OH (500 MHz, $CDCl_3$).

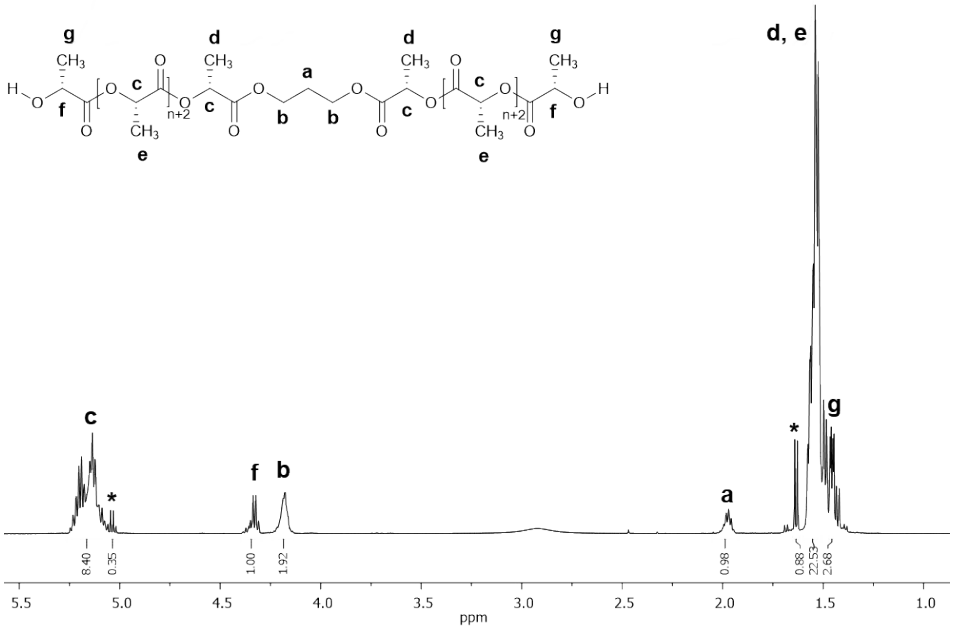


Figure S15. ^{1}H NMR spectrum of HOPDLLA$_3$OH (500 MHz, $CDCl_3$).

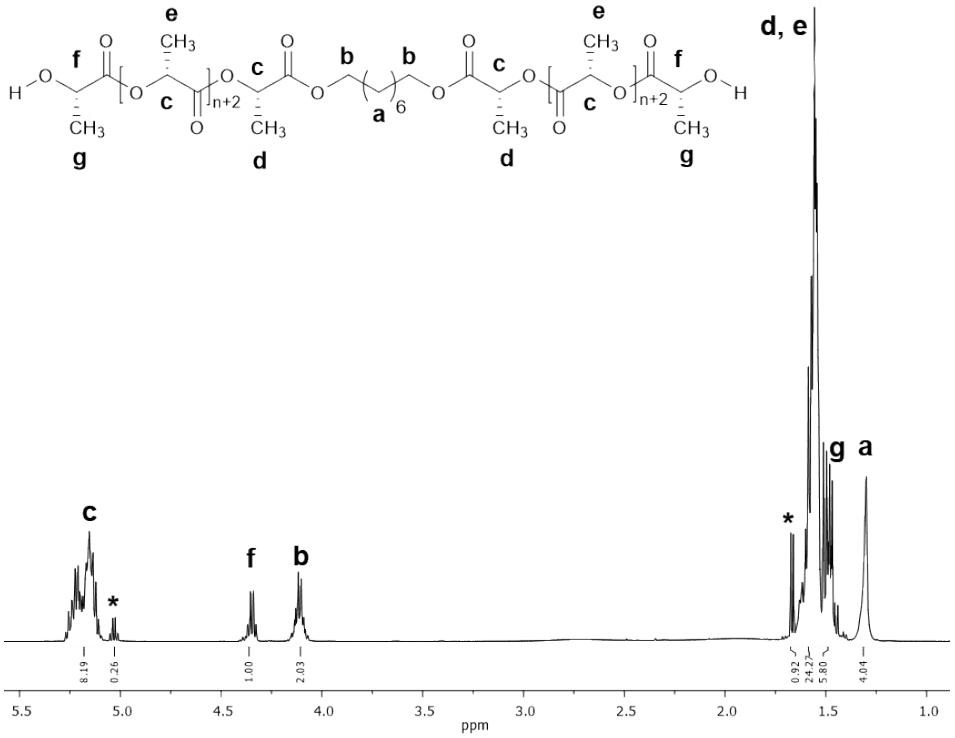


Figure S16. ^{1}H NMR spectrum of HOPDLLA$_8$OH (500 MHz, $CDCl_3$.

^{13}C NMR spectra of Macrodiols (HOPLLAOH) prepared using different types of linear alkyl diols as initiators in the ROP of L-LA.

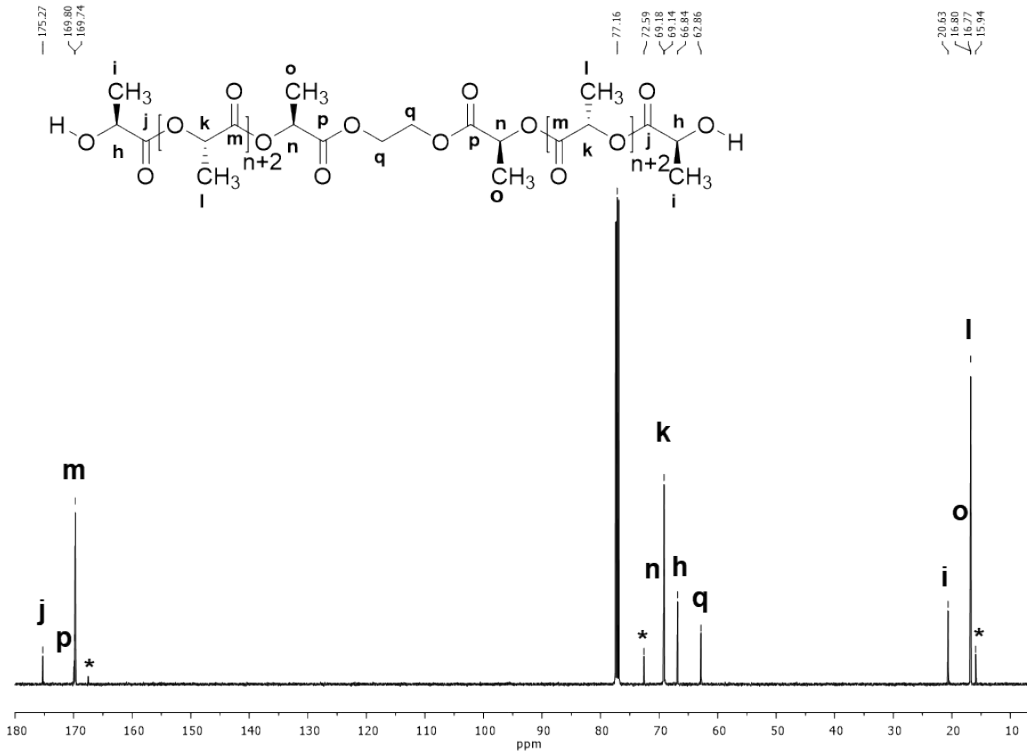


Figure S17. ^{13}C NMR spectrum of HOPLLA$_2$OH (500 MHz, $CDCl_3$).

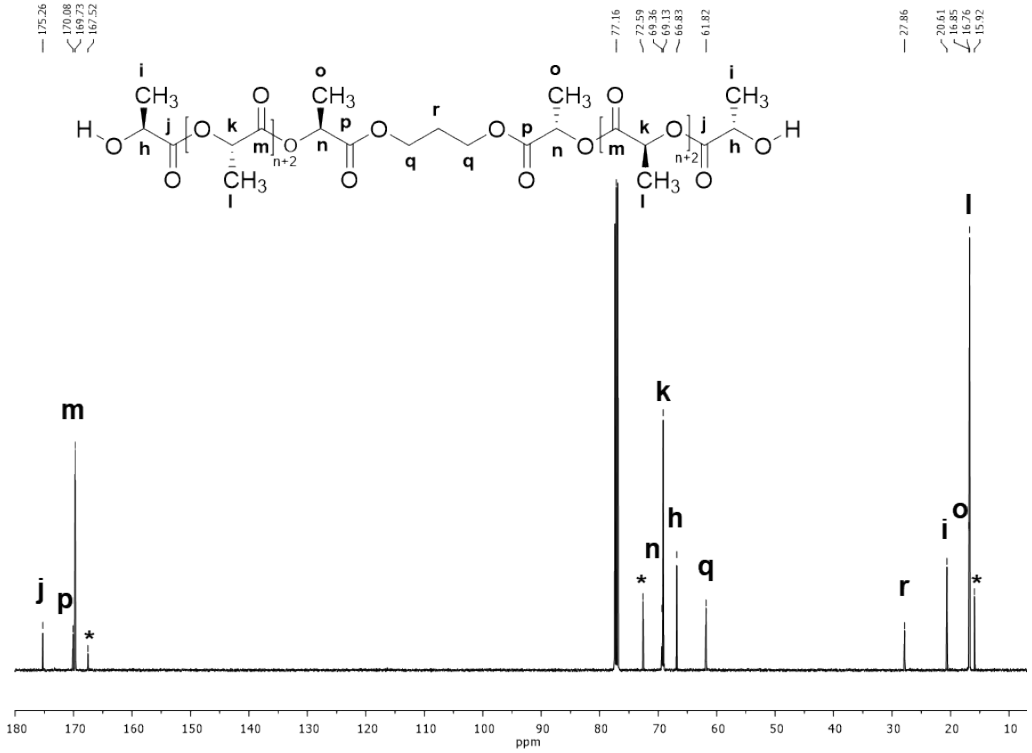


Figure S18. ^{13}C NMR spectrum of HOPLLA$_3$OH (500 MHz, $CDCl_3$).

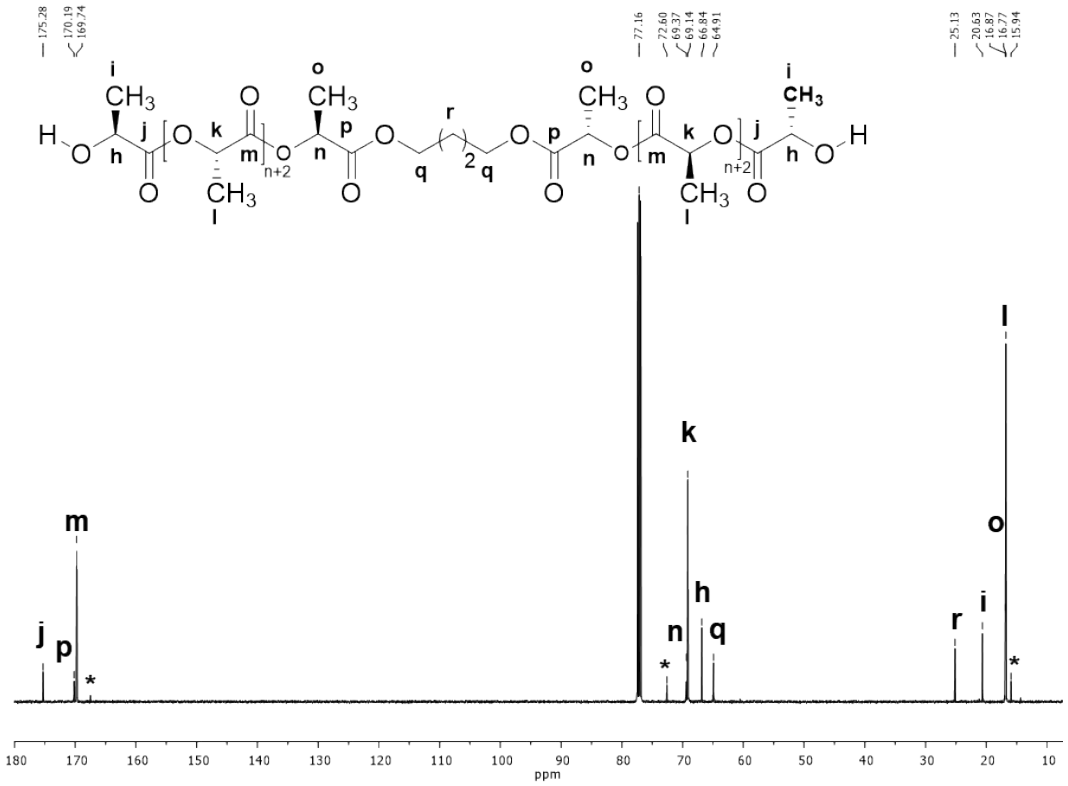


Figure S19. ^{13}C NMR spectrum of $HOPLLA_4OH$ (500 MHz, $CDCl_3$).

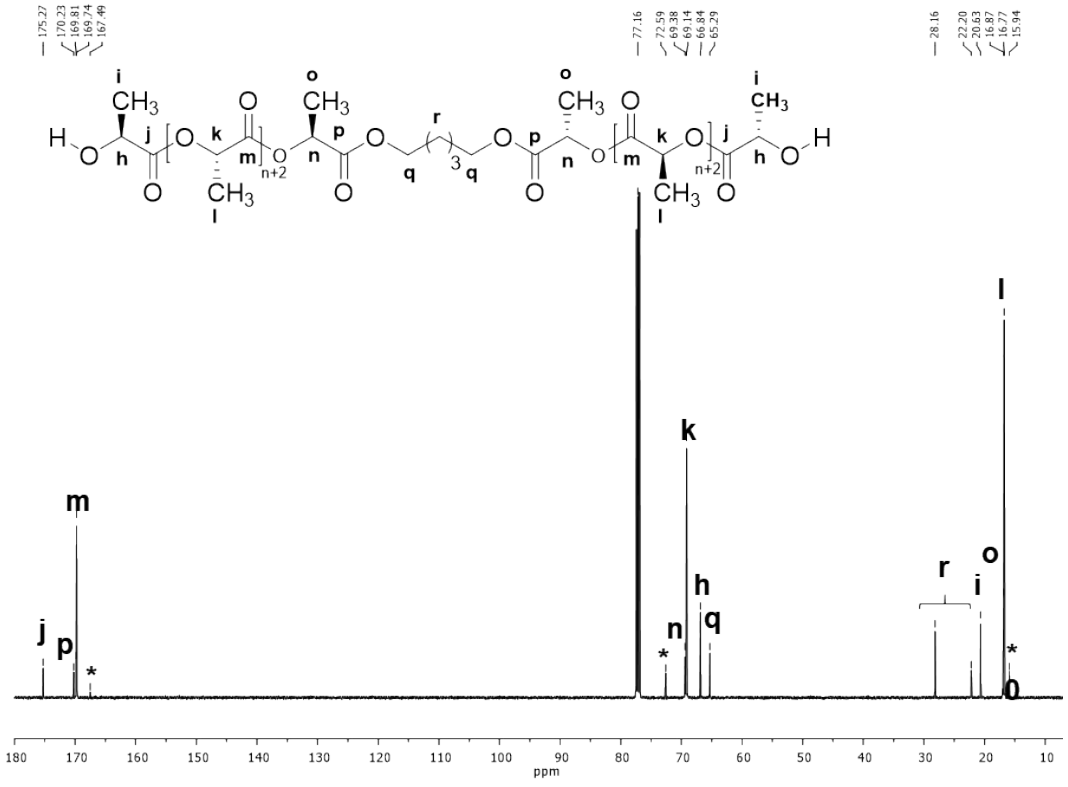


Figure S20. ^{13}C NMR spectrum of $HOPLLA_5OH$ (500 MHz, $CDCl_3$).

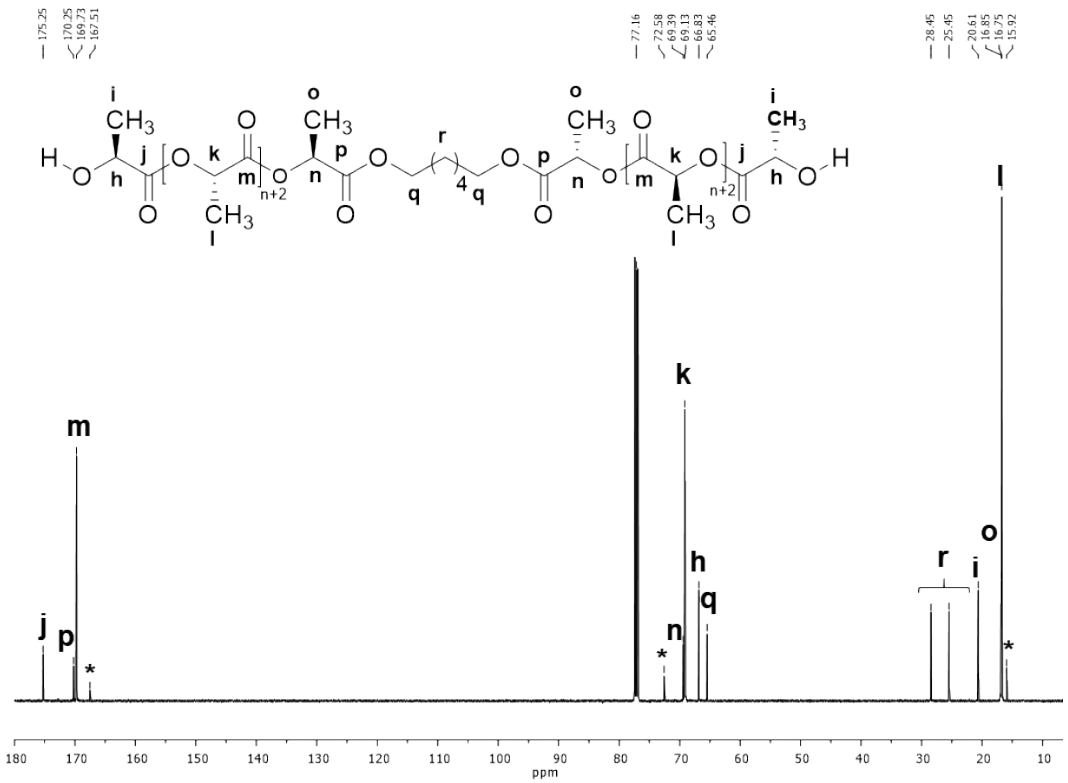


Figure S21. ^{13}C NMR spectrum of $HOPLLA_6OH$ (500 MHz, $CDCl_3$).

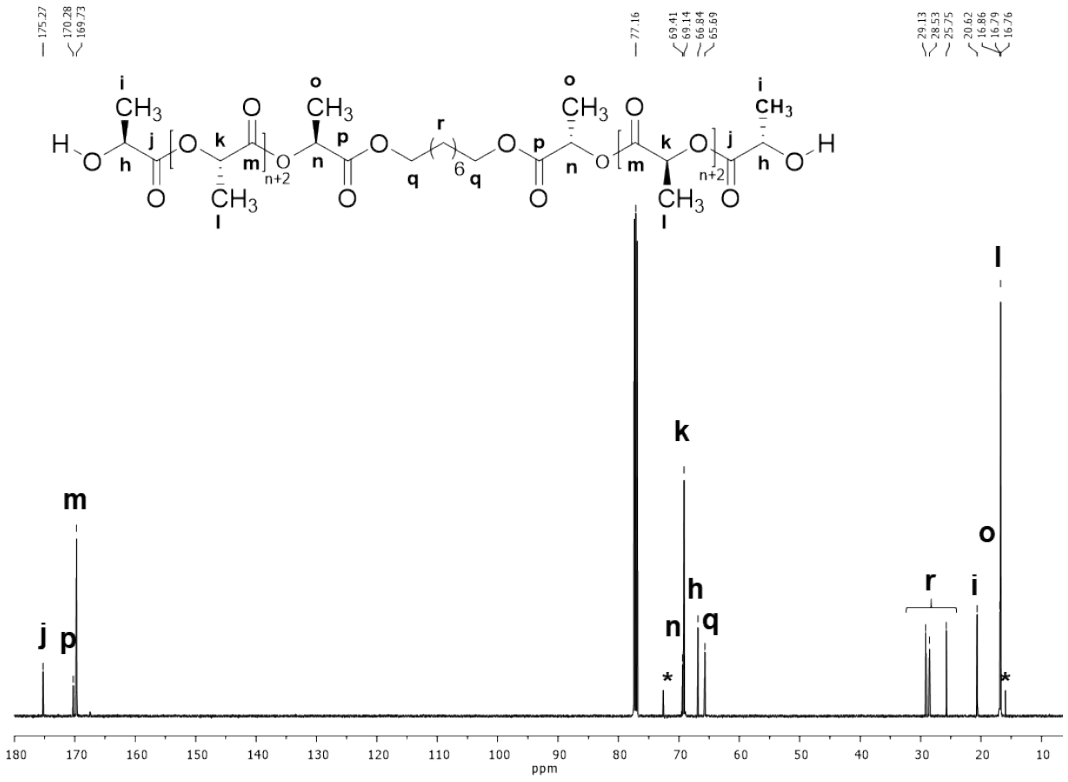


Figure S22. ^{13}C NMR spectrum of $HOPLLA_8OH$ (500 MHz, $CDCl_3$).

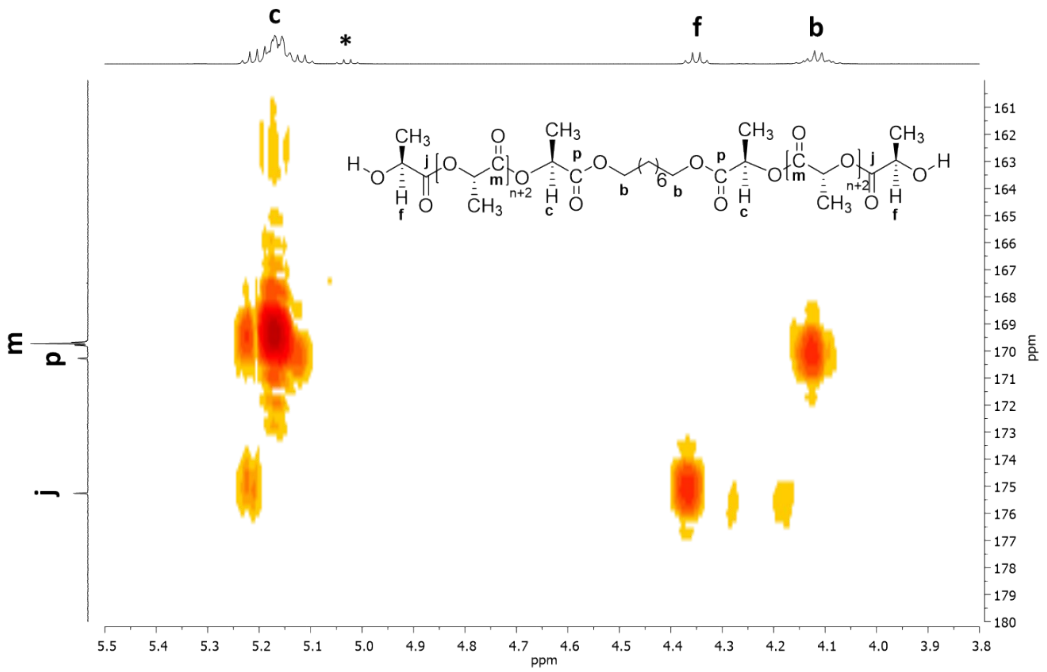


Figure S23. ^{1}H-^{13}C HMBC NMR spectrum of $HOPLLA_8OH$ (500 MHz, $CDCl_3$).

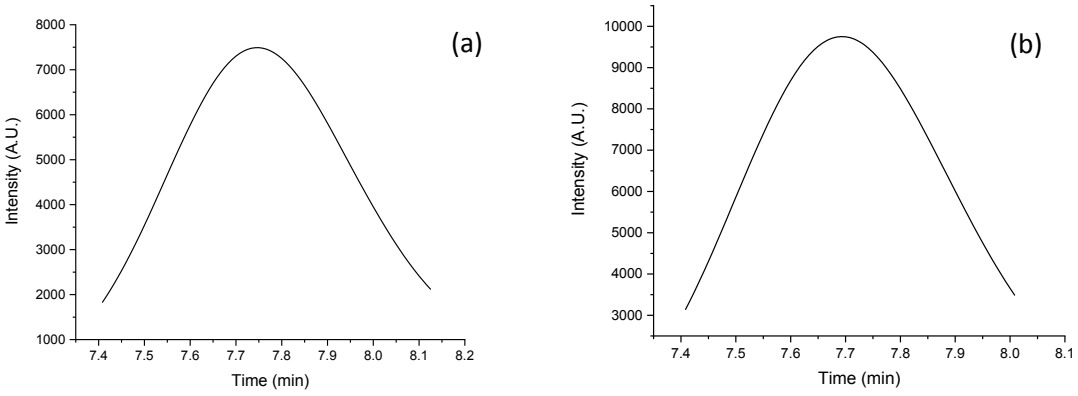


Figure S24. SEC chromatograms profile for a) $HOPLLA_2OH$, b) $HOPLLA_8OH$.

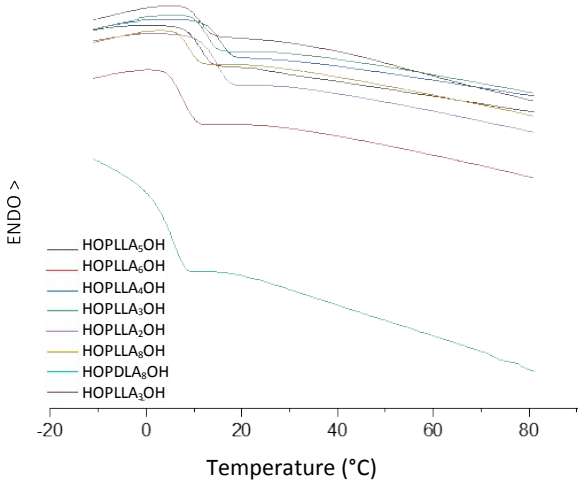
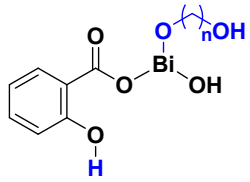
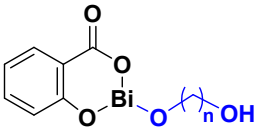


Figure S25. DSC thermograms of the different poly(L-lactide) macrodiols (HOPLLAOH) (all samples).

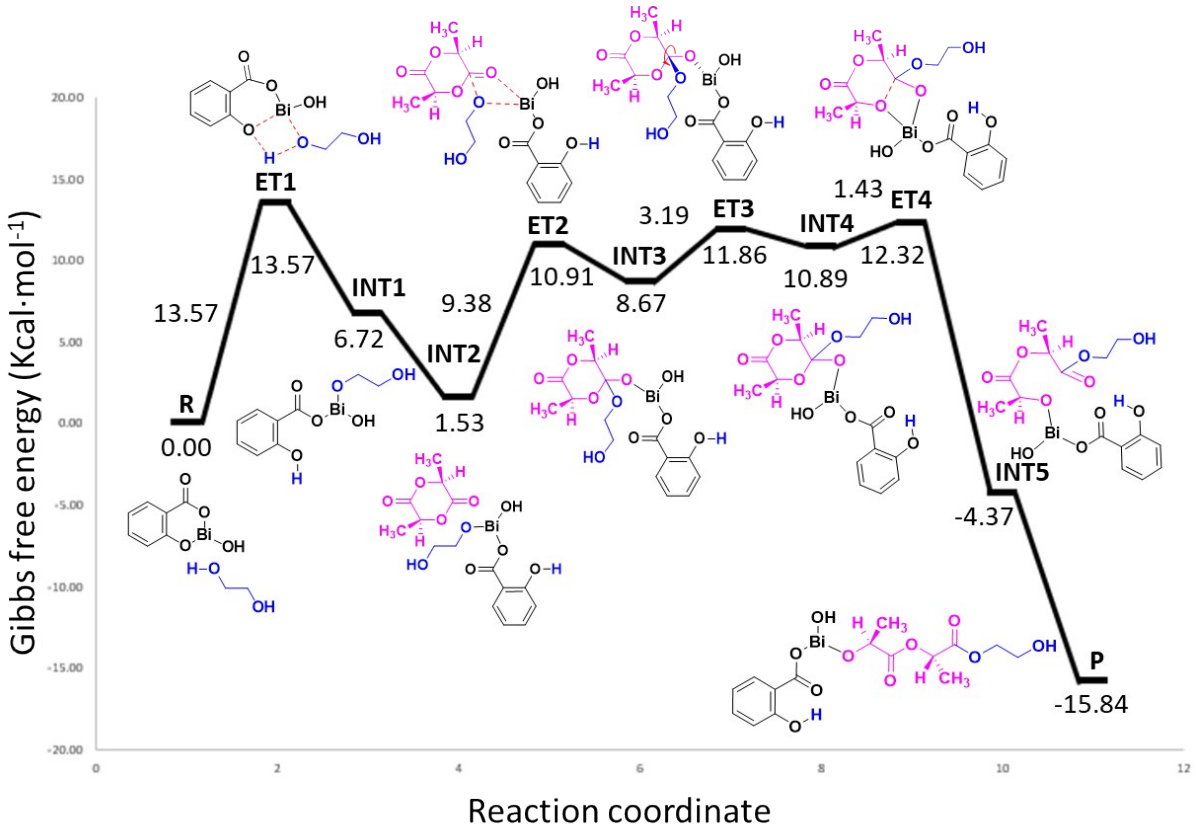
Computational Details

Geometry optimizations were performed in the gas phase using the hybrid PBE0 density functional which mixes 25% of HF exchange in its formulation.[1] Grimme's D3 method[2] for incorporating dispersion effects was explicitly included in the geometry optimizations. The electronic configurations of light atoms such as hydrogen and carbon were described with Pople's double-ζ 6-31G(d) basis set containing one polarization function. On the other hand, the pseudopotential LANL2DZ containing a polarization function was used for bismuth.[3] Thus, this level of theory to show the energy values can be written as D3-PBE0/[6-31G(d),LANL2DZ].

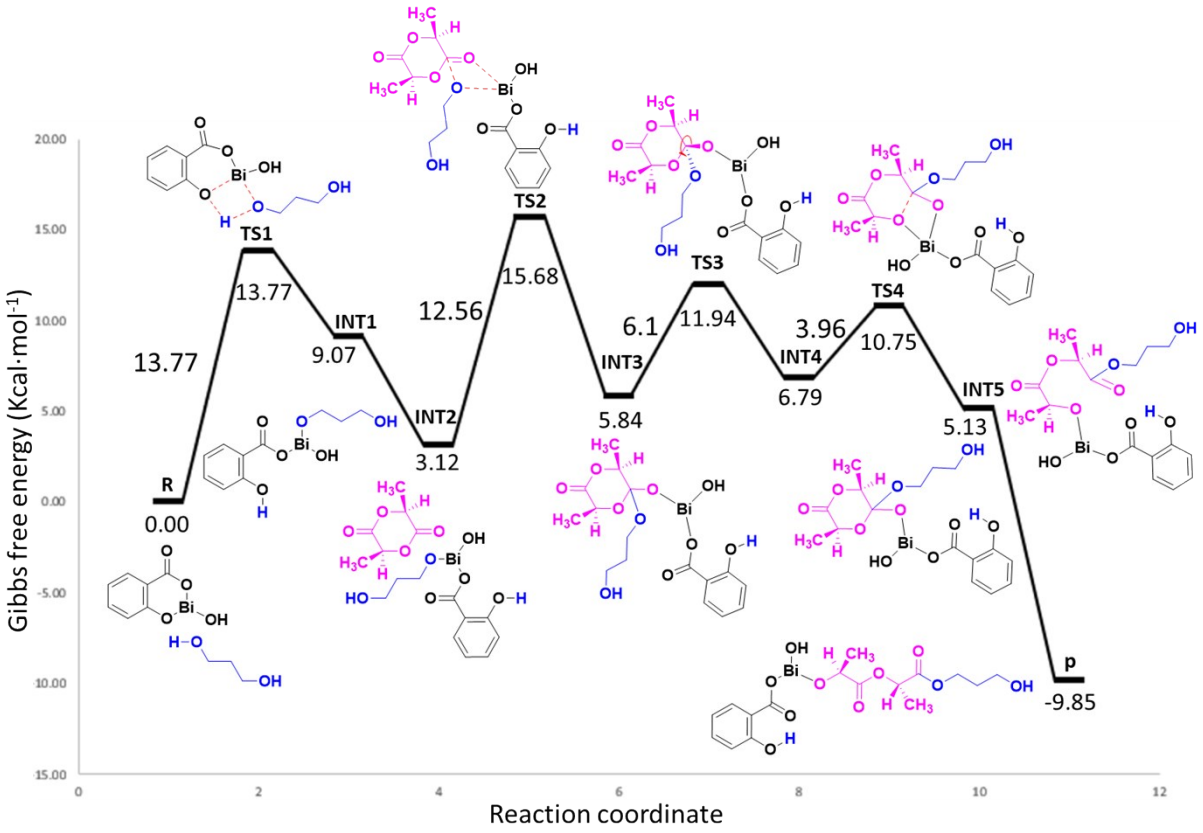
Table S1. Total energy barrier using the following diols as initiators of the ROP of L-Lactide catalyst with bismuth subsalicylate.

Alkoxides	**Total energy barrier (Kcal/mol) with:**			
	ethylen glycol	**1,3-propanediol**	**1,4-butanediol**	**1,5-pentanediol**
 **(1)**	13.57	15.68	17.35	20.52
 **(2)**	46.18	46.39	46.57	46.97

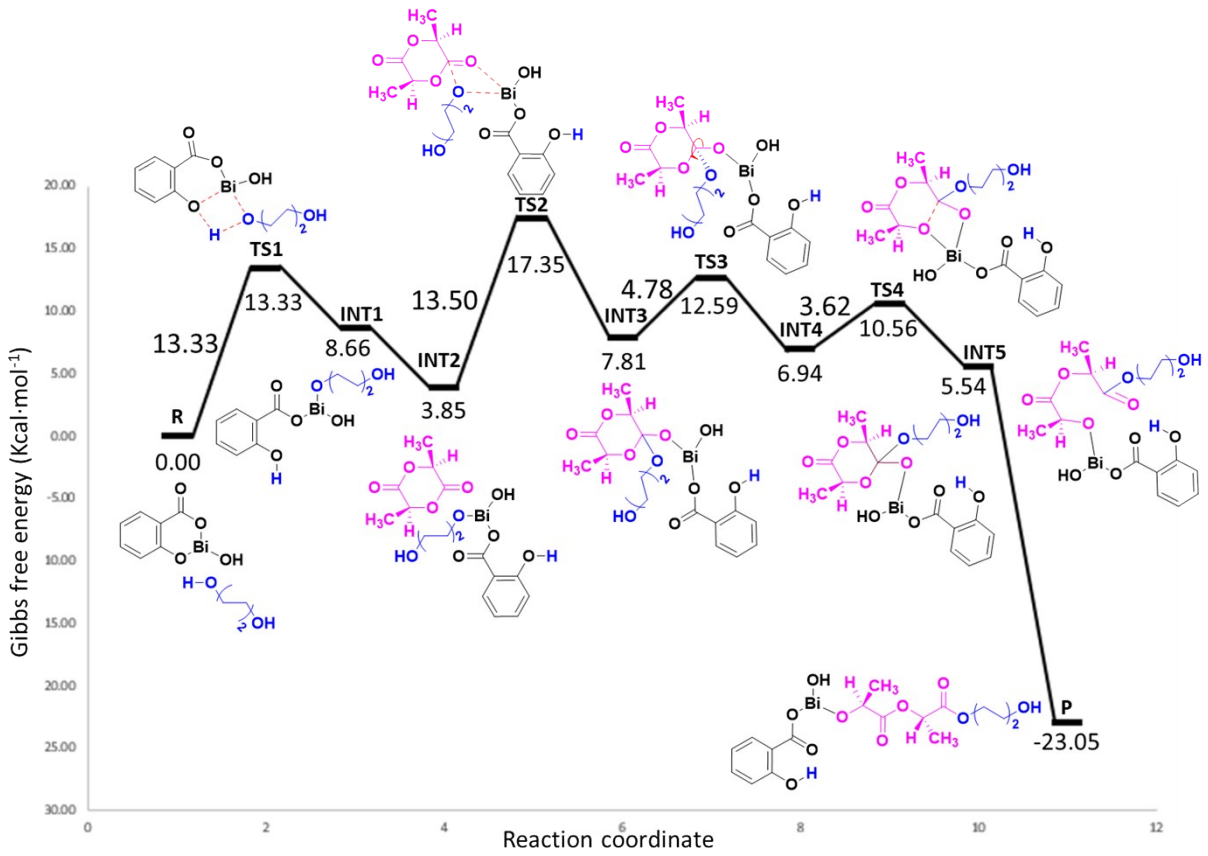
Note of Table S1: There is a trend, as the aliphatic chain of the diol used increases the total barrier in the two cases. However, the difference in energies obtained with alkoxide (2) is more significant. Therefore, the alkoxide (1) is the most reactive to carry out the polymerization of L-lactide.



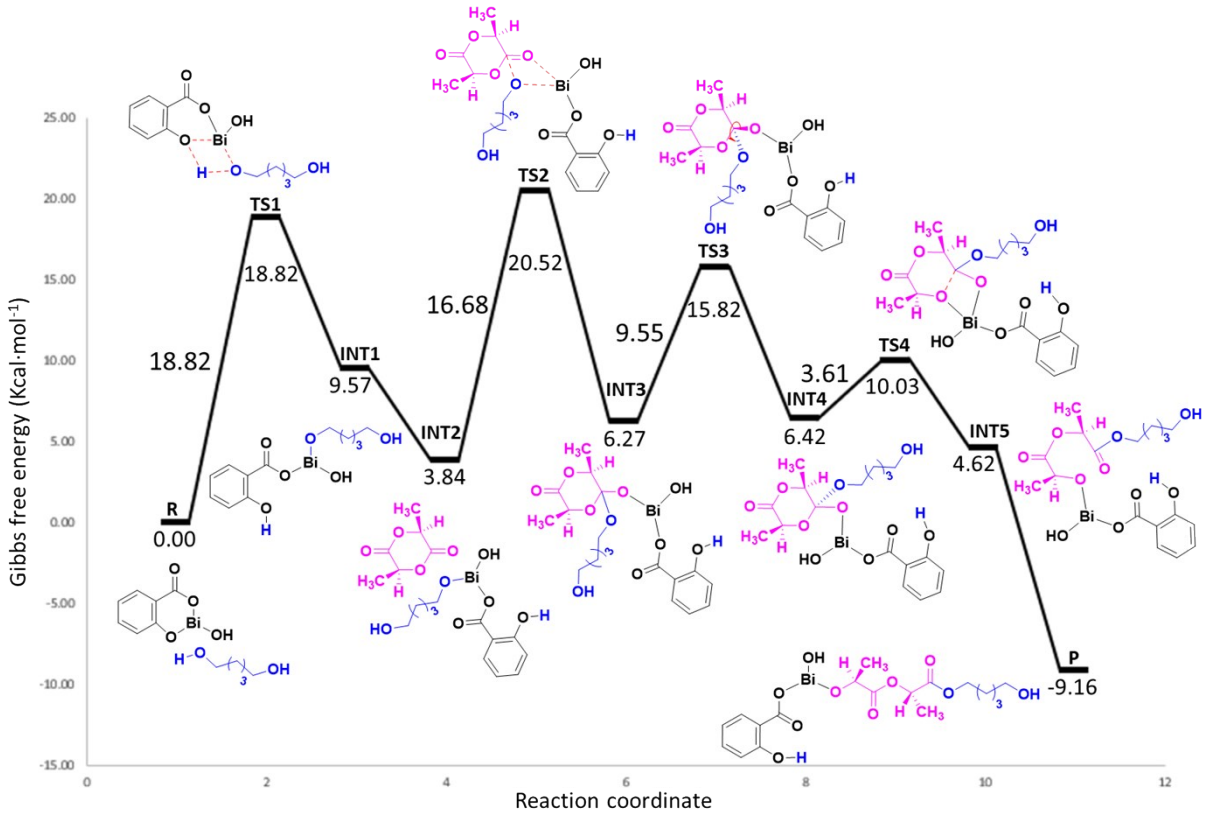
Scheme S1. Energy profile in gas phase at 140°C of the ROP of the L-lactide initiated with ethyleneglycol using bismuth subsalicylate as catalyst.



Scheme S2. Energy profile in gas phase at 140°C of the ROP of the L-lactide initiated with 1,3-propanediol using bismuth subsalicylate as catalyst.



Scheme S3. Energy profile in gas phase at 140°C of the ROP of the L-lactide initiated with 1,4-butanediol using bismuth subsalicylate as catalyst.



Scheme S4. Energy profile in gas phase at 140°C of the ROP of the L-lactide initiated with 1,5-pentanediol using bismuth subsalicylate as catalyst.

Table S2. Cartesian coordinates (xyz format) of the optimized geometries for all the species involved in the energy profile of the **Scheme S1** calculated at the D3-PBE0/[6-31G(d), LANL2DZ] level.

R

E(scf) = -805.501842111 a.u.

C	1.087312	1.204866	-0.876220
C	2.412341	-0.421903	0.599567
C	2.359273	0.634415	-0.318417
C	3.562087	1.191432	-0.764298
H	3.509277	2.035836	-1.444958
C	4.786172	0.670812	-0.364404
C	4.821075	-0.408311	0.516577
C	3.635913	-0.943360	1.009194
H	5.709324	1.104447	-0.737690
H	5.772634	-0.823373	0.837427
H	3.635519	-1.759602	1.725160
O	0.960047	2.400942	-1.030001
O	0.180040	0.326700	-1.297311
O	1.270789	-0.977369	1.138909
Bi	-1.050607	-0.959915	-0.226904
O	-2.763332	-0.191753	-0.905310
H	-2.746495	0.791217	-0.870434
C	-1.882080	2.499761	1.030649
C	-1.828838	1.229768	1.877836
H	-2.192322	3.339936	1.669119
H	-0.890714	2.724655	0.628608
H	-1.528659	1.508355	2.897453
H	-2.844259	0.805768	1.949245
O	-2.748089	2.418893	-0.096872
O	-0.902791	0.258482	1.449830
H	-3.658323	2.402055	0.230567
H	0.741543	-0.288384	1.611669

ET1

E(scf) = -805.490134714 a.u.

C	-1.311543	-1.538855	0.963805
C	-1.915335	0.231590	-0.827183
C	-2.251266	-0.629989	0.233102
C	-3.582821	-0.654486	0.673042
H	-3.819196	-1.341598	1.479052
C	-4.554280	0.162040	0.117490
C	-4.202616	1.028424	-0.918587
C	-2.897775	1.056840	-1.389310
H	-5.575343	0.127330	0.485341
H	-4.950599	1.674492	-1.373125
H	-2.613168	1.700818	-2.216899
O	-1.734859	-2.396290	1.706858
O	0.004784	-1.363975	0.842559
O	-0.672887	0.290809	-1.366155
Bi	1.361362	-0.539021	-0.476767
O	2.471495	-0.112228	1.151129
H	1.836498	0.149147	1.853911
C	0.271875	2.642532	1.377021
C	1.274563	2.640972	0.230651
H	0.285106	3.634528	1.854444
H	-0.739450	2.485835	0.984244
H	1.221504	3.602317	-0.298243
H	2.291495	2.522584	0.625889
O	0.491875	1.622251	2.337068
O	1.060273	1.622285	-0.727013
H	1.149789	1.954614	2.971796
H	-0.029914	1.291432	-1.110540

INT1

E(scf) = -805.514760750 a.u.

C	-2.140762	-1.572894	0.097835
C	-1.743611	0.941826	-0.428867
C	-2.527580	-0.121915	0.074993
C	-3.813150	0.166512	0.559174

INT2

E(scf) = -1339.28768843 a.u.

C	2.779911	2.329077	0.648331
C	2.819930	2.269953	-0.872205
C	3.143806	-0.081269	-0.662338
C	4.098411	0.351185	0.444052

H	-4.395301	-0.675811	0.919730
C	-4.329580	1.450477	0.564569
C	-3.552985	2.493115	0.055512
C	-2.282510	2.238955	-0.432936
H	-5.327584	1.639904	0.948342
H	-3.939901	3.509062	0.039329
H	-1.669746	3.038182	-0.841321
O	-2.970825	-2.432031	0.312072
O	-0.867350	-1.894378	-0.113390
O	-0.505578	0.813673	-0.947104
Bi	0.817061	-0.667611	-0.268630
O	0.672064	-0.054426	1.655460
H	-0.253132	-0.076614	1.944692
C	3.308882	1.285793	1.163923
C	2.982740	2.159430	-0.036169
H	4.213388	1.660086	1.664698
H	2.479856	1.282036	1.874129
H	2.713936	3.171656	0.287641
H	3.855099	2.244104	-0.697936
O	3.455078	-0.072096	0.774133
O	1.939851	1.572572	-0.806211
H	4.220058	-0.140826	0.184950
H	1.092719	2.045647	-0.735872
O	3.444882	1.329170	1.264519
O	2.537438	0.927140	-1.299379
O	2.242042	3.198205	1.282286
O	2.923934	-1.227801	-0.978785
C	1.830026	3.189182	-1.541015
H	1.993194	3.185698	-2.612757
H	0.807517	2.856395	-1.333165
H	1.963840	4.206019	-1.147985
H	3.843598	2.520540	-1.194323
C	4.525515	-0.788716	1.320668
H	5.054147	-1.546778	0.719361
H	5.192664	-0.423579	2.111806
H	3.658555	-1.277335	1.781281
H	4.972809	0.820094	-0.029588
C	-3.131844	-0.936876	-0.080435
C	-2.330831	1.525177	-0.412996
C	-3.301915	0.563640	-0.095407
C	-4.580851	1.027648	0.269345
H	-5.318538	0.269545	0.530650
C	-4.886064	2.380189	0.306946
C	-3.912369	3.320033	-0.019226
C	-2.634493	2.887688	-0.369801
H	-5.892036	2.703542	0.579085
H	-4.141264	4.389946	-0.003914
H	-1.863603	3.603744	-0.631877
O	-3.974140	-1.641457	0.463714
O	-2.118701	-1.456735	-0.752796
O	-1.048968	1.172309	-0.782654
Bi	-0.009137	-1.296379	-0.691870
O	0.287334	-2.918712	0.464379
H	-0.335201	-2.837293	1.209775
C	0.625018	-0.208777	2.179941
C	-0.772473	-0.332521	2.785695
H	1.175278	0.594509	2.690780
H	1.174383	-1.152162	2.332253
H	-0.704944	-0.563142	3.864092
H	-1.322412	0.612542	2.661218
O	0.555258	0.115787	0.808418
O	-1.387779	-1.384352	2.059442
H	-0.457068	1.200731	0.020944
H	-2.363593	-1.445705	2.235114

ET2

E(scf) = -1339.27719490 a.u.

C	2.122911	3.201694	0.491516
C	0.889124	3.101561	-0.403590
C	1.638918	0.852138	-0.960784
C	3.057094	1.321125	-0.683016
O	3.115262	2.312993	0.356754
O	0.791958	1.914404	-1.205127
O	2.206249	4.072562	1.317418
O	1.507763	-0.092372	-1.806019
C	-0.376575	3.278821	0.418974
H	-1.247024	3.347968	-0.244168
H	-0.518522	2.429342	1.087206
H	-0.301937	4.192018	1.008023
H	0.981940	3.926560	-1.117315
C	4.041959	0.200497	-0.371648
H	4.642827	-0.051365	-1.290829
H	4.745939	0.556379	0.437489
H	3.513215	-0.725705	-0.031485
H	3.344600	1.818442	-1.617966
C	-2.202787	-0.806188	1.165984
C	-2.513730	0.672766	-0.892544
C	-2.952388	0.197817	0.350673
C	-4.128345	0.731616	0.889868
H	-4.436950	0.375635	1.867829
C	-4.867900	1.687427	0.208256
C	-4.421221	2.144533	-1.030642
C	-3.247095	1.640867	-1.577941
H	-5.783493	2.079409	0.640602
H	-4.987985	2.894005	-1.576179
H	-2.891655	1.982622	-2.546703
O	-2.313784	-0.796801	2.389918
O	-1.493245	-1.703604	0.539251
O	-1.34973	0.200421	-1.447655
Bi	0.249196	-1.712061	-0.678043
O	1.374759	-2.735920	0.643371
H	1.068714	-2.550530	1.558377
C	1.645217	0.028748	1.723036
C	0.723871	-0.253697	2.892603

INT3

E(scf) = -1339.28647826 a.u.

C	1.819987	-0.221655	-0.406675
C	3.186637	-0.227730	-1.136282
C	3.444177	2.114596	-0.932053
C	1.934209	2.086819	-1.131575
O	1.381965	1.132673	-0.217434
O	3.999731	0.896693	-0.771370
O	0.959005	-0.906766	-1.204425
O	4.109213	3.113627	-0.879544
C	3.985634	-1.480753	-0.872090
H	3.382084	-2.356970	-1.123071
H	4.890053	-1.481750	-1.486487
H	4.276069	-1.544182	0.179549
H	2.957367	-0.155385	-2.206311
C	1.307007	3.433349	-0.855528
H	1.767612	4.190058	-1.494393
H	0.232421	3.402931	-1.057935
H	1.470925	3.720963	0.186463
H	1.713883	1.772143	-2.164206
C	-1.911634	0.404518	1.648308
C	-2.385036	1.336893	-0.695577
C	-2.763024	1.111171	0.635117
C	-4.004060	1.595210	1.065105
H	-4.264124	1.446009	2.108531
C	-4.869321	2.235658	0.190024
C	-4.489463	2.423225	-1.138827
C	-3.246623	1.983851	-1.578344
H	-5.833893	2.590931	0.540000
H	-5.156814	2.926085	-1.833292
H	-2.916753	2.139924	-2.600893
O	-2.039699	0.636971	2.831746
O	-1.015881	-0.475667	1.217329
O	-1.184959	0.896833	-1.208691
Bi	-0.859089	-1.653458	-0.513356
O	-0.023787	-3.117574	0.566617
H	0.725117	-2.748976	1.064120
C	1.522917	0.455816	2.884330
C	2.511104	-0.179414	1.924349

H	2.162562	0.969637	1.911932
H	2.390641	-0.770159	1.660565
H	1.308134	-0.062507	3.804511
H	-0.123006	0.444116	2.887900
O	0.946471	0.154143	0.469861
O	0.272769	-1.591676	2.914908
H	-0.763692	0.944854	-1.691746
H	-0.709671	-1.571205	2.823643

H	0.759206	-0.280713	3.166255
H	1.006080	1.287480	2.386395
H	3.074450	-0.956097	2.452032
H	3.224697	0.562281	1.557030
O	2.289178	0.890716	3.988171
O	1.835206	-0.828358	0.843596
H	1.677156	1.250893	4.641615
H	-0.415965	1.128841	-0.636470

ET3

E(scf) = -1339.27719490 a.u.

C	-1.385728	0.522987	0.556044
C	-1.596330	1.682447	1.561992
C	-2.355677	3.137478	-0.145228
C	-1.337924	2.363110	-0.969528
O	-1.610971	0.973354	-0.755088
O	-2.572840	2.613420	1.086723
O	-0.100153	0.069929	0.720245
O	-2.972892	4.096674	-0.519592
C	-2.024760	1.218817	2.933707
H	-1.296150	0.504226	3.326662
H	-2.084757	2.074345	3.611816
H	-3.002195	0.731650	2.895200
H	-0.631843	2.200879	1.633791
C	-1.439715	2.645850	-2.447446
H	-1.332504	3.718903	-2.621749
H	-0.637926	2.117489	-2.969293
H	-2.414299	2.331959	-2.832510
H	-0.317332	2.590272	-0.628254
C	2.676569	1.132516	1.371080
C	2.566935	-1.123900	2.556403
C	3.053859	0.187135	2.471206
C	3.963608	0.628255	3.435887
H	4.307870	1.656805	3.380833
C	4.431626	-0.230973	4.422745
C	3.972064	-1.545412	4.467113
C	3.028670	-1.986657	3.544337
H	5.154029	0.122069	5.152784
H	4.332719	-2.225796	5.233611
H	2.627046	-2.994716	3.581730
O	2.456325	2.305658	1.587070

INT4

E(scf) = -1339.28282663 a.u.

C	-1.405269	0.525532	0.556053
C	-1.615871	1.684992	1.562001
C	-2.375218	3.140023	-0.145219
C	-1.357465	2.365655	-0.969519
O	-1.630512	0.975899	-0.755079
O	-2.592381	2.615965	1.086732
O	-0.119694	0.072474	0.720254
O	-2.992433	4.099219	-0.519583
C	-2.044301	1.221362	2.933716
H	-1.315691	0.506771	3.326671
H	-2.104298	2.076890	3.611825
H	-3.021736	0.734195	2.895209
H	-0.651384	2.203424	1.633800
C	-1.459256	2.648395	-2.447437
H	-1.352045	3.721448	-2.621740
H	-0.657467	2.120034	-2.969284
H	-2.433840	2.334504	-2.832501
H	-0.336873	2.592817	-0.628245
C	2.203459	0.673319	-1.151860
C	3.314783	0.047541	1.057616
C	3.315464	0.757245	-0.150476
C	4.420376	1.555551	-0.458234
H	4.395506	2.128587	-1.380445
C	5.528055	1.596677	0.379954
C	5.530858	0.849745	1.555965
C	4.418766	0.088390	1.902077
H	6.386989	2.206581	0.115925
H	6.392410	0.873626	2.217532
H	4.381921	-0.471879	2.831392
O	1.805526	1.653545	-1.745347

O	2.721442	0.607725	0.147667
O	1.600686	-1.596392	1.686289
Bi	1.238899	-0.469429	-0.817951
O	0.847784	0.963779	-2.163220
H	0.559184	1.783220	-1.727018
C	-4.284895	-1.687408	0.915235
C	-3.557699	-0.500037	0.320506
H	-4.215002	-1.645682	2.014289
H	-3.786092	-2.611783	0.583091
H	-3.600874	-0.544113	-0.771281
H	-4.025375	0.433194	0.654183
O	-5.615347	-1.607993	0.463023
O	-2.207700	-0.585705	0.768502
H	-6.093014	-2.377005	0.796527
H	0.779176	-1.079012	1.821082

O	1.783371	-0.563317	-1.413424
O	2.218259	-0.692048	1.463360
Bi	0.379177	-1.666860	-0.364117
O	-0.998645	-1.599770	-1.818047
H	-1.247757	-0.682371	-2.021437
C	-4.304436	-1.684863	0.915244
C	-3.577240	-0.497492	0.320515
H	-4.234543	-1.643137	2.014298
H	-3.805633	-2.609238	0.583100
H	-3.620415	-0.541568	-0.771272
H	-4.044916	0.435739	0.654192
O	-5.634888	-1.605448	0.463032
O	-2.227241	-0.583160	0.768511
H	-6.112555	-2.374460	0.796536
H	1.463484	-0.081935	1.600500

ET4

E(scf) = -1339.28676053 a.u.

C	-1.418318	1.166956	0.601006
C	-1.703184	1.865134	-0.719332
C	-3.693390	0.695562	-1.422386
C	-2.942490	-0.604297	-1.148677
O	-2.215000	-0.528978	0.067756
O	-3.081740	1.858309	-1.067687
O	-0.206907	0.747298	0.772791
O	-4.785877	0.747200	-1.916565
C	-1.231766	3.323981	-0.674504
H	-0.572134	3.510366	0.222500
H	-0.648520	3.572792	-1.608829
H	-2.140854	3.988478	-0.622867
H	-1.127182	1.294520	-1.456081
C	-3.906920	-1.777493	-1.107738
H	-4.507240	-1.813043	-2.019629
H	-3.346945	-2.713863	-1.016683
H	-4.579193	-1.686916	-0.248638
H	-2.237491	-0.730217	-1.987442
C	2.744910	-0.034945	-0.687291
C	4.712732	0.109252	0.921013
C	4.115815	0.387977	-0.328995
C	4.848192	1.102420	-1.289819

INT5

E(scf) = -1339.31061838 a.u.

C	-3.099904	0.830145	-0.349082
C	-3.941947	-0.365192	-0.798309
C	-2.820481	-2.375590	0.012496
C	-1.524987	-1.907997	-0.659145
O	-1.129781	-0.769682	0.062912
O	-3.873897	-1.505177	0.046917
O	-2.420382	1.409999	-1.199237
O	-2.949003	-3.432982	0.564738
C	-5.407409	0.025782	-0.920850
H	-5.512216	0.876086	-1.601698
H	-5.973035	-0.820035	-1.320904
H	-5.833028	0.299303	0.048373
H	-3.558448	-0.611181	-1.792548
C	-0.485916	-3.013599	-0.627259
H	-0.846086	-3.908384	-1.143331
H	0.433770	-2.671465	-1.112139
H	-0.262200	-3.278799	0.408824
H	-1.755247	-1.670745	-1.717295
C	2.693215	0.412757	-0.181760
C	5.059737	1.040602	0.126867
C	4.075255	0.038767	0.118794
C	4.437470	-1.298421	0.403357

H	4.362871	1.299894	-2.240486	H	2.676352	-1.940756	0.227553
C	6.135723	1.537656	-1.036717	C	5.778817	-1.592677	0.684242
C	6.715858	1.257517	0.205845	C	6.729818	-0.587616	0.682195
C	6.017340	0.554916	1.172249	C	6.379167	0.739925	0.403395
H	6.688657	2.088181	-1.791535	H	6.039843	-2.623255	0.902689
H	7.727502	1.593003	0.419969	H	7.764450	-0.837374	0.903066
H	6.454304	0.329997	2.140137	H	7.133311	1.520490	0.405883
O	2.244405	0.256373	-1.773775	O	1.787532	-0.524713	-0.232495
O	2.109269	-0.752842	0.229417	O	2.338197	1.596459	-0.396324
O	4.094896	-0.567660	1.898797	O	3.565346	-2.311309	0.424817
Bi	-0.020310	-1.288441	0.128295	Bi	0.014885	0.746971	-0.796206
O	-0.084071	-1.042519	-1.853013	O	-0.127464	1.679809	0.992162
H	0.753810	-0.573235	-2.096932	H	0.723116	2.112131	1.166546
C	-4.431161	0.967465	1.742980	C	-2.566393	0.231894	2.897748
C	-3.332376	2.029088	1.872854	C	-3.721491	0.697932	2.025185
H	-5.292594	1.317349	2.323068	H	-2.998960	-0.186944	3.815543
H	-4.769770	0.889161	0.702732	H	-2.027248	-0.573692	2.379788
H	-3.301281	2.418437	2.891860	H	-4.276530	1.493637	2.527200
H	-3.483639	2.855437	1.172927	H	-4.387334	-0.123692	1.757984
O	-4.045798	-0.273250	2.260425	O	-1.723870	1.284635	3.254260
O	-2.018618	1.459309	1.728221	O	-3.174006	1.340979	0.850539
H	-3.371225	-0.611032	1.642241	H	-1.173343	1.485215	2.469459
H	3.206436	-0.801761	1.551351	H	4.746332	2.056480	-0.093411

p

E(scf) = -1339.32358607 a.u.

C	3.926179	0.565060	0.504665
C	2.828248	1.251215	1.309466
C	1.266653	-0.490750	1.211037
C	0.530482	-1.574400	1.978966
O	-0.267605	-2.340894	1.149804
O	2.059456	0.253113	1.977677
O	4.206021	-0.604297	0.569286
O	1.121526	-0.294422	0.015593
C	3.395678	2.170655	2.375405
H	3.992985	2.957053	1.907249
H	2.580723	2.633011	2.938946
H	4.027482	1.609082	3.070152
H	2.185487	1.800706	0.614404
C	1.527102	-2.470300	2.714061

H	2.104059	-1.903019	3.449533
H	0.968662	-3.260592	3.221972
H	2.217360	-2.931524	2.001298
H	-0.083579	-1.041566	2.729187
C	-2.671698	0.524085	-0.559214
C	-4.401875	2.157095	-1.220451
C	-3.410145	1.767525	-0.307161
C	-3.146460	2.577026	0.820976
H	-1.814186	1.424169	1.472105
C	-3.883534	3.755156	1.000240
C	-4.855850	4.117316	0.084046
C	-5.124591	3.320867	-1.035796
H	-3.669126	4.363918	1.872932
H	-5.417484	5.034604	0.241883
H	-5.889736	3.612775	-1.748251
O	-1.740331	0.180172	0.293068
O	-2.884908	-0.206225	-1.546565
O	-2.220008	2.279698	1.740271
Bi	-1.030581	-1.713183	-0.652259
O	-2.669165	-2.805969	-0.187644
H	-3.419042	-2.463509	-0.696140
C	6.140591	2.104736	-1.892625
C	5.623407	0.949329	-1.063952
H	5.324240	2.494113	-2.520586
H	6.463166	2.916995	-1.222297
H	6.409179	0.548238	-0.416734
H	5.259602	0.138666	-1.701664
O	7.204275	1.590027	-2.657139
O	4.548795	1.461444	-0.267611
H	7.546908	2.300495	-3.212889
H	-4.578059	1.511678	-2.075524

Table S3. Cartesian coordinates (xyz format) of the optimized geometries for all the species involved in the energy profile of the **Scheme S2** calculated at the D3-PBE0/[6-31G(d), LANL2DZ] level.

R

E(scf) = -844.776731998 a.u.

C	-2.538121	-1.298298	0.680305
C	-2.077701	1.095903	-0.231338
C	-2.893342	0.128890	0.396281
C	-4.181345	0.512351	0.804786
H	-4.782557	-0.252474	1.285804
C	-4.671023	1.791010	0.609240
C	-3.857664	2.736856	-0.017512
C	-2.582505	2.390966	-0.429979
H	-5.672671	2.051659	0.937475
H	-4.218791	3.748345	-0.185907
H	-1.936780	3.113047	-0.921575
O	-3.313565	-2.033815	1.253737
O	-1.351965	-1.763799	0.281119
O	-0.820936	0.896013	-0.678451
Bi	0.329292	-0.835999	0.516418
O	1.079826	-0.617812	1.350361
H	0.419134	-0.915289	1.995069
C	4.937063	1.242313	1.037274
C	3.867899	0.791924	0.059438
H	4.536214	1.209001	2.063678
H	5.218307	2.288857	0.828054
C	2.636229	1.667827	0.115577
H	4.284182	0.801816	-0.954673
H	3.592228	-0.240545	0.303281
H	2.168610	1.614332	1.104757
H	2.889760	2.711864	-0.110949
O	6.037977	0.374902	0.884012
O	1.708767	1.208177	-0.879139
H	6.707770	0.624700	1.532791
H	0.905552	1.764831	-0.852627

ET1

E(scf) = -844.752929915 a.u.

C	-1.287728	0.462857	1.573434
C	-2.248863	0.758410	-0.807228
C	-2.320127	0.919660	0.582579
C	-3.451520	1.548811	1.116548
H	-3.480368	1.702222	2.190692
C	-4.504494	1.951315	0.306876
C	-4.431124	1.748851	-1.069931
C	-3.299059	1.164679	-1.625398
H	-5.378954	2.421514	0.746883
H	-5.247943	2.059928	-1.715325
H	-3.200243	1.022911	-2.697193
O	-1.119424	1.071893	2.607418
O	-0.651480	-0.685131	1.346603
O	-1.152960	0.194615	-1.428495
Bi	0.390049	-1.535814	-0.238698
O	1.754217	-2.097749	1.141867
H	1.597858	-1.607970	1.965358
C	3.864941	2.761694	0.308363
C	2.863930	2.037548	-0.571924
H	4.642875	2.055773	0.645996
H	3.358460	3.143428	1.210817
C	2.197886	0.876180	0.142257
H	2.101172	2.752659	-0.902869
H	3.373881	1.669803	-1.469752
H	2.948785	0.141863	0.466372
H	1.678222	1.230922	1.046652
O	4.421310	3.812862	-0.451791
O	1.274911	0.263905	-0.745731
H	5.046267	4.287148	0.110777
H	-0.329676	0.729181	-1.278901

INT1

E(scf) = -844.761349720 a.u.

C	-1.287728	0.462857	1.573434

INT2

E(scf) = -1378.54792441 a.u.

C	3.072326	2.350215	0.686509

C	-2.248863	0.758410	-0.807228
C	-2.320127	0.919660	0.582579
C	-3.451520	1.548811	1.116548
H	-3.480368	1.702222	2.190692
C	-4.504494	1.951315	0.306876
C	-4.431124	1.748851	-1.069931
C	-3.299059	1.164679	-1.625398
H	-5.378954	2.421514	0.746883
H	-5.247943	2.059928	-1.715325
H	-3.200243	1.022911	-2.697193
O	-1.119424	1.071893	2.607418
O	-0.651480	-0.685131	1.346603
O	-1.152960	0.194615	-1.428495
Bi	0.390049	-1.535814	-0.238698
O	1.754217	-2.097749	1.141867
H	1.597858	-1.607970	1.965358
C	3.864941	2.761694	0.308363
C	2.863930	2.037548	-0.571924
H	4.642875	2.055773	0.645996
H	3.358460	3.143428	1.210817
C	2.197886	0.876180	0.142257
H	2.101172	2.752659	-0.902869
H	3.373881	1.669803	-1.469752
H	2.948785	0.141863	0.466372
H	1.678222	1.230922	1.046652
O	4.421310	3.812862	-0.451791
O	1.274911	0.263905	-0.745731
H	5.046267	4.287148	0.110777
H	-0.329676	0.729181	-1.278901
C	2.512836	2.631281	-0.702572
C	2.707474	0.301877	-1.172675
C	3.995386	0.422969	-0.381915
O	3.756813	1.194222	0.802320
O	1.998331	1.420188	-1.296465
O	2.952078	3.096310	1.616595
O	2.313026	-0.726924	-1.678715
C	1.396129	3.645482	-0.690540
H	1.102798	3.891062	-1.714514
H	0.528454	3.242976	-0.161478
H	1.736045	4.550486	-0.182783
H	3.345923	2.980203	-1.331919
C	4.548617	-0.917100	0.036435
H	4.761719	-1.523485	-0.846780
H	5.468072	-0.772144	0.608690
H	3.821108	-1.449010	0.654346
H	4.725152	0.959378	-1.009531
C	-2.911111	-1.049362	0.529035
C	-2.615412	1.498996	0.276782
C	-3.374886	0.376034	0.635497
C	-4.677387	0.576370	1.106527
H	-5.239039	-0.298480	1.419576
C	-5.241232	1.844003	1.156573
C	-4.488498	2.945403	0.753797
C	-3.176139	2.773371	0.330476
H	-6.260786	1.973383	1.507698
H	-4.915322	3.944170	0.788895
H	-2.557268	3.620450	0.049923
O	-3.245565	-1.869635	1.359675
O	-2.236208	-1.387891	-0.561746
O	-1.306312	1.406853	-0.129403
Bi	-0.382612	-0.862316	-1.405875
O	0.017811	-2.840882	-1.350292
H	-0.699246	-3.253466	-0.840675
C	1.274376	-2.032667	3.755873
C	1.096359	-0.943731	2.714452
H	1.901543	-2.842707	3.344044
H	0.294066	-2.474096	3.999826
C	0.490936	-1.478984	1.429148
H	0.451035	-0.159699	3.128486
H	2.06899	-0.481437	2.506579

H	1.133422	-2.25724	0.99292
H	-0.48426	-1.944234	1.638548
O	1.874229	-1.449528	4.892673
O	0.344746	-0.409806	0.503993
H	1.92927	-2.126791	5.578395
H	-0.765123	0.864655	0.507916

ET2

E(scf) = 1378.52715869 a.u.

C	3.116032	2.369008	-0.204409
C	2.406709	2.159751	-1.535553
C	1.980352	-0.122446	-0.870352
C	3.373401	0.014199	-0.285363
O	3.510184	1.247323	0.430916
O	1.550854	1.007229	-1.533718
O	3.346242	3.452798	0.260979
O	1.643114	-1.217945	-1.417301
C	1.571593	3.360561	-1.930009
H	1.125580	3.193804	-2.910488
H	0.780389	3.534246	-1.192728
H	2.206061	4.250590	-1.969981
H	3.191395	1.992137	-2.288712
C	3.762018	-1.128253	0.623887
H	4.744549	-0.927702	1.058188
H	3.029818	-1.272778	1.418417
H	3.807047	-2.050862	0.039588
H	4.054606	0.037815	-1.150637
C	-2.496533	-0.293456	1.134220
C	-2.218248	0.598886	-1.296089
C	-2.895749	0.516746	-0.074472
C	-4.037205	1.324707	0.085832
H	-4.539589	1.274940	1.047285
C	-4.489441	2.165174	-0.916394
C	-3.788125	2.235995	-2.118547
C	-2.656612	1.455795	-2.305335
H	-5.376221	2.772120	-0.757046
H	-4.128445	2.898080	-2.914533
H	-2.107838	1.483448	-3.244597
O	-2.915638	0.036212	2.224289
O	-1.746672	-1.367105	0.992862

INT3

E(scf) = -1378.54831271 a.u.

C	3.432044	1.076717	-2.014769
C	1.912174	1.105587	-2.115821
C	1.702558	-0.633823	-0.448121
C	3.004621	-1.086519	-1.157469
O	3.919014	0.000848	-1.362423
O	1.383320	0.707950	-0.846879
O	4.164669	1.935229	-2.427100
O	0.738211	-1.505079	-0.842508
C	1.396935	2.488350	-2.440213
H	0.309648	2.471088	-2.557735
H	1.663074	3.189023	-1.644130
H	1.849832	2.840443	-3.369760
H	1.586456	0.390982	-2.888427
C	3.734484	-2.175312	-0.408931
H	4.580375	-2.532481	-1.002567
H	4.109393	-1.810840	0.550703
H	3.050486	-3.007728	-0.223937
H	2.693643	-1.463343	-2.139024
C	-1.923569	1.022322	1.372591
C	-2.411677	1.045593	-1.154387
C	-2.751703	1.366331	0.167908
C	-3.936570	2.077380	0.393270
H	-4.165644	2.347597	1.419448
C	-4.782907	2.420062	-0.650871
C	-4.442399	2.066738	-1.956376
C	-3.256408	1.388229	-2.207845
H	-5.702607	2.961877	-0.451450
H	-5.095591	2.330464	-2.783677
H	-2.957470	1.119263	-3.216391
O	-2.062897	1.629728	2.410748
O	-1.028121	0.043252	1.263014

O	-1.097201	-0.168392	-1.541410
Bi	-0.152583	-2.110209	-0.183200
O	0.630583	-2.976658	1.473375
H	0.280893	-2.570046	2.281612
C	-0.352330	2.479936	2.860840
C	0.176198	1.925956	1.546935
H	-1.200689	1.866030	3.191268
H	0.436643	2.421413	3.634244
C	0.754666	0.528493	1.720213
H	-0.650163	1.894025	0.823887
H	0.929053	2.620763	1.163298
H	1.724960	0.566919	2.226463
H	0.080333	-0.073245	2.351565
O	-0.736471	3.819508	2.627917
O	0.882471	-0.188840	0.505696
H	-1.160062	4.146431	3.434922
H	-0.344045	0.389835	-1.837696

O	-1.275163	0.337364	-1.479755
Bi	-1.067344	-1.74077	0.167438
O	-0.245284	-2.715128	1.713658
H	0.535136	-2.220729	2.013849
C	2.747205	2.389678	2.976304
C	1.852453	1.516801	2.114507
H	3.664398	2.651051	2.418697
H	3.064281	1.827827	3.872035
C	2.611316	0.307103	1.598579
H	0.976902	1.197448	2.689112
H	1.483629	2.111057	1.273499
H	3.426573	0.607382	0.931924
H	3.058833	-0.246403	2.433261
O	2.017142	3.543913	3.324806
O	1.765792	-0.644721	0.939462
H	2.572833	4.084735	3.899826
H	-0.459457	0.716937	-1.076960

ET3

E(scf) = -1378.54772519 a.u.

C	-1.810699	3.462210	-0.088099
C	-0.853450	2.623932	-0.922406
C	-1.131740	0.734994	0.514356
C	-1.245509	1.864870	1.568043
O	-2.108947	2.913422	1.115510
O	-1.279856	1.264547	-0.779574
O	-2.325778	4.489575	-0.436205
O	0.096126	0.145124	0.678334
C	-0.880786	2.980346	-2.387629
H	-0.127328	2.388440	-2.913395
H	-1.872203	2.793282	-2.810355
H	-0.651161	4.041274	-2.510589
H	0.175066	2.725560	-0.546092
C	-1.753785	1.389096	2.907763
H	-1.745909	2.216318	3.622610
H	-2.772575	1.002531	2.826220
H	-1.110383	0.588677	3.283473
H	-0.234912	2.276499	1.682672
C	2.792837	-0.510877	1.831802
C	1.967243	-2.727452	0.878639

INT4

E(scf) = -1378.54909419 a.u.

C	-1.810699	3.462210	-0.088099
C	-0.853450	2.623932	-0.922406
C	-1.131740	0.734994	0.514356
C	-1.245509	1.864870	1.568043
O	-2.108947	2.913422	1.115510
O	-1.279856	1.264547	-0.779574
O	-2.325778	4.489575	-0.436205
O	0.096126	0.145124	0.678334
C	-0.880786	2.980346	-2.387629
H	-0.127328	2.388440	-2.913395
H	-1.872203	2.793282	-2.810355
H	-0.651161	4.041274	-2.510589
H	0.175066	2.725560	-0.546092
C	-1.753785	1.389096	2.907763
H	-1.745909	2.216318	3.622610
H	-2.772575	1.002531	2.826220
H	-1.110383	0.588677	3.283473
H	-0.234912	2.276499	1.682672
C	2.497802	0.488623	-1.095655
C	3.471471	-0.303258	1.124305

C	2.711681	-2.006928	1.822696
C	3.444830	-2.712874	2.780117
H	3.989848	-2.144177	3.527811
C	3.493888	-4.101477	2.761412
C	2.784722	-4.803166	1.788867
C	2.009887	-4.117342	0.858475
H	4.084885	-4.634653	3.500293
H	2.817512	-5.888925	1.764418
H	1.418601	-4.643143	0.114980
O	2.765955	0.125108	2.864492
O	3.010700	0.034987	0.635863
O	1.151321	-2.092389	-0.039727
Bi	1.579503	0.576987	-0.759432
O	1.807387	2.548034	-0.466837
H	1.611032	2.782021	0.456021
C	-5.704529	-1.041446	0.252458
C	-4.267577	-1.168052	0.721959
H	-5.738993	-1.063917	-0.849694
H	-6.116759	-0.069103	0.571391
C	-3.389739	-0.060139	0.179012
H	-4.248324	-1.159223	1.818193
H	-3.873970	-2.138547	0.397575
H	-3.379332	-0.066480	-0.916047
H	-3.741976	0.923861	0.513652
O	-6.428204	-2.115091	0.812353
O	-2.065671	-0.292910	0.662333
H	-7.343320	-2.045503	0.512769
H	0.443469	-1.622842	0.448877

ET4

E(scf) = -1378.54880646 a.u.

C	-1.287728	0.462857	1.573434
C	-2.248863	0.758410	-0.807228
C	-2.320127	0.919660	0.582579
C	-3.451520	1.548811	1.116548
H	-3.480368	1.702222	2.190692
C	-4.504494	1.951315	0.306876
C	-4.431124	1.748851	-1.069931
C	-3.299059	1.164679	-1.625398
H	-5.378954	2.421514	0.746883
C	3.581734	0.433882	-0.062731
C	4.770859	1.121997	-0.317685
H	4.832223	1.717875	-1.223594
C	5.851379	1.027424	0.550939
C	5.742537	0.254148	1.704769
C	4.548712	-0.397542	1.998767
H	6.775761	1.552131	0.328002
H	6.581905	0.172279	2.389827
H	4.427173	-0.974819	2.910277
O	2.215935	1.517368	-1.673480
O	1.965608	-0.695269	-1.397106
O	2.293417	-0.934501	1.479481
Bi	0.378853	-1.621365	-0.441338
O	-0.915630	-1.312553	-1.941844
H	-1.019792	-0.361462	-2.113742
C	-5.704529	-1.041446	0.252458
C	-4.267577	-1.168052	0.721959
H	-5.738993	-1.063917	-0.849694
H	-6.116759	-0.069103	0.571391
C	-3.389739	-0.060139	0.179012
H	-4.248324	-1.159223	1.818193
H	-3.87397	-2.138547	0.397575
H	-3.379332	-0.066480	-0.916047
H	-3.741976	0.923861	0.513652
O	-6.428204	-2.115091	0.812353
O	-2.065671	-0.292910	0.662333
H	-7.343320	-2.045503	0.512769
H	1.603955	-0.250580	1.610467

INT5

E(scf) = -1378.55283654 a.u.

C	3.264607	-1.487046	1.293219
C	2.236687	-2.306697	0.518551
C	1.424495	0.851190	0.188159
C	1.564321	0.229012	1.568895
O	2.865503	-0.275594	1.798690
O	1.709861	-1.489521	-0.498005
O	4.403593	-1.813521	1.492542
O	0.322360	0.806093	-0.400966
C	2.885430	-3.553823	-0.056083

H	-5.247943	2.059928	-1.715325
C	3.342399	-1.366475	1.476548
C	2.427269	-2.017104	0.441159
C	1.372468	0.685280	0.427208
C	1.539669	0.193569	1.854108
O	2.855577	-0.275840	2.126435
O	1.861931	-1.015869	-0.383123
O	4.444203	-1.753915	1.767027
O	0.158079	0.757406	-0.014788
C	3.177891	-3.051283	-0.400914
H	3.275596	-2.654538	-1.445228
H	4.194616	-3.228670	0.020875
H	2.621540	-4.024012	-0.431120
H	1.633203	-2.507644	1.022679
C	1.229850	1.300506	2.843243
H	1.313948	0.913833	3.864198
H	1.925770	2.140922	2.731446
H	0.211138	1.665817	2.681935
H	0.813764	-0.618930	1.967785
C	-3.035794	-0.238823	0.439256
C	-4.686590	1.369104	-0.641300
C	-4.262874	0.588414	0.457592
C	-5.031254	0.591231	1.631810
H	-4.679635	-0.018733	2.458113
C	-6.188793	1.340852	1.733579
C	-6.597791	2.111202	0.639137
C	-5.859893	2.127432	-0.531774
H	-6.771746	1.331152	2.649393
H	-7.505565	2.705976	0.703497
H	-6.164585	2.720287	-1.388576
O	-2.678047	-0.882069	1.426321
O	-2.369726	-0.245360	-0.706271
O	-4.020634	1.429178	-1.802629
Bi	-0.352959	-1.092536	-0.978330
O	-0.550153	-2.282083	0.617722
H	-1.355434	-1.965607	1.095347
C	5.651557	2.894950	-0.478413
C	4.151018	2.757008	-0.662641
H	6.152461	1.962285	-0.788080
H	5.884479	3.049058	0.588823
C	3.593226	1.609521	0.143908
H	3.667826	-3.278842	-0.768646
H	3.333460	-4.166560	0.731162
H	2.126330	-4.147781	-0.575188
H	1.452330	-2.605894	1.234072
C	1.252830	1.264413	2.644120
H	1.311208	0.778596	3.621689
H	1.957431	2.100856	2.631913
H	0.239730	1.653253	2.505391
H	0.812769	-0.565227	1.628571
C	-3.127293	-0.201496	0.442767
C	-4.420199	1.746860	-0.555668
C	-4.261501	0.753316	0.436263
C	-5.208497	0.661108	1.466362
H	-5.057779	-0.112005	2.213566
C	-6.291916	1.519337	1.528165
C	-6.439175	2.499651	0.540620
C	-5.518307	2.615195	-0.486746
H	-7.017362	1.432914	2.331377
H	-7.285121	3.181799	0.575332
H	-5.619169	3.371329	-1.259232
O	-2.996236	-1.020753	1.360053
O	-2.301981	-0.117164	-0.575455
O	-3.563162	1.910442	-1.572232
Bi	-0.379682	-1.29178	-0.916386
O	-0.690761	-2.173871	0.843719
H	-1.589072	-1.884754	1.173789
C	5.673858	3.275341	-0.18631
C	4.243836	2.979699	-0.604361
H	6.306879	2.392232	-0.374663
H	5.713334	3.478281	0.897498
C	3.676036	1.803906	0.157245
H	3.630098	3.871125	-0.432569
H	4.222253	2.770613	-1.679453
H	4.253733	0.890423	-0.003433
H	3.627735	1.993645	1.230886
O	6.100729	4.38858	-0.935715
O	2.343764	1.580902	-0.368334
H	7.016052	4.579179	-0.694812
H	-2.86967	1.220036	-1.452777

H	3.666512	3.696656	-0.360773
H	3.932409	2.605457	-1.725395
H	4.028960	0.650531	-0.163994
H	3.764222	1.737733	1.215085
O	6.069461	3.989995	-1.260865
O	2.183604	1.555662	-0.129663
H	7.023963	4.086940	-1.153147
H	-3.238526	0.842800	-1.697866

p

E(scf) = -1378.59748690 a.u.

C	-0.851512	-0.786487	-1.311740
C	0.006172	-1.888527	-1.908514
C	-3.632232	0.117773	-0.930048
C	-2.513488	0.818671	-1.693925
O	-1.621518	-0.172121	-2.202862
O	0.751576	-2.528966	-0.932552
O	-0.815326	-0.472010	-0.132542
O	-3.793626	-1.075578	-0.879679
C	-0.868767	-2.901093	-2.645907
H	-1.596502	-3.342135	-1.958227
H	-1.404593	-2.432967	-3.476073
H	-0.227158	-3.696929	-3.033104
H	0.664722	-1.383626	-2.638733
C	-3.037668	1.607231	-2.879544
H	-2.207015	2.086662	-3.404555
H	-3.559911	0.947806	-3.579393
H	-3.730231	2.378066	-2.533049
H	-1.975922	1.466513	-0.994183
C	2.677062	0.777175	0.391639
C	4.011976	2.840782	0.806347
C	3.321629	1.998915	-0.096583
C	3.262221	2.339594	-1.456277
H	2.729940	1.669948	-2.124626
C	3.866941	3.489581	-1.928355
C	4.546836	4.319600	-1.027574
C	4.621250	4.005417	0.318140
H	3.818628	3.744963	-2.982351
H	5.027341	5.226136	-1.387063
H	5.147793	4.640829	1.023187

O	2.048731	0.020920	-0.445291
O	2.719083	0.451572	1.608637
O	4.112235	2.578246	2.110844
Bi	1.333632	-1.617013	0.834605
O	3.021445	-2.713606	0.664364
H	3.073664	-3.032024	-0.250456
C	-7.485416	1.216971	1.793849
C	-6.292323	1.666646	0.970272
H	-7.143367	0.584305	2.630229
H	-8.156407	0.599679	1.172511
C	-5.520854	0.494246	0.407301
H	-6.646271	2.306904	0.154144
H	-5.635411	2.277112	1.600122
H	-5.128274	-0.159295	1.194232
H	-6.133493	-0.123247	-0.259025
O	-8.135762	2.378078	2.257533
O	-4.415292	1.024281	-0.340912
H	-8.891101	2.104572	2.792993
H	3.638822	1.723293	2.266404

Table S4. Cartesian coordinates (xyz format) of the optimized geometries for all the species involved in the energy profile of the **Scheme S3** calculated at the D3-PBE0/[6-31G(d), LANL2DZ] level.

R

E(scf) = -884.042376469 a.u.

C	-2.823199	-1.153539	0.881366
C	-2.313136	1.133812	-0.250784
C	-3.117424	0.271685	0.526505
C	-4.331078	0.770104	1.027818
H	-4.926494	0.083670	1.621177
C	-4.758833	2.062505	0.783173
C	-3.958446	2.903381	0.007695
C	-2.756015	2.442579	-0.499933
H	-5.703458	2.414012	1.187055
H	-4.272640	3.922738	-0.202186
H	-2.122012	3.081928	-1.107671
O	-3.597472	-1.804370	1.550700
O	-1.691581	-1.711397	0.443773
O	-1.125386	0.815058	-0.805670
Bi	-0.029061	-0.937921	-0.536669
O	0.847846	-0.586986	1.252835
H	0.216120	-0.780034	1.962896
C	5.933725	0.237498	0.598528
H	5.634129	-0.741076	1.010184
H	6.293534	0.062033	-0.429917
C	4.731423	1.161247	0.565115
C	3.594835	0.607936	-0.286947
H	4.391244	1.321342	1.596040
H	5.058072	2.137322	0.183160
C	2.395640	1.530197	-0.289509
H	3.281625	-0.368552	0.105033
H	3.930190	0.459660	-1.322207
H	2.677245	2.527511	-0.651368
H	1.977904	1.614880	0.719409
O	1.402561	0.995937	-1.180484
O	6.924887	0.850381	1.393128
H	0.620960	1.583214	-1.177309
H	7.683840	0.255406	1.436841

ET1

E(scf) = -884.018808297 a.u.

C	-1.962220	0.140711	1.700453
C	-2.422405	0.911682	-0.734251
C	-2.716619	0.883676	0.643698
C	-3.809857	1.633222	1.107065
H	-4.016711	1.594080	2.171525
C	-4.587503	2.397755	0.254358
C	-4.280436	2.425381	-1.106875
C	-3.211891	1.687921	-1.592126
H	-5.425287	2.968820	0.643202
H	-4.879493	3.018856	-1.792889
H	-2.963783	1.681765	-2.649380
O	-2.294585	0.201658	2.863863
O	-0.873604	-0.578138	1.382423
O	-1.418790	0.199289	-1.296516
Bi	-0.021754	-1.446047	-0.283798
O	1.547181	-1.685346	0.979324
H	1.335374	-1.249777	1.820939
C	5.540384	1.412273	0.049057
H	5.693362	0.397387	0.452843
H	5.817498	1.383126	-1.018707
C	4.078994	1.794086	0.182811
C	3.155890	0.831259	-0.555666
H	3.827961	1.822829	1.251232
H	3.954206	2.816731	-0.197320
C	1.698199	1.213628	-0.395957
H	3.283601	-0.189532	-0.175127
H	3.395414	0.817953	-1.627201
H	1.520437	2.230924	-0.765958
H	1.403500	1.187498	0.662307
O	0.864149	0.342678	-1.166524
O	6.303561	2.368425	0.752504
H	-0.292071	0.646165	-1.340706
H	7.233080	2.116943	0.684463

INT1

E(scf) = -884.026651081 a.u.

C	-1.521845	0.694539	1.643561
C	-2.175741	1.312298	-0.794741
C	-2.323549	1.418023	0.594970
C	-3.314111	2.281738	1.082213
H	-3.399931	2.379946	2.159503
C	-4.155877	2.979873	0.228858
C	-4.009022	2.839733	-1.149822
C	-3.014386	2.013579	-1.657347
H	-4.923293	3.631328	0.636395
H	-4.660497	3.380326	-1.830911
H	-2.861749	1.898022	-2.725973
O	-1.444205	1.154013	2.762721
O	-0.964578	-0.478252	1.364379
O	-1.229817	0.498349	-1.384756
Bi	-0.331007	-1.628777	-0.253198
O	0.792726	-2.607789	1.109468
H	0.834931	-2.088099	1.928351
C	5.364203	2.197866	-0.425547
H	5.684653	1.778821	-1.394823
H	4.849753	3.150560	-0.638163
C	4.398969	1.240514	0.245914
C	3.171175	0.951907	-0.610232
H	4.936139	0.309696	0.469784
H	4.101003	1.670983	1.210846
C	2.203368	0.003399	0.074420
H	3.468777	0.510908	-1.570843
H	2.642955	1.886891	-0.843120
H	1.864540	0.436930	1.028707
H	2.705435	-0.944963	0.311203
O	1.098161	-0.228925	-0.784341
O	6.462094	2.387895	0.440739
H	-0.296319	0.780230	-1.201915
H	7.073024	3.003766	0.017252

INT2

E(scf) = -1417.81369917 a.u.

C	-2.889951	-0.876745	2.403264
C	-2.104114	-2.165795	2.197835
C	-2.349088	-1.845210	-0.153004
C	-3.741084	-1.377978	0.226335
O	-3.655777	-0.502121	1.358625
O	-1.572868	-2.226621	0.857432
O	-2.870517	-0.236406	3.416560
O	-1.931961	-1.887890	-1.290378
C	-0.946388	-2.305477	3.154896
H	-0.482530	-3.288461	3.039188
H	-0.196480	-1.536051	2.953513
H	-1.308079	-2.192822	4.179048
H	-2.806946	-3.005040	2.314732
C	-4.430398	-0.634291	-0.890830
H	-4.535038	-1.285788	-1.761373
H	-5.420023	-0.309550	-0.560268
H	-3.843547	0.239889	-1.183408
H	-4.326672	-2.265817	0.513944
C	2.784627	1.215499	-0.797551
C	2.762288	0.024125	1.486768
C	3.342892	0.904650	0.562197
C	4.549384	1.526842	0.901106
H	4.965219	2.237697	0.193489
C	5.204710	1.234148	2.089613
C	4.638916	0.320575	2.976901
C	3.415303	-0.268855	2.682462
H	6.150636	1.714053	2.322940
H	5.139467	0.081295	3.911345
H	2.935164	-0.951977	3.376821
O	2.874415	2.333504	-1.262037
O	2.313192	0.193158	-1.500944
O	1.544495	-0.573026	1.273528
Bi	0.661870	-1.091177	-1.321389
O	0.093613	-0.394389	-3.128419
H	0.673011	0.356597	-3.338835
C	-0.736273	1.555110	-0.807597
C	-1.519241	2.400387	0.181701
H	-1.353977	1.319958	-1.686119

H	0.137975	2.117701	-1.166912
C	-2.014731	3.700999	-0.440877
H	-2.366386	1.813245	0.560620
H	-0.876379	2.616568	1.046117
C	-2.782746	4.559590	0.544934
H	-1.171243	4.286366	-0.828584
H	-2.669627	3.490032	-1.296943
H	-3.630768	3.983975	0.953936
H	-2.128366	4.819511	1.393907
O	-0.330173	0.347841	-0.172496
O	-3.226812	5.714613	-0.135573
H	0.858471	0.094727	0.997157
H	-3.684603	6.276854	0.501715

ET2

E(scf) = -1417.792871800 a.u.

C	1.806552	3.227392	0.641905
C	1.364879	2.621620	1.970209
C	-0.634401	1.868847	0.859465
C	-0.520053	3.222424	0.182540
O	0.826302	3.459451	-0.249054
O	0.307049	1.667420	1.831888
O	2.947119	3.518963	0.396792
O	-1.797235	1.434145	1.159209
C	2.506918	1.947572	2.694160
H	2.167987	1.591564	3.672102
H	2.866585	1.091853	2.114787
H	3.328596	2.650878	2.830509
H	0.981765	3.460146	2.578748
C	-1.462572	3.416279	-0.980893
H	-2.485188	3.489199	-0.602476
H	-1.215126	4.348965	-1.495789
H	-1.426691	2.584876	-1.687171
H	-0.759199	3.958455	0.966503
C	-0.043933	-2.668509	-0.769096
C	0.224023	-1.937577	1.726782
C	0.605630	-2.670936	0.596147
C	1.760979	-3.461092	0.704583
H	2.049216	-4.017934	-0.181296
C	2.512708	-3.516153	1.866616

INT3

E(scf) = -1417.81629945 a.u.

C	-3.113825	-0.885839	2.511724
C	-1.616974	-0.603433	2.534322
C	-1.398103	-1.279496	0.213999
C	-2.492489	-2.265565	0.693239
O	-3.520831	-1.607437	1.448180
O	-1.212972	-0.253000	1.206225
O	-3.898871	-0.484730	3.328059
O	-0.266735	-2.014437	0.057549
C	-1.276168	0.543621	3.456927
H	-0.193123	0.692417	3.497774
H	-1.754045	1.463727	3.109912
H	-1.643171	0.327405	4.462674
H	-1.082894	-1.513406	2.851375
C	-3.155084	-3.003928	-0.444179
H	-2.391563	-3.499814	-1.049252
H	-3.842574	-3.756731	-0.048959
H	-3.716464	-2.316955	-1.082407
H	-1.986123	-2.981616	1.351506
C	1.526299	1.793576	-0.630310
C	2.447414	0.628981	1.466989
C	2.487762	1.657006	0.515170
C	3.472648	2.643156	0.646080
H	3.466997	3.452778	-0.077121
C	4.420988	2.584851	1.657272

C	2.122485	-2.760445	2.970670
C	0.979692	-1.978899	2.899829
H	3.401246	-4.140199	1.912516
H	2.699167	-2.786673	3.891929
H	0.648807	-1.399333	3.758916
O	0.502676	-3.259930	-1.682583
O	-1.198261	-2.053686	-0.955279
O	-0.923416	-1.178769	1.725294
Bi	-2.257239	-0.373286	-0.269150
O	-2.496271	0.290794	-2.182804
H	-1.912878	-0.170573	-2.803072
C	0.666673	0.664782	-1.460847
C	2.085910	0.257850	-1.102615
H	0.653249	1.645737	-1.950441
H	0.255964	-0.062072	-2.174479
C	2.925155	0.028470	-2.357028
H	2.555785	1.031989	-0.484701
H	2.050359	-0.658177	-0.502787
C	4.366967	-0.311271	-2.029322
H	2.498376	-0.793496	-2.946201
H	2.918222	0.921200	-2.994577
H	4.812800	0.508145	-1.440712
H	4.395979	-1.221053	-1.403475
O	-0.213875	0.663191	-0.342563
O	5.054779	-0.501412	-3.248538
H	-0.780885	-0.352527	2.222091
H	5.970067	-0.721719	-3.039022

C	4.383262	1.537260	2.577108
C	3.393128	0.566537	2.487475
H	5.185137	3.352783	1.731836
H	5.118826	1.482048	3.374863
H	3.327067	-0.246845	3.203627
O	1.309145	2.880818	-1.122419
O	0.923965	0.703497	-1.088343
O	1.518755	-0.387598	1.417512
Bi	1.375127	-1.345348	-1.040881
O	0.463774	-1.571481	-2.809983
H	-0.431153	-1.198281	-2.746863
C	-2.710685	0.355451	-1.028318
C	-2.134033	1.758275	-1.045832
H	-3.405018	0.217533	-0.193679
H	-3.265824	0.159164	-1.953305
C	-3.209602	2.810536	-1.289120
H	-1.627010	1.945071	-0.092698
H	-1.358651	1.815170	-1.817883
C	-2.634071	4.213498	-1.303093
H	-3.711458	2.634900	-2.250283
H	-3.987930	2.761197	-0.515539
H	-2.148203	4.421156	-0.335030
H	-1.851374	4.282059	-2.075820
O	-1.680974	-0.645545	-0.987382
O	-3.691879	5.116657	-1.552848
H	0.591554	-0.057035	1.341068
H	-3.318363	6.006297	-1.581755

ET3

E(scf) = 1478.816071610 a.u.

C	-1.333483	3.627545	-0.079596
C	-0.435782	2.731118	-0.919405
C	-0.848641	0.855284	0.505817
C	-0.880082	1.984353	1.565622
O	-1.668417	3.093169	1.121057
O	-0.950778	1.401843	-0.785248
O	-1.774589	4.691058	-0.420072
O	0.331563	0.173425	0.670579
C	-0.440099	3.097590	-2.382465
H	0.270518	2.459107	-2.913374

INT4

E(scf) = -1417.81418429 a.u.

C	-1.333483	3.627545	-0.079596
C	-0.435782	2.731118	-0.919405
C	-0.848641	0.855284	0.505817
C	-0.880082	1.984353	1.565622
O	-1.668417	3.093169	1.121057
O	-0.950778	1.401843	-0.785248
O	-1.774589	4.691058	-0.420072
O	0.331563	0.173425	0.670579
C	-0.440099	3.097590	-2.382465
H	0.270518	2.459107	-2.913374

H	-1.442264	2.981382	-2.805261	H	-1.442264	2.981382	-2.805261
H	-0.138727	4.141118	-2.499090	H	-0.138727	4.141118	-2.499090
H	0.597306	2.762673	-0.543364	H	0.597306	2.762673	-0.543364
C	-1.417586	1.538044	2.904106	C	-1.417586	1.538044	2.904106
H	-0.830220	0.693222	3.274440	H	-0.830220	0.693222	3.274440
H	-1.351078	2.359183	3.622932	H	-1.351078	2.359183	3.622932
H	-2.461100	1.224081	2.822867	H	-2.461100	1.224081	2.822867
H	0.157384	2.322804	1.680142	H	0.157384	2.322804	1.680142
C	2.893487	-0.729357	1.936166	C	2.764693	0.367553	-1.067919
C	2.610241	-2.291853	-0.057171	C	3.661922	-0.521254	1.145680
C	3.075013	-2.044748	1.241923	C	3.835795	0.221329	-0.030355
C	3.774356	-3.054192	1.908330	C	5.075019	0.820962	-0.268934
H	4.099468	-2.864380	2.927076	H	5.187835	1.422719	-1.166002
C	4.067136	-4.256975	1.276533	C	6.139788	0.631931	0.604055
C	3.638787	-4.470502	-0.031835	C	5.965265	-0.147389	1.745591
C	2.897422	-3.495393	-0.692043	C	4.723381	-0.709928	2.024172
H	4.629800	-5.023647	1.801054	H	7.102792	1.087822	0.393613
H	3.863969	-5.406640	-0.535314	H	6.791777	-0.302758	2.433552
H	2.519517	-3.654068	-1.697483	H	4.552495	-1.288656	2.926819
O	2.596551	-0.658512	3.109913	O	2.552445	1.422520	-1.627264
O	3.196766	0.330193	1.186281	O	2.159781	-0.774991	-1.392923
O	1.836316	-1.370674	-0.738213	O	2.437312	-1.065416	1.485633
Bi	1.913123	1.352014	-0.077619	Bi	0.498245	-1.594927	-0.467557
O	1.751745	2.967855	1.098073	O	-0.765131	-1.183020	-1.968706
H	1.369510	2.729395	1.959664	H	-0.816626	-0.224211	-2.121482
C	-3.163425	0.237042	0.170563	C	-3.163425	0.237042	0.170563
C	-4.116808	-0.828641	0.670496	C	-4.116808	-0.828641	0.670496
H	-3.155931	0.270139	-0.923684	H	-3.155931	0.270139	-0.923684
H	-3.453252	1.227773	0.542414	H	-3.453252	1.227773	0.542414
C	-5.544466	-0.582663	0.196623	C	-5.544466	-0.582663	0.196623
H	-3.763055	-1.805652	0.314380	H	-3.763055	-1.805652	0.314380
H	-4.078207	-0.858069	1.767878	H	-4.078207	-0.858069	1.767878
C	-6.508633	-1.648535	0.680389	C	-6.508633	-1.648535	0.680389
H	-5.903949	0.392722	0.549494	H	-5.903949	0.392722	0.549494
H	-5.583633	-0.554146	-0.899825	H	-5.583633	-0.554146	-0.899825
H	-6.178015	-2.636525	0.316939	H	-6.178015	-2.636525	0.316939
H	-6.493815	-1.686431	1.783218	H	-6.493815	-1.686431	1.783218
O	-1.857263	-0.100236	0.643790	O	-1.857263	-0.100236	0.643790
O	-7.791797	-1.323201	0.193399	O	-7.791797	-1.323201	0.193399
H	1.001153	-1.241183	-0.241920	H	1.796811	-0.333670	1.607608
H	-8.407566	-2.002967	0.494418	H	-8.407566	-2.002967	0.494418

ET4

E(scf) = -1417.81506078 a.u.

C	2.879029	-2.177520	1.290617
C	2.072027	-2.331054	0.006946
C	1.193066	0.293131	0.848995
C	1.140515	-0.679728	2.017917
O	2.379758	-1.340010	2.234619
O	1.658735	-1.055411	-0.452978
O	3.915599	-2.746476	1.515048
O	0.051007	0.641457	0.343474
C	2.892532	-3.030755	-1.061250
H	2.280862	-3.184250	-1.957739
H	3.768056	-2.427843	-1.331928
H	3.242443	-4.003046	-0.703609
H	1.192193	-2.945329	0.258554
C	0.747385	0.022829	3.305113
H	-0.223742	0.508742	3.178273
H	0.673098	-0.714381	4.110342
H	1.487479	0.774428	3.595693
H	0.362609	-1.407949	1.747483
C	-3.265638	-0.235589	0.180635
C	-4.716545	1.783350	-0.360708
C	-4.451247	0.621628	0.392562
C	-5.354817	0.243167	1.402828
H	-5.127093	-0.653612	1.963092
C	-6.484895	0.992204	1.675223
C	-6.732137	2.146399	0.923537
C	-5.862868	2.538969	-0.079702
H	-7.170531	0.688358	2.460227
H	-7.616419	2.745967	1.124888
H	-6.041879	3.431535	-0.671105
O	-3.057122	-1.228427	0.879580
O	-2.467670	0.129235	-0.811506
O	-3.916949	2.221659	-1.344966
Bi	-0.467179	-0.735829	-1.220361
O	-0.896708	-2.384182	-0.168770
H	-1.752351	-2.194971	0.301935
C	3.449493	1.079252	1.266393
C	4.208103	2.372052	0.985288
H	3.936754	0.218127	0.782109

INT5

E(scf) = -1417.81898164 a.u.

C	2.716758	-2.050380	1.298784
C	1.560926	-2.839019	0.683186
C	1.172939	0.418932	0.015696
C	1.234139	-0.130127	1.432418
O	2.480155	-0.752288	1.681055
O	1.098146	-2.133343	-0.441682
O	3.825147	-2.476829	1.477911
O	0.110051	0.377331	-0.634006
C	2.028232	-4.232385	0.300031
H	1.182437	-4.796005	-0.106491
H	2.812051	-4.172434	-0.459750
H	2.426124	-4.769775	1.165587
H	0.772958	-2.923152	1.450895
C	1.004818	0.979729	2.451848
H	-0.007080	1.376781	2.329075
H	1.086271	0.543531	3.451211
H	1.729640	1.793986	2.370178
H	0.409351	-0.838998	1.536202
C	-2.844197	0.512891	0.579462
C	-4.290733	2.148797	-0.718853
C	-3.749969	1.682107	0.500296
C	-4.074829	2.350011	1.689947
H	-3.647207	1.963760	2.610121
C	-4.906864	3.455113	1.691949
C	-5.432912	3.911223	0.477917
C	-5.131268	3.270377	-0.711547
H	-5.149747	3.959951	2.622004
H	-6.088825	4.778207	0.462867
H	-5.533898	3.612033	-1.660093
O	-2.351789	0.158333	1.659205
O	-2.606975	-0.112600	-0.550107
O	-4.039027	1.568879	-1.899514
Bi	-0.937519	-1.641792	-0.808705
O	-1.347117	-2.259172	1.054639
H	-1.857469	-1.530026	1.486129
C	3.478388	1.250104	0.034180
C	4.129843	2.359528	-0.760545
H	4.026328	0.308623	-0.045680

H	3.376106	0.867141	2.342781	H	3.389319	1.505182	1.091093
C	5.227958	2.239437	-0.155746	C	5.537886	2.649443	-0.251387
H	3.466113	3.158586	0.761461	H	4.157453	2.068533	-1.818209
H	4.732682	2.691775	1.907182	H	3.506476	3.260602	-0.694197
C	5.979203	3.532212	-0.413522	C	6.218949	3.752075	-1.040133
H	5.969942	1.458477	0.089830	H	5.511899	2.948270	0.804512
H	4.724345	1.921099	-1.090711	H	6.161262	1.748016	-0.307622
H	5.266513	4.311717	-0.751557	H	6.282110	3.460375	-2.102155
H	6.424644	3.888811	0.535147	H	5.610220	4.671009	-0.990635
O	2.121098	1.215335	0.721157	O	2.162445	1.047039	-0.545276
O	6.964262	3.272494	-1.385125	O	7.497363	3.948221	-0.480434
H	-3.172955	1.577208	-1.394076	H	-3.448475	0.804246	-1.702428
H	7.433917	4.097914	-1.563353	H	7.943043	4.640927	-0.983933

p

E(scf) = -1417.83985041 a.u.

C	-1.265655	0.023488	-0.052064
C	-0.083299	-0.683654	-0.692699
C	-4.093024	0.565771	-0.674935
C	-2.960448	1.572013	-0.506677
O	-1.740669	0.963391	-0.900816
O	0.615684	-1.348922	0.333697
O	-1.743048	-0.208766	1.027721
O	-4.006665	-0.484808	-1.260387
C	-0.597824	-1.662151	-1.747462
H	0.250025	-2.133486	-2.254469
H	-1.204730	-2.435451	-1.266271
H	-1.218783	-1.146350	-2.484985
H	0.542870	0.079410	-1.171276
C	-3.166276	2.793768	-1.384880
H	-4.099738	3.294909	-1.115560
H	-2.336018	3.492404	-1.248834
H	-3.208179	2.504726	-2.439596
H	-2.909794	1.850099	0.550953
C	3.443104	0.779753	-0.313456
C	4.905969	2.250571	1.158092
C	4.180110	2.025396	-0.033660
C	4.145125	3.030488	-1.014127
H	3.577841	2.826673	-1.916873
C	4.805028	4.231280	-0.835854

C	5.520498	4.443844	0.348564
C	5.571742	3.471420	1.331663
H	4.768810	4.998228	-1.603129
H	6.044667	5.383424	0.503760
H	6.122298	3.623472	2.254632
O	2.799374	0.602230	-1.343838
O	3.520002	-0.156839	0.633389
O	5.000246	1.356819	2.151577
Bi	2.504218	-2.027137	0.278884
O	2.887597	-2.174586	-1.684137
H	2.846363	-1.276195	-2.061419
C	-6.358790	0.178133	-0.211767
C	-7.506323	0.859016	0.501735
H	-6.119050	-0.793073	0.234330
H	-6.579676	0.009026	-1.271635
C	-8.779818	0.022636	0.444487
H	-7.217070	1.040852	1.545013
H	-7.676963	1.842740	0.044658
C	-9.943073	0.686716	1.155450
H	-9.072283	-0.160440	-0.597646
H	-8.612870	-0.961412	0.901241
H	-9.678020	0.861874	2.211995
H	-10.138242	1.673331	0.701468
O	-5.209640	1.031405	-0.104912
O	-11.062168	-0.164298	1.038781
H	4.483951	0.569502	1.877360
H	-11.803483	0.252155	1.495850

Table S5. Cartesian coordinates (xyz format) of the optimized geometries for all the species involved in the energy profile of the **Scheme S4** calculated at the D3-PBE0/[6-31G(d), LANL2DZ] level.

R

E(scf) = -923.307013398 a.u.

C	-3.077636	-1.180731	0.952296
C	-2.643601	1.119371	-0.185968
C	-3.400879	0.244685	0.623988
C	-4.591732	0.728978	1.189641
H	-5.150704	0.032916	1.806777
C	-5.041990	2.019431	0.977167
C	-4.288818	2.872739	0.168693
C	-3.109813	2.426002	-0.402426
H	-5.967982	2.359662	1.430795
H	-4.621774	3.890743	-0.017570
H	-2.512942	3.075048	-1.036932
O	-3.814662	-1.844480	1.650507
O	-1.962006	-1.723353	0.458992
O	-1.482948	0.815149	-0.802555
Bi	-0.350672	-0.921974	-0.583569
O	0.586059	-0.556267	1.172671
H	-0.012403	-0.772145	1.904628
C	6.809609	0.759682	1.102262
C	5.648659	0.255631	0.267448
H	7.098829	1.769095	0.762274
H	6.494324	0.850334	2.155753
H	5.381090	-0.749636	0.617696
H	5.990407	0.146193	-0.770074
C	4.432722	1.173237	0.327775
C	3.263004	0.647427	-0.498752
H	4.112329	1.291535	1.372769
H	4.711491	2.176721	-0.026291
C	2.059390	1.561286	-0.430345
H	2.972885	-0.342734	-0.124378
H	3.564108	0.529663	-1.548023
H	2.315765	2.565832	-0.791644
H	1.688950	1.629144	0.598308
O	7.874705	-0.155252	0.960512
O	1.028000	1.031078	-1.279458

ET1

E(scf) = -923.277934045 a.u.

C	-2.363650	0.278703	1.557086
C	-2.094566	1.506360	-0.713800
C	-2.633810	1.382615	0.584340
C	-3.492813	2.390941	1.050144
H	-3.893669	2.271072	2.051320
C	-3.810559	3.496097	0.279425
C	-3.265609	3.613600	-1.000149
C	-2.418637	2.627134	-1.488912
H	-4.475248	4.261399	0.668912
H	-3.503236	4.473341	-1.621510
H	-1.997414	2.688652	-2.488027
O	-2.887231	0.267759	2.649728
O	-1.490669	-0.698806	1.252125
O	-1.292704	0.575648	-1.280578
Bi	-0.654602	-1.555502	-0.426212
O	0.554028	-2.417473	0.951864
H	0.323440	-2.066036	1.830114
C	6.229897	1.267421	0.124562
C	4.795401	1.418864	0.626433
H	6.847477	0.795219	0.915185
H	6.242835	0.586733	-0.758303
H	4.813101	2.093798	1.506819
H	4.208132	1.947668	-0.152325
C	4.159656	0.061829	0.972735
C	3.106492	-0.421586	-0.030870
H	4.948453	-0.701977	1.041346
H	3.704035	0.098436	1.969181
C	1.814751	0.367042	0.080632
H	2.862783	-1.478859	0.158366
H	3.487935	-0.345991	-1.058936
H	1.987202	1.438843	-0.099057
H	1.390120	0.263801	1.090899
O	6.706339	2.556038	-0.206541
O	0.872028	-0.063257	-0.901668

H	8.610610	0.156736	1.501799
H	0.244094	1.613280	-1.235709

H	7.627125	2.459247	-0.507895
H	-0.094701	0.627898	-1.139720

INT1

E(scf) = -923.291465206 a.u.

C	-1.746773	0.818766	1.643021
C	-2.245042	1.577415	-0.792350
C	-2.393248	1.686717	0.597053
C	-3.223732	2.704116	1.086826
H	-3.307621	2.799807	2.164479
C	-3.914976	3.553342	0.235272
C	-3.773517	3.410559	-1.143682
C	-2.933152	2.428805	-1.653007
H	-4.561309	4.324203	0.644473
H	-4.308019	4.068529	-1.823319
H	-2.786448	2.304563	-2.721490
O	-1.609899	1.239805	2.771769
O	-1.399395	-0.429488	1.350814
O	-1.443229	0.621239	-1.383235
Bi	-0.877678	-1.626013	-0.273014
O	0.069833	-2.762502	1.102735
H	0.139453	-2.263506	1.932634
C	6.630734	1.280515	0.489094
C	5.401521	1.159024	-0.389925
H	6.376522	1.843411	1.403512
H	6.957400	0.275659	0.807661
H	5.679477	0.613191	-1.301008
H	5.101690	2.166149	-0.707678
C	4.240747	0.459952	0.308878
C	3.005197	0.336243	-0.577703
H	4.557318	-0.542176	0.633725
H	3.978939	1.009432	1.225096
C	1.854842	-0.361445	0.125347
H	3.249102	-0.222878	-1.490419
H	2.674773	1.333219	-0.899423
H	1.577457	0.192539	1.036404
H	2.157690	-1.369753	0.441078
O	7.636500	1.935779	-0.254500
O	0.746888	-0.438921	-0.758125
H	8.416357	2.018521	0.308384

INT2

E(scf) = -1457.07824395 a.u.

C	-2.219567	-1.914396	2.410914
C	-1.007390	-2.830685	2.299370
C	-1.282037	-2.769858	-0.068621
C	-2.758357	-2.833721	0.271545
O	-3.038772	-1.919533	1.339584
O	-0.450341	-2.771869	0.969272
O	-2.467575	-1.249651	3.376874
O	-0.844030	-2.720495	-1.198067
C	0.090467	-2.472195	3.269948
H	0.887608	-3.218763	3.224564
H	0.508052	-1.493459	3.019572
H	-0.318179	-2.438097	4.281989
H	-1.353421	-3.861873	2.469020
C	-3.640525	-2.472257	-0.897858
H	-3.467383	-3.167061	-1.722799
H	-4.689536	-2.521687	-0.595832
H	-3.412416	-1.461392	-1.244602
H	-2.979935	-3.856054	0.617492
C	2.287321	2.012471	-0.862025
C	2.641074	1.021037	1.491411
C	2.876759	2.004782	0.520189
C	3.748276	3.053903	0.833627
H	3.889252	3.830300	0.087822
C	4.424544	3.095049	2.045345
C	4.214852	2.084648	2.981832
C	3.314800	1.061156	2.710478
H	5.111065	3.909085	2.258791
H	4.736081	2.103152	3.935203
H	3.104504	0.285115	3.440418
O	1.980881	3.059528	-1.395223
O	2.237263	0.853776	-1.506065
O	1.748656	-0.005666	1.301716
Bi	1.230750	-0.972846	-1.242911
O	0.512583	-0.660603	-3.103675
H	0.764034	0.244731	-3.351017

H	-0.476722	0.756792	-1.202587

C	-4.994074	4.146525	-0.477133
C	-4.111234	3.126812	0.215010
H	-4.373118	4.978597	-0.850382
H	-5.475979	3.682898	-1.355456
H	-4.748690	2.323430	0.606766
H	-3.643441	3.605943	1.084773
C	-3.042176	2.549563	-0.705973
C	-2.144655	1.533656	-0.005069
H	-3.523671	2.074667	-1.574167
H	-2.423085	3.364313	-1.108550
C	-1.090312	0.957226	-0.933207
H	-2.749882	0.715360	0.406883
H	-1.642308	2.009912	0.847831
H	-0.468724	1.769154	-1.339381
H	-1.561936	0.452308	-1.788700
O	-5.954526	4.599807	0.453968
O	-0.291156	0.026310	-0.212190
H	-6.498115	5.267706	0.017814
H	0.866546	0.332807	0.985323

ET2

E(scf) = -1457.05532141 a.u.

C	-0.126525	3.855369	1.090431
C	-0.835994	3.122033	2.218623
C	-1.782510	1.663600	0.553800
C	-1.910182	2.970242	-0.218393
O	-0.704087	3.743033	-0.117749
O	-1.309902	1.831726	1.821500
O	0.866432	4.519385	1.241220
O	-2.739102	0.814615	0.450556
C	0.053473	2.937779	3.425552
H	-0.500204	2.420467	4.214656
H	0.935583	2.348224	3.162814
H	0.388428	3.910084	3.792850
H	-1.713053	3.732153	2.492208
C	-2.274749	2.831385	-1.689572
H	-1.448403	3.219634	-2.301993
H	-2.456295	1.783900	-1.968055
H	-3.170600	3.419847	-1.926756
H	-2.703777	3.508301	0.318458

INT3

E(scf) = -1457.07972799 a.u.

C	-1.989707	-2.567623	2.476182
C	-0.815331	-1.597863	2.519618
C	-0.394902	-1.910428	0.151626
C	-0.859074	-3.335444	0.545026
O	-2.042895	-3.316557	1.356291
O	-0.693995	-0.998610	1.225403
O	-2.836551	-2.657641	3.323930
O	0.944500	-1.991330	-0.056154
C	-1.027318	-0.502582	3.538343
H	-0.151964	0.151982	3.580995
H	-1.908876	0.090498	3.280396
H	-1.190037	-0.943879	4.524149
H	0.105468	-2.156238	2.752476
C	-1.130788	-4.215250	-0.651164
H	-0.249335	-4.231184	-1.297553
H	-1.350841	-5.234301	-0.321462
H	-1.980869	-3.842286	-1.227866
H	-0.042193	-3.764627	1.137334

C	1.079951	-2.236546	-1.044223
C	0.606128	-2.369032	1.499042
C	1.267941	-2.799953	0.342225
C	2.192677	-3.843702	0.468720
H	2.731280	-4.144614	-0.424342
C	2.410237	-4.476265	1.685039
C	1.715239	-4.053968	2.816610
C	0.822897	-2.992521	2.724105
H	3.121364	-5.294391	1.751764
H	1.878062	-4.538929	3.775068
H	0.288296	-2.620817	3.592813
O	2.019244	-2.230382	-1.817734
O	-0.119309	-1.827994	-1.404333
O	-0.305627	-1.325839	1.489417
Bi	-1.923486	-1.067476	-0.516772
O	-2.280566	-0.420552	-2.405845
H	-1.508444	-0.651696	-2.946118
C	5.561447	1.577135	-1.549167
C	4.400735	1.420030	-0.586688
H	5.582792	0.719074	-2.241780
H	5.416947	2.485165	-2.159095
H	4.407547	2.269590	0.108554
H	4.570299	0.516439	0.013249
C	3.056245	1.331671	-1.301279
C	1.891439	1.143346	-0.333836
H	2.894810	2.241413	-1.894729
H	3.065335	0.486540	-2.003866
C	0.557629	1.104539	-1.060764
H	1.889047	1.948590	0.412709
H	2.035153	0.198455	0.208871
H	0.590559	0.365934	-1.868955
H	0.328453	2.078320	-1.499145
O	6.750557	1.655813	-0.790622
O	-0.512709	0.718279	-0.187083
H	7.489292	1.741511	-1.406004
H	0.100935	-0.478199	1.212916

C	0.619808	2.229993	-0.564859
C	2.035940	1.588062	1.484066
C	1.535000	2.539318	0.584825
C	1.889010	3.880430	0.773678
H	1.462652	4.609067	0.091177
C	2.753045	4.261796	1.790000
C	3.265985	3.296743	2.656174
C	2.900956	1.964030	2.508822
H	3.024811	5.306258	1.910108
H	3.942135	3.582955	3.457089
H	3.267347	1.195484	3.182597
O	-0.103518	3.089345	-1.021227
O	0.619455	1.001022	-1.067029
O	1.746440	0.244419	1.375743
Bi	2.019491	-0.555366	-1.121190
O	1.286056	-1.124941	-2.896854
H	0.321449	-1.211060	-2.820558
C	-2.385116	-1.062455	-0.967400
C	-2.620846	0.427436	-0.794949
H	-2.898573	-1.639339	-0.191220
H	-2.775718	-1.397141	-1.936027
C	-4.089412	0.787415	-0.999570
H	-2.298058	0.729655	0.207555
H	-1.990398	0.978566	-1.501558
C	-4.366354	2.268439	-0.762345
H	-4.392773	0.516302	-2.022282
H	-4.718471	0.185638	-0.325788
H	-4.116291	2.537276	0.272108
H	-3.723235	2.881872	-1.405693
O	-0.990625	-1.404956	-0.994468
C	-5.813691	2.640289	-1.016261
H	0.776219	0.063126	1.337845
H	-6.074784	2.414226	-2.064635
H	-6.890839	4.250414	-0.907407
O	-5.970978	4.014914	-0.733714
H	-6.470914	2.022959	-0.379269

ET3

E(scf) = 1457.08100521 a.u.

C	-0.704415	3.777878	-0.010198

INT4

E(scf) = -1457.07908328 a.u.

C	-0.780387	3.797258	-0.022232

C	0.131718	2.828700	-0.855575	C	0.055746	2.848080	-0.867609
C	-0.444699	0.965101	0.519350	C	-0.520671	0.984481	0.507316
C	-0.415958	2.068804	1.605891	C	-0.491930	2.088184	1.593857
O	-1.105522	3.245719	1.170748	O	-1.181494	3.265099	1.158714
O	-0.496862	1.546089	-0.758839	O	-0.572834	1.565469	-0.770873
O	-1.051746	4.880946	-0.333487	O	-1.127718	4.900326	-0.345521
O	0.607848	0.220047	0.664182	O	0.607848	0.220047	0.664182
C	0.186221	3.225781	-2.309544	C	0.110249	3.245161	-2.321578
H	0.850703	2.541242	-2.842830	H	0.774731	2.560622	-2.854864
H	-0.813941	3.203664	-2.752074	H	-0.889913	3.223044	-2.764108
H	0.575912	4.242619	-2.396777	H	0.499940	4.261999	-2.408811
H	1.156146	2.763284	-0.460703	H	1.080174	2.782664	-0.472737
C	-1.019659	1.635933	2.920337	C	-1.095631	1.655313	2.908303
H	-2.082187	1.406763	2.807496	H	-2.158159	1.426143	2.795462
H	-0.509725	0.739422	3.283755	H	-0.585697	0.758802	3.271721
H	-0.907201	2.432986	3.660249	H	-0.983173	2.452366	3.648215
H	0.641187	2.323547	1.752453	H	0.565215	2.342927	1.740419
C	2.980007	0.219848	2.466581	C	3.039223	0.185766	-1.057161
C	2.201290	-2.204824	2.491513	C	3.851269	-0.778317	1.155796
C	2.804249	-1.111920	3.129723	C	4.091962	-0.050261	-0.017793
C	3.301139	-1.279732	4.424623	C	5.378186	0.442528	-0.251484
H	3.735112	-0.417109	4.921816	H	5.544447	1.034211	-1.146984
C	3.264581	-2.521276	5.048283	C	6.420623	0.161444	0.623752
C	2.704851	-3.609978	4.383238	C	6.176850	-0.603569	1.762253
C	2.159365	-3.448159	3.113319	C	4.890740	-1.058897	2.036170
H	3.673944	-2.640345	6.047148	H	7.419561	0.534234	0.417262
H	2.673062	-4.585411	4.860867	H	6.985081	-0.830867	2.451970
H	1.682919	-4.272655	2.591641	H	4.668930	-1.623290	2.936838
O	2.792453	1.262882	3.056294	O	2.913275	1.255124	-1.615254
O	3.461797	0.148070	1.225496	O	2.343976	-0.904528	-1.381905
O	1.610435	-2.083758	1.248034	O	2.584182	-1.216592	1.491077
Bi	2.346229	-0.005913	-0.512403	Bi	0.595691	-1.553366	-0.481347
O	2.663022	1.889164	-1.089069	O	-0.593321	-1.013269	-2.004096
H	2.318412	2.512920	-0.428081	H	-0.537907	-0.055814	-2.162031
C	-7.654096	-0.869226	0.023690	C	-7.730068	-0.849846	0.011656
C	-6.267102	-1.178892	0.551858	C	-6.343074	-1.159512	0.539824
H	-7.954847	0.142681	0.345210	H	-8.030819	0.162061	0.333176
H	-7.636327	-0.866767	-1.079601	H	-7.712299	-0.847387	-1.091635
H	-5.993165	-2.192600	0.231428	H	-6.069137	-2.173220	0.219394
H	-6.310118	-1.197889	1.648700	H	-6.386090	-1.178509	1.636666
C	-5.217926	-0.177359	0.082531	C	-5.293898	-0.157979	0.070497

C	-3.821219	-0.502151	0.603082
H	-5.198732	-0.152506	-1.016663
H	-5.503977	0.833999	0.406803
C	-2.787822	0.497138	0.126227
H	-3.522436	-1.503304	0.264823
H	-3.823828	-0.526879	1.700903
H	-3.014934	1.505654	0.494276
H	-2.753318	0.530298	-0.967563
O	-8.537817	-1.850852	0.521713
O	-1.515972	0.073377	0.624765
H	-9.420869	-1.655874	0.183918
H	0.868530	-1.447644	1.319811

C	-3.897191	-0.482771	0.591048
H	-5.274704	-0.133126	-1.028697
H	-5.579949	0.853379	0.394769
C	-2.863794	0.516518	0.114193
H	-3.598408	-1.483924	0.252789
H	-3.899800	-0.507499	1.688869
H	-3.090906	1.525034	0.482242
H	-2.829290	0.549678	-0.979597
O	-8.613789	-1.831472	0.509679
O	-1.591944	0.092757	0.612731
H	-9.496841	-1.636494	0.171884
H	2.007957	-0.432817	1.608884

ET4

E(scf) = -1457.08036081 a.u.

C	2.404578	-2.404904	1.426088
C	1.503508	-2.679041	0.228415
C	0.964637	0.140200	0.639483
C	0.884270	-0.613738	1.959876
O	2.066563	-1.360224	2.225377
O	1.199414	-1.462539	-0.433264
O	3.388352	-3.041708	1.696244
O	-0.161359	0.525988	0.129780
C	2.170872	-3.650669	-0.734564
H	1.491364	-3.877317	-1.562609
H	3.086666	-3.211795	-1.140465
H	2.429373	-4.583900	-0.221200
H	0.579912	-3.133018	0.626546
C	0.656787	0.339305	3.118098
H	1.486247	1.036911	3.238664
H	-0.267516	0.901150	2.957814
H	0.563391	-0.240853	4.039932
H	0.023872	-1.279707	1.859024
C	-3.477489	0.128718	0.303625
C	-4.723088	2.169782	-0.566867
C	-4.517536	1.175918	0.416220
C	-5.328014	1.172690	1.561559
H	-5.146117	0.396044	2.297982
C	-6.317905	2.120615	1.746447
C	-6.510155	3.101994	0.767461

INT5

E(scf) = -1457.07908328 a.u.

C	-0.780387	3.797258	-0.022232
C	0.055746	2.848080	-0.867609
C	-0.520671	0.984481	0.507316
C	-0.491930	2.088184	1.593857
O	-1.181494	3.265099	1.158714
O	-0.572834	1.565469	-0.770873
O	-1.127718	4.900326	-0.345521
O	0.607848	0.220047	0.664182
C	0.110249	3.245161	-2.321578
H	0.774731	2.560622	-2.854864
H	-0.889913	3.223044	-2.764108
H	0.499940	4.261999	-2.408811
H	1.080174	2.782664	-0.472737
C	-1.095631	1.655313	2.908303
H	-2.158159	1.426143	2.795462
H	-0.585697	0.758802	3.271721
H	-0.983173	2.452366	3.648215
H	0.565215	2.342927	1.740419
C	3.039223	0.185766	-1.057161
C	3.851269	-0.778317	1.155796
C	4.091962	-0.050261	-0.017793
C	5.378186	0.442528	-0.251484
H	5.544447	1.034211	-1.146984
C	6.420623	0.161444	0.623752
C	6.176850	-0.603569	1.762253

C	-5.725948	3.129172	-0.372788	C	4.890740	-1.058897	2.036170
H	-6.936683	2.103129	2.638359	H	7.419561	0.534234	0.417262
H	-7.283891	3.854445	0.898387	H	6.985081	-0.830867	2.451970
H	-5.864131	3.883834	-1.140817	H	4.668930	-1.623290	2.936838
O	-3.299214	-0.699880	1.197445	O	2.913275	1.255124	-1.615254
O	-2.768508	0.141451	-0.817708	O	2.343976	-0.904528	-1.381905
O	-4.002340	2.250579	-1.693690	O	2.584182	-1.216592	1.491077
Bi	-0.927083	-1.031635	-1.139447	Bi	0.595691	-1.553366	-0.481347
O	-1.482036	-2.394498	0.215988	O	-0.593321	-1.013269	-2.004096
H	-2.233841	-1.992635	0.712841	H	-0.537907	-0.055814	-2.162031
C	7.441563	2.384759	-0.922306	C	-7.730068	-0.849846	0.011656
C	6.511304	2.872498	0.184730	C	-6.343074	-1.159512	0.539824
H	8.102150	1.584497	-0.517606	H	-8.030819	0.162061	0.333176
H	6.850108	1.939277	-1.750936	H	-7.712299	-0.847387	-1.091635
H	5.904489	3.706284	-0.209752	H	-6.069137	-2.173220	0.219394
H	7.138321	3.300329	0.988850	H	-6.386090	-1.178509	1.636666
C	5.604214	1.755530	0.732610	C	-5.293898	-0.157979	0.070497
C	4.160614	1.836910	0.213252	C	-3.897191	-0.482771	0.591048
H	6.031681	0.771900	0.477781	H	-5.274704	-0.133126	-1.028697
H	5.583029	1.797442	1.833683	H	-5.579949	0.853379	0.394769
C	3.324800	0.698780	0.748477	C	-2.863794	0.516518	0.114193
H	4.144085	1.822495	-0.887228	H	-3.598408	-1.483924	0.252789
H	3.707520	2.787806	0.525916	H	-3.899800	-0.507499	1.688869
H	3.360231	0.655492	1.843008	H	-3.090906	1.525034	0.482242
H	3.661951	-0.265809	0.357033	H	-2.829290	0.549678	-0.979597
O	8.201725	3.489442	-1.363897	O	-8.613789	-1.831472	0.509679
O	1.972763	0.915689	0.308598	O	-1.591944	0.092757	0.612731
H	8.812242	3.178929	-2.049481	H	-9.496841	-1.636494	0.171884
H	-3.361494	1.505307	-1.659492	H	2.007957	-0.432817	1.608884

p

E(scf) = -1457.08373899 a.u.

C	2.039566	-2.614841	1.326226
C	0.794960	-3.173342	0.635614
C	0.968859	0.116139	0.095114
C	0.891922	-0.481024	1.491349
O	2.007868	-1.310061	1.753986
O	0.497823	-2.351882	-0.465935
O	3.052078	-3.229257	1.527107
O	-0.068163	0.285526	-0.576962

C	1.041962	-4.606563	0.197686
H	0.132418	-5.001724	-0.265949
H	1.855745	-4.643793	-0.531435
H	1.308910	-5.241679	1.047157
H	-0.024849	-3.159481	1.374215
C	0.814666	0.619545	2.542997
H	1.665329	1.305756	2.509964
H	-0.113658	1.181851	2.406141
H	0.790066	0.146070	3.528311
H	-0.041150	-1.046814	1.546134
C	-3.006812	0.861021	0.553515
C	-4.089772	2.772739	-0.721404
C	-3.694713	2.171239	0.494617
C	-3.955553	2.837342	1.700996
H	-3.643696	2.346578	2.617859
C	-4.584695	4.069116	1.722433
C	-4.967133	4.657524	0.511538
C	-4.724736	4.021984	-0.694172
H	-4.780593	4.571189	2.664994
H	-5.462688	5.625261	0.511917
H	-5.017605	4.465916	-1.640562
O	-2.634546	0.383468	1.634061
O	-2.825727	0.250376	-0.594697
O	-3.886259	2.205472	-1.917315
Bi	-1.421718	-1.521457	-0.869850
O	-1.984998	-2.126539	0.956383
H	-2.390612	-1.339202	1.398836
C	7.978124	2.567634	-0.201585
C	6.560039	2.541750	-0.738360
H	7.962586	2.827436	0.870849
H	8.423281	1.561446	-0.285030
H	6.598381	2.295865	-1.807346
H	6.142999	3.554436	-0.664221
C	5.668300	1.548993	-0.001250
C	4.241953	1.532915	-0.545079
H	6.099785	0.540358	-0.074932
H	5.650291	1.796715	1.070170
C	3.380299	0.536742	0.197806
H	4.247510	1.275457	-1.611382
H	3.794543	2.531458	-0.461404
H	3.304531	0.776433	1.259684

H	3.756833	-0.484402	0.104141
O	8.704727	3.516523	-0.950872
O	2.066428	0.582100	-0.419395
H	9.610103	3.532504	-0.616231
H	-3.443146	1.344046	-1.733505

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