Electronic Supplementary Information (ESI)

Structural subtleties and catalytic activity of sodium aminophenolate complexes in polylactide degradation: towards sustainable waste management solutions

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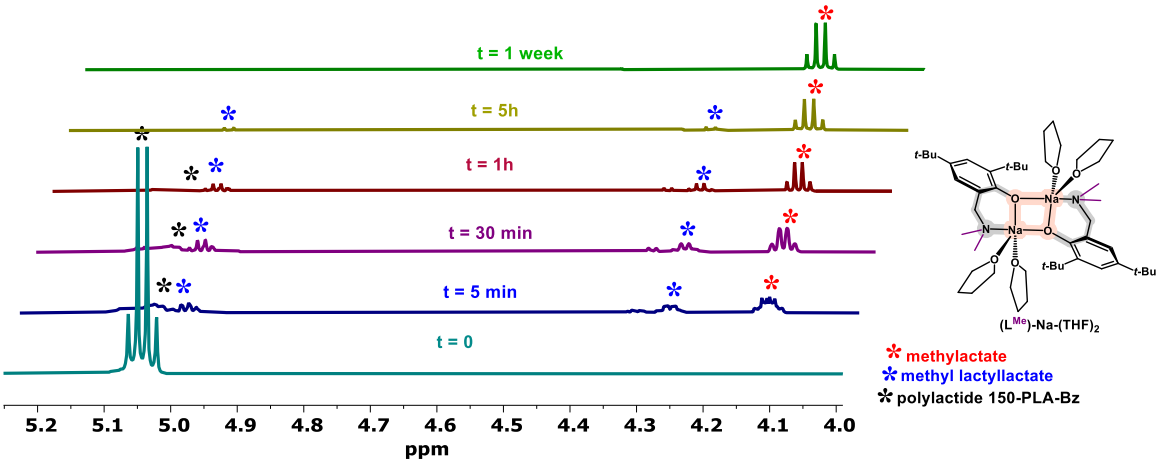


Figure S1. PLA degradation process in the presence of (L^{Me})-Na-$(THF)_2$ monitored by ^1H NMR (C_6D_6).

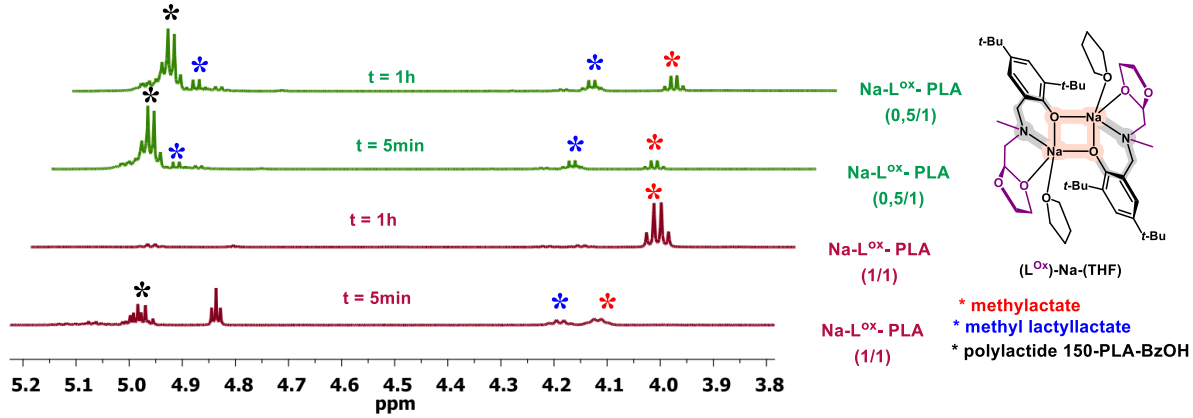


Figure S2. Comparison of PLA depolymerization spectra in the presence of (L^{Ox})-Na-(THF) with different molar ratio [Na]/PLA monitored by ^1H NMR (C_6D_6).

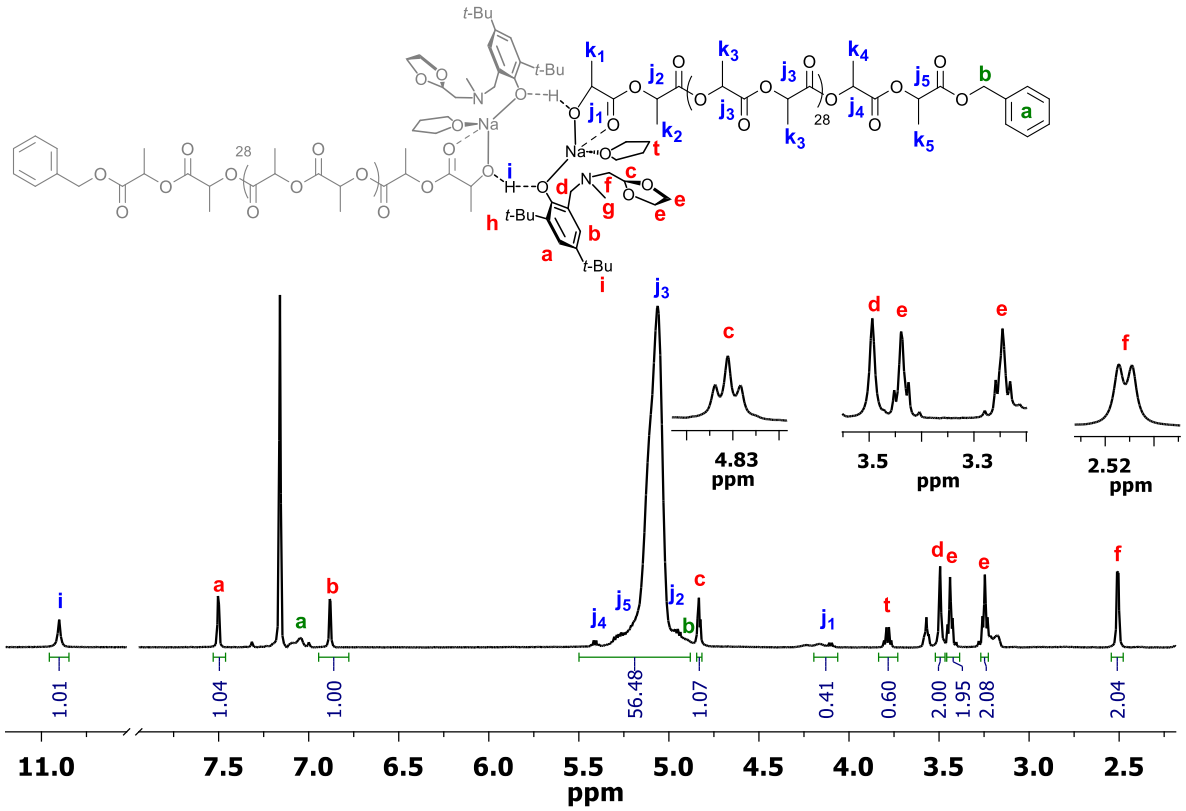
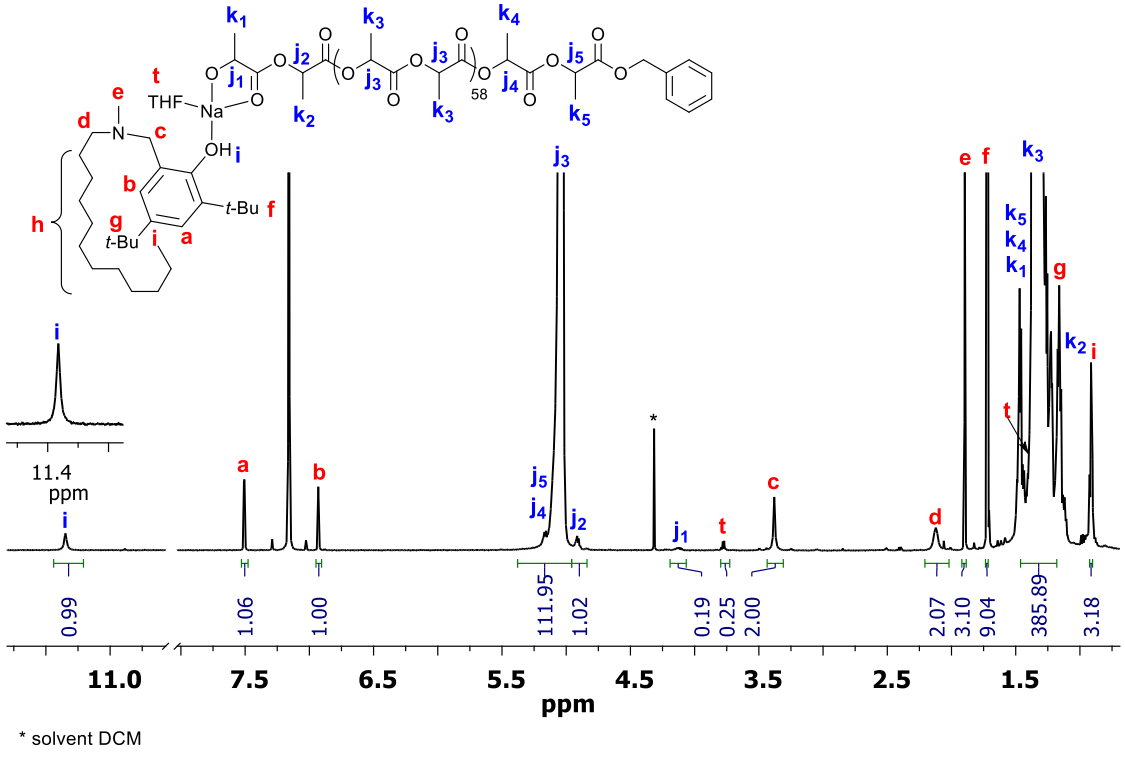


Figure S3. ^{1}H NMR of adduct (L^{Ox})-Na-(THF) with PLA in C_6D_6.



* solvent DCM

Figure S4. ^{1}H NMR of adduct (L^{C12})-Na-(THF) with PLA in C_6D_6.

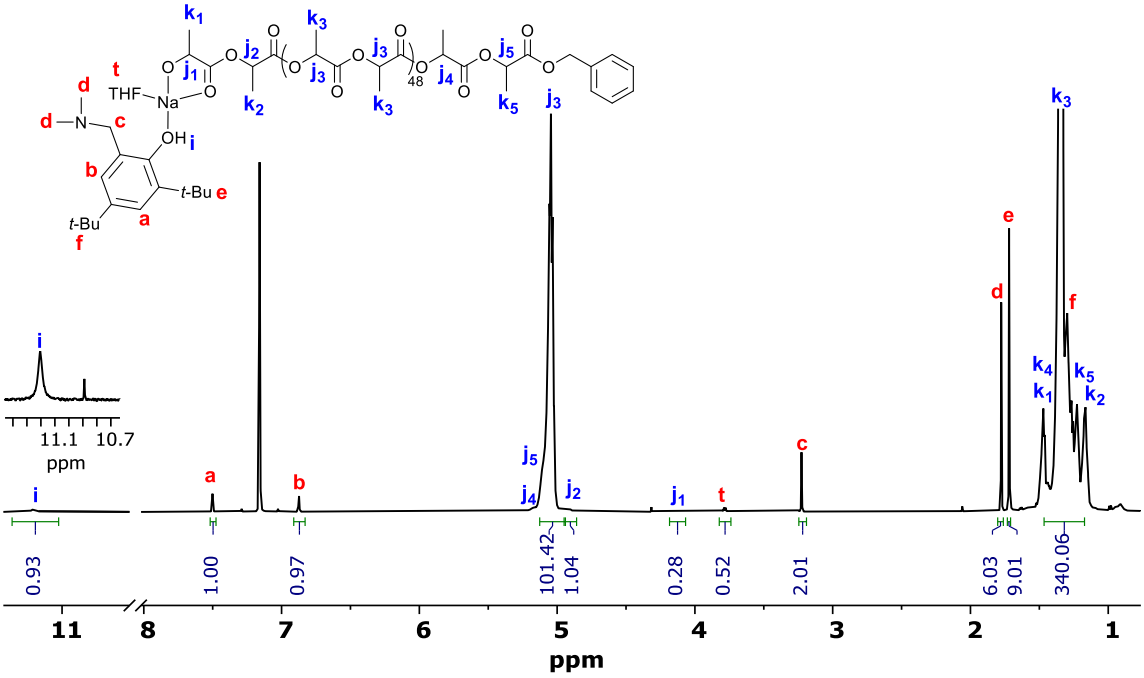


Figure S5. ^{1}H NMR of adduct (L^{Me})-Na-$(THF)_2$ with PLA in C_6D_6.

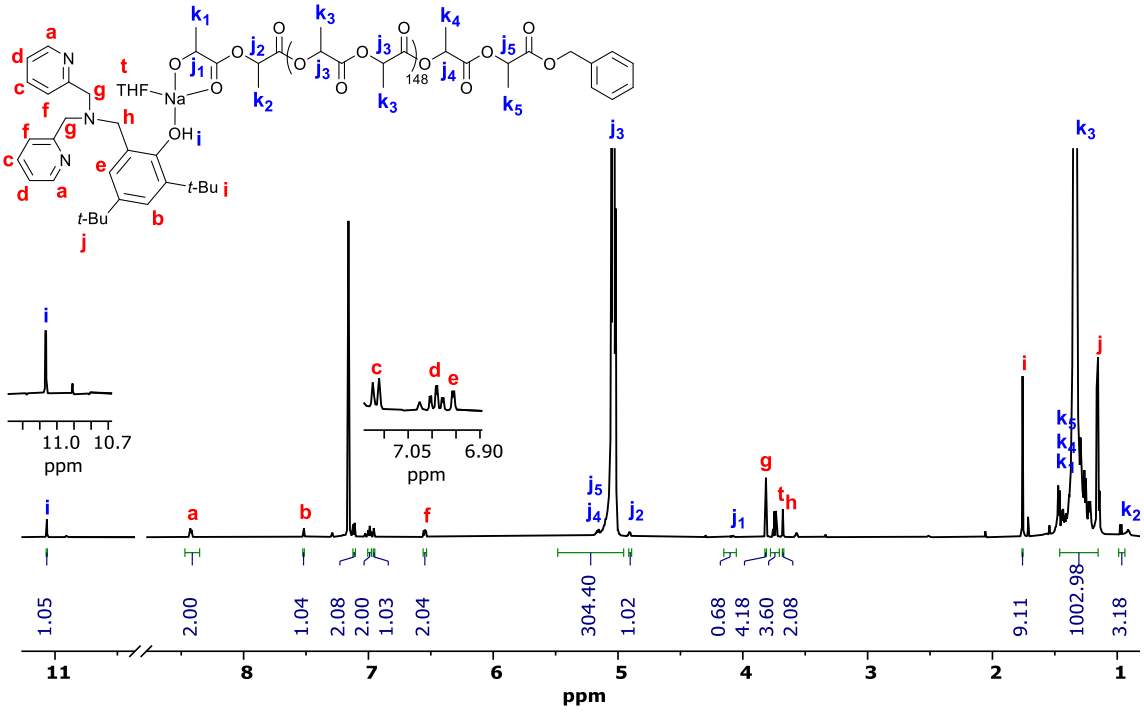


Figure S6. ^{1}H NMR of adduct (L^{Pic})-Na with PLA in C_6D_6.

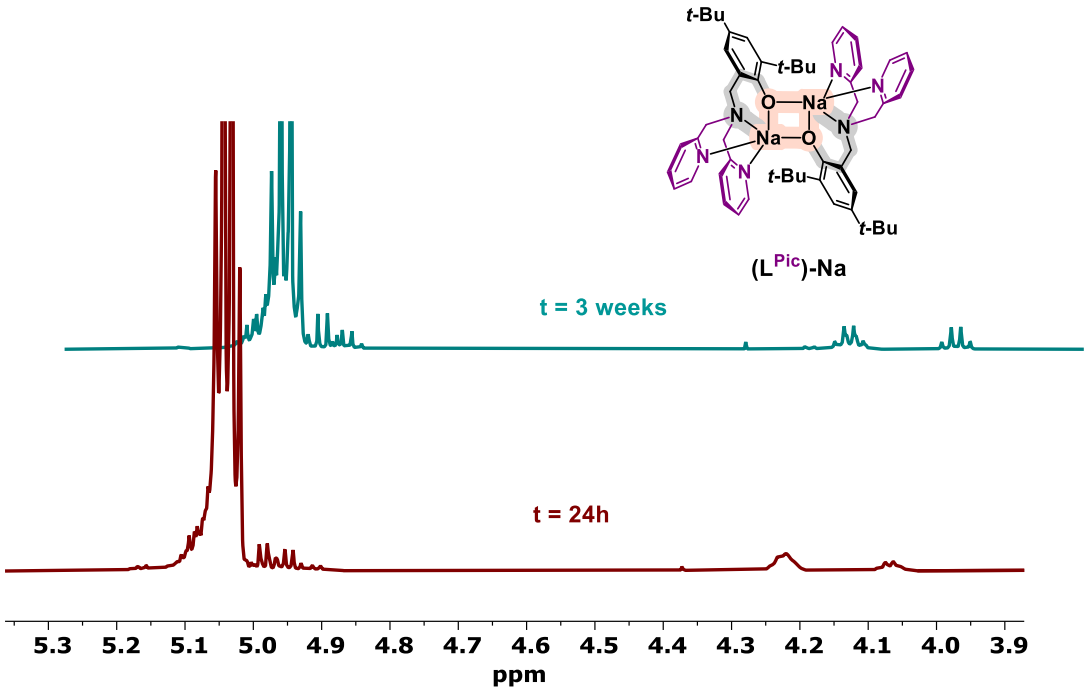


Figure S7. Comparison of PLA depolymerization spectra in the presence of (L^{Pic})-Na in ^{1}H NMR C_6D_6.

Table S1. Energies of calculated models for two proposed versions of the structural motifs of the active sodium catalysts in the PLA degradation reaction. Data are given in Hartree.

	E_{tot}	E_{tot} with ZPE correction	H	G	S[a]
(L^{Bn})-Na-(THF)	-3303.460549	-3302.045167	-3301.967236	-3302.164135	414.408
(L^{Bn})-Na-(THF)(PLA)	-4603.784366	-4601.973558	-4601.865839	-4602.126575	548.764
(L^{Bn})-Na-(THF)(PLA)(ROH)	-4835.254965	-4833.334068	-4833.218221	-4833.499149	591.262
(L^{Bn})-Na-(THF)(LA-Me)	-4069.359803	-4067.692481	-4067.596080	-4067.831676	495.853
(L^{Bn})-Na-(THF)(PLA)	-4603.808076	-4601.997814	-4601.890120	-4602.151032	549.134
(L^{Bn})-Na-(THF)(PLA)(ROH)	-4835.280945	-4833.361123	-4833.245841	-4833.522993	583.314
(L^{Bn})-Na-(THF)(LA-Me)	-4069.393970	-4067.726537	-4067.629907	-4067.866598	498.157
(L^{Me})-Na-$(THF)_2$	-2844.167564	-2842.840519	-2842.767187	-2842.951596	388.120
(L^{Me})-Na-$(THF)_2$(PLA)	-4144.456252	-4142.733063	-4142.630242	-4142.878734	522.995
(L^{Me})-Na-$(THF)_2$(PLA)(ROH)	-4375.951451	-4374.118976	-4374.007996	-4374.275665	563.356
(L^{Me})-Na-$(THF)_2$(LA-Me)	-3610.047353	-3608.467104	-3608.375772	-3608.597440	466.540
(L^{Me})-Na-$(THF)_2$(PLA)	-4144.488641	-4142.764941	-4142.662396	-4142.911159	523.567
(L^{Me})-Na-$(THF)_2$(PLA)(ROH)	-4375.959765	-4374.128818	-4374.017476	-4374.286701	566.630
(L^{Me})-Na-$(THF)_2$(LA-Me)	-3610.065810	-3608.485679	-3608.394186	-3608.618956	473.070
(L^{C12})-Na-(THF)	-3244.188363	-3242.466504	-3242.377570	-3242.597035	461.903
(L^{C12})-Na-(THF)(PLA)	-4544.475057	-4542.360346	-4542.240561	-4542.537995	626.001
(L^{C12})-Na-(THF)(PLA)(ROH)	-4776.001223	-4773.774446	-4773.648273	-4773.948492	631.864
(L^{C12})-Na-(THF)(LA-Me)	-4010.051711	-4008.080648	-4007.971800	-4008.246065	577.240

(L^{C12})-Na-(THF)(PLA)	-4544.491270	-4542.376354	-4542.257090	-4542.551691	620.040
(L^{C12})-Na-(THF)(PLA)(ROH)	-4775.961398	-4773.738489	-4773.610486	-4773.924201	660.268
(L^{C12})-Na-(THF)(LA-Me)	-4010.071539	-4008.102042	-4007.992783	-4008.269421	582.235
(L^{Pic})-Na	-2902.677795	-2901.549981	-2901.485433	-2901.650461	347.331
(L^{Pic})-Na-(PLA)	-4202.974183	-4201.452226	-4201.357809	-4201.588408	485.337
(L^{Pic})-Na-(PLA)(ROH)	-4434.464773	-4432.834103	-4432.731604	-4432.979461	521.660
(L^{Pic})-Na-(LA-Me)	-3668.553897	-3667.174855	-3667.091202	-3667.299903	439.249
(L^{Pic})-Na-(PLA)	-4202.995834	-4201.473053	-4201.378584	-4201.610442	487.985
(L^{Pic})-Na-(PLA)(ROH)	-4434.469430	-4432.838152	-4432.735510	-4432.987607	530.581
(L^{Pic})-Na-(LA-Me)	-3668.585781	-3667.205850	-3667.122586	-3667.328051	432.439
(L^{Ox})-Na-(THF)	-2913.552811	-2912.315754	-2912.246484	-2912.422298	370.032
(L^{Ox})-Na-(THF)(PLA)	-4213.852174	-4212.218845	-4212.119971	-4212.361620	508.593
(L^{Ox})-Na-(THF)(PLA)(ROH)	-4445.362308	-4443.619223	-4443.512612	-4443.768545	538.657
(L^{Ox})-Na-(THF)(LA-Me)	-3679.432804	-3677.943526	-3677.855614	-3678.072777	457.058
(L^{Ox})-Na-(THF)(PLA)	-4213.871562	-4212.238951	-4212.140064	-4212.381994	509.186
(L^{Ox})-Na-(THF)(PLA)(ROH)	-4445.343817	-4443.602680	-4443.495994	-4443.755417	546.002
(L^{Ox})-Na-(THF)(LA-Me)	-3679.461323	-3677.971559	-3677.883960	-3678.098296	451.107

[a] data are given in cal/mol*K

Table S2. Energies of calculated models for two proposed versions of the active catalyst (L^{Ox})-Na-(THF)(PLA) structural motif with decoordination of amine arm in the degradation reaction of PLA. Data are given in Hartree.

		E_{tot}	E_{tot} with ZPE correction	H	G	S[a]
Path A	(L^{Ox})-Na-(THF)(PLA)	-4213.866080	-4212.233286	-4212.134725	-4212.375577	506.916
	(L^{Ox})-Na-(THF)(PLA)*	-4213.845786	-4212.214269	-4212.115027	-4212.361145	517.999
Path B	(L^{Ox})-Na-(THF)(PLA)	-4213.866608	-4212.233981	-4212.135208	-4212.378009	511.018
	(L^{Ox})-Na-(THF)(PLA)*	-4213.859906	-4212.225599	-4212.127171	-4212.366199	503.078

[a] data are given in cal/mol*K

Table S3 Energies of calculated models for the proposed version of the active catalyst (L^{Ox})-Na-(THF) structural motif with one active centre in the degradation reaction of PLA. Data are given in Hartree.

	E_{tot}	E_{tot} with ZPE correction	H	G	S[a]
(L^{Ox})-Na-(THF)(PLA)	-3563.720827	-3562.284897	-3562.201327	-3562.406838	432.534
(L^{Ox})-Na-(THF)(PLA)(ROH)	-3679.471069	-3677.980285	-3677.892936	-3678.106586	449.664
(L^{Ox})-Na-(THF)(LA-Me)	-3296.515150	-3295.150354	-3295.072508	-3295.264337	403.738

[a] data are given in cal/mol*K