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Supporting Information

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Supporting Information

for

Influence of the Nucleophile on the *Candida antarctica* Lipase B-Catalysed Resolution of a Chiral Acyl Donor

Eduardo García-Urdiales, Nicolás Ríos-Lombardía, Juan Mangas-Sánchez, Vicente Gotor-Fernández and Vicente Gotor*

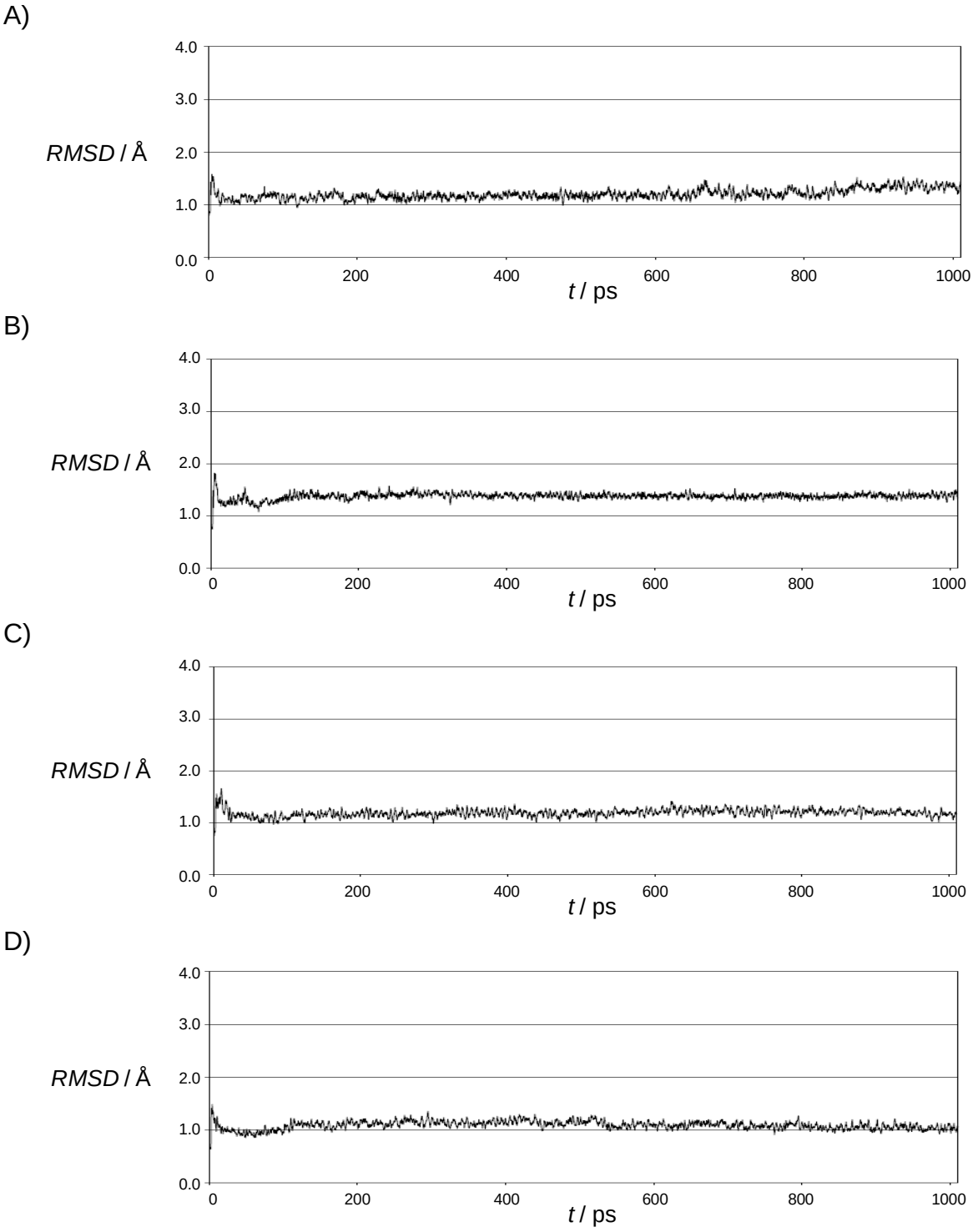
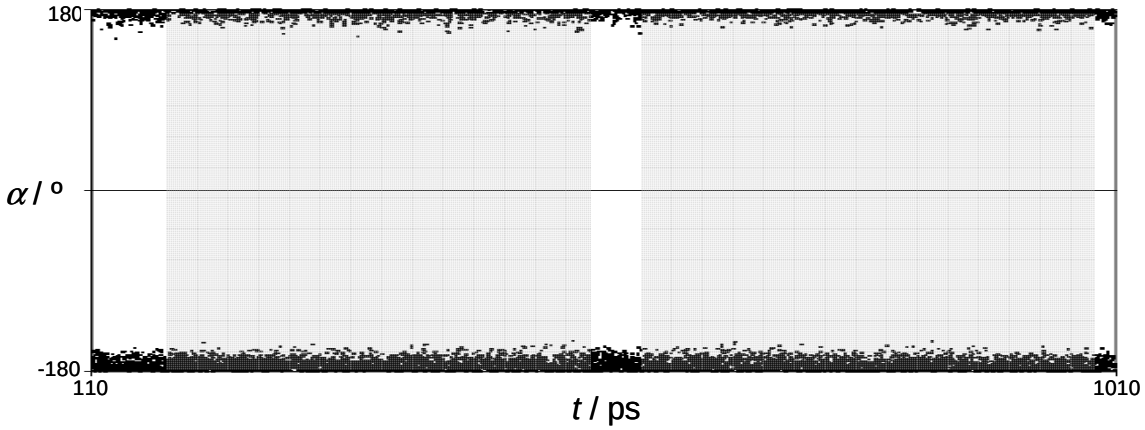


Figure S1. Time dependence of the RMSD (Å) of the CALB backbone atoms with respect to the coordinates of the original crystal structure (PDB entry number: 1TCA) during the 1ns MDS of A) IT_2-(*R*)-**3a**, B) IT_2-(*S*)-**3a**, C) IT_2-(*R*)-**3b** and D) IT_2-(*S*)-**3b**.

OG-CD-CH-CI



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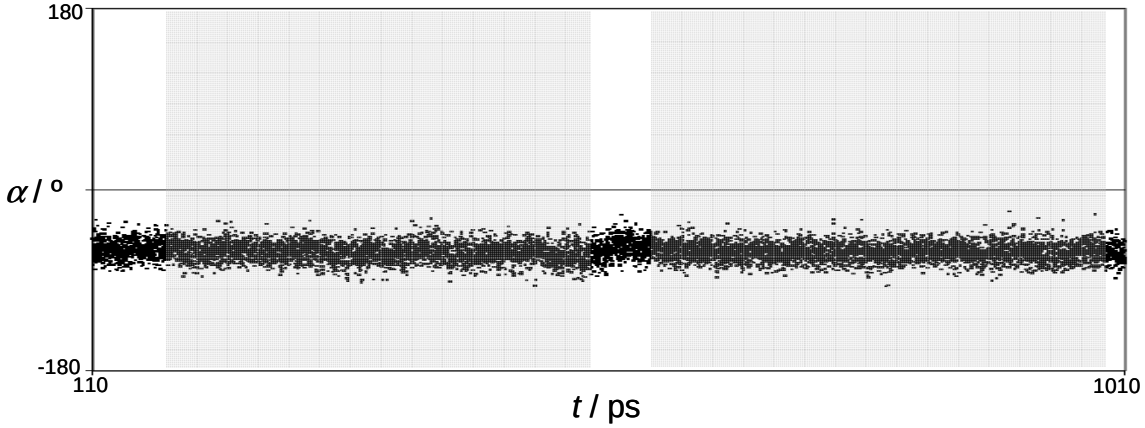

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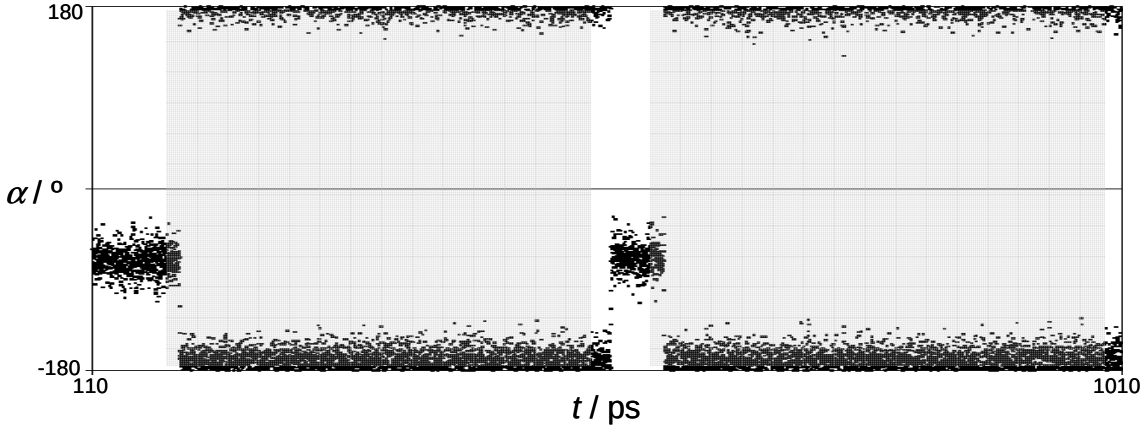
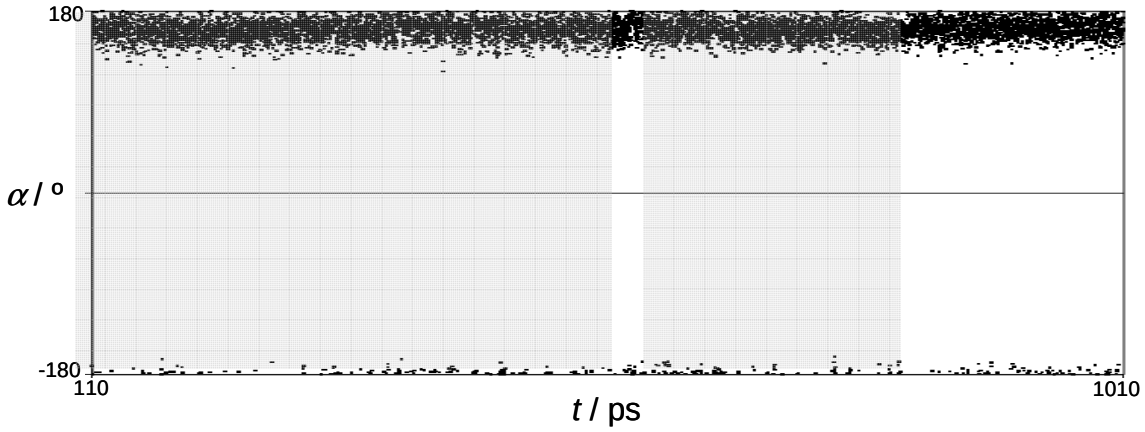


Figure S2. Time dependence of the torsions formed by the heavy atoms of the acyl chain and the nucleophile in IT_2-(*R*)-**3a** during the 1ns MDS. Snapshots corresponding to the major conformation are shaded in grey.

OG-CD-CH-CI



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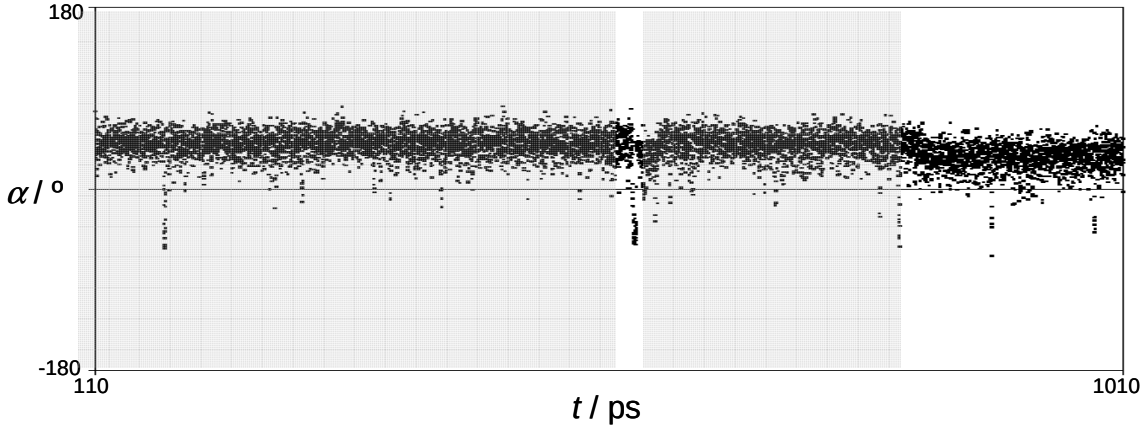

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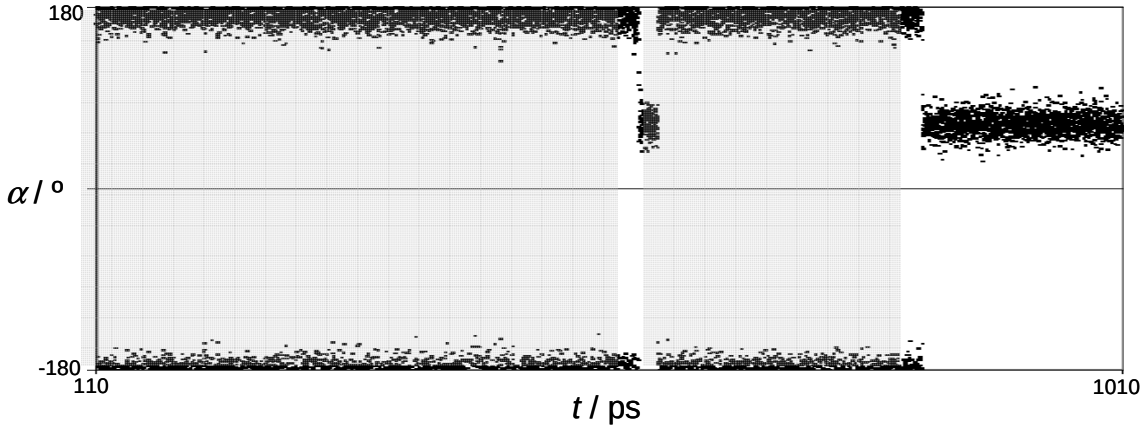
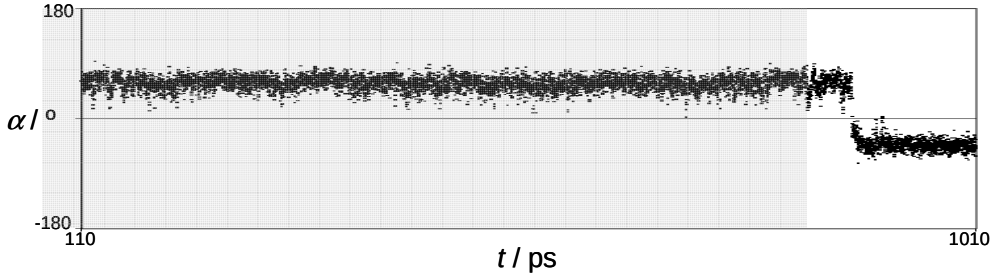


Figure S3. Time dependence of the torsions formed by the heavy atoms of the acyl chain and the nucleophile in IT_2-(*S*)-**3a** during the 1ns MDS. Snapshots corresponding to the major conformation are shaded in grey.

OG-CD-CH-CI



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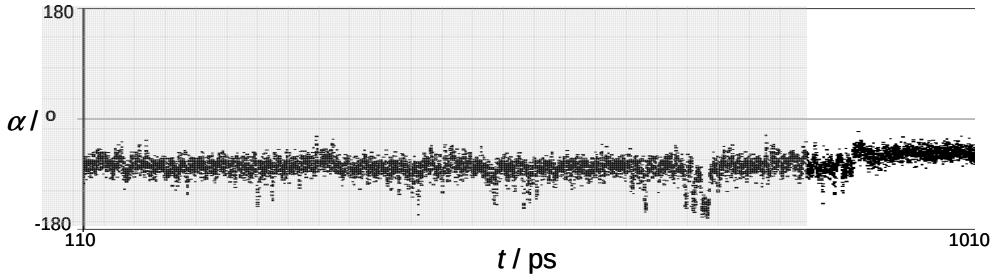
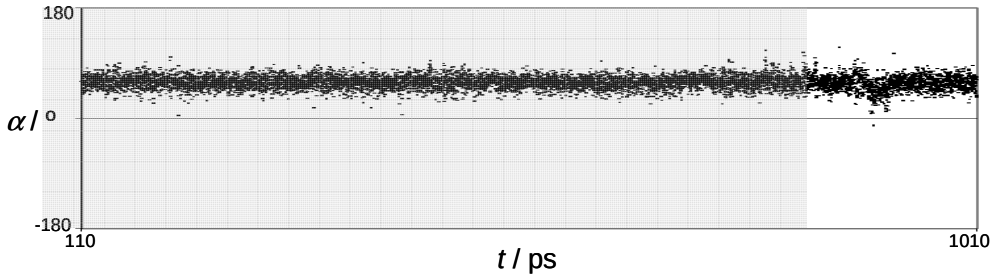
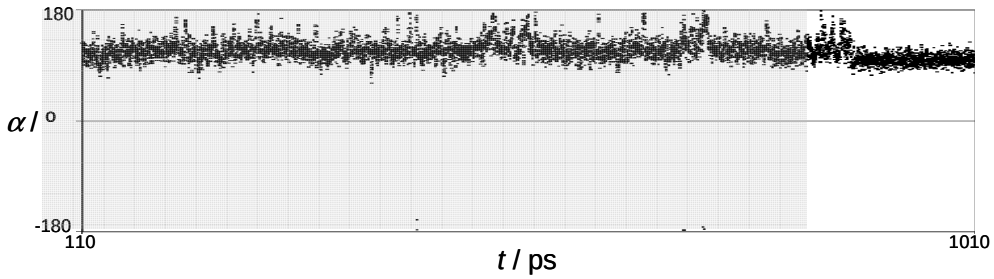


CH-CI-CK-CL



CD-NZ-CN-CO



NZ-CN-CO-CT

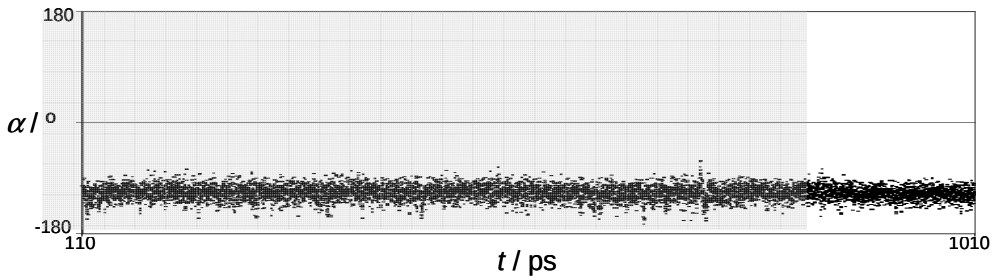
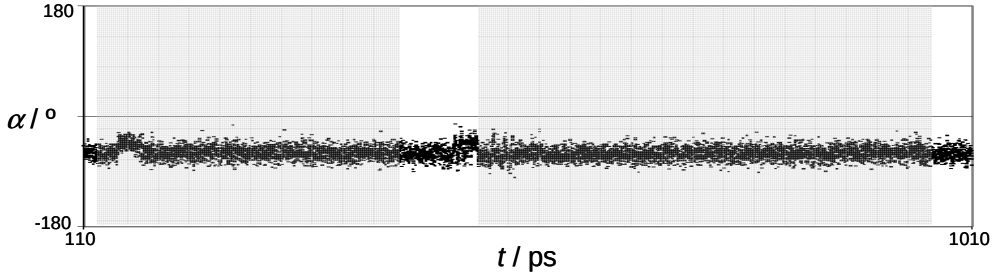
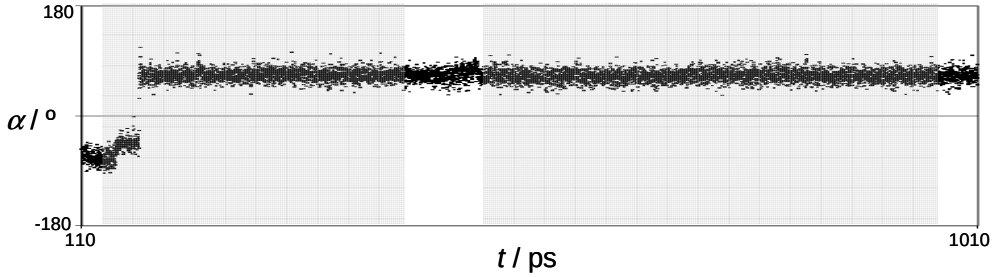


Figure S4. Time dependence of the torsions formed by the heavy atoms of the acyl chain and the nucleophile in IT_2-(*R*)-**3b** during the 1ns MDS. Snapshots corresponding to the major conformation are shaded in grey.

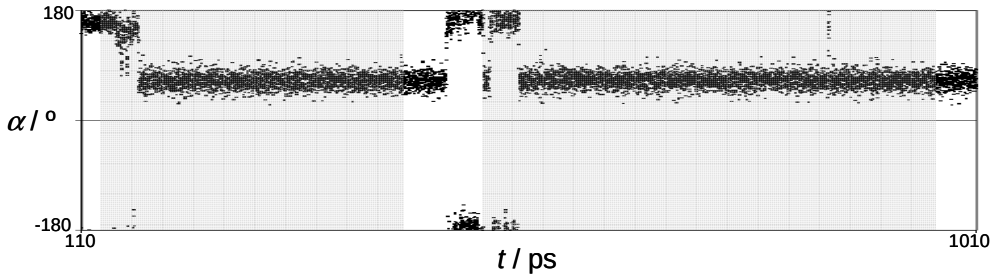
OG-CD-CH-CI



CD-CH-CI-OM



CH-CK-CI-CL



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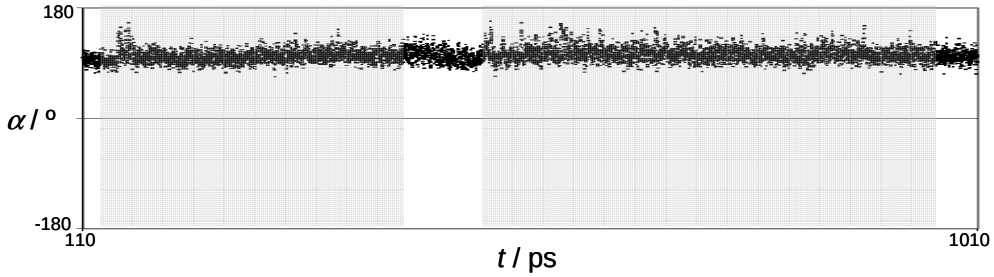

NZ-CN-CO-CT

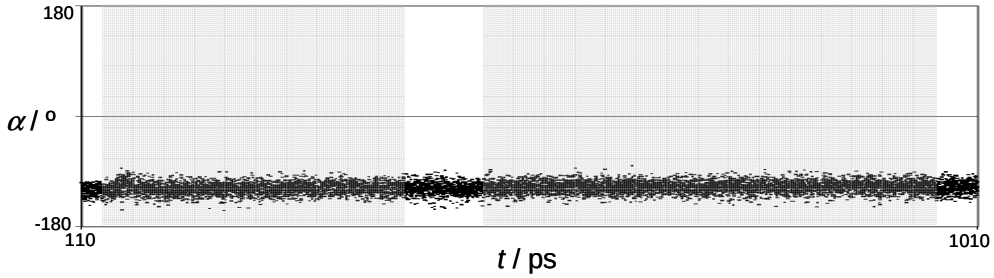

Figure S5. Time dependence of the torsions formed by the heavy atoms of the acyl chain and the nucleophile in IT_2-(*S*)-**3b** during the 1ns MDS. Snapshots corresponding to the major conformation are shaded in grey.

Table S1. Number of "normal" contacts between the acyl chain of IT_2-(*R*/*S*)-**3a** and the binding site of CALB

Atom[a]	Amino acid	IT_2-(*R*)-**3a**[b]	IT_2-(S)-**3a**[b]
CH	Asp134	400	423
CH	Gln157	3850	5404
CH	His224	54	49
CH	Ile189	23	34
CH	Thr40	47	1326
CI	Ala281	96	43
CI	Gln157	2379	102
CI	Ile189	4	399
CI	Thr40	3150	152
CK	Ala281	25	16
CK	Gln157	2005	534
CK	Ile189	90	312
CK	Thr138	13	3
CK	Thr40	4	237
CL	Ala281	183	306
CL	Gln157	766	116
CL	Ile189	2	85
CL	Ile285	318	0
CL	Thr138	43	124
CL	Val154	55	1
OM	Ala281	5409	4566
OM	Gln157	0	170
OM	Ile189	2832	10
OM	Ile285	369	0
OM	Thr40	215	7599

[a] See atom names in Scheme 4 of the main text. [b] Maximum number of contacts: 9000.

Table S2. Number of "normal" contacts between the acyl chain of IT_2-(*R*/*S*)-**3b** and the binding site of CALB

Atom[a]	Amino acid	IT_2-(*R*)-**3b**[b]	IT_2-(S)-**3b**[b]
CH	Asp134	97	0
CH	Gln157	4793	3
CH	His224	23	186
CH	Ile189	2	409
CH	Thr40	6809	148
CI	Asp134	641	644
CI	Gln157	396	7816
CI	His224	46	0
CI	Ile189	1963	20
CI	Thr40	0	431
CI	Val190	19	0
CK	Asp134	234	591
CK	Gln157	12	3201
CK	Ile189	2511	128
CK	Thr138	94	480
CK	Val190	2	20
CL	Asp134	221	454
CL	Gln157	3458	1876
CL	Ile189	8	102
CL	Ile285	0	58
CL	Thr138	405	363
CL	Thr40	7	181
OM	Asp134	6349	7062
OM	Gln106	571	536
OM	His224	699	45
OM	Ile189	907	58
OM	Thr138	185	13
OM	Thr40	821	368
OM	Val190	3664	3609

[a] See atom names in Scheme 4 of the main text. [b] Maximum number of contacts: 9000.