Electronic Supplementary Material (ESI) for Chemical Communications

Asymmetric H/D exchange reaction of fluorinated aromatic ketones

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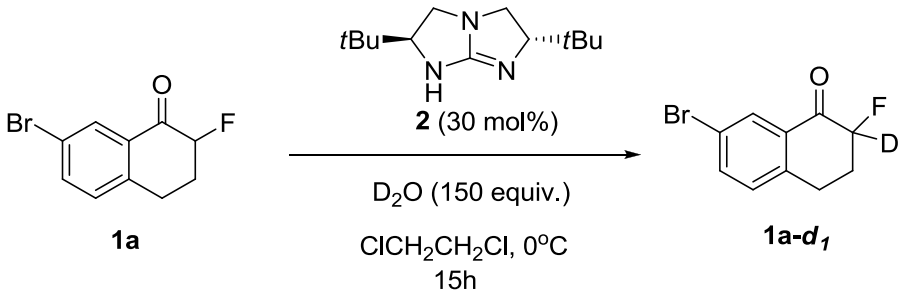
Supporting Information

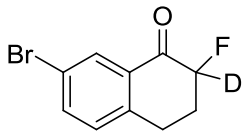
General procedures and methods

^{1}H and ^{13}C NMR spectra were recorded on a Bruker ACF300 (300MHz), Bruker DPX300 (300MHz) or AMX500 (500MHz) spectrometer. Chemical shifts are reported in parts per million (ppm). The residual solvent peak was used as an internal reference. Low resolution mass spectra were obtained on a Finnigan/MAT LCQ spectrometer in ESI mode and a Finnigan/MAT 95XL-T mass spectrometer in FAB mode. All high resolution mass spectra were obtained on a Finnigan/MAT 95XL-T spectrometer. Enantiomeric excess values were determined by chiral HPLC analysis on two sets: Jasco HPLC units, including a Jasco DG-980-50 Degasser, a LG-980-02 Ternary Gradient Unit, a PU-980 Intelligient HPLC Pump, UV-975 Intelligient UV/VIS Detectors, and an AS-950 Intelligient Sampler; Dionex Ultimate 3000 HPLC units, including a Ultimate 3000 Pump, Ultimate 3000 variable Detectors. Optical rotations were recorded on Jasco DIP-1000 polarimeter. Analytical thin layer chromatography (TLC) was performed with Merck pre-coated TLC plates, silica gel 60F-254, layer thickness 0.25 mm. Flash chromatography separations were performed on Merck 60 (0.040 - 0.063mm) mesh silica gel. Dichloromethane was distilled from CaH_2 and stored under N_2 atmosphere. Other reagents and solvents were commercial grade and were used as supplied without further purification, unless otherwise stated.

Typical experimental procedure for deuteration of 1a.



To a solution of 30 mol% chiral guanidine **2** (2.7 mg, 0.012 mmol) in 0.8 mL of $ClCH_2CH_2Cl$ (DCE), D_2O (0.12 mL, 6 mmol) was added. Then, the reaction mixture was cooled to 0 ^oC. After stirring at 0 ^oC for 20 min, **1a** (9.7 mg, 0.04 mmol) was added in two batches. This resulting solution was stirred for 15 hours at 0 ^oC. The reaction mixture was purified by flash chromatography on silica gel eluting with hexane/EA (30/1 to 5/1) to give **1a-*d*$_1$** (13 mg) as an off-white solid with 96% yield. The deuteration incorporation was determined by ^1H NMR spectroscopy by comparing the relative intensity to a non-exchangeable proton in the molecule.

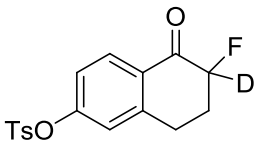


1a-*d*$_1$

The product **1a-*d*$_1$** was obtained as an off-white solid. Yield: 96%. *ee*: 24%; 100%D

^1H NMR (500 MHz, $CDCl_3$, ppm): δ = 8.2 (s, 1H), 7.63 (d, *J* = 8.2 Hz, 1H), 7.16 (d, *J* = 8.2 Hz, 1H), 3.12-3.02 (m, 2H), 2.61-2.54 (m, 1H), 2.40-2.31 (m, 1H)

The *ee* was determined by HPLC analysis. PHENOMENEX Lux 5u Amylose-2 (4.6 mm i.d. x 250 mm, 4.6 mm i.d. x 250 mm); Hexane/2-propanol = 95/5; flow rate 0.5 ml/min; 25°C; 254 nm; retention time: major isomer: 50.0 min; minor isomer: 46.8 min



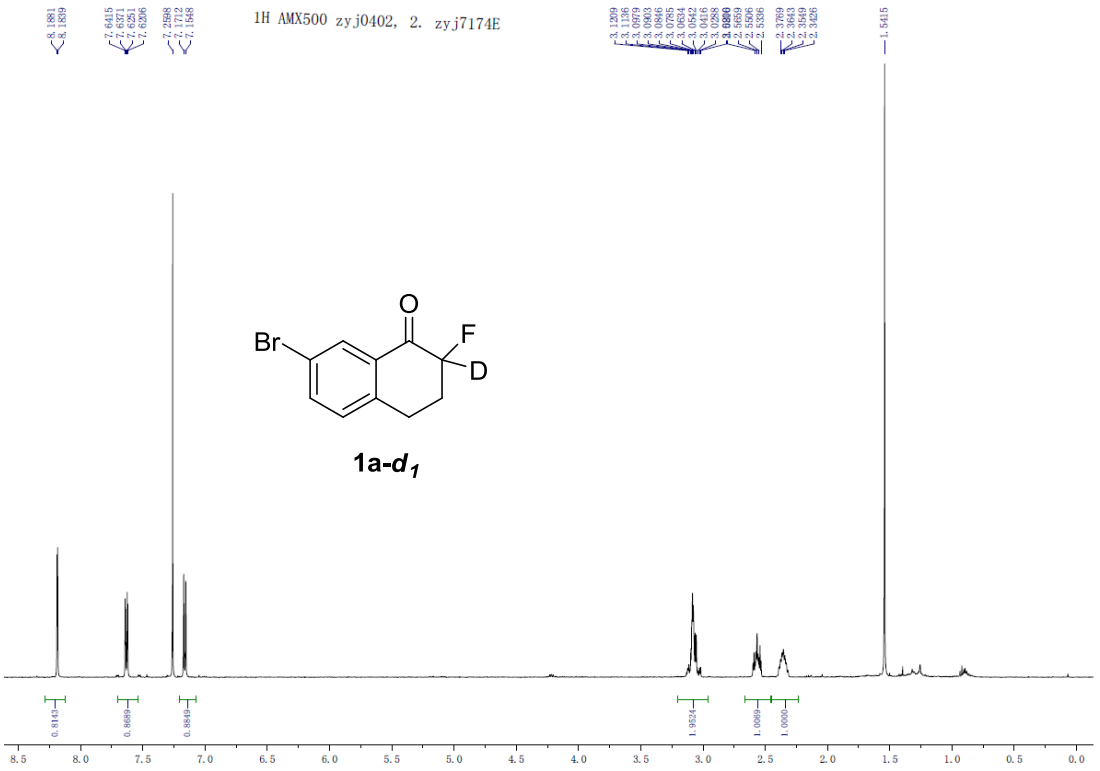
1b-*d*$_1$

The product **1b-*d*$_1$** was obtained as white solid. Yield: 98%. *ee*: 30%; 95%D

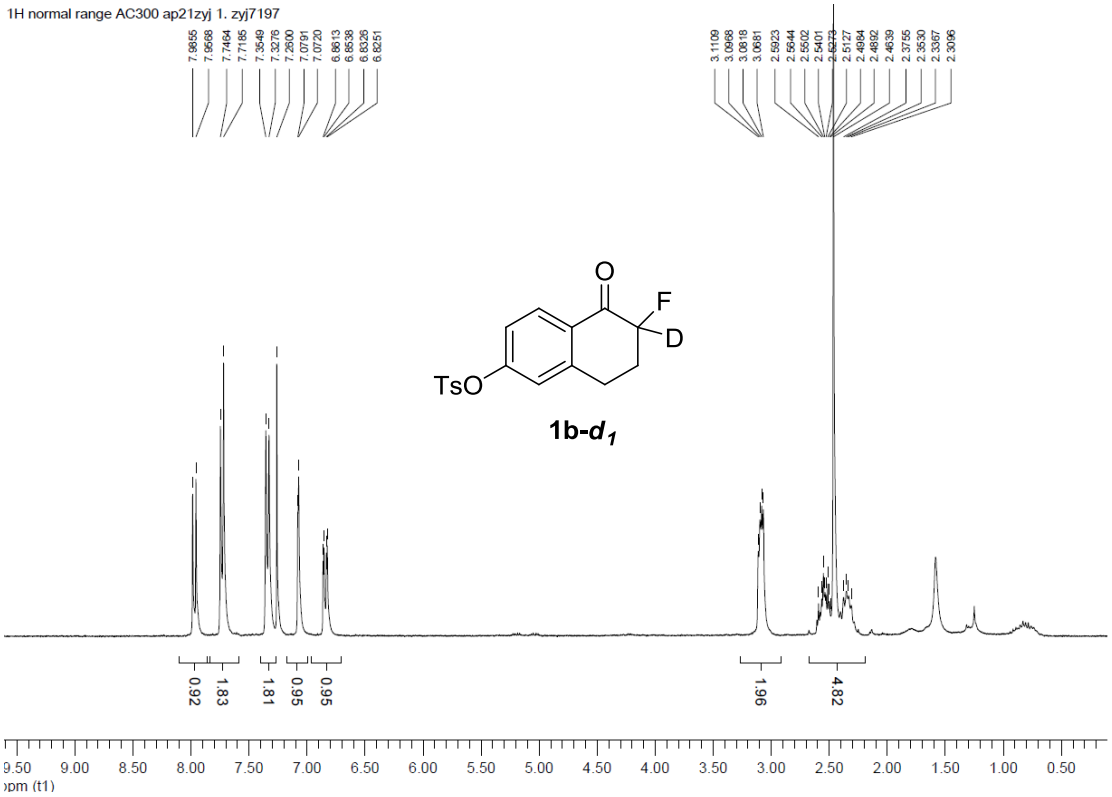
^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.97 (d, *J* = 8.6 Hz, 1H), 7.73 (d, *J* = 8.3 Hz, 1H), 7.34(d, *J* = 8.1 Hz, 2H), 6.86-6.84 (m, 1H), 3.10-3.08 (m, 2H), 2.59-2.34 (m, 5H)

The *ee* was determined by HPLC analysis. PHENOMENEX Lux 5u Amylose-2 (4.6 mm i.d. x 250 mm, 4.6 mm i.d. x 250 mm); Hexane/2-propanol = 92/8; flow rate 0.8 ml/min; 25°C; 254 nm; retention time: major isomer: 124.3 min; minor isomer: 132.8 min

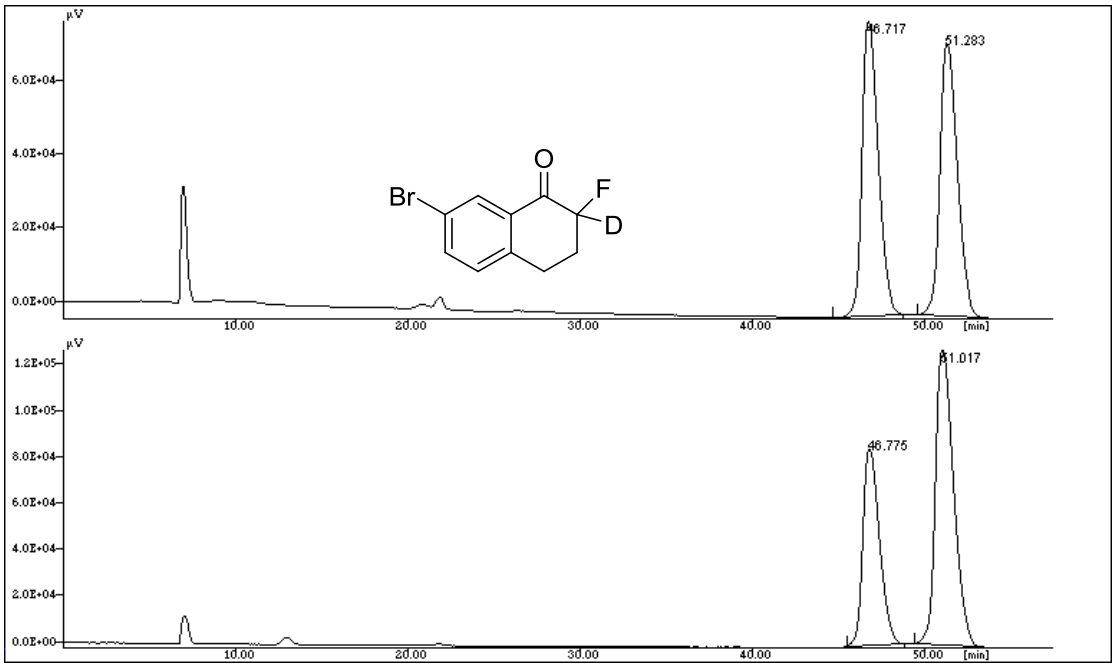
1H NMR and HPLC spectrum



1a-*d*$_1$



1b-*d*$_1$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O
F
D
Br
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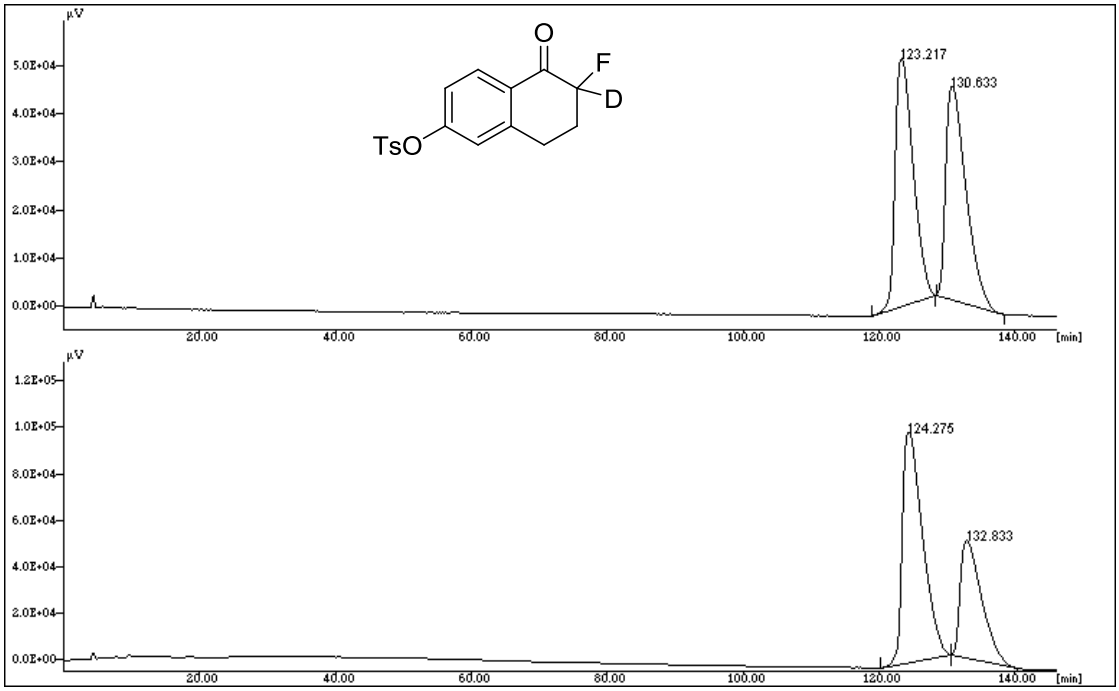
μV
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2.0E+04
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20.00
40.00
60.00
80.00
100.00
120.00
140.00
[min]
123.217
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O
F
D
TsO
μV
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6.0E+04
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2.0E+04
0.0E+00
20.00
40.00
60.00
80.00
100.00
120.00
140.00
[min]
124.275
132.833

DFT computational details

DFT calculations were performed using the Gaussian 09 program.[1] Becke[2] three parameter functional with the non local Lee-Yang-Parr[3] correlation functional (B3LYP) theory was applied with 6-31G(d) Pople basis set[4] for all atoms.

Cartesian coordinates and thermodynamic data for transition states presented

S-H_2O-TS

Imaginary Frequency= -835.62 cm^{-1}
Zero-point correction= 0.548848 (Hartree/Particle)
Sum of electronic and thermal Enthalpies= -1312.149613
Sum of electronic and thermal Free Energies= -1312.241616

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C	1.89628000	0.27492700	-0.27095700
O	-1.67690300	0.95759500	-0.92631900

[1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Comperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz J. C., J. V.; Fox, D. J. **2009**, Gaussian.

[2] Becke, A. D. *J. Chem. Phys.* **1983**, *98*, 5648.

[3] Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

[4] (a) Ditchfield, R.; Hehre, W. J.; Pople, J. A. *J. Chem. Phys.* **1971**, *54*, 724. (b) Hariharan, P. C.; Pople, J. A. *Theo. Chem. Acc.* **1973**, *28*, 213. (c) Hehre, W.J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.* **1972**, *56*, 2257.

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R-H_2O-TS

Imaginary Frequency= -855.30 cm^{-1}
Zero-point correction= 0.551730 (Hartree/Particle)
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C	4.45500600	-1.09512400	0.18284300
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S -TS

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Zero-point correction= 0.531037 (Hartree/Particle)

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Sum of electronic and thermal Free Energies= - 1235.813559

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R -TS

Imaginary Frequency= -902.14 cm^{-1}
Zero-point correction= 0.531158 (Hartree/Particle)
Sum of electronic and thermal Enthalpies= - 1235.725722
Sum of electronic and thermal Free Energies= - 1235.811618

C	3.63750600	-0.49247600	-0.53694100
C	2.88053800	-1.47735900	0.41200400
C	1.20833300	2.31846600	-1.08627400
C	2.65714600	1.79872200	-1.40024000
H	3.68053500	-0.87106500	-1.56998100
H	4.65682300	-0.29689400	-0.19663200
H	0.63619400	-1.37139700	0.73591100
H	2.72336900	1.43578000	-2.43773800
N	2.79489200	0.69992200	-0.45004000
N	1.51482200	-0.93375400	0.37988600
N	0.56701200	1.13225700	-0.46180900
H	3.42941400	2.55595600	-1.25243200
C	1.52435700	0.28958900	-0.13274200
O	-0.96539100	-1.84438500	0.74491300
C	-1.76515200	-0.87282100	0.68361400
C	-3.07391200	-1.04443600	-0.02401800
C	-1.46375800	0.44674800	1.16344500
C	-3.38926000	-2.30100900	-0.55951900
C	-4.00579400	0.01024000	-0.10961200

H	-0.52121700	0.96102600	0.08202500
C	-2.63555900	1.31350600	1.57025000
F	-0.47552700	0.44109000	2.17531500
H	-2.64876600	-3.08845400	-0.46909700
C	-4.61733300	-2.52167300	-1.17438400
C	-5.23764300	-0.22725200	-0.72806900
C	-3.64491000	1.38151700	0.41721600
H	-3.12304300	0.90984500	2.47200200
H	-2.29378800	2.32176300	1.82886700
C	-5.54607900	-1.48044900	-1.25667300
H	-4.85544800	-3.49930500	-1.58376200
H	-5.96328700	0.58021200	-0.79263300
H	-3.20003500	1.96404300	-0.40417400
H	-4.54976100	1.91877600	0.72245900
H	-6.51111100	-1.64556000	-1.72793200
C	2.94672500	-2.98588000	0.05483600
C	2.27030900	-3.28658800	-1.29567900
H	2.76373500	-2.77804400	-2.13105500
H	1.21901800	-2.98589300	-1.28462700
H	2.31255700	-4.36129200	-1.50073300
C	2.22074700	-3.77726100	1.16389900
H	2.66680300	-3.58440000	2.14627100
H	2.29458300	-4.85254400	0.97021600
H	1.15778000	-3.52310500	1.21582300
C	4.42710400	-3.41233300	0.01555900
H	4.50721500	-4.49009900	-0.15890300
H	4.93267800	-3.19248800	0.96310600
H	4.97814900	-2.90945700	-0.78701200
C	1.11566900	3.60938800	-0.21464300
C	-0.36819500	4.01750900	-0.12443800
H	-0.78380400	4.22794300	-1.11705400
H	-0.47928900	4.92286100	0.48167500
H	-0.97150400	3.23268400	0.33665500
C	1.66963300	3.37440300	1.20262100
H	2.72303600	3.07619300	1.18194500
H	1.10524800	2.59335800	1.72005200
H	1.59617200	4.29408200	1.79306000
C	1.88380600	4.75329200	-0.90727900
H	1.70260700	5.69770000	-0.38386900
H	1.55755000	4.88496800	-1.94606000
H	2.96625800	4.59074100	-0.91112300
H	3.29352700	-1.36155400	1.42577300
H	0.69793800	2.53685800	-2.03202600

Computer Simulations by CKS

Reaction conditions:

A: 1 M

B: 1 M

C: 0 M

D: 0 M

Kinetic Isotope Effect = 7

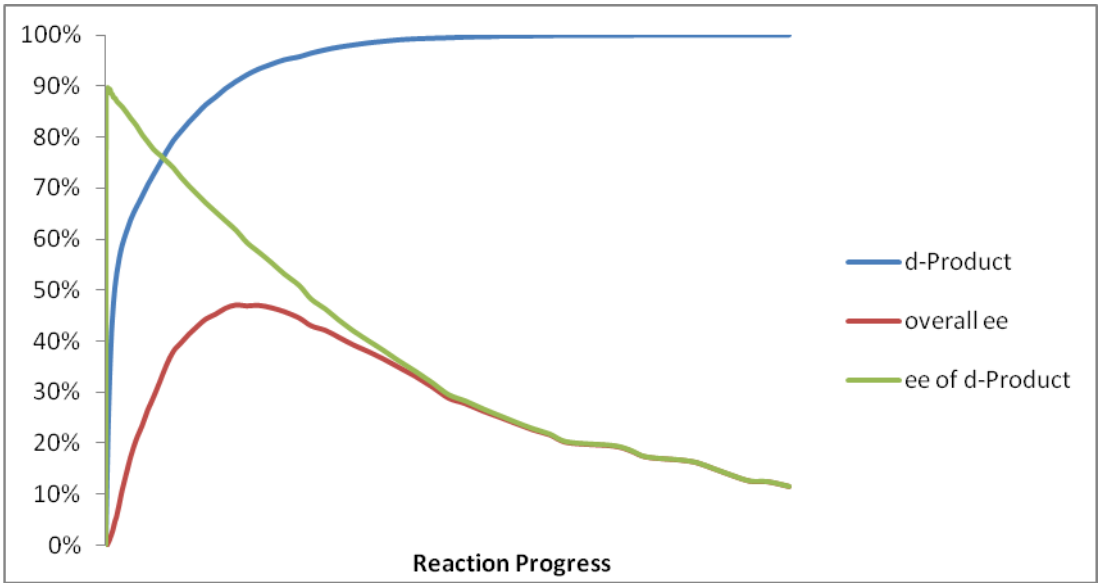
Catalyst Selectivity = 20:1

Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.00005
B -> C	Rate constant: 0.00005
B -> D	Rate constant: 0.0000025
C <=> D	Rate constant: 0.00000714

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.016	0.944	0.997	0.056	0.003	3.0%	0.0%	88.6%
0.050	0.829	0.991	0.170	0.010	9.0%	-0.1%	88.9%
0.090	0.717	0.984	0.284	0.016	15.0%	0.1%	89.6%
0.135	0.606	0.975	0.397	0.022	20.9%	0.3%	89.7%
0.190	0.497	0.965	0.509	0.029	26.9%	0.6%	89.4%
0.255	0.388	0.954	0.623	0.035	32.9%	1.1%	89.4%
0.337	0.285	0.939	0.732	0.044	38.8%	1.7%	88.7%
0.446	0.186	0.921	0.841	0.052	44.6%	2.7%	88.4%
0.611	0.099	0.892	0.947	0.062	50.5%	4.6%	87.7%
0.896	0.033	0.847	1.045	0.075	56.0%	7.8%	86.6%
1.383	0.006	0.769	1.133	0.092	61.3%	13.8%	84.9%
2.076	0.000	0.676	1.206	0.117	66.2%	20.7%	82.3%
2.867	0.000	0.587	1.265	0.148	70.6%	26.5%	79.0%
4.135	0.000	0.457	1.352	0.191	77.1%	35.2%	75.3%
5.675	0.000	0.342	1.413	0.245	82.9%	41.3%	70.4%
7.514	0.000	0.243	1.452	0.305	87.9%	45.2%	65.3%
10.419	0.000	0.134	1.469	0.396	93.3%	46.9%	57.5%
12.214	0.000	0.097	1.457	0.446	95.2%	45.7%	53.1%
14.054	0.000	0.071	1.429	0.500	96.5%	42.9%	48.2%
16.918	0.000	0.039	1.392	0.569	98.0%	39.2%	42.0%
19.993	0.000	0.019	1.349	0.632	99.0%	34.9%	36.2%
31.600	0.000	0.002	1.200	0.798	99.9%	20.0%	20.2%



Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 7 and catalyst selectivity of 20 to 1.

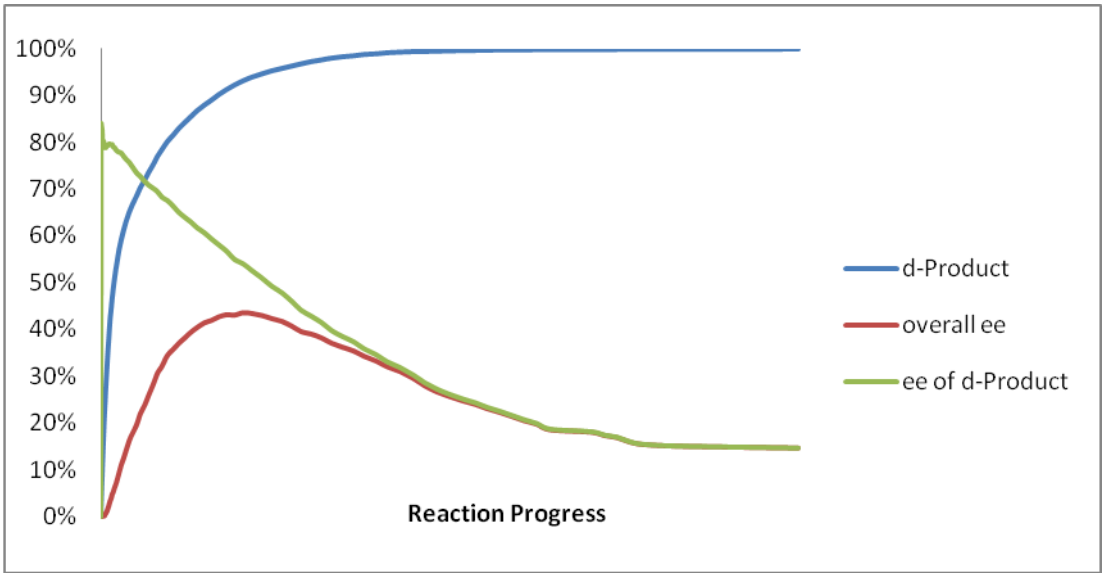
Kinetic Isotope Effect = 7
Catalyst Selectivity = 10:1
Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.0001
B -> C	Rate constant: 0.0001
B -> D	Rate constant: 0.000001
C <=> D	Rate constant: 0.00001428

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.022	0.919	0.991	0.082	0.007	4.5%	0.2%	83.5%
0.045	0.839	0.982	0.164	0.016	9.0%	0.3%	82.4%
0.072	0.758	0.973	0.243	0.027	13.5%	0.1%	80.1%
0.099	0.680	0.961	0.323	0.036	17.9%	0.3%	80.1%
0.130	0.602	0.951	0.400	0.047	22.4%	0.2%	78.8%
0.166	0.526	0.937	0.480	0.057	26.8%	0.6%	78.8%
0.207	0.449	0.924	0.561	0.065	31.3%	1.1%	79.2%
0.249	0.378	0.908	0.641	0.073	35.7%	1.8%	79.5%
0.299	0.308	0.890	0.720	0.082	40.1%	2.8%	79.6%
0.392	0.211	0.857	0.837	0.095	46.6%	4.7%	79.5%
0.526	0.124	0.816	0.945	0.114	53.0%	6.9%	78.4%
0.713	0.058	0.757	1.053	0.132	59.2%	11.1%	77.7%
0.985	0.018	0.681	1.143	0.158	65.1%	16.1%	75.7%
1.378	0.004	0.588	1.216	0.192	70.4%	22.0%	72.7%

1.828	0.001	0.492	1.282	0.225	75.3%	28.3%	70.2%
2.324	0.000	0.395	1.344	0.260	80.2%	34.5%	67.5%
2.926	0.000	0.314	1.382	0.304	84.3%	38.2%	64.0%
3.610	0.000	0.239	1.414	0.346	88.0%	41.4%	60.7%
4.970	0.000	0.135	1.436	0.429	93.3%	43.6%	54.0%
5.966	0.000	0.092	1.423	0.484	95.4%	42.3%	49.2%
7.707	0.000	0.046	1.382	0.572	97.7%	38.2%	41.4%
9.619	0.000	0.020	1.332	0.648	99.0%	33.2%	34.6%
20.135	0.000	0.000	1.151	0.849	100.0%	15.1%	15.1%



Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 7 and catalyst selectivity of 10 to 1.

Kinetic Isotope Effect = 7
Catalyst Selectivity = 5:1
Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.0002
B -> C	Rate constant: 0.0002
B -> D	Rate constant: 0.00004
C <=> D	Rate constant: 0.00002857

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.012	0.952	0.988	0.051	0.008	3.0%	0.3%	71.9%
0.038	0.853	0.968	0.152	0.028	9.0%	0.4%	69.0%
0.066	0.759	0.943	0.249	0.050	14.9%	0.7%	66.6%
0.097	0.667	0.917	0.346	0.070	20.8%	1.3%	66.2%

0.133	0.576	0.890	0.441	0.094	26.7%	1.6%	64.8%
0.172	0.487	0.859	0.542	0.112	32.7%	2.9%	65.8%
0.216	0.403	0.827	0.637	0.133	38.5%	4.0%	65.4%
0.265	0.320	0.794	0.728	0.157	44.3%	4.9%	64.5%
0.325	0.247	0.753	0.819	0.181	50.0%	6.6%	63.8%
0.397	0.181	0.709	0.908	0.203	55.5%	8.8%	63.5%
0.484	0.120	0.660	0.992	0.228	61.0%	11.2%	62.7%
0.598	0.072	0.603	1.069	0.257	66.3%	14.1%	61.3%
0.739	0.039	0.534	1.135	0.292	71.3%	17.4%	59.1%
0.908	0.019	0.462	1.197	0.322	76.0%	21.6%	57.6%
1.102	0.006	0.384	1.257	0.353	80.5%	26.3%	56.2%
1.352	0.003	0.312	1.293	0.393	84.3%	29.5%	53.4%
1.797	0.001	0.213	1.338	0.449	89.3%	33.9%	49.8%
2.328	0.000	0.129	1.355	0.516	93.5%	35.5%	44.9%
2.757	0.000	0.090	1.353	0.557	95.5%	35.3%	41.7%
3.711	0.000	0.040	1.318	0.642	98.0%	31.8%	34.5%
4.734	0.000	0.014	1.275	0.711	99.3%	27.5%	28.4%
7.927	0.000	0.001	1.145	0.854	100.0%	14.5%	14.6%

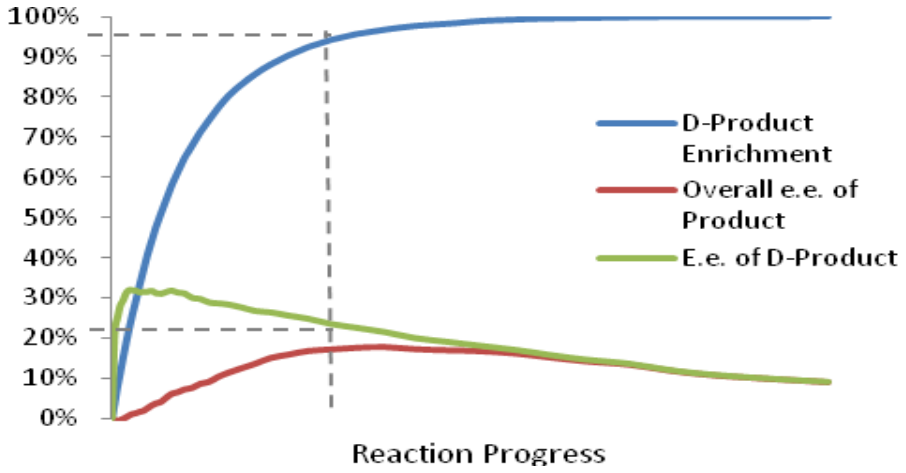
Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 7 and catalyst selectivity of 5 to 1.

Kinetic Isotope Effect = 7
Catalyst Selectivity = 2:1
Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.0005
B -> C	Rate constant: 0.0005
B -> D	Rate constant: 0.00025
C <=> D	Rate constant: 0.00007142

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.010	0.950	0.975	0.046	0.029	3.7%	-0.4%	21.9%
0.019	0.899	0.951	0.093	0.056	7.5%	-0.7%	25.0%
0.030	0.852	0.924	0.143	0.080	11.2%	-0.4%	28.2%
0.052	0.758	0.870	0.244	0.128	18.6%	0.2%	31.3%
0.064	0.713	0.842	0.294	0.151	22.3%	0.7%	32.2%
0.091	0.623	0.786	0.390	0.201	29.6%	1.3%	31.9%
0.118	0.533	0.730	0.485	0.252	36.9%	1.9%	31.7%
0.133	0.492	0.699	0.533	0.277	40.5%	2.5%	31.7%
0.149	0.451	0.668	0.581	0.300	44.0%	3.2%	32.0%
0.185	0.371	0.608	0.670	0.351	51.1%	4.1%	31.2%
0.205	0.334	0.576	0.718	0.372	54.5%	5.2%	31.7%
0.249	0.258	0.514	0.807	0.420	61.4%	6.5%	31.5%
0.274	0.222	0.483	0.850	0.445	64.8%	7.2%	31.3%
0.334	0.161	0.414	0.925	0.499	71.2%	8.6%	29.9%
0.402	0.108	0.345	0.996	0.551	77.3%	10.4%	28.8%
0.441	0.083	0.311	1.032	0.574	80.3%	11.5%	28.5%
0.540	0.050	0.238	1.086	0.625	85.6%	13.6%	26.9%
0.600	0.037	0.202	1.114	0.647	88.0%	15.1%	26.6%
0.742	0.015	0.138	1.154	0.693	92.4%	16.9%	25.0%
0.925	0.004	0.084	1.173	0.739	95.6%	17.7%	22.7%
1.031	0.003	0.064	1.176	0.758	96.7%	17.8%	21.6%
1.393	0.000	0.023	1.168	0.809	98.8%	16.8%	18.2%
2.443	0.000	0.001	1.100	0.899	100.0%	10.0%	10.1%



Kinetic Isotope Effect = 5

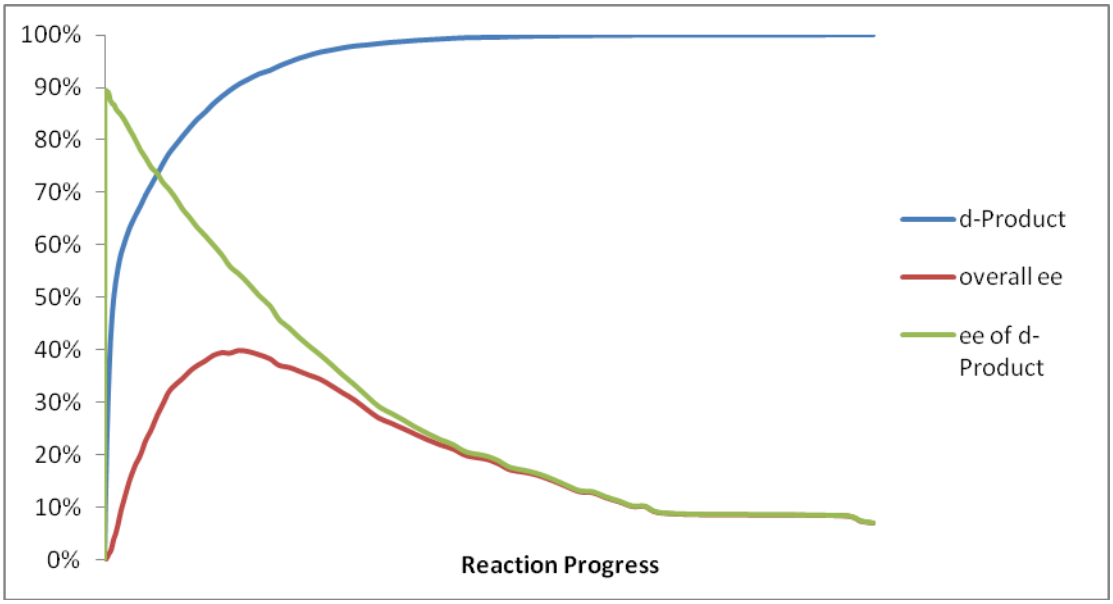
Catalyst Selectivity = 20:1

Reaction Scheme:

A -> C Rate constant: 0.001
A -> D Rate constant: 0.00005
B -> C Rate constant: 0.00005
B -> D Rate constant: 0.0000025
C <=> D Rate constant: 0.00001

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.032	0.886	0.995	0.113	0.007	6.0%	-0.2%	88.3%
0.070	0.773	0.988	0.227	0.013	12.0%	0.0%	89.5%
0.111	0.662	0.979	0.340	0.019	17.9%	0.2%	89.4%
0.161	0.553	0.969	0.451	0.026	23.9%	0.4%	89.0%
0.223	0.443	0.960	0.564	0.032	29.8%	0.7%	89.1%
0.292	0.337	0.948	0.674	0.041	35.8%	1.1%	88.6%
0.380	0.235	0.932	0.780	0.052	41.6%	1.5%	87.5%
0.513	0.144	0.909	0.885	0.062	47.3%	2.9%	86.9%
0.723	0.065	0.876	0.985	0.074	53.0%	5.0%	86.0%
1.069	0.017	0.818	1.077	0.089	58.3%	9.4%	84.8%
1.598	0.001	0.738	1.148	0.113	63.0%	14.9%	82.1%
2.317	0.000	0.653	1.199	0.147	67.3%	19.9%	78.1%
3.413	0.000	0.531	1.275	0.194	73.5%	27.5%	73.6%
4.173	0.000	0.452	1.320	0.227	77.4%	32.0%	70.6%
5.065	0.000	0.386	1.346	0.268	80.7%	34.6%	66.8%
5.990	0.000	0.323	1.370	0.307	83.9%	37.0%	63.4%
7.044	0.000	0.263	1.390	0.348	86.9%	39.0%	60.0%
8.716	0.000	0.188	1.399	0.413	90.6%	39.9%	54.4%
10.731	0.000	0.135	1.383	0.482	93.3%	38.3%	48.3%
12.603	0.000	0.089	1.360	0.551	95.5%	36.0%	42.3%
15.403	0.000	0.050	1.319	0.631	97.5%	31.9%	35.2%
20.971	0.000	0.018	1.228	0.754	99.1%	22.8%	23.9%
34.225	0.000	0.001	1.101	0.898	100.0%	10.1%	10.2%



Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 5 and catalyst selectivity of 20 to 1.

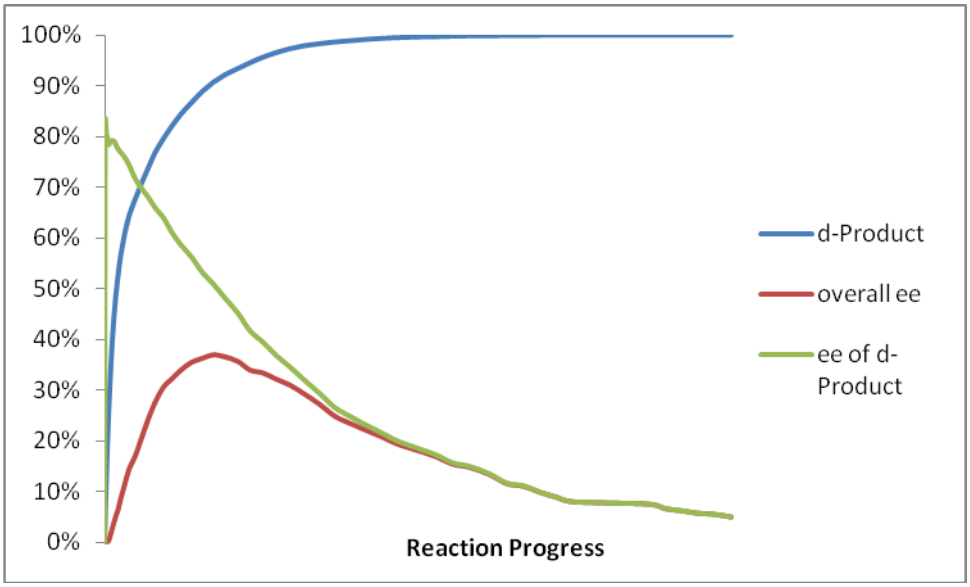
Kinetic Isotope Effect = 5
Catalyst Selectivity = 10:1
Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.0001
B -> C	Rate constant: 0.0001
B -> D	Rate constant: 0.00001
C <=> D	Rate constant: 0.00002

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.022	0.919	0.991	0.082	0.007	4.5%	0.2%	83.5%
0.045	0.839	0.982	0.164	0.016	9.0%	0.3%	82.4%
0.072	0.758	0.973	0.242	0.027	13.5%	0.0%	79.9%
0.099	0.681	0.961	0.322	0.036	17.9%	0.3%	80.1%
0.130	0.602	0.951	0.399	0.048	22.3%	0.1%	78.7%
0.166	0.527	0.938	0.477	0.058	26.8%	0.4%	78.4%
0.206	0.452	0.924	0.559	0.066	31.2%	1.1%	78.9%
0.248	0.381	0.907	0.638	0.074	35.6%	1.8%	79.1%
0.297	0.311	0.889	0.716	0.083	40.0%	2.8%	79.2%
0.357	0.246	0.869	0.793	0.092	44.3%	3.8%	79.1%
0.427	0.185	0.845	0.866	0.104	48.5%	5.1%	78.5%
0.516	0.129	0.818	0.935	0.118	52.6%	6.4%	77.5%
0.625	0.082	0.782	1.004	0.131	56.8%	8.6%	76.9%

0.764	0.046	0.742	1.067	0.146	60.6%	11.2%	75.9%
0.941	0.021	0.692	1.122	0.165	64.3%	14.4%	74.4%
1.425	0.004	0.580	1.202	0.214	70.8%	20.6%	69.7%
1.952	0.001	0.461	1.276	0.262	76.9%	27.6%	65.9%
2.603	0.000	0.357	1.322	0.320	82.1%	32.2%	61.0%
3.344	0.000	0.267	1.354	0.379	86.7%	35.4%	56.3%
4.175	0.000	0.187	1.369	0.444	90.7%	36.9%	51.0%
4.634	0.000	0.157	1.365	0.478	92.2%	36.5%	48.1%
6.104	0.000	0.087	1.333	0.580	95.6%	33.3%	39.4%
7.119	0.000	0.054	1.310	0.636	97.3%	31.0%	34.6%
8.867	0.000	0.027	1.248	0.724	98.6%	24.8%	26.6%
17.394	0.000	0.000	1.089	0.911	100.0%	8.9%	8.9%



Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 5 and catalyst selectivity of 10 to 1.

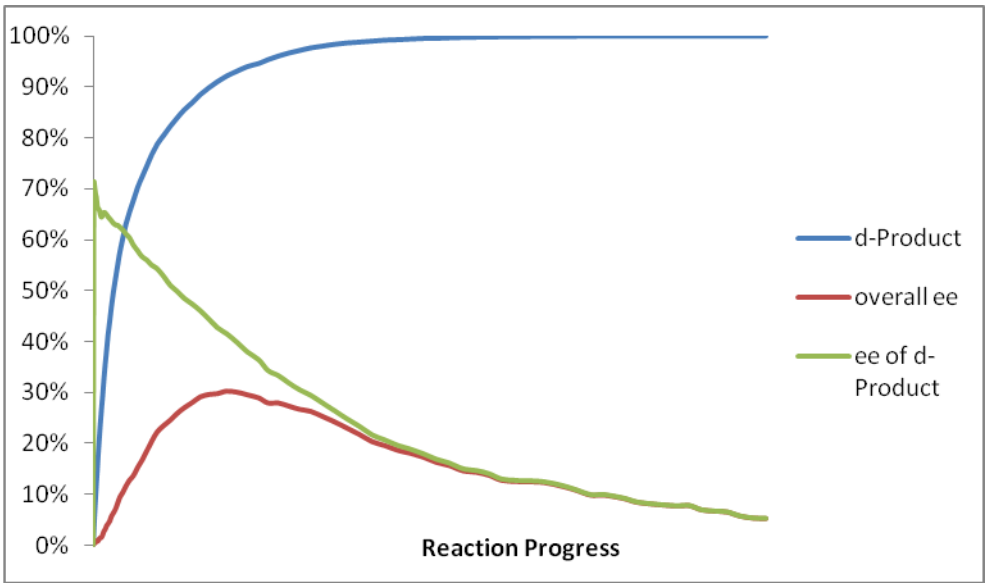
Kinetic Isotope Effect = 5
Catalyst Selectivity = 5:1
Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.0002
B -> C	Rate constant: 0.0002
B -> D	Rate constant: 0.00004
C <=> D	Rate constant: 0.00004

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.024	0.901	0.979	0.102	0.018	6.0%	0.3%	70.2%

0.052	0.807	0.954	0.201	0.038	12.0%	0.8%	68.2%
0.080	0.712	0.932	0.296	0.061	17.8%	0.8%	66.0%
0.114	0.622	0.903	0.391	0.083	23.7%	1.4%	64.9%
0.152	0.532	0.876	0.488	0.104	29.6%	2.0%	64.9%
0.192	0.445	0.846	0.585	0.123	35.4%	3.0%	65.2%
0.235	0.364	0.812	0.677	0.146	41.2%	4.1%	64.4%
0.290	0.290	0.774	0.766	0.170	46.8%	5.6%	63.6%
0.355	0.218	0.735	0.852	0.195	52.3%	7.1%	62.8%
0.429	0.156	0.687	0.939	0.218	57.8%	9.5%	62.3%
0.518	0.102	0.640	1.013	0.245	62.9%	11.5%	61.1%
0.640	0.061	0.584	1.076	0.279	67.8%	13.7%	58.8%
0.775	0.035	0.519	1.132	0.314	72.3%	16.7%	56.6%
0.929	0.016	0.450	1.188	0.346	76.7%	20.4%	54.9%
1.120	0.006	0.384	1.229	0.381	80.5%	23.5%	52.7%
1.333	0.003	0.319	1.257	0.421	83.9%	25.9%	49.8%
1.574	0.001	0.260	1.280	0.459	86.9%	28.1%	47.2%
1.836	0.000	0.203	1.296	0.500	89.8%	29.7%	44.3%
2.116	0.000	0.158	1.303	0.539	92.1%	30.3%	41.4%
2.770	0.000	0.093	1.280	0.627	95.3%	28.0%	34.2%
3.275	0.000	0.057	1.267	0.676	97.2%	26.7%	30.4%
4.222	0.000	0.024	1.218	0.758	98.8%	21.8%	23.3%
7.667	0.000	0.001	1.107	0.892	100.0%	10.7%	10.8%



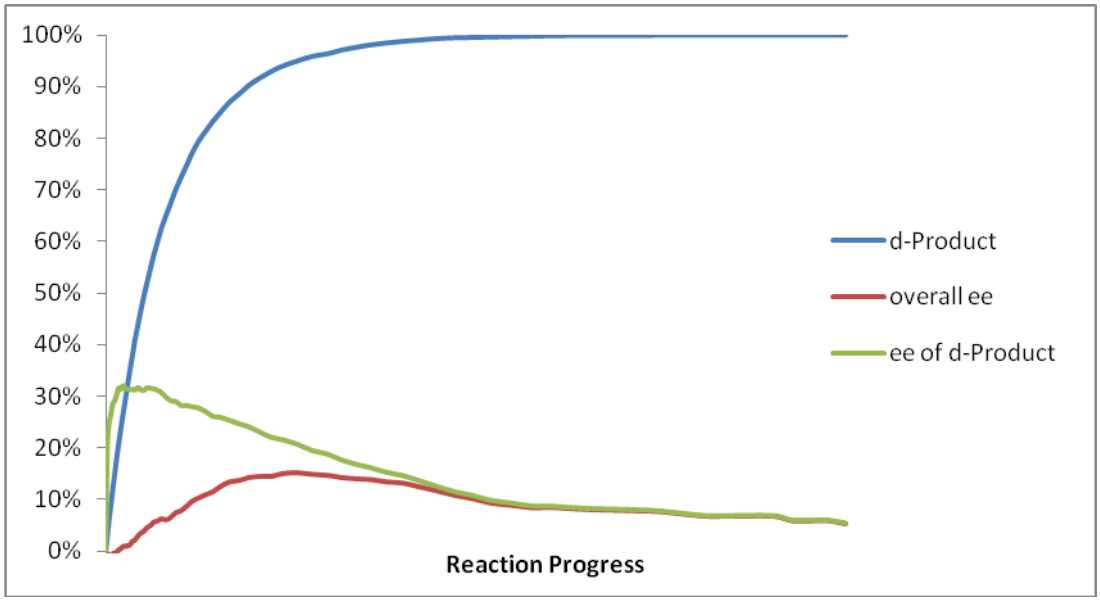
Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 5 and catalyst selectivity of 5 to 1.

Kinetic Isotope Effect = 5
Catalyst Selectivity = 2:1
Reaction Scheme:

A -> C Rate constant: 0.001
A -> D Rate constant: 0.0005
B -> C Rate constant: 0.0005
B -> D Rate constant: 0.00025
C <=> D Rate constant: 0.0001

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.015	0.918	0.962	0.074	0.045	6.0%	-0.7%	24.6%
0.032	0.843	0.919	0.153	0.085	11.9%	-0.4%	28.5%
0.050	0.767	0.878	0.231	0.124	17.8%	-0.2%	30.2%
0.069	0.696	0.832	0.310	0.162	23.6%	0.5%	31.3%
0.091	0.623	0.788	0.387	0.202	29.5%	1.1%	31.5%
0.112	0.551	0.744	0.462	0.242	35.2%	1.3%	31.2%
0.134	0.485	0.696	0.537	0.282	41.0%	2.2%	31.1%
0.161	0.425	0.644	0.611	0.320	46.5%	3.6%	31.2%
0.190	0.362	0.598	0.685	0.355	52.0%	4.6%	31.7%
0.221	0.302	0.549	0.755	0.394	57.5%	5.7%	31.4%
0.256	0.246	0.503	0.818	0.434	62.6%	6.3%	30.7%
0.300	0.194	0.454	0.872	0.479	67.6%	6.7%	29.1%
0.346	0.151	0.402	0.928	0.520	72.4%	7.9%	28.2%
0.397	0.110	0.347	0.986	0.556	77.1%	9.7%	27.9%
0.459	0.076	0.297	1.033	0.594	81.4%	11.0%	27.0%
0.530	0.055	0.243	1.071	0.631	85.1%	12.6%	25.9%
0.613	0.033	0.195	1.104	0.667	88.6%	13.7%	24.6%
0.709	0.017	0.149	1.128	0.706	91.7%	14.5%	23.0%
0.761	0.011	0.130	1.134	0.725	93.0%	14.5%	22.0%
0.882	0.006	0.094	1.146	0.754	95.0%	15.2%	20.6%
1.151	0.000	0.047	1.140	0.812	97.6%	14.0%	16.8%
1.363	0.000	0.024	1.132	0.843	98.8%	13.2%	14.6%
2.543	0.000	0.001	1.077	0.922	100.0%	7.7%	7.8%



Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 5 and catalyst selectivity of 2 to 1.

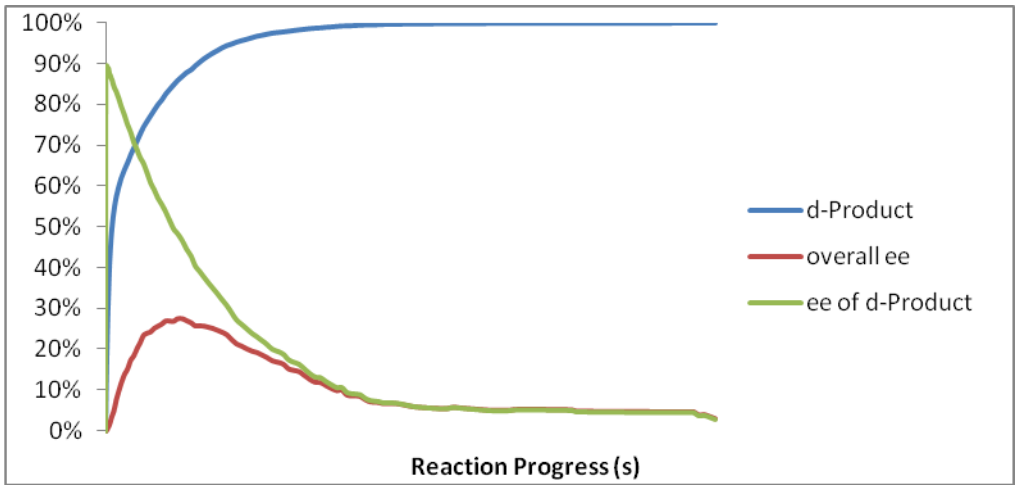
Kinetic Isotope Effect = 3
Catalyst Selectivity = 20:1
Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.00005
B -> C	Rate constant: 0.00005
B -> D	Rate constant: 0.0000025
C <=> D	Rate constant: 0.00001666

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.032	0.886	0.995	0.112	0.007	6.0%	-0.2%	88.0%
0.070	0.773	0.988	0.227	0.013	12.0%	-0.1%	89.1%
0.110	0.663	0.980	0.339	0.019	17.9%	0.1%	89.4%
0.161	0.554	0.970	0.449	0.027	23.8%	0.3%	88.8%
0.222	0.445	0.961	0.562	0.033	29.7%	0.6%	88.8%
0.290	0.339	0.949	0.670	0.042	35.6%	1.0%	88.3%
0.376	0.240	0.932	0.776	0.053	41.4%	1.5%	87.3%
0.503	0.150	0.909	0.877	0.064	47.0%	2.7%	86.4%
0.696	0.072	0.879	0.970	0.079	52.5%	4.2%	84.9%
0.996	0.023	0.826	1.053	0.098	57.6%	7.6%	83.0%
1.436	0.004	0.758	1.112	0.127	61.9%	11.5%	79.5%
2.028	0.000	0.685	1.151	0.165	65.8%	15.1%	75.0%
2.608	0.000	0.613	1.183	0.204	69.4%	18.3%	70.6%

3.195	0.000	0.543	1.216	0.241	72.8%	21.6%	66.9%
3.841	0.000	0.481	1.239	0.280	76.0%	23.9%	63.1%
5.212	0.000	0.376	1.262	0.362	81.2%	26.2%	55.4%
6.296	0.000	0.302	1.269	0.429	84.9%	26.9%	49.5%
7.490	0.000	0.242	1.270	0.487	87.9%	27.0%	44.5%
8.700	0.000	0.192	1.258	0.551	90.4%	25.8%	39.1%
9.894	0.000	0.148	1.251	0.601	92.6%	25.1%	35.1%
11.674	0.000	0.102	1.223	0.674	94.9%	22.3%	28.9%
15.433	0.000	0.049	1.171	0.780	97.6%	17.1%	20.0%
19.902	0.000	0.023	1.118	0.859	98.9%	11.8%	13.1%
38.261	0.000	0.001	1.052	0.947	100.0%	5.2%	5.3%



Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 3 and catalyst selectivity of 20 to 1.

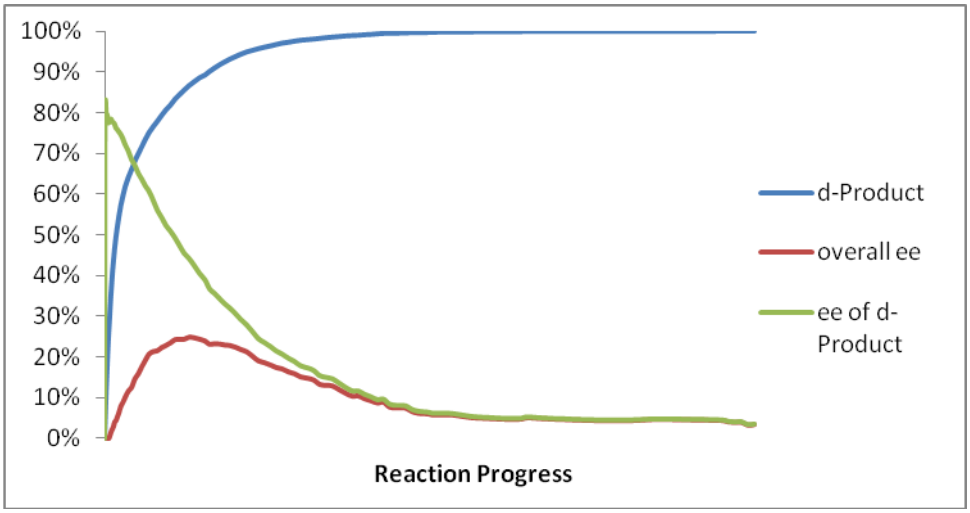
Kinetic Isotope Effect = 3
Catalyst Selectivity = 10:1
Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.0001
B -> C	Rate constant: 0.0001
B -> D	Rate constant: 0.00001
C <=> D	Rate constant: 0.00003333

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.029	0.893	0.988	0.110	0.010	6.0%	0.2%	83.3%
0.063	0.785	0.976	0.214	0.025	12.0%	-0.1%	78.7%
0.098	0.681	0.962	0.320	0.036	17.8%	0.1%	79.6%
0.141	0.580	0.946	0.421	0.053	23.7%	0.1%	77.6%

0.192	0.479	0.929	0.527	0.065	29.6%	0.6%	78.0%
0.246	0.384	0.908	0.632	0.076	35.4%	1.6%	78.5%
0.309	0.294	0.884	0.731	0.091	41.1%	2.5%	77.8%
0.393	0.214	0.853	0.827	0.106	46.7%	4.1%	77.2%
0.500	0.139	0.821	0.915	0.125	52.0%	5.4%	75.9%
0.634	0.080	0.775	1.000	0.145	57.2%	8.0%	74.7%
0.809	0.037	0.725	1.066	0.172	61.9%	10.3%	72.2%
1.057	0.014	0.666	1.113	0.207	66.0%	12.7%	68.6%
1.320	0.006	0.597	1.154	0.243	69.8%	16.0%	65.2%
1.745	0.001	0.497	1.208	0.295	75.1%	20.9%	60.8%
2.239	0.000	0.413	1.224	0.362	79.3%	22.4%	54.3%
2.762	0.000	0.334	1.244	0.422	83.3%	24.4%	49.3%
3.312	0.000	0.267	1.250	0.483	86.6%	25.0%	44.3%
4.122	0.000	0.197	1.233	0.570	90.1%	23.3%	36.8%
4.720	0.000	0.150	1.231	0.619	92.5%	23.1%	33.1%
5.580	0.000	0.102	1.214	0.684	94.9%	21.4%	27.9%
7.213	0.000	0.054	1.165	0.781	97.3%	16.5%	19.7%
9.448	0.000	0.024	1.113	0.863	98.8%	11.3%	12.6%
17.485	0.000	0.001	1.049	0.950	100.0%	4.9%	5.0%



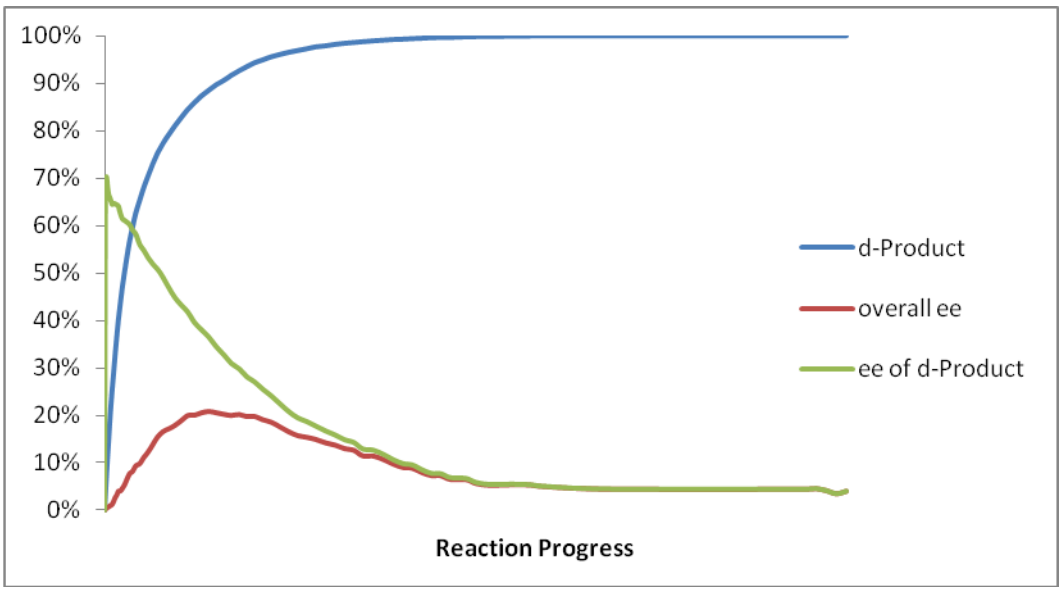
Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 3 and catalyst selectivity of 10 to 1.

Kinetic Isotope Effect = 3
Catalyst Selectivity = 5:1
Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.0002
B -> C	Rate constant: 0.0002
B -> D	Rate constant: 0.00004
C <=> D	Rate constant: 0.00006666

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.030	0.878	0.973	0.127	0.022	7.5%	0.4%	70.2%
0.066	0.760	0.943	0.247	0.050	14.8%	0.7%	66.4%
0.104	0.645	0.913	0.365	0.077	22.1%	1.0%	65.2%
0.151	0.536	0.876	0.484	0.104	29.4%	2.0%	64.6%
0.199	0.430	0.838	0.601	0.131	36.6%	3.2%	64.3%
0.226	0.382	0.816	0.658	0.144	40.1%	4.0%	64.0%
0.257	0.333	0.797	0.707	0.163	43.5%	4.0%	62.5%
0.290	0.290	0.773	0.756	0.181	46.9%	4.6%	61.4%
0.327	0.245	0.751	0.808	0.196	50.2%	5.4%	61.0%
0.368	0.207	0.724	0.858	0.210	53.4%	6.5%	60.6%
0.410	0.169	0.697	0.908	0.226	56.7%	7.7%	60.2%
0.578	0.079	0.614	1.019	0.288	65.3%	9.8%	56.0%
0.717	0.044	0.547	1.079	0.330	70.5%	12.3%	53.1%
0.870	0.020	0.475	1.135	0.371	75.3%	15.5%	50.8%
1.054	0.009	0.408	1.163	0.420	79.2%	17.2%	46.9%
1.259	0.004	0.342	1.185	0.470	82.7%	18.9%	43.2%
1.478	0.002	0.280	1.199	0.520	85.9%	20.1%	39.5%
1.839	0.000	0.206	1.205	0.588	89.7%	20.6%	34.4%
2.215	0.000	0.147	1.202	0.651	92.6%	20.2%	29.8%
2.601	0.000	0.102	1.191	0.707	94.9%	19.1%	25.5%
3.470	0.000	0.047	1.150	0.803	97.6%	15.0%	17.7%
4.426	0.000	0.022	1.114	0.864	98.9%	11.4%	12.6%
7.183	0.000	0.001	1.050	0.949	100.0%	5.0%	5.1%



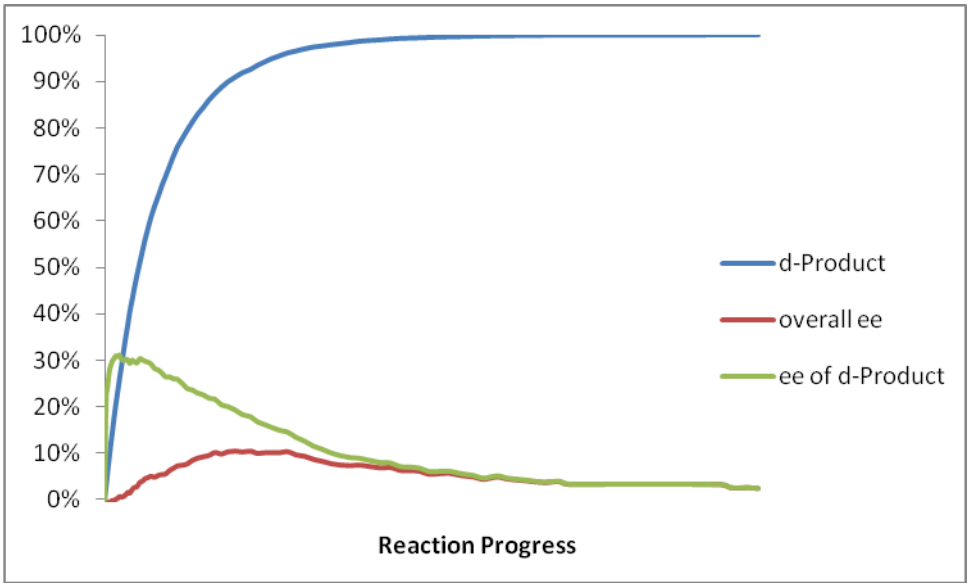
Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 3 and catalyst selectivity of 5 to 1.

Kinetic Isotope Effect = 3
Catalyst Selectivity = 2:1
Reaction Scheme:

A -> C	Rate constant: 0.001
A -> D	Rate constant: 0.0005
B -> C	Rate constant: 0.0005
B -> D	Rate constant: 0.00025
C <=> D	Rate constant: 0.0001667

Table of selected values:

Time /h	[A] /molcm^{-3}	[B] /molcm^{-3}	[C] /molcm^{-3}	[D] /molcm^{-3}	d-Product	overall ee	ee of D-Product
0.000	1.000	1.000	0.000	0.000	0.0%	0.0%	NA
0.015	0.918	0.963	0.074	0.045	6.0%	-0.8%	24.4%
0.032	0.844	0.919	0.153	0.084	11.9%	-0.3%	28.8%
0.049	0.768	0.879	0.230	0.123	17.7%	-0.2%	30.3%
0.069	0.698	0.835	0.305	0.162	23.4%	0.3%	30.7%
0.090	0.627	0.791	0.379	0.204	29.1%	0.6%	30.1%
0.110	0.558	0.746	0.453	0.243	34.8%	1.1%	30.1%
0.131	0.493	0.700	0.522	0.285	40.4%	1.4%	29.3%
0.156	0.435	0.651	0.592	0.322	45.7%	2.7%	29.6%
0.184	0.374	0.608	0.663	0.355	50.9%	3.7%	30.3%
0.212	0.319	0.560	0.727	0.394	56.1%	4.6%	29.7%
0.243	0.265	0.518	0.786	0.431	60.9%	5.1%	29.1%
0.282	0.217	0.475	0.836	0.472	65.4%	5.3%	27.8%
0.320	0.176	0.432	0.880	0.513	69.6%	5.6%	26.4%
0.361	0.136	0.384	0.932	0.548	74.0%	6.8%	26.0%
0.433	0.092	0.317	0.985	0.606	79.5%	7.7%	23.9%
0.547	0.048	0.232	1.048	0.673	86.0%	9.6%	21.8%
0.646	0.025	0.177	1.079	0.719	89.9%	10.3%	20.0%
0.766	0.014	0.134	1.091	0.761	92.6%	10.5%	17.8%
0.878	0.005	0.096	1.097	0.802	95.0%	10.2%	15.5%
1.096	0.001	0.051	1.086	0.862	97.4%	8.7%	11.5%
1.386	0.000	0.023	1.072	0.904	98.8%	7.2%	8.5%
2.383	0.000	0.001	1.039	0.960	100.0%	3.9%	4.0%



Graph: Simulation result of asymmetric H/D reaction, assuming kinetic isotope effect of 3 and catalyst selectivity of 2 to 1.