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Supporting Information

Chiral Bidented Bis(N-Heterocyclic Carbene) Based Palladium Complexes Bearing Carboxylate Ligands: Highly Effective Catalysts for the Enantioselective Conjugate Addition of Arylboronic Acids to Cyclic Enones

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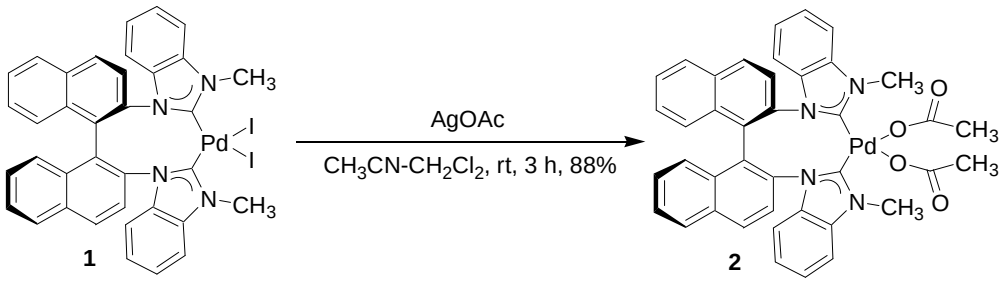
CONTENTS:

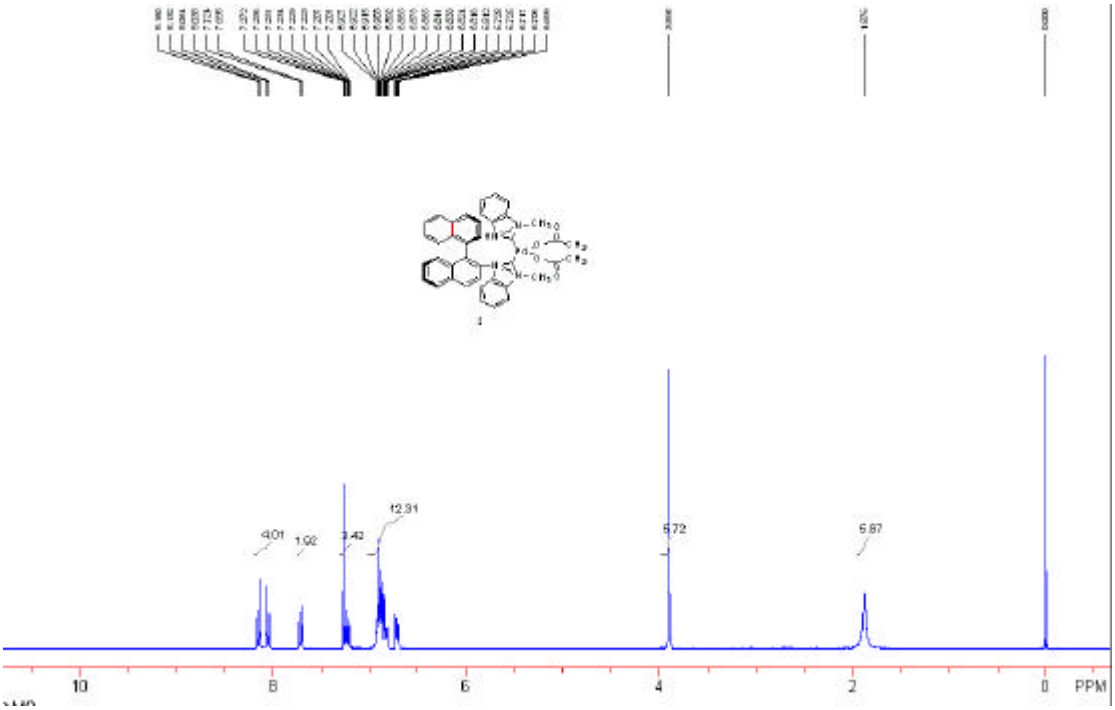
General Remarks: Melting points are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a Varian Mercury vx 300 MHz spectrometer for solution in $CDCl_3$ with tetramethylsilane (TMS) as an internal standard at 300 and 75 MHz, respectively. Mass spectra were recorded with a HP-5989 instrument by EI/ESI/Maldi methods. Organic solvents used were dried by standard methods when necessary. Satisfactory CHN microanalyses were obtained with a Carlo-Erba 1106 analyzer. X-ray diffraction analysis was performed on a Bruker smart-1000 X-ray diffraction meter. Optical rotations were determined at 589 nm (sodium D line) by using a Perkin-Elmer-341 MC digital polarimeter; $[\alpha]_D$-values are given in unit of 10 deg^{-1} cm_2 g^{-1}. Chiral HPLC was performed on a SHIMADZU SPD-10A *vp* series with chiral columns (Chiralpak AS-H, OD-H and AD-H columns 4.6×250 mm, (Daicel Chemical Ind., Ltd.)). Commercially obtained reagents were used without further purification. All reactions were monitored by TLC plate with Huanghai GF254 silica gel coated plates. Flash column chromatography was carried out using 300-400 mesh silica gel at increased pressure.

1. Synthesis of Complexes 2 and 3



Synthesis of NHC-Pd(II) complex 2.

The NHC-Pd(II) complex **1** (174 mg, 0.20 mmol) was suspended in a mixed solution of CH_2Cl_2 (15 mL) and CH_3CN (5 mL). AgOAc (70 mg, 0.42 mmol) was added and the mixture was stirred at room temperature for 3 h. The resulting suspension was filtered from the precipitated AgI over Celite and the solvent was removed under reduced pressure to give the product NHC-Pd(II) complex **2** (131 mg, 88%) as a white powder. Crystals suitable for X-ray diffraction study were grown from CH_2Cl_2/hexane solutions. M.p. 268 ^oC (Dec.); $[\alpha]^{20}_D$ = 52.0 (c 0.12 in DMSO); IR (KBr) *n* = 3408, 3053, 2924, 2847, 1580, 1510, 1385, 751 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.88 (br, 6H, CH_3), 3.90 (s, 6H, CH_3), 6.70-6.73 (m, 2H, ArH), 6.83-6.92 (m, 10H, ArH), 7.20-7.26 (m, 2H, ArH), 7.71 (d, *J* = 8.4 Hz, 2H, ArH), 8.05 (d, *J* = 8.4 Hz, 2H, ArH), 8.15 (d, *J* = 8.4 Hz, 2H, ArH); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* = 23.7, 35.0, 109.1, 112.4, 123.1, 123.4, 124.9, 126.4, 126.9, 127.5, 130.1, 131.2, 132.5, 132.7, 133.1, 135.1, 135.8, 171.6, 177.3; MS (MALDI) *m/e* 620.2.0 (M^+-$2O_2CCH_3$); Anal. Calcd. for $C_{40}H_{32}N_4O_4Pd \cdot 1.5H_2O$ requires: C 62.71, H 4.60, N 7.31; found: C 62.75, H 4.62, N 7.30%.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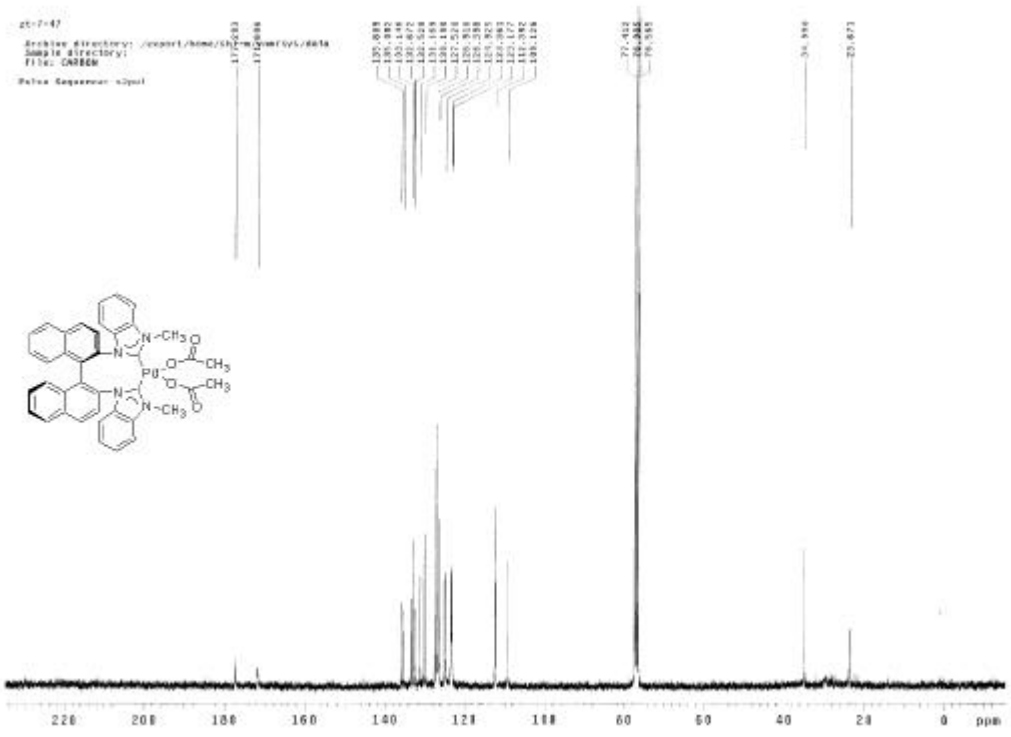
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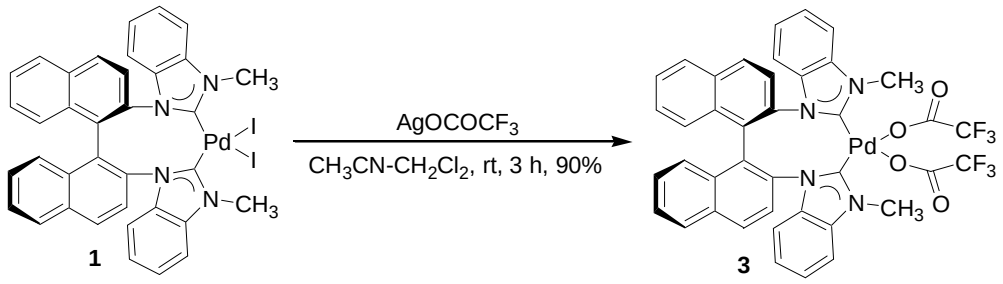
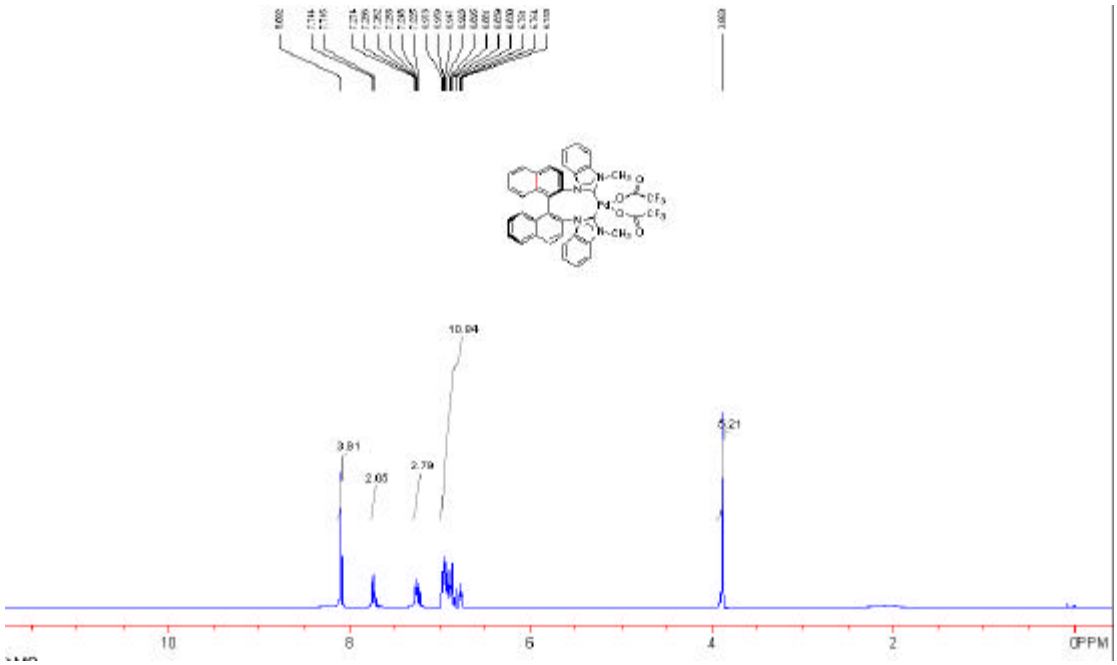


Synthesis of NHC-Pd(II) complex 3.

The NHC-Pd(II) complex **1** (174 mg, 0.20 mmol) was suspended in a mixed solution of CH_2Cl_2 (15 mL) and CH_3CN (5 mL). $AgOCOCF_3$ (93 mg, 0.42 mmol) was added and the reaction mixture was stirred at room temperature for 3 h. The resulting suspension was filtered from the precipitated AgI over Celite and the solvent was removed under reduced pressure to give the product NHC-Pd(II) complex **3** (153 mg, 90%) as a white powder. Crystals suitable for diffraction study were grown from CH_2Cl_2/hexane solutions. M.p. 248 ^oC (Dec.); $[\alpha]^{20}_D$ = 49.0 (c 0.55 in DMSO); IR (KBr) n = 3558, 2924, 1680, 1510, 1393, 745 cm^{-1}; ^1H NMR (300 MHz, $CDCl_3$, TMS) d = 3.88 (s, 6H, CH_3), 6.75-6.78 (m 2H, ArH), 6.83-6.97 (m, 10H, ArH), 7.22-7.27 (m, 2H, ArH), 7.73 (d, J = 8.1 Hz, 2H, ArH), 8.09 (s, 4H, ArH); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) d = 34.9, 109.4, 112.6, 115.9 (q, J = 287.9 Hz, CF_3), 123.8, 124.0, 124.4, 126.8, 127.3, 127.7, 130.5, 131.1, 132.5, 132.8, 133.0, 134.6, 135.7, 161.7 (q, J = 36.7 Hz, CO), 166.7; ^{19}F NMR (282 MHz, $CDCl_3$, $CFCl_3$) d = -74.9; MS (MALDI) m/e 515.2 (M^+-2OCOCF$_3$-Pd); Anal. Calcd. for $C_{40}H_{26}F_6N_4O_4Pd \cdot H_2O$ requires: C 55.54, H 3.26, N 6.48; found: C 55.64, H 3.11, N 6.27%.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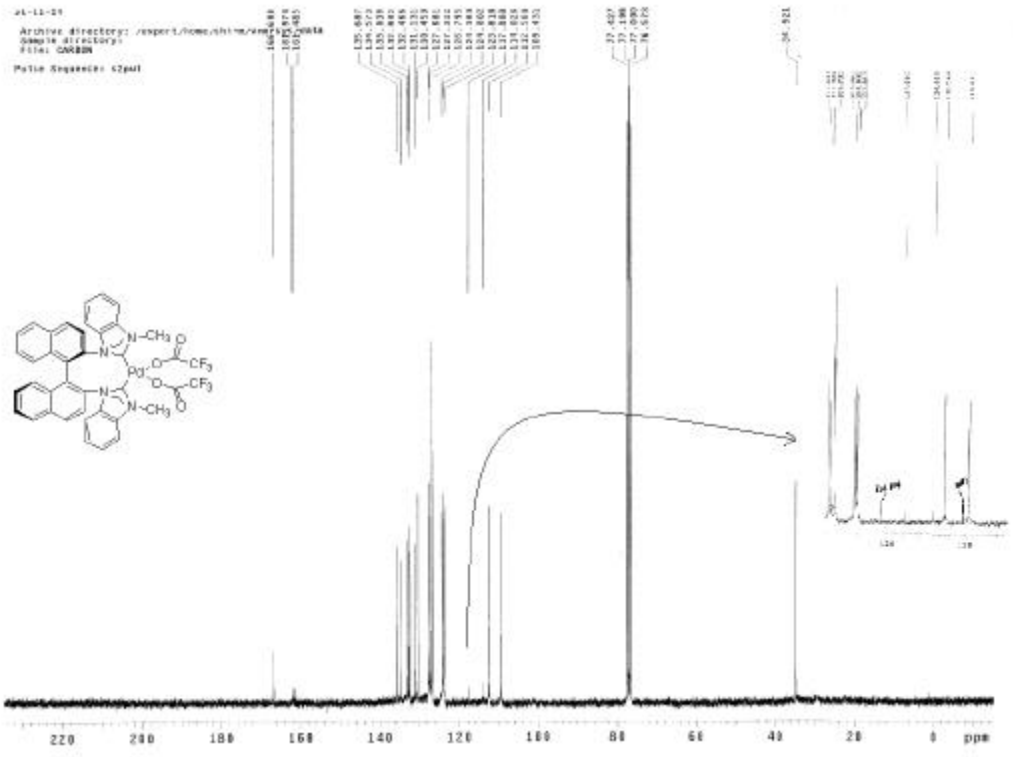
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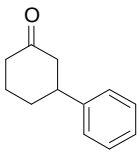
80
60
40
20
0
ppm

2. General Procedure for the Palladium Catalyzed Asymmetric Conjugate Addition of Arylboronic Acids and the Analytical Data of Products

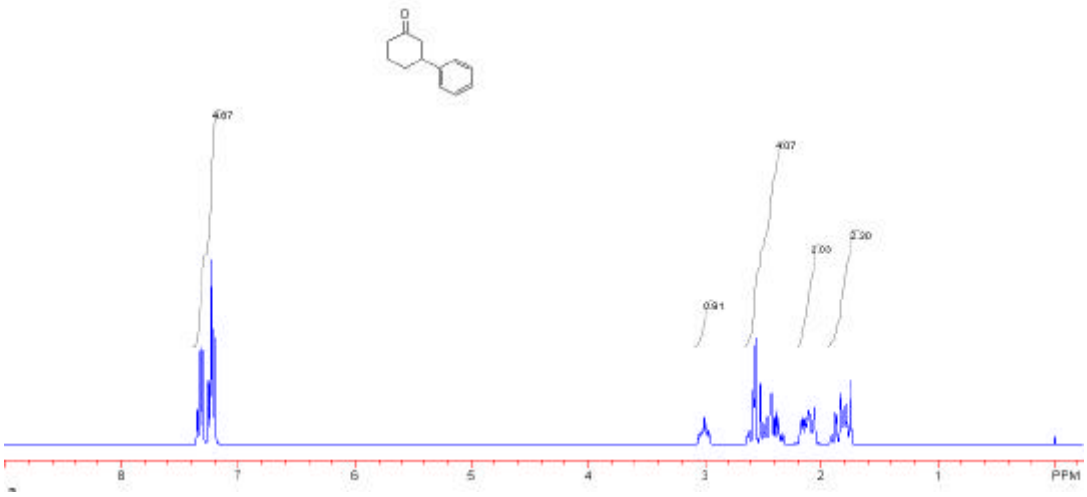
General procedure for the palladium catalyzed asymmetric conjugate addition of arylboronic acids to cyclic enones.

In a flame dried Schlenk tube equipped with septum and stirring bar, NHC-Pd(II)-cat (3 mol %, 7.5 μmol), and KOH (40 mol %, 0.1 mmol, 5.6 mg) were dissolved in dry THF (1.0 mL) and stirred under argon at room temperature for 10 min. Arylboronic acid **5** (1.5 equiv, 0.375 mmol) was added, followed by the addition of enone **4** (0.25 mmol). After the addition of H_2O (0.1 mL), the reaction mixture was stirred at the room temperature for 36 h. Saturated aqueous $NaHCO_3$ solution was added. The organic phase was separated and the resulting aqueous layer was extracted with Et_2O. The combined organic phases were filtered over a plug of silica, dried over anhydrous Na_2SO_4, concentrated under reduced pressure and purified by flash chromatography (eluent: EA/PE) to yield the corresponding products **6**.

Analytical Data of the Products.



3-Phenylcyclohexanone (6aa).[1] Ketone **6aa** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 97% yield, 96% ee. $[\alpha]^{25}_{D}$ = -20.4 (c 1.0 in $CHCl_3$) (for 96% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) d = 1.70-1.92 (2H, m), 2.06-2.18 (2H, m), 2.32-2.63 (4H, m), 2.96-3.05 (1H, m), 7.21-7.36 (5H, m); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) d = 25.5, 32.7, 41.1, 44.7, 48.9, 126.5, 126.6, 128.6, 144.3, 211.0; E.e. was determined by HPLC analysis, Chiralpak AD column, Hexane/*i*-PrOH = 100:1, detection at 209 nm, retention times: 19.5 (Maj) / 23.6 (Min) min.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8
7
6
5
4
3
2
1
PPM


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140
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100
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60
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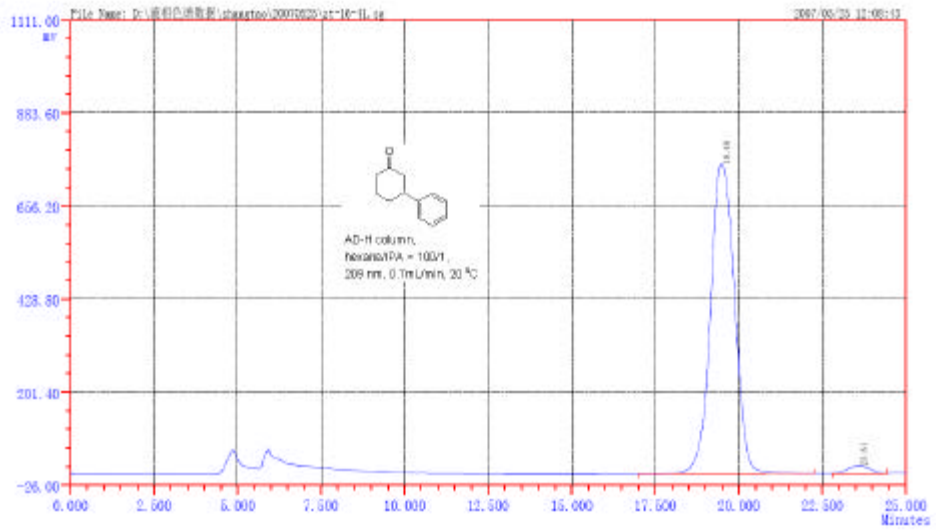

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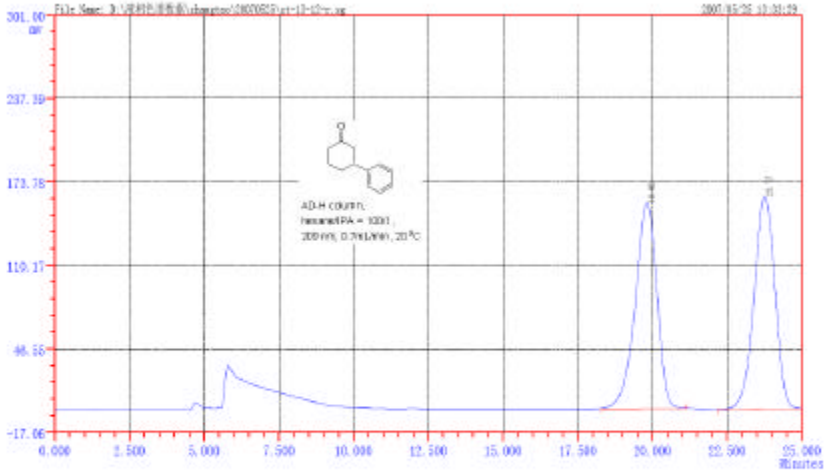
Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation



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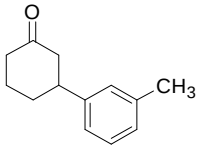
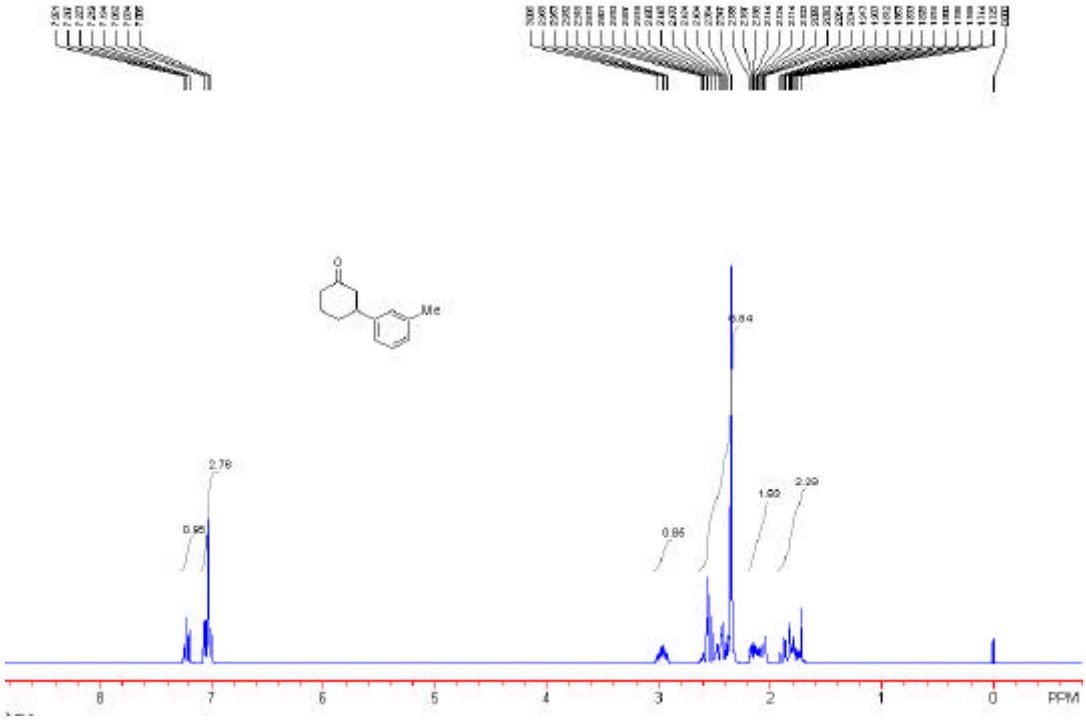
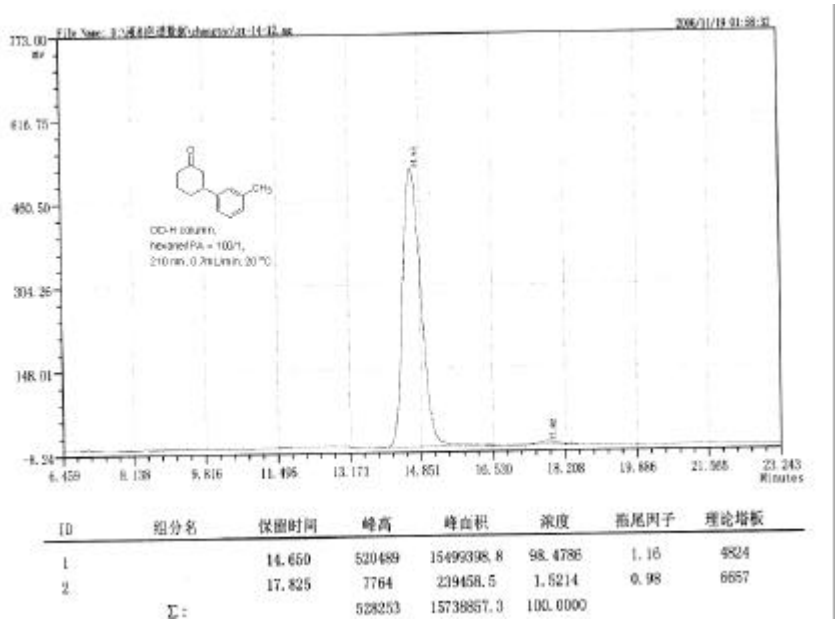


3-(3-Methylphenyl)cyclohexanone (6ab).[1] Ketone **6ab** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 97% yield, 97% ee. $[\alpha]^{25}_{D}$ = -20.8 (c 1.0 in $CHCl_3$) (for 97% ee); ^{1}H NMR (300 MHz, $CDCl_3$,

TMS) *d* = 1.78-1.87 (2H, m), 2.04-2.16 (2H, m), 2.34 (3H, s), 2.35-2.55 (4H, m), 2.95-2.96 (1H, m), 7.00-7.06 (3H, m), 7.19-7.24 (1H, m); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* = 21.4, 25.5, 32.7, 41.1, 44.7, 48.9, 123.5, 127.32, 127.34, 128.2, 138.2, 144.3, 211.1; E.e. was determined by chiral HPLC analysis, Chiralpak OD column, Hexane/*i*-PrOH = 100:1, detection at 210 nm, retention times: 14.65 (Maj) / 17.83 (Min) min.





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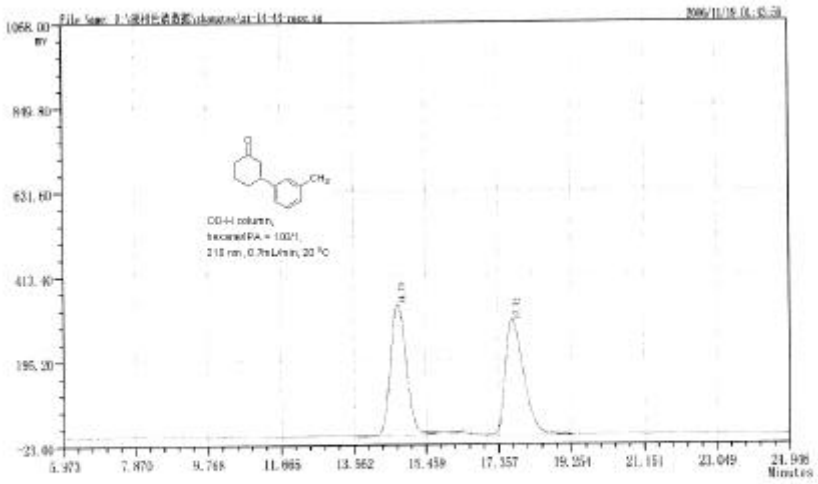
Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation



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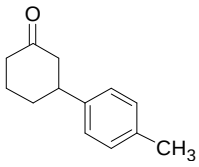
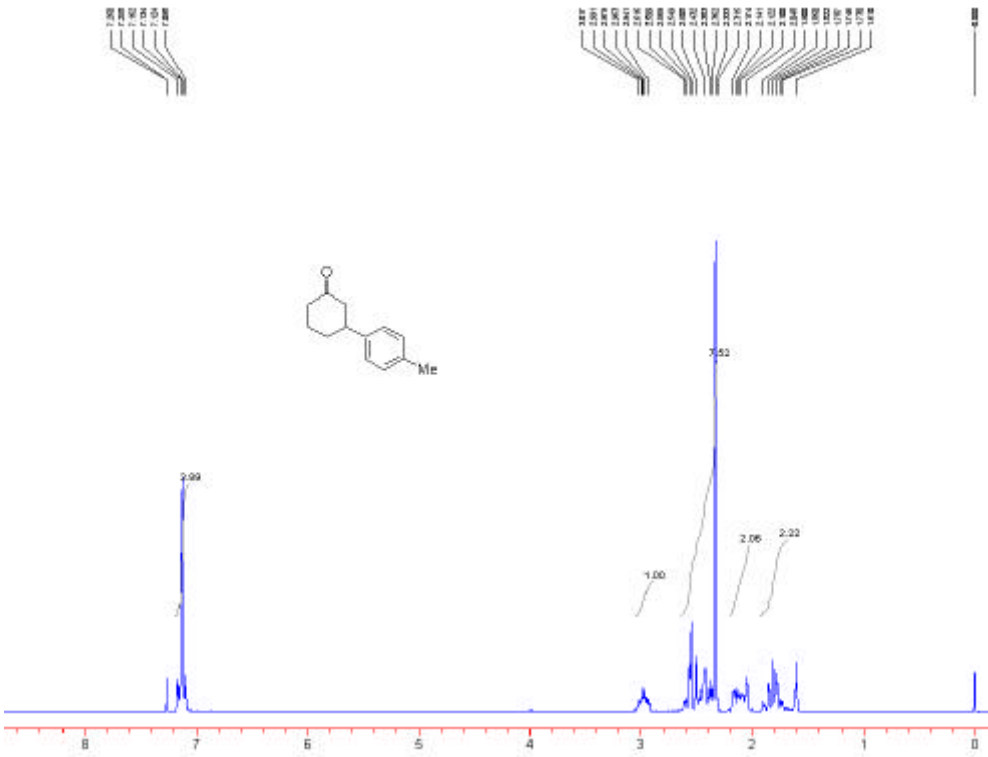


3-(4-Methylphenyl)cyclohexanone (6ac).[1] Ketone **6ac** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 89% yield, 92% ee. $[\alpha]^{25}_{D}$ = -16.4 (c 0.5 in $CHCl_3$) (for 92% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.73-1.90 (2H, m), 2.04-2.18 (2H, m), 2.33 (3H, s), 2.36-2.62 (4H, m), 2.93-3.02 (1H, m), 7.10-7.16 (4H, m); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* = 20.90, 25.5, 32.8, 41.1, 44.3, 49.0, 126.3, 129.2, 136.2, 141.3, 211.2. E.e. was determined by chiral HPLC analysis, Chiralpak AD column, Hexane/*i*-PrOH = 150:1, detection at 209 nm, retention times: 8.11 (Maj) / 8.77 (Min) min.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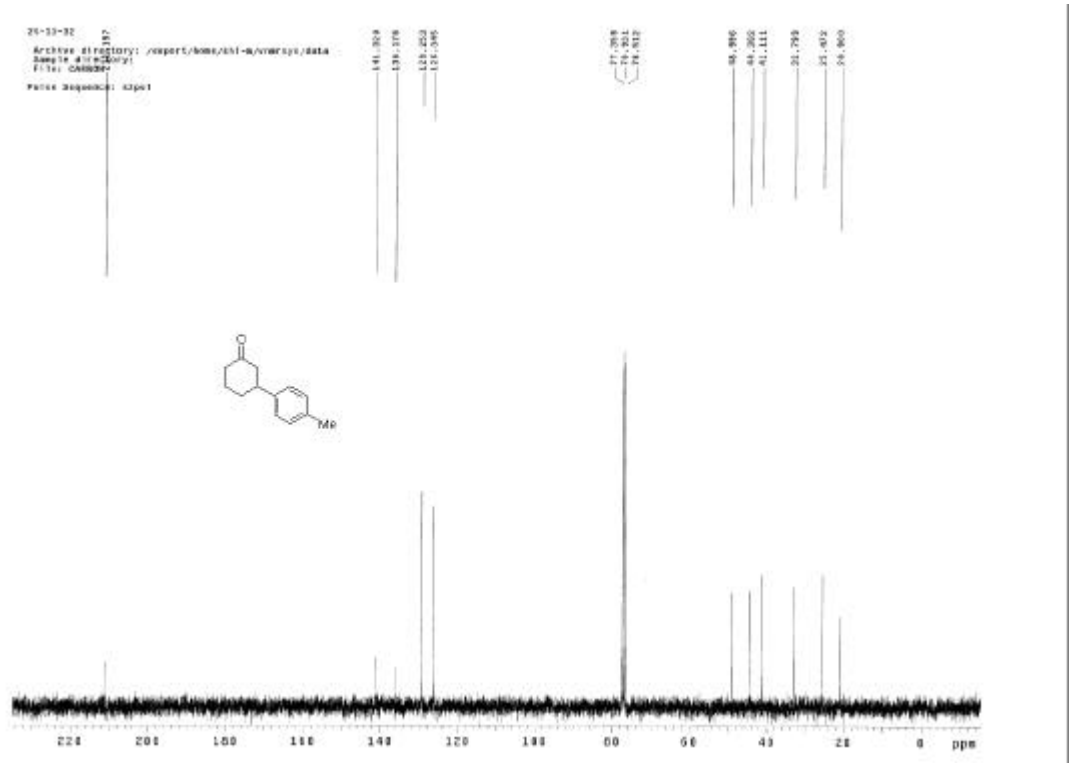
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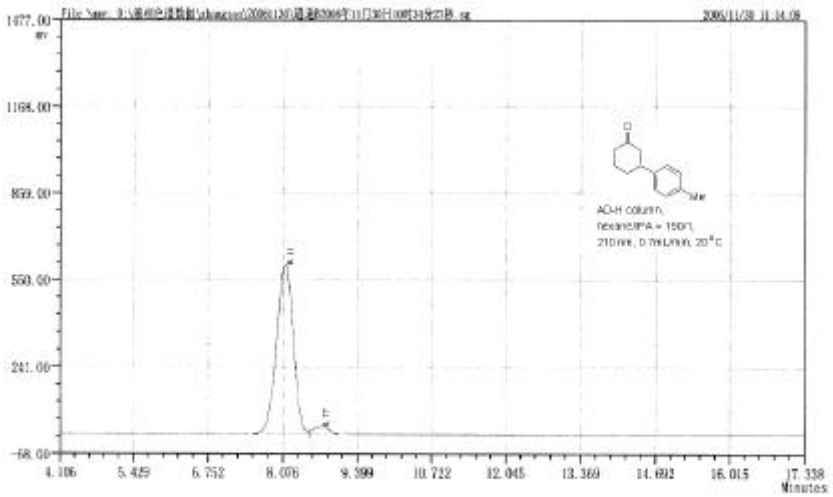

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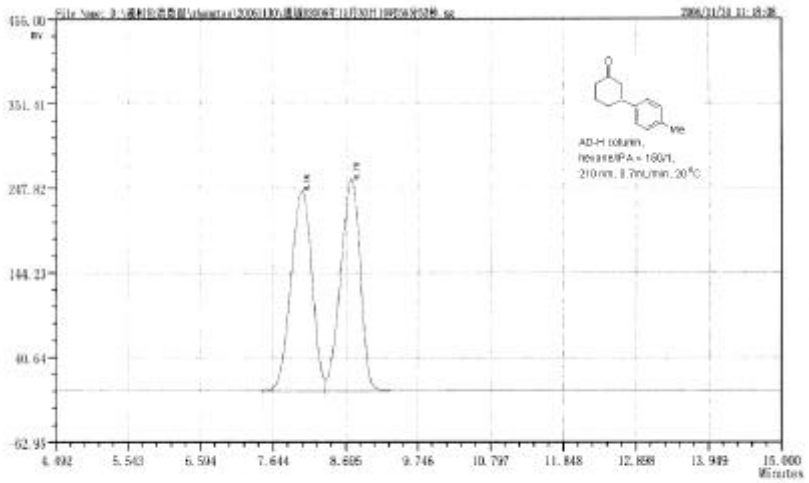

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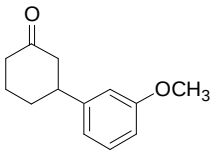
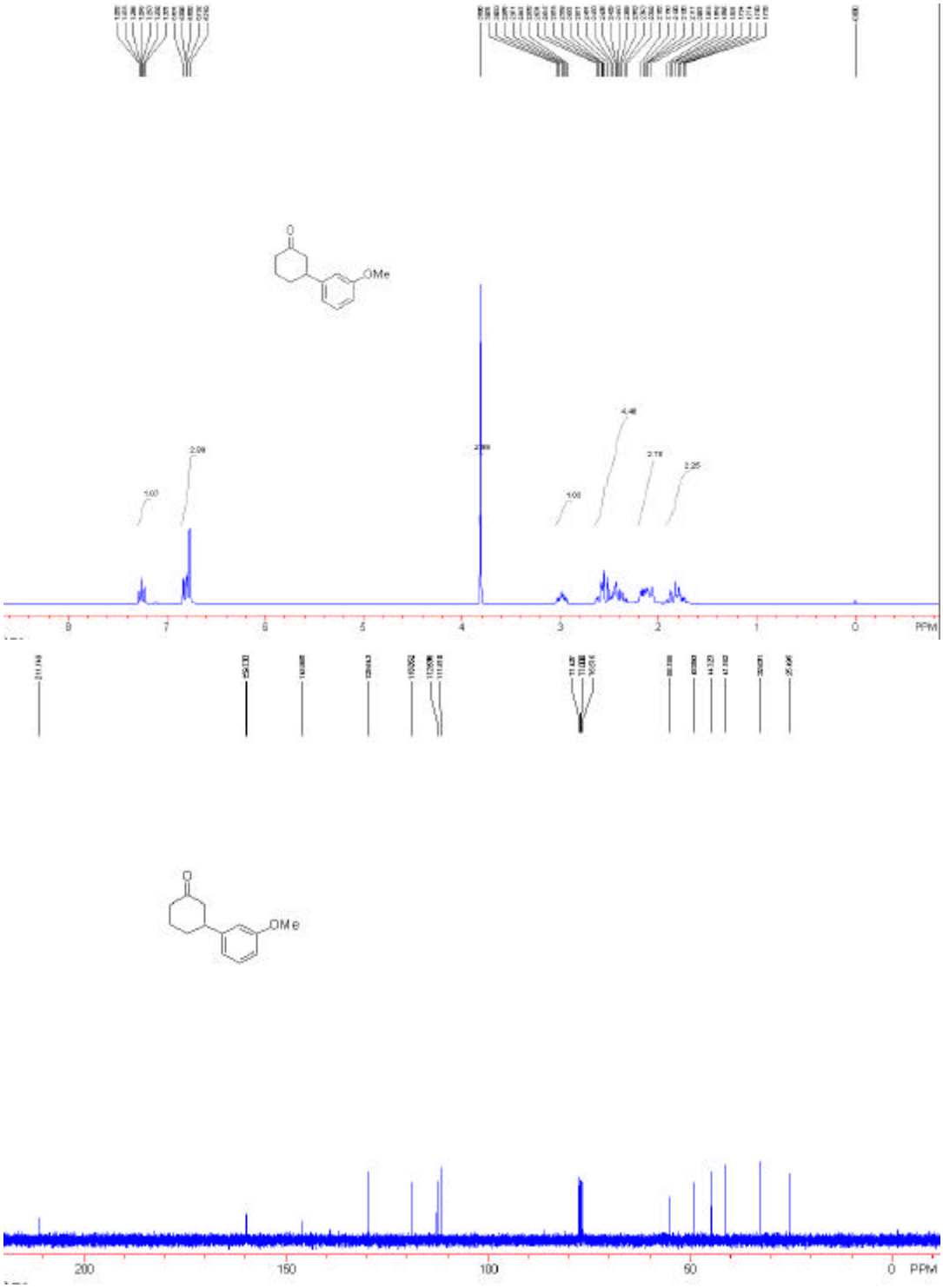
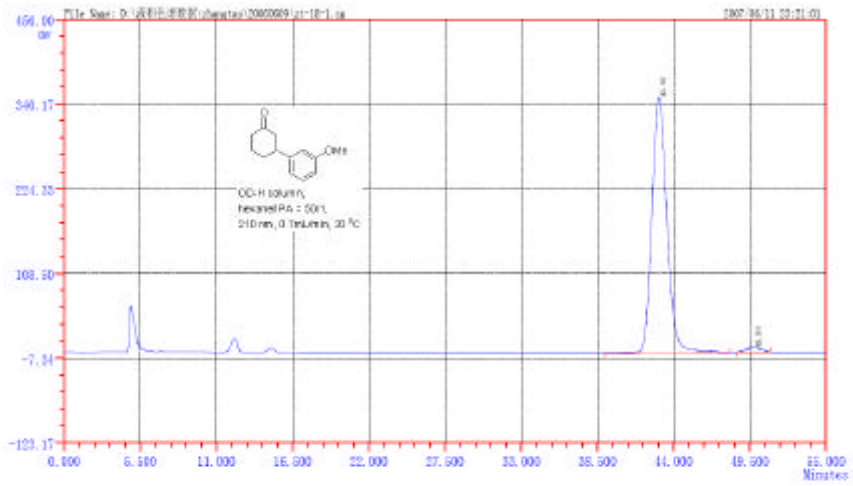


3-(3-Methoxylphenyl)cyclohexanone (3ad).[3,5] Ketone **3ad** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 90% yield, 97% ee. $[\alpha]^{25}_{D}$ = -11.8 (c 1.1 in $CHCl_3$) (for 97% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.73-1.88 (2H, m), 2.06-2.18 (2H, m), 2.34-2.63 (4H, m), 2.95-3.02 (1H, m), 3.80 (3H, s), 6.77-6.83 (3H, m), 7.22-7.28 (1H, m); ^{13}C NMR (75 MHz,

$CDCl_3$, TMS) *d* = 25.5, 32.6, 41.2, 44.7, 48.9, 55.1, 111.7, 112.6, 118.8, 129.6, 145.9, 159.7, 211.1; E.e. was determined by chiral HPLC analysis, Chiralpak OD column, Hexane/*i*-PrOH = 50:1, detection at 210 nm, retention times: 42.95 (Maj) / 49.80 (Min) min.





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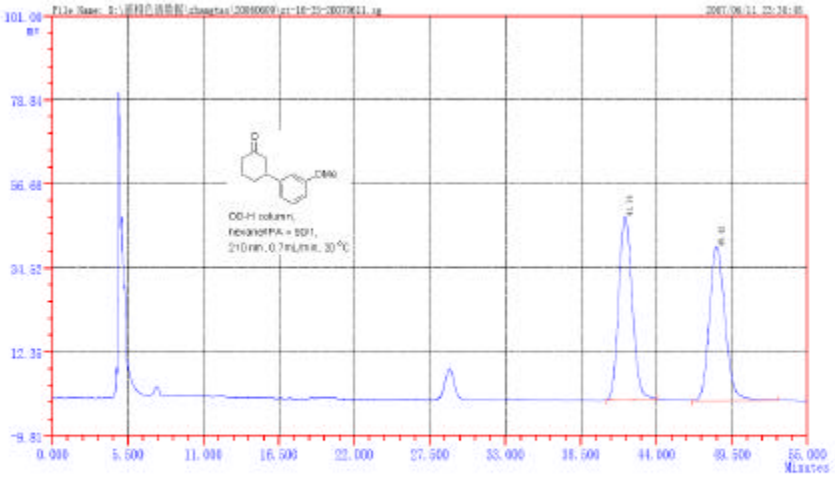
Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation



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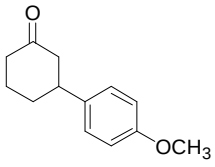
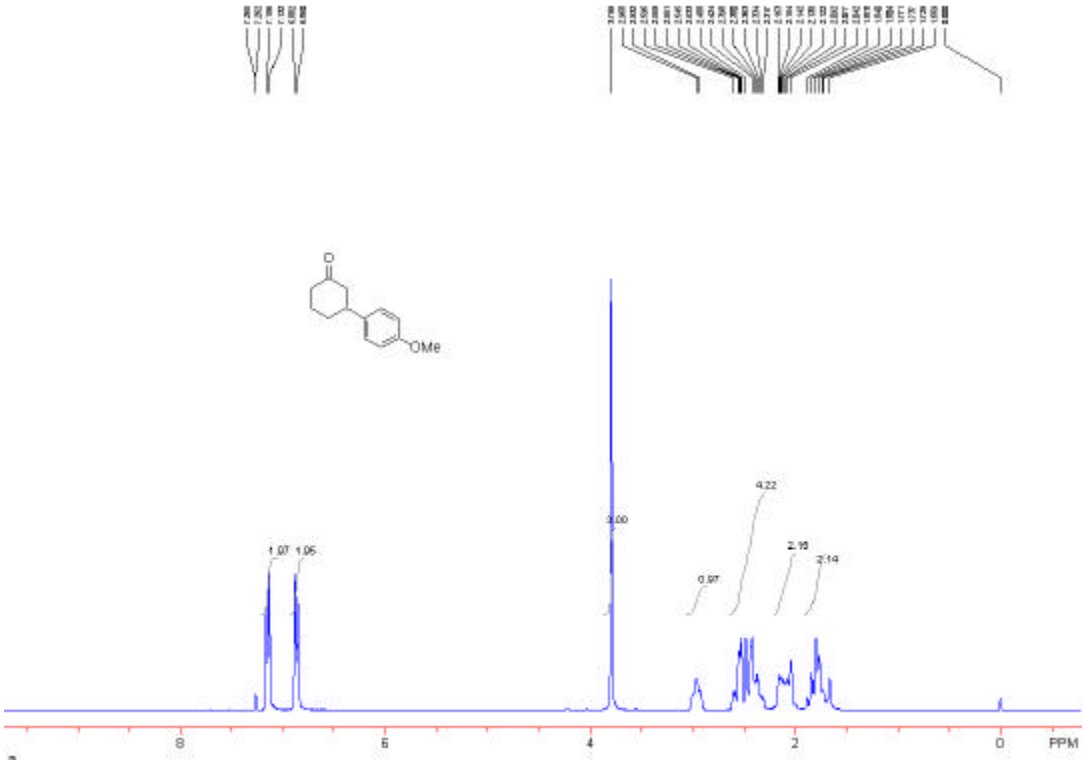
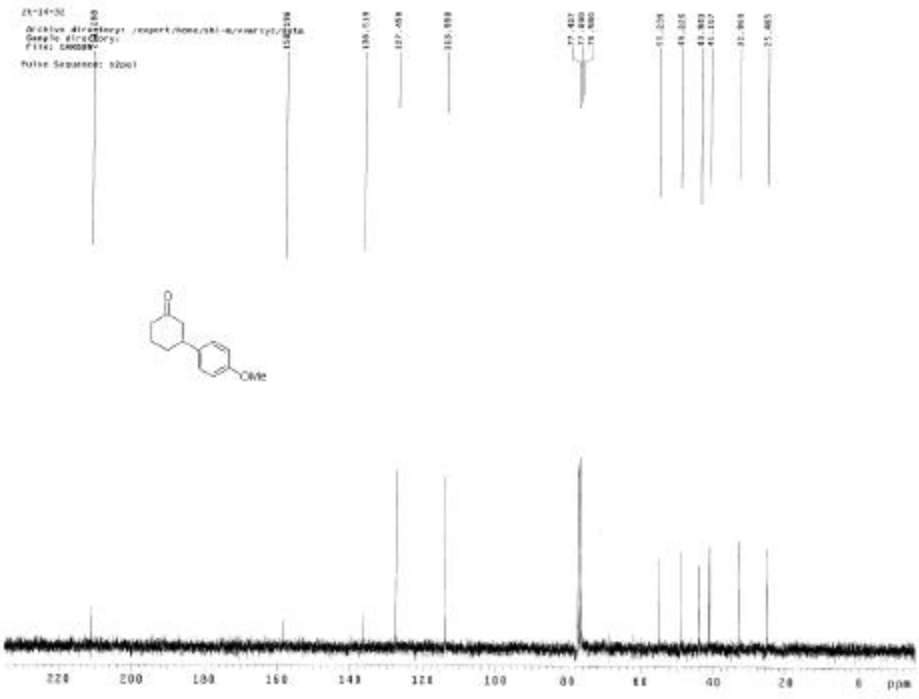
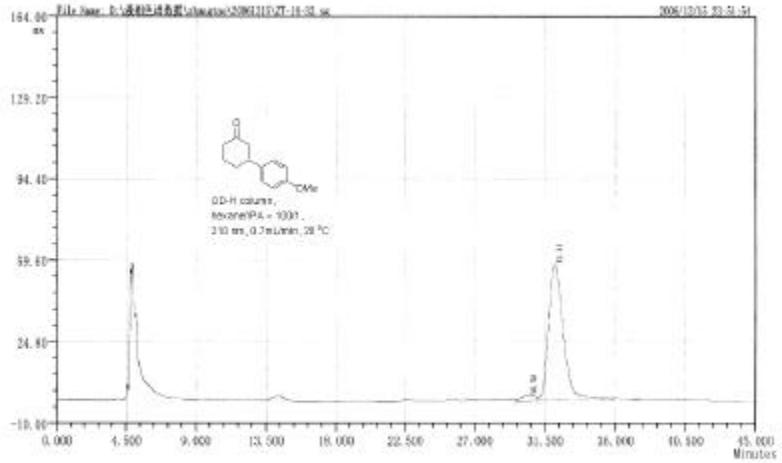


3-(4-Methoxylphenyl)cyclohexanone (6ae).[2] Ketone **6ae** was obtained after purification by flash chromatography (eluent: PE:EA = 20:1) in 90% yield, 94% ee. $[\alpha]^{25}_{D}$ = -19.1 (c 0.35 in $CHCl_3$) (for 94% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.72-1.88 (2H, m), 2.03-2.17 (2H, m), 2.31-2.60 (4H, m), 2.91-3.01 (1H, m), 3.79 (3H, s), 6.87 (2H, d, *J* = 10.2 Hz), 7.18 (2H, d, *J* = 10.2 Hz); ^{13}C NMR (75 MHz,

$CDCl_3$, TMS) *d* = 25.5, 33.0, 41.2, 43.9, 49.2, 55.2, 114.0, 127.5, 136.5, 158.2, 211.3; E.e. was determined by chiral HPLC analysis, Chiralpak OD column, Hexane/*i*-PrOH = 100:1, detection at 210 nm, retention times: 30.50 (Min) / 32.11 (Maj) min.

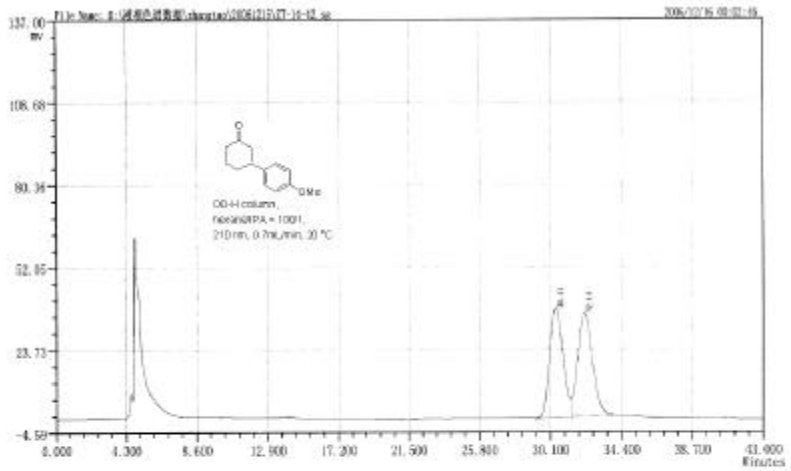




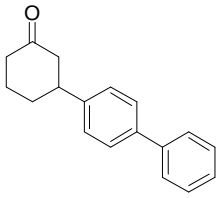


ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		30.500	2369	124381.7	3.1782	0.81	6726
2		32.108	57978	3789176.9	96.8218	1.35	4811
	Σ:		60347	3913558.5	100.0000		

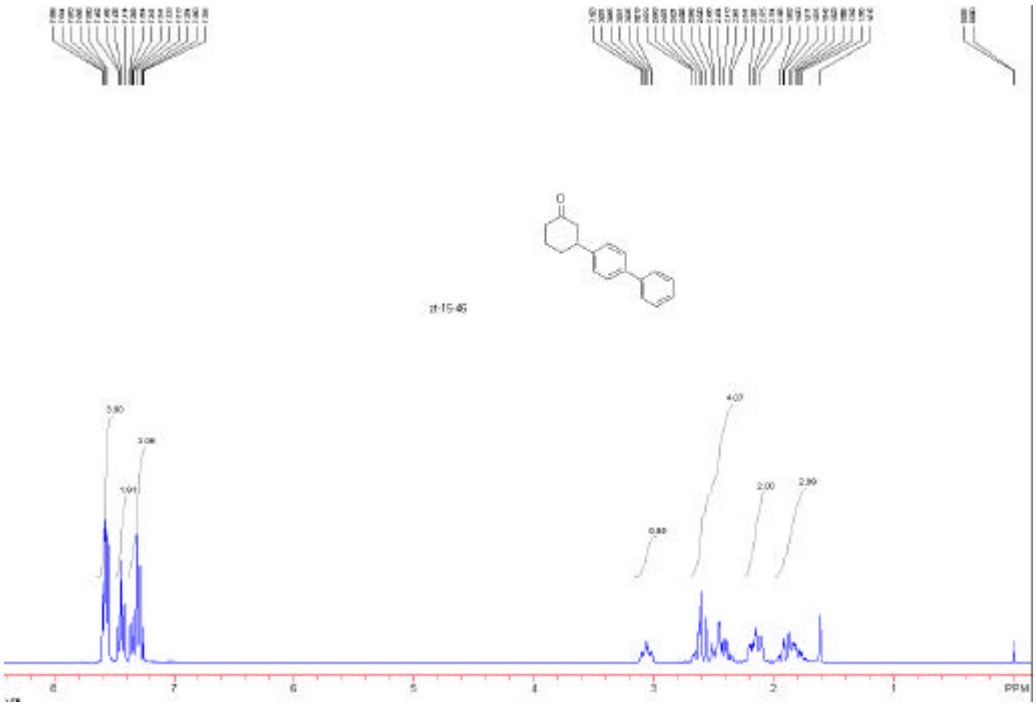
Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation



ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		30.408	37434	2110644.2	49.2473	1.13	5797
2		32.142	35237	2175162.0	50.7527	1.29	5404
Σ:			72671	4285806.2	100.0000		



3-Biphenyl-4-yl-cyclohexanone (6ag).[1] Ketone **6ag** was obtained after purification by flash chromatography (eluent: PE:EA = 20:1) in 97% yield, 93% ee. $[\alpha]^{25}_{D}$ = -5.5 (c 0.5 in $CHCl_3$) (for 93% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.77-1.92 (2H, m), 2.11-2.21 (2H, m), 2.37-2.67 (4H, m), 3.03-3.10 (1H, m), 7.26-7.37 (3H, m), 7.44 (2H, t, *J* = 7.2), 7.55-7.60 (4H, m); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* = 25.5, 32.7, 41.2, 44.4, 48.9, 126.98, 126.99, 127.2, 127.4, 128.7, 139.6, 140.7, 143.4, 211.1; E.e. was determined by chiral HPLC analysis, Chiralpak OD column, Hexane/*i*-PrOH = 50:1, detection at 209 nm, retention times: 25.25 (Min) / 34.62 (Maj) min.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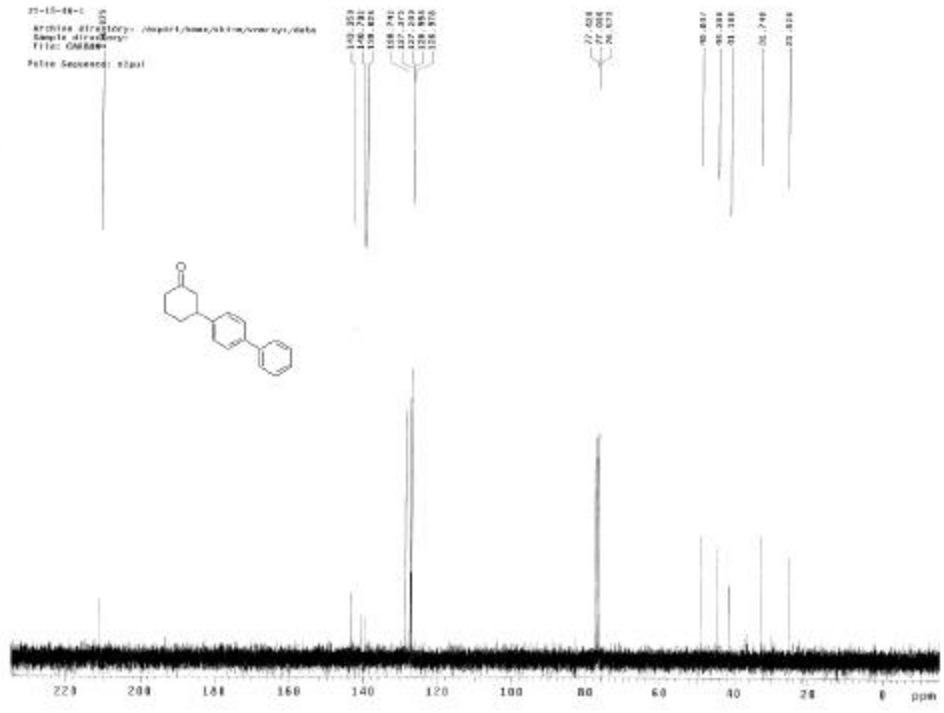
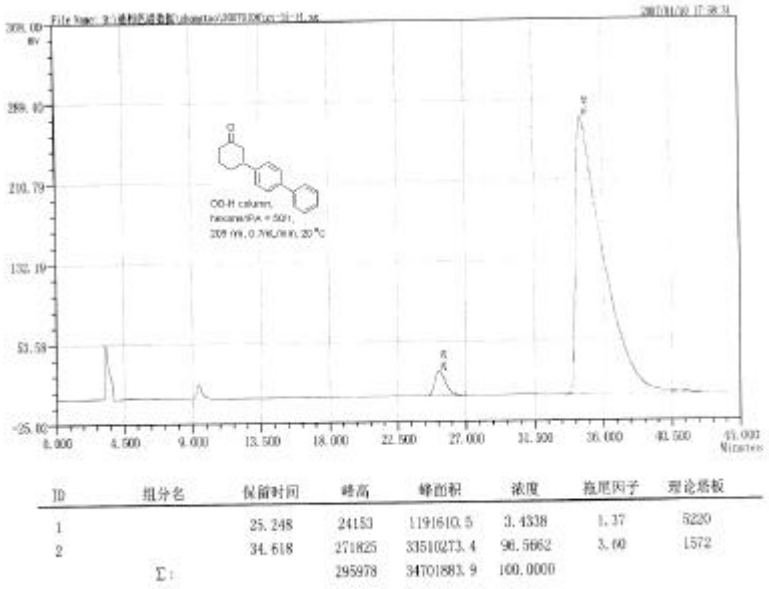
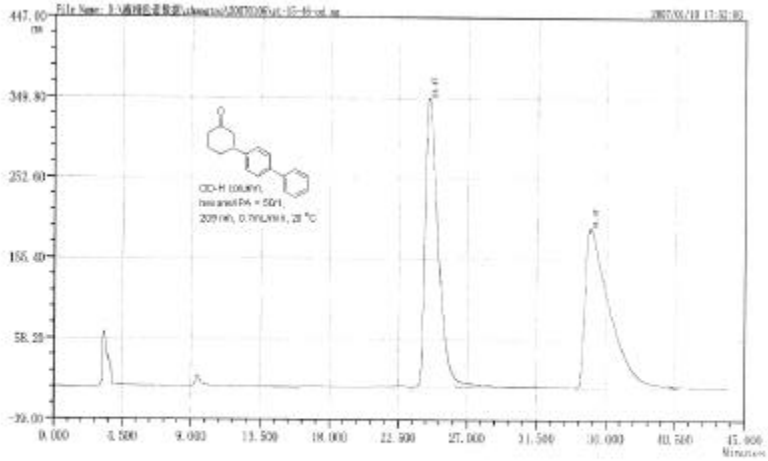
4.07
2.00
2.99
PPM


ppm

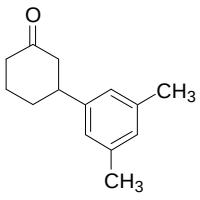


ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		25.248	24153	1191610.5	3.4338	1.17	5220
2		34.618	271825	33510273.4	96.5662	3.00	1572
Σ:			295978	34701883.9	100.0000		

Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation

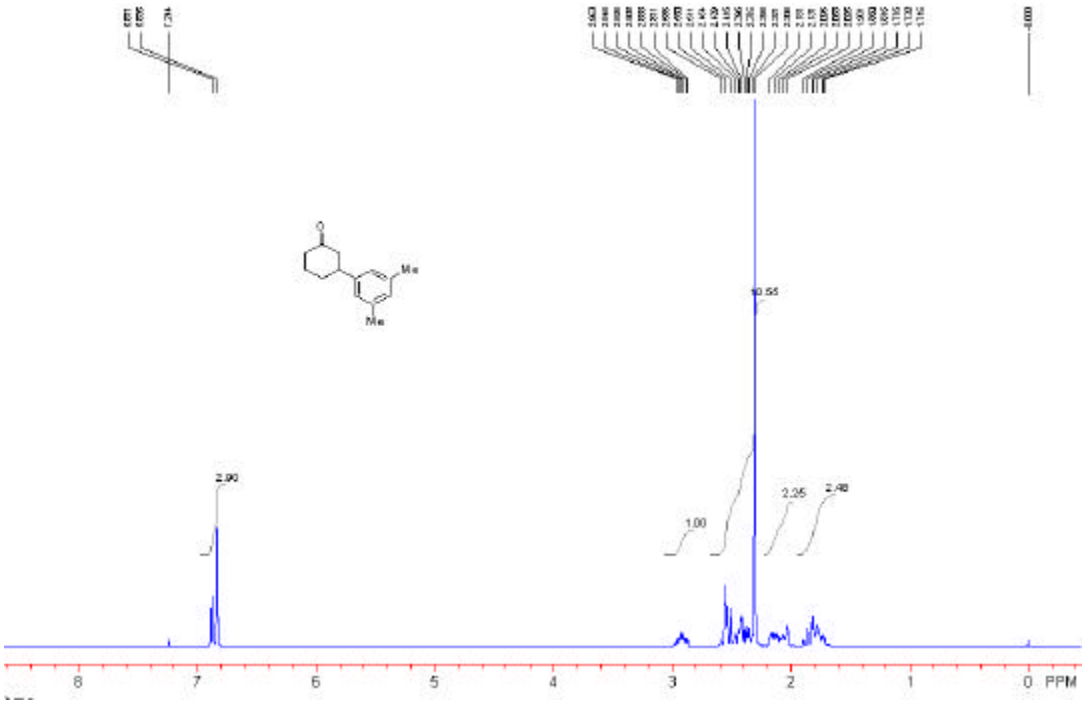


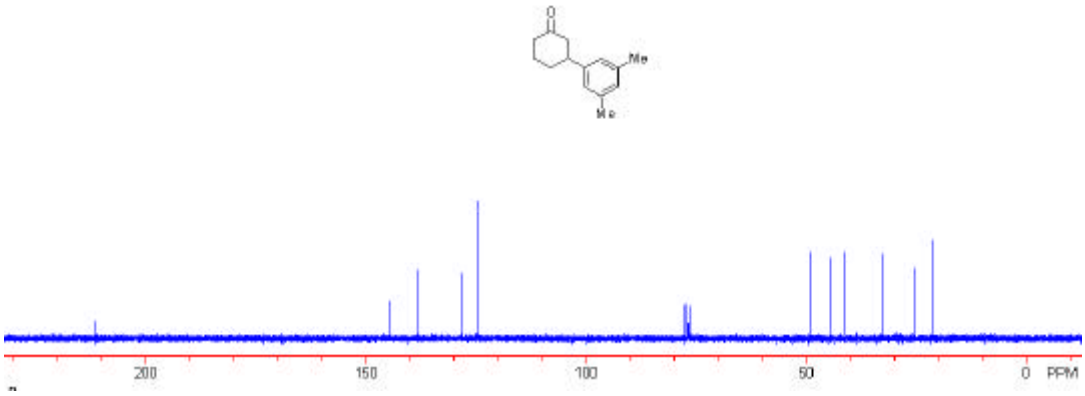
ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		24.465	350317	21182975.8	49.7945	2.13	3263
2		34.965	192799	21357782.6	50.2055	3.22	1986
Σ:			543116	42540758.4	100.0000		

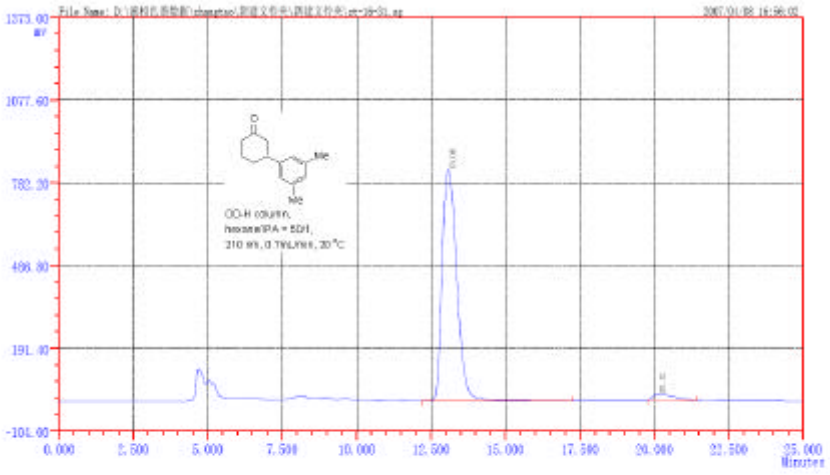


3-(3,5-Dimethylphenyl)cyclohexanone (6ai). Ketone **6ai** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 90% yield, 92% ee. $[\alpha]^{25}_{D}$ = -4.2 (c 0.8 in $CHCl_3$) (for 92% ee). ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.72-1.89 (2H, m), 2.03-2.18 (2H, m), 2.30 (6H, s), 2.33-2.59 (4H, m), 2.87-2.96 (1H, m), 6.83 (2H, s), 6.88 (1H, s); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* = 21.3, 25.6, 32.8, 41.2, 44.7, 49.0, 124.3, 128.3, 138.1, 144.3, 211.2; E.e. was determined by chiral HPLC

analysis, Chiralpak OD column, Hexane/*i*-PrOH = 50:1, detection at 210 nm, retention times: 13.08 (Maj) / 20.12 (Min) min.







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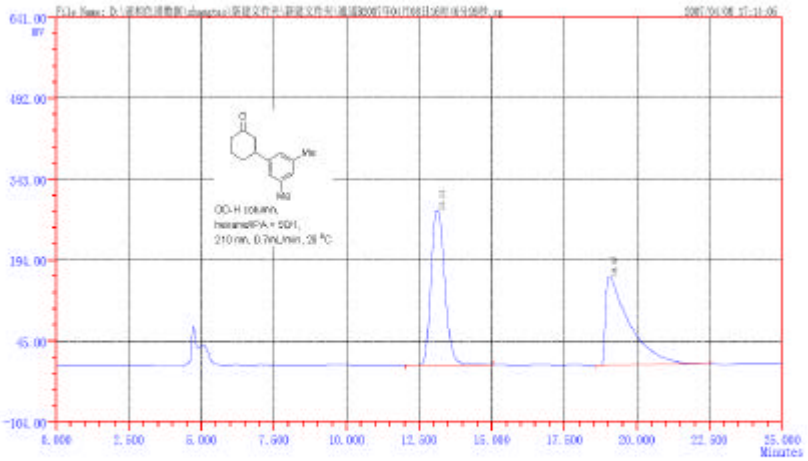
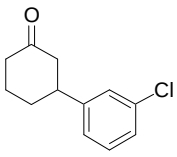
1		13.083	825594	28350434.0	96.0639	1.35	2893
2		20.117	24291	1161633.2	3.9361	2.59	3527
Σ:			849885	29512067.2	100.0000		

Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation

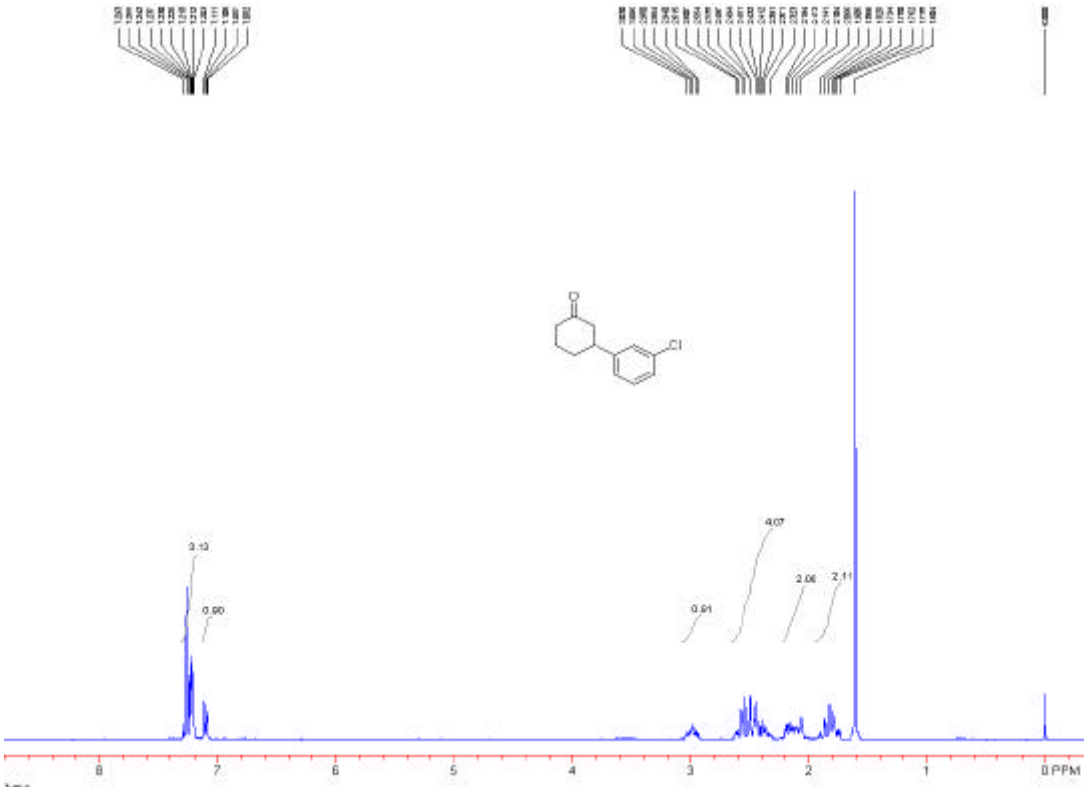


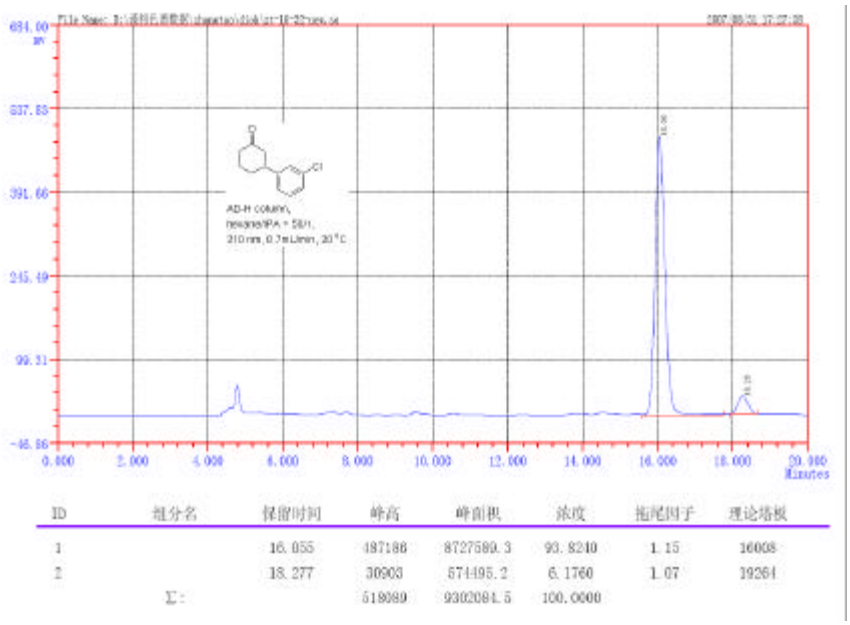
ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		13.133	284359	9343116.6	50.2070	1.19	3184
2		19.067	162314	9266067.4	49.7930	4.86	2223
Σ:			446673	18609184.0	100.0000		



3-(3-Chlorophenyl)cyclohexanone (6ah).[1] Ketone **6ah** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 78% yield, 88% ee. $[\alpha]^{25}_{D}$ = -5.4 (c 1.0 in $CHCl_3$) (for 88% ee); ^{1}H-NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.74-1.91 (2H, m), 2.07-2.19 (2H, m), 2.34-2.62 (4H, m), 2.95-3.03 (1H, m), 7.09-7.29 (4H, m); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* = 20.96, 25.6, 32.9, 41.2, 44.4, 49.1, 126.4, 129.3,

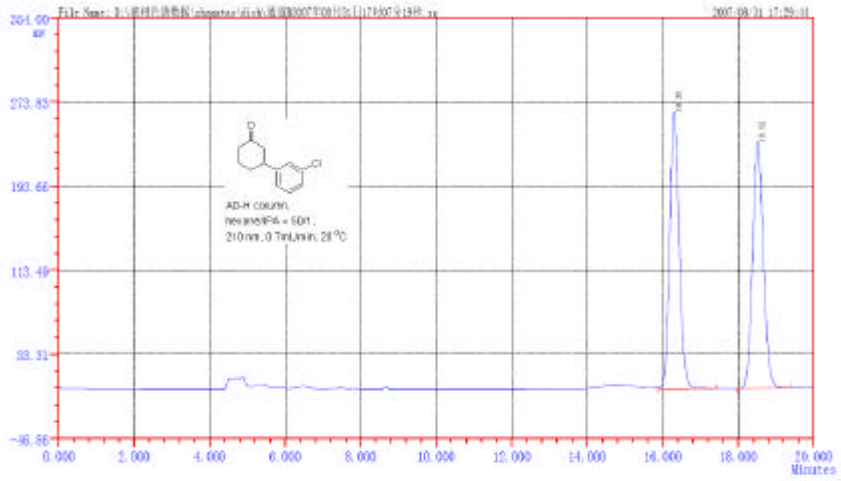
136.2, 141.4, 211.05; E.e. was determined by chiral HPLC analysis, Chiralpak AD column, Hexane/*i*-PrOH = 50:1, detection at 210 nm, retention times: 16.06 (Maj) / 18.28 (Min) min.



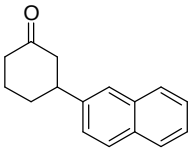


ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		16.055	487186	8727589.3	93.8240	1.15	16008
2		18.277	30903	574495.2	6.1760	1.07	19264
Σ:			518089	9302084.5	100.0000		

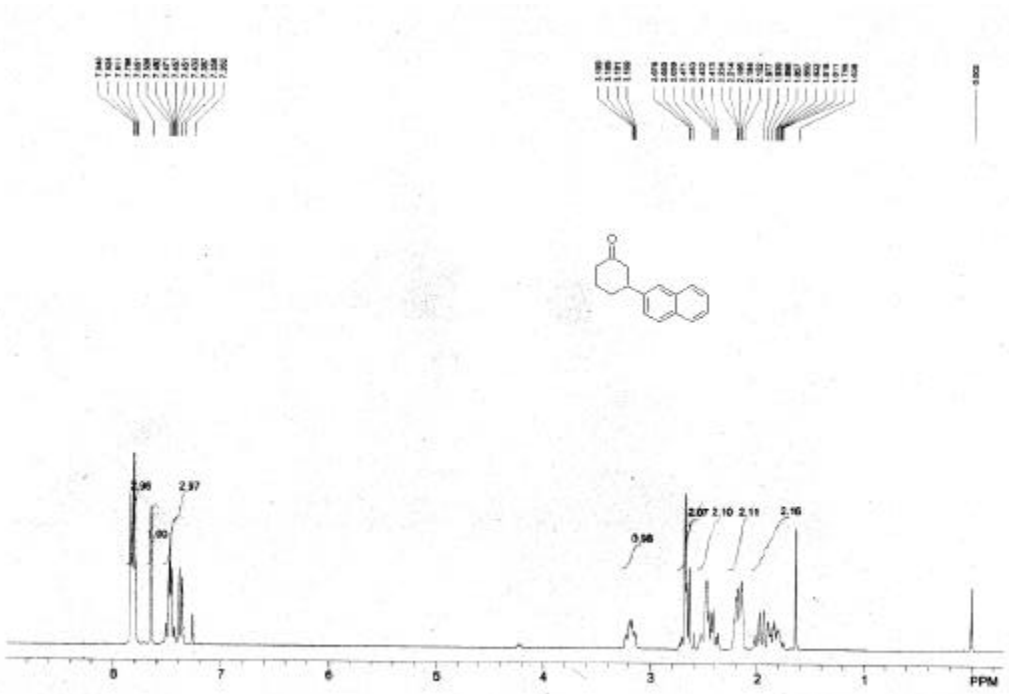
Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation



ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		16.303	264457	4635913.0	49.9452	1.13	17239
2		18.518	234826	4646094.1	50.0548	1.12	17460
Σ:			499283	9282007.0	100.0000		



3-(2-Naphthyl)cyclohexanone (6af).[1] Ketone **6af** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 99% yield, 97% ee. $[\alpha]^{25}_{D}$ = -8.4 (c 1.0 in $CHCl_3$) (for 97% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) d = 1.80-1.98 (2H, m), 2.15-2.22 (2H, m), 2.41-2.47 (2H, m), 2.64-2.68 (2H, m), 3.17-3.20 (1H, m), 7.36 (1H, d, *J* = 8.7 Hz), 7.43-7.51 (2H, m), 7.65 (1H, s), 7.80-7.84 (3H, m); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* = 25.5, 32.7, 41.2, 44.8, 48.8, 124.7, 125.3, 125.6, 126.2, 127.57, 127.64, 128.3, 132.3, 133.5, 141.7, 211.0; E.e. was determined by chiral HPLC analysis, Chiralpak OD column, Hexane/*i*-PrOH = 50:1, detection at 210 nm, retention times: 40.42 (Maj) / 49.07 (Min) min.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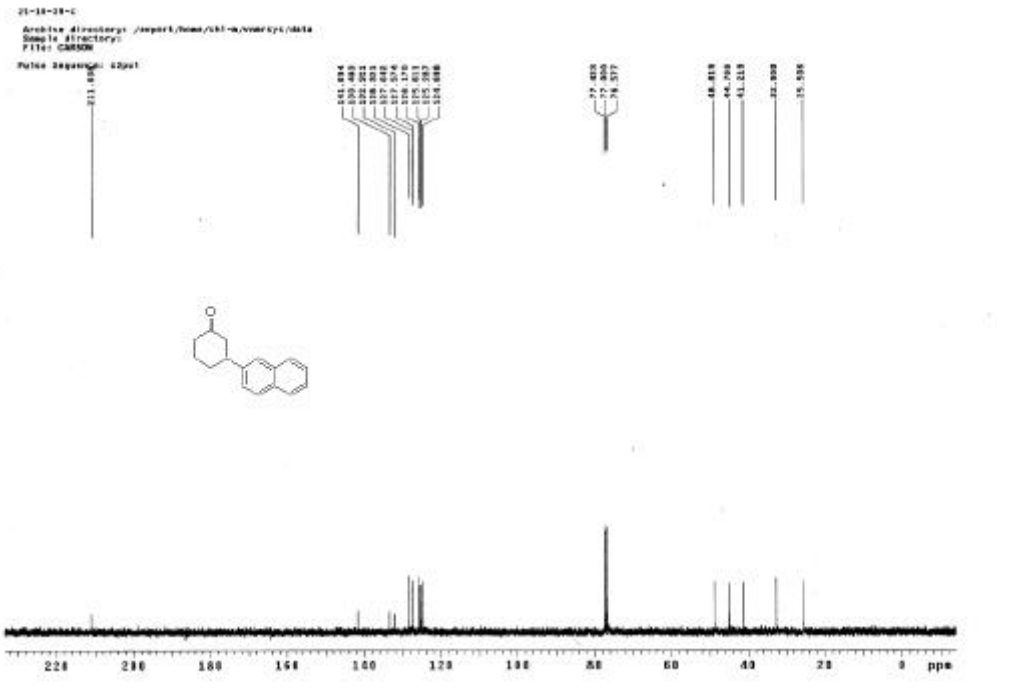
2.10
2.11
2.16
PPM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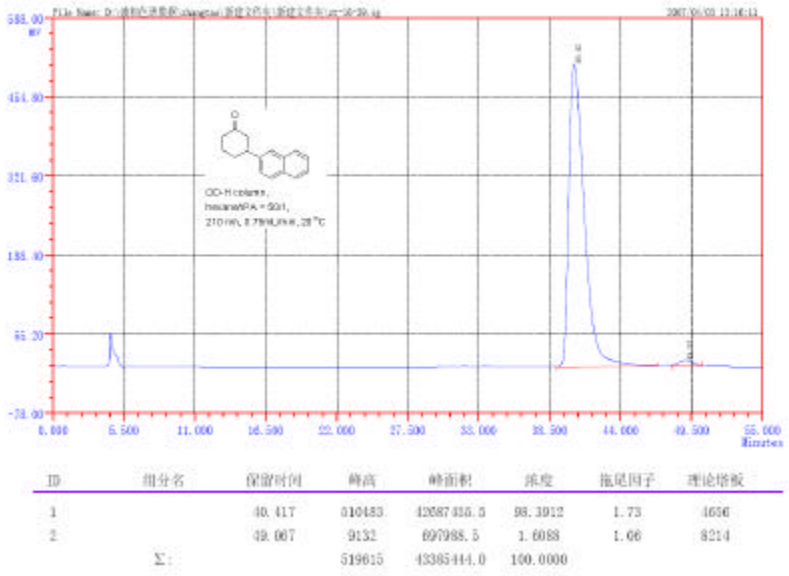
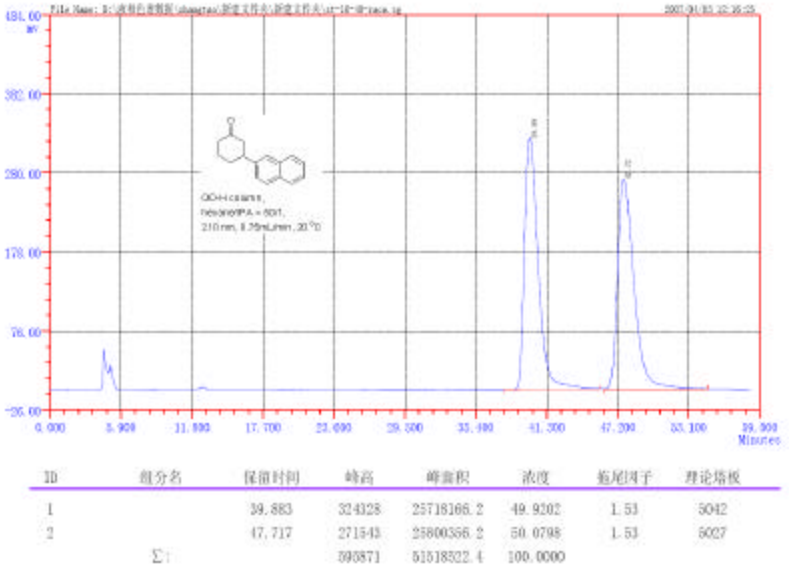
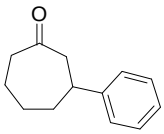


ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		40.417	510483	42687456.5	98.3912	1.73	4656
2		49.067	9132	697988.5	1.6088	1.66	8214
Σ:			519615	43385444.0	100.0000		

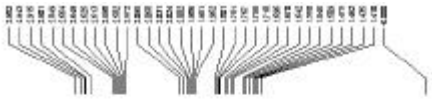
Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation

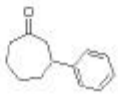


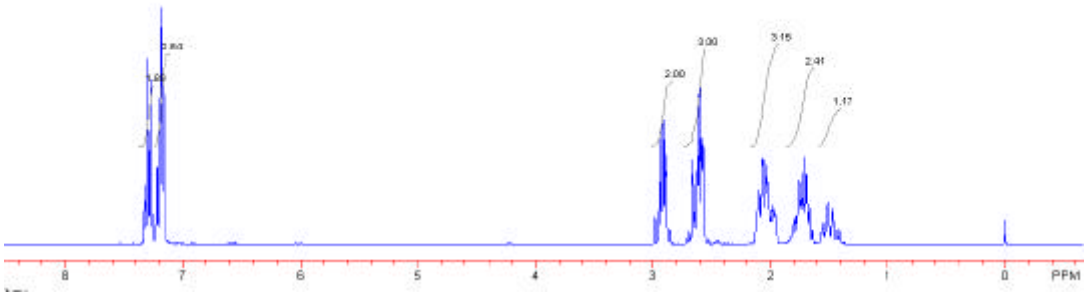
ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		39.883	324328	25718166.2	49.9202	1.53	5042
2		47.717	271543	25800366.2	50.0798	1.53	5027
Σ:			595871	51518532.4	100.0000		



3-Phenylcycloheptanone (6ba).[1] Ketone **6ba** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 88% yield, 91% ee. $[\alpha]^{25}_{D}$ = -50.8 (c 1.0 in $CHCl_3$) (for 91% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) δ = 1.41-1.48 (1H, m), 1.64-1.80 (2H, m), 1.96-2.10 (3H, m), 2.57-2.66 (3H, m), 2.85-2.96 (2H, m), 7.16-7.32 (5H, m); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) δ = 24.1, 29.2, 39.2, 42.7, 43.9, 51.2, 126.3, 126.4, 128.6, 146.9, 213.5; E.e. was determined by chiral HPLC analysis, Chiralpak OD column, Hexane/*i*-PrOH = 50/1, detection at 210 nm, retention times: 12.68 (Maj) / 13.66 (Min) min.



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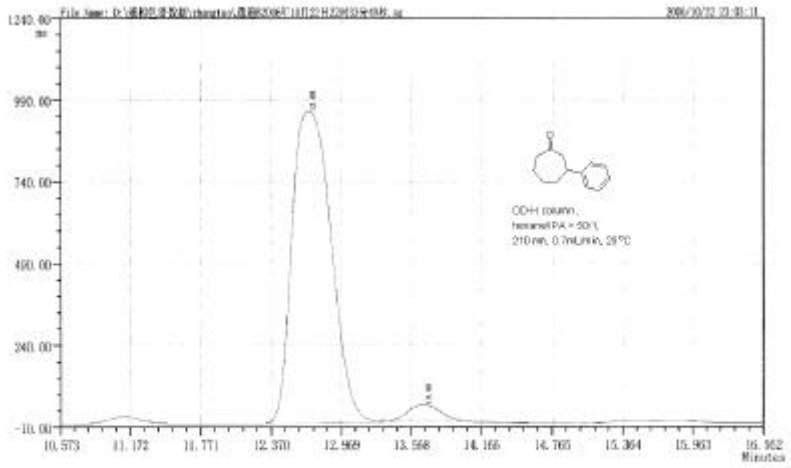
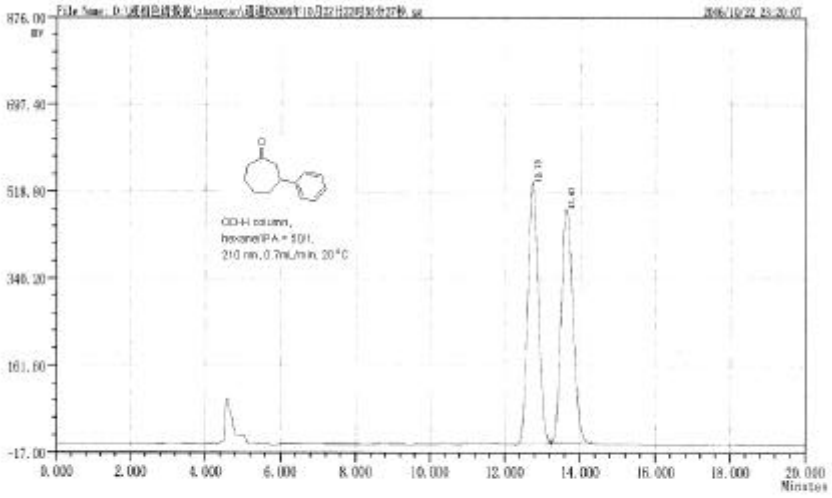
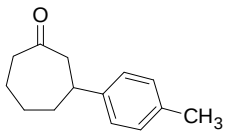


ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		12.683	953016	22079543.3	95.6650	1.30	5973
2		13.675	52380	1000513.0	4.3350	1.06	10216
Σ:			1005396	23080056.3	100.0000		

Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation

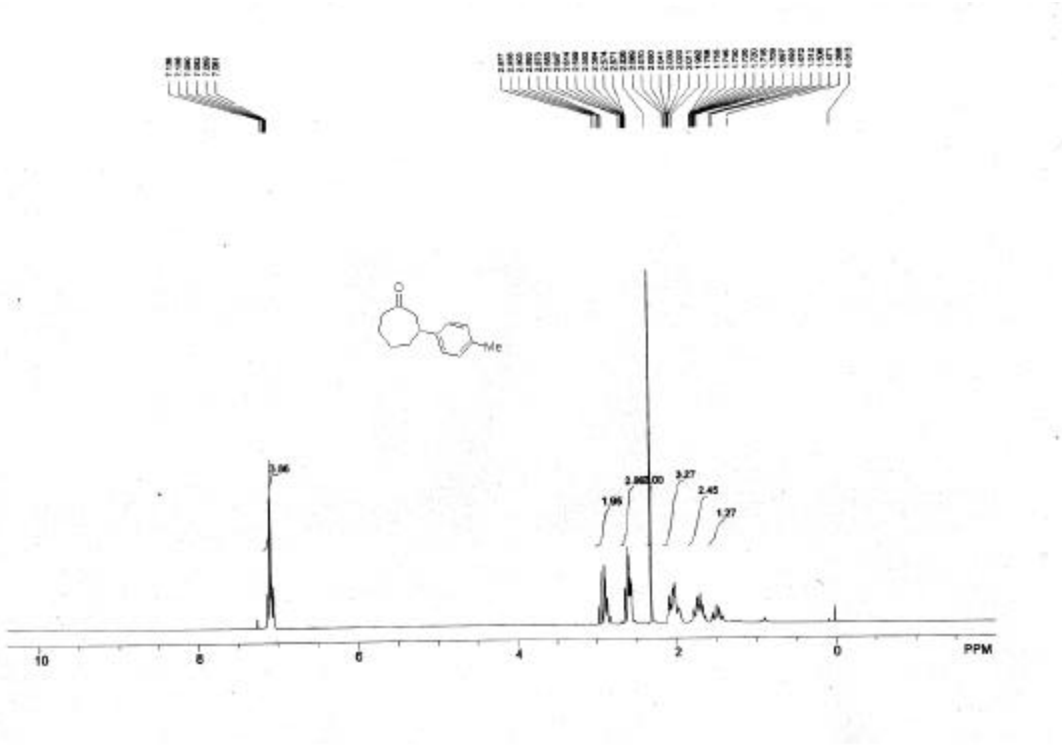


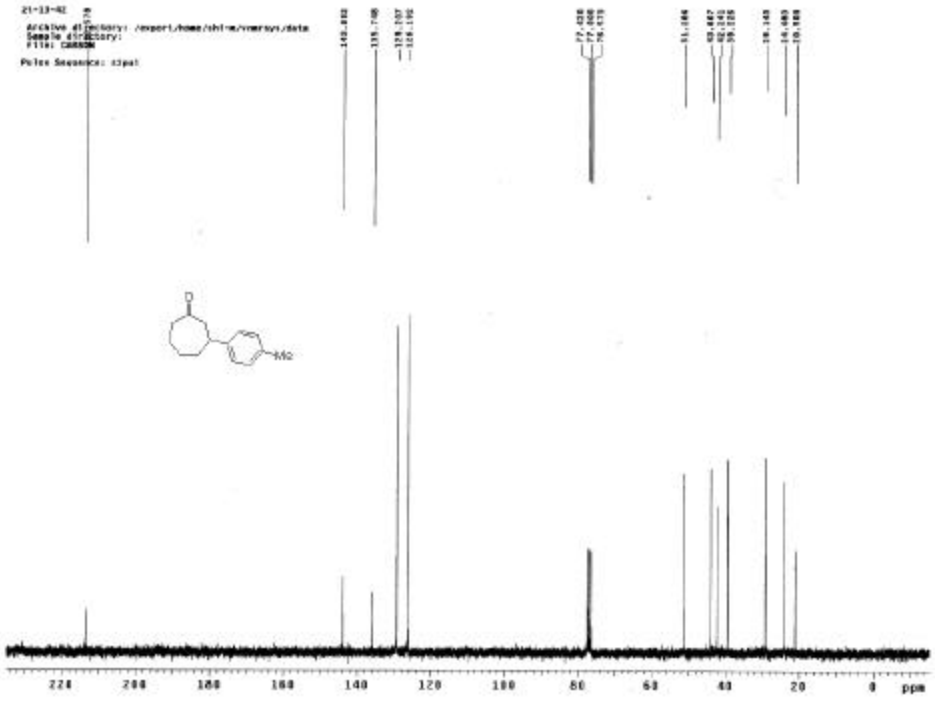
ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		12.733	537404	10466136.0	49.9919	1.17	8520
2		13.633	481609	10469532.8	50.0081	1.22	7839
Σ:			1019013	20935668.8	100.0000		

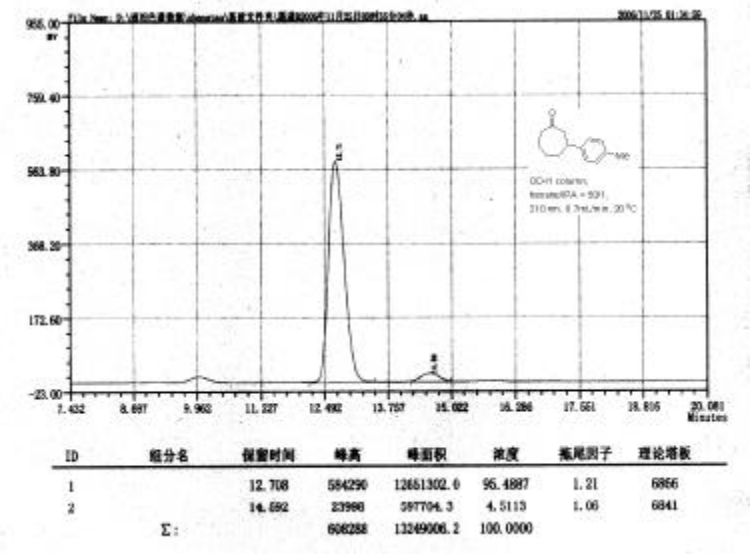


3-(4-Methylphenyl)cycloheptanone (6bb). Ketone **6bb** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 90% yield, 91% ee. $[\alpha]^{25}_{D}$ = -51.4 (c 0.5 in $CHCl_3$) (for 91% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.47-1.51 (1H, m), 1.67-1.76 (2H, m), 1.98-2.09 (3H, m), 2.33 (3H, s), 2.57-2.65 (3H, m), 2.87-2.98 (2H, m), 7.06-7.14 (4H, m); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* =

20.9, 24.1, 29.1, 39.2, 42.2, 43.9, 51.3, 126.2, 129.2, 135.7, 143.9, 213.6; E.e. was determined by chiral HPLC analysis, Chiralpak OD column, Hexane/*i*-PrOH = 50:1, detection at 210 nm, retention times: 12.71 (Maj) / 14.59 (Min) min.







ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
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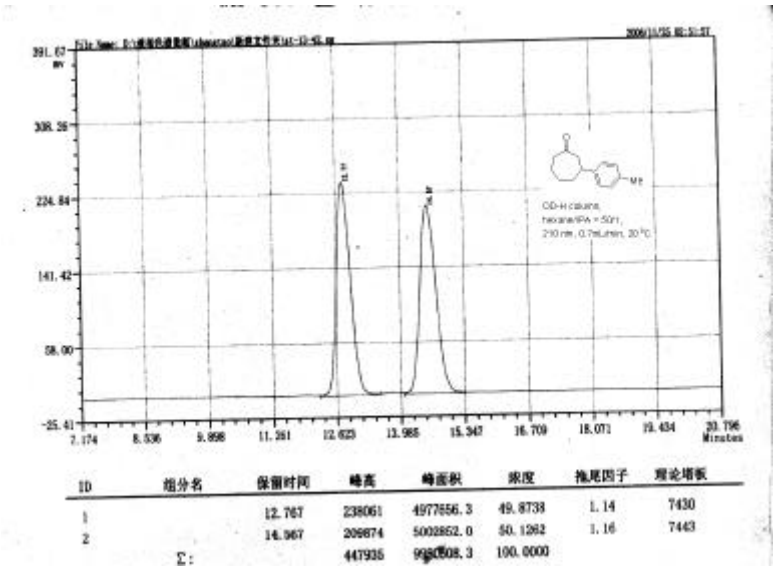
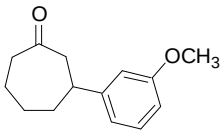
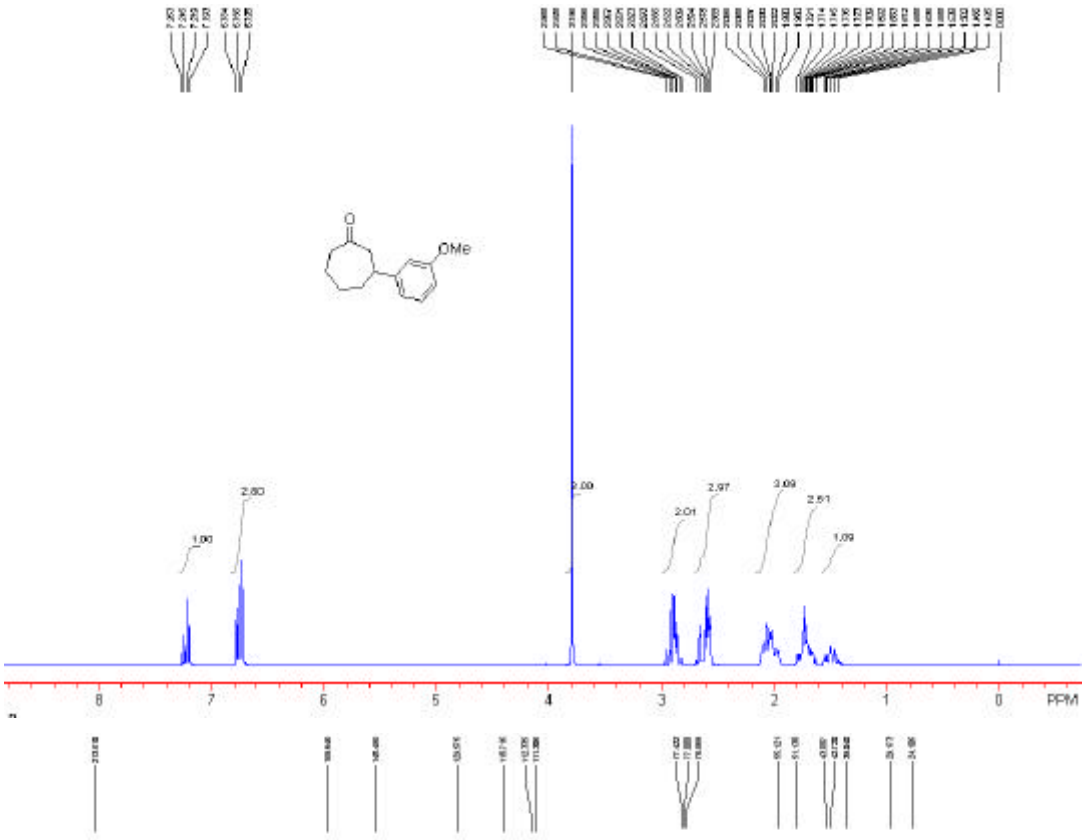
2		14.692	23990	597704.3	4.5113	1.06	6841
	Σ:		608288	13249006.2	100.0000		

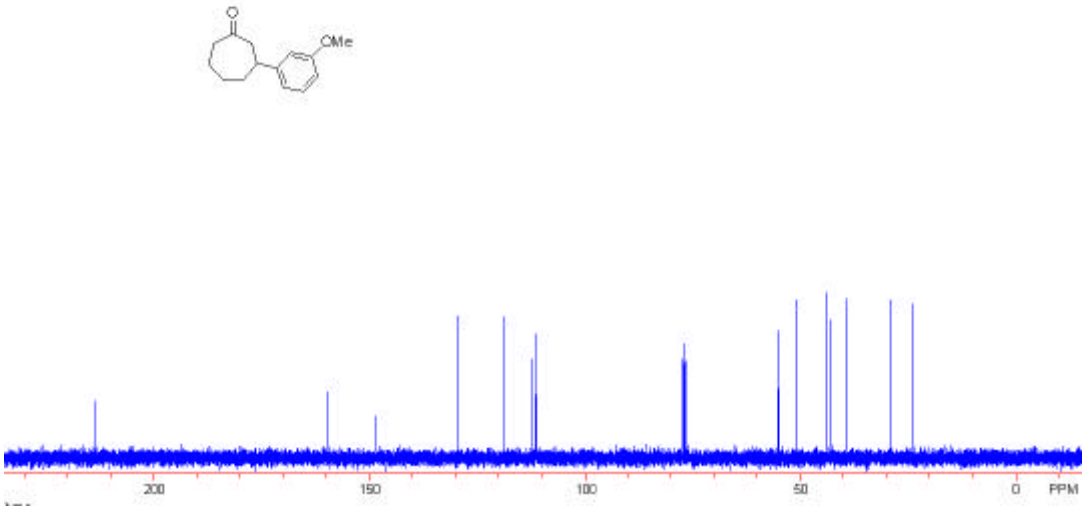
Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation

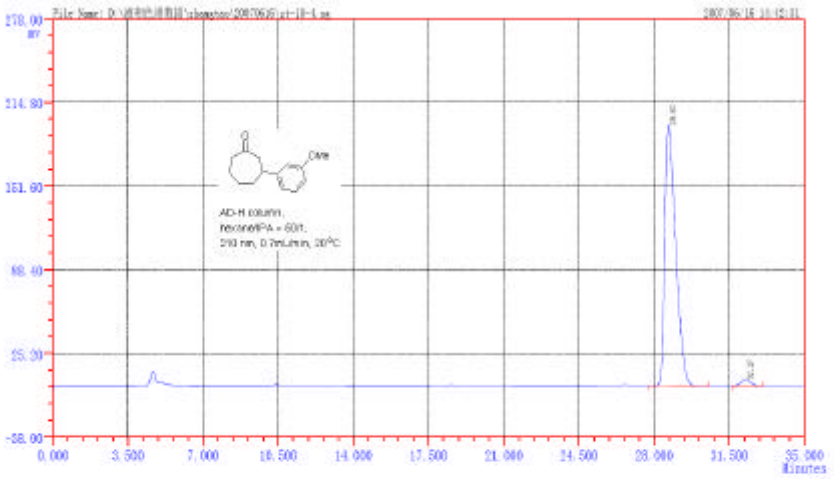




3-(3-Methoxylphenyl)cycloheptanone (6bd). Ketone **6bd** was obtained after purification by flash chromatography (eluent: PE:EA = 25:1) in 86% yield, 96% ee. $[\alpha]^{25}_{D}$ = -15.9 (c 0.4 in $CHCl_3$) (for 96% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.42-1.56 (1H, m), 1.64-1.79 (2H, m), 1.96-2.07 (3H, m), 2.57-2.70 (3H, m), 2.82-2.97 (2H, m), 2.80 (3H, s), 6.73-6.78 (3H, m), 7.22 (1H, t, *J* = 7.8 Hz); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* = 24.1, 29.2, 39.0, 42.7, 43.9, 51.1, 55.1, 111.3,112.3, 118.7, 129.6, 148.6, 159.6, 213.5; E.e. was determined by chiral HPLC analysis, Chiralpak AD column, Hexane/*i*-PrOH = 50:1, detection at 210 nm, retention times: 28.67 (Maj) / 32.28 (Min) min.

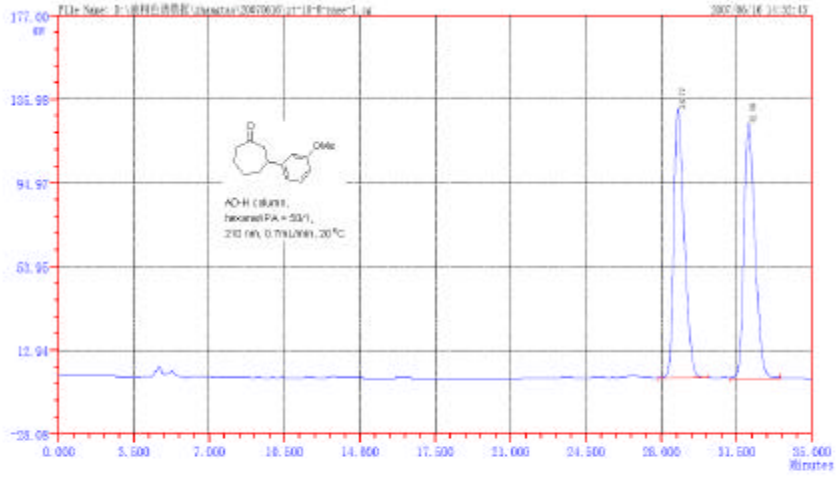

OMe
1.00
2.80
2.00
2.01
2.97
3.09
2.51
1.09
8
7
6
5
4
3
2
1
0
PPM


OMe
200
150
100
50
0
PPM

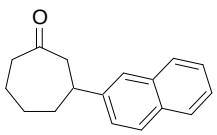


ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		28.672	197405	6920609.9	97.7904	1.64	13331
2		32.275	4674	156373.7	2.2096	1.04	18648
Σ:			202079	7076983.6	100.0000		

Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation

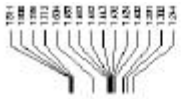


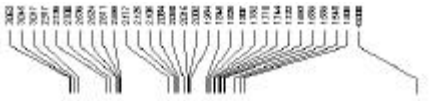
ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		28.770	132029	4414890.3	50.0463	1.42	14754
2		32.082	124515	4406712.9	49.9537	1.27	16357
Σ:			256544	8821603.2	100.0000		

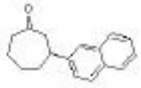


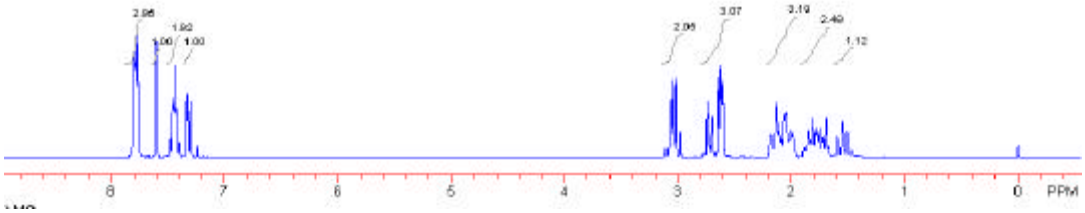
3-(2-Naphthyl)cycloheptanone (6bf). Ketone **6bf** was obtained after purification by flash chromatography (eluent: PE:EA = 20:1) in 99% yield, 97% ee. $[\alpha]^{25}_{D}$ = -35.3 (c 0.8 in $CHCl_3$) (for 97% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 1.70-1.81 (2H, m), 2.00-2.13 (2H, m), 2.29 (3H, s), 2.30-2.55 (4H, m), 2.89-2.96 (1H, m), 7.06-7.22 (4H, m); ^{13}C NMR (75 MHz, $CDCl_3$, TMS) *d* = 20.96, 25.6, 32.9,

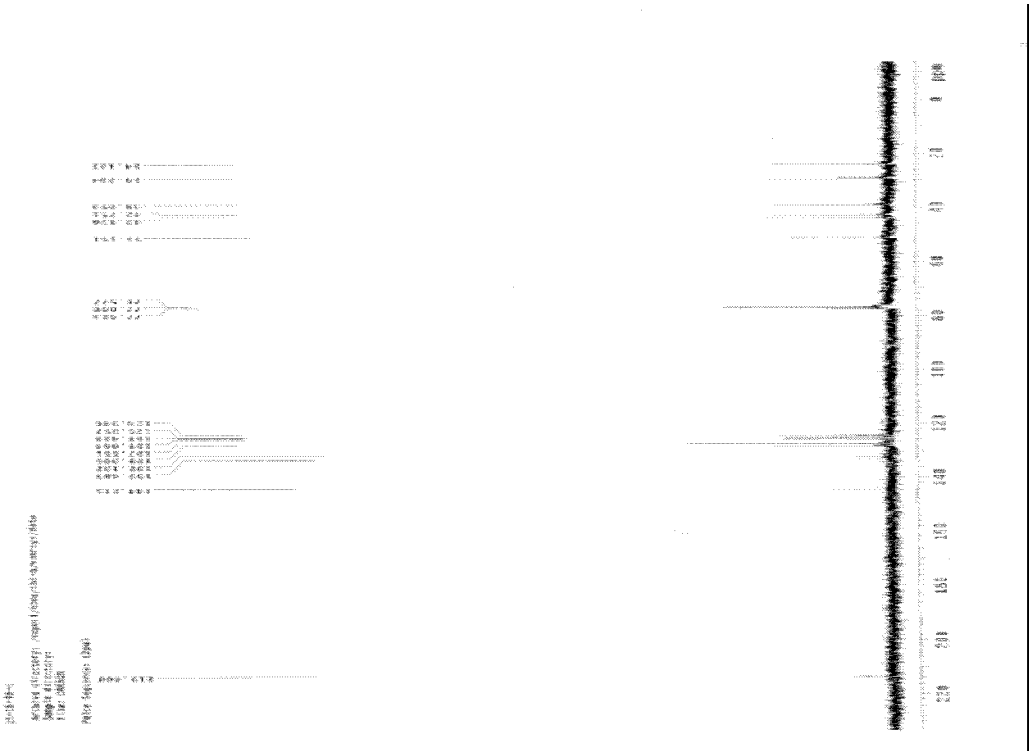
41.2, 44.4, 49.1, 126.4, 129.3, 136.2, 141.4, 211.05; E.e. was determined by chiral HPLC analysis, Chiralpak AD column, Hexane/*i*-PrOH = 100:1, detection at 210 nm, retention times: 31.10 (Maj) / 35.80 (Min) min.

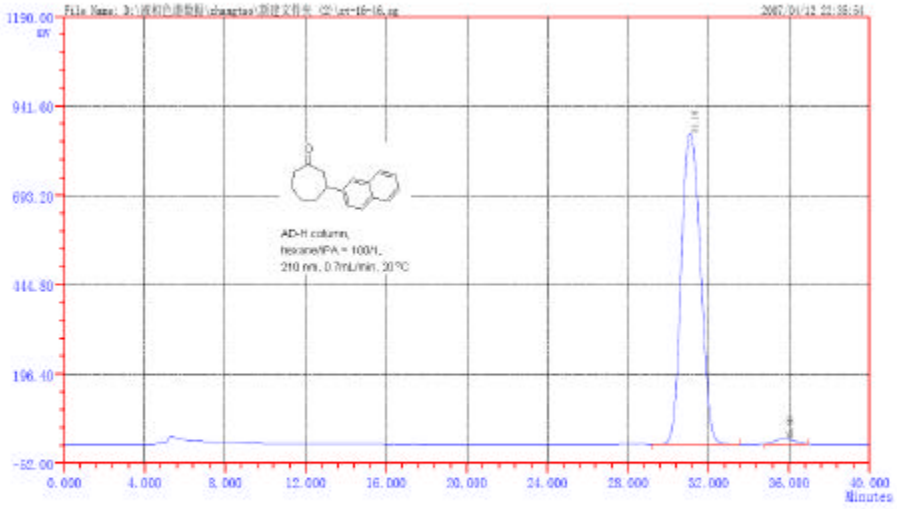






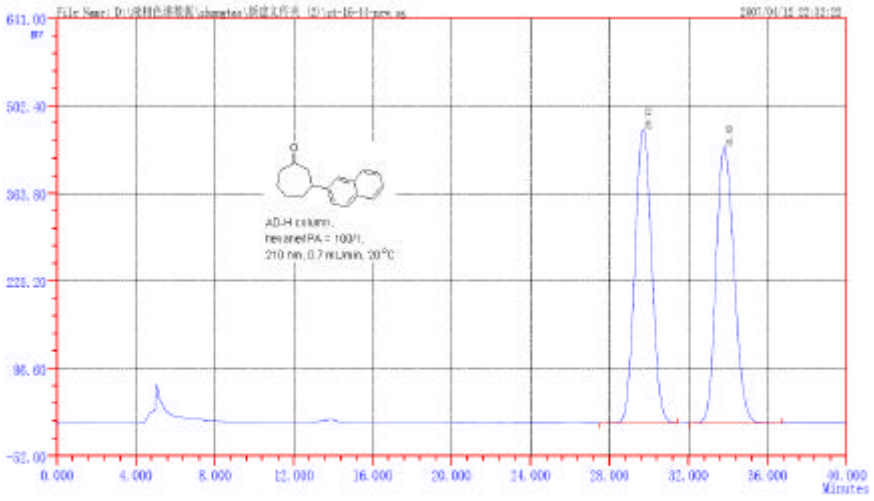




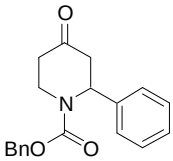


ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		31.100	865009	56546173.5	98.3439	1.11	4511
2		35.800	15231	952223.0	1.6561	1.05	6535
Σ:			880240	57498396.5	100.0000		

Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation

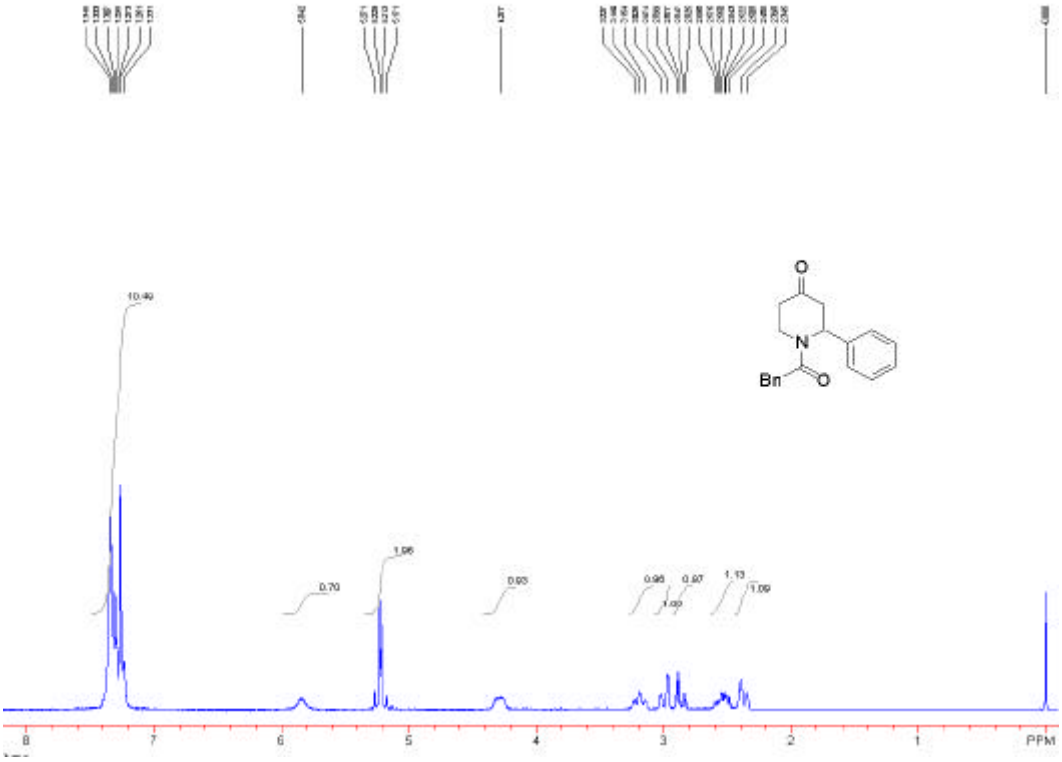


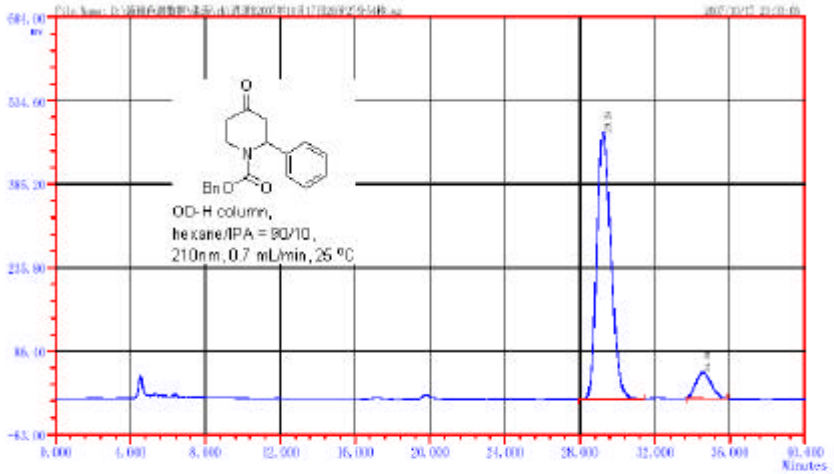
ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		29.717	464922	27646340.6	49.8295	1.04	4977
2		33.833	437616	27835525.1	50.1705	1.15	5639
Σ:			902538	55481865.7	100.0000		



4-Oxo-2-phenylpiperidine-1-carboxylic acid benzyl ester (6ca).[4,5] Ketone **6ca** was obtained after purification by flash chromatography (eluent: PE:EA = 4:1) in 53% yield, 81% ee. $[\alpha]^{25}_{D}$ = -30.5 (c 0.9 in $CHCl_3$) (for 81% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 2.37 (1H, d, *J* = 15.9 Hz), 2.49-2.60 (1H, m), 2.86 (1H, dd, J_1 = 15.6 Hz, J_2 = 6.6 Hz), 3.00 (1H, d, *J* = 15.6 Hz), 3.19 (1H, t, *J* = 11.1 Hz), 4.28 (1H, br), 5.19 (1H, d, *J* =

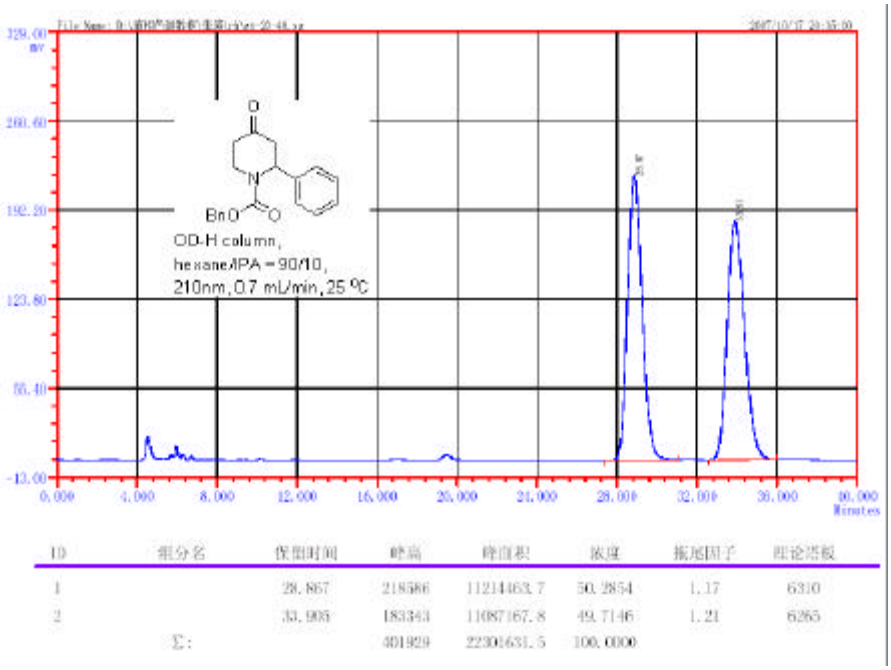
12.6 Hz), 5.25 (1H, d, *J* = 12.6 Hz), 5.84 (1H, br), 7.23-7.35 (10H, m); E.e. was determined by chiral HPLC analysis, Chiralpak OD column, Hexane/*i*-PrOH = 90:10, detection at 210 nm, retention times: 29.24 (Maj) / 34.59 (Min) min.



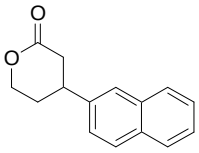


ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		29.237	479144	35402562.7	90.9011	1.24	6018
2		34.585	46791	2706841.8	9.5989	1.10	7086
Σ:			525815	38109404.5	100.0000		

Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation



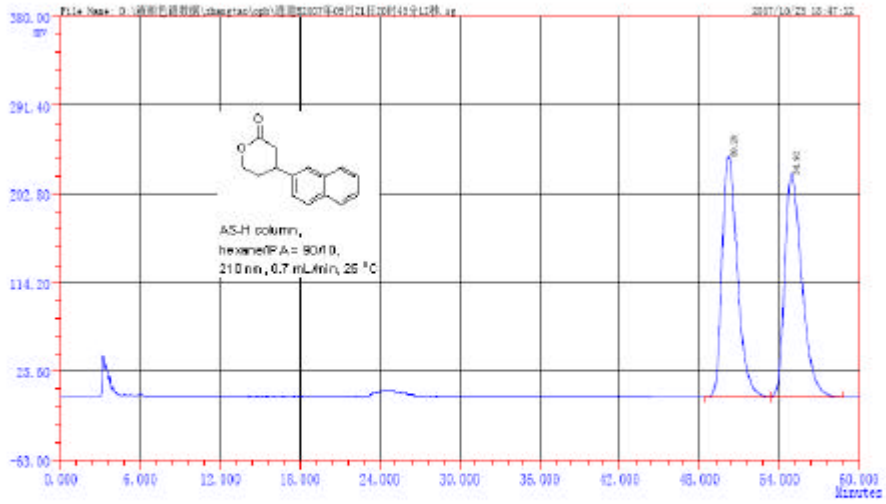
ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		28.867	218586	11214463.7	50.2854	1.17	6310
2		33.905	183343	11087167.8	49.7146	1.21	6265
Σ:			401929	22301631.5	100.0000		



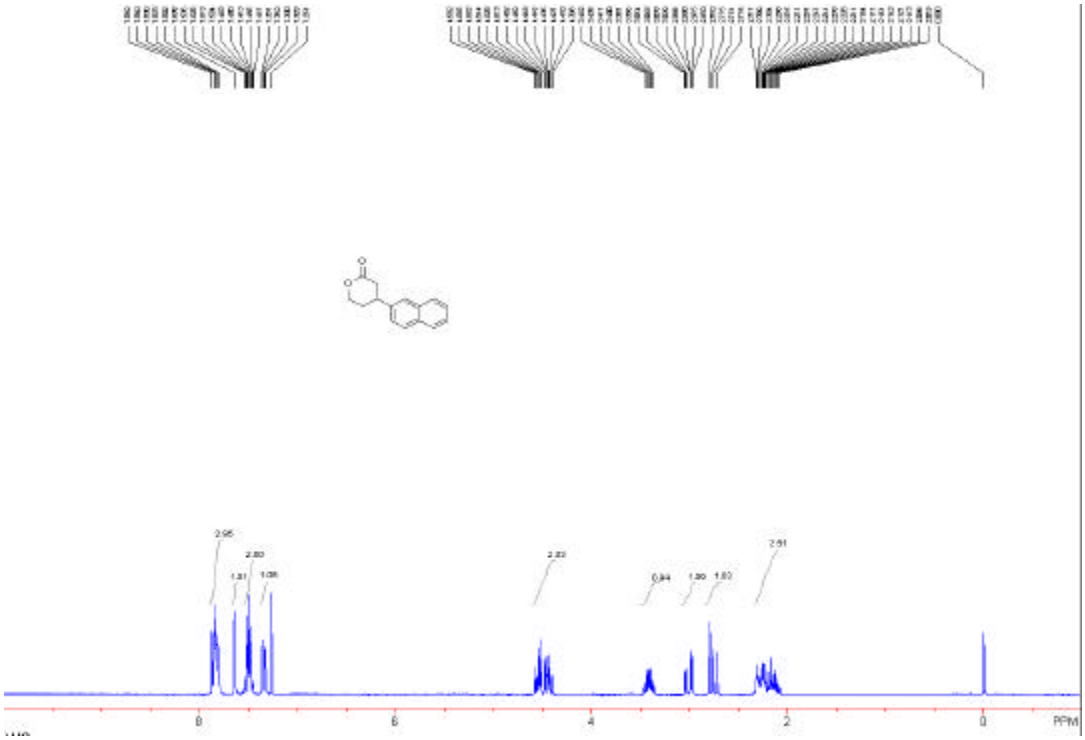
4-Naphthalen-2-yl-tetrahydropyran-2-one (6df).[2] Ketone **6ca** was obtained after purification by flash chromatography (eluent: PE:EA = 4:1) in 62% yield, 38% ee. $[\alpha]^{25}_{D}$ = +12.9 (c 0.4 in $CHCl_3$) (for 38% ee); ^{1}H NMR (300 MHz, $CDCl_3$, TMS) *d* = 2.14-2.32 (2H, m), 2.76 (1H, dd, J_1 = 17.7 Hz, J_2 = 10.5 Hz), 3.03 (1H, dd, J_1 = 11.4 Hz, J_2 = 6.3 Hz),, 3.36-3.47 (1H, m), 4.40-4.57 (2H, m), 7.34 (1H, d, *J* = 8.7 Hz), 7.47-7.53 (2H, m), 7.64 (1H, s), 7.80-7.87 (3H, m); E.e. was determined by chiral HPLC analysis, Chiralpak AS column, Hexane/*i*-PrOH = 90:10, detection at 210 nm, retention times: 49.85 (Min) / 54.42 (Maj) min.

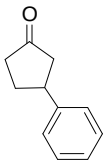
ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		49.847	211274	16687190.5	31.2378	1.34	7938
2		54.420	382927	36732957.4	68.7624	1.58	6414
Σ:			594201	53420147.9	100.0000		

Translation: ID, Content, R time, Peak height, Peak area, Percentage, Tailing factor, Theoretic separation

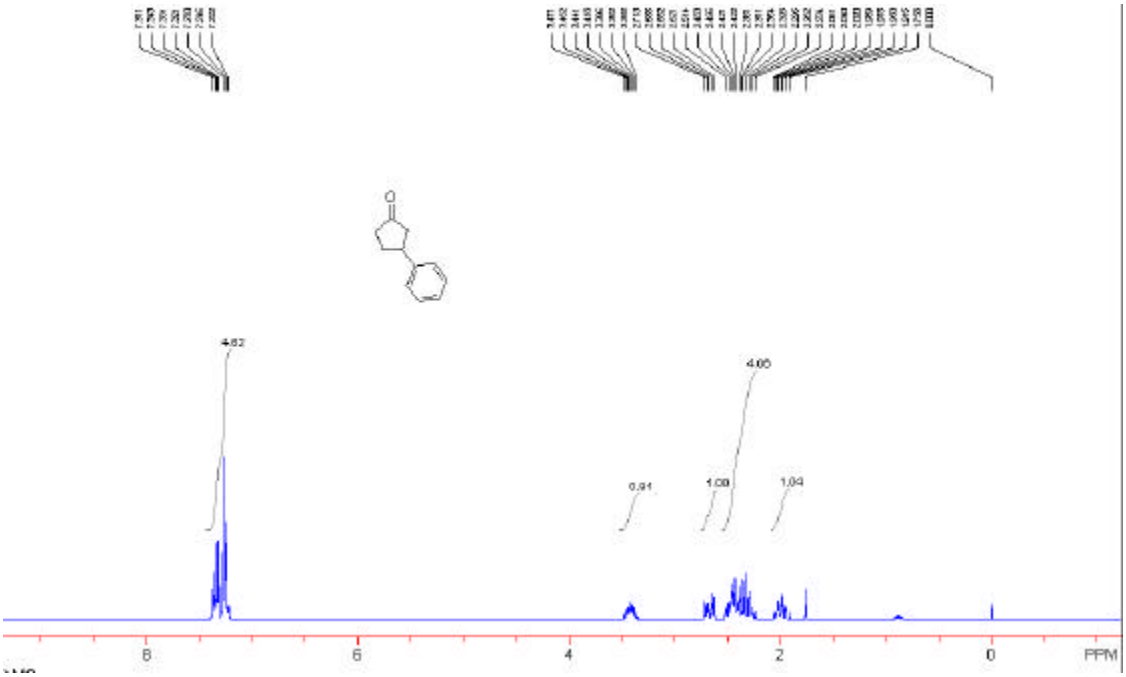


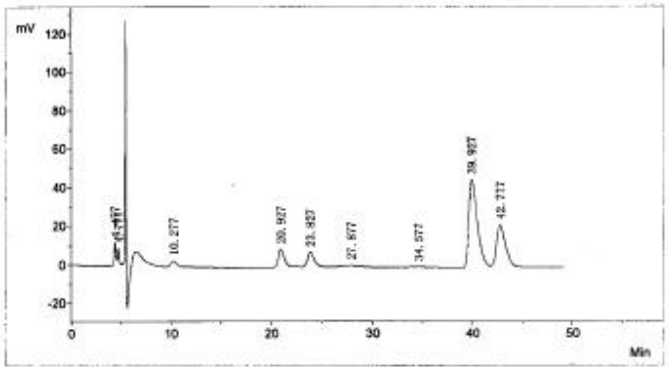
ID	组分名	保留时间	峰高	峰面积	浓度	拖尾因子	理论塔板
1		50.200	239812	19029699.2	48.7792	1.36	7976
2		54.923	222355	19982253.7	51.2208	1.46	7445
Σ:			462167	39011952.9	100.0000		

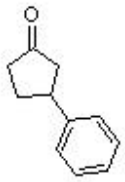




3-Phenylcyclopentanone (**6ea**).[1] Ketone **6ea** was obtained after purification by flash chromatography (eluent: PE:EA = 20:1) in 58% yield, 32% ee. ^{1}H NMR (300 MHz, $CDCl_3$, TMS) d = 1.94-2.02 (1H, m), 2.26-2.48 (4H, m), 2.62-2.71 (1H, dd, J_1 = 7.8 Hz, J_2 = 18 Hz), 3.38-3.44 (1H, m), 7.22-7.37 (5H, m); e.e. was determined by chiral HPLC analysis, Chiralpak OB column, Hexane/*i*-PrOH = 99.5:0.5, detection at 210 nm, retention times: 39.93 (Maj) / 42.78 (Min).



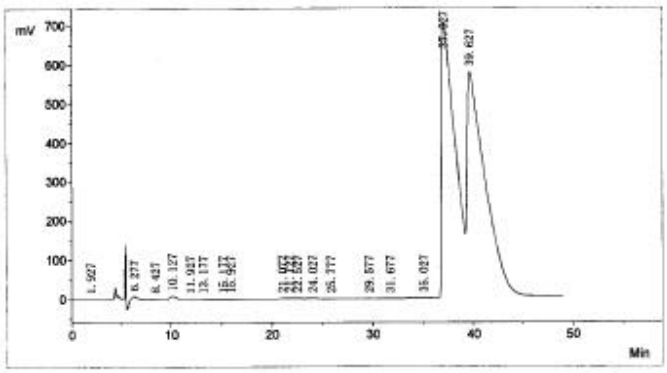


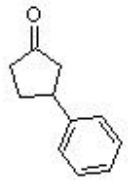


OB column,
hexane/i-PrOH = 99.5:0.5,
0.7 mL/min, 210 nm, 20 °C,

序号	峰号	组份名	保留时间	峰高	峰面积	面积百分比(%)
1	1		4.477	11809.9	127720.9	2.4265
2	2		4.777	8913.4	96351.0	1.8305
3	3		10.277	2733.6	104281.9	1.9812
4	4		20.927	9365.2	381753.3	7.2528
5	5		23.827	7687.5	379223.1	7.2047
6	6		27.877	488.0	20586.3	0.3911
7	7		34.577	403.8	62420.0	1.1859
√8	8		39.927	45399.3	2705669.2	51.4042
√9	9		42.777	21872.6	1385512.0	26.3229
合计:				108673.4	5263517.7	100.0000

Translation: ID, Content, R time, Peak height, Peak area, Percentage.





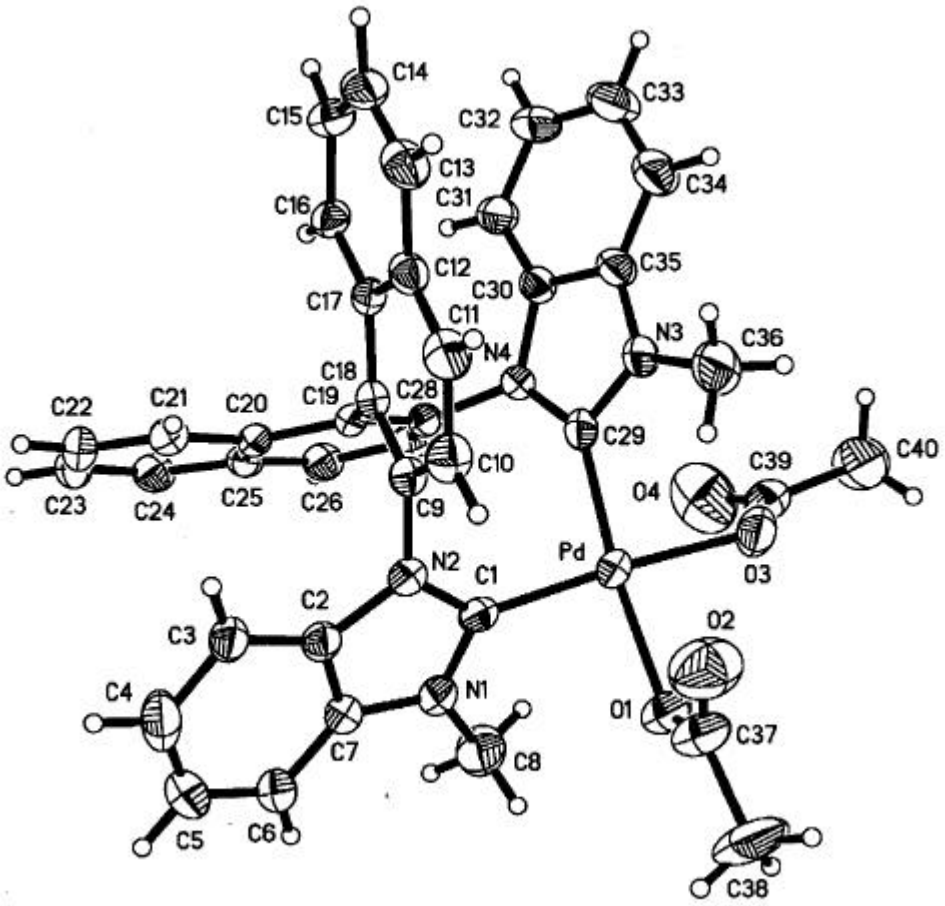
OB column,
hexane/*i*-PrOH = 99.5:0.5,
0.7 mL/min, 210 nm, 20 °C,

序号	峰号	组份名	保留时间	峰高	峰面积	面积百分比(%)
1	1		1.927	458.7	34796.7	0.0247
2	2		6.277	7434.2	1085012.9	0.7712
3	3		8.427	830.2	35610.9	0.0253
4	4		10.127	7193.8	287324.7	0.2042
5	5		11.927	330.8	12794.2	0.0091
6	6		13.177	77.9	1136.2	0.0008
7	7		15.177	115.7	4105.6	0.0029
8	8		15.927	186.4	9935.6	0.0071
9	9		21.077	1157.7	65840.0	0.0468
10	10		21.727	742.0	17897.2	0.0127
11	11		22.527	1156.1	58295.4	0.0414
12	12		24.027	792.5	54068.1	0.0384
13	13		25.777	175.4	5662.4	0.0040
14	14		29.577	234.3	18030.1	0.0128
15	15		31.677	150.2	7167.3	0.0051
16	16		35.027	310.2	28166.2	0.0200
√ 17	17		37.027	704547.2	64399291.7	45.7738
√ 18	18		39.627	577451.3	74565006.2	52.9995
合计:				1303344.6	140690141.4	100.0000

Reference

1. Takaya, Y.; Ogasawara, M.; Hayashi, T.; Sakai, M.; Miyaura, M. *J. Am. Chem. Soc.* **1998**, *120*, 5579.
2. Takaya, Y.; Ogasawara, M.; Hayashi, T. *Tetrahedron Lett.* **1999**, *40*, 6957.
3. Boiteau, J-G.; Imbos, R.; Minnaard, A. J.; Feringa, B. L. *Org. Lett.* **2003**, *5*, 681.
4. Shintani, R.; Tokunaga, N.; Doi, H.; Hayashi, T. *J. Am. Chem. Soc.* **2004**, *126*, 6240.
5. Gini, F.; Hessen, B.; Minnaard A. J. *Org. Lett*. **2005**, *7*, 5309.

3. X-ray Structure of Pd(II)-NHC Complex 2



The crystal data of **2** have been deposited in CCDC with number 605041. Empirical Formula: $C_{40}H_{34}N_4O_5Pd$; Formula Weight: 757.11; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.503 x 0.387 x 0.050 mm; Crystal System: Orthorhombic; Lattice Type: Primitive; Lattice Parameters: a = 9.5879(12)Å, b = 16.684(2)Å, c = 22.540(3)Å, $\alpha = 90^o$, $\beta = 90^o$, $\gamma = 90^o$, V = 3605.4(8)Å^3; Space group: P2(1)2(1)2(1); Z = 4; D_{calc}= 1.395 g/cm^3; F_{000} = 1552; Diffractometer: Rigaku AFC7R; Residuals: R; Rw: 0.0556, 0.1079.

Table 1. Crystal data and structure refinement for cd26139.

Identification code	cd26139
Empirical formula	C40 H34 N4 O5 Pd
Formula weight	757.11
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 9.5879(12) A alpha = 90 deg. b = 16.684(2) A beta = 90 deg. c = 22.540(3) A gamma = 90 deg.
Volume	3605.4(8) A^3
Z, Calculated density	4, 1.395 Mg/m^3
Absorption coefficient	0.564 mm^-1
F(000)	1552
Crystal size	0.503 x 0.387 x 0.050 mm
Theta range for data collection	1.52 to 27.50 deg.
Limiting indices	-11<=h<=12, -21<=k<=18, -29<=l<=28
Reflections collected / unique	21484 / 8117 [R(int) = 0.1449]
Completeness to theta = 27.50	99.3 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.71464
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8117 / 2 / 463
Goodness-of-fit on F^2	0.852
Final R indices [I>2sigma(I)]	R1 = 0.0556, wR2 = 0.1079
R indices (all data)	R1 = 0.0990, wR2 = 0.1229
Absolute structure parameter	0.06(3)
Largest diff. peak and hole	0.916 and -0.532 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cd26139.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd	8398(1)	8833(1)	1297(1)	56(1)
O(1)	7411(6)	7752(3)	1432(2)	76(1)
O(2)	5788(7)	8491(4)	1848(3)	134(2)
O(3)	9232(6)	8689(3)	2128(2)	87(2)
O(4)	11263(7)	8615(5)	1746(3)	148(3)
O(5)	3607(9)	9048(6)	1150(4)	182(4)
N(1)	7579(5)	8267(3)	111(2)	56(1)
N(2)	6895(5)	9496(3)	235(2)	49(1)
N(3)	9231(6)	10398(3)	1746(2)	59(1)
N(4)	10263(5)	10216(3)	898(2)	44(1)
C(1)	7627(6)	8877(4)	494(2)	52(1)
C(2)	6354(6)	9243(4)	-313(2)	50(1)
C(3)	5530(6)	9619(4)	-723(3)	59(2)
C(4)	5190(7)	9157(5)	-1220(3)	84(2)
C(5)	5619(8)	8381(5)	-1287(3)	84(2)
C(6)	6497(9)	8018(4)	-888(3)	79(2)
C(7)	6843(7)	8465(4)	-391(2)	56(2)
C(8)	8354(10)	7494(4)	176(3)	98(2)
C(9)	6909(6)	10314(3)	418(2)	46(1)
C(10)	5831(6)	10611(4)	788(3)	61(2)
C(11)	5849(7)	11406(4)	949(3)	62(2)
C(12)	6921(6)	11912(3)	775(2)	49(2)
C(13)	6920(7)	12739(4)	938(3)	66(2)
C(14)	7951(7)	13240(4)	746(3)	62(2)
C(15)	9037(7)	12942(4)	403(3)	66(2)
C(16)	9062(6)	12153(3)	214(2)	48(1)
C(17)	7996(6)	11628(3)	403(2)	44(1)
C(18)	8011(6)	10789(3)	237(2)	42(1)
C(19)	9241(6)	10422(3)	-66(2)	39(1)
C(20)	9376(6)	10409(3)	-702(2)	42(1)
C(21)	8387(8)	10800(3)	-1077(2)	57(1)
C(22)	8624(8)	10820(4)	-1674(2)	67(2)
C(23)	9743(8)	10459(4)	-1931(3)	69(2)
C(24)	10704(8)	10065(4)	-1585(3)	61(2)
C(25)	10527(6)	10024(3)	-959(2)	47(1)
C(26)	11530(8)	9658(3)	-593(2)	56(1)
C(27)	11433(7)	9685(3)	14(2)	53(1)
C(28)	10265(6)	10077(3)	264(2)	43(1)
C(29)	9283(6)	9887(3)	1273(2)	56(1)
C(30)	10864(6)	10902(3)	1142(2)	46(1)
C(31)	11873(6)	11413(3)	940(2)	58(2)
C(32)	12233(6)	12040(4)	1310(3)	70(2)
C(33)	11604(9)	12150(4)	1852(3)	82(2)
C(34)	10552(8)	11651(5)	2049(3)	83(2)
C(35)	10195(6)	11007(4)	1688(2)	57(2)
C(36)	8197(9)	10367(5)	2221(3)	96(3)
C(37)	6266(11)	7827(5)	1686(4)	93(3)
C(38)	5445(12)	7072(6)	1848(4)	156(5)
C(39)	10469(12)	8652(5)	2175(4)	89(3)
C(40)	11165(11)	8643(6)	2767(4)	160(5)

Table 3. Bond lengths [A] and angles [deg] for cd26139.

Pd-C(29)	1.953(5)
Pd-C(1)	1.955(5)
Pd-O(3)	2.053(4)
Pd-O(1)	2.060(4)
O(1)-C(37)	1.243(10)
O(2)-C(37)	1.254(10)
O(3)-C(39)	1.192(10)
O(4)-C(39)	1.232(10)
O(5)-H(5A)	0.92(2)
O(5)-H(5B)	0.891(19)
N(1)-C(1)	1.336(7)
N(1)-C(7)	1.373(7)
N(1)-C(8)	1.496(8)
N(2)-C(1)	1.379(7)
N(2)-C(2)	1.405(7)
N(2)-C(9)	1.426(7)
N(3)-C(29)	1.368(7)
N(3)-C(35)	1.379(7)
N(3)-C(36)	1.461(8)
N(4)-C(29)	1.377(6)
N(4)-C(30)	1.394(7)
N(4)-C(28)	1.448(6)
C(2)-C(3)	1.368(8)
C(2)-C(7)	1.391(8)
C(3)-C(4)	1.399(9)
C(3)-H(3)	0.9300
C(4)-C(5)	1.365(10)
C(4)-H(4)	0.9300
C(5)-C(6)	1.374(10)
C(5)-H(5)	0.9300
C(6)-C(7)	1.386(8)
C(6)-H(6)	0.9300
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(9)-C(18)	1.383(7)
C(9)-C(10)	1.418(8)
C(10)-C(11)	1.375(9)
C(10)-H(10)	0.9300
C(11)-C(12)	1.386(8)
C(11)-H(11)	0.9300
C(12)-C(17)	1.411(7)
C(12)-C(13)	1.428(8)
C(13)-C(14)	1.366(9)
C(13)-H(13)	0.9300
C(14)-C(15)	1.388(8)
C(14)-H(14)	0.9300
C(15)-C(16)	1.384(8)
C(15)-H(15)	0.9300
C(16)-C(17)	1.412(7)
C(16)-H(16)	0.9300
C(17)-C(18)	1.448(7)
C(18)-C(19)	1.494(7)
C(19)-C(28)	1.360(7)
C(19)-C(20)	1.438(6)
C(20)-C(25)	1.402(8)
C(20)-C(21)	1.427(8)
C(21)-C(22)	1.366(8)
C(21)-H(21)	0.9300
C(22)-C(23)	1.360(9)
C(22)-H(22)	0.9300
C(23)-C(24)	1.375(9)
C(23)-H(23)	0.9300
C(24)-C(25)	1.422(7)
C(24)-H(24)	0.9300
C(25)-C(26)	1.407(8)
C(26)-C(27)	1.372(7)
C(26)-H(26)	0.9300

C(27)-C(28)	1.414(8)
C(27)-H(27)	0.9300
C(30)-C(31)	1.368(8)
C(30)-C(35)	1.399(7)
C(31)-C(32)	1.381(8)
C(31)-H(31)	0.9300
C(32)-C(33)	1.376(9)
C(32)-H(32)	0.9300
C(33)-C(34)	1.380(9)
C(33)-H(33)	0.9300
C(34)-C(35)	1.391(8)
C(34)-H(34)	0.9300
C(36)-H(36A)	0.9600
C(36)-H(36B)	0.9600
C(36)-H(36C)	0.9600
C(37)-C(38)	1.530(11)
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
C(39)-C(40)	1.493(10)
C(40)-H(40A)	0.9600
C(40)-H(40B)	0.9600
C(40)-H(40C)	0.9600

C(29)-Pd-C(1)	96.0(2)
C(29)-Pd-O(3)	87.8(2)
C(1)-Pd-O(3)	175.3(3)
C(29)-Pd-O(1)	172.8(2)
C(1)-Pd-O(1)	89.8(2)
O(3)-Pd-O(1)	86.61(19)
C(37)-O(1)-Pd	112.7(5)
C(39)-O(3)-Pd	118.3(5)
H(5A)-O(5)-H(5B)	132(7)
C(1)-N(1)-C(7)	111.6(5)
C(1)-N(1)-C(8)	125.1(5)
C(7)-N(1)-C(8)	122.9(5)
C(1)-N(2)-C(2)	109.6(5)
C(1)-N(2)-C(9)	126.1(5)
C(2)-N(2)-C(9)	123.1(4)
C(29)-N(3)-C(35)	111.2(4)
C(29)-N(3)-C(36)	125.0(5)
C(35)-N(3)-C(36)	123.4(5)
C(29)-N(4)-C(30)	111.6(4)
C(29)-N(4)-C(28)	122.8(4)
C(30)-N(4)-C(28)	121.3(4)
N(1)-C(1)-N(2)	106.2(4)
N(1)-C(1)-Pd	125.7(4)
N(2)-C(1)-Pd	127.8(5)
C(3)-C(2)-C(7)	122.6(6)
C(3)-C(2)-N(2)	131.9(6)
C(7)-C(2)-N(2)	105.5(5)
C(2)-C(3)-C(4)	115.0(7)
C(2)-C(3)-H(3)	122.5
C(4)-C(3)-H(3)	122.5
C(5)-C(4)-C(3)	122.7(7)
C(5)-C(4)-H(4)	118.6
C(3)-C(4)-H(4)	118.6
C(4)-C(5)-C(6)	122.1(7)
C(4)-C(5)-H(5)	119.0
C(6)-C(5)-H(5)	119.0
C(5)-C(6)-C(7)	116.0(7)
C(5)-C(6)-H(6)	122.0
C(7)-C(6)-H(6)	122.0
N(1)-C(7)-C(6)	131.2(6)
N(1)-C(7)-C(2)	107.1(5)
C(6)-C(7)-C(2)	121.6(6)
N(1)-C(8)-H(8A)	109.5
N(1)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
N(1)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5

C(18)-C(9)-C(10)	122.1(5)
C(18)-C(9)-N(2)	118.1(5)
C(10)-C(9)-N(2)	119.8(5)
C(11)-C(10)-C(9)	118.8(6)
C(11)-C(10)-H(10)	120.6
C(9)-C(10)-H(10)	120.6
C(10)-C(11)-C(12)	121.5(6)
C(10)-C(11)-H(11)	119.3
C(12)-C(11)-H(11)	119.3
C(11)-C(12)-C(17)	120.4(5)
C(11)-C(12)-C(13)	121.0(6)
C(17)-C(12)-C(13)	118.6(6)
C(14)-C(13)-C(12)	120.6(6)
C(14)-C(13)-H(13)	119.7
C(12)-C(13)-H(13)	119.7
C(13)-C(14)-C(15)	120.0(6)
C(13)-C(14)-H(14)	120.0
C(15)-C(14)-H(14)	120.0
C(16)-C(15)-C(14)	121.7(6)
C(16)-C(15)-H(15)	119.1
C(14)-C(15)-H(15)	119.1
C(15)-C(16)-C(17)	119.0(5)
C(15)-C(16)-H(16)	120.5
C(17)-C(16)-H(16)	120.5
C(12)-C(17)-C(16)	119.9(5)
C(12)-C(17)-C(18)	119.0(5)
C(16)-C(17)-C(18)	121.0(5)
C(9)-C(18)-C(17)	118.0(5)
C(9)-C(18)-C(19)	120.2(5)
C(17)-C(18)-C(19)	121.5(5)
C(28)-C(19)-C(20)	118.3(5)
C(28)-C(19)-C(18)	119.5(4)
C(20)-C(19)-C(18)	122.1(5)
C(25)-C(20)-C(21)	119.1(5)
C(25)-C(20)-C(19)	119.3(5)
C(21)-C(20)-C(19)	121.5(5)
C(22)-C(21)-C(20)	119.0(7)
C(22)-C(21)-H(21)	120.5
C(20)-C(21)-H(21)	120.5
C(23)-C(22)-C(21)	122.7(7)
C(23)-C(22)-H(22)	118.7
C(21)-C(22)-H(22)	118.7
C(22)-C(23)-C(24)	119.9(6)
C(22)-C(23)-H(23)	120.1
C(24)-C(23)-H(23)	120.1
C(23)-C(24)-C(25)	120.4(7)
C(23)-C(24)-H(24)	119.8
C(25)-C(24)-H(24)	119.8
C(20)-C(25)-C(26)	119.6(5)
C(20)-C(25)-C(24)	118.8(6)
C(26)-C(25)-C(24)	121.4(6)
C(27)-C(26)-C(25)	121.6(6)
C(27)-C(26)-H(26)	119.2
C(25)-C(26)-H(26)	119.2
C(26)-C(27)-C(28)	117.8(6)
C(26)-C(27)-H(27)	121.1
C(28)-C(27)-H(27)	121.1
C(19)-C(28)-C(27)	123.3(4)
C(19)-C(28)-N(4)	118.2(5)
C(27)-C(28)-N(4)	117.9(5)
N(3)-C(29)-N(4)	104.7(5)
N(3)-C(29)-Pd	121.6(4)
N(4)-C(29)-Pd	132.2(4)
C(31)-C(30)-N(4)	132.3(5)
C(31)-C(30)-C(35)	122.6(5)
N(4)-C(30)-C(35)	105.1(5)
C(30)-C(31)-C(32)	116.6(5)
C(30)-C(31)-H(31)	121.7
C(32)-C(31)-H(31)	121.7
C(33)-C(32)-C(31)	121.9(6)
C(33)-C(32)-H(32)	119.1
C(31)-C(32)-H(32)	119.1

C(32)-C(33)-C(34)	121.7(6)
C(32)-C(33)-H(33)	119.1
C(34)-C(33)-H(33)	119.1
C(33)-C(34)-C(35)	117.2(6)
C(33)-C(34)-H(34)	121.4
C(35)-C(34)-H(34)	121.4
N(3)-C(35)-C(34)	132.7(5)
N(3)-C(35)-C(30)	107.3(5)
C(34)-C(35)-C(30)	119.9(6)
N(3)-C(36)-H(36A)	109.5
N(3)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
N(3)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
O(1)-C(37)-O(2)	123.1(8)
O(1)-C(37)-C(38)	118.8(9)
O(2)-C(37)-C(38)	118.0(10)
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
O(3)-C(39)-O(4)	123.2(8)
O(3)-C(39)-C(40)	121.6(10)
O(4)-C(39)-C(40)	115.2(10)
C(39)-C(40)-H(40A)	109.5
C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(39)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for cd26139.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd	73(1)	49(1)	46(1)	12(1)	-8(1)	-13(1)
O(1)	91(4)	55(3)	81(3)	8(2)	6(3)	-14(3)
O(2)	152(6)	100(5)	148(5)	-15(5)	39(5)	-8(4)
O(3)	95(4)	101(5)	65(3)	30(3)	-21(3)	-34(4)
O(4)	119(6)	172(8)	154(6)	-12(6)	-50(5)	41(5)
O(5)	134(8)	208(10)	204(9)	102(7)	-12(8)	-32(7)
N(1)	73(3)	43(3)	52(3)	5(2)	-4(3)	-1(2)
N(2)	55(3)	42(3)	49(2)	6(2)	-3(2)	-5(2)
N(3)	78(4)	63(3)	36(2)	-2(2)	10(3)	-16(3)
N(4)	55(3)	39(3)	38(2)	-1(2)	-5(2)	-3(2)
C(1)	57(3)	43(3)	55(3)	10(3)	-8(3)	-13(3)
C(2)	44(4)	56(4)	50(3)	8(3)	-1(3)	-11(3)
C(3)	61(4)	61(4)	54(4)	13(3)	-10(3)	-6(3)
C(4)	69(5)	126(7)	56(4)	26(5)	-11(4)	-14(4)
C(5)	110(6)	88(6)	55(4)	-7(5)	-15(5)	-20(4)
C(6)	119(6)	69(4)	48(3)	4(3)	-8(5)	-24(5)
C(7)	70(5)	49(3)	48(3)	6(3)	-8(3)	-10(3)
C(8)	156(7)	51(4)	86(5)	-1(4)	-13(6)	18(5)
C(9)	48(4)	47(3)	44(3)	3(2)	-6(3)	-1(3)
C(10)	51(4)	72(5)	59(4)	4(3)	5(3)	-1(3)
C(11)	66(4)	59(4)	61(4)	-5(3)	-4(3)	24(3)
C(12)	56(4)	47(3)	44(3)	-4(3)	-7(3)	10(3)
C(13)	77(5)	60(4)	61(4)	-14(3)	-10(3)	23(4)
C(14)	78(5)	44(4)	64(4)	-8(3)	-11(4)	13(3)
C(15)	89(5)	41(4)	69(4)	0(3)	3(4)	-7(3)
C(16)	62(4)	38(3)	45(3)	0(2)	7(3)	4(3)
C(17)	56(4)	39(3)	36(3)	2(2)	-3(2)	3(3)
C(18)	47(4)	45(3)	35(3)	2(2)	-5(2)	-1(2)
C(19)	48(3)	35(3)	33(3)	3(2)	0(2)	-4(2)
C(20)	55(4)	35(3)	37(3)	2(2)	1(3)	-4(3)
C(21)	75(4)	43(3)	54(3)	3(2)	-10(4)	-1(3)
C(22)	93(6)	61(4)	47(3)	10(3)	-13(4)	-3(4)
C(23)	103(6)	66(5)	37(3)	1(3)	6(4)	-17(4)
C(24)	82(5)	52(4)	50(3)	-13(3)	14(4)	-1(3)
C(25)	56(4)	44(3)	42(3)	-5(2)	4(3)	-11(3)
C(26)	66(4)	50(3)	52(3)	-9(3)	13(4)	3(3)
C(27)	67(4)	39(3)	53(3)	-1(2)	-2(3)	3(3)
C(28)	58(4)	37(3)	34(3)	-2(2)	6(3)	-2(3)
C(29)	69(4)	64(4)	35(3)	6(3)	0(3)	-14(3)
C(30)	45(3)	50(3)	44(3)	-2(2)	-1(3)	-3(3)
C(31)	62(4)	54(4)	57(3)	-5(3)	4(3)	-6(3)
C(32)	66(4)	56(4)	89(4)	-10(4)	-8(4)	-16(3)
C(33)	95(5)	71(5)	80(4)	-28(4)	4(5)	-16(5)
C(34)	108(6)	84(6)	57(4)	-17(4)	15(4)	-24(5)
C(35)	68(4)	59(4)	44(3)	-10(3)	6(3)	-13(3)
C(36)	113(7)	116(7)	59(4)	-8(4)	28(5)	-42(6)
C(37)	112(8)	60(5)	106(6)	7(5)	5(6)	-25(5)
C(38)	187(11)	104(8)	178(9)	19(7)	35(9)	-87(8)
C(39)	121(8)	63(5)	83(5)	18(4)	-27(6)	-24(6)
C(40)	204(12)	140(10)	135(7)	43(7)	-115(8)	-72(9)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for cd26139.

	x	y	z	U(eq)
H(3)	5219	10143	-675	70
H(4)	4649	9387	-1517	100
H(5)	5306	8091	-1613	101
H(6)	6839	7502	-947	95
H(8A)	9162	7576	420	146
H(8B)	8640	7307	-208	146
H(8C)	7758	7102	358	146
H(10)	5123	10274	920	73
H(11)	5127	11609	1180	74
H(13)	6211	12938	1178	79
H(14)	7926	13781	844	74
H(15)	9766	13281	299	80
H(16)	9771	11972	-34	58
H(21)	7594	11036	-917	69
H(22)	7994	11092	-1915	80
H(23)	9858	10478	-2341	82
H(24)	11475	9825	-1761	73
H(26)	12278	9392	-767	67
H(27)	12113	9453	253	64
H(31)	12296	11342	573	69
H(32)	12919	12398	1189	84
H(33)	11894	12571	2093	99
H(34)	10101	11742	2408	99
H(36A)	7460	10007	2112	144
H(36B)	7820	10893	2286	144
H(36C)	8631	10180	2579	144
H(38A)	4762	6966	1547	234
H(38B)	4985	7151	2222	234
H(38C)	6072	6625	1878	234
H(40A)	10567	8387	3051	240
H(40B)	11348	9184	2892	240
H(40C)	12028	8354	2740	240
H(5A)	2760(40)	8800(40)	1190(30)	90(20)
H(5B)	4300(40)	8980(30)	893(17)	29(15)

Table 6. Torsion angles [deg] for cd26139.

C(29)-Pd-O(1)-C(37)	48(2)
C(1)-Pd-O(1)-C(37)	-95.5(6)
O(3)-Pd-O(1)-C(37)	87.4(5)
C(29)-Pd-O(3)-C(39)	-65.4(7)
C(1)-Pd-O(3)-C(39)	80(3)
O(1)-Pd-O(3)-C(39)	119.1(7)
C(7)-N(1)-C(1)-N(2)	0.1(7)
C(8)-N(1)-C(1)-N(2)	173.4(6)
C(7)-N(1)-C(1)-Pd	173.6(4)
C(8)-N(1)-C(1)-Pd	-13.1(9)
C(2)-N(2)-C(1)-N(1)	1.8(6)
C(9)-N(2)-C(1)-N(1)	-165.9(5)
C(2)-N(2)-C(1)-Pd	-171.4(4)
C(9)-N(2)-C(1)-Pd	20.9(8)
C(29)-Pd-C(1)-N(1)	140.3(5)
O(3)-Pd-C(1)-N(1)	-5(3)
O(1)-Pd-C(1)-N(1)	-44.0(5)
C(29)-Pd-C(1)-N(2)	-47.7(5)
O(3)-Pd-C(1)-N(2)	167(3)
O(1)-Pd-C(1)-N(2)	128.1(5)
C(1)-N(2)-C(2)-C(3)	177.5(6)
C(9)-N(2)-C(2)-C(3)	-14.3(9)
C(1)-N(2)-C(2)-C(7)	-3.0(6)
C(9)-N(2)-C(2)-C(7)	165.1(5)
C(7)-C(2)-C(3)-C(4)	1.4(9)
N(2)-C(2)-C(3)-C(4)	-179.2(6)
C(2)-C(3)-C(4)-C(5)	1.5(10)
C(3)-C(4)-C(5)-C(6)	-4.6(12)
C(4)-C(5)-C(6)-C(7)	4.4(11)
C(1)-N(1)-C(7)-C(6)	-177.7(7)
C(8)-N(1)-C(7)-C(6)	8.8(11)
C(1)-N(1)-C(7)-C(2)	-2.0(7)
C(8)-N(1)-C(7)-C(2)	-175.5(6)
C(5)-C(6)-C(7)-N(1)	173.5(7)
C(5)-C(6)-C(7)-C(2)	-1.6(10)
C(3)-C(2)-C(7)-N(1)	-177.5(5)
N(2)-C(2)-C(7)-N(1)	3.0(6)
C(3)-C(2)-C(7)-C(6)	-1.3(10)
N(2)-C(2)-C(7)-C(6)	179.2(6)
C(1)-N(2)-C(9)-C(18)	80.9(7)
C(2)-N(2)-C(9)-C(18)	-85.2(6)
C(1)-N(2)-C(9)-C(10)	-97.3(7)
C(2)-N(2)-C(9)-C(10)	96.5(6)
C(18)-C(9)-C(10)-C(11)	3.1(8)
N(2)-C(9)-C(10)-C(11)	-178.7(5)
C(9)-C(10)-C(11)-C(12)	-2.3(9)
C(10)-C(11)-C(12)-C(17)	2.8(9)
C(10)-C(11)-C(12)-C(13)	179.2(5)
C(11)-C(12)-C(13)-C(14)	-177.5(6)
C(17)-C(12)-C(13)-C(14)	-1.1(8)
C(12)-C(13)-C(14)-C(15)	-2.0(9)
C(13)-C(14)-C(15)-C(16)	4.5(9)
C(14)-C(15)-C(16)-C(17)	-3.7(9)
C(11)-C(12)-C(17)-C(16)	178.2(5)
C(13)-C(12)-C(17)-C(16)	1.8(7)
C(11)-C(12)-C(17)-C(18)	-3.9(8)
C(13)-C(12)-C(17)-C(18)	179.7(5)
C(15)-C(16)-C(17)-C(12)	0.5(8)
C(15)-C(16)-C(17)-C(18)	-177.4(5)
C(10)-C(9)-C(18)-C(17)	-4.2(7)
N(2)-C(9)-C(18)-C(17)	177.6(4)
C(10)-C(9)-C(18)-C(19)	169.7(5)
N(2)-C(9)-C(18)-C(19)	-8.6(7)
C(12)-C(17)-C(18)-C(9)	4.5(7)
C(16)-C(17)-C(18)-C(9)	-177.6(5)
C(12)-C(17)-C(18)-C(19)	-169.3(4)
C(16)-C(17)-C(18)-C(19)	8.6(7)
C(9)-C(18)-C(19)-C(28)	-82.4(6)

C(17)-C(18)-C(19)-C(28)	91.2(6)
C(9)-C(18)-C(19)-C(20)	96.8(6)
C(17)-C(18)-C(19)-C(20)	-89.6(6)
C(28)-C(19)-C(20)-C(25)	1.9(8)
C(18)-C(19)-C(20)-C(25)	-177.3(5)
C(28)-C(19)-C(20)-C(21)	-176.2(5)
C(18)-C(19)-C(20)-C(21)	4.6(8)
C(25)-C(20)-C(21)-C(22)	-3.1(8)
C(19)-C(20)-C(21)-C(22)	175.1(5)
C(20)-C(21)-C(22)-C(23)	2.3(10)
C(21)-C(22)-C(23)-C(24)	-1.2(11)
C(22)-C(23)-C(24)-C(25)	0.8(10)
C(21)-C(20)-C(25)-C(26)	178.1(5)
C(19)-C(20)-C(25)-C(26)	-0.1(8)
C(21)-C(20)-C(25)-C(24)	2.7(8)
C(19)-C(20)-C(25)-C(24)	-175.5(5)
C(23)-C(24)-C(25)-C(20)	-1.6(10)
C(23)-C(24)-C(25)-C(26)	-176.9(5)
C(20)-C(25)-C(26)-C(27)	-1.7(9)
C(24)-C(25)-C(26)-C(27)	173.5(6)
C(25)-C(26)-C(27)-C(28)	1.6(9)
C(20)-C(19)-C(28)-C(27)	-2.1(8)
C(18)-C(19)-C(28)-C(27)	177.1(5)
C(20)-C(19)-C(28)-N(4)	168.9(4)
C(18)-C(19)-C(28)-N(4)	-11.9(7)
C(26)-C(27)-C(28)-C(19)	0.4(8)
C(26)-C(27)-C(28)-N(4)	-170.7(5)
C(29)-N(4)-C(28)-C(19)	70.7(7)
C(30)-N(4)-C(28)-C(19)	-84.0(7)
C(29)-N(4)-C(28)-C(27)	-117.8(6)
C(30)-N(4)-C(28)-C(27)	87.5(6)
C(35)-N(3)-C(29)-N(4)	-3.0(7)
C(36)-N(3)-C(29)-N(4)	170.6(6)
C(35)-N(3)-C(29)-Pd	165.0(4)
C(36)-N(3)-C(29)-Pd	-21.4(9)
C(30)-N(4)-C(29)-N(3)	2.6(6)
C(28)-N(4)-C(29)-N(3)	-154.3(5)
C(30)-N(4)-C(29)-Pd	-163.6(4)
C(28)-N(4)-C(29)-Pd	39.5(8)
C(1)-Pd-C(29)-N(3)	138.1(5)
O(3)-Pd-C(29)-N(3)	-44.6(5)
O(1)-Pd-C(29)-N(3)	-5(2)
C(1)-Pd-C(29)-N(4)	-57.6(6)
O(3)-Pd-C(29)-N(4)	119.7(5)
O(1)-Pd-C(29)-N(4)	158.9(16)
C(29)-N(4)-C(30)-C(31)	179.1(6)
C(28)-N(4)-C(30)-C(31)	-23.6(9)
C(29)-N(4)-C(30)-C(35)	-1.2(6)
C(28)-N(4)-C(30)-C(35)	156.1(5)
N(4)-C(30)-C(31)-C(32)	-179.2(6)
C(35)-C(30)-C(31)-C(32)	1.2(9)
C(30)-C(31)-C(32)-C(33)	-0.4(10)
C(31)-C(32)-C(33)-C(34)	-1.8(11)
C(32)-C(33)-C(34)-C(35)	3.0(12)
C(29)-N(3)-C(35)-C(34)	-178.8(8)
C(36)-N(3)-C(35)-C(34)	7.5(12)
C(29)-N(3)-C(35)-C(30)	2.3(7)
C(36)-N(3)-C(35)-C(30)	-171.3(6)
C(33)-C(34)-C(35)-N(3)	179.2(7)
C(33)-C(34)-C(35)-C(30)	-2.1(11)
C(31)-C(30)-C(35)-N(3)	179.0(6)
N(4)-C(30)-C(35)-N(3)	-0.7(6)
C(31)-C(30)-C(35)-C(34)	0.0(10)
N(4)-C(30)-C(35)-C(34)	-179.7(6)
Pd-O(1)-C(37)-O(2)	-1.1(11)
Pd-O(1)-C(37)-C(38)	-176.6(6)
Pd-O(3)-C(39)-O(4)	-7.7(13)
Pd-O(3)-C(39)-C(40)	172.8(6)

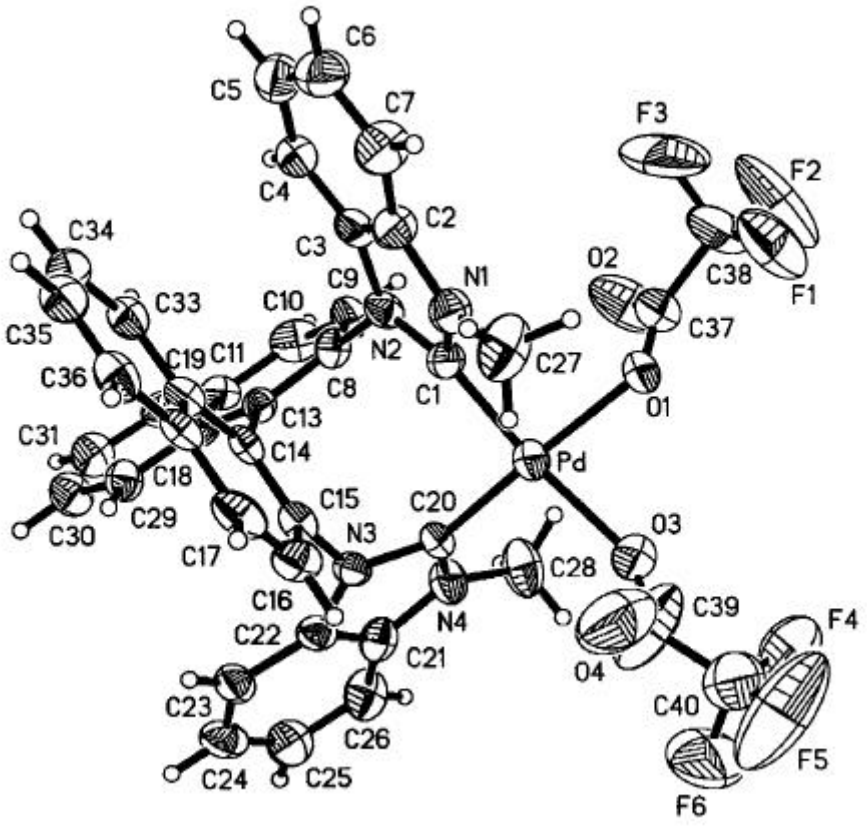
Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd26139 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5A)...O(4)#1	0.92(2)	1.93(5)	2.717(12)	143(7)

Symmetry transformations used to generate equivalent atoms:
#1 x-1,y,z

X-ray Structure of Pd(II)-NHC Complex 3



The crystal data of **3** have been deposited in CCDC with number 633231. Empirical Formula: $C_{40}H_{28}F_6N_4O_5Pd$; Formula Weight: 865.06; Crystal Color, Habit: colorless, prismatic; Crystal Dimensions: 0.234 x 0.168 x 0.109 mm; Crystal System: Orthorhombic; Lattice Type: Primitive; Lattice Parameters: a = 9.6346(7)Å, b = 17.2104(13)Å, c = 22.7713(18)Å, $\alpha = 90^o$, $\beta = 90^o$, $\gamma = 90^o$, V = 3775.8(5)Å^3; Space group: P2(1)2(1)2(1); Z = 4; D_{calc}= 1.522 g/cm^3; F_{000} = 1744; Diffractometer: Rigaku AFC7R; Residuals: R; Rw: 0.0536, 0.1018.

Table 1. Crystal data and structure refinement for cd26541.

Identification code	cd26541
Empirical formula	C40 H28 F6 N4 O5 Pd
Formula weight	865.06
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 9.6346(7) A alpha = 90 deg. b = 17.2104(13) A beta = 90 deg. c = 22.7713(18) A gamma = 90 deg.
Volume	3775.8(5) A^3
Z, Calculated density	4, 1.522 Mg/m^3
Absorption coefficient	0.571 mm^-1
F(000)	1744
Crystal size	0.234 x 0.168 x 0.109 mm
Theta range for data collection	1.48 to 25.50 deg.
Limiting indices	-11<=h<=10, -20<=k<=20, -25<=l<=27
Reflections collected / unique	19937 / 7027 [R(int) = 0.1410]
Completeness to theta = 25.50	99.9 %
Absorption correction	Empirical
Max. and min. transmission	1.00000 and 0.71289
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7027 / 3 / 510
Goodness-of-fit on F^2	0.808
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1018
R indices (all data)	R1 = 0.1047, wR2 = 0.1169
Absolute structure parameter	-0.03(4)
Largest diff. peak and hole	0.341 and -0.473 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for cd26541. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Pd	1775(1)	6040(1)	1314(1)	63(1)
O(1)	820(6)	6157(4)	2131(2)	75(2)
O(2)	-1090(7)	6482(5)	1653(3)	117(3)
O(3)	2658(6)	7111(4)	1474(3)	88(2)
O(4)	4359(10)	6564(7)	1827(4)	125(4)
O(5)	6585(13)	6082(7)	1010(4)	131(3)
N(1)	952(6)	4506(4)	1748(2)	65(2)
N(2)	12(5)	4692(3)	902(2)	52(2)
N(3)	3359(6)	5430(3)	269(2)	54(1)
N(4)	2573(6)	6610(4)	147(3)	69(2)
F(1)	-496(7)	6170(5)	3137(3)	169(3)
F(2)	-2151(11)	6716(7)	2742(3)	209(6)
F(3)	-1886(12)	5535(8)	2634(4)	204(6)
F(4)	3481(10)	8412(5)	1945(4)	189(3)
F(5)	5094(17)	7873(7)	2303(6)	238(11)
F(6)	5181(12)	8170(5)	1474(5)	214(7)
C(1)	917(6)	5018(4)	1286(3)	56(2)
C(2)	27(7)	3905(5)	1668(3)	62(2)
C(3)	-606(6)	4034(5)	1132(3)	55(2)
C(4)	-1599(8)	3535(4)	916(3)	65(2)
C(5)	-1965(8)	2900(4)	1267(4)	76(2)
C(6)	-1362(9)	2808(5)	1819(4)	90(3)
C(7)	-367(10)	3298(5)	2032(3)	86(3)
C(8)	16(7)	4838(4)	279(3)	50(2)
C(9)	-1116(7)	5212(4)	14(3)	63(2)
C(10)	-1228(7)	5245(5)	-584(4)	78(3)
C(11)	-213(7)	4883(4)	-940(3)	49(2)
C(12)	943(7)	4535(4)	-677(3)	48(2)
C(13)	1055(6)	4510(4)	-53(2)	44(2)
C(14)	2297(6)	4163(4)	264(2)	46(2)
C(15)	3336(8)	4630(4)	449(3)	52(2)
C(16)	4433(7)	4347(5)	801(3)	64(2)
C(17)	4437(8)	3586(6)	965(3)	68(2)
C(18)	3382(7)	3077(4)	780(2)	53(2)
C(19)	2297(7)	3356(4)	417(3)	50(2)
C(20)	2585(6)	6016(5)	527(3)	54(2)
C(21)	3380(8)	6453(5)	-343(3)	61(2)
C(22)	3875(7)	5708(5)	-267(3)	58(2)
C(23)	4735(7)	5354(5)	-682(3)	65(2)
C(24)	5071(7)	5800(6)	-1169(3)	83(3)
C(25)	4558(9)	6564(6)	-1236(4)	82(2)
C(26)	3698(9)	6907(5)	-835(3)	82(3)
C(27)	1939(10)	4561(5)	2245(3)	100(3)
C(28)	1802(11)	7349(5)	223(3)	95(3)
C(29)	1930(8)	4166(4)	-1048(3)	61(2)
C(30)	1752(9)	4147(4)	-1639(3)	73(2)
C(31)	560(10)	4479(5)	-1888(3)	76(3)
C(32)	-396(9)	4860(5)	-1557(3)	74(2)
C(33)	1267(7)	2840(4)	225(3)	59(2)
C(34)	1306(8)	2088(5)	384(3)	68(2)
C(35)	2362(9)	1824(5)	752(3)	69(2)
C(36)	3358(9)	2277(5)	939(3)	69(2)
C(37)	-422(11)	6306(6)	2096(4)	84(3)
C(38)	-1244(11)	6210(10)	2642(5)	117(4)
C(39)	3839(18)	7184(8)	1608(7)	136(7)
C(40)	4377(15)	7881(9)	1875(9)	139(5)

Table 3. Bond lengths [A] and angles [deg] for cd26541.

Pd-C(1)	1.944(6)
Pd-C(20)	1.956(6)
Pd-O(3)	2.062(6)
Pd-O(1)	2.084(4)
O(1)-C(37)	1.226(10)
O(2)-C(37)	1.235(10)
O(3)-C(39)	1.185(14)
O(4)-C(39)	1.280(13)
O(5)-H(5B)	0.884(19)
O(5)-H(5A)	0.92(2)
N(1)-C(1)	1.373(8)
N(1)-C(2)	1.377(9)
N(1)-C(27)	1.483(8)
N(2)-C(1)	1.357(7)
N(2)-C(3)	1.384(9)
N(2)-C(8)	1.440(7)
N(3)-C(20)	1.384(8)
N(3)-C(22)	1.402(8)
N(3)-C(15)	1.437(8)
N(4)-C(20)	1.339(9)
N(4)-C(21)	1.387(8)
N(4)-C(28)	1.483(9)
F(1)-C(38)	1.340(11)
F(2)-C(38)	1.254(14)
F(3)-C(38)	1.317(16)
F(4)-C(40)	1.267(13)
F(5)-C(40)	1.194(17)
F(6)-C(40)	1.297(16)
C(2)-C(3)	1.382(8)
C(2)-C(7)	1.388(10)
C(3)-C(4)	1.376(9)
C(4)-C(5)	1.399(9)
C(4)-H(4)	0.9300
C(5)-C(6)	1.393(10)
C(5)-H(5)	0.9300
C(6)-C(7)	1.366(10)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-C(13)	1.375(8)
C(8)-C(9)	1.403(8)
C(9)-C(10)	1.367(9)
C(9)-H(9)	0.9300
C(10)-C(11)	1.414(9)
C(10)-H(10)	0.9300
C(11)-C(12)	1.399(8)
C(11)-C(32)	1.417(8)
C(12)-C(29)	1.422(8)
C(12)-C(13)	1.427(8)
C(13)-C(14)	1.520(8)
C(14)-C(15)	1.352(9)
C(14)-C(19)	1.431(9)
C(15)-C(16)	1.413(9)
C(16)-C(17)	1.361(10)
C(16)-H(16)	0.9300
C(17)-C(18)	1.407(10)
C(17)-H(17)	0.9300
C(18)-C(19)	1.416(9)
C(18)-C(36)	1.423(9)
C(19)-C(33)	1.402(9)
C(21)-C(22)	1.378(9)
C(21)-C(26)	1.400(10)
C(22)-C(23)	1.396(9)
C(23)-C(24)	1.388(10)
C(23)-H(23)	0.9300
C(24)-C(25)	1.414(11)
C(24)-H(24)	0.9300
C(25)-C(26)	1.367(10)
C(25)-H(25)	0.9300

C(26)-H(26)	0.9300
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-C(30)	1.358(7)
C(29)-H(29)	0.9300
C(30)-C(31)	1.401(11)
C(30)-H(30)	0.9300
C(31)-C(32)	1.359(11)
C(31)-H(31)	0.9300
C(32)-H(32)	0.9300
C(33)-C(34)	1.346(10)
C(33)-H(33)	0.9300
C(34)-C(35)	1.394(10)
C(34)-H(34)	0.9300
C(35)-C(36)	1.308(10)
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300
C(37)-C(38)	1.482(12)
C(39)-C(40)	1.441(18)

C(1)-Pd-C(20)	96.9(3)
C(1)-Pd-O(3)	171.7(3)
C(20)-Pd-O(3)	90.9(3)
C(1)-Pd-O(1)	85.9(3)
C(20)-Pd-O(1)	174.8(3)
O(3)-Pd-O(1)	86.5(2)
C(37)-O(1)-Pd	113.3(5)
C(39)-O(3)-Pd	122.5(8)
H(5B)-O(5)-H(5A)	101(3)
C(1)-N(1)-C(2)	111.4(5)
C(1)-N(1)-C(27)	124.1(7)
C(2)-N(1)-C(27)	124.4(6)
C(1)-N(2)-C(3)	111.8(6)
C(1)-N(2)-C(8)	124.1(6)
C(3)-N(2)-C(8)	121.1(6)
C(20)-N(3)-C(22)	108.2(6)
C(20)-N(3)-C(15)	124.6(6)
C(22)-N(3)-C(15)	125.5(6)
C(20)-N(4)-C(21)	111.5(6)
C(20)-N(4)-C(28)	125.7(6)
C(21)-N(4)-C(28)	122.8(6)
N(2)-C(1)-N(1)	104.1(6)
N(2)-C(1)-Pd	132.0(6)
N(1)-C(1)-Pd	123.0(5)
N(1)-C(2)-C(3)	106.4(7)
N(1)-C(2)-C(7)	131.5(7)
C(3)-C(2)-C(7)	121.9(8)
C(4)-C(3)-C(2)	121.5(8)
C(4)-C(3)-N(2)	132.5(6)
C(2)-C(3)-N(2)	106.0(6)
C(3)-C(4)-C(5)	117.3(7)
C(3)-C(4)-H(4)	121.4
C(5)-C(4)-H(4)	121.4
C(6)-C(5)-C(4)	119.9(7)
C(6)-C(5)-H(5)	120.0
C(4)-C(5)-H(5)	120.0
C(7)-C(6)-C(5)	123.0(8)
C(7)-C(6)-H(6)	118.5
C(5)-C(6)-H(6)	118.5
C(6)-C(7)-C(2)	116.3(8)
C(6)-C(7)-H(7)	121.8
C(2)-C(7)-H(7)	121.9
C(13)-C(8)-C(9)	121.2(6)
C(13)-C(8)-N(2)	118.1(6)
C(9)-C(8)-N(2)	120.1(6)
C(10)-C(9)-C(8)	120.6(7)
C(10)-C(9)-H(9)	119.7
C(8)-C(9)-H(9)	119.7

C(9)-C(10)-C(11)	119.8(7)
C(9)-C(10)-H(10)	120.1
C(11)-C(10)-H(10)	120.1
C(12)-C(11)-C(10)	119.7(6)
C(12)-C(11)-C(32)	120.7(7)
C(10)-C(11)-C(32)	119.6(7)
C(11)-C(12)-C(29)	118.0(6)
C(11)-C(12)-C(13)	119.9(6)
C(29)-C(12)-C(13)	121.9(6)
C(8)-C(13)-C(12)	118.7(6)
C(8)-C(13)-C(14)	118.3(5)
C(12)-C(13)-C(14)	122.9(5)
C(15)-C(14)-C(19)	120.0(6)
C(15)-C(14)-C(13)	119.8(6)
C(19)-C(14)-C(13)	119.8(6)
C(14)-C(15)-C(16)	121.7(7)
C(14)-C(15)-N(3)	119.4(6)
C(16)-C(15)-N(3)	118.8(7)
C(17)-C(16)-C(15)	119.3(8)
C(17)-C(16)-H(16)	120.3
C(15)-C(16)-H(16)	120.3
C(16)-C(17)-C(18)	121.0(7)
C(16)-C(17)-H(17)	119.5
C(18)-C(17)-H(17)	119.5
C(17)-C(18)-C(19)	119.8(7)
C(17)-C(18)-C(36)	122.5(7)
C(19)-C(18)-C(36)	117.7(7)
C(33)-C(19)-C(18)	119.3(7)
C(33)-C(19)-C(14)	122.5(6)
C(18)-C(19)-C(14)	118.2(7)
N(4)-C(20)-N(3)	106.7(5)
N(4)-C(20)-Pd	124.9(5)
N(3)-C(20)-Pd	128.3(6)
C(22)-C(21)-N(4)	105.9(7)
C(22)-C(21)-C(26)	123.0(8)
N(4)-C(21)-C(26)	131.1(8)
C(21)-C(22)-C(23)	121.7(8)
C(21)-C(22)-N(3)	107.7(7)
C(23)-C(22)-N(3)	130.6(8)
C(24)-C(23)-C(22)	116.0(8)
C(24)-C(23)-H(23)	122.0
C(22)-C(23)-H(23)	122.0
C(23)-C(24)-C(25)	121.2(8)
C(23)-C(24)-H(24)	119.4
C(25)-C(24)-H(24)	119.4
C(26)-C(25)-C(24)	122.8(8)
C(26)-C(25)-H(25)	118.6
C(24)-C(25)-H(25)	118.6
C(25)-C(26)-C(21)	115.2(8)
C(25)-C(26)-H(26)	122.4
C(21)-C(26)-H(26)	122.4
N(1)-C(27)-H(27A)	109.5
N(1)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
N(1)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
N(4)-C(28)-H(28A)	109.5
N(4)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
N(4)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-C(12)	121.0(8)
C(30)-C(29)-H(29)	119.5
C(12)-C(29)-H(29)	119.5
C(29)-C(30)-C(31)	119.6(8)
C(29)-C(30)-H(30)	120.2
C(31)-C(30)-H(30)	120.2
C(32)-C(31)-C(30)	121.9(7)
C(32)-C(31)-H(31)	119.1
C(30)-C(31)-H(31)	119.1

C(31)-C(32)-C(11)	118.6(8)
C(31)-C(32)-H(32)	120.7
C(11)-C(32)-H(32)	120.7
C(34)-C(33)-C(19)	120.4(7)
C(34)-C(33)-H(33)	119.8
C(19)-C(33)-H(33)	119.8
C(33)-C(34)-C(35)	119.7(8)
C(33)-C(34)-H(34)	120.1
C(35)-C(34)-H(34)	120.1
C(36)-C(35)-C(34)	122.5(8)
C(36)-C(35)-H(35)	118.7
C(34)-C(35)-H(35)	118.7
C(35)-C(36)-C(18)	120.3(8)
C(35)-C(36)-H(36)	119.8
C(18)-C(36)-H(36)	119.8
O(1)-C(37)-O(2)	127.7(8)
O(1)-C(37)-C(38)	116.5(10)
O(2)-C(37)-C(38)	115.7(10)
F(2)-C(38)-F(3)	106.8(10)
F(2)-C(38)-F(1)	105.0(12)
F(3)-C(38)-F(1)	102.6(11)
F(2)-C(38)-C(37)	116.5(12)
F(3)-C(38)-C(37)	109.7(11)
F(1)-C(38)-C(37)	115.0(9)
O(3)-C(39)-O(4)	112.8(14)
O(3)-C(39)-C(40)	122.9(14)
O(4)-C(39)-C(40)	112.9(13)
F(5)-C(40)-F(4)	107.4(17)
F(5)-C(40)-F(6)	103.5(14)
F(4)-C(40)-F(6)	102.6(15)
F(5)-C(40)-C(39)	122.9(16)
F(4)-C(40)-C(39)	114.1(13)
F(6)-C(40)-C(39)	103.7(16)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for cd26541.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Pd	64(1)	72(1)	52(1)	-14(1)	7(1)	-6(1)
O(1)	68(3)	93(4)	62(3)	-28(3)	18(3)	-14(4)
O(2)	97(5)	207(9)	107(5)	59(5)	21(4)	42(5)
O(3)	77(3)	82(4)	104(5)	-21(4)	8(3)	-6(3)
O(4)	164(8)	212(12)	179(9)	2(8)	-31(6)	-75(8)
N(1)	79(4)	75(5)	41(3)	-5(3)	0(3)	-13(4)
N(2)	52(3)	69(4)	35(3)	3(3)	4(3)	-2(3)
N(3)	43(3)	70(4)	49(3)	-8(3)	6(3)	-8(4)
N(4)	84(4)	70(5)	52(4)	-5(3)	6(3)	5(4)
F(1)	172(6)	244(9)	90(4)	11(5)	54(4)	25(7)
F(2)	154(8)	205(15)	139(6)	30(7)	89(6)	168(10)
F(3)	155(11)	231(14)	157(9)	13(8)	101(8)	-102(11)
F(4)	208(8)	112(6)	246(9)	-47(6)	39(8)	-61(6)
F(5)	207(19)	167(14)	171(17)	-46(11)	-168(17)	-64(13)
F(6)	171(11)	136(9)	235(16)	-39(9)	106(13)	-53(8)
C(1)	59(4)	68(5)	41(4)	-8(4)	2(4)	-15(4)
C(2)	74(5)	65(5)	47(4)	4(4)	-2(3)	-11(5)
C(3)	45(4)	66(5)	53(4)	-3(4)	8(3)	4(4)
C(4)	61(5)	69(5)	66(5)	-7(4)	6(4)	-2(5)
C(5)	75(5)	76(6)	78(5)	-8(5)	-1(5)	0(5)
C(6)	95(7)	90(7)	84(6)	5(5)	9(5)	-21(6)
C(7)	109(7)	90(7)	59(5)	12(5)	-10(5)	-13(6)
C(8)	54(4)	52(4)	42(4)	-2(3)	-10(3)	3(4)
C(9)	60(4)	69(5)	59(5)	-5(4)	3(4)	13(4)
C(10)	64(5)	92(7)	77(6)	17(5)	-23(4)	-2(5)
C(11)	47(4)	67(5)	34(4)	9(3)	-6(3)	-4(4)
C(12)	57(4)	45(4)	43(4)	-3(3)	-2(3)	-2(4)
C(13)	51(4)	47(4)	34(4)	-2(3)	0(3)	-4(3)
C(14)	42(4)	63(5)	33(3)	-4(3)	5(3)	13(3)
C(15)	49(4)	61(5)	45(4)	1(3)	6(4)	10(4)
C(16)	50(4)	88(6)	53(5)	4(4)	-10(4)	-2(4)
C(17)	45(5)	103(7)	56(5)	15(5)	1(4)	26(5)
C(18)	47(4)	72(5)	41(4)	2(3)	11(4)	12(4)
C(19)	44(4)	63(5)	42(4)	5(3)	3(3)	8(4)
C(20)	52(4)	54(4)	54(4)	-8(4)	15(3)	0(4)
C(21)	68(5)	62(5)	52(4)	-4(4)	-17(4)	1(5)
C(22)	46(4)	79(6)	49(4)	-5(4)	0(3)	-12(4)
C(23)	48(4)	91(7)	57(5)	-16(5)	-1(4)	-2(4)
C(24)	60(5)	136(9)	54(5)	-13(5)	7(4)	-24(5)
C(25)	99(6)	94(7)	53(5)	3(5)	5(5)	-10(6)
C(26)	113(7)	85(7)	49(5)	4(5)	-13(5)	-2(6)
C(27)	124(7)	117(8)	58(5)	-10(5)	-46(5)	-5(7)
C(28)	125(7)	77(6)	83(6)	-6(4)	5(6)	42(7)
C(29)	67(5)	66(5)	49(4)	-6(3)	-2(4)	-1(5)
C(30)	83(5)	86(6)	51(5)	3(4)	7(5)	1(6)
C(31)	106(7)	93(7)	29(4)	3(4)	1(4)	-15(6)
C(32)	73(6)	85(6)	63(5)	13(4)	-15(4)	-24(5)
C(33)	58(5)	61(5)	59(5)	3(4)	7(3)	10(4)
C(34)	76(6)	57(6)	71(5)	2(4)	14(4)	-1(4)
C(35)	85(6)	53(5)	70(5)	20(4)	19(5)	12(5)
C(36)	72(5)	73(6)	63(5)	7(4)	11(4)	25(5)
C(37)	84(6)	86(7)	83(7)	-6(5)	26(6)	-8(6)
C(38)	82(7)	176(14)	94(8)	15(9)	35(6)	0(9)
C(39)	181(16)	59(8)	168(16)	12(8)	-78(13)	11(10)
C(40)	112(11)	93(11)	212(16)	-27(12)	14(11)	11(9)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for cd26541.

	x	y	z	U(eq)
H(4)	-2010	3616	551	78
H(5)	-2611	2540	1132	92
H(6)	-1650	2395	2052	108
H(7)	25	3228	2402	103
H(9)	-1796	5439	247	75
H(10)	-1970	5505	-757	93
H(16)	5144	4676	920	76
H(17)	5147	3400	1203	81
H(23)	5062	4850	-634	78
H(24)	5646	5592	-1457	100
H(25)	4815	6846	-1567	99
H(26)	3350	7407	-885	99
H(27A)	2751	4841	2123	129
H(27B)	2200	4048	2369	129
H(27C)	1506	4830	2566	129
H(28A)	1112	7285	523	132
H(28B)	1360	7486	-140	132
H(28C)	2437	7752	336	142
H(29)	2710	3934	-883	73
H(30)	2417	3916	-1878	88
H(31)	419	4436	-2291	91
H(32)	-1155	5101	-1732	89
H(33)	552	3019	-14	71
H(34)	631	1745	250	82
H(35)	2358	1306	869	83
H(36)	4055	2076	1177	83
H(5B)	6790(60)	5614(17)	1140(20)	87(15)
H(5A)	5720(40)	6150(40)	1170(30)	120(40)

Table 6. Torsion angles [deg] for cd26541.

C(1)-Pd-O(1)-C(37)	-77.4(7)
C(20)-Pd-O(1)-C(37)	46(3)
O(3)-Pd-O(1)-C(37)	105.9(7)
C(1)-Pd-O(3)-C(39)	82(2)
C(20)-Pd-O(3)-C(39)	-79.5(12)
O(1)-Pd-O(3)-C(39)	104.9(12)
C(3)-N(2)-C(1)-N(1)	5.4(7)
C(8)-N(2)-C(1)-N(1)	-155.3(6)
C(3)-N(2)-C(1)-Pd	-163.9(5)
C(8)-N(2)-C(1)-Pd	35.5(9)
C(2)-N(1)-C(1)-N(2)	-3.8(8)
C(27)-N(1)-C(1)-N(2)	171.7(6)
C(2)-N(1)-C(1)-Pd	166.8(5)
C(27)-N(1)-C(1)-Pd	-17.7(10)
C(20)-Pd-C(1)-N(2)	-55.0(7)
O(3)-Pd-C(1)-N(2)	144.1(16)
O(1)-Pd-C(1)-N(2)	120.7(6)
C(20)-Pd-C(1)-N(1)	137.5(6)
O(3)-Pd-C(1)-N(1)	-23(2)
O(1)-Pd-C(1)-N(1)	-46.9(6)
C(1)-N(1)-C(2)-C(3)	0.8(8)
C(27)-N(1)-C(2)-C(3)	-174.6(6)
C(1)-N(1)-C(2)-C(7)	-174.3(8)
C(27)-N(1)-C(2)-C(7)	10.2(13)
N(1)-C(2)-C(3)-C(4)	180.0(6)
C(7)-C(2)-C(3)-C(4)	-4.3(11)
N(1)-C(2)-C(3)-N(2)	2.4(7)
C(7)-C(2)-C(3)-N(2)	178.1(7)
C(1)-N(2)-C(3)-C(4)	177.8(7)
C(8)-N(2)-C(3)-C(4)	-20.9(11)
C(1)-N(2)-C(3)-C(2)	-5.0(7)
C(8)-N(2)-C(3)-C(2)	156.3(6)
C(2)-C(3)-C(4)-C(5)	1.4(10)
N(2)-C(3)-C(4)-C(5)	178.2(7)
C(3)-C(4)-C(5)-C(6)	2.0(11)
C(4)-C(5)-C(6)-C(7)	-2.8(13)
C(5)-C(6)-C(7)-C(2)	0.0(13)
N(1)-C(2)-C(7)-C(6)	178.0(8)
C(3)-C(2)-C(7)-C(6)	3.5(12)
C(1)-N(2)-C(8)-C(13)	73.3(9)
C(3)-N(2)-C(8)-C(13)	-85.6(8)
C(1)-N(2)-C(8)-C(9)	-115.3(7)
C(3)-N(2)-C(8)-C(9)	85.8(8)
C(13)-C(8)-C(9)-C(10)	1.4(11)
N(2)-C(8)-C(9)-C(10)	-169.7(7)
C(8)-C(9)-C(10)-C(11)	1.6(11)
C(9)-C(10)-C(11)-C(12)	-3.9(11)
C(9)-C(10)-C(11)-C(32)	174.5(7)
C(10)-C(11)-C(12)-C(29)	179.0(7)
C(32)-C(11)-C(12)-C(29)	0.7(10)
C(10)-C(11)-C(12)-C(13)	3.3(10)
C(32)-C(11)-C(12)-C(13)	-175.0(7)
C(9)-C(8)-C(13)-C(12)	-2.0(10)
N(2)-C(8)-C(13)-C(12)	169.3(6)
C(9)-C(8)-C(13)-C(14)	175.9(6)
N(2)-C(8)-C(13)-C(14)	-12.8(9)
C(11)-C(12)-C(13)-C(8)	-0.4(9)
C(29)-C(12)-C(13)-C(8)	-175.9(6)
C(11)-C(12)-C(13)-C(14)	-178.2(6)
C(29)-C(12)-C(13)-C(14)	6.3(9)
C(8)-C(13)-C(14)-C(15)	-81.5(7)
C(12)-C(13)-C(14)-C(15)	96.3(8)
C(8)-C(13)-C(14)-C(19)	92.0(8)
C(12)-C(13)-C(14)-C(19)	-90.1(7)
C(19)-C(14)-C(15)-C(16)	-0.7(9)
C(13)-C(14)-C(15)-C(16)	172.8(6)
C(19)-C(14)-C(15)-N(3)	177.1(5)
C(13)-C(14)-C(15)-N(3)	-9.4(8)

C(20)-N(3)-C(15)-C(14)	81.0(8)
C(22)-N(3)-C(15)-C(14)	-82.5(9)
C(20)-N(3)-C(15)-C(16)	-101.2(8)
C(22)-N(3)-C(15)-C(16)	95.3(8)
C(14)-C(15)-C(16)-C(17)	-0.9(10)
N(3)-C(15)-C(16)-C(17)	-178.7(6)
C(15)-C(16)-C(17)-C(18)	1.3(11)
C(16)-C(17)-C(18)-C(19)	0.0(10)
C(16)-C(17)-C(18)-C(36)	179.5(7)
C(17)-C(18)-C(19)-C(33)	178.7(6)
C(36)-C(18)-C(19)-C(33)	-0.8(9)
C(17)-C(18)-C(19)-C(14)	-1.6(9)
C(36)-C(18)-C(19)-C(14)	178.9(6)
C(15)-C(14)-C(19)-C(33)	-178.3(5)
C(13)-C(14)-C(19)-C(33)	8.1(9)
C(15)-C(14)-C(19)-C(18)	2.0(9)
C(13)-C(14)-C(19)-C(18)	-171.6(5)
C(21)-N(4)-C(20)-N(3)	-3.3(8)
C(28)-N(4)-C(20)-N(3)	176.4(7)
C(21)-N(4)-C(20)-Pd	172.2(5)
C(28)-N(4)-C(20)-Pd	-8.1(10)
C(22)-N(3)-C(20)-N(4)	3.1(7)
C(15)-N(3)-C(20)-N(4)	-162.8(6)
C(22)-N(3)-C(20)-Pd	-172.2(5)
C(15)-N(3)-C(20)-Pd	21.9(9)
C(1)-Pd-C(20)-N(4)	137.1(6)
O(3)-Pd-C(20)-N(4)	-45.6(6)
O(1)-Pd-C(20)-N(4)	14(3)
C(1)-Pd-C(20)-N(3)	-48.4(6)
O(3)-Pd-C(20)-N(3)	128.9(6)
O(1)-Pd-C(20)-N(3)	-171(2)
C(20)-N(4)-C(21)-C(22)	2.2(8)
C(28)-N(4)-C(21)-C(22)	-177.6(7)
C(20)-N(4)-C(21)-C(26)	-177.8(8)
C(28)-N(4)-C(21)-C(26)	2.5(12)
N(4)-C(21)-C(22)-C(23)	179.9(6)
C(26)-C(21)-C(22)-C(23)	-0.1(11)
N(4)-C(21)-C(22)-N(3)	-0.1(7)
C(26)-C(21)-C(22)-N(3)	179.8(7)
C(20)-N(3)-C(22)-C(21)	-1.8(7)
C(15)-N(3)-C(22)-C(21)	163.9(7)
C(20)-N(3)-C(22)-C(23)	178.1(7)
C(15)-N(3)-C(22)-C(23)	-16.1(11)
C(21)-C(22)-C(23)-C(24)	0.7(10)
N(3)-C(22)-C(23)-C(24)	-179.2(6)
C(22)-C(23)-C(24)-C(25)	-0.4(10)
C(23)-C(24)-C(25)-C(26)	-0.7(12)
C(24)-C(25)-C(26)-C(21)	1.2(12)
C(22)-C(21)-C(26)-C(25)	-0.9(11)
N(4)-C(21)-C(26)-C(25)	179.1(7)
C(11)-C(12)-C(29)-C(30)	-0.5(10)
C(13)-C(12)-C(29)-C(30)	175.1(7)
C(12)-C(29)-C(30)-C(31)	-1.7(12)
C(29)-C(30)-C(31)-C(32)	3.8(13)
C(30)-C(31)-C(32)-C(11)	-3.5(13)
C(12)-C(11)-C(32)-C(31)	1.3(12)
C(10)-C(11)-C(32)-C(31)	-177.0(7)
C(18)-C(19)-C(33)-C(34)	0.2(9)
C(14)-C(19)-C(33)-C(34)	-179.5(6)
C(19)-C(33)-C(34)-C(35)	1.3(10)
C(33)-C(34)-C(35)-C(36)	-2.1(11)
C(34)-C(35)-C(36)-C(18)	1.4(12)
C(17)-C(18)-C(36)-C(35)	-179.4(7)
C(19)-C(18)-C(36)-C(35)	0.1(10)
Pd-O(1)-C(37)-O(2)	-9.7(14)
Pd-O(1)-C(37)-C(38)	165.6(9)
O(1)-C(37)-C(38)-F(2)	140.1(13)
O(2)-C(37)-C(38)-F(2)	-44.1(17)
O(1)-C(37)-C(38)-F(3)	-98.5(13)
O(2)-C(37)-C(38)-F(3)	77.4(15)
O(1)-C(37)-C(38)-F(1)	16.6(18)
O(2)-C(37)-C(38)-F(1)	-167.6(11)

Pd-O(3)-C(39)-O(4)	-22(2)
Pd-O(3)-C(39)-C(40)	-162.4(12)
O(3)-C(39)-C(40)-F(5)	132(2)
O(4)-C(39)-C(40)-F(5)	-9(3)
O(3)-C(39)-C(40)-F(4)	-1(3)
O(4)-C(39)-C(40)-F(4)	-141.7(17)
O(3)-C(39)-C(40)-F(6)	-111.9(18)
O(4)-C(39)-C(40)-F(6)	107.5(19)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for cd26541 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(5)-H(5A)...O(4)	0.92(2)	2.11(4)	2.958(16)	152(8)

Symmetry transformations used to generate equivalent atoms: