Supplementary Material (ESI) for Chemical Communications
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Supporting Information for:

A highly enantioselective abiotic receptor for malate dianion in aqueous solution

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Electromotive Force (emf) Measurements

Potentiometric titrations were carried out using a reaction vessel water-thermostated at 25.0 ± 0.1ºC in an argon atmosphere. As it is present in biological systems in similar concentrations, NaCl 0.15 mol dm^{-3} was used as supporting electrolyte. The titrant was delivered by a Metrohm burette-765. The potentiometric measurements were made using a Metrohm 713 pH-mV meter.

The reference electrode was an Ag/AgCl electrode in saturated KCl solution. The glass electrode was calibrated as a hydrogen ion concentration probe by titration of previously standardized amounts of HCl with CO_2-free NaOH solutions and determining the equivalent point by Gran's method, which gives the standard potential, E^{o}', and the ionic product of water [pK_w = 13.73(1)].

The acquisition of the emf data was performed with the computer program PASAT. The HYPERQUAD program was used to process the data and calculate both the protonation and stability constants. The pH range investigated was 2.0-12.0, and the concentration of the anions and of the ligand ranged from 1 x 10^{-3} to 5 x 10^{-3} M with L:A molar ratios from 3:1 to 1:3. The different titrations for each system (at least two) were treated either as a single set or as separate curves without significant variations in the values of the stability constants.

Finally, the sets of data were merged together and treated simultaneously to give the final stability constants.

Table S1. Protonation constants for (*R*,*R*)-**2** (L) and (*R*/*S*)-**1** (A) determined by pHmetric titration in an aqueous 0.15 M NaCl solution at 298.1 K in an argon atmosphere.

Reaction[a]	Log K
L + H ⇆ HL	9.07 (1)[b]
L + 2H ⇆ H_2L	17.60 (1)
L + 3H ⇆ H_3L	22.57 (2)
L + 4H ⇆ H_4L	25.63 (2)
A + H ⇆ HA	4.77 (3)
A + 2H ⇆ H_2A	8.05 (3)

[a]Charges omitted for clarity. [b]Standard deviations in the last significant figure.

Table S2. Binding constants between (*R*,*R*)-**2** (L) and (*R*/*S*)-**1** (A) determined by pHmetric titration in an aqueous 0.15 M NaCl solution at 298.1 K in an argon atmosphere.

Reaction[a]	Log *K* (*R*)-**1**	Log *K* (*S*)-**1**
A + L ⇆ AL	4.40	5.47
A + HL ⇆ HAL	4.34	5.30
A + H_2L ⇆ H_2AL	4.14	4.97
A + H_3L ⇆ H_3AL	3.95	4.65
HA + H_2L ⇆ H_3AL	4.15	4.85
HA + H_3L ⇆ H_4AL	3.25	3.94
HA + H_4L ⇆ H_5AL	3.22	3.79
H_2A + H_3L ⇆ H_5AL	3.00	3.57

[a]Charges omitted for clarity.

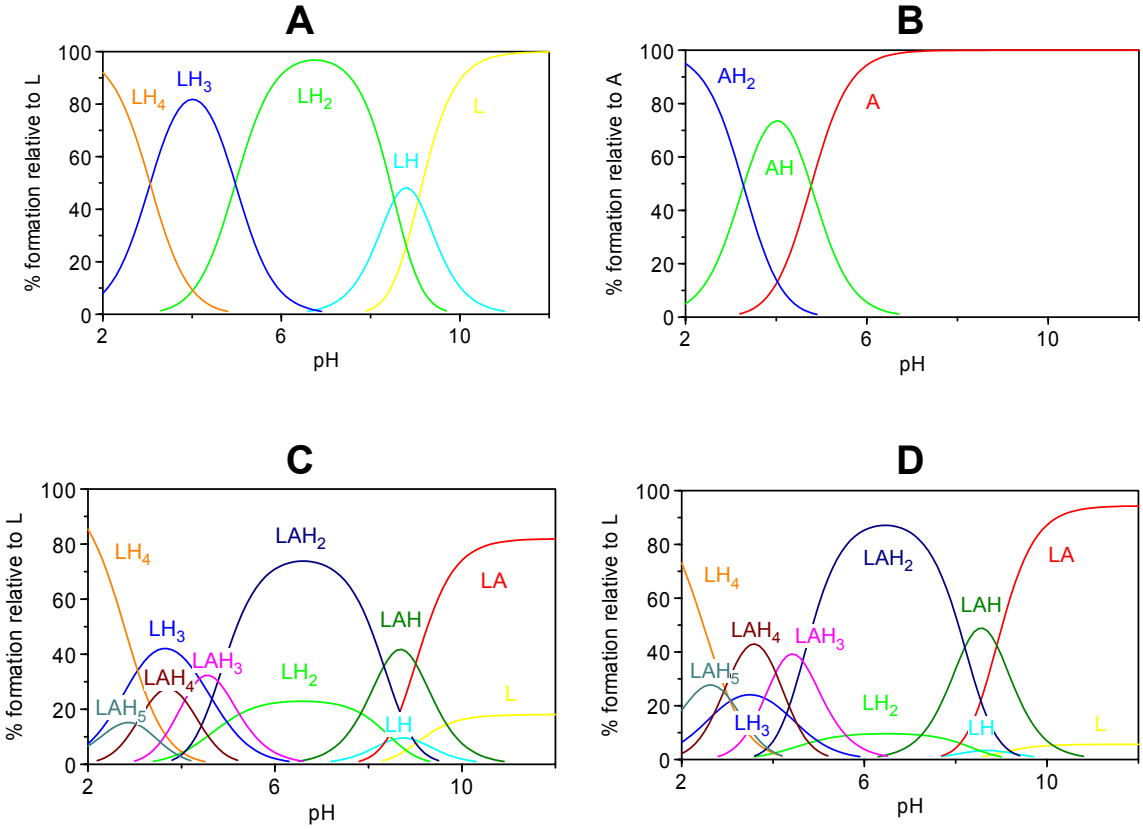


Figure S1. Speciation diagrams provided by HySS program: (A) protonation of (*R*,*R*)-**2**; (B) protonation of (*R*/*S*)-**1**; (C) [(*R*,*R*)-**2** + (*R*)-**1**] complexes; (D) [(*R*,*R*)-**2** + (*S*)-**1**] complexes.

Electrospray Ionization Mass Spectrometry (ESI-MS) analysis.

A Quattro LC (quadrupole-hexapole-quadrupole) mass spectrometer with an orthogonal Z-spray electrospray interface (Micromass, Manchester, UK) was used. Equimolar amounts of compounds **1** and **2** in MeOH:water 1:1 (aprox. $5x10^{-5}$ M) were infused via syringe pump directly to the interface at a flow rate of 10 µL/min. The temperature of the source block was set to 120 ºC and the interface to 150ºC. A capillary voltage of 3.5 kV was used in the positive scan mode and the cone voltage was kept at 15 V. The drying gas as well as nebulizing gas was nitrogen at flow rates of 400 L/h and 80 L/h respectively. The CID spectra were obtained at various collision energies (typically varied from E_{lab} 0-10 eV) by selecting the precursor ion of interest with MS1 and scanning MS2 at a cone voltage kept at 15 V. Argon was used as collision gas and the pressure in the collision cell was maintained at 1×10^{-3} mbar.

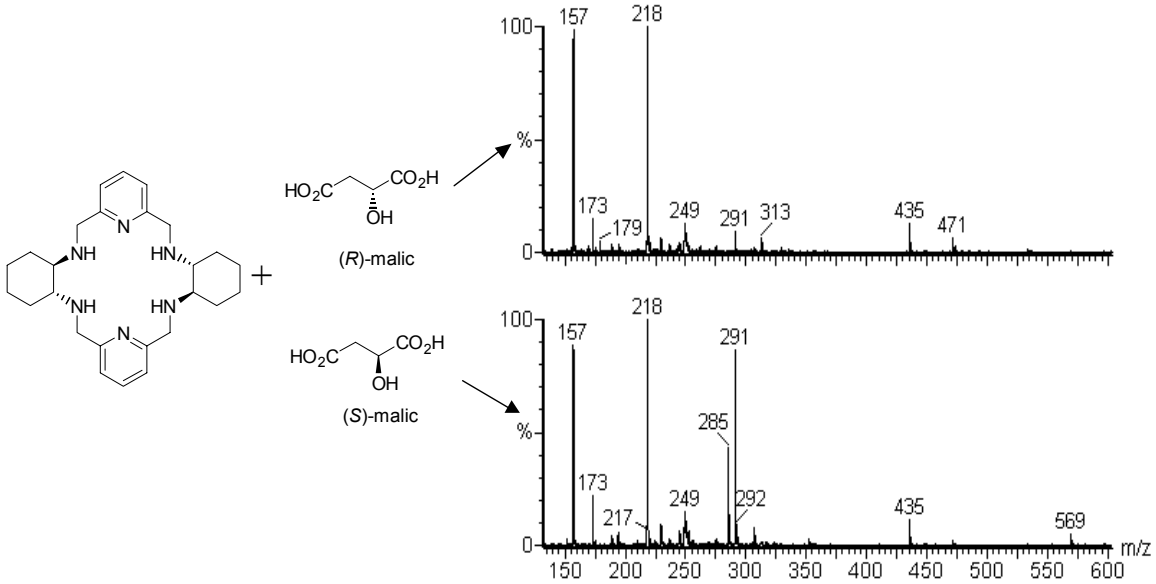


Figure S2. ESI-MS spectra of sample containing an equimolar amount of the receptor and either (*R*) or (*S*)-malic acid.

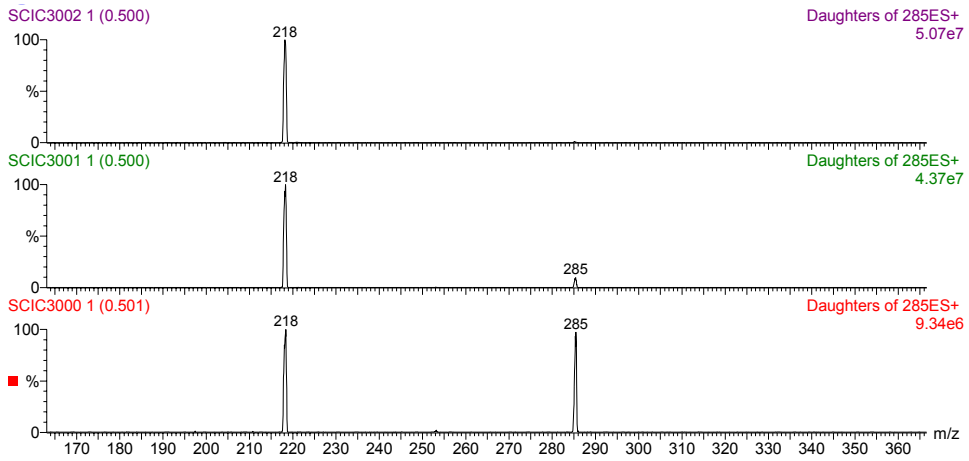


Figure S3. Collision induced dissociation experiments performed on the peak at *m/z* = 285. Collision energies were settled at 1 (bottom), 3 (middle) and 5 (upper) eV, respectively.

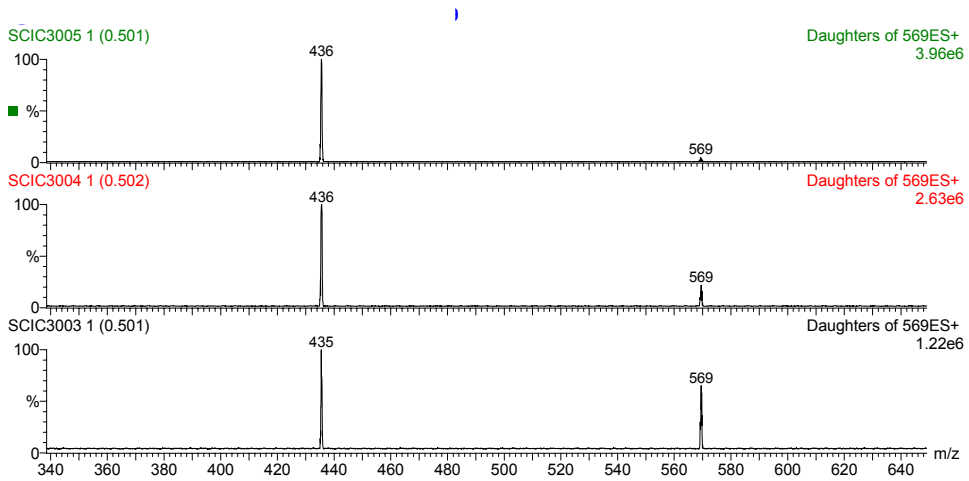


Figure S4. Collision induced dissociation experiments performed on the peak at *m/z* = 569. Collision energies were settled at 1 (bottom), 3 (middle) and 5 (upper) eV, respectively.

Self-diffusion rates measurement by NMR.

PGSE experiments were performed in a Varian INOVA 500 operating at 500 MHz for proton. Samples were prepared by mixing equimolar amounts of (*R*,*R*)-**2** and either (*R*) or (*S*)-**1** (10^{-2} M and pD = 6.5). For PGSE measurements, the Dbppste (DOSY bipolar pulse pair stimulated echo) sequence available in VARIAN software was applied and the gradient strength increments (typically an array of 15) calculated depending on the actual signal attenuation. For the accurate value of *D*, a linear regression of $\ln(I/I_o)$ vs G^2 was used for selected non-overlapped signals of either receptor or substrate (following the Stejskal-Tanner equation: $\ln(I/I_o) = -\gamma_x^2\delta^2(\Delta - \delta/3)DG^2$). All the linear fittings (figure S4) showed excellent correlation coefficients ($R^2 > 0.99$). For the calibration of self diffusion coefficients, the value of the HDO signal in deuterium oxide at 303 K ($D_{HDO} = 1.9 \times 10^{-9}$ m^2/s) was used as an internal standard for every sample. The measurements were repeated at least three times to ensure reproducibility.

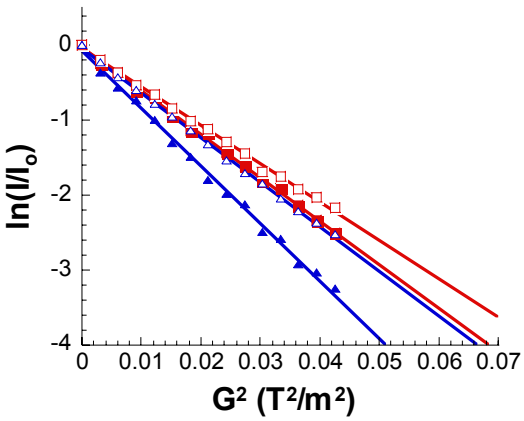


Figure S5. Plots of $\ln(I/I_o)$ vs G^2 for samples containing [(*S*)-**1**+(*R*,*R*)-**2**] (red squares) or [(*R*)-**1**+(*R*,*R*)-**2**] (blue triangles). Open symbols correspond to signal *H*eqβ from the receptor and solid symbols to signal C3*H* from the substrate (see manuscript for atom labeling).

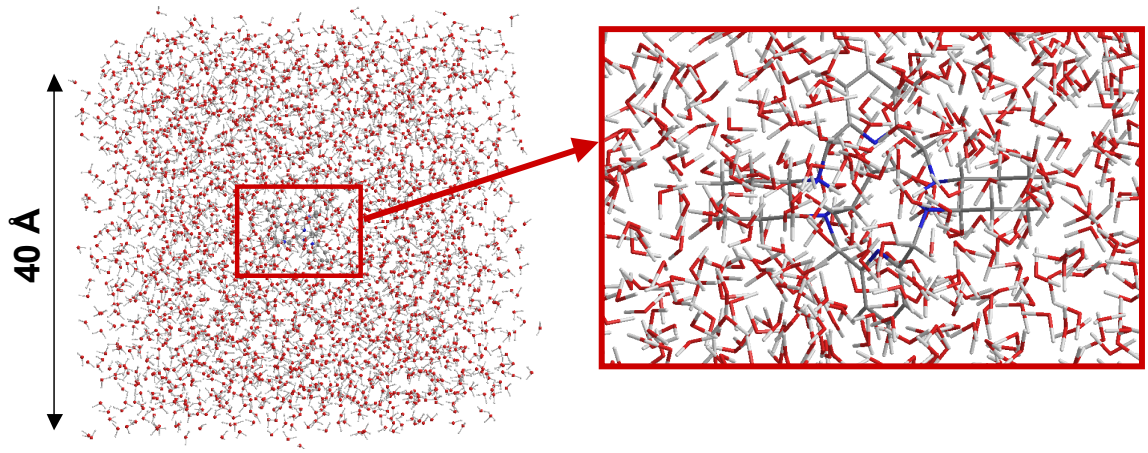
For the estimation of the hydrodynamic radius (r_H), the Stokes-Einstein equation ($D = k_bT/6\pi\eta r_H$) was used. The theoretical calculated value of *D* and r_H (entry 5 in table 2 of the manuscript) was obtained from the optimized geometries. The volume of the solute was obtained from the volume of water molecules excluded from the cube generated by the QM/MM calculations. This volume was approximated to a sphere of radius equal to r_H and *D* was accordingly estimated by the Stokes-Einstein equation. Considering the proposed equilibrium, this value would be the upper limit corresponding to 100% complex.

Molecular modeling.

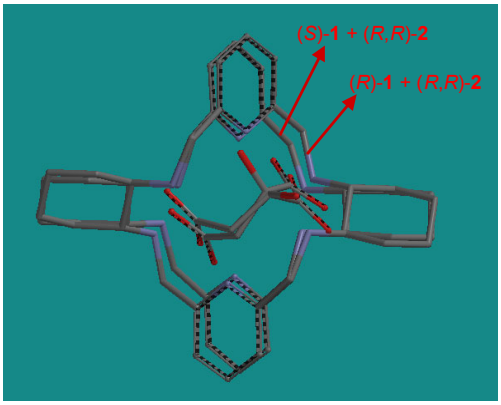
All the theoretical calculations were performed using Spartan '04 program. The optimized geometries for the supramolecular diasteromeric complexes were obtained as follows. A stochastic conformational search was applied (Monte Carlo Search followed by MMFFaq force field minimization) without restrictions to each diasteromeric complex. This method considers the presence of an aqueous solvent and generates a large number of possible conformations. More than 100 conformers were obtained in this way (ca. 40 kJ/mol cut off). The obtained structures were ordered by their energies and analyzed. The global minimum thus obtained for each diasteromeric complex was fully minimized using the PM3 semiempirical quantum mechanics calculations (see Figure 2 in manuscript). Frequencies analyses showed that both structures were minima of energy. For a more accurate value of energy, a single point energy calculation at the HF/6-31G* level of theory was performed using the optimized PM3 geometries. For considering the effect of the solvent a QM/MM mixed method was applied for each minimized structure. The complex was immersed in the center of a 64000 $Å^3$ cube (40x40x40) filled with water molecules. The dynamic configuration of these solvent molecules was minimized with the MMFF force field, while the energy of the solute was calculated at the *ab initio* HF/6-31G* level of theory. The obtained energy differences between complexes are shown in the following table.

Method	Theoretical level	Solvent	$\Delta E_{(R\text{-}S)}$ (kJ/mol)
Molecular Mechanics	MMFFaq	water	3.21
QM/MM	PM3(HF/6-31G*)/MMFF	water	6.54

Representation of dynamic configuration obtained from the QM/MM calculations at the PM3(HF/6-31G*)/MMFF level of theory:



Superimposed optimized geometries (PM3 full minimization and QM/MM using HF/6-31G*//MMFF single point energy calculation) for the diasteromeric complexes, showing the larger distortion produced in the receptor upon interaction with (*R*)-malate. Hydrogen atoms have been omitted for clarity of the picture.



Cartesian coordinates and energies for the optimized geometries:

[(*S*)-**1** + (*R*,*R*)-**2** + $2H^+$] complex.

HF/6-31G* Energy = -1862.6254753 hartrees

```
85
  H   -1.165283    4.638245    0.025192
  C   -0.663422    4.092422   -0.782135
  C    0.628189    2.670029   -2.768372
  C   -0.565674    2.696625   -0.739578
  C   -0.087479    4.775589   -1.847931
  C    0.571518    4.067551   -2.845947
  N    0.057373    2.005722   -1.731094
  H   -0.145447    5.869095   -1.895050
  H    1.044128    4.591415   -3.683868
  C   -1.035172    1.939041    0.459305
  H   -1.744522    2.545334    1.061325
  H   -0.102753    1.770721    1.132355
  C    1.302185    1.875839   -3.854721
  H    2.151154    2.458420   -4.270569
  H    0.578613    1.732544   -4.684418
  N    1.784851    0.524734   -3.502975
  H    1.084000    0.026672   -2.992157
  C   -3.013718    0.664230   -0.488449
  C   -4.695648   -0.484985   -1.981079
  C   -5.481674    0.746658    0.031982
  C   -5.716568   -0.458145   -0.859955
  C   -4.081436    0.697769    0.615509
  C   -3.254150   -0.532455   -1.446945
  H   -4.831345    0.403610   -2.632248
  H   -5.629272    1.684372   -0.541138
  H   -5.661667   -1.391159   -0.264313
  H   -3.987091   -0.193893    1.273560
  H   -3.109177   -1.487213   -0.874283
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  H   -1.491653   -0.002121   -2.433731
  C   -2.082947   -1.767578   -3.295685
  H   -1.785095   -1.530884   -4.337738
```

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  H   -1.776459   -4.468658   -3.564453
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  C    4.700592   -0.913116   -1.396759
  C    5.588959    0.392288   -3.317734
  C    5.719360   -0.892578   -2.520370
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  H    0.346725   -1.093246    4.684433
  H    1.482224   -1.865891    3.562134
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  H    2.523193    0.221863    4.311386
  C    2.137024    0.512894    2.174850
  O    3.137558   -0.132034    1.734955
  O    1.545059    1.252213    1.341461
  O    0.970978    1.412430    4.140945
  H    0.199997    1.541031    3.600067
```

[(*R*)-**1** + (*R*,*R*)-**2** + $2H^+$] complex.

HF/6-31G* Energy = -1862.6229680 hartrees

```
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  H   -1.230576    4.478119    0.493378
  C   -0.589279    4.102448   -0.312576
  C    1.040039    3.092285   -2.304214
  C   -0.536331    2.734634   -0.593842
  C    0.206207    4.972076   -1.052734
  C    1.033630    4.469559   -2.050522
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H	-0.610809	1.481583	1.131241
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N	1.992157	-0.770798	-0.928680

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  O    2.838104   -1.070190    2.097214
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  H    0.643066    0.774948    3.775223
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  O    1.888748   -0.416900    4.738983
  H    2.463272   -1.152023    4.560425
```

[(*S*)-**1** + (*R*,*R*)-**2**] complex.

HF/6-31G* Energy = -1861.4282172 hartrees

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  H   -2.017500    3.991000    2.379500
  C   -2.270500    2.968000    2.085500
  C   -2.860500    0.408000    1.264500
  C   -1.276500    2.133000    1.544500
  C   -3.572500    2.501000    2.203500
  C   -3.884500    1.214000    1.778500
  N   -1.588500    0.860000    1.182500
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  N   -2.229500   -1.603000   -0.182500
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  C    1.777500    1.627000    2.777500
  C    2.996500    0.128000    4.411500
  C    3.569500    2.554000    4.305500
  C    4.110500    1.153000    4.533500
  C    2.912500    2.652000    2.940500
  C    2.327500    0.196000    3.028500
  H    2.246500    0.294000    5.210500
  H    2.842500    2.812000    5.102500
  H    4.909500    0.934000    3.797500
  H    3.669500    2.506000    2.138500
  H    3.094500   -0.033000    2.242500
  H    0.982500    1.847000    3.534500
  H    3.404500   -0.888000    4.589500
  H    4.385500    3.297000    4.391500
  H    4.588500    1.082000    5.530500
  H    2.513500    3.675000    2.790500
  N    1.217500   -0.814000    3.001500
  H    0.520500   -0.530000    2.339500
```

```
  C    1.658500   -2.197000    2.712500
  H    0.836500   -2.857000    3.058500
  H    2.538500   -2.426000    3.349500
  C    1.977500   -2.549000    1.282500
  C    2.543500   -3.140000   -1.345500
  C    2.790500   -3.653000    0.989500
  N    1.456500   -1.784000    0.298500
  C    1.749500   -2.030000   -1.006500
  C    3.057500   -3.950000   -0.342500
  H    3.210500   -4.260000    1.794500
  H    3.683500   -4.810000   -0.596500
  H    2.774500   -3.342000   -2.395500
  C   -2.426500   -1.130000   -1.593500
  C   -1.402500   -0.972000   -3.897500
  C   -3.813500   -1.558000   -3.657500
  C   -2.552500   -1.777000   -4.475500
  C   -3.578500   -1.943000   -2.207500
  C   -1.132500   -1.336000   -2.428500
  H   -1.617500    0.116000   -3.982500
  H   -4.123500   -0.496000   -3.722500
  H   -2.296500   -2.856000   -4.493500
  H   -3.362500   -3.029000   -2.139500
  H   -0.835500   -2.414000   -2.375500
  H   -2.695500   -0.042000   -1.616500
  H   -0.487500   -1.143000   -4.498500
  H   -4.652500   -2.146000   -4.078500
  H   -2.727500   -1.492000   -5.530500
  H   -4.509500   -1.785000   -1.625500
  C    1.316500   -1.048000   -2.052500
  H    1.436500   -1.503000   -3.060500
  H    2.087500   -0.195000   -1.987500
  N   -0.041500   -0.511000   -1.835500
  N    1.171500    1.674000    1.416500
  H    1.884500    1.805000    0.693500
  C    3.131500    1.970000   -1.557500
  O    3.544500    0.779000   -1.646500
  O    3.106500    2.545000   -0.436500
  H   -0.106500    0.467000   -2.133500
  C    2.730500    2.688000   -2.861500
  H    3.637500    3.191000   -3.249500
  H    2.453500    1.925000   -3.616500
  C    1.582500    3.699000   -2.780500
  H    1.452500    4.176000   -3.780500
  C    0.222500    3.042000   -2.381500
  O   -0.202500    2.052000   -3.035500
  O   -0.466500    3.541000   -1.452500
  O    1.920500    4.810000   -1.978500
  H    1.899500    4.486000   -1.083500
```

[(*R*)-**1** + (*R*,*R*)-**2**] complex.

HF/6-31G* Energy = -1861.4222224 hartrees

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83
  H   -2.005500    4.183000    2.433500
  C   -2.258500    3.165000    2.122500
  C   -2.852500    0.618000    1.265500
  C   -1.272500    2.347000    1.541500
  C   -3.554500    2.687000    2.261500
```

C	-3.868500	1.407000	1.818500
N	-1.586500	1.080000	1.159500
H	-4.329500	3.320000	2.702500
H	-4.889500	1.024000	1.891500
C	0.087500	2.895000	1.232500
H	0.258500	3.821000	1.823500
H	0.031500	3.218000	0.130500
C	-3.149500	-0.779000	0.785500
H	-4.175500	-0.808000	0.361500
H	-3.150500	-1.455000	1.663500
N	-2.219500	-1.387000	-0.192500
H	-1.271500	-1.217000	0.084500
C	1.767500	1.858000	2.762500
C	2.971500	0.350000	4.399500
C	3.544500	2.776000	4.312500
C	4.084500	1.374000	4.537500
C	2.901500	2.881000	2.941500
C	2.313500	0.425000	3.012500
H	2.215500	0.511000	5.194500
H	2.810500	3.029000	5.103500
H	4.889500	1.159000	3.806500
H	3.666500	2.739000	2.146500
H	3.085500	0.197000	2.230500
H	0.964500	2.076000	3.511500
H	3.377500	-0.668000	4.573500
H	4.360500	3.519000	4.410500
H	4.553500	1.297000	5.537500
H	2.504500	3.905000	2.792500
N	1.200500	-0.581000	2.975500
H	0.514500	-0.300000	2.300500
C	1.640500	-1.968000	2.703500
H	0.822500	-2.623000	3.065500
H	2.525500	-2.186000	3.339500
C	1.951500	-2.343000	1.278500
C	2.499500	-2.981000	-1.342500
C	2.740500	-3.467000	0.998500
N	1.445500	-1.580000	0.284500
C	1.730500	-1.850000	-1.017500
C	2.999500	-3.788000	-0.328500
H	3.149500	-4.073000	1.811500
H	3.606500	-4.664000	-0.572500
H	2.724500	-3.203000	-2.390500
C	-2.422500	-0.932000	-1.607500
C	-1.411500	-0.814000	-3.920500
C	-3.824500	-1.384000	-3.657500
C	-2.568500	-1.623000	-4.478500
C	-3.583500	-1.747000	-2.202500
C	-1.134500	-1.155000	-2.447500
H	-1.622500	0.273000	-4.022500
H	-4.128500	-0.321000	-3.737500
H	-2.318500	-2.703000	-4.479500
H	-3.373500	-2.833000	-2.119500
H	-0.840500	-2.233000	-2.377500
H	-2.686500	0.158000	-1.643500
H	-0.500500	-1.000000	-4.523500
H	-4.668500	-1.974000	-4.064500
H	-2.748500	-1.355000	-5.537500
H	-4.509500	-1.574000	-1.617500
C	1.316500	-0.872000	-2.074500
H	1.441500	-1.335000	-3.078500
H	2.096500	-0.027000	-2.005500

N	-0.039500	-0.322000	-1.874500
N	1.176500	1.912000	1.394500
H	1.898500	2.053000	0.681500
C	3.153500	2.121000	-1.532500
O	3.556500	0.925000	-1.622500
O	3.188500	2.719000	-0.425500
H	-0.099500	0.649000	-2.196500
C	2.689500	2.815000	-2.826500
H	3.578500	3.305000	-3.272500
H	2.371500	2.043000	-3.557500
C	1.568500	3.841000	-2.654500
C	0.171500	3.190000	-2.383500
O	-0.228500	2.237000	-3.106500
O	-0.561500	3.676000	-1.485500
H	1.827500	4.570000	-1.854500
O	1.490500	4.664000	-3.813500
H	1.067500	4.128000	-4.473500