Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Quantification of the P=O···HN hydrogen bond in the binding of creatinine with phosphonate calix[4]pyrroles.

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Contents

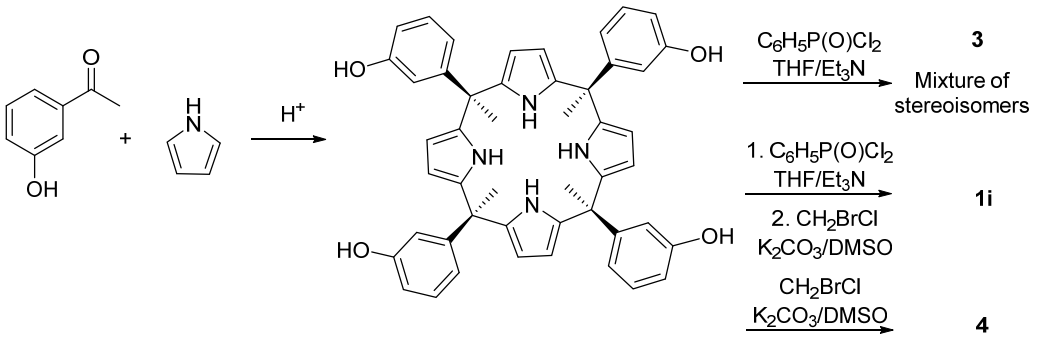
General methods and instrumentation

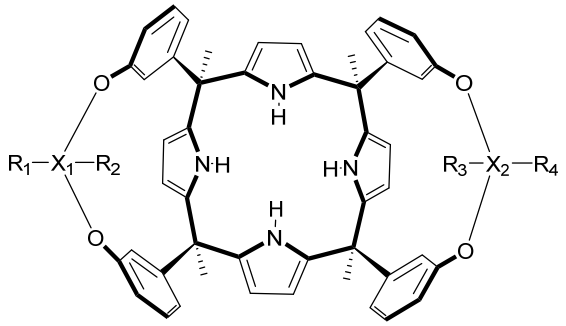
Reagents and solvents used in the synthesis were obtained from commercial suppliers and were used without further purification unless otherwise stated. Pyrrole was distilled under vacuum and freshly used. THF and triethylamine (Et_3N) were dried and distilled from sodium and CaH_2, respectively, under argon atmosphere and freshly used. Flash column chromatography was performed with silica gel, technical grade, pore size 60 Å, and 230–400 mesh particle size. Automatic column chromatography purifications were done with a Combi-flash® RF+ Routine. ^1H, ^{31}P and ^{13}C NMR spectra were recorded on a Bruker Avance 400 (400 MHz for ^1H-NMR), Bruker Avance 500 (500 MHz for ^1H-NMR) ultra-shield spectrometer. Deuterated solvents were purchased from Aldrich.

Crystal structure determination was carried out using a Rigaku MicroMax-007HF diffractometer equipped with a PILATUS 200K detector and a Bruker Apex II Duo equipped with an APEX II detector, both using Mo Kα radiation. Crystal structure solution was achieved using VLD and Patterson methods as implemented in SIR2014 v14.10. Least-squares refinement on F2 using all measured intensities was carried out using the program SHELX-2018/3.

Synthesis and characterization data

Cavitands were synthesized by following the published protocols.[1,2] Hexylcreatinine (**2b**) was also prepared using a known protocol.[3]





	R_1	R_2	R_3	R_4	X_1	X_2
3ii	Ph	=O	=O	Ph	P	P
3io	Ph	=O	Ph	=O	P	P
3oo	=O	Ph	Ph	=O	P	P
1i	Ph	=O	H	H	C	C
4	H	H	H	H	C	C

Scheme S1 Reaction scheme for the preparation of the receptors **1i**, **3** and **4**.

^{1}H and ^{31}P NMR titration experiments.

We prepared a stock solution for each receptor (~ 2.0 mM) in CD_2Cl_2. A stock solution of **2b** (~ 12 mM) was prepared in methanol (HPLC grade) due to solubility issues. We placed different amounts of the solution of **2b** in small vials using high-precision Hamilton Glass microsyringes (33 µL for 0.5 equiv., 66 µL for 1 equiv., and 170 µL for 2.5 equiv.). The methanol was removed under reduced pressure and the residual solid was re-dissolved in 0.4 mL of the stock solution of each receptor. We sonicated the solution for five minutes and transferred it to an NMR tube to acquire the corresponding spectra.

3ii vs **2b**

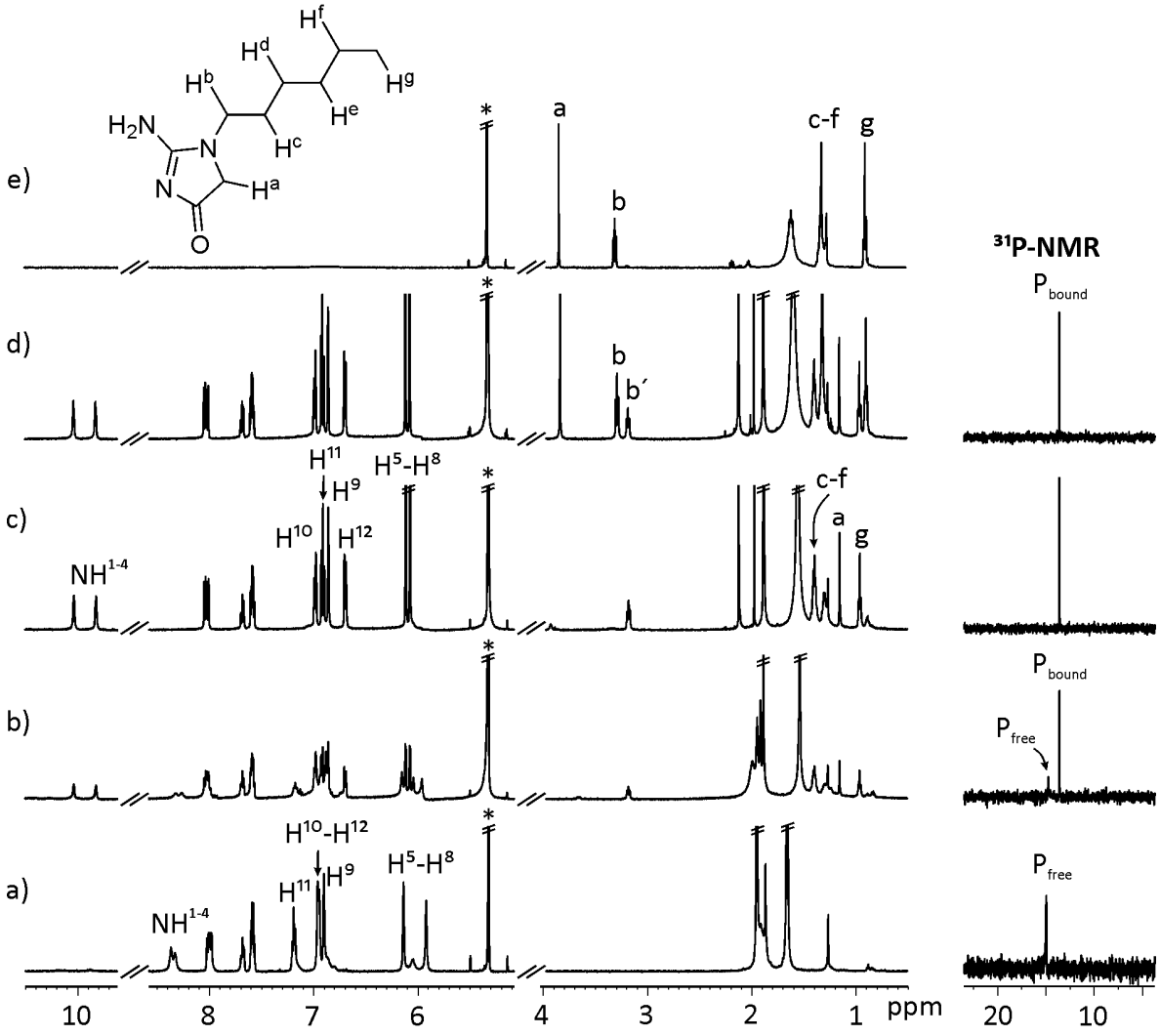


Figure S1 Selected regions of the ^{1}H NMR spectra (500 MHz, 298 K) (left panel) and the corresponding ^{31}P NMR spectra (202 MHz, 298 K) (right panel) of CD_2Cl_2 solutions containing receptor **3ii** and **2b** in different molar ratios: a) Free **3ii**; b) **3ii** + 0.5 equiv. of **2b**; c) **3ii** + 1.0 equiv. of **2b**; d) **3ii** + 2.5 equiv. of **2b**. Trace e) shows the same regions of the ^{1}H NMR spectrum of **2b**. * Residual solvent peak

3io vs **2b**

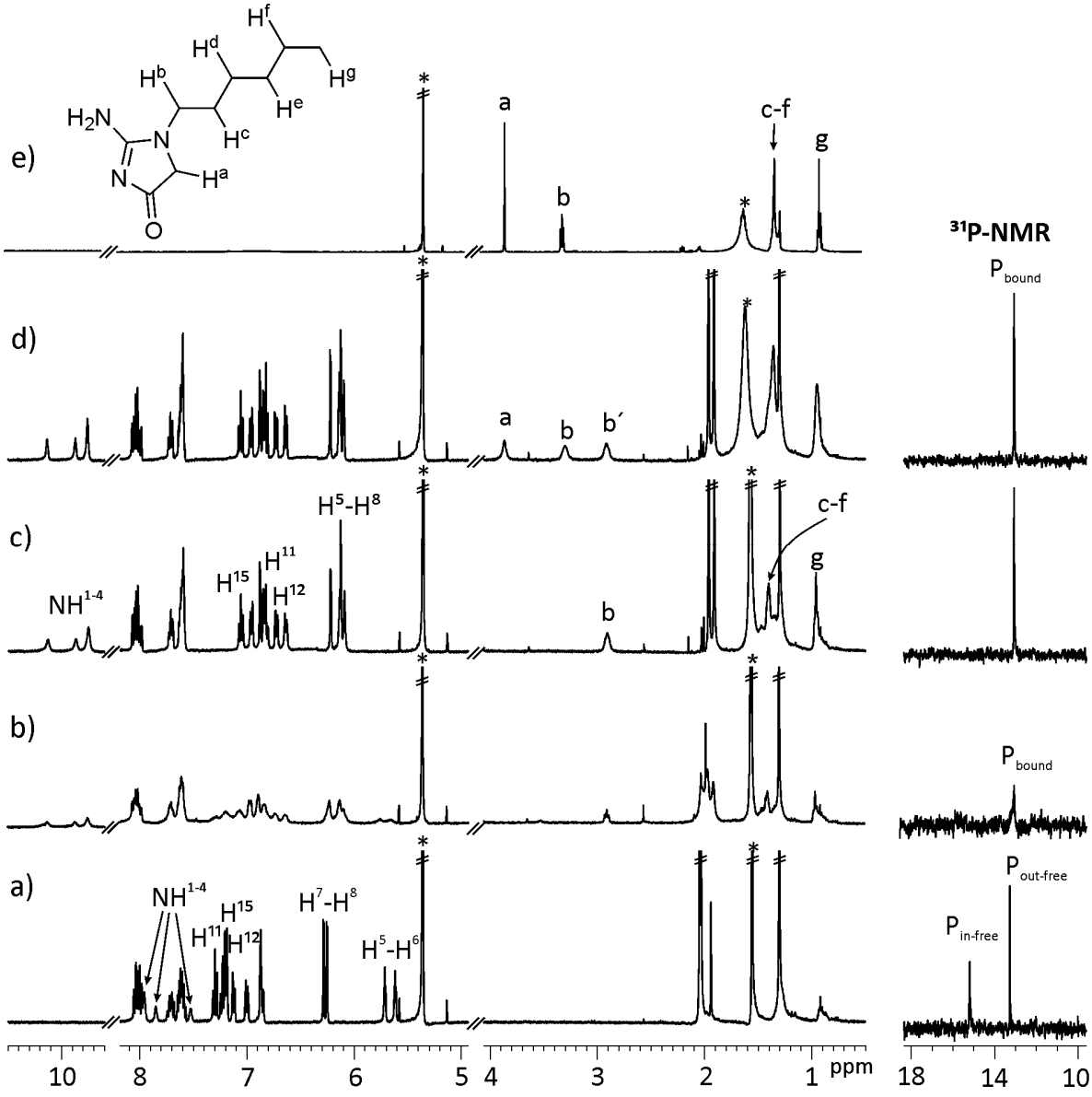


Figure S2 Selected regions of the ^{1}H NMR spectra (500 MHz, 298 K) (left panel) and the corresponding ^{31}P NMR spectra (202 MHz, 298 K) (right panel) of CD_2Cl_2 solutions containing receptor **3io** and **2b** in different molar ratios: a) Free **3io**; b) **3io** + 0.5 equiv. of **2b**; c) **3io** + 1.0 equiv. of **2b**; d) **3io** + 2.5 equiv. of **2b**. Trace e) shows the same regions of the ^{1}H NMR spectrum of **2b**. * Residual solvent peak

3oo vs **2b**

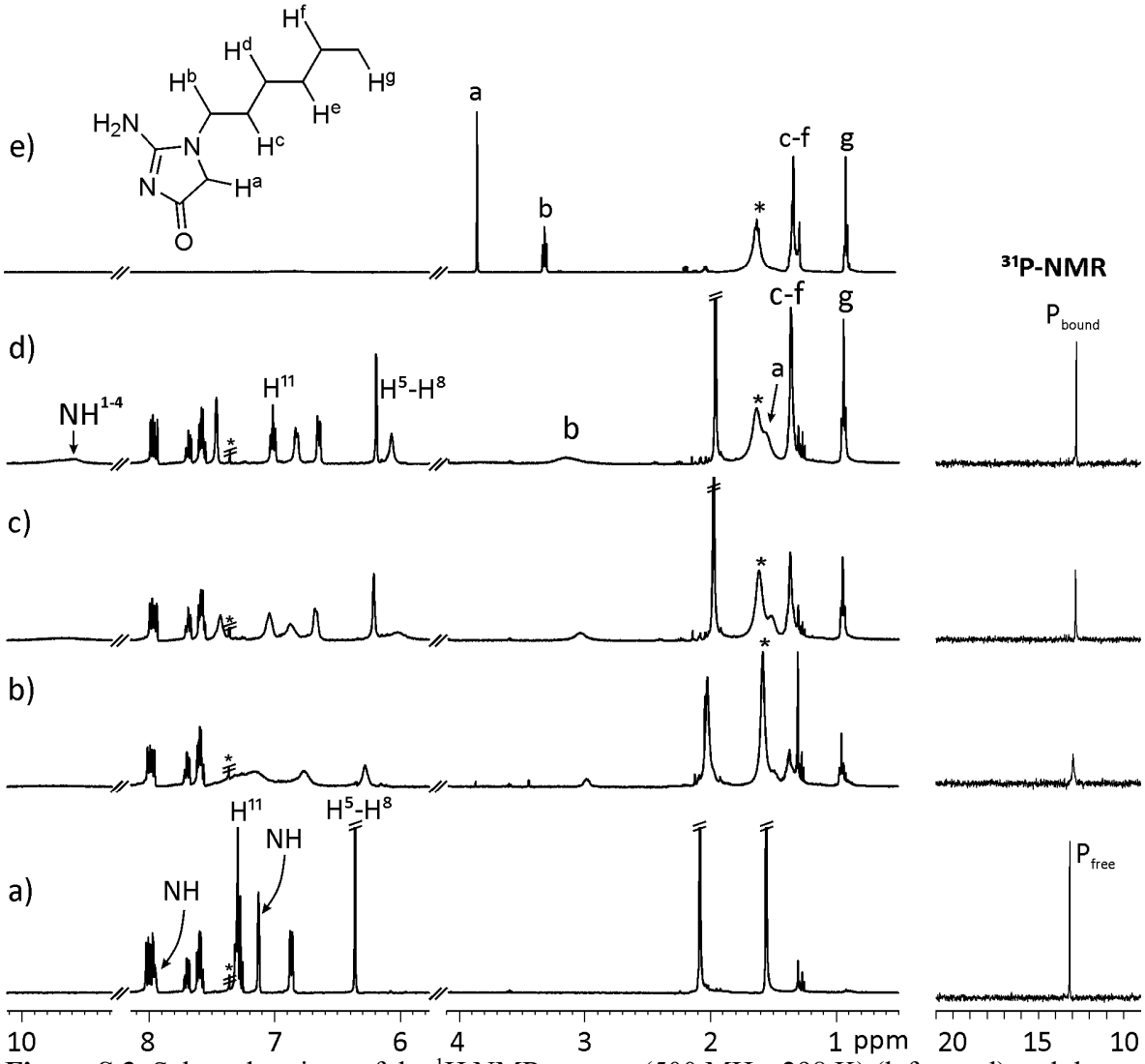


Figure S 3. Selected regions of the ^{1}H NMR spectra (500 MHz, 298 K) (left panel) and the corresponding ^{31}P NMR spectra (202 MHz, 298 K) (right panel) of CD_2Cl_2 solutions containing receptor **3oo** and **2b** in different molar ratios: a) Free **3oo**; b) **3oo** + 0.5 equiv. of **2b**; c) **3oo** + 1.0 equiv. of **2b**; d) **3oo** + 2.5 equiv. of **2b**. Trace e) shows the same regions of the ^{1}H NMR spectrum of **2b**. * Residual solvent peak.

1i vs **2b**

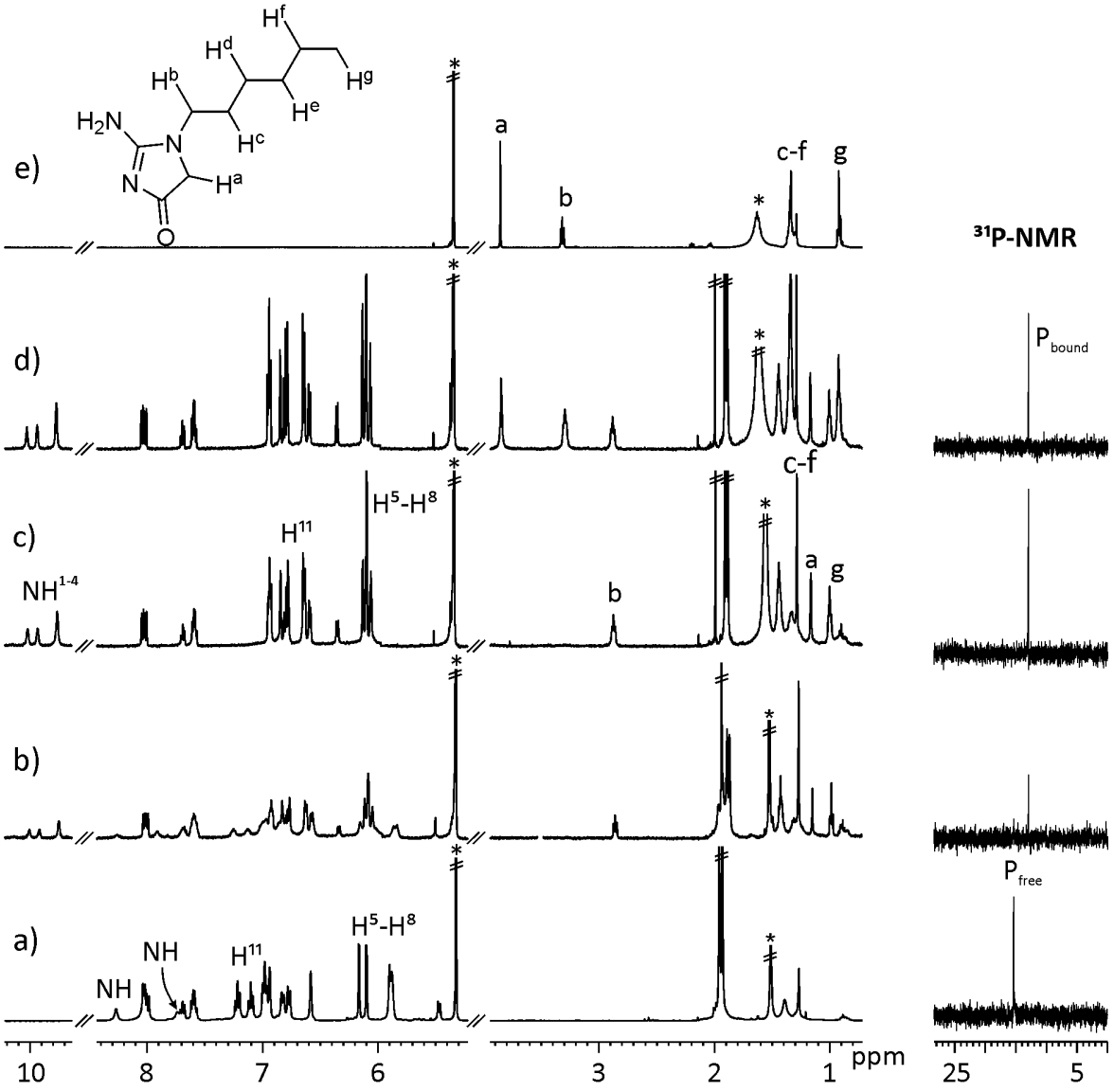


Figure S4 *S*elected regions of the ^{1}H NMR spectra (500 MHz, 298 K) (left panel) and the corresponding ^{31}P NMR spectra (202 MHz, 298 K) (right panel) of CD_2Cl_2 solutions containing receptor **1i** and **2b** in different molar ratios: a) Free **1i**; b) **1i** + 0.5 equiv. of **2b**; c) **1i** + 1.0 equiv. of **2b**; d) **1i** + 2.5 equiv. of **2b**. Trace e) shows the same regions of the ^{1}H NMR spectrum of **2b**. * Residual solvent peak.

4 vs **2b**

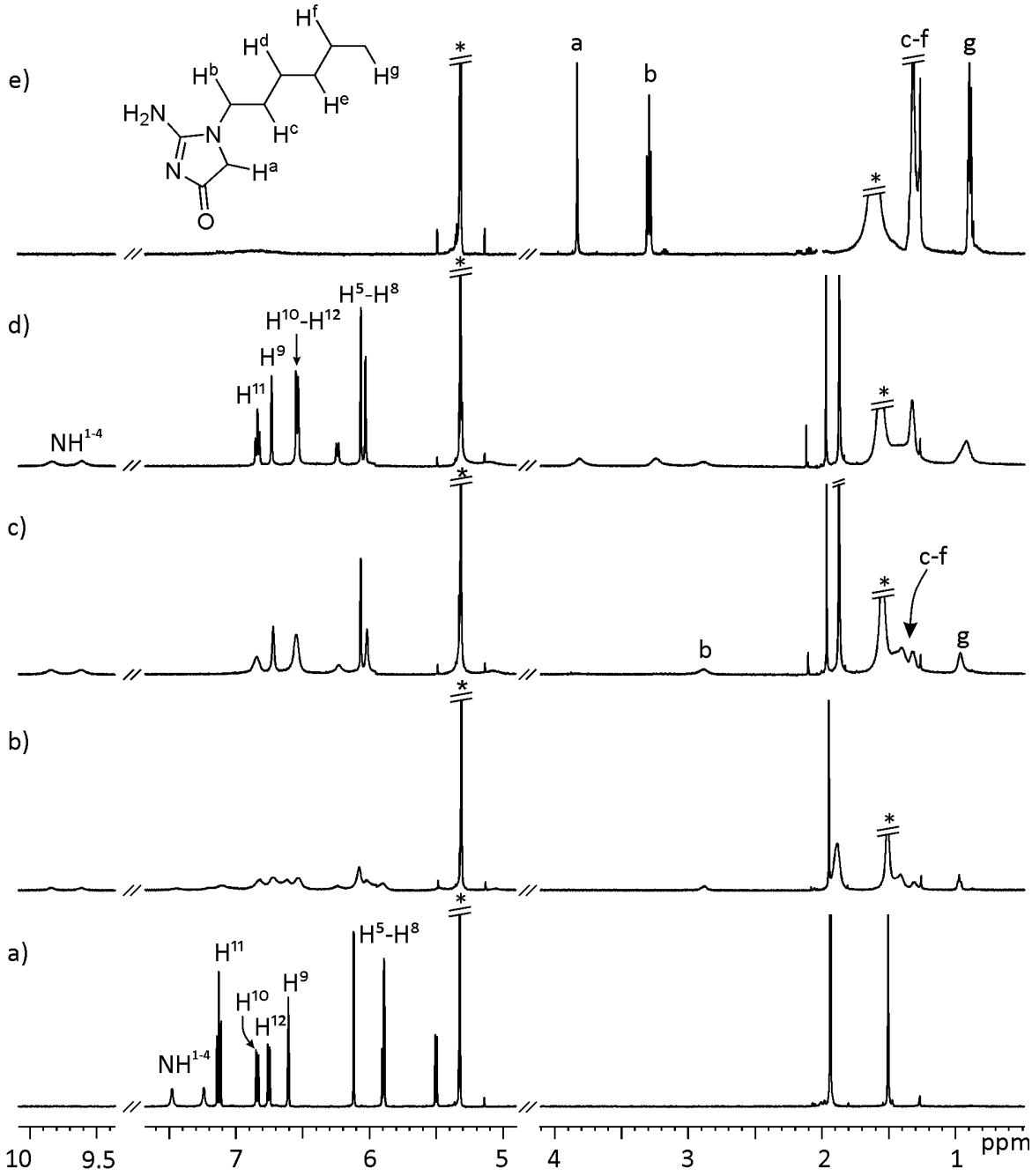


Figure S5 Selected regions of the ^{1}H NMR spectra (500 MHz, 298 K) of CD_2Cl_2 solutions containing receptor **4** and **2b** in different molar ratios: a) Free **4**; b) **4** + 0.5 equiv. of **2b**; c) **4** + 1.0 equiv. of **2b**; d) **4** + 2.5 equiv. of **2b**. Trace e) shows the same regions of the ^{1}H NMR spectrum of **2b**. * Residual solvent peak.

ITC Experiments

ITC experiments were performed in a MicroCal VP-ITC Micro Calorimeter with the VP Viewer 2000 software. Due to the low solubility of the hexyl creatinine **2b** in methylene chloride, reverse ITC experiments were performed. The concentration of the solution in the syringe was approximately seven to ten times more concentrated than the cell solution. The association constants and the thermodynamic parameters were obtained from the fit of the titration data to the "one set of sites" binding model implemented in the Microcal ITC Data Analysis module. The enthalpy of binding for each injection is plotted against the molar ratio of guest/host in the cell. The continuous line represents the least-squares-fit of the data to a single-site binding model.

3ii vs **2b**

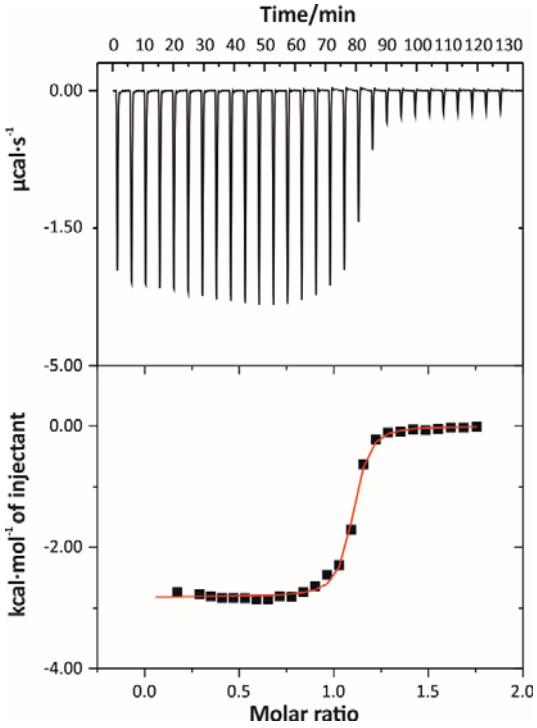


Figure S6 Top) Raw data (heat *vs.* time) for the titration of **2b** with **3ii** in CH_2Cl_2. The titration was performed at 288 K. Bottom) Integrated data fitted to a theoretical binding isotherm (red line) for a 1:1 binding model. [**2ii**] = 3.4 mM over [**2b**] = 0.4 mM.

3io vs **2b**

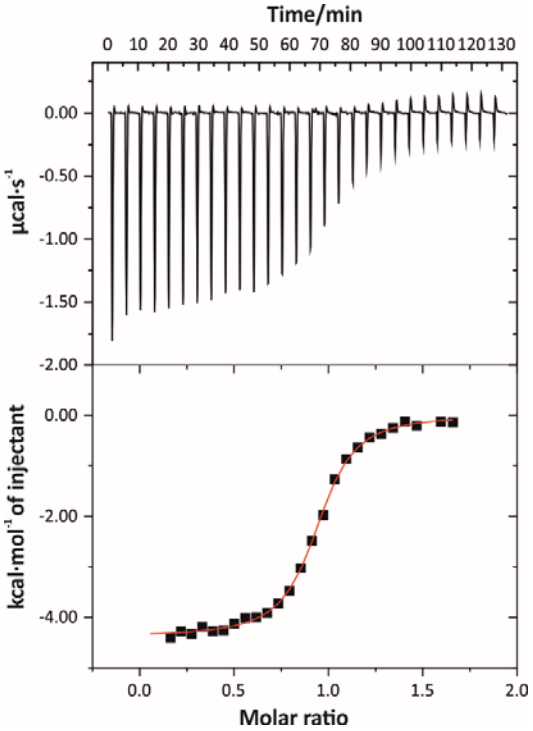


Figure S7 Top) Raw data (heat *vs.* time) for the titration of **2b** with **3io** in CH_2Cl_2. The titration was performed at 288 K. Bottom) Integrated data fitted to a theoretical binding isotherm (red line) for a 1:1 binding model. [**2io**] = 0.9 mM over [**2b**] = 0.1 mM.

3oo vs **2b**

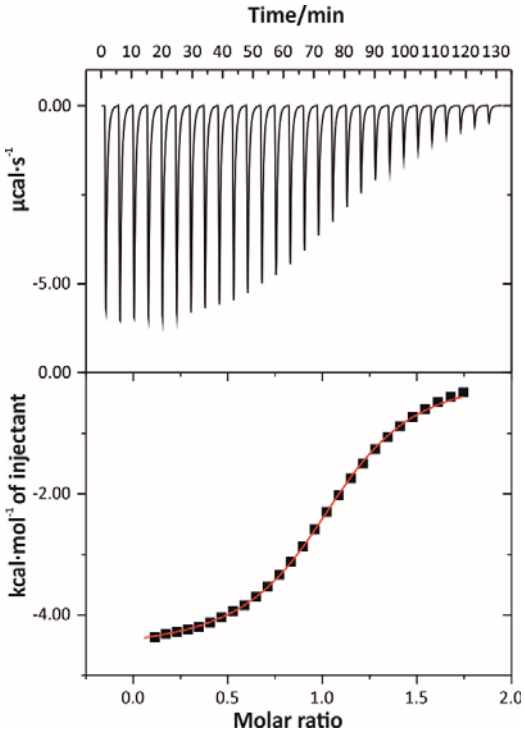


Figure S8 Top) Raw data (heat vs. time) for the titration of **2b** with **3oo** in CH_2Cl_2. The titration was performed at 288 K. Bottom) Integrated data fitted to a theoretical binding isotherm (red line) for a 1:1 binding model. [**2oo**] = 6.5 mM over [**2b**] = 0.8 mM.

1i vs **2b**

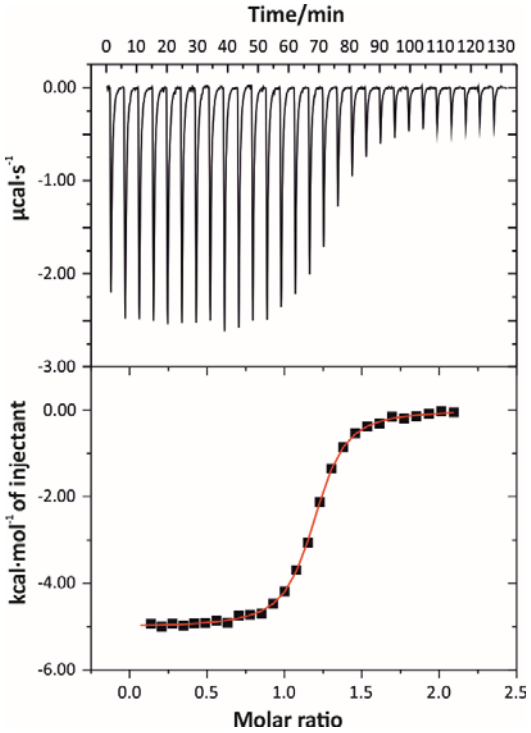


Figure S9 Top) Raw data (heat *vs*. time) for the titration of **2b** with **1i** in CH_2Cl_2. The titration was performed at 288 K. Bottom) Integrated data fitted to a theoretical binding isotherm (red line) for a 1:1 binding model. [**1i**] = 2 mM over [**2b**] = 0.2 mM.

4 vs **2b**

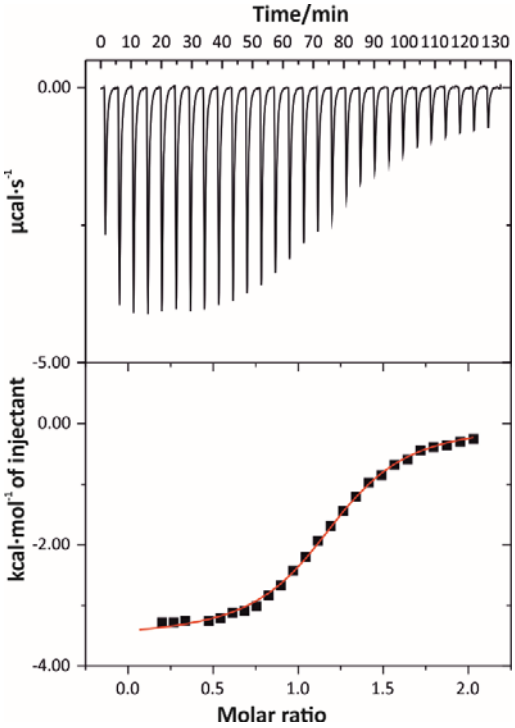


Figure S10 Top) Raw data (heat *vs.* time) for the titration of **2b** with **4** in CH_2Cl_2. The titration was performed at 288 K. Bottom) Integrated data fitted to a theoretical binding isotherm (red line) for a 1:1 binding model. [**4**] = 5.0 mM over [**2b**] = 0.5 mM.

Estimation of hydrogen bond interaction energy

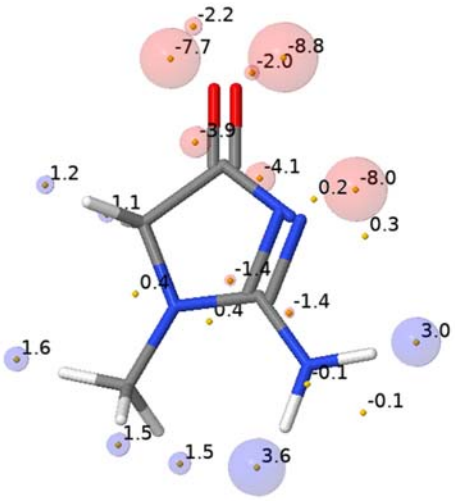


Figure S 11. Surface Site Interaction Point (SSIP) molecular descriptor of creatinine. Blue is used for positive SSIPs and red for negative SSIPs; the size of each sphere represents its magnitude. Image provided by Prof. Christopher A. Hunter, University of Cambridge.

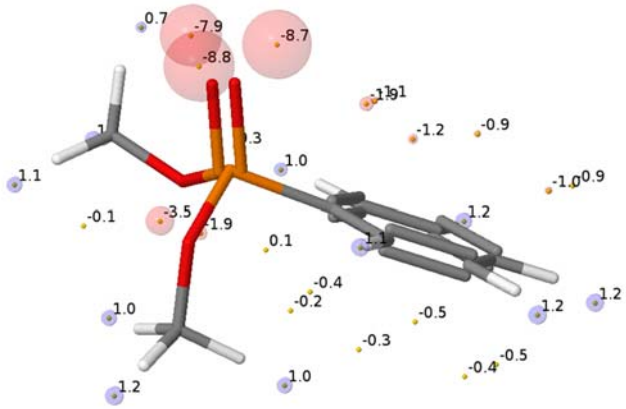


Figure S 12. Surface Site Interaction Point (SSIP) molecular descriptor of dimethylphenylphosphonate. Blue is used for positive SSIPs and red for negative SSIPs; the size of each sphere represents its magnitude. Image provided by Prof. Christopher A. Hunter, University of Cambridge.

Computed energy minimized structures

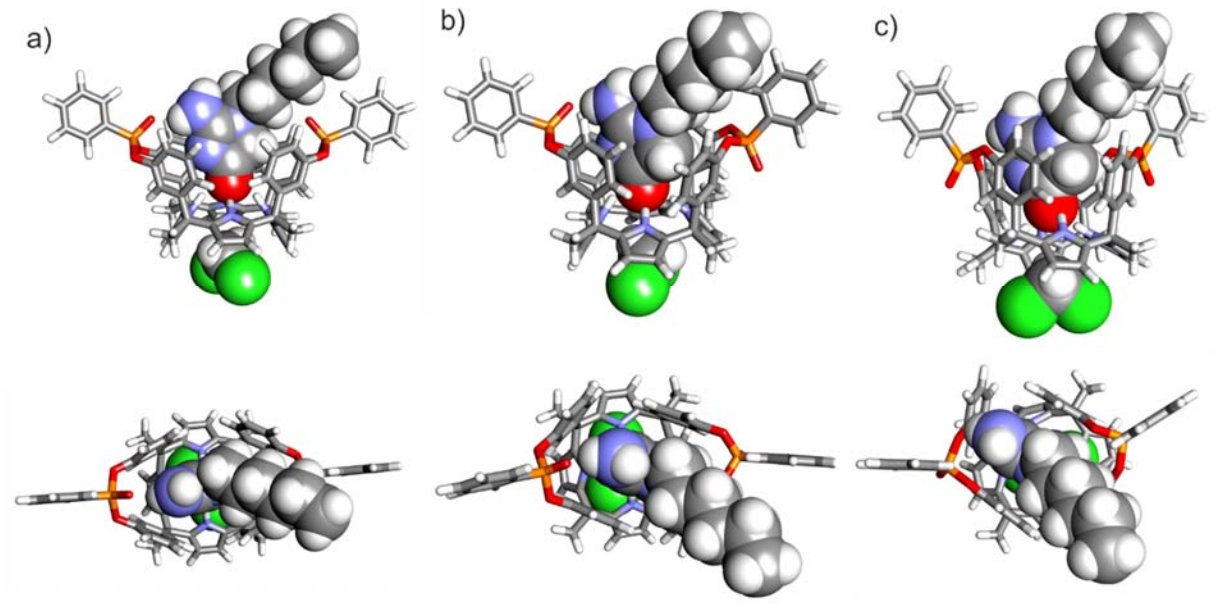


Figure S 13. Side and top views of the energy minimized structures of the **2b⊂3ii** (a), **2b⊂3io** (b) and **2b⊂3oo** (c) inclusion complexes at the RI-BP86-D3BJ-def2-SVP level of theory (solvent COSMO model as implemented in Turbomole version 7.0).

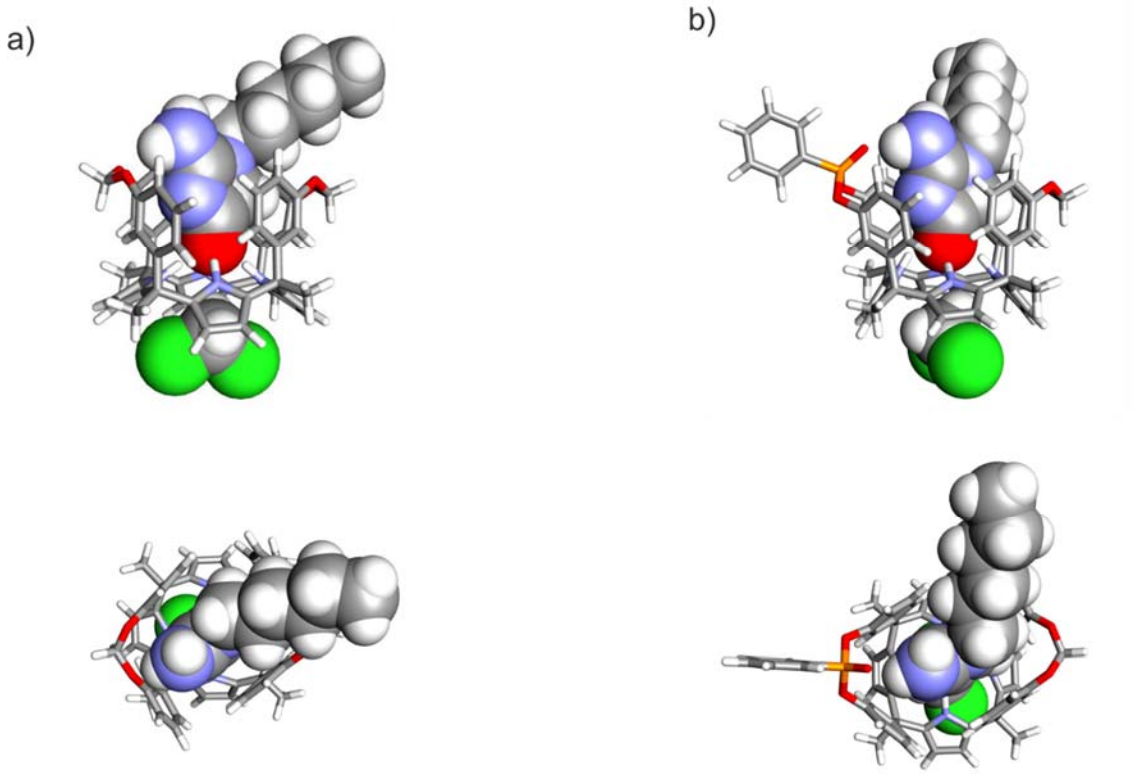


Figure S 14. Side and top views of the energy minimized structures of the **2b⊂4** (a) and **2b⊂1i** (b) inclusion complexes at the RI-BP86-D3BJ-def2-SVP level of theory (solvent COSMO model as implemented in Turbomole version 7.0).

Cartesian coordinates of the full optimized structures for the free receptors and the corresponding inclusion complexes with 2b

3ii

Energy = -4627.478111018

C	-4.2653467	0.4784972	3.4474994
C	-4.8779800	-0.3757123	2.4757939
C	-2.9036440	0.5458675	3.1579203
C	-3.8806061	-0.8175956	1.6065147
N	-2.6973358	-0.2228074	2.0186590
C	-1.7741974	1.2565538	3.8874740
C	-1.4150940	2.5737392	3.2180474
C	-3.9765383	-1.7138618	0.3815237
C	-4.0381073	-0.8725686	-0.8813895
C	-0.5212738	3.8767046	1.5687379
N	-2.9560865	-0.1215430	-1.3104247
C	-3.2042698	0.4300002	-2.5563762
C	-5.0205733	-0.7679740	-1.8649426
C	-4.4968922	0.0512214	-2.9172298
C	-2.1727601	1.2705614	-3.2858219
H	-4.7690673	0.9831391	4.2786219
H	-5.9395075	-0.6386942	2.4214546
C	-2.2080726	1.5327939	5.3472121
C	-5.2664849	-2.5643037	0.4860197
H	-6.0070784	-1.2418772	-1.8395077
H	-5.0128794	0.3285164	-3.8421215
C	-0.8651029	0.4816423	-3.5247832
C	-2.7338218	1.6565542	-4.6762145
C	0.0782623	4.1766004	0.2061250
C	-0.9078118	3.8372752	-0.8996460
N	-0.9902355	2.5618886	-1.4409386
C	-1.8976158	2.5344939	-2.4883378
C	-1.8294584	4.6287561	-1.5820244
C	-2.4509409	3.8106492	-2.5804871
C	1.3802477	3.3656729	-0.0150636
C	0.4321298	5.6815764	0.1365803
H	-2.0287317	5.6886795	-1.3904395
H	-3.2192090	4.1254946	-3.2946429
N	-1.0633705	2.6412787	1.8800269
C	-1.1105295	3.8164060	3.7746667
C	-0.5494620	4.6335237	2.7400332
H	-1.2410045	4.0969809	4.8247754
H	-0.1849324	5.6601642	2.8475349
C	-0.5083673	0.3616418	3.9334548

C	0.7794782	0.9311493	3.9126413
C	-0.6235895	-1.0381811	4.0363654
C	1.9258247	0.1229421	3.9405649
C	0.5296571	-1.8333849	4.0611655
C	1.8138064	-1.2733562	3.9972111
H	0.8806938	2.0247113	3.8776050
H	-1.6069364	-1.5243018	4.0993441
H	2.9234188	0.5867067	3.9176673
H	2.6996403	-1.9224098	4.0010763
C	-2.7952308	-2.7065488	0.2738980
C	-2.3856539	-3.1727961	-0.9933128
C	-2.1872890	-3.2521398	1.4215831
C	-1.3784997	-4.1416932	-1.1173633
C	-1.1889624	-4.2288363	1.2831226
C	-0.7615077	-4.6744976	0.0243464
C	0.3106274	1.1764913	-3.8747036
C	-0.8376141	-0.9269796	-3.5131202
C	1.4739060	0.4686255	-4.2042635
C	0.3394871	-1.6252020	-3.8325541
C	1.5094260	-0.9342464	-4.1788178
C	1.9530203	3.3262101	-1.3035312
C	2.0264852	2.6809967	1.0291711
H	-2.8833025	-2.7832991	-1.8926035
H	-2.5032404	-2.9467076	2.4287379
O	-0.6344707	-4.8062255	2.4302962
H	0.0339449	-5.4286541	-0.0472119
H	0.3252291	2.2746506	-3.9186514
H	-1.7539848	-1.4812688	-3.2717558
H	0.3457221	-2.7253630	-3.8162862
H	2.4410948	-1.4612510	-4.4227347
C	3.2044641	1.9548463	0.7911986
C	3.1333816	2.6063246	-1.5252176
C	3.7721899	1.9073851	-0.4880877
H	1.4866583	3.8521496	-2.1489698
H	1.5928085	2.7010792	2.0353249
H	3.6801190	1.4028157	1.6147872
H	4.6829107	1.3316645	-0.6969195
H	-1.3742157	1.9881800	5.9137578
H	-2.4908466	0.5852901	5.8431151
H	-3.0715323	2.2250243	5.3796816
H	-5.2441883	-3.1714443	1.4103684
H	-5.3471459	-3.2434601	-0.3833893
H	-6.1655090	-1.9191728	0.5089734
H	-2.0069055	2.2921130	-5.2156844
H	-3.6848614	2.2146193	-4.5799124
H	-2.9212677	0.7455317	-5.2757508

H	0.8370285	5.9332947	-0.8613875
H	1.1957593	5.9289355	0.8979751
H	-0.4623687	6.3066743	0.3231371
O	2.5872029	1.1936108	-4.6307321
O	3.6906858	2.6589624	-2.8033737
O	0.3715241	-3.2155808	4.1957900
H	-1.0726950	-4.4908151	-2.1148483
H	-1.7706156	-0.5005350	1.6778609
H	-2.0503263	-0.0867610	-0.8339773
H	-0.3005090	1.8250300	-1.2603285
H	-1.2557994	1.9105324	1.1937883
P	3.9825776	1.3399311	-3.7544948
P	0.8189986	-4.2751219	3.0121877
O	1.7374676	-3.7080231	1.9625464
O	4.4343450	0.0973265	-3.0400714
C	1.3966945	-5.6885701	3.9474751
C	5.0887809	2.0455969	-4.9778586
C	0.6573655	-6.2085642	5.0319380
C	2.6275663	-6.2640846	3.5717986
C	4.7678930	3.2341267	-5.6682749
C	6.3055999	1.3781190	-5.2225544
H	1.1794675	-2.3330181	0.5392024
C	0.9991400	-1.6400030	-0.3062801
Cl	0.1596578	-0.1719135	0.3986557
H	0.3120269	-2.0423745	-1.0698483
Cl	2.5285488	-1.1871944	-1.0613205
C	1.1588320	-7.3122359	5.7364403
C	3.1190034	-7.3688770	4.2846946
C	2.3863016	-7.8913048	5.3640332
C	7.2050590	1.9021671	-6.1643502
C	5.6732755	3.7487038	-6.6072232
C	6.8890053	3.0843055	-6.8552007
H	-0.2994901	-5.7533009	5.3265355
H	3.1922960	-5.8412128	2.7278287
H	3.8193881	3.7547758	-5.4707586
H	6.5394094	0.4545495	-4.6720639
H	0.5898801	-7.7220674	6.5841898
H	4.0797118	-7.8207380	3.9963211
H	2.7750113	-8.7561763	5.9226363
H	8.1568488	1.3850629	-6.3575149
H	5.4304624	4.6752514	-7.1487796
H	7.5954986	3.4934926	-7.5932391

2b⊂3ii

Energy = -5219.915754727

C	-4.4273773	0.5733974	3.9944298
C	-5.2196798	-0.1739220	3.0636200
C	-3.1061565	0.5426950	3.5423499
C	-4.3655282	-0.6415198	2.0609358
N	-3.0981131	-0.1848864	2.3682643
C	-1.8293903	1.1195311	4.1395636
C	-1.5417221	2.4905205	3.5573715
C	-4.6223302	-1.5371522	0.8597026
C	-4.6779944	-0.7350217	-0.4271058
C	-1.0680386	4.0231865	1.9482803
N	-3.6291257	0.0680550	-0.8368790
C	-3.8752642	0.5801587	-2.0982835
C	-5.6320933	-0.7189198	-1.4449880
C	-5.1268599	0.1083428	-2.4968094
C	-2.8925450	1.4875846	-2.8164616
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H	-6.5922522	-1.2448298	-1.4347316
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C	-0.6706185	4.5243760	0.5728076
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C	-3.2260160	4.0449221	-2.1720572
C	0.7346140	3.9917357	0.1984520
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H	-2.8040930	5.9633834	-1.0545115
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C	-1.1633587	4.7033947	3.1624219
H	-1.6158717	3.9411626	5.2401546
H	-1.0377670	5.7812165	3.3064388
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C	1.6610119	-0.3969689	3.3533925

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H	-1.8378723	-1.5805969	4.5912047
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C	-3.0250645	-3.1984985	1.9581971
C	-2.0425722	-4.0794569	-0.5112874
C	-2.0611598	-4.2079250	1.8915171
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H	-1.2353706	1.9181235	1.5210962
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H	5.1582630	-2.8335186	-3.8643057
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H	7.5907551	-2.2385598	-3.6090535
H	6.3686894	-0.9222157	-6.1474073
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C	-1.8723794	-4.0915130	0.1656915
C	-2.8115230	-3.1534383	-0.5758793
C	2.4807979	-2.8362503	-2.0739376
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N	1.2951949	-0.7131426	-2.8852123
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C	1.9791853	-2.0481307	-4.5434627
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H	1.2622450	-0.6639952	-6.1796254
C	1.0175505	2.2804510	-3.0815110
C	0.5295749	1.9477413	-5.4961317
C	-3.7784084	0.3750095	-1.3168026
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C	-1.1456528	1.2022673	-3.8065363
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C	-2.2578481	1.5703653	-4.5626365
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H	-2.2353612	1.9949149	-5.5712478
N	-2.6395090	-1.7753500	-0.5538429
C	-3.9945664	-3.4000902	-1.2711640
C	-4.5552303	-2.1351772	-1.6413898
H	-4.4235181	-4.3865684	-1.4770685
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C	-1.5207978	-3.4632021	1.5422942
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C	0.2710595	3.3028327	-2.4640194
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H	4.4405764	-2.9896993	-3.0338466
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O	1.3454215	-3.1966804	3.8524311
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H	-0.2045401	-2.3901893	-1.3532459
H	1.3071871	-0.2674837	-1.9617106
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P	2.5062345	-2.0317066	3.9697237
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C	3.4121287	-2.5493444	5.4279332
C	3.6000870	-1.5988865	6.4521765
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C	4.2944524	-1.9646746	7.6163019
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H	3.2011216	-0.5808821	6.3309921
H	3.7652353	-4.6011022	4.7615130
H	4.4431004	-1.2263769	8.4182703
H	5.0003219	-5.2371317	6.8410128
H	5.3383506	-3.5556407	8.6684672
C	-1.4490337	6.9358647	0.1636313
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H	-3.0516629	7.5525947	-1.1713082
C	-2.5053789	9.1232994	0.2428720
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C	-1.6654329	9.4819995	1.3107445
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C	-0.7175800	8.5671978	1.8072014
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O	0.2395583	5.2565097	-0.9775382
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H	-0.5064748	1.0312163	1.9973647

2b⊂3io

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C	1.0666717	-5.2905087	-2.2878969
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C	-1.9462286	-4.7691551	-0.0548876
C	-3.0607425	-3.9294765	-0.6528228
C	2.3926584	-3.0034280	-1.9787245
C	2.0420838	-2.0469420	-3.1044310
C	-4.0803298	-1.9973724	-1.2837982
N	0.9873802	-1.1602223	-3.0017477
C	0.8870867	-0.3856538	-4.1433768
C	2.6211320	-1.8532026	-4.3586429
C	1.8937138	-0.8090720	-5.0131795
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H	-0.6198958	-6.7609469	-1.9595230
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H	2.0917706	-0.4045417	-6.0109370
C	0.3955494	1.8704473	-3.1799847
C	0.0932402	1.4656054	-5.6165252
C	-4.1935795	-0.5213851	-1.6218195
C	-3.3707139	-0.1781810	-2.8556810
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C	-1.5010661	0.4149609	-4.0154716
C	-3.7524167	0.0541349	-4.1765575
C	-2.5786395	0.4277076	-4.9053985
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H	-2.9164746	-2.3775590	3.9332830
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C	-0.5438409	2.7305829	-2.5793569
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C	1.2590079	3.8980141	-1.4031969
C	-3.6384710	1.7787266	-0.6872907
C	-3.4773836	-0.0986604	0.8407837
H	2.8336070	-0.2609026	-1.5377318
H	2.6413923	-4.0636143	0.5475376
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H	3.6265349	-0.4656577	2.7343528
H	-1.6116992	2.6339344	-2.8085417
H	2.4976341	1.3526633	-3.3471029
H	3.2641064	3.1689893	-1.7963238
H	1.5646098	4.6923839	-0.7089643
C	-3.1231104	0.7788589	1.8809581
C	-3.2922999	2.6444840	0.3609031
C	-3.0327535	2.1586707	1.6546210
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H	-3.5349436	-1.1749244	1.0394802
H	-2.9025490	0.3755123	2.8801905
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H	-1.6526138	-6.8478002	0.5675421
H	-2.7623364	-6.6521876	-0.8363846
H	3.9534378	-4.4880238	-1.5704851
H	4.5206648	-3.0557023	-2.5003883
H	3.5411211	-4.3241006	-3.3095344
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H	-0.1678418	0.7451404	-6.4154085
H	1.1340300	1.8038859	-5.7756682
H	-5.8017429	0.8647006	-2.1806261
H	-6.2918479	-0.4050164	-1.0057930
H	-6.0636461	-0.8205085	-2.7374397

O	1.2438480	-4.3256266	3.7036528
H	3.4024086	0.8750565	0.6037947
H	0.0276868	-2.8166277	-0.4967355
H	0.4222189	-1.0494092	-2.1435986
H	-1.4465751	-0.1382613	-1.9307491
H	-2.0023433	-2.0692662	-0.7692506
P	2.3969624	-3.2535976	4.1646215
O	1.8731538	-1.9531330	4.7273501
C	3.4111045	-4.2305285	5.2703442
C	3.6074096	-3.7559344	6.5831430
C	3.9931291	-5.4451343	4.8477467
H	-1.0085923	-3.3068262	-3.0550013
C	-1.4448357	-3.0953492	-4.0443216
Cl	-3.0423750	-3.9016342	-4.1250800
Cl	-0.2984619	-3.6915526	-5.2874595
C	4.3905826	-4.5025640	7.4773858
C	4.7731673	-6.1826232	5.7496994
C	4.9717026	-5.7125995	7.0614008
H	3.1467287	-2.8069559	6.8947220
H	3.8385234	-5.8103564	3.8219966
H	4.5471669	-4.1368996	8.5030958
H	5.2298584	-7.1301156	5.4272504
H	5.5854404	-6.2961316	7.7642318
H	-1.5978199	-2.0174630	-4.2203093
C	0.3257599	0.3115512	2.3863331
N	0.0636899	-0.8057652	1.6388212
N	0.2021888	1.4781002	1.6954456
C	-0.2105779	-0.3631547	0.4076224
C	-0.0930674	1.1449150	0.3178654
O	-0.5256930	-1.0726402	-0.5995846
C	0.4479490	2.8339594	2.1563022
N	0.6465036	0.2482364	3.6776867
H	0.9690153	-0.6654177	4.0679814
H	0.9355315	1.0938863	4.1697728
H	-1.0315876	1.6105788	-0.0419015
H	0.7277405	1.4300900	-0.3740402
H	-0.2120357	3.4981727	1.5605155
C	1.9079022	3.2778285	2.0048906
C	2.0894552	4.7785298	2.2478197
C	3.5174206	5.2691559	1.9895816
C	3.6961756	6.7781637	2.1984860
C	5.1223185	7.2649907	1.9258125
H	0.1061209	2.9255869	3.2092099
H	2.2404945	3.0260647	0.9759447
H	2.5530117	2.6917324	2.6944432
H	1.3837308	5.3391424	1.5920521

H	1.7888257	5.0295677	3.2893361
H	3.8117379	5.0049784	0.9479430
H	4.2229856	4.7152836	2.6491710
H	2.9819866	7.3222456	1.5403881
H	3.4027528	7.0384439	3.2398825
H	5.4268025	7.0480584	0.8802587
H	5.8535666	6.7625440	2.5935856
H	5.2201813	8.3584847	2.0837244
C	-2.7456677	6.4974966	-0.6533122
C	-3.3039575	7.3982866	-1.5827153
H	-3.6530346	7.0278336	-2.5577953
C	-3.4072335	8.7583843	-1.2500372
H	-3.8427825	9.4655982	-1.9714309
C	-2.9555484	9.2126437	0.0008098
H	-3.0367992	10.2794688	0.2584417
C	-2.4006075	8.3095838	0.9273109
H	-2.0503102	8.6685564	1.9064545
C	-2.2933017	6.9493795	0.6056994
H	-1.8641689	6.2414180	1.3295134
P	-2.5923078	4.7796801	-1.1413629
O	-0.9695065	4.5108351	-0.9354897
O	-3.1567091	4.3882974	-2.4780076
O	-3.2227989	4.0284995	0.1858838

3oo

Energy = -4627.480850672

C	2.5053725	-0.8885340	3.0976936
C	3.7945757	-0.7587526	3.6131701
H	4.3088376	-1.4931209	4.2425952
C	4.3206513	0.4983369	3.1699680
H	5.3012397	0.9178516	3.4187333
C	3.3455154	1.1138363	2.3880553
C	3.2448647	2.5166436	1.8088162
C	1.7979654	3.0126693	2.0809018
C	1.2939052	3.0200546	3.4000630
H	1.9374303	2.6980163	4.2325630
C	-0.0313643	3.4060109	3.6504682
H	-0.4162845	3.4059900	4.6814295
C	-0.8786215	3.7870134	2.5959564
H	-1.9230686	4.0816989	2.7689164
C	-0.3701124	3.7798093	1.2898362
C	0.9560853	3.4018518	1.0277659
H	1.3264774	3.4050343	-0.0012780
C	-2.1951486	6.1773645	-1.1924816
C	-1.8232026	7.5244188	-1.3742553
H	-0.7592567	7.7860317	-1.4726389
C	-2.8170085	8.5147801	-1.4300834
H	-2.5321134	9.5675711	-1.5745264
C	-4.1708712	8.1598878	-1.3036429
H	-4.9484558	8.9376155	-1.3488854
C	-4.5380871	6.8133207	-1.1191523
H	-5.5990711	6.5396423	-1.0194876
C	-3.5538093	5.8166275	-1.0617667
H	-3.8365353	4.7637901	-0.9166667
C	4.2453680	3.4499070	2.5299611
H	4.1227122	4.4905899	2.1751555
H	5.2869451	3.1336520	2.3284634
H	4.0767238	3.4335598	3.6227290
C	3.5332071	2.5465630	0.3186927
C	4.0761373	3.5565021	-0.4759453
H	4.5161447	4.4909134	-0.1126877
C	3.9085693	3.1733223	-1.8459178
H	4.2052008	3.7552487	-2.7247994
C	3.2637950	1.9364302	-1.8644061
C	2.6961765	1.1228706	-3.0135902
C	1.1631865	1.3540414	-3.1191490
C	0.5906719	2.5413705	-2.6220454
H	1.2299987	3.3183029	-2.1803808

C	-0.7969224	2.7392331	-2.7058926
C	-1.6362671	1.7735917	-3.2850970
H	-2.7202464	1.9492028	-3.3151257
C	-1.0582843	0.6131980	-3.8179789
H	-1.6989657	-0.1451159	-4.2909081
C	0.3295030	0.4064447	-3.7478762
H	0.7601579	-0.5080489	-4.1778231
C	3.3318183	1.5982085	-4.3430117
H	2.9434835	0.9945217	-5.1850142
H	4.4343978	1.5036132	-4.3121012
H	3.0777392	2.6588428	-4.5299232
C	3.0035655	-0.3536996	-2.8070320
C	4.0755336	-1.1334272	-3.2383242
H	4.9352143	-0.7759370	-3.8149675
C	3.8407132	-2.4802926	-2.8061955
H	4.4821659	-3.3468290	-2.9997735
C	2.6303970	-2.4989195	-2.1152477
C	1.8050557	-3.6428734	-1.5450282
C	0.3192662	-3.3932647	-1.9160578
C	-0.0475954	-3.1661850	-3.2600656
H	0.7262324	-3.1584475	-4.0426197
C	-1.3886786	-2.9371998	-3.6023836
H	-1.6630653	-2.7679712	-4.6544303
C	-2.3898725	-2.9155083	-2.6150375
H	-3.4430452	-2.7210291	-2.8615628
C	-2.0162459	-3.1356573	-1.2820042
C	-0.6800124	-3.3817593	-0.9298037
H	-0.4265464	-3.5723849	0.1169818
C	2.2555357	-4.9753817	-2.1866229
H	1.6134588	-5.8046687	-1.8344083
H	3.3040877	-5.2041677	-1.9154332
H	2.1814478	-4.9189865	-3.2884137
C	-4.8711091	-4.5907366	0.9009068
C	-5.0820363	-5.9847309	0.8892282
H	-4.2226173	-6.6655054	0.9789074
C	-6.3877210	-6.4846821	0.7641769
H	-6.5581746	-7.5716211	0.7561126
C	-7.4717923	-5.5973766	0.6519230
H	-8.4947266	-5.9914154	0.5544672
C	-7.2567319	-4.2061310	0.6639243
H	-8.1086347	-3.5153567	0.5773613
C	-5.9568830	-3.6955817	0.7868428
H	-5.7859423	-2.6091619	0.7953748
C	1.9611770	-3.7459358	-0.0387871
C	2.1617240	-4.8499651	0.7900549
H	2.3484409	-5.8758800	0.4570316

C	2.0519564	-4.4039927	2.1480412
H	2.1533864	-5.0205396	3.0471131
C	1.7829079	-3.0365089	2.1215155
C	1.5067529	-2.0309735	3.2243227
C	0.0383307	-1.5420813	3.1389778
C	-0.9508695	-2.4227884	2.6526125
H	-0.6760078	-3.4390619	2.3357260
C	-2.2960425	-2.0189226	2.6192569
C	-2.6822184	-0.7354459	3.0387943
H	-3.7372467	-0.4369364	2.9711722
C	-1.7001027	0.1289124	3.5407988
H	-1.9833177	1.1367292	3.8764357
C	-0.3565993	-0.2745548	3.6126211
H	0.3847832	0.4165602	4.0358966
C	1.6834215	-2.7145527	4.6018548
H	0.9599852	-3.5447945	4.7106811
H	1.5036653	-1.9828381	5.4115486
H	2.7051607	-3.1254939	4.7133821
P	-0.8903883	4.9475745	-1.1142180
P	-3.1812056	-4.0075409	1.0190032
O	-1.2468802	4.1164510	0.2691615
O	0.5214086	5.4469761	-1.2364946
O	-1.4231563	3.9002116	-2.2691559
O	-3.0033093	-3.0170014	-0.3078950
O	-2.1178416	-5.0546889	1.1851830
O	-3.3222766	-2.8683499	2.2006448
N	2.2721063	0.2338099	2.3177098
H	1.3384132	0.5113969	1.9992670
N	3.0529882	1.5763834	-0.5442870
H	2.6931389	0.6682940	-0.2456756
N	2.1638233	-1.1927038	-2.0875664
H	1.2070178	-0.9332775	-1.8274524
N	1.7520054	-2.6584921	0.7919232
H	1.5065643	-1.7201795	0.4721218
H	-2.0719925	-0.9070316	0.3399188
C	-1.8175733	-0.0578601	-0.3120543
Cl	-0.0613962	0.3044357	-0.0543553
Cl	-2.8470190	1.3221852	0.1020125
H	-1.9261180	-0.2870642	-1.3850314

2b⊂3oo

Energy = -5219.910896521

C	3.0856544	-1.4015906	2.7580400
C	4.2321229	-1.0812016	3.4894522
H	4.7400464	-1.7347798	4.2062852
C	4.6049320	0.2595370	3.1463191
H	5.4474509	0.8250505	3.5574413
C	3.6794159	0.7312859	2.2108978
C	3.5027414	2.1079196	1.5864865
C	2.0511193	2.6059065	1.8233906
C	1.3931322	2.3109779	3.0348603
H	1.8938273	1.6746624	3.7785505
C	0.1230780	2.8435719	3.3056214
H	-0.3732696	2.6209124	4.2621869
C	-0.5221660	3.6606087	2.3653158
H	-1.5152256	4.0899390	2.5547674
C	0.1287348	3.9423547	1.1542051
C	1.4126366	3.4388238	0.8813385
H	1.9302715	3.7130581	-0.0486756
C	-1.6751232	6.0256929	-1.7640030
C	-1.3138296	7.1496065	-2.5334506
H	-0.2720322	7.2688540	-2.8654531
C	-2.2891334	8.1044047	-2.8634996
H	-2.0105239	8.9841372	-3.4622392
C	-3.6143825	7.9358859	-2.4279641
H	-4.3765725	8.6860834	-2.6873205
C	-3.9727557	6.8106498	-1.6613416
H	-5.0119125	6.6812451	-1.3238632
C	-3.0062898	5.8522816	-1.3268213
H	-3.2853513	4.9723336	-0.7292972
C	4.4412914	3.1066154	2.3059038
H	4.2930138	4.1267315	1.9049875
H	5.4998196	2.8190341	2.1560880
H	4.2241959	3.1227490	3.3904143
C	3.8307855	2.1113162	0.1054634
C	4.6586907	2.9505269	-0.6420637
H	5.3125378	3.7323733	-0.2419204
C	4.5000566	2.6007870	-2.0219544
H	5.0068762	3.0639115	-2.8749416
C	3.5812570	1.5553188	-2.0847058
C	2.9601956	0.8203551	-3.2601331
C	1.4201624	0.9835376	-3.2054969
C	0.8917192	2.1449135	-2.6071850
H	1.5686613	2.9066390	-2.2029064

C	-0.4945875	2.3263887	-2.5267390
C	-1.3850389	1.3779444	-3.0576957
H	-2.4686199	1.5366164	-2.9682878
C	-0.8546755	0.2346214	-3.6733317
H	-1.5348266	-0.5312114	-4.0737269
C	0.5338632	0.0376556	-3.7567691
H	0.9197184	-0.8764837	-4.2263255
C	3.4515741	1.4583827	-4.5810401
H	3.0090288	0.9281582	-5.4456636
H	4.5544488	1.4038695	-4.6597908
H	3.1521003	2.5230403	-4.6246811
C	3.3759971	-0.6427084	-3.2258464
C	4.4648920	-1.2962818	-3.8072796
H	5.2361095	-0.8278310	-4.4274956
C	4.3923820	-2.6778560	-3.4368108
H	5.0825127	-3.4715475	-3.7400449
C	3.2637634	-2.8416847	-2.6324276
C	2.5684072	-4.0850006	-2.0973800
C	1.0834130	-3.9898924	-2.5367043
C	0.7750366	-3.6828620	-3.8806311
H	1.5918050	-3.5207009	-4.6002495
C	-0.5580341	-3.5520065	-4.2913141
H	-0.7900104	-3.3122023	-5.3401310
C	-1.6071949	-3.7045453	-3.3681877
H	-2.6583194	-3.5795167	-3.6650888
C	-1.2900394	-3.9991824	-2.0374038
C	0.0386640	-4.1641540	-1.6192493
H	0.2641265	-4.4002891	-0.5751973
C	3.1951373	-5.3385584	-2.7485724
H	2.6622537	-6.2490516	-2.4148564
H	4.2609204	-5.4291748	-2.4630961
H	3.1267682	-5.2781640	-3.8507045
C	-4.1068807	-5.3409419	0.4118635
C	-4.3039739	-6.7341013	0.4950935
H	-3.4336418	-7.4052149	0.5431330
C	-5.6103045	-7.2480498	0.5204952
H	-5.7680910	-8.3348196	0.5876806
C	-6.7109377	-6.3761638	0.4643469
H	-7.7337728	-6.7817254	0.4846187
C	-6.5109113	-4.9849958	0.3872828
H	-7.3743296	-4.3041234	0.3502701
C	-5.2104946	-4.4619008	0.3634001
H	-5.0521155	-3.3746727	0.3184340
C	2.7045632	-4.2054051	-0.5886063
C	3.1247016	-5.2791904	0.1975269
H	3.4738912	-6.2485117	-0.1724078

C	3.0379067	-4.8764581	1.5674279
H	3.3021112	-5.4812417	2.4409576
C	2.5654417	-3.5640658	1.5902487
C	2.2154013	-2.6543199	2.7568277
C	0.7167703	-2.2607793	2.7151285
C	-0.2135118	-3.0747862	2.0409998
H	0.1198702	-3.9947295	1.5439719
C	-1.5688021	-2.7100925	2.0154659
C	-2.0287185	-1.5627291	2.6809974
H	-3.0960588	-1.3061560	2.6394587
C	-1.1050108	-0.7789366	3.3878533
H	-1.4528218	0.1152740	3.9260934
C	0.2557403	-1.1206553	3.4052490
H	0.9697454	-0.4909602	3.9522911
C	2.4494397	-3.4250437	4.0789428
H	1.8022537	-4.3215519	4.1145889
H	2.2099211	-2.7784237	4.9439077
H	3.5039197	-3.7514399	4.1627861
P	-0.3930687	4.8337778	-1.3717602
P	-2.4144188	-4.7434278	0.3565055
O	-0.5751757	4.7542860	0.2670173
O	0.9878186	5.1185043	-1.8890559
O	-1.0753092	3.3984084	-1.8468105
O	-2.3717933	-4.0479729	-1.1528221
O	-1.3262587	-5.7366522	0.6444170
O	-2.5472627	-3.4426130	1.3542097
N	2.7822918	-0.2962670	1.9869074
H	2.0111531	-0.2782143	1.2998322
N	3.1982296	1.2666822	-0.7884393
H	2.4500301	0.5943899	-0.5524333
N	2.6813285	-1.5934119	-2.5018011
H	1.8332659	-1.3944299	-1.9547371
N	2.3804266	-3.1743079	0.2758638
H	1.9194473	-2.2883071	0.0043500
N	-1.0319955	-1.3063878	-0.7046351
N	-3.3638421	-1.2290285	-0.9708966
N	-2.1298982	0.5574766	0.0258126
C	-2.2251678	-0.6679555	-0.5517361
C	-3.1475214	1.5839107	0.1871980
C	-3.5236115	1.8516560	1.6487415
H	-4.0368574	1.3037109	-0.4127560
O	1.1526531	-0.6796373	-0.2379773
C	-0.0972183	-0.4735229	-0.2309014
C	-0.7287619	0.7865098	0.3363718
H	-3.3042682	-2.2023003	-1.2898319
H	-4.2746544	-0.7974561	-0.8246933

H	-0.3329145	1.6982101	-0.1457058
H	-0.5411665	0.8632803	1.4288884
H	-2.5938150	1.8659131	2.2543491
H	-4.1398388	1.0155743	2.0420858
C	-4.2518692	3.1880244	1.8129803
H	-5.1876689	3.1850858	1.2112961
H	-3.6173211	3.9932980	1.3758663
C	-4.5752721	3.5427629	3.2672870
H	-3.6368417	3.5202519	3.8668552
H	-5.2281166	2.7544762	3.7052194
C	-5.2448040	4.9131203	3.4272543
H	-6.1811357	4.9322733	2.8266830
H	-4.5864152	5.6921653	2.9811832
C	-5.5556138	5.2726723	4.8830265
H	-2.7444729	2.5113076	-0.2733659
H	-4.6308473	5.2945827	5.4970772
H	-6.2404162	4.5298484	5.3439546
H	-6.0370558	6.2682819	4.9653698
H	4.9382397	-1.0512399	0.9127092
C	5.2156032	-1.3878695	-0.0985546
Cl	5.8932040	-3.0414144	0.0416415
Cl	6.3853433	-0.2051463	-0.7651770
H	4.3548997	-1.4347594	-0.7832480

4

Energy = -3409.895249548

C	0.0591764	-4.6208516	-0.2928687
C	1.2163167	-4.3309843	-1.0883712
C	-0.2327788	-3.4869751	0.4647430
C	1.6103140	-3.0250534	-0.8017703
N	0.6959222	-2.5211294	0.1108769
C	-1.3012875	-3.2309719	1.5171924
C	-2.4768665	-2.4892170	0.9081717
C	2.8132542	-2.2089914	-1.2490968
C	2.4521325	-1.2896589	-2.4036862
C	-3.5535115	-0.7043881	-0.0130707
N	1.3534321	-0.4485889	-2.3634525
C	1.3280717	0.3924061	-3.4619017
C	3.1418092	-0.9907252	-3.5797287
C	2.4359188	0.0643488	-4.2443301
C	0.3589618	1.5594919	-3.5537495
H	-0.4938440	-5.5659354	-0.2704398
H	1.7167734	-5.0137814	-1.7834492
C	-1.7946767	-4.5844026	2.0812158
C	3.9411015	-3.1646981	-1.7069415
H	4.0681029	-1.4665835	-3.9174268
H	2.7258561	0.5529064	-5.1803748
C	0.7968694	2.6794875	-2.5697778
C	0.3966638	2.1375602	-4.9891033
C	-3.6681623	0.6930748	-0.5930561
C	-2.8779003	0.7498319	-1.8959519
N	-1.5414643	1.1136892	-1.9258854
C	-1.0573661	1.1114982	-3.2260095
C	-3.2403562	0.4383461	-3.2057740
C	-2.0972074	0.6659882	-4.0411047
C	-3.1277006	1.7497345	0.4006981
C	-5.1561372	1.0067529	-0.8759044
H	-4.2249289	0.0852874	-3.5317361
H	-2.0455310	0.5267537	-5.1264627
N	-2.3297359	-1.2252109	0.3674576
C	-3.8334743	-2.8054797	0.8347207
C	-4.5107864	-1.6823437	0.2542184
H	-4.2936424	-3.7408301	1.1696189
H	-5.5843794	-1.6013831	0.0553761
C	-0.7139869	-2.4205892	2.7010549
C	-1.5086735	-1.5012850	3.4114104
C	0.6017640	-2.6765912	3.1386314
C	-0.9832812	-0.8300544	4.5287981

C	1.1210197	-2.0116846	4.2653187
C	0.3294170	-1.0695573	4.9542792
H	-2.5478503	-1.3296040	3.1000467
H	1.1956865	-3.4251041	2.5990385
H	-1.6080032	-0.1104486	5.0793741
H	0.7588667	-0.5525632	5.8241719
C	3.3345332	-1.3899211	-0.0364369
C	3.6468111	-0.0237571	-0.1409311
C	3.5193834	-2.0397347	1.2025562
C	4.0980015	0.6939511	0.9784362
C	3.9844673	-1.3212859	2.3178255
C	4.2582798	0.0564096	2.2149338
C	-0.0917809	3.7318210	-2.2609824
C	2.0885276	2.6960259	-2.0125430
C	0.3021735	4.7568545	-1.3819243
C	2.4719825	3.7140615	-1.1257621
C	1.5790318	4.7389036	-0.7922002
C	-2.8587683	3.0535842	-0.0663349
C	-2.9359070	1.4597619	1.7635537
H	3.5163166	0.4869814	-1.1012778
H	3.3084352	-3.1162144	1.2825993
O	4.2727024	-1.9138272	3.5336545
H	4.6010893	0.5989346	3.1074440
H	-1.0858322	3.7523173	-2.7310835
H	2.8014190	1.9080976	-2.2867738
H	3.4792016	3.7040617	-0.6837456
H	1.8502749	5.5410721	-0.0919046
C	-2.4350980	2.4447216	2.6326766
C	-2.3568248	4.0360627	0.8050449
C	-2.1214567	3.7241310	2.1594878
H	-3.0582465	3.2874139	-1.1207853
H	-3.1753193	0.4607937	2.1464990
H	-2.2836901	2.2091952	3.6972397
H	-1.7130656	4.5013502	2.8201857
H	-2.5476636	-4.4123302	2.8728804
H	-0.9469487	-5.1468544	2.5154676
H	-2.2577886	-5.1991490	1.2854432
H	4.1987097	-3.8704160	-0.8956403
H	4.8480245	-2.5873820	-1.9689167
H	3.6278056	-3.7465971	-2.5951576
H	-0.3245468	2.9711312	-5.0832914
H	0.1413727	1.3598719	-5.7343925
H	1.4076528	2.5233466	-5.2203279
H	-5.2560815	2.0149471	-1.3198789
H	-5.7369637	0.9745309	0.0654069
H	-5.5894628	0.2700230	-1.5795275

O	-0.4803272	5.8635584	-1.1056159
O	-2.1307158	5.3460379	0.4466113
O	2.3604639	-2.2514933	4.8130149
H	4.3082365	1.7695699	0.8898274
H	0.8427035	-1.6500240	0.6289704
H	0.6166569	-0.4934534	-1.6578374
H	-1.0782446	1.5999474	-1.1519236
H	-1.4640011	-0.6805630	0.3955617
C	-1.8661420	5.7104843	-0.8965458
C	3.3951730	-2.8764396	4.0741372
H	-2.3204949	4.9996046	-1.6145432
H	-2.3038144	6.7148423	-1.0388384
H	3.9906215	-3.4503662	4.8060145
H	2.9953248	-3.5600495	3.2992098
H	1.6040413	0.5197689	2.6728652
C	0.8385791	1.2469693	2.3516330
Cl	1.4906644	2.8856030	2.4827877
H	-0.0998954	1.1696315	2.9246431
Cl	0.4265217	0.8319911	0.6335225

2b⊂4

Energy = -4002.328945938

C	-0.3388800	-5.7195226	-0.1179177
C	0.7509699	-5.7242428	-1.0473277
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C	1.0532757	-4.3961417	-1.3513722
N	0.1682458	-3.6062736	-0.6408558
C	-1.6728811	-3.7682025	1.0890098
C	-2.7345247	-2.9689292	0.3437850
C	2.1610355	-3.8031131	-2.2019031
C	1.6204221	-2.8191920	-3.2297477
C	-3.6572375	-1.1519458	-0.6836676
N	1.2107905	-1.5521124	-2.8608623
C	0.9434648	-0.7729637	-3.9690500
C	1.5798838	-2.8681184	-4.6250300
C	1.1520473	-1.5824065	-5.0908603
C	0.4695749	0.6705984	-3.8675785
H	-0.8259851	-6.5975742	0.3191510
H	1.2515751	-6.6073767	-1.4577119
C	-2.3705959	-4.8977330	1.8853258
C	2.8970556	-4.9488997	-2.9327320
H	1.8531069	-3.7278116	-5.2456401
H	1.0192730	-1.2796352	-6.1349603
C	1.1539629	1.4401308	-2.7059682
C	0.8104842	1.4043411	-5.1856576
C	-3.7418047	0.2950364	-1.1465781
C	-2.9290434	0.5352088	-2.4043918
N	-1.5713375	0.2854082	-2.4442439
C	-1.0331501	0.7052876	-3.6451856
C	-3.2761183	1.1112363	-3.6271498
C	-2.0807785	1.2170842	-4.4111947
C	-3.2614875	1.2485112	-0.0184815
C	-5.2210989	0.6423345	-1.4378201
H	-4.2833250	1.4122937	-3.9326322
H	-1.9981251	1.6248328	-5.4242286
N	-2.5225616	-1.6692552	-0.0810350
C	-4.0386213	-3.3054938	-0.0246915
C	-4.6174323	-2.1652906	-0.6686174
H	-4.5304303	-4.2667896	0.1583797
H	-5.6343115	-2.0903641	-1.0666977
C	-0.9251484	-2.8827034	2.1200775
C	-1.5847280	-1.8419205	2.8030621
C	0.4136428	-3.1758274	2.4478526
C	-0.9047711	-1.0981386	3.7821584

C	1.0949902	-2.4186480	3.4139279
C	0.4343670	-1.3738325	4.0888813
H	-2.6322936	-1.6121444	2.5676821
H	0.9024549	-4.0116329	1.9316983
H	-1.4262367	-0.2847912	4.3092827
H	0.9870336	-0.7940224	4.8411643
C	3.1928615	-3.0480780	-1.3206355
C	4.1258276	-2.1812000	-1.9252669
C	3.2050727	-3.2061781	0.0745482
C	5.0439646	-1.4748982	-1.1345554
C	4.0987881	-2.4652439	0.8627335
C	5.0338305	-1.6065512	0.2619257
C	0.4917933	2.5698721	-2.1748411
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C	1.0594831	3.3057420	-1.1232569
C	2.9729455	1.8157661	-1.1290473
C	2.3076305	2.9212576	-0.5877919
C	-2.6040297	2.4518164	-0.3427548
C	-3.5601269	0.9713853	1.3304112
H	4.1155703	-2.0499299	-3.0175601
H	2.4617614	-3.8724921	0.5251783
O	4.1164234	-2.4701722	2.2501626
H	5.7259485	-1.0343797	0.8963845
H	-0.4771772	2.8501559	-2.6095255
H	2.9519576	0.2149820	-2.5885667
H	3.9378168	1.4986778	-0.7065616
H	2.7291792	3.4968552	0.2474082
C	-3.2093727	1.8913174	2.3329976
C	-2.2404807	3.3629006	0.6648623
C	-2.5462360	3.0851202	2.0112899
H	-2.4020974	2.6607913	-1.4012411
H	-4.0800564	0.0377554	1.5890506
H	-3.4495816	1.6730242	3.3847372
H	-2.2591746	3.8105389	2.7856243
H	-3.1054819	-4.4660697	2.5908077
H	-1.6234749	-5.4757364	2.4618596
H	-2.8999134	-5.5922865	1.2048334
H	3.3410165	-5.6459133	-2.1969996
H	3.7109637	-4.5434985	-3.5627464
H	2.1969066	-5.5149310	-3.5773692
H	0.4844709	2.4602244	-5.1307360
H	0.3025807	0.9291932	-6.0471493
H	1.9024112	1.3776504	-5.3619716
H	-5.3116185	1.7040975	-1.7349630
H	-5.8384812	0.4777562	-0.5351833
H	-5.6115422	0.0113440	-2.2595365

O	0.4947990	4.4294144	-0.5507835
O	-1.6115253	4.5700173	0.4303475
O	2.4000619	-2.6421308	3.8105240
H	5.7710108	-0.7983760	-1.6093096
H	0.2207644	-2.5755521	-0.5632128
H	1.1201425	-1.2186309	-1.8881300
H	-0.9952554	-0.0327696	-1.6456482
H	-1.6198132	-1.1766419	0.0120623
C	-0.8587693	4.7932527	-0.7476790
C	3.3174603	-3.3631413	3.0227101
C	2.1113706	0.3972162	2.1008439
N	1.8872485	-0.4766316	1.0773156
C	0.6961495	-0.1566415	0.5659823
C	0.0971417	1.0385684	1.2819093
N	1.1276456	1.3173375	2.2674410
O	0.1098296	-0.7571489	-0.3887097
N	3.2216462	0.3156826	2.8416521
C	0.9453666	2.2853085	3.3373518
C	1.0014532	3.7332222	2.8425971
C	0.5396897	4.7469173	3.8922100
C	0.4239584	6.1672052	3.3276446
C	-0.0443898	7.2060320	4.3534217
C	-0.1812615	8.6157131	3.7699990
H	-0.8742485	0.7913683	1.7572692
H	-0.0646862	1.8763546	0.5775614
H	3.3476914	0.8909548	3.6739658
H	3.7454106	-0.5690921	2.7721141
H	-0.0429811	2.0846239	3.8080044
H	1.7054049	2.0980049	4.1227605
H	0.3624753	3.8313423	1.9418649
H	2.0349895	3.9675784	2.5092315
H	-0.4513093	4.4324439	4.2925321
H	1.2309928	4.7386937	4.7649666
H	-0.2800344	6.1497137	2.4654046
H	1.4069770	6.4781871	2.9070328
H	-1.0201061	6.8811866	4.7794607
H	0.6666527	7.2211731	5.2098954
H	-0.9144852	8.6350742	2.9358910
H	0.7869502	8.9797851	3.3661182
H	-0.5210389	9.3455097	4.5328694
H	-1.3031387	4.2903573	-1.6271986
H	-0.8735929	5.8878236	-0.8975571
H	4.0003370	-3.8561074	3.7395489
H	2.8324397	-4.1242959	2.3848214
H	-2.0432264	-2.4933358	-2.2936100
C	-1.9177022	-2.8837870	-3.3155260

Cl	-1.8128046	-4.6684490	-3.2166435
H	-0.9993573	-2.5114797	-3.7989564
Cl	-3.3172432	-2.3278863	-4.2909028

1i

Energy = -4018.684515082

C	-1.2165260	3.7904400	-1.1867187
C	-2.3580983	4.5521167	-0.9292258
H	-2.4233934	5.6441449	-0.9757471
C	-3.4143634	3.6510125	-0.5739647
H	-4.4365281	3.9245714	-0.2921079
C	-2.8994091	2.3551149	-0.6198839
C	-3.4860434	1.0274672	-0.1699708
C	-2.9747023	0.6784026	1.2520617
C	-2.2433335	1.5982686	2.0252132
H	-2.0674654	2.6061264	1.6317585
C	-1.7307747	1.2384119	3.2810617
H	-1.1376782	1.9638652	3.8564393
C	-1.9591381	-0.0382614	3.8100553
H	-1.5516952	-0.3474446	4.7807371
C	-2.7363648	-0.9375028	3.0604578
C	-3.2343663	-0.5976799	1.7947587
H	-3.8194744	-1.3455842	1.2398594
C	-3.1087415	-4.4667575	4.9568601
C	-2.8673403	-4.7529028	6.3158926
H	-2.0254199	-4.2679579	6.8315277
C	-3.7055878	-5.6526638	6.9929010
H	-3.5215608	-5.8784391	8.0538550
C	-4.7752624	-6.2616301	6.3144671
H	-5.4315767	-6.9662034	6.8472621
C	-5.0118560	-5.9754557	4.9567516
H	-5.8494190	-6.4558144	4.4293216
C	-4.1810323	-5.0774624	4.2713064
H	-4.3637070	-4.8528659	3.2104551
C	-5.0295462	1.1395377	-0.1278400
H	-5.3393060	1.9068188	0.6070962
H	-5.4762269	0.1718470	0.1688909
H	-5.4293979	1.4247782	-1.1199925
C	-3.0794627	-0.0785302	-1.1367753
C	-3.6262049	-0.4829206	-2.3547474
H	-4.4938151	-0.0304091	-2.8480215
C	-2.8543297	-1.5899404	-2.8355044
H	-3.0128933	-2.1385845	-3.7705904
C	-1.8493745	-1.8443045	-1.9018241
C	-0.7132036	-2.8630617	-1.9077274
C	-0.1965488	-3.0810013	-0.4648964
O	5.8301106	2.4221686	0.0537802
O	4.6634937	4.2650774	0.8578344

C	-1.1107349	-3.4537399	0.5427173
H	-2.1776011	-3.5981401	0.3189108
C	-0.6686377	-3.6562554	1.8576042
C	0.6736560	-3.4569104	2.2201401
H	0.9823749	-3.5869609	3.2651393
C	1.5843112	-3.1072934	1.2141538
H	2.6460169	-2.9720906	1.4700506
C	1.1597834	-2.9344565	-0.1138261
H	1.8933954	-2.6680882	-0.8836350
C	-1.2297256	-4.2139819	-2.4582517
H	-2.0581360	-4.5951061	-1.8324121
H	-0.4149134	-4.9635824	-2.4613317
H	-1.6016316	-4.0974754	-3.4939995
C	0.3855644	-2.3458301	-2.8164477
C	1.0018257	-2.8959266	-3.9396827
H	0.7665421	-3.8650071	-4.3919422
C	1.9915708	-1.9622763	-4.3926493
H	2.6638235	-2.0907804	-5.2471407
C	1.9577225	-0.8608993	-3.5365601
C	2.8566746	0.3564612	-3.4304154
C	3.7097086	0.2674464	-2.1383071
C	3.9919740	-0.9784046	-1.5458327
H	3.5694528	-1.8939968	-1.9828614
C	4.8376285	-1.0514032	-0.4248458
H	5.0531146	-2.0275594	0.0355511
C	5.4117926	0.1069620	0.1145214
H	6.0708146	0.0693866	0.9933866
C	5.1530591	1.3548633	-0.4894144
C	4.2991753	1.4325358	-1.6059098
H	4.1020711	2.3918207	-2.1009637
C	5.4468702	3.7621794	-0.2017705
H	6.3791797	4.3539813	-0.1942120
H	4.9443427	3.8689567	-1.1830559
C	3.8371095	0.3648728	-4.6278009
H	4.4749334	-0.5386179	-4.6034056
H	4.4881258	1.2577736	-4.5792414
H	3.2867987	0.3781882	-5.5882098
C	2.0386478	1.6389076	-3.4487484
C	1.7668091	2.5369103	-4.4809367
H	2.0881645	2.4317702	-5.5226013
C	1.0119073	3.6237838	-3.9303276
H	0.6529691	4.5065698	-4.4701157
C	0.8349006	3.3715309	-2.5709348
C	0.2184168	4.2096000	-1.4606858
C	1.0863537	4.0644053	-0.1796723
C	2.4893356	4.1801996	-0.2804205

H	2.9425309	4.3774029	-1.2627018
C	3.2953068	4.0714033	0.8670835
C	2.7119714	3.8301364	2.1266798
H	3.3652243	3.7261713	3.0043755
C	1.3178635	3.7387039	2.2283981
H	0.8556656	3.5568278	3.2096234
C	0.5098277	3.8613312	1.0861570
H	-0.5809644	3.7972829	1.1748124
C	0.2316770	5.7005252	-1.8768698
H	1.2624394	6.0240514	-2.1140570
H	-0.1496747	6.3303409	-1.0509749
H	-0.4060527	5.8652366	-2.7664500
N	-1.5758390	2.4668900	-1.0049289
H	-0.9593642	1.6717646	-1.1761145
N	-1.9821934	-0.8951005	-0.9033393
H	-1.4934371	-0.9485020	-0.0047809
N	0.9657234	-1.1080559	-2.6059079
H	0.7638792	-0.5141040	-1.7984719
N	1.4301254	2.1459766	-2.3109513
H	1.5943696	1.7936621	-1.3641140
O	-3.0944167	-2.1854106	3.5713063
O	-0.8718407	-2.7452515	4.9525626
O	-1.5961335	-4.1316618	2.7854824
P	-2.0163657	-3.2976168	4.1499592
H	2.6416615	1.3587397	1.2792423
C	2.1677793	0.3702589	1.4073854
Cl	0.6060459	0.4233268	0.4856412
Cl	1.8927908	0.0739667	3.1294383
H	2.7634274	-0.4494101	0.9728413

2b⊂1i

Energy = -4611.124955087

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C	-3.7007574	3.1309593	-1.6681302
H	-4.7715312	3.3439518	-1.5856576
C	-3.0832449	1.9112321	-1.3901204
C	-3.6500864	0.6025785	-0.8688078
C	-2.9856659	0.1973179	0.4727414
C	-2.2360931	1.1052747	1.2472129
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C	-1.7140836	0.7269381	2.4963035
H	-1.1296396	1.4508679	3.0829958
C	-1.9423238	-0.5571989	3.0116032
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C	-3.2071764	-1.0960591	0.9863499
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C	-3.1210417	-5.1189480	3.8526828
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H	-2.9528227	-7.0245983	6.6971441
C	-4.6848575	-6.8626270	5.3875248
H	-5.3008254	-7.5471526	5.9901862
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H	-4.8599465	-4.9538551	2.5393648
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H	-5.6081196	-0.1492003	-0.2281945
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C	-3.4734993	-0.5080102	-1.8983580
C	-4.3441138	-1.0091807	-2.8700260
H	-5.3600868	-0.6525237	-3.0694018
C	-3.6669971	-2.0757705	-3.5462629
H	-4.0716838	-2.6969227	-4.3524321
C	-2.3959684	-2.1993127	-2.9743424
C	-1.2691139	-3.1910665	-3.2273112
C	-0.7439912	-3.7387466	-1.8754504
O	5.2760661	1.8838572	-0.1419253
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C	-1.6336476	-3.9440081	-0.8055079
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C	-1.8200185	-4.3828479	-4.0439370
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H	2.6492041	3.6096758	-1.7986368
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H	2.6252612	4.2394278	2.4979246
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H	-0.6216018	5.9667395	-2.0308662
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N	1.1582577	1.7495196	-3.0058746
H	0.9224797	1.2008512	-2.1621578
O	-3.0571619	-2.6970901	2.7727845
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C	0.5540194	-0.2418701	0.0482279
C	1.1671286	-1.0646123	1.9457216
C	1.3999788	0.8250246	0.7113585
H	2.2648436	1.1094795	0.0805310
H	0.7978813	1.7373418	0.9095335
C	2.5859784	0.7554130	2.9807096
C	1.7397229	1.5192625	4.0065051
H	3.3106426	1.4384139	2.4904148
H	3.1950527	-0.0317287	3.4745893
N	0.4322522	-1.3263262	0.8201405
N	1.7949689	0.1428119	1.9264710
N	1.2682861	-1.9349507	2.9501626
H	1.7383897	-1.6601403	3.8126137
H	0.5696807	-2.7085114	3.0142098
O	0.0397686	-0.0714343	-1.1034817
H	1.0378808	0.8139664	4.5028957
H	1.1100052	2.2534783	3.4606636
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C	2.5806213	3.7809940	7.1123228
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C	1.7327506	4.5837492	8.1038306
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H	1.1333615	5.3599264	7.5830544
H	2.3611126	5.0969563	8.8598106
H	-0.7745782	0.9697413	-4.1123253
C	-1.5747708	0.6320493	-4.7880663
Cl	-0.8126350	0.1679247	-6.3441382
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H	-2.1125571	-0.2500474	-4.4012347

2b

Energy = -592.3662703110

C	-2.2261080	-2.5514426	-0.6618734
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N	-1.4506451	-1.7213302	-1.4230601
C	-1.2962248	-3.9601531	-2.0456764
C	-0.7175782	-2.5560538	-2.3606779
O	-0.9872424	-4.9898571	-2.6482873
C	-1.1417852	-0.3268540	-1.1445339
N	-2.9607382	-2.0931761	0.3703870
H	-3.6043303	-2.7410364	0.8241936
H	-3.0844762	-1.0966636	0.5425362
H	-0.9014449	-2.2697462	-3.4178343
H	0.3797541	-2.5365664	-2.1810744
H	-0.8551607	0.1487031	-2.1051543
C	-0.0327672	-0.1329613	-0.0999618
C	0.3115268	1.3416181	0.1317662
C	1.4288822	1.5513409	1.1600170
C	1.8011952	3.0232857	1.3775210
C	2.9301661	3.2198730	2.3939693
H	-2.0730913	0.1895258	-0.8234592
H	0.8748262	-0.6822913	-0.4333178
H	-0.3499605	-0.6035590	0.8564683
H	0.6102905	1.8052578	-0.8357481
H	-0.6015986	1.8883292	0.4604306
H	2.3336957	0.9881937	0.8358291
H	1.1251558	1.0995019	2.1317466
H	2.0941692	3.4707666	0.4012145
H	0.8975550	3.5838999	1.7069885
H	3.8559539	2.6979345	2.0714870
H	2.6514906	2.8129147	3.3890335
H	3.1806999	4.2918222	2.5286187

Computed thermodynamic parameters of complexes 2b⊂3io and 2b⊂3oo

Frequency calculations at BP86 def2-SVP level of theory have been performed using ORCA version 4.1.2.[4] The D4 dispersion correction and RI approximation were applied. The optimization of the geometries was done in CH_2Cl_2 after the application of the conductor-like polarizable continuum model (CPCM) implemented in ORCA.

Table S 1. Computed thermodynamic parameters at 288 K for the formation of the 1:1 complexes **2b⊂3io** and **2b⊂3oo**. ΔH enthalpy (kcal·mol^{-1}), TΔS entropy (kcal·mol^{-1}) and free energy ΔG (kcal·mol^{-1}).

	ΔH	**TΔS**	**ΔG**
2b⊂3io	-40.39	-16.92	-23.47
2b⊂3oo	-37.96	-18.18	-19.78

References

[1] M. Ciardi, F. Tancini, G. Gil-Ramírez, E. C. Escudero Adán, C. Massera, E. Dalcanale and P. Ballester, Switching from Separated to Contact Ion-Pair Binding Modes with Diastereomeric Calix[4]pyrrole Bis-phosphonate Receptors, *J. Am. Chem. Soc.*, 2012, **134**, 13121-13132.
[2] T. Guinovart, D. Hernández-Alonso, L. Adriaenssens, P. Blondeau, M. Martínez-Belmonte, F. X. Rius, F. J. Andrade and P. Ballester, Recognition and Sensing of Creatinine, *Angew. Chem., Int. Ed.*, 2016, **55**, 2435-2440.
[3] A. F. Sierra, D. Hernández-Alonso, M. A. Romero, J. A. González-Delgado, U. Pischel and P. Ballester, Optical Supramolecular Sensing of Creatinine, *J. Am. Chem. Soc.*, 2020, **142**, 4276-4284.
[4] F. Neese, The ORCA program system, *WIREs Computational Molecular Science*, 2012, **2**, 73-78.