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X-ray Studies of Conformation: Observation of Conformational Polymorphism of Glycoluril Based Clip

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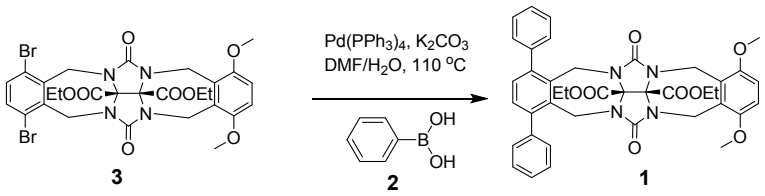
S1. Materials and Instrumental.

The reagents and solvents employed were commercially available and used as received without further purification. Compound **S1** was prepared according to the reported methods.[1] IR spectras were recorded on a Perkin-Elmer PE-983 infrared spectrometer as KBr pellets with absorption in 4000-400 cm^{-1}. NMR spectrawere recorded on a Varian Mercury 400 or 600 MHz spectrometer and resonances (δ) are given in parts per million relative to tetramethylsilane (TMS). HRMS were obtained on a Bruker Apex-Ultra 7.0T FTMS equipped with an electrospray source (ESI). Melting points were determined using XT-4 apparatus and were not corrected.

S2. Synthesis of compound 1

Scheme S1. Synthesis of compound **1**



The coupling reaction between **3** and phenylboronic acid (**2**) was readily accomplished using $Pd(PPh_3)_4$ as catalysts and K_2CO_3 as base in the presence of H_2O in DMF at 110 °C (monitored by TLC), and then the solvent was removed under reduced pressure. The solid residue was purified by flash chromatography (SiO_2, petroleum ether\EtOAc = 30\1) to give **1** (86% yield). M.p. 247.8-248.5 ℃. IR (KBr, cm-1): 2933m, 1725s, 1459s, 1260s, 1080m, 918w, 705w, 668w. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46-7.44 (m, 6H), 7.39-7.36 (m, 2H), 7.31 (s, 2H), 6.81 (s, 1H), 5.37 (d, *J* = 15.6 Hz, 2H), 4.76 (d, *J* = 14.4 Hz, 2H), 4.37 (d, *J* = 13.8 Hz, 2H), 4.17 – 4.13 (m, 4H), 3.83-3.79 (m, 8H), 1.26 (t, *J* = 7.2 Hz, 3H), 0.97 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.3, 151.4, 142.3, 140.1, 132.0, 130.3, 129.2, 128.5, 127.6, 126.7, 112.7, 63.3, 63.1, 57.2, 43.7, 37.4, 14.0, 13.8. HRMS (ESI): m/z$[M+H]^+$ calcd for $C_{40}H_{39}N_4O_8$: 703.2779; found: 703.2762.

S3. Single-crystal X-ray crystallography and the refinements details

Diffraction data for **1**·$CHCl_3$ (**1**a), **1**·CH_2Cl_2 (**1**b), **1**·MeOH (**1**c), **1**·EtOAc (**1**d) and **1**·EtOAc (**1**e) were collected on Bruker Apex CCD area detector diffractometer (MoKα radiation, λ = 0.71073 Å). SMART and SAINT software packages were used for data collection and data integration. Collected data were corrected for absorbance by using SADABS. Structure solution and refinement were carried out with the SHELXTL-PLUS software package and the structure solved by the direct method. Full-matrix least-squares refinement was carried out by minimizing $(F_o^2 - F_c^2)^2$.[2] All non-hydrogen atoms were refined anisotropically; hydrogen atoms were located and refined isotropically or assigned isotropic displacement coefficients U(H) = 1.5U(O-H), and their coordinates were allowed to ride on their respective atoms. The crystal parameters, data collection, and refinement results for all compounds are summarized in Table S1.

Comments: Details of the refinements of complexes 1a-e.

For **1**a, In the refinement, one of the ethoxy groups (C31-C32) was found to be disordered. The commands DFIX, and EADP were used in the refinement to restrain some distances (eg. C36-C37=1.51(1) Å and C36-O6=1.45(1) Å) and thermal factors. The final most satisfactory occupancies for the C36-, C36'-involved ethoxy were 0.62:0.38 for the major and minor components.

For **1**b, In the refinement, the dichloromethane solvent molecule (C41-Cl1-Cl2) was found to be disordered over two sites. The commands DFIX and EADP were used in the refinement to restrain some distances (eg. C41-Cl1=1.73(1) Å and Cl1-Cl2=2.89(2) Å) and thermal factors. The final most satisfactory occupancies for the C41, C41'-involved ethanol were 0.91:0.09 for the major and minor components, respectively.

For **1**c, In the refinement, the methanol solvent molecule (C41-O9; C42-O10) was found to be disordered over three sites. The commands DFIX and EADP were used in the refinement to restrain some distances (eg. C41-O9=1.38(1) Å and C42-O10=1.38(1) Å) and thermal factors. The final most satisfactory occupancies for the C41, C42, C42'-involved methanol were 0.32:0.26:0.42 for each components, respectively.

For **1**d, In the refinement, the ethyl acetate solvent molecule (C1S-C4S-O2S) was found to be disordered over two sites. The commands DFIX and ISOR were used in the refinement to restrain some distances (eg. C1S-C2S=1.51(1) Å and C2S-O2S=1.32(1) Å) and thermal factors. The final

most satisfactory occupancies for the C1S, C1S'-involved ethanol were 0.63:0.37 for the major and minor components, respectively.

For **1**e, In the refinement, the two ethoxycarbonyl groups (O5-O6-C36-C37; O7-O8-C39-C40) were found to be disordered. The commands DFIX were used in the refinement to restrain some distances (eg. C36-C37=1.51(1) Å and C36-O6=1.45(1) Å) and thermal factors. The final most satisfactory occupancies for the O5-, O5' ethyl acetate and O7-, O7' ethoxycarbonyl involved were 0.64:0.36; 0.55:0.45 for the major and minor components, respectively.

Table S1. Crystallographic data and structure refinement details for compounds **1**a−e solvates

empirical formula	**1**-$CHCl_3$ (**1**a)	**1**-CH_2Cl_2 (**1**b)	**1**-MeOH (**1**c)	**1**-EtOAc (**1**d)	**1**-EtOAc (**1**e)
CCDC deposition number	1032703	1032704	1032705	1032706	1032707
formula	$C_{41}H_{39}N_4O_8Cl_3$	$C_{41}H_{40}N_4O_8Cl_2$	$C_{41}H_{42}N_4O_9$	$C_{43}H_{44}N_4O_{9.5}$	$C_{42}H_{42}N_4O_9$
formula weight	820.10	787.67	734.79	768.82	746.80
crystal system	Triclinic	Triclinic	Triclinic	Triclinic	Monoclinic
space group	P-1	P-1	P-1	P-1	P2(1)/c
a (Å)	10.0139(7)	11.2616(7)	8.7063(10)	9.9019(12)	13.3706(17)
b (Å)	11.6799(9)	12.4270(8)	11.0579(13)	14.5729(18)	24.587(3)
c (Å)	17.703(13)	15.9572(10)	20.271(2)	27.372(3)	13.4860(17)
α (deg)	82.3600(10)	68.1700(10)	99.383(2)	94.424(2)	90.00
β (deg)	87.0380(10)	74.5220(10)	98.246(2)	97.048(2)	117.750(2)
γ (deg)	69.4400(10)	65.9000(10)	95.472(2)	100.801(2)	90.00
Z	2	2	2	2	4
V(Å^3)	1921.5(2)	1874.8(2)	1891.4(4)	3830.2(8)	3923.5(9)
temp (K)	150(2)	298(2)	220(2)	100(2)	298(2)
Dcalcd(g cm^{-3})	1.417	1.395	1.290	1.333	1.264
μ (Mo Kα) (mm^{-1})	0.298	0.234	0.092	0.095	0.090
F(000)	852	824	776	1624	1576
θ min−max (deg)	1.16，26.00	1.39，25.00	1.88，25.01	0.75, 26.00	1.90, 25.00
tot., unique data	14870，7460	13311，6532	13231，6602	28344, 14855	26425, 6819
R(int)	0.0306	0.0206	0.0261	0.0249	0.0527
obsd data [I > 2σ(I)]	5224	5267	4785	12139	4428
Nref, Npar	7460, 523	6532, 510	6602, 524	14855, 1114	6819, 603
R1,wR2 (all data)	0.0765, 0.11316	0.0722, 0.2031	0.0857，0.2025	0.0692, 0.1771	0.1003, 0.2110
S	1.031	1.071	1.100	1.088	1.042
min and max resd dens (e Å^{-3})	-0.567，0.398	-0.728, 1.396	-0.279，0.811	-0.352, 0.619	-0.390, 0.916

S4. ^{1}H NMR Spectroscopy

Figure S1 ^{1}H NMR Spectrum of **1** in various solvents

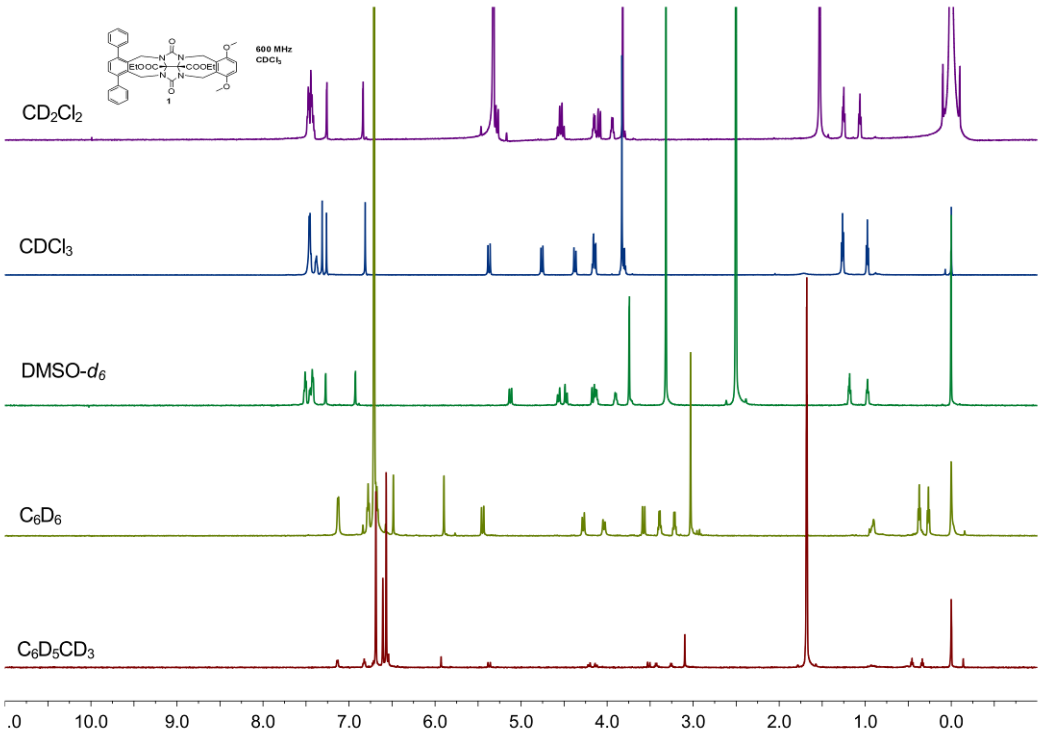


Figure S2. Variable-temperature ^{1}H NMR spectra

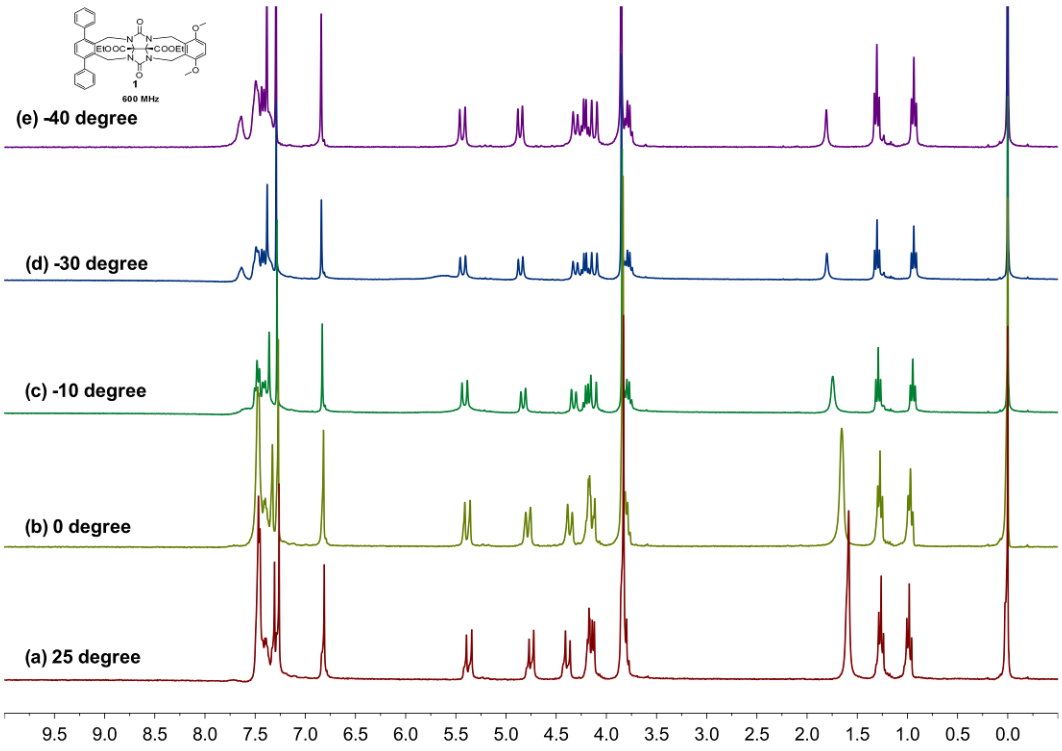
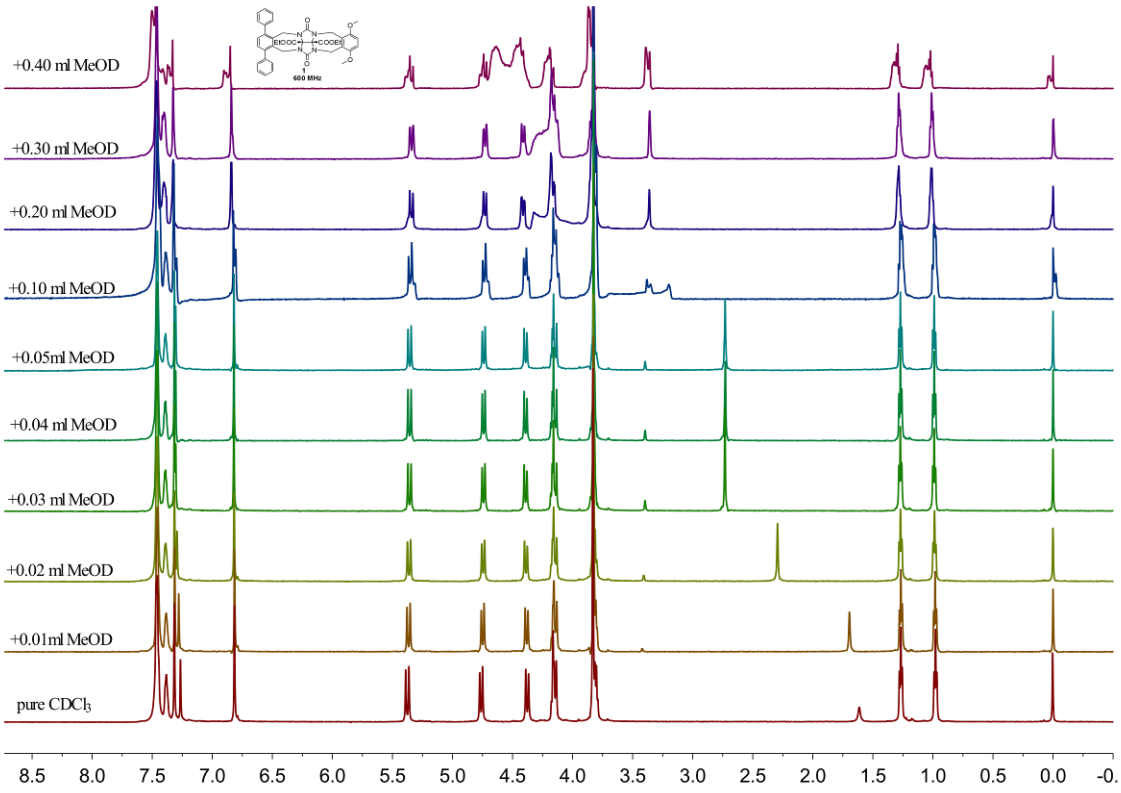
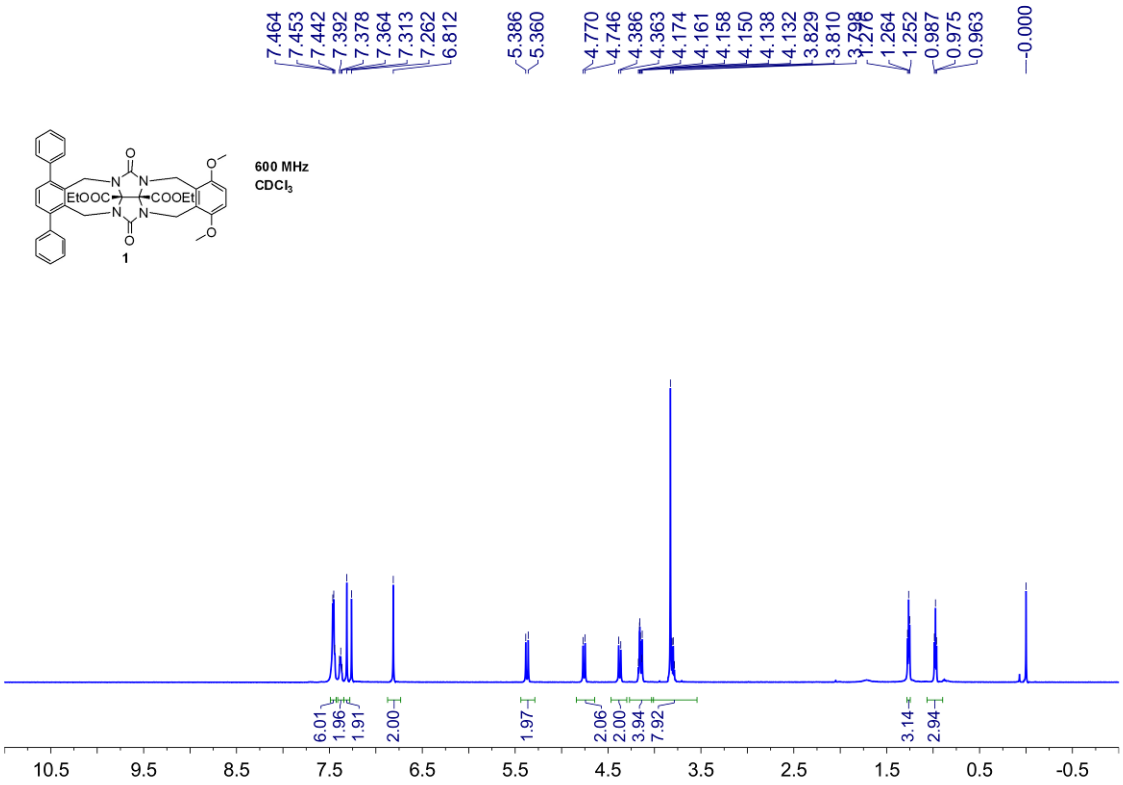


Figure S3. ^{1}H NMR spectra of MeOD titration $CDCl_3$ solution experiments

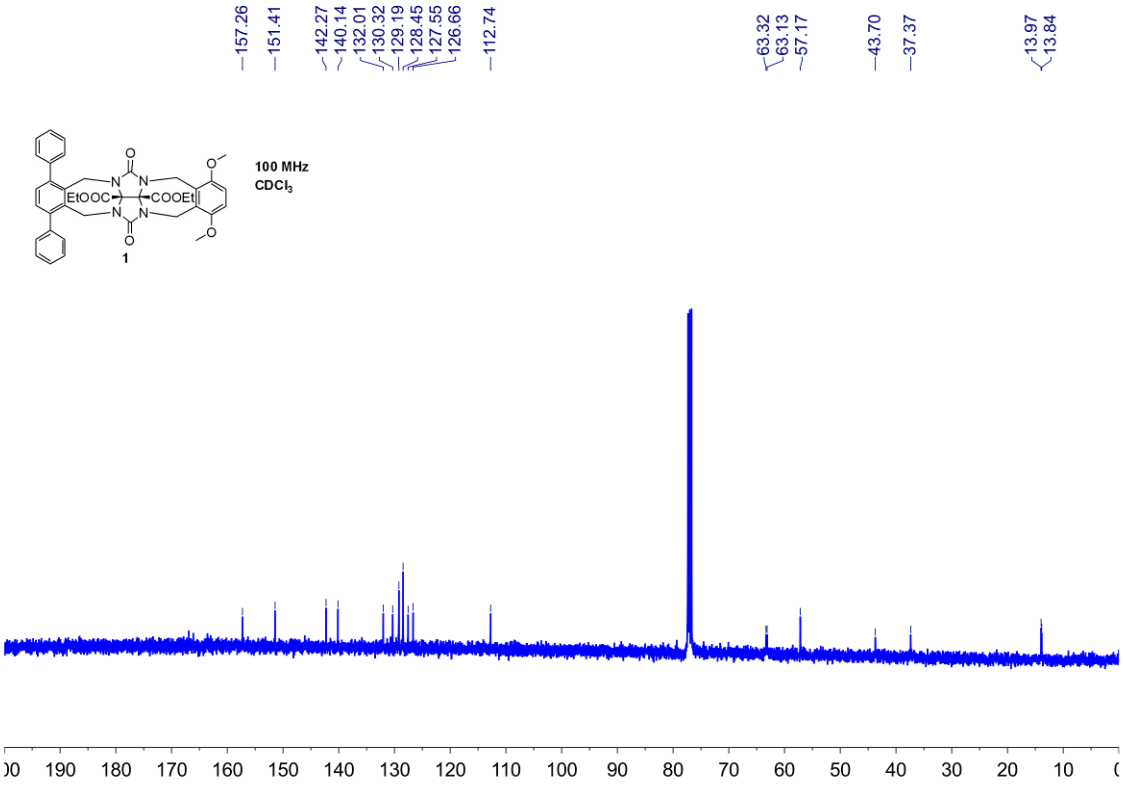


S5. Copies of ^{1}H, ^{13}C NMR and HRMS of 1

a. ^{1}H NMR Spectrum of **1** in $CDCl_3$



b. ^{13}C NMR Spectrum of **1** in $CDCl_3$



c. High Resolution Mass Spectrum of **1**

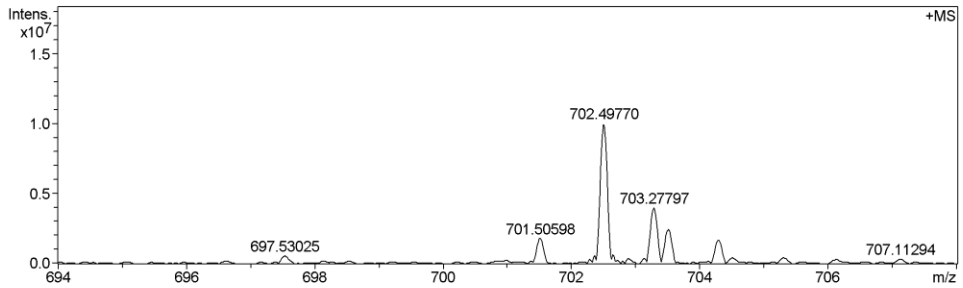
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\User\20111207\W315_ESI_POS_000002.d	Acquisition Date	12/8/2011 1:03:08 AM
Method	Metal_Trypsin digestion	Operator	
Sample Name	W315_ESI_POS	Instrument	apex-Ultra
Comment			

Acquisition Parameter

Polarity	Positive	Source	ESI	No. of Laser Shots	20
Averaged Scans	4	No. of Cell Fills	1	Laser Power	51.0 %
Broadband Low Mass	100.3 m/z	End Plate	3500.0 V	MALDI Plate	300.0 V
Broadband High Mass	1600.0 m/z	Capillary Entrance	4000.0 V	Imaging Spot Diameter	2000.0 µm
Acquisition Mode	Single MS	Skimmer 1	20.0 V		
Pulse Program	basic	Drying Gas Temperature	180.0 °C	Calibration Date	Wed Dec 7 10:47:13 2011
Source Accumulation	0.0 sec	Drying Gas Flow Rate	4.0 L/min	Data Acquisition Size	131072
Ion Accumulation Time	0.0 sec	Nebulizer Gas Flow Rate	1.0 L/min	Apodization	Sine-Bell Multiplication
Flight Time to Acq. Cell	0.0 sec				



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
703.27797	1	C 40 H 39 N 4 O 8	100.00	703.27624	-1.7	-2.5	15.6	23.5	even	ok
	2	C 35 H 44 N O 14	0.00	702.27563	1.0	1.4	609.0	14.5	even	ok
	3	C 32 H 36 N 11 O 8	0.00	702.27428	-1.0	-1.4	611.5	20.5	even	ok
	4	C 34 H 42 N 3 O 13	0.00	700.27121	1.7	2.5	728.5	15.5	even	ok
	5	C 31 H 34 N 13 O 7	0.00	700.26987	-0.7	-1.0	729.6	21.5	even	ok
	6	C 38 H 41 N 2 O 11	0.00	701.27049	-1.4	-2.0	731.3	19.5	even	ok
	7	C 39 H 37 N 6 O 7	0.00	701.27182	-0.2	-0.3	734.4	24.5	even	ok
	8	C 46 H 38 N O 6	0.00	700.26936	0.8	1.2	745.4	28.5	even	ok

Bruker Compass DataAnalysis 4.0 printed: 12/8/2011 2:12:03 AM Page 1 of 1

Figure S6. High Resolution Mass Spectrum of **1**.

References

(1). Wang, Z.-G, Wang, Y.-Z.; Yin, G.-D.; Wu A.-X. *J Chem Crystallogr.* **2008**, *38*, 591–594.

(2). G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr*., **2008**, *64*, 112–122.

S6. Computational methods

All calculations were performed with the Gaussian 09 program. Density functional theory calculations using the B3LYP functional were used to locate all the minima points involved. The 6-31G(d) basis set was applied for all elements. Frequency calculations at the same level had been performed to confirm each stationary point to be a minimum and to evaluate its zero-point energy and the thermal corrections at 298 K. Solvation energies based on the geometry structures obtained at the B3LYP level were obtained at the same level. Solvation energies in each solvent were evaluated by a self-consistent reaction field (SCRF) using the SMD model with radii and non-electrostatic terms.

a. Full citation of Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C. ; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

b. Computed Energies of All Stationary Points

Thermal correction to Gibbs Free Energy (*TCGFE* in Hartree)

Sum of electronic and zero-point Energies (*E*, in Hartree)

Sum of electronic and thermal Free Energies (*G*, in Hartree)

Total free energy in solutions (*E* (sol), in Hartree)

	aa	*as*	*sa*	*ss*
TCGFE	0.643739	0.643762	0.643956	0.64457
E	-2367.268680	-2367.263446	-2367.263320	-2367.258839
G	-2367.351595	-2367.346123	-2367.345862	-2367.340865
E ($CHCl_3$)	-2368.046728	-2368.043385	-2368.041756	-2368.038909
E (CH_2Cl_2)	-2368.050195	-2368.047258	-2368.045459	-2368.042795
E (EtOAc)	-2368.045376	-2368.042727	-2368.040828	-2368.038351
E (MeOH)	-2368.043696	-2368.042720	-2368.040226	-2368.038970

c. Coordinates of All Stationary Points

aa

Cartesian coordinates

ATOM	X	Y	Z
C	3.69654500	5.62586600	-1.55171100
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C	4.69084300	4.70896800	-1.89678300

H	5.57073800	5.03627100	-2.44496400
C	4.55646700	3.36682000	-1.54216100
H	5.32983600	2.65455100	-1.81829900
C	3.42621100	2.91301600	-0.84007100
C	2.43515500	3.84536200	-0.49471100
H	1.54719000	3.52050900	0.03619300
C	2.57106800	5.18786200	-0.85219700
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H	5.19380900	1.70256900	0.67928000
C	4.51159900	-0.32949900	0.72320000
H	5.34465500	-0.67285300	1.32988900
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C	3.78679400	-2.68526100	0.70329400
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H	2.56513800	-5.27669200	2.55039500
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as

Cartesian coordinates

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C	-5.48833100	-4.31134500	-0.87605700
H	-6.58138600	-4.21147700	-0.82438600
H	-5.18991100	-5.24151700	-0.38908600
H	-5.17680600	-4.33656000	-1.92847100
C	-4.95486600	-1.99067200	-0.62529600
C	-4.14643700	-1.02044400	0.00868500
C	-4.25067800	0.32517100	-0.37570600
C	-5.15891500	0.69346200	-1.39308400
C	-5.93195800	-0.27767000	-2.02640700
H	-6.62420800	-0.00966200	-2.81603000
C	-5.83023800	-1.61616800	-1.64312900
H	-6.44635200	-2.35298200	-2.14509300
C	-6.00749000	2.43750600	-2.79896100
H	-5.67786200	1.94499500	-3.72330600
H	-5.85634500	3.51460300	-2.89050400
H	-7.07603200	2.23423200	-2.64322000
C	-3.18597300	-1.48324900	1.10089700
H	-3.48041500	-1.07964400	2.07759100
H	-3.22618700	-2.56855400	1.17338800
C	-3.42026700	1.42248900	0.28094500
H	-3.59370000	2.36530600	-0.23610700
H	-3.72236600	1.55823600	1.32850400
C	-0.99668800	-1.82899400	-0.01893400
C	-1.13968500	1.82218600	-0.64973600
C	-1.32198500	0.22021700	1.07071900
C	0.13913800	0.18743100	0.43878400
C	-1.31842200	0.60862800	2.57760400
C	-1.31181400	2.41824200	4.10014900
H	-0.31296300	2.13613400	4.44567000
H	-2.04708000	1.92014700	4.73958400
C	-1.50141700	3.92159100	4.06010700
H	-0.76114800	4.38783500	3.40310600
H	-1.38113900	4.33513100	5.06735500
H	-2.50063800	4.18251700	3.69715600
C	1.21921800	0.25636600	1.55003100
C	2.39410100	-1.03436000	3.14708200
H	1.94160500	-0.41429400	3.92589400
H	3.37088300	-0.60878100	2.89573100
C	2.48098100	-2.49236500	3.55295400
H	1.48756100	-2.88343600	3.79220100
H	3.11656300	-2.59098800	4.44005100

H	2.90881900	-3.09870100	2.74851600
C	1.18477100	-1.56305800	-1.16088100
H	0.79106800	-1.60437600	-2.18771000
H	1.39143000	-2.59223700	-0.86740400
C	1.05570600	1.31181500	-1.58566700
H	1.18066100	2.33403200	-1.93763000
H	0.56768700	0.74890000	-2.39560100
C	2.46260200	-0.73405000	-1.12489400
C	2.39521600	0.67309000	-1.27010800
C	3.56168300	1.46209100	-1.17371400
C	4.79207100	0.81499700	-0.99345100
H	5.69635500	1.41194300	-0.91799700
C	4.86634300	-0.56626100	-0.89603000
H	5.83355700	-1.04683700	-0.77881900
C	3.71521200	-1.36657100	-0.95482300
C	3.55314700	2.95178900	-1.25133100
C	2.76039300	3.72369100	-0.38462900
H	2.12388800	3.22823700	0.34284800
C	2.80494400	5.11682800	-0.44159800
H	2.18709900	5.69937900	0.23665900
C	3.63852600	5.76208400	-1.35681200
H	3.66815700	6.84769500	-1.39893200
C	4.43409100	5.00457100	-2.21806100
H	5.08386400	5.49697200	-2.93698200
C	4.39339600	3.61161500	-2.16303900
H	5.00569300	3.02484300	-2.84318300
C	3.89873800	-2.84432500	-0.85471200
C	4.62183000	-3.39154000	0.21871200
H	4.99955800	-2.73075600	0.99455000
C	4.84976300	-4.76508100	0.30538500
H	5.40529300	-5.16653600	1.14890300
C	4.36467100	-5.62047100	-0.68528200
H	4.54018200	-6.69065200	-0.61842300
C	3.65497800	-5.09076400	-1.76392700
H	3.28120100	-5.74613700	-2.54594200
C	3.42722500	-3.71726700	-1.84893400
H	2.89398900	-3.31475700	-2.70594000
N	-1.78557800	-1.13042800	0.89355500
N	-1.98389800	1.19826600	0.24420900
N	0.12185300	-1.06177800	-0.28347900
N	0.16436300	1.35639200	-0.41447100
O	-4.83389900	-3.27535900	-0.16636300
O	-5.22937700	2.03035400	-1.68796500
O	-1.23814100	-2.92516300	-0.49279100

O	-1.45323600	2.63271000	-1.50216800
O	-1.15444300	-0.19169200	3.47129100
O	-1.46938700	1.92604700	2.74374500
O	1.62141600	1.29343600	2.03123200
O	1.54966200	-0.96616500	1.96967600

sa

Cartesian coordinates

ATOM	X	Y	Z
C	4.87062400	-5.40264000	-1.17436400
H	5.06778700	-6.46486900	-1.29378900
C	5.82071200	-4.57483900	-0.57379800
H	6.76177800	-4.98872600	-0.22035700
C	5.56412200	-3.21235800	-0.42196800
H	6.30414900	-2.57245500	0.05196300
C	4.35332500	-2.65063100	-0.86266500
C	3.40744200	-3.49313800	-1.46805800
H	2.45946600	-3.09027600	-1.80672500
C	3.66523800	-4.85650400	-1.61768900
H	2.91655700	-5.49030000	-2.08527300
C	4.15200100	-1.17190300	-0.74390400
C	5.11701000	-0.35618200	-1.35385700
H	5.91759200	-0.82368300	-1.91986600
C	5.05713800	1.02321100	-1.25384700
H	5.81375000	1.63459800	-1.73721800
C	4.02273100	1.65735200	-0.54941800
C	3.02870500	0.85872300	0.05974600
C	3.10019900	-0.55642200	-0.02811700
C	4.10433900	3.15001700	-0.44583700
C	3.12361700	4.00079700	-0.98063700
H	2.23155900	3.57804100	-1.43059800
C	3.28128200	5.38642300	-0.91878400
H	2.51103000	6.02826400	-1.33853600
C	4.41547800	5.94703300	-0.32928600
H	4.53318900	7.02669200	-0.28432500
C	5.39766800	5.11055400	0.20328500
H	6.28440400	5.53426500	0.66804500
C	5.24359400	3.72552400	0.14210200
H	6.00927400	3.07742400	0.56109400
C	1.95276700	1.53639000	0.91392700
H	2.11144200	1.30033400	1.97429400
H	2.03678800	2.61780900	0.82510800
C	2.13024900	-1.43071200	0.77044200
H	2.32105500	-2.48451000	0.57494600

H	2.29989100	-1.27316600	1.84494400
C	-0.12046700	1.70167300	-0.48229600
C	-0.07407400	-1.99792500	-0.29631300
C	0.01659900	-0.06728700	1.04268500
C	-0.14587900	-0.11235300	2.58876200
C	-0.39938100	-1.54225100	4.45506600
H	-1.41792600	-1.17455600	4.60930600
H	0.28055300	-0.92775100	5.05303800
C	-0.27021500	-3.02065100	4.76305200
H	-0.95076600	-3.60653600	4.13813700
H	-0.52105700	-3.20078400	5.81408500
H	0.75171600	-3.37150600	4.58750600
C	-1.37591800	-0.14062700	0.28275400
C	-2.56007200	0.05428000	1.26709600
C	-3.91394000	1.68098300	2.32530800
H	-3.51793000	1.42216200	3.31200800
H	-4.80337700	1.07054800	2.14190900
C	-4.19051000	3.16512600	2.18501000
H	-3.28722200	3.74910500	2.38597400
H	-4.96608200	3.46886200	2.89668500
H	-4.53190400	3.39647700	1.17107600
C	-2.15179500	-1.68982700	-1.52976900
C	-2.23612000	1.26702600	-1.70362700
C	-3.51019200	0.44642100	-1.59714000
C	-3.47421700	-0.95374200	-1.51143900
C	-4.67803700	-1.68634600	-1.41947800
C	-5.89984400	-1.01699700	-1.43365200
H	-6.83403200	-1.56220000	-1.37053900
C	-5.93743000	0.37666800	-1.52952900
H	-6.90089600	0.87254400	-1.53887600
C	-4.75655300	1.11185600	-1.60793700
C	-5.94364000	3.18249600	-1.82031700
H	-6.50780100	2.85834100	-2.70480000
H	-5.67464600	4.23479000	-1.92793300
H	-6.57158600	3.05959400	-0.92759700
C	-5.72694500	-3.82499000	-1.19183700
H	-6.27921200	-3.55766000	-0.28131400
H	-5.38908700	-4.86007100	-1.11801000
H	-6.39015200	-3.72168200	-2.06139200
N	0.56373100	1.19456700	0.61883300
N	-1.24021100	0.92307500	-0.68331300
N	-1.36825300	-1.46590900	-0.30092600
N	0.71445600	-1.21119300	0.51477400
O	0.19203800	2.67262100	-1.15359800

O	0.27734300	-2.98500500	-0.92198000
O	-0.36075900	0.87146700	3.26082700
O	-0.07189900	-1.36266100	3.05175200
O	-3.02785600	-0.83730800	1.93800400
O	-2.91193200	1.34169800	1.33574600
O	-4.71776500	2.48007200	-1.70004200
O	-4.55253700	-3.04461600	-1.33495800
H	-2.31126300	-2.76130400	-1.62510300
H	-1.56415100	-1.36439800	-2.40157900
H	-1.78129000	1.11947000	-2.69376000
H	-2.47038900	2.32781000	-1.61615100

ss

Cartesian coordinates

ATOM	X	Y	Z
C	-5.54953300	-4.26667600	0.46703000
H	-5.64417200	-3.97880700	1.52234100
H	-5.12577900	-5.27035800	0.40336800
H	-6.54370700	-4.26294000	-0.00018100
C	-4.91667700	-2.08277800	-0.27710800
C	-3.95999600	-1.27852000	-0.93394800
C	-4.15898200	0.10660400	-1.03423100
C	-5.32476100	0.68623500	-0.48647400
C	-6.26725100	-0.11991400	0.14870300
H	-7.16850700	0.30791900	0.57174500
C	-6.06434800	-1.49866000	0.25483800
H	-6.81292100	-2.09968600	0.75730700
C	-6.66095100	2.65322500	-0.19492600
H	-7.53006900	2.23287900	-0.71810100
H	-6.56565200	3.71178500	-0.44326400
H	-6.80763600	2.54829200	0.88856100
C	-2.72820800	-1.91983700	-1.53618700
C	-3.15019600	0.99331900	-1.74193100
C	-0.29276300	-1.98321700	-1.38768800
C	-0.76676400	1.66656300	-1.62719000
C	-1.35957800	-0.19751300	-0.31169600
C	0.22020800	0.02699800	-0.27261800
C	-1.99197700	-0.05307300	1.09957800
C	-2.89853800	1.49662700	2.63877800
H	-2.10326900	1.29000600	3.36137900
H	-3.73466600	0.82212800	2.84760800
C	-3.31715400	2.95404700	2.64176800
H	-2.45966800	3.60416600	2.44312200
H	-3.73595800	3.22017500	3.61854700

H	-4.07371000	3.13700500	1.87209800
C	0.74733900	0.05814000	1.18725100
C	1.40836400	-1.29944300	3.00701900
H	0.60918100	-0.83242200	3.58898200
H	2.33636100	-0.75061200	3.19778700
C	1.53809500	-2.78171300	3.29766600
H	0.59510700	-3.29584000	3.08910500
H	1.78969000	-2.93000000	4.35381400
H	2.32405600	-3.23492800	2.68541500
C	2.08751600	-1.31678800	-1.46948100
H	2.12565000	-1.21250100	-2.56434400
H	2.33577400	-2.35482000	-1.24931600
C	1.67606100	1.55062000	-1.61650900
H	1.75884000	2.62441100	-1.77393900
H	1.65630900	1.08036500	-2.61140000
C	3.09415600	-0.37839800	-0.81828200
C	2.86300100	1.01841200	-0.83538200
C	3.74808500	1.90079300	-0.17940900
C	4.88890400	1.36591400	0.43533000
H	5.57687100	2.03534300	0.94362500
C	5.14077100	0.00240600	0.41509800
H	6.04328300	-0.38564300	0.87889100
C	4.25687500	-0.89496800	-0.20336400
C	3.53100000	3.37457200	-0.10220100
C	2.34331000	3.91056800	0.42434500
H	1.55868400	3.24049300	0.76355600
C	2.18123400	5.29192400	0.53306400
H	1.25753400	5.69078300	0.94393200
C	3.19642500	6.15860600	0.12417300
H	3.06465800	7.23410300	0.20894400
C	4.38217100	5.63593100	-0.39472000
H	5.17722200	6.30217200	-0.71956600
C	4.54832200	4.25555100	-0.50407700
H	5.46818700	3.85228000	-0.92000400
C	4.62038300	-2.34241300	-0.18646300
C	4.91405900	-2.97917700	1.03098400
H	4.82435300	-2.41790400	1.95733500
C	5.30677500	-4.31727200	1.06515400
H	5.52183800	-4.79119600	2.01933600
C	5.42129900	-5.04508900	-0.12044500
H	5.72611700	-6.08769500	-0.09544500
C	5.14391900	-4.42317100	-1.33875300
H	5.23885800	-4.97747500	-2.26853100
C	4.75027500	-3.08542300	-1.37129300

H	4.55988400	-2.60553700	-2.32754000
N	-1.49484200	-1.54614400	-0.82214300
N	-1.78404400	0.82781000	-1.23503400
N	0.70315100	-1.09890100	-1.03420300
N	0.39646000	1.30475300	-0.93203300
O	-4.64539400	-3.42105900	-0.22285900
O	-5.45359600	2.04512200	-0.62248900
O	-0.15386500	-2.97088700	-2.08923300
O	-0.85311300	2.56402900	-2.44737600
O	-2.03918600	-0.94997100	1.91007000
O	-2.39354700	1.20406900	1.31395800
O	0.76202400	1.05661300	1.87365700
O	1.08200400	-1.16499400	1.60075600
H	-2.80802900	-3.00417800	-1.50522200
H	-2.64334600	-1.62692900	-2.59389400
H	-3.43230500	2.04025200	-1.63346400
H	-3.15196900	0.77084300	-2.81898400