Supporting Information

Exclusive recognition of sarcosine in water and urine by a cavitand-functionalized silicon surface.

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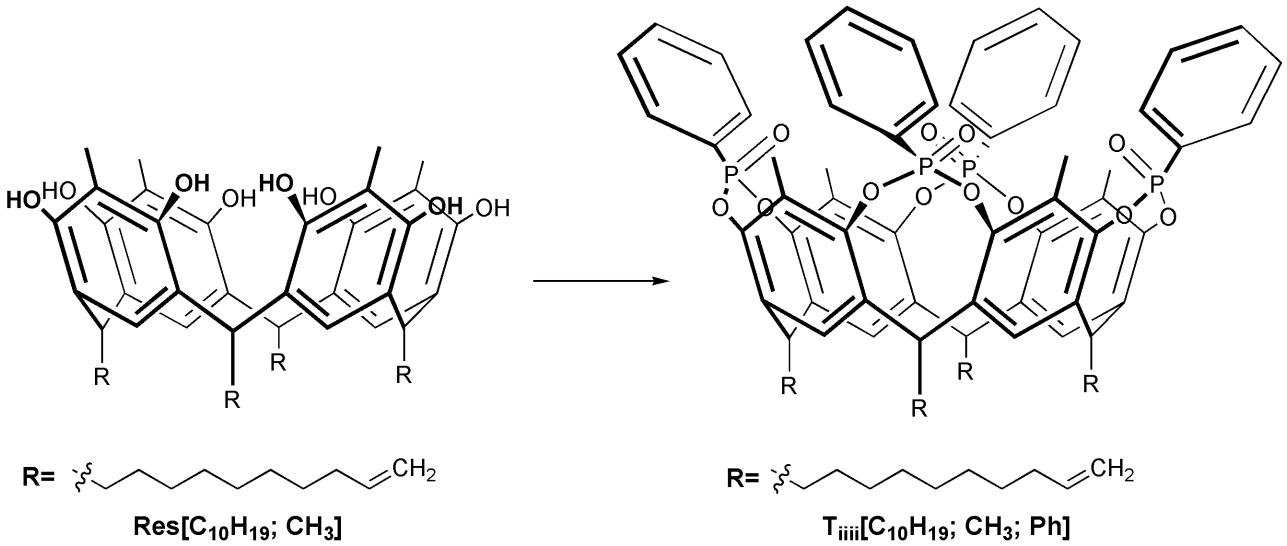
Materials and Methods.

^{1}H NMR and ^{13}C NMR spectra were obtained using a Bruker AVANCE 400 spectrometer. All chemical shifts (δ) were reported in ppm relative to the proton resonances resulting from incomplete deuteration of the NMR solvents. ^{31}P NMR spectra were obtained using a Bruker AVANCE 400 (162 MHz) spectrometer. All chemical shifts (δ) were recorded in ppm relative to external 85% H_3PO_4 at 0.00 ppm. Electrospray ionization ESI-MS experiments were performed on a LTQ Orbitrap XL (Thermo Scientific) mass spectrometer equipped with an Desorption electrospray ionization (DESI) interface or an electrospray ionization (ESI) interface. All solvents were dried and distilled using standard procedures. All commercial reagents were ACS reagent grade and used as received. XPS spectra were run with a PHI 5600 multi-technique ESCA-Auger spectrometer adopting a standard Mg *K*α X-ray source. Analyses were carried out with a photoelectron angle of 45° (relative to the sample surface) with an acceptance angle of ± 7°. The XPS binding energy (BE) scale was calibrated by centering the C 1s peak due to hydrocarbon moieties and "adventitious" carbon at 285.0 eV.[1]. Fluorescence spectra on Si monolayers were obtained with a spectrofluorimeter SPEX FLUOROLOG 111, equipped with a solid plate sample holder for detection in front face. The acquisition mode used was signal/reference, thus correcting the emission spectra for the detection/optical response of the spectrometer. The excitation wavelengths (λ_{ex}) was: λ_{ex} = 340 nm and the spectrum registered in the 390-500 nm range.

Synthesis of Tiiii[$C_{10}H_{19}$, CH_3, Ph].



Scheme S1. Synthesis of **Tiiii[$C_{10}H_{19}$, CH_3, Ph]**.

To a solution of resorcinarene (2) (1g, 0.91 mmol) in freshly distilled pyridine (10 mL) dichlorophenylphosphine (0.504 mL, 3.72 mmol) was added slowly, at room temperature. After 3 hours of stirring at 80 °C, the solution was allowed to cool at room temperature and 4 mL of 35% H_2O_2 were added. The resulting mixture was stirred for 30 min at room temperature, then the solvent was removed under reduced pressure and water added. The precipitate obtained in this way was collected by vacuum filtration, and profusely rinsed with diethyl ether to give the product in a quantitative yield. The detailed physical data of the product are shown in Supplementary Information.

^{1}H NMR: (400 MHz, $CDCl_3$): δ (ppm) 8.17-8.12 (m, 8H), 7.68-7.64 (m, 4H), 7.60-7.55 (m, 8H), 7.27 (s, 4H), 5.89-5.79 (m, 4H), 5.05-4.95 (m, 8H), 4.86 (t, 4H, J=7.2 Hz), 2.43-2.37 (m, 8H), 2.31 (s, 12H), 2.09-2.05 (m, 8H), 1.50-1.28 (m, 48H).

^{13}C NMR: ($CDCl_3$, 162 MHz) δ (ppm): 145.1, 139.1, 134.4, 133.6, 131.5, 128.8, 126.6, 125.1, 124.6, 119.1, 114.2, 36.8, 33.8, 31.4, 29.6, 29.1, 28.0, 11.53, 1.02.

^{31}P NMR: (162 MHz, $CDCl_3$): δ (ppm) 6.54 (s).

HR-DESI-MS (m/z): $[M+NH_4]^+$ calcd. for $C_{96}H_{120}O_{12}NP_4$, 1603.77891, found, 1603.78737 (100%); $[M+Na]^+$ calcd. for $C_{96}H_{116}O_{12}NaP_4$, 1608.73430, found, 1608.74493 (30%).

Tiiii grafting on Si.

For grafting monolayers, a cavitand/1-octene mixtures (χ_{cav} = 0.05) were dissolved in mesitylene (solution concentration = 50 mM). Cavitand solutions (2.0 mL) were placed in a quartz cell and deoxygenated by stirring in a dry box for at least 1 h. A Si(100) substrate was dipped in H_2SO_4/H_2O_2 (3:1 v/v) solution for 12 min to remove organic contaminants, then it was etched in a hydrofluoric acid solution (1% v/v) for 90 s and quickly rinsed with water. The resulting hydrogenated silicon substrate was immediately placed in the mesitylene solution. The cell remained under UV irradiation (254 nm) for two hours. The sample was then removed from the solution and sonicated in dichloromethane for 10 min to remove residual physisorbed material.

Crystal structures.

Crystal data and experimental details for data collection and structure refinement are reported in Table S1. The crystal structures of compounds **Tiiii[C_3H_7, CH_3, Ph]•$CH_3OOCCH_2NH_3Cl$•3CH_3OH•3H_2O** (**1**) and **Tiiii[C_3H_7, CH_3, Ph]•$HOOCCH_2NH_2CH_3Cl$•4CH_3OH•H_2O** (**2**) were determined by X-ray diffraction methods. Intensity data and cell parameters were recorded at 193 K due to the instability of the crystals at room temperature on a Bruker AXS Smart 1000 single-crystal diffractometer (MoK_α radiation) equipped with a CCD area detector. The raw frame data were processed using SAINT and SADABS to yield the reflection data file (3). The structures were solved by Direct Methods using the SIR97 program (4) and refined on F_o^2 by full-matrix least-squares procedures, using the SHELXL-97 program (5) in the WinGX suite (6).

The PLATON SQUEEZE procedure (7) was used for both compounds to treat regions of diffuse solvent which could be seen in the difference Fourier map but could not be sensibly modelled in terms of atomic sites. Their contribution to the diffraction pattern was removed and modified F_o^2 written to a new HKL file. The number of electrons located were included in the formula, formula weight, calculated density, μ and F(000). In compound **1** the residual electron density of 77 electrons per unit cell corresponds to four molecules of methanol per unit cell (four molecules of methanol would give 72 e). In compound **2** the residual electron density of 95 electrons per unit cell corresponds to four molecules of methanol and two molecules of water per unit cell (four molecules of methanol and two molecules of water would give 92 e).

All non-hydrogen atoms were refined with anisotropic atomic displacements with the exception of: i) one disordered phenyl group of the cavitand, the glycine methyl ester and the solvent molecules in compound **1**; ii) the methanol molecules in compound **2**. The hydrogen atoms were included in the refinement at idealized geometry (C-H 0.95 Å) and refined "riding" on the corresponding parent atoms.

The weighting schemes used in the last cycle of refinement were $w = 1/ [\sigma^2 F_o^2 + (0.0729P)^2]$ and $w = 1/ [\sigma^2 F_o^2 + (0.10280P)^2]$, where $P = (F_o^2 + 2F_c^2)/3$ for **1** and **2**, respectively. Molecular geometry calculations were carried out using the PARST97 program (8) Crystallographic data (excluding structure factors) for the structure reported have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-828311 (**1**) and 828312 (**2**) and can be obtained free of charge on application to the

CCDC, 12 Union Road, Cambridge CB2 1EZ, U.K. [Fax: (internat.) + 44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk]

Table S1. Crystal data and structure refinement information for compounds **Tiiii[C_3H_7, CH_3, Ph]•$CH_3OOCCH_2NH_3Cl$•$3CH_3OH$•$3H_2O$** (**1**) and **Tiiii[C_3H_7, CH_3, Ph]•$HOOCCH_2NH_2CH_3Cl$•$4CH_3OH$•H_2O** (**2**).

Compound	**1**	**2**
Formula	$C_{74}H_{94}ClNO_{20}P_4$	$C_{75}H_{94}ClNO_{19}P_4$
Molecular weight	1476.83	1472.84
Crystal system	Triclinic	Triclinic
Space group	*P*-1	*P*-1
a / Å	14.237(1)	14.8953(9)
b / Å	15.190(1)	15.3987(9)
c / Å	20.000(2)	19.2381(11)
α / º	89.952(2)	91.021(1)
β / º	77.113(2)	100.114(1)
γ / º	62.271(2)	118.891(1)
V / Å^3	3705.3(5)	3776.3(4)
Z	2	2
T / K	193(2)	193(2)
ρ / g cm^{-3}	1.324	1.295
μ / mm^{-1}	0.210	0.205
F(000)	1564	1560
Data / parameters	16548 / 809	17955 / 851
Total reflections	23605	47456
Unique reflections (R_{int})	16548 (0.0432)	17955 (0.0634)
Observed reflections [$I>2\sigma(I)$]	5823	7001
Goodness–of–fit on F^{2a}	0.965	0.882
R indices [$I>2\sigma(I)$][b] R1, wR2	0.0855, 0.1922	0.0561, 0.0973
Largest diff. peak and hole / eÅ^{-3}	1.346, -0.653	0.655, -0.397

[a]Goodness-of-fit S = $[\Sigma w(F_o^2-F_c^2)^2/(n-p)]^{1/2}$, where n is the number of reflections and p the number of parameters. [b]R1 = $\Sigma \| F_o | - | F_c \| / \Sigma | F_o |$, wR2 = $[\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.

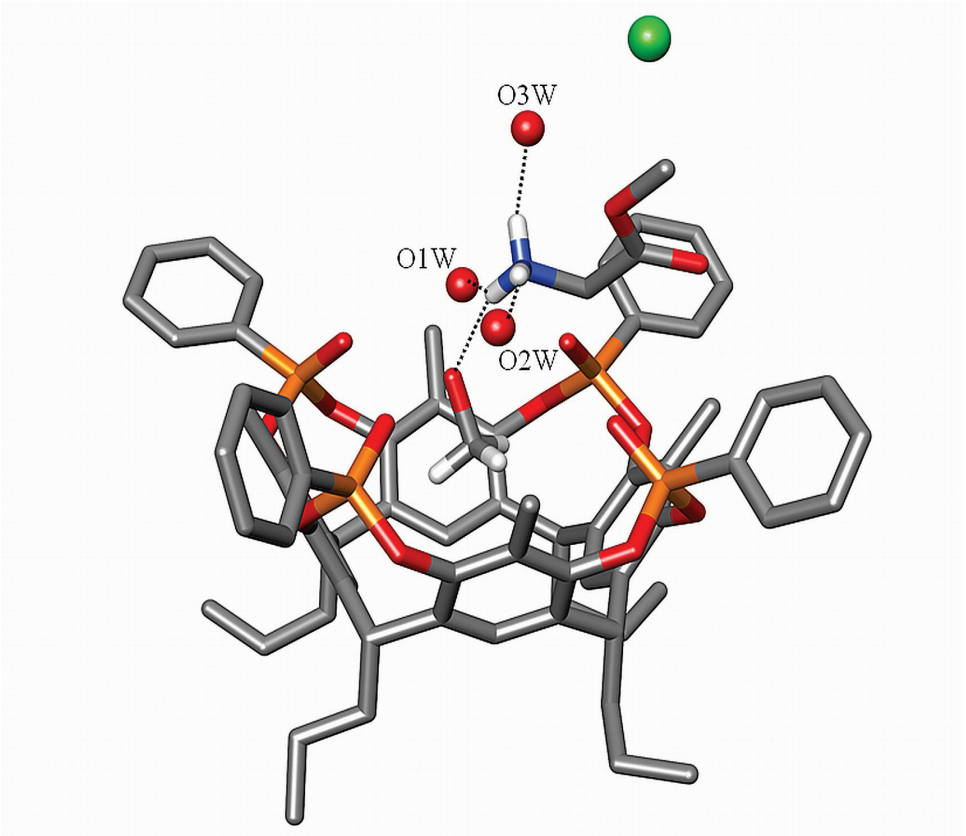


Figure S1. Molecular structure of complex **Tiiii[C_3H_7, CH_3, Ph]•$CH_3OOCCH_2NH_3Cl$•3CH_3OH•3H_2O** showing the network of hydrogen bonds involving the NH_3^+ group of the amino acid, the methanol hosted inside the cavity and the three lattice water molecules. Geometrical parameters: N1···O1S, 2.737(9)Å, N1 -H1H···O1S, 149.54(7)°; N1···O1W, 2.870(9)Å, N1 -H1H···O1W, 129.23(5)°; N1···O2W, 2.521(9)Å, N1 -H1G···O2W, 152.87(8)°; N1···O3W, 2.872(9) Å, N1-H1H···O3W, 162.39(8)°.

Color code: P, orange; O, red; N, blue; Cl, green; C: grey; H, white; hydrogen bonds, black dotted lines. The water molecules and the chloride ion are represented as balls.

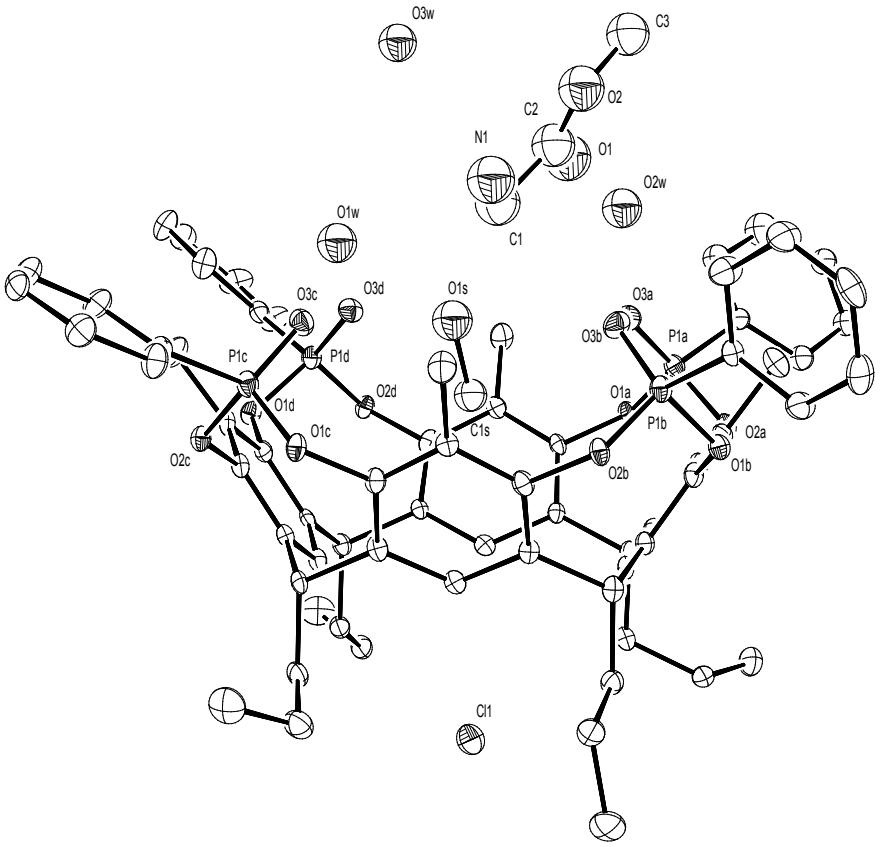


Figure S2. Ortep view (20% ellipsoid probability) of the molecular structure of compound **Tiiii[C_3H_7, CH_3, Ph]•$CH_3OOCCH_2NH_3Cl$•$3CH_3OH$•$3H_2O$ (1)**. Hydrogen atoms and disordered solvent molecules are omitted for clarity.

Description of the weak interactions in complex Tiiii[C_3H_7, CH_3, Ph]•$CH_3OOCCH_2NH_3Cl$ •$3CH_3OH$•$3H_2O$.

The alcohol is stabilized within the cavity by a weak hydrogen bond with one P=O group at the upper rim [O3C···O1S, 3.055(9) Å] and by two CH-π interactions between two methyl hydrogens of the guest and two aromatic rings of the host [C-H···centroid 2.780(4) and 3.052(5) Å; C-H···centroid 158.18(6) and 142.49(8)°]. O1W is involved in two hydrogen bonds with two adjacent PO groups [O1W···O3C, 2.795(9) and O1W···O3D, 2.710(9) Å] and the oxydrilic group of the methanol [O1W···O1S, 2.598(9) Å]; O2W forms a hydrogen bond with a third PO group [O2W···O3B, 2.894(9) Å] and O3W acts as intermediate between the NH_3^+ moiety and the chloride counterion [O3W···Cl1, 3.072(9) Å]. The distance between Cl^- and the positive nitrogen of the guest is thus of 5.155(9) Å. At the same time, each chloride ion is found roughly in the middle of the four alkyl chains at the lower rim of the cavitand situated above. The distance between the ion and the least square plane defined by the four α CH_2 carbons is of 1.462(5) Å. This position is stabilized by C-H···Cl^- interactions ranging in length from 2.866(1) to 3.008(2) Å.

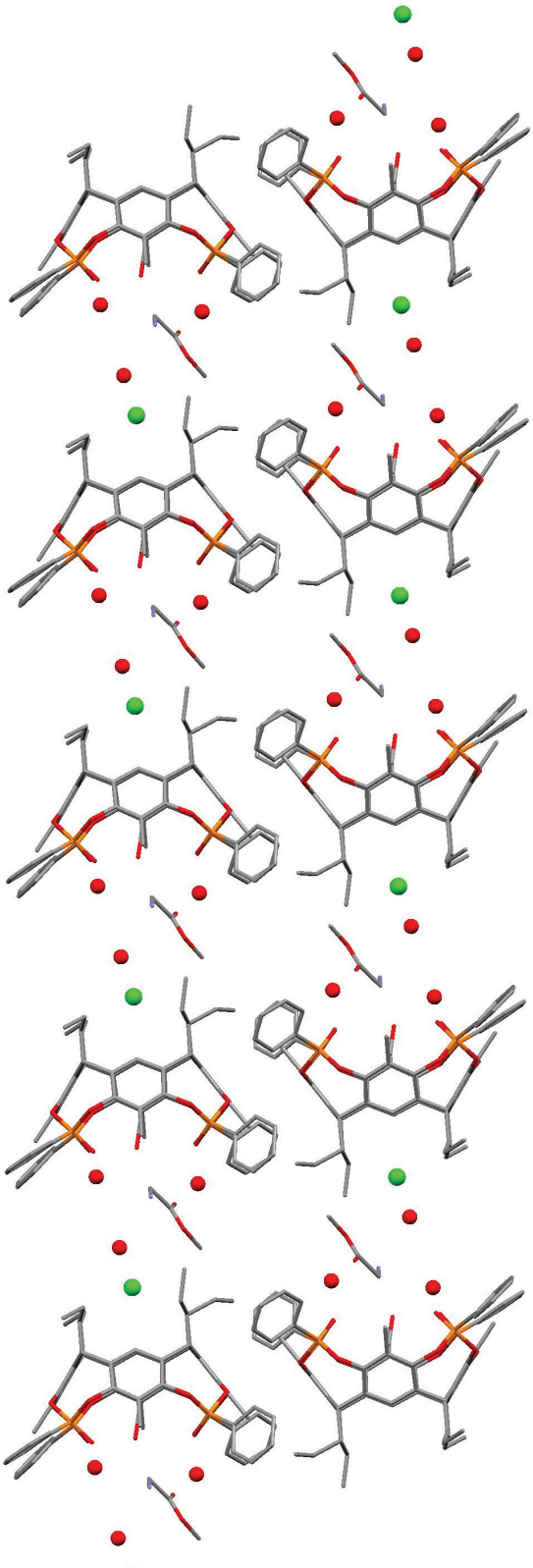


Figure S3. Columnar arrangement of complex **1** in the crystal lattice showing couples of "up-down" rows parallel to the crystallographic a axis.

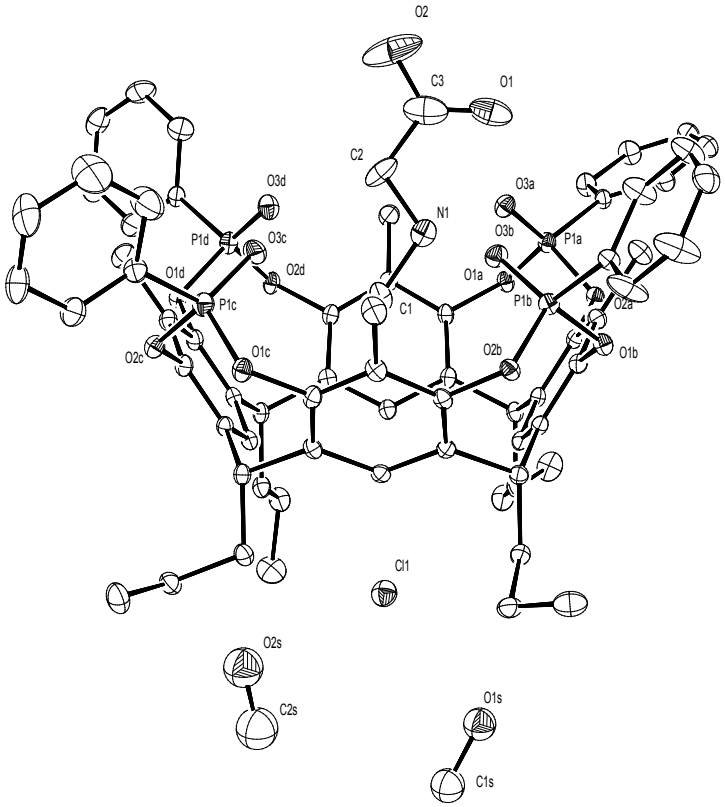


Figure S4. Ortep view (20% ellipsoid probability) of the molecular structure of compound **Tiiii[C_3H_7, CH_3, Ph] •$HOOCCH_2NH_2CH_3Cl$•$4CH_3OH$•H_2O** (**2**). Hydrogen atoms and disordered solvent molecules are omitted for clarity.

Description of the weak interactions in complex Tiiii[C_3H_7, CH_3, Ph]•$HOOCCH_2NH_2CH_3Cl$ •$4CH_3OH$•H_2O.

Sarcosine enters the cavity with its methyl group forming two CH-π interactions with two aromatic rings of the host [C-H···centroid 2.949(3) and 3.103(3) Å; C-H···centroid 142.29(6) and 117.22(6)°]. The complex is further stabilized by two hydrogen bonds involving the positively charged NH_2 moiety and two adjacent P=O groups [N1···O3A, 2.880(3) Å, N1-H1F···O3A, 175.08(3); N1···O3B, 2.740(3) Å, N1-H1E···O3B, 162.96(5)°]. The chloride ion is located among the four alkyl chains at the lower rim of the cavitand, separated by a distance of 7.136(4) Å from the positive nitrogen atom. The distance between the ion and the least square plane defined by the four α CH_2 carbons is of 1.488(3) Å. This position is stabilized by C-H···Cl^- interactions ranging in length from 2.896(1) to 3.015(1) Å. The ion is also involved in to two hydrogen bonds with two methanol molecules of the crystal lattice [Cl···O1S, 3.163(3); Cl···O2S, 3.162(5) Å]

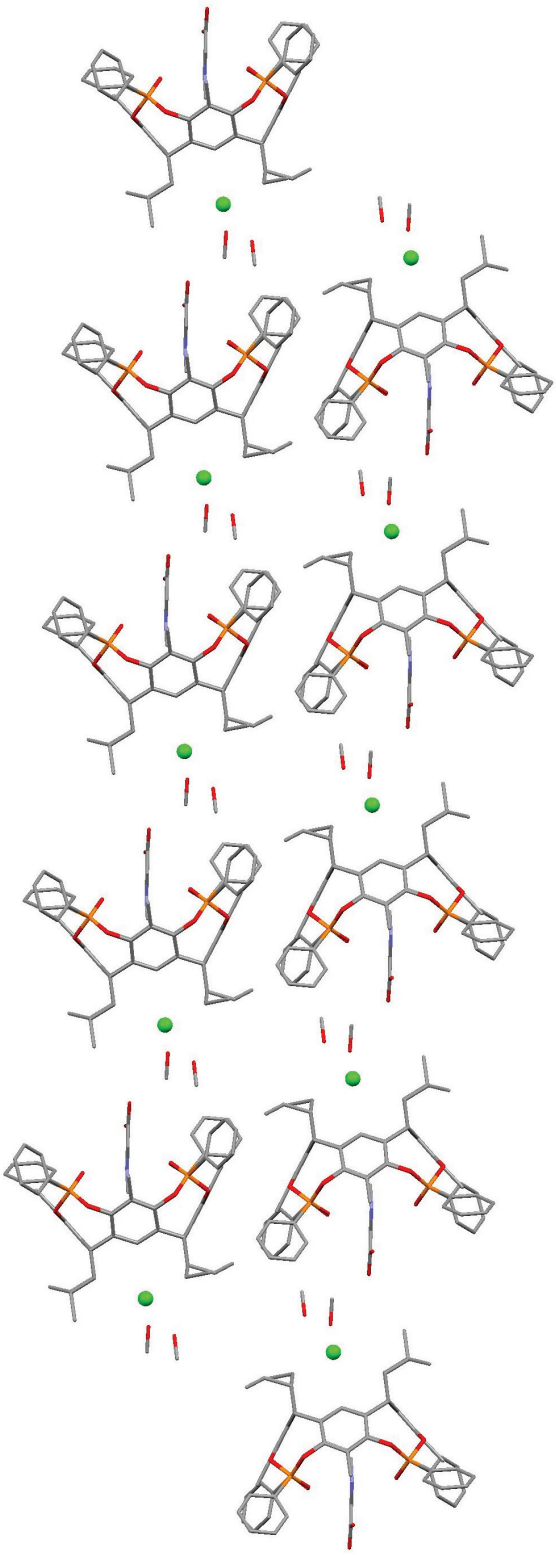


Figure S5. Columnar arrangement of complex **2** in the crystal lattice showing couples of "up-down" rows parallel to the crystallographic a axis.

Job Plot, ^{1}H NMR and ^{31}P NMR of complex Tiiii•sarcosine methyl ester.

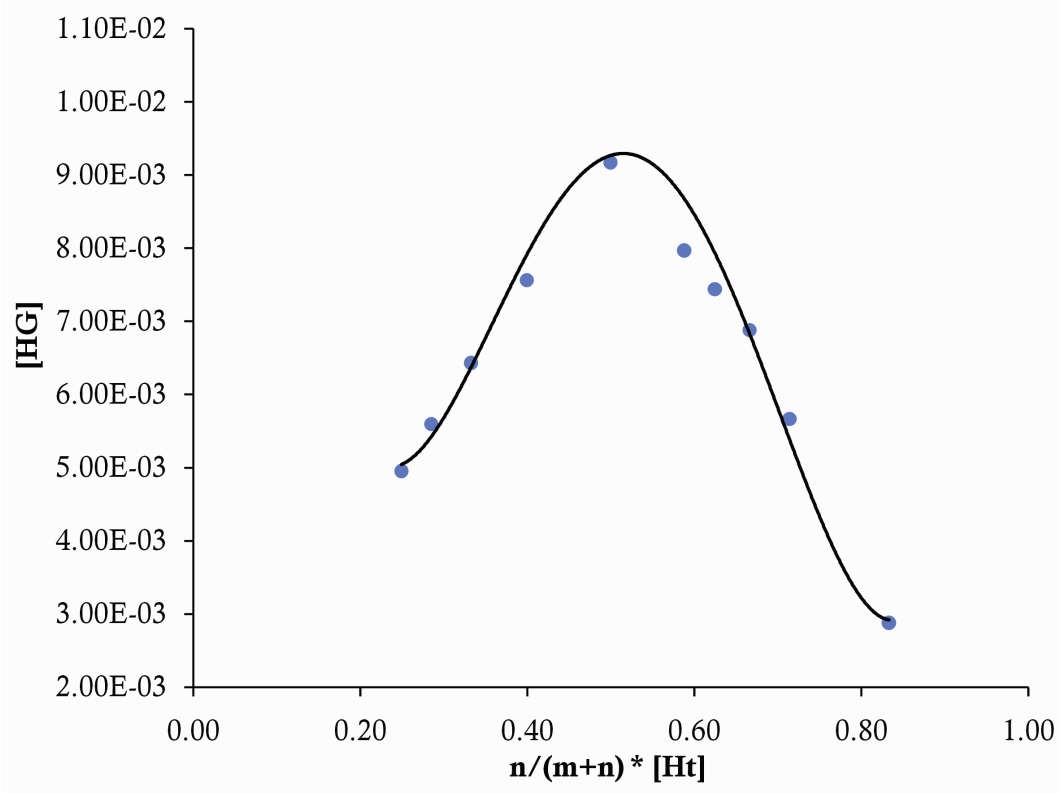


Figure S6. Job Plot for complexation of receptor **Tiiii[C_3H_7, CH_3, Ph]** with sarcosine methyl ester hydrochloride determined in MeOD with ^{31}P NMR by varying the mole fractions of the host and the guest, [**x**]+[**y**] = $1.59*10^{-2}$ M. Integration ratios between complexed and uncomplexed phosphorous peak of **Tiiii[C_3H_7, CH_3, Ph]** were utilized.

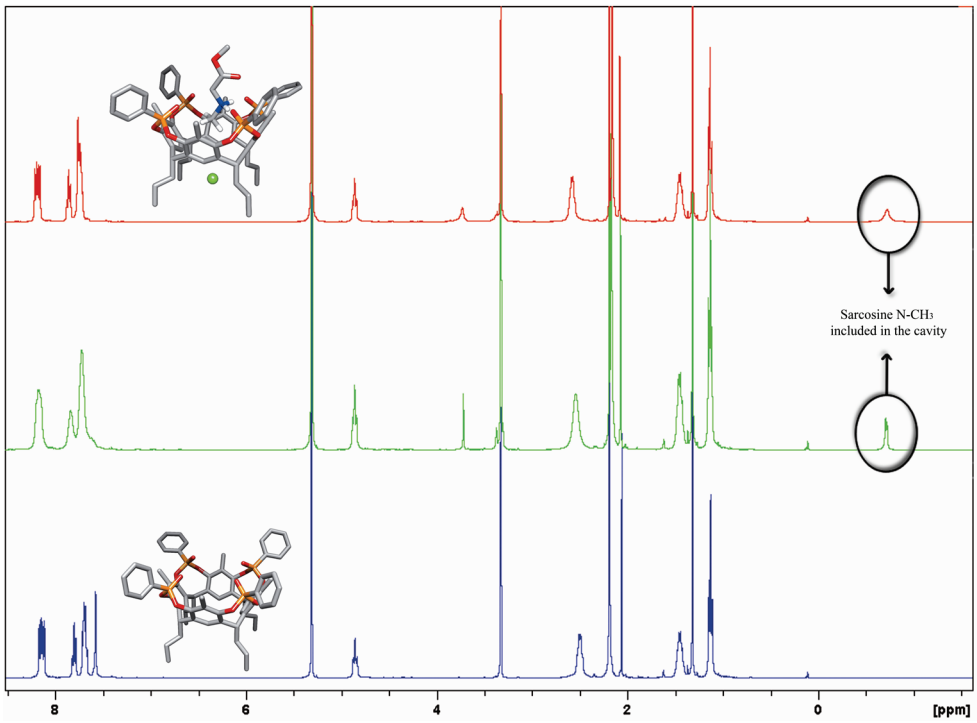


Figure S7. ^{1}H NMR spectra (400 MHz, MeOD, 253K) of free **Tiiii[C_3H_7, CH_3, Ph]** (blue spectrum), 0.5eq. of sarcosine methyl ester hydrochloride added (green spectrum) and the 1:1 complex (red spectum).

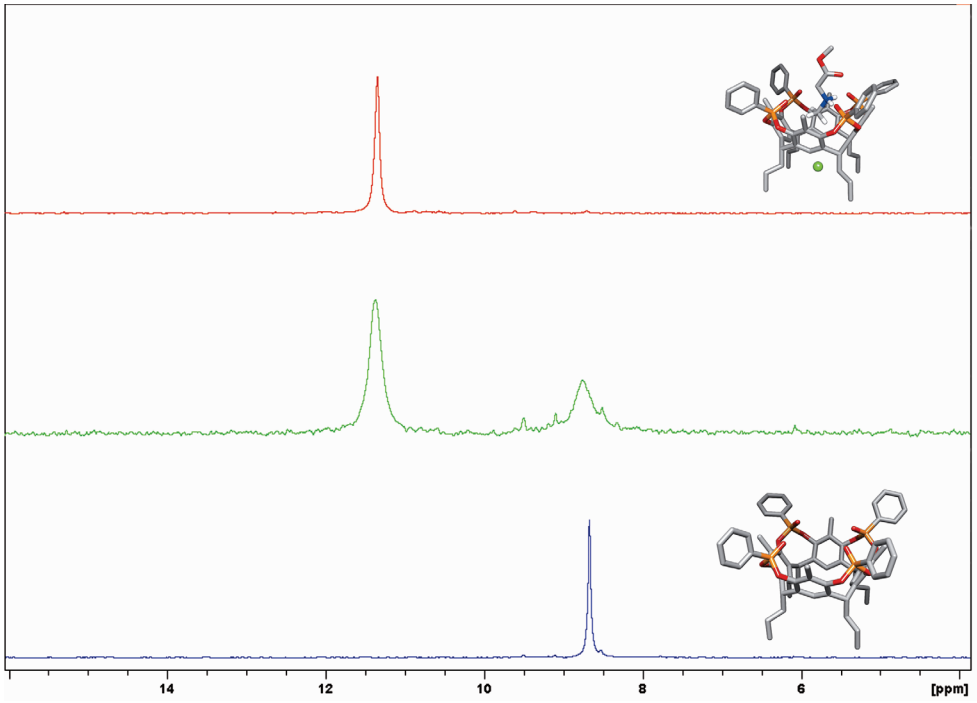
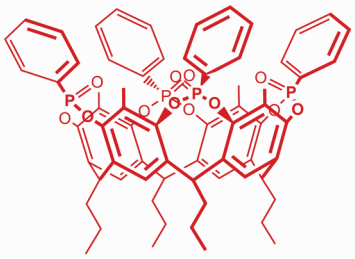
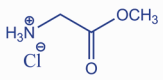


Figure S8. ^{31}P NMR spectra (400 MHz, MeOD, 253K) of free **Tiiii[C_3H_7, CH_3, Ph]** (blue spectrum), plus 0.5eq. of sarcosine methyl ester hydrochloride (green spectrum) and the 1:1 complex (red spectum).

ITC measurements.

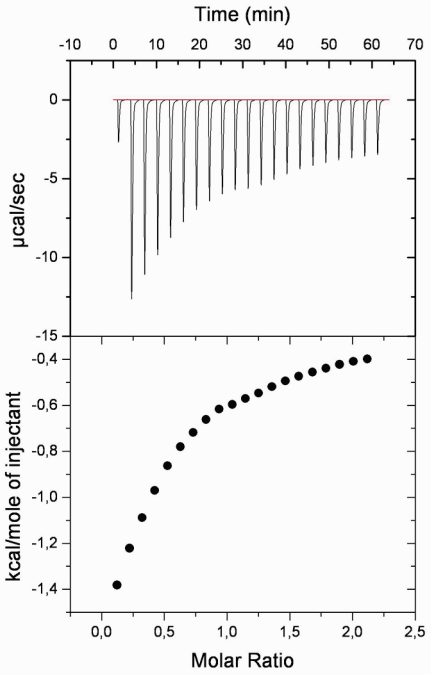


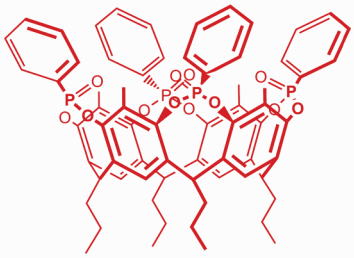
Tiiii[C3H7, CH3, Ph]



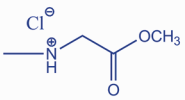
Glycine methyl ester hydrochloride

Solv	Output
MeOH	The shape of the curve indicates an interaction that is too low to be determined.

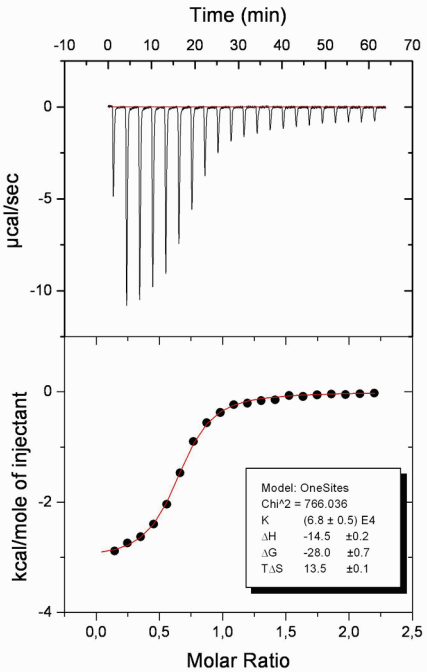




Tiiii[C3H7, CH3, Ph]



Sarcosine methyl ester hydrochloride



Solv	K_{ass}± δK_{ass} (M^{-1})	ΔH± δH ($KJ*mol^{-1}$)	ΔG± δG ($KJ*mol^{-1}$)	TΔS± TδS ($KJ*mol^{-1}$)
MeOH	$6.8 \pm 0.5 \cdot 10^4$	-14.5 ± 0.2	-28.0 ± 0.7	13.5 ± 0.1

Figure S9. ITC data obtained with glycine methyl ester (top) and sarcosine methyl ester (bottom).

Sarcosine complexation at the chloroform-water interface

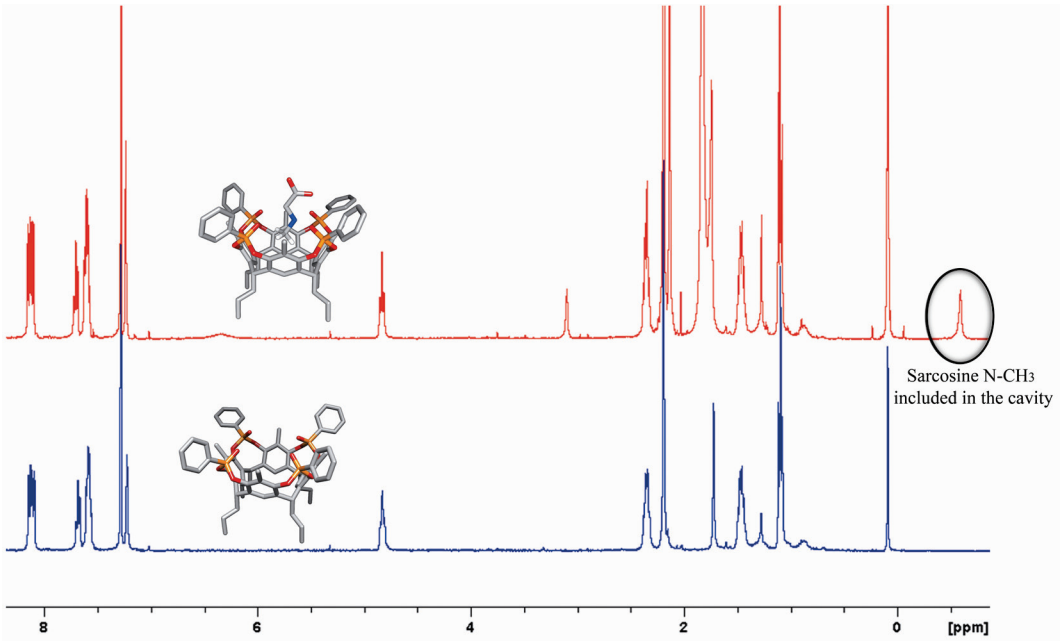


Figure S10. ^{1}H NMR spectra (400 MHz, $CDCl_3$ /D_2O, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (bottom) and the complex **Tiiii[C_3H_7, CH_3, Ph]•sarcosine** (top). 1eq. of sarcosine in D_2O has been added to a 10 mM solution of **Tiiii** in $CDCl_3$/D_2O.

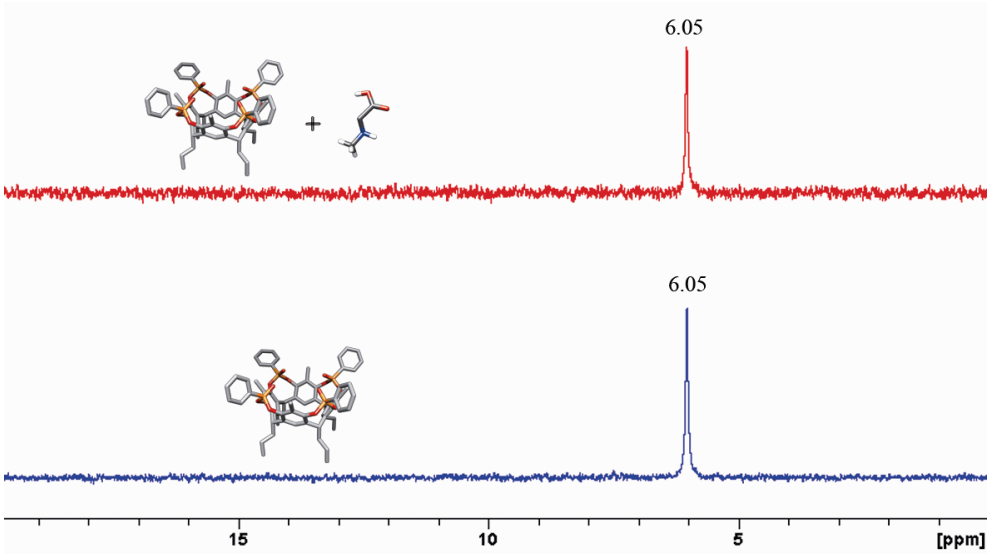


Figure S11. ^{31}P NMR spectra (161 MHz, $CDCl_3$, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (bottom) and the **Tiiii[C_3H_7, CH_3, Ph]** after addition of 1 eq of sarcosine as solid powder (top). Sarcosine has been added as solid powder to a 10 mM solution of **Tiiii** in $CDCl_3$.

Solid sarcosine dissolution in chloroform upon complexation

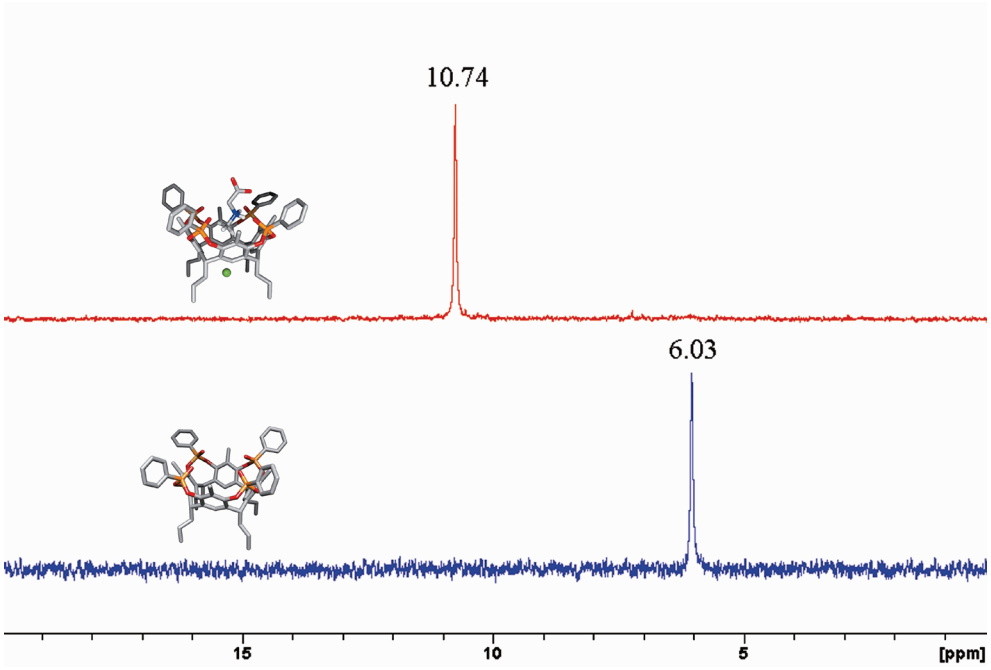


Figure S12. ^{31}P NMR spectra (161 MHz, $CDCl_3$, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (bottom) and the complex **Tiiii[C_3H_7, CH_3, Ph]•sarcosine hydrochloride** (top). 1 eq of sarcosine hydrochloride has been added as solid powder to a 10 mM solution of **Tiiii** in $CDCl_3$.

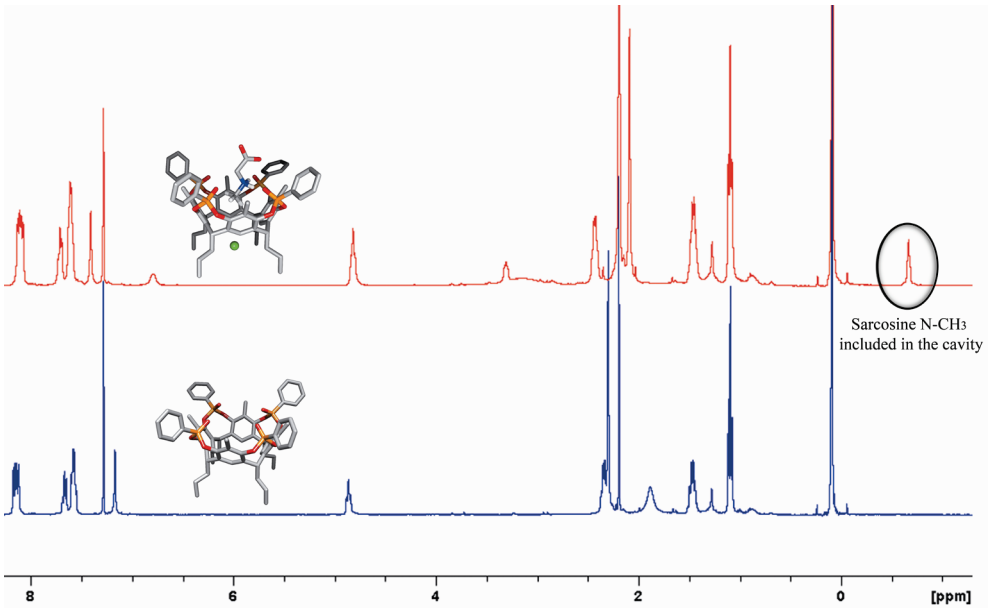


Figure S13. ^{1}H NMR spectra (400 MHz, $CDCl_3$, 298K) of free **Tiiii[C_3H_7, CH_3, Ph]** (bottom) and the complex **Tiiii[C_3H_7, CH_3, Ph]•sarcosine hydrochloride** (top). 1 eq of sarcosine hydrochloride has been added as solid powder to a 10 mM solution of **Tiiii** in $CDCl_3$.

HR-ESI-MS for the complex Tiiii[C3H7, CH3, Ph]•sarcosine.

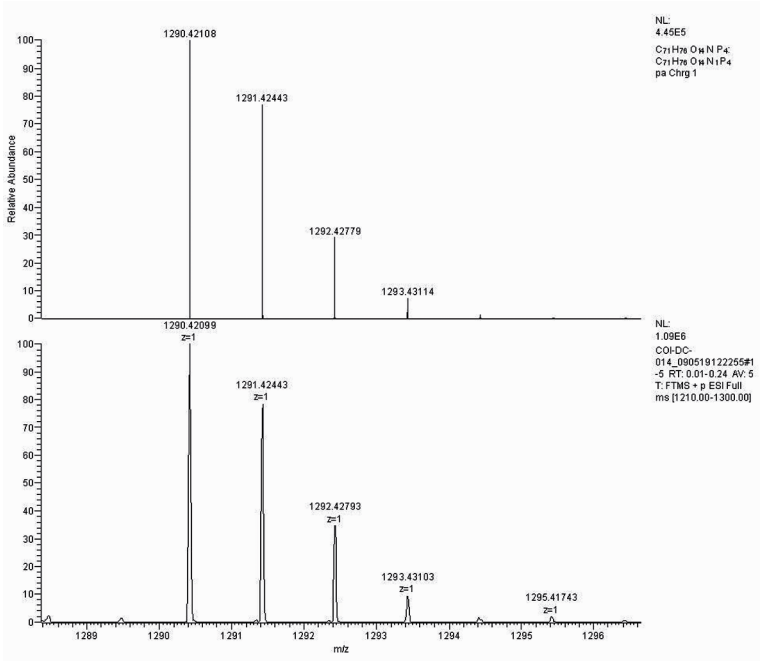


Figure S14. Simulated mass spectrum (top), acquired high resolution mass spectrum (bottom) for the complex **Tiiii[C_3H_7, CH_3, Ph]•sarcosine**.

GC-SIM-MS analyses of urine samples containing sarcosine before and after filtration.

The urine samples added with 1mM and 0.1 mM sarcosine were analyzed to determine if filtration after sarcosine addition would lead to a change in sarcosine concentration in the filtered urine. To this purpose GC-SIM-MS (Gas Chromatography-Selected Ion Monitoring-Mass Spectrometry) was used, following a published procedure (9). In detail the sarcosine spiked urine samples (1mM and 0.1 mM) were added with norvaline (internal standard) and treated with hexyl chloroformate for amino acids derivatization. The samples were then divided in two portions, one filtered as described in the Materials and Methods section, and the other not filtered. GC-SIM-MS was performed on all four samples, two of them filtered and two not. The chromatograms and corresponding histograms are reported in Figure S15 for the 1mM concentration and in Figure S16 for the 0.1mM concentration. In both cases the filtration did not change the sarcosine concentration.

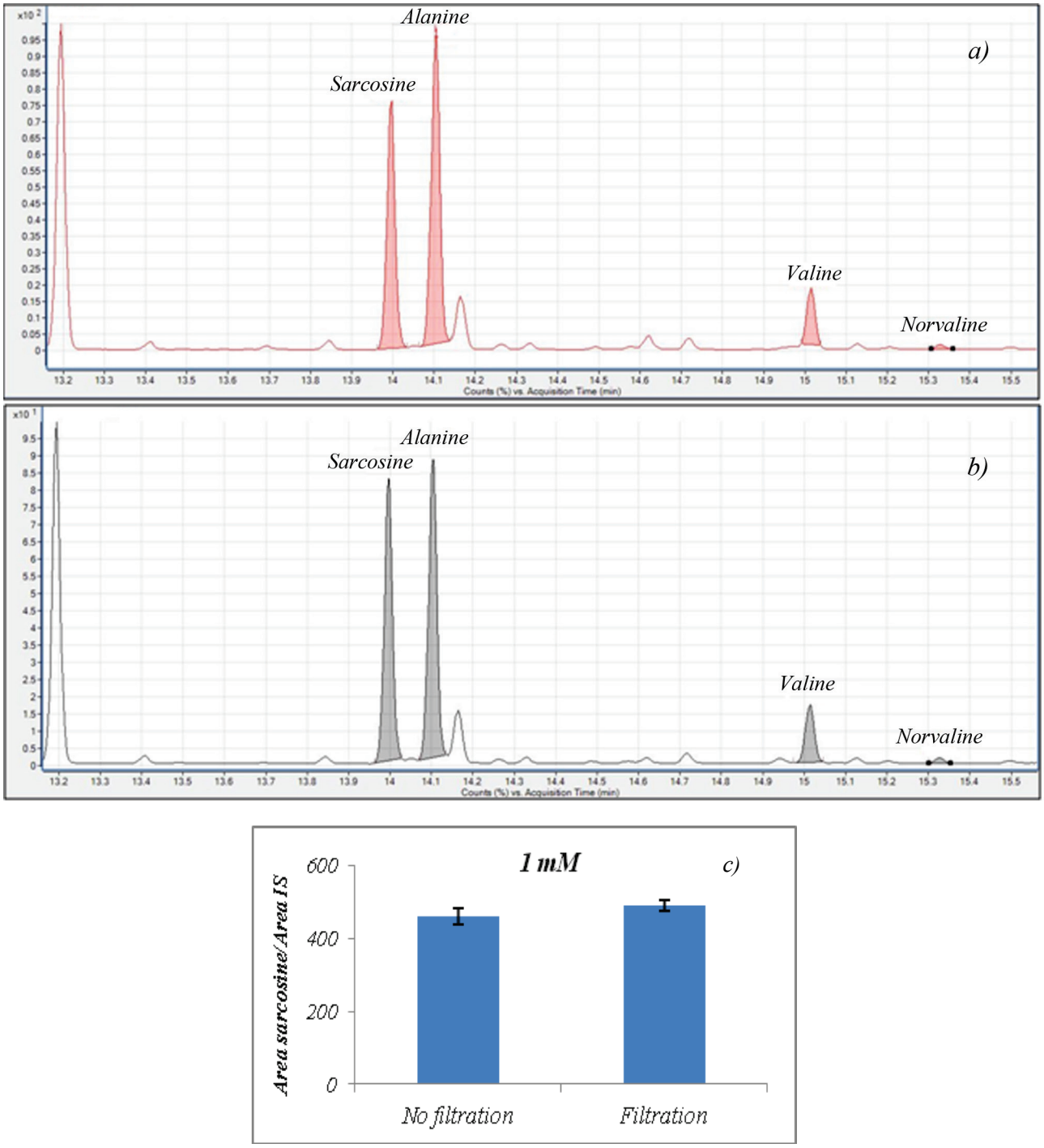
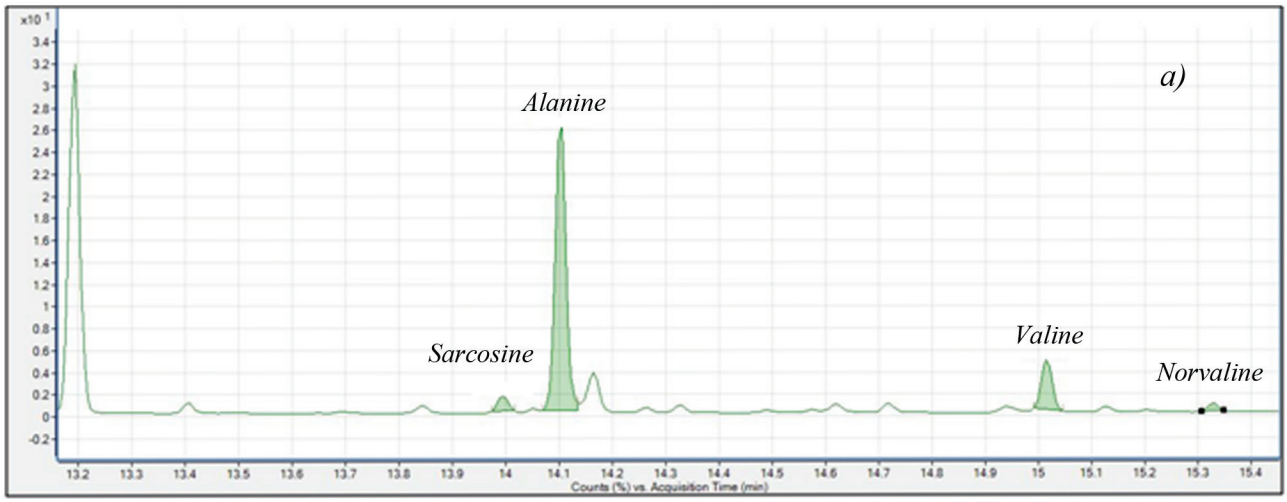
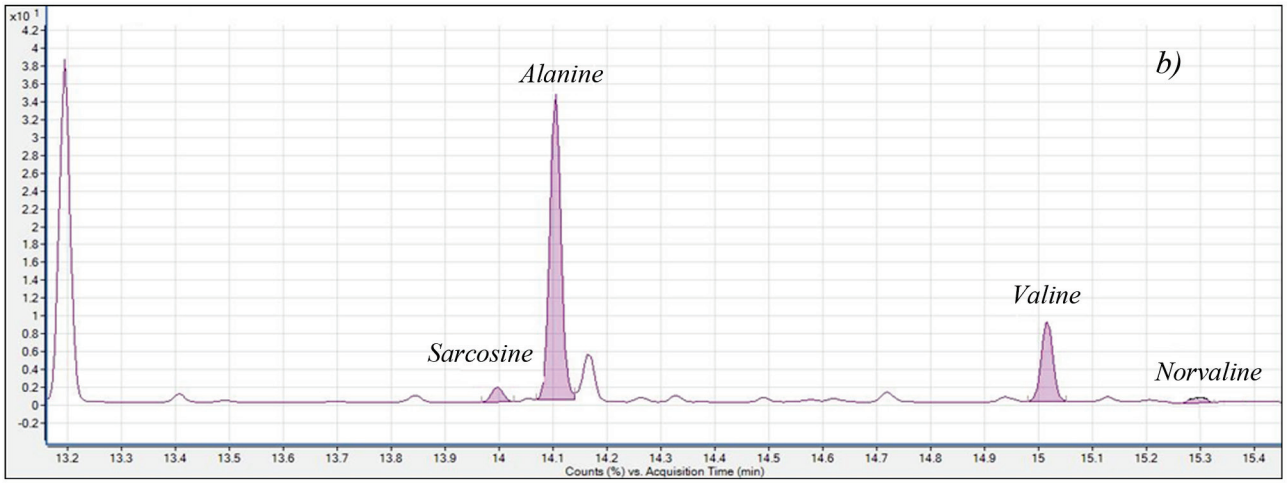


Figure S15. GC-SIM-MS chromatograms of a urinary sample spiked with 1 mM of sarcosine: a) after filtration; b) without filtration; c) histogram reporting the sarcosine peak area normalization with respect to the internal standard (norvaline).





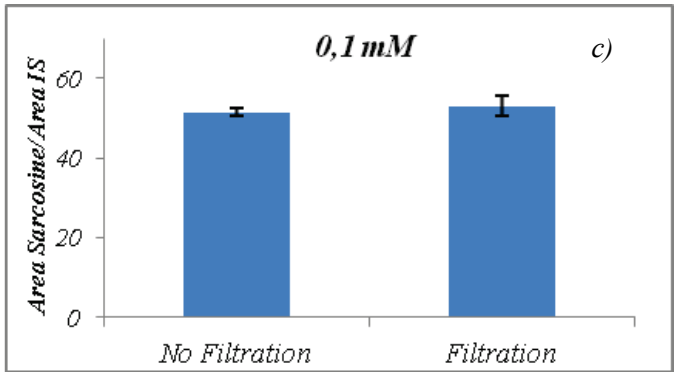


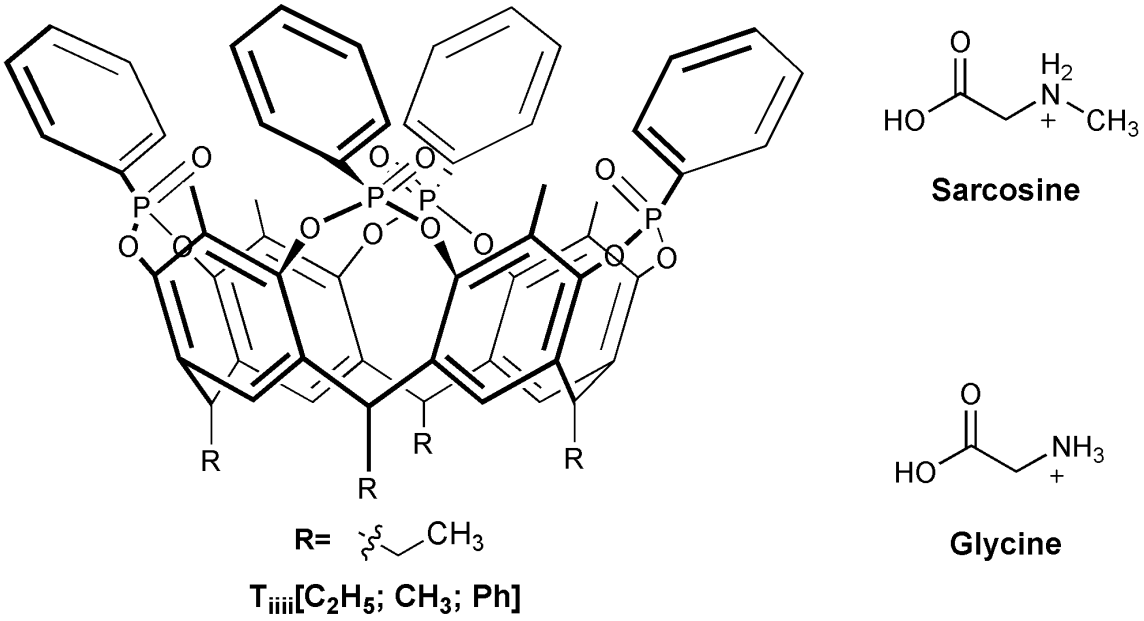
Figure S16. GC-SIM-MS chromatograms of a urinary sample spiked with 0.1 mM of sarcosine: a) after filtration; b) without filtration; c) histogram reporting the sarcosine peak area normalization with respect to the internal standard (norvaline).

DFT Calculations.

DFT calculations have been performed to obtain geometric and energetic details on sarcosine and glycine adducts (both guests as protonated amino acids, Scheme S2) with **Tiiii[$C_{10}H_{19}$, CH_3, Ph]**.

The difference in energy stabilization between **T_{iiii}•glycine** and **T_{iiii}•sarcosine** adducts is computed 3.8 kcal/mol and arises mainly from the CH-π interaction.

Similar calculations have been performed exchanging the methyl groups on the apical positions of **T_{iiii}** with hydride groups **Tiiii[$C_{10}H_{19}$, H, Ph]**, in order to highlight the effect of the methyl groups of the cavity on the sarcosine/glycine selectivity. In this case, it was found a smaller energy difference between the two adducts (3.3 kcal/mol) with respect to adducts with **Tiiii[C_2H_5, CH_3, Ph]**. The methyl groups donate electron density on the cavitand ring enhancing the CH-π interactions, and hence, the sarcosine/glycine selectivity.



Scheme S2. Compounds taken into account for DFT calculations.

Computational details

The Gaussian and plane wave mixed-basis method, as implemented in the QUICKSTEP module (10) within the CP2K simulation package (11), was used. A triple quality TZVP Gaussian basis set was employed for all the atoms. The dispersion correction of Grimme was added to take into account VdW interactions (12). The Goedecker-Teter-Hutter pseudopotentials (13) together with a 320 Ry plane wave cutoff were used to expand the densities obtained with the Perdew-Burke-Ernzerhof (PBE) (14) exchange-correlation density functional. Molecular geometry optimization of stationary points used the Broyden-Fletcher-Goldfarb-Shanno (BFGS) method.

Coordinates in Angstrom and relative energies in a.u. of all structures investigates by DFT calculations.

T_{iiii}[C_2H_5, H, Ph] E=-590.830788 a.u.

C	9.277605587	6.664673958	12.205613789
C	8.167622468	7.556473220	11.665219049
C	10.609473006	7.016048426	11.549345366
C	7.417595095	7.167945201	10.542520321
C	7.866890233	8.801268428	12.233898885
C	11.009517067	6.392881703	10.356823866
C	11.482048003	7.969415513	12.092906710
C	6.415872168	7.975698755	10.012718254
O	7.661077484	5.932845381	9.909406532
C	6.866881763	9.648270035	11.736252105
C	12.217663622	6.696124633	9.735753221
O	10.209971486	5.402158200	9.755512565
C	12.714253156	8.300663185	11.511798418
C	6.153448439	9.204565756	10.611664669
C	6.582507261	11.013770416	12.352904576
C	13.057470238	7.638261522	10.321156516
C	13.643697753	9.343673391	12.119577081
O	5.136939114	10.001517244	10.045119395
C	7.470554473	12.075195289	11.714626108
O	14.291503655	7.884864957	9.686738384
C	13.321643293	10.719637786	11.547861806
C	7.051426402	12.771763041	10.568273075
C	8.736531243	12.394425532	12.224935414
C	13.955914639	11.180902954	10.383301100
C	12.356288179	11.556334881	12.125686197
O	5.787600751	12.528369543	9.994976622
C	7.846369620	13.743085550	9.967686427
C	9.569300779	13.369695995	11.658418799
O	14.945353028	10.406835261	9.742987718
C	13.639996742	12.411255945	9.815727745
C	12.009637659	12.806730306	11.595085604
C	9.090046797	14.036230821	10.519574629
C	10.945194783	13.693112255	12.232352307
C	12.674223636	13.206288937	10.423368474
O	9.856450999	15.042517831	9.895704754
O	12.391210810	14.446344817	9.817738958
C	13.652663117	9.315810738	13.659128333
C	6.671690846	11.006785931	13.891035336
C	9.348795355	6.663812082	13.744067806
C	10.978291024	13.649806276	13.772685641
C	14.710442735	10.258471696	14.241211775
C	10.003304820	14.652151554	14.397884038
C	5.653758901	10.051801954	14.521937321
C	10.364708639	5.644190065	14.267777464
C	4.172498564	11.589762551	8.047630338
C	3.064824507	12.238745948	8.615003015
C	4.197135361	11.266173583	6.680650427
C	1.976894746	12.569507595	7.800676825
C	3.099546192	11.592946693	5.877306657
C	1.994591072	12.247343972	6.436176274
C	11.384708267	15.936251786	7.808210003
C	12.229634470	16.977727722	8.221450759
C	10.828267980	15.926894569	6.517850468
C	12.518670062	18.016121272	7.329797011
C	11.115479689	16.975394701	5.638649628
C	11.962366707	18.015359438	6.043050818
C	15.807796968	8.851368469	7.673937868
C	15.739189848	9.254326649	6.329714268

C	16.917417993	8.142109543	8.158797229
C	16.796998818	8.950089565	5.466502850
C	17.965146787	7.836001191	7.285102765
C	17.906084581	8.239865375	5.943440494
C	8.586629415	4.457778839	7.821405730
C	8.231332792	4.677425364	6.480448673
C	8.681500503	3.157040284	8.339700425
C	7.958324205	3.581757255	5.654226292
C	8.410227880	2.069093047	7.504326640
C	8.046562702	2.280785152	6.166631651
P	8.931230304	5.926624245	8.812711784
P	5.662673650	11.194111270	8.989591490
P	11.035858861	14.493454355	8.837114213
P	14.367667887	9.230339976	8.695440999
O	10.686888662	13.221082948	8.119562072
O	6.891691551	10.845606055	8.200004759
O	9.133024878	7.222183329	8.081611494
O	13.099191142	9.591588227	7.977431837
H	9.037615551	5.633445325	11.895518458
H	8.439130940	9.127474666	13.104342782
H	11.194508255	8.466597170	13.021113777
H	5.872021690	7.668370369	9.120324187
H	12.491141917	6.218089807	8.795573382
H	5.541326359	11.268122521	12.091195846
H	14.665735319	9.094538837	11.787745315
H	9.087963358	11.865698482	13.112794343
H	11.851128726	11.216216595	13.031714383
H	7.510455438	14.249219049	9.063322861
H	14.118707508	12.732659493	8.891382700
H	11.173813563	14.730649657	11.934802291
H	13.844419077	8.276667907	13.975625497
H	12.658879363	9.579727730	14.059123364
H	6.504524789	12.038676471	14.242815486
H	7.688676327	10.731602784	14.218704983
H	8.339634826	6.436036776	14.126279238
H	9.599385058	7.669212555	14.123102444
H	12.011597369	13.864778870	14.093064926
H	10.749598696	12.633957806	14.137417793
H	15.712889446	9.993424216	13.864988508
H	14.730389636	10.206234764	15.341290579
H	10.225215679	15.676224417	14.053275794
H	10.067466087	14.637564979	15.497476461
H	4.628116624	10.324296172	14.221660035
H	5.709603000	10.079919070	15.621713947
H	10.110289751	4.630632532	13.915005029
H	10.385657851	5.629388426	15.368935649
H	3.066976891	12.498602928	9.675312908
H	5.082262558	10.781004200	6.261669239
H	1.118513911	13.087724126	8.231730231
H	3.113162276	11.347006870	4.813163732
H	1.147143501	12.514841406	5.801954519
H	12.674701860	16.956697604	9.217798348
H	10.200930732	15.087363484	6.208429968
H	13.192648013	18.817590792	7.637796797
H	10.691710605	16.971604493	4.632018164
H	12.199592973	18.820770441	5.345636985
H	14.851282744	9.781463828	5.972364920
H	16.946652858	7.816900731	9.200355875
H	16.749028550	9.256331686	4.419152823
H	18.823287883	7.270033456	7.651084919
H	18.724272914	7.992323365	5.263689927
H	8.185978206	5.700343407	6.098833213

H	8.975734562	3.001894227	9.379369526
H	7.683038497	3.744437286	4.609555298
H	8.486550025	1.054611554	7.898331832
H	7.836458740	1.426327766	5.518824594
H	5.836142028	9.016863126	14.190101025
H	8.966836318	14.418010936	14.106570312
H	14.505230120	11.299669898	13.944488342
H	11.376557223	5.882118333	13.901963970

$T_{iiii}[C_2H_5, CH_3, Ph]$ E: -618.396256 a.u.

C	9.211988732	6.726187004	12.147999998
C	8.136154293	7.653637972	11.595468715
C	10.555445867	7.042587369	11.497039656
C	7.399772410	7.295612576	10.455947476
C	7.858951180	8.898161058	12.174050312
C	10.944475498	6.416294420	10.302996954
C	11.431022355	7.989204293	12.043619336
C	6.421140731	8.119275969	9.885439258
O	7.613533181	6.038707884	9.850682321
C	6.874000364	9.757738989	11.671503567
C	12.147962383	6.706890090	9.646033834
O	10.124592072	5.419012999	9.731512681
C	12.664930924	8.300588936	11.459768347
C	6.168889100	9.335163866	10.534335660
C	6.597249790	11.120153662	12.303347899
C	12.992716916	7.635989258	10.267633292
C	13.605091346	9.340675187	12.060501145
O	5.146251244	10.151220270	10.000282159
C	7.496700179	12.181331112	11.677174338
O	14.241897404	7.872296039	9.654483592
C	13.294845539	10.719854411	11.484082033
C	7.087402544	12.884741953	10.534330843
C	8.767732262	12.476237854	12.186675684
C	13.933520651	11.170949289	10.319514789
C	12.342709752	11.566591214	12.065969596
O	5.806881904	12.652248701	9.985223081
C	7.884461435	13.841677352	9.893290840
C	9.604367850	13.441917244	11.612495066
O	14.924380375	10.370843336	9.707514940
C	13.642200282	12.401121992	9.715722525
C	12.031817345	12.824879606	11.536260853
C	9.130811246	14.112998173	10.473644740
C	10.992148031	13.738731057	12.176562137
C	12.698511358	13.208399855	10.362218878
O	9.924096528	15.114795827	9.867300064
O	12.430671384	14.467851221	9.782611771
C	13.612223158	9.325022212	13.601102372
C	6.681499195	11.095680887	13.841258101
C	9.269412672	6.730909712	13.687983474
C	11.034388897	13.698315651	13.716243494
C	14.670583255	10.270817200	14.176777619
C	10.095572544	14.733885584	14.341828863
C	5.659964350	10.131717573	14.452293373
C	10.245868811	5.681301886	14.227792637
C	4.162083372	11.770481395	8.044532932
C	3.086911461	12.454803823	8.633032124
C	4.139522023	11.424000740	6.683701587
C	1.981797867	12.795058806	7.846933749
C	3.026332447	11.763338178	5.907824613
C	1.952317004	12.450289676	6.487954514
C	11.467722343	15.982948340	7.775328989
C	12.409966279	16.953662336	8.149256008

C	10.844654611	16.030747193	6.516555310
C	12.732247074	17.975409960	7.249724162
C	11.165099439	17.063232676	5.630130041
C	12.112152157	18.029558863	5.994140790
C	15.821105483	8.790098633	7.679549887
C	15.868311799	9.307132738	6.374442963
C	16.836083685	7.945955256	8.157144007
C	16.945505638	8.979944558	5.544417526
C	17.902596461	7.615396646	7.315080767
C	17.957313014	8.131822946	6.012871748
C	8.450040678	4.407333656	7.872086466
C	8.285754389	4.507707676	6.481466297
C	8.287068119	3.178039840	8.530575704
C	7.952245255	3.364913312	5.745037210
C	7.950945113	2.043569075	7.785966998
C	7.783179008	2.136683456	6.396609319
P	8.868930709	5.926176041	8.756014404
P	5.662260508	11.348529866	8.955619193
P	11.083030177	14.548148124	8.803358531
P	14.358057570	9.201080906	8.656343527
O	10.700957365	13.287580638	8.079217113
O	6.874585535	11.001895033	8.136869767
O	9.124579982	7.152912680	7.925659010
O	13.116300244	9.581204995	7.898838670
H	8.942593064	5.701975051	11.840163152
H	8.426492766	9.207113227	13.053377017
H	11.144280966	8.496343651	12.966034280
H	5.558866106	11.384651548	12.043082754
H	14.625112767	9.081784381	11.730990892
H	9.117795469	11.936298948	13.067927449
H	11.827490569	11.235143154	12.968967020
H	11.241672892	14.770139556	11.875855161
H	13.800212121	8.288031518	13.927439461
H	12.618873394	9.596279601	13.997348598
H	6.512392448	12.123172188	14.205260289
H	7.697186354	10.817311737	14.170293749
H	8.249202556	6.539933734	14.061617297
H	9.551678456	7.728853962	14.064324273
H	12.076545235	13.880639932	14.028828747
H	10.775978055	12.691542754	14.086153685
H	15.675145070	9.996555816	13.813222914
H	14.681343305	10.235327240	15.277706290
H	10.358098015	15.749518702	14.001018322
H	10.153163097	14.713569120	15.441653538
H	4.636553332	10.408548355	14.148366099
H	5.707909169	10.142849833	15.552690808
H	9.961884374	4.674160472	13.879132745
H	10.256431255	5.674111812	15.329186479
H	3.127984776	12.732171376	9.687959061
H	5.000396661	10.911567424	6.247417176
H	1.148500231	13.340584818	8.293633550
H	3.002275063	11.501457193	4.847707674
H	1.093371719	12.727051097	5.873732540
H	12.900835149	16.889780674	9.121817710
H	10.140659626	15.244414753	6.233619525
H	13.478671418	18.722630037	7.526485814
H	10.688095529	17.103855624	4.648394439
H	12.376544954	18.819384623	5.288423204
H	15.051244332	9.938260656	6.016253732
H	16.774500765	7.536983348	9.167085049
H	16.987206400	9.374563371	4.526751075
H	18.686634400	6.945175650	7.673089436

H	18.784922984	7.861996216	5.353626517
H	8.424193313	5.476697881	5.995656081
H	8.425001343	3.114049448	9.611694059
H	7.823471835	3.434566193	4.662702813
H	7.818580176	1.086225396	8.292435461
H	7.520230009	1.247672334	5.818969150
H	5.845825992	9.102575545	14.105366169
H	9.052978087	14.539310296	14.043066165
H	14.472541454	11.308504940	13.863458516
H	11.267888622	5.885076451	13.869776844
C	12.492926535	6.099894999	8.315640279
H	13.580931775	5.988863173	8.204258023
H	12.005665067	5.122894364	8.190933646
H	12.133385434	6.770020809	7.515316934
C	14.258165045	12.799433517	8.404459917
H	15.262183051	12.364983689	8.296387087
H	13.625740334	12.415451702	7.584846445
H	14.315025756	13.893112265	8.311931970
C	7.443211941	14.483271609	8.608164432
H	7.666183832	13.794096677	7.774701217
H	6.359009545	14.667774152	8.614431381
H	7.978348485	15.427088592	8.436089678
C	5.730878722	7.739871980	8.606158234
H	6.369386335	8.040495862	7.757348556
H	5.580887404	6.651909562	8.551329985
H	4.763650308	8.252689461	8.514021784

Glycine E= -56.676346 a.u.

C	9.733720487	10.553569818	10.130830578
H	10.177722982	11.560402458	10.125971395
H	8.649379987	10.639362494	10.287736750
N	10.328134810	9.784646105	11.304648056
H	9.962160763	8.817048032	11.328848608
H	11.356069902	9.710167556	11.209687776
C	10.001215984	9.873952491	8.787393361
O	9.496986073	10.255924084	7.762169613
O	10.868237736	8.827437420	8.941162459
H	11.028660116	8.415733906	8.060351828
H	10.108096314	10.245532153	12.204002087

Sarcosine E=-63.560257 a.u.

C	9.710644334	10.561243304	9.519223809
H	10.150946053	11.570017601	9.508266177
H	8.623690530	10.654158434	9.656028302
N	10.275732368	9.822972116	10.714099850
H	9.937190960	8.846741607	10.693365958
H	11.300992753	9.752925104	10.603182057
C	9.928061091	10.467660837	12.034898703
H	10.369362236	9.870080936	12.843263702
H	10.338263638	11.485889313	12.037607734
H	8.834272979	10.494602380	12.125535831
C	10.001929223	9.870088951	8.188287089
O	9.514348836	10.235171649	7.148268717
O	10.873878173	8.829753187	8.367224333
H	11.054932539	8.416070015	7.491898902

T_{iiii}[C_2H_5, H, Ph]•glycine adduct E=-647.653125

C	9.276616108	6.665802608	12.214484112
C	8.166172879	7.558348064	11.674557172
C	10.601787881	7.028541098	11.552083086

C	7.408788530	7.173850785	10.556334215
C	7.865782235	8.803014568	12.246069486
C	10.999097504	6.416165132	10.353100114
C	11.476780106	7.979333191	12.098675887
C	6.399771375	7.974272216	10.034096833
O	7.651107073	5.944179514	9.905017510
C	6.862838453	9.649868418	11.752818355
C	12.201598963	6.728491125	9.724207650
O	10.205892180	5.421412351	9.749905699
C	12.705426321	8.319717124	11.513580702
C	6.140905900	9.202904786	10.634250883
C	6.584077428	11.015960461	12.371229020
C	13.040356643	7.669500890	10.313639473
C	13.643607850	9.347913972	12.132270881
O	5.130493969	9.996012756	10.060529121
C	7.478879316	12.066923311	11.724553237
O	14.272622953	7.910277015	9.676220659
C	13.331059967	10.726548882	11.561811150
C	7.065162413	12.753160619	10.570038951
C	8.744015691	12.391328576	12.235834572
C	13.982301232	11.200971214	10.413220785
C	12.358613436	11.560024099	12.133160364
O	5.803028081	12.513637926	9.996578531
C	7.863945246	13.711707106	9.955744831
C	9.582653766	13.356023482	11.657520511
O	14.968682295	10.422948334	9.764950215
C	13.685155436	12.438956545	9.853982388
C	12.023709049	12.816485774	11.610152922
C	9.108642241	14.003265299	10.504591143
C	10.951146863	13.695487295	12.241288025
C	12.709841791	13.228052163	10.455339271
O	9.870154602	15.000882376	9.864806909
O	12.422794942	14.462919677	9.847529600
C	13.645932987	9.320641600	13.672876070
C	6.674104915	11.007198237	13.909375480
C	9.352564400	6.662547767	13.753444900
C	10.980109382	13.652358116	13.782388054
C	14.707561830	10.257745373	14.256023594
C	10.000748592	14.653734817	14.400635091
C	5.653201443	10.051633592	14.534450817
C	10.370786890	5.644402992	14.275113190
C	4.218717633	11.575820296	8.026458415
C	3.105761941	12.219620338	8.593261715
C	4.253319873	11.247619519	6.660827482
C	2.017621213	12.535197407	7.775247487
C	3.154963448	11.566083912	5.854907486
C	2.042037489	12.209153164	6.411396104
C	11.407511600	15.879516116	7.784139512
C	12.239441555	16.934984769	8.194190063
C	10.832843879	15.862854338	6.501582975
C	12.501284540	17.977931814	7.301400834
C	11.094957070	16.918489385	5.623218742
C	11.931758577	17.969056618	6.020710290
C	15.778230370	8.875327152	7.656140691
C	15.706344472	9.292904987	6.316060611
C	16.880877175	8.148029717	8.135492814
C	16.758114109	8.980608019	5.448909826
C	17.920806135	7.838161605	7.254897512
C	17.860031689	8.253629042	5.917448390
C	8.587585255	4.510084400	7.792478823
C	8.220614960	4.736071331	6.455718124
C	8.691108992	3.207919736	8.310957154

C	7.950492380	3.639169624	5.630467268
C	8.419213581	2.122563049	7.473953820
C	8.049350047	2.337418635	6.138435659
P	8.917701228	5.933072153	8.829987503
P	5.669255861	11.178530332	9.006464837
P	11.083062662	14.469738783	8.849505634
P	14.390255076	9.265541125	8.721172347
O	10.780160199	13.138015768	8.201527707
O	6.937767038	10.795979356	8.281159642
O	9.133866227	7.268966544	8.143989302
O	13.095462186	9.668522146	8.041579990
H	9.040485074	5.634057136	11.903939691
H	8.435667235	9.125997264	13.119276830
H	11.199125811	8.458475791	13.038856248
H	5.843529368	7.662185341	9.150724299
H	12.484705151	6.238452035	8.792599007
H	5.544193083	11.275189997	12.109997622
H	14.664812602	9.090553616	11.804136524
H	9.082937072	11.886032773	13.141907208
H	11.841793094	11.215403851	13.030461915
H	7.523710692	14.218467165	9.052969026
H	14.182284748	12.772408686	8.943391404
H	11.170965078	14.734790769	11.943798986
H	13.829868626	8.280932325	13.991121519
H	12.652880394	9.592390186	14.069314994
H	6.505859423	12.038334172	14.262576187
H	7.691190470	10.732158637	14.238473445
H	8.344637100	6.431358712	14.135740237
H	9.599815271	7.668301029	14.133712418
H	12.012246149	13.870875160	14.103684736
H	10.755022011	12.635697213	14.148172709
H	15.709633964	9.989521147	13.882897404
H	14.724535140	10.201682066	15.355104811
H	10.222597020	15.676409677	14.053413334
H	10.062158367	14.643556906	15.499696032
H	4.629397632	10.324946001	14.229847515
H	5.703611488	10.080150039	15.633781584
H	10.119372771	4.629807139	13.924290378
H	10.388923708	5.630523811	15.375763413
H	3.099737711	12.481942340	9.652774725
H	5.138010797	10.763527395	6.240853555
H	1.151973534	13.044309946	8.202020911
H	3.171682815	11.318350521	4.791739463
H	1.190766552	12.463324583	5.776743844
H	12.689557416	16.927147863	9.188364936
H	10.203949801	15.024011827	6.194873075
H	13.160183921	18.793087352	7.604463176
H	10.654664335	16.915131758	4.624260348
H	12.146401243	18.781527142	5.324235037
H	14.830157408	9.841734657	5.963337713
H	16.915555012	7.817116562	9.174813227
H	16.714624938	9.298648025	4.405287432
H	18.775759707	7.263097308	7.612606437
H	18.673144631	8.004070415	5.233047913
H	8.156678116	5.757338104	6.073375269
H	8.991582816	3.048140005	9.348151751
H	7.663958290	3.801105166	4.589550206
H	8.499233030	1.107354066	7.864903074
H	7.840378333	1.484512765	5.489162735
H	5.835386094	9.015480460	14.206227220
H	8.965023592	14.417467286	14.108743352
H	14.508974280	11.301725819	13.965514273

H	11.385006480	5.882467057	13.915888074
C	9.803956183	10.417489125	7.108653041
H	10.235245350	11.429670685	7.064242896
H	8.715132555	10.513415673	7.238283083
N	10.359380242	9.734105665	8.323057460
H	9.945360809	8.764979617	8.402169199
H	11.414659436	9.667280748	8.271616747
H	10.103910998	10.289858845	9.151886392
C	10.087569763	9.695464002	5.814157619
O	9.592019274	10.031559509	4.753636704
O	10.960012963	8.652811212	5.956882865
H	11.069955243	8.258693206	5.064263213

T_{iiii}[C_2H_5, H, Ph]•sarcosine adduct E= -654.542345

C	9.279505875	6.559031030	12.499464960
C	8.168950007	7.446640332	11.952590154
C	10.603316501	6.923457482	11.836219370
C	7.415145755	7.057245665	10.833644576
C	7.866989653	8.692555887	12.519426364
C	10.995602816	6.323668968	10.629038978
C	11.478584289	7.871728931	12.386712377
C	6.409196789	7.858656243	10.305038521
O	7.654894153	5.818692376	10.195734096
C	6.861429824	9.535359726	12.025773636
C	12.191672658	6.651687402	9.994754615
O	10.212970098	5.317242346	10.030596975
C	12.701437951	8.224948676	11.797385899
C	6.141841541	9.085574665	10.906668654
C	6.576877813	10.898095962	12.647402729
C	13.032705417	7.588542658	10.588870949
C	13.633791889	9.256949222	12.417375808
O	5.120710851	9.870338789	10.339342230
C	7.469109773	11.950975234	12.002141735
O	14.265595645	7.829911660	9.955252608
C	13.316940607	10.635071585	11.847012612
C	7.056580758	12.631355395	10.844011414
C	8.730618176	12.280460208	12.516686757
C	13.969473404	11.114104133	10.701414116
C	12.340896071	11.464253631	12.417122852
O	5.792042990	12.389686451	10.276598407
C	7.854443517	13.592188247	10.229641014
C	9.564955775	13.250023943	11.941760691
O	14.963805116	10.342599986	10.057765967
C	13.669205081	12.352580762	10.143804012
C	12.005142533	12.721768160	11.897897775
C	9.094435887	13.894287879	10.785689446
C	10.929212591	13.594729503	12.531051847
C	12.691147778	13.139105434	10.744672187
O	9.850873622	14.904448140	10.160134783
O	12.409904111	14.381059300	10.146829616
C	13.632364533	9.230412977	13.958097143
C	6.666209506	10.884853142	14.185445614
C	9.351620467	6.566169800	14.038560662
C	10.955165678	13.542487349	14.071746360
C	14.682796065	10.179513628	14.541925112
C	9.980084409	14.542328482	14.699095987
C	5.653129086	9.919063990	14.807727995
C	10.374357753	5.556770910	14.567244022
C	4.191171560	11.462789938	8.311185963
C	3.076496995	12.106159080	8.874720323
C	4.238124824	11.150229824	6.941896736
C	1.999364914	12.438414538	8.048999911

C	3.150107818	11.484167535	6.128802974
C	2.036182227	12.128326361	6.681689571
C	11.387582941	15.840819944	8.108104854
C	12.197482433	16.905548782	8.535401636
C	10.810161656	15.833982439	6.826589252
C	12.428828076	17.972689811	7.663298431
C	11.043506163	16.911721265	5.967320514
C	11.853800868	17.975410595	6.384917239
C	15.795873988	8.797037957	7.953177224
C	15.715779341	9.186863849	6.605325071
C	16.906238523	8.089767669	8.443684755
C	16.766376103	8.865230587	5.740243755
C	17.944426880	7.768183893	7.565668528
C	17.874286795	8.154157987	6.219173673
C	8.584642416	4.368466650	8.084059852
C	8.222756341	4.609187975	6.747937246
C	8.679337975	3.063099367	8.593258332
C	7.948330893	3.522210644	5.912064656
C	8.404971137	1.988015257	7.744567545
C	8.039878629	2.216328299	6.409939681
P	8.913423849	5.797715919	9.110323053
P	5.643948018	11.059049935	9.284150800
P	11.076145806	14.407064174	9.141835916
P	14.397472247	9.188257873	9.003714578
O	10.785140646	13.091725208	8.458552226
O	6.905546291	10.681911113	8.545352638
O	9.113113693	7.117235843	8.390894880
O	13.112665565	9.591166986	8.307970114
H	9.046555840	5.525060339	12.193820246
H	8.436937459	9.019601679	13.390988429
H	11.203726220	8.341319290	13.332206429
H	5.853919785	7.543626693	9.422075604
H	12.472033758	6.171332847	9.057243823
H	5.536417828	11.153923070	12.385734825
H	14.656655157	9.003634303	12.091118548
H	9.068911863	11.776230169	13.423373074
H	11.822788395	11.116103852	13.312260837
H	7.514463219	14.097881325	9.325986534
H	14.171525539	12.690214571	9.237632300
H	11.146048954	14.635929396	12.238620504
H	13.826446475	8.192701503	14.278371704
H	12.635309916	9.493047584	14.351502457
H	6.489806883	11.913477016	14.541702043
H	7.685265019	10.616944634	14.514072380
H	8.344427666	6.330721648	14.420161528
H	9.591586235	7.575870678	14.413669964
H	11.987686745	13.754916178	14.396321089
H	10.725711162	12.524346200	14.430466053
H	15.689756507	9.915193603	14.179045211
H	14.690044026	10.132675676	15.641526369
H	10.214754118	15.569143989	14.374007380
H	10.032564219	14.510638050	15.798176415
H	4.627102429	10.183558308	14.503212697
H	5.701974633	9.946430674	15.907043131
H	10.131931926	4.540731937	14.214775224
H	10.386857950	5.543567277	15.667835542
H	3.061108859	12.357033931	9.936847116
H	5.124649450	10.667177387	6.524806211
H	1.133612715	12.949734119	8.472593445
H	3.176022507	11.248797977	5.063054167
H	1.193413797	12.396510050	6.041634852
H	12.652050602	16.887526043	9.526996431

H	10.202661374	14.984401500	6.505808471
H	13.067448611	18.798415310	7.980468715
H	10.601866016	16.915438116	4.968692057
H	12.045784509	18.806123722	5.703564839
H	14.833012732	9.720802525	6.246329836
H	16.947518459	7.782439611	9.490070666
H	16.715871594	9.161592751	4.690561495
H	18.804532466	7.206320264	7.931978359
H	18.685956322	7.894121153	5.536848615
H	8.165171608	5.634584994	6.376479640
H	8.971749904	2.892577869	9.630992596
H	7.663366685	3.694377316	4.872228657
H	8.477385615	0.970741831	8.127696651
H	7.826183405	1.370287373	5.753425814
H	5.845040028	8.885384557	14.477963067
H	8.944295585	14.321898950	14.395023643
H	14.478723973	11.219551781	14.240743341
H	11.388332398	5.802158158	14.212828639
C	9.818028446	10.265349834	7.436646124
H	10.250666997	11.278453062	7.422965135
H	8.730170058	10.362767389	7.572685879
N	10.372014062	9.538890010	8.621570982
H	9.991586278	8.557647217	8.608255168
H	11.419963403	9.489437708	8.538977031
C	9.995900158	10.197622669	9.913391389
H	10.424912511	9.604410101	10.731594471
H	10.399804034	11.218117020	9.913022197
H	8.900089719	10.222357652	9.979863572
C	10.091140160	9.583075464	6.116219543
O	9.592702211	9.942754755	5.064899486
O	10.963702363	8.533866108	6.227233818
H	11.068426592	8.163745827	5.323876660

T_{iiii}[C_2H_5, CH_3, Ph]•glycine adduct E= -675.218942

C	9.243214707	6.727846965	12.248197816
C	8.142105766	7.627007177	11.695284397
C	10.572195654	7.068529471	11.579431893
C	7.381979095	7.238824854	10.580625174
C	7.864643160	8.882568469	12.252121167
C	10.961731203	6.444760819	10.384218335
C	11.447312925	8.021208251	12.118739822
C	6.384636940	8.039597774	10.012101037
O	7.620004456	5.983095374	9.967633513
C	6.870462066	9.729112691	11.744050689
C	12.157830648	6.741969299	9.715367977
O	10.148694531	5.438330735	9.816022506
C	12.678076480	8.337413880	11.528683264
C	6.150388967	9.277024715	10.627692822
C	6.601702226	11.105279912	12.348406519
C	13.000280911	7.677599671	10.331829512
C	13.625895558	9.362871981	12.140519288
O	5.146269414	10.087988585	10.059177261
C	7.511146011	12.146220331	11.702702233
O	14.247305339	7.908691809	9.709877392
C	13.326798874	10.744692685	11.564892886
C	7.108155813	12.831719051	10.545099585
C	8.776391244	12.453697069	12.220908834
C	13.985968193	11.207077147	10.416599641
C	12.361053471	11.586252437	12.132281159
O	5.834942776	12.584570785	9.990731150
C	7.905457798	13.784394109	9.899148146
C	9.615069693	13.415329291	11.640136158

O	14.971255332	10.398925945	9.798671497
C	13.710924920	12.440594618	9.814767083
C	12.050776385	12.843504255	11.597259632
C	9.147463673	14.060903365	10.485554550
C	10.989340076	13.743489592	12.219506181
C	12.741604174	13.234987921	10.439773677
O	9.935299908	15.050856325	9.859365907
O	12.458470969	14.476610819	9.834777537
C	13.625304077	9.344413057	13.681652661
C	6.682772635	11.110311416	13.887501267
C	9.318931800	6.752703097	13.787732769
C	11.015421443	13.715055357	13.760385381
C	14.701891592	10.268356665	14.258836807
C	10.048963174	14.736590908	14.365973165
C	5.645066171	10.177461608	14.518128127
C	10.330254749	5.739308040	14.331562311
C	4.244913840	11.651254150	8.017906078
C	3.137791120	12.311927174	8.576869350
C	4.264378206	11.284287535	6.662062754
C	2.040254007	12.603830299	7.762092193
C	3.157812133	11.579183690	5.858538299
C	2.050150566	12.237549933	6.408090581
C	11.459671093	15.880341334	7.748270484
C	12.319338815	16.926007819	8.124193300
C	10.853163253	15.859245489	6.480243234
C	12.573876753	17.956005923	7.213515066
C	11.109667940	16.899964244	5.582304331
C	11.970327543	17.943513462	5.948025001
C	15.764788387	8.860633089	7.681050952
C	15.728857499	9.372776855	6.372742317
C	16.831178320	8.057026290	8.119735776
C	16.777151281	9.077600900	5.495597143
C	17.869518078	7.766092962	7.230071355
C	17.843048899	8.275405995	5.924071839
C	8.534054536	4.545031415	7.830891329
C	8.117358627	4.804300037	6.513684043
C	8.689491149	3.229426864	8.299900781
C	7.848435799	3.728975887	5.660087193
C	8.419296343	2.165233701	7.434414131
C	7.998318406	2.414061288	6.120302275
P	8.875592352	5.953969299	8.886761957
P	5.694746603	11.256915948	9.001411006
P	11.124155329	14.491234056	8.837825985
P	14.383696145	9.254047155	8.754129536
O	10.793713436	13.161199463	8.197848484
O	6.960493513	10.869647199	8.272382408
O	9.107768436	7.284973307	8.192906038
O	13.095241087	9.675226223	8.070058418
H	8.995107502	5.693949163	11.956258484
H	8.437966957	9.211299575	13.120437647
H	11.172110749	8.514479676	13.051709643
H	5.566058039	11.372734666	12.081219467
H	14.645247165	9.094728391	11.817090007
H	9.111165817	11.943970837	13.125777546
H	11.836422764	11.254415723	13.029570749
H	11.223065438	14.776643911	11.913303367
H	13.791870022	8.303928870	14.007597909
H	12.636303802	9.635404899	14.074632195
H	6.527663154	12.147986737	14.227402682
H	7.693700198	10.824913811	14.225884392
H	8.309104379	6.535095752	14.173368942
H	9.572082816	7.763615766	14.150019304

H	12.049496898	13.923558063	14.082137657
H	10.774917656	12.705831319	14.136319331
H	15.700799430	9.974139159	13.896517297
H	14.710560592	10.228490831	15.358870736
H	10.289140774	15.753482192	14.013927809
H	10.104302713	14.732638660	15.465510353
H	4.626767290	10.462328491	14.205743087
H	5.690250222	10.217847197	15.617288665
H	10.073508540	4.719106021	14.001415071
H	10.347198141	5.748308067	15.432222242
H	3.142576578	12.602769606	9.628886852
H	5.144241243	10.786840004	6.247548947
H	1.178273159	13.123921093	8.183517282
H	3.163438066	11.300913044	4.802724798
H	1.192063176	12.473155665	5.775308822
H	12.793854475	16.920696164	9.106833152
H	10.203554532	15.026920874	6.199823768
H	13.251673440	18.764980369	7.490973038
H	10.645496666	16.891796234	4.594055066
H	12.178273249	18.746644678	5.238259725
H	14.881123239	9.981612790	6.050338378
H	16.838440404	7.654728956	9.134279865
H	16.759690919	9.469250372	4.476545179
H	18.697663674	7.134458923	7.555662166
H	18.655272487	8.040926496	5.233191580
H	8.016012879	5.835729506	6.168453957
H	9.027472885	3.043309967	9.320921255
H	7.524091955	3.918129407	4.634787995
H	8.540933664	1.139886731	7.786536378
H	7.790082355	1.577489286	5.449654103
H	5.813479347	9.135214992	14.202362223
H	9.010996845	14.515416481	14.070014889
H	14.525506962	11.311611029	13.951027747
H	11.345765506	5.965158547	13.968207134
C	9.833354185	10.366253145	7.211440638
H	10.279922643	11.370708786	7.143451244
H	8.747246791	10.483718584	7.343978009
N	10.385852066	9.698493307	8.435559500
H	9.964147719	8.732580905	8.521756342
H	11.442471717	9.630898460	8.378761386
H	10.134185836	10.260685452	9.261027768
C	10.096121117	9.613441964	5.928822240
O	9.582984633	9.923147958	4.868675605
O	10.976330023	8.575776705	6.073429358
H	11.069382072	8.168818691	5.184655244
C	14.361341024	12.868443456	8.529113398
H	15.332949201	12.373906334	8.394638375
H	13.710230813	12.592938093	7.681107714
H	14.498374532	13.958735004	8.505553888
C	7.484158283	14.442315263	8.615238108
H	7.909952233	13.885433612	7.762016586
H	6.390794470	14.440766614	8.511671677
H	7.857800368	15.475011201	8.565117653
C	5.646329143	7.629491349	8.768948858
H	6.166217063	8.037746553	7.884396890
H	5.609699814	6.535574876	8.674296591
H	4.623885191	8.032503987	8.773363163
C	12.509436172	6.115460604	8.394613195
H	13.597315256	5.993304266	8.297664379
H	12.019064323	5.139274300	8.280242494
H	12.167455029	6.771210414	7.573951194

T_{iiii}[C_2H_5, CH_3, Ph]•sarcosine adduct E= -682.108819

C	9.262634231	6.658563951	12.228126475
C	8.150611018	7.551477767	11.687632885
C	10.584661840	7.023989265	11.559120326
C	7.386732817	7.161343851	10.576824305
C	7.867638364	8.802324082	12.250202607
C	10.962449665	6.436109683	10.341698917
C	11.459901601	7.968324589	12.113957881
C	6.377098322	7.953638893	10.018497573
O	7.628415132	5.908563224	9.961217421
C	6.863300295	9.641901027	11.751080194
C	12.148751717	6.760438537	9.667150835
O	10.163479703	5.422859641	9.768108538
C	12.677988255	8.315955201	11.514015950
C	6.135209883	9.186032757	10.641163954
C	6.591652228	11.016758627	12.356659603
C	12.992413321	7.685333994	10.299107448
C	13.618716961	9.347208419	12.129228833
O	5.114561059	9.989102411	10.090032786
C	7.490566243	12.061491421	11.703119680
O	14.239300238	7.922507828	9.683321947
C	13.308055767	10.730107271	11.559421177
C	7.078656668	12.737444610	10.542934738
C	8.751102008	12.386200754	12.219506439
C	13.962761454	11.203551370	10.412765798
C	12.336330295	11.561705574	12.131328879
O	5.801288825	12.484056337	10.001892261
C	7.865927068	13.695967242	9.891596751
C	9.577002384	13.356302036	11.636040988
O	14.957410909	10.408899620	9.791878436
C	13.679046715	12.438967131	9.817486850
C	12.015951159	12.817881199	11.601317130
C	9.104238499	13.991893420	10.477814316
C	10.943087384	13.705820560	12.220460933
C	12.702326597	13.222396413	10.445907791
O	9.872160526	15.005107018	9.862129039
O	12.413624672	14.471558393	9.858633894
C	13.621539664	9.324659085	13.669964573
C	6.683462079	11.021825617	13.894454374
C	9.340619028	6.663534712	13.767027367
C	10.965875597	13.683105795	13.760935317
C	14.688344700	10.258315471	14.250116160
C	9.987846960	14.697854983	14.359702540
C	5.650914894	10.086402056	14.529240713
C	10.362638554	5.650826567	14.291609740
C	4.197070524	11.561092206	8.039895006
C	3.097475338	12.235837878	8.596585949
C	4.229770037	11.221706339	6.676640644
C	2.021436016	12.573379760	7.771094396
C	3.143440345	11.560712568	5.863161313
C	2.044490268	12.236105464	6.409675344
C	11.428598677	15.913185615	7.794291082
C	12.318939725	16.929374236	8.178543863
C	10.816672198	15.924274182	6.528904288
C	12.598914540	17.962419487	7.279254544
C	11.099242961	16.967117999	5.642338854
C	11.992267502	17.980064896	6.015770392
C	15.772890199	8.874864102	7.671806310
C	15.732164421	9.356315362	6.351903643
C	16.841087755	8.082226793	8.125534327
C	16.777538217	9.041139522	5.478185480
C	17.876210716	7.770657131	7.239222347

C	17.844608697	8.248590176	5.921509962
C	8.527886214	4.462868846	7.828253935
C	8.147611570	4.700191794	6.495942699
C	8.647629848	3.156655177	8.331568841
C	7.880702026	3.610828572	5.660073649
C	8.381814321	2.078504545	7.483401229
C	7.998765765	2.304939727	6.153523519
P	8.861824959	5.893686487	8.854812101
P	5.645982477	11.153510714	9.018436548
P	11.090022728	14.497223113	8.847154391
P	14.382047889	9.271190532	8.731236385
O	10.789214434	13.181628493	8.165876644
O	6.901370902	10.757865881	8.276519621
O	9.047083559	7.213910144	8.129492896
O	13.100936173	9.689315595	8.034133900
H	9.026361125	5.625745228	11.922811580
H	8.448160772	9.134726032	13.112456118
H	11.191539209	8.435009999	13.062611088
H	5.552852198	11.278828250	12.096741550
H	14.639315152	9.088783479	11.801637001
H	9.091969730	11.885231074	13.126818919
H	11.811131704	11.221087768	13.025204219
H	11.163812452	14.741176068	11.912724339
H	13.800114067	8.285092360	13.992405833
H	12.629941877	9.603826586	14.065145063
H	6.528269542	12.058831729	14.236195874
H	7.697020395	10.737997206	14.226177324
H	8.333902575	6.429645717	14.151077612
H	9.583698978	7.672023569	14.143268108
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H	10.736035103	12.672282733	14.139707925
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H	14.700233026	10.211269329	15.349823122
H	10.218428181	15.715271339	14.002673536
H	10.040457269	14.699384242	15.459401858
H	4.630624364	10.372813317	14.225084401
H	5.704445118	10.121691395	15.628155170
H	10.116019875	4.635027516	13.940811580
H	10.379382676	5.637742055	15.392253636
H	3.094594301	12.506953451	9.653864999
H	5.105641461	10.715615113	6.264215000
H	1.166778952	13.107558122	8.189828826
H	3.158760268	11.305308870	4.801632619
H	1.203619741	12.508798254	5.768670150
H	12.798787738	16.897336979	9.158012801
H	10.145766037	15.112226109	6.239571639
H	13.301576792	18.747901350	7.562380157
H	10.632040326	16.983356044	4.655635638
H	12.222589155	18.782933837	5.312805616
H	14.881628581	9.954915005	6.018013610
H	16.851681144	7.703447067	9.149085424
H	16.755632547	9.407349705	4.449790528
H	18.705434181	7.146678330	7.576648791
H	18.653544566	7.996363904	5.233040097
H	8.072314994	5.725675234	6.127275743
H	8.954522700	2.988425956	9.365502140
H	7.585006233	3.781167896	4.622888168
H	8.478083035	1.060092538	7.860749433
H	7.795836517	1.456782795	5.496095738
H	5.817077076	9.045627460	14.207716092
H	8.952911805	14.464124074	14.062292722
H	14.498528123	11.301214188	13.949464625

H	11.375899498	5.893559659	13.933286022
C	9.830538128	10.314025802	7.224489246
H	10.276365355	11.321560321	7.199179509
H	8.743848638	10.427902230	7.356739457
N	10.372607994	9.599089100	8.420402404
H	9.976682375	8.623638960	8.418059683
H	11.420848900	9.542434642	8.338074766
C	9.999791003	10.289452000	9.697238492
H	10.425919614	9.714192667	10.528751820
H	10.409763730	11.307278144	9.673005446
H	8.904379801	10.322008002	9.764066042
C	10.093371140	9.615481315	5.911689207
O	9.585349499	9.963525223	4.861246006
O	10.969400977	8.566618831	6.019143116
H	11.061448058	8.192878605	5.115826906
C	5.633282455	7.535109492	8.781891384
H	6.161767247	7.918977416	7.891818367
H	5.580966318	6.440225860	8.706092346
H	4.616850097	7.952645523	8.778648993
C	12.496726138	6.165161172	8.331063211
H	13.584357779	6.043551241	8.230113548
H	12.004557632	5.192754166	8.194695103
H	12.155730947	6.839926337	7.525651751
C	14.336022808	12.876639261	8.538579877
H	15.330242082	12.421562140	8.431395568
H	13.714827832	12.559490835	7.682878991
H	14.427158507	13.971108979	8.501497163
C	7.431476649	14.352858263	8.611428290
H	7.888123140	13.824770483	7.755817489
H	6.340199879	14.312014524	8.496441371
H	7.766462807	15.399723539	8.578462249

References.

1 (a) I. L.Swift *Surf. Interface Anal.* **1982**, *4*, 47–51. (b) D. Briggs & G. Beamson *Anal. Chem.* **1992**, *64,* 1729–1736.

2. E. U. Thoden van Velzen, J. F. J. Engbersen & D. N. Reinhoudt, Synthesis of self-assembling resorcin[4]arene tetrasulfide adsorbates. *Synthesis* **1995**, 989-997.

3. SADABS Bruker AXS; Madison, Wisconsin, USA, 2004; SAINT, Software Users Guide, Version 6.0; Bruker Analytical X-ray Systems. In *Software Users Guide, Version 6.0; Bruker Analytical X-ray Systems*, Madison, WI **1999**. Sheldrick, G. M. *SADABS v2.03: Area-Detector Absorption Correction*. University of Göttingen, Germany **1999**.

4. A. Altomare, M. C. Burla, M. Camalli, G. L. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, SIR97: a new tool for crystal structure determination and refinement. *J. Appl. Crystallogr.***1999**, *32,* 115–119.

5. G. M. Sheldrick, *SHELXL-97. Program for Crystal Structure Refinement*. University of Göttingen, Germany, **1997**; G. M. Sheldrick, A short history of SHELX. *Acta Cryst*. **2008**, *A64***,** 112–122.

6. L. J. Farrugia, WinGX suite for small-molecule single-crystal crystallography. *J. Appl. Crystallogr*. **1999**, *32*, 837-838**.**

7. SQUEEZE -. P. v.d Sluis, A. L. Spek, BYPASS: an effective method for the refinement of crystal structures containing disordered solvent regions. *Acta Crystallogr.* **1990**, *A46***,** 194–201.

8. PARST – M. Nardelli, Parst: A system of fortran routines for calculating molecular structure parameters from results of crystal structure analyses. *Comput. Chem*. **1983**, *7,* 95–98; M. Nardelli, PARST95 - an update to PARST: a system of Fortran routines for calculating molecular structure parameters from the results of crystal structure analyses. *J. Appl. Crystallogr.* **1995**, *28,* 659.

9. F. Bianchi et al. Fully Automated Solid-Phase Microextraction-Fast Gas Chromatography-Mass Spectrometry Method Using a New Ionic Liquid Column for High-Throughput Analysis of Sarcosine and N-ethylglycine in Human Urine and Urinary Sediments. *Anal. Chim. Acta* **2011**, *707*, 197-203.

10. J. Vande Vondele, M. Krack, F. Mohamed, M. Parrinello, T. Chassaing, J. Hutter, QUICKSTEP: Fast and accurate density functional calculations using a mixed Gaussian and plane waves approach. *Comput. Phys. Commun*. **2005**, *67,* 103-128.

11. The CP2K developers group. http://cp2k.berlios.de/

12. S. Grimme, Semiempirical GGA-type density functional constructed with a long-range dispersion correction. *J. Comput. Chem.* **2006**, *27*, 1787-1799.

13. S. Goedecker, M. Teter, J. Hutter, Separable dual-space Gaussian pseudopotentials. *Phys. Rev. B* **1996**, *54*, 1703-1710.

14. J.P. Perdew, K. Burke, M. Ernzerhof, Generalized Gradient Approximation Made Simple. *Phys. Rev. Lett.* **1996**, *77*, 3865-3868.