Supporting Information to

Macrocyclic versus open-chain carbazole receptors for carboxylate binding

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Contents

1. Synthesis and characterization of compounds

1.1 Instruments and methods

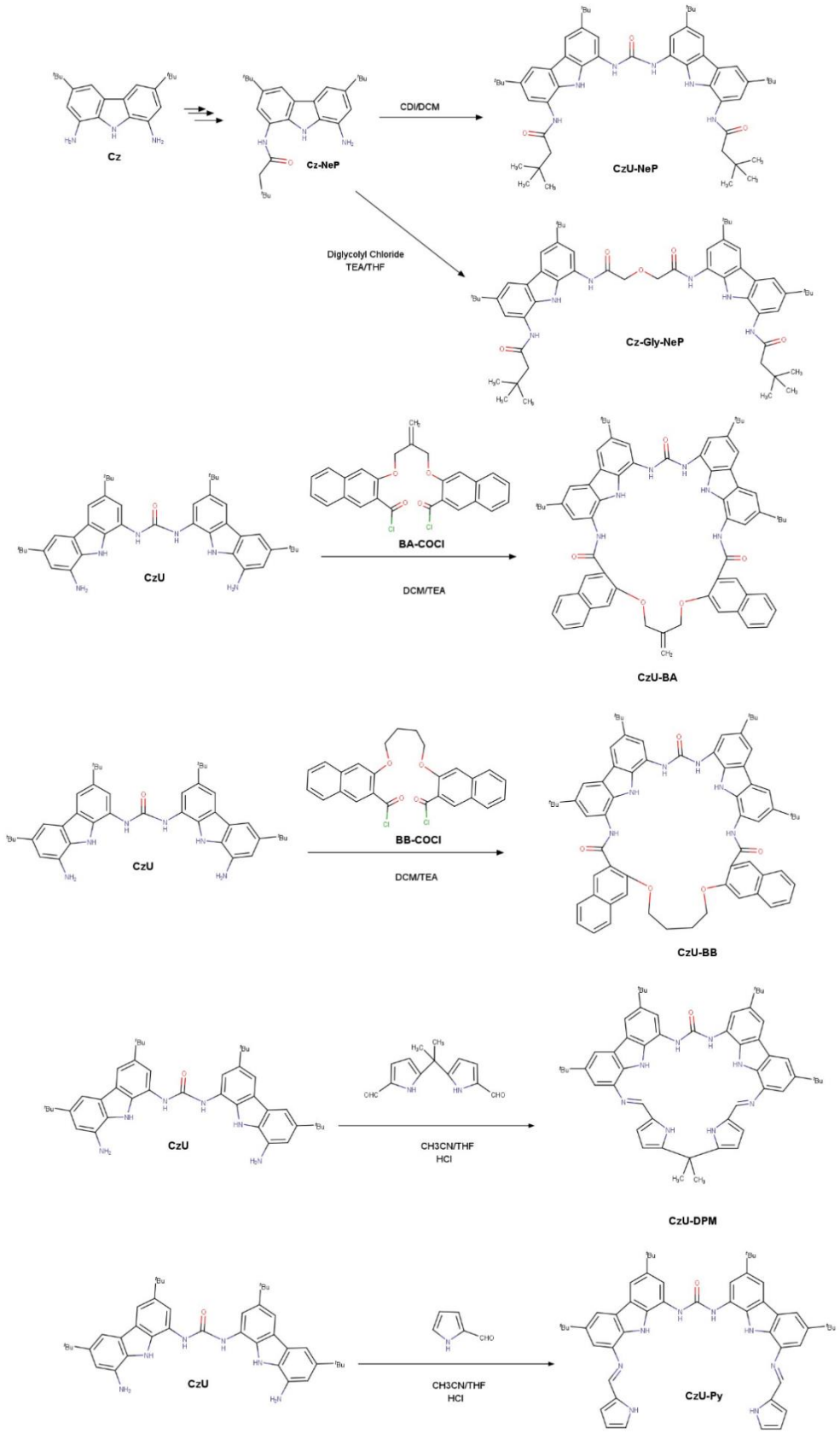
NMR measurements, characterization and assessment of purity of all synthesis products were carried out on a Bruker Avance-III 700 MHz NMR spectrometer. All spectra were recorded using TopSpin 3.2 software and the chemical shifts calibrated against the residual solvent signal. Chemical shifts were reported in parts per million (ppm) and coupling constants J were given in hertz (Hz). Data was reported as follows: chemical shift, multiplicity (s-singlet, bs – broad singlet, d – doublet, dd – doublet of doublets), coupling constant and integration. The residual signal of DMSO-d_6 solvent was used as an internal reference standard (δ_H = 2.500 ppm and δ_C = 39.50 ppm).

High-resolution mass spectrometric analyses of the substances were done using ESI ionization. For ESI-measurements a hybrid mass spectrometer Varian J-320 triple quadrupole instrument coupled with Varian 910 FT-ICR instrument with 7 T magnet were used. The ions from the ion source are first directed through the quadrupole system (which can also be used for low-resolution MS analysis) into the FT-ICR mass spectrometer for high resolution mass spectral analysis. For ionization, a modified nano-ESI source was used with the following parameters: spray chamber temperature, 40 °C; API-drying gas (N_2), 10 psi at 150 °C; ESI needle voltage 1800-2500 V, shield voltage, 300 V; and capillary voltage, 40 V. Solvents used for different receptors were MeOH, and 50% MeOH/50% DCM with 0.1% HCOOH with an analyte concentration of approximately 0.5-1 mg/ml. Sample infusion rate was generally 5 ml/min. For calibration of the m/z axis, samples were spiked with an in-house internal calibration solution, which contained ions with the following exact m/z values: $C_{16}H_{36}N^+$ (m/z = 242.28423); $C_{19}H_{29}N_4PF_3^+$ (m/z = 401.20765); $C_{26}H_{45}N_7P_2Cl^+$ (m/z = 552.28947); $C_{26}H_{64}N_{13}P_4^+$ (m/z = 682.43526); $C_{42}H_{78}N_{13}P_4^+$ (m/z = 888.54481); and $C_{44}H_{82}N_{13}P_4^+$ (m/z = 916.57611). The concentration of the calibrants in the infused solutions remained within 0.5–1.0 μM.

COSMO-RS calculations were done using COSMOThermX19 parametrization BP_TZVP_C19 (solvent: DMSO with 0.5% water).

1.2 Synthesis

Unless stated otherwise, reagents were obtained from commercial sources and used without purification. DMSO-d6 for NMR was obtained from Deutero with at least 99.8% purity. Dry solvents were prepared at least 72 h before use in round-bottomed flasks supplied with 3 Å molecular sieves under an argon atmosphere. Water used in this work was obtained from a MilliQ Advantage A10 system or from an ELGA PURELAB® Ultra system.

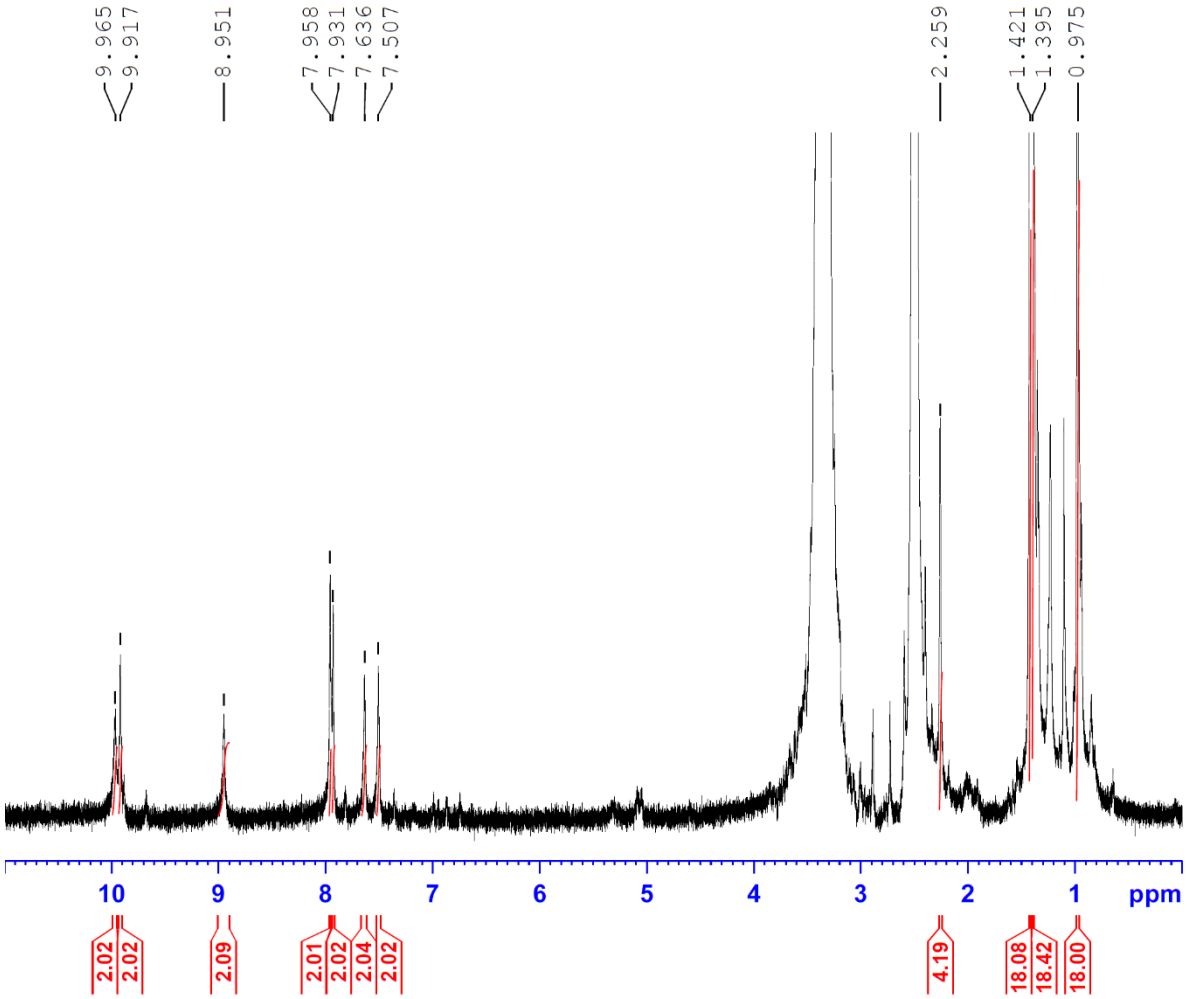


Scheme 1 Synthesis procedure

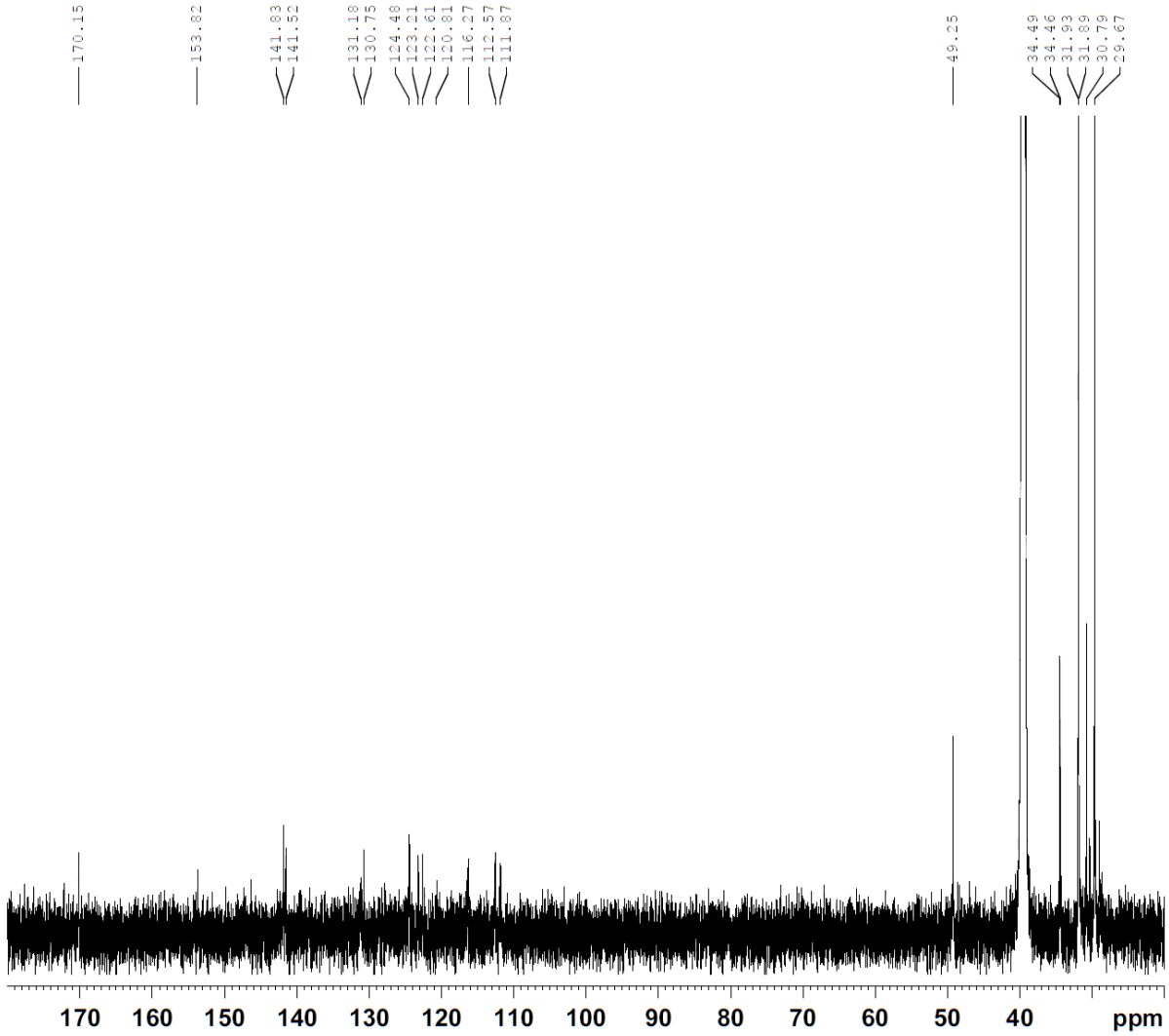
Compounds Cz and Cz-NeP were prepared as described in references.[1–3]

1.3 **Analytical spectra**

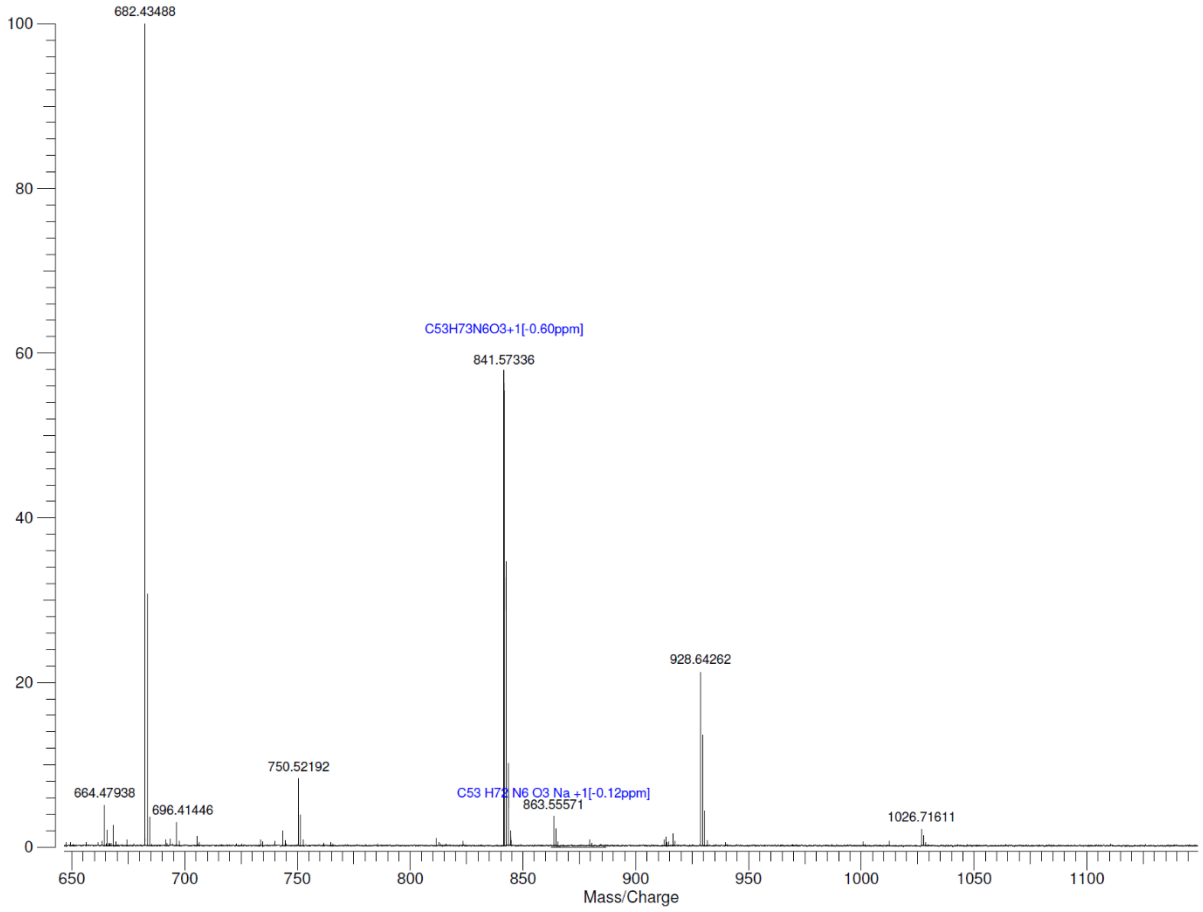
1.3.1. ^{1}H NMR of CzU-NeP in DMSO-d_6



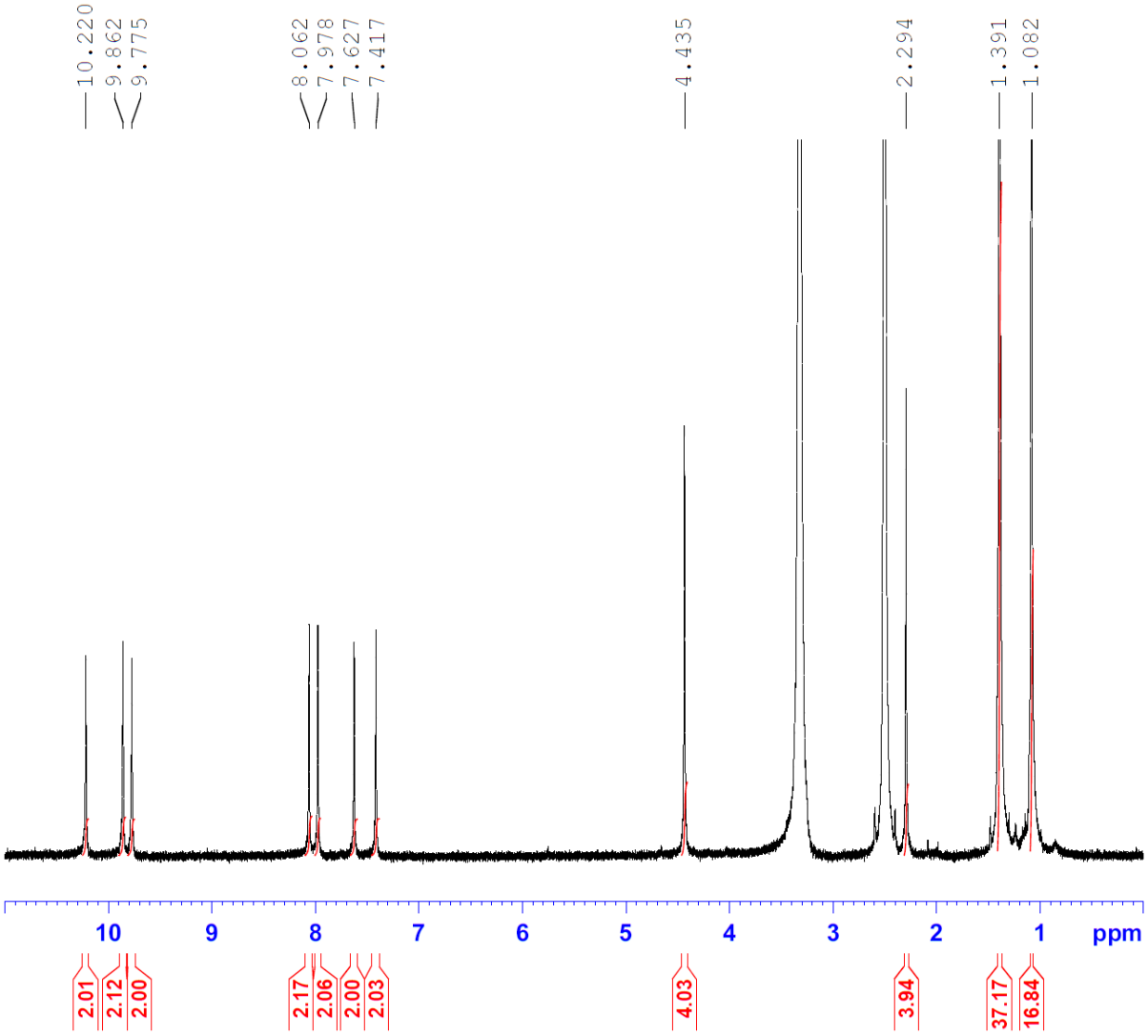
1.3.2. ^{13}C NMR of CzU-NeP in DMSO-d_6



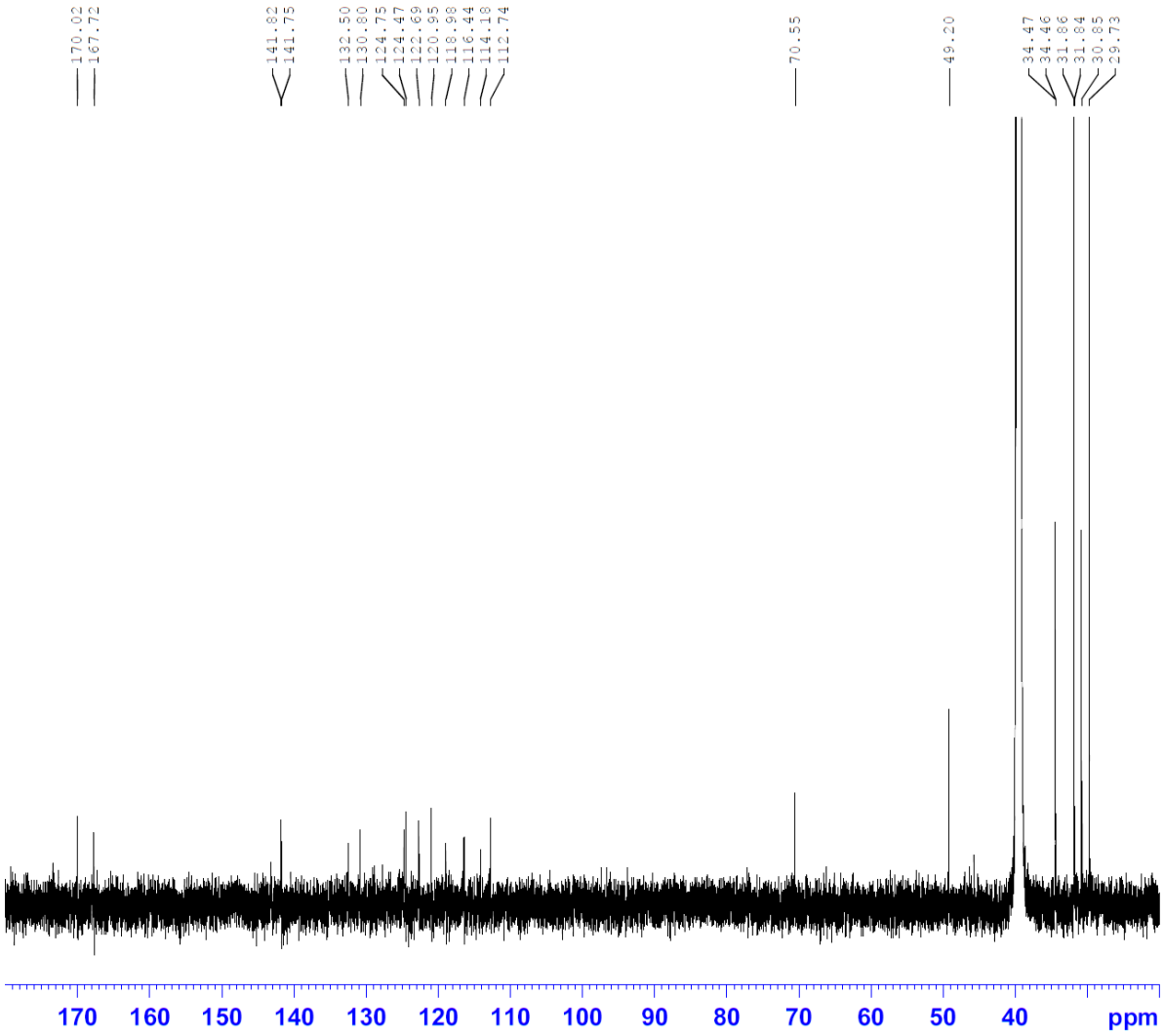
1.3.3. HRMS spectrum of CzU-NeP



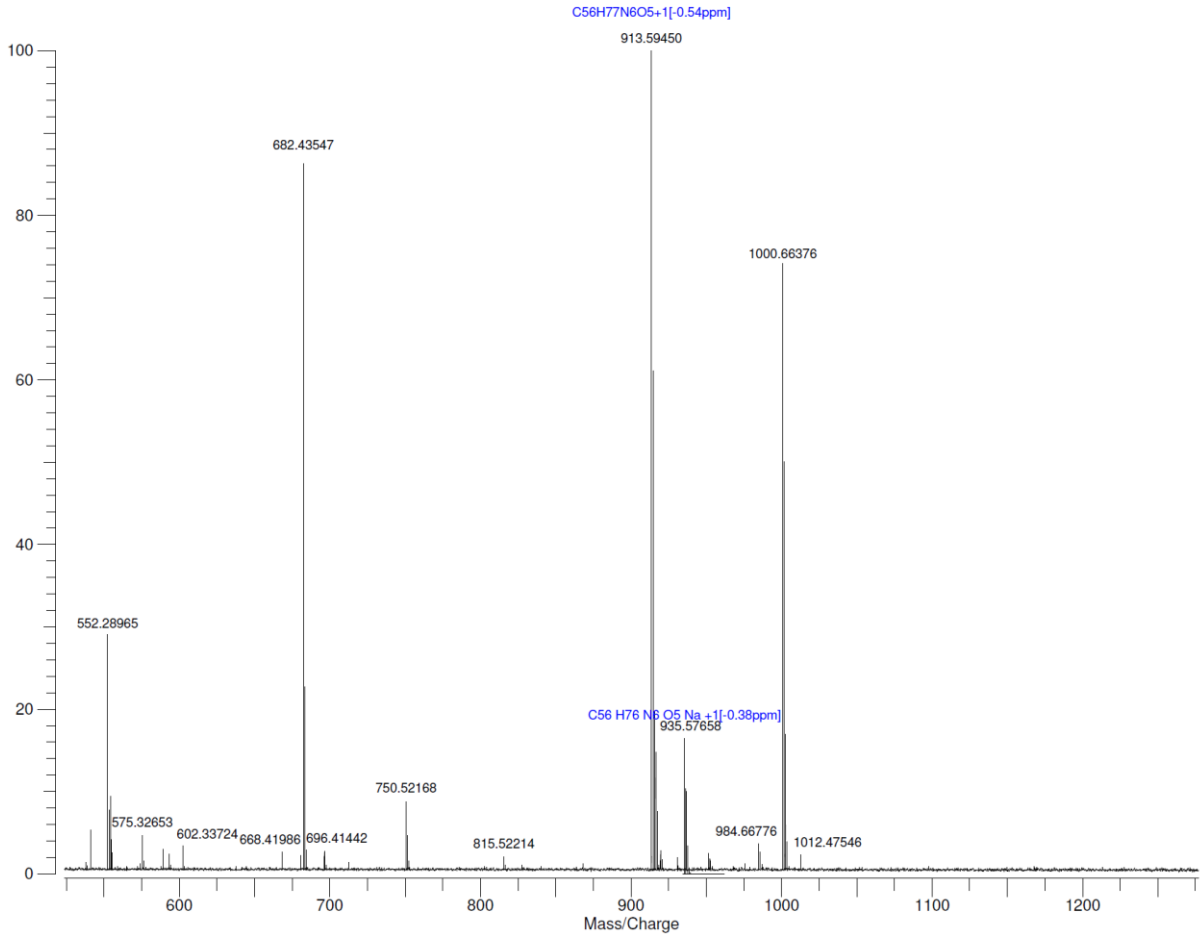
1.3.4. ^{1}H NMR of Cz-Gly-NeP in DMSO-d_6



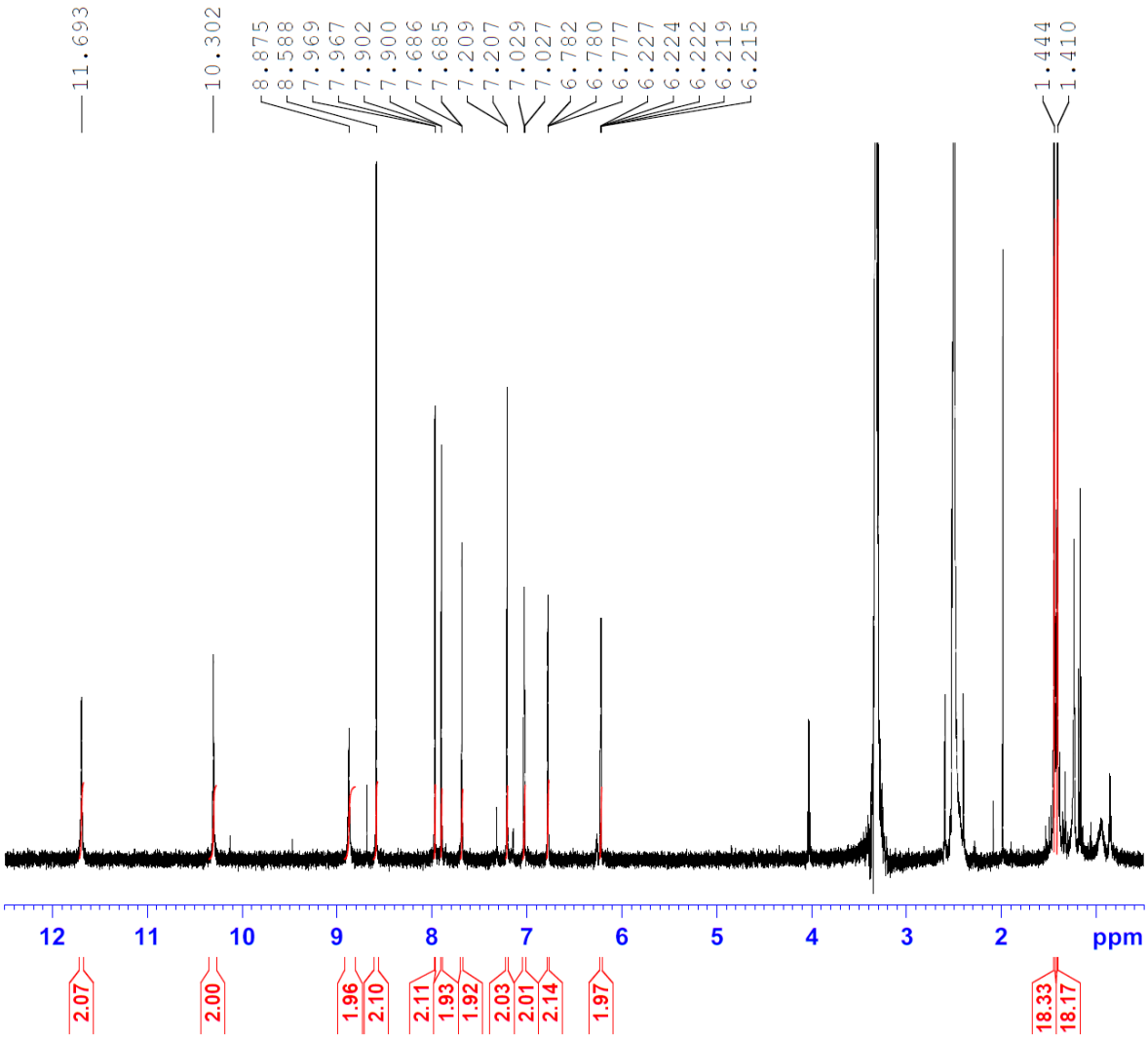
1.3.5. ^{13}C NMR of Cz-Gly-NeP in DMSO-d_6



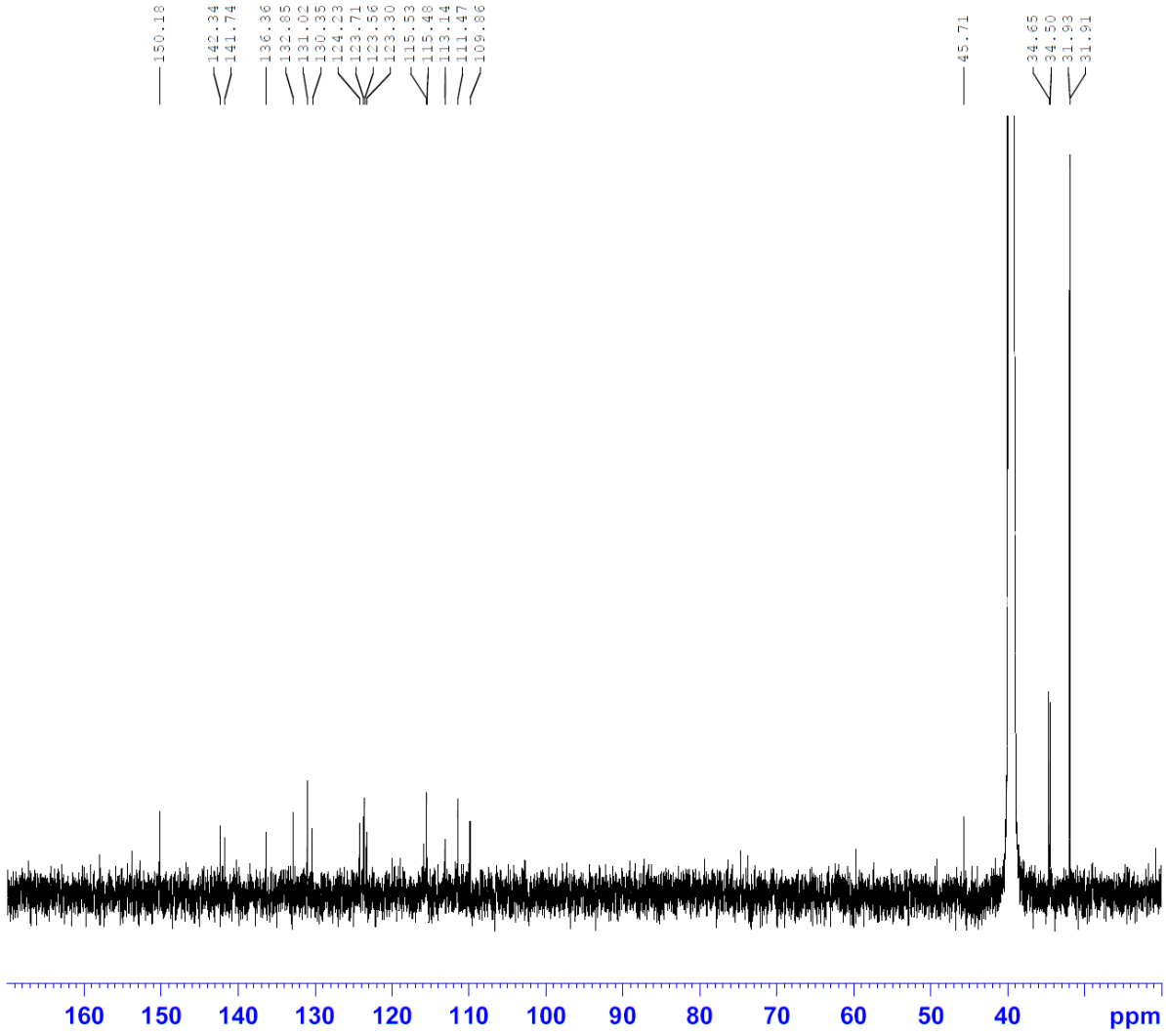
1.3.6. HRMS spectrum of Cz-Gly-NeP



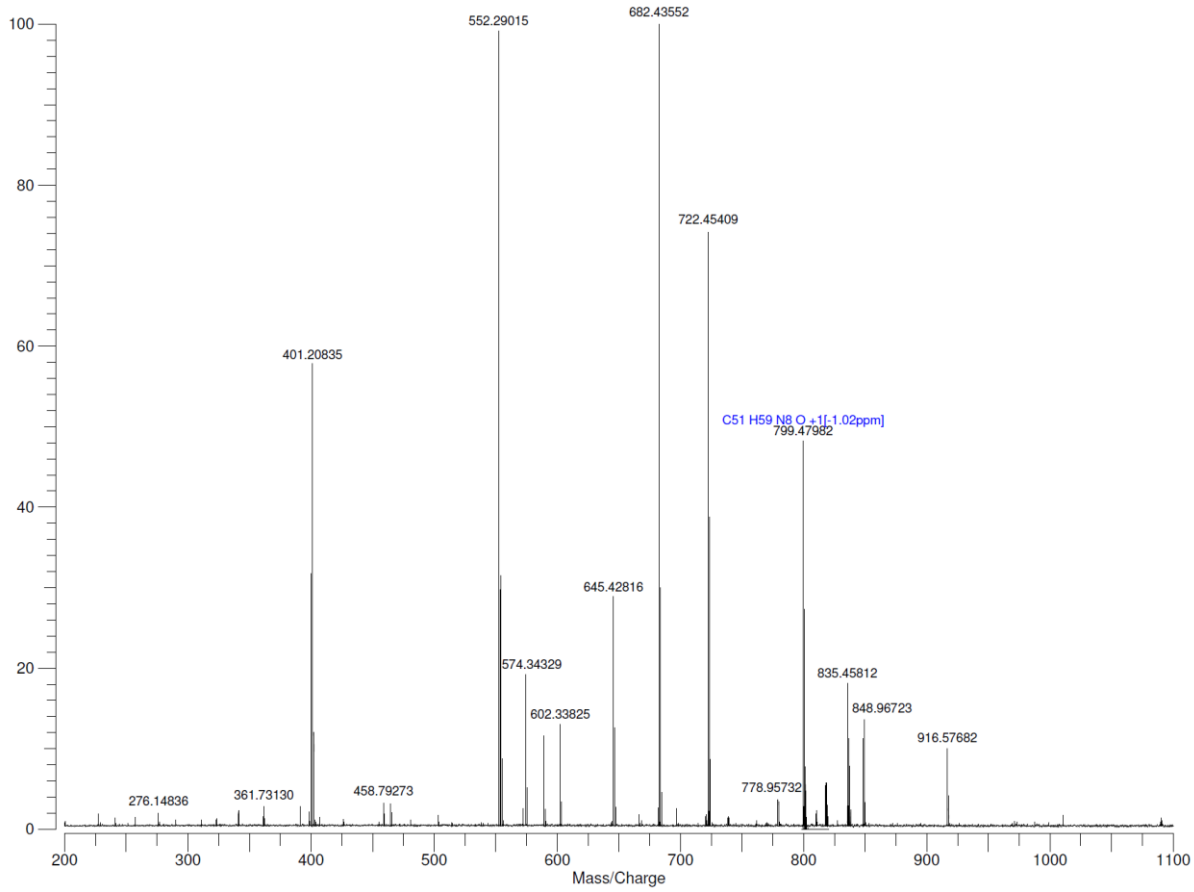
1.3.7. ^{1}H NMR of CzU-Py in DMSO-d_6



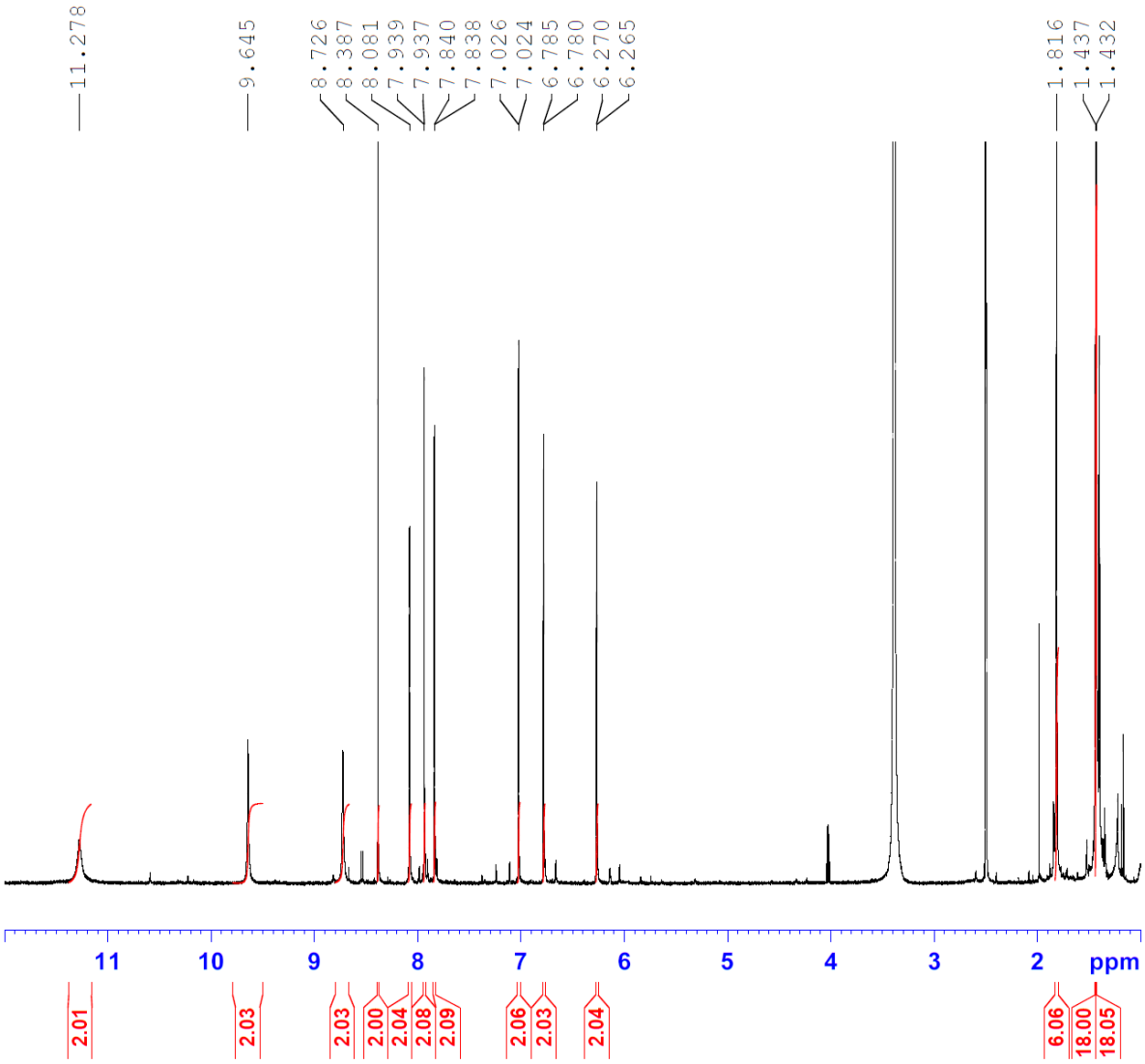
1.3.8. ^{13}C NMR of CzU-Py in DMSO-d_6



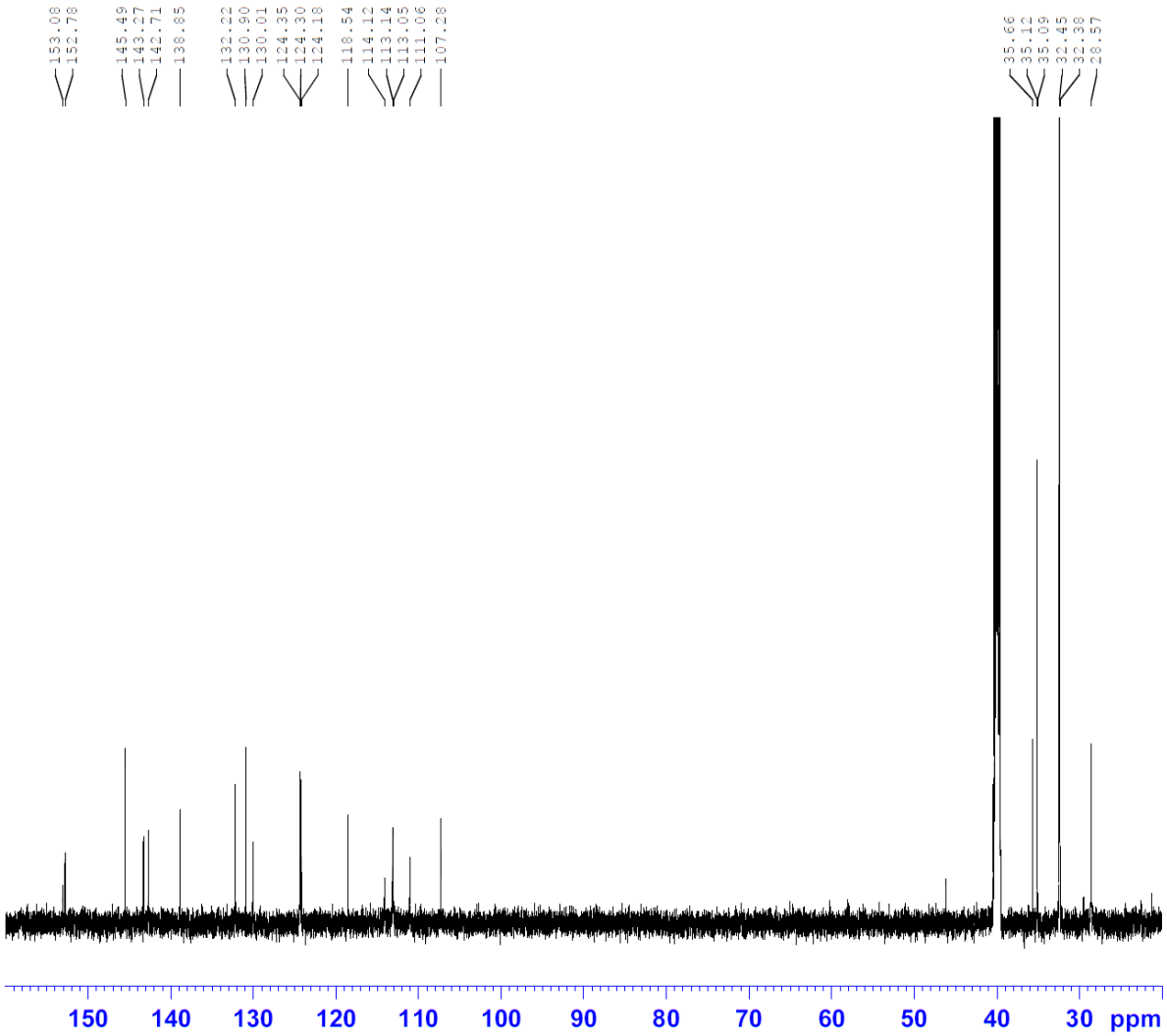
1.3.9. HRMS spectrum of CzU-Py



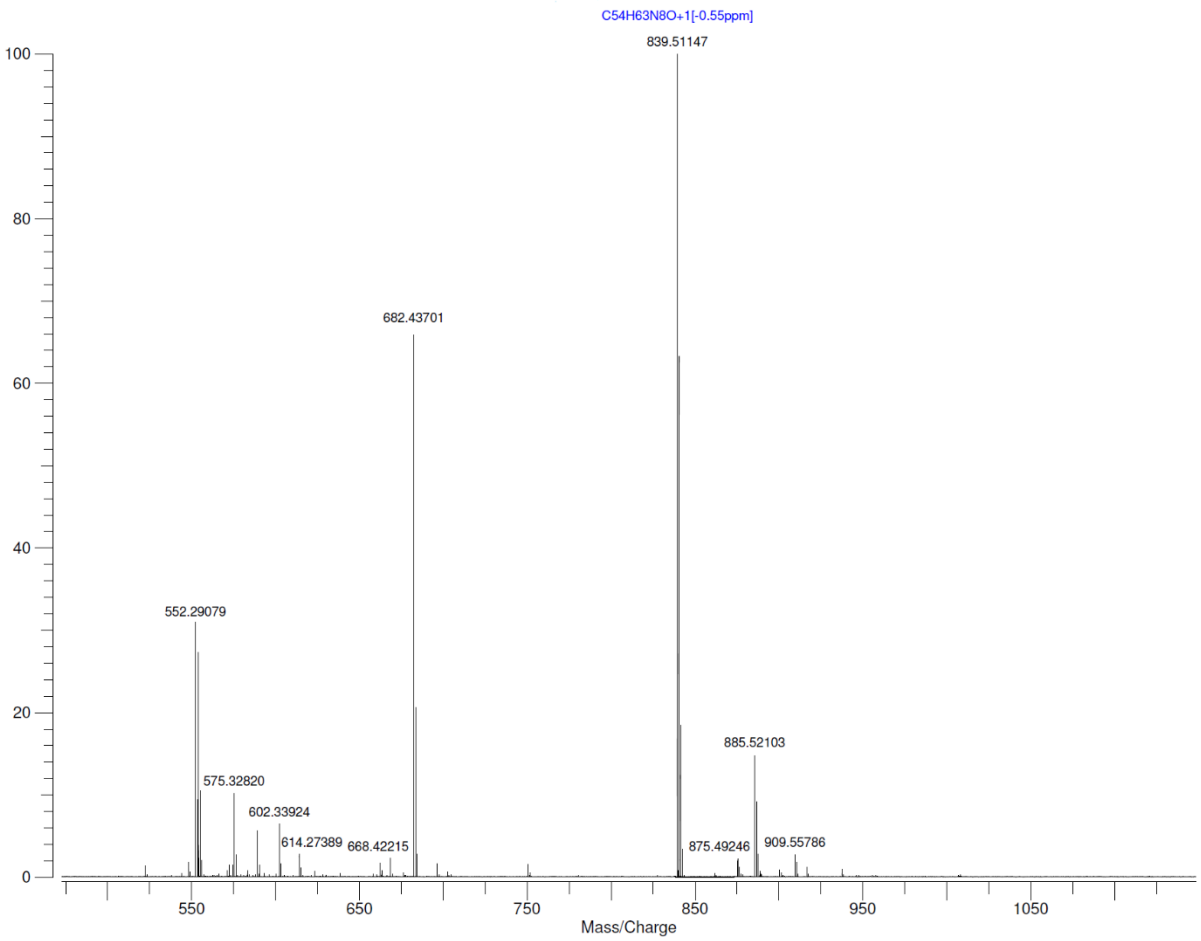
1.3.10. ^{1}H NMR of CzU-DPM in DMSO-d_6



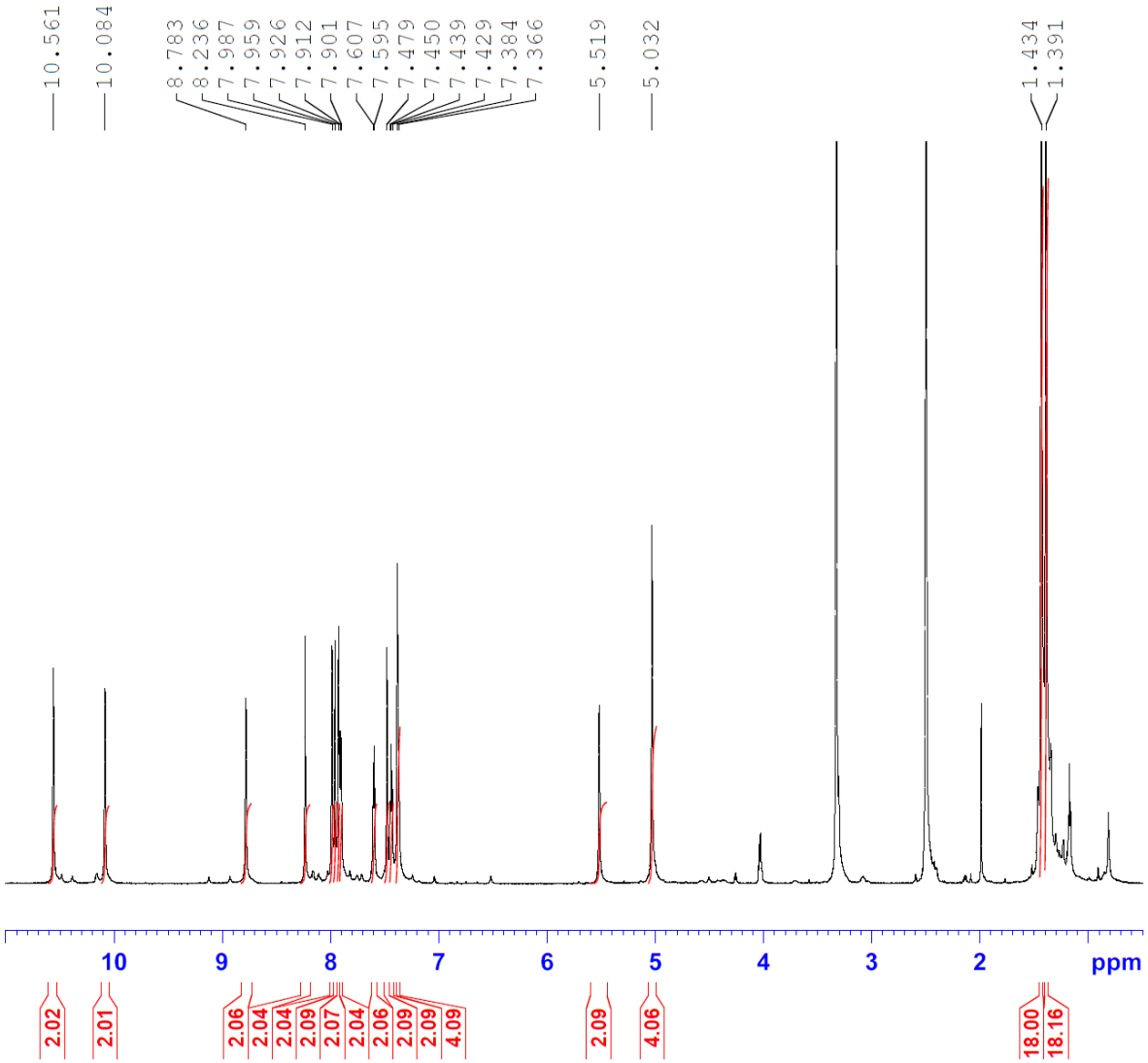
1.3.11. ^{13}C NMR of CzU-DPM in DMSO-d_6



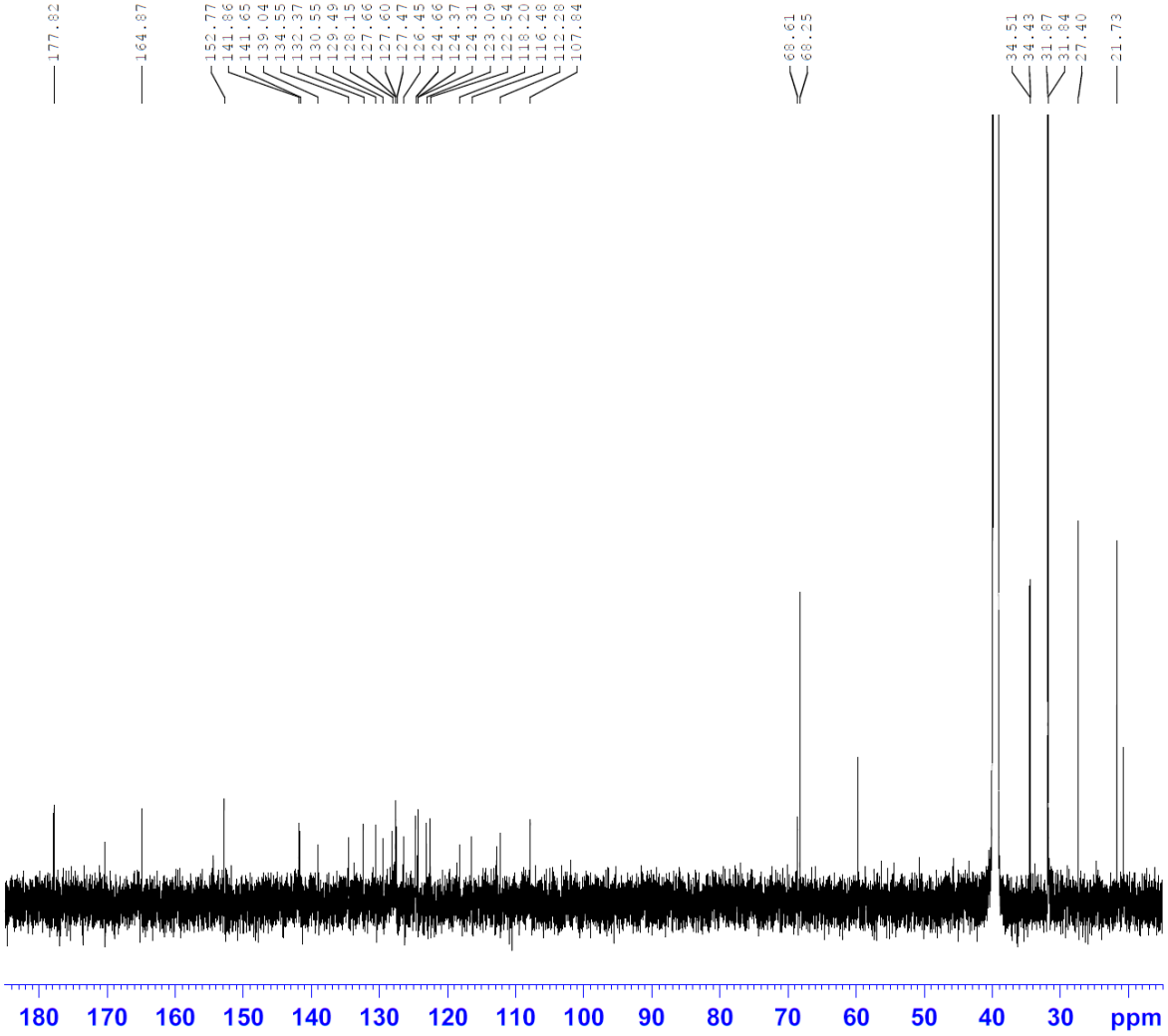
1.3.12. HRMS spectrum of CzU-DPM



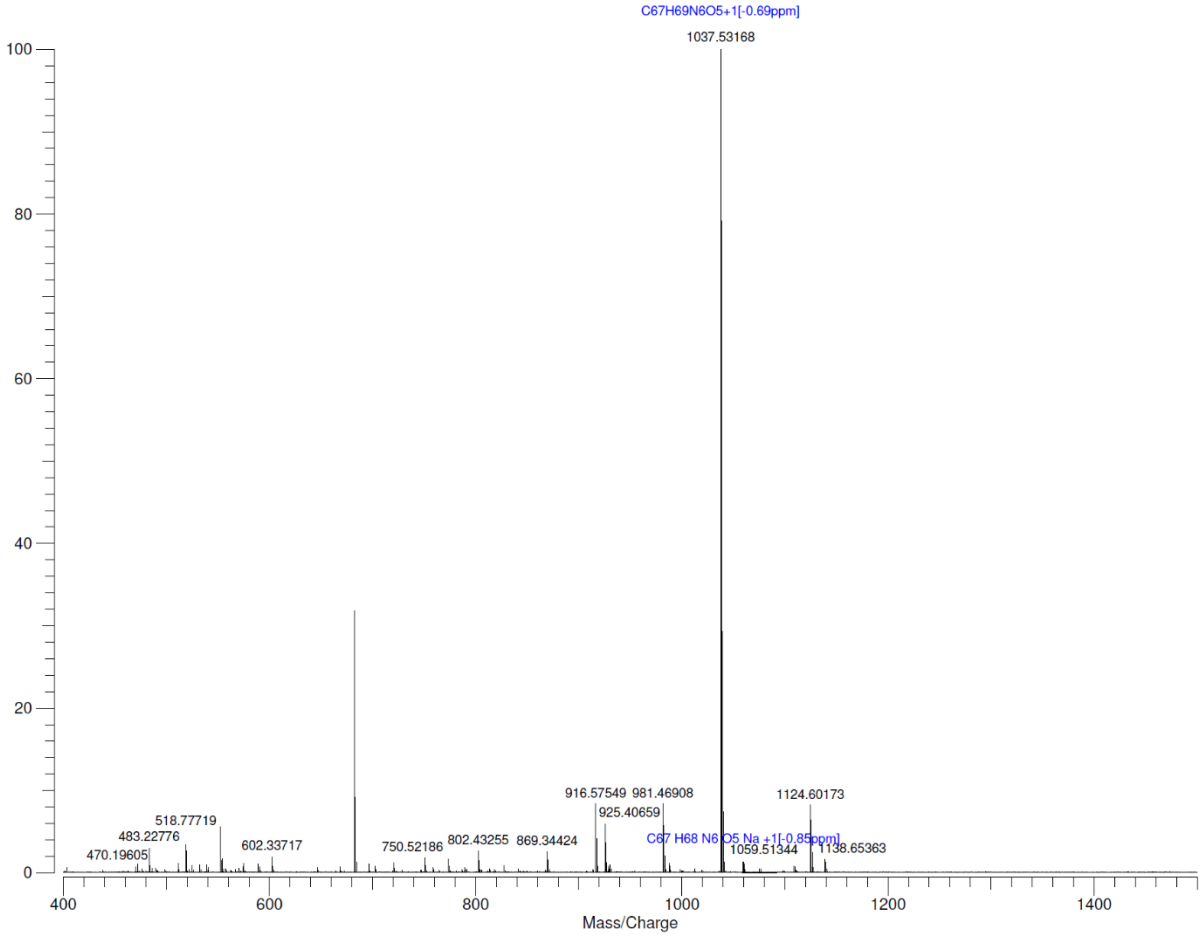
1.3.13. ^{1}H NMR of CzU-BA in DMSO-d_6



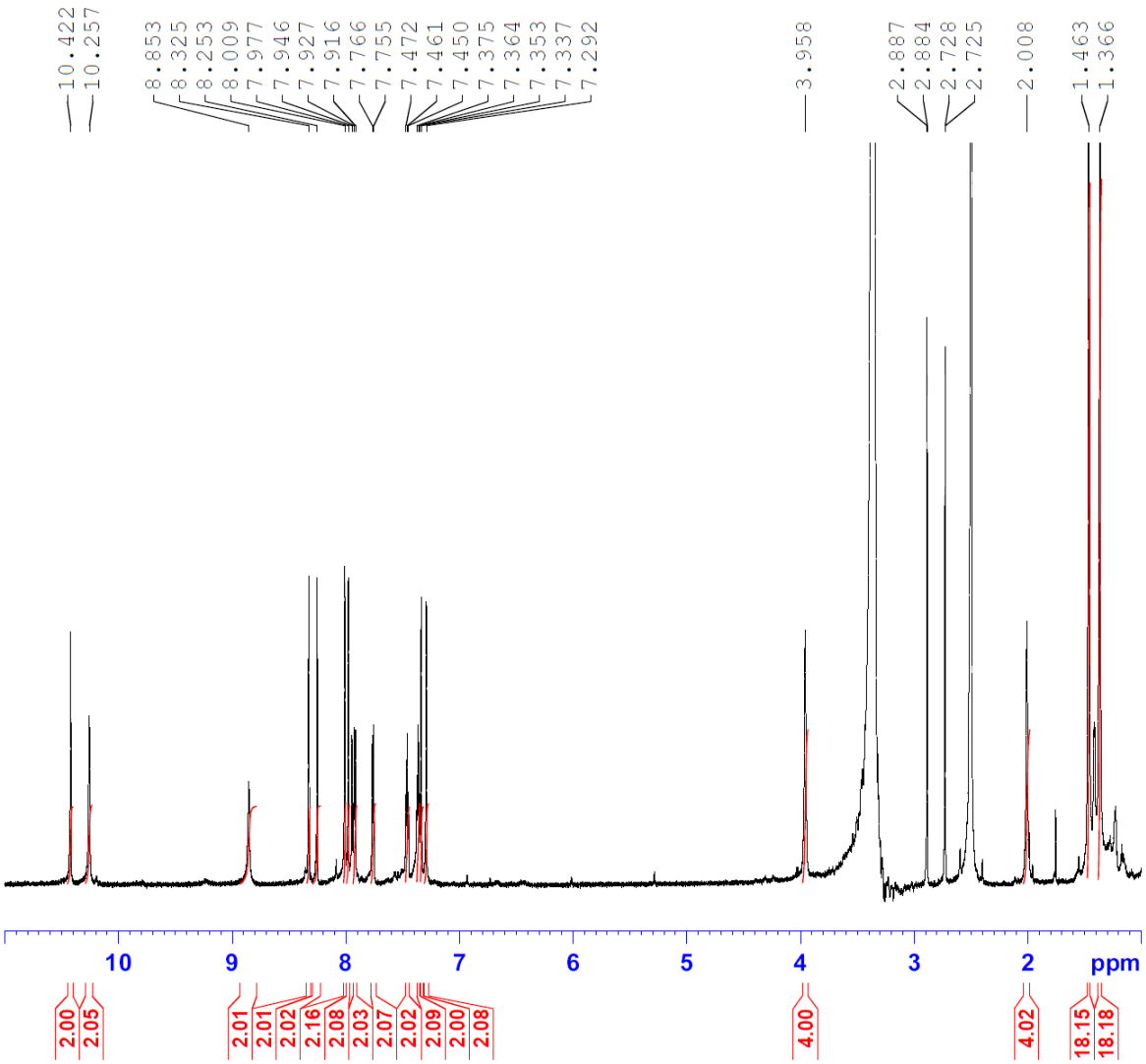
1.3.14. ^{13}C NMR of CzU-BA in DMSO-d_6



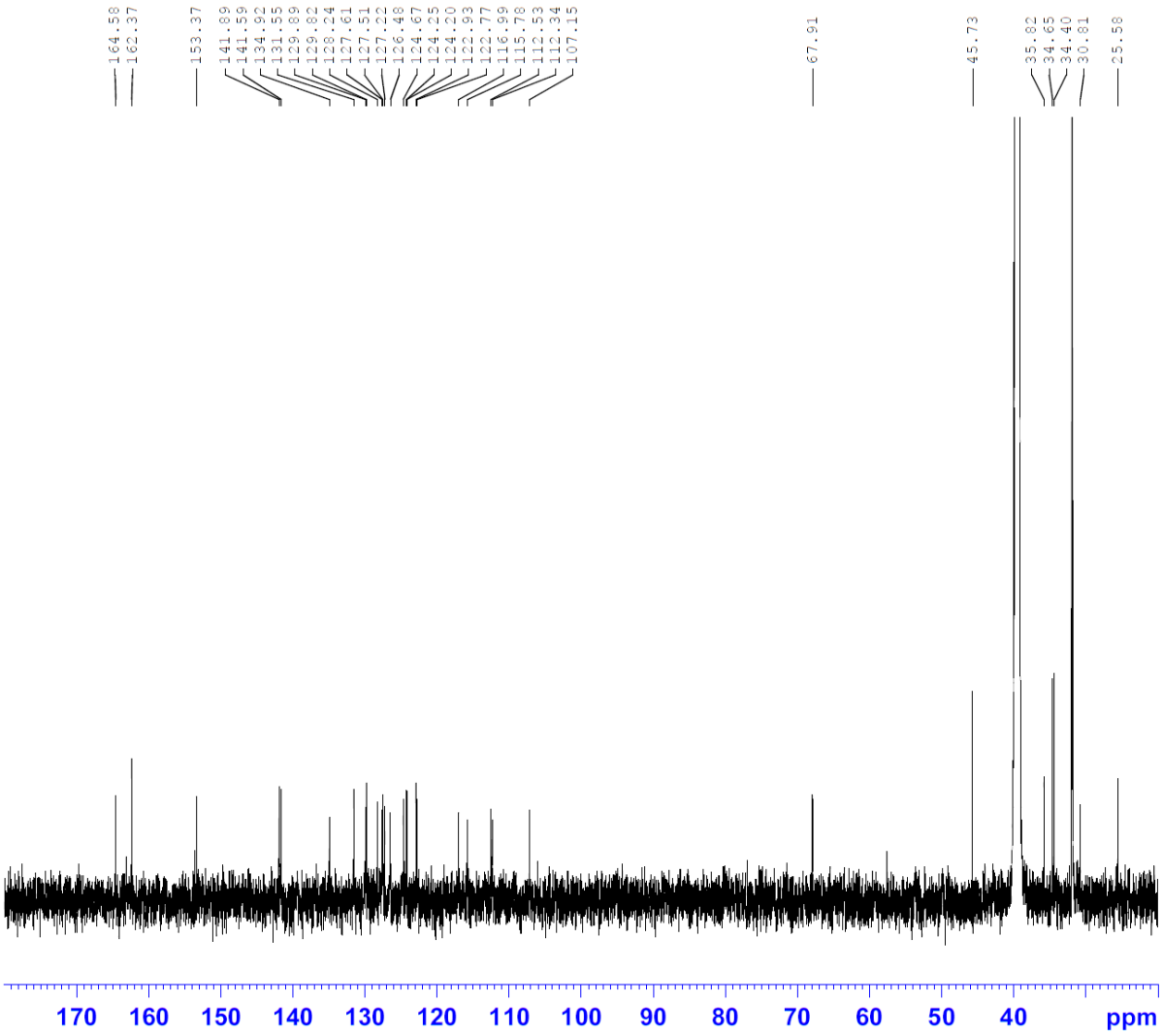
1.3.15. HRMS spectrum of CzU-BA



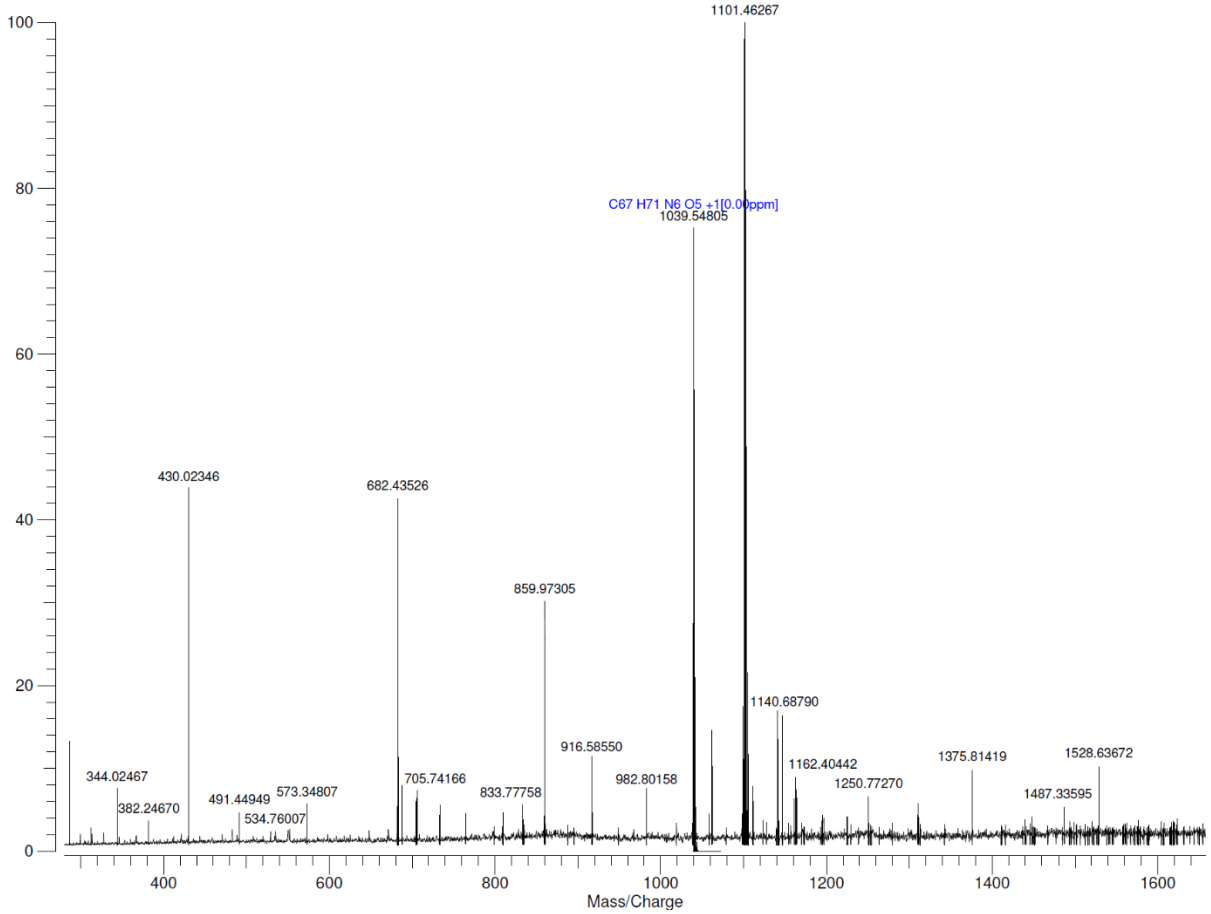
1.3.16. ^{1}H NMR of CzU-BB in DMSO-d_6



1.3.17. ^{13}C NMR of CzU-BB in DMSO-d_6



1.3.18. HRMS spectrum of CzU-BB

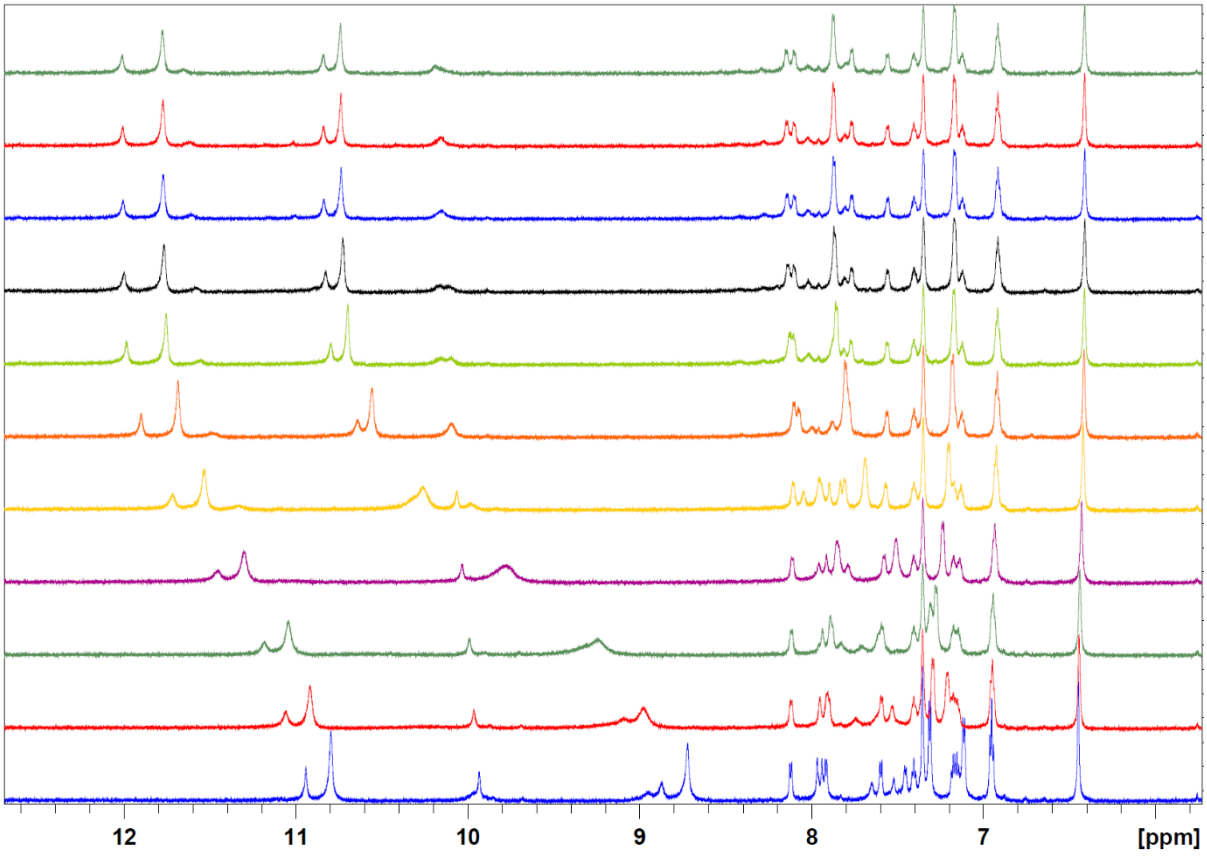


2. Relative binding affinity measurements

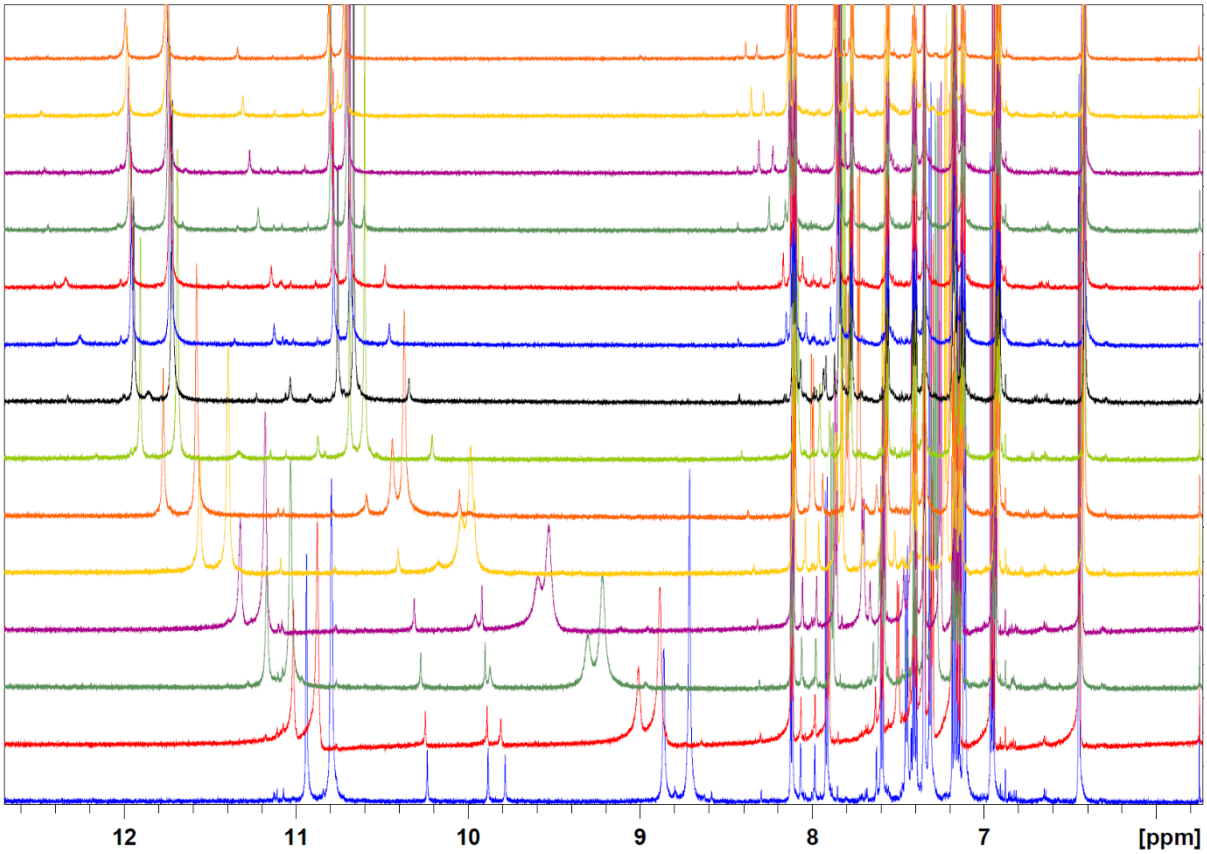
For sample preparation, a few milligrams of receptors were weighed into a NMR tube alongside an anchor molecule, to which binding had previously been quantified using absolute binding measurements.[5] The compounds were dissolved in 700 µL DMSO-d_6 with a water content of 0.5% H_2O (m/m). DMSO-d_6 99.8% and water from MilliQ Advantage A10 system were used. Solutions of carboxylates were prepared by weighing the corresponding tetrabutylammonium salts into vials and dissolving them in 1 mL DMSO-d_6 with a water content of 0.5% H_2O (m/m). Some of the earlier measurements (specifically with receptors Cz-Gly-NeP and CzU-NeP) were made with DMSO-d_6 with a water content of 0.5% (v/v) H_2O. In order to see how much this affects the results, some of the measurements were repeated in DMSO-d_6/H_2O 0.5 % (m/m), and the findings were exactly the same as when using DMSO-d_6/H_2O 0.5 % (v/v). Thus, all reported results refer to DMSO-d_6 with a water content of 0.5% (m/m) H_2O.

For each anion, two solutions were prepared: a dilute and a concentrated solution. During the titration, a blank spectrum of pure receptors was initially obtained. Then, the anion solution was added using an automatic titration syringe. The chemical shifts of the formed host–guest complexes were recorded for each titration step. The dilute solution was used during the first part of the titration, where complexation was partial. The concentrated solution was used towards the end of the titration to ensure full complexation of all host molecules in solution. The recorded chemical shifts of all titration steps were used to calculate the differences of binding affinity with respect to the anchor molecules, $\Delta\log K_{ass}$, as described in reference.[4] NMR spectra of all titration experiments are available below.

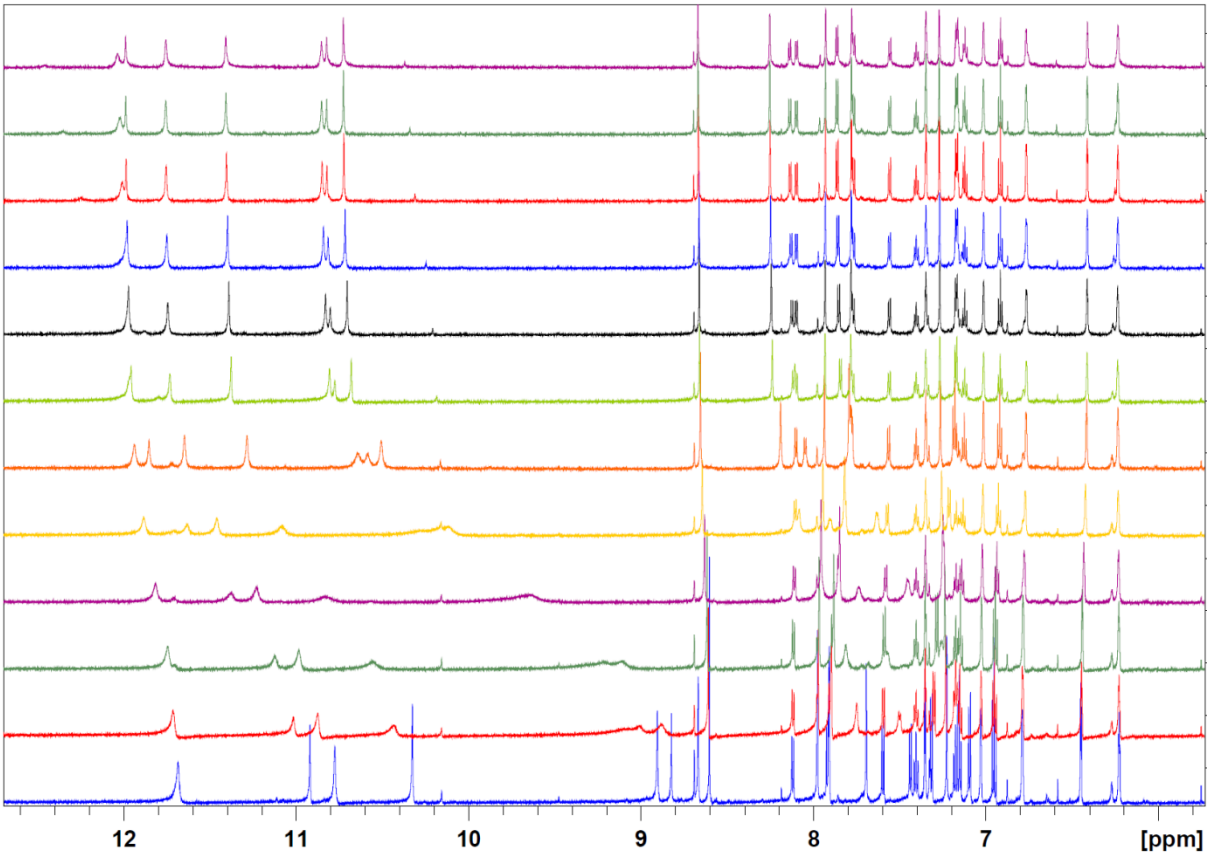
2.1 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-acetate



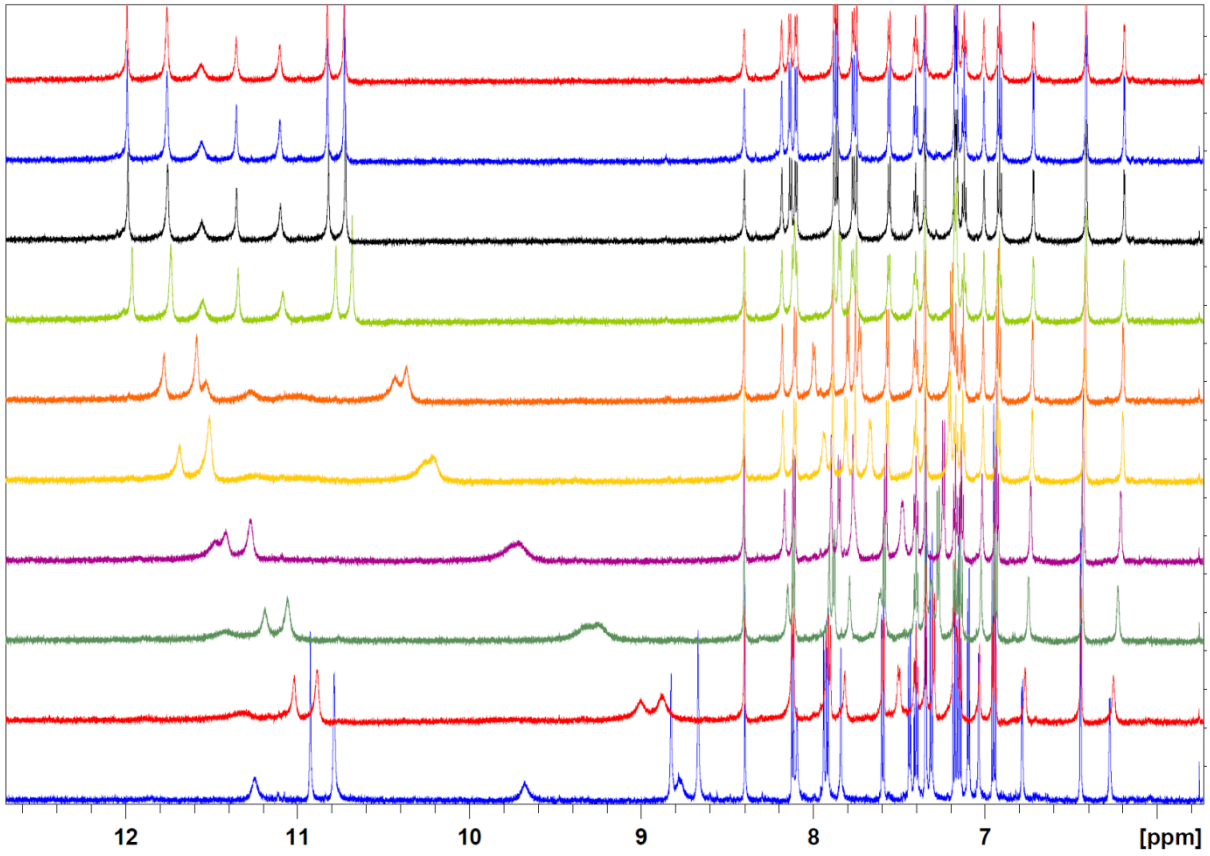
2.2 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors Cz-Gly-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-acetate



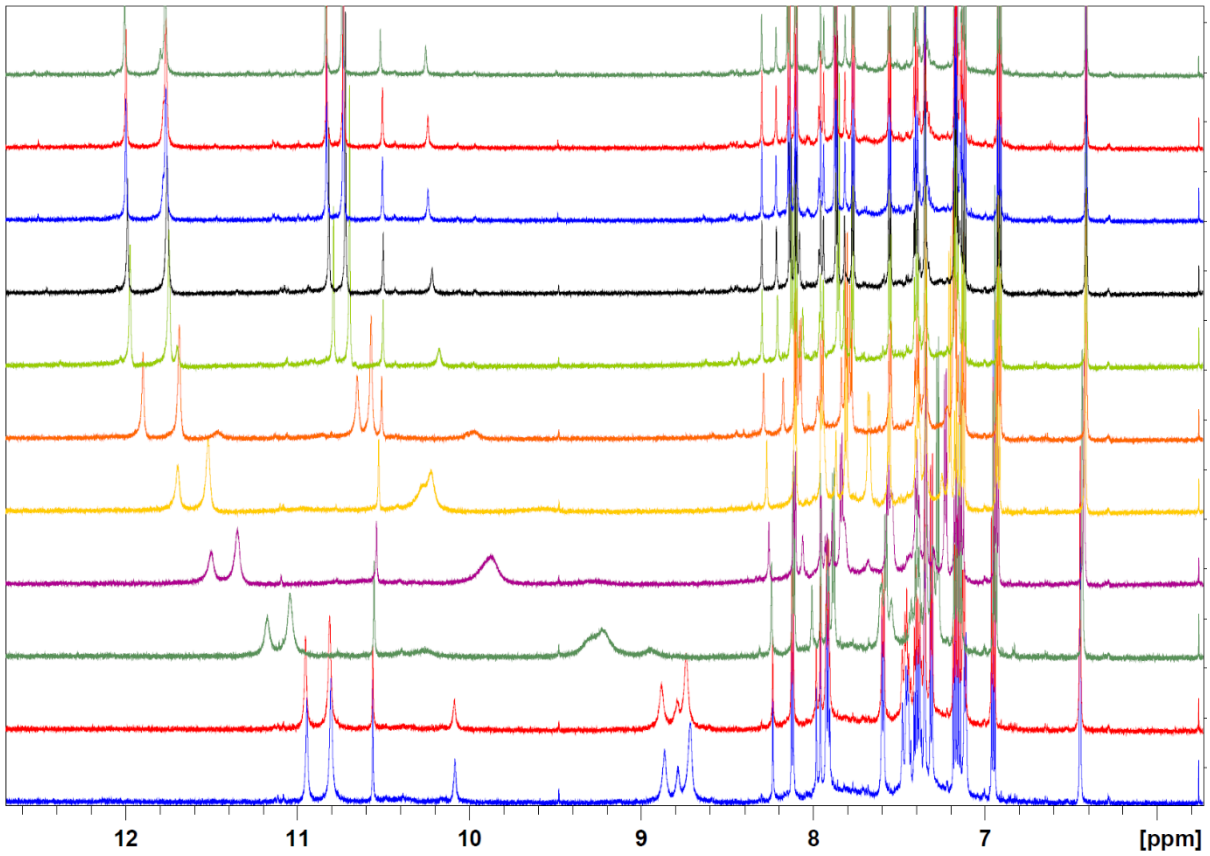
2.3 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-Py; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-acetate



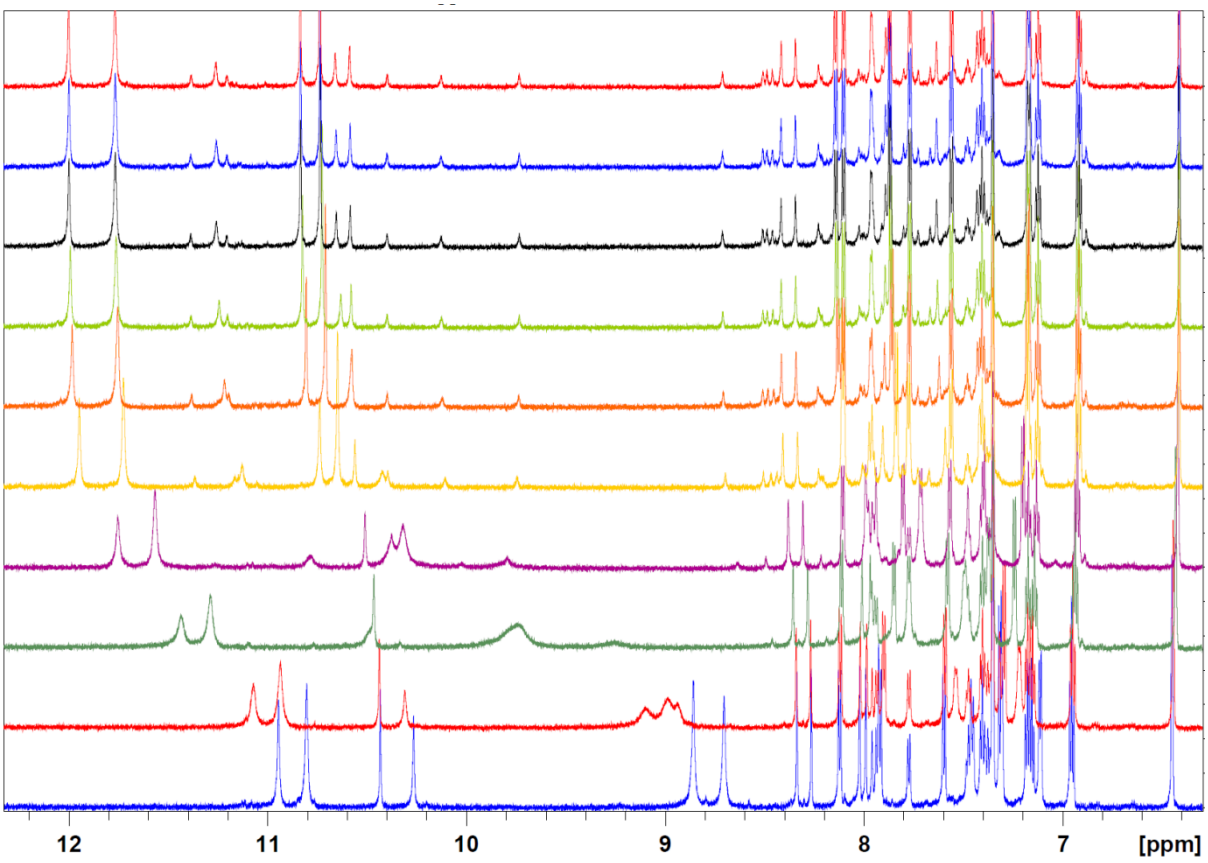
2.4 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-DPM; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-acetate



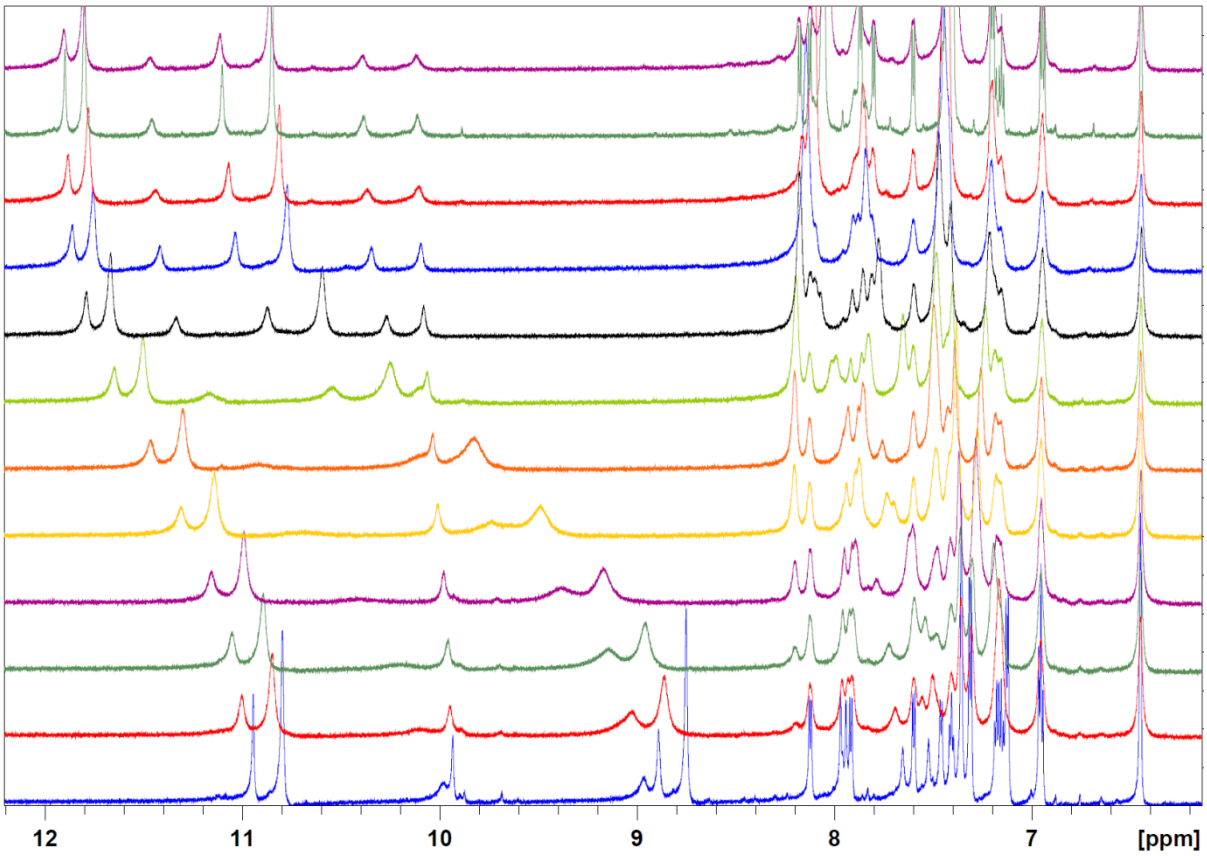
2.5 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BA; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-acetate



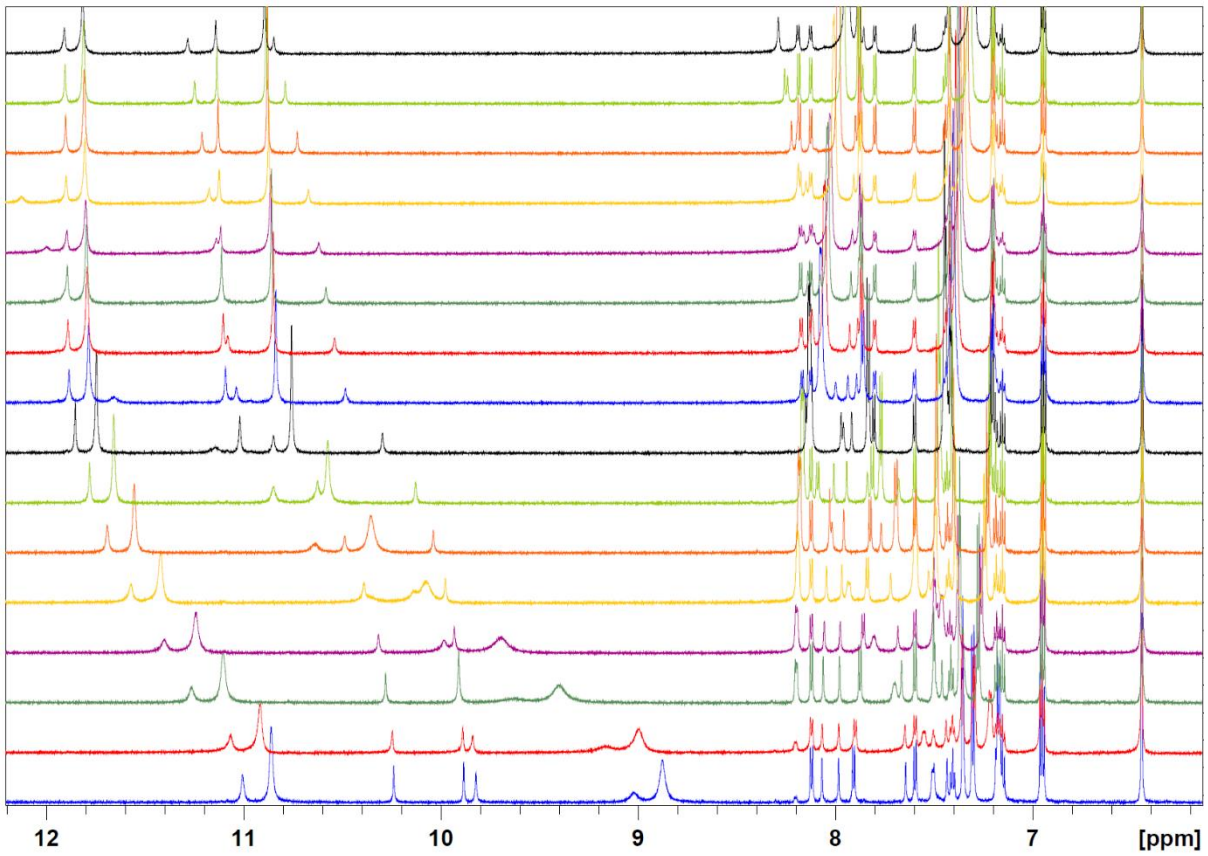
2.6 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BB; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-acetate



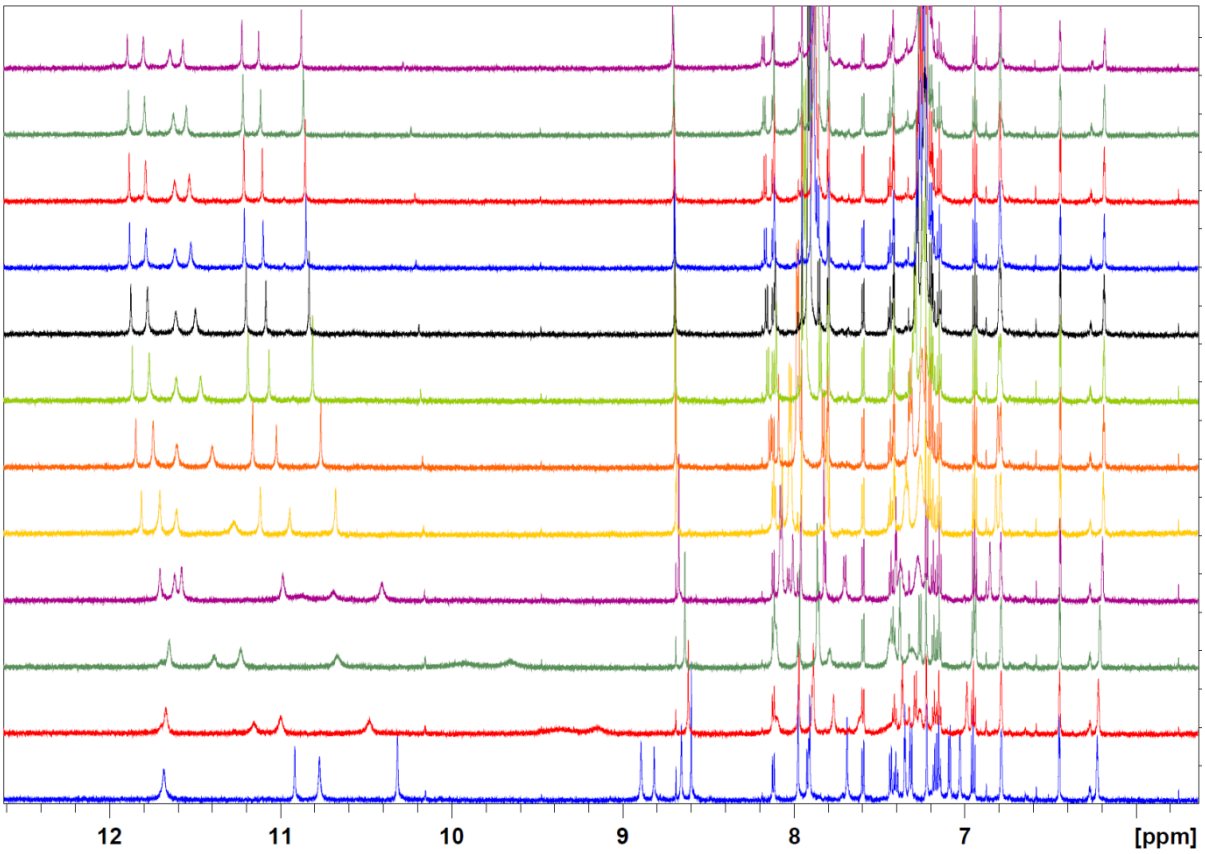
2.7 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-benzoate



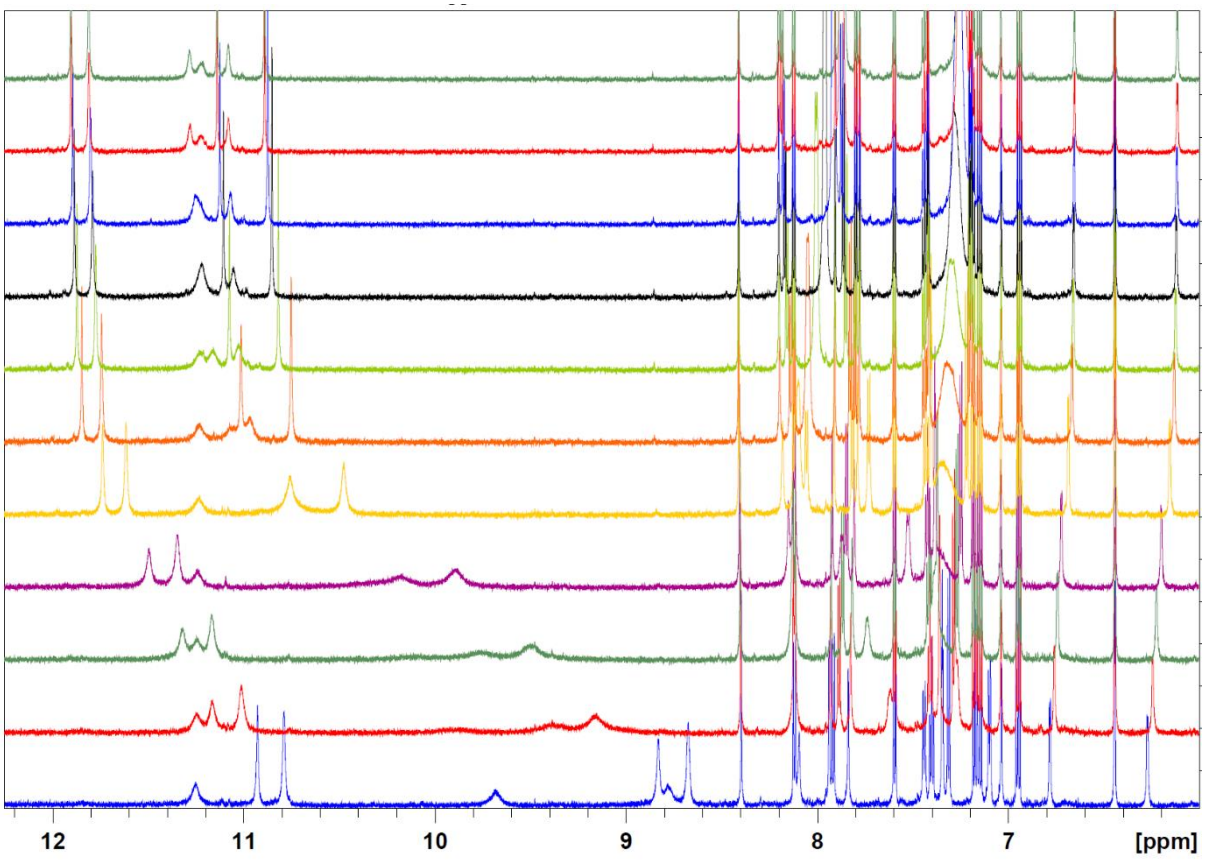
2.8 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors Cz-Gly-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-benzoate



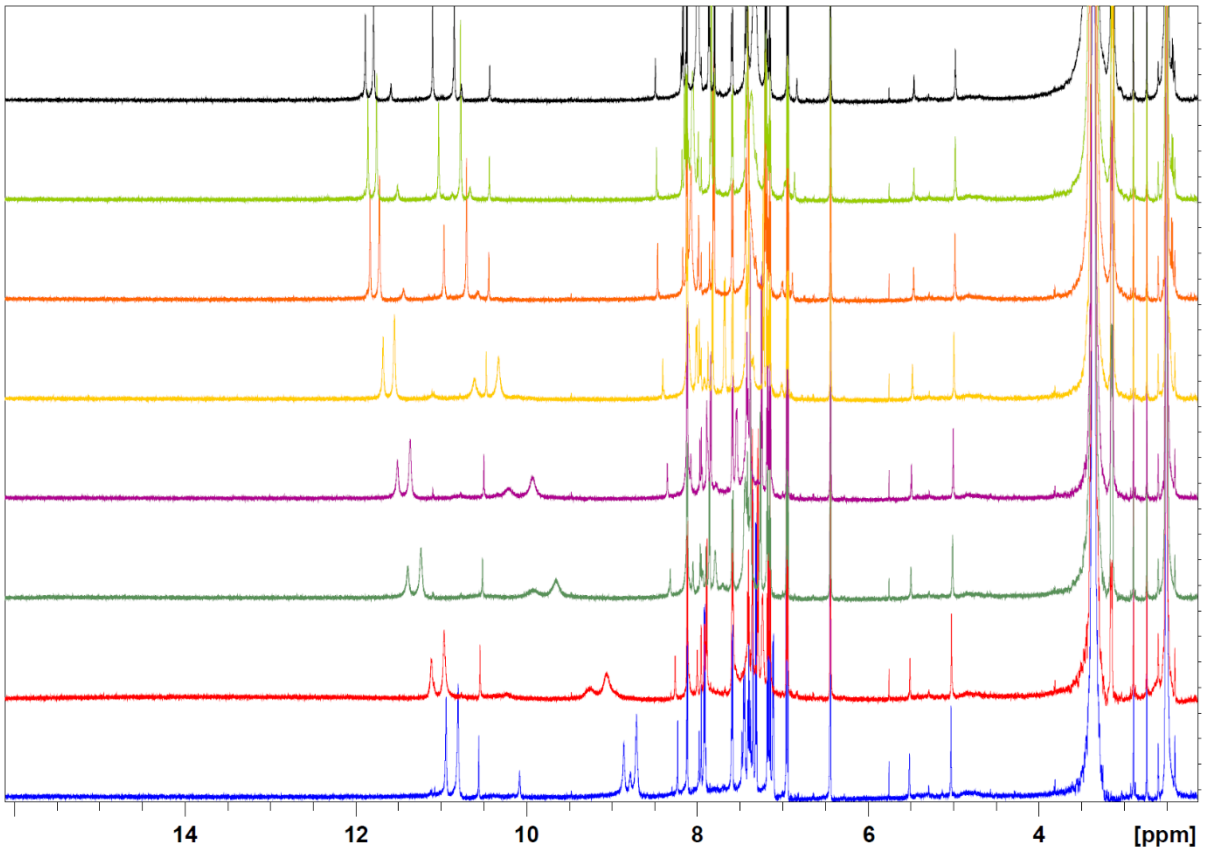
2.9 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-Py; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-benzoate



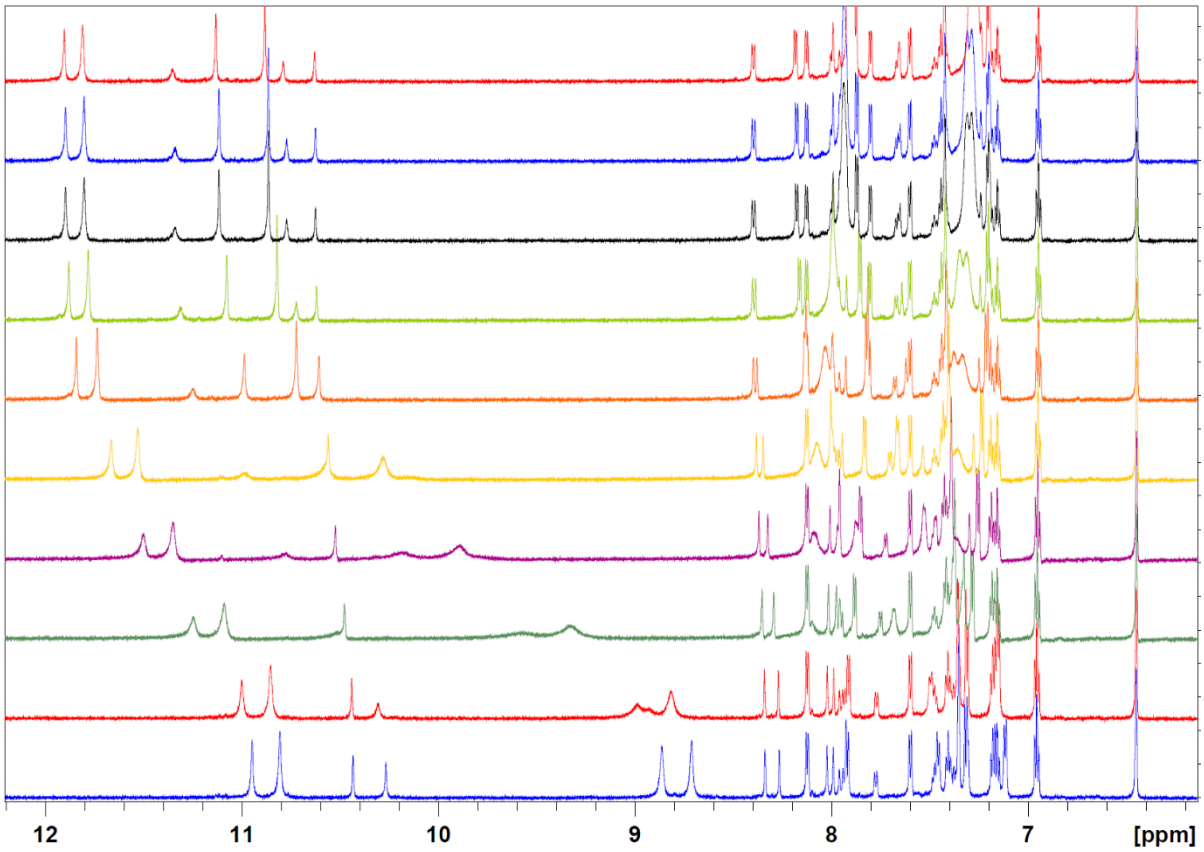
2.10 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-DPM; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-benzoate



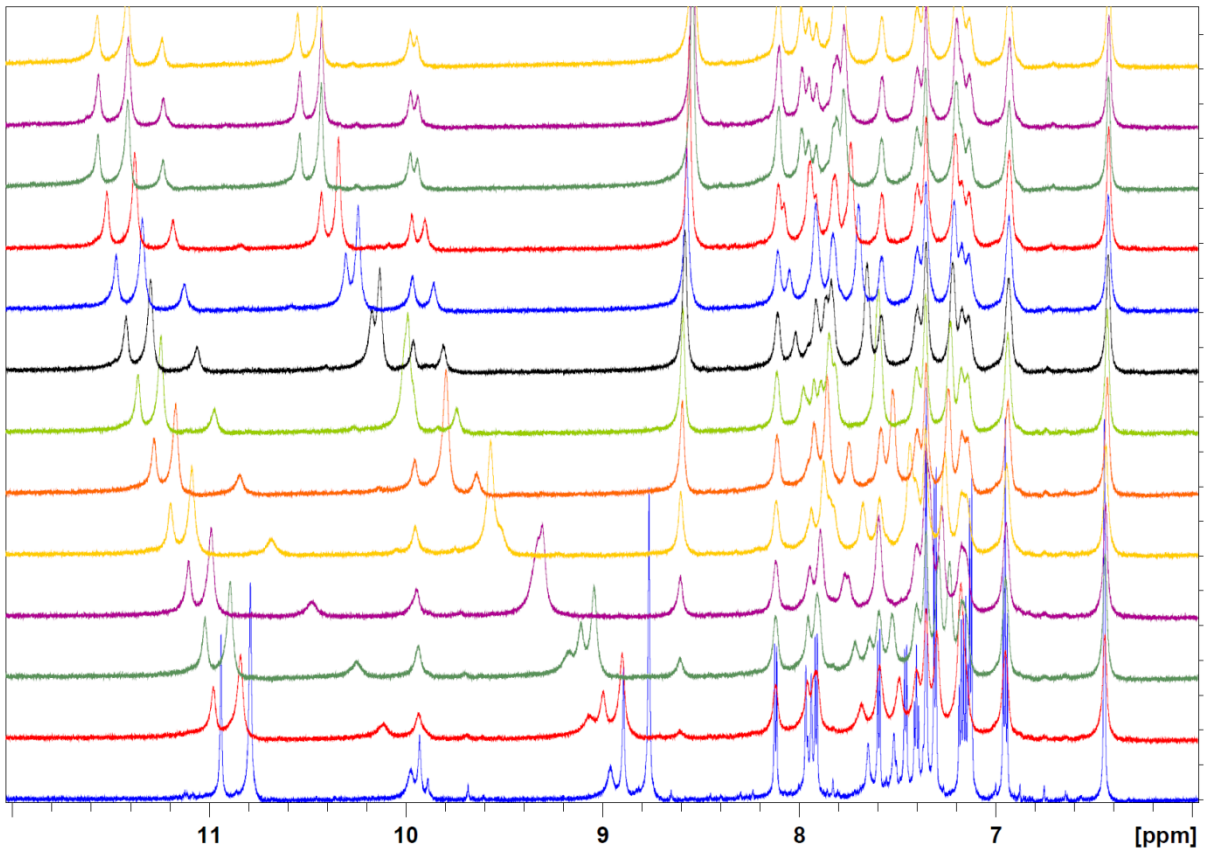
2.11 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BA; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-benzoate



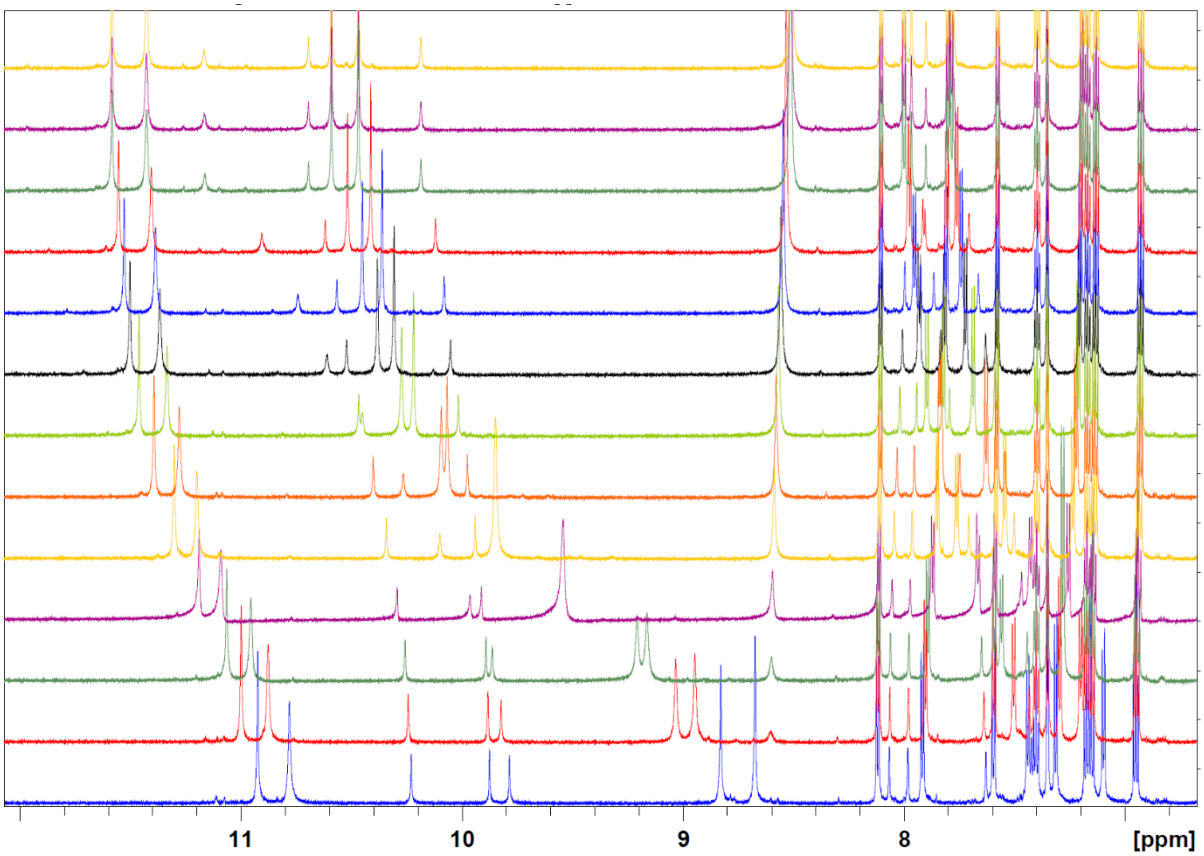
2.12 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BB; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-benzoate



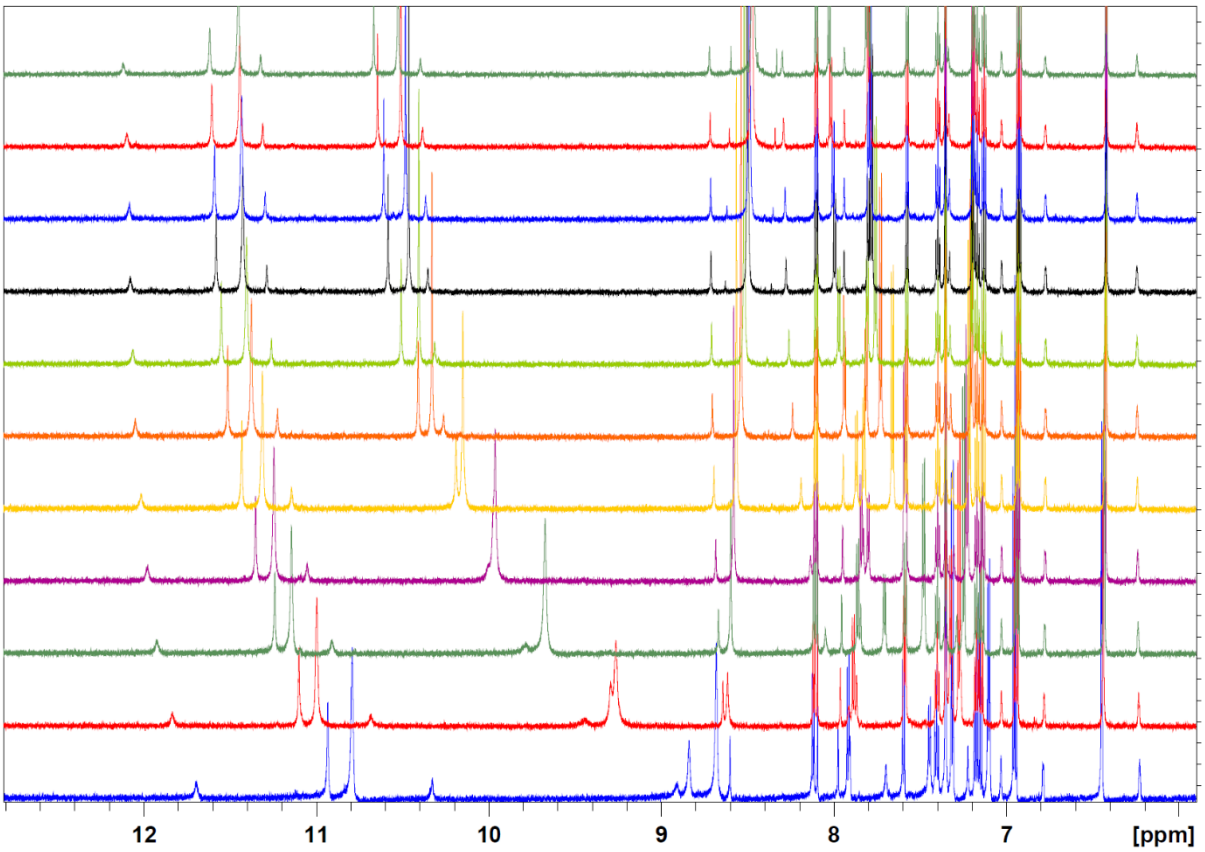
2.13 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-formate



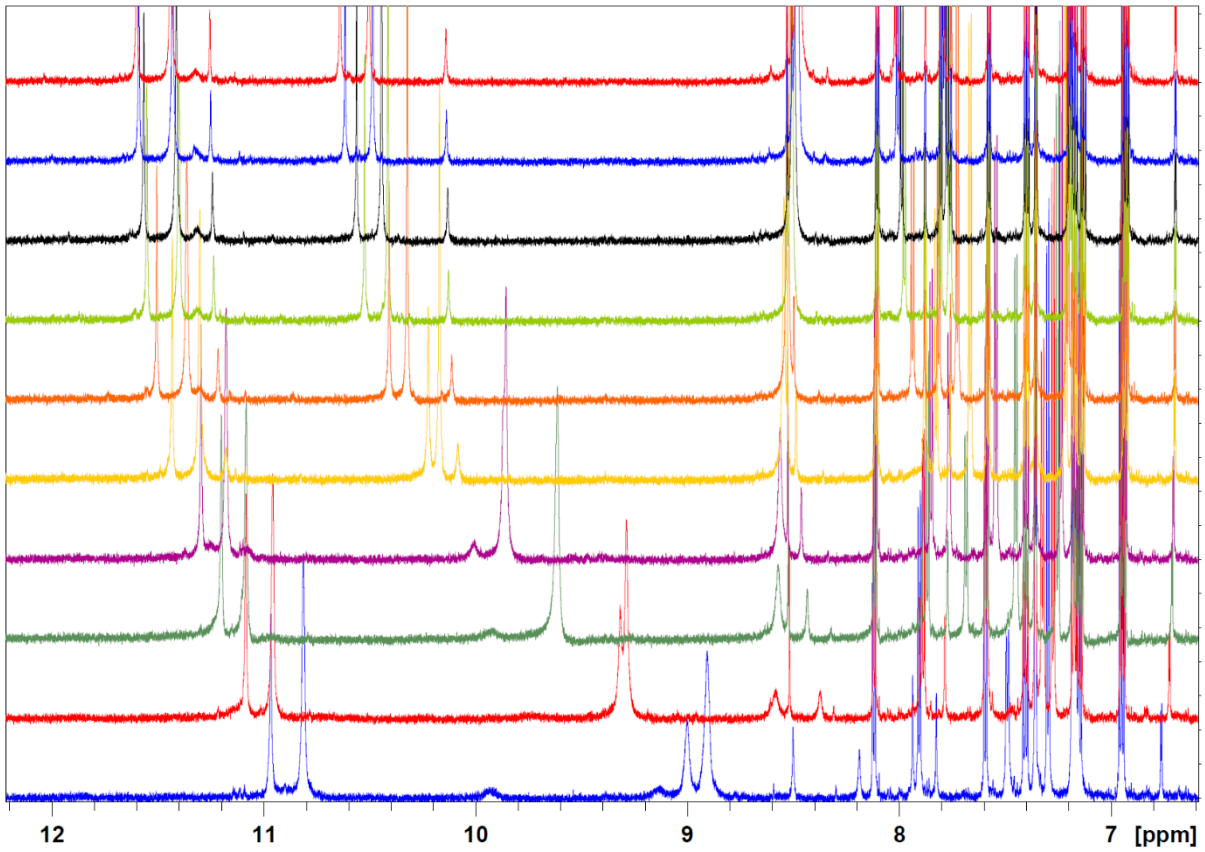
2.14 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors Cz-Gly-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-formate



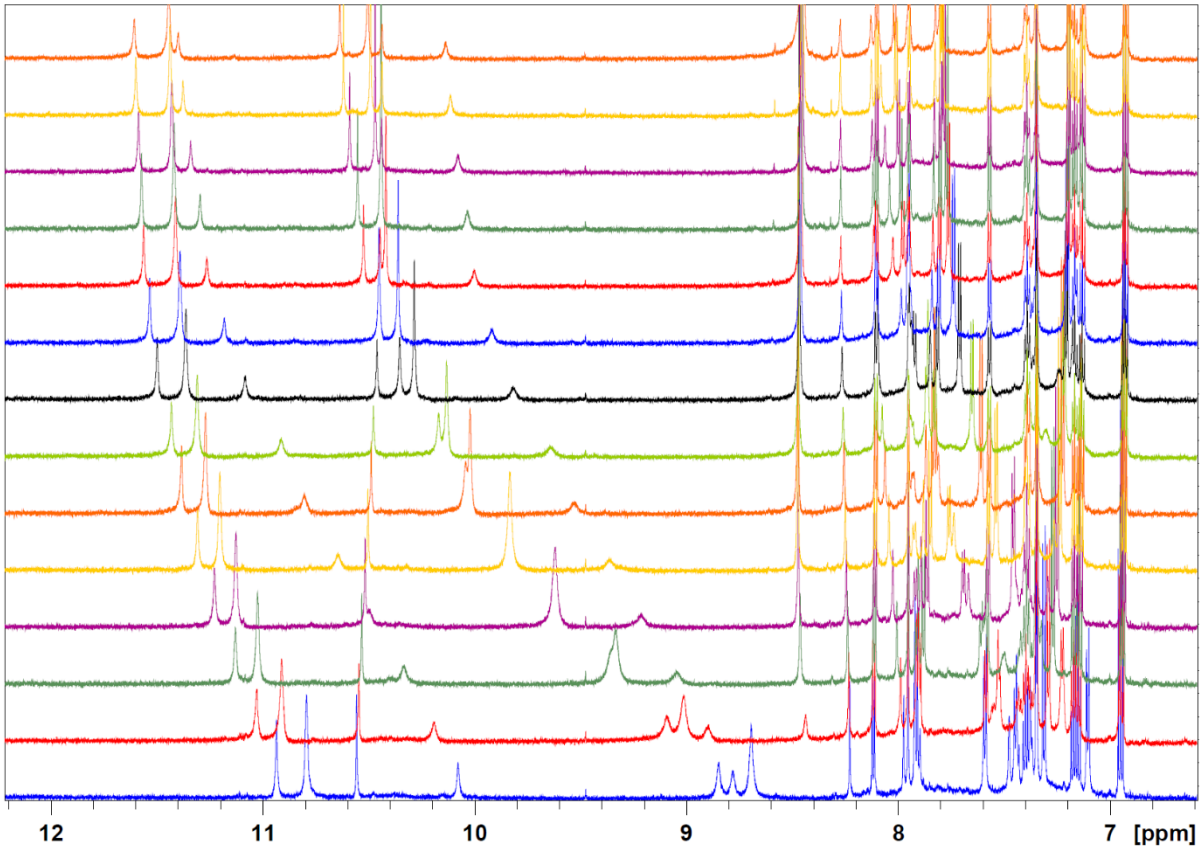
2.15 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-Py; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-formate



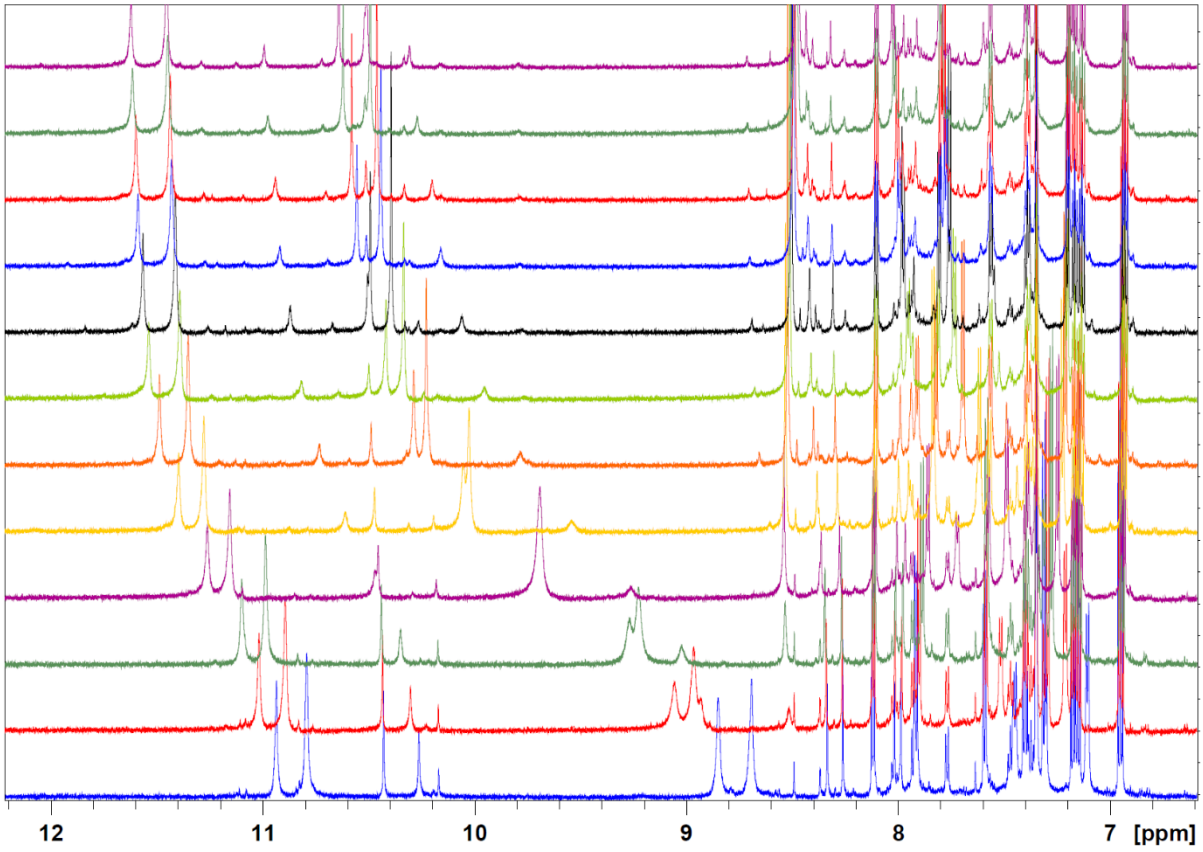
2.16 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-DPM; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-formate



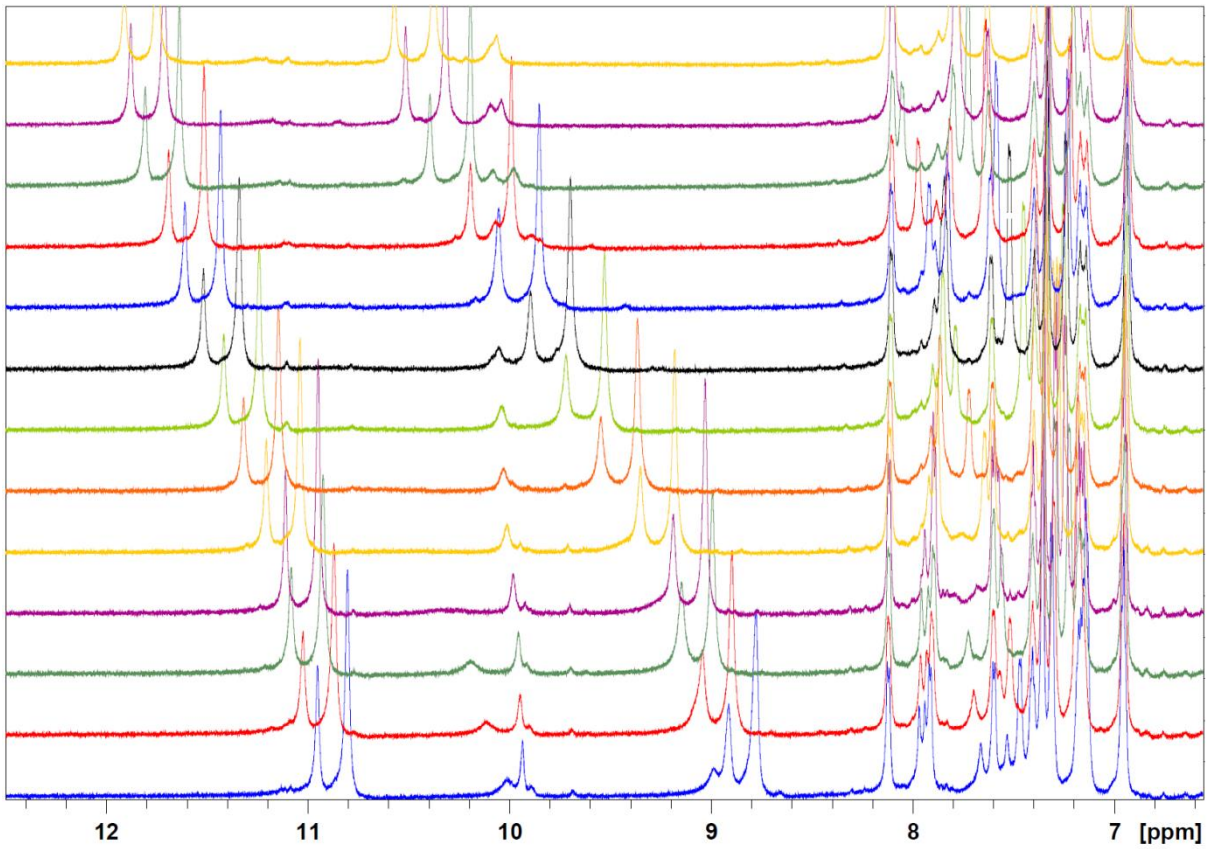
2.17 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BA; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-formate



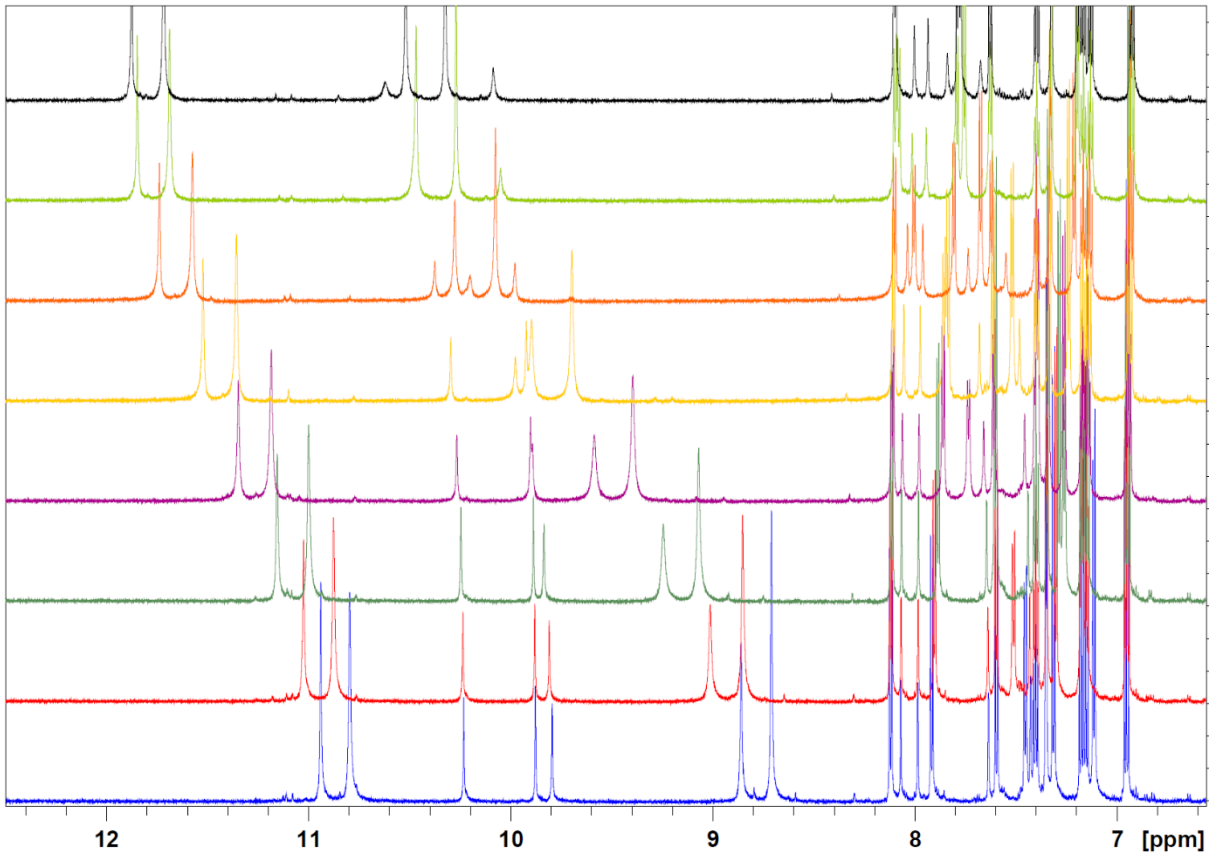
2.18 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BB; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-formate



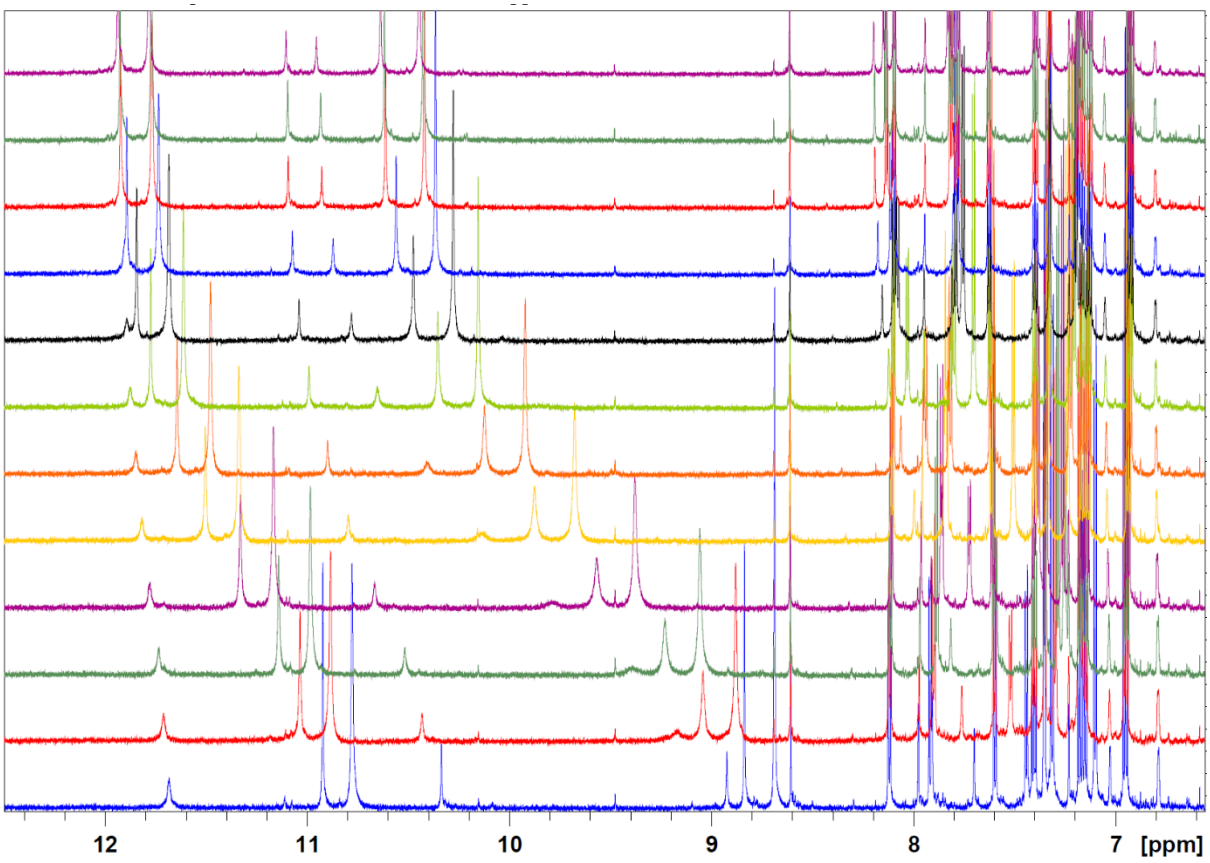
2.19 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-lactate



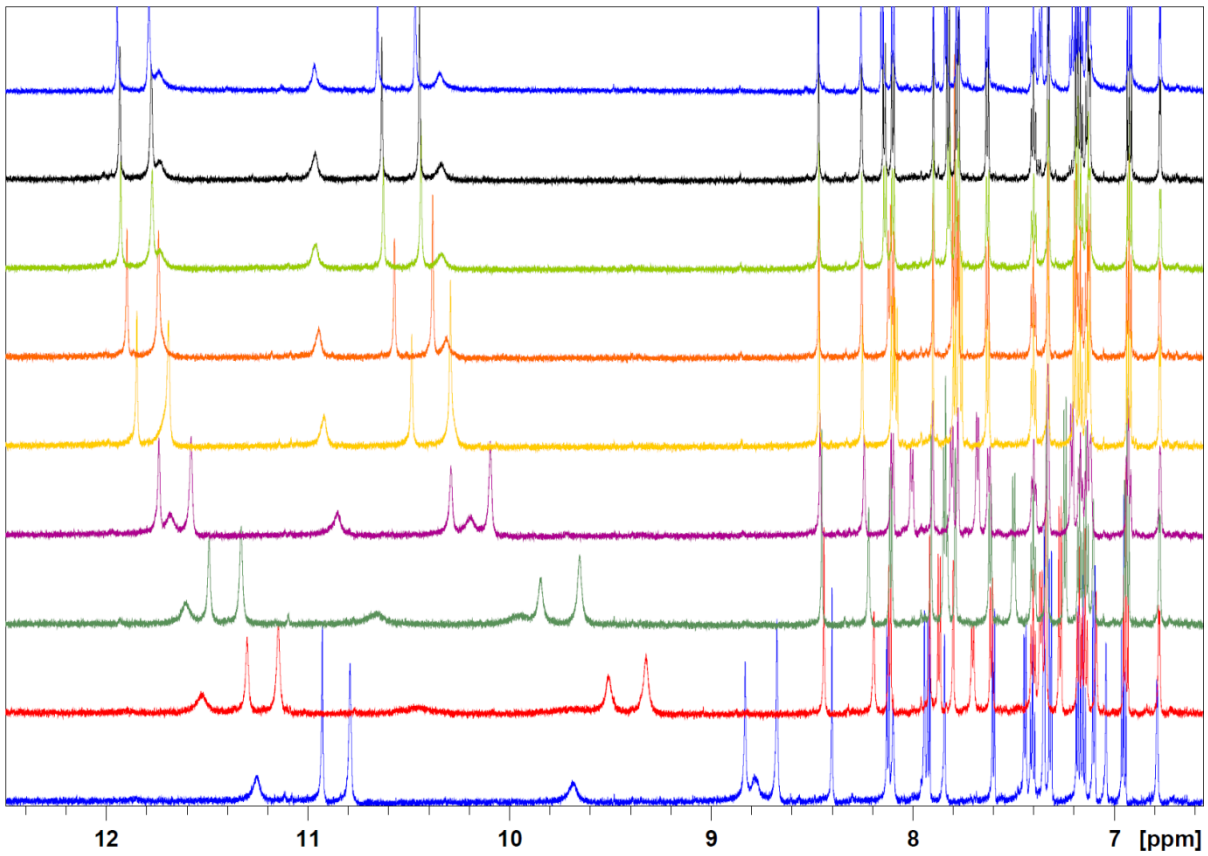
2.20 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors Cz-Gly-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-lactate



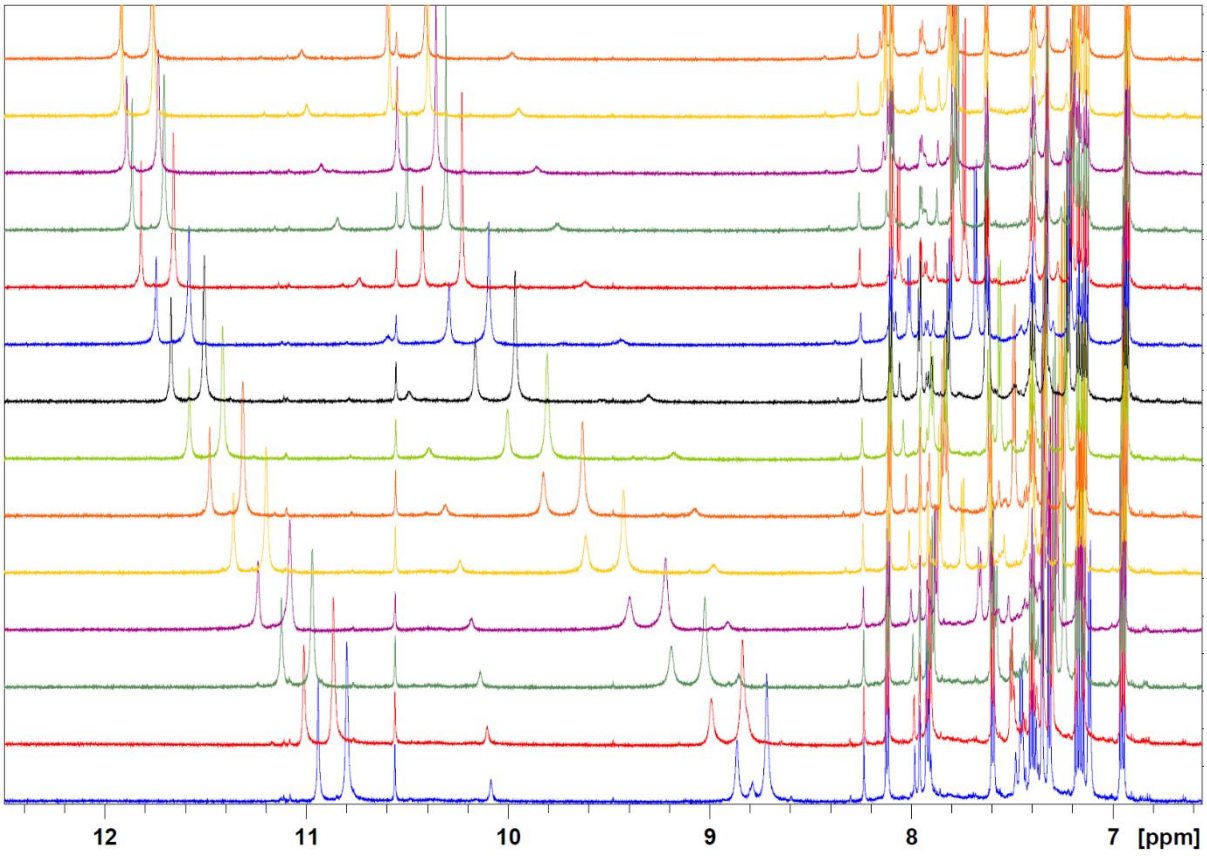
2.21 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-Py; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-lactate



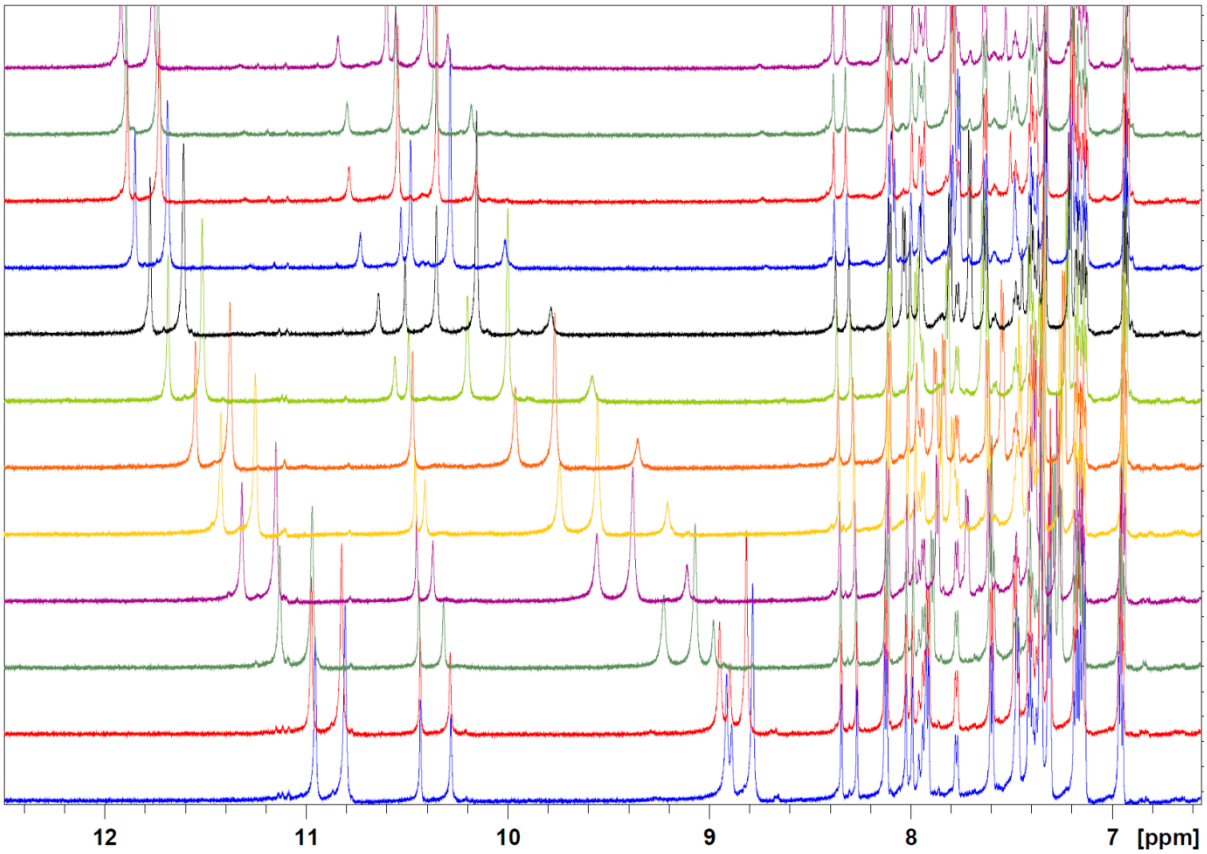
2.22 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-DPM; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-lactate



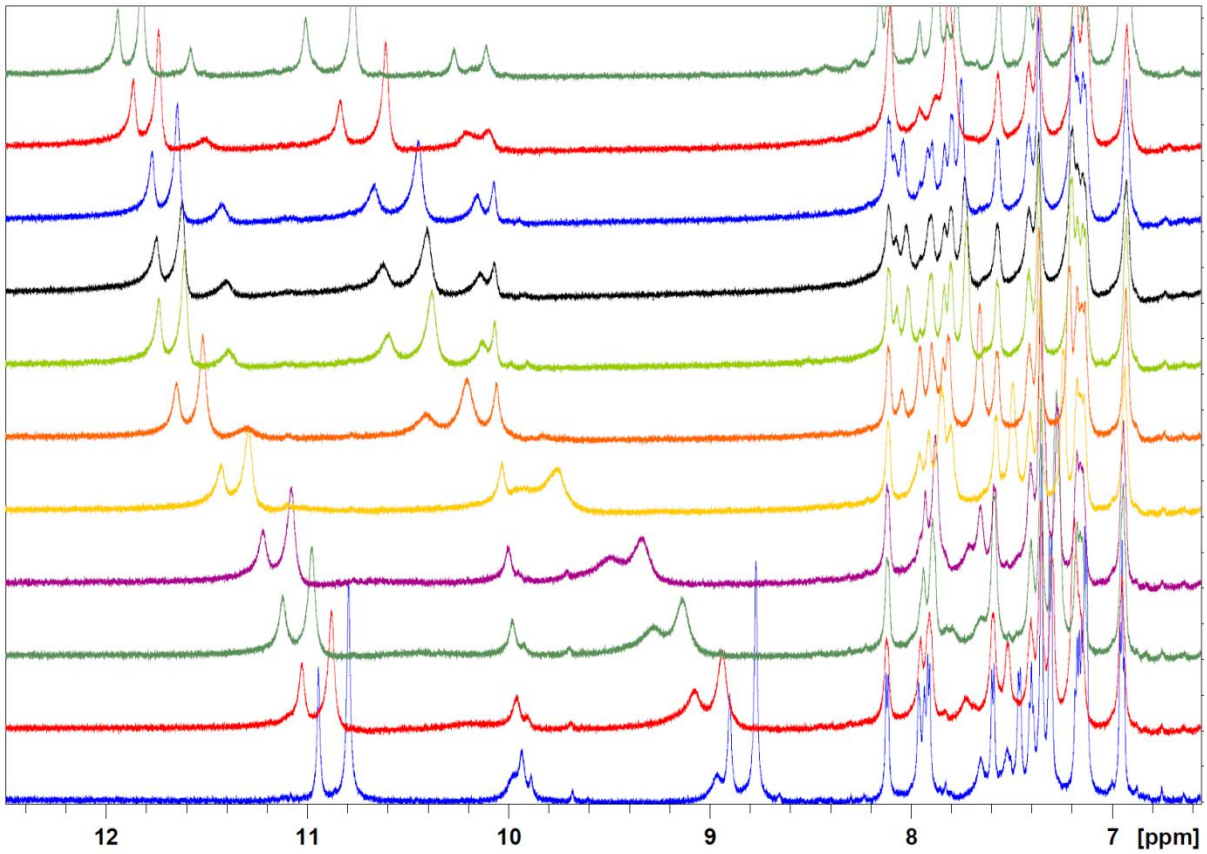
2.23 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BA; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-lactate



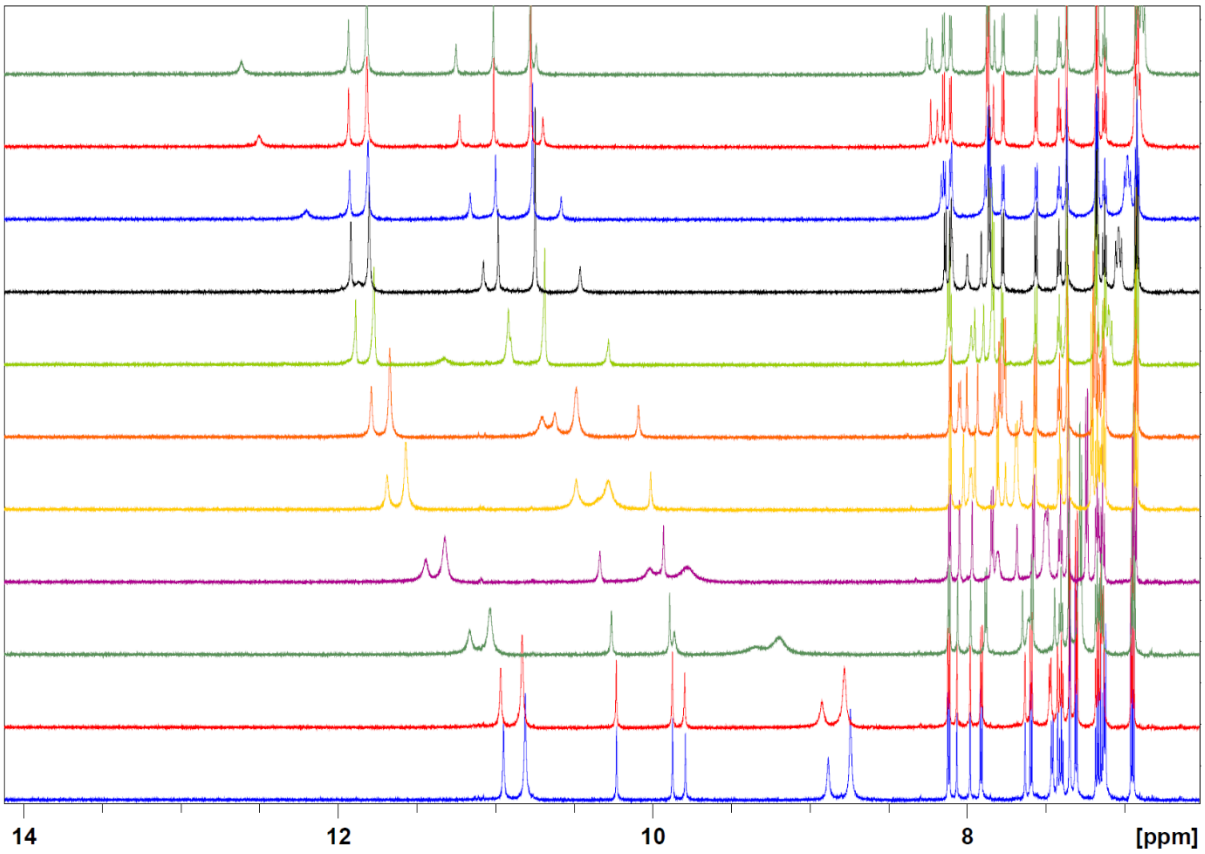
2.24 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BB; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-lactate



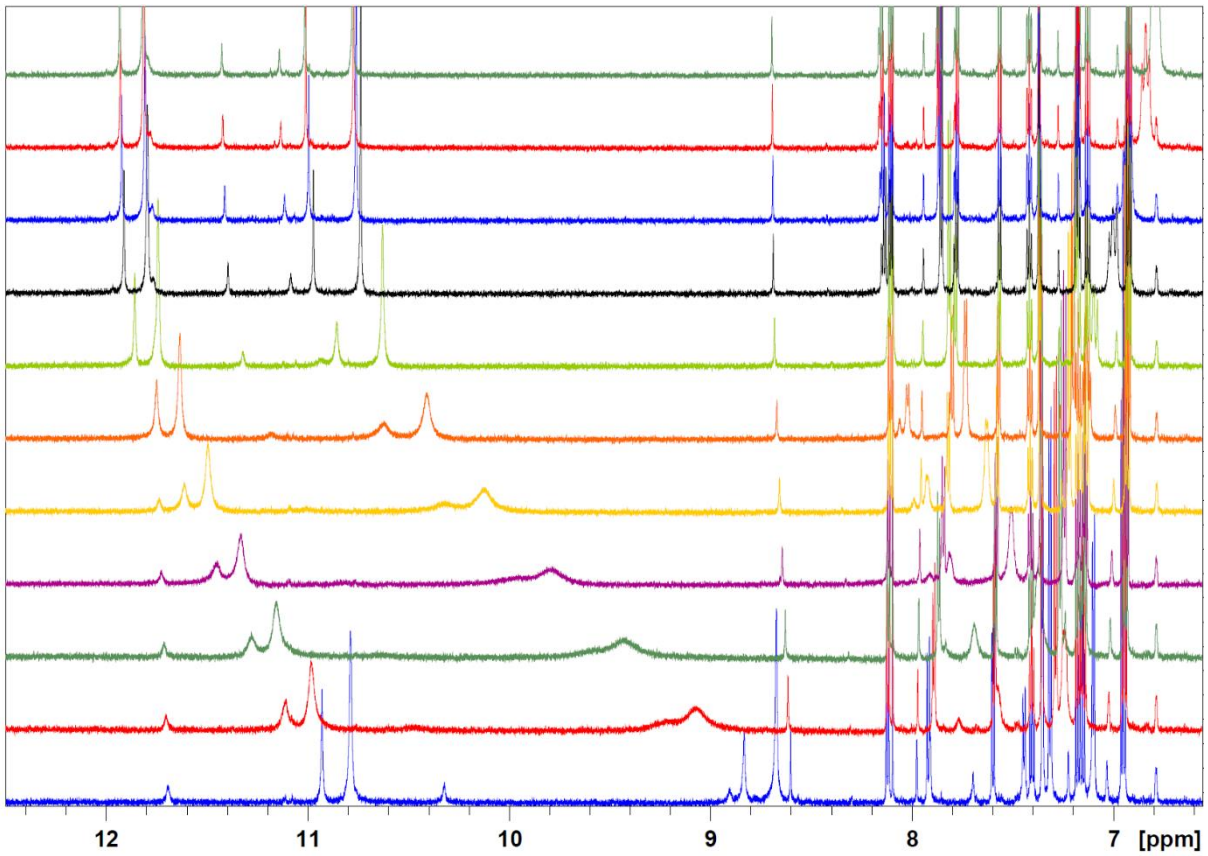
2.25 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-sorbate



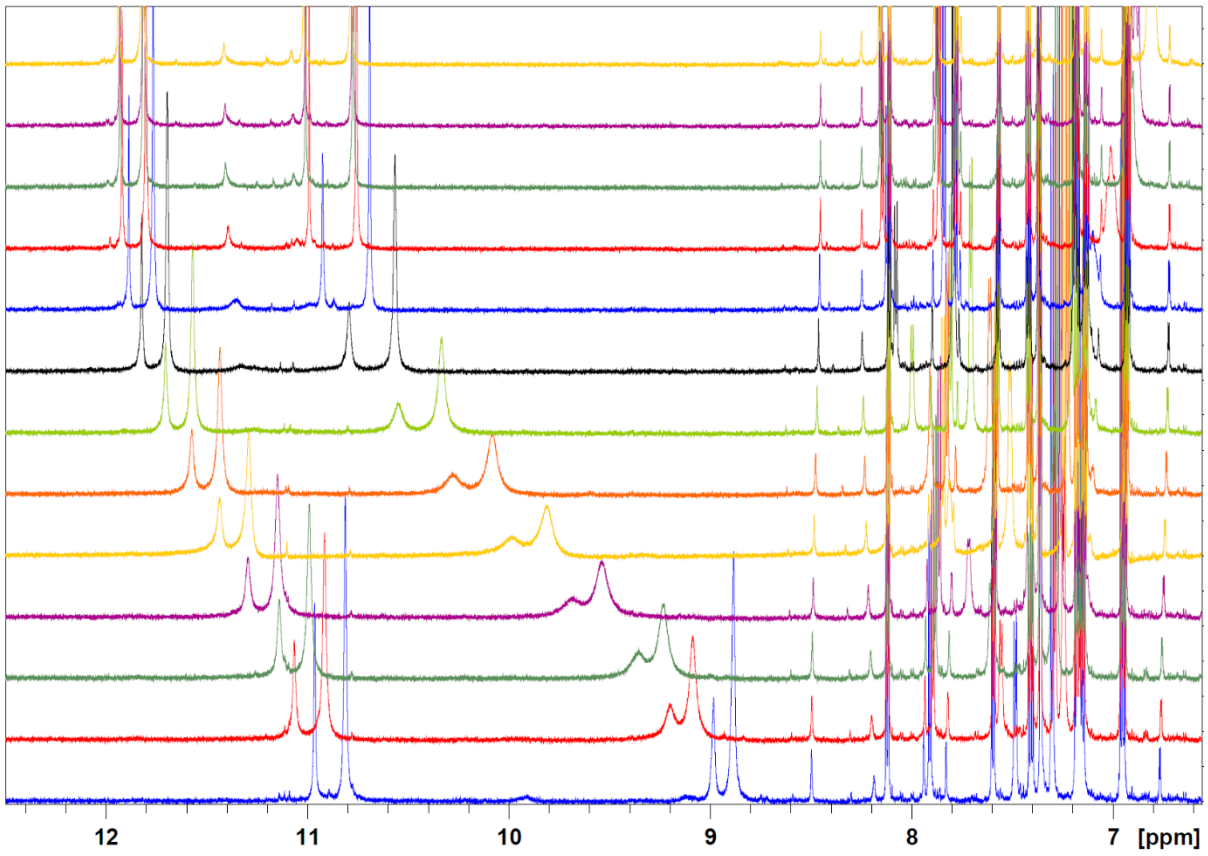
2.26 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors Cz-Gly-NeP; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-sorbate



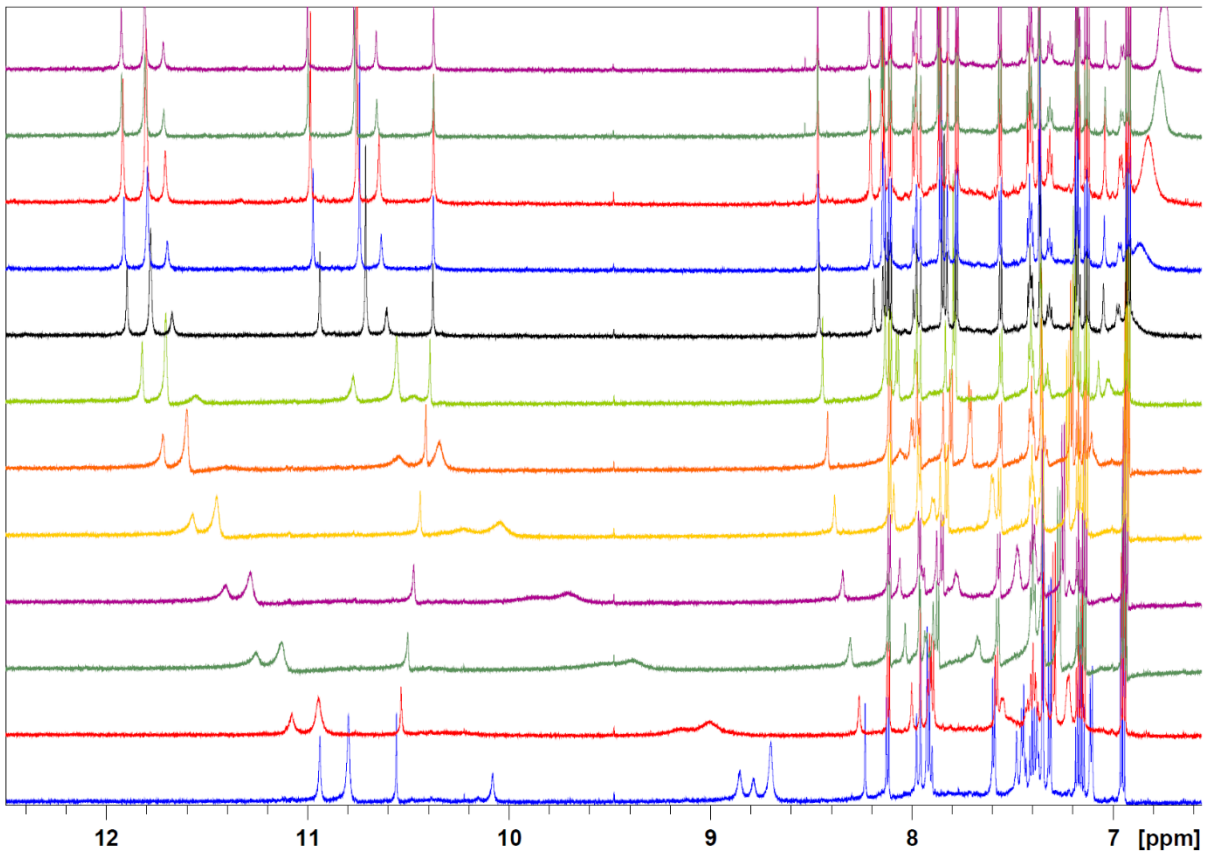
2.27 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-Py; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-sorbate



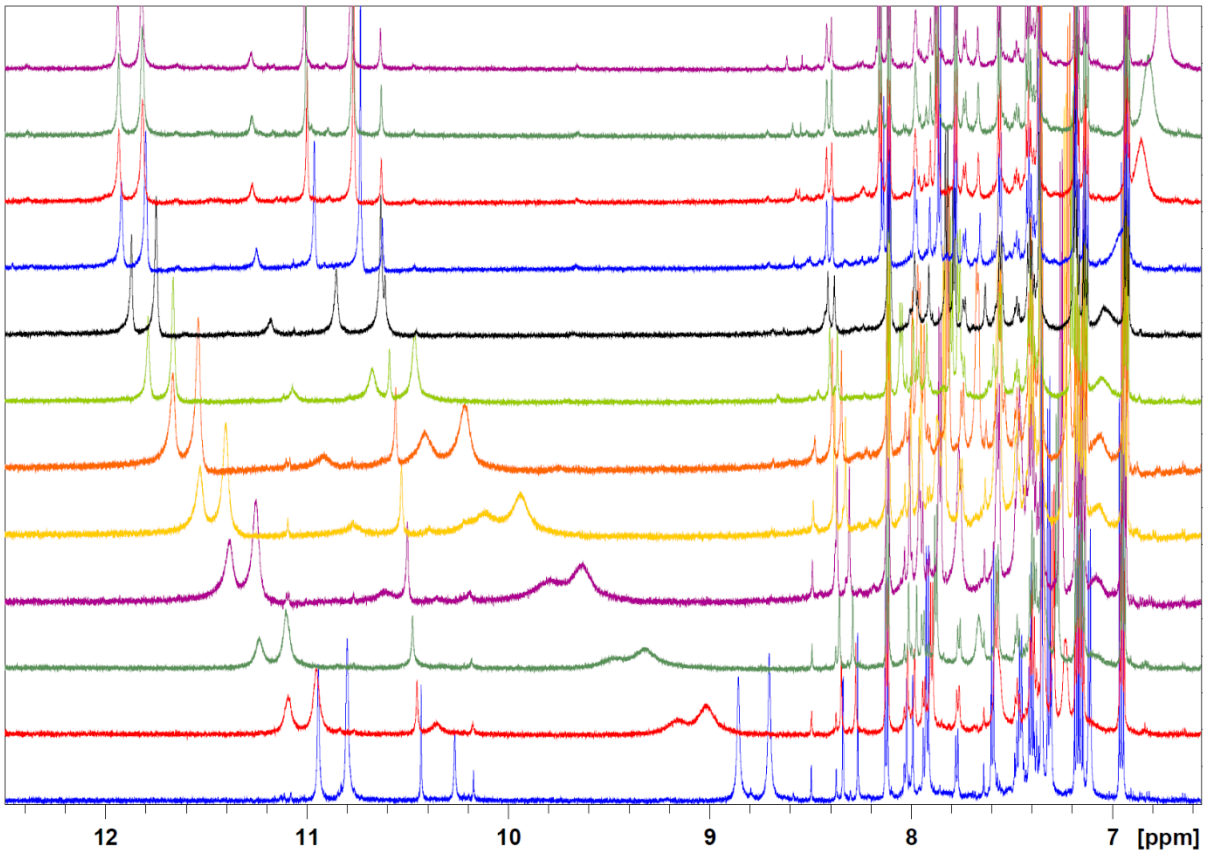
2.28 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-DPM; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-sorbate



2.29 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BA; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-sorbate



2.30 ^{1}H NMR spectra (700.1 MHz) of a mixture of receptors CzU-BB; 1,3-diindolylurea; 1,3-dicarbazolylurea + TBA-sorbate



3. Computational investigation of binding

3.1 Used computational parameters

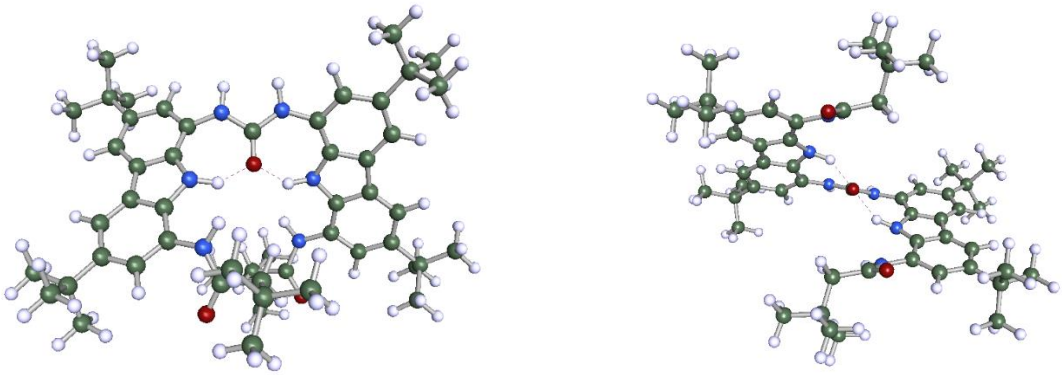
The computational investigation was carried out on DFT level using Turbomole v.6.5 (geometry optimization) and COSMO-RS method[6–8] (using COSMOTherm2021[9]) was applied to study the conformer stability in solution). The Becke-Perdew functional, TZVP basis set, and the following wave function convergence criteria - max difference 10^{-6} Hartree, geometry convergence: max gradient |dE/dxyz| 10^{-3} Hartree $Bohr^{-1}$ - were applied for the geometry optimization. The conformer stability was investigated using COSMOTherm 2021 with the parametrization BP_TZVP_21.

Frequency calculations were carried out on the DFT optimized geometries of the structures of the determined most stable conformers to test whether the geometry optimization reached a true minimum. For the majority of the studied structures, either no negative frequencies were detected, or the minimum negative frequency value observed remained higher than -20 (the exceptions were the acetate complexes of CzU-NEP (-40) and CzU-DPM (-43).

The conformer stability was investigated in the solvent mixture of 99.5% DMSO and 0.5% H_2O. Images of most stable conformers and respective Gibbs free energies in 99.5%DMSO-0.5% H2O are presented in section 3.2. Coordinates of computational geometries for the most stable conformers are presented in SI section 3.3.

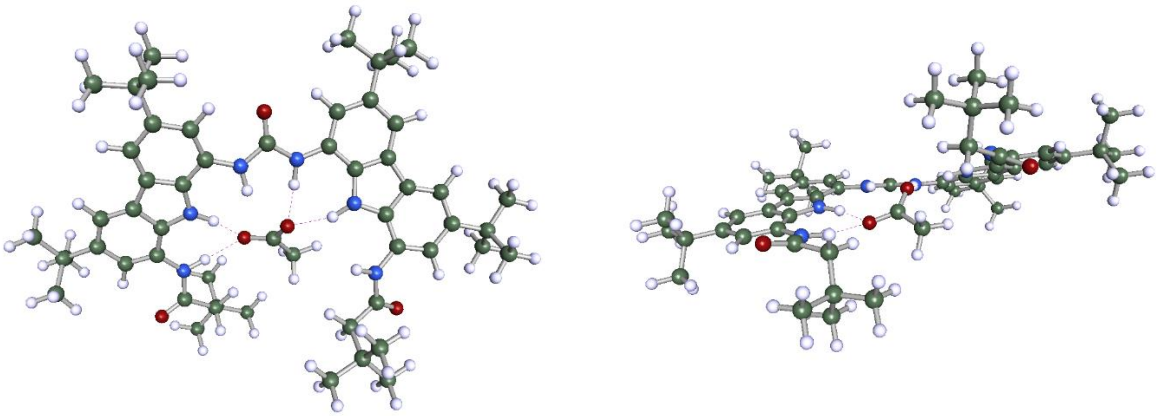
3.2 Images of the geometries of most stable conformers (detemined using COSMO-RS, solvent: 99.5% DMSO with 0.5% water). COSMOTherm 2021, parametrization BP_TZVP_21.

3.2.1 Lowest energy conformation of receptor CzU-NeP



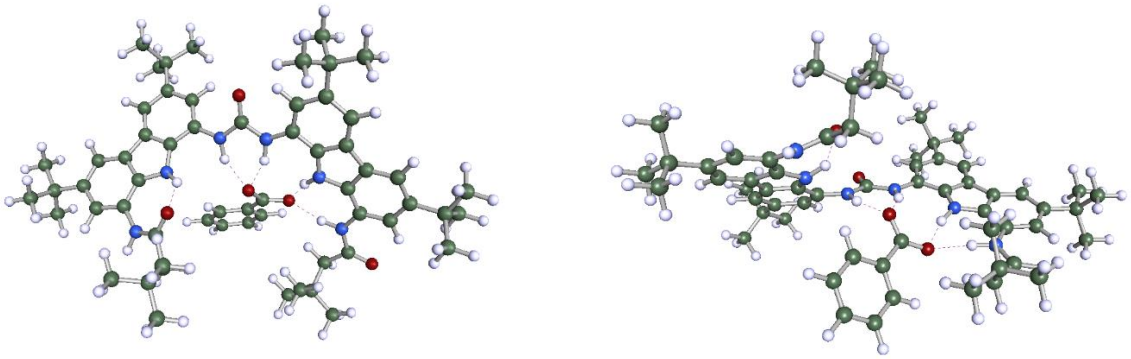
G = -1643073.61922 kcal/mol

3.2.2 Lowest energy conformation of receptor CzU-NeP with acetate anion



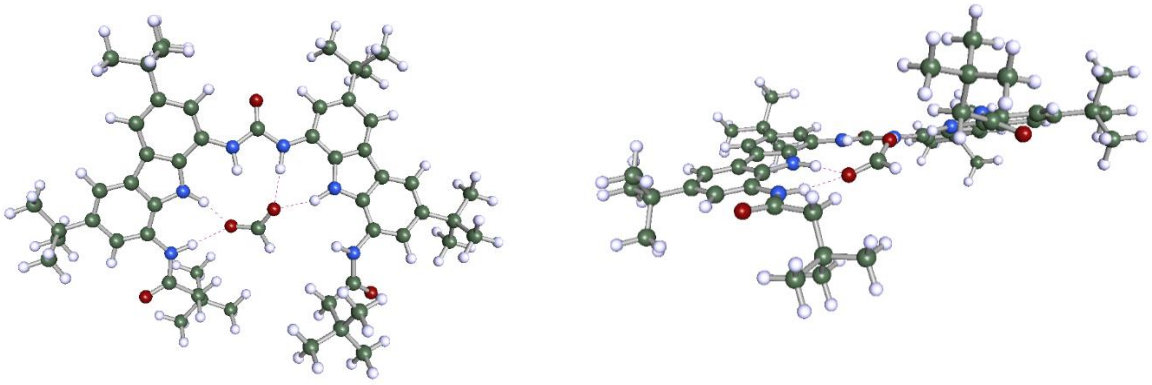
G = -1786625.33635 kcal/mol

3.2.3 Lowest energy conformation of receptor CzU-NeP with benzoate anion



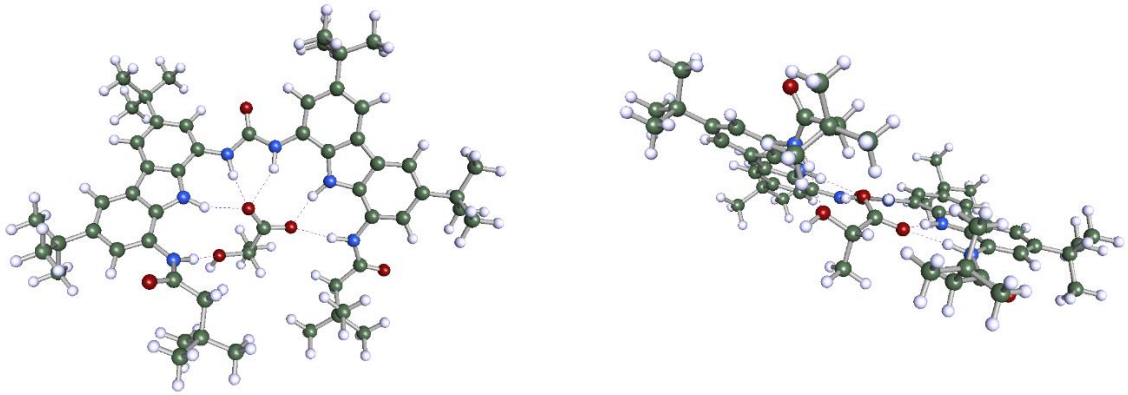
G = -1906988.68199 kcal/mol

3.2.4 Lowest energy conformation of receptor CzU-NeP with formate anion



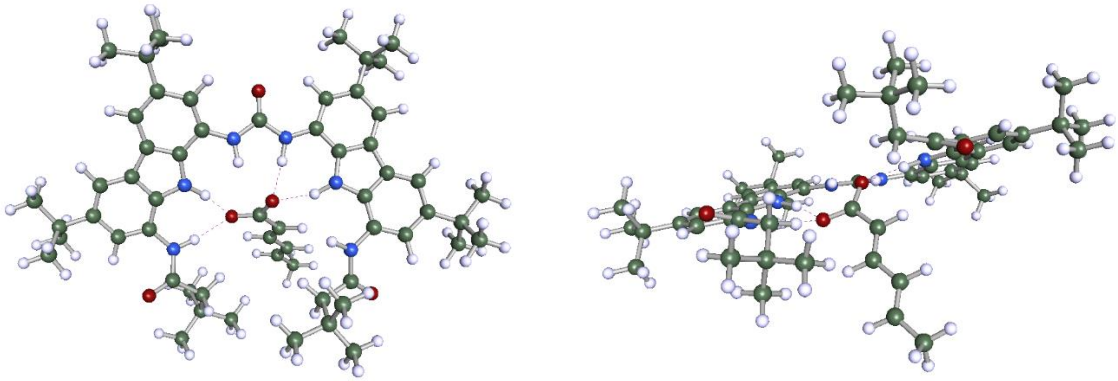
G = -1761943.71261 kcal/mol

3.2.5 Lowest energy conformation of receptor CzU-NeP with lactate anion



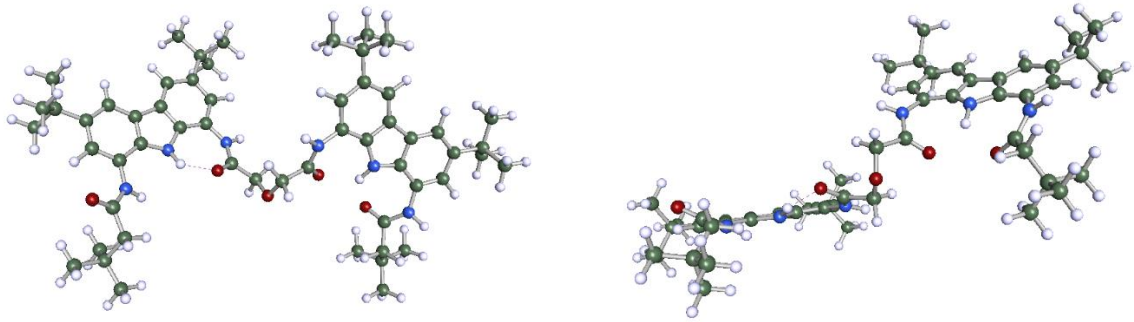
G = -1858530.57751kcal/mol

3.2.6 Lowest energy conformation of receptor CzU-NeP with sorbate anion



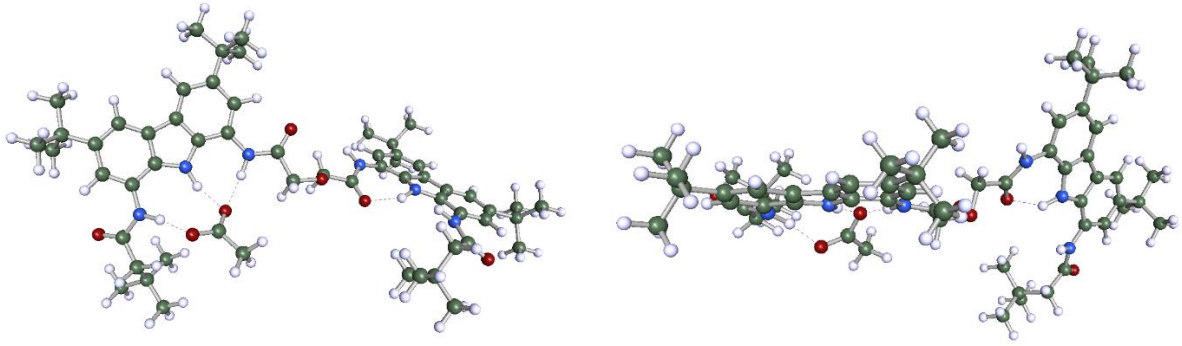
G = -1883801.67397 kcal/mol

3.2.7 Lowest energy conformation of receptor Cz-Gly-NeP



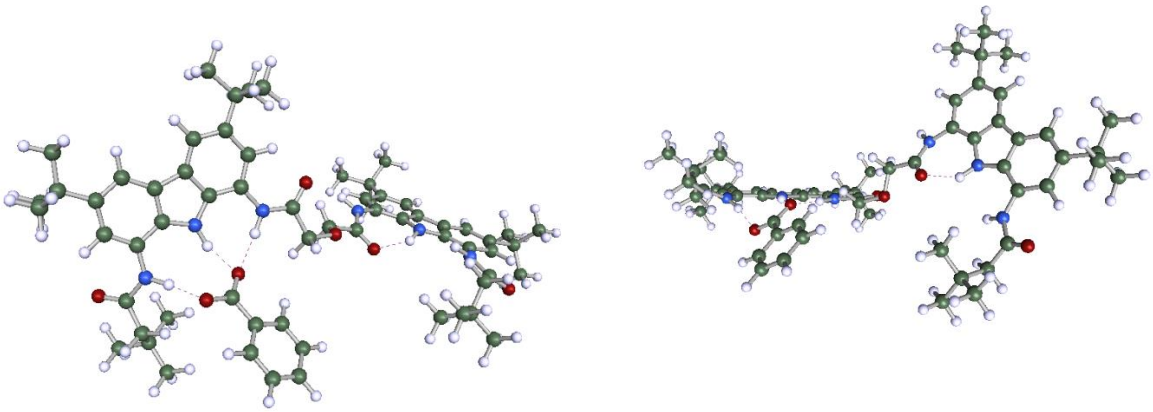
G = -1810796.99183 kcal/mol

3.2.8 Lowest energy conformation of receptor Cz-Gly-NeP with acetate anion



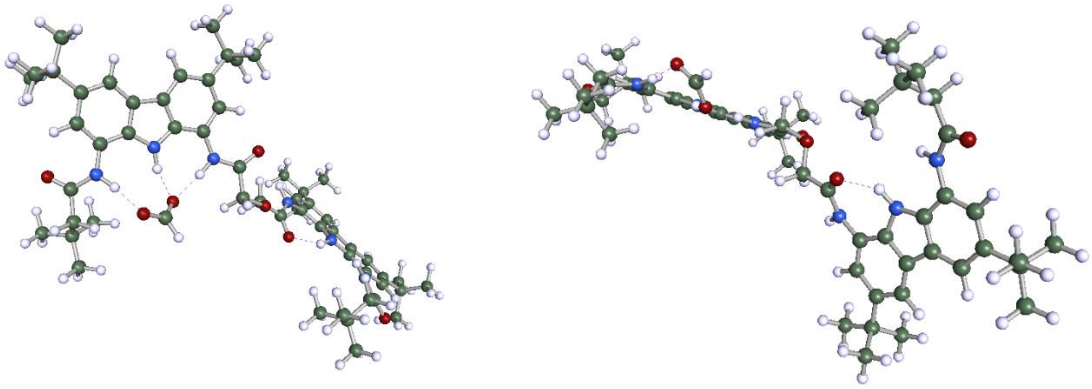
G = -1954346.83059 kcal/mol

3.2.9 Lowest energy conformation of receptor Cz-Gly-NeP with benzoate anion



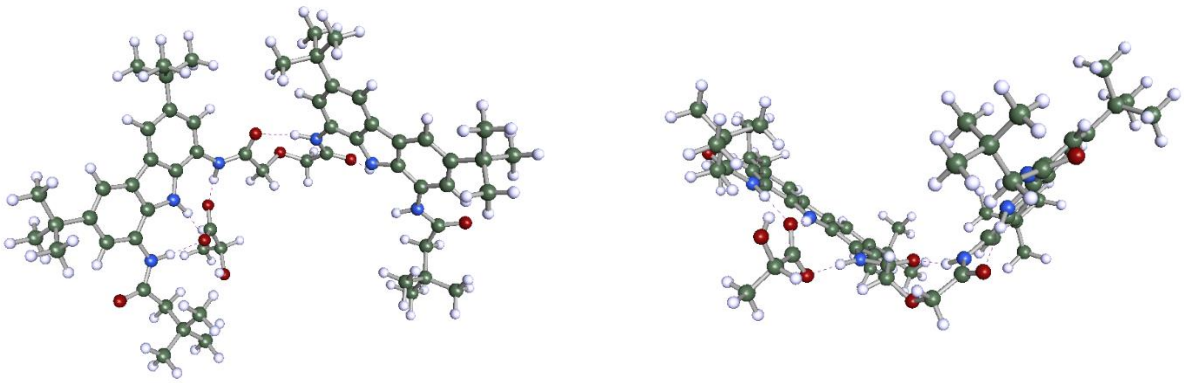
G = -2074709.80141 kcal/mol

3.2.10 Lowest energy conformation of receptor Cz-Gly-NeP with formate anion



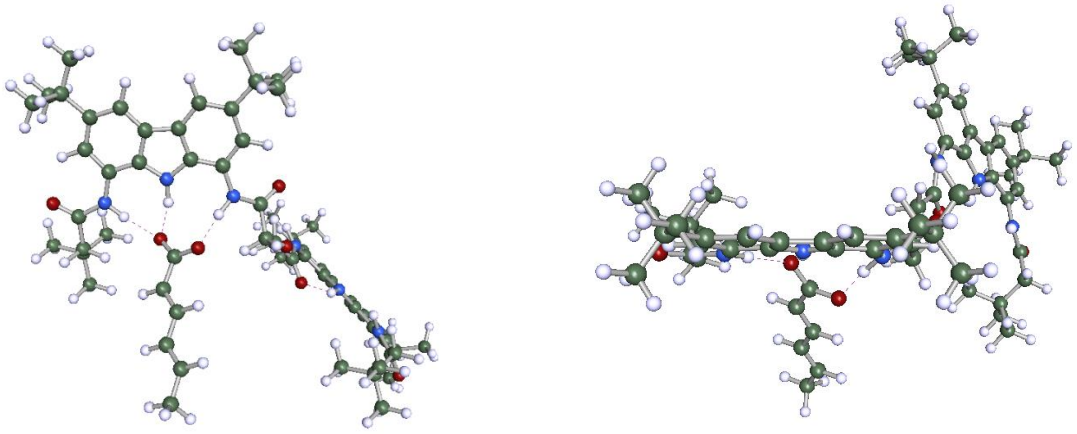
G = -1929664.74222 kcal/mol

3.2.11 Lowest energy conformation of receptor Cz-Gly-NeP with lactate anion



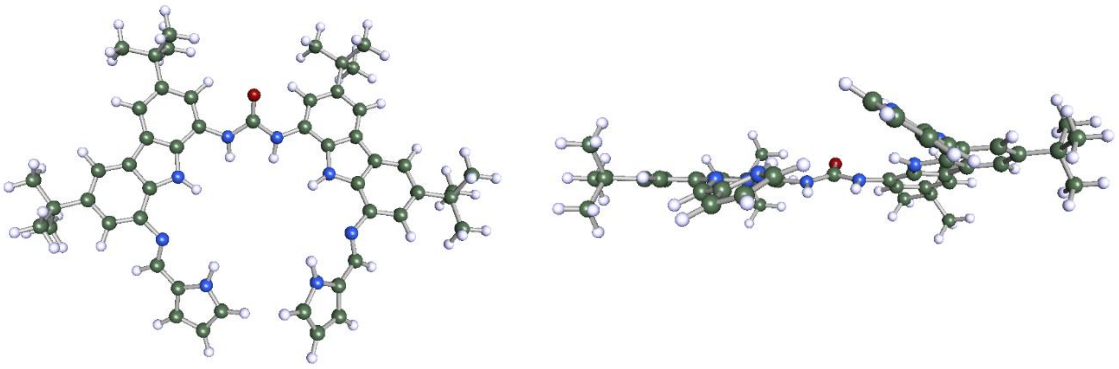
G = -2026255.07778 kcal/mol

3.2.12 Lowest energy conformation of receptor Cz-Gly-NeP with sorbate anion



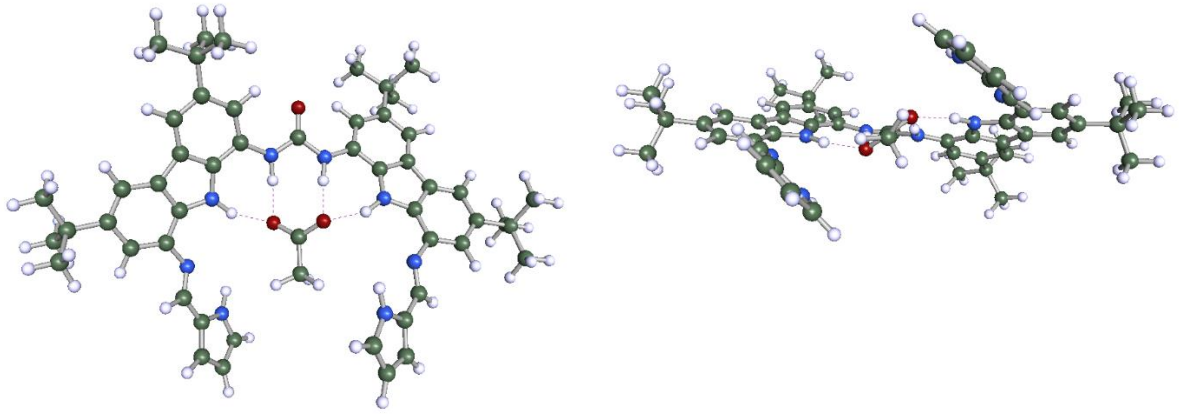
G = -2051526.02421 kcal/mol

3.2.13 Lowest energy conformation of receptor CzU-Py



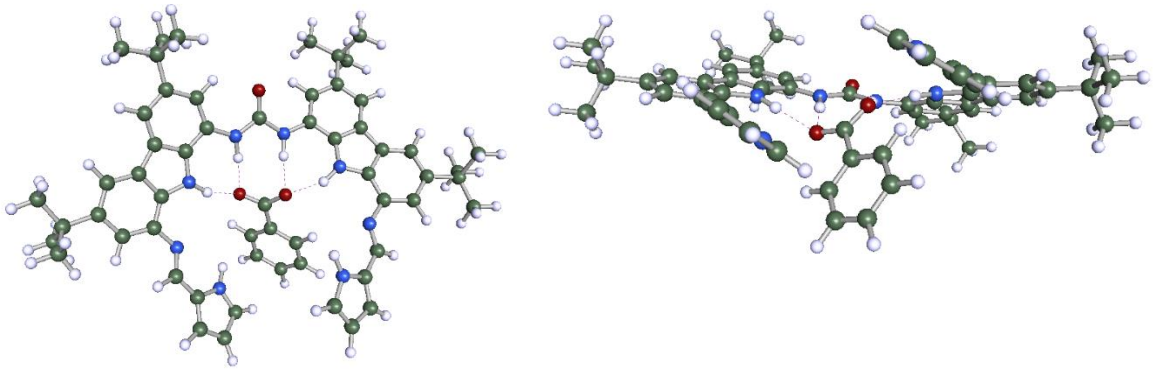
G = -1564185.49168 kcal/mol

3.2.14 Lowest energy conformation of receptor CzU-Py with acetate anion



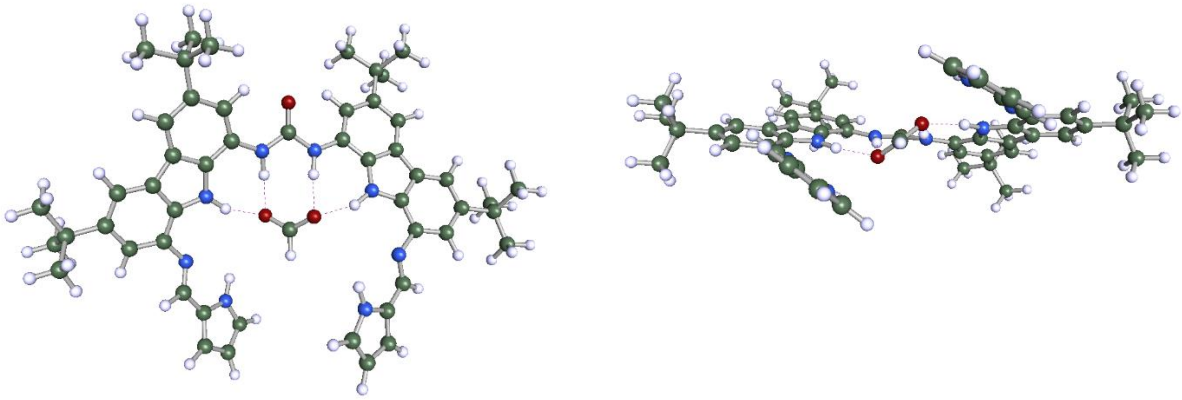
G = -1707738.51842 kcal/mol

3.2.15 Lowest energy conformation of receptor CzU-Py with benzoate anion



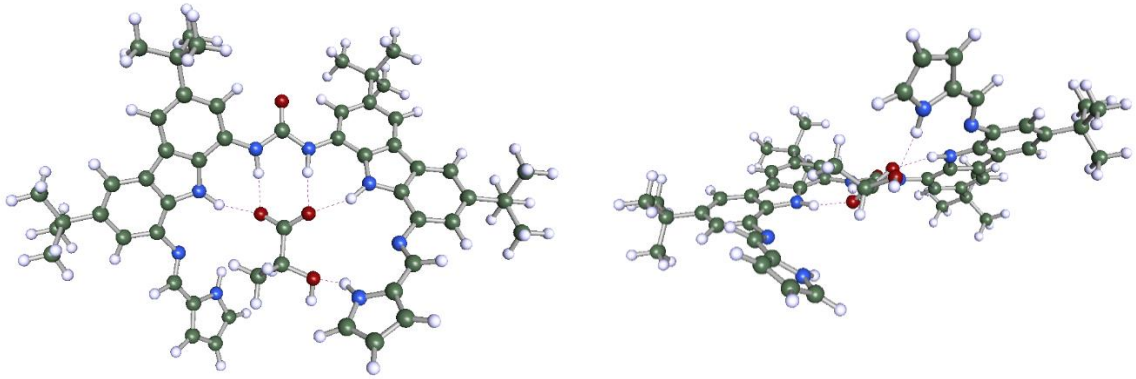
G = -1828098.08974 kcal/mol

3.2.16 Lowest energy conformation of receptor CzU-Py with formate anion



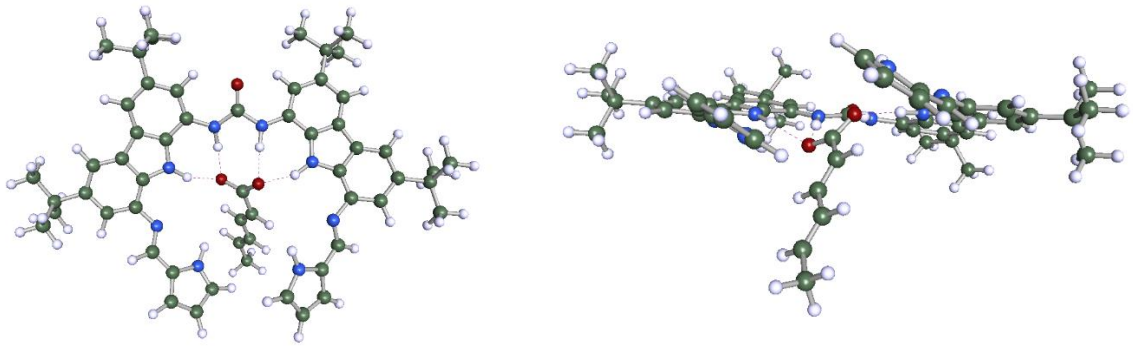
G = -1683055.75883 kcal/mol

3.2.17 Lowest energy conformation of receptor CzU-Py with lactate anion



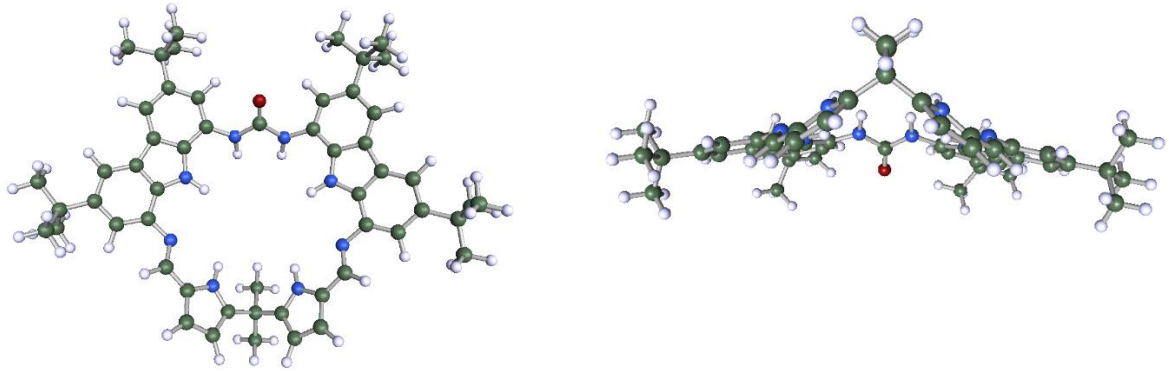
G = -1779642.71785 kcal/mol

3.2.18 Lowest energy conformation of receptor CzU-Py with sorbate anion



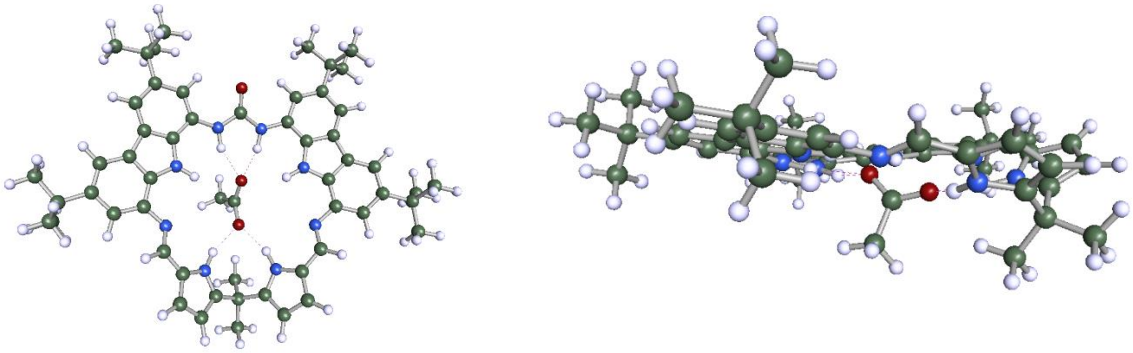
G = -1804914.14324 kcal/mol

3.2.19 Lowest energy conformation of receptor CzU-DPM



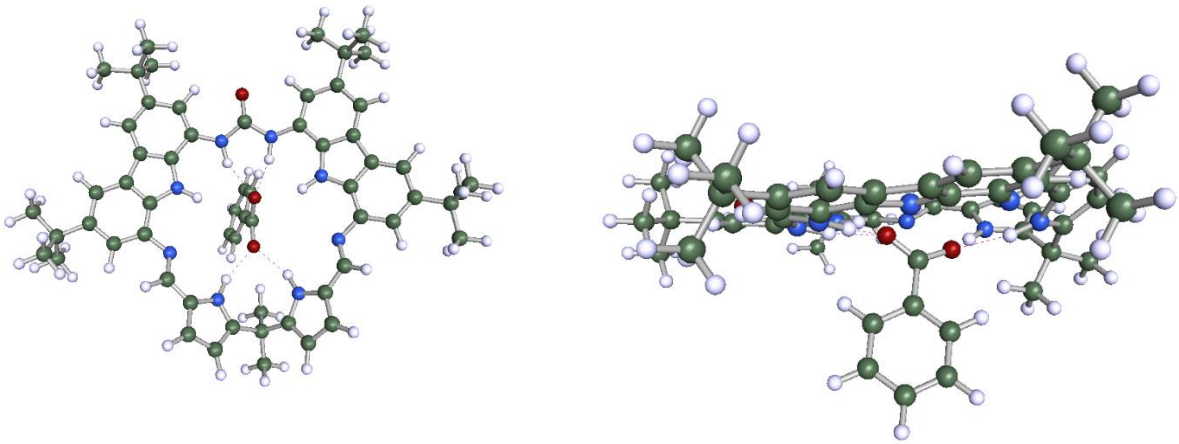
G = -1637465.63173 kcal/mol

3.2.20 Lowest energy conformation of receptor CzU-DPM with acetate anion



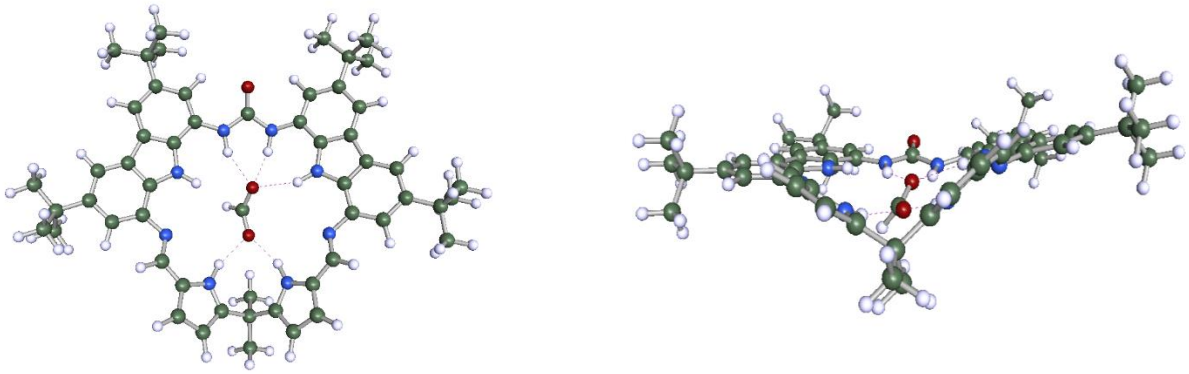
G = -1781015.75558kcal/mol

3.2.21 Lowest energy conformation of receptor CzU-DPM with benzoate anion



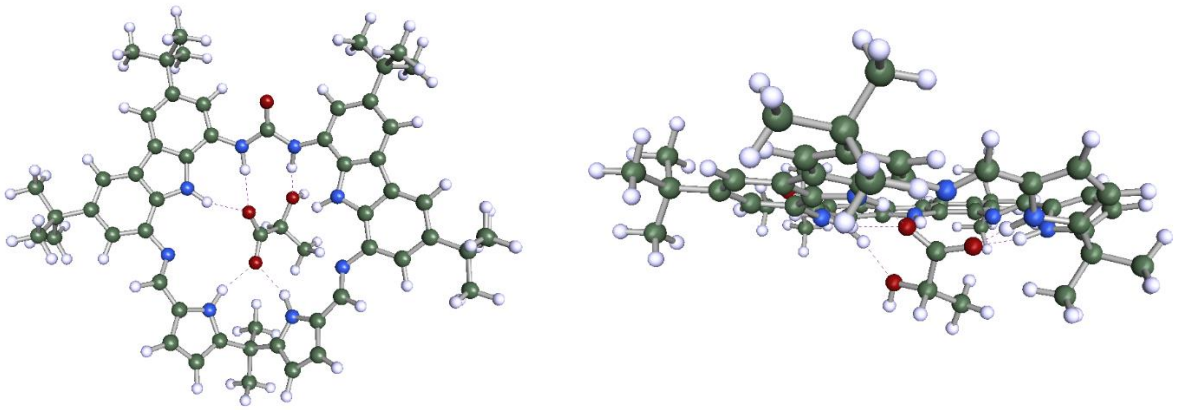
G = -1901377.40925kcal/mol

3.2.22 Lowest energy conformation of receptor CzU-DPM with formate anion



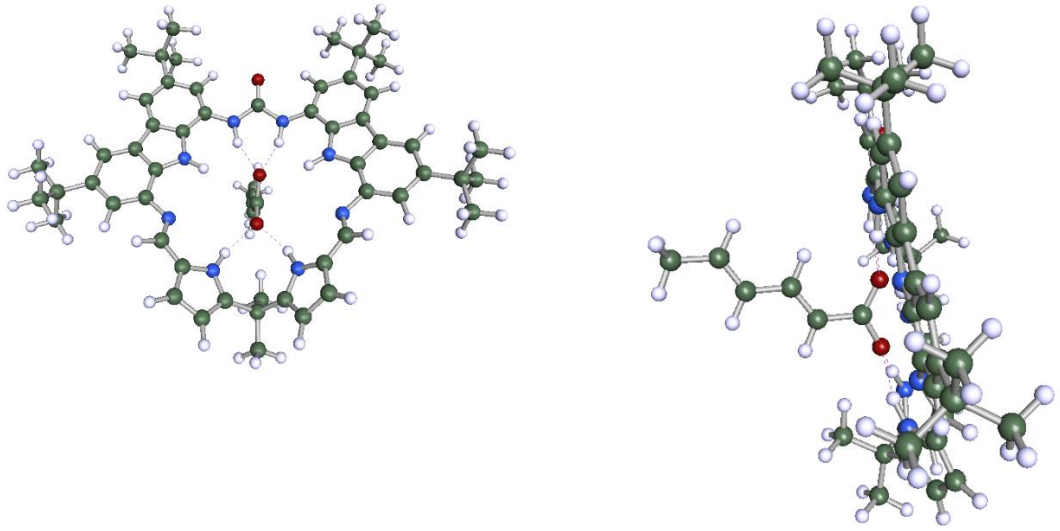
G = -1756333.8839 kcal/mol

3.2.23 Lowest energy conformation of receptor CzU-DPM with lactate anion



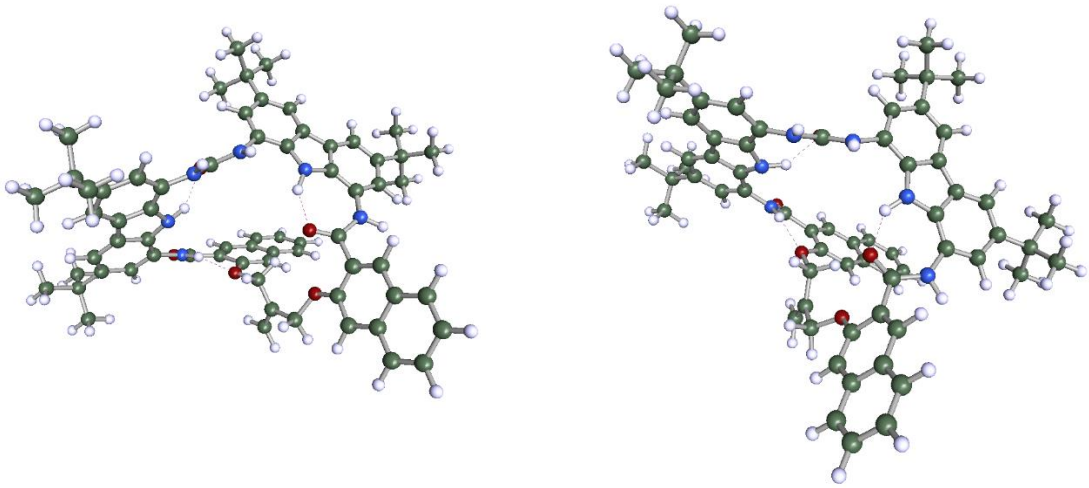
G = -1852920.79124 kcal/mol

3.2.24 Lowest energy conformation of receptor CzU-DPM with sorbate anion



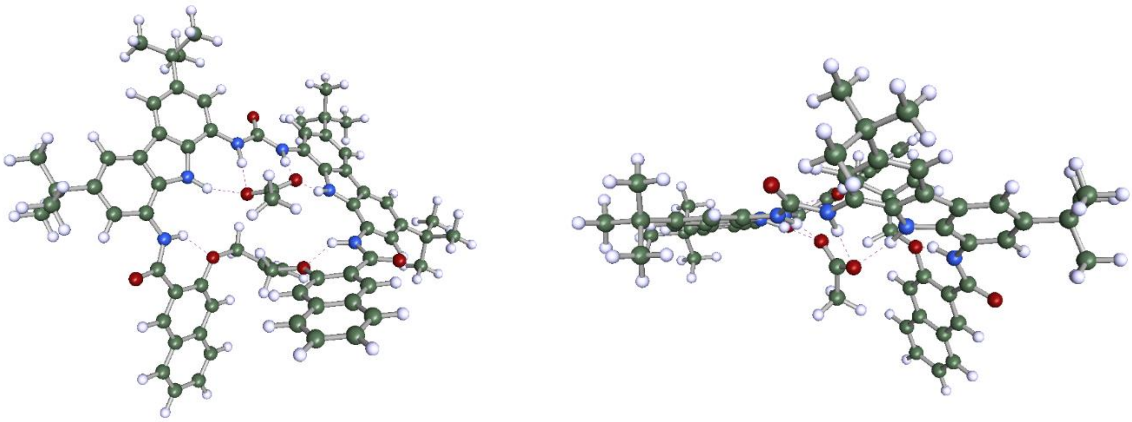
G = -1878193.7422 kcal/mol

3.2.25 Lowest energy conformation of receptor CzU-BA



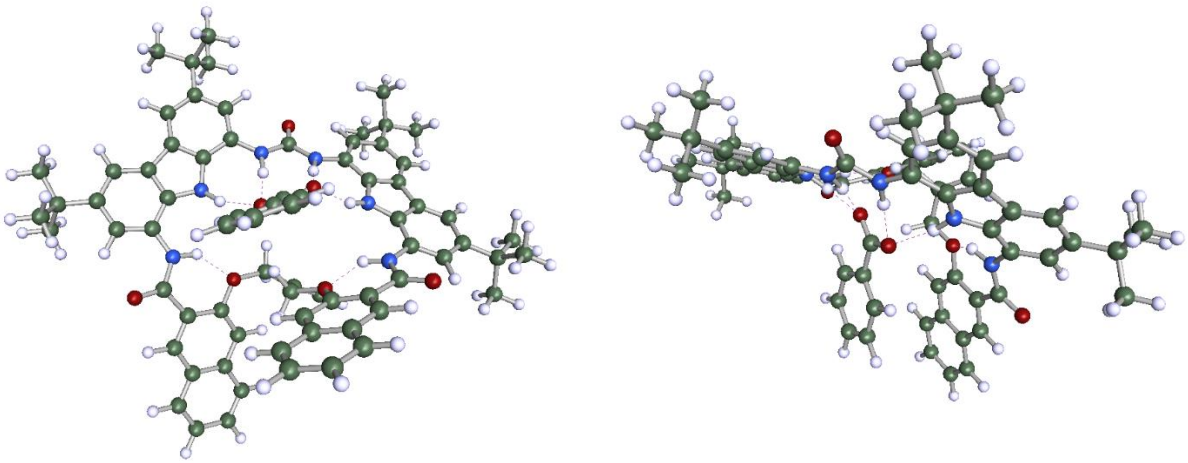
G = -2070891.58366 kcal/mol

3.2.26 Lowest energy conformation of receptor CzU-BA with acetate anion



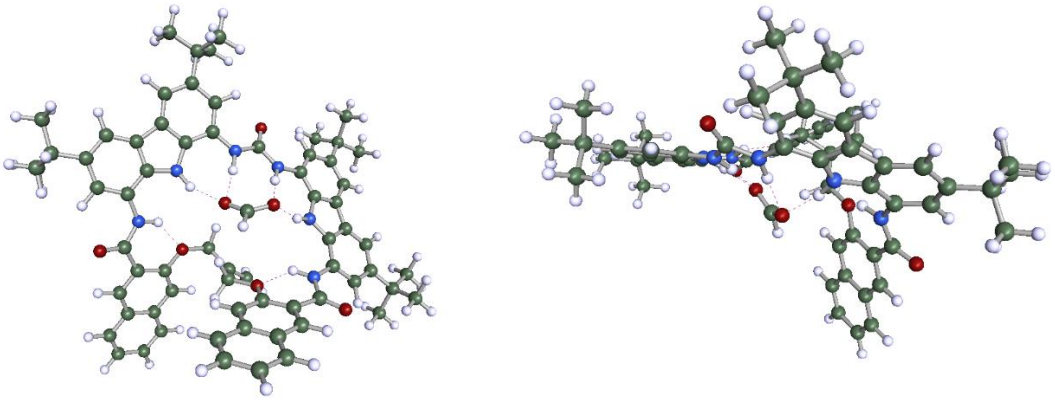
G = -2214440.89509 kcal/mol

3.2.27 Lowest energy conformation of receptor CzU-BA with benzoate anion



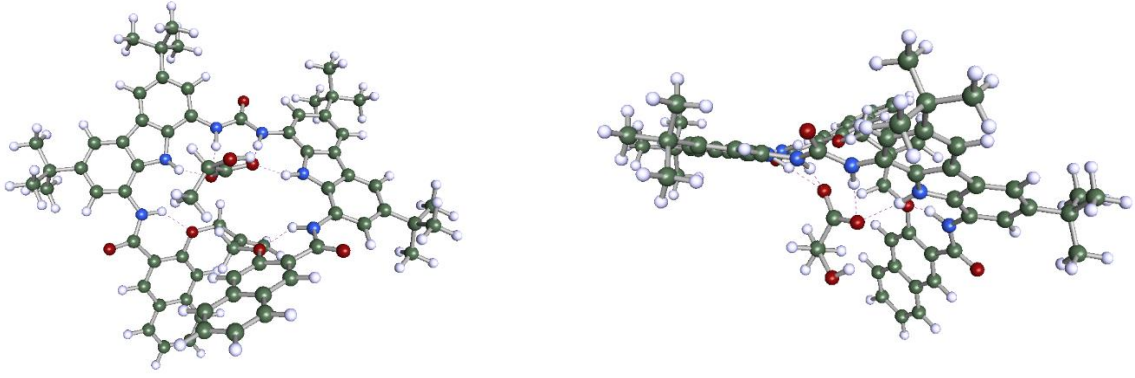
G = -2334802.53378 kcal/mol

3.2.28 Lowest energy conformation of receptor CzU-BA with formate anion



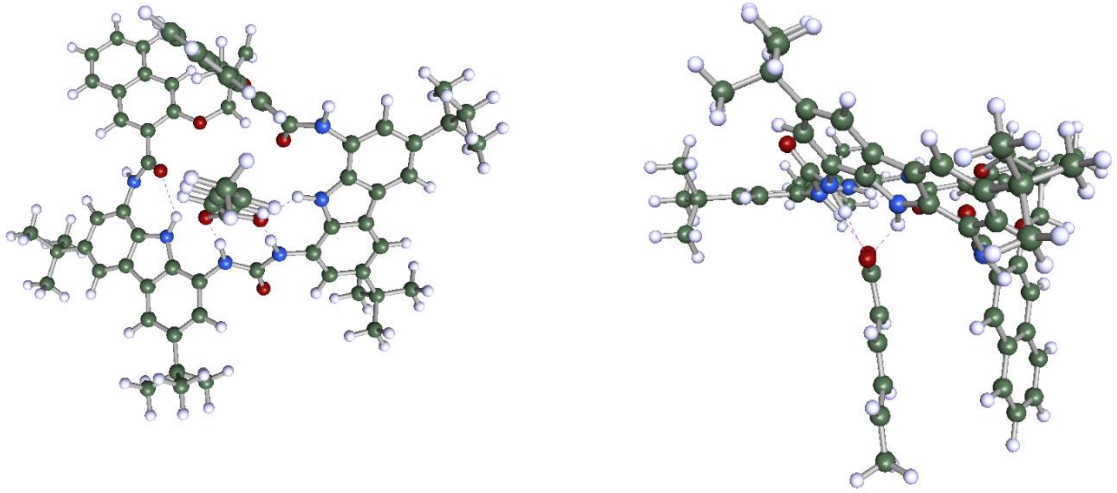
G = -2189759.17786 kcal/mol

3.2.29 Lowest energy conformation of receptor CzU-BA with lactate anion



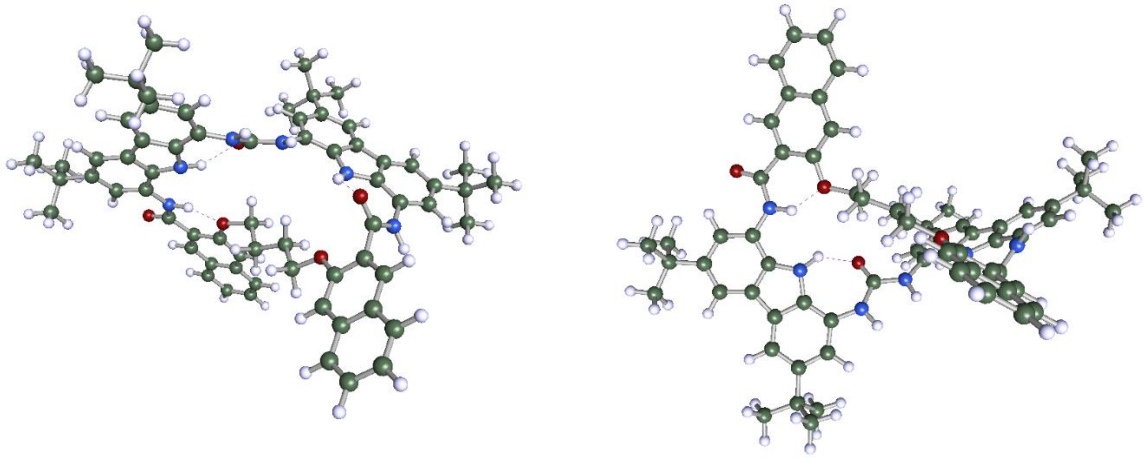
G = -2286344.56364 kcal/mol

3.2.30 Lowest energy conformation of receptor CzU-BA with sorbate anion



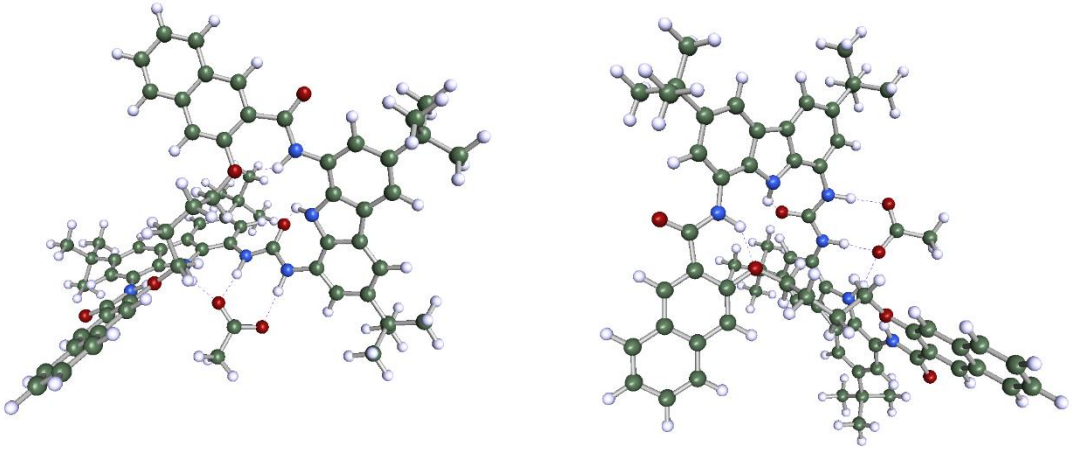
G = -2311606.75936 kcal/mol

3.2.31 Lowest energy conformation of receptor CzU-BB



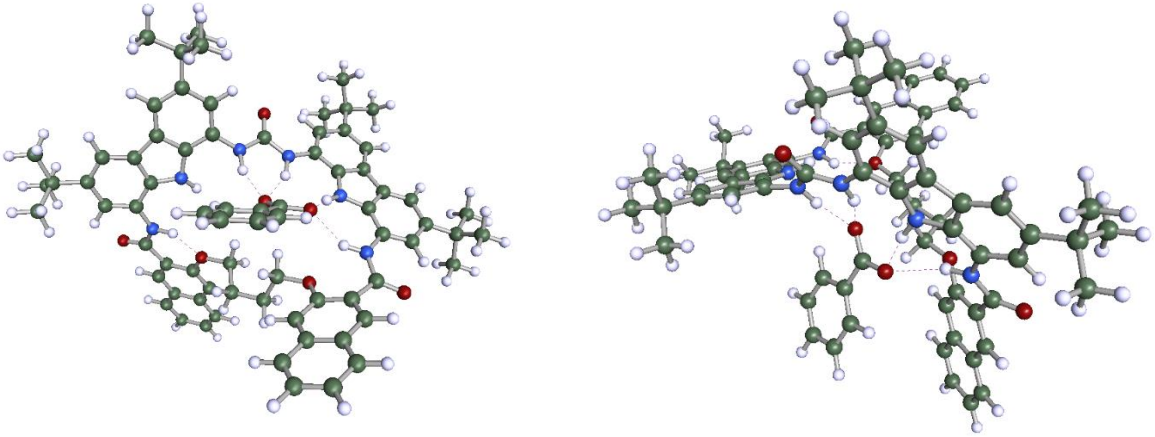
G = -2071664.41086 kcal/mol

3.2.32 Lowest energy conformation of receptor CzU-BB with acetate anion



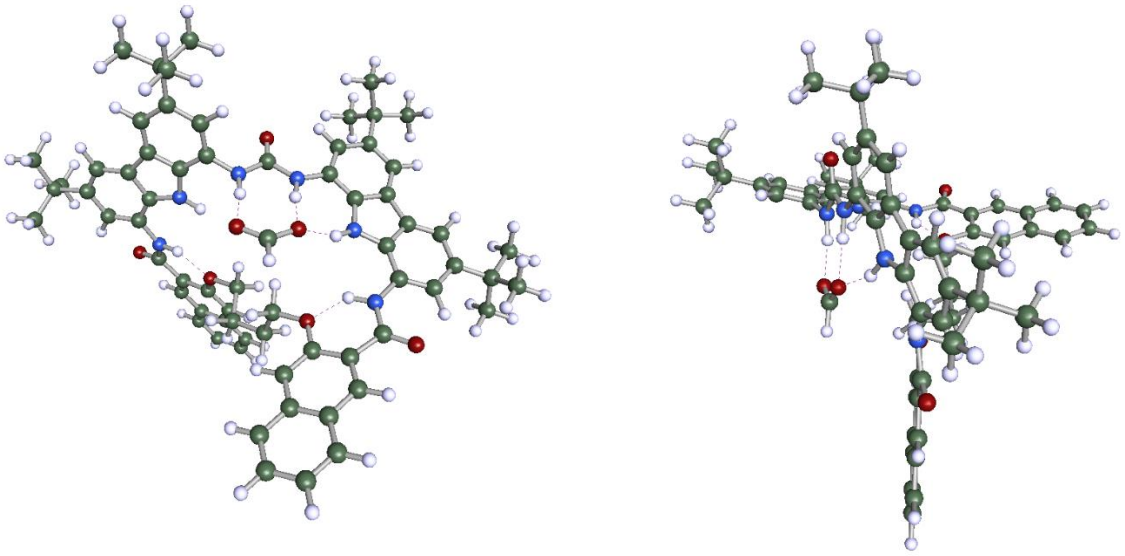
G = -2215214.80803 kcal/mol

3.2.33 Lowest energy conformation of receptor CzU-BB with benzoate anion



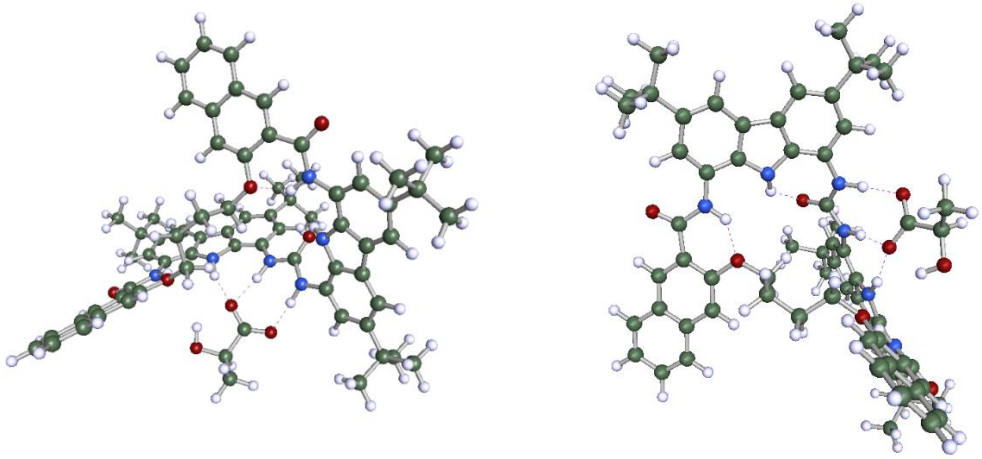
G = -2335574.26789 kcal/mol

3.2.34 Lowest energy conformation of receptor CzU-BB with formate anion



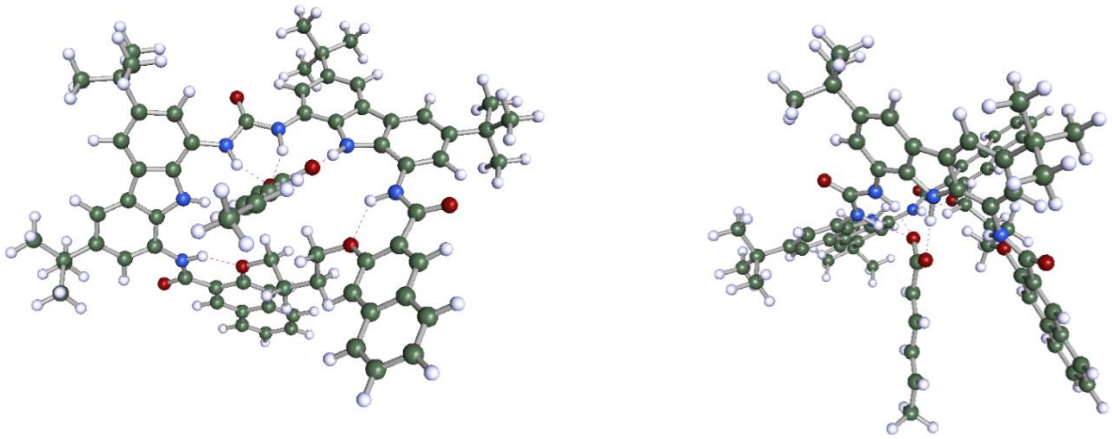
G = -2190528.87343 kcal/mol

3.2.35 Lowest energy conformation of receptor CzU-BB with lactate anion



G = -2287119.60643 kcal/mol

3.2.36 Lowest energy conformation of receptor CzU-BB with sorbate anion



G = -2312389.97268 kcal/mol

3.3 Coordinates of most stable conformer geometries

3.3.1 CzU-NeP free receptor

134 0

C 6.317868 5.075862 1.015234

C 5.169949 4.343863 1.335209

C 3.899789 4.632499 0.776501

H 5.276082 3.524024 2.042239

C 3.784217 5.696319 -0.125848

C 6.183796 6.127643 0.090467

C 4.922136 6.444516 -0.473414

H 2.821912 5.948059 -0.570501

C 5.146568 7.555052 -1.382854

C 2.693665 3.770536 1.198283

C 1.394058 4.203287 0.494442

H 1.471412 4.112936 -0.599518

H 1.122616 5.241574 0.737167

H 0.567770 3.556875 0.825118

C 2.480225 3.894389 2.726347

H 2.278485 4.938299 3.010630

H 3.360495 3.552013 3.289512

H 1.620874 3.281549 3.040370

C 2.966278 2.289692 0.841216

H 2.113803 1.663198 1.146621

H 3.863544 1.906550 1.347964

H 3.109908 2.168153 -0.243173

N 7.146633 7.013835 -0.385213

C 6.537261 7.847249 -1.321410

H 8.143213 6.801017 -0.511808

C 4.286790 8.310625 -2.196099

C 4.805832 9.349320 -2.977327

H 3.222309 8.079837 -2.209534

C 6.195770 9.603118 -2.918985

C 7.080901 8.880647 -2.106748

H 6.619422 10.405612 -3.527043

C 3.926614 10.215438 -3.900147

C 2.441947 9.812124 -3.831736

H 2.032346 9.928297 -2.816878

H 2.284122 8.770949 -4.150749

H 1.857561 10.458331 -4.503234

C 4.404028 10.058524 -5.363642

H 4.327097 9.010488 -5.690868

H 5.448806 10.377879 -5.488263

H 3.782273 10.673351 -6.032855

C 4.043771 11.701035 -3.483373

H 3.420898 12.328343 -4.139780

H 5.079005 12.064774 -3.555411

H 3.703333 11.846509 -2.446922

N 8.436004 9.298166 -2.069357

C 9.559936 8.513280 -1.930990

H 8.583425 10.256819 -2.381551

O 9.513611 7.280225 -1.717362

H 14.303948 12.137493 -1.165646

H 16.338640 2.966507 -5.594449

H 16.013067 11.033564 -2.732595

H 15.166260 1.649831 -5.346193

C 16.094158 2.098199 -4.963788

C 14.793075 11.628074 -0.321884

H 15.574362 12.299429 0.063858

H 16.898927 1.355171 -5.078089

C 16.486450 10.590581 -1.843499

H 17.237225 11.301424 -1.464618

H 14.049201 11.488698 0.476925

C 15.433479 10.293736 -0.748310

N 7.587391 4.837794 1.597852

N 11.128076 3.759562 -4.075800

C 12.437984 4.075736 -3.638257

C 13.521462 3.196094 -3.732973

C 14.398486 9.290636 -1.296887

C 12.682918 5.356864 -3.110604

C 13.030403 9.613392 -1.397253

C 12.063700 8.729424 -1.909180

C 12.501736 7.462479 -2.327905

H 17.013153 9.677772 -2.156775

N 11.799632 6.417565 -2.926227

C 14.814274 8.015233 -1.712082

C 13.876275 7.103310 -2.210049

C 13.987421 5.744096 -2.714814

C 14.833030 3.555102 -3.333727

N 10.738429 9.214984 -2.047963

C 15.058482 4.842154 -2.830710

C 15.960851 2.514797 -3.479202

H 13.330683 2.201799 -4.131112

H 10.798811 6.328393 -2.714073

H 17.636712 3.936721 -3.600348

H 12.682047 10.595234 -1.075694

H 15.865270 7.727764 -1.651542

H 16.055299 5.151994 -2.518801

C 17.321532 3.062804 -3.010711

H 18.089351 2.284526 -3.132892

H 14.677764 0.802810 -2.945563

C 15.623430 1.266414 -2.629649

C 16.140744 9.681230 0.484173

H 16.889017 10.385539 0.879992

H 16.418889 0.511596 -2.731747

H 17.303518 3.350517 -1.948862

H 15.417107 9.464139 1.284156

H 16.660586 8.745973 0.231326

H 15.534625 1.528454 -1.564319

H 10.667196 10.230831 -2.078470

C 10.503534 2.530886 -4.062419

H 10.581225 4.537291 -4.440436

C 8.113213 3.634883 2.018009

H 8.178100 5.656733 1.729246

O 11.045442 1.510883 -3.613973

O 7.509955 2.560503 1.887776

C 9.494066 3.734952 2.647600

C 9.095022 2.534194 -4.637203

C 9.528218 3.601077 4.203665

H 9.970032 4.689541 2.371579

H 10.101687 2.926651 2.212618

C 8.952811 1.906632 -6.060251

H 8.701558 3.562224 -4.671688

H 8.464107 1.963909 -3.938140

C 8.639008 4.676023 4.855311

H 7.578301 4.539737 4.594663

H 8.940292 5.687752 4.541480

H 8.720954 4.625456 5.951735

C 9.066506 2.201138 4.648660

H 9.132133 2.114895 5.744385

H 9.702087 1.418155 4.207100

H 8.028355 2.002219 4.349219

C 10.989911 3.813972 4.644157

H 11.079421 3.715323 5.737134

H 11.347902 4.816213 4.362467

H 11.655677 3.069521 4.180745

C 9.279436 0.402516 -6.035195

H 10.316515 0.218554 -5.722642

H 9.139461 -0.029917 -7.038182

H 8.616065 -0.133333 -5.338619

C 7.486269 2.097508 -6.494567

H 6.797016 1.609390 -5.788300

H 7.321293 1.655958 -7.489535

H 7.222604 3.164924 -6.548106

C 9.877359 2.624962 -7.060943

H 9.673261 3.706690 -7.088406

H 9.722740 2.227139 -8.075521

H 10.939050 2.484345 -6.807004

3.3.2 CzU-NeP acetate complex

141 -1

C -4.891467 -1.103869 1.567529

C -6.172165 -1.293059 2.103329

C -6.979177 -0.223134 2.569337

H -6.540361 -2.313618 2.163118

C -6.487346 1.082925 2.489591

C -4.410874 0.223991 1.503430

C -5.207840 1.312544 1.953076

H -7.082454 1.927783 2.835167

C -4.426648 2.513588 1.724568

C -8.372195 -0.548599 3.143533

C -9.124627 0.715776 3.598182

H -9.293838 1.414371 2.764741

H -8.582872 1.250808 4.392443

H -10.108877 0.430898 3.998698

C	-8.221301	-1.486013	4.365353
H	-7.627611	-1.004721	5.157569
H	-7.725080	-2.428921	4.094144
H	-9.210900	-1.732895	4.780828
C	-9.227237	-1.255215	2.063962
H	-10.224204	-1.495176	2.465400
H	-8.764983	-2.194762	1.728913
H	-9.358596	-0.607781	1.183807
N	-3.197787	0.703268	1.033345
C	-3.202775	2.085739	1.148512
H	-2.472260	0.119239	0.559127
C	-4.668856	3.884116	1.937978
C	-3.693107	4.820340	1.583539
H	-5.616428	4.200070	2.373433
C	-2.468925	4.367671	1.023430
C	-2.197203	3.012999	0.796600
H	-1.701735	5.085516	0.744509
C	-3.891323	6.336086	1.784534
C	-5.264397	6.668386	2.397357
H	-5.391492	6.209334	3.389549
H	-6.091867	6.334178	1.753568
H	-5.356160	7.757815	2.520028
C	-3.785673	7.057832	0.419215
H	-4.559115	6.696343	-0.275468
H	-2.804953	6.896772	-0.051450
H	-3.922209	8.142370	0.551138
C	-2.796345	6.881275	2.732763
H	-2.923694	7.965608	2.877214
H	-1.787852	6.711612	2.329648
H	-2.855022	6.395083	3.718448
N	-0.997670	2.509299	0.258853

C	-0.021851	3.196508	-0.455800
H	-0.821058	1.508264	0.392141
O	-0.058057	4.411088	-0.697443
H	1.845874	6.014058	-3.916695
H	7.440477	-2.691170	-4.463233
H	3.275833	4.681945	-5.586454
H	7.570887	-3.682648	-2.991035
C	8.059967	-2.890139	-3.575506
C	2.777783	6.400657	-3.478011
H	3.033485	7.332080	-4.005198
H	9.033751	-3.274923	-3.916708
C	4.166622	5.138786	-5.129228
H	4.372027	6.086346	-5.651835
H	2.583483	6.656206	-2.425535
C	3.939131	5.399137	-3.620623
N	-4.077608	-2.152770	1.074034
N	4.050184	-2.337543	-0.092668
C	4.832957	-1.540694	-0.964899
C	6.089869	-1.925038	-1.445119
C	3.660331	4.060443	-2.904706
C	4.351020	-0.269401	-1.337016
C	2.446414	3.834131	-2.214095
C	2.169239	2.626901	-1.551093
C	3.157688	1.623005	-1.597016
H	5.019732	4.466934	-5.300819
N	3.159174	0.361132	-1.002329
C	4.626336	3.044520	-2.940820
C	4.378151	1.824340	-2.292256
C	5.145442	0.601871	-2.129618
C	6.886585	-1.084475	-2.262282
N	0.984600	2.336933	-0.856326

C 6.406757 0.188044 -2.591453

C 8.257318 -1.602191 -2.741240

H 6.452790 -2.911428 -1.167019

H 2.308836 -0.095646 -0.627656

H 8.425507 -0.322794 -4.524115

H 1.685485 4.607472 -2.172255

H 5.570463 3.192456 -3.467963

H 6.998930 0.865824 -3.205771

C 8.995136 -0.571484 -3.616069

H 9.962977 -0.987542 -3.932581

H 8.697807 -2.691277 -0.874094

C 9.148185 -1.921051 -1.516692

C 5.209575 6.048345 -3.021014

H 5.424314 7.003120 -3.526623

H 10.130169 -2.292650 -1.848649

H 9.196392 0.361767 -3.068840

H 5.076116 6.252448 -1.947701

H 6.089645 5.399903 -3.137362

H 9.311511 -1.020642 -0.905126

H 0.843105 1.348244 -0.590976

C 4.048167 -3.709659 0.038807

H 3.431989 -1.830507 0.537629

C -4.198101 -3.502859 1.316258

H -3.269977 -1.880762 0.498857

O 4.727882 -4.452742 -0.683339

O -5.063332 -3.985823 2.065003

C -3.181302 -4.369628 0.587658

C 3.142919 -4.237609 1.140942

C -3.761503 -5.229545 -0.580484

H -2.740777 -5.047912 1.335444

H -2.369962 -3.741505 0.188268

C	3.878790	-4.733377	2.427722
H	2.579426	-5.082174	0.715384
H	2.413371	-3.468164	1.437448
C	-4.749447	-6.288307	-0.057203
H	-5.614782	-5.825480	0.435933
H	-4.262018	-6.955118	0.671275
H	-5.114209	-6.906214	-0.892301
C	-4.463450	-4.326520	-1.611680
H	-4.810886	-4.923595	-2.468723
H	-3.781718	-3.550997	-1.994201
H	-5.340957	-3.823043	-1.178272
C	-2.573837	-5.945280	-1.253626
H	-2.928005	-6.584328	-2.077095
H	-2.036736	-6.584035	-0.535480
H	-1.856057	-5.222223	-1.670123
C	4.733149	-3.601892	3.027599
H	5.546997	-3.302952	2.349375
H	5.191850	-3.930545	3.972568
H	4.122500	-2.710754	3.241791
C	2.790930	-5.142525	3.440614
H	2.148529	-4.287830	3.702700
H	3.252790	-5.518620	4.366293
H	2.150094	-5.940063	3.033400
C	4.766189	-5.953470	2.121836
H	4.170033	-6.779926	1.704831
H	5.243292	-6.312328	3.047047
H	5.555867	-5.708381	1.399035
O	0.513281	-0.325000	-0.075274
C	-0.339581	-1.192912	-0.475056
O	-1.589309	-1.105493	-0.259865
H	-0.572862	-2.759875	-1.955697

C 0.170504 -2.414649 -1.226694

H 1.120929 -2.209173 -1.734016

H 0.337346 -3.229469 -0.505787

3.3.3 CzU-NeP benzoate complex

148 -1

C -5.014783 -0.895242 2.331110

C -6.388504 -1.036670 2.574664

C -7.356951 -0.121342 2.086793

H -6.699526 -1.895425 3.162869

C -6.935263 0.975884 1.331482

C -4.610156 0.221595 1.561123

C -5.564278 1.151850 1.069134

H -7.652175 1.697719 0.941008

C -4.817354 2.152858 0.332390

C -8.841907 -0.384111 2.407771

C -9.764730 0.703009 1.826131

H -9.695500 0.755502 0.729253

H -9.532309 1.698208 2.234286

H -10.809247 0.472082 2.083636

C -9.045567 -0.418067 3.941454

H -8.762082 0.543669 4.395740

H -8.444460 -1.207684 4.414549

H -10.103047 -0.611319 4.180215

C -9.265964 -1.747247 1.809502

H -10.324106 -1.950560 2.036926

H -8.667807 -2.573650 2.219465

H -9.144051 -1.749336 0.715561

N -3.340027 0.595908 1.143556

C -3.451539 1.773707 0.412843

H	-2.463829	0.167229	1.519945
C	-5.197785	3.316804	-0.362035
C	-4.218142	4.098655	-0.979440
H	-6.250304	3.595256	-0.406324
C	-2.860631	3.690699	-0.906359
C	-2.445809	2.534465	-0.230124
H	-2.089688	4.286058	-1.388414
C	-4.555660	5.392269	-1.747260
C	-6.064990	5.697954	-1.738986
H	-6.449211	5.836144	-0.717031
H	-6.647455	4.898155	-2.220881
H	-6.252461	6.628444	-2.295190
C	-4.100019	5.256997	-3.220066
H	-4.613549	4.417551	-3.712886
H	-3.016836	5.084372	-3.295964
H	-4.334282	6.177390	-3.777467
C	-3.818769	6.587242	-1.095664
H	-4.047584	7.517447	-1.638914
H	-2.728395	6.448133	-1.109241
H	-4.132033	6.716203	-0.048361
N	-1.118188	2.073812	-0.165198
C	0.029500	2.740112	-0.568874
H	-0.966126	1.093901	0.144170
O	0.060057	3.916603	-0.961109
H	2.950726	6.412784	-0.262839
H	8.049944	-0.830814	-5.625883
H	4.571973	6.175253	-2.238524
H	7.707622	-2.539730	-5.262160
C	8.379276	-1.699363	-5.035346
C	3.798552	6.239186	0.416328
H	4.234367	7.219262	0.661345

H 9.390651 -1.977756 -5.369965

C 5.386094 6.054483 -1.507592

H 5.775643 7.054659 -1.261166

H 3.410779 5.803634 1.349238

C 4.877609 5.348025 -0.227415

N -4.025675 -1.795054 2.793511

N 3.650661 -2.707712 -2.970267

C 4.599290 -1.657719 -2.834343

C 5.921547 -1.911408 -3.223480

C 4.345609 3.947627 -0.598224

C 4.320170 -0.402432 -2.264174

C 2.993257 3.590992 -0.394744

C 2.482346 2.327282 -0.734136

C 3.374436 1.403277 -1.304695

H 6.194252 5.485350 -1.989211

N 3.141471 0.093876 -1.719178

C 5.221534 2.999484 -1.150858

C 4.742173 1.730703 -1.505873

C 5.355425 0.563679 -2.119077

C 6.970942 -0.976774 -3.070795

N 1.151219 1.925897 -0.491451

C 6.670685 0.271752 -2.511703

C 8.391198 -1.366295 -3.524130

H 6.134889 -2.889431 -3.660582

H 2.247885 -0.269976 -2.071809

H 9.143321 0.676005 -3.852294

H 2.302308 4.307197 0.041134

H 6.272078 3.244962 -1.316112

H 7.449001 1.021460 -2.372532

C 9.405969 -0.232260 -3.288951

H 10.401180 -0.557357 -3.626534

H	8.201135	-3.472589	-2.896836
C	8.863091	-2.610143	-2.733074
C	6.048203	5.210804	0.774980
H	6.439284	6.205583	1.039998
H	9.876829	-2.898650	-3.051135
H	9.485244	0.032262	-2.223719
H	5.715813	4.716325	1.700388
H	6.878089	4.625011	0.354680
H	8.889288	-2.401550	-1.652666
H	0.997762	0.958300	-0.162273
C	2.309945	-2.635613	-3.249597
H	4.052292	-3.643799	-2.967848
C	-4.190354	-2.957902	3.511671
H	-3.048461	-1.542743	2.590236
O	1.700565	-1.554612	-3.364571
O	-5.295985	-3.372836	3.898695
C	-2.898481	-3.710351	3.796747
C	1.618923	-3.979096	-3.411462
C	-2.718228	-5.042633	3.000839
H	-2.891987	-3.943876	4.873146
H	-2.033192	-3.062539	3.589949
C	1.244111	-4.360978	-4.879740
H	0.695806	-3.939581	-2.813709
H	2.247909	-4.779770	-2.992665
C	-3.770737	-6.087988	3.413415
H	-4.789999	-5.741957	3.196089
H	-3.709156	-6.303765	4.491483
H	-3.599899	-7.029591	2.868200
C	-2.812728	-4.778667	1.486598
H	-2.614247	-5.703802	0.924287
H	-2.077701	-4.024191	1.166574

H	-3.813420	-4.421902	1.198970
C	-1.315689	-5.585895	3.336929
H	-1.135402	-6.535487	2.809511
H	-1.212187	-5.772786	4.417095
H	-0.530551	-4.874582	3.038440
C	2.495928	-4.339875	-5.776551
H	2.917359	-3.326740	-5.862068
H	2.243024	-4.681506	-6.791826
H	3.280165	-5.006452	-5.384459
C	0.669668	-5.791044	-4.840000
H	1.413835	-6.509000	-4.461999
H	0.370717	-6.110656	-5.849915
H	-0.217933	-5.843541	-4.190804
C	0.178243	-3.405660	-5.447046
H	-0.732147	-3.419554	-4.828232
H	-0.099165	-3.715782	-6.466382
H	0.543260	-2.370495	-5.488725
C	2.007925	-2.473170	4.457413
C	0.917942	-1.874469	3.819615
H	-0.000538	-1.665438	4.369323
H	1.943017	-2.736096	5.514974
O	-1.284397	-0.783712	2.418831
C	3.181383	-2.737231	3.740221
C	0.990069	-1.525777	2.460499
C	-0.185597	-0.866496	1.773631
H	4.032094	-3.208465	4.236421
C	3.261769	-2.393089	2.384664
C	2.174014	-1.786542	1.750384
O	-0.019588	-0.415960	0.593748
H	4.176196	-2.597421	1.824289
H	2.228024	-1.506820	0.697383

3.3.4 CzU-NeP lactate complex

145 -1

C -4.750454 -0.648037 2.560762

C -6.103775 -0.865183 2.853625

C -7.133790 0.023566 2.451479

H -6.350184 -1.751284 3.431846

C -6.794806 1.171942 1.730806

C -4.432014 0.507947 1.810680

C -5.447949 1.417671 1.408730

H -7.558625 1.881703 1.414475

C -4.779722 2.489569 0.696498

C -8.589291 -0.319078 2.826432

C -9.585199 0.743022 2.324369

H -9.564218 0.838445 1.228374

H -9.383258 1.732960 2.760812

H -10.605967 0.452803 2.614602

C -8.721546 -0.414815 4.365288

H -8.463769 0.543770 4.840999

H -8.062418 -1.189521 4.782764

H -9.756602 -0.667813 4.643043

C -8.978275 -1.678985 2.197887

H -10.015981 -1.936450 2.461218

H -8.328430 -2.491347 2.553274

H -8.903210 -1.638688 1.100541

N -3.198889 0.974902 1.378868

C -3.396960 2.168321 0.697183

H -2.302992 0.455261 1.486518

C -5.234856 3.678308 0.095616

C -4.316360 4.540582 -0.509670

H -6.298502 3.914123 0.112781

C -2.940846 4.190279 -0.514899

C	-2.453544	3.017934	0.076471
H	-2.215500	4.849684	-0.984916
C	-4.740456	5.861715	-1.181609
C	-6.260505	6.095229	-1.099721
H	-6.609585	6.155780	-0.057881
H	-6.825269	5.298576	-1.607108
H	-6.511476	7.046920	-1.591516
C	-4.337092	5.838110	-2.675412
H	-4.832409	5.007755	-3.201126
H	-3.251267	5.721471	-2.802601
H	-4.634058	6.779331	-3.164105
C	-4.032347	7.047244	-0.482814
H	-4.320367	7.997187	-0.959594
H	-2.938094	6.958355	-0.541574
H	-4.312548	7.098845	0.580280
N	-1.099859	2.626653	0.077420
C	0.017451	3.421163	-0.155114
H	-0.905366	1.625745	0.205544
O	-0.022947	4.628888	-0.426489
H	2.822153	7.077083	-1.291228
H	7.494737	-1.313644	-4.932108
H	4.343252	6.293907	-3.210610
H	7.282105	-2.851465	-4.061827
C	7.944490	-1.982305	-4.182424
C	3.715042	7.128856	-0.650202
H	4.131357	8.143298	-0.740086
H	8.906251	-2.343965	-4.578475
C	5.198883	6.406941	-2.527570
H	5.568345	7.441213	-2.609105
H	3.398682	6.990021	0.394466
C	4.783227	6.100791	-1.068592

N	-3.707266	-1.515855	2.966127
N	3.536323	-2.331290	-1.239684
C	4.541154	-1.366718	-1.517028
C	5.801736	-1.711051	-2.014009
C	4.275859	4.646126	-0.973295
C	4.285113	-0.002796	-1.277576
C	2.963960	4.349717	-0.533352
C	2.478533	3.035338	-0.446324
C	3.359718	1.992070	-0.791772
H	5.998759	5.735242	-2.871088
N	3.126408	0.619377	-0.835388
C	5.131068	3.591968	-1.326153
C	4.679716	2.265524	-1.237814
C	5.277254	0.979397	-1.550608
C	6.807487	-0.753155	-2.295343
N	1.182605	2.681469	-0.029262
C	6.530257	0.598399	-2.060178
C	8.163549	-1.239175	-2.843078
H	5.996711	-2.766113	-2.198207
H	2.318511	0.146945	-0.402330
H	8.749348	0.636368	-3.835476
H	2.281376	5.149869	-0.263158
H	6.145809	3.793001	-1.674843
H	7.275768	1.364600	-2.271278
C	9.140744	-0.075184	-3.092715
H	10.090425	-0.472455	-3.480153
H	8.184228	-3.087049	-1.639992
C	8.815602	-2.206449	-1.826134
C	6.010996	6.279216	-0.143549
H	6.389093	7.311735	-0.206761
H	9.785126	-2.562247	-2.207959

H	9.363738	0.478109	-2.167757
H	5.744322	6.076117	0.904900
H	6.830514	5.601792	-0.423197
H	8.990540	-1.703418	-0.862795
H	1.038422	1.683213	0.183647
C	3.210450	-3.406039	-2.032835
H	2.967311	-2.175221	-0.395293
C	-3.743847	-2.482924	3.946668
H	-2.786120	-1.363747	2.538123
O	3.773396	-3.643487	-3.112704
O	-4.754855	-2.730045	4.623689
C	-2.433675	-3.232913	4.141131
C	2.091848	-4.280968	-1.483915
C	-2.456063	-4.732422	3.706866
H	-2.191130	-3.183053	5.214765
H	-1.626269	-2.721688	3.594189
C	2.520806	-5.718085	-1.051727
H	1.329768	-4.366262	-2.275152
H	1.618045	-3.785124	-0.622760
C	-3.387226	-5.562996	4.609416
H	-4.425029	-5.209640	4.549926
H	-3.069121	-5.503951	5.661823
H	-3.360371	-6.620724	4.304742
C	-2.905953	-4.856275	2.239566
H	-2.849398	-5.904276	1.908185
H	-2.267185	-4.256427	1.572661
H	-3.945446	-4.519737	2.105569
C	-1.018579	-5.268674	3.848789
H	-0.976211	-6.334514	3.577306
H	-0.656273	-5.166584	4.883520
H	-0.322720	-4.725157	3.190590

C 3.674709 -5.649720 -0.034524

H 4.582883 -5.218182 -0.481784

H 3.927495 -6.658215 0.326906

H 3.401847 -5.037634 0.839342

C 1.295859 -6.379766 -0.390548

H 0.978822 -5.827236 0.507556

H 1.533603 -7.410558 -0.086539

H 0.442578 -6.418465 -1.085108

C 2.946871 -6.560850 -2.267914

H 2.125961 -6.641801 -2.998060

H 3.214716 -7.579218 -1.945614

H 3.811631 -6.117583 -2.779175

O 0.489729 -0.009122 0.372321

H 0.719769 -2.536492 2.297362

C 0.126975 -0.694755 1.379738

H 3.063956 -2.006996 1.943453

C 1.166705 -1.539021 2.140242

O 2.367183 -1.671528 1.349172

H 0.562405 -0.819294 4.098982

C 1.476896 -0.901850 3.497800

H 2.197798 -1.520860 4.052256

H 1.905424 0.101860 3.363943

O -1.048675 -0.724397 1.855041

3.3.5 CzU-NeP formate complex

138 -1

C -4.895686 -1.150598 1.660458

C -6.179508 -1.332452 2.193165

C -7.005667 -0.252879 2.600664

H -6.533966 -2.354866 2.290978

C -6.532232 1.055001 2.465611

C -4.432765 0.181351 1.543787

C -5.248657 1.277782 1.935284

H -7.142970 1.906297 2.764982

C -4.479748 2.478721 1.665985

C -8.398584 -0.572134 3.178639

C -9.171631 0.699956 3.572454

H -9.344479 1.359231 2.708292

H -8.643150 1.276775 4.346203

H -10.154828 0.419172 3.978560

C -8.244418 -1.452962 4.441458

H -7.661832 -0.930173 5.215297

H -7.735280 -2.400991 4.215621

H -9.233800 -1.693454 4.861135

C -9.235330 -1.337490 2.125340

H -10.231454 -1.575041 2.530261

H -8.756618 -2.283592 1.834334

H -9.369898 -0.730987 1.216918

N -3.223102 0.658925 1.062986

C -3.241042 2.043691 1.128619

H -2.453924 0.067705 0.686425

C -4.741844 3.853905 1.815921

C -3.770020 4.786262 1.440563

H -5.701015 4.176470 2.219976

C -2.529109 4.325822 0.925294

C -2.237355 2.966465 0.760380

H -1.765213 5.041431 0.632294

C -3.990891 6.306620 1.570387

C -5.379432 6.647110 2.142745

H -5.519443 6.231334 3.152080

H -6.190249 6.272938 1.499751

H	-5.487288	7.739538	2.214328
C	-3.869073	6.968359	0.176407
H	-4.625513	6.566837	-0.515092
H	-2.878201	6.799123	-0.269521
H	-4.020962	8.055897	0.257282
C	-2.921254	6.908133	2.513428
H	-3.065935	7.995755	2.607787
H	-1.903083	6.735563	2.136763
H	-2.991937	6.464698	3.518331
N	-1.018931	2.455367	0.271443
C	-0.036705	3.126253	-0.450404
H	-0.832017	1.466386	0.458659
O	-0.104418	4.321325	-0.768930
H	1.815326	5.942028	-3.846076
H	7.389370	-2.742005	-4.548096
H	3.211740	4.608805	-5.542624
H	7.537401	-3.753510	-3.091266
C	8.021435	-2.955739	-3.672798
C	2.755630	6.330086	-3.427136
H	2.999835	7.260749	-3.961078
H	8.987877	-3.340912	-4.033949
C	4.111488	5.066525	-5.104223
H	4.306003	6.013285	-5.632407
H	2.582584	6.587340	-2.371370
C	3.914536	5.329041	-3.591656
N	-4.053859	-2.203524	1.229723
N	4.066092	-2.437956	-0.128528
C	4.844843	-1.625346	-0.990409
C	6.090328	-2.009857	-1.497990
C	3.651501	3.991245	-2.868250
C	4.367949	-0.343122	-1.328787

C	2.452460	3.765687	-2.152386
C	2.185505	2.559404	-1.482262
C	3.173630	1.554612	-1.546859
H	4.961071	4.394495	-5.291936
N	3.186545	0.287227	-0.966709
C	4.616717	2.976137	-2.922013
C	4.380745	1.757135	-2.267375
C	5.149132	0.532709	-2.129186
C	6.877908	-1.161895	-2.316795
N	1.013137	2.279670	-0.760120
C	6.398417	0.116956	-2.621497
C	8.238031	-1.679688	-2.825153
H	6.450908	-3.003760	-1.243939
H	2.365047	-0.162913	-0.529097
H	8.384020	-0.378156	-4.593953
H	1.692238	4.538491	-2.097960
H	5.549798	3.122250	-3.469004
H	6.981833	0.798026	-3.240555
C	8.966576	-0.640906	-3.698112
H	9.927593	-1.056787	-4.034945
H	8.702879	-2.794960	-0.979504
C	9.146877	-2.018582	-1.619159
C	5.196473	5.979907	-3.019088
H	5.400350	6.933953	-3.530534
H	10.121601	-2.390417	-1.971527
H	9.180271	0.284349	-3.142068
H	5.084683	6.185744	-1.943643
H	6.074340	5.331715	-3.152242
H	9.324154	-1.127022	-0.998567
H	0.898186	1.307667	-0.432570
C	4.017288	-3.813945	-0.073114

H	3.478495	-1.943914	0.540312
C	-4.252650	-3.562105	1.333711
H	-3.161561	-1.934229	0.795945
O	4.654659	-4.538789	-0.850439
O	-5.247490	-4.068840	1.878589
C	-3.144943	-4.405849	0.718472
C	3.115799	-4.371023	1.017942
C	-3.534272	-5.152477	-0.597515
H	-2.851579	-5.153755	1.471685
H	-2.265743	-3.776168	0.512350
C	3.858102	-4.962609	2.259247
H	2.513153	-5.169236	0.558114
H	2.420563	-3.593556	1.372053
C	-4.597560	-6.233869	-0.330715
H	-5.525372	-5.797612	0.062420
H	-4.233387	-6.971446	0.401447
H	-4.832497	-6.769187	-1.264054
C	-4.058124	-4.152882	-1.645348
H	-4.260794	-4.667641	-2.597080
H	-3.322374	-3.357670	-1.840201
H	-4.995473	-3.677194	-1.317919
C	-2.256281	-5.828605	-1.132179
H	-2.477273	-6.394407	-2.050406
H	-1.840804	-6.531059	-0.393016
H	-1.480661	-5.084592	-1.370402
C	4.766279	-3.897341	2.899845
H	5.576721	-3.591701	2.220629
H	5.231006	-4.293284	3.815524
H	4.194086	-2.997290	3.175234
C	2.776904	-5.386923	3.273056
H	2.172359	-4.525031	3.594760

H 3.243227 -5.828829 4.166890

H 2.098726 -6.137802 2.838480

C 4.693168 -6.195116 1.868186

H 4.058094 -6.976051 1.422166

H 5.176647 -6.619712 2.761623

H 5.475353 -5.939626 1.140800

O 0.661377 -0.383751 0.177070

C -0.182217 -1.325802 0.051817

O -1.437828 -1.225750 0.151693

H 0.226262 -2.340216 -0.165326

3.3.6 CzU-NeP sorbate complex

149 -1

C -4.759088 -0.770723 1.600373

C -6.010796 -0.987942 2.189295

C -6.828955 0.066775 2.670181

H -6.346277 -2.017295 2.284403

C -6.378144 1.384955 2.547451

C -4.322185 0.567329 1.489961

C -5.129784 1.641639 1.953012

H -6.982594 2.218272 2.904465

C -4.388819 2.858318 1.674720

C -8.187070 -0.285970 3.308399

C -8.957454 0.966064 3.767074

H -9.179412 1.641625 2.927084

H -8.400952 1.533065 4.528223

H -9.916397 0.661807 4.212185

C -7.958306 -1.191155 4.542285

H -7.346322 -0.675877 5.298355

H -7.446683 -2.125750 4.270812

H -8.922148 -1.456358 5.004483

C -9.064530 -1.040399 2.280485

H -10.037271 -1.298505 2.727529

H -8.590331 -1.974639 1.947088

H -9.249876 -0.417086 1.392589

N -3.134425 1.065954 0.975078

C -3.176835 2.451763 1.060500

H -2.471467 0.497024 0.399626

C -4.656991 4.225720 1.877295

C -3.719169 5.179532 1.471220

H -5.594788 4.525193 2.344364

C -2.503793 4.748953 0.875384

C -2.204203 3.397166 0.665518

H -1.762396 5.479820 0.562553

C -3.950747 6.693156 1.651381

C -5.308453 7.001374 2.309567

H -5.385952 6.559033 3.314163

H -6.150092 6.632691 1.704063

H -5.425004 8.090295 2.414628

C -3.916676 7.389262 0.269229

H -4.706600 6.993974 -0.387525

H -2.950937 7.243708 -0.235820

H -4.077017 8.472350 0.385316

C -2.836138 7.286607 2.546094

H -2.988646 8.369568 2.675429

H -1.839381 7.137568 2.107078

H -2.843131 6.818190 3.541999

N -1.011600 2.907313 0.102864

C -0.003814 3.613053 -0.546442

H -0.837149 1.903091 0.215258

O -0.003072 4.840120 -0.716724

H 2.147411 6.600297 -3.725907

H 7.314805 -2.337802 -4.684611

H 3.586972 5.318374 -5.426580

H 7.329687 -3.434549 -3.282971

C 7.884997 -2.632622 -3.790572

C 3.075722 6.908734 -3.221710

H 3.396911 7.861509 -3.668581

H 8.849838 -3.048257 -4.120853

C 4.476446 5.699698 -4.902082

H 4.746365 6.670681 -5.346442

H 2.846517 7.098481 -2.162310

C 4.194949 5.864162 -3.389152

N -3.933392 -1.807932 1.098732

N 3.762473 -2.090658 -0.436148

C 4.632247 -1.285775 -1.212717

C 5.884901 -1.707217 -1.672352

C 3.823321 4.493409 -2.783689

C 4.237585 0.034396 -1.510103

C 2.571001 4.280392 -2.159389

C 2.211637 3.043436 -1.599725

C 3.155254 2.000106 -1.678345

H 5.305602 5.002062 -5.087082

N 3.067729 0.703077 -1.175534

C 4.741813 3.435579 -2.858476

C 4.411383 2.185398 -2.310622

C 5.108187 0.913891 -2.208122

C 6.758290 -0.856935 -2.396530

N 0.988407 2.751342 -0.976933

C 6.363455 0.461385 -2.650749

C 8.117372 -1.418019 -2.860370

H 6.180052 -2.730545 -1.454682

H	2.180017	0.271543	-0.859081
H	8.428875	-0.030362	-4.540567
H	1.844939	5.085098	-2.093421
H	5.711690	3.574302	-3.339318
H	7.016879	1.144799	-3.192377
C	8.945706	-0.373522	-3.631810
H	9.901750	-0.821538	-3.940844
H	8.419925	-2.654070	-1.058812
C	8.938844	-1.870511	-1.629238
C	5.466529	6.406386	-2.692616
H	5.746576	7.383156	-3.117357
H	9.911025	-2.275707	-1.950439
H	9.174788	0.506014	-3.011641
H	5.295696	6.539052	-1.613268
H	6.320092	5.725491	-2.820488
H	9.127612	-1.024675	-0.950688
H	0.810839	1.752345	-0.781826
C	3.709193	-3.465912	-0.350917
H	3.116117	-1.586498	0.167668
C	-3.917845	-3.127653	1.492074
H	-3.208826	-1.534741	0.422471
O	4.423338	-4.208221	-1.039168
O	-4.663820	-3.580324	2.374784
C	-2.904195	-3.993793	0.756664
C	2.700599	-3.996755	0.656666
C	-3.516820	-5.115913	-0.139203
H	-2.269801	-4.467437	1.523587
H	-2.252456	-3.363308	0.132447
C	3.310297	-4.526357	1.995030
H	2.165537	-4.823848	0.165875
H	1.957927	-3.220996	0.899247

C	-4.206469	-6.197301	0.712833
H	-5.036625	-5.779457	1.297288
H	-3.494151	-6.656358	1.416484
H	-4.601048	-6.993305	0.062289
C	-4.526653	-4.513074	-1.133278
H	-4.905542	-5.290744	-1.813680
H	-4.062658	-3.725246	-1.746510
H	-5.392156	-4.073175	-0.614495
C	-2.355245	-5.762163	-0.918977
H	-2.727943	-6.579435	-1.555375
H	-1.604325	-6.182872	-0.232483
H	-1.851155	-5.029448	-1.567521
C	4.124011	-3.419990	2.690861
H	5.000690	-3.122859	2.095097
H	4.489827	-3.772970	3.666773
H	3.510271	-2.522536	2.866738
C	2.130489	-4.935504	2.898713
H	1.477726	-4.076262	3.117379
H	2.502285	-5.332352	3.855675
H	1.519020	-5.717698	2.422748
C	4.203966	-5.754766	1.746559
H	3.637205	-6.563631	1.260204
H	4.589793	-6.138349	2.703873
H	5.060678	-5.509210	1.104235
H	1.066158	-1.592251	-2.191455
C	-0.015750	-1.553052	-2.038242
O	0.380183	0.065047	-0.352595
C	-0.495336	-0.683706	-0.933401
O	-1.729821	-0.688291	-0.616495
H	0.246548	-4.563127	-6.100467
H	0.676575	-3.122139	-4.154922

C -0.845589 -4.510952 -5.993331

C -0.403853 -3.033079 -3.990841

H -1.271987 -4.115041 -6.930270

H -1.237979 -5.536652 -5.891798

C -1.253822 -3.669853 -4.829616

C -0.841819 -2.225896 -2.875806

H -2.331354 -3.566827 -4.654602

H -1.921425 -2.142718 -2.707166

3.3.7 Cz-Gly-NeP free receptor

143 0

C -4.992198 4.181691 2.534171

C -6.133322 4.673652 3.176089

C -6.675195 5.953315 2.896015

H -6.609425 4.035346 3.916813

C -6.052466 6.756799 1.933739

C -4.365920 5.016707 1.589784

C -4.896975 6.294392 1.280543

H -6.446778 7.742804 1.690112

C -4.011032 6.877195 0.287293

C -7.936177 6.404250 3.659302

C -8.394725 7.814596 3.244576

H -8.653769 7.863158 2.176306

H -7.623628 8.572409 3.448302

H -9.292378 8.089667 3.818028

C -7.640925 6.418969 5.178254

H -6.826088 7.120657 5.412508

H -7.349494 5.424676 5.545921

H -8.536598 6.735384 5.735315

C -9.094433 5.417534 3.375807

H -9.998799 5.728263 3.921812

H -8.845773 4.394591 3.693234

H -9.334138 5.392596 2.302054

N -3.239671 4.776057 0.808583

C -2.983814 5.918665 0.057701

H -2.443553 4.171281 1.052679

C -4.029462 8.094296 -0.411976

C -3.015425 8.383113 -1.333399

H -4.836633 8.802958 -0.230384

C -1.993540 7.426156 -1.526758

C -1.947374 6.198508 -0.851799

H -1.190127 7.637284 -2.235592

C -2.972241 9.696800 -2.137952

C -4.153343 10.624319 -1.795718

H -4.153168 10.912520 -0.733746

H -5.121876 10.156501 -2.027536

H -4.077120 11.545709 -2.391262

C -3.029796 9.376297 -3.651031

H -3.960176 8.845678 -3.904218

H -2.183536 8.749366 -3.967110

H -2.995857 10.307876 -4.236293

C -1.657829 10.452252 -1.826402

H -1.619549 11.393026 -2.396371

H -0.772193 9.859256 -2.096467

H -1.590268 10.696819 -0.755468

N -0.884045 5.313076 -1.177682

H 3.647071 10.351458 0.211758

H 11.090922 6.228876 -5.777705

H 5.003118 10.907537 -1.899690

H 11.714180 4.624076 -5.324341

C 11.865316 5.705706 -5.196721

C	4.537135	10.599140	0.809658
H	4.484020	11.669837	1.056309
H	12.846918	5.960655	-5.625673
C	5.843497	11.179887	-1.243571
H	5.745171	12.245362	-0.984065
H	4.488222	10.037589	1.754597
C	5.841663	10.317121	0.041285
N	-4.458852	2.888387	2.754984
N	8.522326	2.583520	-2.589571
C	8.783353	3.979622	-2.616985
C	10.014331	4.410255	-3.129575
C	5.990629	8.831471	-0.341963
C	7.922098	4.955264	-2.077803
C	5.017579	7.871173	-0.004109
C	5.131377	6.508817	-0.331129
C	6.270186	6.094331	-1.042599
H	6.775277	11.056308	-1.813645
N	6.698998	4.823128	-1.421259
C	7.126547	8.400754	-1.045909
C	7.264124	7.053676	-1.397028
C	8.325208	6.318628	-2.062339
C	10.434193	5.759940	-3.121846
N	4.123512	5.633317	0.154167
C	9.569725	6.715239	-2.574475
C	11.812351	6.121703	-3.707192
H	10.675627	3.646003	-3.543228
H	6.032422	4.085227	-1.683430
H	11.360507	8.223873	-4.177438
H	4.126994	8.173987	0.547040
H	7.912280	9.108592	-1.315803
H	9.854535	7.766117	-2.532291

C	12.100664	7.631783	-3.618386
H	13.090186	7.840481	-4.051176
H	12.792103	4.279914	-2.990270
C	12.918908	5.370386	-2.928753
C	7.031580	10.737044	0.937647
H	6.941877	11.799443	1.212817
H	13.908084	5.617998	-3.343899
H	12.111385	7.986187	-2.576635
H	7.052836	10.143778	1.864121
H	7.994151	10.602667	0.423789
H	12.912354	5.654860	-1.865766
C	7.330742	1.947148	-2.835799
H	9.344252	1.989848	-2.494453
C	-4.511269	2.129965	3.905072
H	-3.987227	2.461294	1.960245
O	6.284799	2.572670	-3.076295
O	-5.032475	2.539121	4.952140
C	-3.872951	0.754369	3.783514
C	7.393134	0.429220	-2.785635
C	-4.873438	-0.437148	3.640083
H	-3.274195	0.600769	4.693985
H	-3.181484	0.729756	2.926184
C	7.276091	-0.288197	-4.167976
H	6.562073	0.095402	-2.145006
H	8.328500	0.107027	-2.302260
C	-5.750792	-0.576246	4.897405
H	-6.370925	0.315999	5.060560
H	-5.132104	-0.726987	5.795432
H	-6.418629	-1.445478	4.794769
C	-5.765019	-0.246527	2.399007
H	-6.417694	-1.121918	2.260346

H	-5.159854	-0.130509	1.486140
H	-6.411800	0.638713	2.494419
C	-4.029806	-1.715978	3.468759
H	-4.684015	-2.595956	3.371665
H	-3.371502	-1.876131	4.336679
H	-3.400298	-1.659532	2.567202
C	8.363428	0.223646	-5.131226
H	8.227788	1.290527	-5.366560
H	8.325506	-0.333356	-6.079575
H	9.369942	0.092515	-4.704138
C	7.486566	-1.794026	-3.914924
H	8.487944	-1.992226	-3.502467
H	7.388154	-2.357570	-4.855030
H	6.740682	-2.184020	-3.205165
C	5.884274	-0.071437	-4.789243
H	5.093822	-0.460338	-4.128643
H	5.815322	-0.602297	-5.751235
H	5.682062	0.993817	-4.965962
C	-0.298875	4.325883	-0.443641
H	-0.431691	5.520886	-2.068821
C	3.606637	4.522804	-0.446481
H	3.657095	5.945697	1.005789
O	-0.625191	4.004652	0.711794
O	3.957117	4.105798	-1.558482
C	0.820529	3.589603	-1.202696
C	2.559761	3.796142	0.418260
O	1.727831	2.922229	-0.336040
H	1.345710	4.278556	-1.886296
H	0.351439	2.805208	-1.815180
H	1.964127	4.521778	0.998851
H	3.097078	3.158504	1.135485

3.3.8 Cz-Gly-NeP acetate complex

150 -1

C -7.503983 -1.209700 0.959300

C -8.874189 -0.924335 0.995642

C -9.402195 0.268467 1.553390

H -9.549691 -1.659289 0.564441

C -8.520550 1.203368 2.105322

C -6.631309 -0.248146 1.514289

C -7.137591 0.947965 2.095328

H -8.890624 2.129228 2.545330

C -5.985573 1.691507 2.568851

C -10.928888 0.480166 1.534975

C -11.340033 1.815772 2.182424

H -10.905594 2.677963 1.654359

H -11.035566 1.869814 3.238415

H -12.434775 1.918079 2.145001

C -11.620916 -0.664742 2.313107

H -11.286231 -0.683542 3.361394

H -11.404492 -1.647118 1.869418

H -12.713086 -0.524450 2.304466

C -11.433932 0.477638 0.072202

H -12.526361 0.615251 0.046471

H -11.201799 -0.469015 -0.436662

H -10.971859 1.294621 -0.502439

N -5.247693 -0.251404 1.597294

C -4.846131 0.905358 2.248349

H -4.600343 -1.036105 1.347158

C -5.835590 2.928072 3.222549

C -4.557369 3.381749 3.561853

H -6.719992 3.519508 3.458584

C -3.432524 2.580384 3.236144

C	-3.544352	1.345269	2.584133
H	-2.431483	2.922097	3.486475
C	-4.319229	4.725726	4.278235
C	-5.633866	5.472687	4.568584
H	-6.299635	4.890316	5.223147
H	-6.181732	5.712706	3.644860
H	-5.410313	6.421443	5.079019
C	-3.433856	5.634743	3.392054
H	-3.925393	5.841810	2.429190
H	-2.458143	5.172883	3.182897
H	-3.250214	6.596143	3.896772
C	-3.600338	4.475297	5.625485
H	-3.420981	5.430379	6.143579
H	-2.627804	3.982481	5.483085
H	-4.211228	3.838281	6.283002
N	-2.448122	0.515238	2.248387
H	2.117491	3.999186	-5.117191
H	10.521636	-1.829461	-3.979882
H	3.911452	2.789659	-6.509161
H	11.100272	-2.181379	-2.334074
C	11.221575	-1.507067	-3.194054
C	2.838160	4.815571	-4.959386
H	2.699233	5.542842	-5.772727
H	12.246870	-1.629612	-3.576240
C	4.567772	3.658044	-6.348083
H	4.380533	4.383776	-7.154623
H	2.587862	5.321707	-4.014738
C	4.292855	4.309514	-4.971672
N	-6.967249	-2.409307	0.427323
N	7.488039	-1.232624	0.621480
C	7.880906	-0.551139	-0.554450

C	9.160696	-0.624238	-1.116706
C	4.570668	3.283150	-3.855135
C	6.940167	0.285485	-1.187597
C	3.571787	2.882134	-2.946034
C	3.796469	1.955776	-1.912736
C	5.087738	1.419302	-1.788055
H	5.609909	3.318484	-6.435758
N	5.619080	0.552289	-0.838880
C	5.850455	2.719739	-3.727209
C	6.107800	1.789631	-2.713688
C	7.297365	1.051087	-2.325382
C	9.535627	0.120549	-2.263138
N	2.708511	1.679723	-1.038879
C	8.595054	0.968167	-2.858273
C	10.970776	-0.030659	-2.804228
H	9.880177	-1.284570	-0.638891
H	4.965281	-0.074485	-0.347397
H	10.548240	0.576382	-4.876866
H	2.566937	3.296899	-3.030154
H	6.650729	3.001839	-4.413418
H	8.852036	1.560282	-3.736026
C	11.219449	0.843828	-4.047002
H	12.253238	0.699089	-4.394233
H	11.889258	-0.234458	-0.808290
C	11.984104	0.386016	-1.710923
C	5.230008	5.527571	-4.789252
H	5.048023	6.267064	-5.584280
H	13.013223	0.277267	-2.087246
H	11.088621	1.914152	-3.827771
H	5.053813	6.017254	-3.819391
H	6.288929	5.235399	-4.835763

H	11.835724	1.436771	-1.418942
C	8.048827	-2.350783	1.200986
H	6.707899	-0.820224	1.128229
C	-7.480469	-3.135724	-0.619492
H	-6.092196	-2.772553	0.868263
O	9.015193	-2.949111	0.706304
O	-8.511430	-2.812109	-1.235557
C	-6.686007	-4.386466	-0.972124
C	7.384005	-2.786758	2.498930
C	-5.946931	-4.341116	-2.346419
H	-7.398491	-5.227652	-0.986855
H	-5.945441	-4.588265	-0.184280
C	6.522413	-4.085774	2.408548
H	6.749694	-1.975778	2.890315
H	8.190942	-2.951313	3.229987
C	-6.944804	-4.337359	-3.518841
H	-7.599510	-3.456151	-3.483820
H	-7.583004	-5.234770	-3.493754
H	-6.403479	-4.333014	-4.478052
C	-5.044174	-3.096063	-2.427277
H	-4.461893	-3.104710	-3.361623
H	-4.336054	-3.059464	-1.584692
H	-5.635658	-2.167837	-2.410361
C	-5.074919	-5.609163	-2.435848
H	-4.542130	-5.643064	-3.398881
H	-5.690022	-6.519050	-2.356363
H	-4.323858	-5.634811	-1.630911
C	7.397198	-5.311270	2.086165
H	7.892958	-5.208937	1.111130
H	6.776931	-6.220859	2.065151
H	8.177371	-5.450051	2.850500

C	5.862417	-4.287244	3.787087
H	6.620996	-4.385821	4.579146
H	5.250836	-5.202495	3.788634
H	5.207886	-3.439712	4.042877
C	5.427249	-3.930015	1.337672
H	4.791317	-3.054501	1.540352
H	4.779300	-4.819659	1.322735
H	5.857058	-3.815286	0.330854
C	-1.113138	0.766333	2.394500
H	-2.688539	-0.410119	1.848393
C	2.415550	0.552120	-0.330107
H	1.973570	2.387102	-1.056693
O	-0.623665	1.827969	2.805382
O	3.166038	-0.429986	-0.207557
C	-0.225742	-0.440434	2.029602
C	1.013142	0.561954	0.277013
O	1.062877	-0.061230	1.557442
H	-0.739418	-1.098397	1.305907
H	-0.049974	-1.016812	2.950521
H	0.361262	-0.012986	-0.409935
H	0.614586	1.588357	0.347747
H	-1.783612	-4.364459	1.001978
C	-2.386072	-4.198498	1.907480
H	-2.772754	-5.159963	2.264791
H	-1.716216	-3.767241	2.665118
O	-3.179063	-2.041471	1.219914
C	-3.515118	-3.222434	1.592461
O	-4.715436	-3.616155	1.696481

3.3.9 Cz-Gly-NeP benzoate complex

157 -1

C -7.769984 -1.304837 0.892932

C -9.107838 -0.961058 1.126034

C -9.498961 0.235485 1.778945

H -9.867518 -1.654176 0.774156

C -8.508042 1.116287 2.221064

C -6.783216 -0.396520 1.340258

C -7.153667 0.803871 2.007213

H -8.768964 2.045443 2.727487

C -5.920431 1.495413 2.323853

C -11.002341 0.510033 1.979205

C -11.259726 1.850062 2.693177

H -10.864736 2.701947 2.119382

H -10.809873 1.871721 3.697019

H -12.343404 2.000355 2.809812

C -11.626299 -0.619458 2.833768

H -11.152851 -0.666107 3.826288

H -11.510900 -1.602441 2.354971

H -12.703266 -0.438248 2.975820

C -11.708160 0.553509 0.602589

H -12.785193 0.741276 0.733600

H -11.594482 -0.394341 0.057645

H -11.293999 1.358053 -0.024211

N -5.400293 -0.452520 1.232127

C -4.866488 0.679523 1.830631

H -4.825417 -1.226644 0.833035

C -5.642540 2.714064 2.967811

C -4.316284 3.123416 3.126979

H -6.466579 3.325809 3.333695

C -3.276750 2.294961 2.631276

C	-3.516853	1.075920	1.981697
H	-2.240738	2.602914	2.741393
C	-3.936352	4.446068	3.821599
C	-5.174283	5.230541	4.294670
H	-5.765865	4.659451	5.025762
H	-5.832259	5.502973	3.455619
H	-4.851497	6.162765	4.781510
C	-3.146860	5.341415	2.836510
H	-3.754822	5.577786	1.949927
H	-2.222404	4.854194	2.494777
H	-2.867705	6.289063	3.323171
C	-3.053109	4.148051	5.056590
H	-2.772318	5.086696	5.559693
H	-2.126625	3.626430	4.776612
H	-3.592106	3.519277	5.781653
N	-2.496910	0.237255	1.468254
H	2.795853	4.517094	-5.376102
H	11.256923	-1.143768	-3.618627
H	4.798496	3.498329	-6.621510
H	11.594055	-1.655400	-1.947481
C	11.806139	-0.883357	-2.700916
C	3.459540	5.325730	-5.034341
H	3.406684	6.134779	-5.777965
H	12.883608	-0.917643	-2.925106
C	5.398680	4.356480	-6.283150
H	5.298645	5.159844	-7.029577
H	3.065546	5.720070	-4.085652
C	4.919236	4.853804	-4.898287
N	-7.367627	-2.509167	0.266503
N	7.511853	-1.211356	0.458944
C	8.044000	-0.375805	-0.550587

C	9.397061	-0.334892	-0.908152
C	5.078934	3.718844	-3.866960
C	7.167724	0.500024	-1.222314
C	3.977595	3.188379	-3.166438
C	4.091697	2.155457	-2.220021
C	5.372957	1.640924	-1.967459
H	6.453379	4.046943	-6.259620
N	5.797221	0.683505	-1.051121
C	6.350842	3.181566	-3.610874
C	6.499656	2.147638	-2.679437
C	7.652740	1.406512	-2.197438
C	9.902075	0.556547	-1.887671
N	2.906201	1.756213	-1.543070
C	9.019110	1.434411	-2.525174
C	11.410544	0.527140	-2.202606
H	10.069385	-1.022411	-0.400874
H	5.109887	-0.023416	-0.752657
H	11.281281	1.349416	-4.240083
H	2.978265	3.583428	-3.351172
H	7.229086	3.564713	-4.133235
H	9.374705	2.136757	-3.278424
C	11.798463	1.547208	-3.289051
H	12.880303	1.485140	-3.478276
H	12.013374	0.133076	-0.118123
C	12.213082	0.857088	-0.921214
C	5.779847	6.064941	-4.466466
H	5.679928	6.881083	-5.199160
H	13.293336	0.835163	-1.133658
H	11.572690	2.579396	-2.981499
H	5.458031	6.444852	-3.485180
H	6.845503	5.803327	-4.398166

H	11.958055	1.859872	-0.546266
C	8.052908	-2.350957	1.015314
H	6.625176	-0.909216	0.856038
C	-8.093525	-3.254586	-0.631012
H	-6.439429	-2.890521	0.551227
O	9.140477	-2.822632	0.653021
O	-9.229653	-2.935124	-1.025014
C	-7.397063	-4.519249	-1.116051
C	7.202916	-2.981832	2.108365
C	-6.993897	-4.521527	-2.624312
H	-8.092210	-5.356346	-0.940404
H	-6.495698	-4.702027	-0.511558
C	6.513073	-4.329478	1.723296
H	6.425929	-2.274878	2.439748
H	7.867495	-3.160963	2.967719
C	-8.233907	-4.542199	-3.537439
H	-8.857046	-3.651123	-3.386162
H	-8.855019	-5.428642	-3.335212
H	-7.924069	-4.578278	-4.593859
C	-6.130104	-3.288268	-2.949303
H	-5.778032	-3.330993	-3.991497
H	-5.246948	-3.235294	-2.294726
H	-6.699905	-2.354295	-2.826872
C	-6.169887	-5.800773	-2.873609
H	-5.862657	-5.860705	-3.929213
H	-6.758434	-6.701875	-2.640315
H	-5.260992	-5.815977	-2.252917
C	7.555067	-5.441086	1.500505
H	8.235637	-5.196972	0.674124
H	7.047532	-6.389228	1.264163
H	8.162739	-5.597323	2.405316

C	5.600976	-4.724178	2.901856
H	6.180560	-4.836517	3.831217
H	5.102451	-5.683744	2.694858
H	4.822112	-3.965553	3.073960
C	5.658291	-4.151980	0.455168
H	4.907397	-3.357393	0.587642
H	5.120554	-5.083921	0.223418
H	6.276531	-3.897849	-0.419220
C	-1.148618	0.465648	1.446752
H	-2.799752	-0.674275	1.082319
C	2.558798	0.541347	-1.029635
H	2.159967	2.451349	-1.566482
O	-0.588305	1.491018	1.856135
O	3.316668	-0.438717	-0.943832
C	-0.340352	-0.715521	0.868392
C	1.093804	0.462826	-0.602951
O	0.998850	-0.368836	0.551065
H	-0.863894	-1.135026	-0.009463
H	-0.278402	-1.500526	1.636854
H	0.528735	0.019599	-1.446628
H	0.684375	1.467128	-0.404437
H	-0.300300	-7.536065	0.131698
C	-1.007762	-6.712270	0.245484
C	-2.270489	-6.942303	0.806713
H	-2.549112	-7.946977	1.130946
C	-3.175550	-5.887164	0.950243
H	-4.163267	-6.054077	1.381215
C	-2.829653	-4.588112	0.540919
C	-3.821090	-3.451780	0.699541
O	-3.451642	-2.276536	0.347371
O	-4.972837	-3.730966	1.153162

C -1.562707 -4.368173 -0.022907

H -1.301512 -3.362244 -0.351489

C -0.656381 -5.422135 -0.171432

H 0.324770 -5.239320 -0.614085

3.3.10 Cz-Gly-NeP lactate complex

154 -1

C -6.528572 -1.049668 1.511459

C -7.749044 -0.984848 0.828806

C -8.129366 0.137103 0.050037

H -8.415774 -1.839106 0.913960

C -7.252114 1.222581 -0.049606

C -5.672167 0.065363 1.420773

C -6.025457 1.191611 0.636342

H -7.510983 2.097211 -0.645448

C -4.933133 2.140159 0.767395

C -9.494973 0.109902 -0.664706

C -9.757881 1.398408 -1.466661

H -9.004559 1.552206 -2.253648

H -9.768192 2.288578 -0.819991

H -10.741429 1.329306 -1.954772

C -10.622658 -0.044270 0.383581

H -10.620301 0.801108 1.088651

H -10.515036 -0.971514 0.964381

H -11.603957 -0.070928 -0.115092

C -9.543064 -1.085985 -1.645334

H -10.516442 -1.116206 -2.159088

H -9.407529 -2.045684 -1.126206

H -8.755389 -0.997840 -2.409197

N -4.408957 0.256664 1.977074

C	-3.979257	1.536000	1.632512
H	-4.078303	-0.118524	2.878839
C	-4.698511	3.408059	0.213989
C	-3.521975	4.097749	0.529217
H	-5.437601	3.842951	-0.458155
C	-2.598440	3.484712	1.407281
C	-2.796349	2.218017	1.974117
H	-1.675371	4.006278	1.666831
C	-3.199720	5.491305	-0.042603
C	-4.325933	6.021919	-0.949027
H	-5.276243	6.124371	-0.403802
H	-4.494882	5.368977	-1.818084
H	-4.049581	7.016836	-1.328271
C	-1.900557	5.414876	-0.879220
H	-2.016942	4.717617	-1.722679
H	-1.047803	5.075274	-0.273994
H	-1.651540	6.407009	-1.286035
C	-3.001756	6.495712	1.117870
H	-2.771861	7.495130	0.717520
H	-2.174011	6.200843	1.778505
H	-3.913799	6.573004	1.728912
N	-1.767646	1.693745	2.804473
H	1.748560	5.971685	0.303855
H	6.306681	-0.012276	-6.773246
H	2.066149	5.798985	-2.245260
H	7.245231	-1.414553	-6.206333
C	7.315829	-0.358145	-6.502476
C	2.757072	6.406787	0.364343
H	2.656525	7.497994	0.269398
H	7.950046	-0.301450	-7.400895
C	3.052245	6.270018	-2.114794

H	2.920924	7.361747	-2.172655
H	3.164436	6.195707	1.364411
C	3.674460	5.878146	-0.753585
N	-6.095220	-2.172345	2.255418
N	5.787353	-2.303831	-1.783655
C	6.011233	-1.045532	-2.392408
C	6.807637	-0.851414	-3.530688
C	3.857767	4.347637	-0.692171
C	5.400444	0.101495	-1.833160
C	3.256711	3.566044	0.319573
C	3.426669	2.176065	0.405163
C	4.230546	1.551190	-0.565468
H	3.689351	5.962710	-2.956414
N	4.565848	0.215483	-0.728378
C	4.658447	3.706931	-1.650041
C	4.850311	2.320239	-1.592716
C	5.601431	1.384665	-2.407766
C	7.016110	0.421432	-4.120444
N	2.870543	1.397219	1.455018
C	6.406058	1.541245	-3.549861
C	7.912170	0.513977	-5.371590
H	7.276486	-1.731772	-3.960420
H	4.279641	-0.575012	-0.116494
H	7.058205	2.372222	-6.184385
H	2.634437	4.038904	1.073993
H	5.140825	4.282391	-2.442485
H	6.545277	2.535095	-3.974284
C	8.035108	1.957985	-5.893163
H	8.681724	1.971469	-6.783007
H	9.316403	-1.044035	-4.691533
C	9.332402	0.001528	-5.031066

C	5.054226	6.564906	-0.610084
H	4.941318	7.659076	-0.658863
H	9.979441	0.057837	-5.920172
H	8.484706	2.627231	-5.144003
H	5.519873	6.311617	0.354822
H	5.743641	6.260046	-1.410400
H	9.788627	0.610678	-4.235946
C	6.269353	-3.537523	-2.164998
H	5.202654	-2.303920	-0.939100
C	-6.852249	-3.178281	2.817514
H	-5.087413	-2.265070	2.364368
O	7.028970	-3.703566	-3.133345
O	-8.090643	-3.189813	2.772630
C	-6.043076	-4.270257	3.500412
C	5.793515	-4.699633	-1.306277
C	-5.880924	-5.592907	2.684160
H	-6.558934	-4.503334	4.444564
H	-5.039276	-3.896904	3.757088
C	4.755381	-5.645165	-1.991069
H	5.359609	-4.321874	-0.368413
H	6.684246	-5.290568	-1.040675
C	-7.244752	-6.264983	2.444303
H	-7.912055	-5.627983	1.847441
H	-7.749759	-6.484523	3.397754
H	-7.106557	-7.216047	1.906788
C	-5.191500	-5.314368	1.335699
H	-5.014219	-6.257792	0.797190
H	-4.216909	-4.821422	1.478853
H	-5.806999	-4.672383	0.687515
C	-4.994166	-6.534033	3.523345
H	-4.854121	-7.493303	3.001943

H	-5.453223	-6.743424	4.501959
H	-4.000414	-6.093601	3.698709
C	5.393872	-6.412099	-3.163407
H	5.754082	-5.727686	-3.942999
H	4.655952	-7.094376	-3.613418
H	6.248542	-7.015601	-2.820094
C	4.287100	-6.656832	-0.926502
H	5.137449	-7.225279	-0.520262
H	3.576254	-7.373670	-1.365911
H	3.781704	-6.152089	-0.088396
C	3.543374	-4.839330	-2.494134
H	3.078655	-4.264153	-1.678187
H	2.779699	-5.516587	-2.905686
H	3.826537	-4.133253	-3.289273
C	-1.880251	0.836345	3.846166
H	-0.815661	2.070653	2.615529
C	1.659667	1.580437	2.040741
H	3.447723	0.592487	1.800250
O	-2.940456	0.311305	4.250207
O	0.850510	2.483538	1.755814
C	-0.589304	0.515612	4.606102
C	1.307815	0.536545	3.106688
O	0.579776	1.191257	4.154261
H	-0.461401	-0.579873	4.603310
H	-0.754806	0.824910	5.648511
H	2.211212	0.058264	3.515062
H	0.692185	-0.240443	2.621522
O	4.089790	-2.149952	0.750228
H	3.461325	-2.981743	3.666607
C	4.242603	-1.898471	1.997371
H	3.889204	-3.990729	1.282766

C 4.285285 -3.117399 2.942210

O 4.050924 -4.325438 2.196285

H 5.760636 -2.303935 4.311701

C 5.608571 -3.205460 3.702919

H 5.600108 -4.078867 4.369962

H 6.451467 -3.308135 3.003674

O 4.333220 -0.748438 2.511005

3.3.11 Cz-Gly-NeP formate complex

147 -1

C -7.691640 -1.358958 1.117452

C -9.054811 -1.066538 1.248671

C -9.537094 0.147069 1.802632

H -9.762112 -1.812953 0.895843

C -8.614976 1.096735 2.253460

C -6.777836 -0.380973 1.569256

C -7.237327 0.836590 2.144099

H -8.948919 2.038677 2.688279

C -6.052583 1.592185 2.503021

C -11.060459 0.364551 1.891182

C -11.419415 1.724948 2.517357

H -11.023008 2.564801 1.927015

H -11.037876 1.815817 3.545514

H -12.513577 1.831742 2.556881

C -11.693771 -0.748057 2.760784

H -11.282833 -0.728236 3.781572

H -11.511086 -1.747076 2.339869

H -12.783562 -0.604652 2.827122

C -11.673779 0.310254 0.471139

H -12.764290 0.453877 0.522247

H -11.483723 -0.656272 -0.017646

H -11.253113 1.102029 -0.167334

N -5.392129 -0.387413 1.555054

C -4.939807 0.792965 2.124475

H -4.766297 -1.150454 1.210482

C -5.856391 2.850013 3.100779

C -4.557162 3.312216 3.329150

H -6.721597 3.450293 3.381127

C -3.459460 2.496432 2.951643

C -3.616678 1.238207 2.354949

H -2.443219 2.842927 3.120040

C -4.267575 4.678555 3.980992

C -5.557790 5.440926 4.333950

H -6.177966 4.885033 5.053073

H -6.167561 5.650349 3.442035

H -5.297866 6.406173 4.793566

C -3.442070 5.553144 3.006859

H -3.996221 5.727521 2.072006

H -2.482629 5.081429 2.749960

H -3.224525 6.531010 3.464211

C -3.459579 4.469586 5.284018

H -3.242986 5.440230 5.757057

H -2.500118 3.968004 5.091925

H -4.025604 3.857114 6.002237

N -2.541088 0.397755 1.978082

H 2.439276 4.212028 -5.102582

H 10.810131 -1.626060 -3.749518

H 4.339226 3.106591 -6.437432

H 11.266989 -2.087842 -2.092500

C 11.443483 -1.353498 -2.891599

C 3.138608 5.020302 -4.841115

H	3.051517	5.797916	-5.614421
H	12.496523	-1.439168	-3.201850
C	4.974612	3.965231	-6.172672
H	4.839160	4.741529	-6.941708
H	2.815492	5.463121	-3.886966
C	4.595330	4.523739	-4.780306
N	-7.199458	-2.580540	0.591604
N	7.423082	-1.390392	0.627051
C	7.897920	-0.616761	-0.457658
C	9.217138	-0.640184	-0.925850
C	4.801331	3.426906	-3.716354
C	6.997596	0.259796	-1.096353
C	3.743425	2.962718	-2.909831
C	3.901332	1.969597	-1.927518
C	5.183896	1.427308	-1.748808
H	6.023285	3.636501	-6.206543
N	5.652340	0.497746	-0.826157
C	6.073298	2.860826	-3.534122
C	6.264774	1.864473	-2.570123
C	7.429639	1.106007	-2.147742
C	9.667858	0.189392	-1.983207
N	2.757540	1.636276	-1.150242
C	8.764450	1.070622	-2.586227
C	11.142324	0.089309	-2.420179
H	9.906258	-1.329732	-0.444886
H	4.968679	-0.163787	-0.430005
H	10.871998	0.839149	-4.471693
H	2.744201	3.380311	-3.036346
H	6.918539	3.191935	-4.139846
H	9.078974	1.726337	-3.397562
C	11.474010	1.051816	-3.575388

H	12.533180	0.940388	-3.850569
H	11.904005	-0.249429	-0.378165
C	12.061012	0.435401	-1.223974
C	5.504504	5.731864	-4.451759
H	5.373571	6.521259	-5.208432
H	13.118105	0.363052	-1.523931
H	11.312218	2.102894	-3.292350
H	5.253325	6.156528	-3.467957
H	6.566987	5.449424	-4.439891
H	11.874941	1.460956	-0.870446
C	7.979605	-2.513983	1.200590
H	6.579720	-1.042655	1.077458
C	-7.815719	-3.375643	-0.345604
H	-6.290072	-2.924450	0.966075
O	9.024487	-3.033246	0.782021
O	-8.905245	-3.089972	-0.872431
C	-7.058782	-4.651830	-0.689996
C	7.205167	-3.061548	2.390785
C	-6.505461	-4.729096	-2.147696
H	-7.757362	-5.490684	-0.537133
H	-6.220719	-4.785715	0.009840
C	6.478640	-4.422658	2.149193
H	6.460335	-2.324678	2.730634
H	7.929736	-3.191908	3.209931
C	-7.646683	-4.848157	-3.174401
H	-8.313708	-3.976904	-3.131711
H	-8.251945	-5.748515	-2.985401
H	-7.233850	-4.923768	-4.192736
C	-5.650145	-3.487024	-2.461612
H	-5.191035	-3.579923	-3.458038
H	-4.842421	-3.361892	-1.724577

H	-6.257460	-2.568794	-2.457861
C	-5.622190	-5.989951	-2.232682
H	-5.223719	-6.112533	-3.251666
H	-6.198919	-6.894352	-1.983258
H	-4.769032	-5.927248	-1.539424
C	7.490591	-5.559539	1.915661
H	8.100924	-5.379272	1.020754
H	6.958640	-6.514985	1.787096
H	8.171097	-5.663157	2.775150
C	5.661652	-4.730873	3.419897
H	6.313867	-4.793863	4.304763
H	5.139556	-5.694374	3.314535
H	4.906257	-3.952109	3.606532
C	5.525653	-4.314931	0.944873
H	4.792591	-3.505587	1.087192
H	4.965858	-5.253603	0.814689
H	6.073186	-4.121282	0.009724
C	-1.198719	0.646923	2.052311
H	-2.791860	-0.543569	1.628029
C	2.420642	0.464518	-0.540037
H	2.025207	2.346202	-1.165697
O	-0.685661	1.715320	2.411860
O	3.162014	-0.527728	-0.441205
C	-0.336621	-0.574167	1.670091
C	0.986121	0.440671	-0.014645
O	0.975073	-0.219145	1.249764
H	-0.849276	-1.186717	0.906743
H	-0.206602	-1.191808	2.571550
H	0.379779	-0.122394	-0.750906
H	0.571513	1.459401	0.065470
O	-3.369259	-2.153048	0.922295

C -3.637375 -3.302402 1.407452

O -4.785272 -3.749379 1.676595

H -2.765374 -3.971440 1.607186

3.3.12 Cz-Gly-NeP sorbate complex

158 -1

C -7.235596 -0.981389 0.421950

C -8.600485 -0.659067 0.424214

C -9.149079 0.376977 1.223990

H -9.246935 -1.248422 -0.220402

C -8.300681 1.120344 2.048350

C -6.394314 -0.214509 1.264317

C -6.924805 0.827966 2.071922

H -8.688358 1.922941 2.675648

C -5.802039 1.397162 2.790985

C -10.666752 0.637206 1.149374

C -11.105876 1.792094 2.068704

H -10.616390 2.739611 1.797899

H -10.885718 1.580309 3.126070

H -12.192336 1.939481 1.977419

C -11.432861 -0.637611 1.577334

H -11.182991 -0.915264 2.612513

H -11.193041 -1.492344 0.928651

H -12.519285 -0.466139 1.521201

C -11.060534 1.001269 -0.302503

H -12.144507 1.184424 -0.367543

H -10.812581 0.193259 -1.005694

H -10.538745 1.912093 -0.633791

N -5.023866 -0.299724 1.460372

C -4.652350 0.665195 2.381531

H	-4.398333	-0.989926	0.973647
C	-5.682910	2.450171	3.715236
C	-4.427842	2.775082	4.240162
H	-6.572831	3.004289	4.012756
C	-3.298959	2.022308	3.827384
C	-3.379138	0.968381	2.910152
H	-2.317792	2.262681	4.231380
C	-4.225056	3.915724	5.257011
C	-5.546402	4.625705	5.606411
H	-6.273966	3.936080	6.060247
H	-6.011824	5.084386	4.721084
H	-5.348768	5.427731	6.332906
C	-3.253639	4.966341	4.667877
H	-3.661024	5.399442	3.741767
H	-2.273048	4.527128	4.434332
H	-3.094401	5.783701	5.388332
C	-3.624031	3.345676	6.564404
H	-3.471451	4.153804	7.296815
H	-2.651629	2.863696	6.388600
H	-4.297749	2.599594	7.012786
N	-2.261749	0.186362	2.520965
H	1.798058	3.508518	-5.412341
H	10.709460	-1.468610	-4.091074
H	3.646460	2.332160	-6.755571
H	11.348726	-1.642533	-2.438820
C	11.393658	-1.028561	-3.349540
C	2.450404	4.392491	-5.349742
H	2.227619	5.031946	-6.216387
H	12.417855	-1.091394	-3.748741
C	4.232270	3.261417	-6.693403
H	3.963670	3.895201	-7.552789

H	2.184111	4.957035	-4.443290
C	3.941715	4.008599	-5.369707
N	-6.658743	-2.006100	-0.364430
N	7.730713	-0.792102	0.532709
C	8.039458	-0.162431	-0.695982
C	9.307489	-0.170987	-1.289479
C	4.335897	3.110525	-4.179876
C	7.017457	0.547220	-1.358918
C	3.397576	2.703276	-3.211100
C	3.726187	1.887978	-2.114008
C	5.061545	1.473479	-1.987548
H	5.296357	3.000737	-6.787158
N	5.687537	0.732114	-0.990665
C	5.662943	2.671010	-4.045959
C	6.023991	1.852532	-2.969677
C	7.281326	1.249256	-2.561456
C	9.591001	0.516016	-2.496824
N	2.687247	1.594590	-1.187516
C	8.568763	1.235085	-3.124915
C	11.022537	0.446499	-3.064357
H	10.091094	-0.733023	-0.787683
H	5.099500	0.095354	-0.433010
H	10.503692	0.854997	-5.163847
H	2.358793	3.022887	-3.297820
H	6.419209	2.962327	-4.776757
H	8.754077	1.778143	-4.051105
C	11.167825	1.240627	-4.375790
H	12.202246	1.156316	-4.740877
H	11.992996	0.477278	-1.084465
C	12.017549	1.031492	-2.033307
C	4.777051	5.310843	-5.326540

H 4.510480 5.959266 -6.175197

H 13.044591 0.981484 -2.427221

H 10.950934 2.309796 -4.233102

H 4.587653 5.868120 -4.396655

H 5.854926 5.103168 -5.385660

H 11.784713 2.085645 -1.818413

C 8.424123 -1.781973 1.196846

H 6.916027 -0.426340 1.020604

C -7.273669 -2.850903 -1.259529

H -5.644522 -2.164100 -0.248908

O 9.456442 -2.297032 0.743867

O -8.497840 -2.849443 -1.478012

C -6.324605 -3.797684 -1.981556

C 7.816315 -2.189215 2.531095

C -6.054942 -3.452472 -3.481436

H -6.770680 -4.803282 -1.929784

H -5.357090 -3.827108 -1.457936

C 7.149902 -3.601374 2.559785

H 7.069780 -1.445299 2.850950

H 8.631552 -2.170685 3.271687

C -7.336702 -3.582923 -4.324666

H -8.115256 -2.885987 -3.986391

H -7.746582 -4.603272 -4.263546

H -7.114713 -3.368880 -5.381905

C -5.488170 -2.026111 -3.609211

H -5.209873 -1.817546 -4.653763

H -4.590474 -1.899561 -2.985042

H -6.225523 -1.268292 -3.303145

C -5.010887 -4.462428 -3.998271

H -4.795625 -4.281218 -5.062775

H -5.375424 -5.496508 -3.897338

H -4.064488 -4.377524 -3.442003

C 8.195994 -4.712894 2.357406

H 8.689321 -4.630732 1.379484

H 7.712520 -5.700101 2.420441

H 8.975305 -4.666159 3.134324

C 6.502416 -3.767584 3.948819

H 7.253512 -3.678976 4.749173

H 6.030317 -4.758348 4.034654

H 5.727788 -3.004747 4.121431

C 6.061895 -3.703308 1.475006

H 5.300808 -2.917001 1.597797

H 5.551091 -4.676141 1.536633

H 6.486674 -3.613892 0.463359

C -0.967503 0.612382 2.440335

H -2.439815 -0.822421 2.277598

C 2.509208 0.508849 -0.382035

H 1.894694 2.234985 -1.237628

O -0.582375 1.776957 2.620712

O 3.344301 -0.393879 -0.205995

C 0.028030 -0.523292 2.126704

C 1.127277 0.453166 0.267923

O 1.261434 -0.057483 1.591020

H -0.437703 -1.275790 1.466854

H 0.280369 -1.021490 3.075062

H 0.509105 -0.227491 -0.350326

H 0.644762 1.444838 0.271216

C -1.685648 -6.620001 0.868853

C -0.870847 -7.419171 1.595949

C -0.547093 -8.841208 1.273221

C -1.973713 -5.246272 1.216810

C -2.782200 -4.420997 0.509292

C -3.050905 -3.006094 0.894213

O -3.794296 -2.320111 0.095948

H -1.053250 -9.180810 0.358973

H -0.837377 -9.507629 2.102832

H 0.539854 -8.975878 1.142584

H -2.160328 -7.020507 -0.035032

H -0.404129 -7.002892 2.496926

H -1.501234 -4.845104 2.120866

H -3.270212 -4.775108 -0.403124

O -2.542272 -2.539713 1.962924

3.3.13 CzU-Py free receptor

118 0

C -5.081711 -1.353948 2.125626

C -6.266159 -1.296779 2.881388

C -6.931709 -0.085618 3.192852

H -6.664961 -2.234967 3.271842

C -6.386438 1.121304 2.733431

C -4.551722 -0.117787 1.699151

C -5.193134 1.113197 1.988611

H -6.867857 2.071447 2.962553

C -4.366187 2.154184 1.404168

C -8.218125 -0.138878 4.041657

C -8.817810 1.259383 4.281682

H -9.089661 1.755611 3.337907

H -8.124428 1.914720 4.829888

H -9.733593 1.165244 4.884089

C -7.903987 -0.772000 5.418598

H -7.155956 -0.175606 5.962540

H -7.515272 -1.795617 5.318149

H -8.817783 -0.817952 6.031188

C -9.280599 -1.000412 3.317450

H -10.203201 -1.047424 3.916338

H -8.929820 -2.030347 3.158500

H -9.531293 -0.571076 2.335482

N -3.407872 0.124466 0.956529

C -3.265385 1.498006 0.791010

H -2.721492 -0.593482 0.745069

C -4.462705 3.556899 1.371004

C -3.471231 4.303097 0.727223

H -5.309954 4.045835 1.850646

C -2.390861 3.624775 0.107328

C -2.263115 2.230486 0.121047

H -1.615186 4.192411 -0.400049

C -3.510610 5.842647 0.656027

C -4.744232 6.426939 1.369158

H -4.760913 6.166551 2.438004

H -5.683713 6.077925 0.914690

H -4.724126 7.524202 1.292778

C -3.551659 6.292762 -0.823975

H -4.449156 5.902092 -1.327201

H -2.670191 5.943407 -1.380265

H -3.575264 7.392098 -0.886308

C -2.244216 6.423743 1.329187

H -2.259471 7.523700 1.281146

H -1.325505 6.077374 0.834419

H -2.192472 6.127615 2.387934

N -1.219666 1.519203 -0.510267

C 0.030201 1.999292 -0.875900

H -1.417975 0.547067 -0.734877

O 0.399826 3.166299 -0.701247

H	1.763361	4.178033	-4.977943
H	8.442915	-1.947217	-4.157379
H	3.402232	2.699673	-6.294165
H	8.032335	-3.659931	-3.897056
C	8.687742	-2.840380	-3.564766
C	2.630795	4.693603	-4.539557
H	2.876352	5.545177	-5.191235
H	9.728298	-3.120545	-3.791303
C	4.224259	3.283975	-5.853174
H	5.125147	2.654046	-5.848063
H	2.333255	5.098660	-3.560613
C	3.855535	3.766560	-4.429860
N	-4.356834	-2.514441	1.818012
N	4.072784	-3.244941	0.320857
C	4.908952	-2.574998	-0.582957
C	6.244307	-2.924563	-0.877385
C	3.592330	2.545795	-3.524874
C	4.413764	-1.410663	-1.201045
C	2.348348	2.346651	-2.887768
C	2.091589	1.248781	-2.053398
C	3.126630	0.322032	-1.858331
H	4.420682	4.147031	-6.508273
N	3.154766	-0.839322	-1.097656
C	4.607602	1.593874	-3.332613
C	4.384081	0.483844	-2.508492
C	5.210304	-0.637024	-2.087607
C	7.061199	-2.180656	-1.755554
N	0.830553	1.021495	-1.447412
C	6.527205	-1.030144	-2.363753
C	8.522255	-2.582458	-2.047729
H	6.661488	-3.791118	-0.365198

H	2.451763	-1.137913	-0.428095
H	9.250549	-0.504960	-2.166308
H	1.542192	3.061118	-3.036147
H	5.577935	1.714627	-3.817747
H	7.138947	-0.427621	-3.037514
C	9.468937	-1.434731	-1.621591
H	10.515471	-1.708280	-1.828630
H	8.888802	-3.729764	-0.204173
C	8.945486	-3.858103	-1.295613
C	5.032475	4.588207	-3.851240
H	5.237781	5.460752	-4.490980
H	9.988564	-4.099815	-1.547703
H	9.375401	-1.228712	-0.544531
H	4.796175	4.952971	-2.840040
H	5.953432	3.990621	-3.791001
H	8.326500	-4.723819	-1.575421
H	0.475896	0.067311	-1.477382
C	-4.968555	-3.655987	1.699877
C	4.203431	-4.525776	0.507884
C	3.439786	-5.236313	1.489429
H	4.899279	-5.140264	-0.086872
C	-4.263005	-4.879536	1.461954
H	-6.065720	-3.747125	1.760123
N	2.533455	-4.621694	2.336829
C	3.431554	-6.605115	1.804973
C	2.503978	-6.796723	2.854819
C	1.962861	-5.547478	3.162383
N	-2.885005	-4.949627	1.345561
C	-2.500240	-6.239882	1.116225
C	-4.754220	-6.185484	1.302431
C	-3.645474	-7.036601	1.087240

H -5.802494 -6.469305 1.343486

H 4.037969 -7.363564 1.316676

H 1.224066 -5.257018 3.902875

H 2.248452 -7.733777 3.341010

H -3.664807 -8.110599 0.926601

H -1.454614 -6.499901 0.984874

H 2.340300 -3.623464 2.331357

H -2.273225 -4.139625 1.404494

3.3.14 CzU-Py acetate complex

125 -1

C -5.303742 -1.177871 1.811742

C -6.524476 -1.110636 2.506158

C -7.114201 0.105057 2.933503

H -7.054776 -2.049202 2.678578

C -6.452047 1.305794 2.648754

C -4.662016 0.051483 1.537723

C -5.227827 1.285647 1.954757

H -6.878300 2.261653 2.952634

C -4.312338 2.322895 1.520909

C -8.466232 0.059879 3.673473

C -8.951116 1.461642 4.088597

H -9.112658 2.114368 3.217572

H -8.237931 1.957773 4.764109

H -9.909753 1.373985 4.621294

C -8.327845 -0.799192 4.953614

H -7.575718 -0.370830 5.633691

H -8.026620 -1.831069 4.721978

H -9.289606 -0.841399 5.488095

C -9.539521 -0.569753 2.753428

H -10.508528 -0.615313 3.274775

H -9.269597 -1.593001 2.454832

H -9.670376 0.028152 1.838709

N -3.463378 0.289582 0.888950

C -3.232281 1.662629 0.874072

H -2.810896 -0.433976 0.550784

C -4.333969 3.725546 1.634688

C -3.277176 4.471753 1.108279

H -5.174481 4.210137 2.130642

C -2.202422 3.794824 0.476853

C -2.142657 2.398588 0.344023

H -1.378263 4.366162 0.058233

C -3.232645 6.011051 1.185117

C -4.459131 6.593812 1.911627

H -4.527234 6.235900 2.949985

H -5.398402 6.340209 1.397175

H -4.380627 7.690619 1.940770

C -3.196271 6.598546 -0.246269

H -4.094262 6.306825 -0.812142

H -2.315138 6.251505 -0.805012

H -3.159092 7.698411 -0.206023

C -1.964006 6.458865 1.949679

H -1.922409 7.557832 2.006648

H -1.046224 6.112679 1.453290

H -1.965644 6.062416 2.976304

N -1.073818 1.697650 -0.243698

C 0.016277 2.238005 -0.913608

H -1.102739 0.654431 -0.183916

O 0.093650 3.422658 -1.281074

H 1.495497 4.033836 -5.075583

H 8.223001 -1.966892 -4.500907

H	2.977649	2.420628	-6.421668
H	7.835736	-3.656827	-4.096698
C	8.529298	-2.827858	-3.889142
C	2.406910	4.586397	-4.801333
H	2.569463	5.361480	-5.565101
H	9.535758	-3.132806	-4.216163
C	3.843378	3.039117	-6.139190
H	4.739952	2.404027	-6.173003
H	2.226438	5.096501	-3.843137
C	3.639153	3.665244	-4.738716
N	-4.739367	-2.361320	1.314094
N	4.425842	-2.928023	0.554215
C	5.125556	-2.324454	-0.499701
C	6.409042	-2.718118	-0.935131
C	3.489130	2.543281	-3.689797
C	4.561882	-1.191894	-1.124465
C	2.330338	2.431784	-2.889274
C	2.161459	1.430527	-1.914379
C	3.214591	0.499388	-1.766786
H	3.961773	3.829856	-6.896797
N	3.341250	-0.581268	-0.895627
C	4.523623	1.612553	-3.520279
C	4.388951	0.593516	-2.566570
C	5.254614	-0.498469	-2.155617
C	7.123974	-2.042040	-1.947574
N	1.008315	1.289416	-1.120595
C	6.528549	-0.924615	-2.558264
C	8.538684	-2.481831	-2.380836
H	6.873971	-3.558398	-0.420224
H	2.592773	-0.954899	-0.292239
H	9.266021	-0.425889	-2.701195

H	1.526477	3.152421	-2.999389
H	5.433758	1.672225	-4.120058
H	7.058542	-0.374523	-3.338168
C	9.537839	-1.326522	-2.131984
H	10.551888	-1.626820	-2.439631
H	9.101935	-3.528843	-0.526658
C	9.034461	-3.719106	-1.608461
C	4.871766	4.533591	-4.388138
H	4.996494	5.337004	-5.131077
H	10.040619	-3.989730	-1.961437
H	9.568724	-1.058322	-1.065034
H	4.753922	4.998511	-3.397200
H	5.795988	3.938180	-4.376305
H	8.380703	-4.590165	-1.766158
H	0.930592	0.414830	-0.551625
C	-4.838081	-3.461318	1.998529
C	4.519118	-4.209294	0.749281
C	3.914366	-4.855436	1.877170
H	5.057389	-4.873302	0.051917
C	-4.389558	-4.723890	1.488912
H	-5.263396	-3.482547	3.016025
N	3.223681	-4.167537	2.860030
C	3.883673	-6.213818	2.230060
C	3.160205	-6.325181	3.441245
C	2.762980	-5.038538	3.806332
N	-3.867959	-4.884102	0.216663
C	-3.534300	-6.192076	0.008395
C	-4.382249	-5.989426	2.096783
C	-3.844256	-6.908514	1.165149
H	-4.731928	-6.202464	3.103717
H	4.340837	-7.019144	1.660972

H 2.194395 -4.686388 4.661446

H 2.945987 -7.234683 3.995207

H -3.694815 -7.974951 1.307880

H -3.107982 -6.517621 -0.935466

H 3.092594 -3.159278 2.856085

H -3.759801 -4.123209 -0.449016

H 0.577877 -3.436935 1.313764

C -0.233978 -3.162797 0.630463

H -1.206594 -3.438055 1.056752

C -0.192377 -1.679991 0.294531

O -1.259372 -1.130381 -0.138971

H -0.105315 -3.735926 -0.300981

O 0.910487 -1.054620 0.431836

3.3.15 CzU-Py benzoate complex

132 -1

C 4.923985 3.407918 -0.474636

C 3.695205 3.467778 0.208024

C 3.038371 4.680459 0.529852

H 3.217004 2.522876 0.472635

C 3.638482 5.888386 0.150297

C 5.482753 4.642631 -0.877018

C 4.856693 5.876122 -0.552857

H 3.164593 6.841939 0.382011

C 5.708919 6.921250 -1.086104

C 1.687693 4.625334 1.272177

C 1.116942 6.028602 1.550450

H 0.927078 6.584943 0.620259

H 1.791755 6.628087 2.179750

H 0.159385 5.934474 2.084100

C	1.869769	3.902204	2.628541
H	2.591505	4.437568	3.263942
H	2.232184	2.872553	2.496249
H	0.909451	3.854654	3.165084
C	0.659169	3.847485	0.416608
H	-0.309313	3.798080	0.938274
H	0.988952	2.816852	0.220938
H	0.500948	4.343676	-0.553138
N	6.665214	4.890430	-1.552365
C	6.807997	6.267123	-1.704556
H	7.238439	4.177960	-2.025918
C	5.626435	8.326040	-1.068740
C	6.635498	9.078791	-1.673230
H	4.777387	8.807089	-0.584019
C	7.723252	8.407670	-2.289626
C	7.846079	7.009891	-2.319356
H	8.516221	8.981561	-2.760627
C	6.614737	10.620325	-1.698282
C	5.371736	11.197654	-0.995641
H	5.329621	10.908081	0.065009
H	4.439084	10.869878	-1.479273
H	5.403226	12.296392	-1.041011
C	6.612027	11.115849	-3.164206
H	5.721778	10.751123	-3.699091
H	7.501711	10.772353	-3.711088
H	6.602088	12.216828	-3.194118
C	7.871184	11.168026	-0.979874
H	7.868889	12.269132	-0.995257
H	8.797134	10.825787	-1.463817
H	7.895467	10.840164	0.070471
N	8.917770	6.306443	-2.903279

C	10.097491	6.835760	-3.406007
H	8.790480	5.277922	-3.004701
O	10.329535	8.051098	-3.509369
H	11.930337	9.075787	-7.252871
H	18.465657	2.840502	-6.867499
H	13.503859	7.612100	-8.664639
H	18.010506	1.122660	-6.757455
C	18.688516	1.892110	-6.357720
C	12.821213	9.550590	-6.815576
H	13.077824	10.418832	-7.440884
H	19.720507	1.606140	-6.614424
C	14.349937	8.154339	-8.215427
H	15.232124	7.499425	-8.253271
H	12.555547	9.926696	-5.816249
C	14.020502	8.585773	-6.766199
N	5.602095	2.229315	-0.819729
N	14.114722	1.281697	-2.440094
C	14.935829	2.003109	-3.317224
C	16.257290	1.642616	-3.661269
C	13.740810	7.334392	-5.908253
C	14.459087	3.227759	-3.831167
C	12.506478	7.153250	-5.245795
C	12.220711	6.032626	-4.444054
C	13.222085	5.041894	-4.349389
H	14.559171	9.038348	-8.838171
N	13.234710	3.845425	-3.632368
C	14.731660	6.351012	-5.775320
C	14.475183	5.208973	-5.004000
C	15.270494	4.039732	-4.671515
C	17.086086	2.431264	-4.486635
N	10.992083	5.840127	-3.781983

C	16.574571	3.638941	-4.993596
C	18.534709	2.018642	-4.823004
H	16.656874	0.728958	-3.222424
H	12.396445	3.382128	-3.251406
H	19.316797	4.078715	-4.759401
H	11.736489	7.914030	-5.324491
H	15.700791	6.464608	-6.264483
H	17.193579	4.278504	-5.625819
C	19.513784	3.098233	-4.302253
H	20.551886	2.817581	-4.540332
H	18.876730	0.702733	-3.090597
C	18.926868	0.670400	-4.189474
C	15.230167	9.351427	-6.178380
H	15.448023	10.244591	-6.785147
H	19.962506	0.424935	-4.467211
H	19.430514	3.208817	-3.210426
H	15.022933	9.679726	-5.148415
H	16.134983	8.727048	-6.160765
H	18.284072	-0.150716	-4.541444
H	10.807856	4.885184	-3.409633
C	5.474651	1.169878	-0.076727
C	14.232833	-0.010096	-2.343559
C	13.504216	-0.770061	-1.372442
H	14.891634	-0.594983	-3.006825
C	6.083038	-0.081878	-0.415120
H	4.907666	1.176630	0.869268
N	12.648414	-0.193313	-0.449740
C	13.495080	-2.153250	-1.129981
C	12.617919	-2.391750	-0.046373
C	12.106309	-1.156218	0.352193
N	6.847081	-0.271492	-1.554628

C 7.296819 -1.560604 -1.607007

C 6.053757 -1.309337 0.266041

C 6.814944 -2.234838 -0.485306

H 5.531726 -1.493597 1.201458

H 14.068532 -2.890065 -1.686458

H 11.403872 -0.899234 1.138780

H 12.375633 -3.351003 0.401976

H 7.002122 -3.277452 -0.245316

H 7.922760 -1.902236 -2.425240

H 12.463856 0.805277 -0.399403

H 7.042795 0.461152 -2.234501

C 8.125773 -0.241934 -5.232716

C 9.203101 -1.132079 -5.130755

H 7.224439 -0.534193 -5.774646

C 8.206060 1.023427 -4.642766

H 9.141266 -2.120542 -5.589953

C 10.358337 -0.751691 -4.435811

H 7.375369 1.726948 -4.718021

C 9.365833 1.414090 -3.949478

C 10.442102 0.516563 -3.854013

C 9.459940 2.797814 -3.343433

O 10.587088 3.187712 -2.892350

O 8.405987 3.513505 -3.333797

H 11.339939 0.825526 -3.317032

H 11.196216 -1.445929 -4.351322

3.3.16 CzU-Py lactate complex

129 -1

C -5.464040 -1.071161 1.562070

C -6.688013 -0.968617 2.247003

C -7.188813 0.248079 2.773151

H -7.293244 -1.873274 2.330676

C -6.431749 1.413860 2.600857

C -4.725211 0.123567 1.404516

C -5.201054 1.357798 1.920753

H -6.788847 2.370337 2.982140

C -4.202467 2.354196 1.584496

C -8.552083 0.245548 3.494105

C -8.937167 1.641544 4.018765

H -9.034643 2.373838 3.203156

H -8.200138 2.024637 4.740651

H -9.908511 1.583840 4.532032

C -8.498003 -0.723226 4.700103

H -7.727328 -0.409478 5.420418

H -8.270307 -1.751969 4.385669

H -9.468670 -0.737510 5.219991

C -9.655700 -0.223742 2.515672

H -10.633468 -0.234012 3.022316

H -9.461465 -1.238569 2.139395

H -9.724976 0.452543 1.650185

N -3.505929 0.322939 0.780555

C -3.167267 1.669497 0.891461

H -2.880112 -0.425064 0.449133

C -4.118968 3.739894 1.814651

C -3.002191 4.444792 1.359111

H -4.926072 4.244824 2.344618

C -1.977117 3.743162 0.674680

C -2.026235 2.364203 0.419093

H -1.108861 4.283913 0.306992

C -2.838210 5.962846 1.573539

C -4.026648 6.575332 2.337849

H -4.139289 6.134095 3.339886

H -4.974607 6.444499 1.794378

H -3.862343 7.655591 2.465741

C -2.730607 6.671727 0.201851

H -3.639252 6.506174 -0.396387

H -1.870876 6.305857 -0.377933

H -2.605465 7.756663 0.342933

C -1.550981 6.236521 2.388098

H -1.422202 7.319262 2.543874

H -0.655637 5.862203 1.871630

H -1.602229 5.751948 3.374822

N -1.013393 1.640775 -0.237810

C 0.045813 2.162724 -0.967314

H -1.080513 0.598995 -0.204499

O 0.151721 3.357162 -1.289023

H 1.266902 3.845383 -5.332707

H 8.248740 -1.870582 -4.697618

H 2.802469 2.270947 -6.661876

H 7.916608 -3.551908 -4.216193

C 8.594831 -2.698889 -4.062462

C 2.154988 4.446380 -5.085265

H 2.270065 5.209656 -5.869523

H 9.598487 -2.992468 -4.407995

C 3.642785 2.934867 -6.407629

H 4.566985 2.340652 -6.439659

H 1.964259 4.970582 -4.136783

C 3.429974 3.585624 -5.019746

N -4.981874 -2.243291 0.962590

N 4.547682 -2.807328 0.409248

C 5.268809 -2.181936 -0.614527

C 6.561036 -2.539740 -1.053093

C	3.348120	2.484279	-3.941849
C	4.635814	-1.126235	-1.301545
C	2.206387	2.334312	-3.123024
C	2.104329	1.350827	-2.122482
C	3.198872	0.472985	-1.974374
H	3.713953	3.711331	-7.185790
N	3.391409	-0.567846	-1.069472
C	4.430908	1.610682	-3.764007
C	4.359556	0.605096	-2.789706
C	5.287759	-0.424740	-2.351746
C	7.228494	-1.874266	-2.105065
N	0.975269	1.183535	-1.296533
C	6.579337	-0.803812	-2.746764
C	8.639880	-2.293152	-2.569712
H	7.040654	-3.387862	-0.565346
H	2.665706	-0.994810	-0.479399
H	9.293513	-0.229734	-2.988179
H	1.366616	3.012376	-3.238455
H	5.330700	1.705874	-4.374876
H	7.072486	-0.269583	-3.561082
C	9.611413	-1.100838	-2.397465
H	10.622802	-1.383149	-2.729925
H	9.286471	-3.250041	-0.694635
C	9.196473	-3.483922	-1.766180
C	4.625459	4.519118	-4.710003
H	4.700998	5.309007	-5.473992
H	10.201089	-3.736032	-2.137060
H	9.670924	-0.793307	-1.342382
H	4.500567	5.002587	-3.728975
H	5.576875	3.968362	-4.699102
H	8.567885	-4.380948	-1.872555

H	0.905849	0.283796	-0.775789
C	-5.201777	-3.396579	1.519353
C	5.162258	-3.333782	1.425025
C	4.459074	-4.014129	2.472702
H	6.256162	-3.265563	1.556052
C	-4.835267	-4.631345	0.890939
H	-5.673038	-3.489508	2.512400
N	3.083491	-4.176832	2.492241
C	4.965303	-4.609438	3.640651
C	3.868526	-5.135927	4.361602
C	2.718728	-4.850698	3.623098
N	-4.258414	-4.698325	-0.365734
C	-4.026306	-6.000703	-0.705844
C	-4.969211	-5.950944	1.350604
C	-4.460242	-6.807889	0.346492
H	-5.391717	-6.240168	2.309452
H	6.015260	-4.646999	3.920008
H	1.677193	-5.080738	3.826712
H	3.898761	-5.663036	5.311043
H	-4.409424	-7.892595	0.374377
H	-3.576495	-6.258368	-1.659732
H	2.426033	-3.855001	1.764875
H	-4.053013	-3.882475	-0.936642
O	0.806321	-3.939622	0.686081
C	-0.440701	-3.205523	0.743628
C	-1.005249	-3.164455	2.168092
C	-0.233605	-1.777582	0.207160
O	-1.295520	-1.169006	-0.150442
H	-1.169681	-3.690215	0.074121
O	0.927981	-1.277952	0.172830
H	-1.964873	-2.631013	2.182346

H -0.304448 -2.655353 2.845574

H -1.174803 -4.185236 2.539870

H 0.572372 -4.883348 0.761676

3.3.17 CzU-Py formate complex

122 -1

C -5.225596 -1.267213 1.972790

C -6.456412 -1.205049 2.649665

C -7.085658 0.012253 3.011111

H -6.960146 -2.148530 2.868446

C -6.456076 1.218647 2.676625

C -4.624470 -0.032581 1.639186

C -5.226565 1.203724 1.992092

H -6.913649 2.173836 2.933110

C -4.337693 2.243051 1.508945

C -8.443898 -0.036970 3.739900

C -8.977796 1.368320 4.075222

H -9.148279 1.968667 3.168947

H -8.289769 1.921944 4.731713

H -9.940100 1.277895 4.600878

C -8.293154 -0.822750 5.065007

H -7.562392 -0.335500 5.728362

H -7.957735 -1.855430 4.891218

H -9.258989 -0.866834 5.591854

C -9.486369 -0.748039 2.844095

H -10.459360 -0.796474 3.357546

H -9.181504 -1.776658 2.602918

H -9.625221 -0.203846 1.897479

N -3.430866 0.205466 0.983602

C -3.239577 1.580958 0.893893

H	-2.784050	-0.521462	0.645020
C	-4.393580	3.648280	1.557903
C	-3.354815	4.394726	0.997426
H	-5.245850	4.134553	2.031598
C	-2.264490	3.716543	0.394453
C	-2.170327	2.317661	0.325764
H	-1.455154	4.288110	-0.051034
C	-3.345752	5.936541	1.006721
C	-4.587400	6.522080	1.704824
H	-4.650613	6.208317	2.757593
H	-5.519156	6.224787	1.200215
H	-4.533718	7.620664	1.686159
C	-3.318351	6.462385	-0.448412
H	-4.207736	6.126100	-1.003059
H	-2.427728	6.112305	-0.989794
H	-3.306543	7.563674	-0.455725
C	-2.089900	6.445715	1.753937
H	-2.073599	7.546751	1.763905
H	-1.163060	6.099534	1.274611
H	-2.085382	6.093623	2.796631
N	-1.087700	1.615201	-0.238594
C	0.007854	2.154298	-0.901165
H	-1.116353	0.576673	-0.172179
O	0.087423	3.339111	-1.264899
H	1.597157	4.094588	-4.949440
H	8.261407	-2.000799	-4.469206
H	3.093189	2.519532	-6.326836
H	7.846101	-3.702461	-4.150496
C	8.541045	-2.890704	-3.886869
C	2.507692	4.626772	-4.635224
H	2.693579	5.429128	-5.364678

H 9.553782 -3.192115 -4.197307

C 3.957810 3.118918 -6.002781

H 4.849938 2.477977 -6.043652

H 2.311881 5.101167 -3.661812

C 3.729774 3.691459 -4.583148

N -4.591631 -2.443448 1.549560

N 4.270024 -3.152502 0.386044

C 5.039159 -2.504542 -0.589407

C 6.332847 -2.891594 -0.999681

C 3.547071 2.530461 -3.583040

C 4.514982 -1.330045 -1.168424

C 2.371650 2.401979 -2.809407

C 2.171392 1.363914 -1.879964

C 3.208105 0.411825 -1.755269

H 4.097749 3.937655 -6.726131

N 3.297354 -0.715451 -0.942178

C 4.567469 1.581479 -3.431660

C 4.401444 0.525311 -2.524737

C 5.243020 -0.597087 -2.146012

C 7.086152 -2.175188 -1.954642

N 1.003466 1.207862 -1.107843

C 6.522267 -1.022722 -2.531125

C 8.509048 -2.610307 -2.365246

H 6.771733 -3.765330 -0.518928

H 2.556910 -1.078659 -0.325641

H 9.264232 -0.549886 -2.574625

H 1.579972 3.137657 -2.904274

H 5.490066 1.654526 -4.010441

H 7.082335 -0.445585 -3.269316

C 9.510711 -1.477037 -2.037349

H 10.530599 -1.774212 -2.328172

H	9.006333	-3.742359	-0.542688
C	8.970840	-3.884697	-1.633311
C	4.962539	4.532748	-4.172756
H	5.110867	5.363008	-4.880916
H	9.985223	-4.148863	-1.966978
H	9.512464	-1.255375	-0.959339
H	4.827666	4.960209	-3.167177
H	5.880696	3.927890	-4.164404
H	8.315650	-4.742025	-1.849372
H	0.926025	0.333763	-0.546812
C	-4.702720	-3.536642	2.242925
C	4.377992	-4.434154	0.571961
C	3.652657	-5.109085	1.608333
H	5.013465	-5.075016	-0.061837
C	-4.132629	-4.774785	1.799416
H	-5.223458	-3.570686	3.214535
N	2.791134	-4.452561	2.470430
C	3.638300	-6.465724	1.969459
C	2.752291	-6.607592	3.063934
C	2.240200	-5.341371	3.349515
N	-3.431531	-4.895885	0.611695
C	-3.005261	-6.183354	0.448699
C	-4.144188	-6.043995	2.399545
C	-3.437142	-6.925848	1.548335
H	-4.619746	-6.284688	3.346878
H	4.214745	-7.249329	1.484604
H	1.531098	-5.015923	4.104397
H	2.505485	-7.523794	3.592681
H	-3.254759	-7.984769	1.707611
H	-2.431081	-6.476607	-0.424686
H	2.601417	-3.454411	2.421321

H -3.261485 -4.118847 -0.022326

C -0.207081 -1.763778 0.368046

O -1.270848 -1.254500 -0.098353

O 0.906989 -1.171840 0.487011

H -0.256587 -2.826671 0.702522

3.3.18 CzU-Py sorbate complex

133 -1

C -4.910735 -0.763919 2.350136

C -6.180998 -0.733039 2.953958

C -6.892612 0.463576 3.214395

H -6.644122 -1.688972 3.205754

C -6.306177 1.683923 2.853540

C -4.367804 0.480604 1.957992

C -5.047209 1.699153 2.226033

H -6.821204 2.625793 3.040949

C -4.196166 2.761398 1.724653

C -8.287272 0.377512 3.867435

C -8.912479 1.766799 4.093070

H -9.056007 2.309402 3.146679

H -8.296250 2.389983 4.758344

H -9.899963 1.651130 4.564402

C -8.176023 -0.328876 5.240202

H -7.513057 0.231809 5.916492

H -7.777927 -1.348972 5.142571

H -9.168271 -0.398273 5.712582

C -9.235442 -0.435731 2.953851

H -10.234170 -0.509090 3.411824

H -8.864609 -1.457935 2.789835

H -9.343460 0.048561 1.971368

N	-3.155904	0.752727	1.346777
C	-3.048731	2.130260	1.174282
H	-2.553578	0.053658	0.887193
C	-4.314708	4.163757	1.720291
C	-3.294373	4.935311	1.159802
H	-5.199646	4.628446	2.154006
C	-2.160750	4.286010	0.605421
C	-2.002314	2.891454	0.597809
H	-1.361928	4.874959	0.163936
C	-3.351791	6.475549	1.116509
C	-4.636414	7.029159	1.761089
H	-4.715886	6.747843	2.821918
H	-5.540309	6.675318	1.242534
H	-4.628672	8.127909	1.706331
C	-3.305745	6.955431	-0.353888
H	-4.163778	6.562850	-0.920666
H	-2.385911	6.628039	-0.859257
H	-3.341106	8.055489	-0.397286
C	-2.140200	7.062058	1.879827
H	-2.169841	8.162569	1.853219
H	-1.186702	6.739709	1.437636
H	-2.150645	6.744674	2.933631
N	-0.890103	2.206011	0.071089
C	0.293415	2.758744	-0.396799
H	-0.994645	1.173883	-0.038252
O	0.492372	3.978673	-0.522027
H	2.239058	5.229151	-3.939767
H	8.332831	-1.413516	-4.375799
H	3.650176	3.783301	-5.530693
H	7.757115	-3.098221	-4.373946
C	8.511992	-2.414405	-3.957021

C	3.177393	5.614120	-3.513531
H	3.461289	6.510392	-4.085434
H	9.503993	-2.749695	-4.298120
C	4.548323	4.238312	-5.086014
H	5.384728	3.536658	-5.216005
H	2.981609	5.928233	-2.477420
C	4.312908	4.576940	-3.594330
N	-4.174767	-1.926672	2.073387
N	4.120711	-3.041602	0.151473
C	4.947361	-2.299113	-0.702730
C	6.217893	-2.719873	-1.151845
C	3.992393	3.282625	-2.817602
C	4.535586	-1.004622	-1.084714
C	2.776154	3.125809	-2.116009
C	2.448947	1.964679	-1.390111
C	3.398132	0.917126	-1.400523
H	4.784604	5.153485	-5.651697
N	3.363784	-0.332127	-0.782520
C	4.924525	2.235984	-2.802346
C	4.630361	1.058498	-2.100311
C	5.360640	-0.180723	-1.899925
C	7.059974	-1.921284	-1.954617
N	1.232480	1.781957	-0.704772
C	6.614408	-0.640983	-2.327113
C	8.452870	-2.405303	-2.410651
H	6.567475	-3.695566	-0.816072
H	2.529593	-0.756817	-0.342670
H	9.390885	-0.418579	-2.233367
H	2.051208	3.932847	-2.105218
H	5.875663	2.325712	-3.330274
H	7.245042	0.006362	-2.939852

C	9.537831	-1.444909	-1.867338
H	10.537044	-1.778143	-2.188961
H	8.788913	-3.882145	-0.811493
C	8.776656	-3.826083	-1.910605
C	5.594720	5.220899	-3.013378
H	5.842181	6.142826	-3.563201
H	9.774266	-4.119812	-2.269012
H	9.523156	-1.419268	-0.767145
H	5.455901	5.481915	-1.953120
H	6.457099	4.542849	-3.086732
H	8.055764	-4.567671	-2.286924
H	1.043126	0.828038	-0.329224
C	-4.295420	-2.961555	2.850826
C	4.113881	-4.339927	0.086091
C	3.376158	-5.147789	1.011140
H	4.667272	-4.893588	-0.690961
C	-3.621210	-4.199857	2.597984
H	-4.911865	-2.942173	3.765344
N	2.634669	-4.618258	2.053418
C	3.251513	-6.544148	1.088546
C	2.421487	-6.839070	2.195350
C	2.052725	-5.623291	2.772031
N	-2.770951	-4.402018	1.523613
C	-2.281268	-5.677457	1.549786
C	-3.663321	-5.404202	3.318510
C	-2.824036	-6.330042	2.656064
H	-4.248288	-5.574187	4.218664
H	3.719602	-7.252872	0.410260
H	1.425847	-5.406203	3.630960
H	2.116611	-7.822115	2.542514
H	-2.625915	-7.358270	2.944159

H -1.589207 -6.028678 0.791564

H 2.546462 -3.621440 2.233336

H -2.533690 -3.683784 0.840988

C -1.284129 -4.546455 -2.099712

C -2.295649 -5.034720 -2.854412

C -2.335611 -6.397629 -3.462365

C -1.285322 -3.216719 -1.531509

C -0.285762 -2.693693 -0.778439

C -0.288274 -1.293338 -0.272625

O 0.806108 -0.851746 0.228464

H -1.434698 -6.980483 -3.226873

H -2.435934 -6.333476 -4.558831

H -3.218464 -6.957058 -3.109864

H -0.408810 -5.177405 -1.905794

H -3.161357 -4.388614 -3.042430

H -2.155111 -2.582715 -1.739445

H 0.613873 -3.276622 -0.563042

O -1.346436 -0.585193 -0.379302

3.3.19 CzU-DPM free receptor

125 0

C -4.505625 -0.781991 2.544536

C -5.634422 -0.703992 3.380159

C -6.461366 0.443373 3.465361

H -5.895120 -1.588956 3.963762

C -6.147042 1.561743 2.680981

C -4.237298 0.352723 1.749894

C -5.032862 1.525156 1.822692

H -6.760467 2.461199 2.722865

C -4.436410 2.482646 0.907234

C	-7.680999	0.415178	4.408835
C	-8.467184	1.739410	4.386049
H	-8.867864	1.961131	3.385615
H	-7.846264	2.589828	4.705946
H	-9.319521	1.670085	5.078377
C	-7.206796	0.162270	5.860150
H	-6.527435	0.960676	6.195187
H	-6.677083	-0.796457	5.954777
H	-8.070879	0.138085	6.542428
C	-8.639735	-0.722459	3.982279
H	-9.513525	-0.752691	4.651598
H	-8.149390	-1.705545	4.024209
H	-9.001171	-0.565690	2.954530
N	-3.211337	0.550409	0.840597
C	-3.309030	1.835937	0.329359
H	-2.456641	-0.109538	0.681065
C	-4.735357	3.812783	0.564144
C	-3.929484	4.496091	-0.354782
H	-5.594336	4.301691	1.022370
C	-2.829057	3.816338	-0.934716
C	-2.499551	2.497088	-0.611816
H	-2.201537	4.328179	-1.662673
C	-4.204435	5.954163	-0.773187
C	-5.430807	6.544957	-0.052651
H	-5.297162	6.558077	1.039484
H	-6.349895	5.984921	-0.282049
H	-5.582858	7.583394	-0.382570
C	-4.465033	6.015246	-2.297613
H	-5.340835	5.406657	-2.569742
H	-3.603105	5.648033	-2.873303
H	-4.659497	7.053672	-2.608279

C	-2.975399	6.830035	-0.432002
H	-3.157595	7.873618	-0.732434
H	-2.071434	6.482605	-0.952383
H	-2.771626	6.815265	0.649496
N	-1.420533	1.800604	-1.211288
C	-0.150900	2.317863	-1.420387
H	-1.597198	0.837654	-1.490869
O	0.190526	3.453539	-1.072303
H	2.293552	4.954071	-4.925443
H	8.571104	-1.492538	-3.807704
H	4.142881	3.605268	-6.094474
H	8.060154	-3.197687	-3.834720
C	8.690251	-2.464811	-3.308367
C	3.066445	5.384859	-4.270866
H	3.434401	6.303866	-4.750348
H	9.741320	-2.774456	-3.419036
C	4.870393	4.105121	-5.436949
H	5.751246	3.453410	-5.346368
H	2.593336	5.672845	-3.319883
C	4.243569	4.415076	-4.056597
N	-3.669966	-1.898143	2.395683
N	3.498546	-3.174388	-0.362027
C	4.510738	-2.391654	-0.934183
C	5.867284	-2.762291	-1.057331
C	3.807347	3.098448	-3.381571
C	4.148093	-1.150098	-1.491349
C	2.464804	2.860322	-3.014388
C	2.050375	1.675592	-2.389133
C	3.023345	0.698671	-2.130666
H	5.191223	5.037807	-5.926658
N	2.901917	-0.544592	-1.526327

C 4.761841 2.098206 -3.131068

C 4.380631 0.899038 -2.515563

C 5.103935 -0.293643 -2.102211

C 6.838566 -1.945473 -1.675307

N 0.698083 1.419800 -2.048990

C 6.442792 -0.698883 -2.193678

C 8.310826 -2.387842 -1.809804

H 6.156640 -3.743580 -0.682191

H 2.075910 -0.916587 -1.068046

H 9.119221 -0.352832 -1.548311

H 1.704539 3.611804 -3.212997

H 5.806373 2.249032 -3.410033

H 7.171327 -0.045089 -2.676595

C 9.224010 -1.354318 -1.107307

H 10.279187 -1.654962 -1.201208

H 8.348065 -3.773963 -0.100070

C 8.573431 -3.766954 -1.177108

C 5.295927 5.121574 -3.168190

H 5.622118 6.062065 -3.639136

H 9.635952 -4.025570 -1.296576

H 8.982676 -1.282163 -0.035921

H 4.876864 5.361685 -2.179142

H 6.185333 4.493167 -3.017827

H 7.982374 -4.560268 -1.659263

H 0.340726 0.490000 -2.259440

C -3.480141 -2.704301 3.400375

C 3.785089 -4.017249 0.588617

C 2.813656 -4.904812 1.147347

H 4.793741 -4.088158 1.028624

C -2.706272 -3.901086 3.289833

H -3.893468 -2.502049 4.402485

N 1.496990 -4.963220 0.718548

C 2.954352 -5.871150 2.155856

C 1.705981 -6.507612 2.314831

C 0.807633 -5.926911 1.406971

N -2.111995 -4.318435 2.109201

C -1.457887 -5.508124 2.292652

C -2.405908 -4.871113 4.259246

C -1.630823 -5.871066 3.636918

H -2.729311 -4.842293 5.296694

H 3.872617 -6.082713 2.697817

H 1.471996 -7.303550 3.014755

H -1.230334 -6.763533 4.107686

H 1.131585 -4.378635 -0.028961

H -2.192515 -3.803593 1.236027

C -0.675035 -6.207046 1.186979

C -0.921496 -7.731761 1.279593

H -0.617098 -8.136868 2.252888

H -0.350086 -8.250778 0.497454

H -1.989980 -7.946134 1.137560

C -1.129755 -5.722040 -0.206065

H -0.989168 -4.640974 -0.358279

H -2.195851 -5.943335 -0.351679

H -0.563616 -6.245322 -0.988223

3.3.20 CzU-DPM acetate complex

132 -1

C -4.304823 -0.635082 2.585382

C -5.492348 -0.649035 3.340838

C -6.382658 0.450452 3.416015

H -5.752110 -1.572716 3.861237

C	-6.078361	1.615037	2.698170
C	-4.042411	0.548282	1.864122
C	-4.908477	1.670655	1.918570
H	-6.744164	2.477218	2.726542
C	-4.319017	2.687161	1.065180
C	-7.660287	0.317528	4.269554
C	-8.511083	1.601183	4.251403
H	-8.854970	1.850758	3.236454
H	-7.958057	2.464788	4.650469
H	-9.402761	1.457369	4.879645
C	-7.272605	0.018461	5.737715
H	-6.658522	0.831447	6.154182
H	-6.702284	-0.917234	5.826109
H	-8.177914	-0.078884	6.356851
C	-8.528049	-0.843358	3.727070
H	-9.440621	-0.950245	4.333959
H	-7.990769	-1.802203	3.756093
H	-8.829855	-0.653637	2.685722
N	-2.977213	0.830543	1.025794
C	-3.124835	2.126926	0.543442
H	-2.160611	0.230830	0.924195
C	-4.694154	3.999275	0.718851
C	-3.887582	4.740473	-0.150214
H	-5.608526	4.421867	1.133157
C	-2.710158	4.149198	-0.677954
C	-2.308781	2.846193	-0.354771
H	-2.076678	4.713480	-1.357560
C	-4.231107	6.185998	-0.563842
C	-5.533475	6.685418	0.089757
H	-5.464949	6.688426	1.187989
H	-6.399164	6.071484	-0.201109

H	-5.732837	7.717513	-0.234741
C	-4.404118	6.260405	-2.099965
H	-5.221681	5.603633	-2.434304
H	-3.487880	5.958650	-2.627619
H	-4.645422	7.290413	-2.405926
C	-3.083937	7.132347	-0.135829
H	-3.315591	8.168161	-0.429714
H	-2.130415	6.853814	-0.606948
H	-2.943421	7.108979	0.955537
N	-1.173838	2.197528	-0.866214
C	-0.075223	2.765942	-1.494379
H	-1.068607	1.193409	-0.653774
O	0.051770	3.972751	-1.740679
H	2.452834	5.064482	-5.022025
H	8.491375	-1.512333	-3.747268
H	4.182252	3.547600	-6.169263
H	7.889916	-3.187445	-3.708085
C	8.577979	-2.476306	-3.225987
C	3.274550	5.503913	-4.436772
H	3.660364	6.367253	-4.999056
H	9.605974	-2.845293	-3.367181
C	4.961664	4.059718	-5.584608
H	5.816927	3.376056	-5.484791
H	2.860596	5.881058	-3.489691
C	4.416430	4.496448	-4.203835
N	-3.420171	-1.712512	2.427468
N	3.471875	-2.867010	-0.102128
C	4.501358	-2.125346	-0.697282
C	5.833358	-2.565876	-0.861253
C	3.956398	3.251628	-3.415446
C	4.179636	-0.879225	-1.270011

C	2.619166	3.108016	-2.978999
C	2.178248	1.988379	-2.253790
C	3.123358	0.985708	-1.969496
H	5.297758	4.938396	-6.157302
N	2.963034	-0.215971	-1.285638
C	4.879967	2.234969	-3.127973
C	4.468928	1.100447	-2.412042
C	5.151084	-0.099573	-1.956696
C	6.819869	-1.818691	-1.539303
N	0.858284	1.790152	-1.813198
C	6.464266	-0.572937	-2.085971
C	8.261024	-2.340661	-1.717089
H	6.086430	-3.554153	-0.478562
H	2.123703	-0.528972	-0.793000
H	9.177926	-0.343716	-1.540877
H	1.887421	3.880854	-3.192523
H	5.917536	2.317513	-3.455979
H	7.200597	0.024498	-2.626912
C	9.252275	-1.338248	-1.078575
H	10.286800	-1.693478	-1.206321
H	8.294016	-3.682768	0.027324
C	8.477695	-3.714875	-1.057123
C	5.539739	5.216024	-3.419146
H	5.882765	6.104367	-3.972677
H	9.520255	-4.031714	-1.209025
H	9.059070	-1.228531	-0.000542
H	5.179149	5.545683	-2.433012
H	6.407651	4.559931	-3.262379
H	7.828962	-4.488614	-1.495185
H	0.622318	0.846501	-1.467281
C	-3.315955	-2.591092	3.382200

C	3.760999	-3.744385	0.814943
C	2.822725	-4.682401	1.346566
H	4.780612	-3.842577	1.225871
C	-2.580173	-3.811913	3.282040
H	-3.823698	-2.454361	4.352783
N	1.483952	-4.766268	0.987700
C	3.099991	-5.781584	2.175396
C	1.913792	-6.530505	2.300115
C	0.917064	-5.879852	1.557947
N	-1.850426	-4.232560	2.177093
C	-1.393162	-5.511386	2.380736
C	-2.575351	-4.868146	4.208157
C	-1.841507	-5.928089	3.642901
H	-3.089176	-4.860789	5.166348
H	4.074552	-6.017959	2.595533
H	1.788841	-7.454720	2.855194
H	-1.661823	-6.900530	4.090352
H	0.970516	-4.019046	0.496329
H	-1.577985	-3.624860	1.388370
C	-0.544225	-6.267150	1.366834
C	-0.698203	-7.784162	1.613083
H	-0.383111	-8.079617	2.621866
H	-0.089698	-8.341576	0.887720
H	-1.749501	-8.075460	1.483549
C	-1.011396	-5.969285	-0.078566
H	-0.935570	-4.903862	-0.333960
H	-2.059405	-6.279028	-0.199296
H	-0.397873	-6.540818	-0.789351
O	-0.383834	-2.659034	0.187870
O	-0.131963	-0.492732	-0.364781
C	-0.619113	-1.666635	-0.563638

H -1.428652 -2.854129 -2.192129

C -1.564350 -1.860623 -1.745673

H -1.427464 -1.084911 -2.509030

H -2.601459 -1.804893 -1.379036

3.3.21 CzU-DPM benzoate complex

139 -1

C -4.406936 -0.709982 2.366796

C -5.611409 -0.737557 3.093870

C -6.528073 0.342860 3.124866

H -5.860074 -1.656703 3.627693

C -6.230621 1.501469 2.394578

C -4.154151 0.464281 1.628379

C -5.042726 1.569563 1.642831

H -6.914860 2.349580 2.392028

C -4.447776 2.585776 0.792806

C -7.821796 0.198681 3.951938

C -8.716178 1.449278 3.860379

H -9.035298 1.649235 2.826434

H -8.207510 2.346375 4.244067

H -9.621852 1.295761 4.465837

C -7.458998 -0.026562 5.439720

H -6.880830 0.822565 5.834718

H -6.860945 -0.938716 5.578312

H -8.374560 -0.128160 6.042933

C -8.636245 -1.013115 3.438993

H -9.562490 -1.121645 4.024481

H -8.071388 -1.952189 3.527334

H -8.913316 -0.880560 2.382041

N -3.068817 0.757557 0.821365

C	-3.226931	2.042394	0.314597
H	-2.256228	0.153058	0.726061
C	-4.835895	3.886479	0.419155
C	-4.016094	4.634157	-0.431883
H	-5.770634	4.296047	0.799684
C	-2.809990	4.060941	-0.912058
C	-2.393082	2.771157	-0.558452
H	-2.164893	4.631317	-1.575592
C	-4.375230	6.066767	-0.876045
C	-5.711190	6.545197	-0.276838
H	-5.683414	6.562012	0.823061
H	-6.552291	5.909327	-0.591938
H	-5.920274	7.569015	-0.620763
C	-4.493547	6.118610	-2.418272
H	-5.283419	5.439353	-2.773403
H	-3.552122	5.831677	-2.908514
H	-4.746566	7.139102	-2.745919
C	-3.265107	7.043183	-0.418799
H	-3.506455	8.069499	-0.737205
H	-2.288486	6.777983	-0.848560
H	-3.166593	7.038604	0.677372
N	-1.223426	2.146090	-1.021974
C	-0.091860	2.746859	-1.556908
H	-1.134863	1.133345	-0.858573
O	0.029866	3.961728	-1.762783
H	2.496293	5.245107	-4.854544
H	8.376476	-1.566150	-4.117201
H	4.186930	3.778638	-6.124892
H	7.727241	-3.223264	-4.152081
C	8.447389	-2.559067	-3.650353
C	3.334225	5.628489	-4.252931

H	3.731656	6.518481	-4.762983
H	9.460438	-2.948254	-3.837697
C	4.981400	4.233075	-5.513341
H	5.823066	3.527022	-5.469498
H	2.939998	5.952228	-3.277980
C	4.456600	4.584528	-4.100766
N	-3.492886	-1.766963	2.255632
N	3.424198	-2.961665	-0.373082
C	4.448383	-2.232423	-0.993991
C	5.762675	-2.699210	-1.213904
C	3.978177	3.298507	-3.393741
C	4.140403	-0.960651	-1.513193
C	2.646087	3.159860	-2.939322
C	2.190706	2.003726	-2.283582
C	3.117253	0.964174	-2.083069
H	5.331378	5.142392	-6.026651
N	2.940994	-0.269881	-1.465114
C	4.881034	2.242626	-3.195677
C	4.455867	1.073534	-2.546424
C	5.116397	-0.168118	-2.178323
C	6.749502	-1.946888	-1.886753
N	0.877992	1.796038	-1.830145
C	6.413779	-0.666852	-2.362042
C	8.171109	-2.496044	-2.128756
H	6.000741	-3.707218	-0.875467
H	2.093870	-0.607622	-1.002596
H	9.146645	-0.536076	-1.871896
H	1.930745	3.963148	-3.084883
H	5.913763	2.322276	-3.539245
H	7.153893	-0.060300	-2.887487
C	9.204653	-1.555243	-1.464197

H 10.225628 -1.930171 -1.636641

H 8.212853 -3.929440 -0.458248

C 8.365808 -3.908682 -1.547906

C 5.601591 5.225600 -3.279452

H 5.957748 6.143324 -3.773383

H 9.394297 -4.245351 -1.745879

H 9.040417 -1.497546 -0.377460

H 5.256503 5.492706 -2.269088

H 6.457171 4.542839 -3.177456

H 7.683119 -4.639899 -2.006970

H 0.635830 0.836434 -1.537516

C -3.358401 -2.594604 3.250249

C 3.734834 -3.825571 0.549330

C 2.809843 -4.739582 1.141340

H 4.767115 -3.923008 0.927484

C -2.586500 -3.796378 3.199745

H -3.863084 -2.424964 4.217464

N 1.457756 -4.832367 0.836960

C 3.112806 -5.800921 2.008689

C 1.929874 -6.537283 2.211608

C 0.909073 -5.918250 1.476642

N -1.878357 -4.257760 2.096469

C -1.376330 -5.510227 2.355925

C -2.517325 -4.795662 4.183633

C -1.767553 -5.863686 3.655455

H -2.999007 -4.747766 5.157208

H 4.100880 -6.020418 2.405686

H 1.821880 -7.433581 2.813826

H -1.543105 -6.802640 4.151374

H 0.933200 -4.121881 0.309613

H -1.663357 -3.688635 1.264797

C -0.556179 -6.312292 1.352942

C -0.702762 -7.815862 1.675966

H -0.361203 -8.063706 2.688915

H -0.113604 -8.407597 0.961966

H -1.757182 -8.111505 1.588760

C -1.067415 -6.082448 -0.088261

H -0.948325 -5.039990 -0.412340

H -2.132094 -6.348760 -0.152449

H -0.509232 -6.723186 -0.785577

C -2.284992 -1.181707 -4.319334

C -3.188333 -2.248372 -4.396650

C -1.489366 -1.018678 -3.181607

C -1.568533 -1.928394 -2.113655

C -2.474373 -2.998765 -2.205621

C -3.284085 -3.154992 -3.333585

H -2.202560 -0.473303 -5.145916

H -0.789220 -0.184354 -3.126445

H -2.542598 -3.704226 -1.377658

H -3.990588 -3.985756 -3.385585

H -3.815711 -2.372388 -5.281422

C -0.699593 -1.766521 -0.879106

O -0.561447 -2.761612 -0.108056

O -0.157886 -0.617606 -0.677264

3.3.22 CzU-DPM lactate complex

136 -1

C -4.367708 -0.631755 2.588736

C -5.510029 -0.588929 3.409986

C -6.368994 0.534245 3.497282

H -5.759951 -1.487978 3.976565

C -6.077629 1.664265 2.721938

C -4.114190 0.517968 1.807761

C -4.954485 1.661710 1.874642

H -6.719797 2.544096 2.755889

C -4.398424 2.632262 0.951228

C -7.598580 0.463586 4.425403

C -8.418316 1.767327 4.408465

H -8.814467 1.989411 3.406266

H -7.822216 2.629869 4.742907

H -9.275504 1.669428 5.091349

C -7.136093 0.205575 5.879591

H -6.481508 1.017116 6.232256

H -6.582680 -0.740112 5.969269

H -8.007180 0.150997 6.551221

C -8.523194 -0.692868 3.974772

H -9.403195 -0.754307 4.633809

H -8.007864 -1.663399 4.009818

H -8.877422 -0.532629 2.944967

N -3.084774 0.751343 0.913978

C -3.246641 2.024505 0.380158

H -2.347661 0.074837 0.658724

C -4.769516 3.940119 0.587797

C -4.005898 4.638082 -0.353241

H -5.648458 4.393878 1.044350

C -2.871769 4.004927 -0.922475

C -2.464269 2.710572 -0.574604

H -2.271057 4.539754 -1.654618

C -4.354023 6.071603 -0.802655

C -5.606607 6.617112 -0.091124

H -5.470914 6.661393 0.999975

H -6.496774 6.006119 -0.303863

H -5.811703 7.638993 -0.443586

C -4.621316 6.087756 -2.327029

H -5.467574 5.432040 -2.582756

H -3.744138 5.749033 -2.897189

H -4.866168 7.108631 -2.660015

C -3.170079 7.016043 -0.485236

H -3.404409 8.042582 -0.808346

H -2.250804 6.701914 -0.999923

H -2.964062 7.035702 0.595817

N -1.351491 2.062952 -1.145588

C -0.183123 2.686755 -1.567644

H -1.289271 1.035874 -1.023927

O 0.046900 3.899708 -1.458827

H 2.528890 5.349563 -4.860500

H 8.424675 -1.430694 -3.821840

H 4.352861 3.954398 -6.016915

H 7.804647 -3.094572 -3.947324

C 8.471079 -2.433385 -3.372818

C 3.299734 5.723661 -4.169891

H 3.724711 6.638417 -4.608634

H 9.501735 -2.805376 -3.483828

C 5.080341 4.399203 -5.320914

H 5.927472 3.704917 -5.224592

H 2.810742 6.004381 -3.224720

C 4.423665 4.693147 -3.951035

N -3.525129 -1.741481 2.428484

N 3.201015 -2.954512 -0.495564

C 4.263546 -2.212924 -1.041401

C 5.595924 -2.662346 -1.173547

C 3.906995 3.376842 -3.332725

C 3.987077 -0.932477 -1.557367

C 2.541546 3.194587 -3.012641

C 2.053603 2.011440 -2.436819

C 2.980003 0.986988 -2.180911

H 5.458518 5.331101 -5.769590

N 2.784402 -0.248347 -1.578628

C 4.809133 2.328766 -3.086756

C 4.353785 1.129239 -2.520152

C 5.002205 -0.111858 -2.123839

C 6.625500 -1.881651 -1.742301

N 0.697923 1.776482 -2.124184

C 6.316588 -0.591382 -2.208855

C 8.069165 -2.409538 -1.878357

H 5.821526 -3.675792 -0.843020

H 1.889080 -0.658089 -1.329626

H 8.996101 -0.445764 -1.497914

H 1.824111 3.987480 -3.204801

H 5.867069 2.440522 -3.331109

H 7.091052 0.035895 -2.654086

C 9.031965 -1.473286 -1.109087

H 10.068180 -1.833768 -1.203265

H 7.991810 -3.880989 -0.242811

C 8.234053 -3.833063 -1.315202

C 5.477400 5.323119 -3.008336

H 5.858760 6.263002 -3.437274

H 9.279906 -4.153120 -1.434525

H 8.776472 -1.442019 -0.039061

H 5.038132 5.549566 -2.024762

H 6.333321 4.651133 -2.852064

H 7.601562 -4.561162 -1.845339

H 0.359521 0.807882 -2.237499

C -3.376377 -2.577296 3.414003

C	3.472182	-3.850087	0.410594
C	2.546542	-4.776363	0.984587
H	4.495319	-3.966636	0.808213
C	-2.670648	-3.817255	3.314331
H	-3.814058	-2.386257	4.409488
N	1.185623	-4.886541	0.720319
C	2.884269	-5.829536	1.851444
C	1.716756	-6.573742	2.098720
C	0.667102	-5.968297	1.392893
N	-2.017047	-4.280228	2.179653
C	-1.568623	-5.561590	2.392313
C	-2.626089	-4.845210	4.269920
C	-1.945590	-5.934053	3.691241
H	-3.079571	-4.802071	5.257207
H	3.885855	-6.033814	2.222135
H	1.635785	-7.463533	2.714588
H	-1.755800	-6.896758	4.155094
H	0.621576	-4.187661	0.211230
H	-1.780027	-3.686801	1.364891
C	-0.802816	-6.368560	1.349851
C	-0.921203	-7.870352	1.692181
H	-0.521430	-8.108789	2.685938
H	-0.370035	-8.464202	0.950260
H	-1.976835	-8.173344	1.666717
C	-1.401017	-6.159376	-0.061866
H	-1.360205	-5.111327	-0.384987
H	-2.451977	-6.481657	-0.066905
H	-0.849122	-6.770205	-0.790638
O	-0.960638	-0.678527	-0.347516
H	-1.752267	-2.222251	-2.668905
H	-0.159654	-0.955527	-3.856038

C -0.830891 -1.863939 -0.784403

H 0.214160 -3.305928 -3.825377

C -0.715208 -2.062744 -2.315420

O -0.216960 -0.830379 -2.891036

C 0.147368 -3.251501 -2.728249

O -0.826344 -2.914804 -0.073246

H -0.299090 -4.188867 -2.373346

H 1.160238 -3.165910 -2.308510

3.3.23 CzU-DPM formate complex

129 -1

C -4.369157 -0.693113 2.514893

C -5.566061 -0.712821 3.254759

C -6.454302 0.388705 3.330157

H -5.834716 -1.641482 3.761598

C -6.137644 1.561330 2.630611

C -4.095909 0.498084 1.811503

C -4.956756 1.623553 1.867991

H -6.801568 2.424864 2.661263

C -4.349768 2.647884 1.035261

C -7.744280 0.248844 4.163885

C -8.591319 1.535045 4.149903

H -8.919977 1.798466 3.133427

H -8.041849 2.391929 4.567849

H -9.492268 1.385697 4.763464

C -7.378374 -0.069835 5.633496

H -6.768317 0.736150 6.069017

H -6.811802 -1.008137 5.718235

H -8.292746 -0.172417 6.238244

C -8.607268 -0.902558 3.594252

H	-9.528605	-1.014726	4.186828
H	-8.072995	-1.863237	3.618483
H	-8.893842	-0.698562	2.551329
N	-3.019643	0.784634	0.989050
C	-3.150523	2.088611	0.523482
H	-2.197762	0.191522	0.917051
C	-4.713968	3.965195	0.698011
C	-3.892009	4.711413	-0.152321
H	-5.632079	4.387777	1.103904
C	-2.711087	4.119986	-0.671628
C	-2.320677	2.810989	-0.359099
H	-2.067307	4.688583	-1.337790
C	-4.222711	6.163109	-0.554732
C	-5.532280	6.661403	0.085141
H	-5.479888	6.652164	1.184233
H	-6.396385	6.054759	-0.225122
H	-5.722189	7.697891	-0.230892
C	-4.372638	6.255609	-2.092307
H	-5.187660	5.605997	-2.446267
H	-3.449855	5.956439	-2.609868
H	-4.605525	7.290003	-2.389794
C	-3.077517	7.098938	-0.099227
H	-3.299771	8.139041	-0.385073
H	-2.118427	6.820824	-0.559208
H	-2.953391	7.062910	0.993781
N	-1.185169	2.161672	-0.870720
C	-0.097107	2.725929	-1.521998
H	-1.095177	1.152477	-0.688663
O	0.051644	3.938038	-1.724782
H	2.405097	5.002367	-5.131438
H	8.450976	-1.555280	-3.799855

H	4.141028	3.483654	-6.265296
H	7.858433	-3.233318	-3.751201
C	8.540422	-2.514947	-3.271188
C	3.223465	5.444617	-4.543602
H	3.610924	6.306668	-5.106728
H	9.571034	-2.879404	-3.404987
C	4.917361	3.998288	-5.678763
H	5.772590	3.315523	-5.572616
H	2.804475	5.824172	-3.599707
C	4.365386	4.439219	-4.301992
N	-3.482240	-1.769563	2.356086
N	3.425991	-2.910283	-0.162690
C	4.449919	-2.165717	-0.763645
C	5.784804	-2.600648	-0.919045
C	3.902728	3.196744	-3.511600
C	4.122061	-0.925648	-1.347593
C	2.563642	3.051439	-3.081516
C	2.121803	1.934041	-2.354737
C	3.063784	0.930020	-2.064377
H	5.255530	4.875247	-6.252876
N	2.904356	-0.264315	-1.367903
C	4.825251	2.181604	-3.215536
C	4.411970	1.047633	-2.500113
C	5.095309	-0.146733	-2.033917
C	6.771277	-1.853830	-1.597400
N	0.797500	1.743038	-1.919041
C	6.411725	-0.613604	-2.153271
C	8.215738	-2.369950	-1.764792
H	6.040432	-3.584759	-0.527354
H	2.044481	-0.598040	-0.917880
H	9.122270	-0.367378	-1.598974

H	1.831422	3.822472	-3.300967
H	5.865000	2.265313	-3.536493
H	7.147399	-0.015224	-2.694128
C	9.199248	-1.358151	-1.129067
H	10.236078	-1.709255	-1.249419
H	8.247087	-3.699089	-0.010523
C	8.436022	-3.738268	-1.093812
C	5.484376	5.162625	-3.514709
H	5.829163	6.049300	-4.069825
H	9.480800	-4.051156	-1.238538
H	9.000484	-1.241491	-0.052762
H	5.118970	5.495465	-2.531420
H	6.352168	4.507911	-3.351631
H	7.793044	-4.518286	-1.529173
H	0.552633	0.790651	-1.615268
C	-3.383233	-2.652374	3.307863
C	3.720613	-3.768745	0.770172
C	2.789217	-4.707915	1.312586
H	4.739258	-3.848439	1.187624
C	-2.640944	-3.869831	3.215624
H	-3.898806	-2.518664	4.274683
N	1.452563	-4.806547	0.949877
C	3.072278	-5.792758	2.157756
C	1.891403	-6.549269	2.287999
C	0.891987	-5.917102	1.533385
N	-1.902858	-4.297243	2.118371
C	-1.427975	-5.566050	2.342002
C	-2.623726	-4.912911	4.156747
C	-1.873279	-5.970269	3.609486
H	-3.137713	-4.897527	5.114760
H	4.046889	-6.015749	2.585037

H 1.772150 -7.467015 2.854903

H -1.679809 -6.932702 4.072491

H 0.939395 -4.064275 0.449083

H -1.643429 -3.704715 1.313657

C -0.564416 -6.324612 1.342122

C -0.700100 -7.839794 1.611146

H -0.386084 -8.116210 2.625598

H -0.081382 -8.400375 0.896944

H -1.747071 -8.146266 1.481438

C -1.030388 -6.058302 -0.109913

H -0.972186 -4.997675 -0.386390

H -2.072694 -6.387687 -0.228774

H -0.405297 -6.632917 -0.808064

O -0.450201 -2.772814 0.065771

O -0.067979 -0.607987 -0.495709

C -0.770184 -1.672922 -0.461053

H -1.780759 -1.615655 -0.935540

3.3.24 CzU-DPM sorbate complex

140 -1

C -4.454806 -0.718885 2.353390

C -5.644798 -0.730089 3.104925

C -6.534994 0.369891 3.174029

H -5.905366 -1.651652 3.628680

C -6.226532 1.532878 2.455540

C -4.191292 0.460464 1.625690

C -5.054729 1.585079 1.678455

H -6.890360 2.396673 2.481418

C -4.460894 2.600061 0.826843

C -7.816594 0.239229 4.021902

C -8.665226 1.524270 3.999617

H -9.003811 1.774327 2.983008

H -8.112666 2.386991 4.401245

H -9.560158 1.381982 4.623570

C -7.436761 -0.060588 5.491925

H -6.823369 0.751301 5.911527

H -6.868585 -0.997306 5.583250

H -8.345356 -0.156338 6.106451

C -8.683459 -0.920268 3.474953

H -9.599063 -1.026180 4.077458

H -8.147446 -1.879771 3.506124

H -8.980047 -0.729762 2.432250

N -3.123151 0.740945 0.790863

C -3.267425 2.036537 0.306079

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H -5.854030 7.639906 -0.459021

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H -3.607696 5.882468 -2.851576

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H 4.047485 3.480799 -6.404442

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H 5.681356 3.304907 -5.719182

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C 6.678073 -1.906645 -1.786668

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H 1.750541 3.802864 -3.424113

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H 8.152304 -3.768459 -0.216994

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N	-1.980070	-4.305323	1.990573
C	-1.518132	-5.580412	2.207336
C	-2.711957	-4.927477	4.023729
C	-1.970679	-5.988843	3.470672
H	-3.231014	-4.914834	4.979049
H	3.957321	-6.051205	2.407032
H	1.679610	-7.493939	2.701459
H	-1.789588	-6.957081	3.926603
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C	-0.808512	-7.857719	1.466280
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H	-0.197461	-8.419560	0.746497
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H	-1.061499	-5.002425	-0.513121
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C	-2.909445	-0.851139	-5.228603
C	-3.731510	-1.180641	-6.430781
C	-1.866935	-1.333364	-3.045806
C	-1.606214	-2.157674	-2.002245
C	-0.760792	-1.800380	-0.828884
O	-0.523765	-2.723203	0.016863
H	-4.134161	-2.201824	-6.386195
H	-3.134388	-1.078302	-7.352452

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H -3.099523 -2.698463 -4.211091

H -2.471159 0.153642 -5.196588

H -1.440942 -0.323885 -3.033658

H -2.012553 -3.172820 -1.998660

O -0.311082 -0.598040 -0.706912

3.3.25 CzU-BA free receptor

146 0

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C 2.415850 3.464590 -2.176255

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H 2.229381 4.187311 -4.246444

H 1.247892 5.100932 -3.070119

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H 1.967982 2.849151 -0.105407

H 0.585913 2.747760 -1.218672

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C	6.959769	7.580043	-1.771977
H	7.924166	6.364411	-0.370654
C	5.432747	8.331274	-3.552628
C	6.273935	9.418237	-3.817025
H	4.512103	8.187605	-4.117235
C	7.460508	9.544863	-3.059572
C	7.834271	8.651206	-2.045170
H	8.137742	10.376840	-3.263960
C	5.961543	10.469722	-4.899414
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C	12.607604	-3.877063	-0.305493
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H	12.999738	-4.314230	1.815938
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C	14.078050	-3.482874	-0.585142
H	14.501825	-2.923392	0.262606
H	14.169903	-2.858329	-1.485194
H	14.688651	-4.386068	-0.739031
C	12.052600	-4.663919	-1.516858
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C	11.006920	1.768610	-4.112622
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C	10.812205	4.104328	-5.738232
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H	11.474851	5.179802	-3.983203
C	10.128388	2.704463	-7.653441
C	10.703217	5.246728	-6.579262
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H	10.926334	6.232921	-6.166576
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H	10.012557	10.409444	0.782281
C	12.117666	10.536653	1.282421
C	13.505024	8.717985	0.353015
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C	12.011546	11.722250	2.060084
H	11.033614	12.197167	2.166545
H	14.488620	8.264785	0.229037
C	14.525581	10.484185	1.779566
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3.3.26 CzU-BA acetate complex

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H	7.541211	10.886320	-2.599586
C	5.005339	11.665379	-3.226678
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H	2.927940	11.648419	-2.500404
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H	6.110715	-3.457302	5.170524
C	4.967903	-2.025851	3.168973
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N	9.946339	0.882678	0.345971
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H	10.037785	1.893045	0.140425
C	11.668989	-2.048135	1.607527
C	12.911876	-2.018547	0.965908
H	11.419084	-2.843015	2.309611
C	13.179052	-0.987074	0.032515
C	12.252112	0.021258	-0.271162
H	14.127733	-0.968607	-0.496776
C	14.000499	-3.079949	1.223124
C	13.555657	-4.130860	2.257773
H	12.666493	-4.685854	1.922215
H	13.330062	-3.674788	3.233295
H	14.365518	-4.859794	2.408849

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H 15.073849 -1.865509 2.703644

H 15.669351 -1.651467 1.040057

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H 13.444088 -4.324370 -0.497902

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H 11.576698 1.445594 -1.642180

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N 7.313179 2.170438 0.877291

H 8.097174 2.751260 0.512910

C 13.369519 1.967286 -3.346441

C 14.440907 1.895282 -4.226708

C 12.193072 2.678188 -3.778766

C 12.120855 3.221364 -5.049534

C 14.409691 2.456258 -5.525953

C 13.213331 3.126826 -5.952401

H 15.332951 1.361080 -3.895648

H 11.227041 3.754350 -5.369747

C 15.513944 2.364475 -6.419445

C 13.168319 3.681730 -7.261536

C 15.440678 2.914609 -7.685138

H 16.419465 1.851935 -6.087383

C 14.258264 3.576439 -8.106654

H 12.260954 4.192182 -7.591721

H 16.290588 2.841093 -8.365469

H 14.211082 4.006185 -9.108966

O 11.179677 2.787394 -2.855217

C 9.948025 3.483859 -3.190144

C 10.098608 4.982560 -3.335059

H 9.315398 3.272567 -2.316858

H 9.494053 3.037651 -4.086834

C 11.065236 9.100772 -1.070568

C 11.945190 9.986610 -0.464410

C 11.568334 7.803350 -1.446617

H 11.561793 10.970654 -0.189771

C 13.295188 9.665035 -0.187233

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C 15.493240 10.228552 0.698425

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O 10.683807 6.965036 -2.087788

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H 15.493128 7.030659 -0.538204

H 16.170183 10.937773 1.177464

H 17.001082 8.667696 0.553528

H 11.232995 5.037456 -1.499736

H 12.086502 5.671704 -2.935385

C 9.324436 5.671532 -4.182157

H 8.617588 5.160995 -4.839148

H 9.358787 6.759944 -4.233456

C 10.811252 5.193676 1.473137

O 9.565257 3.645070 0.109405

C 9.551071 4.754049 0.742187

O 8.518615 5.496744 0.831592

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H 11.702598 4.690773 1.079861

H 10.706345 4.919619 2.534800

3.3.27 CzU-BA benzoate complex

160 -1

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C 2.633419 5.255373 -0.779815

H 3.416567 3.463367 0.175211

C 2.964325 6.507344 -1.304094

C 5.316975 6.102803 -0.733835

C 4.305617 6.933362 -1.278936

H 2.202727 7.158342 -1.731931

C 4.968311 8.139410 -1.737249

C 1.186369 4.722836 -0.764514

C 0.193009 5.716865 -1.394662

H 0.433174 5.922913 -2.448717

H 0.172318 6.673889 -0.852240

H -0.821026 5.291512 -1.360810

C 0.746091 4.462711 0.696280

H 0.780232 5.390979 1.286364

H 1.392126 3.722127 1.189316

H -0.285857 4.078889 0.719899

C 1.111680 3.397516 -1.560389

H 0.082603 3.005272 -1.549985

H 1.769440 2.628245 -1.131138

H 1.408576 3.553184 -2.608684

N 6.553774 6.734346 -0.861360

C 6.351198 7.975788 -1.448293

H 7.400615 6.428808 -0.358421

C 4.500548 9.319895 -2.339206

C 5.401365 10.339749 -2.664703

H 3.435761 9.428797 -2.543811

C 6.776878 10.147248 -2.387260

C 7.277398 8.983684 -1.790762

H 7.491084 10.926271 -2.642617

C 4.956484 11.661717 -3.320719

C 3.436655 11.707469 -3.564814

H 2.868562 11.624358 -2.626417

H 3.106605 10.904908 -4.241515

H 3.170635 12.667419 -4.031626

C 5.668913 11.831254 -4.684068

H 5.412638 11.005943 -5.365489

H 6.762205 11.854362 -4.572142

H 5.359410 12.775595 -5.159043

C 5.334393 12.846690 -2.399659

H 5.029418 13.798827 -2.861012

H 6.418224 12.890982 -2.219647

H 4.830790 12.761397 -1.424891

N 8.658077 8.759081 -1.563515

C 9.613097 9.709689 -1.304681

H 9.007787 7.801240 -1.665102

O 9.335971 10.914219 -1.172149

N 6.059382 4.046597 0.307571

C 6.018073 2.716389 0.699198

H 6.973011 4.530137 0.426005

O 4.979269 2.047573 0.817740

C 7.628463 0.991208 1.527664

C 6.791234 0.280309 2.398552

C 7.172315 -0.940295 3.010463

H	5.803118	0.692280	2.591837
C	8.444269	-1.462285	2.751851
C	8.904401	0.439919	1.275740
C	9.314104	-0.768237	1.891111
H	8.770985	-2.396598	3.206853
C	10.661721	-1.033367	1.417588
C	6.167583	-1.638733	3.948386
C	6.721673	-2.958431	4.516988
H	7.632657	-2.797320	5.112992
H	6.952862	-3.682023	3.720925
H	5.969432	-3.416515	5.176300
C	4.867776	-1.957454	3.171782
H	5.072740	-2.628994	2.324221
H	4.395279	-1.046695	2.776501
H	4.141401	-2.453559	3.834210
C	5.833616	-0.704524	5.136206
H	5.111879	-1.191080	5.811129
H	5.391535	0.242669	4.796127
H	6.738987	-0.469283	5.716411
N	9.911413	0.899196	0.417974
C	10.989062	0.020279	0.525596
H	10.016768	1.907832	0.223412
C	11.587155	-2.057888	1.681329
C	12.837175	-2.038774	1.053107
H	11.320961	-2.853928	2.376010
C	13.126935	-1.004116	0.129940
C	12.215067	0.016932	-0.176161
H	14.081785	-0.992354	-0.388452
C	13.909810	-3.115465	1.313806
C	13.442923	-4.165911	2.339093
H	12.550069	-4.708283	1.992903

H	13.214272	-3.712025	3.314943
H	14.242452	-4.905441	2.493510
C	15.191352	-2.442907	1.861133
H	14.986663	-1.922916	2.809451
H	15.598977	-1.708089	1.152103
H	15.968295	-3.200636	2.046446
C	14.244167	-3.847849	-0.008001
H	15.012284	-4.616548	0.168892
H	14.629515	-3.156098	-0.770697
H	13.351277	-4.343415	-0.418354
N	12.406142	0.974042	-1.198637
C	13.548738	1.221491	-1.920547
H	11.570952	1.460723	-1.541474
O	14.661560	0.779855	-1.586595
N	7.293196	2.219761	0.930151
H	8.090079	2.803382	0.603062
C	13.386416	1.992069	-3.211957
C	14.462368	1.917608	-4.086257
C	12.221439	2.722992	-3.642064
C	12.162339	3.279876	-4.907461
C	14.445587	2.494358	-5.378908
C	13.259055	3.182429	-5.805060
H	15.345531	1.367955	-3.756676
H	11.276807	3.827421	-5.226274
C	15.554248	2.400431	-6.266695
C	13.228135	3.752191	-7.108198
C	15.494798	2.965514	-7.526531
H	16.452075	1.874395	-5.934872
C	14.322183	3.644703	-7.947750
H	12.328312	4.275894	-7.438239
H	16.348080	2.890477	-8.202446

H 14.285862 4.086258 -8.945364

O 11.206707 2.838085 -2.720511

C 9.969664 3.520387 -3.064523

C 10.100541 5.019802 -3.219337

H 9.335294 3.306681 -2.193008

H 9.524878 3.063275 -3.960395

C 11.036393 9.229345 -1.138541

C 11.920377 10.166002 -0.620639

C 11.550749 7.919190 -1.449022

H 11.528123 11.159171 -0.395463

C 13.285173 9.886526 -0.376169

C 12.877017 7.607478 -1.204818

C 13.773198 8.568366 -0.667210

C 14.178332 10.860349 0.152691

H 13.798272 11.860562 0.372481

H 13.263276 6.611297 -1.413253

C 15.141934 8.274060 -0.417877

C 15.504054 10.545323 0.382398

C 11.101307 5.688620 -2.310643

O 10.661843 7.031199 -2.012496

C 15.986171 9.241771 0.094587

H 15.518123 7.272722 -0.638100

H 16.185178 11.296396 0.786030

H 17.035175 9.003671 0.280836

H 11.221808 5.124938 -1.372531

H 12.079367 5.727394 -2.818847

C 9.318451 5.688048 -4.075925

H 8.622811 5.159749 -4.730775

H 9.335787 6.776212 -4.137644

C 11.803018 7.048245 2.938626

C 10.687159 6.578023 2.241985

H 9.766339 7.160812 2.203765

H 11.759573 8.011370 3.450405

O 8.455376 5.531398 0.871323

C 12.977082 6.285964 2.979576

C 10.732113 5.340372 1.577855

C 9.515183 4.823610 0.845968

H 13.849292 6.653865 3.522992

C 13.031440 5.051638 2.320183

C 11.914885 4.583172 1.622839

O 9.595987 3.695037 0.252927

H 13.945420 4.455556 2.350752

H 11.945236 3.623180 1.106707

3.3.28 CzU-BA lactate complex

157 -1

C 5.025331 4.811980 -0.175059

C 3.676202 4.431838 -0.194297

C 2.648673 5.262964 -0.711030

H 3.432268 3.450817 0.205245

C 2.981117 6.521120 -1.219688

C 5.337568 6.091515 -0.690246

C 4.325189 6.938155 -1.207259

H 2.217804 7.184036 -1.625486

C 4.990925 8.147200 -1.654023

C 1.198330 4.740304 -0.683623

C 0.203194 5.751999 -1.282128

H 0.429021 5.973996 -2.336095

H 0.197456 6.699808 -0.723432

H -0.813262 5.333233 -1.240157

C 0.777709 4.458396 0.778912

H	0.827261	5.376165	1.384090
H	1.425238	3.704829	1.249912
H	-0.256532	4.081593	0.811013
C	1.102944	3.429419	-1.500830
H	0.071298	3.044394	-1.482390
H	1.760980	2.648218	-1.094171
H	1.386048	3.600908	-2.550464
N	6.578574	6.713422	-0.827182
C	6.375805	7.967420	-1.388304
H	7.426595	6.405637	-0.330231
C	4.525844	9.343553	-2.225840
C	5.430848	10.362870	-2.542501
H	3.459421	9.465766	-2.413734
C	6.808442	10.153083	-2.289001
C	7.305331	8.972841	-1.724141
H	7.526408	10.930429	-2.539731
C	4.987629	11.702085	-3.163628
C	3.464940	11.765018	-3.385043
H	2.909261	11.665932	-2.440770
H	3.118996	10.980111	-4.074340
H	3.200279	12.737038	-3.826912
C	5.682187	11.895444	-4.532978
H	5.409348	11.087480	-5.228676
H	6.777147	11.907214	-4.436528
H	5.373869	12.852494	-4.982460
C	5.388329	12.863632	-2.222531
H	5.084105	13.827814	-2.658540
H	6.474956	12.895854	-2.057538
H	4.898399	12.760874	-1.242461
N	8.686753	8.727649	-1.523203
C	9.649842	9.657998	-1.227483

H 9.028036 7.773296 -1.674122

O 9.384154 10.856551 -1.036146

N 6.082144 4.016720 0.306569

C 6.041023 2.682370 0.688709

H 6.990676 4.495162 0.411291

O 4.999731 2.024962 0.830487

C 7.665877 0.947002 1.480622

C 6.833156 0.222019 2.343531

C 7.229892 -0.994410 2.953774

H 5.837240 0.617488 2.530149

C 8.510421 -1.497278 2.699355

C 8.951553 0.417535 1.234630

C 9.374549 -0.787799 1.845691

H 8.847843 -2.428843 3.152046

C 10.727817 -1.032486 1.376019

C 6.230530 -1.711014 3.883606

C 6.803050 -3.021910 4.454366

H 7.707434 -2.846032 5.056199

H 7.051063 -3.740850 3.659166

H 6.054470 -3.493083 5.108529

C 4.941923 -2.050458 3.097128

H 5.164463 -2.716337 2.249588

H 4.456178 -1.147154 2.700700

H 4.219816 -2.560660 3.753420

C 5.872451 -0.784326 5.070307

H 5.154470 -1.284324 5.739291

H 5.416559 0.155692 4.728600

H 6.769504 -0.534551 5.657261

N 9.955593 0.897113 0.382987

C 11.043410 0.028899 0.490225

H 10.063576 1.912336 0.224620

C	11.666621	-2.045509	1.636899
C	12.917145	-2.006680	1.010248
H	11.410256	-2.848447	2.327291
C	13.192926	-0.967101	0.088274
C	12.266386	0.041288	-0.215715
H	14.146379	-0.943114	-0.432384
C	14.005177	-3.067739	1.271312
C	13.551958	-4.126898	2.293798
H	12.668208	-4.682194	1.944720
H	13.314322	-3.678203	3.269884
H	14.362230	-4.854547	2.448790
C	15.274769	-2.376228	1.822907
H	15.059539	-1.860619	2.771303
H	15.672771	-1.634287	1.115810
H	16.062780	-3.122132	2.009335
C	14.353966	-3.792823	-0.050788
H	15.133043	-4.550114	0.127132
H	14.730971	-3.094355	-0.811490
H	13.469700	-4.301116	-0.464217
N	12.435297	0.997273	-1.242627
C	13.564331	1.251376	-1.982512
H	11.588769	1.468822	-1.578782
O	14.686703	0.825482	-1.659932
N	7.316750	2.171536	0.880500
H	8.104192	2.750214	0.541255
C	13.375222	2.009766	-3.277646
C	14.444542	1.949247	-4.161187
C	12.193025	2.715590	-3.703175
C	12.113608	3.264155	-4.971033
C	14.406179	2.516690	-5.457383
C	13.204055	3.180836	-5.877500

H 15.340578 1.418286 -3.835620

H 11.215393 3.792874 -5.286207

C 15.508499 2.436497 -6.354308

C 13.151477 3.741422 -7.183867

C 15.427856 2.991940 -7.617195

H 16.418387 1.928572 -6.027171

C 14.239773 3.647507 -8.032419

H 12.239593 4.246848 -7.509272

H 16.276301 2.927316 -8.300251

H 14.186878 4.081457 -9.032628

O 11.181254 2.815819 -2.775914

C 9.937371 3.490506 -3.110484

C 10.060964 4.991716 -3.255332

H 9.307601 3.266605 -2.238507

H 9.490812 3.036176 -4.006758

C 11.070392 9.157536 -1.094654

C 11.964913 10.059396 -0.535301

C 11.571194 7.860329 -1.474537

H 11.581725 11.042367 -0.256514

C 13.328743 9.756560 -0.311121

C 12.898241 7.528382 -1.259182

C 13.806247 8.453484 -0.678595

C 14.231552 10.693479 0.265972

H 13.859896 11.682351 0.543306

H 13.280232 6.546934 -1.535250

C 15.174099 8.135427 -0.453051

C 15.555972 10.356277 0.471282

C 11.071614 5.645775 -2.348687

O 10.670099 7.004254 -2.068121

C 16.027605 9.067864 0.108241

H 15.542669 7.146028 -0.732425

H 16.244363 11.078675 0.912823

H 17.075686 8.812715 0.275261

H 11.164328 5.089056 -1.403117

H 12.053273 5.646978 -2.851042

C 9.271079 5.667152 -4.098599

H 8.569538 5.144166 -4.751359

H 9.288438 6.755730 -4.152160

H 10.415471 4.080136 2.826470

C 10.516993 4.957063 2.158315

O 9.632902 3.715780 0.270121

C 9.495840 4.727979 1.024135

O 10.172250 6.141826 2.892642

O 8.531339 5.559409 0.960060

H 9.342012 6.444327 2.452887

C 11.959919 5.033382 1.664193

H 12.229708 4.118746 1.119495

H 12.641972 5.141988 2.518825

H 12.095949 5.899350 1.000615

3.3.29 CzU-BA formate complex

150 -1

C 5.041756 4.833825 -0.117260

C 3.694745 4.444299 -0.123527

C 2.661019 5.248699 -0.670386

H 3.458143 3.474681 0.307343

C 2.982561 6.491144 -1.223430

C 5.340787 6.098502 -0.677091

C 4.323115 6.920311 -1.224960

H 2.213516 7.131923 -1.653300

C 4.982351 8.118224 -1.713282

C	1.214949	4.715026	-0.625782
C	0.211678	5.696486	-1.259938
H	0.436432	5.883177	-2.320998
H	0.197602	6.663314	-0.734914
H	-0.801285	5.270989	-1.203842
C	0.794779	4.480461	0.845231
H	0.835057	5.419056	1.418341
H	1.448461	3.749684	1.342798
H	-0.236093	4.095587	0.889286
C	1.131534	3.375700	-1.396868
H	0.103249	2.982371	-1.365734
H	1.796049	2.614946	-0.962870
H	1.414123	3.513148	-2.451579
N	6.575859	6.724506	-0.833473
C	6.366929	7.954510	-1.438086
H	7.426261	6.442744	-0.324225
C	4.518809	9.295296	-2.326312
C	5.423783	10.306234	-2.671197
H	3.453355	9.410655	-2.523683
C	6.801927	10.110115	-2.405038
C	7.296669	8.949695	-1.800378
H	7.519180	10.881096	-2.677250
C	4.980141	11.623152	-3.338467
C	3.458266	11.675910	-3.567767
H	2.899051	11.607376	-2.622902
H	3.116269	10.867899	-4.231956
H	3.193859	12.632134	-4.043048
C	5.679653	11.771682	-4.710959
H	5.411325	10.939831	-5.379696
H	6.774140	11.789278	-4.610512
H	5.371194	12.712180	-5.194159

C	5.374733	12.816647	-2.435613
H	5.070659	13.764974	-2.905295
H	6.460586	12.856825	-2.267303
H	4.880742	12.746017	-1.454810
N	8.674884	8.707164	-1.573983
C	9.633625	9.635722	-1.259865
H	9.011758	7.747310	-1.693401
O	9.374440	10.842100	-1.116535
N	6.104804	4.065268	0.392799
C	6.085964	2.727349	0.761082
H	7.014178	4.554765	0.501654
O	5.057176	2.042753	0.870630
C	7.716821	1.006037	1.549627
C	6.904075	0.298789	2.446125
C	7.291040	-0.930709	3.035254
H	5.929934	0.722735	2.680674
C	8.547110	-1.464294	2.727608
C	8.975488	0.441730	1.245289
C	9.393193	-0.774172	1.840950
H	8.880101	-2.404913	3.164697
C	10.719574	-1.053744	1.319368
C	6.313718	-1.623586	4.005712
C	6.869147	-2.957993	4.537567
H	7.804940	-2.818013	5.099491
H	7.058459	-3.675428	3.724931
H	6.135966	-3.412486	5.220505
C	4.978436	-1.913456	3.279790
H	5.137208	-2.579651	2.418078
H	4.505293	-0.991442	2.912595
H	4.271618	-2.404405	3.966812
C	6.043786	-0.696915	5.215472

H	5.342314	-1.178716	5.914697
H	5.603885	0.260915	4.903061
H	6.976012	-0.482198	5.760031
N	9.958048	0.889750	0.353850
C	11.029302	-0.000661	0.420248
H	10.065547	1.889490	0.136549
C	11.640933	-2.089336	1.550693
C	12.870279	-2.082761	0.882788
H	11.387674	-2.884313	2.251409
C	13.142126	-1.047297	-0.044422
C	12.233530	-0.014144	-0.317922
H	14.081065	-1.044188	-0.591254
C	13.936942	-3.174019	1.103726
C	13.489347	-4.224101	2.137970
H	12.578776	-4.752779	1.817765
H	13.298426	-3.772808	3.123005
H	14.283562	-4.974967	2.262688
C	15.244135	-2.521258	1.613016
H	15.077570	-2.005077	2.570790
H	15.637770	-1.787174	0.895400
H	16.016928	-3.290033	1.768244
C	14.219355	-3.903231	-0.231813
H	14.982217	-4.683279	-0.083225
H	14.589858	-3.212549	-1.002747
H	13.307461	-4.384668	-0.616322
N	12.409889	0.943884	-1.342903
C	13.549620	1.202130	-2.065596
H	11.569210	1.422119	-1.683047
O	14.667059	0.773798	-1.729983
N	7.369155	2.245293	0.980158
H	8.159495	2.837356	0.652788

C 13.380149 1.966179 -3.359790

C 14.452361 1.889198 -4.238473

C 12.213574 2.695387 -3.786991

C 12.149052 3.249412 -5.053257

C 14.429653 2.461541 -5.532988

C 13.241552 3.148882 -5.955652

H 15.337388 1.341412 -3.910862

H 11.262440 3.795925 -5.370535

C 15.534028 2.364353 -6.425715

C 13.204384 3.714359 -7.260442

C 15.468595 2.925222 -7.687128

H 16.433282 1.839123 -6.096528

C 14.294229 3.603425 -8.104985

H 12.303248 4.237502 -7.587765

H 16.318557 2.847572 -8.366921

H 14.253137 4.041354 -9.104009

O 11.201079 2.810670 -2.861940

C 9.975056 3.514334 -3.198221

C 10.131138 5.013398 -3.340284

H 9.334860 3.297794 -2.331706

H 9.521220 3.073310 -4.097581

C 11.035295 9.117251 -1.029373

C 11.896341 9.998730 -0.391048

C 11.545074 7.816264 -1.384275

H 11.509023 10.985668 -0.132611

C 13.232661 9.668912 -0.061008

C 12.844315 7.457573 -1.066934

C 13.715818 8.360026 -0.400294

C 14.100737 10.583155 0.599639

H 13.725349 11.576535 0.854927

H 13.228106 6.470634 -1.320330

C 15.054046 8.014397 -0.064272

C 15.396934 10.219180 0.911902

C 11.141773 5.661446 -2.426740

O 10.681862 6.981342 -2.057823

C 15.873897 8.925125 0.577264

H 15.425897 7.020147 -0.321190

H 16.058487 10.924571 1.417362

H 16.899121 8.648346 0.829801

H 11.295683 5.055727 -1.520442

H 12.109366 5.748764 -2.949504

C 9.359850 5.702871 -4.189809

H 8.652479 5.193528 -4.847156

H 9.397703 6.791100 -4.243174

O 9.673006 3.717072 0.229507

C 9.610048 4.910874 0.649653

O 8.548628 5.579225 0.840358

H 10.575044 5.421226 0.878670

3.3.30 CzU-BA sorbate complex

161 -1

C 5.061203 4.756726 0.174031

C 3.756705 4.249510 0.093113

C 2.668787 4.992976 -0.437078

H 3.601596 3.229100 0.435224

C 2.891066 6.293524 -0.898075

C 5.254962 6.082184 -0.283020

C 4.186815 6.840173 -0.827549

H 2.081116 6.885195 -1.323867

C 4.761620 8.101309 -1.256857

C 1.279482 4.325930 -0.487154

C	0.206336	5.255147	-1.084427
H	0.443669	5.542787	-2.119719
H	0.084906	6.173733	-0.491029
H	-0.762885	4.734389	-1.096735
C	0.838073	3.939180	0.944823
H	0.769047	4.830695	1.586663
H	1.544489	3.237921	1.411849
H	-0.151245	3.455863	0.921713
C	1.348900	3.048449	-1.358548
H	0.362909	2.559436	-1.396709
H	2.070602	2.322279	-0.957593
H	1.650197	3.293118	-2.388747
N	6.429460	6.814204	-0.369077
C	6.158386	8.028062	-0.967732
H	7.320471	6.536923	0.061847
C	4.205165	9.261452	-1.820270
C	5.022907	10.358776	-2.115552
H	3.133777	9.297156	-2.016462
C	6.409656	10.248677	-1.856091
C	7.003502	9.106864	-1.303358
H	7.070750	11.080763	-2.108071
C	4.476635	11.664410	-2.725337
C	2.951265	11.614115	-2.932996
H	2.414078	11.463850	-1.984549
H	2.658597	10.812120	-3.627183
H	2.609816	12.567567	-3.362329
C	5.143072	11.914667	-4.099550
H	4.926505	11.090627	-4.796152
H	6.235020	12.008419	-4.011410
H	4.759925	12.847205	-4.542773
C	4.797154	12.849497	-1.782962

H	4.415297	13.789104	-2.211486
H	5.879729	12.965687	-1.629126
H	4.326799	12.706006	-0.798311
N	8.404551	9.104374	-1.081108
C	9.257258	8.053869	-1.372180
H	8.831887	10.018309	-0.941869
O	8.850276	6.977576	-1.819550
N	6.180001	4.056527	0.661826
C	6.313544	2.685997	0.798410
H	7.001693	4.640955	0.954570
O	5.383968	1.874128	0.640554
C	7.926606	1.035883	1.641476
C	7.181734	0.465673	2.680915
C	7.473698	-0.794962	3.254301
H	6.328628	1.035881	3.049286
C	8.576207	-1.505153	2.767509
C	9.034626	0.304925	1.168158
C	9.355622	-0.958793	1.733963
H	8.838357	-2.481191	3.175212
C	10.502083	-1.462058	1.005366
C	6.577191	-1.326574	4.389284
C	7.051896	-2.694379	4.913708
H	8.072875	-2.644568	5.321231
H	7.031570	-3.464118	4.127491
H	6.385099	-3.027149	5.723099
C	5.127702	-1.482979	3.870331
H	5.085125	-2.201678	3.037493
H	4.719242	-0.526586	3.513916
H	4.472647	-1.851901	4.675166
C	6.588060	-0.327185	5.571192
H	5.948955	-0.698247	6.387504

H 6.211176 0.661460 5.272195

H 7.607393 -0.197981 5.965738

N 9.912881 0.570696 0.117658

C 10.821487 -0.477888 0.024669

H 10.127487 1.486838 -0.284469

C 11.212578 -2.669675 1.089315

C 12.260366 -2.924196 0.198585

H 10.930253 -3.402385 1.844533

C 12.554711 -1.942235 -0.773114

C 11.860184 -0.729184 -0.893295

H 13.359205 -2.124972 -1.488170

C 13.091200 -4.221298 0.233440

C 12.630885 -5.172257 1.354100

H 11.584331 -5.485431 1.221836

H 12.730630 -4.711166 2.348298

H 13.254044 -6.078446 1.341851

C 14.580019 -3.874626 0.474447

H 14.710875 -3.351875 1.434071

H 14.982508 -3.230938 -0.320966

H 15.183234 -4.795078 0.499771

C 12.952594 -4.962308 -1.118363

H 13.546362 -5.889126 -1.104507

H 13.307671 -4.348072 -1.958386

H 11.902829 -5.229994 -1.312363

N 12.217782 0.097637 -1.992928

C 12.291127 1.468226 -2.090608

H 12.647044 -0.412812 -2.762940

O 11.798321 2.244112 -1.258161

N 7.612087 2.306792 1.103150

H 8.375982 3.031134 1.131436

C 13.071068 1.906086 -3.307451

C	14.265554	1.260678	-3.595140
C	12.625715	2.959569	-4.181624
C	13.337353	3.234437	-5.340432
C	15.045482	1.567626	-4.738223
C	14.549226	2.560995	-5.646500
H	14.635985	0.488440	-2.916784
H	12.986521	3.998477	-6.030854
C	16.272108	0.907330	-5.023260
C	15.303391	2.851709	-6.817816
C	16.983439	1.213867	-6.167862
H	16.640504	0.152332	-4.324904
C	16.492214	2.192247	-7.070104
H	14.931757	3.606060	-7.514959
H	17.923438	0.703100	-6.383285
H	17.061840	2.425690	-7.971674
O	11.488471	3.614519	-3.805767
C	10.861415	4.541194	-4.729615
C	11.627255	5.818426	-5.014392
H	9.917956	4.785509	-4.222096
H	10.626509	4.022904	-5.673249
C	10.704231	8.326190	-1.076085
C	11.071175	9.061126	0.039349
C	11.737218	7.774260	-1.915578
H	10.296743	9.453163	0.701586
C	12.428202	9.294507	0.384180
C	13.071731	7.978524	-1.597758
C	13.449825	8.734953	-0.455432
C	12.802476	10.057523	1.523697
H	12.017656	10.474271	2.158187
H	13.862495	7.575219	-2.229172
C	14.812899	8.966351	-0.118133

C 14.135647 10.269235 1.823351

C 12.327871 6.511823 -3.877528

O 11.316585 7.104734 -3.026044

C 15.146032 9.717125 0.995074

H 15.594500 8.543924 -0.753668

H 14.416013 10.859306 2.697390

H 16.196039 9.887648 1.240699

H 12.922882 5.797729 -3.283903

H 12.996081 7.294589 -4.269244

C 11.624641 6.354079 -6.243139

H 11.143620 5.852227 -7.086255

H 12.104210 7.314187 -6.443990

C 10.799038 7.869672 4.260055

C 10.407168 8.968194 4.944920

C 11.264754 9.747962 5.888183

C 9.936367 7.137748 3.359094

C 10.283979 6.012016 2.692421

C 9.339206 5.243852 1.829954

O 9.718356 4.089880 1.441264

H 12.277334 9.327810 5.964180

H 10.819917 9.771549 6.897344

H 11.346657 10.800343 5.568345

H 11.823088 7.498571 4.387732

H 9.379648 9.326576 4.807549

H 8.919851 7.520398 3.213137

H 11.283561 5.583145 2.811757

O 8.194268 5.755930 1.560637

3.3.31 CzU-BB free recceptor

148 0

C	6.038726	4.618674	-0.734647
C	5.125827	3.751873	-1.340878
C	4.191335	4.181669	-2.316029
H	5.151720	2.704341	-1.045716
C	4.153348	5.537167	-2.662582
C	6.010055	5.970253	-1.125597
C	5.051303	6.436708	-2.063386
H	3.437702	5.904844	-3.397354
C	5.285590	7.862107	-2.216933
C	3.245841	3.140260	-2.944524
C	2.290236	3.769159	-3.975007
H	2.835744	4.235120	-4.809270
H	1.639778	4.530697	-3.519033
H	1.641690	2.987015	-4.396717
C	2.392284	2.476993	-1.837449
H	1.777940	3.225370	-1.313923
H	3.017120	1.967325	-1.090341
H	1.716559	1.727485	-2.278372
C	4.082961	2.053434	-3.660464
H	3.419491	1.296142	-4.106060
H	4.762609	1.539659	-2.965378
H	4.691019	2.493950	-4.465032
N	6.835819	7.023120	-0.751609
C	6.393119	8.177256	-1.380174
H	7.422876	7.083660	0.083649
C	4.688626	8.851258	-3.014862
C	5.181350	10.161960	-2.991553
H	3.848798	8.584494	-3.655873
C	6.300771	10.443589	-2.173522

C	6.930475	9.478630	-1.379103
H	6.722249	11.450824	-2.164329
C	4.562601	11.297886	-3.828256
C	3.355318	10.817887	-4.654639
H	2.550672	10.427561	-4.013408
H	3.635483	10.034282	-5.374119
H	2.945662	11.663778	-5.225700
C	5.623372	11.862821	-4.802824
H	5.980312	11.081132	-5.490166
H	6.493617	12.270365	-4.268608
H	5.188533	12.675789	-5.404869
C	4.084392	12.428150	-2.885313
H	3.641866	13.248545	-3.471308
H	4.914044	12.844864	-2.296554
H	3.320973	12.057977	-2.184313
N	8.149330	9.822990	-0.731816
C	8.676814	9.312141	0.414436
H	8.727900	10.503167	-1.223852
O	8.059024	8.560123	1.191747
N	6.936577	4.222443	0.290383
C	7.479311	2.961056	0.464585
H	7.027207	4.871183	1.069638
O	7.488275	2.091886	-0.424189
C	8.513495	1.577257	2.287347
C	8.302951	1.377390	3.659345
C	8.785648	0.254600	4.369610
H	7.736183	2.143811	4.192707
C	9.500236	-0.719190	3.663284
C	9.247961	0.594175	1.598559
C	9.720545	-0.556123	2.286435
H	9.891013	-1.602421	4.167178

C 10.426027 -1.359841 1.304431

C 8.500136 0.145536 5.879995

C 9.097861 -1.135295 6.491449

H 10.192390 -1.168260 6.383400

H 8.677989 -2.043173 6.033153

H 8.867354 -1.167373 7.566611

C 6.970753 0.126789 6.117228

H 6.506277 -0.733286 5.611700

H 6.489153 1.041902 5.743909

H 6.756022 0.048679 7.194293

C 9.114299 1.362877 6.611763

H 8.913592 1.295806 7.692269

H 8.692718 2.311798 6.250126

H 10.204897 1.397811 6.467413

N 9.678183 0.553211 0.270268

C 10.354436 -0.654098 0.078011

H 9.084822 1.019944 -0.427141

C 11.087750 -2.597410 1.380735

C 11.678635 -3.136099 0.233436

H 11.128853 -3.124625 2.333290

C 11.618909 -2.404089 -0.977869

C 10.986801 -1.156286 -1.080444

H 12.086071 -2.800163 -1.875403

C 12.406166 -4.495458 0.238415

C 12.388022 -5.159751 1.628013

H 11.362242 -5.356822 1.974066

H 12.895367 -4.541872 2.384022

H 12.914705 -6.124073 1.578099

C 13.882280 -4.295876 -0.182269

H 14.401742 -3.623945 0.517770

H 13.963280 -3.864891 -1.190403

H 14.409536 -5.262220 -0.185037

C 11.716549 -5.451626 -0.763839

H 12.230170 -6.425443 -0.773517

H 11.735453 -5.050186 -1.787280

H 10.665543 -5.621391 -0.484370

N 10.993363 -0.350503 -2.238020

C 11.368293 -0.692928 -3.512877

H 10.761088 0.641802 -2.118186

O 11.652361 -1.858800 -3.838984

N 8.036747 2.785557 1.718789

H 7.822043 3.502126 2.410531

C 11.454079 0.429730 -4.522492

C 11.933628 0.065997 -5.774003

C 11.107764 1.814004 -4.311792

C 11.277171 2.743879 -5.323481

C 12.103553 0.987540 -6.833412

C 11.768795 2.364581 -6.599687

H 12.190281 -0.983307 -5.929754

H 11.034105 3.793036 -5.159304

C 12.595994 0.596294 -8.110529

C 11.944992 3.301536 -7.656051

C 12.753660 1.528845 -9.117708

H 12.847409 -0.453199 -8.279583

C 12.425817 2.890149 -8.885541

H 11.693313 4.350246 -7.483205

H 13.130950 1.223227 -10.094927

H 12.555301 3.618075 -9.688648

O 10.602333 2.137612 -3.075540

C 10.088962 3.469733 -2.803274

C 11.156740 4.422622 -2.271932

H 9.315289 3.298564 -2.042033

H 9.591419 3.860409 -3.702805

C 10.123904 9.671010 0.653762

C 10.515572 10.758050 1.403957

C 11.105651 8.767545 0.126551

H 9.765354 11.441126 1.808760

C 11.892954 11.008982 1.666756

C 12.451657 8.978419 0.366089

H 11.962560 6.215849 -0.283193

C 12.873956 10.098807 1.138008

C 12.322028 12.125680 2.434163

H 11.569737 12.810305 2.832681

H 13.205253 8.298003 -0.031652

C 14.249009 10.352814 1.403069

C 13.666755 12.344057 2.674117

C 10.483252 5.720823 -1.808990

C 11.424289 6.696765 -1.117017

O 10.571117 7.743760 -0.597553

C 14.635003 11.449570 2.152774

H 14.998779 9.666227 1.003520

H 13.986046 13.204461 3.264613

H 15.694288 11.629680 2.345836

H 12.160600 7.125997 -1.816625

H 10.009902 6.228355 -2.663668

H 9.678334 5.476026 -1.097545

H 11.913909 4.628748 -3.043296

H 11.671656 3.940163 -1.426063

3.3.32 CzU-BB acetate complex

155 -1

C -2.940476 0.394785 -0.022952

C	-3.903909	-0.399191	-0.660379
C	-4.807929	0.110025	-1.627384
H	-3.939005	-1.453804	-0.394180
C	-4.758242	1.468452	-1.958130
C	-2.889662	1.756827	-0.398395
C	-3.803476	2.296862	-1.339112
H	-5.444502	1.892864	-2.690148
C	-3.476821	3.707549	-1.463645
C	-5.817706	-0.860223	-2.272224
C	-6.732075	-0.157395	-3.292394
H	-6.158122	0.285254	-4.120236
H	-7.332026	0.637301	-2.824109
H	-7.429680	-0.890153	-3.725060
C	-6.712649	-1.485211	-1.175670
H	-7.278350	-0.707037	-0.640773
H	-6.121168	-2.043693	-0.436328
H	-7.434853	-2.183860	-1.626903
C	-5.053482	-1.987829	-3.006613
H	-5.764332	-2.693593	-3.464150
H	-4.408822	-2.555972	-2.320710
H	-4.418615	-1.574825	-3.805414
N	-2.001842	2.750070	0.016963
C	-2.365947	3.934399	-0.611749
H	-1.487812	2.691955	0.914379
C	-4.021994	4.770881	-2.206549
C	-3.456750	6.047890	-2.110430
H	-4.883063	4.588943	-2.849004
C	-2.309186	6.237262	-1.297724
C	-1.726948	5.192712	-0.568079
H	-1.833760	7.213608	-1.242901
C	-4.023693	7.260631	-2.875700

C	-5.269649	6.896752	-3.704613
H	-6.085606	6.517802	-3.070690
H	-5.046120	6.138930	-4.469931
H	-5.638834	7.794615	-4.221935
C	-2.949046	7.817297	-3.840022
H	-2.649966	7.054973	-4.575141
H	-2.047560	8.143290	-3.301500
H	-3.344988	8.685965	-4.389194
C	-4.421922	8.364713	-1.866761
H	-4.823184	9.240375	-2.400546
H	-3.561223	8.698503	-1.270059
H	-5.196460	8.001977	-1.174061
N	-0.504633	5.267088	0.131427
C	0.272923	6.362555	0.398112
H	-0.034888	4.371078	0.311198
O	-0.125760	7.529755	0.232897
N	-2.073557	-0.053166	0.987528
C	-1.746151	-1.359185	1.291217
H	-1.634197	0.684729	1.596598
O	-1.928516	-2.327697	0.520596
C	-0.662542	-2.671614	3.092351
C	-0.841309	-2.937455	4.458369
C	-0.285062	-4.063671	5.110863
H	-1.432666	-2.220937	5.030967
C	0.471359	-4.970772	4.357334
C	0.114444	-3.590077	2.363548
C	0.666891	-4.739316	2.985188
H	0.918948	-5.847857	4.823406
C	1.423510	-5.435876	1.955193
C	-0.533152	-4.247478	6.621396
C	0.128020	-5.526436	7.168363

H 1.220832 -5.509669 7.040455

H -0.263262 -6.431154 6.679454

H -0.080222 -5.612594 8.245221

C -2.054606 -4.338229 6.890720

H -2.495983 -5.195872 6.360807

H -2.580725 -3.429448 6.565241

H -2.241520 -4.467935 7.968111

C 0.048167 -3.036882 7.390460

H -0.127514 -3.153648 8.471215

H -0.416819 -2.092149 7.073986

H 1.133394 -2.953203 7.226767

N 0.538850 -3.517118 1.033713

C 1.303145 -4.658556 0.778388

H -0.125867 -3.120620 0.357353

C 2.176796 -6.622638 1.940169

C 2.808405 -7.029388 0.758024

H 2.260138 -7.216238 2.850037

C 2.707841 -6.211953 -0.395322

C 1.985862 -5.010832 -0.401526

H 3.216442 -6.498640 -1.312561

C 3.631823 -8.329933 0.668326

C 3.650678 -9.101537 2.001204

H 2.639146 -9.396985 2.317424

H 4.107230 -8.511623 2.810102

H 4.245092 -10.019701 1.883125

C 5.093200 -7.994432 0.284968

H 5.556855 -7.342871 1.041231

H 5.153129 -7.483448 -0.686515

H 5.688062 -8.918309 0.217457

C 3.020486 -9.251047 -0.414314

H 3.604719 -10.180775 -0.494969

H 3.015362 -8.768931 -1.402458

H 1.983477 -9.519232 -0.161148

N 1.954687 -4.086168 -1.466986

C 2.296387 -4.283967 -2.778491

H 1.755514 -3.109931 -1.218801

O 2.583272 -5.404461 -3.234848

N -1.178843 -1.478866 2.544555

H -1.242165 -0.654569 3.196180

C 2.300382 -3.060258 -3.667810

C 2.523433 -3.311318 -5.015192

C 2.107431 -1.688338 -3.260964

C 2.153573 -0.668012 -4.196104

C 2.571138 -2.292221 -5.994396

C 2.379379 -0.933355 -5.571971

H 2.670415 -4.350356 -5.315608

H 2.019462 0.369467 -3.893511

C 2.800592 -2.569131 -7.371738

C 2.428657 0.101278 -6.547277

C 2.841917 -1.542985 -8.296078

H 2.944873 -3.605726 -7.684382

C 2.654226 -0.199663 -7.877922

H 2.284257 1.136618 -6.230886

H 3.018822 -1.760601 -9.350682

H 2.689154 0.602732 -8.617229

O 1.873676 -1.465320 -1.922526

C 1.651782 -0.114419 -1.429057

C 2.958932 0.639951 -1.180176

H 1.092832 -0.273242 -0.498452

H 0.995686 0.424438 -2.129274

C 1.673815 6.084745 0.900189

C 2.404116 7.200930 1.284444

C	2.328895	4.797883	0.959999
H	1.907264	8.171629	1.233729
C	3.750130	7.131371	1.714774
C	3.652619	4.699558	1.352907
H	1.236551	1.735137	0.702558
C	4.392988	5.846357	1.741447
C	4.483160	8.286211	2.108937
H	3.986437	9.258883	2.085483
H	4.152088	3.731158	1.376946
C	5.751230	5.769125	2.159216
C	5.800244	8.178551	2.512507
C	2.723573	2.129654	-0.862202
C	2.112323	2.369735	0.518526
O	1.562419	3.711418	0.625209
C	6.436011	6.909793	2.536198
H	6.245374	4.795233	2.179737
H	6.356959	9.067548	2.813381
H	7.477385	6.836938	2.855383
H	2.829432	2.187443	1.331372
H	3.678337	2.668245	-0.944342
H	2.049334	2.562384	-1.619149
H	3.589674	0.575482	-2.078215
H	3.515118	0.150237	-0.365959
C	-0.761988	3.080916	4.555274
O	-1.236326	0.732943	4.285542
C	-0.979274	1.834247	3.706140
O	-0.904550	1.968058	2.435073
H	0.075154	3.670885	4.159679
H	-0.580253	2.825481	5.606144
H	-1.662593	3.711483	4.497186

3.3.33 CzU-BB benzoate complex

162 -1

C -3.808054 0.546757 -0.108289

C -5.046912 -0.042912 -0.399409

C -6.125467 0.667088 -0.986564

H -5.163335 -1.094852 -0.150948

C -5.956055 2.017242 -1.300489

C -3.663799 1.922019 -0.416289

C -4.727899 2.642843 -1.017256

H -6.759171 2.594962 -1.757350

C -4.250567 3.997252 -1.206165

C -7.443025 -0.086003 -1.256613

C -8.512993 0.820393 -1.892898

H -8.185764 1.220080 -2.864387

H -8.771006 1.668225 -1.240517

H -9.431405 0.238893 -2.063114

C -8.006633 -0.634386 0.076448

H -8.215223 0.185444 0.780525

H -7.302547 -1.326365 0.560462

H -8.946429 -1.179849 -0.103066

C -7.179019 -1.268600 -2.219321

H -8.114198 -1.817187 -2.413184

H -6.452176 -1.979710 -1.800925

H -6.786749 -0.908879 -3.182637

N -2.562528 2.762273 -0.258227

C -2.919046 4.028327 -0.709894

H -1.749994 2.596976 0.388818

C -4.848996 5.149251 -1.744977

C -4.124954 6.342511 -1.790607

H -5.871468 5.096822 -2.118273

C -2.796388 6.358141 -1.297009

C	-2.161291	5.225272	-0.763807
H	-2.218972	7.276763	-1.329797
C	-4.712628	7.648369	-2.361451
C	-6.161768	7.468258	-2.851199
H	-6.833657	7.157145	-2.037056
H	-6.231749	6.724426	-3.659277
H	-6.535749	8.424760	-3.245408
C	-3.854891	8.122652	-3.559144
H	-3.848821	7.367958	-4.360759
H	-2.812910	8.311303	-3.263320
H	-4.263325	9.057966	-3.972341
C	-4.705978	8.742722	-1.267413
H	-5.118140	9.682437	-1.666824
H	-3.688715	8.948485	-0.904779
H	-5.319442	8.438622	-0.405570
N	-0.820811	5.215809	-0.307703
C	0.080144	6.251616	-0.314689
H	-0.455936	4.317556	0.026957
O	-0.215896	7.415178	-0.642393
N	-2.711817	-0.139219	0.443880
C	-2.691109	-1.421081	0.976572
H	-1.790441	0.338724	0.436524
O	-3.690791	-2.139252	1.131558
C	-1.070198	-2.960292	2.068793
C	-1.782958	-3.373016	3.198968
C	-1.379991	-4.465652	4.006235
H	-2.680002	-2.811652	3.459256
C	-0.206519	-5.152087	3.672571
C	0.079802	-3.694746	1.731531
C	0.527407	-4.771381	2.536354
H	0.141059	-5.988829	4.277955

C	1.721277	-5.295526	1.897799
C	-2.238303	-4.842298	5.229113
C	-1.656240	-6.039419	6.002848
H	-0.649714	-5.824980	6.392385
H	-1.599217	-6.942807	5.377410
H	-2.304105	-6.269026	6.861918
C	-3.665255	-5.215923	4.761263
H	-3.641097	-6.081668	4.082107
H	-4.150732	-4.382760	4.233294
H	-4.292854	-5.477922	5.627355
C	-2.320594	-3.637315	6.196736
H	-2.934083	-3.896801	7.073645
H	-2.775459	-2.759016	5.716875
H	-1.319109	-3.350722	6.552258
N	0.953407	-3.526461	0.657206
C	1.924050	-4.524470	0.722428
H	0.684161	-3.040169	-0.193675
C	2.594434	-6.348758	2.217489
C	3.665733	-6.645174	1.368020
H	2.422246	-6.928323	3.123955
C	3.838132	-5.873911	0.192632
C	2.985235	-4.819170	-0.158050
H	4.656189	-6.101420	-0.485558
C	4.665059	-7.781859	1.660246
C	4.338361	-8.520610	2.971705
H	3.343029	-8.988931	2.941338
H	4.377021	-7.847796	3.841590
H	5.077906	-9.318392	3.134434
C	6.093291	-7.197124	1.778498
H	6.151829	-6.468072	2.601140
H	6.403918	-6.691454	0.852931

H	6.816825	-8.001676	1.982439
C	4.630388	-8.810169	0.504726
H	5.346395	-9.623535	0.699872
H	4.897005	-8.350132	-0.457556
H	3.627866	-9.253046	0.403836
N	3.144611	-4.043971	-1.331859
C	3.654079	-4.472804	-2.532999
H	2.812171	-3.074299	-1.325369
O	4.085171	-5.625971	-2.700521
N	-1.401019	-1.822559	1.294596
H	-0.662111	-1.104302	1.183924
C	3.652987	-3.482924	-3.676801
C	4.125760	-3.981563	-4.884049
C	3.192889	-2.116436	-3.646639
C	3.214067	-1.344770	-4.797144
C	4.167917	-3.217373	-6.073062
C	3.693299	-1.862746	-6.028293
H	4.471814	-5.016202	-4.899693
H	2.865288	-0.313521	-4.780404
C	4.655754	-3.746037	-7.301648
C	3.727277	-1.084572	-7.219266
C	4.675409	-2.966192	-8.442061
H	5.014205	-4.777472	-7.326667
C	4.207163	-1.626715	-8.397416
H	3.368579	-0.053545	-7.190032
H	5.050092	-3.376210	-9.381353
H	4.227888	-1.020344	-9.304837
O	2.731215	-1.645181	-2.439523
C	2.259029	-0.272501	-2.324124
C	3.405416	0.730774	-2.190698
H	1.638902	-0.293081	-1.419252

H	1.603414	-0.039459	-3.176897
C	1.480694	5.944434	0.154345
C	2.126988	6.952112	0.853705
C	2.196445	4.731353	-0.128222
H	1.584501	7.879749	1.046830
C	3.453309	6.815301	1.330754
C	3.501975	4.574747	0.309324
H	1.109887	1.828409	-0.971509
C	4.154918	5.592517	1.052366
C	4.107197	7.842882	2.066863
H	3.564745	8.768027	2.275485
H	4.060050	3.667379	0.079900
C	5.492317	5.451988	1.518310
C	5.406175	7.675033	2.507744
C	2.906715	2.188310	-2.149426
C	2.018867	2.440084	-0.933610
O	1.515492	3.798636	-0.862319
C	6.101430	6.469800	2.228780
H	6.031629	4.525599	1.308192
H	5.901825	8.467445	3.071124
H	7.127553	6.347423	2.580998
H	2.544284	2.194679	0.002924
H	3.777819	2.859571	-2.132742
H	2.339981	2.419426	-3.065534
H	4.099200	0.618833	-3.035757
H	3.977046	0.500972	-1.277427
C	2.325912	2.467273	4.672761
C	1.388141	2.558285	3.641196
H	0.788352	3.459476	3.509008
H	2.461758	3.303607	5.361382
O	-0.460584	2.681996	1.517057

C 3.093501 1.305400 4.822527

C 1.200999 1.487240 2.751495

C 0.170495 1.583780 1.647699

H 3.827413 1.233924 5.627801

C 2.919104 0.235558 3.935499

C 1.976668 0.326530 2.907548

O -0.014215 0.563609 0.901581

H 3.519077 -0.669743 4.047613

H 1.832056 -0.500422 2.211093

3.3.34 CzU-BB lactate complex

159 -1

C -2.952612 0.339957 -0.151740

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C -4.848451 0.075081 -1.722028

H -3.989699 -1.495069 -0.490993

C -4.782223 1.431261 -2.060821

C -2.885804 1.695742 -0.535391

C -3.805549 2.247707 -1.461669

H -5.474596 1.862869 -2.782635

C -3.461672 3.654366 -1.591354

C -5.886229 -0.880910 -2.343184

C -6.807473 -0.166833 -3.349219

H -6.241859 0.261887 -4.190045

H -7.384644 0.640172 -2.873483

H -7.525636 -0.889457 -3.764798

C -6.770670 -1.485266 -1.226580

H -7.311042 -0.694712 -0.683819

H -6.175505 -2.052595 -0.496929

H -7.514384 -2.171769 -1.661004

C	-5.154720	-2.024523	-3.086091
H	-5.886151	-2.720334	-3.525981
H	-4.506752	-2.600088	-2.409657
H	-4.528618	-1.626264	-3.899127
N	-1.973531	2.674976	-0.137944
C	-2.335598	3.867858	-0.757380
H	-1.467988	2.615390	0.756237
C	-4.007082	4.725121	-2.322579
C	-3.428324	5.996575	-2.230749
H	-4.880193	4.553842	-2.951400
C	-2.266824	6.171558	-1.435683
C	-1.684629	5.118760	-0.718519
H	-1.781665	7.143416	-1.384176
C	-3.996010	7.217122	-2.982653
C	-5.258298	6.867616	-3.792679
H	-6.067319	6.493335	-3.147243
H	-5.053652	6.111185	-4.564640
H	-5.627780	7.770830	-4.300350
C	-2.931139	7.766720	-3.961778
H	-2.650843	7.004181	-4.703972
H	-2.018330	8.082473	-3.436357
H	-3.327513	8.640995	-4.501576
C	-4.367358	8.321160	-1.963330
H	-4.768812	9.202196	-2.487863
H	-3.494058	8.645047	-1.379535
H	-5.133970	7.963257	-1.259471
N	-0.451766	5.180205	-0.035844
C	0.309205	6.276291	0.277252
H	0.033442	4.284883	0.103444
O	-0.109773	7.441565	0.164716
N	-2.077805	-0.116371	0.851074

C	-1.750697	-1.430208	1.134866
H	-1.665380	0.606213	1.477059
O	-1.902999	-2.374504	0.331320
C	-0.705091	-2.772274	2.941051
C	-0.906466	-3.055449	4.300398
C	-0.352679	-4.184360	4.949750
H	-1.513639	-2.350548	4.870957
C	0.425863	-5.075068	4.199392
C	0.091603	-3.675182	2.213990
C	0.643227	-4.826104	2.833943
H	0.873231	-5.953513	4.662984
C	1.421010	-5.507671	1.810164
C	-0.627088	-4.389424	6.452925
C	0.034256	-5.670216	6.995441
H	1.129151	-5.642751	6.889003
H	-0.340132	-6.571401	6.487162
H	-0.193799	-5.772544	8.066813
C	-2.152461	-4.495525	6.692790
H	-2.577386	-5.349525	6.143832
H	-2.679873	-3.586608	6.369722
H	-2.357792	-4.640890	7.764771
C	-0.070061	-3.184363	7.248045
H	-0.263655	-3.317184	8.323851
H	-0.538390	-2.239942	6.935795
H	1.017010	-3.088764	7.104597
N	0.536250	-3.588103	0.891628
C	1.311961	-4.722349	0.637833
H	-0.117812	-3.185880	0.208232
C	2.181808	-6.689679	1.797933
C	2.831344	-7.084658	0.621834
H	2.256083	-7.288766	2.704970

C 2.738591 -6.261662 -0.528274

C 2.008874 -5.065152 -0.537030

H 3.259226 -6.540044 -1.441150

C 3.664279 -8.379238 0.534534

C 3.672830 -9.158017 1.863335

H 2.659738 -9.462140 2.166087

H 4.115756 -8.569424 2.680748

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C 5.127622 -8.032000 0.169811

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H 5.729266 -8.951590 0.103870

C 3.071557 -9.298434 -0.560052

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N 1.973406 -4.141269 -1.602818

C 2.344875 -4.328136 -2.908214

H 1.751766 -3.169368 -1.357282

O 2.677404 -5.438055 -3.359061

N -1.223992 -1.576407 2.401059

H -1.355567 -0.778903 3.068550

C 2.313254 -3.107246 -3.800627

C 2.524234 -3.356781 -5.150186

C 2.094065 -1.739442 -3.394368

C 2.102174 -0.720610 -4.332005

C 2.532211 -2.339399 -6.132421

C 2.313027 -0.984467 -5.710560

H 2.692002 -4.392722 -5.450397

H 1.947953 0.314195 -4.029739

C 2.746542 -2.614563 -7.512549

C	2.320991	0.048170	-6.689178
C	2.747111	-1.590480	-8.440113
H	2.911559	-3.648161	-7.824840
C	2.532285	-0.251059	-8.022559
H	2.155921	1.080525	-6.373141
H	2.912488	-1.806787	-9.496851
H	2.534847	0.549701	-8.764443
O	1.875936	-1.519694	-2.052668
C	1.638425	-0.173269	-1.556277
C	2.936183	0.603777	-1.330694
H	1.099838	-0.341723	-0.615345
H	0.960221	0.354068	-2.244110
C	1.719758	5.997462	0.750862
C	2.476818	7.118848	1.062562
C	2.358617	4.706127	0.851919
H	1.991392	8.093332	0.983312
C	3.834777	7.048589	1.452473
C	3.691194	4.604828	1.209574
H	1.260015	1.627732	0.635424
C	4.460748	5.756831	1.517871
C	4.596001	8.209081	1.769367
H	4.112484	9.187162	1.716336
H	4.175543	3.630443	1.271098
C	5.830172	5.677461	1.896399
C	5.923507	8.099474	2.136330
C	2.678436	2.081108	-0.974799
C	2.121606	2.276310	0.435244
O	1.564068	3.609404	0.609654
C	6.542117	6.823562	2.199157
H	6.311069	4.698042	1.946355
H	6.501828	8.992591	2.378390

H 7.591864 6.749505 2.489215

H 2.872474 2.075742 1.212490

H 3.615940 2.644257 -1.083879

H 1.964067 2.512236 -1.694973

H 3.542162 0.570582 -2.247130

H 3.525506 0.110168 -0.542356

H -1.702586 3.102234 5.172551

C -0.768964 2.869672 4.629989

O -1.507916 0.623850 4.140662

C -1.089412 1.711980 3.659725

O -0.375696 4.036513 3.886026

O -0.890240 1.948631 2.415139

H -0.297095 3.691819 2.965127

C 0.312053 2.473769 5.638953

H -0.014411 1.607591 6.230342

H 0.511361 3.310641 6.322741

H 1.247219 2.215358 5.120345

3.3.35 CzU-BB formate complex

152 -1

C 5.557104 4.517081 -0.377149

C 4.363435 3.850096 -0.692406

C 3.297580 4.458141 -1.404135

H 4.281189 2.814488 -0.373181

C 3.421590 5.789467 -1.808017

C 5.660712 5.864485 -0.802563

C 4.599616 6.494946 -1.501050

H 2.623025 6.290155 -2.354600

C 5.032708 7.852845 -1.772173

C 2.036292 3.620509 -1.694159

C	0.978172	4.414200	-2.483034
H	1.359742	4.745500	-3.460473
H	0.633733	5.300739	-1.929315
H	0.102352	3.773992	-2.665385
C	1.400101	3.165343	-0.358557
H	1.109568	4.033293	0.252993
H	2.093879	2.550602	0.232534
H	0.497352	2.564992	-0.552139
C	2.420006	2.372383	-2.524255
H	1.526662	1.761354	-2.728691
H	3.146360	1.739595	-1.994708
H	2.862606	2.664584	-3.488778
N	6.725592	6.760280	-0.673473
C	6.338973	7.973496	-1.231222
H	7.464667	6.647116	0.037827
C	4.419835	8.950399	-2.401482
C	5.103602	10.166918	-2.498449
H	3.412934	8.842243	-2.803978
C	6.417032	10.258983	-1.973851
C	7.061449	9.180496	-1.353767
H	6.968308	11.192603	-2.051766
C	4.488763	11.411475	-3.168765
C	3.056522	11.153823	-3.672620
H	2.377408	10.875943	-2.852537
H	3.025593	10.357079	-4.431285
H	2.662212	12.070135	-4.136330
C	5.357718	11.829775	-4.379125
H	5.404283	11.022950	-5.126834
H	6.386726	12.071765	-4.077071
H	4.929660	12.721293	-4.863431
C	4.440326	12.576734	-2.151776

H	4.010455	13.474396	-2.622684
H	5.442961	12.837256	-1.783585
H	3.816890	12.313478	-1.283734
N	8.398541	9.207162	-0.896916
C	9.176535	10.299559	-0.611762
H	8.894238	8.309892	-0.852516
O	8.737472	11.462569	-0.634373
N	6.634440	3.945062	0.325283
C	6.836974	2.602690	0.615064
H	7.333510	4.611993	0.716472
O	6.039219	1.694730	0.323924
C	8.333716	1.117052	1.868480
C	7.702013	0.714030	3.047313
C	8.026002	-0.485649	3.728539
H	6.929565	1.373399	3.447695
C	9.037069	-1.298645	3.200397
C	9.327373	0.273180	1.350900
C	9.689632	-0.930056	2.012281
H	9.320557	-2.225539	3.698783
C	10.724807	-1.550417	1.204667
C	7.265054	-0.842016	5.019716
C	7.742744	-2.172876	5.628786
H	8.807551	-2.138726	5.903819
H	7.590278	-3.016530	4.939230
H	7.169011	-2.382402	6.543871
C	5.754202	-0.966743	4.708329
H	5.569885	-1.763192	3.971405
H	5.343484	-0.029819	4.305950
H	5.197156	-1.213105	5.625812
C	7.476214	0.274196	6.070711
H	6.929962	0.031993	6.995733

H 7.111960 1.247090 5.710716

H 8.542698 0.380642 6.320754

N 10.103597 0.415996 0.206884

C 10.927271 -0.699799 0.084920

H 9.871229 1.066252 -0.537322

C 11.459922 -2.741313 1.335075

C 12.394568 -3.090077 0.354685

H 11.288837 -3.382184 2.199254

C 12.576871 -2.229300 -0.755716

C 11.861475 -1.034899 -0.918387

H 13.291195 -2.492045 -1.530730

C 13.237612 -4.378434 0.435496

C 12.920671 -5.202257 1.697833

H 11.868563 -5.523565 1.723992

H 13.132895 -4.638089 2.618666

H 13.546023 -6.106846 1.709030

C 14.740792 -4.011217 0.463492

H 14.975996 -3.389184 1.340456

H 15.040852 -3.456691 -0.437213

H 15.352800 -4.924864 0.516489

C 12.951788 -5.261656 -0.802826

H 13.552862 -6.182882 -0.758358

H 13.200537 -4.741554 -1.738889

H 11.889585 -5.546754 -0.843612

N 12.031862 -0.155026 -2.011454

C 12.491187 -0.464764 -3.267315

H 11.757870 0.824886 -1.887275

O 12.862011 -1.608714 -3.580872

N 8.048605 2.366001 1.238323

H 8.660167 3.166565 1.526782

C 12.511713 0.652978 -4.285952

C	12.944391	0.282898	-5.552891
C	12.103656	2.021922	-4.088509
C	12.131885	2.921139	-5.141635
C	12.993933	1.178279	-6.645923
C	12.569277	2.533443	-6.434911
H	13.250514	-0.754790	-5.695717
H	11.821827	3.955238	-4.999142
C	13.440885	0.779581	-7.937396
C	12.609580	3.442791	-7.528589
C	13.468618	1.685357	-8.980291
H	13.761318	-0.253663	-8.088679
C	13.049099	3.025204	-8.771376
H	12.287932	4.475000	-7.373592
H	13.812266	1.374922	-9.968333
H	13.075253	3.731665	-9.603096
O	11.684653	2.366256	-2.822641
C	11.241454	3.722783	-2.547092
C	12.405870	4.687159	-2.318587
H	10.631530	3.609555	-1.641857
H	10.578341	4.062080	-3.357407
C	10.617902	10.028370	-0.238811
C	11.326573	11.126351	0.230229
C	11.312745	8.767513	-0.328497
H	10.797164	12.078733	0.293735
C	12.684413	11.058998	0.621028
C	12.644691	8.670394	0.036329
H	10.287202	5.713178	-0.796438
C	13.360475	9.795650	0.522132
C	13.394021	12.193840	1.105810
H	12.871568	13.150387	1.178899
H	13.174591	7.722026	-0.043933

C 14.727696 9.717982 0.908424

C 14.720950 12.086628 1.475574

C 11.933792 6.145225 -2.162527

C 11.163227 6.370075 -0.863434

O 10.581233 7.698440 -0.787397

C 15.389650 10.838929 1.374767

H 15.247102 8.760089 0.833134

H 15.260052 12.959949 1.846340

H 16.438369 10.766515 1.669006

H 11.788763 6.186159 0.023014

H 12.810139 6.807371 -2.197384

H 11.288553 6.423111 -3.011033

H 13.097430 4.635287 -3.171345

H 12.973352 4.368291 -1.430297

O 9.796721 4.377642 2.215710

C 9.404877 5.562764 2.041342

O 8.353864 5.927755 1.420498

H 10.030379 6.380001 2.476141

3.3.36 CzU-BB sorbate complex

163 -1

C -3.792083 0.363454 -0.383120

C -5.000570 -0.253017 -0.741486

C -6.057292 0.428911 -1.396031

H -5.109203 -1.305624 -0.492467

C -5.896711 1.780008 -1.710191

C -3.656007 1.740046 -0.693091

C -4.699616 2.431575 -1.360778

H -6.682560 2.338362 -2.218371

C -4.241409 3.793886 -1.536379

C -7.339474 -0.354771 -1.739029

C -8.390775 0.525721 -2.439373

H -8.017483 0.929429 -3.392369

H -8.704067 1.369921 -1.806453

H -9.285009 -0.076474 -2.659083

C -7.967250 -0.912802 -0.439074

H -8.234037 -0.096203 0.249012

H -7.277667 -1.588025 0.087414

H -8.882793 -1.479095 -0.671324

C -6.993025 -1.533230 -2.680839

H -7.902288 -2.104229 -2.926466

H -6.275338 -2.226176 -2.218506

H -6.554138 -1.166374 -3.621033

N -2.578621 2.604422 -0.480155

C -2.939281 3.857545 -0.968371

H -1.843346 2.457443 0.265864

C -4.838409 4.928813 -2.110580

C -4.142333 6.140461 -2.129509

H -5.840883 4.850897 -2.530983

C -2.838690 6.185109 -1.578250

C -2.208982 5.070234 -1.005434

H -2.280711 7.117060 -1.591266

C -4.732578 7.428838 -2.735509

C -6.156949 7.215293 -3.281005

H -6.854116 6.895735 -2.491840

H -6.179432 6.464959 -4.085870

H -6.534554 8.161034 -3.697064

C -3.837016 7.910620 -3.902284

H -3.783759 7.149681 -4.696134

H -2.811814 8.123219 -3.566880

H -4.247428 8.834024 -4.339755

C	-4.790805	8.531771	-1.651609
H	-5.203953	9.460182	-2.075532
H	-3.792972	8.759563	-1.250167
H	-5.432693	8.222795	-0.812596
N	-0.878623	5.093688	-0.523575
C	-0.120013	6.193776	-0.212255
H	-0.381655	4.198249	-0.473273
O	-0.582365	7.349313	-0.200132
N	-2.718289	-0.303325	0.231379
C	-2.712835	-1.579258	0.778377
H	-1.796749	0.180788	0.260269
O	-3.714320	-2.301887	0.903922
C	-1.121993	-3.098030	1.942964
C	-1.878940	-3.529023	3.037449
C	-1.493717	-4.618802	3.858186
H	-2.797580	-2.985928	3.257323
C	-0.295054	-5.284773	3.576470
C	0.057181	-3.809765	1.659917
C	0.485204	-4.885121	2.477519
H	0.037540	-6.119060	4.193521
C	1.716335	-5.383713	1.891079
C	-2.399694	-5.013680	5.040422
C	-1.833987	-6.204542	5.835838
H	-0.849123	-5.976071	6.270453
H	-1.735219	-7.104755	5.211041
H	-2.515677	-6.446915	6.664600
C	-3.798468	-5.407585	4.508509
H	-3.730232	-6.270247	3.828460
H	-4.272938	-4.580071	3.961939
H	-4.459890	-5.682331	5.344890
C	-2.543267	-3.813502	6.007156

H -3.190172 -4.085702 6.855618

H -2.990567 -2.940809 5.510198

H -1.562804 -3.512308 6.406585

N 0.976278 -3.618949 0.630575

C 1.962070 -4.596282 0.734906

H 0.756447 -3.103196 -0.216712

C 2.590567 -6.428237 2.236657

C 3.703049 -6.698681 1.432759

H 2.386263 -7.022686 3.126726

C 3.920060 -5.907942 0.277210

C 3.068875 -4.860586 -0.097463

H 4.771749 -6.114133 -0.365577

C 4.701265 -7.828642 1.753083

C 4.328205 -8.586754 3.040850

H 3.340093 -9.065027 2.963529

H 4.323125 -7.924240 3.919448

H 5.068858 -9.378872 3.224875

C 6.117549 -7.232409 1.937086

H 6.134705 -6.512061 2.769278

H 6.461877 -6.713855 1.030855

H 6.839561 -8.032540 2.162437

C 4.724116 -8.842828 0.584710

H 5.439952 -9.651525 0.798741

H 5.024559 -8.367922 -0.360256

H 3.731033 -9.294136 0.437749

N 3.263521 -4.062669 -1.249818

C 3.830283 -4.457429 -2.436451

H 2.901217 -3.103514 -1.243090

O 4.314277 -5.589917 -2.600597

N -1.434576 -1.968240 1.153412

H -0.691934 -1.249357 1.043496

C	3.816835	-3.457316	-3.571269
C	4.318986	-3.931106	-4.776575
C	3.308757	-2.107658	-3.536722
C	3.309977	-1.329881	-4.683386
C	4.343801	-3.158734	-5.960886
C	3.817733	-1.823254	-5.913202
H	4.701042	-4.952985	-4.795250
H	2.923103	-0.312350	-4.663909
C	4.860864	-3.662096	-7.188134
C	3.831494	-1.038231	-7.100133
C	4.860084	-2.876044	-8.324491
H	5.257990	-4.679239	-7.215453
C	4.340809	-1.555613	-8.277043
H	3.433423	-0.021791	-7.068818
H	5.257520	-3.266624	-9.262718
H	4.345522	-0.944228	-9.181314
O	2.825602	-1.659022	-2.329718
C	2.305861	-0.303515	-2.207601
C	3.417904	0.738070	-2.075351
H	1.689390	-0.347300	-1.300627
H	1.641911	-0.090481	-3.059209
C	1.327248	5.956032	0.153929
C	1.965038	7.018923	0.779482
C	2.092960	4.763257	-0.101914
H	1.381665	7.922598	0.964334
C	3.320596	6.974123	1.181784
C	3.426859	4.694317	0.266198
H	1.160339	1.740203	-0.745968
C	4.070147	5.777383	0.918285
C	3.958432	8.067760	1.832647
H	3.379911	8.972990	2.030823

H	4.012967	3.800248	0.057373
C	5.437128	5.725769	1.310920
C	5.286653	7.986300	2.204933
C	2.868079	2.177133	-2.028080
C	2.026638	2.411082	-0.776808
O	1.433133	3.738389	-0.729690
C	6.028886	6.805840	1.939628
H	6.012651	4.819341	1.110591
H	5.770149	8.828146	2.703406
H	7.077961	6.752939	2.236989
H	2.609241	2.241481	0.141730
H	3.712971	2.880282	-2.061196
H	2.251539	2.373799	-2.919691
H	4.110646	0.654042	-2.924556
H	4.001805	0.525191	-1.165870
C	2.051405	2.024800	4.826488
C	2.186058	2.968207	5.786954
C	3.137410	2.898754	6.936404
C	1.116436	2.130902	3.729291
C	0.955987	1.203896	2.754582
C	-0.027233	1.343032	1.644654
O	-0.058058	0.396269	0.772602
H	3.735332	1.976988	6.919524
H	2.597980	2.948363	7.897240
H	3.824341	3.761829	6.930080
H	2.677580	1.125109	4.868874
H	1.552469	3.861723	5.729327
H	0.491809	3.030509	3.684762
H	1.560329	0.292419	2.748519
O	-0.781245	2.368145	1.593899

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