Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

INTERACTION BETWEEN GUANIDINIUM CATION AND AROMATIC AMINO ACIDS.

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Figure S1. Minima found for the complexes formed by the amino acids and guanidinium not included in the text.

Table S1. Cartesian coordinates of the minima found for Phe-guanidinium complex at the M06-2X/6-31+G* level.

Table S2. Cartesian coordinates of the minima found for Tyr-guanidinium complex at the M06-2X/6-31+G* level.

Table S3. Cartesian coordinates of the minima found for Trp-guanidinium complex at the M06-2X/6-31+G* level.

Table S4. Complexation energies (kJ/mol) for phenylalanine complexes with guanidinium obtained with different methods.

Table S5. Complexation energies (kJ/mol) for tyrosine complexes with guanidinium obtained with different methods.

Table S6. Complexation energies (kJ/mol) for tryptophan complexes with guanidinium obtained with different methods.

Table S7. SAPT(DFT) partitioning (kJ/mol) for complexes with phenylalanine.

Table S8. SAPT(DFT) partitioning (kJ/mol) for complexes with tyrosine.

Table S9. SAPT(DFT) partitioning (kJ/mol) for complexes with tryptophan

Table S10. Ionization potential and HOMO energies employed for obtaining the shift parameter employed in SAPT(DFT) calculations.

Table S11. Complexation energies (kJ/mol) at the CSD(T)/CBS level. Zero point energy correction and Gibbs energy correction (298 K) to the complexation energy as obtained at the M06-2X/6-31+G*

Figure S2. Selected most stable minima found for Phe and Trp as obtained at the M06-2X/6-31+G* level. M06-2X/6-31+G* relative energies (kJ/mol) in blue italics; MP2/CBS ones in black. Values including ZPE and relative Gibbs energies in the Tables obtained at the M06-2X/6-31+G* level.

Figure S3. Selected most stable minima found for Tyr as obtained at the M06-2X/6-31+G* level. M06-2X/6-31+G* relative energies (kJ/mol) in blue italics; MP2/CBS ones in black. Values including ZPE and relative Gibbs energies in the Tables obtained at the M06-2X/6-31+G* level. Top and bottom structures differ in the orientation of the O-H group. M06-2X/6-31+G* values in blue italics; MP2/CBS ones in black.

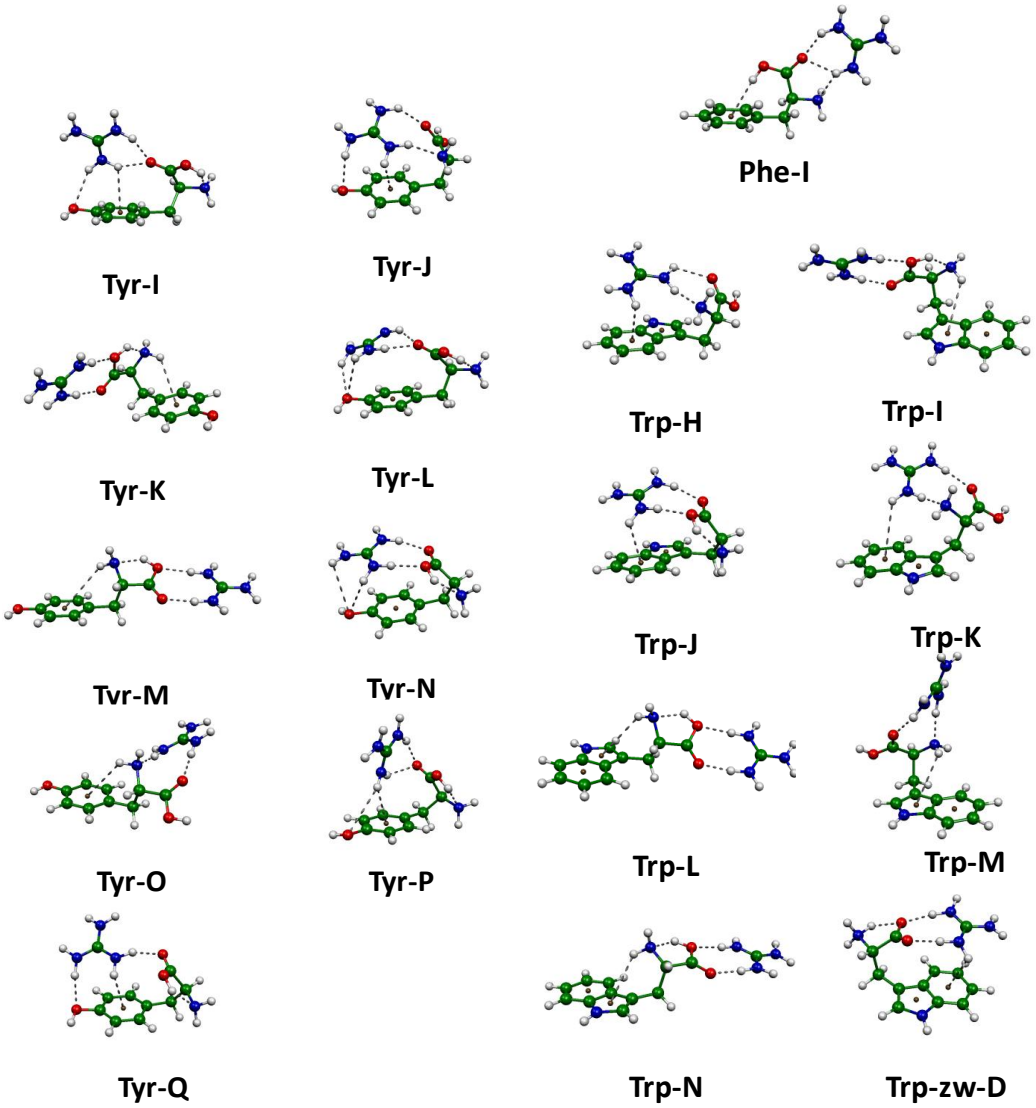

Figure S1. Other minima not included in the text

Table S1. Cartesian coordinates of the minima found for the complexes with Phenylalanine studied in this work as obtained at the M06-2X/6-31+G* level of calculation.

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Phe-A
  N -1.747994 -2.676878  0.021748
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  O -1.576630  1.202100  0.167997
  H  0.166354 -1.759186  1.013363
  X  4.109248  0.090330 -0.311370
 34
Phe-I
  N  3.857534 -1.351213  0.643197
  C  4.287045 -0.481017 -0.265734
  N  3.521282  0.539350 -0.634606
  N  5.502419 -0.638914 -0.813768
  H  4.457616 -2.084396  0.991725
  H  2.599092  0.719741 -0.216950
  H  3.815544  1.159627 -1.375388
  H  5.881108  0.037278 -1.461007
  H  6.077670 -1.440991 -0.599975
  H  2.925625 -1.247287  1.043107
  N  0.983032  2.134555 -0.000445
  C -0.225625  1.393128  0.345531
  C  0.195261  0.112058  1.065364
  O  1.355784 -0.247960  1.108703
  C -1.021367  1.068679 -0.938583
  C -2.306268  0.316706 -0.679288
  C -2.473374 -0.993414 -1.135345
  C -3.337858  0.912044  0.060187
  C -3.644826 -1.697504 -0.859800
  C -4.507134  0.206984  0.342858
  C -4.661090 -1.101075 -0.116130
  H  0.744633  2.898891 -0.629940
  H -0.887236  1.946200  1.030834
  H -1.242001  2.025629 -1.428571
  H -0.372640  0.499909 -1.614537
  H -1.680317 -1.467749 -1.708784
  H -3.237578  1.941335  0.401353
  H -3.761139 -2.713141 -1.225188
  H -5.300318  0.683223  0.911051
  H -5.571993 -1.649813  0.101247
  H  1.385127  2.562777  0.832955
  O -0.739834 -0.602675  1.666169
  H -1.639243 -0.272131  1.474091
  X -3.488425 -0.392710 -0.397920
```

Table S2. Cartesian coordinates of the minima found for the complexes with Tyrosine studied in this work as obtained at the M06-2X/6-31+G* level of calculation.

35
Tyr-A
N -0.713165 1.106138 1.214298
C -1.214894 2.064630 0.450188
N -2.517866 2.063212 0.131060
N -0.435016 3.076905 0.055228
H 0.298490 0.935838 1.320446
H -3.079679 1.219416 0.209796
H -2.907829 2.805828 -0.431724
H -0.768469 3.741819 -0.627788
H 0.571351 2.969820 0.140105
H -1.294382 0.307760 1.442383
N 1.927468 -0.126635 1.800802
C 2.578271 -0.594208 0.580264
C 2.550325 0.540292 -0.429806
O 2.017834 1.616202 -0.253199
C 1.886591 -1.859838 0.020002
C 0.399764 -1.686596 -0.175243
C -0.511497 -2.193575 0.753601
C -0.102585 -0.979369 -1.274822
C -1.880219 -1.943311 0.639487
C -1.461954 -0.721680 -1.407612
C -2.344544 -1.174619 -0.426852
O -3.647611 -0.750414 -0.519759
H 2.515511 0.557773 2.275112
H 3.640583 -0.844065 0.720803
H 2.378920 -2.126671 -0.920375
H 2.079388 -2.677737 0.723400
H -0.155000 -2.789037 1.591217
H 0.580104 -0.626872 -2.045645
H -2.573763 -2.333284 1.381356
H -1.855519 -0.170501 -2.256648
H -4.244943 -1.345310 -0.040015
H 3.203242 0.995111 -2.147389
H 1.810832 -0.903331 2.449738
O 3.201734 0.226180 -1.548258
X -0.983506 -1.449858 -0.315240
35
Tyr-B
N -1.182219 2.670073 0.316197
C -1.962369 1.799361 -0.322223
N -3.257330 1.669384 0.002907
N -1.463058 1.097816 -1.334848
H -1.478855 3.090316 1.185277
H -3.658638 2.253181 0.723629
H -3.726703 0.784059 -0.174578
H -0.451467 0.977863 -1.398018
H -2.056251 0.454489 -1.839020
H -0.190110 2.700360 0.081875
N 4.246263 -0.370550 -0.253988
C 2.807862 -0.381610 -0.502896
C 2.265415 1.006992 -0.161230
O 1.215712 1.441442 -0.603840
C 2.147490 -1.428291 0.427574
C 0.640224 -1.468802 0.370778
C -0.130684 -0.834381 1.349632
C -0.021182 -2.151918 -0.654039
C -1.520694 -0.846911 1.293664
C -1.412471 -2.162061 -0.733749
C -2.155617 -1.484409 0.230844
O -3.519865 -1.325180 0.129608
H 4.596509 -1.283110 0.026147
H 2.530906 -0.594164 -1.542882
H 2.556049 -2.405324 0.142297
H 2.480394 -1.228362 1.453816
H 0.362028 -0.327833 2.177033
H 0.553941 -2.686568 -1.407102
H -2.121747 -0.365365 2.059779
H -1.911468 -2.684315 -1.547340
H -3.919768 -2.053867 -0.370218
H 3.826660 1.186217 0.829581
H 4.778409 -0.071970 -1.068195
O 2.988739 1.696178 0.694972
X -0.766737 -1.491414 0.309522
35
Tyr-C
N -1.688558 2.834457 -0.002218
C -2.581202 1.863610 -0.170005
N -2.175206 0.642890 -0.504111
N -3.889181 2.112550 -0.012655
H -0.693021 2.605001 -0.064887
H -1.175602 0.462069 -0.596615
H -2.784325 -0.163039 -0.396538
H -4.219560 3.000520 0.336827
H -4.583221 1.411210 -0.229201
H -1.970086 3.798863 0.097687
N 4.166654 0.744636 -0.318281
C 2.818327 0.226332 -0.537200
C 1.823893 1.305676 -0.096411
O 0.656098 1.326808 -0.450354
C 2.614126 -1.055735 0.306351
C 1.194971 -1.560636 0.282165
C 0.671969 -2.155579 -0.867887
C 0.349107 -1.363109 1.376393
C -0.678881 -2.481734 -0.956906
C -0.998938 -1.698482 1.311134
C -1.514426 -2.223031 0.128510
O -2.880862 -2.352838 0.050741
H 4.546850 1.201308 -1.143768
H 2.594966 0.001159 -1.586831
H 3.301725 -1.811098 -0.092848
H 2.924630 -0.843583 1.337034
H 1.317784 -2.345457 -1.722667
H 0.743191 -0.925006 2.290596
H -1.081662 -2.908351 -1.872611
H -1.665944 -1.534195 2.152039
H -3.127118 -2.989431 -0.637997
H 3.282695 2.033606 0.790106
H 4.818902 0.015952 -0.040280
O 2.309784 2.214141 0.722606
X -0.162700 -1.913762 0.212235
35
Tyr-D
N 5.217561 1.788505 0.053917
C 4.164260 0.958988 0.046361
N 3.348929 0.919982 1.098857
N 3.928985 0.181664 -1.001442
H 5.517557 2.250997 0.900468
H 3.400980 1.624337 1.821137
H 2.610034 0.220134 1.173386
H 4.612527 0.080798 -1.738572
H 3.052674 -0.353816 -1.064020
H 5.772070 1.939952 -0.776871
N -0.968305 -2.434193 1.362471
C -0.426426 -2.393460 0.003034
C 0.821150 -1.504772 0.035572
O 1.468328 -1.201610 -0.947512
C -1.410352 -1.902105 -1.079281
C -2.056341 -0.588717 -0.709662
C -1.391472 0.627789 -0.922538
C -3.318466 -0.550554 -0.112287
C -1.958035 1.835192 -0.539332
C -3.900748 0.654228 0.279311
C -3.215895 1.850931 0.070279
O -3.713031 3.062895 0.422357
H -1.196793 -3.375112 1.667630
H -0.063193 -3.389951 -0.275461
H -0.860610 -1.817497 -2.022105
H -2.173568 -2.675930 -1.211237
H -0.424969 0.628918 -1.422180
H -3.875549 -1.475245 0.030555
H -1.456168 2.780686 -0.719070
H -4.889416 0.660780 0.732418
H -4.606405 2.977294 0.786152
H 0.468277 -1.490387 1.854409
H -1.804321 -1.854953 1.443917
O 1.167282 -1.092265 1.249415

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  X -2.640160  0.638145 -0.322372
 35
Tyr-E
  N  3.362487  1.226351 -0.049353
  C  2.078248  1.578024 -0.222370
  N  1.486504  2.438248  0.602749
  N  1.414905  1.098334 -1.268256
  H  3.681004  0.336923 -0.425808
  H  1.931739  2.695584  1.472470
  H  0.473829  2.577412  0.545448
  H  0.408389  1.222167 -1.371315
  H  1.875450  0.466027 -1.907861
  H  3.878904  1.582743  0.742914
  N -3.542888 -0.326296 -0.966409
  C -3.001601  0.243446  0.271686
  C -1.904915  1.240470 -0.109213
  O -1.359185  1.983807  0.675098
  C -2.358913 -0.837064  1.181876
  C -0.952892 -1.227921  0.781453
  C -0.675307 -1.936241 -0.392919
  C  0.124483 -0.829969  1.580171
  C  0.636899 -2.176175 -0.797987
  C  1.438267 -1.088088  1.205799
  C  1.690175 -1.718153 -0.008951
  O  3.001819 -1.767081 -0.425494
  H -4.361078  0.188052 -1.287208
  H -3.754516  0.786292  0.853689
  H -2.337660 -0.439649  2.199893
  H -3.028192 -1.705942  1.196908
  H -1.488344 -2.295175 -1.019898
  H -0.068468 -0.304294  2.512185
  H  0.834485 -2.699184 -1.731170
  H  2.273801 -0.792244  1.833506
  H  3.147659 -2.504072 -1.038852
  H -2.096561  0.480244 -1.804961
  H -3.831982 -1.293234 -0.844763
  O -1.521657  1.177262 -1.386301
  X  0.376937 -1.496091  0.394594
 35
Tyr-F
  N -4.718684 -1.306572  0.273944
  C -5.448270 -0.199748  0.275497
  N -4.871335  0.976233  0.032884
  N -6.764958 -0.254309  0.520787
  H -5.106593 -2.187923  0.579736
  H -3.861332  1.061411 -0.083479
  H -5.428262  1.804508 -0.122406
  H -7.249548 -1.137668  0.593911
  H -7.311010  0.584025  0.659936
  H -3.729416 -1.273282 -0.003045
  N  0.502758  1.531908 -1.018094
  C  0.142000  0.138249 -0.755303
  C -1.363680  0.084708 -0.523563
  O -2.010504 -0.940570 -0.456118
  C  0.831719 -0.395456  0.522422
  C  2.334092 -0.323534  0.415882
  C  3.034677 -1.189919 -0.434613
  C  3.059693  0.630992  1.129264
  C  4.411382 -1.104143 -0.572610
  C  4.445136  0.729931  1.002732
  C  5.122495 -0.137704  0.147656
  O  6.465768 -0.105607 -0.030986
  H  0.610754  1.713231 -2.013350
  H  0.373683 -0.532323 -1.590751
  H  0.490727  0.198331  1.380714
  H  0.489590 -1.423492  0.679940
  H  2.495499 -1.956319 -0.988644
  H  2.544160  1.302823  1.813474
  H  4.960147 -1.778149 -1.222530
  H  4.993281  1.475748  1.573496
  H  6.871532  0.577009  0.522959
  H -1.183275  1.933575 -0.475611
  H  1.393175  1.764560 -0.578932
  O -1.930644  1.276533 -0.342428
  X  3.734579 -0.232396  0.281385
 35
Tyr-G
  N -3.690073 -0.084510  0.348717
  C -3.194010  1.074818 -0.063125
  N -3.986885  1.999827 -0.620123
  N -1.894865  1.322280  0.095722
  H -4.684276 -0.259696  0.370455
  H -3.654447  2.937530 -0.795942
  H -4.958767  1.809137 -0.818854
  H -1.300113  0.615585  0.522313
  H -1.435972  2.090494 -0.374603
  H -3.041197 -0.808861  0.669145
  N  1.069330 -2.855438 -1.288006
  C  0.619996 -2.663487  0.090623
  C -0.718683 -1.921042  0.035100
  O -1.268598 -1.444970  1.016869
  C  1.605232 -1.939547  1.034282
  C  1.842230 -0.498315  0.650045
  C  1.127027  0.530037  1.280261
  C  2.762454 -0.137306 -0.339128
  C  1.287252  1.859695  0.908897
  C  2.928640  1.189976 -0.731299
  C  2.177707  2.191813 -0.115899
  O  2.267837  3.504263 -0.450050
  H  1.518489 -3.755357 -1.427769
  H  0.392252 -3.648120  0.517269
  H  1.202129 -1.991145  2.049974
  H  2.543021 -2.505911  1.025051
  H  0.455252  0.280196  2.099490
  H  3.397485 -0.896098 -0.793871
  H  0.763467  2.659032  1.426454
  H  3.654008  1.444067 -1.500735
  H  2.981937  3.652910 -1.087512
  H -0.616885 -2.262672 -1.782077
  H  1.721143 -2.126821 -1.573959
  O -1.255132 -1.812947 -1.164012
  X  2.020885  0.855983  0.275480
 35
Tyr-H
  N  1.288507  1.154427  1.398821
  C  1.510008  1.927378  0.340693
  N  0.558871  2.772329 -0.056165
  N  2.700133  1.900425 -0.275848
  H  2.006405  0.525367  1.729674
  H -0.347399  2.740864  0.408727
  H  0.601550  3.212408 -0.964406
  H  3.281927  1.066398 -0.242881
  H  2.902774  2.559333 -1.014828
  H  0.329131  0.987738  1.698463
  N -3.382126 -0.694810 -1.177764
  C -2.882466 -0.505997  0.189063
  C -2.207410  0.871479  0.275474
  O -1.561726  1.242406  1.238846
  C -1.949813 -1.604523  0.725011
  C -0.515049 -1.550473  0.232136
  C -0.131621 -0.910228 -0.951620
  C  0.489168 -2.139737  1.007762
  C  1.207346 -0.802084 -1.316651
  C  1.834530 -2.037992  0.660864
  C  2.191340 -1.331506 -0.487389
  O  3.495325 -1.031996 -0.800366
  H -4.365750 -0.948004 -1.192167
  H -3.741733 -0.440711  0.867034
  H -1.936827 -1.530865  1.816897
  H -2.407282 -2.573443  0.487663
  H -0.871271 -0.462770 -1.611455
  H  0.219815 -2.669174  1.918950
  H  1.502676 -0.293826 -2.229954
  H  2.598423 -2.481814  1.296165
  H  4.107329 -1.674138 -0.408133
  H -2.898725  1.110763 -1.430778
  H -2.876981 -1.422514 -1.678051
  O -2.375843  1.648323 -0.779266
  X  0.845952 -1.462003 -0.142483
 35
Tyr-zw-A
  N  3.901810  0.298648 -1.075095
  C  4.280262  0.919859  0.033211
  N  3.544748  0.818753  1.134922
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  N  5.404647  1.659242  0.045304
  H  4.518875  0.246157 -1.872707
  H  2.721350  0.189551  1.175380
  H  3.736556  1.407312  1.932651
  H  5.926114  1.834564 -0.801094
  H  5.797760  2.000763  0.910150
  H  2.987159 -0.194672 -1.118410
  N -0.827909 -2.176699  1.412502
  C -0.250633 -2.234740  0.021840
  C  0.966015 -1.270508  0.038213
  O  1.470861 -1.010690 -1.064176
  C -1.310242 -1.892496 -1.032774
  C -2.077163 -0.639952 -0.678495
  C -1.489268  0.628620 -0.807064
  C -3.376787 -0.716976 -0.169087
  C -2.175521  1.775363 -0.437792
  C -4.078173  0.428955  0.207936
  C -3.474849  1.679204  0.074062
  O -4.085362  2.838676  0.414554
  H -1.619007 -1.513058  1.425654
  H  0.138171 -3.246243 -0.128555
  H -0.769987 -1.777665 -1.977274
  H -1.999812 -2.736384 -1.148118
  H -0.487648  0.713525 -1.221990
  H -3.871597 -1.684461 -0.092292
  H -1.732881  2.759951 -0.549468
  H -5.093698  0.346837  0.587709
  H -4.992956  2.680020  0.712876
  H -1.140402 -3.078332  1.778096
  O  1.326343 -0.883036  1.183734
  H -0.057657 -1.771039  1.990763
  X -2.778627  0.525869 -0.301740
 35
Tyr-zw-B
  N -6.670077 -0.067624 -0.520602
  C -5.352443 -0.003498 -0.253572
  N -4.753078  1.171611 -0.128346
  N -4.651474 -1.124412 -0.118286
  H -7.174974 -0.939823 -0.463746
  H -3.719461  1.229520 -0.016797
  H -5.292459  2.024902 -0.101631
  H -5.061014 -2.014407 -0.362311
  H -3.650092 -1.103081  0.150385
  H -7.206051  0.764875 -0.717177
  N  0.501714 -1.076093  1.291866
  C  0.077375  0.230940  0.673355
  C -1.450812  0.142207  0.468788
  O -2.018592  1.206763  0.184930
  C  0.799676  0.418622 -0.670405
  C  2.295709  0.282693 -0.528449
  C  2.950455 -0.893129 -0.919198
  C  3.057055  1.297382  0.060851
  C  4.318229 -1.059148 -0.726124
  C  4.425709  1.148598  0.256017
  C  5.060239 -0.035145 -0.134631
  O  6.386084 -0.251002  0.027472
  H  1.442293 -1.356254  0.976521
  H  0.332905  1.035457  1.365764
  H  0.414929 -0.317866 -1.387452
  H  0.508826  1.406367 -1.040495
  H  2.389734 -1.683124 -1.417893
  H  2.578575  2.228711  0.358455
  H  4.830612 -1.962300 -1.041692
  H  5.002477  1.954131  0.704489
  H  6.824731  0.528212  0.399453
  H  0.495477 -1.042010  2.314506
  O -1.937321 -1.018504  0.568332
  H -0.234621 -1.752870  1.001520
  X  3.684566  0.123542 -0.331922
 35
Tyr-I
  N -3.752626  2.263373 -0.192826
  C -2.438005  1.994261 -0.189076
  N -2.010535  0.795114 -0.568584
  N -1.565079  2.918570  0.199040
  H -4.409815  1.633692 -0.631493
  H -2.650991  0.014353 -0.653635
  H -1.010364  0.589874 -0.565814
  H -1.844855  3.876804  0.350263
  H -0.572851  2.673588  0.245472
  H -4.109950  3.148919  0.135823
  N  4.197533  0.491688 -0.438903
  C  2.788154  0.139037 -0.592331
  C  1.953246  1.248219  0.055339
  O  0.764143  1.405004 -0.171563
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  O  0.747417  1.357427 -0.299158
  C  2.463440 -1.253705  0.192285
  C  1.000372 -1.623294  0.184850
  C  0.370406 -2.026152 -0.996531
  C  0.237996 -1.521461  1.347987
  C -0.995430 -2.282404 -1.028872
  C -1.129977 -1.781470  1.334866
  C -1.746938 -2.139610  0.138363
  O -3.103046 -2.280701  0.022019
  H  4.047915  1.219182  0.397617
  H  2.549116 -0.039936 -1.625873
  H  3.060126 -2.052929 -0.268004
  H  2.804725 -1.141085  1.229774
  H  0.948679 -2.138557 -1.911644
  H  0.708424 -1.212288  2.278210
  H -1.493134 -2.591837 -1.942913
  H -1.714729 -1.677299  2.245949
  H -3.507165 -2.426872  0.890822
  H  4.774446 -0.311202 -0.000750
  O  2.621177  2.005076  0.782983
  H  4.614782  0.866839 -1.165566
  X -0.377262 -1.895732  0.163444
 35
Tyr-zw-F
  N -1.586028  1.099329 -1.348439
  C -1.932818  1.790156 -0.266942
  N -3.199662  1.721217  0.182050
  N -1.036393  2.579584  0.315540
  H -2.267481  0.519475 -1.815576
  H -3.728887  0.869520  0.016526
  H -3.477375  2.270343  0.983420
  H -0.065209  2.516531 -0.016495
  H -1.214360  2.984740  1.223053
  H -0.590262  0.959669 -1.536594
  N  4.211512 -0.079970 -0.079953
  C  2.782372 -0.313408 -0.507318
  C  2.084113  1.044032 -0.196325
  O  2.572722  1.646465  0.779662
  C  2.215644 -1.449216  0.363591
  C  0.707350 -1.516755  0.331902
  C  0.029348 -2.212803 -0.670015
  C -0.038803 -0.853481  1.310956
  C -1.363200 -2.205267 -0.730996
  C -1.427671 -0.854353  1.275295
  C -2.084100 -1.499624  0.229783
  O -3.445579 -1.322331  0.145866
  H  4.084969  0.620820  0.696031
  H  2.754150 -0.548800 -1.572457
  H  2.649569 -2.403578  0.039592
  H  2.535919 -1.271798  1.398881
  H  0.587944 -2.761874 -1.424891
  H  0.473944 -0.321793  2.109704
  H -1.878861 -2.729943 -1.532264
  H -2.012366 -0.349541  2.038790
  H -3.858093 -2.035424 -0.365683
  H  4.697654 -0.920874  0.244411
  O  1.119910  1.353380 -0.925354
  H  4.772907  0.365617 -0.811802
  X -0.696179 -1.523714  0.291154
```

Table S3. Cartesian coordinates of the minima found for the complexes with Tryptophan studied in this work as obtained at the M06-2X/6-31+G* level of calculation.

```
39
Trp-A
  N  1.978676  2.463159 -5.051808
  C  1.911027  2.624831 -3.743260
  N  2.338999  3.764146 -3.174125
  N  1.398457  1.654903 -2.982926
  H  1.500563  1.671477 -5.523738
  H  2.474109  3.837710 -2.176305
  H  2.610255  4.554473 -3.741851
  H  1.296279  0.715490 -3.369967
  H  1.222956  1.797606 -1.999225
  H  2.493888  3.113923 -5.637650
  N  0.344396  0.396649 -6.358949
  C  0.897685 -0.928851 -6.639069
  C  1.499598 -1.468671 -5.355965
  O  1.464716 -0.912078 -4.277850
  C  1.962436 -0.870694 -7.755444
  C  3.140109 -0.014477 -7.402090
  C  4.289118 -0.420168 -6.771728
  C  3.265742  1.406634 -7.593195
  N  5.103728  0.662127 -6.536095
  C  4.503107  1.797738 -7.023606
  C  2.440707  2.389152 -8.168293
  C  4.914090  3.135297 -6.973869
  C  2.842322  3.715379 -8.127996
  C  4.065405  4.085848 -7.524740
  H -0.031105  0.792576 -7.219761
  H  0.129050 -1.655384 -6.944789
  H  2.280390 -1.894372 -7.973153
  H  1.474182 -0.496390 -8.663981
  H  4.599155 -1.415972 -6.481834
  H  6.028360  0.615828 -6.132815
  H  1.500113  2.119030 -8.642302
  H  5.864746  3.419076 -6.531263
  H  2.216995  4.482018 -8.574747
  H  4.360472  5.130832 -7.518737
  H  2.388166 -2.986465 -4.670962
  O  2.061847 -2.662766 -5.530842
  H -0.444739  0.315884 -5.717371
  X  4.060361  0.686371 -7.065343
  X  3.671896  2.755008 -7.568617
 39
Trp-B
  N -1.730135 -0.661789 -1.293399
  C -2.594204 -1.356313 -0.550762
  N -3.886846 -1.005296 -0.558375
  N -2.186344 -2.407027  0.149557
  H -1.887117  0.335980 -1.405252
  H -4.538442 -1.375098  0.118749
  H -4.233174 -0.332509 -1.227834
  H -2.850018 -3.058585  0.544685
  H -1.192539 -2.507081  0.391117
  H -0.759266 -0.968523 -1.333309
  N  3.558015 -1.137471 -0.713436
  C  2.759891 -1.294385  0.503746
  C  1.375564 -1.789930  0.094659
  O  0.555783 -2.224913  0.875752
  C  2.559423  0.058030  1.228998
  C  1.702420  1.026314  0.465291
  C  2.083731  1.875211 -0.542000
  C  0.282678  1.218680  0.637082
  N  0.992595  2.563861 -1.018050
  C -0.124093  2.194259 -0.306948
  C -0.670390  0.695351  1.530940
  C -1.449422  2.645253 -0.396217
  C -1.977385  1.148062  1.458505
  C -2.365062  2.110348  0.499582
  H  4.201043 -0.352791 -0.647443
  H  3.180388 -2.018270  1.210230
  H  2.101144 -0.149442  2.201168
  H  3.551496  0.478003  1.433179
  H  3.065040  2.060749 -0.959531
  H  1.030366  3.299715 -1.709057
  H -0.383999 -0.045186  2.273522
  H -1.741412  3.410159 -1.110543
  H -2.716446  0.772763  2.160668
  H -3.392530  2.463311  0.483163
  H  1.921799 -1.277574 -1.612381
  O  1.091114 -1.639436 -1.197795
  H  4.114739 -1.966848 -0.908241
  X  0.987466  1.775665 -0.152925
  X -1.050612  1.668659  0.570491
 39
Trp-C
  N  0.796235  2.283761 -3.279605
  C  1.921528  2.941139 -3.559977
  N  2.823881  2.393093 -4.359032
  N  2.137381  4.156783 -3.033036
  H  0.170308  2.597192 -2.552276
  H  3.585454  2.931896 -4.761701
  H  2.636384  1.472399 -4.760148
  H  1.439716  4.621100 -2.469947
  H  3.033232  4.612241 -3.132818
  H  0.627212  1.379574 -3.722006
  N  2.219808 -3.164286 -6.191685
  C  2.486048 -1.730024 -6.125370
  C  1.318170 -1.066237 -5.397933
  O  1.407664  0.029346 -4.868495
  C  2.590312 -1.172461 -7.565648
  C  2.633268  0.317836 -7.685451
  C  1.687513  1.100859 -8.292439
  C  3.660670  1.212750 -7.218123
  N  2.055312  2.423692 -8.226466
  C  3.263196  2.525978 -7.579369
  C  4.871936  1.036715 -6.525065
  C  4.032028  3.653447 -7.268798
  C  5.635627  2.149898 -6.206798
  C  5.218592  3.448029 -6.576378
  H  2.594912 -3.584520 -7.038334
  H  3.393436 -1.472029 -5.565797
  H  3.493231 -1.615841 -8.006587
  H  1.735402 -1.557874 -8.136334
  H  0.767777  0.809580 -8.783218
  H  1.550724  3.187827 -8.652080
  H  5.216288  0.042776 -6.249436
  H  3.722634  4.650043 -7.571511
  H  6.577511  2.024290 -5.681976
  H  5.851793  4.297897 -6.339052
  H  0.396386 -2.624260 -5.800766
  O  0.191477 -1.742536 -5.399445
  H  2.605854 -3.670573 -5.398498
  X  2.659992  1.516223 -7.800370
  X  4.447008  2.337803 -6.895755
 39
Trp-D
  N  3.277416  1.492784 -3.950483
  C  2.438956  2.080997 -3.107282
  N  1.248073  1.536523 -2.863891
  N  2.795984  3.223640 -2.499861
  H  4.043516  2.016487 -4.365864
  H  0.961456  0.712500 -3.394163
  H  0.661624  1.862758 -2.109728
  H  3.749500  3.553399 -2.554152
  H  2.185552  3.682538 -1.839245
  H  2.938478  0.685416 -4.476287
  N  1.568375 -3.020638 -7.299559
  C  2.023061 -1.716357 -6.827325
  C  1.131101 -1.297259 -5.661266
  O  1.476716 -0.476488 -4.827483
  C  1.875294 -0.690048 -7.978256
  C  2.042176  0.745232 -7.591978
  C  1.058850  1.698612 -7.601885
  C  3.241314  1.404656 -7.143038
  N  1.565376  2.904882 -7.178641
  C  2.903181  2.760553 -6.898701
  C  4.563566  0.983250 -6.916622
  C  3.837935  3.695673 -6.440201
```

```
  C  5.494899  1.902610 -6.455075
  C  5.134311  3.248347 -6.219687
  H  1.716501 -3.138547 -8.298717
  H  3.056109 -1.709766 -6.457914
  H  2.612225 -0.967493 -8.743530
  H  0.882614 -0.832103 -8.424584
  H  0.018829  1.609004 -7.888056
  H  1.055366  3.776311 -7.170343
  H  4.862058 -0.044236 -7.110348
  H  3.565014  4.734821 -6.278131
  H  6.521632  1.592065 -6.288479
  H  5.892683  3.950864 -5.886578
  H -0.064076 -2.541877 -6.342383
  O -0.060284 -1.851933 -5.632716
  H  2.032422 -3.791376 -6.824948
  X  2.162179  1.902787 -7.282849
  X  4.195868  2.332515 -6.678887
 39
Trp-E
  N  1.112426  2.126029 -3.436312
  C  2.225788  2.825621 -3.621618
  N  3.344333  2.213542 -4.015922
  N  2.246459  4.141528 -3.373843
  H  0.313524  2.516468 -2.957687
  H  4.017004  2.754561 -4.550637
  H  3.266144  1.234089 -4.287650
  H  3.111049  4.661701 -3.422080
  H  1.399143  4.658522 -3.189047
  H  1.095248  1.148215 -3.734694
  N  1.033237 -2.929155 -6.719200
  C  2.057258 -1.956103 -6.342668
  C  1.412292 -0.958733 -5.385969
  O  2.042109 -0.265878 -4.606301
  C  2.530761 -1.211618 -7.614426
  C  3.517534 -0.104799 -7.403830
  C  4.882650 -0.211320 -7.466911
  C  3.231991  1.289057 -7.177391
  N  5.461953  1.020687 -7.278297
  C  4.476431  1.965174 -7.114801
  C  2.045238  2.032159 -7.043937
  C  4.567226  3.352529 -6.931724
  C  2.127432  3.403650 -6.862812
  C  3.377495  4.058284 -6.809616
  H  1.166505 -3.277813 -7.665153
  H  2.926079 -2.386553 -5.831813
  H  2.972460 -1.970927 -8.270723
  H  1.641918 -0.827714 -8.133813
  H  5.497786 -1.082919 -7.649860
  H  6.451986  1.209890 -7.341670
  H  1.074010  1.543004 -7.089877
  H  5.527611  3.861011 -6.921249
  H  1.217583  3.990906 -6.778552
  H  3.409536  5.138843 -6.700758
  H -0.187800 -1.581784 -6.095929
  O  0.099642 -0.855489 -5.484774
  H  1.013859 -3.732064 -6.094854
  X  4.314112  0.791760 -7.288246
  X  3.304302  2.683476 -6.990047
 39
Trp-F
  N  0.351601  1.772825 -3.328087
  C  1.173828  2.709815 -3.803427
  N  0.855703  4.005929 -3.665473
  N  2.294747  2.357924 -4.409118
  H  0.470795  0.802350 -3.614176
  H  1.537651  4.728456 -3.848896
  H -0.075292  4.295418 -3.402076
  H  2.652788  1.400920 -4.333825
  H  2.846191  3.015060 -4.954818
  H -0.374898  1.999223 -2.664321
  N  1.161758 -2.242055 -6.831539
  C  2.436057 -1.998270 -6.152165
  C  2.172221 -0.988022 -5.031863
  O  3.038663 -0.438049 -4.389128
  C  3.581446 -1.494370 -7.056008
  C  3.340198 -0.112369 -7.592942
  C  2.555702  0.253145 -8.659604
  C  3.889497  1.113112 -7.064193
  N  2.551531  1.621681 -8.797426
  C  3.366787  2.176294 -7.839907
  C  4.815052  1.402063 -6.044554
  C  3.700209  3.515510 -7.596976
  C  5.171120  2.722103 -5.816880
  C  4.607889  3.771700 -6.578822
  H  1.078344 -1.670697 -7.671024
  H  2.750338 -2.926214 -5.659948
  H  4.509379 -1.502737 -6.475974
  H  3.705173 -2.220406 -7.867143
  H  2.024907 -0.362133 -9.375828
  H  2.100704  2.126485 -9.546933
  H  5.241107  0.604687 -5.442272
  H  3.292731  4.319361 -8.203556
  H  5.898303  2.957353 -5.045680
  H  4.918153  4.794928 -6.387673
  H  0.388353 -1.283353 -5.483776
  O  0.881074 -0.727588 -4.815904
  H  1.042989 -3.215077 -7.096863
  X  3.140743  1.010373 -7.990814
  X  4.258426  2.450130 -6.823555
 39
Trp-G
  N  0.454586  2.316776 -5.938263
  C  1.309267  3.015875 -5.206788
  N  2.028453  2.435606 -4.245254
  N  1.446247  4.340840 -5.401375
  H  0.479448  1.285927 -6.026471
  H  2.943354  2.821006 -4.032940
  H  1.937472  1.427097 -4.136234
  H  0.910114  4.818223 -6.111408
  H  1.847642  4.913235 -4.671352
  H -0.174738  2.794917 -6.568162
  N  0.030257 -0.469577 -6.835458
  C  1.144401 -1.394910 -6.647796
  C  1.630692 -1.265299 -5.218346
  O  1.360941 -0.343397 -4.476118
  C  2.294741 -1.080084 -7.637620
  C  2.757077  0.345755 -7.621464
  C  2.404629  1.324282 -8.513307
  C  3.655739  0.965388 -6.678605
  N  2.993244  2.520044 -8.165115
  C  3.782349  2.325084 -7.052995
  C  4.389186  0.494614 -5.574078
  C  4.589880  3.226127 -6.347854
  C  5.187512  1.379816 -4.868662
  C  5.282489  2.737666 -5.249936
  H -0.229040 -0.449939 -7.820892
  H  0.868684 -2.448224 -6.793957
  H  3.125546 -1.761885 -7.423069
  H  1.934423 -1.338955 -8.640359
  H  1.776452  1.257492 -9.392732
  H  3.008609  3.345365 -8.747305
  H  4.352413 -0.555246 -5.292886
  H  4.688254  4.262152 -6.660680
  H  5.772363  1.025159 -4.025501
  H  5.937949  3.401653 -4.694028
  H  2.682920 -2.165833 -3.932706
  O  2.408754 -2.284646 -4.860947
  H -0.790110 -0.798702 -6.327136
  X  3.118608  1.496111 -7.606297
  X  4.481192  1.854783 -5.962022
 39
Trp-zw-A
  N  1.496030  1.075128 -0.221514
  C  0.241382  1.261183  0.165423
  N -0.030762  1.593217  1.441425
  N -0.748468  1.129738 -0.709922
  H  2.241581  1.029613  0.457984
  H  0.707862  1.789320  2.100883
  H -0.976836  1.593158  1.793317
  H -1.690439  1.393852 -0.460409
  H -0.568761  0.789761 -1.675170
  H  1.721217  0.888640 -1.221387
  N  0.064576 -0.514860 -5.688810
  C  1.365194 -0.496052 -4.926451
```

```
  C  1.030084  0.148858 -3.556003
  O -0.198308  0.190047 -3.270832
  C  2.453805  0.252351 -5.699758
  C  1.982039  1.603785 -6.142178
  C  2.037306  2.778352 -5.434201
  C  1.290202  1.900597 -7.373423
  N  1.427358  3.778584 -6.148980
  C  0.953886  3.275590 -7.338940
  C  0.928657  1.136831 -8.501972
  C  0.265253  3.902047 -8.383459
  C  0.241173  1.752328 -9.534607
  C -0.088773  3.122823 -9.472445
  H -0.672758 -0.472467 -4.954456
  H  1.647355 -1.538129 -4.743962
  H  3.308285  0.331424 -5.022768
  H  2.775265 -0.343282 -6.562593
  H  2.476495  2.969591 -4.463825
  H  1.364380  4.743464 -5.858253
  H  1.215908  0.089082 -8.584386
  H  0.019636  4.959325 -8.345804
  H -0.034287  1.179634  -10.414526
  H -0.621654  3.577918  -10.301224
  O  1.996827  0.522727 -2.873034
  H -0.014039  0.338671 -6.267214
  H -0.054069 -1.330146 -6.293724
  X  1.538158  2.667382 -6.487544
  X  0.598400  2.515036 -8.434141
 39
Trp-zw-B
  N -0.960977  0.282504 -0.283510
  C -0.097262  0.448738  0.712408
  N  1.188115  0.633710  0.449479
  N -0.534130  0.432843  1.985973
  H -1.954292  0.291061 -0.103195
  H  1.870662  0.640302  1.193541
  H  1.517597  0.739224 -0.533582
  H  0.087911  0.632255  2.755428
  H -1.470445  0.133186  2.214855
  H -0.641302  0.234719 -1.270237
  N  0.612722 -0.014423 -5.375409
  C  1.632360  0.685101 -4.512335
  C  1.134621  0.560961 -3.056849
  O -0.067578  0.196905 -2.927875
  C  1.748624  2.162059 -4.925475
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  H  2.073178  3.678837  -10.261663
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  H  0.470400  0.448215 -5.611051
  O  0.601583  0.425548 -4.613073
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  X  3.929652  2.160639 -9.670894
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  N -1.689058  3.293918 -2.290263
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  H -0.069473  0.482800 -2.491317
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  H -1.574575  4.293112 -2.378805
  H  0.437398  3.742113 -3.619068
  H  1.282466  2.300583 -3.107458
  H -1.506501  0.869980 -1.563181
  N  2.581891 -2.309642 -4.522026
  C  2.818850 -0.846661 -4.821795
  C  2.021027 -0.090168 -3.732104
  O  2.434840  1.027856 -3.411003
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  C  2.055283  0.917291 -6.460274
  C  2.979954  1.828359 -6.896247
  C  0.849806  1.653820 -6.181793
  N  2.429194  3.085884 -6.895211
  C  1.123028  3.012815 -6.470213
  C -0.438706  1.292994 -5.750029
  C  0.154210  4.016027 -6.336702
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Table S4. Complexation energies (kJ/mol) for phenylalanine complexes with guanidinium obtained with different methods.

	6-31+G*	CBS					Aug-cc-pVDZ				cc-pVTZ			
	M062X	MP2	SCS-MP2	SCSN-MP2	MP2.X	CCSD(T)	SAPT	MP2	SCS-MP2	SCSN-MP2	M062X	B3LYP-D3	B2PLYP-D3	B2PLYP
Phe-A	-127.7	-129.3	-112.7	-127.1	-123.6	-123.0	-122.7	-122.7	-107.6	-123.5	-126.6	-127.5	-135.1	-119.9
Phe-B	-121.2	-122.4	-107.4	-123.1	-120.2	-118.8	-120.3	-115.6	-102.2	-119.0	-120.5	-124.7	-131.7	-121.0
Phe-C	-116.6	-118.4	-104.8	-119.4	-118.0	-118.2	-117.2	-114.3	-102.1	-117.2	-115.9	-121.9	-130.1	-123.7
Phe-D	-113.0	-114.1	-102.3	-116.0	-113.7	-113.9	-113.4	-109.7	-99.3	-113.5	-112.7	-118.1	-126.8	-123.1
Phe-E	-113.8	-114.3	-101.4	-114.4	-111.9	-112.0	-113.1	-110.4	-98.9	-112.6	-113.3	-115.9	-124.9	-116.3
Phe-F	-112.4	-113.3	-101.5	-115.1	-110.0	-110.8	-111.8	-108.3	-97.8	-112.6	-111.7	-115.9	-124.5	-117.6
Phe-G	-112.4	-111.2	-99.9	-113.2	-108.4	-108.8	-110.3	-106.5	-96.5	-111.1	-111.7	-114.6	-122.8	-117.1
Phe-H	-102.1	-103.3	-92.0	-104.4	-100.8	-101.5	-101.7	-100.2	-90.2	-102.8	-101.9	-106.0	-114.7	-107.5
Phe-I	-99.0	-98.3	-86.7	-99.7	-97.5	-97.1	-96.6	-94.4	-84.2	-97.8	-98.9	-98.5	-107.5	-100.5
Phe-zw-A	-119.7	-124.1	-106.7	-120.5	-125.1	-123.6	-116.5	-120.5	-104.7	-119.3	-109.4	-124.1	-130.9	-123.1
Phe-zw-B	-116.7	-119.7	-104.2	-117.3	-120.8	-119.1	-112.3	-115.7	-101.9	-115.8	-105.6	-120.4	-127.8	-122.5
Sum. Squares	**74.6**	**76.2**	**1534.1**	**112.8**	**8.6**	**0.0**	**104.8**	**87.7**	**2425.3**	**42.2**	**421.5**	**185.8**	**1582.8**	**321.2**
Standard Dev.	**2.6**	**2.6**	**11.8**	**3.2**	**0.9**	**0.0**	**3.1**	**2.8**	**14.8**	**2.0**	**6.2**	**4.1**	**12.0**	**5.4**
Average Dev.	**-0.7**	**-2.0**	**11.6**	**-2.1**	**-0.3**	**0.0**	**1.0**	**2.6**	**14.7**	**0.1**	**1.7**	**-3.7**	**-11.8**	**-4.1**
MUE	**2.3**	**2.0**	**11.6**	**3.0**	**0.7**	**0.0**	**2.0**	**2.6**	**14.7**	**1.5**	**4.0**	**3.7**	**11.8**	**4.8**
MUE-NozW	**2.1**	**2.3**	**10.6**	**3.1**	**0.5**	**0.0**	**0.8**	**2.4**	**13.9**	**1.0**	**1.8**	**4.3**	**12.7**	**5.4**

Table S5. Complexation energies (kJ/mol) for tyrosine complexes with guanidinium obtained with different methods.

	6-31+G*	CBS					Aug-cc-pVDZ				cc-pVTZ			
	M062X	MP2	SCS-MP2	SCSN-MP2	MP2.X	CCSD(T)	SAPT	MP2	SCS-MP2	SCSN-MP2	M062X	B3LYP-D3	B2PLYP-D3	B2PLYP
Tyr-A	-132.6	-131.7	-111.8	-126.6	-124.6	-124.4	-123.4	-124.0	-106.1	-122.6	-130.2	-127.5	-134.8	-114.5
Tyr-B	-129.8	-128.5	-109.1	-124.6	-123.7	-123.2	-123.9	-120.7	-103.3	-120.1	-126.2	-127.3	-134.1	-116.4
Tyr-C	-124.8	-126.2	-109.9	-124.7	-123.8	-123.1	-123.4	-120.3	-105.8	-121.3	-123.0	-126.3	-134.7	-122.7
Tyr-D	-117.4	-119.6	-105.2	-120.6	-118.8	-119.2	-117.4	-115.4	-102.5	-118.2	-117.1	-123.8	-132.5	-125.9
Tyr-E	-120.4	-120.7	-99.5	-112.9	-115.0	-115.0	-113.6	-114.0	-94.8	-109.2	-117.0	-119.4	-126.1	-105.1
Tyr-F	-112.7	-114.2	-101.7	-116.3	-113.4	-114.0	-113.7	-109.6	-98.7	-113.6	-113.1	-118.9	-127.7	-124.0
Tyr-G	-113.7	-113.8	-97.7	-113.5	-111.8	-111.9	-111.5	-108.4	-94.1	-110.7	-113.8	-116.1	-123.8	-112.4
Tyr-H	-120.6	-117.6	-96.1	-110.6	-112.0	-111.7	-112.2	-110.8	-91.5	-107.2	-118.0	-115.5	-121.8	-100.8
Tyr-O	-112.8	-114.0	-101.3	-116.0	-110.1	-111.2	-111.5	-109.0	-97.7	-113.3	-112.7	-117.4	-126.1	-119.0
Tyr-Q	-112.4	-113.6	-94.1	-106.7	-108.8	-108.7	-107.1	-108.4	-90.9	-104.2	-110.2	-112.3	-119.4	-101.7
Tyr-P	-113.6	-112.6	-94.3	-109.0	-108.9	-108.5	-108.3	-107.0	-90.6	-106.3	-112.6	-112.9	-120.0	-104.1
Tyr-zw-A	-120.3	-125.2	-107.0	-121.9	-125.7	-124.5	-118.2	-121.5	-105.1	-120.4	-110.6	-126.1	-133.4	-125.6
Tyr-zw-B	-116.9	-120.3	-104.0	-118.1	-121.0	-119.7	-113.7	-116.2	-101.7	-116.4	-106.5	-121.8	-129.3	-124.0
Tyr-zw-E	-89.1	-95.6	-75.4	-87.8	-93.8	-91.9	-89.2	-90.4	-72.3	-84.8	-79.6	-93.0	-100.5	-88.1
Tyr-I	-124.2	-125.4	-109.4	-124.8	-123.0	-122.2	-123.1	-119.3	-105.2	-121.3	-122.7	-125.8	-134.0	-122.4
Tyr-J	-129.3	-128.0	-108.3	-123.2	-121.1	-120.9	-119.9	-120.5	-102.8	-119.3	-126.5	-123.6	-131.3	-111.1
Tyr-K	-114.9	-117.2	-103.0	-118.4	-116.4	-116.8	-115.1	-112.9	-100.1	-116.0	-114.8	-121.4	-129.7	-123.4
Tyr-L	-120.6	-119.4	-100.7	-116.1	-115.1	-114.6	-115.7	-111.8	-95.0	-111.5	-117.3	-117.8	-124.4	-107.0
Tyr-M	-112.6	-114.1	-101.6	-116.4	-113.4	-113.9	-113.6	-109.5	-98.6	-113.6	-113.1	-119.1	-128.4	-124.7
Tyr-N	-114.0	-116.6	-96.1	-109.7	-111.4	-111.8	-110.4	-110.6	-92.1	-106.6	-111.6	-115.7	-122.3	-102.5

Tyr-zw-C	-119.6	-124.5	-106.4	-121.4	-125.0	-123.8	-117.5	-120.8	-104.4	-120.0	-110.0	-125.3	-132.4	-124.7
Tyr-zw-D	-116.5	-120.2	-104.0	-118.1	-120.9	-119.6	-113.7	-116.1	-101.6	-116.3	-106.4	-121.7	-129.2	-123.9
Tyr-zw-F	-93.2	-94.4	-71.1	-83.0	-90.2	-88.8	-85.3	-88.2	-67.1	-79.5	-78.9	-88.4	-95.0	-75.8
Sum. Squares	**473.61**	**363.48**	**4864.35**	**147.88**	**16.12**	**0.00**	**186.49**	**165.96**	**7661.37**	**332.61**	**1138.72**	**312.37**	**2836.01**	**1259.39**
Standard Dev.	**4.54**	**3.98**	**14.54**	**2.54**	**0.84**	**0.00**	**2.85**	**2.69**	**18.25**	**3.80**	**7.04**	**3.69**	**11.10**	**7.40**
Average Dev.	**-1.86**	**-3.22**	**14.42**	**-0.05**	**-0.36**	**0.00**	**1.64**	**2.34**	**18.16**	**2.92**	**2.06**	**-3.38**	**-10.92**	**1.71**
MUE	**3.89**	**3.22**	**14.42**	**2.25**	**0.67**	**0.00**	**1.98**	**2.34**	**18.16**	**3.09**	**5.09**	**3.41**	**10.92**	**6.34**
MUE-NozW	**4.00**	**3.65**	**13.60**	**1.99**	**0.42**	**0.00**	**0.89**	**2.29**	**17.74**	**2.37**	**2.40**	**4.10**	**11.75**	**6.98**

Table S6. Complexation energies (kJ/mol) for tryptophan complexes with guanidinium obtained with different methods.

	6-31+G*	CBS					Aug-cc-pVDZ				cc-pVTZ			
	M062X	MP2	SCS-MP2	SCSN-MP2	MP2.X	CCSD(T)	SAPT	MP2	SCS-MP2	SCSN-MP2	M062X	B3LYP-D3	B2PLYP-D3	B2PLYP
Trp-A	-137.0	-141.7	-122.7	-139.4	-134.3	-134.2	-132.7	-134.6	-117.4	-135.5	-137.3	-138.9	-148.2	-131.5
Trp-B	-136.1	-139.9	-117.4	-133.0	-133.9	-133.7	-132.1	-133.8	-113.2	-129.8	-133.6	-137.7	-145.8	-125.2
Trp-C	-133.3	-137.9	-119.8	-137.9	-133.6	-132.5	-132.5	-130.2	-114.0	-133.2	-132.7	-137.6	-145.4	-132.2
Trp-D	-132.8	-138.4	-119.6	-137.5	-133.6	-132.5	-132.8	-130.4	-113.5	-132.8	-131.9	-137.7	-145.8	-131.0
Trp-E	-134.4	-136.8	-116.5	-133.4	-131.4	-130.5	-131.7	-129.0	-110.6	-128.8	-132.9	-136.0	-144.0	-126.2
Trp-F	-128.3	-133.1	-112.7	-128.6	-128.0	-127.8	-125.9	-126.8	-108.4	-125.2	-126.9	-131.9	-141.0	-125.8
Trp-G	-133.1	-134.6	-111.8	-127.8	-125.2	-125.1	-125.3	-127.7	-106.8	-124.2	-130.7	-129.6	-137.5	-113.2
Trp-H	-128.0	-131.4	-111.0	-125.2	-121.6	-121.6	-120.9	-123.4	-105.0	-121.2	-126.2	-125.3	-134.9	-114.6
Trp-I	-117.5	-120.3	-105.3	-120.9	-119.7	-120.0	-117.7	-115.8	-102.4	-118.6	-116.9	-124.2	-133.8	-127.8
Trp-J	-118.5	-125.8	-103.2	-118.3	-119.0	-118.9	-117.3	-119.6	-98.8	-115.0	-117.3	-126.1	-133.3	-112.3
Trp-K	-119.7	-123.0	-107.5	-122.3	-117.6	-118.4	-118.3	-116.4	-102.5	-118.9	-118.4	-125.7	-134.0	-123.8
Trp-L	-115.7	-117.9	-104.8	-120.4	-117.1	-117.6	-116.4	-112.9	-101.3	-117.5	-115.8	-122.8	-132.0	-128.4
Trp-M	-117.2	-118.6	-104.2	-118.5	-115.7	-116.0	-116.2	-114.8	-101.9	-116.8	-117.0	-121.0	-131.2	-122.4
Trp-N	-113.9	-116.2	-102.6	-117.4	-115.5	-116.0	-115.2	-111.7	-99.6	-114.8	-114.0	-120.8	-130.6	-126.7
Trp-zw-A	-127.6	-132.9	-113.8	-129.2	-133.6	-132.3	-125.1	-129.5	-112.2	-128.1	-116.9	-132.7	-141.2	-133.2
Trp-zw-B	-124.1	-128.2	-110.8	-125.0	-128.9	-127.6	-121.7	-124.7	-109.0	-123.8	-113.0	-129.2	-137.5	-131.7
Trp-zw-C	-122.7	-127.0	-110.0	-125.0	-127.6	-126.3	-120.0	-122.5	-107.3	-123.2	-95.7	-110.4	-117.4	-97.5
Trp-zw-D	-107.9	-114.0	-89.0	-102.9	-109.6	-107.9	-103.6	-108.0	-85.1	-99.4	-95.7	-110.5	-117.5	-97.6
Sum. Squares	**199.90**	**529.87**	**3751.17**	**186.50**	**13.16**	**0.00**	**165.41**	**118.21**	**6111.78**	**160.53**	**1620.90**	**631.62**	**3016.32**	**1649.01**
Standard Dev.	**3.33**	**5.43**	**14.44**	**3.22**	**0.86**	**0.00**	**3.03**	**2.56**	**18.43**	**2.99**	**9.49**	**5.92**	**12.95**	**9.57**

Average Dev.	**-0.50**	**-4.39**	**14.24**	**-1.33**	**-0.40**	**0.00**	**1.86**	**1.51**	**18.32**	**1.78**	**3.66**	**-3.29**	**-11.79**	**2.09**
MUE	**2.57**	**4.39**	**14.24**	**2.80**	**0.68**	**0.00**	**2.06**	**2.14**	**18.32**	**2.18**	**5.53**	**5.06**	**12.78**	**7.22**
MUE-NozW	**2.46**	**5.07**	**13.27**	**2.75**	**0.46**	**0.00**	**0.95**	**2.07**	**17.81**	**1.40**	**1.92**	**5.04**	**13.77**	**6.13**

Table S7. SAPT(DFT) partitioning (kJ/mol) for complexes with phenylalanine.

	E_{def}	E_{tot}	E_{ele}	E_{exch}	E_{ind}	$E_{exch-ind}$	E_{disp}	$E_{exch-dis}$	δHF
Phe-A	31.45	-122.66	-158.91	137.78	-95.48	45.07	-58.19	9.30	-24.20
Phe-B	26.26	-120.34	-145.42	104.94	-74.31	29.80	-45.48	6.82	-15.46
Phe-C	4.15	-117.21	-127.31	87.85	-62.94	26.71	-30.57	4.97	-15.11
Phe-D	8.07	-113.38	-127.02	84.74	-61.15	25.60	-29.32	4.79	-14.33
Phe-E	23.89	-113.08	-152.33	126.33	-89.63	42.54	-40.86	7.33	-23.85
Phe-F	23.45	-111.79	-150.43	134.60	-96.50	45.86	-43.46	7.76	-26.14
Phe-G	24.88	-110.25	-152.56	130.80	-92.89	44.44	-40.75	7.45	-25.17
Phe-H	30.48	-101.66	-144.81	122.82	-87.91	40.70	-40.28	7.08	-23.28
Phe-I	43.95	-96.59	-146.09	98.56	-71.11	29.50	-36.13	6.01	-15.44
Phe-zw-A	77.47	-116.50	-215.55	147.32	-105.07	50.12	-42.76	8.48	-29.85
Phe-zw-B	87.66	-112.32	-221.22	147.94	-107.12	50.81	-42.42	8.51	-29.90

Table S8. SAPT(DFT) partitioning (kJ/mol) for complexes with tyrosine.

	E_{def}	E_{tot}	E_{ele}	E_{exch}	E_{ind}	$E_{exch-ind}$	E_{disp}	$E_{exch-dis}$	δHF
Tyr-A	42.94	-123.45	-169.88	143.43	-98.91	49.48	-70.96	11.24	-19.21
Tyr-B	32.45	-123.93	-162.33	129.37	-87.00	42.20	-64.07	10.03	-14.10
Tyr-C	29.59	-123.42	-149.31	100.94	-73.77	30.10	-46.09	6.76	-14.01
Tyr-D	5.94	-117.42	-129.02	88.23	-63.24	26.72	-30.77	4.98	-15.26
Tyr-E	34.62	-113.62	-152.81	127.29	-86.06	44.21	-65.14	10.00	-15.02
Tyr-F	9.37	-113.67	-128.58	85.41	-61.70	25.76	-29.46	4.82	-14.50
Tyr-G	14.56	-111.49	-121.20	86.50	-70.07	31.68	-39.95	6.00	-12.41
Tyr-H	38.40	-112.25	-149.94	118.72	-82.53	41.91	-65.41	9.90	-12.53
Tyr-O	25.63	-111.51	-151.72	134.92	-96.88	45.76	-43.63	7.76	-26.38
Tyr-Q	31.49	-107.13	-133.12	107.05	-77.36	35.80	-54.64	7.86	-15.15
Tyr-P	28.58	-108.28	-132.40	99.13	-74.39	35.75	-50.82	7.55	-13.28
Tyr-zw-A	78.99	-118.22	-218.62	148.02	-105.83	50.32	-42.98	8.52	-29.96
Tyr-zw-B	89.68	-113.75	-225.01	149.62	-108.35	51.37	-42.74	8.61	-30.32
Tyr-zw-E	108.47	-89.20	-200.39	127.94	-94.27	40.04	-51.16	8.40	-19.94
Tyr-I	27.35	-123.12	-145.39	98.05	-71.79	28.60	-45.10	6.54	-13.91
Tyr-J	41.69	-119.89	-164.56	140.42	-96.62	48.34	-69.72	11.01	-19.06
Tyr-K	4.77	-115.08	-125.89	88.64	-63.38	26.79	-30.63	4.99	-15.39
Tyr-L	34.28	-115.69	-150.58	118.43	-80.73	38.04	-61.26	9.28	-13.08
Tyr-M	9.20	-113.62	-128.25	85.15	-61.59	25.68	-29.41	4.81	-14.44
Tyr-N	28.16	-110.35	-138.14	117.47	-81.25	40.23	-59.28	8.86	-16.62
Tyr-zw-C	77.22	-117.50	-216.64	149.19	-106.52	50.72	-43.07	8.57	-30.27
Tyr-zw-D	89.35	-113.72	-224.60	149.47	-108.13	51.19	-42.66	8.59	-30.31
Tyr-zw-F	121.83	-85.34	-219.82	155.35	-109.56	55.39	-70.33	11.93	-18.79

Table S9. SAPT(DFT) partitioning (kJ/mol) for complexes with tryptophan.

	E_{def}	E_{tot}	E_{ele}	E_{exch}	E_{ind}	$E_{exch-ind}$	E_{disp}	$E_{exch-dis}$	δHF
Trp-A	36.14	-132.67	-166.94	137.73	-98.28	44.89	-60.96	9.43	-24.67
Trp-B	24.69	-132.12	-153.18	122.77	-88.94	43.16	-61.92	9.53	-18.07
Trp-C	28.13	-132.54	-153.75	111.31	-79.77	31.17	-51.70	7.50	-16.87
Trp-D	28.44	-132.75	-154.80	115.07	-82.12	33.38	-54.80	8.07	-16.93
Trp-E	31.76	-131.66	-159.09	119.99	-88.12	41.20	-60.80	9.41	-16.04
Trp-F	21.44	-125.93	-137.64	103.22	-77.21	33.31	-50.35	7.14	-17.45
Trp-G	45.77	-125.26	-165.65	144.13	-99.76	49.78	-76.22	11.80	-22.60
Trp-H	39.53	-120.91	-158.13	138.74	-98.13	49.33	-68.40	10.60	-23.22
Trp-I	5.42	-117.74	-129.92	91.83	-65.87	27.99	-31.14	5.16	-16.16
Trp-J	36.23	-117.35	-147.75	124.19	-86.98	40.40	-62.94	9.22	-19.28
Trp-K	39.76	-118.32	-170.52	146.93	-106.70	51.31	-52.78	9.08	-26.92
Trp-L	10.32	-116.37	-132.08	86.59	-62.86	26.19	-29.76	4.88	-14.82
Trp-M	29.46	-116.17	-161.79	132.38	-94.30	44.80	-42.09	7.63	-25.57
Trp-N	12.84	-115.22	-133.99	87.80	-63.53	26.64	-29.97	4.95	-15.09
Trp-zw-A	75.61	-125.06	-223.86	154.73	-110.90	53.07	-44.07	8.91	-31.72
Trp-zw-B	89.23	-121.70	-234.03	154.10	-111.31	53.19	-43.59	8.89	-31.44
Trp-zw-C	88.31	-119.98	-230.58	152.56	-110.48	52.50	-43.31	8.78	-31.09
Trp-zw-D	121.14	-103.56	-232.91	166.29	-120.46	60.73	-70.22	12.18	-29.05

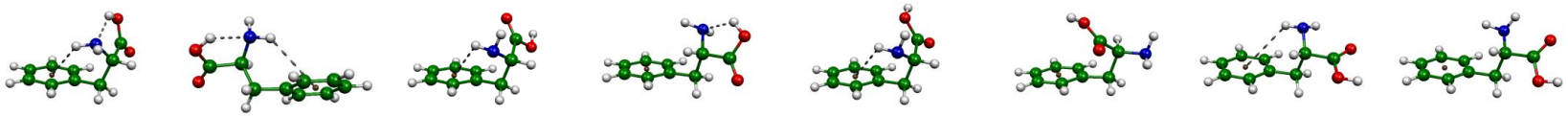
Table S10. Ionization potential and HOMO energies employed for obtaining the shift parameter employed in SAPT(DFT) calculations.

	IP (a.u.)	E_{HOMO} (a. u.)
Guanidinium	0.61316673	-0.501141
Phenylalanine	0.33759606	-0.266596
Tyrosine	0.31044500	-0.237391
Tryptophan	0.29440145	-0.223551

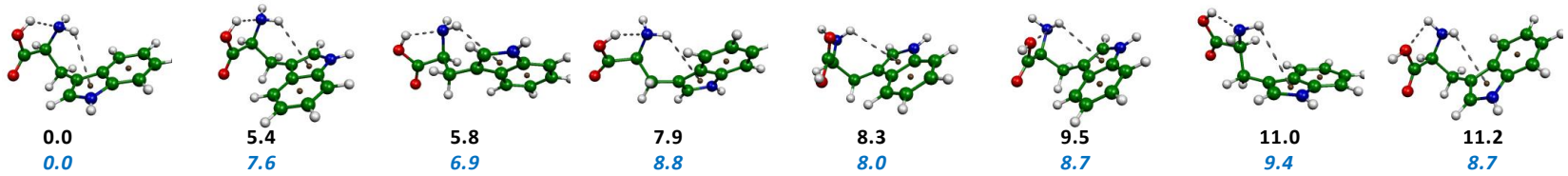
Table S11. Complexation energies (kJ/mol) at the CSD(T)/CBS level. Zero point energy correction and Gibbs energy correction (298 K) to the complexation energy as obtained at the M06-2X/6-31+G*

	$\Delta E_{CCSD(T)}$	ZPE correction	Gibbs energy correction
Phe-A	-122.97	4.86	13.40
Phe-B	-118.81	4.44	12.33
Phe-C	-118.21	3.31	11.34
Phe-D	-113.90	3.15	10.96
Phe-E	-111.99	4.89	12.01
Phe-F	-110.77	3.38	11.14
Phe-G	-108.81	3.91	11.60
Phe-H	-101.51	3.60	11.35
Phe-I	-97.14	3.84	11.65
Phe-zw-A	-123.60	5.79	12.33
Phe-zw-B	-119.11	4.52	11.26
Tyr-A	-124.45	4.73	14.06
Tyr-B	-123.24	5.67	13.88
Tyr-C	-123.09	3.78	12.26
Tyr-D	-119.19	2.56	11.07
Tyr-E	-115.03	4.92	14.09
Tyr-F	-113.96	2.31	10.62
Tyr-G	-111.91	2.29	11.34
Tyr-H	-111.69	5.09	14.23
Tyr-O	-111.25	3.98	12.02
Tyr-Q	-108.71	4.22	13.82
Tyr-P	-108.53	2.94	11.19
Tyr-zw-A	-124.50	4.42	13.25
Tyr-zw-B	-119.66	2.13	10.43
Tyr-zw-E	-91.86	4.63	13.50
Tyr-I	-122.16	3.35	11.17
Tyr-J	-120.86	2.26	11.85
Tyr-K	-116.85	4.68	13.41
Tyr-L	-114.58	5.23	11.89
Tyr-M	-113.89	3.89	11.05
Tyr-N	-111.78	5.23	11.86
Tyr-zw-C	-123.81	3.51	10.74
Tyr-zw-D	-119.61	2.69	11.49
Tyr-zw-F	-88.82	7.70	14.45
Trp-A	-134.20	4.65	13.09
Trp-B	-133.70	6.36	14.38

Trp-C	-132.52	4.08	12.41
Trp-D	-132.51	5.32	12.50
Trp-E	-130.46	5.74	13.59
Trp-F	-127.78	4.30	13.06
Trp-G	-125.06	6.27	14.78
Trp-H	-121.64	4.58	13.45
Trp-I	-120.01	3.04	10.90
Trp-J	-118.86	5.93	13.99
Trp-K	-118.43	4.96	12.26
Trp-L	-117.60	3.20	10.63
Trp-M	-116.04	5.06	12.02
Trp-N	-115.98	3.47	10.94
Trp-zw-A	-132.30	6.05	12.31
Trp-zw-B	-127.60	5.08	11.53
Trp-zw-C	-126.30	6.81	14.45
Trp-zw-D	-107.87	6.88	14.49

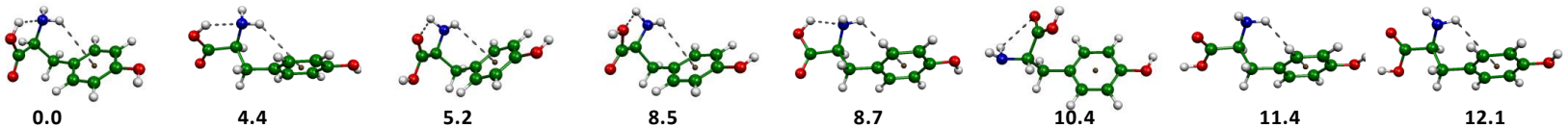


ΔE	0.0	3.3	2.3	4.1	5.1	8.6	9.1	8.4
ΔE+ZPE	0.0	3.7	1.4	4.2	4.7	6.7	7.2	7.5
ΔG_{298}	0.0	3.9	1.4	3.8	3.9	4.9	6.2	6.7

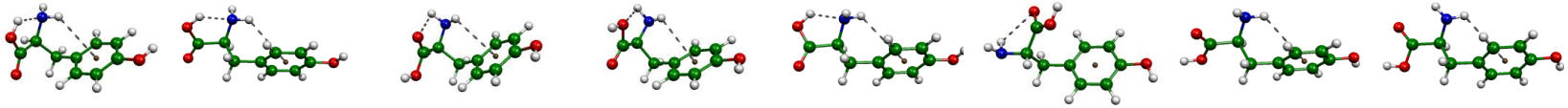


ΔE	0.0	7.6	6.9	8.8	8.0	8.7	9.4	8.7
ΔE+ZPE	0.0	7.9	7.3	9.4	6.4	7.9	9.0	7.8
ΔG_{298}	0.0	8.1	6.5	8.8	5.7	8.3	6.0	6.3

Figure S2. Selected most stable minima found for Phe and Trp as obtained at the M06-2X/6-31+G* level. M06-2X/6-31+G* relative energies (kJ/mol) in blue italics; MP2/CBS ones in black. Values including ZPE and relative Gibbs energies in the Tables obtained at the M06-2X/6-31+G* level.



ΔE	0.0	4.8	3.5	6.3	5.9	9.8	10.6	9.8
ΔE+ZPE	0.0	3.6	2.0	5.3	5.0	6.9	7.7	7.8
ΔG_{298}	0.0	2.2	1.3	3.6	3.2	4.0	5.5	5.7



ΔE	1.8	4.8	3.6	6.2	6.1	9.8	10.7	10.6
ΔE+ZPE	1.1	4.2	1.8	5.0	5.4	6.8	7.5	7.7
ΔG_{298}	0.6	2.9	0.7	3.4	3.9	4.2	5.0	5.5

Figure S3. Selected most stable minima found for Tyr as obtained at the M06-2X/6-31+G* level. M06-2X/6-31+G* relative energies (kJ/mol) in blue italics; MP2/CBS ones in black. Values including ZPE and relative Gibbs energies in the Tables obtained at the M06-2X/6-31+G* level. Top and bottom structures differ in the orientation of the O-H group. M06-2X/6-31+G* values in blue italics; MP2/CBS ones in black.