

Supporting Information for

Ion-peptide interactions between alkali metal ions and a terminally-protected dipeptide; Modeling a portion of the selectivity filter in K⁺ channels

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Contents

Table S1

Table S2

Table S3

Figure S1

Figure S2

Figure S3

Figure S4

Figure S5

Cartesian coordinates of optimized structures

Table S1 Calculated distances (Å): between metal ion and oxygen atoms; between two oxygen atoms of the two C=O groups; and between two hydrogen atoms of the two NH groups for each complex of the more stable OH rotamer.

	Na ⁺ Ac-Tyr-NHMe			K ⁺ Ac-Tyr-NHMe		
	O/O/R	O/O	O/O'	O/O/R	O/O	O/O'
M ⁺ ...O(Ac)	2.209	2.187	2.180	2.589	2.573	2.581
M ⁺ ...O(Y)	2.258	2.202	2.204	2.664	2.606	2.603
O...O	3.017	3.137	3.093	3.099	3.236	3.212
H...H	3.279	2.990	3.198	3.231	2.844	3.054

Table S2 Relative stabilization energies (kJ/mol) of the conformers calculated at B3LYP-D3/cc-pVTZ with zero point energy correction. The relative energies of phenolic OH rotamer of each isomer is presented in the parenthesis.

	O/O/R	O/O	O/O'	O/R	OH
Na ⁺ Ac-Tyr-NHMe	0	6.2	9.8	44	132
	(1.7)	(6.3)	(9.9)	(45)	(139)
K ⁺ Ac-Tyr-NHMe	0	3.8	6.3	30	101
	(1.1)	(4.0)	(6.4)	(38)	(102)

Table S3 Observed and calculated vibrational frequencies and their assignments.

	obs.				calc.				Isomer assignment
	OH str.	NH str.	NH str.	CO str.	OH str.	NH str.(Nt)	NH str.(Ct)	CO str.	
Na ⁺ Ac-Tyr-NHMe	3631	3476	3463	1701	3637	3465	3458	1678	O/O/R
	3637	3429	3423	1684	3640	3412	3428	1660	O/O
	3640	3475	3410	1686	3641	3469	3422	1664	O/O'
K ⁺ Ac-Tyr-NHMe	3642	3481	3466	1701	3639	3469	3462	1684	O/O/R
	3642	3453	3432	1682	3641	3440	3427	1665	O/O
	3642	3473	3411	1686	3643	3464	3414	1665	O/O'

Fig. S1 Skeletal formulas of a) GYG and b) Ac-Tyr-NHMe.

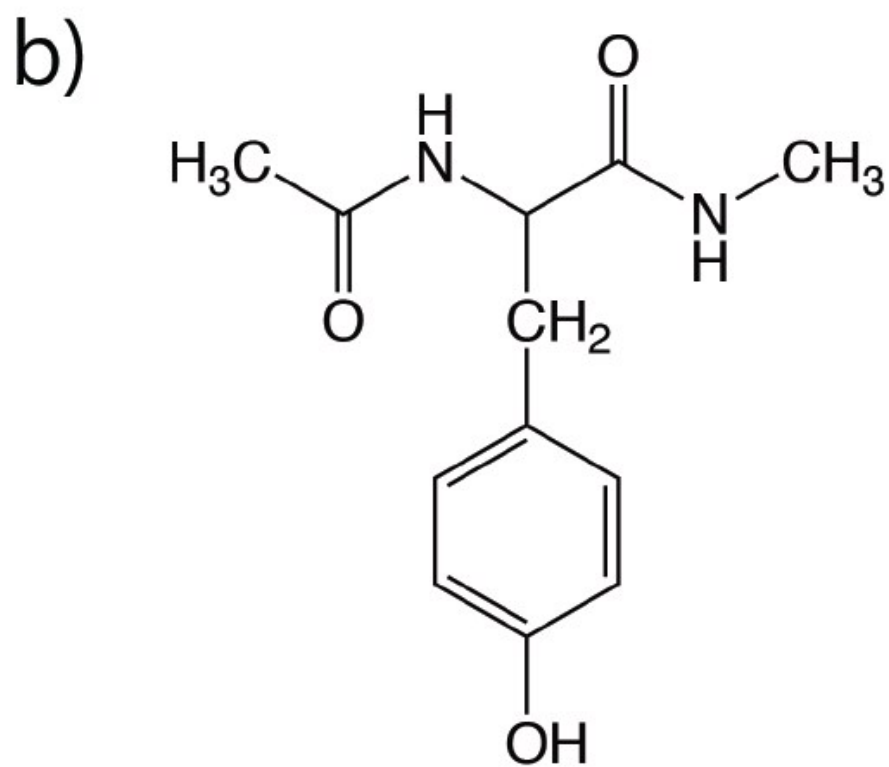
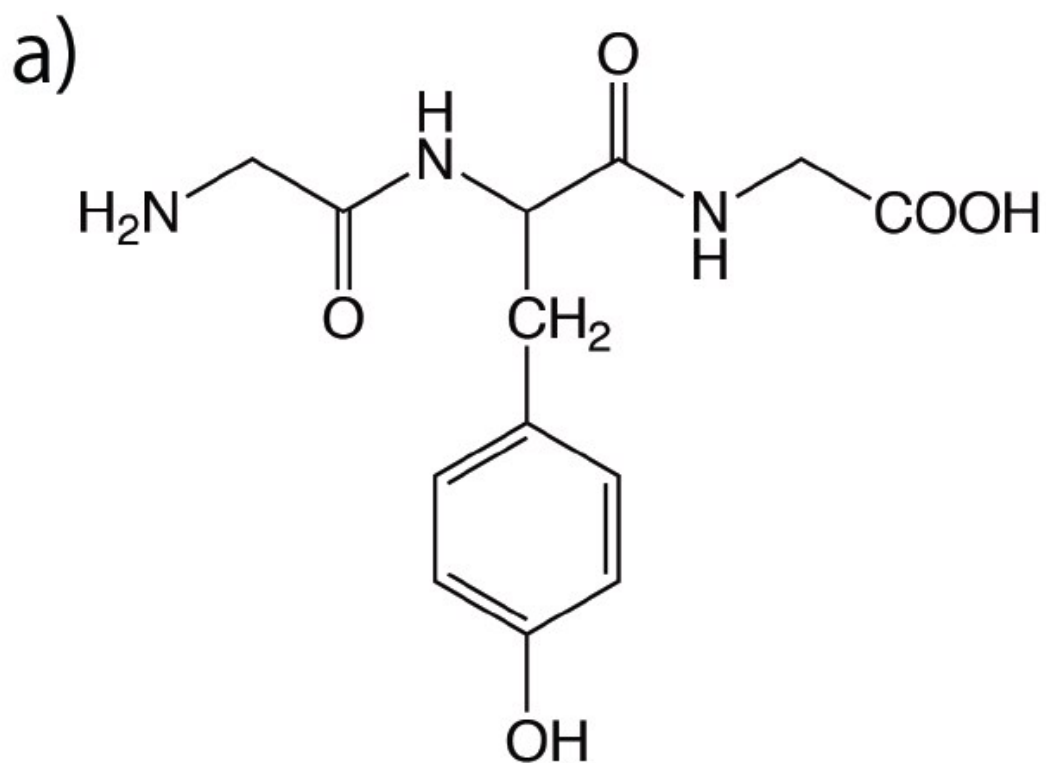


Fig. S2 Optimized structures of each complex. Each conformer has opposite OH rotamers and more stable one is presented.

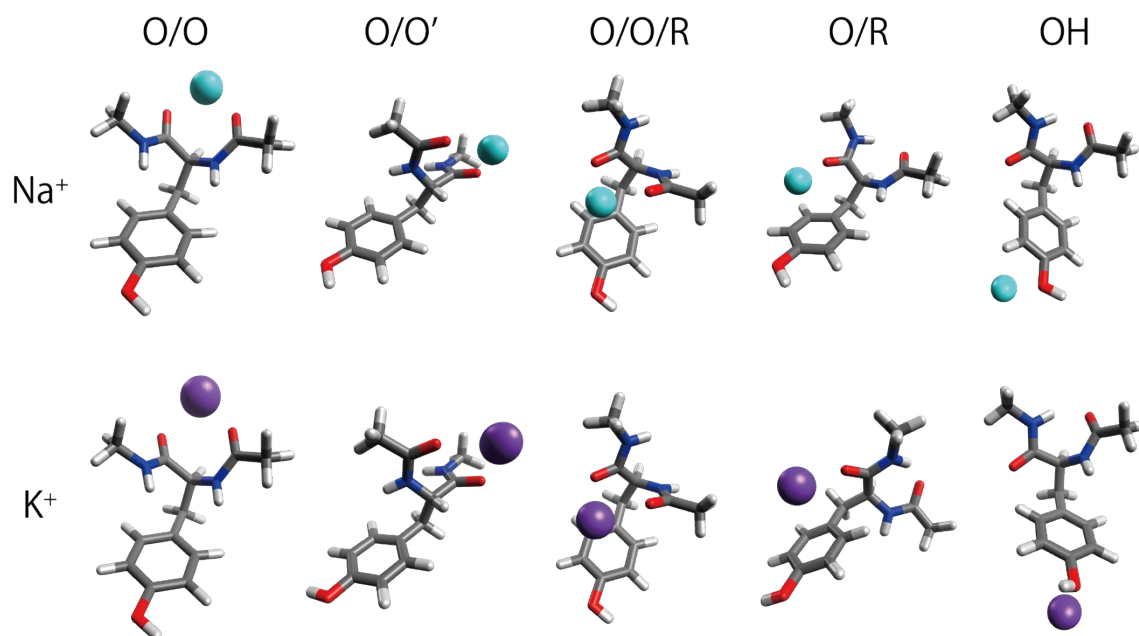


Fig. S3 a) IRPD and b)~d) IR-UV dip spectra of K^+ complex. To measure the IR-UV dip spectra, frequencies of UV laser were fixed to b) 35371, c) 35425 and d) 35563 cm^{-1} , respectively.

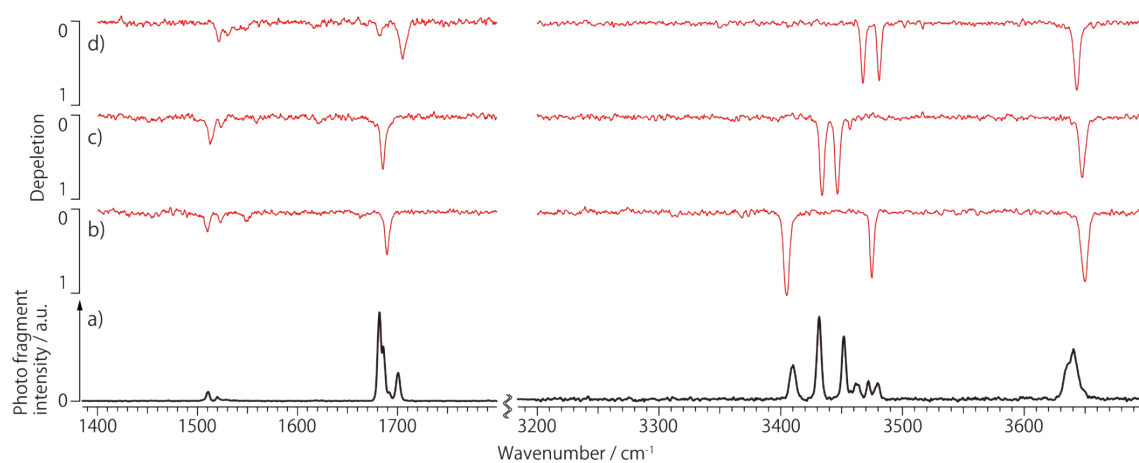


Fig. S4 a) IRPD and b)~d) IR² dip spectra of Na⁺ complex compared with calculated IR spectra at B3-LYP-D3/cc-pVTZ (scaling factor: 0.956 (for OH and NH stretches) and 0.975 (for others)). Each IR² dip spectrum was measured by probing a band indicated by an arrow.

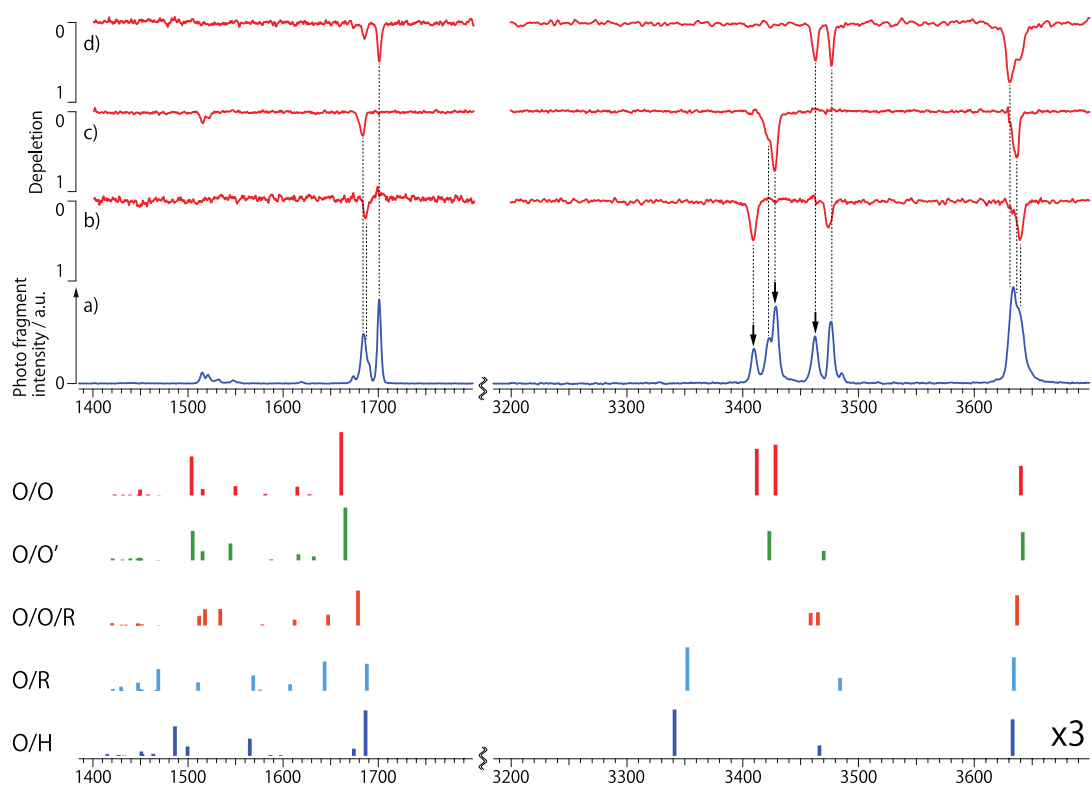
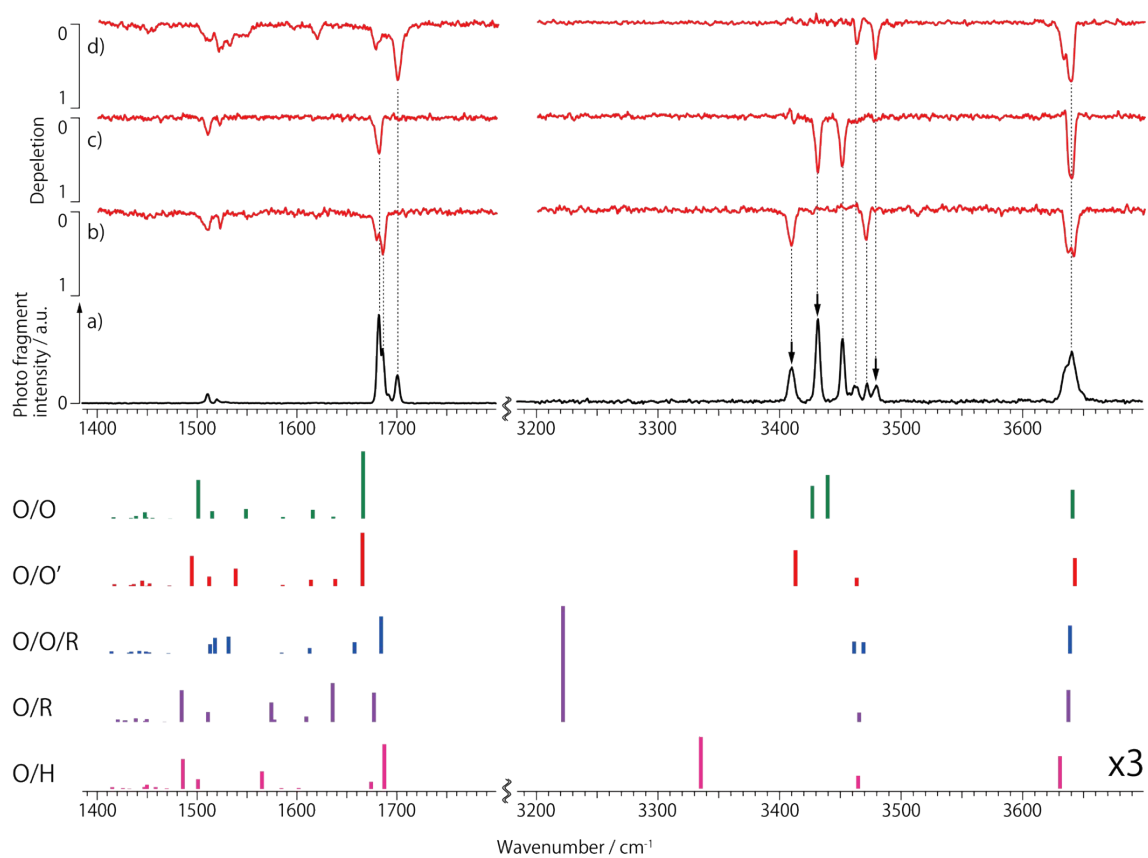


Fig. S5 a) IRPD and b)~d) IR² dip spectra of K⁺ complex compared with calculated IR spectra at B3-LYP-D3/cc-pVTZ (scaling factor: 0.956 (for OH and NH stretches) and 0.975 (for others)). Each IR² dip spectrum was measured by probing a band indicated by an arrow.



Cartesian coordinates of optimized structures

Na⁺Ac-Tyr-NHMe

O/O/R

C 4.478494 -1.049705 -2.246446
C 3.230868 -1.192892 -1.415472
O 2.117691 -1.218746 -1.943325
N 3.399743 -1.296759 -0.076396
C 2.331798 -1.374143 0.928679
C 1.847014 0.004548 1.439791
C 1.192156 -2.308433 0.457502
O 0.069185 -1.891049 0.166453
H 4.446424 -0.079563 -2.743138
H 5.402174 -1.128476 -1.676473
H 4.466672 -1.812323 -3.024030
H 4.340792 -1.235636 0.275446
H 2.786032 -1.868112 1.790113
H 2.690799 0.446833 1.974213
H 1.075419 -0.188432 2.185320
C 1.338930 0.992050 0.418613
N 1.506799 -3.607926 0.422497
C 0.572863 -4.633262 -0.030140
H 2.446768 -3.885375 0.650235
H 0.889712 -5.596970 0.359503
H 0.540112 -4.681919 -1.119829
H -0.422401 -4.403200 0.341331
C -0.031532 1.218922 0.248682
C -0.509378 2.106137 -0.709466
H -0.737405 0.694828 0.879895
O -0.134876 3.659813 -2.432821
C 0.390448 2.811768 -1.515531
C 1.761006 2.625106 -1.333597
H -1.567945 2.302514 -0.813585
H 3.286251 1.621784 -0.233026
C 2.218593 1.734061 -0.370880
H 2.467183 3.190363 -1.929515
H 0.558930 4.152360 -2.884901
Na -0.017322 -0.686967 -1.742099

O/O/R rotamer

C 4.508245 -1.103669 -2.228611
C 3.252743 -1.226270 -1.406832
O 2.143375 -1.246623 -1.943111
N 3.408261 -1.316746 -0.065144
C 2.330741 -1.380400 0.931047
C 1.853322 0.002516 1.435930
C 1.185764 -2.305595 0.454659
O 0.069000 -1.878022 0.153881
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H 4.497963 -1.877983 -2.994663
H 4.346567 -1.261095 0.295048
H 2.773733 -1.875301 1.797835
H 2.704510 0.448761 1.955414
H 1.092995 -0.185293 2.194314
C 1.328177 0.987257 0.419696
N 1.487506 -3.608122 0.426636
C 0.547194 -4.624813 -0.032287
H 2.423122 -3.894220 0.661516
H 0.857580 -5.592573 0.352410
H 0.515298 -4.667027 -1.122213
H -0.447092 -4.390574 0.339303
C -0.039268 1.245349 0.303399
C -0.532449 2.147281 -0.638741
H -0.734393 0.736323 0.958325
O -0.049281 3.725560 -2.414601
C 0.352089 2.831454 -1.478224
C 1.724250 2.602878 -1.356403
H -1.595542 2.351840 -0.687830
H 3.263972 1.564735 -0.316161
C 2.194997 1.703847 -0.412747
H 2.401643 3.158835 -1.989066
H -0.993608 3.902496 -2.342392
Na 0.028264 -0.655377 -1.742363

O/O

C 5.771936 0.061552 -2.934215
C 4.753372 -0.914060 -2.411244
O 4.924501 -2.135428 -2.519342
N 3.659017 -0.402013 -1.813185
C 2.614272 -1.225137 -1.210183
C 1.842853 -0.444856 -0.114505
C 1.759307 -1.886419 -2.311479
O 1.935169 -3.083233 -2.589624
H 6.713300 -0.113896 -2.413203
H 5.482689 1.102982 -2.807913
H 5.942770 -0.141946 -3.990789
H 3.526095 0.597374 -1.809683
H 3.107844 -2.060484 -0.717482
H 2.537375 -0.326735 0.718785
H 1.042404 -1.095817 0.239185
C 1.287492 0.907606 -0.494749
N 0.880226 -1.128415 -2.962934
C 0.052465 -1.638553 -4.050789
H 0.770193 -0.166021 -2.682687
H 0.638321 -1.761463 -4.962383
H -0.751157 -0.931443 -4.237078
H -0.367708 -2.603432 -3.776116
C -0.051211 1.071603 -0.871289
C -0.556843 2.309062 -1.235840
H -0.718253 0.218459 -0.856967
O -0.279721 4.613022 -1.590779
C 0.271888 3.432528 -1.222043
C 1.600364 3.298220 -0.818229
H -1.594506 2.430982 -1.512546
H 3.110194 1.980407 -0.090936
C 2.091027 2.050835 -0.453978
H 2.241696 4.169366 -0.766037
H 0.355461 5.332081 -1.504909
Na 3.902470 -4.043632 -2.827930

O/O rotamer

C 5.778340 0.087033 -2.908720
C 4.762166 -0.899109 -2.401237
O 4.943672 -2.118564 -2.513562
N 3.658340 -0.398071 -1.810778
C 2.615410 -1.231015 -1.217634
C 1.836272 -0.465902 -0.117106
C 1.766967 -1.884730 -2.327956
O 1.959232 -3.073253 -2.629412
H 6.712259 -0.076967 -2.370707
H 5.475678 1.125427 -2.789171
H 5.970050 -0.116444 -3.961641
H 3.518552 0.600269 -1.805853
H 3.111989 -2.068522 -0.731650
H 2.528952 -0.347788 0.717832
H 1.041633 -1.126997 0.230852
C 1.268836 0.884869 -0.485876
N 0.874264 -1.127537 -2.961971
C 0.054305 -1.628294 -4.059786
H 0.752265 -0.172201 -2.662753
H 0.642236 -1.726125 -4.973074
H -0.758827 -0.928904 -4.233669
H -0.353070 -2.603800 -3.803896
C -0.074663 1.046301 -0.832456
C -0.590138 2.288590 -1.182275
H -0.740397 0.192330 -0.809135
O -0.190311 4.653413 -1.514167
C 0.237347 3.411735 -1.183986
C 1.575734 3.277034 -0.810473
H -1.638944 2.387984 -1.433790
H 3.098277 1.962588 -0.116053
C 2.072424 2.032779 -0.459911
H 2.198261 4.159799 -0.776530
H -1.133863 4.652872 -1.707897
Na 3.932253 -4.024499 -2.858460

O/O'

C -1.994465 1.259792 2.270997
C -1.853220 0.351082 1.081488
O -2.843067 -0.169996 0.551774
N -0.605887 0.121490 0.620309
C -0.345581 -0.591299 -0.629378
C 1.124788 -0.399313 -1.056826
C -0.751356 -2.074319 -0.520448
O -1.731636 -2.505433 -1.143671
H -2.525807 0.725653 3.058047
H -1.044139 1.621586 2.657909
H -2.611722 2.110393 1.981577
H 0.143818 0.692218 0.981175
H -0.988924 -0.176423 -1.406348
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H 1.787893 -0.875589 -0.331120
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C 2.560430 3.051508 -0.314643
H 2.626836 1.142417 0.631691
O 2.456325 5.096334 -1.464169
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H 0.502328 1.321715 -3.086031
C 1.071365 1.800222 -2.297845
H 1.046501 3.707135 -3.280188
H 2.137113 5.501124 -2.277617
Na -3.720951 -1.610325 -0.829498

O/O' rotamer

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C -1.860724 0.352601 1.074229
O -2.845670 -0.148646 0.517408
N -0.606891 0.109005 0.638148
C -0.330506 -0.595389 -0.612776
C 1.145881 -0.402559 -1.015430
C -0.745609 -2.076863 -0.522899
O -1.724207 -2.494268 -1.157879
H -2.576421 0.719359 3.037143
H -1.067918 1.589935 2.684727
H -2.607782 2.117059 1.974188
H 0.143471 0.665097 1.019789
H -0.960640 -0.171557 -1.395415
H 1.300476 -0.939370 -1.952884
H 1.798458 -0.873260 -0.276467
C 1.514102 1.052923 -1.158584
N -0.008628 -2.871193 0.255035
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H 0.613621 -4.791018 0.772277
H -0.623856 -4.719604 -0.497615
H -1.073639 -4.439138 1.192375
C 2.297876 1.696139 -0.202904
C 2.604485 3.048579 -0.311071
H 2.702835 1.134473 0.631476
O 2.379523 5.102338 -1.571933
C 2.124301 3.782635 -1.393334
C 1.341818 3.149843 -2.363139
H 3.225689 3.526164 0.436697
H 0.449352 1.327020 -3.008843
C 1.045317 1.804880 -2.240306
H 0.989999 3.728390 -3.205563
H 2.953355 5.436937 -0.874611
Na -3.707621 -1.570974 -0.892262

O/R

C 5.836119 -0.631731 -3.067233
C 4.612376 -1.385076 -2.609902
O 4.492152 -2.591156 -2.767723
N 3.635875 -0.647795 -1.991672
C 2.426515 -1.288711 -1.489741
C 1.847143 -0.601750 -0.237290
C 1.445237 -1.470195 -2.660401
O 0.571319 -0.629082 -2.942571
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H 5.804299 0.434654 -2.847801
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H 1.049054 -1.244441 0.135758
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N 1.634705 -2.569999 -3.380779
C 0.880212 -2.861614 -4.592402
H 2.474557 -3.102980 -3.183057
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C -0.560844 2.363348 -0.357964
H -0.729903 0.254809 -0.050030
O -0.252161 4.671876 -0.681538
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H -1.615921 2.561859 -0.220828
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H 2.366096 4.035399 -0.758321
H 0.422438 5.359304 -0.718650
Na -0.345990 1.278237 -2.933707

O/R rotamer

C 5.908293 -0.749981 -3.020285
C 4.643010 -1.450131 -2.592733
O 4.476864 -2.650951 -2.747406
N 3.683735 -0.670997 -1.998134
C 2.446559 -1.266149 -1.506160
C 1.876522 -0.561943 -0.259144
C 1.472196 -1.419911 -2.687302
O 0.642284 -0.543581 -2.993056
H 6.737725 -1.167410 -2.449463
H 5.885799 0.329141 -2.873677
H 6.092885 -0.971950 -4.070222
H 3.785883 0.327564 -2.008599
H 2.721763 -2.269326 -1.182664
H 2.686518 -0.548747 0.474095
H 1.108799 -1.220072 0.148598
C 1.296959 0.828725 -0.385624
N 1.621217 -2.537477 -3.389774
C 0.872683 -2.809225 -4.609882
H 2.436233 -3.101753 -3.176852
H -0.183424 -2.607595 -4.446962
H 1.002715 -3.855072 -4.872908
H 1.224030 -2.186663 -5.434627
C -0.064393 1.048535 -0.159986
C -0.633032 2.319373 -0.260141
H -0.701125 0.214114 0.105196
O -0.302247 4.684286 -0.698363
C 0.169663 3.419634 -0.581463
C 1.537796 3.222315 -0.795576
H -1.685773 2.459602 -0.044117
H 3.156769 1.848173 -0.779567
C 2.084189 1.950485 -0.677548
H 2.159918 4.081250 -1.004753
H -1.207893 4.751828 -0.375300
Na -0.110604 1.437405 -2.913051

OH

C 5.471767 -0.401416 -3.381891
C 4.462249 -1.299974 -2.707309
O 4.581305 -2.518022 -2.706891
N 3.412434 -0.681445 -2.095524
C 2.384439 -1.415480 -1.366655
C 1.823192 -0.579293 -0.199153
C 1.269835 -1.962940 -2.295304
O 0.101256 -1.604293 -2.185671
H 5.258611 0.661475 -3.273048
H 5.510210 -0.655506 -4.440652
H 6.453640 -0.615240 -2.961162
H 3.278613 0.304755 -2.239142
H 2.884741 -2.285384 -0.938465
H 2.573948 -0.576423 0.591590
H 0.947133 -1.103193 0.179297
C 1.454986 0.853226 -0.518238
N 1.709278 -2.865064 -3.189123
C 0.844962 -3.509497 -4.164280
H 2.693440 -3.106047 -3.165676
H 0.864819 -4.591836 -4.034268
H 1.165952 -3.273002 -5.179612
H -0.170539 -3.153000 -4.018054
C 0.247757 1.179322 -1.143590
C -0.075259 2.503961 -1.418556
H -0.408250 0.379056 -1.453481
O 0.348955 4.833714 -1.239836
C 0.801322 3.520221 -1.047883
C 2.009386 3.228559 -0.436262
H -0.962570 2.738707 -1.999868
H 3.268886 1.667021 0.293193
C 2.326954 1.895407 -0.188930
H 2.687839 4.020493 -0.145071
H 1.085285 5.446342 -1.348377
Na -1.503109 4.406705 -0.007042

OH rotamer

C 5.460600 -0.398467 -3.491152
C 4.463386 -1.291581 -2.782029
O 4.583997 -2.515770 -2.756827
N 3.417186 -0.661378 -2.163435
C 2.405738 -1.397847 -1.407497
C 1.840924 -0.554678 -0.241977
C 1.290160 -1.996956 -2.308097
O 0.112737 -1.639521 -2.217774
H 5.267165 0.676572 -3.359269
H 5.452682 -0.639959 -4.565509
H 6.467818 -0.635213 -3.116385
H 3.270035 0.327744 -2.327880
H 2.936929 -2.258355 -0.970062
H 2.596691 -0.544578 0.558161
H 0.959445 -1.089282 0.141638
C 1.454741 0.883595 -0.546691
N 1.735778 -2.950087 -3.154374
C 0.868383 -3.647354 -4.090558
H 2.733609 -3.170767 -3.125549
H 0.865144 -4.730856 -3.888070
H 1.201050 -3.487302 -5.129471
H -0.150340 -3.257465 -3.971542
C 0.318244 1.201045 -1.320335
C -0.060006 2.526041 -1.545837
H -0.263670 0.377299 -1.739829
O 0.339158 4.910374 -1.116844
C 0.716666 3.557598 -1.013690
C 1.865544 3.280870 -0.267388
H -0.958120 2.749969 -2.128722
H 3.118088 1.728488 0.550530
C 2.219505 1.942288 -0.033717
H 2.523948 4.094055 0.060117
H -0.170812 5.059167 -1.929683
Na 0.187296 5.164513 1.082549

K⁺Ac-Tyr-NHMe

O/O/R

C 4.599100 -1.018819 -2.180905
C 3.307225 -1.216152 -1.428546
O 2.234638 -1.319356 -2.022277
N 3.397704 -1.279536 -0.077888
C 2.271667 -1.380289 0.858432
C 1.744810 -0.017107 1.359968
C 1.174909 -2.321922 0.311799
O 0.033062 -1.936302 0.069337
H 4.551032 -0.058070 -2.694466
H 5.487056 -1.040726 -1.551727
H 4.678462 -1.791683 -2.943991
H 4.308057 -1.148866 0.331409
H 2.676963 -1.882964 1.739994
H 2.569653 0.446846 1.906810
H 0.971146 -0.232833 2.096831
C 1.214102 0.963203 0.343426
N 1.555195 -3.601990 0.176543
C 0.675053 -4.631746 -0.357345
H 2.517894 -3.838936 0.347213
H 1.023893 -5.606277 -0.025348
H 0.659994 -4.614808 -1.449230
H -0.334239 -4.468167 0.011572
C -0.156582 1.222579 0.245626
C -0.662675 2.130369 -0.676170
H -0.840880 0.704902 0.904694
O -0.346446 3.669324 -2.428495
C 0.207302 2.809330 -1.533665
C 1.580119 2.580745 -1.436064
H -1.720371 2.351997 -0.722528
H 3.138474 1.543389 -0.415934
C 2.067894 1.679602 -0.496063
H 2.266211 3.124693 -2.074122
H 0.335897 4.163178 -2.896105
K -0.279528 -0.770219 -2.305798

O/O/R rotamer

C 4.659749 -1.053986 -2.152915
C 3.351730 -1.234690 -1.424895
O 2.290629 -1.339605 -2.038759
N 3.413481 -1.277717 -0.071906
C 2.271070 -1.374619 0.845537
C 1.739337 -0.012792 1.343734
C 1.179725 -2.313553 0.283265
O 0.045776 -1.922605 0.013065
H 4.629989 -0.097436 -2.675761
H 5.534769 -1.077303 -1.505875
H 4.747778 -1.834093 -2.907579
H 4.316533 -1.148943 0.353956
H 2.661995 -1.878161 1.733191
H 2.567534 0.460972 1.877438
H 0.979102 -0.232149 2.093558
C 1.181253 0.963848 0.337406
N 1.553944 -3.597215 0.167725
C 0.679198 -4.625234 -0.378375
H 2.511005 -3.839236 0.361555
H 1.017888 -5.599842 -0.036299
H 0.684380 -4.611952 -1.470339
H -0.336054 -4.455963 -0.028872
C -0.182969 1.257674 0.311902
C -0.713705 2.179575 -0.586743
H -0.847040 0.757096 1.003962
O -0.318645 3.735611 -2.404955
C 0.126921 2.834173 -1.490215
C 1.496109 2.561626 -1.471487
H -1.772575 2.409701 -0.565479
H 3.077105 1.488707 -0.532333
C 2.007848 1.652183 -0.556681
H 2.143024 3.096805 -2.152359
H -1.239703 3.963999 -2.239105
K -0.201511 -0.732553 -2.353573

O/O

C 5.741414 0.090251 -3.024692
C 4.727998 -0.894582 -2.504931
O 4.854320 -2.109335 -2.692758
N 3.679316 -0.395616 -1.816714
C 2.645800 -1.248693 -1.242415
C 1.870523 -0.512629 -0.118954
C 1.765362 -1.870097 -2.346365
O 1.775513 -3.092905 -2.529478
H 6.708468 -0.141313 -2.578305
H 5.489807 1.127693 -2.812381
H 5.839616 -0.044059 -4.101441
H 3.572661 0.603028 -1.732292
H 3.142508 -2.102745 -0.786903
H 2.562545 -0.414076 0.718974
H 1.074102 -1.180300 0.212148
C 1.307856 0.845437 -0.464266
N 1.034945 -1.034872 -3.091090
C 0.161467 -1.487328 -4.166400
H 1.048046 -0.053414 -2.865093
H 0.717903 -1.630906 -5.094039
H -0.610317 -0.739594 -4.330604
H -0.301201 -2.431280 -3.888235
C -0.010628 1.001532 -0.908173
C -0.520156 2.244500 -1.246005
H -0.655770 0.134991 -0.976328
O -0.269873 4.567001 -1.487934
C 0.284667 3.380532 -1.139376
C 1.592337 3.252308 -0.672414
H -1.543154 2.360362 -1.575098
H 3.088843 1.928121 0.073722
C 2.086943 1.998361 -0.334840
H 2.213771 4.131141 -0.551732
H 0.347815 5.291049 -1.340086
K 3.920693 -4.482658 -3.035836

O/O rotamer

C 5.728247 0.110099 -3.025835
C 4.724024 -0.882599 -2.503480
O 4.860535 -2.096657 -2.688928
N 3.670792 -0.391322 -1.816554
C 2.644064 -1.252211 -1.241920
C 1.855091 -0.520768 -0.124912
C 1.772501 -1.885842 -2.345394
O 1.793831 -3.108785 -2.525788
H 6.697300 -0.111126 -2.578505
H 5.466983 1.145756 -2.816712
H 5.828058 -0.026589 -4.102148
H 3.556195 0.606650 -1.734922
H 3.147455 -2.099716 -0.781438
H 2.538847 -0.418896 0.719411
H 1.059314 -1.192792 0.198697
C 1.289946 0.835465 -0.473610
N 1.034234 -1.059014 -3.092260
C 0.170049 -1.521992 -4.170251
H 1.040715 -0.076725 -2.869457
H 0.731672 -1.662352 -5.095288
H -0.608297 -0.782268 -4.339868
H -0.284872 -2.469720 -3.892120
C -0.027836 0.992136 -0.908345
C -0.537200 2.240507 -1.243179
H -0.675699 0.127428 -0.973762
O -0.155109 4.622602 -1.452681
C 0.270789 3.373758 -1.143245
C 1.583122 3.241897 -0.687818
H -1.567318 2.336595 -1.564121
H 3.077894 1.917417 0.050191
C 2.073708 1.990348 -0.352440
H 2.189711 4.129947 -0.580950
H -1.083444 4.614521 -1.709053
K 3.952566 -4.480082 -3.026764

O/O'

C -1.974750 1.132545 2.307164
C -1.803567 0.256849 1.095467
O -2.761609 -0.328782 0.579872
N -0.554347 0.123582 0.594938
C -0.316377 -0.563455 -0.670623
C 1.152285 -0.384764 -1.109471
C -0.708455 -2.047082 -0.587323
O -1.508354 -2.531820 -1.392888
H -2.457656 0.552294 3.092730
H -1.038982 1.540579 2.683895
H -2.645323 1.952378 2.049312
H 0.164328 0.756511 0.914263
H -0.966225 -0.136113 -1.435089
H 1.265774 -0.889571 -2.070246
H 1.807823 -0.900874 -0.405352
C 1.546773 1.067170 -1.211289
N -0.118413 -2.764561 0.377073
C -0.367148 -4.185027 0.584387
H 0.468482 -2.280294 1.035528
H 0.516277 -4.643159 1.022643
H -0.575514 -4.652381 -0.374184
H -1.216941 -4.348344 1.250192
C 2.369537 1.659103 -0.254955
C 2.698796 3.009239 -0.320125
H 2.785338 1.057707 0.545455
O 2.476234 5.115459 -1.492162
C 2.201549 3.793508 -1.358236
C 1.379399 3.213324 -2.327944
H 3.350247 3.446017 0.426978
H 0.433070 1.433026 -3.015706
C 1.061299 1.869906 -2.248487
H 1.013592 3.830965 -3.136023
H 3.076486 5.410195 -0.799275
K -3.999463 -1.829386 -1.116421

O/O' rotamer

C -1.892755 1.280840 2.310086
C -1.852342 0.536363 1.002872
O -2.879924 0.093592 0.478007
N -0.643123 0.359388 0.424620
C -0.519120 -0.193894 -0.920542
C 0.949211 -0.131564 -1.394535
C -1.072898 -1.625335 -0.992302
O -1.934063 -1.927387 -1.823950
H -2.391829 0.658547 3.052084
H -0.909318 1.564592 2.679435
H -2.497890 2.178061 2.178148
H 0.142409 0.886978 0.776499
H -1.135179 0.389910 -1.605334
H 0.974903 -0.519658 -2.413937
H 1.554538 -0.806682 -0.786876
C 1.516772 1.264125 -1.332356
N -0.551512 -2.507663 -0.130965
C -0.959110 -3.905205 -0.077562
H 0.094908 -2.169552 0.562258
H -0.149816 -4.496954 0.343031
H -1.173790 -4.253986 -1.084203
H -1.850383 -4.037516 0.539220
C 2.381981 1.643590 -0.302790
C 2.870312 2.938507 -0.206995
H 2.704334 0.908701 0.426210
O 3.006887 5.139398 -1.016219
C 2.498797 3.889080 -1.156272
C 1.641123 3.525225 -2.196618
H 3.549275 3.226363 0.583007
H 0.503954 1.959460 -3.096482
C 1.159219 2.227175 -2.276349
H 1.360576 4.255676 -2.945796
H 2.722855 5.705700 -1.741484
K -4.332638 -1.050686 -1.323597

O/R

C 5.603996 -0.408184 -3.659067
C 4.509206 -1.246249 -3.048982
O 4.459943 -2.461564 -3.204055
N 3.567855 -0.585835 -2.315338
C 2.601948 -1.283030 -1.460571
C 2.193297 -0.411519 -0.273560
C 1.386872 -1.858606 -2.232276
O 0.218280 -1.574382 -1.917099
H 6.547805 -0.683583 -3.187419
H 5.450688 0.664283 -3.547890
H 5.684232 -0.656881 -4.715743
H 3.691971 0.400521 -2.162957
H 3.121382 -2.157752 -1.059172
H 3.106141 -0.178818 0.282009
H 1.596398 -1.036029 0.392495
C 1.436533 0.881915 -0.529046
N 1.683152 -2.704517 -3.210334
C 0.663063 -3.362619 -4.012065
H 2.671641 -2.904677 -3.365020
H -0.000910 -3.954948 -3.382467
H 1.153577 -4.015645 -4.728126
H 0.062504 -2.630272 -4.552565
C 1.181625 1.423582 -1.793611
C 0.468207 2.608237 -1.952011
H 1.526547 0.919389 -2.684961
O -0.708627 4.435953 -1.053453
C -0.012907 3.291637 -0.834405
C 0.229702 2.768309 0.438097
H 0.294991 3.026218 -2.934128
H 1.137830 1.206980 1.574130
C 0.950094 1.587276 0.577174
H -0.125588 3.292299 1.317272
H -0.905190 4.884157 -0.223533
K -1.679659 -0.090598 -1.240458

O/R rotamer

C 5.678552 -0.557611 -3.757642
C 4.529111 -1.320780 -3.139698
O 4.403172 -2.537933 -3.273542
N 3.620781 -0.583761 -2.417599
C 2.657243 -1.228079 -1.507989
C 2.314146 -0.318478 -0.319778
C 1.401238 -1.780309 -2.240444
O 0.246140 -1.386833 -1.968510
H 6.605689 -0.830932 -3.228027
H 5.553279 0.534246 -3.719874
H 5.796004 -0.879670 -4.802238
H 3.871870 0.377196 -2.213310
H 3.165756 -2.119154 -1.099465
H 3.272563 -0.032098 0.150892
H 1.802593 -0.941946 0.429869
C 1.478317 0.936207 -0.543101
N 1.647301 -2.738426 -3.134033
C 0.596969 -3.393529 -3.900267
H 2.637069 -2.974538 -3.291095
H -0.190362 -3.773441 -3.231604
H 1.037250 -4.234595 -4.450581
H 0.133355 -2.700625 -4.622468
C 1.371185 1.618360 -1.766271
C 0.583383 2.770819 -1.899785
H 1.883707 1.246056 -2.655100
O -0.909814 4.384880 -0.852176
C -0.115925 3.284893 -0.795665
C -0.018095 2.619035 0.439364
H 0.530547 3.280017 -2.867191
H 0.842429 0.981160 1.528341
C 0.771500 1.471878 0.553010
H -0.545295 3.030317 1.302870
H -0.807897 4.826901 -1.709715
K -1.519059 0.235976 -1.337081

OH

C -0.579579 0.073832 3.675357
C -0.926268 -0.265872 2.244703
O -2.084943 -0.288474 1.850415
N 0.120290 -0.541403 1.416723
C -0.052428 -0.840796 -0.000257
C 1.165065 -0.369872 -0.820794
C -0.398679 -2.330304 -0.258224
O 0.330621 -3.059186 -0.922555
H -0.991810 1.056509 3.902202
H -1.071354 -0.643381 4.331589
H 0.490186 0.077808 3.880789
H 1.039061 -0.645335 1.812349
H -0.918276 -0.261686 -0.326212
H 1.092153 0.713068 -0.922363
H 1.068980 -0.804168 -1.814789
C 2.524324 -0.710068 -0.249142
N -1.566507 -2.715507 0.284605
C -2.081693 -4.070437 0.176026
H -2.100488 -2.020284 0.792731
H -3.142221 -4.043249 -0.070339
H -1.953172 -4.619575 1.110998
H -1.542101 -4.588471 -0.611797
C 3.080889 -1.988362 -0.383341
C 4.339330 -2.280377 0.126727
H 2.504418 -2.752472 -0.884000
O 6.365994 -1.505963 1.236873
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C 4.519546 -0.023470 0.968265
H 4.759735 -3.271888 0.007500
H 2.847480 1.249483 0.567647
C 3.261871 0.258111 0.435529
H 5.064364 0.717422 1.539283
H 6.457272 -2.389736 1.611432
K 7.228136 -0.257944 -1.030683

OH rotamer

C -0.565854 0.050375 3.684744
C -0.921571 -0.293562 2.257384
O -2.083632 -0.327704 1.873189
N 0.119694 -0.559039 1.420429
C -0.059433 -0.845075 0.001327
C 1.155356 -0.366311 -0.817943
C -0.408451 -2.332107 -0.270345
O 0.316010 -3.055167 -0.947703
H -0.967232 1.038474 3.907856
H -1.061932 -0.658350 4.346731
H 0.504750 0.045341 3.885835
H 1.045782 -0.639092 1.804311
H -0.926907 -0.263516 -0.316288
H 1.077136 0.715981 -0.920518
H 1.062461 -0.800993 -1.812233
C 2.516927 -0.698463 -0.246150
N -1.573260 -2.721267 0.274572
C -2.092888 -4.073457 0.155352
H -2.101162 -2.030410 0.795758
H -3.148210 -4.042160 -0.112467
H -1.985783 -4.622169 1.093181
H -1.539824 -4.593822 -0.621422
C 3.051104 -1.989950 -0.314940
C 4.306589 -2.271961 0.211194
H 2.450794 -2.774520 -0.753055
O 6.356349 -1.577268 1.188061
C 5.057906 -1.255911 0.796004
C 4.548406 0.031261 0.887964
H 4.681747 -3.289290 0.224259
H 2.884886 1.298044 0.453424
C 3.279043 0.292654 0.377888
H 5.129516 0.821703 1.346816
H 6.647794 -1.001614 1.904306
K 6.977058 -1.991191 -1.457103