Supporting Information:

Quantum Mechanics Study on Hydrophilic and Hydrophobic Interactions in the Trivaline-Water System

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Table S1. M06-2X/6-31+G*/PCM=water relative energy, kcal mol^{-1}, and optimized dihedral angles, deg, for the bare Val_3H^+ in the β-β conformation.

	ΔE	ψ_N	$\phi_{central}$	$\psi_{central}$	ϕ_C	χ_N	$\chi_{central}$	χ_C
β-β_A	0.0	157.5	-155.5	159.5	-154.8	-55.2	-51.1	-47.1
β-β_B	0.6	145.2	-153.6	159.1	-156.0	51.3	-50.7	-47.0
β-β_C	0.3	163.6	-159.1	158.5	-155.6	-177.2	-50.9	-46.9
β-β_D	0.0	154.9	-133.8	136.2	-156.8	-54.7	56.2	-46.9
β-β_E	0.4	144.6	-118.9	125.3	-160.1	47.4	55.7	-46.6
β-β_F	0.4	163.3	-134.5	135.2	-156.3	-176.2	56.0	-46.6
β-β_G	-0.3	156.7	-137.7	165.4	-158.1	-54.7	-177.5	-46.8
β-β_H	0.2	144.9	-136.3	166.5	-157.3	49.3	-177.4	-46.8
β-β_I	0.1	163.3	-139.7	166.1	-158.1	-177.2	-177.5	-46.2
β-β_J	0.3	157.8	-154.0	157.9	-132.5	-55.5	-50.9	55.2
β-β_K	0.9	146.0	-152.0	157.7	-132.4	50.0	-50.7	55.1
β-β_L	0.7	163.6	-159.1	158.0	-132.0	-179.1	-50.5	55.0
β-β_M	0.2	158.9	-128.1	138.3	-130.8	-52.0	55.1	56.1
β-β_N	1.0	146.3	-131.7	138.7	-130.5	47.4	55.6	53.9
β-β_O	0.7	163.8	-133.0	133.2	-134.5	-177.3	55.8	55.9
β-β_P	0.0	154.8	-137.7	165.1	-134.5	-56.0	-177.4	55.6
β-β_Q	0.6	145.1	-135.9	165.4	-134.4	49.1	-177.3	55.7
β-β_R	0.5	163.7	-138.1	166.1	-133.6	-177.1	-177.5	55.6
β-β_S	-1.0	156.9	-154.4	157.4	-136.7	-55.7	-50.6	-177.7
β-β_T	-0.3	145.1	-152.4	157.0	-137.0	50.5	-50.4	-177.8
β-β_U	-0.6	164.4	-158.8	158.2	-135.7	-179.5	-49.8	-177.9
β-β_V	-1.1	158.5	-128.3	137.2	-136.0	-51.7	55.0	-176.3
β-β_W	-0.4	145.4	-131.5	135.9	-136.3	47.0	55.7	-178.8
β-β_X	-0.6	164.6	-134.3	135.6	-136.4	-178.5	55.7	-177.4
β-β_Y	-1.3	154.1	-138.4	166.0	-136.0	-55.4	-176.7	-177.6
β-β_Z	-0.7	144.9	-136.0	166.1	-136.2	51.2	-176.7	-177.5
β-β_AA	-0.7	162.7	-140.0	167.4	-134.3	-178.3	-176.5	-177.9

Table S2. M06-2X/6-31+G*/PCM=water relative energy, kcal mol^{-1}, and optimized dihedral angles, deg, for the bare Val_3H^+ in the β-PPII conformation.

	ΔE	ψ_N	$\phi_{central}$	$\psi_{central}$	ϕ_C	χ_N	$\chi_{central}$	χ_C
β-PPII_A	-0.2	155.4	-156.9	154.7	-60.0	-55.2	-54.2	-50.8
β-PPII_B	0.4	141.4	-158.1	155.0	-59.5	54.5	-53.6	-51.4
β-PPII_C	0.1	165.3	-155.8	153.2	-59.6	-175.2	-54.0	-50.8
β-PPII_D	0.1	155.1	-136.3	141.7	-57.5	-53.9	58.2	-52.5
β-PPII_E	0.7	141.3	-135.8	141.9	-57.4	51.0	58.1	-52.3
β-PPII_F	0.5	164.5	-137.0	140.8	-57.2	-178.0	58.1	-52.5
β-PPII_G	-0.4	155.7	-138.4	165.9	-59.1	-56.0	-178.0	-52.2
β-PPII_H	0.2	144.4	-137.5	166.8	-59.5	50.4	-177.7	-52.6
β-PPII_I	0.1	162.1	-140.0	166.8	-59.1	-177.4	-178.2	-52.9
β-PPII_J	-0.3	157.0	-155.6	155.4	-57.4	-53.9	-53.1	53.9
β-PPII_K	0.4	143.0	-154.3	155.4	-58.2	53.4	-52.8	53.7
β-PPII_L	0.0	164.6	-158.6	155.1	-57.8	-178.3	-52.9	53.8
β-PPII_M	0.0	156.0	-133.3	135.9	-59.0	-54.1	57.4	54.4
β-PPII_N	0.6	143.5	-133.7	138.2	-58.3	49.8	57.8	54.0
β-PPII_O	0.4	163.0	-136.3	135.6	-58.9	-177.3	58.1	54.4
β-PPII_P	-0.5	156.2	-137.6	164.5	-59.7	-54.3	-178.1	53.6
β-PPII_Q	0.1	141.5	-138.6	164.8	-60.3	52.2	-178.2	53.4
β-PPII_R	-0.1	164.7	-137.4	164.4	-59.6	-176.9	-178.0	53.7
β-PPII_S	-0.7	156.4	-156.1	154.9	-67.9	-54.3	-53.9	-177.0
β-PPII_T	0.0	140.3	-157.5	155.3	-68.1	53.9	-53.4	-177.3
β-PPII_U	-0.4	163.4	-158.9	154.5	-67.9	-177.1	-53.6	-177.0
β-PPII_V	-0.1	157.1	-133.6	138.9	-67.1	-52.5	58.9	-176.4
β-PPII_W	0.4	144.0	-133.3	140.0	-67.2	51.0	59.2	-177.1
β-PPII_X	0.3	164.1	-134.8	136.6	-69.1	-176.6	59.2	-175.8
β-PPII_Y	-0.7	156.0	-137.6	161.4	-70.6	-54.9	-179.9	-176.5
β-PPII_Z	-0.1	146.1	-134.6	162.1	-69.7	51.6	-179.2	-175.7
β-PPII_AA	-0.3	162.8	-139.2	162.5	-69.2	-177.9	-179.8	-175.9

Table S3. M06-2X/6-31+G*/PCM=water relative energy, kcal mol^{-1}, and optimized dihedral angles, deg, for the bare Val_3H^+ in the PPII-β conformation.

	ΔE	ψ_N	$\phi_{central}$	$\psi_{central}$	ϕ_C	χ_N,	$\chi_{central}$	χ_C
PPII-β_A	-0.1	154.3	-57.0	147.4	-159.6	-56.0	-50.7	-47.1
PPII-β_B	1.1	143.3	-57.7	146.5	-158.3	57.0	-51.1	-46.8
PPII-β_C	0.7	161.6	-58.7	146.2	-159.7	-179.1	-51.0	-47.0
PPII-β_D	-0.4	155.0	-57.2	137.0	-158.5	-55.2	54.5	-46.2
PPII-β_E	0.9	138.5	-71.9	129.7	-158.8	54.7	56.5	-46.3
PPII-β_F	0.2	162.8	-59.7	137.0	-158.5	-178.1	54.6	-46.4
PPII-β_G	0.0	154.7	-59.6	154.5	-161.5	-56.6	-177.9	-46.7
PPII-β_H	1.3	143.3	-62.2	156.1	-159.9	59.8	-175.9	-46.7
PPII-β_I	0.9	159.4	-62.4	157.0	-161.1	176.8	-175.6	-47.1
PPII-β_J	0.0	155.4	-58.2	146.4	-136.2	-55.4	-51.2	54.6
PPII-β_K	1.3	143.0	-58.9	147.6	-133.0	56.5	-50.8	54.4
PPII-β_L	0.8	161.5	-59.9	144.0	-136.8	-177.6	-52.3	55.0
PPII-β_M	-0.4	156.7	-57.4	138.3	-133.5	-54.3	54.3	55.6
PPII-β_N	0.8	140.1	-72.3	123.8	-137.4	56.4	57.5	57.9
PPII-β_O	0.1	163.8	-60.7	136.8	-134.5	-177.7	54.7	56.3
PPII-β_P	0.2	155.2	-60.7	153.7	-138.4	-56.2	-176.1	55.5
PPII-β_Q	1.6	144.1	-62.0	157.1	-135.2	60.9	-176.3	55.7
PPII-β_R	0.9	157.7	-63.7	157.1	-138.9	177.0	-175.9	55.6
PPII-β_S	-1.3	154.6	-58.1	145.9	-139.4	-55.1	-51.4	-178.6
PPII-β_T	0.1	141.6	-59.0	147.4	-136.7	58.7	-50.8	-178.6
PPII-β_U	-0.5	161.7	-59.0	146.0	-139.4	-177.7	-51.0	-179.0
PPII-β_V	-1.7	156.5	-57.1	137.5	-137.5	-53.8	54.1	-178.1
PPII-β_W	-0.6	140.3	-69.4	126.7	-139.4	55.0	56.6	-176.5
PPII-β_X	-1.2	163.9	-60.0	135.1	-138.6	-175.6	54.9	-178.2
PPII-β_Y	-1.1	155.1	-60.8	151.9	-141.2	-55.3	-177.6	-178.4
PPII-β_Z	0.4	141.9	-62.8	155.2	-138.3	61.0	-176.3	-178.1
PPII-β_AA	-0.3	157.8	-63.3	157.0	-140.6	175.8	-175.6	-177.6

Table S4. M06-2X/6-31+G*/PCM=water relative energy, kcal mol^{-1}, and optimized dihedral angles, deg, for the bare Val_3H^+ in the PPII-PPII conformation.

	ΔE	ψ_N	$\phi_{central}$	$\psi_{central}$	ϕ_C	χ_N,	$\chi_{central}$	χ_C
PPII-PPII_A	-0.2	154.8	-57.4	149.4	-58.4	-57.7	-52.0	-51.2
PPII-PPII_B	0.8	145.2	-56.4	147.8	-58.4	55.6	-51.7	-51.4
PPII-PPII_C	0.6	161.6	-59.2	149.7	-57.6	-179.9	-51.4	-52.2
PPII-PPII_D	0.0	154.4	-58.3	140.7	-57.6	-55.5	56.1	-53.7
PPII-PPII_E	1.0	142.9	-60.6	139.5	-57.1	57.2	56.7	-53.9
PPII-PPII_F	0.6	163.7	-60.5	140.6	-57.1	180.0	56.6	-54.0
PPII-PPII_G	0.2	154.4	-63.6	160.7	-59.0	-56.0	-176.6	-52.4
PPII-PPII_H	1.3	145.6	-61.6	157.2	-58.9	58.0	-176.2	-51.8
PPII-PPII_I	1.0	162.9	-64.3	159.3	-59.0	179.0	-175.9	-51.9
PPII-PPII_J	-0.3	155.6	-57.2	148.7	-57.7	-57.1	-51.2	54.1
PPII-PPII_K	0.8	145.3	-57.6	148.6	-57.1	56.2	-50.9	53.9
PPII-PPII_L	0.5	163.9	-58.5	147.6	-57.7	-179.8	-50.8	53.7
PPII-PPII_M	0.0	156.1	-56.9	137.2	-60.4	-56.3	56.5	53.3
PPII-PPII_N	1.0	143.5	-59.8	136.2	-60.1	58.0	57.0	53.3
PPII-PPII_O	0.5	164.5	-59.5	137.1	-59.7	-177.9	56.6	53.9
PPII-PPII_P	-0.1	154.6	-62.2	159.6	-58.4	-56.3	-176.0	54.1
PPII-PPII_Q	1.1	144.5	-63.5	158.2	-57.9	58.5	-176.0	54.0
PPII-PPII_R	0.8	161.0	-65.0	160.1	-58.2	179.1	-175.2	53.9
PPII-PPII_S	-0.6	154.4	-58.6	151.0	-65.5	-56.7	-50.5	-176.7
PPII-PPII_T	0.4	143.8	-59.4	148.9	-65.3	56.6	-50.2	-177.1
PPII-PPII_U	0.2	163.4	-59.7	149.4	-65.1	-178.0	-50.7	-176.4
PPII-PPII_V	-0.1	154.2	-60.4	138.6	-68.4	-54.8	57.6	-176.0
PPII-PPII_W	0.8	142.1	-60.9	135.9	-71.6	58.4	57.7	-176.3
PPII-PPII_X	0.4	161.7	-62.0	139.7	-68.1	-179.8	57.8	-176.3
PPII-PPII_Y	-0.3	154.5	-61.3	156.9	-68.8	-55.5	-178.3	-175.9
PPII-PPII_Z	0.9	145.8	-60.7	154.8	-68.8	58.3	-177.2	-175.5
PPII-PPII_AA	0.5	160.3	-63.9	157.6	-69.5	178.7	-177.7	-175.9

Table S5. M06-2X/6-31+G*/PCM=water optimized dihedral angles, deg, of the $Val_3H^+ \cdot nH_2O$ (n=10, 14, 18 and 22) complexes in the β-β conformation.

	ψ_N	$\phi_{central}$	$\psi_{central}$	ϕ_C	χ_N	$\chi_{central}$	χ_C
10h2o_β-β_A	150.4	-153.1	149.7	-155.8	-45.2	-49.2	-45.2
10h2o_β-β_B	136.3	-153.0	148.1	-154.0	61.7	-52.4	-43.3
10h2o_β-β_C	158.8	-148.6	155.1	-156.3	-172.9	-50.3	-46.7
10h2o_β-β_D	155.3	-125.6	107.6	-157.4	-46.5	53.0	-44.8
10h2o_β-β_E	136.6	-91.9	95.7	-158.8	67.5	55.2	-54.1
10h2o_β-β_F	161.7	-107.7	113.3	-156.2	-167.8	50.4	-41.3
14h2o_β-β_A	143.3	-139.3	141.7	-132.9	-47.7	-72.1	-49.8
14h2o_β-β_B	130.3	-133.7	141.0	-142.1	62.6	-58.8	-47.6
14h2o_β-β_C	151.1	-135.7	148.5	-144.5	-172.3	-55.7	-48.4
18h2o_β-β_A	145.8	-144.1	142.0	-144.8	-47.0	-68.8	-45.3
18h2o_β-β_B	133.6	-140.7	138.7	-144.5	62.1	-64.3	-45.5
18h2o_β-β_C	153.6	-139.2	146.2	-146.8	-171.4	-60.9	-46.7
22h2o_β-β_A	146.1	-142.7	141.6	-140.1	-47.1	-69.1	-46.3
22h2o_β-β_B	133.9	-133.9	139.6	-146.6	62.5	-60.0	-44.1
22h2o_β-β_C	154.4	-131.8	145.2	-144.8	-174.5	-63.6	-46.3
22h2o_β-β_D	148.6	-112.9	127.7	-124.6	-48.7	52.3	-48.3
22h2o_β-β_E	133.3	-108.6	124.5	-128.4	59.1	52.9	-52.7
22h2o_β-β_F	159.9	-99.3	130.4	-122.0	-169.1	53.0	-50.2
22h2o_β-β_J	146.1	-142.0	139.1	-125.2	-47.4	-68.8	53.8
22h2o_β-β_K	135.2	-137.5	141.4	-130.9	62.4	-62.1	58.2
22h2o_β-β_S	146.1	-144.0	140.8	-134.7	-48.3	-68.7	-178.3

Table S6. M06-2X/6-31+G*/PCM=water optimized dihedral angles, deg, of the $Val_3H^+ \cdot nH_2O$ (n=10, 14, 18 and 22) complexes in the β-PPII conformation.

	ψ_N	$\phi_{central}$	$\psi_{central}$	ϕ_C	χ_N	$\chi_{central}$	χ_C
10h2o_β-PPII_A	142.2	-128.7	159.3	-55.7	-71.5	-52.5	-54.1
10h2o_β-PPII_B	138.9	-141.1	158.6	-56.3	59.1	-54.9	-51.1
10h2o_β-PPII_C	162.2	-152.0	159.6	-56.5	-173.9	-53.6	-51.7
14h2o_β-PPII_A	148.4	-142.4	149.4	-52.2	-48.2	-68.2	-54.3
14h2o_β-PPII_B	136.4	-130.9	151.8	-53.1	67.0	-59.9	-54.6
14h2o_β-PPII_C	155.7	-134.8	154.9	-54.2	-171.5	-56.0	-55.3
14h2o_β-PPII_J	148.2	-142.3	147.0	-52.8	-48.4	-69.0	52.3
14h2o_β-PPII_S	146.0	-140.2	153.1	-58.5	-48.7	-63.5	-179.3
18h2o_β-PPII_A	144.7	-136.8	150.9	-56.7	-49.6	-61.4	-50.3
18h2o_β-PPII_B	135.9	-131.9	151.0	-57.0	61.6	-57.2	-50.7
18h2o_β-PPII_C	158.4	-129.4	154.7	-58.9	-169.2	-52.3	-50.3
18h2o_β-PPII_J	147.9	-141.8	146.9	-56.1	-48.5	-67.9	52.2
18h2o_β-PPII_S	144.9	-139.2	151.8	-59.7	-49.5	-62.9	-178.7
22h2o_β-PPII_A	143.9	-138.0	128.7	-58.0	-50.0	-72.8	-46.6
22h2o_β-PPII_B	136.0	-134.6	128.8	-56.3	62.1	-72.1	-47.6
22h2o_β-PPII_C	154.9	-139.1	130.8	-57.3	-168.6	-73.6	-46.7
22h2o_β-PPII_D	149.3	-116.2	134.6	-56.6	-49.6	51.8	-48.7
22h2o_β-PPII_E	132.7	-107.7	131.1	-55.7	60.0	51.6	-49.3
22h2o_β-PPII_F	159.7	-109.2	136.5	-55.4	-170.7	51.8	-48.0
22h2o_β-PPII_J	146.4	-137.6	135.4	-50.5	-48.7	-71.4	49.9
22h2o_β-PPII_K	137.8	-130.5	125.9	-52.4	64.6	-71.9	52.0
22h2o_β-PPII_S	146.8	-139.2	137.0	-59.9	-48.6	-73.1	-174.0

Table S7. M06-2X/6-31+G*/PCM=water optimized dihedral angles, deg, of the $Val_3H^+ \cdot nH_2O$ (n=10, 14, 18 and 22) complexes in the PPII-PPII conformation.

	ψ_N	$\phi_{central}$	$\psi_{central}$	ϕ_C	χ_N	$\chi_{central}$	χ_C
10h2o_PPII-PPII_A	137.7	-66.4	141.6	-56.8	-72.5	-50.3	-50.6
10h2o_PPII-PPII_B	133.6	-66.1	142.6	-57.2	54.0	-49.4	-52.0
10h2o_PPII-PPII_C	159.2	-63.9	143.0	-60.8	-169.4	-47.6	-48.2
10h2o_PPII-PPII_D	144.2	-62.3	133.4	-58.3	-71.3	56.6	-51.3
10h2o_PPII-PPII_E	141.2	-62.2	129.3	-59.6	64.5	56.0	-51.8
10h2o_PPII-PPII_F	165.0	-60.2	133.2	-63.6	-169.8	56.5	-47.9
10h2o_PPII-PPII_G	137.7	-68.5	150.0	-56.8	-71.6	-169.6	-52.3
10h2o_PPII-PPII_H	134.8	-69.3	151.1	-57.5	65.6	-170.1	-51.8
10h2o_PPII-PPII_I	157.6	-63.7	146.9	-61.2	-168.5	-171.3	-47.4
10h2o_PPII-PPII_J	136.9	-65.5	142.5	-54.6	-72.8	-48.3	53.9
10h2o_PPII-PPII_S	136.2	-66.1	144.1	-60.8	-72.3	-48.8	176.1
14h2o_PPII-PPII_A	138.6	-66.7	137.0	-80.2	-71.5	-55.1	-33.5
14h2o_PPII-PPII_B	140.8	-68.1	130.3	-78.2	68.6	-57.6	-36.7
14h2o_PPII-PPII_C	161.7	-63.4	138.1	89.5	-169.1	-51.0	-38.1
14h2o_PPII-PPII_D	146.1	-63.7	130.2	-74.5	-71.4	57.1	-37.7
14h2o_PPII-PPII_E	145.6	-64.7	125.1	-73.0	68.2	58.8	-39.6
14h2o_PPII-PPII_F	165.9	-60.2	131.7	-82.2	-170.3	56.0	-39.8
14h2o_PPII-PPII_G	138.4	-70.3	150.4	-65.5	-71.0	-166.3	-39.1
14h2o_PPII-PPII_H	140.1	-75.5	150.6	-63.7	-68.6	-165.2	-42.2
14h2o_PPII-PPII_I	161.7	-66.4	147.7	-68.8	-170.2	-166.0	-41.1
14h2o_PPII-PPII_J	135.5	-66.7	142.3	-62.7	-72.4	-48.7	55.7
14h2o_PPII-PPII_S	137.3	-68.3	143.9	-73.7	-72.8	-42.1	-164.5
18h2o_PPII-PPII_A	137.9	-66.0	137.9	-75.3	-72.0	-55.0	-32.5
18h2o_PPII-PPII_B	139.4	-67.4	132.7	-73.3	67.8	56.6	-35.7
18h2o_PPII-PPII_C	160.7	-63.6	138.5	-80.0	-168.9	-53.8	-35.4
18h2o_PPII-PPII_D	145.5	-62.5	131.5	-73.2	-71.5	56.5	-37.3
18h2o_PPII-PPII_E	144.9	-63.8	127.0	-71.0	68.1	57.7	-39.7
18h2o_PPII-PPII_F	165.4	-59.1	132.4	-77.1	-169.0	56.1	-40.1
18h2o_PPII-PPII_G	139.2	-69.9	149.8	-66.1	-70.4	-165.5	-38.8
18h2o_PPII-PPII_H	139.9	-74.5	150.4	-64.8	68.4	-164.6	-41.0
18h2o_PPII-PPII_I	160.9	-65.9	149.8	-69.1	-170.0	-166.8	-40.0
18h2o_PPII-PPII_J	133.5	-65.7	143.8	-62.2	-72.4	-52.0	55.5
18h2o_PPII-PPII_S	139.9	-68.1	143.6	-70.4	-71.3	-24.1	-167.0
22h2o_PPII-PPII_A	137.2	-66.5	138.6	-74.0	-71.5	-56.4	-29.4
22h2o_PPII-PPII_B	139.5	-69.3	133.9	-72.9	67.8	-58.4	-31.6
22h2o_PPII-PPII_C	159.5	-64.6	142.5	-78.7	-169.0	-50.6	-32.2
22h2o_PPII-PPII_D	144.8	-64.7	133.1	-74.1	-70.0	56.5	-31.6
22h2o_PPII-PPII_E	144.2	-66.1	128.6	-71.6	67.9	57.3	-33.1
22h2o_PPII-PPII_F	163.9	-62.7	134.7	-78.2	-168.8	57.5	-35.3
22h2o_PPII-PPII_G	139.9	-69.9	147.2	-67.5	-68.6	-165.7	-36.1
22h2o_PPII-PPII_H	142.1	-73.8	144.0	-66.1	68.3	-165.9	-38.1
22h2o_PPII-PPII_I	161.0	-67.5	150.6	-68.3	-170.6	-168.0	-39.5

Table S8. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $10H_2O$_β-β_A.

N	3.917707	-0.725891	0.021192
C	2.731323	0.130832	-0.239124
C	1.503476	-0.752951	-0.050890
N	0.386716	-0.161444	0.363132
C	-0.826350	-0.940141	0.552960
C	-2.018368	-0.015274	0.360809
N	-3.132683	-0.570585	-0.116847
C	-4.370688	0.179130	-0.246155
C	-5.499054	-0.835228	-0.218555
O	-6.689643	-0.258372	-0.068767
O	1.573382	-1.964122	-0.330060
O	-1.956310	1.185705	0.674657
C	-4.383644	1.032903	-1.543409
O	-5.337994	-2.028558	-0.348184
C	2.807914	0.750458	-1.652608
C	-0.838341	-1.623948	1.946148
C	-1.914040	-2.704973	2.042713
C	-4.534592	0.159111	-2.788372
C	-5.432501	2.143194	-1.499359
C	1.875088	1.955212	-1.770016
C	2.538330	-0.264134	-2.765708
C	-0.955554	-0.615167	3.087004
H	3.953392	-1.567272	-0.594497
H	3.861984	-1.064432	0.999644
H	2.739697	0.929003	0.510348
H	0.415487	0.819735	0.671246
H	-0.837414	-1.719273	-0.215862
H	-3.155967	-1.556390	-0.362616
H	-4.466245	0.841311	0.621159
H	-7.381222	-0.946740	-0.092910
H	-3.393217	1.503915	-1.565530
H	3.839300	1.112916	-1.753641
H	0.144626	-2.105524	2.015438
H	-2.921832	-2.273843	2.029966
H	-1.804013	-3.252336	2.983860
H	-1.834418	-3.427906	1.222884
H	-5.535623	-0.287671	-2.835916
H	-3.795600	-0.649110	-2.811105
H	-4.399758	0.763959	-3.689758
H	-6.447891	1.737994	-1.529303
H	-5.303747	2.800075	-2.365088
H	-5.330706	2.750804	-0.593758
H	2.107480	2.714797	-1.016207
H	0.824247	1.666554	-1.652068
H	1.984478	2.412010	-2.758462
H	2.733112	0.199193	-3.737179
H	1.489973	-0.586644	-2.753903
H	3.171643	-1.153607	-2.684118
H	-0.783154	-1.114665	4.045043
H	-1.959420	-0.173414	3.119211

H	-0.220585	0.192375	2.992529
O	2.824918	-1.445713	2.485393
H	2.570392	-2.392034	2.410220
H	3.192001	-1.326950	3.373464
O	2.051004	-3.922827	1.585140
H	1.726858	-3.459629	0.788632
H	1.308817	-4.449098	1.917398
O	4.319404	-3.120975	-1.437533
H	5.024508	-3.121521	-2.100776
H	3.512381	-3.458093	-1.887898
O	1.822220	-3.780119	-2.393624
H	1.611413	-3.553135	-3.311261
H	1.453126	-3.064438	-1.841936
O	0.834080	2.586504	1.208154
H	0.330536	3.043313	0.494108
H	0.250100	2.693931	1.992457
O	6.104903	0.915024	-0.582030
H	6.876225	0.920091	0.003211
H	5.788792	1.849536	-0.635867
O	5.026341	3.403186	-0.706227
H	4.577364	3.666900	-1.522429
H	4.367672	3.484289	0.024121
O	3.372479	3.541188	1.455153
H	2.439888	3.221567	1.418149
H	3.783183	3.091234	2.207799
O	-1.343174	2.836200	2.851364
H	-1.448999	2.542048	3.767833
H	-1.781548	2.166279	2.292814
O	-1.014593	3.467573	-0.631739
H	-1.594829	2.752477	-0.307082
H	-1.471546	4.295957	-0.423905
H	4.792742	-0.174770	-0.117013

Table S9. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $10H_2O$_β-β_B.

N	-3.763029	-0.879297	-0.115590
C	-2.610798	-0.045251	0.327534
C	-1.365949	-0.916909	0.215045
N	-0.283366	-0.357171	-0.312993
C	0.960463	-1.101060	-0.434761
C	2.105260	-0.100941	-0.410669
N	3.251052	-0.513899	0.131636
C	4.442525	0.317190	0.134121
C	5.632654	-0.621636	0.199374
O	6.780788	0.007163	-0.044870
O	-1.396345	-2.087695	0.640600

O	1.974594	1.032439	-0.905391
C	4.428498	1.322666	1.318401
O	5.551019	-1.798215	0.473785
C	-2.814997	0.438302	1.774853
C	0.974543	-1.968347	-1.720650
C	2.144976	-2.950788	-1.726998
C	4.700740	0.625550	2.651230
C	5.370940	2.502880	1.088836
C	-4.126189	1.216344	1.902838
C	-1.633975	1.301571	2.223109
C	0.940473	-1.123413	-2.991886
H	-4.028487	-1.572798	0.616752
H	-3.505348	-1.391330	-0.984032
H	-2.535938	0.811987	-0.349126
H	-0.331827	0.616566	-0.634574
H	1.033066	-1.766499	0.432211
H	3.332644	-1.450284	0.517537
H	4.477982	0.871822	-0.809650
H	7.516385	-0.628258	0.044151
H	3.401851	1.708458	1.335715
H	-2.866289	-0.455503	2.412567
H	0.044517	-2.544571	-1.669306
H	3.106817	-2.435304	-1.831974
H	2.045533	-3.636551	-2.573834
H	2.170994	-3.552252	-0.811031
H	5.739300	0.276431	2.708014
H	4.039555	-0.234613	2.803093
H	4.540800	1.322967	3.478551
H	6.418554	2.188683	1.100377
H	5.229270	3.242769	1.882688
H	5.167686	2.991202	0.129526
H	-5.005258	0.605920	1.672674
H	-4.122212	2.084918	1.232447
H	-4.238442	1.581989	2.927949
H	-1.793418	1.637727	3.251573
H	-1.545298	2.189565	1.586615
H	-0.683216	0.759633	2.190934
H	0.789325	-1.769333	-3.862162
H	1.885149	-0.584682	-3.137108
H	0.118556	-0.399534	-2.967611
O	-2.486295	-2.061143	-2.300025
H	-2.207668	-2.971113	-2.051414
H	-2.847788	-2.114454	-3.196720
O	-1.506285	-4.301484	-1.048904
H	-1.401558	-3.726993	-0.265214
H	-2.143628	-4.985851	-0.796555
O	-4.573185	-2.634380	1.954253
H	-5.245280	-2.256016	2.539564
H	-3.798897	-2.852120	2.521801
O	-2.142176	-3.147075	3.102733
H	-1.856941	-2.663869	3.891905
H	-1.685495	-2.730977	2.344890
O	-0.891733	2.460094	-0.930180
H	-0.193479	2.872416	-0.368600
H	-0.521686	2.526297	-1.838336
O	-6.032155	0.623508	-0.744071
H	-6.387510	0.377941	-1.610852

H	-5.910399	1.605128	-0.768107
O	-5.673582	3.312993	-0.783834
H	-6.169074	3.731978	-0.064995
H	-4.728697	3.556514	-0.636299
O	-3.078766	3.985957	-0.286930
H	-2.323376	3.434041	-0.598605
H	-2.870498	4.893178	-0.553964
O	0.839596	2.426001	-3.058769
H	0.708433	2.019766	-3.927910
H	1.369958	1.794996	-2.535233
O	1.326111	3.346031	0.449999
H	1.857986	2.668515	-0.010083
H	1.692738	4.203346	0.187807
H	-4.599655	-0.289781	-0.326857

Table S10. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $10H_2O$_β-β_C.

N	3.760774	-0.962335	-0.167569
C	2.599774	-0.050157	-0.330404
C	1.348587	-0.844324	0.018727
N	0.285104	-0.120658	0.357295
C	-0.969885	-0.746298	0.730980
C	-2.101995	0.178495	0.304168
N	-3.285464	-0.392544	0.081967
C	-4.476549	0.384742	-0.218073
C	-5.663440	-0.475571	0.175560
O	-6.801284	0.215054	0.196562
O	1.343936	-2.085306	-0.071838
O	-1.930202	1.407060	0.212385
C	-4.522965	0.798897	-1.713756
O	-5.587750	-1.660597	0.414640
C	2.496902	0.553938	-1.743846
C	-1.003670	-1.043129	2.254518
C	-2.149872	-1.978162	2.638779
C	-4.787194	-0.402942	-2.620192
C	-5.514159	1.932674	-1.973886
C	2.108769	-0.476723	-2.806191
C	3.785129	1.288184	-2.115849
C	-1.026256	0.239084	3.085579
H	3.750349	-1.775980	-0.818995
H	3.719499	-1.333076	0.799989
H	2.731366	0.756619	0.397490
H	0.401843	0.891327	0.488021
H	-1.040645	-1.693253	0.185860
H	-3.397816	-1.398961	0.167613
H	-4.468761	1.286198	0.404135
H	-7.535204	-0.388472	0.420035

H	-3.514300	1.178434	-1.917606
H	1.688383	1.292229	-1.681230
H	-0.059775	-1.567667	2.447953
H	-3.123801	-1.481846	2.558932
H	-2.030025	-2.297104	3.678596
H	-2.163203	-2.878074	2.013153
H	-5.809282	-0.779134	-2.486837
H	-4.089710	-1.223920	-2.422105
H	-4.676509	-0.113137	-3.669195
H	-6.548221	1.599559	-1.848350
H	-5.395820	2.290565	-3.001260
H	-5.340213	2.776835	-1.298069
H	1.121663	-0.910174	-2.610499
H	2.837378	-1.293514	-2.866908
H	2.069391	0.006336	-3.787046
H	3.633774	1.854552	-3.039386
H	4.614898	0.592477	-2.286021
H	4.084382	1.990740	-1.329816
H	-0.903167	-0.000114	4.146016
H	-1.984186	0.762896	2.973592
H	-0.219367	0.924798	2.801668
O	2.837854	-1.340577	2.448799
H	2.364316	-2.191986	2.581355
H	3.328207	-1.166614	3.265343
O	1.271616	-3.605215	2.258154
H	1.144430	-3.332824	1.328440
H	1.728314	-4.458919	2.226563
O	3.989105	-3.312985	-1.727399
H	4.542545	-3.295069	-2.521494
H	3.108123	-3.652198	-2.006245
O	1.356542	-3.974890	-2.111367
H	0.944032	-3.739103	-2.955204
H	1.102277	-3.276177	-1.477768
O	1.093667	2.672869	0.595139
H	0.787548	2.904132	-0.309903
H	0.412479	3.074688	1.183270
O	6.256435	0.326413	-0.302049
H	6.861254	-0.032967	0.363486
H	6.211150	1.298684	-0.130116
O	6.019389	2.986895	0.227562
H	6.076292	3.582073	-0.533800
H	5.133418	3.134551	0.633528
O	3.616358	3.250243	1.496849
H	2.717850	3.089098	1.126538
H	3.634804	2.799920	2.353656
O	-1.184002	3.554434	1.838071
H	-1.325434	3.508986	2.795069
H	-1.673673	2.803676	1.450241
O	-0.333261	2.666486	-1.741805
H	-1.061636	2.273379	-1.222234
H	-0.706907	3.441138	-2.187129
H	4.668501	-0.456163	-0.271487

Table S11. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $10H_2O$_β-β_D.

N	3.573367	-0.306180	-0.840467
C	2.288472	0.337967	-0.471395
C	1.379646	-0.742518	0.101027
N	0.428964	-0.321174	0.932995
C	-0.689361	-1.160351	1.348493
C	-1.940882	-0.353031	1.008488
N	-2.668808	-0.772201	-0.027228
C	-3.837149	-0.042632	-0.490951
C	-4.704314	-1.032119	-1.245394
O	-5.923593	-0.551812	-1.481513
O	1.501009	-1.919759	-0.278616
O	-2.222792	0.675775	1.646900
C	-3.429656	1.164943	-1.379734
O	-4.321470	-2.118569	-1.618836
C	1.643916	1.022061	-1.701280
C	-0.622817	-1.535740	2.835282
C	0.602930	-2.412451	3.086937
C	-2.916226	0.711918	-2.745903
C	-4.545377	2.200877	-1.503885
C	0.568526	2.022521	-1.277193
C	1.084308	0.017576	-2.710351
C	-1.908867	-2.244007	3.263148
H	3.452860	-1.116011	-1.487391
H	4.010441	-0.662526	0.030585
H	2.513517	1.093864	0.289227
H	0.459958	0.648049	1.283781
H	-0.651769	-2.071740	0.743000
H	-2.434382	-1.636822	-0.506198
H	-4.387694	0.321782	0.382989
H	-6.428983	-1.207937	-1.998075
H	-2.600138	1.635720	-0.838884
H	2.456957	1.584654	-2.178080
H	-0.515155	-0.604012	3.406189
H	0.498942	-3.366432	2.554690
H	0.700933	-2.631477	4.154569
H	1.524897	-1.925340	2.752591
H	-3.732332	0.315906	-3.363234
H	-2.148355	-0.064117	-2.654872
H	-2.474959	1.558575	-3.280740
H	-5.390975	1.815053	-2.080510
H	-4.161483	3.088991	-2.015515
H	-4.911764	2.509419	-0.518760
H	0.952420	2.745147	-0.549031
H	-0.297290	1.517321	-0.832059
H	0.211231	2.575749	-2.151261
H	0.737146	0.546834	-3.602641
H	0.225854	-0.518837	-2.286494
H	1.828040	-0.722793	-3.023193
H	-1.839641	-2.550952	4.310881
H	-2.072761	-3.144817	2.659028

H	-2.787172	-1.597630	3.161315
O	3.850932	-1.164192	1.784126
H	3.748413	-2.141589	1.736291
H	4.601570	-0.990695	2.370841
O	3.174689	-3.712037	1.073230
H	2.434651	-3.315498	0.573974
H	2.776874	-4.333195	1.700723
O	3.607822	-2.549186	-2.567581
H	3.942136	-2.412491	-3.465729
H	2.739570	-3.002817	-2.658806
O	1.066926	-3.605238	-2.427835
H	0.442353	-3.361654	-3.126917
H	0.885336	-3.006692	-1.678567
O	0.552473	2.346906	1.995140
H	-0.170194	2.828812	1.526947
H	0.182002	2.210065	2.894514
O	4.980661	1.765088	-2.085336
H	5.933916	1.849681	-1.938349
H	4.569423	2.596369	-1.745736
O	3.652986	3.897914	-1.066668
H	2.883130	4.235961	-1.546416
H	3.366895	3.741959	-0.135813
O	3.015828	3.412920	1.541370
H	2.135778	3.051331	1.798616
H	3.678666	2.889896	2.015205
O	-1.277166	1.887216	3.975663
H	-1.304956	1.434661	4.830972
H	-1.737828	1.309690	3.334542
O	-1.758552	3.310048	0.862372
H	-2.235767	2.504883	1.141651
H	-2.186628	4.049072	1.319849
H	4.204722	0.392840	-1.289882

Table S12. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $10H_2O$_β-β_E.

N	3.003419	-1.570735	0.679080
C	2.078181	-0.726658	-0.123398
C	0.893998	-0.366392	0.767122
N	0.467061	0.893124	0.725000
C	-0.743525	1.332606	1.413199
C	-1.876848	1.193402	0.391737
N	-2.574173	0.057569	0.463496
C	-3.610611	-0.299910	-0.490222
C	-4.491790	-1.327491	0.196654
O	-5.673108	-1.460948	-0.401271
O	0.357409	-1.250394	1.461353

O	-2.075369	2.048884	-0.486817
C	-2.998331	-0.852941	-1.805860
O	-4.143350	-1.973381	1.160361
C	1.586684	-1.476310	-1.376885
C	-0.583985	2.751774	1.963585
C	0.527876	2.777694	3.012920
C	-2.215426	-2.141545	-1.559222
C	-4.037515	-1.023625	-2.913284
C	2.754385	-2.056304	-2.176655
C	0.765033	-0.526070	-2.247290
C	-1.907903	3.242916	2.551223
H	2.653272	-2.549454	0.762474
H	3.110186	-1.151214	1.625428
H	2.629930	0.175496	-0.415401
H	0.881853	1.558236	0.058189
H	-0.918678	0.643133	2.244908
H	-2.383021	-0.606633	1.208916
H	-4.204379	0.591329	-0.717491
H	-6.182293	-2.159666	0.052052
H	-2.295288	-0.074389	-2.127227
H	0.948288	-2.302813	-1.031156
H	-0.296999	3.406127	1.130839
H	0.250611	2.162835	3.878414
H	0.688434	3.801208	3.364963
H	1.472124	2.393489	2.616040
H	-2.882540	-2.962816	-1.268495
H	-1.465049	-2.005906	-0.770406
H	-1.689798	-2.445937	-2.469366
H	-4.716011	-1.855904	-2.705020
H	-3.527956	-1.230418	-3.859195
H	-4.637671	-0.116631	-3.040630
H	3.323496	-2.802229	-1.612941
H	3.441561	-1.262398	-2.491143
H	2.367674	-2.548486	-3.074079
H	0.372438	-1.050968	-3.123091
H	1.392180	0.300071	-2.605080
H	-0.088103	-0.095208	-1.712374
H	-1.781769	4.244067	2.973776
H	-2.240994	2.577608	3.357176
H	-2.700563	3.293759	1.797796
O	2.882840	0.096499	2.898267
H	2.191830	-0.181714	3.541128
H	3.675135	0.299847	3.416731
O	0.749742	-0.999935	4.222635
H	0.319696	-1.180764	3.365452
H	0.106219	-0.512057	4.756882
O	2.124576	-4.254329	0.722705
H	2.331591	-4.780087	-0.063428
H	1.148738	-4.301084	0.841590
O	-0.525240	-3.893094	1.273971
H	-1.222505	-4.062737	0.623624
H	-0.402655	-2.924710	1.304550
O	1.119778	2.789045	-1.335158
H	0.572246	2.438308	-2.075356
H	0.643999	3.613421	-1.094393
O	5.481013	-1.340843	-0.589160
H	6.179797	-1.048023	0.013982

H	5.411762	-0.643878	-1.286644
O	5.030644	0.553763	-2.489495
H	5.794269	0.884149	-2.984872
H	4.616326	1.342016	-2.063106
O	3.855753	2.661896	-1.228031
H	2.881638	2.762032	-1.323679
H	4.035935	2.694012	-0.277084
O	-0.955726	4.567422	-0.991353
H	-1.148252	5.323131	-0.417090
H	-1.508642	3.826153	-0.671728
O	-0.915236	2.033651	-3.050063
H	-1.543935	2.043631	-2.302677
H	-1.176184	2.773745	-3.618767
H	3.946769	-1.584153	0.228690

Table S13. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $10H_2O$_β-β_F.

N	3.140233	-1.481824	0.421793
C	2.216958	-0.489901	-0.183315
C	1.113621	-0.214465	0.828313
N	0.424209	0.906714	0.623658
C	-0.813270	1.228767	1.321673
C	-1.923802	1.069226	0.285321
N	-2.800534	0.082674	0.473328
C	-3.856223	-0.187274	-0.488434
C	-4.966489	-0.900721	0.258349
O	-6.088037	-0.965220	-0.456812
O	0.858009	-1.041425	1.720167
O	-1.964362	1.808645	-0.714686
C	-3.326815	-1.033234	-1.680413
O	-4.836520	-1.386370	1.359790
C	1.602661	-0.965992	-1.517253
C	-0.765680	2.646753	1.909170
C	0.266028	2.699671	3.035736
C	-3.135963	-2.497705	-1.286716
C	-4.199161	-0.887343	-2.925724
C	0.504251	-2.015153	-1.329337
C	2.686602	-1.450290	-2.480121
C	-2.148168	3.073151	2.403842
H	2.703006	-2.411250	0.600916
H	3.448292	-1.087706	1.329689
H	2.805620	0.417563	-0.357563
H	0.713159	1.534831	-0.140171
H	-0.940140	0.498603	2.127556
H	-2.775063	-0.479499	1.319332
H	-4.233926	0.769806	-0.863346
H	-6.758645	-1.465699	0.045875
H	-2.341914	-0.604623	-1.907231

H	1.135272	-0.075719	-1.953380
H	-0.447917	3.323474	1.104159
H	-0.086876	2.116925	3.895448
H	0.413749	3.731063	3.369290
H	1.234919	2.298770	2.718822
H	-4.102627	-2.996984	-1.146317
H	-2.564215	-2.594873	-0.357102
H	-2.594635	-3.033255	-2.072187
H	-5.193696	-1.315800	-2.770571
H	-3.730348	-1.410840	-3.764752
H	-4.315853	0.165546	-3.204286
H	-0.336514	-1.621668	-0.744688
H	0.877215	-2.914805	-0.825697
H	0.111631	-2.313886	-2.306400
H	2.245131	-1.634671	-3.463930
H	3.138189	-2.389934	-2.140517
H	3.483795	-0.708427	-2.598723
H	-2.091868	4.058955	2.874639
H	-2.526252	2.364383	3.150703
H	-2.876688	3.133244	1.588052
O	3.479023	0.416565	2.444149
H	2.967183	0.212166	3.258728
H	4.345919	0.734500	2.735592
O	1.692113	-0.492186	4.315539
H	1.121542	-0.730212	3.559365
H	1.173058	0.109462	4.868494
O	2.217838	-4.067719	1.079726
H	2.284325	-4.770045	0.416760
H	1.280750	-4.052138	1.381027
O	-0.319437	-3.540968	1.972861
H	-1.071369	-3.801822	1.421684
H	-0.188140	-2.583748	1.829949
O	1.208657	2.572989	-1.600920
H	0.723790	2.102274	-2.316636
H	0.678937	3.389177	-1.458913
O	5.552050	-1.636066	-1.009873
H	6.296756	-1.635847	-0.390765
H	5.642913	-0.811019	-1.545366
O	5.538607	0.652257	-2.489582
H	6.386564	1.082307	-2.672578
H	4.982166	1.324511	-2.033161
O	3.914339	2.448746	-1.214821
H	2.958271	2.568643	-1.413627
H	4.033424	2.680503	-0.282511
O	-0.889713	4.308837	-1.339327
H	-1.064025	5.066860	-0.762732
H	-1.430544	3.567028	-1.001000
O	-0.625779	1.164127	-3.084145
H	-1.302898	1.366440	-2.408665
H	-0.977176	1.491636	-3.925512
H	3.996794	-1.607788	-0.162297

Table S14. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $14H_2O$_β-β_A.

N	-4.008570	1.185937	0.066337
C	-3.112926	0.055649	-0.300085
C	-1.688193	0.540479	-0.047114
N	-0.820838	-0.343940	0.426572
C	0.525468	0.032192	0.829370
C	1.489324	-1.049104	0.359617
N	2.664374	-0.610754	-0.090041
C	3.717569	-1.514969	-0.505976
C	5.016405	-1.055108	0.127934
O	5.939226	-2.011841	0.143549
O	-1.403229	1.727186	-0.300954
O	1.185510	-2.254360	0.426516
C	3.825414	-1.568808	-2.054314
O	5.210495	0.068025	0.546550
C	-3.359041	-0.387377	-1.756877
C	0.609279	0.266227	2.364636
C	2.059260	0.431194	2.825519
C	4.307852	-0.236195	-2.629387
C	4.685049	-2.733610	-2.544523
C	-2.744172	-1.764568	-2.000470
C	-2.865646	0.625787	-2.791866
C	-0.092898	-0.824114	3.172894
H	-3.803731	2.055305	-0.470188
H	-3.858610	1.409933	1.067901
H	-5.004328	0.919364	-0.098041
H	-3.353792	-0.772188	0.375576
H	-1.149786	-1.290611	0.660539
H	0.773096	0.970842	0.325864
H	2.830832	0.402585	-0.123048
H	3.474313	-2.512027	-0.128602
H	6.766795	-1.653506	0.518004
H	2.792469	-1.741977	-2.382625
H	-4.448753	-0.479339	-1.851942
H	0.076054	1.210925	2.530942
H	2.588371	-0.529849	2.803774
H	2.079951	0.801041	3.855080
H	2.618279	1.131207	2.197194
H	5.358227	-0.054086	-2.368341
H	3.713630	0.610218	-2.266525
H	4.238172	-0.251579	-3.721055
H	5.742098	-2.580969	-2.307536
H	4.592589	-2.821898	-3.631340
H	4.367467	-3.681572	-2.097538
H	-3.153860	-2.512395	-1.312715
H	-1.655277	-1.747433	-1.875842
H	-2.955641	-2.092928	-3.022602
H	-3.201664	0.321174	-3.787186
H	-1.769987	0.664650	-2.808308
H	-3.245504	1.636501	-2.606279
H	-0.011069	-0.595498	4.240543

H	0.369383	-1.802846	3.005556
H	-1.157175	-0.889654	2.927636
O	-2.727617	1.407332	2.534197
H	-2.131857	2.191327	2.532027
H	-3.034399	1.290316	3.444706
O	-1.094394	3.485844	1.822521
H	-1.121848	3.022265	0.963029
H	-0.139496	3.570313	2.024923
O	-3.730747	3.759137	-1.099907
H	-4.417801	4.044848	-1.719385
H	-2.872500	3.944189	-1.535360
O	-1.125667	3.729804	-2.079030
H	-1.002561	3.654891	-3.037836
H	-1.123467	2.818853	-1.718922
O	-1.890631	-2.991963	0.916749
H	-1.534167	-3.405043	0.094663
H	-1.331554	-3.398799	1.614174
O	-6.558396	0.273733	-0.629362
H	-7.312050	0.447857	-0.047009
H	-6.507425	-0.706977	-0.736576
O	-6.177075	-2.399946	-0.904050
H	-5.841657	-2.737057	-1.747305
H	-5.556485	-2.709684	-0.202205
O	-4.594137	-3.143251	1.184986
H	-3.609256	-3.131903	1.134028
H	-4.830462	-2.640984	1.978399
O	2.844080	2.288840	-0.076817
H	3.790467	2.522505	-0.221419
H	2.319591	2.921518	-0.619720
O	1.670255	3.811459	1.911414
H	2.221414	3.168611	1.410783
H	2.160912	4.039036	2.714569
O	1.307599	4.414987	-0.859886
H	0.423667	4.302376	-1.265457
H	1.166379	4.639649	0.076636
O	0.235941	-4.276440	2.088493
H	0.573617	-4.414737	2.985146
H	0.816627	-3.611567	1.671158
O	-0.362651	-3.934933	-1.170775
H	0.370251	-3.402491	-0.803179
H	-0.097173	-4.859327	-1.053906
O	5.556296	2.695719	-0.366493
H	5.873672	2.820359	-1.273100
H	5.774918	1.776825	-0.129578

Table S15. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $14H_2O$_β-β_B.

N	-3.831629	1.313506	0.155326
C	-2.965264	0.203033	-0.337450

C	-1.534566	0.624746	-0.021894
N	-0.754669	-0.249284	0.600640
C	0.600117	0.084915	1.015553
C	1.525414	-1.051293	0.608410
N	2.722131	-0.687277	0.153929
C	3.717754	-1.667285	-0.233937
C	5.076137	-1.153874	0.199027
O	5.997993	-2.110913	0.212070
O	-1.169400	1.770732	-0.349849
O	1.170946	-2.240236	0.727410
C	3.668484	-1.932804	-1.764298
O	5.310325	0.006368	0.470156
C	-3.161919	-0.007502	-1.847324
C	0.668019	0.378412	2.535445
C	2.069409	0.833337	2.943728
C	4.154678	-0.718196	-2.556180
C	4.414054	-3.204248	-2.167061
C	-4.634157	-0.265578	-2.173597
C	-2.292314	-1.166120	-2.337166
C	0.202375	-0.794206	3.396898
H	-3.789258	2.131981	-0.488769
H	-3.504951	1.629041	1.092745
H	-4.827587	1.006646	0.243526
H	-3.233347	-0.703978	0.214314
H	-1.126040	-1.190039	0.780210
H	0.891278	0.993512	0.480039
H	2.926530	0.313870	0.035651
H	3.504087	-2.598567	0.298746
H	6.860690	-1.722633	0.454271
H	2.600937	-2.082339	-1.971847
H	-2.843638	0.918483	-2.347353
H	-0.028232	1.213104	2.679997
H	2.788402	0.007368	2.888463
H	2.056226	1.196213	3.976012
H	2.432671	1.640979	2.300698
H	5.235939	-0.576501	-2.430670
H	3.649541	0.203924	-2.245889
H	3.964195	-0.863933	-3.623477
H	5.494892	-3.094314	-2.039726
H	4.218607	-3.422111	-3.221537
H	4.084232	-4.064502	-1.574932
H	-5.278416	0.584126	-1.926052
H	-4.997182	-1.146381	-1.629321
H	-4.744055	-0.461842	-3.244388
H	-2.373158	-1.255790	-3.424276
H	-2.631884	-2.110143	-1.896484
H	-1.233650	-1.034173	-2.089030
H	0.118515	-0.473282	4.439860
H	0.926406	-1.616392	3.361955
H	-0.777891	-1.174370	3.087841
O	-2.505755	1.930045	2.560004
H	-1.816344	2.620169	2.424385
H	-3.006382	2.191109	3.346922
O	-0.581701	3.624439	1.605187
H	-0.608604	3.074533	0.798289
H	0.367542	3.809146	1.760556
O	-3.795114	3.534334	-1.618306

H	-4.441111	3.501831	-2.338952
H	-2.920513	3.673537	-2.039279
O	-1.130652	3.475909	-2.428004
H	-0.968663	3.196265	-3.342062
H	-1.106109	2.665174	-1.875775
O	-2.050548	-2.846928	0.559419
H	-1.480335	-3.174529	-0.177622
H	-1.694279	-3.324838	1.341220
O	-6.483232	0.511335	0.459270
H	-6.832068	0.774015	1.323728
H	-6.624440	-0.465947	0.394778
O	-6.848404	-2.169054	0.256167
H	-7.437011	-2.372711	-0.485351
H	-6.008436	-2.653366	0.072552
O	-4.549251	-3.502221	-0.352960
H	-3.680396	-3.289900	0.062043
H	-4.648622	-4.462964	-0.283606
O	2.987553	2.179143	-0.238524
H	3.909209	2.337030	-0.549490
H	2.401296	2.671279	-0.856987
O	2.126696	4.220027	1.402497
H	2.627060	3.463428	1.022358
H	2.697006	4.638494	2.063644
O	1.396022	4.124257	-1.339360
H	0.486879	4.073848	-1.696164
H	1.352469	4.583561	-0.482414
O	-0.304253	-4.034923	2.296948
H	-0.293657	-3.951007	3.261551
H	0.350492	-3.393767	1.956455
O	-0.140045	-3.661613	-1.249907
H	0.558941	-3.296220	-0.672533
H	0.015634	-4.616993	-1.286876
O	5.651325	2.427915	-0.905902
H	5.886849	2.394721	-1.844841
H	5.889535	1.558572	-0.537816

Table S16. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $14H_2O$_β-β_C.

N	-3.842511	1.417854	-0.107851
C	-3.011100	0.199977	-0.305637
C	-1.574510	0.607293	-0.002979
N	-0.776496	-0.346415	0.461737
C	0.578676	-0.078254	0.914980
C	1.499862	-1.155228	0.358967
N	2.747857	-0.774624	0.099522
C	3.741600	-1.716375	-0.380015
C	5.077499	-1.333017	0.223350
O	5.970792	-2.313360	0.138904

O	-1.213690	1.780536	-0.214898
O	1.096552	-2.324279	0.197177
C	3.795901	-1.727560	-1.932790
O	5.321114	-0.243436	0.700883
C	-3.153354	-0.402354	-1.716092
C	0.626957	-0.007445	2.464435
C	1.993462	0.454575	2.968761
C	4.355387	-0.413727	-2.479840
C	4.549363	-2.935116	-2.489056
C	-2.505749	0.457075	-2.804340
C	-4.620038	-0.699095	-2.033534
C	0.217979	-1.321371	3.129268
H	-3.637597	2.178540	-0.788008
H	-3.626270	1.787487	0.837516
H	-4.862620	1.192736	-0.131188
H	-3.346894	-0.532632	0.434945
H	-1.181987	-1.276077	0.619237
H	0.877077	0.895343	0.512907
H	2.997380	0.220519	0.181259
H	3.465569	-2.713494	-0.024735
H	6.823011	-2.003378	0.501053
H	2.743125	-1.814578	-2.231008
H	-2.610132	-1.353506	-1.676683
H	-0.113833	0.761047	2.718200
H	2.763585	-0.305811	2.795146
H	1.944498	0.641214	4.046008
H	2.311058	1.377239	2.474607
H	5.427278	-0.323976	-2.261023
H	3.844722	0.458460	-2.055811
H	4.238030	-0.378198	-3.566905
H	5.621478	-2.870815	-2.281866
H	4.417440	-2.977491	-3.574615
H	4.173314	-3.871534	-2.063654
H	-1.421088	0.529467	-2.669365
H	-2.922844	1.471187	-2.828047
H	-2.685545	0.002822	-3.783204
H	-4.685953	-1.270651	-2.963839
H	-5.200291	0.220994	-2.169697
H	-5.093341	-1.287981	-1.239915
H	0.132630	-1.176178	4.210525
H	0.974479	-2.096806	2.959487
H	-0.748426	-1.692084	2.769166
O	-2.686447	1.666862	2.444868
H	-1.939461	2.297551	2.539522
H	-3.189828	1.709725	3.270917
O	-0.543000	3.321739	1.981143
H	-0.579677	2.909264	1.097272
H	0.401949	3.529379	2.132927
O	-3.446417	3.755738	-1.673580
H	-4.025328	3.939125	-2.427670
H	-2.527960	3.877942	-1.993158
O	-0.718910	3.553856	-2.202699
H	-0.503926	3.272469	-3.105467
H	-0.811553	2.736990	-1.668173
O	-2.249355	-2.857904	0.467470
H	-1.898098	-3.034311	-0.436032
H	-1.719884	-3.464332	1.034896

O	-6.571623	0.821121	0.047657
H	-6.976807	1.319509	0.772506
H	-6.753557	-0.131453	0.239635
O	-7.053620	-1.809103	0.552185
H	-7.645149	-2.185684	-0.115548
H	-6.261760	-2.396800	0.569835
O	-4.920214	-3.512047	0.537506
H	-3.966848	-3.260959	0.531018
H	-5.004526	-4.215583	1.197304
O	3.171322	2.100233	0.137483
H	4.126995	2.247717	-0.051192
H	2.676453	2.661094	-0.502572
O	2.155272	4.017025	1.833836
H	2.694743	3.289344	1.450121
H	2.680603	4.421781	2.539410
O	1.745310	4.162113	-0.974243
H	0.860765	4.092786	-1.386541
H	1.620126	4.522325	-0.078182
O	-0.245889	-4.366836	1.560267
H	-0.086044	-4.473516	2.509394
H	0.395168	-3.698900	1.245404
O	-0.747915	-2.930855	-1.820381
H	0.053034	-2.781579	-1.278804
H	-0.582392	-3.736198	-2.332484
O	5.900144	2.335622	-0.221869
H	6.224199	2.439394	-1.128690
H	6.079942	1.410883	0.023475

Table S17. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $18H_2O$_β-β_A.

N	-4.746640	1.428885	0.190779
C	-3.957592	0.222812	-0.179452
C	-2.490099	0.605079	-0.009016
N	-1.656617	-0.340769	0.403910
C	-0.262961	-0.047155	0.699864
C	0.588264	-1.234509	0.278017
N	1.763922	-0.928664	-0.259962
C	2.749761	-1.940873	-0.588497
C	4.121365	-1.339820	-0.323173
O	5.105438	-2.191721	-0.430758
O	-2.135549	1.769041	-0.279633
O	0.207454	-2.406669	0.468435
C	2.581437	-2.429241	-2.050994
O	4.265057	-0.150898	-0.056635
C	-4.304306	-0.236715	-1.611331
C	-0.066045	0.306241	2.200495
C	1.416507	0.464752	2.549566
C	3.023300	-1.354488	-3.044423

C	3.278819	-3.762956	-2.314907
C	-3.829555	-1.670348	-1.842278
C	-3.765717	0.701909	-2.692812
C	-0.732107	-0.695348	3.142400
H	-4.480412	2.267548	-0.366927
H	-4.549433	1.649446	1.184464
H	-5.765735	1.243775	0.060930
H	-4.227421	-0.565250	0.531556
H	-2.036421	-1.256273	0.680263
H	0.025836	0.824050	0.105560
H	2.013383	0.059147	-0.388445
H	2.607803	-2.789993	0.089473
H	6.014789	-1.695042	-0.353568
H	1.500112	-2.584583	-2.159844
H	-5.400907	-0.231438	-1.660537
H	-0.566534	1.275826	2.321719
H	1.916122	-0.511513	2.584527
H	1.518514	0.927955	3.535638
H	1.955915	1.078675	1.821104
H	4.112135	-1.221294	-3.010529
H	2.551193	-0.387869	-2.834951
H	2.758085	-1.646221	-4.064979
H	4.366290	-3.660835	-2.268010
H	3.011815	-4.124290	-3.313131
H	2.972934	-4.521743	-1.586353
H	-4.274908	-2.359293	-1.116493
H	-2.739209	-1.752403	-1.766534
H	-4.118427	-2.000647	-2.844715
H	-4.164286	0.403142	-3.666536
H	-2.671966	0.642525	-2.749191
H	-4.048615	1.746260	-2.521217
H	-0.621291	-0.353208	4.176616
H	-0.259903	-1.680395	3.065829
H	-1.802311	-0.797490	2.939030
O	-3.355042	1.515994	2.605337
H	-2.735483	2.281399	2.583879
H	-3.628436	1.401427	3.526687
O	-1.772465	3.593876	1.816611
H	-1.945650	3.188966	0.945897
H	-0.790683	3.629049	1.851152
O	-4.208326	3.935462	-1.056541
H	-4.901744	4.340544	-1.597469
H	-3.379567	4.004525	-1.573544
O	-1.690482	3.569299	-2.240863
H	-1.710679	3.333220	-3.181259
H	-1.743235	2.728965	-1.737299
O	-2.929592	-2.864406	1.043810
H	-2.633365	-3.341678	0.233031
H	-2.380639	-3.279126	1.745956
O	-7.388460	0.708044	-0.374926
H	-8.091459	0.955508	0.243155
H	-7.420677	-0.276116	-0.456171
O	-7.249556	-1.993186	-0.587722
H	-6.998217	-2.383067	-1.437397
H	-6.621108	-2.344259	0.087185
O	-5.624558	-2.846873	1.425561
H	-4.643993	-2.893131	1.328887

H	-5.792994	-2.331259	2.227635
O	2.153639	1.947487	-0.502984
H	3.115890	2.137834	-0.460706
H	1.768151	2.651083	-1.064885
O	0.954253	3.747452	1.364789
H	1.388167	2.927654	1.059709
H	0.869647	4.245898	0.527411
O	0.847019	4.277532	-1.397580
H	-0.051088	4.145243	-1.776982
H	1.267761	4.978704	-1.916463
O	-0.887752	-4.195471	2.295391
H	-0.581785	-4.242728	3.212621
H	-0.272680	-3.599336	1.825494
O	-1.518505	-3.996598	-1.029658
H	-0.735629	-3.535849	-0.667344
H	-1.337356	-4.942725	-0.928288
O	4.846669	2.747869	-0.239022
H	4.969248	3.708173	-0.284216
H	5.100541	2.470563	0.668705
O	6.529572	1.249178	-1.878123
H	5.887304	1.753568	-1.331144
H	6.022520	0.916493	-2.633287
O	7.917599	0.053440	2.084859
H	8.665844	0.667761	2.099074
H	7.111050	0.598044	2.209339
O	5.426326	1.252944	1.984785
H	4.897443	1.333500	2.793468
H	4.986087	0.575936	1.427057
O	7.311779	-0.933201	-0.409602
H	7.597139	-0.623950	0.482296
H	7.085290	-0.120365	-0.925037

Table S18. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $18H_2O$_β-β_B.

N	-4.628721	1.439213	0.233761
C	-3.811049	0.295829	-0.263342
C	-2.359613	0.677354	0.002763
N	-1.571572	-0.233366	0.555159
C	-0.179259	0.053358	0.865704
C	0.649427	-1.176954	0.538733
N	1.813928	-0.938366	-0.052192
C	2.768472	-1.991486	-0.341228
C	4.159108	-1.406652	-0.151225
O	5.117719	-2.292890	-0.184108
O	-1.974936	1.819695	-0.319010
O	0.253504	-2.321802	0.840541
C	2.555052	-2.554277	-1.771447
O	4.337281	-0.201041	-0.013538

C	-4.051729	0.069361	-1.765983
C	0.006820	0.506053	2.336760
C	1.483522	0.763869	2.647237
C	2.995086	-1.544926	-2.832221
C	3.218381	-3.915271	-1.975405
C	-5.537378	-0.157531	-2.053189
C	-3.223095	-1.115291	-2.266147
C	-0.592643	-0.468010	3.348991
H	-4.521533	2.265201	-0.392363
H	-4.299673	1.705574	1.184827
H	-5.641166	1.187374	0.301042
H	-4.090711	-0.594558	0.309160
H	-1.962342	-1.160980	0.758310
H	0.136382	0.877012	0.219028
H	2.067687	0.030131	-0.284034
H	2.623684	-2.796883	0.386827
H	6.041753	-1.816927	-0.163763
H	1.468394	-2.690787	-1.850186
H	-3.725396	0.981518	-2.285616
H	-0.542430	1.453831	2.401986
H	2.040210	-0.178784	2.717381
H	1.579233	1.280828	3.606791
H	1.968749	1.372078	1.877084
H	4.086630	-1.430706	-2.829226
H	2.546450	-0.558795	-2.666744
H	2.701462	-1.887939	-3.828689
H	4.308638	-3.835536	-1.950317
H	2.927385	-4.322386	-2.948966
H	2.907934	-4.627293	-1.202898
H	-6.154067	0.712823	-1.808212
H	-5.909637	-1.018840	-1.484559
H	-5.676286	-0.370890	-3.117373
H	-3.355040	-1.227175	-3.346147
H	-3.557844	-2.042704	-1.788102
H	-2.152481	-0.994443	-2.069523
H	-0.570489	-0.019520	4.347395
H	-0.007967	-1.394165	3.390834
H	-1.634692	-0.710808	3.117027
O	-3.198555	1.802761	2.616712
H	-2.587633	2.568309	2.507477
H	-3.617206	1.902403	3.484089
O	-1.618320	3.790163	1.627836
H	-1.800369	3.311928	0.796768
H	-0.637062	3.839521	1.633917
O	-4.369982	3.660397	-1.536708
H	-5.074354	3.754154	-2.194500
H	-3.526296	3.682173	-2.033552
O	-1.775618	3.279335	-2.571474
H	-1.759735	2.849605	-3.440657
H	-1.786389	2.560233	-1.902073
O	-2.993939	-2.776491	0.648542
H	-2.432657	-3.203423	-0.042168
H	-2.669956	-3.183758	1.483115
O	-7.322532	0.769650	0.532611
H	-7.660760	1.088539	1.382248
H	-7.491005	-0.205273	0.522588
O	-7.755757	-1.910202	0.489745

H	-8.399550	-2.141559	-0.195677
H	-6.942034	-2.426935	0.278006
O	-5.534567	-3.335338	-0.199768
H	-4.646141	-3.152251	0.187608
H	-5.669426	-4.290363	-0.113030
O	2.214201	1.880630	-0.626889
H	3.177242	2.061122	-0.695341
H	1.781817	2.467849	-1.280609
O	1.069573	3.932058	0.983030
H	1.528199	3.094445	0.778968
H	0.899878	4.283773	0.086456
O	0.802249	4.019215	-1.827770
H	-0.101041	3.875233	-2.188837
H	1.237548	4.650356	-2.419669
O	-1.354795	-3.803734	2.579428
H	-1.393411	-3.566758	3.517464
H	-0.663956	-3.238673	2.179005
O	-1.084597	-3.849662	-1.025027
H	-0.386528	-3.492041	-0.440761
H	-0.986115	-4.813031	-1.005182
O	4.934372	2.615193	-0.661894
H	5.082256	3.551880	-0.862233
H	5.200732	2.480002	0.274388
O	6.617892	0.877627	-2.049304
H	5.964476	1.451342	-1.591045
H	6.136684	0.462561	-2.780000
O	7.930858	0.205866	2.054379
H	8.713150	0.774859	2.013717
H	7.154686	0.804802	2.092098
O	5.497781	1.497887	1.781127
H	4.984217	1.735192	2.568479
H	5.030496	0.747820	1.355419
O	7.356049	-1.099312	-0.296822
H	7.623456	-0.674859	0.552419
H	7.148855	-0.360392	-0.920085

Table S19. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $18H_2O$_β-β_C.

N	-4.657910	1.494928	0.013519
C	-3.879558	0.243557	-0.186275
C	-2.414815	0.618430	0.002602
N	-1.602669	-0.350485	0.405292
C	-0.206237	-0.107746	0.728153
C	0.627123	-1.256609	0.181069
N	1.840971	-0.932036	-0.245694
C	2.801835	-1.930123	-0.678461
C	4.183957	-1.418449	-0.304110
O	5.133085	-2.305453	-0.436330

O	-2.044319	1.780041	-0.253042
O	0.190255	-2.426696	0.176574
C	2.668302	-2.209659	-2.198497
O	4.366827	-0.260743	0.057061
C	-4.126969	-0.406306	-1.561361
C	-0.017752	0.075392	2.258247
C	1.438289	0.379529	2.616124
C	3.154662	-1.017062	-3.022149
C	3.355326	-3.506630	-2.623282
C	-3.508716	0.382882	-2.717674
C	-5.618474	-0.657351	-1.788697
C	-0.527431	-1.115825	3.068962
H	-4.433207	2.234322	-0.684133
H	-4.398317	1.865024	0.947338
H	-5.687094	1.315364	0.023101
H	-4.186831	-0.449872	0.602547
H	-2.014711	-1.267246	0.612665
H	0.092170	0.821946	0.233460
H	2.125673	0.055876	-0.256350
H	2.608943	-2.856064	-0.126311
H	6.059112	-1.862906	-0.268869
H	1.588573	-2.329772	-2.356535
H	-3.623827	-1.379207	-1.505773
H	-0.631274	0.953124	2.500511
H	2.068769	-0.510085	2.499480
H	1.503868	0.702011	3.659738
H	1.859293	1.167087	1.984069
H	4.243107	-0.905485	-2.936013
H	2.687528	-0.080532	-2.697080
H	2.920064	-1.164455	-4.080552
H	4.442585	-3.429008	-2.537611
H	3.109830	-3.725765	-3.667284
H	3.022191	-4.351793	-2.011293
H	-2.416471	0.420425	-2.642938
H	-3.889780	1.410330	-2.757864
H	-3.758310	-0.101243	-3.666339
H	-5.754899	-1.265962	-2.687241
H	-6.168087	0.279182	-1.937149
H	-6.071426	-1.190999	-0.945922
H	-0.493419	-0.875679	4.136167
H	0.107533	-1.994726	2.908904
H	-1.561576	-1.380687	2.822721
O	-3.368304	1.677032	2.504473
H	-2.642312	2.337844	2.559218
H	-3.814278	1.682485	3.363782
O	-1.407013	3.465851	1.868299
H	-1.546347	3.042823	0.999783
H	-0.433051	3.587095	1.913918
O	-4.127149	3.758991	-1.629090
H	-4.734522	4.015213	-2.338183
H	-3.225414	3.798986	-2.009157
O	-1.434697	3.381761	-2.351184
H	-1.333141	3.005984	-3.239590
H	-1.527534	2.623474	-1.735432
O	-3.176328	-2.792163	0.627553
H	-2.883048	-3.073267	-0.269151
H	-2.645967	-3.368844	1.224836

O	-7.408771	1.043880	0.275752
H	-7.762848	1.605113	0.981216
H	-7.612486	0.113988	0.542290
O	-7.938506	-1.530599	0.987303
H	-8.594716	-1.925812	0.395027
H	-7.166768	-2.144191	0.977530
O	-5.866938	-3.310209	0.892685
H	-4.904872	-3.109397	0.817196
H	-5.941041	-4.004490	1.563420
O	2.353964	1.926170	-0.355264
H	3.325152	2.070858	-0.351252
H	1.983269	2.588758	-0.974416
O	1.285425	3.889871	1.383412
H	1.722755	3.067115	1.088190
H	1.128875	4.341509	0.531147
O	1.058809	4.186559	-1.423145
H	0.174814	4.021888	-1.821370
H	1.497985	4.838193	-1.989307
O	-1.183446	-4.281730	1.750756
H	-0.980193	-4.332076	2.696091
H	-0.530920	-3.667624	1.358603
O	-1.729131	-3.358062	-1.637124
H	-0.929762	-3.013151	-1.190846
H	-1.784045	-2.897669	-2.487435
O	5.076301	2.604665	-0.084980
H	5.227269	3.561775	-0.106921
H	5.254972	2.310970	0.835646
O	6.879619	1.113471	-1.592406
H	6.189022	1.616037	-1.105715
H	6.485871	0.881551	-2.446136
O	7.776802	-0.305287	2.410688
H	8.570575	0.234745	2.535585
H	7.012073	0.303584	2.493599
O	5.397904	1.096633	2.187218
H	4.828693	1.227734	2.961120
H	4.949770	0.438426	1.614613
O	7.391211	-1.175262	-0.171245
H	7.588336	-0.908989	0.757747
H	7.259032	-0.334652	-0.674532

Table S20. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $22H_2O$_β-β_A.

N	5.282205	-1.190297	0.161264
C	4.286069	-0.138188	-0.179139
C	2.913118	-0.781428	-0.012870
N	1.925247	-0.008462	0.417394
C	0.605456	-0.548732	0.703326
C	-0.438098	0.470169	0.271239

N	-1.532733	-0.039495	-0.284846
C	-2.670579	0.780689	-0.649588
C	-3.925885	0.001634	-0.293249
O	-5.031851	0.703694	-0.353460
O	2.773572	-1.985467	-0.304233
O	-0.269935	1.690244	0.460309
C	-2.623297	1.157877	-2.154505
O	-3.891523	-1.189330	-0.012883
C	4.532165	0.406779	-1.601692
C	0.463591	-0.935272	2.201470
C	-0.970892	-1.352682	2.536718
C	-2.902891	-0.058297	-3.037695
C	-3.539357	2.330478	-2.498832
C	3.801429	1.734027	-1.798477
C	4.164702	-0.590623	-2.702188
C	0.937796	0.163367	3.151165
H	5.171354	-2.048790	-0.418233
H	5.131126	-1.468403	1.148307
H	6.249449	-0.817120	0.039843
H	4.415071	0.670141	0.548661
H	2.131159	0.958926	0.702170
H	0.482439	-1.456794	0.106159
H	-1.601950	-1.056508	-0.413896
H	-2.638260	1.696984	-0.049431
H	-5.881557	0.070814	-0.240151
H	-1.586284	1.479519	-2.316458
H	5.610788	0.603182	-1.655235
H	1.124827	-1.802823	2.324938
H	-1.634875	-0.479635	2.568486
H	-0.999361	-1.830550	3.520659
H	-1.385950	-2.048942	1.800900
H	-3.952024	-0.368412	-2.949869
H	-2.269963	-0.911920	-2.770038
H	-2.717259	0.184885	-4.088020
H	-4.595254	2.059370	-2.400980
H	-3.366715	2.638488	-3.535106
H	-3.342519	3.193246	-1.854118
H	4.107823	2.473561	-1.051182
H	2.714569	1.610375	-1.728760
H	4.026137	2.139086	-2.789869
H	4.493174	-0.202170	-3.670431
H	3.078166	-0.730925	-2.751908
H	4.634778	-1.569372	-2.557159
H	0.878061	-0.195715	4.183786
H	0.303583	1.052629	3.072536
H	1.976095	0.449450	2.958186
O	3.933882	-1.567849	2.574927
H	3.442788	-2.420990	2.553871
H	4.165532	-1.399181	3.499364
O	2.690771	-3.861022	1.768965
H	2.780721	-3.409482	0.908309
H	1.733289	-4.079405	1.805292
O	5.195244	-3.720876	-1.153405
H	5.934519	-3.977324	-1.723698
H	4.378311	-3.931217	-1.650515
O	2.624141	-3.805001	-2.291122
H	2.594536	-3.551001	-3.226643

H	2.533967	-2.977841	-1.771526
O	2.691005	2.704361	1.092222
H	2.282658	3.127834	0.292127
H	2.100977	2.996830	1.816581
O	7.737292	0.042946	-0.362085
H	8.468849	-0.066278	0.262678
H	7.581147	1.015145	-0.443304
O	7.090635	2.670643	-0.582086
H	6.762887	2.999364	-1.431655
H	6.410434	2.897602	0.095799
O	5.345693	3.195740	1.443076
H	4.373199	3.056006	1.353803
H	5.615602	2.715071	2.239171
O	-1.474495	-2.927652	-0.524181
H	-2.396007	-3.265972	-0.502564
H	-0.975093	-3.540313	-1.102607
O	0.038052	-4.515978	1.307391
H	-0.548209	-3.789388	1.021736
H	0.216320	-4.967105	0.457957
O	0.241795	-4.951548	-1.466652
H	1.103340	-4.655318	-1.838143
H	-0.040161	-5.713916	-1.993252
O	0.361886	3.635182	2.315575
H	-0.030953	3.619272	3.200918
H	-0.060018	2.915060	1.801824
O	1.176591	3.684613	-0.943097
H	0.508142	3.000879	-0.751377
H	0.803463	4.515259	-0.560685
O	-4.026385	-4.117384	-0.295551
H	-4.004620	-5.082648	-0.381199
H	-4.284334	-3.921745	0.632051
O	-6.090372	-2.901037	-1.718135
H	-5.306955	-3.290451	-1.269516
H	-5.774769	-2.580999	-2.575800
O	-7.326909	-1.872025	2.267193
H	-8.023079	-2.541911	2.330699
H	-6.473397	-2.350787	2.338241
O	-4.739640	-2.818641	2.019142
H	-4.181918	-2.863430	2.811218
H	-4.413002	-2.062071	1.487670
O	-7.003164	-0.812178	-0.229342
H	-7.190396	-1.155147	0.678933
H	-6.714347	-1.594224	-0.766034
O	0.235855	5.786105	0.520395
H	0.153124	5.203298	1.300673
H	-0.655934	6.159954	0.345084
O	-2.207421	6.964082	-0.015453
H	-2.570068	7.479800	0.718734
H	-2.964575	6.457152	-0.391849
O	-5.235392	3.463810	0.338651
H	-4.969548	3.462779	1.269837
H	-5.167982	2.536042	0.042944
O	-4.288155	5.580495	-1.146291
H	-5.052980	6.141821	-1.338646
H	-4.634424	4.817947	-0.630026

Table S21. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $22H_2O$_β-β_B.

N	5.107534	-1.362841	0.177325
C	4.127285	-0.334922	-0.276516
C	2.751880	-0.919010	0.022098
N	1.858475	-0.134998	0.607780
C	0.524884	-0.610364	0.945785
C	-0.481781	0.438273	0.500576
N	-1.597018	-0.028306	-0.049621
C	-2.671040	0.853830	-0.462521
C	-3.979499	0.113683	-0.244637
O	-5.048629	0.862407	-0.373984
O	2.530173	-2.103051	-0.302960
O	-0.262880	1.653958	0.672817
C	-2.488821	1.291909	-1.941213
O	-4.015942	-1.086375	-0.010011
C	4.288530	-0.057190	-1.781293
C	0.398748	-0.938009	2.454178
C	-0.985317	-1.505711	2.774369
C	-2.793331	0.140440	-2.899686
C	-3.286095	2.547661	-2.285736
C	5.722880	0.363387	-2.107926
C	3.299835	1.019149	-2.232948
C	0.717543	0.250641	3.359916
H	5.104143	-2.182026	-0.466771
H	4.840900	-1.693129	1.127412
H	6.076547	-0.974011	0.230510
H	4.300011	0.577511	0.303800
H	2.117021	0.840386	0.802489
H	0.356016	-1.533765	0.383425
H	-1.703035	-1.040152	-0.201191
H	-2.652452	1.741712	0.179616
H	-5.927876	0.260031	-0.329528
H	-1.421724	1.537888	-2.020265
H	4.065096	-0.995967	-2.307838
H	1.149758	-1.719201	2.625505
H	-1.758166	-0.730971	2.700712
H	-1.001747	-1.898513	3.795456
H	-1.261363	-2.314355	2.090155
H	-3.866716	-0.088399	-2.901199
H	-2.248817	-0.770914	-2.627200
H	-2.511768	0.411899	-3.921284
H	-4.364252	2.360101	-2.260899
H	-3.027051	2.882319	-3.295428
H	-3.060894	3.364485	-1.592135
H	6.453377	-0.423968	-1.897402
H	5.998929	1.257138	-1.534586
H	5.799395	0.608563	-3.171557
H	3.373937	1.156718	-3.315536
H	3.535116	1.976940	-1.755897
H	2.260513	0.764767	-1.997877

H	0.778401	-0.085136	4.399857
H	-0.073562	1.006906	3.303340
H	1.673429	0.722845	3.107709
O	3.836512	-1.924589	2.619793
H	3.259470	-2.719454	2.550967
H	4.336706	-2.016562	3.443925
O	2.287724	-3.983003	1.733879
H	2.349312	-3.491844	0.891958
H	1.345711	-4.259388	1.766018
O	5.141233	-3.557570	-1.641822
H	5.804623	-3.500425	-2.344892
H	4.283412	-3.716956	-2.087046
O	2.468834	-3.613855	-2.528780
H	2.335844	-3.211948	-3.401227
H	2.392264	-2.888652	-1.870848
O	2.873635	2.582740	0.696282
H	2.274763	2.912477	-0.025846
H	2.496777	2.999730	1.497374
O	7.693872	-0.342719	0.426434
H	8.096275	-0.624186	1.261216
H	7.723247	0.646247	0.431089
O	7.737843	2.372028	0.420486
H	8.317118	2.701068	-0.282339
H	6.850766	2.765512	0.241911
O	5.312482	3.464548	-0.185302
H	4.463054	3.169048	0.218951
H	5.314989	4.430660	-0.118960
O	-1.627701	-2.888763	-0.464891
H	-2.558166	-3.184479	-0.572074
H	-1.104762	-3.395932	-1.120053
O	-0.290181	-4.796672	1.136234
H	-0.869374	-4.045243	0.901466
H	-0.022257	-5.117488	0.252813
O	0.085150	-4.778444	-1.675139
H	0.942377	-4.483004	-2.055724
H	-0.265248	-5.448271	-2.280808
O	0.858367	3.596232	2.304448
H	0.675209	3.601626	3.255654
H	0.350533	2.851812	1.917923
O	1.001601	3.454199	-1.073108
H	0.344901	2.831075	-0.710069
H	0.756834	4.325467	-0.677195
O	-4.233518	-3.956800	-0.528201
H	-4.252885	-4.915561	-0.669616
H	-4.488552	-3.804897	0.408748
O	-6.132554	-2.559611	-2.005751
H	-5.407292	-3.009158	-1.516736
H	-5.721923	-2.168813	-2.790826
O	-7.349420	-1.792546	2.054116
H	-8.062790	-2.446010	2.093328
H	-6.510572	-2.293546	2.142654
O	-4.786322	-2.845197	1.927738
H	-4.266040	-3.049545	2.719734
H	-4.378670	-2.058087	1.513472
O	-7.073165	-0.586753	-0.382309
H	-7.229918	-0.996616	0.504162
H	-6.790606	-1.326872	-0.978233

O	0.446399	5.654846	0.440844
H	0.485963	5.112998	1.253322
H	-0.452098	6.051146	0.402993
O	-2.023624	6.888600	0.277832
H	-2.354231	7.257458	1.109118
H	-2.796991	6.455792	-0.154361
O	-5.222245	3.600273	0.401578
H	-4.976585	3.577009	1.338006
H	-5.159542	2.678062	0.087836
O	-4.153370	5.718224	-0.994440
H	-4.881035	6.339151	-1.143001
H	-4.545111	4.950457	-0.519522

Table S22. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $22H_2O$_β-β_C.

N	5.127658	-1.292984	-0.360989
C	4.130990	-0.192448	-0.274837
C	2.776832	-0.853162	-0.060304
N	1.858619	-0.117720	0.551370
C	0.524779	-0.606993	0.854026
C	-0.476620	0.446226	0.396579
N	-1.626024	-0.016040	-0.080681
C	-2.696557	0.870279	-0.494529
C	-4.010484	0.194349	-0.142184
O	-5.059014	0.977584	-0.226263
O	2.582213	-2.007035	-0.489277
O	-0.216838	1.662512	0.492350
C	-2.591891	1.189508	-2.010362
O	-4.070588	-0.991194	0.154245
C	4.119912	0.716834	-1.517574
C	0.386409	-0.945121	2.361532
C	-1.020705	-1.444144	2.696718
C	-2.940553	-0.034172	-2.857968
C	-3.412611	2.412566	-2.413223
C	3.599340	0.012176	-2.772423
C	5.499157	1.335017	-1.748899
C	0.771945	0.219995	3.273216
H	4.944317	-1.951541	-1.146671
H	5.049875	-1.833310	0.519556
H	6.107743	-0.936218	-0.426129
H	4.397860	0.400101	0.605493
H	2.130007	0.812267	0.893879
H	0.369289	-1.526040	0.279717
H	-1.766550	-1.030712	-0.176740
H	-2.610204	1.802549	0.074503
H	-5.954515	0.415387	-0.088127
H	-1.531264	1.430411	-2.159460
H	3.421532	1.526979	-1.273197

H	1.099789	-1.765021	2.521066
H	-1.747585	-0.623428	2.668767
H	-1.033963	-1.868725	3.705010
H	-1.362385	-2.211204	1.994655
H	-4.010994	-0.265107	-2.784989
H	-2.377929	-0.921142	-2.545146
H	-2.714963	0.157839	-3.911083
H	-4.487223	2.226695	-2.318829
H	-3.206358	2.664904	-3.458401
H	-3.157364	3.283025	-1.800434
H	2.552842	-0.292127	-2.661051
H	4.193277	-0.876052	-3.018700
H	3.654944	0.695520	-3.624891
H	5.430891	2.112292	-2.515480
H	6.225035	0.590569	-2.094813
H	5.888761	1.792564	-0.832354
H	0.743723	-0.106921	4.317304
H	0.065182	1.050681	3.168533
H	1.781692	0.593766	3.071911
O	4.132870	-1.976686	2.188335
H	3.497843	-2.726867	2.214136
H	4.668823	-2.042001	2.992030
O	2.370832	-3.947611	1.493405
H	2.389154	-3.444598	0.656891
H	1.429660	-4.214463	1.580810
O	4.815051	-3.333256	-2.324805
H	5.380151	-3.347425	-3.110903
H	3.898625	-3.471194	-2.641459
O	2.036440	-3.349798	-2.768708
H	1.769086	-2.867693	-3.566593
H	2.068568	-2.691434	-2.041672
O	2.948571	2.486452	1.233174
H	2.671137	2.862329	0.360041
H	2.326703	2.912374	1.859741
O	7.804432	-0.440870	-0.367287
H	8.353695	-1.070973	0.121868
H	7.895521	0.422404	0.105505
O	7.904384	1.917250	0.988725
H	8.081178	2.707784	0.458722
H	7.024017	2.053917	1.408147
O	5.473222	2.133015	2.226216
H	4.589624	2.344304	1.847224
H	5.318449	1.468578	2.913305
O	-1.786421	-2.881264	-0.403839
H	-2.731958	-3.145088	-0.427065
H	-1.338000	-3.405183	-1.099894
O	-0.250370	-4.733208	1.083430
H	-0.870069	-3.997754	0.911161
H	-0.065614	-5.047827	0.176707
O	-0.150932	-4.726282	-1.750507
H	0.639569	-4.346945	-2.196224
H	-0.493853	-5.415328	-2.338496
O	0.627622	3.651867	2.197347
H	0.221015	3.758131	3.070180
H	0.155748	2.920015	1.746507
O	1.635478	3.223741	-1.026726
H	0.918334	2.614936	-0.766462

H	1.288945	4.117931	-0.790065
O	-4.425213	-3.872103	-0.259194
H	-4.471101	-4.833446	-0.374870
H	-4.631236	-3.692017	0.684670
O	-6.444838	-2.491349	-1.587338
H	-5.673674	-2.938311	-1.172029
H	-6.144357	-2.189815	-2.456968
O	-7.365240	-1.474710	2.471179
H	-8.109555	-2.087606	2.560442
H	-6.551196	-2.020828	2.513120
O	-4.875347	-2.651435	2.165431
H	-4.302536	-2.817555	2.929882
H	-4.486427	-1.895716	1.678613
O	-7.138487	-0.376277	-0.023007
H	-7.275712	-0.730627	0.889925
H	-6.937721	-1.162220	-0.592995
O	0.707099	5.525884	0.104722
H	0.559890	5.068054	0.955477
H	-0.148746	5.933106	-0.153761
O	-1.612037	6.830050	-0.655348
H	-1.817747	7.576472	-0.074669
H	-2.476717	6.407697	-0.868534
O	-5.031860	3.773497	0.342387
H	-4.698557	3.798105	1.251339
H	-5.048821	2.830220	0.091521
O	-4.027729	5.711895	-1.337173
H	-4.723785	6.379178	-1.422952
H	-4.391609	5.015797	-0.744582

Table S23. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $22H_2O$_β-β_D.

N	5.044686	-1.328834	-0.372385
C	4.085927	-0.193524	-0.342815
C	2.731752	-0.766462	0.058252
N	1.922916	0.027192	0.749616
C	0.561951	-0.350057	1.104891
C	-0.388326	0.565913	0.336137
N	-1.334707	-0.049311	-0.365098
C	-2.357122	0.648358	-1.121366
C	-3.711677	0.147783	-0.638493
O	-4.739647	0.815958	-1.107905
O	2.432531	-1.919919	-0.306412
O	-0.256007	1.803061	0.398128
C	-2.149179	0.410503	-2.641435
O	-3.819958	-0.823439	0.097355
C	4.032264	0.516985	-1.713371
C	0.331359	-0.241454	2.623521
C	1.191554	-1.273839	3.349801
C	-2.412874	-1.047894	-3.019330
C	-2.961242	1.363664	-3.517070

C	3.346514	1.875787	-1.583670
C	3.368160	-0.326421	-2.804129
C	-1.151378	-0.427177	2.952417
H	4.732574	-2.103328	-0.995390
H	5.116280	-1.716216	0.589717
H	5.981184	-0.991854	-0.686574
H	4.446438	0.510468	0.415706
H	2.240011	0.967931	1.026238
H	0.412175	-1.387614	0.791064
H	-1.423037	-1.069732	-0.265871
H	-2.274691	1.720835	-0.907325
H	-5.646173	0.322647	-0.853166
H	-1.084948	0.628110	-2.800116
H	5.080189	0.688387	-1.991352
H	0.644784	0.764545	2.935636
H	0.863771	-2.289702	3.095332
H	1.097854	-1.151224	4.433472
H	2.248720	-1.181724	3.082184
H	-3.475114	-1.295411	-2.896116
H	-1.827150	-1.746333	-2.411649
H	-2.154253	-1.217922	-4.068770
H	-4.031836	1.144169	-3.468113
H	-2.643996	1.258399	-4.559376
H	-2.808758	2.406715	-3.221395
H	3.820342	2.496089	-0.815076
H	2.286434	1.766006	-1.326736
H	3.401028	2.414540	-2.534350
H	3.491879	0.167885	-3.772007
H	2.291702	-0.426311	-2.617632
H	3.798535	-1.330508	-2.882607
H	-1.299210	-0.427399	4.036523
H	-1.514256	-1.385053	2.557452
H	-1.773835	0.369373	2.528379
O	4.489014	-1.968981	2.278794
H	3.903632	-2.763135	2.252860
H	5.152105	-2.134416	2.964956
O	2.832358	-3.986870	1.537823
H	2.695569	-3.437789	0.742595
H	1.915973	-4.173508	1.838566
O	4.467776	-3.661287	-1.898691
H	5.023071	-3.854467	-2.667971
H	3.539825	-3.765320	-2.194934
O	1.704714	-3.543646	-2.340232
H	1.400712	-3.212918	-3.199657
H	1.747745	-2.770368	-1.739147
O	2.671548	2.697710	1.529535
H	2.283418	3.227335	0.783030
H	2.078192	2.898434	2.279580
O	7.385484	-0.108633	-1.293355
H	8.238937	-0.378941	-0.924564
H	7.268489	0.843994	-1.060904
O	6.802242	2.456995	-0.633134
H	6.390997	3.020673	-1.304091
H	6.260842	2.545653	0.185895
O	5.388423	2.619971	1.698383
H	4.406024	2.695329	1.718053
H	5.628622	1.965322	2.370086

O	-1.518978	-2.848267	0.231897
H	-2.465841	-3.008498	0.438218
H	-1.253612	-3.556423	-0.391994
O	0.128677	-4.552161	1.781663
H	-0.441587	-3.781810	1.589661
H	0.108753	-5.029443	0.928940
O	-0.229718	-4.993353	-0.995816
H	0.476813	-4.606202	-1.560202
H	-0.628194	-5.715769	-1.502908
O	0.205061	3.332308	2.673188
H	-0.355453	3.139750	3.439868
H	-0.107381	2.755154	1.941687
O	1.304315	4.052353	-0.384085
H	0.594983	3.385318	-0.427311
H	0.928326	4.797124	0.144606
O	-4.142456	-3.587195	0.967795
H	-4.182829	-4.498238	1.296161
H	-4.451006	-3.008880	1.699656
O	-5.975459	-2.985598	-1.044229
H	-5.272789	-3.188634	-0.387225
H	-5.553085	-3.049678	-1.913261
O	-7.497341	-0.400488	2.027073
H	-8.244440	-0.973493	2.253052
H	-6.695000	-0.837331	2.384973
O	-4.977762	-1.448441	2.491976
H	-4.505465	-1.193268	3.299501
H	-4.545479	-0.973156	1.751308
O	-6.842449	-0.435703	-0.627721
H	-7.142142	-0.376987	0.312361
H	-6.572200	-1.378370	-0.771851
O	0.296784	5.841075	1.422054
H	0.152306	5.094520	2.037271
H	-0.596134	6.147150	1.145623
O	-2.160541	6.563716	0.400273
H	-2.915057	6.548120	1.006231
H	-2.296436	5.817734	-0.230182
O	-4.813937	3.552531	-1.874710
H	-5.459711	3.986552	-1.297422
H	-4.837459	2.606141	-1.633548
O	-2.280202	4.459441	-1.353033
H	-1.849123	4.706203	-2.184212
H	-3.193705	4.175319	-1.589331

Table S24. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $22H_2O$_β-β_E.

N	4.823708	-1.565345	-0.260595
C	3.840442	-0.467183	-0.464822
C	2.495757	-0.960339	0.050897
N	1.812314	-0.134499	0.833476
C	0.438931	-0.398637	1.242541

C	-0.452564	0.591706	0.495814
N	-1.430466	0.054562	-0.224200
C	-2.399693	0.833040	-0.972533
C	-3.784525	0.339992	-0.575878
O	-4.774791	1.086405	-1.004122
O	2.085047	-2.080745	-0.309033
O	-0.241713	1.817045	0.582572
C	-2.133824	0.695627	-2.495892
O	-3.945732	-0.690947	0.063361
C	3.724030	-0.111377	-1.958563
C	0.257428	-0.273691	2.764478
C	1.057706	-1.366297	3.470648
C	-2.339111	-0.742821	-2.973052
C	-2.945438	1.676938	-3.340544
C	5.075810	0.334737	-2.517171
C	2.666566	0.974540	-2.163661
C	-1.228278	-0.357492	3.121525
H	4.646433	-2.352145	-0.921402
H	4.746761	-1.931101	0.714287
H	5.801841	-1.221213	-0.393359
H	4.182521	0.400806	0.109869
H	2.215393	0.790346	1.039774
H	0.194785	-1.420347	0.935417
H	-1.571086	-0.963953	-0.171074
H	-2.296984	1.885830	-0.683489
H	-5.707340	0.609101	-0.813063
H	-1.072092	0.954032	-2.603412
H	3.405539	-1.023963	-2.482076
H	0.647370	0.707426	3.069622
H	0.657828	-2.356001	3.214769
H	0.988441	-1.245597	4.556399
H	2.114267	-1.343997	3.187830
H	-3.392993	-1.036814	-2.884858
H	-1.736230	-1.458211	-2.403629
H	-2.058963	-0.831990	-4.027005
H	-4.008493	1.418783	-3.350055
H	-2.583556	1.651742	-4.373172
H	-2.844162	2.702479	-2.972128
H	5.829316	-0.457816	-2.480271
H	5.457243	1.196297	-1.955426
H	4.961997	0.634680	-3.562967
H	2.608666	1.240458	-3.222984
H	2.922131	1.881301	-1.603605
H	1.667854	0.651227	-1.848666
H	-1.356425	-0.353784	4.207957
H	-1.662474	-1.286909	2.730369
H	-1.801141	0.482588	2.712747
O	4.202589	-2.333967	2.351827
H	3.563316	-3.082207	2.263308
H	4.921221	-2.650071	2.919218
O	2.425719	-4.186690	1.506717
H	2.292282	-3.610411	0.730245
H	1.509001	-4.353994	1.817312
O	4.384707	-3.690172	-2.096364
H	4.904945	-3.632832	-2.911162
H	3.450064	-3.788221	-2.374566
O	1.610819	-3.609492	-2.476114

H	1.303119	-3.240239	-3.318286
H	1.649638	-2.864496	-1.838598
O	2.973236	2.487715	1.174356
H	2.511179	2.957021	0.430625
H	2.484361	2.795484	1.964705
O	7.436856	-0.594521	-0.498556
H	8.006231	-0.919443	0.214320
H	7.484263	0.392356	-0.454993
O	7.529223	2.119282	-0.345788
H	7.497865	2.592397	-1.189509
H	6.808601	2.495865	0.213456
O	5.643491	3.101446	1.357919
H	4.681181	2.905846	1.273139
H	5.709652	4.055131	1.510097
O	-1.726480	-2.765181	0.173522
H	-2.689145	-2.922691	0.287415
H	-1.420879	-3.424650	-0.484370
O	-0.289884	-4.660000	1.703895
H	-0.803797	-3.844885	1.540873
H	-0.280005	-5.068817	0.816281
O	-0.458118	-4.891807	-1.131014
H	0.288307	-4.569276	-1.684169
H	-0.924746	-5.556058	-1.659308
O	0.772436	3.357420	2.632297
H	0.357228	3.273259	3.503633
H	0.273695	2.774525	2.016764
O	1.415284	3.739760	-0.673341
H	0.664042	3.132437	-0.537383
H	1.185746	4.549445	-0.156630
O	-4.410995	-3.505656	0.659405
H	-4.490144	-4.443819	0.889550
H	-4.719057	-2.995969	1.440721
O	-6.169923	-2.639671	-1.320098
H	-5.490082	-2.932212	-0.672769
H	-5.731185	-2.635446	-2.183335
O	-7.630476	-0.282535	1.960322
H	-8.406963	-0.836683	2.126361
H	-6.855192	-0.785878	2.289646
O	-5.174413	-1.487714	2.372409
H	-4.707492	-1.338525	3.209001
H	-4.700636	-0.967935	1.689456
O	-6.936616	-0.107452	-0.676910
H	-7.248654	-0.122405	0.261101
H	-6.706647	-1.044208	-0.905709
O	0.886674	5.726206	1.136668
H	0.785226	5.049570	1.835720
H	-0.003084	6.126558	1.013190
O	-1.642254	6.685242	0.578336
H	-2.261993	6.688161	1.321763
H	-1.926574	5.951452	-0.015743
O	-4.727930	3.869568	-1.576465
H	-5.334927	4.297478	-0.954349
H	-4.794735	2.911666	-1.396322
O	-2.124064	4.596068	-1.122849
H	-1.704857	4.797469	-1.972235
H	-3.066685	4.389647	-1.321971

Table S25. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $22H_2O$_β-β_F.

N	-4.770425	1.007251	-0.420266
C	-3.995278	-0.257471	-0.334586
C	-2.629320	0.099710	0.237945
O	-2.222234	1.274908	0.210628
N	-1.891742	-0.901234	0.708318
C	-0.524114	-0.683723	1.159412
C	0.324120	-0.203105	-0.028819
O	0.242474	-0.760091	-1.138125
N	1.140533	0.830949	0.192100
C	2.031283	1.316071	-0.846604
C	3.244980	0.407894	-0.960281
O	3.586379	-0.346271	-0.049238
O	3.924852	0.527944	-2.066728
C	-3.854266	-0.964964	-1.700470
C	0.021995	-1.994130	1.759344
C	2.455485	2.784631	-0.593624
C	-2.866978	-0.252552	-2.624953
C	-5.213121	-1.153727	-2.375163
C	-0.809454	-2.415593	2.973030
C	1.489093	-1.846302	2.152315
C	2.759210	3.502469	-1.908315
C	3.622459	2.916418	0.385702
H	-4.810377	1.418966	0.538007
H	-5.755507	0.818863	-0.693954
H	-4.338395	1.712473	-1.054012
H	-4.538877	-0.905815	0.361707
H	-2.251502	-1.861721	0.676982
H	-0.520229	0.096763	1.933469
H	1.204989	1.215503	1.143055
H	1.494818	1.276549	-1.797258
H	4.857098	-0.003079	-1.968190
H	-3.453580	-1.960266	-1.467582
H	-0.050809	-2.768393	0.984191
H	1.572597	3.256592	-0.150261
H	-3.192371	0.768297	-2.856552
H	-2.780989	-0.798104	-3.569627
H	-1.869127	-0.201519	-2.179636
H	-5.625124	-0.197946	-2.720663
H	-5.933010	-1.632195	-1.705358
H	-5.094504	-1.794832	-3.253649
H	-1.876620	-2.508865	2.751227
H	-0.695929	-1.685356	3.782645
H	-0.457636	-3.383205	3.343873
H	1.855652	-2.782141	2.586020
H	1.613388	-1.051246	2.898568
H	2.117749	-1.607474	1.290169
H	1.916399	3.426711	-2.604225
H	3.646854	3.084828	-2.395316
H	2.948907	4.563050	-1.714379

H	3.412499	2.441256	1.348225
H	3.828048	3.973981	0.577163
H	4.538975	2.470600	-0.022719
O	-4.769964	1.641100	2.299137
H	-4.945021	0.858822	2.842121
H	-3.881150	1.980888	2.572037
O	-3.642410	3.127986	-1.948457
H	-3.952672	3.331163	-2.842760
H	-2.662986	3.064800	-2.001554
O	-0.893845	2.681913	-1.734661
H	-0.544688	2.126569	-2.474020
H	-1.142551	2.051576	-1.028800
O	-2.272551	2.607396	2.692631
H	-1.949441	2.255894	1.842991
H	-1.743650	2.162749	3.393177
O	0.028138	0.856971	-3.574304
H	0.909485	1.018170	-3.981024
H	0.148107	0.092193	-2.981343
O	-0.657217	-3.387557	-1.491094
H	-0.456946	-2.429281	-1.439407
H	0.136066	-3.817447	-1.095957
O	-2.641763	-3.654219	0.273065
H	-1.926298	-3.688686	-0.422660
H	-2.404122	-4.312671	0.944200
O	-6.580070	-1.809482	0.999340
H	-6.196148	-2.597016	0.544104
H	-7.084907	-2.146100	1.753954
O	-7.491855	0.311598	-0.456368
H	-8.015116	0.078402	-1.236595
H	-7.345521	-0.524984	0.041709
O	-5.310740	-3.768293	-0.409531
H	-4.355875	-3.824668	-0.181082
H	-5.654314	-4.672339	-0.358725
O	3.850539	0.252147	2.645427
H	4.720992	0.682578	2.688738
H	3.698978	0.113424	1.684816
O	2.600554	1.306267	-4.479111
H	2.847289	0.725293	-5.214236
H	3.179809	1.052146	-3.735980
O	1.443175	1.683058	2.908846
H	1.472498	2.661287	2.775286
H	2.354848	1.354165	3.052431
O	-0.670855	1.446876	4.609068
H	-0.869884	0.563504	4.949328
H	0.183576	1.385290	4.125808
O	3.919930	-3.117893	-0.035147
H	4.253463	-3.083359	0.887165
H	3.766157	-2.173367	-0.238456
O	1.490315	-4.481104	-0.123201
H	1.725450	-5.379531	-0.398806
H	2.339300	-3.984135	-0.097708
O	5.856066	-3.303637	-1.988759
H	6.650086	-3.818411	-1.783839
H	5.224075	-3.457318	-1.251752
O	6.095992	-0.607858	-1.696711
H	6.070387	-1.580578	-1.882238
H	6.228533	-0.524614	-0.718564

O	6.393270	-0.372180	1.027037
H	7.319681	-0.292244	1.300613
H	6.047610	-1.167614	1.485373
O	4.912021	-2.296853	2.430258
H	4.389797	-1.564819	2.822482
H	5.229443	-2.844867	3.163886
O	-0.250443	4.834180	-0.083062
H	-0.405401	4.138422	-0.758041
H	0.136859	5.584360	-0.557782
O	1.128361	4.318658	2.290608
H	0.626448	4.480271	1.459710
H	1.884314	4.922781	2.266442

Table S26. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $22H_2O$_β-β_J.

N	5.094119	-1.470704	0.234855
C	4.175817	-0.351181	-0.108183
C	2.761926	-0.911117	-0.000163
N	1.811060	-0.088035	0.421239
C	0.450271	-0.550594	0.634848
C	-0.518095	0.536096	0.187370
N	-1.582491	0.083120	-0.469225
C	-2.718952	0.898391	-0.851724
C	-3.955853	0.218781	-0.281550
O	-4.977040	1.009152	-0.057104
O	2.556729	-2.095502	-0.330361
O	-0.319396	1.737851	0.445431
C	-2.796020	1.020789	-2.394661
O	-3.979786	-0.990059	-0.087431
C	4.495913	0.210028	-1.509619
C	0.214885	-0.973692	2.110260
C	-1.257210	-1.315657	2.359868
C	-4.070718	1.723828	-2.863133
C	-1.552439	1.756998	-2.896359
C	3.847400	1.581000	-1.695678
C	4.106063	-0.739777	-2.644187
C	0.704515	0.063173	3.119038
H	4.947082	-2.307824	-0.367590
H	4.896162	-1.760391	1.210122
H	6.086134	-1.157889	0.148485
H	4.331368	0.430712	0.642660
H	2.071321	0.852811	0.747705
H	0.303408	-1.433261	0.006000
H	-1.663041	-0.927378	-0.638575
H	-2.605762	1.895573	-0.411217
H	-5.849211	0.432757	0.149597
H	-2.791111	-0.004206	-2.792900
H	5.585016	0.345011	-1.526810
H	0.817086	-1.883129	2.234955

H	-1.869507	-0.405383	2.397101
H	-1.361288	-1.829171	3.320915
H	-1.671149	-1.954997	1.572558
H	-4.168219	2.710986	-2.395984
H	-4.973303	1.151043	-2.632313
H	-4.031729	1.868429	-3.946960
H	-1.532726	2.777131	-2.495309
H	-1.564307	1.815605	-3.989097
H	-0.630254	1.249190	-2.595765
H	4.175972	2.286927	-0.925498
H	2.753618	1.519106	-1.656253
H	4.121417	1.992318	-2.671995
H	4.487323	-0.350103	-3.592398
H	3.015258	-0.815068	-2.730516
H	4.513495	-1.747500	-2.507998
H	0.577915	-0.325980	4.134544
H	0.125526	0.989176	3.043760
H	1.764917	0.295484	2.981487
O	3.641575	-1.817320	2.595005
H	3.101586	-2.638442	2.533788
H	3.865904	-1.697929	3.528905
O	2.291690	-4.011309	1.690753
H	2.436636	-3.547500	0.844279
H	1.321989	-4.170922	1.693430
O	4.894657	-3.961103	-1.138648
H	5.634627	-4.251411	-1.691512
H	4.082514	-4.108370	-1.665570
O	2.362349	-3.870126	-2.353661
H	2.372588	-3.603889	-3.286130
H	2.299351	-3.045899	-1.825695
O	2.728801	2.524709	1.202832
H	2.361918	2.986990	0.403229
H	2.141101	2.831574	1.923220
O	7.637352	-0.396375	-0.211327
H	8.352040	-0.570016	0.418336
H	7.548887	0.585706	-0.271174
O	7.168729	2.272707	-0.378752
H	6.905726	2.654772	-1.228470
H	6.481923	2.533891	0.279681
O	5.398967	2.887117	1.599654
H	4.422718	2.792278	1.495734
H	5.633000	2.401893	2.404245
O	-1.697147	-2.803465	-0.747260
H	-2.640448	-3.074950	-0.738471
H	-1.229429	-3.461363	-1.302405
O	-0.382355	-4.495165	1.144023
H	-0.896142	-3.727957	0.826565
H	-0.201342	-4.967199	0.306810
O	-0.088182	-4.937371	-1.622873
H	0.797542	-4.669487	-1.957176
H	-0.384318	-5.672583	-2.179433
O	0.436661	3.552223	2.401833
H	0.004146	3.538410	3.268517
H	-0.028358	2.899353	1.837856
O	1.347419	3.674099	-0.830520
H	0.590049	3.077815	-0.681973
H	1.097191	4.526956	-0.399033

O	-4.319362	-3.847004	-0.498692
H	-4.387657	-4.796714	-0.679775
H	-4.448910	-3.732317	0.467662
O	-6.347727	-2.277002	-1.618133
H	-5.589588	-2.786965	-1.255494
H	-5.990380	-1.784306	-2.372147
O	-7.082731	-1.659259	2.653078
H	-7.795218	-2.308564	2.744300
H	-6.249712	-2.171226	2.571379
O	-4.605493	-2.677549	1.970433
H	-3.933024	-2.778735	2.661727
H	-4.334298	-1.911315	1.420669
O	-7.016415	-0.387701	0.238866
H	-7.105052	-0.812774	1.127450
H	-6.839695	-1.118696	-0.406797
O	0.779670	5.808228	0.772932
H	0.570908	5.191205	1.501936
H	-0.054972	6.285609	0.565793
O	-1.585395	7.002952	0.016701
H	-2.167320	7.326165	0.719207
H	-2.045566	6.233295	-0.393333
O	-4.964632	3.833179	-0.156330
H	-5.117608	4.169997	0.739027
H	-5.010991	2.859706	-0.086923
O	-2.603255	4.766575	-1.190718
H	-2.762568	4.948524	-2.128651
H	-3.460474	4.442494	-0.828951

Table S27. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $22H_2O$_β-β_K.

N	5.125274	-1.285090	0.336016
C	4.195334	-0.238703	-0.175440
C	2.794803	-0.814065	-0.008250
N	1.855605	-0.025005	0.493101
C	0.501614	-0.504811	0.716255
C	-0.485416	0.561122	0.266779
N	-1.571501	0.092595	-0.338915
C	-2.734331	0.897355	-0.668208
C	-3.942488	0.121635	-0.161254
O	-5.007254	0.838603	0.104125
O	2.592632	-1.993277	-0.361907
O	-0.280694	1.770102	0.489039
C	-2.822307	1.149151	-2.195048
O	-3.905886	-1.096935	-0.046380
C	4.484349	0.071979	-1.654460
C	0.276802	-0.909555	2.196329
C	-1.145577	-1.431694	2.414439
C	-4.069875	1.949398	-2.572387
C	-1.560991	1.880657	-2.656960

C	5.943096	0.491067	-1.847523
C	3.541989	1.165304	-2.160887
C	0.597219	0.212098	3.182694
H	5.154649	-2.098723	-0.314487
H	4.784181	-1.617101	1.261286
H	6.093972	-0.913708	0.464066
H	4.324675	0.658681	0.438579
H	2.109306	0.936618	0.751124
H	0.368634	-1.399197	0.100366
H	-1.640530	-0.917531	-0.517796
H	-2.662285	1.859309	-0.148675
H	-5.838885	0.199420	0.268135
H	-2.863913	0.163976	-2.681898
H	4.301410	-0.852972	-2.219862
H	0.984752	-1.730886	2.362740
H	-1.874782	-0.612321	2.395588
H	-1.218575	-1.922564	3.389838
H	-1.435990	-2.149370	1.639655
H	-4.099257	2.896115	-2.018471
H	-4.996070	1.403322	-2.372712
H	-4.044388	2.186101	-3.640490
H	-1.490107	2.853566	-2.156648
H	-1.600125	2.051054	-3.737321
H	-0.653476	1.307212	-2.441295
H	6.649364	-0.306401	-1.596533
H	6.173652	1.367542	-1.229004
H	6.111243	0.763123	-2.893906
H	3.720609	1.342383	-3.225449
H	3.725691	2.105556	-1.629010
H	2.485384	0.904063	-2.037670
H	0.571599	-0.178295	4.204992
H	-0.146736	1.013896	3.117382
H	1.591953	0.638544	3.015636
O	3.637150	-1.832918	2.650138
H	3.106832	-2.653159	2.521423
H	4.043191	-1.899391	3.526725
O	2.282910	-3.947671	1.603611
H	2.406999	-3.441644	0.777772
H	1.332284	-4.194116	1.574185
O	5.250707	-3.471104	-1.489833
H	5.971617	-3.437314	-2.135412
H	4.428990	-3.611988	-2.003893
O	2.654891	-3.489728	-2.594796
H	2.598260	-3.087922	-3.475559
H	2.538348	-2.761677	-1.946249
O	2.912441	2.654148	0.821552
H	2.392701	3.005214	0.048953
H	2.459303	3.054472	1.590944
O	7.708846	-0.329115	0.795919
H	8.037412	-0.634713	1.654186
H	7.761164	0.658576	0.821218
O	7.812944	2.383799	0.838182
H	8.416304	2.709437	0.154271
H	6.938243	2.795011	0.640730
O	5.427878	3.532971	0.177503
H	4.547388	3.231370	0.502649
H	5.434912	4.495091	0.286958

O	-1.562098	-2.772445	-0.818630
H	-2.488724	-3.078596	-0.925532
H	-1.023217	-3.302095	-1.442113
O	-0.288856	-4.659981	0.870838
H	-0.843504	-3.897825	0.614095
H	0.007387	-4.986049	-0.001908
O	0.219927	-4.667884	-1.917117
H	1.098367	-4.358855	-2.233542
H	-0.070996	-5.347603	-2.542896
O	0.743759	3.641616	2.240716
H	0.458627	3.650595	3.166502
H	0.277723	2.897271	1.803312
O	1.262141	3.521664	-1.137230
H	0.575174	2.871159	-0.898784
H	0.918168	4.366451	-0.758167
O	-4.159350	-3.888382	-0.845334
H	-4.207612	-4.811484	-1.136773
H	-4.298749	-3.890643	0.126805
O	-6.202866	-2.244361	-1.812185
H	-5.438786	-2.777014	-1.497365
H	-5.836648	-1.623975	-2.460300
O	-6.947690	-2.213308	2.539891
H	-7.635532	-2.893655	2.577645
H	-6.097896	-2.684786	2.405857
O	-4.436810	-3.073548	1.764603
H	-3.764068	-3.284030	2.430362
H	-4.170393	-2.227997	1.345638
O	-6.983941	-0.674140	0.283196
H	-7.030945	-1.207237	1.114494
H	-6.782571	-1.309273	-0.449712
O	-2.342582	4.798928	-0.700451
H	-2.443469	5.097970	-1.615949
H	-3.168501	5.076304	-0.236407
O	0.115488	5.565519	0.279390
H	0.258893	5.072472	1.111699
H	-0.812862	5.377586	0.013136
O	-4.659930	5.491773	0.571920
H	-4.568715	5.512341	1.535411
H	-5.280663	4.753498	0.370518
O	-6.239243	3.396525	-0.202921
H	-7.047045	3.249998	0.311435
H	-5.730435	2.566863	-0.133131

Table S28. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-β conformation, $22H_2O$_β-β_S.

N	5.125642	-1.391827	0.172795
C	4.198883	-0.268637	-0.133866
C	2.788187	-0.839451	-0.033094
N	1.833382	-0.035088	0.415883
C	0.482170	-0.522460	0.640782

C	-0.508196	0.571894	0.274784
N	-1.608376	0.150106	-0.344898
C	-2.763995	0.995310	-0.570059
C	-4.001263	0.188421	-0.200720
O	-5.120994	0.864693	-0.292738
O	2.587424	-2.015763	-0.393222
O	-0.300120	1.762211	0.573952
C	-2.853192	1.515584	-2.024064
O	-3.943926	-0.991732	0.116804
C	4.510351	0.333140	-1.519957
C	0.292047	-1.003571	2.106538
C	-1.166782	-1.374382	2.389663
C	-1.625284	2.360189	-2.356173
C	-3.026995	0.362361	-3.012545
C	3.834559	1.694596	-1.672988
C	4.141823	-0.596494	-2.677998
C	0.797958	0.004070	3.137882
H	4.971204	-2.215979	-0.445396
H	4.942695	-1.702469	1.144626
H	6.116475	-1.076511	0.077979
H	4.354368	0.493726	0.636805
H	2.087551	0.895459	0.774925
H	0.325792	-1.379098	-0.020323
H	-1.701635	-0.852741	-0.545353
H	-2.695004	1.854600	0.108337
H	-5.963198	0.226731	-0.136410
H	-3.739271	2.160736	-2.067419
H	5.596813	0.489787	-1.531168
H	0.910032	-1.908160	2.180635
H	-1.790914	-0.474768	2.467610
H	-1.233629	-1.912512	3.340368
H	-1.598356	-2.001159	1.602013
H	-0.712371	1.753072	-2.318902
H	-1.523601	3.197822	-1.658988
H	-1.714755	2.771686	-3.366347
H	-2.174768	-0.325924	-2.962351
H	-3.087724	0.746139	-4.035279
H	-3.941130	-0.210378	-2.816734
H	4.141895	2.386143	-0.881260
H	2.742334	1.608686	-1.643239
H	4.106382	2.139108	-2.635167
H	4.512450	-0.174181	-3.616385
H	3.053081	-0.695174	-2.765508
H	4.572725	-1.597641	-2.568098
H	0.698335	-0.420658	4.142124
H	0.210219	0.927876	3.108378
H	1.853090	0.248877	2.984140
O	3.704587	-1.812448	2.534518
H	3.191898	-2.648680	2.445216
H	3.935283	-1.722915	3.470220
O	2.432660	-4.020044	1.559802
H	2.571820	-3.533309	0.725664
H	1.464049	-4.187830	1.556347
O	4.904422	-3.848725	-1.263347
H	5.653898	-4.144491	-1.800287
H	4.104841	-3.967551	-1.815928
O	2.386482	-3.686024	-2.502345

H	2.393313	-3.361400	-3.416248
H	2.325030	-2.895950	-1.923965
O	2.735756	2.567447	1.297788
H	2.382680	3.048917	0.503647
H	2.139648	2.866484	2.014664
O	7.668774	-0.323845	-0.283432
H	8.396112	-0.551296	0.313823
H	7.586418	0.660671	-0.262104
O	7.210319	2.348456	-0.220107
H	6.948680	2.792916	-1.039307
H	6.512790	2.544888	0.449378
O	5.406187	2.772691	1.777274
H	4.429673	2.741471	1.641148
H	5.592963	2.198510	2.534234
O	-1.635539	-2.717256	-0.756556
H	-2.550671	-3.055417	-0.644701
H	-1.187658	-3.341074	-1.364625
O	-0.239696	-4.483570	1.005598
H	-0.744031	-3.691911	0.736807
H	-0.085940	-4.917218	0.142574
O	-0.048790	-4.797987	-1.789952
H	0.827760	-4.510615	-2.132095
H	-0.353644	-5.510434	-2.370838
O	0.429683	3.597581	2.490669
H	0.032985	3.573483	3.374085
H	-0.022262	2.912371	1.955410
O	1.351837	3.691112	-0.740264
H	0.638359	3.042876	-0.591191
H	1.010770	4.529013	-0.341621
O	-4.118120	-3.922653	-0.217086
H	-4.090324	-4.889522	-0.279387
H	-4.288892	-3.704704	0.725824
O	-6.207423	-2.719615	-1.597636
H	-5.427030	-3.117866	-1.150974
H	-5.885808	-2.385328	-2.447681
O	-7.210698	-1.720657	2.457119
H	-7.892897	-2.400746	2.555106
H	-6.347960	-2.184687	2.509459
O	-4.615265	-2.652024	2.175717
H	-4.043099	-2.741061	2.953454
H	-4.296705	-1.874537	1.672093
O	-7.071855	-0.655920	-0.054375
H	-7.181027	-1.005534	0.864408
H	-6.810524	-1.431599	-0.614252
O	0.411872	5.784544	0.724169
H	0.270732	5.193749	1.489805
H	-0.471443	6.107947	0.437912
O	-1.972708	6.778832	-0.237637
H	-2.569571	7.199529	0.397347
H	-2.536975	6.191594	-0.794437
O	-5.075359	3.678203	-0.066351
H	-4.866210	3.855280	0.862546
H	-5.171107	2.709166	-0.139494
O	-3.514080	5.130667	-1.795871
H	-4.125385	5.627908	-2.358444
H	-4.079206	4.574654	-1.212715

Table S29. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $10H_2O$_β-PPII_A.

N	4.078083	-0.458890	0.429251
C	2.865241	0.156191	-0.167356
C	1.702537	-0.790907	0.102802
N	0.540570	-0.211370	0.387711
C	-0.692586	-0.953160	0.570969
C	-1.753257	-0.313440	-0.321788
N	-2.818933	-1.065582	-0.638098
C	-3.928828	-0.492280	-1.372850
C	-4.447693	0.726873	-0.617017
O	-4.947174	1.642630	-1.442383
O	1.871528	-2.021837	0.033333
O	-1.657190	0.856970	-0.704201
C	-5.039839	-1.544935	-1.589039
O	-4.438046	0.842799	0.591409
C	3.065526	0.451121	-1.671013
C	-1.114202	-0.958302	2.064377
C	3.678643	-0.722613	-2.436106
C	-6.106722	-1.032102	-2.557400
C	-5.675088	-2.016754	-0.278787
C	1.746144	0.890901	-2.310601
C	-2.252685	-1.938918	2.348892
C	-1.475168	0.443272	2.555895
H	4.224815	-1.442640	0.109188
H	3.951940	-0.480378	1.455233
H	4.927640	0.094006	0.175194
H	2.689110	1.101316	0.355107
H	0.508088	0.810358	0.463334
H	-0.506348	-1.982537	0.248256
H	-2.861327	-2.034913	-0.346568
H	-3.574318	-0.142617	-2.348750
H	-5.314625	2.383143	-0.923388
H	-4.532337	-2.394863	-2.064420
H	3.766449	1.295249	-1.711509
H	-0.221973	-1.312465	2.595106
H	3.744992	-0.466872	-3.497999
H	3.062176	-1.623636	-2.343127
H	4.689862	-0.958292	-2.090521
H	-5.663011	-0.669208	-3.489815
H	-6.687871	-0.216370	-2.115096
H	-6.799105	-1.843117	-2.800569
H	-6.234270	-1.206250	0.201255
H	-4.939459	-2.388323	0.442259
H	-6.375085	-2.831434	-0.485752
H	1.227326	1.647735	-1.712547
H	1.064013	0.040811	-2.429908
H	1.939135	1.309757	-3.302354
H	-2.361690	-2.067379	3.430004
H	-2.061357	-2.927357	1.914316
H	-3.207331	-1.559751	1.967199

H	-0.663717	1.160876	2.395693
H	-1.693847	0.419404	3.628220
H	-2.367713	0.812105	2.036982
O	2.796681	-0.539280	2.936162
H	2.319874	-1.398582	2.983036
H	2.154575	0.145089	3.176092
O	1.555000	-2.990801	2.625371
H	1.640501	-2.946210	1.652261
H	2.098711	-3.740902	2.908695
O	4.806262	-3.113443	-0.219442
H	5.622566	-3.203314	-0.732057
H	4.112249	-3.601321	-0.717401
O	2.585883	-4.281599	-1.371829
H	2.495270	-4.343612	-2.333757
H	2.049665	-3.516551	-1.091803
O	0.846329	2.679926	0.860145
H	1.161763	2.830062	1.765234
H	-0.076760	3.051963	0.821278
O	6.175135	1.053166	-0.595341
H	7.049868	0.984354	-0.185501
H	5.925598	2.008904	-0.557296
O	5.313888	3.630428	-0.541077
H	4.341453	3.740049	-0.655792
H	5.543451	4.118230	0.262850
O	2.617258	3.934668	-0.858781
H	1.948375	3.517834	-0.270850
H	2.253665	3.913980	-1.755545
O	-1.704532	3.380783	0.451397
H	-2.370059	3.389023	1.173353
H	-1.854583	2.534987	-0.014310
O	-3.853213	3.115801	2.203238
H	-4.243711	2.330550	1.774682
H	-3.675298	2.858610	3.119880

Table S30. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $10H_2O$_β-PPII_B.

N	4.045300	-0.441513	0.288570
C	2.881157	-0.218305	-0.612704
C	1.686050	-0.920283	0.019267
N	0.529804	-0.271817	-0.025589
C	-0.686031	-0.811589	0.554999
C	-1.841741	-0.474147	-0.379068
N	-2.945490	-1.230749	-0.274116
C	-4.147006	-0.885368	-1.006507
C	-4.556728	0.538422	-0.643675
O	-5.227935	1.125844	-1.630172
O	1.832183	-2.057546	0.507572
O	-1.780072	0.474125	-1.167905

C	-5.275995	-1.896939	-0.700634
O	-4.325385	1.068393	0.423714
C	3.167885	-0.771116	-2.020901
C	-0.896382	-0.233784	1.981266
C	1.947704	-0.601724	-2.928645
C	-6.441938	-1.745454	-1.678391
C	-5.764069	-1.814032	0.747908
C	4.397299	-0.088727	-2.623327
C	-2.056800	-0.897549	2.722992
C	-1.066681	1.284774	1.955163
H	4.416843	-1.411472	0.188670
H	3.747017	-0.296173	1.274490
H	4.818520	0.232335	0.084334
H	2.702683	0.862338	-0.657965
H	0.499413	0.675927	-0.418784
H	-0.569639	-1.898355	0.621913
H	-2.961470	-2.016069	0.366004
H	-3.932123	-0.900441	-2.080665
H	-5.513521	2.015248	-1.346766
H	-4.821390	-2.882455	-0.867672
H	3.376162	-1.844533	-1.909785
H	0.037394	-0.470976	2.506116
H	2.188465	-0.952592	-3.935992
H	1.655664	0.453136	-3.002581
H	1.083315	-1.170650	-2.573010
H	-6.102723	-1.791211	-2.718026
H	-6.965997	-0.795963	-1.530434
H	-7.160243	-2.554448	-1.517079
H	-6.291501	-0.870959	0.930122
H	-4.949482	-1.886822	1.476429
H	-6.462168	-2.632145	0.947000
H	5.307915	-0.276917	-2.047151
H	4.248658	0.997116	-2.675133
H	4.563998	-0.458113	-3.639320
H	-2.023915	-0.614930	3.779584
H	-2.006610	-1.992028	2.671083
H	-3.021595	-0.566545	2.322875
H	-0.221084	1.786016	1.471891
H	-1.141645	1.668945	2.977564
H	-1.985046	1.560029	1.423589
O	2.632513	0.022028	2.658276
H	2.325876	-0.809456	3.084170
H	2.953837	0.597931	3.367349
O	1.699451	-2.497804	3.234324
H	1.548277	-2.588895	2.272800
H	0.852346	-2.684092	3.665112
O	5.128116	-3.022315	-0.114554
H	5.805305	-3.051174	-0.806059
H	4.411704	-3.634781	-0.398953
O	2.818080	-4.387853	-0.652572
H	2.547064	-4.551560	-1.567671
H	2.287307	-3.628008	-0.340616
O	0.754972	2.552517	-0.804675
H	1.120631	2.804273	-1.666997
H	-0.174445	2.909057	-0.796800
O	6.066001	1.434961	-0.195784
H	6.683430	1.496789	0.547899

H	5.643302	2.326108	-0.271537
O	4.785153	3.825214	-0.352015
H	4.532635	4.087408	-1.248935
H	3.944871	3.752829	0.161140
O	2.497158	3.487438	1.101029
H	1.792504	3.211002	0.472403
H	2.171688	4.288363	1.537045
O	-1.839297	3.234502	-0.936308
H	-2.356747	3.534068	-0.157751
H	-2.068767	2.292011	-1.048237
O	-3.624117	3.723658	1.142082
H	-4.056497	2.852122	1.068322
H	-3.302422	3.786910	2.053432

Table S31. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $10H_2O$_β-PPII_C.

N	4.065609	-0.581545	0.124922
C	2.841845	-0.009118	-0.492639
C	1.658142	-0.827899	0.007507
N	0.467002	-0.255574	-0.134037
C	-0.737748	-0.854693	0.411001
C	-1.908285	-0.411052	-0.455485
N	-3.023689	-1.155176	-0.401993
C	-4.227365	-0.721474	-1.082532
C	-4.606932	0.668730	-0.582351
O	-5.264124	1.362666	-1.507353
O	1.830515	-1.968913	0.473611
O	-1.848487	0.612532	-1.144645
C	-5.370572	-1.738664	-0.862147
O	-4.366747	1.088673	0.530978
C	2.897032	0.020294	-2.031401
C	-0.912697	-0.426942	1.894755
C	4.111338	0.809817	-2.520202
C	-6.549628	-1.463241	-1.796108
C	-5.832330	-1.801306	0.595825
C	2.845135	-1.377711	-2.650475
C	-2.028412	-1.192990	2.604226
C	-1.117929	1.082243	2.022288
H	4.269301	-1.560093	-0.170419
H	3.910193	-0.589378	1.150873
H	4.901952	0.016713	-0.057972
H	2.753778	1.013189	-0.108718
H	0.412565	0.707844	-0.483197
H	-0.628432	-1.943188	0.362484
H	-3.039335	-2.009183	0.143222
H	-4.024634	-0.637525	-2.155901
H	-5.531885	2.225749	-1.138329
H	-4.938671	-2.708973	-1.140910

H	1.992371	0.561800	-2.336350
H	0.040008	-0.696115	2.367713
H	4.043698	0.959843	-3.601498
H	5.047563	0.278358	-2.316407
H	4.166570	1.793552	-2.040174
H	-6.228418	-1.398073	-2.840386
H	-7.056041	-0.528667	-1.534736
H	-7.278394	-2.274616	-1.712333
H	-6.332666	-0.871584	0.888954
H	-5.008094	-1.972183	1.296330
H	-6.547450	-2.619779	0.718605
H	1.921078	-1.904568	-2.388091
H	3.693782	-1.992739	-2.330674
H	2.884277	-1.298961	-3.740820
H	-1.969813	-1.008922	3.681331
H	-1.944479	-2.275188	2.448334
H	-3.015883	-0.858549	2.266692
H	-0.312569	1.650223	1.542683
H	-1.144792	1.368165	3.078714
H	-2.070057	1.379620	1.567916
O	2.840094	-0.154692	2.604256
H	2.433116	-0.944952	3.023503
H	3.160080	0.409710	3.322850
O	1.508469	-2.500764	3.184707
H	1.498656	-2.610947	2.213875
H	2.028205	-3.240540	3.532398
O	4.814906	-3.261843	-0.383425
H	5.466429	-3.462822	-1.070654
H	4.027760	-3.823054	-0.568799
O	2.362660	-4.458201	-0.650640
H	2.024685	-4.633937	-1.541048
H	1.935146	-3.631306	-0.354035
O	0.764402	2.603402	-0.795994
H	1.032750	2.863801	-1.690946
H	-0.143350	2.988901	-0.670055
O	6.275738	1.131029	-0.176164
H	6.851052	1.080827	0.601339
H	5.936311	2.058886	-0.200873
O	5.186834	3.626346	-0.176534
H	5.107399	4.086600	-1.024233
H	4.274132	3.551898	0.189970
O	2.745309	3.241442	0.979233
H	1.969623	3.131985	0.383520
H	2.494776	3.905262	1.637986
O	-1.820862	3.338308	-0.651370
H	-2.308794	3.575019	0.166461
H	-2.067579	2.411086	-0.833106
O	-3.571765	3.649952	1.493020
H	-4.033548	2.806136	1.330001
H	-3.239930	3.601273	2.401643

Table S32. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $14H_2O$_β-PPII_A.

N	-4.223935	0.462078	0.064383
C	-3.105272	-0.300178	-0.553459
C	-1.832283	0.470694	-0.222400
N	-0.717573	-0.229267	-0.066701
C	0.519170	0.396731	0.372839
C	1.675092	-0.249411	-0.375716
N	2.731515	0.527901	-0.610856
C	3.932485	-0.012367	-1.214294
C	4.382932	-1.240032	-0.431313
O	4.955944	-2.148027	-1.217125
O	-1.886363	1.713388	-0.136866
O	1.648010	-1.444557	-0.717352
C	5.032973	1.072772	-1.240293
O	4.273703	-1.365909	0.770683
C	-3.335055	-0.471198	-2.069353
C	0.665602	0.288505	1.918023
C	-3.179045	0.836690	-2.848296
C	6.238403	0.623345	-2.065727
C	5.459973	1.509454	0.163778
C	-2.410070	-1.550198	-2.630667
C	2.019281	0.804172	2.410075
C	0.421584	-1.131306	2.426421
H	-4.260957	1.451837	-0.257135
H	-4.071914	0.477149	1.089795
H	-5.127111	-0.016048	-0.144512
H	-3.084966	-1.283887	-0.070764
H	-0.758304	-1.258335	-0.074183
H	0.470321	1.457690	0.106666
H	2.688529	1.524598	-0.376743
H	3.719807	-0.336178	-2.239493
H	5.274453	-2.890988	-0.669870
H	4.568309	1.927405	-1.750605
H	-4.370462	-0.822317	-2.165714
H	-0.127319	0.938210	2.310353
H	-3.490405	0.683580	-3.885507
H	-2.129753	1.156131	-2.861284
H	-3.783721	1.650843	-2.434260
H	5.941901	0.300924	-3.068806
H	6.764341	-0.206189	-1.581068
H	6.944651	1.452435	-2.167395
H	6.031443	0.719421	0.662812
H	4.606964	1.755593	0.806004
H	6.099223	2.394658	0.094105
H	-2.556914	-2.507828	-2.120421
H	-1.358129	-1.258059	-2.530276
H	-2.613907	-1.698147	-3.695326
H	1.997679	0.907593	3.499248
H	2.276305	1.777050	1.979268
H	2.823146	0.107183	2.146404
H	-0.591536	-1.477664	2.200730
H	0.548507	-1.157931	3.513949

H	1.139283	-1.833476	1.987533
O	-2.840069	0.289057	2.478599
H	-2.469482	1.168222	2.721666
H	-2.986775	-0.192835	3.305075
O	-1.950613	2.867051	2.412436
H	-1.999697	2.691183	1.453592
H	-1.041528	3.218846	2.531237
O	-4.523194	3.245815	-0.516064
H	-5.302885	3.560447	-0.996250
H	-3.753556	3.701003	-0.913934
O	-1.998404	3.995424	-1.551170
H	-1.970645	4.010498	-2.520563
H	-1.813527	3.071573	-1.276856
O	-0.936257	-3.132739	-0.101048
H	-0.614669	-3.276757	-1.021063
H	-0.179087	-3.456876	0.438076
O	-6.314568	-1.284879	-0.495296
H	-7.241599	-1.055093	-0.335971
H	-6.060989	-1.933601	0.205581
O	-5.282094	-2.890223	1.428055
H	-4.531986	-3.436751	1.090573
H	-4.938410	-2.390752	2.182803
O	-3.272766	-4.439943	0.443009
H	-2.417697	-3.996131	0.230965
H	-3.536060	-4.914556	-0.358685
O	1.611976	-3.929746	0.619528
H	2.140372	-3.868428	1.442451
H	1.854855	-3.125812	0.122888
O	3.404143	-3.284433	2.670197
H	3.848923	-2.604396	2.129902
H	3.044165	-2.816396	3.438098
O	2.423241	3.342285	0.098168
H	1.757904	3.922200	-0.333451
H	3.236545	3.869016	0.141139
O	0.290743	5.060883	-0.423993
H	0.450348	5.986062	-0.662981
H	-0.539303	4.790541	-0.880242
O	0.530941	4.082829	2.200337
H	0.303716	4.604527	1.403404
H	1.311327	3.582300	1.905625
O	0.515090	-3.301463	-2.435357
H	1.025929	-2.515252	-2.165236
H	0.213966	-3.137576	-3.340773

Table S33. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $14H_2O$_β-PPII_B.

N	-4.102688	0.721120	0.389925
C	-3.071709	-0.032635	-0.376705
C	-1.739511	0.628058	-0.045425

N	-0.699691	-0.153938	0.207033
C	0.608872	0.392581	0.529287
C	1.650816	-0.297173	-0.338919
N	2.742166	0.411949	-0.622000
C	3.869193	-0.200062	-1.294771
C	4.286064	-1.452649	-0.531004
O	4.816527	-2.368570	-1.336808
O	-1.687320	1.874032	-0.046566
O	1.510678	-1.472826	-0.718061
C	5.028783	0.817574	-1.396239
O	4.180256	-1.593551	0.670135
C	-3.341710	0.044523	-1.890933
C	0.909863	0.236524	2.044367
C	-2.346132	-0.846852	-2.633670
C	6.156739	0.296351	-2.286592
C	5.561563	1.237658	-0.023732
C	-4.778561	-0.358470	-2.226002
C	2.242617	0.875150	2.437050
C	0.864445	-1.220181	2.501548
H	-4.223899	1.677219	-0.006572
H	-3.791387	0.807808	1.377335
H	-5.017495	0.214795	0.385810
H	-3.094047	-1.073311	-0.032808
H	-0.815845	-1.177679	0.188757
H	0.588428	1.461564	0.291331
H	2.781667	1.405817	-0.374315
H	3.576032	-0.514202	-2.303008
H	5.116576	-3.131441	-0.806904
H	4.584965	1.694183	-1.887588
H	-3.188737	1.089930	-2.193459
H	0.103063	0.796996	2.533764
H	-2.509681	-0.773838	-3.712564
H	-2.487290	-1.894852	-2.341312
H	-1.305964	-0.569872	-2.431642
H	5.782695	-0.025024	-3.263787
H	6.671660	-0.550938	-1.821959
H	6.893373	1.089092	-2.445972
H	6.085271	0.408188	0.464308
H	4.768201	1.573778	0.653058
H	6.273344	2.060057	-0.142993
H	-5.516926	0.329024	-1.801796
H	-4.997211	-1.369198	-1.861438
H	-4.911546	-0.351677	-3.312052
H	2.313774	0.931533	3.527513
H	2.342359	1.888611	2.035996
H	3.085375	0.278521	2.070629
H	-0.086519	-1.708689	2.262472
H	1.001294	-1.271746	3.586511
H	1.671883	-1.794338	2.034658
O	-2.762228	0.762859	2.879236
H	-2.124050	1.507806	2.953567
H	-2.298287	-0.036953	3.167119
O	-1.284478	3.011076	2.461810
H	-1.397856	2.811310	1.512555
H	-0.403140	3.441352	2.510884
O	-4.419010	3.297335	-0.791802
H	-5.130592	3.422820	-1.436276

H	-3.611266	3.671395	-1.198788
O	-1.814113	3.925297	-1.763059
H	-1.741464	3.803435	-2.722420
H	-1.650710	3.047735	-1.354997
O	-1.153913	-3.017315	0.083430
H	-0.975762	-3.152397	-0.874708
H	-0.360916	-3.423849	0.505072
O	-6.452715	-0.792797	0.482200
H	-6.780289	-0.874113	1.389966
H	-6.240418	-1.712092	0.185953
O	-5.657871	-3.236067	-0.412263
H	-4.896001	-3.523157	0.147407
H	-6.307194	-3.953312	-0.375784
O	-3.523469	-3.832537	1.176741
H	-2.656022	-3.613584	0.762605
H	-3.460876	-4.756550	1.458974
O	1.378092	-3.990054	0.531272
H	1.993453	-4.052427	1.291310
H	1.642364	-3.169461	0.073991
O	3.482956	-3.770727	2.363960
H	3.901969	-3.022393	1.898157
H	3.311653	-3.460373	3.265199
O	2.675511	3.273455	-0.068425
H	2.001077	3.796808	-0.555276
H	3.515466	3.738623	-0.206324
O	0.558534	4.974621	-0.739434
H	0.774968	5.842683	-1.111733
H	-0.294962	4.704231	-1.148626
O	1.041361	4.440202	1.994593
H	0.700743	4.835769	1.167131
H	1.801751	3.922370	1.675127
O	0.064018	-3.171767	-2.383102
H	0.649743	-2.445417	-2.097007
H	-0.265804	-2.928196	-3.260203

Table S34. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $14H_2O$_β-PPII_C.

N	-4.173036	0.562935	0.046889
C	-3.068791	-0.347717	-0.357506
C	-1.777594	0.422033	-0.119261
N	-0.682464	-0.303495	0.072979
C	0.582276	0.297099	0.458806
C	1.693774	-0.302337	-0.387597
N	2.782277	0.446174	-0.551927
C	3.955412	-0.094940	-1.207316
C	4.368447	-1.383965	-0.504331
O	4.952466	-2.236514	-1.342315
O	-1.793491	1.667495	-0.143484

O	1.612523	-1.452200	-0.858589
C	5.091606	0.952789	-1.197358
O	4.215346	-1.601763	0.680152
C	-3.189861	-0.829056	-1.813734
C	0.826032	0.089754	1.979490
C	-4.554086	-1.477575	-2.055152
C	6.275725	0.501970	-2.052850
C	5.545508	1.315919	0.218827
C	-2.901045	0.276395	-2.831559
C	2.058023	0.842605	2.479937
C	0.917537	-1.388769	2.353986
H	-4.160490	1.466939	-0.470029
H	-4.031107	0.775429	1.051163
H	-5.111125	0.127703	-0.054616
H	-3.117034	-1.204914	0.320050
H	-0.771771	-1.326823	0.111389
H	0.516654	1.372051	0.258006
H	2.785587	1.421432	-0.235049
H	3.714261	-0.353026	-2.244736
H	5.247089	-3.026302	-0.850309
H	4.651112	1.842042	-1.668491
H	-2.417187	-1.598388	-1.927336
H	-0.064047	0.526171	2.449885
H	-4.546362	-2.008793	-3.011277
H	-5.355517	-0.731783	-2.096738
H	-4.802036	-2.196531	-1.265456
H	5.958930	0.215699	-3.060674
H	6.790491	-0.352165	-1.600650
H	6.997042	1.319598	-2.139976
H	6.052540	0.470515	0.696932
H	4.714046	1.615318	0.866169
H	6.252774	2.149641	0.173907
H	-1.863153	0.621759	-2.766292
H	-3.562250	1.140681	-2.692976
H	-3.058564	-0.105084	-3.844812
H	2.073687	0.829473	3.574261
H	2.055500	1.886891	2.153218
H	2.980016	0.369411	2.123727
H	0.036242	-1.959784	2.042695
H	1.010056	-1.489485	3.440209
H	1.803615	-1.846102	1.899502
O	-2.837823	0.691185	2.514912
H	-2.275526	1.470615	2.711404
H	-3.130088	0.334298	3.365782
O	-1.273334	2.943465	2.264923
H	-1.328548	2.705764	1.319909
H	-0.406808	3.383453	2.378166
O	-4.365784	3.150793	-1.144738
H	-5.037936	3.323964	-1.819663
H	-3.526296	3.516834	-1.491960
O	-1.706069	3.723965	-1.876708
H	-1.513860	3.627510	-2.822212
H	-1.570353	2.842809	-1.469189
O	-1.158112	-3.168657	-0.089994
H	-1.005253	-3.146665	-1.062257
H	-0.351831	-3.616936	0.257480
O	-6.799428	-0.598717	0.120370

H	-7.436354	-0.028492	0.575002
H	-6.421985	-1.190488	0.807163
O	-4.996550	-1.846344	1.711666
H	-4.553271	-2.673559	1.406228
H	-5.066388	-1.915143	2.674776
O	-3.638330	-3.982635	0.713652
H	-2.733222	-3.754471	0.395899
H	-4.064030	-4.473434	-0.003808
O	1.416242	-4.042261	0.222088
H	2.024946	-4.153576	0.982307
H	1.648820	-3.169211	-0.148531
O	3.482702	-3.955993	2.109849
H	3.902958	-3.154824	1.743399
H	3.273172	-3.747851	3.032207
O	2.659960	3.287414	0.114413
H	1.956293	3.765492	-0.392010
H	3.487905	3.754140	-0.080337
O	0.562170	4.834212	-0.617244
H	0.359548	4.989638	0.323034
H	-0.265651	4.534966	-1.046681
O	1.100085	4.441046	2.129322
H	1.440795	4.954674	2.876541
H	1.872250	4.026420	1.692014
O	-0.308422	-2.498450	-2.607724
H	0.448185	-2.055270	-2.173683
H	0.075097	-3.135071	-3.228957

Table S35. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $14H_2O$_β-PPII_J.

N	-4.194610	0.435117	-0.027601
C	-3.044269	-0.297804	-0.621818
C	-1.791858	0.467871	-0.210449
N	-0.682169	-0.234410	-0.029988
C	0.535113	0.379062	0.477289
C	1.715626	-0.246779	-0.250274
N	2.768375	0.539956	-0.473109
C	3.975894	-0.007994	-1.062153
C	4.414889	-1.222565	-0.251791
O	4.864963	-2.206790	-1.023780
O	-1.854610	1.706674	-0.087318
O	1.709614	-1.441052	-0.596994
C	5.085758	1.061688	-1.089517
O	4.399445	-1.272733	0.961574
C	-3.206044	-0.419057	-2.151246
C	0.622225	0.222890	2.022658
C	-3.032658	0.916020	-2.878957
C	4.697482	2.190795	-2.047633

C	6.430959	0.457331	-1.495801
C	-2.245392	-1.469310	-2.707760
C	1.964956	0.703124	2.576395
C	0.342285	-1.207864	2.480001
H	-4.225619	1.435779	-0.314493
H	-4.087903	0.412289	1.003401
H	-5.083707	-0.041662	-0.292542
H	-3.037524	-1.297133	-0.172073
H	-0.721162	-1.262661	-0.066822
H	0.496115	1.446865	0.240584
H	2.730570	1.523657	-0.189770
H	3.769525	-0.350160	-2.083850
H	5.186697	-2.936876	-0.461376
H	5.172068	1.459777	-0.068322
H	-4.232000	-0.777509	-2.304533
H	-0.176758	0.871084	2.406711
H	-3.297546	0.794018	-3.933094
H	-1.988040	1.247932	-2.836360
H	-3.664561	1.709389	-2.465230
H	3.734319	2.645306	-1.796786
H	4.639561	1.810601	-3.074213
H	5.455989	2.978806	-2.020086
H	6.355812	-0.038674	-2.470439
H	6.795841	-0.273433	-0.767241
H	7.180176	1.250008	-1.575712
H	-2.404953	-2.445847	-2.238696
H	-1.201954	-1.172052	-2.550008
H	-2.400176	-1.581250	-3.785000
H	1.910647	0.764290	3.667572
H	2.250377	1.686598	2.190777
H	2.767900	0.005565	2.312281
H	-0.666209	-1.533811	2.208405
H	0.429300	-1.266685	3.570245
H	1.066905	-1.906705	2.047216
O	-2.910833	0.173063	2.431822
H	-2.573885	1.052609	2.720120
H	-3.090102	-0.337371	3.234349
O	-2.099541	2.769242	2.494839
H	-2.107434	2.632436	1.528593
H	-1.195721	3.115011	2.664576
O	-4.482349	3.235485	-0.512943
H	-5.245489	3.567608	-1.007699
H	-3.700275	3.707608	-0.864514
O	-1.926841	4.044637	-1.409688
H	-1.852500	4.107712	-2.374647
H	-1.738266	3.111729	-1.171419
O	-0.899994	-3.138935	-0.147871
H	-0.526054	-3.258033	-1.051821
H	-0.176631	-3.479182	0.425311
O	-6.243169	-1.310751	-0.729249
H	-7.178537	-1.090438	-0.610422
H	-6.021638	-1.980831	-0.037474
O	-5.303366	-2.984976	1.184614
H	-4.541783	-3.517320	0.850175
H	-4.981892	-2.508819	1.963890
O	-3.254637	-4.485370	0.201015
H	-2.393117	-4.025436	0.062926

H	-3.477403	-4.899281	-0.645397
O	1.621531	-3.966522	0.661076
H	2.139693	-3.894334	1.489508
H	1.864207	-3.161096	0.167520
O	3.380202	-3.272017	2.727406
H	3.842085	-2.572425	2.227430
H	3.002308	-2.835411	3.505082
O	2.344671	3.301170	0.396107
H	1.729662	3.935759	-0.033237
H	3.158492	3.800949	0.565331
O	0.281227	5.098583	-0.118545
H	0.448361	6.031503	-0.318892
H	-0.521303	4.839497	-0.627138
O	0.396104	3.959611	2.452731
H	0.209445	4.544150	1.689774
H	1.158169	3.444085	2.135376
O	0.657919	-3.247391	-2.415373
H	1.157281	-2.464918	-2.115228
H	0.384973	-3.067783	-3.326787

Table S36. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $14H_2O$_β-PPII_S.

N	-4.167132	0.463004	0.125387
C	-3.065148	-0.273429	-0.550057
C	-1.779993	0.471315	-0.204025
N	-0.678060	-0.251716	-0.057664
C	0.579760	0.340472	0.370616
C	1.705104	-0.297623	-0.430569
N	2.801861	0.443129	-0.605054
C	3.986814	-0.136369	-1.201186
C	4.451656	-1.327842	-0.370640
O	5.320721	-2.074438	-1.047675
O	-1.814574	1.711987	-0.087532
O	1.615676	-1.458470	-0.861490
C	5.122314	0.900761	-1.329455
O	4.109040	-1.561477	0.769272
C	-3.325246	-0.370552	-2.067348
C	0.762848	0.160002	1.905167
C	-3.188472	0.972590	-2.787611
C	5.583897	1.418534	0.035415
C	4.700989	2.039377	-2.260501
C	-2.409192	-1.419590	-2.695556
C	2.079448	0.746127	2.419593
C	0.642145	-1.300557	2.338149
H	-4.209167	1.468005	-0.145945
H	-3.998152	0.425837	1.146443
H	-5.076047	-0.003135	-0.087355
H	-3.044141	-1.280785	-0.118428
H	-0.728506	-1.278425	-0.127935

H	0.539207	1.412527	0.152122
H	2.799182	1.416878	-0.291514
H	3.743013	-0.521399	-2.198787
H	5.628347	-2.807671	-0.482148
H	5.956372	0.366699	-1.798500
H	-4.361723	-0.719894	-2.158771
H	-0.067042	0.734010	2.339241
H	-3.529800	0.867709	-3.821357
H	-2.139601	1.291979	-2.816443
H	-3.780381	1.766519	-2.319351
H	5.967580	0.612542	0.669890
H	4.771135	1.912634	0.581422
H	6.385068	2.151177	-0.097862
H	3.881132	2.628023	-1.834979
H	4.377031	1.654933	-3.233026
H	5.545577	2.715354	-2.423772
H	-2.555435	-2.403347	-2.237557
H	-1.355351	-1.136484	-2.587855
H	-2.622166	-1.508231	-3.764979
H	2.050912	0.799973	3.512229
H	2.266188	1.751036	2.031349
H	2.925834	0.114395	2.129546
H	-0.306535	-1.756810	2.035119
H	0.712815	-1.369003	3.428611
H	1.457068	-1.895997	1.912327
O	-2.912006	0.207310	2.637505
H	-2.399781	1.025439	2.832069
H	-2.384965	-0.540473	2.953721
O	-1.806828	2.691048	2.532681
H	-1.849282	2.557592	1.566444
H	-0.925102	3.101819	2.669623
O	-4.495154	3.261762	-0.298235
H	-5.293526	3.584755	-0.740718
H	-3.743731	3.744147	-0.699264
O	-2.020841	4.061286	-1.381760
H	-2.026579	4.137015	-2.348634
H	-1.824645	3.123357	-1.171721
O	-0.935121	-3.143092	-0.253667
H	-0.653932	-3.246876	-1.191919
H	-0.158175	-3.501414	0.235534
O	-6.267702	-1.263882	-0.439796
H	-7.192320	-1.033034	-0.268376
H	-6.005337	-1.912601	0.257542
O	-5.190618	-2.871791	1.457811
H	-4.461910	-3.425048	1.086006
H	-4.816378	-2.391556	2.210462
O	-3.262361	-4.439042	0.347613
H	-2.411327	-4.000436	0.109859
H	-3.581141	-4.863219	-0.462228
O	1.605784	-3.994427	0.372076
H	2.142435	-4.044061	1.190736
H	1.877303	-3.157232	-0.049180
O	3.442036	-3.727814	2.465236
H	3.868985	-2.958641	2.043880
H	3.126169	-3.418334	3.326827
O	2.410385	3.286188	0.208868
H	1.731946	3.860732	-0.209587

H	3.193687	3.850604	0.303311
O	0.299485	5.053496	-0.252121
H	0.494215	5.969133	-0.501613
H	-0.542509	4.812368	-0.702390
O	0.590636	4.067578	2.365471
H	0.334136	4.602505	1.586748
H	1.352072	3.564855	2.027637
O	0.440927	-3.239904	-2.640360
H	0.974281	-2.480982	-2.338169
H	0.128913	-3.020225	-3.530138

Table S37. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $18H_2O$_β-PPII_A.

N	-4.792749	-0.717035	0.108011
C	-3.478575	-1.098113	-0.477145
C	-2.537121	0.065787	-0.188075
N	-1.267140	-0.219099	0.072238
C	-0.321362	0.812682	0.469304
C	0.986256	0.595656	-0.275994
N	1.710555	1.685879	-0.517789
C	3.042863	1.588279	-1.077276
C	3.916357	0.707796	-0.186605
O	4.933742	0.181705	-0.843807
O	-2.994809	1.224572	-0.211801
O	1.369842	-0.541076	-0.604004
C	3.637632	3.009097	-1.222659
O	3.720900	0.549260	1.005897
C	-3.621540	-1.412457	-1.979938
C	-0.129812	0.808680	2.011749
C	-3.931364	-0.176345	-2.826961
C	4.894405	3.020535	-2.092215
C	3.899739	3.663302	0.136899
C	-2.370449	-2.122567	-2.492832
C	0.827872	1.904729	2.481498
C	0.324374	-0.548764	2.545807
H	-5.153156	0.185765	-0.266767
H	-4.668202	-0.593919	1.129517
H	-5.486135	-1.477303	-0.065795
H	-3.140965	-1.996769	0.051645
H	-0.959468	-1.201565	0.100514
H	-0.746225	1.779560	0.180060
H	1.321925	2.608891	-0.300781
H	2.994395	1.113406	-2.064526
H	5.596127	-0.287665	-0.217758
H	2.860253	3.581229	-1.747125
H	-4.466779	-2.109714	-2.046725
H	-1.130888	1.032603	2.402700
H	-4.166381	-0.486010	-3.849295
H	-3.060451	0.488489	-2.874575

H	-4.784018	0.396770	-2.447083
H	4.716380	2.538479	-3.058895
H	5.724844	2.505121	-1.600407
H	5.200734	4.054467	-2.277132
H	4.747288	3.185904	0.642251
H	3.035722	3.598791	0.808381
H	4.145098	4.720609	-0.000881
H	-2.173100	-3.042431	-1.933365
H	-1.486859	-1.478348	-2.419625
H	-2.497303	-2.388248	-3.546416
H	0.761621	2.006709	3.569033
H	0.592735	2.873629	2.032038
H	1.862727	1.656164	2.222102
H	-0.343877	-1.365492	2.251849
H	0.355390	-0.522543	3.639811
H	1.334412	-0.783602	2.192499
O	-3.689092	-0.242465	2.661063
H	-3.444393	0.705327	2.760691
H	-2.968813	-0.762947	3.045175
O	-3.311303	2.435190	2.283348
H	-3.264773	2.202697	1.336216
H	-2.653205	3.157496	2.384491
O	-5.996682	1.771984	-0.593299
H	-6.842711	1.792981	-1.063679
H	-5.421877	2.432065	-1.031394
O	-3.879354	3.253937	-1.737676
H	-3.874698	3.241984	-2.707443
H	-3.388285	2.458517	-1.441780
O	-0.478165	-3.027944	0.071083
H	-0.108704	-3.041723	-0.850282
H	0.329370	-3.100315	0.621620
O	-6.208285	-3.073183	-0.309321
H	-7.158784	-3.138751	-0.136716
H	-5.753968	-3.550140	0.426668
O	-4.664026	-4.099300	1.667473
H	-3.793726	-4.394602	1.306561
H	-4.469239	-3.473658	2.380179
O	-2.321419	-4.972990	0.591523
H	-1.630721	-4.300328	0.383629
H	-2.452505	-5.487496	-0.217990
O	2.240069	-2.798219	0.718313
H	2.752243	-2.594470	1.527060
H	2.048898	-1.924487	0.317092
O	3.850454	-1.655229	2.703700
H	3.943836	-0.803596	2.226328
H	3.558369	-1.442873	3.602873
O	0.451753	4.282841	0.012991
H	-0.353471	4.546781	-0.484794
H	1.048749	5.045705	-0.037761
O	-2.111447	5.117853	-0.705173
H	-2.244122	6.004368	-1.072701
H	-2.785671	4.536588	-1.126377
O	-1.626435	4.624927	2.019020
H	-2.031593	4.937258	1.184678
H	-0.712277	4.436171	1.742903
O	6.760832	-0.946358	0.558854
H	7.115688	-0.352292	1.237625

H	6.533662	-1.793709	1.021976
O	5.967851	-3.175326	1.850760
H	5.238302	-2.773850	2.368993
H	6.593838	-3.544278	2.490887
O	3.252156	-3.821758	-1.671836
H	3.823801	-3.130029	-2.068186
H	3.117956	-3.563117	-0.736629
O	0.804357	-2.754938	-2.312915
H	1.022372	-1.834455	-2.078034
H	1.657152	-3.239154	-2.197817
O	4.560325	-1.721878	-2.961426
H	5.399432	-1.903584	-3.409531
H	4.743601	-0.991908	-2.342470

Table S38. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $18H_2O$_β-PPII_B.

N	-4.711492	-0.229560	0.517069
C	-3.492263	-0.706055	-0.195212
C	-2.442496	0.376018	0.023852
N	-1.212382	-0.003430	0.340465
C	-0.156082	0.963006	0.597550
C	1.081876	0.559218	-0.188123
N	1.890192	1.548482	-0.560175
C	3.178872	1.273271	-1.160733
C	4.013171	0.402934	-0.223165
O	4.963550	-0.252164	-0.865379
O	-2.788689	1.566455	-0.111045
O	1.341080	-0.633223	-0.428591
C	3.888737	2.611529	-1.475125
O	3.849544	0.353828	0.983733
C	-3.777861	-0.895754	-1.695080
C	0.130926	1.067184	2.119001
C	-2.520362	-1.389643	-2.410023
C	5.102206	2.422208	-2.384968
C	4.265883	3.373755	-0.201834
C	-4.936172	-1.871661	-1.910157
C	1.127379	2.181124	2.440448
C	0.598710	-0.258619	2.716007
H	-5.119141	0.593295	0.023920
H	-4.451794	0.063049	1.480128
H	-5.434837	-0.980564	0.594967
H	-3.182026	-1.653720	0.259486
H	-1.000542	-1.008695	0.403518
H	-0.509460	1.938018	0.245279
H	1.593908	2.520722	-0.428292
H	3.039625	0.711329	-2.092306
H	5.614524	-0.714855	-0.222561
H	3.141603	3.195440	-2.029741
H	-4.060714	0.087567	-2.097185

H	-0.838850	1.340334	2.552879
H	-2.722154	-1.508570	-3.478336
H	-2.212375	-2.365279	-2.017317
H	-1.676560	-0.699535	-2.304060
H	4.844701	1.848729	-3.281334
H	5.912733	1.901306	-1.866802
H	5.476623	3.400511	-2.700880
H	5.074798	2.862929	0.333362
H	3.423519	3.478318	0.491625
H	4.617789	4.377024	-0.460153
H	-5.883060	-1.501061	-1.505629
H	-4.715488	-2.839582	-1.442677
H	-5.079398	-2.039935	-2.981646
H	1.154125	2.347564	3.521731
H	0.849267	3.123228	1.957694
H	2.137093	1.911142	2.112050
H	-0.083392	-1.086779	2.492353
H	0.668722	-0.171245	3.804916
H	1.594026	-0.517389	2.338744
O	-3.536466	0.551173	2.967375
H	-3.157439	1.457917	2.935029
H	-2.858925	-0.024754	3.350554
O	-2.778812	3.064059	2.234772
H	-2.801622	2.723607	1.319716
H	-2.108310	3.781013	2.207967
O	-5.825001	1.986464	-0.898597
H	-6.536732	1.795607	-1.526822
H	-5.171888	2.531307	-1.383040
O	-3.544259	3.237945	-2.061736
H	-3.439663	3.029727	-3.003033
H	-3.115314	2.509815	-1.563037
O	-0.847900	-2.881064	0.259689
H	-0.418695	-2.885031	-0.638507
H	-0.112552	-3.126180	0.856286
O	-6.629268	-2.228473	0.859535
H	-6.932652	-2.238335	1.779259
H	-6.261127	-3.129436	0.684762
O	-5.561339	-4.659363	0.281017
H	-4.579872	-4.652580	0.192007
H	-5.768637	-5.360528	0.915594
O	-2.863217	-4.709681	-0.113501
H	-2.149758	-4.065667	0.101996
H	-2.642494	-5.067366	-0.985760
O	1.864790	-2.943624	0.983049
H	2.477986	-2.763332	1.723810
H	1.727001	-2.067666	0.564340
O	3.838782	-1.881242	2.680145
H	3.988323	-1.055736	2.171318
H	3.694793	-1.616107	3.601137
O	0.879286	4.280576	-0.362502
H	0.086726	4.483793	-0.907028
H	1.529233	4.965546	-0.584862
O	-1.648653	5.107312	-1.232884
H	-1.702208	5.936402	-1.731578
H	-2.362663	4.528245	-1.584884
O	-1.087869	5.146386	1.539544
H	-1.526899	5.297576	0.678556

H	-0.195545	4.866898	1.265969
O	6.747711	-1.391524	0.582501
H	7.087110	-0.813191	1.282467
H	6.479688	-2.238407	1.024345
O	5.793709	-3.595424	1.799737
H	5.090523	-3.133029	2.304491
H	6.367292	-4.025003	2.451028
O	2.738529	-4.087382	-1.409897
H	3.397817	-3.489769	-1.822562
H	2.635164	-3.791027	-0.481350
O	0.462653	-2.736203	-2.106549
H	0.793852	-1.841065	-1.909766
H	1.251787	-3.316370	-1.974189
O	4.288516	-2.245317	-2.813431
H	5.066085	-2.564970	-3.294134
H	4.603567	-1.510841	-2.255833

Table S39. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $18H_2O$_β-PPII_C.

N	-4.807404	-0.237186	-0.071720
C	-3.470533	-0.864545	-0.256122
C	-2.455370	0.239771	0.009828
N	-1.226970	-0.136022	0.341607
C	-0.199786	0.825016	0.710267
C	1.053534	0.542742	-0.105334
N	1.882644	1.563647	-0.306132
C	3.159759	1.351338	-0.956640
C	3.984270	0.343334	-0.159415
O	4.890583	-0.260416	-0.907132
O	-2.808590	1.426995	-0.126498
O	1.308236	-0.600472	-0.527431
C	3.898562	2.701642	-1.102502
O	3.849555	0.151309	1.036770
C	-3.288371	-1.485633	-1.653769
C	0.068607	0.758684	2.237355
C	-4.438712	-2.440502	-1.976802
C	5.088334	2.602603	-2.057209
C	4.323621	3.276971	0.251094
C	-3.100391	-0.436484	-2.751791
C	0.936913	1.920337	2.717482
C	0.677288	-0.578005	2.659646
H	-4.979798	0.547157	-0.734872
H	-4.822557	0.159874	0.885083
H	-5.582646	-0.933074	-0.132162
H	-3.381498	-1.645849	0.506254
H	-1.024106	-1.139519	0.439025
H	-0.576533	1.823444	0.464240
H	1.607219	2.514309	-0.037521
H	2.994543	0.922954	-1.952670

H	5.547517	-0.816034	-0.350598
H	3.158182	3.373291	-1.557375
H	-2.365114	-2.073125	-1.590519
H	-0.927538	0.863097	2.685638
H	-4.194012	-3.021536	-2.870515
H	-5.369490	-1.898174	-2.178513
H	-4.625396	-3.139366	-1.153688
H	4.794179	2.169875	-3.019028
H	5.888658	1.986976	-1.635823
H	5.492563	3.602443	-2.241502
H	5.137486	2.686530	0.687613
H	3.502571	3.297018	0.976683
H	4.686514	4.301252	0.121902
H	-2.185839	0.147913	-2.598914
H	-3.949390	0.255670	-2.802067
H	-3.014827	-0.933313	-3.722623
H	0.958932	1.934365	3.811558
H	0.545113	2.882074	2.372305
H	1.968302	1.817561	2.361624
H	0.080123	-1.436101	2.331824
H	0.751221	-0.624950	3.750721
H	1.689373	-0.682338	2.251663
O	-3.862417	0.346115	2.515526
H	-3.488640	1.231166	2.712283
H	-4.255499	0.024259	3.339719
O	-2.754630	2.844105	2.263611
H	-2.734359	2.586290	1.323071
H	-2.143888	3.610182	2.330067
O	-5.449091	2.042667	-1.667918
H	-6.033095	1.981493	-2.437730
H	-4.686076	2.590474	-1.943561
O	-2.920351	3.258051	-2.104656
H	-2.556435	3.045549	-2.978291
H	-2.654289	2.526990	-1.506462
O	-0.825743	-3.011877	0.261743
H	-0.586189	-2.944435	-0.699295
H	0.027629	-3.242954	0.685104
O	-6.837713	-2.167529	0.153959
H	-7.605248	-1.823498	0.633961
H	-6.335342	-2.719425	0.798854
O	-5.142779	-3.498589	1.815686
H	-4.349098	-3.916463	1.404311
H	-4.823971	-2.998546	2.580959
O	-2.970003	-4.651196	0.645931
H	-2.168193	-4.094871	0.502797
H	-3.135736	-5.107941	-0.191419
O	1.931801	-3.031742	0.592269
H	2.562075	-2.962709	1.338223
H	1.788767	-2.106041	0.301732
O	3.880294	-2.259367	2.459223
H	4.034395	-1.377531	2.057456
H	3.661191	-2.105222	3.390690
O	1.031863	4.304542	0.195763
H	0.323503	4.594792	-0.421614
H	1.736839	4.965692	0.115365
O	-1.350793	5.215508	-0.911314
H	-1.385920	6.059216	-1.386229

H	-1.950177	4.600146	-1.392522
O	-1.127924	5.062581	1.906807
H	-1.474123	5.281310	1.018854
H	-0.208696	4.805525	1.708538
O	6.705720	-1.579296	0.336452
H	7.094153	-1.057889	1.055452
H	6.465476	-2.458573	0.727898
O	5.851599	-3.878863	1.450320
H	5.151198	-3.468339	2.000979
H	6.462912	-4.317878	2.059656
O	2.408849	-3.729803	-2.083080
H	3.013150	-3.048303	-2.448563
H	2.443831	-3.630398	-1.109482
O	-0.001955	-2.436390	-2.251263
H	0.329959	-1.578031	-1.926904
H	0.820601	-2.977709	-2.337045
O	3.889768	-1.641378	-3.197999
H	4.552530	-1.879900	-3.862681
H	4.368534	-1.145181	-2.508880

Table S40. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $18H_2O$_β-PPII_J.

N	-4.732990	-0.805161	0.022410
C	-3.392740	-1.105886	-0.549650
C	-2.496909	0.068799	-0.173419
N	-1.212782	-0.186486	0.035525
C	-0.301558	0.839178	0.518987
C	1.033567	0.658959	-0.188015
N	1.731293	1.764664	-0.440054
C	3.063419	1.677209	-1.007981
C	3.941418	0.802267	-0.117298
O	4.800151	0.070242	-0.799127
O	-2.995815	1.208830	-0.101127
O	1.461358	-0.467624	-0.499399
C	3.661796	3.091882	-1.152722
O	3.885178	0.824842	1.101026
C	-3.487947	-1.333978	-2.072096
C	-0.186116	0.777571	2.068770
C	-3.795945	-0.052856	-2.850371
C	2.868093	3.886818	-2.193087
C	5.141926	3.043879	-1.535509
C	-2.212198	-1.993367	-2.593249
C	0.868190	1.745172	2.608729
C	0.080135	-0.636865	2.581388
H	-5.110091	0.111423	-0.297497
H	-4.634366	-0.754422	1.053411
H	-5.398348	-1.569827	-0.224157
H	-3.036052	-2.020501	-0.062890
H	-0.884732	-1.162097	0.038027

H	-0.719283	1.812967	0.244885
H	1.336507	2.676040	-0.188769
H	3.013268	1.198982	-1.994369
H	5.484968	-0.390918	-0.193877
H	3.569148	3.579928	-0.171739
H	-4.318613	-2.039123	-2.205163
H	-1.176137	1.091472	2.425314
H	-3.997684	-0.300659	-3.896406
H	-2.935591	0.627330	-2.831670
H	-4.668262	0.481834	-2.458950
H	1.800958	3.940629	-1.957327
H	2.977886	3.427005	-3.182221
H	3.249985	4.910546	-2.250419
H	5.286636	2.473119	-2.460119
H	5.759618	2.590127	-0.754485
H	5.509032	4.060468	-1.703096
H	-2.011708	-2.940373	-2.082264
H	-1.341571	-1.340949	-2.461984
H	-2.310536	-2.200656	-3.662958
H	0.774176	1.819840	3.696417
H	0.769782	2.749448	2.185699
H	1.879078	1.392907	2.375217
H	-0.718500	-1.330718	2.302651
H	0.142609	-0.623089	3.674661
H	1.033134	-1.021157	2.200209
O	-3.465650	-0.509839	2.489139
H	-3.471393	0.443356	2.737182
H	-3.516086	-1.014855	3.313326
O	-3.634174	2.208253	2.438240
H	-3.582382	2.040352	1.478277
H	-2.921126	2.867041	2.589230
O	-5.987550	1.695707	-0.549998
H	-6.827717	1.725784	-1.030306
H	-5.424854	2.398121	-0.934907
O	-3.884894	3.308346	-1.524577
H	-3.837619	3.353424	-2.492193
H	-3.379109	2.512919	-1.252474
O	-0.394676	-2.988090	0.013165
H	0.024263	-2.971413	-0.887292
H	0.378605	-3.061860	0.608989
O	-6.070639	-3.162595	-0.614096
H	-7.025598	-3.261099	-0.487873
H	-5.635984	-3.695011	0.095889
O	-4.608313	-4.350326	1.334994
H	-3.709796	-4.581257	0.996705
H	-4.470592	-3.768791	2.096709
O	-2.168914	-5.041284	0.342127
H	-1.508048	-4.321531	0.207636
H	-2.232311	-5.511565	-0.501736
O	2.326455	-2.752070	0.768149
H	2.798714	-2.503521	1.588063
H	2.113543	-1.892376	0.348795
O	3.692811	-1.380862	2.809472
H	3.829123	-0.547657	2.310131
H	3.255430	-1.139659	3.640006
O	0.343774	4.227350	0.317990
H	-0.449851	4.574950	-0.145261

H	0.922115	4.993907	0.454682
O	-2.216884	5.134912	-0.290476
H	-2.387758	6.055601	-0.538548
H	-2.864796	4.583492	-0.786506
O	-1.751153	4.232239	2.333610
H	-2.125743	4.672520	1.543461
H	-0.846821	4.021690	2.041835
O	6.698128	-1.076892	0.494868
H	7.279145	-0.418202	0.904806
H	6.483808	-1.738335	1.202519
O	5.977860	-2.838276	2.408695
H	5.189690	-2.386638	2.779893
H	6.608223	-2.940041	3.136676
O	3.354780	-3.824105	-1.595824
H	3.962531	-3.173133	-2.007062
H	3.230574	-3.541421	-0.666314
O	0.982207	-2.646787	-2.300210
H	1.209638	-1.734489	-2.044428
H	1.816999	-3.156376	-2.160841
O	4.688852	-1.797789	-2.957854
H	5.594447	-1.921112	-3.278160
H	4.722872	-1.029652	-2.359350

Table S41. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $18H_2O$_β-PPII_S.

N	-4.702313	-0.871007	0.138745
C	-3.383235	-1.163467	-0.484235
C	-2.489810	0.031117	-0.168096
N	-1.204316	-0.211669	0.050933
C	-0.279108	0.837197	0.452448
C	1.027273	0.632844	-0.299071
N	1.757116	1.722242	-0.536973
C	3.083701	1.599873	-1.105039
C	3.974794	0.762772	-0.190150
O	5.066768	0.353335	-0.810732
O	-2.993932	1.170584	-0.137286
O	1.402975	-0.501587	-0.641481
C	3.722850	2.983227	-1.347913
O	3.730411	0.538493	0.981996
C	-3.539560	-1.427243	-1.995597
C	-0.084970	0.825204	1.995336
C	-3.924089	-0.176320	-2.788378
C	3.939688	3.753468	-0.042616
C	2.895169	3.785671	-2.353938
C	-2.266986	-2.057563	-2.558589
C	0.885087	1.906783	2.475355
C	0.359560	-0.539657	2.519717
H	-5.112686	0.030060	-0.185729
H	-4.563179	-0.794531	1.162327

H	-5.363743	-1.653933	-0.059301
H	-2.992199	-2.063644	0.003499
H	-0.862875	-1.183083	0.041597
H	-0.717614	1.799235	0.168586
H	1.372703	2.639686	-0.297494
H	3.018228	1.068162	-2.062508
H	5.729793	-0.095349	-0.169718
H	4.701541	2.778595	-1.796385
H	-4.351953	-2.161257	-2.074916
H	-1.084851	1.052424	2.389163
H	-4.167227	-0.457997	-3.816879
H	-3.085543	0.529374	-2.828248
H	-4.793966	0.341263	-2.369585
H	4.617218	3.224225	0.635599
H	2.998063	3.921725	0.494068
H	4.376705	4.732874	-0.257833
H	1.911361	4.049523	-1.950876
H	2.744988	3.221825	-3.280337
H	3.413481	4.717144	-2.600371
H	-2.019736	-2.991552	-2.044770
H	-1.411013	-1.378659	-2.469562
H	-2.400580	-2.281492	-3.621014
H	0.813735	2.004129	3.563017
H	0.672416	2.881685	2.028540
H	1.917284	1.643105	2.221096
H	-0.308038	-1.351619	2.211440
H	0.383326	-0.524489	3.614099
H	1.371127	-0.774942	2.170725
O	-3.536606	-0.491192	2.677905
H	-3.373261	0.469150	2.821014
H	-2.773610	-0.966903	3.036603
O	-3.439128	2.215526	2.417608
H	-3.397777	2.023224	1.461213
H	-2.788407	2.942149	2.534179
O	-6.054505	1.571037	-0.431048
H	-6.913231	1.543144	-0.877460
H	-5.538969	2.278743	-0.868727
O	-4.050803	3.188714	-1.569464
H	-4.057399	3.210563	-2.539028
H	-3.517111	2.408875	-1.306498
O	-0.371927	-3.013252	-0.008549
H	0.004868	-3.008919	-0.926812
H	0.433523	-3.071208	0.547005
O	-6.031955	-3.262738	-0.355817
H	-6.981301	-3.361673	-0.192952
H	-5.568840	-3.754344	0.365312
O	-4.476049	-4.327409	1.592187
H	-3.597884	-4.574766	1.214165
H	-4.298560	-3.708342	2.315176
O	-2.108715	-5.067490	0.470218
H	-1.461112	-4.349621	0.274711
H	-2.235740	-5.550270	-0.359310
O	2.330365	-2.740793	0.675197
H	2.834770	-2.550796	1.492261
H	2.138037	-1.862036	0.286169
O	3.922483	-1.642065	2.695201
H	3.995207	-0.781700	2.231018

H	3.636195	-1.450859	3.600962
O	0.282254	4.233734	0.089413
H	-0.549203	4.484792	-0.370572
H	0.791554	5.056869	0.153195
O	-2.318543	5.053479	-0.494172
H	-2.469965	5.955676	-0.812994
H	-2.992848	4.484005	-0.930977
O	-1.752499	4.398311	2.181282
H	-2.178392	4.758317	1.376873
H	-0.852527	4.203765	1.866366
O	6.887465	-0.722201	0.637252
H	7.188132	-0.133923	1.346480
H	6.672636	-1.590538	1.066570
O	6.124790	-3.022748	1.815018
H	5.363361	-2.679202	2.329309
H	6.742915	-3.405122	2.454901
O	3.382354	-3.713985	-1.716385
H	3.971394	-3.018385	-2.078887
H	3.225854	-3.476822	-0.778937
O	0.920669	-2.697111	-2.386795
H	1.110876	-1.772323	-2.145450
H	1.786028	-3.156980	-2.264961
O	4.801967	-1.621587	-2.902903
H	5.659543	-1.825561	-3.303999
H	4.966190	-0.884293	-2.287668

Table S42. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $22H_2O$_β-PPII_A.

N	5.187333	0.251171	-0.136933
C	4.014961	-0.482195	0.412327
C	2.801194	0.408151	0.169959
N	1.657384	-0.195659	-0.133876
C	0.462134	0.563473	-0.471865
C	-0.728294	-0.093297	0.216862
N	-1.504676	0.716433	0.933882
C	-2.638784	0.212442	1.683870
C	-3.602136	-0.499257	0.748524
O	-4.365694	-1.388265	1.337498
O	2.924256	1.642723	0.279289
O	-0.952262	-1.317488	0.120788
C	-3.347798	1.385242	2.401840
O	-3.687665	-0.240111	-0.444496
C	4.233069	-0.821671	1.901284
C	0.275982	0.697405	-2.004210
C	4.225314	0.409945	2.809659
C	-4.278528	0.889447	3.507866
C	-4.087688	2.286473	1.410177
C	3.203747	-1.848324	2.372703
C	-1.105559	1.274527	-2.323352

C	0.500186	-0.611548	-2.759048
H	5.307823	1.197101	0.281865
H	5.032663	0.384884	-1.154017
H	6.055827	-0.309864	0.009165
H	3.918587	-1.409276	-0.162646
H	1.666772	-1.211593	-0.296276
H	0.591818	1.566715	-0.057270
H	-1.308382	1.725264	0.932550
H	-2.287592	-0.516356	2.425116
H	-4.988831	-1.837500	0.624678
H	-2.538852	1.962170	2.869329
H	5.226708	-1.286752	1.944700
H	1.046785	1.412468	-2.320181
H	4.538571	0.120547	3.816871
H	3.214972	0.829336	2.884702
H	4.902739	1.198096	2.463404
H	-3.744805	0.255038	4.223035
H	-5.115055	0.315582	3.096813
H	-4.691551	1.744238	4.051676
H	-4.989807	1.793684	1.026864
H	-3.460354	2.557255	0.553211
H	-4.398567	3.214262	1.899260
H	3.251355	-2.766446	1.779926
H	2.184072	-1.450857	2.309303
H	3.392652	-2.109930	3.418019
H	-1.155981	1.575898	-3.374253
H	-1.351360	2.142084	-1.698798
H	-1.875399	0.510721	-2.153167
H	1.511570	-0.998161	-2.601295
H	0.373530	-0.438868	-3.833051
H	-0.226515	-1.371178	-2.455243
O	3.809166	0.467487	-2.548337
H	3.513166	1.400797	-2.658919
H	3.996814	0.124865	-3.434028
O	3.148130	3.075593	-2.127325
H	3.208793	2.794769	-1.194891
H	2.248816	3.468704	-2.178981
O	5.750470	2.922087	0.666588
H	6.584322	3.103879	1.123942
H	5.052935	3.394522	1.165920
O	3.377955	3.755691	1.896724
H	3.367324	3.694610	2.864529
H	3.072838	2.888462	1.555253
O	1.942063	-3.071330	-0.422568
H	1.444990	-3.309071	0.402357
H	1.310892	-3.341253	-1.123037
O	7.237944	-1.605156	0.195780
H	8.163607	-1.342699	0.086593
H	7.007597	-2.161672	-0.588230
O	6.236056	-2.998539	-1.904111
H	5.498819	-3.531479	-1.519684
H	5.825941	-2.388976	-2.535159
O	4.269211	-4.481315	-0.737377
H	3.420117	-4.001971	-0.591186
H	4.543936	-4.819426	0.127214
O	-0.509482	-3.747855	-1.392115
H	-1.032374	-3.544555	-2.185035

H	-0.730349	-3.017718	-0.782887
O	-2.728522	-2.247993	-2.197824
H	-2.498291	-1.662777	-1.452224
H	-3.548195	-1.846084	-2.561287
O	-0.945154	3.487796	0.462701
H	-0.254736	4.042747	0.881703
H	-1.716916	4.089217	0.324823
O	1.241514	5.204816	0.898341
H	1.149722	6.097134	1.263546
H	2.047144	4.814509	1.306351
O	0.709775	4.309262	-1.719730
H	1.039289	4.857719	-0.979300
H	0.017439	3.781725	-1.278250
O	-5.752361	-2.522699	-0.442315
H	-5.660948	-1.973602	-1.254344
H	-5.220933	-3.334157	-0.608964
O	-3.742516	-4.369574	-0.799364
H	-3.284141	-3.722878	-1.388631
H	-3.809473	-5.199041	-1.296407
O	-2.117832	-4.715315	1.510090
H	-2.588230	-4.186035	2.189100
H	-2.626286	-4.601501	0.681236
O	0.252537	-3.372059	1.685578
H	-0.150776	-2.500215	1.526348
H	-0.509241	-3.989550	1.562928
O	-3.254000	-2.982661	3.385916
H	-3.818733	-3.330883	4.091233
H	-3.822957	-2.409595	2.839974
O	-5.214341	-1.073587	-2.782894
H	-5.725899	-1.210186	-3.594814
H	-5.112757	-0.103038	-2.673121
O	-3.025176	5.217358	-0.014837
H	-3.295055	5.671194	0.796963
H	-3.845338	4.804041	-0.374193
O	-5.297883	4.031911	-1.014956
H	-5.744520	4.584299	-1.673331
H	-5.101431	3.183018	-1.466350
O	-4.506129	1.619222	-2.215163
H	-3.878556	1.903912	-2.898788
H	-3.969334	1.201205	-1.510383

Table S43. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $22H_2O$_β-PPII_B.

N	5.038238	0.617133	-0.499883
C	3.958087	-0.162804	0.166417
C	2.684683	0.655555	-0.008647
N	1.581096	0.009049	-0.360675
C	0.325782	0.709374	-0.587254

C	-0.781292	-0.067969	0.113192
N	-1.569136	0.635553	0.921294
C	-2.626885	0.007970	1.690708
C	-3.568245	-0.740403	0.761602
O	-4.203720	-1.737802	1.329153
O	2.730413	1.882806	0.203084
O	-0.928615	-1.297551	-0.054425
C	-3.396391	1.087996	2.487419
O	-3.749620	-0.418019	-0.404598
C	4.270319	-0.370521	1.658896
C	0.049651	0.937876	-2.093595
C	3.158496	-1.186919	2.320620
C	-4.255489	0.469088	3.589295
C	-4.229196	1.982562	1.566004
C	5.623812	-1.060377	1.840257
C	-1.374601	1.460742	-2.293362
C	0.294884	-0.300359	-2.953332
H	5.242498	1.491677	0.029307
H	4.718556	0.873742	-1.455860
H	5.919037	0.062513	-0.595573
H	3.875104	-1.127891	-0.344786
H	1.644678	-1.000247	-0.543477
H	0.415672	1.688589	-0.109024
H	-1.433802	1.652975	0.989727
H	-2.187954	-0.718248	2.386207
H	-4.818802	-2.205049	0.620767
H	-2.617381	1.698578	2.963002
H	4.311963	0.624618	2.124408
H	0.765766	1.713408	-2.395595
H	3.383961	-1.328559	3.381334
H	3.081702	-2.177648	1.857618
H	2.179496	-0.701997	2.247540
H	-3.656677	-0.157718	4.258064
H	-5.058682	-0.145238	3.170106
H	-4.715341	1.262525	4.185846
H	-5.106458	1.446677	1.183177
H	-3.649631	2.341083	0.707543
H	-4.587824	2.859321	2.113028
H	6.459653	-0.453194	1.479121
H	5.638439	-2.019885	1.307889
H	5.795527	-1.259652	2.902241
H	-1.508029	1.814751	-3.320161
H	-1.620058	2.280553	-1.607069
H	-2.092861	0.648969	-2.118245
H	1.318304	-0.671048	-2.843696
H	0.145285	-0.045409	-4.007842
H	-0.407052	-1.101665	-2.702956
O	3.496075	1.065493	-2.789245
H	3.172291	1.996786	-2.766923
H	3.787992	0.892477	-3.696049
O	2.767280	3.565281	-2.039477
H	2.872061	3.188764	-1.145164
H	1.852450	3.924016	-2.019173
O	5.655829	2.966968	0.988130
H	6.381450	2.879976	1.623449
H	4.900160	3.341008	1.486405
O	3.178727	3.673404	2.150778

H	3.112610	3.455335	3.093276
H	2.889469	2.876212	1.656999
O	2.124992	-2.843795	-0.538085
H	1.565478	-3.091275	0.246200
H	1.600571	-3.187944	-1.289724
O	7.406009	-0.815088	-0.892143
H	7.745019	-0.667465	-1.787278
H	7.299290	-1.794301	-0.800737
O	7.061385	-3.493692	-0.625336
H	6.124254	-3.725372	-0.426981
H	7.584336	-3.854120	0.105590
O	4.476914	-4.177502	-0.051337
H	3.647956	-3.698168	-0.284328
H	4.340829	-4.531184	0.839578
O	-0.239774	-3.584091	-1.674118
H	-0.788210	-3.446851	-2.463080
H	-0.502589	-2.853143	-1.082445
O	-2.671663	-2.266137	-2.285933
H	-2.439612	-1.706715	-1.521447
H	-3.537208	-1.908647	-2.582268
O	-1.196877	3.453678	0.704795
H	-0.522874	3.982142	1.180790
H	-2.003004	4.023111	0.653100
O	0.967287	5.150318	1.323827
H	0.852674	5.990134	1.792588
H	1.793718	4.746962	1.672904
O	0.322318	4.650446	-1.384698
H	0.679837	5.080065	-0.581570
H	-0.331526	4.035035	-1.002230
O	-5.567568	-2.901893	-0.448188
H	-5.568499	-2.302434	-1.229087
H	-4.975402	-3.651159	-0.686823
O	-3.426566	-4.545902	-0.993179
H	-3.043221	-3.821149	-1.545549
H	-3.440082	-5.340509	-1.548129
O	-1.754467	-4.912449	1.273078
H	-2.274828	-4.500010	1.995326
H	-2.281638	-4.785247	0.457675
O	0.403182	-3.260517	1.500302
H	-0.087360	-2.437895	1.325516
H	-0.280353	-3.960877	1.356209
O	-3.036307	-3.441808	3.269827
H	-3.636053	-3.864783	3.901483
H	-3.582321	-2.822750	2.751291
O	-5.277211	-1.275150	-2.713652
H	-5.803660	-1.414475	-3.515539
H	-5.265567	-0.307571	-2.549020
O	-3.390483	5.071592	0.401514
H	-3.701013	5.439826	1.241574
H	-4.173147	4.625747	0.000419
O	-5.575132	3.817042	-0.714658
H	-6.039398	4.383323	-1.348582
H	-5.371379	2.987277	-1.196973
O	-4.789021	1.458319	-2.038088
H	-4.218232	1.797928	-2.746080
H	-4.190528	1.046767	-1.380912

Table S44. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $22H_2O$_β-PPII_C.

N	5.116707	0.629861	-0.160948
C	3.963746	-0.251842	0.163539
C	2.715150	0.605533	-0.002850
N	1.585332	-0.037633	-0.272947
C	0.343662	0.670001	-0.545546
C	-0.783407	-0.075593	0.157612
N	-1.605370	0.663049	0.897425
C	-2.677276	0.064200	1.669981
C	-3.592781	-0.733145	0.756137
O	-4.253039	-1.690731	1.362347
O	2.792246	1.837534	0.159971
O	-0.913422	-1.313958	0.054009
C	-3.471269	1.173741	2.399218
O	-3.733318	-0.481825	-0.433208
C	4.049562	-0.857365	1.578313
C	0.103259	0.842551	-2.067308
C	5.403678	-1.534875	1.798674
C	-4.335972	0.602605	3.522324
C	-4.303192	2.006175	1.420543
C	3.754965	0.160042	2.683606
C	-1.321804	1.334335	-2.331163
C	0.391007	-0.424184	-2.871979
H	5.192573	1.454510	0.470579
H	4.957071	0.984686	-1.121345
H	6.021715	0.107452	-0.170695
H	3.962759	-1.057897	-0.576585
H	1.639483	-1.049026	-0.444656
H	0.433296	1.664763	-0.099721
H	-1.487129	1.684727	0.909305
H	-2.249490	-0.627708	2.406397
H	-4.844855	-2.201581	0.664671
H	-2.706738	1.819352	2.851359
H	3.269817	-1.629619	1.600889
H	0.816548	1.617441	-2.378925
H	5.370124	-2.135722	2.712129
H	6.206421	-0.798027	1.916207
H	5.666746	-2.194887	0.964977
H	-3.736856	0.020322	4.229998
H	-5.125953	-0.043834	3.127141
H	-4.813160	1.420196	4.070771
H	-5.168070	1.438370	1.055599
H	-3.716798	2.325465	0.551444
H	-4.680780	2.906499	1.914003
H	2.725717	0.531475	2.631478
H	4.436408	1.017942	2.632081
H	3.887505	-0.311623	3.661673
H	-1.424619	1.653051	-3.372951
H	-1.605134	2.170575	-1.680812
H	-2.033101	0.516513	-2.155299
H	1.427553	-0.753966	-2.751125

H	0.227526	-0.224006	-3.936007
H	-0.279495	-1.239161	-2.580780
O	3.760796	0.969468	-2.598555
H	3.357273	1.860908	-2.705068
H	4.053354	0.687378	-3.477080
O	2.806777	3.470023	-2.114829
H	2.889703	3.127930	-1.204860
H	1.885864	3.810930	-2.138664
O	5.494284	3.033023	1.317806
H	6.183201	3.086372	1.995947
H	4.685279	3.417041	1.714278
O	2.880582	3.693623	2.121884
H	2.684364	3.459649	3.042439
H	2.670543	2.902643	1.580552
O	2.176548	-2.876097	-0.433378
H	1.667838	-3.100851	0.389591
H	1.598874	-3.234928	-1.139222
O	7.530318	-0.766354	-0.474749
H	8.064072	-0.312181	-1.143306
H	7.290347	-1.640339	-0.869064
O	6.700597	-3.125709	-1.547503
H	5.923595	-3.539913	-1.101154
H	7.371256	-3.820427	-1.616239
O	4.541295	-4.255457	-0.322612
H	3.689737	-3.759428	-0.366682
H	4.666200	-4.490762	0.608331
O	-0.216047	-3.674055	-1.447738
H	-0.755748	-3.554235	-2.245904
H	-0.490159	-2.932470	-0.874732
O	-2.606391	-2.401569	-2.193815
H	-2.409914	-1.787592	-1.461922
H	-3.471034	-2.084560	-2.535525
O	-1.289285	3.471939	0.512844
H	-0.653384	4.057218	0.974951
H	-2.106924	4.011194	0.382100
O	0.812419	5.238679	1.103560
H	0.700928	6.100627	1.530911
H	1.597120	4.816918	1.520650
O	0.315607	4.535740	-1.590054
H	0.629721	5.031552	-0.807463
H	-0.346973	3.940286	-1.191360
O	-5.552584	-2.970223	-0.383173
H	-5.535540	-2.419673	-1.199188
H	-4.939399	-3.720870	-0.553970
O	-3.353145	-4.590527	-0.732777
H	-2.971409	-3.906661	-1.335020
H	-3.328308	-5.429763	-1.217204
O	-1.686710	-4.764354	1.569048
H	-2.203992	-4.285121	2.251163
H	-2.208724	-4.698457	0.743222
O	0.517928	-3.159679	1.681775
H	0.028548	-2.346632	1.463975
H	-0.175572	-3.859226	1.595060
O	-2.987482	-3.138030	3.431906
H	-3.515410	-3.525283	4.145348
H	-3.609160	-2.631851	2.877414
O	-5.213146	-1.480298	-2.732148

H	-5.723875	-1.666651	-3.534642
H	-5.209288	-0.504829	-2.620685
O	-3.501868	5.016581	0.009666
H	-3.816932	5.467723	0.806541
H	-4.283101	4.532951	-0.348348
O	-5.678684	3.652159	-0.983077
H	-6.171143	4.170436	-1.636482
H	-5.439254	2.813204	-1.432166
O	-4.767986	1.280611	-2.188353
H	-4.187835	1.608330	-2.894243
H	-4.176772	0.919013	-1.496142

Table S45. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $22H_2O$_β-PPII_D.

N	5.277432	0.123538	-0.106361
C	4.047822	-0.683205	0.105640
C	2.861263	0.259774	-0.063769
N	1.735853	-0.265644	-0.533803
C	0.517151	0.509960	-0.718819
C	-0.553833	-0.048686	0.214176
N	-1.267132	0.837195	0.905981
C	-2.324333	0.401954	1.797310
C	-3.339941	-0.435466	1.034888
O	-3.966671	-1.321113	1.764978
O	2.985255	1.453552	0.270379
O	-0.760888	-1.273711	0.298214
C	-3.004305	1.634888	2.438382
O	-3.592659	-0.253132	-0.153351
C	4.066576	-1.355183	1.495633
C	0.064633	0.452041	-2.194002
C	3.922951	-0.358170	2.647468
C	-3.869960	1.242988	3.635234
C	-3.805589	2.444939	1.416289
C	2.993534	-2.439014	1.575116
C	1.084489	1.174109	-3.072023
C	-1.332956	1.048614	-2.362990
H	5.330073	0.952212	0.522234
H	5.273884	0.479126	-1.084911
H	6.119105	-0.475349	0.042718
H	4.035974	-1.458301	-0.669236
H	1.713256	-1.253870	-0.825451
H	0.736168	1.547531	-0.446565
H	-1.092271	1.842565	0.769497
H	-1.898807	-0.230010	2.585648
H	-4.726930	-1.780010	1.201780
H	-2.173297	2.252540	2.804225
H	5.048927	-1.839176	1.569438
H	0.025950	-0.607779	-2.481218
H	4.077954	-0.875668	3.598551

H	2.914631	0.073027	2.665017
H	4.647271	0.461524	2.590500
H	-3.297792	0.670660	4.372365
H	-4.729115	0.639759	3.324651
H	-4.251526	2.144629	4.123495
H	-4.734268	1.927475	1.144847
H	-3.236549	2.630002	0.497838
H	-4.079729	3.417092	1.836210
H	3.078861	-3.154943	0.750231
H	1.988788	-2.002965	1.545993
H	3.086115	-2.991612	2.514745
H	0.815540	1.067879	-4.127848
H	2.095589	0.778821	-2.935483
H	1.102912	2.245420	-2.834827
H	-2.083852	0.455377	-1.831982
H	-1.602167	1.073471	-3.423675
H	-1.371315	2.075240	-1.973931
O	4.552215	0.951967	-2.662699
H	4.225584	1.877272	-2.551967
H	5.162868	0.959810	-3.414346
O	3.660785	3.324548	-1.705436
H	3.502639	2.829456	-0.879460
H	2.795527	3.758256	-1.873708
O	5.710359	2.526716	1.357297
H	6.436778	2.554737	1.996766
H	4.930243	2.910352	1.808692
O	3.168048	3.237928	2.292867
H	2.968334	3.026242	3.217919
H	2.882788	2.467144	1.758923
O	1.537608	-3.021402	-1.401213
H	1.137169	-3.464164	-0.607595
H	0.797703	-3.002407	-2.040591
O	7.297582	-1.748061	0.387633
H	8.090527	-1.738346	-0.167966
H	6.864161	-2.623325	0.241056
O	5.884342	-4.030211	-0.002216
H	5.194552	-3.941149	-0.701005
H	5.461919	-4.454179	0.758546
O	4.088182	-3.718467	-2.031739
H	3.137544	-3.505657	-1.879829
H	4.387912	-3.145446	-2.752287
O	-1.111446	-2.851885	-2.043463
H	-1.948971	-2.624442	-2.484847
H	-1.103694	-2.324784	-1.219665
O	-3.811681	-2.087611	-2.257800
H	-3.692768	-1.500603	-1.482572
H	-4.694986	-1.830117	-2.585835
O	-0.704576	3.547919	0.228634
H	-0.096603	4.056670	0.805368
H	-1.478780	4.140797	0.069914
O	1.414848	5.093309	1.214651
H	1.323261	5.908364	1.729627
H	2.092261	4.544971	1.670788
O	1.219741	4.625586	-1.567030
H	1.457115	5.057496	-0.722392
H	0.467103	4.064714	-1.296426
O	-5.789184	-2.414759	0.409880

H	-6.026898	-1.825847	-0.343725
H	-5.407484	-3.229275	0.009703
O	-4.294526	-4.369594	-0.840214
H	-4.034606	-3.693004	-1.509335
H	-4.666400	-5.120852	-1.326637
O	-2.219987	-5.032012	0.963118
H	-2.465337	-4.536038	1.773088
H	-2.902108	-4.813617	0.296558
O	0.246483	-3.851158	0.825499
H	-0.072218	-2.939404	0.957693
H	-0.583953	-4.375343	0.733855
O	-2.625345	-3.407466	3.197561
H	-3.127524	-3.747696	3.952494
H	-3.117594	-2.629178	2.879271
O	-6.270665	-0.850353	-1.851335
H	-7.166691	-0.840937	-2.220144
H	-5.957664	0.080872	-1.843829
O	-2.775943	5.279642	-0.272964
H	-2.916327	5.859619	0.489715
H	-3.657019	4.883455	-0.471725
O	-5.222440	4.162673	-0.832784
H	-5.707315	4.661350	-1.506808
H	-5.143463	3.248695	-1.180991
O	-4.839151	1.554894	-1.788652
H	-4.411576	1.639186	-2.656229
H	-4.179777	1.126408	-1.205365

Table S46. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $22H_2O$_β-PPII_E.

N	5.101541	0.377412	-0.089916
C	3.893184	-0.368142	0.355034
C	2.682094	0.493223	0.022910
N	1.661992	-0.101462	-0.583110
C	0.391220	0.569316	-0.822284
C	-0.639289	-0.029911	0.132359
N	-1.380871	0.824606	0.831787
C	-2.391630	0.341310	1.752346
C	-3.361352	-0.573442	1.019973
O	-3.912452	-1.492447	1.769620
O	2.685157	1.691310	0.364208
O	-0.780556	-1.263628	0.237232
C	-3.137686	1.539395	2.384295
O	-3.645700	-0.426268	-0.165780
C	3.942287	-0.626656	1.872295
C	-0.041268	0.417318	-2.293633
C	2.676383	-1.356698	2.323309
C	-3.965429	1.110503	3.595286
C	-3.996769	2.284402	1.359946
C	5.193356	-1.420315	2.251553

C	0.924973	1.185742	-3.192815
C	-1.479886	0.899144	-2.482930
H	5.266192	1.211362	0.514153
H	4.974293	0.705857	-1.073389
H	5.947061	-0.236887	-0.071729
H	3.862663	-1.315463	-0.195564
H	1.740371	-1.095907	-0.841131
H	0.526136	1.631406	-0.592979
H	-1.256762	1.837275	0.689333
H	-1.911541	-0.247414	2.543093
H	-4.625633	-2.025831	1.210542
H	-2.342372	2.211694	2.732798
H	3.983523	0.356372	2.362413
H	0.004154	-0.652079	-2.542418
H	2.730697	-1.565477	3.395541
H	2.567779	-2.313866	1.799762
H	1.769331	-0.767149	2.147141
H	-3.352760	0.579605	4.330981
H	-4.791723	0.455365	3.300827
H	-4.393319	1.993284	4.079553
H	-4.891901	1.705463	1.100623
H	-3.446274	2.494734	0.435808
H	-4.329501	3.241913	1.771216
H	6.118135	-0.873905	2.044213
H	5.228345	-2.370490	1.704719
H	5.174693	-1.645698	3.321767
H	0.666763	1.029908	-4.245120
H	1.961350	0.869382	-3.043013
H	0.864331	2.262197	-2.986126
H	-2.183729	0.267855	-1.931683
H	-1.750074	0.867386	-3.543110
H	-1.596172	1.932659	-2.128702
O	4.334815	1.203349	-2.640017
H	3.972645	2.113156	-2.503175
H	5.022440	1.277169	-3.318283
O	3.349462	3.516626	-1.663007
H	3.173416	3.041843	-0.828614
H	2.484052	3.934384	-1.869062
O	5.574323	2.651884	1.547265
H	6.195171	2.524103	2.279349
H	4.769517	3.051922	1.937684
O	3.003399	3.462796	2.359127
H	2.790678	3.282604	3.287850
H	2.720622	2.675521	1.847687
O	1.853001	-2.913867	-1.247803
H	1.486800	-3.307638	-0.413926
H	1.109690	-3.007914	-1.878478
O	7.294266	-1.362662	-0.186655
H	7.841140	-1.207664	-0.970797
H	6.976586	-2.296118	-0.259049
O	6.348903	-3.902567	-0.438954
H	5.542177	-3.934747	-1.007497
H	6.139256	-4.398222	0.365220
O	4.237599	-3.903844	-2.155966
H	3.359886	-3.594171	-1.830432
H	4.081559	-4.764531	-2.570661
O	-0.782028	-3.020850	-1.968864

H	-1.608046	-2.867572	-2.460579
H	-0.855863	-2.445852	-1.180252
O	-3.503742	-2.358005	-2.204397
H	-3.437923	-1.733407	-1.453591
H	-4.399889	-2.175053	-2.549114
O	-0.951920	3.551224	0.170401
H	-0.364021	4.067926	0.760502
H	-1.755560	4.108541	0.029822
O	1.114143	5.156661	1.198843
H	0.959190	5.968004	1.704620
H	1.829063	4.669489	1.666605
O	0.895780	4.771017	-1.601376
H	1.119962	5.183800	-0.743680
H	0.171180	4.167644	-1.346336
O	-5.597715	-2.770651	0.397777
H	-5.834438	-2.224406	-0.387466
H	-5.120453	-3.557546	0.048187
O	-3.840522	-4.604362	-0.687656
H	-3.616898	-3.934740	-1.376844
H	-4.104042	-5.411935	-1.154276
O	-1.767329	-4.988067	1.202509
H	-2.082672	-4.489240	1.986173
H	-2.446642	-4.859580	0.509966
O	0.584681	-3.596595	1.044523
H	0.179261	-2.710097	1.074470
H	-0.193007	-4.201067	0.981613
O	-2.413721	-3.335253	3.357163
H	-2.894098	-3.700466	4.114566
H	-2.988441	-2.641707	2.985478
O	-6.078082	-1.319642	-1.945305
H	-6.937955	-1.414880	-2.381955
H	-5.869315	-0.359766	-1.940958
O	-3.126116	5.154086	-0.319100
H	-3.329745	5.706369	0.449792
H	-3.967916	4.693941	-0.547183
O	-5.470612	3.865087	-0.957373
H	-5.966940	4.327806	-1.648484
H	-5.343346	2.949592	-1.286747
O	-4.950264	1.258446	-1.867324
H	-4.503925	1.373340	-2.721889
H	-4.275128	0.892368	-1.259707

Table S47. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $22H_2O$_β-PPII_F.

N	5.094687	0.484195	0.327715
C	3.927630	-0.421455	0.163451
C	2.709465	0.465804	-0.048783
N	1.659454	-0.112309	-0.621216
C	0.390864	0.567857	-0.830148

C	-0.637983	-0.030636	0.126559
N	-1.438856	0.821786	0.759841
C	-2.445515	0.340822	1.685600
C	-3.348920	-0.668728	0.994833
O	-3.862935	-1.566072	1.794586
O	2.721936	1.639809	0.364542
O	-0.727438	-1.263145	0.291086
C	-3.269065	1.533363	2.225653
O	-3.616467	-0.610768	-0.202741
C	3.711003	-1.352089	1.373547
C	-0.046330	0.431811	-2.303364
C	4.978438	-2.144428	1.694395
C	-4.078803	1.142711	3.461395
C	-4.163805	2.146957	1.146133
C	3.183848	-0.613658	2.606595
C	0.931655	1.199117	-3.192759
C	-1.480480	0.923769	-2.498564
H	4.995444	1.139023	1.130746
H	5.150989	1.051426	-0.539010
H	5.987900	-0.049981	0.401234
H	4.121581	-1.015929	-0.735778
H	1.753510	-1.081648	-0.954218
H	0.534610	1.627909	-0.592249
H	-1.371106	1.830583	0.560678
H	-1.953821	-0.170942	2.521452
H	-4.528599	-2.185923	1.265737
H	-2.519754	2.277442	2.527394
H	2.943293	-2.065927	1.053574
H	-0.005973	-0.637026	-2.558016
H	4.748798	-2.917130	2.433841
H	5.762370	-1.505352	2.116278
H	5.381211	-2.635086	0.801549
H	-3.438670	0.715993	4.240281
H	-4.853292	0.409410	3.214233
H	-4.573530	2.027928	3.871998
H	-5.026260	1.501547	0.937398
H	-3.623079	2.309116	0.206544
H	-4.548010	3.115852	1.478179
H	2.193085	-0.179483	2.428814
H	3.860143	0.191473	2.918027
H	3.091225	-1.315045	3.441106
H	0.686178	1.044125	-4.248010
H	1.966645	0.882216	-3.028641
H	0.869690	2.275200	-2.985162
H	-2.191415	0.301473	-1.945594
H	-1.746753	0.889579	-3.559542
H	-1.589632	1.959251	-2.149992
O	4.437876	1.378737	-2.234955
H	4.025315	2.273433	-2.227558
H	5.046563	1.358377	-2.987636
O	3.268275	3.692938	-1.458205
H	3.082230	3.151138	-0.668496
H	2.400353	4.105768	-1.662856
O	4.975852	2.503162	2.340895
H	5.447405	2.427274	3.182972
H	4.073305	2.815530	2.557633
O	2.222937	3.138183	2.547659

H	1.781410	2.766139	3.326879
H	2.139273	2.469320	1.835195
O	2.013105	-2.897549	-1.368474
H	1.747652	-3.265558	-0.488451
H	1.220591	-3.048958	-1.924091
O	7.521366	-0.942346	0.200345
H	8.182377	-0.430492	-0.288455
H	7.357264	-1.754436	-0.337074
O	6.905031	-3.129138	-1.315717
H	6.009080	-3.008297	-1.707483
H	6.901382	-3.992921	-0.879047
O	4.492941	-2.519748	-2.444969
H	3.611349	-2.799123	-2.108152
H	4.468491	-2.642324	-3.405127
O	-0.644806	-3.073429	-1.884699
H	-1.486974	-2.992986	-2.366264
H	-0.741763	-2.483467	-1.109869
O	-3.393662	-2.630573	-2.131139
H	-3.363871	-1.942025	-1.435806
H	-4.312116	-2.562259	-2.458540
O	-1.214208	3.550949	0.025745
H	-0.766401	4.107478	0.697103
H	-2.049708	4.019314	-0.215107
O	0.652058	5.117272	1.387016
H	0.493357	5.883580	1.957537
H	1.252830	4.516140	1.882547
O	0.787919	4.895672	-1.443994
H	0.915393	5.255486	-0.544133
H	0.054625	4.265397	-1.303649
O	-5.421095	-3.072706	0.513604
H	-5.716660	-2.609473	-0.304352
H	-4.858407	-3.823793	0.216250
O	-3.444643	-4.763213	-0.413820
H	-3.303703	-4.138014	-1.163232
H	-3.605812	-5.635909	-0.803772
O	-1.325030	-4.813433	1.478979
H	-1.660335	-4.258424	2.215220
H	-2.013455	-4.782307	0.784354
O	0.968268	-3.364435	1.084929
H	0.504004	-2.507002	1.029557
H	0.224383	-4.010679	1.144264
O	-2.098019	-3.028028	3.485177
H	-2.453705	-3.388981	4.310359
H	-2.814068	-2.495063	3.094347
O	-6.051753	-1.822639	-1.901533
H	-6.905837	-2.015880	-2.316685
H	-5.925414	-0.849867	-1.955219
O	-3.465840	4.911288	-0.764195
H	-3.709934	5.586052	-0.114002
H	-4.285997	4.388510	-0.926032
O	-5.759335	3.459703	-1.228464
H	-6.293039	3.846198	-1.938322
H	-5.594034	2.530142	-1.495227
O	-5.120617	0.826312	-1.977258
H	-4.690245	0.917912	-2.842762
H	-4.416668	0.547550	-1.356499

Table S48. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $22H_2O$_β-PPII_J.

N	5.258705	0.176310	-0.160710
C	4.070803	-0.516436	0.407746
C	2.877990	0.389422	0.125744
N	1.711629	-0.195805	-0.113699
C	0.535611	0.575893	-0.485104
C	-0.663362	0.021412	0.275610
N	-1.464035	0.935819	0.821657
C	-2.679658	0.572955	1.523080
C	-3.508022	-0.365782	0.663447
O	-4.178539	-1.267133	1.332106
O	3.042013	1.624630	0.149803
O	-0.879518	-1.200482	0.377416
C	-3.481306	1.857953	1.833770
O	-3.585435	-0.248388	-0.556206
C	4.273889	-0.802609	1.910024
C	0.333608	0.599983	-2.023505
C	4.248580	0.463030	2.770222
C	-2.738356	2.701443	2.871642
C	-4.902120	1.554987	2.310044
C	3.244749	-1.817701	2.406116
C	-1.016222	1.218961	-2.391711
C	0.478258	-0.774209	-2.673090
H	5.385776	1.136806	0.221451
H	5.113127	0.270328	-1.182850
H	6.117003	-0.390376	0.016666
H	3.959813	-1.461507	-0.134978
H	1.679303	-1.221166	-0.200615
H	0.707310	1.604443	-0.154229
H	-1.264612	1.930860	0.655097
H	-2.437432	0.049834	2.457287
H	-4.815944	-1.795908	0.683389
H	-3.545795	2.418810	0.890018
H	5.269170	-1.260325	1.982410
H	1.139881	1.244355	-2.397358
H	4.543504	0.213996	3.793607
H	3.236867	0.884707	2.810031
H	4.931101	1.237922	2.404625
H	-1.712723	2.932347	2.568899
H	-2.704266	2.173586	3.831986
H	-3.262228	3.650311	3.017948
H	-4.891195	0.910985	3.197113
H	-5.504533	1.061627	1.540145
H	-5.401246	2.491353	2.578036
H	3.305986	-2.756381	1.847015
H	2.223635	-1.429179	2.316571
H	3.422409	-2.040106	3.462455
H	-1.055871	1.421551	-3.466227
H	-1.212772	2.152296	-1.853628
H	-1.825233	0.519125	-2.148992
H	1.458425	-1.219023	-2.476146

H	0.368487	-0.677431	-3.758314
H	-0.300873	-1.456937	-2.320148
O	3.876276	0.282795	-2.581562
H	3.572400	1.202457	-2.759319
H	4.030312	-0.133893	-3.441495
O	3.195940	2.911607	-2.332670
H	3.236896	2.674222	-1.386729
H	2.318421	3.345824	-2.416954
O	5.834519	2.873938	0.569416
H	6.645200	3.073301	1.059815
H	5.117015	3.374811	1.008673
O	3.417054	3.813054	1.671166
H	3.380980	3.790790	2.640039
H	3.118929	2.932815	1.357589
O	1.822636	-3.087164	-0.274500
H	1.369266	-3.276629	0.588252
H	1.129432	-3.338941	-0.921905
O	7.260084	-1.711144	0.283261
H	8.193784	-1.487897	0.156772
H	7.006121	-2.299018	-0.469627
O	6.205509	-3.157420	-1.753543
H	5.422001	-3.638197	-1.393236
H	5.869786	-2.576896	-2.452166
O	4.109246	-4.526987	-0.676521
H	3.271465	-4.033426	-0.510013
H	4.339106	-4.961904	0.157212
O	-0.720120	-3.638892	-1.107127
H	-1.241984	-3.465143	-1.908514
H	-0.883203	-2.853820	-0.547983
O	-2.974468	-2.415819	-2.258554
H	-2.963741	-1.697760	-1.595328
H	-3.780220	-2.204201	-2.771957
O	-0.939909	3.646501	0.083305
H	-0.274644	4.210115	0.529761
H	-1.799006	4.130567	0.134012
O	1.311967	5.255829	0.581606
H	1.264578	6.172637	0.890245
H	2.096477	4.853412	1.018238
O	0.832725	4.317169	-2.032632
H	1.171215	4.852075	-1.286430
H	0.062737	3.878179	-1.623656
O	-5.684292	-2.540312	-0.233357
H	-5.692794	-2.067051	-1.098135
H	-5.199495	-3.382928	-0.388315
O	-3.789287	-4.481181	-0.618985
H	-3.378521	-3.886819	-1.288778
H	-3.914526	-5.340140	-1.050134
O	-2.085030	-4.708940	1.667548
H	-2.602062	-4.179883	2.311875
H	-2.553589	-4.620809	0.813159
O	0.239638	-3.297123	1.919020
H	-0.145165	-2.418349	1.749083
H	-0.521712	-3.910184	1.769239
O	-3.286031	-2.942497	3.458465
H	-3.999664	-3.237365	4.042754
H	-3.679913	-2.270770	2.872525
O	-5.500817	-1.281160	-2.716581

H	-6.204798	-1.428272	-3.366277
H	-5.357839	-0.309922	-2.673705
O	-3.376695	4.901669	0.275850
H	-3.397943	5.778326	-0.135287
H	-4.156240	4.417286	-0.083592
O	-5.545195	3.522624	-0.696590
H	-6.179251	3.202825	-0.038551
H	-5.349010	2.762345	-1.284695
O	-4.722616	1.408923	-2.342592
H	-4.269738	1.793610	-3.109595
H	-4.026139	1.054844	-1.753373

Table S49. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $22H_2O$_β-PPII_K.

N	5.130534	0.406139	-0.180139
C	3.973630	-0.298791	0.439203
C	2.744008	0.520449	0.064946
N	1.651407	-0.133789	-0.305528
C	0.441359	0.566868	-0.709848
C	-0.732864	-0.034105	0.055067
N	-1.479659	0.829711	0.735790
C	-2.635450	0.410776	1.507239
C	-3.558152	-0.419326	0.630863
O	-4.185842	-1.382182	1.264548
O	2.817620	1.762585	0.140774
O	-0.969517	-1.261326	0.050584
C	-3.375122	1.661734	2.030225
O	-3.729330	-0.185059	-0.556627
C	4.130842	-0.375742	1.968559
C	0.246391	0.556979	-2.244940
C	2.973951	-1.170545	2.576482
C	-2.501575	2.406832	3.041538
C	-4.726814	1.308903	2.651961
C	5.473763	-1.002312	2.348559
C	-1.136318	1.107394	-2.600822
C	0.471074	-0.811723	-2.883803
H	5.291375	1.327018	0.281813
H	4.915512	0.567357	-1.184084
H	6.007689	-0.159503	-0.130958
H	3.921925	-1.304981	0.007410
H	1.688876	-1.160290	-0.366326
H	0.557802	1.607775	-0.394251
H	-1.301064	1.836853	0.618537
H	-2.314261	-0.212650	2.352076
H	-4.823204	-1.879288	0.603891
H	-3.550664	2.308176	1.158294
H	4.100494	0.654480	2.351251
H	1.013598	1.242871	-2.626931
H	3.077837	-1.202845	3.664656

H	2.981631	-2.202745	2.207220
H	1.996661	-0.733910	2.346931
H	-1.524780	2.682151	2.632893
H	-2.340081	1.785922	3.930624
H	-3.002331	3.327924	3.354056
H	-4.605237	0.594506	3.474829
H	-5.420931	0.873730	1.926227
H	-5.188346	2.215277	3.055102
H	6.326361	-0.381807	2.057458
H	5.592673	-1.984071	1.874027
H	5.520069	-1.140626	3.432653
H	-1.205871	1.297594	-3.675885
H	-1.357579	2.039959	-2.068031
H	-1.912381	0.375681	-2.340381
H	1.473448	-1.196648	-2.671423
H	0.372736	-0.725345	-3.971043
H	-0.272132	-1.536945	-2.540091
O	3.804846	0.542869	-2.643269
H	3.445089	1.449367	-2.784785
H	4.191764	0.262926	-3.485629
O	2.934275	3.095468	-2.316777
H	2.952599	2.848550	-1.372429
H	2.053167	3.517474	-2.421562
O	5.650032	2.864735	1.154516
H	6.298040	2.817254	1.872411
H	4.857710	3.302448	1.528576
O	3.083382	3.743407	1.935108
H	2.882553	3.626122	2.876474
H	2.824054	2.910007	1.486609
O	1.985819	-3.004328	-0.169860
H	1.439756	-3.138846	0.648707
H	1.410780	-3.388694	-0.864658
O	7.413235	-1.216683	-0.320796
H	8.133488	-0.804713	-0.820285
H	7.024000	-1.905077	-0.913942
O	6.036929	-2.998193	-1.835479
H	5.433764	-3.489524	-1.227104
H	5.461629	-2.522817	-2.452936
O	4.370964	-4.337470	-0.141676
H	3.493698	-3.889903	-0.090586
H	4.685703	-4.429779	0.769084
O	-0.404825	-3.811630	-1.197569
H	-0.891267	-3.725871	-2.033186
H	-0.651674	-3.006497	-0.703759
O	-2.677351	-2.390029	-2.107585
H	-2.412015	-1.762975	-1.409749
H	-3.497671	-1.999098	-2.481240
O	-1.103880	3.561469	0.082437
H	-0.451025	4.123194	0.550692
H	-1.980110	4.005507	0.186620
O	1.078552	5.219282	0.687017
H	0.961464	6.109695	1.050003
H	1.833808	4.818162	1.173113
O	0.564168	4.470456	-2.003380
H	0.915283	4.956550	-1.230913
H	-0.179548	3.978839	-1.604631
O	-5.649005	-2.627214	-0.386950

H	-5.589179	-2.131462	-1.235031
H	-5.131157	-3.452819	-0.519282
O	-3.624997	-4.477350	-0.624371
H	-3.179188	-3.836989	-1.230565
H	-3.650851	-5.327414	-1.089190
O	-2.033815	-4.676697	1.725205
H	-2.551855	-4.155759	2.375360
H	-2.524218	-4.611318	0.880079
O	0.202980	-3.117801	1.868446
H	-0.240815	-2.294148	1.599354
H	-0.508823	-3.797052	1.769169
O	-3.274917	-2.898386	3.479232
H	-3.960736	-3.187651	4.098505
H	-3.714478	-2.296209	2.851055
O	-5.170383	-1.289916	-2.805261
H	-5.646573	-1.494001	-3.624428
H	-5.114111	-0.310984	-2.747531
O	-3.566595	4.713913	0.442947
H	-3.636301	5.617603	0.101720
H	-4.340082	4.225130	0.074960
O	-5.698663	3.301685	-0.550229
H	-6.218795	2.819361	0.108910
H	-5.444566	2.646299	-1.234312
O	-4.662309	1.475417	-2.404952
H	-4.215066	1.946137	-3.125526
H	-3.967380	1.168409	-1.789181

Table S50. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the β-PPII conformation, $22H_2O$_β-PPII_S.

N	5.221384	0.111816	-0.234510
C	4.036505	-0.581977	0.338183
C	2.851102	0.352221	0.125219
N	1.670352	-0.209609	-0.094984
C	0.487568	0.583908	-0.393386
C	-0.685057	-0.029194	0.363542
N	-1.510090	0.826889	0.969494
C	-2.643074	0.337309	1.727282
C	-3.566354	-0.467724	0.828825
O	-4.378046	-1.259999	1.479569
O	3.032322	1.583831	0.188223
O	-0.850364	-1.260476	0.422556
C	-3.443136	1.492280	2.369353
O	-3.592630	-0.340420	-0.391973
C	4.272049	-0.932290	1.822015
C	0.250051	0.685915	-1.924189
C	4.290199	0.297665	2.732483
C	-4.152951	2.341914	1.311981
C	-2.541972	2.342685	3.267269
C	3.237909	-1.950214	2.302190

C	-1.125850	1.280710	-2.230670
C	0.416992	-0.650231	-2.645509
H	5.377319	1.054269	0.180266
H	5.050352	0.246123	-1.248581
H	6.072150	-0.478097	-0.102691
H	3.894897	-1.503087	-0.237718
H	1.619567	-1.230209	-0.220818
H	0.662825	1.592178	-0.008093
H	-1.340276	1.834821	0.871643
H	-2.284251	-0.334155	2.517517
H	-5.023321	-1.748109	0.803740
H	-4.199074	1.008976	2.999009
H	5.260495	-1.409146	1.850485
H	1.029706	1.370560	-2.283768
H	4.605421	0.003017	3.737541
H	3.287352	0.734161	2.814351
H	4.977597	1.074794	2.380916
H	-4.953765	1.788240	0.809031
H	-3.449963	2.694977	0.547430
H	-4.603818	3.225505	1.773983
H	-1.831441	2.934163	2.679570
H	-1.977853	1.720295	3.969671
H	-3.154788	3.041528	3.844320
H	3.260969	-2.860972	1.695971
H	2.223204	-1.537034	2.265154
H	3.444250	-2.227705	3.340094
H	-1.193453	1.539743	-3.291890
H	-1.342918	2.176415	-1.638142
H	-1.900746	0.536411	-2.009738
H	1.426472	-1.053475	-2.523148
H	0.240600	-0.510512	-3.717189
H	-0.308078	-1.385335	-2.281072
O	3.780380	0.320346	-2.612641
H	3.507359	1.258883	-2.738317
H	3.936423	-0.046692	-3.494684
O	3.214917	2.957487	-2.248313
H	3.286274	2.692834	-1.311634
H	2.329797	3.382718	-2.290737
O	5.866990	2.767763	0.580349
H	6.700510	2.933224	1.044397
H	5.176745	3.261252	1.069041
O	3.505635	3.689547	1.795468
H	3.487846	3.628688	2.763137
H	3.182913	2.829064	1.452214
O	1.730384	-3.101655	-0.409825
H	1.302803	-3.344199	0.452147
H	1.014295	-3.299983	-1.050425
O	7.178016	-1.846359	0.072575
H	8.115373	-1.647703	-0.067206
H	6.888610	-2.395112	-0.697106
O	6.051883	-3.180557	-2.002344
H	5.270221	-3.674255	-1.654950
H	5.707755	-2.558384	-2.659723
O	3.955501	-4.585338	-0.976278
H	3.143195	-4.073881	-0.748205
H	4.199757	-5.076292	-0.178441
O	-0.850108	-3.601161	-1.197591

H	-1.417831	-3.387254	-1.957600
H	-0.989265	-2.855981	-0.580953
O	-3.147654	-2.376368	-2.267679
H	-3.122501	-1.690965	-1.570427
H	-3.953747	-2.132158	-2.764644
O	-0.875337	3.570134	0.334927
H	-0.169632	4.098339	0.763012
H	-1.640480	4.185824	0.225568
O	1.392743	5.174405	0.789948
H	1.338701	6.078031	1.134309
H	2.187699	4.764405	1.199803
O	0.835407	4.293919	-1.829911
H	1.185369	4.822490	-1.084392
H	0.108873	3.805353	-1.398535
O	-5.855105	-2.463765	-0.157608
H	-5.847242	-1.957640	-1.003748
H	-5.360004	-3.296714	-0.333834
O	-3.974929	-4.414402	-0.618533
H	-3.575645	-3.841074	-1.313561
H	-4.141777	-5.275842	-1.030438
O	-2.191991	-4.685105	1.602049
H	-2.668678	-4.156607	2.277036
H	-2.697011	-4.577481	0.771240
O	0.232983	-3.442144	1.835537
H	-0.116054	-2.538392	1.733253
H	-0.564217	-4.004872	1.679204
O	-3.322826	-2.969228	3.491225
H	-3.925758	-3.324021	4.160685
H	-3.845017	-2.336295	2.965861
O	-5.633970	-1.113475	-2.586282
H	-6.367073	-1.173184	-3.217476
H	-5.411176	-0.160199	-2.506615
O	-2.995107	5.274731	-0.032232
H	-3.304782	5.625085	0.815900
H	-3.779416	4.840576	-0.442954
O	-5.182748	4.046383	-1.163156
H	-5.560951	4.558502	-1.893101
H	-5.021443	3.147910	-1.522645
O	-4.579437	1.481785	-2.164976
H	-4.011088	1.667650	-2.929887
H	-3.999837	1.065457	-1.494632

Table S51. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_A.

N	3.275462	-1.536492	0.570688
C	2.670083	-0.336622	-0.073252
C	1.254688	-0.249609	0.485803
O	0.597866	-1.295827	0.615154
N	0.754424	0.936069	0.844756
C	-0.603495	0.950387	1.368429

C	-1.553020	0.550910	0.237218
O	-1.371817	0.928544	-0.933127
N	-2.587109	-0.228290	0.568076
C	-3.614981	-0.578351	-0.394903
C	-4.223961	0.704000	-0.955235
O	-4.300081	1.751204	-0.357200
O	-4.698758	0.515882	-2.190229
C	2.733176	-0.466317	-1.612974
C	-0.990801	2.284503	2.038380
C	-4.680117	-1.476838	0.273966
C	1.922704	0.642656	-2.274960
C	2.283319	-1.833477	-2.131291
C	-2.283947	2.110480	2.840656
C	-1.133577	3.453890	1.066151
C	-5.594395	-2.124521	-0.766074
C	-5.495928	-0.731853	1.333474
H	3.334680	-1.362810	1.590855
H	4.231555	-1.713405	0.186742
H	3.252316	0.537146	0.236600
H	1.283471	1.800410	0.690978
H	-0.653203	0.172749	2.139624
H	-2.691875	-0.533108	1.529718
H	-3.161088	-1.129592	-1.226182
H	-5.121963	1.340738	-2.494456
H	3.790774	-0.318218	-1.866405
H	-0.173545	2.498815	2.739782
H	-4.105451	-2.275939	0.761715
H	0.856553	0.535124	-2.043898
H	2.038205	0.592639	-3.361781
H	2.246775	1.632121	-1.950055
H	1.253729	-2.052400	-1.827351
H	2.922664	-2.652086	-1.787039
H	2.321482	-1.826870	-3.225183
H	-2.223793	1.265654	3.535603
H	-3.139769	1.957462	2.172589
H	-2.477703	3.013693	3.426248
H	-1.369802	4.364617	1.624818
H	-1.949348	3.272682	0.356175
H	-0.217518	3.639104	0.501778
H	-5.017592	-2.652578	-1.532188
H	-6.222796	-1.378835	-1.263123
H	-6.252967	-2.846646	-0.274761
H	-4.869194	-0.217558	2.070334
H	-6.131510	-1.439922	1.872818
H	-6.146051	0.017817	0.868791
O	2.748894	-0.628161	3.183440
H	2.571641	0.316170	3.304606
H	1.918371	-1.100639	3.414516
O	1.638245	-3.918075	0.269608
H	1.985528	-4.709072	-0.167443
H	0.797816	-3.701744	-0.188600
O	-0.967016	-3.133164	-0.712434
H	-1.060598	-2.652659	-1.560972
H	-0.826187	-2.410715	-0.076231
O	0.545702	-2.257277	3.275788
H	0.362830	-2.132713	2.325401
H	-0.291661	-2.098709	3.736099

O	-1.320811	-1.239509	-2.772870
H	-0.675215	-1.170800	-3.492047
H	-1.290658	-0.387258	-2.294487
O	0.138769	3.124611	-1.954398
H	-0.389127	2.381460	-1.591386
H	-0.468211	3.878883	-1.997484
O	2.213422	3.249444	-0.162062
H	1.531657	3.381655	-0.866415
H	2.279484	4.085354	0.325131
O	6.495542	0.819009	0.259674
H	5.816544	1.409889	-0.139427
H	6.437395	0.942655	1.218030
O	5.866733	-1.732265	-0.432390
H	5.991505	-1.878183	-1.381414
H	6.189789	-0.817973	-0.241331
O	4.630313	2.268013	-1.109406
H	3.833154	2.731606	-0.771974
H	5.027585	2.857621	-1.766769
H	2.677369	-2.379508	0.426103

Table S52. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_B.

N	3.247971	-1.557138	0.636232
C	2.556067	-0.432713	-0.058167
C	1.164382	-0.363918	0.558502
O	0.522931	-1.419801	0.699777
N	0.667066	0.816655	0.930242
C	-0.695075	0.847753	1.441676
C	-1.642089	0.471573	0.300745
O	-1.441776	0.856276	-0.864849
N	-2.702284	-0.275546	0.613414
C	-3.712656	-0.599150	-0.376510
C	-4.274420	0.700357	-0.947434
O	-4.354664	1.742913	-0.341827
O	-4.703199	0.533755	-2.202150
C	2.468832	-0.717767	-1.569798
C	-1.061415	2.194650	2.099374
C	-4.818575	-1.471127	0.260078
C	3.854005	-1.000686	-2.153294
C	1.798780	0.446768	-2.292965
C	-2.352062	2.052469	2.910918
C	-1.191332	3.351636	1.109577
C	-5.741340	-2.064199	-0.804933
C	-5.623450	-0.717748	1.322129
H	3.091090	-1.478414	1.661112
H	4.279515	-1.532448	0.468434
H	3.123614	0.485389	0.132269
H	1.180807	1.678670	0.720435
H	-0.763760	0.073846	2.214224
H	-2.815028	-0.612880	1.562961

H	-3.248081	-1.156737	-1.198117
H	-5.097836	1.369866	-2.513900
H	1.840538	-1.610276	-1.687793
H	-0.236766	2.406148	2.792675
H	-4.280814	-2.299465	0.740822
H	4.538602	-0.172223	-1.934916
H	3.777533	-1.103309	-3.240045
H	4.287456	-1.929707	-1.768857
H	2.414304	1.350208	-2.231563
H	0.811790	0.666119	-1.876268
H	1.670378	0.201142	-3.351748
H	-2.295698	1.225387	3.626985
H	-3.212347	1.890251	2.250833
H	-2.535215	2.972260	3.473795
H	-1.383663	4.279329	1.656871
H	-2.030256	3.184002	0.423718
H	-0.284868	3.498095	0.517757
H	-5.174643	-2.590554	-1.579479
H	-6.341522	-1.286895	-1.288369
H	-6.427046	-2.777172	-0.338038
H	-4.990749	-0.246990	2.082414
H	-6.296556	-1.412352	1.832824
H	-6.234338	0.068069	0.864339
O	2.457508	-0.986826	3.286788
H	2.300695	-0.050564	3.478934
H	1.607181	-1.451171	3.456285
O	2.168062	-3.921883	-0.546439
H	2.713002	-4.367808	-1.210634
H	1.295754	-3.750319	-0.969122
O	-0.395606	-3.159913	-1.261856
H	-0.660706	-2.559353	-1.989972
H	-0.304914	-2.558961	-0.499283
O	0.159486	-2.489975	3.248655
H	-0.011132	-2.249306	2.318385
H	-0.664035	-2.327945	3.731909
O	-1.316976	-1.097110	-2.916414
H	-0.808956	-0.805807	-3.687814
H	-1.347768	-0.332145	-2.307991
O	-0.017472	3.015472	-2.007248
H	-0.580737	2.327198	-1.594497
H	-0.556486	3.820429	-2.031952
O	2.096337	3.045383	-0.274592
H	1.406992	3.155283	-0.977374
H	2.147482	3.893639	0.193469
O	6.350341	1.360942	0.573909
H	5.703419	1.786566	-0.036934
H	6.169737	1.719639	1.454651
O	6.019700	-1.330005	0.455922
H	6.488511	-1.664416	-0.322349
H	6.200386	-0.358231	0.490028
O	4.594587	2.379116	-1.245633
H	3.723593	2.701057	-0.922930
H	4.966653	3.097250	-1.778490
H	2.863639	-2.466347	0.301367

Table S53. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_C.

N	3.170231	-1.618475	0.211108
C	2.657562	-0.255764	-0.091515
C	1.263258	-0.175235	0.515624
O	0.621354	-1.218164	0.731648
N	0.749927	1.030940	0.762424
C	-0.601811	1.115551	1.292259
C	-1.571575	0.556141	0.250137
O	-1.407234	0.757519	-0.964805
N	-2.611081	-0.142474	0.714281
C	-3.678971	-0.594521	-0.157037
C	-4.344759	0.623166	-0.793083
O	-4.331468	1.738819	-0.328720
O	-4.978517	0.296515	-1.922945
C	2.637016	0.038527	-1.606069
C	-0.970947	2.554180	1.716374
C	-4.687393	-1.449692	0.644996
C	1.525001	-0.710623	-2.340982
C	4.003757	-0.235099	-2.236210
C	-2.212503	2.543793	2.611762
C	-1.180903	3.505801	0.537589
C	-5.603600	-2.253657	-0.277586
C	-5.500724	-0.612801	1.635592
H	3.169746	-1.739996	1.246774
H	4.154433	-1.737412	-0.102265
H	3.327275	0.447302	0.413368
H	1.294292	1.878166	0.569650
H	-0.648728	0.478191	2.183176
H	-2.694750	-0.298471	1.712533
H	-3.254689	-1.210195	-0.957811
H	-5.424058	1.089796	-2.275650
H	2.433475	1.111227	-1.690739
H	-0.117560	2.903017	2.313056
H	-4.065692	-2.162308	1.203719
H	1.658865	-1.796492	-2.278319
H	1.531582	-0.428987	-3.398559
H	0.537200	-0.465839	-1.937225
H	4.211935	-1.310202	-2.291442
H	4.806880	0.257138	-1.678905
H	4.015428	0.151435	-3.259679
H	-2.093362	1.868197	3.465759
H	-3.100227	2.244535	2.042499
H	-2.393012	3.550053	3.001104
H	-1.331830	4.522270	0.913446
H	-2.069147	3.219735	-0.036880
H	-0.326721	3.524410	-0.143838
H	-5.026396	-2.844009	-0.996524
H	-6.280902	-1.600130	-0.835354
H	-6.210871	-2.939978	0.319849
H	-4.873125	0.009488	2.283236
H	-6.092415	-1.271288	2.277771
H	-6.193984	0.051071	1.106197
O	3.024803	-1.520120	3.010472

H	3.186103	-0.625582	3.344528
H	2.113076	-1.764553	3.287810
O	1.583780	-3.793997	-0.724995
H	1.874803	-4.330698	-1.476153
H	0.649843	-3.538672	-0.907879
O	-0.995634	-2.795602	-0.911473
H	-1.247151	-2.328810	-1.737213
H	-0.679039	-2.095567	-0.310960
O	0.423665	-2.360700	3.271508
H	0.198363	-1.996680	2.394188
H	-0.207294	-1.974538	3.896590
O	-1.893364	-1.145396	-2.982164
H	-1.365150	-1.047974	-3.788373
H	-1.778136	-0.316736	-2.477193
O	0.467829	2.408294	-2.284778
H	-0.170886	1.847334	-1.792547
H	-0.068542	3.065558	-2.753509
O	2.249079	3.216032	-0.385863
H	1.666961	3.120738	-1.178986
H	2.149378	4.128208	-0.072042
O	5.487115	0.531350	1.260377
H	5.389436	1.326093	0.685082
H	5.988886	0.812760	2.039287
O	5.976626	-1.804272	-0.035356
H	6.497978	-1.744183	-0.848609
H	6.052299	-0.931032	0.411717
O	4.920309	2.487881	-0.553540
H	3.995719	2.819028	-0.528044
H	5.485184	3.271788	-0.620240
H	2.573797	-2.371022	-0.197128

Table S54. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_D.

N	3.314051	-2.006537	0.032260
C	2.706153	-0.702998	-0.351200
C	1.356909	-0.636615	0.341452
O	0.698849	-1.680331	0.506227
N	0.902980	0.551239	0.734379
C	-0.445524	0.642409	1.273155
C	-1.422757	0.243454	0.163145
O	-1.267197	0.620920	-1.003400
N	-2.466700	-0.522381	0.511930
C	-3.477718	-0.879433	-0.463262
C	-4.028942	0.390244	-1.102305
O	-4.134516	1.459207	-0.537358
O	-4.428834	0.179032	-2.352922
C	2.592778	-0.583983	-1.886979
C	-0.731317	2.055048	1.813651
C	-4.594615	-1.709933	0.209062
C	1.515351	-1.491729	-2.484177

C	2.362455	0.869583	-2.295732
C	0.256019	2.395251	2.933015
C	-2.169315	2.160223	2.326333
C	-5.516212	-2.348586	-0.829963
C	-5.397002	-0.898310	1.229540
H	3.412593	-2.015705	1.064466
H	4.259196	-2.066264	-0.393743
H	3.376700	0.074066	0.031487
H	1.426781	1.413123	0.545582
H	-0.532453	-0.071801	2.102542
H	-2.564107	-0.844042	1.468066
H	-3.016096	-1.474488	-1.259995
H	-4.816502	1.001443	-2.708121
H	3.574047	-0.894044	-2.269741
H	-0.604344	2.761520	0.982191
H	-4.065137	-2.517181	0.733534
H	1.624349	-2.536493	-2.177454
H	1.574765	-1.453860	-3.576017
H	0.514850	-1.152078	-2.190320
H	2.359232	0.950324	-3.386921
H	3.144485	1.530092	-1.908426
H	1.390626	1.225993	-1.938169
H	1.300387	2.316538	2.616299
H	0.111430	1.716580	3.782225
H	0.085325	3.417533	3.284021
H	-2.342547	3.161830	2.732051
H	-2.344913	1.440956	3.136748
H	-2.908224	1.975272	1.540699
H	-4.949825	-2.923081	-1.569821
H	-6.103256	-1.591554	-1.359954
H	-6.215059	-3.026693	-0.331710
H	-4.760196	-0.380508	1.954953
H	-6.064838	-1.563842	1.783930
H	-6.013587	-0.143264	0.729480
O	3.065719	-1.384143	2.773100
H	3.051285	-0.444268	3.006585
H	2.214101	-1.761861	3.087288
O	1.791079	-4.366650	-0.446740
H	2.081071	-5.017347	-1.102285
H	0.842131	-4.190629	-0.633699
O	-0.829465	-3.493944	-0.889806
H	-1.514921	-3.921772	-0.355043
H	-0.576865	-2.686126	-0.403740
O	0.655058	-2.665171	3.113025
H	0.391277	-2.422782	2.204358
H	-0.067604	-2.382593	3.692672
O	-2.719184	3.960499	-0.675777
H	-3.241442	3.137353	-0.634470
H	-2.817756	4.381201	0.190887
O	-0.227006	3.136045	-1.591102
H	-0.493984	2.199034	-1.477874
H	-1.021924	3.621568	-1.281162
O	1.916142	3.202111	0.032312
H	1.156160	3.321868	-0.599337
H	1.797069	3.870508	0.725091
O	5.424093	1.009224	0.300792
H	5.180255	1.862312	-0.132920

H	6.022999	1.234372	1.027487
O	5.871430	-1.386740	-0.919406
H	6.169057	-1.366652	-1.839893
H	5.857907	-0.454524	-0.603172
O	4.505329	3.268860	-0.925810
H	3.577367	3.359532	-0.611016
H	4.950103	4.101169	-0.708435
H	2.728164	-2.826087	-0.238664

Table S55. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_E.

N	3.066313	-1.673911	0.758913
C	2.453261	-0.639051	-0.118487
C	1.133446	-0.258144	0.536361
O	0.423272	-1.146636	1.039565
N	0.764551	1.020390	0.516954
C	-0.559887	1.400751	0.987103
C	-1.594723	0.721300	0.088351
O	-1.520711	0.813827	-1.150675
N	-2.574649	0.036147	0.677617
C	-3.601119	-0.638525	-0.097483
C	-4.343591	0.384096	-0.951422
O	-4.533731	1.536793	-0.642919
O	-4.797462	-0.167524	-2.080901
C	2.220345	-1.197298	-1.537226
C	-0.719374	2.930066	0.971489
C	-4.557609	-1.403125	0.844765
C	3.519400	-1.765301	-2.111708
C	1.660338	-0.108697	-2.451718
C	0.280471	3.569729	1.936982
C	-2.152867	3.321195	1.333686
C	-5.461659	-2.355067	0.061531
C	-5.382159	-0.467732	1.732453
H	3.037655	-1.331588	1.737719
H	4.069576	-1.825914	0.514882
H	3.138545	0.215547	-0.161768
H	1.348004	1.724262	0.050308
H	-0.681786	1.043113	2.017393
H	-2.584610	-0.051746	1.687787
H	-3.125515	-1.358913	-0.772987
H	-5.309025	0.500647	-2.574823
H	1.481021	-2.005720	-1.450176
H	-0.507601	3.274391	-0.050384
H	-3.898339	-2.011000	1.479593
H	4.302779	-0.997909	-2.106050
H	3.355194	-2.080359	-3.146357
H	3.876719	-2.639966	-1.558491
H	2.370600	0.720663	-2.542819
H	0.708971	0.286280	-2.085327
H	1.494222	-0.515823	-3.454207

H	1.317291	3.304963	1.706437
H	0.071204	3.251318	2.965188
H	0.194799	4.659593	1.895254
H	-2.245145	4.410955	1.352565
H	-2.414783	2.945010	2.330652
H	-2.882862	2.929626	0.617978
H	-4.878787	-3.020076	-0.583881
H	-6.171280	-1.804891	-0.564613
H	-6.035917	-2.971279	0.759384
H	-4.766176	0.262442	2.268379
H	-5.928225	-1.054911	2.476251
H	-6.115037	0.088390	1.137693
O	2.719471	-0.134071	3.102321
H	2.716718	0.825392	2.968378
H	1.858884	-0.359907	3.520908
O	1.583182	-4.042903	0.257514
H	1.967079	-4.668389	-0.373808
H	0.674738	-3.839895	-0.065627
O	-0.963448	-3.126613	-0.337280
H	-1.104889	-2.719191	-1.218585
H	-0.721766	-2.374149	0.234229
O	0.303941	-1.213425	3.827756
H	0.057365	-1.292525	2.886377
H	-0.438027	-0.775988	4.270195
O	-1.473764	-1.604007	-2.622468
H	-0.836288	-1.618377	-3.351675
H	-1.478965	-0.688019	-2.280732
O	-0.065144	2.670722	-2.666244
H	-0.639262	2.065829	-2.149569
H	-0.596142	3.461866	-2.841756
O	2.115404	2.990834	-1.086230
H	1.385636	2.983096	-1.756685
H	2.180962	3.903077	-0.763705
O	5.985771	1.003602	0.674370
H	5.445435	1.370688	-0.062888
H	5.571698	1.305499	1.495978
O	5.829955	-1.701932	0.392223
H	6.256212	-1.971463	-0.434143
H	5.993254	-0.732216	0.486287
O	4.519111	1.715153	-1.520106
H	3.725626	2.291079	-1.459061
H	5.055655	2.062476	-2.247843
H	2.538672	-2.570132	0.680291

Table S56. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_F.

N	3.168542	-1.848585	-0.183580
C	2.649739	-0.456092	-0.213750
C	1.283787	-0.474410	0.456394
O	0.658402	-1.542525	0.581823

N	0.785000	0.694587	0.850330
C	-0.578917	0.779338	1.349065
C	-1.524574	0.270252	0.256880
O	-1.342114	0.538186	-0.935179
N	-2.577417	-0.461455	0.648478
C	-3.553787	-0.920069	-0.321175
C	-4.104168	0.274077	-1.090545
O	-4.197543	1.403196	-0.654470
O	-4.513226	-0.075331	-2.307561
C	2.559441	0.112811	-1.646586
C	-0.906102	2.232587	1.744830
C	-4.674026	-1.713342	0.388581
C	3.915336	0.052184	-2.351448
C	1.472751	-0.563695	-2.485946
C	0.020008	2.693097	2.873590
C	-2.368590	2.373609	2.171131
C	-5.534330	-2.486356	-0.611098
C	-5.537875	-0.826479	1.289044
H	3.157644	-2.180782	0.805917
H	4.163333	-1.870020	-0.484816
H	3.348948	0.146930	0.376823
H	1.309648	1.562126	0.693611
H	-0.673925	0.138139	2.235774
H	-2.707862	-0.678731	1.629793
H	-3.050816	-1.571467	-1.045236
H	-4.898285	0.703942	-2.751666
H	2.294087	1.171093	-1.518403
H	-0.738836	2.855271	0.854378
H	-4.143501	-2.446468	1.011580
H	4.704774	0.509582	-1.748582
H	3.856251	0.597133	-3.298302
H	4.198120	-0.980940	-2.585743
H	1.424617	-0.085544	-3.469235
H	0.481836	-0.485781	-2.026774
H	1.694537	-1.625107	-2.643479
H	1.080120	2.611311	2.615861
H	-0.155816	2.092983	3.774256
H	-0.184951	3.739571	3.118632
H	-2.561186	3.404576	2.483466
H	-2.586766	1.721137	3.026407
H	-3.066390	2.123962	1.366588
H	-4.920391	-3.113091	-1.265895
H	-6.123537	-1.809829	-1.238174
H	-6.229902	-3.134603	-0.070163
H	-4.943532	-0.217067	1.978718
H	-6.210468	-1.449355	1.885648
H	-6.153642	-0.146240	0.689717
O	3.128838	-2.371633	2.574767
H	3.468803	-1.624447	3.088351
H	2.213311	-2.536637	2.895860
O	1.601214	-3.868353	-1.417352
H	1.796877	-4.220237	-2.297767
H	0.642480	-3.649770	-1.411840
O	-1.020094	-2.988463	-1.086459
H	-1.538154	-3.638503	-0.587439
H	-0.665710	-2.367546	-0.420909
O	0.457999	-2.856761	3.027150

H	0.221237	-2.367012	2.216389
H	-0.015566	-2.425701	3.753785
O	-2.529570	3.717835	-1.164994
H	-3.074898	2.924065	-1.008507
H	-2.689788	4.300263	-0.407872
O	0.025359	2.786724	-1.792581
H	-0.262624	1.880121	-1.552518
H	-0.793532	3.303181	-1.627989
O	1.941598	3.211324	0.014427
H	1.248231	3.219154	-0.701381
H	1.806981	4.011785	0.544603
O	5.483218	0.813685	0.909375
H	5.249155	1.611639	0.376589
H	6.056701	1.119219	1.627279
O	5.956365	-1.582127	-0.312582
H	6.493134	-1.527268	-1.116218
H	5.964963	-0.683230	0.089489
O	4.581519	2.827576	-0.687589
H	3.651429	3.055902	-0.463622
H	5.068285	3.664478	-0.706528
H	2.593815	-2.515727	-0.741059

Table S57. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_G.

N	3.286105	-1.502911	0.562139
C	2.606255	-0.383064	-0.147567
C	1.212917	-0.297674	0.465848
O	0.599067	-1.347580	0.717412
N	0.694611	0.901535	0.745026
C	-0.639718	0.938670	1.320028
C	-1.641166	0.479498	0.259402
O	-1.451855	0.677735	-0.953170
N	-2.742503	-0.132729	0.700495
C	-3.789378	-0.549025	-0.215566
C	-4.273169	0.665645	-1.002499
O	-4.305123	1.797035	-0.579477
O	-4.697447	0.315163	-2.220501
C	2.613948	-0.628440	-1.673507
C	-1.020002	2.302823	1.930375
C	-4.942407	-1.222327	0.562477
C	1.748631	0.406533	-2.384856
C	2.182625	-2.042064	-2.067658
C	-1.297499	3.395031	0.898713
C	0.042489	2.737694	2.941657
C	-5.919174	-1.915217	-0.388109
C	-5.678259	-0.250337	1.488352
H	3.376689	-1.243871	1.561604
H	4.235397	-1.667965	0.156605
H	3.165998	0.532855	0.068527
H	1.191318	1.759255	0.484155
H	-0.655095	0.204976	2.134371

H	-2.850263	-0.320298	1.691184
H	-3.376588	-1.270192	-0.930628
H	-5.044433	1.106668	-2.673389
H	3.656851	-0.474452	-1.979221
H	-1.952243	2.113680	2.477892
H	-4.456920	-1.997054	1.171249
H	0.693187	0.277611	-2.119638
H	1.840963	0.288929	-3.468632
H	2.045065	1.426145	-2.133394
H	1.174790	-2.265108	-1.700390
H	2.861095	-2.814433	-1.693276
H	2.171337	-2.117809	-3.159543
H	-2.090231	3.104341	0.200748
H	-0.398672	3.639224	0.324684
H	-1.618437	4.306564	1.412199
H	-0.306343	3.614366	3.494906
H	0.979352	3.013264	2.443554
H	0.257552	1.941166	3.662487
H	-5.402144	-2.604461	-1.063272
H	-6.466214	-1.186964	-0.995494
H	-6.650241	-2.486685	0.191069
H	-5.002821	0.303270	2.149144
H	-6.380691	-0.805156	2.116968
H	-6.250798	0.481974	0.908741
O	2.846049	-0.360917	3.099618
H	2.660150	0.588963	3.128159
H	2.033810	-0.815276	3.416465
O	1.788830	-3.973090	0.514916
H	2.187219	-4.766720	0.129271
H	0.924603	-3.855877	0.064078
O	-0.861615	-3.405820	-0.404487
H	-1.064289	-2.992869	-1.269512
H	-0.718048	-2.631214	0.166152
O	0.684192	-2.003051	3.463400
H	0.437054	-1.977226	2.519921
H	-0.128443	-1.840143	3.964410
O	-1.475478	-1.679417	-2.545878
H	-0.879110	-1.645728	-3.308738
H	-1.436548	-0.794553	-2.131575
O	-0.097482	2.874018	-2.153296
H	-0.571692	2.122674	-1.737038
H	-0.746109	3.591671	-2.211299
O	2.023964	3.191577	-0.459047
H	1.310877	3.253342	-1.142744
H	2.090213	4.064868	-0.042484
O	6.403918	0.967273	-0.038881
H	5.688415	1.497119	-0.459424
H	6.373610	1.168458	0.907536
O	5.855073	-1.652962	-0.506544
H	5.961990	-1.867582	-1.444570
H	6.142819	-0.713848	-0.396318
O	4.432304	2.224302	-1.445807
H	3.632188	2.681904	-1.107564
H	4.770902	2.771350	-2.169467
H	2.723701	-2.381024	0.509323

Table S58. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_H.

N	3.278351	-1.445164	0.704629
C	2.495378	-0.480845	-0.120018
C	1.140865	-0.350236	0.567183
O	0.561921	-1.381682	0.950538
N	0.612595	0.862958	0.738207
C	-0.722352	0.956127	1.305517
C	-1.726329	0.420167	0.283400
O	-1.525901	0.510139	-0.940258
N	-2.844705	-0.124637	0.764910
C	-3.889516	-0.597434	-0.125186
C	-4.347685	0.557308	-1.011726
O	-4.353925	1.720722	-0.685405
O	-4.781216	0.115142	-2.196024
C	2.332849	-1.016716	-1.555782
C	-1.091475	2.375643	1.783223
C	-5.058915	-1.190408	0.692664
C	3.690284	-1.379224	-2.160320
C	1.609072	0.009027	-2.423717
C	-1.349007	3.362044	0.644867
C	-0.029702	2.893339	2.755216
C	-6.032902	-1.953813	-0.205290
C	-5.793255	-0.133969	1.522149
H	3.194107	-1.182417	1.706262
H	4.293265	-1.420393	0.456916
H	3.034442	0.473382	-0.125367
H	1.078228	1.682253	0.333769
H	-0.744966	0.299643	2.181950
H	-2.967790	-0.221261	1.766684
H	-3.479006	-1.377768	-0.776432
H	-5.111577	0.873135	-2.714048
H	1.714771	-1.922250	-1.490990
H	-2.029599	2.251870	2.339166
H	-4.588920	-1.914213	1.372069
H	4.366052	-0.516451	-2.123602
H	3.557250	-1.666077	-3.207838
H	4.163933	-2.224163	-1.649764
H	2.210067	0.918089	-2.532008
H	0.637234	0.278886	-2.002566
H	1.441718	-0.402191	-3.424178
H	-2.163480	3.026260	-0.006108
H	-0.453377	3.510985	0.033792
H	-1.629454	4.334444	1.060979
H	-0.365380	3.830451	3.208498
H	0.918622	3.093363	2.243244
H	0.160187	2.173188	3.558659
H	-5.516350	-2.705966	-0.809871
H	-6.564496	-1.276898	-0.881691
H	-6.776822	-2.463787	0.413587
H	-5.118281	0.463622	2.144044
H	-6.512481	-0.623788	2.184815
H	-6.346947	0.554689	0.874582

O	2.690670	-0.316353	3.220812
H	2.544772	0.641015	3.210159
H	1.863164	-0.722274	3.563781
O	2.273804	-4.018049	0.010691
H	2.799630	-4.524455	-0.624912
H	1.364068	-3.957249	-0.362351
O	-0.358688	-3.498252	-0.609198
H	-0.682775	-3.043599	-1.415469
H	-0.256426	-2.771093	0.032585
O	0.451974	-1.817612	3.711107
H	0.206736	-1.829966	2.766612
H	-0.349957	-1.590299	4.204032
O	-1.420781	-1.810796	-2.566926
H	-0.950174	-1.650501	-3.397975
H	-1.461447	-0.948252	-2.108659
O	-0.296954	2.564709	-2.450205
H	-0.797305	1.904103	-1.926872
H	-0.886885	3.327432	-2.547747
O	1.882823	2.935896	-0.853203
H	1.160420	2.917137	-1.531016
H	1.934986	3.850016	-0.532455
O	6.144139	1.549540	0.305048
H	5.488197	1.832813	-0.374503
H	5.851582	1.933849	1.144029
O	6.025381	-1.164752	0.308991
H	6.449718	-1.493481	-0.496743
H	6.147790	-0.183563	0.304660
O	4.372770	2.094324	-1.694318
H	3.504535	2.491438	-1.461201
H	4.739334	2.639841	-2.405745
H	2.913397	-2.411510	0.564732

Table S59. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_I.

N	3.039211	-1.756156	0.554032
C	2.587056	-0.462937	-0.026322
C	1.199795	-0.210807	0.550801
O	0.518900	-1.173250	0.945265
N	0.738233	1.040035	0.580631
C	-0.603521	1.267906	1.094680
C	-1.609485	0.568292	0.181825
O	-1.432211	0.480776	-1.044830
N	-2.702909	0.079205	0.772047
C	-3.792732	-0.491507	0.003373
C	-4.366364	0.582515	-0.917673
O	-4.275874	1.773373	-0.733612
O	-5.018586	0.038872	-1.949259
C	2.573624	-0.480253	-1.569281
C	-0.943125	2.763717	1.261694
C	-4.867833	-1.064353	0.956344

C	1.416260	-1.295746	-2.147974
C	3.918015	-0.955656	-2.122919
C	-1.133109	3.508137	-0.060286
C	0.103076	3.443818	2.148209
C	-5.821329	-2.012259	0.228792
C	-5.638797	0.036305	1.689403
H	2.983991	-1.661290	1.584435
H	4.036796	-1.950898	0.324873
H	3.290001	0.301325	0.323656
H	1.309985	1.811758	0.224386
H	-0.659992	0.803398	2.086662
H	-2.797106	0.153633	1.779155
H	-3.404176	-1.304094	-0.621293
H	-5.406029	0.753358	-2.489194
H	2.432630	0.564687	-1.868284
H	-1.901271	2.775604	1.797276
H	-4.303266	-1.655061	1.690205
H	1.487813	-2.352772	-1.868633
H	1.437368	-1.231980	-3.240410
H	0.445535	-0.919181	-1.810112
H	4.062204	-2.029836	-1.954598
H	4.753101	-0.407741	-1.676289
H	3.944839	-0.788840	-3.203802
H	-1.945754	3.080119	-0.655234
H	-0.220175	3.492876	-0.663861
H	-1.376555	4.555281	0.144452
H	-0.232307	4.451163	2.411120
H	1.064731	3.542418	1.631514
H	0.269139	2.883335	3.074276
H	-5.274546	-2.798190	-0.302138
H	-6.441188	-1.475883	-0.495752
H	-6.485628	-2.488984	0.955628
H	-4.980153	0.761251	2.180004
H	-6.278246	-0.408361	2.457133
H	-6.283195	0.587685	0.994767
O	2.717491	-0.669677	3.137352
H	3.092034	0.198443	3.344935
H	1.796900	-0.668964	3.480818
O	1.403481	-4.020966	0.006187
H	1.672214	-4.691173	-0.638502
H	0.474581	-3.775931	-0.214023
O	-1.145657	-2.991036	-0.341494
H	-1.415613	-2.686540	-1.234396
H	-0.790378	-2.196613	0.098991
O	0.011107	-0.914566	3.651582
H	-0.091169	-1.294423	2.758677
H	-0.246844	-1.607681	4.277198
O	-2.053868	-1.733092	-2.663092
H	-1.538109	-1.809083	-3.479602
H	-1.888645	-0.833929	-2.317782
O	0.438327	1.832326	-2.648393
H	-0.199028	1.383305	-2.050254
H	-0.094862	2.423343	-3.201484
O	2.281578	2.915868	-0.984853
H	1.665102	2.680656	-1.723097
H	2.249382	3.880429	-0.888545
O	5.934308	0.741881	0.810947

H	5.560693	1.301989	0.090283
H	5.600803	1.099438	1.646282
O	5.823112	-1.958236	0.453127
H	6.336250	-2.227028	-0.322472
H	5.987974	-0.994118	0.575473
O	4.896798	2.094031	-1.313661
H	3.982002	2.444878	-1.234782
H	5.441818	2.831997	-1.624253
H	2.434191	-2.558813	0.273497

Table S60. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_J.

N	3.216764	-1.592815	0.450348
C	2.632755	-0.348531	-0.125464
C	1.223474	-0.262041	0.449332
O	0.539982	-1.296194	0.521502
N	0.760561	0.912143	0.888574
C	-0.584521	0.929554	1.443097
C	-1.565927	0.600248	0.316980
O	-1.396216	1.015288	-0.842404
N	-2.619112	-0.158457	0.635599
C	-3.680395	-0.414541	-0.323344
C	-4.208839	0.924376	-0.831579
O	-4.368771	1.900159	-0.135838
O	-4.512570	0.876496	-2.130672
C	2.684941	-0.393687	-1.670038
C	-0.923983	2.242489	2.179033
C	-4.803469	-1.236343	0.340123
C	1.886482	0.762257	-2.262620
C	2.209273	-1.721666	-2.261544
C	-2.173029	2.053553	3.044769
C	-1.105640	3.444793	1.254353
C	-4.281538	-2.623657	0.722672
C	-6.017290	-1.359944	-0.582415
H	3.269128	-1.483850	1.480476
H	4.173771	-1.757985	0.064399
H	3.234620	0.495125	0.227784
H	1.306169	1.772368	0.775682
H	-0.634504	0.118312	2.178930
H	-2.749265	-0.446454	1.599492
H	-3.277992	-0.974655	-1.176848
H	-4.897739	1.732453	-2.397105
H	3.743062	-0.248067	-1.922716
H	-0.068709	2.426430	2.842768
H	-5.107346	-0.694259	1.247093
H	0.819822	0.652982	-2.033831
H	1.997176	0.774623	-3.351007
H	2.223360	1.727204	-1.881702
H	1.177811	-1.939409	-1.963248
H	2.836940	-2.568799	-1.968808

H	2.240760	-1.653427	-3.353506
H	-2.077673	1.194609	3.717745
H	-3.065113	1.918067	2.421942
H	-2.332261	2.944680	3.658628
H	-1.299088	4.339490	1.853781
H	-1.961364	3.296226	0.584589
H	-0.219922	3.637406	0.645983
H	-3.412308	-2.585322	1.387220
H	-3.989450	-3.178365	-0.175954
H	-5.066705	-3.186966	1.235342
H	-6.486912	-0.392326	-0.782938
H	-6.767077	-2.004755	-0.115470
H	-5.732906	-1.808020	-1.541436
O	2.691883	-0.899148	3.130529
H	2.522218	0.035277	3.320316
H	1.852482	-1.376686	3.316068
O	1.553650	-3.920689	0.020431
H	1.894639	-4.685375	-0.465701
H	0.718212	-3.664297	-0.427617
O	-1.023150	-3.067403	-0.915586
H	-1.129384	-2.518002	-1.720126
H	-0.916560	-2.398127	-0.218090
O	0.429512	-2.451591	3.097449
H	0.259005	-2.234536	2.161295
H	-0.393306	-2.264850	3.573433
O	-1.420374	-1.031793	-2.821922
H	-0.784529	-0.905951	-3.542081
H	-1.382007	-0.220023	-2.278116
O	0.127606	3.233039	-1.802986
H	-0.402525	2.480216	-1.464585
H	-0.474355	3.992485	-1.812608
O	2.218334	3.265334	-0.023218
H	1.531056	3.431719	-0.714632
H	2.291287	4.077940	0.500979
O	6.423141	0.766058	0.342366
H	5.768989	1.385202	-0.055767
H	6.314836	0.832585	1.302063
O	5.819841	-1.735405	-0.533897
H	5.957389	-1.814444	-1.489011
H	6.136321	-0.835594	-0.275633
O	4.619968	2.297421	-1.018838
H	3.828848	2.757207	-0.662388
H	5.038148	2.916587	-1.634757
H	2.609010	-2.418468	0.252572

Table S61. M06-2X/6-31+G*/PCM/Integral=SuperFineGrid optimized Cartesian coordinates of the $Val_3H^+ \cdot 10H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $10H_2O$_PPII-PPII_S.

N	3.235642	-1.541183	0.499781
C	2.639796	-0.301733	-0.074261
C	1.199582	-0.276366	0.426460
O	0.544655	-1.330976	0.428451

N	0.681444	0.869637	0.878775
C	-0.691797	0.837157	1.357148
C	-1.606084	0.539880	0.166138
O	-1.362674	0.979242	-0.969753
N	-2.675858	-0.225042	0.410135
C	-3.689620	-0.456407	-0.599084
C	-4.318811	0.873139	-1.002623
O	-4.241130	1.902699	-0.375691
O	-5.013708	0.741117	-2.137161
C	2.775370	-0.304012	-1.614170
C	-1.095475	2.109709	2.130533
C	-4.772883	-1.437901	-0.100876
C	1.984421	0.850697	-2.219290
C	2.363973	-1.626255	-2.263915
C	-2.392252	1.868926	2.909198
C	-1.237751	3.350649	1.250998
C	-5.599113	-0.863008	1.052302
C	-4.148625	-2.785601	0.265547
H	3.236670	-1.454817	1.533070
H	4.214440	-1.667954	0.156081
H	3.192955	0.551175	0.332639
H	1.210411	1.745588	0.822594
H	-0.764723	-0.006317	2.053686
H	-2.840044	-0.547211	1.357128
H	-3.216313	-0.885931	-1.490319
H	-5.439211	1.592748	-2.349395
H	3.842057	-0.129628	-1.805525
H	-0.284750	2.271587	2.853207
H	-5.437138	-1.590403	-0.958786
H	0.910238	0.717418	-2.046288
H	2.148642	0.890831	-3.300226
H	2.283536	1.812467	-1.800289
H	1.323327	-1.874623	-2.028457
H	2.994472	-2.466364	-1.957325
H	2.453633	-1.529184	-3.350474
H	-2.334939	0.970690	3.534329
H	-3.245342	1.773650	2.227245
H	-2.589127	2.721418	3.565635
H	-1.487597	4.213563	1.875842
H	-2.044389	3.217418	0.520289
H	-0.317014	3.586042	0.713437
H	-6.114203	0.060389	0.768395
H	-4.982775	-0.646947	1.933573
H	-6.357258	-1.589678	1.358291
H	-3.522245	-3.169155	-0.545611
H	-4.938463	-3.513869	0.471973
H	-3.526430	-2.715550	1.165934
O	2.552087	-0.906939	3.160786
H	2.326858	0.017070	3.344020
H	1.725937	-1.424217	3.290989
O	1.673165	-3.903406	-0.067263
H	2.058215	-4.646009	-0.554652
H	0.854234	-3.656144	-0.550233
O	-0.877033	-3.129884	-1.118461
H	-0.952251	-2.542725	-1.899929
H	-0.866554	-2.494511	-0.382302
O	0.366660	-2.555583	2.970267

H	0.239809	-2.327685	2.029641
H	-0.488932	-2.412198	3.401469
O	-1.235758	-1.036727	-2.962254
H	-0.592952	-0.882964	-3.670630
H	-1.221441	-0.236383	-2.400424
O	0.145350	3.267808	-1.750864
H	-0.382717	2.489525	-1.470922
H	-0.473443	4.013597	-1.758710
O	2.147240	3.271894	0.122910
H	1.487637	3.451063	-0.592358
H	2.179933	4.065172	0.679789
O	6.397992	0.911322	0.574050
H	5.745345	1.523516	0.162273
H	6.254236	0.960285	1.530120
O	5.886477	-1.588611	-0.360807
H	6.073479	-1.650860	-1.308741
H	6.168718	-0.685489	-0.075336
O	4.620697	2.442354	-0.818630
H	3.795007	2.846498	-0.473006
H	5.050527	3.123889	-1.355706
H	2.664793	-2.380377	0.253890

Table S62. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_A.

N	3.580132	0.154360	1.639771
C	3.042073	-0.195000	0.295096
C	1.607144	0.329531	0.277589
O	0.909032	0.203562	1.295363
N	1.138205	0.933570	-0.819882
C	-0.246557	1.391923	-0.807197
C	-1.157901	0.158982	-0.746560
O	-0.915692	-0.852130	-1.428589
N	-2.203583	0.221168	0.088747
C	-3.114523	-0.899737	0.213760
C	-4.104579	-0.892681	-0.939578
O	-4.447656	0.084354	-1.568252
O	-4.607859	-2.111599	-1.167364
C	3.171219	-1.719010	0.060726
C	-0.570201	2.334080	-1.985078
C	-3.848313	-0.910443	1.582444
C	2.454902	-2.133340	-1.218896
C	2.685589	-2.560222	1.242110
C	-1.963292	2.936936	-1.805249
C	-0.471266	1.686300	-3.364780
C	-4.164783	-2.344669	2.007788
C	-5.111051	-0.047304	1.597452
H	3.658839	1.189663	1.708901
H	4.523613	-0.272510	1.777569
H	2.939369	-0.175517	2.394641
H	3.641846	0.335075	-0.452182
H	1.716252	0.997263	-1.662993

H	-0.392888	1.963252	0.118466
H	-2.383009	1.075052	0.627934
H	-2.523757	-1.815640	0.138295
H	-5.282456	-2.062818	-1.872524
H	4.246901	-1.890003	-0.078393
H	0.172733	3.139992	-1.916354
H	-3.120722	-0.501335	2.293987
H	1.379889	-1.937671	-1.145653
H	2.586629	-3.205770	-1.390274
H	2.843574	-1.605861	-2.090125
H	1.627852	-2.373774	1.453719
H	3.259815	-2.380802	2.156123
H	2.794538	-3.619300	0.989065
H	-2.085285	3.415455	-0.829521
H	-2.735009	2.165527	-1.905318
H	-2.146565	3.691530	-2.575424
H	-0.676716	2.439003	-4.131915
H	-1.211103	0.884944	-3.475043
H	0.517940	1.272450	-3.565598
H	-3.256476	-2.954852	2.043539
H	-4.872854	-2.816453	1.317470
H	-4.618394	-2.344304	3.003595
H	-4.925851	0.970407	1.243601
H	-5.504584	0.015609	2.615993
H	-5.894111	-0.486167	0.966192
O	3.298527	2.927685	1.474620
H	3.184873	3.268234	0.575138
H	2.411529	2.986876	1.910725
O	1.845632	-0.734916	3.797912
H	2.177065	-1.352768	4.465503
H	1.048120	-1.156704	3.411010
O	-0.649125	-1.629846	2.632620
H	-0.644480	-2.322350	1.936195
H	-0.531236	-0.811128	2.119821
O	0.905460	2.700543	2.711323
H	0.687012	1.803324	2.399761
H	0.254931	3.308820	2.291196
O	-0.608453	-3.218385	0.314517
H	-1.414027	-3.735925	0.097370
H	-0.555612	-2.538806	-0.382432
O	0.818498	-1.279770	-3.656142
H	0.218004	-1.111078	-2.898218
H	0.282824	-1.137569	-4.451003
O	2.841740	0.515301	-3.177584
H	2.196102	-0.148349	-3.526074
H	2.956917	1.184164	-3.870472
O	6.877031	0.463183	-0.491163
H	6.280593	0.165312	-1.216683
H	6.726375	1.413708	-0.386066
O	6.174761	-0.869941	1.771080
H	6.320735	-1.823109	1.683954
H	6.534270	-0.451784	0.951210
O	5.249778	-0.620177	-2.394032
H	4.447407	-0.191104	-2.763907
H	5.743600	-0.966164	-3.151855
O	-4.899746	2.759841	-0.594928
H	-5.836642	2.842226	-0.361519

H	-4.800508	1.877465	-1.002652
O	-3.010377	-4.451204	-0.401206
H	-2.884953	-5.084128	-1.124162
H	-3.656904	-3.803255	-0.731943
O	-3.007162	2.717499	1.359849
H	-3.388114	2.653235	2.249793
H	-3.762662	2.868945	0.739492
O	-0.874477	4.442812	1.563459
H	-0.619879	4.849301	0.722532
H	-1.708704	3.949927	1.405416

Table S63. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_B.

N	-3.493341	-0.027981	-1.692919
C	-2.865878	-0.341007	-0.379462
C	-1.517202	0.374394	-0.379151
O	-0.840979	0.359638	-1.421690
N	-1.081441	0.962368	0.739863
C	0.293116	1.457461	0.773181
C	1.223772	0.238648	0.739210
O	1.038379	-0.733490	1.493166
N	2.214181	0.259980	-0.160848
C	3.109016	-0.872182	-0.297541
C	4.137432	-0.850290	0.822380
O	4.511124	0.138943	1.413348
O	4.636339	-2.067263	1.069547
C	-2.666113	-1.866666	-0.241413
C	0.566485	2.398542	1.962528
C	3.789535	-0.901315	-1.691010
C	-3.956237	-2.623148	-0.564603
C	-2.185390	-2.221356	1.161691
C	1.974610	2.982517	1.841053
C	0.396194	1.763158	3.341232
C	4.151877	-2.333091	-2.085772
C	5.009413	0.016526	-1.781977
H	-3.494161	1.004360	-1.835362
H	-4.487844	-0.340012	-1.726330
H	-2.957459	-0.493035	-2.456018
H	-3.524626	0.034474	0.411306
H	-1.643599	0.900914	1.594334
H	0.453312	2.039638	-0.140960
H	2.343771	1.085740	-0.754582
H	2.514984	-1.784048	-0.188134
H	5.331687	-2.003193	1.753100
H	-1.891471	-2.155060	-0.964655
H	-0.161870	3.212558	1.852647
H	3.016341	-0.547377	-2.384366
H	-4.777424	-2.257269	0.063574
H	-3.813114	-3.687146	-0.353211
H	-4.245734	-2.537557	-1.617053
H	-2.974336	-2.034085	1.897211

H	-1.301217	-1.645270	1.444076
H	-1.917365	-3.280265	1.205497
H	2.127256	3.473645	0.876743
H	2.729030	2.194607	1.957094
H	2.141428	3.721930	2.630025
H	0.517455	2.533185	4.109232
H	1.158358	0.995428	3.514379
H	-0.587310	1.310984	3.480965
H	3.268595	-2.980006	-2.065767
H	4.911042	-2.750658	-1.414958
H	4.561979	-2.344639	-3.100145
H	4.793893	1.037440	-1.455263
H	5.362036	0.062468	-2.816287
H	5.834324	-0.365152	-1.167118
O	-3.318933	2.759006	-1.661130
H	-3.315423	3.121865	-0.763087
H	-2.423205	2.944270	-2.041531
O	-1.988321	-1.579671	-3.556754
H	-2.377026	-2.408738	-3.870579
H	-1.107343	-1.810262	-3.180614
O	0.520332	-1.881063	-2.370850
H	0.547118	-2.464625	-1.578516
H	0.365590	-0.991187	-2.003860
O	-0.839033	2.886064	-2.722116
H	-0.599359	1.986907	-2.430218
H	-0.295446	3.496733	-2.173218
O	0.605578	-3.253787	0.038622
H	1.436317	-3.755191	0.189921
H	0.622149	-2.529054	0.690396
O	-0.612393	-1.340403	3.731976
H	0.026138	-1.086835	3.032715
H	-0.185162	-1.124435	4.574507
O	-2.747643	0.258510	3.073740
H	-2.083935	-0.382638	3.431297
H	-2.897449	0.912771	3.774254
O	-6.505556	1.066927	0.559885
H	-6.014773	0.528416	1.223950
H	-6.033368	1.909081	0.485463
O	-6.264493	-0.412039	-1.713170
H	-6.684327	-1.275249	-1.587237
H	-6.469630	0.116926	-0.904650
O	-5.191243	-0.673624	2.200250
H	-4.354553	-0.381628	2.625745
H	-5.749581	-1.023561	2.910277
O	4.922235	2.737678	0.279704
H	4.771881	1.907116	0.772834
H	4.935936	3.445141	0.941909
O	2.832528	2.796906	-1.454680
H	3.638212	2.913555	-0.892084
H	3.133860	2.799713	-2.376621
O	0.688807	4.453853	-1.064883
H	1.572506	4.054138	-1.219657
H	0.760614	5.388117	-1.309932
O	3.064643	-4.466436	0.517377
H	3.424848	-4.993778	-0.211117
H	3.736895	-3.791861	0.716202

Table S64. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_C.

N	-3.421793	-0.565587	-1.645147
C	-3.024982	-0.268203	-0.243124
C	-1.605995	0.287857	-0.300971
O	-0.894907	0.061528	-1.295671
N	-1.149780	0.971421	0.751345
C	0.228688	1.447037	0.742994
C	1.162936	0.233493	0.706335
O	0.935837	-0.769701	1.403981
N	2.220999	0.327849	-0.108793
C	3.202523	-0.733060	-0.207079
C	4.301927	-0.512072	0.820202
O	4.591755	0.551399	1.322963
O	4.971587	-1.638712	1.090882
C	-3.106020	-1.520839	0.655800
C	0.520067	2.377007	1.941309
C	3.789355	-0.839024	-1.639954
C	-1.977252	-2.515273	0.386082
C	-4.475317	-2.193973	0.545899
C	1.853846	3.097455	1.742104
C	0.512161	1.673277	3.299025
C	4.288634	-2.254916	-1.926099
C	4.882090	0.196758	-1.909711
H	-3.358675	0.315005	-2.204109
H	-4.412875	-0.874257	-1.702018
H	-2.803808	-1.273140	-2.097733
H	-3.719538	0.496505	0.120966
H	-1.758325	1.140530	1.558136
H	0.379320	2.029930	-0.173031
H	2.334713	1.174095	-0.677235
H	2.701342	-1.675538	0.027791
H	5.704822	-1.442734	1.706475
H	-2.991532	-1.153125	1.680181
H	-0.283880	3.125180	1.921434
H	2.933480	-0.644947	-2.297316
H	-2.023746	-2.914887	-0.633273
H	-2.052400	-3.355721	1.082454
H	-0.992987	-2.058987	0.527282
H	-4.598929	-2.697307	-0.420472
H	-5.290933	-1.477175	0.681605
H	-4.566371	-2.957664	1.324097
H	1.876034	3.660939	0.806032
H	2.685779	2.383704	1.739917
H	2.022465	3.799058	2.564586
H	0.617507	2.418896	4.092891
H	1.349495	0.971212	3.381774
H	-0.409353	1.117961	3.482989
H	3.497886	-2.992173	-1.752844
H	5.148749	-2.511587	-1.298473
H	4.604509	-2.329429	-2.971236
H	4.561659	1.214691	-1.667479
H	5.161808	0.175998	-2.966842

H	5.784241	-0.019953	-1.323582
O	-3.265194	1.991821	-2.723384
H	-3.790567	2.181113	-3.514453
H	-2.322789	2.186997	-2.954953
O	-1.768745	-2.383301	-3.093184
H	-2.065937	-3.292515	-3.241567
H	-0.866016	-2.444749	-2.699909
O	0.701700	-2.173605	-1.880984
H	0.833039	-2.735151	-1.083137
H	0.389045	-1.313984	-1.542208
O	-0.593875	2.273782	-3.037881
H	-0.417969	1.466980	-2.519012
H	-0.352692	3.019352	-2.443241
O	1.152576	-3.505451	0.518499
H	2.063751	-3.858396	0.619009
H	1.110813	-2.714844	1.087026
O	-1.139528	-1.274743	3.261335
H	-0.433335	-1.055195	2.614149
H	-0.681713	-1.445649	4.098367
O	-2.894170	0.810713	3.082963
H	-2.338479	0.043745	3.365108
H	-2.843625	1.469802	3.792697
O	-5.972473	1.146752	-0.061994
H	-5.919658	0.907753	0.893922
H	-6.456549	1.983758	-0.112170
O	-6.222478	-0.802977	-1.934032
H	-6.762650	-1.567734	-1.688734
H	-6.371041	-0.120707	-1.240556
O	-5.546058	0.267041	2.482104
H	-4.623038	0.457513	2.761085
H	-6.114417	0.608125	3.188298
O	4.713805	3.169770	0.171178
H	5.598413	3.277108	-0.209537
H	4.720486	2.304180	0.624199
O	3.804866	-4.298154	0.762068
H	3.960895	-4.870822	1.528027
H	4.340979	-3.501234	0.918216
O	2.583521	2.890743	-1.482552
H	2.824608	2.851232	-2.421123
H	3.404561	3.134395	-0.987364
O	0.202750	4.214518	-1.236511
H	0.105213	5.141174	-1.500881
H	1.158517	4.002364	-1.301157

Table S65. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_D.

N	-3.555098	-0.678761	-1.608964
C	-3.012510	-0.454092	-0.242683
C	-1.605289	0.105654	-0.426416
O	-0.906923	-0.252672	-1.388414

N	-1.173866	0.994156	0.469530
C	0.187677	1.508122	0.404656
C	1.154672	0.341314	0.633104
O	0.997410	-0.432109	1.595534
N	2.156775	0.187295	-0.239179
C	3.098749	-0.905521	-0.085432
C	4.049508	-0.606011	1.063588
O	4.351682	0.499094	1.457274
O	4.570868	-1.720648	1.589233
C	-3.093411	-1.756962	0.586463
C	0.380074	2.618543	1.452476
C	3.869021	-1.189545	-1.400207
C	-2.367816	-1.607723	1.920379
C	-2.580066	-2.981016	-0.172493
C	-0.557534	3.791477	1.155630
C	1.834136	3.086020	1.465048
C	4.327288	-2.647118	-1.453568
C	5.043285	-0.235778	-1.624087
H	-3.707865	0.250065	-2.049289
H	-4.459214	-1.191740	-1.563745
H	-2.885397	-1.223404	-2.195857
H	-3.640374	0.307240	0.228921
H	-1.766509	1.267110	1.259856
H	0.363576	1.932040	-0.593245
H	2.291823	0.875514	-0.987069
H	2.533097	-1.804197	0.176180
H	5.215986	-1.482731	2.283698
H	-4.163650	-1.891545	0.793665
H	0.136299	2.193130	2.435477
H	3.125782	-1.042676	-2.193717
H	-1.289726	-1.492453	1.768241
H	-2.526553	-2.502263	2.529643
H	-2.731339	-0.748664	2.488455
H	-1.536443	-2.847912	-0.476100
H	-3.175646	-3.205342	-1.062839
H	-2.625967	-3.855339	0.483952
H	-1.610696	3.493835	1.133787
H	-0.307225	4.229406	0.183096
H	-0.443197	4.560793	1.925811
H	1.959669	3.903672	2.180972
H	2.126139	3.459698	0.476197
H	2.523757	2.283569	1.747978
H	3.477470	-3.328502	-1.340990
H	5.059874	-2.863622	-0.668168
H	4.803346	-2.850134	-2.417544
H	4.748119	0.813853	-1.540167
H	5.461250	-0.389702	-2.622970
H	5.843963	-0.419658	-0.896719
O	-3.475329	2.025087	-2.305141
H	-3.568460	2.630148	-1.554776
H	-2.549847	2.131758	-2.639143
O	-1.805906	-2.275511	-3.274526
H	-2.130673	-3.138708	-3.568785
H	-0.968762	-2.451443	-2.790973
O	0.694475	-2.449147	-1.899961
H	0.697501	-2.865637	-1.009520
H	0.504035	-1.513116	-1.708555

O	-0.917723	1.965908	-3.193608
H	-0.644234	1.170223	-2.701184
H	-0.389118	2.713844	-2.831743
O	0.701311	-3.229863	0.790224
H	1.533182	-3.673618	1.065189
H	0.708395	-2.366492	1.243451
O	-0.547812	0.098191	3.882576
H	-0.002677	-0.101419	3.090220
H	0.058581	0.486625	4.530699
O	-2.593559	1.613823	2.934506
H	-1.898624	1.125895	3.443952
H	-2.600321	2.521783	3.274614
O	-6.009474	0.477653	0.002172
H	-5.777632	0.535214	0.958021
H	-6.647984	1.184500	-0.170756
O	-6.091174	-1.899624	-1.280144
H	-6.218459	-2.717942	-0.779109
H	-6.338551	-1.157159	-0.686212
O	-5.065950	0.391971	2.560188
H	-4.251512	0.890838	2.788279
H	-5.683273	0.531480	3.293310
O	3.176393	-4.271412	1.514219
H	3.557160	-4.910103	0.893394
H	3.810856	-3.535721	1.563148
O	4.662293	2.924587	-0.026591
H	5.596625	2.949818	-0.282365
H	4.562683	2.136832	0.543857
O	2.790501	2.461051	-1.934550
H	3.168335	2.310815	-2.815133
H	3.537041	2.742308	-1.348864
O	0.556406	4.020605	-2.094938
H	0.615397	4.808328	-2.655598
H	1.458695	3.632014	-2.065804

Table S66. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_E.

N	-3.422205	-0.583387	-1.771225
C	-2.829908	-0.534189	-0.408003
C	-1.499559	0.198533	-0.545880
O	-0.805724	0.019318	-1.561203
N	-1.106868	0.975220	0.463269
C	0.250128	1.507853	0.507649
C	1.213696	0.324279	0.651636
O	1.069502	-0.500664	1.573205
N	2.190658	0.202835	-0.250854
C	3.100780	-0.924943	-0.187144
C	4.056437	-0.744593	0.982525
O	4.390801	0.317457	1.460156
O	4.538967	-1.911998	1.421549
C	-2.609309	-1.959747	0.144439

C	0.398315	2.488499	1.681469
C	3.860007	-1.120603	-1.522211
C	-3.883630	-2.797181	0.016969
C	-2.161419	-1.909995	1.604236
C	-0.568183	3.663356	1.519728
C	1.841680	2.984241	1.763068
C	4.318497	-2.570761	-1.676205
C	5.029747	-0.149687	-1.688508
H	-3.420024	0.378599	-2.168018
H	-4.416160	-0.897085	-1.739808
H	-2.868464	-1.224146	-2.379664
H	-3.522517	0.019119	0.238806
H	-1.695025	1.066616	1.299137
H	0.458884	2.039153	-0.429528
H	2.318493	0.931920	-0.959858
H	2.509453	-1.825524	0.004131
H	5.189254	-1.750208	2.132876
H	-1.814616	-2.423231	-0.456311
H	0.159126	1.941331	2.604117
H	3.109623	-0.921218	-2.297832
H	-4.720474	-2.299309	0.522472
H	-3.728571	-3.768711	0.495261
H	-4.164498	-2.987555	-1.023787
H	-2.954626	-1.491663	2.233808
H	-1.256428	-1.312724	1.737754
H	-1.942985	-2.922326	1.955250
H	-1.613348	3.341185	1.473796
H	-0.337791	4.210295	0.598828
H	-0.465449	4.347468	2.367835
H	1.949253	3.699378	2.583751
H	2.119566	3.494052	0.832003
H	2.549777	2.165565	1.934300
H	3.473424	-3.260970	-1.587018
H	5.064909	-2.836120	-0.919728
H	4.775675	-2.710425	-2.660401
H	4.735969	0.892299	-1.532638
H	5.441806	-0.234680	-2.698042
H	5.835239	-0.380527	-0.980176
O	-3.294916	2.163519	-2.282824
H	-3.455429	2.692695	-1.487740
H	-2.377337	2.382972	-2.583032
O	-1.890492	-2.511750	-3.181441
H	-2.251893	-3.409416	-3.208848
H	-0.991402	-2.584897	-2.781848
O	0.605720	-2.356240	-1.997503
H	0.594845	-2.752126	-1.095367
H	0.411970	-1.412457	-1.846477
O	-0.725238	2.411282	-3.083491
H	-0.452732	1.574726	-2.662593
H	-0.255815	3.128875	-2.600108
O	0.595509	-3.225416	0.626996
H	1.431853	-3.706420	0.814454
H	0.651827	-2.398718	1.140717
O	-0.426905	-0.338547	3.927587
H	0.171976	-0.376180	3.150916
H	0.084870	0.063291	4.645379
O	-2.532142	1.080645	2.975380

H	-1.833894	0.570667	3.460161
H	-2.586586	1.946073	3.409934
O	-6.330444	0.861359	0.405438
H	-5.844262	0.577220	1.215164
H	-5.969359	1.724742	0.157446
O	-6.188116	-0.949231	-1.618759
H	-6.612137	-1.785105	-1.376905
H	-6.348526	-0.326807	-0.869337
O	-5.004075	-0.090870	2.590846
H	-4.157604	0.347053	2.832018
H	-5.552348	-0.076187	3.389309
O	2.792805	2.631702	-1.713886
H	3.141569	2.591198	-2.618115
H	3.564898	2.812472	-1.120543
O	0.651278	4.322479	-1.644290
H	1.538107	3.899423	-1.660936
H	0.746616	5.176992	-2.090432
O	4.800505	2.775247	0.093352
H	4.638930	1.987067	0.649183
H	4.792742	3.535363	0.694527
O	3.076551	-4.401633	1.022419
H	3.110431	-5.028023	1.760996
H	3.715758	-3.701370	1.241591

Table S67. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_F.

N	3.332430	-1.003946	1.633751
C	2.979640	-0.453155	0.299954
C	1.580318	0.139245	0.414429
O	0.840663	-0.159089	1.366832
N	1.183612	0.938422	-0.576044
C	-0.172811	1.466582	-0.621451
C	-1.162823	0.298398	-0.686733
O	-1.005812	-0.616308	-1.514045
N	-2.195066	0.330242	0.161678
C	-3.200845	-0.714312	0.161121
C	-4.224420	-0.446735	-0.931887
O	-4.466607	0.634963	-1.420536
O	-4.886978	-1.554019	-1.285391
C	3.039290	-1.518226	-0.816555
C	-0.330361	2.373557	-1.856982
C	-3.878794	-0.840932	1.549109
C	1.883726	-2.514636	-0.730115
C	4.391941	-2.230468	-0.837295
C	0.600069	3.585039	-1.764154
C	-1.779385	2.833500	-2.008783
C	-4.461750	-2.238919	1.753418
C	-4.935078	0.239719	1.787315
H	3.255625	-0.234350	2.335588
H	4.327129	-1.305079	1.651287

H	2.708497	-1.780971	1.941468
H	3.706583	0.340711	0.093049
H	1.816519	1.146990	-1.354821
H	-0.366537	2.050347	0.289250
H	-2.283216	1.122514	0.806745
H	-2.705668	-1.662556	-0.064655
H	-5.571503	-1.325695	-1.944596
H	2.937653	-0.960939	-1.756123
H	-0.056235	1.771163	-2.734858
H	-3.057442	-0.710910	2.264919
H	1.915093	-3.091716	0.201268
H	1.937914	-3.220041	-1.564587
H	0.912259	-2.013959	-0.786587
H	4.515124	-2.885028	0.033922
H	5.221215	-1.517873	-0.868788
H	4.455585	-2.860001	-1.729895
H	1.642159	3.314198	-1.570839
H	0.269236	4.255152	-0.962531
H	0.567837	4.149377	-2.701083
H	-1.866304	3.516242	-2.859168
H	-2.105890	3.373835	-1.112115
H	-2.467378	1.998545	-2.176076
H	-3.699783	-3.008577	1.593675
H	-5.298080	-2.428131	1.072219
H	-4.837409	-2.334053	2.776770
H	-4.553518	1.247159	1.593744
H	-5.278146	0.203973	2.825116
H	-5.809000	0.083160	1.142505
O	3.231323	1.316526	3.185514
H	3.719651	2.030353	2.750095
H	2.296995	1.629780	3.276362
O	1.649672	-3.000718	2.738914
H	1.899880	-3.935020	2.700233
H	0.737226	-2.937927	2.366900
O	-0.797762	-2.432911	1.631080
H	-0.911758	-2.863142	0.751979
H	-0.453036	-1.540229	1.441744
O	0.579409	1.868028	3.313148
H	0.356046	1.183533	2.655965
H	0.349269	2.728858	2.897115
O	-1.225113	-3.437966	-0.914787
H	-2.136887	-3.795355	-0.996285
H	-1.218630	-2.597594	-1.407779
O	0.976528	-0.801292	-3.462328
H	0.283871	-0.717332	-2.769691
H	0.502381	-0.868300	-4.304663
O	2.712049	1.205108	-3.026601
H	2.112579	0.506333	-3.391944
H	2.618323	1.983066	-3.597566
O	5.895823	1.054832	0.074164
H	5.782650	0.908203	-0.895621
H	6.474357	1.825224	0.171355
O	6.138907	-1.088955	1.745561
H	6.704344	-1.800119	1.411629
H	6.242784	-0.334693	1.121249
O	5.323443	0.451067	-2.520103
H	4.426455	0.750449	-2.788082

H	5.928414	0.757269	-3.211558
O	-4.483506	3.230825	-0.245099
H	-5.389091	3.347055	0.079677
H	-4.475470	2.371808	-0.712115
O	-3.866815	-4.267115	-1.000811
H	-4.087196	-4.846447	-1.745598
H	-4.389038	-3.457185	-1.134065
O	-2.510337	2.860406	1.577629
H	-2.856058	2.806258	2.482647
H	-3.268331	3.141129	1.007109
O	-0.221583	4.250444	2.175334
H	0.300250	4.685342	1.486536
H	-1.067859	3.969614	1.767731

Table S68. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_G.

N	-3.706491	-0.515714	-1.466983
C	-3.017608	-0.448349	-0.148121
C	-1.609146	0.060420	-0.445037
O	-1.013624	-0.352877	-1.451232
N	-1.064397	0.967165	0.372825
C	0.286141	1.422799	0.086967
C	1.261315	0.278464	0.376805
O	1.023627	-0.580333	1.244696
N	2.385901	0.243330	-0.345046
C	3.342011	-0.825588	-0.131805
C	3.922810	-0.701266	1.269517
O	4.012975	0.329393	1.900015
O	4.381235	-1.869544	1.729281
C	-3.069057	-1.824994	0.551076
C	0.660406	2.724811	0.822219
C	4.455306	-0.811249	-1.208381
C	-2.213604	-1.817846	1.813529
C	-2.669899	-2.984836	-0.362625
C	0.974377	2.540080	2.305778
C	-0.427348	3.779201	0.605151
C	5.074630	-2.199852	-1.370154
C	5.531361	0.241249	-0.934151
H	-3.812187	0.453681	-1.823332
H	-4.651938	-0.946969	-1.363732
H	-3.146104	-1.062961	-2.157464
H	-3.553397	0.282369	0.466988
H	-1.557501	1.266246	1.219329
H	0.336050	1.638451	-0.986691
H	2.582948	0.971562	-1.038421
H	2.810608	-1.782128	-0.193492
H	4.794984	-1.737751	2.604730
H	-4.118577	-1.949630	0.848706
H	1.576638	3.073775	0.331352

H	3.939132	-0.559674	-2.144159
H	-1.152555	-1.713688	1.563798
H	-2.339574	-2.760609	2.354238
H	-2.492959	-1.006129	2.487869
H	-1.651743	-2.856004	-0.744450
H	-3.347734	-3.105729	-1.213204
H	-2.696420	-3.915162	0.213309
H	1.772769	1.807233	2.469740
H	0.090043	2.215173	2.862701
H	1.304691	3.493189	2.729987
H	-0.068945	4.758917	0.934549
H	-1.330901	3.546115	1.180217
H	-0.707222	3.849453	-0.451575
H	4.313308	-2.950095	-1.605861
H	5.593511	-2.511769	-0.457306
H	5.807127	-2.183839	-2.182579
H	5.107081	1.229003	-0.731347
H	6.194420	0.327766	-1.799540
H	6.145422	-0.044389	-0.071209
O	-3.433977	2.232958	-1.943158
H	-3.315122	2.771978	-1.147393
H	-2.571282	2.251525	-2.426841
O	-2.227623	-2.009341	-3.449840
H	-2.605147	-2.817455	-3.825952
H	-1.353268	-2.264052	-3.079960
O	0.440368	-2.450329	-2.502078
H	0.546890	-2.873357	-1.620578
H	0.390500	-1.506656	-2.273967
O	-1.114990	1.861471	-3.289709
H	-0.861689	1.024686	-2.859763
H	-0.408365	2.513403	-3.082256
O	0.749809	-3.263130	0.148435
H	1.606122	-3.702432	0.343483
H	0.776088	-2.417402	0.633712
O	-0.344050	-0.205545	3.697333
H	0.130895	-0.333265	2.847833
H	0.313660	0.151074	4.313188
O	-2.407046	1.401985	2.920988
H	-1.711659	0.873066	3.386620
H	-2.460342	2.257665	3.374134
O	-6.728375	0.576592	0.791266
H	-6.041632	0.514097	1.494503
H	-6.603952	1.435667	0.362520
O	-6.296376	-1.444810	-0.976744
H	-6.433027	-2.311852	-0.568269
H	-6.556290	-0.770157	-0.303532
O	-4.852340	0.103984	2.717201
H	-4.033033	0.618976	2.884322
H	-5.242669	-0.071421	3.585909
O	3.963906	2.983502	0.839425
H	3.941335	2.085119	1.228337
H	4.845173	3.334578	1.038531
O	3.269071	-4.342303	0.666016
H	3.238128	-5.116437	1.248158
H	3.790944	-3.674641	1.144125
O	3.127087	2.663171	-1.723457
H	3.821187	2.695798	-2.399891

H	3.542338	2.943356	-0.871594
O	0.817416	3.742487	-2.736262
H	1.668804	3.472701	-2.328006
H	0.592435	4.608657	-2.368108

Table S69. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_H.

N	-3.747096	-0.357777	-1.505753
C	-2.916384	-0.499081	-0.278249
C	-1.574852	0.152671	-0.602178
O	-1.071909	-0.028058	-1.723888
N	-0.979762	0.886352	0.341327
C	0.368122	1.382891	0.116312
C	1.351517	0.221422	0.289475
O	1.109212	-0.723612	1.062033
N	2.485445	0.263749	-0.414229
C	3.434878	-0.826973	-0.295648
C	3.952907	-0.877192	1.135318
O	4.057680	0.078038	1.873718
O	4.334911	-2.107253	1.490159
C	-2.733080	-1.988178	0.082026
C	0.719019	2.586146	1.016386
C	4.593008	-0.681746	-1.312495
C	-4.079783	-2.713650	0.109251
C	-2.031120	-2.126464	1.430560
C	1.048974	2.204879	2.459433
C	-0.397623	3.630257	0.952404
C	5.271969	-2.029031	-1.562082
C	5.616654	0.377651	-0.900459
H	-3.722106	0.636119	-1.805940
H	-4.746132	-0.595684	-1.320434
H	-3.378899	-0.976185	-2.259344
H	-3.428572	0.027330	0.535468
H	-1.412645	0.961738	1.267741
H	0.422066	1.726046	-0.922017
H	2.692110	1.064202	-1.019358
H	2.909077	-1.768276	-0.496235
H	4.707247	-2.087479	2.393408
H	-2.099326	-2.434216	-0.696418
H	1.621190	3.020774	0.569308
H	4.109019	-0.367253	-2.246434
H	-4.767257	-2.209074	0.799163
H	-3.932752	-3.738507	0.463153
H	-4.548086	-2.774730	-0.878616
H	-2.673533	-1.754853	2.236109
H	-1.086320	-1.579158	1.453934
H	-1.809869	-3.179353	1.626883
H	1.886608	1.500365	2.519846
H	0.188063	1.749049	2.959154

H	1.320564	3.102668	3.023967
H	-0.059420	4.567549	1.404077
H	-1.286345	3.297635	1.500842
H	-0.693713	3.831018	-0.082809
H	4.552088	-2.785300	-1.888975
H	5.768205	-2.396959	-0.657409
H	6.034063	-1.917178	-2.338956
H	5.152429	1.332424	-0.638538
H	6.314129	0.556388	-1.723731
H	6.201238	0.041327	-0.035628
O	-3.385737	2.418302	-1.682723
H	-3.306855	2.829606	-0.809391
H	-2.534074	2.593666	-2.154683
O	-2.734815	-2.317732	-3.298963
H	-3.220551	-3.154407	-3.328543
H	-1.802460	-2.542171	-3.066816
O	-0.077277	-2.487998	-2.607360
H	0.173851	-2.899532	-1.748293
H	-0.155203	-1.540691	-2.391233
O	-1.072352	2.479930	-3.077525
H	-0.807705	1.579357	-2.815213
H	-0.363297	3.087448	-2.769570
O	0.626585	-3.335630	-0.073870
H	1.515951	-3.750195	-0.044790
H	0.723113	-2.495192	0.411581
O	-0.076532	-0.823598	3.619902
H	0.433876	-0.770057	2.785204
H	0.515196	-0.501795	4.316501
O	-2.200066	0.760954	2.983864
H	-1.503100	0.169033	3.365365
H	-2.222810	1.552906	3.543773
O	-6.350132	1.201313	1.081632
H	-5.746298	0.757711	1.722599
H	-5.914953	2.026352	0.821668
O	-6.484524	-0.563117	-0.986089
H	-6.903008	-1.383617	-0.687946
H	-6.545384	0.070807	-0.230643
O	-4.744942	-0.276098	2.719407
H	-3.856649	0.083851	2.937149
H	-5.163002	-0.497530	3.564719
O	4.185324	2.811522	1.066683
H	4.076684	1.899534	1.405197
H	3.920329	3.407314	1.783182
O	0.905745	4.200423	-2.227605
H	0.719290	4.975671	-1.679124
H	1.748181	3.817348	-1.898907
O	3.227797	-4.346523	0.011906
H	3.754432	-3.805062	0.625037
H	3.283632	-5.254383	0.345930
O	3.179318	2.862785	-1.458787
H	3.863633	3.003913	-2.131526
H	3.602423	3.032627	-0.583126

Table S70. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_I.

N	3.473214	-1.009154	1.488963
C	2.998453	-0.463778	0.190094
C	1.604388	0.098698	0.445553
O	0.958907	-0.282697	1.436473
N	1.100966	0.966249	-0.434283
C	-0.246666	1.471229	-0.221734
C	-1.241310	0.318284	-0.379479
O	-1.045697	-0.608969	-1.183322
N	-2.343663	0.374871	0.375317
C	-3.369445	-0.640989	0.250890
C	-4.050686	-0.496954	-1.103563
O	-4.078507	0.516333	-1.767414
O	-4.671914	-1.617735	-1.482377
C	2.984288	-1.530279	-0.924725
C	-0.597960	2.653691	-1.149970
C	-4.391349	-0.540594	1.410336
C	1.861348	-2.551581	-0.746078
C	4.346317	-2.214538	-1.051657
C	-0.916733	2.237746	-2.586812
C	0.499121	3.720038	-1.097702
C	-5.120507	-1.866471	1.627561
C	-5.384937	0.606851	1.216681
H	3.449235	-0.236078	2.188988
H	4.465068	-1.317228	1.429609
H	2.871149	-1.781420	1.848685
H	3.689134	0.341658	-0.084294
H	1.644490	1.250252	-1.254720
H	-0.304246	1.835851	0.810523
H	-2.480794	1.165546	1.012804
H	-2.892079	-1.627286	0.289923
H	-5.135214	-1.460894	-2.328525
H	2.794981	-0.978223	-1.852398
H	-1.507411	3.089462	-0.720295
H	-3.780587	-0.340782	2.300420
H	1.984102	-3.130821	0.176215
H	1.864255	-3.251904	-1.586688
H	0.877408	-2.074067	-0.718112
H	4.540531	-2.881709	-0.203289
H	5.158328	-1.484825	-1.124691
H	4.360761	-2.827647	-1.957680
H	-1.781467	1.567504	-2.638339
H	-0.067584	1.730535	-3.057273
H	-1.144900	3.128222	-3.180766
H	0.148160	4.629586	-1.594751
H	1.406065	3.392571	-1.618390
H	0.756198	3.966265	-0.063224
H	-4.415420	-2.691801	1.768521
H	-5.769861	-2.107436	0.779367
H	-5.750491	-1.795670	2.519178
H	-4.889562	1.556361	0.991481
H	-5.978318	0.742535	2.125201
H	-6.078665	0.387269	0.395604

O	3.385863	1.353855	2.987522
H	3.723078	2.107611	2.481762
H	2.449607	1.570541	3.222159
O	1.851328	-3.001548	2.710544
H	2.099435	-3.937016	2.693469
H	0.916144	-2.954039	2.399483
O	-0.704452	-2.498326	1.782976
H	-0.888182	-2.922165	0.912645
H	-0.375379	-1.606536	1.565770
O	0.730551	1.630063	3.510315
H	0.512610	0.914070	2.885868
H	0.374791	2.453589	3.105324
O	-1.309237	-3.438076	-0.744217
H	-2.227270	-3.787776	-0.746371
H	-1.347376	-2.561203	-1.167655
O	0.781256	-0.765252	-3.300975
H	0.159747	-0.679329	-2.544264
H	0.227041	-0.774082	-4.096015
O	2.542804	1.251641	-2.936156
H	1.946674	0.539169	-3.278979
H	2.453754	2.005570	-3.539496
O	6.239016	0.995466	-0.133388
H	5.866945	0.935603	-1.044549
H	5.967175	1.851348	0.227407
O	6.268538	-1.199522	1.490681
H	6.793930	-1.917062	1.108537
H	6.392269	-0.420664	0.901131
O	5.207284	0.580527	-2.620891
H	4.273473	0.833113	-2.794555
H	5.726751	0.960340	-3.344735
O	-3.871023	3.202553	-0.849163
H	-3.897746	2.285952	-1.192219
H	-4.770782	3.548061	-0.952129
O	-3.948009	-4.271219	-0.568081
H	-4.188133	-5.038174	-1.109454
H	-4.458956	-3.524558	-0.924178
O	-2.755105	2.959191	1.617535
H	-3.365915	3.069130	2.362781
H	-3.245853	3.229391	0.803821
O	-0.235998	3.875924	2.223675
H	-1.184493	3.725682	2.017860
H	-0.190994	4.708053	2.717256

Table S71. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_J.

N	-3.649415	0.263203	-1.583539
C	-3.086824	-0.166900	-0.272708
C	-1.632567	0.299236	-0.281307
O	-0.952537	0.152266	-1.306670
N	-1.136118	0.892169	0.811096

C	0.243123	1.353879	0.769797
C	1.160431	0.131330	0.672102
O	0.911557	-0.918961	1.290995
N	2.245925	0.241046	-0.101089
C	3.204912	-0.848362	-0.169717
C	3.809089	-1.057608	1.212589
O	4.181338	-0.158581	1.937103
O	3.935128	-2.346026	1.536163
C	-3.271537	-1.689414	-0.084353
C	0.582476	2.277169	1.959637
C	4.313191	-0.546581	-1.197921
C	-2.511130	-2.168476	1.147166
C	-2.874241	-2.510555	-1.311795
C	1.889731	3.023078	1.696348
C	0.656240	1.560640	3.306772
C	3.704464	-0.440027	-2.596736
C	5.394537	-1.628564	-1.162194
H	-3.653162	1.300792	-1.610371
H	-4.624629	-0.093459	-1.697497
H	-3.059911	-0.078619	-2.375566
H	-3.639672	0.359573	0.512545
H	-1.693498	0.960071	1.667736
H	0.365482	1.940868	-0.149760
H	2.470027	1.122104	-0.574153
H	2.689003	-1.768006	-0.468970
H	4.382218	-2.424564	2.401479
H	-4.345392	-1.823004	0.101316
H	-0.234562	3.010348	1.989910
H	4.768745	0.413176	-0.920248
H	-1.430947	-2.046990	1.009750
H	-2.706444	-3.231349	1.317813
H	-2.810497	-1.625539	2.044498
H	-1.821597	-2.353448	-1.567444
H	-3.484591	-2.281638	-2.190925
H	-3.010982	-3.572580	-1.085467
H	1.870268	3.553234	0.739482
H	2.739339	2.332221	1.692244
H	2.066984	3.756719	2.488001
H	0.845703	2.292463	4.097758
H	1.476281	0.832470	3.319518
H	-0.269568	1.037770	3.552227
H	2.923907	0.325538	-2.659387
H	3.257082	-1.396912	-2.888835
H	4.482829	-0.186412	-3.322903
H	5.928112	-1.651367	-0.206275
H	6.131153	-1.436645	-1.947339
H	4.957397	-2.618398	-1.336892
O	-3.037770	2.977921	-1.209548
H	-2.819940	3.220891	-0.297522
H	-2.187724	3.007626	-1.715206
O	-2.064586	-0.612141	-3.823452
H	-2.455275	-1.207497	-4.479264
H	-1.266490	-1.072350	-3.479213
O	0.420383	-1.655572	-2.888710
H	0.410622	-2.289953	-2.136227
H	0.508994	-0.802432	-2.432068
O	-0.789609	2.659898	-2.684926

H	-0.617702	1.744394	-2.399374
H	-0.025004	3.201683	-2.384806
O	0.513741	-3.152642	-0.541546
H	1.363330	-3.643154	-0.506301
H	0.581852	-2.478751	0.160836
O	-0.747987	-1.417638	3.550378
H	-0.179073	-1.236611	2.771237
H	-0.165131	-1.348999	4.321495
O	-2.714123	0.469386	3.237353
H	-2.076437	-0.227657	3.530539
H	-2.764011	1.122142	3.952760
O	-6.879123	0.625706	0.715867
H	-6.250831	0.292913	1.397890
H	-6.729386	1.579697	0.647881
O	-6.302750	-0.605565	-1.635984
H	-6.487626	-1.554921	-1.591957
H	-6.611171	-0.217079	-0.781213
O	-5.177623	-0.558676	2.487551
H	-4.353339	-0.167011	2.850783
H	-5.638271	-0.960971	3.238322
O	5.073032	2.373441	0.930022
H	6.020729	2.314411	0.736540
H	4.825395	1.516750	1.331542
O	3.066673	-4.268671	-0.439883
H	3.134105	-5.233447	-0.380438
H	3.499983	-3.919051	0.357776
O	3.404367	2.679071	-1.210328
H	3.922860	2.585214	-2.024939
H	4.061585	2.714976	-0.472630
O	1.268934	4.290319	-1.867014
H	1.057788	4.987096	-1.229567
H	2.084603	3.847397	-1.549471

Table S72. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 14H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $14H_2O$_PPII-PPII_S.

C	-3.094378	-0.130949	-0.234042
C	-1.625321	0.285506	-0.299736
O	-0.984957	0.109958	-1.347800
N	-1.080063	0.872214	0.769089
C	0.308250	1.307828	0.706902
C	1.202684	0.063484	0.639805
O	0.899504	-0.967862	1.265693
N	2.311504	0.121957	-0.112308
C	3.178530	-1.042102	-0.157269
C	3.937494	-1.157232	1.154324
O	4.209873	-0.233823	1.890771
O	4.330086	-2.413336	1.387811
C	-3.333548	-1.634142	0.036186
C	0.643538	2.245109	1.890840
C	4.165465	-1.082419	-1.349356

C	-2.545120	-2.087336	1.259258
C	-3.021473	-2.530675	-1.162138
C	1.865589	3.100195	1.571407
C	0.854986	1.518679	3.218427
C	5.391362	-0.185409	-1.179126
C	3.425889	-0.801004	-2.656784
H	-3.637926	1.293948	-1.631866
H	-4.676592	-0.053825	-1.604103
H	-3.141532	-0.152786	-2.338933
H	-3.605383	0.451384	0.540263
H	-1.611191	0.962170	1.640851
H	0.436185	1.874565	-0.224475
H	2.571198	0.983966	-0.601186
H	2.537834	-1.922311	-0.250124
H	4.867197	-2.445788	2.202891
H	-4.403454	-1.711352	0.269466
H	-0.226781	2.908771	1.981891
H	4.510952	-2.123004	-1.375838
H	-1.467343	-2.023874	1.072738
H	-2.781882	-3.129548	1.492994
H	-2.780612	-1.486469	2.138144
H	-1.976864	-2.426831	-1.472435
H	-3.661452	-2.324036	-2.025539
H	-3.185264	-3.574001	-0.875144
H	1.737267	3.661181	0.641602
H	2.761401	2.478863	1.483098
H	2.043324	3.815331	2.380030
H	1.021441	2.253249	4.012027
H	1.736165	0.867102	3.171783
H	-0.003928	0.909262	3.501994
H	5.991872	-0.467827	-0.307031
H	5.111386	0.865281	-1.070036
H	6.031684	-0.271879	-2.061953
H	2.552734	-1.451249	-2.769756
H	4.098396	-0.971950	-3.502800
H	3.082983	0.239002	-2.710572
O	-3.002942	2.973531	-1.425650
H	-2.795651	3.308289	-0.540808
H	-2.146263	2.945778	-1.921264
O	-2.267048	-0.822982	-3.811618
H	-2.756277	-1.398519	-4.417158
H	-1.500003	-1.349969	-3.495889
O	0.147117	-1.929962	-2.821972
H	0.219381	-2.573728	-2.083029
H	0.162869	-1.078230	-2.351101
O	-0.733450	2.530679	-2.830137
H	-0.572931	1.637287	-2.475891
H	0.013728	3.096159	-2.530046
O	0.442946	-3.330853	-0.416770
H	1.319968	-3.769224	-0.388551
H	0.503461	-2.602475	0.229113
O	-0.686923	-1.417715	3.588333
H	-0.136912	-1.272544	2.788737
H	-0.071388	-1.398673	4.336513
O	-2.532306	0.598687	3.292481
H	-1.931024	-0.126448	3.592417
H	-2.498664	1.289965	3.971675

O	-6.820587	0.858623	0.885257
H	-6.169345	0.540085	1.551911
H	-6.658608	1.806705	0.775728
O	-6.373123	-0.480505	-1.436808
H	-6.598980	-1.417603	-1.346060
H	-6.631398	-0.044078	-0.588566
O	-5.067164	-0.304274	2.621434
H	-4.220490	0.056639	2.963743
H	-5.506842	-0.722025	3.376228
O	5.025143	2.408119	1.005769
H	5.981642	2.404762	0.849377
H	4.808130	1.521778	1.356198
O	3.073453	-4.299505	-0.414829
H	3.200037	-5.259071	-0.459508
H	3.617962	-3.991106	0.329830
O	3.381899	2.651412	-1.200894
H	3.924088	2.639758	-2.005467
H	4.014710	2.744328	-0.448894
O	1.266323	4.226068	-2.002144
H	1.009102	4.949468	-1.413003
H	2.053667	3.796752	-1.604860

Table S73. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_A.

N	-4.497630	-1.020185	0.291873
C	-3.607816	0.174903	0.324713
C	-2.262398	-0.305529	-0.215779
O	-1.841572	-1.419798	0.130422
N	-1.577675	0.464749	-1.068194
C	-0.285793	-0.024675	-1.536563
C	0.668900	-0.073322	-0.334827
O	0.677201	0.833462	0.515700
N	1.463910	-1.146384	-0.229708
C	2.389163	-1.254569	0.881840
C	3.577576	-0.328326	0.665925
O	3.929218	0.073622	-0.439182
O	4.208020	-0.034607	1.776823
C	-3.553299	0.748849	1.760210
C	0.256317	0.793750	-2.726053
C	2.840277	-2.717750	1.134291
C	-2.491913	1.837666	1.867171
C	-3.334145	-0.317740	2.834571
C	1.502833	0.121676	-3.298088
C	0.579597	2.246058	-2.388698
C	3.118892	-2.940889	2.621214
C	4.046569	-3.133260	0.290922
H	-4.660551	-1.283256	-0.700847
H	-5.411884	-0.808000	0.750259
H	-4.048749	-1.830336	0.773090
H	-4.034510	0.926604	-0.347916

H	-1.909223	1.405884	-1.300601
H	-0.433248	-1.054284	-1.887122
H	1.468796	-1.865698	-0.959842
H	1.868759	-0.906870	1.777840
H	5.077273	0.507065	1.609157
H	-4.536790	1.211754	1.915705
H	-0.540306	0.763747	-3.481496
H	1.975529	-3.333835	0.856941
H	-1.493041	1.425270	1.690270
H	-2.500202	2.269445	2.872319
H	-2.663613	2.644777	1.154565
H	-2.388182	-0.846610	2.680460
H	-4.142484	-1.054369	2.874067
H	-3.288365	0.171510	3.812364
H	1.329152	-0.926963	-3.554813
H	2.325525	0.163565	-2.576108
H	1.828682	0.641829	-4.203381
H	0.954919	2.755269	-3.282496
H	1.360290	2.296818	-1.622948
H	-0.286686	2.801560	-2.028040
H	2.244997	-2.685016	3.229034
H	3.965882	-2.333744	2.958685
H	3.366998	-3.991834	2.799020
H	3.892396	-2.950243	-0.775176
H	4.244226	-4.200718	0.425107
H	4.947148	-2.588133	0.601279
O	-4.318662	-1.500853	-2.455529
H	-3.988762	-0.752755	-2.974610
H	-3.586496	-2.166714	-2.427079
O	-3.300889	-3.327609	1.598161
H	-3.723991	-3.736254	2.367068
H	-2.393116	-3.087220	1.884642
O	-0.514832	-2.731593	2.153472
H	-0.315457	-1.922022	2.673570
H	-0.535030	-2.397741	1.239793
O	-2.345366	-3.286649	-1.979553
H	-2.003590	-2.863524	-1.170816
H	-1.630345	-3.222375	-2.653028
O	0.108708	-0.210030	3.217722
H	0.979579	-0.135416	3.666499
H	0.205989	0.312159	2.399990
O	-0.309533	3.526337	0.439893
H	-0.033136	2.587447	0.475096
H	0.465392	3.997440	0.059334
O	-2.501264	3.267474	-1.130336
H	-1.719400	3.530995	-0.573480
H	-2.476564	3.819116	-1.927533
O	-7.058961	1.821338	-0.444719
H	-6.280836	2.413713	-0.322031
H	-7.007619	1.484167	-1.350731
O	-6.951418	-0.212502	1.352598
H	-7.000659	0.105563	2.265725
H	-7.089534	0.573346	0.770156
O	-4.943668	3.431092	0.154991
H	-4.094358	3.460582	-0.339645
H	-5.209743	4.352709	0.287961
O	4.153830	-1.534127	-2.832348

H	5.018532	-1.970692	-2.861594
H	4.169071	-0.958299	-2.042773
O	2.693110	0.004585	4.236386
H	2.817425	0.844092	4.703930
H	3.321324	0.025566	3.490933
O	1.899273	-3.034745	-2.418191
H	2.115223	-3.950497	-2.182227
H	2.747059	-2.608967	-2.694892
O	-0.411264	-3.098435	-3.920250
H	-0.483880	-2.368704	-4.552186
H	0.484663	-3.047573	-3.522645
O	3.943731	2.777557	-1.297153
H	4.051372	2.755439	-2.261032
H	3.906156	1.841652	-1.011756
O	1.995713	4.714837	-0.582784
H	1.841864	5.207407	-1.402384
H	2.654293	4.026691	-0.810631
O	6.046544	3.611850	0.296199
H	6.818037	3.958479	-0.175515
H	5.356406	3.445881	-0.382016
O	6.389178	1.233518	1.503719
H	6.312808	2.116835	1.054387
H	7.029021	0.718182	0.988946

Table S74. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_B.

N	4.432467	-1.077183	-0.447988
C	3.478663	0.066668	-0.411322
C	2.208302	-0.476741	0.237108
O	1.814737	-1.606768	-0.096724
N	1.540083	0.276143	1.115999
C	0.234431	-0.192111	1.573638
C	-0.720901	-0.134930	0.373555
O	-0.754423	0.859799	-0.373270
N	-1.482152	-1.210230	0.141242
C	-2.379277	-1.221908	-0.997917
C	-3.569352	-0.310241	-0.727805
O	-3.940973	-0.003619	0.401002
O	-4.177816	0.086024	-1.818835
C	3.183608	0.552494	-1.847162
C	-0.276559	0.582669	2.804542
C	-2.821413	-2.658770	-1.373918
C	4.479124	0.801801	-2.621793
C	2.329063	1.815649	-1.823576
C	-1.559927	-0.064147	3.322561
C	-0.522029	2.068552	2.558371
C	-3.140389	-2.753643	-2.866313
C	-3.994663	-3.165375	-0.534482
H	4.492357	-1.510413	0.498461
H	5.394103	-0.766085	-0.707037

H	4.096037	-1.786736	-1.133072
H	3.928220	0.868523	0.185668
H	1.853017	1.234597	1.300487
H	0.348090	-1.240162	1.873436
H	-1.469231	-2.003453	0.789913
H	-1.838308	-0.803002	-1.851906
H	-5.044242	0.621422	-1.615497
H	2.618010	-0.247479	-2.343717
H	0.509550	0.466369	3.562314
H	-1.941062	-3.284233	-1.177302
H	5.120266	1.505672	-2.076992
H	4.239649	1.243188	-3.593978
H	5.042077	-0.117778	-2.812011
H	2.898427	2.659443	-1.421795
H	1.430388	1.681215	-1.217253
H	2.009492	2.065969	-2.838671
H	-1.419318	-1.122026	3.557038
H	-2.360056	0.023214	2.578724
H	-1.896451	0.444082	4.231222
H	-0.841660	2.545014	3.490744
H	-1.319341	2.208389	1.821779
H	0.365294	2.595183	2.203977
H	-2.288991	-2.424710	-3.471515
H	-4.012836	-2.142751	-3.123034
H	-3.369334	-3.790328	-3.131306
H	-3.800833	-3.087041	0.538173
H	-4.192417	-4.216055	-0.765542
H	-4.908285	-2.599021	-0.756177
O	4.302252	-1.990044	2.195344
H	4.080101	-1.296603	2.834048
H	3.540761	-2.623398	2.196916
O	3.369044	-2.777809	-2.483970
H	3.765971	-2.753887	-3.366451
H	2.405569	-2.612248	-2.607766
O	0.610306	-2.300297	-2.508084
H	0.364457	-1.414484	-2.860685
H	0.697232	-2.151942	-1.548833
O	2.171125	-3.622028	1.855950
H	1.846783	-3.107356	1.093671
H	1.529242	-3.452362	2.583110
O	-0.108551	0.287554	-3.182866
H	-0.977743	0.355476	-3.635904
H	-0.248904	0.685119	-2.303624
O	0.156505	3.560466	-0.245309
H	-0.166427	2.637748	-0.290009
H	-0.548086	4.037751	0.247152
O	2.462583	3.088138	1.097050
H	1.663581	3.405411	0.594612
H	2.471159	3.580617	1.932706
O	6.876598	1.824982	1.015647
H	6.156577	2.415341	0.689493
H	6.603208	1.521798	1.893478
O	7.084933	-0.241807	-0.735803
H	7.434317	0.079569	-1.579547
H	7.095971	0.530517	-0.118957
O	4.935343	3.392699	-0.080444
H	4.046357	3.374733	0.341207

H	5.190456	4.325663	-0.132173
O	-4.142342	-1.774629	2.662895
H	-4.138447	-1.149841	1.910803
H	-4.995615	-2.232458	2.624007
O	-1.852410	-3.213082	2.237197
H	-2.714077	-2.811096	2.507575
H	-2.041781	-4.130195	1.984910
O	0.368762	-2.976008	3.828065
H	-0.505425	-3.154987	3.417508
H	0.413286	-3.518975	4.628866
O	-2.673100	0.457870	-4.240139
H	-2.896874	-0.196290	-4.918633
H	-3.308783	0.319747	-3.514200
O	-6.047789	3.552837	0.054677
H	-5.364969	3.323345	0.721369
H	-6.834286	3.826741	0.548942
O	-2.026749	4.635582	1.107762
H	-2.687147	3.921424	1.224714
H	-2.483845	5.337208	0.621182
O	-3.932758	2.589206	1.558886
H	-3.886796	1.696501	1.159563
H	-4.042971	2.448657	2.512498
O	-6.347345	1.350591	-1.461850
H	-7.012896	0.779888	-1.047950
H	-6.280890	2.163678	-0.893869

Table S75. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_C.

N	-4.274726	-0.936550	1.051746
C	-3.574391	0.164335	0.339595
C	-2.249817	-0.415690	-0.149368
O	-1.781503	-1.426411	0.400424
N	-1.605320	0.214255	-1.134648
C	-0.301105	-0.281816	-1.559108
C	0.679813	-0.146226	-0.385148
O	0.672484	0.862859	0.339688
N	1.521603	-1.166277	-0.180370
C	2.499597	-1.115140	0.889159
C	3.699734	-0.281593	0.460531
O	3.942787	0.003149	-0.708819
O	4.465831	0.079964	1.460562
C	-3.355424	1.395896	1.244821
C	0.182566	0.437749	-2.837088
C	2.916175	-2.533782	1.356043
C	-2.260007	1.175118	2.286700
C	-4.663732	1.841052	1.900945
C	1.430425	-0.244423	-3.393818
C	0.466144	1.925559	-2.640095
C	3.338052	-2.527760	2.825441
C	4.006622	-3.150843	0.478904

H	-4.402324	-1.726394	0.381692
H	-5.230082	-0.652761	1.351082
H	-3.734619	-1.295124	1.869598
H	-4.205435	0.444156	-0.511612
H	-2.008817	1.056999	-1.555272
H	-0.405084	-1.349481	-1.793282
H	1.505144	-1.975221	-0.809922
H	2.037528	-0.605625	1.739399
H	5.320428	0.575994	1.137878
H	-3.025722	2.195045	0.572928
H	-0.635852	0.317564	-3.559921
H	2.000819	-3.133204	1.271040
H	-2.521124	0.374482	2.988009
H	-2.109862	2.092962	2.862938
H	-1.303954	0.917235	1.821980
H	-4.979085	1.138980	2.681847
H	-5.469659	1.944691	1.168202
H	-4.515548	2.814102	2.378573
H	1.279971	-1.313763	-3.565515
H	2.272833	-0.123067	-2.704235
H	1.712192	0.213460	-4.346418
H	0.770896	2.367898	-3.594071
H	1.281248	2.070989	-1.924930
H	-0.398745	2.480700	-2.275927
H	2.558192	-2.089403	3.456601
H	4.264060	-1.961916	2.969815
H	3.517135	-3.553861	3.161466
H	3.741958	-3.140907	-0.581737
H	4.180778	-4.189963	0.772776
H	4.954376	-2.609789	0.595985
O	-4.522311	-2.749776	-1.058932
H	-4.746285	-2.309678	-1.891796
H	-3.646807	-3.189454	-1.199612
O	-2.893847	-2.122591	3.237064
H	-3.160778	-1.927236	4.146730
H	-1.921539	-1.962034	3.189543
O	-0.218793	-1.668139	2.721735
H	0.103104	-0.781222	3.003484
H	-0.480256	-1.559812	1.788602
O	-2.024389	-3.792608	-1.125587
H	-1.670278	-3.094853	-0.544084
H	-1.580927	-3.671138	-1.994657
O	0.807934	0.864442	3.240855
H	1.723294	0.838249	3.598472
H	0.890657	1.155802	2.314528
O	-0.778605	3.271173	0.127015
H	-0.419038	2.362187	0.203554
H	0.005233	3.794044	-0.154718
O	-2.725795	2.867961	-1.691071
H	-2.035020	3.209168	-1.061599
H	-2.582543	3.320054	-2.536911
O	-6.799388	0.813984	-1.093545
H	-6.292337	1.656957	-1.164409
H	-6.603820	0.298141	-1.888616
O	-7.025354	-0.450439	1.312818
H	-7.444962	0.113054	1.978650
H	-7.086705	0.035885	0.458986

O	-5.394192	3.146669	-1.047901
H	-4.437491	3.101810	-1.272335
H	-5.763944	3.853624	-1.597088
O	4.042382	-1.953083	-2.831553
H	4.886399	-2.427206	-2.786947
H	4.087050	-1.261490	-2.142551
O	3.435943	0.643277	4.083130
H	3.802899	1.473448	4.422095
H	3.926200	0.455103	3.261917
O	1.741889	-3.287876	-2.189185
H	1.919448	-4.184600	-1.864363
H	2.599064	-2.940164	-2.537006
O	-0.668784	-3.496925	-3.509619
H	-0.868552	-2.802536	-4.153853
H	0.264768	-3.378793	-3.232678
O	3.705323	2.725307	-1.529796
H	3.731933	2.761778	-2.499006
H	3.772578	1.776643	-1.298292
O	1.644626	4.468587	-0.584433
H	1.618909	5.143339	-1.278397
H	2.321723	3.823277	-0.873049
O	5.908118	3.693354	-0.156237
H	6.561947	4.154961	-0.701428
H	5.146040	3.493770	-0.742303
O	6.596857	1.278381	0.790783
H	6.416970	2.184725	0.423567
H	7.082935	0.794739	0.105245

Table S76. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_D.

N	4.460908	-1.203137	0.010874
C	3.572188	-0.137512	-0.524794
C	2.264547	-0.241548	0.253488
O	1.847307	-1.346737	0.635902
N	1.611954	0.891254	0.513430
C	0.312560	0.863067	1.171030
C	-0.669829	0.111561	0.264517
O	-0.748827	0.383473	-0.946885
N	-1.419714	-0.844482	0.823905
C	-2.355641	-1.602502	0.014311
C	-3.558358	-0.741175	-0.346584
O	-3.926642	0.216141	0.327484
O	-4.185363	-1.148057	-1.422008
C	3.431906	-0.277328	-2.058349
C	-0.153286	2.301542	1.457687
C	-2.783220	-2.918099	0.712133
C	2.373904	0.676221	-2.607148
C	3.144674	-1.711587	-2.503505
C	0.814107	2.988119	2.424795
C	-1.569394	2.296839	2.027117

C	-3.188927	-3.970447	-0.319831
C	-3.889337	-2.713905	1.748070
H	4.715399	-0.946996	0.984950
H	5.324681	-1.283775	-0.563473
H	3.975133	-2.127059	0.023768
H	4.048385	0.820575	-0.297423
H	1.972537	1.789071	0.174214
H	0.403295	0.325436	2.124686
H	-1.373540	-1.003314	1.835267
H	-1.853484	-1.867185	-0.920711
H	-5.055167	-0.608745	-1.604219
H	4.407560	0.030050	-2.458403
H	-0.161765	2.841191	0.501915
H	-1.876416	-3.274548	1.217194
H	1.375039	0.389249	-2.262324
H	2.375355	0.637924	-3.700352
H	2.561893	1.710117	-2.308654
H	2.219510	-2.086320	-2.053489
H	3.957300	-2.400967	-2.254357
H	3.016923	-1.731084	-3.590166
H	1.842087	3.006424	2.048809
H	0.812908	2.464074	3.386881
H	0.499706	4.023768	2.589306
H	-1.889768	3.317608	2.259222
H	-1.610936	1.716221	2.956595
H	-2.291386	1.870580	1.322702
H	-2.381100	-4.144947	-1.038317
H	-4.087808	-3.664116	-0.865974
H	-3.410336	-4.916665	0.183126
H	-3.634466	-1.943102	2.480264
H	-4.069043	-3.646891	2.289902
H	-4.830790	-2.423225	1.264760
O	4.517429	-0.127828	2.592412
H	4.391018	0.831686	2.627840
H	3.717642	-0.530714	3.013404
O	3.232545	-3.823331	-0.000583
H	3.624472	-4.500606	-0.570482
H	2.294190	-3.742103	-0.281771
O	0.455330	-3.429624	-0.529015
H	0.220449	-3.009345	-1.386383
H	0.575624	-2.668062	0.066464
O	2.288482	-1.408283	3.455673
H	1.907914	-1.563393	2.571489
H	1.679866	-0.786545	3.916922
O	-0.257485	-1.869676	-2.737869
H	-1.133388	-2.117910	-3.107350
H	-0.395335	-1.004209	-2.309589
O	0.063480	2.887457	-2.019203
H	-0.138904	1.978321	-1.715477
H	-0.685373	3.428676	-1.680641
O	2.317198	3.451879	-0.669376
H	1.494968	3.379847	-1.227935
H	2.225504	4.260901	-0.143024
O	6.396266	1.247343	-0.370573
H	5.917795	1.965669	-0.845841
H	7.055627	1.678882	0.191731
O	6.825748	-1.145965	-1.550490

H	6.818325	-1.219768	-2.515620
H	6.904851	-0.190568	-1.335914
O	4.805158	2.947491	-1.789219
H	3.951464	3.250982	-1.409029
H	5.201329	3.719794	-2.218625
O	-2.834872	-2.508681	-3.553409
H	-3.028832	-3.456693	-3.596666
H	-3.427815	-2.142755	-2.871926
O	-3.947863	0.522491	3.163952
H	-4.793557	0.163221	3.472069
H	-3.963509	0.445062	2.188954
O	-1.659889	-0.834898	3.725320
H	-1.818451	-1.669081	4.193997
H	-2.526519	-0.359190	3.692427
O	0.587953	0.388780	4.677254
H	0.683602	0.421764	5.640642
H	-0.303421	0.014714	4.499886
O	-5.766588	2.569696	-2.721302
H	-5.300809	2.893762	-1.920336
H	-6.507444	3.174084	-2.875112
O	-4.370600	2.901982	-0.355237
H	-4.271381	1.955053	-0.124762
H	-4.871291	3.300874	0.373549
O	-2.018711	4.318961	-0.893580
H	-2.817865	3.800773	-0.658457
H	-1.779583	4.820188	-0.100475
O	-6.343494	0.063262	-1.959799
H	-6.938337	0.115164	-1.195836
H	-6.204423	0.996245	-2.274490

Table S77. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_E.

N	4.359192	-1.381306	0.064783
C	3.429336	-0.378306	-0.519900
C	2.200190	-0.361916	0.382528
O	1.791304	-1.426762	0.876042
N	1.579073	0.800976	0.572616
C	0.273044	0.847854	1.219834
C	-0.720351	0.100777	0.321958
O	-0.819893	0.388462	-0.885189
N	-1.452042	-0.873219	0.869356
C	-2.371255	-1.630585	0.040296
C	-3.556531	-0.758655	-0.353550
O	-3.929218	0.207693	0.305144
O	-4.160847	-1.164360	-1.441682
C	3.040010	-0.767608	-1.962626
C	-0.152868	2.309075	1.435231
C	-2.817720	-2.940690	0.731757
C	4.284795	-1.066054	-2.800902
C	2.222754	0.343947	-2.619988

C	0.840151	3.024366	2.353202
C	-1.564157	2.360069	2.015984
C	-3.257966	-3.977516	-0.301877
C	-3.903127	-2.716772	1.785063
H	4.479271	-1.164164	1.074145
H	5.303310	-1.321957	-0.373917
H	3.971585	-2.342385	-0.053569
H	3.939220	0.593299	-0.514966
H	1.925921	1.650336	0.112039
H	0.334950	0.346811	2.194357
H	-1.398226	-1.047022	1.877460
H	-1.847501	-1.899439	-0.882624
H	-5.017934	-0.614763	-1.650822
H	2.423329	-1.674943	-1.900683
H	-0.160170	2.798031	0.451827
H	-1.911483	-3.318716	1.222515
H	4.966548	-0.206529	-2.791385
H	3.988492	-1.252325	-3.837333
H	4.828830	-1.950280	-2.453894
H	2.828387	1.250580	-2.727637
H	1.324563	0.587078	-2.047322
H	1.903053	0.023411	-3.615400
H	1.860748	3.009002	1.956937
H	0.848704	2.545134	3.338354
H	0.543792	4.071085	2.475473
H	-1.866305	3.396611	2.196906
H	-1.607690	1.829064	2.974578
H	-2.299697	1.909705	1.340656
H	-2.469217	-4.155290	-1.040112
H	-4.161227	-3.654722	-0.830178
H	-3.481731	-4.924637	0.198283
H	-3.615162	-1.962684	2.522844
H	-4.102815	-3.650216	2.319043
H	-4.842091	-2.392622	1.318556
O	4.380231	-0.227618	2.619067
H	4.299935	0.737324	2.591617
H	3.590525	-0.557459	3.116728
O	3.203545	-3.902393	-0.527590
H	3.535042	-4.363035	-1.311824
H	2.228861	-3.808784	-0.649630
O	0.484576	-3.394115	-0.615361
H	0.251744	-2.887428	-1.427954
H	0.649790	-2.705455	0.054953
O	2.151409	-1.325796	3.686742
H	1.759552	-1.517971	2.814532
H	1.571267	-0.652070	4.109513
O	-0.206973	-1.770043	-2.738255
H	-1.077636	-2.062118	-3.089666
H	-0.379841	-0.917622	-2.297036
O	-0.082500	2.810326	-2.124382
H	-0.339059	1.940118	-1.755690
H	-0.751334	3.432244	-1.757699
O	2.269195	3.191912	-0.894536
H	1.429560	3.147375	-1.431748
H	2.229091	4.024894	-0.399370
O	6.622930	1.784409	-0.323479
H	5.923267	2.178668	-0.896025

H	6.371843	1.977164	0.591368
O	6.973840	-0.873368	-0.775312
H	7.292205	-1.036283	-1.674867
H	6.943774	0.107203	-0.662761
O	4.728751	2.729358	-2.042176
H	3.853626	2.997976	-1.681965
H	5.046350	3.477707	-2.568694
O	-1.686618	-0.766644	3.769076
H	-1.844878	-1.573765	4.282987
H	-2.556872	-0.301008	3.697078
O	0.471068	0.580332	4.760962
H	-0.402259	0.172841	4.567623
H	0.524326	0.669698	5.723998
O	-3.970717	0.552521	3.126735
H	-3.973839	0.447911	2.153924
H	-4.814551	0.188884	3.434912
O	-2.741971	-2.609453	-3.478985
H	-3.008553	-2.330728	-4.367846
H	-3.356632	-2.162939	-2.867834
O	-5.658106	2.571291	-2.796898
H	-5.214737	2.893136	-1.982416
H	-6.387717	3.182581	-2.975332
O	-6.285739	0.072143	-2.051016
H	-6.126376	1.003417	-2.361099
H	-6.907026	0.130379	-1.308901
O	-4.333941	2.901552	-0.389419
H	-4.865774	3.287539	0.324111
H	-4.233161	1.953641	-0.163724
O	-2.011997	4.372065	-0.911891
H	-1.735964	4.838426	-0.109622
H	-2.802021	3.844928	-0.665915

Table S78. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_F.

N	4.211080	-1.397419	-0.804274
C	3.553099	-0.094134	-0.529416
C	2.240835	-0.396711	0.184273
O	1.751924	-1.538424	0.155900
N	1.637129	0.627229	0.785629
C	0.324309	0.481468	1.400176
C	-0.680344	0.029212	0.332205
O	-0.739834	0.609028	-0.765584
N	-1.485224	-0.992728	0.640762
C	-2.471604	-1.467960	-0.311377
C	-3.668758	-0.526961	-0.346084
O	-3.960608	0.228008	0.576942
O	-4.379441	-0.624692	-1.441643
C	3.309850	0.732589	-1.811590
C	-0.095140	1.831354	2.014296
C	-2.895544	-2.925230	-0.005182
C	2.171213	0.168089	-2.660894

C	4.592164	0.888416	-2.629331
C	0.864421	2.242278	3.133189
C	-1.524017	1.768244	2.544813
C	-3.439298	-3.615408	-1.256204
C	-3.892221	-3.018743	1.150891
H	4.308039	-1.909421	0.100498
H	5.179145	-1.246473	-1.151380
H	3.674594	-2.006214	-1.459536
H	4.225677	0.454704	0.140066
H	2.059739	1.560992	0.755108
H	0.374839	-0.281630	2.189956
H	-1.425001	-1.415279	1.572373
H	-2.015719	-1.454568	-1.305534
H	-5.231606	-0.029500	-1.412795
H	3.015091	1.729433	-1.459311
H	-0.058289	2.578811	1.210826
H	-1.962847	-3.428950	0.280071
H	2.399126	-0.840258	-3.025098
H	2.003668	0.808525	-3.532209
H	1.232461	0.119584	-2.100689
H	4.895855	-0.061714	-3.085209
H	5.415340	1.271042	-2.019582
H	4.418296	1.599687	-3.442226
H	1.914171	2.236235	2.825363
H	0.758904	1.566961	3.989771
H	0.620814	3.252808	3.475655
H	-1.807283	2.733909	2.974912
H	-1.613162	1.009070	3.330809
H	-2.242698	1.529980	1.755227
H	-2.726082	-3.548548	-2.084176
H	-4.386991	-3.170294	-1.576455
H	-3.621636	-4.673050	-1.042785
H	-3.536045	-2.506839	2.049596
H	-4.068932	-4.066854	1.408814
H	-4.857559	-2.577191	0.872246
O	4.495106	-2.361425	1.806385
H	4.894172	-1.682837	2.370135
H	3.616482	-2.578000	2.206392
O	2.826163	-3.279451	-2.404738
H	3.027554	-3.377105	-3.346515
H	1.850581	-3.139411	-2.338309
O	0.198271	-2.704769	-1.877512
H	-0.137027	-1.996340	-2.475362
H	0.499047	-2.242586	-1.072716
O	1.959461	-2.948545	2.581895
H	1.579301	-2.536898	1.784070
H	1.637515	-2.415986	3.343156
O	-0.867130	-0.632697	-3.368973
H	-1.766866	-0.890343	-3.669994
H	-0.994307	0.006539	-2.644418
O	0.424142	3.094425	-1.330256
H	0.159102	2.158804	-1.208364
H	-0.322891	3.592605	-0.926005
O	2.491229	3.362531	0.340171
H	1.742826	3.401125	-0.318461
H	2.303099	4.036652	1.011485
O	6.332696	1.277928	0.608213

H	5.964778	2.110845	0.225696
H	6.939795	1.543288	1.314351
O	6.949781	-0.824140	-1.021742
H	7.419722	-0.581928	-1.832580
H	6.901092	-0.007567	-0.473500
O	5.090492	3.394742	-0.576728
H	4.166795	3.487125	-0.251641
H	5.497539	4.269016	-0.488318
O	-3.830135	-0.261079	3.386906
H	-4.654136	-0.718430	3.612972
H	-3.888399	-0.063325	2.430617
O	-3.419065	-1.491304	-3.997496
H	-3.850027	-1.006020	-4.716939
H	-3.911014	-1.257613	-3.189266
O	-1.520919	-1.707273	3.474242
H	-1.701479	-2.636725	3.686063
H	-2.371355	-1.223042	3.614257
O	0.922439	-1.531559	4.711176
H	1.290853	-0.688944	5.011264
H	-0.002936	-1.364759	4.433988
O	-4.109823	3.039240	0.444738
H	-4.476537	3.359400	1.284011
H	-4.125603	2.061812	0.504317
O	-1.609099	4.299624	0.110055
H	-1.872202	5.186045	-0.179036
H	-2.447047	3.798371	0.204983
O	-5.746672	3.334014	-1.767313
H	-6.434079	4.012689	-1.698956
H	-5.174104	3.433811	-0.976087
O	-6.492264	0.771085	-1.492784
H	-6.299471	1.738626	-1.616786
H	-7.011072	0.695422	-0.677045

Table S79. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_G.

N	4.542225	-0.865505	-0.532533
C	3.519678	0.212660	-0.635722
C	2.268070	-0.344244	0.038922
O	1.971390	-1.537423	-0.127837
N	1.541222	0.458505	0.821846
C	0.341028	-0.090277	1.432333
C	-0.704171	-0.319446	0.336557
O	-0.753237	0.395147	-0.679414
N	-1.564872	-1.324779	0.527122
C	-2.570428	-1.614319	-0.476513
C	-3.557702	-0.457643	-0.567420
O	-3.783320	0.300686	0.369735
O	-4.176110	-0.394965	-1.719341
C	3.328247	0.623887	-2.112192
C	-0.199794	0.759038	2.599884

C	-3.296202	-2.949003	-0.172974
C	2.168797	1.604715	-2.251380
C	3.142894	-0.567412	-3.053406
C	-0.951470	2.016155	2.166625
C	0.931728	1.087366	3.576729
C	-3.869830	-3.561899	-1.450812
C	-4.378272	-2.805284	0.899232
H	4.785712	-0.977787	0.469964
H	5.402161	-0.608607	-1.064637
H	4.169861	-1.773614	-0.889360
H	3.891889	1.075124	-0.072946
H	1.779261	1.450822	0.917543
H	0.608323	-1.068792	1.848278
H	-1.519124	-1.890569	1.379675
H	-2.072770	-1.705366	-1.448831
H	-4.953000	0.292169	-1.731521
H	4.255411	1.148048	-2.380099
H	-0.915547	0.106691	3.114339
H	-2.511073	-3.619726	0.200253
H	1.217890	1.121489	-2.002949
H	2.104853	1.960454	-3.283998
H	2.293997	2.475363	-1.604414
H	2.267993	-1.162358	-2.771367
H	4.017199	-1.224993	-3.080585
H	2.980119	-0.194790	-4.069541
H	-1.768727	1.787388	1.472077
H	-0.285370	2.735834	1.682056
H	-1.388933	2.504439	3.043326
H	0.518680	1.494566	4.504352
H	1.614553	1.836957	3.160351
H	1.518048	0.194454	3.820016
H	-3.091019	-3.705981	-2.206506
H	-4.651100	-2.925364	-1.879403
H	-4.315459	-4.535381	-1.225233
H	-4.010229	-2.304188	1.799469
H	-4.747525	-3.793194	1.188767
H	-5.230737	-2.229312	0.518284
O	4.509342	-0.784199	2.271777
H	4.168088	0.043120	2.642319
H	3.827638	-1.476224	2.460185
O	3.618731	-3.420337	-1.521392
H	4.054864	-3.825346	-2.284805
H	2.666341	-3.354592	-1.755167
O	0.774298	-3.309765	-1.867996
H	0.415902	-2.594347	-2.440221
H	0.809132	-2.881202	-0.995804
O	2.678598	-2.773777	2.372537
H	2.274131	-2.612821	1.500852
H	1.969645	-2.651083	3.043246
O	-0.273395	-1.061666	-3.140671
H	-1.165112	-1.199585	-3.529045
H	-0.411093	-0.450375	-2.392601
O	-0.116240	3.195146	-0.830302
H	-0.330930	2.241001	-0.785480
H	-0.861153	3.661785	-0.385305
O	2.087767	3.304627	0.691046
H	1.275958	3.410695	0.119998

H	1.988525	3.913781	1.438707
O	6.631438	1.997750	0.239625
H	5.854341	2.572493	0.047985
H	6.500656	1.633921	1.127371
O	6.886710	0.109484	-1.702647
H	6.889681	0.487272	-2.594007
H	6.923347	0.867692	-1.072972
O	4.514894	3.492744	-0.603449
H	3.659645	3.546976	-0.121012
H	4.758272	4.403110	-0.827050
O	-3.332078	-0.151003	3.134406
H	-3.438777	0.001298	2.172347
H	-4.229951	-0.164250	3.499629
O	-2.875830	-1.465329	-4.049243
H	-3.061518	-0.978445	-4.866134
H	-3.468805	-1.085139	-3.375325
O	-1.771777	-2.368490	3.213775
H	-2.228051	-3.198505	3.421640
H	-2.416896	-1.637555	3.375338
O	0.744655	-2.417050	4.297690
H	-0.193440	-2.339277	4.017339
H	0.867264	-1.807865	5.039482
O	-5.780882	3.737936	-1.351192
H	-5.356332	3.668555	-0.469258
H	-6.581839	4.269386	-1.233192
O	-4.356377	2.984053	0.882179
H	-4.226056	2.038532	0.659525
H	-4.740332	3.002343	1.772308
O	-2.086136	4.564865	0.520102
H	-2.878739	4.011117	0.687642
H	-2.405733	5.332329	0.023072
O	-6.183602	1.138250	-1.896922
H	-6.072930	2.111786	-1.730034
H	-6.897242	0.838875	-1.312876

Table S80. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_H.

N	-4.549351	-0.817070	0.682382
C	-3.433432	0.166816	0.618191
C	-2.256514	-0.578012	-0.005821
O	-2.039598	-1.752766	0.337377
N	-1.490366	0.063307	-0.890691
C	-0.272223	-0.573323	-1.365235
C	0.778195	-0.505848	-0.251942
O	0.792734	0.427359	0.569846
N	1.683407	-1.486419	-0.205919
C	2.682443	-1.485399	0.845563
C	3.592685	-0.272938	0.691496
O	3.815590	0.259864	-0.390705
O	4.151446	0.098605	1.815052

C	-3.077024	0.671301	2.032167
C	0.244595	0.024013	-2.690602
C	3.497942	-2.801782	0.842958
C	-4.328320	1.141099	2.776915
C	-2.053995	1.801538	1.951930
C	0.966479	1.360996	-2.525681
C	-0.897019	0.122142	-3.704292
C	4.129298	-3.060094	2.211343
C	4.555026	-2.841446	-0.262457
H	-4.663087	-1.245269	-0.256831
H	-5.454102	-0.355998	0.922129
H	-4.337208	-1.549371	1.392943
H	-3.757948	1.002130	-0.013389
H	-1.680683	1.049583	-1.100034
H	-0.505795	-1.626504	-1.552778
H	1.675755	-2.231472	-0.908604
H	2.168642	-1.394006	1.810313
H	4.883127	0.822918	1.691864
H	-2.632078	-0.174098	2.574428
H	0.970352	-0.708739	-3.064166
H	2.758719	-3.591870	0.656822
H	-4.855843	1.902407	2.189189
H	-4.035628	1.589656	3.731000
H	-5.019966	0.322481	3.001257
H	-2.494821	2.682963	1.473918
H	-1.164852	1.505789	1.390995
H	-1.733100	2.082292	2.959125
H	1.810325	1.291280	-1.828066
H	0.291538	2.139902	-2.157422
H	1.356202	1.696715	-3.492574
H	-0.496239	0.335394	-4.699701
H	-1.591855	0.929043	-3.444981
H	-1.466140	-0.812586	-3.752225
H	3.375073	-3.066249	3.004166
H	4.875167	-2.295966	2.454413
H	4.632879	-4.031399	2.205864
H	4.143962	-2.596246	-1.245983
H	4.991843	-3.842489	-0.320514
H	5.367394	-2.134920	-0.052684
O	-4.400554	-1.467312	-2.046239
H	-4.101452	-0.716229	-2.579848
H	-3.716290	-2.174331	-2.151049
O	-3.888132	-2.529279	2.854045
H	-4.314388	-2.321915	3.697988
H	-2.915550	-2.513785	3.019551
O	-1.134073	-2.520733	2.864625
H	-0.657016	-1.706236	3.146977
H	-1.213411	-2.413961	1.898886
O	-2.535766	-3.420114	-1.914784
H	-2.159645	-3.097000	-1.075563
H	-1.811795	-3.397387	-2.579761
O	0.214079	-0.157132	3.333989
H	1.105165	-0.298161	3.722026
H	0.380533	0.163233	2.427514
O	0.274848	3.223404	0.211611
H	0.537261	2.288619	0.327438
H	0.933622	3.614497	-0.408557

O	-2.016297	2.902194	-1.140685
H	-1.198647	3.148999	-0.623310
H	-1.931938	3.329264	-2.007467
O	-6.499934	2.073417	-1.166083
H	-5.738443	2.610455	-0.842624
H	-6.178118	1.578664	-1.933791
O	-7.059208	0.400078	0.904736
H	-7.323003	0.911670	1.683133
H	-6.965133	1.048039	0.164859
O	-4.462404	3.481098	-0.024088
H	-3.571925	3.392022	-0.433034
H	-4.638592	4.431507	0.038658
O	3.576806	-0.903927	-2.967357
H	3.592187	-0.468446	-2.090264
H	3.412973	-0.205524	-3.618955
O	-0.523204	-3.371821	-3.795084
H	-0.610966	-2.900372	-4.635683
H	0.395291	-3.221935	-3.480952
O	2.810843	-0.588482	4.262975
H	3.424507	-0.298901	3.563139
H	3.023105	-0.049349	5.039518
O	1.939783	-3.048791	-2.625236
H	2.413095	-3.894492	-2.663046
H	2.571424	-2.355402	-2.933232
O	2.008554	4.279742	-1.645143
H	2.292502	5.179912	-1.427669
H	2.829320	3.742414	-1.666111
O	4.340063	2.759218	-1.514038
H	4.819698	2.584380	-2.338183
H	4.233513	1.893007	-1.067808
O	5.494333	4.143406	0.570005
H	6.254248	4.716176	0.390112
H	5.161560	3.834587	-0.299776
O	6.051555	1.769546	1.698879
H	6.805123	1.403894	1.210519
H	5.883187	2.672996	1.320726

Table S81. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_I.

N	-4.290988	-0.898554	1.172769
C	-3.510075	0.190439	0.528660
C	-2.248227	-0.460982	-0.027990
O	-1.866926	-1.552769	0.426789
N	-1.567861	0.188821	-0.973261
C	-0.330483	-0.392075	-1.469458
C	0.705413	-0.404115	-0.340027
O	0.718762	0.468247	0.543708
N	1.607373	-1.390959	-0.371368
C	2.656389	-1.459105	0.626339
C	3.640884	-0.312447	0.424074

O	3.761800	0.287252	-0.639346
O	4.377115	-0.068058	1.478544
C	-3.176621	1.334518	1.508888
C	0.206880	0.329173	-2.723587
C	3.374201	-2.831121	0.574577
C	-2.108042	0.943490	2.529276
C	-4.438811	1.856575	2.197287
C	0.867695	1.673822	-2.420585
C	-0.891049	0.461690	-3.781668
C	4.040911	-3.166368	1.908506
C	4.376833	-2.921502	-0.577768
H	-4.473762	-1.626291	0.449353
H	-5.222408	-0.562033	1.492326
H	-3.777814	-1.352713	1.959659
H	-4.127376	0.580138	-0.288754
H	-1.893147	1.099381	-1.312268
H	-0.541216	-1.430180	-1.752513
H	1.573583	-2.084813	-1.124308
H	2.203173	-1.340424	1.618075
H	5.141535	0.609097	1.290529
H	-2.772251	2.140915	0.886435
H	0.978535	-0.337794	-3.124229
H	2.570466	-3.560126	0.407400
H	-2.445994	0.124435	3.174257
H	-1.878226	1.802219	3.167432
H	-1.177838	0.631329	2.045790
H	-4.823332	1.134427	2.927312
H	-5.227080	2.087066	1.474409
H	-4.201060	2.775276	2.741726
H	1.696619	1.570221	-1.712312
H	0.153515	2.389199	-2.000097
H	1.267951	2.104576	-3.344173
H	-0.450870	0.800335	-4.724677
H	-1.646273	1.200372	-3.489969
H	-1.386092	-0.498652	-3.953943
H	3.327157	-3.108752	2.736595
H	4.871539	-2.485428	2.120110
H	4.443127	-4.183266	1.871606
H	3.938019	-2.628079	-1.536439
H	4.743535	-3.947348	-0.674135
H	5.243131	-2.274245	-0.391953
O	-4.627971	-2.474313	-1.121098
H	-4.816677	-1.936655	-1.904028
H	-3.796067	-2.971749	-1.317792
O	-2.976241	-2.354831	3.233923
H	-3.184873	-2.202635	4.166807
H	-1.994346	-2.296778	3.153498
O	-0.283259	-2.152735	2.642996
H	0.135439	-1.335955	3.001536
H	-0.567236	-1.915347	1.740849
O	-2.223385	-3.730571	-1.344579
H	-1.835674	-3.141509	-0.671570
H	-1.773694	-3.503015	-2.189829
O	0.983843	0.187740	3.387536
H	1.884818	-0.025508	3.716869
H	1.095078	0.514920	2.476010
O	-0.448075	3.044419	0.459802

H	-0.131039	2.117393	0.493651
H	0.319365	3.560508	0.119266
O	-2.355525	2.942280	-1.403968
H	-1.652567	3.141853	-0.724115
H	-2.138593	3.463216	-2.192557
O	-6.648814	1.252655	-0.861900
H	-6.042975	2.030681	-0.880980
H	-6.505133	0.763295	-1.684426
O	-6.984616	-0.167953	1.444376
H	-7.352935	0.379394	2.152732
H	-6.991794	0.387904	0.631386
O	-4.976915	3.396380	-0.682754
H	-4.036171	3.288478	-0.950132
H	-5.295106	4.189435	-1.138706
O	3.303084	-0.715424	-3.257099
H	3.423479	-0.360390	-2.352178
H	4.196299	-0.834638	-3.614104
O	3.530221	-0.582674	4.165020
H	3.942158	-0.014987	4.833502
H	4.040674	-0.443320	3.347100
O	1.664990	-2.857257	-2.876630
H	2.092809	-3.724888	-2.945383
H	2.318301	-2.191014	-3.199912
O	-0.967148	-2.941076	-3.678125
H	0.006972	-2.946354	-3.552873
H	-1.144967	-3.490254	-4.455919
O	5.713131	4.009197	0.559428
H	5.130739	3.844984	-0.213315
H	6.437344	4.571120	0.246908
O	3.958555	3.005368	-1.312224
H	3.967397	2.056175	-1.069018
H	4.153091	3.040558	-2.261649
O	1.643647	4.447070	-0.657571
H	2.428283	3.906899	-0.891841
H	1.982125	5.174201	-0.114665
O	6.359078	1.474506	1.162149
H	6.176871	2.432089	0.966766
H	6.943594	1.156326	0.456946

Table S82. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_J.

N	4.540148	-0.861935	-0.162906
C	3.578177	0.270500	-0.275121
C	2.237229	-0.285298	0.200362
O	1.866455	-1.400555	-0.191926
N	1.510755	0.433363	1.065213
C	0.243379	-0.119212	1.519761
C	-0.707960	-0.197490	0.320459
O	-0.710290	0.676494	-0.564470
N	-1.540105	-1.242958	0.263704

C	-2.515655	-1.331831	-0.808650
C	-3.475735	-0.151278	-0.718947
O	-3.923967	0.247015	0.353094
O	-3.811320	0.350447	-1.879266
C	3.566187	0.821144	-1.719079
C	-0.336054	0.671821	2.711932
C	-3.285996	-2.666535	-0.747003
C	2.436146	1.830147	-1.895896
C	3.485413	-0.269927	-2.788197
C	-1.506999	-0.082433	3.339614
C	-0.775238	2.088107	2.351498
C	-2.316963	-3.828614	-0.970753
C	-4.409482	-2.700528	-1.785223
H	4.642506	-1.107723	0.840990
H	5.469632	-0.593366	-0.556822
H	4.185208	-1.706957	-0.665179
H	3.915366	1.058371	0.406494
H	1.801929	1.380925	1.322500
H	0.433962	-1.143779	1.864612
H	-1.561690	-1.943689	1.010145
H	-1.997057	-1.276805	-1.772622
H	-4.594919	1.023197	-1.822620
H	4.520402	1.353600	-1.827594
H	0.480454	0.719621	3.444709
H	-3.731858	-2.746992	0.252917
H	1.459473	1.348230	-1.778696
H	2.475300	2.261643	-2.900550
H	2.506290	2.647939	-1.177734
H	2.576327	-0.868335	-2.673751
H	4.349923	-0.941200	-2.774233
H	3.455098	0.203890	-3.774339
H	-1.247212	-1.117309	3.580353
H	-2.370035	-0.090630	2.665502
H	-1.816121	0.413566	4.264218
H	-1.183410	2.585856	3.237406
H	-1.563005	2.064394	1.590236
H	0.043755	2.701020	1.972146
H	-1.497083	-3.839440	-0.245155
H	-1.877101	-3.765423	-1.972902
H	-2.850365	-4.780600	-0.888414
H	-5.185523	-1.955333	-1.583526
H	-4.884904	-3.685445	-1.776690
H	-4.013349	-2.520548	-2.791419
O	4.104380	-1.340443	2.567653
H	3.672661	-0.606735	3.029597
H	3.423670	-2.053617	2.483533
O	3.632780	-3.250834	-1.473542
H	4.147289	-3.616375	-2.207567
H	2.728079	-3.092514	-1.826989
O	0.912400	-2.993801	-2.251376
H	0.651701	-2.140795	-2.669035
H	0.723846	-2.823296	-1.314039
O	2.301912	-3.263062	1.936428
H	1.995087	-2.843094	1.112254
H	1.525428	-3.308181	2.538647
O	0.035874	-0.507338	-3.131990
H	-0.827201	-0.580998	-3.594907

H	-0.159363	-0.012571	-2.313873
O	0.151678	3.415731	-0.466332
H	-0.094490	2.468954	-0.512002
H	-0.624024	3.865374	-0.060460
O	2.314450	3.257145	1.143324
H	1.530383	3.472073	0.567581
H	2.239181	3.807866	1.937811
O	7.000854	2.263793	0.482557
H	6.163807	2.765874	0.344416
H	7.016018	2.009485	1.416407
O	6.996463	0.069280	-1.114367
H	7.072275	0.315851	-2.047540
H	7.078388	0.905169	-0.593217
O	4.728450	3.624723	-0.150685
H	3.882732	3.576406	0.348885
H	4.889410	4.564927	-0.317366
O	-4.368270	-1.533697	2.550907
H	-5.234676	-1.952883	2.438301
H	-4.275405	-0.902354	1.809223
O	-2.530212	-0.757212	-4.190115
H	-2.663151	-0.367463	-5.067081
H	-3.112826	-0.263284	-3.584468
O	-2.180118	-3.165985	2.380637
H	-2.459209	-4.057001	2.117814
H	-3.009056	-2.664782	2.576839
O	0.216686	-3.407681	3.724036
H	0.276626	-2.899427	4.545428
H	-0.699425	-3.305821	3.388860
O	-4.095650	2.856338	1.390630
H	-4.201098	2.764335	2.350259
H	-4.056603	1.944698	1.032660
O	-2.041757	4.662540	0.698287
H	-1.786015	5.110236	1.518152
H	-2.736260	4.019971	0.953630
O	-5.922591	4.010689	-0.309367
H	-6.802532	4.206380	0.044734
H	-5.375190	3.714606	0.449590
O	-5.826595	1.893638	-1.970729
H	-5.897639	2.680959	-1.368953
H	-6.631591	1.370837	-1.834841

Table S83. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 18H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $18H_2O$_PPII-PPII_S.

N	-4.599489	-0.585589	0.488202
C	-3.576613	0.488940	0.371312
C	-2.290642	-0.199517	-0.079176
O	-1.994812	-1.320913	0.363553
N	-1.538001	0.424300	-0.986396
C	-0.314526	-0.201123	-1.465699
C	0.691244	-0.229343	-0.304965

O	0.742217	0.703450	0.514546
N	1.499417	-1.293667	-0.193498
C	2.413250	-1.349121	0.934795
C	3.514117	-0.311763	0.768897
O	3.858028	0.134254	-0.321053
O	4.091275	0.002875	1.901236
C	-3.469635	1.275161	1.695895
C	0.195383	0.531959	-2.738478
C	3.030691	-2.742037	1.197676
C	-2.297429	2.248848	1.647526
C	-3.373554	0.375497	2.928091
C	0.727376	-0.465513	-3.764614
C	1.236281	1.612828	-2.449218
C	4.136383	-3.127748	0.214860
C	1.932796	-3.803200	1.276501
H	-4.793512	-0.951474	-0.464267
H	-5.477371	-0.211641	0.902893
H	-4.254498	-1.373094	1.081108
H	-3.914764	1.166752	-0.417373
H	-1.766391	1.374461	-1.296677
H	-0.556498	-1.238843	-1.729434
H	1.448002	-2.066389	-0.862701
H	1.846764	-1.082944	1.832736
H	4.937168	0.587490	1.782654
H	-4.398486	1.858647	1.753458
H	-0.691112	1.010643	-3.173943
H	3.482062	-2.651416	2.193205
H	-1.346061	1.708561	1.598120
H	-2.285497	2.865538	2.551030
H	-2.360674	2.917303	0.786621
H	-2.499318	-0.280957	2.868908
H	-4.264506	-0.244289	3.068822
H	-3.263243	1.000850	3.819433
H	-0.025028	-1.222904	-4.005088
H	1.629116	-0.963645	-3.399404
H	0.994451	0.057199	-4.688375
H	1.531564	2.102260	-3.382831
H	2.136953	1.179003	-1.996995
H	0.854616	2.379840	-1.772931
H	4.972836	-2.420003	0.237092
H	3.765682	-3.176759	-0.812055
H	4.530422	-4.114349	0.476307
H	1.145786	-3.508035	1.978168
H	2.361624	-4.751941	1.612912
H	1.468872	-3.979070	0.299031
O	-4.400853	-1.404057	-2.185258
H	-4.014636	-0.744079	-2.779369
H	-3.731322	-2.127384	-2.098232
O	-3.788922	-2.779028	2.168713
H	-4.325212	-2.951390	2.956042
H	-2.872251	-2.627710	2.490490
O	-1.025830	-2.451852	2.685082
H	-0.669556	-1.612663	3.053608
H	-1.020780	-2.274152	1.727954
O	-2.606517	-3.329785	-1.547667
H	-2.199351	-2.842309	-0.808491
H	-1.895102	-3.499566	-2.205345

O	0.103774	0.028906	3.298129
H	0.980290	-0.170710	3.693202
H	0.295886	0.384202	2.410057
O	0.150363	3.500214	0.235426
H	0.349607	2.554245	0.387759
H	0.968917	3.888111	-0.150638
O	-1.841977	3.245412	-1.562255
H	-1.095718	3.473836	-0.943097
H	-1.605916	3.603984	-2.431427
O	-6.199995	1.709582	-0.923288
H	-5.633597	2.515474	-0.925228
H	-6.779612	1.776025	-1.695880
O	-6.971303	0.640710	1.437005
H	-6.995753	1.190282	2.233458
H	-6.921905	1.250513	0.668357
O	-4.404784	3.738164	-0.622827
H	-3.511460	3.677532	-1.027919
H	-4.693655	4.655507	-0.735682
O	3.783235	-1.419023	-2.721252
H	4.697724	-1.728601	-2.807443
H	3.764517	-0.875394	-1.906820
O	2.605386	-0.812972	4.191631
H	2.859450	-0.606404	5.103359
H	3.307337	-0.446096	3.624038
O	1.783755	-3.274393	-2.354160
H	2.126432	-4.166778	-2.189455
H	2.552655	-2.734627	-2.655218
O	-0.679641	-3.848467	-3.445446
H	-0.847616	-3.576882	-4.358924
H	0.231145	-3.560424	-3.223457
O	4.451439	2.696277	-1.287677
H	4.768504	2.574894	-2.195916
H	4.293910	1.796835	-0.931403
O	2.381920	4.554626	-1.004329
H	2.129527	4.862279	-1.887286
H	3.072621	3.873005	-1.147422
O	6.051635	3.764688	0.682657
H	6.882959	4.180199	0.410474
H	5.566488	3.539755	-0.140535
O	6.252879	1.327809	1.793991
H	6.229123	2.244689	1.411301
H	6.932994	0.842667	1.302047

Table S84. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $22H_2O$_PPII-PPII_A.

N	-4.889277	0.825896	0.145359
C	-4.004632	-0.336152	-0.150987
C	-2.617788	0.075726	0.333448
O	-2.226316	1.232599	0.107524
N	-1.863764	-0.797947	1.004702

C	-0.524882	-0.376613	1.401763
C	0.310450	-0.186823	0.125711
O	0.207103	-0.970661	-0.835032
N	1.118202	0.878763	0.084979
C	1.969964	1.099544	-1.068385
C	3.128322	0.117007	-1.050236
O	3.512020	-0.426835	-0.014062
O	3.705304	-0.064654	-2.205909
C	-4.070684	-0.681932	-1.657358
C	0.109504	-1.334412	2.430563
C	2.469904	2.565763	-1.159964
C	-3.031045	-1.738847	-2.016422
C	-3.931082	0.536933	-2.571668
C	1.437323	-0.765880	2.927284
C	0.341230	-2.747183	1.905250
C	2.584786	2.996837	-2.622364
C	3.784738	2.820349	-0.421411
H	-4.948277	0.939288	1.177492
H	-5.846250	0.667518	-0.243698
H	-4.492854	1.704772	-0.251252
H	-4.368778	-1.189602	0.430254
H	-2.182423	-1.763443	1.131713
H	-0.620796	0.604572	1.883744
H	1.233797	1.476368	0.913705
H	1.378920	0.889652	-1.961823
H	4.614924	-0.623805	-2.068090
H	-5.066980	-1.120234	-1.800382
H	-0.600232	-1.367275	3.267902
H	1.683098	3.166807	-0.690514
H	-2.016158	-1.357423	-1.861099
H	-3.127611	-2.011951	-3.071362
H	-3.151247	-2.646054	-1.422993
H	-2.968022	1.036980	-2.425226
H	-4.729526	1.271248	-2.427357
H	-3.977813	0.203031	-3.612779
H	1.345683	0.260359	3.293671
H	2.172619	-0.773149	2.115156
H	1.829153	-1.385017	3.739967
H	0.803645	-3.358945	2.686660
H	1.026586	-2.725372	1.052147
H	-0.578597	-3.244244	1.594838
H	1.632046	2.873961	-3.149274
H	3.345243	2.408463	-3.148129
H	2.877673	4.050165	-2.679885
H	3.722315	2.569381	0.640190
H	4.048599	3.879576	-0.496239
H	4.608247	2.244360	-0.863254
O	-4.407848	0.911424	2.897763
H	-4.031716	0.102164	3.273993
H	-3.682024	1.584972	2.898937
O	-3.807970	3.335764	-0.883917
H	-4.292211	3.876700	-1.524575
H	-2.933717	3.160204	-1.286634
O	-1.007102	2.828775	-1.720657
H	-0.807608	2.175469	-2.430380
H	-1.056187	2.273672	-0.919645
O	-2.503429	2.787502	2.501417

H	-2.253267	2.496100	1.606129
H	-1.705928	2.664912	3.066804
O	-0.519261	0.577652	-3.276847
H	0.307462	0.495326	-3.801864
H	-0.426063	-0.091527	-2.573224
O	-0.764309	-3.661565	-0.966982
H	-0.485307	-2.723302	-0.929331
H	0.020481	-4.165850	-0.655188
O	-2.846532	-3.568481	0.757674
H	-2.107273	-3.767267	0.120776
H	-2.783636	-4.220772	1.472430
O	-7.490045	-2.145375	0.676874
H	-6.705434	-2.676323	0.405852
H	-7.387250	-1.966680	1.622718
O	-7.438461	0.156331	-0.764599
H	-7.579853	-0.018315	-1.706334
H	-7.551923	-0.706504	-0.296002
O	-5.375697	-3.518601	-0.356862
H	-4.494468	-3.638764	0.062269
H	-5.625359	-4.383513	-0.713571
O	4.074847	0.822485	2.421765
H	4.976082	1.182883	2.384864
H	3.908828	0.480377	1.516957
O	1.972179	0.251504	-4.487517
H	1.983210	-0.540751	-5.045302
H	2.665898	0.108178	-3.816126
O	1.774359	2.493276	2.360447
H	1.893386	3.411419	2.012920
H	2.656603	2.113488	2.554349
O	-0.318608	2.437506	4.119639
H	-0.310354	1.628190	4.650799
H	0.507684	2.437689	3.584613
O	3.616447	-3.168033	0.551301
H	3.970833	-2.983504	1.445641
H	3.484213	-2.269639	0.187570
O	1.545438	-4.966262	-0.070950
H	1.936456	-5.557228	-0.731061
H	2.264250	-4.351544	0.191665
O	5.426431	-3.905198	-1.395331
H	6.204743	-4.405597	-1.109947
H	4.843809	-3.820898	-0.608004
O	5.841759	-1.242975	-1.772757
H	5.742854	-2.227452	-1.731514
H	6.066034	-0.962547	-0.849108
O	6.377604	-0.482974	0.804953
H	7.320757	-0.475822	1.027723
H	5.958408	-1.104666	1.437835
O	4.821630	-1.852910	2.705761
H	4.430663	-0.993706	2.970351
H	5.206885	-2.241971	3.505642
O	0.254635	5.183728	-1.017394
H	-0.162541	4.357493	-1.351981
H	0.703546	5.585032	-1.775716
O	1.767776	4.996930	1.292142
H	1.250015	5.079138	0.457734
H	2.603611	5.460229	1.138668

Table S85. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $22H_2O$_PPII-PPII_B.

N	4.828352	0.932788	-0.068174
C	3.885342	-0.185067	0.214558
C	2.559406	0.229117	-0.414820
O	2.190428	1.408886	-0.279903
N	1.818753	-0.676264	-1.057162
C	0.464875	-0.301330	-1.454802
C	-0.373391	-0.170910	-0.173827
O	-0.292132	-1.013129	0.739362
N	-1.151134	0.909729	-0.065923
C	-1.974762	1.090732	1.113929
C	-3.142265	0.118548	1.078599
O	-3.540830	-0.391036	0.030855
O	-3.708096	-0.095240	2.234115
C	3.717044	-0.365962	1.739080
C	-0.136877	-1.263186	-2.497453
C	-2.453042	2.556311	1.271127
C	5.076224	-0.461326	2.434930
C	2.876807	-1.602691	2.047546
C	-1.503970	-0.747187	-2.944605
C	-0.281676	-2.702991	-2.015185
C	-2.584015	2.921320	2.749881
C	-3.747983	2.864990	0.519003
H	4.799372	1.144737	-1.087022
H	5.812575	0.677901	0.169165
H	4.541025	1.775228	0.471931
H	4.286773	-1.095906	-0.244081
H	2.125331	-1.654520	-1.074612
H	0.525052	0.689285	-1.919749
H	-1.250781	1.553484	-0.861253
H	-1.365812	0.837448	1.985137
H	-4.621233	-0.648526	2.087790
H	3.189222	0.524006	2.108734
H	0.554699	-1.232608	-3.349812
H	-1.648155	3.165508	0.844935
H	5.677854	-1.263724	1.990630
H	4.925338	-0.695814	3.492982
H	5.641282	0.475067	2.386838
H	3.421889	-2.513671	1.781619
H	1.927591	-1.595309	1.505637
H	2.651365	-1.638101	3.117111
H	-1.471391	0.292682	-3.282256
H	-2.216742	-0.810725	-2.114187
H	-1.889461	-1.361978	-3.763618
H	-0.692180	-3.319664	-2.821248
H	-0.977792	-2.752120	-1.172765
H	0.664760	-3.149950	-1.705835
H	-1.640826	2.757351	3.282892
H	-3.362549	2.324668	3.238151
H	-2.857127	3.976685	2.850505
H	-3.666458	2.658536	-0.551259
H	-3.997150	3.924324	0.633238

H	-4.589352	2.283106	0.917573
O	4.359643	1.121412	-2.822906
H	4.048097	0.294418	-3.219287
H	3.618818	1.772427	-2.913230
O	3.912711	3.043005	1.646899
H	4.361253	3.192982	2.491562
H	2.957355	2.958806	1.854055
O	1.095560	2.664213	1.887281
H	0.860514	1.929309	2.502854
H	1.202740	2.220595	1.022545
O	2.372665	2.941655	-2.655895
H	2.098528	2.631637	-1.773618
H	1.603803	2.784879	-3.251209
O	0.551356	0.335916	3.257343
H	-0.274722	0.267492	3.785864
H	0.430288	-0.302128	2.529645
O	0.610431	-3.696538	0.951301
H	0.279742	-2.777451	0.887183
H	-0.107679	-4.243155	0.560290
O	2.810498	-3.416339	-0.591428
H	2.049077	-3.655589	0.005300
H	2.784338	-4.044642	-1.329889
O	7.220558	-2.244574	-1.041985
H	6.521456	-2.743003	-0.556071
H	6.909074	-2.157792	-1.954496
O	7.502774	0.171733	0.165176
H	7.938490	0.057629	1.022116
H	7.485299	-0.721374	-0.258280
O	5.350378	-3.525156	0.472616
H	4.437011	-3.574912	0.109822
H	5.603400	-4.434184	0.691320
O	-4.067118	0.937062	-2.363116
H	-4.959605	1.312860	-2.286274
H	-3.880685	0.561458	-1.475185
O	-1.932606	0.095672	4.492847
H	-1.976275	-0.701800	5.041581
H	-2.640423	-0.005077	3.828364
O	-1.738408	2.562753	-2.328417
H	-1.811794	3.471372	-1.945832
H	-2.640048	2.217216	-2.495910
O	0.195899	2.499442	-4.268318
H	0.189232	1.652523	-4.737381
H	-0.581061	2.497868	-3.663932
O	-3.590245	-3.112437	-0.657735
H	-3.983895	-2.871798	-1.522471
H	-3.434608	-2.239310	-0.246437
O	-1.583532	-5.024009	-0.168968
H	-1.997634	-5.666766	0.425435
H	-2.286502	-4.374690	-0.386975
O	-5.398509	-3.894433	1.279095
H	-6.171320	-4.393816	0.977473
H	-4.814993	-3.782309	0.495846
O	-5.848321	-1.258796	1.784366
H	-5.735791	-2.238258	1.689681
H	-6.084434	-0.933743	0.878245
O	-6.404382	-0.378726	-0.749669
H	-7.347566	-0.363467	-0.971840

H	-5.986383	-0.981011	-1.401795
O	-4.878741	-1.708840	-2.704275
H	-4.480471	-0.848833	-2.955593
H	-5.281482	-2.075196	-3.506297
O	-0.120751	5.061369	1.215704
H	0.268534	4.222786	1.551326
H	-0.572464	5.469101	1.969030
O	-1.611419	5.005655	-1.126143
H	-1.090673	5.031576	-0.290476
H	-2.428248	5.493826	-0.948789

Table S86. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $22H_2O$_PPII-PPII_C.

N	-4.783784	0.891285	-0.430782
C	-3.988821	-0.333883	-0.152469
C	-2.627302	0.146424	0.339391
O	-2.237718	1.288284	0.039236
N	-1.870827	-0.695694	1.041976
C	-0.527819	-0.285059	1.431307
C	0.316772	-0.101075	0.158681
O	0.172710	-0.851840	-0.822387
N	1.190231	0.910310	0.156868
C	2.078580	1.114678	-0.972510
C	3.241122	0.138151	-0.899804
O	3.560453	-0.423759	0.149406
O	3.894248	-0.019016	-2.016839
C	-3.851305	-1.238739	-1.396696
C	0.083199	-1.286017	2.435910
C	2.575991	2.580094	-1.063684
C	-2.886720	-0.669868	-2.436737
C	-5.217478	-1.540975	-2.014550
C	1.348926	-0.711518	3.065115
C	0.404142	-2.644316	1.818978
C	2.804930	2.986916	-2.519270
C	3.821928	2.858819	-0.221963
H	-4.827287	1.448032	0.450203
H	-5.767170	0.661121	-0.684437
H	-4.349610	1.492135	-1.163455
H	-4.511849	-0.880891	0.639996
H	-2.208773	-1.642405	1.242651
H	-0.604200	0.690264	1.929142
H	1.307030	1.485245	1.001401
H	1.517267	0.892407	-1.882577
H	4.792594	-0.596575	-1.841503
H	-3.431826	-2.180036	-1.023699
H	-0.677675	-1.408118	3.218467
H	1.748188	3.181308	-0.674166
H	-3.239707	0.286155	-2.840173
H	-2.788831	-1.371459	-3.270710
H	-1.890094	-0.512939	-2.015207

H	-5.634433	-0.657366	-2.512034
H	-5.930654	-1.898205	-1.265942
H	-5.106671	-2.320950	-2.773610
H	1.180601	0.262413	3.532126
H	2.124935	-0.596087	2.301710
H	1.728711	-1.396669	3.829279
H	0.805975	-3.314052	2.586133
H	1.165825	-2.533719	1.040896
H	-0.465172	-3.128077	1.372739
H	1.908558	2.814451	-3.125393
H	3.633726	2.425003	-2.963358
H	3.054211	4.051709	-2.571315
H	3.678422	2.609552	0.832531
H	4.075698	3.921723	-0.278291
H	4.686995	2.293268	-0.592576
O	-4.690256	1.975998	2.145348
H	-4.736870	1.299843	2.836795
H	-3.826599	2.443645	2.267261
O	-3.651502	2.742041	-2.290701
H	-3.975249	2.822832	-3.199531
H	-2.673663	2.671333	-2.350617
O	-0.869254	2.365094	-2.080843
H	-0.524677	1.686837	-2.711073
H	-1.102169	1.869962	-1.270329
O	-2.276586	3.209684	2.110410
H	-1.986710	2.694889	1.335695
H	-1.670331	2.959036	2.843788
O	0.024165	0.219163	-3.556801
H	0.905243	0.251666	-3.993818
H	0.119448	-0.415667	-2.823137
O	-1.065312	-3.359698	-1.057617
H	-0.751942	-2.434014	-0.974400
H	-0.257779	-3.890881	-0.876457
O	-2.868615	-3.442969	0.943690
H	-2.234228	-3.588602	0.190231
H	-2.636234	-4.086154	1.631544
O	-7.086534	-1.632066	1.329934
H	-6.523908	-2.404329	1.084821
H	-6.806065	-1.348992	2.211891
O	-7.526314	0.329235	-0.512947
H	-8.007409	-0.010023	-1.281422
H	-7.490223	-0.408081	0.139805
O	-5.566673	-3.710997	0.440035
H	-4.597746	-3.668489	0.604801
H	-5.854779	-4.577120	0.763932
O	4.060281	0.819024	2.607297
H	4.968937	1.158155	2.652296
H	3.955122	0.508529	1.683192
O	2.601778	0.299244	-4.546150
H	2.790462	-0.448734	-5.132392
H	3.163924	0.166636	-3.759456
O	1.715721	2.457005	2.510062
H	1.799084	3.368413	2.138979
H	2.606268	2.114464	2.730421
O	-0.506345	2.532291	4.111206
H	-0.649461	1.717791	4.614476
H	0.369050	2.450373	3.670666

O	3.567638	-3.197082	0.511247
H	3.829945	-3.112828	1.449431
H	3.530745	-2.261074	0.227419
O	1.340593	-4.689155	-0.440889
H	1.720031	-5.231796	-1.147481
H	2.090237	-4.174219	-0.073414
O	5.483740	-3.914505	-1.332751
H	6.224796	-4.451427	-1.016278
H	4.844519	-3.853076	-0.588331
O	5.980159	-1.249537	-1.529912
H	5.862815	-2.233134	-1.546800
H	6.175260	-1.019325	-0.584778
O	6.395996	-0.608605	1.082148
H	7.314363	-0.680311	1.383076
H	5.876351	-1.210946	1.657796
O	4.627408	-1.938264	2.805014
H	4.267085	-1.068581	3.076964
H	4.977506	-2.351060	3.609376
O	-0.002169	4.808385	-1.053456
H	-0.247889	3.963738	-1.491473
H	0.379540	5.366182	-1.747081
O	1.474101	4.891955	1.312768
H	0.947316	4.863433	0.481917
H	2.241185	5.451492	1.124184

Table S87. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $22H_2O$_PPII-PPII_D.

N	-4.922012	0.825534	0.058962
C	-4.019595	-0.287615	-0.339089
C	-2.651306	0.040403	0.245359
O	-2.267857	1.220692	0.317688
N	-1.904042	-0.973541	0.674036
C	-0.543619	-0.742274	1.138438
C	0.292535	-0.244469	-0.048576
O	0.224083	-0.805627	-1.157378
N	1.070279	0.821294	0.160994
C	1.919584	1.331987	-0.899074
C	3.109498	0.410348	-1.101265
O	3.484040	-0.377587	-0.234586
O	3.733335	0.561702	-2.238421
C	-4.034494	-0.469753	-1.873705
C	0.017157	-2.034048	1.759094
C	2.376120	2.787685	-0.620558
C	-2.998878	-1.500331	-2.317592
C	-3.850183	0.844651	-2.633512
C	-0.816316	-2.426595	2.980674
C	1.485218	-1.856960	2.138693
C	2.539330	3.562068	-1.928197
C	3.645394	2.880386	0.227270
H	-5.071981	0.756100	1.083278

H	-5.836831	0.753128	-0.431732
H	-4.495241	1.752274	-0.157999
H	-4.404702	-1.196436	0.131844
H	-2.246849	-1.937546	0.598996
H	-0.558729	0.040520	1.910105
H	1.154451	1.210885	1.108922
H	1.339621	1.329291	-1.824623
H	4.671914	0.052214	-2.187624
H	-5.031655	-0.872067	-2.097999
H	-0.049643	-2.829125	1.005566
H	1.549753	3.239974	-0.061847
H	-1.981668	-1.131554	-2.149234
H	-3.113147	-1.699028	-3.387154
H	-3.114584	-2.448614	-1.786726
H	-2.900200	1.324290	-2.373388
H	-4.659831	1.556791	-2.446008
H	-3.834189	0.639149	-3.708226
H	-1.872653	-2.579220	2.738841
H	-0.758729	-1.644124	3.746625
H	-0.432029	-3.355122	3.413408
H	1.862340	-2.766013	2.617375
H	1.610381	-1.023133	2.842028
H	2.105360	-1.661038	1.258367
H	1.616533	3.543745	-2.518566
H	3.346319	3.142425	-2.538838
H	2.789798	4.606055	-1.713628
H	3.542919	2.364997	1.185585
H	3.872648	3.929920	0.437526
H	4.508934	2.454199	-0.299929
O	-4.590990	0.205215	2.765760
H	-4.385972	-0.723045	2.949737
H	-3.790438	0.727729	3.019603
O	-3.863212	3.447414	-0.607689
H	-4.345601	3.993043	-1.245642
H	-2.954223	3.359541	-0.961278
O	-1.058981	3.047324	-1.287015
H	-0.821032	2.540293	-2.097614
H	-1.167557	2.354332	-0.606609
O	-2.466589	1.840431	3.098228
H	-2.151353	1.841517	2.176411
H	-1.710105	1.555892	3.660259
O	-0.479263	1.166202	-3.253341
H	0.359130	1.245151	-3.760445
H	-0.365265	0.363858	-2.709865
O	-0.533704	-3.523454	-1.410534
H	-0.344990	-2.561981	-1.390722
H	0.251798	-3.938040	-0.983926
O	-2.642257	-3.735177	0.229103
H	-1.872216	-3.803122	-0.401766
H	-2.488008	-4.388744	0.928485
O	-6.741522	-1.675902	0.379622
H	-6.278161	-2.467850	0.019795
H	-7.306544	-1.990095	1.100218
O	-7.414642	0.392056	-1.220934
H	-7.501721	0.266756	-2.176845
H	-7.431243	-0.500172	-0.810665
O	-5.216032	-3.606743	-0.790123

H	-4.324903	-3.782222	-0.414544
H	-5.611224	-4.472558	-0.969312
O	3.926346	0.203349	2.434110
H	4.814025	0.586599	2.315564
H	3.641513	0.019816	1.512416
O	2.036740	1.329205	-4.436687
H	2.126539	0.718264	-5.183315
H	2.727638	1.066872	-3.799683
O	1.604071	1.735696	2.814482
H	1.660403	2.717223	2.710643
H	2.511820	1.376076	2.900064
O	-0.310066	1.174085	4.661323
H	-0.199632	0.318891	5.099813
H	0.477954	1.305011	4.085316
O	3.956735	-3.121756	-0.183416
H	4.353054	-3.047518	0.712282
H	3.735595	-2.193388	-0.399018
O	1.594921	-4.570148	0.002252
H	1.819318	-5.480998	-0.239504
H	2.434860	-4.062273	-0.072350
O	5.825132	-3.221267	-2.209707
H	6.647382	-3.697976	-2.025011
H	5.222267	-3.400246	-1.454194
O	5.956993	-0.513137	-1.936712
H	5.965460	-1.487402	-2.113541
H	6.107012	-0.416486	-0.964385
O	6.336526	-0.247817	0.804784
H	7.266215	-0.063302	1.008797
H	6.130408	-1.098458	1.246954
O	5.069088	-2.304114	2.224589
H	4.533250	-1.596645	2.642046
H	5.394084	-2.876414	2.935973
O	0.050201	5.178902	0.089601
H	-0.302094	4.467988	-0.491517
H	0.546177	5.777689	-0.487831
O	1.445953	4.421270	2.367420
H	0.955364	4.693091	1.557591
H	2.258086	4.947962	2.377611

Table S88. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $22H_2O$_PPII-PPII_E.

N	-4.824072	0.993686	-0.012989
C	-3.890278	-0.084706	-0.434872
C	-2.582744	0.177748	0.300996
O	-2.195367	1.350346	0.453217
N	-1.871936	-0.867720	0.712673
C	-0.505364	-0.690291	1.187723
C	0.347047	-0.230766	-0.002662
O	0.308662	-0.844681	-1.085587

N	1.099513	0.858769	0.160562
C	1.940890	1.326489	-0.925451
C	3.113497	0.378147	-1.111421
O	3.480398	-0.393090	-0.226842
O	3.729783	0.487231	-2.257536
C	-3.665166	-0.052738	-1.962431
C	0.012007	-2.003760	1.795575
C	2.417572	2.783124	-0.700113
C	-5.001518	-0.027797	-2.707276
C	-2.840700	-1.259903	-2.411325
C	-0.848058	-2.399655	2.996646
C	1.479642	-1.860479	2.192303
C	2.606708	3.502246	-2.035609
C	3.677941	2.885945	0.159307
H	-4.834196	1.019497	1.024992
H	-5.800264	0.796117	-0.323665
H	-4.505838	1.910508	-0.391977
H	-4.329945	-1.045123	-0.140254
H	-2.214309	-1.820958	0.541603
H	-0.493705	0.089877	1.960827
H	1.169837	1.293036	1.089709
H	1.348741	1.300720	-1.843892
H	4.662103	-0.031659	-2.197835
H	-3.108990	0.867295	-2.192068
H	-0.061795	-2.784783	1.027315
H	1.592485	3.271435	-0.170290
H	-5.617071	-0.885445	-2.409245
H	-4.819180	-0.097190	-3.783655
H	-5.567614	0.892571	-2.531861
H	-3.393452	-2.187444	-2.225967
H	-1.877914	-1.318628	-1.897576
H	-2.641361	-1.187919	-3.484540
H	-1.900469	-2.538805	2.729941
H	-0.799533	-1.626907	3.773186
H	-0.482182	-3.336896	3.426502
H	1.837875	-2.783340	2.658494
H	1.614220	-1.039306	2.908637
H	2.109862	-1.661585	1.319392
H	1.688653	3.474024	-2.632919
H	3.412502	3.046380	-2.621093
H	2.870300	4.550028	-1.859255
H	3.554231	2.409211	1.135212
H	3.922243	3.938384	0.332761
H	4.539520	2.423625	-0.340069
O	-4.451711	0.430968	2.710726
H	-4.270381	-0.502593	2.893922
H	-3.663545	0.936605	3.031334
O	-3.853741	3.344738	-1.299819
H	-4.260712	3.588645	-2.143784
H	-2.886486	3.297689	-1.463082
O	-1.057827	2.975472	-1.429340
H	-0.820899	2.373344	-2.175108
H	-1.217220	2.371213	-0.676239
O	-2.321023	2.005004	3.206234
H	-1.991812	1.973642	2.289450
H	-1.588163	1.691978	3.784046
O	-0.517634	0.975965	-3.248989

H	0.315069	1.059340	-3.764947
H	-0.373294	0.202885	-2.671556
O	-0.405856	-3.541979	-1.432359
H	-0.163059	-2.594358	-1.380319
H	0.310041	-4.004045	-0.937297
O	-2.627961	-3.565035	0.058136
H	-1.838673	-3.677638	-0.542898
H	-2.527994	-4.222635	0.763925
O	-7.040028	-2.176720	0.755786
H	-6.347939	-2.648501	0.236079
H	-6.689481	-2.076893	1.652772
O	-7.479015	0.239042	-0.417142
H	-7.882285	0.125935	-1.289901
H	-7.422404	-0.662243	-0.016633
O	-5.200151	-3.334339	-0.897328
H	-4.293122	-3.548366	-0.583055
H	-5.534354	-4.134092	-1.329542
O	3.914075	0.261900	2.423639
H	4.803115	0.637926	2.292785
H	3.626184	0.054916	1.507690
O	1.986980	1.175573	-4.450600
H	2.089155	0.564351	-5.195422
H	2.694232	0.940826	-3.820821
O	1.610229	1.818970	2.801051
H	1.665865	2.796256	2.665849
H	2.519056	1.458445	2.872476
O	-0.185932	1.274638	4.772632
H	-0.086714	0.386732	5.144063
H	0.564677	1.406745	4.148821
O	3.931246	-3.143853	-0.096738
H	4.332721	-3.037431	0.793493
H	3.706098	-2.224198	-0.343059
O	1.590390	-4.623874	0.137848
H	1.826841	-5.539601	-0.071823
H	2.425142	-4.109009	0.053646
O	5.793690	-3.312719	-2.123248
H	6.613267	-3.789205	-1.926488
H	5.191534	-3.465221	-1.361345
O	5.945223	-0.598817	-1.933011
H	5.945829	-1.578238	-2.078698
H	6.097317	-0.471978	-0.964495
O	6.325547	-0.243744	0.799292
H	7.255542	-0.057365	1.000187
H	6.114346	-1.079274	1.267123
O	5.053281	-2.253220	2.280590
H	4.518802	-1.534242	2.679582
H	5.378236	-2.806793	3.006669
O	0.012941	5.141408	-0.064415
H	-0.309978	4.428580	-0.658570
H	0.459736	5.785414	-0.633042
O	1.437416	4.483303	2.234159
H	0.933904	4.714200	1.420217
H	2.244729	5.016891	2.208688

Table S89. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $22H_2O$_PPII-PPII_F.

N	-4.770425	1.007251	-0.420266
C	-3.995278	-0.257471	-0.334586
C	-2.629320	0.099710	0.237945
O	-2.222234	1.274908	0.210628
N	-1.891742	-0.901234	0.708318
C	-0.524114	-0.683723	1.159412
C	0.324120	-0.203105	-0.028819
O	0.242474	-0.760091	-1.138125
N	1.140533	0.830949	0.192100
C	2.031283	1.316071	-0.846604
C	3.244980	0.407894	-0.960281
O	3.586379	-0.346271	-0.049238
O	3.924852	0.527944	-2.066728
C	-3.854266	-0.964964	-1.700470
C	0.021995	-1.994130	1.759344
C	2.455485	2.784631	-0.593624
C	-2.866978	-0.252552	-2.624953
C	-5.213121	-1.153727	-2.375163
C	-0.809454	-2.415593	2.973030
C	1.489093	-1.846302	2.152315
C	2.759210	3.502469	-1.908315
C	3.622459	2.916418	0.385702
H	-4.810377	1.418966	0.538007
H	-5.755507	0.818863	-0.693954
H	-4.338395	1.712473	-1.054012
H	-4.538877	-0.905815	0.361707
H	-2.251502	-1.861721	0.676982
H	-0.520229	0.096763	1.933469
H	1.204989	1.215503	1.143055
H	1.494818	1.276549	-1.797258
H	4.857098	-0.003079	-1.968190
H	-3.453580	-1.960266	-1.467582
H	-0.050809	-2.768393	0.984191
H	1.572597	3.256592	-0.150261
H	-3.192371	0.768297	-2.856552
H	-2.780989	-0.798104	-3.569627
H	-1.869127	-0.201519	-2.179636
H	-5.625124	-0.197946	-2.720663
H	-5.933010	-1.632195	-1.705358
H	-5.094504	-1.794832	-3.253649
H	-1.876620	-2.508865	2.751227
H	-0.695929	-1.685356	3.782645
H	-0.457636	-3.383205	3.343873
H	1.855652	-2.782141	2.586020
H	1.613388	-1.051246	2.898568
H	2.117749	-1.607474	1.290169
H	1.916399	3.426711	-2.604225
H	3.646854	3.084828	-2.395316
H	2.948907	4.563050	-1.714379
H	3.412499	2.441256	1.348225
H	3.828048	3.973981	0.577163
H	4.538975	2.470600	-0.022719

O	-4.769964	1.641100	2.299137
H	-4.945021	0.858822	2.842121
H	-3.881150	1.980888	2.572037
O	-3.642410	3.127986	-1.948457
H	-3.952672	3.331163	-2.842760
H	-2.662986	3.064800	-2.001554
O	-0.893845	2.681913	-1.734661
H	-0.544688	2.126569	-2.474020
H	-1.142551	2.051576	-1.028800
O	-2.272551	2.607396	2.692631
H	-1.949441	2.255894	1.842991
H	-1.743650	2.162749	3.393177
O	0.028138	0.856971	-3.574304
H	0.909485	1.018170	-3.981024
H	0.148107	0.092193	-2.981343
O	-0.657217	-3.387557	-1.491094
H	-0.456946	-2.429281	-1.439407
H	0.136066	-3.817447	-1.095957
O	-2.641763	-3.654219	0.273065
H	-1.926298	-3.688686	-0.422660
H	-2.404122	-4.312671	0.944200
O	-6.580070	-1.809482	0.999340
H	-6.196148	-2.597016	0.544104
H	-7.084907	-2.146100	1.753954
O	-7.491855	0.311598	-0.456368
H	-8.015116	0.078402	-1.236595
H	-7.345521	-0.524984	0.041709
O	-5.310740	-3.768293	-0.409531
H	-4.355875	-3.824668	-0.181082
H	-5.654314	-4.672339	-0.358725
O	3.850539	0.252147	2.645427
H	4.720992	0.682578	2.688738
H	3.698978	0.113424	1.684816
O	2.600554	1.306267	-4.479111
H	2.847289	0.725293	-5.214236
H	3.179809	1.052146	-3.735980
O	1.443175	1.683058	2.908846
H	1.472498	2.661287	2.775286
H	2.354848	1.354165	3.052431
O	-0.670855	1.446876	4.609068
H	-0.869884	0.563504	4.949328
H	0.183576	1.385290	4.125808
O	3.919930	-3.117893	-0.035147
H	4.253463	-3.083359	0.887165
H	3.766157	-2.173367	-0.238456
O	1.490315	-4.481104	-0.123201
H	1.725450	-5.379531	-0.398806
H	2.339300	-3.984135	-0.097708
O	5.856066	-3.303637	-1.988759
H	6.650086	-3.818411	-1.783839
H	5.224075	-3.457318	-1.251752
O	6.095992	-0.607858	-1.696711
H	6.070387	-1.580578	-1.882238
H	6.228533	-0.524614	-0.718564
O	6.393270	-0.372180	1.027037
H	7.319681	-0.292244	1.300613
H	6.047610	-1.167614	1.485373

O	4.912021	-2.296853	2.430258
H	4.389797	-1.564819	2.822482
H	5.229443	-2.844867	3.163886
O	-0.250443	4.834180	-0.083062
H	-0.405401	4.138422	-0.758041
H	0.136859	5.584360	-0.557782
O	1.128361	4.318658	2.290608
H	0.626448	4.480271	1.459710
H	1.884314	4.922781	2.266442

Table S90. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $22H_2O$_PPII-PPII_G.

N	-4.993127	0.586052	-0.057605
C	-3.984477	-0.470767	-0.349494
C	-2.662270	0.061660	0.187909
O	-2.400669	1.269286	0.048680
N	-1.825161	-0.766701	0.813392
C	-0.543244	-0.227196	1.240782
C	0.304473	0.045990	-0.006196
O	0.212152	-0.657349	-1.027164
N	1.137896	1.086755	0.067436
C	2.052677	1.375242	-1.018866
C	3.094927	0.270986	-1.110188
O	3.275207	-0.541335	-0.208415
O	3.817592	0.297653	-2.201749
C	-3.974359	-0.783834	-1.862271
C	0.185790	-1.098501	2.282162
C	2.707317	2.767646	-0.843744
C	-2.863752	-1.770940	-2.206282
C	-3.874244	0.466661	-2.738352
C	0.850653	-2.348119	1.707313
C	-0.768633	-1.445600	3.427229
C	3.086491	3.376874	-2.193284
C	3.900393	2.749050	0.112439
H	-5.151521	0.599485	0.967487
H	-5.890049	0.390012	-0.546995
H	-4.645153	1.521637	-0.356799
H	-4.280138	-1.365549	0.205012
H	-2.039703	-1.767331	0.885632
H	-0.743546	0.735687	1.724456
H	1.211887	1.602666	0.953327
H	1.487800	1.378338	-1.955747
H	4.694761	-0.267037	-2.040801
H	-4.939574	-1.272906	-2.052208
H	0.973577	-0.446727	2.683681
H	1.918505	3.393432	-0.410163
H	-1.878510	-1.320134	-2.047192
H	-2.936518	-2.058220	-3.259459
H	-2.928178	-2.680918	-1.606019
H	-2.948123	1.017759	-2.540027

H	-4.717941	1.150112	-2.600918
H	-3.863705	0.164127	-3.790038
H	1.547036	-2.105847	0.896190
H	0.110413	-3.053953	1.318177
H	1.416111	-2.862190	2.491835
H	-0.210224	-1.870288	4.266558
H	-1.512677	-2.186937	3.113688
H	-1.306313	-0.558397	3.779840
H	2.220905	3.417245	-2.863743
H	3.877093	2.800448	-2.684578
H	3.453502	4.397624	-2.046134
H	3.638891	2.334410	1.090490
H	4.268457	3.767303	0.270109
H	4.729697	2.157726	-0.296742
O	-4.593859	0.364740	2.704224
H	-4.214081	-0.474230	3.003711
H	-3.896183	1.053360	2.835887
O	-4.118524	3.242871	-0.952908
H	-4.613017	3.747659	-1.614778
H	-3.202733	3.183545	-1.289479
O	-1.177374	3.055025	-1.578599
H	-0.853672	2.504406	-2.328021
H	-1.305240	2.403389	-0.862681
O	-2.790873	2.381938	2.674565
H	-2.483031	2.276375	1.756715
H	-2.003494	2.275476	3.256442
O	-0.412187	1.026246	-3.322710
H	0.438653	1.045179	-3.812026
H	-0.305579	0.306637	-2.671746
O	-0.412155	-3.450273	-1.168668
H	-0.190549	-2.497696	-1.120821
H	0.387973	-3.930885	-0.851779
O	-2.411557	-3.594966	0.607359
H	-1.675932	-3.691526	-0.060766
H	-2.225898	-4.221705	1.323511
O	-6.642889	-1.901334	0.544549
H	-6.122145	-2.691923	0.270517
H	-7.183939	-2.174113	1.299506
O	-7.434986	-0.121539	-1.321854
H	-7.491821	-0.373384	-2.254738
H	-7.413836	-0.952976	-0.800384
O	-4.970659	-3.812252	-0.430756
H	-4.071819	-3.854292	-0.034458
H	-5.280880	-4.727123	-0.499610
O	3.481317	0.140631	2.453917
H	4.407430	0.383366	2.253550
H	3.141153	-0.099233	1.565783
O	2.151629	1.003599	-4.468163
H	2.209812	0.357362	-5.187726
H	2.848848	0.751426	-3.834762
O	1.529951	2.144824	2.682371
H	1.756917	3.089919	2.504090
H	2.352990	1.637063	2.838808
O	-0.623849	2.108484	4.339907
H	-0.597890	1.413768	5.013018
H	0.225033	2.057199	3.843692
O	3.964749	-3.222415	0.091647

H	4.209356	-3.115474	1.037091
H	3.740139	-2.312152	-0.191928
O	1.747064	-4.846042	-0.183645
H	2.009206	-5.578901	-0.759967
H	2.550683	-4.286644	-0.081281
O	5.994799	-3.548580	-1.723285
H	6.808517	-3.973849	-1.415920
H	5.332863	-3.654416	-1.004145
O	5.964569	-0.830018	-1.582542
H	6.043190	-1.807213	-1.716218
H	5.997327	-0.683807	-0.607989
O	6.011937	-0.372825	1.194667
H	6.889750	-0.053510	1.455431
H	5.876412	-1.211472	1.683421
O	4.685872	-2.361080	2.621235
H	4.068926	-1.649906	2.893726
H	4.850887	-2.915265	3.398869
O	0.202900	5.126018	-0.377593
H	-0.248526	4.394998	-0.860124
H	0.647113	5.659281	-1.052902
O	1.701207	4.741626	1.923562
H	1.168158	4.883024	1.107518
H	2.543535	5.195576	1.777489

Table S91. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $22H_2O$_PPII-PPII_H.

N	-4.942780	0.797436	-0.135687
C	-3.897581	-0.217218	-0.446821
C	-2.634365	0.278499	0.246885
O	-2.397896	1.500731	0.227510
N	-1.807269	-0.595504	0.819795
C	-0.504872	-0.115531	1.261703
C	0.362835	0.102059	0.018236
O	0.275755	-0.643901	-0.972924
N	1.203843	1.137711	0.048739
C	2.122757	1.359062	-1.050393
C	3.128715	0.218241	-1.103185
O	3.293032	-0.560219	-0.168842
O	3.840232	0.175122	-2.201146
C	-3.674661	-0.307428	-1.972441
C	0.169897	-1.024629	2.307566
C	2.822187	2.734138	-0.926803
C	-5.003690	-0.475427	-2.711683
C	-2.732856	-1.461083	-2.309861
C	0.773848	-2.305115	1.732235
C	-0.816292	-1.327348	3.438178
C	3.260297	3.264152	-2.291963
C	3.986529	2.718968	0.063878
H	-4.969067	0.925580	0.894073
H	-5.891365	0.478601	-0.430297

H	-4.704146	1.696369	-0.601914
H	-4.230883	-1.182628	-0.049470
H	-2.010867	-1.600485	0.763310
H	-0.663396	0.855247	1.741243
H	1.282642	1.685160	0.914087
H	1.552743	1.343982	-1.984943
H	4.702786	-0.406685	-2.022024
H	-3.209562	0.637771	-2.285547
H	0.986903	-0.416321	2.719739
H	2.044502	3.406937	-0.547848
H	-5.545367	-1.348206	-2.327129
H	-4.808020	-0.638382	-3.775706
H	-5.647379	0.406573	-2.631366
H	-3.201044	-2.420997	-2.067135
H	-1.786644	-1.386116	-1.769944
H	-2.507670	-1.451344	-3.380561
H	1.518563	-2.093931	0.956591
H	0.005272	-2.952175	1.296756
H	1.270372	-2.871405	2.527181
H	-0.291399	-1.779181	4.284978
H	-1.589898	-2.031233	3.110425
H	-1.317378	-0.416397	3.784695
H	2.417361	3.297306	-2.990743
H	4.047575	2.642641	-2.730416
H	3.653214	4.279778	-2.181430
H	3.682709	2.360649	1.051911
H	4.386527	3.730033	0.185740
H	4.804734	2.079321	-0.292003
O	-4.519508	0.550198	2.629416
H	-4.195475	-0.325589	2.886724
H	-3.810825	1.194288	2.878424
O	-4.110324	3.071225	-1.694733
H	-4.524103	3.250686	-2.551335
H	-3.142043	3.096285	-1.847005
O	-1.236851	2.960425	-1.758068
H	-0.883536	2.318216	-2.419238
H	-1.413293	2.415901	-0.964556
O	-2.645439	2.473607	2.897640
H	-2.338416	2.406406	1.975460
H	-1.860881	2.324510	3.473588
O	-0.408000	0.858189	-3.338514
H	0.446558	0.891754	-3.820421
H	-0.277765	0.173520	-2.654979
O	-0.303686	-3.409696	-1.274344
H	-0.021449	-2.478536	-1.173040
H	0.418467	-3.951039	-0.877044
O	-2.433366	-3.379160	0.345334
H	-1.678094	-3.516785	-0.293853
H	-2.300842	-4.013387	1.067055
O	-6.900958	-2.413839	0.998351
H	-6.182859	-2.864857	0.495126
H	-6.526771	-2.180940	1.860535
O	-7.528146	-0.201855	-0.459066
H	-7.903012	-0.458902	-1.313797
H	-7.408920	-1.036641	0.055676
O	-5.006439	-3.528523	-0.618094
H	-4.080041	-3.593509	-0.292794

H	-5.248502	-4.413916	-0.927514
O	3.521530	0.206079	2.467133
H	4.454572	0.421501	2.269659
H	3.183615	-0.051230	1.582807
O	2.164675	0.864434	-4.470825
H	2.224842	0.225106	-5.196415
H	2.865266	0.610817	-3.841716
O	1.577635	2.214000	2.663224
H	1.791302	3.153964	2.449993
H	2.408549	1.716895	2.813163
O	-0.434414	2.126474	4.493110
H	-0.357853	1.380164	5.104544
H	0.367473	2.107918	3.921483
O	3.906027	-3.255811	0.207587
H	4.146616	-3.124532	1.150944
H	3.703209	-2.350179	-0.105437
O	1.685161	-4.879222	-0.066391
H	1.965506	-5.647693	-0.584911
H	2.490083	-4.323026	0.042558
O	5.925411	-3.704879	-1.593991
H	6.728563	-4.138277	-1.270567
H	5.262212	-3.765730	-0.870889
O	5.959528	-0.982856	-1.546457
H	6.016362	-1.965317	-1.647767
H	5.998397	-0.805186	-0.577195
O	6.033185	-0.439124	1.213181
H	6.925670	-0.152538	1.461809
H	5.860394	-1.253440	1.730504
O	4.638046	-2.329066	2.710049
H	4.046159	-1.588535	2.959083
H	4.791593	-2.857996	3.507362
O	0.236458	5.010309	-0.611288
H	-0.236527	4.287237	-1.083967
H	0.670362	5.540555	-1.295534
O	1.693767	4.765844	1.745797
H	1.167570	4.851962	0.918592
H	2.519653	5.246208	1.590316

Table S92. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $Val_3H^+ \cdot 22H_2O$ trivaline-water complex with the backbone chain in the PPII-PPII conformation, $22H_2O$_PPII-PPII_I.

N	-4.824212	0.819187	-0.587359
C	-3.939140	-0.346684	-0.318026
C	-2.633759	0.231311	0.211826
O	-2.343440	1.416758	-0.031534
N	-1.811289	-0.570509	0.886309
C	-0.513868	-0.055856	1.293787
C	0.345110	0.183772	0.044532
O	0.208835	-0.503101	-0.981561
N	1.252252	1.161450	0.131306

C	2.216890	1.376744	-0.930972
C	3.191745	0.207096	-0.974386
O	3.282951	-0.605856	-0.057950
O	3.965834	0.175791	-2.027522
C	-3.708490	-1.208559	-1.576777
C	0.195407	-0.972187	2.311506
C	2.963991	2.720000	-0.741041
C	-2.804768	-0.526040	-2.604360
C	-5.036864	-1.631914	-2.206239
C	0.759112	-2.253628	1.697933
C	-0.736203	-1.276105	3.487247
C	3.499669	3.261023	-2.066400
C	4.069695	2.636324	0.311875
H	-4.930204	1.326624	0.313432
H	-5.776088	0.522791	-0.886337
H	-4.414219	1.479831	-1.280098
H	-4.435163	-0.939774	0.457312
H	-2.073380	-1.546706	1.056148
H	-0.674561	0.911550	1.785280
H	1.352953	1.651456	1.027686
H	1.682589	1.412723	-1.886495
H	4.799108	-0.452077	-1.824392
H	-3.197262	-2.110446	-1.220010
H	1.032839	-0.374700	2.691606
H	2.192499	3.414100	-0.391968
H	-3.252428	0.398571	-2.986831
H	-2.641813	-1.196353	-3.454035
H	-1.825975	-0.281230	-2.182298
H	-5.541670	-0.785463	-2.685338
H	-5.715141	-2.071844	-1.469361
H	-4.847788	-2.382582	-2.979480
H	1.463123	-2.040778	0.886961
H	-0.034422	-2.890854	1.294667
H	1.289403	-2.831033	2.462821
H	-0.169339	-1.732494	4.303844
H	-1.526963	-1.978936	3.201306
H	-1.215659	-0.366123	3.862930
H	2.704679	3.325078	-2.817331
H	4.300645	2.630666	-2.465050
H	3.906228	4.265542	-1.912473
H	3.700994	2.261779	1.271585
H	4.495963	3.628977	0.485349
H	4.884330	1.977716	-0.017120
O	-4.597447	1.417804	2.109183
H	-5.342292	1.614537	2.695349
H	-3.904377	2.099672	2.289267
O	-3.756053	2.825038	-2.348701
H	-4.057643	2.926483	-3.263017
H	-2.775169	2.832546	-2.380020
O	-0.945060	2.629138	-2.035027
H	-0.514184	2.022776	-2.685173
H	-1.226852	2.056752	-1.293091
O	-2.500386	3.131413	2.225252
H	-2.155616	2.742315	1.401421
H	-1.870146	2.879537	2.937311
O	0.160829	0.666201	-3.608854
H	1.054512	0.790204	-3.999504

H	0.275089	0.021157	-2.886085
O	-0.860620	-3.107287	-1.200068
H	-0.558455	-2.178456	-1.115229
H	-0.062794	-3.656057	-1.015116
O	-2.578998	-3.362557	0.826577
H	-1.945654	-3.429731	0.058200
H	-2.286827	-4.008242	1.488444
O	-6.607660	-1.682538	1.064264
H	-6.188757	-2.544411	0.827146
H	-7.090273	-1.828839	1.890691
O	-7.503453	-0.049466	-0.928370
H	-8.128830	0.617887	-0.610218
H	-7.394760	-0.694217	-0.192579
O	-5.227263	-3.872890	0.220236
H	-4.273979	-3.751685	0.431645
H	-5.474662	-4.734556	0.586855
O	3.467822	0.046166	2.614084
H	4.424367	0.210723	2.502995
H	3.181345	-0.134324	1.692980
O	2.768191	1.007708	-4.495206
H	2.980360	0.424280	-5.239144
H	3.338979	0.716241	-3.759951
O	1.570190	2.116171	2.817774
H	1.806119	3.051278	2.613273
H	2.382377	1.604434	3.007863
O	-0.729004	2.471603	4.232131
H	-0.938908	1.846223	4.939668
H	0.153825	2.224385	3.877967
O	3.658262	-3.363274	0.096925
H	3.840369	-3.330851	1.060838
H	3.562894	-2.418100	-0.141650
O	1.291106	-4.683912	-0.499694
H	1.526606	-5.356629	-1.155249
H	2.131046	-4.220399	-0.280920
O	5.780416	-3.812622	-1.584133
H	6.525245	-4.324476	-1.236615
H	5.057944	-3.882327	-0.921127
O	5.986933	-1.111874	-1.345831
H	5.989434	-2.088547	-1.507564
H	5.999714	-0.995896	-0.365539
O	5.975505	-0.767710	1.428171
H	6.878942	-0.628810	1.752238
H	5.659389	-1.589384	1.860340
O	4.306618	-2.608715	2.689467
H	3.788651	-1.824921	2.969790
H	4.420402	-3.171577	3.470171
O	0.181275	4.696395	-0.548683
H	-0.141639	3.966192	-1.123562
H	0.485360	5.392654	-1.148771
O	1.590555	4.647303	1.861761
H	1.070486	4.658773	1.027356
H	2.369185	5.199209	1.699648