

Supplementary Tables

Table S1. Experimental PAs of the most stable conformers of benzene, toluene, naphthalene and 1-methylnaphthalene. All values of energy are listed in kJ mol⁻¹ at 298 K and 1 atm

	experimental ^a	B3LYP-D3 / 6-311++G(d,p)	B3LYP-D3 / 6-31+G(d,p)
benzene	750.4	762.3 ^b	773.2
toluene	784.0	802.8 ^c	803.0
naphthalene	802.9	820.9 ^b	825.5
1-methylnaphthalene	834.8	832.3	835.9

a Experimental PA values from ref. 64. b Computed PA values from ref. 65. c Computed PA values from ref. 66.

Table S2. Computational proton affinities (kJ mol⁻¹) of TMnTP (n=7-9) at aromatic carbons under B3LYP-D3/6-31+G(d,p)

Protonation Position		TM7TP	TM8TP	TM9TP
1	-	971.5	975.7	979.1
2	exo	888.6	897.6	898.1
	endo	843.1	839.7	833.3
3	-	963.9	967.5	971.6
3a	exo	855.9	854.4	851.7
	endo	823.6	822.5	822.2
4	-	950.1	952.3	954.7
5	-	905.8	904.2	901.5
5a	exo	947.0	943.6	941.6
	endo	861.9	867.8	874.2
5b	exo	946.0	937.9	927.4
	endo	859.3	862.9	864.7
6	-	945.0	941.3	939.7
16	-	945.0	943.4	939.6
16a	exo	946.4	935.9	927.8
	endo	859.3	861.1	864.6
16b	exo	899.2	889.7	854.5
	endo	809.9	815.2	820.1
17	-	902.4	900.0	898.4
18	-	951.5	954.8	956.1
18a	exo	849.4	848.0	845.7
	endo	820.1	819.3	819.5
18b	exo	860.7	861.1	861.2
	endo	819.6	821.7	825.9
18c	exo	884.6	877.8	871.3
	endo	821.3	822.1	823.6
18d	exo	947.7	946.9	942.9
	endo	863.3	870.1	875.6

Table S3. Rate constants of [(TMnTP)(Gly)]H⁺ (n=7, 8, 9), at the temperature (T) ranging from 329 K to 371K, the unit of all rate constant values is s⁻¹ and all temperature listed are in K

[(TM7TP)(Gly)]H ⁺			[(TM8TP)(Gly)]H ⁺			[(TM9TP)(Gly)]H ⁺		
T	FD	SD	T	FD	SD	T	FD	SD
/ K		× 10 ⁻²	/ K		× 10 ⁻²	/ K		× 10 ⁻²
334.8	0.37 ± 0.03	0.12 ± 0.006	330.0	0.23 ± 0.01	0.25 ± 0.004	328.9	0.36 ± 0.03	0.97 ± 0.02
341.6	0.47 ± 0.02	0.18 ± 0.004	335.3	0.44 ± 0.05	0.35 ± 0.03	342.2	0.75 ± 0.08	2.83 ± 0.23
353.3	0.79 ± 0.04	0.72 ± 0.03	354.1	0.71 ± 0.02	1.74 ± 0.03	350.9	1.02 ± 0.07	3.71 ± 0.14
356.7	0.83 ± 0.02	0.65 ± 0.02	356.7	1.02 ± 0.10	2.95 ± 0.20	357.0	1.47 ± 0.13	9.02 ± 0.55
363.9	1.30 ± 0.07	1.52 ± 0.03	364.9	1.22 ± 0.04	3.31 ± 0.08	370.6	3.20 ± 0.35	14.18 ± 0.65

Table S4. Natural energy decomposition analysis (NEDA) components in kJ mol^{-1} under B3LYP-D3/6-31+G(d,p)

complex	<i>endo</i> -(TMnTP)(GlyH ⁺)			<i>endo</i> -(TMnTPH ⁺)(Gly)			<i>exo</i> -(TMnTP)(GlyH ⁺)			<i>exo</i> -(TMnTPH ⁺)(Gly)			
	n	7	8	9	7	8	9	7	8	9	7	8	9
E _{tot}		-183.97	-197.97	-199.30	-77.40	-82.62	-84.78	-131.48	-135.41	-136.58	-53.09	-51.89	-51.40
ES		-70.68	-94.50	-85.84	-61.69	-56.04	-56.87	-66.63	-67.09	-67.28	-51.70	-51.63	-49.90
POL		-460.20	-598.47	-571.57	-215.13	-235.44	-237.59	-386.44	-385.78	-389.49	-87.66	-88.96	-76.71
XC		-241.25	-316.68	-296.20	-197.72	-231.76	-225.10	-148.16	-138.00	-138.54	-56.77	-56.32	-52.06
CT		-2.00	-1.69	-1.54	-1.57	-1.75	-1.35	-2.22	-1.67	-1.31	-1.16	-1.10	-1.21
DEF _{host}		418.58	559.25	528.60	176.76	204.89	206.46	368.49	365.92	367.10	45.84	46.74	36.21
DEF _{guest}		171.85	254.11	227.25	221.97	237.48	229.66	103.47	91.20	92.94	98.36	99.37	92.28
SE _{host}		194.20	247.01	238.11	56.87	65.76	68.16	173.54	175.82	177.29	14.98	15.46	12.04
SE _{guest}		40.63	56.79	52.01	52.81	53.56	52.92	25.71	22.87	23.37	29.84	30.02	27.11
EL		-296.06	-389.15	-367.28	-167.15	-172.17	-173.39	-253.81	-254.18	-256.11	-94.54	-95.11	-87.46
CT		-2.00	-1.69	-1.54	-1.57	-1.75	-1.35	-2.22	-1.67	-1.31	-1.16	-1.10	-1.21
CORE		114.08	192.87	169.52	91.33	91.29	89.96	124.55	120.44	120.83	42.61	44.31	37.28

Table S5. Relative enthalpies and Gibbs energies (in parentheses) of the lowest energy *endo*-(TMnTP)(GlyH⁺), *endo*-(TMnTPH⁺)(Gly), *exo*-(TMnTP)(GlyH⁺), and *exo*-(TMnTPH⁺)(Gly) structures at the B3LYP-D3/6-31+G(d,p) and wB97xD/6-31+G(d,p) levels and basis set.

Species	B3LYP/6-31+G(d,p)	wB97xD/6-31+G(d,p)
<i>endo</i> -(TM7TP)(GlyH ⁺)	0.0 (0.0)	0.0 (0.0)
<i>endo</i> -(TM7TPH ⁺)(Gly)	24.9 (27.0)	44.9 (47.3)
<i>exo</i> -(TM7TPH ⁺)(Gly)	48.4 (30.5)	72.8 (53.6)
<i>exo</i> -(TM7TP)(GlyH ⁺)	51.6 (45.9)	59.5 (51.0)
<i>endo</i> -(TM8TP)(GlyH ⁺)	0.0 (0.0)	0.0 (0.0)
<i>endo</i> -(TM8TPH ⁺)(Gly)	26.3 (20.4)	41.9 (36.5)
<i>exo</i> -(TM8TPH ⁺)(Gly)	57.9 (31.2)	80.4 (50.6)
<i>exo</i> -(TM8TP)(GlyH ⁺)	63.5 (48.3)	69.5 (46.6)
<i>endo</i> -(TM9TP)(GlyH ⁺)	0.0 (0.0)	0.0 (0.0)
<i>endo</i> -(TM9TPH ⁺)(Gly)	26.5 (24.8)	40.6 (35.6)
<i>exo</i> -(TM9TPH ⁺)(Gly)	57.0 (30.5)	78.5 (49.7)
<i>exo</i> -(TM9TP)(GlyH ⁺)	64.3 (46.1)	70.9 (52.3)

Coordinates of the lowest-energy TMnTP/Glycine/H⁺ complex types

endo-(TM7TP)(GlyH⁺)

C	-4.17939534	1.70117786	0.32294321
C	-4.05817810	1.06605434	-0.92421518
H	-4.09146754	1.65129279	-1.83702614
C	-3.77565667	-0.30392687	-1.03827103
C	-3.59266616	-1.07869338	0.14699166
C	-3.90868294	-0.48776848	1.40354926
C	-4.19810849	0.88720189	1.46423205
H	-4.35986880	1.32228518	2.44374432
C	-3.50085326	-0.93623799	-2.30530754
H	-3.77601501	-0.41709587	-3.21867107
C	-2.82441203	-2.11903504	-2.36244041
H	-2.56450332	-2.53500624	-3.32937701
C	-2.33298360	-2.75289541	-1.16053738
C	-2.86604280	-2.31426490	0.09298240
C	-2.43073063	-2.90591396	1.31960328
C	-3.05635100	-2.46411023	2.54219008
H	-2.88172777	-3.01328894	3.46025542
C	-3.76110013	-1.29790074	2.58438014
H	-4.15041028	-0.92658388	3.52811401
C	-1.12429744	-3.50130420	-1.15618542
C	-0.47039911	-3.71061690	0.09569227
C	-1.20247533	-3.62327888	1.31803034
C	-0.34869732	-3.75231589	-2.34966629
H	-0.85021425	-3.90225507	-3.29963859
C	1.01309681	-3.69797838	-2.30449445
H	1.58521989	-3.80222281	-3.22000746
C	1.68243639	-3.37038958	-1.06620057
C	0.96899152	-3.62993705	0.14170176
C	1.59403232	-3.43290550	1.40818302
C	0.86145189	-3.85993742	2.57563396
H	1.37998363	-4.00541209	3.51685473
C	-0.49613981	-3.95861047	2.53137616
H	-1.04847638	-4.18272183	3.43688281
C	2.80575116	-2.50211377	-1.00931592
C	3.15245054	-1.94070532	0.25882189
C	2.69755575	-2.53987227	1.47407318
C	3.36462189	-1.89021440	-2.19157729
H	3.27035065	-2.39115889	-3.14874275
C	3.89852497	-0.63573689	-2.14364856
H	4.22693267	-0.14507566	-3.05540193
C	3.94071127	0.09841110	-0.90355162
C	3.71574808	-0.62638492	0.30404492
C	3.83214806	0.05753810	1.54648106
C	3.67289952	-0.70723229	2.75479608
H	3.91331256	-0.24147172	3.70641092
C	3.13825412	-1.96149871	2.71892305
H	2.94792555	-2.48472642	3.64906532
C	4.03806733	1.49731536	-0.84971032
H	4.11318527	2.03628183	-1.78893702
C	3.94421738	2.20388349	0.36254965

C	3.94478653	1.45880164	1.54931379
H	3.95163776	1.95985719	2.51038416
C	3.72063635	3.72518658	0.35050428
C	3.83800413	4.35027773	1.75494531
H	3.09726268	3.96192908	2.45936612
H	3.68770610	5.43220948	1.68795412
H	4.83191014	4.17951900	2.18106221
C	4.76409120	4.42068315	-0.55538737
H	5.77931378	4.22381088	-0.19702757
H	4.60614890	5.50417449	-0.55035557
H	4.70308726	4.08758719	-1.59550473
C	2.29695653	4.01789033	-0.23626192
H	2.28801833	3.71191964	-1.29133392
H	2.16609428	5.10823221	-0.23561860
C	1.07907832	3.38234749	0.46356476
H	1.14489769	2.28498219	0.36709253
H	1.10565595	3.58749723	1.54049167
C	-0.25656501	3.88824293	-0.11494809
H	-0.28738455	3.68342177	-1.19249276
H	-0.28722192	4.98120217	-0.01483885
C	-1.52156275	3.30358881	0.54100740
H	-1.48855074	2.20451714	0.50971807
H	-1.53625977	3.57459572	1.60356964
C	-2.81161702	3.77059871	-0.15838247
H	-2.73772321	3.50162395	-1.21879380
H	-2.85117861	4.86740862	-0.12145404
C	-4.17548046	3.23812687	0.39887990
C	-5.31079548	3.81298308	-0.48162889
H	-5.19810607	3.53771751	-1.53434807
H	-5.31527573	4.90661904	-0.42636529
H	-6.28597029	3.45139609	-0.14048905
C	-4.38626680	3.75743429	1.83422020
H	-5.35799120	3.44649318	2.23161777
H	-4.36630637	4.85163769	1.83320939
H	-3.61158241	3.41656103	2.52724006
N	-0.49106714	-0.23951178	-0.31458052
H	-1.46970133	-0.14715386	-0.63641613
C	0.45990152	-0.14496000	-1.46508374
C	-0.00171602	0.96106130	-2.39129907
H	1.46641805	0.04249583	-1.09114966
H	0.45468104	-1.10039929	-1.99365546
O	-1.06928051	1.52204778	-2.27903547
O	0.91269816	1.20360606	-3.33392405
H	0.57438733	1.89315028	-3.93297346
H	-0.33785960	0.51803754	0.36001130
H	-0.39649376	-1.14265868	0.16723086

endo-(TM7TPH⁺)(Gly)

C	-4.19131100	1.82992600	0.38949100
C	-4.35001000	1.16462000	-0.95201500
H	-3.77209400	1.68887800	-1.71948700
C	-3.97860800	-0.28711600	-1.01855200
C	-3.70055700	-1.00068800	0.16415000
C	-3.94901100	-0.37688500	1.42726700
C	-4.17454500	1.04285300	1.49886200
H	-4.16595700	1.48219800	2.48961800
C	-3.77658600	-0.91896100	-2.25300500
H	-4.06611900	-0.41510100	-3.17000500
C	-3.03866100	-2.09077000	-2.32021900
H	-2.77542700	-2.47833800	-3.29821300
C	-2.49537500	-2.68268200	-1.15453100
C	-2.97104900	-2.22302600	0.10696400
C	-2.51077300	-2.81472700	1.32027200
C	-3.05078000	-2.33055100	2.54199500
H	-2.80884400	-2.82992300	3.47359100
C	-3.75334600	-1.14114400	2.59730600
H	-4.04116500	-0.72887100	3.55955600
C	-1.25428000	-3.41519100	-1.18121900
C	-0.57826500	-3.63498900	0.05249300
C	-1.29284200	-3.56653400	1.28884100
C	-0.50836600	-3.63593700	-2.38142400
H	-1.01748400	-3.70393700	-3.33613900
C	0.86277500	-3.60181800	-2.35515700
H	1.40690800	-3.64778200	-3.29257200
C	1.56524100	-3.36035600	-1.13036300
C	0.85505600	-3.61131300	0.07932100
C	1.50924800	-3.49408900	1.33927000
C	0.77496600	-3.91576700	2.49681200
H	1.29377700	-4.09408900	3.43246600
C	-0.59188100	-3.96720100	2.47129800
H	-1.13542900	-4.18022300	3.38475000
C	2.75504500	-2.57447700	-1.06434000
C	3.14277000	-2.06472500	0.21141500
C	2.66225200	-2.66369100	1.41726100
C	3.37283500	-1.99545500	-2.23029000
H	3.25850900	-2.47980400	-3.19429600
C	4.00116500	-0.78395900	-2.15722300
H	4.39299400	-0.31545100	-3.05647600
C	4.06785300	-0.06631500	-0.91175400
C	3.78742400	-0.79231000	0.27958400
C	3.92668700	-0.13381600	1.53147000
C	3.73190500	-0.91007300	2.72515300
H	3.98858900	-0.47112700	3.68522200
C	3.14034000	-2.13893000	2.66872000
H	2.92280700	-2.66547100	3.59089700
C	4.22243800	1.32728700	-0.83770500
H	4.34438700	1.87471300	-1.76738800
C	4.11211700	2.02419100	0.37913000

C	4.08084600	1.26257400	1.55580600
H	4.08705000	1.75095000	2.52325600
C	3.90663100	3.54929500	0.38496500
C	4.05797300	4.15850500	1.79268500
H	3.33248300	3.76257400	2.50795800
H	3.90487000	5.24100300	1.74109400
H	5.06205500	3.98273500	2.19264800
C	4.94251200	4.23780500	-0.53517400
H	5.96267300	3.99848400	-0.21881500
H	4.81989600	5.32483300	-0.49376200
H	4.83494700	3.94040000	-1.58272700
C	2.47552800	3.86645700	-0.17515800
H	2.42503200	3.47715000	-1.20269500
H	2.40206600	4.95842600	-0.26874500
C	1.24536000	3.36129600	0.60672600
H	1.29778600	2.27260400	0.73930300
H	1.24434500	3.79150000	1.61552300
C	-0.07526300	3.73804300	-0.09645600
H	-0.08964900	3.28817000	-1.09944500
H	-0.08752800	4.82446000	-0.26385500
C	-1.36530500	3.33543300	0.65024800
H	-1.36683100	2.25526100	0.82827500
H	-1.36896800	3.82383500	1.63251300
C	-2.62154200	3.73876700	-0.14805700
H	-2.53105800	3.33293800	-1.16229800
H	-2.63188100	4.83138700	-0.25914300
C	-4.03547700	3.34797500	0.42503200
C	-5.10704400	4.00247900	-0.48443800
H	-4.98325200	3.72857600	-1.53635100
H	-5.03187400	5.09214500	-0.42078100
H	-6.11643700	3.71659100	-0.16955000
C	-4.19859900	3.92277400	1.84446200
H	-5.19632400	3.71361300	2.24424900
H	-4.07197100	5.00926800	1.81371600
H	-3.45863500	3.52963600	2.54613200
H	-5.40454900	1.28633500	-1.25315100
N	1.19558700	1.13298400	-3.04186900
H	-0.67699200	1.45101300	-3.12911400
C	0.84014000	0.38395100	-1.83273400
C	-0.62087800	0.61108300	-1.46957500
H	0.95415100	-0.68948000	-2.00172700
H	1.44819700	0.62943100	-0.95849800
O	-1.33302600	1.24677700	-2.41435500
O	-1.10715500	0.23696000	-0.42382000
H	1.77034000	0.58543400	-3.67283500
H	1.70443700	1.98336600	-2.81988000

exo-(TM7TPH⁺)(Gly)

C	-4.42884402	1.68410393	0.63282052
C	-4.65866558	0.96948308	-0.66981287
H	-4.26169369	1.53776639	-1.51721529
C	-4.13366896	-0.43241749	-0.75083996
C	-3.67686195	-1.08584101	0.41456028
C	-3.86173087	-0.45443650	1.68809105
C	-4.21186017	0.94189238	1.75217592
H	-4.13547525	1.41354078	2.72526583
C	-4.00245109	-1.07744990	-1.98790385
H	-4.42152265	-0.61421351	-2.87546182
C	-3.21140524	-2.21358483	-2.09839765
H	-3.02073057	-2.61218437	-3.08861442
C	-2.53595642	-2.75492348	-0.98006609
C	-2.88735536	-2.26817135	0.31264515
C	-2.28184385	-2.80800701	1.48862473
C	-2.72040663	-2.31617041	2.74313348
H	-2.35277092	-2.76959580	3.65707488
C	-3.49393779	-1.17084816	2.84378847
H	-3.71248044	-0.75396966	3.82222218
C	-1.28437772	-3.46081511	-1.11706227
C	-0.46579487	-3.60048375	0.04106985
C	-1.04037145	-3.51578960	1.34673338
C	-0.67131784	-3.71259042	-2.38112840
H	-1.27923052	-3.85349763	-3.26750471
C	0.68916378	-3.58698507	-2.51236203
H	1.12784025	-3.63599501	-3.50314954
C	1.49921788	-3.23747792	-1.38682635
C	0.95722764	-3.50384036	-0.09644116
C	1.74408256	-3.30778071	1.07431203
C	1.16715341	-3.72058335	2.31801092
H	1.79260359	-3.82759030	3.19769749
C	-0.19264383	-3.83707064	2.45159891
H	-0.61622087	-4.02791342	3.43113642
C	2.59549181	-2.32770381	-1.47617350
C	3.10554894	-1.77568354	-0.26101558
C	2.84565049	-2.40439652	0.99688742
C	2.95701112	-1.68762926	-2.71199241
H	2.72270042	-2.16823767	-3.65514314
C	3.45800343	-0.41683102	-2.71574137
H	3.62807879	0.09941134	-3.65659607
C	3.66698552	0.29408430	-1.48478964
C	3.64364128	-0.45375988	-0.27400757
C	3.92698815	0.21314453	0.94829958
C	3.96748978	-0.57485139	2.14816873
H	4.33280668	-0.11933112	3.06452329
C	3.45886516	-1.84312783	2.16935494
H	3.41534403	-2.38142709	3.10945078
C	3.73054168	1.69353410	-1.41873095
H	3.64551681	2.24959795	-2.34728513
C	3.77662292	2.37936079	-0.19280593

C	3.98823826	1.61830622	0.96455874
H	4.11399380	2.10529892	1.92479201
C	3.47030564	3.88518821	-0.14952848
C	3.66540530	4.48498669	1.25651490
H	3.01552667	4.02545581	2.00639001
H	3.43218751	5.55411507	1.23284770
H	4.70223586	4.38035917	1.59352662
C	4.40226361	4.65069995	-1.11865035
H	5.45169430	4.50847018	-0.84095783
H	4.18358201	5.72324944	-1.08457820
H	4.28060268	4.32547402	-2.15607347
C	1.98927089	4.10909850	-0.61522013
H	1.91024237	3.81112685	-1.66909344
H	1.80864736	5.19273198	-0.59391429
C	0.86619032	3.40512939	0.17298954
H	1.00191051	2.31662212	0.12029385
H	0.92591291	3.67407347	1.23543750
C	-0.53178186	3.78195404	-0.35829736
H	-0.60587997	3.49722074	-1.41731098
H	-0.63306321	4.87641872	-0.33241126
C	-1.71586961	3.16125576	0.41162775
H	-1.66043539	2.06572742	0.34933184
H	-1.62171128	3.41374610	1.47574118
C	-3.06951857	3.65311900	-0.13804862
H	-3.14622553	3.36876092	-1.19305522
H	-3.07663688	4.75136152	-0.12224231
C	-4.38467932	3.20586101	0.60603182
C	-5.58904849	3.76066208	-0.19578354
H	-5.58044007	3.42302266	-1.23561893
H	-5.55263567	4.85453103	-0.20584921
H	-6.53697919	3.45911353	0.26320646
C	-4.42135908	3.82189149	2.01722441
H	-5.33384282	3.53698509	2.55168407
H	-4.40808237	4.91316396	1.93898180
H	-3.56246443	3.52974368	2.62720875
H	-5.74734814	0.95741417	-0.85133930
N	-6.33565127	2.52115925	-6.17754493
H	-6.26798508	1.25333643	-4.80478211
C	-5.18602437	3.11371028	-5.48166900
C	-4.84138787	2.29686345	-4.22963237
H	-4.28821098	3.14104552	-6.10698410
H	-5.37269859	4.14212242	-5.15683775
O	-5.62995421	1.22989461	-4.04203252
O	-3.93848314	2.58639804	-3.47119337
H	-6.12010270	2.23408821	-7.12588951
H	-7.14023202	3.13782052	-6.20841401

exo-(TM7TP)(GlyH⁺)

C	2.43715506	4.33111151	0.01811103
C	1.68269541	4.24362073	-1.16495443
H	2.17007400	4.36413946	-2.12743616
C	0.32919093	3.88241455	-1.15714066
C	-0.30188085	3.59295994	0.08655913
C	0.38666167	3.89999213	1.29208906
C	1.74371709	4.26375997	1.23337575
H	2.26842813	4.40297979	2.17157888
C	-0.41413560	3.63474681	-2.36366734
H	-0.01211637	3.98809206	-3.30922353
C	-1.55167555	2.88288443	-2.34059127
H	-2.04192241	2.63344011	-3.27480774
C	-2.01645487	2.29270162	-1.11066445
C	-1.48434401	2.79343095	0.11928029
C	-1.95239757	2.30189765	1.37772379
C	-1.42769838	2.90222411	2.57667346
H	-1.86635537	2.65888175	3.53809730
C	-0.29377492	3.66117872	2.53523097
H	0.15363917	4.02374803	3.45660656
C	-2.69509268	1.04497894	-1.08762974
C	-2.76105014	0.34570538	0.15480668
C	-2.62379297	1.04791233	1.39038147
C	-3.00160336	0.28950109	-2.28022453
H	-3.23165974	0.80702018	-3.20531224
C	-2.86183372	-1.06699847	-2.28575960
H	-2.98311870	-1.61435611	-3.21415204
C	-2.39952438	-1.75085237	-1.09955430
C	-2.61001658	-1.09125723	0.14878968
C	-2.30869204	-1.75450622	1.38014055
C	-2.68675377	-1.07313147	2.59502417
H	-2.71889853	-1.61348411	3.53537972
C	-2.84767377	0.28903841	2.59898820
H	-2.99952138	0.80124024	3.54341817
C	-1.45905505	-2.81508004	-1.13583695
C	-0.81815616	-3.19070743	0.08674319
C	-1.37481932	-2.82614194	1.35249406
C	-0.88207375	-3.27684793	-2.37298467
H	-1.42378697	-3.14011946	-3.30199587
C	0.39595140	-3.75178356	-2.40863457
H	0.86011881	-3.99921807	-3.35934845
C	1.18452255	-3.83465733	-1.20840856
C	0.51297153	-3.70447562	0.04090548
C	1.26054604	-3.86033382	1.24031513
C	0.55215154	-3.79118223	2.48897669
H	1.07508626	-4.05384769	3.40444804
C	-0.72207864	-3.30498528	2.54318321
H	-1.19852418	-3.17488567	3.50860020
C	2.58467086	-3.88347402	-1.22584863
H	3.08020564	-3.88364287	-2.19169717
C	3.34718422	-3.81144213	-0.04698573

C	2.66385767	-3.91159681	1.17197397
H	3.21243511	-3.93940553	2.10640747
C	4.85009743	-3.49961105	-0.13036895
C	5.54269776	-3.56619859	1.24461463
H	5.12817063	-2.85268477	1.96202454
H	6.60580257	-3.33286949	1.12914514
H	5.46923134	-4.56902395	1.67899367
C	5.55818334	-4.51282607	-1.06081447
H	5.44170449	-5.53389384	-0.68307032
H	6.62902848	-4.29010916	-1.11521530
H	5.16677510	-4.48366663	-2.08192112
C	5.02808228	-2.06567314	-0.74027493
H	4.65274718	-2.08127155	-1.77206778
H	6.10862229	-1.88095816	-0.81497710
C	4.37285624	-0.88146203	-0.00246446
H	3.28778792	-1.03802751	0.06190319
H	4.74060665	-0.83223180	1.03048123
C	4.66047448	0.46464228	-0.69727678
H	4.26763577	0.43054110	-1.72376818
H	5.74884230	0.58647023	-0.79446724
C	4.08569454	1.70180294	0.02142632
H	2.99266119	1.61609584	0.08440881
H	4.45553056	1.71462804	1.05472452
C	4.46593786	3.01443041	-0.69162482
H	4.10104237	2.96479263	-1.72607899
H	5.56086267	3.07462612	-0.76061945
C	3.97200726	4.36227861	-0.05989055
C	4.43986658	5.52339718	-0.96909368
H	4.06584085	5.42651610	-1.99258560
H	5.53353828	5.54411278	-1.02156495
H	4.09975188	6.48652401	-0.57466559
C	4.62806565	4.55697294	1.32080319
H	4.33352414	5.51134893	1.77042889
H	5.71685047	4.56616866	1.20928363
H	4.37869606	3.75743971	2.02385541
N	-5.50452656	-0.82653622	1.01600375
H	-4.88010882	-1.33832174	0.37413496
C	-6.12231412	0.34982439	0.33171993
C	-7.24683488	-0.16109260	-0.55462719
H	-6.51568565	1.03777110	1.08444000
H	-5.34883997	0.86349001	-0.24276904
O	-7.63087256	-1.31043855	-0.52212656
O	-7.73107011	0.81239212	-1.32268257
H	-8.46657399	0.46796513	-1.86153295
H	-6.22904658	-1.48142527	1.33254276
H	-4.89092889	-0.54700770	1.80476791

endo-(TM8TP)(GlyH⁺)

C	4.29666698	2.21985121	0.02556910
C	4.28619556	1.51188918	1.24049474
H	4.26710801	2.05343802	2.18105821
C	4.19062389	0.11326247	1.29284288
C	4.09352701	-0.62055469	0.07480750
C	4.33713671	0.06089887	-1.15383985
C	4.42315085	1.46945897	-1.15539274
H	4.53398883	1.96780257	-2.11224705
C	4.00889276	-0.60635077	2.52743534
H	4.24867620	-0.11206106	3.46447284
C	3.44737544	-1.84856397	2.52783938
H	3.23840536	-2.33421413	3.47394269
C	2.99373486	-2.45646554	1.29976181
C	3.48602064	-1.91961903	0.07107629
C	3.09328661	-2.48789821	-1.18137312
C	3.69275788	-1.94524589	-2.37951625
H	3.58850549	-2.47749921	-3.31848524
C	4.28775762	-0.71632093	-2.36982469
H	4.65738060	-0.27707091	-3.29222739
C	1.83522393	-3.28416695	1.26155459
C	1.18219924	-3.47119778	0.00487306
C	1.89959290	-3.26733569	-1.21534587
C	1.10046990	-3.64722723	2.44549261
H	1.61894208	-3.75796483	3.39099902
C	-0.25977791	-3.73454416	2.41110117
H	-0.80057210	-3.91790209	3.33256206
C	-0.98367191	-3.46909197	1.19584814
C	-0.25544107	-3.55115562	-0.02851604
C	-0.92681428	-3.41063480	-1.28071914
C	-0.15155516	-3.63720733	-2.47291392
H	-0.65371793	-3.78216923	-3.42278229
C	1.21155893	-3.57826967	-2.44468336
H	1.76958810	-3.67299212	-3.36939263
C	-2.27656489	-2.87526232	1.18284619
C	-2.79094974	-2.39392690	-0.06035541
C	-2.21255607	-2.80396935	-1.30139179
C	-2.95778581	-2.48078468	2.39000119
H	-2.70091754	-2.95464762	3.33031196
C	-3.84147160	-1.44084824	2.39122692
H	-4.28008656	-1.09589141	3.32356369
C	-4.12595555	-0.71828553	1.17670778
C	-3.72604927	-1.31208423	-0.05469646
C	-4.07429463	-0.66071093	-1.27005881
C	-3.71205179	-1.30089403	-2.50542909
H	-4.09884256	-0.89917409	-3.43782839
C	-2.82345533	-2.33468668	-2.51903943
H	-2.50919133	-2.74808559	-3.47060641
C	-4.62943340	0.60034844	1.17228278
H	-4.85422022	1.05902691	2.12931110
C	-4.77079564	1.33326195	-0.01694462

C	-4.59322311	0.63957021	-1.22488465
H	-4.75988744	1.14808721	-2.16907429
C	-4.99689383	2.85704355	-0.04244955
C	-6.17853605	3.20133308	-0.97996631
H	-5.97898622	2.92382332	-2.01908543
H	-6.37158499	4.27884626	-0.96183567
H	-7.09065228	2.68672998	-0.66139851
C	-5.31807317	3.42852316	1.35117755
H	-6.24757317	3.00699543	1.74821614
H	-5.44883332	4.51300137	1.28121192
H	-4.52208952	3.24355123	2.07817702
C	-3.70273878	3.54046628	-0.61018487
H	-3.46758293	3.07628231	-1.57592565
H	-3.94769707	4.58846100	-0.82683756
C	-2.44882238	3.49658596	0.28481445
H	-2.38519766	2.51722419	0.77155969
H	-2.54357775	4.23106516	1.09428578
C	-1.13566877	3.75042642	-0.48072894
H	-1.01583129	2.95997446	-1.23346614
H	-1.20813990	4.69407902	-1.03786347
C	0.10908516	3.80149417	0.42814454
H	0.06947051	2.97817183	1.15762050
H	0.07223881	4.71835496	1.03126678
C	1.45603430	3.74986222	-0.32230258
H	1.58399694	2.75639595	-0.78111919
H	1.42626591	4.45372507	-1.16244696
C	2.66191559	4.07275237	0.58242440
H	2.53607808	3.56095653	1.54553351
H	2.63310896	5.14591705	0.81054171
C	4.09464531	3.74736291	0.03257957
C	5.13182448	4.40293650	0.97702070
H	4.99571104	4.09787861	2.01863478
H	5.03727248	5.49289755	0.94102458
H	6.15108037	4.13966749	0.67752694
C	4.26934607	4.37073595	-1.36475420
H	5.28717136	4.22331105	-1.74041347
H	4.09014433	5.44895516	-1.30978297
H	3.57153984	3.96280083	-2.10189223
N	1.21856940	-0.00500573	-1.13264926
H	0.46142964	0.40980370	-1.70064146
C	0.81310778	0.11767604	0.30293445
C	-0.68912263	0.32715694	0.30734744
H	1.08879009	-0.78458603	0.84536183
H	1.32828506	0.96765353	0.75242218
O	-1.30308423	0.51247081	-0.72522055
O	-1.18859961	0.28707617	1.52927907
H	-2.16806208	0.35530766	1.49092151
H	1.31892081	-0.99342009	-1.40354887
H	2.12221780	0.45235503	-1.31812531

endo-(TM8TPH⁺)(Gly)

C	-4.67689400	1.64347600	0.14398000
C	-4.79334000	0.84771100	-1.12835300
H	-4.30544800	1.37094300	-1.95739400
C	-4.25150500	-0.54949300	-1.09264300
C	-3.82881600	-1.11410300	0.12930000
C	-4.08628500	-0.41155400	1.34791300
C	-4.49525700	0.97085400	1.31202600
H	-4.50523700	1.49645200	2.26017000
C	-4.05200000	-1.26799600	-2.27620700
H	-4.44360600	-0.88397700	-3.21340300
C	-3.20484500	-2.36575600	-2.28860500
H	-2.95689800	-2.81268700	-3.24442400
C	-2.55092200	-2.80099200	-1.11352800
C	-2.99016700	-2.26623200	0.13216600
C	-2.42890900	-2.72277000	1.36328800
C	-2.93612600	-2.16819600	2.56596900
H	-2.60178300	-2.55656300	3.52165000
C	-3.74093800	-1.04050700	2.56180300
H	-4.01538600	-0.57242300	3.50234700
C	-1.27080500	-3.46320400	-1.15211300
C	-0.52113000	-3.56017000	0.05846000
C	-1.17189000	-3.42056800	1.32303700
C	-0.58776300	-3.75177000	-2.36877400
H	-1.14279500	-3.88994900	-3.28901300
C	0.78157400	-3.67840400	-2.42185300
H	1.27175900	-3.76679900	-3.38490100
C	1.54490300	-3.35084600	-1.26079700
C	0.91056000	-3.52538400	0.00278300
C	1.64878000	-3.36156700	1.21094500
C	0.97189900	-3.66863200	2.43336500
H	1.53567600	-3.77375800	3.35384900
C	-0.39839000	-3.70390700	2.49013900
H	-0.88537400	-3.83091200	3.45030300
C	2.74062500	-2.57066500	-1.31362700
C	3.26895900	-2.06329700	-0.08681800
C	2.86273700	-2.61287700	1.16823900
C	3.22902100	-2.00834300	-2.54142800
H	2.95760700	-2.46195000	-3.48730700
C	3.89968200	-0.81788400	-2.54435600
H	4.16139300	-0.34356300	-3.48588700
C	4.16415700	-0.12067900	-1.31775200
C	3.99114200	-0.83119400	-0.09946200
C	4.31319300	-0.17850500	1.12301100
C	4.19034500	-0.93550500	2.33833500
H	4.58713700	-0.51995100	3.26075100
C	3.49966700	-2.11476000	2.35867200
H	3.34924000	-2.62476000	3.30362700
C	4.41614500	1.26379000	-1.27594400
H	4.45052000	1.79654200	-2.21924800
C	4.51085200	1.96289500	-0.06526100

C	4.56669900	1.20060500	1.11554400
H	4.72143800	1.69206500	2.07101600
C	4.42920600	3.49800400	0.01545700
C	5.52119300	4.04614400	0.96449900
H	5.38196300	3.71465900	1.99780500
H	5.49763000	5.14050900	0.97087200
H	6.51668300	3.72951000	0.63735200
C	4.62135600	4.16997300	-1.35760500
H	5.61132900	3.94765600	-1.76963000
H	4.54201200	5.25610900	-1.24794500
H	3.87058300	3.86284500	-2.09027800
C	3.02806900	3.88572400	0.60711500
H	2.91336400	3.36996800	1.57138100
H	3.05607600	4.95760000	0.84437600
C	1.78866600	3.61158300	-0.26603400
H	1.82995300	2.59444700	-0.67817900
H	1.79388400	4.28514000	-1.13144500
C	0.45969100	3.79889900	0.49481100
H	0.37663300	3.02778700	1.27603600
H	0.47875400	4.75386700	1.03723200
C	-0.78888300	3.75402200	-0.40971100
H	-0.69000500	2.94404800	-1.14148600
H	-0.83234000	4.68365500	-0.99330500
C	-2.11309500	3.56605600	0.35634800
H	-2.10423900	2.58675900	0.84994500
H	-2.18081600	4.31699000	1.15358500
C	-3.34785400	3.65822000	-0.55742600
H	-3.14289800	3.10332700	-1.48046200
H	-3.49173200	4.70432300	-0.85684900
C	-4.72222900	3.16584600	0.03641800
C	-5.84562300	3.59651300	-0.93947000
H	-5.66172100	3.25944500	-1.96369100
H	-5.91316400	4.68803800	-0.96535900
H	-6.81783800	3.20821100	-0.61705000
C	-4.98218000	3.84561300	1.39362300
H	-5.95263800	3.54715500	1.80352300
H	-4.99269600	4.93178700	1.26136300
H	-4.21278900	3.61863600	2.13571500
H	-5.86171200	0.81899100	-1.40147100
N	1.13932100	0.23226000	1.15243400
H	1.34170100	-0.01698400	-0.71946200
C	-0.28509000	0.19768600	0.83592000
C	-0.49118100	0.29216900	-0.68068200
H	-0.71058800	-0.75870300	1.14857000
H	-0.88400900	0.98151800	1.30745700
O	0.62202900	0.09165500	-1.39218000
O	-1.56916400	0.51594500	-1.19220100
H	1.40732800	-0.40440700	1.89319300
H	1.47286800	1.16164000	1.38575600

exo-(TM8TPH⁺)(Gly)

C	-4.85893518	1.70167294	0.60803993
C	-5.09867674	0.91970059	-0.65526096
H	-4.78102784	1.47270578	-1.54399188
C	-4.48570841	-0.44815172	-0.69903878
C	-3.98103879	-1.03412679	0.48218491
C	-4.18403286	-0.36729014	1.73521178
C	-4.59502514	1.01428508	1.75237215
H	-4.51654513	1.52910995	2.70332567
C	-4.32645343	-1.12228018	-1.91609208
H	-4.77033325	-0.70942823	-2.81648591
C	-3.48096839	-2.22180364	-1.99598537
H	-3.27941863	-2.64262083	-2.97467684
C	-2.77830116	-2.69839390	-0.86660049
C	-3.13484498	-2.17880681	0.41180576
C	-2.50561025	-2.65946039	1.60087037
C	-2.94793975	-2.13734950	2.84094851
H	-2.55426120	-2.54212649	3.76665985
C	-3.76770424	-1.02182344	2.91028873
H	-3.99172913	-0.57859709	3.87583474
C	-1.51791880	-3.39373543	-0.98835293
C	-0.69494372	-3.50638043	0.17001550
C	-1.26012073	-3.36427651	1.47551556
C	-0.92101178	-3.69979428	-2.24497224
H	-1.53783033	-3.83623714	-3.12562788
C	0.44471117	-3.65123184	-2.38667886
H	0.87085257	-3.75460748	-3.37857654
C	1.28448646	-3.32712118	-1.27954116
C	0.72944931	-3.48863118	0.02241841
C	1.54069475	-3.31990454	1.18184427
C	0.94513629	-3.63350857	2.44299492
H	1.56720880	-3.74011059	3.32486888
C	-0.41866610	-3.66830217	2.58723204
H	-0.84304423	-3.79641383	3.57639761
C	2.48310074	-2.55866418	-1.41234274
C	3.07512528	-2.02946662	-0.22494332
C	2.73989465	-2.55701542	1.06154698
C	2.92256814	-2.03538964	-2.67460590
H	2.60283591	-2.51049727	-3.59500301
C	3.62494652	-0.86346281	-2.73941552
H	3.86308313	-0.42488794	-3.70463106
C	3.96327569	-0.14234812	-1.54661481
C	3.81701712	-0.81326904	-0.30265276
C	4.21325651	-0.14225819	0.88790483
C	4.13436226	-0.86644636	2.12562285
H	4.57192038	-0.42977918	3.01918353
C	3.43621748	-2.03774572	2.20648721
H	3.31910976	-2.51817560	3.17109162
C	4.26268827	1.23338389	-1.55354728
H	4.27511719	1.74183116	-2.51100117
C	4.41690166	1.95943098	-0.36577231

C	4.50420116	1.22761582	0.83165447
H	4.70428051	1.74119627	1.76662312
C	4.32527470	3.49355080	-0.31203933
C	5.46951342	4.07948018	0.54716078
H	5.42256690	3.74639457	1.58811609
H	5.41174845	5.17279314	0.55448366
H	6.44594762	3.79313281	0.14300692
C	4.40580055	4.13967877	-1.70793839
H	5.36381431	3.92014135	-2.19152942
H	4.32213471	5.22694298	-1.61267667
H	3.60356665	3.80973735	-2.37349716
C	2.95784136	3.85909991	0.36605552
H	2.93691280	3.39328708	1.36006613
H	2.95342226	4.94376751	0.53984733
C	1.67135201	3.47496021	-0.39191241
H	1.75835377	2.45512573	-0.78996104
H	1.54820740	4.13423466	-1.26081519
C	0.40787377	3.56048319	0.48838338
H	0.43926125	2.75283637	1.23418329
H	0.42226706	4.50001863	1.05913123
C	-0.91162003	3.48524157	-0.30252781
H	-0.88124543	2.63181411	-0.99511662
H	-0.99535183	4.38176433	-0.93297998
C	-2.16774793	3.36425545	0.58517264
H	-2.18151148	2.36779108	1.04688222
H	-2.09308137	4.08328911	1.41097106
C	-3.47211111	3.60935075	-0.19817823
H	-3.42038550	3.09751182	-1.16546641
H	-3.54235342	4.67898938	-0.43613883
C	-4.82845384	3.22071224	0.50708728
C	-5.99126176	3.72816204	-0.38111027
H	-5.90570789	3.37562570	-1.41200086
H	-5.98120903	4.82220322	-0.40813704
H	-6.95923170	3.41124655	0.02283781
C	-4.92808882	3.91095081	1.87936083
H	-5.87461193	3.66889757	2.37433087
H	-4.88695252	4.99630157	1.74535801
H	-4.11082447	3.63765919	2.55147605
H	-6.19276997	0.82872121	-0.77519811
N	-6.43826333	2.13578455	-6.52748188
H	-6.33191572	0.84414621	-5.17863631
C	-5.52996311	2.89697084	-5.65988558
C	-5.22895352	2.10813593	-4.37881805
H	-4.57043503	3.10480939	-6.14352423
H	-5.94368496	3.86379710	-5.35641525
O	-5.82106443	0.90789077	-4.32769340
O	-4.52035099	2.53017784	-3.48769656
H	-6.04373773	1.94110064	-7.44101905
H	-7.33398898	2.59274616	-6.65985127

exo-(TM8TP)(GlyH⁺)

C	1.37468505	5.08236271	0.00475711
C	0.64796889	4.82200899	-1.17000706
H	1.07117652	5.07759111	-2.13613765
C	-0.56374995	4.11961744	-1.15340490
C	-1.07719008	3.65641886	0.09134463
C	-0.47430260	4.11672081	1.29418771
C	0.74024701	4.82298761	1.22668661
H	1.22631507	5.08098739	2.16074954
C	-1.23227470	3.70347517	-2.35628223
H	-0.94624972	4.15964869	-3.30000725
C	-2.13799401	2.68382316	-2.33423487
H	-2.55961297	2.33044737	-3.26826177
C	-2.42696009	1.98256087	-1.11000422
C	-2.01530844	2.58082400	0.12236749
C	-2.33725582	1.97727672	1.37804085
C	-1.95474755	2.66993003	2.58033807
H	-2.30079158	2.31047989	3.54302110
C	-1.04917795	3.69103277	2.54001571
H	-0.69202611	4.13930426	3.46309659
C	-2.80894396	0.61300796	-1.09850822
C	-2.72687690	-0.09721751	0.13711154
C	-2.72173199	0.60769542	1.37994707
C	-2.97183139	-0.17251955	-2.29659476
H	-3.27628524	0.30708221	-3.22033336
C	-2.61580911	-1.48999779	-2.31375313
H	-2.64375108	-2.03660049	-3.24983323
C	-2.06805243	-2.11307560	-1.13410787
C	-2.35206553	-1.49081670	0.11856103
C	-1.97088636	-2.12205867	1.34587061
C	-2.43222413	-1.50791067	2.56568833
H	-2.37634956	-2.05142571	3.50287554
C	-2.80138208	-0.18648692	2.58157675
H	-3.02526199	0.28685382	3.53177491
C	-1.02843901	-3.08398809	-1.17783888
C	-0.35865446	-3.41329982	0.04203575
C	-0.93918667	-3.09793326	1.31067943
C	-0.42054613	-3.49586078	-2.41537299
H	-0.96629006	-3.38445889	-3.34528203
C	0.88406706	-3.89704661	-2.45331360
H	1.36132885	-4.10879838	-3.40618101
C	1.67546618	-3.94440919	-1.25552274
C	1.00053935	-3.84611898	-0.00781863
C	1.75842636	-3.95939759	1.19236481
C	1.04983906	-3.93506612	2.44323597
H	1.59006557	-4.16683694	3.35697442
C	-0.25202867	-3.53226162	2.49950480
H	-0.73487059	-3.43864024	3.46583134
C	3.08167118	-3.91936854	-1.27883515
H	3.56976371	-3.90226106	-2.24667554
C	3.83603311	-3.79630740	-0.10472268

C	3.15680498	-3.93276788	1.11855738
H	3.71251553	-3.91965572	2.05068169
C	5.31183905	-3.36401090	-0.10746790
C	6.14626489	-4.26759860	0.82978918
H	5.82349550	-4.19800368	1.87275923
H	7.19979599	-3.97140171	0.79658794
H	6.07789890	-5.31636119	0.52262753
C	5.94444431	-3.42798387	-1.51033282
H	5.93846635	-4.45103537	-1.90181725
H	6.98664805	-3.09765558	-1.45648917
H	5.43676071	-2.78266808	-2.23220273
C	5.37190347	-1.89351227	0.43650727
H	4.91638748	-1.88224455	1.43535161
H	6.42975880	-1.63648924	0.58334815
C	4.71216359	-0.79877806	-0.42553817
H	3.74476477	-1.15102981	-0.80773170
H	5.33652258	-0.60143463	-1.30645886
C	4.49242707	0.51962442	0.34327533
H	3.69911691	0.36676811	1.08946039
H	5.39954542	0.76818853	0.91255976
C	4.13256739	1.71575002	-0.55743310
H	3.33221134	1.42642418	-1.25395381
H	5.00357879	1.96033000	-1.18209238
C	3.68633211	2.97152776	0.21801617
H	2.70049590	2.78092557	0.66280686
H	4.37410430	3.13963356	1.05679946
C	3.63420373	4.23453723	-0.66453472
H	3.18971963	3.97273029	-1.63363789
H	4.66207575	4.55652128	-0.88009287
C	2.85865549	5.47349302	-0.09397050
C	3.04605507	6.65989513	-1.06785260
H	2.73829456	6.41452034	-2.08856198
H	4.10128569	6.94903980	-1.10852039
H	2.46753262	7.52935679	-0.73874419
C	3.45469735	5.88147333	1.26638436
H	2.94639230	6.76199194	1.67417160
H	4.51200292	6.13545105	1.14064679
H	3.39977708	5.08054691	2.00852443
N	-5.26388301	-1.64649383	0.99558583
H	-5.88557419	-2.40867897	1.29083973
C	-6.05555370	-0.53255379	0.39020604
C	-7.14936022	-1.14723902	-0.46847528
H	-6.49576779	0.06985129	1.18892518
H	-5.38156202	0.09817373	-0.19266898
O	-7.38935215	-2.33557386	-0.46549298
O	-7.78318057	-0.21511219	-1.17640672
H	-8.49615314	-0.62848960	-1.69675632
H	-4.67334835	-1.32461598	1.78657446
H	-4.59506676	-2.03586276	0.31481105

endo-(TM9TP)(GlyH⁺)

C	-5.07351229	1.46286931	0.02465855
C	-4.87612216	0.79146364	-1.19410703
H	-5.02071091	1.31921362	-2.13152247
C	-4.39328931	-0.52423021	-1.25521856
C	-4.08891198	-1.21022094	-0.04268028
C	-4.47767252	-0.61543977	1.19426421
C	-4.95637875	0.71082397	1.20273466
H	-5.17642459	1.16049647	2.16446174
C	-4.04993825	-1.16711554	-2.49645446
H	-4.40722253	-0.73579290	-3.42715987
C	-3.21675398	-2.24627136	-2.51351561
H	-2.91286091	-2.66171648	-3.46712097
C	-2.63513530	-2.75909093	-1.29741257
C	-3.20321590	-2.33739449	-0.05628657
C	-2.69406420	-2.83218902	1.18584897
C	-3.36010512	-2.41828508	2.39781421
H	-3.11939607	-2.90862123	3.33420090
C	-4.21112081	-1.35044675	2.40576203
H	-4.64429976	-1.00097516	3.33878720
C	-1.35875036	-3.38970683	-1.28243111
C	-0.67154556	-3.50780067	-0.03509546
C	-1.39273321	-3.41740610	1.19643615
C	-0.60239869	-3.64255762	-2.47968416
H	-1.11610850	-3.79350242	-3.42202800
C	0.75975696	-3.58836013	-2.46096439
H	1.30447563	-3.69878265	-3.39158448
C	1.46893151	-3.27993369	-1.24864284
C	0.76606740	-3.44568852	-0.01722468
C	1.44111489	-3.27878302	1.22884161
C	0.70423128	-3.58678878	2.42401040
H	1.22746494	-3.68943464	3.36781354
C	-0.65876650	-3.66100084	2.41152299
H	-1.19024168	-3.82080441	3.34265868
C	2.70923072	-2.58681224	-1.23790388
C	3.20646805	-2.09985044	0.00985539
C	2.68142336	-2.58126572	1.24755169
C	3.33514662	-2.11218036	-2.44702015
H	3.09668532	-2.58106157	-3.39451547
C	4.13597834	-1.00925662	-2.43637350
H	4.53017063	-0.60735858	-3.36556709
C	4.39287385	-0.30209037	-1.20631474
C	4.06109277	-0.95392833	0.01860234
C	4.39123141	-0.31345695	1.24268940
C	4.09329462	-1.00631067	2.46499273
H	4.46506214	-0.60127909	3.40202985
C	3.27749477	-2.09960472	2.46551403
H	3.00616748	-2.55321196	3.41182199
C	4.81806897	1.03657816	-1.17305494
H	4.98136811	1.54012413	-2.12098083
C	4.95214967	1.74722551	0.03433018

C	4.83772225	1.02025485	1.22533081
H	5.00068058	1.50696022	2.17997571
C	5.07708048	3.28093482	0.00535470
C	5.36707162	3.87512906	1.39679623
H	4.58453170	3.64666036	2.12554164
H	5.43509811	4.96500679	1.32176405
H	6.31993527	3.50920182	1.79346771
C	6.22107031	3.71284108	-0.94138695
H	7.17468597	3.28208394	-0.61986763
H	6.32187915	4.80305468	-0.93743911
H	6.04381022	3.40692136	-1.97667284
C	1.16613558	3.90496434	-0.47202065
H	1.12505205	3.25864769	-1.36070654
H	1.18630140	4.93589370	-0.85042472
C	-0.11693533	3.70094178	0.35539398
H	-0.08604160	2.70209192	0.81748436
H	-0.12879074	4.40566255	1.19732668
C	-1.41426008	3.85547817	-0.45914960
H	-1.34426252	3.25105994	-1.37712460
H	-1.50094193	4.89411278	-0.80380221
C	-2.69289778	3.46432702	0.30387094
H	-2.62197144	2.40963715	0.61189424
H	-2.74878321	4.03980951	1.23572035
C	-3.97920448	3.66203464	-0.51982822
H	-3.80591850	3.29402214	-1.53922800
H	-4.17349166	4.73796743	-0.61598178
C	-5.28271264	2.98791507	0.02981099
C	-6.45786267	3.36866583	-0.90105770
H	-6.27301177	3.08654618	-1.94158713
H	-6.61972199	4.45119678	-0.87985335
H	-7.38246225	2.88028729	-0.57764253
C	-5.59628554	3.53606831	1.43493234
H	-6.52757524	3.11464536	1.82733621
H	-5.72053197	4.62215674	1.38423592
H	-4.80006018	3.33334741	2.15717465
C	2.46699606	3.60863625	0.29800791
H	2.49603167	4.22510586	1.20514946
H	2.45170590	2.56647455	0.63981022
C	3.73068456	3.86344707	-0.54681396
H	3.86272745	4.94562974	-0.67801174
H	3.57250406	3.45519985	-1.55412571
N	-1.32127328	-0.05943237	1.04452056
H	-1.21490764	-1.04590673	1.32414252
C	-0.77864502	0.15812154	-0.33264483
C	0.72615165	0.32292387	-0.19684283
H	-1.03804022	-0.69539090	-0.95936319
H	-1.22654140	1.05897195	-0.75430721
O	1.26711597	0.34582001	0.88992362
O	1.30890445	0.45778277	-1.37680880
H	2.28235850	0.53156915	-1.26792338
H	-2.32628996	0.15930118	1.10483408
H	-0.78436950	0.50702352	1.71296699

endo-(TM9TPH⁺)(Gly)

C	-5.17921975	1.49226431	0.03391619
C	-5.19247204	0.76273612	-1.28265454
H	-4.75107360	1.37529435	-2.07549808
C	-4.52502618	-0.58000419	-1.30499015
C	-4.11514799	-1.18471712	-0.10018117
C	-4.47684948	-0.57792138	1.14337089
C	-4.98976923	0.76729806	1.16867203
H	-5.06559356	1.23583603	2.14304773
C	-4.22438335	-1.20864020	-2.51962865
H	-4.60033152	-0.79307879	-3.44985675
C	-3.32423801	-2.26065804	-2.55463373
H	-3.01817479	-2.64284240	-3.52142130
C	-2.70091173	-2.73350408	-1.37583323
C	-3.20143605	-2.27745887	-0.12351009
C	-2.65170240	-2.75526339	1.10321789
C	-3.24325115	-2.30587175	2.31236432
H	-2.91981637	-2.72462505	3.25888039
C	-4.13605332	-1.25006075	2.33489304
H	-4.48543690	-0.86002095	3.28596450
C	-1.41480463	-3.37990586	-1.40309128
C	-0.69241389	-3.51162066	-0.18057942
C	-1.36984402	-3.39863282	1.07355291
C	-0.71209391	-3.65245602	-2.61439228
H	-1.25372626	-3.76750124	-3.54569550
C	0.65765155	-3.62199987	-2.64061081
H	1.16498665	-3.71655245	-3.59407909
C	1.40951941	-3.34620406	-1.45666095
C	0.74183127	-3.51301444	-0.20750306
C	1.46351233	-3.40232460	1.01671803
C	0.75109499	-3.69609061	2.22264622
H	1.29254348	-3.82304659	3.15344390
C	-0.61904352	-3.70032003	2.25128680
H	-1.12429669	-3.82768034	3.20156460
C	2.64835612	-2.63776474	-1.47469109
C	3.19432502	-2.19438468	-0.23016321
C	2.72752287	-2.73664156	1.00811226
C	3.19742136	-2.09164116	-2.68585091
H	2.90399978	-2.50518705	-3.64351255
C	3.97757639	-0.97136005	-2.65781406
H	4.30314008	-0.51111153	-3.58651040
C	4.30076323	-0.32942803	-1.41438068
C	4.03108353	-1.03661815	-0.20887536
C	4.41906231	-0.45126046	1.02701008
C	4.19694055	-1.21203625	2.22480449
H	4.61862811	-0.85560811	3.16066170
C	3.38988616	-2.31663963	2.21497418
H	3.17460648	-2.82155016	3.14973095
C	4.73187343	1.00281696	-1.34190746
H	4.84401359	1.54925331	-2.27309889
C	4.91430238	1.66480019	-0.11535711

C	4.85385972	0.88788699	1.04966934
H	5.06798353	1.33212059	2.01532616
C	5.04764428	3.19832950	-0.09274550
C	5.33840610	3.74234293	1.31865105
H	4.55647491	3.48650092	2.03945659
H	5.40368988	4.83423081	1.28292921
H	6.29285210	3.36602280	1.70183492
C	6.19967639	3.64768835	-1.02190971
H	7.14918573	3.20332101	-0.70662263
H	6.30643369	4.73684023	-0.98949578
H	6.02543116	3.36814354	-2.06511941
C	1.13530947	3.86648661	-0.55451983
H	1.07519950	3.23112072	-1.45039877
H	1.17640800	4.89961873	-0.92519400
C	-0.14352809	3.68084930	0.28493790
H	-0.11787209	2.70135203	0.78103868
H	-0.15574233	4.41976633	1.09791193
C	-1.44350623	3.78860922	-0.53417010
H	-1.38402880	3.09897598	-1.38663253
H	-1.52042791	4.80066280	-0.95565989
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H	-2.64664605	2.43204545	0.63846089
H	-2.76849477	4.11016668	1.15086939
C	-3.99727189	3.62262184	-0.57369552
H	-3.82050821	3.19500252	-1.56848670
H	-4.18975537	4.69064709	-0.73893795
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C	-6.49274431	3.41545884	-0.92694845
H	-6.31528253	3.12464190	-1.96656989
H	-6.61887203	4.50212265	-0.91151961
H	-7.43467946	2.96323984	-0.59809886
C	-5.60088802	3.59972374	1.40391354
H	-6.53874591	3.21517603	1.81831261
H	-5.68917126	4.68778750	1.32869840
H	-4.79825753	3.38789956	2.11476234
C	2.43928462	3.54056711	0.19850366
H	2.47069648	4.11203965	1.13449388
H	2.43000503	2.48080886	0.48721032
C	3.70913541	3.81411203	-0.62947017
H	3.85226088	4.89911683	-0.71581489
H	3.54841293	3.44846893	-1.65182042
H	-6.24927647	0.64400528	-1.57761627
N	1.00002946	0.18062316	1.29656148
H	1.52968627	1.01259345	1.53327461
C	0.60039909	0.16134666	-0.11580317
C	-0.92191063	0.28610142	-0.22619600
H	1.05262797	0.96313302	-0.70473997
H	0.87973713	-0.77753176	-0.59730922
O	-1.51964200	0.37771318	-1.27840205
O	-1.53815954	0.26668118	0.96206497
H	-0.78903596	0.21145138	1.61780464
H	1.55902803	-0.62396068	1.55293575

exo-(TM9TPH⁺)(Gly)

C	-5.23228881	1.45753429	0.54313191
C	-5.28455659	0.73403406	-0.77218601
H	-4.96288147	1.36366324	-1.60572454
C	-4.52781157	-0.55905634	-0.83337610
C	-4.05121702	-1.15622087	0.35486585
C	-4.41142761	-0.58382049	1.61872492
C	-4.97989663	0.74018997	1.67023590
H	-5.02362360	1.20738678	2.64759906
C	-4.21541228	-1.14433503	-2.06579458
H	-4.61665342	-0.70877113	-2.97523838
C	-3.27998863	-2.16901482	-2.13237519
H	-2.97602349	-2.51949015	-3.11208794
C	-2.62591095	-2.65173896	-0.97730535
C	-3.09724014	-2.21405768	0.29439497
C	-2.50315253	-2.69280073	1.50221628
C	-3.06663780	-2.26990807	2.72951368
H	-2.69489926	-2.67841597	3.66250376
C	-4.00084704	-1.24732203	2.78984930
H	-4.33179806	-0.87815873	3.75583956
C	-1.33289822	-3.29163561	-1.04583857
C	-0.56914702	-3.40812129	0.15283054
C	-1.20730151	-3.31259832	1.42870213
C	-0.67146492	-3.57011832	-2.27446840
H	-1.24232471	-3.69200924	-3.18745230
C	0.70006204	-3.53386487	-2.34536522
H	1.17370872	-3.63134173	-3.31581398
C	1.48773881	-3.24361412	-1.19337580
C	0.86071203	-3.39088015	0.07822263
C	1.61714158	-3.25546705	1.27807728
C	0.95371056	-3.55985711	2.50395160
H	1.52735004	-3.66667499	3.41784933
C	-0.41665197	-3.60255412	2.57786722
H	-0.88618147	-3.73746046	3.54521792
C	2.73554450	-2.55038779	-1.26193604
C	3.30735928	-2.06788293	-0.04481070
C	2.86579012	-2.56286734	1.22181760
C	3.28069554	-2.07236044	-2.50092320
H	2.96592983	-2.52042459	-3.43621736
C	4.09319299	-0.97371337	-2.53138698
H	4.42034012	-0.56447778	-3.48326978
C	4.44446701	-0.28574754	-1.32240200
C	4.16848032	-0.93139643	-0.08464711
C	4.58058627	-0.30239951	1.12084216
C	4.35783707	-1.00190523	2.35263056
H	4.78549713	-0.60305620	3.26841111
C	3.54089370	-2.09767931	2.39936471
H	3.32496328	-2.55237938	3.35919979
C	4.89033008	1.04415237	-1.31249630
H	4.99045571	1.55267745	-2.26626274
C	5.06816734	1.75796142	-0.11576066

C	5.02616766	1.03129401	1.08108497
H	5.23897234	1.51961840	2.02519488
C	5.09300985	3.29348312	-0.14437262
C	5.39993297	3.90493116	1.23649563
H	4.64930407	3.64778921	1.98909808
H	5.41932476	4.99614712	1.15566809
H	6.37940456	3.58274521	1.60613283
C	6.15585598	3.81536856	-1.13715997
H	7.15984107	3.50331877	-0.83140522
H	6.13491856	4.90979500	-1.16914331
H	5.98638260	3.45736435	-2.15683934
C	1.11426035	3.73727578	-0.42593610
H	1.06432057	3.52716853	-1.50414695
H	1.07733601	4.83126100	-0.32646347
C	-0.11808623	3.12103383	0.26155056
H	-0.08522989	2.02791340	0.14195547
H	-0.06273922	3.31119711	1.34319652
C	-1.46207826	3.64719810	-0.27519218
H	-1.50763681	3.48156362	-1.36115658
H	-1.50811524	4.73569218	-0.13004467
C	-2.68859511	2.99198811	0.38632653
H	-2.63059186	1.90531644	0.23768467
H	-2.63907406	3.15069422	1.47145160
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H	-4.07237964	3.30947191	-1.23894389
H	-4.05572805	4.61224367	-0.06710203
C	-5.34253489	2.97462360	0.51625337
C	-6.55525341	3.42493054	-0.33246674
H	-6.52559132	3.02738857	-1.34996938
H	-6.57307449	4.51769141	-0.39875572
H	-7.49335556	3.09914325	0.12989137
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H	-6.37428859	3.20060427	2.43441723
H	-5.59350270	4.67064911	1.84042713
H	-4.61552511	3.39136309	2.55694165
C	2.45423624	3.21761967	0.12819416
H	2.52243003	3.47285686	1.19372970
H	2.45732770	2.12135457	0.07532081
C	3.67685999	3.76994749	-0.62918445
H	3.66658166	4.86762738	-0.58591265
H	3.57229789	3.50578178	-1.68993030
H	-6.34611501	0.54433503	-1.00558167
N	-8.68457385	2.19345293	-5.33825293
H	-8.39196710	1.59675987	-3.58712651
C	-7.22919765	2.04668478	-5.46859545
C	-6.62291744	1.53800061	-4.15386711
H	-6.94514409	1.33783277	-6.25269759
H	-6.73366026	2.99291070	-5.70746106
O	-7.52034972	1.34797141	-3.17891110
O	-5.43573641	1.32864125	-4.00402037
H	-9.20170978	1.58580019	-5.96412078
H	-9.00186674	3.14517491	-5.48559759

exo-(TM9TP)(GlyH⁺)

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C	3.43049182	-3.86410137	-1.15632714
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C	3.62690847	-2.47686371	-1.15923852
C	3.60668050	-1.77233053	0.07840386
C	3.62067649	-2.51718601	1.28958620
C	3.42504712	-3.90866219	1.24184119
H	3.34138814	-4.43812278	2.18397871
C	3.68929898	-1.70840040	-2.37199149
H	3.83991050	-2.22776783	-3.31437457
C	3.46850456	-0.36224360	-2.35913839
H	3.43798799	0.17564459	-3.29960315
C	3.14193510	0.32144230	-1.13513316
C	3.35834528	-0.36684768	0.10001347
C	3.12406215	0.27841650	1.35428752
C	3.43680541	-0.44481271	2.55764651
H	3.39055595	0.05835170	3.51689030
C	3.66618307	-1.79048621	2.52706416
H	3.80766277	-2.34043044	3.45338689
C	2.36649377	1.51351306	-1.11936497
C	1.80462889	1.93976742	0.12269041
C	2.33939785	1.46597015	1.36059037
C	1.89331587	2.16512710	-2.31316967
H	2.43311679	2.04145363	-3.24533672
C	0.70683328	2.84000345	-2.31577118
H	0.32730857	3.24010472	-3.24915092
C	-0.10116438	2.90933473	-1.12523144
C	0.54957723	2.65048192	0.11966211
C	-0.14464739	2.84899641	1.35590159
C	0.62655999	2.72835098	2.56477565
H	0.21138670	3.06486419	3.50859745
C	1.82947702	2.06657385	2.56650328
H	2.33088896	1.89315500	3.51255278
C	-1.52301274	2.93719155	-1.14940036
C	-2.22910233	2.74807595	0.08002918
C	-1.56677883	2.88570490	1.33989326
C	-2.26784354	2.85764201	-2.37840099
H	-1.79080170	3.12523080	-3.31405417
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H	-4.03977982	2.18700726	-3.34861402
C	-4.15159432	1.86258529	-1.19600248
C	-3.55216952	2.21398647	0.04717569
C	-4.20006016	1.82737983	1.25246900
C	-3.61696660	2.24698177	2.49569438
H	-4.16576590	2.07394104	3.41731541
C	-2.35432343	2.76460489	2.53725810
H	-1.91015920	2.99033263	3.50017020
C	-5.22426521	0.96097899	-1.20392228
H	-5.59745469	0.62528973	-2.16629250
C	-5.72391414	0.39079418	-0.02097623

C	-5.27699606	0.92578557	1.19391187
H	-5.68968706	0.57235847	2.13184281
C	-6.56309760	-0.89371426	-0.09406926
C	-7.11944143	-1.31562802	1.27969325
H	-6.33170501	-1.52958192	2.00728734
H	-7.71481563	-2.22705263	1.16736461
H	-7.77232519	-0.54261865	1.69941330
C	-7.76181758	-0.72011703	-1.05385909
H	-8.43394481	0.06777195	-0.69817312
H	-8.33276131	-1.65264047	-1.11415230
H	-7.44917395	-0.46451179	-2.07046954
C	-3.42654928	-3.34616798	-0.58258927
H	-3.25019048	-3.06805742	-1.63186237
H	-3.97410825	-4.29887411	-0.60759007
C	-2.07027225	-3.55551438	0.11500191
H	-1.53523384	-2.59493360	0.15211661
H	-2.24181898	-3.84924410	1.16065589
C	-1.17100714	-4.60320938	-0.56579884
H	-1.01601942	-4.31402647	-1.61545499
H	-1.69262781	-5.57038405	-0.58988737
C	0.19966700	-4.77428216	0.11503135
H	0.69604457	-3.79623915	0.15678859
H	0.04501872	-5.08439049	1.15668795
C	1.11264138	-5.78265530	-0.60736909
H	1.20051089	-5.47717593	-1.65843412
H	0.62957896	-6.76927919	-0.61628572
C	2.56135184	-5.97192713	-0.03196902
C	3.34927725	-6.90749409	-0.97650614
H	3.40989753	-6.51628494	-1.99626130
H	2.85903214	-7.88515996	-1.03179057
H	4.37024297	-7.05916899	-0.61087747
C	2.48590117	-6.65296269	1.34827879
H	3.48371454	-6.79639746	1.77697531
H	2.02576050	-7.64034203	1.24279604
H	1.88363622	-6.08842418	2.06546527
C	-4.30099324	-2.26707443	0.08251593
H	-4.49526801	-2.55642240	1.12352807
H	-3.73094869	-1.33015806	0.12600091
C	-5.63047048	-2.02493783	-0.65647622
H	-6.21324683	-2.95608848	-0.67107212
H	-5.40456069	-1.79043499	-1.70519580
N	2.51397696	4.82735052	0.96328435
H	2.41495686	5.80709651	1.25476043
C	3.85918747	4.59897609	0.35291839
C	4.19479969	5.80651876	-0.50772631
H	4.59925291	4.48487011	1.14908345
H	3.82698830	3.67616378	-0.22935443
O	3.52480271	6.81691165	-0.50209912
O	5.29878213	5.59477637	-1.22051294
H	5.50878723	6.39095836	-1.74200652
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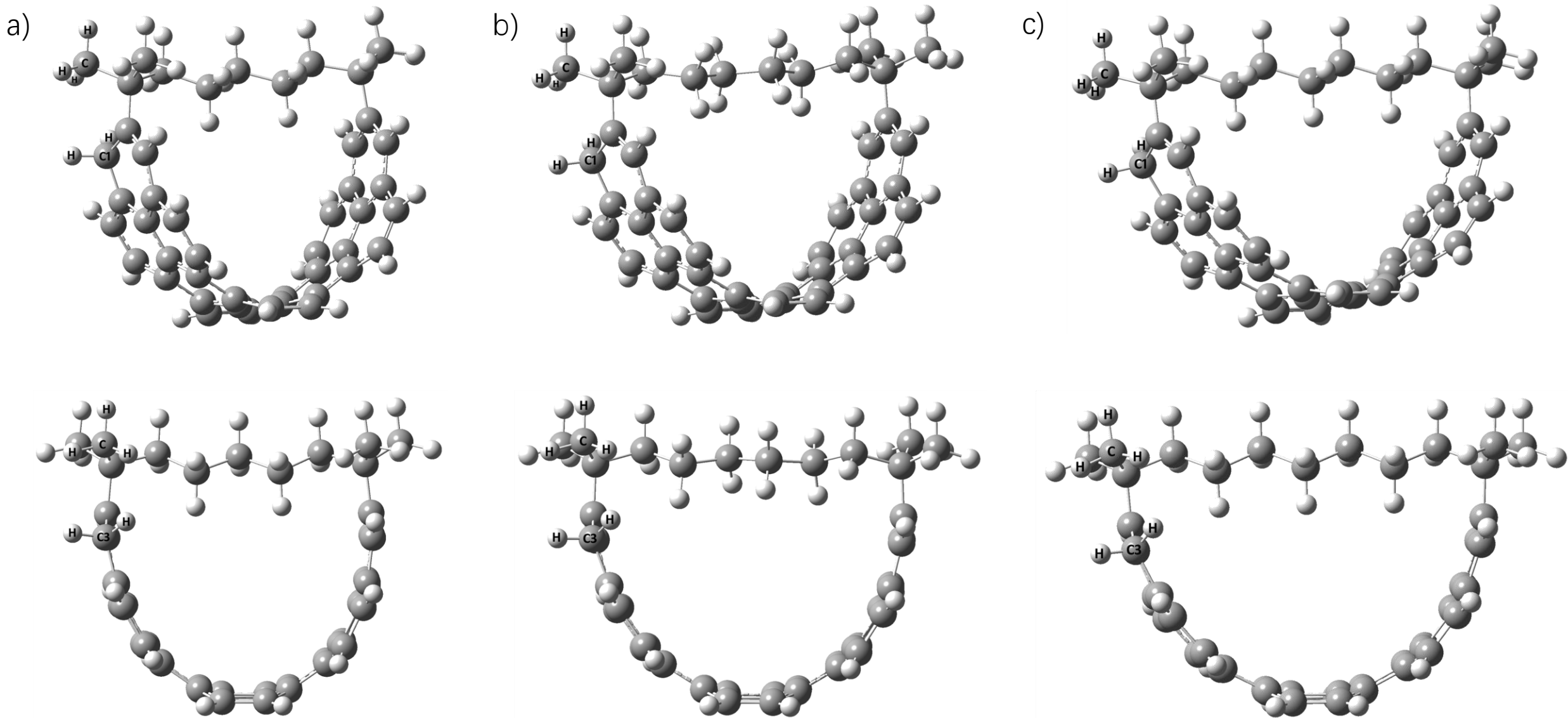
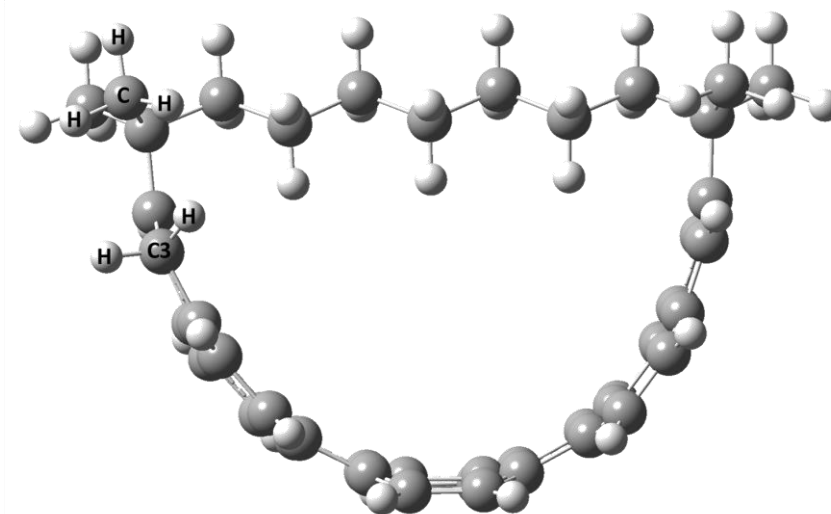
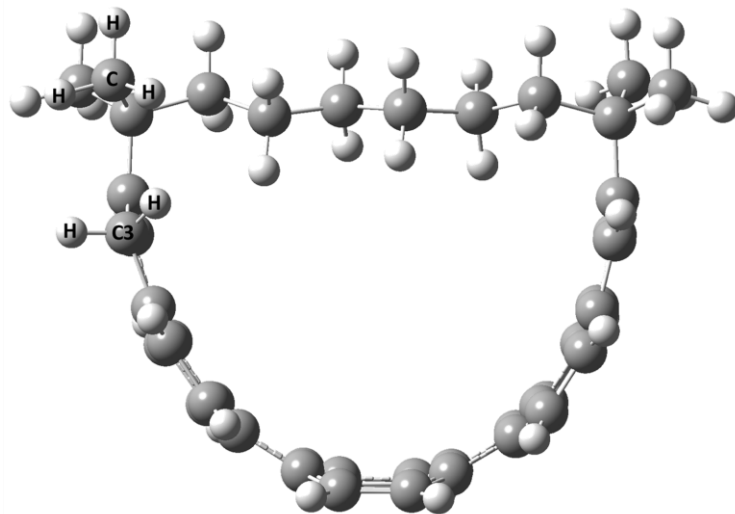
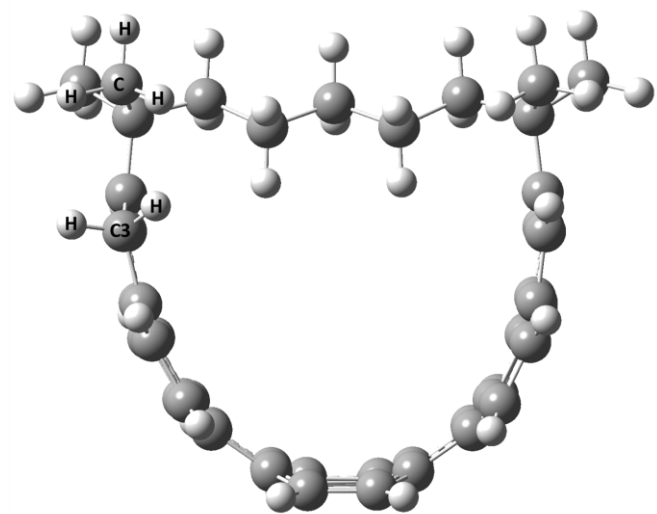
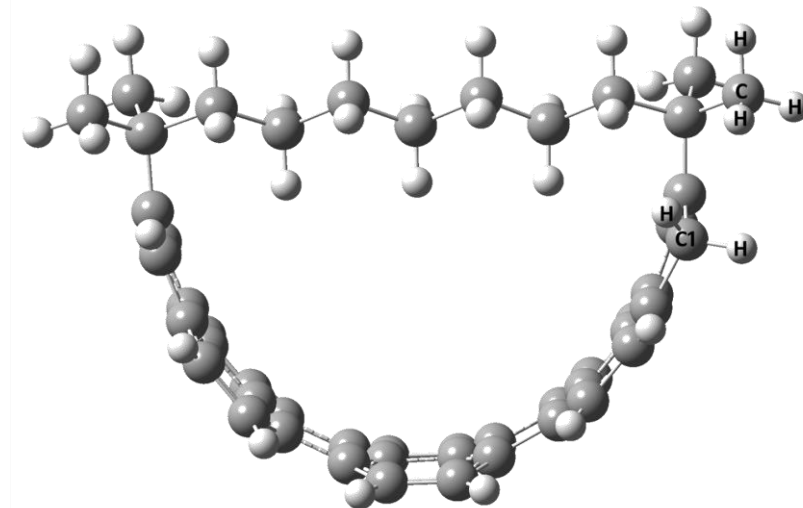
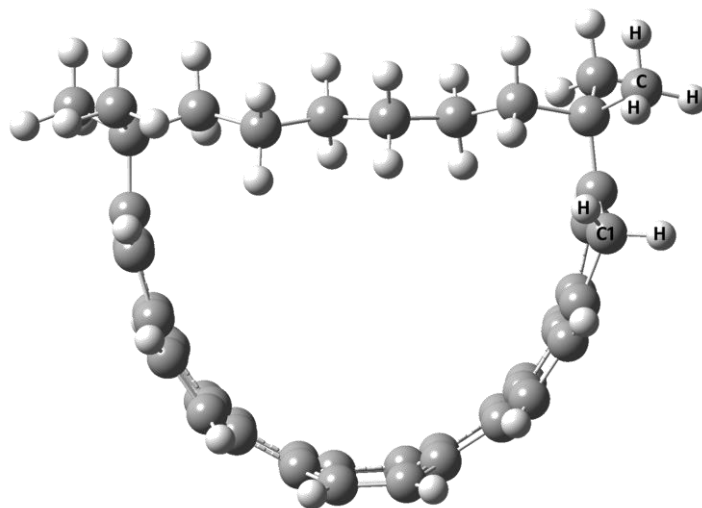
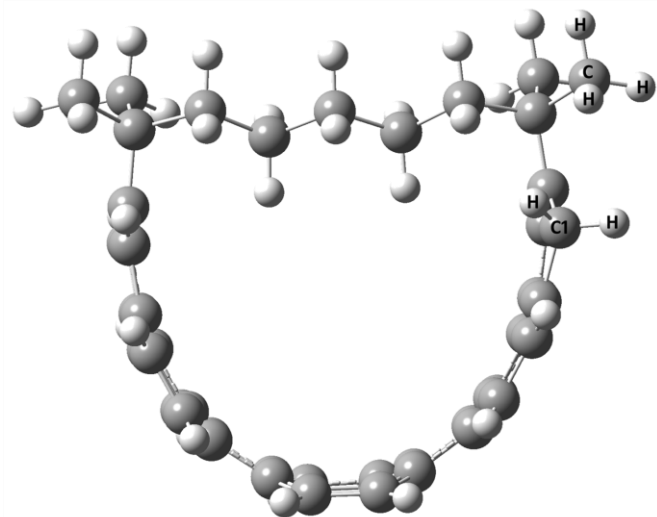


Figure S1. Computed structures of a) TM7TPH⁺; b) TM8TPH⁺; c) TM9TPH⁺ where the protonation sites are at carbon 1 (C1) and carbon 3 (C3) at the level of B3LYP-D3/6-31+G(d,p). The two hydrogens on C1 and the two hydrogens of methyl group close to C1 are staggered. When the protonation site is on C3, the two hydrogens on C3 are face to face with the two hydrogens of the methyl group right above C3.

Another perspective view of protonation on C1



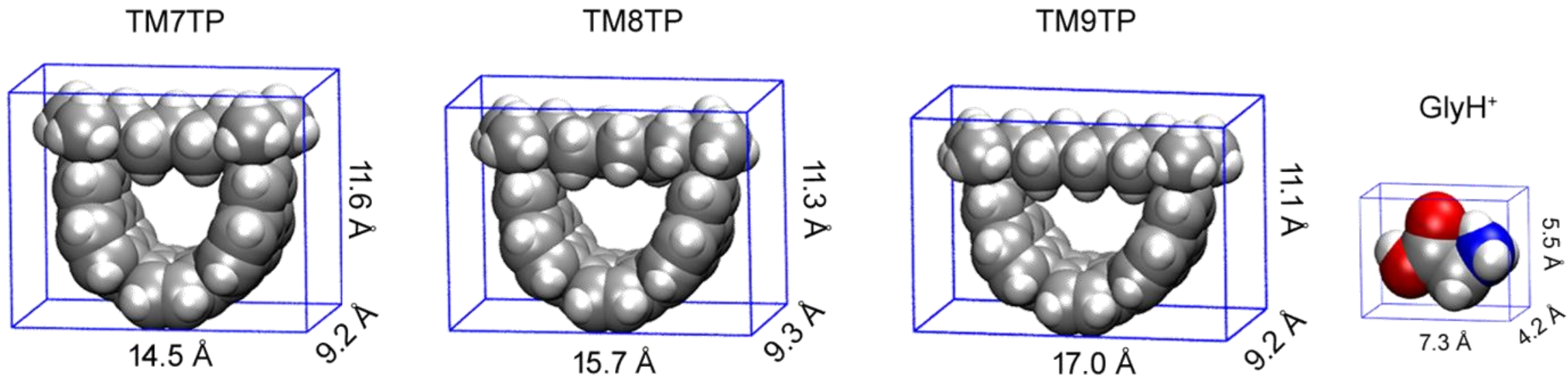


Figure S2. Boxes that enclose the Van de Waals surfaces ($\rho = 0.001$ a.u.) of TM_nTP ($n=7, 8, 9$), and protonated glycine.

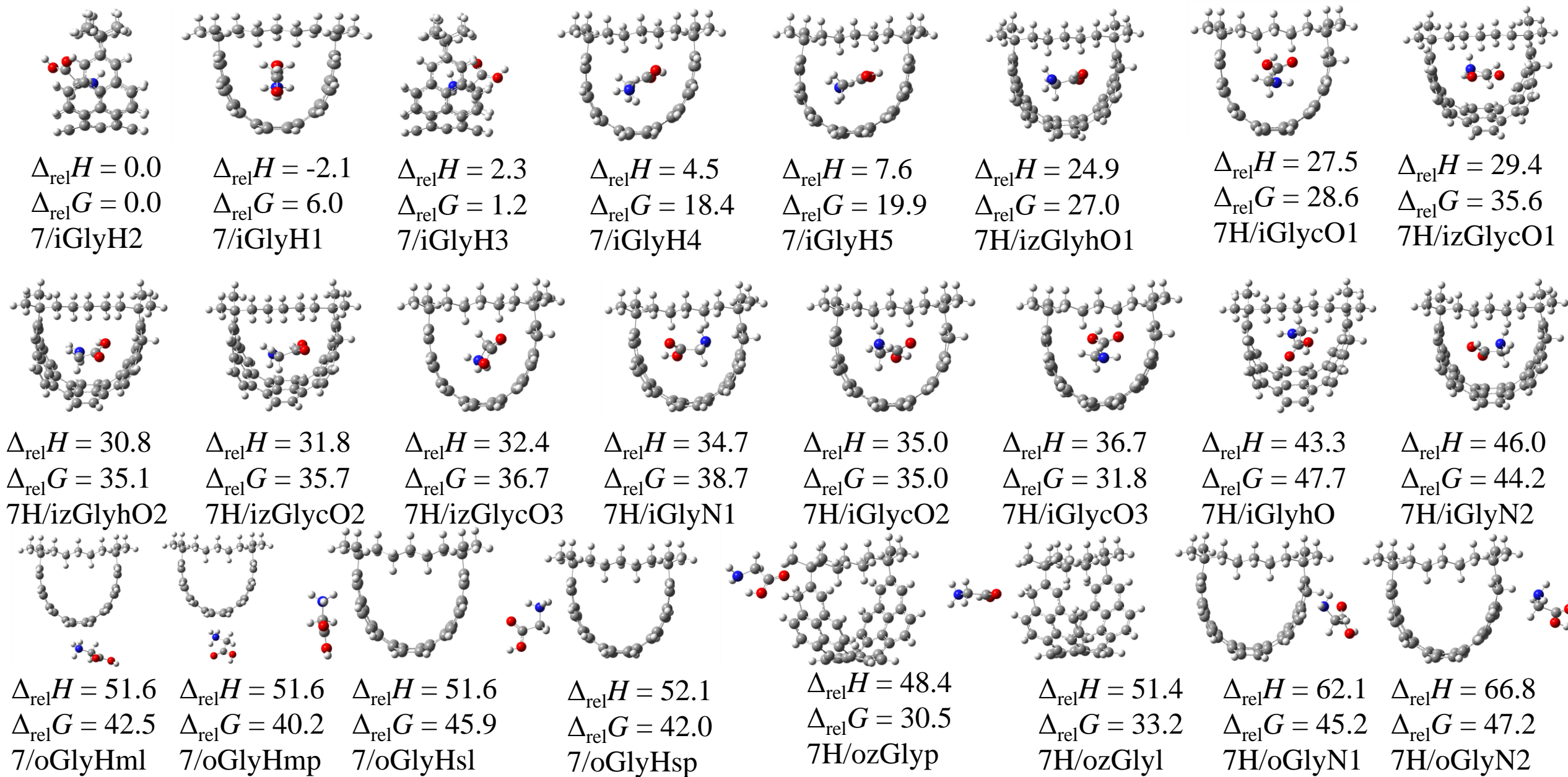


Figure S3. Computed structures and relative energies to the global minimum structure of [(TM7TP)(Gly)]H⁺ at the level of B3LYP-D3/6-31+G(d,p). Energies are listed in kJ mol⁻¹ at 298 K and 1 atm.

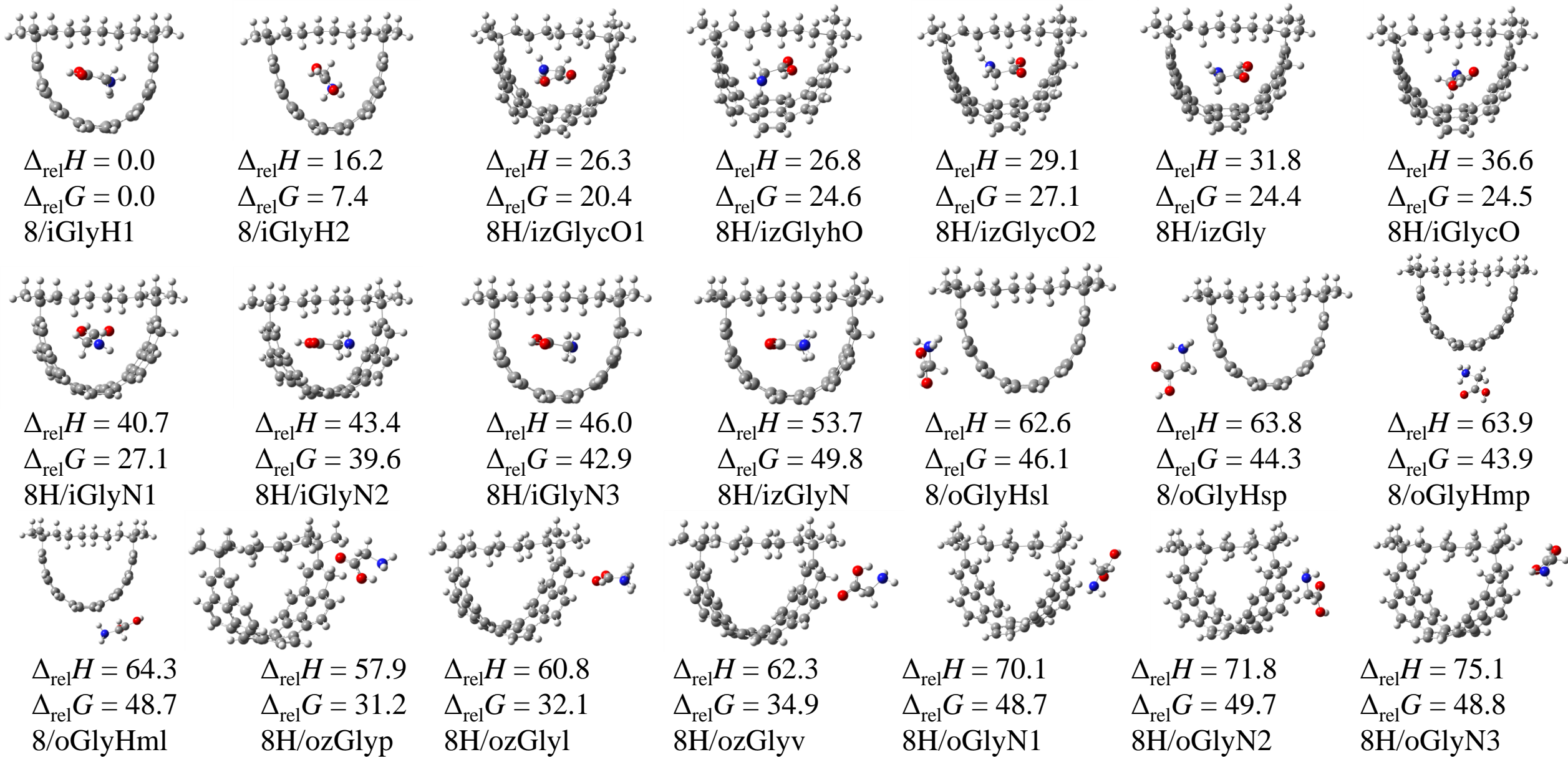


Figure S4. Computed structures and relative energies to the global minimum structure of $[(\text{TM8TP})(\text{Gly})]\text{H}^+$ at the level of B3LYP-D3/6-31+G(d,p). Energies are listed in kJ mol^{-1} at 298 K and 1 atm.

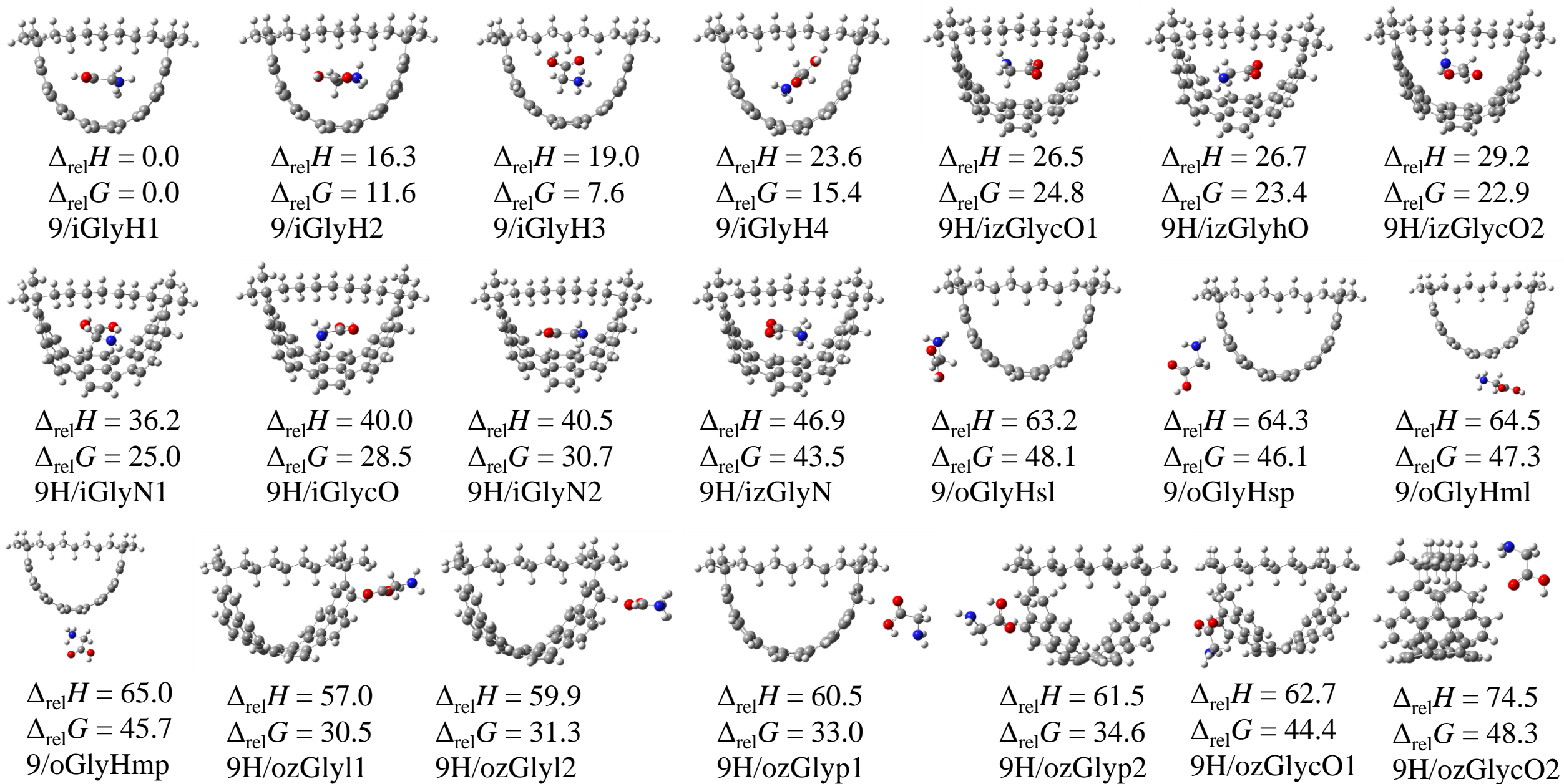


Figure S5. Computed structures and relative energies to the global minimum structure of $[(\text{TM9TP})(\text{Gly})]\text{H}^+$ at the level of B3LYP-D3/6-31+G(d,p). Energies are listed in kJ mol^{-1} at 298 K and 1 atm.

Energy kJ/mol

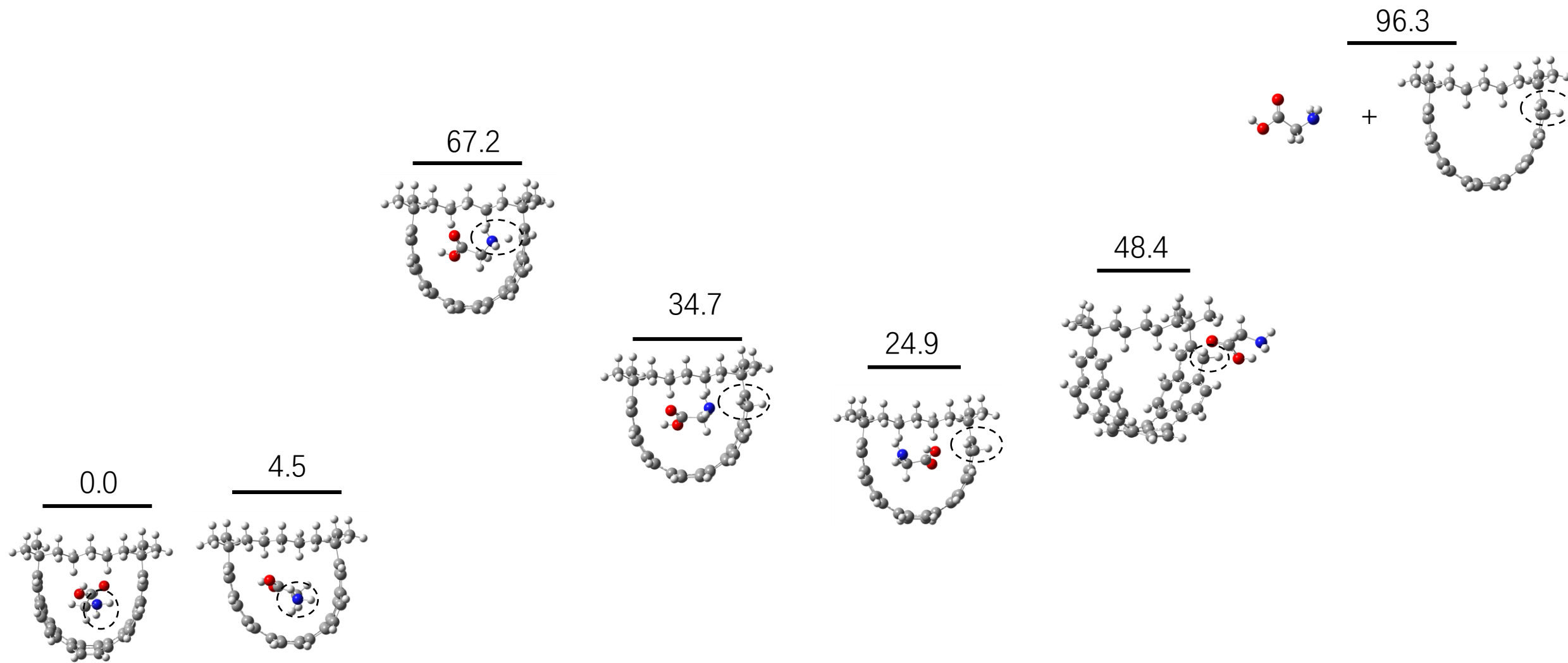


Figure S6. A possible dissociation pathway for *endo*-(TM7TP)(GlyH⁺) at the level of B3LYP-D3/6-31+G(d,p) at 298K₁₇ 1 atm. Black dashed line circles the protonation site.

Energy kJ/mol

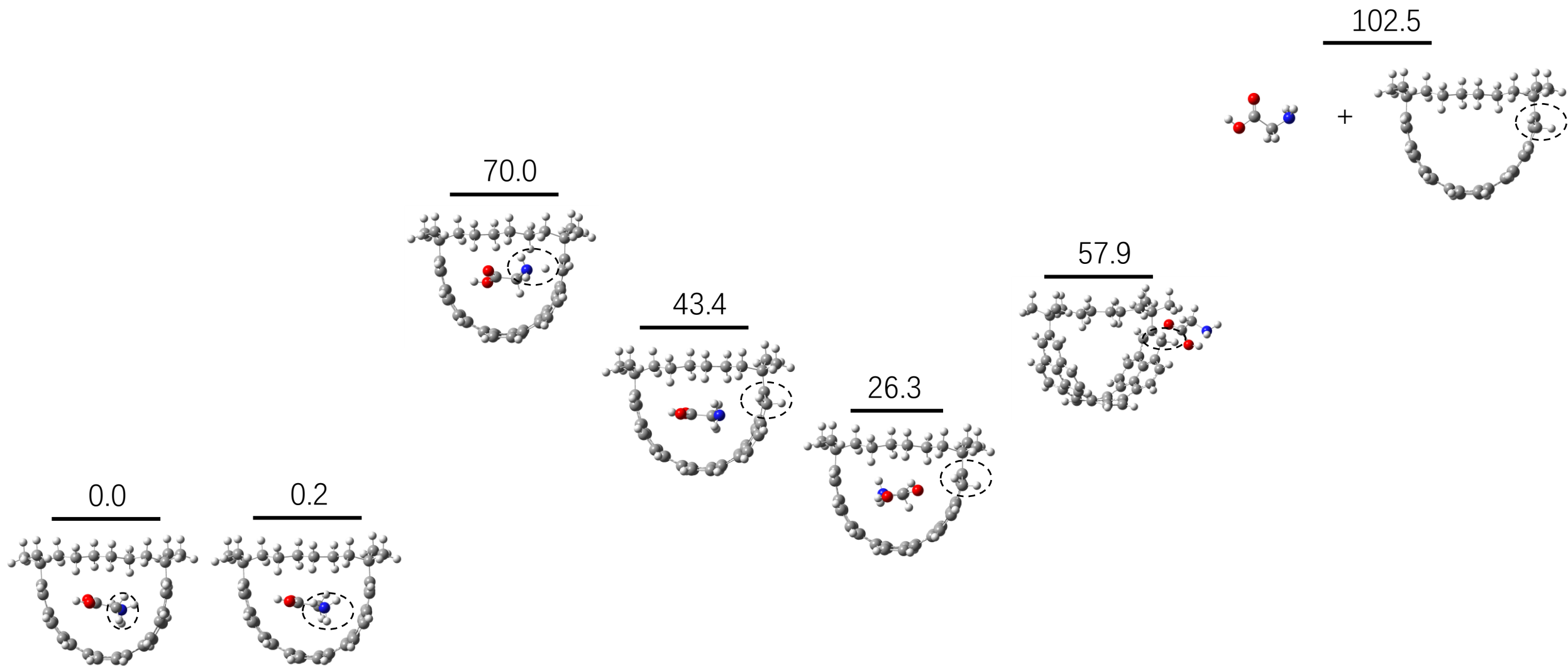


Figure S7. A possible dissociation pathway for *endo*-(TM8TP)(GlyH⁺) at the level of B3LYP-D3/6-31+G(d,p) at 298K, 1 atm. Black dashed line circles the protonation site.

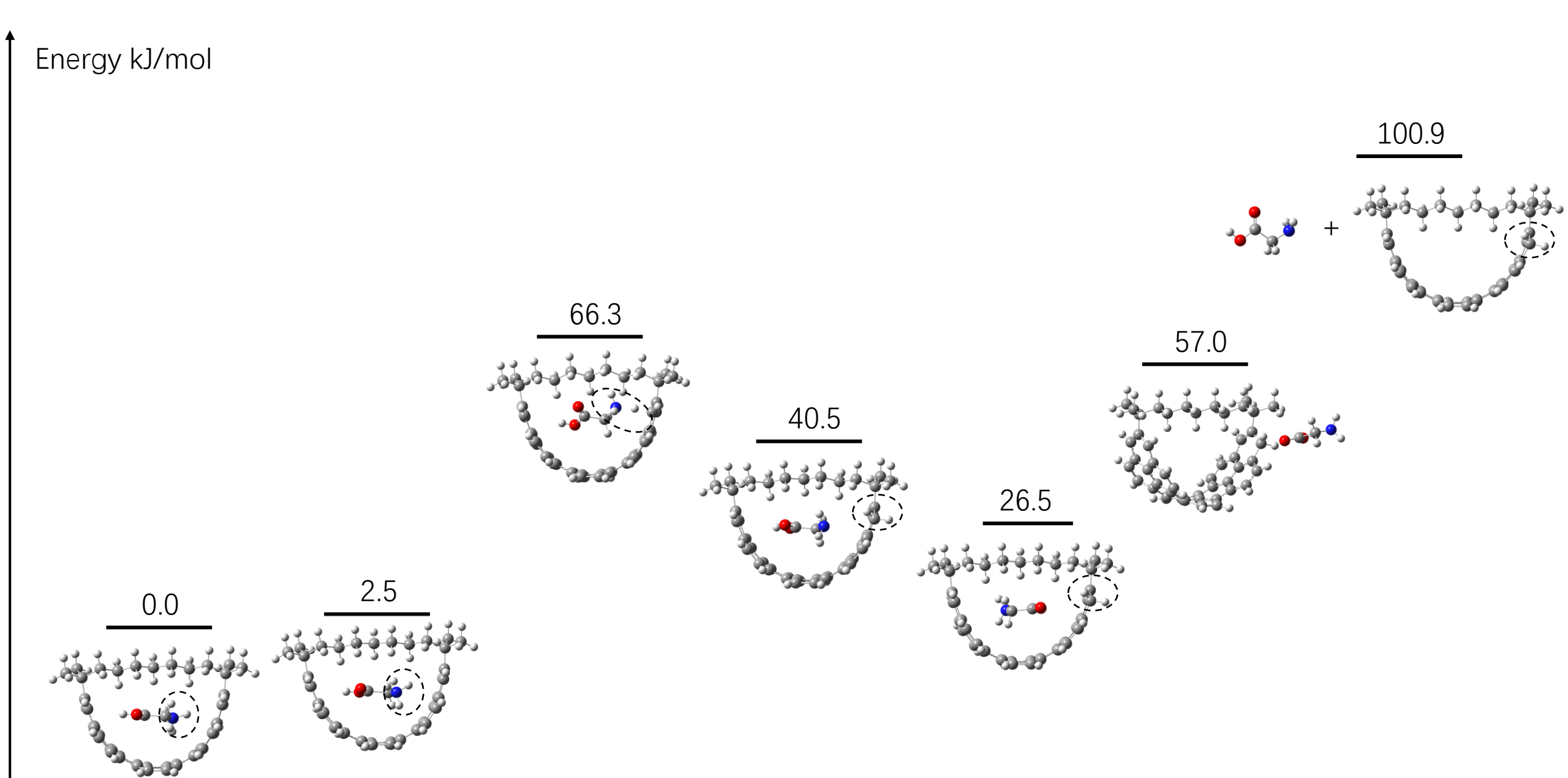
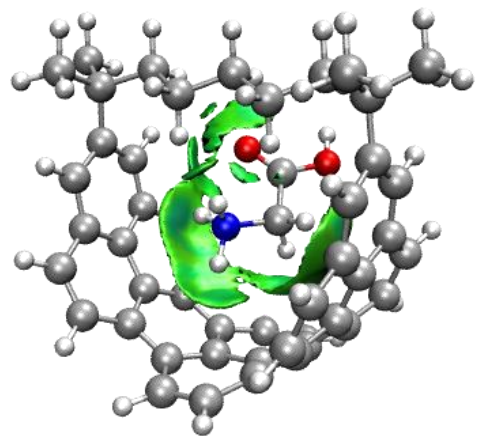
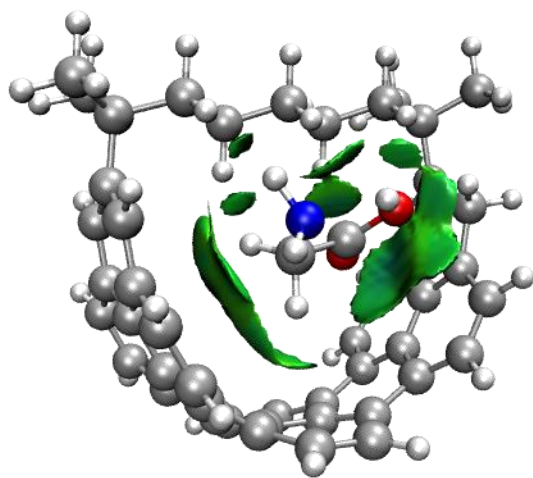
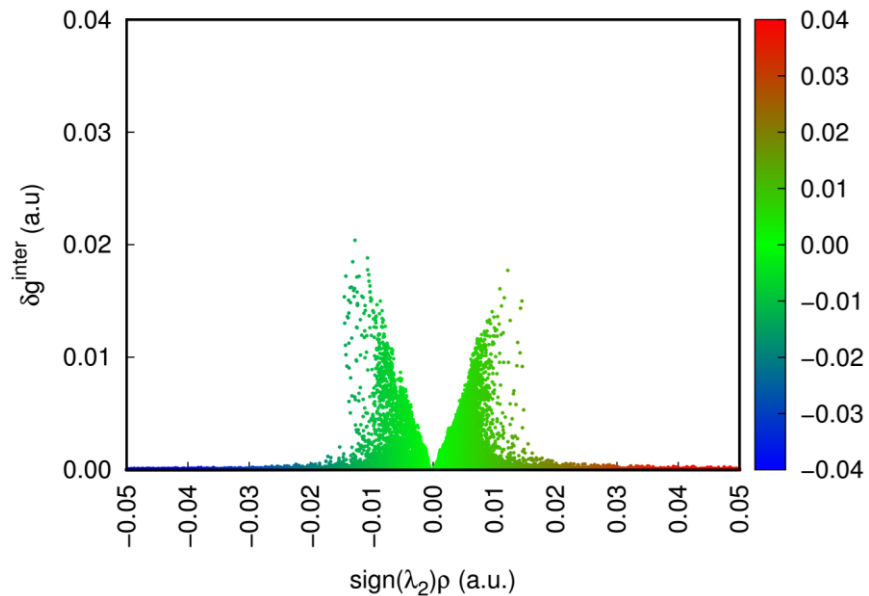


Figure S8. A possible dissociation pathway for *endo*-(TM9TP)(GlyH⁺) at the level of B3LYP-D3/6-31+G(d,p) at 298K₁₉ atm. Black dashed line circles the protonation site.



endo-(GlyH⁺)(TM7TP)



endo-(Gly)[(TM7TP)H⁺]

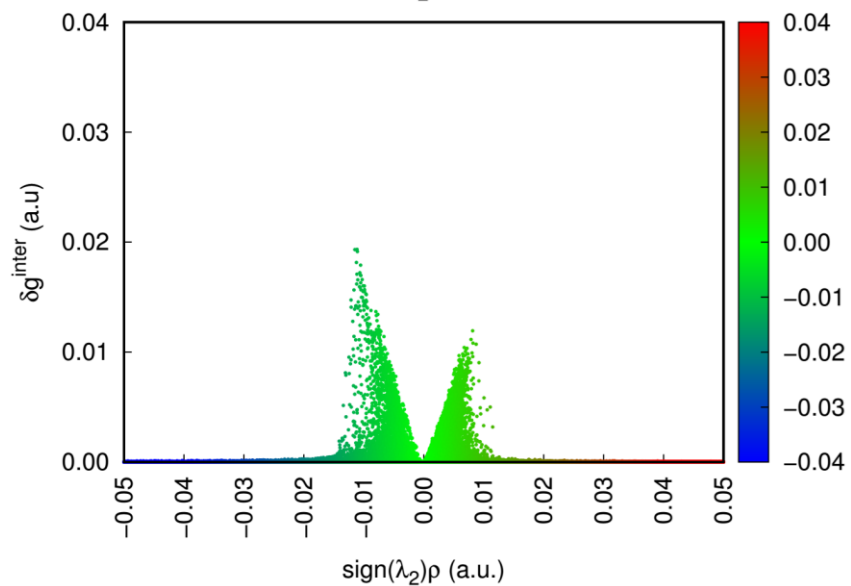
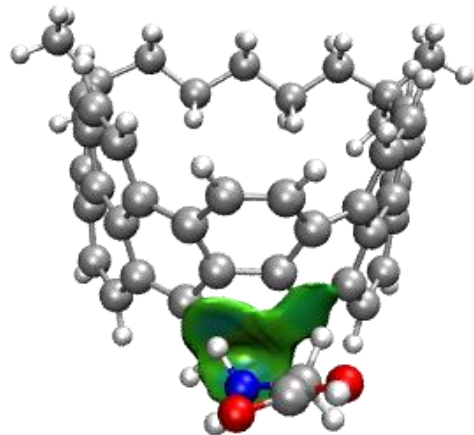
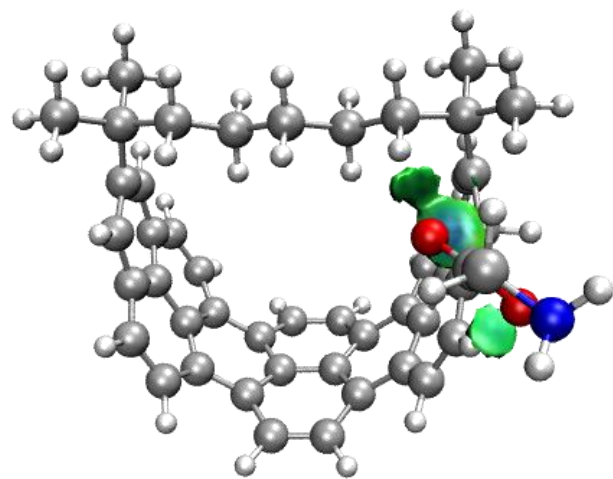
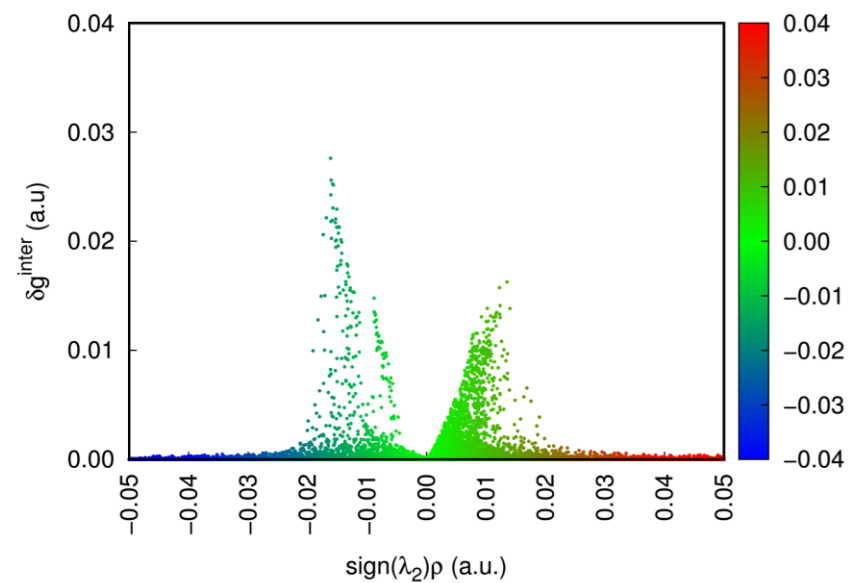


Figure S9. IGMH analysis of the lowest energy structures of each type of [(TM7TP)(Gly)]H⁺ complexes. Upper figures are three dimensional isosurfaces (isovalue = 0.005 a.u.), lower figures are IGMH scatter plots. Both are colored according BGR scheme over the range of $-0.04 < \text{sign}(\lambda_2)\rho < 0.04$ a.u., where the color blue, green and red correspond to strong attraction, weak attraction, and strong repulsion respectively.



exo-(GlyH⁺)(TM7TP)



exo-(Gly)[(TM7TP)H⁺]

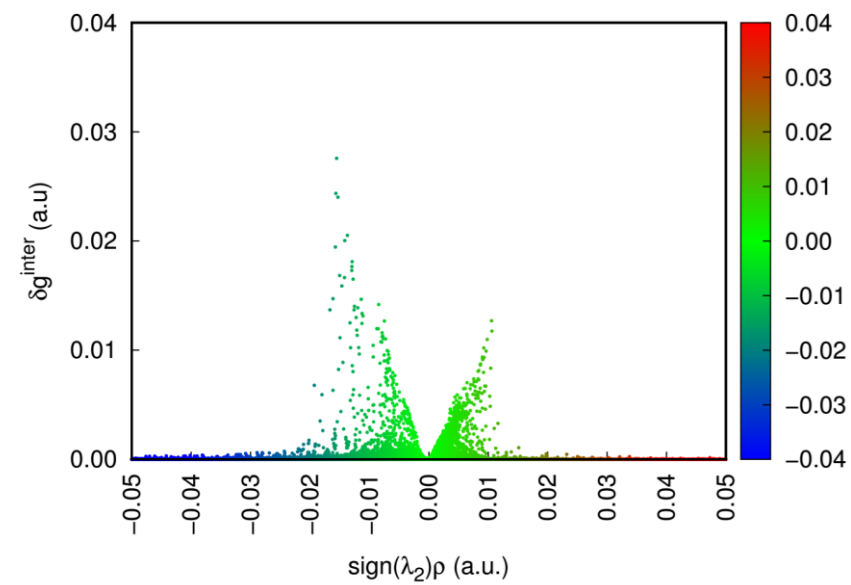
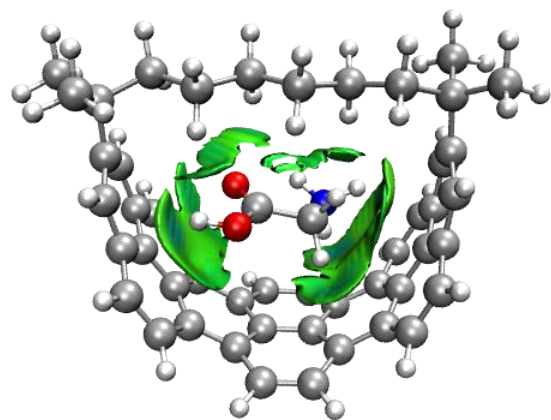
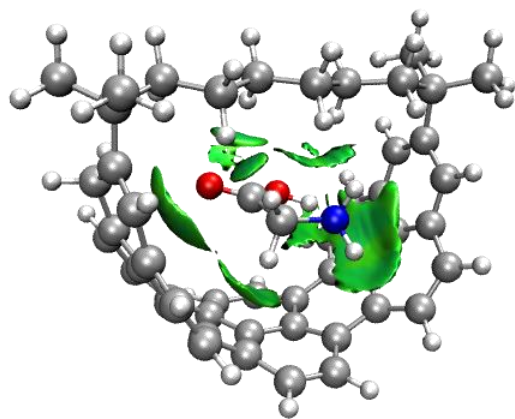
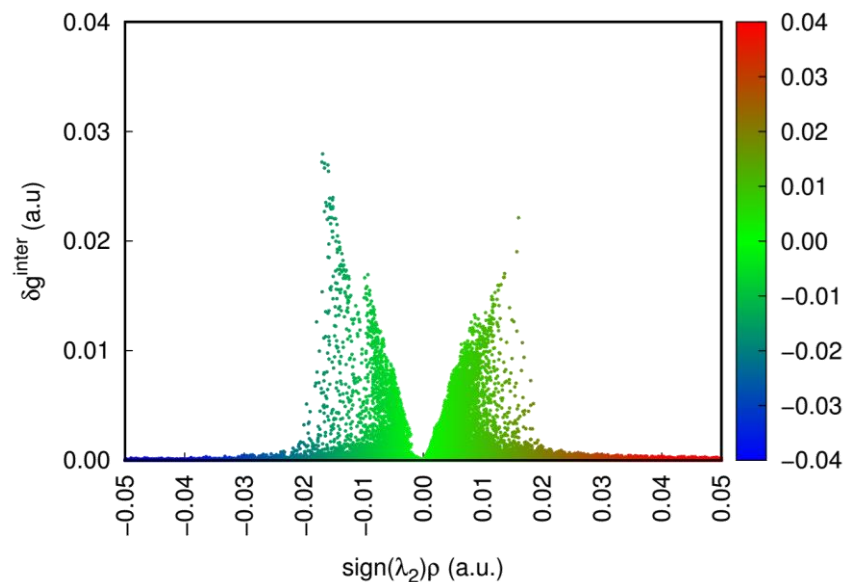


Figure S9. continued



endo-(GlyH⁺)(TM8TP)



endo-(Gly)[(TM8TP)H⁺]

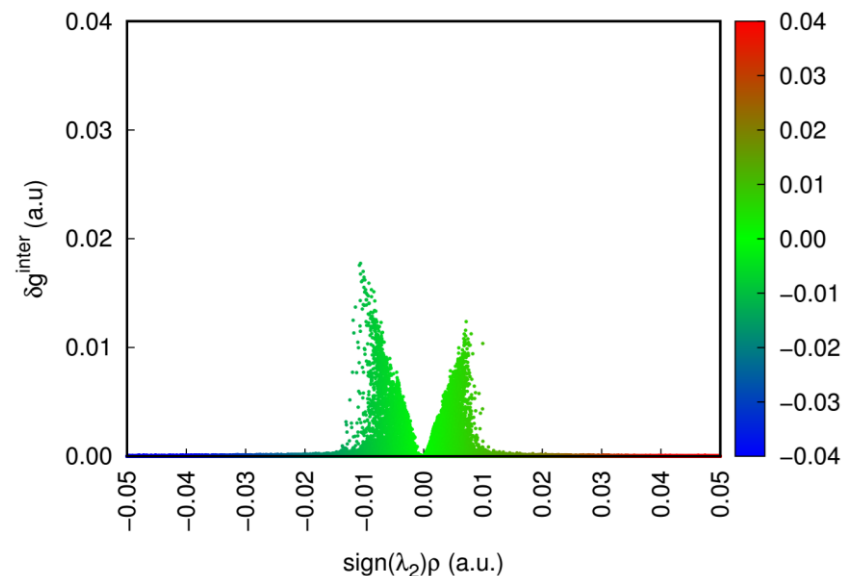
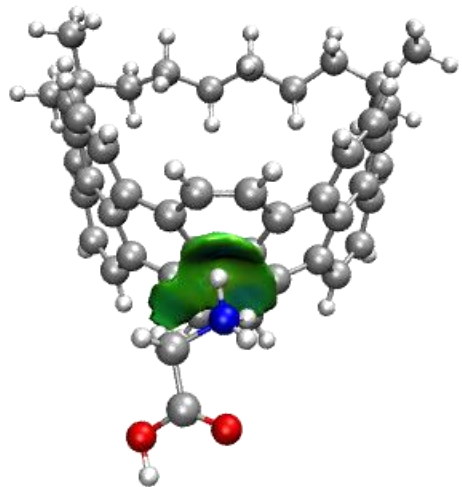
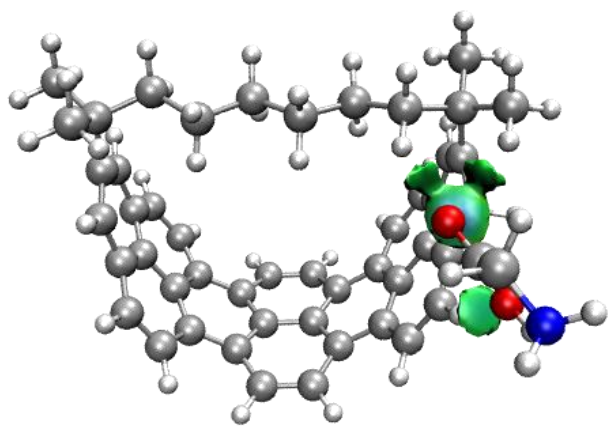
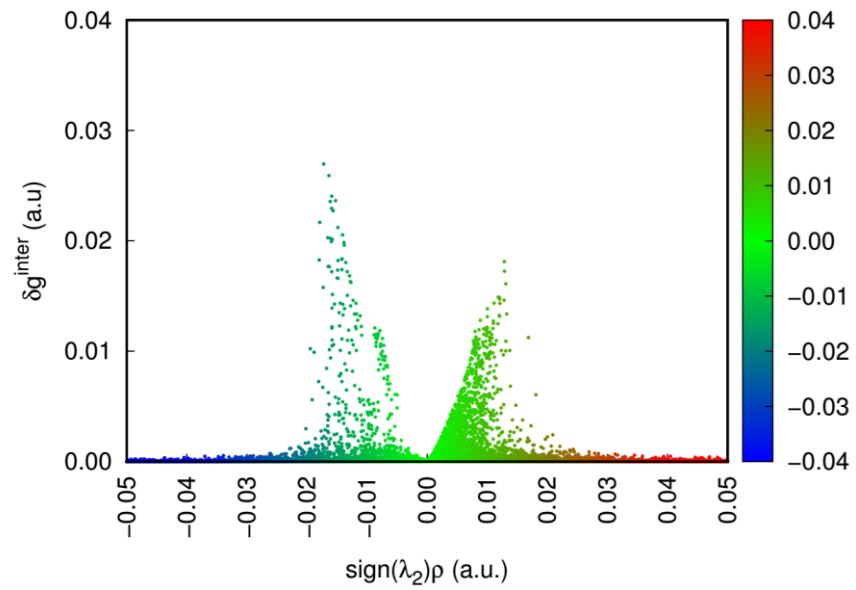


Figure S10. IGMH analysis of the lowest energy structures of each type of [(TM8TP)(Gly)]H⁺ complexes. Upper figures are three dimensional isosurfaces (isovalue = 0.005 a.u.), lower figures are IGMH scatter plots. Both are colored according BGR scheme over the range of $-0.04 < \text{sign}(\lambda_2)\rho < 0.04$ a.u., where the color blue, green and red correspond to strong attraction, weak attraction, and strong repulsion respectively.



exo-(GlyH⁺)(TM8TP)



exo-(Gly)[(TM8TP)H⁺]

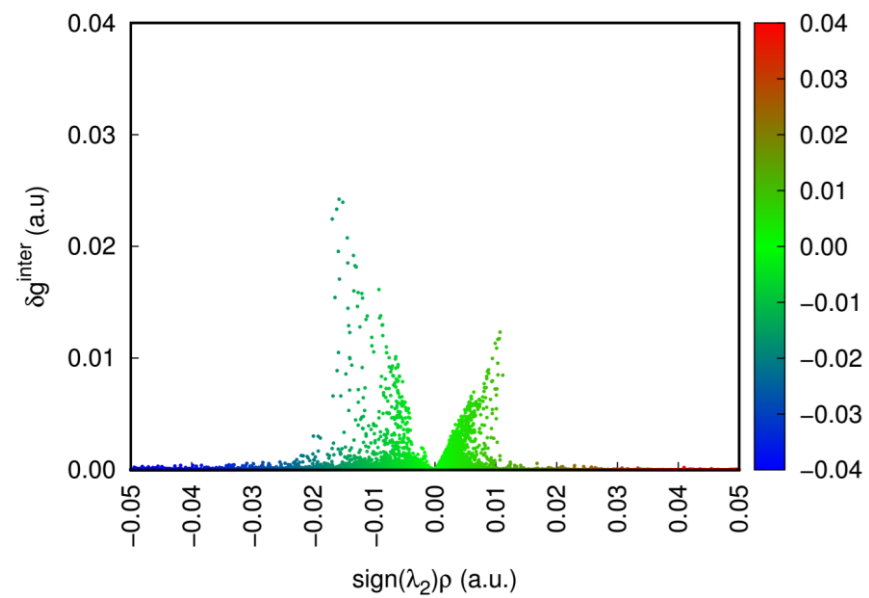


Figure S10. continued