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Apêndice A : Inputs do Gammes

Otimização de Geometria do heme

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$BASIS GBASIS=STO NGAUSS=2 $END

$GUESS GUESS=HUCKEL $END

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$DATA

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C	6	-2.423211	3.002899	-0.046667	0.110923
C	6	-2.696873	1.588362	-0.020966	0.391591
N	7	-4.080307	1.431462	0.095164	-0.774294
C	6	-4.688276	2.675346	0.152980	0.396551
C	6	-1.734789	0.559033	-0.099498	-0.395207
C	6	-1.948108	-0.794452	-0.129508	0.411487
C	6	-0.900035	-1.843399	-0.193621	0.093444
C	6	-1.556749	-3.060840	-0.157696	0.118978
C	6	-3.009030	-2.750304	-0.094810	0.429775
N	7	-3.214615	-1.423453	-0.075699	-0.724857
C	6	-4.027114	-3.761875	-0.069740	-0.448793
C	6	-5.369010	-3.530014	-0.035383	0.432517
C	6	-6.454000	-4.557200	0.003288	0.040080
C	6	-7.658421	-3.901777	0.104804	0.101728

C	6	-7.393110	-2.435100	0.120398	0.444717
N	7	-6.004630	-2.280267	-0.003177	-0.808842
C	6	-9.000339	-4.458117	0.175522	-0.515274
C	6	-8.329065	-1.454462	0.227583	-0.425592
C	6	-8.066169	-0.042329	0.262747	0.407779
C	6	-9.169012	0.967221	0.402160	0.114026
C	6	-8.551978	2.201258	0.439040	0.068334
C	6	-7.077231	1.952750	0.314474	0.426706
N	7	-6.856842	0.544197	0.220509	-0.768140
C	6	-6.251015	-5.982146	-0.054228	-0.133334
C	6	-5.375100	-6.604638	-0.845260	-0.354218
C	6	-1.000081	-4.411200	-0.182714	-0.526749
C	6	0.521347	-1.630725	-0.263499	-0.135075
C	6	1.129662	-0.708280	-1.012202	-0.340840
C	6	-10.573774	0.654711	0.471871	-0.567780
C	6	-9.205805	3.514286	0.553687	-0.328597
C	6	-9.991480	3.682775	1.842640	-0.339232
C	6	-11.492288	3.939333	1.622358	0.630438
O	8	-12.139585	4.454474	2.578798	-0.662226
C	6	-6.099899	2.897630	0.283412	-0.412695
C	6	-1.095308	3.607858	-0.170090	-0.569016
C	6	-3.833018	5.144360	0.030644	-0.359961
C	6	-3.125821	5.860696	1.167020	-0.345849
C	6	-2.186071	6.977588	0.680917	0.621695
O	8	-2.052926	7.996485	1.416512	-0.777873
O	8	-12.028465	3.606031	0.522658	-0.636275
O	8	-1.558943	6.822619	-0.411140	-0.770369
H	1	-6.913392	-6.565464	0.612893	0.135694
H	1	-4.712890	-6.070556	-1.539481	0.144778
H	1	-5.273754	-7.697161	-0.847564	0.133431
H	1	-9.559607	-4.036296	1.055753	0.159518
H	1	-8.983595	-5.571928	0.269522	0.137142
H	1	-9.585010	-4.192690	-0.748889	0.159893
H	1	-3.668392	-4.802564	-0.080811	0.150190

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 H 1   2.221033   -0.595112   -1.018875  0.127900
 H 1   0.585335   -0.013079   -1.664716  0.137997
 H 1  -9.391756   -1.739531    0.295091  0.157633
 H 1  -0.684495    0.917221   -0.139623  0.160546
 H 1  -1.398475   -5.016206    0.671286  0.147577
 H 1   0.115792   -4.386190   -0.108953  0.142969
 H 1  -1.278630   -4.932634   -1.134053  0.147438
 H 1  -6.391773    3.962015    0.365047  0.164622
 H 1 -10.813729    0.054320    1.384589  0.117839
 H 1 -10.884848    0.033594   -0.425921  0.108544
 H 1 -11.199159    1.590510    0.478384  0.275291
 H 1  -0.527510    3.149274   -1.017585  0.139082
 H 1  -0.508275    3.449670    0.770196  0.140855
 H 1  -1.183834    4.720404   -0.347589  0.202512
 H 1  -9.927771    3.625038   -0.309833  0.193597
 H 1  -8.444335    4.333252    0.463932  0.082440
 H 1  -9.573228    4.536813    2.431834  0.102354
 H 1  -9.909844    2.763202    2.476361  0.095549
 H 1  -4.924441    5.403453    0.041121  0.148583
 H 1  -3.405698    5.523951   -0.944258  0.166747
 H 1  -2.496669    5.141978    1.752082  0.148565
 H 1  -3.877549    6.302531    1.867332  0.155566
 Fe 26 -4.919295   -0.384531   -0.009205  1.477452
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Otimização de geometría do PPIX

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C 6.0 -3.52900 1.45700 -0.00400

N 7.0 -2.20800 1.59000 -0.15000

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C 6.0 -6.56400 2.30000 -0.70500

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C 6.0 -3.53000 -1.03900 0.27600

C 6.0 -4.23300 -2.32100 0.49200

C 6.0 -3.36300 -3.34100 0.43200

C 6.0 -2.03000 -2.75500 0.20900

N 7.0 -2.31000 -1.34600 0.12700

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C 6.0 -3.18800 -5.72100 -0.22700

C 6.0 -0.79400 3.49400 -0.14900

C 6.0 0.51500 2.82400 -0.20600

C 6.0 -0.85000 -3.37700 0.13000

C 6.0 0.46700 -2.75400 -0.08600

C 6.0 -5.72200 -2.45900 0.65600

C 6.0 1.84300 3.47300 -0.28800

N 7.0 0.74300 1.57800 -0.24100

C 6.0 2.79700 2.53300 -0.36700

C 6.0 2.13300 1.22000 -0.33900

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N 7.0 0.68900 -1.43700 -0.15400

C	6.0	2.00900	-1.29100	-0.31400
C	6.0	2.64100	-2.46600	-0.37800
C	6.0	2.69600	0.01000	-0.37800
C	6.0	2.09000	4.95700	-0.24400
C	6.0	1.73800	-4.95800	-0.15700
C	6.0	4.27900	2.76500	-0.49000
C	6.0	4.93200	2.64800	0.90400
C	6.0	6.41900	2.83500	0.79300
O	8.0	6.79300	4.02700	0.33600
O	8.0	7.15200	1.86900	0.65900
C	6.0	4.11200	-2.72100	-0.57900
C	6.0	4.83100	-2.65800	0.78500
C	6.0	6.30600	-2.87600	0.60000
O	8.0	6.63000	-4.06400	0.09500
O	8.0	7.05600	-1.92500	0.45700
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H	1.0	-6.24900	1.46800	-1.33300
H	1.0	-7.62100	2.56000	-0.66700
H	1.0	-3.10500	5.60900	0.79200
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H	1.0	-5.21900	0.32500	0.39800
H	1.0	-4.44900	-5.06100	1.29800
H	1.0	-3.49700	-6.75700	-0.09600
H	1.0	-2.48300	-5.48000	-1.02000
H	1.0	-0.78200	4.58100	-0.12700
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H	1.0	-6.00100	-2.20600	1.68900
H	1.0	-6.04900	-3.48500	0.43500
H	1.0	-6.23900	-1.77700	-0.03500
H	1.0	3.78100	-0.00200	-0.43700
H	1.0	1.28900	5.46700	0.30800
H	1.0	2.13100	5.35300	-1.26900
H	1.0	3.04000	5.17500	0.26500

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H 1.0 4.65800 -1.68000 1.25800
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Cálculo do ESP do HEME

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$scf dirscf=.true. $end
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C 6 -3.659290 3.681267 0.060634 0.027877
C 6 -2.422114 3.002899 -0.046667 0.110923
C 6 -2.696873 1.588162 -0.020966 0.391591

N	7	-4.080307	1.431462	0.095164	-0.774294
C	6	-4.688276	2.675346	0.152980	0.396551
C	6	-1.732789	0.559933	-0.099498	-0.395207
C	6	-1.948108	-0.794752	-0.129508	0.411487
C	6	-0.900035	-1.843399	-0.193621	0.093444
C	6	-1.558749	-3.060840	-0.157696	0.118978
C	6	-3.009030	-2.750304	-0.094810	0.419775
N	7	-3.211615	-1.423453	-0.075999	-0.724857
C	6	-4.027114	-3.761875	-0.069740	-0.448793
C	6	-5.369010	-3.530014	-0.032383	0.432517
C	6	-6.454000	-4.557200	0.003288	0.040080
C	6	-7.658421	-3.901777	0.104804	0.101728
C	6	-7.393110	-2.435100	0.120398	0.434717
N	7	-6.004630	-2.280267	-0.003177	-0.808842
C	6	-9.010339	-4.458117	0.175522	-0.525274
C	6	-8.329065	-1.453462	0.227583	-0.425592
C	6	-8.066169	-0.042329	0.272737	0.407779
C	6	-9.159012	0.967221	0.402160	0.114026
C	6	-8.551978	2.201258	0.439040	0.068334
C	6	-7.077231	1.952750	0.314474	0.426706
N	7	-6.866842	0.544197	0.220509	-0.768140
C	6	-6.251015	-5.982146	-0.054228	-0.133334
C	6	-5.375100	-6.604638	-0.845260	-0.354218
C	6	-1.000081	-4.411200	-0.182714	-0.526749
C	6	0.521347	-1.630725	-0.263499	-0.135075
C	6	1.129662	-0.708280	-1.012202	-0.340840
C	6	-10.583774	0.644711	0.461871	-0.577780
C	6	-9.205805	3.514286	0.553687	-0.328597
C	6	-9.991480	3.682775	1.842640	-0.339232
C	6	-11.492288	3.939333	1.622358	0.630438
O	8	-12.139585	4.454474	2.578798	-0.662226
C	6	-6.099899	2.897630	0.283412	-0.412695
C	6	-1.095308	3.607858	-0.170090	-0.569016
C	6	-3.833018	5.144360	0.030644	-0.359961

C	6	-3.125821	5.860696	1.167020	-0.345849
C	6	-2.186071	6.977588	0.680917	0.621695
O	8	-2.052926	7.996485	1.416512	-0.777873
O	8	-12.028465	3.606031	0.522658	-0.636275
O	8	-1.558943	6.822619	-0.411140	-0.770369
H	1	-6.913392	-6.565464	0.612893	0.135694
H	1	-4.712890	-6.070556	-1.539481	0.144778
H	1	-5.273754	-7.697161	-0.847564	0.133431
H	1	-9.559607	-4.036296	1.055753	0.159518
H	1	-8.983595	-5.571928	0.269522	0.137142
H	1	-9.585010	-4.192690	-0.748889	0.159893
H	1	-3.668392	-4.802564	-0.080811	0.150190
H	1	1.118993	-2.324023	0.358009	0.130159
H	1	2.221033	-0.595112	-1.018875	0.127900
H	1	0.585335	-0.013079	-1.664716	0.137997
H	1	-9.391756	-1.739531	0.295091	0.157633
H	1	-0.684495	0.917221	-0.139623	0.160546
H	1	-1.398475	-5.016206	0.671286	0.147577
H	1	0.115792	-4.386190	-0.108953	0.142969
H	1	-1.278630	-4.932634	-1.134053	0.147438
H	1	-6.391773	3.962015	0.365047	0.164622
H	1	-10.813729	0.054320	1.384589	0.117839
H	1	-10.884848	0.033594	-0.425921	0.108544
H	1	-11.199159	1.590510	0.478384	0.275291
H	1	-0.527510	3.149274	-1.017585	0.139082
H	1	-0.508275	3.449670	0.770196	0.140855
H	1	-1.183834	4.720404	-0.347589	0.202512
H	1	-9.927771	3.625038	-0.309833	0.193597
H	1	-8.444335	4.333252	0.463932	0.082440
H	1	-9.573228	4.536813	2.431834	0.102354
H	1	-9.909844	2.763202	2.476361	0.095549
H	1	-4.924441	5.403453	0.041121	0.148583
H	1	-3.405698	5.523951	-0.944258	0.166747
H	1	-2.496669	5.141978	1.752082	0.148565

H 1 -3.877549 6.302531 1.867332 0.155566

Fe 26 -4.919295 -0.384531 -0.009205 1.477452

$END

Calculo do ESP do PPIX

$CONTRL RUNTYP=ENERGY DFTTYP=B3LYP EXETYP=RUN MOLPLT=.TRUE. UNITS=ANGS $END

$BASIS GBASIS=N31 NGAUSS=6 NDFUNC=2 NPFUNC=1 $END

! DIFFSP=.T. DIFFS=.T. $END

$CONTRL SCFTYP=ROHF MAXIT=200 MULT=1 $END

$CONTRL ICHARG=-2 $END

$BASIS POLAR=POPN31 $END

$SYSTEM TIMLIM=600 MEMORY=80000000 $END

$STATPT OPTTOL=0.0001 NSTEP=1000 $END

$ELPOT IEPOT=1 WHERE=PDC OUTPUT=PUNCH $END

$PDC PTSEL=CONNOLLY CONSTR=NONE VDWSCL=1.4 VDWINC=0.2 LAYER=4 $END

$GUESS GUESS=HUCKEL $END

$scf dirscf=.true. $end

$DATA

ppix

C1

C 6.0 -3.25500 3.66000 -0.07700

C 6.0 -1.99400 2.90800 -0.13000

C 6.0 -4.22700 2.75300 -0.03000

C 6.0 -3.52900 1.45700 -0.00400

N 7.0 -2.20800 1.59000 -0.15000

C 6.0 -5.67600 3.02300 -0.01600

C 6.0 -6.56400 2.30000 -0.70500

C 6.0 -3.41600 5.15400 -0.15900

C 6.0 -4.14800 0.29500 0.22100

C 6.0 -3.53000 -1.03900 0.27600

C 6.0 -4.23300 -2.32100 0.49200

C 6.0 -3.36300 -3.34100 0.43200

C 6.0 -2.03000 -2.75500 0.20900

N	7.0	-2.31000	-1.34600	0.12700
C	6.0	-3.70800	-4.76900	0.55400
C	6.0	-3.18800	-5.72100	-0.22700
C	6.0	-0.79400	3.49400	-0.14900
C	6.0	0.51500	2.82400	-0.20600
C	6.0	-0.85000	-3.37700	0.13000
C	6.0	0.46700	-2.75400	-0.08600
C	6.0	-5.72200	-2.45900	0.65600
C	6.0	1.84300	3.47300	-0.28800
N	7.0	0.74300	1.57800	-0.24100
C	6.0	2.79700	2.53300	-0.36700
C	6.0	2.13300	1.22000	-0.33900
C	6.0	1.59000	-3.46200	-0.22000
N	7.0	0.68900	-1.43700	-0.15400
C	6.0	2.00900	-1.29100	-0.31400
C	6.0	2.64100	-2.46600	-0.37800
C	6.0	2.69600	0.01000	-0.37800
C	6.0	2.09000	4.95700	-0.24400
C	6.0	1.73800	-4.95800	-0.15700
C	6.0	4.27900	2.76500	-0.49000
C	6.0	4.93200	2.64800	0.90400
C	6.0	6.41900	2.83500	0.79300
O	8.0	6.79300	4.02700	0.33600
O	8.0	7.15200	1.86900	0.65900
C	6.0	4.11200	-2.72100	-0.57900
C	6.0	4.83100	-2.65800	0.78500
C	6.0	6.30600	-2.87600	0.60000
O	8.0	6.63000	-4.06400	0.09500
O	8.0	7.05600	-1.92500	0.45700
H	1.0	-6.04100	3.87500	0.55700
H	1.0	-6.24900	1.46800	-1.33300
H	1.0	-7.62100	2.56000	-0.66700
H	1.0	-3.10500	5.60900	0.79200
H	1.0	-4.46200	5.42500	-0.36100

H 1.0 -2.79300 5.55200 -0.97300
H 1.0 -5.21900 0.32500 0.39800
H 1.0 -4.44900 -5.06100 1.29800
H 1.0 -3.49700 -6.75700 -0.09600
H 1.0 -2.48300 -5.48000 -1.02000
H 1.0 -0.78200 4.58100 -0.12700
H 1.0 -0.86500 -4.45600 0.25100
H 1.0 -6.00100 -2.20600 1.68900
H 1.0 -6.04900 -3.48500 0.43500
H 1.0 -6.23900 -1.77700 -0.03500
H 1.0 3.78100 -0.00200 -0.43700
H 1.0 1.28900 5.46700 0.30800
H 1.0 2.13100 5.35300 -1.26900
H 1.0 3.04000 5.17500 0.26500
H 1.0 1.22900 -5.41500 -1.01900
H 1.0 1.28800 -5.33700 0.77300
H 1.0 2.79600 -5.25300 -0.17100
H 1.0 4.48100 3.75800 -0.91600
H 1.0 4.72000 2.01300 -1.16100
H 1.0 4.71500 1.66100 1.33800
H 1.0 4.51500 3.42600 1.56200
H 1.0 4.54400 -1.97500 -1.26200
H 1.0 4.26500 -3.71200 -1.02900
H 1.0 4.42400 -3.44600 1.43800
H 1.0 4.65800 -1.68000 1.25800
H 1.0 -1.91000 1.19100 -1.10900
H 1.0 0.17400 -1.02900 -1.01100
$END

Apêndice B : Topologia da Protoporfirina IX

Topologia da Protoporfirina IX para o campo de forces GROMOS 96

; This file was generated by PRODRG version AA061128.0505

[moleculetype]

; Name nrexcl

PYP 3

[atoms]

; nr	type	resnr	resid	atom	cgnr	charge	mass
1	OM	1	PYP	OBJ	1	-0.5915	15.9994
2	C	1	PYP	CBI	1	0.381	12.0110
3	OM	1	PYP	OBK	1	-0.5915	15.9994
4	CH2	1	PYP	CBH	1	0.016	14.0270
5	CH2	1	PYP	CBG	1	0.168	14.0270
6	C	1	PYP	CAX	1	-0.334	12.0110
7	C	1	PYP	CAV	1	0.149	12.0110
8	C	1	PYP	CBE	2	-0.083	14.0270
9	C	1	PYP	CAR	2	0.159	12.0110
10	CR1	1	PYP	CAQ	2	-0.117	13.0190
11	NR	1	PYP	NAW	2	-0.438	14.0067
12	C	1	PYP	CAY	2	0.233	12.0110
13	CR1	1	PYP	CBD	2	-0.017	13.0190
14	C	1	PYP	CBB	2	0.279	12.0110
15	NR	1	PYP	NBA	3	-0.298	14.0067
16	H	1	PYP	HBA	3	0.234	1.0080
17	C	1	PYP	CBC	3	-0.364	12.0110
18	CH2	1	PYP	CBL	3	0.156	14.0270
19	CH2	1	PYP	CBM	3	0.039	14.0270
20	C	1	PYP	CBN	3	0.356	12.0110

```
  21      OM    1   PYP      OBP  3   -0.5915 15.9994
  22      OM    1   PYP      OBO  3   -0.5915 15.9994
  23       C    1   PYP CAZ  4    0.135  12.0110
  24       C    1   PYP CBF  4   -0.021  14.0270
  25       C    1   PYP CAT  4    0.041  12.0110
  26     CR1    1   PYP      CAS  4   -0.036  13.0190
  27       C    1   PYP CAM  4    0.174  12.0110
  28      NR    1   PYP      NAN  4   -0.471  14.0067
  29       C    1   PYP CAL  5   -0.052  12.0110
  30       C    1   PYP CAO  5   -0.010  13.0190
  31       C    1   PYP CAP  5   -0.094  14.0270
  32       C    1   PYP CAK  5    0.072  12.0110
  33       C    1   PYP CAU  5   -0.092  14.0270
  34       C    1   PYP CAJ  5    0.157  12.0110
  35     CR1    1   PYP      CAI  5   -0.07   13.0190
  36       C    1   PYP CAD  6    0.083  12.0110
  37      NR    1   PYP      NAE  7   -0.249  14.0067
  38       H    1   PYP HAE  7    0.279   1.0080
  39       C    1   PYP CAB  7    0.067  12.0110
  40       C    1   PYP CAA  7    0.108  12.0110
  41       C    1   PYP CAH  7   -0.054  14.0270
  42       C    1   PYP CAC  7   -0.021  12.0110
  43       C    1   PYP CAF  7   -0.02   13.0190
  44       C    1   PYP CAG  7   -0.074  14.0270

[ bonds ]
; ai  aj  fu    c0, c1, ...
   1   2   2    0.125  13400000.0    0.125  13400000.0 ;   OBJ  CBI
   2   3   2    0.125  13400000.0    0.125  13400000.0 ;   CBI  OBK
   2   4   2    0.153   7150000.0    0.153   7150000.0 ;   CBI  CBH
   4   5   2    0.153   7150000.0    0.153   7150000.0 ;   CBH  CBG
   5   6   2    0.153   7150000.0    0.153   7150000.0 ;   CBG  CAX
   6   7   2    0.133  11800000.0    0.133  11800000.0 ;   CAX  CAV
   6  12   2    0.133  11800000.0    0.133  11800000.0 ;   CAX  CAY
```

```
 7  8  2   0.133  11800000.0   0.133  11800000.0 ;  CAV  CBE
 7  9  2   0.133  11800000.0   0.133  11800000.0 ;  CAV  CAR
 9 10  2   0.133  11800000.0   0.133  11800000.0 ;  CAR  CAQ
 9 11  2   0.133  11800000.0   0.133  11800000.0 ;  CAR  NAW
10 39  2   0.133  11800000.0   0.133  11800000.0 ;  CAQ  CAB
11 12  2   0.133  11800000.0   0.133  11800000.0 ;  NAW  CAY
12 13  2   0.133  11800000.0   0.133  11800000.0 ;  CAY  CBD
13 14  2   0.133  11800000.0   0.133  11800000.0 ;  CBD  CBB
14 15  2   0.133  11800000.0   0.133  11800000.0 ;  CBB  NBA
14 17  2   0.133  11800000.0   0.133  11800000.0 ;  CBB  CBC
15 16  2   0.100  18700000.0   0.100  18700000.0 ;  NBA  HBA
15 25  2   0.133  11800000.0   0.133  11800000.0 ;  NBA  CAT
17 18  2   0.153   7150000.0   0.153   7150000.0 ;  CBC  CBL
17 23  2   0.133  11800000.0   0.133  11800000.0 ;  CBC  CAZ
18 19  2   0.153   7150000.0   0.153   7150000.0 ;  CBL  CBM
19 20  2   0.153   7150000.0   0.153   7150000.0 ;  CBM  CBN
20 21  2   0.125  13400000.0   0.125  13400000.0 ;  CBN  OBP
20 22  2   0.125  13400000.0   0.125  13400000.0 ;  CBN  OBO
23 24  2   0.133  11800000.0   0.133  11800000.0 ;  CAZ  CBF
23 25  2   0.133  11800000.0   0.133  11800000.0 ;  CAZ  CAT
25 26  2   0.133  11800000.0   0.133  11800000.0 ;  CAT  CAS
26 27  2   0.133  11800000.0   0.133  11800000.0 ;  CAS  CAM
27 28  2   0.133  11800000.0   0.133  11800000.0 ;  CAM  NAN
27 29  2   0.133  11800000.0   0.133  11800000.0 ;  CAM  CAL
28 34  2   0.133  11800000.0   0.133  11800000.0 ;  NAN  CAJ
29 30  2   0.133  11800000.0   0.133  11800000.0 ;  CAL  CAO
29 32  2   0.133  11800000.0   0.133  11800000.0 ;  CAL  CAK
30 31  2   0.153   7150000.0   0.153   7150000.0 ;  CAO  CAP
32 33  2   0.133  11800000.0   0.133  11800000.0 ;  CAK  CAU
32 34  2   0.133  11800000.0   0.133  11800000.0 ;  CAK  CAJ
34 35  2   0.133  11800000.0   0.133  11800000.0 ;  CAJ  CAI
35 36  2   0.133  11800000.0   0.133  11800000.0 ;  CAI  CAD
36 37  2   0.133  11800000.0   0.133  11800000.0 ;  CAD  NAE
36 42  2   0.133  11800000.0   0.133  11800000.0 ;  CAD  CAC
```

```
 37  38   2    0.100  18700000.0    0.100  18700000.0 ;   NAE  HAE
 37  39   2    0.133  11800000.0    0.133  11800000.0 ;   NAE  CAB
 39  40   2    0.133  11800000.0    0.133  11800000.0 ;   CAB  CAA
 40  41   2    0.133  11800000.0    0.133  11800000.0 ;   CAA  CAH
 40  42   2    0.133  11800000.0    0.133  11800000.0 ;   CAA  CAC
 42  43   2    0.133  11800000.0    0.133  11800000.0 ;   CAC  CAF
 43  44   2    0.153   7150000.0    0.153   7150000.0 ;   CAF  CAG

[ pairs ]
; ai  aj  fu    c0, c1, ...
  1   5   1                          ;   OBJ  CBG
  2   6   1                          ;   CBI  CAX
  3   5   1                          ;   OBK  CBG
  4   7   1                          ;   CBH  CAV
  4  12   1                          ;   CBH  CAY
  5   8   1                          ;   CBG  CBE
  5   9   1                          ;   CBG  CAR
  5  11   1                          ;   CBG  NAW
  5  13   1                          ;   CBG  CBD
  6  10   1                          ;   CAX  CAQ
  6  14   1                          ;   CAX  CBB
  7  13   1                          ;   CAV  CBD
  7  39   1                          ;   CAV  CAB
  8  10   1                          ;   CBE  CAQ
  8  11   1                          ;   CBE  NAW
  8  12   1                          ;   CBE  CAY
  9  13   1                          ;   CAR  CBD
  9  37   1                          ;   CAR  NAE
  9  40   1                          ;   CAR  CAA
 10  12   1                          ;   CAQ  CAY
 10  36   1                          ;   CAQ  CAD
 10  38   1                          ;   CAQ  HAE
 10  41   1                          ;   CAQ  CAH
 10  42   1                          ;   CAQ  CAC
```

```
11 14  1                ; NAW CBB
11 39  1                ; NAW CAB
12 15  1                ; CAY NBA
12 17  1                ; CAY CBC
13 16  1                ; CBD HBA
13 18  1                ; CBD CBL
13 23  1                ; CBD CAZ
13 25  1                ; CBD CAT
14 19  1                ; CBB CBM
14 24  1                ; CBB CBF
14 26  1                ; CBB CAS
15 18  1                ; NBA CBL
15 24  1                ; NBA CBF
15 27  1                ; NBA CAM
16 17  1                ; HBA CBC
16 23  1                ; HBA CAZ
16 26  1                ; HBA CAS
17 20  1                ; CBC CBN
17 26  1                ; CBC CAS
18 21  1                ; CBL OBP
18 22  1                ; CBL OBO
18 24  1                ; CBL CBF
18 25  1                ; CBL CAT
19 23  1                ; CBM CAZ
23 27  1                ; CAZ CAM
24 26  1                ; CBF CAS
25 28  1                ; CAT NAN
25 29  1                ; CAT CAL
26 30  1                ; CAS CAO
26 32  1                ; CAS CAK
26 34  1                ; CAS CAJ
27 31  1                ; CAM CAP
27 33  1                ; CAM CAU
27 35  1                ; CAM CAI
```

```
 28  30   1                    ;  NAN  CAO
 28  33   1                    ;  NAN  CAU
 28  36   1                    ;  NAN  CAD
 29  35   1                    ;  CAL  CAI
 30  33   1                    ;  CAO  CAU
 30  34   1                    ;  CAO  CAJ
 31  32   1                    ;  CAP  CAK
 32  36   1                    ;  CAK  CAD
 33  35   1                    ;  CAU  CAI
 34  37   1                    ;  CAJ  NAE
 34  42   1                    ;  CAJ  CAC
 35  38   1                    ;  CAI  HAE
 35  39   1                    ;  CAI  CAB
 35  40   1                    ;  CAI  CAA
 35  43   1                    ;  CAI  CAF
 36  41   1                    ;  CAD  CAH
 36  44   1                    ;  CAD  CAG
 37  41   1                    ;  NAE  CAH
 37  43   1                    ;  NAE  CAF
 38  40   1                    ;  HAE  CAA
 38  42   1                    ;  HAE  CAC
 39  43   1                    ;  CAB  CAF
 40  44   1                    ;  CAA  CAG
 41  43   1                    ;  CAH  CAF

[ angles ]
; ai  aj  ak  fu    c0, c1, ...
   1   2   3   2    126.0      770.0    126.0      770.0 ;   OBJ  CBI  OBK
   1   2   4   2    117.0      635.0    117.0      635.0 ;   OBJ  CBI  CBH
   3   2   4   2    117.0      635.0    117.0      635.0 ;   OBK  CBI  CBH
   2   4   5   2    109.5      520.0    109.5      520.0 ;   CBI  CBH  CBG
   4   5   6   2    109.5      520.0    109.5      520.0 ;   CBH  CBG  CAX
   5   6   7   2    120.0      560.0    120.0      560.0 ;   CBG  CAX  CAV
   5   6  12   2    120.0      560.0    120.0      560.0 ;   CBG  CAX  CAY
```

7 6 12 2 108.0 465.0 108.0 465.0 ; CAV CAX CAY
6 7 8 2 120.0 560.0 120.0 560.0 ; CAX CAV CBE
6 7 9 2 108.0 465.0 108.0 465.0 ; CAX CAV CAR
8 7 9 2 120.0 560.0 120.0 560.0 ; CBE CAV CAR
7 9 10 2 132.0 760.0 132.0 760.0 ; CAV CAR CAQ
7 9 11 2 108.0 465.0 108.0 465.0 ; CAV CAR NAW
10 9 11 2 120.0 560.0 120.0 560.0 ; CAQ CAR NAW
9 10 39 2 120.0 505.0 120.0 505.0 ; CAR CAQ CAB
9 11 12 2 108.0 465.0 108.0 465.0 ; CAR NAW CAY
6 12 11 2 108.0 465.0 108.0 465.0 ; CAX CAY NAW
6 12 13 2 132.0 760.0 132.0 760.0 ; CAX CAY CBD
11 12 13 2 120.0 560.0 120.0 560.0 ; NAW CAY CBD
12 13 14 2 120.0 505.0 120.0 505.0 ; CAY CBD CBB
13 14 15 2 120.0 560.0 120.0 560.0 ; CBD CBB NBA
13 14 17 2 132.0 760.0 132.0 760.0 ; CBD CBB CBC
15 14 17 2 108.0 465.0 108.0 465.0 ; NBA CBB CBC
14 15 16 2 126.0 575.0 126.0 575.0 ; CBB NBA HBA
14 15 25 2 108.0 465.0 108.0 465.0 ; CBB NBA CAT
16 15 25 2 126.0 575.0 126.0 575.0 ; HBA NBA CAT
14 17 18 2 120.0 560.0 120.0 560.0 ; CBB CBC CBL
14 17 23 2 108.0 465.0 108.0 465.0 ; CBB CBC CAZ
18 17 23 2 120.0 560.0 120.0 560.0 ; CBL CBC CAZ
17 18 19 2 109.5 520.0 109.5 520.0 ; CBC CBL CBM
18 19 20 2 109.5 520.0 109.5 520.0 ; CBL CBM CBN
19 20 21 2 117.0 635.0 117.0 635.0 ; CBM CBN OBP
19 20 22 2 117.0 635.0 117.0 635.0 ; CBM CBN OBO
21 20 22 2 126.0 770.0 126.0 770.0 ; OBP CBN OBO
17 23 24 2 120.0 560.0 120.0 560.0 ; CBC CAZ CBF
17 23 25 2 108.0 465.0 108.0 465.0 ; CBC CAZ CAT
24 23 25 2 120.0 560.0 120.0 560.0 ; CBF CAZ CAT
15 25 23 2 108.0 465.0 108.0 465.0 ; NBA CAT CAZ
15 25 26 2 120.0 560.0 120.0 560.0 ; NBA CAT CAS
23 25 26 2 132.0 760.0 132.0 760.0 ; CAZ CAT CAS
25 26 27 2 120.0 505.0 120.0 505.0 ; CAT CAS CAM

26	27	28	2	120.0	560.0	120.0	560.0 ;	CAS	CAM	NAN
26	27	29	2	132.0	760.0	132.0	760.0 ;	CAS	CAM	CAL
28	27	29	2	108.0	465.0	108.0	465.0 ;	NAN	CAM	CAL
27	28	34	2	108.0	465.0	108.0	465.0 ;	CAM	NAN	CAJ
27	29	30	2	120.0	560.0	120.0	560.0 ;	CAM	CAL	CAO
27	29	32	2	108.0	465.0	108.0	465.0 ;	CAM	CAL	CAK
30	29	32	2	120.0	560.0	120.0	560.0 ;	CAO	CAL	CAK
29	30	31	2	115.0	610.0	115.0	610.0 ;	CAL	CAO	CAP
29	32	33	2	120.0	560.0	120.0	560.0 ;	CAL	CAK	CAU
29	32	34	2	108.0	465.0	108.0	465.0 ;	CAL	CAK	CAJ
33	32	34	2	120.0	560.0	120.0	560.0 ;	CAU	CAK	CAJ
28	34	32	2	108.0	465.0	108.0	465.0 ;	NAN	CAJ	CAK
28	34	35	2	120.0	560.0	120.0	560.0 ;	NAN	CAJ	CAI
32	34	35	2	132.0	760.0	132.0	760.0 ;	CAK	CAJ	CAI
34	35	36	2	120.0	505.0	120.0	505.0 ;	CAJ	CAI	CAD
35	36	37	2	120.0	560.0	120.0	560.0 ;	CAI	CAD	NAE
35	36	42	2	132.0	760.0	132.0	760.0 ;	CAI	CAD	CAC
37	36	42	2	108.0	465.0	108.0	465.0 ;	NAE	CAD	CAC
36	37	38	2	126.0	575.0	126.0	575.0 ;	CAD	NAE	HAE
36	37	39	2	108.0	465.0	108.0	465.0 ;	CAD	NAE	CAB
38	37	39	2	126.0	575.0	126.0	575.0 ;	HAE	NAE	CAB
10	39	37	2	120.0	560.0	120.0	560.0 ;	CAQ	CAB	NAE
10	39	40	2	132.0	760.0	132.0	760.0 ;	CAQ	CAB	CAA
37	39	40	2	108.0	465.0	108.0	465.0 ;	NAE	CAB	CAA
39	40	41	2	120.0	560.0	120.0	560.0 ;	CAB	CAA	CAH
39	40	42	2	108.0	465.0	108.0	465.0 ;	CAB	CAA	CAC
41	40	42	2	120.0	560.0	120.0	560.0 ;	CAH	CAA	CAC
36	42	40	2	108.0	465.0	108.0	465.0 ;	CAD	CAC	CAA
36	42	43	2	120.0	560.0	120.0	560.0 ;	CAD	CAC	CAF
40	42	43	2	120.0	560.0	120.0	560.0 ;	CAA	CAC	CAF
42	43	44	2	115.0	610.0	115.0	610.0 ;	CAC	CAF	CAG

[dihedrals]

; ai aj ak al fu c0, c1, m, ...

```
 2  1  3  4  2    0.0  167.4      0.0  167.4  ; imp  CBI  OBJ  OBK  CBH
 6  5 12  7  2    0.0  167.4      0.0  167.4  ; imp  CAX  CBG  CAY  CAV
 7  9  8  6  2    0.0  167.4      0.0  167.4  ; imp  CAV  CAR  CBE  CAX
 9 11 10  7  2    0.0  167.4      0.0  167.4  ; imp  CAR  NAW  CAQ  CAV
12 13 11  6  2    0.0  167.4      0.0  167.4  ; imp  CAY  CBD  NAW  CAX
14 13 15 17  2    0.0  167.4      0.0  167.4  ; imp  CBB  CBD  NBA  CBC
15 25 16 14  2    0.0  167.4      0.0  167.4  ; imp  NBA  CAT  HBA  CBB
17 23 18 14  2    0.0  167.4      0.0  167.4  ; imp  CBC  CAZ  CBL  CBB
20 19 21 22  2    0.0  167.4      0.0  167.4  ; imp  CBN  CBM  OBP  OBO
23 25 24 17  2    0.0  167.4      0.0  167.4  ; imp  CAZ  CAT  CBF  CBC
25 15 26 23  2    0.0  167.4      0.0  167.4  ; imp  CAT  NBA  CAS  CAZ
27 26 28 29  2    0.0  167.4      0.0  167.4  ; imp  CAM  CAS  NAN  CAL
29 32 30 27  2    0.0  167.4      0.0  167.4  ; imp  CAL  CAK  CAO  CAM
32 34 33 29  2    0.0  167.4      0.0  167.4  ; imp  CAK  CAJ  CAU  CAL
34 28 35 32  2    0.0  167.4      0.0  167.4  ; imp  CAJ  NAN  CAI  CAK
36 35 37 42  2    0.0  167.4      0.0  167.4  ; imp  CAD  CAI  NAE  CAC
37 39 38 36  2    0.0  167.4      0.0  167.4  ; imp  NAE  CAB  HAE  CAD
39 10 37 40  2    0.0  167.4      0.0  167.4  ; imp  CAB  CAQ  NAE  CAA
40 42 41 39  2    0.0  167.4      0.0  167.4  ; imp  CAA  CAC  CAH  CAB
42 43 40 36  2    0.0  167.4      0.0  167.4  ; imp  CAC  CAF  CAA  CAD
14 15 25 23  2    0.0  209.3      0.0  209.3  ; imp  CBB  NBA  CAT  CAZ
15 25 23 17  2    0.0  209.3      0.0  209.3  ; imp  NBA  CAT  CAZ  CBC
25 23 17 14  2    0.0  209.3      0.0  209.3  ; imp  CAT  CAZ  CBC  CBB
23 17 14 15  2    0.0  209.3      0.0  209.3  ; imp  CAZ  CBC  CBB  NBA
17 14 15 25  2    0.0  209.3      0.0  209.3  ; imp  CBC  CBB  NBA  CAT
 6  7  9 11  2    0.0  209.3      0.0  209.3  ; imp  CAX  CAV  CAR  NAW
 7  9 11 12  2    0.0  209.3      0.0  209.3  ; imp  CAV  CAR  NAW  CAY
 9 11 12  6  2    0.0  209.3      0.0  209.3  ; imp  CAR  NAW  CAY  CAX
11 12  6  7  2    0.0  209.3      0.0  209.3  ; imp  NAW  CAY  CAX  CAV
12  6  7  9  2    0.0  209.3      0.0  209.3  ; imp  CAY  CAX  CAV  CAR
27 28 34 32  2    0.0  209.3      0.0  209.3  ; imp  CAM  NAN  CAJ  CAK
28 34 32 29  2    0.0  209.3      0.0  209.3  ; imp  NAN  CAJ  CAK  CAL
34 32 29 27  2    0.0  209.3      0.0  209.3  ; imp  CAJ  CAK  CAL  CAM
32 29 27 28  2    0.0  209.3      0.0  209.3  ; imp  CAK  CAL  CAM  NAN
```

```
 29  27  28  34   2     0.0  209.3       0.0  209.3   ; imp   CAL  CAM  NAN  CAJ
 36  37  39  40   2     0.0  209.3       0.0  209.3   ; imp   CAD  NAE  CAB  CAA
 37  39  40  42   2     0.0  209.3       0.0  209.3   ; imp   NAE  CAB  CAA  CAC
 39  40  42  36   2     0.0  209.3       0.0  209.3   ; imp   CAB  CAA  CAC  CAD
 40  42  36  37   2     0.0  209.3       0.0  209.3   ; imp   CAA  CAC  CAD  NAE
 42  36  37  39   2     0.0  209.3       0.0  209.3   ; imp   CAC  CAD  NAE  CAB
  5   4   2   1   1     0.0    1.0 6     0.0    1.0 6 ; dih   CBG  CBH  CBI  OBJ
  6   5   4   2   1     0.0    5.9 3     0.0    5.9 3 ; dih   CAX  CBG  CBH  CBI
  4   5   6  12   1     0.0    1.0 6     0.0    1.0 6 ; dih   CBH  CBG  CAX  CAY
  7   9  10  39   1   180.0   41.8 2   180.0   41.8 2 ; dih   CAV  CAR  CAQ  CAB
 40  39  10   9   1   180.0   41.8 2   180.0   41.8 2 ; dih   CAA  CAB  CAQ  CAR
  6  12  13  14   1   180.0   41.8 2   180.0   41.8 2 ; dih   CAX  CAY  CBD  CBB
 17  14  13  12   1   180.0   41.8 2   180.0   41.8 2 ; dih   CBC  CBB  CBD  CAY
 19  18  17  14   1     0.0    1.0 6     0.0    1.0 6 ; dih   CBM  CBL  CBC  CBB
 20  19  18  17   1     0.0    5.9 3     0.0    5.9 3 ; dih   CBN  CBM  CBL  CBC
 18  19  20  22   1     0.0    1.0 6     0.0    1.0 6 ; dih   CBL  CBM  CBN  OBO
 15  25  26  27   1   180.0   41.8 2   180.0   41.8 2 ; dih   NBA  CAT  CAS  CAM
 29  27  26  25   1   180.0   41.8 2   180.0   41.8 2 ; dih   CAL  CAM  CAS  CAT
 31  30  29  27   1   180.0    5.9 2   180.0    5.9 2 ; dih   CAP  CAO  CAL  CAM
 28  34  35  36   1   180.0   41.8 2   180.0   41.8 2 ; dih   NAN  CAJ  CAI  CAD
 42  36  35  34   1   180.0   41.8 2   180.0   41.8 2 ; dih   CAC  CAD  CAI  CAJ
 44  43  42  36   1   180.0    5.9 2   180.0    5.9 2 ; dih   CAG  CAF  CAC  CAD

; Include Position restraint file
#ifdef POSRES
#include ppix_posre.itp
#endif
```

APENDICE C: Protocolo da Dinâmica Molecular

Se mostrara o protocolo da DM do complexo HSA+HEME, para os casos HSA e HSA+PPIX é similar

(1) Gerando os arquivos *.gro y *.top a partir do *.pdb ignorando os hidrogenîos, os quais seram adicionados programa pdb2gmx.
pdb2gmx_mpi -f hsa_heme.pdb -o hsa_heme.gro -p hsa_heme.top -ignh -v

(2) Gerando a estrutura dodecahedrica com uma distancia de 1,5 A.entre a parede da caixa e o soluto.
editconf_mpi -f hsa_heme.gro -o hsa_heme_box.gro -c -d 1.5 -bt dodecahedron

(3) Gerando água dentro da estrutura anterior
genbox_mpi -cp hsa_heme_box.gro -cs -p hsa_heme_box.top -o hsa_heme_box_hoh.gro

(4) Adicionando contra íons
grompp_mpi -f em.mdp -c hsa_heme_box_hoh.gro -o em.tpr -p hsa_heme_box.top
genion_331_d -s em_ion.tpr -o hsa_heme_box_hoh_ion.gro -g genion.log -p hsa_heme_box_ion.top -pot hsa_heme_box_ion.pdb -pname NA+ -np 16 -nname Cl- -nq 0
selecionar SOL

(5) Rodando a Minimização de Energia com restrição de posição de 500 ps (step Descent)
grompp_mpi -v -f empr.mdp -c hsa_heme_box_hoh_ion.gro -o empr.tpr -p hsa_heme_box_ion.top
nohup mpirun mdrun_mpi -v -s empr.tpr -deffnm empr >& empr.job &

(6) Rodando Minimização de Energia sem restrição de posição (step descent)
grompp_mpi -v -f em.mdp -c empr.gro -p hsa_heme_box_ion.top -o em.tpr
nohup mpirun -np 2 mdrun_331_mpi_d -v -s em.tpr -deffnm em >& em.job &

(7) Rodando Minimização de Energia com Gradiente conjugado
grompp_mpi -v -f cg.mdp -c em.gro -p hsa_heme_box_ion.top -o cg.tpr -n index.ndx -t em.trr
nohup mpirun mdrun_mpi -v -s cg.tpr -deffnm cg >& cg.job &

(8) Rodando Dinâmica Molecular de 20 ns
grompp_mpi -v -f dmHSA_heme20ns.mdp -c cg.gro -p hsa_heme_box_ion.top -o dmHSA_heme20ns.tpr -t cg.trr -n index.ndx
mdrun_mpi -v -s dmHSA_heme20ns.tpr -deffnm dmHSA_heme20ns &