# **Geometrías optimizadas de las biomoléculas de la pared celular bacteriana.**

***Geometría optimizada de la D-alanina.***

O N C H

1.00000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O N C H

2 1 3 7

Selective dynamics

Direct

0.4252259544093028 0.5282070269837472 0.4740880836375487 T T T

0.4509222881493528 0.4327798990925765 0.5299709373348102 T T T

0.5852959814081097 0.4388248713866255 0.4795396756226692 T T T

0.5410224528937199 0.4965979557621658 0.4769976782218959 T T T

0.5677634598548600 0.5524818875709390 0.5223464109180669 T T T

0.4688491080956497 0.4808274715682677 0.4969916462516925 T T T

0.5397701942956714 0.5152925630511266 0.4252330206807810 T T T

0.6189451088769576 0.5648408351619465 0.5070522548251450 T T T

0.5365924999999976 0.5975224999999966 0.5192949999999996 F F F

0.5689351265759653 0.5356219577363406 0.5746770470825338 T T T

0.5690885720952502 0.4027572194470806 0.4472534158972241 T T T

0.5831264219904022 0.4177843882180226 0.5260961246131975 T T T

0.3808598586823191 0.5152041757786654 0.4903181268535340 T T T

***Geometría optimizada de la D-glutamina.***

O N C H

1.00000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O N C H

3 2 5 10

Selective dynamics

Direct

0.6577167750101639 0.4165145668224722 0.4981561887946546 T T T

0.6524335752571075 0.4929084970889255 0.5819095646970953 T T T

0.4134908020173577 0.4318652571837216 0.4850378871258465 T T T

0.6165800167790639 0.5943399481805562 0.4877298467429770 T T T

0.3716529798629647 0.5232307756215522 0.5383772596534196 T T T

0.5367513544530442 0.5030589202959319 0.4611506670581506 T T T

0.6104958469699447 0.5234625439458898 0.4712206185647396 T T T

0.4924999999999997 0.5159374999999997 0.5221050000000034 F F F

0.6424582776113563 0.4778790019302094 0.5235748916234829 T T T

0.4229653553093027 0.4861172910936184 0.5127035792209097 T T T

0.5177977816417685 0.5318874565839298 0.4183723266279997 T T T

0.5336667481756771 0.4498739923776330 0.4478839357685626 T T T

0.6363224843917102 0.5142401781079984 0.4235726912284917 T T T

0.5139148390512351 0.4918135087633352 0.5668564720380610 T T T

0.4894500693172145 0.5697776170841027 0.5328991545184621 T T T

0.6645165864771239 0.6099466426076566 0.4797748213691106 T T T

0.6083221329838846 0.6006171152659340 0.5378142101607596 T T T

0.3793203252117435 0.5679333978868458 0.5606684019991690 T T T

0.3245926897903448 0.5047030891933471 0.5356445182832027 T T T

0.6757049492254587 0.3899288608777632 0.5351917827217008 T T T

***Geometría optimizada de la glicina.***

C H N O

1.00000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

C H N O

2 5 1 2

Selective dynamics

Direct

0.4896250078984599 0.4677813288670779 0.4868879823256749 T T T

0.5586121371620610 0.4972250156191423 0.4770610852256675 T T T

0.4377069960798636 0.5565080751317113 0.4868767769773472 T T T

0.3904784651116426 0.4902882016044857 0.4743490266936473 T T T

0.4887404510397831 0.4204561081324801 0.4591243256342356 T T T

0.4875057338048382 0.4543976473265521 0.5407976222417963 T T T

0.6049280913020051 0.5795708374909835 0.4753283085115088 T T T

0.4357166625736104 0.5111845072623936 0.4635914150763169 T T T

0.6096303342436762 0.4647684910234028 0.4696740627445021 T T T

0.5583375000000004 0.5654274999999984 0.4806574999999995 F F F

***Geometría optimizada de la L-alanina.***

O N C H

1.00000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O N C H

2 1 3 7

Selective dynamics

Direct

0.5803423935638885 0.5256875557617184 0.4725639024056750 T T T

0.5525417394459372 0.4317042169639054 0.5297754156575103 T T T

0.4262863335537479 0.4335863327312973 0.4736059651393247 T T T

0.4646864503953196 0.4956433973207656 0.4750461953890140 T T T

0.4379505996174617 0.5496170816240430 0.5233614007662215 T T T

0.5359699999999989 0.4791875000000019 0.4952875000000034 F F F

0.4664242843626014 0.5172069022751263 0.4243641455610174 T T T

0.4680108198845284 0.5955358831522403 0.5209510102293652 T T T

0.3862788230236877 0.5622652353036154 0.5096493114072559 T T T

0.4381666645696735 0.5308381439956624 0.5749982698925302 T T T

0.3764923014562061 0.4432357988866380 0.4786506543895087 T T T

0.4407716926387887 0.4038176277942779 0.5125467240171829 T T T

0.6241150080890401 0.5127168830610215 0.4903425183100089 T T T

***Geometría optimizada de la L-lisina.***

O N C H

1.00000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O N C H

2 2 6 14

Selective dynamics

Direct

0.3053852555204059 0.4151906410468864 0.4753704687226788 T T T

0.2788158788342524 0.4940831447842453 0.5525188482613542 T T T

0.3766417549424306 0.5823030899974094 0.4967537993636896 T T T

0.6901325034146732 0.4676780905703388 0.5215654336685025 T T T

0.5054149999999993 0.5026174999999995 0.4835750000000019 F F F

0.4400099191087140 0.4777586710761834 0.5142565474986428 T T T

0.5670853460234745 0.4738386895953652 0.5183061544066576 T T T

0.3777483186070100 0.5107528570377289 0.4827247227344506 T T T

0.6325752557520894 0.4980253312129231 0.4874727056203969 T T T

0.3154821006838479 0.4744054543965522 0.5079102226499673 T T T

0.5062622974609509 0.5575904347497674 0.4856542254423497 T T T

0.5064269626611148 0.4890175563994386 0.4300826945450753 T T T

0.4394138077807041 0.4883645474953905 0.5684089207139107 T T T

0.4361949610045239 0.4231300937202490 0.5087857465421697 T T T

0.5662564849337316 0.4187708450677604 0.5168116595789102 T T T

0.5660929821311301 0.4878709128460501 0.5717179245384901 T T T

0.3803614534099369 0.5035028993826052 0.4281886130964275 T T T

0.6331014833559873 0.5534706618246668 0.4876617252915874 T T T

0.6344800469527538 0.4825559623619880 0.4346377365412496 T T T

0.3629600491707471 0.5893245316248754 0.5455447717637524 T T T

0.3405908222181431 0.6051940682158554 0.4688104159353175 T T T

0.6927054496800231 0.4841070614864566 0.5698561743049386 T T T

0.7337914917066197 0.4815300373811089 0.4991096663332660 T T T

0.2658900566494695 0.3946604952506338 0.4958698854384038 T T T

***Geometría optimizada de la N-acetilglucosamina.***

O N C H

1.00000000000000

20.0000000000000000 0.0000000000000000 0.0000000000000000

0.0000000000000000 20.0000000000000000 0.0000000000000000

0.0000000000000000 0.0000000000000000 20.0000000000000000

O N C H

6 1 8 15

Selective dynamics

Direct

0.6011969398778112 0.4479333748190096 0.5097111456897117 T T T

0.4779656044866788 0.6129260857438243 0.5257104030165536 T T T

0.6075682310750896 0.6281658064090777 0.4796458882973242 T T T

0.5141091709485049 0.3735438252456454 0.5179721919594368 T T T

0.7368147501323044 0.4590917324875610 0.4720598862456686 T T T

0.3613471660310377 0.5688062487104436 0.4874886093426227 T T T

0.4187962370502216 0.4692847345098997 0.5002883126866192 T T T

0.5099074999999971 0.5581249999999969 0.4942224999999993 F F F

0.4867103723825805 0.4892877287495715 0.5195671610502954 T T T

0.5845827268722666 0.5672359258836190 0.5085887076454569 T T T

0.6258261654315788 0.5094817467099992 0.4807240895601197 T T T

0.5338984656131982 0.4355334296304620 0.4911450050461127 T T T

0.6994843745049110 0.5138252720022677 0.4986606821514162 T T T

0.3633477271523988 0.5065620774910047 0.4879152968994171 T T T

0.3005597299334539 0.4667338100656884 0.4735938922171181 T T T

0.5026310311549310 0.5600248171541610 0.4392677229272515 T T T

0.4915294350945207 0.4882821194408725 0.5745258190774430 T T T

0.5910195584519333 0.5682220112023539 0.5636082583743757 T T T

0.6204562370222821 0.5072913162453085 0.4256756812515627 T T T

0.5302223778902200 0.4353109878421572 0.4356611972891884 T T T

0.7044214427136086 0.5165826011383388 0.5536637029372666 T T T

0.7204637876531087 0.5596653283230200 0.4771045364736067 T T T

0.4120904526791306 0.4189487509367991 0.5021099724929925 T T T

0.4296653334583370 0.6081179406766902 0.5137927789016865 T T T

0.5731065194589124 0.6611697466803969 0.4901751872407747 T T T

0.5409526349238949 0.3385741375335797 0.4973413156490596 T T T

0.7158150689897241 0.4184801180085995 0.4888072190387222 T T T

0.2634982635900475 0.4782629616084274 0.5124153125787937 T T T

0.2797448885447348 0.4834352765207660 0.4256703154425526 T T T

0.3085211658393823 0.4124982222904626 0.4719596573563068 T T T