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## **Molecular structure of basic oligomeric building units of heparan-sulfate glycosaminoglycans**

Milan Remko<sup>\*,1</sup>, Piet Th. Van Duijnen<sup>2</sup>, Ria Broer<sup>2</sup>

<sup>1</sup>*Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Comenius University Bratislava, Odbojarov 10, SK-832 32 Bratislava, Slovakia*

<sup>2</sup>*Department of Theoretical Chemistry, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands*

*E-mail address:* [remko@fpharm.uniba.sk](mailto:remko@fpharm.uniba.sk) (M. Remko); fax: +421-2-50117100

Supporting Information

**Table A.** Cartesian coordinates (Å) of gas-phase species of dimeric and pentameric structural units of heparin, optimized at the Becke3LYP/6-311+G(d,p) and Becke3LYP/6-31G(d) (pentamer) levels of the DFT theory.

**D-E**

C	-0.09519900	0.79003600	-0.36693200
H	0.34806200	1.15734000	-1.29182800
C	-0.78065600	1.93947600	0.39854300
H	-1.46734800	2.40502100	-0.31642800
N	0.16168300	2.93028600	0.92791400
H	-0.20796200	3.40826700	1.74496700
S	0.81654600	4.07270900	-0.11769400
O	0.85479500	5.33604000	0.58425100
O	0.19324700	3.91406000	-1.42515200
O	2.35545100	3.61097900	-0.24588400
C	-1.60306000	1.38008400	1.55838500
H	-0.94115200	0.87151100	2.27172500
O	-2.24822300	2.47285400	2.19733100
H	-2.83916600	2.10588400	2.86631000
C	-2.61025200	0.36813500	1.01952500
H	-3.29694700	0.88309500	0.34045500
O	-3.31681000	-0.16249500	2.13602300
H	-4.21135300	-0.39117300	1.84587400
C	-1.84995700	-0.72901600	0.25868500
H	-1.20272000	-1.25190300	0.97011700
C	-2.71688900	-1.79931500	-0.36733900
H	-2.11550800	-2.43594300	-1.01293000
H	-3.18738000	-2.40530500	0.40752900
O	-3.74453700	-1.19469600	-1.23032300
S	-5.28463500	-1.47229800	-0.84774100
O	-5.95012500	-0.47371700	-1.91765700
O	-5.57632100	-0.90809500	0.45561500
O	-5.62982100	-2.84340000	-1.15132700
O	-1.05694100	-0.15540100	-0.78835100
O	0.89941200	0.20293000	0.46405800
C	1.88689000	-0.58172600	-0.20212800
H	1.46040000	-1.06202900	-1.08772300
C	3.12013200	0.24902100	-0.57441200
H	3.48393100	0.75918700	0.32725600
O	2.78450400	1.24619500	-1.55044300
H	3.59557900	1.44370600	-2.04243900
C	4.22204400	-0.65726700	-1.11051900
H	3.86616300	-1.19112100	-2.00113600
O	5.31870700	0.18516200	-1.43617400
H	6.01633300	-0.35822600	-1.82076200
C	4.57469300	-1.70800000	-0.06026200
H	4.94850500	-1.23395000	0.86402100
O	5.52414400	-2.55049500	-0.60356400
C	6.11204900	-3.47384800	0.31928800
O	3.39704600	-2.46071500	0.24430700
C	2.34618400	-1.66464100	0.79135300
H	2.67269300	-1.18332500	1.72170600
C	1.24197200	-2.66762000	1.12217300
O	0.43120200	-3.08896100	0.33978000
O	1.31032900	-3.05358400	2.41035700
H	5.36754800	-4.18388000	0.68497600
H	6.88754700	-4.00413000	-0.23062300

H	6.56197100	-2.93939300	1.16395600
H	-5.89237200	-0.85416900	-2.80860100
H	2.42677700	2.78396800	-0.78369100
H	0.62786600	-3.72719200	2.55788300

## E-F

C	6.20835200	-2.74471300	-0.12946800
O	5.28520600	-1.76194600	-0.59703900
C	4.08605300	-1.64725800	0.14748500
H	3.80898300	-2.61141100	0.58777700
C	4.18769600	-0.60162200	1.26374300
H	4.60197500	0.32233200	0.83541000
O	5.05619500	-1.09545900	2.27612800
H	5.04804900	-0.45388800	2.99663900
C	2.80725600	-0.29350100	1.84413800
H	2.39724000	-1.19325800	2.31635600
O	2.97939500	0.74698100	2.80611500
H	2.19220000	0.77456600	3.35949500
C	1.85986000	0.11268100	0.71912000
H	2.22398500	1.01944500	0.21305200
O	0.59448200	0.32409400	1.28681600
C	-0.44543400	0.78923600	0.42797600
H	-0.11730900	0.79166600	-0.61389300
C	-1.64133000	-0.16356000	0.56384700
H	-1.78968200	-0.41227700	1.61641400
O	-1.34631400	-1.35849400	-0.19354400
S	-1.13347700	-2.81929600	0.51515300
O	-0.60591500	-2.66486100	1.84882100
O	-0.48915400	-3.61019700	-0.50173200
O	-2.65463200	-3.30552600	0.71206800
C	-2.91818800	0.43066400	-0.05454500
H	-2.79576800	0.43083100	-1.13899700
N	-4.10926600	-0.34914100	0.29080500
H	-4.63750200	-0.01630000	1.09019100
S	-5.01890500	-1.20901900	-0.75949200
O	-6.29794600	-1.43294900	-0.12825100
O	-4.26110300	-2.33006300	-1.31628700
O	-5.17974300	-0.14674800	-2.00043000
C	-3.14997900	1.88993000	0.37763200
H	-3.91618300	2.35046100	-0.25502300
O	-3.57250200	1.86076200	1.72019000
C	-4.12470300	3.09297300	2.19576400
O	-1.99995600	2.67199400	0.18061500
C	-0.83164400	2.21358500	0.86872900
H	-1.01560200	2.19992600	1.95087100
C	0.25343800	3.24210600	0.62562300
H	-0.09443900	4.23389200	0.91597600
H	1.15824900	2.97984100	1.17578500
O	0.53386600	3.26474400	-0.80559800
S	1.90755100	3.90288500	-1.32540700
O	1.86718700	3.83142800	-2.75913000
O	1.63471700	5.43957200	-0.82720600
O	3.03182800	3.38550300	-0.56674400
O	1.76221100	-0.94612100	-0.21480200
C	3.00834800	-1.22306300	-0.86410800
H	3.35542500	-0.34158600	-1.41549600
C	2.67863500	-2.29008200	-1.90931800

O	2.65355800	-3.52705500	-1.38195600
O	2.42919900	-2.04294600	-3.05940300
H	-3.38260700	3.89488900	2.16604600
H	-4.43435300	2.91651500	3.22444900
H	-4.99465200	3.38197200	1.59551600
H	7.02874900	-2.75620000	-0.84728400
H	6.58744300	-2.49466100	0.86412000
H	5.73951200	-3.73594800	-0.10356500
H	-5.15338500	-0.63786100	-2.83669300
H	-3.15585800	-3.21761800	-0.12989400
H	2.30594800	-4.12938300	-2.05678900
H	2.48692800	5.88895900	-0.71892800

## F-G

O	-5.12132400	0.70029800	2.16361500
O	3.93855500	0.36887500	1.50006300
C	3.10932000	0.30493000	0.35968100
H	3.69100900	0.44517700	-0.55838800
C	2.38513700	-1.04430500	0.28709700
H	1.92218800	-1.26561000	1.24998500
O	3.38158700	-2.05478200	-0.00899600
S	3.64200100	-3.33005200	0.98739300
O	5.01988700	-3.68314500	0.75412200
O	2.66508700	-4.43955500	0.36097000
O	3.12500200	-3.05011200	2.30582300
C	1.35474600	-1.04680600	-0.85103100
H	1.89462700	-0.97795000	-1.79725200
N	0.54418200	-2.26629400	-0.85960400
H	-0.31732600	-2.23796900	-0.32566300
S	0.52554500	-3.36219400	-2.06713700
O	-0.64038900	-4.19294800	-1.87771900
O	1.85021100	-3.96046100	-2.24115900
O	0.31679400	-2.40166000	-3.38387100
C	0.42330200	0.17889800	-0.76562000
H	-0.14680500	0.29179000	-1.68881200
O	-0.45639800	-0.08404700	0.32713400
C	-1.60430800	0.76628000	0.43834800
H	-1.31449800	1.79709900	0.21892100
C	-2.71210000	0.33038900	-0.54079900
H	-2.63023600	-0.75535200	-0.67734600
O	-2.50180900	1.00492500	-1.76910900
H	-3.19275400	0.73876700	-2.38799600
C	-4.09337600	0.62569700	0.04514400
H	-4.23806100	1.70101000	0.17369300
O	-5.04017400	0.15080900	-0.95367400
S	-6.53011900	0.83188000	-1.02564900
O	-6.78553200	0.55746500	-2.59881600
O	-6.41150200	2.25584400	-0.86059300
O	-7.44832300	0.02076700	-0.25836600
C	-4.30448900	-0.11062100	1.37974600
H	-4.76138100	-1.09064400	1.20684600
O	-3.05875400	-0.40284600	2.00432800
C	-2.13579600	0.66941400	1.88687300
H	-2.62923600	1.61493500	2.14213600
C	-0.98224700	0.53513500	2.87196700
O	-0.95693800	-0.62735200	3.52772900
O	-0.17685400	1.42161900	3.02381200

O	1.13236500	1.37243700	-0.62074000
C	2.06654000	1.43076300	0.47197100
H	1.53495100	1.33284700	1.42452100
C	2.67381100	2.81465400	0.46997700
H	1.88724300	3.56953900	0.44371400
H	3.30802200	2.94544700	1.34615900
O	3.48764900	2.94526900	-0.73667200
S	4.33284500	4.28595400	-0.95334000
O	5.07578900	4.09206600	-2.16832400
O	3.08470900	5.31134100	-1.22792200
O	4.97336400	4.70314100	0.27987200
C	-5.68996200	0.04549900	3.30352700
H	-6.31340300	-0.79748900	2.98678400
H	-4.90927200	-0.30499700	3.98330100
H	-6.31110200	0.78633900	3.80340700
C	5.34402500	0.24860900	1.25358500
H	5.59277700	-0.71928100	0.81157600
H	5.69623800	1.05359500	0.59892800
H	5.82930500	0.33713900	2.22467900
H	-7.17908800	-0.32185700	-2.71302700
H	-0.18146200	-0.61903300	4.11186400
H	2.67521000	-4.42196200	-0.62186100
H	3.31819900	6.17933200	-0.86568400
H	0.80956000	-2.78102800	-4.12838000

## G-H

C	-3.51660200	-1.31511500	-0.64043700
H	-4.43530800	-1.70481600	-0.18830200
C	-3.29730300	0.15897300	-0.26777300
H	-3.40611700	0.26749500	0.81242800
N	-4.27209300	1.05891200	-0.91317900
H	-4.41773900	0.81291800	-1.89124400
S	-5.74590400	1.29756300	-0.16151300
O	-6.05867000	2.76060400	-0.82603600
O	-5.49266000	1.43817000	1.25515500
O	-6.78876000	0.39893100	-0.64073700
C	-1.88956400	0.63850500	-0.65987300
H	-1.79296000	0.62644200	-1.75394300
O	-1.65207500	1.94616700	-0.16450600
H	-2.41039300	2.49080800	-0.41221600
C	-0.83477600	-0.30628900	-0.08650400
H	-0.81671300	-0.21057500	1.00179800
C	-1.15981000	-1.75519300	-0.50267800
H	-1.06371600	-1.82766600	-1.59320000
C	-0.22463700	-2.79227400	0.08084400
H	-0.57122100	-3.79545900	-0.17090300
H	0.78777500	-2.64224800	-0.29893800
O	-0.23930100	-2.63379100	1.52974800
S	0.81895800	-3.53764600	2.37097100
O	0.27276500	-3.16124200	3.83962700
O	2.13418100	-2.95930600	2.26696400
O	0.56968300	-4.93529800	2.08648300
O	-2.48875400	-2.11819800	-0.10317900
O	0.43186900	0.06006500	-0.64279600
C	3.91105600	4.97541800	0.32425700
O	3.65984000	3.67927100	0.86880500
C	2.88070700	2.81255300	0.05400700

H	2.80447300	3.22861200	-0.95671300
C	3.64340800	1.48409300	-0.02664100
H	3.92916700	1.18544200	0.98577600
O	4.82051000	1.62788200	-0.83326400
H	5.49484900	2.07670900	-0.31204300
C	2.76367200	0.39823400	-0.62873000
H	2.45045700	0.66068200	-1.64185700
O	3.51427300	-0.83913300	-0.65256000
S	3.96890700	-1.48872400	-2.08583000
O	4.98788800	-2.44396500	-1.73887700
O	4.59730300	-0.20220600	-2.82857400
O	2.80326400	-1.86203700	-2.85332300
C	1.51718700	0.19338000	0.25410000
H	1.64845800	-0.69532400	0.87438700
O	1.34828000	1.24120800	1.17658400
C	1.44024800	2.54006600	0.60110500
H	0.71466100	2.62588000	-0.21261600
C	1.02547300	3.53498000	1.67607600
O	0.90916600	3.31546100	2.84570500
O	0.77518700	4.74512100	1.10954900
C	-4.09509500	-2.62290900	-2.54963400
H	-4.11959500	-2.52841600	-3.63409600
H	-3.44327400	-3.45420700	-2.26872400
O	-3.59393700	-1.38182300	-2.04272100
H	-5.10743200	-2.80920000	-2.17462200
H	2.98227900	5.53086000	0.16813600
H	4.45765600	4.90502000	-0.62389400
H	4.52697300	5.49931000	1.05497700
H	-7.01217800	2.80563900	-0.99683200
H	0.51949400	5.34548300	1.82640800
H	5.01591400	0.40028100	-2.17059500
H	-0.56644300	-3.61872000	4.00595100

### D-E-F-G-H

Becke3LYP/6-31g(d)

C	-3.88838200	5.41326200	1.09485900
H	-3.36288400	5.84031000	1.95622500
C	-2.87903200	5.03876700	-0.00611200
H	-2.09967200	4.42173100	0.44937100
N	-2.23694900	6.26951900	-0.45489200
H	-2.86206900	6.96877800	-0.84664500
S	-0.72651500	6.26772600	-1.18025500
O	-0.31310000	7.65217200	-1.29485300
O	-0.99178800	5.77292100	-2.70145500
O	0.06113500	5.26516500	-0.47416400
C	-3.57355100	4.20700800	-1.10368000
H	-4.29524600	4.83302400	-1.64731200
O	-2.57331300	3.71445000	-1.99670200
H	-2.95680000	3.00124500	-2.54698900
C	-4.31658000	3.03880600	-0.45294600
H	-3.57699800	2.37268800	0.00434800
C	-5.28435200	3.52618700	0.63140800
H	-6.05356600	4.16090700	0.16770600
C	-6.01665000	2.40072700	1.34246500
H	-6.51356300	2.77613000	2.23848100
H	-6.74364600	1.93072300	0.68060100
O	-5.11223800	1.31229100	1.71280300

S	-4.64254500	1.11987800	3.25490000
O	-3.21575000	1.82210000	3.30392900
O	-4.42776300	-0.32501900	3.35300500
O	-5.53344400	1.82550100	4.14589100
O	-4.55396900	4.27036300	1.60676000
O	-5.07344900	2.32081300	-1.44145300
C	6.42891700	-0.30085500	-0.52793900
H	6.15871300	-0.63304500	-1.52679600
C	7.53337700	-1.19794300	0.08272500
H	8.32492600	-1.28420200	-0.67305600
N	7.06734600	-2.52318500	0.52035700
H	7.71724800	-2.98058100	1.15570000
S	6.32284400	-3.61459000	-0.46697900
O	6.88230300	-4.94082500	-0.23667200
O	6.21441900	-3.05404700	-1.81047800
O	4.82029700	-3.60786000	0.19718300
C	8.12041900	-0.53638600	1.33209400
H	7.33500100	-0.48223600	2.10108500
O	9.19609900	-1.34515000	1.78393700
H	9.61826600	-0.84110200	2.50090000
C	8.58466600	0.88275300	1.02328500
H	9.37890000	0.84051200	0.26781500
O	9.06910300	1.43299900	2.24215800
H	9.76856200	2.07203100	2.01381800
C	7.39373100	1.67027600	0.45637400
H	6.60227800	1.71189600	1.21938500
C	7.70585500	3.10733500	0.08608700
H	6.87450300	3.55080800	-0.46419900
H	7.89836800	3.69229600	0.98861200
O	8.86279200	3.16928500	-0.81755700
S	10.12567600	4.02656000	-0.28782400
O	11.10508300	3.73900400	-1.53425800
O	10.72330700	3.36003100	0.86041100
O	9.78049300	5.43595500	-0.23279800
O	6.90871500	1.01680600	-0.71908100
O	5.32920100	-0.36117700	0.35249300
C	4.02785100	0.02550400	-0.08315300
H	3.95230700	1.11651800	-0.17465000
C	3.60885400	-0.61002500	-1.42301800
H	3.96786600	-1.64918200	-1.43690200
O	4.19501800	0.13631700	-2.47683200
H	3.88925500	-0.28890700	-3.29711200
C	2.08585300	-0.64732300	-1.61498400
H	1.71523000	0.38791600	-1.67812900
O	1.84373600	-1.36160900	-2.81028100
H	0.97057400	-1.08521700	-3.15689400
C	1.44609600	-1.30588800	-0.39702400
H	1.82743700	-2.32834100	-0.26644900
O	0.04367300	-1.31290600	-0.51104800
C	-0.64241500	-2.51951700	-0.11989100
H	-0.00510600	-3.06025600	0.58419600
C	-1.92376500	-2.12177900	0.65235200
H	-2.08615700	-1.05220100	0.51230600
O	-1.79286600	-2.40012800	2.06982500
S	-1.13820200	-1.30862700	3.08340700
O	-1.31860600	0.04134100	2.51698500
O	0.38808400	-1.71809300	2.95554700
O	-1.66113500	-1.62999800	4.38768000



C	-3.16825100	-2.90597200	0.20859400
H	-3.08539600	-3.94848800	0.52786600
N	-4.40568400	-2.38385800	0.76335200
H	-4.57970100	-1.38307000	0.75317400
S	-5.35771000	-3.23574000	1.81867800
O	-4.77729700	-3.04503200	3.29718000
O	-5.20686200	-4.64308200	1.51125900
O	-6.66514600	-2.55689500	1.75954300
C	-3.24709200	-2.89190500	-1.32453600
H	-4.13053600	-3.44301300	-1.66123700
O	-3.34188700	-1.52615400	-1.68717200
C	-3.77448900	-1.21907100	-3.02378800
H	-3.46302800	-2.00887900	-3.71290500
C	-5.30199000	-1.06622900	-3.03552000
H	-5.73089700	-1.95521600	-2.55444600
O	-5.69009700	-0.97651300	-4.39060700
H	-6.66263500	-0.99317300	-4.41085400
C	-5.75357600	0.18388300	-2.22519600
H	-6.42885000	0.77762100	-2.84469700
O	-6.40922600	-0.16941700	-0.98458300
S	-7.95549600	-0.73801600	-1.08523700
O	-7.74344800	-2.26347000	-0.68109300
O	-8.35033000	-0.73598700	-2.48596000
O	-8.69739800	-0.02327800	-0.06671800
C	-4.58877200	1.07907800	-1.81500500
H	-4.00401500	0.62657500	-1.01058000
O	-3.75809400	1.26513600	-2.97462500
C	-3.08032200	0.10061000	-3.44515100
H	-3.07918500	0.15979600	-4.53545300
C	-1.64086900	0.01847600	-2.94777800
O	-1.44939100	0.66371700	-1.79846200
O	-0.80463200	-0.64701000	-3.53341400
O	-2.16049500	-3.53933200	-1.92654600
C	-0.83903900	-3.42383600	-1.37406400
H	-0.19544100	-3.01062000	-2.15465500
C	-0.41524100	-4.87526300	-1.11656500
H	-0.96606600	-5.33473300	-0.29099700
H	-0.55473300	-5.46031100	-2.02792400
O	1.00159100	-4.83056300	-0.77529500
S	1.78762600	-6.22372200	-0.60816700
O	0.96953300	-7.22293800	0.05262200
O	1.90428200	-6.61563900	-2.18371400
O	3.09422300	-5.85713000	-0.09891100
O	1.74783800	-0.51079500	0.73679000
C	3.12973200	-0.50907100	1.05878800
H	3.48254400	-1.53320200	1.26795600
C	3.17609800	0.24154200	2.38648600
O	4.23964600	1.01924300	2.57253200
O	2.30142800	0.12531100	3.23250400
C	-5.57666600	7.03677000	1.49823400
H	-6.21798400	7.71929000	0.93751700
H	-6.19435900	6.34176100	2.07780400
O	-4.78033700	6.34358600	0.53631200
H	-4.94152800	7.61260600	2.18462200
H	10.87735000	4.35683300	-2.25621600
H	4.39688400	-4.47813400	0.01816200
H	4.15288700	1.41695300	3.46185500
H	1.87187700	-7.59005100	-2.25291800

H	1.01184800	-0.92112500	2.96923300
H	-0.65551100	0.28469400	-1.35843400
H	-2.50582700	1.15731100	3.07253700
H	-1.47307500	4.90354100	-2.63822400
H	-7.44074600	-2.35275500	0.27372700
H	-4.77342200	-2.08445800	3.53624100

END