

ELECTRONIC SUPPLEMENTARY INFORMATION TO ACCOMPANY:

**COMPOSITION AND CHARGE STATE INFLUENCE ON THE
ION-NEUTRAL COLLISION CROSS SECTIONS OF PROTONATED N-LINKED GLYCOPEPTIDES:
AN EXPERIMENTAL AND THEORETICAL DECONSTRUCTION OF
COULOMBIC REPULSION VS. CHARGE SOLVATION EFFECTS**

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Table S1. Atomic charges, 12-6 Lennard-Jones potential, and dipole polarizability used in the computational studies of ions in He drift gas. The covalent terms are all from MMFF94.

Atomic Site	Description	charge (e)	$R_{min}/2$ (Å)	ϵ (kcal/mol)	α (Å ³)
He	He atoms in drift gas	0	1.5000	0.0400	0.2051
H	H atoms in analyte ion	MMFF94	0.6000	0.0160	0
C	C atoms in analyte ion	MMFF94	1.9080	0.0860	0
N	N atoms in analyte ion	MMFF94	1.8240	0.1700	0
O	O atoms in analyte ion	MMFF94	1.7000	0.2000	0

Table S2. Atomic charges, 12-6 Lennard-Jones potential, and dipole polarizability used in the computational studies of ions in N₂ drift gas. The covalent terms are all from MMFF94.

Atomic Site	Description	charge (e)	$R_{min}/2$ (Å)	ϵ (kcal/mol)	α (Å ³)
N ₂ (single site)	N ₂ molecules in drift gas	0	2.0000	0.2500	1.7400
H	H atoms in analyte ion	MMFF94	0.6000	0.0160	0
C	C atoms in analyte ion	MMFF94	1.9000	0.0800	0
N	N atoms in analyte ion	MMFF94	1.8200	0.1500	0
O	O atoms in analyte ion	MMFF94	1.7000	0.1800	0

Table S3. Average CCS values (Ω) and their standard deviations (s) for each glycopeptide ion studied here. All determinations were made on the basis of four replicate measurements.

Peptide	Glycan	m/z	z	$\Omega_{He} (\text{\AA}^2)$	$S_{He} (\text{\AA}^2)$	$\Omega_{N_2} (\text{\AA}^2)$	$S_{N_2} (\text{\AA}^2)$
NLTK	Man1	522.25	2	252	1	354	1
	Man2	603.27	2	268	3	372	4
	Man3	684.30	2	270	6	374	7
	Man4	765.32	2	286	2	392	2
	Man5	846.35	2	318	2	413	1
	Man6	927.38	2	339	2	436	1
	Man7	1008.4	2	352	2	451	3
	Man8	1089.43	2	371	2	474	1
NLTKDR	Man1	657.81	2	265	2	370	4
		438.87	3	308	4	441	5
	Man2	738.84	2	286	2	394	4
		492.89	3	330	2	467	3
	Man3	819.86	2	303	3	412	5
		546.91	3	358	3	500	3
	Man4	900.89	2	320	2	431	4
		600.93	3	368	2	513	3
	Man5	981.92	2	353	2	452	2
		654.94	3	361	4	510	6
	Man6	1062.94	2	368	1	469	2
		708.96	3	371	3	520	5
	Man7	1143.97	2	383	2	489	2
		762.98	3	377	1	528	1
	Man8	1224.99	2	396	1	505	2
		817.00	3	382	4	537	6
SRNLTK	Man1	643.81	2	267	2	369	2
		429.87	3	310	6	442	8
	Man2	724.84	2	285	3	390	4
		483.56	3	329	5	465	6
	Man3	805.86	2	302	4	410	5
		537.58	3	352	4	493	6
	Man4	886.89	2	326	6	436	6
		591.59	3	354	4	496	5
	Man5	967.92	2	351	2	449	2
		645.61	3	339	4	487	4
	Man6	1048.94	2	363	2	464	2
		699.63	3	348	3	497	3
	Man7	1129.97	2	378	1	481	2
		753.65	3	362	3	513	4
	Man8	1211.00	2	391	2	499	2
		807.66	3	378	1	530	3
SRNLTKDR	Man1	779.38	2	296	3	402	3
		519.92	3	327	1	463	1
	Man2	860.40	2	316	3	424	3
		573.94	3	341	3	481	4
	Man3	941.43	2	331	2	441	3
		627.95	3	351	3	493	4
	Man4	1022.46	2	347	1	458	2
		681.97	3	365	1	509	2
	Man5	1103.48	2	375	2	479	2
		735.98	3	373	1	524	1
	Man6	1184.51	2	388	1	495	2
		790.01	3	386	2	538	5
	Man7	1265.54	2	400	1	510	2
		844.02	3	392	1	544	4
	Man8	1346.56	2	413	1	528	1
		898.04	3	407	2	560	6

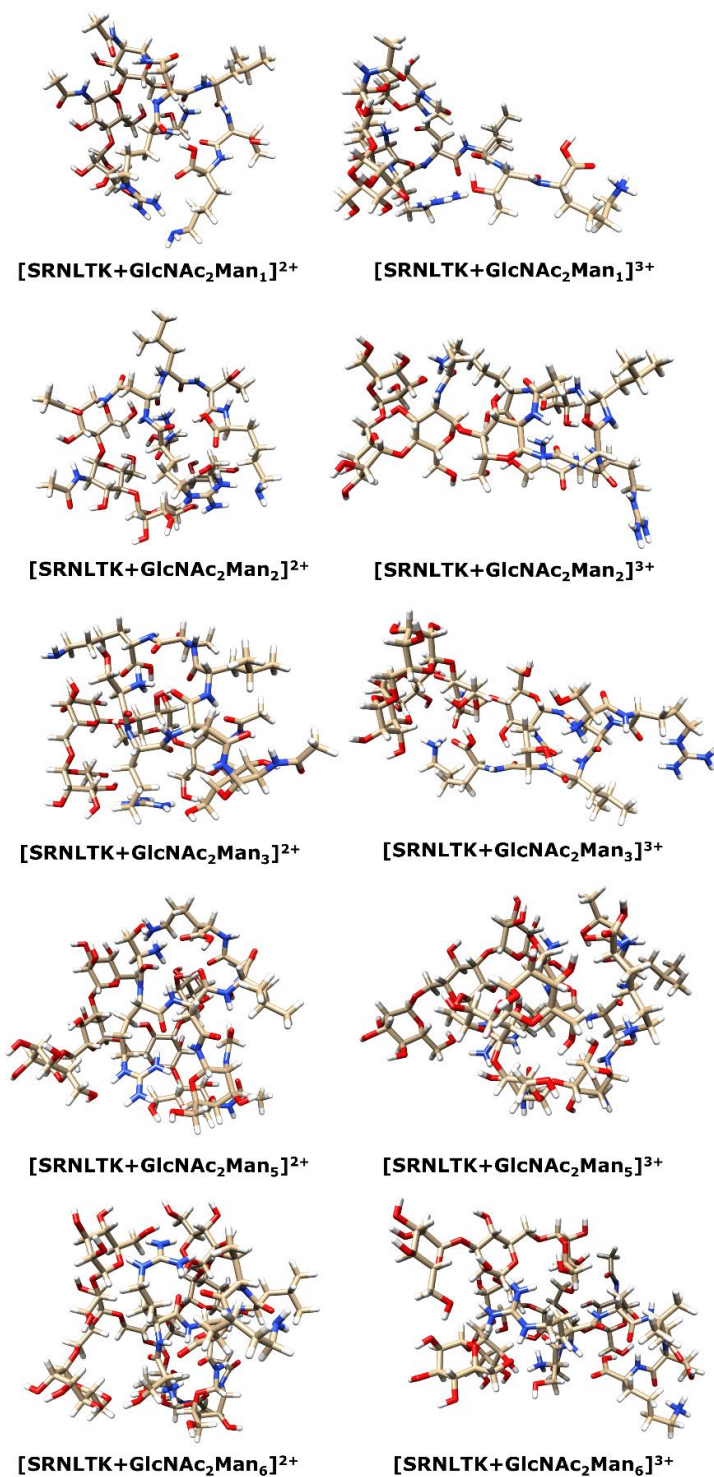


Figure S1. Energy-minimized gas-phase structures of the SRNLTK + GlcNAc₂Man_{1-3,5,6} (top to bottom) with $z = 2+$ (left column) and $z = 3+$ (right column).

Table S4. Experimental (expt) and calculated (calc) He and N₂ CCSs of for the Man1-Man3, Man5, and Man6 glycoforms of SRNLTK with charge states of $z = 2+$ and $z = 3+$. In each case, the percent difference (%D) between the experimental and theoretical values is given.

Peptide	Glycan	z	Ω_{He} (expt, Å ²)	Ω_{He} (calc, Å ²)	%D	Ω_{N_2} (expt, Å ²)	Ω_{N_2} (calc, Å ²)	%D
SRNLTK	Man1	2	266	276	3.7	369	365	1.1
		3	310	285	8.4	442	413	6.8
	Man2	2	285	291	2.1	391	390	0.3
		3	329	315	4.3	465	447	3.9
	Man3	2	302	302	0.0	410	405	1.2
		3	352	343	2.6	493	472	4.4
	Man5	2	351	344	2.0	449	453	0.9
		3	339	351	3.5	487	479	1.7
	Man6	2	363	377	3.8	464	476	2.6
		3	348	376	7.7	497	499	0.4

Table S5. Cartesian coordinates of global optimized gas-phase structures of the SRNLTK + GlcNAc₂Man_n. These coordinates can be visualized by using the MacMolPlt software.

S5.1. Doubly charged SRNLTK + GlcNAc₂Man₁

C	4.0469483181361	-6.5451486427716	-8.4879512520360
O	2.8856750914021	-5.9195352651342	-7.9398729263146
C	4.1117515103754	-8.0434852504400	-8.1336386147441
C	4.0183596789587	-6.3391214690457	-10.0095726463471
O	5.1321253457679	-6.9867680916364	-10.6289796917178
H	5.0870199055247	-6.7434052006827	-11.5755252529107
H	3.0943993291802	-6.7428092026534	-10.4383270593761
H	4.0523260798356	-5.2697673620001	-10.2453806939504
H	4.9504984573212	-6.0488129198174	-8.1087286183623
C	4.0377554035429	-8.2029429679897	-6.6120239031510
C	2.8092241935643	-7.4940473804331	-6.0416429107678
C	2.7748645461883	-6.0242865846929	-6.5140558235099
O	5.3251978815639	-8.6710573705611	-8.6037892143562
O	3.9795993220582	-9.6133475995024	-6.2839664074014
O	1.6566348088171	-8.2435621128877	-6.4692940337681
H	5.4835171805372	-8.2639053761342	-9.4922181228782
H	3.2804011392466	-8.5851880131192	-8.6009490356942
H	3.0236185654058	-9.8326019541990	-6.4016131202490
H	0.8733127460454	-7.7858999605126	-6.1034204776043
H	4.9553847708953	-7.8166884367502	-6.1541530876364
H	2.8426379235788	-7.5636830654738	-4.9494478089811
O	3.8379258898291	-5.2937360516942	-5.9011445806502
C	3.3989976055959	-4.2034153468469	-5.0696201015988
C	2.9134047183935	-4.7121000726764	-3.6905163320400
C	4.5769062994468	-3.2355879714941	-4.8928476615945
C	2.6804494526788	-3.5359284042771	-2.7081946940664
C	3.9202300911123	-2.6028508162261	-2.6957896913055
O	4.2497820966397	-2.1470485686561	-4.0084879092173
C	5.0095279452559	-2.6334452380707	-6.2370998887167
O	6.1021329868529	-1.7252723828654	-6.0306890584481
O	1.7204948376246	-5.4843301676984	-3.9210539803039
N	2.3671911838089	-3.9773348565038	-1.3336357602160
H	2.9260126995640	-3.5622889681284	-0.5843182600764
C	1.1784448332644	-4.5545101661113	-0.9755697804691
C	0.9880059089616	-4.7539572668199	0.5022069016576
O	0.3387859869757	-4.8857901270991	-1.8064919996269
H	5.7377193214364	-1.0485809691317	-5.4220730176745
H	4.1957454591684	-2.0639022430166	-6.6980377054474
H	5.3430015653777	-3.4041824249213	-6.9378350459599
H	2.5772378083490	-3.6730162748524	-5.5707430684239
H	1.8091347862804	-2.9701435686230	-3.0641035145585
H	1.1012013693251	-5.3400034979202	-3.1675851685411
H	3.6479290043346	-5.4125707718968	-3.2746526459331
H	1.9467574652351	-4.7717394215752	1.0279249698850
H	0.3734076316036	-3.9416736679620	0.8981494223109
H	0.4888403313199	-5.7116985728850	0.6736607526440
O	5.0506944955835	-3.2835515981226	-2.1342754250128
C	5.7805308298412	-2.5207730792888	-1.1618205423386
H	5.4435945700096	-3.7637264526074	-4.4831172879416
C	5.4135389395160	-3.0484456209312	0.2404230317190
C	7.2817414914818	-2.7202194420630	-1.4011547453482
C	6.3449065880138	-2.4626760807275	1.3223666615894
C	7.8348176912474	-2.6944152157278	0.9372750468994
O	8.0773382757593	-2.1369958123359	-0.3563708656113
H	5.5398052347125	-1.4516215358185	-1.2282118112145
H	7.5171406729670	-3.7885753111915	-1.4756331789348
O	4.0399461763118	-2.7135550785920	0.5303601596168
N	5.9650968711256	-2.8840699623512	2.6840593548037
H	3.9316833805574	-2.8461376892291	1.4946168979637

H	5.4523307049503	-4.1436659157352	0.2334236238313
H	6.1733489950995	-1.3769748025662	1.3275623078705
C	6.0154281107546	-4.1840819342647	3.1252248655906
C	5.6453009756628	-4.3808441594199	4.5695843191982
O	6.3610621250081	-5.1083413374858	2.3938689460893
H	5.8652408949764	-2.1539206703624	3.3846228689649
H	6.5540927981173	-4.5539766396489	5.1515478271702
H	4.9811731004986	-5.2453789002385	4.6538271951646
H	5.1234106542897	-3.5080621690505	4.9716188424587
H	8.4695928519604	-2.1554200660328	1.6505211043559
N	8.2714798277057	-4.0739981019983	0.9160785693560
H	7.6530962825337	-4.7440852005560	1.3825024211622
C	9.6073080328004	-4.3899353682463	0.8986844695572
C	9.9076236979255	-5.8705966680328	0.9615240127053
O	10.5082351302664	-3.5673343194325	0.7690694989872
C	10.1991896322533	-6.4473592230404	-0.4205405951020
H	9.0827647501094	-6.4092300981245	1.4416942981982
H	10.7821174873534	-5.9882047608160	1.6130536478511
C	11.0988592148095	-5.5314428802524	-1.2895996809474
N	8.9741306601933	-6.6142025204680	-1.2182425297031
H	10.6953014564877	-7.4190507812718	-0.3196276445080
C	8.9290072081477	-7.6074149685985	-2.1843571969231
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C	6.6700990855081	-9.2854598970797	-3.5747367031593
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C	8.5370354980872	-5.3324255126937	-5.0453950673340
C	9.6402777785062	-4.4344462081096	-5.6551536848739
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H	11.3741919078260	-3.4835530583801	-4.7843061569045
H	10.4545735266938	-4.2927944733392	-3.6991893449621
O	7.3365149874827	-5.1859766277518	-5.2498893420991
H	10.0056982657774	-6.5688821738171	-4.2616943985558
H	7.2315998163642	-6.6335527292094	-3.1349449226647
H	8.5943198006092	-8.9982152048352	-4.5240886595919
H	7.3002140605616	-8.0679638711372	-5.2370619994140
H	5.6965120023034	-8.7821548227832	-3.6191618863816
C	6.5631033225349	-10.6651125339621	-4.2140874007750
N	6.3012598676673	-10.5660745766109	-5.6476034666046
C	7.0893611021592	-10.9737997875742	-6.6415273265987
H	5.3665436511404	-10.2468940696479	-5.9363210740251
H	6.9128100432829	-9.4164937513748	-2.5146999766422
H	7.4621449932127	-11.2561266686889	-4.0210947463170
H	5.7259071303658	-11.2123691089163	-3.7673855110220
N	6.6892494031970	-10.8207138619324	-7.8997446203507
N	8.2852850211637	-11.5134474756507	-6.4386520314410
H	7.2576117161886	-11.1572074750034	-8.6631037107734
H	8.7761894410348	-11.4785938750116	-5.5491004313953
H	8.7871230611033	-11.9216825880066	-7.2354449690129
N	12.4187180990995	-5.3989016078149	-0.9138211361486
C	13.2027915666632	-4.3322556423166	-1.5619992746562
C	13.3334835685092	-4.6511067481091	-3.0751316451448
C	14.5803675748946	-4.2065461361372	-0.8950476785911
C	15.4848184870846	-3.1023300486109	-1.4786812532310
C	14.8646781169867	-1.7104978330058	-1.3495856688931
C	16.8466787508129	-3.1279678281258	-0.7793124603956
N	13.8958301307348	-5.8728053397918	-3.3622199772027
C	14.0851685072391	-6.3456122744272	-4.7340857755652
C	15.4868527656364	-6.9803917923891	-4.8805203665261
C	15.8905644847011	-7.2237028195808	-6.3299128480875
O	15.5558124645975	-8.2137809634734	-4.1492614348628
H	14.0401957342091	-5.4807493130760	-5.4080885137369
C	12.8678650180756	-7.2376186668327	-5.1115923796057
N	13.1409438127162	-8.5688710314813	-5.3121392092700

C	12.1221202769423	-9.5409818040541	-5.7178542964453
C	12.8211566484273	-10.7214353583540	-6.4074844808858
C	11.2480258618149	-10.0143123657151	-4.5428660536493
C	11.9176401250603	-11.6522105366538	-7.2267598888707
C	11.1793426909312	-10.9398937719392	-8.3652889580782
C	10.4437164316864	-11.8929154963040	-9.3105913500315
N	9.4163667709129	-12.6795303340669	-8.6069483659569
O	10.2699821471610	-10.7477295256929	-4.6422261649745
O	11.6189727295882	-9.4903068304110	-3.3559619544760
H	10.8471931271264	-9.5860049638540	-2.7392082419782
H	11.4563522239806	-9.0111178037679	-6.4067959122074
H	11.2058576760818	-12.1529211941292	-6.5631963425904
H	12.5478120524101	-12.4431859113535	-7.6528726568229
H	10.4571631611146	-10.2248454923594	-7.9550241337228
H	11.8985813595740	-10.3585399501466	-8.9551441251981
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H	9.9539933153993	-11.3060170740056	-10.0952892309856
H	8.9109790169879	-13.2099432497275	-9.3315631765888
H	9.9159499060165	-13.4386668092012	-8.1181913499330
H	13.9489499046811	-8.9236526721464	-4.7927532088383
O	11.7161134367023	-6.7918547518259	-5.1721085859416
H	14.6082265220693	-1.4850258415034	-0.3089778620805
H	13.9562637083760	-1.6208808165306	-1.9527182171719
H	15.5613044896582	-0.9410827825734	-1.6998558710566
H	15.8598618114902	-6.2965025484314	-6.9100400512689
H	16.9089229204004	-7.6252393889694	-6.3747695061593
H	15.2482277597460	-7.9630348586160	-6.8169733193050
H	16.2231307274822	-6.3037785987080	-4.4280628510723
H	16.4987791337233	-8.4728051185214	-4.1200826236661
H	13.9609577780371	-6.5610967252285	-2.6183392139635
O	12.9712433602196	-3.8630071677926	-3.9519863246733
O	10.6549961072077	-4.9643143238062	-2.2950131148699
H	12.5979760462805	-5.5217978554866	0.0775536187834
H	12.6304967810864	-3.4037118755337	-1.4552103541233
H	14.4360245071103	-4.0213492730799	0.1782736153498
H	15.1078162388964	-5.1677269019307	-0.9617494598914
H	15.6583883665684	-3.3033055304114	-2.5428148049270
H	17.5184121089863	-2.3763276948437	-1.2074441922343
H	17.3253615869803	-4.1061108702483	-0.8954839179550
H	16.7477774760168	-2.9230625711925	0.2921667889922
H	3.6638733625313	-1.7177593853458	-2.1012557640536
H	1.7945905433295	-5.5929150606714	-6.2890453737397
C	7.7541158970596	-2.0717643591205	-2.7040924359380
O	9.1710282403027	-2.2839669764605	-2.8346856242395
H	7.5853108426826	-0.9903272671616	-2.7013525255040
H	7.2631100614644	-2.5115114164861	-3.5730205807942
H	9.5321192445244	-2.0055927694285	-1.9610888064874
C	9.0589813047286	-3.3722929173456	-6.5981575006872
O	8.7091746245863	-2.2034038688439	-5.8530789971634
H	10.3337899000358	-5.0764885759082	-6.2039142802127
H	7.7826518281842	-1.9629121627061	-6.1037263954546
H	9.8188256116460	-3.0669802250975	-7.3250571049122
H	8.1878871701566	-3.7342167415720	-7.1541562350949
H	13.3437254606882	-11.3245352252116	-5.6530747645631
H	13.6010352985419	-10.3358247794495	-7.0782918937889
H	5.9121160382227	-10.1870698130801	-8.1186938896480
H	9.8855582175933	-2.8816971382177	-4.2825946526609

S5.2. Triply charged SRNLTK + GlcNAc₂Man₁

C	3.8114644930095	-9.2344392904312	-1.9369404569524
O	3.6051746665926	-8.7279706492353	-0.6164149877094
C	5.1010880748285	-10.0633915934767	-2.0745471444622
C	2.5820526009368	-10.0718761302193	-2.3230046964745
O	2.7262244500886	-10.6012390350395	-3.6428240642110
H	1.9180356305542	-11.1276760992807	-3.8099286557030
H	2.4453029397471	-10.9026769722351	-1.6218359999720
H	1.6775894622876	-9.4549701738083	-2.2859929443164
H	3.8658811603033	-8.3998966579881	-2.6438788840791
C	6.2979143899930	-9.2892054374095	-1.5152567361421
C	6.0114615078571	-8.7493571684379	-0.1159517116368
C	4.6962601357182	-7.9466713798694	-0.1174454185917
O	5.3637985345655	-10.3873496222010	-3.4607365355489
O	7.4365276328645	-10.1813678789770	-1.4632744675581
O	5.9671994696311	-9.8846742879852	0.7697495805265
H	4.5073992595878	-10.7685613257616	-3.7777819163431
H	5.0042600760934	-11.0172588294972	-1.5412656639665
H	7.3058703227527	-10.6786406424187	-0.6218909407074
H	5.7113318512167	-9.5600316930990	1.6545033989426
H	6.5706610031674	-8.4757021238998	-2.1947303957438
H	6.8494684971322	-8.1225039018150	0.2094480305464
O	4.8467756915011	-6.7660783159395	-0.9063937130502
C	4.1044442167376	-5.6511517293104	-0.3947135081356
C	5.0048734629716	-4.8005014417852	0.5221916424841
C	3.6317671910840	-4.7760120317268	-1.5620478969473
C	4.2842017022502	-3.5010255753603	0.9379714732939
C	3.7271623901176	-2.7494278914818	-0.3076446051757
O	2.9007372087724	-3.6286656853313	-1.0792488780320
C	2.7102996717504	-5.5514324781956	-2.5092984576567
O	2.1604733107754	-4.6560953249337	-3.4903461378701
O	5.3459502153758	-5.5600537443936	1.6957287430062
N	5.0890127083676	-2.6657108606842	1.8510009971660
H	4.6317132422334	-2.3349660448664	2.6951653736036
C	6.3328435495563	-2.1604587336320	1.5490431724712
C	6.9122794510630	-1.2613465620571	2.6090120078798
O	6.9484409890882	-2.4320434504860	0.5219845222131
H	1.6254328637491	-4.0396374835010	-2.9418582971641
H	1.8702719998140	-6.0063720876286	-1.9742964122925
H	3.2556122875416	-6.3299996144270	-3.0447412113713
H	3.2293013941595	-6.0019507691615	0.1701007344347
H	3.4211052962700	-3.8030918098441	1.5478714003141
H	5.8856105518445	-4.9667285215597	2.2531866442966
H	5.9481699811635	-4.6005424468626	0.0040877368567
H	6.1568761628842	-0.9515825096221	3.3361692399003
H	7.7110724134509	-1.7942888769476	3.1312719965033
H	7.3164798285812	-0.3638349585460	2.1326198367076
O	4.7874474719128	-2.2246198537299	-1.0989551033655
C	4.4572903492150	-1.1135478602326	-1.9531797466297
H	4.4852241205639	-4.4328751947834	-2.1607179916107
C	5.7851144840014	-0.3733263322267	-2.2201794128234
C	3.8231769597277	-1.6042101363274	-3.2711062048322
C	6.7428888482141	-1.2171524078974	-3.0920243376498
C	5.9631973856739	-1.6812395013216	-4.3628213493541
O	4.7615814815867	-2.3866191114154	-4.0390904600500
H	3.7676720962353	-0.4384360660081	-1.4317195899793
H	3.0273898878725	-2.3065465504471	-3.0299180086698
O	5.5099296584034	0.8786447249651	-2.8535464124039
N	7.3635586949780	-2.3062550060876	-2.3043299753386
H	6.2485361926415	1.4859822684734	-2.6487060853272
H	6.2669883734303	-0.1524644680151	-1.2589856079268
H	7.5771699181577	-0.5894154687413	-3.4322308152356
C	8.4143687553420	-3.0925632924138	-2.7076515765023
C	8.8771597244822	-4.0702737897388	-1.6625843694724
O	8.9197693984703	-3.0418735777248	-3.8303148182168

H	7.0326108377840	-2.4298618138351	-1.3387994812607
H	8.0701643798558	-4.7686997114034	-1.4257561097019
H	9.1869589917141	-3.5352236000295	-0.7611776615290
H	9.7324601189177	-4.6348549172198	-2.0439091921393
H	5.7171024483626	-0.8174559434937	-4.9893345406345
N	6.7521461058546	-2.5532527964389	-5.1906771105606
H	7.7389726126501	-2.6209402560876	-4.9420736538832
C	6.3213711705442	-3.1265830734117	-6.3471221896480
C	7.3544961382384	-4.0002039173017	-7.0121598940844
O	5.1728246491360	-3.0085944776559	-6.7674419069625
C	7.5472675142597	-5.2753397741444	-6.1822684997065
H	8.2769495731999	-3.4145685971446	-7.1014066630384
H	7.0293438125122	-4.2220302367604	-8.0353549998692
C	8.9582763712901	-5.8499431885911	-6.4132957074819
N	6.4934541203674	-6.2394342838396	-6.4874151285848
H	7.4885393609978	-5.0580078851397	-5.1090135977330
C	5.8421663693021	-6.9584252389590	-5.5123287827969
H	6.0356381392071	-6.1657505862154	-7.3991523309105
C	4.5166302712983	-7.6193974034939	-5.9607191462007
O	6.2317992456237	-7.0039973783876	-4.3472455791311
C	4.6247075443739	-8.5555658692249	-7.1708086309504
C	5.3226969370252	-9.8973165602459	-6.9038588991990
N	3.5297811994120	-6.5363795809432	-6.1478728345880
C	3.5541368193124	-5.6345246399661	-7.1950562952569
C	2.5532484268400	-4.4618996208525	-7.0930143467455
N	2.8070379744851	-3.6784702890511	-5.8500074885777
H	2.5878695400188	-4.2082042906535	-4.9828287928623
H	2.3318842259016	-2.7639270792235	-5.7724227375075
O	4.3848537155139	-5.7068811038876	-8.0994251953931
H	2.7053233884880	-6.5376674435045	-5.5449230359044
H	4.1459598570113	-8.1973052157364	-5.1059676874315
H	5.1235969323437	-8.0708765157690	-8.0167867649664
H	3.6069152648127	-8.7828768437662	-7.5159155730607
H	5.1549714980570	-10.5149528160712	-7.7961479048076
C	6.8355439390710	-9.8019322833339	-6.6961273166152
N	7.2144026514306	-9.8131847913673	-5.2816617500244
C	8.4729851087136	-9.6304757545394	-4.8566811769200
H	6.5393252721061	-10.0675214215403	-4.5481219936104
H	4.8371525626285	-10.4206747158960	-6.0747298217074
H	7.3033934487795	-10.6836014857072	-7.1484467646655
H	7.2309308940523	-8.9085044235132	-7.1852204392267
N	8.8258420028236	-9.9418932954174	-3.6164998461194
N	9.4299047887432	-9.1548702202678	-5.6469965965221
H	9.7905256374523	-9.8115013743754	-3.3217353204844
H	10.3563313412925	-9.0446837024556	-5.2500000284921
H	9.2100648970375	-8.5933086187802	-6.4699771389269
N	9.9733490865400	-5.0318840900201	-5.9520242842531
C	11.3779967887052	-5.4029326160427	-6.0961674356476
C	11.7958493582552	-6.3042449864472	-4.9136662488697
C	12.2755683692284	-4.1571731613341	-6.1392881730926
C	11.9486941403686	-3.1640021146748	-7.2734759624554
C	12.8653625519183	-1.9421099496635	-7.1701696507571
C	12.0834414740344	-3.7959725704049	-8.6592378921579
N	12.9891954709153	-6.9702846095221	-5.0673726978031
C	13.5466307147443	-7.8388218700306	-4.0239991484438
C	12.8011495796993	-9.1970719748601	-3.9144962918875
C	12.9425326859668	-10.0704240894852	-5.1581156875848
O	11.3855860299037	-9.0267943126185	-3.6782590240117
H	13.4399736838345	-7.2939233781744	-3.0773522731774
C	15.0516886254043	-8.0445168520375	-4.2916077052818
N	15.7580562640056	-8.6416417353463	-3.2685084122789
C	17.2062910471168	-8.8599120275263	-3.3569521620796
C	17.6371691407534	-9.6901057455379	-4.5811914835947
C	18.0101995832525	-7.5440828867729	-3.2938693043240
C	18.9824214836393	-10.3998234496964	-4.3491198996182
C	19.8318280100605	-10.5644570023556	-5.6149484689608

C	20.3264905648407	-9.2745909711238	-6.2713500021676
N	21.0371437949132	-8.4105956172596	-5.3048430364590
O	19.1647380668838	-7.4011904094338	-3.6904726213921
O	17.3592795289403	-6.5462558278282	-2.6629402424411
H	17.9634149507669	-5.7732455921669	-2.6400295731514
H	17.4543693660287	-9.4134760979425	-2.4425196593005
H	18.7729041102147	-11.3975788690086	-3.9418195652780
H	19.5781180959680	-9.8968820745936	-3.5800923750800
H	20.7045838744631	-11.1779944696797	-5.3564369164592
H	19.2633364113281	-11.1383444273839	-6.3569277475838
H	19.5123627869097	-8.6788403842023	-6.6921278880225
H	21.0390011485131	-9.5043208278103	-7.0696631376312
H	21.7593492906993	-8.9128414235988	-4.7748009078156
H	20.3839790165532	-7.9804643853895	-4.6157456598085
H	15.3919002291242	-8.5219356998807	-2.3294908301820
O	15.5743882892297	-7.7118904389213	-5.3549471474002
H	12.6205087169777	-1.2054138990519	-7.9427150618215
H	13.9173906435817	-2.2224059730126	-7.2905740271363
H	12.7532912607703	-1.4528391481538	-6.1968163466344
H	12.3634853914843	-10.9931961444589	-5.0406835092883
H	12.5457641924871	-9.5655136080170	-6.0452839732897
H	13.9845208896053	-10.3428683650104	-5.3482840582471
H	13.1914720783003	-9.7532969237228	-3.0547707744735
H	11.2590008544079	-8.0970449984806	-3.3612686858987
H	13.5625274965387	-6.8279939379220	-5.8970356850889
O	11.1213459612771	-6.4481752293010	-3.8918829069766
O	9.1704769664308	-6.9254909503812	-6.9754354720559
H	9.7492132050591	-4.3995320020066	-5.1802993984475
H	11.4938433783750	-5.9970117925038	-7.0098320184655
H	12.1957210502857	-3.6303370854081	-5.1780626451870
H	13.3256437185032	-4.4660446807951	-6.2249749769368
H	10.9166907571237	-2.8112511709296	-7.1562585269853
H	13.0796472276920	-4.2274716927480	-8.8035836353094
H	11.9219201818830	-3.0490364296078	-9.4440648782255
H	11.3427682097066	-4.5870755866739	-8.8101530382171
H	3.0972894402609	-1.9262661381708	0.0497145700975
H	4.4454741703886	-7.7096299872657	0.9217120213652
C	3.1427198802724	-0.5122757287203	-4.1198988760999
O	2.3610545043352	-1.1322133659677	-5.1681423151230
H	3.8514217531442	0.1569409514420	-4.6100551868936
H	2.4569351276788	0.0779792393698	-3.5039441382499
H	1.9407488697981	-0.3760618310759	-5.6318840090352
C	1.1079914740193	-4.9691617655197	-7.1087039702187
O	0.8124962977728	-5.6883335833298	-5.9076523736522
H	2.7287865626147	-3.7838032798977	-7.9346570627018
H	-0.1331280470923	-5.9381367359365	-5.9505238041686
H	0.4115584616673	-4.1269178489366	-7.1772288552724
H	0.9391384729075	-5.6388060494550	-7.9581994251197
H	17.6919491860257	-9.0443166062465	-5.4628621513585
H	16.8802601218145	-10.4530090194589	-4.8037149201243
H	8.1558219966031	-10.2292672593240	-2.8980519743693
H	3.8119047194917	-3.4134141407125	-5.8034696439768
H	21.4963735392018	-7.6219464731383	-5.7771415929271

S5.3. Doubly charged SRNLTK + GlcNAc₂Man₂

C	5.7924480616865	-9.5561202697357	-5.1865644728322
O	5.1026110918443	-10.4168929186531	-4.2732474038513
C	7.3124000488574	-9.7935754747156	-5.1154180402078
C	5.2321083404976	-9.8085015504085	-6.5973093624609
H	5.5474559772669	-10.7996452388147	-6.9436312476198
H	4.1348461406784	-9.8301281775326	-6.5911874828122
H	5.5880140278143	-8.5105289992781	-4.9272331252387
C	7.7795244419860	-9.5462059444397	-3.6742213100981
C	6.9789252804752	-10.3881990512911	-2.6777035847789
C	5.4646091604312	-10.1892370721558	-2.9022786870547
O	8.0546264600398	-8.9286187416723	-5.9940343035583
O	9.1870189693167	-9.8659967074385	-3.5667832254140
O	7.3868814665892	-11.7560707020221	-2.8654186648919
H	7.5925461482418	-8.9744518384501	-6.8583981979939
H	7.5566019549393	-10.8222828841776	-5.4068835965761
H	6.8860537460877	-12.2931734772511	-2.2199270210629
H	7.6859528651781	-8.4810181737773	-3.4368290572449
H	7.2691944506991	-10.1063070524735	-1.6597622672810
O	5.0929410802266	-8.8590899206152	-2.5509379561154
C	4.0214639823714	-8.7785119451086	-1.5984149241730
C	4.6039506270534	-8.8067503948198	-0.1705754485274
C	3.2505146163975	-7.4801046709599	-1.8600266334850
C	3.5364934371115	-8.4196876242256	0.8815769092734
C	2.8226027556552	-7.1111459959868	0.4481292726241
O	2.2507214405256	-7.2347600741769	-0.8548608075024
C	2.5424191033802	-7.5330274452316	-3.2215984108467
O	1.8351740147085	-6.3081676346630	-3.4534938815331
O	5.1350576038993	-10.1312256642928	0.0239311086718
N	4.0911016252018	-8.2627555015970	2.2408465366477
H	3.8811760981887	-7.3853859173710	2.7205522068533
C	4.5215441668832	-9.3111909978090	3.0096575937114
C	4.8788573104684	-8.9541866745600	4.4258128513116
O	4.6110676564275	-10.4527420269848	2.5692229445328
H	1.2027358168375	-6.2455001125913	-2.7079195896735
H	1.8075714244772	-8.3442137127901	-3.2557962272118
H	3.2533401544862	-7.6673349275315	-4.0415412128277
H	3.3343402578199	-9.6263904927096	-1.7281495409661
H	2.8008613580961	-9.2333423578976	0.9314071729620
H	5.0216494610120	-10.3755537825082	0.9711540438004
H	5.4625071735945	-8.1270943413601	-0.1042260578022
H	5.0777692451600	-7.8838839420305	4.5297015044511
H	4.0533057878462	-9.2331018466737	5.0854045043802
H	5.7825993558059	-9.4975381738314	4.7153345111122
O	3.7463334444809	-6.0145406600231	0.4567286932916
C	3.2416614804462	-4.8165056450293	1.0643225142471
H	3.9363064493523	-6.6272290631762	-1.8846763258349
C	3.8732998625209	-4.6909996174465	2.4660370702441
C	3.6567534178461	-3.6124977750716	0.2092498292566
C	3.5963773706212	-3.3052178892930	3.0848564322888
C	4.0217220002141	-2.1775764256455	2.1016295712913
O	3.3507949108029	-2.3654734529559	0.8537385653585
H	2.1475651028906	-4.8420414253892	1.1524200445233
H	4.7314693079048	-3.6510308787517	-0.0047909053035
O	3.3503483970410	-5.7320164336302	3.3169501200439
N	4.1200904730385	-3.1809567834908	4.4577699295490
H	3.5970030604018	-5.4801011694618	4.2300601308794
H	4.9493161762953	-4.8855443175848	2.3929060536699
H	2.5070982282294	-3.2332164300486	3.2134491569183
C	5.4549678719572	-3.2365202073170	4.7781237388117
C	5.7693527802768	-3.0222707573237	6.2334055948820
O	6.3244220830861	-3.4284959766793	3.9321942452728
H	3.4795896471680	-2.8353536959306	5.1675740031194
H	6.2309946627898	-2.0394402783043	6.3583398268153
H	6.4599668126726	-3.8012727235849	6.5677034976947

H	4.8690003328925	-3.0740178827022	6.8517196013580
H	3.6924161470589	-1.2140458461956	2.5082744069781
N	5.4403892134716	-2.0781065246358	1.8340767532971
H	6.0555050399004	-2.5883968142713	2.4728641652515
C	5.9692556917131	-0.9629130165462	1.2326690446329
C	7.4738377368860	-0.9785245184366	1.0862036883597
O	5.2986278650304	-0.0421208012602	0.7770193768528
C	7.9048582677264	-1.3938339925801	-0.3168923859039
H	7.9257556185124	-1.6325335219386	1.8406455955853
H	7.8219986542091	0.0388651243288	1.3028485887692
C	7.0519018392757	-0.7521814273564	-1.4388648962685
N	7.7562237566684	-2.8409603880487	-0.5384097266952
H	8.9509251228104	-1.1113564575132	-0.4796377968712
C	8.6190797727551	-3.4774955204654	-1.4173420750962
H	6.7881429754366	-3.1288737157218	-0.6454311116555
C	7.9467359148765	-4.6179119893272	-2.2173827280872
O	9.7654920940983	-3.0845514956113	-1.6279176338952
C	8.9693635560413	-5.5345739032137	-2.8806333252067
C	9.7525914449778	-6.3789372771982	-1.8722017470091
N	7.1196337643157	-3.9516693844526	-3.2337186683426
C	5.9986873597726	-4.5452596906688	-3.7851299542507
C	5.2202796657905	-3.6327469861550	-4.7640188708688
N	4.8140005646488	-2.3700890079832	-4.0828020646735
H	5.4713773793608	-2.0742078801173	-3.3389301423621
H	3.9215541533917	-2.5270126661577	-3.5661607869764
O	5.6602916400468	-5.6866828618936	-3.4873943092955
H	7.5331464198720	-3.1584364383608	-3.7350205621859
H	7.2943170137409	-5.1963730653660	-1.5523092289120
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H	8.4561104128302	-6.2071760161325	-3.5772968710991
H	9.1002672216030	-7.1785815734281	-1.5005091152855
C	11.0030830215883	-6.9880352127738	-2.4965649704945
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C	11.1156920232983	-7.4322964677180	-4.9580767739831
H	10.1462495593978	-8.5831183029584	-3.6423105056271
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H	11.7572164541449	-6.2189730966296	-2.6820204448762
H	11.4498712806756	-7.7059580097093	-1.8003776237491
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N	11.9188979525440	-6.4084516511397	-5.2260032922563
H	11.0463100275572	-8.0033297266676	-6.9074995273342
H	12.0476241675045	-5.6245435773625	-4.5927155304569
H	12.3258065773931	-6.3215562314909	-6.1616790912744
N	7.1936231782168	0.6029330601270	-1.6464772316717
C	6.2004213646883	1.2593607041936	-2.5096187208045
C	6.3453486196230	0.7155852952312	-3.9565687476607
C	6.3672549927648	2.7863852393545	-2.5111335203071
C	5.9719664237018	3.4792943213632	-1.1900671550118
C	6.3252309050016	4.9677350845112	-1.2641663910232
C	4.4841809182112	3.3223914594164	-0.8708055375738
N	7.5982229726636	0.8567627464542	-4.5063122411638
C	7.9201430117356	0.3859295421686	-5.8537366972901
C	8.7293911348177	1.4647007625759	-6.6083891094401
C	8.8884085399057	1.1703241154957	-8.0952103238364
O	10.0233577890642	1.6296553199131	-6.0093393065257
H	6.9826598630161	0.2329939931735	-6.4034543112336
C	8.5690294049700	-1.0212236809997	-5.7329565927377
N	9.9119990880241	-1.0806334933291	-6.0151602591307
C	10.6904339635179	-2.3241203822048	-6.0025091900833
C	11.9211013021034	-2.1291273265401	-6.9026508113111
C	11.1046978271691	-2.7468111077175	-4.5832926243353
C	12.6628618146147	-3.4052018284293	-7.3209558418371
C	11.7863748835779	-4.3779077716325	-8.1139978462904
C	12.5524587277317	-5.5591417287585	-8.7108761685184
N	13.1697918769845	-6.3903076017224	-7.6663826340949
O	11.6836257363133	-3.7880716657587	-4.2935999286952

O	10.7326681013537	-1.8633579788611	-3.6318987530250
H	10.7980441674452	-2.3360021158576	-2.7627418723042
H	10.0253107326741	-3.1043596228831	-6.3842904930794
H	13.0803431126730	-3.8979088197308	-6.4374440514232
H	13.5182940243746	-3.1105508783392	-7.9418611678812
H	10.9953599984653	-4.7680372625675	-7.4668043469112
H	11.2921632570745	-3.8389431569249	-8.9314756144295
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H	11.8542600915396	-6.1816913534618	-9.2810549932089
H	14.0208778178228	-5.8979958142047	-7.3594503169982
H	13.5643462760994	-7.2146095968300	-8.1390835923426
H	10.4248571607242	-0.2061577005246	-5.8798560833006
O	7.9328969728348	-2.0052378428272	-5.3403062680242
H	7.3959486110265	5.1049620937668	-1.4488333685180
H	6.0833769697265	5.4727739761867	-0.3229019322122
H	5.7747962037551	5.4677975269006	-2.0684159301766
H	7.9154954940453	1.0484126781535	-8.5807367032018
H	9.4189482352703	1.9929904509419	-8.5871999932440
H	9.4848817906628	0.2710773240021	-8.2743871999370
H	8.2090201063098	2.4250379410624	-6.5013435295128
H	10.4192172930173	2.4309180506201	-6.4064216294886
H	8.3754752823981	1.0785785855353	-3.8916952725256
O	5.4035152011415	0.2086269492133	-4.5702883449201
O	6.2942905532923	-1.4355654182620	-2.1369305326586
H	7.4953121711645	1.1354428526400	-0.8379569774357
H	5.2030829319333	0.9683308229783	-2.1619088575868
H	7.4129922053977	3.0344243257077	-2.7382658641404
H	5.7698063717551	3.2124347272889	-3.3285437872498
H	6.5472114052642	3.0451038362169	-0.3640061124132
H	4.2183647993895	3.8904924299768	0.0273669576676
H	4.2226942518155	2.2780735322493	-0.6787053014483
H	3.8607890188934	3.6846092557732	-1.6952273119597
H	1.9983962227246	-6.9325965012137	1.1491563601083
H	4.9172158578153	-10.9432805669492	-2.3267643225860
C	2.9378866245464	-3.5773429481613	-1.1414445453432
O	3.3898297054603	-2.4270543512599	-1.8758410169844
H	1.8543472672937	-3.4821873617868	-1.0191755887150
H	3.1562874133386	-4.4632030213717	-1.7379050071749
H	3.3004625398479	-1.6834650173237	-1.2371948824577
C	3.9538119913993	-4.3111981747826	-5.3033405513937
O	2.8551566978249	-4.0349956089119	-4.4279725606740
H	5.8890393349538	-3.3751306276199	-5.5886923688341
H	2.3670556009812	-4.8834420602307	-4.2971442729470
H	3.6937191642453	-3.8930973292632	-6.2810118009552
H	4.0698083277661	-5.3925877848984	-5.4144819683316
H	12.6365946580790	-1.4657673349434	-6.3984626327421
H	11.6171703629027	-1.6032380288884	-7.8181320036686
O	5.6968196065865	-8.8516565204679	-7.5605974899357
C	5.0729086468386	-7.5720678341404	-7.4096331611148
O	6.0624092960869	-6.6049339277323	-7.0234903726100
C	4.3300848436206	-7.1558818183256	-8.6949194118847
C	5.3219283023281	-6.8482007031938	-9.8160167262160
C	6.3539516395703	-5.8204640567428	-9.3403467497042
C	7.0221312498582	-6.3255234100844	-8.0601826110956
O	3.5417010513580	-5.9789393582725	-8.4353418947626
O	4.6250788641537	-6.2916270226010	-10.9434603933229
O	7.3274512588772	-5.6147503283247	-10.3658955527066
C	7.9951428676776	-5.2881544544246	-7.4913764091031
H	4.3403170092868	-7.5836635107511	-6.5937374415641
H	7.5949311666952	-7.2389518039873	-8.2632943237331
H	6.8169882489245	-5.4376953666035	-11.1832598994029
H	5.8641409876552	-4.8547956497759	-9.1634433323035
H	3.2475823158738	-5.6564564264974	-9.3128635783483
H	3.6387044487731	-7.9431534615673	-9.0151512347425
H	5.8305925709794	-7.7566646508244	-10.1607287277346
O	8.6318713345624	-5.8030640146568	-6.3155920012748

H	7.4663472396655	-4.3771095294475	-7.1955364632322
H	8.7724576955788	-5.0254603646141	-8.2128267268562
H	4.1951017990350	-7.0279839320280	-11.4196268590130
H	9.1921588848607	-10.8421401677344	-3.4225562574041
H	7.9873360074796	-6.4193101832627	-5.9103371799809
H	9.9341823836761	-8.8330098863421	-5.8482010406427
H	4.6925863811448	-1.5401897509261	-4.6803291067107

S5.4. Triply charged SRNLTK + GlcNAc₂Man₂

C	3.2990991399472	-0.2904194182159	-10.1154964186515
O	4.1288667370901	0.4389382129560	-9.1948400231669
C	2.0564548927136	0.5223387455866	-10.4883180567264
C	4.1604633212139	-0.6455670233733	-11.3344573345760
H	3.5536904017462	-1.1008363766229	-12.1239900115904
H	4.6660725094358	0.2468901394294	-11.7198260538681
H	2.9985910882253	-1.2357506944186	-9.6439289460806
C	1.2684380111055	0.8122107948871	-9.2044713367423
C	2.1516482378158	1.5164356514670	-8.1731261713406
C	3.4797647130385	0.7594290625769	-7.9612715490332
O	1.2260312659354	-0.2156909183260	-11.3885118438130
O	0.1464726232825	1.6575710860595	-9.5036375942095
O	2.4185605840071	2.8502662610692	-8.6371945979455
H	0.6639053116602	0.4356198747557	-11.8507957158061
H	2.3412966491283	1.4587007609287	-10.9840065883286
H	1.5476483835930	3.2070131502046	-8.9126623596017
H	0.8695637672559	-0.1193766932767	-8.7839063172607
H	1.6095592776376	1.6135077818119	-7.2255747483269
O	3.2870630528564	-0.4112319423113	-7.1689171337905
C	4.4278595795602	-1.2833629829330	-6.9911062546398
C	5.7574991952019	-0.5658129836541	-6.6356129364251
C	4.0388443390909	-2.2670957344352	-5.8690592435544
C	6.8267100086807	-1.5228387877820	-6.076939790142
C	6.2552271398911	-2.5092458670486	-5.0424301733833
O	5.1061246009793	-3.1756819404747	-5.5620031302642
C	2.8047056801567	-3.1084430083285	-6.2326359351054
O	2.3822839827679	-3.8744067619119	-5.0894018889199
O	6.368557877779	0.0386059756007	-7.7954469762757
N	7.9680383443316	-0.7727666596559	-5.5262174920706
H	7.7480312056612	0.0171365405116	-4.9299953662820
C	9.2173754792669	-1.3224930126695	-5.4370334188772
C	10.2139038318862	-0.5152616040253	-4.6512173363588
O	9.5132833966478	-2.3890990944283	-5.9756816759629
H	1.5763367930090	-4.3454424488791	-5.3800270368881
H	3.0405722356874	-3.8174348784067	-7.0329228819373
H	1.9627398864137	-2.4802653379977	-6.5377409851779
H	4.5745483798169	-1.8434274260713	-7.9230780948306
H	7.2055959038713	-2.1154806295169	-6.9216937450183
H	5.6919468776607	0.2119883936007	-8.4818230633503
H	5.5575564554520	0.2449188314312	-5.9249890442228
H	9.7792829949384	0.4159296817432	-4.2779865671589
H	10.5571462372916	-1.1072209723927	-3.7984629570142
H	11.0611379682512	-0.2690767513413	-5.2968458926103
O	5.9408314285830	-1.8258085440447	-3.8244599635810
C	5.8951679950428	-2.7093116186812	-2.6883495219422
H	3.7803012513961	-1.7009378820050	-4.9671114702186
C	7.2572243485631	-2.7646403108469	-1.9674308306508
C	4.8121557107374	-2.1786415504204	-1.7195179137319
C	7.1946113907058	-3.6454567782582	-0.6891698901352
C	5.7346621593812	-3.7167690865807	-0.1608528280292
O	5.0781241415111	-2.4802637509891	-0.3386036304917
H	5.6531337784254	-3.7241821426937	-3.0279428020587
H	4.7948262152613	-1.0822368985503	-1.7607497742716
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N	8.1521024978131	-3.1743367441616	0.3359514668784
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H	7.5750331814512	-1.7414669786540	-1.7299715487649
H	7.5180889042483	-4.6648152617198	-0.9254698816718
C	9.5120297163788	-3.2015042578433	0.1285036093117
C	10.3398940620805	-2.8502403439823	1.3350641451827
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H	7.8679171828836	-3.3012190480832	1.3043394837155
H	10.8438154197491	-3.7496142947357	1.6978031467856
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C	6.6675390765761	-6.3154608695268	3.9069076710943
H	4.6633306594576	-5.5603967674631	3.5012277040932
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C	4.5325735011329	-8.3159338786790	-0.4946674789570
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H	6.0542817403296	-7.6916397142814	-1.7863034240493
H	6.6154662474949	-8.8162323930603	-0.7095908534829
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H	5.7010103608587	-10.0707101144367	1.1056187515628
H	3.9129732663562	-9.9176199065141	3.2330692044415
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H	6.2925136180021	-10.4303550951007	5.6225148009915
C	4.4330425332085	-11.5428437097415	5.6140736939605
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C	2.5804300870617	-10.2929900060736	6.7337250000322
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H	6.4437293730979	-12.1148107579576	5.1564006994332
H	3.8209123243908	-12.0789052832721	4.8821874414512
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O	7.1276507929503	-6.0960607954682	-4.9204173096533
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H	10.6960583182674	-4.8636434621085	-5.1651468345687
H	9.1486904792362	-5.0550309309073	-5.9945935711869
H	11.7675156779281	-6.3033830772290	-6.9743428141410
H	10.2270446941444	-6.3155644893146	-7.8237099566077
H	11.7560263973905	-4.6251537881916	-8.7908410284890
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H	9.6362357883653	-3.2227088516126	-7.2922477177283
H	9.3542513026871	-4.0956390114701	-8.7108544644047
H	10.2373321991099	-8.5177351982570	-3.2123515159113
O	8.6068942466446	-6.9287318545693	-0.9850444222528
H	13.3679546401871	-7.4722426078895	6.3346599510456
H	13.8064158337766	-8.1823161393585	4.7709752601454
H	12.5808347187629	-8.9590366619307	5.7898535865058
H	10.0465967775986	-11.0869829377678	-2.3710851592505
H	8.5268039036702	-11.8386392241164	-1.8459233974940
H	8.4739757208463	-10.3057386087944	-2.6872914164703
H	9.5717235242735	-10.8708664897468	0.1099319078637
H	7.9152632553699	-9.6224667489726	0.7463162882307
H	11.2261870212064	-7.7060458855508	0.6085735895867
O	8.4628050363243	-8.6483819589020	1.7897754189049
O	8.4635359950413	-4.9297072820605	2.9903134296068
H	8.5533960577003	-7.8807997425077	4.0844855025252
H	10.4533640612251	-6.2905051011932	2.4250548490503
H	10.9551822437371	-8.9283865971745	3.9341699008196
H	12.1007266647593	-8.1461632049107	2.8628725103061
H	11.0825021080079	-7.0025866083673	5.5207625974970
H	11.6423426572494	-5.1376746158973	4.0116855666889
H	13.1850687795076	-5.8995316874230	3.5814457148715
H	12.9070140004756	-5.3033698125570	5.2266167872112
H	7.0104109528167	-3.2788894183200	-4.8629295424952
H	4.1475620089910	1.4360019607596	-7.4162364501898
C	3.3908932880051	-2.6476745090509	-2.0938946233651
O	3.3556567321362	-4.0201309771009	-2.5136416602170
H	2.9938830826080	-2.0311102229424	-2.9056488748418
H	2.7158051824058	-2.5532529676764	-1.2374258558427
H	2.9864295803636	-3.9883052521922	-3.4327397989423
C	3.6879203786378	-7.1279758108296	-0.9931267608088
O	4.2436517088032	-6.5948276391108	-2.2012896748792
H	4.2845143265712	-9.2226989002008	-1.0551237101091
H	3.7720491844986	-5.7421899086385	-2.3630822500256
H	2.6578171578233	-7.4436585106862	-1.1878374681911
H	3.6604106401183	-6.3188877959774	-0.2559695381861
H	9.3837070532791	-7.5716672589391	-5.7625727464908
H	10.9028334422182	-7.3050193061859	-4.9196105856930
O	5.1505686434955	-1.5977460714944	-10.9035592055332
C	6.0112855970861	-1.9988054673279	-11.9662079365448
O	6.9452977942389	-0.9764099092695	-12.3115549957591
C	6.7298213282270	-3.2982011781037	-11.5472215598107
C	7.7272665342757	-3.0089408754231	-10.4218522802602
C	8.6891062388802	-1.8788018660623	-10.8249557912033
C	7.8681337955544	-0.6485185820975	-11.2667708875533
O	7.4795333826551	-3.9032971137230	-12.6166591342865
O	8.4862924719407	-4.2119058895060	-10.1300934523083
O	9.5712375782258	-1.5974599389454	-9.7137453102061
C	8.7788457743316	0.4784888012262	-11.7757925195668
H	5.4197871936786	-2.2090139677930	-12.8653423783860
H	7.3208932248829	-0.2559320158733	-10.4004282835755
H	9.8694705102772	-0.6641821644320	-9.8648748174091
H	9.3305622446954	-2.2222144173748	-11.6456530616354
H	6.9149650280530	-3.9160703045952	-13.4135243131197
H	6.0062002127319	-4.0472144207673	-11.2058553816774
H	7.2074020019655	-2.7416577557181	-9.4945989332083
O	9.7769850219944	0.7968147073359	-10.8056138041783

H	8.1842915571953	1.3745860236303	-11.9854943454111
H	9.2756256115308	0.1862590386692	-12.7074190792578
H	8.6050581929424	-4.6212477835845	-11.0209479319134
H	-0.5182229412562	1.1017303471609	-9.9516960801361
H	10.2068661372581	1.6170378647102	-11.1210190844385
H	1.2031530000912	-9.0306917803420	7.5965228175028
H	6.3339951258662	-7.2497071501983	-0.2226096884576
H	10.2674532132536	-2.7680560159170	-8.7210715060652

S5.5. Doubly charged SRNLTK + GlcNAc₂Man₃

C	4.1093003030360	-4.4229396546423	0.1020249287696
O	3.6249829436593	-5.7039030143474	-0.3462899993933
C	3.8752235702929	-3.3085213806440	-0.9432971232179
C	3.4461879675656	-4.0984467310027	1.4542469217062
H	3.3025538381533	-5.0112665290108	2.0423134547537
H	4.1073875382986	-3.4363610330348	2.0231077825844
H	5.1834843234235	-4.5230374975922	0.3066957537752
C	4.3849487635025	-3.7453573361027	-2.3214833760313
C	3.8089229245656	-5.1179407859423	-2.6863233505197
C	4.2134857077429	-6.1281223651860	-1.5895416178248
O	4.5274099892001	-2.0812609950417	-0.5550627329346
O	4.0259339945972	-2.7531705953746	-3.3053326958789
O	2.3705747374031	-5.0240798039937	-2.8161516099084
H	3.9654677316749	-1.7300786698148	0.1791266253649
H	2.8095411370364	-3.0806399897065	-1.0449752466308
H	2.0422498927896	-5.9452539659440	-2.8492396014391
H	5.4789860456259	-3.7754827678531	-2.3206851114685
H	4.1857678997271	-5.3929255603487	-3.67111058504695
O	5.6228248026253	-6.2058842006034	-1.4106950037482
C	6.2975373993440	-7.3171868660520	-2.0225914774212
C	6.3898834389412	-7.1525219132735	-3.5502183034979
C	7.7002425682877	-7.3555177977552	-1.3841011233691
C	7.4488831847344	-8.0800351887520	-4.1659277217237
C	8.7949940841914	-7.9392110008475	-3.4187461411916
O	8.5998255007192	-8.2717921344461	-2.0343055025179
C	7.6060180668836	-7.7681895987682	0.0930556696478
O	8.9080823098852	-7.7070212610493	0.7020305421626
O	5.1094758062687	-7.4790031980169	-4.1256362575431
N	7.5571784945711	-7.9839527278730	-5.6360508328475
H	7.9640831826921	-8.8033170494961	-6.0780840211056
C	7.6831123683704	-6.8156473077341	-6.3556737267020
C	8.0539030373762	-7.0338333501820	-7.8008096008493
O	7.4667794830017	-5.6883518751843	-5.9161146618038
H	9.4206170661171	-8.3954072316791	0.2226203246097
H	7.2435679517338	-8.7961603627697	0.1986776934763
H	6.9470738586856	-7.1016059315622	0.6565851060879
H	5.7586908675903	-8.2432695571408	-1.7823487077412
H	7.0974441165568	-9.1095474918853	-4.0065394843683
H	5.2437582752022	-7.4487923502249	-5.0942485752255
H	6.5809871222927	-6.0990952029675	-3.7750434096148
H	7.1485151328375	-6.9933967977928	-8.4113436911259
H	8.7481853751939	-6.2488253921853	-8.1135199740673
H	8.5457725617374	-7.9983712744333	-7.9527418552294
O	9.3048536660666	-6.6161971868255	-3.5021689015841
C	10.7186547693139	-6.5247924649688	-3.7568680234223
H	8.1514411729858	-6.3543625021302	-1.4004366154360
C	10.9054455964727	-6.3339079116153	-5.2713782320807
C	11.2422060464612	-5.3563725510396	-2.9014722069621
C	12.2488786770332	-5.6689762509998	-5.6119817122427
C	12.4123185869797	-4.3877790479369	-4.7525237742373
O	12.4689791909580	-4.7684368600454	-3.3721971866537
H	11.2255890314940	-7.4482354646087	-3.4444319066370
H	10.4875178880969	-4.5631431935515	-2.8326349833872
O	10.7344908560406	-7.6297995015805	-5.8813910642396
N	12.4237223945532	-5.4193868389139	-7.0455886180296
H	11.5119955712368	-7.8065730017807	-6.4600677324134
H	10.0953884903808	-5.7157039273025	-5.6684078908698
H	13.0433157655215	-6.3742507125865	-5.3300602736387
C	12.6871508501763	-6.4191528495984	-7.9445629734674
C	12.7571343091308	-5.9793096728053	-9.3798387090784
O	12.8070533292919	-7.5902742443687	-7.5945288029220
H	11.9876734272168	-4.5699163200946	-7.4146753065044
H	12.9177083079707	-4.9002321537717	-9.4570848550460
H	11.8206797240110	-6.2389462336249	-9.8801891848159

H	13.5926464181379	-6.4861913024200	-9.8701756556595
H	13.3664289900100	-3.9085638197668	-4.9989761745844
N	11.4029944084822	-3.3464207522263	-4.8143847026525
H	11.4049613525580	-2.7412201913925	-4.0033470878786
C	10.7415309922121	-2.8887434504317	-5.9217420959918
C	9.7685426506832	-1.7707838115275	-5.6302351770536
O	10.8862450901990	-3.3438415341770	-7.0496941762782
C	8.6222107407648	-2.2583120072586	-4.7326033219341
H	9.4068632161586	-1.3905606865325	-6.5934326659843
H	10.3333071000525	-0.9520045534340	-5.1664700073352
C	7.2846555833374	-2.0026279983686	-5.4567425104007
N	8.6170643323167	-1.5066584303237	-3.4743996182427
H	8.6860667476583	-3.3299297083843	-4.5115640830144
C	8.2517508490719	-2.0895681230419	-2.2763258781932
H	8.4243318536838	-0.5049362130381	-3.5534409480967
C	8.0153266285420	-1.0616064478268	-1.1445919296812
O	8.0701308699512	-3.2962323364349	-2.1446837117027
C	8.2342479574253	-1.6638452522058	0.2507259326435
C	9.6906179570599	-2.1199029316019	0.4301127344268
N	6.6479272266255	-0.5660439898159	-1.3167152542293
C	6.3819214652443	0.4389168140576	-2.2257413993118
C	4.9048556451062	0.6409240214502	-2.5957589207626
N	4.5363180166489	-0.2923552887610	-3.6908513332247
H	5.2820472206553	-0.4199103006421	-4.3991212237254
H	3.7010529387139	0.0151022837236	-4.2260340924804
O	7.2923511761652	1.0412177078745	-2.7960614977252
H	5.8864297466923	-1.2071361653492	-1.0622922702619
H	8.7144104852706	-0.2267733059992	-1.2801558932663
H	7.5562809663317	-2.5102185838721	0.4177121031204
H	7.9880090939112	-0.9083933995118	1.0073867068079
H	10.3681965428289	-1.3415043155695	0.0581234736420
C	10.0756824105441	-2.4195928653655	1.8746538454769
N	9.2216083277535	-3.4058406048864	2.5304476676951
C	9.1140636638987	-4.7030679614635	2.2389248542960
H	8.7525363884132	-3.1183734668047	3.3970511744571
H	9.8618075189829	-3.0036778251904	-0.1892831181161
H	11.1136264235717	-2.7641217589763	1.9389580778325
H	10.0158734060934	-1.4996731834103	2.4675179870936
N	9.8562840596815	-5.2926149502017	1.3099403390282
N	8.2302654627542	-5.4550755060299	2.8933150992941
H	9.6844167008753	-6.2728209349765	1.0848017085969
H	8.1644831993715	-6.4469049894461	2.7079393160873
H	7.5754202510525	-5.0506218801861	3.5701599266817
N	6.9985705517432	-2.9050015739362	-6.4538196036926
C	5.9622440779812	-2.6337728703546	-7.4415779838513
C	4.5403265283807	-2.8576101449394	-6.8735377529300
C	6.1536536077461	-3.4961180075941	-8.7005582252528
C	7.5303340318527	-3.3601813862561	-9.3835952163426
C	7.5904601463306	-4.2739779597107	-10.6108872915195
C	7.8400009737160	-1.9217958412136	-9.7991934961569
N	3.5463382446182	-2.2841412332824	-7.6464073587914
C	2.1293414402194	-2.2889467847711	-7.2647680150410
C	1.5345441121437	-3.6989057588754	-7.0193020665654
C	1.8505901269027	-4.6761673217198	-8.1490000514759
O	0.1023144816746	-3.5917906643336	-6.9321557992578
H	1.5963352750631	-1.8218182455777	-8.1038353953796
C	1.9160996268251	-1.3333817875078	-6.0569120886573
N	0.6208829119380	-1.2737372965676	-5.5855598026082
C	0.3578168003220	-0.8002497163761	-4.2196708184459
C	-1.0997023540794	-0.3411471361787	-4.1196264499609
C	0.6833444690054	-1.9309016069658	-3.2241722551859
C	-1.5547562060872	0.2102090488643	-2.7639570996277
C	-0.6657906157228	1.3185943661741	-2.1966354892750
C	-1.2949784649312	1.9263382215861	-0.9409525998498
N	-0.3347821055654	2.7932190366120	-0.2502084559297
O	0.7566186358985	-1.8150869075450	-2.0113983213271

O	0.9070732976073	-3.1225845370393	-3.8199062511702
H	1.3021539295470	-3.7269093480536	-3.1408066370829
H	1.0476155171374	0.0250183845276	-4.0137124504026
H	-1.6195406297472	-0.6094845474024	-2.0384595263742
H	-2.5768056121892	0.5923095269868	-2.8820835347263
H	0.3205117786443	0.9079348154488	-1.9539253217571
H	-0.5126877448848	2.1017517556681	-2.9493557087456
H	-1.6100920103476	1.1381726203140	-0.2500158926916
H	-2.1830027440933	2.5081300110816	-1.2118029984711
H	-0.8408351660897	3.2942366799102	0.4872642217520
H	-0.0472863644785	3.5320265717003	-0.8987274201976
H	0.0304901900446	-2.0505484435335	-5.8957476920053
O	2.8183610180256	-0.6479597562947	-5.5668616118969
H	7.3922460846655	-5.3144448427127	-10.3350962687792
H	8.5815025981878	-4.2362270266422	-11.0754691198585
H	6.8519172595829	-3.9776896203580	-11.3637006012574
H	1.3488368415210	-5.6348586718974	-7.9765163139943
H	1.4792161310031	-4.2965677005215	-9.1071436915784
H	2.9231620913023	-4.8688104149821	-8.2381610882378
H	1.8851868904927	-4.1128565225758	-6.0689882267225
H	-0.2513476843055	-4.4943232078398	-6.8151560826877
H	3.8195041181702	-1.5691245087667	-8.3107432827394
O	4.3109798800649	-3.4926041683953	-5.8447181341793
H	6.5765313192241	-1.0188200266896	-5.2224823661142
O	7.2546223264350	-3.8852840217510	-6.2926328817665
H	6.0300326232710	-1.5694664402209	-7.6994122612944
H	5.9975690180541	-4.5502697645492	-8.4330266949060
H	5.3686877574816	-3.2548283987456	-9.4294720181306
H	8.3100546598619	-3.6908897891275	-8.6866375961079
H	7.9429381883194	-1.2680169441152	-8.9280227069011
H	7.0507725424104	-1.5157239738784	-10.4408267245275
H	8.7842425290221	-1.8723499706880	-10.3522701070694
H	9.4989488303846	-8.6713384518051	-3.8301480297908
H	3.7823544782156	-7.1135694495106	-1.7965840517230
C	11.5035518645804	-5.8482470687367	-1.4695309760171
O	11.7663347310872	-4.7425840337470	-0.5920709482671
H	12.3760847470673	-6.5091700371472	-1.4299608377828
H	10.6409443916638	-6.3871829004528	-1.0743241903325
H	12.5558328209580	-4.3088668439789	-0.9798346808586
C	4.649537770447	2.0643546537049	-3.1047838614041
O	3.3250635662399	2.1398335230256	-3.6432504521563
H	4.2422173522221	0.4093501580453	-1.7564905125715
H	3.1814025336704	3.0631820912614	-3.9275256739188
H	4.7417462855729	2.7871340981846	-2.2876242659096
H	5.3503745228174	2.3449950261734	-3.8985200007594
H	-1.7643134176195	-1.1748266640215	-4.3833783453841
H	-1.2733598253554	0.4322631932622	-4.8799674718765
O	2.1577569531097	-3.5111593145266	1.2485956665111
C	1.9687494563073	-2.2832217178119	1.9705041276951
O	3.0162932081157	-1.3653958233403	1.6472393629993
C	0.5943594872800	-1.7246436526431	1.5558345874948
C	0.3581865710039	-0.3358248547635	2.1529077210704
C	1.5523968219359	0.5937249429456	1.9184176948305
C	2.8792471056365	-0.0803706677559	2.3029937543541
O	-0.4583057887654	-2.6015582410570	1.9965695348936
O	0.1090394669972	-0.4632596266395	3.5594358714372
O	1.6490667976612	0.9405244713278	0.5293105022173
C	3.1290599128449	-0.1695346186690	3.8204194781903
H	1.9819194124461	-2.5404910339352	3.0350944415201
H	3.6971692736102	0.5150066855598	1.8763345926555
H	0.9185800882351	1.5753494616823	0.3305796146016
H	1.4386464898749	1.5239428221200	2.4868882098166
H	-0.2675964245287	-3.4632079506622	1.5744438213168
H	0.5352656724834	-1.6624081465596	0.4656998003012
H	-0.5498108978162	0.0918675016084	1.7136458395522
O	4.4725611316556	-0.6354688283973	3.9951877459138

H	2.4482840477796	-0.8643660546663	4.3163088222334
H	3.0309702600207	0.8200210404780	4.2798573694683
C	4.8364530440260	-0.8227657113500	5.3594436080210
C	6.3633713648724	-1.0287872218832	5.4084175335500
O	4.1618202813896	-1.9341544321146	5.9519969457761
C	4.4318445198944	-3.1844673398052	5.3138397274680
C	5.9377490779446	-3.5109880974999	5.2401846826518
C	6.7112203693952	-2.3195847413934	4.6630775600113
C	3.6678429070257	-4.2844848169482	6.0652346531945
O	3.9151914661109	-5.5587297474555	5.4691861099820
O	6.1897601332754	-4.6640921752417	4.4062261678545
O	8.1300103772330	-2.5757304008584	4.7616680384737
O	6.8780587961124	-1.1516611708271	6.7435949337126
H	3.3360886133135	-6.1923240188080	5.9385450177142
H	3.9732835978286	-4.3207782832467	7.1167154506094
H	2.5916069691719	-4.0815581866993	6.0392012861434
H	4.0308303558828	-3.1599062760428	4.2949156700328
H	5.5049339669033	-5.3215966205736	4.6852095336197
H	6.3286899881528	-3.7523013047599	6.2361601546651
H	8.3425477921412	-2.3701280569500	5.7022016786226
H	6.4960697371516	-2.2232735600794	3.5921744728429
H	6.8850646141318	-0.1881842187076	4.9368325628385
H	6.5277245299688	-0.4099621649987	7.2726325912511
H	4.5767667557530	0.0672465565448	5.9442835366072
H	-0.6020702605017	-1.1376551936016	3.6244584706786
H	4.0151590785357	-3.2209710905965	-4.1787402788350
H	10.5907615577342	-4.8214082802617	0.7839018234818
H	4.3028234551433	-1.2462024083504	-3.3585111544463

S5.6. Triply charged SRNLTK + GlcNAc₂Man₃

C	0.0692171655918	1.2228359322649	-0.6979608061118
O	1.3669515681949	0.8345488699545	-1.2003309246692
C	0.0467069289372	2.7052781782656	-0.2699192855643
C	-1.0639133634558	0.8547566411583	-1.6736352702447
H	-2.0288575695194	1.1125994683242	-1.2218828597306
H	-0.9694580404644	1.3739641932592	-2.6293810824775
H	-0.0609425844944	0.6042484807254	0.1991654603636
C	0.5795219327138	3.6273750978350	-1.3694495588957
C	1.9114699320860	3.1162374100854	-1.9206860192896
C	1.8164056848674	1.6266030083181	-2.2992995346213
O	0.8730473103849	2.8476348588663	0.8949284383131
O	-0.3725540602825	3.7335224268562	-2.4328132220311
O	2.2677835289305	3.9092604473476	-3.0669060842083
H	0.6579167603815	3.7072039521888	1.3033141081241
H	-0.9751557887078	2.9845735429244	0.0122824682972
H	3.0653153864722	3.4877945932293	-3.4421967515819
H	0.7222779720018	4.6411087584277	-0.9762665620692
H	2.6978279971329	3.2545599270112	-1.1684920306068
O	3.1458585100872	1.2104567925990	-2.6609578608503
C	3.1816378118847	-0.1545788961530	-3.1028682503821
C	3.4727644328592	-0.2017851992567	-4.6091845243607
C	4.2816464992362	-0.8865057752630	-2.3264477469588
C	3.6764838821503	-1.6558932836650	-5.0519997502402
C	4.7361584836580	-2.3597251792001	-4.1616568063694
O	4.4248178040224	-2.2358075804517	-2.7804262247875
C	3.9708061279243	-0.9580509825307	-0.8232719785633
O	2.7336386986175	-1.6525458412247	-0.5903262458139
O	2.3375446092065	0.3504387313745	-5.2963127428415
N	3.9983314502403	-1.7688415717044	-6.4824820017082
H	4.6679838288033	-1.1058532448547	-6.8604516252286
C	3.8639563190191	-2.9772516570813	-7.1279853951948
C	4.5202440955806	-3.0451939929645	-8.4786993211896
O	3.2883766584115	-3.9412667527263	-6.6208937418519
H	2.0438593037196	-0.9479695228387	-0.6222041690035
H	3.9201297452326	0.0325310850209	-0.3602869581973
H	4.7495256586428	-1.5330385508470	-0.3119488888033
H	2.2152935708576	-0.6526056022059	-2.9412117973680
H	2.7181300825797	-2.1741028917055	-4.9062974156838
H	2.6532172467289	0.6150570328465	-6.1899345802786
H	4.3387356042460	0.4262960977285	-4.8518689456758
H	5.5000568284489	-3.5185940531462	-8.3739930472295
H	3.8978758729288	-3.6399027645914	-9.1522419239191
H	4.6498395393187	-2.0494846256442	-8.9098548852644
O	6.0510288477441	-1.8776454997443	-4.4639172465718
C	7.1110379189150	-2.4662877950129	-3.6772734786796
H	5.2390142350978	-0.3620152386103	-2.4385539701601
C	7.3210644631686	-3.9829273498953	-3.8833749856897
C	8.4211429823685	-1.7291796439865	-4.0763622829280
C	8.5488757148556	-4.5077847135099	-3.0967005760820
C	9.5007482704935	-3.3447795891541	-2.7082143329032
O	9.6273008014633	-2.4812230485663	-3.8232778300943
H	6.8839099448941	-2.2926467203302	-2.6191097446419
H	8.4137261438992	-1.5634569337024	-5.1613226879548
O	6.1716367243222	-4.7344066744358	-3.4761236586842
N	9.1974874927465	-5.5677053868792	-3.9046969401022
H	6.4458839098571	-5.6628913476452	-3.3017697393537
H	7.4285832499558	-4.1683479744060	-4.9594316697293
H	8.2328006290838	-4.9907035816886	-2.1667908895346
C	9.7560691810104	-6.6985704361143	-3.3652593402780
C	10.3423589057339	-7.6430782023264	-4.3798166814873
O	9.8170380548752	-6.9200106918144	-2.1572571260777
H	9.3565977500894	-5.3751211135010	-4.8889624980889
H	10.1053719127356	-8.6707332358207	-4.0906556792246
H	11.4266155652317	-7.5082666995546	-4.4093028394050

H	9.9299643524032	-7.4655355334291	-5.3769470162135
H	9.1065497473868	-2.8041278355512	-1.8414536273692
N	10.8279347021488	-3.7972308907359	-2.3875371795903
H	11.4275526616328	-3.9742790683452	-3.1813800611455
C	11.1480246967326	-4.2808999583013	-1.1416244008541
C	12.4379562225886	-5.0815817851976	-1.1434608999661
O	10.4597933121019	-4.0986688654064	-0.1379365049970
C	12.7995331649144	-5.6789834958715	0.2133409056976
H	13.2466605422791	-4.4311760369398	-1.4988518784851
H	12.3235728243546	-5.8912924204363	-1.8734596136978
C	11.6157817904711	-6.3757623254969	0.9547233257997
N	13.3471046026098	-4.6427537773112	1.0923578449062
H	13.5785641045889	-6.4395548013275	0.0790044374492
C	14.1020605476677	-4.9647428685431	2.2039888889463
H	12.8409227448058	-3.7579248851170	1.1346663978689
C	14.0344309732642	-3.8875406722454	3.3249585189749
O	14.7462216843068	-6.0109626396740	2.3044564053184
C	14.9263893231316	-4.2629864682019	4.5162860456165
C	16.4243940680202	-4.1175126827297	4.1967999072741
N	12.6242989529107	-3.7931231986706	3.7544249054535
C	11.7329617286155	-2.9771037516415	3.0833711826037
C	10.2505101466008	-3.1576277303712	3.4312574646156
N	9.6244367661533	-4.1179967944128	2.4776287941393
H	9.7720528711823	-3.8593000847887	1.4852687748064
H	8.5939187319014	-4.1930857512630	2.6144648820205
O	12.0982379916883	-2.2600534050770	2.1523545836749
H	12.2526829796450	-4.6090720487242	4.2337334845919
H	14.3497082963074	-2.9253403150125	2.9043566422508
H	14.6893511221439	-5.2798673939087	4.8540741973257
H	14.6905251181685	-3.6054962949397	5.3633653841017
H	16.8116639397803	-3.2380051784772	4.7252264335916
C	17.2431352830682	-5.3404104634663	4.6140188239794
N	16.8927355534527	-6.5095779393827	3.7960137373981
C	17.5432630760259	-7.6791815951335	3.7977967181847
H	16.1057321944828	-6.4353458366782	3.1440194215493
H	16.5830336036770	-3.9349513696763	3.1273184400807
H	18.3048484657379	-5.1207621231518	4.4610444887081
H	17.0613479055005	-5.5820035350156	5.6660835569717
N	17.1283196886979	-8.6553494627038	2.9860541739072
N	18.5947858022176	-7.9044055377077	4.5877734073191
H	17.5941406451419	-9.5528195705140	2.9540796871982
H	19.0865192179146	-8.7886119601211	4.5815433041132
H	18.9408666703750	-7.1955442398888	5.2205322923187
N	10.9670374199457	-7.3712896063568	0.2661634126376
C	10.0008817268036	-8.2762073904610	0.8957255163496
C	8.7022153764923	-7.5431877487531	1.3104307635688
C	10.5930123598598	-9.0802966940314	2.0697734358588
C	11.8748519208850	-9.8728255647483	1.7400332576747
C	12.4015726627078	-10.5521497545857	3.0072668485420
C	11.6491477541190	-10.9193990122781	0.6485246398939
N	7.9765179715525	-6.9832073285146	0.2794285242704
C	6.5701894843661	-6.5910051990211	0.4807026632508
C	6.4135468431034	-5.2035710203827	1.1613576082207
C	6.7873834013784	-4.0273823508893	0.2688642273040
O	7.2229052530402	-5.0964588403482	2.35064444686964
H	6.1364138056638	-7.3501571181982	1.1456678556263
C	5.8029157761824	-6.6786843150167	-0.8559773247913
N	4.4343961723210	-6.5562504304624	-0.7604319467124
C	3.5800126436251	-6.3221973516839	-1.9370738644232
C	2.4680499326213	-7.3826214042064	-1.9820902129180
C	3.0086537854884	-4.8888324369045	-1.8981365225615
C	1.3903068226485	-7.1896347372608	-3.0580461045391
C	1.9108760298915	-7.1758252576997	-4.5033138274410
C	1.0170563321090	-6.3523075881881	-5.4294251432447
N	1.3014077407030	-4.9246513185584	-5.2395247199219
O	2.3634249545970	-4.3665173187744	-2.8016065510975

O	3.2451430009609	-4.2608658677666	-0.7234231985667
H	2.9210343514238	-3.3214354310648	-0.8073523254115
H	4.2025397260857	-6.3883678246350	-2.8327279181481
H	0.8170735616481	-6.2850371254723	-2.8317793189755
H	0.6656555615533	-8.0095923558604	-2.9663290421460
H	2.9369091049964	-6.8002779969250	-4.5660652399491
H	1.9389767953343	-8.2110446714607	-4.8647432016267
H	-0.0449662386612	-6.5152208469910	-5.2251922733169
H	1.2196475625597	-6.5738639931240	-6.4811618639077
H	1.4452437240953	-4.6502247367789	-4.2526412713080
H	0.5282955743759	-4.3085809791245	-5.5584201684215
H	4.0339576680559	-6.2165315734736	0.1086484233661
O	6.3882591288219	-6.8526323137430	-1.9269792044765
H	12.6102571370485	-9.8120730685471	3.7871802992052
H	13.3333126536730	-11.0900174135972	2.8022369112249
H	11.6760531867558	-11.2698982988997	3.4050878188233
H	6.6748470393982	-3.0847235098821	0.8158655967733
H	7.8355082158908	-4.0844280421986	-0.0318672438336
H	6.1647987488898	-3.9761077495605	-0.6277382240563
H	5.3738543993620	-5.0729400324548	1.4811841070351
H	7.2345254575561	-5.9976537996532	2.7551628533056
H	8.2904069535787	-7.1319213865406	-0.6823940801098
O	8.3077065780486	-7.4693635623796	2.4749687424411
O	11.2987935759961	-6.0763571448369	2.1120662281448
H	10.8862143881731	-7.2988836533032	-0.7485216682030
H	9.7016941286099	-8.9824754652861	0.1113065485808
H	10.8038372439003	-8.4078215419014	2.9108764814877
H	9.8261119047203	-9.7755767251623	2.4383483423235
H	12.6506161516514	-9.1787436962524	1.3947973088855
H	11.4007492054567	-10.4503665769799	-0.3082490922601
H	10.8363515301791	-11.6029975163759	0.9160129415731
H	12.5537874156244	-11.5164566954851	0.4901297855962
H	4.6820705982883	-3.4163717782269	-4.4240976347017
H	1.1722152463197	1.4901416371552	-3.1751817228781
C	8.5212638083138	-0.3382622349044	-3.4272851254512
O	8.4298334774683	-0.4254569371009	-2.0042431000897
H	7.7137495134651	0.3117851229062	-3.7784409141769
H	9.4853258356915	0.1203799651455	-3.6704172415997
H	8.6211757741678	0.4700513948545	-1.6666151904201
C	9.4956408188406	-1.8286206199426	3.3268151441461
O	8.0995107616663	-2.0747469600879	3.4986013931428
H	10.1265862572651	-3.5988686439597	4.4251870243122
H	7.6522083149519	-1.2085122423661	3.5655892767187
H	9.8328163686269	-1.1358323164764	4.1048953137619
H	9.6389305633742	-1.3521679712158	2.3510610708256
H	1.9610739483282	-7.4107066714911	-1.0079586929550
H	2.9270641298013	-8.3714565206533	-2.1109590738045
O	-1.0117803608966	-0.5572420926724	-1.9374003054048
C	-2.1779141761608	-1.0086300285139	-2.6243452718666
O	-2.2914183101397	-0.4317764322885	-3.9248592724504
C	-2.1728232803293	-2.5496378303597	-2.6803896018394
C	-1.0914890732967	-3.0328961135465	-3.6467765973081
C	-1.2549678674267	-2.3753920974193	-5.0246664623312
C	-1.2882856092421	-0.8447316170761	-4.8611303540427
O	-3.4225374722893	-3.0899463839809	-3.1489836116079
O	-1.1760936011646	-4.4654923802963	-3.7971425881264
O	-0.1632177045175	-2.8119822190063	-5.8651238438013
C	-1.5826931231062	-0.1038990109119	-6.1810257114292
H	-3.0672006813272	-0.6963593868025	-2.0636095428462
H	-0.3032527971348	-0.5072988803630	-4.5128384135742
H	-0.2047192605374	-2.2134922265460	-6.6463931509550
H	-2.1775923106473	-2.7334710827313	-5.4973911763261
H	-4.1332490727154	-2.7429658339932	-2.5766780549087
H	-1.9918625829996	-2.9775313770892	-1.6878168978323
H	-0.0918487535680	-2.8203900427449	-3.2502042793056
O	-0.9615676212667	-0.7312050577576	-7.3080651241188

H	-1.2395833171187	0.9342431805295	-6.0821223936541
H	-2.6651269386382	-0.0737648556140	-6.3584182777459
C	-0.9928435774846	0.1164865879817	-8.4636853948535
C	-1.3254311896946	-0.7123201869936	-9.7250128891501
O	0.2577461056529	0.8021223024157	-8.5910545734676
C	1.3633059695550	-0.0806808740008	-8.8563168508382
C	1.1520917577399	-0.8871595911546	-10.1392221250985
C	-0.1685228218694	-1.6555242231327	-10.0491662503812
C	2.6331596771263	0.7715257922800	-8.9419329375329
O	2.8342043262785	1.4396147229196	-7.6880934612527
O	2.2151884336557	-1.8270598380268	-10.3299151822537
O	-0.3914011770615	-2.3219340848538	-11.3007032817993
O	-1.5334777857780	0.1205912785002	-10.8784800350419
H	2.0904146575186	2.0777544375146	-7.6352600599860
H	3.5188452662422	0.1615579154464	-9.1373337610538
H	2.5525160247299	1.5395741528324	-9.7183446383365
H	1.4792638793971	-0.7535343687692	-7.9966212439005
H	1.9184753090804	-2.3926456783978	-11.0749838269108
H	1.1429755612025	-0.2263994072554	-11.0148068401252
H	-0.8094894082871	-1.6541773312568	-11.8857724805474
H	-0.0877742187273	-2.4425304370122	-9.2899369961896
H	-2.2404417919996	-1.2973550635832	-9.5788831714363
H	-2.2990901427403	0.6992209772314	-10.7040716744067
H	-1.7633928268692	0.8906639283921	-8.3592576476479
H	-2.1420731778195	-4.6509047061712	-3.7957698634710
H	0.0745389990898	4.2779906308906	-3.1161501188510
H	16.3319363952990	-8.5180997655102	2.3757231902843
H	10.0102300703271	-5.0737988240061	2.5610764198195
H	2.1374077750516	-4.6018432871916	-5.7628822541415

S5.7. Doubly charged SRNLTK + GlcNAc₂Man₅

C	-0.0943516924508	-2.3581956865668	0.2189649843006
O	-0.7926817422932	-3.4130756659151	0.8814438261180
C	0.1211365820688	-2.6155547075671	-1.2872704441780
C	-0.9010706748100	-1.0598953527843	0.4407506970779
H	-1.9428517086955	-1.2247078341842	0.1380314313031
H	-0.9016721642306	-0.8005999434167	1.5061175021441
H	0.8851569749189	-2.2191831121595	0.6948043906280
C	0.6908778333609	-4.0139559969818	-1.5427442441791
C	-0.1513419784524	-5.0687461960594	-0.8237711929745
C	-0.2426477937519	-4.7207527271444	0.6724404980811
O	1.0433989143683	-1.6548499139320	-1.8429672862285
O	0.6227683614750	-4.2523597948946	-2.9617049145025
O	-1.4553064838846	-5.1274958392887	-1.4211136147312
H	0.6663813012337	-0.7822341782330	-1.6057372319437
H	-0.8232291223400	-2.5022535362983	-1.8347431834391
H	-1.3116936484418	-5.1753354635102	-2.3865500258063
H	1.7342909982483	-4.0458965947210	-1.2043472729363
H	0.3069247010672	-6.0541079255956	-0.9605391401917
O	1.0627586718838	-4.7659002879595	1.2530722680831
C	1.1665147406067	-5.6437579997592	2.3864826079781
C	1.4348689778557	-7.0871344808058	1.9211728516324
C	2.3305005170259	-5.1330755959521	3.2510843739245
C	1.8314858982626	-7.9716497960568	3.1176132130638
C	3.0487679919194	-7.3401262134372	3.8455016723110
O	2.6897096446362	-6.0367400052766	4.3152823964513
C	1.9516074901651	-3.7878000711715	3.8923398570646
O	3.0300928435995	-3.3063866951119	4.6966674457799
O	0.2503681540368	-7.6135463694445	1.3032829321678
N	1.9934153020567	-9.3956283107949	2.7665292532957
H	1.5491157734064	-10.0720818005315	3.3797169129839
C	2.8589676800409	-9.8675472646082	1.8088176482963
C	2.9208310236142	-11.3685683667841	1.7142516616936
O	3.5011211780491	-9.1399835348222	1.0581075014407
H	3.1919819680280	-4.0172480991544	5.3483599456665
H	1.0803977430236	-3.8939158472643	4.5473875429974
H	1.7321751890984	-3.0283442424014	3.1363238976186
H	0.2385279066299	-5.6112484729891	2.9737908094420
H	0.9835489488313	-7.9693506390939	3.8167572593358
H	0.4360763661525	-8.5509332758403	1.1031940974893
H	2.2040916876834	-7.0720084226101	1.1424742388575
H	2.6030224910256	-11.8418921470436	2.6473167110562
H	2.2723354087138	-11.7035224311542	0.9007059681804
H	3.9519911467826	-11.6722358965261	1.5129931355946
O	4.1758347967482	-7.2952695159668	2.9746428792167
C	5.4648856398119	-7.2081494358217	3.6114904561354
H	3.2175612485111	-4.9598378029070	2.6294070104133
C	6.4731273568014	-7.9001701053565	2.6642886891813
C	5.8365732658232	-5.7308096095404	3.8293080024224
C	6.6786630335898	-7.1100831831454	1.3463369687675
C	6.9871944491225	-5.6321074823855	1.7151960360274
O	5.9976432232918	-5.0537134936306	2.5653858865459
H	5.4485659832141	-7.7386383598147	4.5713864039891
H	4.9901198924749	-5.2190345305488	4.2911776347880
O	7.7148859074236	-8.0725082823084	3.3521746220003
N	5.5244178943118	-7.2886212820650	0.4469303024625
H	8.2719260295417	-8.6749711586208	2.8200835002611
H	6.0996050153469	-8.9044173090551	2.4265995587261
H	7.5517994138484	-7.5123266143767	0.8164588072659
C	5.6113686596743	-7.2133000099738	-0.9194022107385
C	4.3488880778596	-7.6179752210456	-1.6296621518500
O	6.6138167138244	-6.8525666164290	-1.5291078268592
H	4.7028758118840	-7.7701116565159	0.8313342074214
H	3.4814836750135	-7.1407669103282	-1.1655264116743
H	4.2412208552645	-8.7049709615520	-1.5944776869770

H	4.4012436660995	-7.3018021915162	-2.6745185536785
H	7.9576276160236	-5.5868106158520	2.2213830944981
N	7.0475058574325	-4.7146763811712	0.6131629560675
H	6.1711731760978	-4.3484926092157	0.2653547354764
C	8.1863818854348	-4.5967166057643	-0.1388619430994
C	8.1570222373189	-3.4962321767032	-1.1706259462189
O	9.1947958040909	-5.2585555970984	0.0837040388742
C	7.0498647961518	-3.6586415685739	-2.2177211448493
H	9.1480642680419	-3.4532374949611	-1.6405436696628
H	8.0488871190712	-2.5572503793180	-0.6119467499976
C	7.7023497474744	-4.1946825116812	-3.5039137571720
N	6.3952250222686	-2.3694297613400	-2.4724018097651
H	6.2629997667537	-4.3533625587589	-1.9112056299565
C	5.5153338954898	-1.8231014829720	-1.5642830372378
H	6.8176576052592	-1.7602882038571	-3.1763402773630
C	5.1496674798025	-0.3282394076295	-1.8053778318127
O	5.1715939840525	-2.4388289540329	-0.5477701903783
C	4.0791094938653	0.1487470431359	-0.8097021301893
C	4.6149039283766	0.2577801839405	0.6260450165872
N	4.7182784063450	-0.0505557643833	-3.1775600284403
C	5.6201250154806	0.2967639113765	-4.1605056761537
C	5.0156035437710	0.7482344144631	-5.5001785056218
N	4.8848115272155	-0.3967903973171	-6.4244301115621
H	4.3529001864897	-1.1903177516596	-6.0219249703079
H	5.8209776693891	-0.7624719233213	-6.6867803962612
O	6.8337251842352	0.1925513302948	-3.9806027561227
H	3.7357883504071	-0.1713948641391	-3.4181143788401
H	6.0698490284159	0.2436343869544	-1.6258683126868
H	3.2147367648087	-0.5223723603590	-0.8589465977218
H	3.7147070351932	1.1371728097971	-1.1118414094490
H	4.7669779462879	1.3144963131482	0.8794236707342
C	3.6601433223890	-0.3634149369232	1.6399714682311
N	4.3190150834584	-0.6535630269201	2.9085981440848
C	5.1141512265630	-1.7047357420667	3.1366403924182
H	4.0699841467604	-0.1145475436209	3.7452282560096
H	5.6056811399728	-0.2010101609997	0.71313566647428
H	2.8382977216036	0.3231587660686	1.8546031248558
H	3.2037836215569	-1.2901842633839	1.2754148000495
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H	6.1867660972967	-2.7237966087497	4.5571065392675
H	5.1549478686976	-2.4258123814560	1.1965200553402
H	5.9145430934337	-3.4194929993194	2.3915065092536
N	7.9167512911824	-5.5543906390409	-3.5089731869411
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C	8.0492482427127	-6.5296548319462	-5.7988745870096
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N	6.6892773123248	-6.7523150856402	-5.6918738586909
C	5.9005982103367	-6.8337091856322	-6.9229203824804
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C	3.7219339585775	-7.6174500648044	-7.9791789982145
O	3.7692272072715	-6.9580871933181	-5.6639485358342
H	6.4706503860565	-7.3863619834460	-7.6800477292192
C	5.7391882561301	-5.3711153646475	-7.3812304830369
N	6.6481509822880	-4.9769638390345	-8.3511133620801
C	6.8060821063620	-3.5527284152329	-8.6845307777090
C	5.5126833965964	-2.9198844360839	-9.2238458174417
C	7.3670907871948	-2.8388063851867	-7.4449507621372
C	5.7577138118839	-1.5870946847790	-9.9419463316982
C	4.5024870509630	-1.0323758442582	-10.6271866519400
C	3.3148444991596	-0.7402718379370	-9.7072950923036
N	3.6226186935866	0.2838309665835	-8.6943970723027
O	6.9692582997296	-1.7841224505241	-6.9681351524888

O	8.3836105761404	-3.5259482039976	-6.8855422392240
H	8.4752050771644	-3.1935715215079	-5.9540731641874
H	7.5794582021874	-3.5107757178269	-9.4607076287937
H	6.5265654292407	-1.7309715780744	-10.7112658298503
H	6.1542804129391	-0.8421651424261	-9.2443955942072
H	4.7775788042861	-0.1137706928285	-11.1612197586418
H	4.1761642500209	-1.7452251432129	-11.3949658652142
H	2.9761619603221	-1.6512658677400	-9.2050723516669
H	2.4767800204201	-0.3831779710481	-10.3169300922912
H	3.8803319826417	1.1350611783330	-9.2111126368348
H	2.7178863641158	0.5298752084045	-8.2574884529158
H	7.5282414034763	-5.4995143685996	-8.3176843721833
O	4.9883421460618	-4.5720453976573	-6.8209113255527
H	11.2848736464642	-9.2740054697020	-2.9310411332628
H	9.7756388918227	-9.4740515790406	-2.0219413798043
H	11.1862856745125	-8.7478499481633	-1.2412928031941
H	2.8116993195288	-8.2032344809992	-7.8104929589328
H	3.3943125060367	-6.6192837903947	-8.2884003525436
H	4.2809451927868	-8.0764888747917	-8.8000562392956
H	4.7721426085898	-8.5805535158686	-6.3737971298780
H	2.9793015581366	-7.5250702666940	-5.5543166688009
H	6.2384622536645	-6.3336022410627	-4.8818226416480
O	8.6373532133991	-6.6775477754585	-6.8702662673506
H	8.0722691672427	-3.4488976008877	-4.4119417671793
O	7.5415023312196	-6.1222053126629	-2.7398592778753
H	9.5991993196477	-5.5328169338015	-4.7364383400941
H	8.4919589330706	-8.2281673552547	-3.7318708307899
H	9.9408257980466	-8.0341653689632	-4.6991863498371
H	9.5322098846023	-7.0195730255745	-1.8391734981512
H	11.0619942135545	-5.4661027687811	-2.9786948601561
H	12.0056968938444	-6.8175331461428	-3.6350730599699
H	11.9877585626918	-6.4974830829355	-1.8923384562834
H	3.2817939805492	-7.9587971098866	4.7200277333888
H	-0.9397808780279	-5.4112700831738	1.1588928768276
C	7.0284266490345	-5.4749681541769	4.7659997387663
O	7.1329086019020	-4.0552618328611	4.9988713114464
H	7.9831957503836	-5.7996879713744	4.3497085126895
H	6.8725976342849	-5.9641097887559	5.7324328537279
H	7.9392919121129	-3.9495789049757	5.5463769154703
C	5.9209044593456	1.8032322041268	-6.1512906192738
O	7.0520126717125	1.2061362818034	-6.7906150348158
H	4.0191036721194	1.1541284638257	-5.3292137997284
H	7.6655777937066	0.9023223993123	-6.0897439023208
H	5.3640012396549	2.3355517662250	-6.9295621229771
H	6.2780960750899	2.5440830774826	-5.4282994042134
H	4.8002987544727	-2.7569380445389	-8.4091667341851
H	5.0385673786393	-3.6175217608123	-9.9260290338385
C	1.7059508372458	-5.0084929911248	-3.4871727841521
C	2.9551984188329	-4.1408057299426	-3.7579691629555
O	1.2696725393832	-5.6412331464087	-4.6993955917804
C	0.8242594675225	-4.6897099227584	-5.6752541561806
C	2.6857542665678	-3.1393320212938	-4.8887972109990
C	1.9608289689503	-3.7460533741021	-6.1020521781949
H	1.9616817579736	-5.8269682798484	-2.8053740265257
H	3.2255682843863	-3.5717925562375	-2.8626224738468
O	4.1106047580459	-4.9425742701128	-4.0550181015057
H	3.8707681236566	-5.5741883262623	-4.7757851378043
O	3.9338639091503	-2.5416013409367	-5.3195632778702
H	2.0777689053288	-2.3181937250863	-4.4929476634753
H	4.4792818824949	-3.3257661160220	-5.5972147389204
O	1.4630822430359	-2.6638440705433	-6.9193129063559
C	0.2635138126269	-5.4594982449123	-6.8814311100106
O	-0.1035972634217	-4.5604684764307	-7.9266962019869
H	-0.0046168831669	-4.0906975339116	-5.2750285070683
H	-0.5926958570296	-5.0883331660236	-8.5884344801954
H	-0.6169544141941	-6.0373172903549	-6.5793982295048

H	1.0032510146824	-6.1672074924920	-7.2697710857801
H	2.6701433648335	-4.2965324874836	-6.7228293108771
H	0.8695070856006	-3.0998189244070	-7.5793567106901
O	-0.3391312766595	0.0122473145137	-0.3240141819069
C	-1.1063069738856	1.2195067200342	-0.2120924861995
O	-0.7707597594435	1.9235672514480	0.9837128596302
C	-0.8468683353745	2.0755356846335	-1.4662660278321
C	0.6239550256802	2.4905048827124	-1.4897185393068
C	0.9748716087796	3.2529476174399	-0.2048272748716
C	0.5671570945084	2.4227629126686	1.0310195163734
O	-1.6869190805904	3.2347224063250	-1.4891209154716
O	0.8442246098978	3.3192117592840	-2.6530230463435
C	2.0439832164311	2.9489814471125	-3.3385667066284
O	2.3922085393157	3.4921218986840	-0.1962200987778
C	0.7091998396917	3.2215757334684	2.3407603288760
H	-2.1778261640509	0.9913298155090	-0.1642742851269
H	1.2497475599086	1.5697846786587	1.1017038471079
H	2.5799396479993	3.9414758487816	0.6546423969108
H	0.4775060643860	4.2301813786268	-0.2065869884241
H	-1.3660470930930	3.7936985669527	-2.2230236133416
H	-1.0747203371367	1.4956345873798	-2.3680924232543
H	1.2488205700269	1.5901635466758	-1.5556109549943
O	1.9668921451937	3.9029607655515	2.4110467496879
H	0.5984888898044	2.5331091993702	3.1884549751664
H	-0.0972889360320	3.9618050870346	2.4137541831617
C	2.2222767298703	4.4001103193382	3.7299932958299
C	3.0694983426183	5.6904286665236	3.6527699320229
O	2.8582056311724	3.3880407587378	4.5221762349171
C	4.1765447145304	3.0460324081026	4.0560720600197
C	5.1095404996774	4.2571141933889	3.9915865799262
C	4.4729109185676	5.3618825278939	3.1467438032834
C	4.7427643999802	1.9813550272294	5.0043197991566
O	3.8808866934395	0.8256567591078	4.9942552818658
O	6.3622534171527	3.8856438204910	3.4069820938737
O	5.3157350203528	6.5222086522896	3.2111042951116
O	3.2118848870564	6.3198368538951	4.9384117133241
H	3.0309752517781	1.1732969744752	5.3479722354402
H	5.7389457195937	1.6514844541348	4.6960567195745
H	4.7897921996278	2.3445161173367	6.0362942976201
H	4.0762986879913	2.5842523435089	3.0652958516979
H	6.8227332562638	4.7328088890288	3.2245901719562
H	5.3228817915439	4.6350277746541	4.9991282879617
H	5.0662239221786	6.9855821540286	4.0391243132683
H	4.4444298999553	5.0561453297030	2.0943279844472
H	2.6062193444410	6.4234378307351	2.9825494683637
H	2.3298065467170	6.6163737127072	5.2309620130664
H	1.2792288899666	4.6476445698563	4.2332974530988
C	2.4651492375606	4.0501376941005	-4.3295586077999
O	1.8675466757126	1.6848079365157	-4.0024838878828
C	0.8856245897137	1.7354177766866	-5.0591839458115
C	1.2652332141221	2.7685074457793	-6.1287675697835
C	1.4612132236503	4.1425558259122	-5.4773397100086
C	0.7331574868094	0.3267478792787	-5.6529209926474
O	0.2431391178610	2.8687042035683	-7.1242170082616
O	1.9648409906544	5.0458001108486	-6.4794327471062
O	3.7698268425940	3.7672273136970	-4.8826332802982
H	1.7305239867194	5.9526029126784	-6.2015352635433
H	0.4955287989556	4.5347078972647	-5.1356765563074
H	2.5365973509389	5.0186165112343	-3.8218523774721
H	3.8717113644559	4.4192905621597	-5.6097525405859
H	2.1873375447095	2.4750139274400	-6.6444818726701
H	0.4920405066359	3.6297277221549	-7.6871242801331
O	1.9460164785257	-0.1146867889408	-6.2693743163888
H	-0.0638409020302	0.2986164750482	-6.4023762499807
H	0.4953148419050	-0.3853565320331	-4.8556415323270
H	1.7508516208950	-1.0295848462301	-6.5921453096784

H	-0.0873147491463	1.9960342081886	-4.6234147590293
H	2.8639486309546	2.8154225206811	-2.6248602285681
H	5.3125133453822	-1.3227960147279	5.1262454787115
H	4.4169925021563	-0.1422281966573	-7.3202780742520

S5.8. Triply charged SRNLTK + GlcNAc₂Man₅

C	2.7910581610374	-4.0673076041548	-6.3576807437210
O	3.5698094564013	-4.3174768463114	-5.1722780449608
C	1.5746078740648	-3.1603975127650	-6.0827446677317
C	3.7256115324385	-3.4283583118059	-7.4051770755164
H	4.5527419709870	-4.1071952296916	-7.6413764670766
H	3.1800906688846	-3.2395152956693	-8.3351790976063
H	2.4534118675008	-5.0278447846468	-6.7675935164400
C	0.7426754419248	-3.6924898630627	-4.9029380399339
C	1.6510987894102	-3.9627619178289	-3.7051202077133
C	2.8188919884761	-4.8818381888051	-4.0944825771542
O	0.7169495062646	-3.1008558763855	-7.2280536789952
O	-0.1886740771687	-2.6489882475744	-4.5197656234542
O	2.1473478339767	-2.6946870995439	-3.2157190402030
H	1.0576883070108	-2.4134184031008	-7.8301716769007
H	1.8891523190051	-2.1342476208797	-5.8544208451791
H	1.3812574967336	-2.0981729847832	-3.3401821868564
H	0.2080613197682	-4.5989202542670	-5.2129389649648
H	1.0728171977633	-4.3993329482968	-2.8882940570062
O	2.4010120519567	-6.1913584932590	-4.4693941528813
C	2.6351938245227	-7.2741327333832	-3.5531323363141
C	4.1264167936722	-7.4419088848147	-3.1769673878221
C	1.7671564301656	-7.2093161657676	-2.2905959626762
C	4.2809204094782	-8.6627324684695	-2.2470692826324
C	3.3603100757501	-8.4860007537295	-1.0052197902250
O	1.9951833665764	-8.3260318321510	-1.4112542850713
C	0.2693390956670	-7.1994160916941	-2.6277607504669
O	-0.4704944550822	-6.8636454302389	-1.4481408112609
O	4.9347484463396	-7.5690067994634	-4.3626205481731
N	5.6621220183335	-9.0290645173518	-1.8992164756126
H	5.8186332521239	-10.0141994825706	-1.7123621144365
C	6.6199306688541	-8.1551424526328	-1.4612540223939
C	7.8720549692464	-8.8066093504214	-0.9355889600330
O	6.5085375112188	-6.9316874918293	-1.5202812973739
H	-0.4655194399491	-7.6762804682922	-0.9026021837483
H	-0.0732678751974	-8.1797668716128	-2.9757367000258
H	0.0224147051688	-6.4548591118018	-3.3876061210343
H	2.3481128128095	-8.1730311444376	-4.1153189580243
H	3.9181354266568	-9.5355114751876	-2.8077226944274
H	4.3849740987797	-7.2606424138914	-5.1148198458837
H	4.4862773918222	-6.5455569277944	-2.6708680531778
H	8.7144565612564	-8.5233384184661	-1.5722982244570
H	8.0484946170341	-8.4620619162089	0.0871352037438
H	7.7936346156038	-9.8969456022314	-0.9248781065012
O	3.7378017289131	-7.3653841596794	-0.1961975884208
C	3.5121679934242	-7.5920582758438	1.2121031543431
H	1.9955422418727	-6.2892650692622	-1.7465109335831
C	4.8257243039852	-8.0527407692653	1.8742083884290
C	3.0432448136722	-6.2803468834379	1.8665208929689
C	4.6766331837255	-8.1055519727518	3.4084886213516
C	4.1251098418345	-6.7592460988044	3.9624702919734
O	2.9160968523327	-6.3960047446493	3.2924887793300
H	2.7394405874089	-8.3597944453659	1.3579007618002
H	3.7436513171687	-5.4691380520720	1.6349259750323
O	5.1772919077731	-9.3587438275704	1.3808520046820
N	5.8878963617056	-8.6194007544671	4.0767164855199
H	5.9338754717322	-9.6612933981069	1.9195654183023
H	5.6389802380661	-7.3842576395880	1.5702167783924
H	3.9181939229519	-8.8730018794074	3.6193389684905
C	7.1043899368648	-7.9839710750597	4.0642807835711
C	8.2047896919290	-8.6837454394286	4.8139104212780
O	7.2714947369526	-6.9147244969920	3.4818613711199
H	5.7820045717713	-9.4384881486084	4.6702098415404
H	8.5969776029010	-8.0109779384772	5.5812155730571
H	8.9999297101215	-8.9496269371616	4.1123612125128

H	7.8484684528290	-9.5957819621824	5.3001796557929
H	3.8733547764372	-6.9035991360173	5.0201916956282
N	5.0219687752658	-5.6269051546994	3.8927535203331
H	6.0015709984012	-5.8523474214498	3.6941977948559
C	4.7853097833676	-4.4880642330209	4.6240820958736
C	5.8974665080100	-3.4611695428013	4.5753330334928
O	3.7146105779488	-4.2700887757676	5.1895997381545
C	5.5836927363069	-2.3288145461091	3.5982960863922
H	6.8309072770418	-3.9525830349759	4.2761677085107
H	6.0501513327605	-3.0805308300656	5.5918025123471
C	4.4632656621141	-1.4164741694601	4.1465356234163
N	5.1669584254901	-2.7965921488131	2.2758192514423
H	6.4886020339213	-1.7214692686209	3.4735515848068
C	5.2826297507947	-1.9486536696360	1.1923845267924
H	4.3523983871928	-3.4007184577944	2.2602373910051
C	4.5818874118874	-2.4503655205814	-0.0871470861415
O	5.9347279126906	-0.9054330223099	1.2256658158910
C	5.4792004155537	-3.4582094618480	-0.8253449495868
C	6.6901736938767	-2.8208030546653	-1.5177639955604
N	4.2089580597065	-1.3100351598691	-0.9180389172398
C	2.9502574452650	-0.7367814109122	-0.8191580895780
C	2.7492307646772	0.4702616239135	-1.7475259449190
N	3.3589353494153	1.7205968676603	-1.2218547374421
H	2.8398056058826	2.0898066112230	-0.3997426963804
H	3.3443258622726	2.4583526951866	-1.9499035654393
O	2.0806410540694	-1.1704760665644	-0.0684969697505
H	4.9655778379149	-0.6786774691666	-1.1809898607932
H	3.6658952500702	-2.9722213422982	0.2163410664716
H	4.8780167923553	-3.9729284486884	-1.5836241285930
H	5.8204958308230	-4.2258175471504	-0.1195177459842
H	7.1866022050174	-2.1248677689383	-0.8350628781102
C	7.7295723525449	-3.8363330462348	-1.9687298979120
N	7.1856674887243	-4.8547905321809	-2.8633866071436
C	7.3977628574323	-4.9334204145839	-4.1795657950260
H	6.8462118591777	-5.7169834985679	-2.4209658147590
H	6.3446641621514	-2.2456386478522	-2.3815996708231
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N	7.1016828059824	-6.0472554699819	-4.8372068964464
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H	7.3827582562503	-6.1196637786951	-5.8154148774604
H	7.8982406385357	-2.9652222964353	-4.5341898200051
H	8.0358240780691	-4.0546577214100	-5.8821088644374
N	4.9012814582311	-0.3375392063668	4.8839237549316
C	3.9726286131667	0.7482024840176	5.2047474701514
C	3.8222306515667	1.6305650654979	3.9358834057979
C	4.4792711382199	1.5853110606343	6.3858539470084
C	4.6893491041931	0.7915172212702	7.6917857716551
C	5.2492006539935	1.7174885854230	8.7748628137813
C	3.4013633559522	0.1335492556917	8.1888399429115
N	2.8234559240432	2.5770524198890	3.9884991309992
C	2.3545631589272	3.3256530167749	2.8051546086313
C	3.4606121218679	4.0598092425989	1.9960022527281
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O	4.1960545336659	3.1956846185881	1.1168770358769
H	1.6783019557478	4.0857017491935	3.2179553293727
C	1.4889217960214	2.3755667483238	1.9426846548629
N	0.4507921283576	1.7625758585543	2.6313879559783
C	-0.5364014758404	0.9654716508840	1.8873574708837
C	-1.1299643231200	-0.1468140882430	2.7632187669917
C	-1.6748480076263	1.8633899185057	1.3710860489964
C	-0.0639624162457	-1.0840473997872	3.3480241122923
C	-0.6934869542503	-2.3402448769822	3.9642068109030
C	0.2520182655943	-3.1488165151485	4.8498947581065
N	1.4801561639116	-3.4942124436604	4.1401696198821
O	-2.5581512269938	1.5384806517633	0.5933840974843

O	-1.6770698211473	3.0990790663494	1.9233815108690
H	-2.4711890976520	3.5310323091190	1.5332926504439
H	-0.0429359986313	0.5268104895128	1.0150497265625
H	0.5105156046276	-0.5470989752237	4.1121906888274
H	0.6357554841273	-1.3795703449056	2.5573394111416
H	-1.5614981940343	-2.0550786405079	4.5712659822810
H	-1.0733018125475	-2.9794093368099	3.1571085684163
H	-0.2153875784700	-4.0867021906664	5.1638386268608
H	0.5460571558204	-2.5818702386434	5.7385319381268
H	2.0606407924293	-2.6602426616944	3.9296051425257
H	1.3426372256199	-3.9965230752666	3.2397178076144
H	0.0553948356295	2.3100040013845	3.3884666642672
O	1.6752848786417	2.1912794942235	0.7399595400840
H	4.5481194750559	2.5259881751748	9.0086170289755
H	6.1928994190664	2.1690934458907	8.4510893842189
H	5.4458684738203	1.1621800690838	9.6981461236346
H	2.2026606698483	4.7934578074789	0.3739825771425
H	2.3442442498456	5.9130001851086	1.7494329775870
H	3.6856167741295	5.7017601447602	0.6042107005881
H	4.1832158720682	4.5022433323774	2.6923769408693
H	4.6133147868557	2.5241082697981	1.7072466944100
H	2.2021229239105	2.5615250351687	4.7886495532979
O	4.5368159157345	1.4862288090398	2.9435204498007
O	3.2685816798561	-1.6499688186028	3.9394066823015
H	5.8511108789520	-0.0313498173860	4.6933253872478
H	2.9857949397145	0.3222881991953	5.4189079345790
H	5.4301015214733	2.0585268254647	6.1040595517060
H	3.7794862787839	2.4093727434260	6.5763673544415
H	5.4313796834947	0.0026696204465	7.5169995810896
H	2.6011145615965	0.8709043973508	8.3126466413434
H	3.5631260843179	-0.3550403689541	9.1558345686971
H	3.0527692162158	-0.6362131021581	7.4935751514885
H	3.4108714503564	-9.4150665946580	-0.4260421553652
H	3.5094601356714	-4.9043080836903	-3.2512237556612
C	1.6704386794041	-5.8730542307008	1.3251875726820
O	1.3089233304957	-4.5532174708469	1.7704781315957
H	0.8874409202906	-6.5584182871658	1.6647241889219
H	1.6866196733010	-5.8480020344117	0.2386857892965
H	0.6148461082247	-4.2921706379402	1.1055867857349
C	1.2695652306936	0.7225640424191	-2.0489176449629
O	1.1561180686558	1.7643797092497	-3.0196664873662
H	3.2683738123561	0.2668662499756	-2.6894019271086
H	0.2024691303478	1.9525055277565	-3.1320758145745
H	0.8099200195638	-0.1767017130299	-2.4639038580846
H	0.7044725505780	1.0113519284644	-1.1614229986514
H	-1.8400021229495	-0.7296262607136	2.1624632275685
H	-1.7092604921046	0.2925598804691	3.5859384990536
C	-1.4859204076310	-3.1385594294355	-4.1667905131148
C	-2.5157869776113	-1.9951048865866	-4.3101849633964
O	-1.4863118256095	-3.6892485048566	-2.8456804594219
C	-1.2624409390478	-2.7309837686091	-1.7996805628649
C	-2.2145107393559	-0.9140217976389	-3.2751870714611
C	-2.1834777251114	-1.5064593798534	-1.8667430570022
H	-1.7864918159876	-3.9427575669044	-4.8486003189460
H	-2.4767363822111	-1.5549742670404	-5.3132271976540
O	-3.8630440286948	-2.4427452353772	-4.0895513774077
H	-4.1000367099945	-3.0520706239953	-4.8142390592355
O	-3.2062830896826	0.1215208851192	-3.3176962682464
H	-1.2600613109844	-0.4265895246425	-3.4985605661161
H	-4.0617673140091	-0.3337595958843	-3.4711340444816
O	-1.6918075971233	-0.5131224140355	-0.9547886994831
C	-1.4558336523150	-3.4370474576451	-0.4482182906951
O	-0.4469573470299	-4.4321451476602	-0.2438155795657
H	-0.2155075285776	-2.4139549705843	-1.8528923036106
H	-0.6698378092105	-5.1625385414531	-0.8740239727996
H	-2.4298745479704	-3.9348891556925	-0.3934271436306

H	-1.3767111540810	-2.7316034241474	0.3841527856367
H	-3.1996030117008	-1.7697159079722	-1.5473515269878
H	-2.3622645410722	0.2096471267849	-0.9498714376081
O	4.2244250078341	-2.1621410846126	-6.9380336577180
C	5.5272005780580	-2.2754629596751	-6.3691523095421
O	6.5374000783038	-2.3549096671316	-7.3752336360882
C	5.8057272763774	-1.0956389196065	-5.4189268063692
C	5.9059098606677	0.2143149281812	-6.2237699751414
C	6.9514801268693	0.0568970527564	-7.3445454643875
C	6.6111866407604	-1.1733964451144	-8.2008110048018
O	7.0319442501603	-1.3117180338997	-4.6754694348729
O	6.2927779658540	1.3447192331831	-5.3971689776329
C	5.3271642440295	1.6543185931571	-4.3929012596358
O	6.9618808799564	1.2379568203098	-8.1461085086033
C	7.6681538404847	-1.4326003808711	-9.2868933395917
H	5.6026988300390	-3.1944608022451	-5.7839546282413
H	5.6449310940274	-1.0319809539928	-8.7030925567135
H	7.1442125576500	1.9885682969974	-7.5501130989315
H	7.9513471798714	-0.0476488707743	-6.9054523040646
H	7.2460536454087	-0.4305600389459	-4.3029976555294
H	4.9999181003806	-1.0314127647747	-4.6802164951943
H	4.9394876629299	0.4631320448231	-6.6828574629165
O	7.1102906836982	-2.3447134608554	-10.2447748324973
H	8.5737920089492	-1.8502177922873	-8.8305094481834
H	7.9276476125758	-0.5166980727782	-9.8262055962407
C	8.0591972373972	-3.2739679977336	-10.7581666145233
C	7.5187914999851	-3.8911920120023	-12.0698676248388
O	8.3434510687971	-4.2903301062226	-9.7817025176611
C	7.1791431919945	-5.0737047950470	-9.4564594683558
C	6.5949172078614	-5.7805945911081	-10.6776155203263
C	6.2909285631644	-4.7548163673030	-11.7723040953473
C	7.5878152495576	-6.0802642891989	-8.3784123718809
O	8.1740622752488	-5.3687403922739	-7.2660427139529
O	5.3872896169420	-6.4678905842232	-10.3251727552207
O	5.8741289874395	-5.4706139873899	-12.9459838388183
O	8.4941558889163	-4.7340606426435	-12.7101867379524
H	8.8860417738168	-4.8585034971185	-7.7203774635234
H	6.7312496171749	-6.6484181618204	-8.0046924179798
H	8.3464021846422	-6.7781663877826	-8.7478528483283
H	6.4307794127829	-4.4111967906807	-9.0089945996391
H	4.9798905439656	-6.7099712037096	-11.1854014429286
H	7.2945412838671	-6.5345078714404	-11.0592793050236
H	6.7006423013545	-5.6987199070785	-13.4227740715689
H	5.4417946380502	-4.1303139499338	-11.4707107920910
H	7.2430308673064	-3.1100209599366	-12.7874493195039
H	9.2214168131158	-4.1636713992486	-13.0222542487679
H	9.0047955197737	-2.7637990204158	-10.9785486317954
C	5.0504905441510	3.1617859418170	-4.2649931049665
O	5.7541683196796	1.0916462305405	-3.1466929427828
C	6.8872050928750	1.7598995514216	-2.5504037423792
C	6.7075459053979	3.2799923509259	-2.4047566904962
C	6.2788748149491	3.8942054129776	-3.7378370112477
C	7.0958481072694	1.1176690476239	-1.1706379641293
O	7.9397562016754	3.8724059672536	-1.9872964521506
O	5.9160002492981	5.2681412412756	-3.5249104171679
O	3.9617685778651	3.3867118778326	-3.3289094789055
H	6.7198539895910	5.8064619355396	-3.6629267124929
H	7.0957244197016	3.8692892962292	-4.4689268187090
H	4.7431596334674	3.5816951062849	-5.2293762963918
H	3.9011975540300	4.3714368820151	-3.2976574654364
H	5.9626950485246	3.5070401269987	-1.6319091321980
H	7.7385721902641	4.7862015766203	-1.7071939942996
O	5.8386876802633	1.0532118353562	-0.4716152802262
H	7.8217688064859	1.6611845511964	-0.5589813259663
H	7.4422454953034	0.0891940429653	-1.2983640296019
H	6.0505555732409	0.6140183062344	0.3930563752119

H	7.7799925571973	1.5554206788933	-3.1551006227971
H	4.3664971167231	1.1800592899181	-4.6270085256431
H	6.5562407321775	-6.8089360517770	-4.4315457259321
H	4.3418581886575	1.6118524966014	-0.9072539874568
H	2.1299138896406	-4.0793118208325	4.7018413211152

S5.9. Doubly charged SRNLTK + GlcNAc₂Man₆

C	1.0232324791403	-0.1919364077787	-4.1794657042792
O	-0.0247292596574	-0.3822930073080	-5.1295888641605
C	2.4300804582661	-0.4529876301839	-4.7540855790083
C	0.8850123542610	1.2591757765064	-3.6838015266387
H	0.8870641536791	1.9375674898730	-4.5469174398511
H	-0.0846513671770	1.3726115426488	-3.1832113011989
H	0.8668834076846	-0.8556281798419	-3.3201405328141
C	2.4849392645857	-1.8259154017927	-5.4446712568528
C	1.3422001369252	-1.9451176440401	-6.4582099071726
C	-0.0212238242562	-1.6420216563798	-5.8028095098156
O	3.4208014744669	-0.4096339407785	-3.7108957703905
C	3.7305786767133	-1.9635356759440	-6.1772998426125
O	1.5873758713101	-1.0386549869432	-7.5476740003607
H	3.2363349390248	0.4094101865238	-3.2052868903378
H	2.7000796608887	0.3251699160847	-5.4786363924113
H	2.5118153022059	-1.1928946485370	-7.8226847593823
H	2.4010311660334	-2.6296573273294	-4.7022185743591
H	1.3388042363513	-2.9556894226792	-6.8836050990734
O	-0.3770607628594	-2.6859764559221	-4.8922864377205
C	-1.8066913703822	-2.8893974773557	-4.7727692992548
C	-2.2986015153496	-3.8540980765564	-5.8791657298679
C	-2.0776731880055	-3.4762070953044	-3.3667688865345
C	-3.7192015500749	-4.3602323012793	-5.5680020788855
C	-3.7135109124014	-5.0453061419536	-4.1807094619954
O	-3.3860309119040	-4.0592230014699	-3.2090266064275
C	-1.9564563175277	-2.3787727221080	-2.2939507303367
O	-2.0700553541577	-2.9376736225343	-0.9724593408611
O	-2.3137828729121	-3.1762667438073	-7.1452342158700
N	-4.3213358495710	-5.1585734933635	-6.6528520634681
H	-5.2483163790429	-4.8813769805874	-6.9590766914522
C	-3.7865625601130	-6.3106085267351	-7.1733177472538
C	-4.6441075689610	-6.9754029166981	-8.2169724069182
O	-2.6879368700679	-6.7544292105391	-6.8566722605365
H	-2.5143224753230	-2.2269483230384	-0.4464371954214
H	-2.7648673696481	-1.6487363352287	-2.4158329147454
H	-0.9978703808474	-1.8596023732807	-2.3527444335094
H	-2.3249423777987	-1.9258826416062	-4.8726418570823
H	-4.3716908788173	-3.4776551481315	-5.5075792349695
H	-2.6440578623311	-3.8193669700332	-7.7998160167795
H	-1.5806722591548	-4.6739587086680	-5.9822243322233
H	-4.6088438294588	-8.0587233011044	-8.0716113623824
H	-5.6873450723034	-6.6561814047091	-8.1433284374479
H	-4.2605275334200	-6.7234850743004	-9.2089813458182
O	-2.8039201160395	-6.1377927583291	-4.1769154556788
C	-2.9547867526718	-7.1179638753742	-3.1358356195889
H	-1.3280010341028	-4.2391906553698	-3.1427631386262
C	-2.3089605812609	-8.4074420614213	-3.6745103657561
C	-2.2305199942395	-6.6650942013416	-1.8608908452184
C	-0.7988227379962	-8.2111929033651	-3.9252102877197
C	-0.1023752488121	-7.4822627168351	-2.7125500718794
O	-0.8428818898591	-6.3998558013269	-2.1467886530632
H	-4.0169994775722	-7.2976650192812	-2.9308471122414
H	-2.6357636458518	-5.6956616509642	-1.5591755455432
O	-2.5369512874374	-9.5001314330953	-2.7829267489730
N	-0.5913035059322	-7.5822521737641	-5.2488419582866
H	-2.4493089162324	-10.3240485565436	-3.3017628325112
H	-2.8020353728806	-8.6710135571122	-4.6196285756205
H	-0.3174646036079	-9.1954612311882	-4.0068692843972
C	0.5707025389438	-7.6462060843721	-5.9696202368094
C	0.4839240645562	-7.0551368804827	-7.3484833399921
O	1.6117676065860	-8.1062431172177	-5.5043498086834
H	-1.4035135478734	-7.1458898009773	-5.7018682277357
H	1.4574852990012	-7.1321600794088	-7.8408007113286
H	0.2047507012030	-6.0000789126810	-7.2848892941584

H	-0.2525401453471	-7.6031255034705	-7.9418813013067
H	0.0961389285256	-8.2068004855513	-1.9149374480456
N	1.1766301397683	-6.9243493610610	-3.1075401959868
H	1.5834250309568	-7.3479752918682	-3.9406916097056
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C	3.1808246446648	-5.6154742011345	-3.1513257072500
O	1.7616255970466	-5.8237979884357	-1.1850847327866
C	4.2911780087817	-4.9524163852074	-2.3350947736691
H	2.7538109444460	-4.8768510830307	-3.8396144189472
H	3.5874301125851	-6.4386406330932	-3.7468046340337
C	5.1400797881727	-6.0624897176964	-1.7023505314711
N	3.7647994596667	-4.0340018687260	-1.3382609089465
H	4.9529862698249	-4.3767437945501	-2.9878735130855
C	4.4266031703489	-2.9473747236435	-0.8154143033394
H	3.0244388364209	-4.4231509630605	-0.7631399049156
C	3.5590044257177	-2.1113929716155	0.1735600466347
O	5.5417330486657	-2.6036363601970	-1.2023192721437
C	4.3831483339720	-1.2152579167335	1.1013693309478
C	5.1204018999658	-1.9656846494281	2.2130187063555
N	2.6319675580846	-2.9691720218963	0.9157317295381
C	1.3351154168453	-3.1388203709089	0.4807455624920
C	0.5740788423312	-4.3231440030275	1.0986897745776
N	-0.4851610966070	-4.7723994824489	0.1628316458647
H	-0.0900406328930	-5.1657784774143	-0.7075406816426
H	-1.0847899081303	-3.9707215775785	-0.1275896550084
O	0.8396987073475	-2.4261475991523	-0.3913211102370
H	3.0628600670833	-3.7204944200950	1.4595849512566
H	2.9776047235337	-1.4423457983765	-0.4747732075799
H	3.7138001520182	-0.4851082022399	1.5718004294091
H	5.0954465321603	-0.6481396631019	0.4924752003777
H	5.6318972000909	-2.8255104387797	1.7794588143902
C	6.1081736306556	-1.0704988109212	2.9646989334876
N	7.1223718961700	-0.4727538728660	2.0914714428415
C	7.9694289995859	-1.1548614182722	1.3134629242401
H	7.2170446793590	0.5475655736226	2.0837651144283
H	4.3967519034689	-2.3595763741141	2.9356987278832
H	5.5672370237420	-0.2458323832841	3.4422199668994
H	6.6185340623098	-1.6229200581825	3.7607020476547
N	8.6450076865119	-0.5399678722649	0.3513026378979
N	8.1480674566521	-2.4597761305862	1.4527709755375
H	9.0880475468587	-1.1154484864657	-0.3602849684461
H	7.6828460229905	-3.0437810410387	2.1416893328888
H	8.7807097522571	-2.9835758505277	0.8420075780221
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C	6.8267021311895	-7.8107384479613	-2.1681326136292
C	7.4176427337994	-7.8103503974105	-0.7383176551302
C	7.9430732101603	-8.0786470354133	-3.1926030234192
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N	8.0106382675572	-6.6280655999468	-0.3522322853150
C	8.5016969361396	-6.4263291762210	1.0137864051855
C	9.7617720834470	-5.5353853509986	0.9855807612212
C	10.3290808722851	-5.2451842771487	2.3689468113710
O	9.5270706525581	-4.2905436900693	0.3103355381472
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H	7.6433813084460	-9.1329692810687	5.8426782057935
H	5.9336604460095	-8.8019060883335	6.0459557765706
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H	6.6623070141937	-7.7991906088334	2.0490993873324
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H	9.6677681925108	-4.6040207072737	2.9587286521606
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H	9.7377585989634	-4.4342243118846	-0.6448644119251
H	7.7763609012891	-5.8018691597915	-0.8915939837256
O	7.4469123481966	-8.8238290411023	-0.0432253984719
O	4.9167488263654	-6.5043934844147	-0.5761569845224
H	6.0685145175689	-6.3450981613059	-3.4977576705983
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C	-2.4050293637785	-7.5915254120320	-0.6416886260678
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H	-1.8125424000066	-8.5050060240848	-0.7135042464281
H	-3.4605449053637	-7.8439768617094	-0.4999352387772
H	-2.2422062041328	-7.4959669203440	1.2887739021610
C	-0.0285394039286	-3.9406562839340	2.4496703151479
O	-1.3104317966425	-3.3488305617130	2.2601416230826
H	1.2656694539108	-5.1619619698287	1.2250833621624
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H	-0.1706707625773	-4.8352290312524	3.0646378221860
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H	5.0602166610112	-6.4630845984972	5.3149062204493
H	6.1991726048966	-5.3281420868117	4.6404638291794
C	4.7630176504722	-2.5817793500702	-5.4098959666874
C	6.1636441105906	-2.1816140168867	-5.9361992737618
O	4.6025144032843	-4.0047576942190	-5.4115326606643
C	4.7692327726529	-4.6183189208360	-6.6984504705478
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H	4.6889744447595	-2.2851060074034	-4.3629373444184
H	6.2800512662466	-1.0919099147852	-5.9828030345861
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H	5.6408834299638	-2.2849796555835	-8.0480745899599
H	8.2715570959489	-2.7598495572511	-7.1326870044191
O	6.1697120045779	-4.7640990508586	-8.6824772319855
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H	5.5671080310234	-7.6123763592437	-5.7250571047961
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H	6.9411775448130	-4.7610843361002	-6.7946806387264
H	6.9207912022857	-4.3050147232140	-9.1113408698083
O	1.9471530633442	1.6234905542966	-2.7913014172538
C	1.7794694605831	2.9740263236813	-2.3383573787170
O	0.6891056582581	3.0721759710914	-1.4247418368026
C	3.0840682154247	3.4880773068440	-1.7084322035800
C	3.3767099171606	2.7463601504748	-0.4034119853039
C	2.1657641331822	2.8086328135586	0.5426182925471
C	0.8806995798113	2.3775988012852	-0.1907450332412
O	2.9958707402685	4.8979396521207	-1.4515743813394
O	4.5085197841490	3.4039453900333	0.2130447096581
C	5.4481377980784	2.4802563909822	0.7535687702610
O	2.4210396324115	1.9532924041961	1.6686989619109
C	-0.3777568442676	2.6568676982532	0.6474636345772
H	1.5397364979746	3.6207618036149	-3.1915102948058
H	0.9213736247063	1.2961825620726	-0.3783211748617
H	1.5857420160014	1.9224582289855	2.1798176790381
H	2.0640104271764	3.8294729498361	0.9310511852689
H	3.7494987944634	5.1166224689967	-0.8693540166686
H	3.9211853737629	3.3439414015613	-2.4013548225953
H	3.6215525265338	1.6992206146771	-0.6285996201350
O	-0.3008200691256	2.0830199260491	1.9590023133329
H	-1.2496327386983	2.2616697994076	0.1105168778409
H	-0.5207594537942	3.7414058157799	0.7397973596544
C	-1.5519350498539	2.2406926190113	2.6419763337907
C	-1.3612086344890	2.0729741447637	4.1655963540635
O	-2.5331787190533	1.3407165599136	2.1181571943202
C	-2.2687619069643	-0.0465549499417	2.4014514856917
C	-2.1830890493045	-0.2963065071761	3.9104248433026
C	-1.1001059786650	0.6079826165414	4.5069523071684
C	-3.3996137656491	-0.8527959719331	1.7508319916558
O	-3.2817010012145	-0.7623084691357	0.3220524658453
O	-1.8439372640218	-1.6600984633167	4.2170468896188
O	-1.0917765401259	0.4111734788593	5.9303058263411
O	-2.5305727786288	2.4754319286961	4.9022406619911
H	-3.3665944419914	0.1934525793400	0.1292886578270
H	-3.3692438549177	-1.9105916953419	2.0162259711795
H	-4.3823247336933	-0.4545162974320	2.0252800631612
H	-1.3278111982040	-0.3284092559994	1.9103555275259
H	-1.6525627772239	-1.6409919388088	5.1823754387239
H	-3.1486564018208	-0.0929650694088	4.3897017035151
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H	-0.1138581194664	0.2957245011567	4.1433500568944
H	-0.5276725526648	2.6859351283990	4.5266247718302
H	-2.6963074555761	3.4187222918958	4.7169284409143
H	-1.9348641587264	3.2542391357022	2.4685035252900
C	6.3306864600306	3.1588690396132	1.8119050571241
O	6.2626166809608	1.9180005530618	-0.2873303284605
C	7.0564662238698	2.9050505019965	-0.9757181578021
C	8.0000218150903	3.6402844399382	-0.0076417751140
C	7.2044208923641	4.2286567725154	1.1620648124457
C	7.8364163671008	2.1890404675781	-2.0880531548255
O	8.6925634033341	4.7122355512387	-0.6549757897857
O	8.1242359069323	4.7177886348072	2.1536893789538
O	7.1949380577824	2.1824405737676	2.4464258036581
H	8.6758523191057	5.3810547576882	1.6901049512582
H	6.5988327087281	5.0803946859078	0.8302859120828
H	5.7166392752086	3.6067524504656	2.6013566903647
H	7.8056077850548	2.7455055258865	2.9784253900947
H	8.7595003048982	2.9620526116838	0.4010661563765
H	9.4770692214390	4.3305174176758	-1.0905302575778
O	8.8354337994004	1.3336659504435	-1.5256239979687
H	8.3333786056398	2.9128096519390	-2.7416312905473
H	7.1650664814445	1.5648237472385	-2.6865327399508
H	9.3563974975569	0.9989343090854	-2.2947127520422
H	6.3847618832797	3.6201083752546	-1.4672040783025

H	4.9325267663749	1.6469683276182	1.2390847988377
C	7.4707199586831	-2.0303896225981	-3.9199121487770
H	6.5360378353728	-1.6441353919445	-3.5036066501927
O	8.2996361873668	-0.8872081930678	-4.1530295438499
C	9.6373274345620	-1.2072455993341	-4.5711364570833
C	8.1019260823786	-2.9914169623591	-2.8873446757990
C	10.3523501501091	-2.0994054311276	-3.5399780610505
C	9.5182758930860	-3.3653345782387	-3.3168122613969
O	11.6470069821206	-2.5143234708776	-3.9893692359880
H	10.4852528739902	-1.5852343252829	-2.5803371264617
H	12.2624675978992	-1.7737159397563	-3.8315230598218
C	10.3838715721222	0.1126799528509	-4.8139399041604
O	10.5748988515419	0.8303006968359	-3.5896331216321
H	9.5880415720610	-1.7223991051660	-5.5384999587592
H	9.8043949875192	0.7575077854063	-5.4827325142514
H	11.3662901653219	-0.0723861486524	-5.2595455626019
H	11.1219263869904	1.6067910276928	-3.8214689311849
O	8.1375312268029	-2.3770630823021	-1.5863187090524
O	10.1507659885794	-4.2070921822352	-2.3294749514247
H	7.1883102325928	-2.3229112213922	-1.3191894238662
H	7.5095884819379	-3.9080931871504	-2.7943079303947
H	11.0836778534004	-4.2594464671275	-2.6332887826557
H	9.4880397426179	-3.9585040768279	-4.2394551581489
H	8.4851966866127	0.4258833515317	0.0730544862700
H	-1.1217885240970	-5.4902209373732	0.5426232873445

S5.10. Triply charged SRNLTK + GlcNAc₂Man₆

C	1.1552684893317	-6.9805073959209	-4.0586085310145
O	2.5585271415092	-7.2266006600724	-3.8996184417679
C	0.2513450021147	-7.9646890872621	-3.2720125342002
C	0.8258197356413	-5.5007635602134	-3.8160838717541
H	0.9469439032075	-5.2142316934461	-2.7674962466918
H	1.5275867489513	-4.8895484354109	-4.3967723684694
H	0.9623896831261	-7.1638053680171	-5.1240430228179
C	0.7261171065529	-8.1672653807088	-1.8259985543612
C	2.2218935800694	-8.5206166902814	-1.8500925428160
C	3.0070262103754	-7.4028583910849	-2.5599471607759
O	0.2746554752847	-9.2551547029197	-3.8980440172090
O	0.54458693365947	-6.9697645116815	-1.0515123323780
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H	-6.3008069509007	-4.2950425325033	0.8575657275997
H	-4.7322895983170	-6.0506156074296	0.9491611489478
H	-6.1303266967202	-5.6191989409345	3.2027203742307
H	-3.9951929208845	-5.2460436747662	3.1693459555188
H	-3.0984705578266	-2.0702318370532	-2.1456644497124
H	4.0390303704257	-5.5705604689616	1.1981591525708
H	11.3423595012022	3.3673626908173	3.6798745257572