

Electronic Supplementary Information (ESI) for New Journal of Chemistry

**EVALUATION AND SYNTHESIS OF AZT PRODRUGS WITH OPTIMIZED
CHEMICAL STABILITIES. EXPERIMENTAL AND THEORETICAL ANALYSES**

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ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

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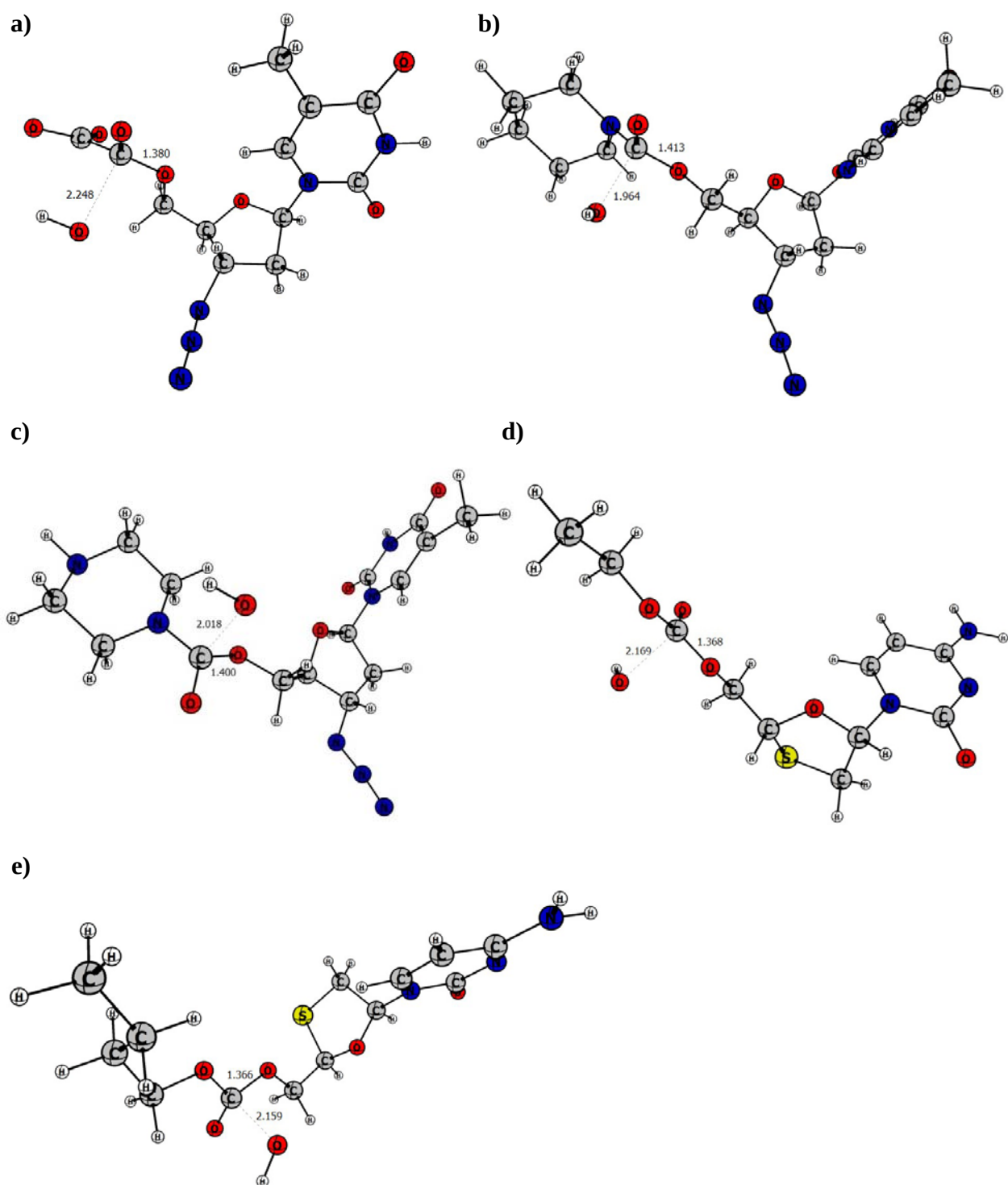


Figure S1. TS1 geometries for the hydrolysis simulation of a) ester **1**, b) carbamate **2**, c) carbamate **3**, d) carbonate **4** and e) carbonate **5** prodrugs, under polarized continuum model.

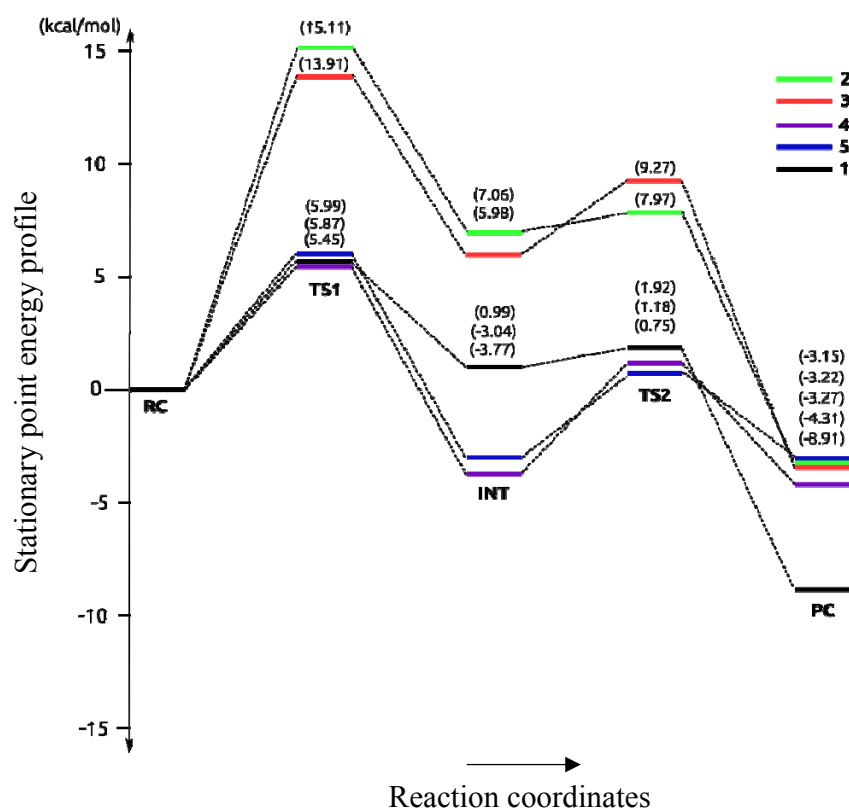


Figure S2. Reaction coordinates energy profile (kcal/mol) for the stationary points corresponding to the simulated hydrolysis of **1-5** under the polarized continuum model (PCM).

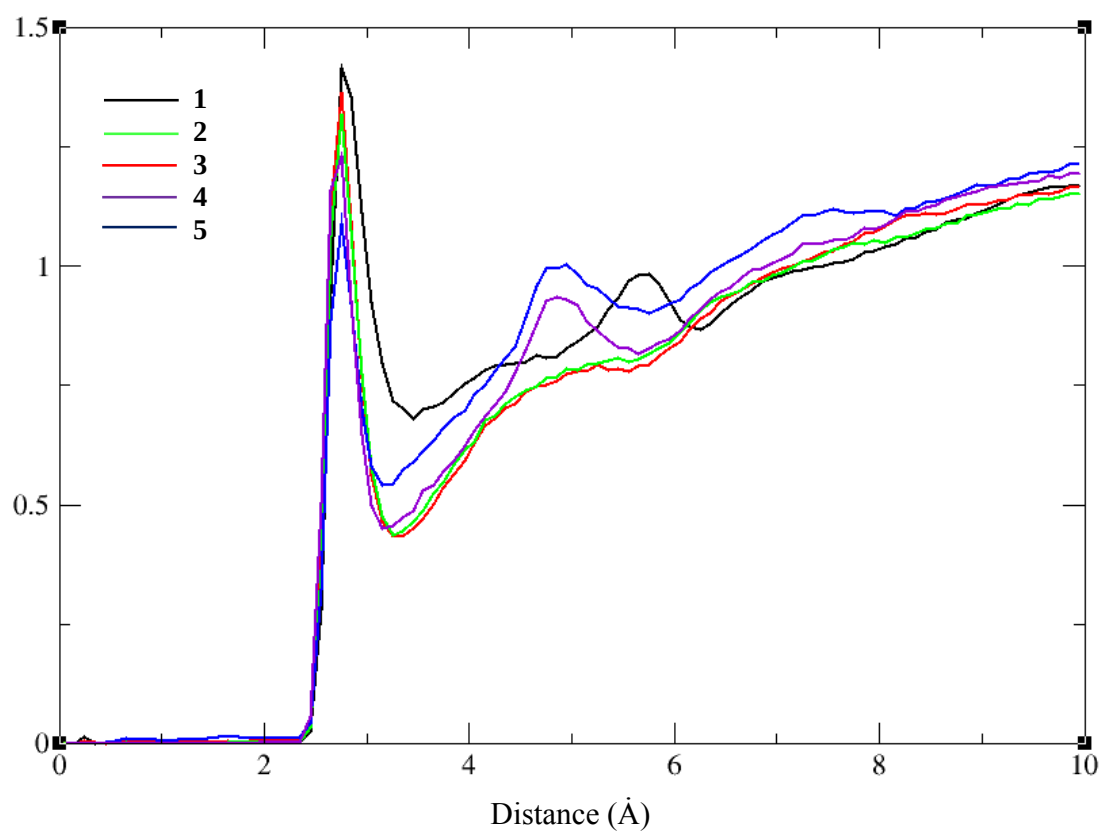


Figure S3. Radial distribution functions of water molecules around the carbonyl oxygen of prodrugs **1-5**.

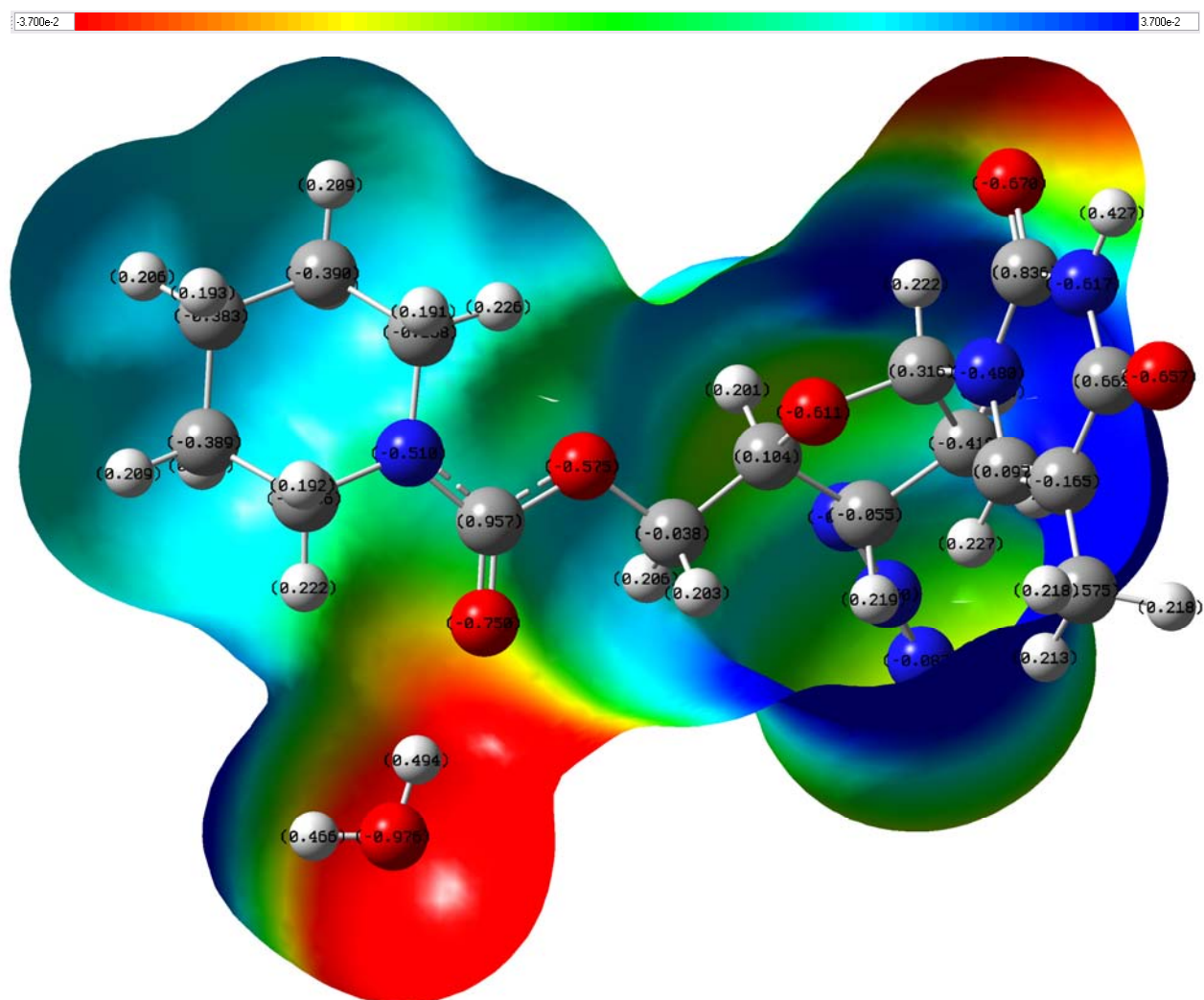


Figure S4. Atomic NBO charges and electrostatic potential calculated for the initial minimum energy conformation of prodrug 2.

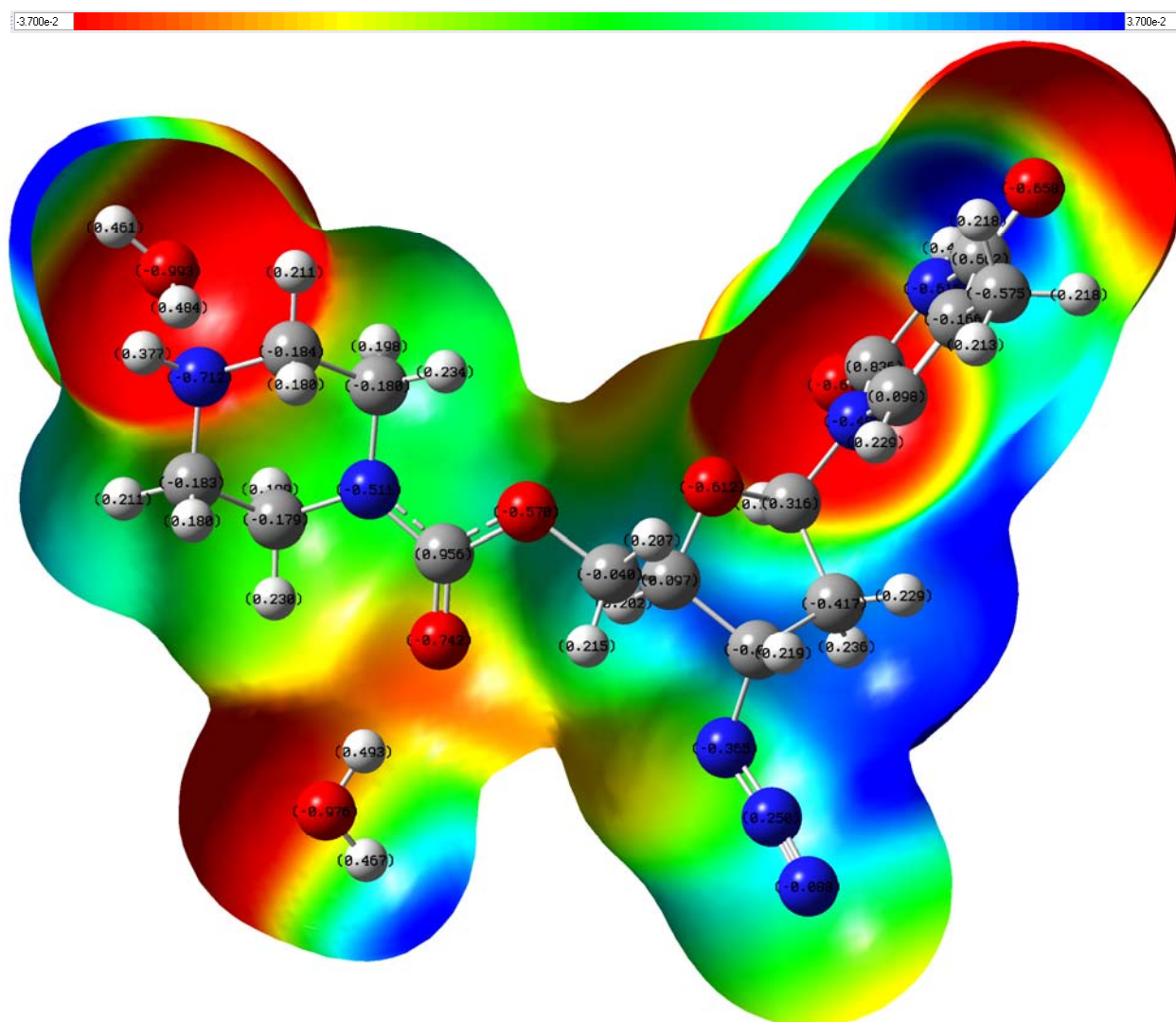


Figure S5. Atomic NBO charges and electrostatic potential calculated for the initial minimum energy conformation of prodrug 3.

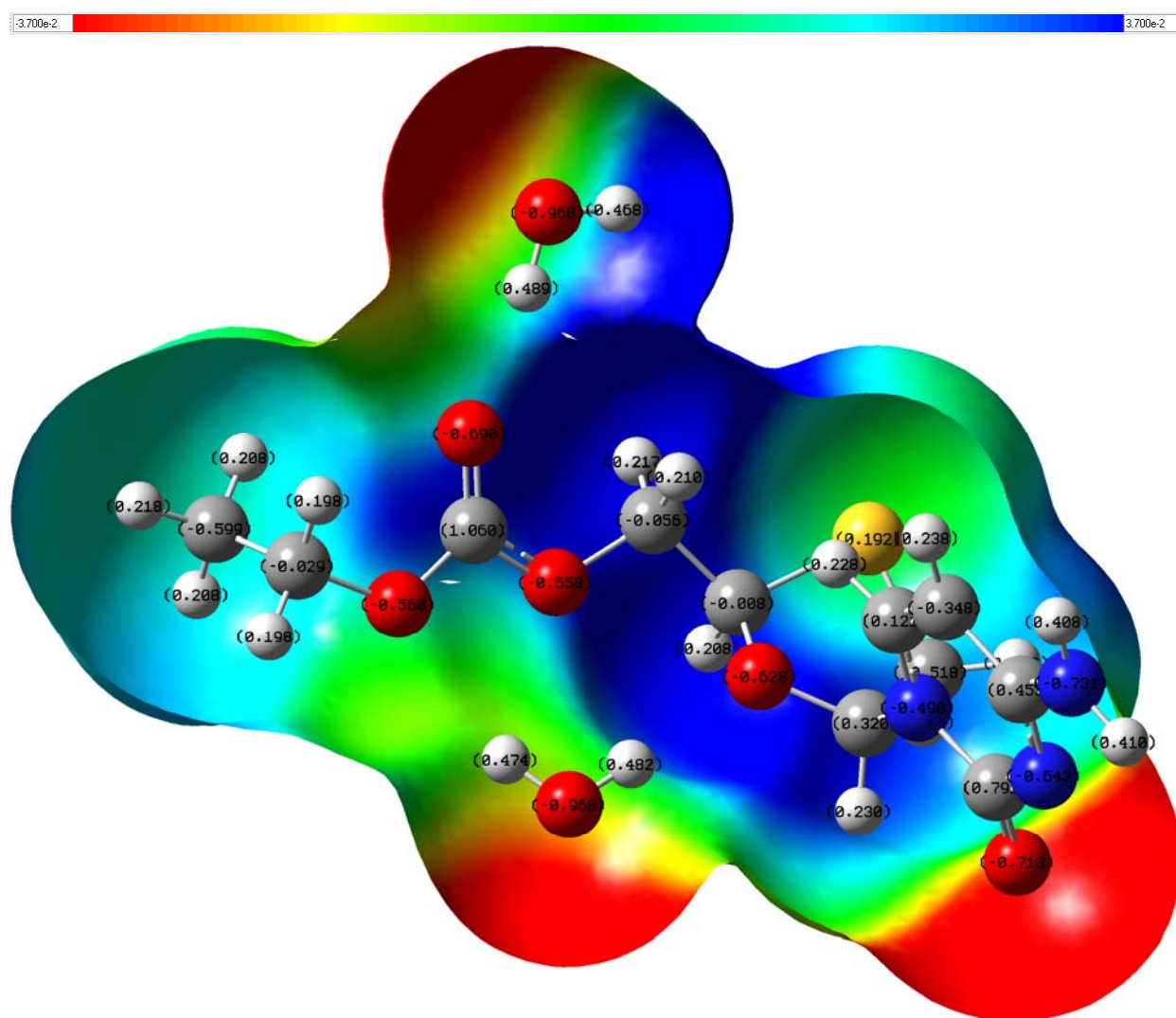


Figure S6. Atomic NBO charges and electrostatic potential calculated for the initial minimum energy conformation of prodrug **4**.

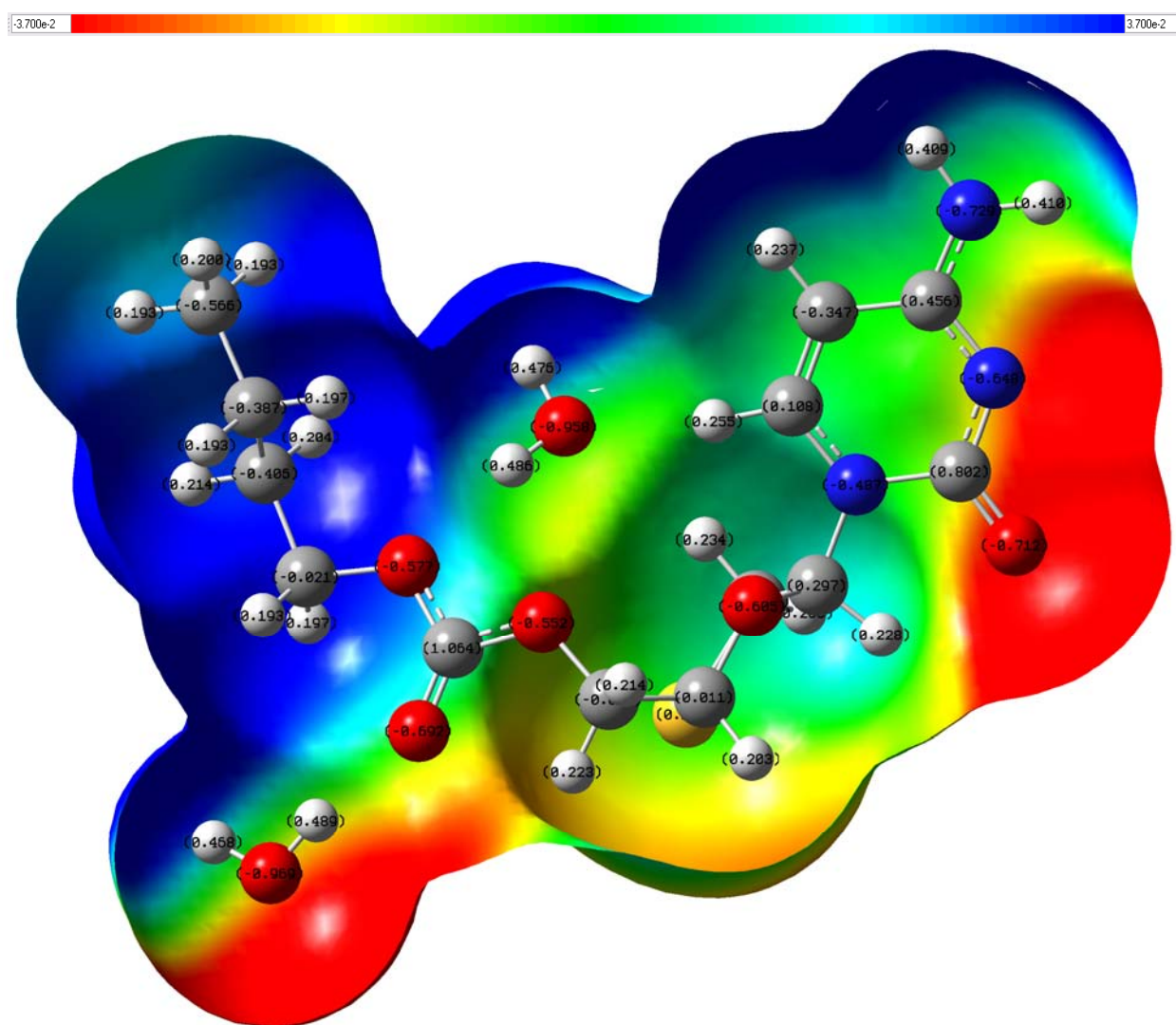


Figure S7. Atomic NBO charges and electrostatic potential calculated for the initial minimum energy conformation of prodrug 5.

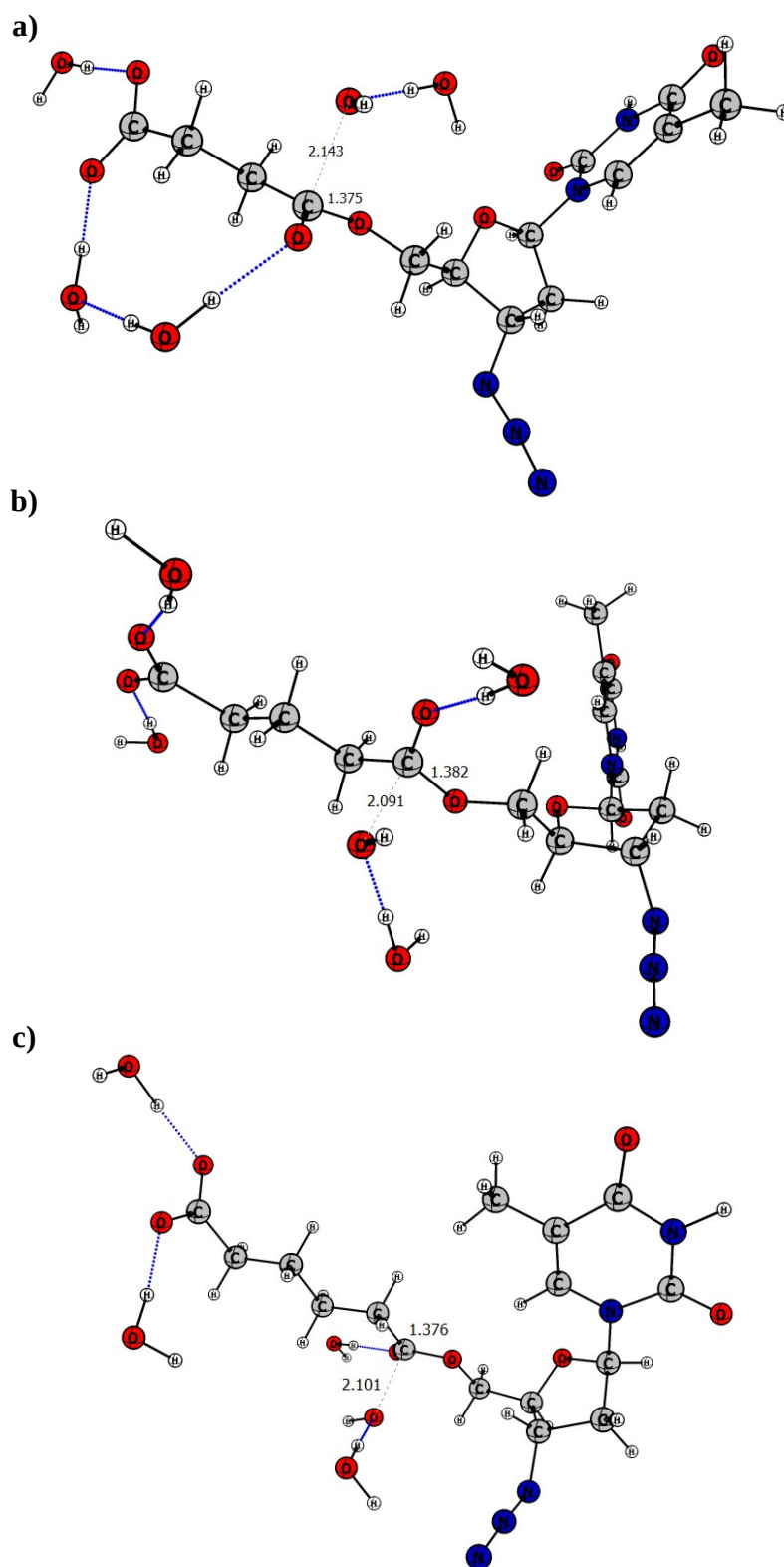


Figure S8. TS1 geometries during the hydrolysis simulation of ester prodrugs: a) **6**, b) **7** and c) **8**, calculated considering an EWM model. S10

Chemical stability experimental data

Stability at pH 7.4

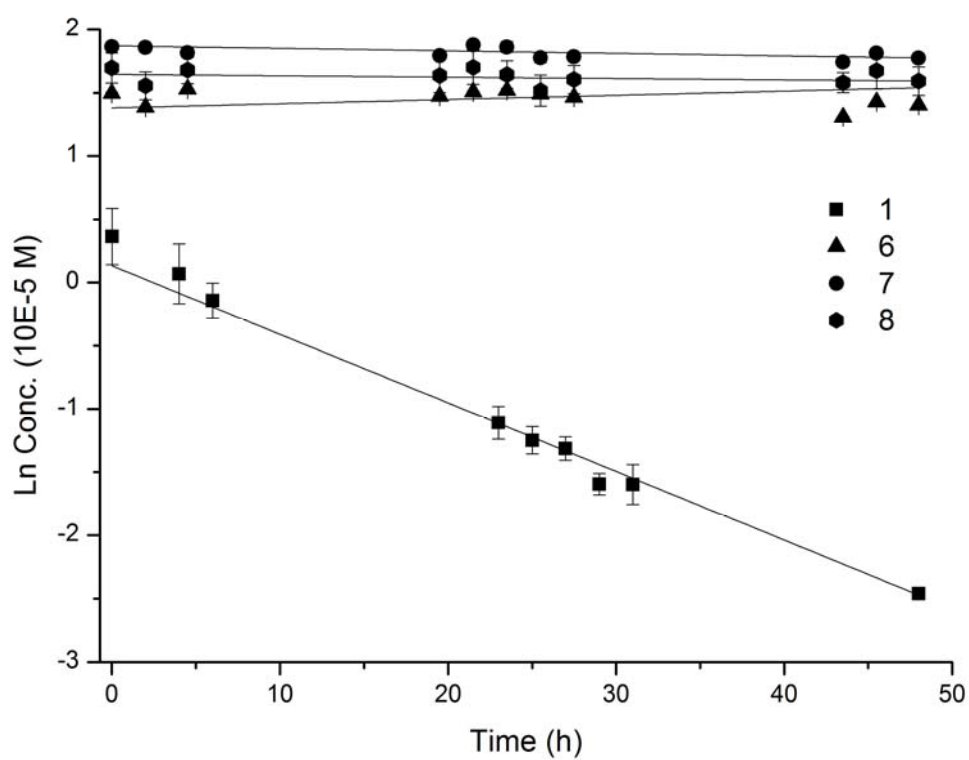


Figure S9. Ln concentration vs. time profiles for hydrolysis studied at pH 7.4 for prodrugs **1**, **6-8**.

Table S1. Table of parameters for the analysis of the Ln concentration vs. time profile obtained at pH 7.4.

Prodrug		Value	Standard error
1	Intercept	0.13193	0.07129
	Slope	-0.05427	0.00169
6	Intercept	1.38169	0.00523
	Slope	0.0033	7.3916E-4
7	Intercept	1.87067	0.02207
	Slope	-0.00199	4.8009E-4
8	Intercept	1.64534	0.0311
	Slope	-0.00108	0.00104

Stability at pH 10.0

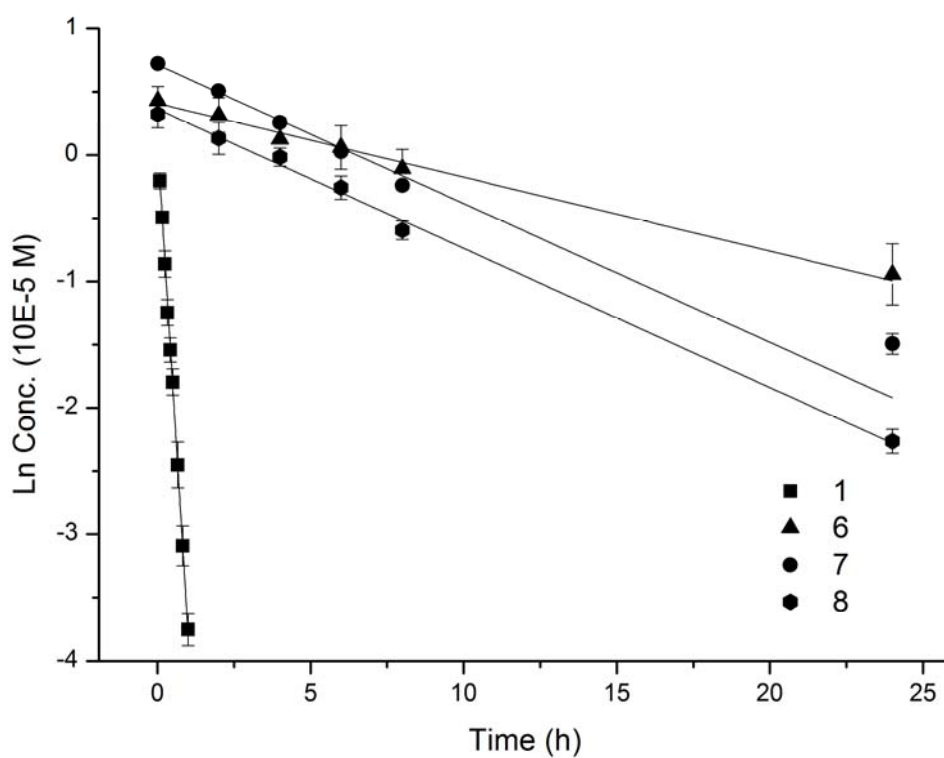


Figure S10. Ln concentration vs. time profiles for hydrolysis studied at pH 10.0 for prodrugs **1**, **6-8**.

Table S2. Table of parameters form the analysis of the Ln concentration vs. time profile obtained at pH 10.0.

Prodrug		Value	Standard error
1	Intercept	0.13545	0,01801
	Slope	-3,90596	0,05144
6	Intercept	0,40941	0,02128
	Slope	-0,0585	0,00286
7	Intercept	0,71403	0,02449
	Slope	-0,1098	0,00665
8	Intercept	0,36376	0,03866
	Slope	-0,11019	0,0037

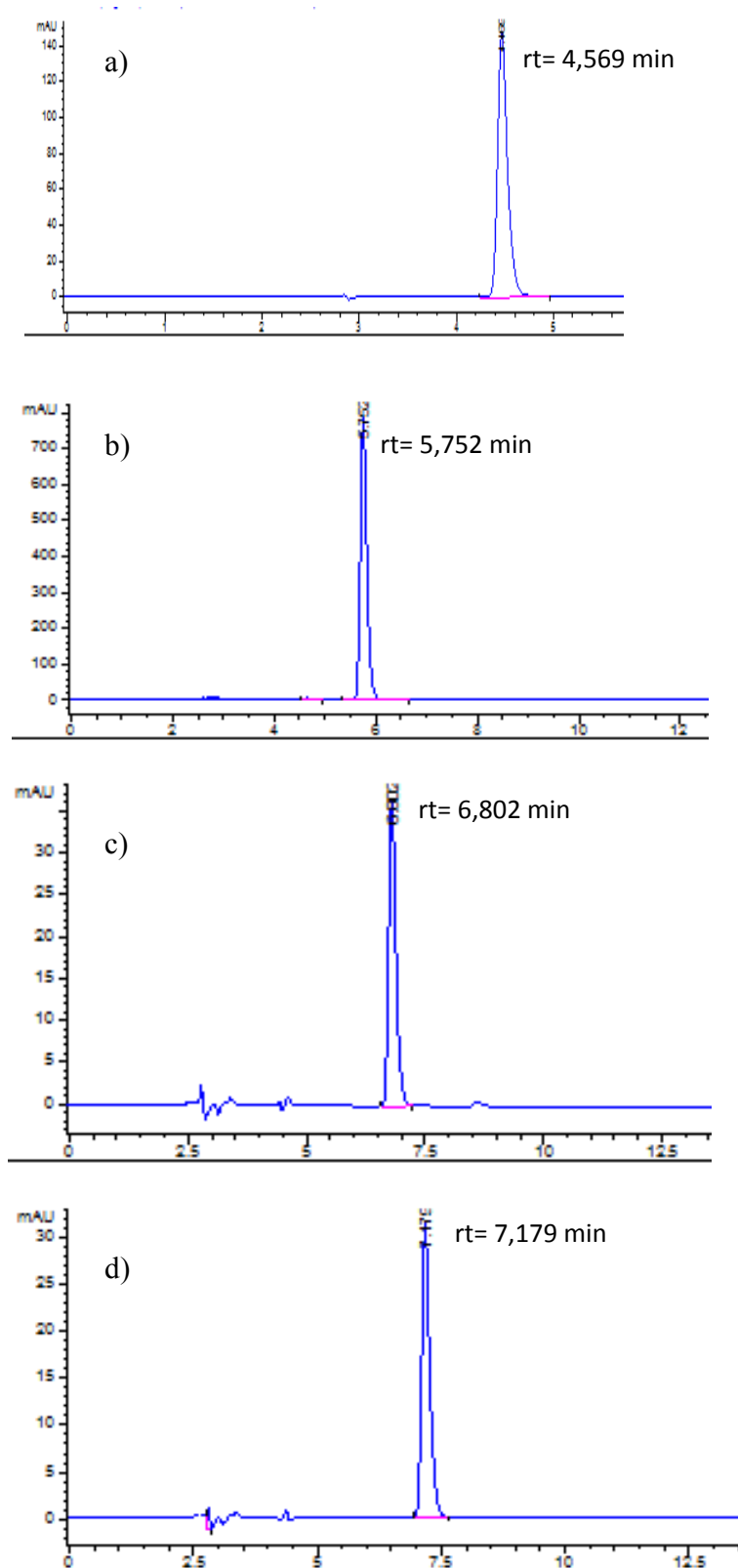


Figure S11. Chromatograms obtained by means of HPLC analyses for: a) AZT, b) **6**, c) **7** and d) **8** after purification stages were applied.

Cartesian coordinates of all stationary point optimized geometries

				O	-1.3407920	-0.9170600	0.3588490
Prodrug 1 (PCM)				C	-1.8718160	0.1261180	1.1831470
RC				H	-1.9166190	-0.2039340	2.2210220
C	-2.6149850	-2.7418690	1.3915280	H	-2.8776660	0.3599870	0.8307240
O	-3.8343570	-2.9221130	1.1929970	C	-0.9850310	1.3463460	1.0617360
C	-1.8009760	-2.2977960	0.1539980	H	-1.4281560	2.1453590	1.6691800
O	-1.3398340	-3.0920380	-0.6417910	O	0.3368220	1.0572870	1.5807120
O	-1.5682770	-0.9830420	-0.0437770	C	-0.7329200	1.8848450	-0.3531240
C	-2.1483270	0.0256860	0.8287760	H	-0.6696160	1.0556600	-1.0603660
H	-2.2216420	-0.3670000	1.8441200	N	-1.8323060	2.7959500	-0.7361730
H	-3.1520700	0.2864190	0.4656920	N	-2.1103520	2.8550150	-1.9298220
C	-1.2379760	1.2330820	0.8338880	N	-2.4622000	2.9952870	-2.9993970
H	-1.7337880	2.0158310	1.4208210	C	0.6181120	2.5979570	-0.1983570
O	0.0156620	0.8938840	1.4660100	H	1.1859770	2.6667710	-1.1254500
C	-0.8326080	1.8216050	-0.5298310	H	0.4533650	3.6096420	0.1792160
H	-0.6865850	1.0215790	-1.2575430	C	1.3337350	1.7661920	0.8779950
N	-1.8540500	2.7732550	-1.0100260	H	1.9011880	2.3902680	1.5646720
N	-2.2453070	2.6367700	-2.1646590	N	2.3213490	0.7924960	0.3250520
N	-2.6849530	2.6162340	-3.2102770	C	1.9587770	-0.4943140	-0.0146120
C	0.4915090	2.5219490	-0.1950110	H	0.9174730	-0.7320380	0.1636430
H	1.1629230	2.6093720	-1.0482400	C	2.8209310	-1.4099230	-0.5193440
H	0.2823540	3.5258290	0.1801190	C	2.4050980	-2.8075690	-0.8781040
C	1.0793610	1.6660800	0.9403470	H	2.9521840	-3.5479700	-0.2868420
H	1.5187720	2.2787120	1.7236210	H	2.6143220	-3.0239810	-1.9297580
N	2.1654090	0.7472060	0.5064650	H	1.3376390	-2.9528270	-0.7071020
C	1.8863540	-0.4926470	-0.0311230	C	4.2060620	-1.0184200	-0.7105530
H	0.8340960	-0.7397520	-0.0663590	O	5.1026370	-1.7351720	-1.1500660
C	2.8319740	-1.3598660	-0.4631480	N	4.4881290	0.3025520	-0.3469670
C	2.5016140	-2.7072900	-1.0370610	H	5.4423370	0.6161700	-0.4776220
H	2.9708830	-3.5079620	-0.4579460	C	3.6164210	1.2494650	0.1515130
H	2.8695900	-2.8002870	-2.0631710	O	3.9693680	2.3936810	0.4116820
H	1.4238330	-2.8758960	-1.0427550	O	-2.9459450	-2.3830140	2.1401880
C	4.2258490	-0.9639230	-0.3516140	O	-3.7720330	-0.6290350	-0.8617870
O	5.1936730	-1.6383290	-0.6938670	H	-4.3451720	-1.3887880	-1.0250640
N	4.4234010	0.3052990	0.2020180	INT			
H	5.3827540	0.6194160	0.2853170	C	-2.5962770	-2.6820760	1.2749130
C	3.4675610	1.2056600	0.6276510	O	-3.7337110	-3.1706990	1.5115760
O	3.7585350	2.3107310	1.0676360	C	-2.3615580	-1.9835390	-0.1281660
O	-1.9398620	-2.8995840	2.4328690	O	-1.7875300	-2.7493650	-1.0019900
O	-5.0748860	0.8499800	-0.0214090	O	-1.5001560	-0.7560420	0.0754830
H	-5.9991710	0.5817850	-0.1234250	C	-1.9971320	0.2257580	0.9540300
TS1				H	-2.0796410	-0.1604760	1.9792120
C	-3.1561620	-2.5979350	0.9202660	H	-2.9948410	0.5640450	0.6457890
O	-4.0327520	-3.3379400	0.4149320	C	-1.0795560	1.4339110	0.9678860
C	-2.1360830	-1.9564400	-0.0777560	H	-1.5394170	2.2157280	1.5848990
O	-1.6901110	-2.6045890	-1.0164690	O	0.1992700	1.0883710	1.5565460

C	-0.7253810	2.0263940	-0.4031870	C	1.8701640	-0.4604410	0.0876900
H	-0.6518310	1.2248230	-1.1403230	H	0.8186050	-0.6578810	0.2896520
N	-1.7707940	2.9913180	-0.8081650	C	2.7039210	-1.4285060	-0.3696500
N	-1.9809480	3.1042660	-2.0116560	C	2.2532290	-2.8401220	-0.6162230
N	-2.2685400	3.2952080	-3.0928080	H	2.8344950	-3.5497960	-0.0199860
C	0.6387240	2.6788730	-0.1423230	H	2.3859150	-3.1239780	-1.6646060
H	1.2588590	2.7722690	-1.0331970	H	1.2003850	-2.9633010	-0.3606630
H	0.4912230	3.6751720	0.2808570	C	4.0906560	-1.0858370	-0.6214680
C	1.2615310	1.7644470	0.9239170	O	4.9610500	-1.8525160	-1.0318410
H	1.8348780	2.3258990	1.6580470	N	4.4122230	0.2499250	-0.3594290
N	2.2158610	0.7589890	0.3677710	H	5.3698250	0.5302030	-0.5331690
C	1.7917230	-0.4852530	-0.0540530	C	3.5749550	1.2473970	0.0974320
H	0.7271100	-0.6652190	0.0582630	O	3.9636510	2.3966640	0.2775610
C	2.6250750	-1.4285050	-0.5588910	O	-2.1143310	-3.8738240	0.8698160
C	2.1494320	-2.7807530	-1.0075810	O	-3.6239930	-1.0713260	-0.7437470
H	2.6199430	-3.5781460	-0.4239600	H	-3.4543320	-0.7168950	-1.6287330
H	2.4093600	-2.9614270	-2.0549650				
H	1.0674020	-2.8707930	-0.9033870	PC			
C	4.0397190	-1.1170930	-0.6566750	C	-5.6123850	-3.6472400	-3.6369070
O	4.9150590	-1.8675420	-1.0842060	O	-5.7612740	-4.5230750	-2.7572370
N	4.3821640	0.1640380	-0.2121740	C	-4.4863060	-2.6306570	-3.3632140
H	5.3600230	0.4205810	-0.2736710	O	-3.3274230	-2.7749880	-3.7000080
C	3.5437040	1.1393530	0.2877280	O	-0.3158450	-0.1680390	2.4768890
O	3.9529310	2.2444390	0.6258920	C	-0.8941580	1.0657190	2.5389200
O	-1.5885700	-2.7770970	2.0265240	H	-0.7451850	1.5845640	3.5162350
O	-3.6431010	-1.4506780	-0.5918590	H	-2.0049340	1.0578820	2.4023030
H	-3.5088140	-1.3630760	-1.5463030	C	-0.3942470	2.0622310	1.4764220
				H	-0.9277480	3.0176790	1.5687770
TS2				O	1.0248030	2.3315490	1.6725100
C	-2.8487470	-2.8603190	0.7424460	C	-0.4936880	1.5599890	0.0307170
O	-3.7844190	-2.5186530	1.5103680	H	-0.4196030	0.4703270	0.0263220
C	-2.5652620	-1.9635130	-0.5109860	N	-1.7939650	1.9747290	-0.5516330
O	-1.9599460	-2.3920240	-1.5133490	N	-2.3029560	1.2321380	-1.3749260
O	-1.3279740	-0.8478020	0.3454600	N	-2.8720950	0.6278490	-2.1521800
C	-1.8128530	0.1530210	1.1708140	C	0.7068100	2.2151420	-0.6632740
H	-1.8409900	-0.1421980	2.2374040	H	1.0718780	1.6646650	-1.5301810
H	-2.8452450	0.4343470	0.9025710	H	0.4379420	3.2246320	-0.9839250
C	-0.9888900	1.4379610	1.0889710	C	1.7419370	2.3086000	0.4659680
H	-1.4710590	2.2222040	1.6865370	H	2.3575400	3.2013910	0.3849130
O	0.3415660	1.2216740	1.6384660	N	2.7137020	1.1691720	0.4755750
C	-0.7375370	1.9617610	-0.3306540	C	2.4328820	-0.0062300	1.1434260
H	-0.6814380	1.1130870	-1.0148990	H	1.4607860	-0.0354310	1.6558560
N	-1.8312550	2.8738850	-0.7371340	C	3.2908510	-1.0584290	1.1832100
N	-2.2637610	2.7490840	-1.8771450	C	2.9743480	-2.3311050	1.9174330
N	-2.7475970	2.7299220	-2.9044770	H	3.7144420	-2.5355030	2.6972270
C	0.6127490	2.6771860	-0.2051700	H	2.9799440	-3.1925720	1.2426840
H	1.1720430	2.7294790	-1.1389170	H	1.9917450	-2.2715170	2.3868000
H	0.4547910	3.6956630	0.1578850	C	4.5623660	-0.9463420	0.4977610
C	1.3338010	1.8635850	0.8786300	O	5.4391870	-1.8094870	0.4490740
H	1.9467880	2.4915760	1.5217890	N	4.7601570	0.2758910	-0.1538330
N	2.2750110	0.8364060	0.3285470	H	5.6330390	0.3884400	-0.6548150

C	3.8952010	1.3492430	-0.2203010	H	20.1215300	20.6874030	10.1448460
O	4.1672610	2.3674810	-0.8490600	C	19.6900050	18.0950630	9.0533880
O	-6.2212300	-3.4852260	-4.7168730	O	19.5751390	18.7555460	8.0265410
O	-4.9241520	-1.5437140	-2.7011000	N	19.9252380	16.7190210	8.9753100
H	-4.1834350	-0.9236550	-2.5497630	H	19.9861980	16.3232650	8.0448710
Prodrug 2 (PCM)				C	20.0787350	15.8170850	10.0090320
				O	20.2728560	14.6272320	9.8111630
				O	17.3405600	15.0862260	19.6056640
				H	16.9245560	15.4866410	18.8289610
RC							
C	13.4452030	14.9661620	16.2515900				
H	12.7835220	15.3074640	15.4435650	TS1			
H	13.5684340	15.7912880	16.9486930	C	13.3143820	14.8783450	15.7795710
C	12.8401070	13.7387010	16.9373090	H	12.6770350	14.6966130	14.9004570
H	13.4353280	13.4953950	17.8252200	H	13.2935570	15.9477890	15.9802020
H	11.8331540	13.9893370	17.2859340	C	12.7493250	14.0779950	16.9621040
C	12.8023680	12.5339580	15.9897910	H	13.2750840	14.3614980	17.8797590
H	12.0951710	12.7341200	15.1741390	H	11.6936120	14.3403890	17.1009750
H	12.4309690	11.6480560	16.5140180	C	12.9027860	12.5712650	16.7179160
C	14.1922070	12.2621540	15.4026720	H	12.2561460	12.2741450	15.8798010
H	14.8712520	11.9253430	16.1947170	H	12.5595330	12.0018380	17.5888330
H	14.1480700	11.4612970	14.6576470	C	14.3598920	12.2245030	16.3873420
C	14.7775860	13.5147840	14.7432740	H	14.9906930	12.4092040	17.2603640
H	14.1835640	13.7831820	13.8589460	H	14.4514160	11.1636730	16.1235760
H	15.7979190	13.3428280	14.4145270	C	14.8844380	13.0775000	15.2223840
N	14.7579230	14.6511180	15.6758220	H	14.3566510	12.7855480	14.3011750
C	15.8071810	15.4742430	15.9082290	H	15.9435090	12.8969610	15.0552300
O	15.7893120	16.4601230	16.6370750	N	14.6807800	14.5111170	15.4236850
O	16.9285830	15.0879150	15.2383640	C	15.7304440	15.3618640	15.7908300
C	18.0956710	15.8997920	15.4453860	O	15.5262900	16.5560640	16.0882520
H	18.4015870	15.8448650	16.4927670	O	16.8533760	15.0225940	15.0033610
H	17.8750210	16.9389810	15.1949660	C	18.0246480	15.7702420	15.2763430
C	19.1965660	15.3623420	14.5619680	H	18.3142970	15.6226660	16.3211180
H	19.3008980	14.2795450	14.7077960	H	17.8540050	16.8384510	15.1074670
O	18.9022470	15.6413050	13.1911340	C	19.1350730	15.2823650	14.3743160
C	20.5633460	16.0305250	14.8009140	H	19.2091190	14.1881720	14.4254430
H	20.4241820	17.0815680	15.0697400	O	18.8881340	15.6812790	13.0181530
N	21.2594050	15.3241800	15.8960660	C	20.5133060	15.8892640	14.6924460
N	22.0866880	15.9719340	16.5321760	H	20.3930900	16.9195580	15.0392340
N	22.8674970	16.4608340	17.1932980	N	21.1687790	15.0858200	15.7474510
C	21.2604020	15.9052540	13.4276040	N	21.9905840	15.6655150	16.4513680
H	21.7688150	16.8258450	13.1428490	N	22.7626640	16.0878240	17.1674130
H	22.0036880	15.1080040	13.4496740	C	21.2446190	15.8490060	13.3329670
C	20.1191810	15.5365280	12.4487530	H	21.7888110	16.7717220	13.1328240
H	20.2382050	14.5242320	12.0682410	H	21.9627270	15.0287470	13.3105470
N	19.9996720	16.3943200	11.2724350	C	20.1186330	15.5944530	12.3016710
C	19.7573800	17.7469370	11.4317660	H	20.2185480	14.6124660	11.8434660
H	19.6852300	18.0710150	12.4616290	N	20.0622570	16.5472260	11.1931520
C	19.6015180	18.6166900	10.4104190	C	19.8610810	17.8901100	11.4540080
C	19.3389710	20.0806560	10.6089130	H	19.7613320	18.1323910	12.5037090
H	19.2972150	20.3308270	11.6700150	C	19.7732870	18.8455030	10.5031080
H	18.3914780	20.3766420	10.1500030	C	19.5546940	20.2971850	10.8141490

H	19.4798640	20.4597150	11.8904120	C	19.1341690	18.7454020	10.6778280
H	18.6369290	20.6662440	10.3478650	C	18.9970350	20.1990720	11.0242810
H	20.3756170	20.9103420	10.4318810	H	19.1781380	20.3664710	12.0870450
C	19.8929140	18.4325940	9.1118740	H	17.9958630	20.5687830	10.7854940
O	19.8403310	19.1779510	8.1391540	H	19.7059430	20.8081350	10.4564600
N	20.0799290	17.0591650	8.9293020	C	18.9334950	18.3271890	9.2978290
H	20.1595960	16.7374030	7.9721520	O	18.6618190	19.0689590	8.3593490
C	20.1660300	16.0716270	9.8906270	N	19.0731600	16.9526400	9.0827850
O	20.3265680	14.8952890	9.6013160	H	18.9350210	16.6275700	8.1334480
O	16.3861140	14.5704510	17.4650160	C	19.3711670	15.9679020	10.0039790
H	16.3950020	15.3781130	17.9940540	O	19.4594630	14.7900510	9.6905980
				O	16.9531800	14.5794430	17.9960110
				H	16.8934210	15.2336650	18.7025200
INT							
C	14.2799210	15.1786380	15.4998020				
H	14.7361900	15.0344000	14.5018290	TS2			
H	14.2535250	16.2508500	15.6902320	C	14.3229920	15.1796180	15.2765710
C	12.8624330	14.5983230	15.4881910	H	14.8356090	14.8091980	14.3731160
H	12.3614290	14.8615830	16.4282100	H	14.3753780	16.2670190	15.2552920
H	12.2852320	15.0608460	14.6790580	C	12.8669960	14.7052030	15.2688940
C	12.8881360	13.0736460	15.3266930	H	12.3290800	15.1891000	16.0935240
H	13.2398740	12.8256010	14.3160750	H	12.3866370	15.0310380	14.3395680
H	11.8788720	12.6562270	15.4152000	C	12.7769130	13.1823000	15.4180140
C	13.8321850	12.4401560	16.3554120	H	13.1829280	12.7058760	14.5155080
H	13.4074800	12.5453200	17.3616940	H	11.7320070	12.8626880	15.4950670
H	13.9418750	11.3659370	16.1659810	C	13.5781170	12.7150070	16.6382570
C	15.2109230	13.1082930	16.3216950	H	13.0901270	13.0638620	17.5567550
H	15.6885770	12.8953270	15.3487450	H	13.6036620	11.6205770	16.6864420
H	15.8548910	12.6921850	17.0959670	C	15.0125480	13.2501470	16.5958650
N	15.0899410	14.5511120	16.5448810	H	15.5485720	12.8016000	15.7455510
C	16.3400680	15.2780980	16.8472820	H	15.5498520	12.9722720	17.5005630
O	16.2121230	16.5403680	17.0532810	N	15.0118730	14.7116180	16.4790380
O	17.2620420	14.9266930	15.7179670	C	16.1838940	15.4246950	16.8278280
C	18.4969610	15.5995870	15.7454890	O	16.2668450	16.6587420	16.6500460
H	19.0382820	15.3862450	16.6778950	O	17.4120960	14.6277400	15.6389730
H	18.3606500	16.6864440	15.6810050	C	18.6439040	15.2346590	15.7056470
C	19.3536990	15.1303970	14.5884580	H	19.2287620	14.9291640	16.6031470
H	19.3839990	14.0328760	14.5664060	H	18.5629180	16.3384370	15.7590440
O	18.8251090	15.6123960	13.3438930	C	19.5383800	14.9076830	14.5133410
C	20.7992310	15.6650820	14.6122700	H	19.5927110	13.8203160	14.3742530
H	20.8194750	16.6579270	15.0701380	O	19.0122600	15.4938120	13.3066910
N	21.6416450	14.7391080	15.4028490	C	20.9805100	15.4599790	14.6341490
N	22.6312550	15.2201150	15.9461230	H	21.0243920	16.2495520	15.3889120
N	23.5677660	15.5459990	16.4979940	N	21.8724530	14.3456290	15.0486470
C	21.1887470	15.7446860	13.1182880	N	22.9326420	14.6622380	15.5788320
H	21.6273360	16.7107140	12.8682770	N	23.9356570	14.8301840	16.0836510
H	21.9155010	14.9736620	12.8615520	C	21.3017630	16.0258310	13.2318460
C	19.8575840	15.5009320	12.3688320	H	21.3775960	17.1138270	13.2696500
H	19.8396870	14.5135610	11.9102230	H	22.2373470	15.6389550	12.8271180
N	19.5650330	16.4483920	11.2939680	C	20.0908650	15.5904770	12.3896260
C	19.4329280	17.7929830	11.5880520	H	20.2730170	14.6316900	11.9031330
H	19.5750540	18.0377730	12.6322920	N	19.7045780	16.5181900	11.3251730

C	19.2365270	17.7766280	11.6537140	H	21.7426510	15.2240740	11.2977330
H	19.1925850	17.9709220	12.7169470	N	20.6956050	16.9432390	10.8846220
C	18.8368670	18.6984530	10.7498770	C	19.7101250	17.8490190	11.2278180
C	18.3290660	20.0578780	11.1324960	H	19.2873580	17.6921400	12.2111900
H	18.3394750	20.1891220	12.2155300	C	19.2728180	18.8399580	10.4192770
H	17.3052500	20.2106100	10.7795010	C	18.1970020	19.8084990	10.8153660
H	18.9407610	20.8473380	10.6868330	H	17.8359990	19.6010170	11.8238360
C	18.9019630	18.3419060	9.3404080	H	17.3460000	19.7554000	10.1304350
O	18.5807510	19.0672160	8.4041320	H	18.5636420	20.8385260	10.7891070
N	19.3766600	17.0507880	9.0908340	C	19.8789330	18.9592410	9.1017740
H	19.4309900	16.7692570	8.1193680	O	19.5965020	19.8054090	8.2587950
C	19.7844310	16.0979210	10.0034590	N	20.8589750	18.0009420	8.8263410
O	20.1825930	14.9950860	9.6576150	H	21.2991210	18.0535850	7.9156240
O	16.6886110	14.9104380	18.0442810	C	21.3124300	16.9818130	9.6411750
H	17.3351230	15.5652830	18.3370950	O	22.1830430	16.2019890	9.2824030
				O	15.7354410	15.2901650	18.5046190
				H	16.1347820	16.0807490	18.8942180
PC				Prodrug 3 (PCM)			
C	13.1751340	15.0072730	15.9352180	RC			
H	13.5778350	14.6815610	14.9672280	C	14.8038390	11.8888110	12.3044290
H	13.0351620	16.0846370	15.8918490	H	15.1471710	11.6185050	11.3087670
C	11.8595540	14.2793960	16.2259450	H	13.9104180	12.5180480	12.2031060
H	11.4027090	14.7121050	17.1237560	C	14.4655700	10.6428050	13.1172730
H	11.1667300	14.4564840	15.3972580	H	13.6120280	10.1369720	12.6595020
C	12.0885880	12.7769470	16.4303690	H	15.3241570	9.9510430	13.0870940
H	12.4144750	12.3264280	15.4838310	N	14.1170680	11.0287310	14.4876800
H	11.1512110	12.2830500	16.7040730	H	13.8468020	10.2071720	15.0182770
C	13.1543580	12.5290430	17.5045390	C	15.2465880	11.6934130	15.1436330
H	12.7793680	12.8514700	18.4830020	H	14.9639280	11.9548960	16.1662300
H	13.3821610	11.4614360	17.5849300	H	16.1371120	11.0448790	15.1950150
C	14.4483230	13.2867520	17.1920720	C	15.6067310	12.9679020	14.3847060
H	14.9070870	12.8830270	16.2801250	H	16.4895940	13.4293860	14.8165520
H	15.1692800	13.1844370	17.9975080	H	14.7765830	13.6825980	14.4490500
N	14.1722330	14.7145070	16.9721130	N	15.8603930	12.6579880	12.9706450
C	14.8170280	15.7223620	17.5926390	C	16.8491790	13.2144390	12.2301040
O	14.6336280	16.9214160	17.4007740	O	17.0073030	13.0516800	11.0266530
O	18.0633470	13.3549740	13.7052630	O	17.6856650	13.9811390	12.9863240
C	18.9488930	14.2140490	14.2754310	C	18.7810820	14.6198780	12.3097320
H	19.3465140	13.8633450	15.2637920	H	19.1312350	13.9903570	11.4923780
H	18.5203940	15.2255650	14.4985510	H	19.5638620	14.7107750	13.0632360
C	20.2219570	14.4995660	13.4592270	C	18.4000520	15.9865850	11.7780680
H	20.6964280	13.5513590	13.1730950	H	17.5170220	15.9086140	11.1318710
O	19.9001800	15.2240200	12.2509310	O	18.1276120	16.8702730	12.8686810
C	21.2639610	15.3791890	14.1898420	C	19.5290690	16.6863810	10.9982610
H	20.8016880	15.8837360	15.0431790	H	20.4982400	16.4192090	11.4287540
N	22.3565340	14.4997550	14.6871260	N	19.4789640	16.2616510	9.5837800
N	23.0296070	14.9371530	15.6143910	N	20.5373000	16.2928170	8.9611390
N	23.7135120	15.2316260	16.4720750	N	21.4458220	16.2732490	8.2827890
C	21.7304620	16.4058320	13.1336270				
H	21.3660370	17.4034570	13.3857060				
H	22.8162420	16.4585280	13.0476420				
C	21.0764770	15.8975180	11.8383850				

C	19.2298880	18.1869230	11.2156320	N	19.6151930	9.6092880	11.8298130
H	20.1317040	18.7525130	11.4478070	C	19.6822090	13.6069540	10.8057990
H	18.7877560	18.6212250	10.3187320	H	20.7680240	13.6535340	10.8898050
C	18.2050980	18.2095780	12.3751280	H	19.4419220	13.0803630	9.8819820
H	17.2265650	18.5361540	12.0288570	C	19.0458980	15.0152810	10.8113440
N	18.5439350	19.0812500	13.4965970	H	18.2730650	15.1007460	10.0488180
C	19.7236330	18.8802310	14.1912300	N	19.9711780	16.1209450	10.5732240
H	20.3325050	18.0675200	13.8179210	C	21.0049960	16.3501190	11.4631040
C	20.1088960	19.6074530	15.2619940	H	21.0449940	15.6540710	12.2903760
C	21.3942800	19.3690780	15.9987160	C	21.8938450	17.3611960	11.3511860
H	22.0258980	20.2617580	15.9882910	C	23.0054520	17.5919220	12.3325170
H	21.9560930	18.5482140	15.5507730	H	23.9810120	17.5495410	11.8401380
H	21.2074090	19.1228910	17.0477130	H	22.9900450	16.8424330	13.1250740
C	19.2222950	20.6690130	15.7179720	H	22.9242210	18.5798530	12.7944820
O	19.4330290	21.4153180	16.6679120	C	21.7524170	18.2690250	10.2217210
N	18.0460240	20.8016400	14.9738610	O	22.4798580	19.2267990	9.9805600
H	17.4034390	21.5265850	15.2698590	N	20.6793980	17.9772170	9.3741630
C	17.6343910	20.0603520	13.8845070	H	20.5494470	18.5934480	8.5808520
O	16.5696010	20.2666260	13.3222560	C	19.7582280	16.9544170	9.4808470
O	20.0058230	12.4707600	15.3862360	O	18.8523980	16.8080520	8.6738370
H	19.2935720	12.7835490	14.8107100	O	17.9973990	15.7705220	16.2615780
				H	17.6053510	16.2224960	17.0199070

TS1

C	14.1096550	15.3971620	16.5165030	INT			
H	14.2935590	14.6183370	17.2541490	C	14.3214550	15.2394710	16.1690800
H	13.4340270	14.9825880	15.7479550	H	14.4668430	14.3469230	16.7767520
C	13.4364390	16.5977440	17.1734300	H	14.1253560	14.9145080	15.1314810
H	12.4457300	16.3097770	17.5361560	C	13.1158870	16.0260520	16.6754200
H	14.0373780	16.9102720	18.0448600	H	12.2071320	15.4270200	16.5626760
N	13.2889390	17.6806520	16.1947270	H	13.2515680	16.2311950	17.7515250
H	12.8228580	18.4720780	16.6267860	N	12.9656920	17.2631270	15.8986430
C	14.5977360	18.0964530	15.6780050	H	12.1688960	17.7899070	16.2427310
H	14.4528160	18.9037360	14.9546210	C	14.1793740	18.0845360	15.9840710
H	15.2540260	18.4761660	16.4799930	H	14.0423280	18.9802250	15.3705570
C	15.2848530	16.9159540	14.9965310	H	14.3815860	18.4137450	17.0181040
H	16.2888310	17.1975630	14.6858510	C	15.3772660	17.2862030	15.4743000
H	14.7140710	16.6370730	14.0959980	H	16.2866140	17.8789300	15.5720500
N	15.3870310	15.7947530	15.9254060	H	15.2284860	17.0684740	14.4039070
C	16.3352540	14.7773740	15.6945470	N	15.5292250	16.0583190	16.2569000
O	16.3286140	13.7352620	16.3633440	C	16.7806990	15.2958440	16.0607340
O	16.6874050	14.7438250	14.3395410	O	16.8837380	14.2219320	16.7582560
C	17.7738680	13.8861750	14.0218820	O	16.8678230	15.0852990	14.5823450
H	17.5551940	12.8596150	14.3332920	C	17.9045840	14.2187960	14.1881070
H	18.6686740	14.2293380	14.5470640	H	17.7347150	13.2042030	14.5707190
C	17.9884530	13.9078860	12.5262920	H	18.8746820	14.5619740	14.5717010
H	17.0430130	13.6981520	12.0086910	C	17.9644960	14.1547080	12.6771580
O	18.4813840	15.1868560	12.1085400	H	16.9627780	13.9627600	12.2702170
C	19.0539730	12.9060050	12.0334740	O	18.4649370	15.3904010	12.1438660
H	19.8063540	12.7470580	12.8104900	C	18.9366210	13.0935690	12.1292770
N	18.3889280	11.6206660	11.7211080	H	19.7905560	12.9906510	12.8047000
N	19.0823830	10.6102560	11.7936410	N	18.2316750	11.7966610	12.0223760

N	18.9160630	10.7846910	12.1372460	N	18.3810570	11.8353520	12.1231050
N	19.4377320	9.7813070	12.2312840	N	19.0657750	10.8444110	12.3527380
C	19.3798960	13.6726220	10.7682100	N	19.5916180	9.8578110	12.5514820
H	20.4551040	13.5798490	10.6152790	C	19.5743100	13.6498870	10.8241820
H	18.8820020	13.1517730	9.9498050	H	20.6613550	13.6033210	10.7541320
C	18.9191990	15.1499230	10.8152250	H	19.1641720	13.0477240	10.0129020
H	18.1185250	15.3347170	10.1015070	C	19.0479760	15.1022350	10.7338240
N	19.9575110	16.1368120	10.5122770	H	18.2612680	15.1900340	9.9860510
C	21.0742240	16.2232730	11.3226380	N	20.0555140	16.1033970	10.3709030
H	21.0880450	15.5164490	12.1416660	C	21.1347890	16.3162140	11.2075260
C	22.0739710	17.1149910	11.1486190	H	21.1391730	15.6968860	12.0947690
C	23.2760820	17.1875390	12.0440910	C	22.1087060	17.2245060	10.9779210
H	24.1989300	17.0293620	11.4789970	C	23.2706670	17.4374330	11.9035190
H	23.2242270	16.4334410	12.8307810	H	24.2203920	17.2538190	11.3932320
H	23.3565410	18.1701780	12.5173190	H	23.2122830	16.7709950	12.7653300
C	21.9646960	18.0499440	10.0381100	H	23.2997590	18.4675170	12.2697370
O	22.7871500	18.9126060	9.7476550	C	22.0118290	18.0334100	9.7714650
N	20.8026690	17.9081940	9.2736540	O	22.8144220	18.8932290	9.4216890
H	20.6934140	18.5466300	8.4949340	N	20.8886760	17.7659980	8.9834600
C	19.7720450	17.0043350	9.4421890	H	20.7887410	18.3147900	8.1380210
O	18.7995560	16.9823150	8.7023120	C	19.8842820	16.8448000	9.2088840
O	17.8829860	16.2464060	16.3138660	O	18.9450720	16.7070680	8.4386040
H	18.2524240	15.9342110	17.1486870	O	17.5460840	15.8061490	16.8937860
				H	18.2487210	15.1535810	17.0078370
TS2							
C	14.0769280	15.2639500	15.9179220	PC			
H	14.0455900	14.2418640	16.2926290	C	12.1890640	14.2956990	15.5098010
H	14.0531680	15.2219820	14.8179190	H	12.2225990	13.6114830	16.3543080
C	12.8680410	16.0465150	16.4223110	H	12.9744390	14.0081470	14.7999060
H	11.9518360	15.6065710	16.0181940	C	10.8283090	14.2453810	14.8216490
H	12.8236160	15.9649260	17.5221260	H	10.6867930	13.2568540	14.3783320
N	12.9593150	17.4429440	15.9808600	H	10.0386070	14.3927920	15.5775920
H	12.1512090	17.9608970	16.3112100	N	10.7750330	15.2583600	13.7635630
C	14.1887090	18.0681720	16.4820960	H	9.8903890	15.1958650	13.2707700
H	14.2331410	19.0999670	16.1218390	C	10.9412260	16.6041950	14.3190380
H	14.2155830	18.0955130	17.5852390	H	10.8823830	17.3355280	13.5093910
C	15.4037550	17.2967890	15.9733010	H	10.1560280	16.8498990	15.0538100
H	16.3150060	17.7273020	16.3843050	C	12.3049690	16.7175860	14.9957890
H	15.4558750	17.3748180	14.8788760	H	12.4096070	17.6840680	15.4801730
N	15.3087150	15.8946410	16.3851310	H	13.0993740	16.6180740	14.2459920
C	16.4672930	15.0860540	16.3413260	N	12.4590730	15.6528260	15.9968550
O	16.4112690	13.8602090	16.5638200	C	13.0153210	15.8300580	17.2143370
O	16.9133150	15.2702730	14.4952990	O	13.2464520	14.9457440	18.0323140
C	17.9173120	14.4006390	14.1392760	O	17.8187830	15.8126640	13.7729580
H	17.7510790	13.3857190	14.5525750	C	19.0155220	15.3599880	14.2316980
H	18.9195930	14.7165660	14.5080600	H	18.9317510	14.6653910	15.1081280
C	18.0505230	14.2245510	12.6309860	H	19.6994550	16.1717630	14.5921890
H	17.0684410	13.9871180	12.1995540	C	19.8543320	14.5617350	13.2189340
O	18.5497760	15.4317010	12.0234080	H	19.2444610	13.7532640	12.7937420
C	19.0624780	13.1497220	12.1927200	O	20.2898560	15.4149930	12.1381240
H	19.8797910	13.0970320	12.9179210	C	21.1547570	13.9565380	13.7971080

H	21.4171290	14.4543220	14.7351580	H	19.8097660	12.2925090	13.2243990
N	20.9242280	12.5120730	14.0680820	H	18.4236170	13.0791980	12.4361620
N	21.6649490	11.9864130	14.8922140	O	18.0053650	12.1262770	14.2387880
N	22.2827100	11.3946240	15.6393880	C	17.5813990	10.9543840	13.7420350
C	22.2303700	14.2189960	12.7181410	O	17.8943780	10.4961940	12.6667060
H	22.9635140	14.9428890	13.0782160	O	16.7664950	10.3986420	14.6331580
H	22.7671740	13.3141990	12.4314840	C	16.2028600	9.1011100	14.2747700
C	21.4187900	14.7971060	11.5461700	H	15.6522300	9.2151940	13.3398910
H	21.1145100	14.0120580	10.8528580	H	17.0279980	8.4059360	14.1126270
N	22.1198220	15.8002980	10.7394150	C	15.3071250	8.6665230	15.4123810
C	22.4691730	17.0091420	11.3104030	H	14.4926960	9.3771090	15.5698030
H	22.1770440	17.1114760	12.3469700	H	14.8683480	7.6944900	15.1737010
C	23.0992920	18.0073990	10.6520330	H	15.8694370	8.5652330	16.3432280
C	23.4641340	19.3133760	11.2953050	O	20.2391920	7.8694590	13.7007150
H	24.5430230	19.4870380	11.2518210	H	19.6021330	8.5049380	13.3448510
H	23.1574580	19.3328970	12.3421790				
H	22.9855470	20.1531870	10.7836610	TS1			
C	23.4295970	17.7952260	9.2509240	O	16.8720800	18.4051920	15.9936500
O	24.0022540	18.5992700	8.5215330	C	16.3703740	18.1171020	14.9013950
N	23.0359030	16.5528840	8.7450810	N	15.3609360	18.8226470	14.3324770
H	23.2484960	16.3737110	7.7711240	C	14.8899560	18.4868640	13.1337280
C	22.3885870	15.5263700	9.4048850	N	13.8910710	19.2347220	12.6243540
O	22.0961330	14.4784320	8.8470440	H	13.5189930	20.0029090	13.1599120
O	13.3020480	17.1348440	17.4830040	H	13.4718730	19.0263410	11.7335380
H	13.6779440	17.1626980	18.3743200	C	15.4047200	17.3784490	12.3912550
Prodrug 4 (PCM)				H	15.0182750	17.1075430	11.4183810
				C	16.3953570	16.6584260	12.9741680
				H	16.8324030	15.7868360	12.5112590
				N	16.8793410	16.9901440	14.2014670
RC				C	17.9641280	16.2210720	14.8554200
O	17.8106430	18.9951850	14.4406160	H	17.7284210	16.2166930	15.9177710
C	17.3692820	18.4671400	13.4141620	C	19.3556280	16.8413040	14.6275110
N	16.6667270	19.1391370	12.4685490	H	19.9888240	16.6726730	15.4991890
C	16.2509790	18.5212080	11.3654340	H	19.3005900	17.9085280	14.4280990
N	15.5658260	19.2504880	10.4629950	S	20.0402410	15.9614510	13.1782690
H	15.3812840	20.2244070	10.6441090	O	17.9444440	14.8988220	14.3569670
H	15.2142610	18.8483960	9.6100590	C	19.1944370	14.4540810	13.8183870
C	16.5047210	17.1350320	11.1220350	H	19.7979010	14.0315040	14.6261470
H	16.1595490	16.6347210	10.2278030	C	18.9703300	13.4294750	12.7286000
C	17.1882810	16.4594590	12.0790000	H	19.9121110	13.2005950	12.2247910
H	17.4066350	15.4053160	12.0029240	H	18.2498730	13.7990140	11.9961820
N	17.6171410	17.0823570	13.2102510	O	18.4907310	12.2391220	13.3493770
C	18.3787510	16.3783310	14.2667720	C	18.2462160	11.2045350	12.4888650
H	18.0224800	16.7803940	15.2130440	O	17.9277790	11.3527080	11.3172390
C	19.9011120	16.5891180	14.1486640	O	17.8691170	10.1600310	13.2642430
H	20.3531920	16.6310840	15.1399070	C	17.4784200	8.9696720	12.5568620
H	20.1474030	17.4979560	13.6056330	H	16.6188760	9.1955710	11.9207230
S	20.5245690	15.1290970	13.2398000	H	18.3085230	8.6621560	11.9167210
O	18.0815570	14.9966870	14.1948570	C	17.1427340	7.9062840	13.5826950
C	19.2330970	14.1575330	14.1245380	H	16.3208320	8.2238270	14.2297260
H	19.5852390	13.9411850	15.1368200	H	16.8370640	6.9875320	13.0748450
C	18.9033970	12.8759290	13.3933450				

H	18.0067800	7.6746990	14.2106120	C	15.5879760	16.6467530	12.2352810
O	20.3320760	10.6395320	12.3013670	H	15.4052200	16.4127790	11.1954260
H	20.4162210	10.5582700	11.3421560	C	16.6230330	16.0829440	12.9084190
INT				H	17.3014090	15.3743380	12.4565990
O	16.8037870	18.3406380	15.9979600	N	16.8494420	16.3686420	14.2181770
C	16.3376990	18.0362830	14.8941570	C	17.9786970	15.7623440	14.9692430
N	15.3182320	18.7079870	14.3023150	H	17.6063390	15.6015240	15.9798000
C	14.8844810	18.3552130	13.0943590	C	19.2206210	16.6750310	15.0038170
N	13.8725820	19.0696680	12.5624430	H	19.7497350	16.5487880	15.9493630
H	13.4653320	19.8267190	13.0881110	H	18.9604050	17.7237030	14.8805080
H	13.4817450	18.8488830	11.6618150	S	20.2668570	16.1048480	13.6182330
C	15.4508860	17.2633240	12.3656430	O	18.3032360	14.5294280	14.3725900
H	15.0940070	16.9776040	11.3856860	C	19.6846090	14.3887610	13.9971330
C	16.4534600	16.5782450	12.9707210	H	20.2420950	14.0278750	14.8672090
H	16.9299120	15.7209030	12.5200100	C	19.8461160	13.4215290	12.8215600
N	16.9003560	16.9282670	14.2065020	H	20.8852550	13.5800040	12.4490610
C	17.9956670	16.1938520	14.8860450	H	19.1792390	13.7771590	12.0114980
H	17.7291510	16.1720390	15.9411140	O	19.5874700	12.1218910	13.1681120
C	19.3667500	16.8712670	14.7023230	C	18.8418000	11.0338330	11.6099040
H	19.9843260	16.7123200	15.5871260	O	18.2204490	11.8539980	10.9383000
H	19.2753210	17.9389980	14.5195040	O	18.2667400	10.0859080	12.3976850
S	20.1160730	16.0397440	13.2573060	C	16.9608470	10.4133650	12.9010740
O	18.0409580	14.8780220	14.3782720	H	17.0213330	11.3770200	13.4105330
C	19.3182010	14.4877000	13.8559450	H	16.2665130	10.5100540	12.0616800
H	19.9212710	14.0822500	14.6730610	C	16.5336410	9.3072840	13.8450490
C	19.1581180	13.4624010	12.7516170	H	17.2220760	9.2206600	14.6896400
H	20.1300980	13.3226340	12.2600580	H	15.5370870	9.5217440	14.2406040
H	18.4480240	13.8278650	12.0029400	H	16.4929940	8.3420150	13.3333370
O	18.7132600	12.2559310	13.3287540	O	20.0335990	10.4945590	11.1735750
C	18.4669590	11.1935290	12.3428900	H	20.4164080	11.1359660	10.5611760
O	17.7253940	11.5024280	11.3522240	PC			
O	17.9746570	10.1831030	13.2539080	O	18.8741360	18.4132470	12.4809400
C	17.5242720	8.9931880	12.6176850	C	18.3675560	17.4322330	11.9233400
H	16.7128700	9.2279380	11.9200370	N	17.5862050	17.5250150	10.8169490
H	18.3419480	8.5476100	12.0366040	C	17.0972850	16.4297050	10.2396830
C	17.0463230	8.0252580	13.6865700	N	16.3342590	16.5928380	9.1393590
H	16.2250240	8.4551400	14.2670870	H	16.1512010	17.5203680	8.7910810
H	16.6865710	7.1000590	13.2264360	H	15.9268090	15.8109330	8.6543290
H	17.8536880	7.7671530	14.3778080	C	17.3515880	15.1183760	10.7467850
O	19.8057880	10.7424540	11.9383650	H	16.9475800	14.2318340	10.2775820
H	19.7944800	10.7897070	10.9749500	C	18.1138060	15.0319420	11.8669020
TS2				H	18.3442530	14.0930270	12.3485470
O	16.2913140	17.5477350	16.0923120	N	18.6174250	16.1444270	12.4631830
C	16.0187950	17.2837890	14.9154340	C	19.4592210	16.0683640	13.6889040
N	14.9656100	17.8275710	14.2535770	H	19.1624140	16.9188170	14.3011240
C	14.7478980	17.5373130	12.9729260	C	20.9621360	16.1443280	13.3685190
N	13.6870750	18.1164600	12.3745720	H	21.4926060	16.6286500	14.1898530
H	13.0904170	18.7330930	12.9027110	H	21.1583750	16.6907470	12.4491640
H	13.4553230	17.9356160	11.4122310	S	21.4959270	14.4032950	13.2153920
				O	19.1726330	14.8701230	14.3644720

C	20.3037330	13.9990680	14.5737910	H	12.7228990	11.7085200	13.1557930
H	20.7678080	14.2714510	15.5273890	H	13.2315880	12.0598910	14.8180790
C	19.8718360	12.5223570	14.6032010	C	12.1625770	13.6878510	13.8501920
H	20.8295000	11.9507110	14.5042990	H	12.0905460	14.1079490	12.8402440
H	19.3418960	12.3474830	13.6355930	H	11.1631930	13.3089580	14.0958860
O	19.1455270	12.1894550	15.7038630	C	12.5608830	14.7775750	14.8515050
C	14.8894410	10.4061220	13.8405440	H	12.6196290	14.3388130	15.8550680
O	15.1829520	10.9678880	12.8093660	H	13.5669110	15.1400070	14.6165740
O	14.5428310	10.9786960	14.9854490	C	11.5824260	15.9538910	14.8626090
C	14.5201080	12.4374930	15.0033680	H	11.5273270	16.4347420	13.8806480
H	15.5217370	12.7953270	14.7615190	H	10.5711170	15.6289860	15.1277090
H	13.8303930	12.7764680	14.2291860	H	11.8853490	16.7155990	15.5864880
C	14.0808110	12.8666860	16.3846010	O	17.9852240	11.6450760	17.1564370
H	14.7754300	12.5124720	17.1493310	H	17.1981700	11.0824310	17.1226750
H	14.0535420	13.9581690	16.4305250				
H	13.0814920	12.4920300	16.6168470	TS1			
O	14.8618450	9.0727530	14.0062840	O	22.1666310	15.9707640	12.1229650
H	15.1167300	8.6553630	13.1704840	C	21.2340150	16.4862770	12.7427660
Prodrug 5 (PCM)				N	21.3713730	17.6050670	13.4994020
				C	20.3313800	18.1309610	14.1395450
				N	20.5443530	19.2388550	14.8732260
				H	21.4721530	19.6279300	14.9331330
RC				H	19.8069850	19.6783020	15.3988450
O	22.0647460	15.9954770	12.1565450	C	19.0169610	17.5634160	14.0725320
C	21.1124660	16.4759820	12.7740540	H	18.1765830	17.9943940	14.5987410
N	21.2116680	17.5839900	13.5518850	C	18.8768300	16.4438920	13.3269290
C	20.1513290	18.0713770	14.1890860	H	17.9340550	15.9220020	13.2324120
N	20.3264620	19.1713000	14.9440580	N	19.9387280	15.8927840	12.6667920
H	21.2429900	19.5832440	15.0222620	C	19.7565640	14.6640920	11.9078480
H	19.5719470	19.5816040	15.4690670	H	20.7515310	14.3152520	11.6338760
C	18.8529300	17.4709190	14.0971340	O	19.1070490	13.7250530	12.7606390
H	17.9959440	17.8698050	14.6217190	C	18.8791900	14.8238160	10.6577740
C	18.7499380	16.3625950	13.3296960	H	19.4606810	15.1986450	9.8166450
H	17.8220190	15.8186420	13.2155090	H	18.0383460	15.4925020	10.8423600
N	19.8331470	15.8513480	12.6711820	S	18.2815010	13.1287920	10.3044190
C	19.6909540	14.6366690	11.8835450	C	18.7563120	12.5649570	12.0411230
H	20.6966300	14.3197220	11.6109980	H	19.6299090	11.9161480	11.9260010
O	19.0593120	13.6608490	12.7118870	C	17.6816310	11.7867310	12.7671580
C	18.8171130	14.7997470	10.6323520	H	18.0387620	11.5244320	13.7668930
H	19.3914920	15.2125720	9.8043530	H	17.4781460	10.8634090	12.2183160
H	17.9532580	15.4353490	10.8265050	O	16.5034200	12.5692350	12.8914170
S	18.2817040	13.0958640	10.2294960	C	15.4578880	11.9385150	13.5031880
C	18.7148380	12.5166470	11.9674950	O	15.3053290	10.7237100	13.5147860
H	19.5761860	11.8492740	11.8701920	O	14.4457010	12.8400600	13.5269590
C	17.6106820	11.7547950	12.6665400	C	13.1991380	12.3667660	14.0650470
H	17.9465290	11.4590930	13.6634340	H	12.8444740	11.5274690	13.4610340
H	17.3630700	10.8556710	12.1009760	H	13.3761440	12.0065840	15.0824860
O	16.4519070	12.5979380	12.7879110	C	12.1977440	13.5103110	14.0491350
C	15.3458180	12.0121110	13.2641500	H	12.0732060	13.8655100	13.0186940
O	15.2438160	10.8462660	13.5738590	H	11.2274420	13.0942170	14.3479860
O	14.3887360	12.9335810	13.3307450	C	12.5548420	14.6835900	14.9675800
C	13.0907620	12.4889910	13.8238870				

H	12.6873450	14.3109170	15.9908830	O	15.8795860	11.6612220	15.1180680
H	13.5215470	15.0999890	14.6675160	H	15.8078500	10.7180760	15.3067640
C	11.4959750	15.7886120	14.9596230				
H	11.3635680	16.2062840	13.9561030	TS2			
H	10.5224710	15.4110020	15.2894450	O	21.6924090	15.9470660	10.8840670
H	11.7732170	16.6116590	15.6247710	C	21.1879020	16.5035000	11.8623090
O	16.1831040	12.3109450	15.5027250	N	21.7152340	17.6146320	12.4382170
H	15.9640080	11.4778620	15.9407120	C	21.1250170	18.1913270	13.4808270
				N	21.7060880	19.2904810	13.9977390
INT				H	22.5548380	19.6468920	13.5875780
O	22.1684120	16.0167310	12.1536810	H	21.3109690	19.7829630	14.7813900
C	21.2234760	16.5358960	12.7516620	C	19.9152990	17.6857000	14.0579190
N	21.3390410	17.6796540	13.4745630	H	19.4420020	18.1562560	14.9087280
C	20.2877500	18.2075380	14.0942550	C	19.3917820	16.5734100	13.4916560
N	20.4782350	19.3425860	14.7920400	H	18.4940050	16.0974210	13.8623910
H	21.3960450	19.7570130	14.8320450	N	19.9909370	15.9712670	12.4227620
H	19.7277830	19.7942540	15.2879540	C	19.4039660	14.7639380	11.8493970
C	18.9843350	17.6139360	14.0430780	H	20.1549350	14.3381180	11.1841350
H	18.1351960	18.0445150	14.5554470	O	19.1081880	13.8750580	12.9161050
C	18.8657370	16.4721430	13.3279070	C	18.0945000	15.0142930	11.0851340
H	17.9323420	15.9317770	13.2445970	H	18.2927780	15.3450060	10.0663010
N	19.9382650	15.9212580	12.6855720	H	17.4773480	15.7572940	11.5913410
C	19.7725220	14.6737340	11.9514710	S	17.2549330	13.3863450	11.0845080
H	20.7719850	14.3340870	11.6820550	C	18.4160230	12.7408760	12.4282140
O	19.1381660	13.7447020	12.8234520	H	19.1249400	12.0754220	11.9216160
C	18.8914900	14.8033720	10.6989980	C	17.7276670	11.9776110	13.5630760
H	19.4728790	15.1549820	9.8477240	H	18.5684400	11.5904050	14.1805260
H	18.0555440	15.4821560	10.8684720	H	17.2786570	11.0811390	13.0894360
S	18.2793370	13.1047750	10.3917690	O	16.8050250	12.6776360	14.2924300
C	18.7895570	12.5677200	12.1270150	C	15.2481090	11.5416540	14.8356720
H	19.6738620	11.9350250	12.0015080	O	15.1578700	10.5894160	14.0705210
C	17.7371610	11.7816560	12.8820240	O	14.3336520	12.5648400	14.8635820
H	18.1769410	11.4822490	13.8441520	C	13.6511160	12.8273350	13.6259310
H	17.5237360	10.8642140	12.3204140	H	14.3971790	13.0084020	12.8483600
O	16.5718710	12.5396670	13.0771140	H	13.0688890	11.9444770	13.3430960
C	15.4849350	11.7828930	13.7060370	C	12.7508270	14.0387630	13.8088010
O	15.1951350	10.6591670	13.1735220	H	13.3629870	14.9005990	14.1018520
O	14.4727090	12.8157060	13.6733830	H	12.3305880	14.2826420	12.8247700
C	13.2012970	12.4044670	14.1590190	C	11.6111770	13.8415770	14.8135920
H	12.8259560	11.5688210	13.5575030	H	11.0156180	12.9695690	14.5147010
H	13.2934880	12.0509730	15.1953920	H	12.0287980	13.6028220	15.7971070
C	12.2312820	13.5775770	14.0904260	C	10.7005970	15.0665550	14.9275980
H	12.1591000	13.9216600	13.0506640	H	11.2595670	15.9484150	15.2575740
H	11.2353550	13.2006010	14.3578850	H	10.2392940	15.3114940	13.9651000
C	12.5890770	14.7560340	15.0018810	H	9.8937160	14.8998910	15.6472430
H	12.6718370	14.3974180	16.0360090	O	15.7586890	11.3720740	16.1162010
H	13.5790620	15.1365510	14.7313510	H	16.3836780	12.1071290	16.2209250
C	11.5673360	15.8939730	14.9371610				
H	11.4847930	16.2968720	13.9221870	PC			
H	10.5704910	15.5532350	15.2365590	O	22.2353650	16.3276270	9.9736690
H	11.8452730	16.7208250	15.5976470	C	22.2281620	16.6300380	11.1695600

N	23.2046190	17.3722430	11.7535160	C	13.3540390	12.5189750	13.9591730
C	23.1437800	17.6894510	13.0433630	H	13.6837100	12.8104400	12.9619120
N	24.1474100	18.4292390	13.5521960	H	12.3803170	12.0266750	13.9103080
H	24.9058000	18.7203320	12.9557900	C	14.3512700	11.5688060	14.5905350
H	24.1645510	18.7092100	14.5186280	H	14.3584190	10.6634170	13.9777430
C	22.0644960	17.2745070	13.8889130	C	14.0611830	11.2001600	16.0596840
H	22.0230280	17.5327000	14.9381770	H	13.0185980	11.3958260	16.3483460
C	21.0941720	16.5280920	13.3112700	N	14.3375780	9.7365030	16.2075360
H	20.2456730	16.1450400	13.8620370	N	13.8986620	9.2024890	17.2195910
N	21.1480740	16.1936470	11.9890970	N	13.5440460	8.5974950	18.1133810
C	20.0857530	15.3779400	11.4065810	C	15.0754180	12.0443170	16.8397110
H	20.4472830	15.0465620	10.4331680	H	14.6463100	13.0272510	17.0419310
O	19.8615000	14.2726450	12.2667430	H	15.3678130	11.5994160	17.7913080
C	18.7495660	16.1245710	11.2542110	O	15.6767190	12.1445610	14.5590200
H	18.7289570	16.7044950	10.3321520	C	16.2515480	12.1521760	15.8655240
H	18.5714000	16.7895500	12.1001020	H	16.9413530	11.3176750	15.9761510
S	17.4887830	14.7951640	11.2163740	N	17.0678990	13.3629400	16.0045940
C	18.7533710	13.5198280	11.8097010	C	16.4964600	14.6025760	15.7828850
H	19.0476030	12.9484220	10.9201290	H	15.4461910	14.5690110	15.5237090
C	18.2306690	12.5548210	12.8949570	C	17.1704030	15.7721320	15.8544790
H	19.0794600	11.8293820	12.9995430	C	16.5260310	17.1052410	15.6087740
H	17.4467480	11.9665570	12.3507620	H	16.9978430	17.6240050	14.7693360
O	17.8179920	13.0862370	14.0676260	H	16.6230960	17.7572310	16.4814510
C	13.7289530	10.8971240	14.6186630	H	15.4643260	16.9907700	15.3854800
O	13.6877750	10.9135830	13.4089250	C	18.5879620	15.7237160	16.1786070
O	13.1140380	11.7309670	15.4454050	O	19.3320080	16.6942950	16.2835960
C	12.3136280	12.7860950	14.8331420	N	19.0932170	14.4346710	16.3728850
H	12.9799700	13.4096170	14.2350490	H	20.0788250	14.3642800	16.5954250
H	11.5827200	12.3186010	14.1704030	C	18.4195090	13.2313590	16.2981770
C	11.6493380	13.5762840	15.9435480	O	18.9807840	12.1611910	16.4851660
H	12.4216000	13.9876340	16.6036750	O	10.1878650	16.5139680	17.0191160
H	11.1619690	14.4368320	15.4695060	H	9.7004770	17.2902870	16.7206620
C	10.6203770	12.7845610	16.7571630	H	10.9134520	16.3702170	16.3852420
H	9.8608470	12.3784740	16.0778330	O	9.0370600	13.9685830	16.4874470
H	11.1073060	11.9216670	17.2231850	H	9.3235800	14.8412450	16.8135140
C	9.9422720	13.6323230	17.8356620	H	9.3861950	13.9166670	15.5770470
H	10.6723620	14.0257760	18.5502310	O	10.0126030	14.4780550	10.1505080
H	9.4153430	14.4866830	17.3986020	H	9.1527600	14.1333760	10.4163670
H	9.2112630	13.0465480	18.3999960	H	10.5677130	14.5017900	10.9614290
O	14.4213480	10.0066770	15.3497310	O	11.0172890	11.2840310	16.8361060
H	14.8749820	9.4017900	14.7447250	H	10.4714210	12.0796020	16.9062680
Prodrug 1 (EWM)				O	10.8803260	10.3376620	14.4687740
RC				H	9.9596160	10.2979660	14.1879620
				H	10.8938600	10.7292840	15.4381460
O	10.1000350	14.0773320	13.8599350	TS1			
C	11.2536210	14.3901340	13.5036910				
O	11.6966390	14.6001280	12.3510260	O	10.1429310	15.3646440	14.3482660
C	12.2940130	14.6050250	14.6276810	C	11.1884690	14.7050780	14.1304910
O	12.2705500	15.5812950	15.3563110	O	11.6842950	14.4479400	13.0044600
O	13.2783880	13.7147550	14.7863520	C	12.0026240	14.2171430	15.3890060

O	12.1058860	14.9744820	16.3753880	C	11.9141780	14.0085570	15.9214760
O	13.1790200	13.5065520	15.1237160	O	12.1538400	14.9169670	16.8260630
C	13.2121420	12.4084500	14.2096560	O	13.0963860	13.1597260	15.7748040
H	13.4509950	12.7643840	13.2072250	C	13.0000370	12.0428930	14.9065570
H	12.2422330	11.9130490	14.1823070	H	12.9197240	12.3673080	13.8638040
C	14.2682110	11.4136130	14.6628340	H	12.1179360	11.4392760	15.1486840
H	14.2052070	10.5368740	14.0127920	C	14.2282690	11.1602180	15.0541790
C	14.1599890	10.9821390	16.1373490	H	14.0781610	10.2692850	14.4389030
H	13.1625300	11.1725720	16.5356150	C	14.5497420	10.7455590	16.5021540
N	14.4524180	9.5193620	16.2030440	H	13.6745370	10.8277420	17.1484320
N	14.2375900	8.9746110	17.2814470	N	15.0137250	9.3259760	16.4740950
N	14.0721080	8.3643910	18.2242100	N	15.1163570	8.7702640	17.5630610
C	15.2305670	11.8254980	16.8372120	N	15.2410640	8.1536090	18.5080290
H	14.7953930	12.7850610	17.1175020	C	15.6644140	11.7133970	16.9090170
H	15.6381160	11.3571130	17.7337590	H	15.2121350	12.6325900	17.2821990
O	15.5944810	11.9758890	14.5060740	H	16.3293030	11.3170710	17.6772320
C	16.2911620	12.0106950	15.7465770	O	15.4138620	11.8314410	14.5606640
H	17.0430670	11.2244550	15.7765920	C	16.3928510	11.9674320	15.5845780
N	17.0360440	13.2750020	15.8294360	H	17.2003600	11.2552900	15.4258820
C	16.3677730	14.4720970	15.6452540	N	17.0099940	13.2961400	15.4738090
H	15.3047360	14.3651880	15.4624300	C	16.2055340	14.4216820	15.4707800
C	16.9682840	15.6835280	15.6694180	H	15.1453360	14.2103450	15.5620270
C	16.2239370	16.9713210	15.4668760	C	16.6770090	15.6835890	15.3459400
H	16.6095880	17.5189810	14.6021980	C	15.7885300	16.8936420	15.3478940
H	16.3304150	17.6296800	16.3337790	H	15.8964920	17.4649930	14.4214790
H	15.1605660	16.7869020	15.3077360	H	16.0430930	17.5692150	16.1697330
C	18.4040150	15.7301740	15.8973680	H	14.7414570	16.6078970	15.4531350
O	19.0885900	16.7481220	15.9488720	C	18.1119350	15.8671250	15.1991340
N	19.0051270	14.4787360	16.0628090	O	18.6888240	16.9448700	15.0802950
H	20.0055190	14.4748320	16.2211530	N	18.8505160	14.6798850	15.1960610
C	18.4075930	13.2337820	16.0390490	H	19.8538150	14.7712990	15.0922610
O	19.0481220	12.2035770	16.1976250	C	18.3866220	13.3852780	15.3215230
O	10.3796950	17.1219570	16.5785930	O	19.1410330	12.4218760	15.3046500
H	9.9583940	16.8432580	15.7502170	O	10.1296500	16.7318050	16.7805760
H	11.0511080	16.4134900	16.6750490	H	9.8041640	16.4039720	15.9268790
O	8.2898790	13.7139160	15.7154870	H	10.9018950	16.1283050	16.9284360
H	9.1668270	13.2834700	15.8701760	O	8.3165560	13.5625280	13.1519910
H	8.5609480	14.4812700	15.1861590	H	8.3844790	12.7987740	13.7559460
O	10.5602180	15.3072610	10.6711680	H	8.9920890	14.1863850	13.4851260
H	11.1738920	15.0025190	9.9935650	O	12.0360410	16.2075370	11.3800650
H	10.9295540	15.0140910	11.5405410	H	12.9362430	16.3555320	11.0697530
O	10.8607860	12.8074370	15.8940180	H	12.1076110	15.6840770	12.2183200
H	11.0897900	12.8150230	16.8329200	O	10.8204990	13.0978580	16.3371300
O	10.0787350	10.3434070	15.1152330	H	10.8549410	13.1165210	17.3038180
H	10.8001600	9.7167810	15.2391080	O	8.8896090	11.5939660	15.0917200
H	10.4122710	11.2332020	15.4082390	H	8.2180430	11.3658910	15.7441220
				H	9.5842730	12.1096810	15.5609540
INT				TS2			
O	10.2946980	15.0542180	14.4365540	O	10.9280170	11.4070760	13.5800740
C	11.4822260	14.6345610	14.5340330	C	11.8275820	12.1860500	13.1447490
O	12.3741080	14.7637340	13.6560940				

O	12.3846550	12.0802220	12.0255940	C	8.9846130	12.3638590	12.6488510
C	12.3051680	13.3757370	14.0405440	O	9.4680340	12.4762130	11.5090520
O	12.6827880	14.4499810	13.5164330	C	7.6456780	13.1236770	12.8764970
O	13.6619450	12.5807310	14.8087960	O	6.7605300	13.2104350	12.0584970
C	14.8352730	12.5286320	14.0426980	O	15.2162780	12.8040020	15.0766790
H	14.7296050	13.1485830	13.1457290	C	16.4889210	12.5327890	14.6168090
H	15.0410030	11.4990870	13.7050100	H	16.6846330	12.9677130	13.6143540
C	16.0807670	13.0099610	14.7899750	H	16.6816330	11.4435950	14.5029560
H	16.9645190	12.6955810	14.2270670	C	17.6178360	13.0519470	15.5200420
C	16.1869450	12.5192680	16.2463970	H	18.5817490	12.7238670	15.1194810
H	15.5637870	11.6428990	16.4263130	C	17.4775290	12.6346830	16.9893350
N	17.6175190	12.1731030	16.5147110	H	16.9073870	11.7092830	17.0903850
N	17.8385450	11.5678630	17.5581150	N	18.8507300	12.4301720	17.5499440
N	18.1607030	11.0031560	18.4893750	N	18.9094520	11.9140360	18.6602040
C	15.7305990	13.7369290	17.0561200	N	19.0835350	11.4377690	19.6769540
H	14.6397080	13.7498230	17.0863090	C	16.7606100	13.8265370	17.6295830
H	16.1163070	13.7585730	18.0760040	H	15.6880400	13.6902900	17.4963690
O	16.1148660	14.4619140	14.8587460	H	16.9718500	13.9464710	18.6932790
C	16.2418790	14.8964080	16.1982840	O	17.6533540	14.5066930	15.5406450
H	17.2802780	15.1337510	16.4310660	C	17.2572880	15.0208810	16.8032300
N	15.4988400	16.1629600	16.3569670	H	18.1017500	15.5189170	17.2749890
C	14.3257400	16.3875500	15.6628700	N	16.2451390	16.0757990	16.6069150
H	14.0219670	15.5831370	15.0008270	C	15.0939820	15.7824720	15.8974520
C	13.6036370	17.5303390	15.7631630	H	15.0318300	14.7430440	15.5587040
C	12.3401890	17.7618640	14.9842640	C	14.1310690	16.6958780	15.6256090
H	12.4265540	18.6475930	14.3475370	C	12.8856770	16.3612870	14.8548990
H	11.4894030	17.9336970	15.6508330	H	12.8001970	16.9738370	13.9525010
H	12.1178870	16.9012480	14.3526960	H	11.9871570	16.5473290	15.4507710
C	14.0859160	18.5754340	16.6481380	H	12.8842680	15.3123610	14.5556310
O	13.5450890	19.6622660	16.8423770	C	14.3172930	18.0556040	16.0989010
N	15.2773210	18.2657240	17.3120090	O	13.5356340	18.9905460	15.9339330
H	15.6407660	18.9682820	17.9445350	N	15.5099650	18.2662380	16.7982830
C	16.0202840	17.1054750	17.2284050	H	15.6742660	19.2049440	17.1408400
O	17.0452060	16.9395580	17.8787380	C	16.5054160	17.3515050	17.0822200
O	9.2434810	11.6528240	15.7251930	O	17.5124930	17.6660070	17.7052500
H	9.8628150	11.5836320	14.9616540	O	8.5277500	11.6093940	16.2658940
H	9.5816310	12.4157530	16.2081250	H	8.8068730	11.6671080	15.3282240
O	11.8248880	8.8653710	14.3876780	H	7.9454420	12.3644210	16.4053360
H	12.3755680	9.2589780	15.0942580	O	11.7603660	10.1214340	13.4538890
H	11.4263090	9.6416540	13.9494180	H	12.4454060	10.3948090	14.1087770
O	11.5169010	10.0898510	10.3777840	H	10.9624850	10.6662980	13.6018840
H	10.8709430	9.5539040	10.8512920	O	11.8633850	11.0744640	10.8432680
H	11.8085960	10.7932640	11.0106830	H	12.0077470	10.6537790	11.7162520
O	11.4781040	13.4770440	15.1827010	H	11.0493670	11.5982550	10.9701300
H	11.6800310	14.3455350	15.5570960	O	7.5720460	13.6794180	14.1003730
O	13.3223360	10.3489330	16.2321920	H	6.7239270	14.1480440	14.1822550
H	13.3906720	11.2049380	15.7197340	O	13.7024320	10.8053130	15.2144340
H	12.8636370	10.5485400	17.0557670	H	14.3467970	11.6396050	15.1640120
				H	13.6220220	10.5410670	16.1364850
PC							
O	9.4161910	11.7040340	13.6291360	Prodrug 2 (EWM)			

RC				O	16.4773140	18.9240050	17.6676340
				H	17.0169470	18.1198180	17.5585160
C	17.7499060	14.3643390	19.0244900	H	15.9979220	18.8218980	18.4974370
H	16.7202030	14.1040100	19.3031340	O	22.3265180	15.4002380	12.9377690
H	17.9405760	15.3787770	19.3654530	H	22.4983010	15.4548880	13.9511540
C	18.7292940	13.3685300	19.6508380	O	22.7475650	15.4574110	15.4838960
H	19.7539230	13.7173030	19.4779190	H	23.3170640	16.1760720	15.7872610
H	18.5736950	13.3561370	20.7341900	H	21.6115300	16.0178300	12.7331140
C	18.5503050	11.9651930	19.0598690				
H	17.5695130	11.5689540	19.3531570	TS1			
H	19.2990100	11.2807230	19.4700700	C	13.2563920	14.8410850	16.2054530
C	18.6469380	12.0054950	17.5303380	H	12.4774750	14.7943390	15.4298740
H	19.6673910	12.2678360	17.2283830	H	13.2505450	15.8512590	16.6100360
H	18.4295770	11.0219840	17.1019860	C	12.9293490	13.8021280	17.2877710
C	17.6722680	13.0248840	16.9333860	H	13.6193840	13.9233860	18.1298930
H	16.6379440	12.7013040	17.1090520	H	11.9183640	13.9861300	17.6701120
H	17.8111430	13.1188420	15.8607850	C	13.0430160	12.3809600	16.7213860
N	17.8503840	14.3449760	17.5587930	H	12.2545580	12.2280840	15.9708270
C	17.9736990	15.5016750	16.8778460	H	12.8698020	11.6368160	17.5066000
O	18.0712190	16.6177380	17.3920250	C	14.4167340	12.1683720	16.0732230
O	17.9967970	15.3251040	15.5334420	H	15.1935770	12.1962530	16.8411770
C	18.1423490	16.5146290	14.7379770	H	14.4633880	11.1876840	15.5845070
H	19.0463840	17.0488370	15.0355230	C	14.7203880	13.2598430	15.0350030
H	17.2781780	17.1653340	14.8854900	H	14.0403710	13.1371190	14.1788320
C	18.2526640	16.0917790	13.2926800	H	15.7342500	13.1620670	14.6535410
H	19.0265640	15.3205040	13.1894340	N	14.5443270	14.6172290	15.5543710
O	16.9984530	15.5855540	12.8307220	C	15.6422150	15.4013320	15.9342460
C	18.5668400	17.2518800	12.3308270	O	15.4568470	16.5266760	16.4779540
H	18.0719770	18.1650140	12.6733360	O	16.6175750	15.2994060	14.9226160
N	20.0289020	17.4671230	12.2876200	C	17.8026050	16.0430180	15.1629760
N	20.4095270	18.6048350	12.0148330	H	18.0732540	15.9626690	16.2174870
N	20.8785520	19.6082920	11.7788730	H	17.6551060	17.1006690	14.9186390
C	17.9632650	16.7670170	10.9956020	C	18.9218830	15.4731090	14.3208660
H	17.4525690	17.5669120	10.4605820	H	18.9152680	14.3780440	14.3935090
H	18.7483560	16.3800260	10.3454720	O	18.7755680	15.8589350	12.9480530
C	17.0036000	15.6212520	11.4007620	C	20.3206110	15.9867770	14.7038080
H	17.3409740	14.6659340	11.0049850	H	20.2594670	17.0280550	15.0327750
N	15.6211430	15.7720620	10.9525080	N	20.8409420	15.1536330	15.8135760
C	14.8780120	16.8620500	11.3689140	N	21.7554630	15.6380800	16.4791850
H	15.4104960	17.5488900	12.0132930	N	22.5945100	15.9788870	17.1595560
C	13.5871100	17.0750360	11.0340090	C	21.1189680	15.8716920	13.3872890
C	12.8019330	18.2655320	11.5008870	H	21.7181600	16.7611190	13.1943720
H	13.4111270	18.9130670	12.1332160	H	21.7943630	15.0160920	13.4169460
H	11.9226950	17.9573760	12.0734890	C	20.0327250	15.6527460	12.3045770
H	12.4402420	18.8559850	10.6544280	H	20.0841930	14.6461010	11.8943380
C	12.9344080	16.0908320	10.1815040	N	20.1040490	16.5556800	11.1572220
O	11.7738660	16.1446830	9.7891300	C	19.9761620	17.9195130	11.3486580
N	13.7466320	15.0144260	9.8118310	H	19.8374510	18.2167060	12.3796710
H	13.3207160	14.3084910	9.2233750	C	19.9992330	18.8325620	10.3535000
C	15.0636600	14.7795490	10.1522280	C	19.8579480	20.3079560	10.5881750
O	15.6681070	13.7891620	9.7698220	H	19.7381340	20.5253850	11.6505100

H	18.9910210	20.7104310	10.0567520	C	20.0211720	15.6809900	12.2856360
H	20.7350600	20.8505990	10.2245890	H	20.0586690	14.6773750	11.8662650
C	20.1646780	18.3485840	8.9900250	N	20.1221630	16.5937170	11.1481660
O	20.2078070	19.0493920	7.9843720	C	20.0147680	17.9572730	11.3529260
N	20.2773560	16.9596050	8.8778900	H	19.8700690	18.2451180	12.3857580
H	20.3870410	16.5891750	7.9415520	C	20.0630350	18.8803370	10.3679300
C	20.2480930	16.0145620	9.8840350	C	19.9435890	20.3552950	10.6171690
O	20.3491800	14.8184990	9.6557080	H	19.8168170	20.5630790	11.6806360
O	15.4273270	16.9304700	19.1396980	H	19.0886620	20.7777580	10.0818340
H	15.4190740	16.8113560	18.1580600	H	20.8329750	20.8873890	10.2680980
H	16.1890700	17.4832630	19.3461060	C	20.2340360	18.4080090	9.0011370
O	18.8771370	13.1109780	17.2538830	O	20.2987000	19.1184880	8.0034050
H	18.0066180	13.6076920	17.2349610	N	20.3249710	17.0186040	8.8752820
O	16.5428070	14.3871910	17.2096880	H	20.4372480	16.6563360	7.9360660
H	16.3361760	14.8501940	18.0309470	C	20.2695070	16.0636030	9.8709220
H	19.5366430	13.6863850	16.8419890	O	20.3524180	14.8684120	9.6307840
INT				O	15.6381790	16.7776230	19.0193800
C	13.2058150	14.7694070	16.1359480	H	15.4809270	16.8301280	18.0319480
H	12.4311170	14.6075750	15.3708590	H	16.3545440	17.3865080	19.2306010
H	13.1429210	15.8117840	16.4434350	O	18.7146540	13.1093920	17.1190290
C	12.9187330	13.8244740	17.3152830	H	17.8820340	13.6292060	17.0709860
H	13.6002340	14.0511300	18.1433850	O	16.3518040	14.5646400	17.0872010
H	11.9000180	14.0004880	17.6822340	H	16.2342110	15.0645350	17.9090290
C	13.0923780	12.3626000	16.8848860	H	19.4118380	13.6653410	16.7415970
H	12.3148390	12.1108100	16.1493360	TS2			
H	12.9443150	11.6852970	17.7335860	C	13.6045620	14.8343900	15.8337530
C	14.4762050	12.1489810	16.2584750	H	13.9067450	14.9202770	14.7784250
H	15.2469870	12.2586650	17.0258460	H	13.3683510	15.8360010	16.1878270
H	14.5599530	11.1334240	15.8516890	C	12.3864750	13.9147540	15.9462150
C	14.7404910	13.1645880	15.1320140	H	12.0093260	13.9409120	16.9759410
H	14.0735500	12.9263380	14.2892340	H	11.5870270	14.2998450	15.3038200
H	15.7603520	13.0716380	14.7605700	C	12.7416740	12.4739110	15.5622960
N	14.5047030	14.5651270	15.4976060	H	12.9766140	12.4324900	14.4903670
C	15.6211210	15.3501780	16.0038680	H	11.8854550	11.8094630	15.7197680
O	15.3225050	16.5414990	16.4221030	C	13.9546790	11.9911660	16.3651740
O	16.5803670	15.3148750	14.8981610	H	13.6798220	11.8881400	17.4220760
C	17.7592500	16.0597630	15.1252060	H	14.2764610	11.0018590	16.0218900
H	18.0512580	16.0005170	16.1781320	C	15.1297830	12.9663090	16.2450370
H	17.6171360	17.1189510	14.8764570	H	15.5093380	12.9730900	15.2130500
C	18.8841510	15.4918600	14.2845380	H	15.9461010	12.6485570	16.8903020
H	18.8571670	14.3957420	14.3340000	N	14.7180990	14.3182240	16.6335370
O	18.7616990	15.9051450	12.9171610	C	15.6877890	15.2522760	17.0120370
C	20.2886340	15.9684680	14.6921980	O	15.3670280	16.4322670	17.3015300
H	20.2461500	17.0021410	15.0472280	O	16.6427750	15.3776680	15.3010610
N	20.7743420	15.0951910	15.7879990	C	17.8287080	16.0642270	15.3826470
N	21.7018000	15.5337440	16.4677750	H	18.2654130	16.0294050	16.4022620
N	22.5491380	15.8321680	17.1574280	H	17.7383980	17.1463020	15.1419140
C	21.0996980	15.8692850	13.3822190	C	18.9114380	15.5065120	14.4579490
H	21.7077720	16.7572090	13.2113200	H	18.8989960	14.4095870	14.5130100
H	21.7679180	15.0077470	13.4014010	O	18.6762220	15.9032900	13.0947970

C	20.3397550	16.0010730	14.7435270	O	21.4519490	16.2143620	13.8160280
H	20.3091450	17.0216170	15.1367410	O	17.6357080	18.6772340	16.5901120
N	20.9456010	15.1080230	15.7656540	C	16.9513680	18.9791400	15.4409070
N	21.9365660	15.5411030	16.3519160	H	17.4034730	19.8306540	14.8851470
N	22.8505410	15.8367350	16.9529590	H	15.8941050	19.2845280	15.6239100
C	21.0382610	15.9622040	13.3660500	C	16.8787470	17.8388990	14.4151750
H	21.5483190	16.9002460	13.1455400	H	17.8889480	17.4516650	14.2291870
H	21.7783840	15.1627390	13.3175410	O	16.0655170	16.7584020	14.9196000
C	19.8820500	15.6868170	12.3735090	C	16.2263390	18.2221960	13.0666450
H	19.9234170	14.6656100	11.9974160	H	15.6067530	19.1140510	13.1885910
N	19.8624150	16.5488180	11.1900690	N	17.2996500	18.5158540	12.0764940
C	19.6819150	17.9108110	11.3422990	N	17.0539270	19.3892550	11.2452770
H	19.5664860	18.2330910	12.3687100	N	16.9345410	20.1801910	10.4434320
C	19.6279740	18.7901570	10.3177680	C	15.3608980	17.0005880	12.6821500
C	19.4300460	20.2652370	10.5099330	H	14.3041330	17.2705760	12.6587330
H	19.3453560	20.5140960	11.5688110	H	15.6243490	16.6007790	11.7028770
H	18.5243090	20.6111730	10.0038820	C	15.6502240	15.9850910	13.8036830
H	20.2658130	20.8328630	10.0911840	H	16.4301410	15.2829220	13.5090320
C	19.7637730	18.2677710	8.9658080	N	14.5056280	15.1708240	14.2156970
O	19.7381360	18.9348490	7.9362990	C	13.4126440	15.7802120	14.8033580
N	19.9340610	16.8820280	8.8947020	H	13.5061950	16.8525000	14.9122960
H	20.0272830	16.4851290	7.9675140	C	12.3165890	15.1196800	15.2373460
C	19.9868270	15.9718480	9.9321290	C	11.1434190	15.8044780	15.8751120
O	20.1374800	14.7743740	9.7384690	H	11.3012030	16.8826860	15.9281740
O	17.1210290	17.0408730	19.2235790	H	10.9736420	15.4335520	16.8898430
H	16.4291060	17.1243070	18.5236900	H	10.2249900	15.6208400	15.3105280
H	17.8328250	17.6550270	19.0113540	C	12.2865380	13.6732240	15.0776970
O	19.0790360	13.1167980	17.2581070	O	11.3654680	12.9363040	15.4157180
H	18.2458210	13.6177520	17.3273840	N	13.4311480	13.1319350	14.4848400
O	16.7029730	14.6494460	17.7651500	H	13.4441540	12.1266100	14.3618630
H	17.0597530	15.3380130	18.3602290	C	14.5595060	13.7934520	14.0413230
H	19.7079710	13.6944180	16.7987530	O	15.5033790	13.2028450	13.5371130
				O	19.6842360	16.8189730	11.6919180
				H	20.3875800	17.1548940	12.2719940
PC				H	18.9086210	17.3999980	11.8000500
C	22.4004450	14.6265680	15.9195530	O	16.4524690	16.8245370	17.9702150
H	21.9447750	14.8097910	16.9021040	H	16.9203950	17.5677990	17.4433740
H	22.8373150	15.5614950	15.5774540	O	19.9225280	14.6469970	13.2612470
C	23.4546270	13.5222400	16.0326670	H	19.6970750	15.3523360	12.6017560
H	23.9985820	13.4479350	15.0836250	H	16.0741900	16.2619280	17.2842470
H	24.1837780	13.8071130	16.7977780				
C	22.8124570	12.1716880	16.3709310				
H	22.3877030	12.2136520	17.3823400	Prodrug 3 (EWM)			
H	23.5696270	11.3816640	16.3830930				
C	21.7035760	11.8320220	15.3680680	RC			
H	22.1393670	11.6531750	14.3780250	C	15.0252040	13.0810450	16.5181380
H	21.1851610	10.9131430	15.6600320	H	15.5317650	12.1686440	16.2140930
C	20.6773920	12.9645560	15.2640740	H	13.9435420	12.9069960	16.4654920
H	20.1325470	13.0618470	16.2129240	C	15.4220930	13.4666920	17.9389160
H	19.9486130	12.7641760	14.4845000	H	15.0585690	12.7068360	18.6340970
N	21.3410400	14.2442800	14.9790240	H	16.5188310	13.5004130	18.0143220
C	20.9426690	15.1051350	14.0168000	N	14.8187520	14.7634420	18.2908950

H	15.0823980	15.0054240	19.2418000	H	20.9299360	15.3911650	15.6146680
C	15.2854180	15.8216310	17.3793160				
H	14.8209690	16.7671380	17.6678030	TS1			
H	16.3762900	15.9478360	17.4346200	C	14.1245580	15.2094270	16.4647810
C	14.8898880	15.4870730	15.9440180	H	14.4226880	14.4667230	17.2020390
H	15.3045290	16.2225090	15.2614760	H	13.5912850	14.6854410	15.6531880
H	13.7978390	15.5010190	15.8437800	C	13.1879670	16.2268260	17.1052580
N	15.3838660	14.1517330	15.5818370	H	12.2611530	15.7349830	17.4114830
C	15.9333590	13.8428260	14.3868590	H	13.6664230	16.6427180	18.0045580
O	16.2567870	12.7077370	14.0399960	N	12.8614680	17.2881010	16.1356330
O	16.1043430	14.9264960	13.5939460	H	12.2516990	17.9680660	16.5813980
C	16.7099680	14.6923270	12.3099320	C	14.0836890	17.9693680	15.6711790
H	16.0891930	14.0033440	11.7336620	H	13.8014140	18.7368750	14.9460610
H	17.7028140	14.2585090	12.4411410	H	14.6034980	18.4642180	16.5052860
C	16.7966120	16.0180560	11.5919110	C	15.0257380	16.9628920	15.0171810
H	15.8316280	16.5367030	11.6481070	H	15.9599700	17.4527040	14.7489890
O	17.8193450	16.8299550	12.1782030	H	14.5659700	16.5795690	14.0928550
C	17.2139160	15.8955770	10.1154500	N	15.3196370	15.8821110	15.9531100
H	17.9218110	15.0708560	9.9939360	C	16.4549160	15.0852410	15.7393810
N	16.0103950	15.6448360	9.2972650	O	16.7145480	14.1190220	16.4839200
N	16.1780340	15.0432770	8.2390750	O	16.7536100	15.0052710	14.3837910
N	16.2004580	14.4964410	7.2463270	C	17.8676530	14.1850000	14.0467530
C	17.8980140	17.2504930	9.8312870	H	17.6970680	13.1611260	14.3897220
H	18.8035650	17.1347410	9.2367640	H	18.7722330	14.5675840	14.5283710
H	17.2218010	17.9069610	9.2833130	C	18.0222620	14.1839250	12.5435710
C	18.1845690	17.8438140	11.2312080	H	17.0466050	14.0121290	12.0715090
H	17.5982530	18.7422850	11.4082970	O	18.5582660	15.4358540	12.0878340
N	19.5724580	18.2136940	11.4856610	C	19.0227590	13.1442680	12.0109730
C	20.5670040	17.2558370	11.3938500	H	19.8627940	13.0478950	12.7047380
H	20.2173200	16.2709730	11.1141610	N	18.3391430	11.8420200	11.8701970
C	21.8732740	17.4910580	11.6411280	N	19.0392030	10.8376930	11.9656490
C	22.9342890	16.4358380	11.5321410	N	19.5739430	9.8402290	12.0383140
H	23.6942510	16.7167010	10.7976590	C	19.4831200	13.7547470	10.6703010
H	22.5056530	15.4788090	11.2311940	H	20.5526700	13.6285570	10.5054720
H	23.4494250	16.2954260	12.4864250	H	18.9607610	13.2781970	9.8403600
C	22.2588150	18.8390750	12.0366020	C	19.0694850	15.2435670	10.7629700
O	23.4002320	19.2082320	12.2898560	H	18.3007850	15.4866230	10.0330850
N	21.1974890	19.7456310	12.1188580	N	20.1438500	16.2074770	10.5479360
H	21.4313710	20.6910740	12.3973970	C	21.2776720	16.1634940	11.3402390
C	19.8580320	19.5191590	11.8757440	H	21.2745580	15.3793560	12.0858940
O	19.0172890	20.3977650	11.9895020	C	22.3148620	17.0210650	11.2318780
O	11.9796330	14.6375000	18.5331970	C	23.5338270	16.9505560	12.1037720
H	11.7564070	15.0626070	19.3691820	H	24.4384950	16.8141910	11.5047480
H	12.9639910	14.6876540	18.4424750	H	23.4633020	16.1213460	12.8092510
O	17.4395910	11.0167360	12.1133630	H	23.6646520	17.8746240	12.6737460
H	17.6252280	10.2032830	12.5956330	C	22.2314710	18.0647410	10.2188880
H	17.0422560	11.6337020	12.7539500	O	23.0890980	18.9120670	9.9955770
O	18.5940490	17.3952200	15.0879030	N	21.0509380	18.0525640	9.4695710
H	18.2675270	17.1701920	14.2066250	H	20.9587320	18.7706780	8.7611020
H	19.1847880	16.6175070	15.4061200	C	19.9802370	17.1877170	9.5728500
O	20.0318810	15.4340810	15.9676190	O	18.9933430	17.2850210	8.8598200

O	11.2008370	16.3911000	14.0194860	C	22.2171410	16.9982280	11.0382940
H	10.3758710	16.8823700	14.1062160	C	23.4990160	16.9469140	11.8163950
H	11.7931520	16.6968210	14.7547450	H	24.3559420	16.7978590	11.1535960
O	16.8219870	14.2722000	19.2204680	H	23.4839570	16.1335470	12.5433900
H	16.8122850	15.1995280	19.4825510	H	23.6707610	17.8834460	12.3542750
H	16.7611110	14.2598110	18.2377540	C	22.0549540	18.0218520	10.0146940
O	18.9495200	17.6524440	14.1211160	O	22.8913820	18.8654660	9.7114560
H	18.8289420	17.0431300	13.3799770	N	20.8215050	17.9936920	9.3568720
H	18.5446610	17.1888000	14.9198960	H	20.6735330	18.6981490	8.6441730
O	17.8419150	16.4428980	16.1877440	C	19.7630290	17.1314130	9.5592290
H	18.4491830	15.9064910	16.7117710	O	18.7236290	17.2166700	8.9236710
INT				O	12.0062780	16.6575430	13.2316250
				H	11.1055830	16.9968380	13.1768890
				H	12.3121930	16.8108330	14.1646440
C	14.3255320	15.1862470	16.1516920	O	16.4357360	14.2284120	19.4165450
H	14.5207690	14.2955410	16.7479940	H	17.2807930	14.0183220	19.8288470
H	14.1671370	14.8640940	15.1085260	H	16.6102320	14.3249600	18.4401230
C	13.0641510	15.8783070	16.6576320	O	19.0302530	17.6750430	14.1028670
H	12.1999400	15.2214570	16.5260750	H	18.8675990	17.0415120	13.3877540
H	13.1717530	16.0860670	17.7329320	H	18.6088630	17.2785300	14.8925450
N	12.8309960	17.1195870	15.8964360	O	17.7958140	16.4647540	16.3078510
H	12.0123320	17.5905330	16.2720300	H	18.3234480	16.1119530	17.0342470
C	13.9932330	18.0210410	15.9926200	TS2			
H	13.7970450	18.9083140	15.3843490	C	14.3759830	15.2004540	16.2400680
H	14.1563990	18.3506020	17.0299250	H	14.5918870	14.2849590	16.7886950
C	15.2449080	17.3098490	15.4876850	H	14.2314150	14.9335280	15.1831170
H	16.1052400	17.9681180	15.6011770	C	13.1065720	15.8434770	16.7878280
H	15.1273000	17.0905940	14.4145490	H	12.2544970	15.1810390	16.6152910
N	15.4729900	16.0890280	16.2659710	H	13.2101920	15.9867430	17.8741470
C	16.7658990	15.4212970	16.0672060	N	12.8557350	17.1240690	16.1033510
O	16.9661120	14.3732890	16.7988480	H	12.0227580	17.5536580	16.4963330
O	16.8674950	15.1682190	14.6181740	C	13.9970560	18.0397600	16.2743130
C	17.9114950	14.2940900	14.2413670	H	13.7863160	18.9664830	15.7343820
H	17.7288140	13.2827890	14.6213340	H	14.1494820	18.2925080	17.3346380
H	18.8776300	14.6299730	14.6396110	C	15.2660590	17.3999640	15.7206240
C	17.9808840	14.2360270	12.7308620	H	16.1101920	18.0623160	15.9016410
H	16.9767890	14.0729790	12.3192660	H	15.1699360	17.2610820	14.6355420
O	18.5145480	15.4630060	12.2014020	N	15.5075130	16.1173250	16.3878670
C	18.9306910	13.1607510	12.1760600	C	16.7839490	15.5246790	16.2712300
H	19.7976770	13.0591600	12.8348080	O	17.0251170	14.4109780	16.8010300
N	18.2123350	11.8710180	12.0956560	O	16.8861660	15.2887250	14.4144800
N	18.8864340	10.8536590	12.2273710	C	17.8453800	14.3559080	14.0724690
N	19.3965670	9.8465020	12.3381170	H	17.6164600	13.3456380	14.4608160
C	19.3476680	13.7237740	10.7999270	H	18.8518110	14.6089760	14.4652950
H	20.4107180	13.5860100	10.6045680	C	17.9781950	14.2234590	12.5611420
H	18.7972690	13.2228750	10.0031770	H	16.9911180	14.0433320	12.1159690
C	18.9440170	15.2164540	10.8571390	O	18.5263680	15.4365340	12.0031030
H	18.1313390	15.4321400	10.1672550	C	18.9531980	13.1344070	12.0820480
N	20.0026090	16.1684460	10.5363760	H	19.7779510	13.0399730	12.7942710
C	21.1935600	16.1413880	11.2410400	N	18.2343720	11.8437230	11.9831690
H	21.2515630	15.3702940	11.9977700				

N	18.8912640	10.8278580	12.1861130	O	17.2183980	16.2161430	13.1219660
N	19.3882270	9.8219270	12.3581350	C	18.0744430	15.0843250	13.1762290
C	19.4592280	13.6602880	10.7208480	H	17.5299500	14.2124030	13.5562540
H	20.5372880	13.5425240	10.6106630	H	18.9293500	15.2654810	13.8411760
H	18.9816760	13.1221660	9.9015120	C	18.5832270	14.7459330	11.7911380
C	19.0285330	15.1464070	10.6998490	H	17.7400470	14.7053820	11.0896630
H	18.2575210	15.3237950	9.9527820	O	19.5272120	15.7326590	11.3450030
N	20.0972030	16.1014280	10.4038160	C	19.3701050	13.4259170	11.7105430
C	21.1897060	16.1899710	11.2471670	H	19.9392280	13.2777650	12.6326560
H	21.1572680	15.5168660	12.0936590	N	18.4209020	12.3075970	11.5273700
C	22.2187040	17.0470970	11.0714360	N	18.7775730	11.2083970	11.9425490
C	23.3915710	17.1255940	12.0042960	N	18.9891040	10.1487160	12.2870790
H	24.3281780	16.9197690	11.4785840	C	20.3177230	13.6455840	10.5108400
H	23.2924790	16.4067300	12.8189410	H	21.3286280	13.2955680	10.7175950
H	23.4829470	18.1248960	12.4391100	H	19.9537890	13.1085640	9.6346040
C	22.1724740	17.9381760	9.9209200	C	20.2642000	15.1705330	10.2552830
O	23.0284570	18.7649830	9.6238010	H	19.7656530	15.3951300	9.3146580
N	21.0322630	17.7972560	9.1241510	N	21.5576310	15.8450230	10.1933550
H	20.9662800	18.4065400	8.3176720	C	22.4093750	15.8004990	11.2829520
C	19.9713600	16.9297600	9.2939960	H	22.0315740	15.2359850	12.1251970
O	19.0232490	16.9035580	8.5235510	C	23.6117330	16.4134190	11.3330490
O	12.0746300	16.8202500	13.3955240	C	24.5182090	16.3506090	12.5272250
H	11.1494010	17.0884810	13.3584550	H	25.4838070	15.9088160	12.2656790
H	12.3614550	16.9173600	14.3407200	H	24.0745160	15.7534470	13.3252420
O	16.5849230	13.8240880	19.4381000	H	24.7212780	17.3505800	12.9205940
H	15.8722190	14.3820450	19.7688080	C	24.0362090	17.1751280	10.1662170
H	16.7167660	14.0673910	18.4926360	O	25.0964400	17.7815290	10.0574500
O	18.6760550	17.7179510	13.8821890	N	23.1170090	17.1827390	9.1127100
H	18.5845680	17.0629350	13.1729570	H	23.3790310	17.7100250	8.2884820
H	18.2464660	17.2941160	14.6467340	C	21.8823100	16.5689230	9.0499050
O	17.7775030	16.5223120	16.4007790	O	21.1599100	16.6584100	8.0688980
H	18.5679360	16.0512400	16.6961520	O	9.4108160	16.1387230	16.1098050
				H	8.6044730	16.5401390	16.4534190
PC				H	10.1518490	16.4406850	16.6963160
C	13.1061250	15.2173520	17.2872470	O	18.2116380	14.1540410	16.9349060
H	13.7449740	14.4487440	17.7148400	H	18.7561080	14.9256880	16.7439970
H	12.4277360	14.7291370	16.5695030	H	17.2899590	14.3817240	16.6593770
C	12.2838890	15.8880150	18.3836410	O	18.5264250	18.4441710	12.0805330
H	11.5923770	15.1640410	18.8221600	H	19.1613600	17.9211870	11.5734860
H	12.9588450	16.2375800	19.1798850	H	17.9803130	17.7594030	12.5192150
N	11.5046900	17.0044370	17.8194870	O	15.7376160	16.6494230	15.2709440
H	10.9736890	17.4480450	18.5636800	H	16.7052680	16.3030530	13.9721000
C	12.3955360	18.0027700	17.2023580				
H	11.7849440	18.8083330	16.7866910	Prodrug 4 (EWM)			
H	13.0761250	18.4426280	17.9474970				
C	13.2174330	17.3537470	16.0927930	RC			
H	13.9335180	18.0651840	15.6894350	O	17.2978920	17.9336200	16.0029820
H	12.5459500	17.0502480	15.2738350	C	16.6675740	17.7201060	14.9624780
N	13.9466350	16.1969230	16.6054100	N	15.5745040	18.4309600	14.5899520
C	15.1629270	15.8086910	16.0307290	C	14.9679850	18.1868200	13.4309790
O	15.6136950	14.6641100	16.3320610	N	13.8912470	18.9341660	13.1204720

H	13.5731980	19.6436430	13.7615200	H	14.8863480	16.7210960	11.5394550
H	13.3830850	18.8039930	12.2615940	C	16.4273200	16.4046640	12.9683230
C	15.4184360	17.1725530	12.5281580	H	16.9282730	15.6081030	12.4398210
H	14.9220670	16.9784260	11.5873790	N	16.9619970	16.7603870	14.1686110
C	16.4921310	16.4412580	12.9150160	C	18.1778430	16.1219890	14.7152830
H	16.8934520	15.6367240	12.3181340	H	18.0309450	16.0665120	15.7916350
N	17.1129930	16.6759340	14.1044750	C	19.4661630	16.9044650	14.3999510
C	18.2878720	15.9003900	14.5466770	H	20.1777810	16.8046830	15.2199560
H	18.2216080	15.8468800	15.6307780	H	19.2704550	17.9591570	14.2236480
C	19.6306640	16.5329800	14.1338260	S	20.1438570	16.1306590	12.8865770
H	20.3837250	16.3520960	14.9008770	O	18.2805830	14.8103230	14.1832010
H	19.5422300	17.6033290	13.9643090	C	19.5428750	14.5297710	13.5595690
S	20.1124870	15.6915770	12.5803920	H	20.2414740	14.1834520	14.3252840
O	18.1965830	14.5911610	13.9998010	C	19.3616990	13.4814070	12.4826500
C	19.3804740	14.1705060	13.3067200	H	20.3147630	13.2905590	11.9815900
H	20.0812440	13.7384190	14.0248430	H	18.6268200	13.8011770	11.7435850
C	19.0165480	13.1504440	12.2516180	O	18.9164870	12.2960840	13.1423530
H	19.9020060	12.8537600	11.6881180	C	18.3859050	11.3224710	12.3519140
H	18.2522650	13.5271900	11.5724480	O	18.0460330	11.4953460	11.1864760
O	18.5018990	12.0042230	12.9696670	O	17.8034010	10.4424400	13.1974530
C	17.9442680	11.0270620	12.2462990	C	17.1548190	9.3072010	12.5781480
O	17.9070470	10.9717360	11.0365250	H	16.3442740	9.6703640	11.9427070
O	17.4351690	10.1388370	13.0902400	H	17.8948020	8.8057510	11.9538350
C	16.7898590	8.9639370	12.5030480	C	16.6400010	8.4069080	13.6812740
H	15.9667440	9.3103620	11.8773020	H	15.9154750	8.9252850	14.3144270
H	17.5224700	8.4581820	11.8734840	H	16.1418590	7.5392240	13.2408050
C	16.3157720	8.0919100	13.6423300	H	17.4561980	8.0453700	14.3113230
H	15.5925060	8.6168140	14.2700310	O	16.7419150	12.4446710	15.2704230
H	15.8283660	7.2034590	13.2335200	H	17.0438720	11.6993270	14.7301110
H	17.1507880	7.7646400	14.2653640	H	17.2407490	13.2091420	14.9429080
O	16.6302440	12.4549290	15.3910780	O	19.4705900	11.9541900	8.8267610
H	16.8553860	11.6359190	14.9317380	H	19.5313860	11.0975420	8.3895100
H	17.1385040	13.1495960	14.9429160	H	18.9942730	11.8041020	9.6663740
O	18.5908610	11.9280480	8.3983300	O	20.1816850	10.1802080	12.1228420
H	19.4422290	12.3800180	8.4037780	H	20.5533130	10.4834690	11.2851380
H	18.4160160	11.6563540	9.3134510	O	21.6248030	10.7445120	14.1968130
O	22.6834720	11.6944010	12.9344160	H	21.1064880	11.3936340	14.6852010
H	22.6876470	12.5551240	12.4960910	H	21.0783380	10.5331190	13.3580640
O	21.0952980	11.6018060	14.9399010				
H	20.2189870	11.3706120	14.6118600	INT			
H	21.7233640	11.6591490	14.1136320	O	16.6991510	18.1084520	16.0099960
				C	16.2704360	17.7832580	14.8972050
				N	15.2154180	18.3867670	14.2955410
TS1				C	14.8197750	18.0088620	13.0821020
O	16.9274110	18.1175980	16.0040160	N	13.7690860	18.6553020	12.5393330
C	16.3765300	17.7979120	14.9452730	H	13.3085970	19.3856450	13.0587920
N	15.2459800	18.3857950	14.4810900	H	13.4091900	18.4155820	11.6306600
C	14.7265320	18.0260620	13.3096560	C	15.4644900	16.9576600	12.3585910
N	13.6055030	18.6543140	12.9051340	H	15.1340790	16.6477300	11.3767500
H	13.1873700	19.3585340	13.4922290	C	16.5081450	16.3434060	12.9698560
H	13.1507380	18.4237680	12.0375380	H	17.0447180	15.5208540	12.5221760
C	15.3132460	17.0113100	12.4896140				

N	16.9210340	16.7241890	14.2088580	C	19.3458080	16.8107260	14.5086370
C	18.0613530	16.0773300	14.9005440	H	20.0461180	16.7291080	15.3408950
H	17.7712530	15.9918010	15.9459570	H	19.1371710	17.8607400	14.3206670
C	19.3657430	16.8827720	14.7772820	S	20.0451760	16.0227150	13.0166120
H	19.9801490	16.7395730	15.6668500	O	18.2228350	14.6821210	14.3631140
H	19.1802420	17.9447690	14.6395330	C	19.4738360	14.4089760	13.7001120
S	20.2133970	16.1917030	13.3112930	H	20.1918990	14.0766200	14.4543670
O	18.2527770	14.7848600	14.3574270	C	19.3057220	13.3602560	12.6101660
C	19.5746470	14.5492720	13.8361460	H	20.2365500	13.3588020	12.0201420
H	20.2006120	14.1732170	14.6495690	H	18.4964010	13.6678280	11.9378250
C	19.5164550	13.5490060	12.6992340	O	19.0565910	12.0890850	13.1494430
H	20.5112490	13.4721590	12.2396730	C	18.8056340	10.8925250	11.8821840
H	18.8073290	13.8793490	11.9370720	O	18.1334440	11.4210330	10.9605510
O	19.1137190	12.3129320	13.2520050	O	18.2715060	9.8828280	12.6641260
C	18.5974520	11.3406880	12.2952790	C	16.8452940	9.9116130	12.8296160
O	17.8574670	11.8080590	11.3563840	H	16.5532580	10.8534380	13.3018400
O	17.9588180	10.4517100	13.2386110	H	16.3688940	9.8631260	11.8472520
C	17.2608520	9.3553330	12.6409940	C	16.4519990	8.7263470	13.6896420
H	16.4341900	9.7353290	12.0326720	H	16.9216500	8.7775860	14.6751960
H	17.9435690	8.8109030	11.9801820	H	15.3677390	8.7137350	13.8314050
C	16.7480300	8.4498440	13.7463240	H	16.7422770	7.7833260	13.2186430
H	16.0664080	8.9848980	14.4133260	O	17.6922920	12.0401500	15.5749720
H	16.2021840	7.6058760	13.3149830	H	18.1395120	11.9502890	14.7042370
H	17.5707830	8.0504260	14.3453830	H	17.5956290	12.9958120	15.6748930
O	16.7082870	12.2902290	15.0973770	O	20.0710670	11.9253560	9.1614100
H	17.1104210	11.6233630	14.5098450	H	20.0225510	11.4286300	8.3367900
H	17.1924220	13.1060420	14.8987040	H	19.1886490	11.8675680	9.5974710
O	19.1647920	11.4030850	9.0936450	O	20.1219650	10.5041180	11.6246590
H	18.7479190	10.7577150	8.5118610	H	20.3928210	10.9359490	10.7923610
H	18.5104580	11.6349730	9.8060240	O	21.3807150	11.0838850	14.2696640
O	19.7721690	10.6123580	11.8128970	H	20.5348680	11.4648430	13.9370920
H	19.8227070	10.7344510	10.8488680	H	21.6680800	10.5204590	13.5411200
O	21.9714510	10.7951950	13.4940720				
H	21.6727260	11.3880780	14.1931080	PC			
H	21.2130180	10.7290480	12.8755650	O	23.1868480	14.3220930	16.5200470
				C	22.9719410	14.2558930	15.3040980
TS2				N	23.9463990	14.3704610	14.3663230
O	16.7977450	18.1337400	15.8665120	C	23.6578380	14.2546460	13.0720880
C	16.2730960	17.7167130	14.8277410	N	24.6746920	14.3709120	12.1938750
N	15.1663200	18.2720230	14.2737280	H	25.6042750	14.5671340	12.5295170
C	14.6645060	17.7939380	13.1373970	H	24.5257470	14.3261130	11.1996520
N	13.5678110	18.3975760	12.6375720	C	22.3294210	14.0159380	12.6020470
H	13.1577400	19.1758860	13.1288210	H	22.0985860	13.9270170	11.5493630
H	13.1311640	18.0864810	11.7860150	C	21.3537790	13.9266420	13.5414370
C	15.2438200	16.6808300	12.4527470	H	20.3135640	13.7778920	13.2925770
H	14.8268520	16.2888720	11.5352190	N	21.6386110	14.0460360	14.8653440
C	16.3412380	16.1172870	13.0177360	C	20.5875470	13.9465890	15.9123890
H	16.8374490	15.2572030	12.5943390	H	20.8476340	14.6902660	16.6638970
N	16.8633400	16.6009370	14.1766650	C	20.5258130	12.5474590	16.5495510
C	18.0683040	16.0118430	14.8131590	H	20.2079710	12.6254500	17.5902230
H	17.8718330	16.0111320	15.8837910	H	21.4837930	12.0351250	16.5076750

S	19.2699810	11.6459820	15.5742660	S	18.4236190	12.9067570	10.2963090
O	19.3415180	14.2650800	15.3391830	C	18.8789220	12.4674430	12.0688840
C	18.3376490	13.2361640	15.4589610	H	19.7555660	11.8152340	12.0143950
H	17.8015230	13.3922760	16.4000300	C	17.7925830	11.7317340	12.8232430
C	17.3600790	13.2919130	14.2806830	H	18.1352790	11.4948830	13.8330850
H	16.7606050	12.3612470	14.3378490	H	17.5361500	10.8049800	12.3104230
H	17.9655700	13.2016510	13.3565190	O	16.6332080	12.5832640	12.9146750
O	16.5683150	14.4207580	14.2972720	C	15.4925900	12.0183430	13.3002660
C	13.2621440	12.4358870	10.8284120	O	15.3378230	10.8435320	13.5611810
O	13.4211830	11.5601120	10.0042210	O	14.5610790	12.9678090	13.3477520
O	13.2089310	13.7433430	10.5754720	C	13.2053210	12.5583300	13.7211280
C	13.3658820	14.1446290	9.1848010	H	12.8138890	11.9420250	12.9105740
H	14.3346730	13.7871240	8.8321360	H	13.2734050	11.9540870	14.6265510
H	12.5832950	13.6616090	8.5976350	C	12.3742920	13.8073910	13.9357940
C	13.2651700	15.6526390	9.1320450	H	12.3856170	14.4124470	13.0218760
H	14.0475540	16.1231140	9.7316190	H	11.3380130	13.4738240	14.0663420
H	13.3826360	15.9866550	8.0981410	C	12.8001130	14.6498670	15.1427710
H	12.2932840	15.9979720	9.4917020	H	12.7729010	14.0242660	16.0430500
O	17.9236210	16.6227630	13.8623650	H	13.8413480	14.9663940	15.0232520
H	17.3795360	15.7829570	14.0131710	C	11.9120550	15.8792390	15.3454460
H	18.7641540	16.4384580	14.2977930	H	11.9424040	16.5410540	14.4738770
O	13.1568670	9.6700700	12.8295770	H	10.8674430	15.5939610	15.5064300
H	13.3209390	9.4846790	13.7620900	H	12.2332200	16.4618170	16.2133060
H	13.7073760	9.0642240	12.3191660	O	15.7242390	15.5654560	12.1774980
O	13.1111290	12.2414610	12.1383870	H	15.0330090	16.2346380	12.2420620
H	13.1450520	11.2695400	12.3525400	H	15.3505460	14.7489670	12.5408090
O	13.9777650	13.9930780	14.4235400	O	13.5822440	8.5827420	13.9197990
H	14.9718250	14.1471740	14.3652420	H	14.1345430	9.3737010	13.8102820
H	13.7184960	13.4774970	13.6478760	H	13.2914110	8.5774200	14.8387430
Prodrug 5 (EWM)				O	17.5191630	13.2544980	17.0706150
				H	17.1656010	12.2858910	16.9333480
				H	18.3133330	13.3467990	16.5330250
				O	16.6480730	10.8619020	16.8253630
				H	16.2294210	10.6838480	15.9735070
				TS1			
RC				O	22.0567920	15.8320280	12.5241300
O	22.1193870	15.8682670	12.3397900	C	21.0526700	16.3855000	12.9771610
C	21.1273250	16.4477810	12.7868090	N	21.1060490	17.5032850	13.7447650
N	21.2019030	17.5969890	13.5050640	C	19.9960380	18.0592470	14.2218380
C	20.1044160	18.1803030	13.9782770	N	20.1280140	19.1661500	14.9763050
N	20.2564330	19.3158260	14.6849160	H	21.0465170	19.5344350	15.1673230
H	21.1805850	19.6831190	14.8486190	H	19.3326500	19.6331040	15.3793110
H	19.4714120	19.8002310	15.0877110	C	18.6934450	17.5248070	13.9606450
C	18.7936220	17.6464090	13.7604160	H	17.7967430	17.9781700	14.3606350
H	17.9067530	18.1258530	14.1516520	C	18.6279610	16.4151340	13.1890720
C	18.7075830	16.5052020	13.0385150	H	17.6827910	15.9431810	12.9420810
H	17.7553410	16.0324740	12.8241830	N	19.7633680	15.8419580	12.6812960
N	19.8297460	15.9011360	12.5384470	C	19.6753450	14.6262030	11.8932920
C	19.7190230	14.6430620	11.8231990	H	20.6909410	14.3795710	11.5898070
H	20.7282400	14.3668680	11.5229630	O	19.1497020	13.5916560	12.7376960
O	19.1897390	13.6696880	12.7325040				
C	18.7837100	14.6742520	10.6096690				
H	19.2828410	15.1039650	9.7423000				
H	17.8599240	15.2119270	10.8158610				

C	18.7525790	14.7170970	10.6746190	C	19.6905180	14.6231280	11.9230590
H	19.2533810	15.2090140	9.8418400	H	20.7146610	14.3996480	11.6306920
H	17.8177140	15.2256040	10.9039430	O	19.1921950	13.5943220	12.7902670
S	18.4264320	12.9678860	10.2485560	C	18.7730480	14.6605340	10.6976080
C	18.8445070	12.4237320	12.0012540	H	19.2670940	15.1447190	9.8562340
H	19.7259910	11.7812250	11.9243320	H	17.8250160	15.1514700	10.9098330
C	17.7404060	11.6475150	12.6897010	S	18.4899060	12.8948480	10.3142220
H	18.0775020	11.3275920	13.6797840	C	18.9071920	12.4001700	12.0819110
H	17.4963620	10.7591690	12.1029550	H	19.8041290	11.7777130	12.0202260
O	16.6016600	12.4879460	12.8356200	C	17.8145710	11.6192190	12.7890060
C	15.4971740	11.9126340	13.3744640	H	18.2054710	11.2914400	13.7615430
O	15.2418750	10.7145780	13.2837470	H	17.5874180	10.7203350	12.2056760
O	14.5678220	12.8979450	13.4360310	O	16.6750750	12.4312980	12.9526930
C	13.2549530	12.5082890	13.8968340	C	15.5924300	11.8151080	13.6815850
H	12.8567390	11.7551660	13.2134320	O	15.2451830	10.6444450	13.2946420
H	13.3665590	12.0620710	14.8875460	O	14.6243750	12.8756910	13.5585630
C	12.3660900	13.7390710	13.9341130	C	13.3163750	12.5444310	14.0316970
H	12.3613450	14.2082060	12.9426660	H	12.8782290	11.7830270	13.3785050
H	11.3411070	13.3899230	14.1087140	H	13.3910330	12.1216500	15.0405670
C	12.7420660	14.7677160	15.0063710	C	12.4489550	13.7950890	14.0467620
H	12.6968150	14.2886560	15.9919370	H	12.4390900	14.2374880	13.0426190
H	13.7822860	15.0810010	14.8704100	H	11.4179690	13.4770110	14.2469930
C	11.8306070	15.9966650	14.9909350	C	12.8636510	14.8463090	15.0821710
H	11.8824000	16.5176090	14.0293360	H	12.8360280	14.3930430	16.0810000
H	10.7847760	15.7193890	15.1589220	H	13.9046640	15.1397360	14.9124290
H	12.1120030	16.7116090	15.7693050	C	11.9702780	16.0886420	15.0598890
O	15.6729320	15.4385660	12.2911410	H	12.0046600	16.5855660	14.0847580
H	14.9421980	16.0619170	12.3731110	H	10.9248960	15.8317330	15.2606940
H	15.3555550	14.5915210	12.6454150	H	12.2811240	16.8185740	15.8130550
O	13.8262640	8.7359600	14.6394770	O	15.6762430	15.2779510	12.2838210
H	14.2854080	9.4851120	14.2108780	H	14.9233490	15.8727850	12.3730720
H	13.6155960	9.0187030	15.5362700	H	15.4055750	14.4253530	12.6742990
O	18.2474480	13.5374110	15.6839440	O	13.8273660	8.6816290	14.4779040
H	17.4196530	12.9564650	15.5864050	H	14.3124070	9.4448590	14.0746940
H	18.5877580	13.6672110	14.7889660	H	12.9240970	8.9766150	14.6365150
O	16.0964600	12.0757200	15.4010250	O	18.1317600	13.6200110	15.6152010
H	16.2268660	11.1577460	15.6684420	H	17.3691720	13.0201350	15.4947580
				H	18.5001090	13.7370240	14.7271020
				O	15.9964280	11.8489290	15.1038630
				H	16.0585920	10.9284540	15.3862860
INT				TS2			
O	22.0330880	15.9048820	12.5565810	O	21.4270270	15.7235170	10.4604020
C	21.0085330	16.4453100	12.9787410	C	21.2456890	16.1856270	11.5898900
N	21.0228070	17.5861090	13.7138330	N	22.1890470	16.8975300	12.2583350
C	19.8927720	18.1259500	14.1613150	C	21.9471660	17.3804310	13.4739040
N	19.9866990	19.2568620	14.8855220	N	22.9316010	18.0761640	14.0748500
H	20.8930480	19.6536050	15.0775890	H	23.8159970	18.1960230	13.6067270
H	19.1748960	19.7131510	15.2672490	H	22.8285650	18.4504060	15.0034490
C	18.6080860	17.5499710	13.8999300	C	20.6975640	17.1859160	14.1447660
H	17.6945370	17.9902190	14.2758520	H	20.5106140	17.5782370	15.1351350
C	18.5814710	16.4178980	13.1587550				
H	17.6520520	15.9132890	12.9143780				
N	19.7379900	15.8606920	12.6816370				

C	19.7513060	16.4750900	13.4866890	H	19.7616000	20.0951010	15.4929920
H	18.7786900	16.2589350	13.9187480	C	19.6123960	17.9672040	13.9723470
N	19.9903790	15.9780040	12.2347620	H	18.6222440	18.2449730	14.3078630
C	18.9708610	15.1779740	11.5732260	C	19.8024060	16.8882910	13.1750800
H	19.4141470	14.8123440	10.6478980	H	18.9839910	16.2514390	12.8475020
O	18.6420140	14.0895050	12.4338130	N	21.0567980	16.5391430	12.7565840
C	17.6678600	15.9365990	11.2812930	C	21.2318860	15.3513220	11.9305670
H	17.7486630	16.5102590	10.3589040	H	22.3058470	15.1996800	11.8273940
H	17.3975670	16.5979580	12.1032200	O	20.6296170	14.2553390	12.6104490
S	16.4097260	14.6173440	11.0996130	C	20.5698770	15.4454330	10.5499830
C	17.5591280	13.3564220	11.9046190	H	21.1960510	15.9978310	9.8502580
H	17.9095210	12.7043500	11.0970470	H	19.5870720	15.9116150	10.6122180
C	16.9176720	12.4951330	12.9833720	S	20.4119570	13.7011450	10.0196770
H	17.6799510	11.7535360	13.2731840	C	20.6247560	13.0978910	11.7993230
H	16.1054280	11.9239610	12.5213260	H	21.6081870	12.6155030	11.8380850
O	16.4676990	13.2183110	14.0980850	C	19.5535830	12.1098640	12.2656250
C	15.0167510	12.6270150	14.8333290	H	19.8730230	11.8140230	13.2867310
O	14.9967210	11.3714890	14.7175590	H	19.7034280	11.2052860	11.6424090
O	14.0086350	13.3829000	14.2474790	O	18.2530040	12.5651900	12.2321110
C	13.2922920	12.8035170	13.1483860	C	13.4546080	12.1049440	14.0407760
H	13.9037640	12.8681210	12.2422360	O	13.1938540	11.1224640	13.3540170
H	13.1021480	11.7482540	13.3568680	O	12.5174370	12.9062720	14.5586420
C	11.9917440	13.5705390	12.9566440	C	11.1312610	12.5724530	14.2752330
H	12.2191030	14.6288230	12.7783680	H	10.9901640	12.5775570	13.1930360
H	11.5267730	13.1986380	12.0348140	H	10.9355710	11.5632580	14.6447080
C	11.0020400	13.4379000	14.1184650	C	10.2493210	13.6015050	14.9572760
H	10.7880860	12.3751200	14.2886560	H	10.5042560	14.5990490	14.5806910
H	11.4692740	13.8061220	15.0372510	H	9.2206450	13.4049560	14.6315170
C	9.6917250	14.1898020	13.8725150	C	10.3166850	13.5805370	16.4879950
H	9.8689500	15.2608920	13.7296030	H	10.0597660	12.5754790	16.8448860
H	9.1809860	13.8191720	12.9776340	H	11.3462840	13.7660600	16.8106760
H	9.0028090	14.0797440	14.7152020	C	9.3843440	14.6076490	17.1340230
O	16.8273040	15.8779040	14.7081200	H	9.6375260	15.6260870	16.8220610
H	16.5207810	15.9364590	15.6198350	H	8.3404440	14.4282830	16.8567940
H	16.6746030	14.9436180	14.4324140	H	9.4475500	14.5716540	18.2252570
O	16.9621360	9.8922450	15.8057350	O	17.3947510	15.0565730	12.1867680
H	16.1842060	10.3635640	15.4076120	H	16.5332390	15.0139570	12.6159040
H	16.6290130	9.3311080	16.5146850	H	17.7754600	14.1246370	12.2057150
O	17.9133990	12.4491990	16.3639750	O	14.9662870	9.3649090	12.0992940
H	17.7048060	12.8149080	15.4798520	H	14.2391400	9.8751070	12.5068210
H	17.7862780	11.4823870	16.2778950	H	14.8568810	8.4440220	12.3611830
O	15.1895640	13.2180070	16.0872890	O	16.5795320	11.1675140	13.5030320
H	16.0385380	12.9010480	16.4521180	H	17.2887170	11.7233380	12.9710220
				H	16.2494950	10.4443840	12.9388250
				O	14.6464760	12.5276690	14.3769090
PC				H	15.4226460	11.9390060	13.9889720
O	23.3166820	16.9505540	12.7526930				
C	22.1997850	17.2931480	13.1511940				
N	22.0001540	18.3710990	13.9530480	Prodrug 6 (EWM)			
C	20.7767080	18.7065350	14.3531720				
N	20.6556460	19.7872770	15.1486370	RC			
H	21.4772680	20.3038570	15.4198200	O	20.7462270	19.5407830	10.8810670

C	21.3865540	18.5023200	10.8212370	H	19.5797560	12.1884600	13.9870680
N	22.7661100	18.4891420	10.8011440	O	20.7581090	15.0872440	14.1390310
H	23.2065910	19.4004520	10.8407480	H	20.2686530	15.7173740	13.5946320
C	23.6219830	17.3847050	10.7442570	H	20.4264830	14.1615170	13.8468030
O	24.8367210	17.5524460	10.7357800				
C	22.9438090	16.0968430	10.7020160	TS1			
C	23.7678080	14.8438030	10.6585470	O	21.8381170	11.1546280	14.7948180
H	23.1318130	13.9580060	10.6298820	C	21.6116440	11.8342030	15.7840790
H	24.4161750	14.8289600	9.7780290	N	22.5334700	11.9830950	16.8006900
H	24.4176540	14.7693450	11.5349750	H	23.4070840	11.4881930	16.6665290
C	21.5936290	16.0932910	10.7129230	C	22.4145110	12.7302740	17.9763820
H	21.0358330	15.1665070	10.7029150	O	23.3378520	12.7541870	18.7827410
N	20.8122120	17.2351600	10.7561860	C	21.1472220	13.4341800	18.1193230
C	19.3589750	17.1250470	10.7678740	C	20.9210870	14.2809360	19.3371030
H	18.9826920	18.1451610	10.8081870	H	19.9365170	14.7500080	19.3107800
O	18.9662880	16.4197670	11.9517370	H	20.9914920	13.6837310	20.2505060
C	18.7392720	16.3479040	9.5822420	H	21.6739840	15.0703660	19.4131790
H	18.2093560	17.0336870	8.9208610	C	20.2331700	13.2925140	17.1356700
H	19.4917360	15.8297820	8.9886880	H	19.2812160	13.8049810	17.1796380
C	17.7552440	15.3588360	10.2474120	N	20.4185170	12.5169590	16.0045440
N	16.4011420	15.3652900	9.6553740	C	19.3735650	12.4517250	14.9861930
N	16.1908670	14.5598940	8.7522160	H	19.7578760	11.7949950	14.2095160
N	15.8728290	13.8628100	7.9162860	O	19.1869090	13.7705910	14.4576300
H	18.1595990	14.3433140	10.2341780	C	17.9856200	11.9846830	15.4865900
C	17.6675520	15.8698980	11.6984430	H	17.6873970	11.0822280	14.9521670
H	16.9179900	16.6708970	11.7442180	H	17.9807830	11.7566870	16.5518440
C	17.3341650	14.7929420	12.7007690	C	17.0361160	13.1463980	15.1284090
H	18.1604830	14.0832010	12.8402650	N	15.7395370	12.7047160	14.5763360
H	16.4394840	14.2588730	12.3757010	N	14.8057890	12.6088270	15.3681990
O	17.0513530	15.4476160	13.9676310	N	13.8690330	12.4860610	15.9953730
C	16.4976700	14.7058770	14.9315940	H	16.8690350	13.7965540	15.9919520
O	16.2106340	13.5308380	14.7813540	C	17.8189050	13.9087030	14.0463190
C	16.2858440	15.4796050	16.2105930	H	17.6733440	13.4077910	13.0807840
H	15.2572090	15.3049790	16.5349110	C	17.4503240	15.3690050	13.9237530
H	16.4083600	16.5465360	16.0186600	H	17.7724080	15.9236390	14.8097740
C	17.2596510	15.0151260	17.3141820	H	16.3653260	15.4623630	13.8304690
H	17.1506970	13.9371170	17.4621170	O	18.0905270	15.8960820	12.7619130
H	18.2890790	15.2139950	17.0111030	C	17.8174380	17.2099020	12.4637020
C	16.9672450	15.7300460	18.6441380	O	16.8360140	17.7733520	12.9562950
O	17.8058180	16.5791310	19.0472240	C	18.4042590	17.5484550	11.1063140
O	15.8968140	15.4295090	19.2461190	H	17.7964950	16.9950430	10.3765810
O	14.6512610	11.8526000	16.5702830	H	19.4160710	17.1470310	11.0454340
H	15.1794580	12.4018650	15.9679170	C	18.3852950	19.0419100	10.7666800
H	14.4603310	12.4069440	17.3545000	H	17.3822160	19.4402090	10.9305300
O	14.1332340	13.4442360	18.7994790	H	19.0720590	19.5582780	11.4364960
H	14.7942920	14.1715050	18.9353420	C	18.7905440	19.2735170	9.3072310
H	13.2583280	13.8461280	18.8344560	O	20.0157830	19.4501090	9.0585770
O	17.1205940	17.7962050	21.4003380	O	17.8809730	19.2494290	8.4245610
H	16.2750150	17.4294700	21.6820500	O	14.5647280	18.8027250	11.5749140
H	17.3445270	17.3395510	20.5516940	H	15.3557680	18.4778870	12.0423990
O	19.8884630	12.7935360	13.3004310	H	14.7960560	18.8390860	10.6247890

O	15.2524960	18.9419050	8.8667430	H	19.1854590	19.6860060	11.4325210
H	16.2316250	19.0442590	8.7207430	C	18.8512760	19.3200190	9.3360950
H	14.9549710	18.2161960	8.3073870	O	20.0677050	19.5363720	9.0699070
O	20.6778240	19.6759380	6.4261780	O	17.9440780	19.2017010	8.4586700
H	19.8764210	19.5672840	5.9021290	O	14.5941640	18.2717710	11.5103080
H	20.3990920	19.5938690	7.3738470	H	15.4287240	18.1383080	12.0246980
O	19.4581240	18.0380880	13.5665330	H	14.8520630	18.4334860	10.5830190
H	18.9696560	18.4569870	14.2857670	O	15.3235380	18.7550100	8.8204950
O	21.0823220	16.1277910	14.2971220	H	16.2998610	18.9158850	8.7195200
H	20.5530490	15.3186990	14.3081710	H	15.0872100	18.0569130	8.2000590
H	20.4423450	16.8727470	14.0346720	O	20.7205300	19.6361750	6.4318680
INT				H	19.9253230	19.4727470	5.9126370
O	21.8117200	11.1518580	14.7227810	H	20.4414150	19.5951260	7.3827610
C	21.5940850	11.8259910	15.7179080	O	19.0653280	17.9813520	13.5302910
N	22.5212680	11.9596900	16.7321550	H	18.6102000	18.4705070	14.2275830
H	23.3901440	11.4584750	16.5908920	O	21.0054810	16.1240000	14.2813610
C	22.4126410	12.6980020	17.9143630	H	20.5125750	15.2896720	14.2926140
O	23.3391900	12.7080390	18.7175110	H	20.3473400	16.7994920	14.0131500
C	21.1516190	13.4108040	18.0676070	TS2			
C	20.9356920	14.2487230	19.2933300	O	21.1230170	10.6965340	14.5747150
H	19.9545500	14.7252830	19.2740460	C	21.2160490	11.3824530	15.5821460
H	21.0041000	13.6430620	20.2013080	N	22.2514100	11.2271630	16.4829080
H	21.6947620	15.0317650	19.3741520	H	22.9236140	10.5070800	16.2472190
C	20.2333810	13.2846790	17.0855720	C	22.4839420	11.9343330	17.6662180
H	19.2858800	13.8048730	17.1364690	O	23.4606130	11.6651200	18.3583330
N	20.4081240	12.5172030	15.9477170	C	21.4947960	12.9615740	17.9594990
C	19.3557490	12.4678760	14.9331270	C	21.6551330	13.7897940	19.2005050
H	19.7303080	11.8101970	14.1526660	H	20.8482440	14.5182830	19.2921960
O	19.1796950	13.7897390	14.4123880	H	21.6527730	13.1625160	20.0963800
C	17.9680150	12.0122560	15.4426760	H	22.6052870	14.3312600	19.1930810
H	17.6352910	11.1458660	14.8699540	C	20.4741000	13.1209320	17.0885160
H	17.9810160	11.7295230	16.4948190	H	19.7168070	13.8788120	17.2397650
C	17.0416070	13.2113510	15.1591640	N	20.3080300	12.3719810	15.9385540
N	15.7079670	12.8186300	14.6588220	C	19.1718760	12.6469900	15.0555980
N	14.8094920	12.7281630	15.4902810	H	19.3209000	12.0229140	14.1759690
N	13.8991320	12.6156000	16.1576330	O	19.2169870	14.0243710	14.7014210
H	16.9327300	13.8438740	16.0451190	C	17.7795060	12.4041140	15.6846880
C	17.7950980	13.9779790	14.0612410	H	17.3038250	11.5362290	15.2272750
H	17.5996460	13.4992890	13.0934240	H	17.8425720	12.2207720	16.7575550
C	17.4705610	15.4538080	13.9750170	C	16.9920690	13.6944640	15.3667860
H	17.8343720	15.9582540	14.8798830	N	15.6638070	13.4405140	14.7612860
H	16.3812370	15.5724480	13.9435100	N	14.7008690	13.4376340	15.5205670
O	18.0709830	15.9813400	12.8108740	N	13.7359680	13.4165250	16.1185370
C	17.9630740	17.4542470	12.6687680	H	16.8714500	14.3064870	16.2651500
O	16.8200780	17.9467270	13.0407110	C	17.8801450	14.4360230	14.3503880
C	18.4102870	17.6808590	11.2099840	H	17.6499490	14.0732060	13.3396860
H	17.7029190	17.1462300	10.5692030	C	17.7667410	15.9572770	14.3874280
H	19.3917570	17.2187470	11.0627130	H	18.0798900	16.2773890	15.4037050
C	18.4602540	19.1608630	10.8080200	H	16.6878150	16.1895600	14.3081860
H	17.4782970	19.6111060	10.9738490	O	18.4738270	16.5896040	13.3849470

C	17.4927200	18.2564060	12.7667460	N	14.5092820	14.2581360	14.3897650
O	16.2869210	17.9643770	12.8396180	H	17.4189360	14.7171800	15.8584060
C	18.2609620	18.3102320	11.4620900	C	19.1392380	14.6830180	14.5331950
H	18.0521340	17.3917870	10.9142250	H	19.2394820	14.4785830	13.4584240
H	19.3311280	18.3377970	11.6735020	C	19.3420910	16.1817610	14.7926920
C	17.8543510	19.5354870	10.6165340	H	19.2866070	16.3028710	15.9000520
H	16.7762990	19.5103450	10.4345340	H	18.4188840	16.6647050	14.4040720
H	18.0877570	20.4543500	11.1579570	O	20.4848170	16.7116700	14.2472050
C	18.5936080	19.5355450	9.2731080	C	17.1127000	19.4644490	12.1573280
O	19.6314060	20.2472140	9.1752830	O	16.1200260	18.8753690	12.5429650
O	18.1387830	18.8025190	8.3464510	C	17.7338710	19.3161770	10.7937010
O	14.7936840	16.6682460	10.8454080	H	17.7163830	18.2576250	10.5307260
H	15.3457420	17.0986960	11.5290660	H	18.7725820	19.6486600	10.8260650
H	15.2095350	16.8616250	9.9821000	C	16.9457350	20.1264110	9.7412670
O	15.9574830	17.2315690	8.3511290	H	15.8962040	19.8166860	9.7577910
H	16.7570380	17.8207380	8.3833480	H	16.9869390	21.1907310	9.9776530
H	16.1955170	16.4621850	7.8223700	C	17.4967250	19.8950860	8.3227380
O	20.9573370	20.0421450	6.8007690	O	17.9769410	20.8899430	7.7185000
H	20.5010400	19.3864910	6.2615690	O	17.4308500	18.7237170	7.8542270
H	20.4508660	20.0961880	7.6505300	O	14.6091150	16.8691070	11.0368880
O	18.0002580	19.1581770	13.6829400	H	15.0964490	17.5230990	11.5630360
H	17.3540400	19.2244980	14.4012300	H	15.1243200	16.7389700	10.2144160
O	21.0649910	16.3701440	13.8909220	O	16.0872190	16.5428180	8.6967320
H	21.0740840	15.4748040	14.2509050	H	16.5812370	17.3544220	8.4141990
H	20.0963030	16.5265290	13.6754560	H	16.7143940	15.8115130	8.6894540
PC				O	18.9313630	20.4911010	5.1889810
				H	18.8339480	19.5614810	4.9546040
				H	18.5748980	20.5859460	6.1068470
O	21.0765440	10.1789670	15.0308990	O	17.7510590	20.3583830	12.9306540
C	21.0470190	10.7156530	16.1288390	H	17.2885650	20.4312940	13.7823890
N	21.6894310	10.1770360	17.2265360	O	22.5781200	15.7961190	15.4697920
H	22.1855400	9.3109690	17.0541040	H	22.3269300	14.8823480	15.6493810
C	21.7414020	10.6764140	18.5312340	H	21.7596520	16.1834740	14.9872570
O	22.3621690	10.0658490	19.3959950	Prodrug 7 (EWM)			
C	21.0198860	11.9250740	18.7279990	RC			
C	21.0191630	12.5574830	20.0888480	O	23.5915530	12.7544210	12.4676530
H	20.4521220	13.4896310	20.0867760	C	23.1285980	13.7790980	11.9900780
H	20.5769220	11.8901290	20.8339660	N	23.2679700	14.0963710	10.6541130
H	22.0372410	12.7774110	20.4222060	H	23.7812950	13.4200650	10.1016920
C	20.3834560	12.4610230	17.6631160	C	22.7908920	15.2224710	9.9763170
H	19.8454290	13.3967120	17.7389430	O	23.0051410	15.3505250	8.7755810
N	20.3724510	11.8992960	16.4001650	C	22.0543140	16.1616900	10.8102440
C	19.6574730	12.5765460	15.3157040	C	21.4838330	17.3982140	10.1798210
H	19.9050760	12.0305290	14.4057860	H	20.7812650	17.1448150	9.3810230
O	20.1331060	13.9124460	15.2413320	H	20.9578700	18.0070490	10.9166490
C	18.1291950	12.6794320	15.5056890	H	22.2709960	18.0098550	9.7301810
H	17.6115600	11.9242450	14.9136140	C	21.9133910	15.8671140	12.1208230
H	17.8456450	12.5356480	16.5490540	H	21.3576380	16.5145410	12.7852440
C	17.7945570	14.1121500	15.0279950	N	22.4290500	14.7331680	12.7230650
N	16.8166070	14.1568240	13.9124600				
N	15.6314350	14.2056380	14.2245450				

C	22.1953480	14.4917780	14.1440850	C	22.8466620	15.0184420	9.7684320
H	22.5914480	13.4981550	14.3498960	O	23.0324430	15.1043510	8.5589930
O	20.7865840	14.5291830	14.3776930	C	22.1171780	15.9788620	10.5839490
C	22.7765150	15.5351440	15.1006030	C	21.5163390	17.1837310	9.9212970
H	23.8288640	15.3648130	15.3234220	H	20.8037540	16.8915840	9.1448780
H	22.6697880	16.5391940	14.6864430	H	20.9936100	17.8099020	10.6457400
C	21.8885100	15.3887620	16.3379550	H	22.2853050	17.7913100	9.4360030
N	22.5255930	14.4194730	17.2672070	C	22.0092150	15.7308720	11.9075330
N	22.1141590	14.4177340	18.4245080	H	21.4604120	16.3948010	12.5617380
N	21.8279300	14.3280560	19.5184690	N	22.5513980	14.6254000	12.5380850
H	21.7482760	16.3424290	16.8511480	C	22.3502680	14.4346660	13.9731880
C	20.5461210	14.8371460	15.7611460	H	22.7524500	13.4487380	14.2044590
H	20.2727910	13.9141000	16.2800320	O	20.9500620	14.4844520	14.2365910
C	19.4125610	15.8377710	15.8694040	C	22.9555240	15.5116520	14.8760980
H	19.6178380	16.7344510	15.2836100	H	24.0126750	15.3479340	15.0808600
H	19.2509280	16.1172660	16.9126570	H	22.8407170	16.4988870	14.4250120
O	18.2142220	15.2020360	15.3659500	C	22.0941270	15.4156130	16.1376030
C	17.1311040	15.9802890	15.1782780	N	22.7600080	14.4992900	17.1014410
O	17.1271550	17.1726460	15.4092250	N	22.4110640	14.5879440	18.2753880
C	15.9573910	15.1820910	14.6682900	N	22.1831010	14.5823240	19.3868390
H	16.3190530	14.5215820	13.8739220	H	21.9545280	16.3917470	16.6065950
H	15.6487710	14.5155800	15.4833680	C	20.7431690	14.8285970	15.6197320
C	14.7816390	16.0371540	14.1934950	H	20.5101240	13.9118010	16.1697460
H	14.4457870	16.6825410	15.0085840	C	19.5932350	15.8099680	15.7416560
H	15.1143250	16.7021060	13.3919080	H	19.7856200	16.7029990	15.1413480
C	13.6231320	15.1699830	13.7034070	H	19.4823090	16.1098530	16.7890890
H	13.9566890	14.5130850	12.8911920	O	18.4022080	15.1632630	15.3017320
H	13.2909370	14.4952410	14.5013370	C	17.2653160	15.9461050	15.2394800
C	12.3783140	15.9196930	13.1960730	O	17.3543240	17.1793830	15.1850980
O	12.3654980	17.1788890	13.2007530	C	16.1559270	15.1546860	14.5743650
O	11.4197470	15.1982170	12.7946890	H	16.5100440	14.9375840	13.5562030
O	13.7464230	19.4766570	13.7155740	H	16.0639250	14.1913620	15.0791150
H	13.1030010	20.1354010	13.4320860	C	14.8099300	15.8734190	14.5072380
H	13.3295470	18.5981690	13.5652090	H	14.4910650	16.1254810	15.5202360
O	18.4200830	19.5120170	16.4652610	H	14.9266300	16.8192260	13.9714790
H	17.7338030	20.1887690	16.4668000	C	13.7493220	15.0157860	13.8171060
H	18.0075410	18.7020680	16.1220790	H	14.0811130	14.7407880	12.8078850
O	11.2105050	12.4926810	12.6655770	H	13.6305850	14.0621670	14.3460920
H	11.3289230	13.4723780	12.7320090	C	12.3453220	15.6275070	13.6740550
H	10.3051270	12.3423220	12.3722630	O	12.1228290	16.7913520	14.1014220
O	18.2223240	13.2611930	19.2168810	O	11.4731810	14.8984560	13.1151990
H	19.1334190	13.4713960	19.4588640	O	13.1070550	18.9998100	15.3592660
O	17.9757170	12.3368050	16.8355540	H	12.3066310	19.5348080	15.3970370
H	18.1022250	12.7208280	17.7899000	H	12.8557100	18.1567280	14.9174410
H	17.9375420	13.0893400	16.2337050	O	18.4458730	19.2686330	16.6294960
TS1				H	17.6838600	19.7329550	16.9932550
O	23.7315810	12.6518290	12.3287130	H	18.0924470	18.4968530	16.1398870
C	23.2460690	13.6537890	11.8251970	O	11.6925790	12.3676610	12.1669760
N	23.3530950	13.9239440	10.4758250	H	11.6597350	13.2897800	12.5257450
H	23.8622380	13.2337420	9.9369480	H	10.7794430	12.0794800	12.0599310
				O	16.5971520	15.5802830	17.1865980

H	16.8976750	16.3795410	17.6368260	O	13.0540520	18.9321630	15.5084250
O	17.7084490	13.3609740	17.9516310	H	12.2474930	19.4584200	15.5376780
H	17.2946560	14.2514420	17.6761110	H	12.8223040	18.0968810	15.0412480
H	18.2153920	13.0678260	17.1863920	O	17.7187780	18.9896630	16.7105750
INT				H	16.9832550	19.6112840	16.6731610
				H	17.6781000	18.4226830	15.8822400
O	23.7700380	12.6359650	12.1922510	O	11.8134080	12.3767780	12.1110740
C	23.2722590	13.6538660	11.7338210	H	11.7501450	13.2843130	12.5022750
N	23.3749710	13.9842480	10.3971710	H	10.9282350	12.1419250	11.8116550
H	23.8910090	13.3241060	9.8280650	O	16.9032580	16.1343210	16.7823070
C	22.8605560	15.1062110	9.7402680	H	17.1259590	17.0345960	17.0703340
O	23.0466520	15.2488500	8.5359500	O	17.5330150	13.9808140	18.3697680
C	22.1238820	16.0225640	10.5983050	H	17.3257370	14.7610930	17.8067040
C	21.5149330	17.2529840	9.9919900	H	18.0608580	13.3957680	17.8147210
H	20.8004760	16.9927800	9.2059470	TS2			
H	20.9926100	17.8440310	10.7456450				
H	22.2794350	17.8849320	9.5313400	O	23.0907800	13.3823550	11.6669900
C	22.0175040	15.7130720	11.9093210	C	22.2128180	14.2348930	11.6238040
H	21.4626190	16.3401460	12.5941560	N	21.8068630	14.8066120	10.4345160
N	22.5672080	14.5840580	12.4882800	H	22.2832970	14.4677890	9.6075100
C	22.3721990	14.3325330	13.9172580	C	20.8456060	15.8031680	10.2395230
H	22.7544600	13.3284590	14.1004010	O	20.6154680	16.2142640	9.1045940
O	20.9788150	14.4051440	14.1933510	C	20.1951880	16.2562210	11.4570070
C	23.0139060	15.3565490	14.8564870	C	19.1343970	17.3153670	11.3667050
H	24.0671130	15.1547630	15.0481150	H	18.3193220	17.0026570	10.7073120
H	22.9262900	16.3619140	14.4406940	H	18.7204760	17.5253690	12.3529800
C	22.1552760	15.2405950	16.1174000	H	19.5387090	18.2437770	10.9516890
N	22.8084950	14.2819040	17.0507100	C	20.5710970	15.6953320	12.6309300
N	22.4278780	14.3053650	18.2173470	H	20.0874980	15.9715530	13.5615980
N	22.1693200	14.2396510	19.3206160	N	21.5447370	14.7195530	12.7385770
H	22.0406870	16.2040610	16.6186050	C	21.9287550	14.1928470	14.0609180
C	20.7870400	14.7044770	15.5926420	H	22.4706350	13.2695610	13.8605430
H	20.5392120	13.7700920	16.1066080	O	20.7566100	13.9265480	14.8130020
C	19.6548730	15.7020630	15.7643610	C	22.7634770	15.1570090	14.9090010
H	19.8694240	16.6126540	15.1933870	H	23.8284210	15.1040950	14.6849230
H	19.6025300	15.9756050	16.8286590	H	22.4274840	16.1848850	14.7576280
O	18.4478960	15.1137900	15.3361530	C	22.4284460	14.7112040	16.3289680
C	17.2740820	16.0280790	15.3431760	N	23.3420150	13.5861340	16.6869800
O	17.5169270	17.1973470	14.8131720	N	23.3134010	13.2133370	17.8550660
C	16.1791820	15.1763230	14.6781150	N	23.3778420	12.7903390	18.9069270
H	16.5345110	14.9343330	13.6701550	H	22.5502070	15.5156350	17.0581500
H	16.0918430	14.2264090	15.2176000	C	20.9527780	14.2672430	16.2115600
C	14.8167160	15.8659600	14.5984560	H	20.7651080	13.3553970	16.7859370
H	14.4665210	16.0995030	15.6079500	C	19.9733630	15.3607670	16.6632590
H	14.9273020	16.8226620	14.0809310	H	20.1801840	16.2751420	16.0797240
C	13.7776770	15.0052700	13.8795830	H	20.2345620	15.5924450	17.7145780
H	14.1264920	14.7568040	12.8692080	O	18.6488290	14.9921020	16.5280090
H	13.6695660	14.0384070	14.3869150	C	17.6065030	16.2743400	15.5340400
C	12.3646900	15.5946940	13.7317860	O	18.4244810	16.9431200	14.8530120
O	12.1151350	16.7442170	14.1830390	C	16.7010600	15.2385250	14.8956990
O	11.5118480	14.8642190	13.1447250	H	17.3235560	14.6057350	14.2601740

H	16.2790530	14.6008940	15.6763200	C	21.2673420	13.6482010	16.2233200
C	15.5753710	15.8786380	14.0673240	H	21.1425450	12.5570980	16.2663360
H	14.9537400	16.5045460	14.7133030	C	20.2275640	14.3162190	17.1287620
H	16.0085410	16.5446210	13.3147710	H	20.3557550	15.4133800	16.9762580
C	14.7071130	14.8258210	13.3795880	H	20.5964120	14.1271850	18.1643180
H	15.3251680	14.1831870	12.7412560	O	18.9397140	13.8909410	16.9301150
H	14.2697420	14.1506940	14.1260640	C	16.4985310	16.7608830	13.1613440
C	13.5468450	15.3451490	12.5126450	O	16.8391620	17.3199860	12.1363690
O	13.3121960	16.5816570	12.4587230	C	15.5450670	15.5943240	13.2278220
O	12.8768760	14.4678070	11.8923450	H	15.5615870	15.0936010	12.2577600
O	13.9772640	19.0573230	13.3905510	H	15.8915830	14.8861640	13.9852410
H	13.3259090	19.5933910	12.9250620	C	14.1121080	16.0590240	13.5629860
H	13.8197240	18.1259380	13.1130080	H	14.1129110	16.5709350	14.5287480
O	18.7684280	19.1554570	16.3518880	H	13.7868020	16.7918830	12.8190490
H	18.4212250	19.9680020	15.9663610	C	13.1342240	14.8860870	13.5965250
H	18.8110710	18.4794970	15.6333030	H	13.1411110	14.3604830	12.6343550
O	13.1674610	11.7713060	11.8549440	H	13.4599860	14.1438820	14.3347300
H	13.1004190	12.7578060	11.8992860	C	11.6687310	15.2334060	13.9150850
H	12.4661650	11.4724520	11.2656780	O	11.3458540	16.4321820	14.1252680
O	16.9559020	16.9106370	16.5875580	O	10.8609810	14.2606090	13.9450670
H	17.4477940	17.7278060	16.7934990	O	12.1777560	19.0319370	14.2428330
O	17.2940030	14.8658890	18.8091670	H	11.3502830	19.4756740	14.4589430
H	16.7010370	15.6184680	18.6977830	H	11.9710330	18.0720620	14.1815360
H	17.8299800	14.8696960	17.9637390	O	18.4791180	19.3510750	14.4833070
PC				H	18.0241890	20.1826650	14.6637030
O	22.5769840	12.7812290	11.5608730	H	19.1111690	19.5267910	13.7758670
C	22.4927630	13.9896800	11.7255300	O	11.2898310	11.6152960	13.5017660
N	22.5229790	14.8777390	10.6679640	H	11.1803920	12.5859240	13.6566090
H	22.6173990	14.4550380	9.7523830	H	10.5009170	11.1880690	13.8530850
C	22.4371280	16.2724650	10.7054790	O	16.9181890	17.1582280	14.3732920
O	22.4817900	16.9168960	9.6620390	H	17.4976630	17.9632050	14.3117420
C	22.2969530	16.8321740	12.0415800	O	17.1121640	15.7328810	17.0309770
C	22.1910370	18.3209330	12.1970190	H	17.0518190	16.1536460	16.1628680
H	21.3250540	18.7140060	11.6569180	H	17.8436850	15.0236330	16.9809020
H	22.0946010	18.5993490	13.2475140	Prodrug 8 (EWM)			
H	23.0738210	18.8229840	11.7910940	RC			
C	22.2685430	15.9744260	13.0854710	O	21.1386480	19.4860270	14.8501480
H	22.1456850	16.3254330	14.1014810	C	20.1904030	18.9530380	15.4094680
N	22.3686630	14.6010850	12.9667000	N	19.3990470	19.6345180	16.3111960
C	22.3048480	13.7671050	14.1693780	H	19.6632280	20.5984670	16.4751470
H	22.2887010	12.7361740	13.8170310	C	18.2734790	19.1694220	16.9981540
O	21.1031980	14.0784060	14.8581400	O	17.6729170	19.9192670	17.7627550
C	23.4498990	13.9911510	15.1819850	C	17.9269860	17.7860760	16.7160450
H	24.1860850	13.1893620	15.1172200	C	16.7348900	17.1784750	17.3975000
H	23.9690060	14.9332280	15.0016040	H	15.8180550	17.7208160	17.1477100
C	22.7329570	13.9959400	16.5523690	H	16.6169790	16.1367160	17.0983180
N	23.2649690	12.9902620	17.5050070	H	16.8402790	17.2185860	18.4858070
N	24.1635760	13.3602530	18.2527450	C	18.7008840	17.0953620	15.8473580
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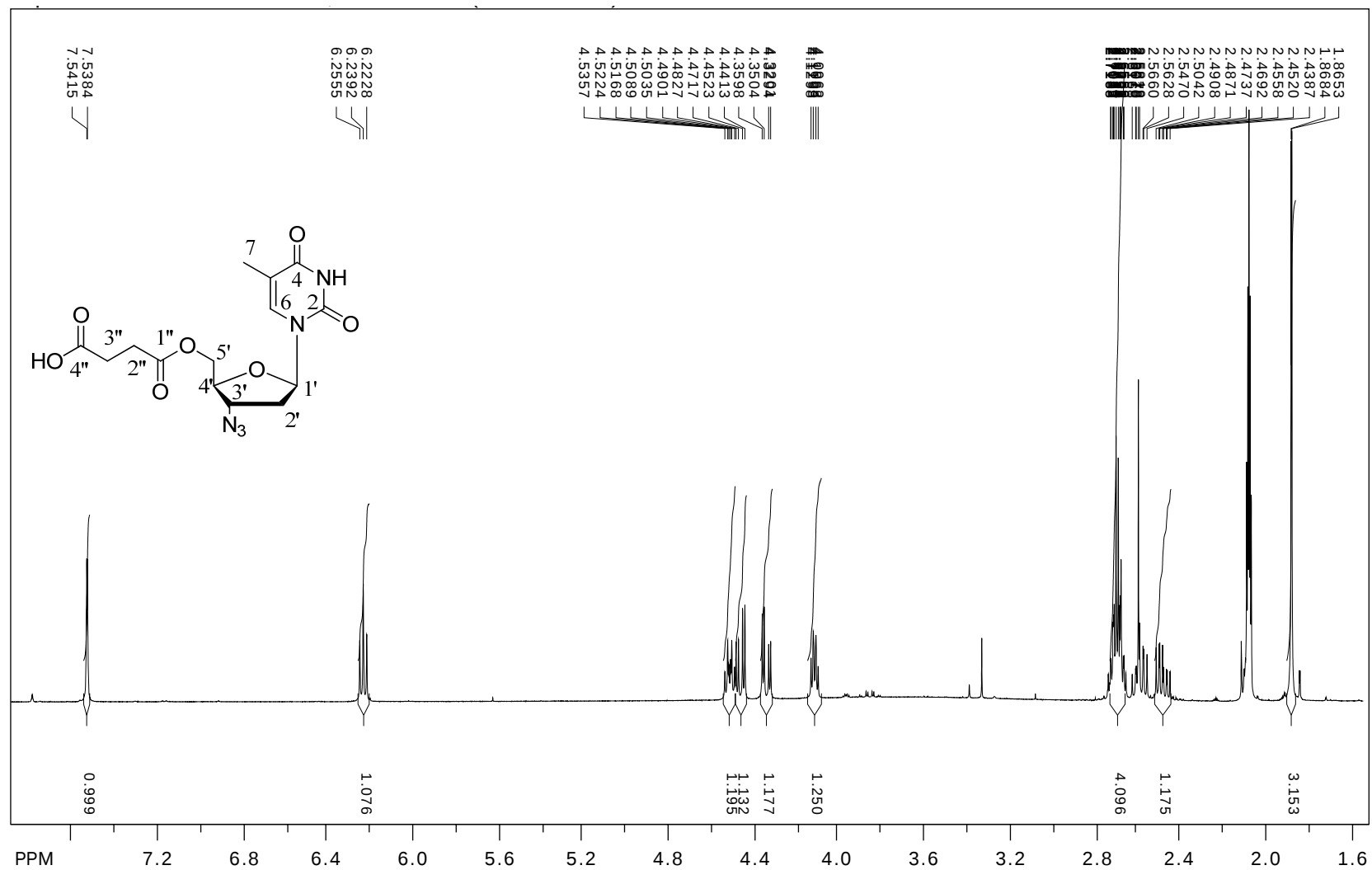
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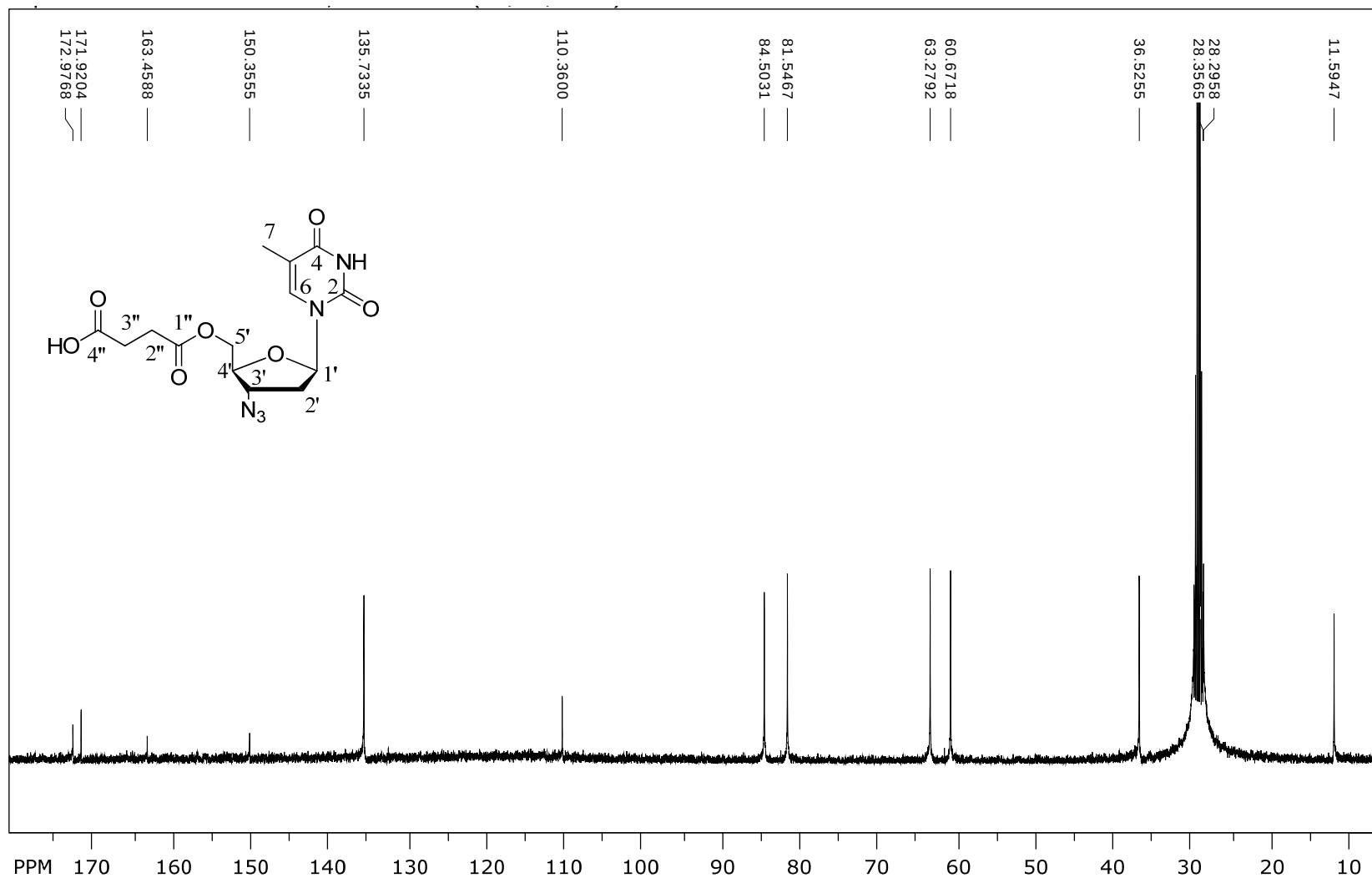
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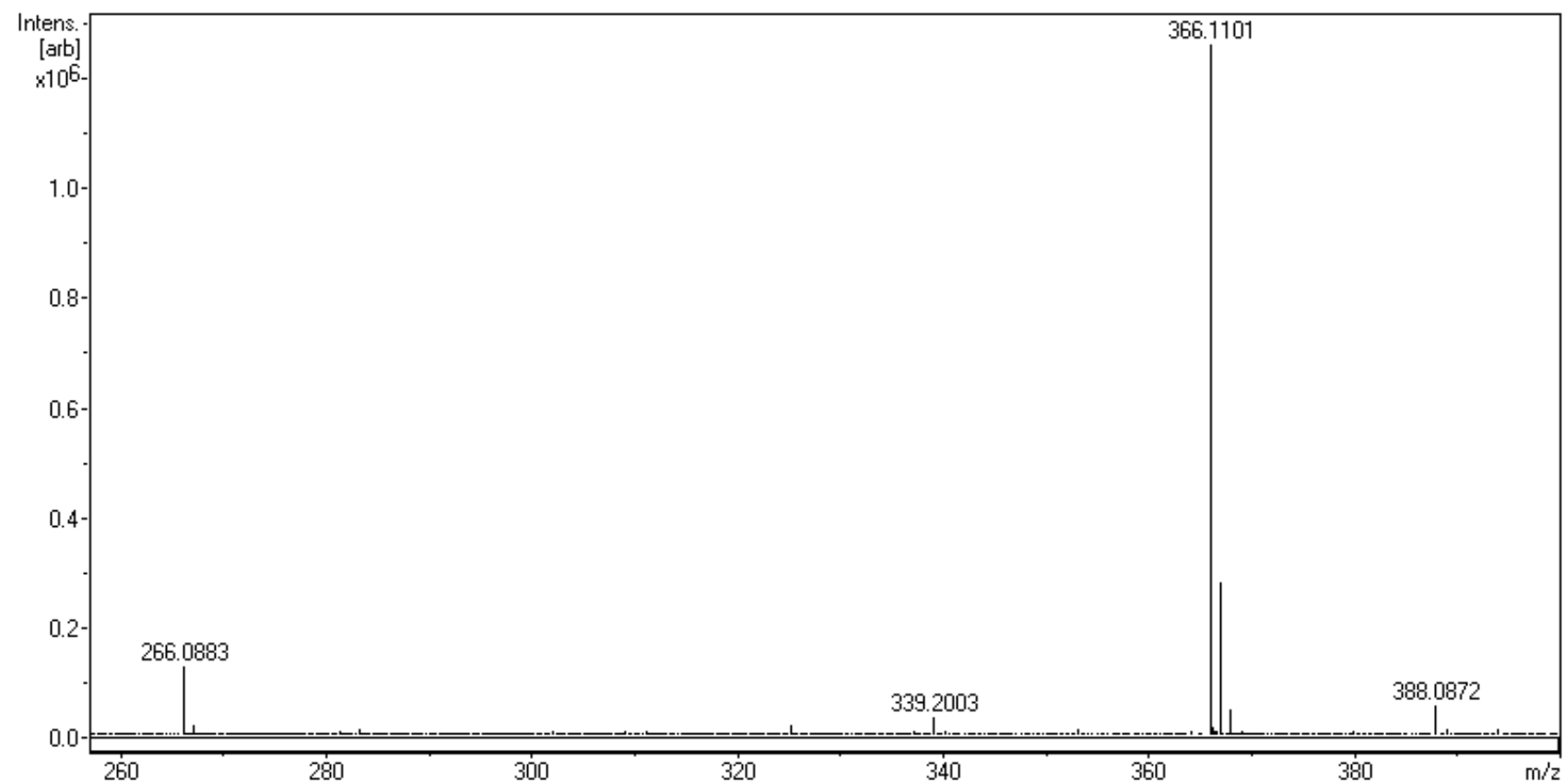
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^1H , ^{13}C and HRMS Spectra

Prodrug 6







Prodrug 7

