

Supporting Information

Fundamental Reaction Pathway and Free Energy Profile for Inhibition of Proteasome by Epoxomicin

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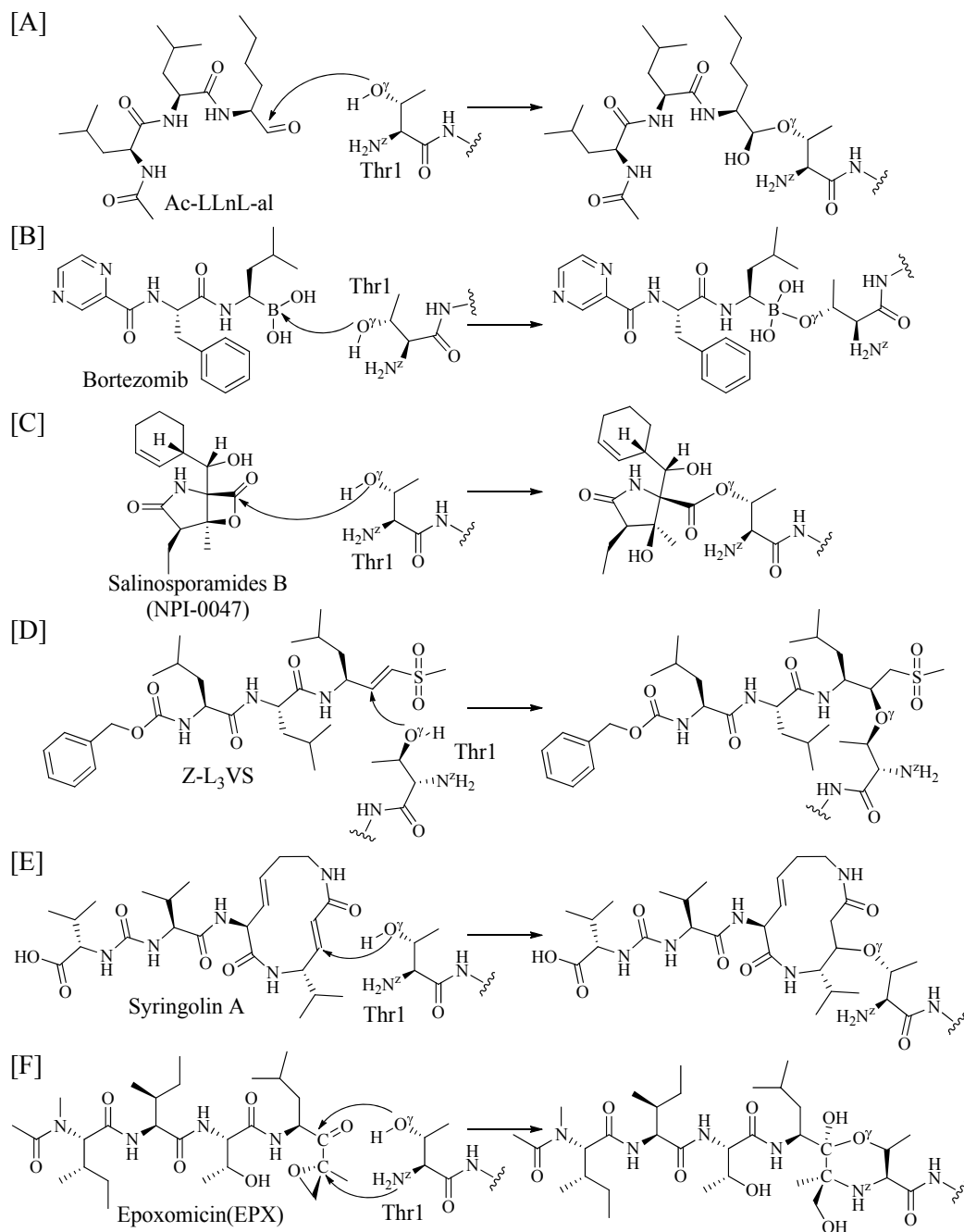
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Supporting Information Available. Molecular structures of selected inhibitors bound to Thr1 residue in the active sites of proteasome; the free energy profiles determined by the QM/MM-FE calculations for the pathways *via* transition state TS6^a or TS6^b; the free energy barriers and absolute QM/MM energies calculated at the QM/MM (Method/6-31++G**:*AMBER*; Method = B3LYP, MP2, M052X, B3PW91, or B3P86) level; coordinates of QM part of the geometries optimized at the QM/MM(B3LYP/6-31G*:*AMBER*) level. This information is available free of charge *via* the Internet at <http://pubs.acs.org/>.



Scheme S1. Molecular structures of selected inhibitors bound to Thr1 residue in the active sites of proteasome.

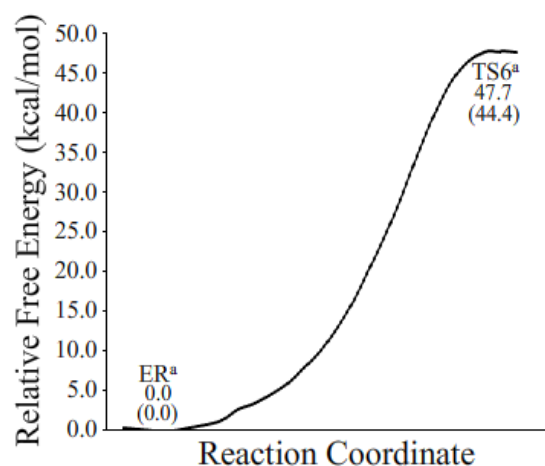


Figure S1. Free energy profile determined by the QM/MM-FE calculations for the possible pathway *via* transition state TS6^a. There were 25 points along the reaction coordinate used in the FEP calculations. The relative free energies were determined first without the zero-point and thermal corrections, and then corrected with the zero-point and thermal corrections for the QM subsystem (values in parentheses). The QM/MM-FE calculations were performed at the B3LYP/6-31++G**:*AMBER* level for each QM/MM optimized geometry along the reaction path.

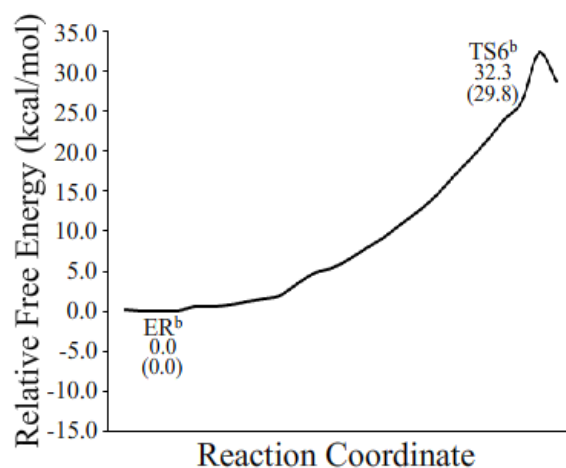


Figure S2. Free energy profile determined by the QM/MM-FE calculations for the pathway *via* transition state TS6^b. There were 26 points along the reaction coordinate used in the FEP calculations. The relative free energies were determined first without the zero-point and thermal corrections, and then corrected with the zero-point and thermal corrections for the QM subsystem (values in parentheses). The QM/MM-FE calculations were performed at the B3LYP/6-31++G**:*AMBER* level for each QM/MM optimized geometry along the reaction path.

Table S1. The free energy barriers (in kcal/mol) calculated by the QM/MM-FE calculations (corrected with the zero-point and thermal corrections for the QM subsystem) using different QM methods. **Note:** The actual free energy barrier associated with transition state ΔG_{TS1}^b should be the ΔG_{TS1}^b value listed in this table plus 1.7 kcal/mol (for the free energy of ER^b relative to ER^a), as discussed in the text of the paper.

Method/Basis set	ΔG_{TS1}^a	ΔG_{TS2}^a	ΔG_{TS3}^a	ΔG_{TS4}^a	ΔG_{TS5}^a	ΔG_{TS6}^a	ΔG_{TS1}^b	ΔG_{TS3}^b	ΔG_{TS6}^b
MP2/6-31+G(d)				26.8					
MP2/6-31+G(d,p)				26.9					
MP2/6-31++G(d)				27.2					
MP2/6-31++G(d,p)	9.4	9.2	-1.7	27.3	1.5	50.5	8.9	-0.8	29.8
B3LYP/6-31+G(d)				23.3					
B3LYP /6-31+G(d,p)				23.5					
B3LYP /6-31++G(d)				23.6					
B3LYP /6-31++G(d,p)	9.9	9.0	-1.7	23.6	1.2	44.4	9.3	-1.6	29.8
M05-2X/6-31++G(d,p)	10.5	9.5	-1.2	26.1	1.4	47.6	10.1	-0.6	28.6
B3PW91/6-31++G(d,p)	8.7	9.3	-1.3	26.0	1.0	44.0	8.7	-0.8	28.0
B3P86/6-31++G(d, p)	8.3	8.6	-1.3	25.5	1.1	42.9	8.6	-0.7	28.1

Table S2. Absolute QM/MM energies (in Hartree) calculated at the QM/MM (Method/6-31++G**:
AMBER; Method=B3LYP, MP2, M052X, B3PW91, or B3P86) level (single-point energy calculations) using the geometries optimized at the QM/MM(B3LYP/6-31G*:
AMBER) level. **Note:** ER^a(1) and ER^a(2) are different conformations of ER^a suitable for different reaction pathways. ER^a(1) is connected to transition state TS1^a, whereas ER^a(2) is connected to transition state TS6^a. Similarly, ER^b(1) and ER^b(2) are different conformations of ER^b. ER^b(1) is connected to transition state TS1^b, whereas ER^b(2) is connected to transition state TS6^b.

State	B3LYP	MP2	M052X	B3PW91	B3P86
ER ^a (1)	-1431.288007	-1426.805455	-1430.974039	-1430.844475	-1435.298045
ER ^a (2)	-1431.277507	-1426.796430	-1430.964780	-1430.834641	-1435.288516
TS1 ^a	-1431.271294	-1426.789587	-1430.956359	-1430.829587	-1435.283813
TS2 ^a	-1431.243770	-1426.762370	-1430.926604	-1430.800912	-1435.256593
TS3 ^a	-1431.266001	-1426.791381	-1430.959045	-1430.826659	-1435.283542
TS4 ^a	-1431.237937	-1426.759214	-1430.932719	-1430.795300	-1435.252816
TS5 ^a	-1431.276810	-1426.807158	-1430.977676	-1430.838649	-1435.297151
TS6 ^a	-1431.198802	-1426.708016	-1430.881031	-1430.756498	-1435.212177
INT1 ^a	-1431.259450	-1426.778332	-1430.943025	-1430.816971	-1435.271575
INT2 ^a	-1431.267251	-1426.792624	-1430.961184	-1430.828553	-1435.285392
INT3 ^a	-1431.277494	-1426.804611	-1430.976168	-1430.838596	-1435.295374
INT4 ^a	-1431.278359	-1426.809298	-1430.979509	-1430.839875	-1435.298507
EP ^a	-1431.316043	-1426.846375	-1431.017758	-1430.877680	-1435.335791
ER ^b (1)	-1431.260175	-1426.778051	-1430.947843	-1430.816556	-1435.273219
ER ^b (2)	-1431.263330	-1426.779976	-1430.953433	-1430.819869	-1435.278207
TS1 ^b	-1431.245195	-1426.763699	-1430.931633	-1430.802535	-1435.259353
TS3 ^b	-1431.244902	-1426.771468	-1430.943526	-1430.806190	-1435.265191
TS6 ^b	-1431.212454	-1426.729121	-1430.904496	-1430.771956	-1435.230039
INT2 ^b	-1431.245637	-1426.773502	-1430.945909	-1430.808339	-1435.267485
INT3 ^b	-1431.257947	-1426.785184	-1430.958289	-1430.818357	-1435.277200

Atomic coordinates of the QM part of the geometries optimized at the QM/MM(B3LYP/6-31G*:AMBER) level.

Note: Atom “F” represents the one-free-valence boundary atom described by the pseudo-potential in the QM subsystem.

ER^a(1)

N	48.83505800	43.73246500	54.15952900
H	49.46406800	44.43722200	53.77352400
H	49.19636500	43.52036500	55.09533500
C	47.47114000	44.24953300	54.23769200
H	47.30394300	44.84933300	53.34327900
C	46.54710600	43.01118700	54.12643900
H	46.71844900	42.37421600	55.01048200
C	45.06870000	43.30598300	53.97225500
H	44.90809000	44.13348800	53.27309400
H	44.55343500	42.42879700	53.57310500
H	44.61654200	43.56428100	54.93285800
O	47.00607000	42.28915200	52.96525100
H	47.98736200	42.44894500	53.02241900
C	47.14494200	45.09132200	55.48062300
O	47.60548600	44.80050000	56.59501600
N	46.25845500	46.05602300	55.21272500
H	46.13783800	46.30180000	54.22458600
F	45.62274800	47.05815400	56.16369800
F	44.59729500	44.11263300	50.08190900
C	46.01178500	43.95445500	49.56259600
H	46.15200500	43.01825000	49.01600900
H	46.30175800	44.78418500	48.90832900
N	47.09121000	43.92316400	50.61809400
H	47.30127700	44.87127800	50.98860100
H	46.88900600	43.28666500	51.42219800
H	47.96225300	43.57289600	50.17794600
F	49.87428300	36.03954800	51.12412200
C	49.64651400	37.47564400	50.84088500
O	50.40617800	38.16892900	50.17807400
N	48.45788300	37.96260600	51.26951000
H	47.85045300	37.42303200	51.87614200
C	48.04980500	39.25836900	50.80153400
C	46.51687400	39.36524500	50.92229500
C	45.78141000	40.31571600	49.95465800
C	44.31446900	39.87074000	49.85203600
H	43.87675200	39.69017500	50.83854300
H	44.23983100	38.94113100	49.27148100
H	43.70341800	40.62899000	49.35334500

C	46.41589000	40.39006400	48.55867700
H	45.78313600	40.96993400	47.87702500
H	46.54099400	39.39354900	48.11325500
H	47.39529100	40.87532600	48.59936400
H	45.80343500	41.31771100	50.39332800
H	46.15318600	38.34711100	50.72950800
H	46.23594300	39.60947400	51.95342700
H	48.31274400	39.29356200	49.73834300
C	48.88498300	40.41315500	51.37727000
O	48.80182800	41.51789700	50.86593500
C	49.93890900	40.22546100	52.47121300
C	51.35041500	40.47593400	51.98891700
H	52.04979700	40.24964200	52.79810900
H	51.45617500	41.52198100	51.68904900
H	51.57021800	39.82186900	51.14744600
C	49.57632100	40.50330500	53.87142300
H	50.34445200	40.89908600	54.53485700
H	48.55105600	40.73997900	54.13669900
O	49.77004300	39.14339000	53.41878700
O	50.61595700	38.11362600	55.83519100
H	49.99215900	38.78862500	56.14407300
H	50.70721300	38.32798000	54.88428400

ER^a(2)

N	48.90780900	43.63184600	54.05208200
H	49.54978800	44.33469500	53.68705100
H	49.22616000	43.44845600	55.00965700
C	47.55271600	44.17927200	54.07012200
H	47.44247300	44.78274700	53.16987200
C	46.57509600	42.98813300	53.92847400
H	46.71382400	42.32516400	54.79974800
C	45.10604200	43.33468200	53.77275400
H	44.97052100	44.16725000	53.07429600
H	44.56690000	42.47267000	53.36988400
H	44.65576100	43.60429200	54.73053600
O	46.99325900	42.27844000	52.74952600
H	47.97565700	42.38847100	52.77183200
C	47.21296800	45.02057800	55.30045600
O	47.65736300	44.73455200	56.42364900
N	46.32985300	45.97859800	55.01555100
H	46.19260600	46.20165000	54.02448500
F	45.67320500	46.94248900	55.98034800
F	44.46224700	44.04275300	49.93461800
C	45.86533500	43.94123500	49.37286300

H	46.02362200	43.01963600	48.80291500
H	46.11244100	44.79037000	48.72702000
N	46.96757000	43.92630400	50.40686900
H	47.17530200	44.87682500	50.77186200
H	46.79482900	43.28466300	51.21247300
H	47.84052300	43.59444300	49.95346900
F	49.80071700	36.13053600	51.06909800
C	49.60354500	37.57466800	50.82561100
O	50.38672500	38.27863300	50.20205600
N	48.41096300	38.05749900	51.24163000
H	47.79681900	37.51615600	51.83937400
C	48.03259500	39.36283300	50.78421000
C	46.49519400	39.49156300	50.83578700
C	45.81323000	40.26301200	49.68061600
C	44.37116600	39.75632000	49.53064500
H	43.84325900	39.74671600	50.48959200
H	44.37180700	38.73495900	49.12878700
H	43.80045500	40.38209800	48.83687700
C	46.55620100	40.17072700	48.33962600
H	45.95774000	40.60990600	47.53373700
H	46.76902700	39.13104300	48.05577100
H	47.50472700	40.71362400	48.38089200
H	45.77012200	41.31819100	49.96442000
H	46.12629700	38.45839000	50.80054700
H	46.17514000	39.91601700	51.79258200
H	48.34780100	39.40905200	49.73807600
C	48.87771100	40.48101900	51.40550500
O	48.88938900	41.58142400	50.87698800
C	49.83811100	40.25609700	52.57811100
C	51.28297900	40.47908600	52.20260100
H	51.91228500	40.29276000	53.07686700
H	51.41838200	41.50588000	51.85329500
H	51.56034400	39.78883300	51.40909700
C	49.38422100	40.52115900	53.95363300
H	50.11067600	40.90558900	54.66901700
H	48.34649100	40.76290000	54.15655200
O	49.59161200	39.16334300	53.50305800
O	50.54707600	38.13366800	55.92679900
H	49.97318100	38.79884100	56.33762000
H	50.56664600	38.40721100	54.98620700
TS1 ^a			
N	48.79033800	43.75577600	54.08654800
H	49.43859000	44.42592300	53.66234600

H	49.19190600	43.46919800	54.99133200
C	47.40900500	44.27514800	54.22413000
H	47.23313100	44.87359800	53.33526300
C	46.57109800	42.96207700	54.05360000
H	46.69962700	42.36774400	54.98408800
C	45.08695500	43.21712500	53.84189000
H	44.92098200	44.00446500	53.09851800
H	44.61159700	42.30957700	53.46418400
H	44.58956100	43.50365200	54.77389700
O	47.20194900	42.31759000	52.97774300
H	48.40540900	42.86644800	53.36359000
C	47.13649500	45.09025400	55.47304000
O	47.62408900	44.79169100	56.57402000
N	46.24842400	46.05342800	55.21250500
H	46.10673700	46.29133500	54.22540700
F	45.61978400	47.04947300	56.16242700
F	44.59843500	44.11233900	50.07921600
C	46.02245300	43.92563100	49.59475800
H	46.15301100	42.98829000	49.05072300
H	46.33734700	44.74987600	48.94460600
N	47.09435200	43.87898900	50.66276400
H	47.29688700	44.83038100	51.02524200
H	46.94709500	43.22311700	51.49301600
H	47.96315200	43.54706100	50.20493400
F	49.86195800	36.05689200	51.11382500
C	49.64037800	37.49492700	50.82604200
O	50.41515800	38.19092200	50.18341100
N	48.43933300	37.97624700	51.22321800
H	47.83814500	37.44511800	51.84309900
C	48.04379600	39.28588900	50.77762500
C	46.51815500	39.41178500	50.95640800
C	45.74803700	40.34296500	49.99509000
C	44.29422700	39.85334000	49.90224500
H	43.87591900	39.63635600	50.88995900
H	44.24286300	38.93310100	49.30401700
H	43.65176200	40.60118100	49.42792900
C	46.36188300	40.44405100	48.59114700
H	45.70516400	41.01672100	47.92596000
H	46.49938000	39.45465000	48.13372900
H	47.33257600	40.94795400	48.61974400
H	45.74368100	41.34203700	50.44023600
H	46.13865900	38.39264100	50.80341000
H	46.28365900	39.68934000	51.99027900
H	48.27088900	39.32609000	49.70688300

C	48.92868900	40.41752500	51.33386200
O	48.93847400	41.49839000	50.77249100
C	49.93428200	40.21188300	52.46924400
C	51.36344500	40.46660200	52.05010800
H	52.03270300	40.24501400	52.88582500
H	51.47620900	41.51163300	51.74862600
H	51.61705200	39.81658200	51.21533900
C	49.50467600	40.46214100	53.85575500
H	50.24484700	40.83856600	54.56387400
H	48.46596400	40.71452300	54.04663900
O	49.72565000	39.11268000	53.39314000
O	50.61286600	38.12167500	55.81543900
H	49.97908300	38.78964300	56.11873000
H	50.68917600	38.32299100	54.85971800

TS2^a

N	48.92441400	43.78009800	53.65806300
H	49.34828900	44.71237900	53.53044500
H	49.36642500	43.39269500	54.50605500
C	47.43908200	43.89888000	53.86417200
H	47.03439800	44.30211500	52.93982700
C	46.81868100	42.47744400	54.11363000
H	47.29936200	42.15200000	55.06761100
C	45.31899900	42.61161100	54.41896700
H	44.76561100	42.86910300	53.50896900
H	44.99827500	41.62227200	54.74176300
H	45.06819500	43.32450100	55.20948600
O	46.98575800	41.59752100	53.07894500
H	49.12989600	43.18900800	52.81306800
C	47.20689000	44.83342500	55.04591700
O	47.74390000	44.59712000	56.14067500
N	46.33614000	45.80812500	54.79014100
H	46.12651500	46.00297800	53.80542900
F	45.74653800	46.77234600	55.79370100
F	44.46904800	44.02418500	49.87348300
C	45.86235600	44.01975900	49.28891700
H	46.03548900	43.18500400	48.60205200
H	46.08944300	44.95232800	48.76264600
N	46.95682300	43.89338100	50.32429200
H	47.14792800	44.80741800	50.77587100
H	46.76783000	43.17554700	51.04346700
H	47.84780900	43.59388200	49.88140700
F	49.50730500	36.48429300	50.97298800
C	49.36580600	37.94119300	50.69199400

O	50.06036000	38.52608100	49.86717400
N	48.36603800	38.57368500	51.35690100
H	47.77501900	38.03725200	51.98145200
C	47.95719900	39.92116100	50.99067900
C	46.42009200	39.95028000	50.75563200
C	45.96516300	40.30743700	49.31820000
C	44.44473500	40.10612400	49.19103600
H	43.88887100	40.68239600	49.93796500
H	44.18971600	39.04601700	49.32935700
H	44.08962300	40.39594500	48.19413700
C	46.67657000	39.55500900	48.18273500
H	46.43052400	40.00505600	47.21346400
H	46.34640200	38.51755400	48.13337500
H	47.76565000	39.53997700	48.28229800
H	46.17466100	41.37299100	49.16951000
H	46.04050700	38.94531200	50.98743600
H	45.95722800	40.63390000	51.46980400
H	48.46165900	40.10333400	50.03884900
C	48.64401600	41.01936700	51.87017100
O	48.86991700	42.13556200	51.35499700
C	49.72660500	40.52424000	52.84675900
C	51.07976800	40.47618200	52.15953200
H	51.83633000	40.10364300	52.85579200
H	51.35259600	41.47680300	51.81524300
H	51.05443600	39.82297000	51.28571400
C	49.66485400	40.72093200	54.30295400
H	50.60011600	40.83258300	54.85194600
H	48.78291700	41.14115300	54.76542600
O	49.44362800	39.41370400	53.73334100
O	50.31281300	38.13883800	56.02497100
H	49.65900700	38.71573700	56.45024100
H	50.29739300	38.44243500	55.09254300

TS3^a

N	48.96203800	43.76544000	53.53250200
H	49.32203100	44.72044700	53.40060700
H	49.47228300	43.37724200	54.33555300
C	47.49497600	43.76758900	53.78699900
H	47.02382900	44.12718100	52.87503200
C	46.97590700	42.33370900	54.14034600
H	47.41140300	42.12999200	55.12755000
C	45.45915800	42.37977300	54.28781100
H	44.97521700	42.54688700	53.31882600
H	45.15578700	41.40541900	54.66609900

H	45.11733500	43.14150100	54.99283200
O	47.22396000	41.17560900	53.30860800
H	49.01882700	43.12999500	52.59818300
C	47.20478600	44.71179100	54.97812300
O	47.70212500	44.46830600	56.08629900
N	46.37675900	45.72347800	54.70970600
H	46.19896400	45.94505700	53.72364000
F	45.79594700	46.69472500	55.72110100
F	44.48714900	44.04353300	49.86200900
C	45.86905400	44.03733100	49.24498800
H	46.04995200	43.16587000	48.60643300
H	46.03343000	44.93976600	48.64477400
N	47.01170500	44.03529900	50.21941700
H	47.03128200	44.89828200	50.78932800
H	47.19165500	43.17621900	50.81904000
H	47.89068400	44.05493000	49.67244500
F	49.49541500	36.51046400	50.95783500
C	49.27148000	37.97249200	50.72674100
O	49.86986300	38.57727700	49.84214200
N	48.33348000	38.57968000	51.50983000
H	47.78121100	37.99176700	52.12549000
C	47.84203600	39.93398000	51.22421000
C	46.33548600	39.89223800	50.83757200
C	46.00756800	40.32773800	49.38794900
C	44.49335600	40.23756000	49.12675800
H	43.91331600	40.85596700	49.82032700
H	44.14786000	39.19991400	49.23509300
H	44.25348700	40.55035800	48.10237400
C	46.76050000	39.57380500	48.27895900
H	46.70402300	40.13625400	47.33987400
H	46.28842500	38.61207600	48.07260700
H	47.81341700	39.38670100	48.50939900
H	46.30058000	41.38091100	49.31060700
H	45.96776700	38.86720200	50.98735700
H	45.76079000	40.52759600	51.51995600
H	48.42191500	40.24190400	50.35516500
C	48.26880200	41.06262800	52.27605700
O	48.42377900	42.23814800	51.61300800
C	49.61768100	40.62714200	52.93683300
C	50.82904000	40.62571900	52.02826100
H	51.70646800	40.28490900	52.58463000
H	51.00853600	41.63042300	51.63954000
H	50.69850300	39.95760500	51.17706600
C	49.84339700	40.76495800	54.39086200

H	50.86327800	40.87919000	54.75578000
H	49.07735700	41.14997300	55.05544500
O	49.53963000	39.47818300	53.83213300
O	50.24499100	38.14349500	56.14466000
H	49.59488400	38.64014500	56.66627800
H	50.10271400	38.46671200	55.22982400
TS4 ^a			
N	49.18575500	43.18030700	53.81183800
H	49.82413800	43.74184900	53.24480600
H	49.52081200	43.19694200	54.78301400
C	47.81143700	43.68155600	53.72659000
H	47.70142100	44.20563600	52.77949300
C	46.80879900	42.49278600	53.78622500
H	46.89343300	42.06380300	54.79009800
C	45.37450200	42.94865400	53.53260400
H	45.32096300	43.65759000	52.69888600
H	44.75232100	42.09791100	53.26581300
H	44.94780500	43.43062900	54.41399500
O	47.02275000	41.37443900	52.85912400
H	49.18357200	42.09349900	50.72934700
C	47.44118700	44.63423900	54.91913300
O	47.84440800	44.35229700	56.05415600
N	46.59574900	45.63454100	54.63458600
H	46.48123200	45.88494100	53.64854100
F	45.90608200	46.57538200	55.62428400
F	44.42374100	44.05404100	49.86102100
C	45.79335700	44.07345200	49.22286400
H	46.02216400	43.15806000	48.66693700
H	45.90364400	44.93766500	48.56028600
N	46.91056100	44.20742200	50.21206700
H	46.78154000	45.01475300	50.85223000
H	47.10546000	43.34588100	50.75275400
H	47.80492100	44.38420200	49.72354000
F	49.59109600	36.50687800	50.94540600
C	49.46248300	37.97493900	50.71395600
O	49.95372200	38.55099600	49.74637900
N	48.68838200	38.63488200	51.61321300
H	48.39957700	38.18172900	52.46724700
C	48.00418300	39.84654900	51.22616700
C	46.53290700	39.49295500	50.88392700
C	45.79311100	40.33494300	49.82791800
C	44.40096200	39.73010600	49.58318500
H	43.84922400	39.59152700	50.51870400

H	44.49112700	38.75326800	49.09192900
H	43.79918000	40.37016400	48.92864100
C	46.56499000	40.42371900	48.50080200
H	45.95361600	40.89102100	47.71895900
H	46.85023200	39.42627400	48.14049800
H	47.48237700	41.01311600	48.59877300
H	45.65170800	41.34726100	50.22441500
H	46.57390300	38.46342700	50.50675900
H	45.94390900	39.45415700	51.80498200
H	48.51224700	40.13115800	50.30445800
C	48.21290100	41.09616900	52.19992700
O	48.42253900	42.22819400	51.31806100
C	49.44378900	40.96523800	53.12163700
C	50.76001900	40.83261100	52.40002900
H	51.54122500	40.48500500	53.07713700
H	51.06692500	41.78585000	51.96231100
H	50.69218500	40.11002800	51.57912100
C	49.35450700	40.49113300	54.51620600
H	50.23781300	40.79382800	55.10437000
H	48.45255300	40.81393700	55.05730600
O	49.34805800	39.17768400	54.09298000
O	50.49717100	38.00559100	56.13863500
H	49.88828600	38.46782000	56.73644600
H	50.26295600	38.40963500	55.24889700

TS5^a

N	49.29977400	43.02141200	53.43701200
H	50.00581700	43.73391800	53.19635900
H	49.49527900	42.67952800	54.40237700
C	47.91302700	43.62755000	53.48279300
H	47.75332800	44.14364300	52.54031500
C	46.95473200	42.43673100	53.67631200
H	47.25167900	41.95281200	54.61148000
C	45.49976000	42.87405900	53.67712000
H	45.28465100	43.55719400	52.84825600
H	44.87296000	42.00015400	53.53756100
H	45.22279500	43.35958400	54.61440800
O	47.08230100	41.41628200	52.66285500
H	48.58745100	42.48552500	50.13573100
C	47.64887400	44.57702000	54.70625000
O	48.02204100	44.23159600	55.82627400
N	46.80345100	45.59337900	54.45329800
H	46.75340200	45.94748300	53.49445200
F	46.05009200	46.44643700	55.47954800

F	44.38001400	44.06196600	49.72988800
C	45.72212400	44.28299400	49.07241400
H	46.11950300	43.38443400	48.59061700
H	45.66948600	45.09995900	48.35010900
N	46.76693000	44.68818600	50.06611500
H	46.44744500	45.41538300	50.73117600
H	47.09527700	43.84841500	50.59103500
H	47.61040900	45.09534000	49.63334800
F	49.63037700	36.70235200	50.98869500
C	49.59355200	38.15939400	50.69074100
O	50.07291800	38.64993300	49.67859000
N	48.92255100	38.94602400	51.59453700
H	48.49241100	38.48208800	52.38518600
C	48.14466500	40.04303100	51.02628700
C	46.72808000	39.47752900	50.75563300
C	45.71556700	40.26256600	49.90916600
C	44.39223500	39.48282000	49.85964400
H	44.06889400	39.16402700	50.85682200
H	44.50432600	38.58753300	49.23803300
H	43.59155200	40.08834100	49.42332900
C	46.22253300	40.52054200	48.48272700
H	45.45025800	41.00159200	47.87059500
H	46.49462100	39.58007300	47.98397000
H	47.10511000	41.16793900	48.47742200
H	45.52775200	41.22069100	50.40139300
H	46.90507100	38.51413300	50.25677700
H	46.27871700	39.23512900	51.72424300
H	48.63466300	40.24900500	50.07506300
C	48.18144700	41.38266500	51.83296900
O	47.89899100	42.41753500	50.82823300
C	49.54507500	41.73123000	52.51938400
C	50.61751100	41.92297700	51.43357700
H	51.61410300	41.99989100	51.87295500
H	50.46717800	42.79708400	50.79270700
H	50.63627600	41.02078600	50.81155700
C	50.06470900	40.71183200	53.58141400
H	50.38919300	39.82131400	53.01777600
H	51.01951800	41.16345800	53.93963100
O	49.14390100	40.51282700	54.55519600
O	49.96803900	38.92651200	56.32603800
H	49.44837000	39.24645400	57.07793700
H	49.68091600	39.58493700	55.56168600

TS6^a

N	49.04433800	43.67470600	53.90364600
H	49.58504600	44.51711300	53.69884000
H	49.33944700	43.41249100	54.85080600
C	47.63288200	44.04512700	53.93095500
H	47.44860800	44.63645200	53.03584900
C	46.74911200	42.76904000	53.77641800
H	46.94876800	42.12784800	54.65742000
C	45.24657500	43.06601200	53.75047200
H	45.01789100	43.88574000	53.05989400
H	44.71919500	42.18481600	53.37990000
H	44.84657700	43.32704600	54.73527000
O	47.16161800	42.13904300	52.59733800
H	48.61567200	42.45766900	51.94151600
C	47.24223600	44.87053800	55.16319100
O	47.66994000	44.58790200	56.29514800
N	46.37603800	45.84661600	54.88043600
H	46.22275400	46.06141700	53.89130400
F	45.73161400	46.81026100	55.85773100
F	44.43137600	44.05850200	49.91330800
C	45.83418900	43.96378400	49.36356700
H	46.00496600	43.04585700	48.78994500
H	46.08330200	44.81946300	48.72665300
N	46.90697700	43.95127700	50.41759200
H	47.03129200	44.88883700	50.84567800
H	46.77970900	43.23394200	51.18268800
H	47.80628100	43.73273400	49.95167500
F	49.68557600	36.28417400	50.98378700
C	49.52757600	37.73611600	50.74248300
O	50.24611000	38.39264300	50.00249900
N	48.44653500	38.28770800	51.35233600
H	47.83951300	37.71357300	51.92751600
C	47.99618700	39.59036200	50.93501700
C	46.44120600	39.58276500	50.86031300
C	45.76128500	40.29365500	49.66865900
C	44.34650200	39.71682400	49.49573100
H	43.79632000	39.69365800	50.44163300
H	44.40131400	38.69361900	49.10352900
H	43.76488200	40.30876400	48.78144300
C	46.53961900	40.18905900	48.34914100
H	45.94095500	40.57119900	47.51458900
H	46.80548900	39.15060400	48.10901900
H	47.46223600	40.77627000	48.38285500
H	45.65956400	41.35222700	49.92185300
H	46.17965100	38.51906900	50.79132800

H	46.03129700	39.97226600	51.79472200
H	48.39843600	39.73659500	49.92559300
C	48.68397700	40.68007200	51.72924700
O	48.87761900	41.81433000	51.13827500
C	49.67071200	40.37180500	52.83393800
C	51.09406000	40.42889700	52.29055600
H	51.78476500	40.13118700	53.08436800
H	51.31763600	41.44873000	51.96822200
H	51.22099100	39.76075700	51.43747400
C	49.41135300	40.66249700	54.24539200
H	50.26047200	40.91504500	54.87809100
H	48.44697000	41.03710200	54.55279500
O	49.37857300	39.29663900	53.74931100
O	50.50686500	38.07652800	55.98534000
H	49.91521200	38.67533100	56.46789800
H	50.45155100	38.40772000	55.06555300

INT1^a

N	48.88995400	43.83519900	53.95866300
H	49.48692400	44.62180900	53.66627300
H	49.25985300	43.50305800	54.86600100
C	47.45102400	44.22210400	54.05612900
H	47.24882700	44.79428400	53.15893200
C	46.65965200	42.88337600	53.92172200
H	46.92959700	42.27507200	54.82221200
C	45.14988200	43.12545600	53.96277800
H	44.86244300	43.90082700	53.24443700
H	44.65252100	42.20578700	53.65427700
H	44.78476700	43.40483900	54.95685100
O	47.10402800	42.29163700	52.76438500
H	48.89327500	43.08011600	53.23891900
C	47.18724300	45.03894700	55.30210800
O	47.71809600	44.75016200	56.38764400
N	46.27688100	45.98078600	55.06932800
H	46.08002100	46.19516900	54.08600400
F	45.65088700	46.95185300	56.04037600
F	44.48830600	43.97768700	50.00715800
C	45.91946200	43.93220500	49.50259000
H	46.10913500	43.07148400	48.85381900
H	46.17271000	44.83675600	48.93752900
N	46.99606100	43.83587200	50.55988600
H	47.23068900	44.77805300	50.92138200
H	46.85074300	43.17742400	51.42238700
H	47.85970300	43.48644700	50.10480200

F	49.64787000	36.37291700	51.02810400
C	49.52837800	37.82023900	50.73551600
O	50.40447300	38.48933700	50.20399600
N	48.29812400	38.33983400	50.97110800
H	47.65070100	37.83988600	51.56937600
C	48.06409000	39.72791900	50.66057900
C	46.54331900	40.00981400	50.74905200
C	45.79729200	40.21904600	49.39456100
C	44.38088500	39.64115100	49.50327200
H	43.84530900	40.05406900	50.36384400
H	44.43175300	38.55336000	49.62517700
H	43.79470700	39.85118800	48.60102800
C	46.51399300	39.67268100	48.15088700
H	45.86493500	39.73480700	47.26996300
H	46.82541800	38.63000900	48.26870900
H	47.41113400	40.25471800	47.92958700
H	45.69026700	41.29660600	49.24035200
H	46.09709500	39.13553700	51.24190500
H	46.36465100	40.85521800	51.41819300
H	48.39727000	39.87438200	49.63025800
C	49.02304700	40.68685700	51.39609300
O	49.23364900	41.79438300	50.93413600
C	49.88208700	40.28077600	52.59594300
C	51.36076900	40.43303000	52.34208500
H	51.92571300	40.19215800	53.24731700
H	51.57192900	41.45617100	52.02208500
H	51.65185700	39.75930600	51.54027100
C	49.31753700	40.45138300	53.94585200
H	49.99786500	40.70709300	54.76037000
H	48.28207700	40.76328300	54.03725500
O	49.49556500	39.12944100	53.39439100
O	50.48251600	38.04853800	55.80294600
H	49.86617300	38.69983500	56.17142400
H	50.49471900	38.28007600	54.85038700
INT2 ^a			
N	48.98871300	43.77869200	53.58320300
H	49.34561100	44.73902900	53.46852100
H	49.47393400	43.39019100	54.40372100
C	47.50740800	43.77558500	53.78625100
H	47.06991900	44.14478700	52.86288600
C	46.96628900	42.34478000	54.12352500
H	47.39389900	42.12774100	55.11177800
C	45.44950500	42.42023800	54.27021100

H	44.97081600	42.60146100	53.30154000
H	45.12894400	41.44900300	54.64047400
H	45.11945700	43.18165700	54.98088500
O	47.18811300	41.19648400	53.28007000
H	49.11732338	43.18623699	52.68345235
C	47.20764000	44.71714000	54.97733600
O	47.70545500	44.46987600	56.08533500
N	46.37822800	45.72710600	54.71129200
H	46.19904200	45.94809000	53.72506000
F	45.79457100	46.69591400	55.72317900
F	44.48829700	44.03997200	49.86297200
C	45.87097700	44.02821500	49.24669500
H	46.04972500	43.15495900	48.60994400
H	46.03655200	44.92838800	48.64305400
N	47.01300800	44.02630900	50.22066100
H	47.03589700	44.89301100	50.78375700
H	47.19766600	43.16683000	50.82650100
H	47.89140200	44.03913000	49.67313400
F	49.49046800	36.50874100	50.95997300
C	49.26806800	37.97061800	50.73038500
O	49.86761500	38.57609500	49.84639900
N	48.33224300	38.57605100	51.51556900
H	47.78097600	37.98586000	52.12975100
C	47.82992700	39.92447400	51.22068300
C	46.32531300	39.86444900	50.82996300
C	45.99606600	40.31617000	49.38572200
C	44.48333000	40.21558400	49.12106600
H	43.89739500	40.81318800	49.82773200
H	44.14868100	39.17218800	49.20700000
H	44.23998500	40.54743600	48.10359300
C	46.75849400	39.58182900	48.27064000
H	46.66887900	40.13498800	47.32834600
H	46.32134000	38.60106500	48.07856100
H	47.82039100	39.43446500	48.48798000
H	46.28139900	41.37202100	49.32160000
H	45.97498100	38.83080000	50.96122000
H	45.73811300	40.47953500	51.51971000
H	48.40841800	40.23115700	50.35088400
C	48.25087800	41.06878600	52.26155900
O	48.41883400	42.22852700	51.59149500
C	49.58617500	40.62242000	52.94805000
C	50.81156300	40.60558900	52.05768600
H	51.67661400	40.24664700	52.62337400
H	51.01362700	41.61094400	51.68114100

H	50.68326600	39.95006900	51.19645600
C	49.79963100	40.77473600	54.40357100
H	50.81942000	40.87883500	54.77463200
H	49.03723700	41.17925100	55.06006100
O	49.47917500	39.48623600	53.85867000
O	50.31028400	38.11882100	56.09329400
H	49.65123500	38.66837400	56.54604600
H	50.27863500	38.45479700	55.17227800

INT3^a

N	49.14434300	43.63535300	53.66866400
H	49.54061000	44.56949800	53.52903100
H	49.52499800	43.32693200	54.56907200
C	47.69190000	43.77238200	53.76953100
H	47.34743800	44.23147700	52.84408500
C	46.92026700	42.43092600	53.96499000
H	47.11549600	42.10793700	54.99347300
C	45.42910300	42.70977200	53.80416900
H	45.21424100	43.22171500	52.85962800
H	44.91359300	41.76083800	53.77493300
H	45.02232900	43.30438700	54.62455900
O	47.15874500	41.25180400	53.12429200
H	49.04891900	42.76205200	52.13267000
C	47.30259800	44.67694100	54.96422200
O	47.71451500	44.40622100	56.10206900
N	46.48480500	45.68877200	54.67074100
H	46.33863100	45.91646800	53.68288600
F	45.85367000	46.63356200	55.67458300
F	44.43551500	44.03824100	49.86948900
C	45.81485500	44.05038400	49.25307100
H	46.02431400	43.16862300	48.63775400
H	45.96733700	44.94693900	48.64321500
N	46.93697100	44.09043000	50.25058400
H	46.89128900	44.93625600	50.85030400
H	47.05497000	43.24072900	50.83135300
H	47.83834500	44.14291100	49.74091200
F	49.56168400	36.49040300	50.96157200
C	49.36644700	37.95617700	50.74610400
O	49.95654300	38.57425200	49.86867300
N	48.44568300	38.55448300	51.55798000
H	47.89636400	37.95254900	52.16175200
C	47.88375800	39.86322200	51.22579700
C	46.37479400	39.69011400	50.87448100
C	45.85522800	40.33990500	49.56970300

C	44.38551500	39.94592300	49.34254000
H	43.75249100	40.21847100	50.19236300
H	44.29970200	38.86258600	49.18489700
H	43.98220800	40.43324300	48.44656900
C	46.68180200	39.99294400	48.32384300
H	46.27092900	40.49325000	47.43817700
H	46.67480200	38.91698400	48.11781100
H	47.72634500	40.29360800	48.42687900
H	45.88581800	41.42887400	49.69477700
H	46.19722700	38.61048800	50.78438400
H	45.75753700	40.04089100	51.70625000
H	48.43440900	40.16728800	50.33716000
C	48.26909900	41.00191200	52.27424900
O	48.56049300	42.14731900	51.50225000
C	49.55880400	40.58511200	53.03946200
C	50.83347900	40.57412300	52.21928200
H	51.65190400	40.17344100	52.82436300
H	51.08997600	41.58920200	51.90676000
H	50.74562000	39.96269300	51.32072200
C	49.66272900	40.74993400	54.49616500
H	50.65423300	40.87226000	54.93020700
H	48.85223300	41.16423800	55.08378300
O	49.38700800	39.45008900	53.93992000
O	50.45253900	38.05767400	56.04426200
H	49.83121400	38.60924100	56.54582300
H	50.37515700	38.42153300	55.13650400

INT4^a

N	49.29549700	43.07355500	53.39762200
H	49.94460600	43.78614100	53.02962400
H	49.61507000	42.89407400	54.36778600
C	47.89416700	43.64253400	53.48101400
H	47.70145300	44.14827400	52.53962900
C	46.96556700	42.43206600	53.68284500
H	47.30013200	41.91595100	54.59094900
C	45.50912500	42.85881700	53.75897400
H	45.26162700	43.56203100	52.95665400
H	44.88505000	41.98441900	53.61684600
H	45.26555400	43.31860300	54.71817300
O	47.05165600	41.46647800	52.62377600
H	48.60235600	42.48229800	50.11342300
C	47.64391700	44.58672700	54.70269700
O	48.03171800	44.23491700	55.81775000
N	46.79816800	45.60087600	54.45573800

H	46.74086700	45.95123200	53.49523300
F	46.04686300	46.44964900	55.48286200
F	44.38869900	44.06576700	49.71957800
C	45.72391900	44.27861800	49.04621700
H	46.11553600	43.37397200	48.57030400
H	45.66591000	45.08632400	48.31373100
N	46.78041100	44.69349500	50.02254200
H	46.47515800	45.43537200	50.67721100
H	47.10780700	43.85980100	50.55834400
H	47.62469100	45.07697200	49.57128700
F	49.62339200	36.71231200	50.98611500
C	49.57272700	38.16789300	50.66412900
O	49.95119400	38.61042000	49.58322900
N	48.99357200	39.00525200	51.57777600
H	48.78225100	38.74309900	52.54227500
C	48.16232600	40.06534200	51.02077400
C	46.74728000	39.47921700	50.77772900
C	45.73001300	40.25990600	49.92783200
C	44.39202100	39.50491400	49.90172100
H	44.06456200	39.21822100	50.90685600
H	44.48276300	38.59211900	49.30244600
H	43.60236200	40.11660500	49.45253800
C	46.22260300	40.48941500	48.49075300
H	45.44855200	40.96941800	47.87933400
H	46.47996900	39.53854800	48.00473400
H	47.11263900	41.12628800	48.46284100
H	45.55879800	41.22999800	50.40375000
H	46.92454400	38.51131800	50.28959700
H	46.31218200	39.24729500	51.75441800
H	48.61849100	40.28930000	50.05623800
C	48.17663800	41.40447300	51.82533400
O	47.93911400	42.45818600	50.83261400
C	49.52290800	41.72353900	52.55062800
C	50.62682900	41.89192400	51.49133800
H	51.61561200	41.95464700	51.95052600
H	50.49724900	42.76345100	50.84177500
H	50.64251800	40.98619800	50.87552900
C	49.99399800	40.63725900	53.58462400
H	50.68502600	39.99528000	53.00123100
H	50.66885200	41.18703400	54.28611100
O	48.97970300	39.96847900	54.18935000
O	49.94530400	38.94157500	56.28687800
H	49.36892700	39.32870500	56.96105700
H	49.58064300	39.35635600	55.40128900

EP^a

N	49.28248700	43.14768100	53.14561100
H	49.89679600	43.86004500	52.75487100
H	49.81965300	42.06895400	55.07424100
C	47.92292100	43.63360300	53.40372100
H	47.50959300	44.17114100	52.54323700
C	47.01771400	42.42348000	53.71423700
H	47.38351600	41.99694600	54.65057800
C	45.54706700	42.78155400	53.81244500
H	45.20713000	43.33327400	52.92991600
H	44.98228400	41.85673000	53.85545400
H	45.32509700	43.36657600	54.70583600
O	47.09779000	41.34950000	52.73214000
H	48.47354800	42.48384800	50.14738500
C	47.69078000	44.55846000	54.67059100
O	48.06253100	44.20315000	55.79148300
N	46.83086500	45.57590000	54.43854300
H	46.79056600	45.94856100	53.48718100
F	46.07079600	46.43205300	55.46429800
F	44.33592700	44.05242800	49.76394000
C	45.68831500	44.30578000	49.13299400
H	46.10478400	43.42219000	48.63950800
H	45.63665300	45.13590000	48.42506300
N	46.71900200	44.70408900	50.14470200
H	46.39543100	45.42504400	50.81447600
H	47.04440700	43.86139200	50.66730300
H	47.56431400	45.12423400	49.72572900
F	49.68183200	36.69620500	51.03790700
C	49.63196900	38.16263500	50.79413800
O	50.24645000	38.71402700	49.89762400
N	48.79287200	38.87330400	51.63149100
H	48.19216000	38.28836400	52.20434600
C	48.08727300	40.01070800	51.02000800
C	46.66275400	39.49260800	50.68652500
C	45.72770900	40.29031100	49.76294500
C	44.38732100	39.54972800	49.63313800
H	43.96826500	39.29044900	50.61186500
H	44.51265400	38.62495800	49.05764600
H	43.64992800	40.16395600	49.10533400
C	46.33620500	40.52141000	48.37338500
H	45.62339300	41.02403500	47.70911400
H	46.61187000	39.57085200	47.89547900
H	47.23326100	41.14418600	48.43092600

H	45.53492500	41.25924200	50.22908900
H	46.82312800	38.50782900	50.22316200
H	46.14660000	39.30073000	51.63424500
H	48.62606600	40.19560800	50.09111400
C	48.13108100	41.36035500	51.81632700
O	47.75799400	42.34595400	50.80075000
C	49.48373600	41.82722400	52.46874600
C	50.56324600	41.84981300	51.35934900
H	51.55210100	42.05151000	51.77384200
H	50.38104500	42.61964400	50.60278100
H	50.63388100	40.87135200	50.87212000
C	50.03503600	40.84846700	53.56431000
H	49.76473400	39.81805500	53.34863600
H	51.13121100	40.91015300	53.54047700
O	49.56883400	41.13591700	54.87456800
O	50.07191600	39.05927900	56.50727500
H	49.55422000	39.30182500	57.28957100
H	49.96672100	39.83962600	55.90273900

ER^b(1)

N	48.73249800	43.24781400	54.51774500
H	49.44329700	43.56927100	53.85435200
H	49.12916700	43.44592900	55.44308900
C	47.47257100	43.99675000	54.34005700
H	47.53183000	44.58041800	53.41816100
C	46.31546600	42.96796800	54.16702900
H	46.37908300	42.26352900	55.00978500
C	44.90706600	43.52491500	54.09657600
H	44.85905300	44.42523800	53.47742200
H	44.25608400	42.77056000	53.64873300
H	44.53695500	43.75114900	55.09727600
O	46.52646300	42.22342900	52.95527600
H	47.24552600	41.58793400	53.13992900
C	47.19066900	44.96432600	55.51697300
O	47.65113500	44.74099000	56.64795500
N	46.33801700	45.94310800	55.19362900
H	46.24007500	46.15390500	54.19545100
F	45.68026800	46.97746400	56.10029000
F	44.62608100	44.11463100	50.06723300
C	46.05242200	43.96802200	49.58392400
H	46.20811700	43.04920400	49.01216000
H	46.36711300	44.81758600	48.96688300
N	47.09244100	43.90345100	50.67488600
H	47.29390000	44.84662000	51.05862600

H	46.86560900	43.25044400	51.45894000
H	47.97500700	43.55733800	50.26159600
F	49.79484900	35.99029500	51.09262400
C	49.63445100	37.42422000	50.75022200
O	50.23895900	37.97048700	49.84432300
N	48.66470200	38.08671200	51.45068900
H	47.97717600	37.54557100	51.96679200
C	48.21888500	39.32513700	50.84150100
C	46.68501800	39.43030100	50.95940900
C	45.91778500	40.36160400	49.99487700
C	44.43859900	39.94431800	49.96260100
H	44.03522300	39.80977400	50.97040000
H	44.31347300	38.99925700	49.41631700
H	43.82520300	40.70366800	49.46687300
C	46.49124300	40.39175500	48.57192300
H	45.85245900	40.99049000	47.91149200
H	46.55633000	39.38661100	48.13389400
H	47.48960700	40.83900600	48.55621900
H	45.96803200	41.37197800	50.40432000
H	46.32659500	38.40749800	50.77519600
H	46.40407600	39.67825400	51.98984100
H	48.46772200	39.24259100	49.77220900
C	49.06998700	40.52305200	51.26783500
O	48.62613300	41.65322800	51.12195700
C	50.53410900	40.40809800	51.70533100
C	51.44229700	41.36886000	50.96468800
H	52.43594200	41.35220900	51.41110900
H	51.03694300	42.38049800	50.96674700
H	51.56215100	41.02243400	49.93594800
C	50.85339700	39.97718900	53.09338000
H	51.73730700	40.38581400	53.57774600
H	50.05062800	39.65303000	53.74912500
O	51.12012800	39.14542300	51.97994400
O	48.21771100	40.51000700	54.46394500
H	47.67507900	40.41020400	55.26139400
H	48.57226700	41.45794600	54.53361200
ER ^b (2)			
N	49.04223700	43.87183800	54.25571900
H	49.58819200	44.72705300	54.13213300
H	49.26993300	43.55929300	55.20419000
C	47.63204300	44.24159300	54.18269300
H	47.51045700	44.85504800	53.28887100
C	46.82226300	42.95206000	53.93656900

H	47.11190600	42.21873500	54.70988400
C	45.31012800	43.10158200	53.92988300
H	44.99605300	43.93797600	53.29753900
H	44.86440400	42.19370700	53.51445500
H	44.91389800	43.25778600	54.93746400
O	47.21739700	42.43815600	52.65100300
H	49.42841100	42.82215100	50.75286900
C	47.15357700	45.03623100	55.40435400
O	47.55597000	44.76495700	56.54822600
N	46.26789200	45.98616600	55.08878000
H	46.16564800	46.21209400	54.09474300
F	45.61422500	46.97513900	56.03675300
F	44.32220700	44.02899000	49.96792600
C	45.72054900	44.00407600	49.38431200
H	45.94319300	43.06089300	48.87272700
H	45.87669700	44.82744500	48.67908900
N	46.80813300	44.14629600	50.39259800
H	46.89911300	45.09736200	50.79528200
H	46.74002200	43.47471800	51.18689400
H	47.74022900	43.97793300	49.97070100
F	49.91047900	35.99626000	51.14960500
C	49.66440800	37.42583900	50.87478800
O	50.45244900	38.15837800	50.29250400
N	48.42093700	37.85592800	51.18719000
H	47.79000400	37.32264400	51.77362000
C	48.03598400	39.11447100	50.62342900
C	46.51615500	39.29035300	50.75395400
C	45.80800800	40.18705300	49.71143100
C	44.35255600	39.71228900	49.58086800
H	43.87498900	39.58711700	50.55851300
H	44.32259200	38.74574600	49.05967800
H	43.75165200	40.41934700	49.00117200
C	46.48596900	40.21175500	48.33205500
H	45.86727700	40.76085600	47.61335200
H	46.63133200	39.20090500	47.92577900
H	47.45786800	40.70781200	48.38586100
H	45.80517100	41.21108300	50.09953300
H	46.11916600	38.27225600	50.64135300
H	46.25176100	39.61733200	51.76625200
H	48.26831500	39.05925300	49.55398800
C	48.95268700	40.25815400	51.06003400
O	48.98398400	41.22827200	50.31244200
C	49.91212400	40.24259000	52.24049500
C	51.30261400	40.71999600	51.87038900

H	51.98091300	40.47736600	52.69081300
H	51.30343700	41.79894700	51.70631500
H	51.64881500	40.21335300	50.97296300
C	49.41473100	40.47773800	53.61174200
H	50.06520500	41.01338500	54.30268300
H	48.34843300	40.57669200	53.79035100
O	49.84490400	39.17401100	53.20199400
O	49.24854500	43.64323100	51.25585900
H	48.14259200	42.76483000	52.49584700
H	50.13437700	43.96844900	51.53647100

TS1^b

N	48.76398900	43.32273800	54.48841900
H	49.48955400	43.64636000	53.82891100
H	49.13356100	43.49524900	55.44118800
C	47.44516900	44.03739400	54.30146800
H	47.52693800	44.61259200	53.38167600
C	46.34698900	42.93365600	54.10529400
H	46.43339800	42.27942700	55.00243100
C	44.92211200	43.47382400	54.08030200
H	44.83647000	44.36197800	53.44655100
H	44.29182900	42.69693700	53.64256000
H	44.55378200	43.70057600	55.08412600
O	46.65058900	42.21779200	52.95864400
H	47.40486200	41.21832900	53.44606900
C	47.20126400	44.97326700	55.49428800
O	47.70907500	44.72577900	56.60284200
N	46.33289100	45.93920300	55.19704800
H	46.19821000	46.13302000	54.19903300
F	45.67367200	46.96821800	56.10046300
F	44.62787200	44.11373800	50.06429100
C	46.06629900	43.94100100	49.62400300
H	46.21978500	43.02126500	49.05595300
H	46.41432500	44.78534600	49.01730600
N	47.06697100	43.85438400	50.74952400
H	47.27973700	44.80109000	51.11330300
H	46.81015700	43.19994700	51.55819700
H	47.94802500	43.47805600	50.36433500
F	49.79295300	36.01141400	51.07877000
C	49.63610300	37.44540200	50.74046400
O	50.25661300	38.00054200	49.84994200
N	48.65067700	38.09153600	51.42596900
H	47.96845400	37.54610700	51.94326400
C	48.20841700	39.33591900	50.83355100

C	46.67505900	39.42884300	50.96206500
C	45.89563000	40.37455500	50.02542500
C	44.42510100	39.92789600	49.97163700
H	44.02491500	39.73447900	50.97162900
H	44.32021800	39.00746800	49.38005500
H	43.79550400	40.69754400	49.51342300
C	46.47389400	40.45666700	48.60584800
H	45.82438500	41.05759000	47.95784800
H	46.56182400	39.46419900	48.14269400
H	47.46256000	40.92557900	48.60676000
H	45.92440300	41.36889500	50.47392300
H	46.32756500	38.40633600	50.75240500
H	46.40480200	39.65075300	51.99946800
H	48.44733700	39.26319000	49.76151200
C	49.07750100	40.51942600	51.26472800
O	48.68583700	41.65721300	51.06204300
C	50.52912900	40.37901100	51.75073400
C	51.46548300	41.31707500	51.01642400
H	52.46149200	41.25418100	51.45132900
H	51.09708200	42.34260300	51.03439800
H	51.56024900	40.98448800	49.98047000
C	50.81762400	39.95217600	53.14657400
H	51.69820000	40.34705100	53.65136600
H	49.98468200	39.65119200	53.77416900
O	51.09711400	39.11085000	52.04421600
O	48.07042600	40.57793400	54.06236600
H	47.52994700	40.28651800	54.81277600
H	48.64777400	42.28029900	54.36772200

TS3^b

N	49.15579400	43.79118400	53.85675100
H	49.44740400	44.72069400	54.19087200
H	49.59098600	43.11481500	54.49065800
C	47.65854000	43.73042300	53.88136900
H	47.32790500	44.12026500	52.92290600
C	47.01821600	42.32139200	54.15958600
H	47.31355700	42.09267300	55.19138100
C	45.50210800	42.49717000	54.10964900
H	45.16977100	42.73060800	53.09200200
H	45.07282900	41.54357600	54.39760700
H	45.12812100	43.26228200	54.79365600
O	47.26189200	41.09294900	53.41232800
H	49.09979400	42.87053100	51.33544500
C	47.24277200	44.67672700	55.04278300

O	47.66484500	44.44625200	56.18670300
N	46.44596600	45.69541400	54.71304600
H	46.33614700	45.91993400	53.71726500
F	45.82048200	46.67606000	55.69124900
F	44.47856200	44.07306700	49.85127300
C	45.87386400	44.12845000	49.26002200
H	46.10671800	43.26253700	48.63005700
H	46.01865400	45.04010000	48.67048600
N	46.97038900	44.15576500	50.27864000
H	46.94231600	45.00073600	50.87595300
H	47.05126700	43.28549700	50.85585000
H	47.89318300	44.19061400	49.80644400
F	49.53053300	36.41031700	50.99049700
C	49.28321400	37.87276500	50.82151400
O	49.89631500	38.52212800	49.97863600
N	48.31813100	38.42495100	51.61010200
H	47.75223600	37.80234300	52.17770100
C	47.81777300	39.76910400	51.32851400
C	46.33187300	39.74823100	50.88032900
C	46.08891600	40.28385300	49.44667000
C	44.58959000	40.26880200	49.10631100
H	43.99691600	40.85618400	49.81599800
H	44.20325500	39.23975200	49.11718200
H	44.41437100	40.66607800	48.09846400
C	46.86692700	39.55138200	48.34043500
H	46.81250000	40.12162600	47.40608100
H	46.41907300	38.57870500	48.12400500
H	47.92124200	39.38438900	48.58111400
H	46.43524800	41.32425900	49.44553300
H	45.96185400	38.71459400	50.93946400
H	45.72434400	40.33855400	51.57525200
H	48.41696200	40.07214000	50.47377700
C	48.20631800	40.95071700	52.32887400
O	48.15853300	42.06110500	51.54086900
C	49.61148300	40.61153200	52.94294300
C	50.81755100	40.68251500	52.02481600
H	51.00028400	41.70831100	51.69206300
H	50.69456500	40.05120300	51.14373200
H	51.70140700	40.32377700	52.55993000
C	49.85992300	40.69714400	54.40451200
H	50.88167700	40.85060700	54.75774000
H	49.08769500	41.02319200	55.09650500
O	49.60406800	39.43444400	53.79357200
O	49.58813300	43.88397900	51.39062100

H	49.49995800	43.77103600	52.75427400
H	50.53807600	43.90479000	51.13451300
TS6 ^b			
N	49.03755800	43.89641000	54.08304100
H	49.52233000	44.79699400	54.14434900
H	49.29100100	43.41443900	54.95135800
C	47.59785500	44.18324100	54.07342800
H	47.42720600	44.81403000	53.20312900
C	46.84838400	42.85958100	53.76378300
H	47.14615900	42.13725600	54.55899800
C	45.32541200	42.99465300	53.82487300
H	44.97082800	43.81914700	53.19651800
H	44.88361300	42.07999800	53.42288900
H	44.95118800	43.14969500	54.84327800
O	47.28836100	42.41786100	52.51466400
H	49.39219100	42.60910700	50.92096000
C	47.15684800	44.95274800	55.31303900
O	47.58489600	44.68568000	56.44956000
N	46.27787600	45.91469800	55.01466200
H	46.13673700	46.12372800	54.02333000
F	45.64617100	46.90150200	55.97348400
F	44.33754900	44.03738400	49.96470800
C	45.75558500	43.94316000	49.44763500
H	45.96309500	42.98359600	48.96284900
H	45.96814500	44.74531300	48.72952700
N	46.80082800	44.06743300	50.50157900
H	46.80853700	45.00769100	50.93247500
H	46.81810800	43.32320700	51.33055800
H	47.71870100	43.98637600	50.04084400
F	49.78463100	36.12535900	51.05946800
C	49.54325500	37.55575100	50.78893000
O	50.34975100	38.29498300	50.23443500
N	48.29028400	37.98645500	51.06644100
H	47.68268800	37.47883300	51.69962300
C	47.97700800	39.31365900	50.62149600
C	46.50958600	39.69636200	50.92300100
C	45.65716500	40.23476900	49.72257000
C	44.38908300	39.39002800	49.54559900
H	43.86165000	39.23389300	50.49273400
H	44.65942800	38.41368900	49.13633300
H	43.69244900	39.85517600	48.84007600
C	46.38801200	40.35331300	48.37462100
H	45.71702900	40.78709200	47.62477400

H	46.70427400	39.37438400	47.98755700
H	47.27145000	40.99538900	48.44515500
H	45.33533700	41.24125700	50.00434700
H	46.03149500	38.78837800	51.30957000
H	46.49900800	40.45009800	51.71687900
H	48.14070200	39.32698200	49.54074500
C	49.00424100	40.33707500	51.08626000
O	49.11932300	41.32351300	50.35153000
C	49.91976300	40.24010600	52.28588800
C	51.34848100	40.63455700	51.97140200
H	51.98005700	40.37314500	52.82258300
H	51.42936000	41.70778600	51.78206300
H	51.69402100	40.09537100	51.09448500
C	49.37585200	40.45348300	53.64111400
H	50.03151200	40.91357800	54.38084800
H	48.31242500	40.62198200	53.76265200
O	49.75231200	39.14214200	53.19794900
O	49.34346000	43.50139000	51.45327800
H	48.85906300	43.25315300	52.36183300
H	50.26744400	43.83748500	51.62802600

INT2^b

N	49.12273300	43.77956700	53.80165000
H	49.43650800	44.71286000	54.11211000
H	49.57488300	43.09563500	54.41824500
C	47.61841500	43.71359400	53.87045800
H	47.26505800	44.08409900	52.91454700
C	47.00772000	42.29974600	54.19260300
H	47.33566200	42.10206000	55.22198500
C	45.48982400	42.46475900	54.18262300
H	45.12990100	42.68970800	53.17239700
H	45.08569500	41.50393200	54.48161000
H	45.12276700	43.22626900	54.87480300
O	47.24443800	41.07142500	53.46087400
H	49.28000900	43.01534400	51.12259300
C	47.24199700	44.67563700	55.03263900
O	47.68988500	44.44935600	56.16756600
N	46.44036700	45.69334800	54.71109200
H	46.31905200	45.91357900	53.71551200
F	45.81929200	46.67693000	55.68946700
F	44.47930200	44.06667800	49.85389600
C	45.87749800	44.11205000	49.26743700
H	46.10569900	43.24627700	48.63607500
H	46.02850100	45.02322500	48.67809300

N	46.97388700	44.13558400	50.28658300
H	46.93296300	44.97566400	50.88910100
H	47.07899000	43.25922600	50.86009600
H	47.89652700	44.19738800	49.81409400
F	49.52210000	36.41609200	50.99611100
C	49.27693900	37.88075700	50.82100400
O	49.89972200	38.52690500	49.98207400
N	48.30515200	38.43785800	51.59642100
H	47.73878900	37.81965400	52.16824100
C	47.81581400	39.79296400	51.33041100
C	46.33226700	39.78476900	50.87517100
C	46.10013700	40.29863300	49.43191400
C	44.60195000	40.29397400	49.08548900
H	44.01132500	40.89182200	49.78805200
H	44.20677400	39.26839200	49.10366400
H	44.43363100	40.68411000	48.07365200
C	46.87387400	39.54336300	48.33850000
H	46.82543900	40.09998600	47.39552600
H	46.41649300	38.57245100	48.13561100
H	47.92602400	39.37036100	48.58432400
H	46.45679900	41.33564500	49.41564700
H	45.94508100	38.75844600	50.95226900
H	45.73213900	40.39767300	51.55685200
H	48.42248300	40.10646700	50.48378900
C	48.20733700	40.95663000	52.35376000
O	48.19248700	42.09377000	51.64266300
C	49.60143200	40.58464200	52.97981300
C	50.80867500	40.67013000	52.06344500
H	50.97862700	41.69916100	51.73113400
H	50.69057500	40.04223900	51.17878300
H	51.69885200	40.31971900	52.59378500
C	49.85010400	40.66026000	54.44300000
H	50.87179300	40.80872400	54.79920100
H	49.07615600	40.97942500	55.13679000
O	49.59606600	39.40151700	53.82031500
O	49.60932700	43.97210400	51.16779700
H	49.42186100	43.69535300	52.78503600
H	50.58096100	43.99780800	51.00001800
INT3 ^b			
N	49.16651300	43.73181000	53.86816100
H	49.45051100	44.70351000	54.04461600
H	49.55546300	43.22090700	54.66532500
C	47.69254800	43.71008400	53.91040300

H	47.32848700	44.10148900	52.96047200
C	47.02001700	42.31947200	54.19234500
H	47.32559100	42.06000900	55.21169400
C	45.50652900	42.49409800	54.15641500
H	45.16531100	42.76570400	53.15097300
H	45.07221700	41.53456500	54.41600400
H	45.14527700	43.23993400	54.86726200
O	47.22604800	41.07019300	53.41816400
H	48.93311300	42.46531300	51.29903600
C	47.25041600	44.65913500	55.06548300
O	47.64121300	44.43671700	56.22219300
N	46.45928600	45.68114300	54.72087000
H	46.36539900	45.90656000	53.72494700
F	45.82624100	46.66945500	55.69065100
F	44.47781500	44.07885100	49.84883100
C	45.87138300	44.15269700	49.25715900
H	46.12134300	43.28666000	48.63414500
H	46.00598800	45.06362100	48.66483700
N	46.95968400	44.20368900	50.28398400
H	46.92672700	45.05791300	50.87066600
H	46.99546200	43.36132800	50.88468400
H	47.89503700	44.21568400	49.83425200
F	49.54100200	36.41208300	50.98147500
C	49.28756200	37.87165200	50.82638700
O	49.89397600	38.53730500	49.99242500
N	48.31729400	38.40418500	51.62522100
H	47.75269100	37.76936100	52.18066000
C	47.80995100	39.74095400	51.35614500
C	46.33057200	39.72900700	50.88160700
C	46.11516300	40.29192800	49.45340000
C	44.62208200	40.29611600	49.08790200
H	44.02182900	40.87246700	49.80014900
H	44.22736500	39.27068000	49.06710300
H	44.46941500	40.71852800	48.08684200
C	46.90471200	39.56999700	48.34885100
H	46.84271800	40.14108100	47.41580500
H	46.47183900	38.59029900	48.13176800
H	47.96110600	39.41749900	48.59024900
H	46.46805000	41.33028000	49.47288500
H	45.96287300	38.69396300	50.91397800
H	45.70989400	40.30437100	51.57706000
H	48.42007300	40.05524600	50.51252400
C	48.17585900	40.89481600	52.38806200
O	48.07841000	42.03037400	51.56181300

C	49.59315300	40.60486900	52.97528100
C	50.78941300	40.70572200	52.04751700
H	50.95918900	41.74003400	51.73411400
H	50.67649100	40.08168100	51.15977800
H	51.67888100	40.35389000	52.57695900
C	49.83742100	40.68519700	54.42897700
H	50.85592400	40.86002600	54.77761200
H	49.06079700	41.00273400	55.11695500
O	49.60146700	39.41663100	53.81213600
O	49.62755300	43.89515800	51.21909800
H	49.57897100	43.83827000	52.22364800
H	50.59245800	44.02442000	51.04502600