

Electronic supplementary information

The Reactivation of Tabun-inhibited mutant AChE with Ortho-7: Steered Molecular Dynamics and Quantum Chemical Studies

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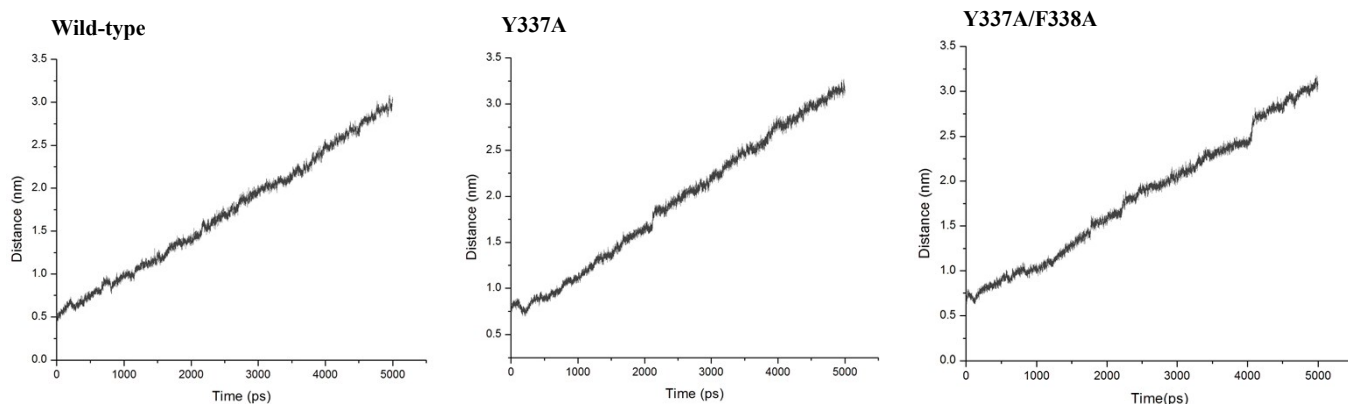


Fig. S1. Center of mass distance between Ortho-7 and *mAChE* during the unbinding of Ortho-7 as a function of time from the active site gorge.

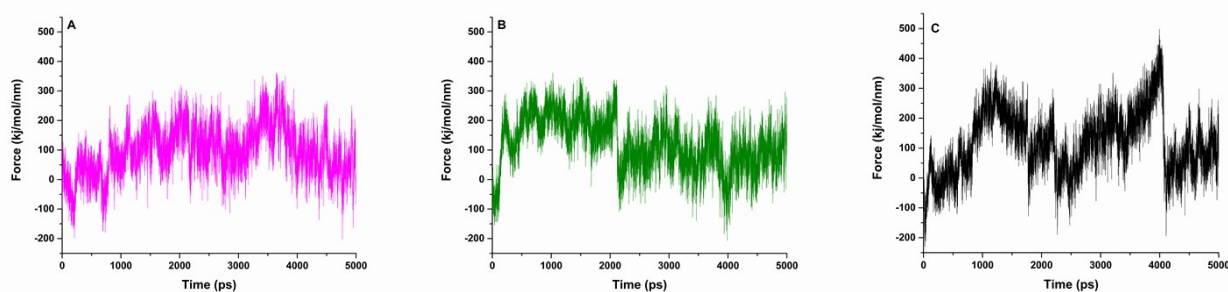
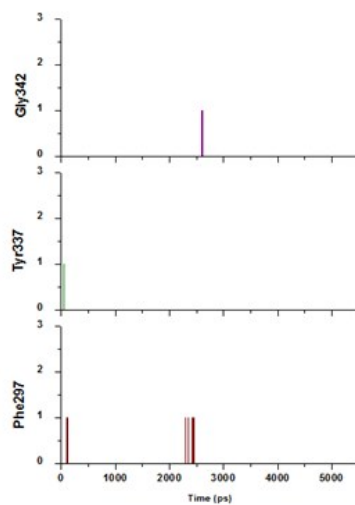
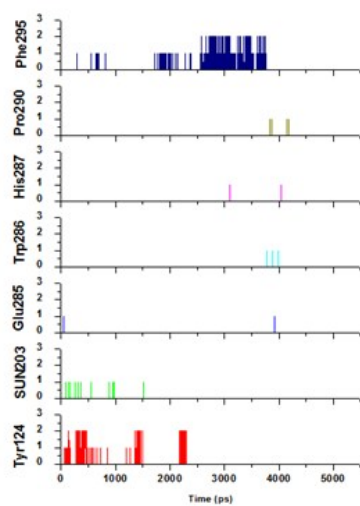
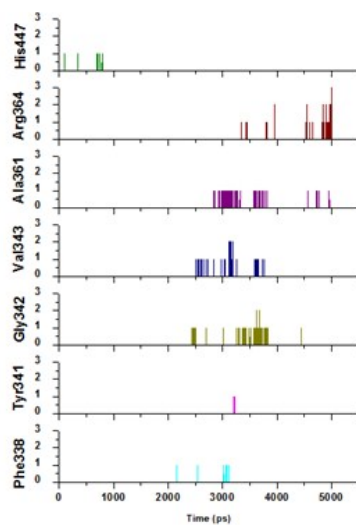
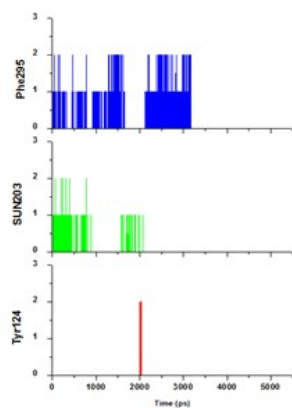


Fig. S2. Force profiles of Ortho-7 and *mAChE* during the unbinding of Ortho-7 as a function of time from the active site gorge in the case of wild type (A), single mutant (Y337A) (B) and double mutant (Y337A/F338A) (C).

Wild-type



Y337A



Y337A/F338A

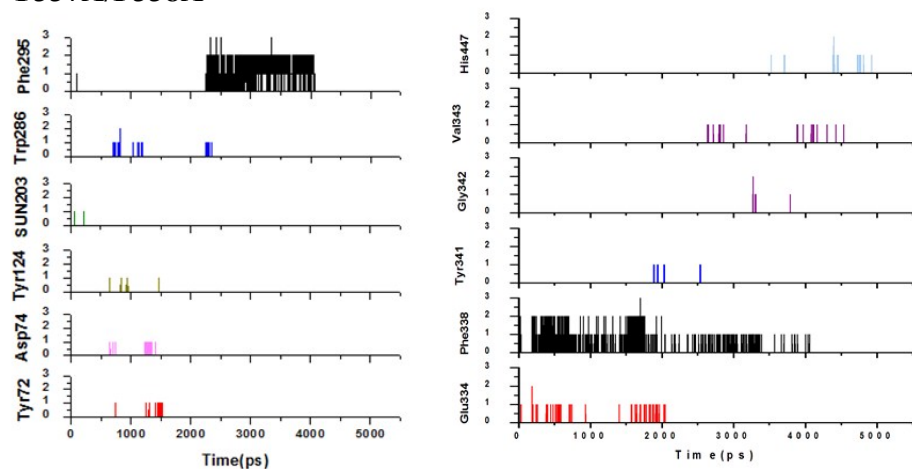


Fig. S3. Number of hydrogen bonds between amino acid residues of wild-type/mutant *mAChE* and Ortho-7 as a function of time during the process of leaving the active site gorge.

M05-2X/6-31+G* calculated Cartesian
coordinates of all geometries. (All energies are
given in Hartee).

Wild type

E = -6363.62276

N	61.430000000	59.200000000	47.640000000
N	50.290000000	62.190000000	49.220000000
N	48.390000000	60.400000000	45.760000000
N	47.790000000	49.400000000	48.680000000
N	48.430000000	49.790000000	45.240000000
N	51.850000000	53.100000000	41.070000000
N	66.490000000	57.550000000	39.100000000
N	61.900000000	61.070000000	37.430000000
N	54.590000000	55.560000000	34.650000000
N	45.770000000	60.340000000	37.020000000
N	48.400000000	59.550000000	36.400000000
N	43.850000000	57.290000000	40.690000000
N	46.820000000	53.690000000	40.140000000
N	47.430000000	53.080000000	42.060000000
N	52.950000000	57.620000000	43.160000000
N	51.490000000	60.220000000	43.130000000
N	58.000000000	59.500000000	39.390000000
N	57.280000000	57.940000000	36.860000000
C	61.260000000	60.440000000	46.880000000
C	61.020000000	60.160000000	45.400000000
C	61.110000000	61.400000000	44.510000000
C	60.030000000	62.120000000	44.020000000
C	62.320000000	61.750000000	43.910000000
C	60.060000000	63.080000000	43.010000000
C	62.470000000	62.700000000	42.900000000
C	61.320000000	63.390000000	42.520000000
C	60.050000000	61.250000000	47.380000000
C	51.270000000	61.100000000	49.120000000
C	51.400000000	60.530000000	47.710000000
C	50.080000000	60.140000000	47.030000000
C	49.460000000	61.020000000	46.240000000
C	49.320000000	59.000000000	47.190000000
C	48.240000000	59.210000000	46.340000000
C	49.460000000	57.900000000	48.040000000
C	47.180000000	58.300000000	46.320000000
C	48.380000000	57.020000000	48.020000000

C	47.310000000	57.190000000	47.150000000
C	52.620000000	61.520000000	49.690000000
C	47.380000000	50.020000000	47.410000000
C	46.800000000	51.360000000	47.870000000
C	46.170000000	52.220000000	46.760000000
C	47.180000000	52.680000000	45.710000000
C	48.610000000	50.120000000	46.520000000
C	49.360000000	49.860000000	44.110000000
C	49.750000000	51.310000000	43.850000000
C	52.700000000	54.280000000	40.840000000
C	52.600000000	51.930000000	40.590000000
C	50.730000000	54.890000000	44.240000000
C	49.570000000	55.880000000	44.280000000
C	50.570000000	48.930000000	44.240000000
C	65.490000000	58.210000000	38.250000000
C	64.770000000	59.370000000	38.950000000
C	63.430000000	59.710000000	38.300000000
C	62.970000000	60.960000000	38.220000000
C	62.620000000	58.950000000	37.470000000
C	61.740000000	59.860000000	36.900000000
C	62.370000000	57.590000000	37.320000000
C	60.630000000	59.420000000	36.190000000
C	61.260000000	57.110000000	36.640000000
C	60.420000000	58.050000000	36.060000000
C	66.200000000	58.670000000	36.970000000
C	54.160000000	54.350000000	35.370000000
C	52.730000000	54.070000000	34.900000000
C	51.710000000	53.650000000	35.960000000
C	52.120000000	52.580000000	36.740000000
C	50.350000000	53.950000000	35.910000000
C	51.190000000	51.840000000	37.470000000
C	49.430000000	53.200000000	36.640000000
C	49.850000000	52.190000000	37.500000000
C	55.120000000	53.170000000	35.240000000
C	46.880000000	60.700000000	37.920000000
C	46.930000000	59.750000000	39.110000000
C	47.070000000	60.430000000	40.480000000
C	46.520000000	59.800000000	41.590000000
C	47.800000000	61.590000000	40.670000000
C	46.590000000	60.420000000	42.830000000
C	47.900000000	62.210000000	41.910000000
C	47.170000000	61.670000000	42.960000000
C	48.220000000	60.620000000	37.170000000
C	49.540000000	59.450000000	35.490000000
C	49.560000000	57.960000000	35.140000000
C	49.770000000	57.050000000	36.360000000

C	48.610000000	56.570000000	36.960000000	P	51.480000000	52.910000000	42.630000000
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C	51.080000000	56.280000000	38.170000000	C	52.474000000	58.295000000	44.165000000
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C	49.570000000	60.390000000	34.280000000	H	59.100000000	61.660000000	44.350000000
C	44.700000000	56.300000000	41.370000000	H	63.160000000	61.100000000	44.130000000
C	46.020000000	56.050000000	40.630000000	H	59.140000000	63.460000000	42.550000000
C	46.600000000	54.680000000	40.990000000	H	63.380000000	62.820000000	42.310000000
C	46.970000000	54.320000000	42.220000000	H	60.560000000	65.000000000	41.780000000
C	44.900000000	56.540000000	42.860000000	H	50.550000000	63.030000000	48.730000000
C	52.220000000	59.620000000	44.080000000	H	49.870000000	61.980000000	45.940000000
C	52.970000000	60.410000000	44.950000000	H	47.880000000	60.750000000	44.980000000
C	52.870000000	61.800000000	44.930000000	H	50.150000000	57.840000000	48.880000000
C	52.100000000	62.370000000	43.930000000	H	46.210000000	58.560000000	45.900000000
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C	50.810000000	58.970000000	40.910000000	H	48.580000000	49.710000000	49.200000000
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C	53.220000000	59.150000000	40.490000000	H	66.450000000	57.950000000	40.010000000
C	54.330000000	59.810000000	39.660000000	H	63.310000000	61.760000000	38.860000000
C	55.660000000	59.510000000	40.330000000	H	61.170000000	61.750000000	37.490000000
C	56.610000000	59.970000000	39.220000000	H	62.950000000	56.790000000	37.780000000
C	58.820000000	60.330000000	40.170000000	H	60.020000000	60.090000000	35.570000000
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C	60.420000000	58.580000000	40.210000000	H	59.410000000	57.720000000	35.840000000
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C	58.380000000	58.300000000	38.940000000	H	53.060000000	52.060000000	36.590000000
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O	53.240000000	60.770000000	50.440000000	H	48.370000000	53.140000000	36.380000000
O	48.160000000	53.320000000	46.140000000	H	49.150000000	51.870000000	38.280000000
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O	50.430000000	51.680000000	42.650000000	H	48.400000000	61.950000000	39.830000000
O	52.600000000	52.600000000	43.540000000	H	46.320000000	59.730000000	43.630000000
O	50.610000000	54.220000000	42.980000000	H	48.720000000	62.920000000	42.060000000
O	50.430000000	47.740000000	43.970000000	H	47.650000000	63.210000000	43.990000000
O	65.700000000	58.530000000	35.860000000	H	47.840000000	58.720000000	36.330000000
O	54.790000000	51.990000000	35.150000000	H	47.640000000	56.660000000	36.470000000
O	46.930000000	62.520000000	44.000000000	H	51.790000000	57.660000000	36.650000000
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O	45.760000000	57.370000000	43.160000000	H	50.010000000	54.990000000	39.580000000
O	53.310000000	56.220000000	43.380000000	H	44.090000000	57.410000000	39.720000000
O	56.730000000	56.940000000	35.950000000	H	46.580000000	53.760000000	39.170000000

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H	60.620000000	60.610000000	41.160000000
H	61.490000000	58.450000000	40.050000000
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H	64.742000000	57.468000000	37.972000000
H	62.160000000	61.046000000	46.985000000
H	56.601000000	61.058000000	39.164000000
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H	54.172000000	60.888000000	39.634000000
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H	53.364000000	59.389000000	41.544000000
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H	53.518000000	51.824000000	41.168000000
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H	52.923000000	54.366000000	39.777000000
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H	48.627000000	55.339000000	44.203000000
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H	52.274000000	57.778000000	45.104000000

Y337A

E= -6058.60229

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C	64.04000	63.93000	52.01000
C	64.65000	65.22000	51.46000
C	64.00000	65.86000	50.41000
H	63.54000	65.20000	49.67000
C	65.78000	65.84000	51.97000
H	66.28000	65.35000	52.80000
C	64.38000	67.14000	49.99000
H	63.91000	67.66000	49.16000
C	66.26000	67.06000	51.50000
H	67.28000	67.39000	51.70000
C	65.49000	67.74000	50.57000
O	65.74000	69.04000	50.27000
H	66.33000	69.40000	50.99000
C	61.80000	64.86000	52.78000
O	60.98000	64.31000	52.04000

N	50.60000	68.79000	57.13000	N	68.36000	61.13000	47.74000
H	50.33000	69.17000	56.25000	H	68.04000	61.55000	48.59000
C	50.82000	67.33000	57.04000	C	67.65000	61.50000	46.51000
C	50.32000	66.80000	55.70000	C	66.49000	62.45000	46.81000
C	49.29000	65.71000	56.02000	C	66.84000	63.82000	47.39000
C	48.06000	65.93000	56.46000	C	66.63000	64.27000	48.62000
H	47.66000	66.92000	56.69000	H	67.05000	63.83000	49.53000
C	49.35000	64.34000	55.81000	C	66.88000	64.93000	46.55000
N	47.34000	64.82000	56.54000	N	66.41000	65.58000	48.56000
H	46.34000	64.80000	56.54000	H	66.10000	66.06000	49.38000
C	48.11000	63.81000	56.14000	C	66.56000	66.04000	47.32000
C	50.30000	63.55000	55.17000	C	67.14000	65.04000	45.19000
H	51.35000	63.82000	55.30000	H	67.01000	64.25000	44.44000
C	47.85000	62.46000	55.90000	C	66.47000	67.28000	46.70000
H	46.86000	62.11000	56.16000	H	66.33000	68.12000	47.38000
C	50.02000	62.23000	54.87000	C	67.16000	66.31000	44.62000
H	50.68000	61.68000	54.20000	H	67.88000	66.40000	43.81000
C	48.80000	61.67000	55.25000	C	66.76000	67.42000	45.35000
H	48.55000	60.65000	54.96000	H	66.60000	68.38000	44.86000
C	52.23000	66.81000	57.31000	C	68.57000	61.89000	45.35000
O	52.37000	65.65000	57.70000	O	68.19000	61.60000	44.22000
N	47.84000	52.16000	54.51000	N	57.10000	58.23000	41.70000
H	48.36000	52.46000	55.31000	H	56.88000	58.99000	42.32000
C	47.71000	53.15000	53.43000	C	56.94000	56.86000	42.21000
C	47.57000	54.54000	54.05000	C	56.07000	55.95000	41.34000
C	46.53000	55.30000	53.23000	C	54.63000	56.45000	41.29000
C	46.79000	55.46000	51.73000	C	53.60000	55.68000	41.83000
O	47.55000	56.29000	51.19000	H	53.81000	54.78000	42.41000
O	46.32000	54.61000	50.94000	C	54.21000	57.38000	40.34000
C	48.99000	53.16000	52.60000	H	54.90000	58.01000	39.78000
O	50.10000	53.03000	53.11000	C	52.25000	55.86000	41.56000
N	48.85000	53.37000	51.29000	H	51.53000	55.11000	41.91000
H	47.93000	53.64000	51.01000	C	52.87000	57.55000	40.00000
C	49.89000	53.41000	50.26000	H	52.67000	58.16000	39.13000
C	50.10000	54.89000	49.93000	C	51.87000	56.82000	40.63000
O	50.87000	55.23000	48.77000	H	50.81000	56.97000	40.43000
P	51.96000	56.41000	48.90000	C	58.29000	56.27000	42.62000
O	53.03000	56.08000	49.87000	O	58.45000	55.26000	43.30000
O	51.23000	57.85000	48.98000	N	47.87000	63.89000	42.63000
N	52.64000	56.47000	47.43000	H	47.24000	63.27000	43.09000
C	53.65000	57.53000	47.34000	C	48.76000	64.66000	43.50000
C	53.19000	55.21000	46.91000	C	47.92000	65.11000	44.69000
C	50.64000	58.30000	50.21000	C	50.16000	64.11000	43.81000
C	49.66000	59.43000	49.93000	O	50.83000	64.46000	44.78000
C	51.21000	52.69000	50.57000	N	50.55000	63.30000	42.83000
O	51.16000	51.47000	50.41000	H	49.89000	63.03000	42.13000

C	51.95000	62.96000	42.55000	C	55.53000	63.21000	46.56000
C	51.96000	61.43000	42.56000	C	56.95000	62.88000	46.10000
C	53.22000	60.64000	42.91000	C	57.89000	63.97000	46.60000
C	53.03000	59.30000	43.23000	C	59.26000	63.61000	46.04000
H	52.31000	58.78000	42.60000	N	59.49000	64.02000	44.63000
C	54.49000	61.20000	42.96000	C	59.81000	65.36000	44.37000
H	54.51000	62.25000	42.66000	H	60.00000	66.03000	45.21000
C	54.11000	58.57000	43.71000	C	60.29000	65.70000	43.12000
H	53.98000	57.53000	43.99000	H	60.68000	66.70000	42.95000
C	55.60000	60.47000	43.37000	C	60.46000	64.74000	42.12000
H	56.56000	60.88000	43.69000	H	61.23000	64.85000	41.35000
C	55.35000	59.19000	43.86000	C	60.06000	63.44000	42.37000
H	56.06000	58.62000	44.46000	H	60.11000	62.74000	41.54000
C	52.54000	63.55000	41.26000	C	59.64000	63.11000	43.66000
O	53.76000	63.67000	41.13000	C	59.69000	61.79000	44.09000
N	44.97000	60.30000	46.14000	N	59.07000	60.90000	43.31000
H	45.19000	60.31000	45.17000	O	59.18000	59.45000	43.50000
C	45.33000	59.11000	46.92000	H	59.55000	59.19000	44.39000
C	46.44000	58.38000	46.16000	H	65.78100	61.95200	47.47100
C	46.74000	57.02000	46.79000	H	65.89500	62.58500	45.90700
N	46.10000	55.89000	46.52000	H	67.17100	60.57700	46.18200
H	45.77000	55.65000	45.61000	H	57.92600	63.94500	47.68900
C	47.52000	56.82000	47.85000	H	57.57600	64.93200	46.19600
H	48.33800	57.46400	48.17100	H	63.47400	63.43200	51.22300
C	46.29100	54.89600	47.57000	H	64.83800	63.25500	52.31900
H	45.92200	53.87400	47.66600	H	63.63700	64.98200	53.77000
N	47.13000	55.70000	48.45000	H	59.41700	62.53500	46.13300
C	45.81000	59.58000	48.30000	H	60.03400	64.04500	46.67300
O	46.72000	60.39000	48.45000	H	56.98000	62.84600	45.01100
O	50.81000	56.74000	44.69000	H	57.25300	61.92000	46.51800
H	50.46000	56.24000	43.89000	H	55.54600	63.49300	47.61300
N	50.44000	58.14000	44.54000	H	55.13100	64.02100	45.95100
C	50.74000	58.93000	45.58000	H	54.08200	57.53700	46.33900
C	50.37000	60.27000	45.50000	H	53.18400	58.49500	47.54100
C	49.07000	60.48000	45.06000	H	54.43600	57.34700	48.07300
H	48.68000	59.92000	44.21000	H	53.61600	55.38000	45.92100
C	48.33000	61.48000	45.68000	H	53.96700	54.84700	47.58300
H	47.45000	61.84000	45.16000	H	52.39500	54.46700	46.84000
C	48.85000	62.27000	46.70000	H	50.52500	55.39200	50.79900
H	48.15000	62.47000	47.51000	H	49.13000	55.38300	49.87100
C	50.20000	62.15000	47.03000	H	47.43800	55.49700	49.39000
H	50.54000	62.43000	48.03000	H	51.15300	66.36100	55.15000
N	50.90000	61.12000	46.39000	H	49.83500	67.60600	55.15000
C	52.36000	61.03000	46.61000	H	54.91200	61.47500	45.43700
C	53.17000	62.31000	46.39000	H	54.87200	61.25200	47.18100
C	54.66000	61.96000	46.38000	H	52.96700	63.01200	47.19900

H	52.89500	62.75400	45.43300
H	52.76900	60.23500	45.98600
H	52.54900	60.65400	47.61600
H	50.18100	66.88100	57.80000
H	51.42300	58.65600	50.87900
H	50.11300	57.47200	50.68400
H	49.21600	59.76700	50.86700
H	50.18700	60.26000	49.45900
H	48.87500	59.07400	49.26400
H	48.53900	65.69100	45.37300
H	47.09100	65.72500	44.33900
H	47.52800	64.23600	45.21000
H	56.08900	54.93700	41.74200
H	56.47800	55.91600	40.33000
H	56.38700	56.97000	43.14300
H	51.57400	61.07000	41.60600
H	51.14000	61.07800	43.18600
H	52.55500	63.30700	43.38700
H	49.47300	52.94100	49.36900
H	46.84800	52.92200	52.80300
H	47.34400	58.98900	46.16400
H	46.13800	58.24000	45.12200
H	44.46300	58.45900	47.02900
H	60.20800	61.53900	45.00400
H	51.25100	58.52100	46.43900
H	46.37400	56.28400	53.67300
H	45.55300	54.84000	53.37700
H	48.52600	55.06000	53.99400
H	47.22200	54.44500	55.07900
H	48.95000	65.57800	42.94380

Y337A/F338A

E= -5827.65487

N	61.77000	60.79000	50.58000
H	62.03000	60.01000	50.02000
C	61.18000	61.92000	49.84000
C	61.12000	61.49000	48.37000
C	60.49000	62.52000	47.43000
C	59.24000	62.30000	46.86000
H	58.79000	61.31000	46.87000
C	61.08000	63.77000	47.35000
H	62.15000	63.94000	47.47000
C	58.56000	63.32000	46.21000

H	57.58000	63.13000	45.78000
C	60.33000	64.79000	46.76000
H	60.83000	65.76000	46.81000
C	59.07000	64.62000	46.21000
O	58.54000	65.48000	45.30000
H	58.05000	64.87000	44.68000
C	59.76000	62.30000	50.29000
O	58.94000	61.43000	50.53000
N	49.55000	61.61000	51.92000
H	49.29000	62.14000	51.11000
C	50.55000	60.59000	51.54000
C	50.62000	60.48000	50.02000
C	49.27000	60.23000	49.34000
C	48.74000	61.02000	48.41000
H	49.28000	61.87000	47.98000
C	48.27000	59.35000	49.73000
N	47.49000	60.64000	48.14000
H	46.91000	61.03000	47.43000
C	47.19000	59.59000	48.90000
C	48.21000	58.33000	50.68000
H	49.10000	58.00000	51.20000
C	46.03000	58.86000	49.12000
H	45.15000	58.92000	48.46000
C	47.02000	57.64000	50.95000
H	46.88000	57.02000	51.83000
C	45.90000	58.00000	50.20000
H	44.94000	58.01000	50.70000
C	51.94000	60.90000	52.10000
O	52.71000	59.99000	52.42000
N	46.91000	50.01000	50.88000
H	47.07000	50.61000	51.66000
C	46.66000	50.59000	49.55000
C	45.79000	51.80000	49.86000
C	45.58000	52.94000	48.86000
C	46.87000	53.68000	48.47000
O	47.82000	53.69000	49.29000
O	46.99000	54.06000	47.29000
C	47.92000	50.90000	48.74000
O	49.04000	50.92000	49.26000
N	47.77000	50.54000	47.47000
H	46.91000	50.17000	47.12000
C	48.84000	50.66000	46.47000
C	49.03000	52.15000	46.19000
O	49.94000	52.53000	45.15000
P	50.81000	53.83000	45.50000
O	51.93000	53.30000	46.32000

O	49.90000	55.07000	45.99000	N	44.99000	59.65000	39.47000
N	51.38000	54.25000	44.04000	H	44.42000	58.83000	39.53000
C	52.22000	55.45000	44.11000	C	45.77000	59.78000	40.71000
C	52.17000	53.17000	43.43000	C	45.57000	58.44000	41.43000
C	49.90000	55.47000	47.36000	C	47.27000	59.96000	40.46000
C	48.95000	56.67000	47.39000	O	48.01000	60.68000	41.14000
C	50.08000	49.81000	46.75000	N	47.80000	59.34000	39.41000
O	50.00000	48.58000	46.73000	H	47.38000	58.57000	38.94000
N	66.47000	59.07000	43.46000	C	49.17000	59.45000	38.89000
H	66.39000	59.68000	44.25000	C	49.64000	58.08000	38.38000
C	65.48000	59.37000	42.41000	C	49.40000	60.54000	37.84000
C	64.87000	60.75000	42.64000	O	50.41000	61.24000	37.84000
C	63.74000	61.10000	41.67000	N	42.27000	56.55000	43.48000
C	63.72000	61.99000	40.67000	H	43.03000	56.45000	42.83000
H	64.48000	62.70000	40.37000	C	42.36000	55.69000	44.66000
C	62.51000	60.46000	41.65000	C	42.93000	54.29000	44.39000
N	62.56000	61.80000	40.04000	C	44.42000	54.19000	44.07000
H	62.29000	62.34000	39.24000	N	44.98000	53.26000	43.30000
C	61.78000	60.85000	40.53000	H	44.40000	52.90000	42.57000
C	61.99000	59.41000	42.40000	C	45.39000	54.46000	44.94000
H	62.26000	59.39000	43.45000	C	46.26000	53.06000	43.61000
C	60.66000	60.18000	40.06000	N	46.53000	53.84000	44.65000
H	60.23000	60.43000	39.09000	C	42.93000	56.31000	45.94000
C	60.82000	58.76000	42.01000	O	43.19000	57.51000	46.00000
H	60.32000	58.04000	42.65000	O	47.89000	55.19000	42.38000
C	60.15000	59.15000	40.86000	H	48.45000	55.34000	41.57000
H	59.66000	58.35000	40.30000	N	47.48000	56.51000	42.85000
C	66.09000	59.31000	41.01000	C	47.64000	56.68000	44.17000
O	65.62000	58.55000	40.17000	C	47.42000	57.99000	44.59000
N	54.67000	56.42000	38.26000	C	46.20000	58.09000	45.27000
H	54.31000	57.15000	38.84000	H	45.87000	57.27000	45.90000
C	54.57000	55.09000	38.88000	C	45.65000	59.35000	45.42000
C	53.38000	54.41000	38.20000	H	44.84000	59.43000	46.15000
C	52.21000	54.19000	39.17000	C	46.29000	60.49000	44.95000
C	51.67000	52.92000	39.27000	H	45.83000	61.48000	45.00000
H	52.14000	52.13000	38.68000	C	47.54000	60.33000	44.38000
C	51.56000	55.26000	39.78000	H	48.08000	61.21000	44.01000
H	51.92000	56.26000	39.56000	N	48.12000	59.07000	44.22000
C	50.55000	52.74000	40.07000	C	49.43000	58.94000	43.54000
H	50.31000	51.71000	40.35000	C	50.61000	59.28000	44.46000
C	50.35000	55.08000	40.45000	C	51.88000	59.13000	43.61000
H	49.92000	55.94000	40.96000	C	53.05000	59.24000	44.58000
C	49.86000	53.80000	40.64000	C	54.30000	59.16000	43.71000
H	49.08000	53.57000	41.38000	C	54.72000	60.54000	43.22000
C	55.86000	54.27000	38.87000	C	55.74000	60.27000	42.11000
O	55.91000	53.28000	39.60000	N	56.78000	61.29000	41.84000

C	56.49000	62.16000	40.79000	H	48.88100	57.05400	48.40800
H	55.45000	62.31000	40.49000	H	49.33000	57.45200	46.73200
C	57.43000	63.11000	40.43000	H	47.96100	56.36000	47.05100
H	57.29000	63.76000	39.56000	H	50.90200	55.79600	47.64000
C	58.61000	63.23000	41.15000	H	49.48600	54.66700	47.97000
H	59.40000	63.85000	40.73000	H	52.58300	55.69900	43.11300
C	58.87000	62.38000	42.22000	H	51.63400	56.28200	44.50100
H	59.90000	62.40000	42.56000	H	53.06900	55.26200	44.76800
C	57.94000	61.38000	42.51000	H	52.53300	53.49200	42.45400
C	58.38000	60.29000	43.25000	H	53.01800	52.93200	44.07200
N	59.29000	60.34000	44.23000	H	51.54500	52.28500	43.31100
O	59.81000	59.05000	44.67000	H	48.41700	50.25100	45.55200
H	60.57000	59.13000	45.32000	H	49.31400	52.65400	47.11400
H	42.36000	53.81900	43.58900	H	48.05800	52.60400	45.99700
H	42.70100	53.64100	45.23500	H	45.20100	55.12300	45.77200
H	41.31800	55.49600	44.91400	H	46.85200	52.36200	43.03600
H	47.35800	54.02400	45.19800	H	44.86400	53.65300	49.27000
H	49.45100	59.59300	42.66700	H	45.10200	52.54900	47.96200
H	49.54400	57.92300	43.16500	H	46.10900	52.22500	50.81200
H	50.64100	58.57000	45.28600	H	44.81500	51.45100	50.20100
H	50.52000	60.31200	44.79800	H	46.06000	49.88100	48.98100
H	51.93100	59.94500	42.88800	H	53.69600	53.45100	37.79000
H	51.88900	58.14500	43.14300	H	53.04500	55.02000	37.36100
H	53.03200	58.39300	45.26600	H	54.29700	55.24400	39.92400
H	53.01700	60.20900	45.07800	H	51.31400	59.68500	49.74700
H	54.10500	58.51500	42.85400	H	51.06700	61.38700	49.61300
H	55.11300	58.71500	44.28400	H	50.22700	59.62800	51.93800
H	55.20500	61.08000	44.03300	H	65.65200	61.50700	42.57200
H	53.85500	61.05300	42.79900	H	64.50100	60.81600	43.66400
H	55.20900	60.04900	41.18400	H	64.68300	58.62900	42.46900
H	56.22200	59.31000	42.29500	H	60.57600	60.54900	48.29100
H	57.98200	59.30600	43.05100	H	62.12500	61.25100	48.02200
H	47.91400	55.84100	44.79300	H	61.83100	62.78900	49.93300
H	50.65600	58.16400	37.99500				
H	49.62100	57.36100	39.19900				
H	48.97700	57.74100	37.58400				
H	49.80500	59.69900	39.74000				
H	46.12000	58.44700	42.37100				
H	44.50900	58.29000	41.63100				
H	45.93900	57.63000	40.80000				
H	45.38500	60.59900	41.31700				