

Supporting Information

Theoretical Study on Mechanism of Ag-catalyzed Synthesis of 3-Alkylideneoxindoles from *N*-Aryl- α -diazoamides: a Lewis Acid or Ag-carbene Pathway?

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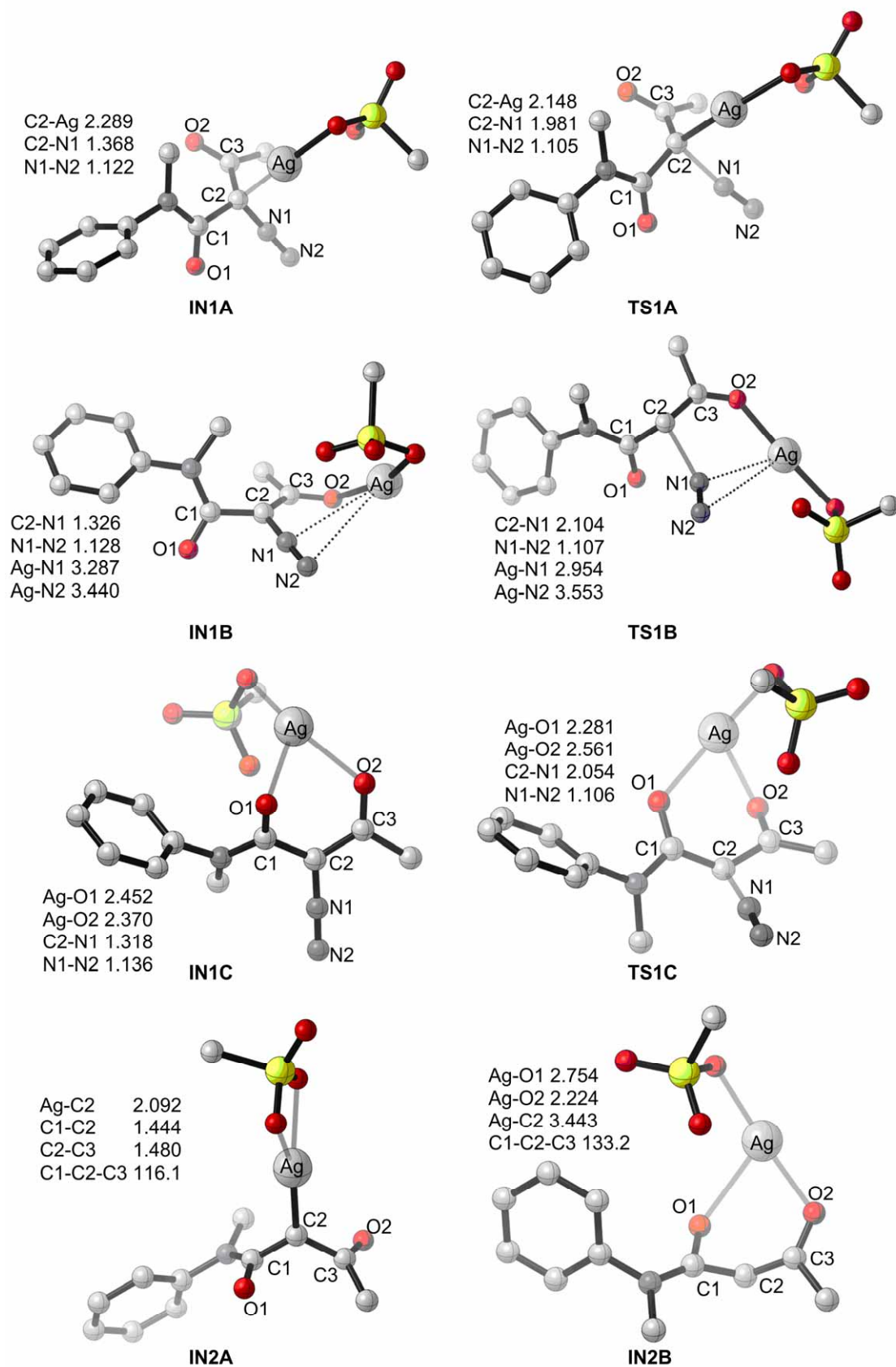


Figure S1. Geometries of key intermediates and transition states in N₂ dissociation step (hydrogens and fluorines are omitted for clarity; bond lengths in angstrom and bond angles in degree).

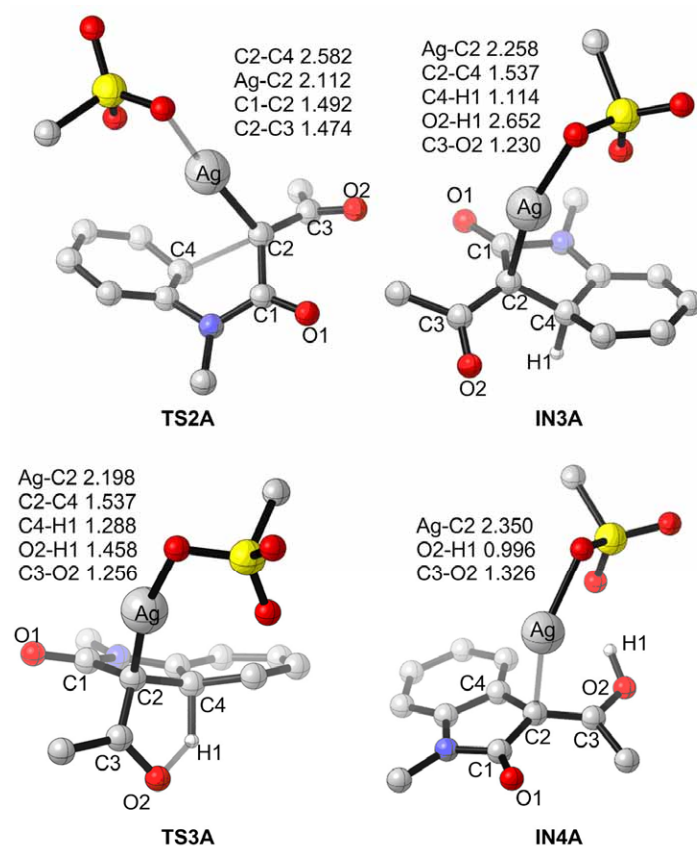


Figure S2. Geometries of key intermediates and transition states in the cyclization step (hydrogens and fluorines are omitted for clarity; bond lengths in angstrom and bond angles in degree).

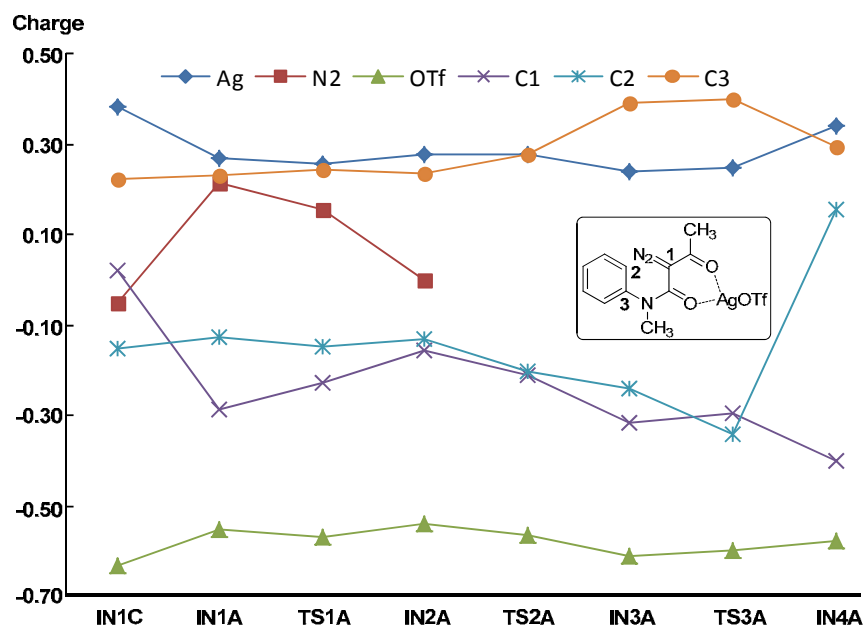


Figure S3. Charge distribution of key atoms along the reaction coordinate. C1, C2, and C3 are defined as in the structure of IN1C in this figure.

3. Computational methodologies

All calculations were performed with Gaussian 03 package.¹ Geometries were optimized in gas phase at the level of B3LYP density functional with LANL2DZ basis set for Ag, and 6-31G* basis sets for the other atoms. The minima and transition states were confirmed by frequency analysis. The thermodynamic correction for gas phase Gibbs free energy (TCG) was obtained in frequency calculation. Single point calculations were calculated by B3LYP functional with LANL2DZ+p basis set² for Ag, and 6-31+G* basis set for the other atoms. The solvation free energy was calculated by CPCM model with UAHF radii.³ The parameters for THF solvent was used to model dioxane solvent that was used in experimental report. The Gibbs free energy was calculated by adding TCG and solvation free energy to the single point energy. All charge distribution discussed in this work was calculated by Mulliken population analysis.

1. M. J. Frisch, et al *Gaussian 03 (Revision D.01)*; Gaussian, Inc.: Wallingford, CT and Pittsburgh, PA., 2004.
2. A. Hollwarth, M. Bohme, S. Dapprich, A. W. Ehlers, A. Gobbi, V. Jonas, K. F. Kohler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 237.
3. Y. Fu, K. Shen, L. Liu and Q. X. Guo, *J. Am. Chem. Soc.*, 2007, **129**, 13510-13519.

4. Energies of Intermediates and Transition States

Table 1. Electronic Energies (E), Thermal Correction for Gibbs Free Energies (TCG), Solvation Free Energies (ΔG_{sol}), and Free Energies in Solution (G_{sol})*.

	E (Hartree)	TCG (Hartree)	ΔG_{sol} (kcal/mol)	G_{sol} (Hartree)
1	-740.458252	0.163406	-0.97	-740.293364
IN1A	-1847.706407	0.171926	2.43	-1847.527581
IN1B	-1847.718288	0.173183	3.11	-1847.537121
IN1C	-1847.728671	0.173416	3.53	-1847.546602
TS1A	-1847.680904	0.168098	2.48	-1847.505826
TS1B	-1847.664758	0.167273	-1.01	-1847.496067
TS1C	-1847.668594	0.168465	2.28	-1847.493468
TS1D	-740.396924	0.158651	-1.62	-740.2378268
IN2A	-1738.182223	0.163396	-0.03	-1738.015847
IN2B	-1738.168413	0.166602	1.66	-1737.996138
TS2A	-1738.174713	0.166216	-0.76	-1738.00668
IN3A	-1738.235331	0.169056	-0.94	-1738.064745
TS3A	-1738.219373	0.167175	-0.7	-1738.050286
IN4A	-1738.27835	0.17338	1.38	-1738.099743
TS4	-1738.151985	0.16469	-2.88	-1737.988857
2	-631.038182	0.162505	-1.52	-630.8750714
3	-631.033108	0.162487	-1.66	-630.8702385
TS5	-631.030054	0.157738	-1.69	-630.8719813

$*G_{\text{sol}} = E + \text{TCG} + (\Delta G + 1.9)/627.51$, where 1.9 kcal/mol comes from the thermal correction from the standard solution state (1mol/L) to the standard state (1/22.4 mol/L), see Fu, Y.; Liu, L.; Li, R. Q.; Liu, R.; Guo, Q. X. *J. Am. Chem. Soc.* **2004**, *126*, 814.

5. Cartesian Coordinates of Intermediates and Transition States

1			
6	-3.719380000	-1.263657000	-0.094618000
6	-2.348338000	-1.198895000	0.155783000
6	-1.705009000	0.045351000	0.175778000
6	-2.447973000	1.211999000	-0.048244000
6	-3.819792000	1.137742000	-0.288757000
6	-4.460851000	-0.101595000	-0.315023000
1	-4.209445000	-2.233289000	-0.112025000
1	-1.775814000	-2.101748000	0.318279000
1	-1.952690000	2.178513000	-0.044608000
1	-4.383147000	2.050342000	-0.463109000
1	-5.528558000	-0.161314000	-0.506530000
7	-0.301246000	0.172314000	0.463277000
6	0.050805000	1.078105000	1.562221000
1	1.070681000	0.877536000	1.891517000
1	-0.023082000	2.132361000	1.275237000
1	-0.628584000	0.899625000	2.401684000
6	0.613955000	-0.667988000	-0.147933000
8	0.297252000	-1.667455000	-0.782350000
6	2.066047000	-0.303075000	-0.005097000
6	2.810645000	0.946836000	-0.288538000
8	4.029169000	0.984982000	-0.188111000
6	2.024930000	2.159168000	-0.761294000
1	0.998151000	1.930608000	-1.054037000
1	2.562120000	2.590517000	-1.610792000
1	2.012597000	2.915490000	0.031854000
7	2.856169000	-1.357582000	0.131313000
7	3.567390000	-2.226561000	0.258344000

IN1A

6	5.683019000	-2.407710000	0.378136000
6	4.388772000	-1.908666000	0.228091000
6	4.203428000	-0.578286000	-0.152156000
6	5.299464000	0.254570000	-0.383954000
6	6.591772000	-0.249733000	-0.231326000
6	6.784239000	-1.579883000	0.147929000
1	5.830042000	-3.441417000	0.677701000
1	3.524425000	-2.540855000	0.410463000
1	5.133766000	1.287621000	-0.675573000
1	7.446468000	0.396903000	-0.408181000
1	7.790942000	-1.970765000	0.265791000
7	2.865764000	-0.069009000	-0.362630000

6	2.359406000	-0.210333000	-1.728891000
1	1.295662000	0.027489000	-1.784807000
1	2.887084000	0.458267000	-2.414292000
1	2.503003000	-1.246989000	-2.048885000
6	2.258130000	0.510459000	0.710358000
8	2.727413000	0.503866000	1.840593000
6	0.890207000	1.203777000	0.497131000
6	0.756320000	2.412766000	-0.440686000
8	1.556394000	2.532718000	-1.344690000
6	-0.378915000	3.385205000	-0.198090000
1	-1.349750000	2.875006000	-0.181137000
1	-0.368407000	4.123395000	-1.001686000
1	-0.249576000	3.907189000	0.758477000
47	-0.724565000	-0.200443000	-0.315593000
8	-3.051618000	1.022662000	-0.345082000
16	-3.624380000	-0.274840000	-0.809877000
8	-4.656476000	-0.248145000	-1.839840000
8	-2.496577000	-1.274345000	-1.055692000
6	-4.414129000	-0.977383000	0.720526000
9	-5.394219000	-0.176525000	1.145166000
9	-4.911498000	-2.191372000	0.480571000
9	-3.487749000	-1.075077000	1.694128000
7	0.379009000	1.461728000	1.739179000
7	-0.019229000	1.679630000	2.764818000

IN1B

6	-6.275886000	1.063299000	1.098964000
6	-4.976445000	0.557634000	1.142662000
6	-4.177541000	0.600940000	-0.007642000
6	-4.690806000	1.158874000	-1.186929000
6	-5.989124000	1.666583000	-1.216689000
6	-6.788804000	1.618821000	-0.074194000
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1	-4.587366000	0.126551000	2.054339000
1	-4.080428000	1.193469000	-2.083957000
1	-6.373729000	2.095248000	-2.137928000
1	-7.800864000	2.012569000	-0.097407000
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6	-1.813270000	0.955309000	-0.687356000
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6	-1.513015000	-2.158798000	-2.117172000
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1	-1.621157000	-3.207571000	-2.415770000
1	-1.037967000	-1.632408000	-2.951694000
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7	0.273852000	-2.033343000	2.307947000
47	2.402313000	-1.556592000	-0.351994000
8	1.344722000	0.707607000	0.685056000
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8	3.113611000	1.784236000	2.138285000
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INIC

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8	-1.763169000	0.574312000	-1.231584000
6	-1.662518000	2.184683000	0.486814000
6	-0.783294000	3.173592000	-0.151215000
8	-0.028883000	2.877933000	-1.079205000
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1	-0.100112000	5.190069000	-0.200398000

1	-0.531038000	4.629552000	1.434870000
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7	-3.126646000	2.942841000	2.304165000
47	0.641113000	0.690619000	-1.698168000
8	1.099580000	-0.153273000	0.887233000
8	2.216634000	-0.853048000	-1.211944000
16	2.064852000	-1.109253000	0.273575000
8	1.917825000	-2.520117000	0.647233000
6	3.716774000	-0.579637000	0.941350000
9	3.736760000	-0.723677000	2.272071000
9	4.696195000	-1.316523000	0.410657000
9	3.937842000	0.710699000	0.647765000

TS1A

6	5.896536000	-2.190799000	0.367311000
6	4.590517000	-1.712621000	0.272499000
6	4.353861000	-0.460184000	-0.305297000
6	5.422357000	0.306041000	-0.783331000
6	6.725154000	-0.184825000	-0.691625000
6	6.966027000	-1.432614000	-0.114972000
1	6.076379000	-3.163587000	0.815968000
1	3.760426000	-2.300125000	0.645388000
1	5.238906000	1.284745000	-1.215800000
1	7.550522000	0.414605000	-1.064957000
1	7.980992000	-1.812316000	-0.040591000
7	3.009838000	0.035973000	-0.458130000
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1	2.930351000	1.598194000	-1.914088000
1	3.135169000	-0.069053000	-2.535124000
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8	2.520586000	-0.319535000	1.756685000
6	0.883772000	0.832640000	0.468986000
6	0.818038000	2.308297000	0.606149000
8	1.580800000	2.866522000	-0.174693000
6	-0.165333000	3.023477000	1.492832000
1	-1.175268000	2.612627000	1.377512000
1	-0.161561000	4.081022000	1.220391000
1	0.127054000	2.928062000	2.545617000
47	-0.792593000	0.114234000	-0.664968000
8	-3.099101000	1.013931000	0.440984000
16	-3.758502000	0.204887000	-0.620111000
8	-4.913074000	0.768869000	-1.310796000
8	-2.705560000	-0.407551000	-1.544679000

6	-4.364872000	-1.305746000	0.279157000
9	-5.274500000	-0.965197000	1.195903000
9	-4.906699000	-2.177016000	-0.573392000
9	-3.329599000	-1.900713000	0.903266000
7	0.118966000	0.209184000	2.186749000
7	-0.421944000	-0.231690000	3.044007000

TS1B

6	-6.584992000	-2.193233000	-0.753095000
6	-5.390230000	-1.670860000	-0.258284000
6	-5.361566000	-0.357559000	0.237409000
6	-6.537526000	0.409366000	0.238502000
6	-7.725595000	-0.128662000	-0.251013000
6	-7.754163000	-1.431505000	-0.752163000
1	-6.597728000	-3.210470000	-1.133675000
1	-4.490238000	-2.268361000	-0.255689000
1	-6.526835000	1.429230000	0.608364000
1	-8.627663000	0.476435000	-0.245592000
1	-8.680339000	-1.849288000	-1.135875000
7	-4.164082000	0.214696000	0.778159000
6	-4.294004000	1.063568000	1.968002000
1	-3.312472000	1.170457000	2.434497000
1	-4.675945000	2.063515000	1.732007000
1	-4.983342000	0.584803000	2.668281000
6	-2.942386000	-0.013698000	0.176490000
8	-2.711838000	-0.884653000	-0.657117000
6	-1.832895000	0.843338000	0.635752000
6	-1.185301000	1.878086000	-0.030631000
8	-0.039524000	1.990697000	-0.512677000
6	-2.082367000	3.126700000	-0.032640000
1	-3.078383000	2.978780000	0.390163000
1	-2.179085000	3.442890000	-1.076250000
1	-1.566238000	3.908712000	0.532204000
7	-0.365039000	-0.653301000	0.820565000
7	0.007480000	-1.519429000	1.399891000
47	1.701909000	0.692105000	-0.805453000
8	2.955802000	-0.761202000	1.100668000
16	3.916875000	-1.123017000	0.023928000
8	4.355569000	-2.512402000	-0.080545000
8	3.477191000	-0.495724000	-1.295752000
6	5.438465000	-0.129758000	0.416940000
9	5.964283000	-0.529115000	1.579367000
9	6.354481000	-0.270929000	-0.545258000
9	5.117655000	1.172313000	0.516610000

TS1C

6	4.461894000	-2.269684000	-1.306398000
6	3.894529000	-1.004240000	-1.156137000
6	3.542870000	-0.555172000	0.120877000
6	3.762325000	-1.364580000	1.239837000
6	4.334299000	-2.626982000	1.081174000
6	4.684405000	-3.081261000	-0.191771000
1	4.731391000	-2.620030000	-2.298578000
1	3.719013000	-0.369745000	-2.016950000
1	3.473296000	-1.013836000	2.226395000
1	4.497832000	-3.256126000	1.951241000
1	5.126625000	-4.065652000	-0.315250000
7	3.000974000	0.766293000	0.318999000
6	3.854135000	1.716839000	1.039740000
1	3.501118000	2.732266000	0.852153000
1	3.857412000	1.529529000	2.119566000
1	4.878076000	1.615045000	0.668927000
6	1.820151000	1.107171000	-0.284631000
8	1.338914000	0.396703000	-1.192483000
6	1.197581000	2.374578000	0.099696000
6	-0.102051000	2.866443000	-0.169727000
8	-0.326399000	2.770106000	-1.396578000
6	-1.051334000	3.516820000	0.792228000
1	-0.536697000	4.126174000	1.540442000
1	-1.627645000	2.728847000	1.293216000
1	-1.740115000	4.142191000	0.219181000
47	-0.894835000	0.284501000	-1.638752000
8	-1.923768000	0.404598000	0.945399000
16	-3.094804000	-0.305204000	0.354128000
8	-4.425532000	0.083459000	0.817201000
8	-2.955402000	-0.426963000	-1.152223000
6	-2.850845000	-2.065352000	0.900009000
9	-2.880320000	-2.146333000	2.235814000
9	-3.804190000	-2.854405000	0.397687000
9	-1.655182000	-2.512956000	0.473467000
7	1.157117000	2.202653000	2.145778000
7	1.242017000	2.184708000	3.248415000

TS1D

6	-3.589869000	-1.446635000	-0.316916000
6	-2.260260000	-1.280094000	0.071668000
6	-1.727649000	0.013731000	0.200187000
6	-2.555694000	1.120445000	-0.054896000

6	-3.883453000	0.939540000	-0.436711000
6	-4.408607000	-0.346365000	-0.572613000
1	-3.987103000	-2.453749000	-0.410685000
1	-1.635492000	-2.137781000	0.270141000
1	-2.161497000	2.127537000	0.030857000
1	-4.504536000	1.809307000	-0.633301000
1	-5.443491000	-0.488035000	-0.871171000
7	-0.378626000	0.252443000	0.615417000
6	-0.163275000	1.374342000	1.536424000
1	0.802486000	1.248476000	2.024278000
1	-0.172251000	2.346394000	1.027970000
1	-0.958814000	1.371269000	2.286881000
6	0.656537000	-0.593505000	0.219370000
8	0.469992000	-1.704234000	-0.266562000
6	2.031566000	-0.074261000	0.475452000
6	3.189163000	-0.761296000	0.004138000
8	3.284246000	-1.823399000	0.629069000
6	4.217530000	-0.272848000	-0.985153000
1	4.573719000	0.730722000	-0.728125000
1	3.792658000	-0.230602000	-1.994765000
1	5.060255000	-0.967952000	-0.977723000
7	2.022541000	1.664204000	-0.551921000
7	2.008119000	2.772946000	-0.602083000

IN2A

6	-4.431098339	-2.832820214	-1.043083078
6	-3.456127264	-1.911264147	-0.661154050
6	-3.787615291	-0.896513066	0.241372018
6	-5.080263386	-0.802505061	0.764477056
6	-6.044284446	-1.736235131	0.385375029
6	-5.722576429	-2.750708209	-0.519002039
1	-4.175202319	-3.619856276	-1.746113135
1	-2.449313185	-1.976388150	-1.059715082
1	-5.334660401	-0.001953000	1.452581113
1	-7.048711549	-1.664541129	0.792101061
1	-6.476527483	-3.474362267	-0.814564063
7	-2.784651215	0.053673004	0.656166051
6	-2.473459188	0.199136015	2.086163160
1	-1.722764131	0.980966077	2.216157171
1	-3.370249258	0.490060038	2.638340204
1	-2.096539162	-0.748706055	2.481826190
6	-2.095503160	0.738746055	-0.255160019
8	-2.197994167	0.752401056	-1.501859115
6	-0.980338076	1.646670125	-0.121829009

6	-1.321227101	3.081456235	0.006819001
8	-1.330191099	3.444802262	1.176089091
6	-1.570581120	3.949053299	-1.189890092
1	-0.655481053	4.018308308	-1.790365138
1	-1.874577146	4.945924376	-0.862427066
1	-2.337279181	3.497077269	-1.828945139
47	1.000715078	0.975908074	-0.111635009
8	2.876431220	0.168576013	-1.272439097
16	3.666606281	-0.134891010	-0.024604002
8	5.095581390	0.155543012	-0.049599004
8	2.879056219	0.367848028	1.159536088
6	3.512021267	-1.981597154	0.129168010
9	4.079795312	-2.588734197	-0.915634071
9	4.095330311	-2.407796182	1.252296097
9	2.209075170	-2.321862178	0.167238013

IN2B

6	-3.904548297	3.503975269	-0.608536045
6	-4.092571313	2.177119167	-0.223511017
6	-2.988382228	1.431630107	0.198597015
6	-1.708776129	1.984630154	0.239806018
6	-1.529882119	3.308018251	-0.169554013
6	-2.624661200	4.066876312	-0.585940045
1	-4.755688361	4.092117311	-0.939482073
1	-5.078793390	1.723260134	-0.266862020
1	-0.859305063	1.400352107	0.580464044
1	-0.526129040	3.720791285	-0.162389012
1	-2.482759187	5.097461388	-0.898838070
7	-3.184702241	0.051972004	0.603527044
6	-3.984097306	-0.249669019	1.796425138
1	-4.122643313	-1.330343100	1.874714144
1	-3.476617266	0.124038009	2.690898205
1	-4.962876378	0.228112018	1.713099132
6	-2.586114198	-0.919672069	-0.052618004
8	-1.808357138	-0.910524071	-1.081117084
6	-2.431850188	-2.286036175	-0.157210012
6	-1.459295113	-3.189370245	0.331498026
8	-0.318099024	-3.341971253	-0.160563012
6	-1.927933146	-4.111517314	1.438938109
1	-2.910003224	-3.833089291	1.834228143
1	-1.185137091	-4.097195311	2.242938170
1	-1.988057154	-5.134178393	1.050473080
47	0.836324065	-1.581242121	-0.899917067
8	2.181582168	0.164258012	-1.244595097

16	2.031570155	1.038216081	-0.013374001
8	1.782187137	2.457001189	-0.288478022
8	1.151218088	0.380446029	0.993362075
6	3.729183285	0.960044076	0.740363057
9	4.636377355	1.472927111	-0.095353007
9	3.751402284	1.652781127	1.884654146
9	4.053762311	-0.314381024	1.002670076

TS2A

6	1.701194000	1.874743000	0.186458000
6	2.024944000	1.319937000	1.443203000
6	1.122900000	1.435740000	2.513397000
6	-0.070124000	2.123229000	2.340798000
6	-0.365753000	2.712639000	1.100467000
6	0.507362000	2.594515000	0.024833000
6	2.927567000	0.276943000	-1.062331000
6	2.263832000	-0.698159000	-0.148964000
1	1.375880000	1.007283000	3.478496000
1	-0.776544000	2.207711000	3.159632000
1	-1.308579000	3.232629000	0.964224000
1	0.246561000	3.009615000	-0.942939000
7	2.563059000	1.594588000	-0.890269000
6	2.895596000	2.572387000	-1.923035000
1	2.075320000	2.694882000	-2.640604000
1	3.123172000	3.534595000	-1.458579000
1	3.770576000	2.200248000	-2.458973000
8	3.663582000	-0.141215000	-1.943904000
6	3.048600000	-1.750467000	0.520685000
8	3.525565000	-2.550065000	-0.272297000
6	3.165475000	-1.867789000	2.018685000
1	3.920738000	-1.165337000	2.393931000
1	2.215701000	-1.640799000	2.512697000
1	3.484307000	-2.883654000	2.264686000
47	0.185894000	-1.037879000	-0.309889000
1	3.029098000	0.945435000	1.611628000
8	-1.891043000	-1.556149000	-0.952507000
16	-2.713108000	-0.999436000	0.195142000
8	-3.864831000	-1.798256000	0.600440000
8	-1.791235000	-0.499353000	1.258927000
6	-3.409788000	0.560296000	-0.542420000
9	-4.056711000	1.267460000	0.392144000
9	-2.407803000	1.325900000	-1.026035000
9	-4.250160000	0.284724000	-1.540080000

IN3A

6	-1.642238000	1.616454000	0.982885000
6	-2.498422000	0.956258000	-0.049310000
6	-2.474495000	1.612003000	-1.389221000
6	-1.960761000	2.856662000	-1.526552000
6	-1.350748000	3.529123000	-0.402711000
6	-1.198917000	2.954223000	0.833332000
6	-1.742665000	-0.627150000	1.557035000
6	-2.239297000	-0.541234000	0.181357000
1	-2.985771000	1.092331000	-2.192289000
1	-1.996439000	3.372259000	-2.480791000
1	-0.952754000	4.527942000	-0.562059000
1	-0.646095000	3.452058000	1.621209000
7	-1.333144000	0.755057000	1.931530000
6	-0.490037000	0.993839000	3.096864000
1	0.542250000	1.138047000	2.763519000
1	-0.843861000	1.867881000	3.649460000
1	-0.559348000	0.104073000	3.724057000
8	-1.619779000	-1.528814000	2.359478000
6	-3.268725000	-1.468489000	-0.345956000
8	-4.108758000	-1.041235000	-1.136396000
6	-3.253657000	-2.923058000	0.083441000
1	-2.396534000	-3.442793000	-0.362436000
1	-3.147072000	-3.015778000	1.168594000
1	-4.173946000	-3.399815000	-0.260364000
47	-0.253583000	-0.924835000	-0.821901000
1	-3.550961000	1.137925000	0.268901000
8	1.826568000	-0.638474000	-1.482831000
16	2.436233000	0.453550000	-0.615669000
8	3.192236000	1.463358000	-1.354736000
8	1.460928000	0.933651000	0.402676000
6	3.681463000	-0.507107000	0.374888000
9	4.297663000	0.304355000	1.243309000
9	3.063529000	-1.479735000	1.064496000
9	4.594654000	-1.060854000	-0.425617000

TS3A

6	2.748078000	1.489279000	-0.085163000
6	1.874856000	0.726908000	0.779446000
6	0.867504000	1.465092000	1.510721000
6	0.963691000	2.837050000	1.599920000
6	1.960487000	3.527570000	0.872418000
6	2.845769000	2.881956000	0.015363000
6	2.780508000	-0.648325000	-0.968059000

6	1.825083000	-0.683878000	0.188515000
1	0.095475000	0.917044000	2.042115000
1	0.257729000	3.392944000	2.207351000
1	2.010271000	4.610469000	0.951676000
1	3.534883000	3.447067000	-0.602764000
7	3.314750000	0.678227000	-1.020892000
6	4.271605000	1.084007000	-2.038271000
1	3.831261000	1.825527000	-2.713913000
1	5.170278000	1.502432000	-1.574185000
1	4.534791000	0.189272000	-2.604006000
8	3.157531000	-1.532442000	-1.711698000
6	2.275481000	-1.620269000	1.238604000
8	2.554223000	-1.111345000	2.352011000
6	2.451267000	-3.089013000	1.002527000
1	1.492984000	-3.600054000	1.154922000
1	2.763035000	-3.267337000	-0.031749000
1	3.176893000	-3.496591000	1.709886000
47	-0.241943000	-1.179384000	-0.372547000
1	2.417468000	0.248255000	1.844662000
8	-2.406730000	-1.384022000	-0.586495000
16	-3.059134000	-0.453420000	0.428566000
8	-4.332471000	-0.936758000	0.954650000
8	-2.056932000	0.077704000	1.387851000
6	-3.464042000	1.012383000	-0.641953000
9	-3.984803000	2.000796000	0.094154000
9	-2.337798000	1.470647000	-1.227779000
9	-4.332680000	0.680501000	-1.599714000

IN4A

6	-2.825177000	1.370393000	-0.139032000
6	-1.851563000	0.820814000	0.729117000
6	-1.063518000	1.673457000	1.503899000
6	-1.274954000	3.054606000	1.416078000
6	-2.245125000	3.578653000	0.557748000
6	-3.034149000	2.739727000	-0.239447000
6	-3.004107000	-0.886556000	-0.440607000
6	-1.910427000	-0.646600000	0.538962000
1	-0.277908000	1.282057000	2.141949000
1	-0.666007000	3.724607000	2.014994000
1	-2.388890000	4.653477000	0.499684000
1	-3.783732000	3.149930000	-0.908734000
7	-3.491036000	0.336656000	-0.823911000
6	-4.570725000	0.511236000	-1.778182000
1	-5.410970000	1.039152000	-1.314590000

1	-4.227456000	1.078590000	-2.650312000
1	-4.896236000	-0.480698000	-2.094563000
8	-3.437431000	-1.996219000	-0.803622000
6	-1.582738000	-1.701370000	1.413548000
8	-2.028348000	-2.915309000	1.169893000
6	-0.770710000	-1.561538000	2.661364000
1	0.283964000	-1.377072000	2.421956000
1	-1.131975000	-0.711048000	3.250527000
1	-0.848668000	-2.478646000	3.248541000
47	0.092602000	-0.823083000	-0.639686000
8	2.093870000	-0.663021000	1.119309000
8	2.186877000	-0.863730000	-1.342517000
16	2.997719000	-0.659552000	-0.067920000
8	4.233076000	-1.432662000	0.004521000
6	3.498701000	1.123943000	-0.228681000
9	4.264949000	1.303523000	-1.306311000
9	2.398170000	1.889903000	-0.349815000
9	4.171820000	1.516041000	0.857225000
1	-2.622529000	-2.877500000	0.350704000

TS4

6	-3.104664000	-3.130567000	-0.523591000
6	-2.551863000	-1.932714000	-0.071535000
6	-3.398292000	-0.846307000	0.191016000
6	-4.782177000	-0.966951000	0.014072000
6	-5.320844000	-2.175515000	-0.424489000
6	-4.483831000	-3.258927000	-0.698797000
1	-2.447787000	-3.970532000	-0.728814000
1	-1.482251000	-1.846132000	0.073957000
1	-5.435239000	-0.121440000	0.207177000
1	-6.394950000	-2.264907000	-0.558672000
1	-4.904671000	-4.198268000	-1.045205000
7	-2.864225000	0.394461000	0.673379000
6	-3.558864000	1.134341000	1.727047000
1	-2.836280000	1.796466000	2.220807000
1	-4.384217000	1.738941000	1.334883000
1	-3.947086000	0.429495000	2.465602000
6	-1.738162000	0.920592000	0.153466000
8	-1.007231000	0.417449000	-0.732293000
6	-1.095894000	2.107746000	0.630450000
6	-0.909529000	3.317480000	-0.087595000
8	0.100719000	3.423301000	-0.815170000
6	-1.868424000	4.464183000	0.117749000
1	-2.378170000	4.663894000	-0.832143000

1	-1.301893000	5.358336000	0.396541000
1	-2.616645000	4.255719000	0.889115000
47	1.335490000	1.434905000	-0.438040000
8	3.160381000	-0.001698000	-0.946847000
16	3.174362000	-0.666448000	0.403734000
8	4.478244000	-1.019691000	0.957781000
8	2.213946000	0.048389000	1.316440000
6	2.306747000	-2.282323000	0.085552000
9	3.007985000	-3.039603000	-0.761788000
9	2.132182000	-2.956141000	1.227588000
9	1.091750000	-2.051855000	-0.457814000

2

6	1.259333000	0.470832000	-0.002317000
6	0.447167000	-0.693564000	0.001713000
6	1.065240000	-1.944477000	0.007659000
6	2.464073000	-2.019456000	0.004525000
6	3.243608000	-0.860372000	-0.002075000
6	2.646440000	0.407479000	-0.004705000
6	-0.889402000	1.238027000	0.003690000
6	-0.933795000	-0.227709000	0.002626000
1	0.476890000	-2.856654000	0.017204000
1	2.946144000	-2.992935000	0.008588000
1	4.327219000	-0.937741000	-0.003889000
1	3.252270000	1.308561000	-0.008040000
7	0.440386000	1.610195000	-0.001521000
6	0.893008000	2.984873000	-0.003634000
1	1.496899000	3.199258000	0.886015000
1	1.490653000	3.198516000	-0.897655000
1	0.006523000	3.621468000	-0.000814000
8	-1.858471000	2.023023000	0.006596000
6	-2.147574000	-0.868000000	-0.002669000
8	-3.283788000	-0.173651000	0.001180000
1	-3.037230000	0.801451000	0.007393000
6	-2.339444000	-2.354996000	-0.010094000
1	-1.794912000	-2.814573000	-0.842324000
1	-1.959022000	-2.800076000	0.917224000
1	-3.401995000	-2.589438000	-0.103592000

3

6	1.256935000	0.479545000	0.000069000
6	0.453740000	-0.694201000	-0.000541000
6	1.098750000	-1.937510000	-0.000628000
6	2.494276000	-1.983672000	-0.000125000

6	3.261877000	-0.810829000	0.000409000
6	2.647102000	0.443878000	0.000516000
6	-0.874518000	1.156401000	-0.000551000
6	-0.927484000	-0.248081000	-0.000822000
1	0.526694000	-2.860003000	-0.000889000
1	2.993889000	-2.948560000	-0.000119000
1	4.346150000	-0.874571000	0.000761000
1	3.237279000	1.355680000	0.000886000
7	0.410229000	1.599799000	-0.000055000
6	0.826804000	2.989424000	0.000301000
1	1.422415000	3.211561000	0.892574000
1	1.423828000	3.211566000	-0.891021000
1	-0.065203000	3.616837000	-0.000394000
8	-1.897752000	1.989246000	-0.000620000
6	-2.211971000	-0.886508000	0.000363000
8	-3.259186000	-0.193094000	0.000890000
6	-2.321584000	-2.394892000	0.000237000
1	-1.825130000	-2.818381000	-0.881371000
1	-1.830150000	-2.817729000	0.885012000
1	-3.375064000	-2.681762000	-0.002465000
1	-2.694375000	1.356223000	-0.000115000

TS5

6	1.257687000	0.486887000	-0.000273000
6	0.478929000	-0.703379000	0.000260000
6	1.140957000	-1.934526000	0.001125000
6	2.538968000	-1.958994000	0.000482000
6	3.283645000	-0.773821000	-0.000499000
6	2.646690000	0.472352000	-0.000710000
6	-0.891868000	1.146494000	0.000676000
6	-0.908156000	-0.278344000	0.000459000
1	0.581370000	-2.865245000	0.002810000
1	3.054671000	-2.915290000	0.001023000
1	4.368950000	-0.817612000	-0.000856000
1	3.222722000	1.393086000	-0.001151000
7	0.393365000	1.598560000	0.000008000
6	0.788084000	2.993341000	-0.000425000
1	1.380562000	3.227706000	0.891041000
1	1.379360000	3.227493000	-0.892746000
1	-0.118444000	3.600450000	0.000105000
8	-1.942094000	1.895302000	0.000890000
6	-2.176931000	-0.886180000	-0.000736000
8	-3.222147000	-0.137949000	-0.000172000
1	-2.759977000	1.049645000	0.000823000

6	-2.374153000	-2.377914000	-0.001360000
1	-1.879863000	-2.832142000	-0.868322000
1	-1.931024000	-2.824084000	0.897226000
1	-3.441072000	-2.608260000	-0.029758000