Supporting Information

Looking inside the intramolecular C–H···O hydrogen bond in lactams derived from α-methylbenzylamine

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Table S1. XYZ coordinates for conformer **1 closed (1a)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) =- -516.08462473024au

E(ZPE) = 0.188714 au

Atomic	Coordinates (Angstroms)		
	X	Y	Z
7	-1.715603000	0.041147000	0.429214000
6	-2.272944000	-1.110241000	-0.068252000
6	-3.215776000	0.020050000	0.126852000
1	-3.860565000	0.146446000	1.001930000
1	-3.547979000	0.526625000	-0.791538000
6	-0.775820000	0.891726000	-0.317005000
1	-1.033522000	0.866135000	-1.396956000
8	-2.021549000	-2.213553000	-0.486380000
6	0.626856000	0.350911000	-0.144124000
6	1.517172000	0.324378000	-1.232274000
6	1.071931000	-0.079959000	1.120541000
6	2.838428000	-0.118935000	-1.061563000
6	2.389985000	-0.528542000	1.290618000
6	3.277752000	-0.545971000	0.201539000
1	1.171959000	0.647283000	-2.220662000
1	0.373199000	-0.080038000	1.962246000
1	3.520895000	-0.139145000	-1.916551000
1	2.724886000	-0.869439000	2.275026000

1	4.304758000	-0.898362000	0.335376000
6	-0.903474000	2.325456000	0.194846000
1	-1.934672000	2.695387000	0.069195000
1	-0.640028000	2.364897000	1.263429000
1	-0.221976000	2.987376000	-0.362011000

Table S2. XYZ coordinates for conformer **2 closed (2a)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = - 555.31599843500au

E(ZPE) = 0.219948 au

Atomic	Coordinates (Angstroms)		
	X	Y	Z
7	-1.524891000	0.395539000	0.023221000
6	-2.259041000	-0.761044000	-0.191442000
6	-2.660524000	-0.824156000	1.298246000
6	-1.672818000	0.360718000	1.488660000
1	-3.717786000	-0.596826000	1.496086000
1	-2.376434000	-1.763711000	1.793757000
1	-0.740510000	0.086588000	2.011977000
1	-2.091176000	1.283557000	1.920732000
8	-2.431950000	-1.435715000	-1.187902000
6	-0.468703000	0.967413000	-0.802926000
1	-0.709963000	0.625728000	-1.824936000
6	0.867461000	0.355178000	-0.406235000
6	1.093504000	-1.000672000	-0.726310000
6	1.853376000	1.057356000	0.310672000
6	2.282912000	-1.637022000	-0.344778000

6	3.046638000	0.420164000	0.694231000
6	3.264399000	-0.926993000	0.368771000
1	0.323610000	-1.551778000	-1.277988000
1	1.704758000	2.109974000	0.566944000
1	2.446531000	-2.686776000	-0.606972000
1	3.806378000	0.979994000	1.248320000
1	4.194545000	-1.420739000	0.665435000
6	-0.525754000	2.491985000	-0.757794000
1	0.263233000	2.932224000	-1.387091000
1	-1.505700000	2.834666000	-1.122635000
1	-0.396344000	2.866476000	0.270467000

Table S3. XYZ coordinates for conformer **3 closed (3a)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = - 594.53169371368au

E(ZPE) = 0.250500 au

Atomic	Coordinates (Angstroms)		
	X	Y	Z
6	-2.740702000	0.017425000	1.634593000
6	-2.836465000	-1.149968000	0.647992000
6	-2.010715000	-0.686510000	-0.549877000
7	-1.288826000	0.419718000	-0.139941000
6	-1.372398000	0.632357000	1.300429000
1	-2.819804000	-0.280155000	2.690439000
1	-3.855823000	-1.425129000	0.342868000
1	-2.345723000	-2.056935000	1.044697000
8	-1.957443000	-1.202055000	-1.661203000

1	-1.315455000	1.703446000	1.550437000
1	-0.548653000	0.111762000	1.828177000
1	-3.530109000	0.755575000	1.419484000
6	-0.170624000	0.911515000	-0.946184000
1	-0.360041000	0.490704000	-1.947334000
6	-0.193284000	2.435071000	-1.040772000
1	-1.147366000	2.761685000	-1.481861000
1	-0.092964000	2.915058000	-0.054594000
1	0.632164000	2.790606000	-1.677151000
6	1.127343000	0.313577000	-0.425158000
6	2.041141000	1.033548000	0.366397000
6	1.389193000	-1.045482000	-0.700995000
6	3.197438000	0.411196000	0.868234000
6	2.541612000	-1.667955000	-0.200223000
6	3.450097000	-0.940309000	0.588008000
1	1.864366000	2.089624000	0.589443000
1	0.677103000	-1.606376000	-1.315981000
1	3.901324000	0.985326000	1.478709000
1	2.734746000	-2.720500000	-0.429447000
1	4.351746000	-1.423065000	0.976663000

Table S4. XYZ coordinates for conformer **4 closed (4a)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = - 633.71481268323au

E(ZPE) = 0.280124 au

Atomic	Coordinates (Angstroms)	
X	Y	Z

7	-1.015400000	0.419663000	-0.242846000
6	-1.814225000	-0.481821000	-0.912024000
6	-3.020889000	-1.042235000	-0.166915000
6	-3.373341000	-0.331083000	1.136498000
6	-2.085648000	-0.121371000	1.927037000
6	-1.179451000	0.825145000	1.152310000
1	-3.853048000	-1.048480000	-0.888145000
1	-2.781095000	-2.101881000	0.034564000
1	-4.110596000	-0.918782000	1.707515000
1	-3.834849000	0.650911000	0.925255000
1	-2.277987000	0.307020000	2.924468000
1	-1.576022000	-1.090974000	2.071331000
1	-0.174720000	0.860664000	1.610241000
1	-1.600248000	1.848048000	1.200257000
8	-1.571689000	-0.855433000	-2.062567000
6	0.162417000	0.953580000	-0.948234000
1	0.035138000	0.613655000	-1.986564000
6	0.171891000	2.480747000	-0.932706000
1	-0.761545000	2.860174000	-1.377025000
1	0.261119000	2.894197000	0.084002000
1	1.019310000	2.857549000	-1.526531000
6	1.413913000	0.291557000	-0.392831000
6	2.393447000	0.976770000	0.349094000
6	1.574319000	-1.093222000	-0.614928000
6	3.511386000	0.293641000	0.860951000
6	2.688508000	-1.774967000	-0.107167000
6	3.660587000	-1.082879000	0.637023000
1	2.299873000	2.052208000	0.524642000

1	0.818374000	-1.622381000	-1.205249000
1	4.265412000	0.840847000	1.435209000
1	2.802987000	-2.846982000	-0.295479000
1	4.531724000	-1.613154000	1.033319000

Table S5. XYZ coordinates for conformer **5 closed (5a)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = -672.89420166620au

E(ZPE) = 0.309329 au

Atomic	Coordinates (Angstroms)		
	X	Y	Z
7	0.986824000	0.904704000	-0.213809000
6	1.970795000	0.594515000	0.707198000
6	3.158645000	-0.176570000	0.143392000
6	0.963434000	0.262593000	-1.525764000
6	2.828629000	-1.663597000	-0.165303000
6	0.645600000	-1.244148000	-1.479295000
6	1.330927000	-1.962247000	-0.312991000
1	3.949240000	-0.108211000	0.903503000
1	3.364973000	-1.980813000	-1.077495000
1	1.933486000	0.427132000	-2.022400000
1	0.966390000	-1.687853000	-2.440183000
1	3.527310000	0.336158000	-0.759246000
1	0.214498000	0.783272000	-2.142474000
1	3.218473000	-2.286472000	0.656927000
1	-0.444184000	-1.392897000	-1.398085000
1	1.186953000	-3.050656000	-0.427342000

1	0.820040000	-1.685775000	0.625716000
6	-0.222783000	1.597206000	0.260951000
1	0.013225000	1.862010000	1.302248000
6	-0.460979000	2.887778000	-0.520933000
1	-1.355097000	3.404239000	-0.136681000
1	0.408617000	3.552508000	-0.404210000
1	-0.609586000	2.711405000	-1.598069000
6	-1.391386000	0.628271000	0.280148000
6	-1.446403000	-0.322923000	1.320867000
6	-2.374695000	0.590298000	-0.725872000
6	-2.448891000	-1.303073000	1.344376000
6	-3.380887000	-0.391314000	-0.705184000
6	-3.416119000	-1.344620000	0.324636000
1	-0.688990000	-0.281610000	2.111824000
1	-2.365564000	1.329073000	-1.532778000
1	-2.479397000	-2.032727000	2.159574000
1	-4.138674000	-0.409561000	-1.494724000
1	-4.199429000	-2.108427000	0.339767000
8	1.904328000	0.921658000	1.894179000

Table S6. XYZ coordinates for conformer **6 closed (6a)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = -712.07715276754au

E(ZPE) = 0.338532 au

Atomic		Coordinates (Angstroms)	
	X	Y	Z
7	-0.706818000	1.090155000	0.285748000

6	-1.763033000	1.014034000	-0.598032000
6	-1.613251000	-1.958704000	1.229912000
6	-3.049354000	0.381833000	-0.099351000
6	-1.939758000	-1.922814000	-0.277331000
6	-3.148394000	-1.051969000	-0.641661000
1	-3.137245000	0.385612000	0.995646000
1	-2.525958000	-1.748221000	1.820399000
1	-2.140973000	-2.947239000	-0.635487000
1	-1.314150000	-2.985166000	1.504664000
1	-3.872893000	0.988693000	-0.506402000
1	-1.049030000	-1.577350000	-0.832559000
1	-4.070568000	-1.519574000	-0.251830000
1	-3.246458000	-1.000972000	-1.739413000
6	-0.693452000	0.481047000	1.617505000
1	-1.610788000	0.754211000	2.165338000
1	0.132472000	0.961181000	2.165776000
6	-0.468887000	-1.038501000	1.682025000
1	0.440580000	-1.286805000	1.109045000
1	-0.242787000	-1.268179000	2.740821000
6	0.552351000	1.674715000	-0.216112000
1	0.303574000	1.994216000	-1.238395000
6	0.955551000	2.914778000	0.580175000
1	0.149771000	3.663007000	0.526285000
1	1.151621000	2.702797000	1.642980000
1	1.871159000	3.352606000	0.151362000
6	1.610975000	0.592617000	-0.315080000
6	2.638465000	0.429211000	0.631302000
6	1.502537000	-0.338113000	-1.370136000

6	3.527950000	-0.655978000	0.539204000
6	2.387603000	-1.421153000	-1.464803000
6	3.400168000	-1.587483000	-0.502810000
1	2.753601000	1.147251000	1.448745000
1	0.708614000	-0.200241000	-2.113093000
1	4.321473000	-0.772925000	1.283911000
1	2.291400000	-2.134338000	-2.289454000
1	4.092010000	-2.432308000	-0.572371000
8	-1.681815000	1.401443000	-1.768131000

Table S7. XYZ coordinates for conformer **1 open (1b)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) =- -516.08719731075au

E(ZPE) = 0.188714 au

Atomic		Coordinates (Angstroms)	
	X	Y	Z
7	1.841156000	0.432227000	0.603121000
6	2.114578000	-0.878833000	0.348047000
6	1.606305000	-0.590073000	1.713529000
1	2.239536000	-0.451397000	2.595557000
1	0.566743000	-0.896797000	1.901050000
6	0.815588000	1.269191000	-0.051134000
1	0.720064000	2.178558000	0.567459000
8	2.419159000	-1.661404000	-0.524278000
6	-0.532422000	0.576863000	-0.084852000
6	-1.572527000	1.022588000	0.752460000
6	-0.758597000	-0.541880000	-0.915815000

6	-2.820635000	0.378457000	0.756363000
6	-2.002885000	-1.190157000	-0.907840000
6	-3.037704000	-0.731250000	-0.075041000
1	-1.402119000	1.887043000	1.403734000
1	0.040174000	-0.917031000	-1.561685000
1	-3.620033000	0.741460000	1.409424000
1	-2.165346000	-2.056355000	-1.556351000
1	-4.007676000	-1.237242000	-0.074556000
6	1.345752000	1.649656000	-1.432983000
1	2.301307000	2.187271000	-1.334620000
1	1.521814000	0.749232000	-2.041528000
1	0.619455000	2.293536000	-1.952509000

Table S8. XYZ coordinates for conformer **2 open (2b)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = -555.31653187919 au

E(ZPE) = 0.219934au

Atomic	Coordinates (Angstroms)		
	X	Y	Z
7	1.511595000	0.336345000	0.480718000
6	2.256666000	-0.442988000	-0.395633000
6	2.766611000	-1.322114000	0.766396000
6	1.770867000	-0.523102000	1.647238000
1	2.545497000	-2.391821000	0.642185000
1	3.829730000	-1.180253000	1.007331000
1	2.195542000	0.015612000	2.509649000
1	0.886223000	-1.103139000	1.962132000

8	2.389667000	-0.431629000	-1.605204000
6	0.398940000	1.253056000	0.268151000
1	0.327218000	1.871783000	1.181838000
6	-0.906145000	0.491842000	0.109619000
6	-1.995016000	0.739792000	0.964012000
6	-1.038445000	-0.476043000	-0.908137000
6	-3.204110000	0.041622000	0.805853000
6	-2.243876000	-1.175990000	-1.064796000
6	-3.330061000	-0.918445000	-0.210051000
1	-1.895885000	1.487497000	1.759137000
1	-0.193556000	-0.680234000	-1.574080000
1	-4.043565000	0.244151000	1.478022000
1	-2.337171000	-1.924418000	-1.857739000
1	-4.269204000	-1.465610000	-0.335117000
6	0.687684000	2.170443000	-0.924001000
1	-0.146518000	2.877669000	-1.050854000
1	1.617287000	2.735955000	-0.752965000
1	0.807206000	1.582977000	-1.844836000

Table S9. XYZ coordinates for conformer **3 open (3b)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = -594.52808242270 au

E(ZPE) = 0.250377 au

Atomic	Coordinates (Angstroms)		
	X	Y	Z
6	-2.591584000	-1.811214000	0.276891000
6	-3.137873000	-0.490230000	0.825098000

6	-2.002712000	0.497491000	0.550430000
7	-1.278954000	-0.022939000	-0.498122000
6	-1.708113000	-1.358491000	-0.896959000
1	-3.365918000	-2.529431000	-0.030277000
1	-3.387926000	-0.499238000	1.894826000
1	-4.028663000	-0.152275000	0.266153000
8	-1.790033000	1.550726000	1.145559000
1	-0.832738000	-2.013477000	-1.045126000
1	-2.273219000	-1.320352000	-1.849209000
1	-1.956912000	-2.290656000	1.040067000
6	-0.113975000	0.583454000	-1.148242000
1	-0.085750000	0.137515000	-2.159392000
6	-0.240639000	2.100255000	-1.321272000
1	-1.175103000	2.346693000	-1.850763000
1	-0.246623000	2.614805000	-0.352918000
1	0.611998000	2.456577000	-1.920820000
6	1.165459000	0.182741000	-0.435591000
6	1.362299000	0.533386000	0.916729000
6	2.169490000	-0.534356000	-1.110878000
6	2.546479000	0.168282000	1.573654000
6	3.357343000	-0.897588000	-0.453657000
6	3.547286000	-0.546163000	0.891558000
1	0.580088000	1.086540000	1.445798000
1	2.021652000	-0.807688000	-2.162065000
1	2.691059000	0.444270000	2.622810000
1	4.130157000	-1.456009000	-0.990817000
1	4.470082000	-0.827908000	1.407544000

Table S10. XYZ coordinates for conformer **4 open (4b)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = -633.71131100369 au

E(ZPE) = 0.279991 au

Atomic	Coordinates (Angstroms)		
	X	Y	Z
7	1.092274000	0.158589000	0.617627000
6	1.608126000	0.860161000	-0.455983000
6	2.893556000	0.321449000	-1.078153000
6	3.034716000	-1.197228000	-1.027976000
6	2.795936000	-1.652066000	0.407041000
6	1.387608000	-1.264153000	0.834485000
1	2.923748000	0.718016000	-2.103626000
1	3.730225000	0.789680000	-0.527443000
1	4.029309000	-1.505737000	-1.389637000
1	2.286267000	-1.668055000	-1.691404000
1	2.909396000	-2.743500000	0.515874000
1	3.531593000	-1.170911000	1.075944000
1	1.249343000	-1.468585000	1.909968000
1	0.647566000	-1.886731000	0.291564000
8	1.125206000	1.916455000	-0.867096000
6	-0.173078000	0.591413000	1.255635000
1	-0.191697000	0.018092000	2.199681000
6	-0.203025000	2.069630000	1.653302000
1	0.724796000	2.331758000	2.186960000
1	-0.304123000	2.733079000	0.788080000
1	-1.055021000	2.225118000	2.334885000
6	-1.386712000	0.145034000	0.457229000

6	-1.759040000	0.782801000	-0.745887000
6	-2.158521000	-0.940854000	0.915525000
6	-2.877040000	0.334820000	-1.465911000
6	-3.279478000	-1.387455000	0.196406000
6	-3.641278000	-0.748565000	-0.999427000
1	-1.158893000	1.615545000	-1.118702000
1	-1.882623000	-1.436061000	1.853826000
1	-3.155644000	0.837788000	-2.397270000
1	-3.868531000	-2.230378000	0.570917000
1	-4.513907000	-1.090799000	-1.563945000

Table S11. XYZ coordinates for conformer **5 open (5b)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = -672.88746672667 au

E(ZPE) = 0.338432 au

Atomic		Coordinates (Angstroms)	
	X	Y	Z
7	0.744192000	-0.134635000	0.005159000
6	1.273397000	1.133319000	-0.060193000
6	2.467576000	1.297225000	-1.001715000
6	1.265931000	-1.198393000	-0.847381000
6	3.713134000	0.415337000	-0.696821000
6	2.534817000	-1.828191000	-0.256983000
6	3.485873000	-0.750794000	0.276420000
1	2.728520000	2.362859000	-0.938665000
1	4.126297000	0.021152000	-1.642682000
1	1.477364000	-0.796269000	-1.849862000

1	3.030859000	-2.428198000	-1.041557000
1	2.114324000	1.123332000	-2.032525000
1	0.468577000	-1.946708000	-0.983807000
1	4.496175000	1.062176000	-0.267785000
1	2.269786000	-2.522946000	0.559874000
1	4.459441000	-1.210432000	0.518986000
1	3.088786000	-0.351154000	1.225663000
6	-0.338784000	-0.512005000	0.935641000
1	-0.225441000	-1.604527000	1.052833000
6	-0.209262000	0.086843000	2.340373000
1	-0.943662000	-0.411911000	2.993524000
1	0.800252000	-0.097075000	2.743412000
1	-0.392810000	1.167031000	2.344261000
6	-1.704056000	-0.271486000	0.317954000
6	-2.564788000	-1.355249000	0.062309000
6	-2.132277000	1.033960000	-0.003841000
6	-3.833721000	-1.148995000	-0.504775000
6	-3.397572000	1.239265000	-0.573384000
6	-4.252354000	0.151531000	-0.824574000
1	-2.240282000	-2.371393000	0.315446000
1	-1.462782000	1.876846000	0.188459000
1	-4.491631000	-2.002162000	-0.696999000
1	-3.720628000	2.255385000	-0.820571000
1	-5.239064000	0.317847000	-1.267281000
8	0.824887000	2.093048000	0.573122000

Table S12. XYZ coordinates for conformer **6 open (6b)** from MP2/cc-pVDZ optimization

E(MP2/cc-pVDZ) = -712.07242607746au

E(ZPE) = 0.309041 au

Atomic	Coordinates (Angstroms)		
	X	Y	Z
7	-0.527376000	0.080702000	-0.024896000
6	-1.014116000	-1.179736000	-0.283747000
6	-3.412871000	1.475595000	-0.296677000
6	-2.254189000	-1.266545000	-1.159256000
6	-3.600541000	0.179898000	0.520886000
6	-3.519723000	-1.118061000	-0.296056000
1	-2.265899000	-0.527645000	-1.972508000
1	-3.695512000	1.298056000	-1.352066000
1	-4.591524000	0.198316000	1.006843000
1	-4.118839000	2.238798000	0.074013000
1	-2.239047000	-2.266908000	-1.617058000
1	-2.861750000	0.154123000	1.340864000
1	-4.401108000	-1.180993000	-0.959862000
1	-3.574106000	-1.980774000	0.390617000
6	-0.870343000	1.260772000	-0.822763000
1	-1.099587000	0.968392000	-1.857976000
1	0.045398000	1.874227000	-0.885635000
6	-2.009520000	2.099279000	-0.237493000
1	-1.767084000	2.337511000	0.815376000
1	-2.026623000	3.063753000	-0.778364000
6	0.532421000	0.324428000	0.978380000
1	0.399052000	1.386303000	1.252902000
6	0.380696000	-0.471468000	2.278616000
1	-0.646201000	-0.376953000	2.668352000

1	0.602251000	-1.535254000	2.140182000
1	1.076251000	-0.045705000	3.020129000
6	1.915765000	0.198164000	0.366610000
6	2.377938000	-1.038401000	-0.132271000
6	2.760947000	1.321750000	0.295511000
6	3.660356000	-1.136616000	-0.691934000
6	4.046887000	1.222350000	-0.262216000
6	4.498854000	-0.009849000	-0.758314000
1	1.721280000	-1.911126000	-0.082483000
1	2.410584000	2.283552000	0.688290000
1	4.009779000	-2.099881000	-1.076636000
1	4.691776000	2.105265000	-0.309745000
1	5.498888000	-0.093082000	-1.194515000
8	-0.553963000	-2.203030000	0.233487000