

Supporting Information

Unified Reaction Pathways for the Prebiotic Formation of RNA and DNA Nucleobases

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Coordinates for optimized structures

Coordinates for DAMN

0 1

C	0.68535400	-0.36242600	0.00071600
C	1.41270600	0.85690000	0.01048600
N	2.07085200	1.80873600	0.03987800
C	-0.67859600	-0.40384600	0.01322200
C	-1.46596400	0.78557700	-0.02573500
N	-2.14621400	1.71885900	-0.04355000
N	1.39138700	-1.59344500	0.00379400
H	1.32503100	-2.08152500	-0.88555800
H	2.36527200	-1.48400700	0.25421400
N	-1.35676900	-1.60998700	-0.00605600
H	-2.31480100	-1.58308700	0.31045700
H	-0.81130600	-2.37776200	0.37028500

Coordinates for DAMN-NH₂

0 2

N	1.73216400	-1.79713900	0.04572800
C	-0.11804800	-0.28690000	-0.09460900
C	1.23778000	-0.45194500	0.00893700
N	-0.98950000	-1.32316600	-0.19329800
H	2.14175900	-2.06754400	-0.84507400
C	2.13889500	0.64148300	0.07878700
N	2.93664900	1.47892200	0.15414400
C	-0.69780400	1.02655900	-0.13901300
N	-1.22522000	2.05274400	-0.16325900
H	-1.98322500	-1.15213800	-0.04171500
H	2.44816100	-1.90631200	0.75632300
H	-0.59037500	-2.23214000	-0.00400300
N	-3.73724200	-0.21394200	0.21777100
H	-4.71634700	-0.40724400	0.45868500
H	-3.68286700	0.80826400	0.12357500

Coordinates for 2

0 2

C	0.72535500	0.33361300	0.02456300
C	-0.69225200	0.60979600	-0.04663900
C	-1.57338100	-0.53561100	0.05364400
N	-1.25463400	1.77152400	-0.17199900
H	-0.55989300	2.51019600	-0.29831900
N	-2.27795600	-1.44453100	0.13597500
C	1.23584900	-0.97840500	-0.05256900
N	1.69206800	-2.04262200	-0.12137200
N	1.62117300	1.36553100	0.10837600
H	1.32426700	2.22414800	0.54945600
H	2.59765900	1.13998700	0.21800000

Coordinates for 3

0 2

C	1.85694700	-0.95382400	0.08171200
C	0.46655900	-0.73878600	-0.18889900
C	-0.01506300	0.54429000	-0.17860800
N	-0.26748700	-1.86214800	-0.48139700
H	-1.25756100	-1.83823600	-0.22912600
N	-1.36680100	0.88233100	-0.41822600
H	-1.51809100	1.80653800	-0.79408300
N	2.96892200	-1.19066000	0.28259800
C	-2.48479700	0.25566200	0.09155000
N	-2.53495700	-0.80272400	0.78322800
H	0.18280900	-2.73669700	-0.25239200
C	0.84444400	1.65549400	0.03539500
N	1.48707700	2.60703300	0.17774100
H	-3.42298000	0.75454800	-0.17890800

Coordinates for 4

0 2

C	1.10458600	1.25002200	-0.53387300
C	0.61513500	0.18106800	0.36910100
C	-0.76319000	-0.31934500	-0.07822500
N	0.58248400	0.70004300	1.72034700
H	0.28661600	-0.03081900	2.36043300
H	1.51185300	1.00588000	1.99453600
N	-0.56990800	-1.61619500	-0.50063600
H	-1.29156300	-2.22595500	-0.85263300
N	1.48396200	2.06133700	-1.25830900
C	0.76482100	-1.94413500	-0.30694400
H	1.11303500	-2.94175000	-0.54596200
N	1.49793700	-1.01140100	0.16749200
C	-1.97879800	0.33756700	-0.05457700
N	-3.00522600	0.88930000	-0.03307500

Coordinates for **5-NH₂**

0 2

C	0.60174700	1.31947600	-0.12272700
C	0.29675500	-0.05231100	0.31911500
C	-1.25006800	-0.27552300	0.64436700
N	1.06804800	-0.33314100	1.51413700
H	0.94091400	-1.31082300	1.76432200
H	2.06012400	-0.20342800	1.29898700
N	-1.46401800	-1.58133600	0.01378200
H	-2.40356400	-1.86489500	-0.22522200
N	0.85870100	2.38245300	-0.48310200
C	-0.42788500	-1.77642800	-0.88123200
H	-0.47875500	-2.61299100	-1.57069100
N	0.57528300	-0.99081300	-0.80538000
C	-2.16973800	0.73351300	0.11217000
N	-2.94043000	1.48398200	-0.30150700
H	-1.36037500	-0.31522500	1.72907400
N	3.56522400	-0.03584900	-0.19596800
H	4.20501000	0.63681100	-0.63631700
H	3.09212300	-0.49888600	-0.98405000

Coordinates for **5**

0 1

C	0.99350600	1.34398900	-0.31222600
C	0.78498400	-0.03373700	0.16157000
C	-0.69809100	-0.29466200	0.69629600
N	1.71172400	-0.28195400	1.25773200
H	1.68275700	-1.27068700	1.49489900
H	2.65876700	-0.08053000	0.94964500
N	-0.95837900	-1.60994200	0.10576100
H	-1.91409800	-1.91406900	-0.01530000
N	1.17771600	2.41763000	-0.68446900
C	-0.03598100	-1.78886100	-0.91106700
H	-0.15012400	-2.63375800	-1.58239200
N	0.94850900	-0.97876100	-0.96890200
C	-1.70586000	0.68737700	0.28842100
N	-2.54346900	1.41630100	-0.02029200
H	-0.66134900	-0.32850600	1.78636400

Coordinates for **6**

0 2

C	1.31394200	0.89542400	-0.61352200
C	0.65759900	-0.30383600	0.08725700
C	-0.76904600	0.05684300	0.71630000
N	1.51739200	-0.79143400	1.14458500

H	1.27351300	-1.75090700	1.36991800
H	2.48481700	-0.78273400	0.83906300
N	-1.55689000	-1.09945200	0.28124500
H	-2.56356500	-1.02845200	0.24053600
N	2.41909100	1.36792800	-0.30351200
C	-0.85521900	-1.69563300	-0.75321300
H	-1.33475700	-2.48211500	-1.32764100
N	0.35329900	-1.32878400	-0.93755400
C	-1.36180500	1.31291800	0.24803100
N	-1.85682500	2.28601500	-0.12361000
H	-0.65312400	0.10054500	1.79979200
H	0.74783200	1.30946300	-1.45886700

Coordinates for **7**

0 2

C	-0.67681800	-0.71320500	0.10174000
C	0.41151500	0.19703600	0.67215000
N	-0.53997500	-2.08269700	0.03477100
H	-0.15697100	-2.53931400	0.85208900
H	-1.36170300	-2.54717600	-0.32712100
N	-0.23854900	1.49474400	0.46325200
H	0.34715800	2.30112500	0.29989900
C	-1.36030100	1.26737800	-0.35007200
H	-1.97777200	2.07816300	-0.70103900
N	-1.63833700	-0.02045100	-0.49602200
C	1.70532200	0.07043100	-0.03839500
N	2.71122800	0.00353600	-0.59847100
H	0.61040900	0.01143700	1.73893200

Coordinates for **AICN**

0 1

C	0.54823400	0.73498700	-0.00825600
C	-0.39854300	-0.28934300	-0.00636400
N	0.34264700	2.08920600	-0.07085100
H	-0.54794000	2.43440700	0.25225400
H	1.13779200	2.64252100	0.21012100
N	0.36095100	-1.46570400	0.00282700
C	1.65810800	-1.09716300	0.00714200
H	2.46445100	-1.81451900	0.01569800
N	1.81014200	0.21353600	0.00310800
C	-1.79858100	-0.25016900	-0.00276600
N	-2.95665800	-0.18696900	0.00507700
H	-0.00918800	-2.40275900	0.00227300

Coordinates for **8**

0 1

C	-0.63013100	-0.85561500	0.41871100
C	0.33022000	0.35112600	0.76646500
N	0.08730100	-2.02222200	-0.01976300
H	-0.54653300	-2.81109900	-0.08743100
H	0.48054700	-1.87116400	-0.94467500
N	-0.50658000	1.49060200	0.36604000
H	-0.04936500	2.35840900	0.12098300
C	-1.46651700	0.97372900	-0.50419400
H	-2.06873800	1.66654500	-1.08438700
N	-1.61639700	-0.28928100	-0.53009200
C	1.59725800	0.32151400	0.01908700
N	2.58003200	0.34408700	-0.58345500
H	0.55908300	0.36992900	1.83233300
H	-1.17046500	-1.11945300	1.33365100

Coordinates for **9**

0 2

C	-0.23362200	-0.97796900	0.46017300
C	0.12697400	0.49366900	0.83119900
N	0.90622500	-1.81093200	0.18633500
H	0.59482700	-2.76479900	0.03545100
H	1.36653900	-1.50100000	-0.66596700
N	-1.09629000	1.17644500	0.39506100
H	-1.06366100	2.17132800	0.21542400
C	-1.66405300	0.34682500	-0.57470500
H	-2.44604400	0.74627000	-1.21388900
N	-1.25372700	-0.85663600	-0.61672200
C	1.35308100	1.09620500	0.09538200
N	1.83592600	0.68971200	-0.97099000
H	0.28943800	0.61308300	1.90282800
H	-0.75286200	-1.40701300	1.32689100
H	1.77254400	1.99963400	0.57117600

Coordinates for **10**

0 2

C	0.73889800	0.03906200	0.41604700
C	-0.20510200	1.16562300	0.08811900
N	1.99336000	0.11370900	-0.32098900
H	2.56119600	-0.69709000	-0.08779100
H	1.79434300	0.05846000	-1.31660100
N	-1.44069300	0.56990700	-0.11713800
H	-2.25614200	1.03647000	-0.48068300
C	-1.25149700	-0.80472600	-0.12265000
H	-2.07955400	-1.46168300	-0.36614600
N	-0.06875900	-1.19480400	0.17067400
H	-0.11389100	2.20784300	0.34954700

H	1.01290100	0.03455800	1.48475000
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Coordinates for **11**

0 1

C	-0.68161300	0.03834000	-0.01296700
C	0.16860700	1.12178900	-0.00983000
N	-2.07719800	0.00796700	-0.08692000
H	-2.42734900	-0.90763700	0.16269800
H	-2.53368000	0.72776300	0.45617500
N	1.44341700	0.56819400	0.00835200
H	2.30996100	1.08012300	0.01729300
H	0.00028600	2.18428900	-0.03564500
C	1.30026800	-0.78020500	0.00951500
H	2.14097900	-1.45663100	0.02100500
N	0.03181400	-1.13436700	0.00116200

Coordinates for **AICN-NH2**

0 2

C	-0.54315400	-0.80463200	-0.08248200
C	-0.39333300	0.58821500	-0.03798100
N	0.40772200	-1.75777500	-0.24546500
H	1.38887900	-1.53458000	-0.08419300
H	0.10740200	-2.70122600	-0.06219700
N	-1.70053600	1.07987100	0.10064100
C	-2.51957400	0.00984300	0.13079300
H	-3.59029200	0.10482000	0.23155000
N	-1.86972600	-1.13220200	0.02644600
C	0.75044400	1.38748600	-0.09540900
N	1.73183000	2.00721400	-0.14158000
H	-1.96024200	2.05107000	0.15974400
N	3.25713300	-0.79224400	0.21328100
H	4.20087100	-1.06678600	0.51060000
H	3.30212200	0.22718100	0.08170000

Coordinates for **12**

0 2

C	-0.58641300	0.81125100	-0.00007900
C	0.41282000	-0.22441200	0.00002200
C	1.80974600	-0.14730800	0.00003000
C	-1.62934500	-1.08381000	0.00007400
H	-2.38647400	-1.85536900	0.00013700
N	-0.33431100	2.09120700	-0.00019300
N	-0.28953400	-1.40605300	0.00013100
N	-1.85003400	0.19244600	-0.00004100
N	2.96776700	-0.09812600	0.00004400
H	-1.22382400	2.59595200	-0.00025200

H	0.11222400	-2.33122800	0.00025300
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Coordinates for **13**

0 2

C	-0.14723800	-0.70039800	0.00000200
C	-0.80453900	0.52939900	0.00059800
C	-0.35434000	1.85790700	0.00021300
C	-2.23887300	-1.15609700	-0.00029800
H	-3.17860400	-1.68637400	-0.00055000
N	1.19360000	-1.01251000	0.00049200
N	-2.16196000	0.18946100	0.00039400
N	-1.04895400	-1.72324000	-0.00059800
N	0.02235800	2.95418600	-0.00048800
H	1.39622200	-2.00276500	0.00033200
H	-2.92609700	0.84717200	0.00063300
H	2.00798200	0.93025900	-0.00122600
C	2.26479400	-0.13379600	-0.00027300
N	3.47805000	-0.47509600	0.00011000

Coordinates for **14**

0 2

C	-0.56547400	-0.80451100	-0.00004800
C	-0.23805300	0.52979800	-0.00019500
C	1.13864600	0.99711900	-0.00007500
C	-2.41751800	0.20805400	0.00015300
H	-3.47111100	0.43904200	0.00016800
N	0.44306000	-1.74647000	-0.00005700
N	-1.45706000	1.17510500	0.00007500
N	-1.90830300	-1.01315200	-0.00007800
N	1.45319600	2.23091900	-0.00001000
H	0.23349000	-2.73250600	0.00012200
H	-1.59210300	2.17433100	0.00004600
H	2.49709700	-2.04649600	0.00080000
C	1.73135900	-1.27504100	-0.00010000
N	2.10323000	-0.04167000	0.00013400

Coordinates for **15**

0 2

C	0.54089900	-0.17126500	-0.00021200
C	-0.77596800	-0.56103500	-0.00020300
C	-1.87969700	0.37268700	-0.00002700
C	-0.21081700	2.03569900	0.00003700
C	0.58744100	-2.28946500	0.00011100
H	0.06500700	3.08713500	0.00017600
H	0.91378200	-3.31746200	0.00024300
N	-1.46661700	1.72441600	0.00013900

N	0.84838200	1.17176700	-0.00021100
N	-0.72627800	-1.93667800	0.00009200
N	1.39417200	-1.23748500	-0.00006900
N	-3.09836300	-0.02578200	0.00007900
H	1.82620600	1.46848500	-0.00031500
H	-1.53698900	-2.53686200	-0.00004500
H	-3.71360900	0.78883200	0.00029600
N	3.71402400	0.80756300	0.00001000
H	3.47854600	-0.19655000	-0.00028500
H	4.73866100	0.86009600	0.00142100

Coordinates for **16**

0 2

C	-0.63821100	-0.84244800	-0.00003800
C	-0.18949800	0.50090300	0.00001800
C	1.21034000	0.77929000	0.00006700
C	1.50276900	-1.52472600	-0.00002000
C	-2.39127300	0.36035500	-0.00000600
H	2.20154700	-2.35557900	-0.00004800
H	-3.41297300	0.71212400	-0.00001100
N	2.03531300	-0.31859500	0.00002700
N	0.19196700	-1.87720600	-0.00005300
N	-1.33261700	1.25471900	-0.00001400
N	-2.02462700	-0.88741200	-0.00005400
N	1.78535200	1.97681200	0.00008100
H	1.06486100	2.70493800	0.00006800
H	-1.40591800	2.26004700	-0.00004700

Coordinates for **17-NH₂**

0 2

C	1.18499800	0.86523300	-0.03874600
C	-0.01853300	0.15185400	0.11585100
C	0.02904100	-1.24598100	0.12840400
C	2.29775300	-1.05990400	-0.20894900
C	-0.36291700	2.31347100	0.14149700
H	3.22953600	-1.59878400	-0.35196600
H	-0.91053600	3.24383700	0.19192500
N	1.20761600	-1.83908100	-0.04581600
N	2.37381700	0.26269100	-0.20320300
N	-1.00712000	1.10785200	0.23916300
N	0.93599900	2.22242000	-0.01062300
N	-1.09875800	-2.04693100	0.26889900
H	-2.01136000	0.93110000	0.22598700
H	-0.84770100	-3.01404900	0.43241200
H	-1.78483700	-1.70332000	0.92815100
N	-3.62742000	-0.13608400	-0.36182900

H	-4.61720000	-0.01504100	-0.60589400
H	-3.32888600	-0.98785600	-0.85510200

Coordinates for **Adenine (17)**

0 1

C	0.73808600	-0.80939900	0.01544100
C	0.18220700	0.48226700	-0.00839200
C	-1.21307100	0.61346700	-0.00575700
C	-1.30872400	-1.68871500	-0.01128400
C	2.38289600	0.54370500	-0.00613100
H	-1.95954900	-2.55775900	-0.02343400
H	3.37543500	0.97101500	-0.01958400
N	-1.94450400	-0.50031200	-0.01405500
N	-0.00533100	-1.92645300	0.01576300
N	1.26582800	1.34433800	-0.01527600
N	2.11848900	-0.73529500	0.02227500
N	-1.87056200	1.82563600	-0.04939300
H	1.25689300	2.34507600	-0.12583600
H	-2.86443700	1.73814800	0.11355600
H	-1.44414200	2.60017900	0.43684800

Coordinates for **18**

0 2

C	0.72412700	-0.82975800	0.06124900
C	0.23456500	0.46299700	-0.18271600
C	-1.22215000	0.73948100	-0.38133400
C	-1.40033500	-1.61515100	-0.00800600
C	2.43400000	0.44221100	0.02934600
H	-2.04827500	-2.48411200	0.08356600
H	3.43570800	0.84445800	0.06620900
N	-1.99661700	-0.48597300	-0.22998000
N	-0.05875900	-1.90749500	0.15364400
N	1.33744500	1.26367900	-0.20733000
N	2.10827200	-0.80491200	0.19477600
N	-1.81085800	1.77443200	0.48104400
H	1.36246500	2.26147200	-0.35119200
H	-1.38857800	1.08435400	-1.41575400
H	-1.65479800	1.53845700	1.45684500
H	-1.38413900	2.67856300	0.30401300

Coordinates for **Purine (19)**

0 1

C	0.21711400	-0.71447300	0.00011800
C	0.23438900	0.70096900	0.00007300
C	-0.97642400	1.37948900	-0.00006700
C	-2.01783200	-0.66574400	-0.00001500

C	2.26584400	-0.14965600	0.00007400
H	-2.96312200	-1.19884100	-0.00002500
H	3.34657300	-0.16319400	0.00006500
N	-2.10906600	0.67849300	-0.00002700
N	-0.91777100	-1.41484500	0.00007100
N	1.57215500	1.03870300	0.00012100
N	1.50631100	-1.21226900	-0.00023700
H	1.97027900	1.96409900	-0.00052500
H	-1.05367500	2.46385400	-0.00011400

Coordinates for **20**

0 2

C	-0.73925800	0.41606700	0.39181500
C	-1.38507400	-0.88420800	0.13128000
N	-1.96494300	-1.85478000	-0.09214200
C	0.74262600	0.40441500	0.06552600
C	1.49217900	-0.76077100	-0.04071800
N	2.13708700	-1.72727900	-0.14645600
N	-1.38063000	1.53678600	-0.31369000
H	-1.51003200	1.30683300	-1.29511700
H	-2.29516300	1.72873000	0.08141500
N	1.34856500	1.64111600	0.10123000
H	2.28937700	1.71012700	-0.25596400
H	0.72733600	2.40859300	-0.12623000
H	-0.85490200	0.62180800	1.46588700

Coordinates for **21**

0 1

C	0.52790600	-0.80088500	-0.00971400
H	0.25406500	-1.84519900	-0.02651200
C	1.89545300	-0.44873700	0.00208800
N	3.00436600	-0.11428900	0.01660700
C	-0.43838500	0.15974500	-0.00808800
C	-1.81629400	-0.24592100	-0.00052200
N	-2.92850600	-0.55250900	0.01512000
N	-0.22125500	1.50634500	-0.04928700
H	-0.97029300	2.13686600	0.18145000
H	0.72191800	1.84629100	0.06539400

Coordinates for **21-NH₂**

0 2

C	1.40612100	0.78902100	0.00666700
H	1.54003200	1.86018600	0.01623000
C	2.54336500	-0.04562700	0.00710000
N	3.45084400	-0.76661200	0.00736400
C	0.14795900	0.25400700	-0.00670900

C	-0.97383400	1.15740100	-0.00440000
N	-1.89344400	1.85434100	-0.00163000
N	-0.17377300	-1.05955200	-0.02510800
H	-1.15073200	-1.35298000	-0.01294400
H	0.56517200	-1.74497400	-0.01657500
N	-3.12864500	-1.34806500	0.01302000
H	-3.89915800	-2.02602700	0.03146100
H	-3.58185200	-0.42580100	0.01035600

Coordinates for **22**

0 2

C	-0.56964100	-0.70734900	-0.00071400
H	-0.31930400	-1.76129500	-0.00179100
C	-1.92272600	-0.35828800	-0.00003800
N	-3.05925500	-0.11937100	0.00072200
N	0.19281800	1.54309600	-0.00028400
H	1.04417900	2.10735200	0.00018700
C	0.46998700	0.27219500	-0.00028400
C	1.83110200	-0.23239100	0.00013500
N	2.92683700	-0.59387600	0.00056300

Coordinates for **23**

0 2

C	0.05021600	-1.22089300	0.19252700
C	0.79994800	1.81138300	-0.06959600
H	-0.42922000	-2.11678200	0.56658400
C	1.43829100	-1.31488000	-0.05586100
N	2.55749400	-1.48011500	-0.29626300
N	1.71452200	1.41875500	0.69604400
N	-0.34648600	1.12052200	-0.47564200
C	-0.73948400	-0.14984800	-0.06816400
C	-2.16088500	-0.30143700	0.06356300
N	-3.30926800	-0.39363700	0.13899300
H	0.85360800	2.82340500	-0.48760900
H	-1.06673000	1.68874100	-0.89571500

Coordinates for **24-NH₂**

0 2

C	-0.77024400	-1.26289700	0.16493600
C	0.45278600	1.60534000	-0.19231300
H	-1.38620300	-2.07725200	0.52495400
C	0.58095200	-1.58505800	-0.09527000
N	1.65101900	-1.94703200	-0.34510200
N	1.20191100	1.01938900	0.63144200
H	2.13627500	1.42489300	0.68268800
N	-0.83402000	1.12522200	-0.48813800

C	-1.38618100	-0.07337400	-0.06551900
C	-2.81227800	-0.02206200	0.10882500
N	-3.95930400	0.04916100	0.21955100
H	0.67707400	2.51243700	-0.76259600
H	-1.47877100	1.79011600	-0.88824700
N	4.08338000	0.42139400	0.11595500
H	5.07594300	0.16826300	0.02454000
H	3.58457800	-0.46708800	-0.04124800

Coordinates for **24**

0 1

C	-0.01081000	-1.24293000	-0.20482200
C	-0.78344300	1.79267900	0.15033000
H	0.48434500	-2.11294900	-0.61801200
C	-1.39256400	-1.38385300	0.05850200
N	-2.49837800	-1.60287600	0.31556400
N	-1.57783500	1.35972000	-0.73040400
H	-2.34098700	2.01110300	-0.89201400
N	0.34352200	1.07592300	0.56333800
C	0.75764200	-0.16475100	0.08458100
C	2.17925100	-0.28103700	-0.08420300
N	3.32796700	-0.34325800	-0.18494200
H	-0.85574200	2.74475200	0.68494100
H	1.04499600	1.60988100	1.05386500

Coordinates for **24-OH**

0 2

C	-0.97485700	1.29759700	0.09466800
C	-0.52748700	-1.82701400	0.14832100
H	-0.87990200	2.33972200	0.37470900
C	-2.26784000	0.89149500	-0.30550400
N	-3.33785900	0.67895200	-0.68922200
N	-1.59659300	-1.63229200	0.79392400
H	-2.09679900	-2.50298700	0.95134000
N	0.33850500	-0.79072800	-0.20125800
C	0.16300100	0.55753600	0.07282800
C	1.40331900	1.23997400	0.32980700
N	2.44182000	1.71910900	0.49215100
H	-0.14115500	-2.78960700	-0.19940200
H	1.28460900	-1.06147500	-0.46036800
O	3.31970400	-1.07264500	-0.64525100
H	3.57769400	-0.18730500	-0.31415700

Coordinates for **25**

0 2

C	0.91592600	1.41829400	-0.22758100
C	-1.33340800	-0.78130500	-0.20394300
H	1.80927400	1.99864300	-0.41200400
C	-0.30557600	2.12257400	-0.17171200
N	-1.30098600	2.71022200	-0.08926700
N	-2.12061200	-0.45687100	0.95230400
H	-2.05291600	0.55386400	1.11474600
N	0.08461000	-0.85998400	0.19942100
C	1.05450900	0.07930300	0.00474800
C	2.39533200	-0.43974100	0.07535000
N	3.46169100	-0.87453400	0.14630100
H	0.37651200	-1.79809000	0.43377800
O	-1.70093500	-2.04327000	-0.67542900
H	-2.34328700	-2.38534900	-0.03950900
H	-1.41572800	-0.04949600	-1.01605900

Coordinates for **26**

0 2

C	-0.49153200	1.30760700	0.01704400
C	1.05519600	-1.04745600	0.36905200
H	-1.07405800	2.21460600	0.03531700
C	0.96811600	1.39888000	-0.02563300
N	1.57645700	2.51492200	0.00073000
N	1.64445000	0.17333500	-0.15965400
H	2.63814000	0.23271600	0.02427800
N	-0.33675000	-1.08987600	-0.06423800
C	-1.07357400	0.08784300	-0.01247800
C	-2.49749200	-0.05556900	-0.02692700
N	-3.64359200	-0.19495700	-0.03231100
H	-0.81919200	-1.92901300	0.22701800
O	1.74524600	-2.15752300	-0.10252800
H	1.71391900	-2.11562900	-1.06887600
H	1.13099000	-1.11428900	1.46445200

Coordinates for **27-NH₂**

0 2

C	0.84112100	0.22740800	0.03228100
C	-1.83865000	-0.65458100	0.37596200
H	1.87139200	0.55471100	0.05169400
C	0.57111100	-1.20834400	-0.01716000
N	1.54524300	-2.04484700	-0.05704100
N	-0.78390400	-1.54494000	-0.08355200
H	-1.00269900	-2.51743600	0.08772700
N	-1.51964700	0.68844100	-0.08039700
C	-0.18846200	1.09975800	-0.00931700
C	0.02513900	2.51485600	-0.03079500

N	0.15868300	3.66159600	-0.04128200
H	-2.20573100	1.37405600	0.20496200
O	-3.07232800	-1.06216100	-0.12598900
H	-3.00591100	-1.02218000	-1.09053600
H	-1.96222600	-0.69001700	1.46891000
N	4.11283000	-0.24295900	0.02338600
H	5.07996200	-0.58980700	-0.02507800
H	3.53215300	-1.09694600	-0.02503900
H	1.21769400	-3.01070700	-0.09835100

Coordinates for **27**

0 1

C	0.43993100	-1.28560500	0.01308700
C	-0.97379600	1.15406400	0.37278900
H	0.98800000	-2.21583000	0.01661700
C	-1.02198300	-1.30951500	-0.02166300
N	-1.77781700	-2.34339000	-0.01703100
N	-1.61566300	-0.04673700	-0.11597200
H	-2.61433600	-0.07072700	0.04764000
N	0.42618700	1.11365300	-0.04344300
C	1.09273900	-0.10058200	-0.00633700
C	2.52319800	-0.03926500	-0.02851900
N	3.67577600	0.02777700	-0.03983800
H	0.95475600	1.92924000	0.23261800
O	-1.59818500	2.28903100	-0.13819600
H	-1.59242800	2.19781000	-1.10147300
H	-1.21894600	-3.19439400	-0.01678000
H	-1.05147900	1.26794800	1.46478600

Coordinates for **28**

0 1

C	0.43993100	-1.28560500	0.01308700
C	-0.97379600	1.15406400	0.37278900
H	0.98800000	-2.21583000	0.01661700
C	-1.02198300	-1.30951500	-0.02166300
N	-1.77781700	-2.34339000	-0.01703100
N	-1.61566300	-0.04673700	-0.11597200
H	-2.61433600	-0.07072700	0.04764000
N	0.42618700	1.11365300	-0.04344300
C	1.09273900	-0.10058200	-0.00633700
C	2.52319800	-0.03926500	-0.02851900
N	3.67577600	0.02777700	-0.03983800
H	0.95475600	1.92924000	0.23261800
O	-1.59818500	2.28903100	-0.13819600
H	-1.59242800	2.19781000	-1.10147300
H	-1.21894600	-3.19439400	-0.01678000

H	-1.05147900	1.26794800	1.46478600
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Coordinates for **29**

0 1

C	-0.36217700	-1.28252600	0.23699000
C	-0.15970800	1.49247600	0.24544200
C	-1.44915600	-0.54772400	-0.04346700
N	-2.71522000	-1.05548600	-0.34156400
N	-1.43749600	0.85787700	-0.02735900
H	-2.19708800	1.23378500	0.52864400
N	0.61856200	0.73545000	1.19645300
C	0.89002700	-0.64837300	0.79007400
C	2.03358400	-0.80252700	-0.15026400
N	2.95218100	-0.97442000	-0.82620200
H	1.47931100	1.22552400	1.41246200
O	0.57046200	1.65450900	-0.96033200
H	-0.06595900	1.84245900	-1.65893000
H	-3.14243800	-0.61738300	-1.14876900
H	-0.35705900	-2.35239700	0.07746500
H	-2.74736000	-2.06359300	-0.40289000
H	-0.36730100	2.47007000	0.69557200
H	1.19259400	-1.18643500	1.69715000

Coordinates for **30**

0 2

C	-0.49355900	-1.28863800	0.07591100
C	-0.07074500	1.43072300	0.32925700
C	-1.54288600	-0.45821300	-0.03984700
N	-2.85849600	-0.84120800	-0.30852000
N	-1.42304800	0.92927700	0.14372600
H	-2.08000500	1.28078400	0.83118100
N	0.72779600	0.53858600	1.13207000
C	0.81829900	-0.83131600	0.64064300
C	2.00171400	-1.10796000	-0.34599100
N	2.98009500	-0.37092400	-0.51781000
H	1.65378300	0.93061800	1.26359800
O	0.53683500	1.63647800	-0.93798600
H	-0.13015700	2.03715300	-1.50675000
H	-3.30698100	-0.26813000	-1.01285800
H	-0.59179600	-2.33165500	-0.20047700
H	-2.97024500	-1.82750400	-0.49716600
H	-0.14632200	2.38205500	0.86921800
H	1.07086300	-1.46673700	1.50340500
H	1.94480800	-2.08609500	-0.85236300

Coordinates for **31**

0 2

C	0.73190600	1.26542600	-0.32623500
C	-1.12359100	-0.68733900	0.36062200
C	1.18851000	0.00865100	0.02120100
N	2.52084100	-0.42723200	0.01839200
N	0.29011800	-0.96564700	0.51767800
H	0.52977900	-1.27481700	1.45539500
N	-1.43918400	0.71211000	0.56405700
C	-0.58580700	1.62846600	-0.07553400
H	-2.42397200	0.89790200	0.42624700
O	-1.55620000	-1.06582600	-0.94048900
H	-1.09068200	-1.88246100	-1.15392800
H	2.65027300	-1.31182200	-0.46468300
H	1.40072900	1.97313800	-0.80081700
H	3.16585900	0.26900700	-0.33057600
H	-1.66060600	-1.27265800	1.11644900
H	-0.99031300	2.60247500	-0.30539100

Coordinates for **32**

0 2

C	1.78158500	1.02333000	-0.08289400
C	0.00851500	-1.16908300	-0.28966100
C	0.33743100	1.24287500	-0.43998100
N	-0.43556500	1.58329100	0.80211800
N	-0.18994900	0.03307400	-1.06385400
H	-1.17718900	0.13982700	-1.27690800
N	1.43576600	-1.34755500	-0.09199400
C	2.22396200	-0.22645600	0.10701700
H	1.66906100	-2.15917300	0.45982600
O	-0.71755200	-1.20175100	0.95074900
H	-0.61547900	-0.30102300	1.32408300
H	0.04245200	2.31419000	1.32159100
H	2.44663100	1.87059900	0.01623500
H	-1.35780300	1.93430900	0.54954300
H	-0.36921200	-2.02330600	-0.85422400
H	3.25330400	-0.43414200	0.37877700
H	0.24771100	2.04422700	-1.18354500
N	-3.30300200	0.00168400	-0.26641900
H	-4.28546400	-0.27097000	-0.13416000
H	-2.77330700	-0.61797900	0.36694500

Coordinates for **33**

0 2

C	0.41978600	1.46351200	-0.09260100
C	-1.02107900	-0.91015300	0.23803200
C	1.16917200	0.28672600	0.46950100

N	2.15649300	-0.34616300	-0.41693500
N	0.23806200	-0.72003400	0.98163900
H	0.72199800	-1.60592200	1.09525200
N	-1.69539100	0.38537700	0.16707700
C	-0.91485800	1.46422000	-0.21591100
H	-2.60784400	0.33431400	-0.26350800
O	-0.64149600	-1.40194600	-0.95310200
H	1.68705900	-0.57770000	-1.29045400
H	0.99639700	2.33650000	-0.36935300
H	2.90888100	0.30396600	-0.62758900
H	-1.66561300	-1.58781200	0.81616700
H	-1.45267600	2.32234800	-0.60292000
H	1.73149500	0.62979200	1.35063200

Coordinates for **34**

0 1

C	1.11769800	1.16196500	0.25796200
C	-1.26134000	-0.39472900	0.02032600
C	1.25503400	-0.32848400	0.42643400
N	2.08407000	-0.99894400	-0.58681600
N	-0.07340000	-0.94060000	0.43669800
H	-0.09166600	-1.94900300	0.48449900
N	-1.20868000	0.97684500	-0.21035200
C	-0.05080400	1.72453900	-0.06419800
H	-2.08656900	1.40422200	-0.45417800
O	-2.28927000	-1.03116500	-0.11963800
H	1.86486500	-0.63543900	-1.51083100
H	2.00625000	1.76821300	0.37089800
H	3.06853500	-0.81879600	-0.41338100
H	-0.16236700	2.78966000	-0.22631700
H	1.73764700	-0.55038900	1.38656300

Coordinates for **35**

0 2

C	1.00203500	1.19635200	0.15078900
C	-1.24792500	-0.49388000	-0.02782400
C	1.15655300	-0.30963900	0.34301000
N	2.38095400	-0.89870700	-0.18653600
N	0.03173600	-1.03312900	-0.19363000
N	-1.32728400	0.89156500	-0.13861000
C	-0.20566800	1.71418500	-0.07534100
H	-2.25682300	1.27908400	-0.19365200
O	-2.22940500	-1.19111300	0.12290100
H	2.41621300	-0.75967900	-1.19225100
H	1.87894700	1.82210200	0.24646600
H	3.19255100	-0.44135200	0.21652200

H	-0.39061400	2.77261200	-0.20850200
H	1.16716300	-0.50407400	1.43584000

Coordinates for Cytosine (**36**)

0 1

C	1.04931200	1.18520000	0.00124600
C	-1.18735000	-0.53182100	0.00001500
C	1.12911000	-0.25288200	0.00274300
N	2.35418400	-0.84333800	0.03533200
N	0.08166400	-1.04938900	-0.00251900
N	-1.27890300	0.89568500	-0.00201500
C	-0.20003100	1.71223900	-0.00133800
H	-2.21857900	1.26431700	-0.00363700
O	-2.21641900	-1.17428100	-0.00086000
H	2.37981800	-1.84428200	-0.07789700
H	1.92832900	1.81328900	0.01190700
H	3.18795100	-0.31496000	-0.15320500
H	-0.39102000	2.77875900	-0.00186700

Coordinates for **37**

0 1

C	1.77749900	-0.00115700	-0.00019300
C	-1.03867200	-0.08822100	0.00008500
C	1.00545200	-1.19811600	-0.00001900
N	-0.29725800	-1.26294800	0.00023200
N	-0.27767400	1.11706100	0.00003700
C	1.07409400	1.16465900	0.00009100
H	-0.82814100	1.96512900	0.00046800
O	-2.24646800	-0.02276600	-0.00022900
H	2.85706500	-0.01726900	-0.00044700
H	1.53020400	2.14752900	0.00008800
H	1.52690400	-2.15504300	0.00005600

Coordinates for **37-OH**

0 2

C	-2.06793200	0.83766100	0.00049400
C	0.25827800	-0.71800600	-0.00006400
C	-2.05229900	-0.58187100	0.00010200
N	-0.97730000	-1.32765200	-0.00023200
N	0.27016200	0.69375000	-0.00081900
C	-0.84886000	1.44943800	0.00000000
H	1.20190300	1.11528800	-0.00088200
O	1.32183900	-1.32769200	0.00019900
H	-2.98971100	1.39987400	0.00087400
H	-2.99966300	-1.11909200	-0.00009000
H	-0.70883800	2.52364500	-0.00012100

O	3.17330700	0.67972000	0.00029300
H	2.74997700	-0.22196100	0.00045000

Coordinates for **38**

0 2

C	-1.12856900	1.10656000	0.26623200
C	1.26249600	-0.30466400	0.00466200
C	0.07253400	1.71684500	-0.07842900
N	1.22440100	1.08962300	-0.23857700
N	0.11075600	-0.92174000	0.46610600
C	-1.20886500	-0.37570100	0.42223500
H	0.18924200	-1.92548700	0.55053200
O	2.29214500	-0.92813900	-0.14490900
H	-2.04345000	1.68122900	0.34448800
H	0.09006400	2.79221000	-0.24753600
H	-1.74846400	-0.64251100	1.34182000
O	-1.91229500	-0.94948300	-0.69948400
H	-2.85787300	-0.91788000	-0.51506800

Coordinates for **39**

0 2

C	-1.92037500	-0.76352200	0.10975200
C	0.19196400	1.15584300	0.22454200
C	-1.89257800	0.55916200	-0.60511500
N	-0.96004500	1.42796900	-0.56929400
N	0.14583200	0.04197000	1.04502300
C	-0.52500800	-1.16125600	0.56974000
H	1.02264700	-0.11190700	1.52585500
O	1.15021700	1.90239000	0.20360900
H	-2.60404900	-0.67048600	0.96361900
H	-2.77359500	0.81596300	-1.19843500
H	-0.57014400	-1.86239700	1.41129200
O	0.13041000	-1.75063600	-0.53526700
H	1.09309200	-1.62271900	-0.43818000
H	-2.32359600	-1.53920800	-0.54543700
N	2.84767600	-0.67994500	-0.43630600
H	3.80231800	-0.83770900	-0.77828100
H	2.75005600	0.34310900	-0.35664800

Coordinates for **40**

0 2

C	1.45469200	0.76714100	-0.47122600
C	-1.23985900	-0.07447700	-0.03399200
C	0.36682200	1.59521600	0.15501200
N	-0.83832200	1.23319500	0.35485900
N	-0.25970000	-0.94864600	-0.51453000

C	1.16736600	-0.72375600	-0.31204700
H	-0.57053300	-1.90981800	-0.58025000
O	-2.39607900	-0.41519900	-0.00171300
H	1.52781200	1.02854700	-1.53528500
H	0.62561500	2.61177700	0.45842000
H	1.72988700	-1.32233600	-1.04028600
O	1.32846600	-1.18355900	0.97746700
H	2.42014100	1.00531200	-0.01741500

Coordinates for Uracil (**41**)

0 1

C	-1.20626100	1.10206900	-0.00012400
C	1.26764100	-0.35200200	-0.00001200
C	0.17053500	1.69692200	0.00006600
N	1.27961500	1.07082700	0.00008500
H	0.22625000	2.78725700	0.00018000
N	0.01707200	-0.99442900	0.00018800
C	-1.23789100	-0.41235500	0.00002500
O	2.28365100	-0.99369800	-0.00015000
H	-1.76792100	1.46172300	0.86973700
O	-2.25593100	-1.06197400	-0.00002200
H	0.04654100	-2.00759800	0.00018500
H	-1.76757600	1.46140500	-0.87037000

Coordinates for **42**

0 2

H	-1.57556500	0.80907500	0.00000000
N	0.27473700	1.67030900	0.00000000
C	0.00000000	-0.68350100	0.00000000
C	-0.48577500	0.67319300	0.00000000
N	0.36672100	-1.77705600	0.00000000

Coordinates for **43a-NH₂**

0 2

N	-0.09806700	-1.39694800	0.00011600
C	-0.16674800	1.01168000	0.00004100
C	0.50332200	-0.27905700	0.00002700
N	-0.74648100	2.00913900	0.00003500
H	-1.12300200	-1.26066100	0.00013200
C	1.95085000	-0.22322500	-0.00003100
N	3.10178300	-0.15675500	-0.00008400
N	-3.02888800	-0.61041300	-0.00009900
H	-3.93173100	-1.09969700	-0.00006600
H	-3.26824500	0.38880600	-0.00006300

Coordinates for **44a**

0 2

N	0.01106700	1.73145200	-0.26577800
C	1.17989400	-0.40780300	0.07454300
C	-0.00363800	0.42107100	0.37202400
N	2.13759800	-1.00024400	-0.16682700
H	0.98947500	2.04674000	-0.25249000
H	-0.00356000	0.59842200	1.46354600
C	-1.24992300	-0.29973800	0.05678600
N	-2.22636600	-0.86354200	-0.17184800

Coordinates for **45**

0 1

N	0.00987800	1.72274000	0.00003600
C	-1.19255600	-0.36974500	-0.00000700
C	0.00194500	0.45030000	-0.00004400
N	-2.16895000	-0.98417600	0.00001900
H	-0.94182600	2.09668600	-0.00001900
C	1.25453800	-0.27314100	-0.00005800
N	2.23882400	-0.87301700	0.00004200

Coordinates for **46**

0 2

N	1.59242200	-1.40706900	-0.47218400
C	-0.68408900	-0.63489700	0.14302100
C	0.81810800	-0.47403100	-0.10972500
N	-1.13662500	-1.72750200	0.57134300
H	1.08729000	-2.28823500	-0.59111300
C	1.34558500	0.85174400	0.11718900
N	1.73397100	1.91906000	0.31654100
C	-1.56653200	0.47293600	-0.12446800
N	-2.27058500	1.35747100	-0.35355500

Coordinates for **47-NH₂**

0 2

N	1.81703600	-1.82660700	0.00005800
C	-0.16945200	-0.39055000	-0.00012700
C	1.32823800	-0.65680100	-0.00000200
N	-0.94988800	-1.38848000	-0.00010900
H	1.04018500	-2.50033900	-0.00007100
C	2.21494400	0.48599800	0.00005500
N	2.89879600	1.41453400	0.00015600
C	-0.63342300	0.98358900	-0.00014800
N	-1.05778400	2.05688700	-0.00018400
H	-1.94386800	-1.10999600	-0.00017400
N	-3.71902300	-0.15953400	0.00020000
H	-3.76356200	0.86707000	0.00103500

H -4.69855200 -0.46774800 -0.00030700

Coordinates for **48**

0 2

N 1.49384000 -1.47785100 -0.00069200
C -0.69827200 -0.53667600 -0.00001200
C 0.72993700 -0.36303500 -0.00020100
N -1.16707600 -1.75172900 0.00037500
H 1.00530100 -2.36378500 0.00146400
C 1.34706100 0.90594100 0.00009500
N 1.87921700 1.93567100 0.00032200
C -1.53423700 0.63883600 -0.00001700
N -2.26102100 1.53599600 -0.00025100
H -2.18513300 -1.76459300 0.00045900
H 2.49818200 -1.43662200 0.00061000

Coordinates for **DAMN**

0 1

C 0.68535400 -0.36242600 0.00071600
C 1.41270600 0.85690000 0.01048600
N 2.07085200 1.80873600 0.03987800
C -0.67859600 -0.40384600 0.01322200
C -1.46596400 0.78557700 -0.02573500
N -2.14621400 1.71885900 -0.04355000
N 1.39138700 -1.59344500 0.00379400
H 1.32503100 -2.08152500 -0.88555800
H 2.36527200 -1.48400700 0.25421400
N -1.35676900 -1.60998700 -0.00605600
H -2.31480100 -1.58308700 0.31045700
H -0.81130600 -2.37776200 0.37028500

Coordinates for **43b** (CNCN)

0 1

N 0.00003000 -1.84267300 0.00000000
C 0.00000000 0.68758600 0.00000000
C 0.00023300 -0.68760300 0.00000000
N -0.00023000 1.84268800 0.00000000

Coordinates for **44b**

0 2

N -0.00143400 -1.74236000 0.00000000
C 1.24069100 0.26330400 0.00000000
C 0.00000000 -0.47551400 0.00000000
N 2.23405800 0.84843300 0.00000000
C -1.24000600 0.26398500 0.00000000
N -2.23321200 0.84954900 0.00000000

Coordinates for **45-NH₂**

0 2

N	0.44304400	-1.62649500	0.00000100
C	0.85812700	0.74775700	-0.00000100
C	1.25156200	-0.65040700	0.00000200
N	0.52661600	1.85390300	-0.00001900
H	-0.53319400	-1.29646100	0.00000300
H	2.32779300	-0.82738300	0.00001600
N	-2.26139700	-0.10439400	0.00001100
H	-3.28026000	-0.23671800	-0.00023100
H	-2.13031000	0.91536100	0.00025800

Coordinates for **45**

0 1

N	1.62956000	-0.32825300	-0.00003100
C	-0.74525800	0.10291900	-0.00017800
C	0.65122900	0.48102000	0.00010300
N	-1.85689200	-0.20842100	0.00007800
H	1.30797100	-1.29996100	0.00011800
H	0.84752600	1.55304400	0.00000500

Coordinates for optimized transition states (TS)

Coordinates for TS **DAMN-NH₂ → 2**

0 2

C	-0.98764200	0.47818600	-0.07053800
C	0.38415800	0.47105000	-0.23729900
C	1.10906200	-0.76341900	-0.18127400
N	1.09939300	1.59266600	-0.51805500
H	0.57410800	2.43082300	-0.27057300
H	2.24744800	1.64493500	-0.19553900
N	1.73686100	-1.72975100	-0.10811800
C	-1.72358800	-0.69214800	0.24175800
N	-2.37674700	-1.60677600	0.52195200
N	-1.67712500	1.69583000	-0.19661300
H	-1.56719600	2.14107200	-1.10174200
H	-2.65265800	1.64465200	0.06150100
N	3.36997600	1.65673800	0.52167400
H	3.33957200	2.28450300	1.32804100
H	3.57326100	0.72739000	0.89782900

Coordinates for TS **2 → 3**

0 2

C	-2.36637100	0.79394900	1.51578400
C	-0.98916700	0.52951500	1.28497200

C	-0.50017900	-0.76513400	1.11867100
N	-0.12768500	1.59437400	1.27045600
H	0.75130700	1.43087200	0.79433800
H	1.61377200	0.26743400	2.81015700
N	0.85192500	-0.91706500	0.98059700
H	1.10449100	-1.86679400	0.71657100
N	-3.47807000	1.05337200	1.69889700
C	1.74993100	-0.76660100	2.52797700
N	2.26525300	-1.77828200	2.88509000
H	-0.51619900	2.52211900	1.19908300
C	-1.38546300	-1.88437400	1.09877400
N	-2.05693100	-2.82423500	1.05444900

Coordinates for TS **3** → **4**

0 2

C	1.24434500	-0.39559500	-1.05026500
C	-0.10324700	0.08597500	-0.94868000
C	-1.15838800	-0.86346400	-0.84196600
N	-0.30533800	1.36455800	-1.47277600
H	-1.27210100	1.66148300	-1.43988900
H	0.29847000	2.06518500	-1.05602800
N	-2.18943200	-0.47189300	0.00822800
H	-3.08632100	-0.93570900	0.01405500
N	2.33754300	-0.76230000	-1.10345400
C	-1.74052400	0.31947600	1.06520900
H	-2.47135500	0.55651000	1.84140500
N	-0.54888900	0.74890300	1.07746800
C	-1.09468100	-2.19528100	-1.28482800
N	-1.10165300	-3.28571700	-1.68252000

Coordinates for TS **4** → **5-NH₂**

0 2

C	1.23725100	1.07900000	-0.07807200
C	0.81939600	-0.15883500	0.61220900
C	-0.72481700	-0.13238000	0.98088400
N	1.61858000	-0.31787600	1.81014800
H	1.48869100	-1.26256800	2.16339400
H	2.60228600	-0.20508600	1.58556900
N	-1.28912000	-0.96292800	-0.04984900
H	-2.21492700	-1.35507700	0.04070400
N	1.57076100	2.03025900	-0.63502000
C	-0.25123800	-1.65696500	-0.63814700
H	-0.47493500	-2.47096200	-1.31930000
N	0.93585100	-1.27691700	-0.35964900
C	-1.37424900	1.14488600	1.16459600
N	-1.92552300	2.13566400	1.37968700

H	-0.78593000	-0.72421000	2.06115500
N	-0.82553700	-1.28705300	3.36956600
H	-0.21145800	-0.62242500	3.85551100
H	-1.76744600	-1.01467200	3.67599400

Coordinates for TS **5** → **6**

0 2

C	1.09811300	1.37189700	-0.09001900
C	0.81988300	-0.04691100	0.25579100
C	-0.69026600	-0.30664000	0.70469900
N	1.68506200	-0.38476100	1.37914000
H	1.63944100	-1.38848400	1.53754100
H	2.64800800	-0.16600300	1.14061500
N	-0.95015700	-1.57432000	0.01718400
H	-1.90396200	-1.85074600	-0.16761000
N	1.50297100	2.45941800	-0.05645400
C	0.02223900	-1.71722600	-0.95647600
H	-0.07210100	-2.51911000	-1.68137900
N	1.02263400	-0.92480100	-0.91637600
C	-1.66352300	0.72249000	0.33193100
N	-2.47882500	1.49046000	0.05963700
H	-0.69904700	-0.41518900	1.79066400
H	0.20472600	1.33839200	-1.79634700

Coordinates for TS **6** → **7**

0 2

C	1.01699800	1.28153000	-0.81915700
C	0.80238800	-0.30862200	0.36499500
C	-0.73187500	-0.36951300	0.64078500
N	1.63938200	-0.15877900	1.46960300
H	2.57594800	-0.47273200	1.24053900
H	1.68225900	0.80678900	1.78426700
N	-1.15556800	-1.12192500	-0.54533900
H	-2.06479500	-1.55987600	-0.57686100
N	1.62415800	2.18842100	-0.35293600
C	-0.02784600	-1.76237100	-1.01382300
H	-0.11140500	-2.52104800	-1.78260100
N	1.09472000	-1.36144900	-0.51921800
C	-1.44979600	0.89161700	0.81240700
N	-2.05117000	1.85853700	0.98778200
H	-0.86740900	-0.95996100	1.56048900
H	0.51704600	0.97215100	-1.73183900

Coordinates for TS **7** → **AICN**

0 2

C	-0.63254600	-0.68941300	-0.02459800
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C	0.43601400	0.20837900	0.22389200
N	-0.57998200	-2.04720100	-0.05516200
H	0.19345200	-2.50385200	0.40222300
H	-1.46950800	-2.51838000	0.00232600
N	-0.14018600	1.46963300	-0.00243200
H	0.31597800	2.34969300	0.17902900
C	-1.46121600	1.27202100	-0.19828500
H	-2.15660600	2.08860300	-0.31855200
N	-1.78800300	-0.00822900	-0.23272800
C	1.82212800	-0.03075600	0.08624200
N	2.95267700	-0.25379900	-0.01802600
H	0.43497600	0.09848500	2.10107600

Coordinates for TS **7** → **8**

0 2

C	-0.82086200	-0.80354400	0.46322800
C	0.31038800	0.23738900	0.82488300
N	-0.36528700	-2.04570900	-0.07183500
H	-0.06478900	-2.69596900	0.64536800
H	-1.09020400	-2.46631200	-0.64084500
N	-0.37617600	1.48421800	0.44824100
H	0.16978300	2.30978500	0.24508700
C	-1.42331700	1.12394600	-0.38174800
H	-1.96492300	1.89521000	-0.91902200
N	-1.73166100	-0.11640300	-0.42410900
C	1.56477100	0.05658100	0.08240700
N	2.56412700	-0.02912900	-0.48558300
H	0.52604200	0.20688100	1.89498000
H	-1.35968600	-0.96052500	1.51075900
N	-1.83935400	-1.13415300	2.96372500
H	-2.31779700	-0.23044600	3.07100700
H	-2.61631900	-1.77656800	2.76215700

Coordinates for TS **8** → **9**

0 2

C	-0.66849200	-0.86900000	0.45798200
C	0.35522100	0.31488100	0.68247600
N	-0.03263000	-2.10478100	0.09662900
H	-0.71078600	-2.85841500	0.11488300
H	0.34040700	-2.05343500	-0.84709200
N	-0.46529900	1.45661600	0.27080500
H	0.00351800	2.30448300	-0.01865100
C	-1.47524600	0.93301000	-0.53679000
H	-2.07645600	1.61714800	-1.12804600
N	-1.66414800	-0.32445300	-0.49476600
C	1.57079100	0.17483400	-0.16198800

N	2.36172700	-0.18629100	-0.93494100
H	0.66003300	0.38175900	1.72569500
H	-1.18382400	-1.02469200	1.41219300
H	2.36899900	1.79177600	0.40563500

Coordinates for TS **9** → **10**

0 2

C	-0.56610300	-0.77195400	0.56101500
C	0.24182100	0.51915700	0.70492500
N	0.23315900	-1.93279300	0.19460500
H	-0.30201400	-2.77807000	0.36657600
H	0.40432400	-1.90630300	-0.80779400
N	-0.55890500	1.49274000	0.10313000
H	-0.15438300	2.35884600	-0.22928900
C	-1.54159900	0.82279100	-0.62036800
H	-2.17959700	1.37940400	-1.29812100
N	-1.63618700	-0.43268100	-0.40815500
C	2.03226800	0.38122300	-0.39504000
N	2.26372500	1.32264200	-1.06278400
H	0.73474500	0.77308400	1.63685100
H	-1.04402700	-1.00344500	1.52412900
H	2.30984100	-0.59387000	-0.02244700

Coordinates for TS **10** → **11**

0 2

C	-0.34852700	-0.74043600	0.12778100
C	0.03589300	0.26542300	1.03450500
N	0.25997300	-1.99542700	-0.05738000
H	0.32974000	-2.51833500	0.80709900
H	-0.28014100	-2.53333200	-0.72534800
N	-0.54438800	1.41651200	0.54638100
H	-0.54626000	2.31535100	1.00031600
C	-1.12919400	1.11011100	-0.64920100
H	-1.62953600	1.85485700	-1.25003400
N	-0.99469700	-0.15021000	-0.96007100
H	0.52734000	0.21932500	1.99042600
H	-1.73559900	-1.15759000	1.02148600

Coordinates for TS **AICN-NH₂** → **12**

0 2

C	0.19173300	-0.75099200	-0.78087500
C	0.26827700	0.40319600	0.02026800
C	1.36169800	1.21122300	0.35576100
C	-1.79616100	-0.37539000	-0.05743400
H	-2.85487100	-0.44891800	0.14168100
N	1.16281000	-1.34586800	-1.51343700

N	-1.03544500	0.62463000	0.45490800
N	-1.10578800	-1.21150000	-0.79556400
N	2.28766900	1.85645700	0.62293100
H	1.12195600	-2.53874500	-1.63088800
H	-1.34135600	1.39098200	1.03372000
H	2.09269500	-1.00484100	-1.28431200
N	1.10812500	-3.81092800	-1.30206700
H	1.85221200	-4.04940600	-0.64196900
H	0.23186900	-3.96338000	-0.79596400

Coordinates for TS **12** → **13**

0 2

C	0.32015600	-1.38850600	0.36354500
C	0.06824900	-0.01233500	0.18974900
C	0.91224100	1.09728200	0.34058400
C	2.90331800	-1.76563300	-0.42449500
C	-1.73797200	-1.21500000	-0.22460400
H	3.29809800	-0.79619100	-0.17149600
H	-2.76269700	-1.43113700	-0.48757300
N	3.00638400	-2.72719900	-1.10825600
N	1.48910500	-1.93814900	0.76949100
N	-1.25659200	0.06215700	-0.19353500
N	-0.82969700	-2.10126500	0.08992400
N	1.62990500	1.99824200	0.46575500
H	1.38479400	-2.95319500	0.79926600
H	-1.76105300	0.90905600	-0.40785700

Coordinates for TS **13** → **14**

0 2

C	-0.48833300	-0.58150400	0.77422400
C	0.19880000	0.21056400	1.67068800
C	1.58842300	0.29488500	1.96890400
C	1.48097500	-1.65970300	0.00444800
C	-1.97754100	0.59581300	1.71997900
H	1.87818000	-2.41246600	-0.68370300
H	-2.92097400	1.03175900	2.00945400
N	2.32916500	-1.05624500	0.73697500
N	0.11642900	-1.50072300	-0.04921600
N	-0.80048800	0.96960900	2.27440200
N	-1.82686700	-0.34556800	0.80356800
N	2.40286400	0.84360200	2.64152300
H	-0.64980000	1.66341900	2.99017500
H	-0.45005800	-2.04464300	-0.67983900

Coordinates for TS **14** → **15**

0 2

C	-0.63350300	-0.58012500	0.09973800
C	-0.25083000	0.73263300	-0.03146200
C	1.12987700	1.17568600	0.00811200
C	1.63676400	-1.11194100	0.32172500
C	-2.43516800	0.48783800	-0.14987200
H	2.37259000	-1.89839700	0.46958100
H	-3.47574100	0.75289100	-0.25154200
N	2.04858800	0.10566500	0.20265400
N	0.33854300	-1.54404300	0.28206200
N	-1.43611700	1.41311400	-0.19301000
N	-1.98047700	-0.74343500	0.02766200
N	1.43326400	2.40865800	-0.11762000
H	0.09531400	-2.51710000	0.38484800
H	-1.51340400	2.41154000	-0.31543200
H	2.60890900	2.64809400	0.00080100
N	3.90210600	2.54250400	-0.03882100
H	4.05664500	1.60320000	0.34033000
H	4.08455500	2.42603500	-1.04151400

Coordinates for TS **15** → **16**

0 2

C	1.38419500	-0.87044300	0.23253100
C	0.83778900	0.37536100	-0.02274900
C	-0.58195000	0.60946500	-0.02360300
C	-0.76308500	-1.68461900	0.42225400
C	3.03430600	0.41780600	-0.08379800
H	-1.39434700	-2.55584400	0.57868000
H	4.03003700	0.81736500	-0.20042800
N	-1.34849400	-0.54290800	0.20731600
N	0.57774400	-1.93583200	0.51223900
N	1.91788100	1.19768700	-0.21700500
N	2.75209900	-0.84032200	0.19123200
N	-1.07235000	1.78458400	-0.23361800
H	0.97611100	-3.05485600	0.41806000
H	1.86344100	2.18635700	-0.40969500
H	-2.09174200	1.72463500	-0.19796500
N	1.45299800	-4.22596900	-0.03545900
H	0.93727600	-4.69716000	-0.78049700
H	2.41608600	-4.12896200	-0.36348500

Coordinates for TS **16** → **17-NH₂**

0 2

C	-0.65404000	-0.75602500	0.12494100
C	-0.12179600	0.54385600	-0.01343200
C	1.27115000	0.70274700	-0.14440900
C	1.42615900	-1.58674400	0.05175600

C	-2.29498100	0.59556800	0.20320200
H	2.08361400	-2.45014700	0.07768600
H	-3.28474600	1.02128400	0.28297900
N	2.03807000	-0.40302200	-0.06554300
N	0.11586600	-1.84691000	0.15371400
N	-1.18779200	1.39677600	0.04408300
N	-2.02849600	-0.68613400	0.24859700
N	1.83162300	1.90577900	-0.41758900
H	-1.09015100	2.41465600	0.08437500
H	2.84120100	1.89416100	-0.29547600
H	1.20797100	2.82742900	-0.05233600
N	0.40807200	3.77847700	0.54980900
H	0.56261200	3.80870700	1.55985700
H	0.74659800	4.67858800	0.20251100

Coordinates for TS **17** → **18**

0 2

C	0.73735400	-0.80147000	0.03936300
C	0.18915600	0.49139600	-0.04370700
C	-1.21540000	0.63384500	-0.15789100
C	-1.32427400	-1.67213700	0.01619500
C	2.38567900	0.54665500	-0.00499100
H	-1.96929200	-2.54498300	0.05198800
H	3.37765500	0.97474100	-0.00599000
N	-1.95918300	-0.49486100	-0.03588300
N	-0.01280800	-1.91118900	0.06621400
N	1.26478200	1.34665800	-0.07594000
N	2.11773400	-0.72890400	0.07428600
N	-1.84454200	1.87943700	-0.01978400
H	1.24471100	2.34474000	-0.21215600
H	-2.84775300	1.76026500	0.05519800
H	-1.48713700	2.42242100	0.75647600
H	-1.13058000	0.60790100	-1.86412400

Coordinates for TS **18** → **19**

0 2

C	0.68452300	-0.91189500	0.04898200
C	0.40488700	0.37372300	-0.45420500
C	-0.92807700	0.71738400	-0.78238000
C	-1.47669600	-1.45838500	-0.19574500
C	2.52942000	0.14627100	0.06653800
H	-2.26285700	-2.20201700	-0.10507100
H	3.56647100	0.42602600	0.18302800
N	-1.85680300	-0.27848700	-0.69463600
N	-0.25451600	-1.85450700	0.18442200
N	1.60110000	1.03972200	-0.42997100

N	2.02948400	-1.02352500	0.35734900
N	-1.43202100	1.93340200	0.76898700
H	1.76030500	2.00536200	-0.67111700
H	-1.15790300	1.53834900	-1.45038200
H	-2.44795100	1.83977700	0.64839000
H	-1.23812900	1.29677700	1.55205000

Coordinates for TS DAMN → **20**

0 2

C	-0.68214500	0.35046000	-0.00315200
C	-1.37311700	-0.89732400	0.00098000
N	-2.00392100	-1.86724400	-0.00905900
C	0.69423600	0.41673600	-0.05823500
C	1.50348400	-0.75223100	0.09166300
N	2.19181300	-1.66977400	0.22126900
N	-1.39370200	1.56912800	-0.26732500
H	-1.78119200	1.56625400	-1.20786600
H	-2.15914800	1.69499100	0.38624400
N	1.34263300	1.59573300	-0.25562400
H	2.31214400	1.67901700	0.00259700
H	0.75298400	2.41736400	-0.21717600
H	-0.88105900	0.59405400	2.06417300

Coordinates for TS **20** → **21**

0 2

C	0.49534100	-0.80447300	-0.30511500
C	0.24583400	-2.20144900	-0.31887300
N	0.09174200	-3.34759800	-0.31195700
C	-0.51945200	0.12810500	-0.11296800
C	-1.87641000	-0.25279900	0.08466600
N	-2.99246400	-0.52007500	0.22990700
N	-0.20324400	1.45538000	-0.03785100
H	-0.92905000	2.09667600	0.24181100
H	0.71627300	1.62847200	0.35699300
H	1.39333000	-0.47477500	-0.80818000
N	1.69280400	-0.27534400	1.47853400
H	1.09092900	-0.72439900	2.17862400
H	2.44620400	-0.96044800	1.34713000

Coordinates for TS **21-NH₂** → **22**

0 2

C	0.43624700	-0.54421800	0.21574500
H	0.23272200	-1.57137500	0.48470000
C	1.77732100	-0.11907500	0.14376100
N	2.87099600	0.26099800	0.08546600
C	-0.60141300	0.31422700	-0.08050300

C	-1.94567300	-0.18605400	0.08146300
N	-3.02323200	-0.56463400	0.24338400
N	-0.50298900	1.57442200	-0.54781800
H	-1.34290300	2.42266000	-0.25210300
H	0.45531900	1.91886800	-0.55713600
N	-2.03764000	3.24562100	0.44307100
H	-2.65792300	2.77390700	1.10411000
H	-1.48140700	3.91105600	0.98268400

Coordinates for TS **22** → **23**

0 2

C	-1.22141900	-1.01154500	0.01780600
H	-1.13637800	-2.02360900	0.39082600
C	-2.51063100	-0.47627000	-0.15857400
N	-3.56894900	-0.02333000	-0.29441300
N	-0.13239700	1.00209700	-0.71363600
H	0.79945900	1.39700800	-0.83172800
C	-0.08338100	-0.27149100	-0.24454100
C	1.19592900	-0.89526700	-0.02934100
N	2.23767800	-1.37064100	0.11710800
C	-0.90195100	2.28363500	0.38461400
H	-1.95411700	2.19592900	0.17177200
N	-0.04226300	2.83232600	0.98745000

Coordinates for TS **23** → **24-NH₂**

0 2

C	0.31340800	-1.50972600	-0.17398800
C	-0.53577500	1.50921900	0.07648000
H	0.84964500	-2.38308400	-0.52384500
C	-1.08329700	-1.66272200	-0.01971000
N	-2.20514200	-1.88934000	0.14598500
N	-1.30806200	1.06332000	-0.81700600
H	-2.12719700	1.92642000	-0.94823100
N	0.58734500	0.83234500	0.55801400
C	1.04641400	-0.41604100	0.15074900
C	2.47796400	-0.52250400	0.10495100
N	3.63128500	-0.57839300	0.10063300
H	-0.67155100	2.48499300	0.55425900
H	1.25006800	1.39825700	1.06681400
N	-2.97718300	2.92202300	-0.94220600
H	-3.12582000	3.06648700	-1.94721400
H	-3.83491200	2.44921400	-0.63612000

Coordinates for TS **24-OH** → **25**

0 2

C	-0.01604600	-1.11968300	-0.40518900
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C	-0.89942000	1.75556000	0.58992700
H	0.50560400	-1.83033700	-1.03399900
C	-1.38043500	-1.38886000	-0.14643200
N	-2.47310000	-1.69305200	0.07742100
N	-1.67329500	1.45291600	-0.41881400
H	-2.47906300	2.07457400	-0.42895200
N	0.18833600	0.94611800	0.91178900
C	0.68963500	-0.08865300	0.11498000
C	2.10544400	-0.04121200	-0.11579700
N	3.24918400	0.01787100	-0.26438000
H	0.87435600	1.40199700	1.49675200
H	-1.16276800	2.42592000	1.40468400
O	-0.20820600	3.32499000	-0.40548600
H	-0.04271800	2.93390200	-1.27972700

Coordinates for TS **25** → **26**

0 2

C	0.30830900	-0.93831400	0.45572600
C	-0.93890300	1.56609800	-0.45982600
H	0.84872700	-1.82878200	0.74359500
C	-1.11228900	-1.04678000	0.36507700
N	-2.12619900	-1.64278300	0.23520800
N	-1.65334300	0.87912300	0.57804200
H	-2.64095800	0.80055800	0.32456900
N	0.47315500	1.40980700	-0.20536800
C	0.99827200	0.19057000	0.14899700
C	2.43225000	0.15435200	0.21605300
N	3.58562100	0.14401500	0.25207300
H	1.08749000	2.04361800	-0.69268900
O	-1.17295200	1.14965500	-1.79907500
H	-2.11883500	1.19245400	-1.98235300
H	-1.17423500	2.63897600	-0.35099200

Coordinates for TS **26** → **27-NH₂**

0 2

C	-1.06477900	1.40820000	0.03140300
C	0.46847800	-0.96916500	0.37546100
H	-1.63644700	2.32212800	0.03958600
C	0.39393500	1.48772400	-0.01045400
N	0.96571300	2.63992300	-0.04334400
N	1.06136800	0.27228700	-0.07197800
H	2.07023500	0.35301300	0.06000400
N	-0.92793800	-0.98769500	-0.05120000
C	-1.65553800	0.19267500	-0.00012500
C	-3.08089000	0.05851800	-0.02595500
N	-4.22771400	-0.07382300	-0.04055900

H	-1.41876800	-1.83082700	0.21142100
O	1.15132600	-2.05965100	-0.15764300
H	1.14347200	-1.95057900	-1.11887100
H	0.54751700	-1.10479800	1.46442800
H	2.12132800	2.48163400	-0.03186900
N	3.39461600	1.97272400	0.03896600
H	3.77278700	2.39927100	-0.81284000
H	3.74248800	2.56697700	0.79798100

Coordinates for TS **27** → **28**

0 2

C	0.28755000	-0.34197000	1.31676800
C	-1.36303100	1.57356200	0.03657100
H	0.87629900	-0.99980100	1.93826000
C	-1.05046100	-0.74050500	0.90525800
N	-1.65130200	-1.83296200	1.21010400
N	-1.69455000	0.16523500	0.05822100
H	-2.68288300	-0.02655600	-0.04634300
N	0.09491400	1.68892100	0.04419500
C	0.78706200	0.88447500	0.93846100
C	2.17686900	1.20365400	1.12679200
N	3.29506900	1.46113300	1.24656000
H	0.40488800	2.65079400	-0.00165200
O	-1.88689400	2.18537200	-1.09701400
H	-1.56156900	1.68488900	-1.85852300
H	-1.04934300	-2.42530300	1.77881000
H	-1.79664500	2.12903400	0.88243800
H	0.37687600	1.70055500	2.63343700

Coordinates for TS **28** → **29**

0 2

C	-0.63755000	1.64548500	-0.32175700
C	-0.14133200	-1.04346700	0.35365200
H	-0.87994600	2.68112300	-0.51180600
C	0.53335100	1.30667700	0.29063000
N	1.42353600	2.20164900	0.81158100
N	0.89727000	-0.02997300	0.46119200
H	1.49626200	-0.17949300	1.26435600
N	-0.96303000	-0.72569800	-0.80233100
C	-1.62357800	0.58771000	-0.75027500
C	-2.16251400	0.89521200	-2.08863700
N	-2.60948500	1.14665000	-3.12051600
H	-1.64625400	-1.46637900	-0.91942100
O	0.42383300	-2.30723600	0.18845900
H	0.92854500	-2.26794500	-0.63597200
H	1.20016100	3.15782700	0.55551600

H	-0.71804100	-1.11862000	1.29056800
H	2.54933400	1.94946600	0.63922700
N	3.75405100	1.69193200	0.03080800
H	3.60382500	0.96640800	-0.67598000
H	4.05485300	2.51247100	-0.50288600
H	-2.49534200	0.58833900	-0.06884000

Coordinates for TS **29** → **30**

0 2

C	-0.44039900	-1.35338400	0.20519100
C	-0.05027500	1.39887400	0.29709400
C	-1.48598900	-0.53859600	-0.01404100
N	-2.78997200	-0.95031200	-0.28821100
N	-1.37420200	0.86018300	0.03791600
H	-2.09633500	1.27695200	0.61396500
N	0.69673100	0.55695700	1.19891500
C	0.85897600	-0.82727200	0.75130000
C	2.02466300	-1.02735200	-0.18558600
N	3.11749300	-1.20121600	-0.54616200
H	1.59247500	0.97807400	1.41708300
O	0.66042500	1.55854100	-0.92166900
H	0.01704000	1.78021900	-1.60403600
H	-3.21286200	-0.45739200	-1.06541000
H	-0.52042500	-2.41715400	0.02689400
H	-2.89408900	-1.95130900	-0.37768300
H	-0.17918700	2.37117100	0.78577300
H	1.14050900	-1.41111000	1.63635500
H	1.01218400	-1.10097700	-1.78277900

Coordinates for TS **30** → **31**

0 2

C	-0.41801300	-1.33076600	0.28257000
C	-0.06870600	1.43346300	0.25855900
C	-1.47609900	-0.53945400	-0.01354500
N	-2.76141900	-0.97352700	-0.32991500
N	-1.38485100	0.86422500	0.04130200
H	-2.10875000	1.27750800	0.61850400
N	0.74173900	0.60770700	1.10944300
C	0.81729900	-0.76807700	0.78694700
C	2.15000300	-1.06663500	-0.68215900
N	2.90934700	-1.97254800	-0.57301300
H	1.62895500	1.03255600	1.34453700
O	0.59239400	1.61654800	-0.99692000
H	-0.07211000	1.93077700	-1.62170200
H	-3.17172500	-0.49552400	-1.12342500
H	-0.46968800	-2.39986100	0.12470800

H	-2.85048200	-1.97696900	-0.40634200
H	-0.20041600	2.40609200	0.74386200
H	1.36075700	-1.34620900	1.52534100
H	1.86471300	-0.23713200	-1.32237900

Coordinates for TS **31** → **32**

0 2

C	0.29740300	1.56380300	0.30544500
C	-0.97419300	-0.92644200	-0.06118300
C	0.99552500	0.30432200	0.67486800
N	1.97913100	-0.09831500	-0.35026900
N	0.03208000	-0.73960900	0.96537600
H	0.49237100	-1.62196800	1.15750400
N	-1.69351900	0.33441000	-0.19371900
C	-0.97629000	1.51054600	-0.12005200
H	-2.43691700	0.30798600	-0.87526700
O	-0.46054500	-1.40102100	-1.29535700
H	0.40720100	-0.97500400	-1.41625000
H	2.48585800	0.71193800	-0.69529200
H	0.82155100	2.50813200	0.36921100
H	2.66551400	-0.73786800	0.04635600
H	-1.68564500	-1.68525600	0.26912200
H	-1.52204000	2.40435900	-0.40208000
H	1.61705700	0.43070100	1.70836900
N	2.37552900	0.40247700	2.96032500
H	2.50900200	1.41503500	3.07430300
H	1.57660500	0.20917800	3.57649800

Coordinates for TS **32** → **33**

0 2

C	0.42669900	1.08700200	-0.37510100
C	-1.00198000	-0.96528200	0.85534100
C	1.19910500	0.12453000	0.48785700
N	2.06467500	-0.83506300	-0.22351000
N	0.28797000	-0.59159800	1.38270500
H	0.76147900	-1.40080500	1.76998300
N	-1.67884100	0.22578300	0.36799800
C	-0.91273900	1.08780800	-0.40364500
H	-2.59823100	0.01727400	-0.00038300
O	-0.79657400	-1.92609400	-0.15214400
H	-1.80953700	-2.09478300	-0.62567600
H	1.49271600	-1.32320400	-0.90937800
H	0.98901600	1.80508100	-0.95804000
H	2.79560200	-0.33683600	-0.72499600
H	-1.60473400	-1.38401200	1.66905400
H	-1.47276200	1.79017000	-1.01118100

H	1.87090500	0.70250200	1.13741900
N	-3.00193900	-2.28795000	-1.14923700
H	-2.82401800	-2.39276900	-2.15276300
H	-3.29584100	-3.22137200	-0.84666100

Coordinates for TS **33** → **34**

0 2

C	0.70216600	1.31423500	-0.10382700
C	-1.25680900	-0.71763900	0.24574800
C	1.17487400	-0.02414100	0.41240500
N	2.36928500	-0.56765200	-0.23523800
N	0.11122000	-1.00853700	0.20712200
H	0.32548600	-1.93837300	0.54006400
N	-1.54596500	0.54964500	-0.31722000
C	-0.57685200	1.53116900	-0.43073300
H	-2.52529000	0.77622000	-0.37857800
O	-2.12548400	-1.61312500	0.27993100
H	2.27857500	-0.48278100	-1.24414200
H	1.43364800	2.10584500	-0.19878100
H	3.19435400	-0.05034200	0.05077100
H	-1.43796300	-0.36203900	1.70024600
H	-0.92639500	2.48513900	-0.80700800
H	1.43317400	0.05917700	1.48123100

Coordinates for TS **34** → **35**

0 2

C	0.76014200	1.18303600	-0.21362400
C	-1.03635000	-0.95754900	0.26413600
C	1.31964800	-0.15293000	0.24964900
N	2.53076200	-0.60383100	-0.43008500
N	0.30515500	-1.18099000	0.05306900
H	0.66070400	-2.41194100	0.30491300
N	-1.44327100	0.36607500	0.09364000
C	-0.55836300	1.37904500	-0.25713200
H	-2.44014500	0.50856200	0.07247000
O	-1.85200600	-1.83335900	0.51273000
H	2.37895400	-0.59705700	-1.43515000
H	1.45649900	1.97337400	-0.46105600
H	3.30355900	0.02180600	-0.22601300
H	-1.01162000	2.31888200	-0.54735400
H	1.58960000	-0.06929200	1.31722000
N	0.67836400	-3.38566100	0.99901800
H	1.20694200	-3.19933500	1.85281500
H	-0.29911200	-3.52237100	1.26853800

Coordinates for TS **35** → **36**

0 2

C	1.02567700	1.23848400	0.17786000
C	-1.16724900	-0.53061000	-0.12779600
C	1.14855700	-0.21700600	0.11138600
N	2.40361500	-0.76076000	-0.06658100
N	0.11096600	-1.02447000	-0.16659400
N	-1.28981300	0.88555800	0.03706000
C	-0.23245100	1.73230600	0.13664700
H	-2.23594300	1.23510700	-0.00464500
O	-2.18026200	-1.18440700	-0.26160500
H	2.40997500	-1.69940100	-0.43463700
H	1.88992000	1.87347100	0.30658600
H	3.15985500	-0.15668700	-0.34019300
H	-0.45403600	2.79117200	0.18891100
H	0.98898900	-0.31008000	1.70754400

Coordinates for TS **35** → **37**

0 2

C	1.08184500	1.25402800	0.69547500
C	-0.91461500	-0.50563300	-0.25808500
C	1.15631100	-0.18790400	0.82802100
N	2.38935100	-0.76889900	-0.62634300
N	0.15281000	-1.00731000	0.47565400
N	-0.97233400	0.90143500	-0.39060400
C	-0.01289900	1.75235000	0.08456500
H	-1.80133300	1.25480700	-0.84596000
O	-1.78947000	-1.19073300	-0.74559700
H	2.22217500	-1.78207600	-0.62066300
H	1.87285000	1.88838200	1.06585800
H	1.90927300	-0.44446600	-1.47416300
H	-0.19499100	2.81099700	-0.05468700
H	1.83398000	-0.58713200	1.57556700

Coordinates for TS **37-OH** → **38**

0 2

C	0.59607000	1.78200000	-0.07598700
C	-1.33211600	-0.24577700	0.19452900
C	0.75940700	0.62227100	0.72797900
N	-0.11924400	-0.33542400	0.86611200
N	-1.52883200	0.93287700	-0.58678300
C	-0.60096500	1.88961600	-0.76624300
H	-2.41061500	0.97145700	-1.08065800
O	-2.20994700	-1.07532400	0.23490500
H	1.35053400	2.54839000	-0.14205300
H	1.68679700	0.50107800	1.28586500
H	-0.88018400	2.75580900	-1.34614700

O	0.77823200	1.48354200	-2.47737200
H	0.98355900	0.54672000	-2.32422400

Coordinates for TS **38** → **39**

0 2

C	-1.49057000	1.18916800	0.21924100
C	1.13186200	0.14463700	0.29232600
C	-0.33050000	1.79400200	-0.46072400
N	0.86655400	1.33730500	-0.44169600
N	0.05177600	-0.50834900	0.88311000
C	-1.30638300	-0.29642100	0.47566000
H	0.28944400	-1.43511000	1.21056800
O	2.26086200	-0.26048200	0.43282600
H	-1.56143700	1.78885000	1.31540200
H	-0.49108400	2.72677900	-1.00407500
H	-1.96957700	-0.63944600	1.27895800
O	-1.55205600	-1.07415500	-0.70211200
H	-2.49762400	-1.06015100	-0.88852100
H	-2.44750800	1.43676600	-0.24383800
N	-1.62286000	2.18850000	2.64587500
H	-2.42312100	1.64869600	2.99766800
H	-0.80806200	1.68340000	3.01572800

Coordinates for TS **39** → **40**

0 2

C	-1.65402500	1.14911300	0.16703600
C	0.94671200	0.00309800	0.27805700
C	-0.40794700	1.76609400	-0.40771300
N	0.76162700	1.26513700	-0.36685800
N	-0.18547700	-0.67802000	0.70583800
C	-1.51745300	-0.37487900	0.23365700
H	0.00406300	-1.63640700	0.96681800
O	2.05495900	-0.43371900	0.47685100
H	-1.80867900	1.55665400	1.17480400
H	-0.50823600	2.73845300	-0.89530500
H	-2.23617500	-0.79156400	0.95135900
O	-1.66066600	-0.99691900	-1.02011000
H	-2.70294000	-0.71502800	-1.54312400
H	-2.52579900	1.43006000	-0.42913200
N	-3.87901500	-0.85125800	-1.83085300
H	-3.96030900	-1.76960000	-2.27290000
H	-4.44451600	-0.90786900	-0.98119500

Coordinates for TS **40** → **41**

0 2

C	1.51066000	0.69317800	-0.07000300
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C	-1.23237000	-0.09363000	-0.02088500
C	0.33864800	1.59251100	-0.34257400
N	-0.88972200	1.25546000	-0.32823900
N	-0.19172200	-1.03053200	0.00465200
C	1.16475500	-0.78297700	-0.25108300
H	-0.46997800	-2.00049100	0.09565300
O	-2.36830000	-0.42326400	0.19728000
H	2.37596500	0.95938800	-0.67760200
H	0.55777100	2.63792400	-0.56623800
H	1.11290700	-0.71385300	-1.90101700
O	2.00338600	-1.68278900	-0.21232800
H	1.81540400	0.81502400	0.97919400

Coordinates for TS **42** → **43a-NH₂**

0 2

N	1.61049100	-0.54467100	0.55582500
C	-0.55342100	-0.28499500	-0.48470000
C	0.68083700	0.18422100	0.10969000
N	-1.53882100	-0.65538900	-0.95898800
H	1.45776200	-1.71556500	0.48541300
H	0.78040500	1.27319400	0.15983200
N	1.01188800	-2.95816700	0.24983300
H	0.06772400	-3.02423400	0.64424100
H	0.86384600	-3.03639600	-0.76187200

Coordinates for TS **43a** → **44a**

0 2

N	0.13939600	1.54805400	-0.44111600
C	1.67179500	-0.77062500	-0.16108300
C	-0.22879300	0.63423800	0.39098100
N	2.69993000	-1.31424100	-0.20775200
H	0.92314000	2.07899400	-0.05317600
H	0.15038100	0.52713400	1.41091100
C	-1.34672900	-0.21907700	0.06978700
N	-2.25231100	-0.90401500	-0.13040700

Coordinates for TS **44a** → **45**

0 2

N	0.01160200	1.73728600	-0.20564200
C	1.19650900	-0.36483500	0.06762600
C	0.00668600	0.47315800	0.06728600
N	2.16780100	-0.98582400	0.03273200
H	0.97041300	2.08833700	-0.26200200
H	-0.00871500	0.44058300	1.94116300
C	-1.25831200	-0.24102500	0.05007300
N	-2.25139400	-0.82442600	0.01506500

Coordinates for TS **45** → **46**

0 2

N	-1.16192400	-0.21424800	1.42601200
C	0.29879200	-1.55534800	0.04656600
C	-0.46481300	-0.34747800	0.37498500
N	0.61273300	-2.64469700	-0.22709000
H	-1.10108300	-1.03512600	2.03217800
C	-0.41272500	0.70526700	-0.61104800
N	-0.36376000	1.52655700	-1.41827600
C	2.44072800	-0.76018200	0.49711400
N	3.41772900	-0.27639700	0.90437800

Coordinates for TS **46** → **47-NH₂**

0 2

N	1.43014900	-1.46182600	-0.41821700
C	-0.89225300	-0.86679100	0.15287500
C	0.58871300	-0.56987100	-0.09913400
N	-1.28444600	-2.06151900	0.03419400
H	0.95189200	-2.36949100	-0.47150400
C	1.02294000	0.80195700	0.04015100
N	1.33944700	1.90459800	0.15887700
C	-1.75847000	0.23723600	0.51208900
N	-2.48278700	1.08864100	0.80030500
H	-2.46224700	-2.32754800	0.22547700
N	-3.71737600	-2.28944200	0.49574700
H	-3.84523800	-1.92579600	1.44477600
H	-4.17373800	-1.60443800	-0.11387900

Coordinates for TS **47** → **48**

0 2

N	1.47663500	-1.47595700	0.00760100
C	-0.79275200	-0.54912100	-0.03477300
C	0.72350700	-0.45359400	-0.00153300
N	-1.30417000	-1.71172600	-0.03812900
H	0.89335800	-2.32146300	-0.01054900
C	1.31070300	0.86562600	0.02410400
N	1.75606600	1.92911300	0.04653800
C	-1.56662400	0.67128200	-0.06320100
N	-2.22193600	1.62095400	-0.08688900
H	-2.32390200	-1.69426900	-0.06222200
H	2.73363700	-2.02585900	1.95637700

Coordinates for TS **48** → **DAMN-NH₂**

0 2

N	1.17938500	-1.70499100	0.02319600
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C	-0.89525700	-0.51489100	0.37767700
C	0.44088200	-0.51582300	0.00724300
N	-1.54108400	-1.59239500	0.88588400
H	0.74876500	-2.47197800	-0.48173200
C	1.12479100	0.68216500	-0.32015500
N	1.73745000	1.62645400	-0.59226100
C	-1.66815700	0.68363300	0.23351100
N	-2.32609700	1.62276000	0.09774500
H	-2.63183100	-1.86285800	0.57360100
H	2.15098700	-1.59647200	-0.22920000
H	-0.93717800	-2.39446400	1.03122500
N	-3.71573300	-2.30774400	-0.13846900
H	-3.93846400	-1.69076400	-0.92352500
H	-3.61593800	-3.24238500	-0.54141800

Coordinates for TS **42** → **43b**

0 2

H	-2.07398600	0.63792900	0.00000000
N	0.03953400	1.87238900	0.00000000
C	-0.06117200	-0.64888700	0.00000000
C	-0.19934000	0.72965500	0.00000000
N	0.05962600	-1.79739100	0.00000000

Coordinates for TS **43b** → **44b**

0 2

N	0.28076300	-1.77577000	0.00000000
C	1.64169100	0.53877400	0.00000000
C	-0.23397800	-0.72340800	0.00000000
N	2.57721900	1.23025600	0.00000000
C	-1.18840000	0.27936600	0.00000000
N	-2.00150000	1.09874500	0.00000000

Coordinates for TS **44b** → **45-NH₂**

0 2

N	-0.14686800	1.84545800	-0.51599200
C	-1.31802200	0.01915700	0.54602600
C	-0.16322000	0.66621500	-0.05195000
N	-2.25486100	-0.46434300	1.01518000
H	-1.17634400	2.48431200	-0.45260700
C	1.04192200	-0.13963500	-0.09878800
N	1.99879700	-0.78216400	-0.13517000
N	-2.39184800	2.90164500	-0.26449800
H	-3.03991900	2.28599400	-0.76520900
H	-2.63819200	2.79625800	0.72433200