Supporting Information

Ultimate Carcinogenic Metabolites from Aromatic and Heterocyclic Aromatic Amines: A Computational Study in Relation to Their Mutagenic Potency

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Table S1. Cartesian coordinates of the optimized structure for the acetic ester of **1**
Charge = 0 Multiplicity = 1

C,0,-3.0855421021,-0.5784918781,-1.3769770251
C,0,-3.0549000927,-0.6422372788,0.0194211749
C,0,-1.8816255675,-0.5209704772,-2.0847004064
H,0,-4.0347407432,-0.5708431123,-1.9054228317
C,0,-1.8378263368,-0.6416049851,0.7014007678
C,0,-0.6561509602,-0.5357445876,-1.4153140455
H,0,-3.9820948552,-0.6799822784,0.5855275693
H,0,-1.8913882229,-0.4702130422,-3.1706286419
C,0,-0.6327024733,-0.5930358908,-0.0154935276
H,0,-1.8209658399,-0.6811802179,1.7884945318
H,0,0.2756121939,-0.5025698845,-1.9692455015
N,0,0.5827536813,-0.7137904916,0.7096356879
O,0,1.6427598036,0.022076744,0.0632911787
H,0,0.5168217567,-0.3089572633,1.6473323944
C,0,2.2618849285,0.9189436609,0.875898653
O,0,1.9183465588,1.1153297635,2.0247578595
C,0,3.4221942093,1.5754407984,0.1759932118
H,0,3.3943503078,1.4085798286,-0.9026232924
H,0,3.4077304997,2.6463533548,0.3956468692
H,0,4.3545586042,1.162297826,0.5777039629

Table S2. Cartesian coordinates of the optimized structure for the transition state for **1a**
Imaginary frequency : -155.2893 cm^{-1}
Charge = 0 Multiplicity = 1

C,0,-2.2332764511,-2.2061228953,-1.3273083217
C,0,-0.8483840989,-2.2565832634,-1.0760054869
C,0,-2.952729533,-1.0029939159,-1.2330411992
H,0,-2.7575560298,-3.1200306775,-1.5958177758
C,0,-0.1708827221,-1.1040584408,-0.7251019106
C,0,-2.2893271823,0.1605416581,-0.8820577977
H,0,-0.3207741908,-3.2028570678,-1.1537704105
H,0,-4.0206931294,-0.9934381617,-1.4300004937
C,0,-0.8783276186,0.1436679725,-0.6390496182
H,0,0.8946342352,-1.1081639991,-0.5144624661
H,0,-2.8008277047,1.114213612,-0.7951934335
N,0,-0.2762476521,1.3155579458,-0.4183607288
O,0,0.8096419725,1.1710570246,1.6272666618
H,0,0.7316507429,1.1911974015,-0.2321766043
C,0,2.0510506314,1.1010343829,1.2713226727
O,0,2.4358238529,0.9809544278,0.0826283701
C,0,3.0520538431,1.1784937759,2.4205210144
H,0,2.8307906701,0.4096051018,3.1678911694
H,0,4.0653310395,1.0479834697,2.0330099103
H,0,2.9663901177,2.1526174383,2.9142088351

Table S3. Cartesian coordinates of the optimized structure for the complex for **1a**
Charge = 0 Multiplicity = 1

C,0,-2.0028312092,-0.0892359337,-2.6538608513
C,0,-1.9870225982,0.0834021266,-1.2608586531
C,0,-0.8120220019,-0.1729273354,-3.4200369549
H,0,-2.9594594791,-0.161096015,-3.1667324341
C,0,-0.7815953029,0.2135562211,-0.5928966523
C,0,0.4016247179,-0.083743716,-2.7862975245
H,0,-2.9219513379,0.128504499,-0.7099900752
H,0,-0.8740914013,-0.3164557955,-4.4946073851
C,0,0.4643007447,0.1230281445,-1.3462812669
H,0,-0.731777172,0.3157554488,0.4971062789
H,0,1.346032671,-0.1620671557,-3.3162928626
N,0,1.6456519029,0.2166068856,-0.7971817444
H,0,1.5897506943,0.3251330672,0.2553698991
O,0,1.6208205243,0.2136683834,1.9249061685
C,0,0.6487043978,-0.050486116,2.7032550752
O,0,-0.5284633659,-0.2766110446,2.3009738803
C,0,0.9397892941,-0.1305964532,4.1949189509
H,0,0.0273598069,0.0142263614,4.7803387299
H,0,1.3445515339,-1.1244273838,4.4243672599
H,0,1.6954758425,0.6097384368,4.4760196717

Table S4. Cartesian coordinates of the optimized structure for the nitrenium ion of **1**
Charge = 1 Multiplicity = 1

C,0,-1.5681918025,0.0000523133,-0.827218311
C,0,-1.5599400189,0.0000304527,0.5870244978
C,0,-0.3806366019,0.0000299651,-1.6113079652
H,0,-2.5265134045,0.0000791268,-1.3426298599
C,0,-0.3543749106,-0.0000110555,1.2436507615
C,0,0.8364307401,-0.0000082857,-0.985963078
H,0,-2.4979199193,0.0000458609,1.1330535647
H,0,-0.455330319,0.0000442196,-2.6942518427
C,0,0.8969003747,-0.000024426,0.4795778938
H,0,-0.2713468189,-0.0000281492,2.3268414715
H,0,1.7671522517,-0.0000257031,-1.5485188703
N,0,1.9896892978,-0.0000638525,1.1749478683
H,0,2.8350064401,-0.0000821713,0.586287665

Table S5. Cartesian coordinates of the optimized structure for the sulfuric acid ester of **1**
Charge = 0 Multiplicity = 1

C,0,-2.934390632,-0.6336435082,-2.5606037649
C,0,-2.9098497599,-0.5286005163,-1.1641987761
C,0,-1.7349512677,-0.6935035256,-3.2728116196
H,0,-3.8837885972,-0.6698327386,-3.0878674678
C,0,-1.6971708102,-0.4992482422,-0.4780370612
C,0,-0.5138671574,-0.6318013743,-2.5951842387
H,0,-3.8414511589,-0.4891101375,-0.6059410637
H,0,-1.7444599167,-0.7715717903,-4.3566568457
C,0,-0.4958487525,-0.5444976815,-1.1985924409
H,0,-1.6663886192,-0.4497194445,0.6059229099
H,0,0.4212247997,-0.654375365,-3.1513280163
N,0,0.7437617708,-0.5832251146,-0.4926533105
O,0,0.9739389294,0.7157553908,0.1586422859
H,0,1.5315445547,-0.6432868954,-1.1362632924
S,0,1.3592118021,0.4352002717,1.7491567527
O,0,2.6406668363,-0.2268812962,1.8431343604
O,0,0.1773198922,-0.0402205472,2.4521573248
O,0,1.6079254449,1.9970240294,2.1102137254
H,0,0.7472591652,2.4196162996,2.2975847432

Table S6. Cartesian coordinates of the optimized structure for the transition state for **1c**
Imaginary frequency: -83.1365 cm^{-1}
Charge = 0 Multiplicity = 1

C,0,3.1133040146,0.9425462937,0.3495849227
C,0,2.8467585037,1.3412770841,-0.9887357881
C,0,2.3959760298,-0.0732861252,0.9799802655
H,0,3.9010542,1.4525420514,0.8990171876
C,0,1.8699773891,0.6998161113,-1.7029839662
C,0,1.3686743914,-0.7103743433,0.2930528039
H,0,3.4218871716,2.148624073,-1.4313921918
H,0,2.6083622024,-0.3358929815,2.0111113766
C,0,1.1196911862,-0.3833451319,-1.0996546629
H,0,1.6287315549,0.957966691,-2.7291837781
H,0,0.8088496105,-1.5203799548,0.7475556625
N,0,0.237495307,-0.9940156815,-1.8503797269
H,0,-0.2424520397,-1.7482401369,-1.3503912055
O,0,-1.8772616325,-0.2059210376,-0.953234841
S,0,-1.8472824953,0.0350561274,0.5217219638
O,0,-3.0602502608,0.6470631765,1.0645136136
O,0,-0.5517835446,0.6151692643,0.9781132927
O,0,-1.7451689713,-1.5031036611,1.1948664516
H,0,-2.6429537392,-1.8828732779,1.1968600318

Table S7. Cartesian coordinates of the optimized structure for the complex for **1c**
Charge = 0 Multiplicity = 1

C,0,-3.8478606401,0.0155646404,0.1857603389
C,0,-3.784711205,-0.1484123053,1.5930688887
C,0,-2.7039397403,0.2352250096,-0.601756907
H,0,-4.8194735283,-0.0336543934,-0.300875754
C,0,-2.5652891135,-0.0936471329,2.2185088035
C,0,-1.462229554,0.3179667521,-0.0025664115
H,0,-4.6968371261,-0.3227062136,2.1553269198
H,0,-2.7971706954,0.3418508071,-1.6781374109
C,0,-1.355035519,0.1523198614,1.4443118909
H,0,-2.4483646857,-0.2251252995,3.2898608896
H,0,-0.5562712223,0.4578149523,-0.5956835378
N,0,-0.2310713775,0.2208858583,2.1009986331
H,0,0.5917798327,0.3737920051,1.470916767
O,0,1.9963437435,0.2750806037,0.4733978308
S,0,2.2037170778,0.0147275123,-0.991080589
O,0,3.2040341936,0.9019689505,-1.6014655294
O,0,0.9148549764,-0.1344327131,-1.7119489898
O,0,2.8354443545,-1.5186420959,-1.0729919539
H,0,3.7933403114,-1.4397119769,-0.9109993636

Table S8. Cartesian coordinates of the optimized structure for the charged sulfuric ester **1d**
Charge = -1 Multiplicity = 1

C,0,-2.7510916415,0.2315237003,-2.9004938953
C,0,-2.8377211323,0.3983208421,-1.5125206485
C,0,-1.7011173702,0.3730742177,-0.7055058628
C,0,-0.432714918,0.1758137513,-1.2854726411
C,0,-0.3414540773,0.015718228,-2.6847537368
C,0,-1.4891132246,0.0380728857,-3.4754106157
N,0,0.7143357126,0.0704691372,-0.511376687
O,0,0.6614215522,0.741072008,0.7208871156
S,0,1.3149382547,-0.2823777032,2.0134796459
O,0,2.6696962018,-0.6159335227,1.5146217439
O,0,0.3772773059,-1.4207534782,2.1054090857
O,0,1.2509638314,0.702089647,3.1112650206
H,0,1.5861406274,0.306864689,-0.9764664735
H,0,-3.6447121708,0.2534481668,-3.5197788459
H,0,-3.8094685999,0.5495520986,-1.0457337983
H,0,-1.7674238198,0.4933533044,0.3693897616
H,0,0.6344094158,-0.1354066008,-3.1435400227
H,0,-1.3939044627,-0.08999135,-4.5524274714

Table S9. Cartesian coordinates of the optimized structure for the complex for **1d**
Charge = -1 Multiplicity = 1

C,0,-2.1107512108,-0.5004802295,-3.191758777
C,0,-2.0549786152,-0.3457788697,-1.7984697267
C,0,-0.8361205848,-0.3001777218,-1.1370306491
C,0,0.3973573313,-0.4073233911,-1.8942529708
C,0,0.3006653267,-0.5569270511,-3.3326083894
C,0,-0.9255280654,-0.6059895529,-3.9572684303
N,0,1.5998253784,-0.3834029244,-1.3524416368
O,0,1.5843280752,0.0800587987,1.3875617495
S,0,0.5195964884,0.4570834652,2.4292151092
O,0,-0.8576604421,0.2390416722,1.8201064657
O,0,0.694532828,1.9096991101,2.7636968961
O,0,0.6930777223,-0.4469596289,3.6133182354
H,0,1.5503648854,-0.262361549,-0.3185085058
H,0,-3.0756091035,-0.5387835864,-3.6931064576
H,0,-0.9909845171,-0.7221520262,-5.0368121824
H,0,1.2329642001,-0.6290625265,-3.8856819602
H,0,-0.7928313111,-0.171531561,-0.0510264982
H,0,-2.9743161742,-0.2602824427,-1.2243477979

Table S10. Cartesian coordinates of the optimized structure for the hydroxylamine of **1**
Charge = 0 Multiplicity = 1

C,0,-1.8981797107,0.0990742516,-1.2906330356
C,0,-1.8974020754,0.0938926501,0.1064090445
C,0,-0.6763096449,0.099993406,-1.9728903545
H,0,-2.8346915697,0.1007454633,-1.8411627274
C,0,-0.6984630171,0.0950643557,0.8239638771
C,0,0.5278830311,0.0878382246,-1.2707825149
H,0,-2.8388764739,0.0974256647,0.6502307888
H,0,-0.6582660035,0.0998824692,-3.0599293006
C,0,0.5243059026,0.0896638617,0.1352992518
H,0,-0.7021446407,0.1189725604,1.9085549592
H,0,1.4734740577,0.0838420399,-1.8098143104
N,0,1.7520592917,0.1622371666,0.8248680483
O,0,1.756212027,-0.4328445488,2.1108841868
H,0,2.5325398279,-0.2180053712,0.2935779476
H,0,1.4228466316,-1.3489270998,2.0091952001

Table S11. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **2**
Charge = 0 Multiplicity = 1

C,0,3.18207,-1.02108,0.36849
C,0,2.13422,-1.90278,0.10346
C,0,0.86805,-1.41377,-0.22694

C,0,0.64623,-0.03323,-0.28535
C,0,1.69496,0.87799,-0.02646
C,0,2.95067,0.35599,0.29887
C,0,1.4636,2.36868,-0.10565
N,0,-0.59812,0.51513,-0.70178
O,0,-1.66585,-0.43215,-0.54399
C,0,-2.72404,0.04751,0.16186
O,0,-2.73864,1.15803,0.65493
C,0,-3.84546,-0.95585,0.21303
H,0,4.16911,-1.39608,0.62471
H,0,3.76373,1.04966,0.50302
H,0,0.05423,-2.09741,-0.4391
H,0,2.29498,-2.97686,0.14956
H,0,-0.88275,1.32868,-0.14982
H,0,-4.12656,-1.11815,1.25804
H,0,-4.71607,-0.53761,-0.30362
H,0,-3.56691,-1.90364,-0.25127
H,0,1.0834,2.66778,-1.09131
H,0,0.73358,2.71494,0.64098
H,0,2.39413,2.91498,0.07587

Table S12. Cartesian coordinates of the optimized structure for the complex for **2**
Charge = 0 Multiplicity = 1

C,0,-2.0769488329,-0.1256233058,-2.3979521648
C,0,-2.1208516967,-0.056586317,-0.9938591061
C,0,-0.9487157885,-0.1552652739,-0.274966652
C,0,0.3273372645,-0.285481461,-0.9786948265
C,0,0.3427508755,-0.3312938036,-2.4534883571
C,0,-0.8683847969,-0.2603905079,-3.1143158214
C,0,1.6436413952,-0.4547051476,-3.1804315227
N,0,1.4650600905,-0.3561663831,-0.3523706216
O,0,-0.7805448171,0.6741946046,2.5585231206
C,0,0.3682644656,0.4388527633,3.0295931433
O,0,1.3544759405,0.0364051539,2.331383181
C,0,0.6124707322,0.6791503524,4.5143088315
H,0,-3.0078509883,-0.0756193191,-2.9591447767
H,0,-3.0716957506,0.0600795549,-0.482391749
H,0,-0.9318930328,-0.0738742743,0.8198082294
H,0,-0.8987569257,-0.300238954,-4.1998525962
H,0,1.356671711,-0.280722321,0.7015254418
H,0,1.2908796896,-0.0800942408,4.9165239906
H,0,1.0954909499,1.6563332276,4.6410422675
H,0,-0.3287869304,0.6826244666,5.0710864777
H,0,2.1403046895,-1.3985430947,-2.9255516951
H,0,1.4963375429,-0.4112725484,-4.2631106008
H,0,2.3350477164,0.3377503227,-2.8737521968

Table S13. Cartesian coordinates of the optimized structure for the nitrenium ion of **2**
Charge = 1 Multiplicity = 1

C,0,-1.8891558717,-0.0003996427,-0.8146229797
C,0,-1.8679192966,0.000315332,0.6141130397
C,0,-0.6850709082,0.0007262825,1.3648801646
C,0,0.5537806395,0.0004467644,0.73768744
C,0,0.5664093352,-0.0004487778,-0.7531231282
C,0,-0.706706647,-0.0007582944,-1.4892414925
N,0,1.7232923205,-0.0010201637,-1.3240183666
C,0,1.8310017994,0.0010180536,1.4938541024
H,0,-2.8403221927,-0.0006483647,-1.3372716049
H,0,-2.8184376138,0.000569239,1.143738905
H,0,-0.7428466244,0.0013051541,2.4490127005
H,0,-0.6691392131,-0.0013263977,-2.5760449619
H,0,2.4408279547,-0.8713397167,1.2237397393
H,0,2.440602405,0.8732323029,1.2227649485
H,0,1.6561824951,0.0016037509,2.5713310427
H,0,1.6560522425,-0.0016531273,-2.3504250804

Table S14. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **3**
Charge = 0 Multiplicity = 1

C,0,-3.4688582452,-0.7330144723,1.1807971047
C,0,-3.4760891278,-0.7450969416,2.560327271
C,0,-2.2587349291,-0.6273473706,3.276438169
C,0,-1.0610789244,-0.4995325146,2.6038144126
C,0,-1.0200634779,-0.4829194691,1.1821593633
C,0,-2.2518660739,-0.6033970591,0.4602185749
C,0,-2.2043806876,-0.5872086198,-0.9623179891
C,0,-1.0133818539,-0.4597625231,-1.634733971
C,0,0.2080639408,-0.3345172035,-0.9117750533
C,0,0.2029620504,-0.3508667038,0.4677946283
N,0,1.3906517883,-0.289935875,-1.6947356741
O,0,2.5036215576,0.20045623,-0.9349435125
C,0,3.143233703,1.2522752301,-1.5149234641
O,0,2.7696620223,1.7568167726,-2.5547730085
C,0,4.3606407109,1.6503919679,-0.7244006768
H,0,-3.1330559502,-0.6767732837,-1.5214424333
H,0,-0.9932041948,-0.458461803,-2.7221611665
H,0,1.1327364713,-0.2635040969,1.0192367234
H,0,-0.128225354,-0.4096744807,3.1562977979
H,0,-2.271817606,-0.638308309,4.3634561228
H,0,-4.4133584304,-0.8449610591,3.1013929907
H,0,-4.3998238117,-0.8235223199,0.6248464558
H,0,1.3109773024,0.3442488747,-2.4947244138
H,0,4.3740840994,1.1869489652,0.2640317337
H,0,5.2553594893,1.3415404078,-1.2769057234

H,0,4.3828143148,2.7398082856,-0.6335364178

Table S15. Cartesian coordinates of the optimized structure for the complex for **3**
Charge = 0 Multiplicity = 1

C,0,-3.6681963296,-0.3941884485,-1.438786589
C,0,-3.5756386718,-0.3677976758,-0.0479752411
C,0,-2.5185735094,-0.3622531863,-2.2587468425
H,0,-4.6503315473,-0.4363592063,-1.9029199008
C,0,-2.322579276,-0.3072744981,0.5791551544
C,0,-1.2686995127,-0.3131226617,-1.6759431285
H,0,-4.4785786626,-0.3888298456,0.5566071988
H,0,-2.6241139785,-0.3725640379,-3.3391921171
C,0,-1.1441932649,-0.2909396684,-0.2527410012
C,0,-2.1797665767,-0.2631699625,2.0188721516
H,0,-0.3591089795,-0.2694735986,-2.2691095175
H,0,-3.0846497722,-0.2733843032,2.621527456
C,0,0.1193126675,-0.2714843606,0.3383751678
C,0,-0.9577779656,-0.1944817562,2.6021677007
C,0,0.2575516056,-0.1717356117,1.7850212609
H,0,-0.8297331801,-0.1331673409,3.6783142115
N,0,1.4180494127,-0.0340179491,2.3559701862
H,0,1.0181530836,-0.2558075778,-0.2921356514
H,0,2.1882556209,0.0139507371,1.6376610402
O,0,2.1911902643,0.6090082864,-1.4259326013
C,0,3.2916752841,0.5850774733,-0.7877914121
C,0,4.5481626439,1.0239520146,-1.5373706198
O,0,3.412721604,0.2494908265,0.4258638014
H,0,4.4278779368,0.906636763,-2.6179738975
H,0,4.731040602,2.085121743,-1.3251187131
H,0,5.4158854745,0.4585194606,-1.1843206198

Table S16. Cartesian coordinates of the optimized structure for the nitrenium ion of **3**
Charge = 1 Multiplicity = 1

C,0,-1.750298465,1.3076594667,-0.0000023456
C,0,-2.8460376369,0.4362972013,-0.0000020898
C,0,-2.6876452222,-0.970213087,-0.0000007021
C,0,-1.4209316904,-1.5056149491,0.0000000319
C,0,-0.2717671151,-0.6404019464,0.000001948
C,0,-0.4493734692,0.8030074149,-0.000001258
C,0,0.710051413,1.6720571519,0.000000639
C,0,1.9692440421,1.1732305245,0.0000012728
C,0,2.1810563147,-0.2754691836,-0.0000030307
C,0,1.0080763459,-1.1522181158,0.0000073877
N,0,3.3206576838,-0.8918373449,-0.0000028491
H,0,0.5409862902,2.7453706769,0.0000002273
H,0,2.8383353487,1.8251864383,0.0000028747

H,0,1.2018762846,-2.2222275953,0.0000076626
H,0,-1.2666696904,-2.581203585,0.0000020679
H,0,-3.5621945491,-1.6125341256,-0.0000002127
H,0,-3.8495212899,0.8539144259,-0.0000032458
H,0,-1.9154221472,2.3811197605,-0.0000029958
H,0,4.1137588645,-0.236771446,0.0000024462

Table S17. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **4**
Charge = 0 Multiplicity = 1

C,0,-3.4331557504,0.5444842195,-1.9288924686
C,0,-3.4810580564,0.617434843,-0.5531507338
C,0,-2.1869935139,0.4154512158,-2.5866790639
H,0,-4.34955413,0.5954999537,-2.5111459818
C,0,-2.296591285,0.5541720983,0.2306770746
C,0,-1.0168870644,0.3481694026,-1.8576631823
H,0,-4.4347941145,0.729263151,-0.0420136089
H,0,-2.1498840988,0.3780735959,-3.6722258846
C,0,-1.0369087996,0.4007412977,-0.4366007286
C,0,-2.3362671891,0.6491320105,1.6499328658
H,0,-0.0696471015,0.2801991471,-2.3842012955
H,0,-3.2969454252,0.7710072552,2.1440785786
C,0,0.151952929,0.3105844543,0.364880104
C,0,-1.1712763051,0.5931443977,2.3786189523
C,0,0.0811068596,0.420253659,1.7400517366
H,0,-1.1997857153,0.6722247895,3.4623098651
N,0,1.3786855474,0.1811756975,-0.3403907928
H,0,0.9861808652,0.3683618516,2.3327584854
H,0,1.3862257358,-0.6109755376,-0.9900164037
O,0,2.4679511224,-0.070105616,0.5557904558
C,0,3.2384830427,-1.1308268937,0.1942387176
C,0,4.4322880673,-1.2691649572,1.1003435586
O,0,2.9811539638,-1.834463424,-0.762084564
H,0,4.3350642683,-0.6566767343,1.9989488215
H,0,4.5530573023,-2.3221254066,1.3689238238
H,0,5.3282852842,-0.9579841137,0.551131021

Table S18. Cartesian coordinates of the optimized structure for the complex for **4**
Charge = 0 Multiplicity = 1

C,0,-2.410064416,-0.0564158627,-0.8343131046
C,0,-2.3589784892,-0.0019336069,0.5865931413
C,0,-1.0914673803,-0.0627196212,1.2362611217
C,0,0.133014478,-0.1908175709,0.407579107
C,0,-0.0169425599,-0.2855716348,-1.0425968668
C,0,-1.2691556319,-0.1744850773,-1.6304594159
N,0,1.2921495929,-0.1927562123,0.9855310857
C,0,-1.0344639184,0.014067016,2.6304191203

C,0,-2.2087935602,0.1353220565,3.3731703845
C,0,-3.4645551482,0.1905438968,2.7404526241
C,0,-3.5410190269,0.1235999149,1.3593019411
O,0,2.2589474204,0.4425158239,-2.6588186286
C,0,3.3158785217,0.1064507635,-2.0387230636
O,0,3.3520464222,-0.3160567422,-0.8463144327
C,0,4.6303686289,0.1951407122,-2.8154330304
H,0,-3.3880929342,-0.0167718271,-1.3112781612
H,0,-0.0640814989,-0.0279978813,3.1138326539
H,0,-2.1524406275,0.1856338971,4.4572357182
H,0,4.6419217435,1.0822241015,-3.4560215027
H,0,5.4805627304,0.2071792775,-2.1281376458
H,0,4.7176133618,-0.6846745912,-3.4654209327
H,0,-4.36872457,0.2861919842,3.3344174979
H,0,-4.5031815258,0.1702295061,0.855221098
H,0,0.8812600552,-0.3742194774,-1.6629375087
H,0,-1.3619774591,-0.2092728923,-2.7118963122
H,0,2.0812138474,-0.2399871823,0.2838202344

Table S19. Cartesian coordinates of the optimized structure for the nitrenium ion of **4**
Charge = 1 Multiplicity = 1

C,0,1.7215068588,-1.3089141087,0.0000118399
C,0,2.7418812038,-0.3698483864,0.0000051357
C,0,2.4203143632,0.9948236211,-0.0000079949
C,0,1.0846524279,1.4306112311,-0.0000128141
C,0,0.0438998855,0.5097070851,-0.0000041792
C,0,0.3642787703,-0.8891645303,0.0000061225
C,0,-0.6734405373,-1.8443317021,0.0000021413
C,0,-2.0456230008,-1.4997146718,-0.0000072098
C,0,-2.3988154784,-0.1765140815,-0.0000093672
C,0,-1.3936974816,0.8924328854,-0.000007798
N,0,-1.8879643419,2.0856149711,0.0000183257
H,0,-0.4011358999,-2.8982730539,0.0000103135
H,0,-2.7982547175,-2.2814163367,-0.0000103145
H,0,-3.4356708961,0.1471674318,-0.0000143899
H,0,0.88958707,2.4991738162,-0.0000271686
H,0,3.2160110996,1.7343180921,-0.000015215
H,0,3.7801835877,-0.6855407298,0.0000095033
H,0,1.9485590063,-2.3715895171,0.0000208302
H,0,-1.1732709249,2.8223314484,0.0000429029

Table S20. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **5**
Charge = 0 Multiplicity = 1

C,0,-1.132197816,0.4608007066,-0.4453168632
C,0,-1.152716966,0.5071881636,0.9513325191
C,0,0.0470396031,0.450950805,1.662275984

C,0,1.268300004,0.3290669034,0.9801853364
C,0,1.2953339065,0.2708503116,-0.4239989008
C,0,0.0989229037,0.3483310534,-1.1251095061
C,0,-0.1359872932,0.3107380195,-2.6227378386
C,0,-1.6460549963,0.4134884642,-2.7266860649
C,0,-2.2148720302,0.5013131699,-1.437183412
C,0,-3.6005922703,0.6037755163,-1.2815694535
C,0,-4.4100078389,0.6183274629,-2.4217091932
C,0,-3.8447749753,0.5313474096,-3.7006353524
C,0,-2.4557621801,0.4278940209,-3.8580878257
N,0,2.5096229546,0.3738614681,1.6712304003
O,0,2.4187727914,-0.3226637127,2.9351749681
C,0,3.3366569368,-1.3138564865,3.0830619981
O,0,4.1286574912,-1.6163660829,2.2123073854
C,0,3.2566722354,-1.9276546705,4.4558982683
H,0,0.2456478714,-0.6154564747,-3.0749643964
H,0,0.3687287759,1.1414690084,-3.1357950121
H,0,-4.0478778919,0.6712072565,-0.2926291161
H,0,-5.4889586201,0.6977541183,-2.3144974504
H,0,-4.4877744433,0.5439593462,-4.5769609008
H,0,-2.0222616992,0.3603592194,-4.8538669017
H,0,2.2448093345,0.1688719914,-0.9470278288
H,0,-2.0914476638,0.5935136002,1.4931129023
H,0,0.0444187128,0.5000319238,2.7456922574
H,0,3.3369763293,-3.0139900466,4.3629466488
H,0,4.1094469043,-1.5766487687,5.0483739815
H,0,2.3317008255,-1.6574316925,4.9692027434
H,0,3.250033282,-0.1137964924,1.1596232692

Table S21. Cartesian coordinates of the optimized structure for the complex for **5**
Charge = 0 Multiplicity = 1

C,0,-1.5092349419,-0.0536955731,0.6609569582
C,0,-1.5875975221,-0.0752579951,2.1011488932
C,0,-0.2680210007,-0.0991269779,2.6275335686
C,0,0.7427791358,-0.0991926018,1.506872395
C,0,-0.1342800903,-0.0719056406,0.2739189814
C,0,0.2307746948,-0.0764991279,-1.045000754
O,0,3.0348696708,0.2867895614,-1.8805460178
C,0,3.0990275993,0.1849975889,-3.1404010706
O,0,2.0949043658,0.0648351929,-3.9117097487
C,0,4.4762396715,0.2415181104,-3.8007877056
C,0,-0.8250480589,-0.0288513859,-2.0588873301
C,0,-2.2245270888,0.0037721871,-1.626879894
C,0,-2.5597349209,-0.0159553649,-0.3031743399
N,0,-0.5870978408,-0.0090576224,-3.3366962631
C,0,-0.0708121501,-0.1182326537,4.0050731305
C,0,-1.1892478263,-0.1142175207,4.8457362401
C,0,-2.4974993058,-0.091049368,4.3258291683

C,0,-2.7085418617,-0.0714172798,2.9523767681
H,0,1.414021825,0.7690540159,1.5456670858
H,0,1.3889050735,-0.9867930909,1.5267336533
H,0,-3.7171467305,-0.053184265,2.548686547
H,0,-3.3444058396,-0.0884709012,5.0058627624
H,0,-1.0470547988,-0.1292183658,5.9231020758
H,0,0.9313756842,-0.135792771,4.4251272567
H,0,1.2857951387,-0.0659191782,-1.3683688087
H,0,-3.5980377827,0.004386199,0.0154159802
H,0,-2.972794701,0.0467645402,-2.412655235
H,0,4.6386229117,1.2525148208,-4.1962448352
H,0,5.2685252376,0.0197573503,-3.0801230691
H,0,4.5236982435,-0.4531309914,-4.645677921
H,0,0.4543303273,-0.0188804218,-3.5384955752

Table S22. Cartesian coordinates of the optimized structure for the nitrenium ion of **5**
Charge = 1 Multiplicity = 1

C,0,-0.3203889985,-1.8551791937,0.0000024204
C,0,-1.5091855633,-0.9252603777,0.0000006635
C,0,-1.0765435694,0.4376969646,0.0000014128
C,0,0.3442503899,0.4704716339,0.0000016477
C,0,0.8465754818,-0.8911901795,0.0000013827
C,0,2.1807607382,-1.1307130457,-0.0000002482
C,0,3.1165763065,0.0021099045,0.0000006009
C,0,2.5693477387,1.366727667,-0.0000013845
C,0,1.2268850744,1.5938655333,0.0000007124
N,0,4.4058764617,-0.1010930166,-0.0000020556
C,0,-2.0108051574,1.50272543,0.0000006924
C,0,-3.3585763966,1.1901616971,-0.0000010833
C,0,-3.7784917248,-0.1595730468,-0.0000022636
C,0,-2.8641346678,-1.2218711847,-0.0000013931
H,0,-0.3104900956,-2.510562907,0.8810925524
H,0,-0.310489206,-2.5105684529,-0.8810833404
H,0,2.5873744936,-2.1398321848,-0.0000013452
H,0,3.294552802,2.1747907273,-0.0000025773
H,0,0.8307492794,2.6043734594,0.0000013027
H,0,-1.6812197472,2.5374052743,0.0000015275
H,0,-4.1027949691,1.9802344692,-0.0000016813
H,0,-4.8429068516,-0.3780655606,-0.0000038943
H,0,-3.2181776007,-2.2486783631,-0.0000023097
H,0,4.7146487541,-1.0812761593,-0.0000048061

Table S23. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **6**
Charge = 0 Multiplicity = 1

N,0,-0.6553,-1.61407,-0.06876
C,0,0.32136,-0.79689,-0.38568
N,0,-0.05241,0.51855,-0.47693
C,0,-1.40617,0.56143,-0.19212
C,0,-1.76849,-0.79049,0.04643
C,0,-3.09404,-1.11323,0.36643
C,0,-4.01901,-0.07463,0.44036
C,0,-3.64213,1.26477,0.20157
C,0,-2.32848,1.60815,-0.11584
N,0,1.61972,-1.20492,-0.73488
O,0,2.60941,-0.82935,0.28731
C,0,3.16158,0.40078,0.09572
C,0,4.35878,0.57306,0.99746
O,0,2.73585,1.22688,-0.68224
H,0,1.64869,-2.22058,-0.65764
H,0,-2.04254,2.64018,-0.29939
H,0,-4.39341,2.04735,0.26581
H,0,5.2451,0.18694,0.47952
H,0,4.50761,1.63542,1.19956
H,0,4.24223,0.01633,1.9305
H,0,0.57819,1.26047,-0.75919
H,0,-5.05391,-0.296,0.68722
H,0,-3.37852,-2.14497,0.55109

Table S24. Cartesian coordinates of the optimized structure for the complex for **6**
Charge = 0 Multiplicity = 1

N,0,3.331533,0.380295,0.242280
C,0,3.248266,-1.022493,0.129535
N,0,1.909562,-1.388636,-0.133016
C,0,1.155493,-0.271757,-0.187087
C,0,2.113211,0.828596,0.054859
C,0,1.636063,2.186228,0.083605
C,0,0.301235,2.381668,-0.120587
C,0,-0.600048,1.279095,-0.403328
C,0,-0.196275,-0.049195,-0.410282
N,0,4.178390,-1.888626,0.237961
O,0,-3.253013,0.688607,0.482585
C,0,-3.651782,-0.451908,0.069626
C,0,-5.104863,-0.816917,0.346276
O,0,-2.900886,-1.268976,-0.525344
H,0,5.065073,-1.416508,0.433669
H,0,-0.963553,-0.817091,-0.549692
H,0,-1.654057,1.474406,-0.582737
H,0,-5.753490,0.059298,0.246399
H,0,-5.431722,-1.610447,-0.332955

H,0,-5.192000,-1.180801,1.377653
H,0,1.596602,-2.347002,-0.229838
H,0,-0.114132,3.384869,-0.097938
H,0,2.334268,2.995100,0.271241

Table S25. Cartesian coordinates of the optimized structure for the nitrenium ion of **6**
Charge = 1 Multiplicity = 1

N,0,-0.7187835533,0.0000271324,-1.4887207448
C,0,-0.7217540453,-0.0000000881,-0.1859579654
C,0,0.6677298066,-0.0000062476,0.3621723248
N,0,1.4570166835,0.0000189885,-0.7030703666
C,0,0.6345056104,0.0000598604,-1.876928954
N,0,1.1531946795,0.0000884641,-3.0311205758
H,0,2.4732240855,0.0000196474,-0.7386533211
C,0,0.9136791116,-0.0000381644,1.7477261084
C,0,-0.2049495349,-0.0000629583,2.5520102319
C,0,-1.5712396609,-0.0000586515,2.0487953971
C,0,-1.8458094549,-0.0000285989,0.7162747705
H,0,0.4372452002,0.0000927981,-3.7658305372
H,0,1.9178489021,-0.0000447819,2.1583324167
H,0,-0.0696835096,-0.0000902713,3.6305258012
H,0,-2.3774601377,-0.0000830443,2.7754740272
H,0,-2.8541402037,-0.0000273521,0.3159819445

Table S26. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **7**
Charge = 0 Multiplicity = 1

N,0,0.51023,0.98711,-0.35729
C,0,-0.2642,-0.12787,-0.59912
N,0,0.37413,-1.2686,-0.47409
C,0,1.66692,-0.9056,-0.13083
C,0,1.76782,0.50547,-0.03143
C,0,2.95686,1.14855,0.32546
C,0,4.0602,0.33287,0.57559
C,0,3.97681,-1.07303,0.47748
C,0,2.78774,-1.70687,0.12503
N,0,-1.58866,0.00732,-1.03956
O,0,-2.41783,0.41612,0.10872
C,0,-3.53366,-0.347,0.26097
O,0,-3.78302,-1.30152,-0.44474
C,0,-4.39568,0.17498,1.38196
C,0,0.10416,2.3784,-0.45182
H,0,2.71753,-2.78808,0.04984
H,0,4.86133,-1.66986,0.68334
H,0,5.00596,0.79077,0.85292
H,0,3.02702,2.22987,0.40538
H,0,-0.84439,2.42857,-0.98835

H,0,-0.02081,2.82097,0.54305
H,0,0.86011,2.94425,-1.00563
H,0,-1.95273,-0.91602,-1.29732
H,0,-3.86707,0.90461,1.99856
H,0,-5.28534,0.64687,0.94967
H,0,-4.72655,-0.66885,1.99351

Table S27. Cartesian coordinates of the optimized structure for the complex for **7**
Charge = 0 Multiplicity = 1

N,0,-0.2415049002,-0.6049144437,0.2253899887
C,0,-0.2303562223,-0.6355762673,1.5503159288
C,0,1.1836242517,-0.6395058414,1.9558319269
N,0,1.9862820657,-0.586021396,0.9235748207
C,0,1.1630444639,-0.5376014343,-0.2115514825
N,0,1.586067786,-0.445151024,-1.3995907514
C,0,1.5183807949,-0.6925693874,3.3517381944
C,0,0.4931557926,-0.72929086,4.2510529283
C,0,-0.8924996896,-0.7226899952,3.8302268083
C,0,-1.2734515251,-0.6771744008,2.5129475108
C,0,-1.3794888399,-0.5445599958,-0.6706305965
O,0,-1.2298370759,1.875064405,-2.2894022257
C,0,-0.6830560534,1.4359927838,-3.3419607306
O,0,0.0522106687,0.4054159093,-3.4272923355
C,0,-0.9271901864,2.2078746261,-4.6450861932
H,0,0.7031889454,-0.763624412,5.3159426221
H,0,-1.6585949949,-0.7550602583,4.6000792244
H,0,-2.318587045,-0.6680423584,2.2232760371
H,0,-2.2965818642,-0.6830286812,-0.0959639488
H,0,-1.2889798966,-1.3249039504,-1.4297900128
H,0,-1.3829926702,0.444325334,-1.1938875455
H,0,0.8679041923,-0.2866080253,-2.1664092018
H,0,-1.5989449516,3.0537447359,-4.4841485181
H,0,0.0339048658,2.5650417564,-5.0318540902
H,0,-1.3500357683,1.5310804242,-5.3956082238
H,0,2.5618390665,-0.6935544005,3.6489959731

Table S28. Cartesian coordinates of the optimized structure for the nitrenium ion for **7**
Charge = 1 Multiplicity = 1

N,0,-0.6218279867,-1.6485437403,-0.0000273357
C,0,0.4725706229,-0.9435103641,0.0000228637
C,0,0.1763847166,0.5182480488,-0.0000410097
N,0,-1.1420659696,0.6288258245,-0.0001972399
C,0,-1.6767918644,-0.7173944971,0.0001762652
N,0,-2.9255993218,-0.9137139669,-0.0001234557
C,0,-1.9579915993,1.8480405664,0.0000300673
C,0,1.2113926885,1.4802535569,0.0000286358

C,0,2.4923414465,0.9821326137,0.0000767021
C,0,2.8099523572,-0.4407751452,0.000057298
C,0,1.8409245045,-1.3951345385,0.0000222938
H,0,-3.1476425327,-1.9147557818,-0.0002108317
H,0,1.0095114827,2.5459000658,0.0000743765
H,0,3.3251795594,1.6803853817,0.0000825367
H,0,3.8578412616,-0.7239845406,0.000028723
H,0,2.0540689642,-2.4588606333,-0.0000330778
H,0,-1.7370665974,2.4365123891,-0.8945328188
H,0,-3.0047349181,1.545648684,-0.004321033
H,0,-1.7434015081,2.432016169,0.8991096472

Table S29. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **8**
Charge = 0 Multiplicity = 1

N,0,-0.7132092877,0.3279672005,0.3279128802
C,0,-0.6876500741,0.3434149276,1.6973664902
N,0,0.5254369841,0.4010550128,2.2023505489
C,0,1.355885556,0.4371201328,1.09508781
C,0,0.6016264215,0.3748764433,-0.0891403822
C,0,1.1863611559,0.3649320737,-1.3838178501
C,0,2.6203508001,0.4349872892,-1.4155060522
C,0,3.3741520941,0.5023430101,-0.1956570353
C,0,2.771293983,0.504235587,1.039464649
C,0,3.2604552741,0.4354467547,-2.6818563393
C,0,2.5328308924,0.3690717239,-3.8546786653
C,0,1.121217854,0.2986453476,-3.8123330886
C,0,0.4602867212,0.2972210452,-2.5987538475
N,0,-1.8760398335,0.4199337151,2.4416916555
O,0,-2.5810766128,-0.8764895813,2.4889602837
C,0,-3.4538932899,-1.0634048995,1.4622564408
O,0,-3.5017485542,-0.368118796,0.4698353759
C,0,-4.3325414061,-2.2577627362,1.7418826155
H,0,-1.6139510657,0.5191154586,3.4214635478
H,0,3.3491937321,0.5532573353,1.957521929
H,0,4.4578436552,0.5521311338,-0.2698630906
H,0,-5.2145958197,-1.9194308689,2.2990195953
H,0,-4.6629832584,-2.6911001565,0.7959238364
H,0,-3.8144778633,-3.005245168,2.3475383237
H,0,-1.5733519747,0.3092963247,-0.2085742781
H,0,4.3465053333,0.4896041562,-2.7158493498
H,0,3.0444252917,0.3708844982,-4.8135566533
H,0,0.554279576,0.2458863274,-4.7380906592
H,0,-0.6258572036,0.2430162842,-2.5754725407

Table S30. Cartesian coordinates of the optimized structure for the complex for **8**
Charge = 0 Multiplicity = 1

N,0,-1.311794,-1.714152,-0.051756
C,0,-1.529866,-0.398810,-0.026238
C,0,-2.997349,-0.255619,0.027794
N,0,-3.592388,-1.429763,0.026308
C,0,-2.571630,-2.383610,-0.021451
N,0,-2.634200,-3.657235,-0.041103
C,0,-3.569448,1.055746,0.078951
C,0,-2.723731,2.126188,0.080253
C,0,-1.275018,2.001220,0.024181
C,0,-0.654677,0.708989,-0.032972
C,0,0.747040,0.580463,-0.109760
C,0,1.556680,1.713161,-0.083445
C,0,0.959007,2.978023,-0.029787
C,0,-0.439412,3.121952,0.012843
H,0,-0.878556,4.115798,0.056203
O,0,4.421339,0.476270,-0.066974
C,0,4.227009,-0.768710,0.021844
O,0,3.067564,-1.289544,0.040104
C,0,5.428613,-1.701648,0.116463
H,0,-3.613204,-3.954292,-0.015453
H,0,-4.647748,1.166016,0.116385
H,0,-3.132958,3.132923,0.114841
H,0,6.364400,-1.151595,-0.018984
H,0,5.422894,-2.207932,1.089633
H,0,5.360547,-2.476454,-0.655752
H,0,-0.418651,-2.197010,-0.081217
H,0,1.583198,3.867646,-0.010291
H,0,2.637131,1.547921,-0.098815
H,0,1.237098,-0.392857,-0.167787

Table S31. Cartesian coordinates of the optimized structure for the Nitrenium ion of **8**
Charge = 1 Multiplicity = 1

N,0,-1.8216918044,-0.0000587229,0.8534308609
C,0,-1.8036009793,-0.0000632052,2.2945629058
N,0,-0.4727953879,-0.0000332249,2.7251079741
C,0,0.2658177381,-0.0000024127,1.6491189237
C,0,-0.576027034,-0.0000191385,0.4128345554
C,0,-0.0100441404,0.0000055417,-0.8889170757
C,0,1.4221585409,0.0000477533,-0.9380275461
C,0,2.2276692738,0.0000629461,0.2842301608
C,0,1.6949937099,0.0000392412,1.5330980957
C,0,2.0377563065,0.0000734824,-2.1923884479
C,0,1.271807244,0.0000584642,-3.3658265205
C,0,-0.1292635765,0.0000173264,-3.3133029062
C,0,-0.7694766668,-0.0000089855,-2.0802840536

N,0,-2.8931413027,-0.0001035544,2.9388387455
H,0,-2.7277032263,-0.0001104152,3.950340199
H,0,2.3023330167,0.0000501253,2.4314004675
H,0,3.3070712837,0.0000943876,0.1593148898
H,0,-2.6884044516,-0.0000813024,0.3239492122
H,0,3.1220794971,0.0001055219,-2.2579946066
H,0,1.7735490866,0.0000788623,-4.3291921284
H,0,-0.7107069086,0.0000062069,-4.2295677601
H,0,-1.8555613291,-0.0000409508,-2.0404818852

Table S32. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **9**
Charge = 0 Multiplicity = 1

N,0,-0.481845418,-0.3036157346,-0.7689387183
C,0,-0.4923306968,-0.4390447685,0.6029259651
C,0,0.7926176766,-0.3569110562,-1.0983255954
C,0,0.8187703051,-0.5529663109,1.0930697968
N,0,1.6366097003,-0.5154025965,-0.0211720418
N,0,1.2990561994,-0.3515481317,-2.4044566847
C,0,-1.6055767372,-0.4587464568,1.4951177231
O,0,1.869516143,0.988334591,-2.672060017
C,0,1.1143145889,-0.6807355255,2.469553427
C,0,-1.3110157697,-0.5926059388,2.8923782779
C,0,-2.9504405229,-0.3530847627,1.0675684464
C,0,3.0844944801,-0.6353663189,-0.0535513393
H,0,0.5211941081,-0.4227870218,-3.0688275756
C,0,1.4295551119,1.5319131652,-3.836994028
C,0,0.0475584918,-0.6998720293,3.3402456724
C,0,-3.9794349331,-0.3797056283,1.9898077897
C,0,-2.3949570947,-0.6145437611,3.8093533183
H,0,2.1359375038,-0.7612631746,2.8302849456
H,0,3.5630682031,0.2855549914,0.2979663772
H,0,3.3990973012,-1.4706700168,0.5797433564
H,0,3.3913083026,-0.8291331074,-1.0823764629
H,0,-3.1524591634,-0.2520727679,0.0052405451
C,0,2.1126371147,2.8473391889,-4.1133085464
O,0,0.6084349701,0.9936812823,-4.5504742414
C,0,-3.700724968,-0.5109222163,3.3708150786
H,0,0.2284981043,-0.7991821435,4.4078890301
H,0,-2.1804478563,-0.7153505957,4.8713413997
H,0,-5.010319606,-0.2990169806,1.6542475236
H,0,2.6608328657,3.2143811784,-3.2434204076
H,0,2.809740405,2.7120784079,-4.9479795638
H,0,1.3586380139,3.5772099331,-4.420763191
H,0,-4.5182427377,-0.5303959337,4.0869642873

Table S33. Cartesian coordinates of the optimized structure for the complex for **9**
Charge = 0 Multiplicity = 1

N,0,-0.5823700135,0.8458377641,1.235309175
C,0,-0.8577480702,-0.3777791374,0.8884027363
C,0,0.1855587127,-0.9482503166,0.0202839666
N,0,1.1097258681,-0.0154625459,-0.1189423899
C,0,0.6396346312,1.1750920074,0.6204287115
N,0,1.2052133223,2.2985311171,0.6935294376
O,0,2.3696503276,2.1150990785,-2.8494274884
C,0,3.0602384424,2.9758670216,-2.2298460281
C,0,3.826241094,4.009928957,-3.0622456305
O,0,3.1827500763,3.0603732404,-0.9688888683
C,0,0.0930170121,-2.2743105007,-0.4864938045
C,0,-1.009230968,-3.0018759912,-0.1313405799
C,0,-2.0726305154,-2.5002452219,0.7225293978
C,0,-2.0131541259,-1.1798694079,1.2486325328
C,0,-3.0398616801,-0.6985617139,2.069340418
C,0,-4.1269234183,-1.5175902577,2.3752251224
C,0,-4.196195859,-2.8202285336,1.8627172435
C,0,-3.1788154406,-3.3071225123,1.0438711787
C,0,2.3310215787,-0.0568750607,-0.9016510968
H,0,0.8600680033,-2.6889517365,-1.1312702787
H,0,-1.110406736,-4.0189656776,-0.5029838459
H,0,2.4733044427,-1.0656513191,-1.2925019872
H,0,2.2633460653,0.6904080114,-1.7302654212
H,0,3.1760745308,0.2264083583,-0.2698280596
H,0,2.0673410696,2.4631832229,0.089410623
H,0,3.6937449684,3.8352611978,-4.1325222435
H,0,3.4685018894,5.0135224699,-2.8046675559
H,0,4.8911056923,3.9697048015,-2.8065477995
H,0,-3.2359749837,-4.3175343158,0.6463262275
H,0,-5.0454408628,-3.4536525143,2.1027486688
H,0,-2.9734766503,0.3133382355,2.4574645017
H,0,-4.92228326,-1.1422696267,3.0127694591

Table S34. Cartesian coordinates of the optimized structure for the nitrenium ion of **9**
Charge = 1 Multiplicity = 1

N,0,-1.0735287126,-1.5655679015,0.0000029116
C,0,-2.3929955898,-1.0850474324,-0.0000071472
C,0,-0.3051353037,-0.5158390525,-0.0000012129
N,0,-2.3760782842,0.3623993528,-0.0000000409
C,0,-1.1067369976,0.7394937944,-0.0000011403
C,0,1.1409986183,-0.4415195104,-0.0000003557
N,0,-3.4906432343,-1.7141984657,-0.0000032769
C,0,1.7155875581,0.8634003789,-0.0000011716
C,0,-0.504417725,2.0122234874,-0.0000010162
C,0,1.9587344867,-1.573432148,0.0000019171

C,0,-3.57506802,1.204006333,0.0000043741
H,0,-3.3382523637,-2.7267840275,0.000003887
C,0,0.8732175928,2.0398507893,-0.0000016574
C,0,3.1142104701,0.9889512953,-0.000000243
C,0,3.3525788712,-1.4241268047,0.0000024095
H,0,-1.0907196166,2.9246455741,-0.0000002476
H,0,-4.4412802426,0.5429003616,-0.0000081735
H,0,-3.5861952661,1.8300307999,0.8964774601
H,0,-3.5861851742,1.8300522263,-0.896453751
H,0,1.5073077242,-2.5609087146,0.0000028661
C,0,3.9267164091,-0.1505546461,0.0000012834
H,0,1.3719953115,3.0064168911,-0.0000007672
H,0,3.5656009019,1.9775245568,-0.000000468
H,0,3.9864547802,-2.3056642162,0.0000037796
H,0,5.0068833411,-0.0410832569,0.0000020186

Table S35. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **10**

Charge = 0 Multiplicity = 1

N,0,-0.3181151362,0.4626561634,-0.6936492057
C,0,-0.3187491639,0.453718733,0.6953642287
C,0,1.0365781889,0.3384995448,1.0587945523
N,0,1.8380625923,0.2462628283,-0.0582437048
C,0,1.0021099159,0.3278415432,-1.0693206665
N,0,1.3658423644,0.3691141263,-2.4224293074
O,0,1.0915761169,-0.9604895941,-3.0121212054
C,0,2.1498677219,-1.4691505427,-3.6964270032
C,0,1.7929198641,-2.779534422,-4.3511872657
O,0,3.223745198,-0.9084468354,-3.7674982445
C,0,1.4298144123,0.3149126329,2.4199443088
C,0,0.4521222931,0.401293126,3.3778898701
C,0,-0.9380791302,0.5052201914,3.0391089002
C,0,-1.3660764748,0.527818393,1.6642120745
C,0,-2.7564840243,0.6100902525,1.386759109
C,0,-3.6849695706,0.6775040721,2.4089772027
C,0,-3.267659429,0.666634095,3.7574413814
C,0,-1.9224416333,0.5808241322,4.0575616855
C,0,-1.429445764,0.6546811154,-1.6141439314
H,0,2.4816129278,0.2292659899,2.6758161929
H,0,0.7184094904,0.3864166084,4.4319624219
H,0,-2.1020368658,-0.2091511011,-1.603414911
H,0,-1.0178793675,0.7742327918,-2.6168213438
H,0,-1.9867957032,1.5573390046,-1.3479676236
H,0,2.3846955205,0.4613098112,-2.4935021157
H,0,1.7741208067,-2.6356234976,-5.437198801
H,0,2.5747317664,-3.5097945581,-4.1236494406
H,0,0.8221143663,-3.1521478681,-4.0188591372
H,0,-1.5943342862,0.5667742774,5.0947084272

H,0,-4.0039709899,0.7223239475,4.5547891599
H,0,-3.1071886811,0.6142028839,0.3614730392
H,0,-4.7436214843,0.7379941188,2.1700285773

Table S36. Cartesian coordinates of the optimized structure for the complex for **10**
Charge = 0 Multiplicity = 1

N,0,0.4557783162,-0.6282521824,-0.4656533216
C,0,0.3801335167,-0.4333233976,0.8384663071
C,0,1.7778692204,-0.3684168884,1.3185080723
N,0,2.6386803463,-0.4302175647,0.3414175408
C,0,1.8916377554,-0.527841552,-0.8381950193
N,0,2.3558722172,-0.476709273,-2.0089181262
C,0,2.0498468901,-0.285530844,2.7271109188
C,0,0.9985160075,-0.2545830195,3.5825752141
C,0,-0.3912035731,-0.2460849081,3.1380186989
C,0,-0.7315228393,-0.3041525962,1.7481699611
C,0,-2.0821924946,-0.179086657,1.3618127973
C,0,-3.0839423251,-0.0565861573,2.3213711851
C,0,-2.7570494073,-0.0502539369,3.6818820075
C,0,-1.4232719764,-0.1345436253,4.0808240866
C,0,-0.5763240647,-0.8986559928,-1.4456804904
O,0,-0.9534418961,1.4080887678,-3.1220203524
C,0,-0.1877978499,1.1142684387,-4.089272267
O,0,0.7424839676,0.2535631853,-4.0710833144
C,0,-0.4198682501,1.845966505,-5.4165806307
H,0,3.0809880385,-0.2591961422,3.0628823814
H,0,1.1722158908,-0.2041611916,4.6545220028
H,0,-0.1614579679,-1.5607923691,-2.2061354373
H,0,-0.8672941534,0.0513750432,-1.969896393
H,0,-1.4233149449,-1.3837934533,-0.9603670352
H,0,1.6551754481,-0.3891523119,-2.7940905869
H,0,-1.1186755164,2.6770323435,-5.2951490361
H,0,0.5360598546,2.2073939381,-5.8095653661
H,0,-0.8271915494,1.1365903381,-6.1472502784
H,0,-3.5397507154,0.040849254,4.4297111032
H,0,-1.1705047015,-0.0988411013,5.1374696553
H,0,-4.1180593369,0.0453765384,2.0063045423
H,0,-2.3518267344,-0.136695582,0.3144060842

Table S37. Cartesian coordinates of the optimized structure for the Nitrenium ion of **10**
Charge = 1 Multiplicity = 1

N,0,-1.5933856012,-0.8526773813,-0.000009688
C,0,-0.5339848855,-0.0604549628,-0.0000028501
C,0,-1.0779601913,1.3359808646,0.0000173204
N,0,-2.3807712845,1.3415769469,0.0000334184
C,0,-2.775660985,0.0046113189,-0.0000193252

N,0,-3.9283193233,-0.5150847268,-0.0000180086
C,0,-0.1888096884,2.4584013479,0.0000092261
C,0,1.1439228884,2.2077717161,-0.000020958
C,0,1.7087598042,0.8590265374,-0.0000208525
C,0,0.8750878283,-0.3094017803,0.0000037882
C,0,1.4710597597,-1.5914192965,0.0000452806
C,0,2.8563277162,-1.7266171057,0.0000456063
C,0,3.6671486845,-0.5870933446,0.0000040635
C,0,3.0957792562,0.6916865018,-0.0000250723
C,0,-1.6949138983,-2.3140151905,-0.0000408926
H,0,3.738101191,1.5678323274,-0.0000465588
H,0,-4.6589338625,0.202739581,0.0000259761
H,0,-0.6011370169,3.461371756,0.0000228251
H,0,1.8490234735,3.0345735259,-0.0000340585
H,0,4.7482808271,-0.6908754172,0.0000003136
H,0,3.3023494812,-2.7160258203,0.0000797249
H,0,0.8597034877,-2.4845030321,0.0000889365
H,0,-1.2225571562,-2.7197858525,0.898585327
H,0,-2.7557280951,-2.5631374683,-0.0001865198
H,0,-1.2223066,-2.7197531091,-0.8985480255

Table S38. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **11**

Charge = 0 Multiplicity = 1

C,0,-2.6735898782,1.059326694,-1.8415099066
C,0,-2.6775945603,0.9444896407,-0.4475710331
C,0,-1.4810910006,0.724778435,0.2284724618
C,0,-0.3123582954,0.6141607534,-0.5413962455
N,0,-0.2901175551,0.7089192958,-1.8741965161
C,0,-1.4506763083,0.9378943116,-2.5014996242
N,0,0.9678219089,0.4865242136,0.036535605
O,0,0.9139864706,-0.2112503263,1.28832139
C,0,1.8326968832,-1.2117371543,1.3972134375
O,0,2.5782647018,-1.5220013793,0.4922573406
C,0,1.8062115621,-1.8181492027,2.7752432318
H,0,-3.5878786493,1.2340789552,-2.4000920605
H,0,-1.3923007101,1.0148059497,-3.5854541013
H,0,-1.4421335949,0.643878377,1.3084614356
H,0,-3.6062237331,1.0313497225,0.1108244865
H,0,1.6177161027,-0.0197881512,-0.5704472337
H,0,1.9042930854,-2.9031518235,2.6863837427
H,0,2.6696794762,-1.4464479663,3.3390803527
H,0,0.893317752,-1.5613968501,3.316525981

Table S39. Cartesian coordinates of the optimized structure for the complex for **11**
Charge = 0 Multiplicity = 1

C,0,3.069277,1.182471,0.026083
C,0,1.733117,1.551193,0.079167
C,0,0.776652,0.536798,0.117279
C,0,1.210783,-0.844162,0.011920
N,0,2.565843,-1.184170,-0.066547
C,0,3.429131,-0.207265,-0.040091
N,0,0.358832,-1.835001,-0.031118
O,0,-2.062720,1.177512,-0.225403
C,0,-2.759168,0.137650,-0.031017
O,0,-2.250189,-1.021244,0.090534
C,0,-4.271068,0.265021,0.052668
H,0,3.858595,1.930145,0.032425
H,0,1.433098,2.594361,0.118895
H,0,-0.298887,0.760715,0.169975
H,0,4.483260,-0.477490,-0.089311
H,0,-0.639691,-1.485788,0.017275
H,0,-4.728624,-0.293438,-0.772157
H,0,-4.625383,-0.185698,0.986607
H,0,-4.584164,1.311010,0.002846

Table S40. Cartesian coordinates of the optimized structure for the nitrenium ion of **11**
Charge = 1 Multiplicity = 1

C,0,-1.5261687336,-0.0000731649,-0.8558444448
C,0,-1.5850722442,-0.0000332403,0.5380238847
C,0,-0.3760819593,0.0000298918,1.2178358151
C,0,0.8651282507,0.000019767,0.4557616517
N,0,0.8921181733,0.0000014667,-0.9412280046
C,0,-0.2547193353,-0.0000425901,-1.5541323211
N,0,1.9658875181,0.0000955845,1.1419128577
H,0,-2.4401936518,-0.0001169305,-1.4462046303
H,0,-2.5354885105,-0.0000493627,1.0626101884
H,0,-0.3040719212,0.0000592501,2.3023619591
H,0,-0.2465894995,-0.0000854199,-2.6422940603
H,0,2.7817878729,0.0001091238,0.5088650578

Table S41. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **12**
Charge = 0 Multiplicity = 1

N,0,-0.8483783571,-0.5345698123,-1.4600864306
C,0,-0.8156391048,-0.4189405952,-0.1508283648
N,0,0.4442022556,-0.3218932245,0.3805718551
C,0,1.3174399385,-0.3862519243,-0.6887606942
C,0,0.4876223904,-0.5343240731,-1.8317976148

C,0,1.1125943616,-0.6293001994,-3.0762953272
C,0,2.5076346437,-0.5697763663,-3.0770680651
C,0,3.2165232334,-0.4197213056,-1.8695340986
N,0,2.6432521416,-0.3218853344,-0.6602627707
N,0,-1.947715542,-0.5124431894,0.6724257478
O,0,-2.2541476112,0.7541892704,1.3430790441
C,0,-1.6517802194,0.894783301,2.5607307966
O,0,-0.7601735185,0.1817329582,2.9628959909
C,0,-2.2547305501,2.06351248,3.2987185169
H,0,-2.7601618248,-0.613513767,0.0658208961
H,0,4.3031725376,-0.3754553147,-1.8810692224
H,0,-3.1280106924,1.7099742043,3.8601936444
H,0,-1.5221367347,2.4595656821,4.0043569756
H,0,-2.5877182881,2.8444714309,2.6107032188
H,0,0.6517690759,-0.2973076787,1.3733388428
H,0,3.0612985005,-0.6369550896,-4.0089967783
H,0,0.5388448171,-0.7425042742,-3.9916775602

Table S42. Cartesian coordinates of the optimized structure for the complex for **12**
Charge = 0 Multiplicity = 1

N,0,0.68538637,-0.1347461952,-2.2876711195
C,0,0.8085970066,-0.1202521453,-0.9752891797
C,0,2.2176614419,0.0632820108,-0.5737301722
N,0,2.9017784491,0.1605184763,-1.7240133115
C,0,1.980459368,0.0367929975,-2.7958403713
N,0,2.3662381682,0.0952481017,-4.0120611274
N,0,2.6863340224,0.1330300661,0.6652098734
C,0,1.7244426949,0.0318237086,1.5954867237
C,0,0.3285815838,-0.1662498622,1.3504057119
C,0,-0.1587394046,-0.2562911425,0.067086324
O,0,-3.0983949463,0.0640553536,0.6816781496
C,0,-3.3295319536,0.009903117,1.9274591717
O,0,-2.391754602,-0.1007952264,2.7692351535
C,0,-4.7620611284,0.116580738,2.4151834399
H,0,1.5569966558,-0.0133865085,-4.6303086994
H,0,2.071622949,0.0929019289,2.6245997677
H,0,-5.4570459497,-0.2691263459,1.6625178732
H,0,-4.8867983628,-0.4244733656,3.3586337531
H,0,-5.0011974964,1.172581376,2.5922774951
H,0,3.8978477554,0.3101985774,-1.8346983521
H,0,-0.3721855989,-0.2441779102,2.1810788748
H,0,-1.2226602868,-0.4024884433,-0.1162272291

Table S43. Cartesian coordinates of the optimized structure for the nitrenium ion of **12**
Charge = 1 Multiplicity = 1

N,0,-0.7220343407,-0.0000500879,-1.4091894405
C,0,-0.7287380853,0.0000313639,-0.087699188
C,0,0.7023584559,-0.0000298816,0.3191474309
N,0,1.4921462353,-0.0001105021,-0.7162162963
C,0,0.6437331196,-0.0000256398,-1.8442797331
N,0,0.9326071449,-0.000036116,-3.0764460909
H,0,-1.5264249115,-0.0000748166,-2.0342231654
C,0,0.992698308,-0.0000160235,1.7296645475
C,0,-0.0930007324,0.0000580739,2.5523380167
C,0,-1.4490687754,0.0001092487,2.0129167452
N,0,-1.7863904683,0.0000882179,0.7349500768
H,0,1.9482358248,-0.000082818,-3.2258513691
H,0,2.0180093587,-0.0000674065,2.0859062226
H,0,0.0168051459,0.0000694691,3.6322407489
H,0,-2.2788191583,0.0001521384,2.7177129046

Table S44. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **13**
Charge = 0 Multiplicity = 1

N,0,-0.9531691135,0.6471344858,0.0387879791
C,0,-0.9851892752,0.6479127684,1.4210123634
C,0,0.3648458163,0.477363746,1.8352091073
N,0,1.185334135,0.3406668212,0.7305760428
C,0,0.3717677844,0.4494785276,-0.2938360709
N,0,0.7798463827,0.48325894,-1.6336705633
O,0,0.2938586935,-0.7327341736,-2.2994145986
C,0,1.2605937272,-1.3684948969,-3.0197888939
O,0,2.4121794756,-0.992118865,-3.0517826606
C,0,0.6902784657,-2.5489868925,-3.7624631977
N,0,0.7523195116,0.4391497697,3.1138553473
C,0,-0.228353019,0.5691144132,4.0120198263
C,0,-1.5921401532,0.7375208124,3.694921552
C,0,-2.0032075389,0.7780311591,2.3621166362
C,0,-2.071826995,0.846951635,-0.8679087648
H,0,0.0776250765,0.5388214291,5.0559480713
H,0,-2.317942207,0.8350698089,4.4968871123
H,0,-3.0474163968,0.9040520391,2.0886666686
H,0,-1.6806859849,1.1142637361,-1.8506226812
H,0,-2.676182472,-0.0627716179,-0.9566612399
H,0,-2.6989684635,1.6640409808,-0.4980963401
H,0,1.8019992317,0.4135867162,-1.6785606817
H,0,-0.3154429717,-2.8012189856,-3.4206596537
H,0,0.6579658294,-2.3084804306,-4.8311133227
H,0,1.3598137214,-3.4033571178,-3.6307468481

Table S45. Cartesian coordinates of the optimized structure for the complex for **13**
Charge = 0 Multiplicity = 1

N,0,-0.2351304461,-0.5347192159,0.4146387143
C,0,-0.1933579407,-0.1262876082,1.6723357948
C,0,1.2257293468,-0.000715637,2.033331097
N,0,2.0099765325,-0.2914493693,1.0286119241
C,0,1.1692754834,-0.6126160888,-0.0405453355
N,0,1.5644966804,-0.9073513935,-1.2067765278
N,0,1.6414290576,0.3814414223,3.2857145714
C,0,0.6850777463,0.6376177205,4.1348734037
C,0,-0.7411262137,0.5428801705,3.860815318
C,0,-1.2019981017,0.1605926108,2.6312857502
C,0,-1.3874428625,-0.7635174198,-0.4291176206
O,0,-1.3629917422,1.0444080785,-2.6798029143
C,0,-0.787936727,0.3459406045,-3.5663385953
O,0,-0.0292668188,-0.646474849,-3.3620686596
C,0,-1.0350878063,0.7294940011,-5.0321288924
H,0,0.9918169218,0.9483081956,5.1325980057
H,0,-1.4339368829,0.7844135897,4.6614790712
H,0,-2.2603063911,0.0862118767,2.4028188249
H,0,-2.2935254006,-0.7246589766,0.178003801
H,0,-1.2994155699,-1.7371570751,-0.9159525069
H,0,-1.4183146253,0.0200300285,-1.2344088652
H,0,0.8268562542,-0.9993004095,-1.9570306455
H,0,-1.7200330627,1.576113822,-5.1099982827
H,0,-0.0757227342,0.9811451022,-5.4974304932
H,0,-1.4435503399,-0.134352217,-5.5674926107

Table S46. Cartesian coordinates of the optimized structure for the nitrenium ion of **13**
Charge = 1 Multiplicity = 1

N,0,-0.5916297446,-1.6438008512,0.0004583594
C,0,0.496611652,-0.9312538697,-0.0001083505
C,0,0.189028092,0.5274925181,-0.0001124305
N,0,-1.122379669,0.638197262,-0.0000006194
C,0,-1.6468624139,-0.7227626731,-0.0005472103
N,0,-2.8961166875,-0.9158961394,-0.0003549734
C,0,-1.9513944442,1.8510900462,0.0004997679
C,0,1.2449957094,1.4804859219,-0.0000900038
C,0,2.4959464392,0.9341868201,-0.0000983102
C,0,2.7122800847,-0.5240967484,-0.0001018499
N,0,1.7767369109,-1.4254317945,0.0000418349
H,0,-3.1224665287,-1.9165551598,0.0002569724
H,0,1.0693225486,2.5514855422,-0.0000072429
H,0,3.3756754285,1.5718688096,0.0000505199
H,0,3.7403639019,-0.8817492879,0.0002316937
H,0,-1.7378366485,2.4392718773,-0.8958903976
H,0,-2.9945232315,1.5364704894,-0.0013956412

H,0,-1.7404418533,2.4368763008,0.8990922104

Table S47. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **14**

Charge = 0 Multiplicity = 1

N,0,-0.9289188731,0.5911446071,0.0665356033
C,0,-0.9438707736,0.602208564,1.4512566012
C,0,0.4128001132,0.4848730029,1.8483100471
N,0,1.2278969015,0.3709868532,0.7362565815
C,0,0.3955232212,0.444096994,-0.2805835185
N,0,0.7961015104,0.5013370298,-1.6205989082
O,0,0.2937778335,-0.6881892931,-2.3158680928
C,0,1.2516471873,-1.3235650331,-3.0471843344
O,0,2.4116637731,-0.971187841,-3.0608388099
C,0,0.6597484958,-2.4659117045,-3.8311665951
C,0,0.6873347391,0.4854966652,3.2169852303
C,0,-0.4109801027,0.6013023366,4.0718890127
C,0,-1.7139966357,0.7115418874,3.5494701689
N,0,-2.0072294264,0.7116145275,2.2397094488
H,0,1.7036348396,0.3992621688,3.590737782
C,0,-2.0772798092,0.7413172086,-0.8147711034
H,0,-0.2723093201,0.6072939713,5.1490635859
H,0,-2.5625774125,0.8038052685,4.2235455852
H,0,-2.8613872381,1.2603986755,-0.2603601362
H,0,-1.7836673396,1.3263489924,-1.6892692143
H,0,-2.4522508682,-0.233806285,-1.1412632116
H,0,1.8174496676,0.4262923055,-1.6743324463
H,0,0.5684278874,-2.1607719878,-4.8799776392
H,0,1.344449172,-3.3167094738,-3.7857067883
H,0,-0.3258116409,-2.7508372114,-3.4573344257

Table S48. Cartesian coordinates of the optimized structure for the complex for **14**

Charge = 0 Multiplicity = 1

N,0,-0.2421984094,0.6131536369,0.2378499439
C,0,-0.2713130403,0.6275890258,1.5636507376
C,0,1.1704826052,0.5194647021,-0.1445918993
C,0,-1.3672373084,0.5748863305,-0.6742808452
C,0,1.1187259747,0.5843151973,2.0188586308
N,0,1.9604232915,0.5200917548,1.0172019552
N,0,1.6407786616,0.4539383432,-1.3192601043
N,0,-1.3636296901,0.6910912936,2.3577588634
H,0,-2.282042063,0.6910730835,-0.0921514426
H,0,-1.3536582752,-0.4019562984,-1.2166953668
H,0,-1.2678388561,1.3735880275,-1.4131093361
C,0,1.3512312099,0.6078272101,3.4324825363
C,0,-1.0850409226,0.7057610567,3.6452186409

H,0,0.9502112168,0.3400171508,-2.1154947042
C,0,0.2401651188,0.6624210854,4.2264100988
H,0,2.3625662804,0.5752129652,3.8253075225
H,0,-1.9412109234,0.7584694939,4.3154917078
H,0,0.3228951958,0.6772101752,5.3088093728
O,0,-1.1149918046,-1.8371270869,-2.3209808295
C,0,-0.5439694345,-1.3866692525,-3.3539609108
O,0,0.1952725928,-0.3586176583,-3.4175144031
C,0,-0.7713425929,-2.141215536,-4.673205949
H,0,-1.3694726858,-3.040555003,-4.5142450018
H,0,0.1991926124,-2.4036001683,-5.1072436507
H,0,-1.2807154412,-1.4777055809,-5.3810480873

Table S49. Cartesian coordinates of the optimized structure for the nitrenium ion of **14**
Charge = 1 Multiplicity = 1

N,0,-0.5115287053,0.000065538,-1.1673677593
C,0,-0.5123376348,-0.0000623116,0.1518531668
C,0,0.9109879811,-0.0000076919,0.5807689324
N,0,1.7159235602,0.0001233606,-0.4406664999
C,0,0.8768442687,0.0001240253,-1.5763531242
N,0,1.1822193799,0.0001758489,-2.8031147826
C,0,-1.6611851752,0.0001825793,-2.0802222217
C,0,1.1811137211,-0.0000857288,1.9956737981
C,0,0.0861588392,-0.0001929906,2.8038107352
C,0,-1.2658155585,-0.0002299131,2.2468343663
N,0,-1.5835572541,-0.0001651159,0.9687890116
H,0,2.1998819736,0.0002281824,-2.9358106673
H,0,2.2015782633,-0.0000574367,2.365461822
H,0,0.1826645401,-0.0002549729,3.8850221516
H,0,-2.1032435945,-0.0003328804,2.9425433849
H,0,-1.614824266,0.8917528051,-2.7090795616
H,0,-2.567927076,-0.0005089109,-1.4756692447
H,0,-1.6141273555,-0.8905920205,-2.7101415901

Table S50. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **15**
Charge = 0 Multiplicity = 1

N,0,-0.7217646348,0.3224275389,0.3196632272
C,0,-0.6878643851,0.3371077705,1.6892488025
N,0,0.527737649,0.3972422014,2.1873631591
C,0,1.3522264514,0.4355783904,1.0761628896
C,0,0.5909919053,0.3725314063,-0.1034843427
C,0,1.176147685,0.3641358436,-1.3962511437
C,0,2.6104703723,0.4356054109,-1.4352450418
C,0,3.3711812129,0.5040993332,-0.2214229855
C,0,2.7679469777,0.5045829626,1.013356869

N,0,3.2936407979,0.4412603415,-2.6139008961
C,0,2.6054291538,0.3779999026,-3.740602266
C,0,1.1937126,0.3036822964,-3.8030308352
C,0,0.4780165447,0.2973797005,-2.6237747275
N,0,-1.8724467609,0.4118033145,2.4394986445
O,0,-2.5817201145,-0.8805957871,2.4826084694
C,0,-3.4581720706,-1.0609466814,1.457402107
O,0,-3.5022792188,-0.3641725194,0.4656385697
C,0,-4.3440875192,-2.2492075065,1.7377724493
H,0,-1.6070612763,0.507306118,3.4187504065
H,0,3.3472728097,0.5542795441,1.9305518616
H,0,4.4506778554,0.5548248783,-0.3227431893
H,0,-5.2217301083,-1.9053907305,2.2985093781
H,0,-4.6808379589,-2.6787672391,0.7923528874
H,0,-3.8293662577,-3.0011569641,2.3407226236
H,0,-1.5865307748,0.302891213,-0.2098219309
H,0,3.188277482,0.3849678065,-4.6607426757
H,0,0.6934342556,0.2534556529,-4.7658089653
H,0,-0.6083042879,0.2413094251,-2.6369063016

Table S51. Cartesian coordinates of the optimized structure for the complex for **15**
Charge = 0 Multiplicity = 1

N,0,1.368574,1.721324,-0.014869
C,0,1.539005,0.399177,-0.010474
C,0,3.000565,0.199524,0.006996
N,0,3.639318,1.349797,0.008960
C,0,2.653907,2.341889,-0.006939
N,0,2.764683,3.612042,-0.011579
C,0,3.526900,-1.134524,0.028669
C,0,2.647231,-2.174816,0.033561
C,0,1.199503,-1.990274,0.009567
C,0,0.625955,-0.678420,-0.011831
C,0,-0.775024,-0.540675,-0.043184
C,0,-1.553239,-1.689923,-0.022467
C,0,-0.899807,-2.929575,-0.012611
N,0,0.436609,-3.090116,0.000179
O,0,-4.418115,-0.472522,-0.016092
C,0,-4.248929,0.779276,0.004381
O,0,-3.098441,1.320498,0.003499
C,0,-5.467386,1.691501,0.041173
H,0,3.754493,3.872646,-0.003612
H,0,4.601457,-1.282364,0.041313
H,0,2.997534,-3.202243,0.044470
H,0,-6.391858,1.114988,-0.056765
H,0,-5.482855,2.243386,0.988424
H,0,-5.404939,2.429488,-0.767275
H,0,0.493990,2.237866,-0.021620
H,0,-1.471580,-3.854824,-0.010374

H,0,-2.637402,-1.558629,-0.023389
H,0,-1.282763,0.425566,-0.070320

Table S52. Cartesian coordinates of the optimized structure for the nitrenium ion of **15**
Charge = 1 Multiplicity = 1

N,0,0.242814148,0.0000090082,-2.0033874445
C,0,0.1976076706,0.0000096325,-0.6839339213
C,0,1.6305115083,0.0000797196,-0.2497364308
N,0,2.4340890148,0.0001175901,-1.2762019949
C,0,1.6244119412,0.0000787954,-2.4181758828
N,0,1.9128378983,0.0001355213,-3.649588491
C,0,1.953548601,0.0000884348,1.1507788855
C,0,0.9276823586,0.0000377017,2.0366703275
C,0,-0.48376603,-0.00002697,1.6280488765
C,0,-0.8711913324,-0.0000447562,0.2496472635
C,0,-2.2464791327,-0.0001128469,-0.0717426708
C,0,-3.1665923253,-0.0001611085,0.962642716
C,0,-2.6858191848,-0.0001405247,2.2848808144
N,0,-1.3872572634,-0.0000755728,2.6133250549
H,0,-0.5225572436,-0.0000268345,-2.6716983309
H,0,2.9273252485,0.0002146011,-3.7975668371
H,0,2.9946959706,0.0001362246,1.4546084233
H,0,1.1018409981,0.0000427826,3.1082301443
H,0,-3.3822406062,-0.0001789215,3.1200822237
H,0,-4.233964478,-0.000214601,0.768441761
H,0,-2.5819709204,-0.0001275457,-1.1056071212

Table S53. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **16**
Charge = 0 Multiplicity = 1

N,0,-0.8447123255,0.383676435,-0.2947642991
C,0,-0.8593599373,0.4004112341,1.0228485667
C,0,0.4927829534,0.4165194021,-0.6252331299
N,0,0.3950294246,0.4377334738,1.5906765871
C,0,1.2858564883,0.430279917,0.5332789599
C,0,1.1022996685,0.4221815771,-1.9130428677
N,0,-2.0062722566,0.470904069,1.8237591268
C,0,2.5340521191,0.4357548192,-1.9578108599
C,0,2.6996053833,0.4392131501,0.494641003
C,0,0.3938872045,0.4144475689,-3.1352091683
C,0,0.7127851009,0.4921068,3.0083401903
O,0,-2.2334243975,-0.8609948047,2.4240071187
H,0,-2.8277320343,0.6154239224,1.2270710479
C,0,3.2990791826,0.4435674947,-0.7447536054
N,0,3.2188376835,0.4406552329,-3.1370411553
C,0,1.1070564457,0.4213937562,-4.3160722582

C,0,-3.505109003,-1.3120536395,2.254758313
H,0,3.2939013325,0.4430433098,1.4041537921
H,0,1.0760362603,-0.4773639369,3.36679444
H,0,1.4789088284,1.2533620107,3.1840245046
H,0,-0.1926243537,0.7606628259,3.5544318795
H,0,-0.692270836,0.4039541449,-3.1213101593
C,0,2.5219128978,0.434213943,-4.2601089579
O,0,-4.3436729027,-0.7032877508,1.6234789746
C,0,-3.7143892603,-2.6223216616,2.9699655077
H,0,4.3799826337,0.4528731426,-0.8438789422
H,0,0.6037003551,0.4168091722,-5.2788562075
H,0,-4.2516066753,-3.3041251055,2.3050654375
H,0,-2.7708575334,-3.0698312889,3.288463016
H,0,-4.3433747189,-2.4449519309,3.8497112747
H,0,3.0997820021,0.4393335351,-5.1835808065

Table S54. Cartesian coordinates of the optimized structure for the complex for **16**
Charge = 0 Multiplicity = 1

N,0,-1.1792815172,0.4393899108,-1.0170750798
C,0,-1.1905527602,0.4310575062,0.2840396537
C,0,0.1684737395,0.4281350707,0.8469962263
N,0,0.9985697329,0.458778697,-0.1793647401
C,0,0.1728497162,0.4310159116,-1.4066427221
N,0,0.5805156949,0.3941309132,-2.5979722995
O,0,3.412272165,-1.8505642704,-1.6988520535
C,0,3.647521316,-1.3149776921,-2.8214657577
C,0,4.6941506368,-1.9790327496,-3.7223298197
O,0,3.0946026551,-0.2651711565,-3.27242399
C,0,0.3973447661,0.4134590124,2.2539048359
C,0,-0.6994489763,0.4047338568,3.0669311866
C,0,-2.070950396,0.4093104155,2.5686967212
C,0,-2.3344667173,0.4243063751,1.1756909728
C,0,-3.6654894994,0.4251541869,0.7402631314
C,0,-4.6720321025,0.4138113274,1.6986477073
C,0,-4.3133338501,0.4008247335,3.0568080678
N,0,-3.0527268421,0.3984453683,3.4923666836
C,0,2.4483314911,0.4313507048,-0.1775273927
H,0,1.402404866,0.4047185377,2.6614582905
H,0,-0.5885841098,0.3933650593,4.1472041401
H,0,2.8096212582,0.5210519539,0.8480252554
H,0,2.7978682945,-0.5235411851,-0.6460544878
H,0,2.8276345738,1.2551391217,-0.7865563215
H,0,1.6258674556,0.2683130352,-2.766648892
H,0,5.1381704657,-2.8518470078,-3.2383824546
H,0,4.2180442432,-2.279188204,-4.6627815659
H,0,5.4755632694,-1.2522712755,-3.9712025208
H,0,-5.0818514957,0.3915655916,3.8268106562
H,0,-3.8844796974,0.4340909304,-0.3233918244

H,0,-5.7191813475,0.414380677,1.4119692594

Table S55. Cartesian coordinates of the optimized structure for the nitrenium ion of **16**
Charge = 1 Multiplicity = 1

N,0,1.0736474585,-1.5743544323,0.0000045959
C,0,0.2977120831,-0.5318656242,-0.0000014764
C,0,1.0889526604,0.7328884081,-0.0000028107
N,0,2.3592274976,0.3686511976,-0.0000006327
C,0,2.38961834,-1.0813055136,-0.000011711
N,0,3.4925687953,-1.698289527,-0.0000067343
C,0,3.5524742532,1.2208779404,0.0000086442
C,0,0.4763025827,2.0064751508,-0.0000027066
C,0,-0.8959414013,2.024804186,-0.0000032716
C,0,-1.729430611,0.8257071475,-0.0000022482
C,0,-1.1481946086,-0.4679341722,-0.0000002693
C,0,-1.9906962938,-1.5860503299,0.0000038667
C,0,-3.3670083774,-1.3691698814,0.0000051082
C,0,-3.8486202964,-0.0503753084,0.0000018517
N,0,-3.0561474325,1.0272553493,-0.0000005284
H,0,3.354239417,-2.7132563502,0.000005691
H,0,1.0591619043,2.921284139,-0.0000011573
H,0,4.4240112457,0.5669399031,-0.0000338328
H,0,3.5569475492,1.8463928373,0.896709314
H,0,3.5569091222,1.8464612747,-0.896644073
H,0,-1.5726219016,-2.5882485245,0.0000062009
H,0,-1.4341918114,2.9689983058,-0.0000020101
H,0,-4.0629168548,-2.202070146,0.0000085611
H,0,-4.9176228865,0.1463484296,0.000004541

Table S56. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **17**
Charge = 0 Multiplicity = 1

N,0,-0.3581497542,0.4294349315,-0.7055836294
C,0,-0.3719694909,0.4368206893,0.682370282
C,0,0.9829974183,0.4364368767,1.0628247958
N,0,1.8012804654,0.3973876765,-0.0451921176
C,0,0.9731068851,0.3984740654,-1.0659193825
N,0,1.3458732862,0.453025492,-2.4158923834
O,0,1.1779574113,-0.8978437954,-2.9927989154
C,0,2.2820098696,-1.3352684075,-3.6561989887
C,0,2.0329382143,-2.6764002075,-4.2977304236
O,0,3.3113596999,-0.6963254954,-3.7189774265
C,0,1.3587053068,0.4583127904,2.4296629853
C,0,0.3694217117,0.4736431712,3.3798806468
C,0,-1.0185231574,0.4608648255,3.0222816019
C,0,-1.4280508086,0.4357648131,1.6408934207

C,0,-2.8195887384,0.4019953088,1.3779026066
C,0,-3.7118211144,0.4045639849,2.4308031594
C,0,-3.208751484,0.4420203879,3.7500110608
N,0,-1.9205018476,0.4672078023,4.0424673708
C,0,-1.4756052733,0.5175946711,-1.6339006423
H,0,2.4112844838,0.4612495708,2.6967216226
H,0,0.6000583291,0.4903283819,4.4402823145
H,0,-2.0746736169,-0.3988863986,-1.6154163483
H,0,-1.0703571782,0.6584221321,-2.6363727754
H,0,-2.1068764225,1.3749099237,-1.3820265499
H,0,2.3552714462,0.6230384689,-2.4800506388
H,0,2.0316028772,-2.550070216,-5.3860210273
H,0,2.8576618073,-3.3469470248,-4.0396560851
H,0,1.0826084431,-3.1111870891,-3.9822903835
H,0,-3.8954693121,0.4486251744,4.5954356305
H,0,-3.1907814239,0.3683118214,0.3596914572
H,0,-4.7835974041,0.3772304505,2.2560321035

Table S57. Cartesian coordinates of the optimized structure for the complex for **17**
Charge = 0 Multiplicity = 1

N,0,0.4311067431,-0.6211386446,-0.5002468259
C,0,0.3640552989,-0.4777425087,0.8106688227
C,0,1.7618162091,-0.4456474306,1.289271074
N,0,2.6189840607,-0.4794304814,0.3076546707
C,0,1.8680726075,-0.5233548144,-0.8727617813
N,0,2.3293614855,-0.4321221278,-2.0421347195
O,0,0.7208210367,0.4199659801,-4.0567375172
C,0,-0.2000932093,1.289508256,-4.0321365309
O,0,-0.9624017401,1.5435628349,-3.0501524006
C,0,-0.4150065385,2.0981146724,-5.3166121776
C,0,2.0388970409,-0.4149129374,2.7010312752
C,0,0.9940378385,-0.4029584733,3.5634133307
C,0,-0.3980934769,-0.366758238,3.1181105357
C,0,-0.7412083572,-0.3721455328,1.7289664665
C,0,-2.0984547879,-0.2134423895,1.386052703
C,0,-3.0428511016,-0.1233054589,2.400115752
C,0,-2.6090144929,-0.1869433375,3.7308205876
N,0,-1.3264996632,-0.2915010805,4.0870359782
C,0,-0.6102505369,-0.8275990017,-1.4834479669
H,0,3.0721821547,-0.4092956117,3.0316438773
H,0,1.1427163533,-0.3894073822,4.6385637917
H,0,-0.2198731554,-1.4758074248,-2.2685551937
H,0,-0.8752814341,0.1507398555,-1.9741476581
H,0,-1.4714615687,-1.301367073,-1.0122318004
H,0,1.6277504935,-0.3049010902,-2.8206459861
H,0,-1.2131162992,2.833967785,-5.1955655146
H,0,0.5202385508,2.6020315332,-5.5846217147
H,0,-0.6627044116,1.4142917074,-6.1364390872

H,0,-3.3255929981,-0.1336255128,4.5476878099
H,0,-4.0958334194,0.0049970101,2.1703834367
H,0,-2.4084859839,-0.1273848103,0.3519311137

Table S58. Cartesian coordinates of the optimized structure for the nitrenium ion of **17**
Charge = 1 Multiplicity = 1

N,0,0.242814148,0.0000090082,-2.0033874445
C,0,0.1976076706,0.0000096325,-0.6839339213
C,0,1.6305115083,0.0000797196,-0.2497364308
N,0,2.4340890148,0.0001175901,-1.2762019949
C,0,1.6244119412,0.0000787954,-2.4181758828
N,0,1.9128378983,0.0001355213,-3.649588491
C,0,1.953548601,0.0000884348,1.1507788855
C,0,0.9276823586,0.0000377017,2.0366703275
C,0,-0.48376603,-0.00002697,1.6280488765
C,0,-0.8711913324,-0.0000447562,0.2496472635
C,0,-2.2464791327,-0.0001128469,-0.0717426708
C,0,-3.1665923253,-0.0001611085,0.962642716
C,0,-2.6858191848,-0.0001405247,2.2848808144
N,0,-1.3872572634,-0.0000755728,2.6133250549
H,0,-0.5225572436,-0.0000268345,-2.6716983309
H,0,2.9273252485,0.0002146011,-3.7975668371
H,0,2.9946959706,0.0001362246,1.4546084233
H,0,1.1018409981,0.0000427826,3.1082301443
H,0,-3.3822406062,-0.0001789215,3.1200822237
H,0,-4.233964478,-0.000214601,0.768441761
H,0,-2.5819709204,-0.0001275457,-1.1056071212

Table S59. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **18**
Charge = 0 Multiplicity = 1

C,0,-3.2841936254,0.0994720517,-1.5900003054
C,0,-3.2308511229,0.0943320748,-0.1932736067
C,0,-2.0186932327,-0.0792767653,0.4758663042
C,0,-0.8454425353,-0.2690265577,-0.2668806381
C,0,-0.8898955374,-0.2712616085,-1.667763651
C,0,-2.1080764938,-0.079342202,-2.322054188
N,0,0.4024144164,-0.4441210073,0.3992074005
O,0,1.5276862642,-0.019748846,-0.3373904198
C,0,1.8812788827,1.3119940033,-0.1123439537
O,0,1.3468011695,2.0112969759,0.7043467498
C,0,2.9963416217,1.6888980629,-1.0517765107
C,0,0.6559055148,-1.2061591278,1.5335416372
C,0,2.1063352328,-1.3156561673,1.9588466456
H,0,-4.2318869856,0.2429051568,-2.1019268966
H,0,-4.1383203473,0.2376406063,0.3873483267

H,0,-1.9794453232,-0.0784203203,1.5572457573
H,0,0.0198767338,-0.4247492827,-2.2380541555
H,0,-2.1345575851,-0.0806485694,-3.4087117294
H,0,2.5710543687,1.9165949901,-2.036567273
H,0,3.499615884,2.5788594986,-0.6702863032
H,0,3.7080978782,0.8680992003,-1.1757423239
O,0,-0.2607957431,-1.7363822954,2.1437553359
H,0,2.1373028625,-1.9492004832,2.8465196936
H,0,2.5204140446,-0.3315287915,2.2049305044
H,0,2.7251618013,-1.7558742146,1.1701288686

Table S60. Cartesian coordinates of the optimized structure for the transition state for **18**
Imaginary frequency: -105.4632
Charge = 0 Multiplicity = 1

C,0,-2.5831921685,-0.9239024838,-2.0696419799
C,0,-2.5494484558,-0.8642896724,-0.6715678186
C,0,-1.3332824839,-0.8867761091,-0.00550575
C,0,-0.1048724894,-1.0002941278,-0.7626884444
C,0,-0.1780626698,-1.0217028195,-2.201722533
C,0,-1.397318852,-0.9999665039,-2.8372136043
N,0,1.1036632656,-1.0035605531,-0.2349365708
O,0,0.1889598721,1.1695867735,0.4155088883
C,0,0.5308099935,2.3546946153,0.8214495301
O,0,1.6903216237,2.6216897897,1.1663206846
C,0,-0.5803647838,3.3951441344,0.8435862591
C,0,1.3655889881,-1.2915049382,1.1287029855
C,0,2.535163761,-0.5599774589,1.7172359539
H,0,-3.5429182451,-0.9041249847,-2.58032957
H,0,-3.4756991689,-0.7897836264,-0.1098260568
H,0,-1.2814613132,-0.8597991908,1.0733263457
H,0,0.7590942857,-1.0690473113,-2.7468646546
H,0,-1.4577831673,-1.0334944419,-3.9208664848
H,0,-1.4004675633,3.0625405684,1.4903666897
H,0,-0.184367094,4.3449973837,1.2131706272
H,0,-0.9883516303,3.5338749901,-0.1641756792
O,0,0.760070214,-2.2039757086,1.6764183616
H,0,2.4339031204,0.5228882606,1.5805921144
H,0,2.6215163598,-0.8153119072,2.7756672206
H,0,3.4459528422,-0.8747705213,1.1917043773

Table S61. Cartesian coordinates of the optimized structure for the complex for **18**
Charge = 0 Multiplicity = 1

C,0,-3.262273,1.004770,0.255252
C,0,-2.335642,0.725801,1.265259
C,0,-1.226063,-0.061324,0.991541
C,0,-1.054534,-0.621123,-0.334889
C,0,-2.010400,-0.275789,-1.359394
C,0,-3.097759,0.509157,-1.061058
N,0,-0.042302,-1.375818,-0.705622
O,0,0.974724,0.792677,-0.015294
C,0,2.037907,1.526680,-0.130028
O,0,3.071991,1.087118,-0.655325
C,0,1.945350,2.946252,0.406316
C,0,0.821090,-2.034333,0.205243
C,0,2.250710,-2.134169,-0.237245
H,0,-4.127550,1.622834,0.482355
H,0,-2.479997,1.133585,2.261195
H,0,-0.510405,-0.312371,1.760764
H,0,-1.838003,-0.674419,-2.353910
H,0,-3.829179,0.756037,-1.824718
H,0,1.690728,2.933622,1.472486
H,0,2.901707,3.457013,0.264653
H,0,1.154363,3.496273,-0.116460
O,0,0.345101,-2.604048,1.178951
H,0,2.659656,-1.144962,-0.474206
H,0,2.835126,-2.620204,0.547123
H,0,2.294821,-2.738211,-1.152567

Table S62. Cartesian coordinates of the optimized structure for the nitrenium ion of **18**
Charge = 1 Multiplicity = 1

C,0,-2.6907222377,-0.2024596899,-1.1591525358
C,0,-2.7656453307,-0.0212911385,0.2399087636
C,0,-1.6007465513,0.1034149236,0.9579724925
C,0,-0.3103422869,0.0294061649,0.2783951493
C,0,-0.2772657186,-0.1555555538,-1.1718414066
C,0,-1.4560659948,-0.2679744033,-1.8603093792
N,0,0.7407991666,0.1211452857,1.0398015433
C,0,2.0809536236,0.2231747836,0.571480867
O,0,2.3486191937,1.2626905214,0.0016721524
C,0,3.0173563322,-0.8671892485,0.9782362619
H,0,-1.5883434458,0.2542540793,2.0333623141
H,0,-3.6148318565,-0.2921433351,-1.7260538302
H,0,-1.4601080978,-0.4028069521,-2.9373760806
H,0,0.6804873249,-0.182410411,-1.6818878573
H,0,-3.733190342,0.0259556264,0.7292201569
H,0,2.6016937043,-1.8580271166,0.7610679529
H,0,3.970084516,-0.7331840338,0.4599828495

H,0,3.1845294659,-0.8103340568,2.0615551965

Table S63. Cartesian coordinates of the optimized structure for the N-acetoxy ester of **19**

Charge = 0 Multiplicity = 1

C,0,-1.7260326741,-0.116055716,-0.4267668713
C,0,-1.7023770414,-0.0715756717,0.9697353549
C,0,-0.4793671114,-0.1187606127,1.6403346633
C,0,0.7169190469,-0.2306236445,0.9133298632
C,0,0.7050481943,-0.2767624511,-0.4903021288
C,0,-0.5177609418,-0.2145536304,-1.1473860847
C,0,-0.8011519418,-0.2463425788,-2.6365651486
H,0,-0.4279098472,-1.1678530294,-3.1049130414
H,0,-0.3187537275,0.5894857006,-3.1625040572
C,0,-2.3140682203,-0.1548849199,-2.6895668132
C,0,-2.8413133999,-0.0778543805,-1.3821551918
C,0,-4.2216106531,0.0127143056,-1.1784870296
C,0,-5.0684174988,0.0257450096,-2.2906450685
C,0,-4.5446564131,-0.0509894116,-3.588091369
C,0,-3.1615404772,-0.1423157228,-3.7933918159
N,0,1.9638871593,-0.2659528425,1.6190540883
C,0,2.2684504552,-1.1660575094,2.6518906994
C,0,3.7359148755,-1.324442123,2.9904391413
O,0,1.3751316438,-1.7432069701,3.2493725662
O,0,3.080230763,0.1133501144,0.8339979777
C,0,3.4440473586,1.4605173062,0.9021827879
C,0,2.6547653526,2.3636506259,1.8143408932
O,0,4.3738348008,1.7879166574,0.2131921972
H,0,-4.6357176997,0.0709386473,-0.1747375025
H,0,-6.1437761475,0.0952937044,-2.1476682768
H,0,-5.2169119229,-0.0400104306,-4.4421665461
H,0,-2.7615780838,-0.202596364,-4.8034132645
H,0,1.6365871338,-0.3595207719,-1.0406053171
H,0,-2.6221886189,0.0056273228,1.5437388815
H,0,-0.4481179018,-0.089328449,2.7223337598
H,0,4.1983346953,-0.3677104716,3.2576765276
H,0,3.8044633965,-2.0084263131,3.8377554644
H,0,4.2953266663,-1.7262710687,2.1394445694
H,0,3.0928212672,3.3608622123,1.7551748785
H,0,1.6033871217,2.4020527245,1.5120886328
H,0,2.6821524306,2.0061948217,2.848539454

Table S64. Cartesian coordinates of the optimized structure for the complex for **19**
Charge = 0 Multiplicity = 1

C,0,-0.688132,-1.348062,0.093774
C,0,0.315674,-2.237676,0.603720
C,0,1.628494,-1.930810,0.428821
C,0,2.019782,-0.701310,-0.278011
C,0,0.975009,0.199108,-0.775106
C,0,-0.334610,-0.133962,-0.583856
C,0,-1.578442,0.639818,-0.911208
H,0,-1.644061,0.987787,-1.948403
H,0,-1.571841,1.583678,-0.285846
C,0,-2.662502,-0.286935,-0.486175
C,0,-2.108172,-1.446742,0.147130
C,0,-2.943940,-2.452854,0.687629
C,0,-4.313642,-2.297952,0.579097
C,0,-4.860113,-1.154639,-0.054779
C,0,-4.049398,-0.152231,-0.583230
N,0,3.251375,-0.348203,-0.485247
C,0,4.370283,-1.112329,-0.126943
C,0,5.297604,-0.414508,0.843100
O,0,4.611299,-2.185075,-0.657638
O,0,-1.294704,3.130463,0.596083
C,0,-0.197202,3.656263,0.225775
C,0,0.112510,5.072722,0.702105
O,0,0.637705,3.080448,-0.526955
H,0,-2.521618,-3.327907,1.174080
H,0,-4.981759,-3.053822,0.981651
H,0,-5.940653,-1.058714,-0.123556
H,0,-4.488375,0.723743,-1.052292
H,0,1.267705,1.137663,-1.232594
H,0,0.025106,-3.148786,1.119561
H,0,2.411224,-2.591674,0.784903
H,0,4.745262,-0.000041,1.693801
H,0,6.056601,-1.120775,1.186676
H,0,5.783727,0.425984,0.333460
H,0,1.178574,5.174019,0.930316
H,0,-0.122817,5.778176,-0.105105
H,0,-0.490325,5.333997,1.577089

Table S65. Cartesian coordinates of the optimized structure for the nitrenium ion of **19**
Charge = 1 Multiplicity = 1

C,0,-2.03805142,0.0699503805,0.1227633788
C,0,-2.0387289173,0.0853406963,1.6317841045
C,0,-0.6984364018,0.0544370463,2.1310012686
C,0,0.2010965265,0.0196288505,1.0319254834
C,0,-0.5600957465,0.0296122327,-0.2017772124
C,0,0.0654246554,-0.0026132102,-1.4045782232

C,0,1.532877401,-0.0552348105,-1.4414406217
C,0,2.2729128964,-0.0579133715,-0.1728838858
C,0,1.6293437636,-0.0215043165,1.0262086381
N,0,2.2479130606,-0.104809834,-2.5208369589
C,0,1.6928202368,-0.2327590455,-3.8232529892
O,0,1.0039168458,-1.199914276,-4.0877187208
C,0,2.153114905,0.8150364216,-4.797658361
C,0,-0.4344149482,0.0600995959,3.523043403
C,0,-1.5099866917,0.0970022097,4.3919223467
C,0,-2.8319512087,0.1280781352,3.8912112446
C,0,-3.1061650551,0.122832467,2.5167295699
H,0,-2.5674839524,-0.8035869075,-0.2805043881
H,0,-2.5273106573,0.9580511059,-0.2988009805
H,0,-0.484207765,-0.0143589673,-2.3400738545
H,0,3.3553011089,-0.0970271638,-0.2460258235
H,0,2.1844849337,-0.0290732897,1.9589323261
H,0,0.5835119713,0.0359511555,3.900345962
H,0,-1.346138194,0.1019701723,5.4648722217
H,0,-3.6589504518,0.1563095466,4.5954685735
H,0,-4.132798911,0.1465519511,2.1631066976
H,0,1.5548377075,0.7485085966,-5.7087438665
H,0,3.2075344167,0.636610804,-5.0426919207
H,0,2.0859336318,1.8211163538,-4.3682653335