

Near IR-emitting DNA-probes exploiting stepwise energy transfer processes

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Absorption and excitation spectra of 1 in CH₂Cl₂

S-I

Emission spectra of 1 in CH₂Cl₂

S-II

Emission spectra of Yb1 with and without DNA

S-II

B3LYP/6-31G(d,p) optimized geometries

S-III-XXXIX

Reference

S-XXXIX

General Procedures. Absorption spectra and fluorescence spectra were collected at room temperature in methanol, unless noted otherwise. Emission spectra were recorded on a FluoromaxP or a Fluorolog 3 Tau spectrofluorimeter. Titrations of **1** with double stranded salmon testis DNA were carried out in HPLC-grade methanol in triplicates. Concentrations were such that $A(\mathbf{1}) < 0.1$. Aliquots of a stock solution of *ds*DNA (in 10 mM HEPES) were added to the methanolic solution of **1**. Excitation of the sample was performed at 328 nm and 525 nm. The emission intensity was monitored between 540 and 750 nm. Emission intensities and luminescent lifetimes of the Nd and Yb complexes were determined in methanol analogously to a reported method in HPLC-grade methanol.¹²

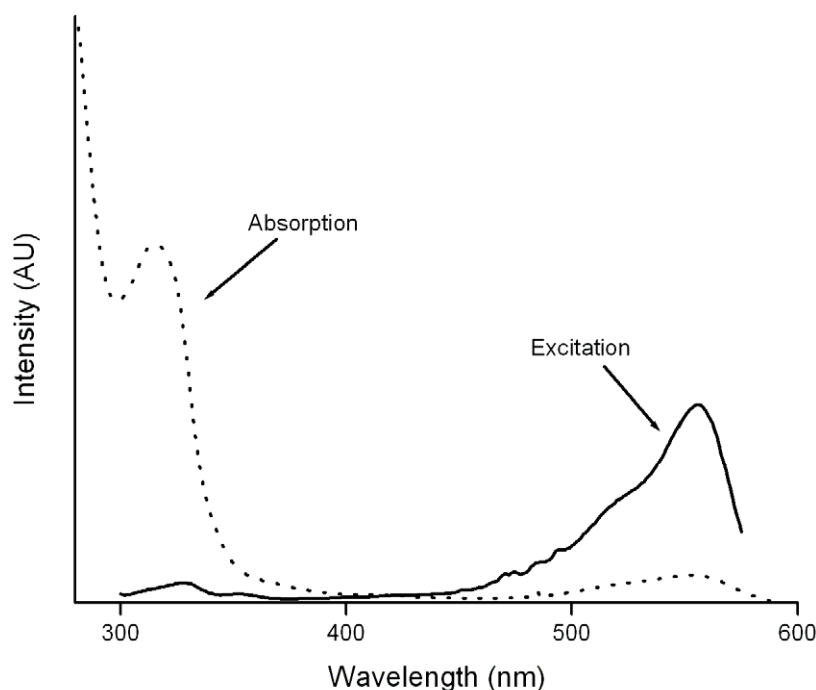


Figure 1. Absorption and excitation spectra of **1** in CH₂Cl₂.

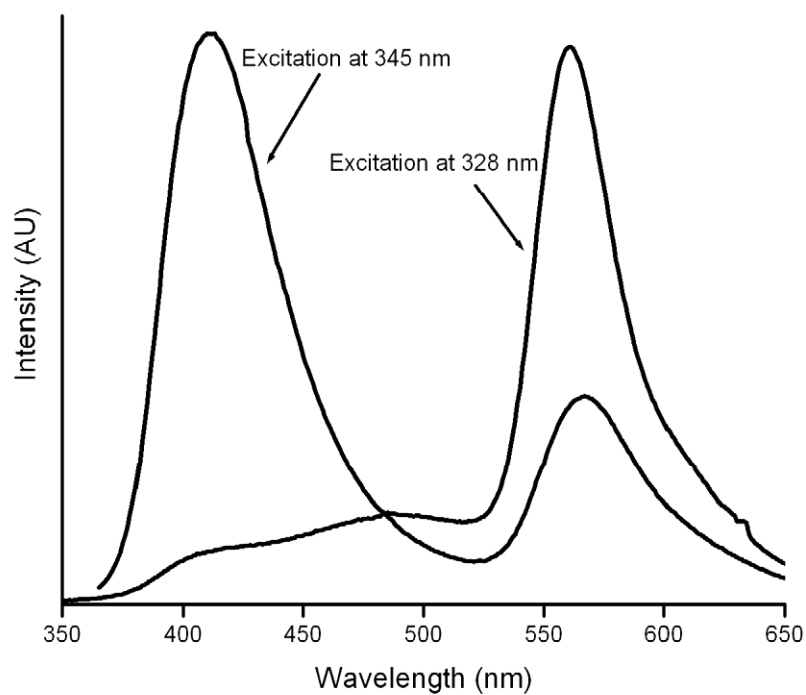


Fig. 2 Emission spectra of **1** in CH₂Cl₂. Excitations were performed at 345 nm and 328 nm.

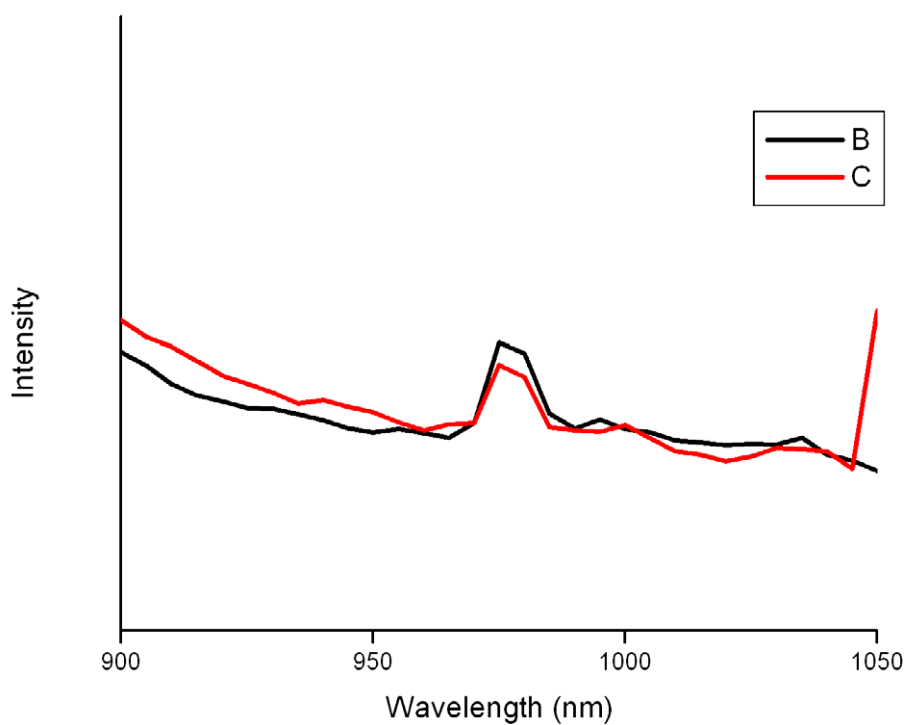


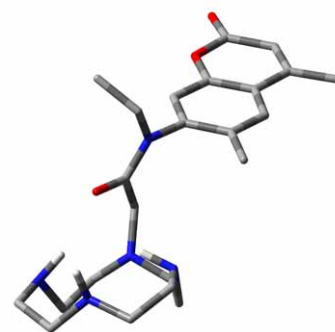
Figure 3. Emission spectra of **Yb1** without (Data set 'B') and with added DNA (1 equiv., Data set 'C'). [Yb1] = 0.033 mM, λ_{exc} = 355 nm.

B3LYP/6-31G(d,p) optimized geometries in Cartesian coordinates (Å) for selected conformers of **4** that have been subjected to frequency analysis and B3LYP/6-311+G(d,p) single point energy calculations with the Gaussian 03 computational chemistry suite.¹ In the graphics hydrogen atoms bound to N's are only shown for clarity.

For the notation see Table 1 in text.

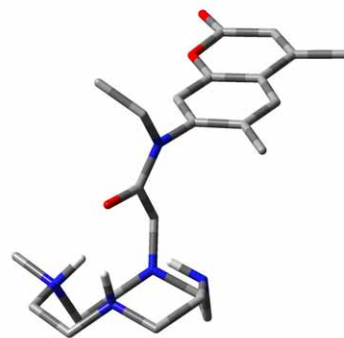
4.[2424].1.iei

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N	5.08526600	0.50220700	0.66654600
C	5.16067000	1.91816000	0.33795700
C	1.74907000	0.74501400	-2.18209500
N	1.72454000	-0.57090600	-1.54627900
C	2.45409400	-1.65022600	-2.21123700
C	5.48526600	-1.86117600	0.05698700
N	4.14271700	-2.05701200	-0.47158900
C	3.95056800	-1.71114200	-1.87111500
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H	5.88601200	2.49108600	0.94432200
H	3.50670400	2.65525400	1.53214200
H	3.80638100	3.59829800	0.07693100
H	2.34845800	-1.56410600	-3.30651400
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H	2.68126500	2.68675200	-2.10530900
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C	0.54418700	-0.89513300	-0.77788000
H	0.28701600	-1.95488500	-0.90980500
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C	0.72489100	-0.70157800	0.74451200
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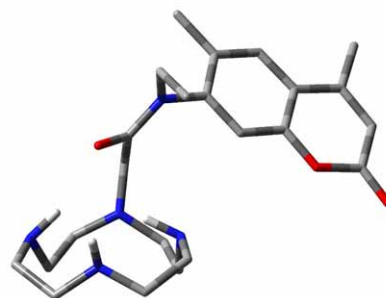
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C	1.64754800	1.18729800	-2.29584000
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C	5.17169000	-1.67441600	0.31986200
N	3.82346900	-1.82646900	-0.35059700
C	3.80550200	-1.40947000	-1.79818800
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H	5.69552600	2.60512900	1.07519300
H	3.31010100	3.00515500	1.49850800
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H	1.82401100	-2.14235600	-2.32644700
H	4.34014200	-2.17266800	-2.37355700
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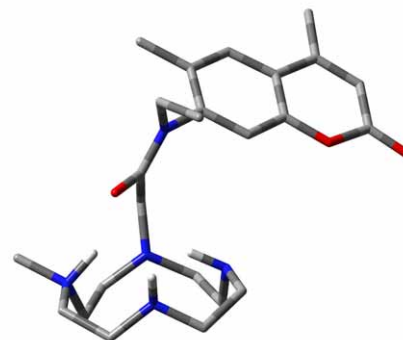
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N	4.55045300	-0.89439800	-1.09322800
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H	-7.35141100	0.35162000	-1.05790000
H	-6.30016900	-0.84744800	-1.83128300
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O	-4.18414300	3.83212600	0.23027700
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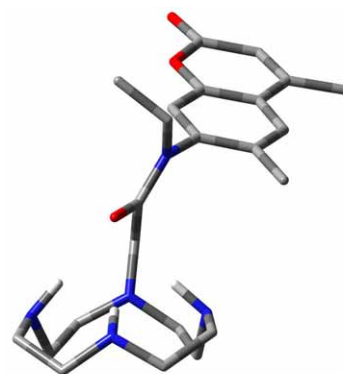
[4.**[2424].2.iei.N4-CH₃**]⁺

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N	4.08992700	1.24086000	1.26617200
C	3.70742400	2.65916800	1.33666500
C	0.98805800	1.42891800	-1.89862800
N	1.54294400	0.07406600	-1.74692800
C	2.68059800	-0.28025200	-2.57221100
C	5.43580100	-0.51225800	0.17625400
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H	1.89124300	3.84084600	1.36851900
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H	4.14910500	0.94934400	-1.58506500
H	1.12319200	1.77306600	-2.93253700
H	-0.08658800	1.37912700	-1.71201100
H	2.64249000	2.65099000	-1.23011600
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H	0.81656900	-1.89356300	-1.89039200
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C	-0.10929700	-2.12801500	2.28781800
H	-0.97762400	-2.74833100	2.51293400
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H	0.91390900	-0.40424100	3.12188800
H	-0.84572600	-0.36969900	3.34571600
H	0.14728800	-1.45853800	4.31887800
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C	-1.62790900	-1.23895000	0.51549100
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H	-6.74478200	1.82054600	-0.69338600
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H	-2.30604400	-4.14998900	1.09469000
H	-2.91999900	-4.22457600	-0.55221200
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C	-6.64164500	-0.89872400	-0.89188600
H	-6.83829700	-1.61603500	-0.08920200
H	-7.56869200	-0.36903000	-1.10934800
H	-6.35998900	-1.47274100	-1.78008700
O	-3.50271200	1.84560700	0.24227500
O	-4.89383800	3.56168700	-0.04280900
H	4.00461600	0.80290800	2.17833600
H	3.38851600	-0.91553600	-0.12795400
H	1.79667900	1.06162800	0.48810000
C	4.45661900	-2.38986600	-1.06011400
H	5.35679700	-2.49919800	-1.66481000
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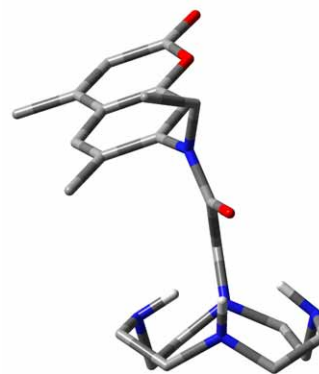
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C	6.01465900	-0.57601300	0.11389900
N	5.13731000	0.39581200	0.75710100
C	5.27834500	1.77392800	0.30027400
C	1.82936800	0.79238400	-2.19962800
N	1.73818800	-0.51352100	-1.54499800
C	2.42568600	-1.63465000	-2.18865400
C	5.39871200	-1.99190100	0.16020800
N	4.06623800	-2.14933000	-0.41862600
C	3.90895400	-1.77720300	-1.81658200
H	5.62767800	1.82243400	-0.74861700
H	6.04135500	2.29907600	0.89295600
H	3.69069000	2.63596500	1.49260500
H	4.09784100	3.56615100	0.05023300
H	2.35122400	-1.54565800	-3.28555800
H	1.91885600	-2.56230300	-1.90142500
H	4.34429700	-2.56305000	-2.45329400
H	4.42669600	-0.84342300	-2.09446400
H	1.97433600	0.65722200	-3.28315100
H	0.87577700	1.31811800	-2.06675800
H	3.92004700	1.23389100	-1.92178000
H	2.91594300	2.65162300	-2.21596500
H	5.33419600	-2.31239200	1.20616300
H	6.08996000	-2.68151700	-0.34325300
H	6.22867000	-0.30148000	-0.93721800
H	6.99010800	-0.60544900	0.62041900
C	0.53640200	-0.77753700	-0.78817300
H	0.23246800	-1.82599600	-0.91028600
H	-0.30423800	-0.17453700	-1.15012400
C	0.71780400	-0.56639500	0.73172100
O	1.81088500	-0.74400400	1.27419800
N	-0.37661700	-0.19524300	1.46805000
C	-0.21848200	-0.05167000	2.93179100
H	0.78262100	0.34507500	3.11202700
H	-0.95127500	0.68828300	3.26555200
C	-0.40647000	-1.37095600	3.68026600
H	-1.40525800	-1.78661100	3.51413200
H	0.33918300	-2.10076200	3.35530000
H	-0.28152800	-1.21178400	4.75627600
C	-2.56981300	-0.90803500	0.67022000
C	-3.82740400	-0.61336500	0.14253200
C	-1.65553300	0.11717700	0.89771300
C	-4.19128600	0.71038900	-0.16124400
C	-1.98251400	1.46537200	0.60981300
C	-5.95592100	-1.49242400	-0.58027500
C	-5.52012000	0.94370200	-0.71069500
C	-3.24581100	1.72407000	0.08395900
C	-6.33691900	-0.12289200	-0.89848700
H	-3.50813500	2.75122700	-0.14796900
H	-7.33630600	-0.01102100	-1.30324200
H	-2.31678500	-1.93766900	0.89544200
C	-1.00094500	2.58566700	0.85889200
H	-0.01438000	2.38915800	0.42479900
H	-1.37570700	3.52285800	0.43970700
H	-0.84274500	2.74704300	1.93170500
C	-5.96318100	2.33866800	-1.05650800
H	-5.30074600	2.78778700	-1.80507600
H	-6.97929600	2.33854400	-1.45530500
H	-5.94091800	2.98897300	-0.17476600
O	-4.67136500	-1.66424400	-0.05831200
O	-6.64130500	-2.47567100	-0.72664200
H	3.35847300	-1.69114400	0.15228500
H	2.56168700	1.07297400	0.21342800
H	4.18083600	0.09658300	0.59383600



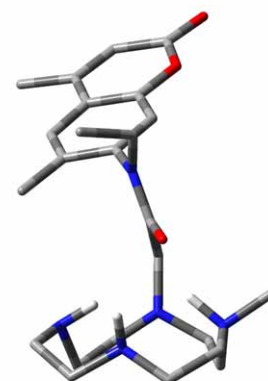
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C	-3.89318200	-2.21367000	-1.32853700
N	-4.05355600	-2.18713300	0.11683800
C	-5.40429200	-1.94939400	0.60559800
C	-5.32338000	1.79395000	-0.06696300
N	-5.14906300	0.50847400	0.59352800
C	-6.04110700	-0.58670200	0.24218800
C	-2.40708800	-2.14076800	-1.70898300
N	-1.75972500	-0.86581200	-1.39827800
C	-1.92158100	0.21812500	-2.36559200
C	-3.96771400	2.53597600	-0.16366500
N	-2.85747700	1.72563000	-0.66584000
C	-3.03732700	1.21940100	-2.02316600
H	-6.20937700	-0.53577400	-0.83994400
H	-7.04267100	-0.52683200	0.70946300
H	-5.37572100	-2.04117400	1.70003300
H	-6.07017700	-2.74824700	0.24949300
H	-2.12147600	-0.20156900	-3.36414500
H	-0.97681000	0.77121000	-2.43442800
H	-2.98584300	2.05639200	-2.73459600
H	-4.01222800	0.73077100	-2.18412700
H	-2.31175500	-2.36547900	-2.78563000
H	-1.88657300	-2.93254900	-1.16010900
H	-4.42720200	-1.40648900	-1.86084200
H	-4.29945700	-3.15763300	-1.72356700
H	-3.68428600	2.89224200	0.83557400
H	-4.08848600	3.42955900	-0.79058200
H	-5.70531900	1.59646700	-1.07463600
H	-6.06602700	2.45728600	0.41287400
C	-0.53747300	-0.88314200	-0.63350700
H	0.22542900	-0.25802000	-1.10770200
H	-0.11023700	-1.89675700	-0.60287200
C	-0.69724500	-0.47132800	0.84860700
O	-1.77671300	-0.53279500	1.43081400
N	0.45500900	-0.13953000	1.53011400
C	0.39764100	-0.07304100	3.00507700
H	-0.39221800	-0.75918500	3.31598800
H	1.35217200	-0.45024500	3.38516400
C	0.11768200	1.32268700	3.56224000
H	0.91332200	2.02812700	3.30398800
H	-0.83200200	1.70319600	3.17801300
H	0.05329900	1.27861400	4.65469500
C	2.71029600	-0.82984000	0.94880800
C	3.94502700	-0.59744700	0.34598400
C	1.70415700	0.13230400	0.87988500
C	4.19399700	0.59921600	-0.34902300
C	1.92096400	1.36232300	0.20781700
C	6.14449700	-1.47106100	-0.12732900
C	5.50085600	0.76945000	-0.96801400
C	3.16119600	1.55351900	-0.39884600
C	6.40811400	-0.23196900	-0.84623000
H	3.33864900	2.48686900	-0.92332900
H	7.39657000	-0.16211600	-1.28577000
H	2.54112300	-1.77099500	1.46013200
C	0.87033200	2.44749100	0.15075200
H	0.67088100	2.85471900	1.14709000
H	1.21398800	3.27186100	-0.47958300
H	-0.09609800	2.10877400	-0.23855600
C	5.82381500	2.02969100	-1.72260400
H	5.73742100	2.90914400	-1.07457500
H	6.83920300	1.99711000	-2.12202400
H	5.13052300	2.17624800	-2.55849600
O	4.87875900	-1.58539500	0.45141400
O	6.91360900	-2.39208000	0.01132400
H	-5.06090500	0.61018600	1.59985000
H	-2.80624200	0.90672400	-0.05853500
H	-3.43215400	-1.47628700	0.50174200



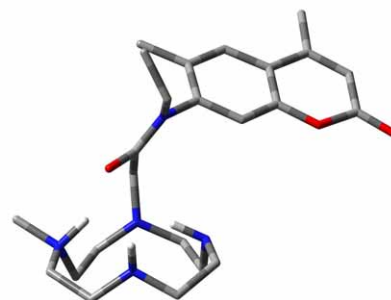
[4.[2424].4.iei.N10-CH₃]⁺

C	-3.77103500	-1.72245100	-1.61011700
N	-3.78270700	-1.94548000	-0.11968100
C	-5.14160000	-1.76731600	0.52182700
C	-5.06349200	2.01436700	0.20831900
N	-4.79507200	0.65620900	0.69902100
C	-5.75303200	-0.37523500	0.34646500
C	-2.35309800	-1.52256400	-2.18600600
N	-1.63922000	-0.36875500	-1.67507700
C	-1.74925900	0.88710500	-2.43400100
C	-3.74400000	2.81526600	0.14486500
N	-2.64436500	2.11058900	-0.51333000
C	-2.85315100	1.82186400	-1.92723500
H	-6.05764000	-0.22097400	-0.69372200
H	-6.68864700	-0.37212200	0.93248900
H	-4.98838800	-1.97896500	1.58387100
H	-5.80472400	-2.53824300	0.11785500
H	-1.92148000	0.66603600	-3.49700400
H	-0.79364000	1.41494500	-2.36337000
H	-2.81341100	2.75622400	-2.50161700
H	-3.83588300	1.36605100	-2.15097500
H	-2.49249500	-1.44073100	-3.27451100
H	-1.75471600	-2.42726500	-2.02978500
H	-4.36213100	-0.82949900	-1.80343800
H	-4.26463800	-2.57952300	-2.08026800
H	-3.41923300	3.05600700	1.16476400
H	-3.92688400	3.77201900	-0.35734500
H	-5.49347900	1.92368600	-0.79487200
H	-5.80346100	2.55968700	0.81413500
C	-0.42676800	-0.58008700	-0.91117500
H	0.34428300	0.12568800	-1.22435000
H	-0.00657100	-1.57954300	-1.10396700
C	-0.62348600	-0.49214300	0.61749800
O	-1.73623500	-0.73459300	1.12935800
N	0.45443900	-0.22275900	1.38637200
C	0.34571800	-0.36971000	2.86035600
H	-0.44084300	-1.10274300	3.04563100
H	1.29490500	-0.78850100	3.20423200
C	0.03632600	0.93200000	3.59682100
H	0.84229400	1.66148300	3.48445800
H	-0.89421900	1.37514200	3.23294800
H	-0.07756900	0.72539500	4.66541400
C	2.68580900	-0.92562500	0.74100400
C	3.96243200	-0.66472600	0.24516100
C	1.74993100	0.10233800	0.83152000
C	4.32025700	0.63101500	-0.17059300
C	2.06448200	1.42105500	0.43037500
C	6.12744400	-1.57356000	-0.31324900
C	5.67238100	0.83766800	-0.68016500
C	3.35001100	1.64223900	-0.06872100
C	6.50648500	-0.22973800	-0.73342400
H	3.61022300	2.64666700	-0.38548200
H	7.52244900	-0.14038900	-1.10070900
H	2.44066600	-1.93512600	1.05281500
C	1.08423700	2.56776500	0.52998300
H	0.95200100	2.89009600	1.56801900
H	1.45463100	3.42918000	-0.03086300
H	0.08681500	2.32748400	0.14755600
C	6.11466000	2.20347800	-1.12637200
H	6.04667600	2.92686600	-0.30603200
H	7.14770400	2.18376300	-1.47730700
H	5.48435500	2.57721300	-1.94129500
O	4.81955700	-1.71534900	0.17834100
O	6.81992900	-2.55780300	-0.34883500
H	-4.62734000	0.66863100	1.70211500
H	-2.55634900	1.21436900	-0.03755200
H	-3.10630200	-1.24137000	0.29802300
C	-3.23603800	-3.28840600	0.25160400
H	-3.17792900	-3.35289400	1.33777600
H	-3.89209900	-4.06867000	-0.13813900
H	-2.23575400	-3.40434100	-0.15999000



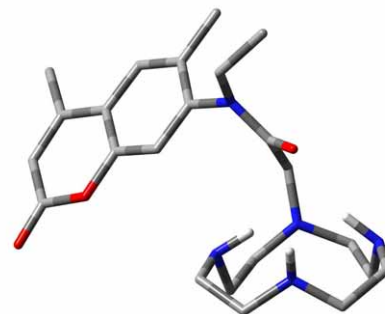
[4.**[2424]**.4.iei.N4-CH₃]⁺

C	1.51889800	2.47136800	-0.92297400
N	1.38271900	2.030005400	0.46214500
C	2.10909400	2.83584400	1.44463100
C	5.35934700	1.04645200	0.69526100
N	4.04415000	1.32686400	1.24268500
C	3.64607700	2.73870700	1.32970800
C	0.94499700	1.41047900	-1.87025700
N	1.57265600	0.08623400	-1.73929000
C	2.72312400	-0.20879700	-2.56767100
C	5.45303800	-0.40298600	0.21015400
N	4.30523000	-0.85044600	-0.67024100
C	4.09239900	0.01105300	-1.88880100
H	3.98619500	3.23207100	0.41257700
H	4.11820400	3.27649600	2.16653500
H	1.80338100	2.49920300	2.44329800
H	1.80366500	3.88477600	1.36480600
H	2.73247700	0.44409000	-3.45261500
H	2.65506900	-1.23271500	-2.95427400
H	4.91118600	-0.19184300	-2.58738800
H	4.15866700	1.04551400	-1.55953400
H	1.03516100	1.76602800	-2.90685200
H	-0.12170500	1.30161800	-1.65416300
H	2.56149600	2.69029800	-1.22132400
H	0.95863800	3.40387700	-1.06476200
H	5.44540600	-1.08921400	1.06185700
H	6.38159400	-0.56533500	-0.34544400
H	5.54109500	1.73636400	-0.13492200
H	6.20096200	1.19631400	1.39311800
C	0.72824400	-1.00442300	-1.28470400
H	1.01993700	-1.93913100	-1.78185100
H	-0.31692700	-0.82176400	-1.54383000
C	0.88746200	-1.26222800	0.22565600
O	2.03836900	-1.37269900	0.70177500
N	-0.21226200	-1.36580800	1.00248900
C	-0.04897800	-1.51373200	2.47232000
H	0.98161800	-1.24174500	2.69967000
H	-0.71217700	-0.78038300	2.93896500
C	-0.35893800	-2.91656100	2.98931600
H	-1.39388400	-3.20456300	2.78582900
H	0.30905200	-3.65876300	2.54268900
H	-0.21483800	-2.94253600	4.07363500
C	-2.00234500	0.23285000	0.67870600
C	-3.30163900	0.56124100	0.29625000
C	-1.54750800	-1.07649600	0.52350400
C	-4.16600800	-0.41484100	-0.23749000
C	-2.36745100	-2.08271200	-0.02824700
C	-4.96423200	2.30179400	0.11617200
C	-5.51979800	-0.00718800	-0.60079000
C	-3.66647400	-1.71815600	-0.39100200
C	-5.86825800	1.28998700	-0.41814600
H	-4.31535800	-2.47985900	-0.81053900
H	-6.85812900	1.65435100	-0.66814200
H	-1.34365000	1.00499800	1.06403400
C	-1.87588400	-3.48791200	-0.28491500
H	-1.17074000	-3.82745900	0.47523500
H	-2.71171600	-4.19123700	-0.30994400
H	-1.36910000	-3.55973600	-1.25605300
C	-6.48993000	-1.01048000	-1.15973100
H	-6.66003600	-1.83017000	-0.45262100
H	-7.45192700	-0.54368900	-1.37739200
H	-6.10888900	-1.45510200	-2.08609800
O	-3.67991600	1.85534000	0.46174400
O	-5.21469700	3.46777300	0.28414500
H	3.92283700	0.86911500	2.14309200
H	3.40909200	-0.81656300	-0.10208800
H	1.79060100	1.09858800	0.51451500
C	4.48808700	-2.29308400	-1.02236500
H	4.55924700	-2.87059300	-0.10101500
H	3.62791300	-2.64283000	-1.58929700
H	5.39815200	-2.41115200	-1.61304700



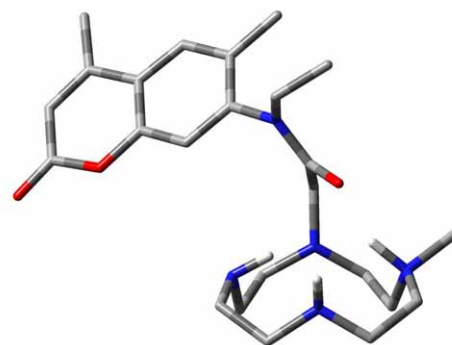
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C	-4.15454700	-0.25409600	2.10901600
N	-4.53775500	0.69529700	1.07517100
C	-5.67290000	0.31044600	0.24805200
C	-3.72814400	-2.23643500	-1.80071400
N	-4.30120800	-0.96840300	-1.36768300
C	-5.52296700	-0.99076900	-0.57525900
C	-2.77566500	0.09782700	2.68542700
N	-1.67178400	-0.05840300	1.73944800
C	-1.07286600	-1.38788400	1.62031800
C	-2.19243100	-2.10719700	-1.94048700
N	-1.53115500	-1.47660000	-0.79575200
C	-1.61463300	-2.23251600	0.45352500
H	-5.45482400	-1.84787300	0.10458200
H	-6.44495600	-1.14425500	-1.16736400
H	-5.87109200	1.14267500	-0.44089500
H	-6.56876000	0.21511900	0.87824600
H	-1.22211500	-1.94859500	2.55620500
H	0.00852900	-1.27308800	1.48702800
H	-1.00462100	-3.14215600	0.36836400
H	-2.63911200	-2.55963400	0.69653600
H	-2.60287800	-0.52382200	3.58057800
H	-2.80825800	1.14246600	3.01242100
H	-4.12788200	-1.30537000	1.77162300
H	-4.88930000	-0.21548900	2.92809900
H	-1.96636400	-1.49717400	-2.82501600
H	-1.75490000	-3.09674700	-2.12304700
H	-3.96618500	-2.98341600	-1.03572100
H	-4.14677600	-2.62616100	-2.74609400
C	-0.79821300	1.06732100	1.48744600
H	0.24057900	0.85111400	1.76350000
H	-1.11555900	1.91960800	2.10174900
C	-0.88202600	1.60316000	0.04180600
O	-1.97244500	1.78079500	-0.49550500
N	0.28833500	1.99889200	-0.57841000
C	0.14601400	2.64818400	-1.90626900
H	1.14118200	2.66240600	-2.35678400
H	-0.49351400	2.01221100	-2.52829100
C	-0.43490900	4.05996900	-1.84086600
H	-1.43948700	4.04031700	-1.41611400
H	0.19144200	4.72430200	-1.23876200
H	-0.49802700	4.47586000	-2.85198000
C	1.67308100	-0.00528700	-0.52230600
C	2.89635400	-0.63176300	-0.28517400
C	1.54971400	1.36712000	-0.30264900
C	4.01894100	0.09692100	0.14859100
C	2.65268700	2.13830000	0.13449400
C	4.11473700	-2.71625100	-0.30551800
C	5.26264600	-0.62690700	0.36812300
C	3.86123700	1.48079500	0.34839800
C	5.27939800	-1.96460100	0.14276800
H	4.71165800	2.06110400	0.69193400
H	6.17599900	-2.55630400	0.28830700
H	0.81873500	-0.59242900	-0.85703500
C	2.53324600	3.62279300	0.37368500
H	1.60487800	3.86762600	0.89713300
H	3.37389300	3.98950600	0.96832800
H	2.52615100	4.18583400	-0.56706700
C	6.49343500	0.10262600	0.83252100
H	6.31868500	0.59707700	1.79479400
H	7.33440300	-0.58369400	0.94871000
H	6.78253800	0.88173900	0.11813300
O	2.94799200	-1.97854800	-0.50066100
O	4.07505700	-3.90546300	-0.51745100
H	-4.36813800	-0.30556900	-2.13395600
H	-2.03562600	-0.60392800	-0.63398800
H	-3.73327700	0.87644700	0.47579400



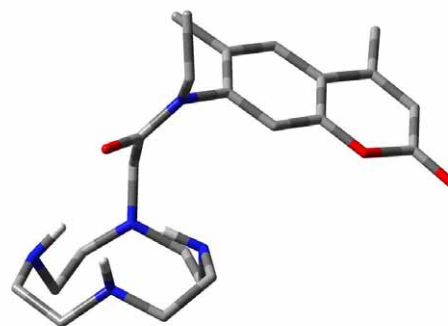
[4.[2424].5.iei.NII-CH₃]⁺

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N	-4.25179800	0.65876900	0.76759600
C	-5.38046000	0.28299700	-0.16971200
C	-3.45393600	-2.61828400	-1.67506200
N	-3.90678700	-1.24748800	-1.40159500
C	-5.23211600	-1.09020000	-0.83085600
C	-2.65799000	-0.15721100	2.58564600
N	-1.49835700	-0.32100000	1.73327600
C	-0.83805200	-1.63612100	1.71391600
C	-1.91336900	-2.64037800	-1.77993900
N	-1.23312700	-1.94725300	-0.68464900
C	-1.36290100	-2.58027000	0.62513500
H	-5.38745100	-1.88532800	-0.09458300
H	-6.06720300	-1.18300800	-1.54642700
H	-5.39548200	1.06914200	-0.93009200
H	-6.31570700	0.34282200	0.39506700
H	-0.94396000	-2.12167800	2.69447500
H	0.23066700	-1.47748600	1.54515100
H	-0.76814800	-3.50165000	0.64507800
H	-2.39915400	-2.87553200	0.87550400
H	-2.65093000	-0.90972500	3.38744300
H	-2.61913800	0.81557300	3.09026300
H	-4.05419100	-1.32372700	1.42742200
H	-4.84566000	-0.23920500	2.58909800
H	-1.61112600	-2.15842700	-2.71819300
H	-1.56578100	-3.67738100	-1.83797200
H	-3.78284500	-3.24579400	-0.83950800
H	-3.89693100	-3.05308800	-2.58442400
C	-0.67850900	0.83625800	1.42306500
H	0.37166500	0.64853500	1.65460100
H	-0.98595300	1.69106400	2.04218200
C	-0.84596000	1.31687900	-0.03177900
O	-1.99457000	1.40463200	-0.51666400
N	0.23854400	1.70664000	-0.73844400
C	0.02245800	2.24155600	-2.11269700
H	1.00257000	2.25157500	-2.59192500
H	-0.60607200	1.52549100	-2.65170100
C	-0.61250600	3.63041900	-2.14933500
H	-1.60325200	3.61885300	-1.69219500
H	0.00545600	4.37042900	-1.63551000
H	-0.72165100	3.94720200	-3.19102500
C	1.88038400	-0.07630700	-0.55574800
C	3.16906400	-0.52899500	-0.27333700
C	1.57924600	1.27658500	-0.40031000
C	4.17678800	0.36234800	0.14079500
C	2.55344200	2.20719000	0.01804500
C	4.64565700	-2.43591200	-0.16198900
C	5.50567200	-0.17973300	0.40550800
C	3.83448600	1.71831600	0.27791200
C	5.69648700	-1.51294400	0.24953500
H	4.59555800	2.41892200	0.60520500
H	6.66041700	-1.97487000	0.42982000
H	1.12126200	-0.78662900	-0.87476400
C	2.25101300	3.67707600	0.17935700
H	1.25880300	3.84428200	0.60756000
H	2.98707900	4.15417900	0.83060400
H	2.28078600	4.20259100	-0.78243900
C	6.62364500	0.72868500	0.83578100
H	6.38030100	1.23725700	1.77555000
H	7.54792900	0.16757600	0.98268300
H	6.81078500	1.50534800	0.08575600
O	3.39183400	-1.86208100	-0.41735200
O	4.75266500	-3.62816600	-0.29848200
H	-3.79912800	-0.66735800	-2.23027400
H	-1.68202400	-1.03568600	-0.61547200
H	-3.35124100	0.71852200	0.20815400
C	-4.48278600	2.04330200	1.28541500
H	-4.56453600	2.72305400	0.43759500
H	-5.40110700	2.06404700	1.87472700
H	-3.63927900	2.34926900	1.90062600



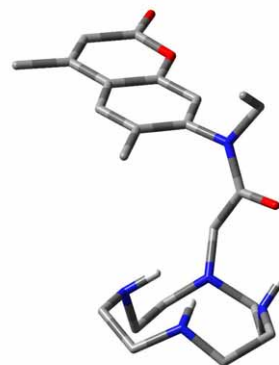
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N	-1.66746500	-1.51671600	0.70582800
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C	-5.66310600	-0.91099600	0.38759700
N	-4.45659500	-1.01260800	1.19764600
C	-3.93127700	-2.33849800	1.49632600
C	-1.08309600	-1.15330600	-1.66021800
N	-1.70584100	0.16953200	-1.70022300
C	-2.77884700	0.38272700	-2.67030200
C	-5.74970600	0.46543900	-0.31389400
N	-4.58046400	0.88740600	-1.07299400
C	-4.17684200	0.00642000	-2.15777400
H	-4.14167800	-2.97691400	0.63109900
H	-4.40608700	-2.83375600	2.36286600
H	-2.21259200	-1.77776600	2.69242800
H	-1.99542800	-3.28188600	1.80669800
H	-2.57764900	-0.19103300	-3.59085500
H	-2.79723400	1.44337100	-2.94287100
H	-4.88800400	0.10786300	-2.99223400
H	-4.16742800	-1.06511200	-1.89160700
H	-1.14323800	-1.62569000	-2.65386900
H	-0.01971500	-1.02877500	-1.42826500
H	-2.69898100	-2.40580200	-0.96113400
H	-1.08707400	-3.03836000	-0.61743500
H	-5.94127100	1.23770400	0.44294600
H	-6.63030800	0.45675900	-0.97237600
H	-5.61570300	-1.70363400	-0.36770200
H	-6.60073100	-1.08298200	0.94884900
C	-0.86595800	1.28829300	-1.32176300
H	-1.22258100	2.19342000	-1.82551000
H	0.17752200	1.13424900	-1.62435200
C	-0.96787900	1.61044000	0.18406600
O	-2.06976500	1.81689700	0.68776100
N	0.19400200	1.68865000	0.92649100
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H	-0.99774400	1.95558500	2.58897500
H	0.44785900	0.97917000	2.88517100
C	0.80676500	3.11330800	2.90863000
H	1.87878900	3.07048500	2.69155600
H	0.39791200	4.02919200	2.47144900
H	0.69123700	3.17777600	3.99548500
C	1.77691000	-0.13831400	0.70728600
C	3.02013200	-0.63906200	0.32458800
C	1.46214800	1.19708000	0.45704500
C	3.96893900	0.18207200	-0.31294200
C	2.38219300	2.05464200	-0.19033400
C	4.46964600	-2.56812400	0.25236900
C	5.24703600	-0.40940500	-0.68257500
C	3.61512200	1.52076700	-0.56022800
C	5.45737500	-1.71952300	-0.40091500
H	4.32959900	2.16742200	-1.05928000
H	6.38835300	-2.21441600	-0.65289900
H	1.03907400	-0.79623300	1.15735300
C	2.03731800	3.48718500	-0.51775500
H	1.65576400	4.02436800	0.35355700
H	2.91544600	4.01971400	-0.89176600
H	1.26190400	3.54488800	-1.29066000
C	6.30008000	0.42223900	-1.36240300
H	6.58678800	1.27930900	-0.74263300
H	7.19549700	-0.16898700	-1.56336100
H	5.93276500	0.82175900	-2.31450000
O	3.26403900	-1.95456400	0.59169800
O	4.60457000	-3.73834900	0.52116900
H	-4.52157000	-0.43874900	2.03299600
H	-3.79531400	1.00874800	-0.43440700
H	-2.15316700	-0.62272900	0.62260100



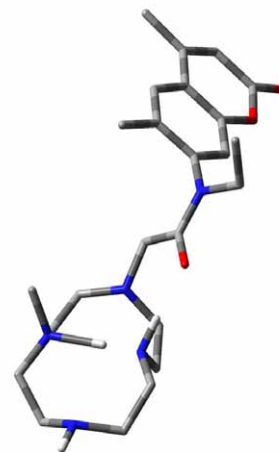
4.[2424].7.ii

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C	-5.08422000	2.31090900	0.80970300
N	-5.17897000	0.89629800	1.15278500
C	-6.17589500	0.11955900	0.42358000
C	-2.72925500	-1.02854000	-2.25256600
N	-1.82963200	-0.10539300	-1.55034500
C	-1.83465400	1.27489300	-2.05052400
C	-3.62812200	2.80500100	0.93654300
N	-2.63012400	2.12294200	0.10443300
C	-2.85642900	2.17299700	-1.33606300
H	-6.40681900	0.56809900	-0.56180100
H	-7.12948600	0.06963600	0.96739500
H	-5.57452900	-1.80474600	1.19494600
H	-6.35214600	-1.88618300	-0.39577000
H	-2.02431000	1.30647700	-3.13732800
H	-0.84328000	1.70848000	-1.88612200
H	-2.71755400	3.20478300	-1.68839400
H	-3.87610900	1.87985100	-1.63263100
H	-2.73287500	-0.82108300	-3.33851000
H	-2.33637300	-2.03765000	-2.11632800
H	-4.66142100	-0.06849300	-1.99510100
H	-4.72795200	-1.78277500	-2.37346400
H	-3.31033300	2.69318000	1.97990800
H	-3.59681900	3.87749900	0.70592400
H	-5.45016700	2.51070800	-0.21504500
H	-5.71362100	2.91866200	1.47631700
C	-0.50897900	-0.65399400	-1.28194100
H	0.17057300	0.16426900	-1.04986300
H	-0.06601800	-1.17738400	-2.15328800
C	-0.50180700	-1.67721500	-0.13518200
O	-1.43533000	-2.45335900	0.05634500
N	0.65152800	-1.76584400	0.61655100
C	0.77858000	-2.91089200	1.54455300
H	0.22294700	-3.73991100	1.10228200
H	1.83710200	-3.18310400	1.58213000
C	0.24978000	-2.62504500	2.95022500
H	0.79808200	-1.80792900	3.42902800
H	-0.81129500	-2.36592200	2.91170300
H	0.36118400	-3.51587500	3.57732300
C	2.91440300	-1.29840400	-0.12059800
C	4.03171400	-0.47210300	-0.20387100
C	1.75575800	-0.85380400	0.51801400
C	4.01335100	0.82316200	0.34512800
C	1.69919400	0.44016300	1.09294100
C	6.30019900	-0.23495000	-0.99240900
C	5.21596600	1.63518100	0.21995700
C	2.83409000	1.24422700	0.98303000
C	6.28754300	1.10553700	-0.42154400
H	2.80276400	2.23674700	1.42091000
H	7.20946000	1.66210000	-0.54619600
H	2.95661900	-2.28772800	-0.56242600
C	0.46619800	0.96923300	1.78602500
H	-0.08107200	0.17548100	2.29801000
H	0.74219100	1.72504400	2.52666900
H	-0.23343000	1.44643300	1.08694900
C	5.25437700	3.02560200	0.79168500
H	5.07197000	3.01155700	1.87212400
H	6.22397200	3.49471500	0.61447100
H	4.47977400	3.65732000	0.34257500
O	5.12608200	-0.97548800	-0.84322100
O	7.22388900	-0.75281300	-1.57339100
H	-4.29884000	0.44808300	0.89828300
H	-2.56917500	1.13658800	0.35234000
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[4.[2424].7.ii.e.N4-CH₃]^{+,1}

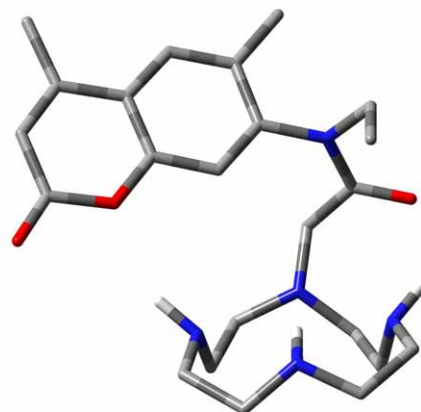
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C	6.47751800	-1.21364200	-0.17263100
N	6.70668400	0.21820300	0.04904100
C	6.26806800	1.17387200	-0.95897700
C	1.98268600	-0.22908500	-1.98816700
N	1.60038800	-0.74375300	-0.66990900
C	1.92783500	-2.14387800	-0.41851300
C	5.54266000	-1.83074400	0.87460500
N	4.10134700	-1.46293200	0.72973900
C	3.42961300	-2.41146600	-0.19202000
H	6.25206400	0.74506500	-1.97443600
H	6.98240300	2.00312000	-0.99808800
H	4.96000900	2.22525300	0.38479500
H	4.69586200	2.62989300	-1.32506400
H	1.60476400	-2.80963900	-1.23782000
H	1.37729100	-2.46331200	0.46916100
H	3.52099400	-3.44327600	0.18448600
H	3.96678900	-2.37980800	-1.14437600
H	1.87606900	-0.98618700	-2.78070700
H	1.30738700	0.58947100	-2.24100600
H	4.15924600	-0.44979200	-2.25333600
H	3.52231600	1.11877200	-2.74695500
H	5.87932300	-1.46788200	1.84826100
H	5.64615400	-2.92615700	0.87553000
H	6.12108700	-1.40961900	-1.19507700
H	7.42676700	-1.75725200	-0.09401400
C	0.26523700	-0.33401100	-0.25305200
H	-0.02855800	-0.91677500	0.62452400
H	-0.50732200	-0.52808800	-1.01434900
C	0.23184600	1.16664600	0.10930300
O	1.25963400	1.85934400	0.06383100
N	-0.97712200	1.68848100	0.44939700
C	-1.13837500	3.16122200	0.55782900
H	-0.14224900	3.58308900	0.42901300
H	-1.75704700	3.49137800	-0.28555700
C	-1.75498800	3.62921600	1.87170300
H	-2.73444400	3.17700900	2.04984200
H	-1.10455100	3.40835600	2.72298300
H	-1.89570700	4.71332800	1.83056300
C	-2.99632400	0.90031200	-0.65587900
C	-4.18709500	0.17603600	-0.65955300
C	-2.17784000	0.88800800	0.47260000
C	-4.58436600	-0.56442500	0.47137000
C	-2.53737600	0.15856800	1.62748600
C	-6.15395300	-0.45384800	-1.91082900
C	-5.85164900	-1.28584200	0.40686700
C	-3.73974100	-0.55101300	1.59302800
C	-6.57086100	-1.21607800	-0.73998100
H	-4.03653500	-1.10519300	2.47704600
H	-7.51937200	-1.72943400	-0.84945300
H	-2.72393400	1.46725700	-1.53941200
C	-1.66370200	0.12575400	2.85910700
H	-1.18600000	1.08883400	3.04566100
H	-2.24867800	-0.14124400	3.74187500
H	-0.86355500	-0.62249700	2.77191700
C	-6.33619700	-2.07386700	1.59247200
H	-6.49993400	-1.41891200	2.45636200
H	-7.27659600	-2.57916900	1.36708900
H	-5.60504600	-2.83149400	1.89521600
O	-4.92588700	0.21913900	-1.79763200
O	-6.75211800	-0.35277200	-2.95050700
H	7.68079000	0.38096100	0.26807800
H	3.95495500	-0.01213000	0.01111200
H	2.90394600	1.30614800	-0.28034700
C	3.45065200	-1.44317300	2.05542800
H	3.98394500	-0.74600700	2.70500900
H	2.42147500	-1.09281900	1.96205700
H	3.45043100	-2.43576100	2.52991900



¹ Structure is more stable and has been optimized with an extraannular N7-H.

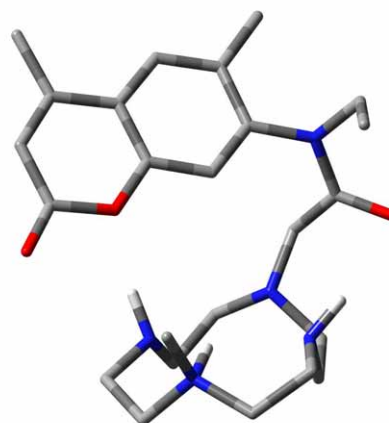
4.[2424].8.eie

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C	4.40999900	-0.19316400	-1.55691600
C	2.89558700	3.12865700	-0.84218900
N	3.00098600	1.83854000	-1.50345400
C	4.36378000	1.34342700	-1.63893500
C	3.08672100	-0.77504600	-1.98706800
N	1.66572500	-0.45225000	1.80132200
C	1.19887500	0.74763600	2.49250100
C	1.47929000	3.36243900	-0.30237700
N	0.99638900	2.23744000	0.50583900
C	1.59267400	2.07946000	1.82659600
H	5.02638900	1.76013500	-0.85567400
H	4.80751900	1.65453300	-2.59584800
H	3.98891700	-0.62012300	-2.47449200
H	5.47295700	-0.49809300	-1.51267700
H	1.55580400	0.78110900	3.54067800
H	0.10422900	0.70866500	2.54227700
H	1.31551000	2.89127200	2.52693300
H	2.68068800	2.13025500	1.72972900
H	3.44781800	-0.37517200	2.95105700
H	3.18084400	-1.86255900	2.03969400
H	4.08246900	0.81508200	0.90412300
H	5.05356000	-0.62926300	1.14591700
H	0.78550200	3.45984600	-1.14317100
H	1.46923700	4.32384400	0.24264500
H	3.62546800	3.22946000	-0.01129700
H	3.13340900	3.94492400	-1.53947400
C	0.78865100	-1.61902100	1.90979000
H	-0.23786200	-1.28144800	2.04957100
H	1.04231400	-2.27386600	2.76190800
C	0.92076900	-2.48739200	0.65055000
O	1.93469600	-3.16094000	0.46690600
N	-0.11576800	-2.50765900	-0.26109000
C	0.10660300	-3.24139800	-1.52538600
H	0.78389800	-4.06390700	-1.29313400
H	-0.84988000	-3.66160000	-1.84729800
C	0.69553600	-2.34988700	-2.61988300
H	0.00660500	-1.54552600	-2.89450800
H	1.62894200	-1.89389700	-2.28084600
H	0.89992100	-2.94271000	-3.51759400
C	-1.15365000	-0.29991700	-0.30246500
C	-2.29181800	0.50242800	-0.24290300
C	-1.28305600	-1.68331200	-0.18293800
C	-3.57711300	-0.04962300	-0.10452800
C	-2.55722400	-2.28196900	-0.01282700
C	-3.15177200	2.76647100	-0.28119200
C	-4.71522300	0.85760600	-0.07600400
C	-3.67206700	-1.44823300	0.01204400
C	-4.48398300	2.19178500	-0.17036500
H	-4.65087700	-1.89828600	0.14414900
H	-5.29285800	2.91320400	-0.15464800
H	-0.17605500	0.16288400	-0.40406800
C	-2.72006600	-3.77238500	0.16386200
H	-1.89790000	-4.19537000	0.74696900
H	-3.65933600	-3.99997300	0.67460700
H	-2.73614900	-4.30108800	-0.79680700
C	-6.11239800	0.31613600	0.05437300
H	-6.23036600	-0.24762700	0.98672800
H	-6.84712100	1.12341500	0.04828200
H	-6.34701000	-0.36880100	-0.76806900
O	-2.09539900	1.85406000	-0.32386000
O	-2.87809200	3.94240300	-0.33239300
H	2.47006600	1.15998300	-0.95724000
H	3.48049700	-1.69544000	-0.48154200
H	-0.01322800	2.31360700	0.58618700



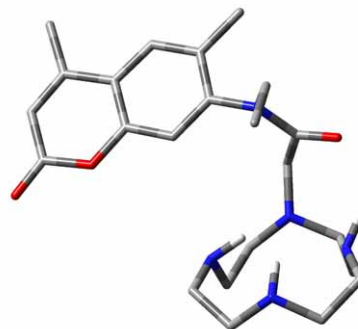
[4.[2424].8.eie.N7-CH₃]⁺

C	3.46325000	-1.56843200	0.38966800
N	2.77323700	-1.20738800	-0.85313700
C	3.62925600	-0.71509300	-1.92404000
C	3.52094500	2.51235300	0.06819200
N	3.06716600	1.54426700	-0.99547000
C	4.16262800	0.68679200	-1.57671400
C	2.51377900	-2.20609600	1.41735600
N	1.25370100	-1.47814900	1.63489100
C	1.29172000	-0.52948500	2.75111000
C	2.35231700	2.74408000	1.04907400
N	1.70404300	1.46461100	1.32778000
C	2.13633700	0.73116000	2.51916800
H	4.94941500	0.61761000	-0.82437500
H	4.57982400	1.18898400	-2.45229400
H	3.03843200	-0.67837800	-2.84480600
H	4.51031100	-1.34513700	-2.13481300
H	1.65061000	-1.00018900	3.68543300
H	0.26298700	-0.20350600	2.94611000
H	2.06154400	1.34434300	3.43316400
H	3.19589700	0.47156200	2.41656800
H	3.07067000	-2.33302000	2.36134700
H	2.26454300	-3.20667400	1.05991600
H	3.91980900	-0.66325100	0.80538200
H	4.29218400	-2.27692000	0.21778400
H	1.61703000	3.41998100	0.60397600
H	2.75270500	3.24099000	1.94425300
H	4.36563600	2.04557600	0.57932700
H	3.86593500	3.43577300	-0.40225400
C	0.08617000	-2.37171500	1.72051500
H	-0.76848000	-1.78907600	2.06511800
H	0.23368800	-3.19615900	2.43947700
C	-0.23606200	-3.05174100	0.38175300
O	0.50275800	-3.92321800	-0.07252400
N	-1.42478600	-2.72640400	-0.24830700
C	-1.78274800	-3.52278500	-1.44838600
H	-1.50840300	-4.55627800	-1.23251000
H	-2.86743600	-3.47484000	-1.55955100
C	-1.09517900	-3.04845000	-2.72859200
H	-1.32633600	-2.00058500	-2.94444200
H	-0.01219600	-3.16839400	-2.64827800
H	-1.43890200	-3.64927400	-3.57610500
C	-1.20646900	-0.31670700	-0.29788500
C	-1.75444300	0.95604100	-0.22015700
C	-2.02179500	-1.43465300	-0.11578400
C	-3.12340600	1.16286500	0.00829700
C	-3.40464300	-1.27964200	0.15656600
C	-1.30694800	3.32881500	-0.37190600
C	-3.61159100	2.53506400	0.03485900
C	-3.91827700	0.01671300	0.20151800
C	-2.72252700	3.54882800	-0.15832200
H	-4.97594500	0.14304100	0.40871000
H	-3.03332900	4.58691800	-0.15354000
H	-0.14397200	-0.43263300	-0.47861200
C	-4.30760100	-2.46081300	0.41788500
H	-3.75722600	-3.28915600	0.87046000
H	-5.12211700	-2.18103600	1.09055400
H	-4.76663100	-2.83583900	-0.50447900
C	-5.06981400	2.81396000	0.26525800
H	-5.39762400	2.41167300	1.23022400
H	-5.27244200	3.88595300	0.25523100
H	-5.68484500	2.34024000	-0.50781900
O	-0.88391900	2.00233000	-0.38644900
O	-0.44335600	4.17091000	-0.52916100
H	2.43379500	0.89190500	-0.45686300
H	2.20816100	-1.99003700	-1.17147100
H	0.69625100	1.56915400	1.31250200
C	2.23457600	2.20559300	-2.05166500
H	2.86650100	2.89316100	-2.61631100
H	1.83464900	1.43755200	-2.71357500
H	1.41108100	2.74730400	-1.58526700



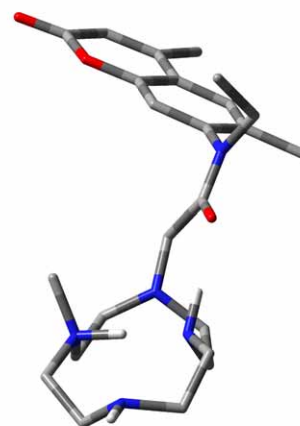
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C	4.19968700	-0.37422300	1.46715600
N	4.10080200	-0.69900100	0.05078100
C	5.25875800	-0.32045100	-0.75762500
C	3.44288600	2.88342400	-1.03826900
N	3.96264200	1.60846800	-1.52908200
C	5.26884500	1.19946300	-1.02050800
C	2.99417100	-0.87615000	2.27683500
N	1.67704200	-0.42511400	1.82402400
C	1.21876300	0.87483700	2.31589000
C	1.90964200	2.81612400	-0.89299200
N	1.39113100	1.82550800	0.05872900
C	1.71124600	2.05858300	1.46352800
H	5.52660500	1.72887600	-0.08511900
H	6.07312800	1.43131200	-1.73267500
H	5.17334500	-0.84333100	-1.71665400
H	6.22399000	-0.61378100	-0.30719500
H	1.52520000	1.03943000	3.36431600
H	0.12539800	0.88223600	2.29255900
H	1.19563000	2.96645600	1.80445000
H	2.78538100	2.22524800	1.64854100
H	3.15876500	-0.59253800	3.33258300
H	3.00040800	-1.96817500	2.23118500
H	4.29749000	0.71146200	1.57324600
H	5.10434500	-0.80551200	1.94070800
H	1.48001700	2.58433800	-1.87501500
H	1.52714000	3.80224200	-0.60482000
H	3.89310500	3.16244900	-0.06750200
H	3.69205900	3.69894600	-1.73257100
C	0.67618800	-1.48712100	1.72502200
H	-0.31878800	-1.06104500	1.84443000
H	0.80117200	-2.25715300	2.50328400
C	0.82958200	-2.19064900	0.37046000
O	1.85207400	-2.82970200	0.11799700
N	-0.17329700	-2.05945000	-0.56280800
C	0.07389300	-2.61886600	-1.90949300
H	0.64929200	-3.53760700	-1.77992300
H	-0.89587900	-2.87354500	-2.34524500
C	0.82646000	-1.64221200	-2.81361000
H	0.26186900	-0.71525200	-2.95280900
H	1.79969200	-1.39666100	-2.38145200
H	0.99131700	-2.09071800	-3.79892900
C	-1.52295200	-0.01752200	-0.38748300
C	-2.76604700	0.59764500	-0.22193200
C	-1.43497800	-1.40820100	-0.34164500
C	-3.93616900	-0.15568000	-0.02060000
C	-2.58809700	-2.20379400	-0.12212100
C	-3.96348900	2.69190400	-0.13124800
C	-5.19521600	0.55926100	0.13292000
C	-3.81009300	-1.55595600	0.03008300
C	-5.17841900	1.91414700	0.07403000
H	-4.69739100	-2.15682900	0.20194100
H	-6.08367200	2.50113300	0.17990700
H	-0.64102900	0.60836800	-0.50587800
C	-2.50306600	-3.70865600	-0.03468800
H	-1.70640300	-4.02778700	0.64412500
H	-3.44590100	-4.12801400	0.32511800
H	-2.28863700	-4.16575300	-1.00731500
C	-6.47637500	-0.19870300	0.34930200
H	-6.42508000	-0.80715000	1.25937100
H	-7.32345700	0.48364900	0.44173500
H	-6.67530800	-0.88198000	-0.48402300
O	-2.78516500	1.96066300	-0.27214100
O	-3.89329100	3.89696000	-0.18748800
H	3.33577800	0.87427500	-1.20558200
H	1.73803500	0.89334200	-0.16416100
H	3.83387900	-1.67040100	-0.07714800



[4.[2424].9.ii.e.N4-CH₃]^{+,2}

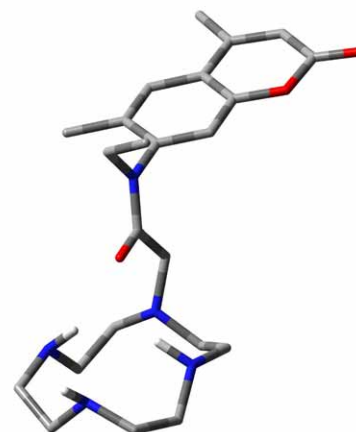
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N	-3.94609400	-0.89681300	-0.13634300
C	-5.13602400	-1.62301200	0.34354000
C	-6.30554500	1.57600400	-0.21126400
N	-6.58338200	0.39226400	0.59412700
C	-6.45285200	-0.93080600	-0.02166700
C	-2.20193100	-0.74645500	-1.89456200
N	-1.58476000	0.26206600	-1.02512500
C	-1.78915300	1.65165600	-1.40238200
C	-5.15916000	2.41450800	0.36975300
N	-3.79834400	1.78158500	0.19248600
C	-3.20895200	2.18345600	-1.13447700
H	-6.56873300	-0.88150000	-1.11584700
H	-7.26581700	-1.56902100	0.33899700
H	-5.06604500	-1.67807600	1.43377800
H	-5.14872600	-2.65306900	-0.04503000
H	-1.58259000	1.85208800	-2.46969200
H	-1.08026000	2.26285000	-0.83761600
H	-3.18685300	3.27775800	-1.17942400
H	-3.91139200	1.84130300	-1.89643900
H	-2.09306300	-0.48968500	-2.96151800
H	-1.65757200	-1.67954500	-1.73779600
H	-4.34384900	-0.33514500	-2.13212800
H	-3.93338700	-2.02918200	-1.95070800
H	-5.32861600	2.52673100	1.44164800
H	-5.12615100	3.41317400	-0.07796400
H	-6.09604800	1.30092000	-1.25429400
H	-7.17856000	2.23972600	-0.25064400
C	-0.22273200	-0.07472100	-0.63435200
H	0.25375300	0.80577100	-0.19347800
H	0.41858300	-0.36232700	-1.48354200
C	-0.21262400	-1.20124000	0.42250800
O	-1.25976700	-1.62638200	0.92001000
N	1.00315600	-1.71364800	0.76241100
C	1.05813400	-2.79214800	1.77768400
H	0.18310700	-3.42549900	1.62116800
H	1.95334200	-3.38224800	1.56668200
C	1.08791700	-2.26539700	3.21170000
H	1.95838200	-1.62586000	3.38495300
H	0.18032700	-1.69748300	3.43182400
H	1.14275800	-3.10351200	3.91303400
C	2.71219600	0.02144200	0.88948400
C	3.92775500	0.57104300	0.48138800
C	2.24786400	-1.15475200	0.30391100
C	4.70945100	-0.05952400	-0.50350600
C	2.99787600	-1.81538800	-0.69623400
C	5.51250600	2.37118600	0.75958900
C	5.97970900	0.55910200	-0.86843500
C	4.21494700	-1.24742000	-1.07098300
C	6.33389300	1.71154200	-0.24771000
H	4.80211900	-1.74316800	-1.83686200
H	7.26562700	2.21697700	-0.47453400
H	2.14815100	0.51663600	1.67202600
C	2.51024800	-3.09023500	-1.34069400
H	1.45687100	-3.02211100	-1.62953000
H	3.09304000	-3.31977300	-2.23555500
H	2.59777300	-3.94844900	-0.66448900
C	6.86381500	-0.07923400	-1.90352900
H	6.34877400	-0.16061000	-2.86747800
H	7.77424100	0.50354300	-2.05235100
H	7.15217600	-1.09298600	-1.60372700
O	4.30722300	1.72849800	1.08324400
O	5.76525000	3.40204700	1.32921500
H	-7.47729300	0.48159700	1.05803700
H	-3.91642300	0.65877400	0.15329200
H	-3.10716100	-1.22930900	0.35444200
C	-2.89995100	2.08720200	1.34280400
H	-3.40763300	1.79334400	2.26187500
H	-1.98964400	1.49994300	1.24051500
H	-2.67393600	3.15617000	1.37417500



² Structure is more stable and has been optimized with an extraannular N7-H.

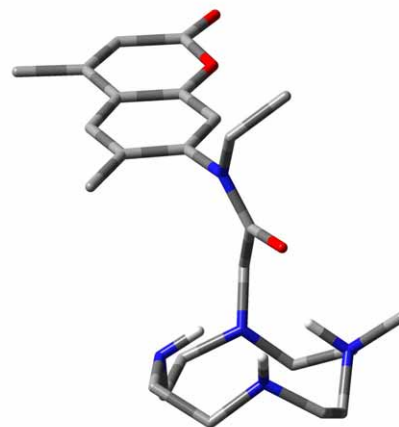
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C	5.22002800	-1.99615700	-0.50438800
C	6.09475900	-0.75148400	-0.25508700
N	5.54862400	0.05905400	0.83142000
C	5.87756400	1.48600300	0.80262200
C	4.91037400	2.25484700	-0.10385400
N	3.56075100	2.17923900	0.43561600
C	2.49966700	2.64757900	-0.44053500
C	2.17092700	1.76085500	-1.66351000
N	1.79709300	0.39864500	-1.29267800
C	2.14854500	-0.64639800	-2.25582200
C	3.60687400	-1.09545900	-2.12883100
N	3.82489700	-1.73057600	-0.83630600
H	1.51735700	-1.51922700	-2.05854100
H	1.94965800	-0.32783000	-3.29469700
H	5.76915800	1.87785900	1.81954900
H	6.91574900	1.68238600	0.48090800
H	5.23645200	-2.62314900	0.39783400
H	5.67250300	-2.59641500	-1.30575400
H	2.74944300	3.65311900	-0.80593200
H	1.59102300	2.76727700	0.16500500
H	3.42590400	-1.13381200	-0.11092100
H	3.36437300	1.21773600	0.71294000
H	1.38483800	2.25869200	-2.26583100
H	3.82036500	-1.82030600	-2.92813800
H	7.14069100	-1.06480000	-0.07930800
H	5.22562200	3.30754700	-0.14717000
H	3.05347500	1.69462600	-2.30662700
H	5.00874200	1.86507900	-1.13576200
H	6.11362400	-0.13413800	-1.15926100
H	4.26137500	-0.22521400	-2.32394100
C	0.51795200	0.25006300	-0.63859700
H	0.03320300	1.22798300	-0.52357900
H	-0.18442500	-0.35159400	-1.23283800
C	0.64633600	-0.36150200	0.77461500
O	1.71436600	-0.40485600	1.37470900
N	-0.50636400	-0.86430800	1.34372600
C	-0.41764800	-1.42733300	2.70635800
H	-1.21252600	-2.17282700	2.80504500
H	0.54515700	-1.93694800	2.77891800
C	-0.53663400	-0.36886700	3.80329700
H	0.27452400	0.35817700	3.71606100
H	-1.49384300	0.15904200	3.74768000
H	-0.46905200	-0.84057300	4.78925100
C	-1.80367700	-0.75314600	0.74648200
C	-2.49509500	0.45383900	0.83080800
C	-2.38683400	-1.87606600	0.10884200
C	-3.77043300	0.56883900	0.27700900
H	-2.05440500	1.31147700	1.32603800
C	-3.66245100	-1.73090600	-0.42921000
C	-4.38286000	-0.52348700	-0.36227600
H	-4.11478100	-2.58329900	-0.92575900
C	-5.66262600	2.01437300	-0.11824500
C	-5.71634900	-0.33148600	-0.91520000
C	-6.29992400	0.88610000	-0.78378200
H	-7.29073700	1.08847300	-1.17424100
C	-1.64412700	-3.18502600	-0.00013400
H	-0.63396900	-3.04230400	-0.39596100
H	-1.53179500	-3.67165700	0.97527700
H	-2.17499700	-3.87859700	-0.65681800
C	-6.41875600	-1.46448700	-1.61159600
H	-5.83727800	-1.82023900	-2.46959200
H	-6.55342800	-2.31775900	-0.93725200
H	-7.40183200	-1.15349600	-1.96995100
O	-4.38390100	1.78034300	0.39295000
O	-6.13542900	3.11602600	0.02708800
H	5.79084900	-0.34593300	1.72914200



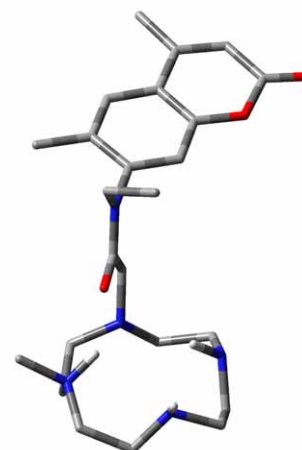
[4.3333].1.1ei.N10-CH₃⁺

C	-3.93863000	2.83816900	0.50526000
C	-5.19702700	1.96909700	0.32737100
N	-4.97235900	0.61535700	0.86159400
C	-5.80819800	-0.43575100	0.29435400
C	-5.10539100	-1.11090600	-0.89104400
N	-3.79287500	-1.74781100	-0.50956400
C	-2.93640900	-2.10778300	-1.70213500
C	-2.33501500	-0.90150700	-2.43298800
N	-1.62533800	0.01465400	-1.55496200
C	-1.55091600	1.40516800	-2.04785900
C	-2.72829400	2.24616400	-1.55676600
N	-2.73051900	2.28162100	-0.09924700
H	-0.63140700	1.85369200	-1.66400300
H	-1.49380300	1.43753700	-3.14581900
H	-6.04476900	-1.17342600	1.06672000
H	-6.77872800	-0.07264700	-0.07843800
H	-3.74842700	2.97747000	1.57690300
H	-4.12797000	3.83551700	0.09200100
H	-3.54245100	-2.71016700	-2.38485900
H	-2.14111200	-2.74396100	-1.30922700
H	-2.63665400	1.32539700	0.23871600
H	-3.20621300	-1.07690600	0.04877500
H	-1.69862600	-1.32227200	-3.23399600
H	-2.62081900	3.26632600	-1.94650200
H	-6.06542000	2.46285300	0.79081500
H	-5.73036900	-1.89076000	-1.33707200
H	-3.12367300	-0.34004500	-2.94095100
H	-4.88608500	-0.36470800	-1.65568800
H	-5.43149000	1.87498200	-0.73855300
H	-3.66119700	1.84854700	-2.00230600
C	-0.41154000	-0.49482600	-0.92598400
H	-0.15311600	-1.49136700	-1.31212800
H	0.44609400	0.14038400	-1.15524300
C	-0.59808900	-0.63805900	0.59663500
O	-1.70025900	-0.99629300	1.05379700
N	0.45126600	-0.38062800	1.40889400
C	0.28732100	-0.55540400	2.87259100
H	0.96453800	0.15378200	3.35394100
H	-0.73822200	-0.27464700	3.11809100
C	0.58390100	-1.98025600	3.33727700
H	-0.10309700	-2.69110100	2.87028600
H	1.61036200	-2.27359100	3.09945800
H	0.45822800	-2.04916600	4.42197000
C	1.74952300	0.01646900	0.92252700
C	2.62739000	-0.96769100	0.47702900
C	2.11660100	1.38161700	0.93543700
C	3.89766900	-0.60897000	0.02385800
H	2.34468100	-2.01427300	0.47669400
C	3.39538700	1.70290500	0.48072500
C	4.30865600	0.73654600	0.02171600
H	3.69441800	2.74579600	0.48015700
C	5.99609300	-1.37918100	-0.88779300
C	5.65319100	1.04006100	-0.45812700
C	6.43009000	0.01252100	-0.88118400
H	7.43747700	0.17433400	-1.24729400
C	1.17181800	2.45784700	1.41685900
H	0.17894400	2.38394000	0.95976500
H	1.02449500	2.40960200	2.50214000
H	1.57283900	3.44816200	1.18956700
C	6.15096300	2.45858700	-0.47456800
H	5.51713500	3.09292500	-1.10457000
H	6.14327400	2.89070500	0.53243800
H	7.17098600	2.50934300	-0.85879900
O	4.69763000	-1.61711600	-0.40830000
O	6.63536000	-2.32853300	-1.26169600
H	-5.04973500	0.62489600	1.87313200
C	-3.97418100	-2.95289000	0.36133600
H	-4.59469300	-2.69636000	1.21724100
H	-4.44483000	-3.74951200	-0.21736600
H	-2.99311300	-3.25966700	0.71943300



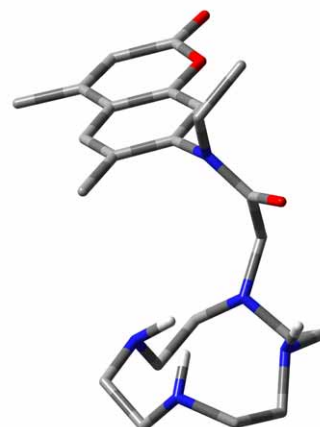
[4.[3333].1.1ei.N4-CH₃]⁺

C	5.49046500	-0.92068800	0.19048400
C	5.69144100	0.58100200	0.37051600
N	4.66106000	1.16089800	1.21921700
C	4.58845900	2.63567400	1.16076300
C	3.74060300	3.09509800	-0.02524900
N	2.37185600	2.63069800	0.15426100
C	1.52748700	2.67381900	-1.02954100
C	1.78601200	1.55645700	-2.06342300
N	1.77827800	0.21374000	-1.45561300
C	2.49620700	-0.79324200	-2.23010800
C	3.97646100	-0.87650600	-1.83397800
N	4.15592100	-1.31737300	-0.40099000
H	2.01689300	-1.76815900	-2.09777100
H	2.46473100	-0.59049200	-3.31239100
H	4.10427300	2.97719200	2.07986000
H	5.58521500	3.10089100	1.11572500
H	5.54665900	-1.42347000	1.16008200
H	6.26752500	-1.34403100	-0.45300700
H	1.65192600	3.63975200	-1.53192500
H	0.47813600	2.64647200	-0.70943100
H	3.36861800	-0.87946100	0.14381100
H	2.41257600	1.67279400	0.49725300
H	1.06014800	1.63900100	-2.89124800
H	4.52534400	-1.57834800	-2.46907800
H	6.71916000	0.71357200	0.75195300
H	3.75558000	4.19137000	-0.06706200
H	2.77738900	1.70239500	-2.50563900
H	4.21381600	2.75018000	-0.96676300
H	5.67212500	1.08957300	-0.59795100
H	4.43521300	0.10691200	-1.93315200
C	0.49096100	-0.21814800	-0.93633500
H	-0.13623000	0.65583100	-0.75464100
H	-0.07955300	-0.83938300	-1.64669300
C	0.63583000	-0.98633500	0.39071900
O	1.75250200	-1.23139700	0.87859200
N	-0.50297200	-1.40870200	0.99254800
C	-0.40855500	-2.14724100	2.27509100
H	-1.28203200	-2.80181000	2.32848800
H	0.48549600	-2.77124200	2.22365200
C	-0.35021900	-1.22662200	3.49316800
H	0.52987900	-0.58003500	3.44743600
H	-1.24440700	-0.60125800	3.56451800
H	-0.28725700	-1.82608200	4.40641400
C	-1.81925200	-1.06281700	0.51440200
C	-2.33999200	0.19031600	0.82860000
C	-2.57410800	-2.00624000	-0.21771500
C	-3.62603900	0.53298700	0.40750300
H	-1.76583100	0.90900000	1.40282100
C	-3.85816800	-1.63541900	-0.61516100
C	-4.41413700	-0.37834100	-0.31947300
H	-4.45030700	-2.34926400	-1.17808200
C	-5.34293900	2.22972000	0.37358200
C	-5.75440600	0.04034000	-0.71804700
C	-6.16588900	1.28471200	-0.37184700
H	-7.15009700	1.65340000	-0.63735100
C	-2.02276100	-3.36886300	-0.56214200
H	-1.04458400	-3.30186800	-1.05054600
H	-1.89052700	-3.99421300	0.32791800
H	-2.69767400	-3.89895000	-1.23752900
C	-6.64372600	-0.89610600	-1.48764600
H	-6.18161500	-1.18968500	-2.43699800
H	-6.83230300	-1.81478200	-0.92076400
H	-7.60510200	-0.42903300	-1.70736900
O	-4.06512300	1.77395200	0.73808400
O	-5.65064000	3.34722400	0.69860500
H	4.80503500	0.86818000	2.18178900
C	3.97206500	-2.79768600	-0.25560100
H	4.80589200	-3.30926600	-0.73937100
H	3.93752200	-3.04102500	0.80536100
H	3.03065000	-3.09295600	-0.71189200



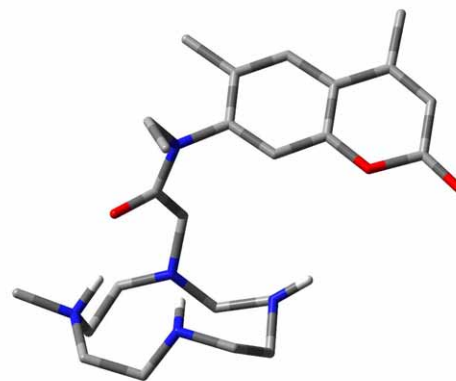
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C	-3.62073900	2.67806100	0.87187800
C	-5.03573700	2.23322600	0.46349100
N	-5.38016200	0.95324100	1.09276700
C	-6.26661600	0.09109500	0.31395700
C	-5.62126200	-0.55113800	-0.93047900
N	-4.38158800	-1.22828500	-0.56156200
C	-3.59216700	-1.76150400	-1.67165500
C	-2.67000600	-0.71121900	-2.30687100
N	-1.62009200	-0.21971200	-1.41389400
C	-1.22395000	1.17191500	-1.65407700
C	-2.26834600	2.16324400	-1.12920700
N	-2.51275200	1.91570400	0.28709600
H	-0.29038000	1.35244400	-1.11387700
H	-1.02848400	1.37859200	-2.72280300
H	-6.62198800	-0.71107900	0.97659500
H	-7.15570400	0.65914500	0.01517700
H	-3.54596400	2.61007100	1.96488700
H	-3.48132700	3.73397500	0.61107600
H	-4.22488400	-2.18154700	-2.47569600
H	-2.97773700	-2.57291100	-1.27528300
H	-2.67014400	0.91172200	0.38333700
H	-2.23922500	-1.14446200	-3.23030800
H	-1.87702800	3.18163000	-1.25825200
H	-5.75769300	2.99708300	0.78669000
H	-6.35734600	-1.21608800	-1.42215100
H	-3.27049000	0.14605400	-2.62559900
H	-5.37797000	0.22737000	-1.66361900
H	-5.09543500	2.20057500	-0.63757500
H	-3.17925400	2.10568900	-1.75148500
C	-0.50544400	-1.14994500	-1.21711900
H	-0.57252800	-1.98717800	-1.92432500
H	0.44521100	-0.64874700	-1.40946600
C	-0.53957300	-1.78438500	0.18553300
O	-1.41752800	-2.58975500	0.48532900
N	0.41228500	-1.40772300	1.11215300
C	0.34171200	-2.04047300	2.44691600
H	0.84083600	-1.37207000	3.15315600
H	-0.71374100	-2.10616500	2.71763000
C	0.98412000	-3.42791600	2.48452500
H	0.46670700	-4.10246200	1.79853000
H	2.04283200	-3.38387700	2.21033100
H	0.91471700	-3.84570500	3.49438600
C	1.56764700	-0.61012700	0.82365600
C	2.61040800	-1.17127200	0.08633400
C	1.66410600	0.71322500	1.32302500
C	3.75537600	-0.42504400	-0.18903000
H	2.54155300	-2.18841400	-0.28222000
C	2.82833600	1.42529200	1.03999800
C	3.89004700	0.89087800	0.28668800
H	2.91209300	2.44082100	1.41323000
C	5.92144300	-0.39110600	-1.25295700
C	5.11647000	1.60870200	-0.03072400
C	6.06491300	0.97337900	-0.76406100
H	6.99797200	1.45653000	-1.03057400
C	0.54739300	1.35534000	2.10992300
H	-0.35785700	1.49720200	1.50509800
H	0.26087300	0.75514800	2.97906800
H	0.85984600	2.33700800	2.47618900
C	5.31478300	3.01991500	0.44996200
H	4.53278100	3.68167200	0.06078900
H	5.26667700	3.07349400	1.54339000
H	6.28316700	3.40972700	0.13058500
O	4.72728600	-1.03618500	-0.92502000
O	6.73174700	-1.00273600	-1.90771900
H	-4.52569600	0.41827200	1.23193200
H	-4.57774800	-1.97753500	0.09627700



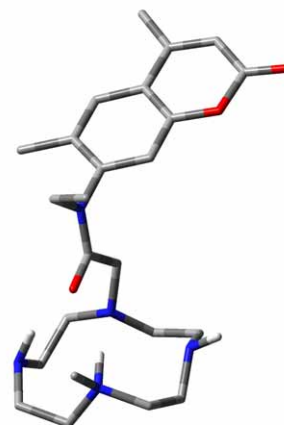
[4.[3333].2.ii.e.N4-CH₃]⁺

C	5.09391900	0.35646600	0.77285800
C	4.32090800	1.66724300	0.88314900
N	2.99243700	1.46541300	1.43793300
C	2.26570500	2.71339200	1.70843600
C	1.62286100	3.32422100	0.45279800
N	0.63522400	2.38487200	-0.10855100
C	0.56955900	2.29215400	-1.56606400
C	1.69127500	1.45374800	-2.20594900
N	1.97242700	0.14579800	-1.58405100
C	3.08238800	-0.54501000	-2.24921300
C	4.43220600	-0.18338500	-1.62233900
N	4.49051700	-0.64955100	-0.18291200
H	2.92939600	-1.62525500	-2.17593100
H	3.13564900	-0.30799200	-3.32391900
H	1.47730100	2.49899500	2.43950200
H	2.94543100	3.43257300	2.17969000
H	5.11264700	-0.13126100	1.74974900
H	6.12066800	0.53476800	0.43918300
H	0.59736900	3.27259700	-2.07168600
H	-0.40374300	1.86057600	-1.82174200
H	3.49219700	-0.85630400	0.09973100
H	1.44486600	1.34791100	-3.27788100
H	5.26264600	-0.64278000	-2.16444900
H	4.89920500	2.28629700	1.57985200
H	1.17307000	4.29807500	0.69345700
H	2.62595100	2.02622100	-2.16896700
H	2.39502200	3.52204300	-0.30000400
H	4.35073500	2.20860000	-0.08096700
H	4.58078300	0.89582800	-1.63462900
C	0.81078600	-0.70077400	-1.33205200
H	-0.08006900	-0.08653100	-1.26207700
H	0.61929800	-1.42370900	-2.14440600
C	0.98590400	-1.50724700	-0.03680000
O	2.12634200	-1.77260300	0.39132700
N	-0.11497600	-1.98626500	0.59026300
C	0.07498400	-2.80408200	1.81636500
H	-0.80993500	-3.43597800	1.91570000
H	0.93812000	-3.44874100	1.64369500
C	0.27671800	-1.95256500	3.06929000
H	1.16718400	-1.32620800	2.97318800
H	-0.58845700	-1.31052800	3.25802800
H	0.40658800	-2.60342400	3.93919100
C	-1.44586400	-1.51133400	0.30688800
C	-1.74441200	-0.18673800	0.62201600
C	-2.42056200	-2.36875200	-0.24626000
C	-3.01153200	0.32226000	0.35338900
H	-0.98422400	0.46447900	1.03762600
C	-3.69186100	-1.83468300	-0.46749000
C	-4.02107300	-0.49787800	-0.18300500
H	-4.45305300	-2.48024000	-0.89313100
C	-4.44259700	2.26874000	0.39298100
C	-5.33258000	0.09841700	-0.41735800
C	-5.50095100	1.41301900	-0.12805800
H	-6.45111100	1.91165200	-0.28148300
C	-2.12152600	-3.80670400	-0.59505100
H	-1.10297500	-3.92774500	-0.97387100
H	-2.22231200	-4.46526600	0.27591200
H	-2.81416900	-4.17215700	-1.35675900
C	-6.45713600	-0.73593100	-0.96384900
H	-6.20043600	-1.15008500	-1.94546800
H	-6.67621300	-1.58159600	-0.30243200
H	-7.36686500	-0.14336200	-1.07240500
O	-3.20733400	1.64097600	0.62744900
O	-4.52029000	3.44633400	0.63400400
H	2.41693900	0.94377100	0.77500300
H	-0.28784000	2.62453800	0.24124600
C	5.18162500	-1.97176500	-0.06233800
H	5.05866300	-2.33876000	0.95643500
H	4.71946000	-2.67615300	-0.75349600
H	6.24060100	-1.85123500	-0.29656300



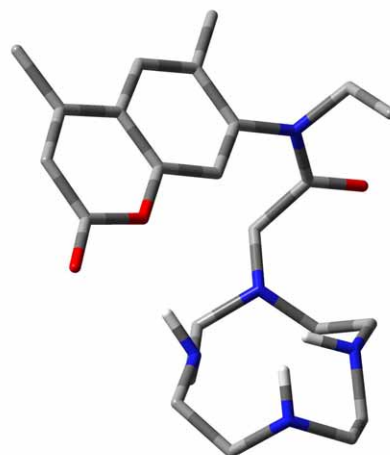
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C	5.18652900	-1.49944700	-0.44902000
C	5.38110500	-0.03177600	-0.01276500
N	4.33748400	0.48474300	0.95984700
C	4.49147800	1.97866000	1.15871600
C	3.88337100	2.79632900	0.02052500
N	2.43233800	2.65631300	0.02540500
C	1.76558000	2.81073300	-1.27107300
C	1.93305100	1.59003300	-2.19230400
N	1.79786400	0.29188200	-1.52413000
C	2.13842000	-0.82491400	-2.42709900
C	3.61800200	-1.20658600	-2.35690000
N	3.92448400	-1.82808400	-1.06838300
H	1.55293300	-1.70443300	-2.13573200
H	1.85881600	-0.59837400	-3.46773000
H	3.98683300	2.22721600	2.09528200
H	5.55920800	2.17914300	1.28214700
H	5.34509900	-2.16699900	0.40492000
H	6.00893500	-1.71158300	-1.14358800
H	2.10230000	3.69639500	-1.83533300
H	0.70447700	2.97874900	-1.06316100
H	3.15978900	-1.69628300	-0.41209500
H	1.22343100	1.71168300	-3.03151100
H	3.84362300	-1.90399100	-3.17522200
H	6.35227900	0.10414300	0.47348600
H	4.23267900	3.83461500	0.13739700
H	2.93023900	1.60924900	-2.64708000
H	4.27411100	2.45913200	-0.94394900
H	5.34101900	0.62766800	-0.88019500
H	4.22675300	-0.30782200	-2.54916900
C	0.53666300	0.09874300	-0.82580000
H	0.13956300	1.06334000	-0.50256500
H	-0.24450500	-0.34807800	-1.45868600
C	0.71748700	-0.73888800	0.45178600
O	1.83828800	-0.89830200	0.96772800
N	-0.39267600	-1.29564400	0.99815500
C	-0.26139300	-2.09131100	2.24140000
H	-1.06976800	-2.82616000	2.23537400
H	0.68810500	-2.62601600	2.18249200
C	-0.32488900	-1.23999000	3.50882900
H	0.48986800	-0.51104800	3.52642800
H	-1.27591400	-0.70532700	3.58438400
H	-0.22942400	-1.88035100	4.39088400
C	-1.72473100	-1.01656400	0.52143700
C	-2.31191500	0.20057400	0.85813800
C	-2.42584600	-1.98163700	-0.23649200
C	-3.60974000	0.48814200	0.43437800
H	-1.78015800	0.93396000	1.45379200
C	-3.72468400	-1.66660100	-0.63445400
C	-4.34617100	-0.44566400	-0.31661400
H	-4.27528900	-2.39566200	-1.21952100
C	-5.40515600	2.10199100	0.41621800
C	-5.70216200	-0.08420000	-0.71798500
C	-6.17626700	1.13226200	-0.35174400
H	-7.17513700	1.45781200	-0.61884100
C	-1.80041600	-3.30182100	-0.61695600
H	-0.80683600	-3.16911500	-1.05722900
H	-1.67764000	-3.96230100	0.24885100
H	-2.42262400	-3.82858600	-1.34359100
C	-6.53883800	-1.04671000	-1.51397700
H	-6.05811200	-1.29265400	-2.46764700
H	-6.68120300	-1.98762200	-0.97067700
H	-7.52232700	-0.62512100	-1.72761600
O	-4.11069000	1.70055900	0.78519100
O	-5.76645300	3.19899700	0.75719000
H	3.38052400	0.29907900	0.57321200
H	2.03014000	3.31226200	0.68844600
C	4.39863300	-0.22764100	2.27701300
H	5.36711700	-0.03208300	2.74066400
H	3.59013400	0.14194400	2.90526300
H	4.25667400	-1.29358300	2.11944500



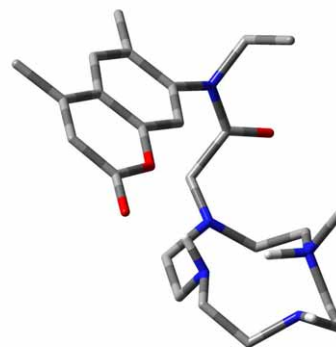
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C	2.54767500	2.92914600	0.41733700
C	3.95595100	2.71950400	-0.14889900
N	3.93510100	2.03370700	-1.44351200
C	4.86870800	0.91931300	-1.59816500
C	4.62872700	-0.30382900	-0.69162300
N	3.28072500	-0.82671300	-0.89282700
C	2.97986400	-2.08354600	-0.21325500
C	2.55875000	-1.96642300	1.26387900
N	1.28213100	-1.22865700	1.43463400
C	1.35063900	-0.11680100	2.39112800
C	2.24917300	1.05436200	1.98173800
N	1.86515500	1.66240900	0.71075600
H	0.33095500	0.27054900	2.51337000
H	1.67614800	-0.45251800	3.39481500
H	4.80814800	0.58392600	-2.63993800
H	5.88888300	1.29172200	-1.43765400
H	1.93741600	3.46508000	-0.31792100
H	2.61748500	3.57991200	1.30775200
H	3.85895600	-2.73811200	-0.27453500
H	2.17948600	-2.60006900	-0.75288000
H	2.46750000	-2.97464300	1.69016000
H	2.21922700	1.77872100	2.81896000
H	4.42952400	3.70747800	-0.25170200
H	5.34981600	-1.08382200	-0.97178700
H	3.34504500	-1.45228400	1.82813500
H	4.85969800	-0.04235200	0.36033100
H	4.55973000	2.17107400	0.58963400
H	3.29154400	0.72355800	1.91364900
C	0.15195300	-2.11291300	1.75157500
H	0.37311100	-2.78822500	2.59581200
H	-0.70232800	-1.49411800	2.03331800
C	-0.21485500	-3.02791000	0.57852400
O	0.39120000	-4.07801400	0.39294900
N	-1.26323500	-2.65658700	-0.24887400
C	-1.53232700	-3.52214300	-1.41807800
H	-1.34869200	-4.55043100	-1.10286500
H	-2.58972300	-3.42228700	-1.67201300
C	-0.66323800	-3.17154200	-2.62640000
H	-0.81592900	-2.13434000	-2.94024400
H	0.39488600	-3.31334100	-2.39487300
H	-0.91776400	-3.82200800	-3.46983700
C	-1.94902300	-1.40451600	-0.17583500
C	-1.23671700	-0.21935900	-0.36366200
C	-3.34621400	-1.37123400	0.07335900
C	-1.89819000	1.00371800	-0.29407900
H	-0.16409800	-0.24039800	-0.51641100
C	-3.97805900	-0.13027300	0.09560300
C	-3.28594700	1.08047300	-0.08844500
H	-5.04615800	-0.09899800	0.28626200
C	-1.66793900	3.41213800	-0.38140900
C	-3.90349900	2.39829100	-0.06159400
C	-3.11077300	3.49019000	-0.21416800
H	-3.51583100	4.49546200	-0.20133300
C	-4.14137100	-2.62633800	0.34280000
H	-4.50114400	-3.09361000	-0.58174900
H	-3.53910000	-3.37263900	0.86720200
H	-5.01983200	-2.40117700	0.95327900
C	-5.38889100	2.53409800	0.13093600
H	-5.93700100	2.00320300	-0.65538500
H	-5.70208300	2.10362600	1.08886100
H	-5.69234300	3.58247400	0.11226700
O	-1.12757700	2.12583900	-0.43217000
O	-0.90171300	4.34352100	-0.47067200
H	0.86241700	1.82225500	0.68923800
H	2.60589200	-0.12378200	-0.58570900
H	2.99534900	1.69380800	-1.62590200



[4.[3333].3.eii.N10-CH₃]⁺³

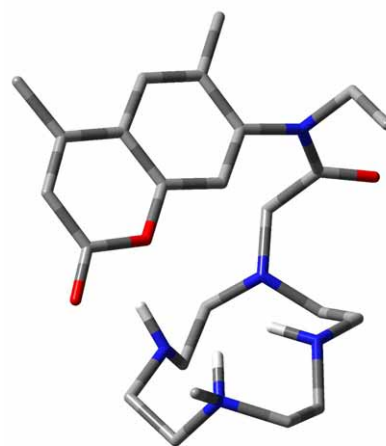
C	2.64363200	2.64692000	0.40817400
C	4.13602100	2.48486400	0.11544400
N	4.35903500	1.71606200	-1.11904200
C	5.23443600	0.55816200	-1.04241100
C	4.59905600	-0.62362500	-0.29520800
N	3.14878700	-0.87691100	-0.63436900
C	2.66571300	-2.16583900	0.00751300
C	2.18212000	-2.01819900	1.45042700
N	0.94347600	-1.22978000	1.54740300
C	1.01211100	-0.09993300	2.48420500
C	2.05097500	0.96307900	2.11756000
N	1.97815000	1.35586200	0.69881100
H	0.02572800	0.37636700	2.47740400
H	1.20050400	-0.42020600	3.52453200
H	5.47112800	0.25146200	-2.06591000
H	6.20243500	0.74564600	-0.54525900
H	2.14626300	3.08621500	-0.46016400
H	2.50910000	3.35273000	1.24163600
H	3.48520900	-2.88790000	-0.05442800
H	1.84385100	-2.54758400	-0.59515700
H	2.02361100	-3.03920800	1.81699900
H	1.88460900	1.82231600	2.78532900
H	4.58574400	3.48269100	0.04178700
H	5.16037800	-1.53682400	-0.51298700
H	2.96381600	-1.57937100	2.08045500
H	4.62938600	-0.46612500	0.78523100
H	4.63918400	1.99409400	0.95881900
H	3.06648600	0.61037700	2.33656000
C	-0.25952700	-2.04761400	1.79382700
H	-0.11129900	-2.75179100	2.62874100
H	-1.07556500	-1.37885100	2.06537400
C	-0.63955900	-2.91471700	0.58622800
O	0.04381000	-3.89684300	0.30151600
N	-1.78726600	-2.60007000	-0.11470200
C	-2.17652700	-3.51846900	-1.21210100
H	-1.96085800	-4.53077500	-0.86761000
H	-3.25528100	-3.42702600	-1.34895000
C	-1.44654700	-3.23540500	-2.52495700
H	-1.62718400	-2.21318900	-2.87195500
H	-0.37106800	-3.39045200	-2.40568600
H	-1.80056600	-3.92066700	-3.30100300
C	-2.33218900	-1.27631100	-0.11641700
C	-1.46284400	-0.21840600	-0.38095800
C	-3.70159800	-1.02598000	0.14460600
C	-1.91878700	1.09164000	-0.34495300
H	-0.41343800	-0.40764900	-0.56379900
C	-4.13492500	0.30133200	0.11388500
C	-3.27256600	1.38816700	-0.12463500
H	-5.18270700	0.50159300	0.31285100
C	-1.30541900	3.42877200	-0.49836400
C	-3.67340200	2.79001800	-0.13908300
C	-2.71576900	3.73612100	-0.33078300
H	-2.95693300	4.79259400	-0.34704900
C	-4.67302300	-2.13109900	0.48171100
H	-5.12895600	-2.56364500	-0.41675700
H	-4.18094700	-2.94343700	1.02262700
H	-5.48751300	-1.75081300	1.10297200
C	-5.11506600	3.16630100	0.05547400
H	-5.74692800	2.70603200	-0.71215000
H	-5.48352700	2.82030000	1.02779600
H	-5.24901800	4.24799800	0.00593900
O	-0.97574500	2.06616900	-0.52336700
O	-0.39145800	4.21282800	-0.60743800
H	0.99792100	1.45828100	0.43821800
H	2.60847100	-0.03603000	-0.21738100
H	4.66558900	2.32704800	-1.86704500
C	2.89406900	-0.89595800	-2.10839300
H	3.14190500	0.08337300	-2.51194500
H	3.49383000	-1.68105900	-2.57393500
H	1.83619800	-1.10280600	-2.27124700



³ Structure is more stable and has been optimized with an extraannular N7-H.

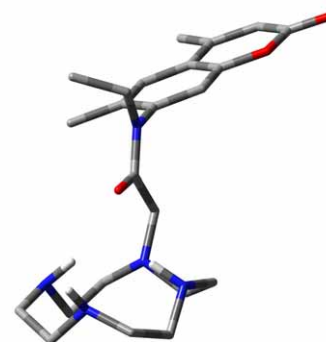
[4.[3333].3.eii.N7-CH₃]⁺

C	3.12361700	1.61241500	1.33156200
C	4.17673200	1.19986800	0.29384100
N	3.48251400	0.87526900	-1.01461900
C	4.02254900	-0.36587000	-1.69653800
C	3.64347200	-1.64805000	-0.95569000
N	2.19581200	-1.76767600	-0.87476600
C	1.67461000	-3.08701800	-0.46905900
C	1.35998400	-3.15650600	1.03653600
N	0.52467300	-2.00651500	1.46177200
C	1.03736700	-1.31266700	2.65042400
C	2.29488100	-0.46860100	2.41144600
N	2.07981100	0.58688200	1.40840000
H	0.24915500	-0.63990600	3.01018300
H	1.25082900	-2.00608100	3.48287100
H	3.57555000	-0.38425700	-2.69184500
H	5.10488700	-0.23925700	-1.78521400
H	2.66472500	2.55661100	1.02469600
H	3.63705800	1.78639700	2.28870800
H	2.39366200	-3.87079500	-0.73201700
H	0.76380100	-3.29939200	-1.03379500
H	0.85998800	-4.10669400	1.25904600
H	2.59518600	-0.04555800	3.38405900
H	4.90694200	1.98964600	0.10772000
H	4.03867600	-2.47100800	-1.56117100
H	2.29581000	-3.14001400	1.60668700
H	4.17515500	-1.70569000	0.01211100
H	4.70958200	0.30374800	0.61396100
H	3.12560400	-1.10534800	2.08434100
C	-0.90102100	-2.34084000	1.63117700
H	-1.04967800	-3.12982700	2.38659100
H	-1.42069300	-1.44399600	1.97439200
C	-1.55873200	-2.88896500	0.35715400
O	-1.40608500	-4.06418200	0.04274700
N	-2.37986000	-2.05125800	-0.37637900
C	-3.05668200	-2.63478300	-1.55916600
H	-3.33769700	-3.65464300	-1.29220200
H	-3.96939400	-2.06061000	-1.73196200
C	-2.18298000	-2.63480400	-2.81327600
H	-1.86895000	-1.62175300	-3.08397100
H	-1.29550600	-3.25402500	-2.66368400
H	-2.74607900	-3.04847600	-3.65558900
C	-2.40019100	-0.63128300	-0.22627400
C	-1.22614400	0.08606200	-0.46161800
C	-3.59332600	0.04270300	0.14307600
C	-1.21760500	1.46743700	-0.30524400
H	-0.32029900	-0.42882200	-0.75438200
C	-3.55228700	1.43130000	0.24983600
C	-2.37924400	2.17961500	0.03406800
H	-4.46059800	1.95301800	0.53266900
C	0.12613900	3.47579000	-0.32422400
C	-2.28946800	3.62722500	0.15163900
C	-1.07836800	4.22104400	-0.03516800
H	-0.94944000	5.29362800	0.04834500
C	-4.87167500	-0.70230500	0.43964800
H	-5.45472700	-0.88646500	-0.47020100
H	-4.66944600	-1.67420800	0.89621700
H	-5.50584600	-0.12670200	1.11804800
C	-3.51032200	4.43967300	0.47727600
H	-4.29207100	4.28840300	-0.27502700
H	-3.93120000	4.14352800	1.44451300
H	-3.27519500	5.50425200	0.51858900
O	-0.01141300	2.10276500	-0.48827500
O	1.25400000	3.92935900	-0.42275900
H	1.17621500	1.02366900	1.55588500
H	1.82703200	-1.11063200	-0.18476500
H	2.51253300	0.65684100	-0.72580200
C	3.43113500	2.05347300	-1.94396000
H	4.44893100	2.30197700	-2.24768400
H	2.84020500	1.77553000	-2.81724600
H	2.94797300	2.88699800	-1.43243100



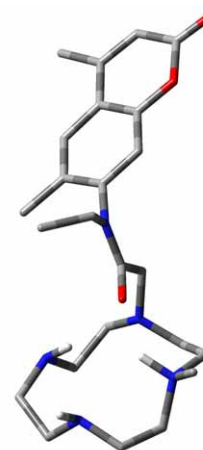
4.[3333].4.iei

C	5.25133700	-1.92836100	-0.45348600
C	6.12462400	-0.68882100	-0.17536900
N	5.56305900	0.11174400	0.91084000
C	5.89294100	1.53873700	0.89993300
C	4.93903800	2.31598700	-0.01347600
N	3.58145000	2.23216200	0.50413900
C	2.53277800	2.71024500	-0.38144100
C	2.22660700	1.84269600	-1.62362900
N	1.84313500	0.47524600	-1.28219500
C	2.21709000	-0.55542300	-2.25178500
C	3.67314300	-1.00447300	-2.09935100
N	3.86390600	-1.65661000	-0.81116500
H	1.58495200	-1.43260400	-2.07874000
H	2.03996000	-0.22367400	-3.29051400
H	5.76979000	1.92121900	1.91873400
H	6.93568800	1.73759600	0.59504400
H	5.24804100	-2.56395900	0.44276200
H	5.71844600	-2.52211400	-1.25134800
H	2.78471600	3.72236300	-0.72678000
H	1.61410300	2.81690300	0.21127800
H	3.44780800	-1.07117000	-0.08623400
H	3.38283500	1.26728400	0.76727500
H	1.45247900	2.35104900	-2.23267400
H	3.90457600	-1.71845800	-2.90343500
H	7.16660200	-1.00695500	0.01436600
H	5.25312600	3.36955700	-0.04052100
H	3.12083700	1.78563300	-2.25137500
H	5.05420900	1.93734900	-1.04782000
H	6.16014200	-0.06187800	-1.07232500
H	4.33072400	-0.13130200	-2.26897000
H	5.79266000	-0.30156500	1.80807400
C	0.55112900	0.32101600	-0.65648200
H	0.05186600	1.29457100	-0.55854900
H	-0.13010800	-0.28776200	-1.26439300
C	0.64409200	-0.26361700	0.77057700
O	1.70735300	-0.34673500	1.37412800
N	-0.54424200	-0.62149100	1.37875500
C	-0.50585600	-0.93052400	2.82506200
H	0.29515200	-0.32691000	3.25663600
H	-1.45722200	-0.60254100	3.25371600
C	-0.25943100	-2.40727000	3.13382600
H	-1.06661400	-3.04053200	2.75265200
H	0.68687600	-2.73212200	2.69417600
H	-0.20194900	-2.55598400	4.21734900
C	-1.82043600	-0.57532600	0.72627800
C	-2.66299400	0.50306400	0.99927000
C	-2.24508200	-1.61936600	-0.13261300
C	-3.93030300	0.56842800	0.42465100
H	-2.34041400	1.30198000	1.65773400
C	-3.51615100	-1.51996600	-0.69655000
C	-4.38368100	-0.44375300	-0.44075900
H	-3.85113400	-2.31529000	-1.35464100
C	-5.97889400	1.82748800	0.21692200
C	-5.71857100	-0.31125500	-1.00761800
C	-6.45371700	0.77983500	-0.67726400
H	-7.45314500	0.93356100	-1.06795500
C	-1.36467300	-2.80215600	-0.45745300
H	-0.62551400	-2.55797500	-1.23017200
H	-0.80605600	-3.14680700	0.41457800
H	-1.96385800	-3.63471100	-0.83499800
C	-6.25602200	-1.36523800	-1.93616000
H	-5.61791500	-1.47301500	-2.82049800
H	-6.29116300	-2.34329200	-1.44308100
H	-7.26442300	-1.11441700	-2.27047000
O	-4.69462900	1.65323000	0.73714200
O	-6.59010400	2.81687100	0.54248000



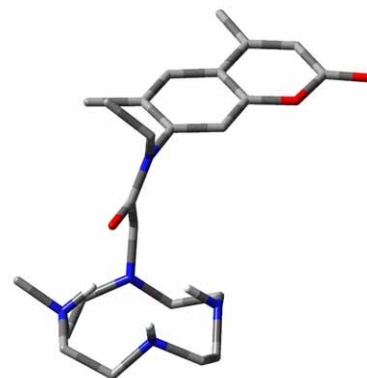
[4.[3333].4.iei.N10-CH₃]⁺

C	-4.13269900	2.75410000	0.19760000
C	-5.34045900	1.80198500	0.12697500
N	-5.03831900	0.52553800	0.79708900
C	-5.81750200	-0.62336800	0.35155300
C	-5.07327300	-1.38949400	-0.75070300
N	-3.72514400	-1.89164700	-0.30008700
C	-2.83507000	-2.32764300	-1.44170900
C	-2.31254200	-1.17797300	-2.31087500
N	-1.65285200	-0.12292300	-1.55766200
C	-1.67906400	1.19960900	-2.21589200
C	-2.90914400	2.00801300	-1.80637900
N	-2.89862200	2.21100200	-0.36329900
H	-0.79063700	1.75442100	-1.90520600
H	-1.63514100	1.10240200	-3.31056500
H	-6.02089800	-1.28168600	1.20128500
H	-6.80271500	-0.35358200	-0.05936100
H	-3.94221200	3.01417700	1.24646200
H	-4.38425600	3.69087200	-0.31304400
H	-3.39272900	-3.04592600	-2.04947200
H	-2.00106300	-2.85699400	-0.97716500
H	-2.73082700	1.30939500	0.07954000
H	-3.19005400	-1.12325500	0.17705600
H	-1.65514700	-1.64935600	-3.06555800
H	-2.87943100	2.98087600	-2.31323200
H	-6.23235900	2.29267700	0.54684800
H	-5.64695400	-2.25401000	-1.09872200
H	-3.13749900	-0.72864300	-2.87053100
H	-4.89865300	-0.72708300	-1.59930500
H	-5.57576600	1.58403100	-0.92037200
H	-3.81436500	1.49531800	-2.18736300
H	-5.11297400	0.63742700	1.80267900
C	-0.40382000	-0.48095400	-0.89882500
H	-0.04160000	-1.46647300	-1.23080500
H	0.39030100	0.21928700	-1.16249000
C	-0.56334500	-0.56582000	0.63208700
O	-1.66213600	-0.87283400	1.13017400
N	0.52880300	-0.36775300	1.40644400
C	0.43283500	-0.65983800	2.85973400
H	-0.27497700	-1.48354800	2.97098500
H	1.41898800	-1.00933700	3.17422500
C	-0.01449100	0.53004900	3.70660300
H	0.71177800	1.34579000	3.67316200
H	-0.98382400	0.90429800	3.36846200
H	-0.11367000	0.21578400	4.75019300
C	1.81296100	0.01994200	0.86959300
C	2.75233200	-0.98640600	0.65592800
C	2.11529700	1.37492600	0.60267000
C	4.01938000	-0.66639700	0.17001800
H	2.51720900	-2.02446800	0.86442900
C	3.39046900	1.65670100	0.10813700
C	4.36394400	0.66800500	-0.11431500
H	3.64008300	2.69061200	-0.10609800
C	6.17928800	-1.49797100	-0.51464800
C	5.70608100	0.93515800	-0.62197100
C	6.54444400	-0.11537100	-0.79926000
H	7.55341700	0.01828100	-1.17226100
C	1.13270000	2.49911600	0.84152100
H	0.11782700	2.27098300	0.50172500
H	1.05792200	2.74454700	1.90618600
H	1.45980700	3.40429500	0.32433400
C	6.13343800	2.34254600	-0.93313000
H	5.48716500	2.79218400	-1.69547300
H	6.07517100	2.97820400	-0.04241700
H	7.16040800	2.36611600	-1.30117600
O	4.88034500	-1.69861900	-0.01998800
O	6.87594500	-2.46857500	-0.66335300
C	-3.83666300	-2.99852700	0.70282200
H	-4.47494500	-2.68328500	1.52542400
H	-4.25765100	-3.88208900	0.21990600
H	-2.84062100	-3.20388500	1.09044000



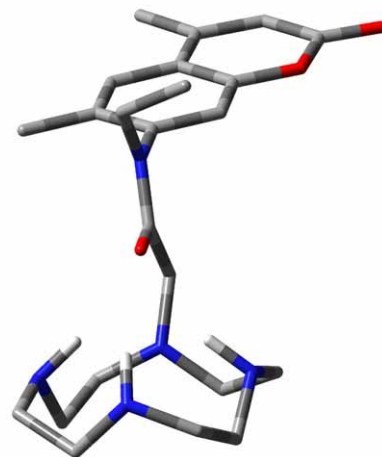
[4.**[3333]**.4.iei.N4-CH₃]⁺

C	5.52590400	-0.69371800	0.25186000
C	5.61732700	0.80904000	0.50617500
N	4.50743300	1.27483100	1.32406200
C	4.28880400	2.73522200	1.29175600
C	3.41196000	3.12615100	0.10156700
N	2.10247300	2.50795100	0.25003100
C	1.25330900	2.51197600	-0.93026100
C	1.65836500	1.53386100	-2.05445800
N	1.80016200	0.14892100	-1.57682000
C	2.68796700	-0.69104900	-2.36660100
C	4.13419900	-0.65178600	-1.85133600
N	4.25085600	-1.14090200	-0.42841500
H	2.31731200	-1.72099200	-2.36935900
H	2.72327300	-0.38460300	-3.42371100
H	3.76146400	3.00914400	2.20969900
H	5.23371100	3.29913700	1.26884800
H	5.56126100	-1.23320000	1.20229500
H	6.36152900	-1.04033900	-0.36363200
H	1.22390800	3.52290800	-1.35311600
H	0.22482900	2.29676300	-0.61358300
H	3.41216700	-0.76743400	0.09315900
H	2.24349500	1.55049400	0.56521900
H	0.93303900	1.60818500	-2.88363800
H	4.80031800	-1.26154400	-2.46969400
H	6.61290300	0.99138800	0.94698900
H	3.30442300	4.21790000	0.08210500
H	2.62829100	1.83772100	-2.46236700
H	3.93629100	2.85681200	-0.83784600
H	5.61139000	1.36054500	-0.43865600
H	4.49336300	0.37667200	-1.86885500
H	4.63471300	0.96913300	2.28448000
C	0.58183500	-0.47281800	-1.08333600
H	-0.25872300	0.21901300	-1.16656700
H	0.29939600	-1.35033700	-1.68316800
C	0.72604000	-0.93177600	0.38190400
O	1.85136800	-1.11995100	0.87842100
N	-0.40480400	-1.12560000	1.10301200
C	-0.28922000	-1.45778000	2.54543800
H	0.66720600	-1.05898900	2.88572800
H	-1.08986000	-0.91865100	3.05784200
C	-0.37937500	-2.95366100	2.84018800
H	-1.33842700	-3.37168300	2.52163600
H	0.42712500	-3.50005300	2.34269100
H	-0.28538300	-3.12033600	3.91752700
C	-1.72751500	-0.89883200	0.57047200
C	-2.35447500	0.30238100	0.90666100
C	-2.38658300	-1.86886300	-0.21510900
C	-3.64839800	0.56266400	0.46187400
H	-1.84812500	1.04498400	1.51380500
C	-3.68559200	-1.57647800	-0.64005900
C	-4.34405100	-0.37912800	-0.32190900
H	-4.20827800	-2.31560700	-1.23842100
C	-5.48603100	2.12698800	0.42590100
C	-5.70184100	-0.04962000	-0.74539600
C	-6.21521000	1.14808900	-0.37267600
H	-7.21680300	1.45127300	-0.65550400
C	-1.74543700	-3.17543100	-0.62182700
H	-1.29585000	-3.10745900	-1.62106200
H	-0.96358700	-3.48578400	0.07313600
H	-2.49105700	-3.97358400	-0.66662300
C	-6.49583700	-1.02327400	-1.57118700
H	-5.99134300	-1.24068400	-2.51954500
H	-6.62156300	-1.97614100	-1.04478000
H	-7.48690300	-0.62634300	-1.79670300
O	-4.19004900	1.75522500	0.81780800
O	-5.88662000	3.20744600	0.77387100
C	4.13692000	-2.63189800	-0.34324500
H	5.00712600	-3.08652300	-0.81982100
H	4.08439600	-2.91598800	0.70689100
H	3.22414000	-2.95553500	-0.83765800



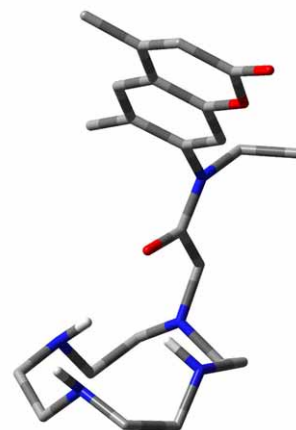
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C	5.67805500	1.51194100	0.93263500
C	4.79533600	2.24050800	-0.09842600
N	3.40011900	2.24459000	0.33335000
C	2.42790200	2.68414900	-0.65586800
C	2.16445900	1.72110400	-1.83688700
N	1.80836600	0.37054800	-1.40675000
C	2.18571500	-0.70739800	-2.32471900
C	3.63419700	-1.16200100	-2.12303600
N	3.78239900	-1.77967700	-0.81203100
H	1.53654400	-1.56863700	-2.13239000
H	2.03213500	-0.41425700	-3.37726800
H	5.47653100	1.94920200	1.91812100
H	6.73213800	1.71086900	0.70340900
H	5.11483900	-2.56052800	0.57807300
H	5.67792800	-2.60942100	-1.08917800
H	2.74226600	3.65181700	-1.06852600
H	1.48082200	2.87746700	-0.13327800
H	3.25972600	-1.22903400	-0.13242900
H	3.12461500	1.31261100	0.63809900
H	1.39381300	2.16675300	-2.49667000
H	3.88696800	-1.89685300	-2.90160600
H	7.03628300	-1.02651700	0.08917300
H	5.13560900	3.28299200	-0.18141300
H	3.07397500	1.63700600	-2.43902300
H	4.95564900	1.78609600	-1.09409700
H	6.02930900	-0.12548600	-1.03478700
H	4.29973200	-0.29621800	-2.29119600
C	0.54310000	0.22174400	-0.72871000
H	0.04257500	1.19343000	-0.63576700
H	-0.15909000	-0.41144000	-1.28954700
C	0.70280900	-0.34544800	0.70133100
O	1.79177000	-0.38556900	1.27348400
N	-0.43247700	-0.80969200	1.32026700
C	-0.31616600	-1.32973000	2.69940800
H	-1.11396100	-2.06555900	2.83714600
H	0.64423500	-1.84418000	2.76732600
C	-0.40583800	-0.23522400	3.76271300
H	0.40615100	0.48509200	3.63584700
H	-1.36175500	0.29518500	3.71109000
H	-0.31867300	-0.67582100	4.76121100
C	-1.74285700	-0.72497900	0.74313200
C	-2.44547300	0.47554200	0.81794600
C	-2.32302600	-1.86794800	0.14085800
C	-3.73322500	0.56397100	0.28784300
H	-2.00513800	1.34821100	1.28654500
C	-3.61088900	-1.74846100	-0.37432600
C	-4.34423200	-0.54851700	-0.31720800
H	-4.06319700	-2.61636100	-0.84305500
C	-5.65044500	1.97829000	-0.09884700
C	-5.69133000	-0.38421100	-0.84677800
C	-6.28689700	0.82868700	-0.72815700
H	-7.28782000	1.01121800	-1.10228400
C	-1.56711800	-3.17050300	0.04501200
H	-0.58325200	-3.03379400	-0.41487500
H	-1.39202700	-3.61369700	1.03152800
H	-2.12320600	-3.89779600	-0.55136100
C	-6.39325000	-1.53981600	-1.50532100
H	-5.82498500	-1.90615100	-2.36770100
H	-6.50377800	-2.38049300	-0.81105000
H	-7.38720500	-1.24830700	-1.84964400
O	-4.35846100	1.76980100	0.39157000
O	-6.13316700	3.07684500	0.03332000
H	4.54086400	-0.16713400	1.24587900



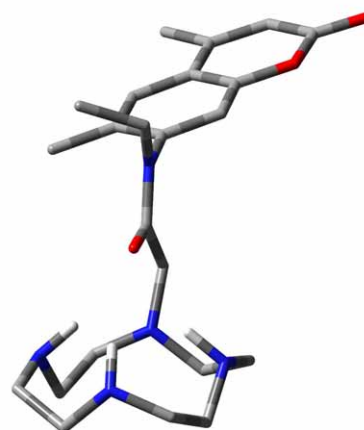
4.[3333].6.iei

C	4.15941300	-2.08473500	-1.97668600
C	4.46656800	-2.82744800	-0.66091100
N	3.29507200	-2.84561900	0.21253700
C	3.55884000	-2.94720200	1.64967200
C	3.84265400	-1.56731100	2.25281400
N	2.66470500	-0.72303100	2.12361500
C	2.85302300	0.68648500	2.41859900
C	3.70216900	1.50288000	1.41724600
N	3.16056900	1.50480200	0.06173300
C	4.14063200	1.57933000	-1.02291700
C	4.75802900	0.21525900	-1.34442000
N	3.73514200	-0.69644200	-1.83697000
H	3.62794900	1.92991300	-1.92409800
H	4.94566000	2.30170300	-0.79936100
H	2.65960000	-3.34676800	2.13038800
H	4.39315700	-3.63037800	1.88822200
H	3.36403800	-2.62678900	-2.50653700
H	5.04553000	-2.12544400	-2.62528300
H	3.31337100	0.78877700	3.41115400
H	1.86014900	1.15006200	2.50131400
H	2.93473600	-0.65769100	-1.20510600
H	2.28207100	-0.82313700	1.18411000
H	3.81700200	2.53355200	1.81118500
H	5.52444000	0.35387000	-2.12119100
H	4.85192800	-3.83825000	-0.89048500
H	4.09002000	-1.68810500	3.31755500
H	4.70859800	1.07696100	1.37074900
H	4.75155400	-1.15416500	1.77338800
H	5.27434100	-2.31112500	-0.13152800
H	5.29539600	-0.14671500	-0.44784900
H	2.64451900	-3.56493200	-0.08377400
C	1.92608700	2.22905900	-0.11133400
H	1.75278900	2.92507600	0.72324000
H	1.97374800	2.85277400	-1.01436900
C	0.69765000	1.29828300	-0.25885200
O	0.81445400	0.08257200	-0.35805800
N	-0.54449500	1.89744300	-0.30012400
C	-0.77867100	3.35224800	-0.25249900
H	0.09650000	3.86127100	-0.66233700
H	-1.60616300	3.56763800	-0.93682300
C	-1.10094100	3.90726800	1.13795600
H	-2.02762300	3.48185600	1.53115500
H	-0.29759800	3.69200200	1.84913700
H	-1.22685500	4.99376100	1.08473700
C	-1.69769600	1.04872400	-0.45294600
C	-2.48161300	0.76700100	0.66042800
C	-2.04037700	0.54461500	-1.72926200
C	-3.63405600	-0.00706500	0.52129600
H	-2.20175000	1.12139300	1.64487300
C	-3.19210100	-0.22832300	-1.83470400
C	-4.01452900	-0.52059500	-0.72987500
H	-3.46306600	-0.62295300	-2.80864900
C	-5.53076900	-0.99497400	1.63989700
C	-5.22634300	-1.32435900	-0.79668800
C	-5.92690500	-1.53401400	0.34627900
H	-6.83578000	-2.12478100	0.35759800
C	-1.16978100	0.80886000	-2.93138700
H	-0.99550200	1.87995200	-3.08114000
H	-0.19216200	0.33204500	-2.80653300
H	-1.63062200	0.41373600	-3.84014000
C	-5.67925200	-1.90543100	-2.10805200
H	-5.86501500	-1.11635700	-2.84553400
H	-4.91410700	-2.56663900	-2.53013400
H	-6.59850700	-2.48109300	-1.98412400
O	-4.36026700	-0.23587200	1.65310700
O	-6.11937200	-1.14450400	2.68479300



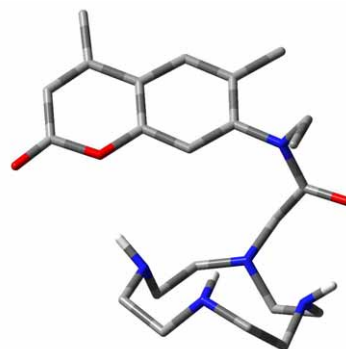
4.[3333].7.iii

C	5.20798300	-1.87473300	-0.35575800
C	6.03677600	-0.61587600	-0.04098500
N	5.52036600	0.11487800	1.11767100
C	5.67381500	1.56814500	1.07886100
C	4.79787400	2.32449600	0.06223800
N	3.39602100	2.29594700	0.47136600
C	2.43513200	2.76706400	-0.51453900
C	2.20425100	1.85400300	-1.74086800
N	1.85240200	0.48326700	-1.37528800
C	2.26040100	-0.55137200	-2.32908500
C	3.71036900	-0.99720100	-2.11822700
N	3.84143800	-1.66256700	-0.82927400
H	1.62022700	-1.42805200	-2.18247800
H	2.12234000	-0.21817700	-3.37190100
H	5.45086600	1.96408600	2.07709700
H	6.72855200	1.78949400	0.87467500
H	5.15474400	-2.49068000	0.55133200
H	5.74725600	-2.46750500	-1.10604800
H	2.74412400	3.75593700	-0.87805400
H	1.47672400	2.92478500	-0.00066600
H	3.30006000	-1.14411200	-0.13899200
H	3.12600800	1.34924500	0.73236900
H	1.44211100	2.32072200	-2.39590600
H	3.98506100	-1.69925200	-2.91932500
H	7.07386500	-0.92643600	0.15959300
H	5.12596300	3.37340500	0.02398300
H	3.12569500	1.80401100	-2.32849600
H	4.97906300	1.90957400	-0.94696300
H	6.08034900	0.01432400	-0.94355000
H	4.36907100	-0.11882000	-2.24201600
C	0.57259400	0.29763400	-0.73493300
H	0.05460000	1.25891400	-0.62174300
H	-0.10505400	-0.32229100	-1.33589100
C	0.69770500	-0.29875800	0.68639200
O	1.77971500	-0.39058200	1.26440500
N	-0.46865600	-0.66348200	1.31857600
C	-0.39809000	-0.99756900	2.75958300
H	0.41734900	-0.40703600	3.18159100
H	-1.33650500	-0.66764500	3.21400900
C	-0.15885800	-2.48113100	3.03864800
H	-0.98157500	-3.10067200	2.66863700
H	0.77321700	-2.80992700	2.57224400
H	-0.07639900	-2.64596300	4.11799600
C	-1.76101900	-0.60477300	0.69563500
C	-2.58805100	0.47755000	0.99739300
C	-2.21112000	-1.63902100	-0.16094100
C	-3.86743300	0.55689000	0.45173500
H	-2.24517600	1.26836100	1.65545100
C	-3.49428000	-1.52562500	-0.69478700
C	-4.34748400	-0.44517600	-0.41125900
H	-3.84944200	-2.31329400	-1.35146300
C	-5.91080800	1.83210800	0.30047400
C	-5.69394900	-0.29835100	-0.94740000
C	-6.41304800	0.79521700	-0.59159800
H	-7.41966500	0.95964100	-0.95870800
C	-1.34677300	-2.82453900	-0.51789700
H	-0.63449800	-2.58171100	-1.31599900
H	-0.76000100	-3.17416700	0.33325800
H	-1.96181800	-3.65392600	-0.87621500
C	-6.25975400	-1.34022500	-1.87260200
H	-5.64284300	-1.44461600	-2.77225200
H	-6.29127400	-2.32230800	-1.38738400
H	-7.27351000	-1.07918200	-2.18186400
O	-4.61583800	1.64418300	0.79025900
O	-6.50684700	2.82284700	0.64779700
H	4.55588400	-0.13713500	1.31214700



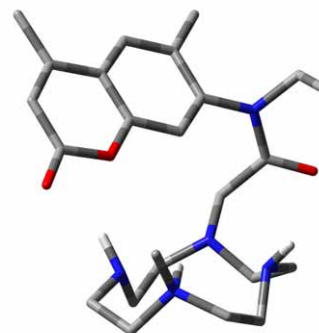
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C	1.57365200	3.41212000	-0.48763400
C	3.02149800	3.02170000	-0.79964600
N	3.06584700	1.79723400	-1.58719000
C	4.39607900	1.21077600	-1.72128900
C	4.89552500	0.47053700	-0.46711200
N	4.00792000	-0.64630900	-0.15561700
C	3.97243300	-1.08813800	1.23477000
C	2.97924400	-0.28881200	2.09148200
N	1.58705500	-0.28553000	1.62854300
C	0.82241900	0.82629500	2.21077800
C	1.17523400	2.21170400	1.64149000
N	0.85203700	2.35071700	0.22408000
H	-0.23969100	0.64482300	2.01832600
H	0.93653200	0.87349800	3.31208400
H	4.38115500	0.50004400	-2.56021500
H	5.11029500	1.99765300	-1.99699900
H	1.04854900	3.57529500	-1.43412700
H	1.57534600	4.37325500	0.05809300
H	4.95620000	-1.01183800	1.73442500
H	3.68832100	-2.14056000	1.24154900
H	3.04951700	-0.66929100	3.13149400
H	0.66611800	2.96384900	2.27179400
H	3.47979200	3.83942100	-1.37347800
H	5.95059900	0.16599300	-0.60142000
H	3.31605900	0.75073200	2.12597200
H	4.88530800	1.16053900	0.38461000
H	3.59397200	2.96636700	0.14771800
H	2.24473800	2.40032400	1.76961700
C	0.92420000	-1.59070600	1.76032900
H	1.38017800	-2.20183200	2.55503000
H	-0.12354800	-1.43870800	2.02970400
C	1.01850400	-2.44004300	0.47855200
O	1.99460900	-3.15150300	0.25420500
N	-0.03459100	-2.41287000	-0.41584500
C	0.15853000	-3.12247800	-1.69879000
H	0.71208400	-4.03779900	-1.48251700
H	-0.82868800	-3.39452600	-2.08120100
C	0.91193200	-2.27080000	-2.72161700
H	0.35324100	-1.36448200	-2.97438900
H	1.88561700	-1.97496500	-2.32400100
H	1.07022900	-2.84085600	-3.64329000
C	-1.23555600	-1.65220400	-0.26275700
C	-1.19863200	-0.26730900	-0.40656900
C	-2.45911900	-2.32375900	-0.00531400
C	-2.37884400	0.46621100	-0.28538400
H	-0.25915900	0.25059100	-0.57454400
C	-3.61843200	-1.55942900	0.08481200
C	-3.61562100	-0.15856800	-0.05347400
H	-4.55802900	-2.06476400	0.28371400
C	-3.37477800	2.67498200	-0.29122700
C	-4.80178400	0.67976600	0.04217400
C	-4.65879100	2.02398400	-0.08254700
H	-5.50682500	2.69602300	-0.01817800
C	-2.51209500	-3.81971500	0.18835600
H	-2.41953600	-4.36021200	-0.76088600
H	-1.69672400	-4.16757200	0.82894200
H	-3.45992900	-4.11762800	0.64370300
C	-6.15170500	0.05876000	0.27544600
H	-6.40015500	-0.65327500	-0.51945100
H	-6.17220100	-0.49427400	1.22136200
H	-6.93249200	0.82090000	0.30897900
O	-2.27124100	1.82546900	-0.39935700
O	-3.17528600	3.86405400	-0.37347000
H	2.46470100	1.11167900	-1.12942000
H	-0.14598300	2.50219600	0.11088500
H	4.19851400	-1.43671000	-0.76167300



[4.**[3333]**.8.eie.N7-CH₃]⁺

C	2.80058700	2.33529100	1.21495200
C	3.90369600	1.97306100	0.20648800
N	3.26656700	1.30070000	-0.98441900
C	4.17604600	0.30462900	-1.66376500
C	4.04000200	-1.07309000	-1.01696000
N	2.64382600	-1.49471200	-1.08456100
C	2.32416900	-2.73875400	-0.35741500
C	2.06657100	-2.56146300	1.14585400
N	0.94382300	-1.66990300	1.49482900
C	1.23242000	-0.83547400	2.67030300
C	2.28892300	0.25114200	2.45966800
N	1.92782300	1.17834900	1.38709400
H	0.29868000	-0.33768800	2.95854900
H	1.53981200	-1.43651300	3.54602100
H	3.87212100	0.25562900	-2.71256200
H	5.19899900	0.68643900	-1.62787000
H	2.20548800	3.16990300	0.83519300
H	3.28289600	2.67025100	2.14537600
H	3.12728500	-3.48690000	-0.46543000
H	1.43804200	-3.17268600	-0.81933000
H	1.91347100	-3.56819800	1.56326400
H	2.41927000	0.76782800	3.42594200
H	4.46585800	2.84350000	-0.13949400
H	4.74811600	-1.75580500	-1.51596500
H	2.97512700	-2.17409000	1.61789800
H	4.34598100	-1.02896200	0.03436900
H	4.60420300	1.25536100	0.63938600
H	3.26267300	-0.19634300	2.22583100
C	-0.32927400	-2.38248000	1.70537800
H	-0.23308600	-3.18108000	2.46047500
H	-1.06186900	-1.66050900	2.07228300
C	-0.86613600	-3.08844900	0.45523200
O	-0.44486400	-4.19851300	0.14439100
N	-1.87880300	-2.48121000	-0.26604900
C	-2.40734400	-3.22674500	-1.43295500
H	-2.42783400	-4.28089100	-1.15333100
H	-3.43361600	-2.89603300	-1.60061600
C	-1.57392500	-3.02842800	-2.69885500
H	-1.51445800	-1.97124600	-2.97692900
H	-0.56318100	-3.41934700	-2.55756400
H	-2.03069900	-3.57055100	-3.53253900
C	-2.21970400	-1.09842100	-0.14875000
C	-1.22224300	-0.14175300	-0.34525000
C	-3.55176200	-0.69915400	0.13786800
C	-1.53664400	1.20882400	-0.25634100
H	-0.19696500	-0.44217800	-0.52505900
C	-3.82965000	0.66590800	0.18399700
C	-2.84586700	1.65325600	-0.01421100
H	-4.84606700	0.97654900	0.40249000
C	-0.67765500	3.46621000	-0.34915100
C	-3.08670800	3.08808800	0.03025200
C	-2.03144000	3.93202700	-0.14119700
H	-2.15203200	5.00857100	-0.11542300
C	-4.64709500	-1.69940200	0.41879800
H	-5.16136200	-2.01216800	-0.49757700
H	-4.25219500	-2.60049600	0.89417000
H	-5.40265900	-1.26588300	1.07856600
C	-4.47382600	3.61699300	0.26107300
H	-5.16272800	3.25733500	-0.51099700
H	-4.86623200	3.27911100	1.22672200
H	-4.48608500	4.70791500	0.25048100
O	-0.49622500	2.09097400	-0.41685100
O	0.32316400	4.15359600	-0.46094900
H	2.48412700	0.74885900	-0.55058200
H	0.95922400	1.46580800	1.46404600
H	2.40057000	-1.63862600	-2.06222200
C	2.67718200	2.28802600	-1.94751100
H	3.49016400	2.83756200	-2.42540000
H	2.11047800	1.73626200	-2.69814200
H	2.00730700	2.96923500	-1.42001900



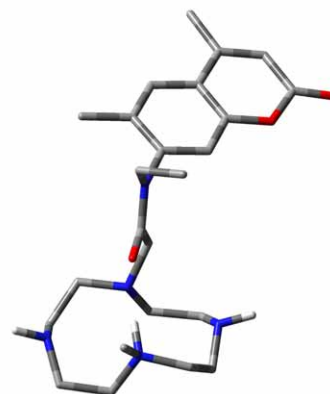
4.[3333].9.eie

C	-1.90443300	-3.51229700	0.20757600
C	-3.35908600	-3.23659100	-0.19426700
N	-3.38864000	-2.23847300	-1.25750700
C	-4.66486000	-1.54582400	-1.41986100
C	-4.90804600	-0.43087900	-0.38684000
N	-3.86174500	0.58799200	-0.48952500
C	-3.73635800	1.49262700	0.65501200
C	-2.93100300	0.88928500	1.81734100
N	-1.50528800	0.63747000	1.55448400
C	-0.97360700	-0.48136800	2.35005300
C	-1.52553900	-1.86958300	2.00515800
N	-1.23778600	-2.28171300	0.63916200
H	0.11129300	-0.50470400	2.19457800
H	-1.12660700	-0.32615100	3.43646100
H	-4.69885000	-1.10308600	-2.42612100
H	-5.48482900	-2.27347200	-1.37847200
H	-1.37235600	-3.88459100	-0.67465400
H	-1.88155500	-4.31201000	0.97024900
H	-4.71988700	1.78465500	1.06826600
H	-3.25621600	2.41424200	0.32069500
H	-3.05319700	1.55541900	2.69204900
H	-1.11992100	-2.57030600	2.76139200
H	-3.81257300	-4.17405100	-0.54515600
H	-5.92702400	-0.01711300	-0.50483300
H	-3.39814500	-0.05884500	2.09422500
H	-4.86803000	-0.86048200	0.62056600
H	-3.93109000	-2.94163200	0.70638900
H	-2.61056300	-1.89124800	2.14507900
C	-0.68534700	1.84253900	1.73595900
H	-1.05400500	2.47605300	2.55841100
H	0.33153900	1.53556100	1.98855800
C	-0.63247600	2.76722600	0.51120900
O	-1.31082000	3.79136800	0.46281100
N	0.20296100	2.42404900	-0.52996000
C	0.25074800	3.33402500	-1.69277600
H	0.53728000	2.73942600	-2.56447700
H	-0.76133800	3.71286100	-1.84893500
C	1.22255800	4.49833200	-1.49709100
H	0.91742200	5.10506400	-0.64113400
H	2.24439600	4.14180600	-1.33327600
H	1.22713000	5.13768400	-2.38623300
C	1.07985500	1.29059800	-0.54213600
C	2.29172900	1.35755500	0.14448000
C	0.73733000	0.14263800	-1.29733700
C	3.17783200	0.28085400	0.10472200
H	2.56063900	2.24235100	0.71045000
C	1.64964100	-0.90966800	-1.32647600
C	2.87773200	-0.87469800	-0.63785700
H	1.39774600	-1.79190100	-1.90636500
C	5.30908900	-0.59179100	0.82882600
C	3.85706200	-1.95212200	-0.64805600
C	5.00408000	-1.78977300	0.05845400
H	5.76944900	-2.55696000	0.08673700
C	-0.57571500	0.05781900	-2.02856300
H	-1.40553600	0.28903400	-1.35375100
H	-0.61726500	0.76321400	-2.86715700
H	-0.73455100	-0.94524600	-2.43090400
C	3.59282500	-3.20898200	-1.43118000
H	2.67937200	-3.70575200	-1.08496100
H	3.45313500	-2.98691100	-2.49504000
H	4.42186500	-3.91255400	-1.33423100
O	4.34121100	0.41336700	0.80561700
O	6.31067900	-0.39677400	1.47589100
H	-4.00940600	1.13226400	-1.33451100
H	-0.23468500	-2.34699700	0.49923100
H	-2.69276900	-1.53411500	-1.01234600



[4.[3333].9.eie.N7-CH₃]⁺

C	5.63549500	-0.81876700	-0.84010800
C	5.27042100	0.53849300	-0.23219200
N	4.20097800	0.47277400	0.82829100
C	3.97786200	1.82899800	1.46092300
C	3.44457000	2.92555000	0.52979800
N	2.03511400	2.73702600	0.19693000
C	1.65533700	2.76629600	-1.21577900
C	2.03941800	1.49620300	-2.00013100
N	1.92177600	0.23483700	-1.24858900
C	2.22588300	-0.92836800	-2.10684500
C	3.71428500	-1.15046900	-2.39805200
N	4.45448600	-1.58139400	-1.20446500
H	1.86426800	-1.82282600	-1.59173400
H	1.67717100	-0.85839400	-3.06318700
H	3.25650000	1.67110500	2.26462100
H	4.93500900	2.12616700	1.90164000
H	6.21254400	-1.40582000	-0.12009400
H	6.31960800	-0.60207500	-1.67994500
H	2.07398600	3.62568900	-1.76642100
H	0.56926100	2.89604800	-1.24367500
H	1.43102800	1.48503700	-2.92264800
H	3.78464600	-1.90654200	-3.19045300
H	6.15428100	1.00271400	0.21584000
H	3.60365600	3.86937900	1.06831200
H	3.07871600	1.57851800	-2.33739600
H	4.05192800	3.00932400	-0.37803200
H	4.89612200	1.20652900	-1.00685300
H	4.16986200	-0.24599800	-2.81912100
C	0.60745300	0.06153200	-0.62357700
H	0.25302700	1.02395300	-0.25456200
H	-0.14890400	-0.30846600	-1.33123600
C	0.70347200	-0.85449600	0.60445800
O	1.78220800	-1.02398500	1.18155000
N	-0.44249300	-1.46034900	1.03002700
C	-0.37892500	-2.32266900	2.23226100
H	-1.17950100	-3.06053100	2.13986400
H	0.57675500	-2.84868200	2.19815400
C	-0.51702100	-1.54488400	3.54049700
H	0.29650600	-0.82234600	3.64635000
H	-1.47084100	-1.01180900	3.59039400
H	-0.47341300	-2.23426600	4.38920200
C	-1.74320600	-1.12157200	0.51527800
C	-2.29635300	0.11137100	0.85609200
C	-2.45474600	-2.03846300	-0.29202100
C	-3.56188600	0.46301900	0.38744700
H	-1.76117200	0.80731100	1.49223200
C	-3.72352000	-1.66192600	-0.73177600
C	-4.30696500	-0.42320200	-0.41125100
H	-4.27940200	-2.35521700	-1.35441800
C	-5.28563900	2.15247900	0.33373200
C	-5.63044400	0.00256600	-0.85437700
C	-6.06743100	1.23081700	-0.48093300
H	-7.04143100	1.60297900	-0.77739100
C	-1.87448300	-3.37779500	-0.67670600
H	-0.81998700	-3.29638200	-0.95633000
H	-1.93041900	-4.09866000	0.14747600
H	-2.41927300	-3.80755100	-1.52037700
C	-6.47691000	-0.90913200	-1.69836400
H	-5.96929300	-1.16476900	-2.63534500
H	-6.68404900	-1.84947600	-1.17522500
H	-7.43059200	-0.43963200	-1.94491500
O	-4.02558300	1.68971700	0.74380900
O	-5.61294700	3.25892800	0.68021200
H	1.46725400	3.40229100	0.70856800
H	4.68160100	-2.56669300	-1.26085900
H	3.30111400	0.16007800	0.37528500
C	4.52130100	-0.53546700	1.88979000
H	5.49942900	-0.30584600	2.31749600
H	3.74405000	-0.49015600	2.64841400
H	4.50369300	-1.52321200	1.43746000



Reference

1 Gaussian 03, Revision C.02, M. J. Frisch *et al.*, Gaussian, Inc., Wallingford CT, 2004.