

Supplementary Information

Efficient Buchwald-Hartwig and nitrene-mediated five-membered ring closure approaches to the total synthesis of quindoline. Unexpected direct conversion of a nitro group into a phosphazene

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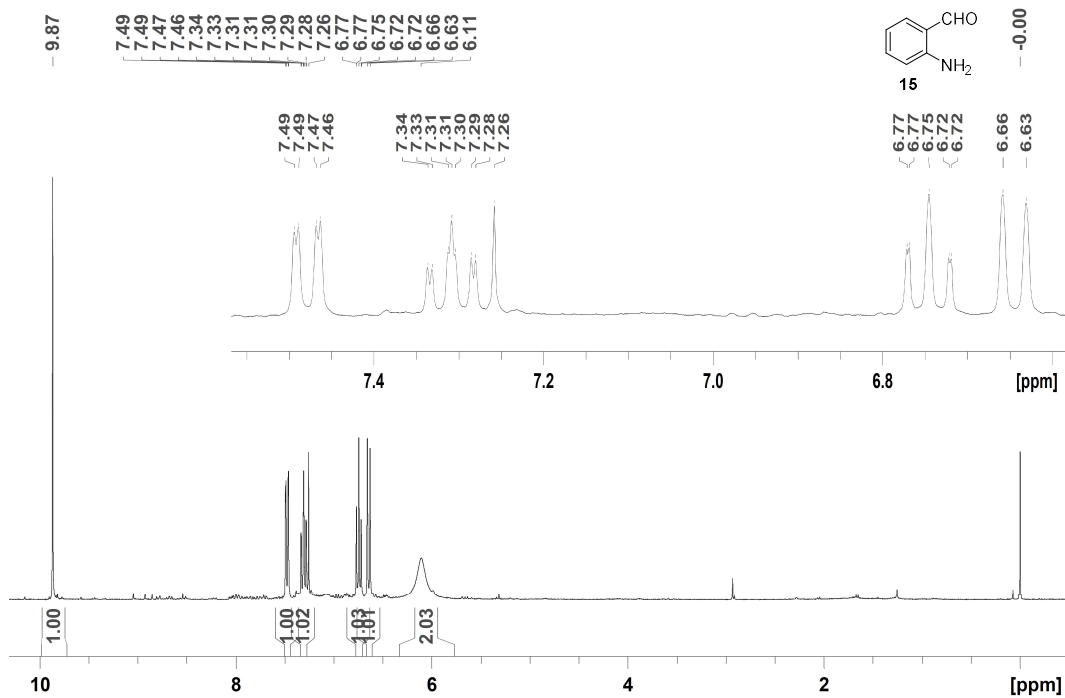


Figure S1. ¹H NMR (300 MHz) spectrum of compound 15 in CDCl₃.

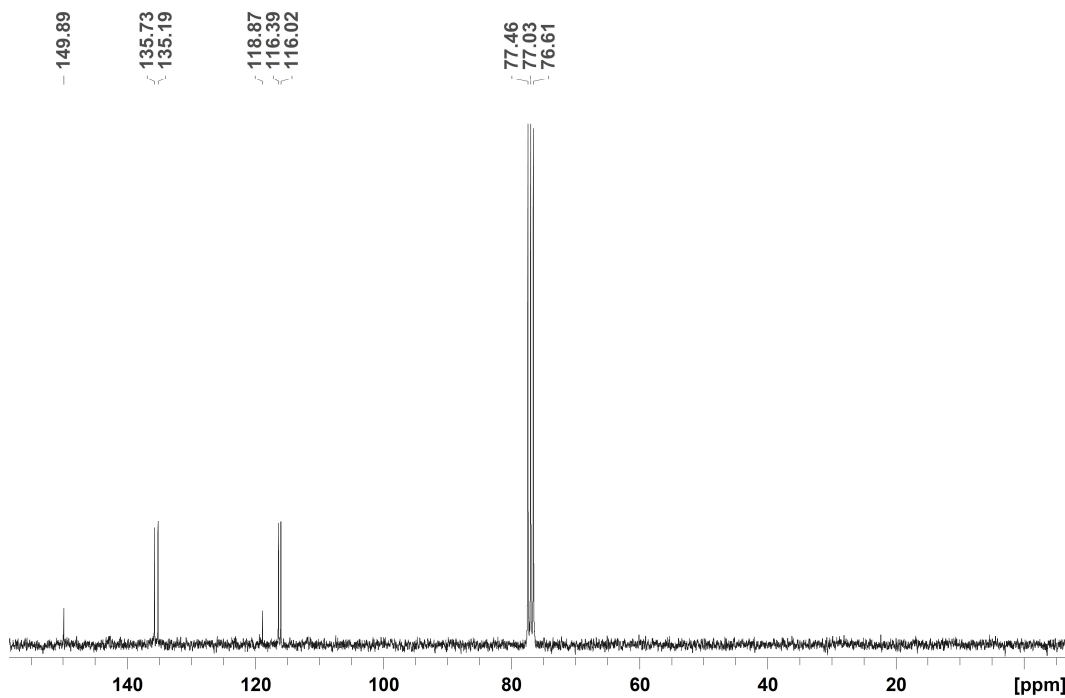


Figure S2. ¹³C NMR (75 MHz) spectrum of compound 15 in CDCl₃.

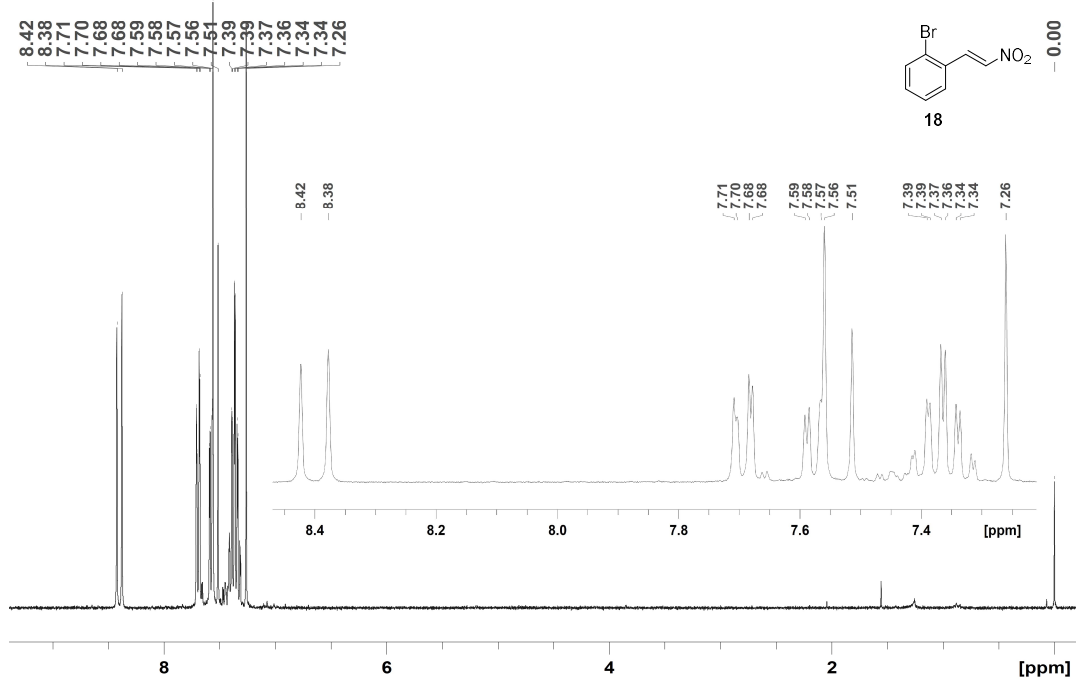


Figure S3. ¹H NMR (300 MHz) spectrum of compound **18** in CDCl₃.

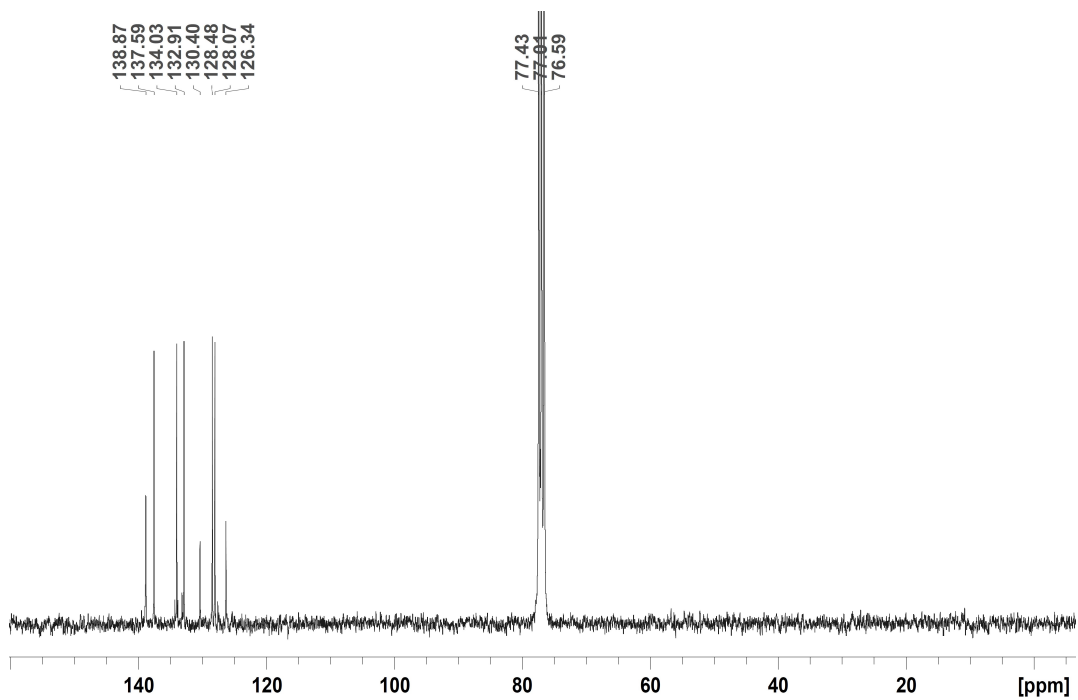


Figure S4. ¹³C NMR (75 MHz) spectrum of compound **18** in CDCl₃.

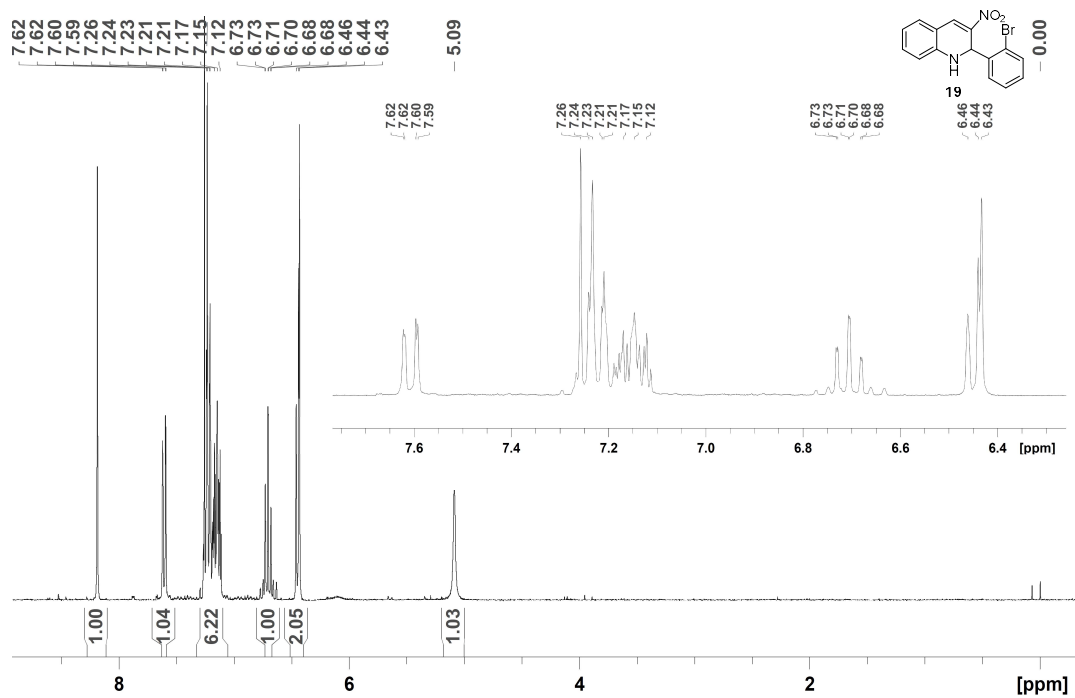


Figure S5. ¹H NMR (300 MHz) spectrum of compound **19** in CDCl₃.

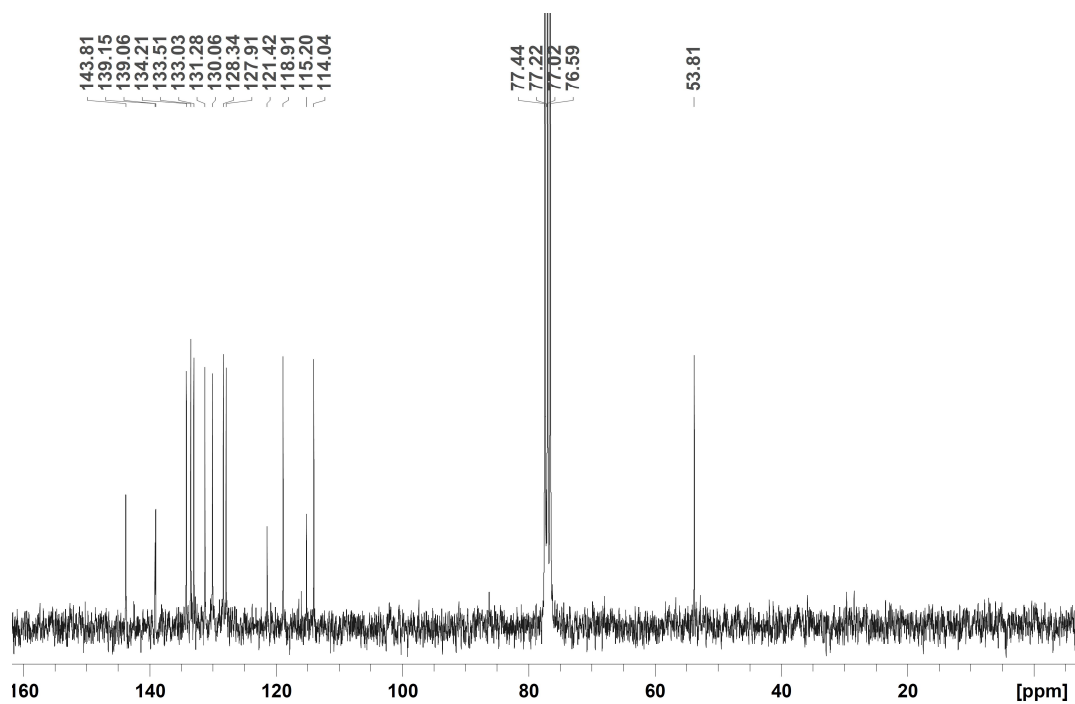


Figure S6. ¹³C NMR (75 MHz) spectrum of compound **19** in CDCl₃.

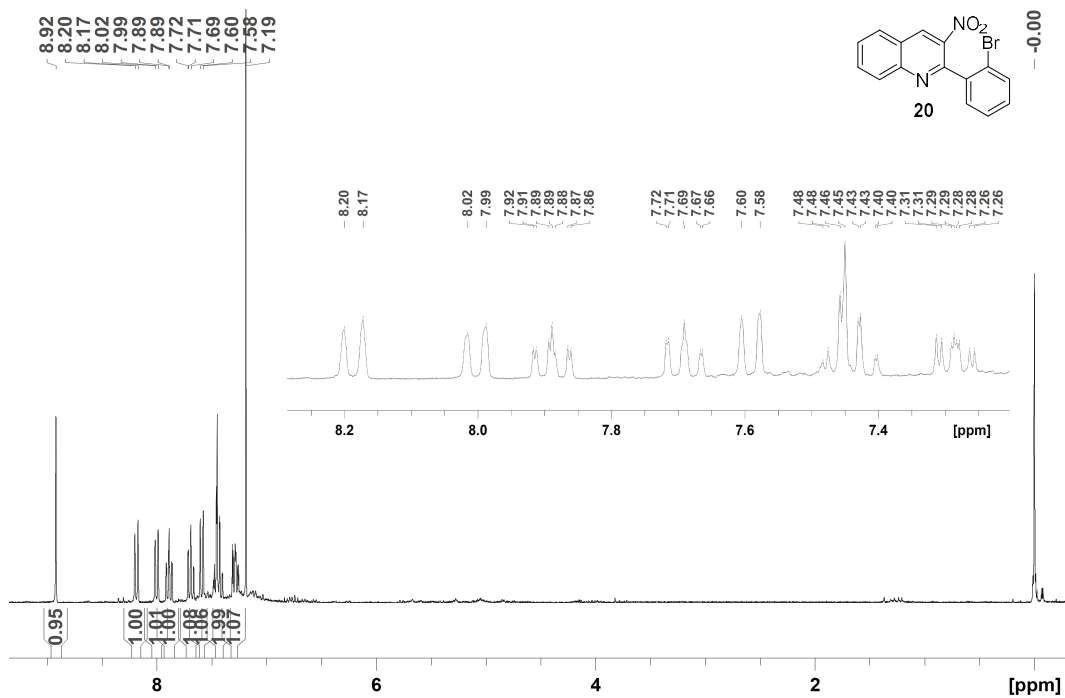


Figure S7. ^1H NMR (300 MHz) spectrum of compound **20** in CDCl_3 .

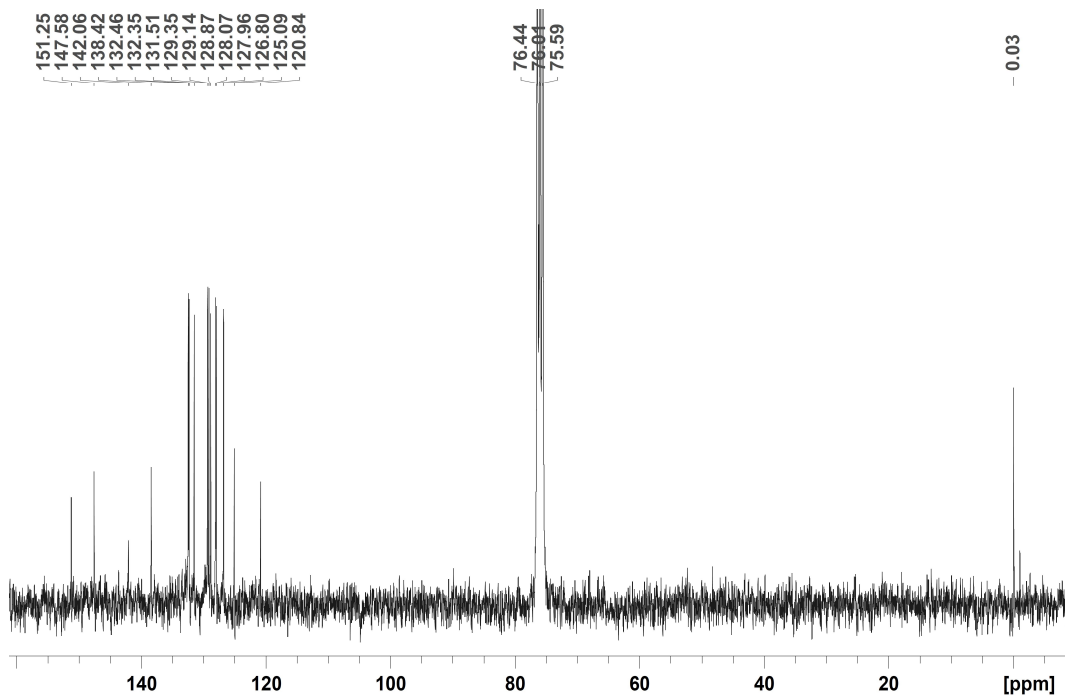


Figure S8. ^{13}C NMR (75 MHz) spectrum of compound **20** in CDCl_3 .

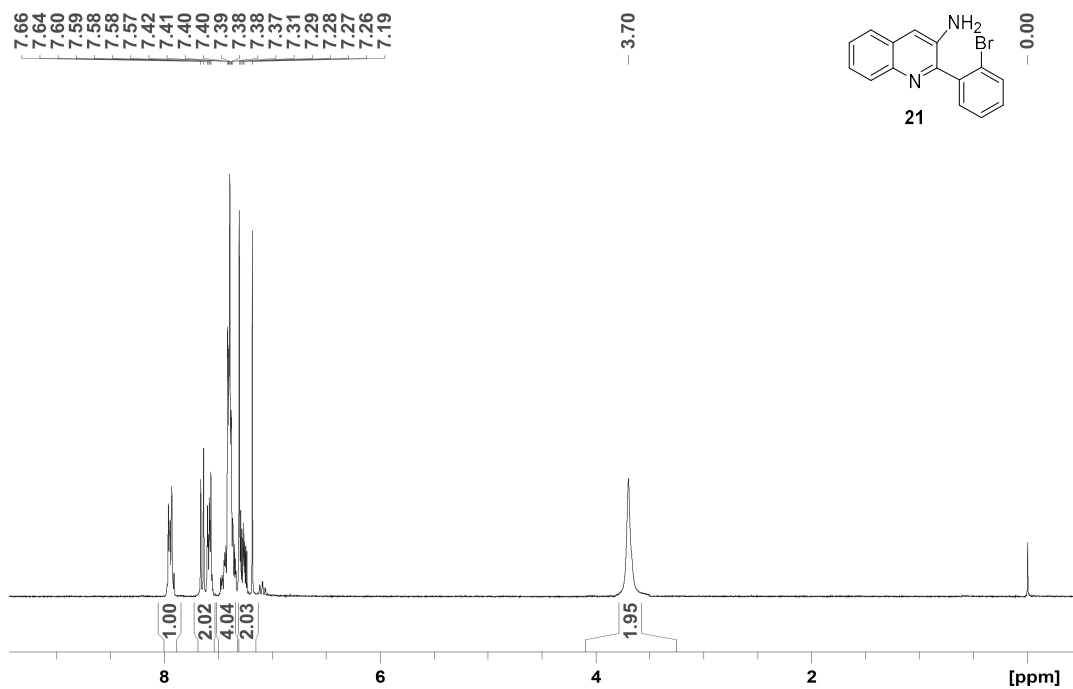


Figure S9. ^1H NMR (300 MHz) spectrum of compound **21** in CDCl_3 .

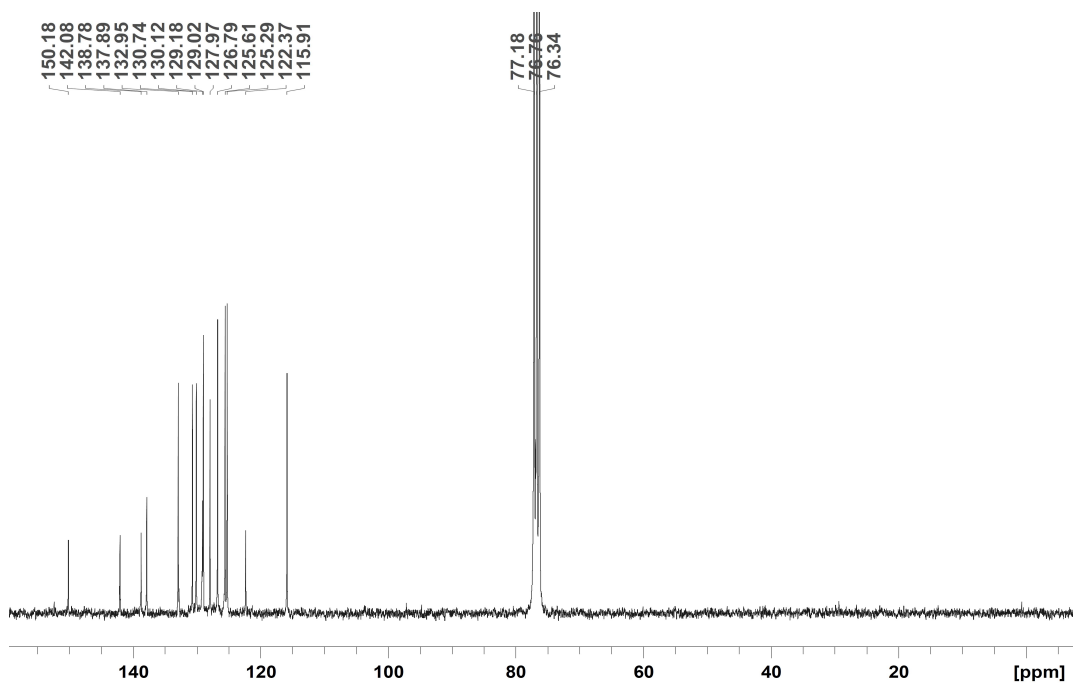


Figure S10. ^{13}C NMR (75 MHz) spectrum of compound **21** in CDCl_3 .

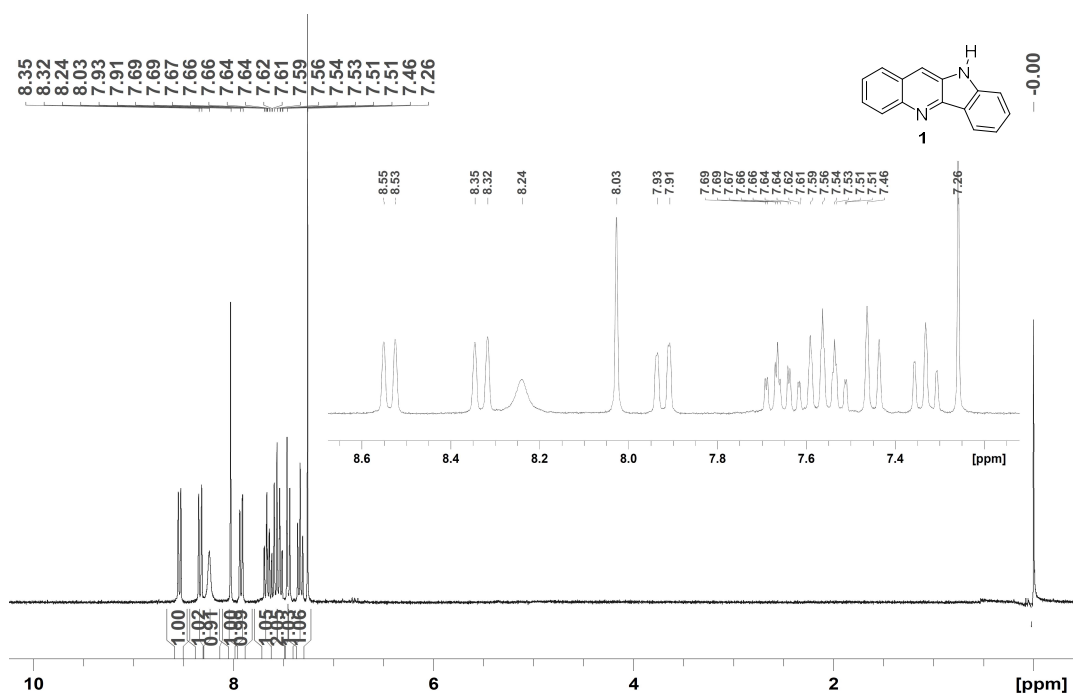


Figure S11. ^1H NMR (300 MHz) spectrum of compound **1** in CDCl_3 .

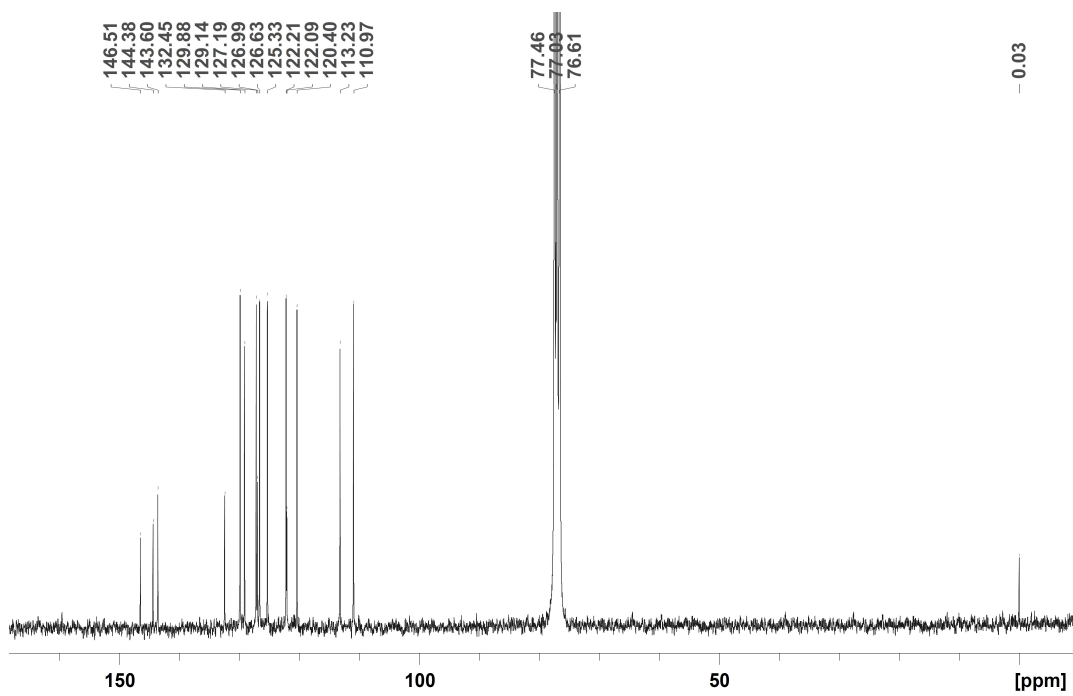


Figure S12. ^{13}C NMR (75 MHz) spectrum of compound **1** in CDCl_3 .

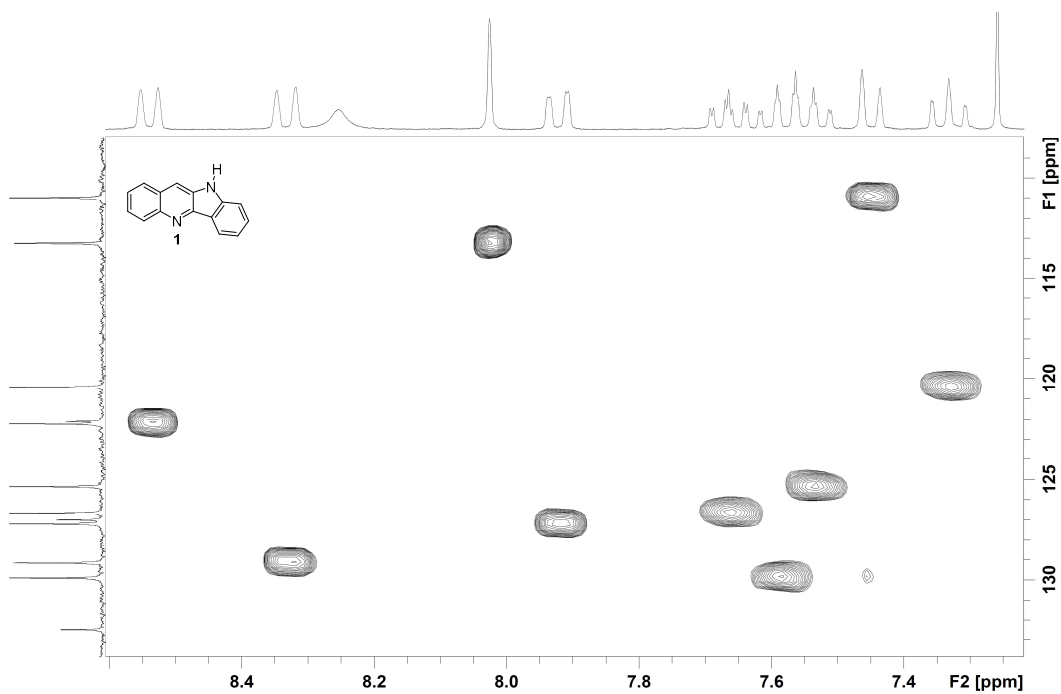


Figure S13. HSQC spectrum of compound **1** in CDCl₃.

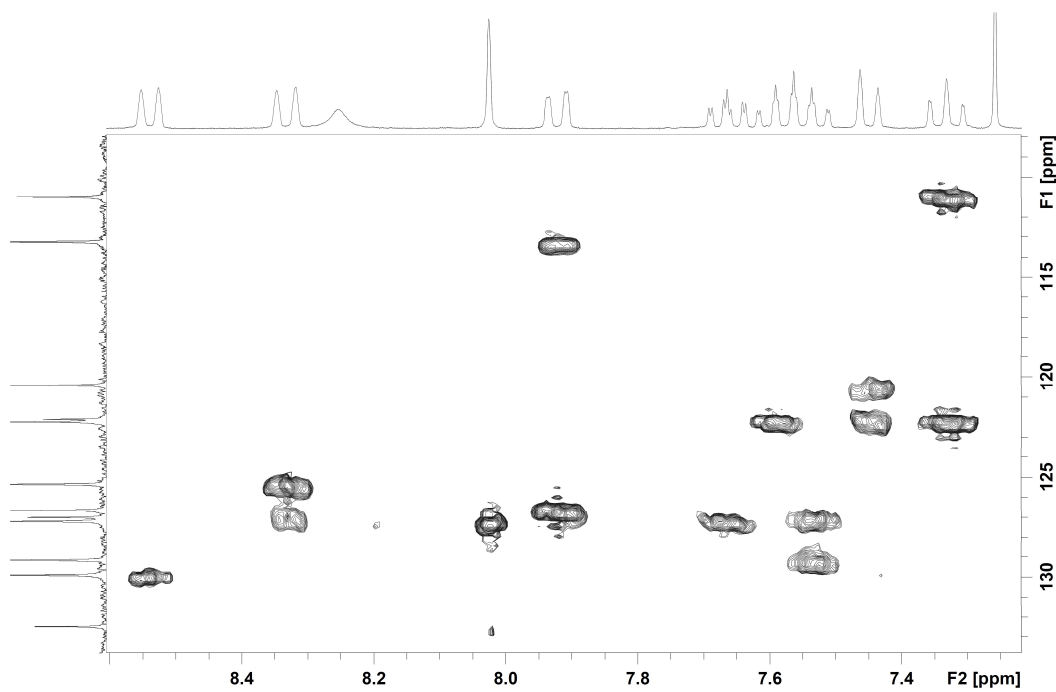


Figure S14. HMBC spectrum of compound **1** in CDCl₃.

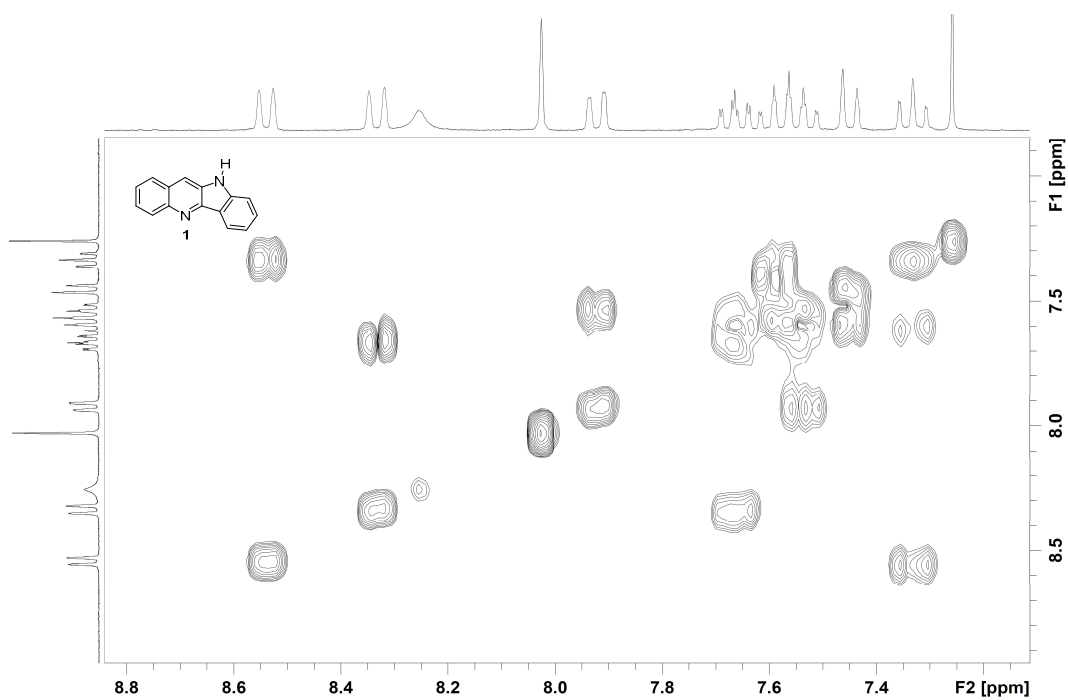


Figure S15. COSY spectrum of compound **1** in CDCl₃.

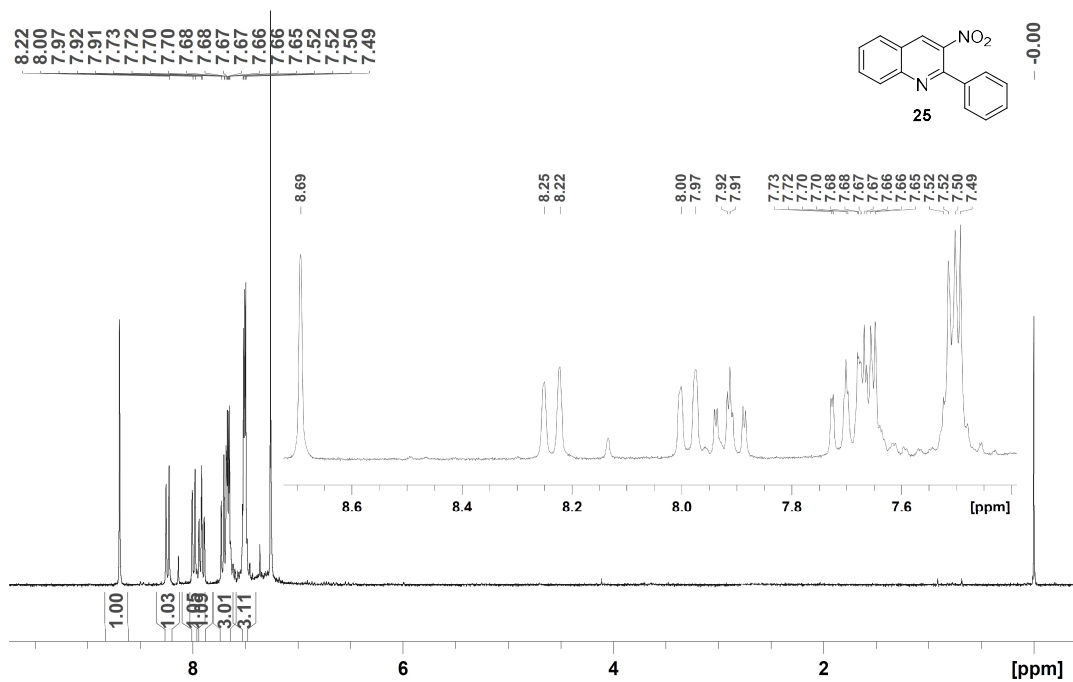


Figure S16. ¹H spectrum of compound 25 in CDCl₃.

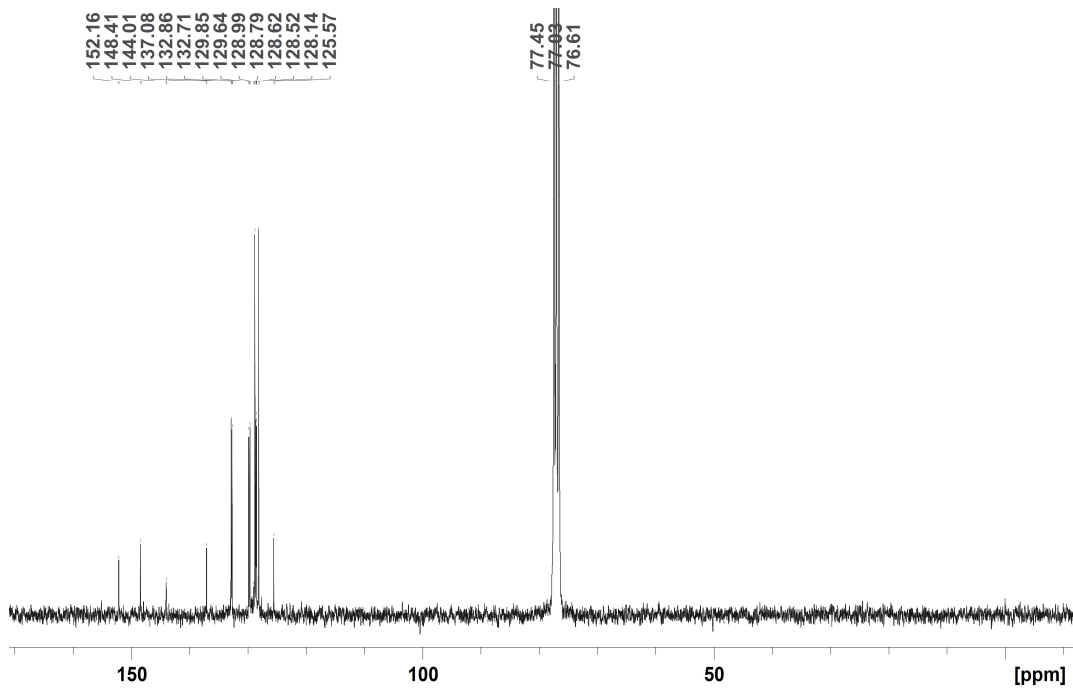


Figure S17. ¹³C spectrum of compound 25 in CDCl₃.

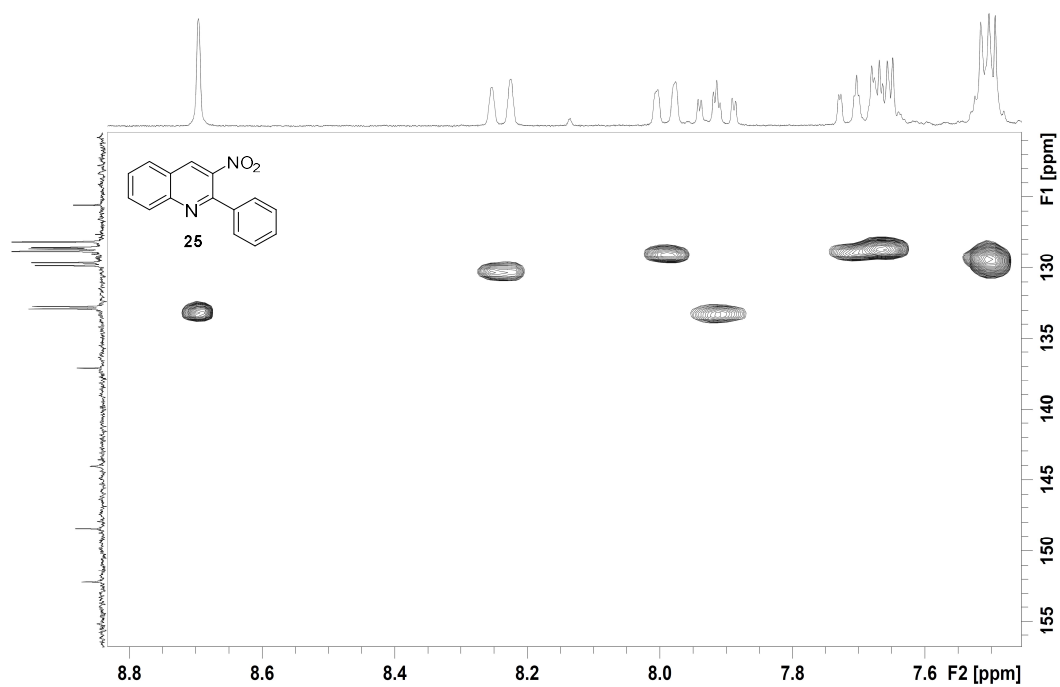


Figure S18. HSQC spectrum of compound 25 in CDCl₃.

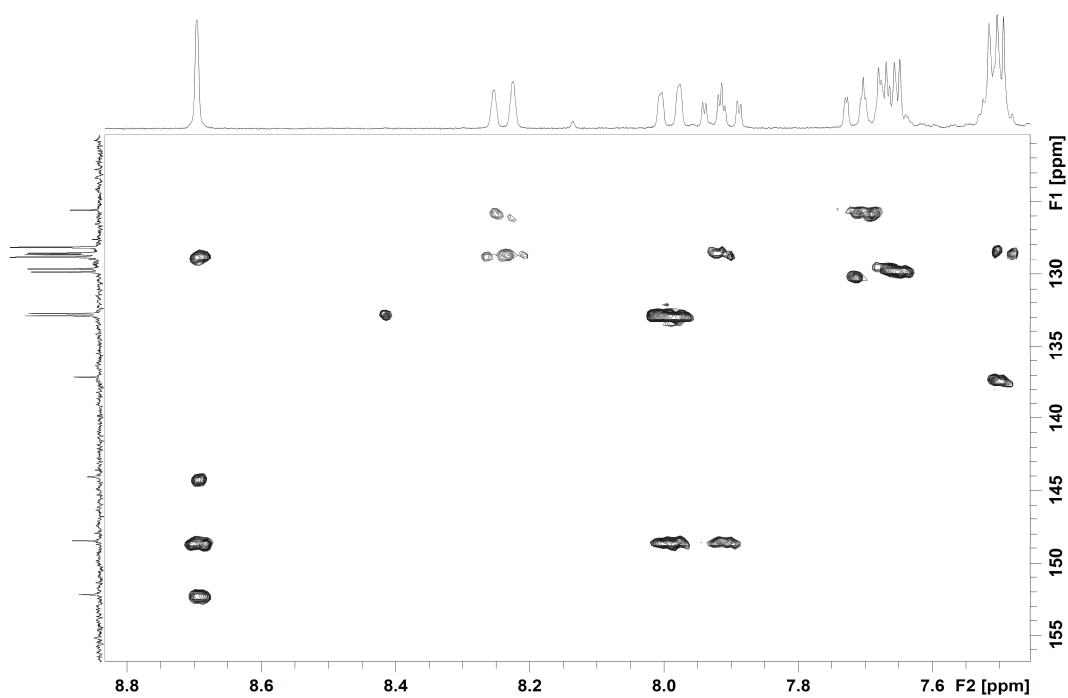
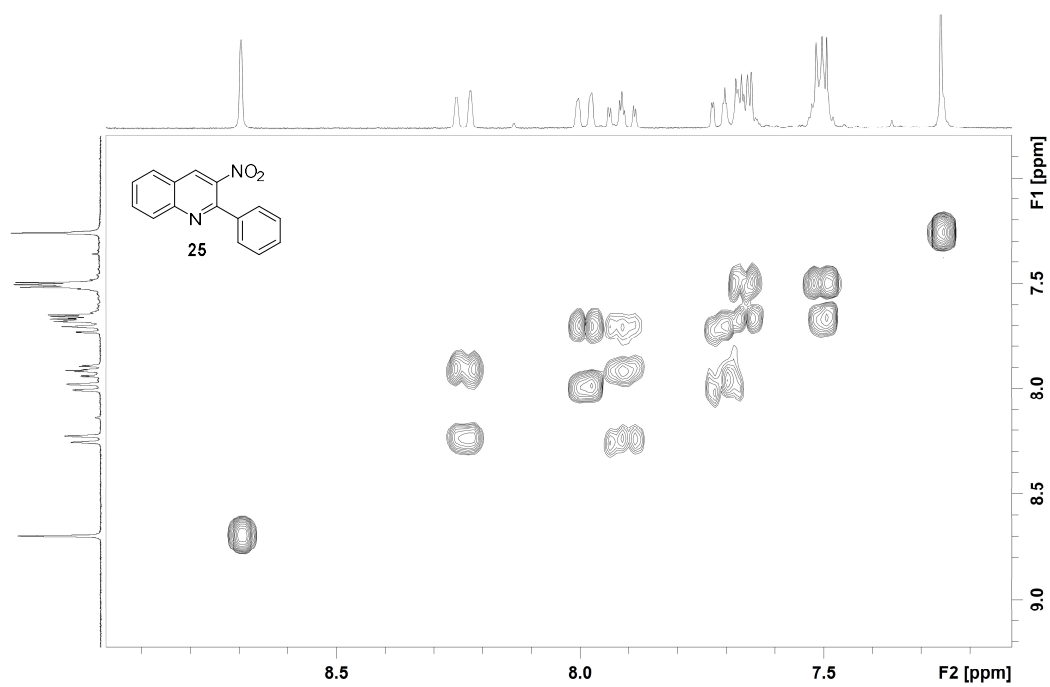


Figure S19. HMBC spectrum of compound 25 in CDCl₃.



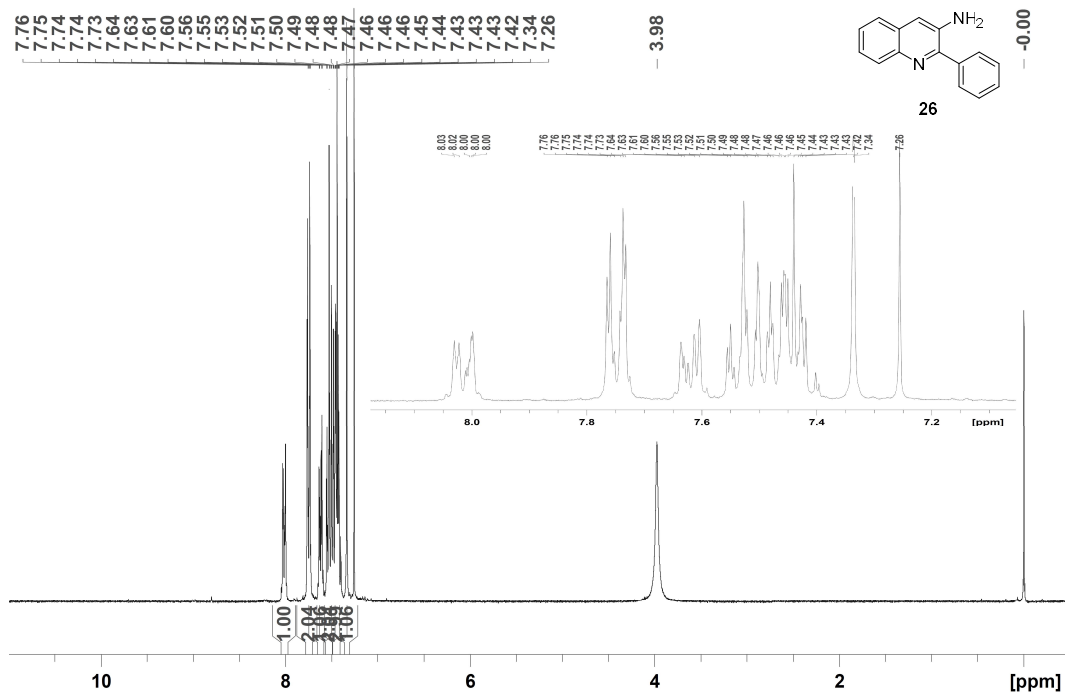


Figure S21. ¹H spectrum of compound 26 in CDCl₃.

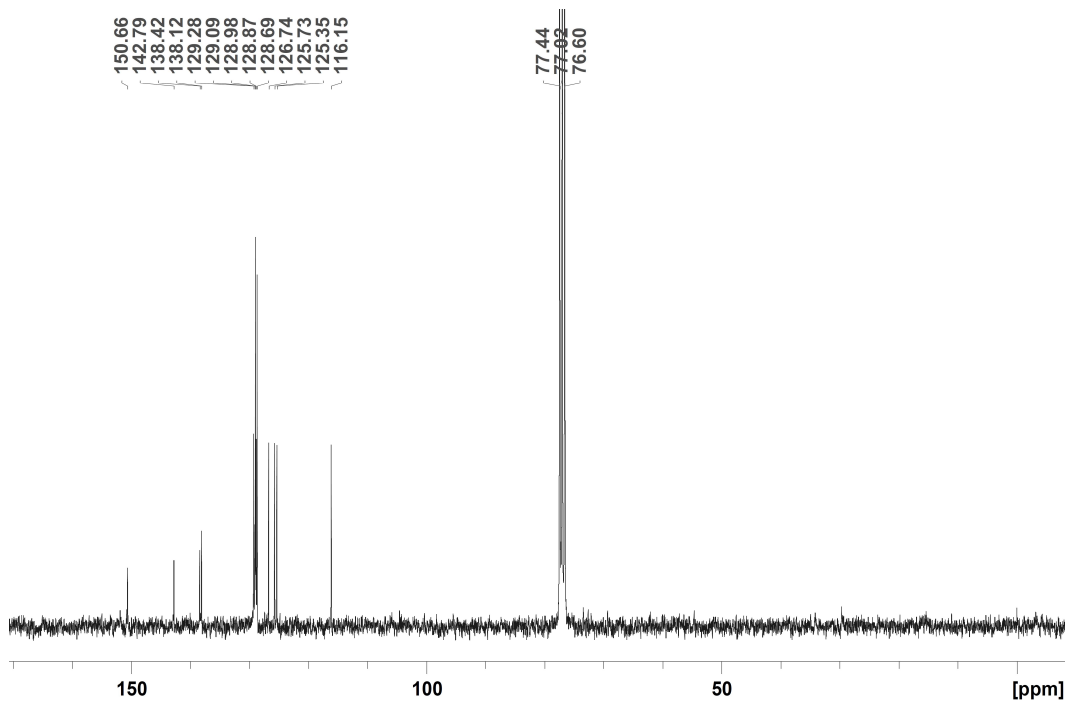
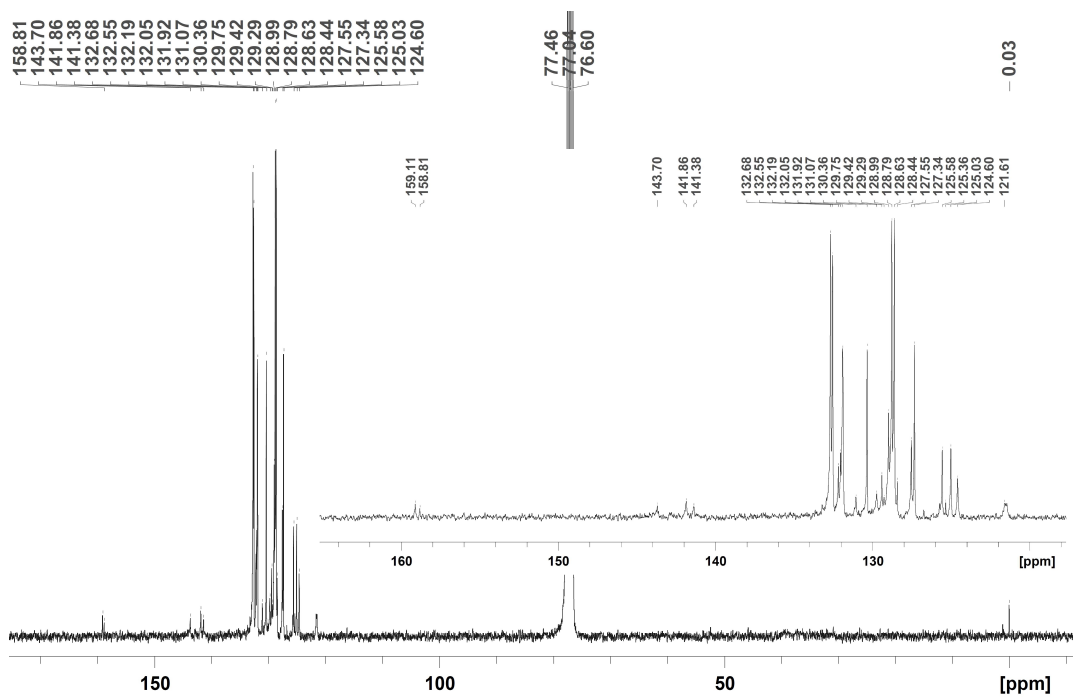
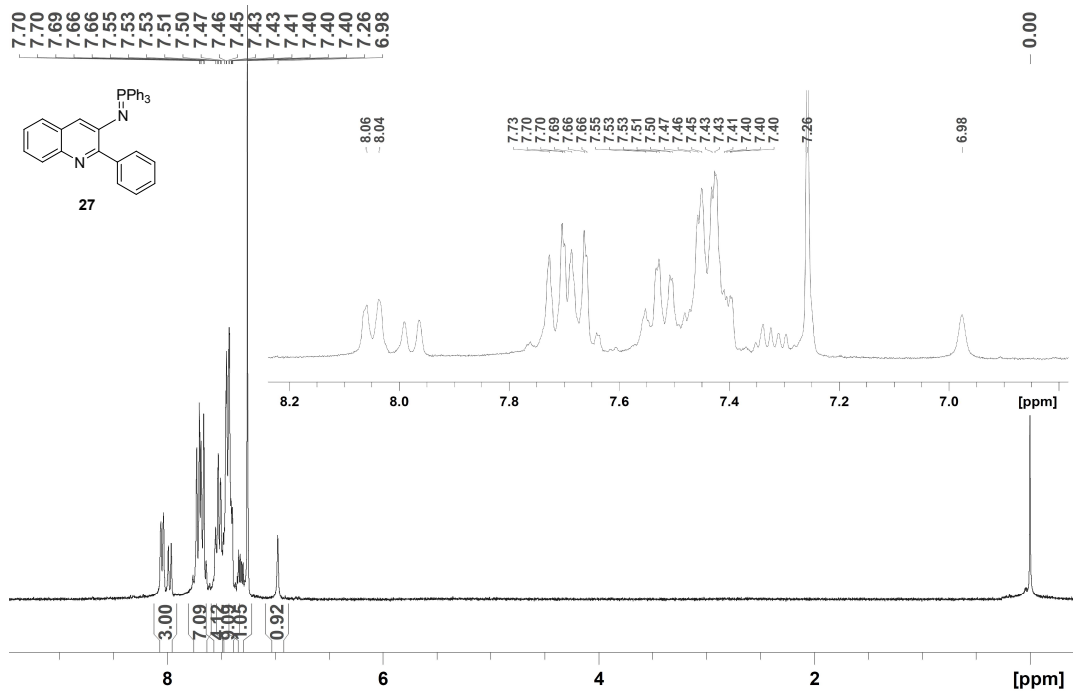
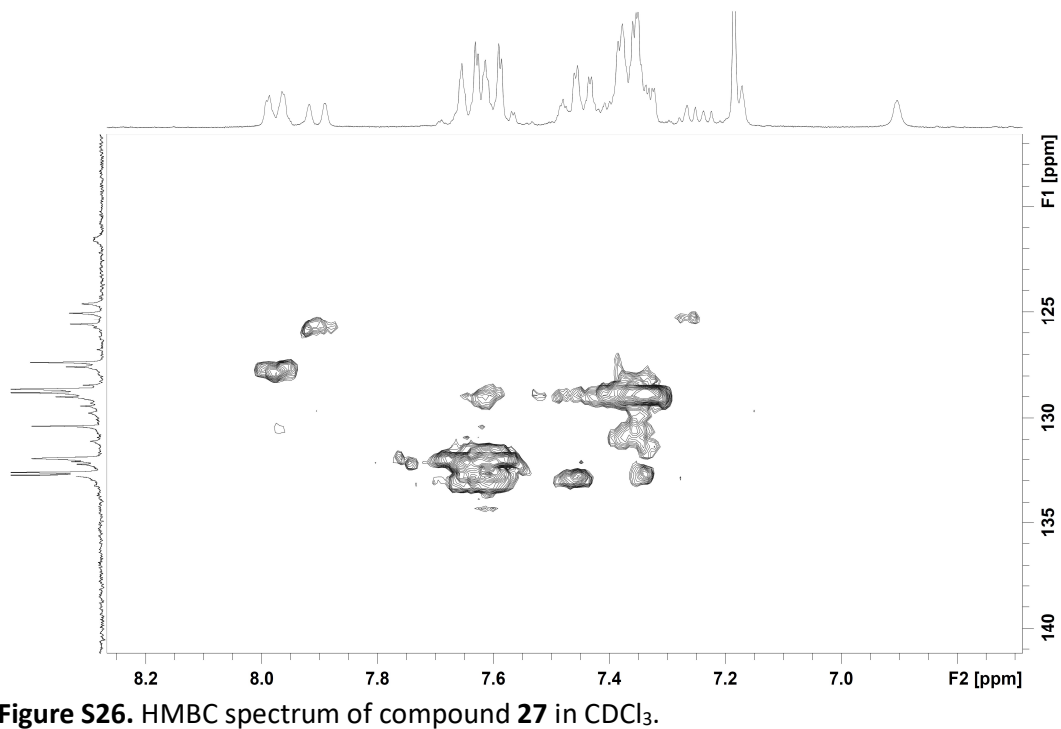
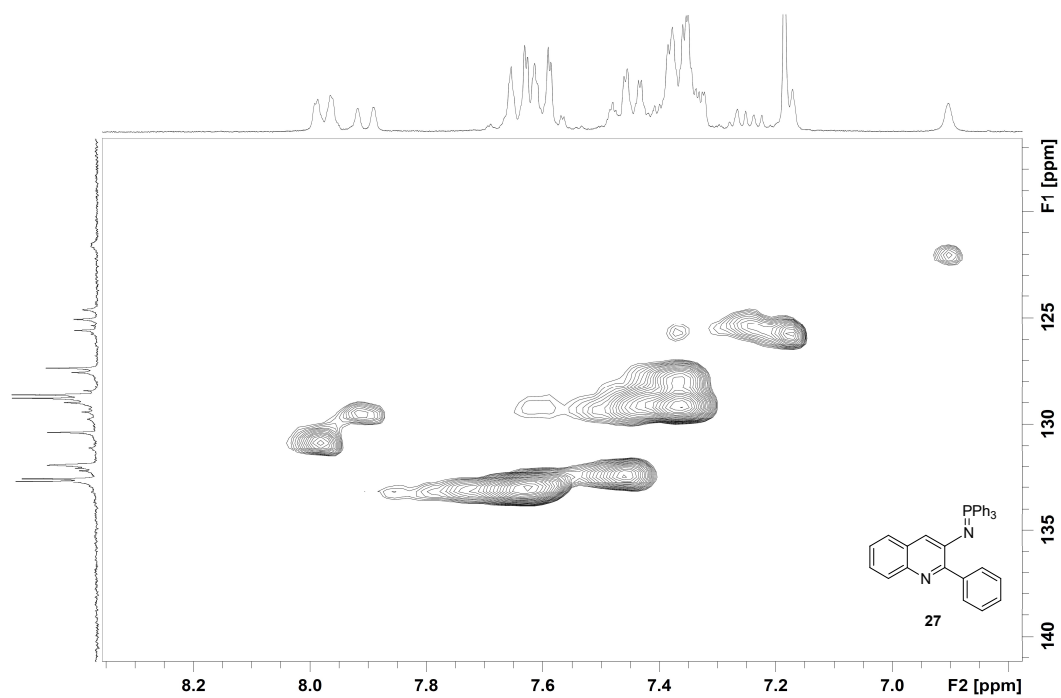


Figure S22. ¹³C NMR (75 MHz) spectrum of compound 26 in CDCl₃.





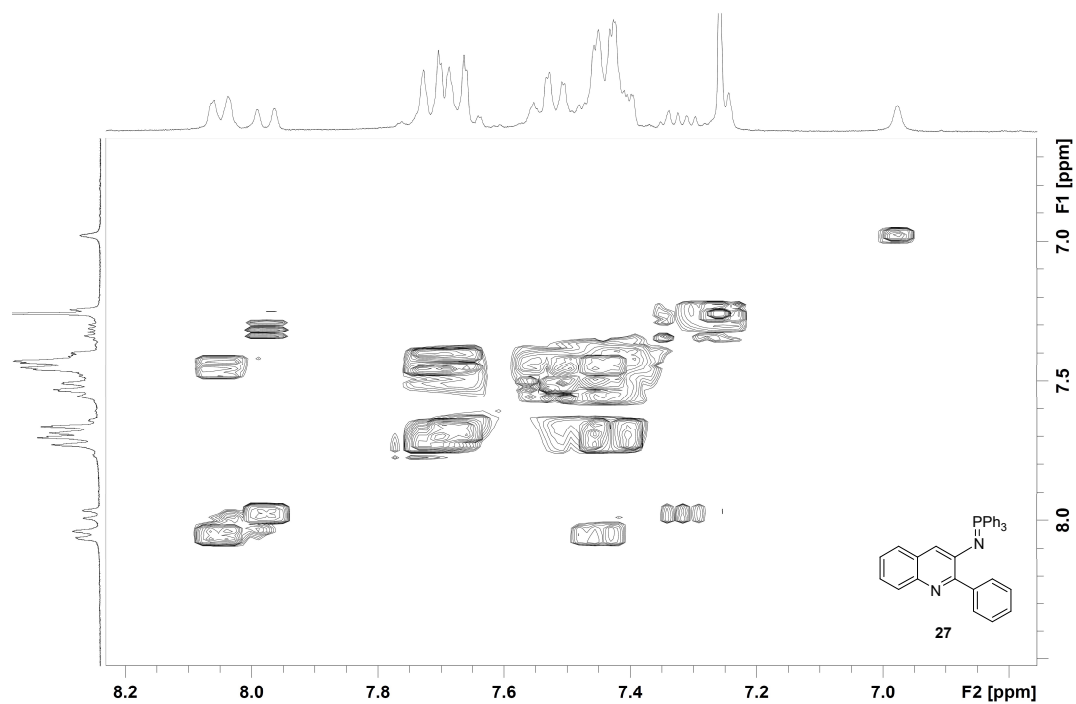


Figure S27. COSY spectrum of compound **27** in CDCl_3 .

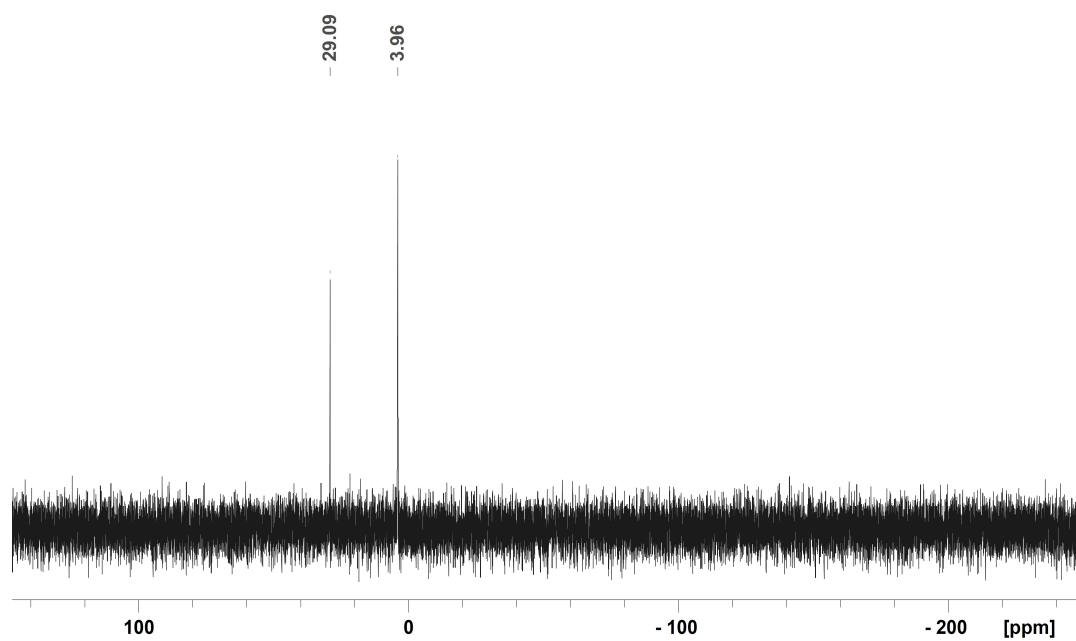
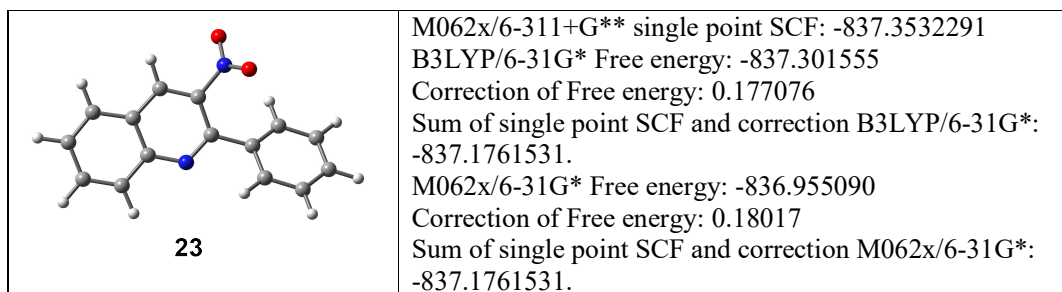


Figure S27. ^{31}P spectrum of compound **27** in CDCl_3 .

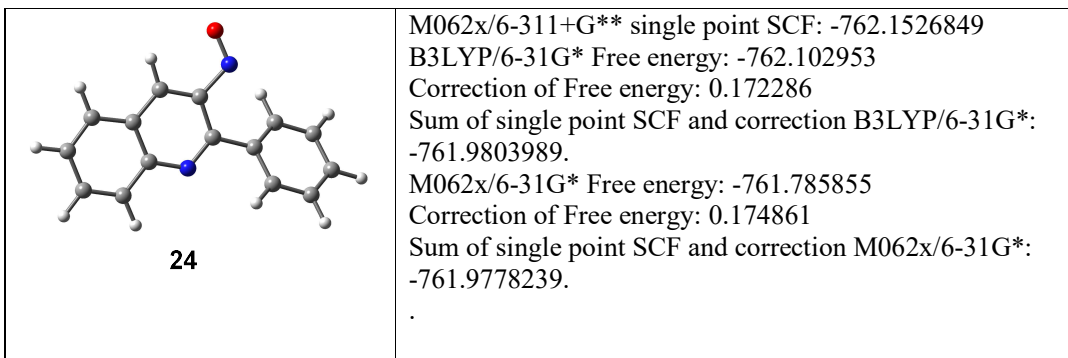
Cartesian Coordinates



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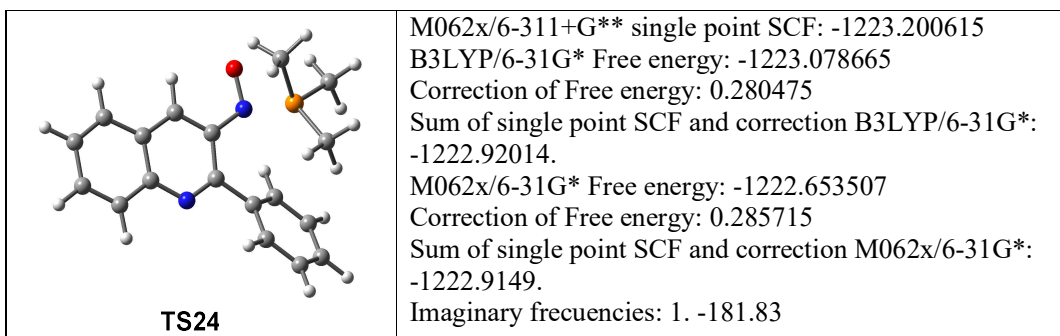
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0 1

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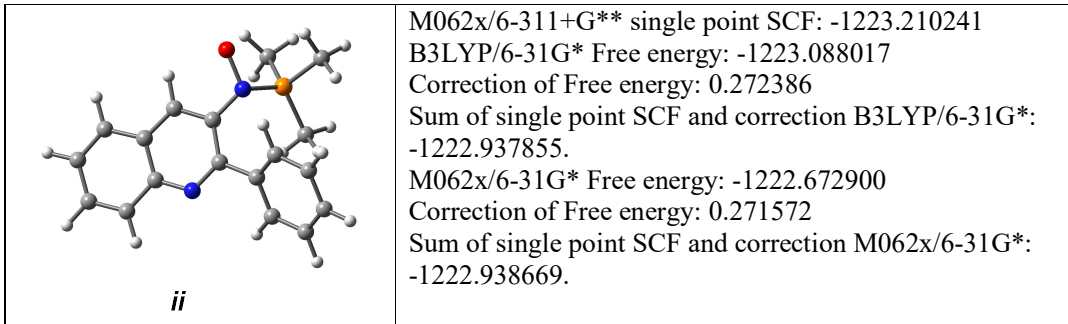
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O 1

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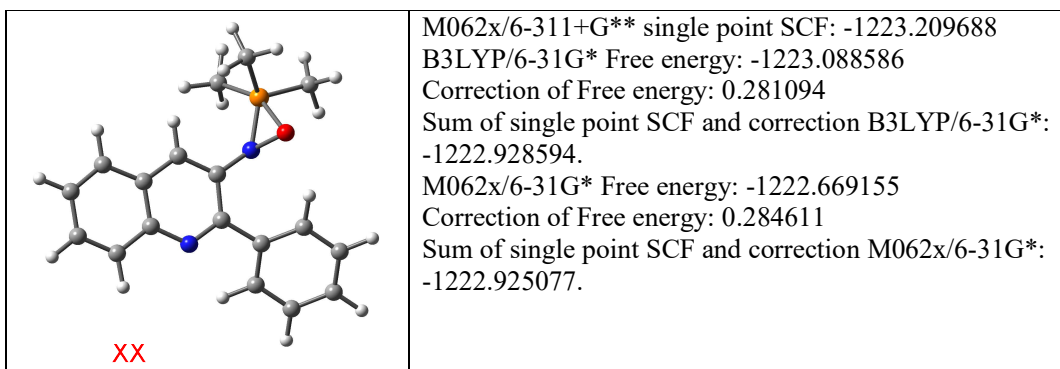
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O 1

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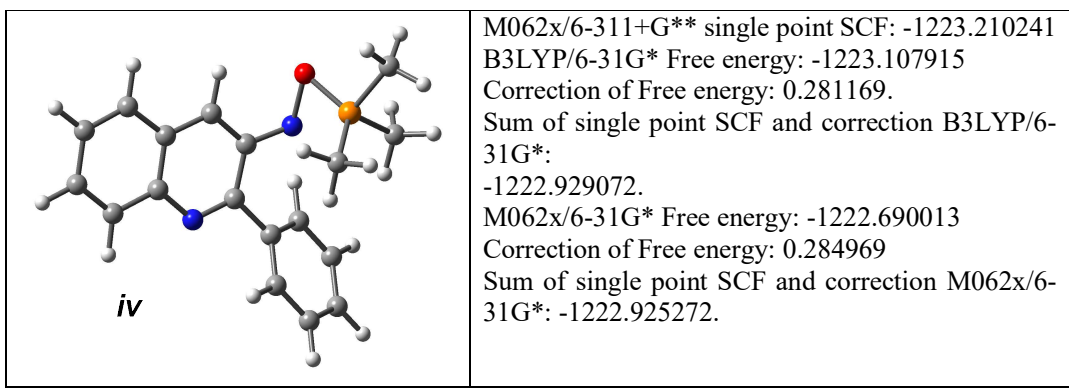
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O 1

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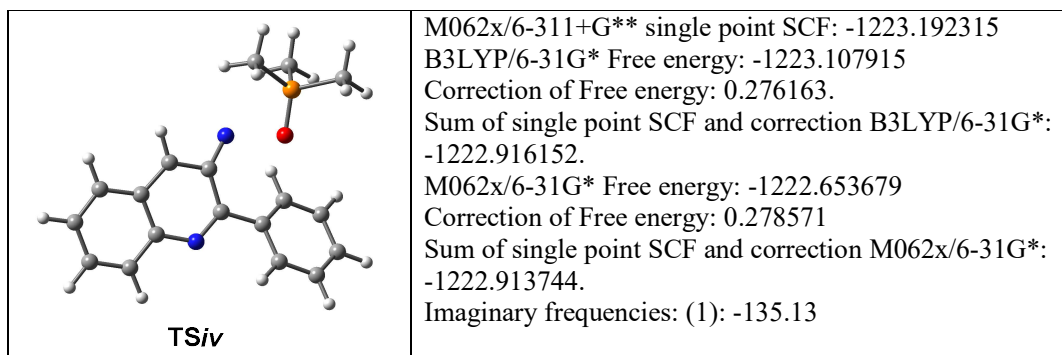
H	1.63919600	-4.55117000	-0.50153900
H	2.27619000	-3.58611500	-1.87079900
H	2.04901000	-3.87694700	1.93339300
H	0.44601900	-3.13672400	1.78980300
H	1.76266400	-2.23592500	2.54915500
H	4.33061500	-2.09831500	-0.60252500
H	4.18754500	-2.89582900	0.99760900
H	4.01536000	-1.13130700	0.84215700
H	-0.92502000	-2.31890400	0.03156700
H	-4.21593200	2.10753300	-0.10858100
H	-6.13071300	0.51696000	-0.09204900
H	-5.71715800	-1.93045600	-0.03720000
H	-3.40626600	-2.80233400	0.00610800
H	2.11372700	1.13135100	-1.14404500
H	3.68783500	3.01545400	-1.07758300
H	3.07908700	5.12860900	0.07217500
H	0.84646800	5.34231900	1.14378900
H	-0.75268800	3.45331800	1.04828200



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P	-2.06706400	-2.05805200	0.23823700
C	-3.63980000	-1.27502500	-0.26483300
C	-1.47124000	-1.41519100	1.84272700
C	-2.63355700	-3.76729500	0.69817100
O	-1.00567800	-2.47453300	-0.90431000
N	-0.98834200	-0.91144300	-0.89255700
C	0.29546200	-0.47074200	-0.59761100
N	1.65367400	1.42213100	0.08004200
C	2.76550400	0.63654500	0.04822300
C	2.69796600	-0.74038800	-0.32489000
C	1.42588700	-1.27371800	-0.63319600
C	4.01797600	1.20767500	0.38962100
C	5.16486800	0.44402700	0.35838000
C	5.10133900	-0.92110700	-0.01576900
C	3.89681300	-1.50178400	-0.34966800
C	0.47278700	0.92907300	-0.24111800
C	-0.66607300	1.89220900	-0.16952600
C	-1.74137700	1.87129400	-1.07473300
C	-2.75822500	2.82463200	-0.99196700
C	-2.72688700	3.80844200	-0.00223000
C	-1.65973300	3.84213000	0.89872000
C	-0.63756600	2.89991300	0.81074400

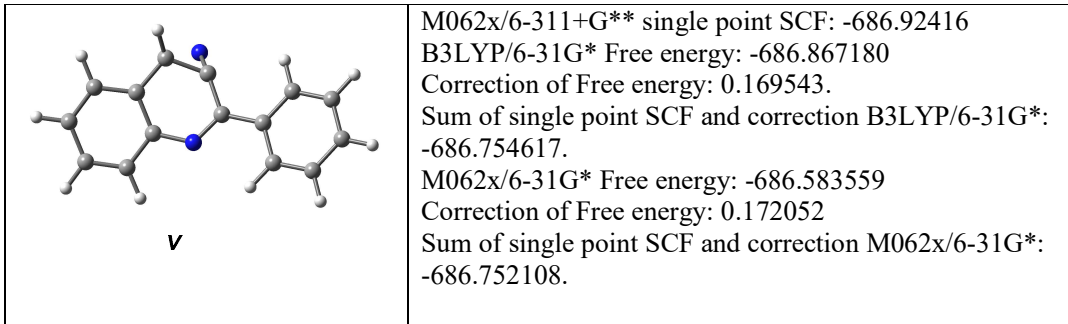
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H	-3.81883000	-1.53591200	-1.31278200
H	-2.04518500	-1.85248400	2.66514000
H	-1.54431500	-0.32571000	1.86698000
H	-0.41890100	-1.69310200	1.95646500
H	-3.04411500	-4.27206300	-0.18244200
H	-3.40329400	-3.73820800	1.47682000
H	-1.78743800	-4.35779100	1.06446000
H	1.32663000	-2.32008700	-0.89900700
H	4.03541100	2.25717300	0.66820000
H	6.12301700	0.88594100	0.61812300
H	6.01275700	-1.51309100	-0.03939400
H	3.84857400	-2.54985700	-0.63689900
H	-1.76944400	1.11379600	-1.84968400
H	-3.57223400	2.80306200	-1.71251100
H	-3.52274100	4.54598100	0.06261900
H	-1.62148000	4.60762800	1.66968400
H	0.20664100	2.93451900	1.49126300



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N	0.66314600	-1.04617900	0.88464000
C	-0.46559700	-0.60640600	0.35946600
C	-0.89377300	0.78986100	0.09601500
N	-2.14852400	1.07779800	-0.14552300
C	-3.12506200	0.12034700	-0.08218900
C	-2.83044400	-1.25510200	0.15618600
C	-1.46812900	-1.59750100	0.25856400
C	-4.46803900	0.51272000	-0.25869300
C	-5.48139100	-0.42357300	-0.22030800
C	-5.19029900	-1.78782500	-0.00572800
C	-3.88905500	-2.19737900	0.18170200
C	0.04884700	1.93811900	0.07087700
C	1.18243500	1.98508400	0.89309700
C	1.98082100	3.12439000	0.92480800
C	1.68194200	4.21954400	0.11718600
C	0.56311100	4.17669200	-0.71453000
C	-0.25244800	3.05223400	-0.72714200
H	-1.16163000	-2.63255500	0.34990800
H	-4.66879100	1.56380300	-0.42732700
H	-6.51057000	-0.11187100	-0.35880300
H	-5.99693600	-2.51186700	0.01519800
H	-3.65742100	-3.24432000	0.34861200
H	1.42111900	1.12418300	1.50039400

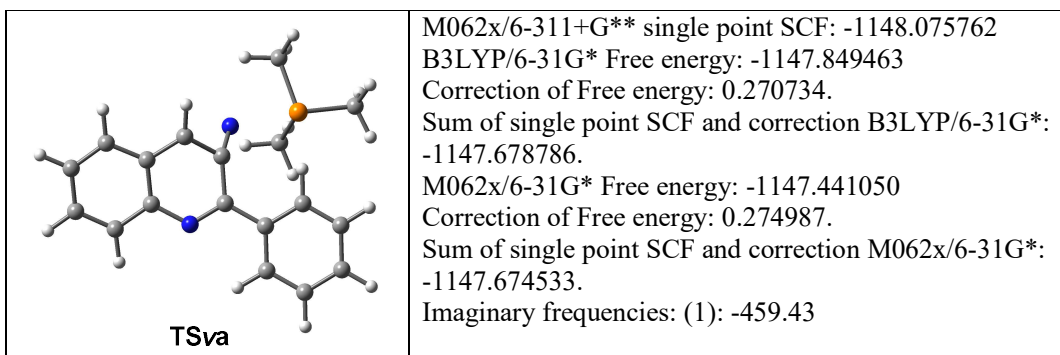
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H	2.31501900	5.10027700	0.13497400
H	0.32319100	5.02376700	-1.34800200
H	-1.13978500	3.02045100	-1.34601800
O	2.11200200	-0.44294800	-0.49070800
P	3.12644500	-1.55625200	-0.24888800
C	3.73112400	-1.63566700	1.46472000
C	2.52354900	-3.22465600	-0.65912800
C	4.59696600	-1.28818600	-1.29353600
H	4.21934100	-0.69200900	1.71503600
H	2.86770700	-1.76779300	2.11596100
H	4.43853000	-2.45696800	1.59890400
H	2.17719000	-3.23204400	-1.69426000
H	3.31074100	-3.97155800	-0.53337500
H	1.68234400	-3.44646000	-0.00391700
H	4.29892200	-1.29417700	-2.34331300
H	5.02612600	-0.31216500	-1.06155600
H	5.34792000	-2.06403800	-1.12601100



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C	-4.47437900	-0.41279800	0.23081700
C	-3.68531200	0.71143700	0.43448000
C	-2.30318900	0.66045800	0.22937000
C	-1.69422600	-0.58650600	-0.10738700
C	-2.51356500	-1.70926000	-0.31775500
C	-3.88708000	-1.62069500	-0.16371900
C	-1.39465200	1.80090800	0.39507200
C	-0.06923900	1.47210400	-0.13228100
C	0.55648500	0.15164700	-0.10044200
N	-0.31152900	-0.80756000	-0.13485600
N	-0.63849600	2.29584400	-0.89412000
C	2.00105800	-0.07350400	-0.00744300
C	2.88350600	1.01514300	-0.01244400
C	4.25700200	0.80744900	0.06463700
C	4.76157500	-0.48817600	0.14824500
C	3.88750700	-1.57798900	0.15412300
C	2.51706600	-1.37586300	0.07819200
H	-5.54803300	-0.35226600	0.36809400
H	-4.13981000	1.65168800	0.72831500
H	-2.03435100	-2.64398700	-0.58260700
H	-4.50647800	-2.49426800	-0.33150800
H	-1.53708900	2.54075000	1.17331100
H	2.49102400	2.02420100	-0.08060500

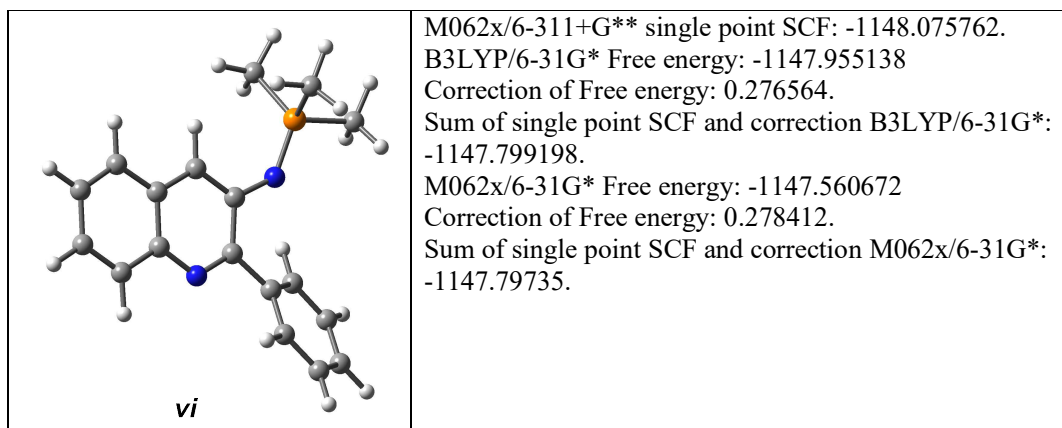
H	4.93205300	1.65539200	0.05868700
H	5.83173500	-0.65072100	0.20891000
H	4.28045900	-2.58624900	0.21912200
H	1.82532600	-2.20865600	0.08032700



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N	0.20372100	-1.53436400	-0.45253900
C	-0.41506700	-0.46367800	-0.72247100
N	-1.71864500	1.20989700	0.32890900
C	-2.79974000	0.34502300	0.25696300
C	-2.81061800	-0.80506900	-0.59431800
C	-1.59578600	-1.09277200	-1.27748000
C	-3.96280200	0.67923600	0.96931200
C	-5.11741200	-0.07166500	0.82474700
C	-5.14802000	-1.16489300	-0.05725000
C	-4.01309000	-1.52370500	-0.76039300
C	-0.55592700	0.90460000	-0.15737300
C	0.52547500	1.90173900	-0.18880200
C	0.37903100	3.12377900	0.48791600
C	1.39201600	4.07168800	0.45121700
C	2.56375900	3.82188600	-0.26624700
C	2.71513100	2.61515300	-0.94589200
C	1.70476200	1.65881500	-0.90651000
H	-1.50885800	-1.80804800	-2.07844200
H	-3.93229800	1.55026100	1.61283300
H	-6.00836700	0.19633400	1.38095600
H	-6.06296700	-1.73332500	-0.17948100
H	-4.02870300	-2.37419700	-1.43360800
H	-0.53776300	3.30449500	1.03406000

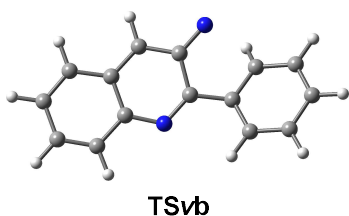
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H	3.35263100	4.56524400	-0.29488800
H	3.62031200	2.41763000	-1.50891700
H	1.83144600	0.71762200	-1.42724000
P	2.68370000	-1.87462600	0.12810700
C	2.36893900	-1.72548800	1.94765500
C	4.55015300	-1.75952500	0.11140300
C	2.46213300	-3.69253100	-0.13399500
H	2.61467100	-0.71334200	2.27752300
H	2.95980800	-2.43980400	2.52886200
H	1.30781800	-1.89504300	2.13416900
H	5.01830400	-2.46578300	0.80500900
H	4.85401800	-0.74596500	0.38297600
H	4.91773200	-1.96116900	-0.89751700
H	1.39758400	-3.92170100	-0.08521200
H	3.00196500	-4.28547100	0.61012800
H	2.82333300	-3.96264400	-1.12916000



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P	1.70520200	2.46436700	0.11236200
C	1.18357800	3.23773700	1.69656300
C	1.30956400	3.73570400	-1.16060200
C	3.52238400	2.42154900	0.16600400
N	1.21468200	0.98482100	-0.14607600
C	-0.05603000	0.45038500	-0.14269400
N	-1.37836700	-1.58723100	-0.02345600
C	-2.52441500	-0.85781300	-0.03596900
C	-2.50132500	0.56394700	-0.12157300
C	-1.23452900	1.18387900	-0.16986900
C	-3.76971700	-1.52955100	0.02869400
C	-4.94804000	-0.82031900	0.00692600
C	-4.92680500	0.59126000	-0.08188400
C	-3.73185900	1.26946600	-0.14501400
C	-0.20118800	-0.99935100	-0.08950600
C	0.96897200	-1.92698500	-0.06457700
C	0.86609900	-3.11393700	0.67663600
C	1.90560200	-4.03665400	0.70027800
C	3.06716600	-3.80289700	-0.03424300
C	3.17526500	-2.63706800	-0.78872000
C	2.14227200	-1.70301400	-0.79873200
H	0.09494000	3.28891600	1.74273200

H	1.59539100	4.24409000	1.80053700
H	1.53276400	2.61509400	2.52203100
H	1.81865300	4.67858100	-0.94629700
H	0.23390100	3.91310000	-1.19766200
H	1.63010100	3.36634500	-2.13641500
H	3.83393900	1.72919800	0.94868900
H	3.93469600	3.41329600	0.36265600
H	3.89742500	2.05333900	-0.78977900
H	-1.19678500	2.26794900	-0.22514600
H	-3.75338100	-2.61127100	0.09097700
H	-5.89825000	-1.34012300	0.05541300
H	-5.86222600	1.13991200	-0.10028800
H	-3.71821500	2.35320100	-0.21219400
H	-0.04849700	-3.30128700	1.22420900
H	1.80713600	-4.94238500	1.28900500
H	3.87733900	-4.52398000	-0.02164100
H	4.06888900	-2.45271100	-1.37585100
H	2.23797500	-0.79793600	-1.37999000

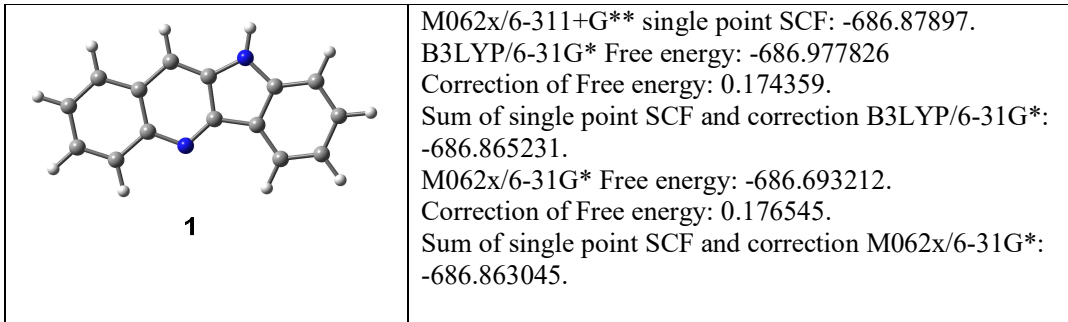


M062x/6-311+G** single point SCF: -686.87897.
 B3LYP/6-31G* Free energy: -686.840002
 Correction of Free energy: 0.169438.
 Sum of single point SCF and correction B3LYP/6-31G*:
 -686.709532.
 M062x/6-31G* Free energy: -686.538314.
 Correction of Free energy: 0.17107.
 Sum of single point SCF and correction M062x/6-31G*:
 -686.7079.
 Imaginary frequencies: (1): -263.95

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C	4.55508100	-0.00995000	-0.06721900
C	3.64108800	1.00691100	-0.07566500
C	2.23858200	0.73113300	-0.01928600
C	1.81106100	-0.64913700	0.05936900
C	2.79201500	-1.67353500	0.04710300
C	4.12700900	-1.36490200	-0.01507500
C	1.27687600	1.73745200	0.01658700
C	-0.10514200	1.37742800	-0.07141700
C	-0.40630000	-0.06068200	0.10337100
N	0.50637600	-0.99946500	0.16173600
C	-1.82430100	-0.29186000	0.21307500
C	-2.63324000	0.85864900	0.37378000
C	-4.01631500	0.78808500	0.12333800
C	-4.58789700	-0.43447100	-0.17281200
C	-3.79698100	-1.60097800	-0.23482400
C	-2.43066500	-1.53539900	-0.04497100
N	-1.03160100	2.23029200	-0.36634600
H	5.61532500	0.21214200	-0.10730800
H	3.96375200	2.04150500	-0.12106200
H	2.44399700	-2.69813000	0.09628800
H	4.86677900	-2.15713700	-0.02261200
H	1.54932300	2.78480100	-0.03171100
H	-4.62878700	1.67566800	0.22455700

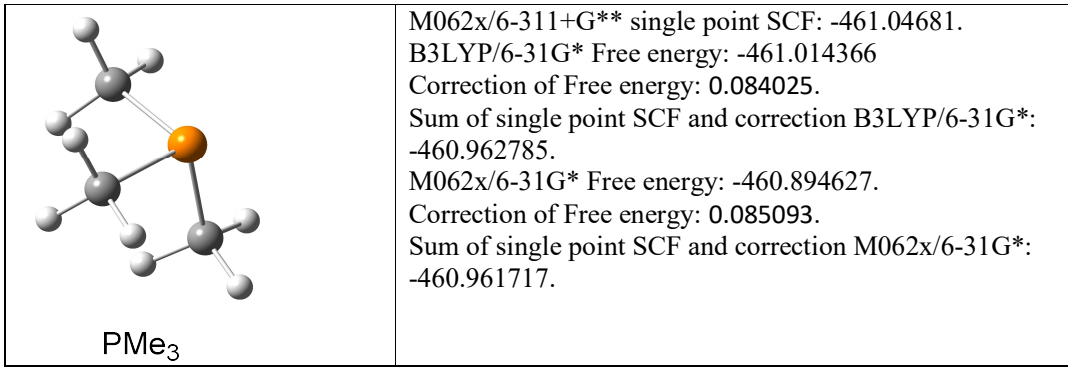
H	-5.65769700	-0.50506500	-0.33455600
H	-4.26444700	-2.55091700	-0.46759500
H	-1.79795600	-2.40699500	-0.15859800
H	-2.25893100	1.71586300	0.94274000



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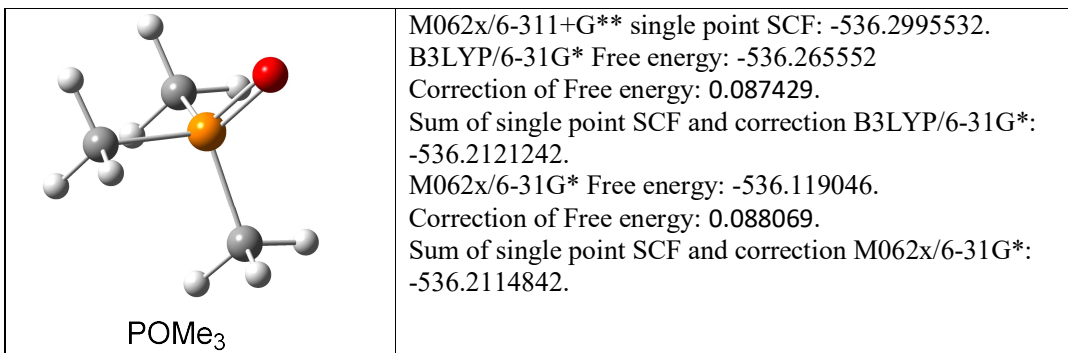
C	-4.55753200	0.19577000	-0.00000600
C	-3.55019600	1.12826500	-0.00000600
C	-2.18694700	0.72983200	-0.00000400
C	-1.87925700	-0.67648500	-0.00000200
C	-2.94903600	-1.61045400	-0.00000200
C	-4.25430800	-1.18777200	-0.00000500
C	-1.12272200	1.66462200	-0.00000300
C	0.15300900	1.16073000	-0.00000100
C	0.36200600	-0.26574300	0.00000100
N	-0.60596200	-1.15494000	0.00000000
C	1.79912800	-0.47262800	0.00000300
C	2.39468900	0.81043900	0.00000200
C	3.77915100	0.96888400	0.00000400
C	4.55893300	-0.18449000	0.00000700
C	3.98146500	-1.46343800	0.00000700
C	2.59969700	-1.61479600	0.00000500
N	1.39212500	1.77550900	0.00000000
H	-5.59308800	0.51705500	-0.00000800
H	-3.78369900	2.18830100	-0.00000700
H	-2.68783500	-2.66186700	-0.00000100
H	-5.06070000	-1.91235600	-0.00000500
H	-1.33029100	2.72975800	-0.00000500
H	4.23658100	1.95185500	0.00000400

H	5.63905700	-0.08955200	0.00000800
H	4.62182200	-2.33754000	0.00000900
H	2.13841100	-2.59520800	0.00000600
H	1.54810700	2.76915300	-0.00000100



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P	-0.00015700	-0.00010000	-0.61585900
C	1.41707100	-0.79393300	0.28433000
C	-1.39599800	-0.82997000	0.28448300
C	-0.02082300	1.62403700	0.28432600
H	1.49189400	-1.84712500	-0.00150700
H	1.29963800	-0.73100200	1.37210400
H	2.35343800	-0.30388400	0.00226900
H	-1.28193000	-0.76140800	1.37227400
H	-1.44172900	-1.88546700	0.00104200
H	-2.34527700	-0.36689300	-0.00001100
H	0.85685700	2.21280900	0.00232800
H	-0.02164900	1.49089100	1.37211000
H	-0.91039400	2.19277500	-0.00156200



O 1

P	-0.00014400	0.00035500	0.19222800
C	0.39278400	-1.61328900	-0.55761800
C	1.20074600	1.14546000	-0.56069100
C	-1.59343700	0.46552200	-0.55987900
O	0.00005200	0.00224400	1.68544100
H	1.38237600	-1.93291200	-0.22065400
H	0.38162100	-1.56494900	-1.65047100
H	-0.33941300	-2.35229600	-0.22188700
H	1.16452000	1.10918200	-1.65346100
H	2.20653200	0.88088400	-0.22392100
H	0.98346900	2.16316200	-0.22602200
H	-2.36499800	-0.23253700	-0.22465000
H	-1.54412400	0.45132500	-1.65266200
H	-1.86879800	1.46869800	-0.22408700