

**S_NAr reactions of 4-halogenotetrahydroquinazolines
with 2-aminophenol accompanied by the Smiles rearrangement**

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1. Experimental Section

^1H and ^{13}C NMR spectra were recorded on a 400 MHz spectrometer Agilent 400-MR (400.0 and 100.6 for ^1H and ^{13}C , respectively) at room temperature; chemical shifts δ were measured with reference to the solvent for ^1H (CDCl_3 , $\delta = 7.26$ ppm) and ^{13}C (CDCl_3 , $\delta = 77.16$ ppm). Accurate mass measurements (HRMS) were obtained on G3 QToF quadrupole-time-of-flight with electrospray ionization (ESI). Analytical thin layer chromatography was carried out with silica gel plates (supported on aluminum); the detection was done by UV lamp (254 nm). Column chromatography was performed on silica gel (Macherey-Nagel, Silica 60, 0.015-0.04 mm). Compounds **1**,^{S1} **5**,^{S2} **9**^{S3} were obtained *via* described methods. All other starting materials were commercially available. All reagents except commercial products of satisfactory quality were purified according to literature procedures prior to use.

1.1. 4-Chloro-2-methyl-5,6,7,8-tetrahydroquinazoline 1-oxide (**8**)

A solution of *m*-chloroperoxybenzoic acid (0.62 g, 3.6 mmol) and 4-chlorotetrahydroquinazoline **1** (0.55 g, 3.0 mmol) in CH_2Cl_2 (10 mL) was stirred at room temperature for 16 hours. The reaction mixture was quenched with 30% aqueous K_2CO_3 . The organic phase was separated and the water phase extracted with DCM (3×5 mL). The combined organic layers were dried over MgSO_4 ; the solvent was evaporated under reduced pressure. The product was isolated via preparative column chromatography (SiO_2).

Yield 0.38 g (64%). Yellowish oil, $R_f = 0.1$ (light petroleum–EtOAc, 1:1).

^1H NMR (400 MHz, CDCl_3) δ_{H} , ppm, *J*, Hz: 1.74–1.83 (2H, m, CH_2), 1.82–1.91 (2H, m, CH_2), 2.66 (3H, s, CH_3), 2.70 (2H, br. t, $^3J_{\text{HH}} 6.1$, CH_2), 2.89 (2H, br. t, $^3J_{\text{HH}} 6.5$, CH_2).

NMR spectrum corresponded to the spectrum of described compound.^{S4}

1.2. Reactions of 4-halogenotetrahydroquinazoline derivatives **1,5,8,9** with 2-aminophenol (general procedures)

Method A. A mixture of the corresponding 4-halogenotetrahydroquinazoline derivative **1,5,8** or **9** (0.5 mmol), 2-aminophenol (109 mg, 1.0 mmol) and Cs_2CO_3 (326 mg, 1.0 mmol) in absolute DMF (3 mL) was stirred for 2–40 h at r.t. or under reflux, in atmosphere of argon. The reaction mixture was allowed to cool down to r.t., if necessary, quenched with an equal volume of icy water and extracted with EtOAc (3×10 mL). The combined organic layers were washed with brine (3×5 mL) and dried over MgSO_4 ; the solvent was evaporated under reduced pressure. The product was isolated via preparative column chromatography (SiO_2).

Method B. A mixture of the corresponding 4-halogenotetrahydroquinazoline derivative **1,5,8** or **9** (0.5 mmol), 2-aminophenol (55 mg, 0.5 mmol) and DIPEA (129 mg, 1.0 mmol) in absolute

ethanol (1 mL) was stirred for 24 h at r.t. under argon. Then reaction mixture was quenched with an equal volume of water and extracted with DCM (3 × 5 mL). The combined organic layers were washed with water (3 × 3 mL) and dried over MgSO₄; the solvent was evaporated under reduced pressure. The product was isolated via preparative column chromatography (SiO₂).

2-[(2-Methyl-5,6,7,8-tetrahydroquinazolin-4-yl)amino]phenol (2)

Yield 26 mg (20%) from **1** (method A, reaction proceeded at r.t. for 40 h); 71 mg (56%) from **1** (method A, reaction proceeded under reflux for 24 h);^{S5} 22 mg (17%) from **9** (method A, reaction proceeded at r.t. for 2 h). Dark-purple solid, m.p. = 236–237 °C, *R*_f = 0.3 (CH₂Cl₂-MeOH, 30:1).

¹H NMR (400 MHz, CDCl₃) δ_H , ppm, *J*, Hz: 1.80–1.98 (4H, m, 2CH₂), 2.52 (2H, br.t, ³*J*_{HH} 6.3, CH₂), 2.54 (3H, s, CH₃), 2.75 (2H, br.t, ³*J*_{HH} 6.1, CH₂), 6.42 (1H, br.s, NH), 6.81–6.91 (1H, m, 1CH), 6.95–7.18 (3H, m, 3CH).

¹³C NMR (101 MHz, CDCl₃) δ_C , ppm: 22.0 (CH₂), 22.2 (CH₂), 22.3 (CH₂), 25.0 (CH₃), 32.0 (CH₂), 110.1 (C(4a), THQ), 120.3 (CH), 120.8 (CH), 122.8 (CH), 126.7 (CH), 127.8 (C, Ar), 149.4 (C,Ar), 158.0 (C(4), C(8a), THQ), 162.9 (C(2), THQ).

NMR spectra corresponded to the spectra of described compound.^{S5}

4-(2-Aminophenoxy)-2-methyl-5,6,7,8-tetrahydroquinazoline 1-oxide (6)

Yield 7 mg (5%) from **8** (method A, reaction proceeded at r.t. for 24 h); 85 mg (63%) from **5** (method A, reaction proceeded at r.t. for 24 h); 92 mg (68%) from **5** (method B, reaction proceeded for 24 h). Yellow oil, *R*_f = 0.3 (light petroleum–EtOAc–MeOH, 3:1:1).

¹H NMR (400 MHz, CDCl₃) δ_H , ppm: 1.69–1.79 (2H, m, CH₂), 1.79–1.87 (2H, m, CH₂), 2.50 (3H, s, CH₃), 2.68–2.76 (2H, m, CH₂), 2.89–2.94 (2H, m, CH₂), 3.78 (2H, br.s, NH₂), 6.68–6.77 (1H, m, CH), 6.77–6.83 (1H, m, CH), 6.89–6.96 (1H, m, CH), 6.97–7.04 (1H, m, CH).

NMR spectrum corresponded to the described compound.^{S5}

2-[(2-Methyl-1-oxido-5,6,7,8-tetrahydroquinazolin-4-yl)amino]phenol (7)

Yield 27 mg (20%) from **8** (method A, reaction proceeded under reflux for 5 h). Yellow oil, *R*_f = 0.2 (light petroleum–EtOAc–MeOH, 3:1:0.1).

¹H NMR (400 MHz, CDCl₃) δ_H , ppm, *J*, Hz: 1.60–1.71 (4H, m, 2CH₂), 2.30–2.38 (2H, m, CH₂), 2.71 (3H, s, CH₃), 2.74–2.80 (2H, m, CH₂), 6.85–6.93 (2H, m, 2CH), 6.95 (1H, br.d, ³*J* 4.2, CH), 8.09 (1H, br.d, ³*J* 8.0, CH).

NMR spectrum corresponded to the described compound.^{S6}

1.3. 4-(2-Nitrophenoxy)-2-methyl-5,6,7,8-tetrahydroquinazoline (10)

A mixture of 4-chlorotetrahydroquinazoline **1** (183 mg, 1.0 mmol), 2-nitrophenol (153 mg, 1.1 mmol), KI (16.6 mg, 0.1 mmol) and Cs₂CO₃ (326 mg, 1.0 mmol) in absolute DMF (3 mL) was stirred for 12 h under reflux in atmosphere of argon. The mixture was allowed to cool down to

r.t., quenched with an equal volume of icy water and extracted with EtOAc (3 × 10 mL). The combined organic layers were washed with brine (3 × 5 mL) and dried over MgSO₄; the solvent was evaporated under reduced pressure. The product was isolated *via* preparative column chromatography (SiO₂).

Yield 91 mg (32%). Yellowish oil, R_f = 0.1 (light petroleum–CH₂Cl₂, 1:3).

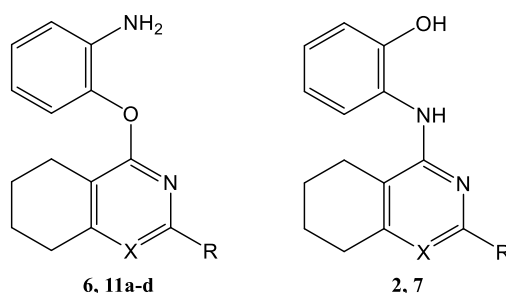
¹H NMR (400 MHz, CDCl₃) δ_H, ppm, *J*, Hz: 1.83–1.94 (4H, m, 2CH₂), 2.36 (3H, s, CH₃), 2.73–2.85 (4H, m, 2CH₂), 7.32 (1H, dd, ³*J* 8.0, ⁴*J* 1.3, CH), 7.35–7.41 (1H, m, CH), 7.62–7.70 (1H, m, CH), 8.07 (1H, dd, ³*J* 8.3, ⁴*J* 1.6, CH).

¹³C NMR (101 MHz, CDCl₃) δ_C, ppm: 21.7 (CH₂), 22.0 (CH₂), 22.3 (CH₂), 25.4 (CH₃), 32.0 (CH₂), 113.9 (C(4a), THQ), 125.6 (CH), 125.7 (CH), 125.8 (CH), 134.5 (CH), 142.3 (C, Ar), 146.3 (C, Ar), 164.0 (C(2), THQ), 165.9 (C(4), THQ), 167.4 (C(8a), THQ).

HRMS (ESI⁺) *m/z*: calcd. for C₁₅H₁₅N₃O₃ 286.1192, found 286.1195 [M+H⁺].

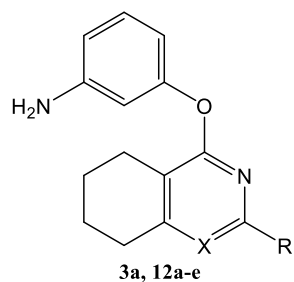
2. Comparison of ¹³C NMR spectra of 4-substituted tetrahydroquinazoline derivatives

Table S1. Chosen NMR data for tetrahydroquinazoline derivatives, containing 2-aminophenyl moiety



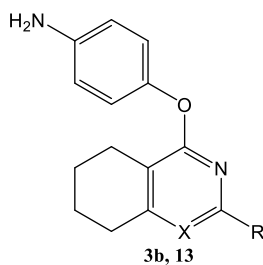
Compound	X	R	δ, ppm	
			C(Ar)-O	C(Ar)-N
6 ^{S5}	N ⁺ –O [–]	CH ₃	140.3	138.7
11a ^{S5}	N ⁺ –O [–]	<i>i</i> -Pr	140.3	138.7
11b ^{S5}	N ⁺ –O [–]	cy-Pr	140.0	138.7
11c ^{S5}	N ⁺ –O [–]	<i>t</i> -Bu	140.3	138.7
11d ^{S5}	N ⁺ –O [–]	cy-Hex	140.4	138.7
7 ^{S6}	N ⁺ –O [–]	CH ₃	146.9	127.3
2 ^{S5}	N	CH ₃	149.4	127.8

Table S2. Selected NMR data for tetrahydroquinazoline derivatives containing 3-aminophenoxy moiety



Compound	X	R	δ , ppm	
			C(Ar)-O	C(Ar)-N
12a ^{S5}	N ⁺ -O ⁻	CH ₃	154.1	148.0
12b ^{S5}	N ⁺ -O ⁻	<i>i</i> -Pr	154.1	147.7
12c ^{S5}	N ⁺ -O ⁻	<i>c</i> -C ₃ H ₅	154.0	147.7
12d ^{S5}	N ⁺ -O ⁻	<i>t</i> -Bu	154.1	147.7
12e ^{S5}	N ⁺ -O ⁻	Cy	154.3	147.7
3a ^{S5}	N	CH ₃	154.3	147.8

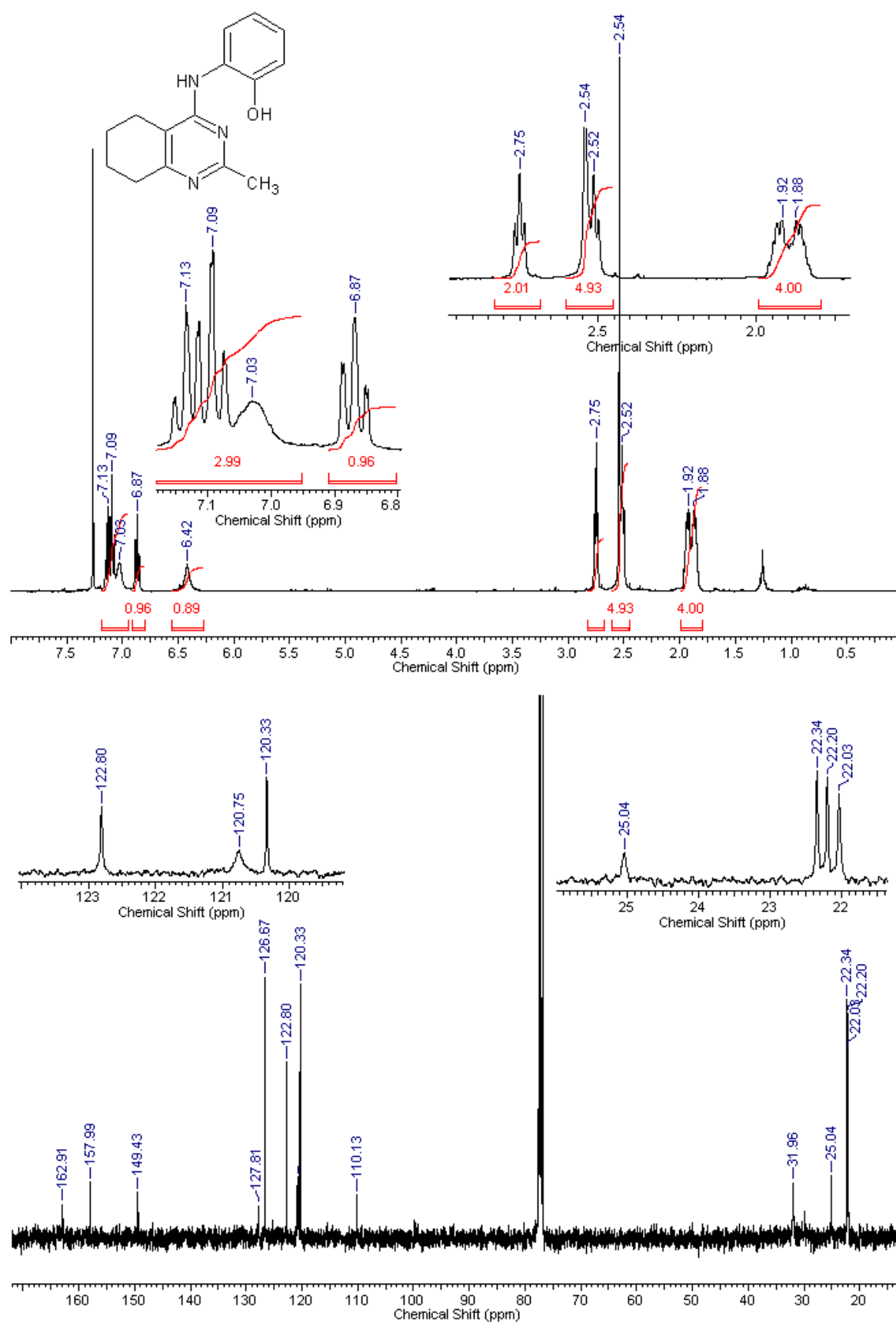
Table S3. Selected NMR data for tetrahydroquinazoline derivatives containing 4-aminophenoxy moiety



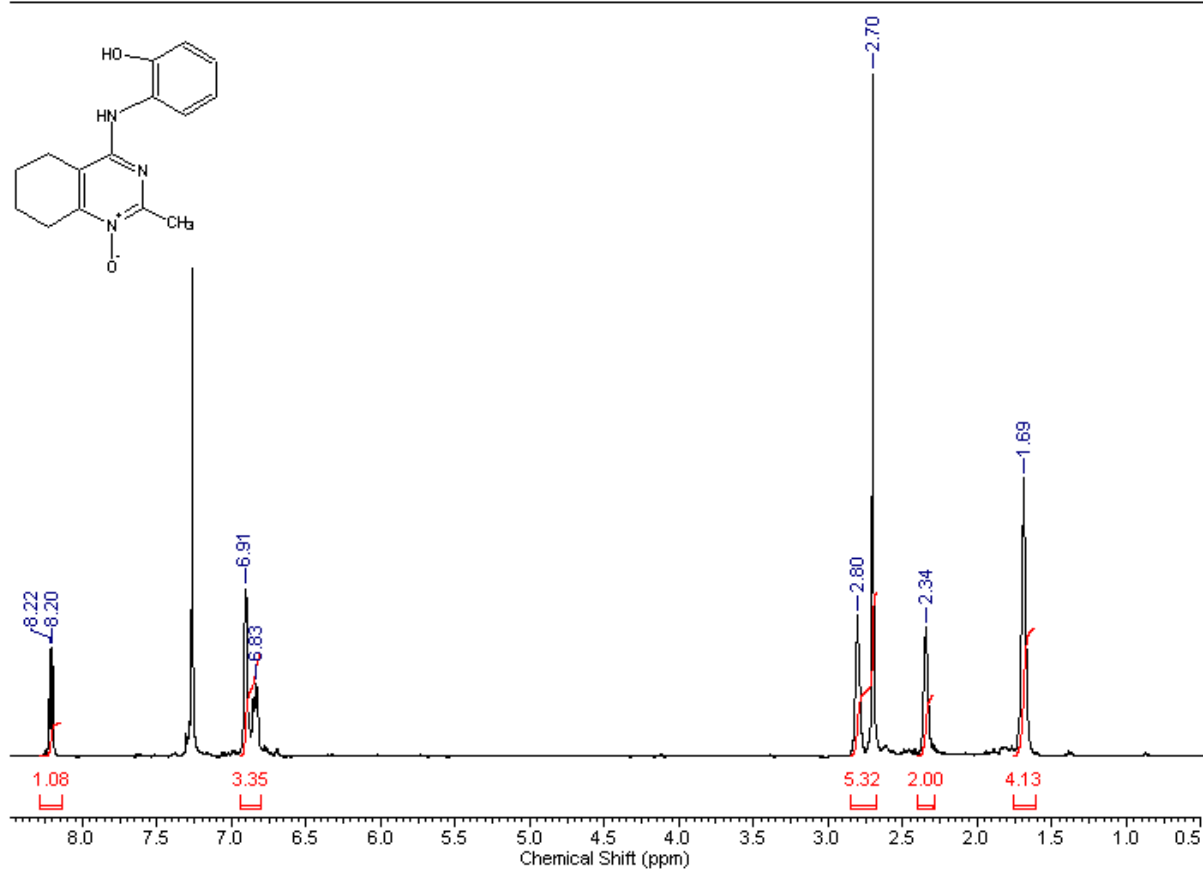
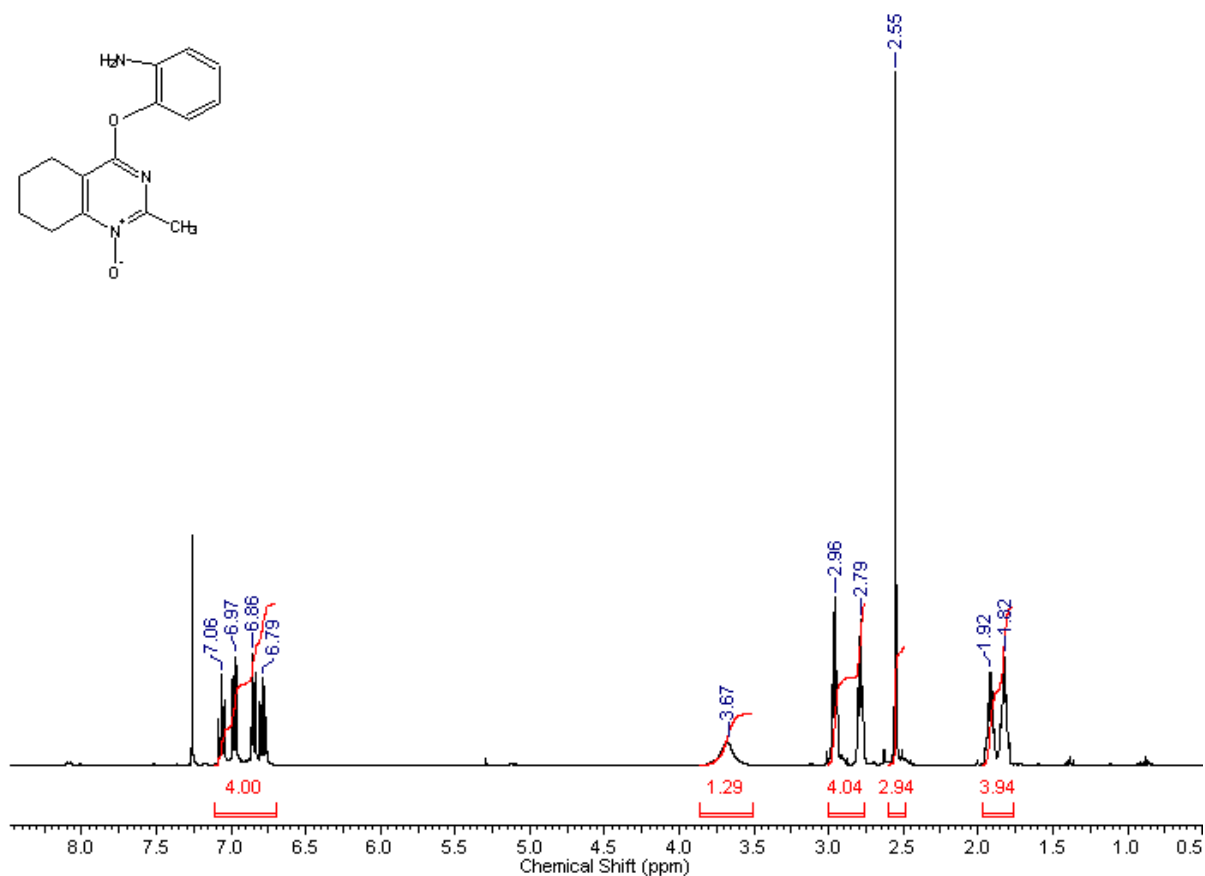
Compound	X	R	δ , ppm	
			C(Ar)-O	C(Ar)-N
13 ^{S5}	N ⁺ -O ⁻	CH ₃	145.0	143.9
3b ^{S5}	N	CH ₃	145.2	143.5

3. Copies of NMR spectra

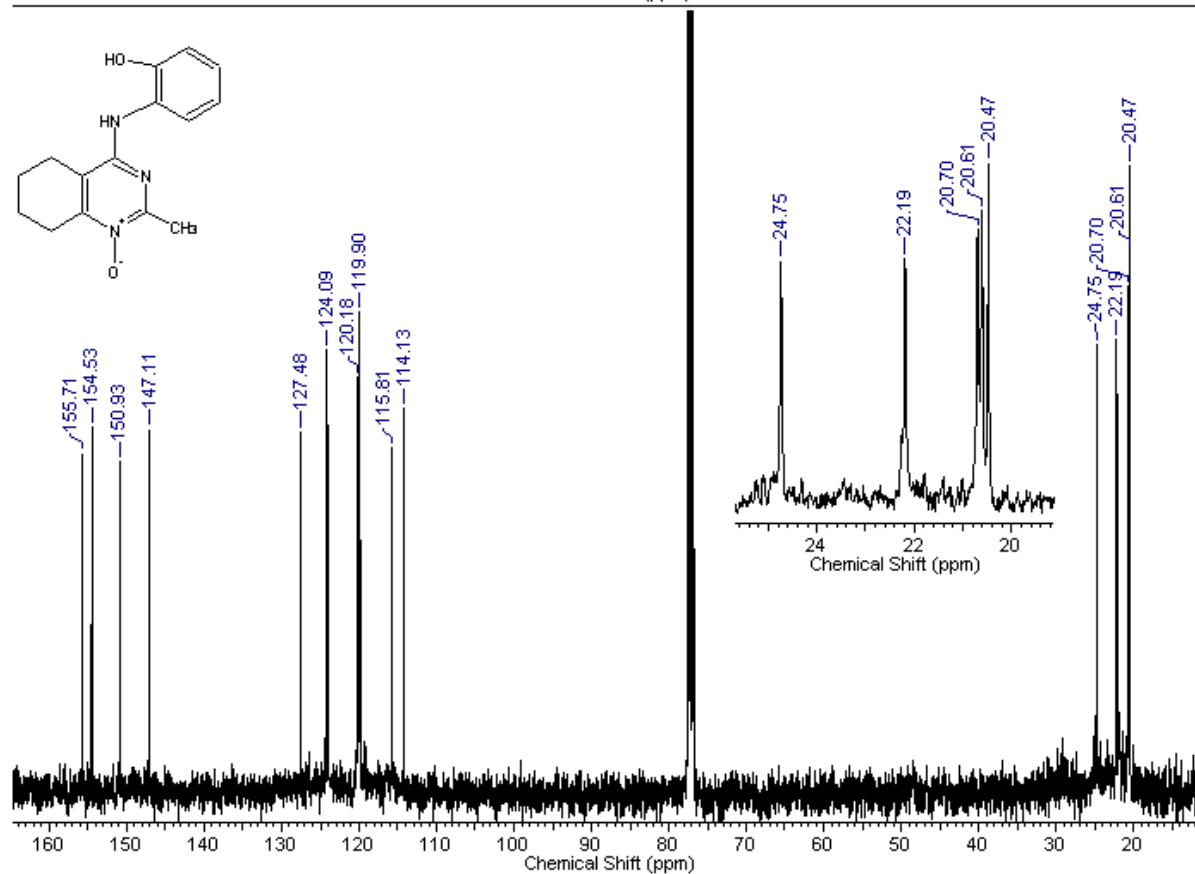
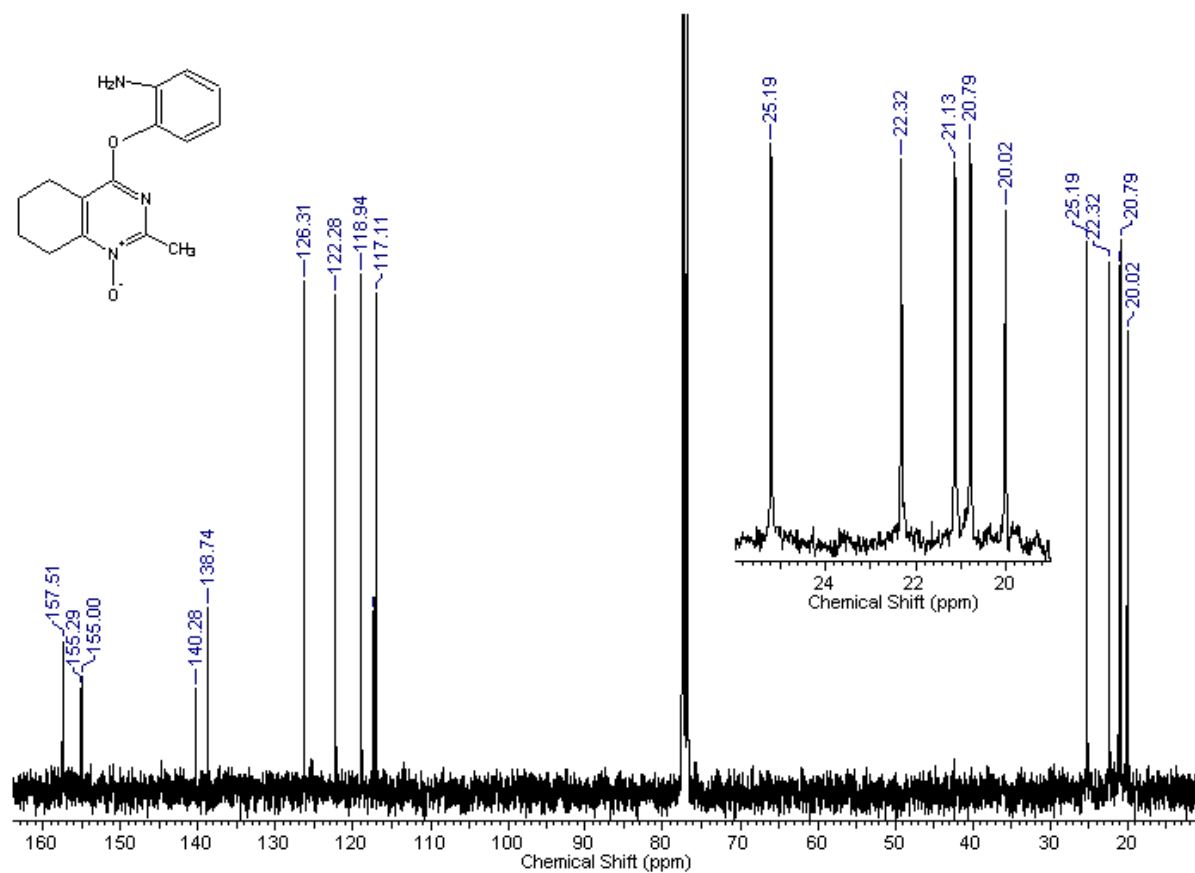
^1H NMR (400MHz, CDCl_3) and ^{13}C NMR (101 MHz, CDCl_3) spectra of compound 2



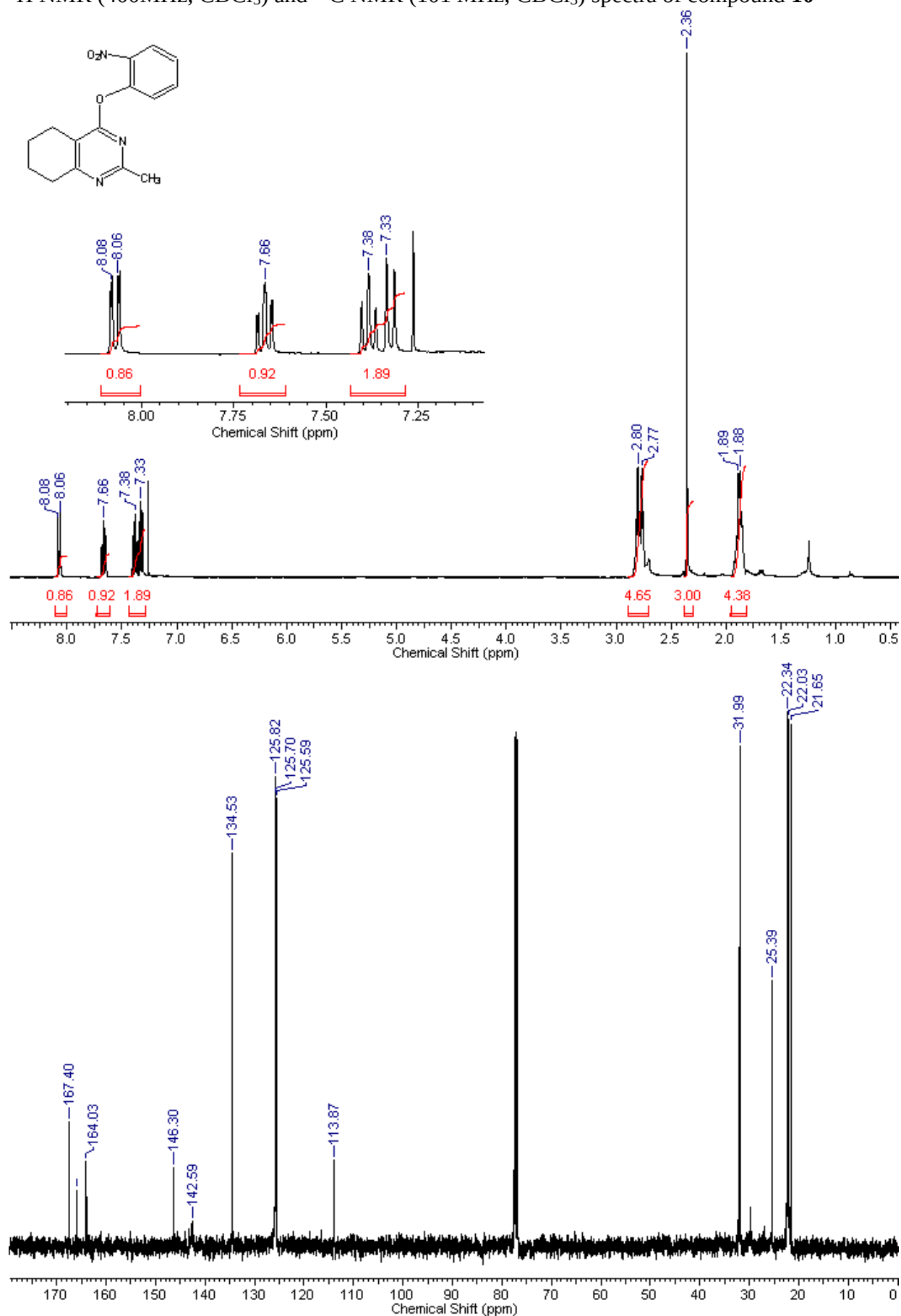
^1H NMR spectra (400MHz, CDCl_3) of compounds **6**^{S5} and **7**^{S6}



^{13}C NMR spectra (101 MHz, CDCl_3) of compounds **6**^{S5} and **7**^{S6}

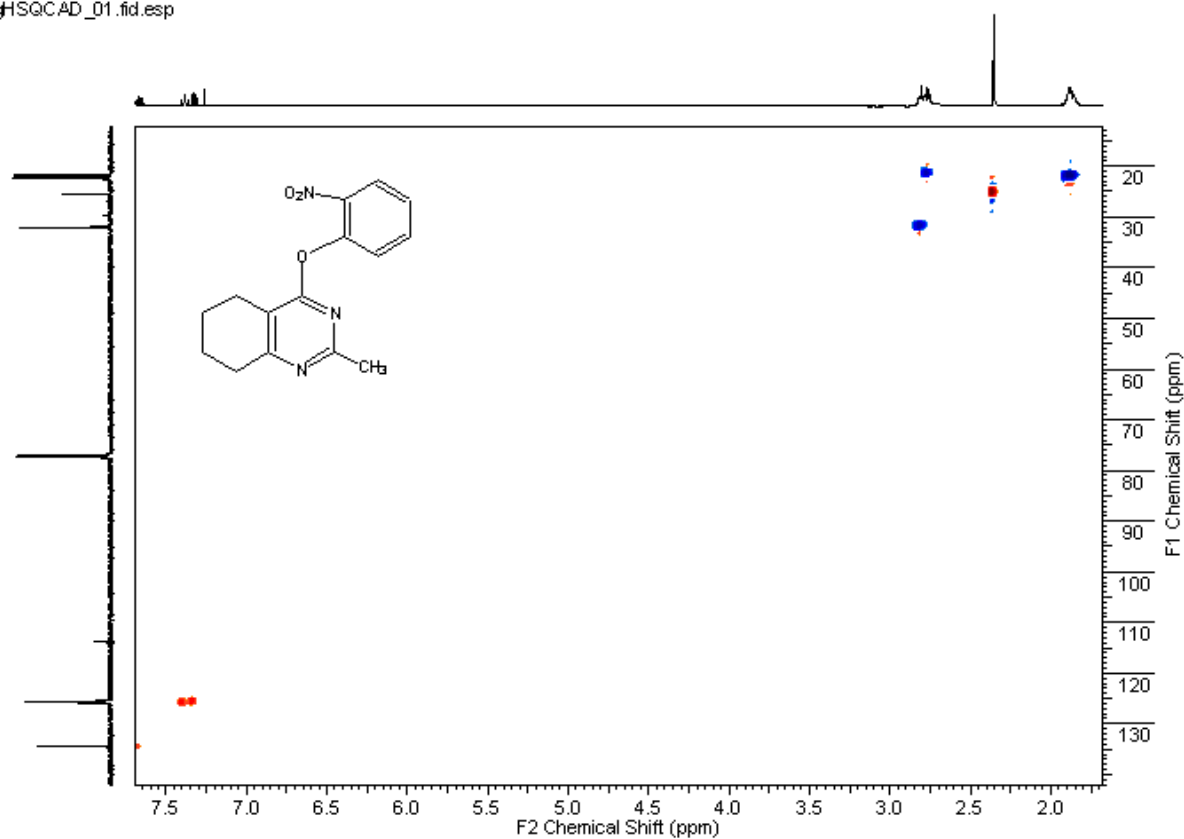


^1H NMR (400MHz, CDCl_3) and ^{13}C NMR (101 MHz, CDCl_3) spectra of compound **10**

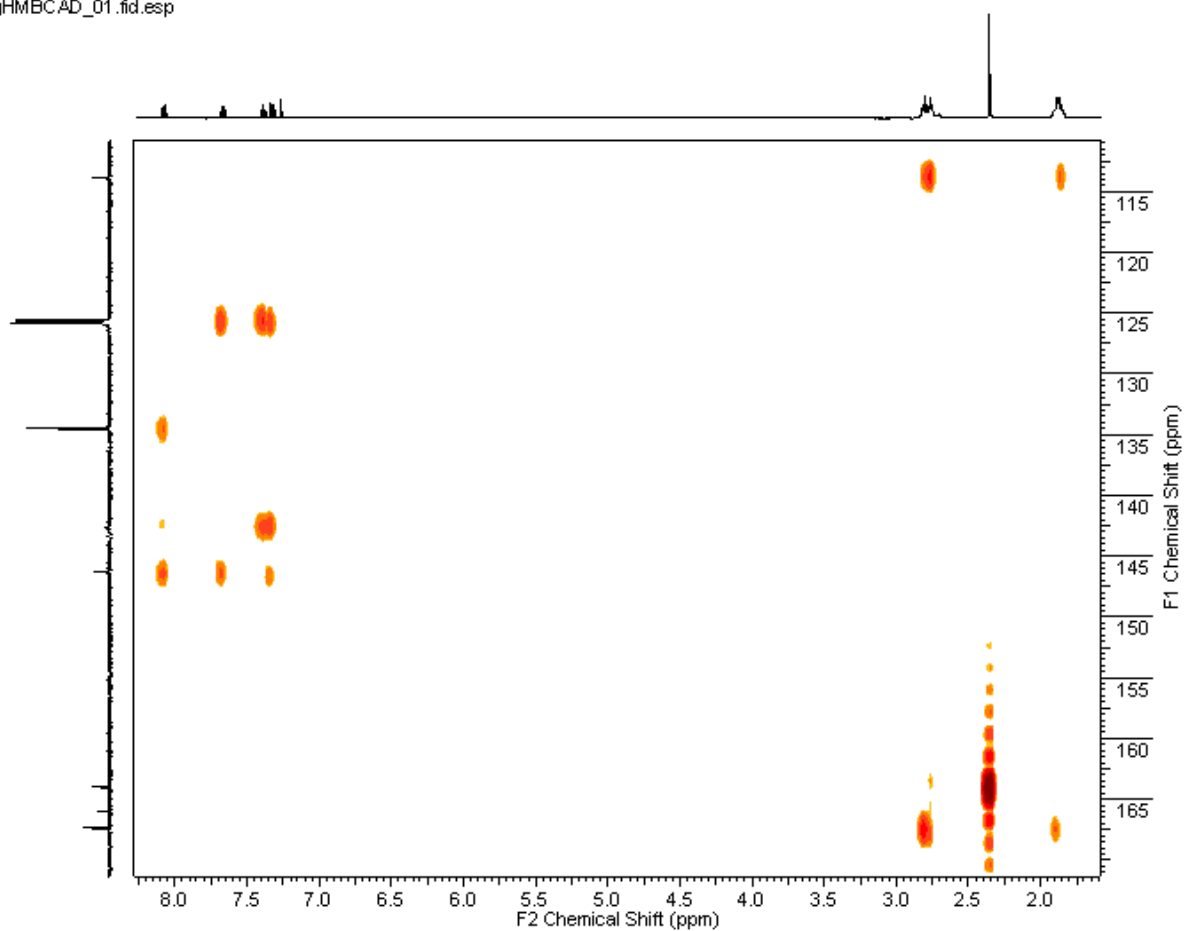


HSQC and HMBC (low field) spectra of compound **10**

gHSQCAD_01.fid.esp



gHMBCAD_01.fid.esp



4. DFT Calculations

Computations were carried out with ORCA 5.0.3^{S7} program package. Geometry optimization was carried out using the DFT functional B3LYP^{S8} utilizes the atom-pairwise dispersion correction based on tight binding partial charges (D4)^{S9,S10} and def2-TZVPP basis set^{S11} with the auxiliary basis: def2/J.^{S12} The uncorrected molecular electronic energies were calculated for an ideal gas under standard conditions (1 atm, 298 K). Vibrational entropies were corrected using the Grimme quasi RRHO model^{S13} at 298.15 K under ideal gas conditions, with the default reference frequency ($\omega_0 = 100 \text{ cm}^{-1}$) interpolating between harmonic and free rotor treatments for low frequency modes. Transition states were located via the NEB-TS method. SCF convergence across all steps employed VeryTightSCF, except during NEB-TS^{S14} transition-state searches – both minimum energy path finding and saddle-point optimizations – where VeryTightSCF was enforced to ensure high accuracy.

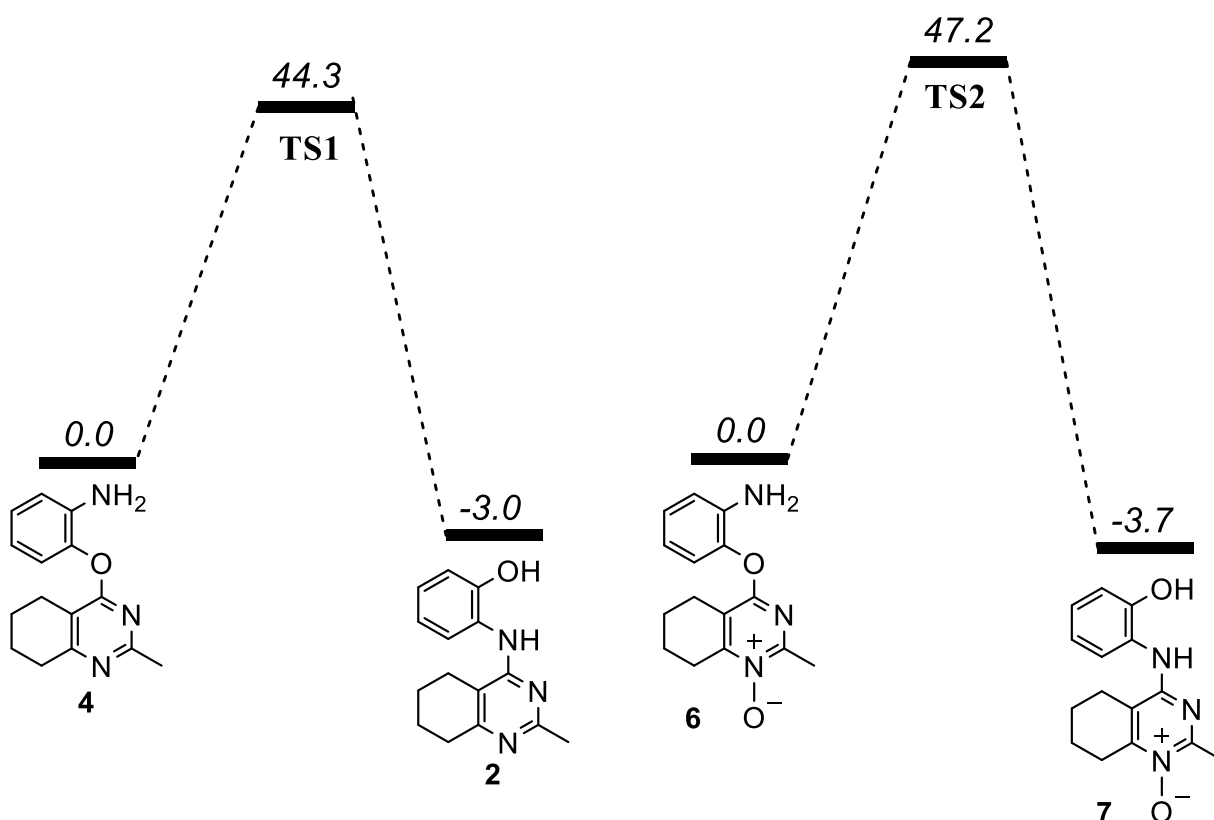
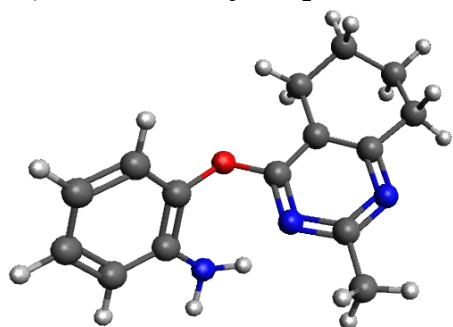


Figure S1. Difference in reactivity of tetrahydroquinazoline **4** and tetrahydroquinazoline N-oxide **6** in the Smiles rearrangement

5. Cartesian Coordinates

2-[(5,6,7,8-Tetrahydroquinazolin-4-yl)oxy]aniline (4)



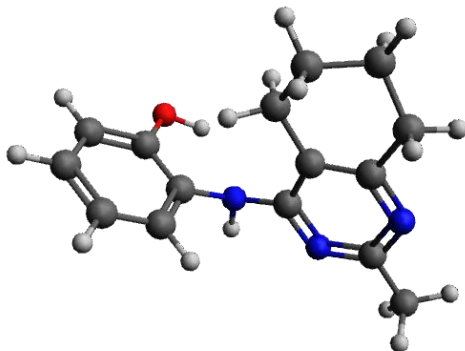
E = -821.22666620 Eh

ZPE = 0.29876294 Eh

G₂₉₈ = -820.97026987 Eh

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C	1.61873756541524	-0.46906359164013	-0.11812304584798
C	1.96581308551361	-1.86364515897546	-0.56505941143099
C	3.42255048109045	-1.98101814728595	-1.01378201272624
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H	1.77396161175443	-2.55877737787108	0.25939940685125
H	3.54052807312665	-1.52074040561889	-1.99976486219074
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H	4.40657880611314	0.71361789601159	-0.84753589853893
H	4.22939819051325	-1.73744689735988	0.96698468906114
H	3.68966914101046	-3.03322228196464	-1.12497480293046
H	1.28802373247174	-2.16790717529407	-1.36410951112110
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O	-0.66505250513845	-0.96437075607275	-0.22318312354775
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H	-5.78824226214325	-0.07475658668921	-0.83002073217555
N	-2.22204439790278	-0.15211203157495	2.02837912527517
H	-2.84971806962073	0.23713831108601	2.71434017218577
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H	-0.12001038066595	3.85216327620599	0.37121836229740
H	0.00806236803368	3.35721310848145	2.04911601652945
H	1.43231139576108	4.02770973147119	1.22675275674181
H	-1.33683265179590	0.33534067831784	2.02859888913536

2-[(5,6,7,8-Tetrahydroquinazolin-4-yl)amino]phenol (2)



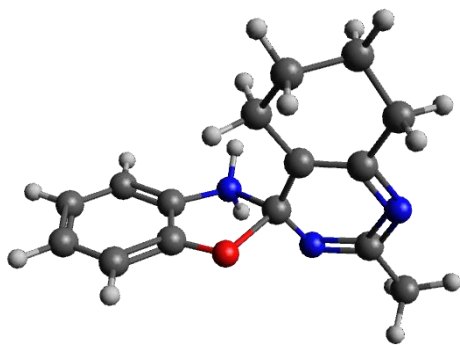
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ZPE = 0.29963872 Eh

G₂₉₈ = -820.97499553 Eh

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C	1.04441074662135	-2.61081985153262	-0.86628592263560
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H	4.19747816947041	-1.23205169745124	-0.53567937357579
C	0.51444607099066	0.94193623386886	0.56856035453189
H	0.14008182383080	-1.89962584630279	0.96293360000463
H	0.92232659548753	-2.40366005554460	-1.93397467586392
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N	3.11391845415644	1.00543305615982	-0.20406457435517
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O	-2.59594604961450	-0.65062287691872	2.27216620968856
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H	2.88543383472957	3.91784374266329	1.29859920341963
H	4.32485898693767	3.11571814954647	0.60549326010318
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TS1



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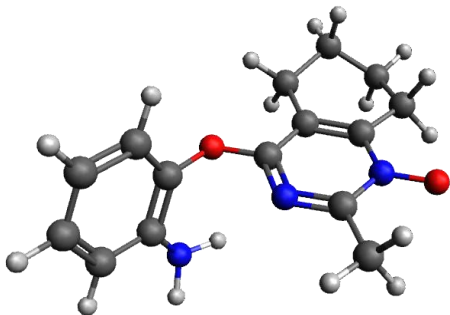
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$\text{ZPE} = 0.29871176 \text{ Eh}$

$G_{298} = -820.89974286 \text{ Eh}$

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C	-2.01094847246013	2.10697920182980	0.00023652271617
H	-3.71645371308922	-1.26653743751049	1.28936904416868
H	-2.93145640725959	-2.61643785419133	-1.33605216109398
H	-1.21722389070662	-3.87284898000158	0.02626357277801
H	0.38369422168804	-1.90624874247048	0.32004791538740
N	-2.88408096414807	1.13368885828386	0.18601317988180
N	-0.71020293288346	1.94755756628520	-0.27595827755791
O	0.85745928170296	0.57649908189318	1.12800207936551
C	2.04297823536440	0.22490529212854	0.70240871926923
C	3.14540351148230	-0.13212584934661	1.49096329253203
C	2.20313845958338	0.19039210678392	-0.68612542974651
C	4.32975514736356	-0.49640499950808	0.86620732543842
H	3.05601385989820	-0.11825296371837	2.56781598469368
C	3.37078034603534	-0.17573158106960	-1.32047135666749
C	4.45710092636954	-0.52594776321009	-0.52411519784799
H	5.18029355488726	-0.76912300716051	1.47773780367160
H	3.44590604319059	-0.18726598186084	-2.40049655341098
H	5.39168748408974	-0.81719296509013	-0.98088056832529
N	0.95755789531088	0.60664459460742	-1.30608327058832
H	0.97856104199056	1.56947538398206	-1.65058494849615
H	0.64647472187542	-0.00716454005418	-2.05527126380682
C	-2.49851120147883	3.52239588279118	0.09209840960804
H	-2.10295361035635	3.98894149467517	0.99727440911308
H	-2.13606567388196	4.10775804906480	-0.75347334595066
H	-3.58431125811498	3.54780861360483	0.12689675790949

4-(2-Aminophenoxy)-5,6,7,8-tetrahydroquinazoline 1-oxide (6)



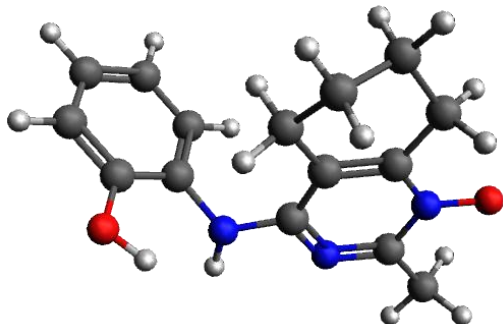
E = -896.39427980 Eh

ZPE = 0.30261964 Eh

G₂₉₈ = -896.13511340 Eh

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C	3.83761217091298	-0.30647682562021	0.08960622778849
C	2.40061072448590	0.08933320832539	0.09924076068247
C	1.35874152856464	-0.77788336610728	-0.16076407338053
C	1.60464842584367	-2.22011719780373	-0.51750927643804
C	3.05195710940767	-2.46897006140914	-0.94111672102816
H	5.05404585675336	-2.05682487299422	-0.21271110918751
H	4.31911512775124	0.14492091957856	0.95869062124504
C	0.07023650062373	-0.23957257711288	-0.08556241199336
H	1.35580842004586	-2.84874481694890	0.34396545424590
H	3.21865190541363	-2.04982536917606	-1.93811875624652
C	0.84524689641852	1.83896340594838	0.42864223595959
H	4.31699096862014	0.17523936552437	-0.76921235928141
H	3.84656726995937	-2.24009740232455	1.04382615661575
H	3.23336795345075	-3.54205885482565	-1.01631847283745
H	0.90904994092280	-2.51355550472490	-1.30449242038282
N	2.14165962594428	1.41109560162774	0.37913331246996
N	-0.16828924194054	1.02127567818902	0.20379275398846
O	-0.96838297177630	-1.08684168771671	-0.31215276194456
C	-2.26007592161342	-0.56080009536577	-0.40411938724839
C	-2.78648931410878	-0.30347944280775	-1.65460175850977
C	-3.00704855591058	-0.38296577343501	0.76366094841943
C	-4.09330064465203	0.15143150384386	-1.77942165062823
H	-2.16102809746565	-0.46293143141423	-2.52251595239439
C	-4.32021393649012	0.07619217629325	0.62123208207926
C	-4.85408555962874	0.33953738282343	-0.63118123428301
H	-4.50815064486256	0.35429744438430	-2.75653618467661
H	-4.92314710486396	0.22111798641075	1.50934752120229
H	-5.87370461216421	0.69288438861656	-0.70857992072232
N	-2.48007071367205	-0.70724292031592	2.00545770080099
H	-1.47630354280435	-0.69161937887446	2.06916453672528
H	-2.91811973181163	-0.24805144306686	2.78667880476935
C	0.62890037627152	3.27335941097275	0.74232055777762
H	1.12690732040910	3.90197593823218	0.00176693333355
H	-0.43728242774657	3.47930632447035	0.75918062099829
H	1.08532851585364	3.52537161618207	1.70133266122846
O	3.11075682468416	2.23314304801712	0.59166286086173

4-((2-Hydroxyphenyl)amino)-5,6,7,8-tetrahydroquinazoline 1-oxide (7)



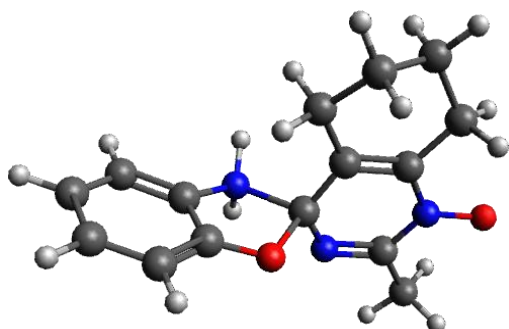
E = -896.40259705 Eh

ZPE = 0.30411060 Eh

G₂₉₈ = -896.14094697 Eh

C	-1.60343329814774	3.07380325295642	0.39926320588421
C	-2.65625975067147	1.96936339920680	0.34121265449087
C	-2.06254507432067	0.62392984619440	0.09316510080246
C	-0.73851515230748	0.40282209709110	-0.24476443212713
C	0.19435282848548	1.56627303032909	-0.47531496576730
C	-0.55569386116295	2.87901555718360	-0.69245964985683
H	-2.09007197874967	4.04546138098901	0.30642732752386
H	-3.25008898536911	1.91331128512285	1.25555558469428
C	-0.34608790219792	-0.93269541989352	-0.41538605523999
H	0.87171652018324	1.67105589664348	0.37622917781133
H	-1.04538746913558	2.86953549179441	-1.67108515842067
C	-2.47633672287058	-1.69741119582528	-0.04112990545016
H	-3.39146972562624	2.16244773703459	-0.44706793177191
H	-1.10934047306228	3.06257664359883	1.37541959196385
H	0.15538479030168	3.70629659897767	-0.70220609380046
H	0.83035415386541	1.34455873073183	-1.33416849242222
N	-2.93611924896419	-0.43006676619754	0.19026423333701
N	-1.21226181819795	-1.93785985554592	-0.31924968651395
O	3.12964591379154	-0.32256555220752	-2.11724599022282
C	3.16205271733574	-0.30449768217151	-0.76178563633195
C	4.27356450769432	0.21543308356856	-0.10725512099491
C	2.07555436367066	-0.78328968138605	-0.02295125545381
C	4.29006349889541	0.26648181395329	1.27917211333293
H	5.10296243660019	0.58339401257267	-0.69510990455984
C	2.10424557961923	-0.72639919699342	1.36460230159659
C	3.20715056155579	-0.19735232476147	2.02112492134053
H	5.15473376472810	0.67562342051336	1.78454287219182
H	1.25327136410705	-1.09335190771529	1.92350038435536
H	3.22525128428710	-0.15325444756330	3.10113929651323
N	0.95971550259019	-1.29786272968310	-0.76248179537702
H	2.25595696326442	-0.65896395971845	-2.36987598479568
H	0.99606152448741	-2.30087653371983	-0.89917438682711
C	-3.47537610243928	-2.79182802952134	0.05188936285897
H	-4.29221261589720	-2.62081542300450	-0.65148098565958
H	-2.98793657818733	-3.74045507025490	-0.15338437343906
H	-3.93293452882869	-2.80376294876619	1.04276216746700
O	-4.17548698932667	-0.22887455353285	0.47916750886811

TS2



Imaginary mode -306.21 cm^{-1}

E = -896.32060792 Eh

ZPE = 0.30262247 Eh

G₂₉₈ = -896.05981679 Eh

C	-2.86435529345122	-2.49661103269076	-0.18669436853668
C	-3.30930375338091	-1.08045751071229	0.17153536352777
C	-2.20870857590356	-0.08373929291924	0.02352368049137
C	-0.89318635703091	-0.42339168748015	-0.14720134710468
C	-0.43423780139347	-1.86055282782984	-0.15843017777839
C	-1.49289389976812	-2.80709828728959	0.40757629290797
H	-3.60845183148721	-3.21355115428184	0.16313987810544
H	-4.15241137384516	-0.74140743674463	-0.43174927113590
C	0.03535345444136	0.65845969051352	-0.21938178785897
H	-0.19075658289238	-2.17611449613779	-1.18315460474143
H	-1.53280953491312	-2.68789510593277	1.49411937750306
C	-1.66584620927413	2.19757066712257	-0.12542297238117
H	-3.67326208142343	-1.02855180386269	1.20260804654972
H	-2.81625917458908	-2.60261756842845	-1.27525090693322
H	-1.20593679477828	-3.84167304526921	0.21151472008295
H	0.48946903183624	-1.95304314949779	0.41430316332201
N	-2.59557541321013	1.24023471716988	0.08576168139743
N	-0.38487188251435	1.91630410302086	-0.32853880487852
O	1.10345550776041	0.51493550276316	1.09237240175240
C	2.26781032602640	0.05834106219465	0.69208247144810
C	3.32248770425112	-0.36161145944565	1.51009033232524
C	2.43914529004203	-0.02820802961457	-0.69180472601470
C	4.48270640743518	-0.83833099736666	0.91523110460660
H	3.21871371984213	-0.30900968172922	2.58433812523879
C	3.58174276760578	-0.50926903279068	-1.29527387176010
C	4.62475831538645	-0.92074945040646	-0.47102651807716
H	5.30022712420533	-1.15919089367348	1.54780863716666
H	3.67013746913934	-0.56101889900560	-2.37296626983752
H	5.53878129166888	-1.30027657569971	-0.90407645873530
N	1.23553894916519	0.45758081289648	-1.33338293740621
H	1.31817862266970	1.41012911152077	-1.69295671558776
H	0.88368122667560	-0.14593648610727	-2.07217282631966
C	-2.14572226811399	3.60236174125371	-0.13598320889142
H	-2.57619161963133	3.85446436480787	0.83516120110529
H	-1.31783651949176	4.26810633885307	-0.36367437128758
H	-2.95534193050995	3.72098363946225	-0.85782202074190
O	-3.84947831054864	1.55033415333755	0.29664768847747

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