Supplementary Material

Study of the regioselectivity of vicarious nucleophilic amination of mononitroquinolines with 1,1,1-trimethylhydrazinium iodide (TMHI)

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Table 1. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-2 carbon atom in 3-nitroquinoline (**1a**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.4155	0.0000	0.0000
3	C	2.1120	1.2380	0.0000
4	C	1.4185	2.4167	0.0000
5	C	0.0019	2.4163	-0.0070
6	C	-0.7010	1.2434	-0.0068
7	C	2.0985	-1.2409	-0.0295
8	C	1.3770	-2.4125	-0.0219
9	C	-0.0665	-2.3663	0.0769
10	N	2.0583	-3.7314	-0.1041
11	N	-0.2511	-2.8377	2.0201
12	N	-0.7208	-1.1774	-0.0107
13	N	-1.3037	-2.3282	2.8438
14	C	-0.9395	-1.0076	3.5186
15	C	-1.6640	-3.3182	3.9481
16	O	3.1849	-3.8456	0.3456
17	O	1.5017	-4.6689	-0.6396
18	H	-1.9146	-4.3031	3.5235
19	H	-2.5294	-2.9730	4.5336
20	H	-0.8230	-3.4685	4.6423
21	H	-0.7089	-0.2346	2.7663
22	H	-0.0526	-1.1142	4.1625
23	H	-1.7617	-0.6287	4.1448

24	H	0.5960	-2.8393	2.5460
25	H	3.1973	-1.2409	-0.0739
26	H	-1.7970	1.2409	-0.0217
27	H	-0.5249	3.3766	-0.0153
28	H	1.9487	3.3744	-0.0002
29	H	3.2080	1.2283	-0.0008
30	H	-0.6768	-3.2538	-0.1769
31	C	-2.5318	-2.0942	1.9844
32	H	-2.2376	-1.4980	1.0733
33	H	-2.9499	-3.0443	1.6204
34	H	-3.3182	-1.5596	2.5343

Table 2. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-4 carbon atom in 3-nitroquinoline (**1a**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.4155	0.0000	0.0000
3	C	2.1120	1.2380	0.0000
4	C	1.4185	2.4167	0.0000
5	C	0.0019	2.4163	-0.0070
6	C	-0.7010	1.2434	-0.0068
72	C	2.0985	-1.2409	-0.0295
8	C	1.3770	-2.4125	-0.0219
9	C	-0.0665	-2.3663	0.0769
10	N	2.0583	-3.7314	-0.1041
11	N	-0.2511	-2.8377	2.0201
12	N	-0.7208	-1.1774	-0.0107
13	N	-1.3037	-2.3282	2.8438
14	C	-0.9395	-1.0076	3.5186
15	C	-1.6640	-3.3182	3.9481
16	O	3.1849	-3.8456	0.3456
17	O	1.5017	-4.6689	-0.6396
18	H	-1.9146	-4.3031	3.5235
19	H	-2.5294	-2.9730	4.5336
20	H	-0.8230	-3.4685	4.6423
21	H	-0.7089	-0.2346	2.7663
22	H	-0.0526	-1.1142	4.1625
23	H	-1.7617	-0.6287	4.1448
24	H	0.5960	-2.8393	2.5460
25	H	3.1973	-1.2409	-0.0739

26	H	-1.7970	1.2409	-0.0217
27	H	-0.5249	3.3766	-0.0153
28	H	1.9487	3.3744	-0.0002
29	H	3.2080	1.2283	-0.0008
30	H	-0.6768	-3.2538	-0.1769
31	C	-2.5318	-2.0942	1.9844
32	H	-2.2376	-1.4980	1.0733
33	H	-2.9499	-3.0443	1.6204
34	H	-3.3182	-1.5596	2.5343

Table 3. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-6 carbon atom in 5-nitroquinoline (**1b**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.4345	0.0000	0.0000
3	C	2.1469	1.2165	0.0000
4	C	1.4180	2.4497	-0.0194
5	C	0.0242	2.4344	-0.2038
6	C	-0.6712	1.1759	-0.0924
7	N	2.1020	3.7377	0.1710
8	C	3.5673	1.1546	0.0286
9	N	-0.2632	2.8842	-2.1104
10	C	4.1944	-0.0625	0.0656
11	C	3.4195	-1.2487	0.0654
12	N	2.0916	-1.2183	0.0320
13	O	1.5069	4.6906	0.6381
14	O	3.2843	3.8566	-0.1351
15	N	0.3228	2.3118	-3.2940
16	C	1.8270	2.5144	-3.2646
17	C	-0.2088	2.9815	-4.5590
18	H	0.2809	2.5866	-5.4625
19	H	-0.0341	4.0687	-4.5299
20	H	-1.2932	2.8267	-4.6742
21	H	2.3039	2.1073	-4.1692
22	H	2.2784	2.0174	-2.3864
23	H	2.0820	3.5838	-3.1959
24	H	3.8808	-2.2422	0.0929
25	H	5.2863	-0.1316	0.0937

26	H	-1.2480	2.9497	-2.2598
27	H	4.1205	2.1165	0.0088
28	H	-0.5594	3.3516	0.0113
29	H	-0.5322	-0.9544	0.0955
30	H	-1.7666	1.1939	-0.0693
31	C	0.0435	0.8180	-3.4152
32	H	0.5733	0.3695	-4.2689
33	H	-1.0319	0.6222	-3.5447
34	H	0.3617	0.2878	-2.4983

Table 4. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-8 carbon atom in 5-nitroquinoline (**1b**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.4404	0.0000	0.0000
3	C	2.1714	1.2076	0.0000
4	C	1.4614	2.4486	0.0478
5	C	0.0718	2.4224	0.1968
6	C	-0.6374	1.2296	0.2048
7	N	2.1550	3.7479	0.0073
8	C	3.5940	1.1258	-0.0175
9	N	-0.4213	-0.4623	-1.9690
10	C	4.2068	-0.0962	-0.0113
11	C	3.4160	-1.2747	0.0146
12	N	2.0916	-1.2267	0.0191
13	O	1.5062	4.7791	-0.0491
14	O	3.3768	3.8102	0.0000
15	N	-0.4256	0.3739	-3.1240
16	C	-1.4798	1.4532	-2.9402
17	C	-0.7684	-0.3998	-4.3955
18	H	-0.8319	0.2642	-5.2712
19	H	-1.7366	-0.9143	-4.2926
20	H	-0.0117	-1.1692	-4.6155
21	H	-1.5226	2.1282	-3.8081
22	H	-1.2665	2.0581	-2.0405
23	H	-2.4773	1.0092	-2.7996
24	H	3.8668	-2.2734	0.0364
25	H	5.2981	-0.1795	-0.0174
26	H	0.0991	-1.2868	-2.1799
27	H	4.1602	2.0804	-0.0217

28	H	-0.4878	3.3611	0.3216
29	H	-0.5434	-0.9390	0.2035
30	H	-1.7204	1.2502	0.3691
31	C	0.9190	1.0569	-3.3581
32	H	0.8752	1.7815	-4.1850
33	H	1.7034	0.3219	-3.5951
34	H	1.2444	1.5945	-2.4488

Table 5. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-5 carbon atom in 6-nitroquinoline (**1c**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.4294	0.0000	0.0000
3	C	2.1340	1.2203	0.0000
4	C	1.4114	2.4692	-0.0280
5	C	0.0167	2.4250	0.1407
6	C	-0.6757	1.1814	0.0887
7	N	-0.7404	3.6625	0.3843
8	C	3.5485	1.1901	0.0481
9	N	1.6770	3.0532	-1.9334
10	C	4.1966	-0.0203	0.0821
11	C	3.4364	-1.2138	0.0642
12	N	2.1065	-1.2097	0.0231
13	O	-1.9285	3.7137	0.1040
14	O	-0.1817	4.6455	0.8402
15	N	1.0830	2.5565	-3.1416
16	C	1.3450	1.0659	-3.2529
17	C	1.6831	3.2292	-4.3743
18	H	1.2834	2.8002	-5.3061
19	H	2.7778	3.1114	-4.3925
20	H	1.4693	4.3096	-4.3874
21	H	0.9133	0.6495	-4.1756
22	H	0.9077	0.5244	-2.3936
23	H	2.4253	0.8537	-3.2522
24	H	3.9124	-2.2011	0.0856
25	H	5.2885	-0.0776	0.1245
26	H	1.6535	4.0504	-1.9693
27	H	4.1066	2.1337	0.0535
28	H	-1.7731	1.1763	0.1407
29	H	-0.5358	-0.9557	-0.0228

30	H	1.9781	3.3811	0.2458
31	C	-0.4254	2.7757	-3.1915
32	H	-0.8682	2.3650	-4.1116
33	H	-0.6784	3.8464	-3.1464
34	H	-0.9188	2.2871	-2.3315

Table 6. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-7 carbon atom in 6-nitroquinoline (**1c**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.3901	0.0000	0.0000
3	C	2.1140	1.2277	0.0000
4	C	1.4062	2.4347	-0.0700
5	C	0.0184	2.4410	-0.0664
6	C	-0.7266	1.2144	0.0903
7	N	-0.7039	3.7182	-0.2555
8	C	3.5425	1.1839	-0.0165
9	N	-1.4129	1.3164	1.8514
10	C	4.1793	-0.0187	-0.0353
11	C	3.4045	-1.2224	-0.0404
12	N	2.0888	-1.2243	-0.0223
13	O	-1.8189	3.7295	-0.7424
14	O	-0.1748	4.7628	0.0910
15	N	-0.7859	0.8522	3.0771
16	C	-0.7071	-0.6639	3.0492
17	C	-1.6022	1.2522	4.3021
18	H	-1.1647	0.8474	5.2278
19	H	-2.6350	0.8767	4.2268
20	H	-1.6574	2.3471	4.4130
21	H	-0.2771	-1.0602	3.9814
22	H	-0.0827	-1.0098	2.2058
23	H	-1.7057	-1.1073	2.9136
24	H	3.8899	-2.2054	-0.0582
25	H	5.2706	-0.0909	-0.0531
26	H	-1.7828	2.2276	2.0221
27	H	4.1005	2.1271	-0.0202
28	H	-1.7868	1.1947	-0.2355
29	H	-0.5513	-0.9424	-0.1058
30	H	1.9737	3.3734	-0.1535
31	C	0.6182	1.4097	3.2582

32	H	1.1191	0.9742	4.1357
33	H	0.5999	2.5032	3.3860
34	H	1.2414	1.1988	2.3680

Table 7. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-6 carbon atom in 7-nitroquinoline (**1d**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.4052	0.0000	0.0000
3	C	2.1156	1.2331	0.0000
4	C	1.4198	2.4296	-0.0998
5	C	0.0112	2.4514	-0.2770
6	C	-0.6905	1.2013	-0.0929
7	N	-2.1647	1.2056	0.0253
8	C	3.5470	1.1814	0.1282
9	N	-0.3037	2.9254	-2.0568
10	C	4.1723	-0.0210	0.2162
11	C	3.4001	-1.2286	0.1787
12	N	2.0883	-1.2204	0.0811
13	O	-2.7996	0.2275	-0.3350
14	O	-2.7438	2.1848	0.4592
15	N	0.3572	2.3964	-3.2453
16	C	1.8190	2.8040	-3.2215
17	C	-0.2651	2.9689	-4.5146
18	H	0.2724	2.6312	-5.4142
19	H	-0.2423	4.0701	-4.5029
20	H	-1.3179	2.6623	-4.6231
21	H	2.3467	2.4564	-4.1225
22	H	2.3288	2.3820	-2.3358
23	H	1.9212	3.8986	-3.1616
24	H	3.8826	-2.2108	0.2374
25	H	5.2594	-0.0952	0.3188
26	H	-1.2852	2.9434	-2.2386
27	H	4.1043	2.1240	0.1603
28	H	-0.5101	3.3923	-0.0024
29	H	-0.5380	-0.9551	0.0994
30	H	1.9580	3.3801	-0.0136
31	C	0.2765	0.8807	-3.3358
32	H	0.8478	0.4934	-4.1928
33	H	-0.7658	0.5410	-3.4426
34	H	0.6767	0.4097	-2.4174

Table 8. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-8 carbon atom in 7-nitroquinoline (**1d**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.4494	0.0000	0.0000
3	C	2.1679	1.2115	0.0000
4	C	1.4580	2.4445	0.0458
5	C	0.0974	2.4491	0.1629
6	C	-0.6374	1.2339	0.1968
7	N	-2.0983	1.2777	0.4142
8	C	3.5870	1.1616	-0.0049
9	N	-0.4490	-0.4528	-1.9124
10	C	4.2178	-0.0550	0.0091
11	C	3.4416	-1.2411	0.0290
12	N	2.1131	-1.2147	0.0236
13	O	-2.6561	0.3848	1.0227
14	O	-2.7395	2.2244	-0.0164
15	N	-0.2337	0.2677	-3.1322
16	C	-0.9721	1.5935	-3.0716
17	C	-0.7585	-0.5002	-4.3432
18	H	-0.6524	0.0827	-5.2710
19	H	-1.8257	-0.7438	-4.2199
20	H	-0.2199	-1.4505	-4.4837
21	H	-0.8312	2.1746	-3.9954
22	H	-0.6176	2.2055	-2.2225
23	H	-2.0534	1.4405	-2.9252
24	H	3.9061	-2.2335	0.0548
25	H	5.3098	-0.1280	0.0139
26	H	-0.1796	-1.4021	-2.0622
27	H	4.1557	2.0981	-0.0071
28	H	-0.4383	3.4044	0.2464
29	H	-0.5259	-0.9433	0.2482
30	H	2.0252	3.3811	0.0323
31	C	1.2426	0.5598	-3.3830
32	H	1.3924	1.1737	-4.2837
33	H	1.8173	-0.3705	-3.5092
34	H	1.6812	1.0998	-2.5245

Table 9. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-5 carbon atom in 8-nitroquinoline (**1e**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.4218	0.0000	0.0000
3	C	2.1229	1.2262	0.0000
4	C	1.3972	2.4690	-0.0452
5	C	0.0013	2.4144	0.1384
6	C	-0.6813	1.2051	0.1256
7	N	-0.7585	-1.2802	-0.0886
8	C	3.5389	1.1959	0.0619
9	N	1.6548	3.0916	-1.8846
10	C	4.1916	-0.0092	0.1011
11	C	3.4351	-1.2082	0.0759
12	N	2.1090	-1.2093	0.0257
13	O	-0.9983	-1.7333	-1.1933
14	O	-1.1812	-1.8116	0.9156
15	N	1.0576	2.5690	-3.0907
16	C	1.3711	1.0911	-3.2191
17	C	1.6176	3.2719	-4.3253
18	H	1.2054	2.8481	-5.2541
19	H	2.7136	3.1740	-4.3681
20	H	1.3843	4.3481	-4.3184
21	H	0.9738	0.6758	-4.1579
22	H	0.9312	0.5186	-2.3814
23	H	2.4576	0.9144	-3.1965
24	H	3.9140	-2.1942	0.0995
25	H	5.2829	-0.0636	0.1530
26	H	1.5298	4.0820	-1.8973
27	H	4.0926	2.1417	0.0725
28	H	-1.7738	1.2127	0.2306
29	H	-0.5540	3.3417	0.3104
30	H	1.9418	3.3811	0.2634
31	C	-0.4567	2.7411	-3.1125
32	H	-0.9091	2.2702	-3.9983
33	H	-0.7394	3.8048	-3.1126
34	H	-0.9082	2.2820	-2.2133

Table 10. Cartesian coordinates of the transition state involved in the reaction of the TMAI with C-7 carbon atom in 8-nitroquinoline (**1e**)

NO.	ATOM	X	Y	Z
1	C	0.0000	0.0000	0.0000
2	C	1.4208	0.0000	0.0000
3	C	2.1277	1.2246	0.0000
4	C	1.3974	2.4483	-0.0659
5	C	0.0392	2.4419	-0.0690
6	C	-0.7119	1.2142	0.0529
7	N	-0.7617	-1.2727	-0.1201
8	C	3.5433	1.2000	-0.0048
9	N	-1.4778	1.3558	1.8134
10	C	4.1999	-0.0036	-0.0227
11	C	3.4426	-1.2015	-0.0522
12	N	2.1154	-1.2043	-0.0432
13	O	-1.4116	-1.4801	-1.1267
14	O	-0.7707	-2.0702	0.7988
15	N	-0.8216	1.2640	3.1001
16	C	-0.1408	-0.0825	3.2433
17	C	-1.8299	1.3967	4.2383
18	H	-1.3469	1.2798	5.2207
19	H	-2.6142	0.6274	4.1562
20	H	-2.3291	2.3782	4.2273
21	H	0.3432	-0.1840	4.2263
22	H	0.6276	-0.2228	2.4624
23	H	-0.8612	-0.9101	3.1257
24	H	3.9222	-2.1868	-0.0879
25	H	5.2924	-0.0565	-0.0268
26	H	-2.0712	2.1588	1.8374
27	H	4.0955	2.1463	-0.0025
28	H	-1.7616	1.2281	-0.3036
29	H	-0.5190	3.3781	-0.1798
30	H	1.9586	3.3862	-0.1523
31	C	0.2279	2.3541	3.2857
32	H	0.7910	2.2246	4.2221
33	H	-0.2321	3.3539	3.3041
34	H	0.9489	2.3423	2.4475