Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Site activation effects promoted by intramolecular Hydrogen Bond interactions in S_NAr reactions.

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Table of contents.

Table S1. Experimental conditions and k_{obs} values for the reactions of benzoic hydrazide with 2-chloro-5-nitropyrimidine in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

pH= 2.7 F_N=0.333		pH= 3.0 F_N=0.500		pH= 3.3 F_N=0.667	
$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$
4,47	1,49	3,54	0,14	18,3	0,73
11,2	3,73	8,86	0,32	25,1	0,90
17,9	5,97	14,2	0,53	32,0	1,60
24,6	8,21	19,5	0,75	38,9	1,86
31,3	10,4	24,8	0,90	45,7	2,18
37,9	12,7	30,1	1,20		
44,7	14,9	35,4	1,41		

Table S2. Experimental conditions and k_{obs} values for the reactions of *p*-toluic hydrazide with 2-chloro-5-nitropyrimidine in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

pH= 3.1 F_N=0.334		pH= 3.5 F_N=0.557		pH= 3.7 F_N=0.666	
$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$
2,67	0,16	2,76	0,18	2,89	0,20
6,68	0,31	6,89	0,45	7,23	0,45
10,7	0,47	11,0	0,75	11,6	0,87
14,7	0,70	15,2	1,00	15,9	1,16
18,7	0,90	19,3	1,09	20,2	1,57
22,7		23,4	1,55	24,6	1,90
26,7	1,38	27,6	1,89	28,9	2,27

Table S3. Experimental conditions and k_{obs} values for the reactions of 4-chlorobenzoic hydrazide with 2-chloro-5-nitropyrimidine in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

pH= 2.5 F_N=0.334		pH= 2.8 F_N=0.500		pH=3.1 F_N=0.666	
$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$
1,58	0,02	1,67	0,04	1,63	0,06
3,94	0,06	4,19	0,10	4,09	0,15
6,31	0,08	6,70	0,17	6,54	0,24
8,68	0,13	9,21	0,22	8,99	0,34
11,0	0,18	11,7	0,29	11,4	0,44
13,4	0,22	14,2	0,35	13,9	0,47
15,8	0,26	16,7	0,43	16,3	0,59

Table S4. Experimental conditions and k_{obs} values for the reactions of 4-methoxy-benzhydrazide with 2-chloro-5-nitropyrimidine in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

pH= 3,2 F_N=0.355		pH= 3,50 F_N=0.523		pH= 3,80 F_N=0.686	
$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$
3,32	0,17	3,48	0,26	3,29	0,29
8,31	0,39	8,70	0,65	8,21	0,68
13,3	0,65	13,9	1,11	13,1	1,10
18,3	0,86	19,1	1,41	18,1	1,50
23,3	1,14	24,4	1,76	23,0	1,87
28,3	1,48	29,6	2,17	27,9	2,38
33,2	1,61	34,8	2,49	32,9	2,81

Table S5. Experimental conditions and k_{obs} values for the reactions of 4-(trifluoromethyl)benzhydrazide with 2-chloro-5-nitropyrimidine in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

pH= 2.4 F_N=0.334		pH= 2.7 F_N=0.500		pH= 3.0 F_N=0.666	
$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$	$10^3[N]_{tot}$/M	$10^3k_{obs}/s^{-1}$
1,11	0,03	0,99	0,03	1,10	0,04
2,77	0,06	2,48	0,08	2,75	0,05
4,43	0,10	3,97	0,13	4,40	0,14
6,09	0,15	5,46	0,20	6,05	0,19
7,75	0,19	6,95	0,23	7,70	0,30
9,41	0,23	8,44	0,29	9,35	0,32
11,1	0,24	9,93	0,32	1,10	0,41

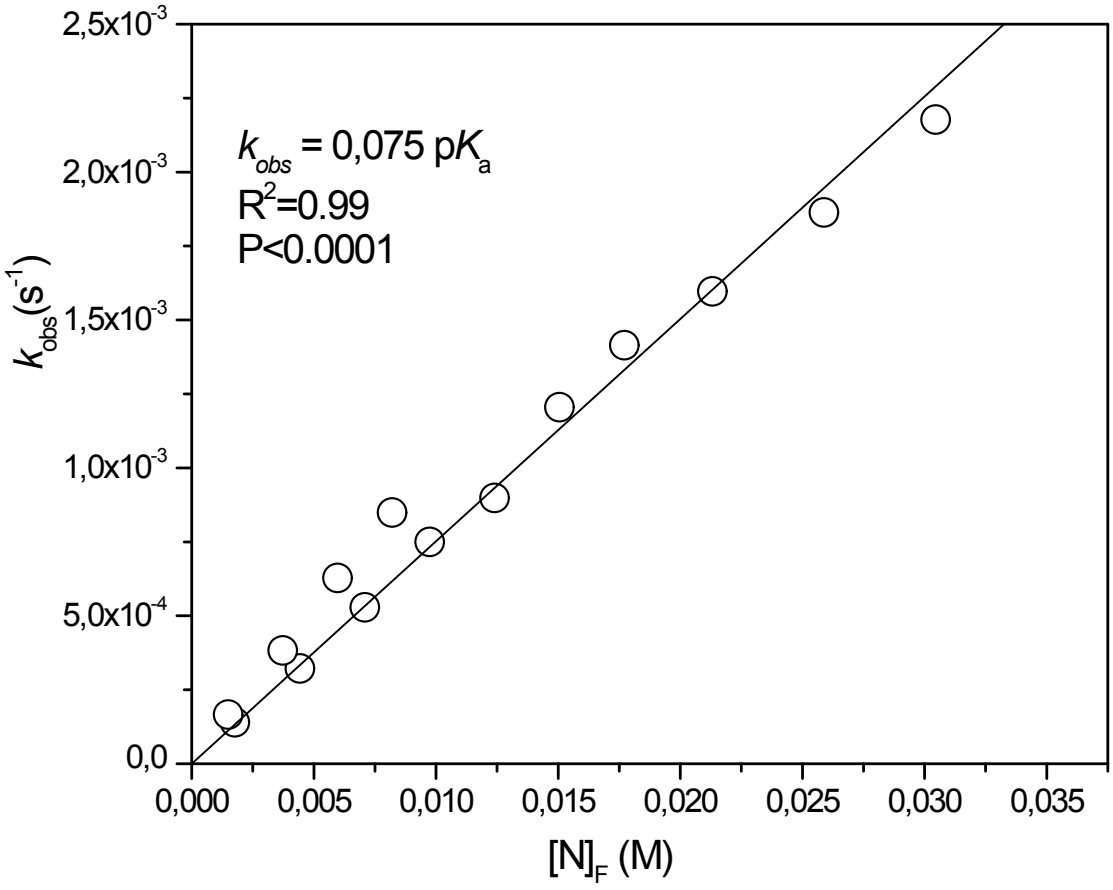


Figure S1. k_{obs} *vs.* free concentration of benzoic hydrazide in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

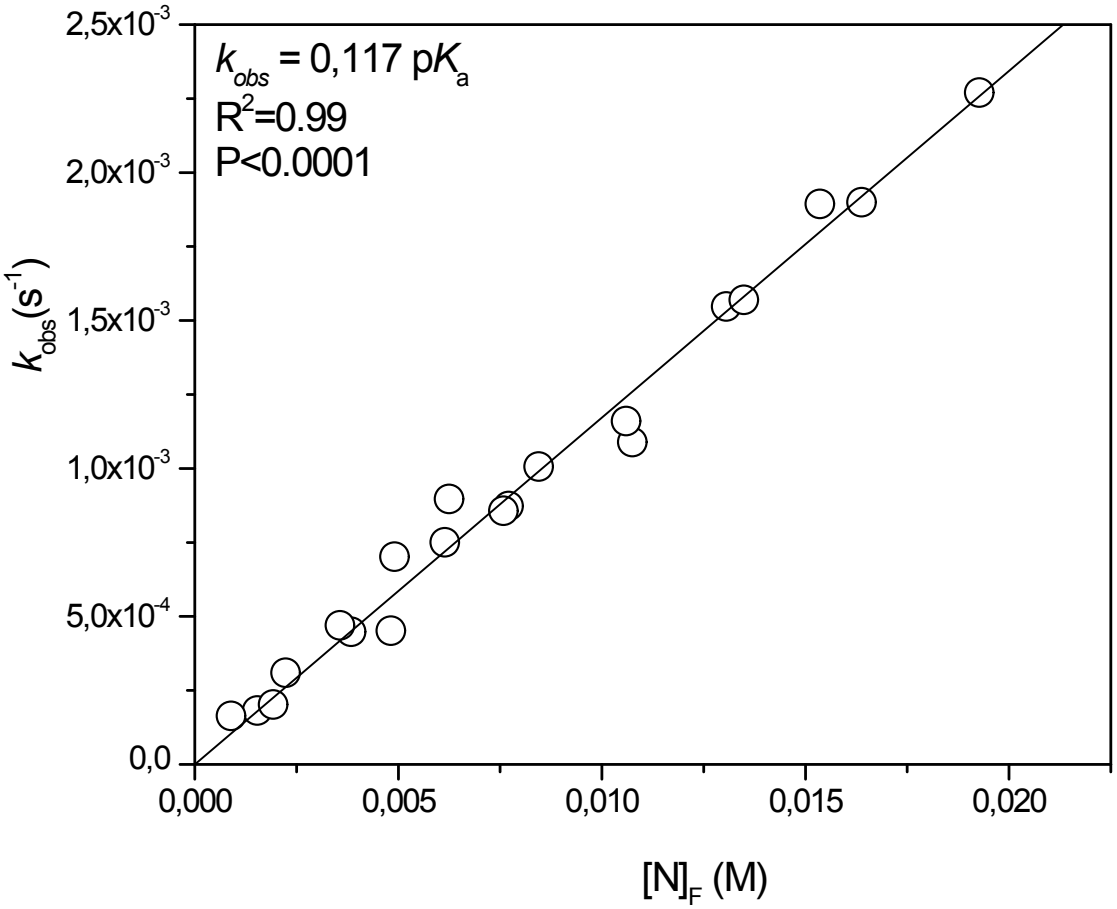


Figure S2. k_{obs} *vs.* free concentration of *p*-toluic hydrazide in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

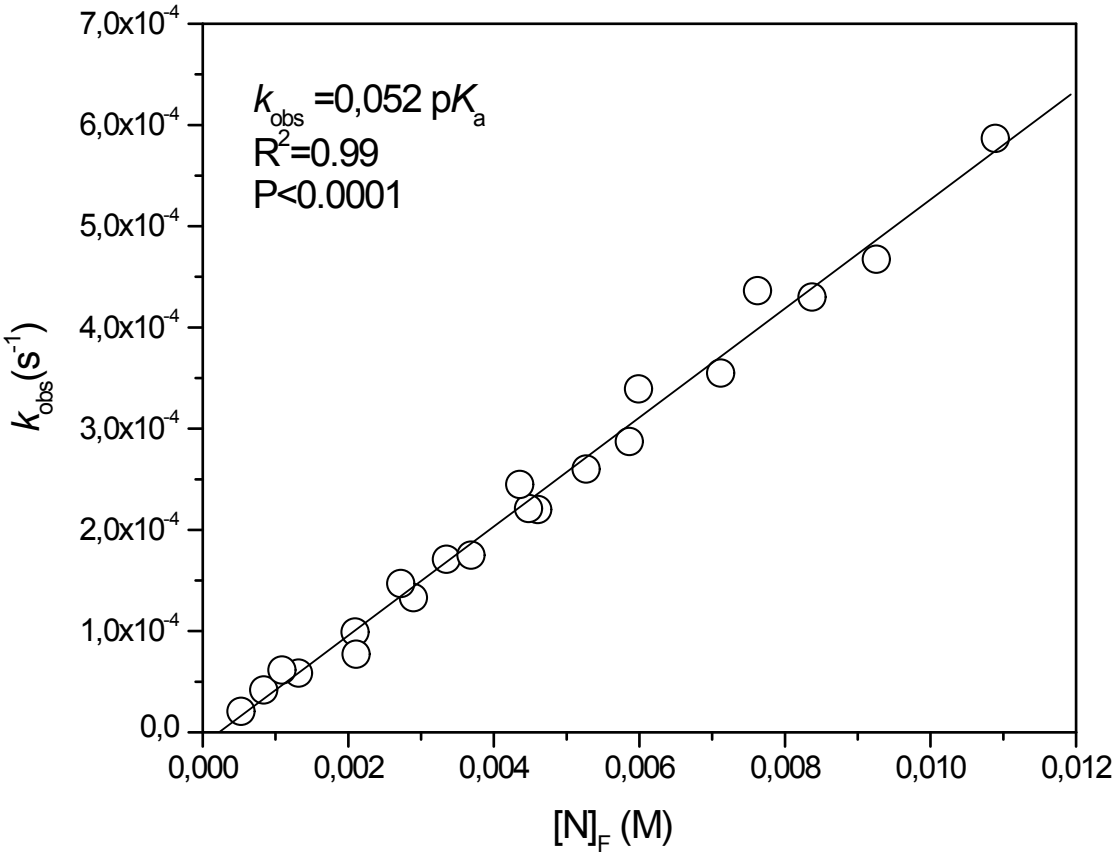


Figure S3. k_{obs} *vs.* free concentration of 4-chlorobenzoic hydrazide in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

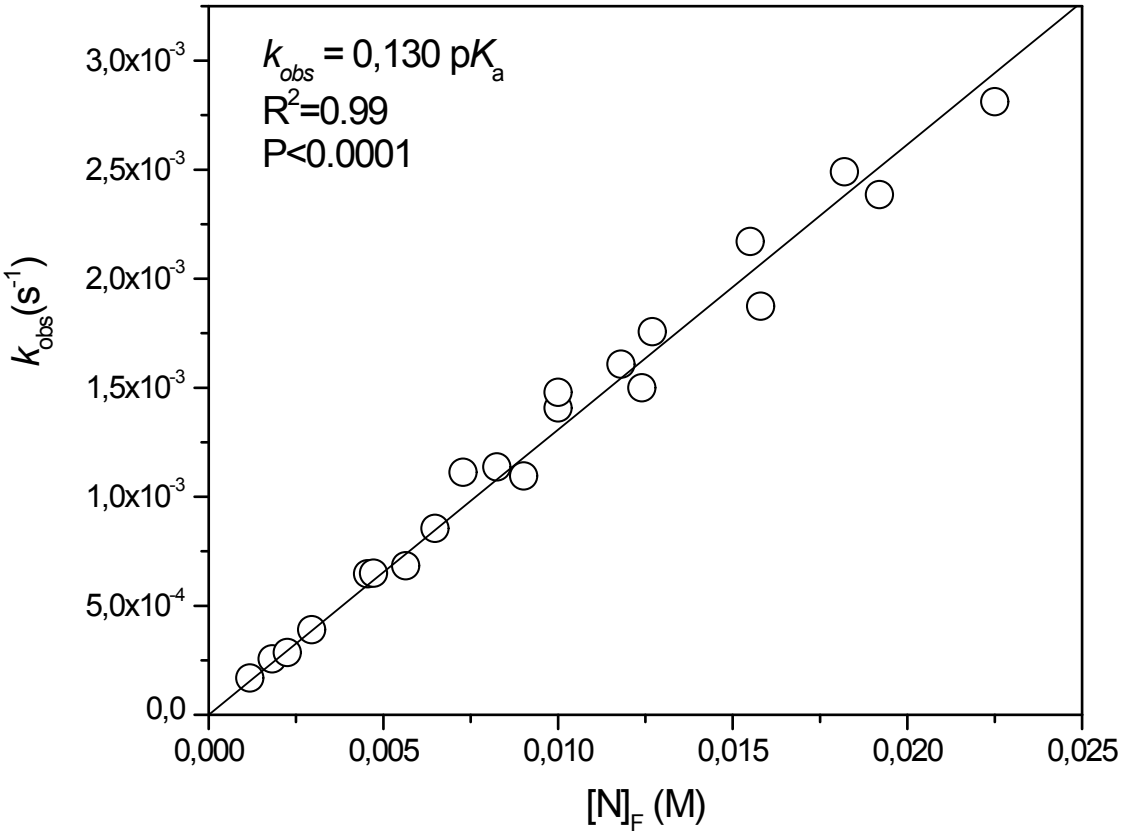


Figure S4. k_{obs} *vs.* free concentration of 4-methoxy-benzhydrazide in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

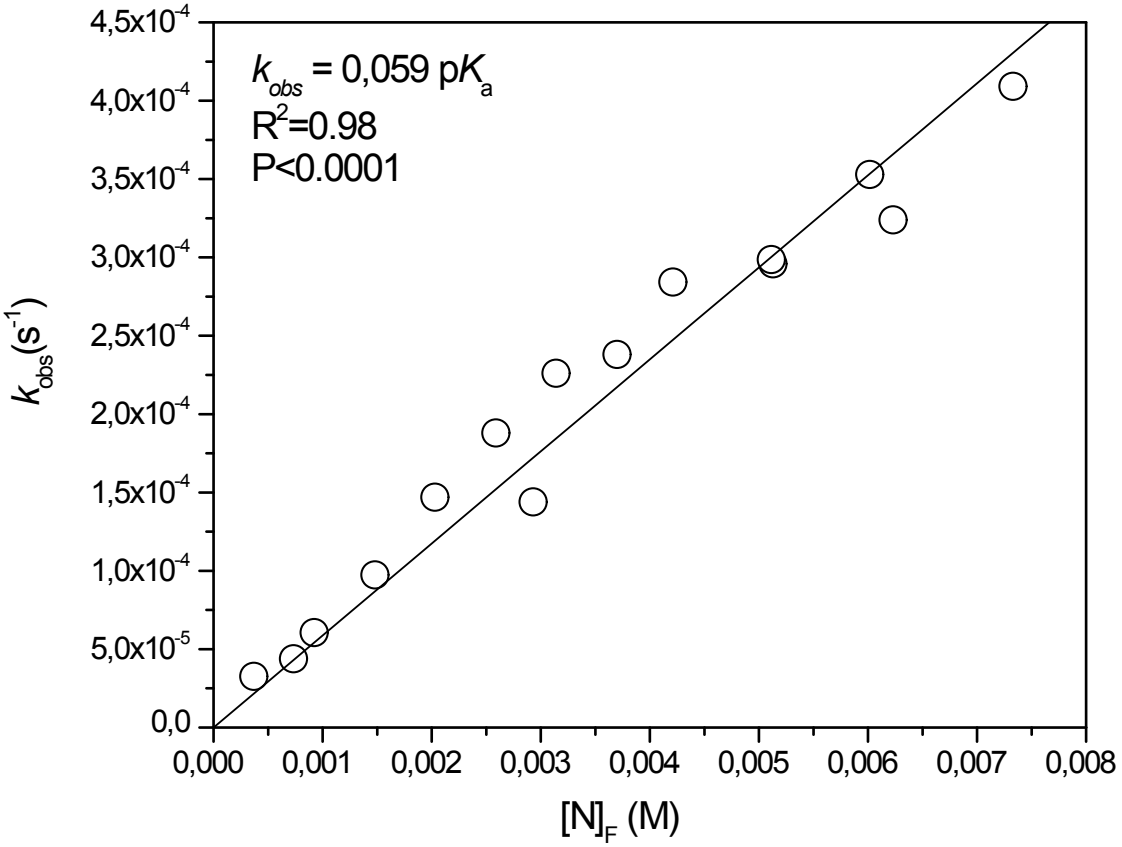


Figure S5. k_{obs} *vs.* free concentration of 4-(trifluoromethyl)benzhydrazide in water, at 25.0 ºC, ionic strength 0.2 M (KCl).

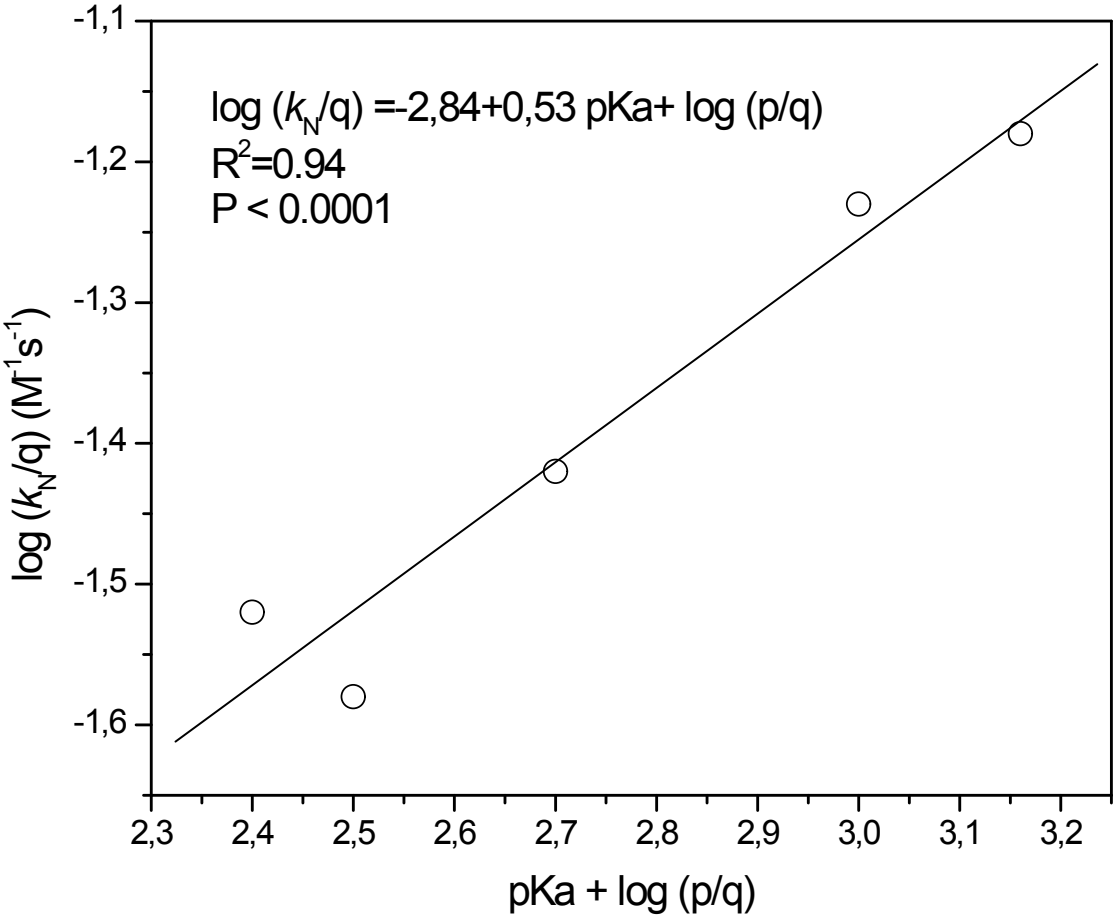


Figure S6. Brønsted-type plot (statistically corrected) for the reactions of benzohydrazides drivatives with 2-chloro-5-nitropyrimidine. in aqueous solution, at 25.0 °C and an ionic strength of 0.2 M.

Cartesian coordinates, total energies and number of imaginary frequencies (NIMAG).

Transition State (**TS-1**) for the reaction between benzohydrazide towards 2-chloro-5-nitropyrimidine calculated at the M05-2X/6–31G(d,p) level of theory in gas phase.

C	3.43374600	-0.98391400	0.03866700
C	1.20848900	-0.75140700	0.44457300
C	2.38924000	1.16576200	0.06529900
C	3.54906100	0.40656400	-0.07709000
H	4.30991800	-1.60944700	-0.08698200
N	2.29159000	-1.57471500	0.29993800
N	1.22307200	0.61778500	0.33593100
Cl	0.10909000	-1.28085300	1.78259800
N	4.80988900	1.02850900	-0.34353300
O	4.83363500	2.24576700	-0.43046400
O	5.78195300	0.30312000	-0.47458000
H	2.43224700	2.24358800	-0.03962300
N	0.13234500	-1.24610600	-0.92228600
H	0.70150800	-1.23360400	-1.76694500
N	-0.94257900	-0.36496100	-1.02060300
H	-0.68503700	0.54031100	-0.63557100
H	-0.24752700	-2.18799500	-0.77165000
C	-2.17867300	-0.92383400	-0.73577300
O	-2.34507200	-2.12514500	-0.84557000
C	-3.24550100	0.03870000	-0.36231400
C	-4.55911300	-0.30405600	-0.68355900
C	-2.97135800	1.22333000	0.32471000
C	-5.59658100	0.55588400	-0.34968300
H	-4.74254300	-1.24229900	-1.19053200
C	-4.01607800	2.07427900	0.66654000
H	-1.96277400	1.46694800	0.64031200
C	-5.32404500	1.74607600	0.32121700
H	-6.61589400	0.29842900	-0.60654200
H	-3.80992000	2.98684000	1.21041400
H	-6.13397400	2.41390000	0.58622400

Energy -1384.54927145 atomic units NIMAG = 1 , ν_I (cm^{-1}) = 240i

Transition State (**TS-2**) for the reaction between benzohydrazide towards 2-chloro-5-nitropyrimidine calculated at the M05-2X/6–31G(d,p) level of theory in gas phase.

C	0.96974800	0.00020900	-0.64112600
N	1.50069900	-1.18807700	-0.92248000
C	2.77655000	-1.29134000	-0.59160900
C	3.47269600	-0.18390200	-0.10676000
C	2.85943000	1.06353500	-0.14978700
N	1.58025900	1.16663000	-0.48113600
H	3.27736100	-2.23953400	-0.73629100
H	3.41931600	1.96661100	0.05306400
N	4.87015600	-0.29902700	0.25948000
O	5.44165600	0.71977800	0.59517900
O	5.36979700	-1.40559400	0.20151700
Cl	-0.05414000	-0.41777500	1.52926300
N	-0.43870300	0.08571400	-1.14857600
H	-0.94160400	-0.55443100	-0.49861700
H	-0.45460000	-0.27437800	-2.10598100
N	-1.01117000	1.37952700	-1.08456900
H	-0.26436000	2.04928800	-0.89805400
C	-2.07370900	1.55390500	-0.15223900
O	-2.16195000	2.60149700	0.43207800
C	-3.06665600	0.44863000	-0.07100800
C	-3.63660400	0.17739800	1.17292000
C	-3.46195200	-0.26439400	-1.20492000
C	-4.58961600	-0.82486400	1.28299700
H	-3.30084900	0.74066200	2.03320600
C	-4.42746700	-1.25925800	-1.08980400
H	-3.05143200	-0.01342800	-2.17730600
C	-4.98367800	-1.54181700	0.15418000
H	-5.02265200	-1.05257100	2.24805400
H	-4.74921400	-1.80543000	-1.96694000
H	-5.72875400	-2.32203400	0.24510700

Energy -1384.54433336 atomic units NIMAG = 1 , ν_I (cm^{-1}) = 225i

Reactive complex for the reaction between benzohydrazide towards 2-chloro-5-nitropyrimidine calculated at the M05-2X/6–31G(d,p) level of theory in gas phase.

C	0.02723400	-0.19917500	-0.11057900
C	-0.04182600	0.05862700	2.12056900
C	2.01989100	0.01270400	1.19348700
C	1.41172500	-0.14955400	-0.04216300
H	-0.47928500	-0.32493500	-1.05894900
N	-0.71335500	-0.09297800	0.98865300
N	1.27317200	0.11715700	2.29362900
Cl	-0.99440000	0.19989500	3.55336600
N	2.21464000	-0.26761700	-1.25260300
O	3.41962700	-0.22680500	-1.12146600
O	1.61378800	-0.39854600	-2.29987400
H	3.09681700	0.06525000	1.32156800
N	4.54932700	0.34629000	3.18760700
H	5.19654300	-0.42591100	3.31017100
N	3.61874600	0.28304100	4.23366200
H	2.65559500	0.33234900	3.93785100
H	5.10745700	1.18492200	3.33043100
C	3.99948800	0.64280000	5.49030700
O	5.15806800	0.93964900	5.74700300
C	2.91437700	0.65225300	6.52103700
C	3.16826800	1.34276300	7.70540400
C	1.69464500	-0.00355400	6.34433000
C	2.20020500	1.39671000	8.70003100
H	4.13072400	1.82367700	7.82076600
C	0.72798400	0.05119800	7.34218700
H	1.49968200	-0.57527400	5.44534200
C	0.97811200	0.75359600	8.51780700
H	2.39739100	1.93693000	9.61724500
H	-0.21600700	-0.46101500	7.20440700
H	0.22394800	0.79434100	9.29396400

Energy -1384.57800550 atomic units NIMAG = 0

Meisenheimer complex for the reaction between benzohydrazide towards 2-chloro-5-nitropyrimidine calculated at the M05-2X/6–31G(d,p) level of theory in gas phase.

C	-0.00078600	0.00301100	0.00046400
C	0.00000100	-0.00050100	1.39608800
C	1.20331000	-0.00306100	2.10525400
C	2.40663900	0.01103400	1.41128600
C	2.40675100	0.02856700	0.01866900
C	1.20521000	0.02253200	-0.68618300
H	-0.94970800	-0.00228900	-0.51897100
H	1.20943000	-0.04672200	3.18739800
H	3.34208400	0.00288100	1.95498300
H	3.34666900	0.04303000	-0.51835600
H	1.20999400	0.03442900	-1.76822100
C	-1.31892100	-0.00435900	2.06590500
O	-2.36821000	-0.30119200	1.52752200
N	-1.31112000	0.32661400	3.42516300
H	-0.68216500	1.04961600	3.77424100
N	-2.60250400	0.57255000	3.92007300
H	-2.82809100	-0.06582200	4.68626100
C	-2.78345000	1.98317800	4.47250400
C	-4.17681500	3.00515300	5.90010400
C	-1.80818200	3.32609700	5.98717100
C	-3.08838900	3.79545500	6.29951100
H	-5.15080000	3.15960900	6.34799800
H	-0.94203800	3.73093700	6.49580000
H	-3.26012100	0.41618100	3.13407500
Cl	-2.82866100	2.97396300	2.73410900
N	-4.02992200	2.02145700	5.04449600
N	-1.63430100	2.34240700	5.13327400
N	-3.26306400	4.85734700	7.24369500
O	-2.26170400	5.42683600	7.64765300
O	-4.40250800	5.13227400	7.58263000

Energy -1384.55886311 atomic units NIMAG = 0

Product complex for the reaction between benzohydrazide towards 2-chloro-5-nitropyrimidine calculated at the M05-2X/6–31G(d,p) level of theory in gas phase.

C	0.02244200	-0.03542100	-0.01538600
N	-0.01870800	0.04338700	1.32643600
C	1.15270400	0.04774800	1.93416800
C	2.34099400	-0.03667700	1.21221900
C	2.26922200	-0.12029700	-0.17142700
N	1.10331400	-0.12088600	-0.80063600
H	1.17207200	0.11419300	3.01500100
H	3.17219000	-0.18693600	-0.76534900
N	3.61867400	-0.03950800	1.88852800
O	4.61668100	-0.12800800	1.19876900
O	3.60783000	0.04331000	3.10248300
Cl	1.30227100	3.37435900	0.37487600
N	-1.19362300	-0.01883500	-0.62530400
H	0.68760200	3.64982000	-0.72004900
H	-2.00560400	-0.04674000	-0.03183200
N	-1.35331800	-0.26847300	-1.96492800
H	-1.11212000	-1.20978600	-2.25453900
C	-0.89475900	0.65027100	-2.90951000
O	-0.52918100	0.25526000	-3.99458100
C	-0.94162000	2.10419600	-2.56620700
C	-0.00235000	2.92196900	-3.19534200
C	-1.91962700	2.66699200	-1.74492000
C	-0.02034600	4.29633600	-2.97869700
H	0.72696900	2.46357600	-3.85013900
C	-1.94676800	4.04291100	-1.54231500
H	-2.66974500	2.03905000	-1.28393600
C	-0.99471500	4.85731800	-2.15213800
H	0.71612900	4.92904100	-3.45714600
H	-2.70855900	4.47976900	-0.90994800
H	-1.01183700	5.92685900	-1.98519900

Energy -1384.59640604 atomic units NIMAG = 0

Transition State (**TS-1a**) for the reaction between benzohydrazide towards 2-chloro-5-nitropyrimidine calculated at the M05-2X/6–31G(d,p) level of theory in water (PCM)

C	-0.04541200	0.00057400	0.00017500
C	-0.04450500	-0.16698000	2.26274200
C	1.99305900	-0.12252000	1.25219600
C	1.35428100	0.05619100	0.02327100
H	-0.57560500	0.05289200	-0.94320600
N	-0.75514100	-0.14459000	1.09431800
N	1.31784200	-0.27627100	2.37107800
Cl	-0.87331100	-1.12016300	3.54265500
N	2.10411200	0.19381300	-1.17957300
O	3.32506300	0.19107800	-1.10313500
O	1.49051900	0.31619600	-2.23085900
H	3.07428700	-0.16400400	1.30503000
N	-0.36590000	1.51061300	2.98963300
H	-0.12690300	2.21033600	2.28773600
N	0.39341000	1.68265800	4.14113500
H	1.30453900	1.24468400	4.07264600
H	-1.35080600	1.61570400	3.25261100
C	-0.29935400	1.73938200	5.32497800
O	-1.49776900	1.98682900	5.32790200
C	0.50507000	1.54061600	6.55858200
C	0.07114600	2.18787800	7.71690900
C	1.62975600	0.71254800	6.59271100
C	0.77857400	2.03194500	8.90186200
H	-0.81282400	2.81026000	7.67095000
C	2.32788500	0.55157600	7.78478500
H	1.94581700	0.16044700	5.71531100
C	1.90781800	1.21528400	8.93495500
H	0.45048200	2.54222200	9.79798200
H	3.19324400	-0.09718700	7.81651200
H	2.45626000	1.09016700	9.85977800

Energy -1384.57033305 atomic units NIMAG = 1, ν_I (cm^{-1}) = 257i

Transition State (**TS-1b**) for the reaction between benzohydrazide towards 2-chloro-5-nitropyrimidine calculated at the M05-2X/6–31G(d,p) level of theory in water (PCM)

C	-0.02754500	0.42551400	0.22942500
C	0.00945000	0.11870600	2.46845900
C	2.00449400	0.53508700	1.49028100
C	1.31864600	0.81686900	0.30283800
H	-0.54149900	0.42322400	-0.72446300
N	-0.68597300	0.01015600	1.28561700
N	1.38025000	0.13418600	2.57544500
Cl	-0.73015900	-0.85611100	3.77567900
N	2.01337400	1.27682500	-0.85167200
O	3.21297800	1.49688400	-0.75616500
O	1.37276800	1.44512400	-1.88091400
H	3.08445700	0.61210600	1.52321500
N	-0.48864500	1.77040100	3.04153600
H	-0.20507100	2.39851700	2.28795100
H	-1.50608400	1.80726100	3.11419600
C	1.86471100	3.44975700	3.08358900
C	1.03108800	4.34331900	2.40482100
C	3.19116700	3.28072600	2.68203100
C	1.51838200	5.03254100	1.29772100
H	0.02076300	4.52632700	2.75444500
C	3.66730100	3.96112000	1.56854800
H	3.82718400	2.60337900	3.23798900
C	2.82889400	4.83121500	0.87285800
H	0.87658800	5.72809900	0.77343200
H	4.68792400	3.81296800	1.24147000
O	2.08409900	2.49021200	5.25660900
N	0.09350500	2.19629600	4.24161700
C	1.40119400	2.66882000	4.26662400
H	3.20068000	5.35888500	0.00405100
H	-0.11517700	1.56294400	5.00543300

Energy -1384.56215085 atomic units NIMAG = 1, ν_I (cm^{-1}) = 231i

Transition State for the reaction between benzohydrazide towards 1-chloro-2,4-dinitrobenzene (**TS-2**) calculated at the M05-2X/6–31G(d,p) level of theory in water (PCM)

C	0.31550500	-0.85083800	0.32238000
C	-0.00736300	0.68313100	2.25458600
C	2.16060300	0.51328700	1.09698800
C	1.62050900	-0.43347000	0.19528600
H	-0.10543000	-1.58160000	-0.35195100
Cl	-0.47479300	0.50786600	3.97298000
N	2.43715400	-0.97690700	-0.84705900
O	3.59421900	-0.58729100	-0.93290500
O	1.94663100	-1.80294100	-1.60502900
H	3.19735700	0.80283300	1.00503500
N	-0.91301500	2.25964100	1.86340300
H	-0.18900700	2.98024900	1.90521700
N	-1.99806700	2.65855100	2.63354800
H	-2.79433200	2.04077300	2.56468500
H	-1.18271700	2.14979400	0.88322100
C	-2.18136600	3.92103600	3.14727900
O	-3.29117400	4.26928400	3.50897700
C	-0.97700300	4.79495300	3.26970600
C	0.20992200	4.32829700	3.84255800
C	-1.09320700	6.12802600	2.87339500
C	1.28880000	5.19479700	3.99380900
H	0.27594400	3.30869200	4.20655200
C	-0.00812700	6.98416800	3.01472900
H	-2.02838800	6.47747800	2.45522900
C	1.18172000	6.51730000	3.57195000
H	2.20475400	4.83896900	4.44685100
H	-0.09001800	8.01493200	2.69574200
H	2.02347200	7.18835500	3.68456600
C	1.39354500	1.02747800	2.09411100
C	-0.48068800	-0.31629500	1.32511700
N	-1.84802900	-0.72135600	1.36282300
O	-2.18807900	-1.73290200	0.77155000
O	-2.63893800	-0.00531400	1.97577000
H	1.82215300	1.71059400	2.81560800

Energy -1556.94791598 atomic units NIMAG = 1, ν_I (cm^{-1}) = 211i

Transition State for the reaction between benzoic hydrazide towards 2-chloro-5-nitropyrimidine (**TS-1wHB**) calculated at the M05-2X/6–31G(d,p) level of theory in water (PCM).

C	-0.10154400	-0.08890700	0.16387500
C	0.03811600	-0.19019900	2.41913300
C	2.00692300	-0.07121500	1.30109600
C	1.28854100	0.07935400	0.11387700
H	-0.68126600	-0.10369100	-0.75103200
N	-0.73707100	-0.26926500	1.29859600
N	1.40382700	-0.25713800	2.45730000
Cl	-0.69349100	-1.02410600	3.82234900
N	1.96162500	0.26037000	-1.13093900
O	3.18176300	0.33693500	-1.12107000
O	1.28366100	0.33986400	-2.14521600
H	3.09008000	-0.06753600	1.28886700
N	-0.28813800	1.58595500	3.02953700
H	-0.07894500	2.23075100	2.26910400
N	0.53417300	1.83699500	4.11849300
H	1.47169300	1.47951500	3.98738900
H	-1.29150300	1.65483700	3.27865500
C	0.00524800	1.95503500	5.36843800
O	-1.18133600	2.20657800	5.55682500
C	0.98283500	1.80513200	6.48160800
C	0.74941600	2.53387800	7.64904300
C	2.07297000	0.93492600	6.39971500
C	1.62374800	2.41767800	8.72212200
H	-0.11272500	3.18614100	7.69771000
C	2.93888200	0.81434600	7.48171800
H	2.23014100	0.32022700	5.52041200
C	2.71950500	1.55986500	8.63735800
H	1.45101300	2.99075800	9.62375000
H	3.77766600	0.13309700	7.42473600
H	3.39766900	1.46611500	9.47595700
H	-2.81403600	1.74988400	4.52449200
O	-3.08614700	1.50421500	3.62802500
H	-3.26199900	0.55816800	3.66945900

Energy -1460.99852893 atomic units NIMAG = 1, ν_I (cm^{-1}) = 252i

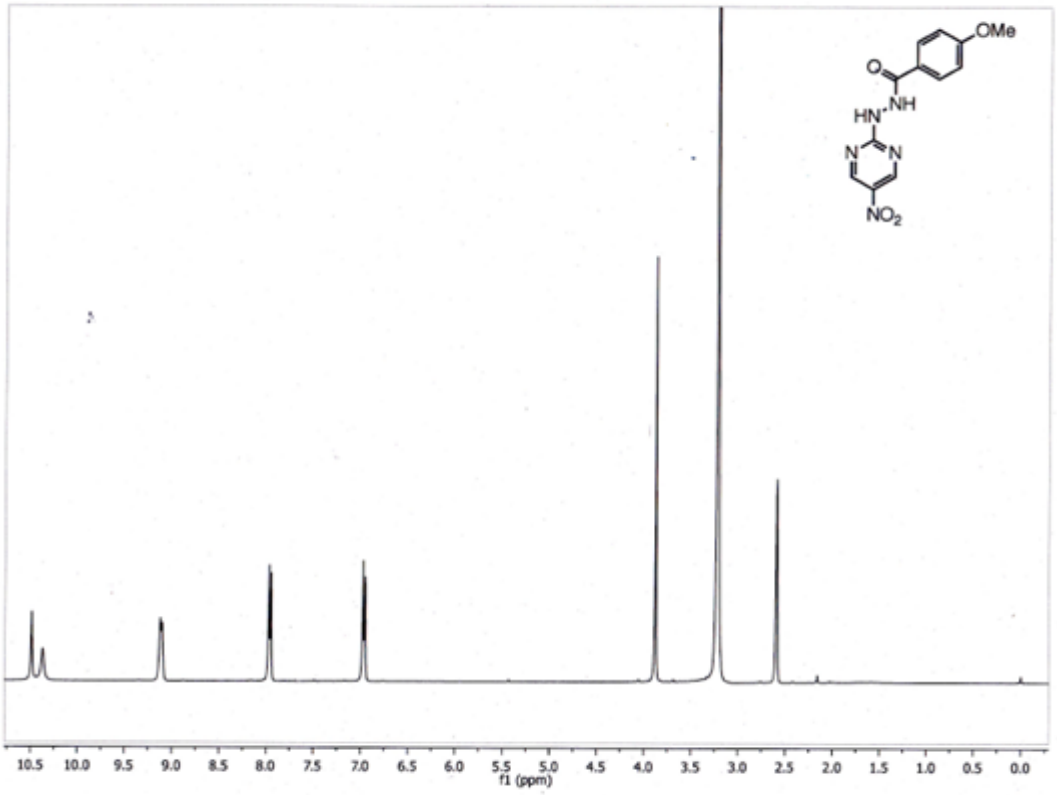
Transition State for the reaction between benzoic hydrazide towards 2-chloro-5-nitropyrimidine (**TS-1nHB**) calculated at the M05-2X/6–31G(d,p) level of theory in water (PCM)

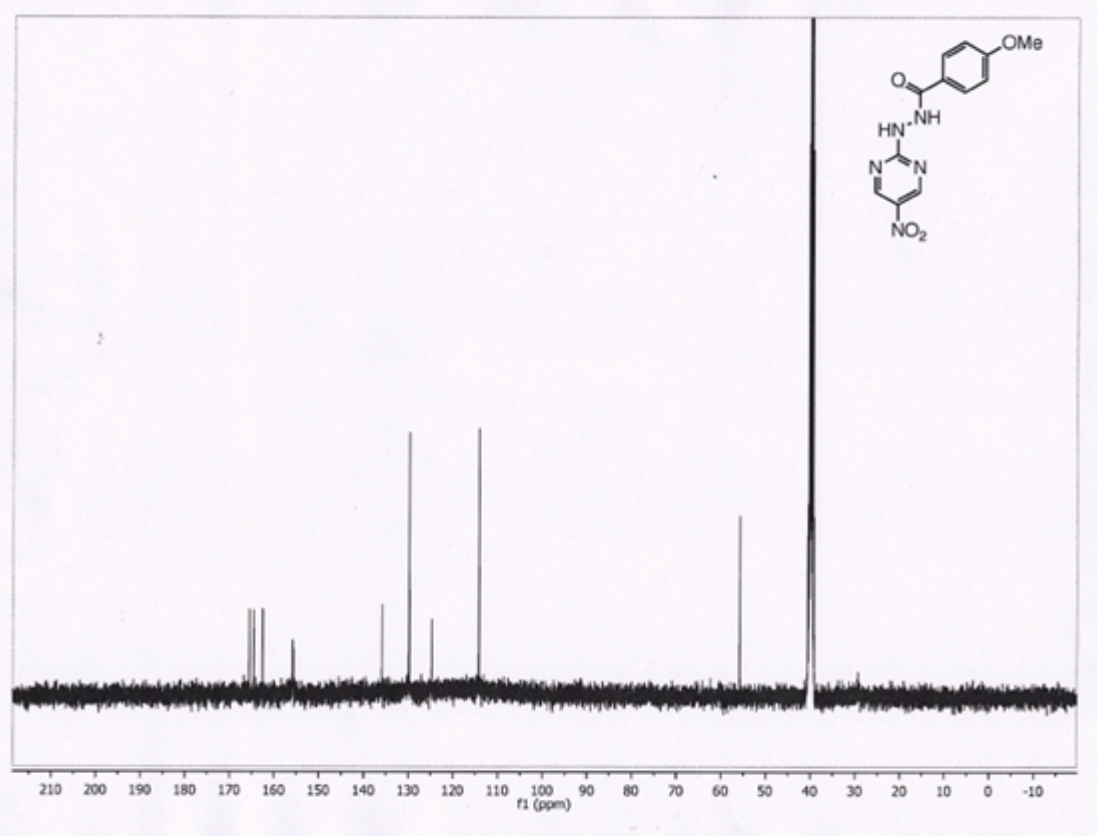
C	-0.19277900	0.10647700	0.22528100
C	0.02312300	-0.15209300	2.47059900
C	1.89221000	0.49198400	1.34052200
C	1.10219200	0.65191600	0.19780600
H	-0.76640500	0.02815100	-0.69076900
N	-0.72829200	-0.35773600	1.32658100
N	1.39497600	0.04240200	2.46975500
Cl	-0.44452800	-1.29423800	3.77692200
N	1.64958600	1.19576700	-0.99343600
O	2.80494900	1.60273900	-0.96677400
O	0.93412400	1.25620300	-1.98436600
H	2.95345600	0.70813700	1.30570300
N	-0.63818400	1.34211200	3.11847300
H	-0.81826700	1.92468000	2.29706300
H	-1.53443400	1.14566400	3.56670600
C	0.80306200	3.65284900	2.25092500
C	-0.47074500	4.19955200	2.05893000
C	1.79820000	3.82483300	1.28592400
C	-0.74986600	4.89296500	0.88566500
H	-1.22723500	4.11283700	2.83118500
C	1.50644600	4.50366500	0.10881200
H	2.78491700	3.41432300	1.45853300
C	0.23278500	5.03267400	-0.09206000
H	-1.73057400	5.32518000	0.73796600
H	2.26894200	4.61345200	-0.65084600
O	2.22143000	3.04478900	4.06559200
H	2.62985100	1.27779200	5.16385500
N	0.20387300	2.03006000	4.00252300
C	1.15861800	2.89673000	3.48436900
H	0.00743400	5.56151200	-1.00902600
H	0.60225300	1.40552100	4.71409200
H	2.18423800	0.04319100	4.39846800
O	2.18127100	0.42992500	5.28997600

Energy -1460.99381666 atomic units NIMAG = 1, ν_I (cm^{-1}) = 139i

4-methoxy-*N*-(5-nitropyrimidin-2-yl)benzohydrazide.

To a stirred solution of 4-methoxybenzhydrazide (91.4 mg, 0.55 mmol) in THF (15 mL) containing potassium carbonate (76 mg, 0.55 mmol) was added 2-chloro-5-nitropyrimidine (79.8 mg, 0.5 mmol) disolved in THF (5.0 mL). The reaction mixture was stirred for 24 hours at room temperature, filtered and concentratated in vacuo. Purification by flash chromatography (ethyl acetate/hexane 1:2) gave of 4-methoxy-*N*-(5-nitropyrimidin-2-yl)benzohydrazide (97 mg, 67%), mp 252-253 ºC. ^{1}H-NMR (400 MHz, DMSO-d_6) d : 3.87 (s, 3H), 6.96 (d, J = 8.7 Hz, 2H), 7.96 (d, J = 8.7 Hz, 2H), 9.10 (s, 1H), 9.12 (s, 1H), 10.4 (s, 1H), 10.5 (s, 1H); ^{13}C-NMR (100 MHz, DMSO-d_6) d : 55.4, 114.2 (2C), 124.7, 129.9 (2C), 135.7, 155.6, 155.8, 162.3, 164.6, 165.6; FT-IR (KBr) 3270, 3108, 1626, 1599, 1538, 1434, 1346 cm-1. Anal. Calcd for $C_{12}H_{11}N_5O_4$: C, 49.83; H, 3.83; N, 24.21. Found: C, 49.70; H, 3.68; N, 24.32.


OMe
O
NH
HN
N
N
NO2
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


OMe
O
NH
HN
N
N
NO2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)