Electronic Supplementary Information: Crawford, Ieva, McNab and Parsons

Structural studies of some push-pull *N*-arylbenzazoles†

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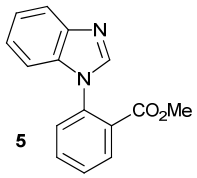
Supplementary Information

NMR spectra of 5.

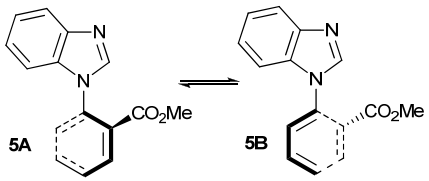


5

The ^{1}H and ^{13}C NMR spectra for compound **5** are shown in Figures S1 and S2 respectively. The proton spectrum shows broad signals between 7.1-7.4 ppm and 7.8-8.0 ppm which would not be expected from the C-H signals in product **5**. This was not observed in the carbazole or indole analogues **1** and **3**, respectively. This broadening was observed when the proton spectrum was recorded in [^{2}H]DMSO and [^{2}H]chloroform so the effect is not due to the NMR solvent.

This compound was therefore subjected to ^{1}H NMR spectroscopy at higher and lower temperatures. The higher temperature spectra are shown in Figures S3 a-c and show that the broadened signals sharpen as the temperature increases. The lower temperature NMR spectra of compound **5** are shown in Figures S3 d-e and also show a sharpening of the broadened signals as the temperature is decreased.

It is unusual for broadened peaks on a proton spectrum to sharpen at both lower and higher temperatures. This suggests that there may be slow exchange at room temperature between two identical sites (*e.g.* **5A** and **5B**) resulting in identical spectra under conditions of fast exchange and slow exchange, at increased and decreased temperatures, respectively.



5A **5B**

Similar line broadening is observed in the ^{13}C NMR spectrum of **5** (Figure S2) resulting in the apparent absence of 3 quaternaries and a C-H signal; the latter may be the broadened peak at around δ_C 143 ppm.

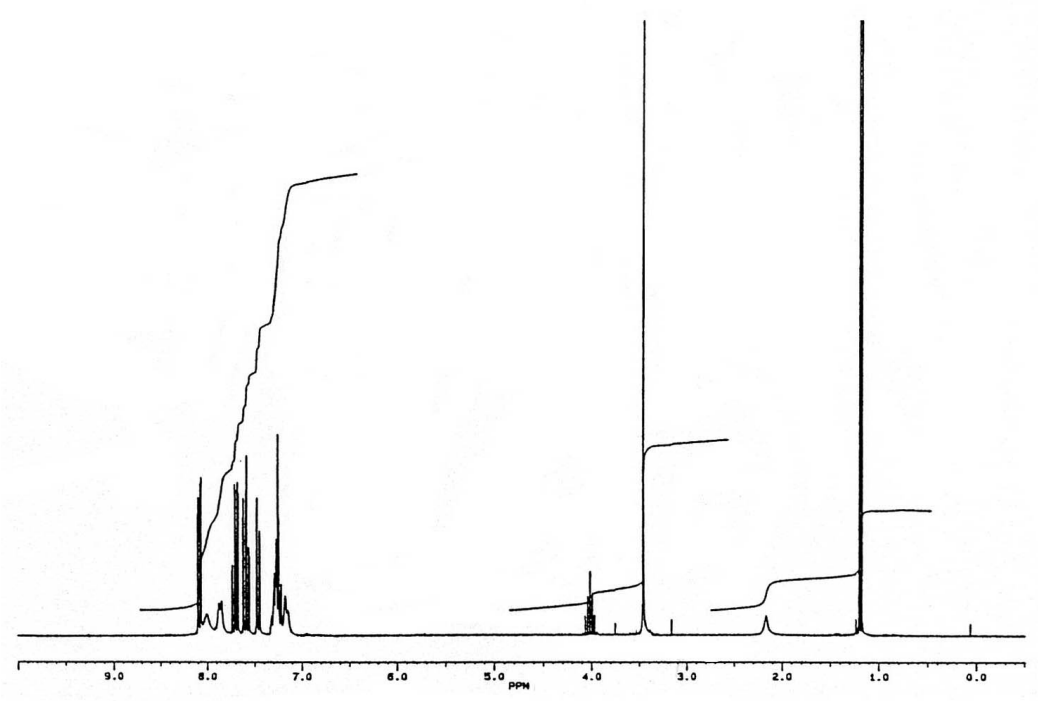


Figure S1. Room temperature ^{1}H NMR spectrum of compound **5**.

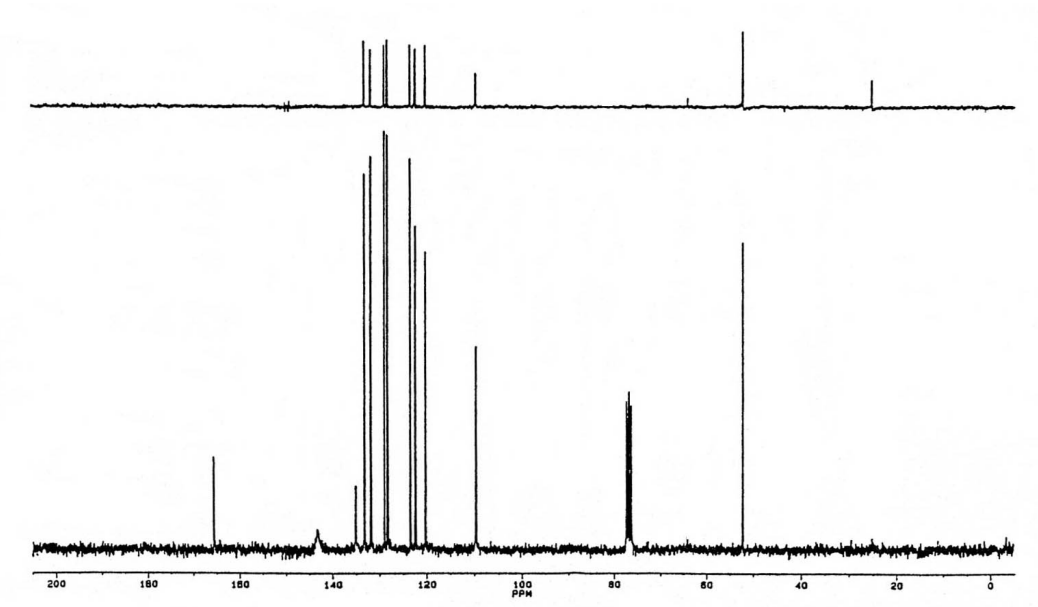


Figure S2. Room temperature ^{13}C NMR spectrum of **5**.

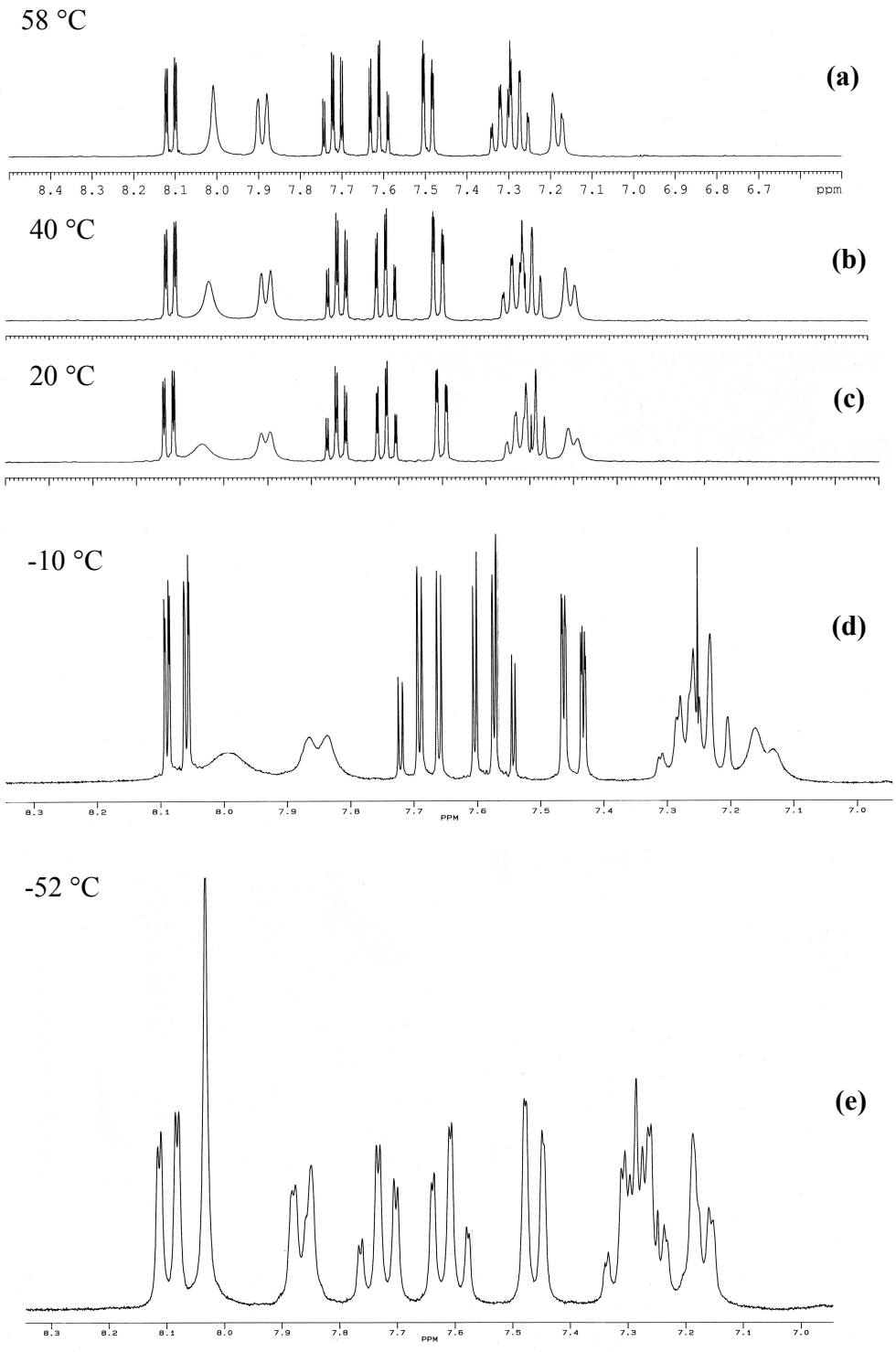


Figure S3. Variable Temperature ^{1}H NMR spectra of **5** (note different scales for the low temperature spectra).

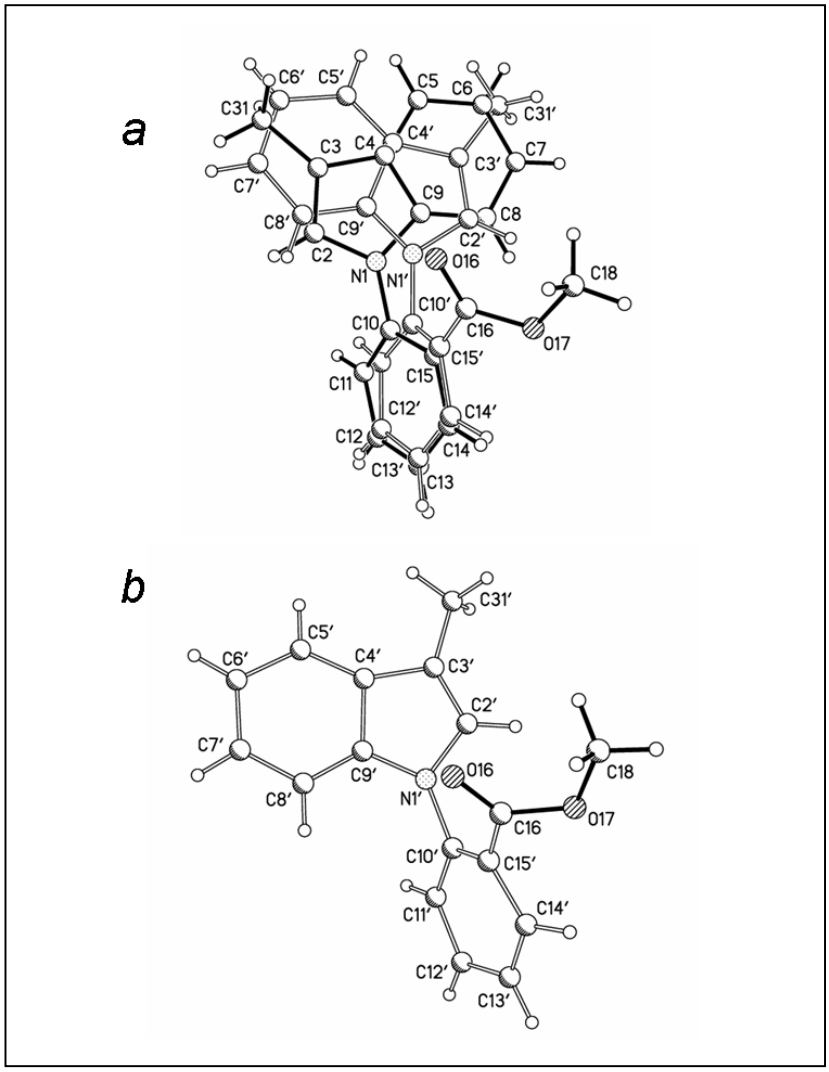


Figure S4. (a) A view of both conformers of **3** showing the crystallographic numbering scheme; (b) a view of the minor conformer of **3**. Equivalent bond distances and angles in the two components were restarined to be equal.

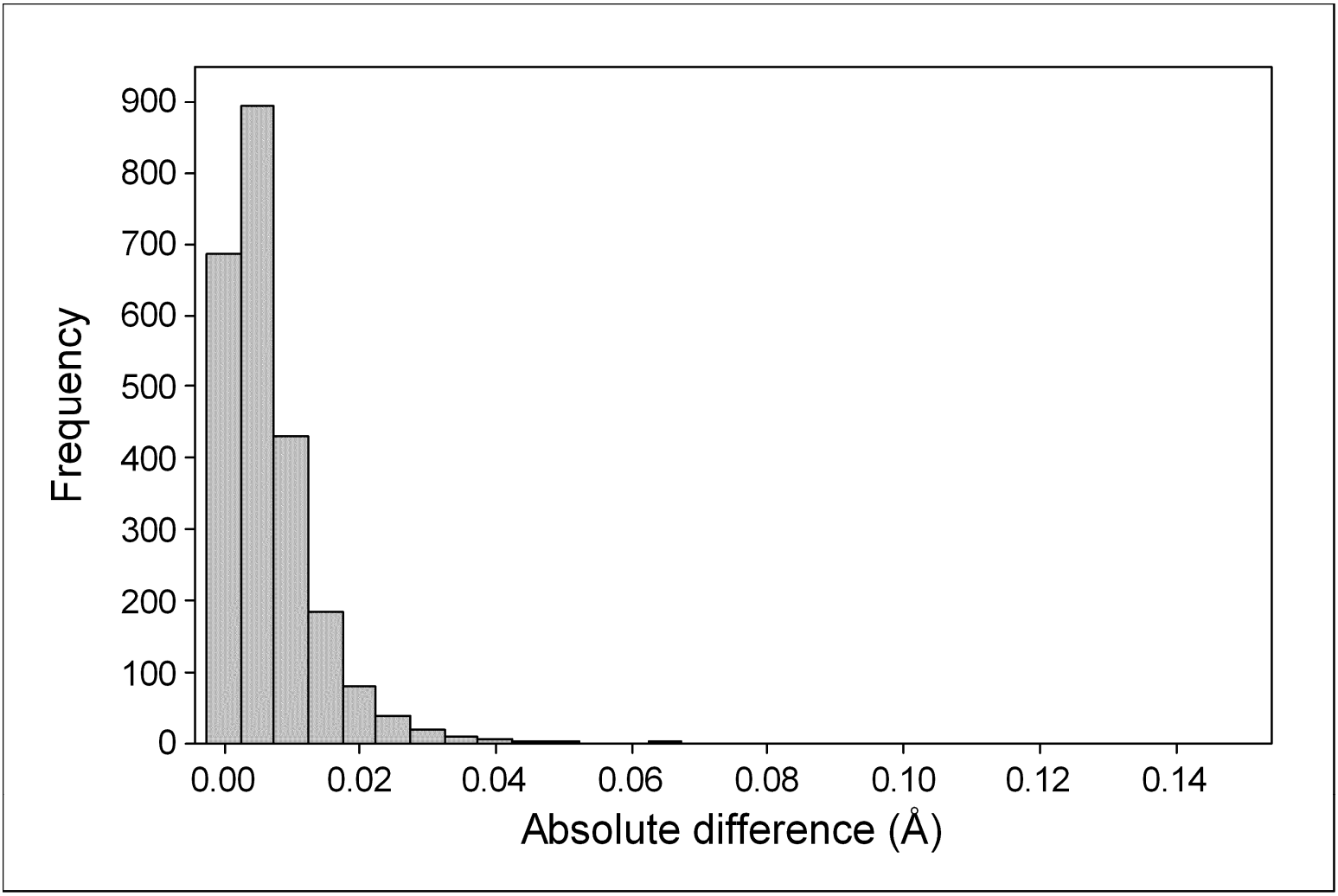


Figure S5. Histogram of the frequency of hits from the Cambridge Crystallographic database, for the difference in length between the two N-O bonds in nitro groups. The search was carried out using version 5.31 (November 2009), with the following parameters specified: R factor <5%, no errors, no disorder, cut-off temperature ≤200 K.

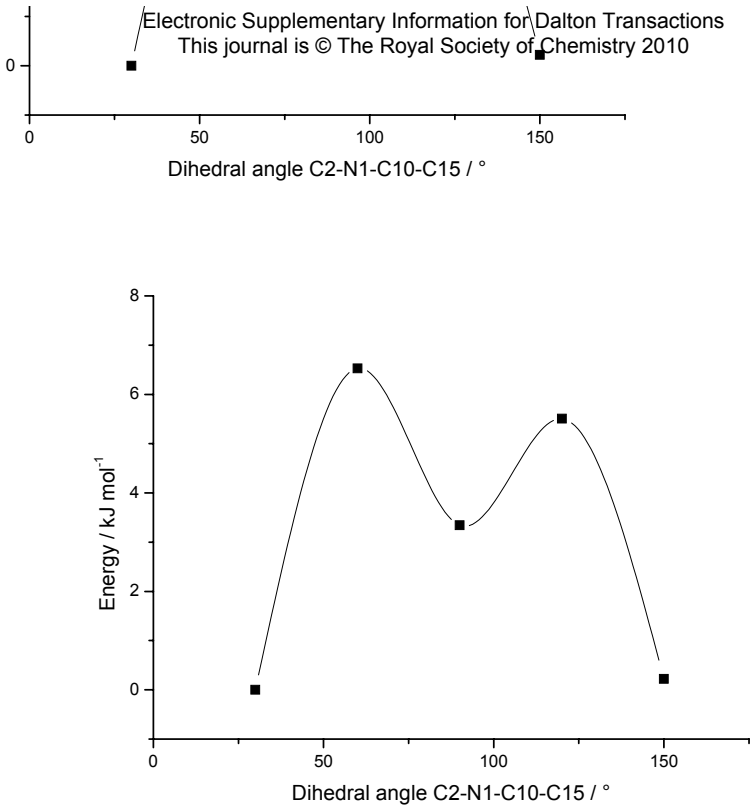


Figure S6. Plot of variation of calculated total energy *versus* dihedral angle C2-N1-C10-C15 for **3**.

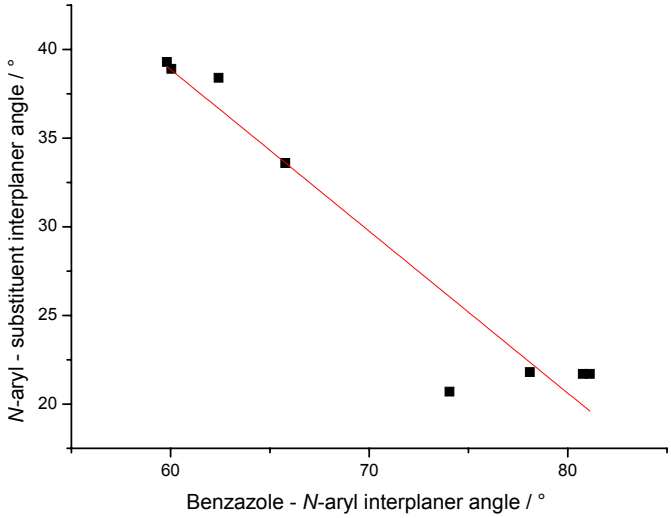


Figure S7. Plot of benzazole – *N*-aryl interplanar angle *versus* *N*-aryl – substituent interplanar angle for **1** (8 molecules) (X-ray data).

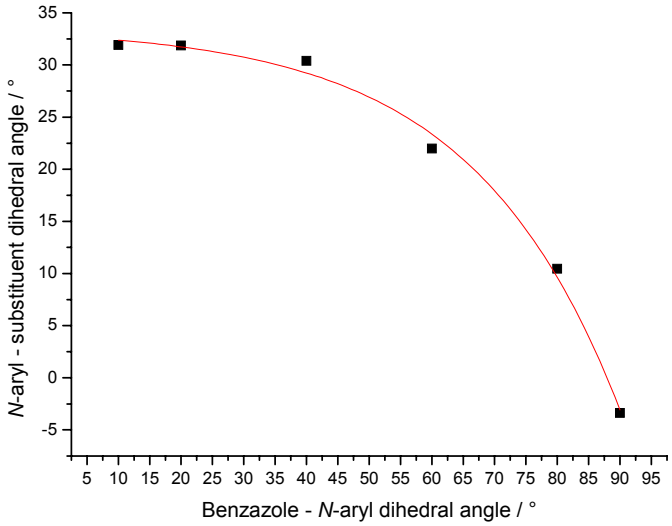


Figure S8. Plot of benzazole – *N*-aryl dihedral angle *versus* *N*-aryl – substituent dihedral angle for **1** (calculated data).

Table 1. Crystallographic experimental details

Experiments were carried out at 150 K with Mo *K*α radiation using a SMART APEX CCD area detector diffractometer.

	(**2**) (SEMTAG)	(**3**) (CARZOL)	(**4**) (PELDUG)	(**5**) (CARZUR)	(**6**) (PELFES)
Crystal data					
Chemical formula	$C_{18}H_{12}N_2O_2$	$C_{17}H_{15}NO_2$	$C_{14}H_{10}N_2O_2$	$C_{15}H_{12}N_2O_2$	$C_{14}H_{11}N_3O_2$
M_r	288.30	265.30	238.24	252.27	253.26
Crystal system, space group	Orthorhombic, *Iba*2	Monoclinic, $P2_1/c$	Orthorhombic, *Pbca*	Monoclinic, $P2_1/c$	Triclinic, $P\bar{1}$
a, *b*, *c* (Å)	14.333 (9), 25.751 (16), 7.859 (5)	7.3474 (6), 7.9170 (7), 23.9413 (19)	7.7628 (6), 7.7446 (6), 38.063 (3)	7.1962 (8), 7.8951 (9), 22.354 (3)	7.7474 (16), 8.2529 (18), 10.230 (2)
α, β, γ (°)	90, 90, 90	90, 92.593 (1), 90	90, 90, 90	90, 95.317 (2), 90	86.580 (3), 82.200 (3), 71.914 (3)
V (Å^3)	2901 (3)	1391.2 (2)	2288.3 (3)	1264.6 (2)	615.9 (2)
Z	8	4	8	4	2
μ (mm^{-1})	0.09	0.08	0.10	0.09	0.10
Crystal size (mm)	0.6 × 0.3 × 0.3	0.24 × 0.24 × 0.16	0.51 × 0.39 × 0.12	0.22 × 0.22 × 0.18	0.33 × 0.30 × 0.18
Data collection					
Absorption correction	*SADABS*	*SADABS*	*SADABS*	*SADABS*	*SADABS*
T_{min}, T_{max}	0.632, 1	0.928, 0.464	0.754, 0.928	0.667, 1.000	0.894, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10745, 2939, 2596	7632, 2830, 2166	11920, 2343, 1945	6900, 2570, 1942	4925, 2471, 2040
R_{int}	0.035	0.021	0.030	0.029	0.020
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.028, 0.061, 0.97	0.039, 0.1012, 0.96	0.042, 0.104, 1.04	0.036, 0.090, 0.94	0.052, 0.121, 1.11
No. of reflections	2939	2830	2343	2570	2471
No. of parameters	248	247	204	173	205
No. of restraints	1	43	0	0	0
H-atom treatment	H atoms treated by a mixture of independent and constrained	–	H atoms treated by a mixture of independent and constrained	–	H atoms treated by a mixture of independent and constrained

	refinement		refinement		refinement
$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.15, -0.12	0.23, -0.24	0.22, -0.16	0.18, -0.17	0.25, -0.23
Absolute structure	Flack H D (1983), Acta Cryst. A39, 876-881	–	–	–	–
Flack parameter	0.5 (10) [Not determined]	–	–	–	–

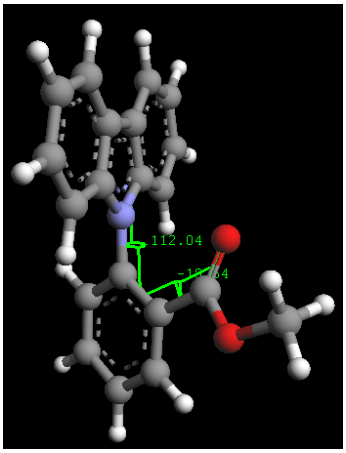
	(**7**) (PELDOA)
Crystal data	
Chemical formula	$C_{13}H_9N_3O_2$
M_r	239.23
Crystal system, space group	Monoclinic, $P2_1$
a, b, c (Å)	7.519 (5), 7.223 (5), 10.049 (7)
α, β, γ (°)	90, 103.631 (11), 90
V (Å^3)	530.4 (6)
Z	2
μ (mm^{-1})	0.11
Crystal size (mm)	0.45 × 0.36 × 0.15
Data collection	
Absorption correction	*SADABS*
T_{min}, T_{max}	0.345, 0.928
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1938, 1412, 1078
R_{int}	0.040
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.119, 0.93
No. of reflections	1412
No. of parameters	163
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement

$\Delta\rangle_{max}$, $\Delta\rangle_{min}$ (e Å^{-3})	0.28, -0.24
Absolute structure	Flack H D (1983), Acta Cryst. A39, 876-881
Flack parameter	-2 (3)

Calculated Data

This section contains the Cartesian coordinates and energies for the energy surfaces shown in this paper. All the structure and energies were calculated at B3LYP/6-31G level, using Gaussian 03;[1] energies are quoted both in Hartrees (Ha) and kJ mol^{-1}.

9-(2-Carbomethoxyphenyl)-9*H*-carbazole 1



Energy = -976.1352403 Ha = -2562857.715 kJ mol^{-1}

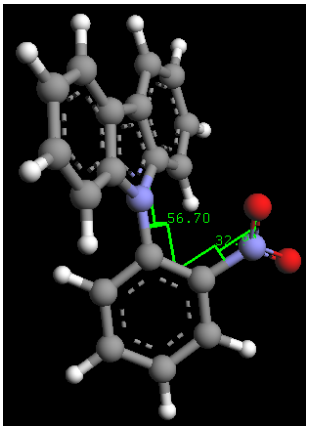
Torsion angle 1 = 112.04°

Torsion angle 2 = –18.64°

C	2.145547	1.035336	-0.356927
C	0.787091	0.909528	-0.758973
N	0.344218	-0.389037	-0.450256
C	1.400483	-1.090959	0.158951
C	2.535094	-0.235459	0.229092
C	-0.963319	-0.903732	-0.682196
C	-2.104746	-0.414722	-0.001060
C	-3.370438	-0.929713	-0.339943
C	-1.112768	-1.912356	-1.645670
C	-2.372326	-2.435409	-1.946317
C	-3.506800	-1.934069	-1.298427
C	-1.994642	0.571760	1.105885
O	-0.983257	0.830109	1.767217
C	2.820741	2.242024	-0.583203
C	0.104945	1.955632	-1.386545
C	3.722809	-0.714067	0.797628
C	3.763985	-2.021466	1.287321
C	2.627807	-2.851133	1.216276
C	1.431320	-2.398026	0.653521
C	2.143416	3.294941	-1.202019
C	0.799962	3.149180	-1.599812
O	-3.205960	1.186001	1.365106
C	-3.218698	2.145863	2.477144
H	-4.239229	-0.538920	0.173330
H	-0.228044	-2.263652	-2.164494
H	-2.467782	-3.215879	-2.693969
H	-4.490666	-2.323762	-1.536423
H	3.857624	2.357139	-0.282694

H	-0.927600	1.848882	-1.700537
H	4.598831	-0.075936	0.861055
H	4.677899	-2.402900	1.730875
H	2.679201	-3.861774	1.609050
H	0.557495	-3.038250	0.609417
H	2.655378	4.234791	-1.381107
H	0.293227	3.978274	-2.083766
H	-4.238914	2.523624	2.505041
H	-2.503571	2.948850	2.287395
H	-2.956427	1.644964	3.411668

9-(2-Nitrophenyl)-9*H*-carbazole 2



Energy = -952.7506593 Ha = -2501461.147 kJ mol^{-1}

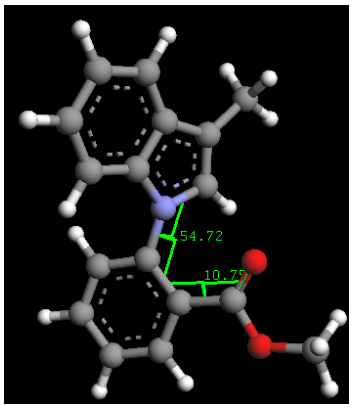
Torsion angle 1 = 56.60°

Trosion angle 2 = 32.94°

C	-3.556712	-1.127118	0.314228
C	-2.365712	-0.446807	0.029964
C	-2.055770	0.941171	-0.269208
C	-0.649573	1.027815	-0.452374
N	-0.094972	-0.260807	-0.288009
C	-1.138833	-1.163887	0.011780
C	-1.081652	-2.532203	0.290078
C	-2.283703	-3.188787	0.571035
C	-3.510107	-2.497527	0.580089
C	-2.841234	2.092498	-0.409820
C	-2.221792	3.302097	-0.730588
C	-0.827754	3.367222	-0.916598
C	-0.023221	2.232027	-0.783920
C	2.295677	0.001159	0.347332
C	3.644097	-0.297535	0.121421
C	3.994588	-1.254898	-0.828387
C	1.271134	-0.604581	-0.410301
C	1.650184	-1.561216	-1.368742
C	2.990662	-1.896671	-1.565463
N	2.011296	0.937508	1.441487
O	2.865614	1.848515	1.657943
O	0.968648	0.767868	2.128100
H	-4.502612	-0.595130	0.334351
H	-0.140584	-3.069897	0.300910
H	-2.267136	-4.251233	0.791759

H	-4.425743	-3.035248	0.802559
H	-3.916940	2.044711	-0.273057
H	-2.818189	4.201897	-0.838318
H	-0.364970	4.316361	-1.166195
H	1.049112	2.297080	-0.931226
H	4.392517	0.217914	0.709366
H	5.038299	-1.497659	-0.990930
H	0.873522	-2.014305	-1.973466
H	3.252679	-2.639015	-2.311600

1-(2-Carbomethoxyphenyl)-3-methyl-1*H*-indole 3



Energy = -861.8254304 = -2262735.595 kJ mol^{-1}

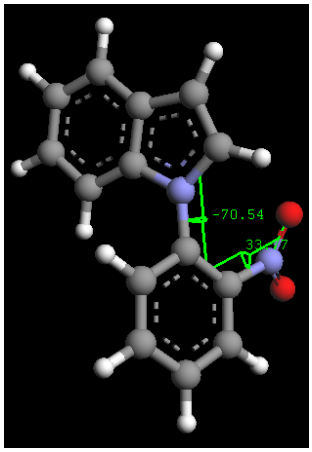
Torsion angle 1 = 54.72°

Torsion angle 2 = 10.75°

C	-3.929749	-0.435083	-0.320405
C	-2.618638	-0.529511	0.175884
C	-1.670250	0.475805	-0.169912
C	-1.999705	1.546718	-1.009094
C	-3.309454	1.615541	-1.488348
C	-4.267114	0.637802	-1.145268
C	-1.944355	-1.497081	1.019078
C	-0.649000	-1.070705	1.146281
N	-0.452668	0.128701	0.440089
C	-2.555132	-2.723038	1.627682
C	0.736577	0.903355	0.427209
C	2.008648	0.378579	0.077122
C	3.137406	1.219254	0.175968
C	0.635905	2.251093	0.817810
C	1.760823	3.071993	0.877195
C	3.022464	2.551127	0.565619
C	2.191063	-0.990027	-0.469603
O	1.307949	-1.763373	-0.861371
O	3.529153	-1.341070	-0.541684
C	3.822408	-2.654327	-1.127353
H	-4.667895	-1.191224	-0.071036
H	-3.593058	2.434782	-2.141511
H	-5.276522	0.721361	-1.535536
H	-1.825591	-3.270051	2.234029
H	-2.926868	-3.412486	0.857846
H	-3.406644	-2.474983	2.275598
H	4.103625	0.806084	-0.080080

H	1.655198	4.106693	1.186697
H	3.906032	3.177273	0.624051
H	3.457350	-2.700529	-2.155731
H	4.906927	-2.737918	-1.090218
H	3.345258	-3.443799	-0.542724
H	-1.265923	2.294010	-1.289226
H	-0.337701	2.633413	1.100727
H	0.166281	-1.516972	1.691736

1-(2-Nitrophenyl)-1*H*-indole 4



Energy = -799.1314919 Ha = -2098131.719 kJ mol^{-1}

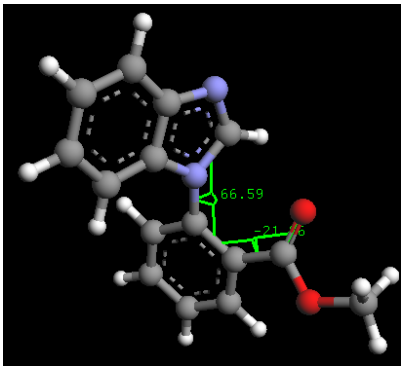
Torsion angle 1 = -70.54°

Torsion angle 2 = -33.77°

C	-3.908934	-0.385242	-0.033737
C	-2.594574	-0.645964	-0.458848
C	-1.537523	0.181884	0.016685
C	-1.761963	1.243205	0.901137
C	-3.077446	1.480816	1.303267
C	-4.140496	0.676340	0.839860
C	-2.002537	-1.635513	-1.327991
C	-0.654360	-1.414502	-1.356044
N	-0.337029	-0.310753	-0.535498
C	0.910914	0.363419	-0.458607
C	2.089578	-0.170478	0.112545
C	3.261940	0.591481	0.202836
C	0.965821	1.691661	-0.922642
C	2.134474	2.448202	-0.843120
C	3.292665	1.895717	-0.281631
N	2.162718	-1.515891	0.680873
O	2.939532	-1.686965	1.666888
O	1.475068	-2.438212	0.160925
H	-4.729969	-1.005652	-0.379040
H	-0.947933	1.857035	1.270591
H	-3.284093	2.295481	1.989785
H	-5.151068	0.887179	1.174643
H	-2.523055	-2.419250	-1.856422

H	0.127983	-1.945080	-1.868309
H	4.130079	0.141345	0.666402
H	0.066249	2.113551	-1.354802
H	2.142633	3.463158	-1.225378
H	4.207191	2.474018	-0.219857

1-(2-Carbomethoxyphenyl)-1*H*-benzimidazole 5



Energy = -838.546089 Ha = -2201615.335kJ mol^{-1}

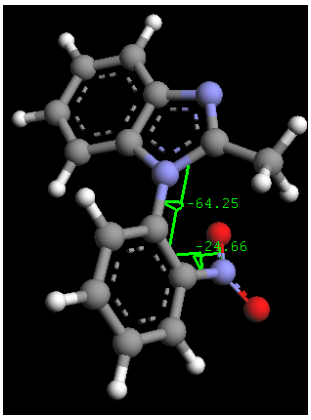
Torsion angle 1 = 66.59°

Torsion angle 2 = -21.86°

C	3.982134	-0.961381	-0.094155
C	2.677567	-0.789503	-0.567916
C	1.802335	0.128943	0.065802
C	2.194081	0.883601	1.175574
C	3.501001	0.699654	1.635301
C	4.383799	-0.208162	1.009909
N	2.021933	-1.416197	-1.644658
C	0.804981	-0.915502	-1.654510
N	0.589929	0.032871	-0.642915
C	-0.551513	0.867740	-0.450945
C	-1.835928	0.376963	-0.105572
C	-2.880874	1.300712	0.095910
C	-0.354450	2.253390	-0.571980
C	-1.402464	3.151249	-0.368268
C	-2.674587	2.672364	-0.036100
C	-2.122997	-1.069043	0.066608
O	-1.476709	-2.014882	-0.402860
O	-3.250594	-1.278974	0.833175
C	-3.642084	-2.680238	1.043582
H	4.646876	-1.666223	-0.580096
H	3.843634	1.265957	2.495453
H	5.390148	-0.320945	1.399789
H	-3.855821	0.917502	0.366382
H	-1.227046	4.216388	-0.476339
H	-3.497517	3.361132	0.120101
H	-2.843335	-3.218538	1.557476
H	-4.539579	-2.626309	1.656369

H	-3.843864	-3.163807	0.085387
H	1.519874	1.577832	1.664667
H	0.633471	2.611789	-0.837272
H	0.022551	-1.185375	-2.340861

2-Methyl-1-(2-nitrophenyl)-1*H*-benzimidazole 6



Energy = -854.4740188 Ha = -2140166.946 kJ mol^{-1}

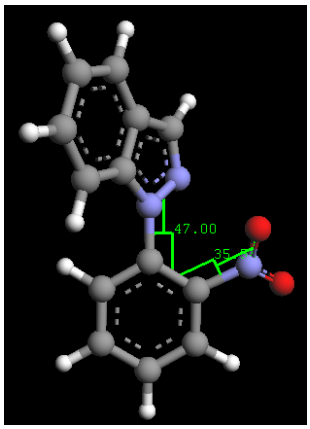
Torsion angle 1 = -64.25°

Torsion angle 2 = -24.66°

C	3.871013	-0.403616	0.010357
C	2.526617	-0.591056	0.346457
C	1.559004	0.376879	-0.018715
C	1.892542	1.534623	-0.725341
C	3.240651	1.706642	-1.053348
C	4.216417	0.753238	-0.690241
N	1.912398	-1.648405	1.037697
C	0.624642	-1.362060	1.087176
N	0.337925	-0.125043	0.465005
C	-0.917040	0.529938	0.361938
C	-2.022970	0.015985	-0.348052
C	-3.252253	0.685480	-0.356417
C	-1.079923	1.756876	1.026951
C	-2.294489	2.444654	0.992549
C	-3.388836	1.903438	0.306556
N	-1.950027	-1.219830	-1.139099
O	-3.037541	-1.832738	-1.356475
O	-0.831365	-1.595430	-1.584540
C	-0.414654	-2.208183	1.737601
H	4.609084	-1.146918	0.288501
H	1.147068	2.266399	-1.016438
H	3.542115	2.591910	-1.603877
H	5.251593	0.924483	-0.966441
H	-4.077018	0.238938	-0.895818
H	-0.237541	2.148500	1.585092
H	-2.390041	3.390748	1.513998
H	-4.338932	2.424508	0.286047

H	0.090478	-2.948024	2.360576
H	-1.019549	-2.749663	1.000207
H	-1.092402	-1.619627	2.366226

1-(2-Nitrophenyl)-1*H*-indazole 6



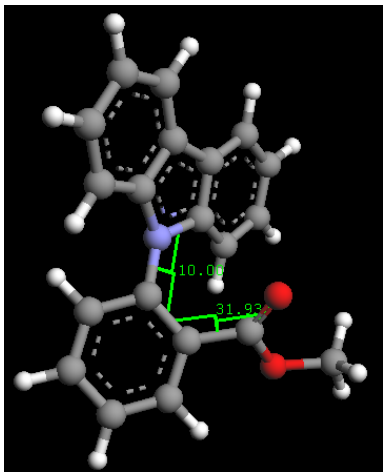
Energy = -818.1417705 Ha = -2140166.946 kJ mol^{-1}

Torsion angle 1 = 47.00°

Torsion angle 2 = 35.55°

C	-3.838213	-0.606629	0.221609
C	-2.466528	-0.712025	0.512645
C	-1.566284	0.285038	0.046868
C	-2.000801	1.374999	-0.723753
C	-3.363347	1.454093	-0.999587
C	-4.275774	0.478827	-0.529775
C	-1.648971	-1.657771	1.215306
N	-0.367528	-1.307131	1.201562
N	-0.307152	-0.103558	0.486678
C	0.939675	0.525828	0.294187
C	2.078807	-0.181021	-0.135469
C	3.330309	0.437346	-0.201172
C	1.082092	1.886944	0.605431
C	2.321745	2.520223	0.492585
C	3.453069	1.793113	0.103168
N	2.007510	-1.570546	-0.603229
O	3.012741	-2.306105	-0.382763
O	0.990064	-1.932547	-1.251815
H	-4.536867	-1.360167	0.569727
H	-1.308339	2.118472	-1.100495
H	-3.735152	2.282118	-1.594417
H	-5.328867	0.581178	-0.768882
H	-1.949567	-2.560525	1.723001
H	4.183513	-0.154268	-0.507265
H	0.218692	2.428721	0.972814
H	2.408339	3.573023	0.738291
H	4.421313	2.275531	0.036529

9-(2-Carbomethoxyphenyl)-9*H*-carbazole 1 at different torsion angles



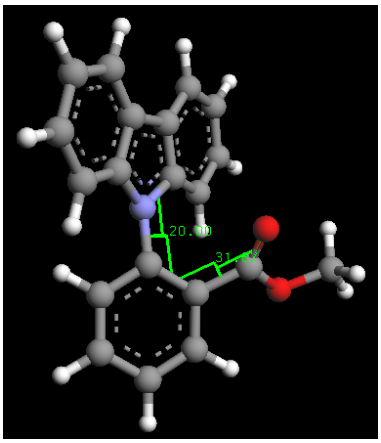
Energy = -976.1204047 Ha = -2562818.764 kJ mol^{-1}

Torsion angle 1 (fixed) = 10°

Torsion angle 2 (free rotation) = 31.93°

C	-2.582418	0.273798	0.076841
C	-1.757267	-0.876140	-0.029801
N	-0.460815	-0.481539	-0.514047
C	-0.481358	0.940664	-0.604366
C	-1.776863	1.419755	-0.294733
C	0.686915	-1.309764	-0.314402
C	1.975300	-0.819449	0.028301
C	3.105624	-1.646164	-0.127213
C	0.607915	-2.620582	-0.834410
C	1.728812	-3.442989	-0.933963
C	2.994462	-2.952590	-0.595380
C	2.158093	0.412979	0.837687
O	1.392239	0.812740	1.721702
C	-3.908593	0.158169	0.509884
C	-2.236366	-2.129517	0.370676
C	-2.072866	2.783629	-0.419233
C	-1.084718	3.653486	-0.879592
C	0.182866	3.159142	-1.240977
C	0.492749	1.801818	-1.126050
C	-4.399075	-1.098028	0.868044
C	-3.560867	-2.224604	0.811080
O	3.347508	1.053716	0.552066
C	3.653744	2.239903	1.366034
H	4.070415	-1.243475	0.155850
H	-0.334353	-2.965358	-1.237870
H	1.617865	-4.448465	-1.327057
H	3.876721	-3.574108	-0.700230
H	-4.539706	1.038282	0.582957
H	-1.611461	-3.011256	0.374338

H	-3.063232	3.154112	-0.174117
H	-1.297708	4.712737	-0.978857
H	0.932043	3.840490	-1.631815
H	1.463562	1.439067	-1.440321
H	-5.423941	-1.204787	1.207622
H	-3.941770	-3.192451	1.121111
H	4.610238	2.595823	0.988200
H	3.721575	1.967555	2.421518
H	2.870929	2.989859	1.236298



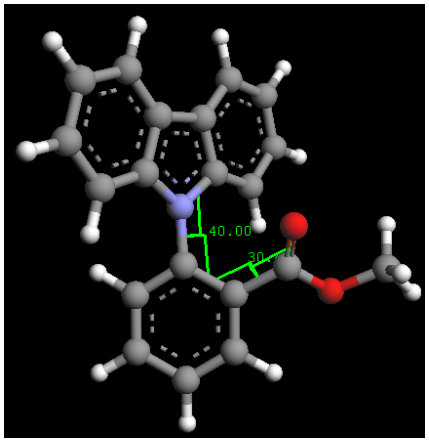
Energy = -976.1259923 Ha = -2562833.435 kJ mol^{-1}

Torsion angle 1 (fixed) = 20°

Torsion angle 2 = 31.87°

C	-2.579287	0.224526	0.085319
C	-1.720286	-0.903155	0.006865
N	-0.445306	-0.482520	-0.485171
C	-0.499757	0.929448	-0.630820
C	-1.808210	1.381831	-0.326291
C	0.725314	-1.285423	-0.358256
C	1.988202	-0.780613	0.044902
C	3.141576	-1.570318	-0.129405
C	0.678694	-2.573395	-0.930644
C	1.822710	-3.361401	-1.049003
C	3.068952	-2.854639	-0.663667
C	2.117608	0.436235	0.886984
O	1.312536	0.806025	1.748708
C	-3.898917	0.074118	0.528520
C	-2.154550	-2.164899	0.428806
C	-2.137830	2.734248	-0.485453
C	-1.170992	3.616962	-0.967225
C	0.111257	3.148142	-1.310937
C	0.457319	1.802671	-1.162225
C	-4.345266	-1.190152	0.916381
C	-3.473366	-2.292781	0.876734
O	3.303565	1.104051	0.655233
C	3.556085	2.283487	1.496852

H	4.091871	-1.160428	0.189895
H	-0.257612	-2.925280	-1.344208
H	1.745509	-4.351970	-1.485472
H	3.968026	-3.449405	-0.780729
H	-4.560171	0.933128	0.584615
H	-1.497026	-3.023915	0.436591
H	-3.136445	3.087053	-0.247607
H	-1.410865	4.667620	-1.093060
H	0.844745	3.840573	-1.711946
H	1.441231	1.458016	-1.456360
H	-5.364515	-1.322358	1.263920
H	-3.824738	-3.265513	1.205825
H	4.521697	2.659434	1.164372
H	3.583614	1.997820	2.550607
H	2.767497	3.022917	1.343601



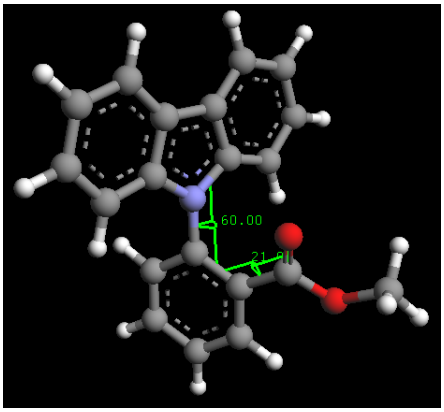
Energy = -976.1329583 Ha = -2562851.724 kJ mol^{-1}

Torsion angle 1(fixed) = 40°

Torsion angle 2 = 30.40°

C	-2.577040	0.101610	0.116396
C	-1.632283	-0.959491	0.087700
N	-0.407486	-0.465277	-0.423536
C	-0.563904	0.916202	-0.676440
C	-1.900715	1.289006	-0.373893
C	0.808483	-1.199767	-0.450268
C	2.025904	-0.688503	0.062264
C	3.219742	-1.399626	-0.163617
C	0.822795	-2.423549	-1.143312
C	2.007856	-3.139655	-1.314732
C	3.217089	-2.619483	-0.838647
C	2.063573	0.481018	0.977411
O	1.185837	0.799940	1.786556
C	-3.876256	-0.137929	0.581622
C	-1.958766	-2.238392	0.549988
C	-2.321682	2.606721	-0.595680
C	-1.417610	3.529672	-1.123764

C	-0.102874	3.139046	-1.442835
C	0.338161	1.829854	-1.232214
C	-4.214414	-1.418305	1.024265
C	-3.260119	-2.453043	1.013692
O	3.250671	1.178602	0.871150
C	3.411055	2.323029	1.780328
H	4.143338	-0.987224	0.223051
H	-0.101099	-2.783490	-1.580387
H	1.990888	-4.084007	-1.848932
H	4.145760	-3.158316	-0.991255
H	-4.607470	0.663992	0.607353
H	-1.229665	-3.039349	0.565131
H	-3.339972	2.904085	-0.365191
H	-1.730130	4.554030	-1.298006
H	0.582710	3.865451	-1.867785
H	1.349323	1.541844	-1.495447
H	-5.216998	-1.617265	1.388252
H	-3.535288	-3.438026	1.377237
H	4.387277	2.736739	1.535199
H	3.371893	1.989387	2.819566
H	2.615810	3.050249	1.604751



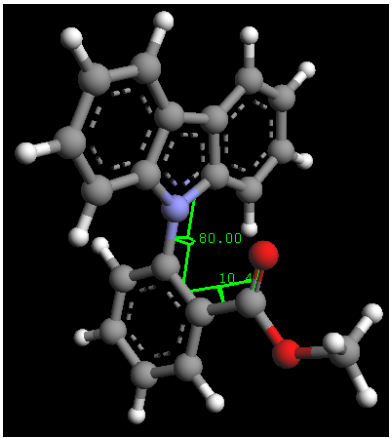
Energy = -976.1351626 Ha = -2562857.511 kJ mol^{-1}

Torsion angle 1(fixed) = 60°

Torsion angle 2 = 21.99°

C	-2.558064	-0.130931	0.199057
C	-1.474465	-1.051377	0.158389
N	-0.361199	-0.412469	-0.421859
C	-0.719825	0.911575	-0.737997
C	-2.079179	1.114957	-0.373897
C	0.920381	-1.001589	-0.607250
C	2.086305	-0.499861	0.020983
C	3.330163	-1.083136	-0.286875
C	1.025155	-2.091844	-1.485049
C	2.262125	-2.682866	-1.749479
C	3.421678	-2.168252	-1.158344
C	2.023274	0.558442	1.062804

O	1.046101	0.845612	1.762537
C	-3.786484	-0.536732	0.736720
C	-1.594915	-2.351719	0.657356
C	-2.679955	2.356909	-0.618350
C	-1.929297	3.368768	-1.220490
C	-0.586913	3.145834	-1.584342
C	0.034315	1.915819	-1.351755
C	-3.917652	-1.837609	1.227664
C	-2.830232	-2.731939	1.189507
O	3.237983	1.201032	1.212762
C	3.300006	2.228582	2.261254
H	4.217420	-0.681079	0.184798
H	0.125326	-2.450829	-1.971495
H	2.321665	-3.525691	-2.430204
H	4.388783	-2.609994	-1.372708
H	-4.624203	0.152604	0.776673
H	-0.759340	-3.042137	0.641364
H	-3.716414	2.529822	-0.345444
H	-2.382659	4.335543	-1.413473
H	-0.022240	3.943088	-2.057520
H	1.066270	1.751255	-1.641466
H	-4.863799	-2.163205	1.647439
H	-2.950168	-3.735914	1.584339
H	4.313209	2.621589	2.204132
H	3.102825	1.783160	3.238901
H	2.560536	3.007747	2.065869



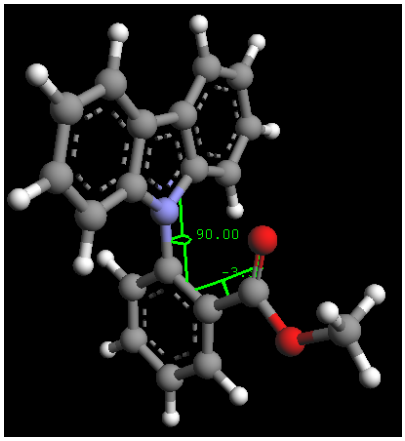
Energy = -976.13498 Ha = -2562857.032 kJ mol^{-1}

Torsion 1(fixed) = 80°

Torsion 2 = 10.45°

C	-2.443301	-0.522492	0.235976
C	-1.202488	-1.178547	0.001478
N	-0.312132	-0.261203	-0.580671
C	-0.960326	0.978120	-0.707734
C	-2.289385	0.849496	-0.215802
C	1.047163	-0.528854	-0.925104

C	2.128902	-0.188093	-0.076185
C	3.440216	-0.466164	-0.505878
C	1.301046	-1.147106	-2.157021
C	2.608150	-1.430530	-2.561851
C	3.680724	-1.083884	-1.733690
C	1.912450	0.428193	1.260408
O	0.836935	0.547198	1.857356
C	-3.502067	-1.241292	0.806645
C	-1.004449	-2.522877	0.327909
C	-3.144717	1.958666	-0.252791
C	-2.671233	3.166376	-0.770852
C	-1.352108	3.273439	-1.253710
C	-0.479474	2.181911	-1.230189
C	-3.313262	-2.585936	1.134077
C	-2.076043	-3.216724	0.896769
O	3.098414	0.870613	1.817250
C	2.999449	1.476217	3.151462
H	4.262939	-0.195746	0.142401
H	0.456437	-1.393196	-2.790562
H	2.785808	-1.910787	-3.518359
H	4.699639	-1.293586	-2.041148
H	-4.456366	-0.759058	0.995096
H	-0.052878	-3.011644	0.150294
H	-4.162382	1.881542	0.117624
H	-3.324219	4.032496	-0.802827
H	-1.005006	4.221394	-1.652947
H	0.534618	2.269290	-1.604817
H	-4.125587	-3.152164	1.578009
H	-1.950132	-4.261823	1.162009
H	4.020235	1.755704	3.404886
H	2.597746	0.753651	3.865130
H	2.345779	2.350345	3.119565



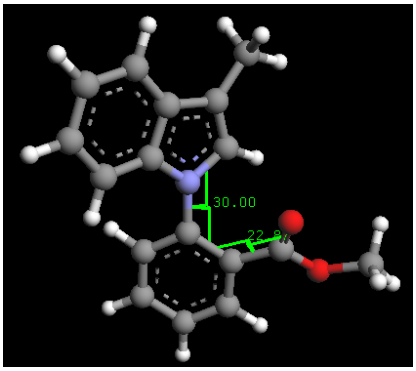
Energy = -976.1349413 Ha = -2562856.93 kJ mol^{-1}

Torsion 1(fixed) = 90°

Torsion 2 = -3.37°

C	2.345557	0.772012	-0.043657
C	1.041917	1.091950	-0.516010
N	0.307771	-0.097714	-0.649665
C	1.114818	-1.173683	-0.245548
C	2.391921	-0.669641	0.128604
C	-1.063791	-0.188072	-1.038091
C	-2.131034	-0.060539	-0.114570
C	-3.452348	-0.155427	-0.591040
C	-1.343100	-0.410104	-2.393272
C	-2.660581	-0.506818	-2.849092
C	-3.717835	-0.377195	-1.942804
C	-1.889998	0.161323	1.336588
O	-0.795753	0.201399	1.909906
C	3.275461	1.801528	0.152733
C	0.657223	2.407392	-0.788990
C	3.383084	-1.562908	0.556271
C	3.092404	-2.928134	0.608236
C	1.820647	-3.407065	0.236486
C	0.815247	-2.537673	-0.195632
C	2.899130	3.119350	-0.117338
C	1.602680	3.415789	-0.582310
O	-3.073327	0.324128	2.033595
C	-2.946230	0.541830	3.480192
H	-4.263343	-0.054263	0.117591
H	-0.508563	-0.502976	-3.078945
H	-2.857461	-0.679466	-3.901957
H	-4.744558	-0.448382	-2.285576
H	4.275370	1.578854	0.512442
H	-0.339443	2.640461	-1.147630
H	4.363912	-1.198963	0.846602
H	3.851748	-3.628993	0.939562
H	1.615612	-4.471918	0.286593
H	-0.162682	-2.910756	-0.479580
H	3.610414	3.925004	0.032916
H	1.330976	4.447134	-0.784821
H	-3.969656	0.645997	3.835311
H	-2.365397	1.445801	3.675031
H	-2.449724	-0.311233	3.947566

1-(2-Carbomethoxyphenyl)-3-methyl-1*H*-indole 3 at different torsion angles



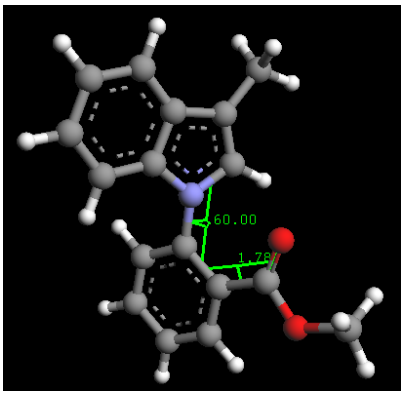
Energy = -861.8228581 Ha = -2262728.841 kJ mol^{-1}

Torsion angle 1(fixed) = 30°

Torsion angle 2 = 22.85°

	3.938734	-0.602771	0.180251
C	2.585616	-0.641127	-0.192328
C	1.753246	0.486412	0.062367
C	2.241156	1.616040	0.731310
C	3.589276	1.626495	1.098181
C	4.434817	0.534655	0.816715
C	1.764759	-1.665274	-0.807712
C	0.499809	-1.153555	-0.894721
N	0.459835	0.168214	-0.412141
C	2.224889	-3.017344	-1.260513
C	-0.696948	0.976668	-0.293088
C	-1.997512	0.456622	-0.049405
C	-3.109580	1.319161	-0.153378
C	-0.568748	2.344467	-0.609968
C	-1.677548	3.185871	-0.662684
C	-2.961615	2.671387	-0.447292
C	-2.237619	-0.904952	0.490047
O	-1.444970	-1.592034	1.147315
O	-3.525856	-1.342421	0.232760
C	-3.901808	-2.633043	0.824176
H	4.585250	-1.453387	-0.012141
H	3.988604	2.492241	1.616892
H	5.478303	0.577183	1.112147
H	1.399724	-3.593107	-1.692253
H	2.634689	-3.602189	-0.426300
H	3.014012	-2.945076	-2.021054
H	-4.091690	0.902905	0.028937
H	-1.540857	4.234102	-0.908205
H	-3.832397	3.314573	-0.508900
H	-3.825847	-2.587620	1.912897
H	-4.930524	-2.793498	0.507270
H	-3.246478	-3.423707	0.452797
H	1.601757	2.453270	0.981955

H	0.408980	2.727385	-0.871760
H	-0.381317	-1.603200	-1.319661



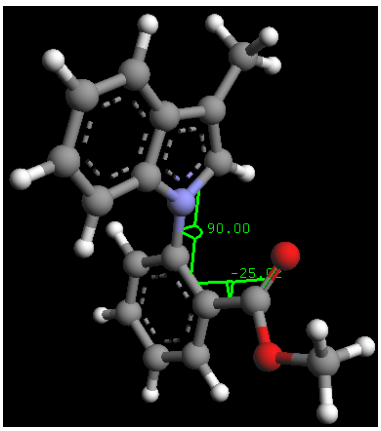
Energy = -861.8253447 Ha = -2262735.37 kJ mol^{-1}

Torsion 1(fixed) = 60°

Torsion 2 = 1.78°

C	3.932441	-0.388045	0.373826
C	2.636202	-0.500988	-0.156707
C	1.651662	0.463496	0.204221
C	1.931931	1.514344	1.085462
C	3.228295	1.602900	1.596872
C	4.220428	0.663894	1.243351
C	2.009105	-1.453268	-1.052106
C	0.705209	-1.058488	-1.194204
N	0.457262	0.103689	-0.442727
C	2.667177	-2.639738	-1.689387
C	-0.738276	0.871635	-0.460906
C	-2.013463	0.355016	-0.107774
C	-3.136579	1.203456	-0.208450
C	-0.631284	2.216432	-0.859828
C	-1.751679	3.042677	-0.928426
C	-3.015209	2.530990	-0.610088
C	-2.208470	-1.019053	0.420544
O	-1.335809	-1.865940	0.651365
O	-3.543453	-1.289231	0.673276
C	-3.839912	-2.613232	1.231817
H	4.697573	-1.113596	0.115050
H	3.474373	2.407048	2.283194
H	5.218085	0.761429	1.659780
H	1.968522	-3.179863	-2.336887
H	3.034477	-3.349951	-0.936406
H	3.529924	-2.346375	-2.302612
H	-4.104629	0.798503	0.052905
H	-1.640705	4.074174	-1.246591
H	-3.895823	3.160911	-0.672850
H	-3.338771	-2.738485	2.194080
H	-4.922116	-2.629001	1.346503

H	-3.503366	-3.395974	0.548527
H	1.171263	2.232177	1.371386
H	0.346380	2.593140	-1.136541
H	-0.087388	-1.510763	-1.766882



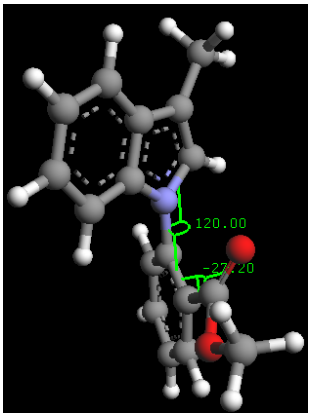
Energy = -861.8241314 Ha = 2262732.184 kJ mol^{-1}

Torsion 1(fixed) = 90°

Torsion 2 = -25.02°

C	-3.735765	0.241487	0.669964
C	-2.600304	0.093737	-0.146791
C	-1.400078	-0.418410	0.427966
C	-1.313909	-0.785117	1.776267
C	-2.456959	-0.627468	2.561156
C	-3.656009	-0.118691	2.014604
C	-2.336652	0.356673	-1.546263
C	-1.027204	0.009904	-1.770365
N	-0.439071	-0.461410	-0.586908
C	-3.306811	0.912797	-2.545223
C	0.883481	-0.987110	-0.453246
C	1.997281	-0.168903	-0.150570
C	3.254201	-0.772618	0.039278
C	1.053979	-2.374078	-0.561807
C	2.311282	-2.958207	-0.386391
C	3.414351	-2.153424	-0.082594
C	1.881669	1.310037	-0.060265
O	1.036848	2.020520	-0.616031
O	2.881951	1.849727	0.725918
C	2.884993	3.313156	0.856157
H	-4.662089	0.631615	0.258995
H	-2.423205	-0.900257	3.611366
H	-4.526103	-0.008085	2.654267
H	-2.847049	1.005388	-3.534901
H	-3.661261	1.910181	-2.252241
H	-4.194618	0.274412	-2.650314
H	4.099090	-0.141352	0.282400
H	2.425746	-4.032977	-0.480861

H	4.393504	-2.597822	0.060460
H	1.948798	3.650912	1.305284
H	3.733242	3.531681	1.501848
H	3.002344	3.780091	-0.124291
H	-0.393846	-1.175836	2.198037
H	0.183780	-2.982985	-0.779602
H	-0.440496	0.080343	-2.672446



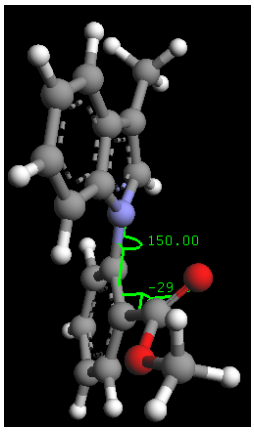
Energy = -861.8249564 Ha = -2262734.35 kJ mol^{-1}

Torsion 1(fixed) = 120°

Torsion 2 = -27.20°

C	3.570527	0.706039	-0.467856
C	2.543650	-0.140072	-0.013345
C	1.228448	0.024289	-0.535577
C	0.927846	0.991541	-1.501708
C	1.966159	1.817257	-1.934103
C	3.274670	1.678852	-1.421349
C	2.507580	-1.240142	0.929029
C	1.215404	-1.701263	0.941866
N	0.418904	-0.949397	0.060527
C	3.659388	-1.756124	1.737996
C	-0.967984	-1.165303	-0.164818
C	-1.940659	-0.169661	0.091140
C	-3.284880	-0.430631	-0.233970
C	-1.370279	-2.406291	-0.681491
C	-2.714420	-2.664584	-0.957543
C	-3.674360	-1.667983	-0.747353
C	-1.600264	1.101232	0.782956
O	-0.683651	1.274332	1.592851
O	-2.482334	2.112951	0.452462
C	-2.269700	3.401052	1.127294
H	4.580526	0.600858	-0.083501
H	1.763688	2.578870	-2.680672
H	4.058444	2.339107	-1.779191
H	3.354973	-2.595645	2.371994
H	4.071661	-0.978592	2.394779

H	4.481552	-2.105099	1.098533
H	-4.018110	0.345481	-0.055331
H	-3.006291	-3.630840	-1.355700
H	-4.717606	-1.854116	-0.978388
H	-1.268064	3.776348	0.908362
H	-3.036002	4.057280	0.719321
H	-2.382159	3.285181	2.207628
H	-0.074114	1.099930	-1.903285
H	-0.609544	-3.151172	-0.886804
H	0.769840	-2.489318	1.529057



Energy = -861.8229432 Ha = -2262729.065 kJ mol^{-1}

Torsion 1 (fixed) = 150°

Torsion 2 = -29.07°

C	3.518688	0.973525	-0.447258
C	2.576531	0.018595	-0.030288
C	1.193627	0.227525	-0.301969
C	0.755615	1.338098	-1.034019
C	1.712938	2.266521	-1.446755
C	3.080513	2.095703	-1.147735
C	2.709296	-1.261824	0.635378
C	1.447294	-1.782756	0.732081
N	0.493225	-0.884818	0.208764
C	3.983374	-1.878187	1.127889
C	-0.857844	-1.237060	-0.034419
C	-1.917990	-0.299605	0.046030
C	-3.206795	-0.681966	-0.373510
C	-1.138778	-2.542486	-0.479182
C	-2.432131	-2.916087	-0.842396
C	-3.471117	-1.978321	-0.811315
C	-1.766413	1.006533	0.735988
O	-1.014833	1.250132	1.685710
O	-2.629881	1.959770	0.225248
C	-2.618149	3.267559	0.896726
H	4.574397	0.830570	-0.238073
H	1.394822	3.136643	-2.012353

H	3.796592	2.841568	-1.477687
H	3.802486	-2.859628	1.578499
H	4.468726	-1.249708	1.886351
H	4.707357	-2.014650	0.313395
H	-4.000566	0.052481	-0.319578
H	-2.620100	-3.929937	-1.180690
H	-4.473369	-2.256019	-1.118294
H	-1.613818	3.694512	0.865356
H	-3.324458	3.874389	0.333503
H	-2.931395	3.160889	1.937759
H	-0.287054	1.484184	-1.288254
H	-0.322201	-3.247421	-0.581472
H	1.121757	-2.697974	1.201055

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