Electronic Supplementary Information

Predicting the regioselectivity of arynes: a simple model based on orbital electronegativity

Saber Mirzaei[a] and Hormoz Khosravi*[b]

[a]Department of Chemistry, Marquette University, Milwaukee, WI 53201-1414, USA.
[b]Faculty of Chemistry, K. N. Toosi University of Technology, P.O. Box: 15875-4416, Tehran, Iran.
*Email: saber.mirzaei@marquette.edu

Table of Contents

Fig. S1. Predicted ^{13}C NMR shifts for 14 different substituted benzynes (using MarvinSketch 17.13). Red value and asterisk show the preferred position based on the NMR shift and experimental data, respectively. The ^{13}C NMR shifts predict incorrect position for compounds 5, 7, 9, 12, 13 and 14.

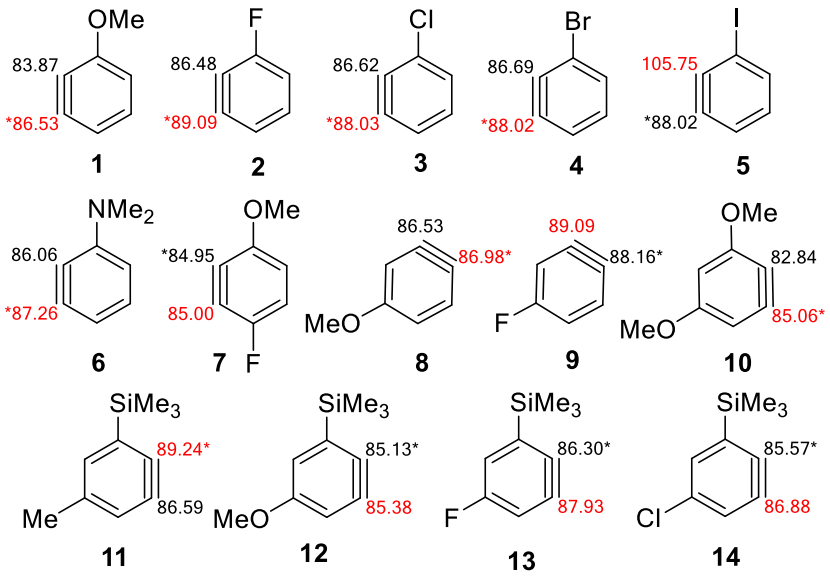


Fig. S2. Predicted ^{13}C NMR shifts for 16 different heterocyclic arynes (using MarvinSketch 17.13). Red value and asterisk show the preferred position based on the NMR shift and experimental data, respectively. The ^{13}C NMR shifts predict incorrect position for compounds 17, 19 and 26.

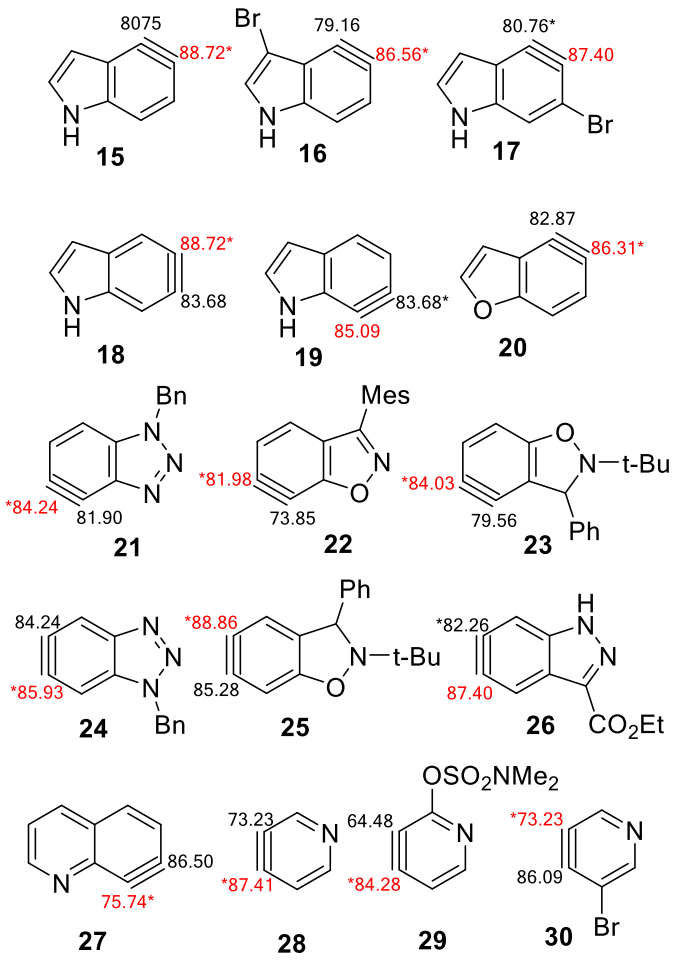


Fig. S3. Predicted ^{13}C NMR shifts for 3 different nonaromatic alkynes (using MarvinSketch 17.13). Red value and asterisk show the preferred position based on the NMR shift and experimental data, respectively.

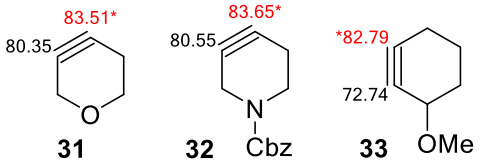


Fig. S4. Linear correlation of Gasteiger calculated charge vs π OE values for 30 arynes at the experimentally predicted carbon (Figures S5 and S6).

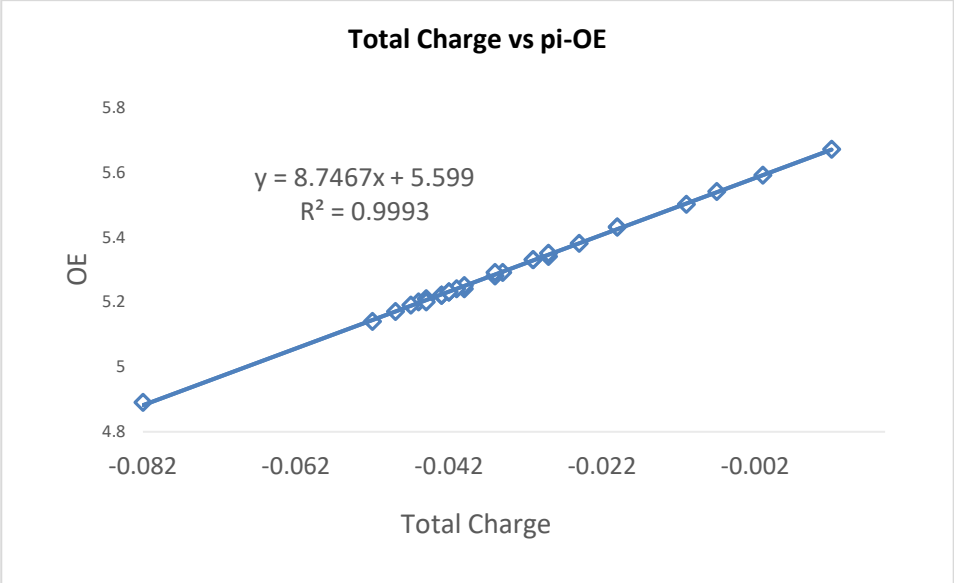


Fig. S5. Calculated total charges for 14 different substituted benzynes (using MarvinSketch 17.13). Red value and asterisk show the preferred position based on the calculated total charge and experimental data, respectively.

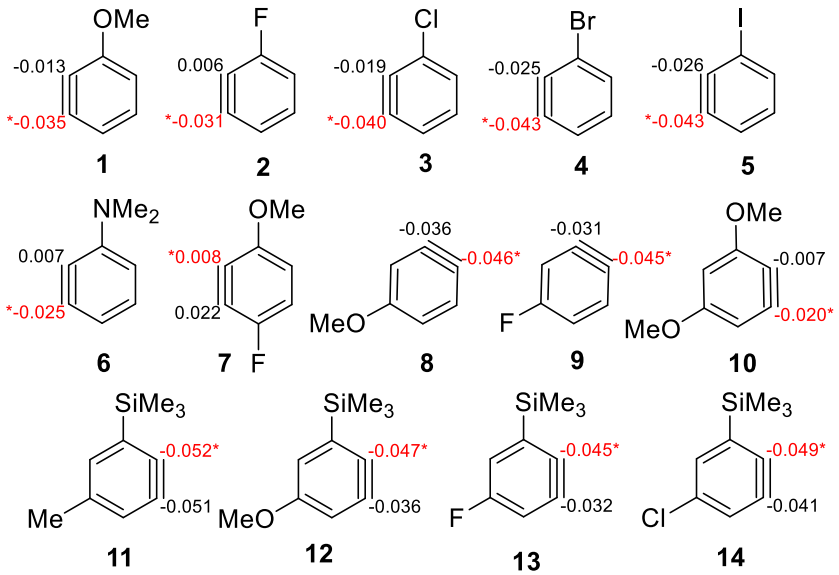


Fig. S6. Calculated total charges for 16 different heterocyclic arynes (using MarvinSketch 17.13). Red value and asterisk show the preferred position based on the calculated total charge and experimental data, respectively.

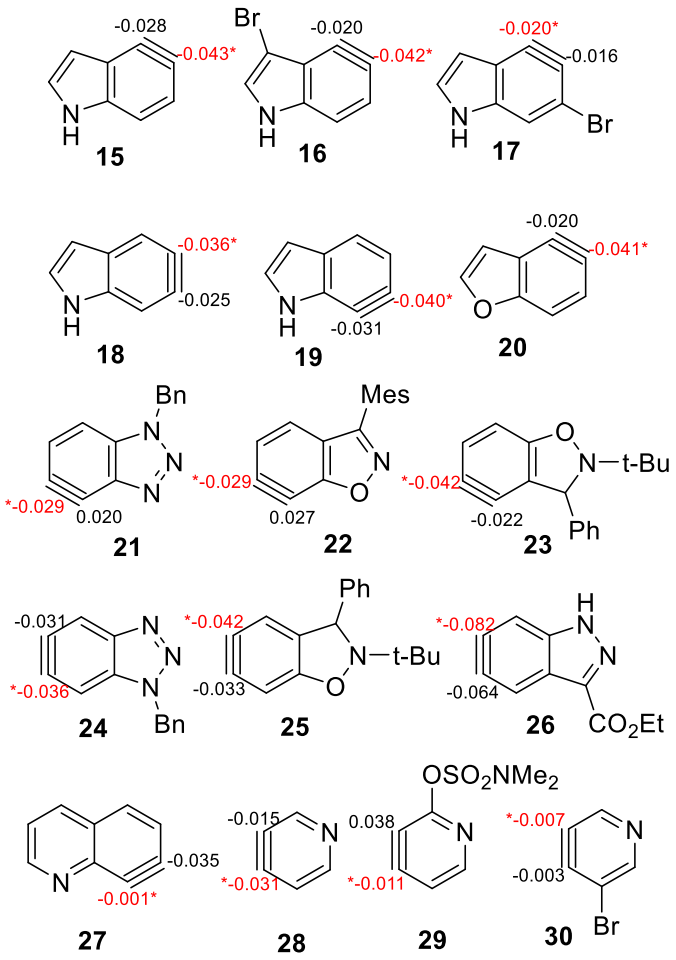


Fig. S7. Calculated total charges for 3 different nonaromatic alkynes (using MarvinSketch 17.13). Red value and asterisk show the preferred position based on the calculated total charge and experimental data, respectively.

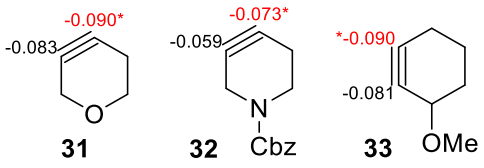


Fig. S8. Calculated NBO charges for 14 different substituted benzynes (B3LYP/6-31G*). Red value and asterisk show the preferred position based on the calculated NBO charge and experimental data, respectively. The NBO charge predicts incorrect position for compounds 7-9.

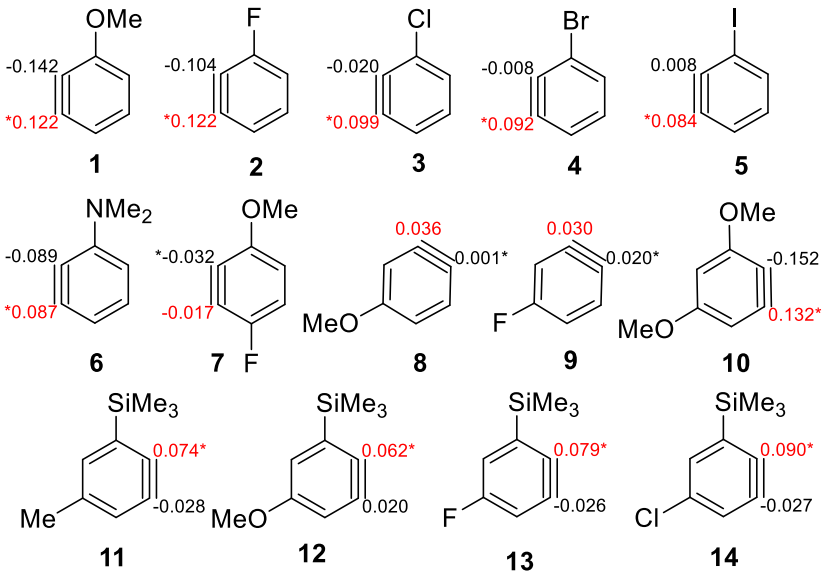


Fig. S9. Calculated NBO charges for 16 different heterocyclic arynes (B3LYP/6-31G*). Red value and asterisk show the preferred position based on the calculated NBO charge and experimental data, respectively. The NBO charge predicts incorrect position for compounds 15, 24-26.

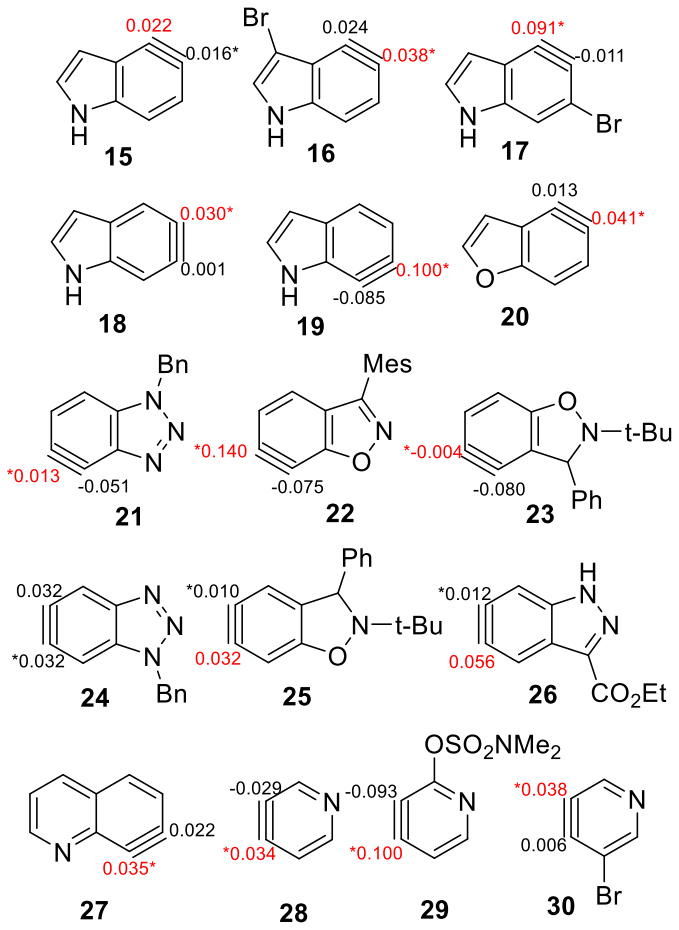


Fig. S10. Calculated NBO charges for 3 different nonaromatic alkynes (B3LYP/6-31G*). Red value and asterisk show the preferred position based on the calculated total charge and experimental data, respectively.

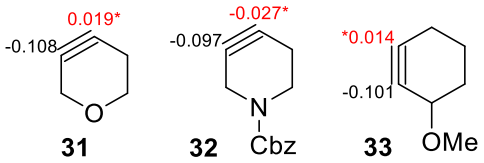


Fig. S11. The energy profile of reaction of 2-methoxyfuran with 7,8-quinolyne (kcal.mol^{-1}, HF/6-31G*).

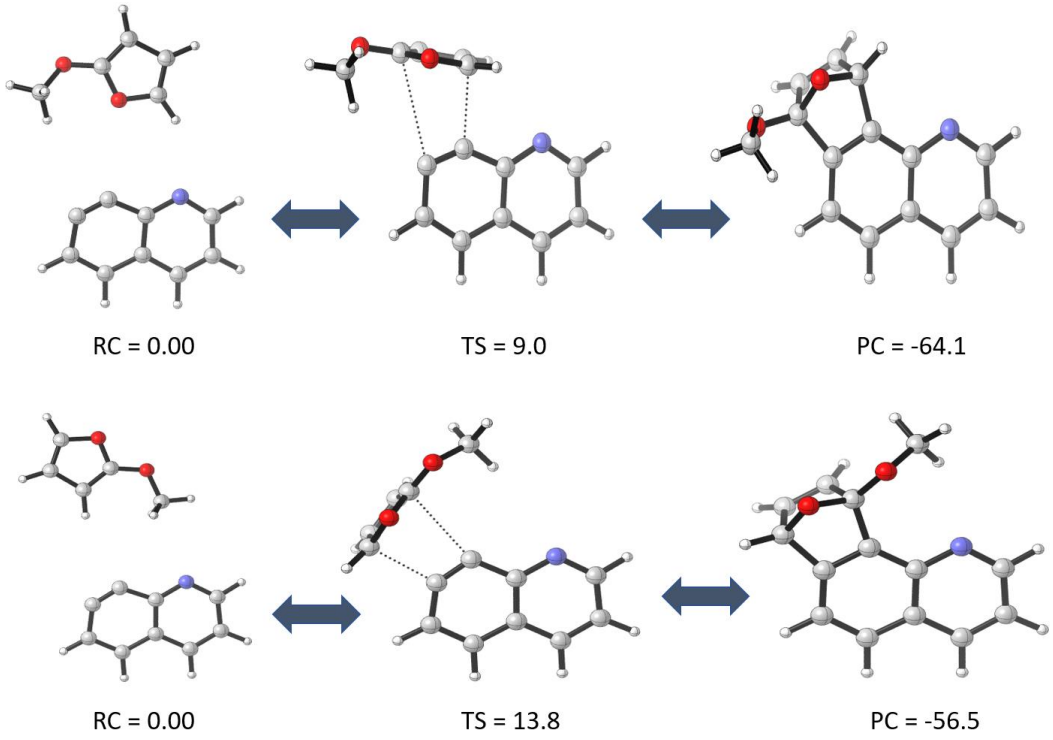


Fig. S12. The highest occupied molecular orbital contribution analysis (HOMO-CA) of 2-methoxyfuran (B3LYP/6-31G*) using Hirshfeld population analysis.

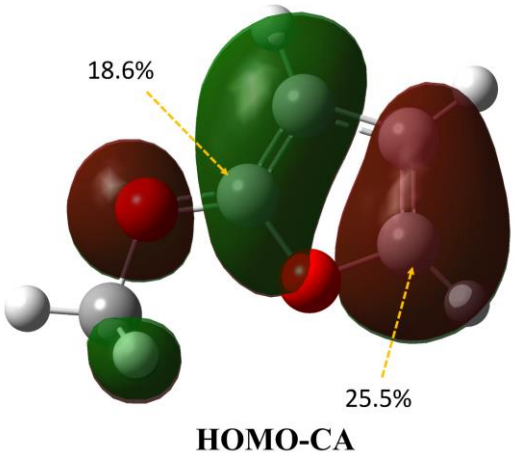


Fig. S13. Comparison between predicted OE and calculated internal angle differences (distortion model).

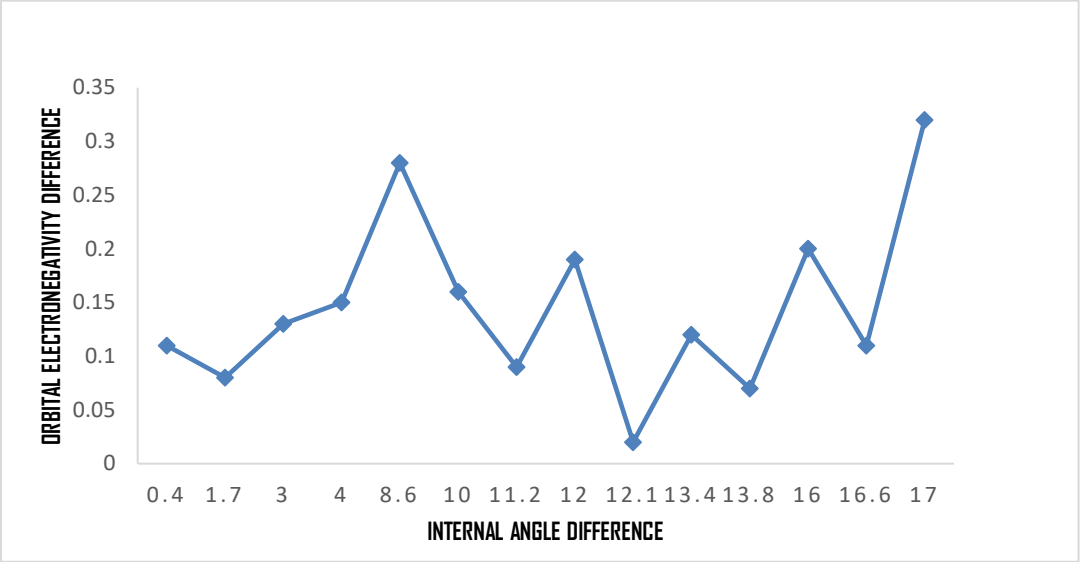


Table S1. OE of some substituted benzynes and indolynes which do not studied experimentally.

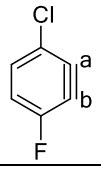
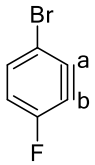
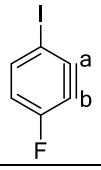
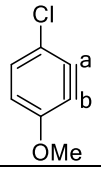
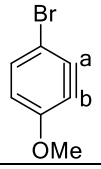
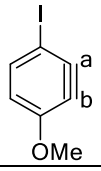
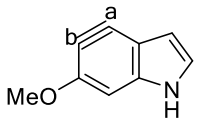
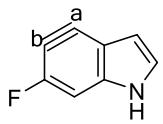
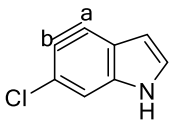
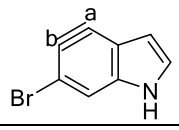
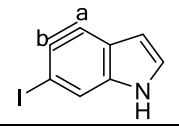
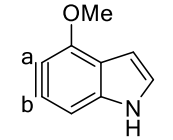
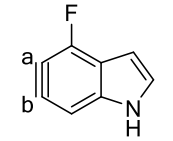
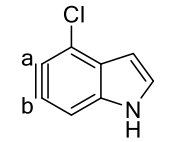
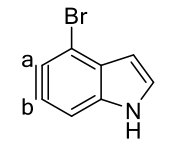
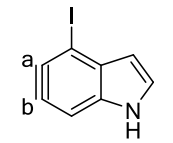
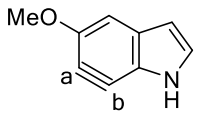
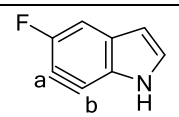
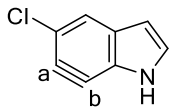
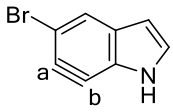
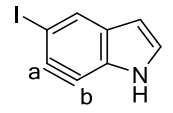
Structure	OE		Distortion[12b]		LUMO-CA[5]	
	a	b	a°	b°	a%	b%
	5.62	5.75	130	122	39.3	36.5
	5.57	5.73	131	122	39.1	36.1
	5.55	5.72	131	121	37.8	35.3
	5.58	5.58	129	124	38.3	35.0
	5.53	5.56	130	123	38.2	34.7
	5.51	5.56	130	123	37.0	33.9
	5.49	5.56	132	122	40.4	32.7
	5.54	5.73	133	120	41.3	34.4
	5.45	5.51	130	123	40.0	35.8

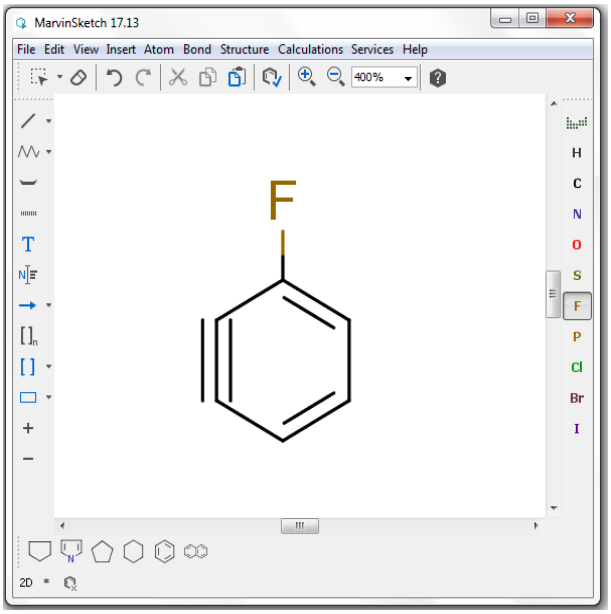
Table S1. Continued

	5.43	5.46	130	124	39.8	36.0
	5.42	5.44	127	127	39.6	35.9
	5.55	5.37	122	135	33.3	40.6
	5.71	5.41	120	135	34.9	41.4
	5.50	5.33	124	132	36.5	40.0
	5.45	5.31	125	131	36.6	39.8
	5.43	5.30	127	129	36.5	39.4
	5.59	5.48	129	123	35.6	37.4
	5.76	5.52	125	126	37.1	38.5
	5.54	5.43	129	123	38.5	37.0
	5.49	5.41	130	122	38.5	36.5
	5.47	5.40	130	122	37.5	35.9

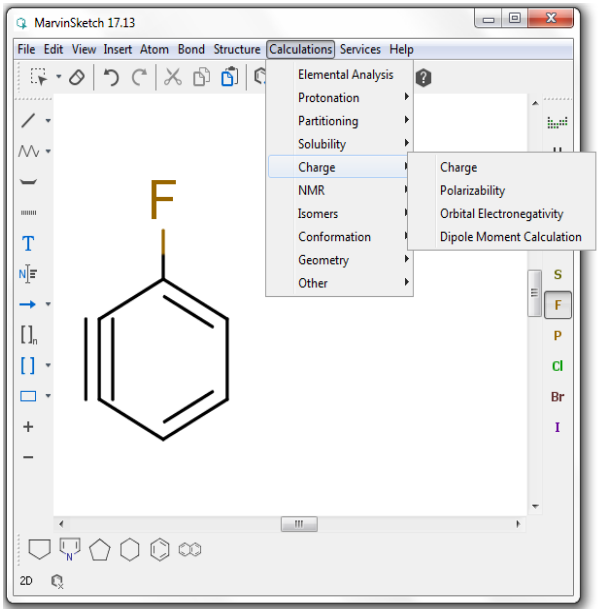
S1. OE (Orbital Electronegativity) calculations setup procedures.

The latest version of MarvinSketch can be downloaded free of charge form ChemAxon (https://www.chemaxon.com/download/marvin-suite/#marvin)

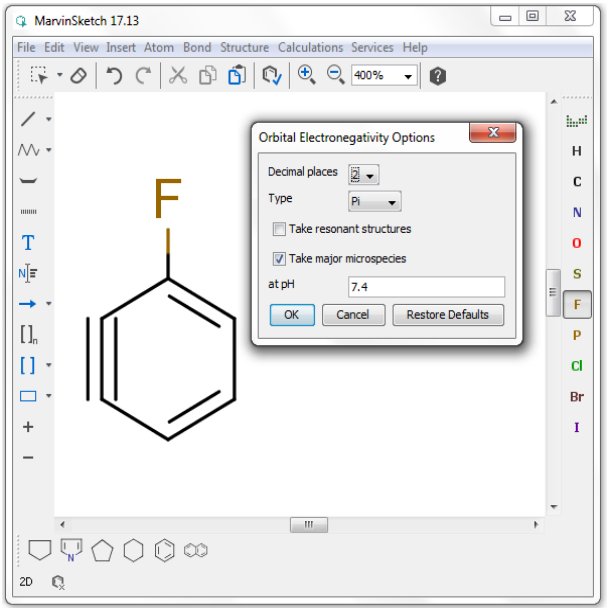
Draw aryne that you want to predict its regioselectivity.

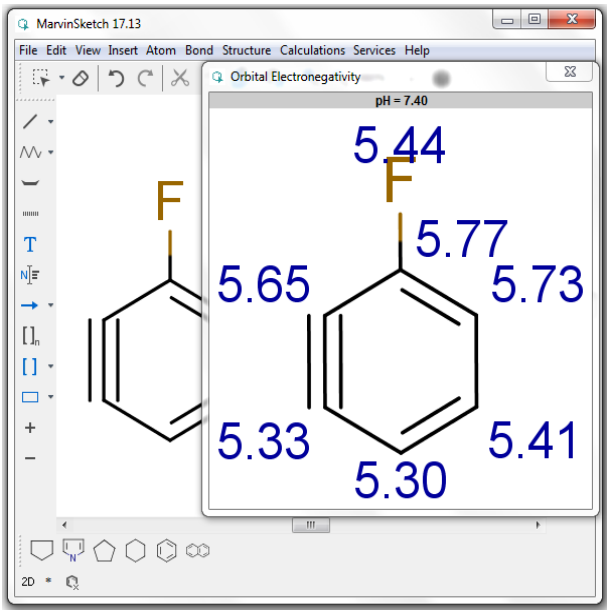


Chose Calculations, Charge and Orbital Electronegativity



Orbital Electronegativity Options window will be open. Select Decimal places 2 (default value), orbital type (pi orbitals) and take major microspecies (this option provide better results compared to experimental data).





S2. Computational details.

All calculations were done using Gaussian 09 software package.[1] For some of the structures with other possible conformations (e.g., 3-methoxybenzyne, Fig. S14), the relative free energies of all conformers have been calculated and the most stable conformer has been selected for the future analysis. Charge analysis were calculated using natural bond orbital (NBO) approach with NBO 3.1 code integrated in Gaussian 09 package.[2] The B3LYP functional of density functional theory is used for the charge and also the orbital contribution analysis calculations.[3] For finding the transition state the Hartree-Fock (HF) method has been used. All the calculations were carried out using the 6-31G* basis set. The frequency calculation performed for all optimized structures to confirm the presence of one imaginary frequency for transition states and no imaginary frequency for minimum structures. Moreover, the correctness of TS structures is checked using the intrinsic reaction coordinate (IRC). For orbital contribution analysis, the Hirshfeld population analysis method is used which showed the lowest basis set dependency.[4,5]

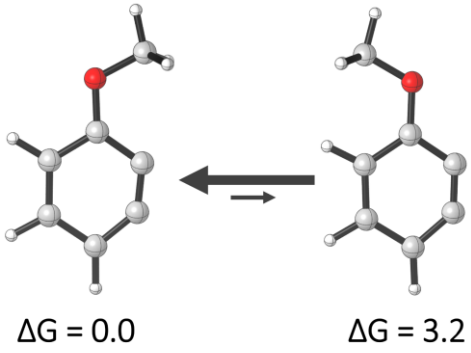


Fig. S14. Relative free energies (ΔG, kcal.mol^{-1}) of 3-methoxybenzyne conformers (B3LYP/6-31G*).

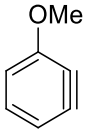
S2. References.

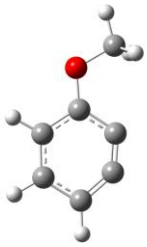
1) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, T. Vreven Jr., K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian-09 suite of programs, Gaussian, Inc.,Pittsburgh, PA, 2009.
2) J. P. Foster and F. Weinhold, *J. Am. Chem. Soc.*, 1980, **102**, 7211.
3) A. D. Becke*, Phys. Rev. A: At., Mol., Opt. Phys*., 1988, **38**, 3098.
4) F. L. Hirshfeld, *Theoret. Chim Acta,* 1977, **44**, 129.
5) S. Mirzaei and H. Khosravi, *Tetrahedron lett*., 2017, **58**, 3362.

S3. Cartesian coordinates of all optimized structures (B3LYP/6-31G*).

3-methoxybenzyne

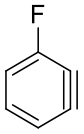
C	-0.01995172	-1.09220863	0.00006372
C	1.91434565	0.82517077	-0.00015911
C	-0.47383697	0.22912693	0.00031977
C	1.21459598	-1.31294640	-0.00003464
C	2.34066250	-0.52747992	0.00005044
C	0.56386235	1.19417600	0.00001279
H	2.67215417	1.60605219	-0.00040370
H	3.37982821	-0.83091368	-0.00006424
H	0.28635124	2.24437862	-0.00014477
O	-1.75837546	0.65063711	0.00014411
C	-2.74726441	-0.37416275	-0.00020115
H	-2.65661637	-1.00502020	-0.89274161
H	-3.71213006	0.13549291	-0.00040942
H	-2.65706375	-1.00514274	0.89229998

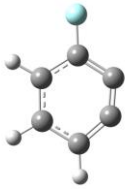




3-FluoroBenzyne

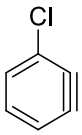
C	-1.24732500	0.35957200	0.00000000
C	0.92528700	-1.30404200	0.00000000
C	0.00000000	0.95959800	0.00000000
C	-1.28969200	-0.89418600	0.00000000
C	-0.35807000	-1.90228000	0.00000000
C	1.10477000	0.08786300	0.00000000
H	1.80005600	-1.95041300	0.00000000
H	-0.52036000	-2.97261400	0.00000000
H	2.10418600	0.51244700	0.00000000
F	0.20070000	2.28571400	0.00000000

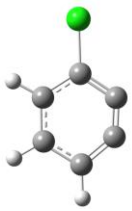




3-ChloroBenzyne

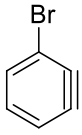
C	1.27445600	-0.01007000	0.00000000
C	-0.73431300	-1.82140500	0.00000000
C	0.00000000	0.52234400	0.00000000
C	1.45719500	-1.24885200	0.00000000
C	0.59115100	-2.31734400	0.00000000
C	-1.02613800	-0.44785400	0.00000000
H	-1.55720700	-2.53273400	0.00000000
H	0.83106200	-3.37375200	0.00000000
H	-2.06081000	-0.11827000	0.00000000
Cl	-0.38748000	2.23316700	0.00000000

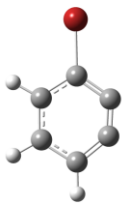




3-BromoBenzyne

C	0.40519500	1.45986200	0.00000000
C	-2.26508900	1.09240600	0.00000000
C	0.00000000	0.14302600	0.00000000
C	-0.41354200	2.40690300	0.00000000

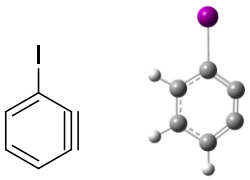




C	-1.79014200	2.42556700	0.00000000
C	-1.40294400	-0.01645700	0.00000000
H	-3.33929300	0.92146300	0.00000000
H	-2.44499400	3.28885300	0.00000000
H	-1.81732100	-1.02009600	0.00000000
Br	1.15430700	-1.37880200	0.00000000

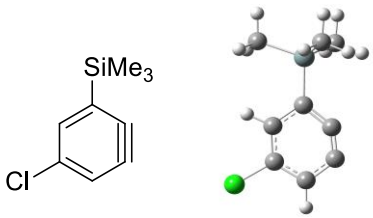
3-IodoBenzyne

C	-1.02388000	1.51909000	0.00000000
C	1.43232400	2.59979000	0.00000000
C	0.00000000	0.60208100	0.00000000
C	-0.83815300	2.75718400	0.00000000
C	0.33113300	3.48742400	0.00000000
C	1.27905800	1.20132300	0.00000000
H	2.43786600	3.01491700	0.00000000
H	0.43980500	4.56575500	0.00000000
H	2.16308800	0.57066100	0.00000000
I	-0.22874800	-1.53118300	0.00000000



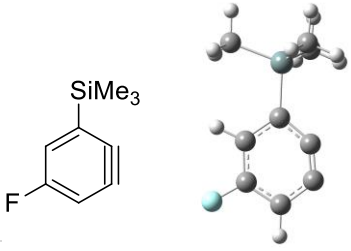
5-chloro-3-(trimethylsilyl)benzyne

C	-1.60858360	-1.23330870	-0.17875558
C	1.10912052	-2.41580030	-0.08867863
C	-1.18441768	-2.54650160	-0.27802641
C	-0.07598090	-3.12623673	-0.25110141
C	0.86016675	-1.03229376	0.03079611
Si	-3.38154166	-0.56276305	-0.24756616
C	-4.36614565	-1.35208245	1.15971997
C	-3.32894329	1.31577233	-0.05517941
C	-4.13019365	-1.04377603	-1.91522013
C	-0.42755947	-0.45751073	-0.01048660
H	2.11604512	-2.81864496	-0.05191495
H	-5.41300012	-1.02514104	1.13902233
H	-3.95143421	-1.08409851	2.13824440
H	-4.35849168	-2.44587231	1.08464598
H	-4.34345761	1.73082061	-0.09148081
H	-2.88733922	1.61624160	0.90221473
H	-2.75227041	1.79257336	-0.85643497
H	-5.17298036	-0.71150040	-1.98878993
H	-3.57651045	-0.59426443	-2.74749718
H	-4.11743797	-2.13085697	-2.05722455
H	-0.50836274	0.62087392	0.09127159
Cl	2.24255174	0.04352479	0.24448310



5-fluoro-3-(trimethylsilyl)benzyne

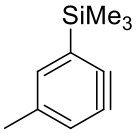
C	-0.83780025	-0.55982296	-0.04437981
C	2.05181175	-1.22998696	-0.04445781
C	-0.18781125	-1.78478896	-0.04429481



C	1.00793675	-2.15114596	-0.04432081
C	1.55497675	0.08538604	-0.04446981
Si	-2.70352725	-0.22783896	-0.04435181
C	-3.44824625	-1.01501296	1.50494219
C	-2.99393625	1.63951804	-0.04447381
C	-3.44834525	-1.01516996	-1.59352081
C	0.18693775	0.42327504	-0.04440581
H	3.11878675	-1.42992896	-0.04444381
H	-4.53727125	-0.88544496	1.52648919
H	-3.04005325	-0.56594796	2.41770919
H	-3.24092725	-2.09090296	1.54329219
H	-4.06901025	1.85664804	-0.04485181
H	-2.56356225	2.12012004	0.84194719
H	-2.56296125	2.12007504	-0.93062881
H	-4.53734525	-0.88539096	-1.61510981
H	-3.04004925	-0.56635296	-2.50636281
H	-3.24123725	-2.09110796	-1.63166881
H	-0.06417925	1.48044104	-0.04437981
F	2.44845575	1.10046304	-0.04442781

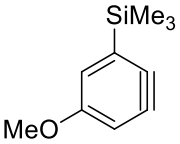
5-methyl-3-(trimethylsilyl)benzyne

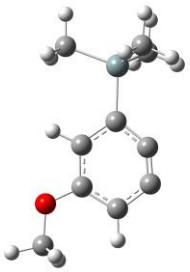
C	0.87176503	0.27776924	-0.05028342
C	-1.97979588	1.01010693	0.02502543
C	0.26973910	1.52555357	-0.05538302
C	-0.91917486	1.91194799	-0.02561870
C	-1.56187523	-0.34182990	0.03799642
C	-2.59712972	-1.44729775	0.09205889
Si	2.72001174	-0.12045241	-0.10064348
C	3.54956395	0.66526948	1.40703762
C	2.95149612	-1.99759807	-0.07187904
C	3.45254357	0.60569394	-1.68642700
C	-0.18723283	-0.67316534	0.00125248
H	-3.03511857	1.27097653	0.05298434
H	-2.47351013	-2.07179661	0.98526592
H	-3.61178321	-1.03735806	0.11289656
H	-2.52504846	-2.10989114	-0.77904039
H	4.63321845	0.49506786	1.39555926
H	3.15547888	0.24974967	2.34172655
H	3.38323687	1.74871245	1.43067359
H	4.01828552	-2.25068558	-0.10118277
H	2.53326736	-2.44643881	0.83680424
H	2.47660972	-2.48039178	-0.93413670
H	4.53492292	0.43435973	-1.73649970
H	3.00088358	0.15537420	-2.57794940
H	3.28416340	1.68770579	-1.74101609
H	0.07893781	-1.72932406	0.01320786



5-methoxy-3-(trimethylsilyl)benzyne

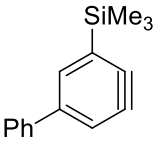
C	0.63824012	-0.24808087	0.02095951
C	-2.16925088	-1.18947087	0.02108651
C	0.12126212	-1.53862187	0.02079951
C	-1.03749788	-2.00318387	0.02075651
C	-1.82428788	0.18416713	0.02107751
Si	2.45727612	0.27403013	0.02087251
C	3.28403512	-0.43235387	-1.52702549
C	2.55779312	2.16176113	0.02109851
C	3.28432412	-0.43276587	1.56842751
C	-0.47297688	0.62663513	0.02095251
H	-3.19692888	-1.53443287	0.02097451
H	4.35402312	-0.19148287	-1.54936649
H	2.83123812	-0.03006687	-2.44062949
H	3.18810712	-1.52398687	-1.56339749
H	3.60401712	2.49085613	0.02119251
H	2.07786912	2.59414613	-0.86468949
H	2.07777212	2.59395513	0.90692651
H	4.35430112	-0.19183287	1.59066851
H	2.83164912	-0.03078187	2.48222451
H	3.18847212	-1.52441487	1.60448651
H	-0.31715388	1.70228913	0.02086351
O	-2.74571388	1.19645413	0.02095051
C	-4.12027188	0.85027813	0.02069851
H	-4.39214688	0.27391113	0.91527651
H	-4.66746788	1.79488413	0.02043451
H	-4.39175488	0.27363513	-0.87382049

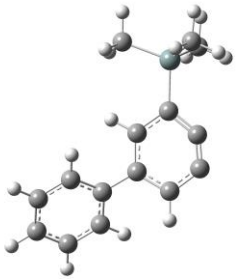




5-phenyl-3-(trimethylsilyl)benzyne

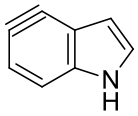
C	1.46801716	-0.39298076	-0.05038372
C	-0.94064484	1.27982124	-0.35866872
C	1.34580416	0.96669024	-0.27889972
C	0.37044316	1.73745424	-0.41966072
C	-1.03050784	-0.11876876	-0.11926772
Si	3.05814416	-1.40185976	0.13853128
C	3.99989516	-0.77185076	1.65320228
C	2.61254516	-3.22686976	0.35516228
C	4.10585316	-1.16059876	-1.41741772
C	0.14044316	-0.90340476	0.02682628
H	-1.83302084	1.88223624	-0.50162272
H	4.94949316	-1.30674676	1.77772528
H	3.41645916	-0.90783776	2.57116828
H	4.22927716	0.29633824	1.56176328
H	3.52234416	-3.83117376	0.45556228
H	2.00657416	-3.39689076	1.25290428
H	2.05493416	-3.61511776	-0.50526972
H	5.06215616	-1.69166576	-1.33573072
H	3.58994716	-1.53562376	-2.30890372

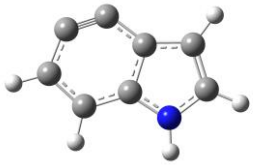




H	4.32785816	-0.10009276	-1.58518872
H	0.01475916	-1.96401576	0.23167428
C	-2.37107084	-0.75980476	-0.02522772
C	-2.62886984	-1.99834776	-0.63740372
C	-3.41782984	-0.13487476	0.67322028
C	-3.88737184	-2.59184476	-0.55128472
H	-1.84105184	-2.48624976	-1.20478272
C	-4.67795084	-0.72628076	0.75612928
H	-3.23305884	0.81073324	1.17543428
C	-4.91820884	-1.95803176	0.14510628
H	-4.06508284	-3.54777476	-1.03718172
H	-5.47052884	-0.22729876	1.30768428
H	-5.89945984	-2.42019776	0.21100828

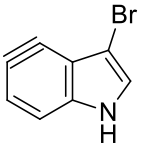
4,5-indolyne

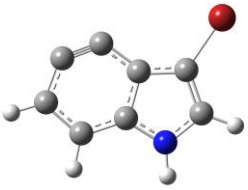




C	0.64029882	-1.43934965	0.00647917
C	1.33745482	1.18640635	0.00647917
C	1.83163282	-1.07206565	0.00647917
C	-0.46164118	-0.58313065	0.00647917
C	-0.01677318	0.79124035	0.00647917
C	2.35760682	0.22105235	0.00647917
N	-1.16427018	1.56059435	0.00647917
C	-2.27546318	0.74218335	0.00647917
C	-1.88894718	-0.57585065	0.00647917
H	1.59913282	2.24202335	0.00647917
H	3.40691982	0.49509335	0.00647917
H	-1.19165318	2.56832435	0.00647917
H	-3.26792218	1.17095235	0.00647917
H	-2.54799218	-1.43204865	0.00647917

3-bromo-4,5-indolyne

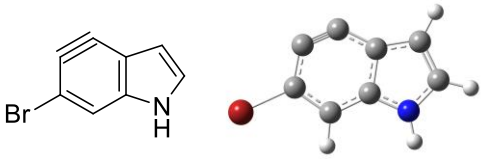




C	0.18414312	2.92454006	0.04076794
C	2.76637012	3.81862206	0.04076794
C	0.48149512	4.13491206	0.04076794
C	1.13323712	1.90425306	0.04076794
C	2.47316912	2.43788806	0.04076794
C	1.72707112	4.76202606	0.04076794
N	3.32507012	1.35080906	0.04076794
C	2.59517812	0.17984906	0.04076794
C	1.25695112	0.48465406	0.04076794
H	3.79932312	4.15843806	0.04076794
H	1.91808212	5.82921406	0.04076794
H	4.33249712	1.39557406	0.04076794
H	3.07914212	-0.78538794	0.04076794
Br	-0.15959788	-0.75470794	0.04076794

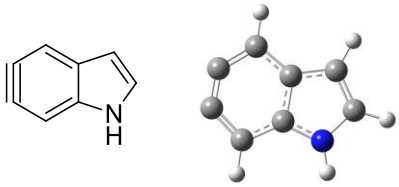
6-bromo-4,5-indolyne

C	1.22022000	1.56123500	0.00000000
C	0.00000000	-0.82544600	0.00000000
C	-0.02579700	1.51767200	0.00000000
C	2.13736500	0.51944100	0.00000000
C	1.40677000	-0.72862600	0.00000000
C	-0.76982300	0.34585100	0.00000000
N	2.36330400	-1.72323400	0.00000000
C	3.62399300	-1.16065000	0.00000000
C	3.52919900	0.20921900	0.00000000
H	-0.49286400	-1.79260700	0.00000000
H	2.17400100	-2.71363500	0.00000000
H	4.50155500	-1.79172800	0.00000000
H	4.35451000	0.90604100	0.00000000
Br	-2.68034000	0.25206900	0.00000000



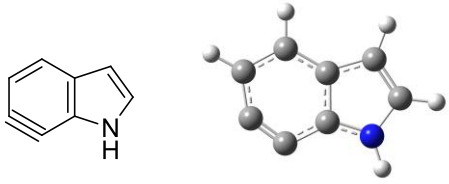
5,6-indolye

C	-0.83423100	-1.65507300	0.00000000
C	-1.29192700	1.27615400	0.00000000
C	-2.02217000	-0.96287400	0.00000000
C	0.24800900	-0.72951300	0.00000000
C	0.00000000	0.69192100	0.00000000
C	-2.24028300	0.27393800	0.00000000
N	1.23582300	1.30838300	0.00000000
C	2.23526500	0.35251400	0.00000000
C	1.67576500	-0.89684600	0.00000000
H	-0.69023400	-2.73065300	0.00000000
H	-1.45965600	2.34956600	0.00000000
H	1.38562000	2.30485800	0.00000000
H	3.27524800	0.64973900	0.00000000
H	2.21569500	-1.83351600	0.00000000



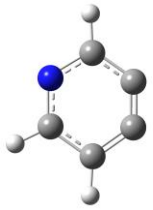
6,7- indolyne

C	0.65318100	-1.63781800	0.00000000
C	1.36845300	1.04294100	0.00000000
C	1.82241400	-1.19276200	0.00000000
C	-0.38316100	-0.70615900	0.00000000
C	0.00000000	0.68188100	0.00000000
C	2.38777500	0.07437000	0.00000000
C	-2.26008300	0.52776600	0.00000000
H	1.64972300	2.09347600	0.00000000
H	3.44076400	0.32800900	0.00000000
H	-1.33319500	2.50564200	0.00000000
H	-3.32804200	0.69512500	0.00000000
H	-2.30321500	-1.60813000	0.00000000
N	-1.75599800	-0.76164800	0.00000000
C	-1.22758800	1.42935100	0.00000000



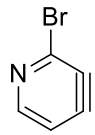
3,4-pyridyne

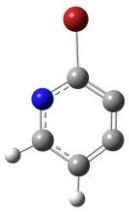
C	1.17312054	-0.05009640	0.01487039
C	0.41253023	-1.21305721	0.00241269
C	-0.84565573	-1.24169654	-0.01693514
C	-1.67104741	-0.13852230	-0.02889263
C	-0.88273288	1.04644060	-0.01600236
N	0.44834257	1.08522163	0.00447979
H	2.25494216	0.02648662	0.03154394
H	-2.75518712	-0.10393602	-0.04552843
H	-1.38822797	2.01032097	-0.02313250



5-bromo-3,4-pyridyne

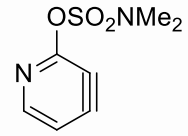
C	2.04419932	3.25466502	-0.16387685
N	3.33571764	0.94834027	-0.05049318
C	3.41321935	3.38688374	-0.22423567
C	1.38883244	2.18698341	-0.06461269
C	2.00216871	0.95019134	-0.00085147
C	4.00666196	2.09520938	-0.15588678
H	4.00794804	4.28869649	-0.30961551
H	5.09086621	2.01289277	-0.19058473
Br	1.09544082	-0.71236433	0.14947235

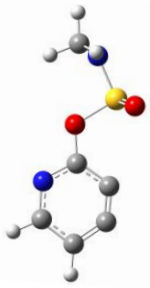




2-sulfamate-3,4-pyridyne

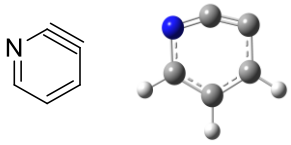
C	0.45288934	-1.12761540	0.08375883
N	-0.33924909	1.38229065	0.17177923
C	1.48871486	-0.24179724	0.27610167
C	-0.77251348	-0.89140067	-0.04912426
C	-1.23994701	0.41467215	-0.01006722
C	0.95068443	1.07259342	0.30709403
O	-2.53470535	0.84369779	-0.13728597
S	-3.76112659	-0.31067929	-0.37156425
N	-5.04611713	0.72172602	-0.45247953
C	-5.13904871	1.56013272	-1.65693122
C	-5.43893877	1.37962340	0.80255334
O	-3.54460957	-0.91213211	-1.67511907
O	-3.85198114	-1.09716287	0.84543098
H	2.54733659	-0.43817012	0.39144252
H	1.62847024	1.91141346	0.45210396
H	-4.88304424	0.96529363	-2.53324399
H	-6.17664722	1.89373184	-1.74698836
H	-4.47935069	2.43577950	-1.59687668
H	-4.79953222	2.24314854	1.02849653
H	-5.38931137	0.66052452	1.61970093
H	-6.47370790	1.71485679	0.68906164





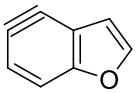
2,3-pyridyne

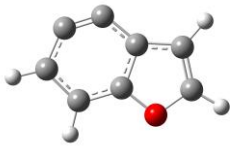
C	1.26598582	-0.46777355	-0.17218085
C	1.32290896	0.95585986	-0.16258081
C	0.02426829	-0.72525478	-0.02964257
C	0.11895782	1.68470397	-0.01319560
H	0.13500342	2.77035766	-0.00266872
H	2.26728326	1.48997898	-0.26712068
C	-1.10719359	1.02718736	0.12294736
N	-1.17539222	-0.35285862	0.11516648
H	-2.05177452	1.54794914	0.23956657



4,5-benzofuranyne

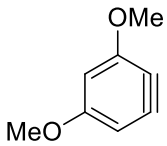
C	0.61143800	-1.65532200	0.00000000
C	1.34662000	0.97586300	0.00000000
C	1.80310200	-1.28456600	0.00000000
C	-0.46461600	-0.76851600	0.00000000
C	0.00000000	0.57863700	0.00000000
C	2.35461200	-0.00508900	0.00000000
C	-2.19511500	0.63094200	0.00000000
C	-1.89927800	-0.69474200	0.00000000
H	1.60091800	2.03126100	0.00000000
H	3.40850800	0.24893500	0.00000000
H	-3.13210300	1.16776200	0.00000000
H	-2.60636300	-1.51160300	0.00000000
O	-1.07644100	1.42505100	0.00000000

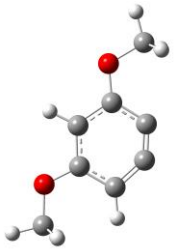




3,5-dimethoxybenzyne

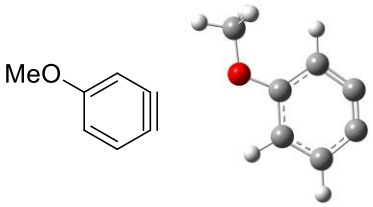
C	0.81998075	1.40613269	-0.01453772
C	-1.54651025	0.03844169	-0.01497072
C	0.91720275	0.00669369	-0.01447972
C	-0.31559625	1.92934769	-0.01459572
C	-1.60751525	1.46090069	-0.01500672
C	-0.31892425	-0.66195331	-0.01474772
H	-2.52465725	2.03241769	-0.01537172
H	-0.34355225	-1.74621831	-0.01489372
O	2.05716475	-0.72112431	-0.01412372
C	3.26910975	0.02571469	-0.01562972
H	3.34007375	0.65646869	-0.91012272
H	4.07694375	-0.70793531	-0.01293772
H	3.33895675	0.66185069	0.87512528
O	-2.65935625	-0.75285331	-0.01509272





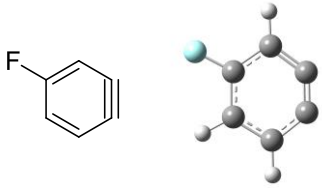
C	-3.93131325	-0.12599431	-0.01493272
H	-4.07579425	0.49328969	-0.91025372
H	-4.66336925	-0.93558031	-0.01466072
H	-4.07546025	0.49350469	0.88027328

4-methoxybenzyne



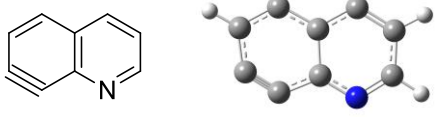
C	-1.09067277	0.23101745	0.08947834
C	1.46200623	-0.53134355	0.09003034
C	-0.93235777	-1.15094755	0.08980634
C	-0.17605377	1.07978945	0.08965034
C	1.19149323	0.86058045	0.09016834
C	0.42345923	-1.50160855	0.08980534
H	1.96795323	1.61540745	0.09018334
H	0.72080523	-2.54629755	0.08963134
O	2.72484323	-1.05338255	0.08990734
C	3.82244823	-0.15504655	0.09003234
H	3.82245723	0.48123745	0.98515834
H	4.71878423	-0.77783955	0.08991134
H	3.82242623	0.48153345	-0.80488266
H	-1.72263477	-1.89471455	0.08953534

4-flouro bnezyne



C	1.78248700	0.34489200	0.00080200
C	-0.80975700	-0.05064600	-0.00054200
C	1.44882600	-1.00163500	-0.00045200
C	1.00416900	1.32248100	0.00067800
C	-0.37843600	1.28944600	-0.00085800
C	0.05236600	-1.16474100	-0.00009500
H	-1.08065900	2.11567600	-0.00055700
H	-0.39284200	-2.15502600	0.00046100
H	2.13415000	-1.84277500	0.00011200
F	-2.13984200	-0.28407300	0.00031000

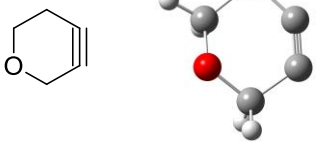
7,8-quinolyne



C	-1.30657778	0.87127457	-0.16110778
N	-1.06642645	-1.93692208	0.07793014
C	-2.41341652	0.05183313	-0.20802789
C	-0.01901913	0.30528177	0.00991270
C	0.02705424	-1.14913008	0.12595175
C	-2.23751278	-1.34501623	-0.08353007
C	1.36345962	-1.56576878	0.29036753
C	2.36691812	-0.83649816	0.33395019

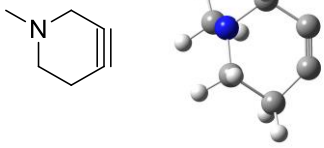
C	2.43652549	0.56144266	0.23370718
C	1.16868267	1.10474479	0.06638030
H	-1.40989282	1.94978762	-0.25401111
H	-3.41066423	0.46084058	-0.33823678
H	-3.10543812	-2.00238569	-0.11918758
H	3.33406012	1.16891051	0.27612462
H	1.06127277	2.18356596	-0.02695259

3,4-oxacyclohexyne



C	0.66814672	1.26806434	0.11565878
C	0.88818234	-1.04382227	0.16359203
C	-1.31368188	-0.03733346	0.03163910
O	-0.38676333	-1.04436099	-0.43592387
C	-0.55732533	1.24817454	0.11891108
C	1.73453696	0.29131516	-0.07330894
H	0.81407670	-1.19316601	1.25136123
H	1.42187124	-1.88745493	-0.28369030
H	-1.71817445	-0.31369590	1.01596217
H	-2.12732462	-0.04263353	-0.69768764
H	2.55666654	0.31974461	0.65115368
H	2.16120003	0.32335880	-1.08263898

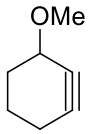
3,4-piperidyne

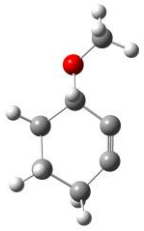


C	1.27248699	0.78365633	-0.50032927
C	0.12174099	-0.81911867	0.79942673
C	-0.87464701	1.39638633	0.44018673
C	0.39858299	1.63140033	-0.33832827
C	1.36259699	-0.64787367	-0.21985427
H	0.48085499	-0.49307067	1.78140173
H	-0.13894701	-1.88098967	0.86205373
H	-0.75442801	1.77994233	1.45997273
H	-1.76818301	1.86042833	0.01268473
H	2.27663299	-0.98420767	0.28400873
H	1.23356399	-1.26564867	-1.11782127
N	-1.07804401	-0.06714167	0.48110973
C	-1.77820501	-0.56986567	-0.70197627
H	-1.94386101	-1.64649667	-0.59325027
H	-2.75705101	-0.08548367	-0.77815027
H	-1.23240701	-0.39252267	-1.64295327

3-methoxycyclohexanyne

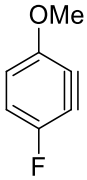
C	-0.28324061	-1.21688547	0.05549856
C	-0.74451561	1.14036853	-0.17096744
C	-2.70021261	-0.61738447	-0.21100444
C	-2.19081461	0.80435853	0.25207156
C	-1.48841861	-1.42635447	-0.01369044
C	0.34007539	0.12936653	0.32212556
O	1.53206639	0.42221453	-0.36427744
C	2.61777939	-0.38572347	0.04615156
H	-0.66791861	1.17141353	-1.26436144
H	-0.47883261	2.13852153	0.19901356
H	-3.00496361	-0.60370947	-1.26496844
H	-3.57141161	-0.92049647	0.38049856
H	-2.87030661	1.56735453	-0.14865844
H	-2.26944461	0.85007253	1.34558956
H	0.50430339	0.23201353	1.40853256
H	3.47535339	-0.10933247	-0.57196844
H	2.86798539	-0.22112547	1.10658956
H	2.38768139	-1.45200647	-0.09739844

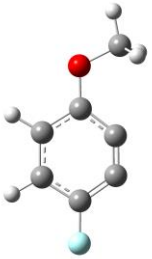




5-methoxy-3-fluorobenzyne

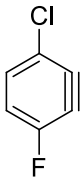
C	0.63705072	-0.91265021	0.01148055
C	-1.05102228	1.13481779	0.01122755
C	1.27534072	0.32009079	0.01118555
C	-0.59488828	-1.14098921	0.01138855
C	-1.57396728	-0.17150321	0.01089355
C	0.32928772	1.37349179	0.01135655
H	-1.74714728	1.96933079	0.01144355
H	0.70576472	2.39293879	0.01157855
O	2.59875472	0.58947679	0.01126255
C	3.45339372	-0.55042121	0.01139455
H	3.28585972	-1.16379821	0.90566055
H	4.47452972	-0.16664321	0.01144255
H	3.28598372	-1.16390421	-0.88282345
F	-2.89815628	-0.38824121	0.01140555

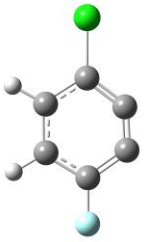




3-chloro-6-fluorobenzyne

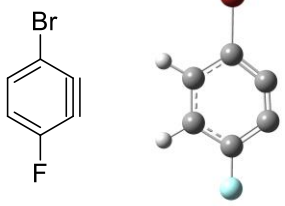
C	-1.30295500	-0.99895000	0.00000000
C	1.13760700	0.15543200	0.00000000
C	-0.23442600	-1.87319400	0.00000000
C	-1.15115900	0.24339200	0.00000000





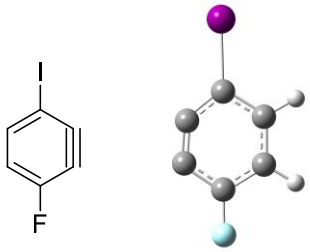
C	0.00000000	0.99340600	0.00000000
C	1.02318900	-1.24265500	0.00000000
H	2.12229200	0.61454800	0.00000000
H	1.91540200	-1.86218200	0.00000000
F	-0.32684000	-3.20678300	0.00000000
Cl	0.12178400	2.73200500	0.00000000

3-bromo-6-fluorobenzyne



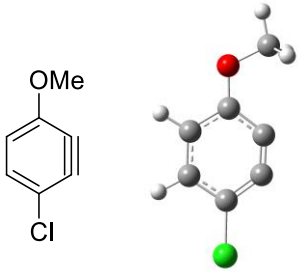
C	1.47617272	-0.76815001	-0.12685424
C	-1.04235491	0.22494645	-0.05703756
C	0.46491060	-1.70555519	-0.03980124
C	1.22553645	0.45783457	-0.16969379
C	0.03480273	1.13505091	-0.14585908
C	-0.83219843	-1.16102366	-0.00530409
H	-2.05460664	0.61766033	-0.02869252
H	-1.67882599	-1.83799994	0.06281415
F	0.64522333	-3.02950638	0.01053990
Br	-0.22195832	3.01239184	-0.21719321

6-fluoro-3-iodobenzyne



C	-0.39931131	4.14915783	-0.15288552
C	1.70984160	2.43334362	-0.05753976
C	0.85507132	4.72970239	-0.10736455
C	-0.51057854	2.90099668	-0.14856365
C	0.40513031	1.88806824	-0.10529623
C	1.92844728	3.82024685	-0.05858856
H	2.56190586	1.76060132	-0.01916424
H	2.94122817	4.21071385	-0.02128849
F	1.08808698	6.04664399	-0.10735508
I	0.01947440	-0.20231486	-0.10593532

3-Chloro-5-methoxybenzyne

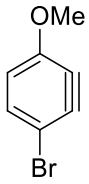


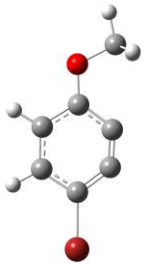
C	-1.72115705	-1.83905464	0.02453395
C	-0.12190905	0.31494536	0.02450595
C	-2.40124405	-0.62474364	0.02404395
C	-0.47414505	-1.94838764	0.02458095
C	0.48353295	-0.96377164	0.02418595
C	-1.51151805	0.47876436	0.02436295
H	0.51928495	1.19242636	0.02482395
H	-1.93836105	1.47793236	0.02457295
O	-3.73244205	-0.41334764	0.02420395
C	-4.54354805	-1.58601064	0.02448095

H	-4.35174805	-2.19184764	-0.86946105
H	-5.57798905	-1.24000864	0.02456195
H	-4.35153805	-2.19162064	0.91853095
Cl	2.21731295	-1.17612464	0.02468895

3-bromo-5-methoxybenzyne

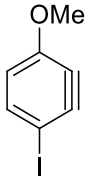
C	1.80446735	0.51875847	-0.04346645
C	0.27190235	2.73160047	-0.04342845
C	2.51834735	1.71489447	-0.04323245
C	0.55340135	0.46580747	-0.04347745
C	-0.37471965	1.47300147	-0.04327845
C	1.66622535	2.84831647	-0.04336445
H	-0.33988065	3.62956147	-0.04356545
H	2.12666635	3.83237847	-0.04344645
O	3.85550835	1.88429947	-0.04326145
C	4.63022935	0.68719747	-0.04338145
H	4.41959235	0.08759347	0.85044755
H	5.67475235	1.00147247	-0.04339045
H	4.41954035	0.08772347	-0.93728545
Br	-2.26711665	1.30002347	-0.04355245

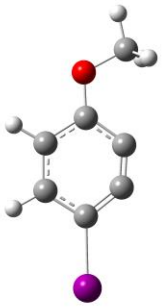




3-iodo-5-methoxybenzyne

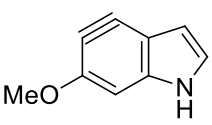
C	2.51610988	0.58010582	-0.15523728
C	1.02208988	2.83578282	-0.15516728
C	3.24678388	1.76812982	-0.15550228
C	1.26305788	0.57607582	-0.15521828
C	0.34781588	1.58942882	-0.15539028
C	2.41994988	2.92072182	-0.15528028
H	0.43686688	3.75152782	-0.15496228
H	2.90121588	3.89477882	-0.15512428
O	4.58665388	1.91140682	-0.15531228
C	5.33898188	0.70068282	-0.15510728
H	5.11699188	0.10475082	0.73846872
H	6.38923488	0.99545282	-0.15499128
H	5.11721788	0.10462882	-1.04865828
I	-1.77458112	1.41192282	-0.15522228

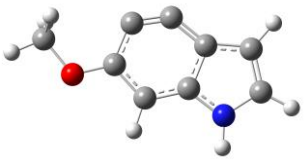




6-methoxy-4,5-indolyne

C	-0.01267792	1.76220839	-0.02318313
C	0.39839008	-0.86089361	-0.02291413
C	1.17435908	1.37438439	-0.02308013
C	-1.21637592	1.08083039	-0.02308513

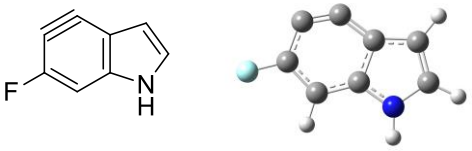




C	-0.90688492	-0.33215861	-0.02303913
C	1.50457508	0.00610239	-0.02275213
N	-2.12624792	-0.97881361	-0.02325913
C	-3.15439492	-0.05213161	-0.02303513
C	-2.63861592	1.21832039	-0.02302213
H	0.57287308	-1.93263061	-0.02297213
H	-2.25181092	-1.97894661	-0.02347613
H	-4.18391592	-0.38107661	-0.02303713
H	-3.20550592	2.13793739	-0.02300613
O	2.75450508	-0.52475561	-0.02312513
C	3.82234508	0.41434039	-0.02317813
H	3.78658708	1.05236739	-0.91508513
H	4.74278308	-0.17248761	-0.02406013
H	3.78759808	1.05126539	0.86955987

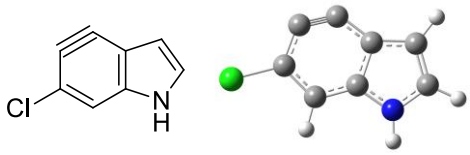
6-Fluoro-4,5-indolyne

C	-0.52236464	-0.84385048	-0.06652726
C	1.58595336	0.76424652	-0.06652726
C	0.59834736	-1.39501448	-0.06652726
C	-0.92081564	0.48075752	-0.06652726
C	0.27699636	1.29024552	-0.06652726
C	1.75867236	-0.62170648	-0.06652726
N	-0.15730064	2.59899652	-0.06652726
C	-1.53934364	2.63751752	-0.06652726
C	-2.04412964	1.36203752	-0.06652726
H	2.45870736	1.40970552	-0.06652726
H	0.44188936	3.40984752	-0.06652726
H	-2.05772264	3.58585852	-0.06652726
H	-3.08887364	1.08786752	-0.06652726
F	3.00255136	-1.13487648	-0.06652726



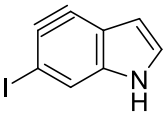
6-chloro-4,5-indolyne

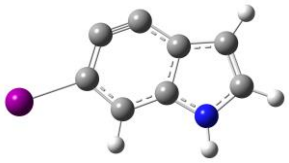
C	-1.15861251	0.42340943	0.01423515
C	1.42112749	1.12312543	0.01423515
C	-0.29827951	-0.47929357	0.01423515
C	-1.01060351	1.80220243	0.01423515
C	0.40429149	2.09974743	0.01423515
C	1.07143149	-0.23431157	0.01423515
N	0.49775849	3.47653243	0.01423515
C	-0.76623251	4.03208043	0.01423515
C	-1.71671851	3.04127543	0.01423515
H	2.46838649	1.40888543	0.01423515
H	1.35829849	4.00207343	0.01423515
H	-0.88872151	5.10600443	0.01423515
H	-2.78740551	3.18366243	0.01423515
Cl	2.31840349	-1.47344357	0.01423515



6-iodo-4,5-indolyne

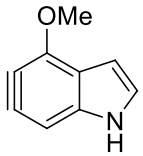
C	2.33116900	0.16315100	0.00000000
C	-0.08549000	-1.01701200	0.00000000
C	1.29877700	0.86291700	0.00000000
C	2.43304600	-1.22260900	0.00000000
C	1.09992800	-1.78302300	0.00000000
C	0.00000000	0.38311100	0.00000000
N	1.26790000	-3.15333700	0.00000000
C	2.61399300	-3.45909600	0.00000000
C	3.36060800	-2.30594900	0.00000000
H	-1.05543100	-1.50433900	0.00000000
H	0.52262400	-3.83245800	0.00000000
H	2.93779600	-4.49039200	0.00000000
H	4.43894900	-2.24415800	0.00000000
I	-1.77417800	1.59275000	0.00000000

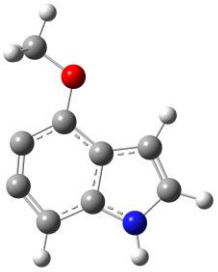




4-methoxy-5,6-indolye

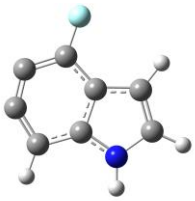
C	-1.06492600	-0.01495300	0.00011000
C	1.12439200	1.97350900	-0.00001200
C	-1.22445800	1.36360800	0.00012100
C	0.30287300	-0.41655800	0.00014400
C	1.34831100	0.56602500	0.00005900
C	-0.23440300	2.13972300	-0.00007100
N	2.53958700	-0.12874100	-0.00003900
C	2.28805500	-1.49271500	-0.00018100
C	0.93694000	-1.70566300	0.00015100
H	1.90720300	2.72255300	-0.00012700
H	3.45464500	0.29287500	-0.00013300
H	3.10738600	-2.19842500	-0.00029900
H	0.43978500	-2.66459900	0.00033600
O	-2.02751500	-0.96594300	-0.00000100
C	-3.36574700	-0.48162000	-0.00014000
H	-3.56042900	0.12728900	-0.89167200
H	-3.56196400	0.12352600	0.89362500
H	-4.00982900	-1.36263900	-0.00252600





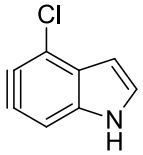
4-Fluoro-5,6-indolye

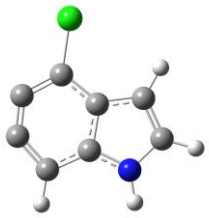
C	-1.41502000	0.43455100	0.00000000
C	0.16385500	-2.03212100	0.00000000
C	-1.94891400	-0.83230200	0.00000000
C	0.00000000	0.48524000	0.00000000
C	0.75447900	-0.73783800	0.00000000
C	-1.19105800	-1.83689200	0.00000000



N	2.08453600	-0.37633500	0.00000000
C	2.19419100	1.00595100	0.00000000
C	0.94627600	1.56556700	0.00000000
H	0.71984700	-2.96204200	0.00000000
H	2.86009800	-1.01977800	0.00000000
H	3.16867800	1.47455100	0.00000000
H	0.71702100	2.62109300	0.00000000
F	-2.12002800	1.57862100	0.00000000

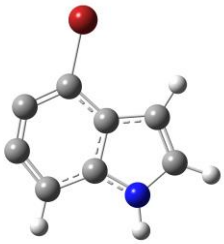
4-chloro-5,6-indolye





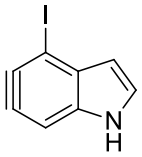
C	0.92366200	-0.70932700	0.00000000
C	-1.97922500	-1.20158200	0.00000000
C	0.30844900	-1.93601800	0.00000000
C	0.00000000	0.37180800	0.00000000
C	-1.41620600	0.10191900	0.00000000
C	-0.93738800	-2.09427300	0.00000000
N	-2.04899200	1.32672200	0.00000000
C	-1.10559700	2.33944600	0.00000000
C	0.15140600	1.79830900	0.00000000
H	-3.04441500	-1.40450900	0.00000000
H	-3.04759300	1.46291400	0.00000000
H	-1.41728300	3.37488100	0.00000000
H	1.08332600	2.34426100	0.00000000
Cl	2.65284100	-0.41684000	0.00000000

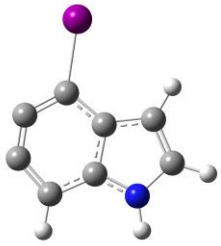
4-bromo-5,6-indolye



C	0.50110266	1.10541764	-0.01588394
C	-1.67390334	-0.87845036	-0.01588394
C	-0.84242234	1.36759664	-0.01588394
C	0.78419866	-0.28699136	-0.01588394
C	-0.30029534	-1.23736436	-0.01588394
C	-1.74371534	0.49313164	-0.01588394
N	0.27667966	-2.48954536	-0.01588394
C	1.65555766	-2.36804136	-0.01588394
C	2.00169666	-1.04395436	-0.01588394
H	-2.48832534	-1.59472336	-0.01588394
H	-0.22960334	-3.36103236	-0.01588394
H	2.28034766	-3.25062336	-0.01588394
H	3.00361066	-0.64061836	-0.01588394
Br	1.91195866	2.38975564	-0.01588394

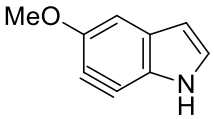
4-iodo-5,6-indolye

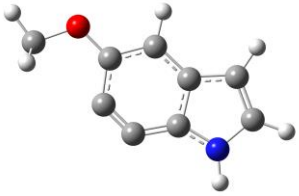




C	-0.55688840	-0.31940498	-0.00855972
C	2.20891460	-1.33572098	-0.00855972
C	-0.15519340	-1.62407798	-0.00855972
C	0.54804860	0.57679202	-0.00855972
C	1.89318460	0.04763802	-0.00855972
C	1.02924460	-2.04194498	-0.00855972
N	2.74294260	1.13360902	-0.00855972
C	2.00517460	2.30341102	-0.00855972
C	0.66873660	2.00637302	-0.00855972
H	3.22240960	-1.72304998	-0.00855972
H	3.74944760	1.08130402	-0.00855972
H	2.50300660	3.26331102	-0.00855972
H	-0.14325540	2.71881502	-0.00855972
I	-2.58020840	0.38402102	-0.00855972

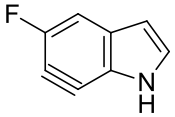
5-methoxy-6,7- indolyne

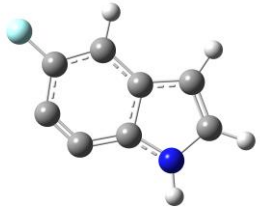




C	-0.06398922	-1.41708275	-0.00633552
C	-0.52410222	1.25186125	-0.00597352
C	-1.23253922	-0.97287375	-0.00630752
C	1.07936778	-0.64146275	-0.00621152
C	0.80593778	0.77300125	-0.00614652
C	-1.62120022	0.37448325	-0.00604152
C	3.04961878	0.42611525	-0.00646752
H	-0.72899722	2.31877925	-0.00596952
H	2.28931178	2.47458925	-0.00670152
H	4.12764178	0.50607925	-0.00658952
H	2.92033178	-1.70483375	-0.00529052
O	-2.88664622	0.86842425	-0.00619052
C	-3.92104922	-0.10561375	-0.00634752
H	-3.86497922	-0.74156475	-0.89958152
H	-4.86238622	0.44696325	-0.00649452
H	-3.86524122	-0.74154375	0.88691648
N	2.44417278	-0.81717175	-0.00572852
C	2.09487678	1.41078325	-0.00649752

5-fluoro-6,7- indolyne

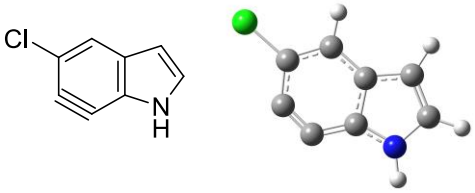




C	-0.72071900	-1.47075600	0.00000000
C	1.33023000	0.28723900	0.00000000
C	0.45566500	-1.89174700	0.00000000
C	-1.11088700	-0.14519700	0.00000000
C	0.00000000	0.77175700	0.00000000

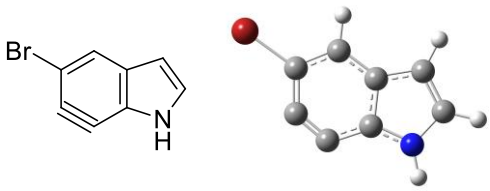
C	1.58933500	-1.08405500	0.00000000
C	-1.94860200	1.93223700	0.00000000
H	2.17389200	0.97126500	0.00000000
H	-0.05718300	3.02647200	0.00000000
H	-2.73015700	2.67875600	0.00000000
H	-3.20566300	0.20581600	0.00000000
F	2.85262800	-1.54329000	0.00000000
C	-0.58585500	2.08368700	0.00000000
N	-2.27279200	0.58690200	0.00000000

5-chloro-6,7- indolyne



C	-2.42402440	-0.40604594	0.03381170
C	0.16127960	0.46987306	0.03381170
C	-1.45580940	-1.19445994	0.03381170
C	-2.26749440	0.97075306	0.03381170
C	-0.89548740	1.41063806	0.03381170
C	-0.09869840	-0.90808694	0.03381170
C	-2.26957440	3.21219106	0.03381170
H	1.19394760	0.80624806	0.03381170
H	-0.10756440	3.52623606	0.03381170
H	-2.71724640	4.19593306	0.03381170
H	-4.07842240	2.07592006	0.03381170
Cl	1.19624260	-2.08898394	0.03381170
N	-3.07048540	2.08272806	0.03381170
C	-0.94860540	2.84683106	0.03381170

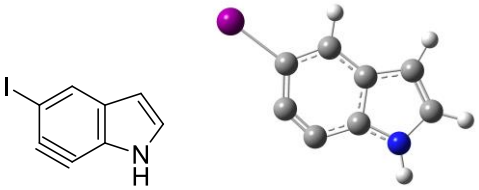
5-bromo-6,7- indolyne



C	3.57571401	1.04507281	0.05802625
C	0.85311701	0.74772581	0.05802625
C	3.01573701	-0.07121519	0.05802625
C	2.84532001	2.22443381	0.05802625
C	1.41537501	2.04618681	0.05802625
C	1.67033801	-0.39190219	0.05802625
C	1.90217801	4.25851781	0.05802625
H	-0.22491099	0.61706281	0.05802625
H	-0.19100899	3.63236281	0.05802625
H	1.89373801	5.33932081	0.05802625
H	4.02155001	3.98968681	0.05802625
Br	0.94190301	-2.15298219	0.05802625
C	0.85802301	3.37074481	0.05802625
N	3.10442801	3.57142681	0.05802625

5-iodo-6,7- indolyne

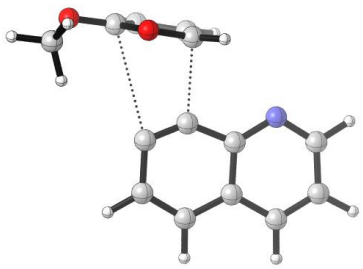
C	0.47555287	0.37631104	0.15414728
C	-2.13328913	-0.50108996	0.15414728
C	-0.51547513	1.13797204	0.15414728
C	0.29736587	-1.00163096	0.15414728
C	-1.07486613	-1.44204796	0.15414728
C	-1.86986613	0.87797304	0.15414728
C	0.29682387	-3.24483396	0.15414728
H	-3.16350313	-0.84483796	0.15414728
H	-1.86555213	-3.55703696	0.15414728
H	0.74483787	-4.22840796	0.15414728
H	2.10684987	-2.10879896	0.15414728
I	-3.42741213	2.34093304	0.15414728
C	-1.02402413	-2.87869696	0.15414728
N	1.09883887	-2.11505696	0.15414728



The Cartesian coordinates of transition state structures of Fig. 5 (HF/6-31G*).

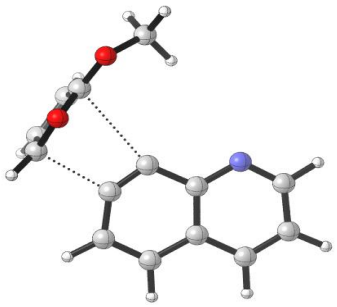
TS1

N	1.99247200	-1.45908800	-0.26155100
C	3.85525500	0.60994900	-0.00699600
C	1.59627600	-0.19561200	-0.06592600
C	3.27333100	-1.68066300	-0.32529600
C	4.25535500	-0.68014000	-0.20401000
C	2.48068600	0.90855100	0.07142400
C	1.96394900	2.23376400	0.27775700
C	0.62843700	2.48632400	0.35040500
C	-0.26950400	1.37205500	0.22384500
C	0.28220000	0.27318400	0.02999700
C	-1.30652600	-1.79486400	0.81955100
C	-1.21323800	-1.49709200	-0.49986400
O	-2.28235500	-0.73539900	-0.86029000
C	-2.96602100	-0.47459700	0.24397900
C	-2.45091800	-1.11617200	1.31843100
H	4.57872200	1.40051700	0.08907800
H	3.57340900	-2.70264600	-0.48201900
H	5.29485000	-0.94205000	-0.26811300
H	2.67260700	3.03841500	0.38029700
H	0.27527200	3.49005100	0.50868900
H	-0.61437700	-2.40092400	1.36576000
H	-2.81126200	-1.06003200	2.32236400



H	-0.60306900	-1.87000200	-1.28991900
O	-4.03621700	0.28188400	0.14843900
C	-4.05389800	1.27446200	-0.86391500
H	-4.93322000	1.86935100	-0.67335900
H	-3.16277300	1.88382100	-0.80097900
H	-4.12119100	0.82033800	-1.84243900

TS2



N	-1.82366100	1.66379200	0.09319400
C	-3.81237900	-0.29062900	-0.01369800
C	-1.47801600	0.35972000	0.02215800
C	-3.08244600	1.97191100	0.10554700
C	-4.13180700	1.02905100	0.05421800
C	-2.45201900	-0.67539600	-0.03351800
C	-2.06017600	-2.05348600	-0.10568400
C	-0.74583700	-2.41700000	-0.12247900
C	0.07758500	-1.28836300	-0.06971000
C	-0.11314900	-0.05589400	0.01498800
C	2.79920100	-0.07000700	1.11732000
C	2.71661700	0.39452700	-0.17072200
O	2.54696900	-0.58422700	-1.02714900
C	2.30019000	-1.71227000	-0.30162400
C	2.55534600	-1.44695600	1.01627700
O	2.87071300	1.57585100	-0.70862100
C	2.53372600	2.69566900	0.08958300
H	-4.58149900	-1.04251700	-0.05382700
H	-3.31987400	3.02153500	0.16046400
H	-5.15306400	1.36248000	0.06996800
H	-2.82834200	-2.80603200	-0.15099200
H	-0.41729100	-3.43680700	-0.18196200
H	2.93587100	0.51194700	2.00243700
H	2.28562900	-2.62464100	-0.85545100
H	2.49839400	-2.15561100	1.81688900
H	3.21593400	2.78911400	0.92573200
H	1.51438400	2.60000800	0.43736000
H	2.63300500	3.55571400	-0.55275200