Click Organocatalysis: Acceleration of Azide–Alkyne Cycloadditions with Mutually Orthogonal Click Reactions

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Content	Page

M06-2X/6-311++G(d,p)//M06-2X/6-31G(d) Energetic Data

E: Electronic energies

G: Gibbs energies

	E	***G***
1	−891.934779	−891.908012
2	−305.174638	−305.13157
3	−1150.875607	−1150.561921
4	−688.843078	−688.682275
TS (1+2) 1,4-triazole	−1197.113848	−1197.020665
TS (1+2) 1,5-triazole	−1197.11494	−1197.02064
TS (1+3) 1,4-triazole	−2042.805805	−2042.43778
TS (1+3) 1,5-triazole	−2042.803379	−2042.435503
TS (1+4) 1,4-triazole	−1580.761377	−1580.548181
TS (1+4) 1,5-triazole	−1580.763967	−1580.550089
5	−1153.282608	−1152.926517
TS-1	−1458.449663	−1458.024118
6	−1458.517387	−1458.088055
TS-2a	−2350.448477	−2349.96399
TS-2b	−2350.44259	−2349.957566
7a	−2350.531488	−2350.040837
7b	−2350.527915	−2350.03732
TS-3a	−2350.503696	−2350.015103
TS-3b	−2350.491073	−2350.003559
8a	−1197.233028	−1197.132273
8b	−1197.228653	−1197.127378

M06-2X/6-31G(d) Optimized Coordinates

1

N	2.09134300	1.06713300	-0.00004500
N	4.08496400	-0.19663800	0.00013600
N	3.08791800	0.32511100	0.00003000
C	0.81925700	0.47966600	-0.00004700
C	-0.26734200	1.36015200	-0.00003500
C	0.53977900	-0.88864000	-0.00005000
C	-1.57308300	0.89456600	-0.00000100
C	-0.76401600	-1.36402100	-0.00002100
C	-1.82675500	-0.47183200	0.00000400
F	1.54440300	-1.76907000	-0.00006900
F	-0.99123400	-2.67271300	0.00000400
F	-3.07641200	-0.91941200	0.00005900
F	-2.58455100	1.75506300	0.00004300
F	-0.04960900	2.66962100	-0.00003100

2

C	2.63100900	-0.40106500	-0.00005600
H	3.66586300	-0.66529700	-0.00000200
C	1.46579800	-0.10206600	0.00002800
C	0.06701300	0.30710500	0.00006300
O	-0.30567400	1.45199300	-0.00001600
O	-0.74350000	-0.75712400	0.00003500
C	-2.13622500	-0.43585600	-0.00003400
H	-2.65636300	-1.39175500	0.00019000
H	-2.39081900	0.14492100	0.88892600
H	-2.39085500	0.14448000	-0.88926900

3

C	1.34330500	0.11051300	-0.10152000
O	0.38764700	-0.71561900	-0.77540200
C	0.66525300	1.47909700	-0.26416600
C	-0.64556600	1.23888200	-0.23508900
C	5.36977300	-0.35444800	-1.49539900
C	5.05069200	0.66116400	-0.59700200
C	3.73952300	0.81299100	-0.15695100
C	2.74129200	-0.05178300	-0.61053700
C	3.06234200	-1.07009600	-1.50564000
C	4.37444500	-1.21682200	-1.94773700
H	6.39167200	-0.47226600	-1.84203800
H	5.82182000	1.33726600	-0.24105100
H	3.48890800	1.60717100	0.54352600
H	2.27939800	-1.73739000	-1.84918500
H	4.61983400	-2.00899500	-2.64836400

C	1.06655100	-0.31646600	1.35501000
C	-0.30499200	-0.58900200	1.38592100
C	-0.91567900	-1.03305700	2.53713100
C	-0.11415600	-1.18999700	3.68160200
C	1.24589900	-0.91326600	3.64882800
C	1.86280800	-0.47005000	2.46625300
H	-1.97340900	-1.27482600	2.56480100
H	-0.56691700	-1.54297700	4.60292300
H	1.84393800	-1.05247300	4.54402500
H	2.93158800	-0.27788300	2.42919500
C	-0.78559400	-0.30118900	-0.05370400
C	-4.27560000	-2.37988800	-1.45323900
C	-4.36142200	-1.54658700	-0.34067100
C	-3.23851500	-0.86113900	0.11173300
C	-2.01607100	-1.00654000	-0.54952600
C	-1.93252500	-1.84005700	-1.66509100
C	-3.05955700	-2.52254600	-2.11472000
H	-5.15377800	-2.91344500	-1.80386300
H	-5.30781600	-1.42415000	0.17690700
H	-3.31725700	-0.18541900	0.95585600
H	-0.98124000	-1.95142000	-2.17272700
H	-2.98459300	-3.16884400	-2.98394200
H	1.17013200	2.43646300	-0.30410400
C	-1.71481100	2.24893800	-0.14748300
O	-2.80212700	2.07145600	0.34988200
O	-1.32262000	3.42756600	-0.66131800
C	-2.29028300	4.47091000	-0.55842500
H	-1.83180700	5.34476900	-1.01832500
H	-3.20551700	4.19294600	-1.08530900
H	-2.53082000	4.66686600	0.48890400

4

C	-0.07025900	0.46959500	1.28525200
C	-0.81376700	1.87313500	-0.14466900
C	-1.73372000	0.65379600	-0.31109800
C	-1.24614600	-0.26386700	0.62882800
C	-1.80592800	-1.51360800	0.76768600
C	-2.89750200	-1.83423500	-0.05815400
C	-3.38268300	-0.92402100	-0.98769100
C	-2.79497900	0.34479200	-1.13186500
H	-1.42582700	-2.23029200	1.48937700
H	-3.36888900	-2.80771400	0.03448400
H	-4.22928900	-1.19402400	-1.61122300
H	-3.17800500	1.05117700	-1.86266600
C	1.02128500	0.57096500	0.20844000
O	-0.56830400	1.81311000	1.26395600

C	0.56029500	1.44316800	-0.68905800
C	2.21226500	-0.28962500	0.18512600
O	2.42120700	-1.16427900	0.99403400
O	3.03826100	0.00024700	-0.83298300
C	4.20723600	-0.81504500	-0.89891200
H	4.76653900	-0.46122500	-1.76335300
H	4.79799400	-0.70715000	0.01337000
H	3.93265400	-1.86520000	-1.01998600
H	0.24125300	0.15949800	2.28016600
H	-1.19822500	2.84620500	-0.44489600
H	0.99589000	1.72579300	-1.63862600

TS (1+2) 1,4-triazole

C	-1.79319500	1.41555300	0.19870600
C	-2.84450100	0.78594800	0.06236200
N	-0.36376200	0.26970100	-0.83087400
C	-4.26890700	0.46908600	0.13108000
O	-5.12333500	1.03271100	-0.50260300
O	-4.49233900	-0.53780000	0.98427900
C	-5.86539300	-0.91504100	1.10288200
H	-5.88302900	-1.73097100	1.82297300
H	-6.46209300	-0.07225600	1.45793700
H	-6.25207400	-1.24339000	0.13598400
N	-2.22106400	-1.00508800	-1.04760800
N	-1.10867700	-0.71764900	-1.10175100
C	3.64988000	-0.11100300	0.35928900
C	2.91116600	-1.26289300	0.12529500
C	1.58021500	-1.17307700	-0.25904200
C	0.96433800	0.06697800	-0.44664000
C	1.72906400	1.21211200	-0.21018400
C	3.05113000	1.13247200	0.19574600
F	4.91799500	-0.19639600	0.74029200
F	3.47412300	-2.45497000	0.28168400
F	0.89636500	-2.29639400	-0.46829800
F	1.16522900	2.41229500	-0.35645700
F	3.74622800	2.24056800	0.42184100
H	-1.10512800	2.19185200	0.46280700

TS (1+2) 1,5-triazole

C	-2.96351200	0.26705600	0.31283100
C	-3.63707800	1.29768700	0.36801100
N	-1.16487700	0.97056500	-0.73651900
N	-2.47593600	2.79708700	-0.50125900
N	-1.53088900	2.17924200	-0.74794700
C	2.76274400	-0.29207000	0.02647100
C	2.40841600	1.01302700	0.34371900

C	1.11788000	1.46056800	0.09855400
C	0.16847000	0.63276800	-0.50405100
C	0.55497300	-0.66719500	-0.83636200
C	1.82616100	-1.13873800	-0.55541500
F	3.98937800	-0.72963200	0.28116300
F	3.29985100	1.82461100	0.90141800
F	0.79113000	2.70675100	0.43341000
F	-0.33162300	-1.48713600	-1.39608800
F	2.15256000	-2.39280600	-0.85103400
H	-4.47844700	1.92020900	0.59039200
C	-2.58228800	-1.14358500	0.42399900
O	-3.19685800	-2.05226400	-0.06706300
O	-1.47320300	-1.28542700	1.16536100
C	-1.03902400	-2.63840200	1.33289800
H	-0.18191800	-2.58762600	2.00282000
H	-1.83680400	-3.24187200	1.76953000
H	-0.75255300	-3.06023000	0.36720500

TS (1+3) 1,4-triazole

C	2.02413000	-0.04454000	-0.48469800
C	0.20120800	1.13931200	-0.36299400
C	1.24275000	2.07397800	-1.00551500
C	2.40566100	1.30661800	-1.10823500
C	3.55564200	1.82988300	-1.65890700
C	3.51385100	3.15832600	-2.11216500
C	2.35527500	3.91886200	-2.00734400
C	1.18809300	3.37774400	-1.44577700
H	4.46051500	1.23905500	-1.75475000
H	4.40199200	3.59563300	-2.55752900
H	2.34928600	4.94089700	-2.37301500
H	0.27321000	3.96030900	-1.37930600
C	1.82850300	0.26134900	1.02648200
O	0.63614300	-0.12280700	-0.87966900
C	0.63822000	0.96080500	1.10137300
H	0.36071900	1.62555000	1.90986900
C	2.93964800	0.46892500	1.97055100
O	4.10832200	0.52872100	1.66561600
O	2.49489600	0.61179300	3.23168700
C	3.51584700	0.85015900	4.20012000
H	4.05699300	1.76947400	3.96584500
H	3.00122300	0.93889500	5.15541100
H	4.22198300	0.01751300	4.21830800
N	1.32537900	-1.71690700	1.75618500
N	-0.68360500	-0.63214000	1.79801300
N	0.18882800	-1.55713900	1.83329500
C	4.14434500	-3.58558100	-1.68267300

C	4.83896700	-2.51116000	-1.13372400
C	4.16044300	-1.36226300	-0.73735500
C	2.77420300	-1.28132500	-0.89333700
C	2.07751400	-2.36290700	-1.43499900
C	2.76222200	-3.50926200	-1.82768500
H	4.67721800	-4.48000900	-1.99068600
H	5.91592300	-2.56601200	-1.00757900
H	4.69886600	-0.54098900	-0.27794000
H	1.00032200	-2.30369900	-1.54013500
H	2.21115100	-4.34531800	-2.24743000
C	-3.83568200	2.19601300	-1.36074100
C	-3.17994900	2.84421300	-0.31683400
C	-1.87422700	2.48963000	0.01392000
C	-1.22165000	1.47633400	-0.69050300
C	-1.87399500	0.83706300	-1.74537000
C	-3.17905100	1.19435800	-2.07422700
H	-4.85689100	2.46460100	-1.61196100
H	-3.68708100	3.62046400	0.24737200
H	-1.36981900	2.99056400	0.83652900
H	-1.35210700	0.05890800	-2.29386400
H	-3.68747100	0.68440600	-2.88742300
C	-4.37249000	-1.22078300	-0.11633900
C	-4.19508500	-0.20732000	0.81655600
C	-2.98038800	-0.07677500	1.46860500
C	-1.90773500	-0.92285500	1.18174900
C	-2.10113100	-1.92147600	0.22445300
C	-3.32673700	-2.08772900	-0.40235300
F	-5.53209800	-1.34275500	-0.75213400
F	-5.18466700	0.64292000	1.06847200
F	-2.81818600	0.90944000	2.34545100
F	-1.09890400	-2.73823600	-0.09798500
F	-3.49009500	-3.04983500	-1.30574100

TS (1+3) 1,5-triazole

C	0.68328600	-0.83675000	-0.57033000
C	2.50506700	0.22515000	-0.01674800
C	2.98972500	-1.04731300	-0.73243000
C	1.82408600	-1.73158400	-1.08421200
C	1.87208100	-2.94207600	-1.73961400
C	3.14035000	-3.46108400	-2.04743900
C	4.30009200	-2.77790400	-1.69950300
C	4.23877000	-1.54622000	-1.02764400
H	0.96705300	-3.47191100	-2.02065500
H	3.21482500	-4.40890300	-2.57128700
H	5.26704000	-3.19932700	-1.95617200
H	5.14127900	-1.00183600	-0.76373200

C	0.77272600	-0.93933400	0.97720200
O	1.28027500	0.45980200	-0.73249900
C	1.91898200	-0.24966500	1.32303900
H	2.50681900	-0.47255900	2.20533200
C	0.24975800	-2.06326000	1.78217400
O	-0.15498600	-3.10890800	1.32923500
O	0.32589900	-1.80584800	3.09524400
C	-0.17723500	-2.84618800	3.93321000
H	-0.05844500	-2.48627500	4.95369600
H	-1.23019900	-3.02908000	3.70772600
H	0.38643300	-3.76872500	3.77939600
N	-0.76028600	0.54360100	1.67040500
N	1.21778200	1.57101600	2.10946500
N	0.07783800	1.43754400	1.97447700
C	-4.38517000	1.29145300	-0.29497300
C	-4.08092100	0.03959200	0.22563700
C	-2.89224900	-0.14982400	0.90796600
C	-1.96111200	0.88214000	1.04764000
C	-2.27749900	2.12791900	0.50363300
C	-3.48618700	2.33783700	-0.14457000
F	-5.52265600	1.47821300	-0.95610400
F	-4.92419300	-0.97242400	0.05478600
F	-2.60241000	-1.35327100	1.39882400
F	-1.41447900	3.13777900	0.60426300
F	-3.77018700	3.53459100	-0.65066600
C	-3.07642500	-1.04326300	-2.65501900
C	-2.62845200	-2.13826100	-1.92117500
C	-1.41280400	-2.08405300	-1.24210700
C	-0.63992000	-0.92019300	-1.28305100
C	-1.08787400	0.17580100	-2.02591300
C	-2.30112400	0.11349800	-2.70587600
H	-4.02785800	-1.08698500	-3.17672100
H	-3.22949300	-3.04071900	-1.86878900
H	-1.07904500	-2.93023900	-0.65240900
H	-0.48357900	1.07599300	-2.05936700
H	-2.64206100	0.97369200	-3.27508200
C	5.24239300	3.51633600	-0.27407500
C	5.10077800	2.83403600	0.93034800
C	4.19586700	1.78019000	1.03418000
C	3.43317000	1.40105100	-0.06855500
C	3.58334000	2.08190200	-1.27874600
C	4.47944500	3.13990300	-1.37824700
H	5.94377100	4.34118300	-0.35275100
H	5.68823100	3.12606500	1.79515300
H	4.07475400	1.26471400	1.98231200
H	2.98608800	1.77582000	-2.13228400

H	4.58521400	3.67059300	-2.31936400

TS (1+4) 1,4-triazole

C	2.73001100	0.37444300	1.17604500
C	1.48265700	-1.33896300	0.83549600
C	2.83909000	-1.73965100	0.24881600
C	3.65368200	-0.62162600	0.47541100
C	4.96040100	-0.58658000	0.04159200
C	5.45846700	-1.72136000	-0.61990300
C	4.65308600	-2.83168300	-0.84080800
C	3.31553500	-2.85094500	-0.41175400
H	5.58906500	0.28366000	0.20438900
H	6.48854100	-1.73099900	-0.96245100
H	5.06247500	-3.69744100	-1.35186400
H	2.68937500	-3.71964100	-0.59314900
C	1.71334400	0.83631100	0.11986800
O	1.89930200	-0.51681100	1.93175400
C	0.91258900	-0.26446600	-0.10386000
H	0.37255300	-0.46416900	-1.02233700
C	1.89378000	1.92919900	-0.84282200
O	1.11334000	2.22286100	-1.71854600
O	3.04863300	2.58345800	-0.61748200
C	3.29462800	3.67649100	-1.50069200
H	3.34385700	3.32650900	-2.53401400
H	2.49822100	4.41887000	-1.41583400
H	4.24926700	4.09914400	-1.19165600
N	0.40643500	2.06144200	1.48487500
N	-0.83571500	0.20901000	1.01543300
N	-0.49920300	1.35801500	1.43584200
H	3.17640800	1.14116000	1.80559700
H	0.80351800	-2.12376000	1.15988300
C	-4.65740500	-0.62219300	-0.52523000
C	-3.67408200	-1.60025500	-0.43784900
C	-2.43255400	-1.28261600	0.08782600
C	-2.12827700	0.00954200	0.52382800
C	-3.12602000	0.98132600	0.41154200
C	-4.38030500	0.66793300	-0.09402900
F	-5.85269500	-0.91959200	-1.01960200
F	-3.92669300	-2.83682200	-0.85091300
F	-1.49587900	-2.23044700	0.15936800
F	-2.89052000	2.22947200	0.81114900
F	-5.31375300	1.60871100	-0.17536700

TS (1+4) 1,5-triazole

C	2.04120600	-0.27772200	-0.94505500
C	3.09765400	1.55286800	-0.56683600

C	4.06874100	0.45975200	-0.11131500
C	3.37809400	-0.73455500	-0.36071200
C	3.92073700	-1.95857800	-0.03743200
C	5.20442000	-1.97283900	0.53304700
C	5.89147900	-0.79008900	0.77572200
C	5.32237400	0.45499200	0.45986700
H	3.38316800	-2.88422100	-0.22021700
H	5.66657800	-2.92202900	0.78566800
H	6.88353300	-0.82722900	1.21482200
H	5.86352100	1.37564500	0.65757000
C	1.28223500	0.38446500	0.21236700
O	2.45134200	0.89390200	-1.66170100
C	1.94253300	1.57193900	0.45183300
H	1.95443900	2.09117600	1.40147700
C	0.36883500	-0.27030600	1.16010000
O	-0.14846200	0.26991000	2.11028000
O	0.10688600	-1.53769000	0.78827300
C	-0.85082000	-2.21270000	1.60434200
H	-1.74906000	-1.59997200	1.71708900
H	-1.07918300	-3.14339500	1.08650400
H	-0.43294700	-2.41180300	2.59366000
N	-0.44696200	1.09185100	-1.00555300
N	0.68849100	2.99248400	-0.46818300
N	-0.17014100	2.32085600	-0.84967500
H	1.47825100	-0.96199400	-1.57516500
H	3.50974000	2.51376200	-0.87013800
C	-4.14634700	-0.59262000	0.02252800
C	-3.83022900	0.66759900	0.51603400
C	-2.61571800	1.25247800	0.18842300
C	-1.72171100	0.62320400	-0.68303000
C	-2.05732000	-0.64684400	-1.16254700
C	-3.25454400	-1.25302200	-0.81499600
F	-5.29995200	-1.16295000	0.34638900
F	-4.68050900	1.29684800	1.31865700
F	-2.31771000	2.44813100	0.68454500
F	-1.20851800	-1.29746600	-1.95004500
F	-3.54948700	-2.46493900	-1.27468400

5

C	1.11156400	0.49736400	0.08546900
C	-1.11142900	0.49746800	0.08534000
C	0.72033700	1.81436500	0.22663400
C	-0.72012800	1.81441200	0.22643900
C	-1.43409100	3.03982900	0.40448600
C	-0.71968700	4.18914000	0.55704800
C	0.71969500	4.18910600	0.55741400

C	1.43418000	3.03980300	0.40510500
H	-2.51946100	3.04149200	0.43538800
H	-1.23804400	5.13225400	0.70009600
H	1.23801500	5.13219200	0.70078300
H	2.51952600	3.04156000	0.43659900
C	5.04223500	-1.10924900	-0.32246700
C	4.09239500	-1.79051400	0.44580400
C	2.79898600	-1.31434200	0.59938500
C	2.43471000	-0.11105200	-0.04608800
C	3.39021100	0.55619500	-0.81649200
C	4.69044700	0.07933400	-0.95866200
H	4.40278900	-2.70868300	0.93603900
H	3.10085800	1.46359300	-1.33888300
H	5.39782300	0.62815400	-1.56854000
C	-5.04212600	-1.10901800	-0.32243400
C	-4.09291500	-1.78916600	0.44761700
C	-2.79955900	-1.31289800	0.60129100
C	-2.43466400	-0.11082900	-0.04608800
C	-3.38956700	0.55543100	-0.81803600
C	-4.68980400	0.07854700	-0.96023500
H	-4.40380300	-2.70641300	0.93926000
H	-3.09974600	1.46208700	-1.34147300
H	-5.39676400	0.62655300	-1.57132700
O	0.00002400	-0.28011000	0.01176400
O	6.27112900	-1.68402600	-0.38440700
O	-6.27105800	-1.68372100	-0.38423300
C	1.82362400	-2.08003600	1.45397500
H	1.11587300	-2.63837100	0.83401600
H	2.35037600	-2.79140400	2.09471000
H	1.23692400	-1.40734500	2.08646500
C	-1.82494200	-2.07685100	1.45828800
H	-1.23899200	-1.40276900	2.09002400
H	-2.35226100	-2.78693000	2.09999100
H	-1.11648500	-2.63641100	0.84027000
C	7.25568300	-1.02699700	-1.15093200
H	6.95649300	-0.95015400	-2.20341400
H	7.45994800	-0.02268200	-0.75992100
H	8.15653000	-1.63581600	-1.07468400
C	-7.25508400	-1.02775900	-1.15235000
H	-6.95525400	-0.95255500	-2.20476600
H	-8.15603800	-1.63637000	-1.07570900
H	-7.45949500	-0.02282800	-0.76299700

TS-1

C	-1.45782600	0.55197600	0.10800800
C	0.71881100	0.42039500	0.41394000

C	-1.01360900	1.89212700	0.41653500
C	0.39185200	1.81118500	0.54961400
C	1.16712000	2.98766100	0.58218700
C	0.51628900	4.20283000	0.56765900
C	-0.88834700	4.27960400	0.46092900
C	-1.65649200	3.13886600	0.34875800
H	2.24915600	2.95057500	0.56185500
H	1.09634100	5.11944200	0.60199600
H	-1.36631200	5.25397700	0.43081000
H	-2.72692900	3.20765600	0.18470000
C	-5.49675600	-0.82932100	0.55397200
C	-4.58598400	-1.58987000	-0.17728200
C	-3.25553300	-1.18628900	-0.32856200
C	-2.83223100	0.01955500	0.25783500
C	-3.75565500	0.75373000	1.02015200
C	-5.06899900	0.35002600	1.16792700
H	-4.89284400	-2.52086200	-0.64153800
H	-3.42259400	1.64992700	1.53222800
H	-5.77700700	0.92006100	1.75954400
C	4.49452600	-1.47549600	1.07258400
C	3.46289600	-2.17629800	0.43869800
C	2.21398300	-1.61353400	0.22091900
C	1.98231500	-0.28342300	0.65562400
C	3.01436100	0.39409800	1.31098900
C	4.26576000	-0.17695800	1.52255900
H	3.66974700	-3.19036000	0.10936000
H	2.83055900	1.38594700	1.70549500
H	5.03025500	0.38917600	2.04051200
O	-0.42845600	-0.28715100	0.45623000
O	-6.80050400	-1.15723500	0.73510400
O	5.66638300	-2.14364900	1.20667500
C	-2.32094000	-2.10748100	-1.06950600
H	-1.74710300	-2.71258100	-0.36049700
H	-2.88435100	-2.78801600	-1.71330400
H	-1.59835000	-1.56403800	-1.68127800
C	1.15935700	-2.44277700	-0.45979000
H	0.41190000	-2.78226700	0.26352300
H	0.63995400	-1.86885100	-1.23032800
H	1.61404400	-3.32078000	-0.92529000
C	-7.26679900	-2.34646900	0.13605000
H	-7.15930500	-2.31163500	-0.95482400
H	-6.73453900	-3.22361600	0.52357900
H	-8.32315200	-2.42042700	0.39402500
C	6.73608200	-1.46226000	1.82595100
H	7.00243100	-0.55422000	1.27177700
H	6.49231000	-1.19589400	2.86132900

H	7.57938600	-2.15251400	1.81870000
C	-0.90797700	0.68967500	-1.85459900
C	0.33653900	0.65787500	-1.91657600
H	-1.83734400	0.81322400	-2.38579600
C	1.74495900	0.79133900	-2.17635800
O	2.37655600	1.81841400	-2.04996000
O	2.31002500	-0.38875700	-2.50551000
C	3.73581700	-0.36640600	-2.53128300
H	4.12354200	-0.02699600	-1.56619900
H	4.04155400	-1.39466100	-2.72240600
H	4.09549500	0.29859000	-3.31989300

6

C	-1.24642200	0.51986900	-0.04723000
C	0.93129500	0.34042000	0.03790000
C	-0.89175700	0.65449400	1.45453600
C	0.50087900	0.55398300	1.50382200
C	1.19090200	0.72137200	2.68297100
C	0.43934000	0.95316100	3.84801500
C	-0.94762400	1.02992200	3.80253600
C	-1.63883600	0.89167900	2.58634500
H	2.27628800	0.66976900	2.70989800
H	0.95060000	1.07709000	4.79780900
H	-1.50432300	1.20860300	4.71741800
H	-2.72249000	0.96467200	2.54210100
C	-5.26649900	-0.70707600	-1.00681900
C	-4.40192500	-1.58617200	-0.35492900
C	-3.09037200	-1.21684100	-0.04357500
C	-2.63443300	0.06333800	-0.40115200
C	-3.51251200	0.92930500	-1.06021500
C	-4.81343700	0.56302600	-1.36236200
H	-4.73346900	-2.58007000	-0.07518900
H	-3.17732800	1.91804100	-1.35397800
H	-5.49172300	1.23820000	-1.87250000
C	4.56097900	-1.77310400	-0.94201100
C	3.69426700	-2.28002500	0.02306100
C	2.51454700	-1.60848800	0.36403700
C	2.20916500	-0.39240500	-0.26808200
C	3.07503900	0.08310800	-1.26002900
C	4.23834800	-0.58350700	-1.59692400
H	3.91021300	-3.21957000	0.52023000
H	2.83320000	0.99538800	-1.79216500
H	4.90746800	-0.20936100	-2.36383600
O	-0.21235700	-0.39016800	-0.45517300
O	-6.55288200	-0.99533000	-1.33201600
O	5.72023300	-2.36919000	-1.32408000

C	-2.20718200	-2.22788300	0.64479500
H	-1.72513700	-1.80112200	1.52964200
H	-2.79326100	-3.09590500	0.95743500
H	-1.41166100	-2.56491300	-0.02520700
C	1.61532500	-2.26316600	1.38742300
H	1.81889900	-1.89514800	2.39845700
H	0.56288500	-2.07108100	1.17492600
H	1.77751200	-3.34471700	1.38564600
C	-7.04501900	-2.27162200	-0.98835300
H	-8.08137000	-2.29637100	-1.32510600
H	-6.47997100	-3.06637000	-1.49018100
H	-7.01063500	-2.43421800	0.09580500
C	6.06549200	-3.58417600	-0.69821800
H	7.01173900	-3.89519100	-1.14136900
H	6.19515500	-3.45344400	0.38315000
H	5.30766800	-4.35620100	-0.87898300
C	-0.69347700	1.82223600	-0.65449100
C	0.63625500	1.72076400	-0.59925400
H	-1.25644000	2.71632800	-0.88847600
C	1.57807100	2.85396900	-0.63689500
O	2.63254700	2.87643800	-0.04714600
O	1.10747300	3.88355400	-1.36265400
C	1.94581000	5.03833600	-1.36703200
H	1.43889100	5.76875800	-1.99573400
H	2.07108400	5.42326800	-0.35247300
H	2.92877300	4.79405000	-1.77599300

TS-2a

C	2.02954700	0.55907800	-0.21553600
C	-0.06261200	1.18665600	-0.37417500
C	2.07795300	1.91849400	-0.92577800
C	0.74644400	2.31661600	-1.04598700
C	0.40750400	3.48912000	-1.68942300
C	1.45264800	4.28250200	-2.18790900
C	2.78048200	3.89808400	-2.03488000
C	3.11457200	2.69440600	-1.39572100
H	-0.62997200	3.78268100	-1.82712200
H	1.21919600	5.20784300	-2.70541400
H	3.56925000	4.53298500	-2.42654700
H	4.14657600	2.37466100	-1.28426000
C	5.28142500	-2.14284500	-1.06367800
C	5.11607100	-1.64171900	0.22307600
C	4.05011100	-0.78087800	0.47838900
C	3.14759000	-0.40458200	-0.51036400
C	3.32126400	-0.91045500	-1.82097100
C	4.38324900	-1.77032100	-2.06742100

H	5.79203200	-1.90288600	1.02811700
H	3.94013800	-0.39264800	1.48171100
H	4.53847600	-2.17849800	-3.06177300
C	-4.13124000	0.57381200	-1.62721300
C	-3.11279400	-0.28627300	-2.05383400
C	-1.81160000	-0.05757600	-1.64841200
C	-1.48999300	1.01835500	-0.81070700
C	-2.49612800	1.90657300	-0.41567300
C	-3.81441600	1.67108100	-0.83027000
H	-3.37467300	-1.12967000	-2.68469200
H	-1.01906600	-0.73076500	-1.95922800
H	-4.58804900	2.35513700	-0.49776600
O	0.75996100	0.05979200	-0.70376800
C	1.59882800	0.90639800	1.23361400
C	0.26636900	1.26898500	1.12942400
C	2.48654900	1.54132700	2.22529600
O	3.62552000	1.88755700	2.01254200
O	1.86775400	1.71255300	3.40864100
C	2.66066500	2.35324900	4.40683300
H	3.56696700	1.77543900	4.60090800
H	2.94418900	3.35754700	4.08394700
H	2.03554900	2.39700200	5.29730300
C	2.39026500	-0.58784800	-2.96639100
H	2.16245200	0.47920500	-3.02596700
H	2.84232100	-0.89838500	-3.91171100
H	1.43766400	-1.11168400	-2.85022200
C	-2.24728700	3.08911000	0.49386100
H	-2.94132300	3.90072300	0.25747500
H	-2.41585800	2.80813100	1.53881800
H	-1.23326200	3.48554100	0.40829200
O	6.27300600	-2.99050400	-1.44351000
O	-5.38609300	0.24694600	-2.02387600
C	7.20254700	-3.37936100	-0.45753000
H	7.91125800	-4.04305000	-0.95324400
H	7.73768100	-2.51291800	-0.04995700
H	6.71240400	-3.91757300	0.36291800
C	-6.44519600	1.07482400	-1.59104800
H	-7.35638000	0.63242700	-1.99311800
H	-6.50225100	1.10182400	-0.49750400
H	-6.33470500	2.09495800	-1.97832800
H	-0.24598900	1.90444400	1.83900900
N	0.35755400	-1.18379100	2.15390400
N	1.50108000	-1.05549100	2.17768900
N	-0.69955000	-0.51943700	1.92527900
C	-4.14710000	-2.35506600	0.36806400
C	-2.92825200	-3.00998100	0.25338000

C	-1.77455100	-2.42274100	0.75201900
C	-1.81752600	-1.20064200	1.42720000
C	-3.05679300	-0.57097200	1.54836200
C	-4.20607600	-1.12719600	1.01289900
F	-5.24556100	-2.89262500	-0.14796200
F	-2.86302100	-4.18281300	-0.36951100
F	-0.61269900	-3.05303900	0.59603600
F	-3.13485000	0.60512000	2.16775900
F	-5.36437000	-0.47592100	1.09734800

TS-2b

C	2.37701400	0.56433200	0.11200500
C	0.32827900	1.08681600	-0.45925800
C	2.50025700	1.88795200	-0.66520300
C	1.19718800	2.21863500	-1.04638900
C	0.93773600	3.35535900	-1.78178100
C	2.02837300	4.16834300	-2.13093400
C	3.32250800	3.84040000	-1.74424400
C	3.57739900	2.67973000	-0.99668900
H	-0.06851400	3.61315500	-2.09609700
H	1.85583400	5.06578800	-2.71673400
H	4.14761400	4.48499300	-2.03100200
H	4.58783800	2.40445500	-0.70654700
C	5.96654100	-1.81431800	0.18934400
C	5.26990400	-1.64117100	-1.00596300
C	4.08989100	-0.89175200	-1.05619400
C	3.59560600	-0.31502200	0.12484700
C	4.30695000	-0.49785300	1.31587100
C	5.47828600	-1.23286200	1.36050600
H	5.63425200	-2.08569700	-1.92562700
H	3.93067900	-0.06637700	2.23719100
H	6.02687700	-1.37556900	2.28486700
C	-3.62402900	0.51559900	-2.10914600
C	-2.70818700	-0.53384400	-2.16345800
C	-1.40672200	-0.40828200	-1.65738100
C	-1.01966200	0.81724100	-1.08475500
C	-1.94638700	1.87051500	-1.05863200
C	-3.23171400	1.73259100	-1.55221100
H	-2.99524200	-1.48700900	-2.59457700
H	-1.66169300	2.80826700	-0.59591900
H	-3.94846100	2.54494000	-1.50399600
O	1.24446300	-0.01209000	-0.56479600
O	7.11829800	-2.52308100	0.31077700
O	-4.90455000	0.44253000	-2.55068400
C	3.38026300	-0.77197200	-2.38326400
H	2.99861200	0.23620400	-2.55880600

H	4.05732800	-1.03549300	-3.19992000
H	2.52247900	-1.45018300	-2.41743700
C	-0.52172000	-1.63040000	-1.76533700
H	-0.10243300	-1.92608200	-0.80215800
H	-1.09751300	-2.46896200	-2.16707800
H	0.32521700	-1.44244500	-2.42982000
C	7.63563500	-3.13438100	-0.85003000
H	8.54413000	-3.65076200	-0.54056200
H	6.92786800	-3.86045300	-1.26778000
H	7.88295300	-2.39028400	-1.61681700
C	-5.35254700	-0.79278800	-3.06625600
H	-6.39179800	-0.63835500	-3.35571800
H	-4.77097300	-1.09368600	-3.94579300
H	-5.30224700	-1.58170800	-2.30707800
C	1.68818800	0.93211700	1.43871300
C	0.41104300	1.31122800	1.08197000
C	-0.32893900	2.33855200	1.85167300
O	-0.88982900	3.29539800	1.37132200
O	-0.24392300	2.11887700	3.17120900
C	-0.93701600	3.07310000	3.97539800
H	-0.78070800	2.75875900	5.00588200
H	-0.53779400	4.07612700	3.81114400
H	-2.00037000	3.06616000	3.72591600
N	0.25226300	-1.11984100	2.17052500
N	-0.75108600	-0.42260400	1.85273900
N	1.39787800	-1.00874600	2.27522900
H	2.19984100	1.32013800	2.31104500
C	-4.40166300	-1.92574300	0.45254700
C	-3.32276300	-2.79280700	0.55121800
C	-2.10522800	-2.33306400	1.03116100
C	-1.94089200	-1.00308600	1.42208700
C	-3.04588500	-0.15246300	1.32821800
C	-4.25731100	-0.59468600	0.82357500
F	-5.56034600	-2.36059100	-0.04137800
F	-3.45440200	-4.06206200	0.17605500
F	-1.07481100	-3.17750700	1.09768900
F	-2.91365700	1.12219300	1.69098000
F	-5.27625100	0.24499500	0.68990800

7a

C	-0.04003400	0.67718900	0.87774600
C	2.07900500	0.31879100	0.43823500
C	0.70551100	1.76907000	1.62571300
C	2.05722800	1.55235000	1.34288700
C	3.03408800	2.35754500	1.90217200
C	2.62837700	3.38955600	2.75458600

C	1.28252400	3.59977300	3.03809000
C	0.29856100	2.78265700	2.47357300
H	4.08952300	2.18264500	1.72725900
H	3.37895700	4.02255000	3.21725900
H	0.99405300	4.39288700	3.72061000
H	-0.74764500	2.92156200	2.72670200
C	-3.84102500	-0.95634600	2.08121300
C	-3.76760100	0.37024200	1.66158900
C	-2.54239200	0.95573800	1.31585600
C	-1.37337600	0.18588600	1.38448700
C	-1.45667500	-1.13628200	1.84460100
C	-2.66680700	-1.70701200	2.19151800
H	-4.66574400	0.97461000	1.57789800
H	-0.55262400	-1.73170600	1.89013200
H	-2.73599500	-2.73785800	2.52124500
C	5.79841300	-1.82963700	0.11634200
C	4.63489400	-2.53404300	0.41532500
C	3.39315700	-1.89543700	0.53227100
C	3.33675300	-0.50389900	0.36451300
C	4.51168500	0.18710300	0.03691900
C	5.73177000	-0.45016600	-0.08451600
H	4.66693200	-3.60889200	0.55327800
H	4.46679100	1.25710700	-0.14606800
H	6.63703400	0.08992300	-0.33855900
O	0.93115700	-0.37833500	0.91090200
O	-4.99245800	-1.60169400	2.38885300
O	7.02808300	-2.39186900	-0.00977100
C	-2.58912500	2.39657400	0.85317400
H	-3.26914000	2.51424000	0.00280300
H	-2.97257200	3.03518900	1.65660700
H	-1.61627100	2.79260500	0.56158500
C	2.19158300	-2.76591400	0.82355700
H	1.40115000	-2.61502500	0.08449300
H	2.48579600	-3.81819400	0.81019900
H	1.76693600	-2.53921100	1.80522000
C	-6.20785500	-0.92708200	2.14076100
H	-6.99993100	-1.62830400	2.40194100
H	-6.30130800	-0.02760800	2.76082900
H	-6.29777100	-0.65381900	1.08265200
C	7.12914800	-3.78784000	0.16441700
H	6.52498100	-4.32673000	-0.57520300
H	8.18113300	-4.03474100	0.02239100
H	6.81734200	-4.08781500	1.17215400
C	0.03259600	1.04134400	-0.65985400
C	1.51083400	0.75655700	-0.99166000
C	2.24949000	1.92092100	-1.61575600

O	2.01671200	3.07137300	-1.33398800
O	3.19680200	1.53081800	-2.46662900
C	3.96722600	2.59143200	-3.03295200
H	4.48391200	3.14577100	-2.24550000
H	4.68061800	2.11115800	-3.69958200
H	3.32033800	3.27779200	-3.58291300
N	0.33096000	-0.80337800	-2.07561600
N	1.49575300	-0.43869700	-1.85979600
N	-0.58661700	0.03489600	-1.50849800
H	-0.29835100	2.05036100	-0.90539400
C	-4.69616800	-0.77307100	-1.47545000
C	-3.79739100	-1.77930100	-1.14327700
C	-2.43310300	-1.53057000	-1.18959100
C	-1.94578300	-0.27688800	-1.56365700
C	-2.86544300	0.70580500	-1.92298700
C	-4.23087700	0.47945200	-1.84882100
F	-6.00611600	-0.99389300	-1.38039600
F	-4.25038500	-2.95730500	-0.72997300
F	-1.59037800	-2.48060900	-0.80720500
F	-2.42852500	1.92192300	-2.25805200
F	-5.08862900	1.45904000	-2.12612300

7b

C	-2.25434800	0.28568400	0.24137800
C	-0.17347900	0.36082100	0.95194200
C	-2.30000700	1.07266700	1.54433600
C	-0.98136400	1.12485900	1.99369500
C	-0.64208700	1.78396100	3.16041900
C	-1.67514000	2.38074300	3.88914400
C	-2.99656400	2.32134000	3.44563100
C	-3.32801100	1.66626500	2.25519400
H	0.38871900	1.83084100	3.49818200
H	-1.44711000	2.89179500	4.81921800
H	-3.78045300	2.78078400	4.03968000
H	-4.35917800	1.59632700	1.91917500
C	-5.76126400	-2.04620800	-0.65631400
C	-5.73088500	-0.69536600	-0.99687800
C	-4.59980600	0.08897500	-0.74373800
C	-3.48516300	-0.49825600	-0.13250600
C	-3.53067600	-1.85363100	0.21302900
C	-4.64791400	-2.62669400	-0.04558700
H	-6.58467200	-0.22691200	-1.47390600
H	-2.66523900	-2.30178100	0.68794100
H	-4.68478200	-3.67876400	0.21513200
C	3.65392100	-1.41239700	1.85915600
C	2.52150200	-2.22186000	1.81293100

C	1.24123700	-1.69200200	1.59359500
C	1.11408000	-0.30846300	1.37808700
C	2.25149100	0.50188300	1.51797000
C	3.50594400	-0.02766900	1.75671300
H	2.61199900	-3.29482900	1.94075000
H	2.15119400	1.57605500	1.40342300
H	4.38523900	0.60360100	1.83230100
O	-1.14008900	-0.58135800	0.48205700
O	-6.81966600	-2.86949100	-0.87413300
O	4.92324600	-1.86932200	1.99587300
C	-4.62613200	1.53479300	-1.18012800
H	-4.00968100	1.67507800	-2.07516900
H	-5.64595000	1.84174900	-1.42465300
H	-4.25480000	2.21039800	-0.40239100
C	0.09115600	-2.67437300	1.60689300
H	-0.73865800	-2.30602800	2.21390300
H	-0.29235400	-2.84813200	0.59916400
H	0.42909100	-3.62740400	2.02173300
C	-7.95369000	-2.32155200	-1.50736700
H	-7.70802400	-1.94062300	-2.50606500
H	-8.67333500	-3.13512900	-1.59692100
H	-8.39232000	-1.51207900	-0.91102200
C	5.12276900	-3.26660400	1.92954900
H	6.20127800	-3.41868800	1.96399300
H	4.65743700	-3.77859700	2.78008400
H	4.72181100	-3.67230500	0.99388500
C	-1.60251700	1.22511400	-0.82733200
C	-0.12440700	1.29912300	-0.33787300
C	0.35174300	2.73702900	-0.15460900
O	0.87457200	3.19631400	0.83057600
O	0.09438100	3.44806100	-1.25507600
C	0.59461200	4.78655800	-1.23763700
H	0.32395800	5.21364300	-2.20123800
H	0.14152400	5.35050700	-0.42000000
H	1.67886900	4.77325700	-1.11013100
N	-0.39136000	0.23104100	-2.42004300
N	0.52079000	0.69112500	-1.49778300
N	-1.54911300	0.54653600	-2.12926000
H	-2.08864300	2.19275600	-0.93281800
C	4.47805000	-0.71599800	-1.51198700
C	4.22387000	0.64468900	-1.61810800
C	2.91171200	1.09454100	-1.65061600
C	1.83846900	0.21119400	-1.55973400
C	2.11653400	-1.15262700	-1.46384700
C	3.42254600	-1.61623900	-1.43730700
F	5.72783000	-1.15862600	-1.46604000

F	5.23364900	1.50778500	-1.68401800
F	2.68459100	2.40768900	-1.71023900
F	1.12062500	-2.01956400	-1.34549400
F	3.67277500	-2.91638100	-1.29505400

TS-3a

C	2.05442100	0.35327500	-0.75092700
C	-0.06596400	0.99031400	-0.68645600
C	2.06966900	1.77106600	-1.01317800
C	0.72375300	2.17803400	-1.01723200
C	0.38216400	3.51636300	-1.23230800
C	1.40305500	4.42599500	-1.44587500
C	2.75155200	4.02013700	-1.44120200
C	3.10154800	2.70043200	-1.22564500
H	-0.65425500	3.83355300	-1.26919300
H	1.16226600	5.46585300	-1.64406600
H	3.52819100	4.75488100	-1.63032900
H	4.13965400	2.39084400	-1.25994900
C	5.44074600	-2.21980500	-0.48085000
C	5.50877800	-0.89184800	-0.06153400
C	4.37898100	-0.09560400	-0.17786500
C	3.17435800	-0.58093800	-0.70544500
C	3.09857200	-1.94035600	-1.09511100
C	4.23884500	-2.72173800	-0.98849600
H	6.40921700	-0.47627900	0.37331700
H	4.42152300	0.91014800	0.22190000
H	4.21528700	-3.76444500	-1.28966900
C	-4.29446100	0.82299500	-1.43622700
C	-3.72064900	1.86880200	-0.71805000
C	-2.33928800	1.87794300	-0.54463900
C	-1.50626300	0.88642600	-1.06807500
C	-2.08734000	-0.14344100	-1.83968100
C	-3.46746800	-0.15447200	-1.99934300
H	-4.32169700	2.64774600	-0.26480300
H	-1.91049300	2.66382500	0.07094000
H	-3.94320700	-0.94792400	-2.56867300
O	0.79195300	-0.08829700	-0.95440700
C	1.42659700	0.68735000	1.49062000
C	0.02385500	0.82659600	1.14950700
C	2.32498300	1.77262000	1.87767000
O	3.47446100	1.66197900	2.24135000
O	1.70808700	2.96922200	1.73825600
C	2.52524300	4.09919500	2.02576300
H	1.93167400	4.97040000	1.75036400
H	2.77994300	4.12347200	3.08836700
H	3.44480000	4.06298000	1.43813000

C	1.84078800	-2.58115900	-1.61652400
H	2.04566900	-3.60658500	-1.93214800
H	1.07361400	-2.60444400	-0.83825600
H	1.43240100	-2.03220000	-2.46903700
C	-1.28410000	-1.24710800	-2.47802400
H	-1.91709900	-1.83089400	-3.15039100
H	-0.44475900	-0.84536800	-3.05162200
H	-0.86783100	-1.92418000	-1.72699200
O	6.46935800	-3.09757400	-0.42742500
O	-5.62424500	0.65408000	-1.62863100
C	7.68016800	-2.65078100	0.14569500
H	8.35873300	-3.50302100	0.11931500
H	8.11135400	-1.82285600	-0.42996400
H	7.53212500	-2.33177600	1.18402200
C	-6.49125100	1.59060200	-1.02163700
H	-6.32905000	2.59835000	-1.42273900
H	-7.50263900	1.26416400	-1.26225300
H	-6.35692400	1.60092300	0.06527200
H	-0.56733400	1.66580600	1.50380700
N	0.62042200	-1.30002600	1.83467200
N	1.67705100	-0.61873400	1.89434000
N	-0.43600900	-0.47063300	1.50222000
C	-4.29461700	-2.02287700	0.84328100
C	-3.17892900	-2.79349600	0.55071400
C	-1.90148200	-2.29586000	0.77271800
C	-1.70288500	-1.02013500	1.31000300
C	-2.84382100	-0.28511100	1.64262100
C	-4.11874200	-0.75274900	1.37387000
F	-5.51569500	-2.48299800	0.59607700
F	-3.33058900	-4.00204700	0.01683900
F	-0.87426600	-3.05066900	0.38629200
F	-2.70947900	0.93451200	2.16884800
F	-5.17699400	0.01492300	1.63128400

TS-3b

C	-2.32084900	0.29798400	0.07208100
C	-0.36388100	0.16182100	1.09894000
C	-2.31720000	1.30780300	1.11783600
C	-1.05874800	1.23821500	1.74080500
C	-0.70247700	2.15553200	2.74482200
C	-1.63177800	3.11601600	3.09374300
C	-2.88942100	3.19385000	2.45430300
C	-3.24066000	2.30117200	1.45814500
H	0.25992900	2.09472100	3.24365000
H	-1.39756400	3.82461900	3.88284500
H	-3.59288400	3.96019700	2.76509400

H	-4.20723300	2.35129600	0.96435200
C	-6.08230000	-1.41937300	-1.11453300
C	-5.47738000	-1.80169200	0.08138600
C	-4.24295600	-1.26968400	0.46578500
C	-3.59466400	-0.34919000	-0.37399100
C	-4.21891100	0.02808400	-1.57019100
C	-5.44584700	-0.49162200	-1.94096500
H	-5.95720200	-2.51554400	0.74207200
H	-3.72848500	0.72087000	-2.24225100
H	-5.92606400	-0.20353600	-2.86964400
C	3.48217100	-1.46441300	1.98917600
C	2.39749600	-2.32682600	1.83130700
C	1.11247500	-1.84128500	1.57327400
C	0.91934300	-0.45181400	1.46278600
C	2.01094500	0.40769800	1.68615400
C	3.27625700	-0.08177600	1.94076800
H	2.53706900	-3.40042800	1.88997700
H	1.87568500	1.47907000	1.59382400
H	4.12375300	0.58126900	2.07759600
O	-1.26702800	-0.55525600	0.38653100
O	-7.27827500	-1.88603000	-1.55345300
O	4.76010800	-1.86594400	2.18112900
C	-3.64082500	-1.73467300	1.76811600
H	-2.92247600	-2.54049400	1.58787700
H	-3.11107500	-0.93065300	2.28672000
H	-4.41723100	-2.11994300	2.43395100
C	-0.01263100	-2.83464300	1.43757100
H	-0.83521200	-2.57421100	2.11007000
H	-0.41280300	-2.85255500	0.42138500
H	0.33576200	-3.83761800	1.69516800
C	-7.95225300	-2.82593200	-0.74606500
H	-8.87536100	-3.06902800	-1.27197100
H	-7.35750900	-3.73801400	-0.61369100
H	-8.19320300	-2.40616800	0.23825400
C	5.01772000	-3.25535300	2.22802700
H	4.49696600	-3.72632200	3.07026500
H	4.72048100	-3.74138700	1.29327700
H	6.09409200	-3.35523100	2.36593300
C	-1.43252400	1.21575000	-1.34516800
C	-0.07992800	1.41378000	-0.89119700
C	0.45599500	2.65864000	-0.34134000
O	1.61840200	2.89107300	-0.07988300
O	-0.53965900	3.53009000	-0.09463100
C	-0.13321900	4.75001200	0.52108300
H	0.43780400	4.54591400	1.42893700
H	0.48090100	5.33429200	-0.16838900

H	-1.05623400	5.27607100	0.76193900
N	-0.17322600	-0.13493200	-2.54191400
N	0.65669000	0.54680200	-1.70866900
N	-1.35604600	0.27908000	-2.41365300
H	-2.10961700	2.05258300	-1.48405100
C	4.68216700	-0.59914800	-1.37406800
C	3.67241000	-1.53216500	-1.18188200
C	2.34762500	-1.15289700	-1.32614500
C	2.00880900	0.16429400	-1.63670000
C	3.03485400	1.06842400	-1.90903500
C	4.36361100	0.70055600	-1.74398400
F	5.95139900	-0.95700200	-1.22438000
F	3.98181600	-2.78096200	-0.83186200
F	1.39595600	-2.05986400	-1.14541300
F	2.76182400	2.28399500	-2.35720600
F	5.33532100	1.57597000	-1.98515400

8a

N	0.94375800	-1.51243200	-0.98693600
N	2.22364400	-1.51159500	-0.97520600
C	2.67063200	-0.44976700	-0.24097800
C	1.58729600	0.24756800	0.23009300
N	0.52869400	-0.44524900	-0.24850600
H	1.49372900	1.13434000	0.83589600
C	-3.57083200	0.36794500	0.13713200
C	-2.68464000	1.39578800	-0.16091800
C	-1.33226100	1.11701800	-0.28948500
C	-0.84562800	-0.17539800	-0.10330200
C	-1.74239700	-1.19589700	0.21178200
C	-3.10066900	-0.92635800	0.32098400
F	-4.86471400	0.62464200	0.25464500
F	-3.13236100	2.63258600	-0.33475300
F	-0.49187300	2.10508100	-0.58421400
F	-1.31580500	-2.42864100	0.42689500
F	-3.94874900	-1.90048000	0.62177700
C	4.10802500	-0.17328900	-0.04093900
O	5.01288900	-0.82721600	-0.48538900
O	4.26668900	0.92710000	0.71884400
C	5.62736500	1.28036900	0.96942900
H	5.59191200	2.17705800	1.58563600
H	6.13846500	0.47049700	1.49405900
H	6.14677000	1.47739900	0.02935400

8b

C	2.33306400	-0.42951200	-0.09333500
C	3.26695900	-1.35806000	-0.47836100

C	2.56827500	0.89977600	0.50571300
O	3.65475600	1.41805800	0.52857200
O	1.45982200	1.43115700	1.03445400
N	1.14100500	-1.04497900	-0.34948300
N	1.34909900	-2.27026200	-0.86949600
N	2.62324700	-2.46205200	-0.93710800
C	-2.81139100	0.33254900	-0.08446300
C	-2.45120800	-0.85986300	0.52865200
C	-1.13689500	-1.30578400	0.45658300
C	-0.18273700	-0.56837200	-0.23761800
C	-0.55897100	0.61985800	-0.85797400
C	-1.86238900	1.08134100	-0.77227400
F	-4.06187100	0.76415500	-0.00861900
F	-3.35870700	-1.56443700	1.19278500
F	-0.80437400	-2.43080500	1.06828400
F	0.34316400	1.33220100	-1.52295600
F	-2.21135300	2.22251400	-1.35480800
C	1.63353900	2.73313800	1.60343400
H	1.98511900	3.43046200	0.84082500
H	0.65202800	3.02433900	1.97241800
H	2.35899000	2.69282300	2.41771800
H	4.34258400	-1.28338100	-0.43685800

General Experimental Procedures

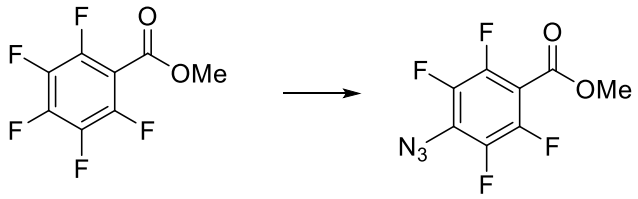
All chemicals were from commercial sources and were used without further purification. HPLC experiments were carried out on a 1200 series HPLC from Agilent Technologies (Santa Clara, CA, USA) equipped with a Varian Microsorb-MV 100-5 C18 250 × 4.6 mm column. Gradients were run with water containing TFA (0.1% v/v) and ACN containing TFA (0.1% v/v). Absorbance was measured at 210 nm. Column chromatography was performed with an Isolera automated purification system from Biotage (Uppsala, Sweden) using prepacked SNAP KP silica gel columns. The phrase "concentrated under reduced pressure" refers to the removal of solvents and other volatile materials using a rotary evaporator at water aspirator pressure (<20 Torr) while maintaining the water-bath temperature of 40 °C. Residual solvent was removed from samples by the vacuum (<0.1 Torr) achieved by a mechanical belt-drive oil pump. All procedures were performed in air at ambient temperature (~22 °C) and pressure (1.0 atm) unless indicated otherwise.

NMR spectra were acquired with an Avance Neo 400 spectrometer from Bruker (Billerica, MA, USA). (Note: Additional peaks might arise in NMR spectra from atropisomers around an oxanorbornadiene–phenyl bond.) Mass spectra were acquired by using positive ionization with an AccuTOF-DART 4G instrument from JEOL (Tokyo, Japan).

Chemical Synthesis

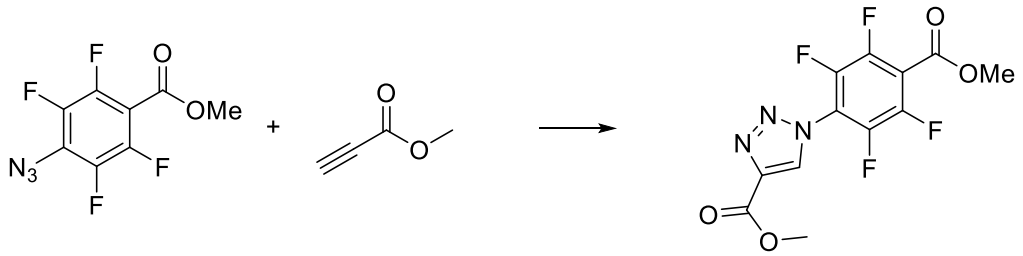
Caution! *Sodium azide is highly toxic.*[1] For example, sodium azide is nearly as toxic to mammals as sodium cyanide. The LD_{50} values for acute dermal toxicity in rabbits are 20 mg/kg (NaN_3) and 10.4 mg/kg (NaCN), respectively (MSDS).

Caution! *Organic azides are explosive.*[2] They can decompose to release N_2(g) upon the input of energy, such as heat, pressure, or impact. The organic azide used in this work has eight carbons along with six atoms of similar size, suggestive of relative stability.[2] Nonetheless, organic azides should be stored in the dark below room temperature (*e.g.*, at –20 °C). Moreover, azide–alkyne cycloadditions are exothermic[3] and should be performed on a small (*e.g.*, mg) scale prior to a cautious scale-up.[4]

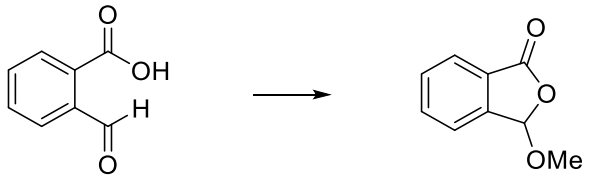


Methyl 4-Azido-2,3,5,6-tetrafluorobenzoate (9). Methyl pentafluorobenzoate (3.2796 g, 14.5 mmol, 1 equiv) was dissolved in 30 mL of 2:1 acetone/water, and sodium azide (1.1312 g, 17.4 mmol, 1.2 equiv) was added to the resulting solution. The reaction mixture was stirred at 90 °C (oil bath) for 3 h, then cooled. The mixture was diluted with 60 mL of water, extracted with Et_2O (3×), washed with sat. aq. sodium bicarbonate, dried over $MgSO_4$(s), filtered, and concentrated under reduced pressure to yield a white crystalline solid which was sufficiently pure

(3.4425 g, 13.8 mmol, 95%). **^{1}H NMR** (400 MHz, acetone-d_6, δ): 3.97 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, acetone-d_6, δ): 159.3, 146.5, 146.5, 146.5, 146.4, 146.4, 146.4, 146.3, 146.3, 144.0, 144.0, 143.9, 143.9, 143.9, 143.8, 143.8, 143.8, 142.1, 142.0, 141.9, 141.9, 141.8, 139.6, 139.6, 139.5, 139.5, 139.4, 139.4, 123.8, 107.5, 107.3, 107.2, 52.7, 29.5, 29.3, 29.1, 28.9, 28.7, 28.5, 28.3. **^{19}F{^{1}H} NMR** (376 MHz, acetone-d_6, δ): −141.67, −141.69, −141.71, −141.73, −141.75, −141.77, −153.03, −153.04, −153.06, −153.09, −153.11, −153.12. **HRMS** (DART–TOF) *m*/*z* calcd for $C_8H_4F_4N_3O_2^+$ [M + H]$^+$, 250.0234; found, 250.0243.



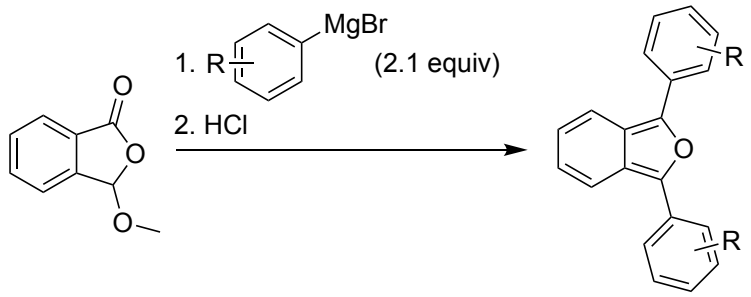
Methyl 1-(2,3,5,6-Tetrafluoro-4-(methoxycarbonyl)phenyl)-1*H*-1,2,3-triazole-4-carboxylate (11a). Methyl 4-azido-2,3,5,6-tetrafluorobenzoate (0.3963 g, 1.59 mmol, 1 equiv) was dissolved in 4 mL of a 1:1 *t*-BuOH/water, and the resulting solution was thoroughly purged with Ar(g). Sodium ascorbate (0.0792 g, 0.4 mmol, 0.25 equiv) and $CuSO_4 \cdot 5H_2O$ (0.0200 g, 0.08 mmol, 0.05 equiv) were added, followed by methyl propiolate (0.15 mL, 1.75 mmol, 1.1 equiv). The reaction mixture was stirred overnight, then diluted with 10 mL of water, extracted with EtOAc (3×), washed with H_2O, dried over $MgSO_4$(s), filtered, and concentrated under reduced pressure. The product was isolated by chromatography on silica gel (EtOAc in hexanes, product eluted at 40%) to yield a white solid (0.4469 g, 1.34 mmol, 84%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 8.49 (d, J = 1.2 Hz, 1H), 4.06 (s, 3H), 4.03 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 160.2, 158.8, 146.4, 146.3, 146.3, 146.2, 146.2, 143.8, 143.8, 143.7, 143.6, 142.8, 142.7, 142.65, 140.4, 140.3, 140.2, 140.1, 130.0, 130.0, 129.9, 118.2, 114.7, 114.5, 114.4, 77.4, 77.0, 53.9, 52.6. **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$, δ): −136.13, −136.14, −136.15, −136.16, −136.18, −136.20, −136.22, −136.23, −136.24, −136.25, −144.62, −144.64, −144.65, −144.67, −144.70, −144.72, −144.73, −144.73, −144.74. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{12}H_8F_4N_3O_4^+$ [M + H]$^+$, 334.0445; found, 334.0488.



3-Methoxyisobenzofuran-1(3*H*)-one. 2-Carboxybenzaldehyde (10.0381 g, 66.9 mmol) was dissolved in 150 mL of MeOH. The resulting solution was stirred at reflux (oil bath) overnight, and then concentrated under reduced pressure to yield a crystalline white solid (10.8967 g, 66.4 mmol, 99%), which was used without further purification. **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 7.90

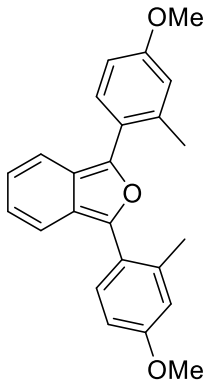
(d, J = 7.6 Hz, 1H), 7.73 (td, J = 7.5, 1.1 Hz, 1H), 7.66–7.56 (m, 2H), 6.32 (s, 1H), 3.65 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 168.5, 144.7, 134.4, 130.8, 127.0, 125.2, 123.5, 103.2, 77.7, 77.3, 77.0, 56.7. **HRMS** (DART–TOF) m/z calcd for $C_9H_9O_3$ $[M + H]^+$, 165.0546; found, 165.0568.

General Procedure for the Synthesis of 1,3-Diarylisobenzofurans

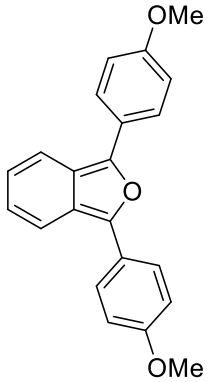


Isobenzofurans were prepared in a single step as reported previously.[5] Briefly, 3-methoxyisobenzofuran-1(3*H*)-one (1 equiv) was dissolved in dry THF (~0.4 M), and the resulting solution was cooled to 0 °C. The appropriate Grignard reagent (2.1 equiv, previously prepared from the corresponding aryl bromide as described below) was added dropwise to the phthalide solution under Ar(g), and the reaction mixture was allowed to stir overnight while warming to room temperature (~18 h). The reaction was quenched by the addition of 4 N HCl(aq) (~7 equiv), and the resulting solution was stirred for 1 h, then extracted with EtOAc (3×), washed with water and brine, dried over $MgSO_4$(s), filtered, and concentrated. In most cases the desired product was a crystalline solid that could be isolated by crystallization of the residue from ethanol. All isobenzofurans displayed strong fluorescence under illumination with a hand-held UV lamp.

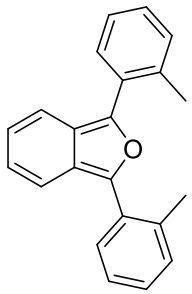
Preparation of Aryl Grignard Reagents. Magnesium turnings (2.2 equiv relative to 3-methoxyisobenzofuran-1(3*H*)-one) were stirred vigorously under N_2(g) for 30 min to remove oxide, then suspended in THF (equal volume as used to dissolve 3-methoxyisobenzofuran-1(3*H*)-one). A crystal of iodine was added, and the reaction mixture was heated to reflux (oil bath) under N_2(g). Aryl bromide (2.1 equiv relative to 3-methoxyisobenzofuran-1(3*H*)-one) was added dropwise (neat for liquids; solution in a minimal THF for solids), and the reaction mixture was stirred at reflux (time is indicated for each substrate) or at room temperature as specified for each substrate, then cooled to room temperature and carried forward. For some substrates, heating at reflux resulted in poor yields; in these cases, the magnesium suspension was heated to reflux, and the bromide was added dropwise until the reaction had initiated as indicated by the disappearance of the iodine color. The reaction mixture was removed from heat, and the addition of the bromide continued (the exothermic reaction generally maintained refluxing of the solvent during addition) and stirred for the time indicated for each substrate, then carried forward.



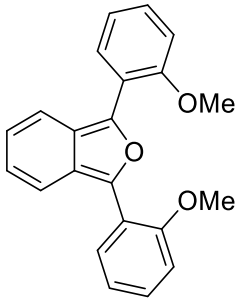
1,3-bis(4-Methoxy-2-methylphenyl)isobenzofuran (5). 1,3-bis(4-Methoxy-2-methylphenyl)isobenzofuran was prepared according to the general procedure starting with 3-methoxyisobenzofuran-1(3*H*)-one (2.7415 g, 16.7 mmol), 4-bromo-3-methylanisole (5.0 mL, 35.4 mmol), and magnesium turnings (0.9019 g, 37.1 mmol). The Grignard reagent was prepared by heating at reflux (oil bath) for 3 h. The product was isolated and purified by crystallization from ethanol, yielding a bright yellow crystalline solid (5.5061 g, 15.4 mmol, 92%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 7.56 (d, J = 8.4 Hz, 2H), 7.51 (dd, J = 6.9, 2.9 Hz, 2H), 6.98–6.85 (m, 6H), 3.90 (s, 6H), 2.53 (s, 6H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 159.3, 144.8, 138.3, 130.7, 124.0, 123.6, 121.7, 119.9, 116.6, 111.3, 55.3, 21.4. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{24}H_{23}O_3^+$ [M + H]$^+$, 359.1642; found, 359.1650.



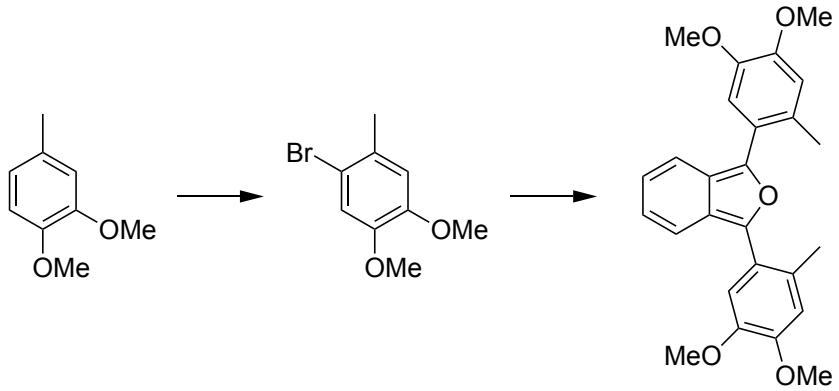
1,3-bis(4-Methoxyphenyl)isobenzofuran. 1,3-bis(4-Methoxyphenyl)isobenzofuran was prepared according to the general procedure from 3-methoxyisobenzofuran-1(3*H*)-one (1.8337 g, 11.2 mmol), 4-bromoanisole (3.0 mL, 24 mmol), and magnesium turnings (0.6928 g, 28.5 mmol). The Grignard reagent was prepared stirring for 3 h after initiation of the reaction. The product was isolated by crystallization from ethanol to give a bright yellow crystalline solid (3.2229 g, 9.7 mmol, 87%) **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 7.93–7.84 (m, 4H), 7.83–7.73 (m, 2H), 7.09–7.02 (m, 4H), 6.98 (dd, J = 6.9, 2.9 Hz, 2H), 3.90 (s, 6H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 158.6, 143.2, 126.1, 125.0, 124.6, 121.0, 120.1, 114.5, 77.4, 77.0, 55.4. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{22}H_{19}O_3$ [M + H]$^+$, 331.1329; found, 331.1346.



1,3-Di-*o*-tolylisobenzofuran. 1,3-Di-*o*-tolylisobenzofuran was prepared according to the general procedure from 3-methoxyisobenzofuran-1(3*H*)-one (3.7180 g, 22.6 mmol), 2-bromotoluene (5.73 mL, 47.6 mmol), and magnesium turnings (1.3298 g, 54.7 mmol). The Grignard reagent was prepared by heating at reflux (oil bath) for 3 h. The product was a crystalline yellow solid (4.4919 g, 15.1 mmol, 67%) that displayed bright blue triboluminecence. **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 7.71–7.62 (m, 2H), 7.62–7.52 (m, 2H), 7.41–7.30 (m, 6H), 7.04–6.95 (m, 2H), 2.57 (s, 6H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 145.3, 136.5, 131.3, 130.6, 129.3, 127.9, 125.9, 124.49, 122.3, 120.0, 77.4, 77.0, 76.7, 21.3. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{22}H_{19}O^+$ $[M + H]^+$, 299.1430; found, 299.1452.

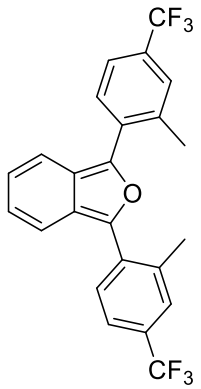


1,3-bis(2-Methoxyphenyl)isobenzofuran. 1,3-bis(2-Methoxyphenyl)isobenzofuran was prepared according to the general procedure from 3-methoxyisobenzofuran-1(3*H*)-one (1.8878 g, 11.5 mmol), 2-bromoanisole (3 mL, 24.1 mmol), and magnesium turnings (0.6150 g, 25.3 mmol). The Grignard reagent was prepared by heating at reflux (oil bath) for 3 h. The product was not crystalline and was purified by chromatography on silica gel (0–50% v/v EtOAc in hexanes, product eluted at 30%) to yield a yellow syrup (2.7791 g, 8.4 mmol, 73%). **^{1}H NMR** (400 MHz, acetone-d_6, δ): 7.78 (dd, J = 7.7, 1.7 Hz, 2H), 7.73–7.63 (m, 2H), 7.38 (ddd, J = 8.3, 7.3, 1.8 Hz, 2H), 7.19 (dd, J = 8.4, 1.1 Hz, 2H), 7.12 (td, J = 7.5, 1.1 Hz, 2H), 7.00–6.89 (m, 2H), 3.96 (s, 6H). **^{13}C{^{1}H} NMR** (101 MHz, acetone-d_6, δ): 156.0, 142.4, 129.3, 129.0, 123.6, 123.2, 121.2, 120.8, 111.8, 55.0, 29.6, 29.4, 29.2, 29.0, 28.8, 28.6, 28.4. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{22}H_{19}O_3$ $[M + H]^+$, 331.1329; found, 331.1399.

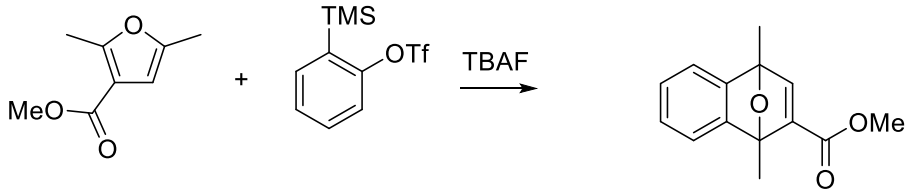


1-Bromo-4,5-dimethoxy-2-methylbenzene. 3,4-Dimethoxytoluene (5.3458 g, 35.1 mmol, 1 equiv) was dissolved in 30 mL of DMF. A solution of *N*-bromosuccinimide (6.9704 g, 38.6 mmol, 1.1 equiv) in 20 mL of DMF was added dropwise, and the reaction mixture was stirred for 1 h, then diluted with 100 mL of water, extracted with Et_2O (3×), washed with water and brine, dried over $MgSO_4$(s), and concentrated under reduced pressure. The residue was passed through a short silica plug, eluting with DCM, and then concentrated under reduced pressure to yield a dark red liquid that crystallized upon standing (7.7117 g, 33.4 mmol, 95%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 6.96 (s, 1H), 6.69 (s, 1H), 3.81 (d, J = 3.0 Hz, 6H), 2.29 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 148.1, 147.6, 129.5, 115.3, 114.4, 113.5, 77.6, 77.2, 76.9, 56.1, 56.0, 22.3. **HRMS** (DART–TOF) *m*/*z* calcd for $C_9H_{12}BrO_2$ $[M + H]^+$, 231.0015; found, 231.0014.

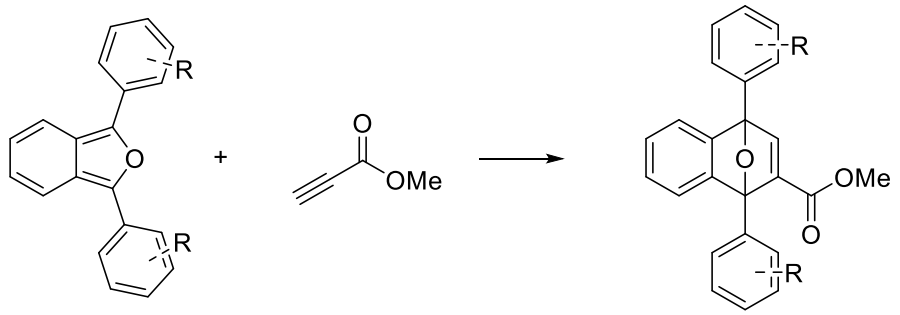
1,3-bis(4,5-Dimethoxy-2-methylphenyl)isobenzofuran. 1,3-bis(4,5-Dimethoxy-2-methylphenyl)isobenzofuran was prepared according to the general procedure from 3-methoxyisobenzofuran-1(3*H*)-one (2.4624 g, 15 mmol), 1-bromo-4,5-dimethoxy-2-methylbenzene (7.2550 g, 31.4 mmol), and magnesium turnings (0.7998 g, 32.9 mmol). The Grignard reagent was prepared by heating at reflux (oil bath) for 3 h. The product was isolated by crystallization from ethanol to yield a crystalline yellow solid (2.1553 g, 35%). **^{1}H NMR** (400 MHz, acetone-d_6, δ): 7.60–7.51 (m, 2H), 7.16 (s, 2H), 7.04–6.91 (m, 4H), 3.89 (d, J = 2.1 Hz, 12H), 2.46 (s, 6H). **^{13}C{^{1}H} NMR** (101 MHz, acetone-d_6, δ): 149.4, 147.5, 144.7, 128.8, 124.3, 122.5, 121.6, 119.8, 114.8, 113.0, 55.4, 55.2, 29.5, 29.4, 29.2, 29.0, 28.8, 28.6, 28.4, 19.8. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{26}H_{27}O_5$ $[M + H]^+$: 419.1853; found, 419.1892.



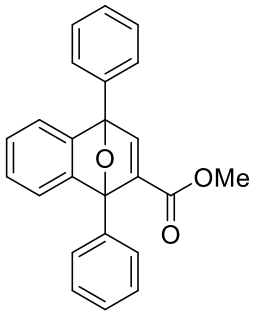
1,3-bis(2-Methyl-4-(trifluoromethyl)phenyl)isobenzofuran. 1,3-bis(2-Methyl-4-(trifluoromethyl)phenyl)isobenzofuran was prepared according to the general procedure from 3-methoxyisobenzofuran-1(3*H*)-one (1.6104 g, 9.81 mmol), 4-bromo-3-methylbenzotrifluoride (4.9140 g, 20.6 mmol), and magnesium turnings (0.5251 g, 21.6 mmol). The Grignard reagent was prepared by heating at reflux (oil bath) for 3 h. The product was purified by chromatography on silica gel (hexanes) to yield an orange crystalline solid (2.8901 g, 6.7 mmol, 68%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 7.77 (d, J = 8.1 Hz, 2H), 7.66–7.53 (m, 6H), 7.14–7.04 (m, 2H), 2.63 (s, 6H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 144.6, 137.0, 133.47, 130.2, 129.9, 129.6, 129.3, 128.2, 128.2, 128.2, 128.1, 125.6, 125.5, 123.3, 122.9, 122.9, 122.8, 122.8, 122.8, 119.6, 77.3, 77.0, 76.7, 21.4. **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$, δ): −62.60. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{24}H_{17}F_6O$ $[M + H]^+$, 435.1178; found, 435.1248.



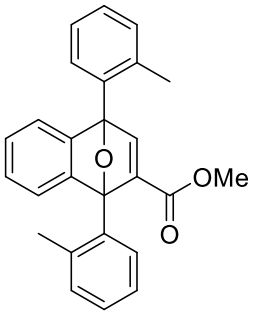
Methyl 1,4-Dimethyl-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate (10). Methyl 2,5-dimethylfuran-3-carboxylate (2.2053 g, 14.3 mmol, 2 equiv) and 2-(trimethylsilyl)phenyl trifluoromethanesulfonate (2.0850 g, 7 mmol, 1 equiv) were placed in a dry flask under N_2(g). Tetrabutylammonium fluoride (1 M in THF, 14 mL, 2 equiv) was added slowly, and the resulting mixture was stirred overnight. The reaction was quenched with 25 mL, extracted Et_2O (3×), washed twice with water, dried over $MgSO_4$(s), filtered, and concentrated under reduced pressure. The residue was purified twice by chromatography on silica gel (0–20% v/v EtOAc in hexanes, product eluted at 15%) to yield a colorless syrup (0.3940 g, 1.7 mmol, 24%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 7.54 (s, 1H), 7.32–7.28 (m, 2H), 7.21–7.17 (m, 1H), 7.07–7.03 (m, 2H), 3.73 (s, 3H), 2.06 (s, 4H), 1.95 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 164.0, 156.9, 151.9, 150.5, 150.4, 125.5, 125.2, 119.3, 119.2, 89.1, 87.8, 51.5, 14.9, 14.6. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{14}H_{15}O_3$ $[M + H]^+$, 231.1016; found, 231.1017.



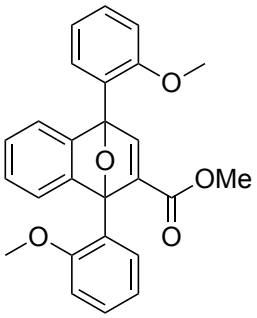
General Procedure for the Synthesis of Propiolate Adducts. 1,3-Diarylsobenzofuran (1 equiv) and methyl propiolate (5 equiv) were stirred in toluene (~0.2 M with respect to isobenzofuran) under an inert atmosphere for 18 h at 70 °C. The reaction mixture was then cooled and concentrated under reduced pressure, and the product was separated by chromatography on silica gel.



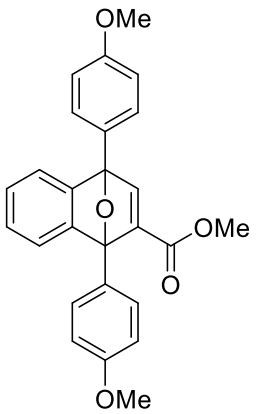
Methyl 1,4-Diphenyl-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate (3). Methyl 1,4-diphenyl-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate proved to be particularly sensitive to oxidation and was prepared by a modified method. Commercially available 1,3-diphenylisobenzofuran (0.7190 g, 2.66 mmol, 1 equiv) was placed in a flask that was then thoroughly purged with N_2(g). Methyl propiolate (3.3 mL, 39.9 mmol, 15 equiv) was added, and the reaction mixture was stirred overnight, and then concentrated under reduced pressure. The product was isolated by chromatography on silica gel (10% v/v EtOAc in hexanes). The resulting white solid was purified further by chromatography on a C18 column (Biotage) (0–100% v/v ACN in water, major product eluted at 70%) to yield a white solid (0.3059 g, 0.86 mmol, 32%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 8.08 (s, 1H), 7.88–7.80 (m, 2H), 7.73–7.66 (m, 2H), 7.60 (dt, J = 7.2, 1.0 Hz, 1H), 7.57–7.41 (m, 6H), 7.16–6.98 (m, 3H), 3.70 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 164.3, 155.9, 151.4, 151.2, 149.7, 134.3, 133.9, 128.9, 128.8, 128.8, 128.8, 128.3, 127.1, 125.7, 125.4, 122.0, 121.1, 93.9, 92.6, 77.4, 77.0, 76.7, 51.7. **HRMS** (DART–TOF) m/z calcd for $C_{24}H_{19}O_3$ $[M + H]^+$, 355.1329; found, 355.1321.



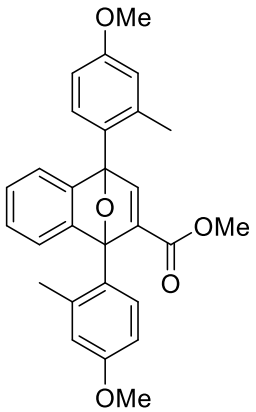
Methyl 1,4-Di-*o*-tolyl-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate. Methyl 1,4-di-*o*-tolyl-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate was prepared according to the general method from the corresponding isobenzofuran (0.5996 g, 2 mmol) and methyl propiolate (0.84 mL, 10 mmol). The product was purified by chromatography on silica gel (0–40% v/v EtOAc in hexanes, product eluted at 30%) to yield a pale yellow solid (0.6463 g, 1.7 mmol, 85%) **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 8.15 (s, 1H), 7.90 (dd, J = 7.6, 1.6 Hz, 1H), 7.76–7.65 (m, 1H), 7.61 (dt, J = 7.3, 0.9 Hz, 1H), 7.41–7.20 (m, 7H), 7.06–6.98 (m, 2H), 3.70 (s, 3H), 2.44 (s, 3H), 2.40 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 164.8, 154.5, 152.1, 150.8, 150.5, 138.9, 137.1, 132.2, 132.0, 129.9, 129.1, 128.9, 128.1, 126.0, 125.5, 125.4, 125.1, 123.5, 121.4, 94.3, 93.3, 51.8, 21.5, 21.4. **HRMS** (DART–TOF) m/z calcd for $C_{26}H_{23}O_3$ $[M + H]^+$, 383.1642; found, 383.1654.



Methyl 1,4-bis(2-Methoxyphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate. Methyl 1,4-bis(2-methoxyphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate was prepared according to the general method from the corresponding isobenzofuran (0.4001 g, 1.21 mmol) and methyl propiolate (0.51 mL). The product was purified by chromatography on silica gel (0–40% v/v EtOAc in hexanes, product eluted at 30%) to yield a colorless solid (0.4575 g, 1.1 mmol, 91%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 7.97 (s, 1H), 7.83 (dd, J = 7.7, 1.7 Hz, 1H), 7.63 (dd, J = 7.6, 1.7 Hz, 1H), 7.46 (dddd, J = 7.1, 6.0, 4.2, 1.7 Hz, 2H), 7.39 (ddd, J = 8.2, 7.4, 1.8 Hz, 1H), 7.14–6.96 (m, 7H), 3.96 (s, 3H), 3.81 (s, 3H), 3.64 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 165.1, 158.5, 156.2, 151.2, 150.2, 131.0, 130.6, 129.3, 127.5, 125.0, 124.9, 123.8, 122.6, 121.2, 121.0, 120.7, 111.7, 110.4, 95.0, 90.6, 77.3, 77.0, 76.7, 55.3, 55.2, 51.2. **HRMS** (DART–TOF) m/z calcd for $C_{26}H_{23}O_5$ $[M + H]^+$, 415.1540; found, 415.1564.

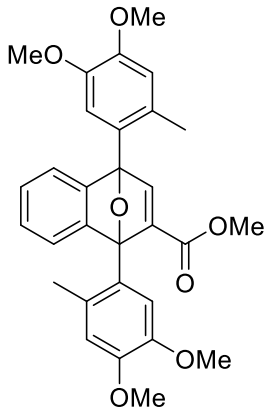


Methyl 1,4-bis(4-Methoxyphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate. The corresponding isobenzofuran (0.3985 g, 1.2 mmol) was dissolved in 4 mL of methyl propiolate, and the reaction mixture was stirred overnight, and then concentrated under reduced pressure. The product was isolated by chromatography on silica gel (0–40% v/v EtOAc in hexanes, product eluted at 30%) to yield a colorless solid (0.2800 g, 0.68 mmol, 57%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 8.08 (s, 1H), 7.78–7.70 (m, 2H), 7.69–7.62 (m, 2H), 7.58 (dt, J = 7.1, 0.9 Hz, 1H), 7.17–6.99 (m, 8H), 3.87 (s, 4H), 3.87 (s, 3H), 3.71 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 171.2, 164.5, 160.1, 160.0, 156.0, 151.7, 151.3, 150.2, 130.3, 129.0, 126.3, 126.1, 125.6, 125.4, 122.0, 121.2, 114.2, 113.8, 93.8, 92.4, 77.4, 77.1, 76.8, 55.4, 55.4, 55.3, 55.3, 51.7. **HRMS** (DART–TOF) m/z calcd for $C_{26}H_{23}O_5$ $[M + H]^+$, 415.1540; found, 415.1555.

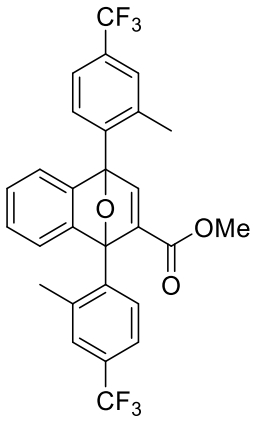


Methyl 1,4-bis(4-Methoxy-2-methylphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate (6). Methyl 1,4-bis(4-methoxy-2-methylphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate was prepared according to the general procedure from isobenzofuran (0.8167 g, 2.28 mmol) and methyl propiolate (0.95 mL, 11.4 mmol). The product was purified by chromatography on silica gel (0–40% v/v EtOAc in hexanes, product eluted at 30%) to yield a pale yellow foam (0.9266 g, 2.1 mmol, 92%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 8.10 (s, 1H), 7.83–7.76 (m, 1H), 7.63 (d, J = 8.5 Hz, 1H), 7.56 (d, J = 7.1 Hz, 1H), 7.15–7.03 (m, 1H), 7.03–6.99 (m, 2H), 6.89–6.78 (m, 4H), 3.86 (s, 3H), 3.85 (s, 3H), 3.70 (s, 3H), 2.38 (s, 3H), 2.36 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 165.0, 159.9, 159.8, 154.9, 152.1, 151.0, 150.8,

140.7, 139.3, 131.3, 129.8, 125.3, 125.0, 124.5, 124.3, 123.5, 121.5, 117.7, 117.6, 110.7, 110.4, 94.1, 93.0, 77.3, 76.7, 55.2, 55.2, 51.7, 21.6, 21.6. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{28}H_{27}O_5$ $[M + H]^+$, 443.1853; found, 443.1876.



Methyl 1,4-bis(4,5-Dimethoxy-2-methylphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate. Methyl 1,4-bis(4,5-dimethoxy-2-methylphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate was prepared according to the general procedure from the corresponding isobenzofuran (0.3177 g, 0.76 mmol) and methyl propiolate (0.32 mL). The product was purified by chromatograph on silica gel (0–40% v/v EtOAc in hexanes, product eluted at 30%) to yield an off-white solid (0.3255 g, 0.65 mmol, 86%) **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 8.06 (s, 1H), 7.60 (d, J = 7.1 Hz, 1H), 7.44 (s, 1H), 7.21 (s, 1H), 7.16–6.99 (m, 3H), 6.83 (s, 1H), 6.79 (s, 1H), 3.94 (s, 3H), 3.93 (s, 3H), 3.90 (s, 3H), 3.90 (s, 3H), 3.70 (s, 3H), 2.40 (s, 3H), 2.34 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 164.9, 154.6, 152.1, 151.0, 150.8, 149.0, 148.9, 146.9, 146.2, 131.8, 129.1, 125.4, 125.1, 124.2, 124.0, 123.2, 121.6, 115.1, 114.8, 113.9, 111.5, 94.0, 92.8, 77.4, 77.1, 76.8, 56.2, 56.1, 55.9, 55.8, 51.8, 21.0, 21.0, 20.9. **HRMS** (DART–TOF) *m*/*z* calcd for $C_{30}H_{31}O_7$ $[M + H]^+$, 503.2064; found, 503.2068.

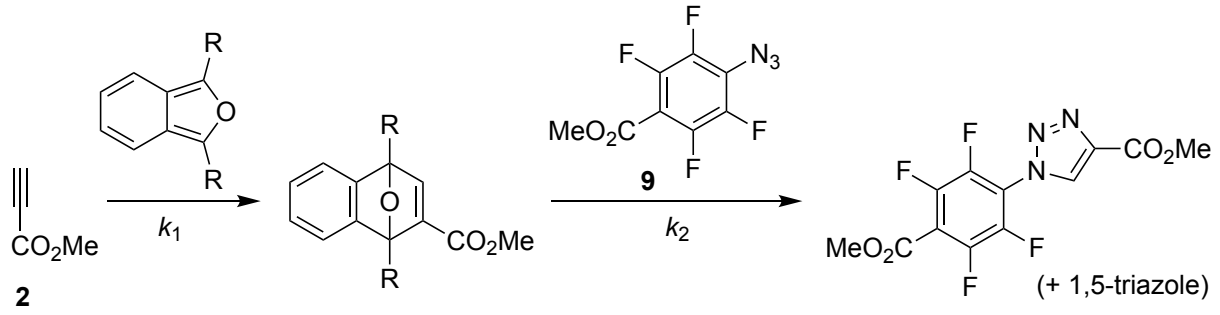


Methyl 1,4-bis(2-Methyl-4-(trifluoromethyl)phenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate. Methyl 1,4-bis(2-methyl-4-(trifluoromethyl)phenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate was synthesized according to the general procedure from the

corresponding isobenzofuran (0.7392 g, 1.7 mmol) and methyl propiolate (0.71 mL, 8.5 mmol) and purified by chromatography on silica gel (0–40% v/v EtOAc in hexanes, product eluted at 20%) to yield an orange solid (0.7996 g, 1.6 mmol, 94%). **^{1}H NMR** (400 MHz, $CDCl_3$, δ): 8.18 (s, 1H), 8.09 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.1 Hz, 1H), 7.69–7.53 (m, 5H), 7.18 (td, J = 7.3, 1.3 Hz, 1H), 7.07 (dt, J = 14.0, 7.1 Hz, 2H), 3.73 (s, 3H), 2.53 (s, 3H), 2.49 (s, 3H). **^{13}C{^{1}H} NMR** (101 MHz, $CDCl_3$, δ): 164.2, 153.7, 151.9, 149.8, 149.5, 140.0, 137.6, 136.0, 135.7, 131.7, 131.6, 131.6, 131.3, 131.2, 131.0, 130.9, 130.7, 130.6, 130.3, 130.2, 130.2, 128.9, 128.9, 128.8, 128.8, 128.7, 128.7, 128.6, 128.6, 128.3, 128.2, 128.1, 128.1, 125.9, 125.6, 125.4, 125.4, 123.6, 123.0, 123.0, 123.0, 122.9, 122.7, 122.7, 122.5, 122.5, 122.4, 122.4, 121.4, 120.0, 93.6, 93.0, 52.0, 21.5, 21.4. **^{19}F{^{1}H} NMR** (376 MHz, $CDCl_3$, δ): −62.75, −62.82. **HRMS** (DART–TOF) m/z calcd for

Reaction Kinetics

Reaction kinetics were assessed by HPLC analysis using absorption at 210 nm. Authentic standards of the benzooxanorbornadiene intermediates and the triazole product were used to obtain calibration curves for quantitation. Reaction temperature was controlled by the HPLC autosampler. The solvents used in the reaction were degassed using three freeze-pump-thaw cycles and stored under N_2(g). All reactions were performed in triplicate, and rate constants are reported as the mean ± SD. Rate constants were determined by initial rates with <10% conversion of the reactants. Reactions for the first step were performed under pseudo first-order conditions with a large excess of methyl propiolate; reactions for the second step were performed under second-order conditions. The isobenzofuran scaffold is highly sensitive to oxidation, especially at elevated temperatures, but oxidation can generally be prevented by addition of an excess of oxygen scavengers such as butylated hydroxytoluene (BHT) or propyl gallate, which did not otherwise affect the reaction kinetics.



Representative Procedure for the Determination of k_1. 1,3-bis(4-Methoxy-2-methylphenyl)isobenzofuran (5.0 mg, 1.4×10^{-5} mol, 1 equiv) and propyl gallate (15 mg, 7.1×10^{-5} mol, ~5 equiv) were dissolved in 1.0 mL of degassed 1:4 H_2O/dioxane. Methyl propiolate (20 µL, 2.2×10^{-4} mol, 15 equiv) was added, and the resulting solution was mixed thoroughly, then immediately transferred to an autosampler vial maintained at 30 °C (heat block) and analyzed

by sequential injections on to an HPLC instrument. The reaction rate was determined by the area of the oxanorbornadiene adduct product peak.

Representative Procedure for the Determination of k_2. Methyl 1,4-bis(4-methoxy-2-methylphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate (7.1 mg, 1.6×10^{-5} mol, 1 equiv) was dissolved in 2.0 mL of degassed 1:4 H_2O/dioxane. In a separate vial, methyl 4-azido-2,3,5,6-tetrafluorobenzoate (4.0 mg, 1.6×10^{-5} mol, 1 equiv) was dissolved in 2.0 mL of degassed 1:4 H_2O/dioxane. Aliquots (0.5 mL) of each solution were added to an autosampler vial, mixed thoroughly, placed in the autosampler maintained at 30 °C, and analyzed by sequential injections on HPLC. The reaction rate was determined by the area of the triazole product peak, combining the areas for both the 1,4- and 1,5-triazoles if both were present in the reaction mixture.

Representative Procedure for the Catalytic Reaction. Methyl 4-azido-2,3,5,6-tetrafluorobenzoate (10.0 mg, 4.0×10^{-5} mol, 1 equiv), BHT (8.8 mg, 4.0×10^{-5} mol, 1 equiv), and 1,3-bis(4-methoxy-2-methylphenyl)isobenzofuran (2.9 mg, 0.8×10^{-5} mol, 0.2 equiv) were dissolved in 1.0 mL of degassed 1:4 H_2O/dioxane. Methyl propiolate (20 µL, 2.2×10^{-4} mol, 5.6 equiv) was added, and the resulting solution was mixed thoroughly and then immediately transferred to an autosampler vial maintained at 30 °C (heat block) and analyzed by sequential injections on to an HPLC instrument. The reaction rate was determined by the area of the triazole product peak, and the reaction was allowed to progress until nearly complete (>95%) conversion of the azide was observed. The reaction rate was compared to that of a background reaction with identical concentrations of reagents, omitting only the isobenzofuran, run under identical conditions, as well as a reaction with identical concentrations using 100 mol% of isobenzofuran.

References

(1) Peer, M. Performing Hazardous Reactions with Sodium Azide. *Spec. Chem*. **1998**, *18*, 256–263.

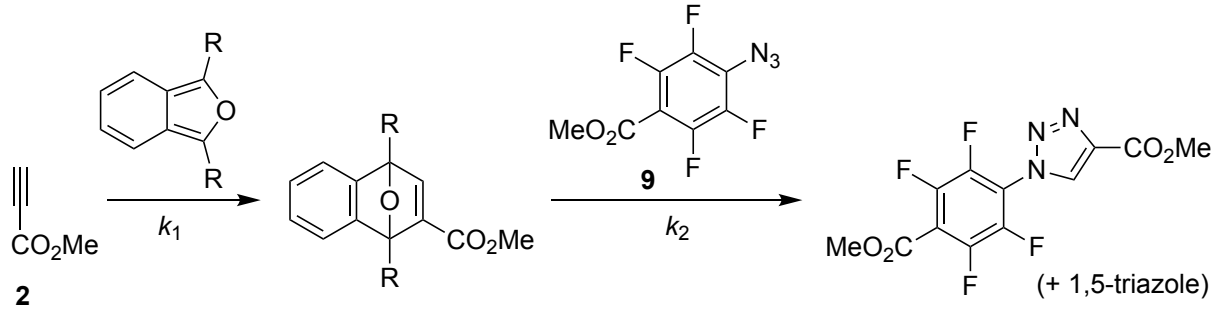
(2) See: Ref. 77 in Kolb, H. C.; Finn, M. G.; Sharpless, K. B. Click Chemistry: Diverse Chemical Function from a Few Good Reactions. *Angew. Chem.*, *Int. Ed.* **2001**, *40*, 2004–2021.

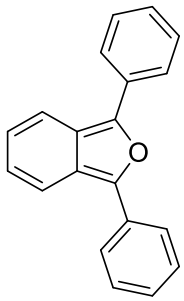
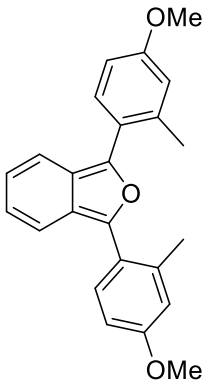
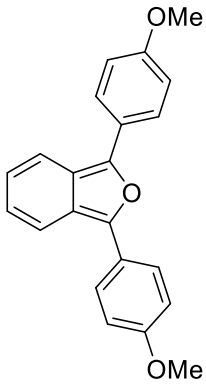
(3) Blomquist, A. T.; Liu, L. H. Many-Membered Carbon Rings. VII. Cycloöctyne. *J. Am. Chem. Soc.* **1953**, *75*, 2153–2154.

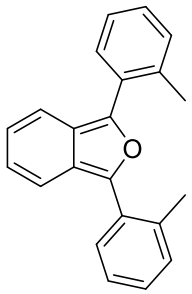
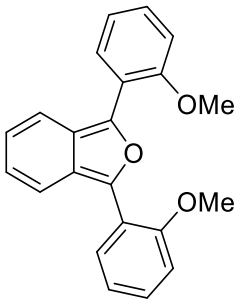
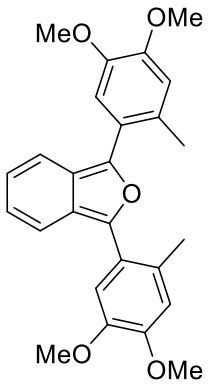
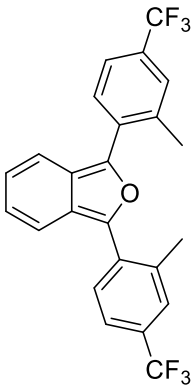
(4) González-Bobes, F.; Kopp, N.; Li, L.; Deerberg, J.; Sharma, P.; Leung, S.; Davies, M.; Bush, J.; Hamm, J.; Hrystak, M. Scale-up of Azide Chemistry: A Case Study. *Org. Process Res. Dev.* **2012**, *16*, 2051–2057.

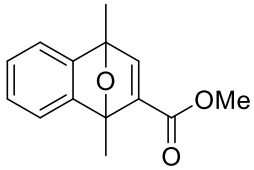
(5) Benderradji, F.; Nechab, M.; Einhorn, C.; Einhorn, J. A Single-Step Synthesis of Symmetrical 1,3-Diarylisobenzofurans. *Synlett* **2006**, 2035–2038.

Table S1. Rate Constants for the Cycloaddition of Alkyne 2 with Isobenzofurans and Corresponding Oxanorbornadiene Adducts with Azide 9 in 1:4 H_2O/dioxane at 30 °C.



Compound	k_1 (M^{-1} min^{-1})	k_2 (M^{-1} min^{-1})	Inactivation by bis Adduct Formation?
	$(8.7 \pm 0.5) \times 10^{-3}$	$(8.7 \pm 0.1) \times 10^{-1}$ **3**	Yes
	$(2.57 \pm 0.04) \times 10^{-3}$ **5**	$(4.4 \pm 0.1) \times 10^{-1}$ **6**	No
	$(1.5 \pm 0.1) \times 10^{-1}$	$(9.4 \pm 0.1) \times 10^{-1}$	Yes (rapid)

	$(9.56 \pm 0.08) \times 10^{-4}$	$(3.0 \pm 0.2) \times 10^{-1}$	No
	$(8.9 \pm 0.3) \times 10^{-3}$	$(4.6 \pm 0.1) \times 10^{-2}$	Yes (slow)
	$(2.06 \pm 0.04) \times 10^{-3}$	$(6.6 \pm 0.1) \times 10^{-1}$	No
	$(4.94 \pm 0.02) \times 10^{-4}$	$(3.9 \pm 0.1) \times 10^{-1}$	No

	—	$(2.9 \pm 0.1) \times 10^{-2}$ **10**	—

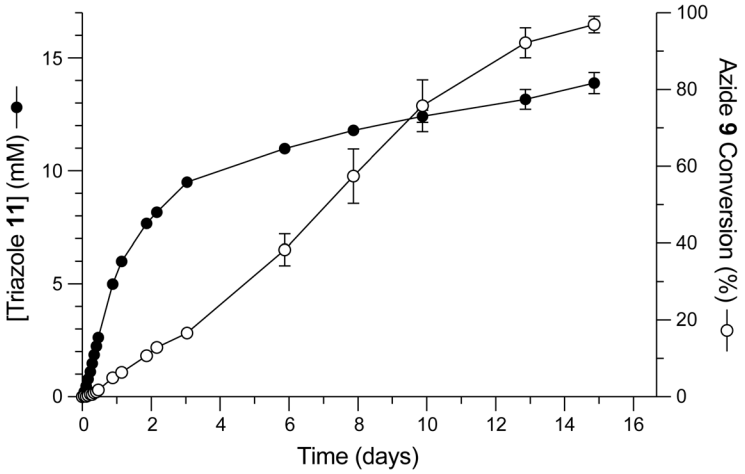


Figure S1. Full reaction progress curves for the reaction of alkyne **2** and azide **9** catalyzed by isobenzofuran **5** (20 mol%). Values are the mean ± SD from three independent experiments. The yield of triazole **11** is likely compromised by product degradation and catalyst degradation during the long time course (see: Figure S3).

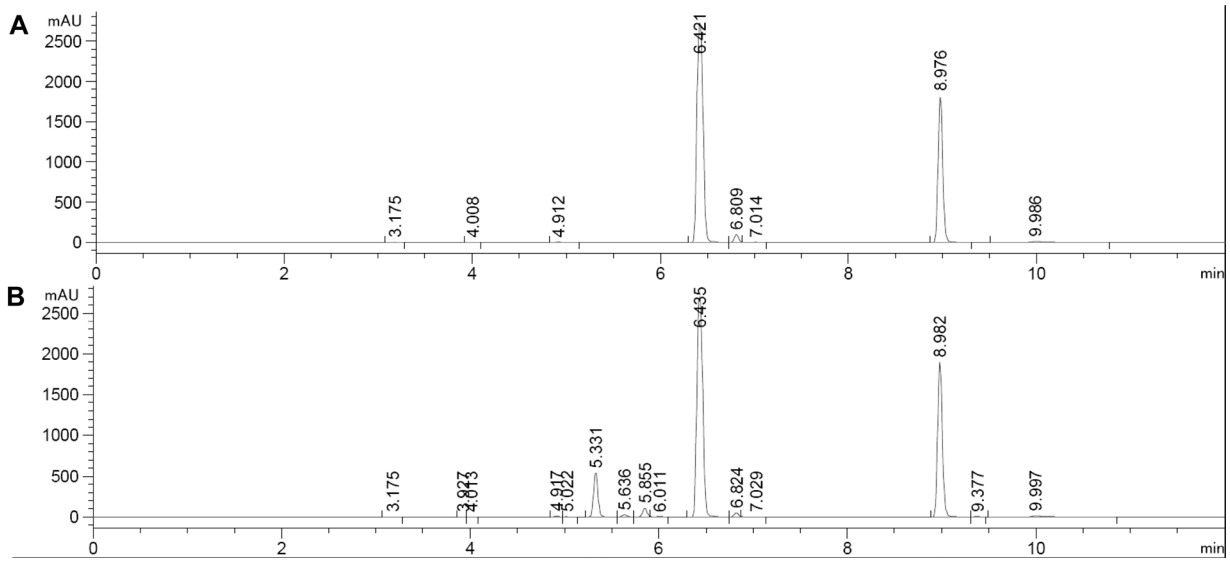


Figure S2. Representative HPLC traces (detected at 280 nm) for the uncatalyzed reaction of alkyne **2** and azide **9**. (A) Initial reaction mixture. The peak at 6.421 min corresponds to azide **9**; the peak at 8.976 min corresponds to the BHT additive. Alkyne **2** has no absorbance at 280 nm and was detected at 210 nm. (B) Reaction mixture after 120 h at 30 °C. The peak at 5.331 min corresponds to the 1,4-triazole product; the peak at 5.855 min corresponds to the 1,5-triazole product. Integration yields 1,4-triazole:1,5-triazole 83:17. No other significant products were observed from the reaction.

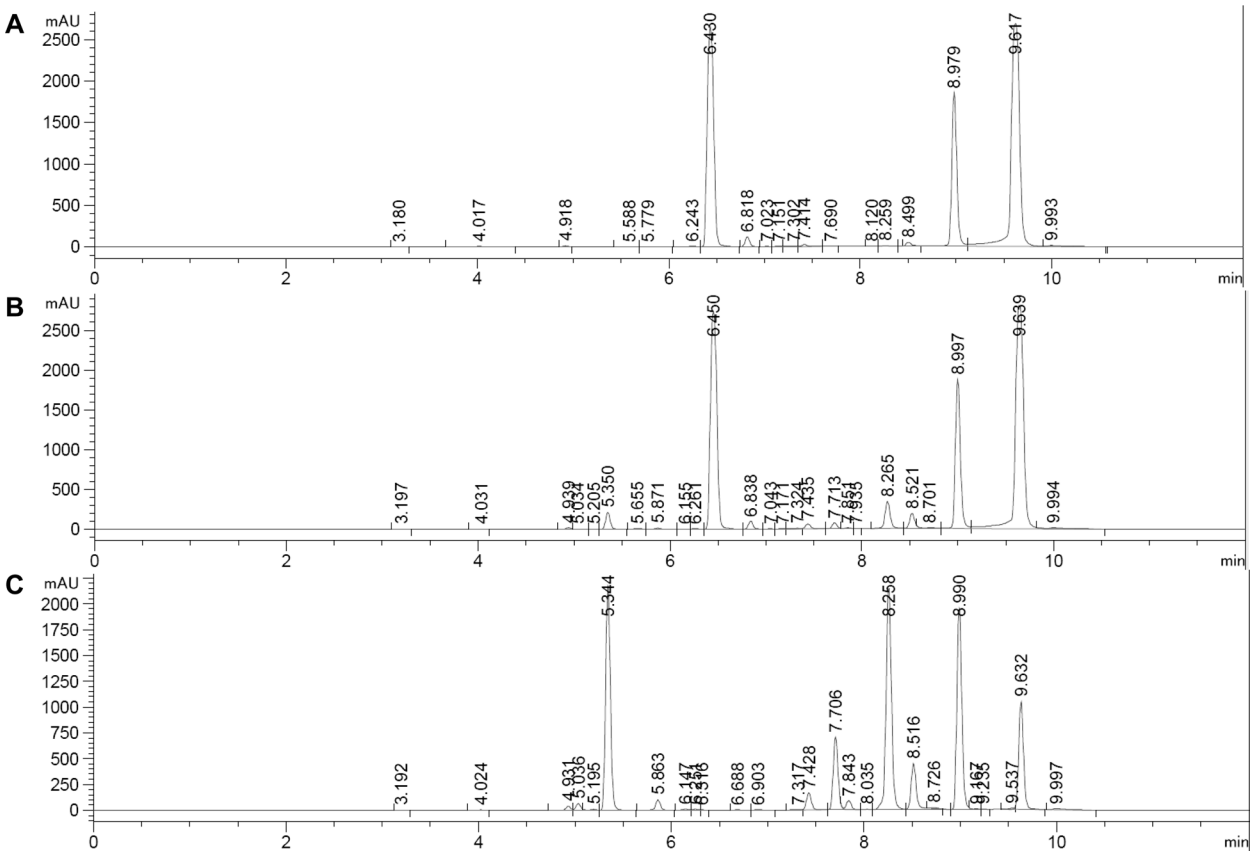
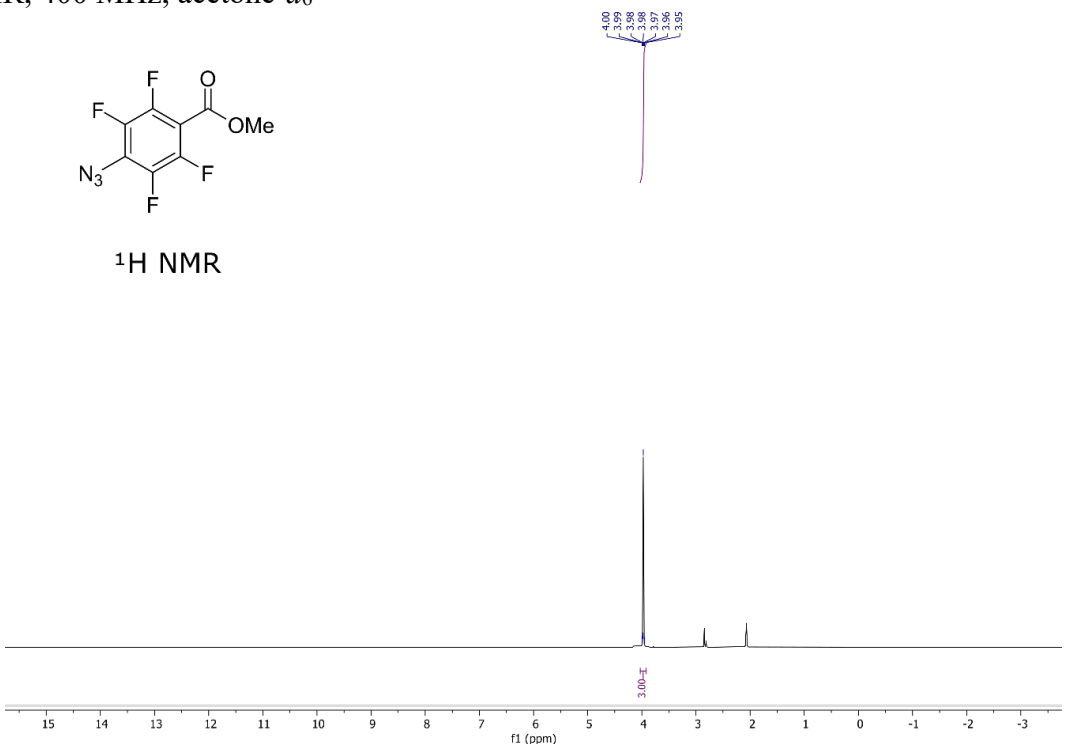


Figure S3. Representative HPLC traces (detected at 280 nm) for the reaction of alkyne **2** and azide **9** catalyzed by isobenzofuran **5** (100 mol%). (A) Initial reaction mixture. The peak at 6.430 min corresponds to azide **9**; the peak at 8.979 min corresponds to the BHT additive; the peak at 9.647 min corresponds to isobenzofuran. Alkyne **2** has no absorbance at 280 nm and was detected at 210 nm. (B) Reaction mixture after 6 h at 30 °C. The peak at 5.350 min corresponds to the 1,4-triazole product; the peak at 5.871 min corresponds to the 1,5-triazole product; the peak at 8.265 min corresponds to the benzooxanorbornadiene adduct. (C) Reaction mixture after 148 h at 30 °C. The peak at 5.344 min corresponds to the 1,4-triazole product; the peak at 5.863 min corresponds to the 1,5-triazole product; the peak at 8.258 min corresponds to the benzooxanorbornadiene adduct. The peaks at 7.706 min and 8.516 min correspond to isobenzofuran degradation products. Integration yields 1,4-triazole:1,5-triazole 96:4.

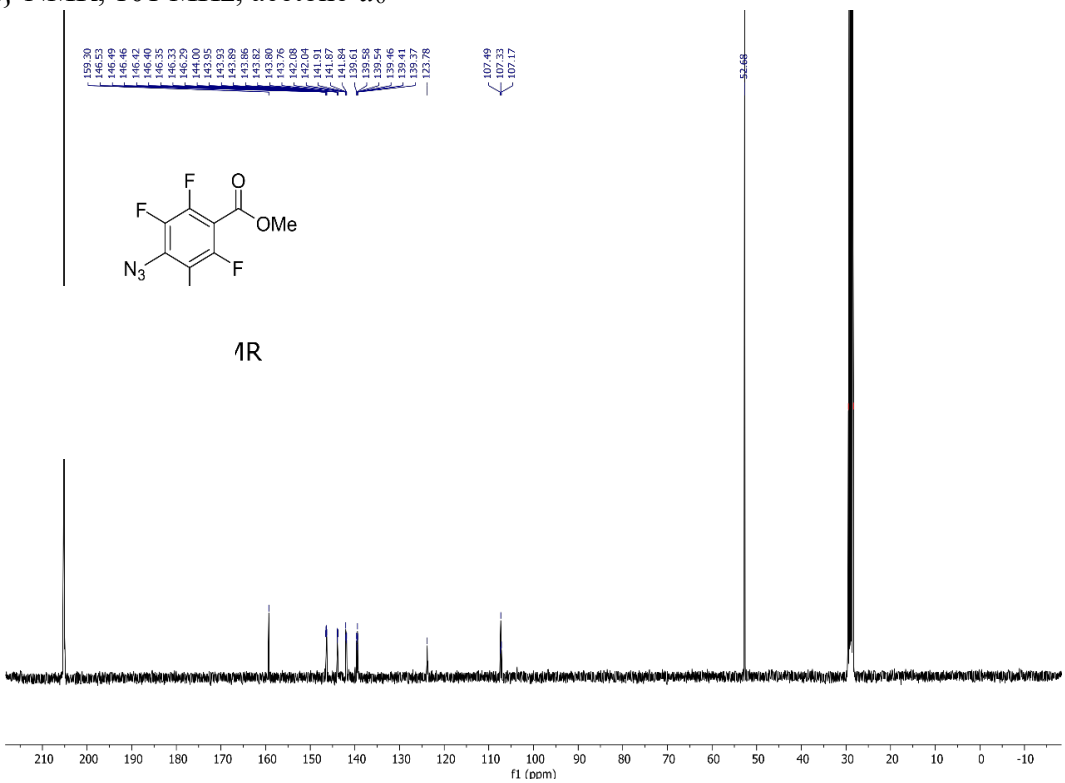
NMR Spectra

Methyl 4-Azido-2,3,5,6-tetrafluorobenzoate (9)

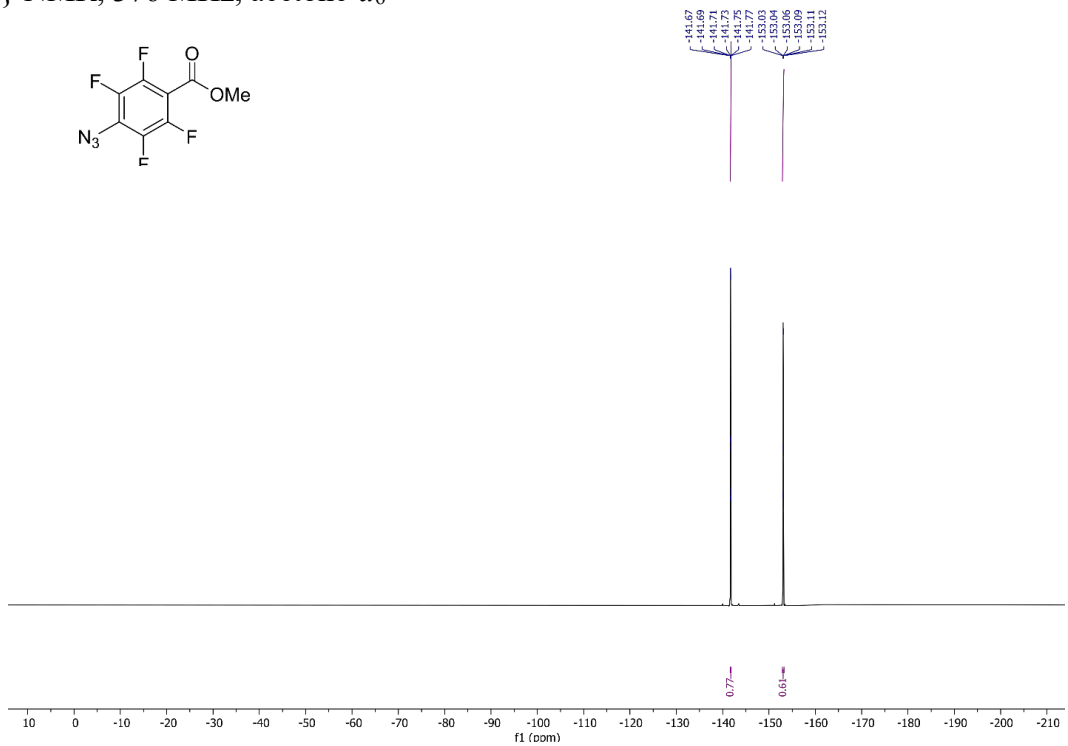
^{1}H NMR, 400 MHz, acetone-d_6



^{13}C{^{1}H} NMR, 101 MHz, acetone-d_6

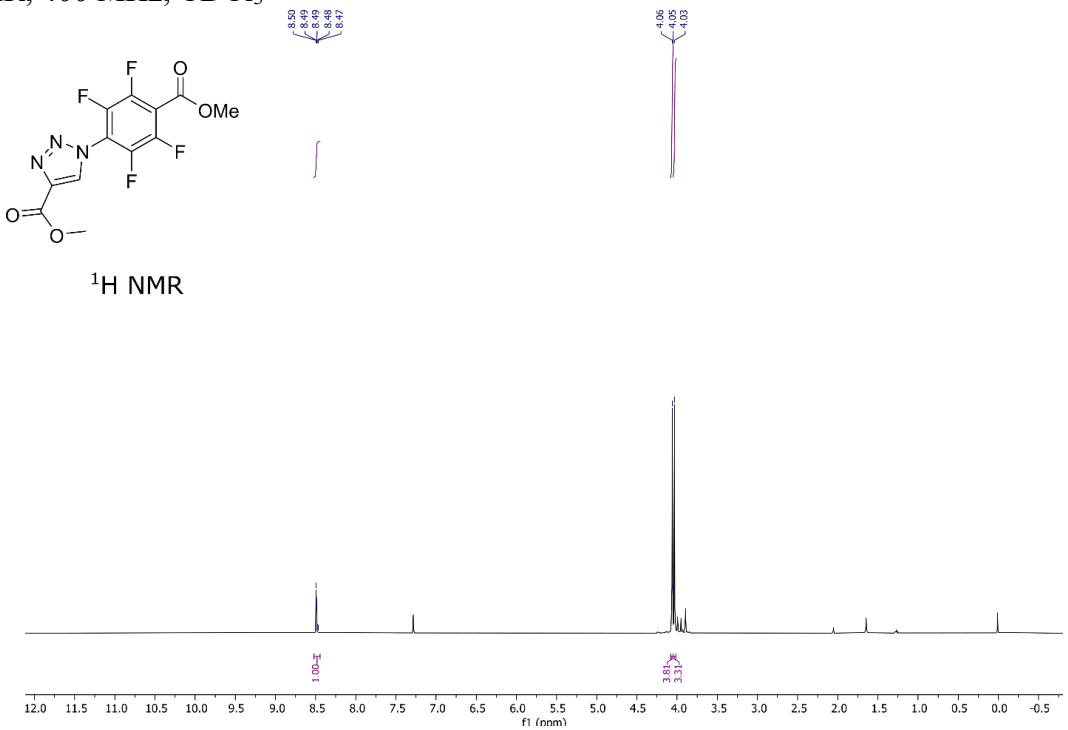


$^{19}F\{^{1}H\}$ NMR, 376 MHz, acetone-d_6



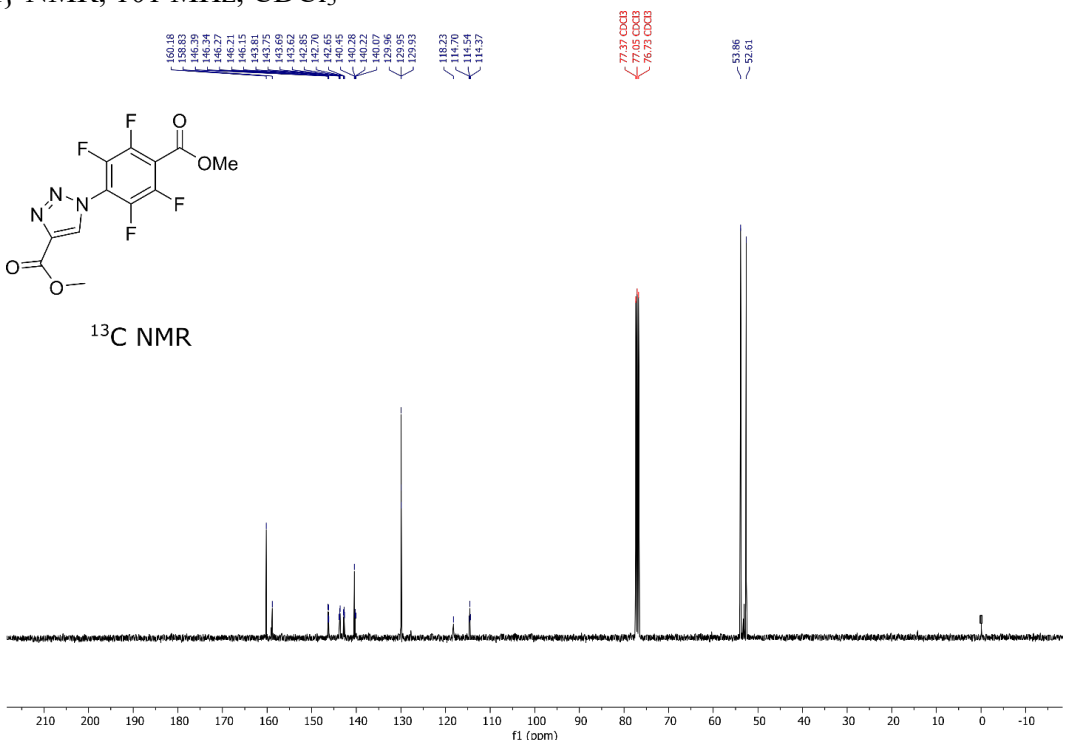
Methyl 1-(2,3,5,6-Tetrafluoro-4-(methoxycarbonyl)phenyl)-1*H*-1,2,3-triazole-4-carboxylate

^{1}H NMR, 400 MHz, $CDCl_3$



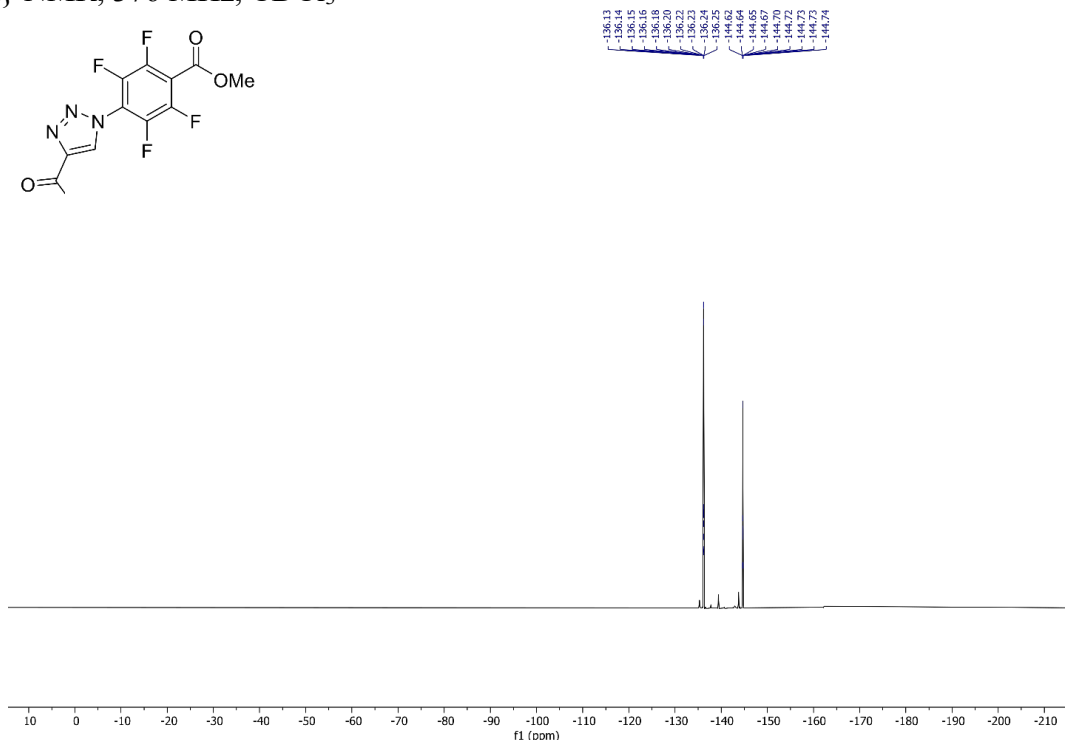
^{1}H NMR

^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$



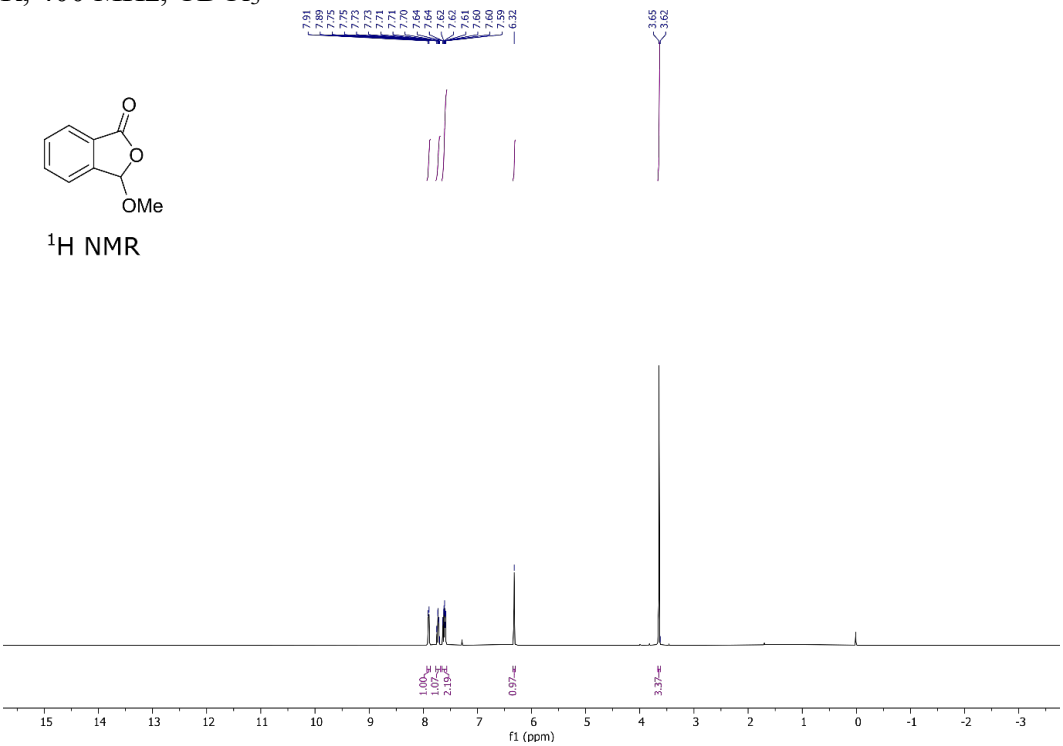
^{13}C NMR

$^{19}F\{^{1}H\}$ NMR, 376 MHz, $CDCl_3$

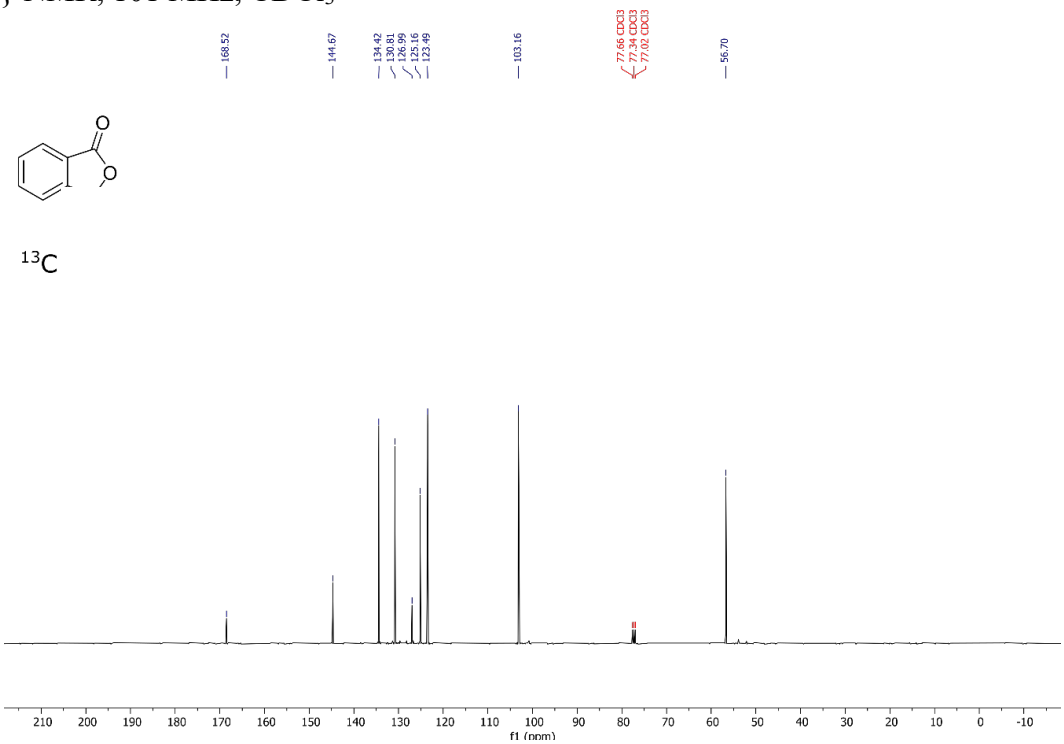


3-Methoxyisobenzofuran-1(3*H*)-one

^{1}H NMR, 400 MHz, $CDCl_3$

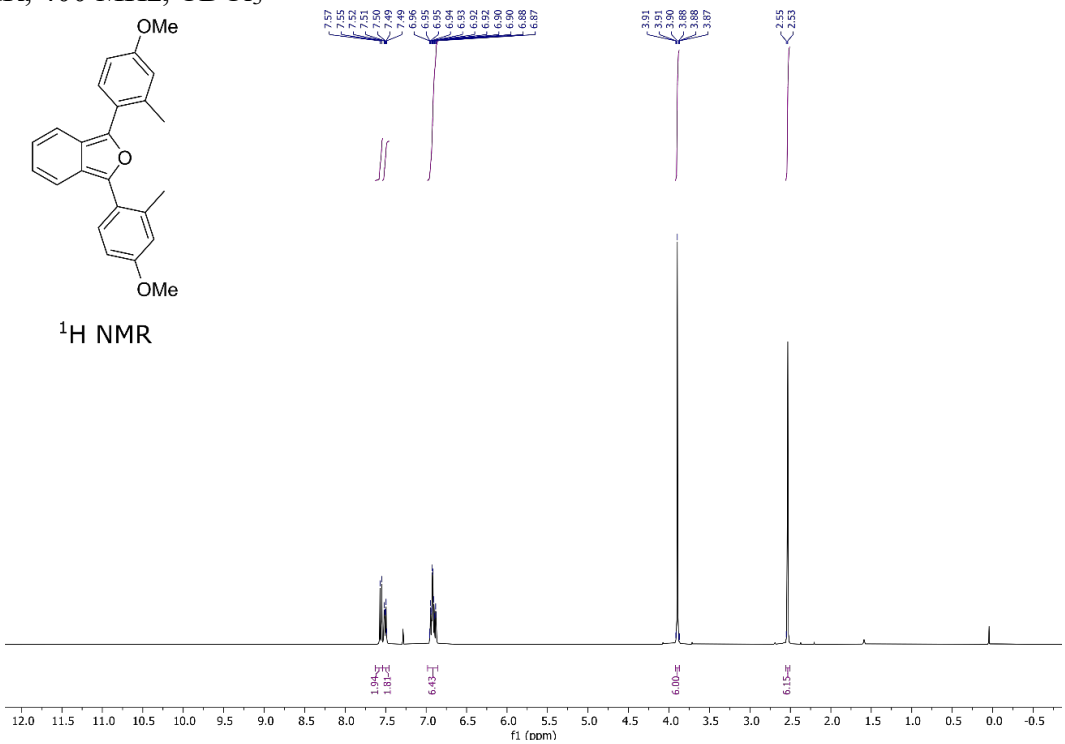


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

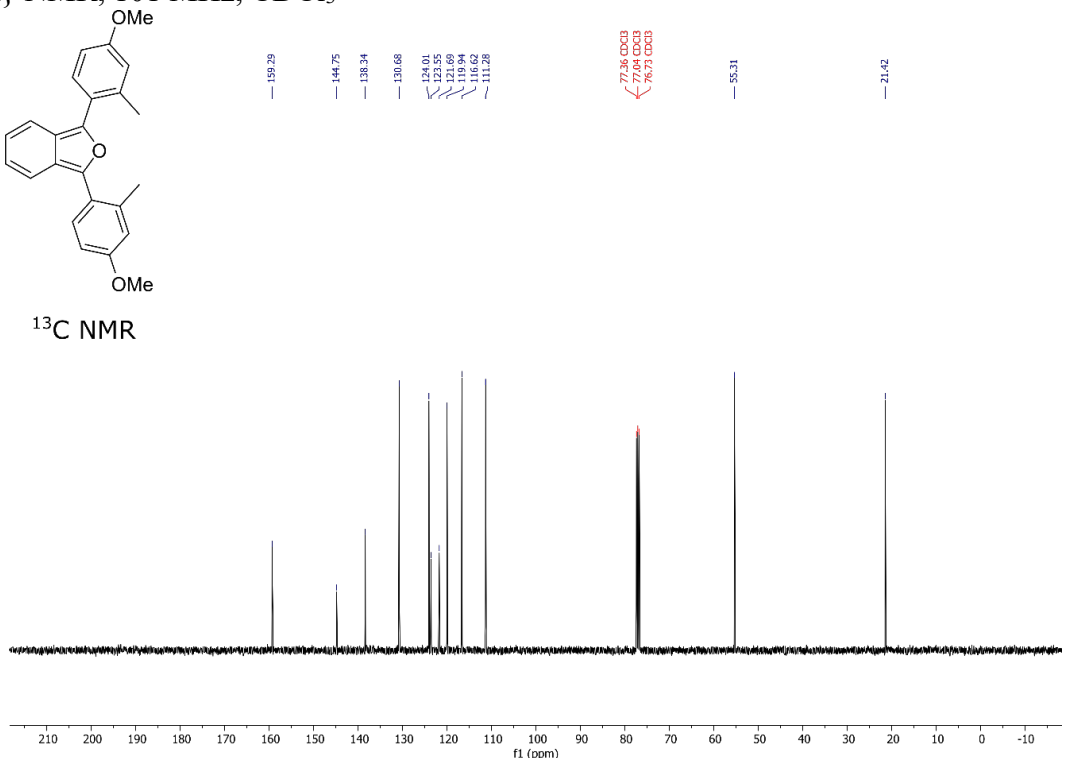


1,3-bis(4-Methoxy-2-methylphenyl)isobenzofuran (5)

^{1}H NMR, 400 MHz, $CDCl_3$

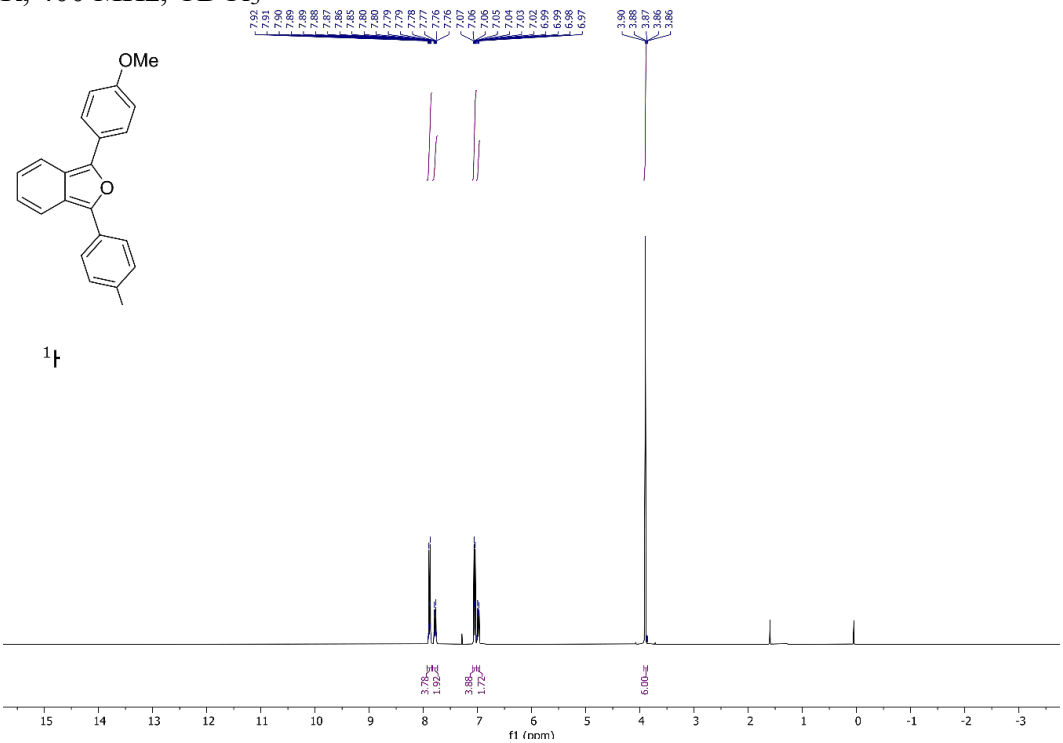


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

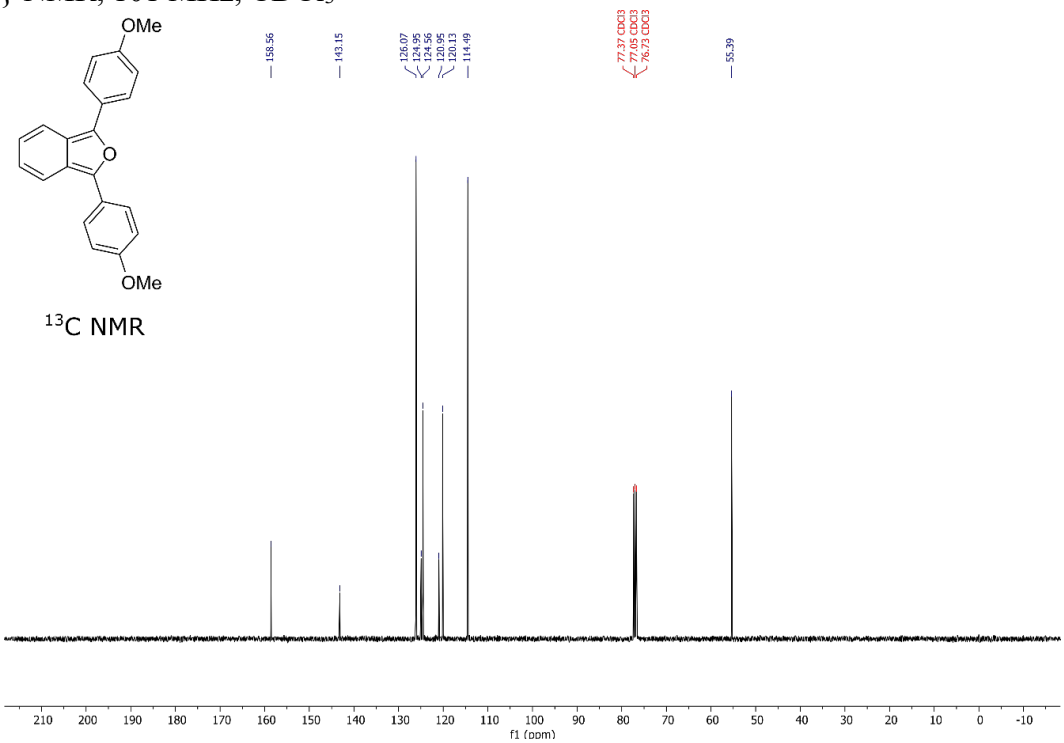


1,3-bis(4-Methoxyphenyl)isobenzofuran

^{1}H NMR, 400 MHz, $CDCl_3$

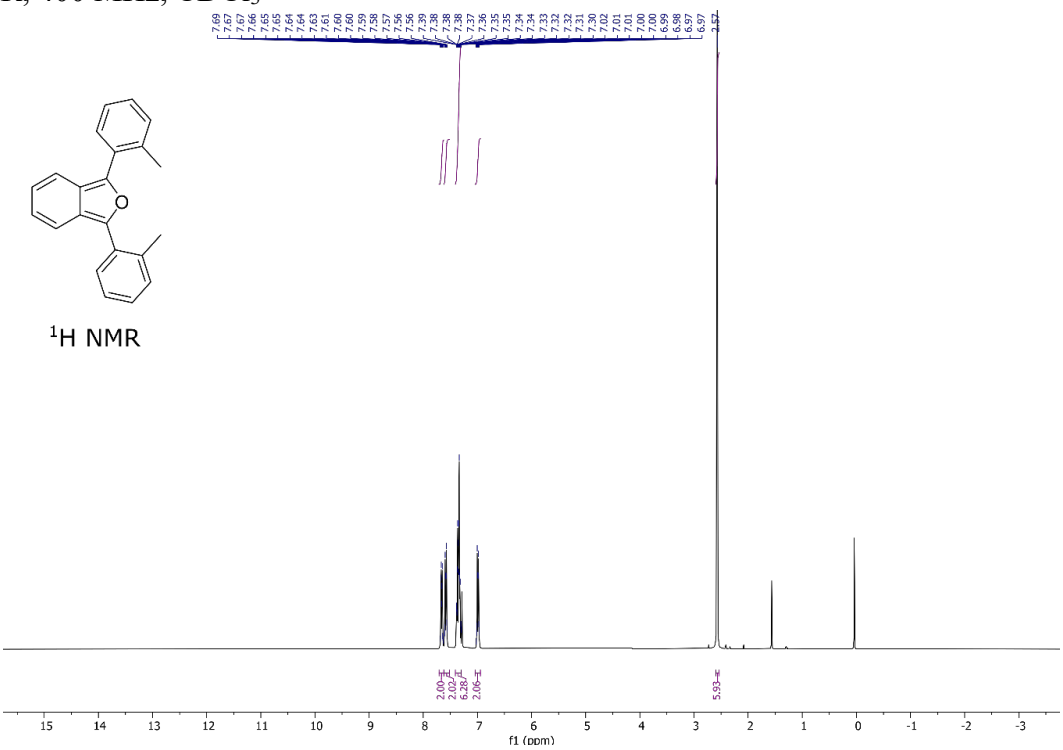


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

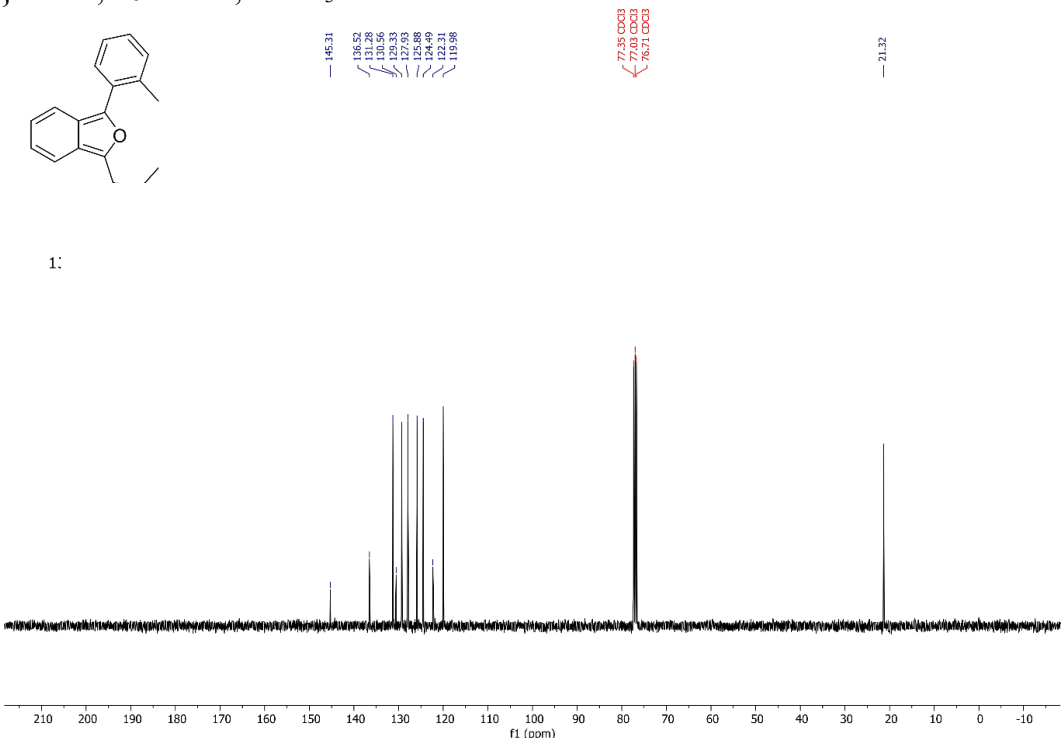


1,3-Di-*o*-tolylisobenzofuran

^{1}H NMR, 400 MHz, $CDCl_3$

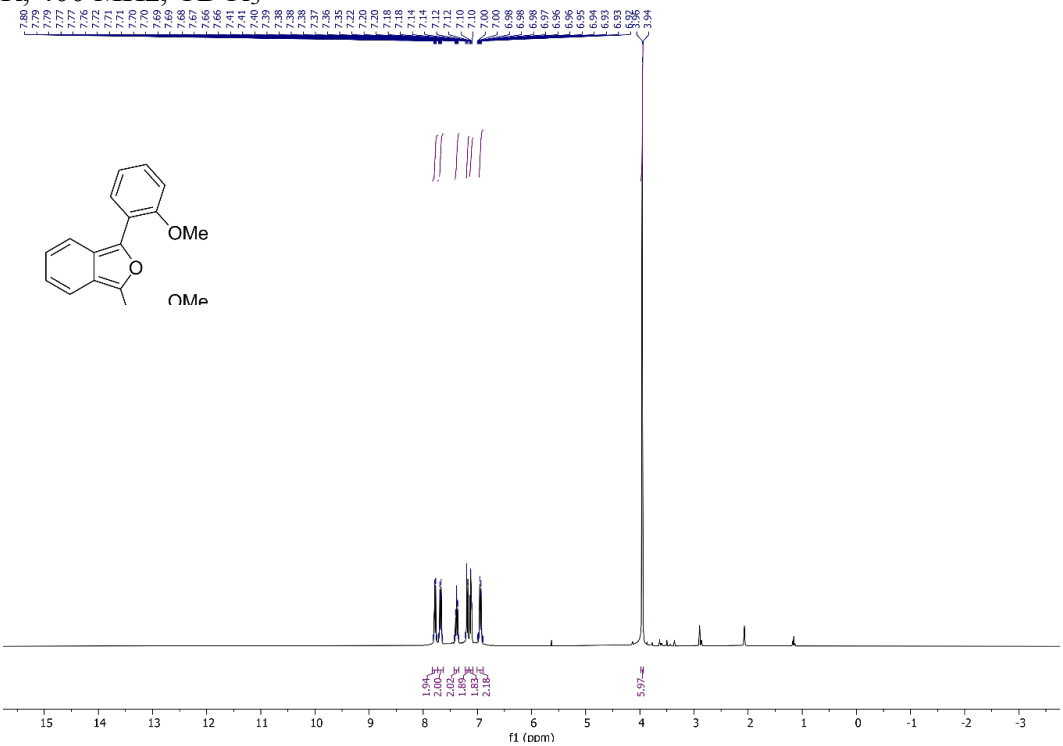


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

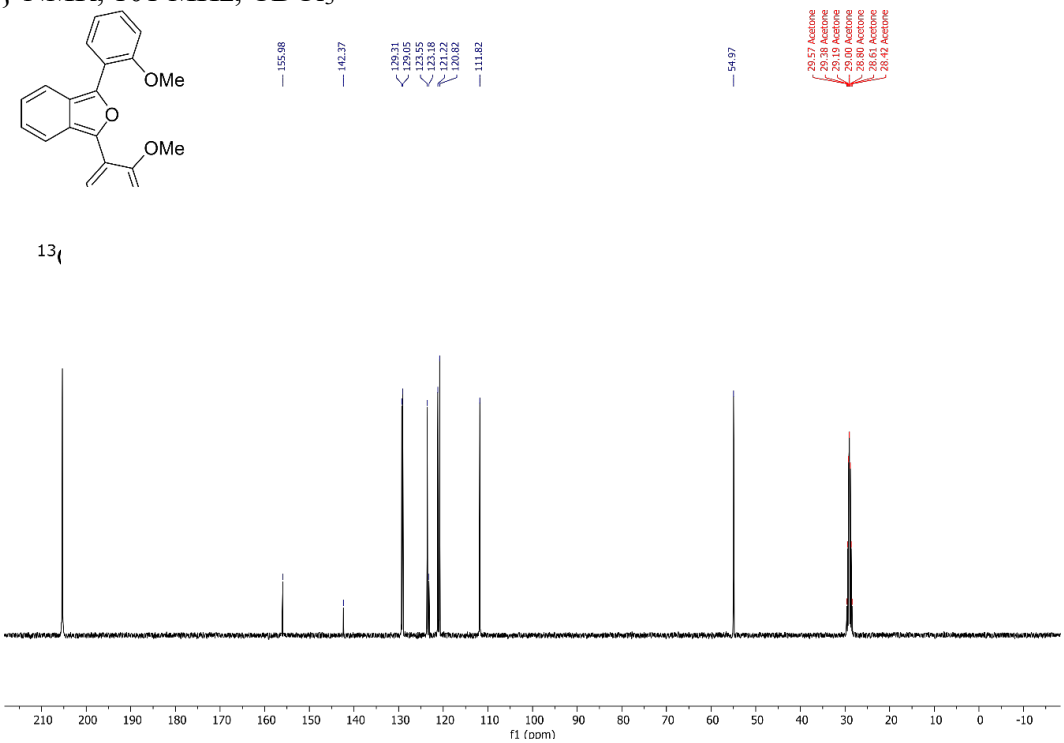


1,3-bis(2-Methoxyphenyl)isobenzofuran

^{1}H NMR, 400 MHz, $CDCl_3$

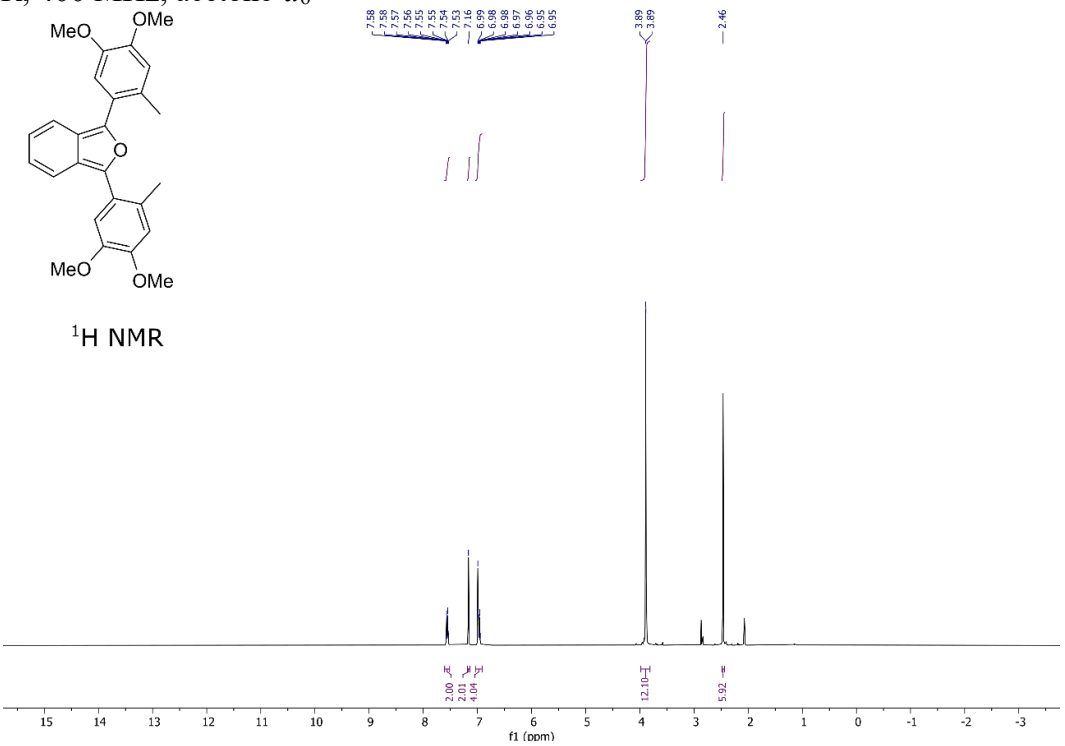


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

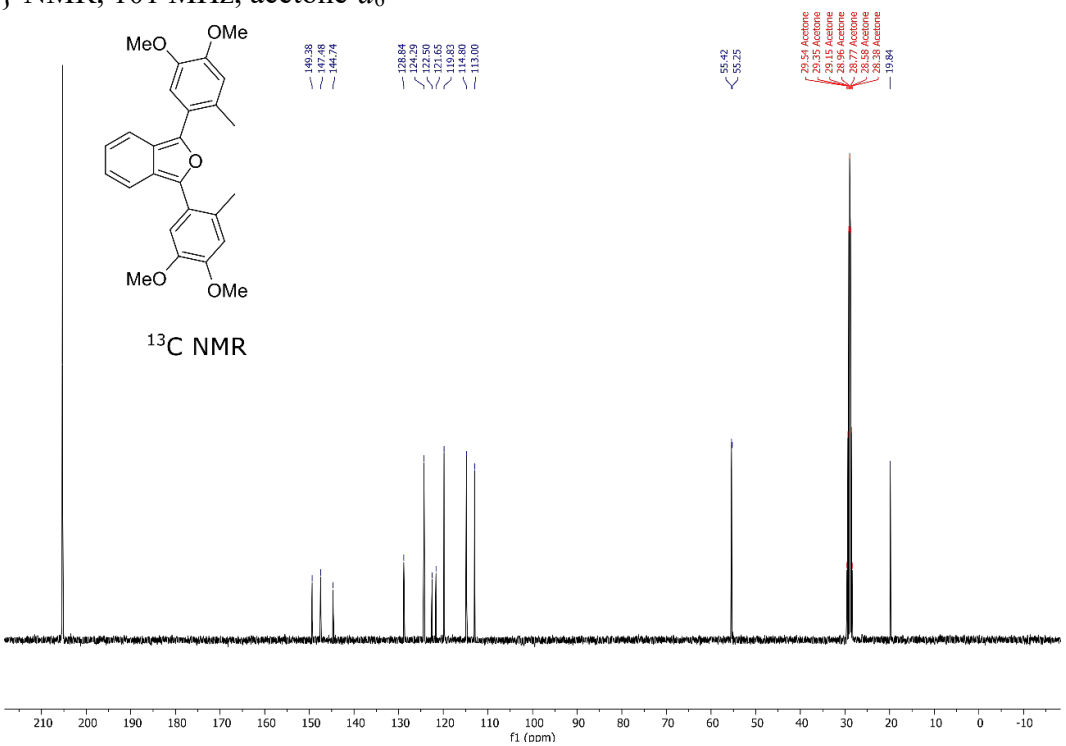


1,3-bis(4,5-Dimethoxy-2-methylphenyl)isobenzofuran

^{1}H NMR, 400 MHz, acetone-d_6

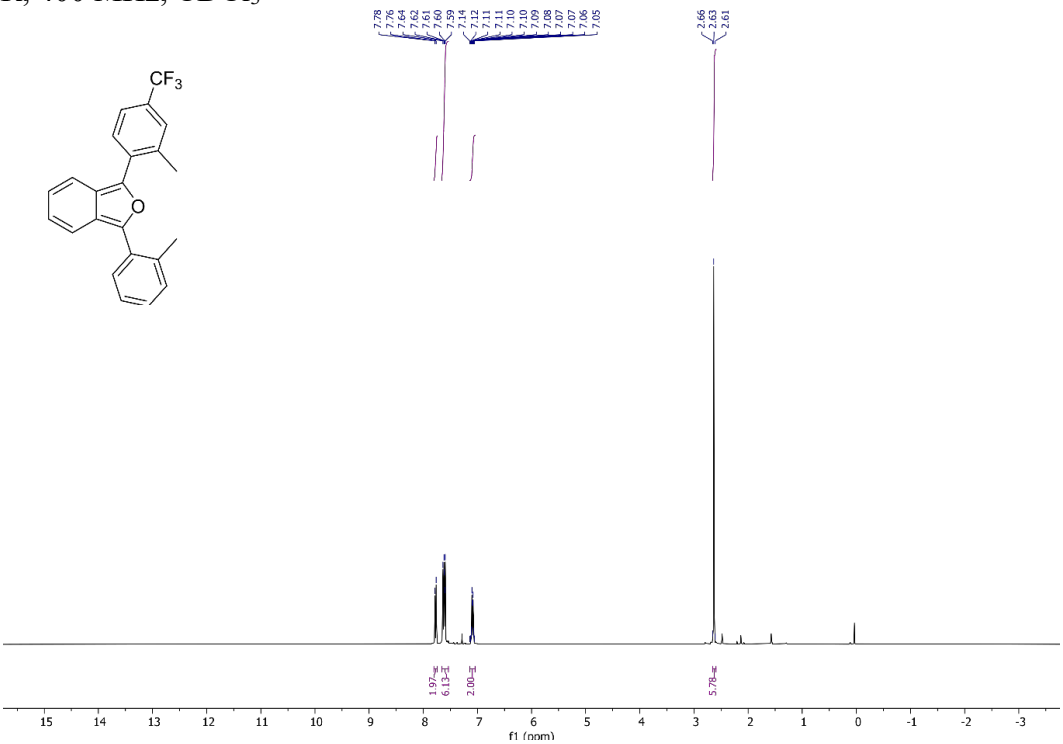


^{13}C{^{1}H} NMR, 101 MHz, acetone-d_6

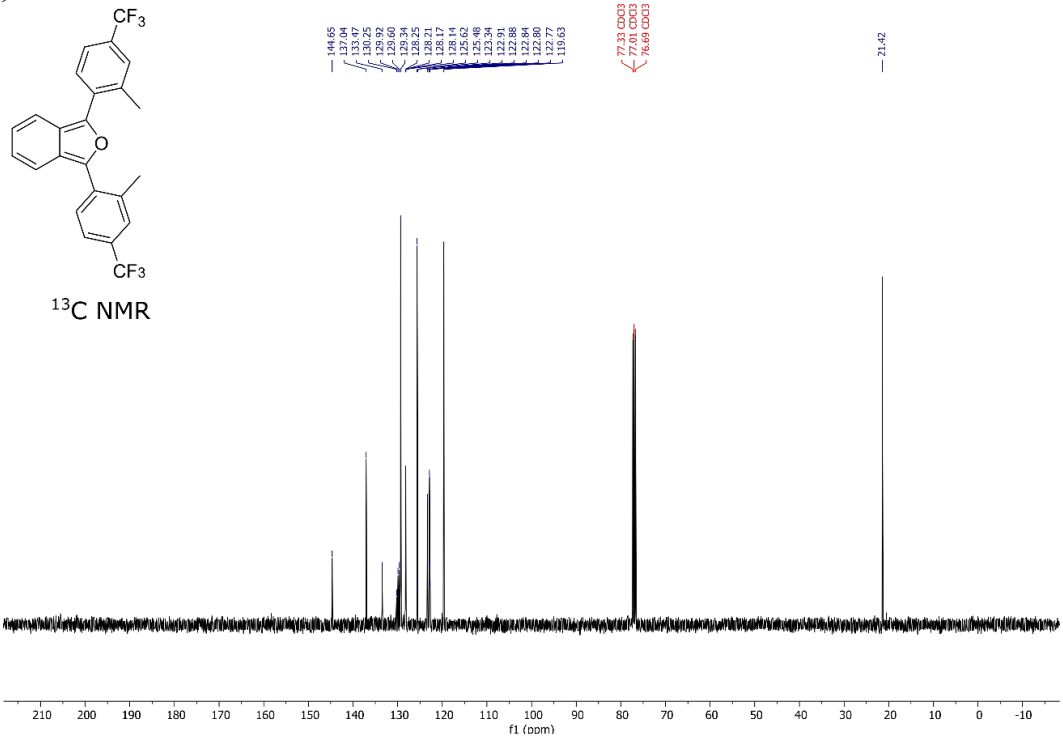


1,3-bis(2-Methyl-4-(trifluoromethyl)phenyl)isobenzofuran

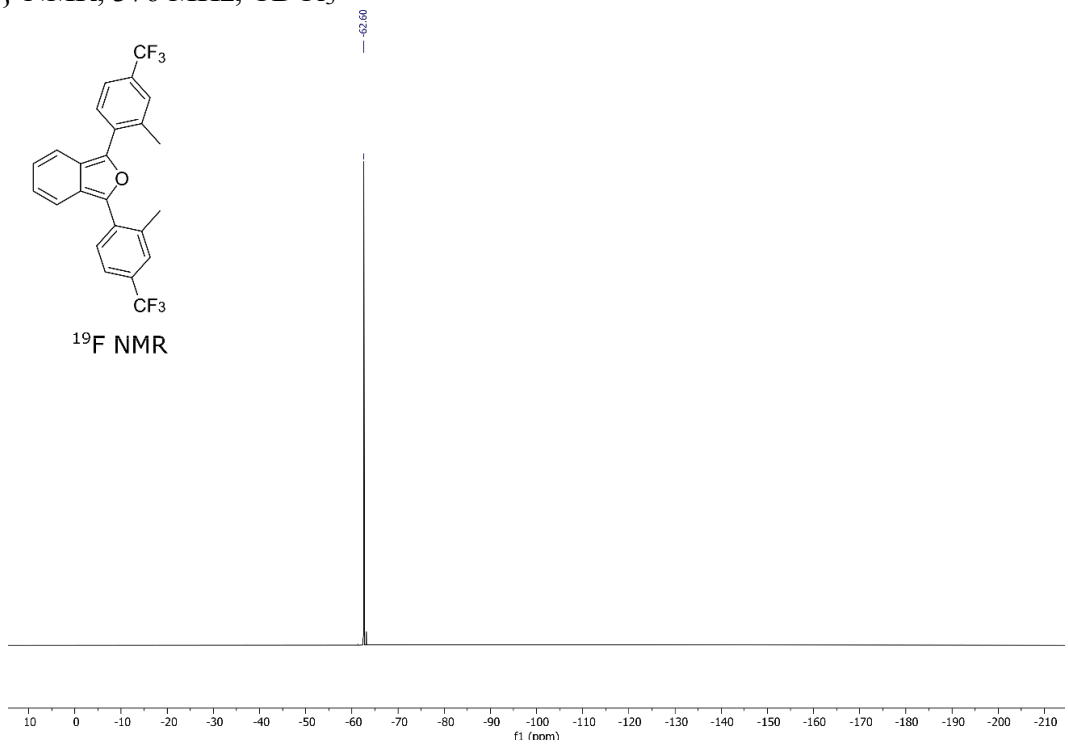
^{1}H NMR, 400 MHz, $CDCl_3$



^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

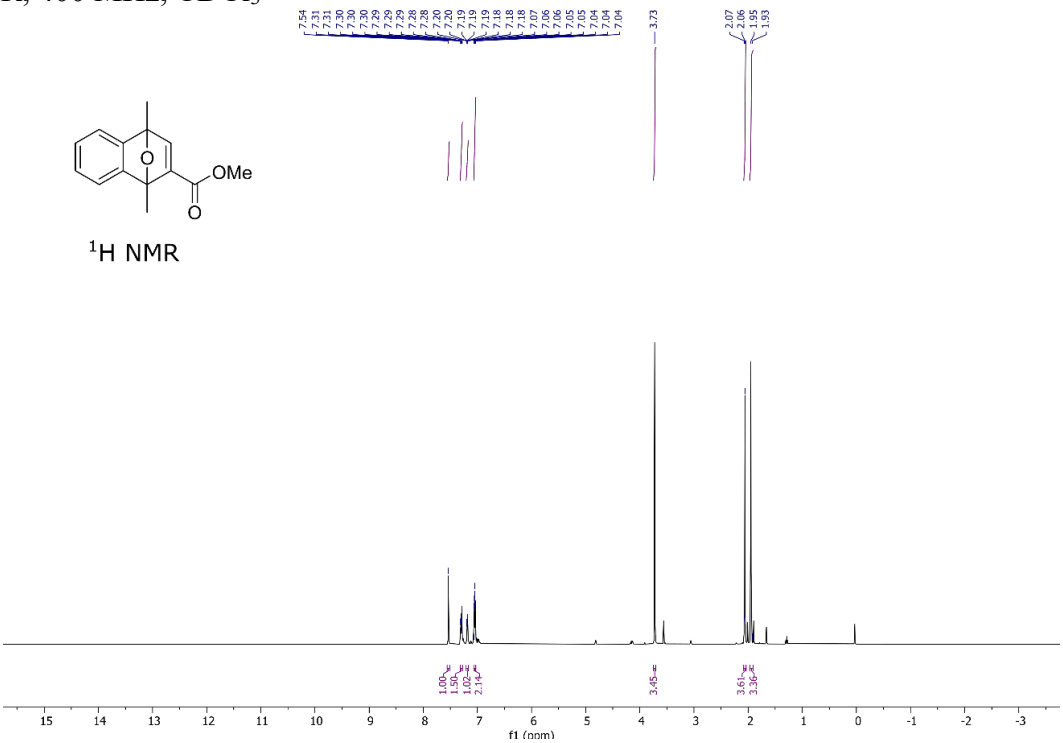


$^{19}F\{^{1}H\}$ NMR, 376 MHz, $CDCl_3$

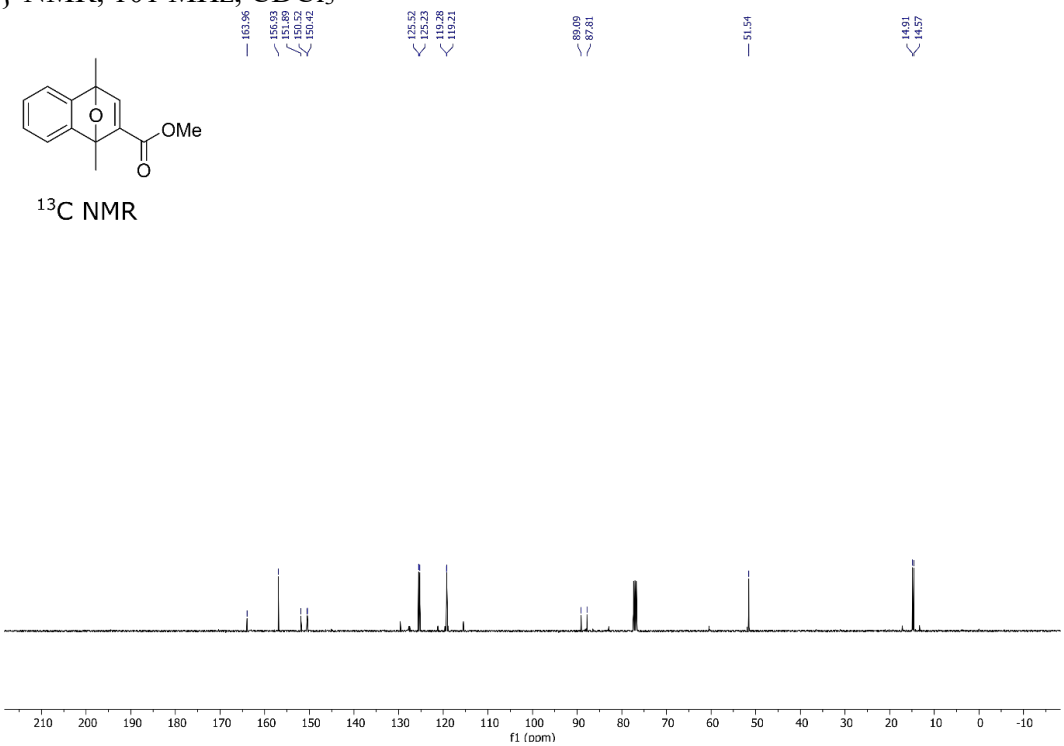


Methyl 1,4-Dimethyl-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate (10)

^{1}H NMR, 400 MHz, $CDCl_3$

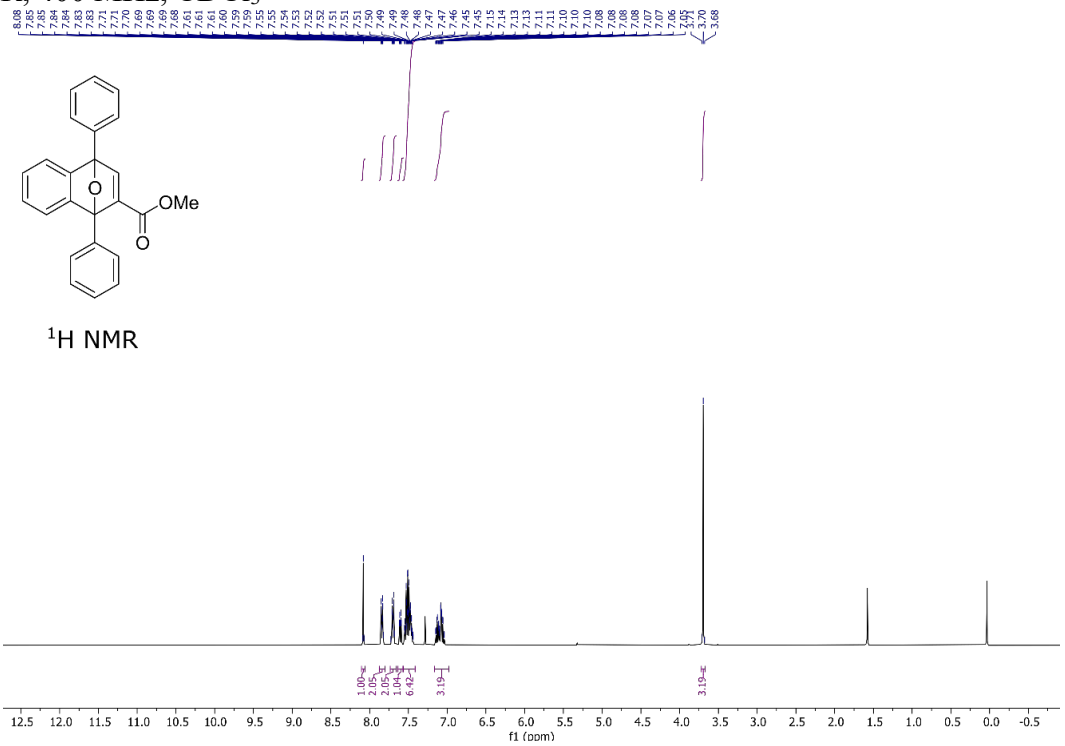


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

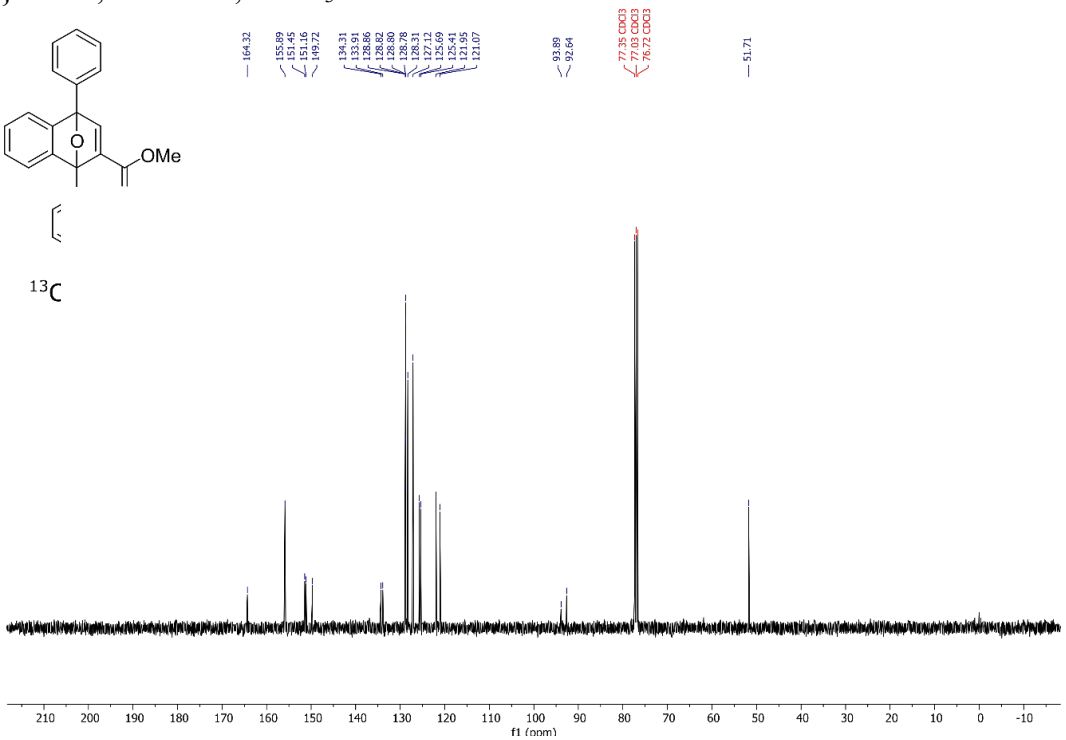


Methyl 1,4-Diphenyl-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate (3)

^{1}H NMR, 400 MHz, $CDCl_3$

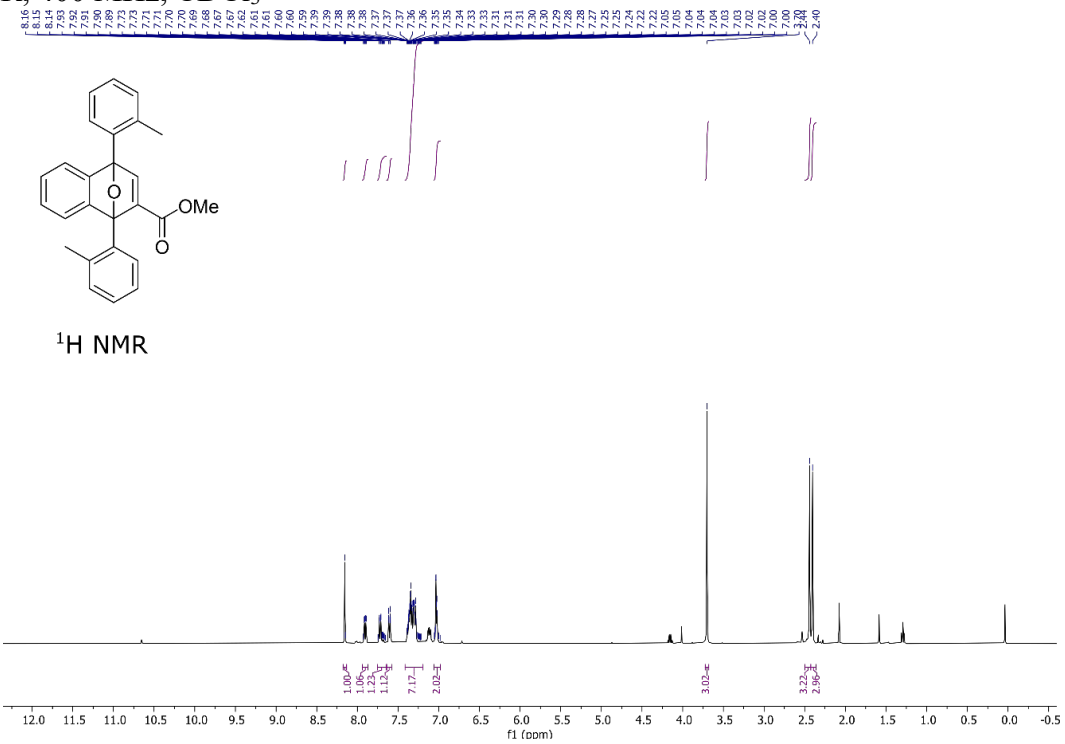


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

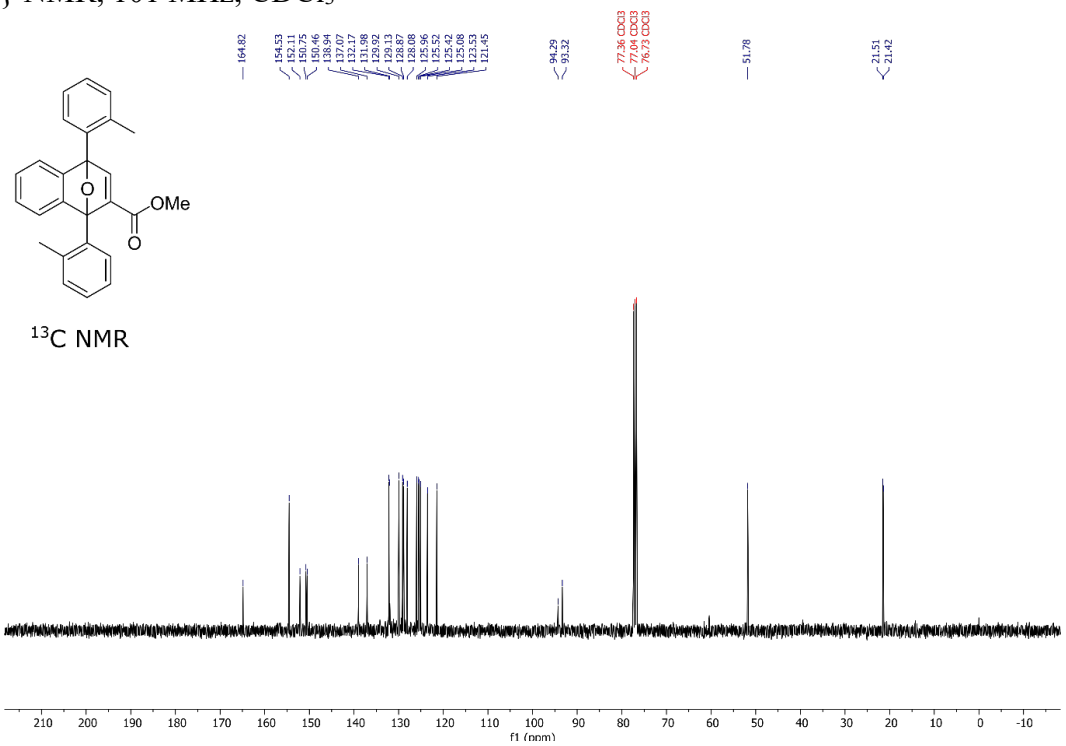


Methyl 1,4-Diphenyl-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate (3)

^{1}H NMR, 400 MHz, $CDCl_3$

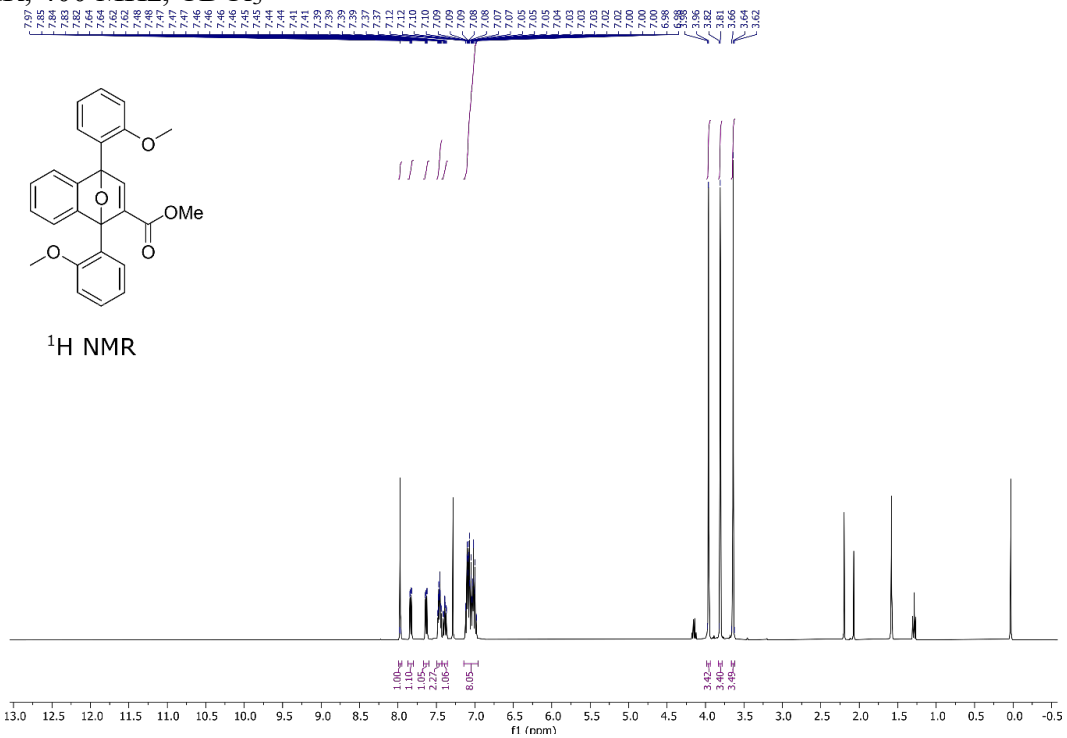


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

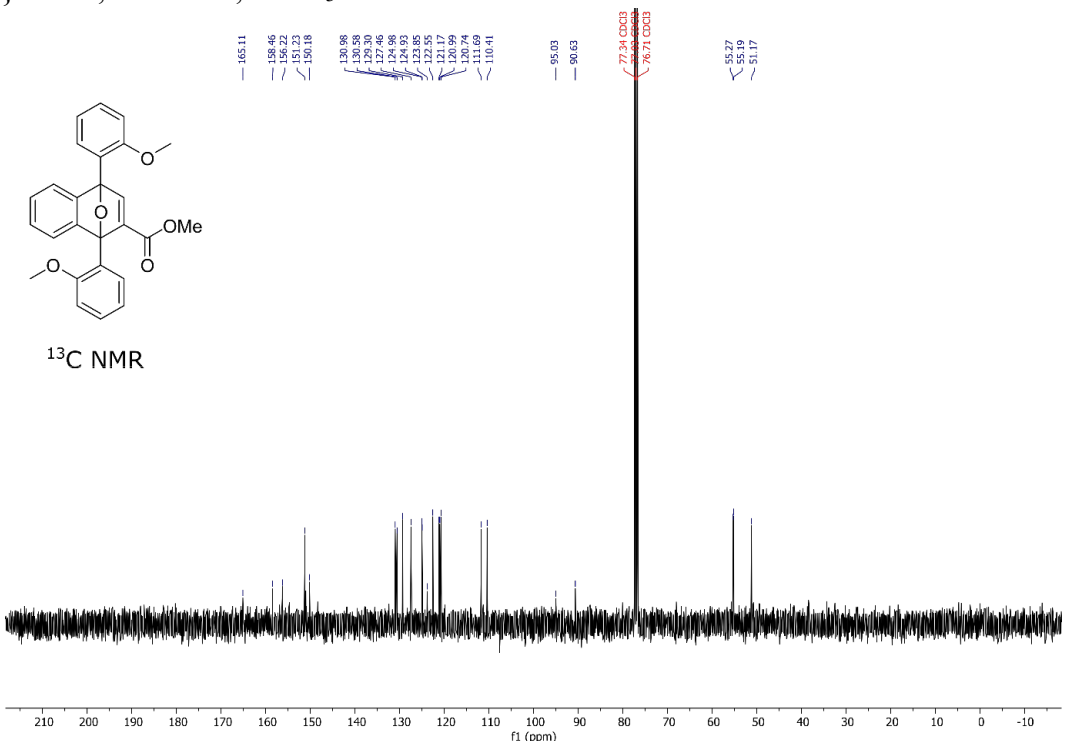


Methyl 1,4-Di-*o*-tolyl-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate

^{1}H NMR, 400 MHz, $CDCl_3$

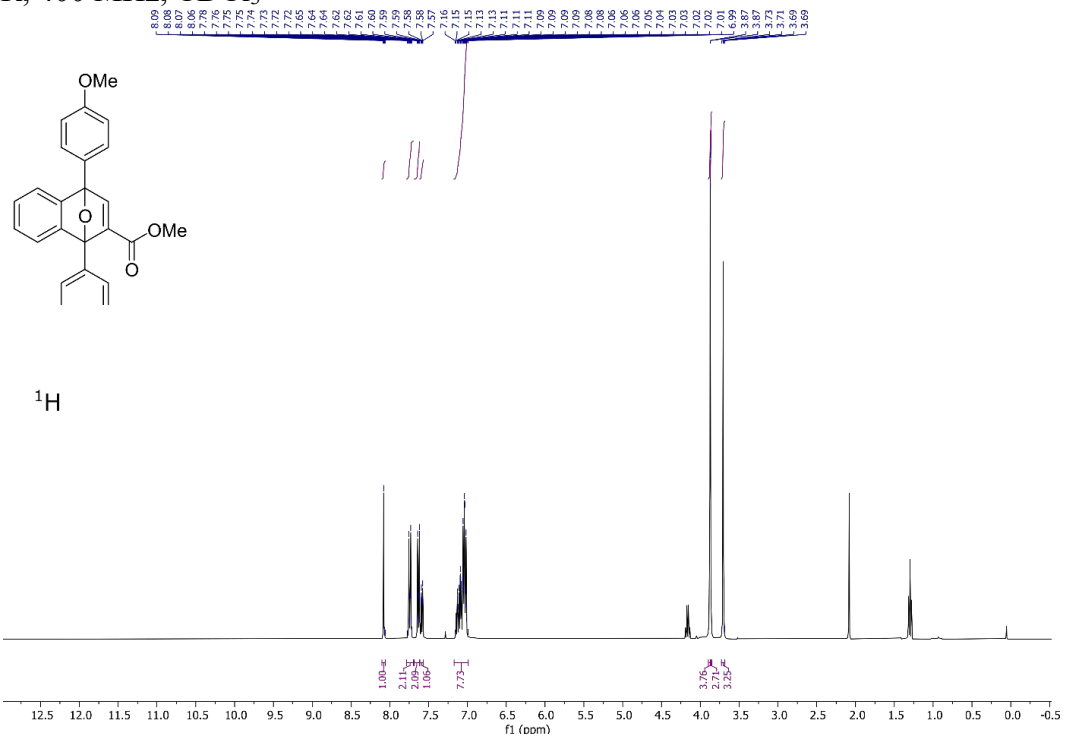


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

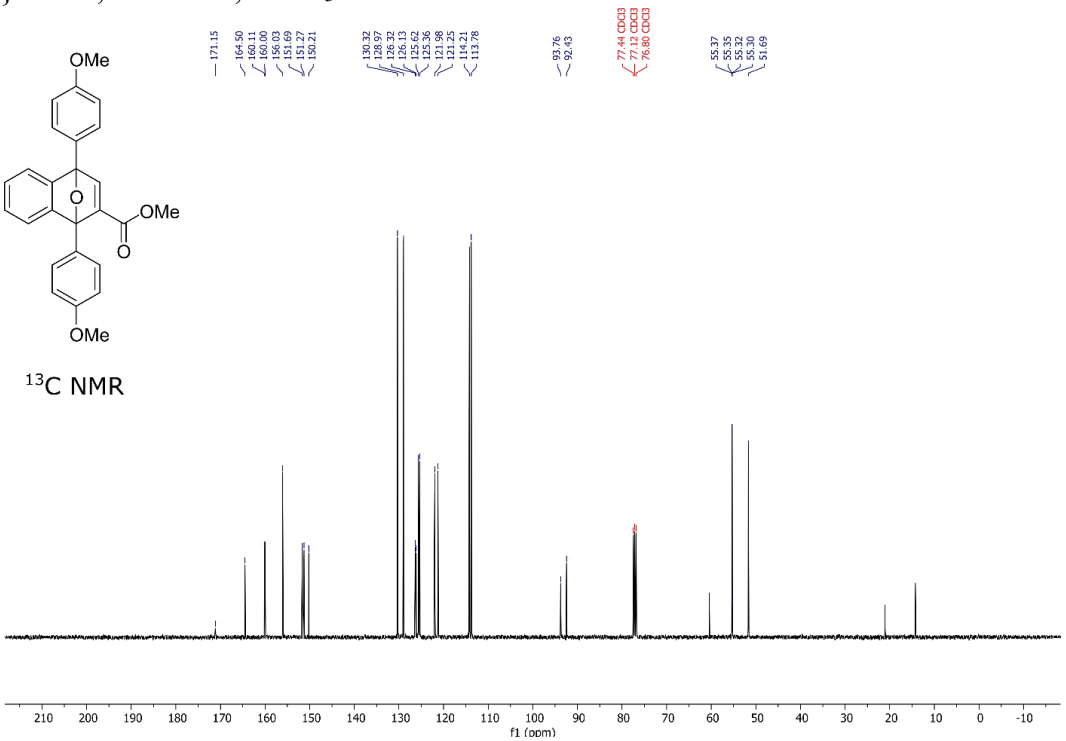


Methyl 1,4-bis(4-Methoxyphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate

^{1}H NMR, 400 MHz, $CDCl_3$

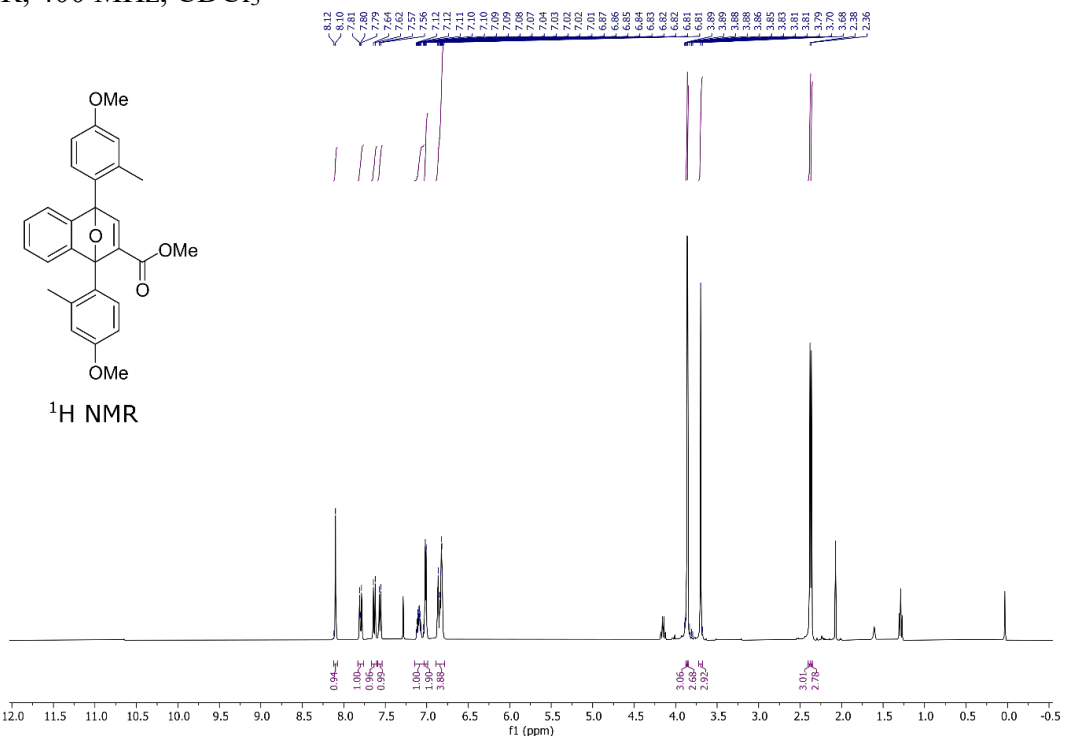


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

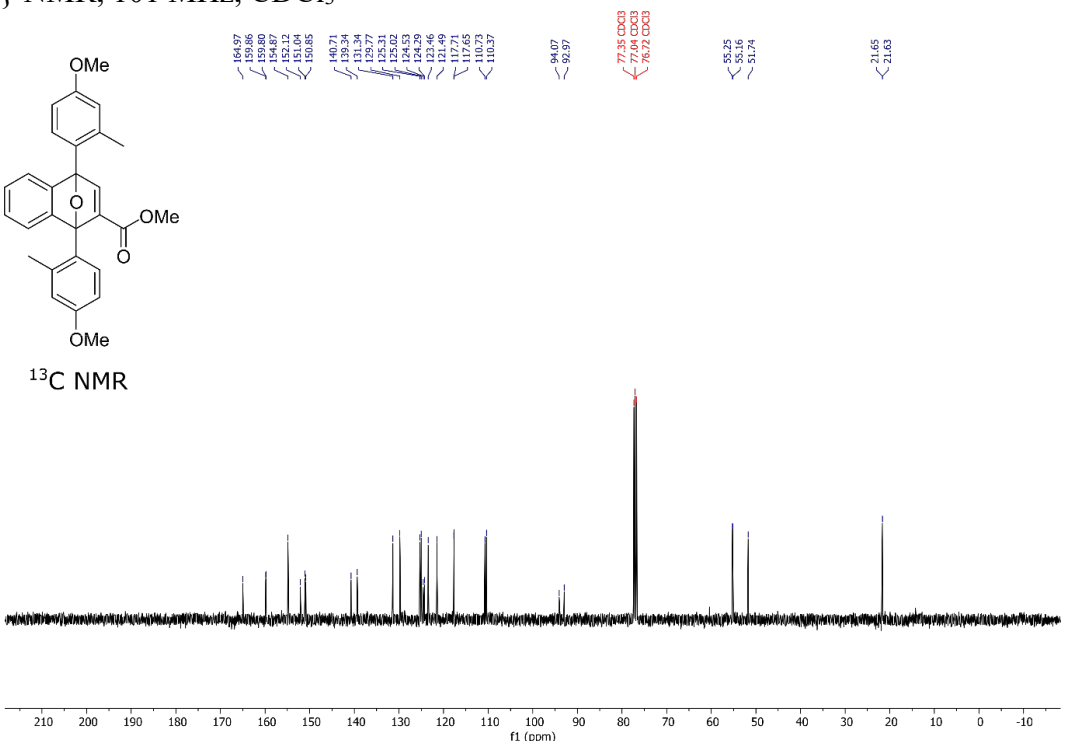


Methyl 1,4-bis(4-Methoxy-2-methylphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate (6)

^{1}H NMR, 400 MHz, $CDCl_3$

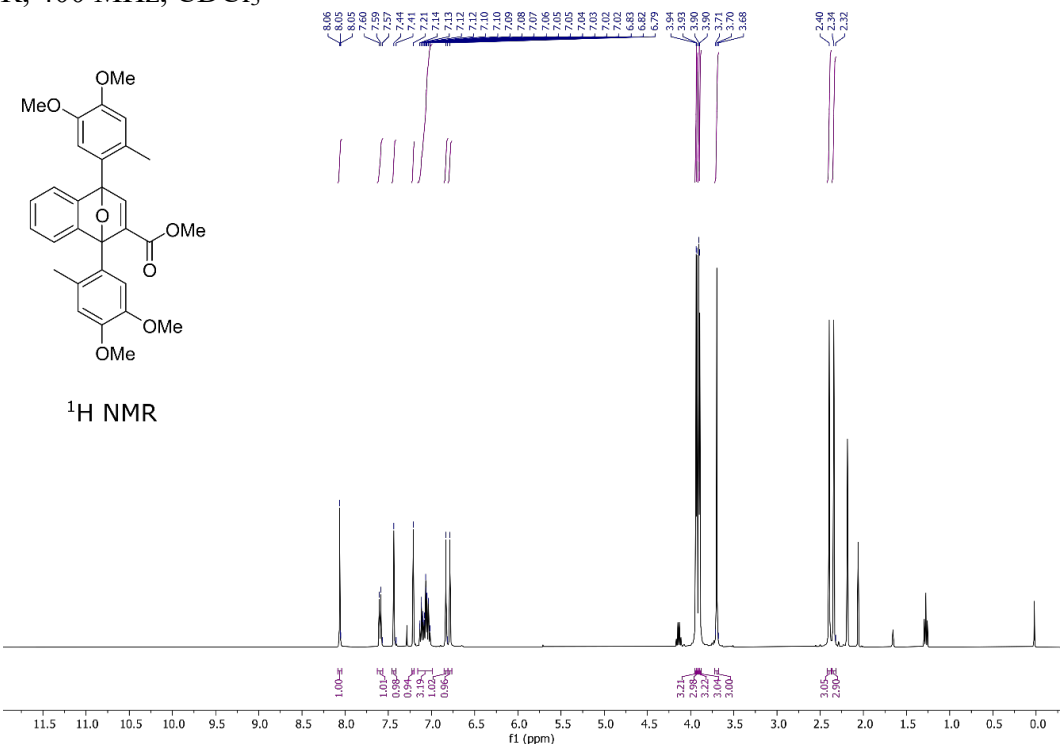


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

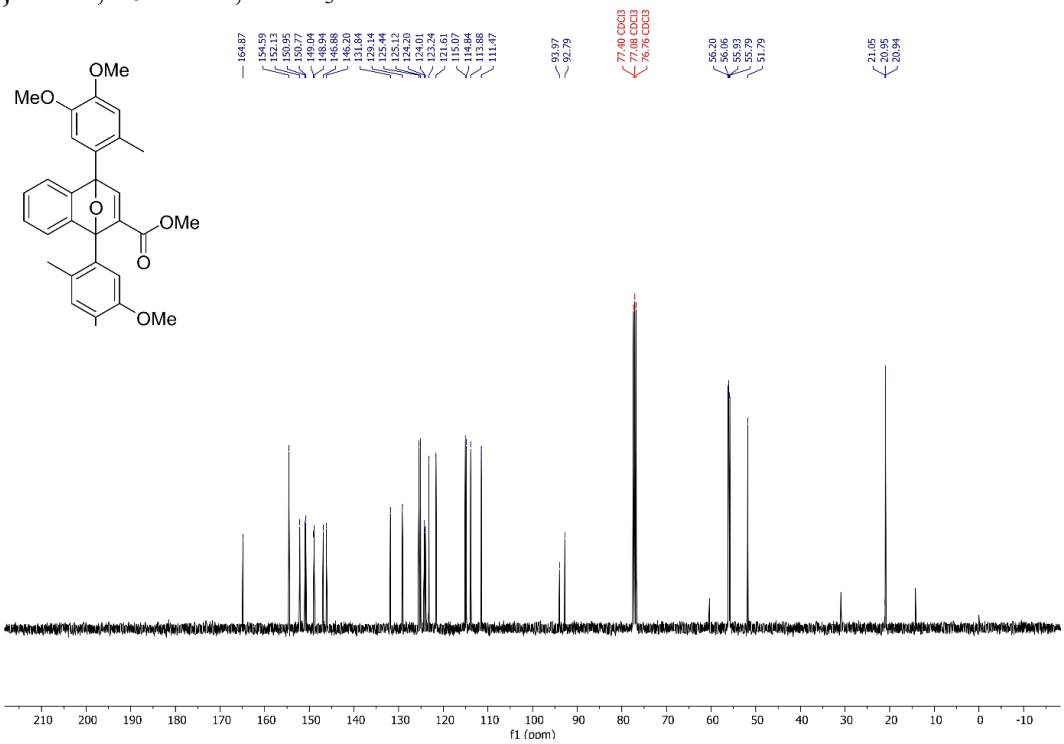


Methyl 1,4-bis(4,5-Dimethoxy-2-methylphenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate

^{1}H NMR, 400 MHz, $CDCl_3$

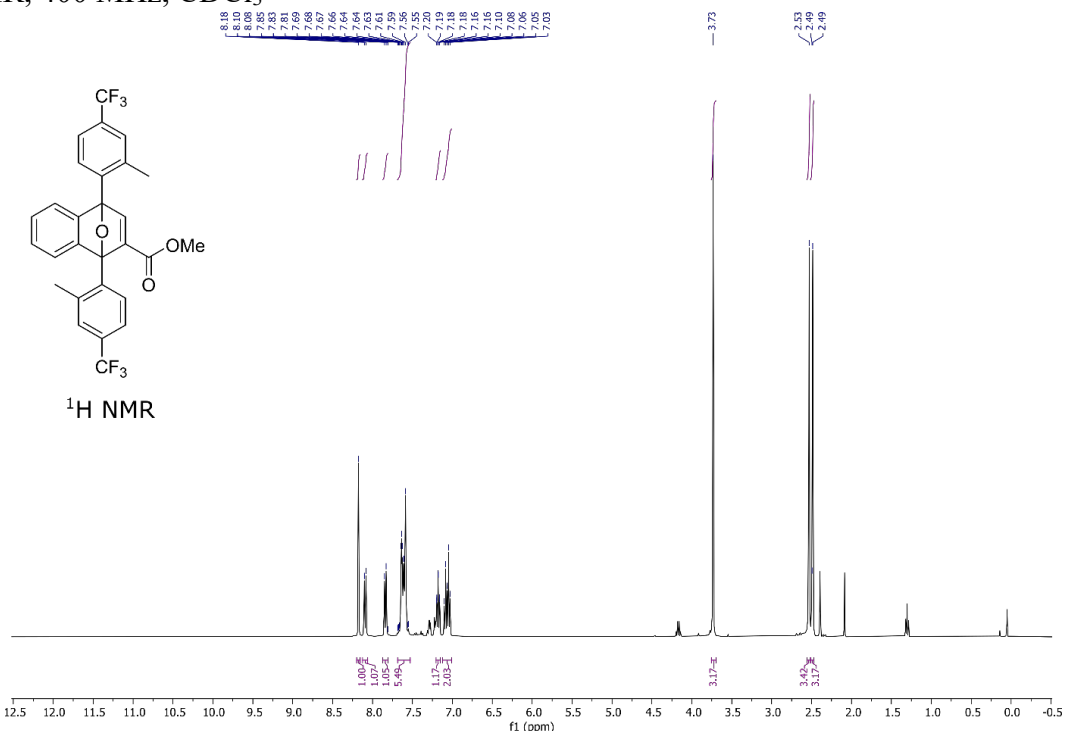


^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$

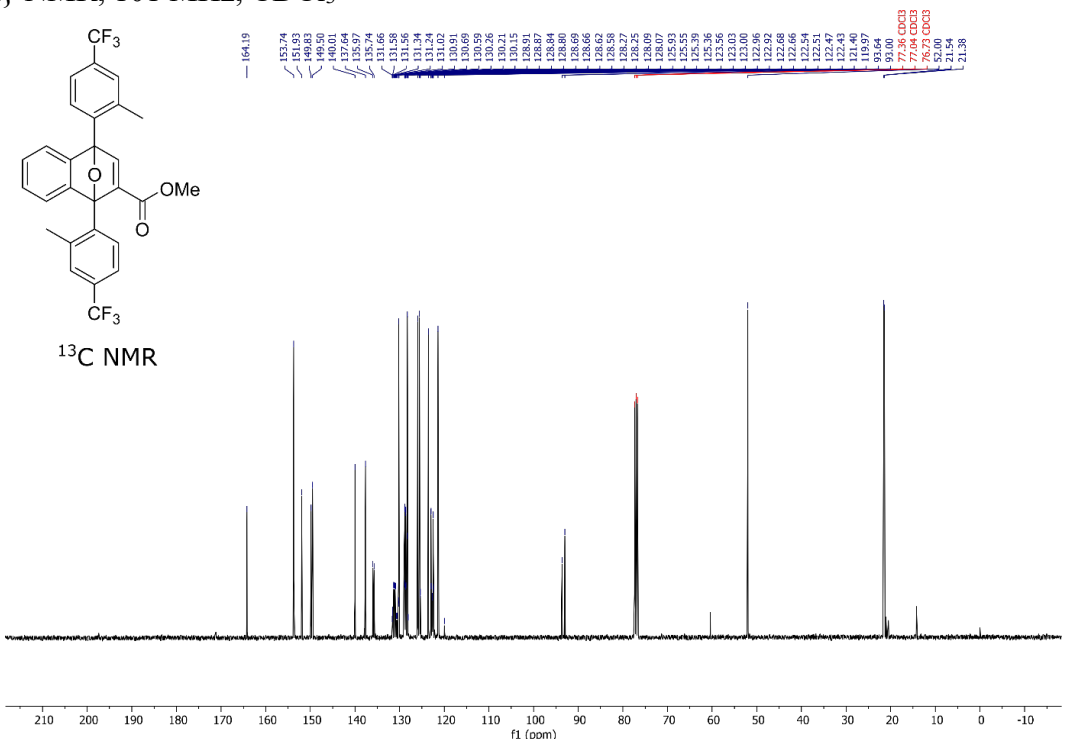


Methyl 1,4-bis(2-Methyl-4-(trifluoromethyl)phenyl)-1,4-dihydro-1,4-epoxynaphthalene-2-carboxylate

^{1}H NMR, 400 MHz, $CDCl_3$



^{13}C{^{1}H} NMR, 101 MHz, $CDCl_3$



$^{19}F\{^{1}H\}$ NMR, 376 MHz, $CDCl_3$