

Appendix A

Supporting Information for

Synthesis, Characterization and Computational Study of Potential Itaconimide-based Initiators for Atom Transfer Radical Polymerization

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Figure S1. FT-IR spectrum of *N*-phenylitaconimide (**III**).

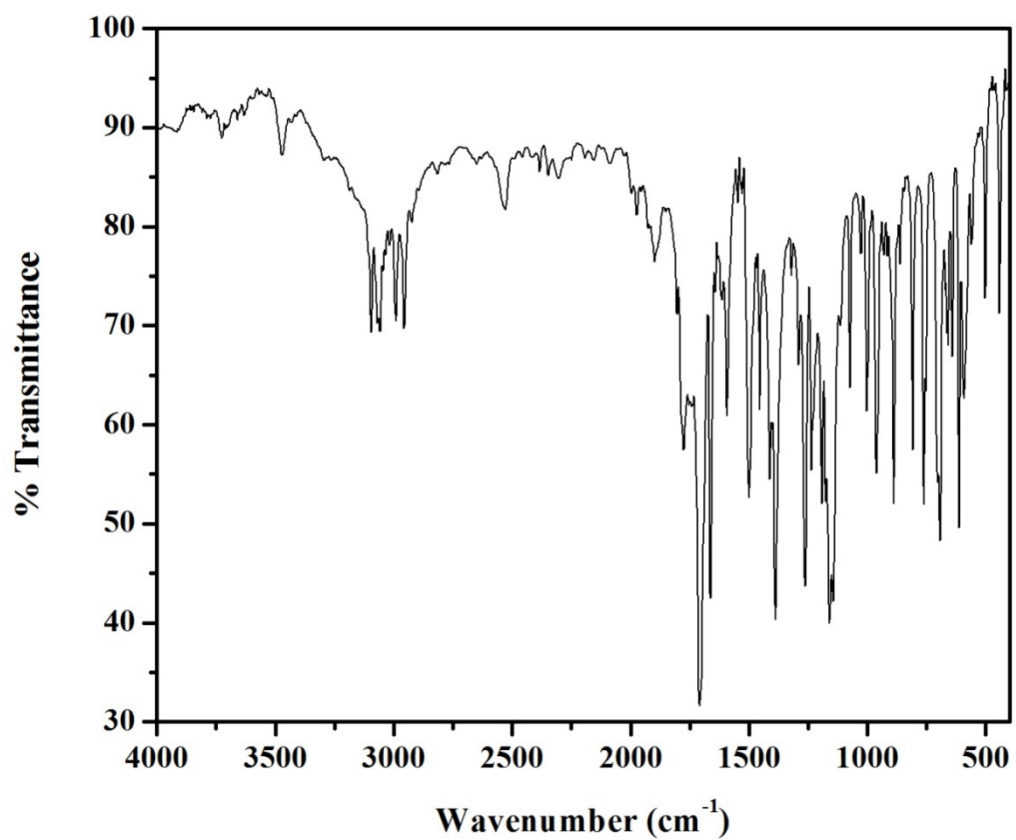


Figure S2. 500 MHz ^1H -NMR spectrum of *N*-phenylitaconimide (**III**) CDCl_3 , using TMS as reference standard.

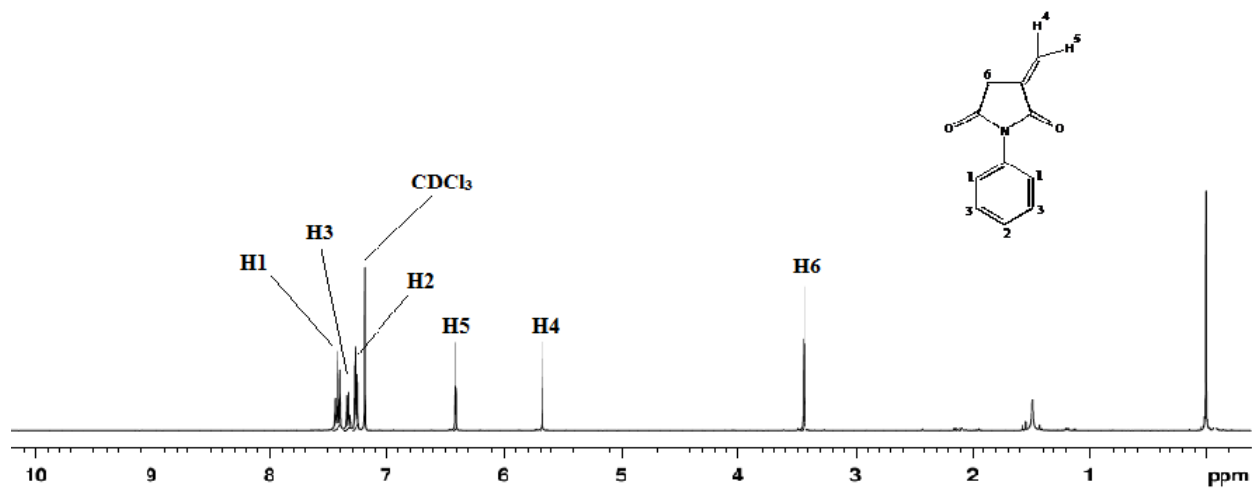


Figure S3. FT-IR spectrum of *N*-phenylcitraconimide (**IV**).

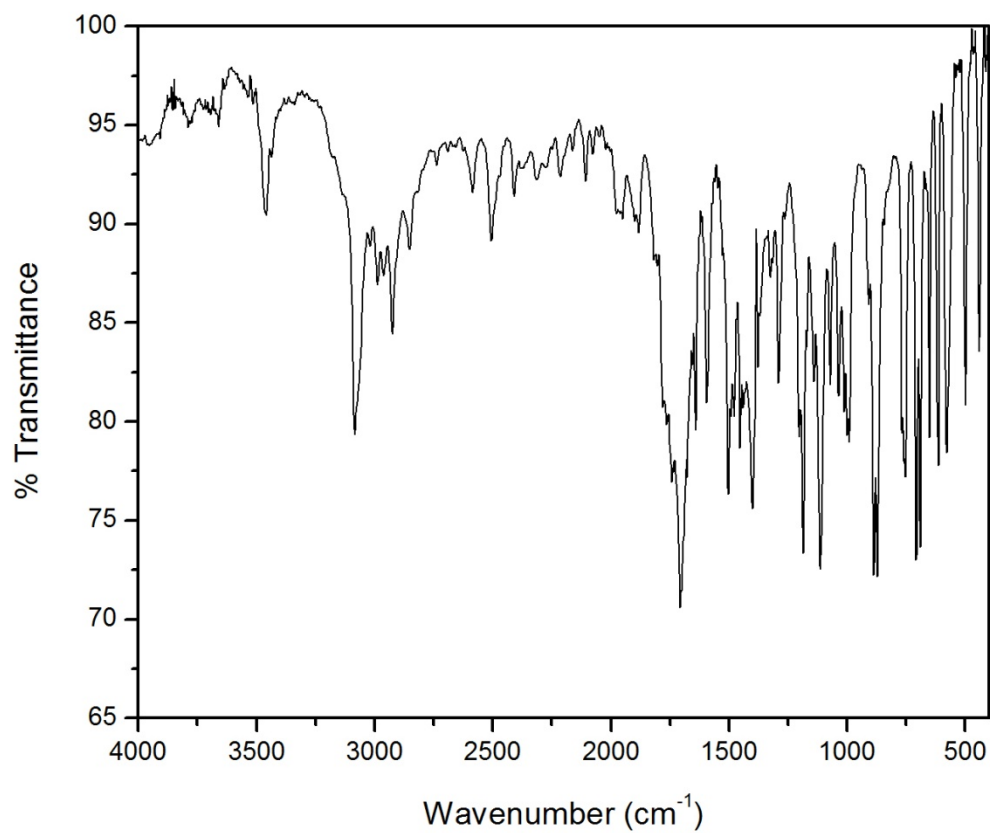


Figure S4. 500 MHz ^1H NMR spectrum of *N*-phenylcitraconimide (**IV**) in CDCl_3 , using TMS as reference standard.

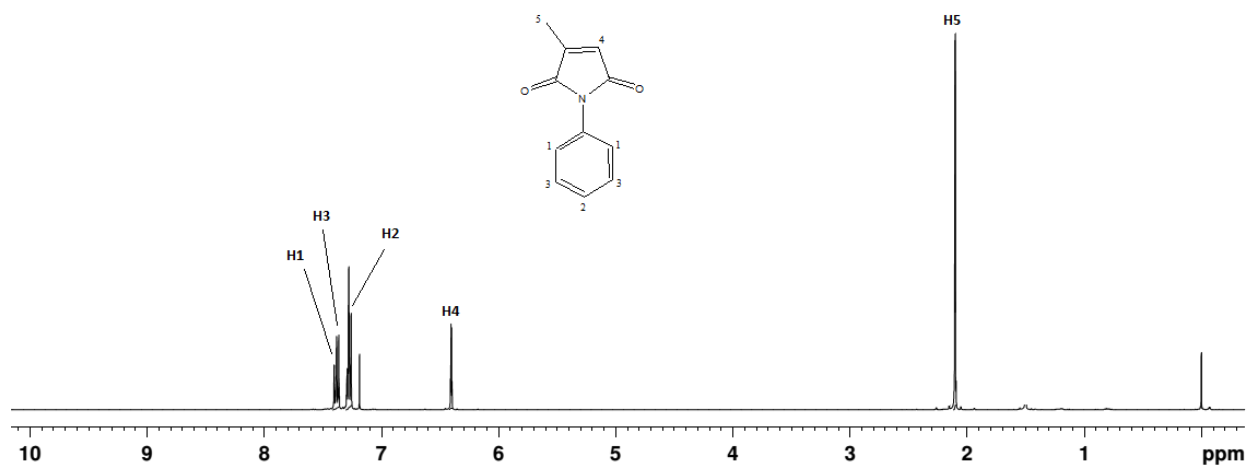


Figure S5. FT-IR spectrum of *N*-phenyl(3-bromomethyl)succinimide (**1a-Br**).

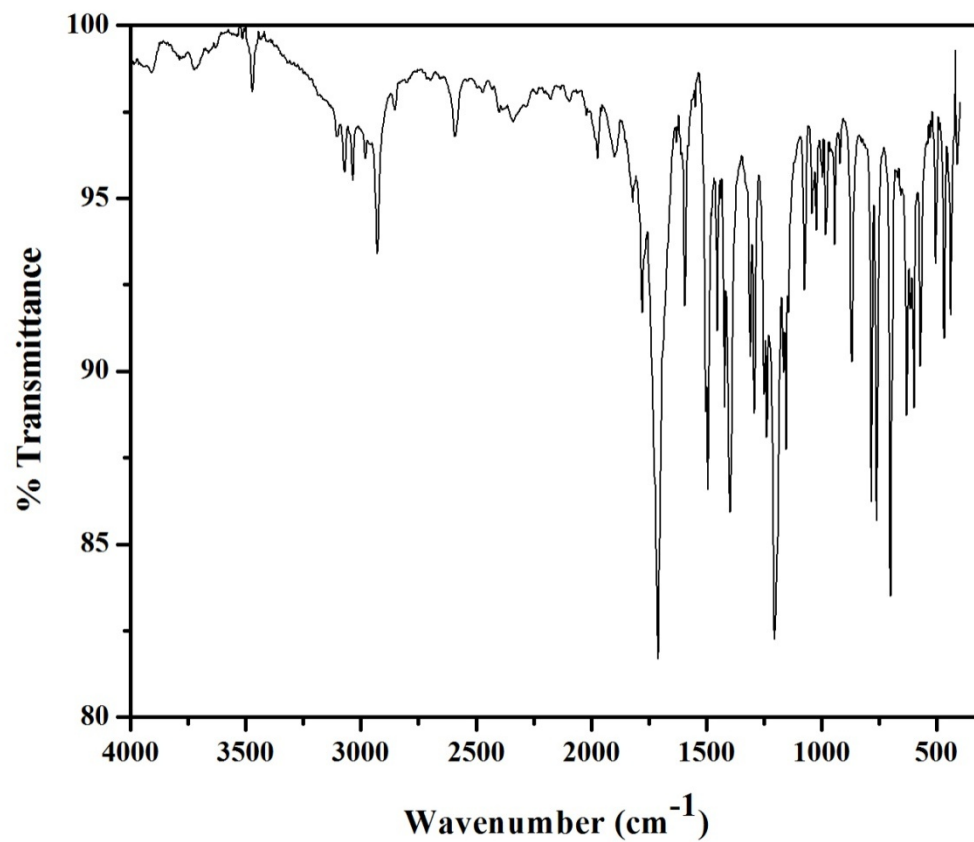


Figure S6. 500 MHz ^1H -NMR spectrum of *N*-phenyl(3-bromomethyl)succinimide (**1a-Br**) in CDCl_3 , using TMS as standard.

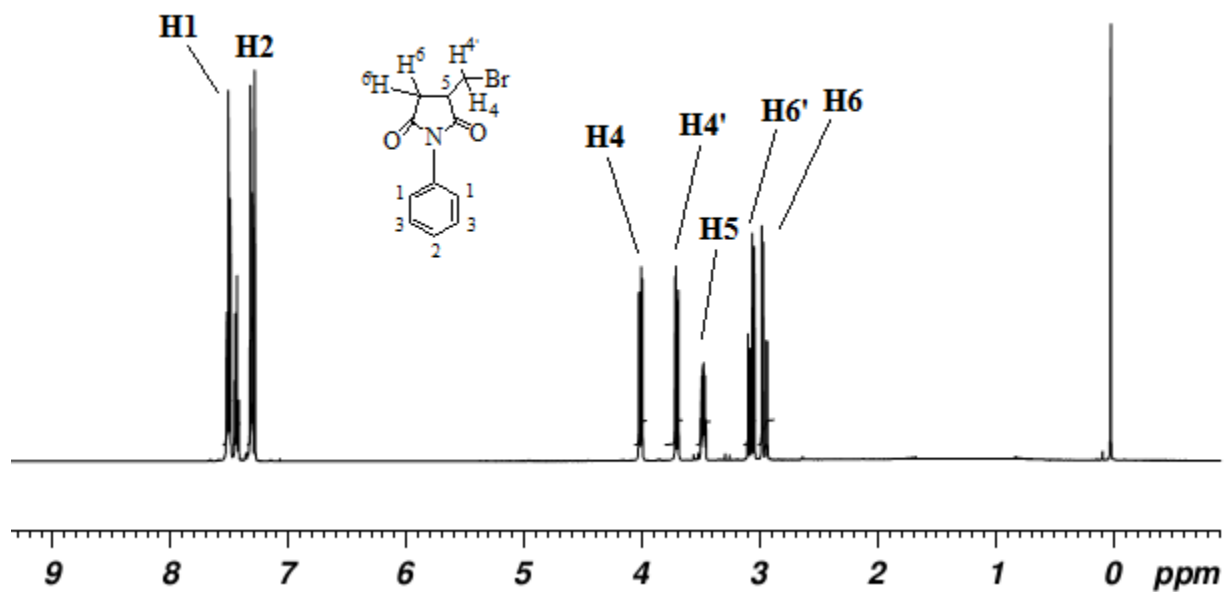


Figure S7. 125 MHz ^{13}C -NMR spectrum of *N*-phenyl(3-bromomethyl)succinimide (**1a-Br**) in CDCl_3 , using TMS as internal standard.

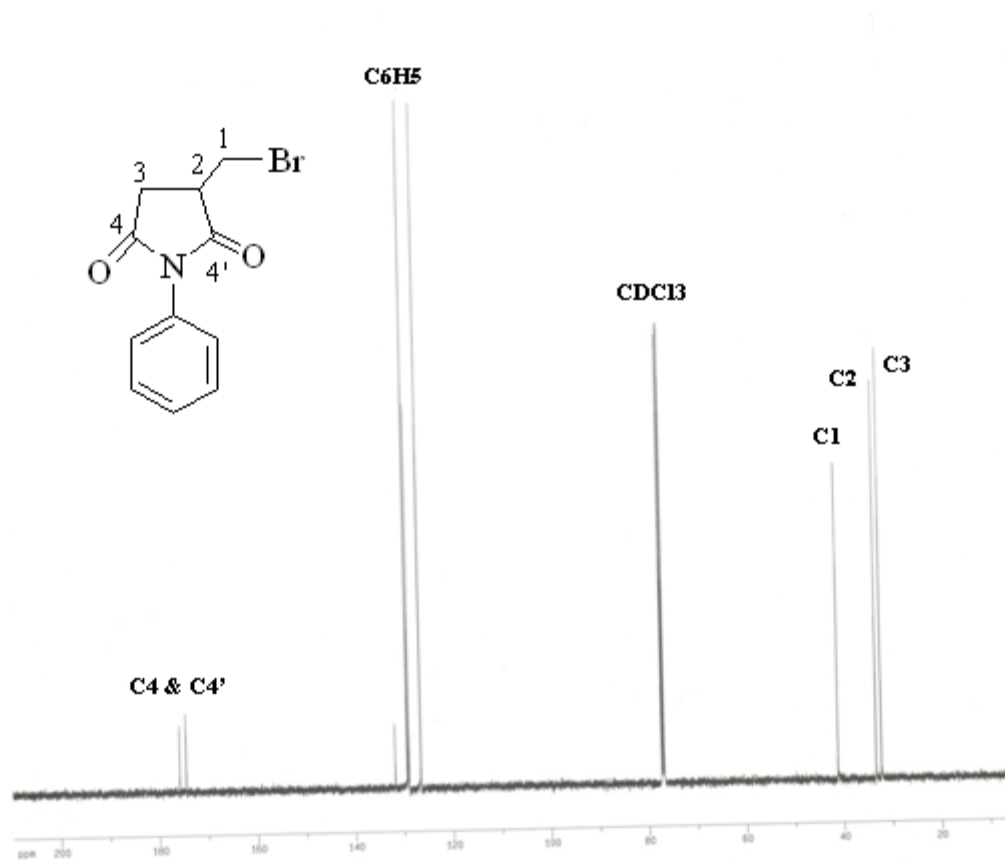


Figure S8. HRMS of *N*-phenyl(3-bromomethyl)succinimide (**1a-Br**).

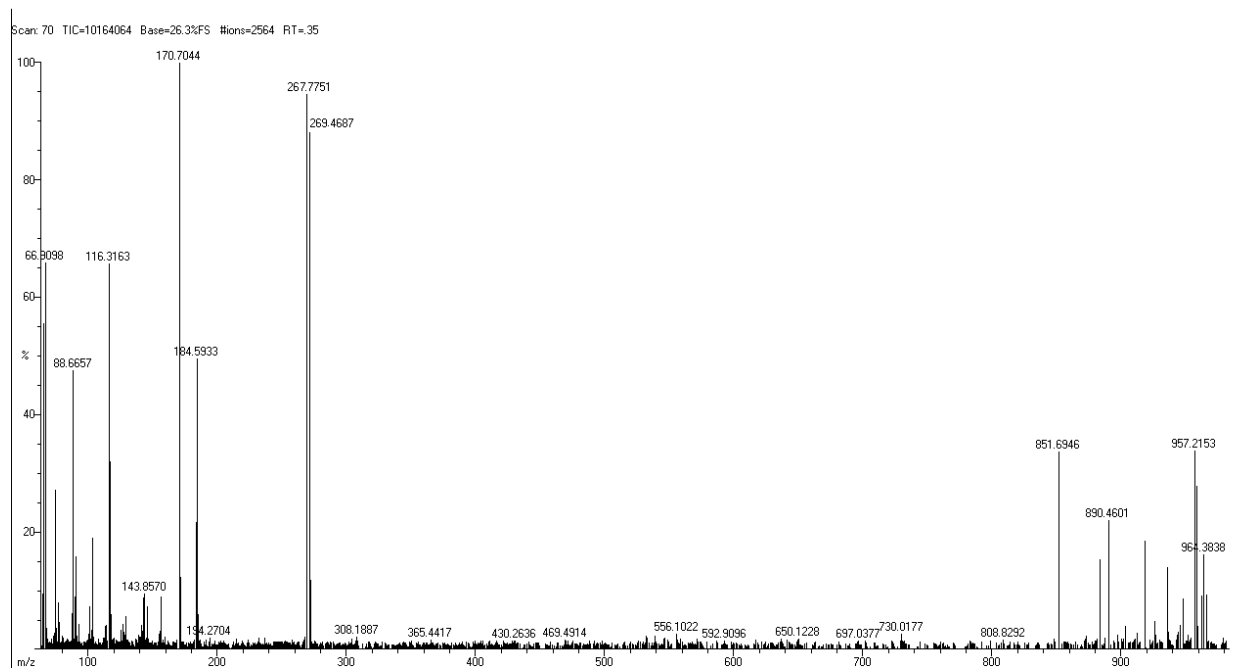


Figure S9. FT-IR spectrum of *N*-phenyl(3-bromo-4-methyl)succinimide (**2a-Br**).

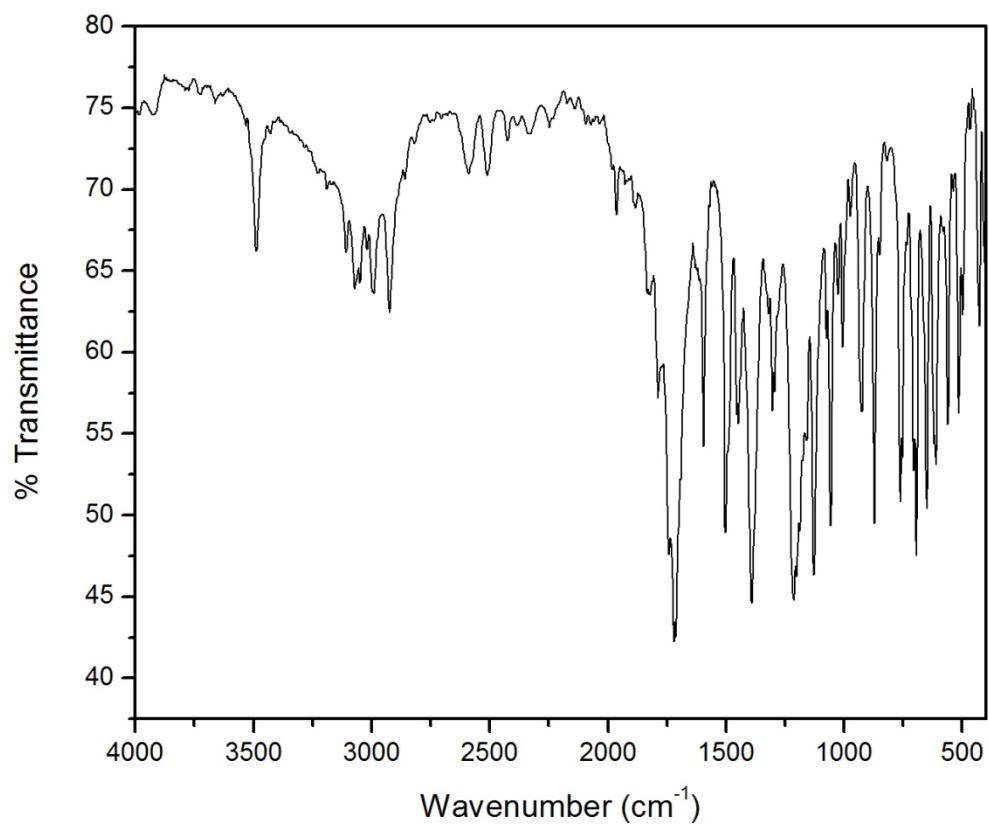


Figure S10. 500 MHz ^1H -NMR spectrum of *N*-phenyl(3-bromo-4-methyl)succinimide (**2a-Br**) in CDCl_3 , using TMS as standard internal solvent.

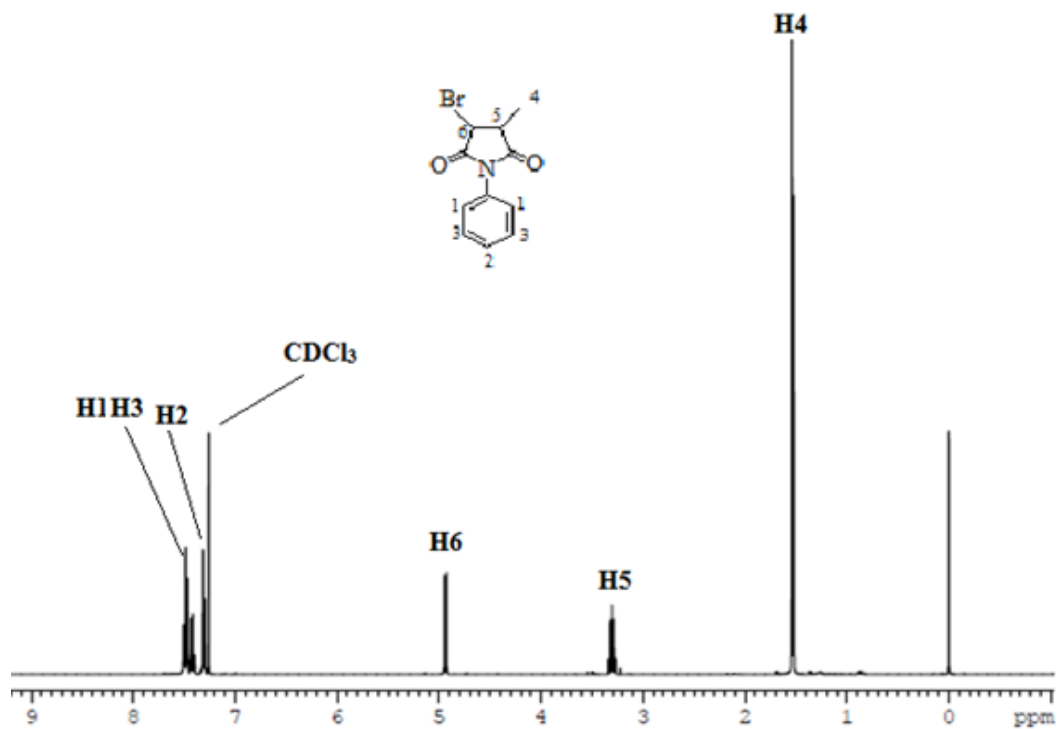


Figure S11. 125 MHz ^{13}C -NMR spectrum of *N*-phenyl(3-bromo-4-methyl)succinimide (**2a-Br**) in CDCl_3 , using TMS as standard.

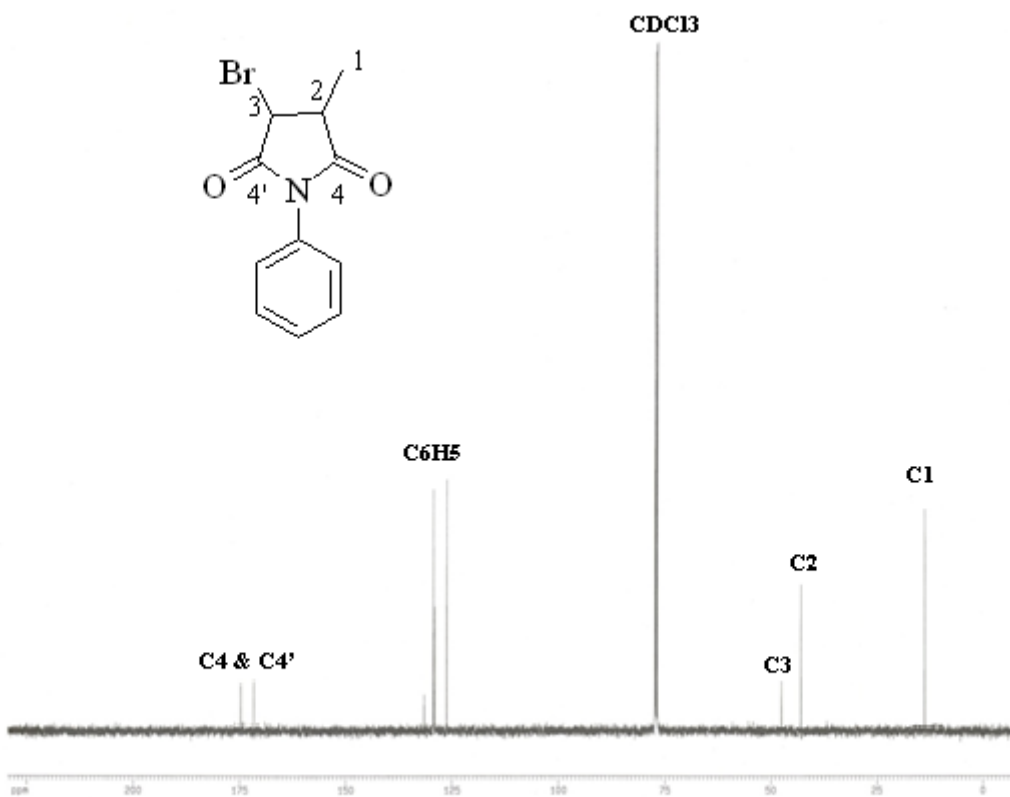


Figure S12. HRMS of *N*-phenyl(3-bromo-4-methyl)succinimide (**2a-Br**).

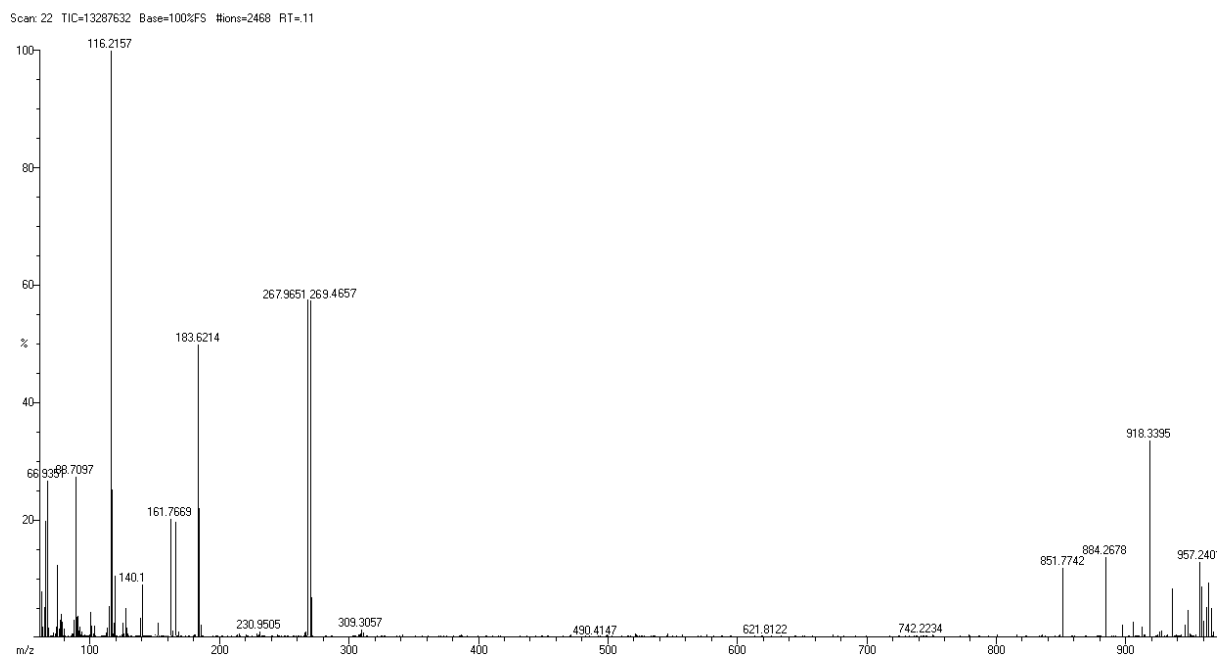


Figure S13. FT-IR spectra of *N*-phenyl(3-bromo-3-methyl)succinimide (**3a-Br**).

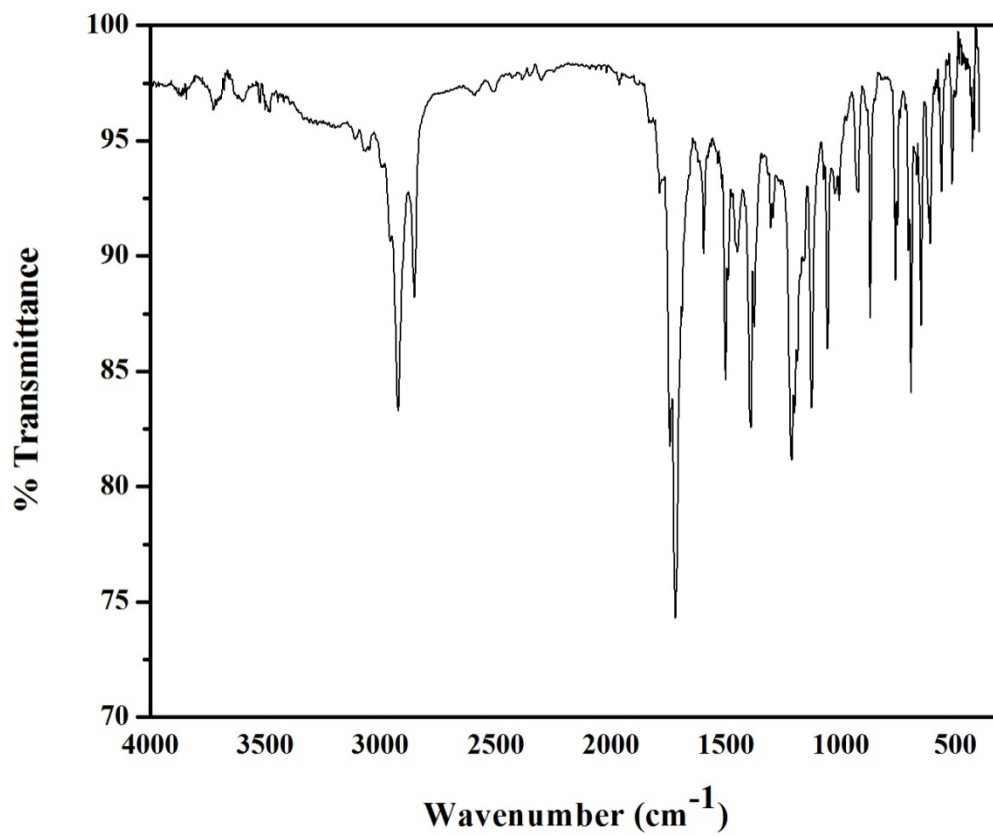


Figure S14. 500 MHz ^1H NMR spectrum of *N*-phenyl(3-bromo-3-methyl)succinimide (**3a-Br**) in CDCl_3 , using TMS as internal standard.

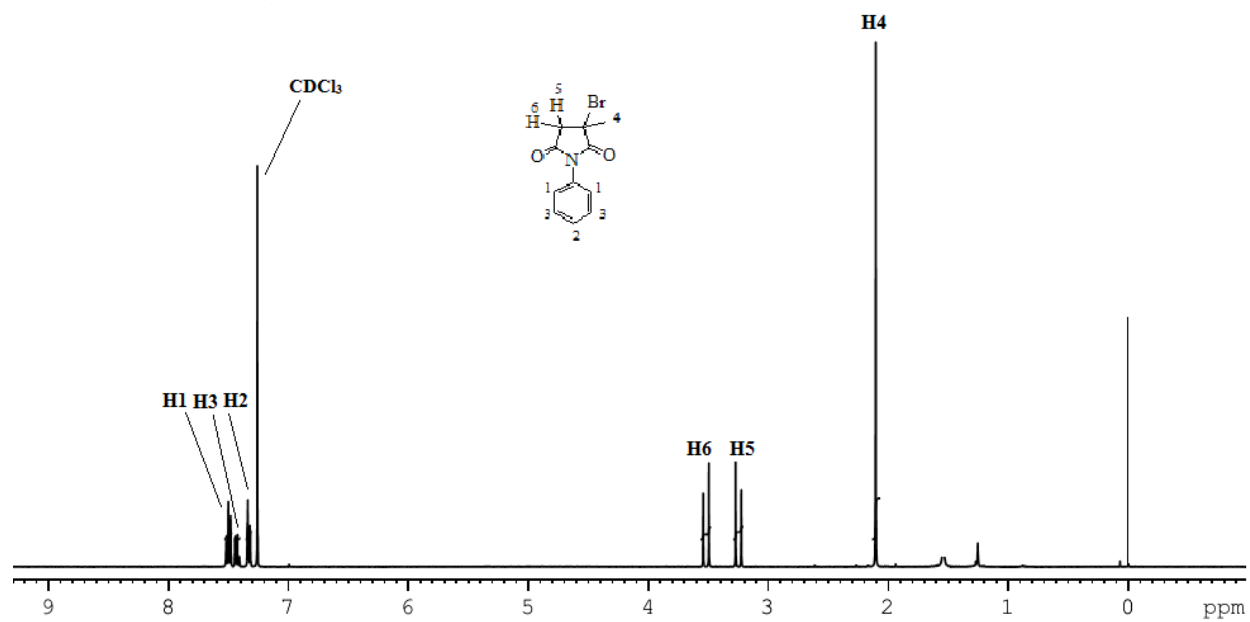


Figure S15. 125 MHz ^{13}C -NMR spectrum of *N*-phenyl(3-bromo-3-methyl)succinimide (**3a-Br**) in CDCl_3 , using TMS as internal standard.

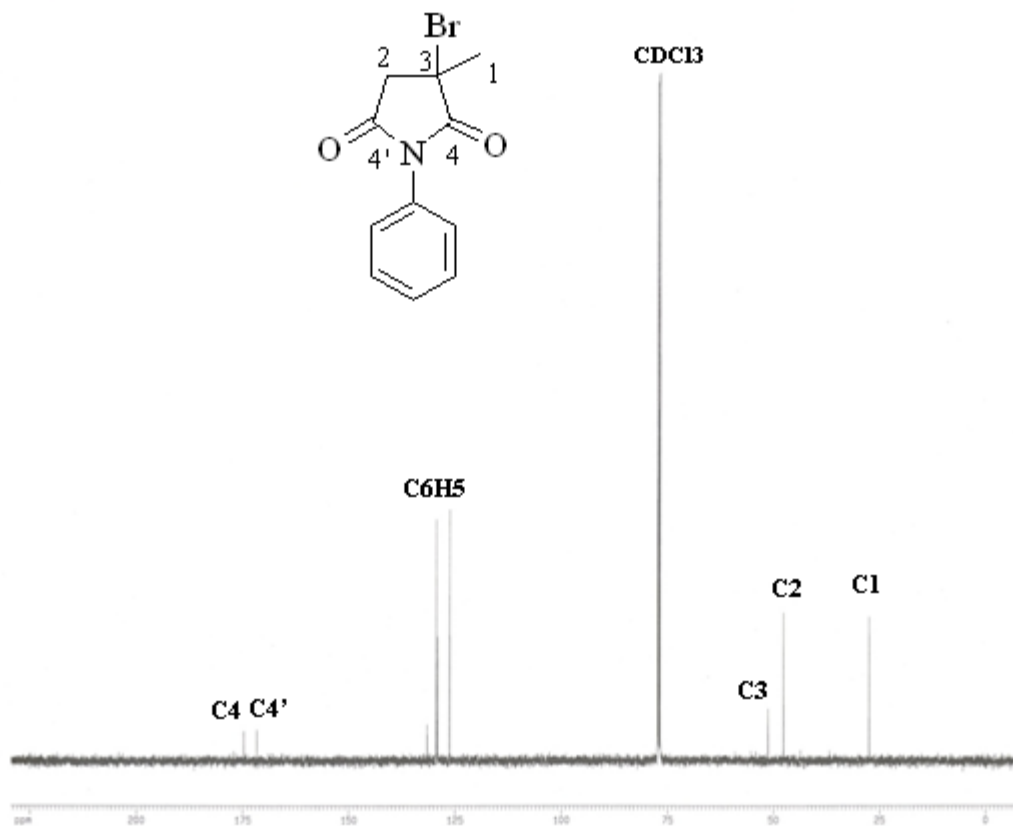


Figure S16. HRMS of *N*-phenyl(3-bromo-3-methyl)succinimide (**3a-Br**).

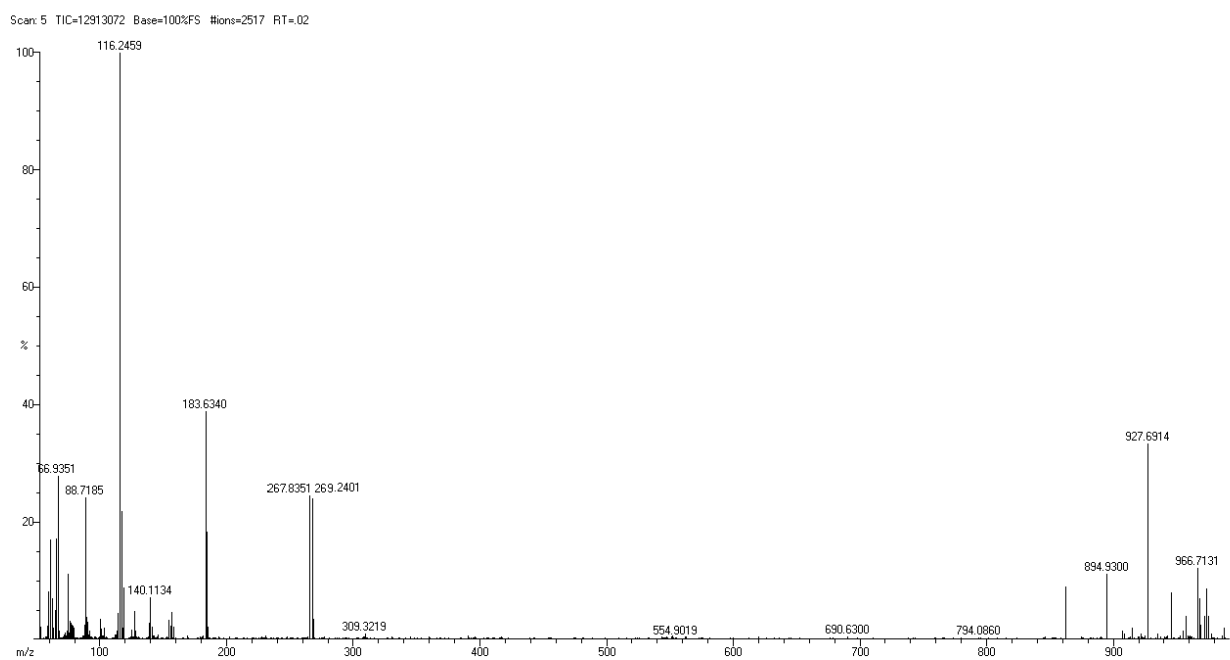


Figure S17. Plot of absorbance with time at 745 nm for (a) 70 mM; (b) 50 mM of 4-Br, alkyl bromide.

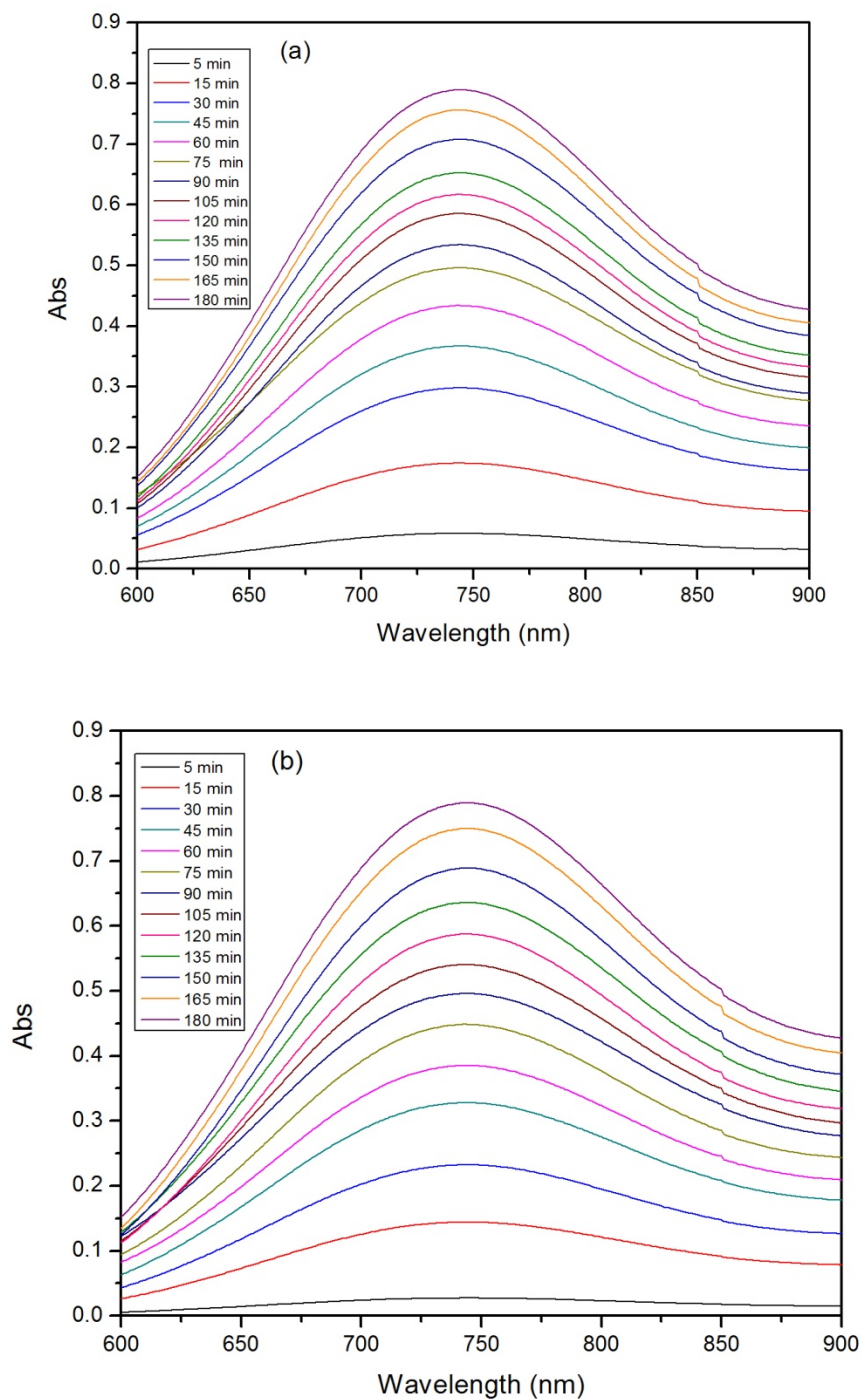


Figure S18. Plot of absorbance with time at 745 nm for (a) 70 mM; (b) 50 mM of **1a-Br**, alkyl bromide.

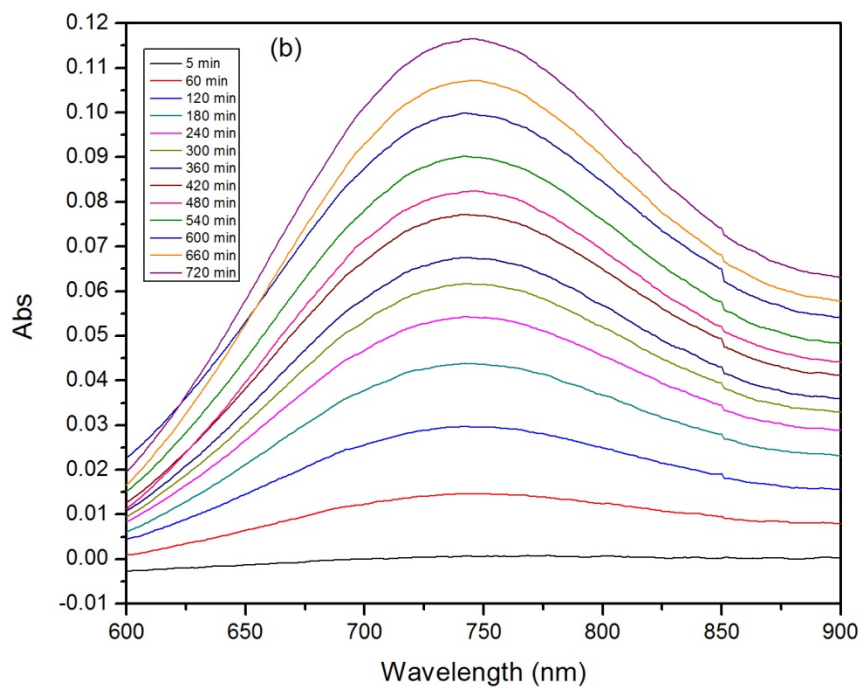
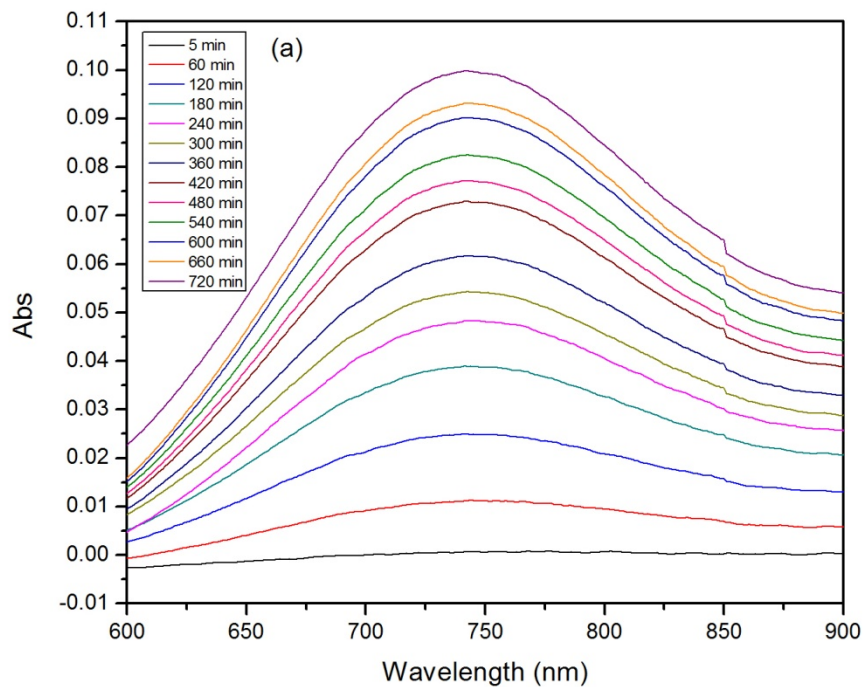


Figure S19. Plot of absorbance with time at 745 nm for (a) 70 mM; (b) 50 mM **2a-Br**, alkyl bromide.

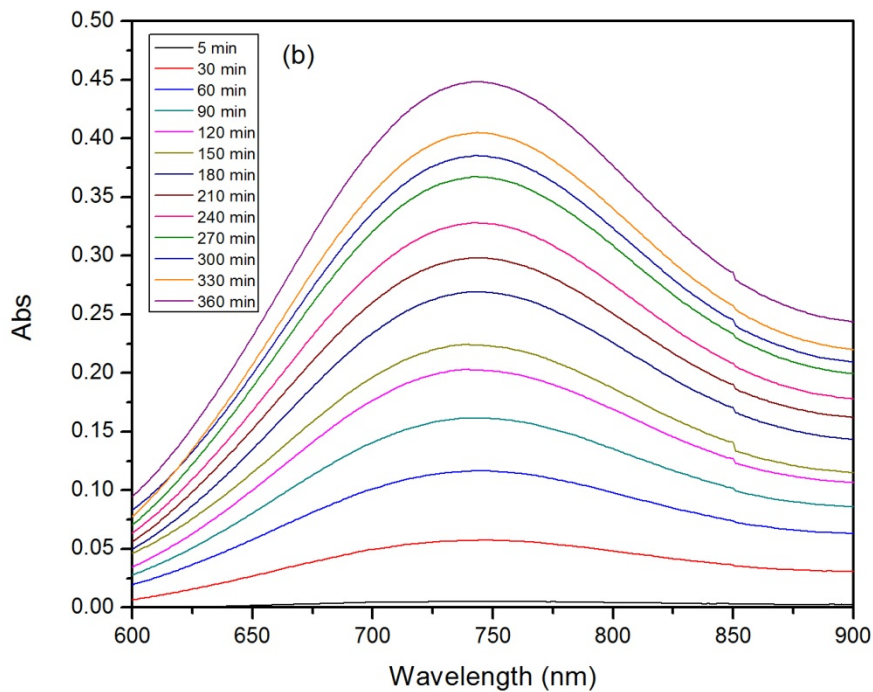
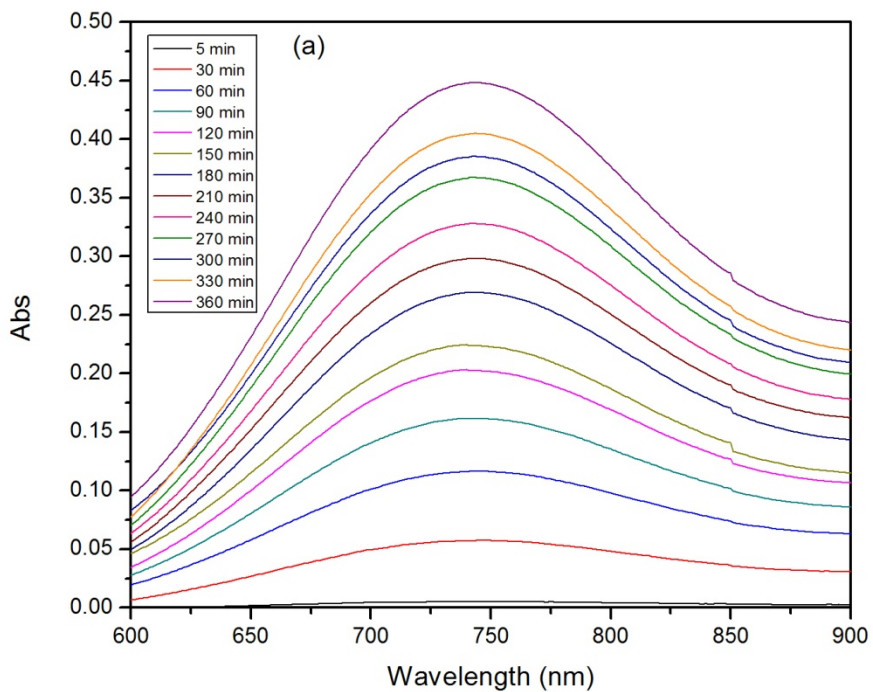


Figure S20. Plot of absorbance with time at 745 nm for (a) 70 mM (b) 50 mM of **3a**-Br, alkyl bromide.

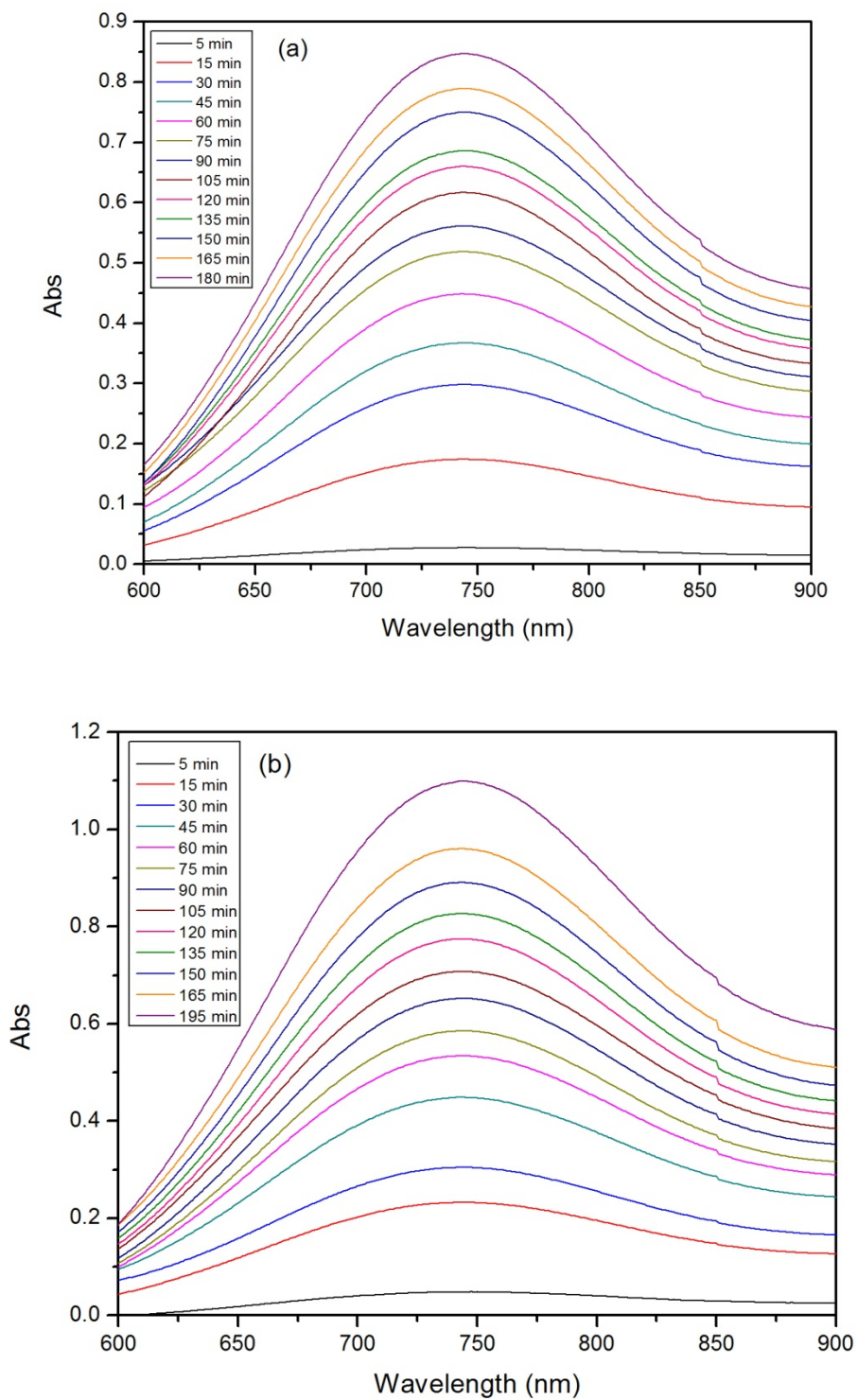


Figure S21. Plot of absorbance vs concentration of $\text{BrCu}^{\text{II}}\text{Bpy}$ complex, to calculate extinction coefficient of $\text{Cu}^{\text{II}}\text{Br}_2/\text{Bpy}$ complex at λ_{max} 745 nm in acetonitrile

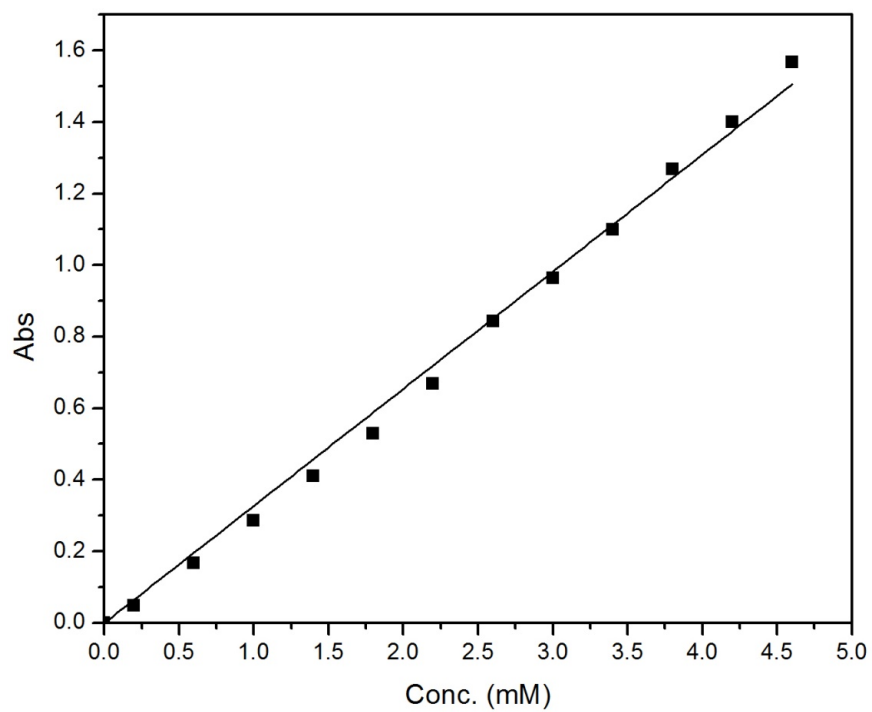


Figure S22. DOSY NMR spectrum of *N*-phenylsuccinimide (SI) in CD₃CN at 25 °C.

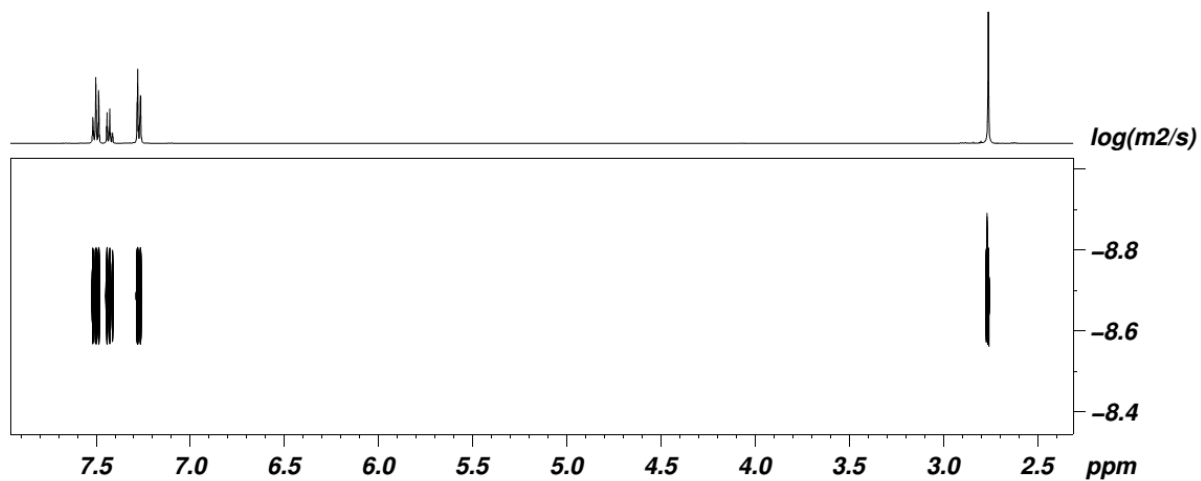


Figure S23. Plot of diffusion time vs gradient strength for *N*-phenylsuccinimide (SI) in CD₃CN at 25 °C for $\delta = 7.556$ ppm.

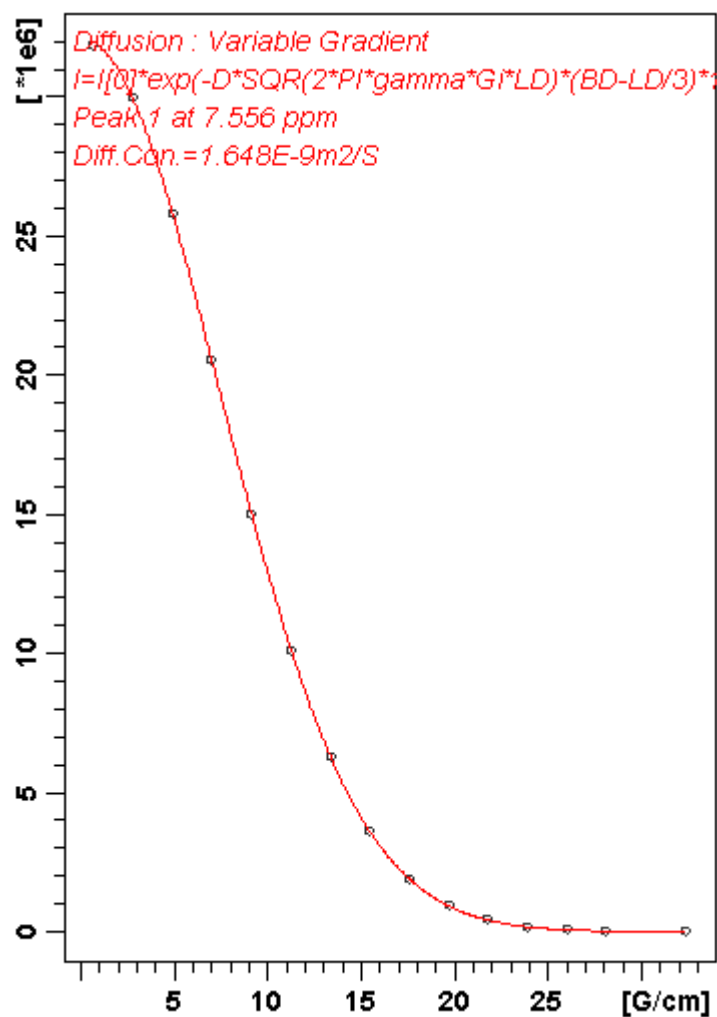


Figure S24. Plot of diffusion time vs gradient strength for *N*-phenylsuccinimide (SI) in CD₃CN at 25 °C for $\delta = 2.816$ ppm.

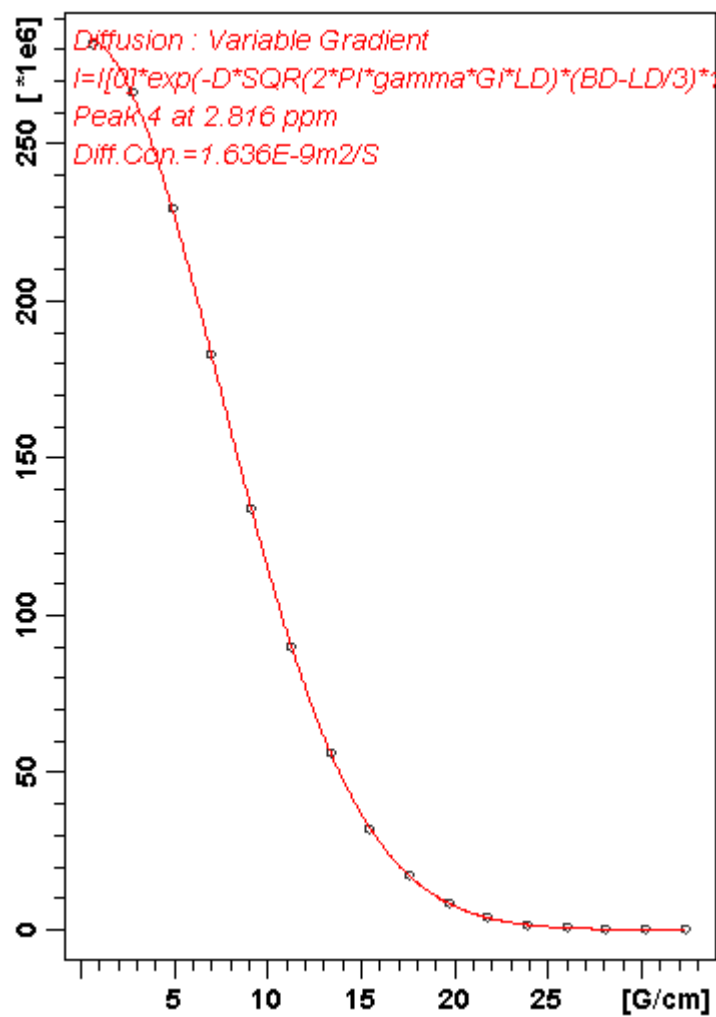


Figure S25. Plots of $F(Y) = F[\text{BrCu}^{\text{II}}\text{Bpy}]$ vs time (s) for (a) **4-Br**, (b) **1a-Br**, (c) **2a-Br** and (d) **3a-Br** alkyl bromides for 50 mM.

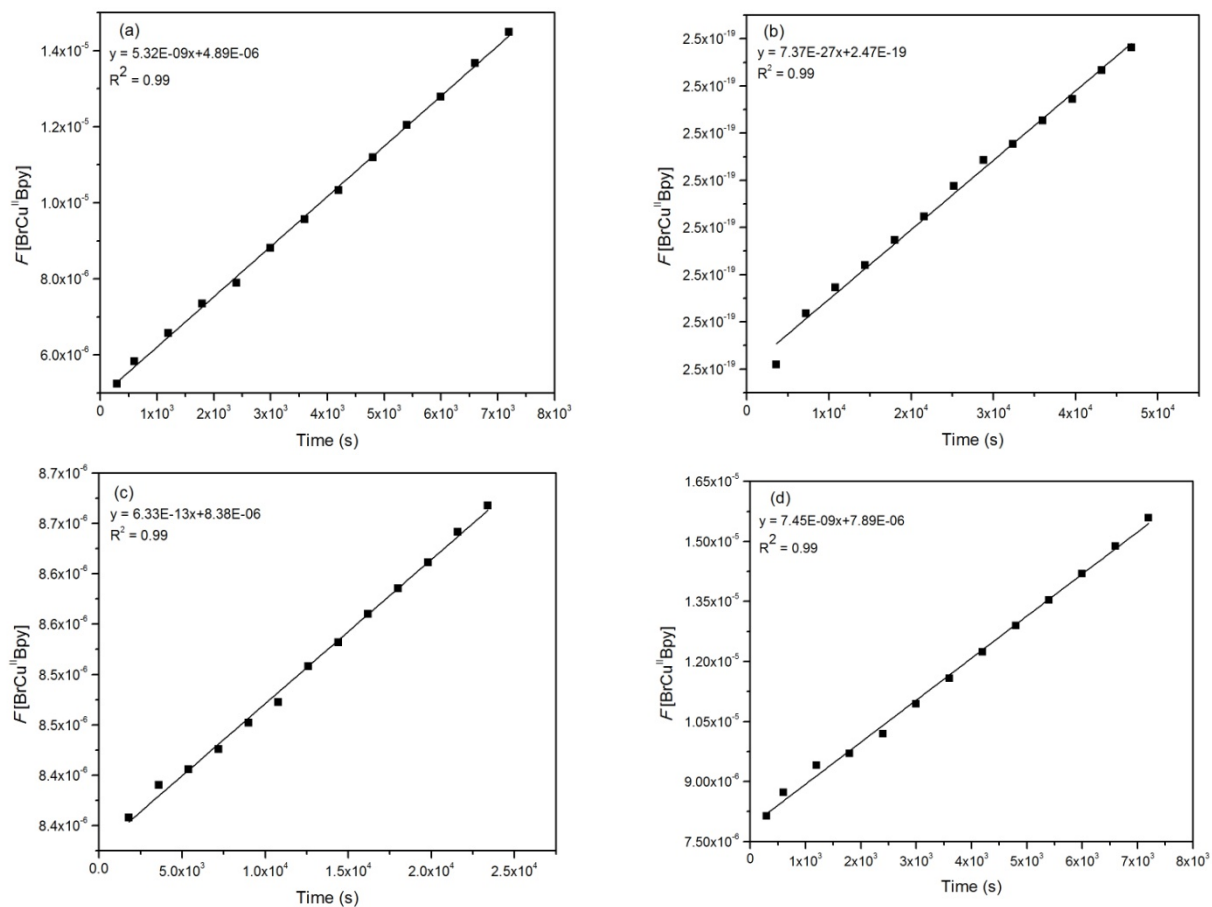


Figure S26. FT-IR spectrum of PI and MMA Copolymer. Polymerization conditions: [PI]/[MMA]/[**3a-Br**]/[CuBr₂]/[Bpy]/[Sn(EH)₂] = 20/80/1/1/3/0.5, in anisole at 80 °C.

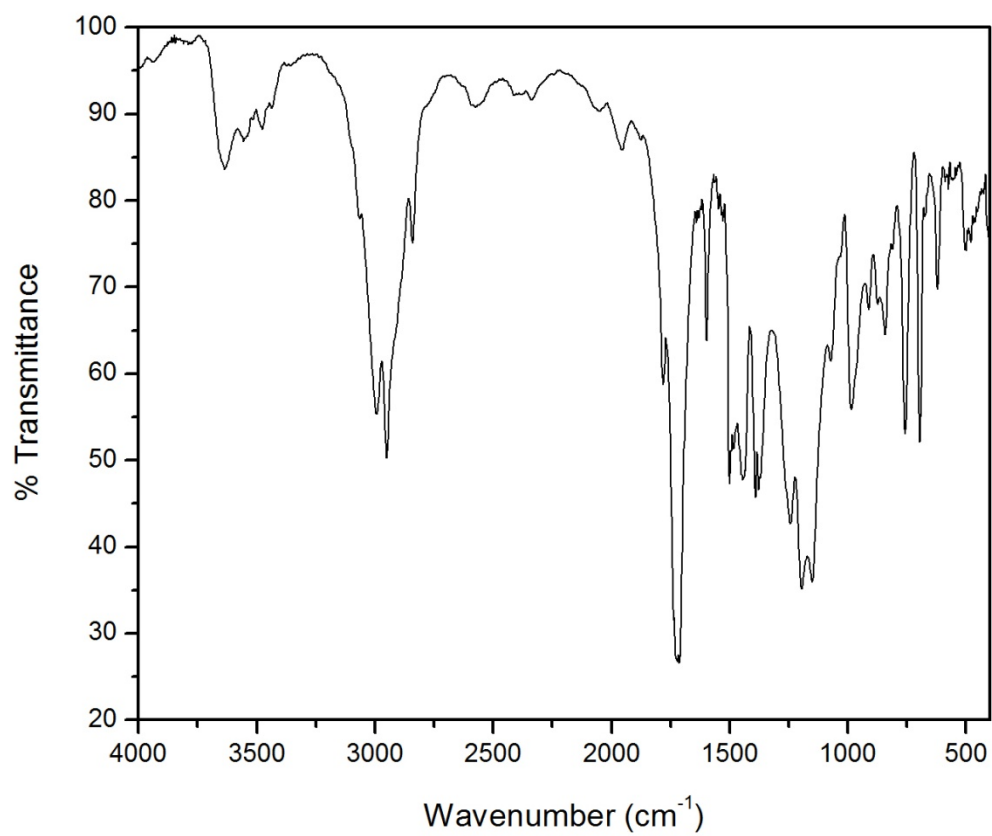


Figure S27. 500 MHz ^1H NMR spectrum of PI and MMA copolymer in CDCl_3 , using TMS as standard. Polymerization conditions: $[\text{PI}]/[\text{MMA}]/[\mathbf{3a}\text{-Br}]/[\text{CuBr}_2]/[\text{Bpy}]/[\text{Sn}(\text{EH})_2] = 20/80/1/1/3/0.5$, in anisole at $80\text{ }^\circ\text{C}$.

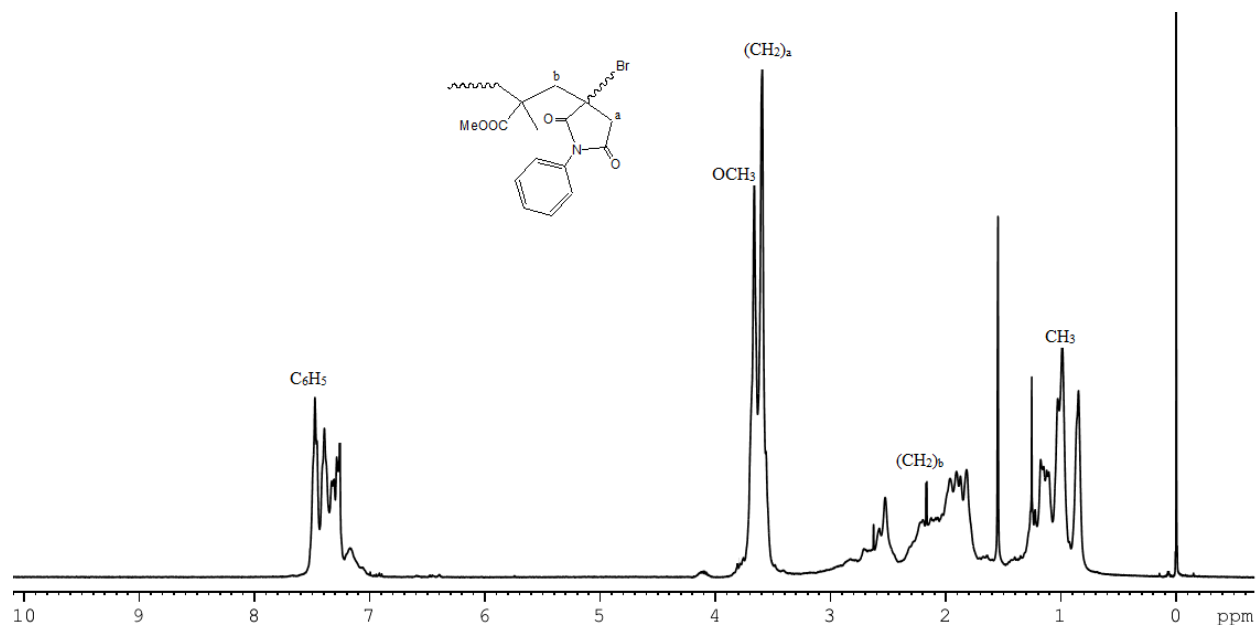


Figure S28. 500 MHz ^1H NMR spectra of the reaction mixture for copolymerization of PI and MMA in CDCl_3 , using TMS as reference standard at various time intervals. Polymerization conditions: $[\text{PI}]/[\text{MMA}]/[\mathbf{3a}\text{-Br}]/[\text{CuBr}_2]/[\text{Bpy}]/[\text{Sn}(\text{EH})_2] = 20/80/1/1/3/0.5$, in anisole at $80\text{ }^\circ\text{C}$.

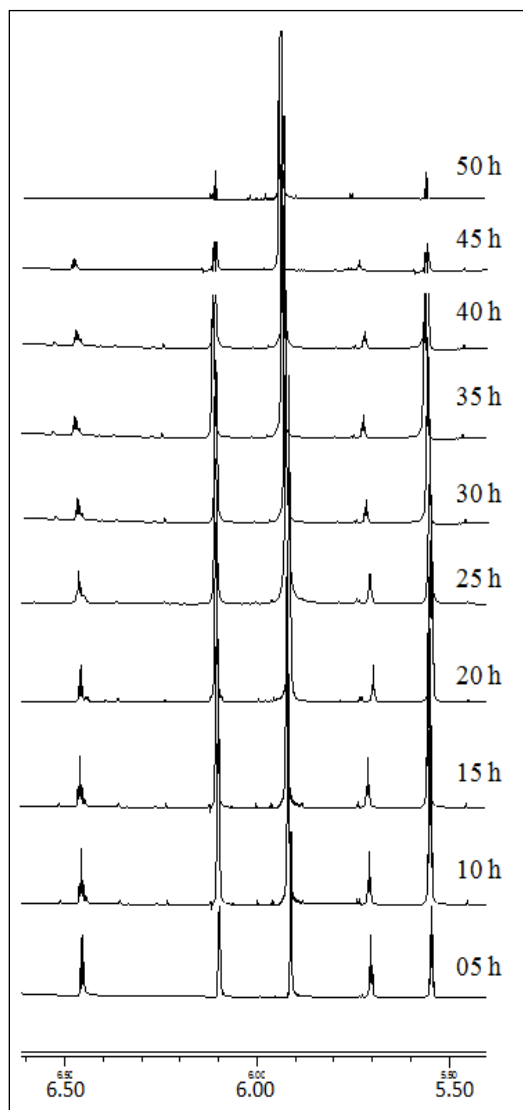
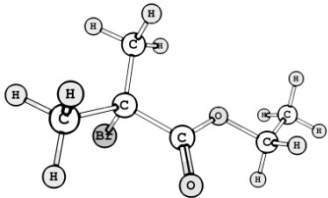
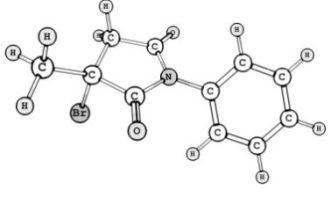
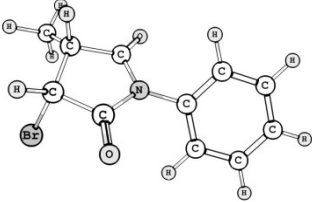
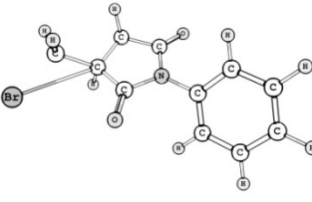
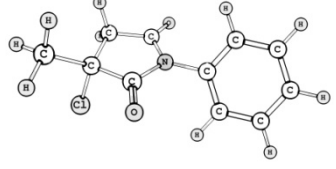
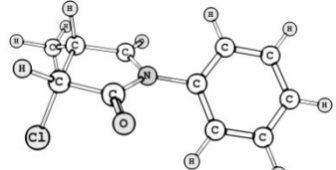


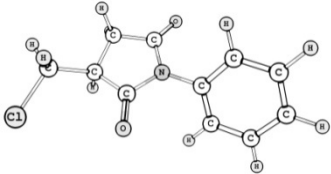
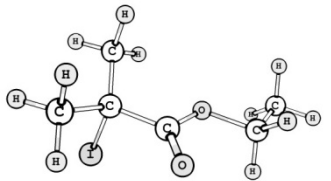
Table S1. B3LYP/ 6-31+G(d)/ LanL2DZ optimized geometries (gas phase) of studied alkyl halides (R-X).

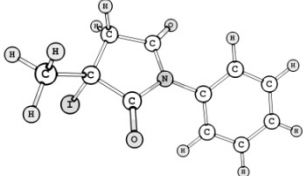
Designation of R-X	Optimized Geometry	Coordinates			
4-Br		6	-0.605133000	0.781232000	-0.343797000
		8	-0.788136000	1.440492000	-1.346524000
		8	-1.552013000	0.035430000	0.249567000
		6	-2.843499000	-0.014395000	-0.411862000
		1	-3.226915000	1.006900000	-0.499968000
		1	-2.694877000	-0.409022000	-1.421982000
		6	-3.749304000	-0.898629000	0.423547000
		1	-3.341110000	-1.911223000	0.508465000
		1	-3.878617000	-0.490211000	1.431668000
		1	-4.735962000	-0.963362000	-0.049760000
		6	0.736702000	0.714461000	0.395686000
		35	1.553953000	-1.007560000	-0.264041000
		6	1.662759000	1.841378000	-0.039488000
		1	1.775266000	1.866350000	-1.124410000
		1	1.243882000	2.803176000	0.284029000
		1	2.645449000	1.713042000	0.422826000
		6	0.602810000	0.594225000	1.909651000
1	0.112480000	1.494447000	2.304747000		
1	0.011991000	-0.276777000	2.195888000		
1	1.595232000	0.514263000	2.363150000		
3a-Br		6	-0.015267000	1.607198000	-0.425315000
		7	0.525350000	0.462945000	0.194659000
		6	4.247485000	0.580793000	0.144973000
		6	2.917715000	0.987515000	0.267435000
		6	1.894121000	0.054916000	0.075846000
		6	2.190296000	-1.275796000	-0.235022000
		6	3.523217000	-1.673421000	-0.347135000
		6	4.553937000	-0.748337000	-0.158824000
		1	5.590619000	-1.061447000	-0.249581000
		1	5.043403000	1.306303000	0.289337000
		1	2.677426000	2.019663000	0.497205000
		1	1.387951000	-1.991406000	-0.378660000
		1	3.753772000	-2.708439000	-0.584185000
		6	-0.433047000	-0.248629000	0.933685000
		6	-1.801771000	0.386551000	0.653653000

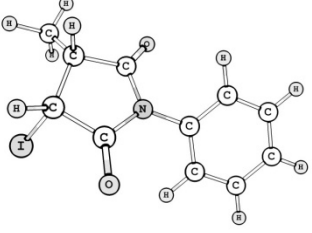
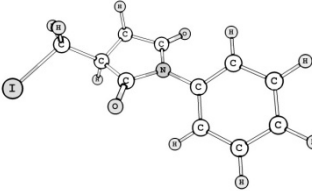
		6	-1.459587000	1.739194000	0.034134000
		8	0.589696000	2.366757000	-1.148801000
		8	-0.216852000	-1.190588000	1.662981000
		1	-1.495426000	2.527752000	0.799674000
		1	-2.103990000	2.044521000	-0.790985000
		6	-2.743735000	0.377759000	1.841058000
		1	-2.314988000	0.982226000	2.651103000
		1	-3.714019000	0.799407000	1.563460000
		1	-2.887736000	-0.639743000	2.211240000
		35	-2.566783000	-0.761579000	-0.805474000
2a-Br		6	-0.324238000	-0.538345000	1.036654000
		7	0.541480000	0.327343000	0.350869000
		6	3.603962000	-1.502405000	-0.703564000
		6	2.263489000	-1.214529000	-0.444126000
		6	1.919364000	0.030825000	0.090538000
		6	2.902231000	0.987074000	0.361811000
		6	4.239387000	0.691454000	0.090843000
		6	4.594235000	-0.552392000	-0.438025000
		1	5.636716000	-0.779669000	-0.644228000
		1	3.872330000	-2.471459000	-1.115331000
		1	1.492845000	-1.950711000	-0.646306000
		1	2.623947000	1.954007000	0.766366000
		1	5.003322000	1.436321000	0.296362000
		6	-0.101467000	1.515928000	-0.051740000
		6	-1.514791000	1.509149000	0.535069000
		6	-1.730230000	0.041733000	0.915570000
		8	-0.010330000	-1.555129000	1.613944000
		8	0.407013000	2.400350000	-0.704260000
		35	-2.665981000	-1.017601000	-0.469064000
		1	-2.303241000	-0.121446000	1.826226000
		1	-1.429538000	2.057225000	1.488182000
		6	-2.544023000	2.230040000	-0.333496000
		1	-2.247333000	3.275075000	-0.458232000
		1	-2.619296000	1.775459000	-1.324156000
		1	-3.531762000	2.196883000	0.137580000
1a-Br		6	0.822055000	1.930105000	-0.314096000
		7	0.999508000	0.545892000	-0.141676000
		6	4.491905000	-0.185227000	0.929532000
		6	3.245802000	0.436199000	0.831635000
		6	2.280904000	-0.089225000	-0.033148000

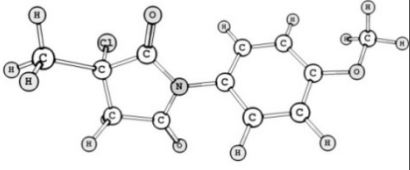
		6	2.553230000	-1.230556000	-0.793794000
		6	3.799535000	-1.848828000	-0.682402000
		6	4.771720000	-1.328340000	0.176096000
		1	5.741885000	-1.811155000	0.257593000
		1	5.243109000	0.226669000	1.597913000
		1	3.029748000	1.327247000	1.410635000
		1	1.795579000	-1.637065000	-1.454749000
		1	4.008642000	-2.738578000	-1.270019000
		6	-0.222418000	-0.151630000	-0.060196000
		6	-1.355796000	0.840627000	-0.344626000
		6	-0.671230000	2.217283000	-0.276398000
		8	1.712998000	2.742235000	-0.443147000
		8	-0.332946000	-1.333355000	0.179391000
		1	-0.885417000	2.740126000	0.665538000
		1	-0.942706000	2.894709000	-1.090399000
		6	-2.555884000	0.696823000	0.587191000
		1	-2.260771000	0.489244000	1.617249000
		1	-3.165741000	1.600740000	0.561850000
		35	-3.767860000	-0.758732000	0.058894000
		1	-1.685126000	0.648010000	-1.373870000
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		8	-0.276203000	1.780636000	-0.673749000
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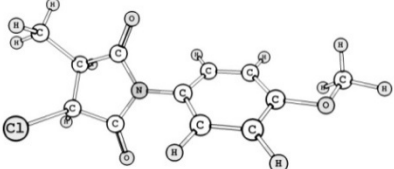
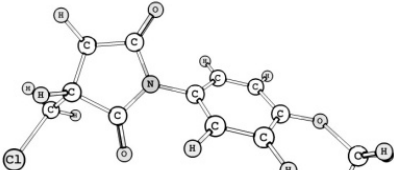
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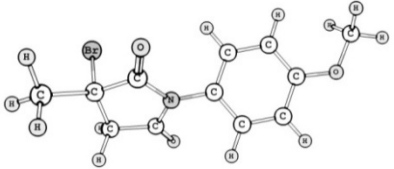
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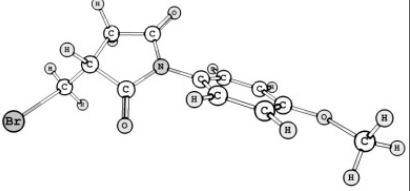
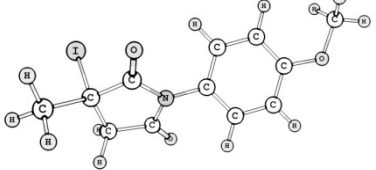
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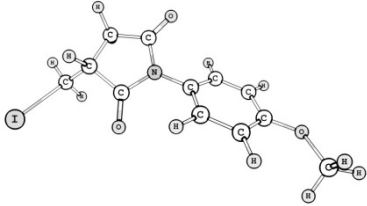
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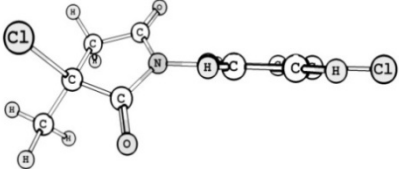
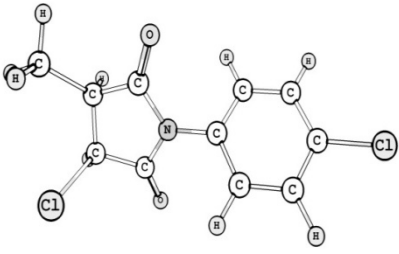
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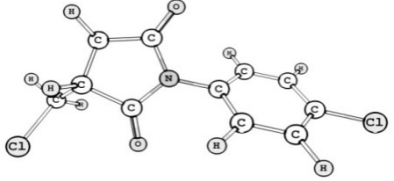
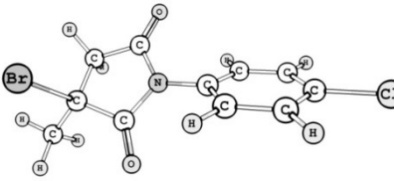
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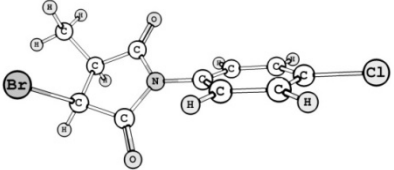
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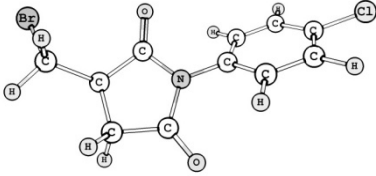
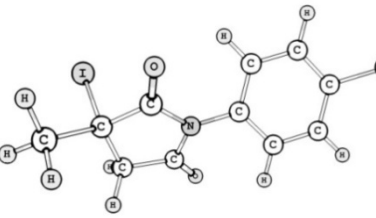
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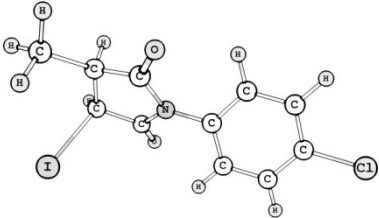
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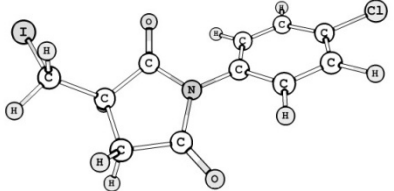
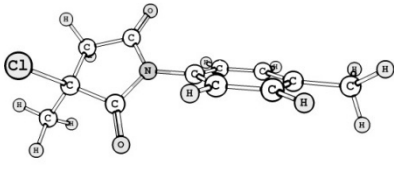
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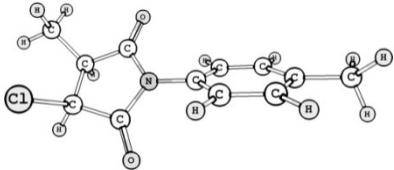
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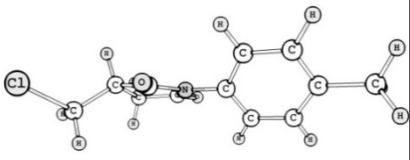
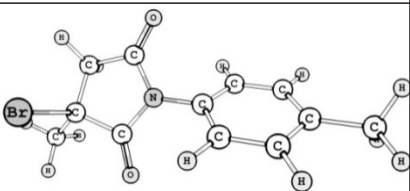
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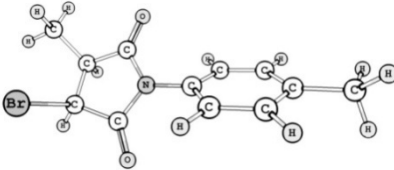
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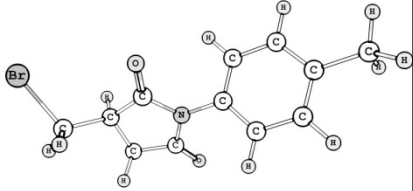
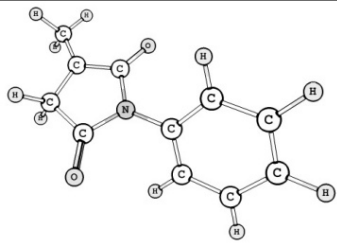
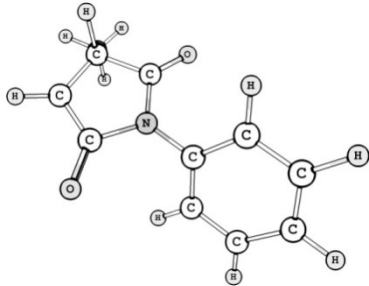
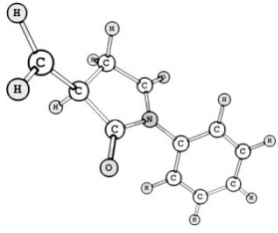
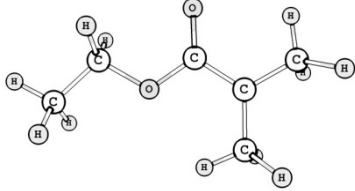
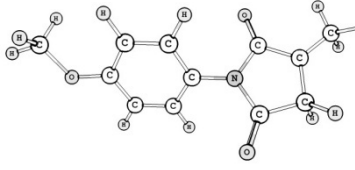
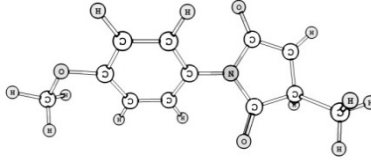
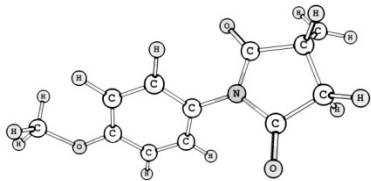
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		1	-4.859362000	0.723007000	1.530934000
		1	-2.572798000	1.638758000	1.386761000
		1	2.652661000	0.372317000	1.632671000
		1	3.651736000	1.418711000	0.596000000
		1	-6.021880000	-2.352648000	-0.355454000
		1	-6.650508000	-0.700692000	-0.265149000
		1	-6.237876000	-1.566616000	1.217703000

Table S2. B3LYP/ 6-31+G(d)/ LanL2DZ optimized geometries (gas phase) of studied alkyl radicals (R[•]).

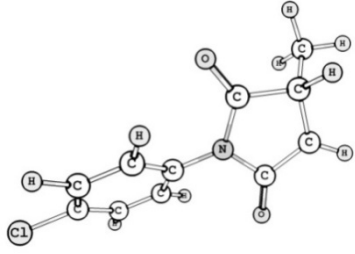
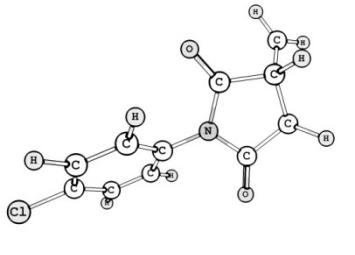
Designation of radicals	Optimized geometry	Optimized coordinate			
Rad_3a		6	-1.005749000	1.425812000	-0.275703000
		7	-0.378218000	0.196855000	-0.037269000
		6	3.232224000	0.730317000	0.700304000
		6	1.849379000	0.918086000	0.680003000
		6	1.038169000	0.007041000	-0.007372000
		6	1.607535000	-1.089279000	-0.666480000
		6	2.990904000	-1.271348000	-0.631521000
		6	3.807595000	-0.363586000	0.048084000
		1	4.884580000	-0.507727000	0.069635000
		1	3.859004000	1.442201000	1.230759000
		1	1.404244000	1.769825000	1.181109000
		1	0.974142000	-1.797548000	-1.187605000
		1	3.428798000	-2.126116000	-1.140078000
		6	-1.329136000	-0.853266000	0.170989000
		6	-2.650552000	-0.263494000	0.065996000
		6	-2.514698000	1.191929000	-0.221208000
		8	-0.448909000	2.484257000	-0.488842000
		8	-1.038600000	-2.021730000	0.396142000
		1	-2.961360000	1.837058000	0.550221000
		1	-2.967422000	1.499349000	-1.175704000
6	-3.911855000	-1.023116000	0.240196000		
1	-4.514477000	-0.610930000	1.063731000		
1	-4.540379000	-0.963693000	-0.661360000		
1	-3.702430000	-2.075201000	0.452037000		
Rad_2a		6	-1.071116000	1.389425000	-0.383772000
		7	-0.403737000	0.143963000	-0.154779000
		6	3.124452000	0.776469000	0.851404000
		6	1.739695000	0.914602000	0.743786000
		6	1.014500000	0.007237000	-0.037922000
		6	1.670325000	-1.033887000	-0.706047000
		6	3.054221000	-1.166440000	-0.584189000
		6	3.785675000	-0.262851000	0.191450000
		1	4.863742000	-0.367604000	0.280476000
		1	3.685329000	1.484811000	1.455214000

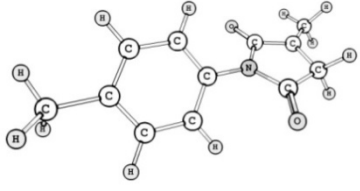
		1	1.228169000	1.725072000	1.249667000
		1	1.102269000	-1.737904000	-1.303109000
		1	3.559698000	-1.978156000	-1.100478000
		6	-1.311406000	-0.919547000	-0.055092000
		6	-2.728881000	-0.361913000	-0.251980000
		6	-2.485539000	1.092057000	-0.444490000
		8	-0.512008000	2.471467000	-0.501032000
		8	-1.026359000	-2.081296000	0.156941000
		1	-3.231285000	1.858266000	-0.617798000
		1	-3.134582000	-0.818199000	-1.170261000
		6	-3.666355000	-0.735759000	0.916049000
		1	-3.700360000	-1.823393000	1.027657000
		1	-3.313939000	-0.300258000	1.857120000
		1	-4.679376000	-0.368093000	0.722510000
Rad_1a		6	-1.078695000	1.363051000	-0.349041000
		7	-0.418412000	0.139644000	-0.123062000
		6	3.111328000	0.726189000	0.911993000
		6	1.723961000	0.854118000	0.825593000
		6	1.007135000	0.010474000	-0.028198000
		6	1.666989000	-0.959202000	-0.789070000
		6	3.053586000	-1.085204000	-0.688640000
		6	3.778996000	-0.243244000	0.158688000
		1	4.858807000	-0.342086000	0.231543000
		1	3.668702000	1.385632000	1.571729000
		1	1.203694000	1.608660000	1.405284000
		1	1.100894000	-1.614997000	-1.441573000
		1	3.565339000	-1.842652000	-1.276156000
		6	-1.306737000	-0.940363000	0.007472000
		6	-2.736269000	-0.421554000	-0.209873000
		6	-2.577876000	1.105736000	-0.328329000
		8	-0.528222000	2.430615000	-0.514939000
		8	-0.988018000	-2.087518000	0.235067000
		1	-3.001457000	1.633844000	0.533972000
		1	-3.029417000	1.534423000	-1.227790000
		6	-3.669576000	-0.909765000	0.846938000
		1	-3.534584000	-1.898542000	1.271578000
		1	-4.571561000	-0.351852000	1.077323000
		1	-3.038663000	-0.836127000	-1.190695000

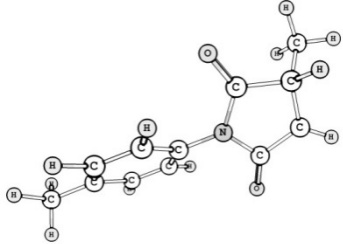
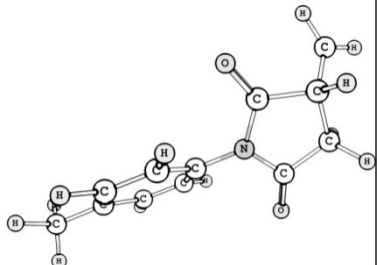
Rad_4		6	-0.288582000	-0.513292000	-0.000021000
		8	-0.237016000	-1.741524000	-0.000021000
		8	0.834332000	0.261854000	-0.000062000
		6	2.092990000	-0.446251000	-0.000092000
		1	2.133424000	-1.091849000	0.883845000
		1	2.133533000	-1.091575000	-0.884226000
		6	3.203796000	0.588231000	0.000127000
		1	3.148240000	1.226854000	-0.888330000
		1	3.148163000	1.226551000	0.888796000
		1	4.177319000	0.083856000	0.000081000
		6	-1.523377000	0.259471000	0.000026000
		6	-2.823055000	-0.476821000	0.000089000
		1	-2.671277000	-1.557980000	0.000171000
		1	-3.426247000	-0.203598000	0.879836000
		1	-3.426253000	-0.203741000	-0.879700000
		6	-1.542170000	1.754555000	-0.000055000
		1	-0.540229000	2.185528000	-0.000047000
		1	-2.086373000	2.133926000	-0.879156000
		1	-2.086445000	2.134030000	0.878953000
		Rad_3c		6	-1.939053000
8	-1.493007000			2.476891000	0.560883000
6	-3.415804000			0.981928000	0.280437000
6	-3.400925000			-0.471662000	-0.045300000
6	-2.026596000			-0.914612000	-0.182599000
8	-1.616980000			-2.040974000	-0.439129000
7	-1.189344000			0.223928000	0.041452000
6	0.237444000			0.189397000	-0.020633000
6	0.942971000			-0.854260000	0.580904000
6	2.338665000			-0.895437000	0.517316000
6	3.036417000			0.120834000	-0.147108000
6	2.325571000			1.171286000	-0.748354000
6	0.938706000			1.203955000	-0.690536000
6	-4.577108000			-1.356353000	-0.225344000
8	4.395568000			0.179264000	-0.264911000
6	5.176153000			-0.852138000	0.325915000
1	-3.939144000			1.596125000	-0.467795000
1	-3.884452000			1.214985000	1.248237000
1	0.408884000			-1.648795000	1.088732000
1	2.860428000			-1.720866000	0.987826000
1	2.879964000	1.952523000	-1.259204000		

		1	0.399315000	2.022737000	-1.152387000
		1	-4.259875000	-2.374533000	-0.466952000
		1	-5.231610000	-0.990782000	-1.031201000
		1	-5.196116000	-1.387042000	0.684276000
		1	6.214924000	-0.597745000	0.108798000
		1	4.940855000	-1.831180000	-0.111599000
		1	5.028952000	-0.890098000	1.413207000
Rad_2c		6	1.983993000	1.335765000	-0.416983000
		8	1.523123000	2.461324000	-0.555748000
		6	3.365666000	0.911675000	-0.467020000
		6	3.476893000	-0.554774000	-0.246672000
		6	2.014411000	-0.977243000	-0.043977000
		8	1.624440000	-2.105468000	0.185559000
		7	1.207212000	0.160917000	-0.165555000
		6	-0.216197000	0.157250000	-0.044391000
		6	-0.973407000	-0.830239000	-0.677006000
		6	-2.365365000	-0.844162000	-0.553460000
		6	-3.007377000	0.144274000	0.203255000
		6	-2.244519000	1.138865000	0.835205000
		6	-0.861175000	1.144751000	0.716409000
		6	4.373173000	-0.988882000	0.932833000
		8	-4.357748000	0.226005000	0.385205000
		6	-5.189715000	-0.747138000	-0.234085000
		1	4.177534000	1.603414000	-0.655825000
		1	3.842772000	-1.063734000	-1.153897000
		1	-0.482280000	-1.602421000	-1.257997000
		1	-2.927988000	-1.625914000	-1.050742000
		1	-2.756289000	1.899302000	1.416942000
		1	-0.281753000	1.921629000	1.201309000
		1	4.311296000	-2.073178000	1.063699000
		1	4.056689000	-0.507370000	1.864243000
		1	5.415396000	-0.714976000	0.738620000
		1	-6.211237000	-0.482261000	0.043648000
		1	-4.962138000	-1.757122000	0.131090000
		1	-5.089281000	-0.719530000	-1.326970000
Rad_1c		6	1.975861000	1.308693000	-0.399705000
		8	1.513973000	2.413132000	-0.595048000
		6	3.448975000	0.928655000	-0.377968000
		6	3.480150000	-0.602650000	-0.215446000
		6	2.013398000	-0.992441000	0.025144000

		8	1.601045000	-2.102948000	0.284697000
		7	1.218548000	0.153341000	-0.131507000
		6	-0.210745000	0.149623000	-0.017779000
		6	-0.969151000	-0.755707000	-0.757486000
		6	-2.362177000	-0.772206000	-0.642225000
		6	-2.998776000	0.134256000	0.215152000
		6	-2.231862000	1.048132000	0.955262000
		6	-0.847726000	1.052749000	0.843534000
		6	4.376945000	-1.136997000	0.850492000
		8	-4.349182000	0.207505000	0.399598000
		6	-5.185966000	-0.689013000	-0.320830000
		1	3.921153000	1.444063000	0.466587000
		1	3.928648000	1.291682000	-1.291686000
		1	3.739409000	-1.069331000	-1.185155000
		1	-0.478742000	-1.462929000	-1.417926000
		1	-2.929486000	-1.490691000	-1.222454000
		1	-2.740985000	1.744740000	1.614051000
		1	-0.261119000	1.764194000	1.414692000
		1	4.163420000	-2.099099000	1.303258000
		1	5.322424000	-0.648401000	1.063402000
		1	-6.206636000	-0.445426000	-0.021419000
		1	-4.968414000	-1.733256000	-0.061177000
		1	-5.079747000	-0.549009000	-1.404481000
Rad_3d		6	-1.864394000	1.412085000	0.262873000
		8	-1.367294000	2.501243000	0.467525000
		6	-3.356940000	1.093881000	0.202399000
		6	-3.410458000	-0.368868000	-0.074269000
		6	-2.059035000	-0.886251000	-0.165337000
		8	-1.701993000	-2.038659000	-0.377019000
		7	-1.167192000	0.216921000	0.039830000
		6	0.255118000	0.105371000	0.020081000
		6	0.880948000	-0.979678000	0.646339000
		6	2.270871000	-1.091550000	0.625525000
		6	3.029124000	-0.111787000	-0.015351000
		6	2.416693000	0.975336000	-0.639000000
		6	1.026207000	1.080614000	-0.624558000
		6	-4.626557000	-1.198633000	-0.248830000
		17	4.781011000	-0.249500000	-0.037890000
		1	-3.834695000	1.707401000	-0.576078000
		1	-3.831343000	1.382703000	1.152159000

		1	0.288028000	-1.742657000	1.135885000
		1	2.758758000	-1.933206000	1.105939000
		1	3.017169000	1.731452000	-1.134013000
		1	0.546953000	1.926667000	-1.102165000
		1	-4.358043000	-2.237718000	-0.457820000
		1	-5.250216000	-0.822398000	-1.073743000
		1	-5.258626000	-1.172976000	0.651881000
Rad_2d		6	1.913496000	1.380018000	-0.359931000
		8	1.401347000	2.485188000	-0.474819000
		6	3.314822000	1.025090000	-0.385377000
		6	3.493569000	-0.440047000	-0.207272000
		6	2.050487000	-0.942493000	-0.060177000
		8	1.711320000	-2.094114000	0.124303000
		7	1.188517000	0.159072000	-0.168869000
		6	-0.234235000	0.079027000	-0.092283000
		6	-0.913234000	-0.956066000	-0.746980000
		6	-2.302858000	-1.039502000	-0.667936000
		6	-3.007572000	-0.080354000	0.059733000
		6	-2.341881000	0.957740000	0.711710000
		6	-0.951351000	1.034771000	0.638059000
		6	4.380062000	-0.867288000	0.982454000
		17	-4.759062000	-0.181289000	0.155630000
		1	4.095720000	1.762270000	-0.526565000
		1	3.908349000	-0.899802000	-1.119700000
		1	-0.361402000	-1.702454000	-1.305629000
		1	-2.832112000	-1.842251000	-1.170616000
		1	-2.901396000	1.698479000	1.273389000
		1	-0.431081000	1.843814000	1.136169000
		1	4.367957000	-1.956827000	1.078410000
		1	4.017285000	-0.431092000	1.919201000
		1	5.411966000	-0.537675000	0.823852000
Rad_1d		6	1.913278000	1.351071000	-0.334433000
		8	1.406555000	2.440124000	-0.498414000
		6	3.399878000	1.035007000	-0.286728000
		6	3.497632000	-0.497665000	-0.169940000
		6	2.044759000	-0.963870000	0.004085000
		8	1.675386000	-2.099798000	0.209144000
		7	1.200651000	0.151234000	-0.135860000
		6	-0.228135000	0.076344000	-0.073517000
		6	-0.908051000	-0.891501000	-0.819053000

		6	-2.299047000	-0.970916000	-0.754660000
		6	-2.999326000	-0.072304000	0.050583000
		6	-2.329910000	0.899790000	0.794389000
		6	-0.938187000	0.969657000	0.734367000
		6	4.379427000	-1.022953000	0.913342000
		17	-4.751847000	-0.166324000	0.128926000
		1	3.828251000	1.545467000	0.583682000
		1	3.883615000	1.447153000	-1.177196000
		1	3.813727000	-0.921252000	-1.142472000
		1	-0.356807000	-1.590367000	-1.437889000
		1	-2.832342000	-1.723000000	-1.326545000
		1	-2.887285000	1.593107000	1.415476000
		1	-0.411508000	1.725624000	1.305469000
		1	4.198086000	-2.009326000	1.326090000
		1	5.291667000	-0.497108000	1.176211000
Rad_3b		6	1.478091000	1.415184000	-0.272287000
		8	0.962654000	2.494723000	-0.485488000
		6	2.977015000	1.125436000	-0.207735000
		6	3.056096000	-0.335117000	0.074354000
		6	1.712746000	-0.875074000	0.168217000
		8	1.377361000	-2.033072000	0.386149000
		7	0.803556000	0.210350000	-0.042280000
		6	-0.618902000	0.074233000	-0.019719000
		6	-1.231867000	-0.994787000	-0.679592000
		6	-2.621863000	-1.121831000	-0.647325000
		6	-3.425998000	-0.194325000	0.026960000
		6	-2.789307000	0.872886000	0.679693000
		6	-1.403097000	1.010849000	0.665607000
		6	4.286500000	-1.142941000	0.252929000
		6	-4.931130000	-0.329158000	0.054091000
		1	3.441630000	1.750298000	0.569806000
		1	3.447971000	1.419750000	-1.157547000
		1	-0.629753000	-1.729725000	-1.201094000
		1	-3.085667000	-1.961397000	-1.160155000
		1	-3.386868000	1.609990000	1.212237000
		1	-0.933032000	1.846255000	1.171745000
		1	4.035397000	-2.186014000	0.464150000
		1	4.902336000	-0.754312000	1.078120000
		1	4.919772000	-1.108950000	-0.646756000
		1	-5.260903000	-1.232025000	-0.470251000

		1	-5.417054000	0.531196000	-0.423824000
		1	-5.308542000	-0.382858000	1.083080000
Rad_2b		6	1.530866000	1.381617000	-0.373183000
		8	1.002806000	2.479137000	-0.492954000
		6	2.937921000	1.047258000	-0.407941000
		6	3.138598000	-0.414175000	-0.221646000
		6	1.702928000	-0.934419000	-0.056625000
		8	1.382697000	-2.089718000	0.141246000
		7	0.826568000	0.153399000	-0.166729000
		6	-0.596487000	0.054806000	-0.076644000
		6	-1.273976000	-0.958711000	-0.760829000
		6	-2.662987000	-1.051935000	-0.659855000
		6	-3.402817000	-0.143260000	0.107948000
		6	-2.701957000	0.867167000	0.784392000
		6	-1.314961000	0.971179000	0.701278000
		6	4.041731000	-0.820814000	0.962367000
		6	-4.908802000	-0.232952000	0.198120000
		1	3.707120000	1.794212000	-0.561826000
		1	3.550715000	-0.875011000	-1.134776000
		1	-0.721373000	-1.677569000	-1.355005000
		1	-3.177619000	-1.848704000	-1.192073000
		1	-3.249057000	1.586509000	1.390227000
		1	-0.794706000	1.763819000	1.226525000
		1	4.044616000	-1.909701000	1.066891000
		1	3.681807000	-0.382324000	1.899233000
		1	5.067955000	-0.479025000	0.792201000
		1	-5.280827000	-1.165529000	-0.238700000
		1	-5.388417000	0.598262000	-0.335565000
		1	-5.250557000	-0.188661000	1.239344000
Rad_1b		6	1.533777000	1.354817000	-0.340755000
		8	1.013138000	2.437165000	-0.509062000
		6	3.025614000	1.060024000	-0.295740000
		6	3.143502000	-0.471499000	-0.183723000
		6	1.697255000	-0.954792000	0.005761000
		8	1.345856000	-2.095072000	0.220343000
		7	0.839521000	0.147808000	-0.133689000
		6	-0.590015000	0.055168000	-0.061226000
		6	-1.269715000	-0.879781000	-0.843526000
		6	-2.660437000	-0.969438000	-0.759061000
		6	-3.395178000	-0.131635000	0.089918000

		6	-2.689619000	0.802167000	0.864636000
		6	-1.300960000	0.898161000	0.798409000
		6	4.045086000	-0.989173000	0.886361000
		6	-4.902453000	-0.215793000	0.164621000
		1	3.447440000	1.572436000	0.576837000
		1	3.503444000	1.481989000	-1.184762000
		1	3.452498000	-0.888226000	-1.161585000
		1	-0.718455000	-1.542589000	-1.501991000
		1	-3.179818000	-1.706307000	-1.367381000
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		1	-0.773353000	1.628943000	1.401907000
		1	3.877761000	-1.976919000	1.301826000
		1	4.955430000	-0.454672000	1.138425000
		1	-5.280699000	-1.095056000	-0.367064000
		1	-5.371725000	0.670402000	-0.282577000
		1	-5.248616000	-0.275670000	1.203544000