

## Supporting Information

### Structural Study of some Unsaturated Malononitriles using Mass Spectrometry and Theoretical Models

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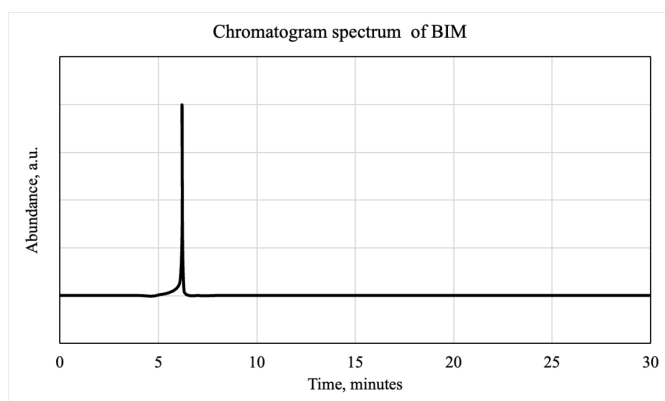


Figure S1. Chromatogram Spectrum of BIM.

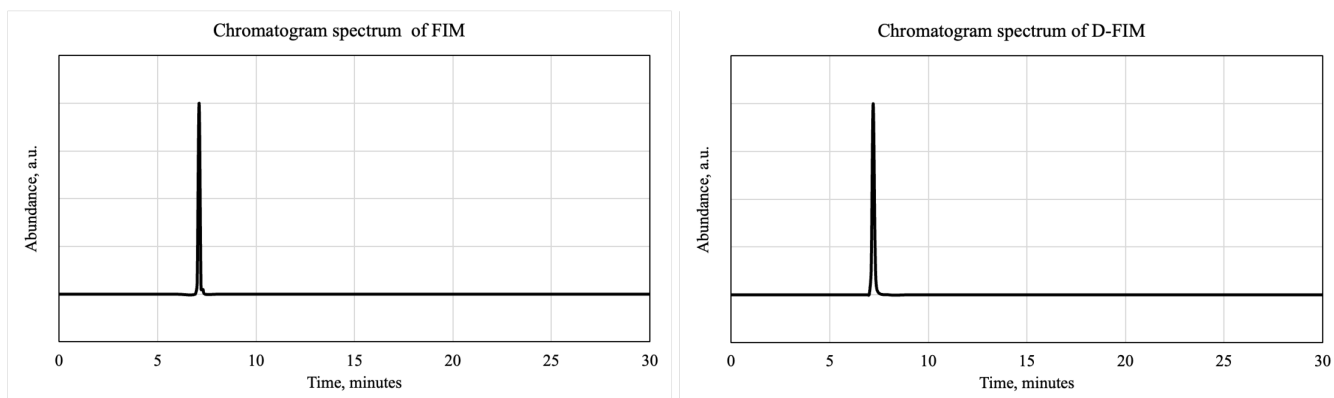


Figure S2. Chromatogram Spectrum of FIM and D-FIM.

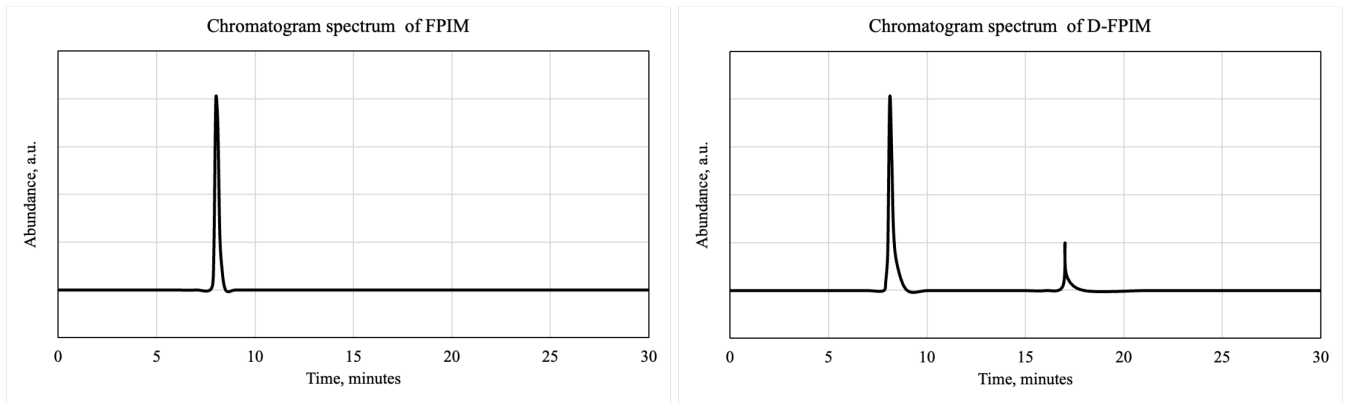


Figure S3. Chromatogram Spectrum of FPIM and D-FPIM.

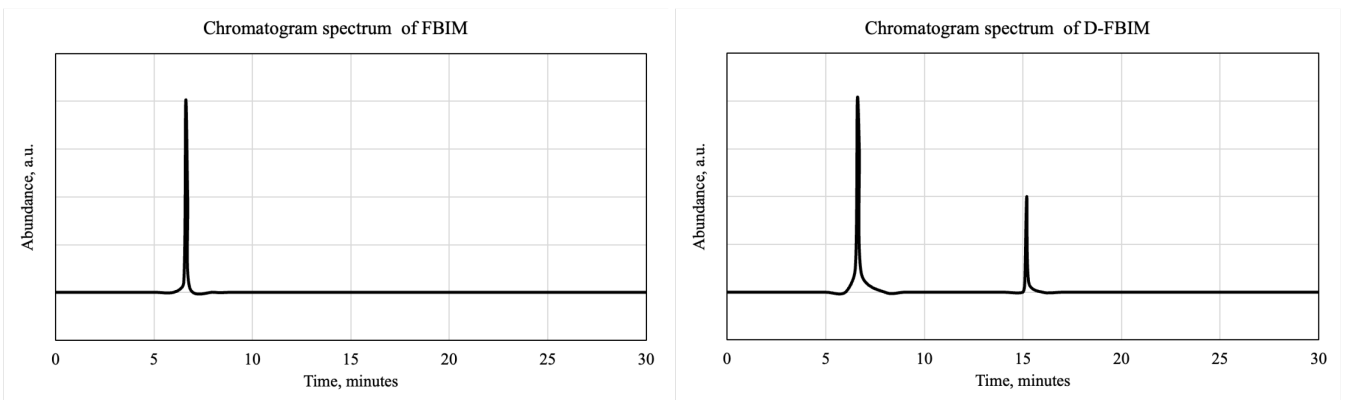
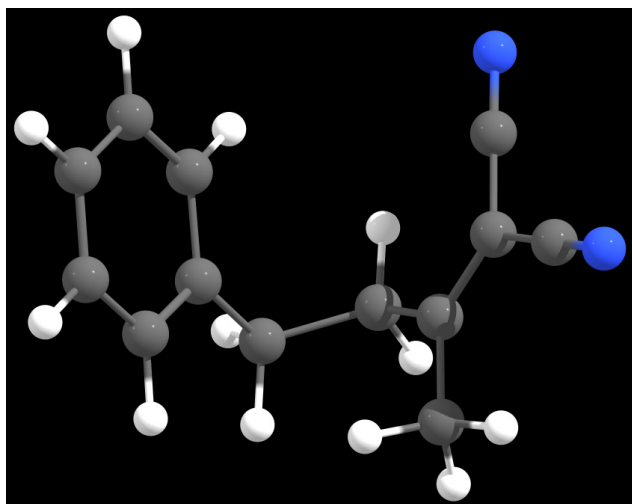
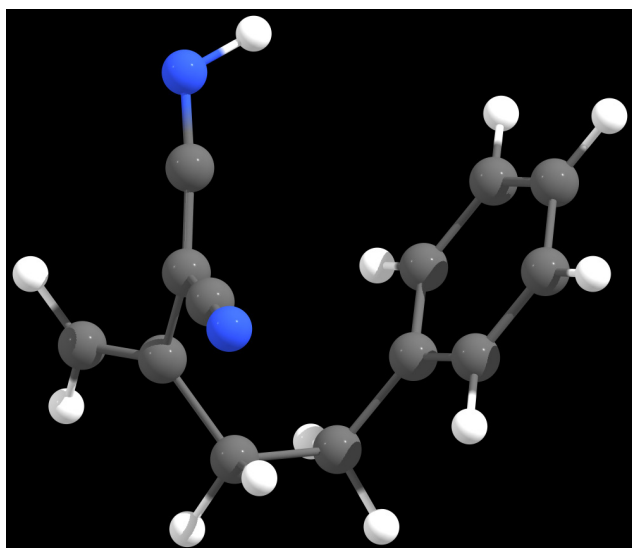


Figure S4. Chromatogram Spectrum of FBIM and D-FBIM.



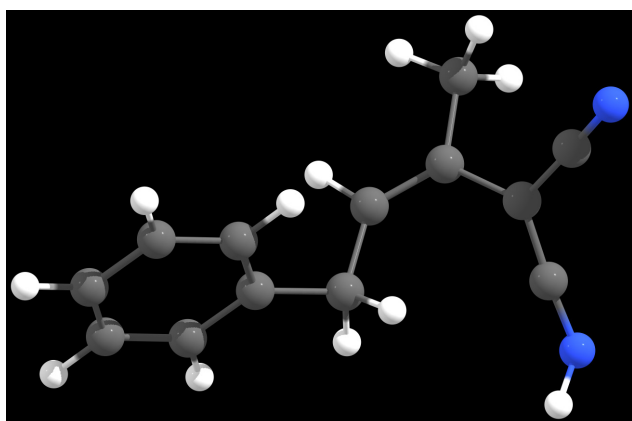
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6	-2.167770000	1.359879000	-2.632171000
6	-2.011680000	0.610313000	-1.468950000
6	-1.104689000	1.019742000	-0.491165000
6	-0.339999000	2.179345000	-0.656332000
6	0.650461000	2.606254000	0.409872000
6	0.433134000	4.036797000	0.968032000
6	-0.915690000	4.271624000	1.594142000
6	-1.339428000	3.340165000	2.688954000
6	-1.713839000	5.297431000	1.190726000
6	-2.990488000	5.551847000	1.790401000
6	-1.332274000	6.202231000	0.146677000
7	-1.026699000	6.943824000	-0.685042000
7	-4.019145000	5.761168000	2.273164000
1	0.079900000	3.821956000	-1.993407000
1	-1.521563000	3.105895000	-3.715024000
1	-2.873251000	1.046649000	-3.393576000
1	-2.594048000	-0.292398000	-1.319857000
1	-0.984021000	0.423592000	0.408597000
1	1.666755000	2.577406000	0.001765000
1	0.633468000	1.882319000	1.229098000
1	0.618797000	4.772028000	0.184006000
1	1.189043000	4.211499000	1.745555000
1	-0.514161000	3.176454000	3.388760000
1	-1.597011000	2.364075000	2.263240000
1	-2.205733000	3.705677000	3.239181000

Figure S5. Optimized structure and final structural coordinates of FBIM Nitrile



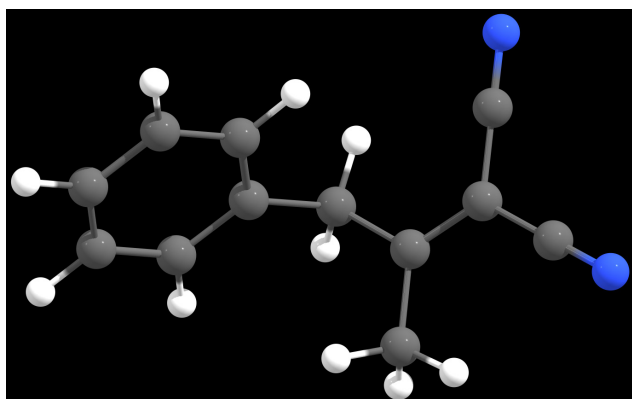
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6	-0.929626000	2.591834000	-2.816399000
6	-1.801308000	1.512016000	-2.670054000
6	-1.884238000	0.859962000	-1.440957000
6	-1.104941000	1.290687000	-0.366079000
6	-0.230162000	2.374950000	-0.498077000
6	0.609702000	2.840083000	0.673267000
6	0.215361000	4.215279000	1.276703000
6	-1.210218000	4.283891000	1.786153000
6	-1.545113000	3.952751000	3.037166000
6	-2.258768000	4.715086000	0.806765000
6	-3.412535000	4.065877000	0.700025000
6	-2.019980000	5.811150000	-0.071477000
7	-1.789813000	6.704609000	-0.770671000
7	-4.496220000	3.525946000	0.687613000
1	0.523647000	3.855225000	-1.872492000
1	-0.854054000	3.103678000	-3.769510000
1	-2.401630000	1.177385000	-3.508979000
1	-2.545976000	0.008354000	-1.319871000
1	-1.171513000	0.773263000	0.586085000
1	1.658767000	2.906807000	0.363177000
1	0.565150000	2.088046000	1.466496000
1	0.379453000	4.999620000	0.531710000
1	0.895520000	4.425313000	2.106959000
1	-0.795063000	3.609602000	3.741754000
1	-2.566133000	4.017163000	3.395421000
1	-4.645533000	2.742843000	0.050092000

Figure S6. Optimized structure and final structural coordinates of FBIM Keto A



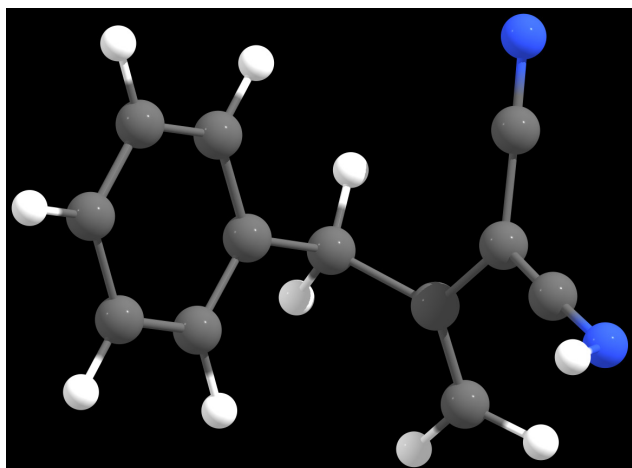
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6	0.857451000	2.140906000	-3.099957000
6	-0.141587000	2.706550000	-3.888856000
6	-1.334047000	3.123188000	-3.295780000
6	-1.521953000	2.976115000	-1.923584000
6	-0.525943000	2.406534000	-1.120731000
6	-0.740739000	2.252324000	0.375477000
6	-0.791750000	3.578199000	1.091769000
6	-1.647851000	3.975727000	2.045241000
6	-1.614011000	5.368719000	2.626337000
6	-2.691927000	3.074462000	2.628510000
6	-2.403159000	1.841578000	3.032049000
6	-4.025755000	3.543895000	2.817659000
7	-5.100314000	3.950781000	2.957278000
7	-2.087983000	0.783343000	3.530259000
1	1.445855000	1.546323000	-1.118705000
1	1.787454000	1.813097000	-3.551785000
1	0.005538000	2.820931000	-4.957089000
1	-2.118369000	3.562367000	-3.902774000
1	-2.451043000	3.306482000	-1.469389000
1	0.073146000	1.641176000	0.785732000
1	-1.667392000	1.696536000	0.552474000
1	-0.046002000	4.301445000	0.769103000
1	-0.857391000	5.977293000	2.128390000
1	-1.391748000	5.342607000	3.698368000
1	-2.583035000	5.865767000	2.513679000
1	-2.127106000	-0.068338000	2.970320000

Figure S7. Optimized structure and final structural coordinates of FBIM Keto B



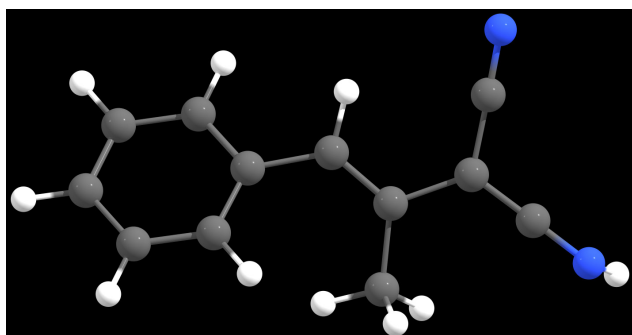
6	-5.784836000	0.978581000	1.973607000
6	-4.453915000	1.139443000	1.570799000
6	-3.778911000	0.046391000	1.020392000
6	-4.417902000	-1.185401000	0.876654000
6	-5.741492000	-1.337185000	1.283996000
6	-6.424180000	-0.250611000	1.830995000
6	-3.763103000	2.488594000	1.731579000
6	-3.444747000	2.803621000	3.175023000
6	-2.394736000	1.963702000	3.833404000
6	-4.084646000	3.803730000	3.839808000
6	-5.091390000	4.614913000	3.220511000
6	-3.801897000	4.111960000	5.210770000
7	-3.578565000	4.363944000	6.315986000
7	-5.908303000	5.269288000	2.730892000
1	-6.327927000	1.819889000	2.391906000
1	-2.750097000	0.158655000	0.692347000
1	-3.881906000	-2.022598000	0.443294000
1	-6.240272000	-2.293251000	1.171519000
1	-7.456969000	-0.358382000	2.143315000
1	-4.383263000	3.276139000	1.298726000
1	-2.820329000	2.474980000	1.174138000
1	-1.439739000	2.096260000	3.311775000
1	-2.656778000	0.904946000	3.745151000
1	-2.253101000	2.207393000	4.885415000

Figure S8. Optimized structure and final structural coordinates of FPIM Nitrile



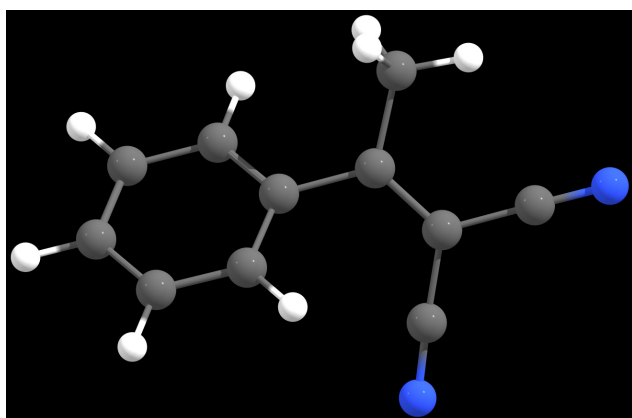
6	-6.138854000	1.225737000	1.834310000
6	-4.769875000	1.139897000	1.565776000
6	-4.103778000	-0.057183000	1.855307000
6	-4.789540000	-1.142525000	2.395183000
6	-6.156613000	-1.046083000	2.659060000
6	-6.828729000	0.140889000	2.377118000
6	-4.012574000	2.315859000	0.965619000
6	-2.981959000	2.916240000	1.902689000
6	-1.666789000	2.847423000	1.673324000
6	-3.514963000	3.586572000	3.129805000
6	-4.710573000	4.360540000	3.074485000
6	-2.915113000	3.455021000	4.308594000
7	-5.685240000	4.980182000	2.998479000
1	-6.669398000	2.148185000	1.622399000
1	-3.039803000	-0.140376000	1.655320000
1	-4.258765000	-2.064530000	2.607380000
1	-6.692089000	-1.890734000	3.078463000
1	-7.890950000	0.226583000	2.578691000
1	-4.729755000	3.090178000	0.674839000
1	-3.499942000	2.001050000	0.052232000
1	-1.281150000	2.328871000	0.802953000
1	-0.941759000	3.305714000	2.336450000
7	-2.289950000	3.424956000	5.344726000
1	-2.496838000	2.703534000	6.035800000

Figure S9. Optimized structure and final structural coordinates of FPIM Keto A



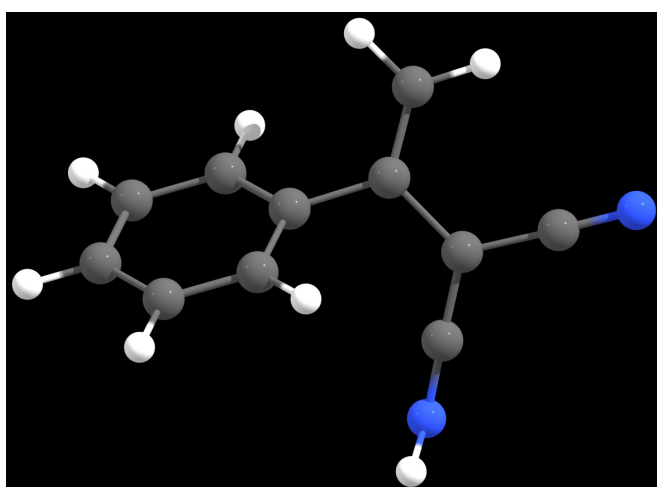
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6	-4.576809000	0.893875000	1.825041000
6	-4.076551000	-0.278637000	2.416452000
6	-3.788983000	-1.402689000	1.645430000
6	-3.998544000	-1.384997000	0.267448000
6	-4.516883000	-0.237104000	-0.332700000
6	-4.920608000	2.105600000	2.586883000
6	-4.264423000	2.658106000	3.629075000
6	-2.962380000	2.157882000	4.201608000
6	-4.822849000	3.871355000	4.275897000
6	-6.059579000	4.440065000	3.844844000
6	-4.206574000	4.509726000	5.272196000
7	-3.736342000	5.002715000	6.274526000
7	-7.060113000	4.890244000	3.478185000
1	-5.221284000	1.768965000	-0.035369000
1	-3.947445000	-0.326012000	3.490744000
1	-3.412592000	-2.299494000	2.125676000
1	-3.774963000	-2.261313000	-0.330665000
1	-4.697216000	-0.216488000	-1.401968000
1	-5.806732000	2.622279000	2.226644000
1	-2.477863000	1.452999000	3.528504000
1	-3.109193000	1.664244000	5.168832000
1	-2.270800000	2.990048000	4.369409000
1	-3.069714000	5.771045000	6.188167000

Figure S10. Optimized structure and final structural coordinates of FPIM Keto B



6	-2.683751000	0.404518000	1.545544000
6	-2.904654000	-0.495298000	0.489036000
6	-2.116938000	-1.633177000	0.350970000
6	-1.114307000	-1.908320000	1.280279000
6	-0.900306000	-1.035455000	2.345487000
6	-1.672515000	0.114629000	2.475164000
6	-3.530411000	1.610655000	1.686645000
6	-3.001420000	2.841617000	1.953269000
6	-1.595266000	3.105971000	2.026634000
6	-3.833020000	3.993746000	2.139286000
6	-5.014387000	1.428571000	1.538016000
7	-0.471490000	3.366994000	2.091111000
7	-4.493974000	4.929618000	2.291174000
1	-3.674244000	-0.292369000	-0.246188000
1	-2.286821000	-2.305268000	-0.482504000
1	-0.505739000	-2.799451000	1.175695000
1	-0.129521000	-1.247353000	3.077518000
1	-1.502395000	0.779007000	3.313075000
1	-5.249381000	1.016210000	0.552280000
1	-5.565778000	2.359508000	1.660424000
1	-5.371682000	0.701645000	2.274085000

Figure S11. Optimized structure and final structural coordinates of FIM Nitrile



6	-2.146201000	0.701355000	1.678134000
6	-1.016217000	0.317967000	0.944689000
6	0.056548000	1.192936000	0.782833000
6	0.016296000	2.464518000	1.351751000
6	-1.103289000	2.856612000	2.085533000
6	-2.177785000	1.984757000	2.243195000
6	-3.277089000	-0.251099000	1.875485000
6	-4.629991000	0.203229000	1.460723000
6	-4.828215000	1.283722000	0.704102000
6	-5.791006000	-0.536663000	1.834201000
6	-3.087186000	-1.469921000	2.401164000
7	-5.011918000	2.177418000	-0.088571000
7	-6.716554000	-1.154641000	2.150176000
1	-0.988937000	-0.666007000	0.490356000
1	0.921017000	0.881861000	0.206687000
1	0.850871000	3.145195000	1.225821000
1	-1.136275000	3.839553000	2.542787000
1	-3.034739000	2.288893000	2.835221000
1	-3.902568000	-2.170916000	2.534856000
1	-2.101754000	-1.779796000	2.725480000
1	-5.169006000	3.130028000	0.240376000

Figure S12. Optimized structure and final structural coordinates of FIM Keto

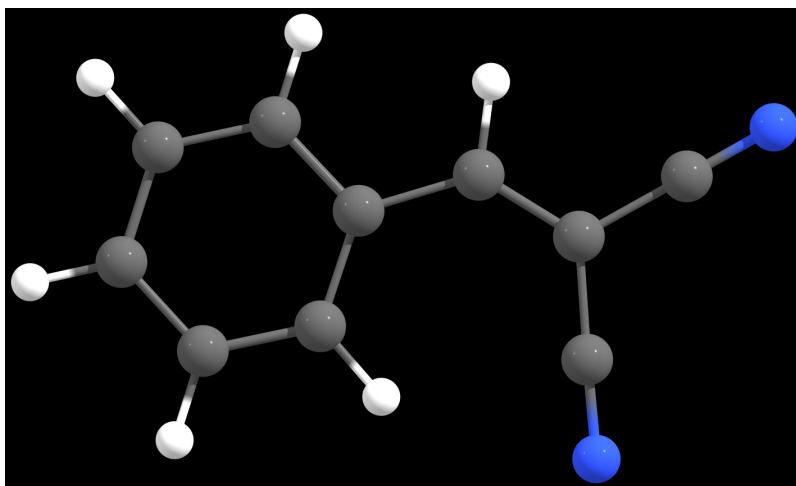


Figure S13. Optimized structure and final structural coordinates of BIM

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