

2-Pyridinyl-Terminated Iminobenzoate: Type and Orientation of Mesogenic Core Effect, Geometrical DFT Investigation

Jehan Y. Al-Humaidi ¹, Shady Nada ², Mariam Gerges ², Marwa Ehab ², Mariusz Jaremko ³, Abdul-Hamid Emwas ⁴ and Mohamed Hagar ^{2,*}

¹ Department of Chemistry, College of Science, Princess Nourah Bint Abdulrahman University, P.O. Box 84428, Riyadh 11671, Saudi Arabia; jyalhamidi@pnu.edu

² Department of Chemistry, Faculty of Science, Alexandria University, Alexandria 21321, Egypt; shadyadel4869@gmail.com (S.N.); mariamgerges1720@gmail.com (M.G.); marwa.ehab2022@gmail.com (M.E.)

³ Smart-Health Initiative (SHI) and Red Sea Research Center (RSRC), Division of Biological and Environmental Sciences and Engineering (BESE), King Abdullah University of Science and Technology (KAUST), P.O. Box 4700, Thuwal 23955-6900, Saudi Arabia; mariusz.jaremko@kaust.edu.sa

⁴ Core Labs, King Abdullah University of Science and Technology, P.O. Box 4700, Thuwal 23955-6900, Saudi Arabia; abdelhamid.emwas@kaust.edu.sa

* Correspondence: mohamed.hagar@alexu.edu.eg

Coordinates of the investigated compounds

A Compound (in Angstrom Å)

6	-9.502094000	0.760297000	0.579498000
6	-8.708339000	0.251763000	-0.451044000
7	-9.167760000	-0.134186000	-1.627911000
6	-10.481152000	-0.022063000	-1.847578000
6	-11.374168000	0.473739000	-0.904472000
6	-10.864851000	0.869360000	0.330074000
8	-7.342301000	0.026985000	-0.329085000
6	-6.510985000	0.784414000	0.448387000
8	-6.871079000	1.704318000	1.137942000
6	-5.102867000	0.321321000	0.323951000
6	-4.130622000	0.977231000	1.094111000
6	-2.803325000	0.595721000	1.017737000
6	-2.416445000	-0.453503000	0.167736000
6	-3.391750000	-1.103729000	-0.600053000
6	-4.725682000	-0.722653000	-0.526958000
6	-1.014082000	-0.877894000	0.067544000
7	-0.087872000	-0.330420000	0.753561000
6	1.253655000	-0.715738000	0.597370000
6	2.076488000	-0.674424000	1.731367000
6	3.413773000	-1.036785000	1.647431000
6	3.989233000	-1.417178000	0.428650000

6	3.169417000	-1.427959000	-0.705085000
6	1.823563000	-1.086930000	-0.630153000
6	5.462555000	-1.739990000	0.331890000
6	6.336124000	-0.497277000	0.069876000
6	7.834679000	-0.811174000	0.004686000
6	8.703202000	0.424950000	-0.255566000
6	10.205993000	0.124663000	-0.295734000
6	11.071264000	1.362750000	-0.556120000
6	12.575416000	1.068272000	-0.586027000
6	13.431017000	2.311331000	-0.846288000
1	-9.067572000	1.071028000	1.515781000
1	-10.826238000	-0.346430000	-2.824803000
1	-12.430651000	0.546392000	-1.130677000
1	-11.520723000	1.260485000	1.099437000
1	-4.442478000	1.785263000	1.743990000
1	-2.041983000	1.092672000	1.605341000
1	-3.099937000	-1.913331000	-1.260961000
1	-5.475871000	-1.221624000	-1.125166000
1	-0.815444000	-1.706563000	-0.625570000
1	1.638214000	-0.367321000	2.673524000
1	4.027572000	-1.015373000	2.542548000
1	3.593795000	-1.701477000	-1.666327000
1	1.221129000	-1.072993000	-1.531367000

1	5.626987000	-2.468983000	-0.469253000
1	5.792875000	-2.218055000	1.260732000
1	6.149990000	0.241270000	0.858582000
1	6.015655000	-0.027050000	-0.867349000
1	8.017560000	-1.555321000	-0.781327000
1	8.146965000	-1.281249000	0.946228000
1	8.505631000	1.174181000	0.521789000
1	8.400473000	0.886069000	-1.204392000
1	10.405457000	-0.625834000	-1.071593000
1	10.508201000	-0.334004000	0.654649000
1	10.866855000	2.115907000	0.216032000
1	10.774054000	1.818590000	-1.509547000
1	12.780276000	0.316024000	-1.357529000
1	12.872458000	0.613772000	0.366944000
1	14.496903000	2.067682000	-0.860362000
1	13.273932000	3.068740000	-0.071876000
1	13.182274000	2.768258000	-1.809275000

B Compound (in Angstrom Å)

6	-11.609197000	1.097658000	0.745029000
6	-10.793267000	0.849122000	-0.362172000
7	-11.215670000	0.854015000	-1.615705000

6	-12.505306000	1.118758000	-1.836851000
6	-13.416640000	1.385228000	-0.820617000
6	-12.948670000	1.371205000	0.490231000
8	-9.443769000	0.528187000	-0.293311000
6	-8.640163000	0.686297000	0.798802000
8	-9.002859000	1.106861000	1.868738000
6	-7.246354000	0.268323000	0.486881000
6	-6.296527000	0.342627000	1.516980000
6	-4.983954000	-0.028336000	1.286432000
6	-4.590366000	-0.484586000	0.017664000
6	-5.543399000	-0.555671000	-1.007184000
6	-6.862080000	-0.182937000	-0.780091000
6	-3.205071000	-0.887100000	-0.256018000
7	-2.295988000	-0.858650000	0.639151000
6	-0.969681000	-1.200456000	0.326420000
6	-0.213893000	-1.848020000	1.312913000
6	1.100579000	-2.220564000	1.064396000
6	1.720542000	-1.930045000	-0.156960000
6	0.971083000	-1.250618000	-1.123952000
6	-0.351685000	-0.890592000	-0.895048000
6	3.166956000	-2.290521000	-0.406084000
6	4.152627000	-1.165669000	-0.033248000
6	5.614654000	-1.535462000	-0.305318000

6	6.606146000	-0.418332000	0.039685000
6	8.066098000	-0.789403000	-0.244872000
6	9.062585000	0.329490000	0.079111000
6	10.519652000	-0.045725000	-0.214469000
6	11.520037000	1.074114000	0.093800000
1	-11.206533000	1.089072000	1.744062000
1	-12.816659000	1.115136000	-2.877294000
1	-14.453709000	1.595278000	-1.050672000
1	-13.618610000	1.571455000	1.318649000
1	-6.613552000	0.696362000	2.490047000
1	-4.240071000	0.023925000	2.071209000
1	-5.246059000	-0.905722000	-1.990267000
1	-7.595475000	-0.235356000	-1.573216000
1	-3.003663000	-1.230168000	-1.279835000
1	-0.686591000	-2.065804000	2.263273000
1	1.659828000	-2.742062000	1.834955000
1	1.432744000	-0.995953000	-2.073097000
1	-0.898611000	-0.339396000	-1.651572000
1	3.301810000	-2.544022000	-1.463636000
1	3.421097000	-3.191069000	0.163611000
1	4.024867000	-0.914012000	1.026173000
1	3.891265000	-0.260570000	-0.594190000
1	5.728190000	-1.803320000	-1.363881000

1	5.872385000	-2.437641000	0.264447000
1	6.498813000	-0.152001000	1.098962000
1	6.345305000	0.484175000	-0.527857000
1	8.167787000	-1.066898000	-1.302089000
1	8.329710000	-1.686540000	0.330071000
1	8.965552000	0.606754000	1.136712000
1	8.797749000	1.226820000	-0.494954000
1	10.612638000	-0.331404000	-1.270306000
1	10.786541000	-0.938900000	0.365147000
1	11.429455000	1.360493000	1.149573000
1	11.253319000	1.967067000	-0.486214000
6	12.975157000	0.694714000	-0.204168000
1	13.063326000	0.402782000	-1.258714000
1	13.243121000	-0.195464000	0.379596000
6	13.978130000	1.814715000	0.093984000
1	13.712284000	2.704795000	-0.491159000
1	13.891040000	2.108650000	1.148161000
6	15.432724000	1.432964000	-0.203672000
1	15.519131000	1.136811000	-1.256195000
1	15.699570000	0.545797000	0.383425000
6	16.428110000	2.558479000	0.092006000
1	16.388946000	2.854776000	1.144988000
1	17.454671000	2.253082000	-0.128514000

1	16.210043000	3.447193000	-0.508586000
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C Compound (in Angstrom Å)

6	12.707980000	-1.216353000	0.736455000
6	11.896441000	-0.978378000	-0.376083000
7	12.321052000	-1.003891000	-1.628285000
6	13.609478000	-1.281182000	-1.842505000
6	14.516410000	-1.539513000	-0.820386000
6	14.045881000	-1.503280000	0.489294000
8	10.551315000	-0.638416000	-0.309922000
6	9.735741000	-0.838270000	0.766827000
8	10.084411000	-1.316871000	1.816715000
6	8.350936000	-0.384064000	0.466449000
6	7.394985000	-0.485648000	1.488512000
6	6.090694000	-0.080459000	1.269324000
6	5.711476000	0.437895000	0.020142000
6	6.670079000	0.534230000	-0.997441000
6	7.980612000	0.127450000	-0.781644000
6	4.336182000	0.882448000	-0.238722000
7	3.423979000	0.832057000	0.652314000
6	2.107416000	1.223446000	0.357174000
6	1.366777000	1.831739000	1.379401000

6	0.064062000	2.255143000	1.151768000
6	-0.559466000	2.056212000	-0.085827000
6	0.173242000	1.413607000	-1.090308000
6	1.484447000	1.002936000	-0.881207000
6	-1.993095000	2.476430000	-0.314874000
6	-3.014305000	1.352918000	-0.048643000
6	-4.464237000	1.799112000	-0.265619000
6	-5.492352000	0.686398000	-0.031029000
6	-6.941985000	1.144742000	-0.227616000
6	-7.975887000	0.033234000	-0.014068000
6	-9.423977000	0.502494000	-0.195256000
6	-10.462500000	-0.607170000	0.004955000
1	12.302996000	-1.192818000	1.734426000
1	13.923303000	-1.294717000	-2.882105000
1	15.552426000	-1.760406000	-1.044982000
1	14.712663000	-1.696269000	1.321957000
1	7.701084000	-0.886631000	2.446633000
1	5.342519000	-0.151772000	2.048487000
1	6.383785000	0.931633000	-1.965685000
1	8.718260000	0.199649000	-1.569273000
1	4.146530000	1.278714000	-1.245431000
1	1.842984000	1.979588000	2.341385000
1	-0.483159000	2.745334000	1.950920000

1	-0.292647000	1.228789000	-2.053455000
1	2.017861000	0.482159000	-1.668305000
1	-2.110606000	2.825288000	-1.347095000
1	-2.227412000	3.330717000	0.329631000
1	-2.888850000	0.990910000	0.978583000
1	-2.788538000	0.500970000	-0.700935000
1	-4.575890000	2.183647000	-1.287751000
1	-4.685693000	2.642744000	0.400901000
1	-5.372391000	0.290235000	0.985426000
1	-5.281181000	-0.150121000	-0.709443000
1	-7.057403000	1.555011000	-1.239202000
1	-7.154422000	1.972923000	0.460802000
1	-7.854629000	-0.385787000	0.993170000
1	-7.771770000	-0.789649000	-0.711237000
1	-9.542317000	0.930609000	-1.199086000
1	-9.628595000	1.319918000	0.508253000
1	-10.340046000	-1.041402000	1.005618000
1	-10.264130000	-1.420783000	-0.704690000
6	-11.909264000	-0.129651000	-0.164901000
1	-12.029993000	0.309981000	-1.163453000
1	-12.107574000	0.680776000	0.548449000
6	-12.951218000	-1.237422000	0.027701000
1	-12.757317000	-2.045257000	-0.689749000

1	-12.827637000	-1.681140000	1.024060000
6	-14.397049000	-0.754250000	-0.134139000
1	-14.519745000	-0.307624000	-1.129359000
1	-14.590730000	0.051908000	0.585322000
6	-15.441263000	-1.860289000	0.054510000
1	-15.317745000	-2.309849000	1.048432000
1	-15.251251000	-2.665378000	-0.667340000
6	-16.886963000	-1.374913000	-0.102196000
1	-17.010191000	-0.924457000	-1.094624000
1	-17.077629000	-0.572276000	0.620564000
6	-17.923409000	-2.486469000	0.085565000
1	-18.942536000	-2.107624000	-0.030880000
1	-17.781385000	-3.287442000	-0.646805000
1	-17.847223000	-2.933703000	1.081653000

D Compound (in Angstrom Å)

6	-14.490854000	-1.001619000	0.000201000
6	-13.254052000	-0.090959000	0.000354000
6	-11.927621000	-0.870383000	0.000146000
6	-10.683306000	0.033534000	0.000268000
6	-9.358636000	-0.747978000	0.000067000
6	-8.114895000	0.157430000	0.000082000

6	-6.795785000	-0.634707000	-0.000030000
6	-5.573257000	0.270179000	-0.000193000
8	-4.395351000	-0.601994000	-0.000257000
6	-3.125048000	-0.054663000	-0.000237000
6	-2.068734000	-0.979979000	0.000000000
6	-0.755872000	-0.536504000	-0.000001000
6	-0.474610000	0.844983000	-0.000252000
6	-1.537338000	1.761379000	-0.000480000
6	-2.858396000	1.322618000	-0.000463000
6	0.893957000	1.372478000	-0.000308000
8	1.204877000	2.568609000	-0.000593000
8	1.831568000	0.334488000	0.000006000
6	3.227604000	0.462588000	0.000066000
7	3.825532000	-0.738782000	0.000542000
6	5.167396000	-0.790420000	0.000628000
6	5.959905000	0.369183000	0.000241000
6	5.314068000	1.611065000	-0.000135000
6	3.923231000	1.676844000	-0.000252000
7	7.381475000	0.390267000	0.000345000
7	7.952611000	-0.754384000	-0.000267000
6	9.377510000	-0.740290000	-0.000046000
6	9.991994000	-1.999672000	-0.000980000
6	11.383512000	-2.097430000	-0.000875000

6	12.162468000	-0.936685000	0.000175000
6	11.546745000	0.323587000	0.001122000
6	10.159332000	0.427416000	0.001019000
1	-15.414534000	-0.419237000	0.000320000
1	-14.504326000	-1.647056000	0.882181000
1	-14.504340000	-1.646724000	-0.882021000
1	-13.284238000	0.566174000	0.876427000
1	-13.284296000	0.566537000	-0.875446000
1	-11.897088000	-1.528028000	-0.876676000
1	-11.897016000	-1.528376000	0.876706000
1	-10.714864000	0.690811000	0.877258000
1	-10.714936000	0.691137000	-0.876477000
1	-9.326116000	-1.404795000	-0.876670000
1	-9.325982000	-1.405027000	0.876624000
1	-8.148989000	0.813798000	0.877441000
1	-8.149071000	0.813921000	-0.877184000
1	-6.748828000	-1.284280000	-0.877586000
1	-6.748659000	-1.284243000	0.877543000
1	-5.551875000	0.906486000	0.889460000
1	-5.552081000	0.906362000	-0.889945000
1	-2.309628000	-2.032585000	0.000192000
1	0.060817000	-1.241564000	0.000197000
1	-1.312575000	2.818443000	-0.000671000

1	-3.659974000	2.044929000	-0.000629000
1	5.621196000	-1.767990000	0.001023000
1	5.915135000	2.508652000	-0.000332000
1	3.394415000	2.612301000	-0.000594000
1	9.360250000	-2.876298000	-0.001780000
1	11.856958000	-3.069630000	-0.001604000
1	13.241779000	-1.009602000	0.000264000
1	12.153177000	1.219424000	0.001945000
1	9.663711000	1.385953000	0.001733000

E Compound (in Angstrom Å)

8	0.011035000	-0.500536000	0.000438000
6	-1.134052000	0.415190000	-0.000019000
6	-2.389399000	-0.443465000	0.000137000
6	-3.678015000	0.397482000	-0.000069000
6	-4.954510000	-0.461201000	-0.000026000
6	-6.249313000	0.368773000	-0.000145000
6	-7.526022000	-0.489227000	-0.000163000
6	-8.822464000	0.338655000	-0.000246000
6	-10.098694000	-0.520049000	-0.000245000
6	-11.396058000	0.306418000	-0.000287000
6	-12.671650000	-0.553250000	-0.000221000

6	-13.969793000	0.272010000	-0.000210000
6	-15.244712000	-0.588676000	-0.000062000
6	-16.543609000	0.235463000	-0.000007000
6	-17.817853000	-0.625823000	0.000208000
6	-19.117921000	0.196841000	0.000285000
6	-20.384472000	-0.672127000	0.000533000
6	1.300297000	-0.000655000	0.000175000
6	1.618991000	1.365279000	-0.000393000
6	2.955686000	1.754179000	-0.000588000
6	3.984825000	0.799949000	-0.000217000
6	3.650011000	-0.568884000	0.000357000
6	2.321783000	-0.964215000	0.000545000
6	5.371509000	1.283597000	-0.000448000
8	5.713997000	2.470122000	-0.001139000
8	6.284108000	0.224778000	0.000230000
6	7.689926000	0.330210000	0.000203000
6	8.417267000	1.524713000	0.000925000
6	9.810668000	1.449494000	0.000985000
6	10.470266000	0.215123000	0.000362000
6	9.720874000	-0.976077000	-0.000346000
6	8.337006000	-0.915625000	-0.000423000
7	11.889594000	0.273195000	0.000511000
7	12.497821000	-0.852647000	-0.000060000

6	13.921209000	-0.782493000	-0.000048000
6	14.670103000	0.407064000	0.000345000
7	16.016478000	0.411844000	0.000335000
6	16.663355000	-0.779706000	-0.000075000
6	15.995037000	-2.004642000	-0.000492000
6	14.600852000	-2.005635000	-0.000486000
1	-1.088566000	1.049614000	-0.889998000
1	-1.088783000	1.050224000	0.889539000
1	-2.366837000	-1.094065000	0.877897000
1	-2.366813000	-1.094474000	-0.877319000
1	-3.687740000	1.054547000	-0.877475000
1	-3.687842000	1.054795000	0.877151000
1	-4.946249000	-1.118798000	0.876707000
1	-4.946194000	-1.118963000	-0.876634000
1	-6.256756000	1.026841000	-0.877036000
1	-6.256847000	1.026942000	0.876668000
1	-7.518424000	-1.147495000	0.876548000
1	-7.518356000	-1.147566000	-0.876818000
1	-8.830401000	0.996941000	-0.877026000
1	-8.830457000	0.997020000	0.876474000
1	-10.090540000	-1.178444000	0.876453000
1	-10.090514000	-1.178494000	-0.876906000
1	-11.404582000	0.964760000	-0.877047000

1	-11.404567000	0.964860000	0.876398000
1	-12.662889000	-1.211673000	0.876480000
1	-12.662941000	-1.211740000	-0.876873000
1	-13.978901000	0.930355000	-0.876972000
1	-13.978795000	0.930488000	0.876452000
1	-15.235370000	-1.247077000	0.876647000
1	-15.235507000	-1.247184000	-0.876693000
1	-16.553213000	0.893808000	-0.876790000
1	-16.553033000	0.893970000	0.876657000
1	-17.809074000	-1.284413000	0.876956000
1	-17.809271000	-1.284563000	-0.876429000
1	-19.126418000	0.854800000	-0.875673000
1	-19.126201000	0.854981000	0.876110000
1	-21.288576000	-0.059600000	0.000580000
1	-20.419035000	-1.316599000	0.882714000
1	-20.419253000	-1.316787000	-0.881502000
1	0.845291000	2.117421000	-0.000671000
1	3.219767000	2.802030000	-0.001032000
1	4.436174000	-1.307315000	0.000654000
1	2.041707000	-2.007132000	0.000977000
1	7.910867000	2.472264000	0.001317000
1	10.409358000	2.348748000	0.001526000
1	10.240596000	-1.921470000	-0.000829000

1	7.734574000	-1.812011000	-0.000962000
1	14.173431000	1.364042000	0.000672000
1	17.742887000	-0.727171000	-0.000062000
1	16.552538000	-2.930488000	-0.000819000
1	14.024599000	-2.919701000	-0.000804000

F Compound (in Angstrom Å)

6	14.838794000	0.624762000	0.097716000
6	13.442243000	1.244871000	0.253211000
6	12.302426000	0.234882000	0.034314000
6	10.900374000	0.848281000	0.187345000
6	9.761009000	-0.159504000	-0.040608000
6	8.360465000	0.458394000	0.112177000
6	7.225795000	-0.550666000	-0.135766000
6	5.846970000	0.074036000	0.018018000
8	4.866766000	-0.973111000	-0.262979000
6	3.508290000	-0.677377000	-0.209006000
6	2.646518000	-1.735800000	-0.531897000
6	1.271333000	-1.548950000	-0.506256000
6	0.723361000	-0.295758000	-0.159350000
6	1.598265000	0.759667000	0.130830000
6	2.981661000	0.576893000	0.122289000

7	-0.663242000	-0.013731000	-0.121973000
6	-1.556453000	-0.915510000	0.106985000
6	-2.990258000	-0.619567000	0.086435000
6	-3.919153000	-1.637278000	0.354010000
6	-5.295506000	-1.398020000	0.342664000
6	-5.737458000	-0.105284000	0.056114000
6	-4.833547000	0.929655000	-0.212822000
6	-3.470751000	0.674018000	-0.199499000
8	-7.093434000	0.309655000	0.017397000
6	-8.207694000	-0.505045000	0.141340000
8	-8.155206000	-1.726330000	0.305513000
6	-9.458522000	0.276119000	0.052411000
6	-10.678953000	-0.411139000	0.145498000
7	-11.872476000	0.209165000	0.077377000
6	-11.882424000	1.552045000	-0.087406000
6	-10.716451000	2.312677000	-0.188937000
6	-9.483030000	1.667588000	-0.118601000
1	15.624284000	1.365724000	0.260262000
1	14.975481000	0.209221000	-0.903964000
1	14.991815000	-0.185165000	0.815527000
1	13.329198000	2.072574000	-0.455516000
1	13.346448000	1.683389000	1.252583000
1	12.414602000	-0.593679000	0.743591000

1	12.398090000	-0.203971000	-0.965969000
1	10.792080000	1.680341000	-0.518379000
1	10.803884000	1.282377000	1.189556000
1	9.866917000	-0.992098000	0.664133000
1	9.856258000	-0.592225000	-1.043071000
1	8.261806000	1.298391000	-0.585313000
1	8.262896000	0.881286000	1.118905000
1	7.309399000	-1.388854000	0.560552000
1	7.308219000	-0.966437000	-1.143117000
1	5.709367000	0.900425000	-0.686493000
1	5.697094000	0.451679000	1.034427000
1	3.081888000	-2.684691000	-0.809863000
1	0.621673000	-2.366987000	-0.786532000
1	1.170860000	1.722890000	0.369927000
1	3.628628000	1.407084000	0.361668000
1	-1.290097000	-1.951590000	0.341948000
1	-3.566095000	-2.636898000	0.574947000
1	-5.997735000	-2.186861000	0.541974000
1	-5.218569000	1.915408000	-0.429008000
1	-2.755027000	1.455992000	-0.405906000
1	-10.690497000	-1.482816000	0.277211000
1	-12.859384000	2.012011000	-0.136809000
1	-10.775171000	3.383710000	-0.319689000

1	-8.557125000	2.216091000	-0.192109000
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G Compound (in Angstrom Å)

6	-13.283298000	-0.033812000	0.526323000
6	-11.910672000	0.619004000	0.712640000
6	-10.756278000	-0.240867000	0.185894000
6	-9.377051000	0.400487000	0.376933000
6	-8.231924000	-0.464379000	-0.161496000
6	-6.867248000	0.169755000	0.054821000
8	-5.886670000	-0.714074000	-0.493928000
6	-4.570268000	-0.382439000	-0.404439000
6	-3.671675000	-1.289085000	-0.985409000
6	-2.309201000	-1.053883000	-0.941890000
6	-1.796976000	0.100883000	-0.319819000
6	-2.706328000	1.017087000	0.218640000
6	-4.077272000	0.780081000	0.197519000
7	-0.433737000	0.422157000	-0.236667000
6	0.463088000	-0.486402000	-0.198766000
6	1.895497000	-0.170231000	-0.156097000
6	2.830555000	-1.211904000	-0.082693000
6	4.192542000	-0.943844000	-0.032912000
6	4.642565000	0.380051000	-0.058151000

6	3.711407000	1.426921000	-0.134608000
6	2.355524000	1.156947000	-0.182975000
6	6.085257000	0.740269000	-0.007067000
8	6.871241000	-0.375729000	0.107598000
8	6.515259000	1.863051000	-0.054947000
6	8.261909000	-0.276533000	0.184592000
6	8.875203000	-1.049381000	1.164960000
6	10.264466000	-1.065455000	1.253424000
6	11.031114000	-0.311023000	0.367947000
6	10.400910000	0.456771000	-0.609399000
6	9.011927000	0.479327000	-0.711740000
1	-14.084091000	0.603696000	0.910497000
1	-13.340086000	-0.991718000	1.052531000
1	-13.489936000	-0.225447000	-0.531219000
1	-11.747740000	0.828946000	1.776727000
1	-11.896880000	1.591343000	0.205561000
1	-10.915528000	-0.445753000	-0.880457000
1	-10.773246000	-1.216288000	0.688468000
1	-9.217286000	0.597662000	1.444744000
1	-9.362579000	1.378811000	-0.120033000
1	-8.366941000	-0.642986000	-1.233380000
1	-8.239868000	-1.445385000	0.325011000
1	-6.674447000	0.320277000	1.124808000

1	-6.807067000	1.146001000	-0.443388000
1	-4.074346000	-2.166669000	-1.476684000
1	-1.637045000	-1.753115000	-1.425399000
1	-2.313969000	1.919469000	0.671960000
1	-4.746582000	1.505899000	0.638663000
1	0.214625000	-1.555993000	-0.177594000
1	2.483805000	-2.240038000	-0.062740000
1	4.909286000	-1.751587000	0.024821000
1	4.078883000	2.445334000	-0.154759000
1	1.626704000	1.955292000	-0.240997000
1	8.258538000	-1.627619000	1.842133000
1	10.745011000	-1.667417000	2.016099000
1	12.112516000	-0.321399000	0.438200000
1	10.991759000	1.045809000	-1.301502000
1	8.521388000	1.081710000	-1.462589000

H Compound (in Angstrom Å)

6	-14.776023000	0.223987000	-0.181545000
6	-13.406316000	0.893647000	-0.323927000
6	-12.234797000	-0.071373000	-0.107762000
6	-10.859640000	0.591717000	-0.243317000
6	-9.689048000	-0.372789000	-0.021911000

6	-8.315198000	0.295553000	-0.148801000
6	-7.149656000	-0.672468000	0.083391000
6	-5.795299000	0.008629000	-0.029586000
8	-4.789664000	-0.978154000	0.213116000
6	-3.480761000	-0.607280000	0.200313000
6	-2.556301000	-1.620505000	0.493294000
6	-1.199469000	-1.351931000	0.505991000
6	-0.718559000	-0.057200000	0.230843000
6	-1.653197000	0.951484000	-0.024757000
6	-3.018797000	0.687172000	-0.059957000
7	0.635816000	0.308342000	0.240066000
6	1.556356000	-0.532210000	-0.038275000
6	2.979672000	-0.179405000	0.019620000
6	3.943591000	-1.139512000	-0.318140000
6	5.298104000	-0.836243000	-0.271419000
6	5.709900000	0.443456000	0.115506000
6	4.750105000	1.408693000	0.456753000
6	3.402211000	1.102438000	0.410393000
6	7.142105000	0.834600000	0.190935000
8	7.541392000	1.912089000	0.553611000
8	7.948458000	-0.197253000	-0.204615000
6	9.336432000	-0.144818000	-0.205893000
7	9.873345000	-1.341199000	-0.043460000

6	11.205802000	-1.433411000	-0.082394000
6	12.042040000	-0.341532000	-0.285575000
6	11.451135000	0.907754000	-0.458571000
6	10.066952000	1.025943000	-0.422931000
1	-15.588862000	0.937048000	-0.343857000
1	-14.904708000	-0.204367000	0.817424000
1	-14.896626000	-0.587486000	-0.906084000
1	-13.327910000	1.720914000	0.391862000
1	-13.322106000	1.345254000	-1.319849000
1	-12.311425000	-0.898291000	-0.825676000
1	-12.321331000	-0.525639000	0.887870000
1	-10.785766000	1.419854000	0.473348000
1	-10.772592000	1.044007000	-1.239682000
1	-9.757473000	-1.198443000	-0.741397000
1	-9.777782000	-0.827952000	0.972603000
1	-8.251127000	1.123762000	0.568510000
1	-8.224430000	0.746846000	-1.145082000
1	-7.190268000	-1.492731000	-0.640910000
1	-7.228917000	-1.125067000	1.077357000
1	-5.705532000	0.818047000	0.706282000
1	-5.658634000	0.440339000	-1.029562000
1	-2.934895000	-2.609214000	0.723011000
1	-0.507426000	-2.143669000	0.768278000

1	-1.284818000	1.953306000	-0.210224000
1	-3.708163000	1.491696000	-0.276566000
1	1.337248000	-1.562161000	-0.350042000
1	3.626084000	-2.132957000	-0.617680000
1	6.039487000	-1.581300000	-0.526185000
1	5.088627000	2.392425000	0.757222000
1	2.650768000	1.836354000	0.672181000
1	11.614726000	-2.429951000	0.055591000
1	13.117370000	-0.467332000	-0.307341000
1	12.059899000	1.789672000	-0.622065000
1	9.572894000	1.977187000	-0.536150000

I Compound (in Angstrom Å)

6	13.056379000	-0.935373000	0.197218000
6	11.810075000	-0.075689000	-0.059878000
6	10.492380000	-0.834898000	0.170668000
6	9.240957000	0.024871000	-0.075131000
6	7.927565000	-0.744249000	0.150215000
6	6.700061000	0.126566000	-0.069372000
8	5.525825000	-0.720954000	0.156536000
6	4.253831000	-0.187897000	0.045553000
6	3.199835000	-1.085753000	0.278744000

6	1.886151000	-0.651829000	0.194404000
6	1.599030000	0.690527000	-0.123016000
6	2.660115000	1.578999000	-0.353799000
6	3.982574000	1.150474000	-0.273633000
6	0.228181000	1.210871000	-0.221790000
8	-0.074307000	2.383306000	-0.466428000
8	-0.717213000	0.208071000	-0.002114000
6	-2.120571000	0.371209000	-0.020403000
6	-2.824142000	-0.838427000	-0.085635000
6	-4.210633000	-0.831745000	-0.072659000
6	-4.916554000	0.385025000	0.006458000
6	-4.187838000	1.583031000	0.071363000
6	-2.791370000	1.593601000	0.059837000
6	-6.379583000	0.418823000	0.022212000
7	-7.099060000	-0.647387000	-0.062673000
6	-8.512549000	-0.613664000	0.019717000
6	-9.232475000	-1.520835000	-0.775310000
6	-10.625119000	-1.542873000	-0.733409000
6	-11.319340000	-0.680185000	0.122676000
6	-10.607327000	0.204556000	0.937606000
6	-9.212874000	0.242808000	0.888875000
1	13.972986000	-0.367116000	0.026919000
1	13.077849000	-1.806335000	-0.462725000

1	13.077746000	-1.299961000	1.227335000
1	11.832438000	0.301585000	-1.088119000
1	11.835078000	0.806239000	0.589675000
1	10.471265000	-1.217568000	1.197590000
1	10.462443000	-1.713388000	-0.484259000
1	9.267364000	0.412692000	-1.100119000
1	9.272429000	0.899221000	0.585625000
1	7.895486000	-1.141730000	1.167703000
1	7.873494000	-1.600724000	-0.526384000
1	6.670438000	0.519482000	-1.089977000
1	6.681143000	0.965527000	0.632488000
1	3.443136000	-2.109195000	0.522704000
1	1.074148000	-1.338785000	0.373685000
1	2.432487000	2.607161000	-0.596405000
1	4.781414000	1.852130000	-0.457216000
1	-2.266046000	-1.761256000	-0.144832000
1	-4.772696000	-1.752707000	-0.123427000
1	-4.716758000	2.526273000	0.131091000
1	-2.243132000	2.517519000	0.094049000
1	-6.834502000	1.412771000	0.098206000
1	-8.677882000	-2.190840000	-1.416642000
1	-11.169289000	-2.238392000	-1.358562000
1	-12.399802000	-0.707797000	0.164161000

1	-11.136443000	0.859137000	1.617849000
1	-8.666352000	0.906734000	1.545294000

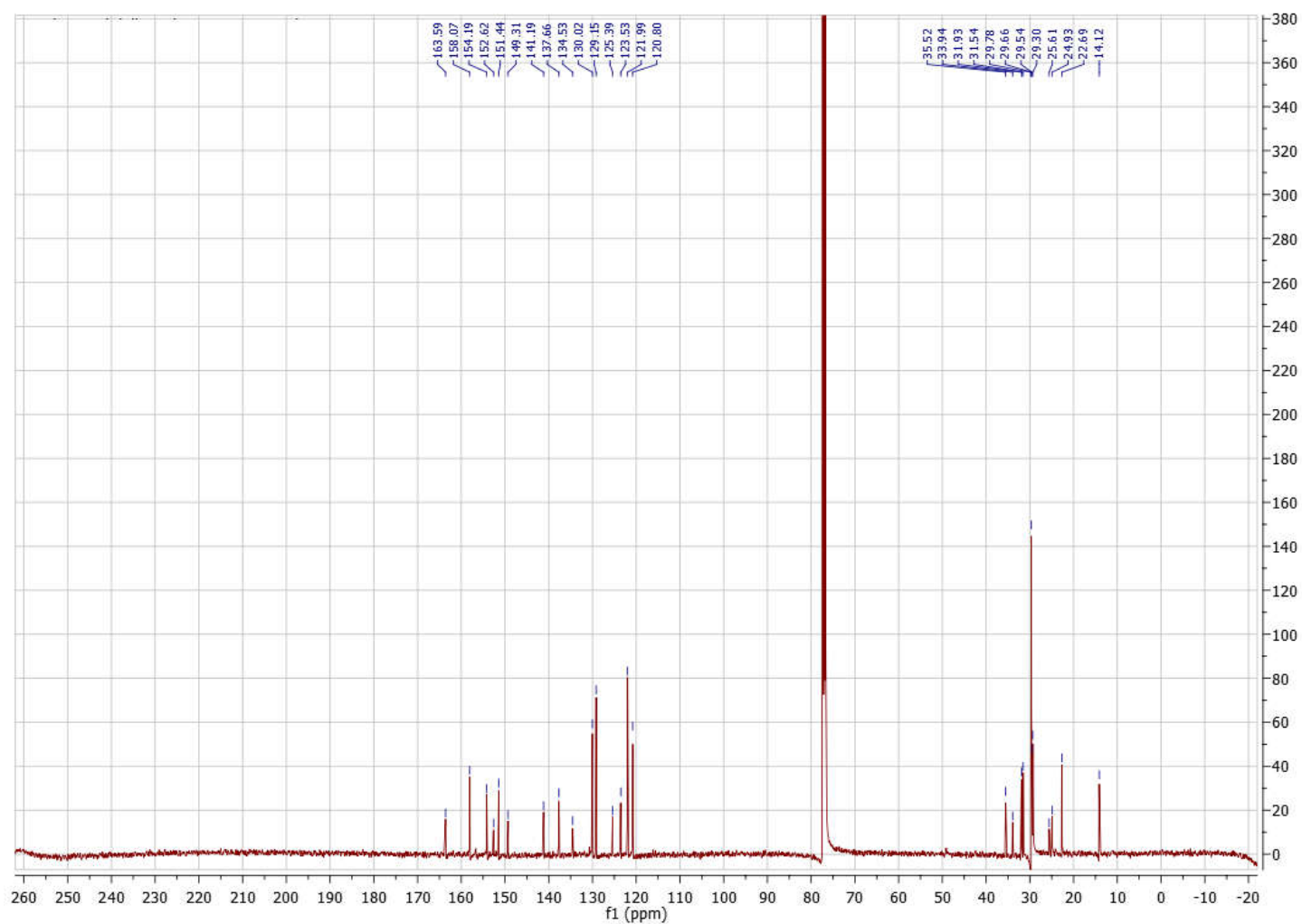


Figure S2. ¹³C NMR of Pyridin-2-yl 4-[4-(tetradecylphenyl)iminomethyl]benzoate (C).