

Silica vanadic acid [SiO₂–VO(OH)₂] as an efficient heterogeneous catalyst for the synthesis of 1,2-dihydro-1-aryl-3*H*-naphth[1,2-*e*][1,3]oxazin-3-one and 2,4,6-triarylpyridine derivatives *via* anomeric based oxidation

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† Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/b000000x/

Table S1. Electronic energy, zero point energy and corrected electronic energy at B3LYP/SVP level of theory

Compounds	E _{el}	ZPE	E ₀
15-cis	-941.9617862	0.3542272	-941.607559
15-trans	-941.9622843	0.354279	-941.608006
16	-2703.6437212	0.4124422	-2703.231279
4	-940.7921804	0.3316914	-940.460489
TS-1	-2704.7504257	0.427422	-2704.323004
TS-2	-2704.7536123	0.4264023	-2704.327210
H₂	-1.1737901	0.0099631	-1.163827
(OH)₃SiOV(O)(OH)₂	-1762.835353	0.07878	-1762.756573

Figure S1. Total Energy along IRC of TS-1

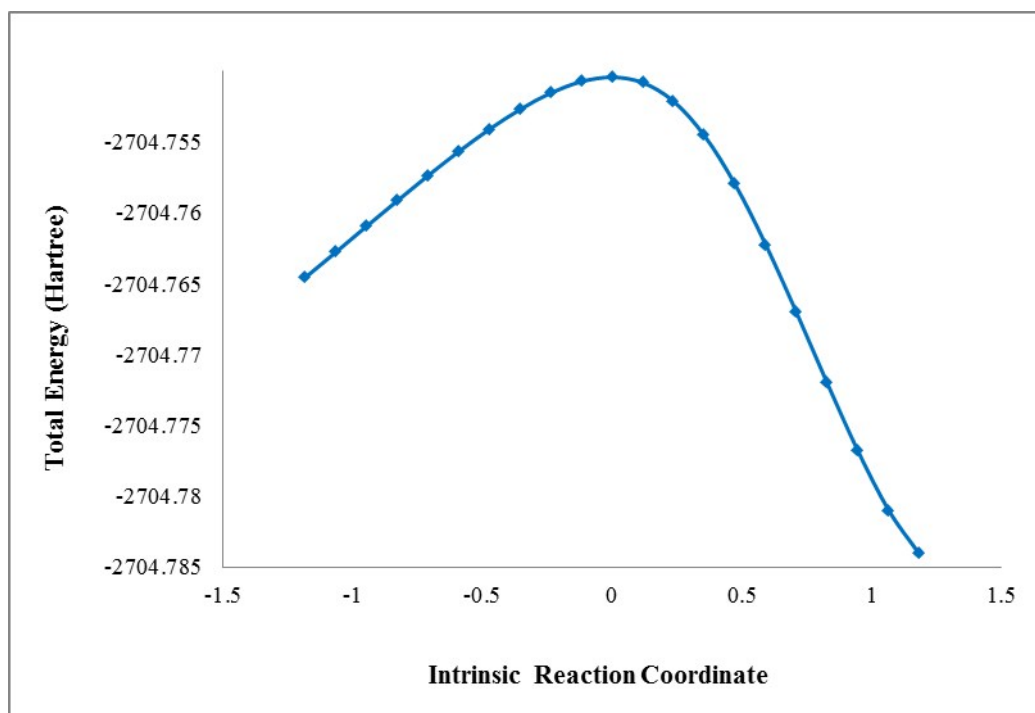


Figure S2. Total Energy along IRC of TS-2

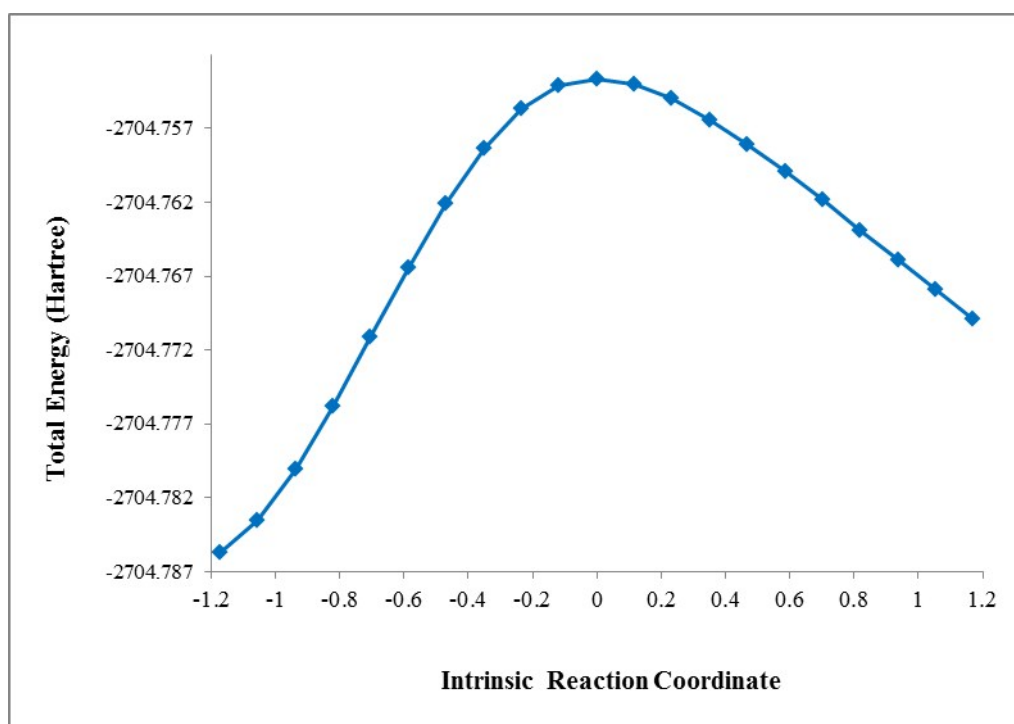


Table S2. Cartesian atomic coordinates of calculated structures at B3LYP/SVP level of theory

“15-cis”			
C	-0.977259000	1.111581000	-0.124002000
C	-1.065232000	1.120409000	1.225420000
C	-1.023319000	-1.306018000	1.291430000
C	-0.934705000	-1.367614000	-0.056461000
H	-1.001457000	2.063654000	-0.656786000
H	-0.924613000	-2.347497000	-0.536693000
C	-1.126336000	2.365212000	2.034452000
C	-1.884760000	2.417574000	3.219732000
C	-0.429579000	3.522886000	1.639852000
C	-1.952769000	3.589694000	3.976984000
C	-0.502198000	4.694419000	2.394187000
C	-1.263537000	4.733974000	3.567317000
H	-2.450492000	1.538330000	3.536122000
H	0.191102000	3.493498000	0.741963000
H	-2.555616000	3.609910000	4.888713000
H	0.050299000	5.580308000	2.070290000
H	-1.315216000	5.650681000	4.160119000
C	-1.040682000	-2.505859000	2.167780000
C	-1.799313000	-2.519975000	3.353876000
C	-0.299948000	-3.656673000	1.838699000
C	-1.824061000	-3.648945000	4.176494000
C	-0.329320000	-4.785455000	2.658392000
C	-1.090687000	-4.787363000	3.832120000
H	-2.398322000	-1.645944000	3.619125000
H	0.321201000	-3.654150000	0.940630000
H	-2.427665000	-3.640559000	5.087897000
H	0.257156000	-5.666613000	2.385320000
H	-1.108402000	-5.670276000	4.476018000
N	-1.146291000	-0.075732000	1.949355000
H	-0.812184000	-0.043895000	2.906403000
C	-0.923282000	-0.151245000	-0.958444000
H	0.014764000	-0.151184000	-1.551920000
C	-2.056239000	-0.197844000	-1.992255000
C	-1.777181000	-0.212289000	-3.365748000
C	-3.398819000	-0.226278000	-1.582541000
C	-2.809068000	-0.254293000	-4.309780000
C	-4.432471000	-0.268567000	-2.520539000
C	-4.141048000	-0.282755000	-3.889369000
H	-0.735517000	-0.190896000	-3.701225000
H	-3.631656000	-0.215905000	-0.514417000
H	-2.570155000	-0.265019000	-5.376755000
H	-5.472269000	-0.290606000	-2.182916000
H	-4.949797000	-0.315837000	-4.624113000
“15-trans”			
C	0.696750000	1.240171000	-0.914835000
C	-0.555251000	1.214572000	-0.404442000
C	-0.556701000	-1.213932000	-0.404572000
C	0.695255000	-1.240984000	-0.914990000
H	1.144339000	2.205656000	-1.156461000
H	1.141716000	-2.206967000	-1.156709000
C	-1.337577000	2.438693000	-0.092469000
C	-2.732752000	2.470040000	-0.279402000
C	-0.705347000	3.596515000	0.398434000
C	-3.468445000	3.623195000	0.004719000

C	-1.440693000	4.749201000	0.677412000
C	-2.825996000	4.768428000	0.482782000
H	-3.241649000	1.589815000	-0.678679000
H	0.371091000	3.580312000	0.581558000
H	-4.549646000	3.628262000	-0.156702000
H	-0.929845000	5.635842000	1.061956000
H	-3.401379000	5.670241000	0.706776000
C	-1.340461000	-2.437137000	-0.092608000
C	-2.735661000	-2.466884000	-0.279613000
C	-0.709561000	-3.595675000	0.398318000
C	-3.472690000	-3.619172000	0.004560000
C	-1.446246000	-4.747495000	0.677342000
C	-2.831567000	-4.765118000	0.482701000
H	-3.243513000	-1.586070000	-0.678925000
H	0.366892000	-3.580695000	0.581451000
H	-4.553894000	-3.623018000	-0.156876000
H	-0.936439000	-5.634717000	1.061927000
H	-3.407999000	-5.666257000	0.706713000
N	-1.217089000	0.000708000	-0.185887000
H	-1.943307000	0.001093000	0.521627000
C	1.512669000	-0.000878000	-1.210967000
H	1.782827000	-0.000942000	-2.286603000
C	2.849730000	-0.001715000	-0.456685000
C	2.878852000	-0.002249000	0.947041000
C	4.068304000	-0.001857000	-1.149420000
C	4.092367000	-0.002910000	1.638238000
C	5.286968000	-0.002512000	-0.461982000
C	5.302524000	-0.003037000	0.935096000
H	1.935753000	-0.002138000	1.500032000
H	4.062428000	-0.001457000	-2.243887000
H	4.095619000	-0.003315000	2.731752000
H	6.226816000	-0.002613000	-1.020813000
H	6.252994000	-0.003548000	1.475129000

“16”

C	3.121135000	0.873650000	-0.226593000
C	1.786160000	1.221131000	-0.474246000
C	1.160290000	-1.027878000	-0.540234000
C	2.480102000	-1.432210000	-0.290900000
C	1.375095000	2.646831000	-0.595567000
C	0.370719000	3.023688000	-1.505208000
C	1.991926000	3.647188000	0.177866000
C	0.002253000	4.362484000	-1.643657000
C	1.617387000	4.985342000	0.043577000
C	0.623595000	5.348179000	-0.870418000
C	0.073925000	-2.021673000	-0.739731000
C	-0.954524000	-1.774315000	-1.667020000
C	0.044244000	-3.218654000	-0.002674000
C	-1.993458000	-2.688239000	-1.839798000
C	-0.993888000	-4.135379000	-0.179686000
C	-2.017496000	-3.870116000	-1.093481000
N	0.835442000	0.277707000	-0.620439000
C	3.491800000	-0.475904000	-0.122937000
C	4.900643000	-0.874558000	0.131645000
C	5.197979000	-1.992333000	0.933574000
C	5.970177000	-0.144611000	-0.419890000
C	6.520738000	-2.364963000	1.179074000
C	7.292710000	-0.521418000	-0.179229000
C	7.573161000	-1.632004000	0.622460000
H	3.868837000	1.658836000	-0.116861000

H	2.719660000	-2.495389000	-0.279783000
H	-0.113602000	2.259562000	-2.114752000
H	2.752243000	3.374487000	0.913276000
H	-0.773520000	4.637763000	-2.362623000
H	2.099111000	5.746936000	0.661865000
H	0.332354000	6.396135000	-0.977916000
H	-0.935091000	-0.856192000	-2.256752000
H	0.815358000	-3.416549000	0.745266000
H	-2.801442000	-2.462850000	-2.537698000
H	-1.013977000	-5.051129000	0.416513000
H	-2.845880000	-4.571571000	-1.213433000
H	-0.738376000	0.689545000	-0.314643000
H	4.385469000	-2.560043000	1.392587000
H	5.764692000	0.711624000	-1.066360000
H	6.730228000	-3.229430000	1.814037000
H	8.108598000	0.052338000	-0.625939000
H	8.608539000	-1.925409000	0.812671000
Si	-4.829206000	-0.557960000	-0.170970000
O	-3.959980000	-0.120506000	1.187490000
V	-2.374957000	0.612208000	1.534735000
O	-2.545576000	2.102415000	2.501158000
O	-1.437703000	-0.351503000	2.344955000
O	-1.686958000	0.962504000	-0.039669000
O	-6.377986000	0.006733000	-0.036614000
O	-4.030768000	0.047121000	-1.477731000
O	-4.968646000	-2.193191000	-0.329376000
H	-3.008289000	2.835087000	2.065316000
H	-6.489549000	0.942654000	0.162788000
H	-3.154618000	0.412691000	-1.254625000
H	-5.673039000	-2.596422000	0.191533000

“4”

C	0.771692000	1.197908000	0.007969000
C	-0.633333000	1.160973000	-0.008723000
C	-0.633416000	-1.160952000	0.008642000
C	0.771604000	-1.197984000	-0.008041000
H	1.297814000	2.152198000	0.015818000
H	1.297667000	-2.152304000	-0.015842000
C	-1.450689000	2.409132000	-0.020832000
C	-2.791088000	2.366904000	0.404975000
C	-0.926267000	3.640857000	-0.453165000
C	-3.575111000	3.520755000	0.412713000
C	-1.713236000	4.794586000	-0.450927000
C	-3.040044000	4.740678000	-0.014441000
H	-3.200320000	1.410504000	0.732800000
H	0.100173000	3.702093000	-0.820635000
H	-4.612023000	3.468417000	0.755164000
H	-1.288363000	5.739639000	-0.799147000
H	-3.655254000	5.644187000	-0.011106000
C	-1.450897000	-2.409038000	0.020793000
C	-2.791360000	-2.366618000	-0.404788000
C	-0.926554000	-3.640871000	0.452942000
C	-3.575527000	-3.520378000	-0.412495000
C	-1.713662000	-4.794499000	0.450735000
C	-3.040541000	-4.740397000	0.014465000
H	-3.200545000	-1.410132000	-0.732417000
H	0.099939000	-3.702289000	0.820226000
H	-4.612485000	-3.467880000	-0.754785000
H	-1.288864000	-5.739639000	0.798807000
H	-3.655841000	-5.643845000	0.011144000

N	-1.301470000	0.000037000	-0.000040000
C	1.500400000	-0.000063000	-0.000024000
C	2.988116000	-0.000117000	0.000019000
C	3.710249000	0.941490000	0.756532000
C	3.710199000	-0.941789000	-0.756475000
C	5.106614000	0.939700000	0.758663000
C	5.106555000	-0.940102000	-0.758578000
C	5.810689000	-0.000219000	0.000047000
H	3.171691000	1.667069000	1.370541000
H	3.171572000	-1.667317000	-1.370485000
H	5.647631000	1.673224000	1.361973000
H	5.647542000	-1.673659000	-1.361875000
H	6.903583000	-0.000257000	0.000054000

“TS-1”

C	-2.937806000	0.966428000	0.100514000
C	-3.268294000	-0.358345000	0.235198000
C	-1.186718000	-0.995104000	-0.818843000
C	-0.842168000	0.326784000	-0.961467000
C	-4.546129000	-0.841507000	0.807875000
C	-5.183414000	-1.986291000	0.292360000
C	-5.148198000	-0.159749000	1.881473000
C	-6.388505000	-2.435476000	0.835506000
C	-6.353876000	-0.609923000	2.420759000
C	-6.977426000	-1.748830000	1.901096000
C	-0.372652000	-2.131970000	-1.301534000
C	-0.985389000	-3.237117000	-1.925069000
C	1.022514000	-2.130142000	-1.122445000
C	-0.216304000	-4.315074000	-2.364831000
C	1.787524000	-3.215806000	-1.557782000
C	1.170466000	-4.305817000	-2.179646000
N	-2.373004000	-1.305271000	-0.197098000
C	-1.643901000	1.376767000	-0.385764000
C	-1.479798000	2.771798000	-0.926344000
C	-0.251642000	3.452435000	-0.860078000
C	-2.559633000	3.386291000	-1.583598000
C	-0.114687000	4.714293000	-1.439981000
C	-2.418541000	4.652211000	-2.160300000
C	-1.194629000	5.320475000	-2.091129000
H	-3.656796000	1.723674000	0.410779000
H	0.072711000	0.577923000	-1.496171000
H	-4.754884000	-2.515449000	-0.562881000
H	-4.652829000	0.712710000	2.312367000
H	-6.874144000	-3.320384000	0.417208000
H	-6.803286000	-0.073891000	3.260128000
H	-7.919960000	-2.101205000	2.326951000
H	-2.064743000	-3.239825000	-2.102512000
H	1.515807000	-1.299547000	-0.612867000
H	-0.700085000	-5.160149000	-2.861168000
H	2.865799000	-3.199394000	-1.380755000
H	1.771788000	-5.152539000	-2.520708000
H	-2.562911000	-2.281907000	0.001764000
H	-0.862760000	1.709062000	1.054381000
H	0.597603000	3.021342000	-0.325003000
H	-3.514436000	2.862451000	-1.669060000
H	0.846323000	5.230031000	-1.370858000
H	-3.269481000	5.111895000	-2.669503000
H	-1.082181000	6.310586000	-2.540290000
O	3.454223000	-0.016684000	0.205595000
V	2.591170000	1.047498000	1.389455000

O	0.983152000	0.587179000	1.534151000
O	2.633485000	2.758274000	0.820286000
O	3.355709000	0.908463000	2.787857000
H	-0.090412000	1.274342000	1.336247000
H	3.072238000	3.421589000	1.370682000
Si	4.877219000	-0.872261000	0.297873000
O	5.923297000	-0.297984000	-0.844449000
H	5.867765000	0.649846000	-1.009917000
O	5.460424000	-0.801462000	1.840398000
H	4.922032000	-0.250287000	2.438949000
O	4.664805000	-2.472576000	-0.094221000
H	4.744386000	-3.054458000	0.671509000

“TS-2”

C	-2.601309000	0.283520000	0.053584000
C	-1.759735000	1.182255000	0.657459000
C	-0.395590000	-0.618196000	1.488766000
C	-1.200950000	-1.533167000	0.860213000
C	-1.946814000	2.649449000	0.602888000
C	-1.723101000	3.449730000	1.738385000
C	-2.339164000	3.264830000	-0.599439000
C	-1.905292000	4.832231000	1.676476000
C	-2.519717000	4.647824000	-0.657109000
C	-2.306553000	5.434169000	0.479573000
C	0.766420000	-0.973586000	2.333884000
C	0.969137000	-0.336367000	3.573161000
C	1.694042000	-1.934210000	1.897239000
C	2.069837000	-0.667191000	4.364182000
C	2.802297000	-2.249129000	2.685338000
C	2.989159000	-1.624399000	3.920953000
N	-0.667556000	0.720396000	1.346224000
C	-2.241973000	-1.108032000	-0.046665000
C	-3.278706000	-2.120953000	-0.444858000
C	-2.901170000	-3.346189000	-1.021317000
C	-4.640347000	-1.887515000	-0.195581000
C	-3.857603000	-4.309095000	-1.340948000
C	-5.600303000	-2.852342000	-0.518383000
C	-5.213251000	-4.065100000	-1.091239000
H	-3.482968000	0.655868000	-0.466958000
H	-1.017934000	-2.595546000	1.019241000
H	-1.428695000	2.983511000	2.681884000
H	-2.460447000	2.656623000	-1.497991000
H	-1.739224000	5.441569000	2.568298000
H	-2.814064000	5.115160000	-1.599924000
H	-2.447045000	6.516918000	0.431491000
H	0.247403000	0.403981000	3.927659000
H	1.592145000	-2.393681000	0.912441000
H	2.211276000	-0.176032000	5.330222000
H	3.534537000	-2.966970000	2.310291000
H	3.859061000	-1.871907000	4.534527000
H	0.116200000	1.361778000	1.471559000
H	-1.847531000	-3.529967000	-1.246117000
H	-4.955228000	-0.953968000	0.275166000
H	-3.545442000	-5.252029000	-1.796868000
H	-6.655477000	-2.652951000	-0.314901000
H	-5.963304000	-4.818184000	-1.345437000
Si	3.787837000	-0.885163000	-1.301125000
O	2.704501000	-0.004643000	-2.199649000
V	1.391923000	1.144273000	-1.755875000
O	1.560506000	2.683403000	-2.652965000

O	-0.096521000	0.462599000	-2.100856000
O	1.572461000	1.422565000	-0.172510000
O	5.196999000	-1.075536000	-2.144852000
O	4.021547000	-0.136192000	0.146339000
O	3.230468000	-2.422072000	-1.006691000
H	1.962433000	3.433984000	-2.193344000
H	-0.871602000	-0.486906000	-1.822157000
H	5.537417000	-0.285389000	-2.579737000
H	3.291973000	0.464614000	0.380647000
H	3.312831000	-3.027974000	-1.752926000
H	-1.482929000	-1.143496000	-1.499666000

“H₂”

H	0.000000000	0.000000000	0.380307000
H	0.000000000	0.000000000	-0.380307000

“(OH)₃SiOV(O)(OH)₂”

Si	-1.749341000	-0.007453000	-0.027365000
O	-0.198909000	-0.025304000	-0.690287000
V	1.441722000	0.004611000	-0.054313000
O	2.357054000	-1.386983000	-0.645445000
H	2.710978000	-2.061691000	-0.047682000
O	2.261548000	1.499706000	-0.514145000
H	2.512684000	2.171671000	0.136556000
O	1.325668000	-0.069681000	1.516834000
O	-2.744583000	-0.943552000	-0.943381000
H	-2.509253000	-1.871215000	-1.057784000
O	-1.641796000	-0.559321000	1.515673000
H	-0.799471000	-0.393532000	1.964725000
O	-2.343681000	1.524632000	-0.048929000
H	-2.706175000	1.837091000	-0.886073000

Fig S3. The IR spectrum of 2,6-bis(4-methoxyphenyl)-4-(p-tolyl)pyridine (Table 3, entry 6)

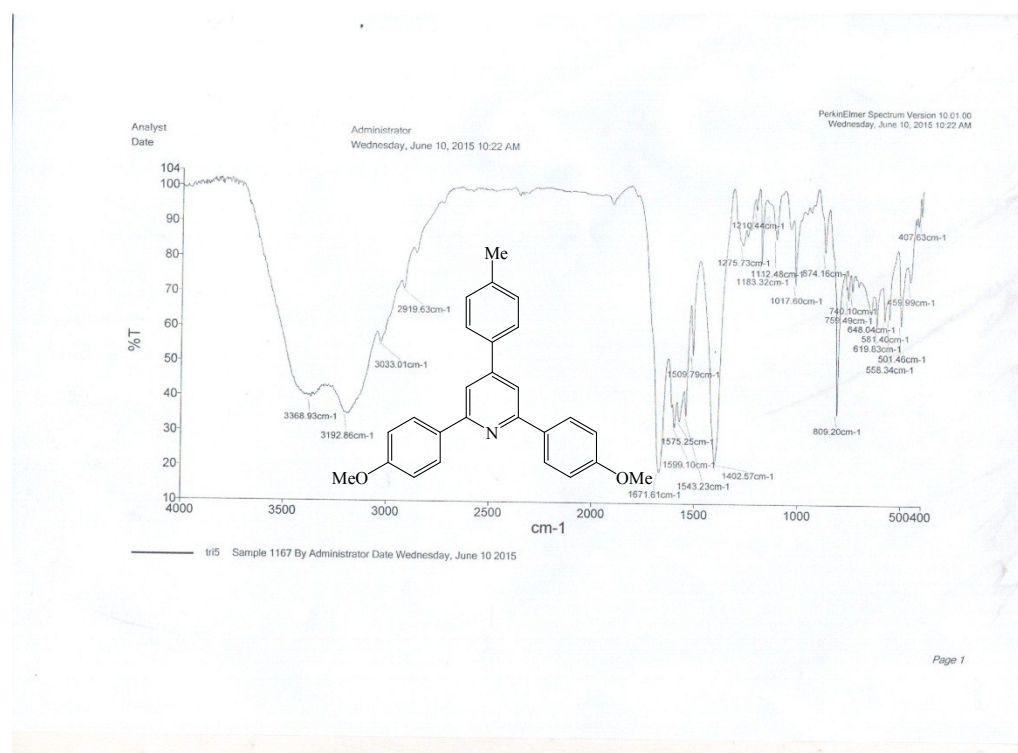


Fig S4. The ^1H NMR spectrum of 2,6-bis(4-methoxyphenyl)-4-(p-tolyl)pyridine (Table 3, entry 6)

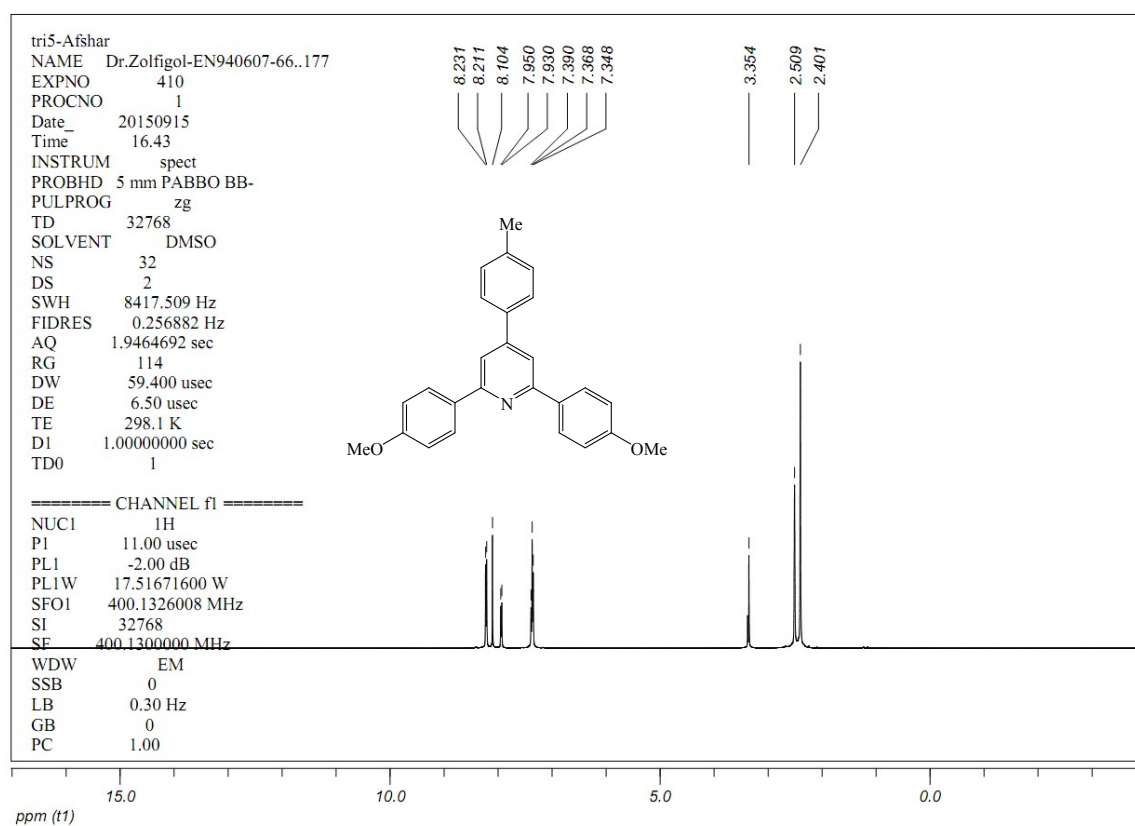


Fig S5. The ^1H NMR spectrum of 2,6-bis(4-methoxyphenyl)-4-(p-tolyl)pyridine (Table 3, entry 6)

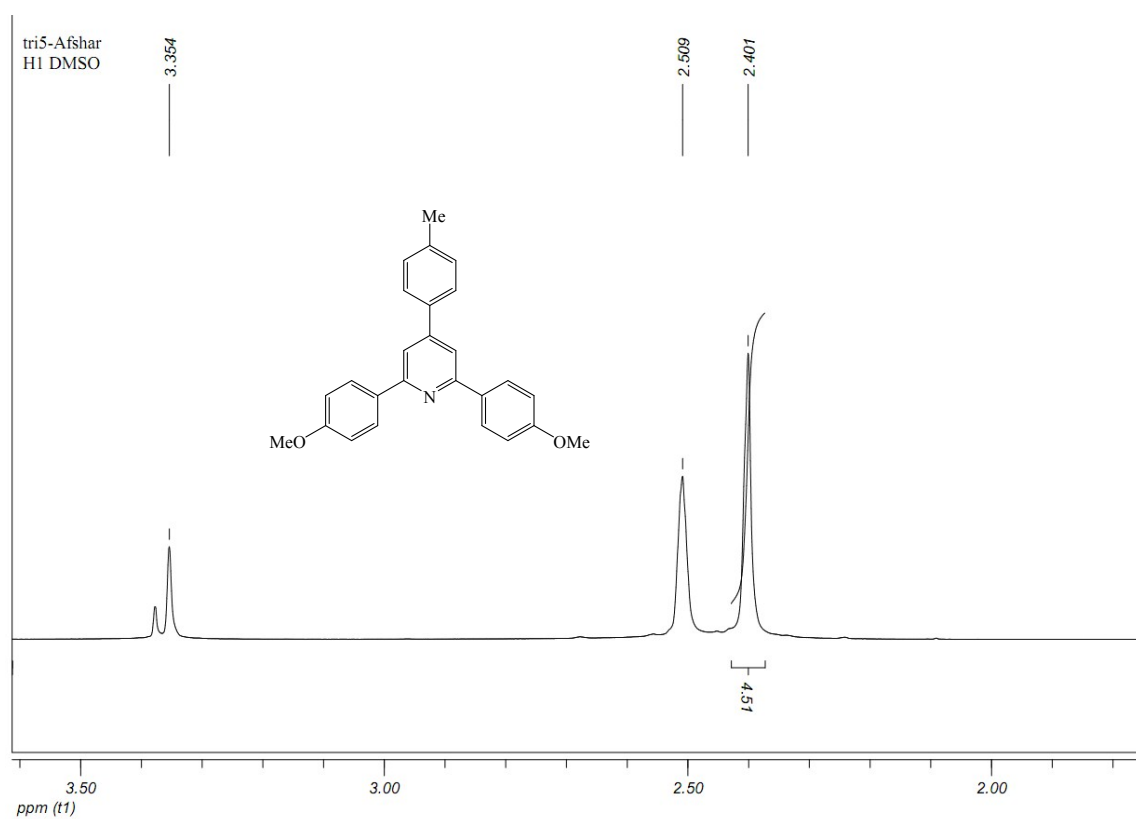


Fig S6. The ^1H NMR spectrum of 2,6-bis(4-methoxyphenyl)-4-(p-tolyl)pyridine (Table 3, entry 6)

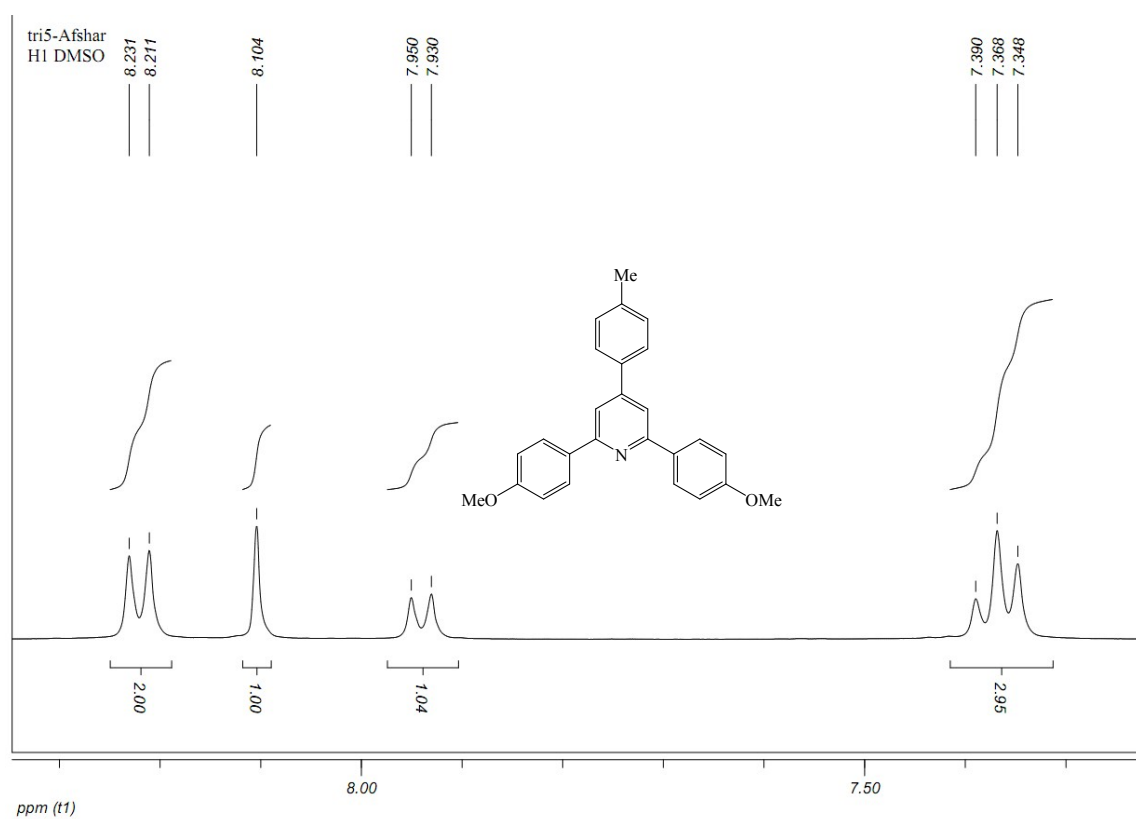


Fig S7. The ^{13}C NMR spectrum of 2,6-bis(4-methoxyphenyl)-4-(p-tolyl)pyridine (Table 3, entry 6)

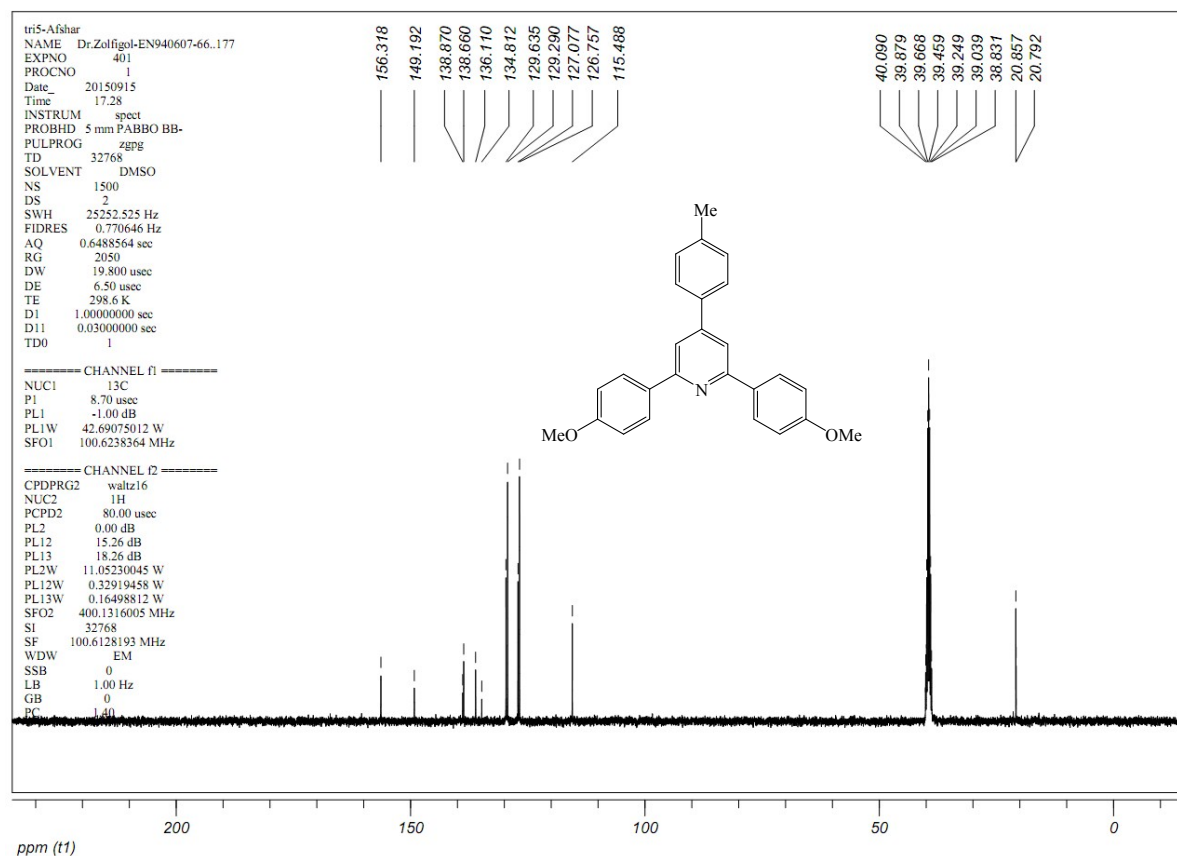


Fig S8. The IR spectrum of 4-(4-nitrophenyl)-2,6-di-*p*-tolylpyridine (Table 3, entry 8)

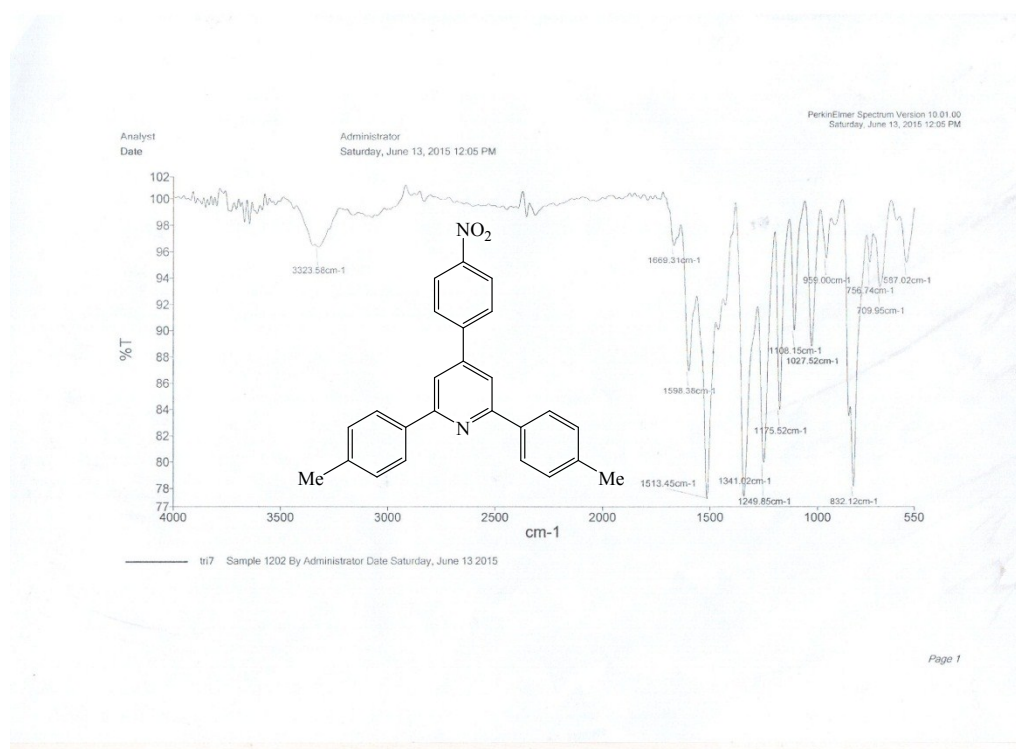


Fig S9. The ^1H NMR spectrum of 4-(4-nitrophenyl)-2,6-di-*p*-tolylpyridine (Table 3, entry 8)

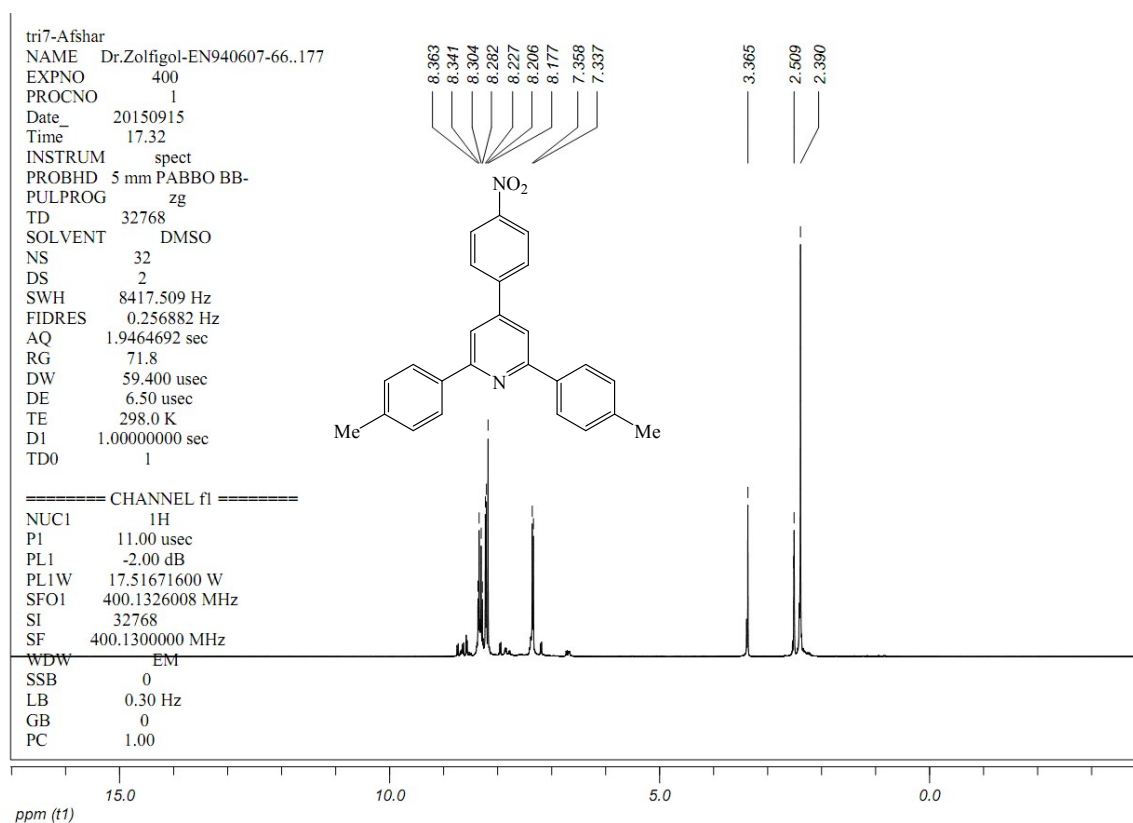


Fig S10. The ^1H NMR spectrum of 4-(4-nitrophenyl)-2,6-di-*p*-tolylpyridine (Table 3, entry 8)

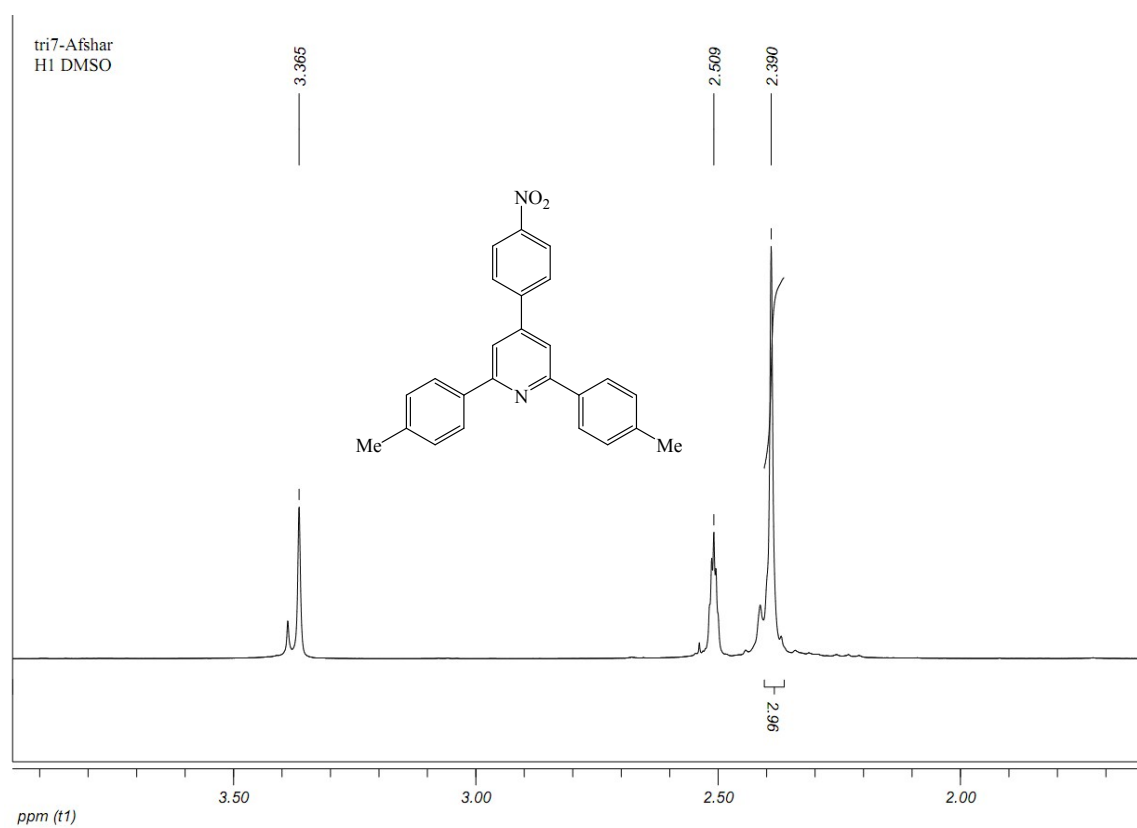


Fig S11. The ^1H NMR spectrum of 4-(4-nitrophenyl)-2,6-di-*p*-tolylpyridine (Table 3, entry 8)

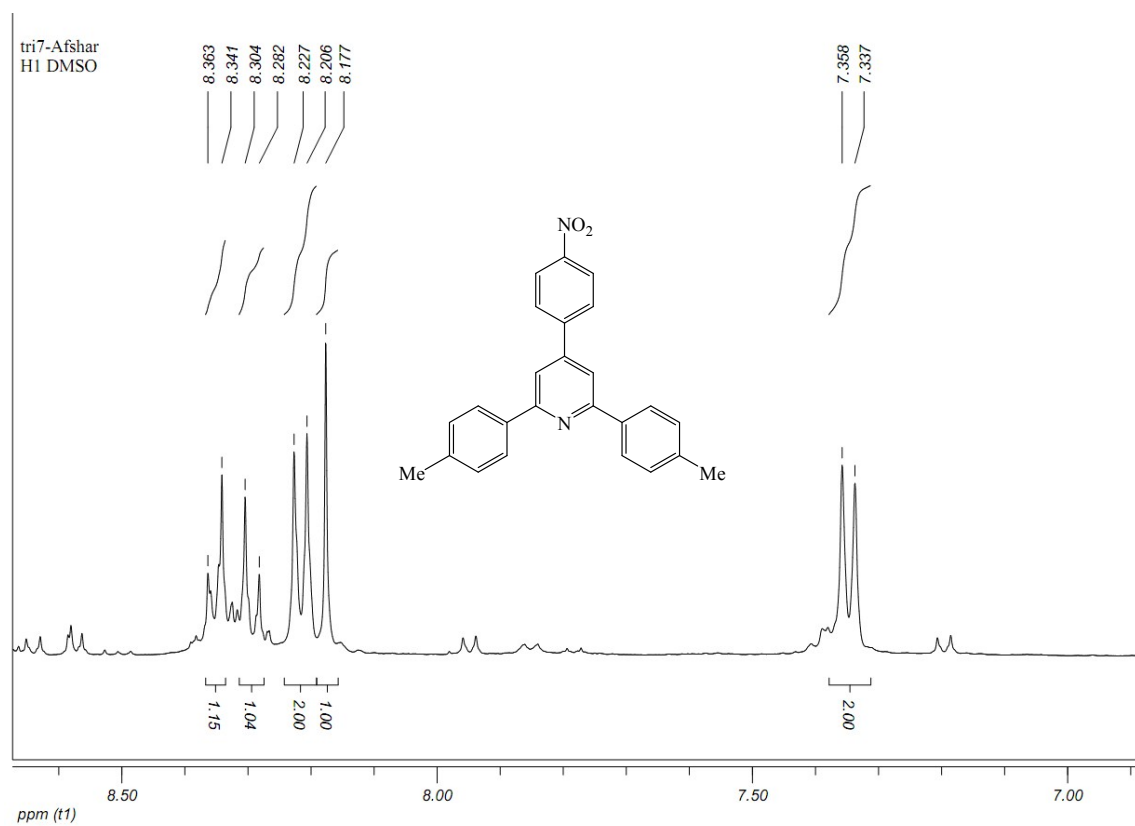


Fig S12. The ^{13}C NMR spectrum of 4-(4-nitrophenyl)-2,6-di-*p*-tolylpyridine (Table 3, entry 8)

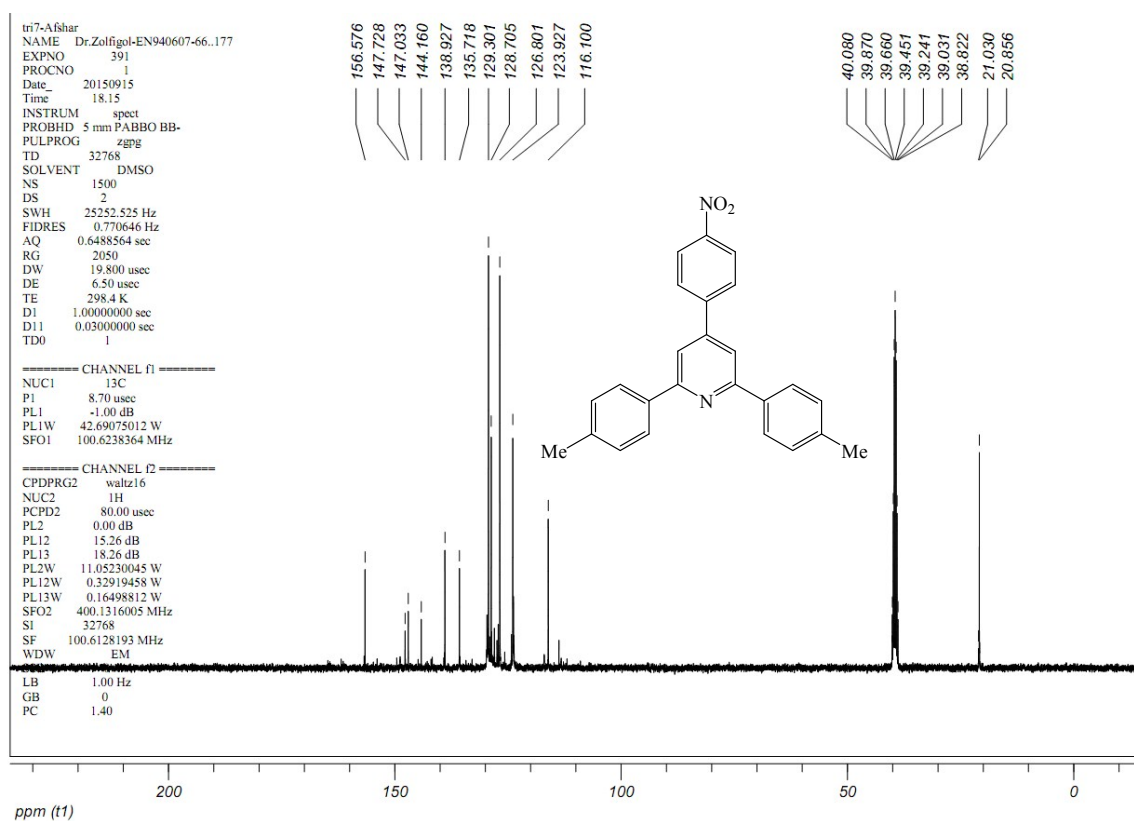


Fig S13. The FT-IR spectrum of *SVA catalyst*

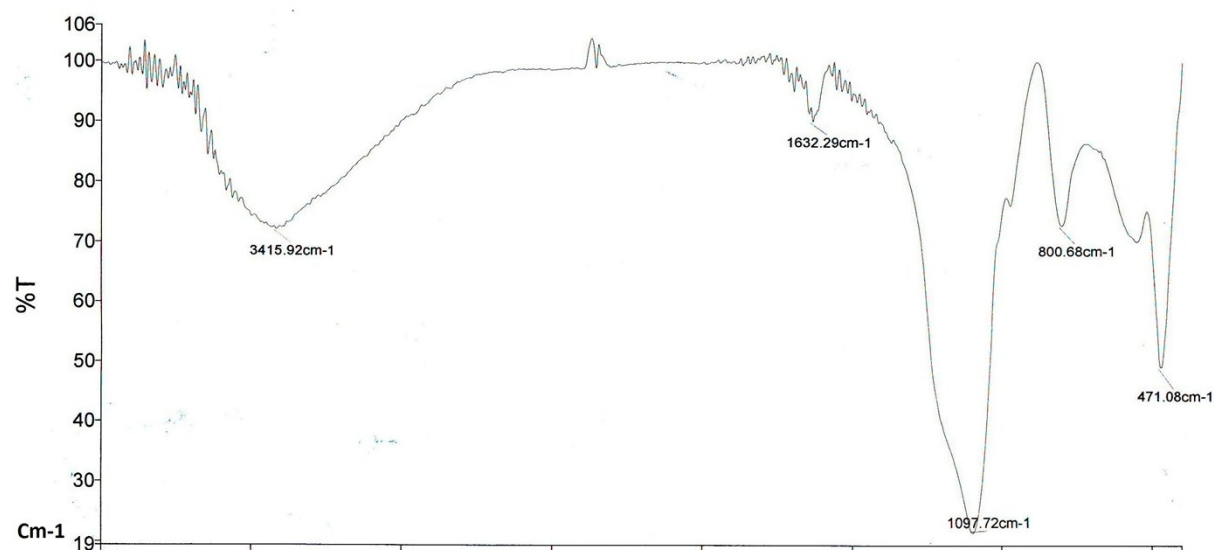


Fig S14. The TG, DTG and DTA analysis of *SVA catalyst*

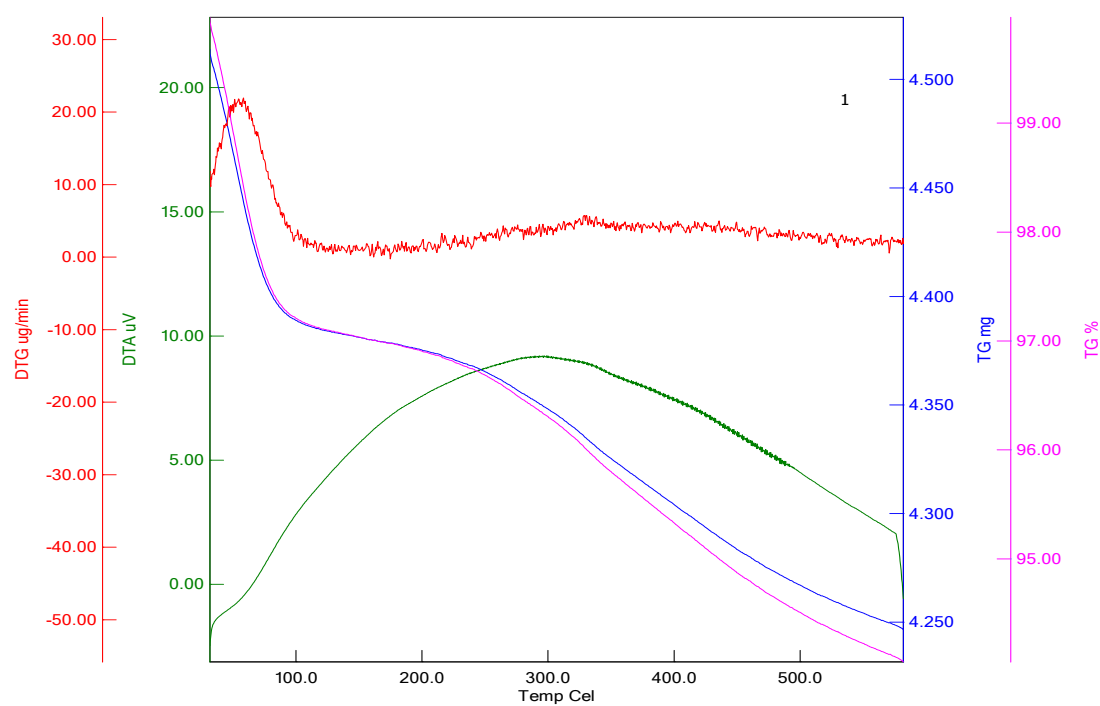


Fig S15. The XRD pattern of *SVA catalyst*

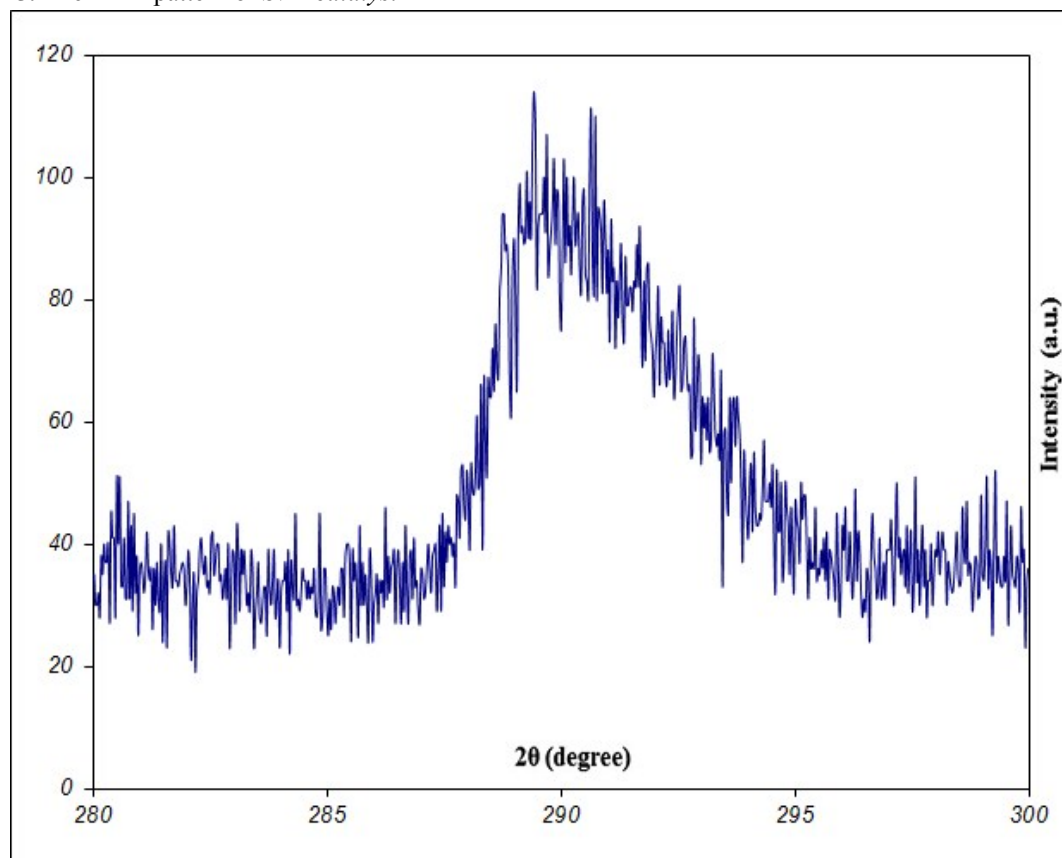


Fig S16. The SEM analysis of *SVA catalyst*

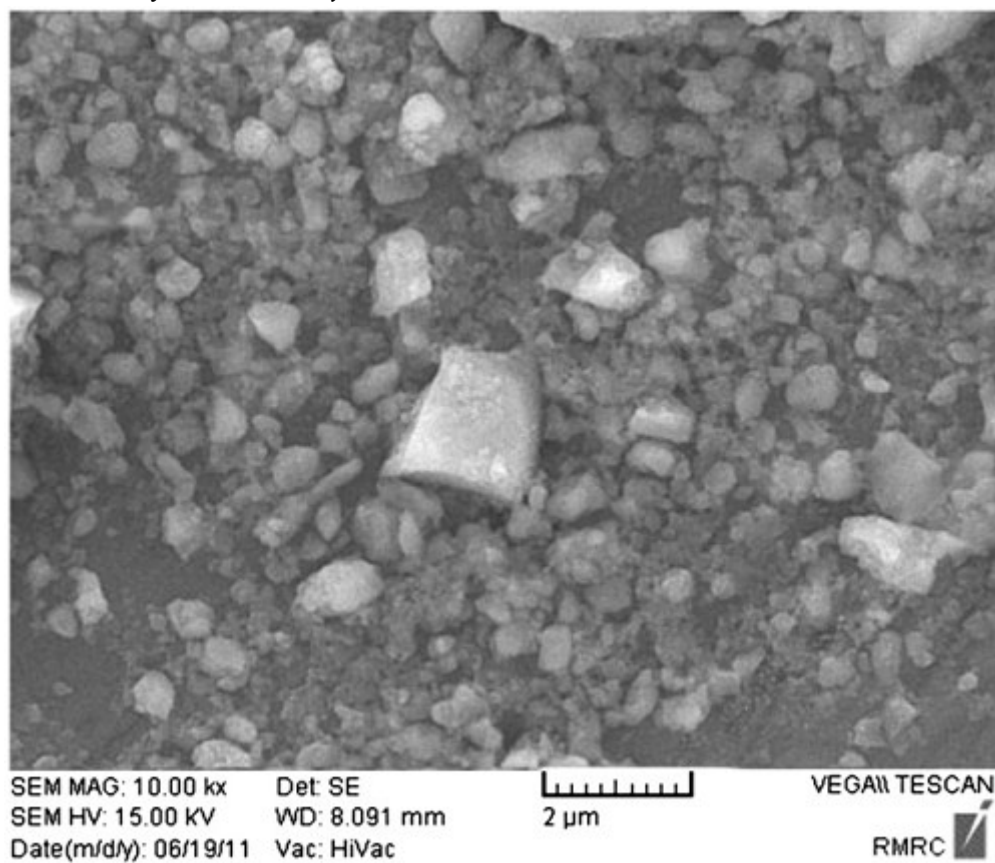


Fig S17. The EDX analysis of *SVA catalyst*

