# Supplementary Data

## Synthesis, crystal structure, DFT and anticancer activity of some imine-type compounds *via* routine Schiff base reaction: An example of unexpected cyclization to oxazine derivative

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**Figure S1**. $^{1}H$ NMR spectrum of **1** in $CDCl_3$.

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**Figure S7**. $^{1}H$ NMR spectrum of **3** in $CDCl_3$.

**Figure S8**. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in $CDCl_3$.

**Figure S9**. $^{1}H$ NMR spectrum of **4** in $CDCl_3$.

**Figure S10**. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in $CDCl_3$.

**Figure S11**. FT-IR spectrum of **3**.

**Figure S12**. FT-IR spectrum of **4**.

**Table S1**. Cartesian coordinates for the calculated structure of **3**.

| | | | |
|---|---|---|---|
| O | -0.771478000 | 0.553378000 | 1.956593000 |
| O | 0.928649000 | 0.863779000 | -0.629474000 |
| N | -0.871486000 | -1.655184000 | -0.120258000 |
| N | 2.630452000 | -0.730312000 | -0.442532000 |
| N | 2.687135000 | -2.103754000 | -0.106065000 |
| C | -2.490685000 | 4.337235000 | -0.874233000 |
| H | -2.784005000 | 5.290668000 | -1.304519000 |
| C | -1.948711000 | 4.288560000 | 0.413357000 |
| H | -1.818397000 | 5.203777000 | 0.983516000 |
| C | -1.572681000 | 3.067103000 | 0.963416000 |
| H | -1.141645000 | 3.002822000 | 1.956865000 |
| C | -1.740632000 | 1.881918000 | 0.233403000 |
| C | -1.329406000 | 0.597594000 | 0.870030000 |
| C | -1.713694000 | -0.743473000 | 0.228654000 |
| C | 0.500473000 | -1.498780000 | -0.169895000 |
| C | 1.286865000 | -0.291610000 | -0.434459000 |
| C | 3.735694000 | 0.105981000 | -0.129299000 |
| C | 4.663516000 | -0.261864000 | 0.853807000 |
| H | 4.518704000 | -1.181384000 | 1.409958000 |
| C | 5.747106000 | 0.572220000 | 1.126858000 |
| H | 6.464126000 | 0.280413000 | 1.888678000 |
| C | 5.900133000 | 1.779737000 | 0.445050000 |
| H | 6.741483000 | 2.429485000 | 0.665447000 |
| C | -2.653227000 | 3.161099000 | -1.609542000 |
| H | -3.068093000 | 3.198815000 | -2.612405000 |
| C | -2.282016000 | 1.936821000 | -1.057849000 |
| H | -2.404566000 | 1.025289000 | -1.633738000 |
| C | -3.159779000 | -1.083427000 | 0.181221000 |
| C | -3.602557000 | -2.157655000 | -0.611374000 |
| H | -2.869136000 | -2.708524000 | -1.189474000 |
| C | -4.949293000 | -2.502381000 | -0.649691000 |
| H | -5.276043000 | -3.330935000 | -1.271680000 |
| C | -5.881875000 | -1.784299000 | 0.104997000 |
| H | -6.933623000 | -2.053557000 | 0.073028000 |
| C | -5.454780000 | -0.718818000 | 0.897562000 |
| H | -6.171192000 | -0.159066000 | 1.491453000 |
| C | -4.106271000 | -0.366506000 | 0.932932000 |
| H | -3.790358000 | 0.460598000 | 1.559850000 |
| C | 1.374015000 | -2.549863000 | -0.058725000 |
| C | 1.040317000 | -3.992710000 | 0.113298000 |
| H | 1.405998000 | -4.600160000 | -0.722581000 |
| H | -0.044932000 | -4.088833000 | 0.163873000 |
| H | 1.473239000 | -4.397601000 | 1.034622000 |
| C | 3.677693000 | -2.869744000 | -0.873139000 |
| H | 3.710785000 | -3.884552000 | -0.474860000 |
| H | 4.659145000 | -2.414558000 | -0.740425000 |
| H | 3.433151000 | -2.898279000 | -1.942658000 |
| C | 4.959511000 | 2.148324000 | -0.518800000 |
| H | 5.065819000 | 3.089061000 | -1.050807000 |
| C | 3.883701000 | 1.315746000 | -0.820221000 |
| H | 3.148970000 | 1.596769000 | -1.563250000 |

**Table S2**. Cartesian coordinates for the calculated structure of **4**.

| | | | |
|---|---|---|---|
| O | -1.406610000 | 1.299074000 | 0.132544000 |
| O | -0.271185000 | 0.577804000 | 2.029147000 |
| H | -0.414697000 | 1.481814000 | 2.351035000 |
| N | -1.239567000 | -1.467659000 | -0.187894000 |
| C | -2.475979000 | -0.824300000 | -0.133833000 |
| C | -3.658770000 | -1.559670000 | -0.289583000 |
| H | -3.576382000 | -2.633956000 | -0.420017000 |
| C | -4.892616000 | -0.915858000 | -0.276367000 |
| H | -5.806430000 | -1.489756000 | -0.392543000 |
| C | -4.951911000 | 0.474406000 | -0.123230000 |
| H | -5.913019000 | 0.979851000 | -0.120680000 |
| C | -3.784591000 | 1.223047000 | 0.030168000 |
| H | -3.808831000 | 2.301629000 | 0.146345000 |
| C | -2.557838000 | 0.564730000 | 0.036036000 |
| C | -0.222665000 | 0.643620000 | 0.623722000 |
| C | 0.913116000 | 1.520619000 | 0.094089000 |
| C | 0.998850000 | 1.774021000 | -1.280811000 |
| H | 0.264940000 | 1.339207000 | -1.951817000 |
| C | 2.010322000 | 2.586646000 | -1.786797000 |
| H | 2.067192000 | 2.773375000 | -2.855098000 |
| C | 2.944801000 | 3.164115000 | -0.923609000 |
| H | 3.732289000 | 3.799457000 | -1.318032000 |
| C | 2.861306000 | 2.919802000 | 0.445984000 |
| H | 3.583009000 | 3.364518000 | 1.124903000 |
| C | 1.851478000 | 2.098439000 | 0.952112000 |
| H | 1.802284000 | 1.900042000 | 2.017658000 |
| C | -0.171709000 | -0.827969000 | 0.143519000 |
| C | 1.120295000 | -1.554345000 | 0.076839000 |
| C | 2.154687000 | -1.326490000 | 0.998238000 |
| H | 2.018899000 | -0.596479000 | 1.786684000 |
| C | 3.335202000 | -2.064648000 | 0.931043000 |
| H | 4.121984000 | -1.885164000 | 1.657944000 |
| C | 3.505018000 | -3.033117000 | -0.059083000 |
| H | 4.429120000 | -3.601299000 | -0.113923000 |
| C | 2.478528000 | -3.271716000 | -0.976319000 |
| H | 2.602167000 | -4.025953000 | -1.748120000 |
| C | 1.294235000 | -2.544474000 | -0.905161000 |
| H | 0.486248000 | -2.729837000 | -1.604347000 |

**Table S3**. NMR chemical shifts (C.S) for **3**.

| Atom | C.S(calc) | C.S(exp) | Atom | C.S(calc) | C.S(exp) |
|---|---|---|---|---|---|
| C6 | 119.839 | 132.887 | H7 | 7.823 | 7.308 |
| C8 | 115.620 | 128.356 | H9 | 7.850 | 7.365 |
| C10 | 116.316 | 129.042 | H11 | 8.575 | 7.803 |
| C12 | 126.056 | 136.738 | H19 | 7.420 | 7.139 |
| C13 | 182.059 | 194.462 | H21 | 7.779 | 7.295 |
| C14 | 152.046 | 162.143 | H23 | 7.583 | 7.251 |
| C15 | 110.180 | 122.833 | H25 | 7.605 | 7.269 |
| C16 | 145.596 | 158.694 | H27 | 7.919 | 7.702 |
| C17 | 124.556 | 134.891 | H30 | 8.679 | 7.821 |
| C18 | 108.309 | 120.01 | H32 | 7.853 | 7.685 |
| C20 | 116.388 | 129.418 | H34 | 7.711 | 7.281 |
| C22 | 112.589 | 124.536 | H36 | 7.493 | 7.142 |
| C24 | 115.028 | 127.924 | H38 | 7.313 | 7.119 |
| C26 | 119.974 | 132.887 | H41 | 2.353 | 2.319 |
| C28 | 127.335 | 137.129 | H42 | 3.416 | 2.319 |
| C29 | 113.943 | 126.769 | H43 | 2.269 | 2.319 |
| C31 | 115.978 | 128.356 | H45 | 3.530 | 2.939 |
| C33 | 116.980 | 129.918 | H46 | 3.546 | 2.939 |
| C35 | 115.119 | 127.924 | H47 | 2.902 | 2.939 |
| C37 | 117.496 | 136.326 | H49 | 7.687 | 7.275 |
| C39 | 144.263 | 149.959 | H51 | 7.758 | 7.291 |
| C40 | 3.180 | 10.989 | | | |
| C44 | 27.255 | 36.107 | | | |
| C48 | 116.361 | 129.087 | | | |
| C50 | 112.070 | 124.536 | | | |

**Table S4**. NMR chemical shifts (C.S) for **4**.

| Atom | C.S(calc) | C.S(exp) | Atom | C.S(calc) | C.S(exp) |
|---|---|---|---|---|---|
| C5 | 121.105 | 131.948 | H3 | 2.787 | 3.823 |
| C6 | 116.967 | 129.027 | H7 | 7.905 | 7.538 |
| C8 | 109.802 | 122.601 | H9 | 7.541 | 6.811 |
| C10 | 117.107 | 129.459 | H11 | 7.676 | 6.887 |
| C12 | 103.992 | 116.58 | H13 | 7.302 | 6.52 |
| C14 | 132.208 | 143.914 | H18 | 7.681 | 7.039 |
| C15 | 88.609 | 94.723 | H20 | 7.599 | 6.91 |
| C16 | 131.212 | 139.995 | H22 | 7.657 | 7 |
| C17 | 116.516 | 128.322 | H24 | 7.794 | 7.197 |
| C19 | 115.955 | 127.899 | H26 | 8.158 | 7.79 |
| C21 | 116.007 | 127.899 | H30 | 8.091 | 7.747 |
| C23 | 115.206 | 127.899 | H32 | 7.472 | 6.793 |
| C25 | 112.449 | 126.272 | H34 | 7.591 | 6.907 |
| C27 | 147.966 | 159.869 | H36 | 7.678 | 7.016 |
| C28 | 125.823 | 135.809 | H38 | 8.258 | 7.916 |
| C29 | 117.377 | 129.922 | | | |
| C31 | 114.360 | 127.899 | | | |
| C33 | 116.829 | 128.89 | | | |
| C35 | 115.466 | 127.899 | | | |
| C37 | 116.979 | 129.027 | | | |

**Figure S1**. $^{1}H$ NMR spectrum of **1** in $CDCl_3$.

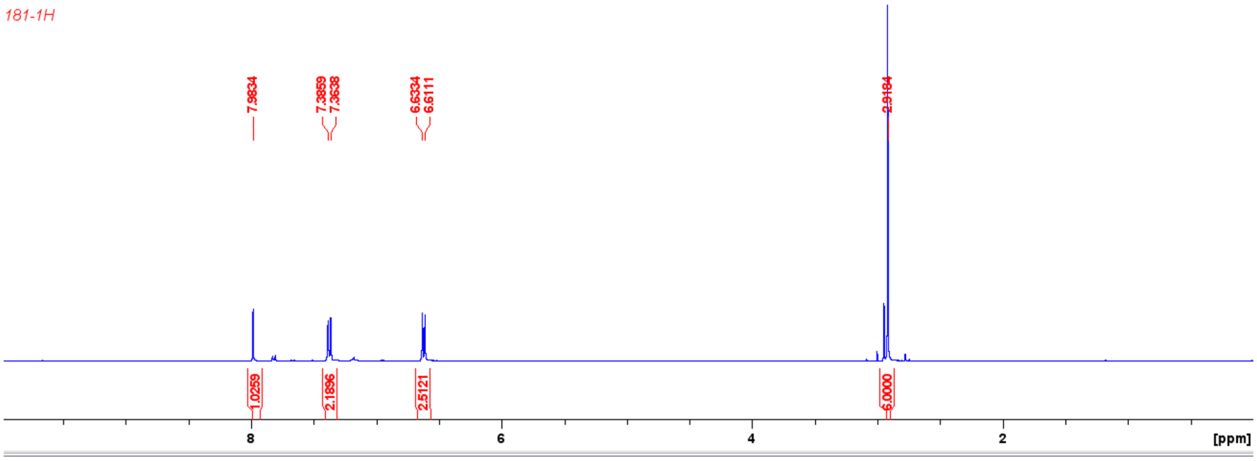



**Figure S2**. $^{13}C\{^{1}H\}$ NMR spectrum of **1** in $CDCl_3$.

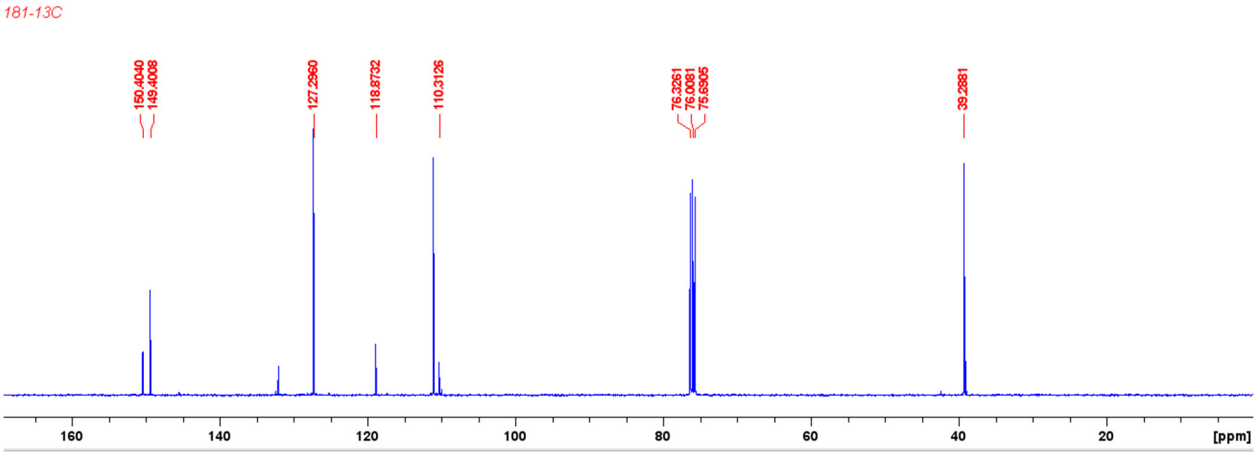


**Figure S3**. $^{1}H$ NMR spectrum of **2** in $CDCl_3$.

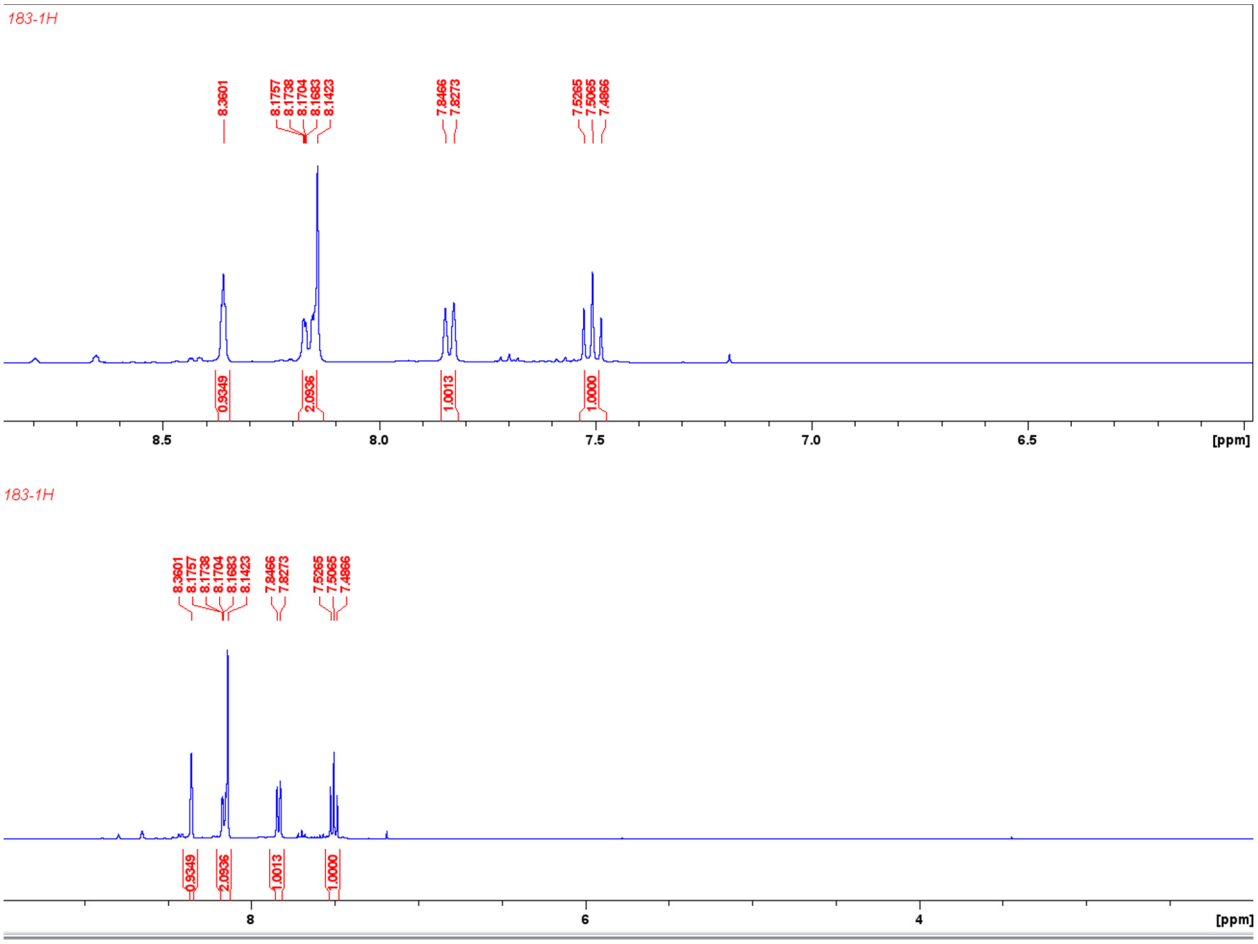



**Figure S4**. $^{13}C\{^{1}H\}$ NMR spectrum of **2** in $CDCl_3$.

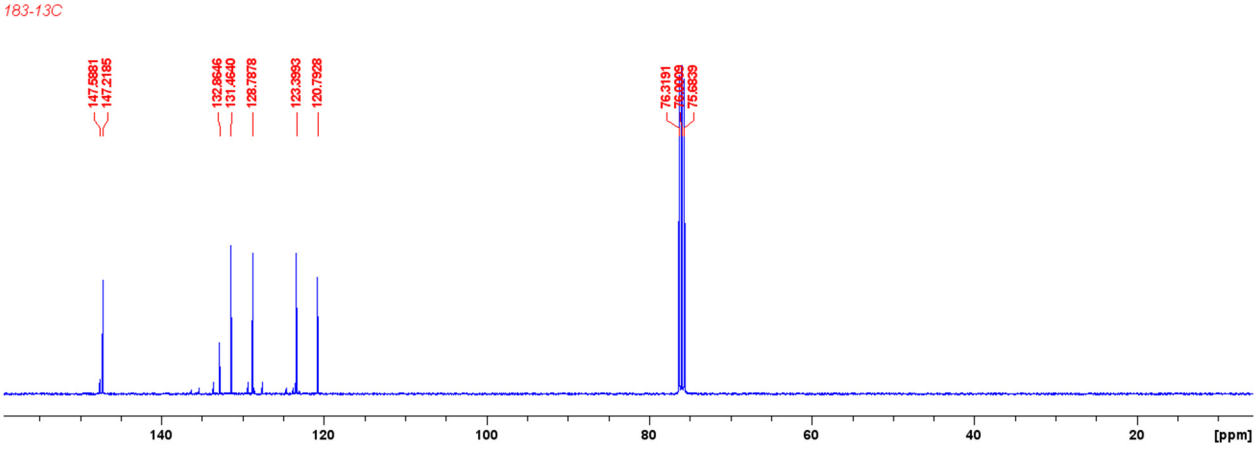


**Figure S5**. FT-IR spectrum of **1**.

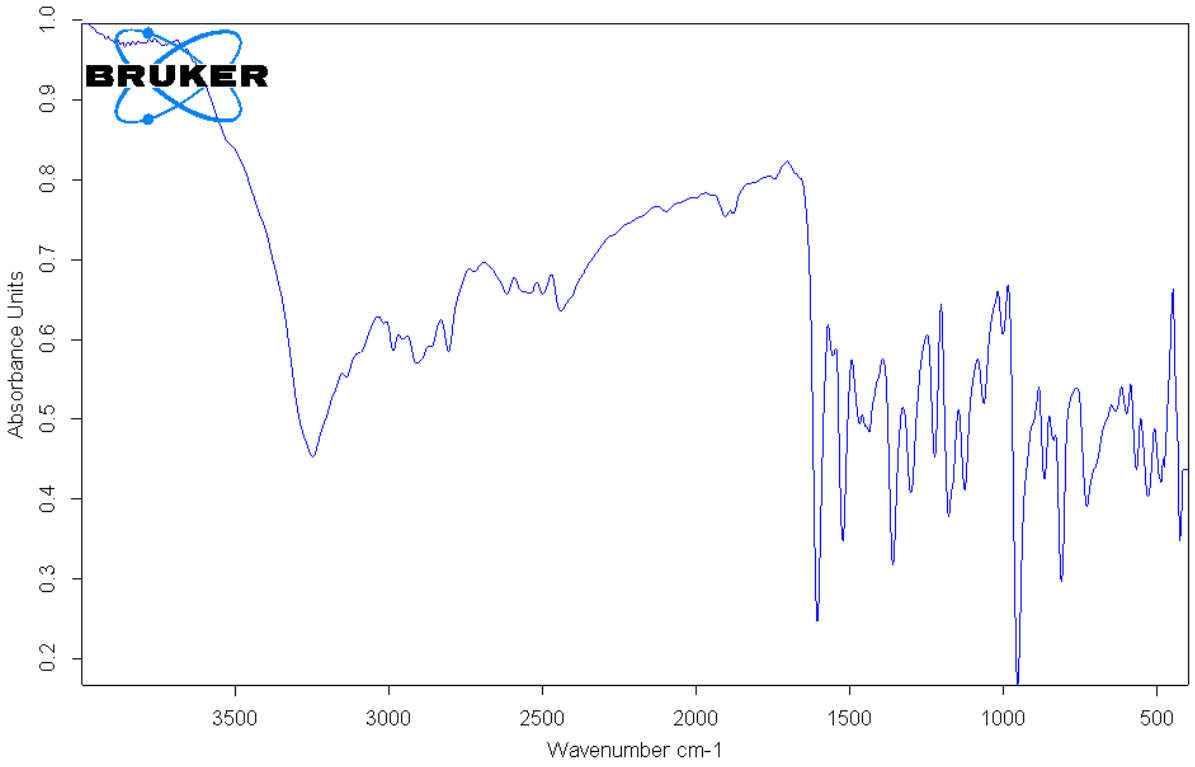



**Figure S6**. FT-IR spectrum of **2**.

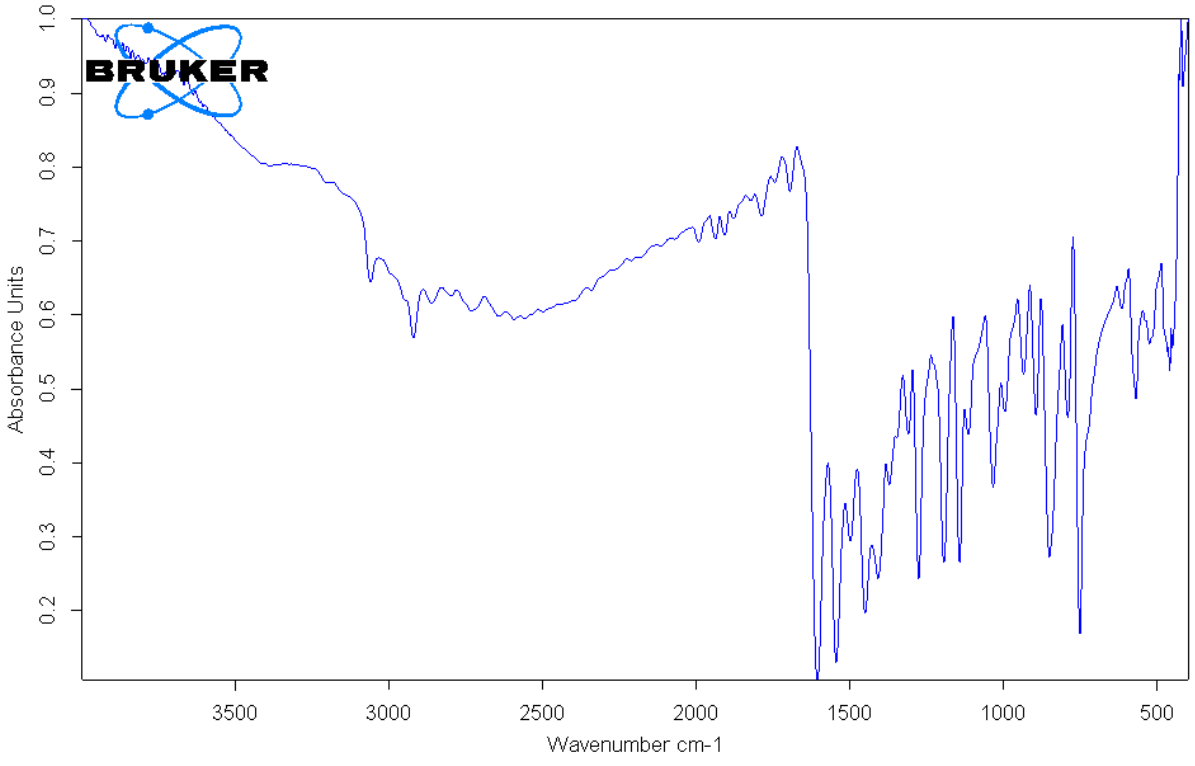


**Figure S7**. $^{1}H$ NMR spectrum of **3** in $CDCl_3$.

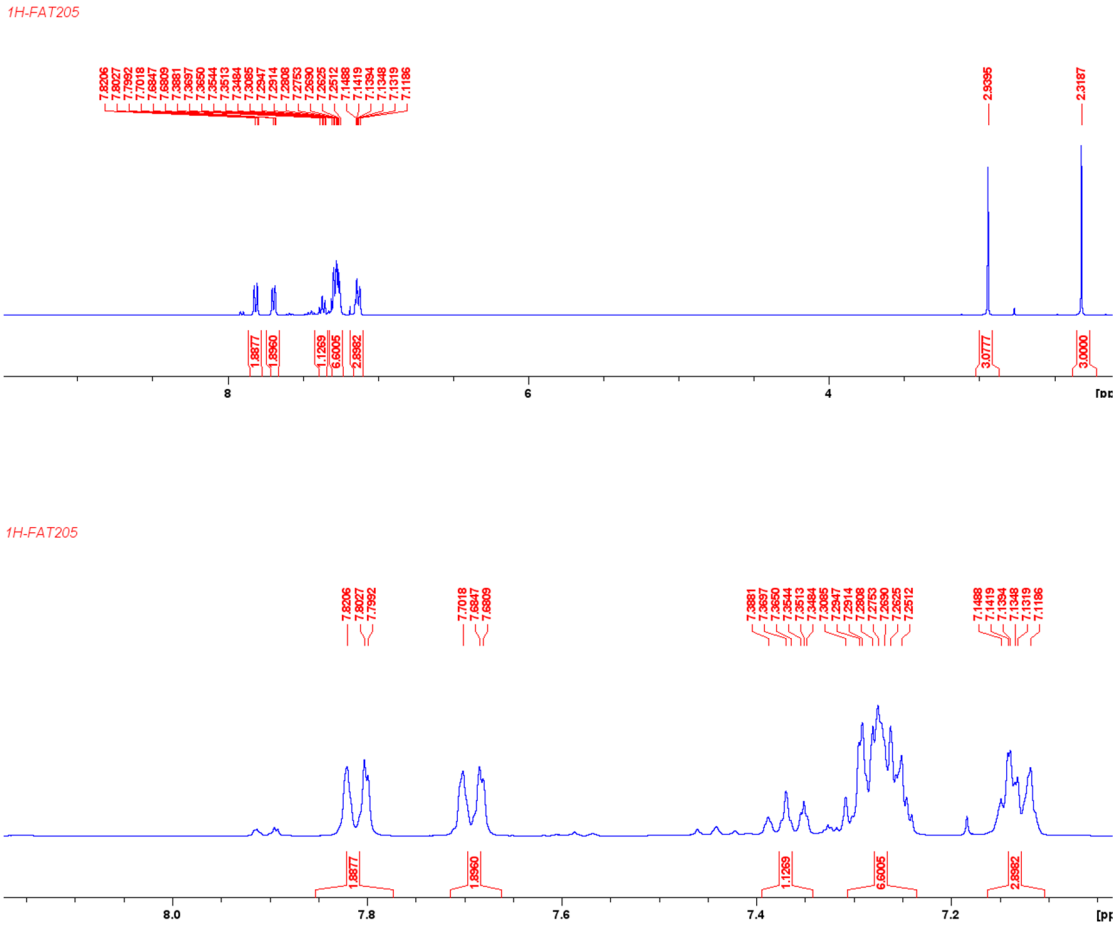



**Figure S8**. $^{13}C\{^{1}H\}$ NMR spectrum of **3** in $CDCl_3$.

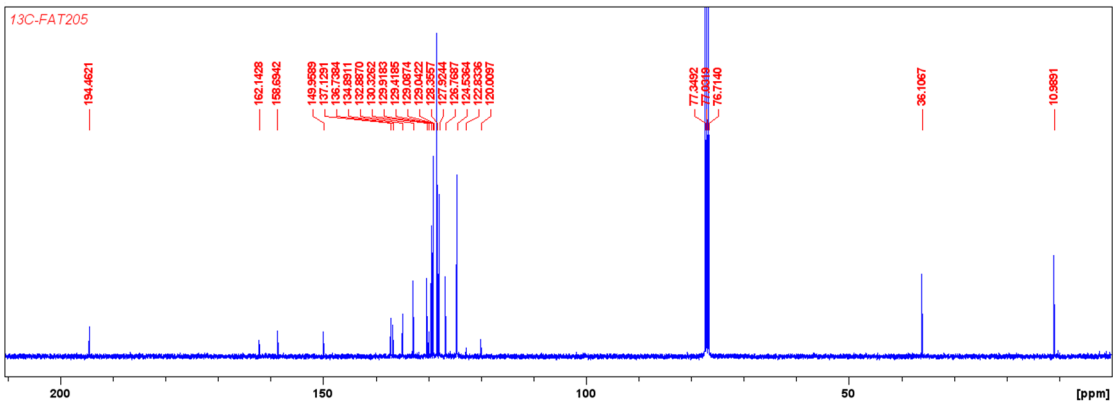


**Figure S9**. $^{1}H$ NMR spectrum of **4** in $CDCl_3$.

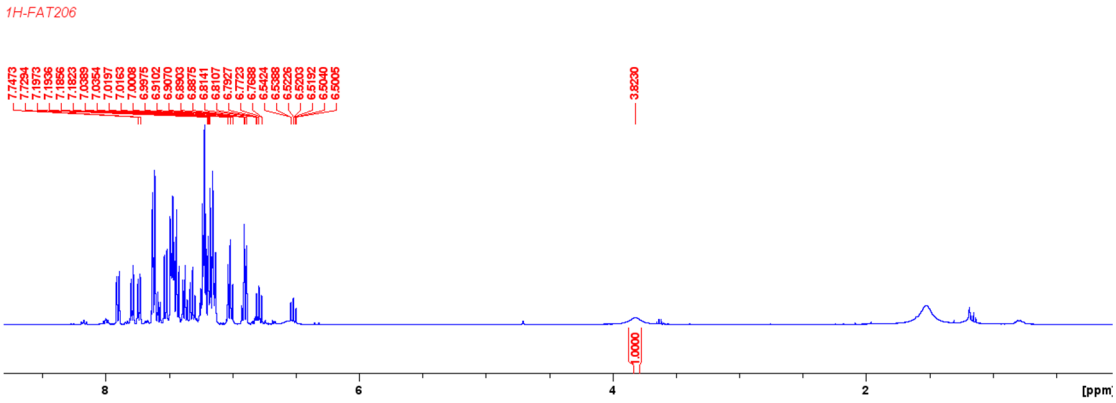



**Figure S10**. $^{13}C\{^{1}H\}$ NMR spectrum of **4** in $CDCl_3$.

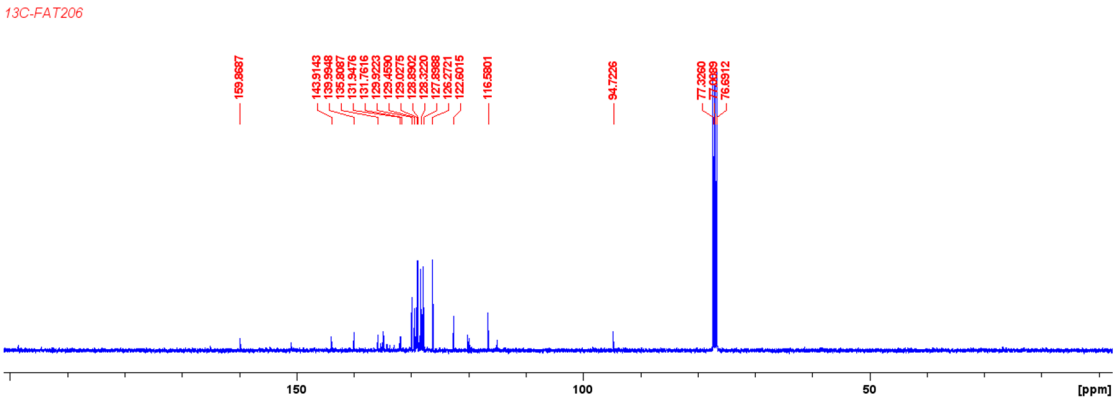


**Figure S11**. FT-IR spectrum of **3**.

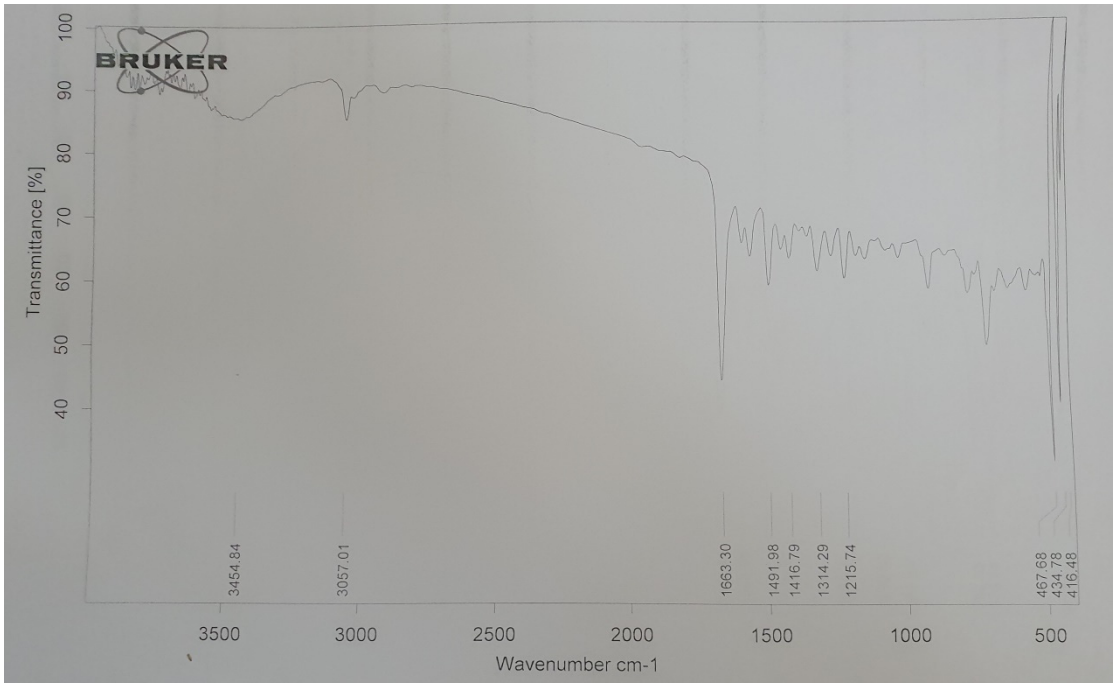



**Figure S12**. FT-IR spectrum of **4**.

