

Supporting Information

**Synthesis of fullereryl-1,2,3-triazoles by reaction of fullereryl
azide with terminal acetylenes**

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Federation

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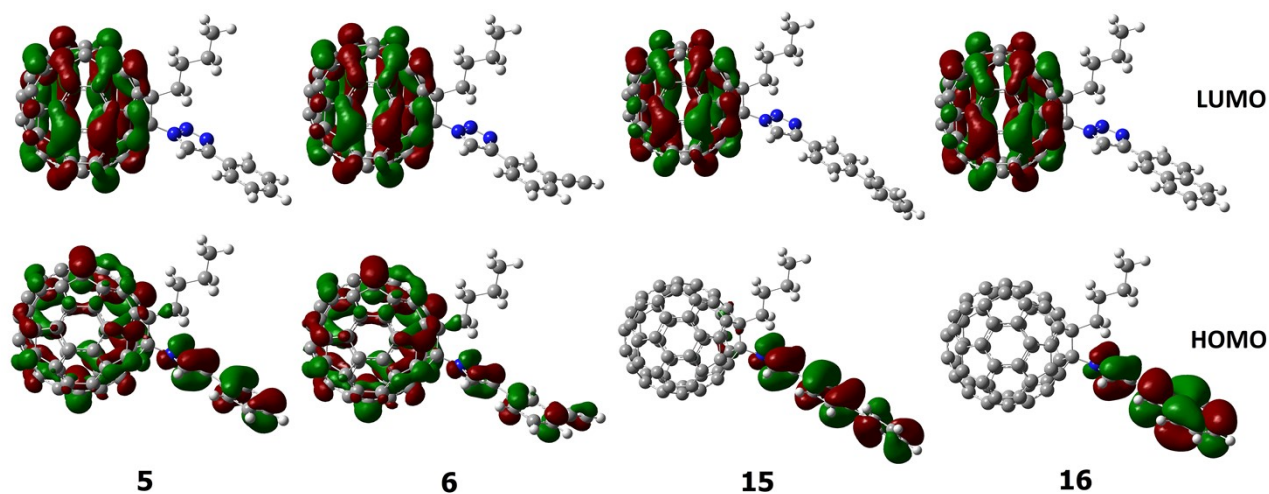


Figure S1. Distribution of the boundary orbitals of compounds **5**, **6**, **15**, and **16** calculated at the PBE/PBE/6-311G(d,p) level of theory.

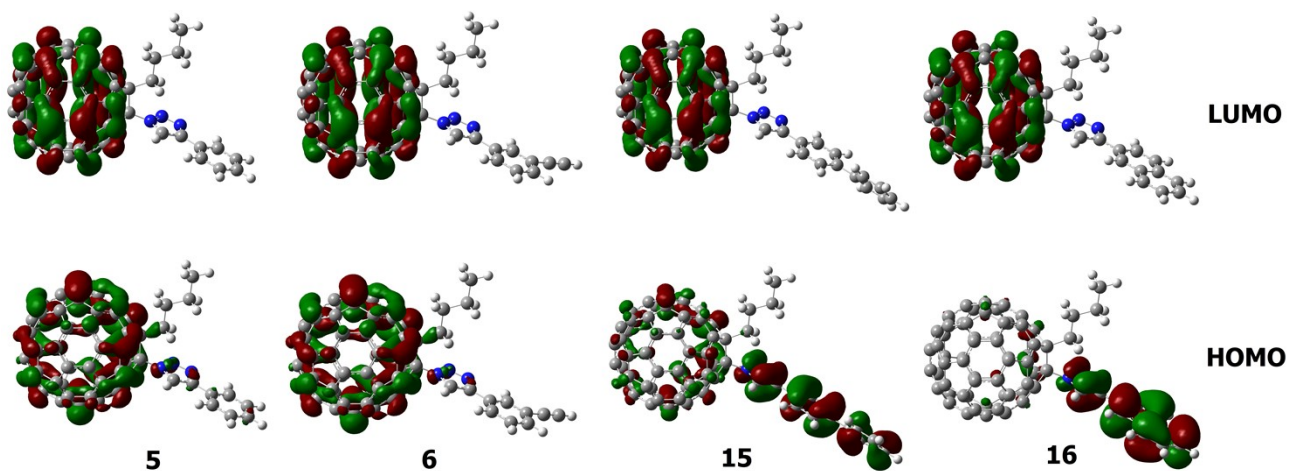


Figure S2. Distribution of the boundary orbitals of compounds **5**, **6**, **15**, and **16** calculated at the B3LYP / 6-31G (d, p) level of theory.

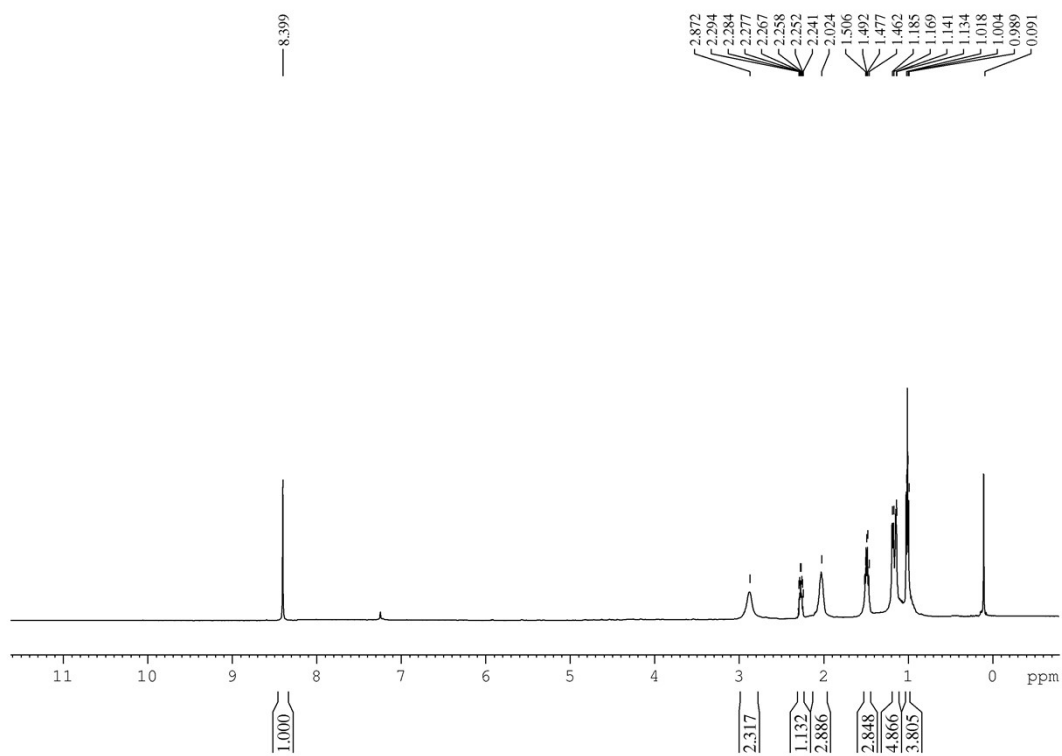


Figure S1. Copy of ^1H NMR spectra of compound 2

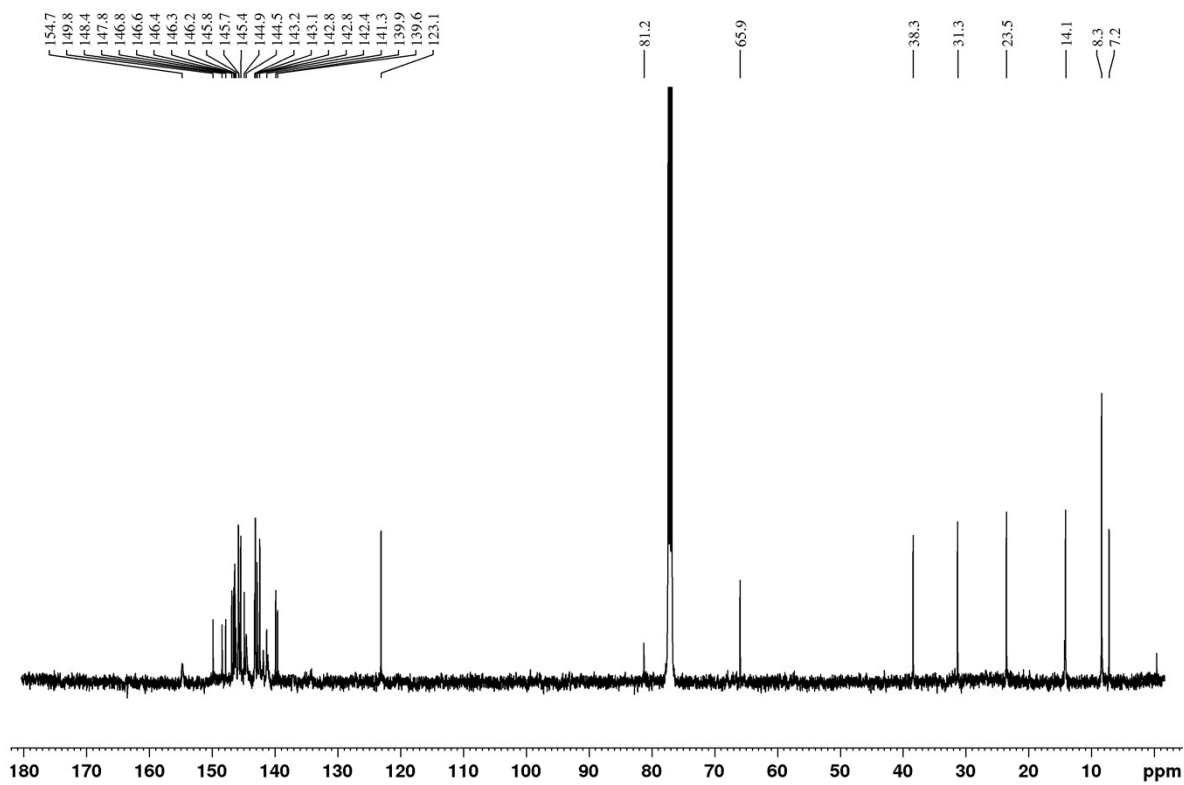


Figure S2. Copy of ^{13}C NMR spectra of compound 2

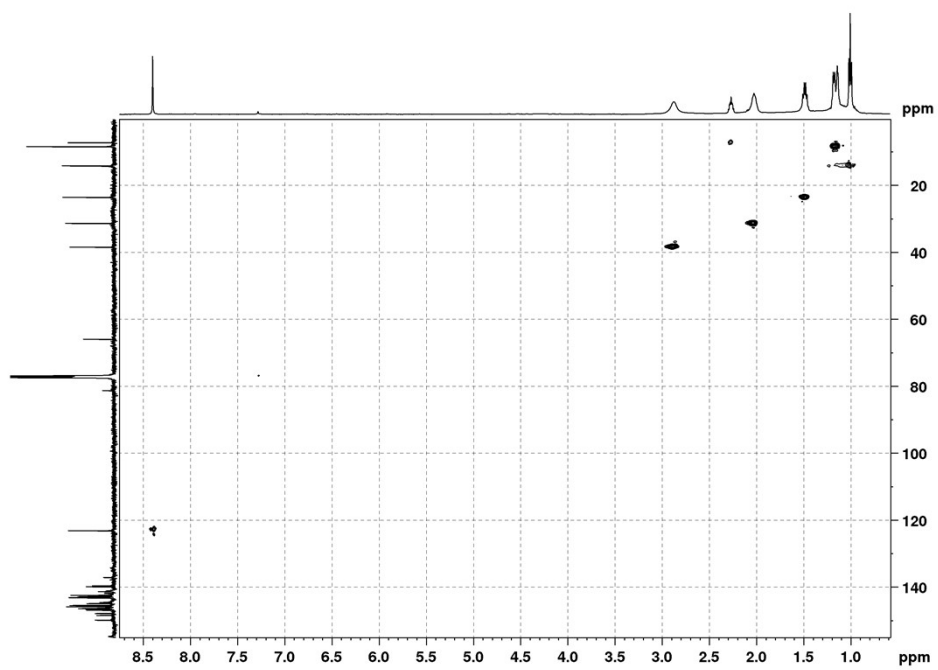


Figure S3. Copy of HSQC spectra of compound 2

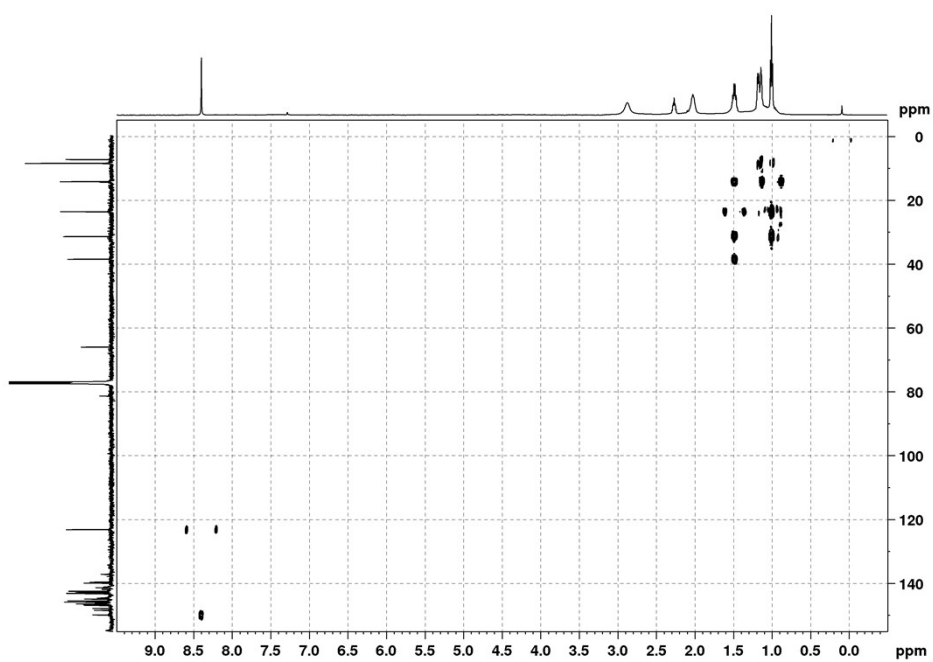


Figure S4. Copy of HMBC spectra of compound 2

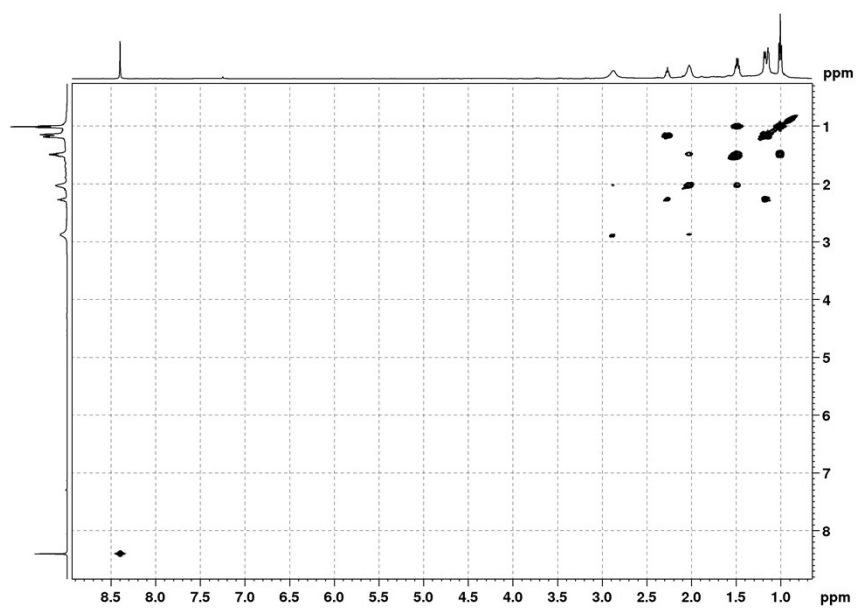


Figure S5. Copy of COSY spectra of compound 2

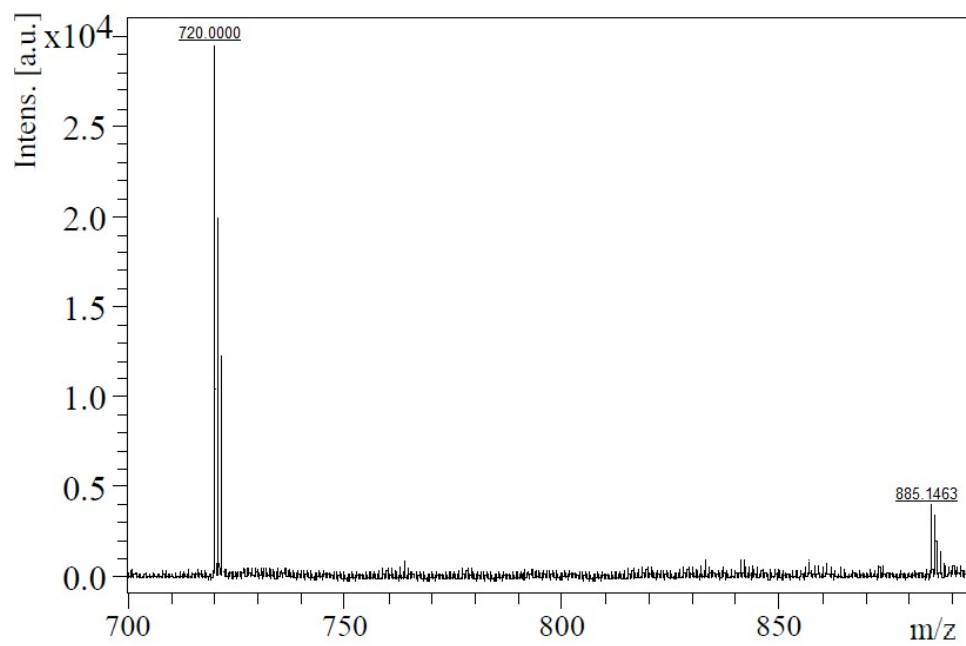


Figure S6. Copy of MALDI TOF spectra of compound 2

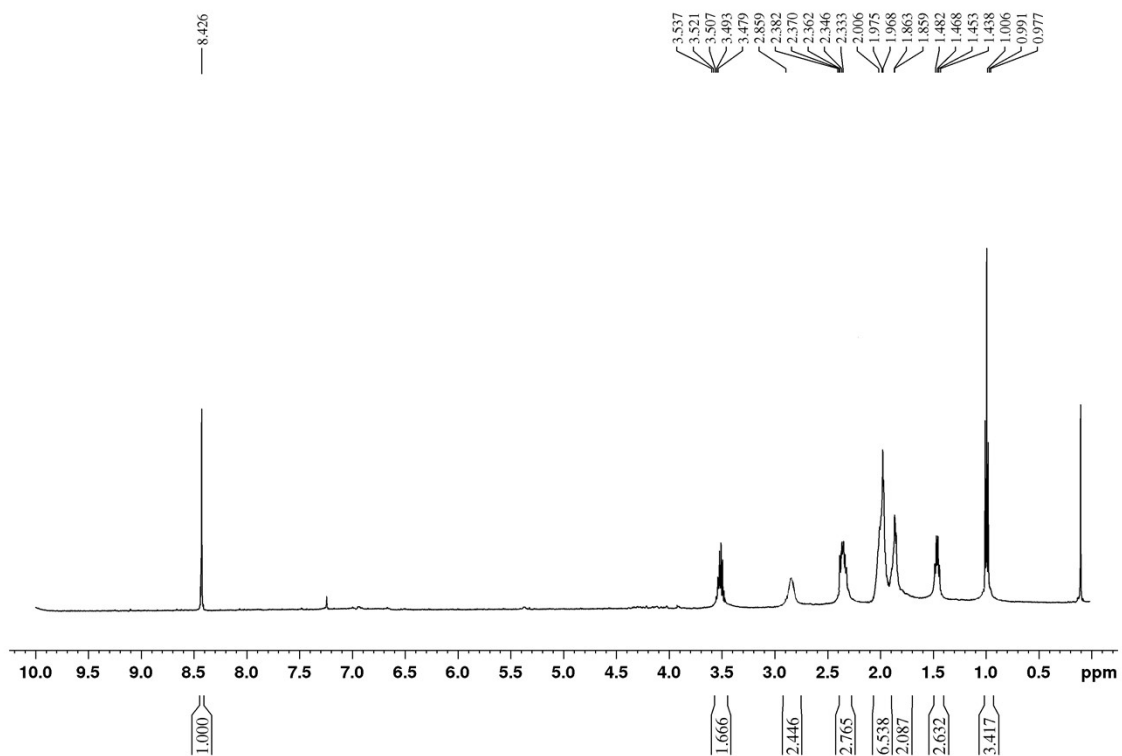


Figure S7. Copy of ^1H NMR spectra of compound 3

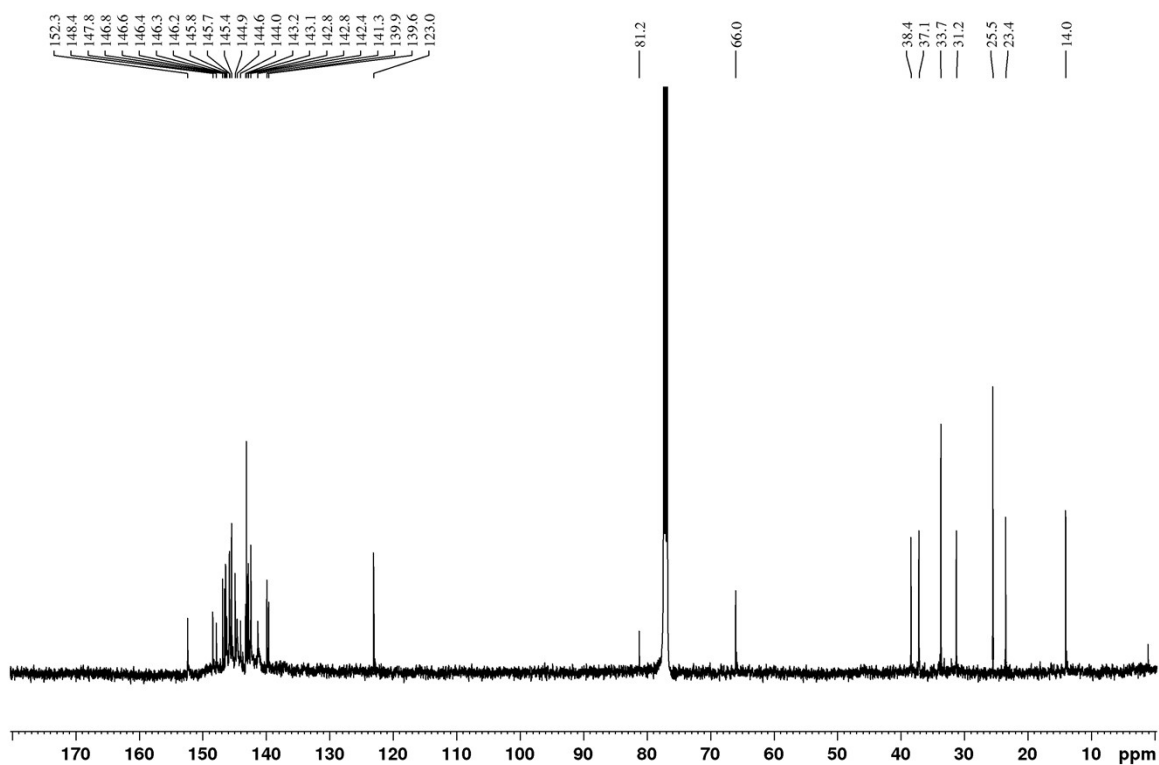


Figure S8. Copy of ^{13}C NMR spectra of compound 3

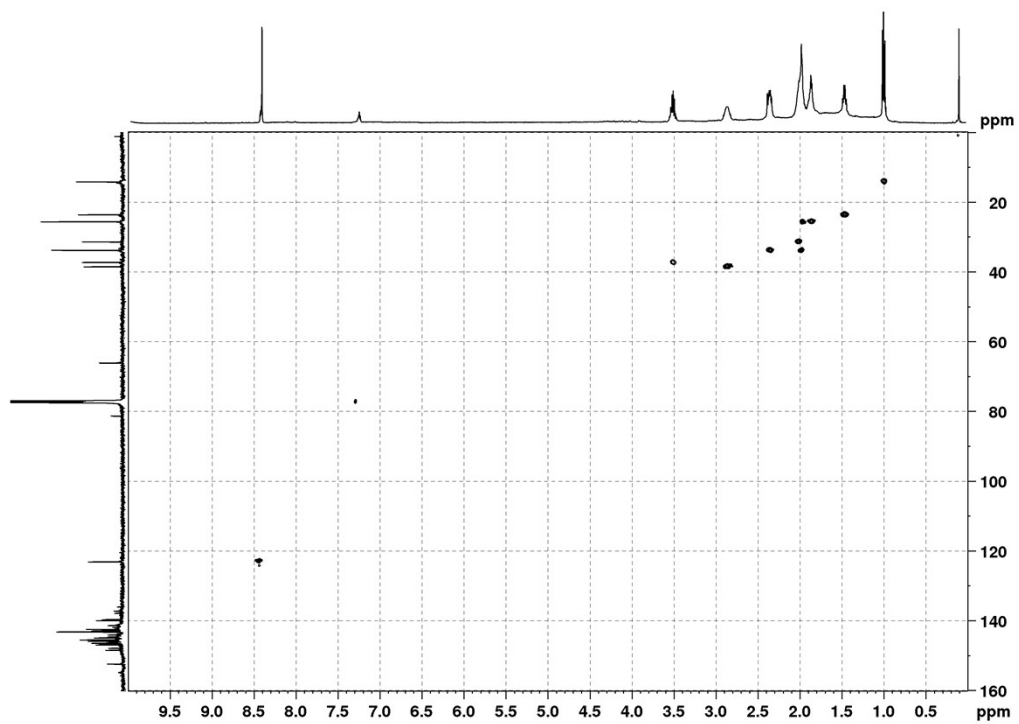


Figure S9. Copy of HSQC spectra of compound **3**

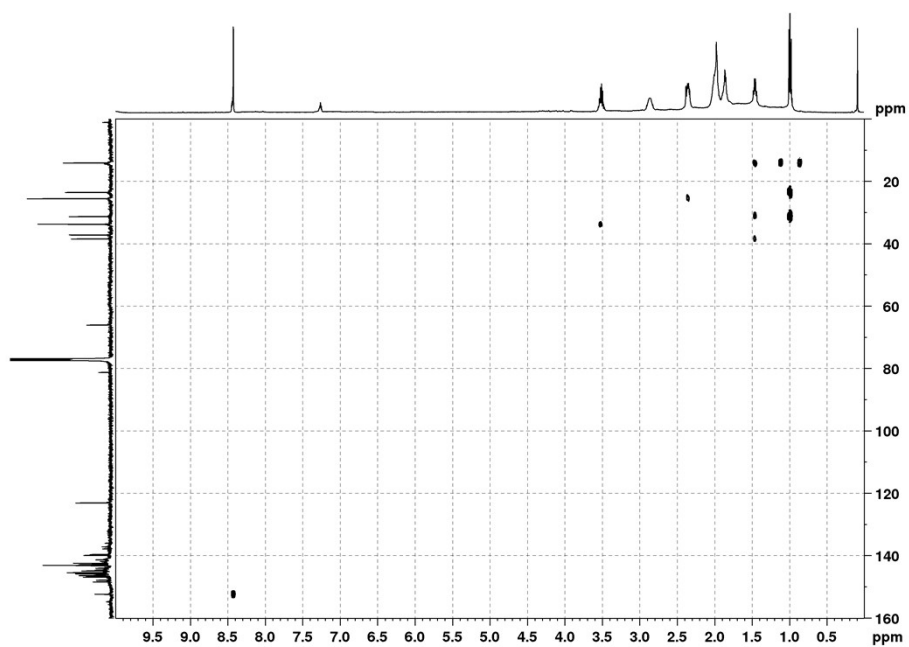


Figure S10. Copy of HMBC spectra of compound **3**

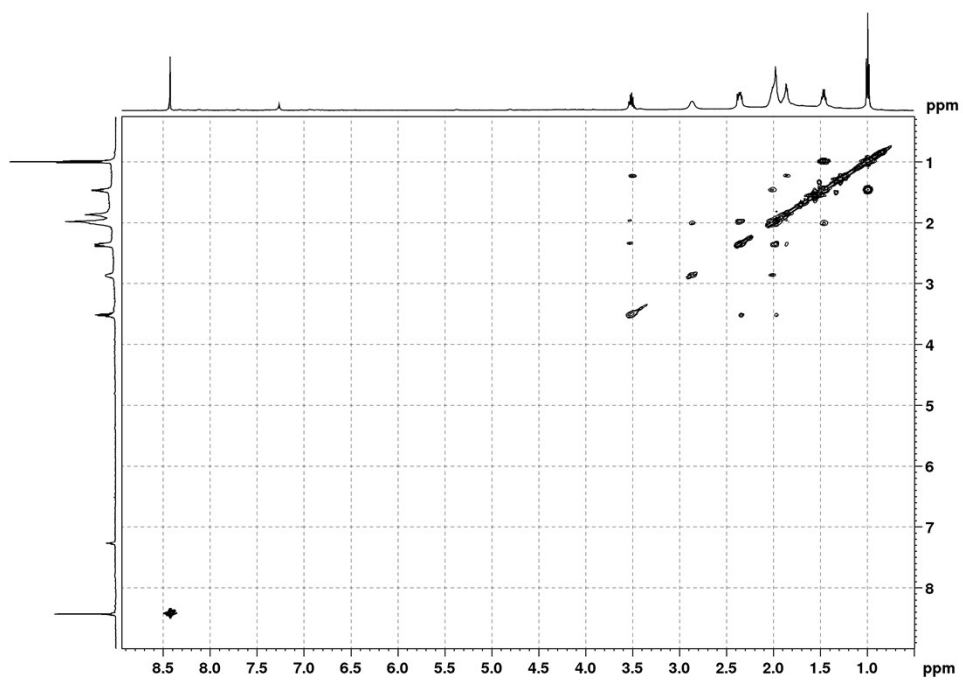


Figure S11. Copy of COSY spectra of compound **3**

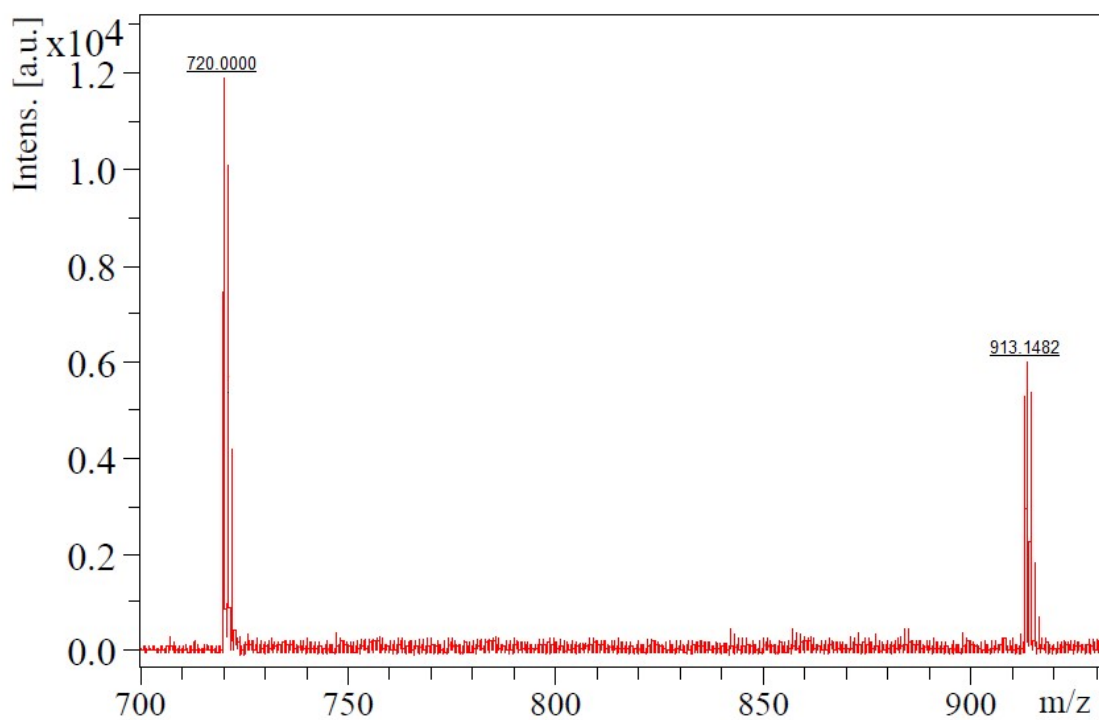


Figure S12. Copy of MALDI TOF spectra of compound **3**

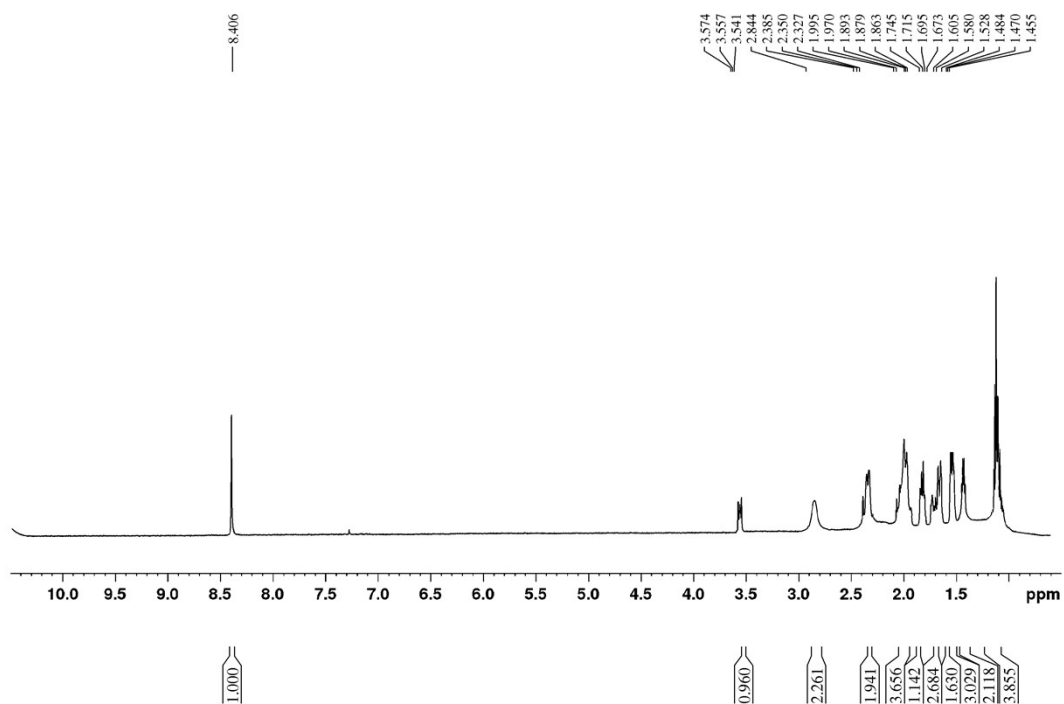


Figure S13. Copy of ^1H NMR spectra of compound 4

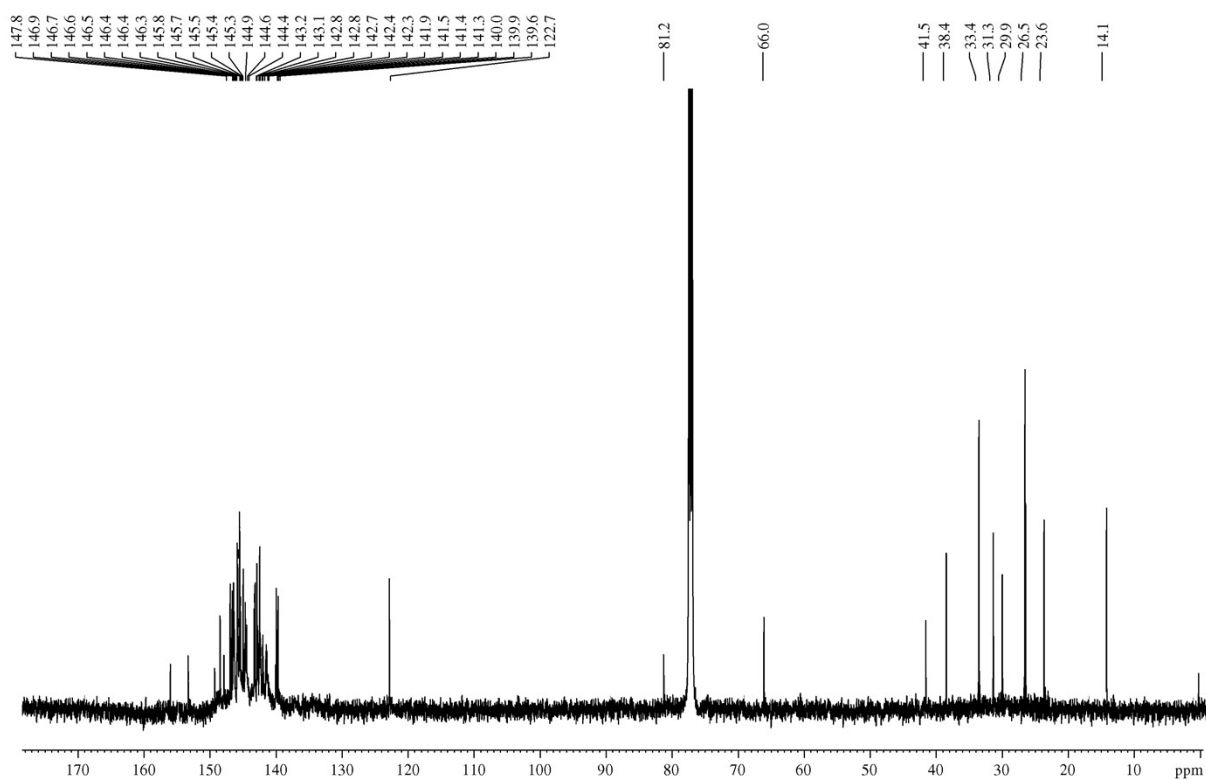


Figure S14. Copy of ^{13}C NMR spectra of compound 4

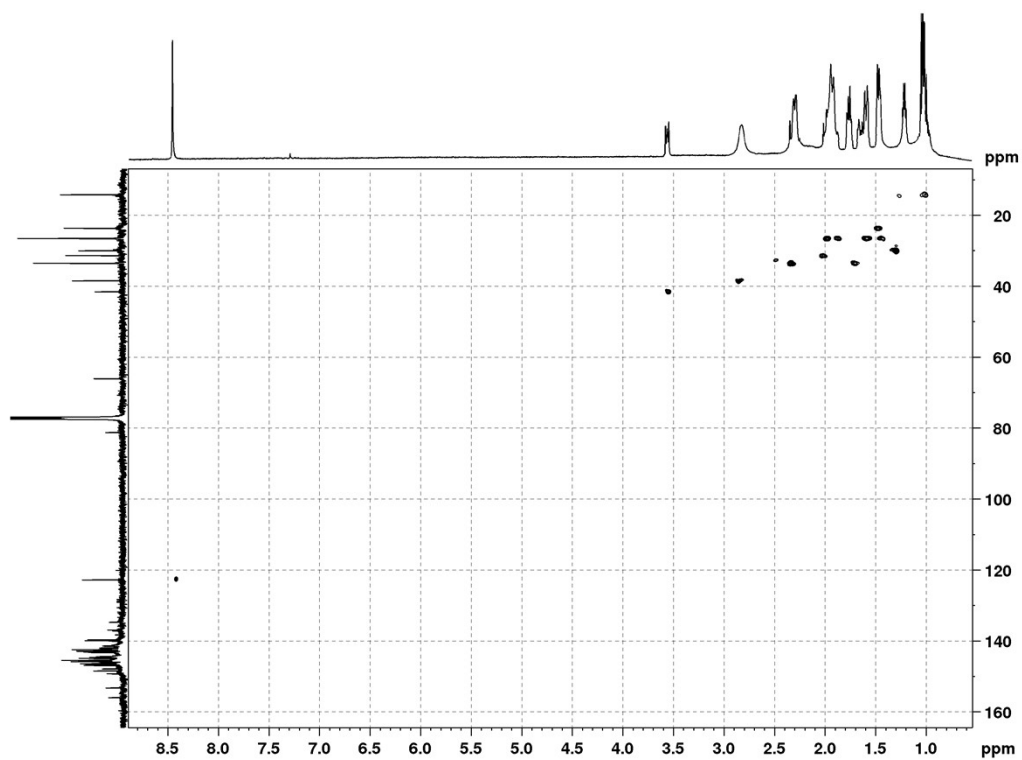


Figure S15. Copy of HSQC NMR spectra of compound 4

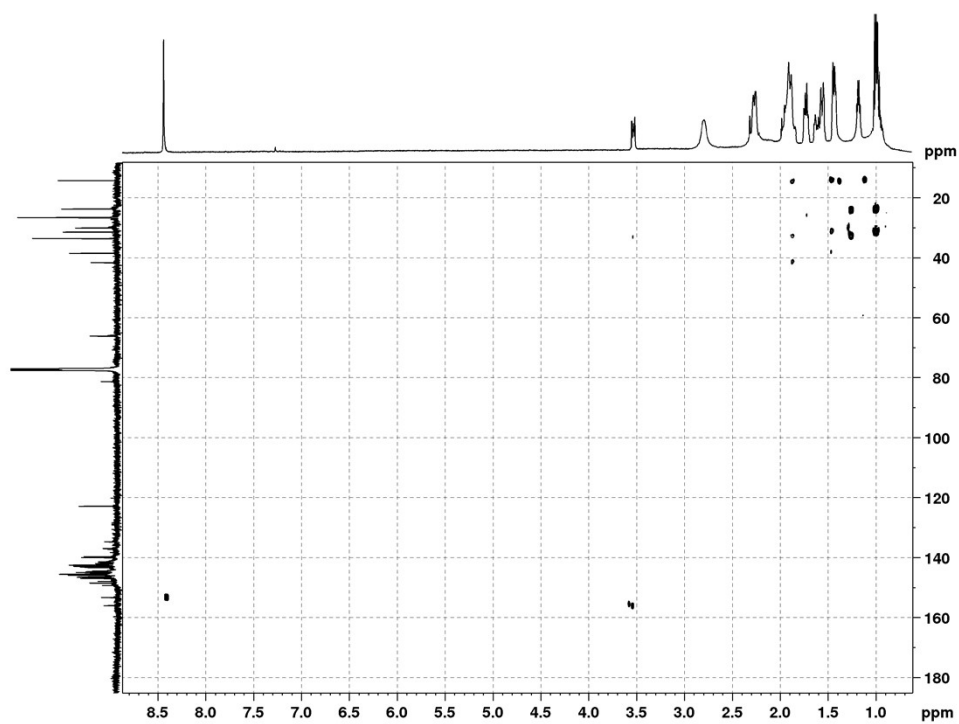


Figure S16. Copy of HMBC NMR spectra of compound 4

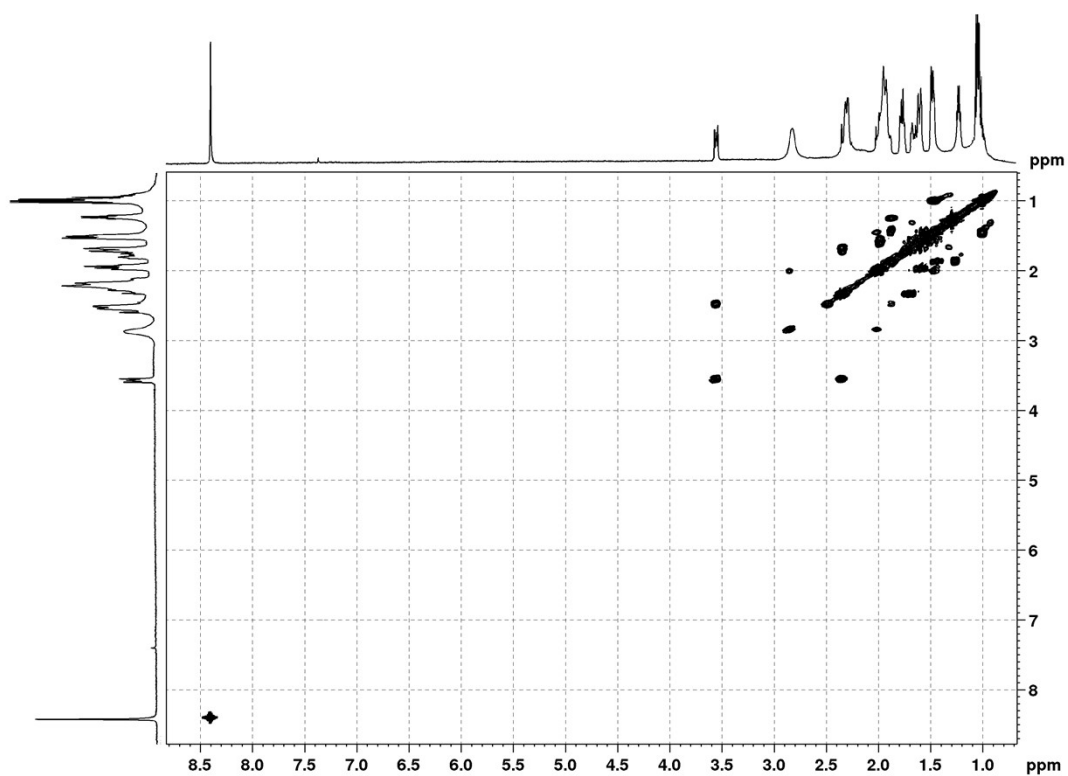


Figure S17. Copy of COSY NMR spectra of compound 4

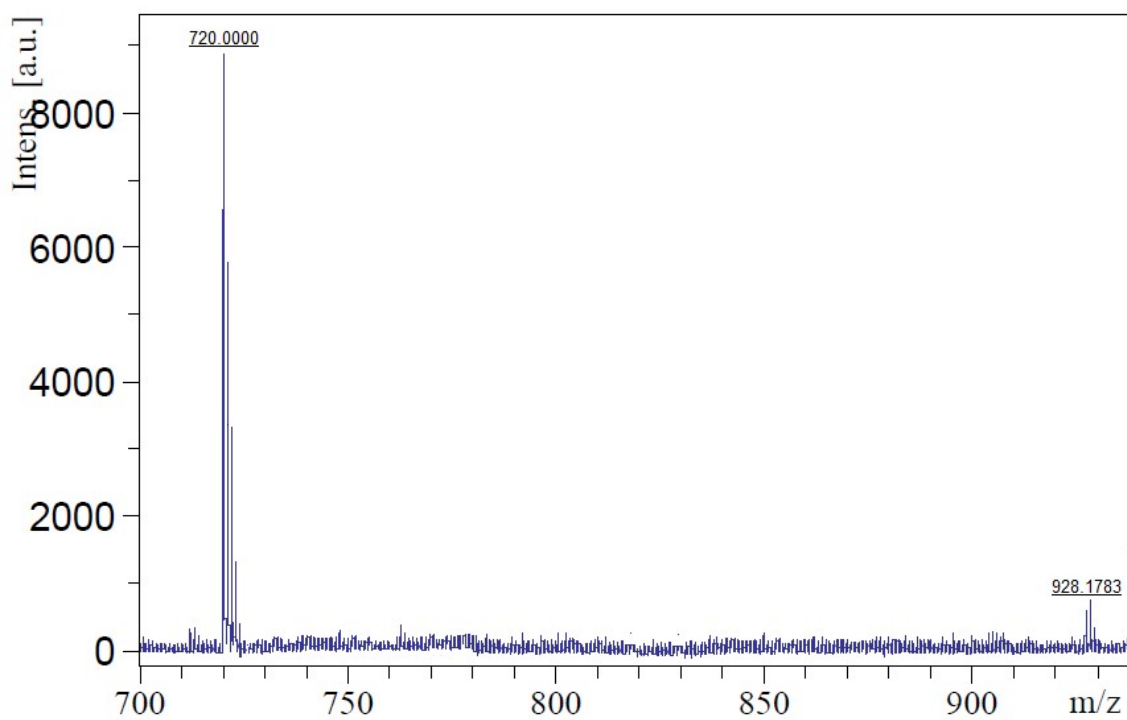


Figure S18. Copy of MALDI TOF spectra of compound 4

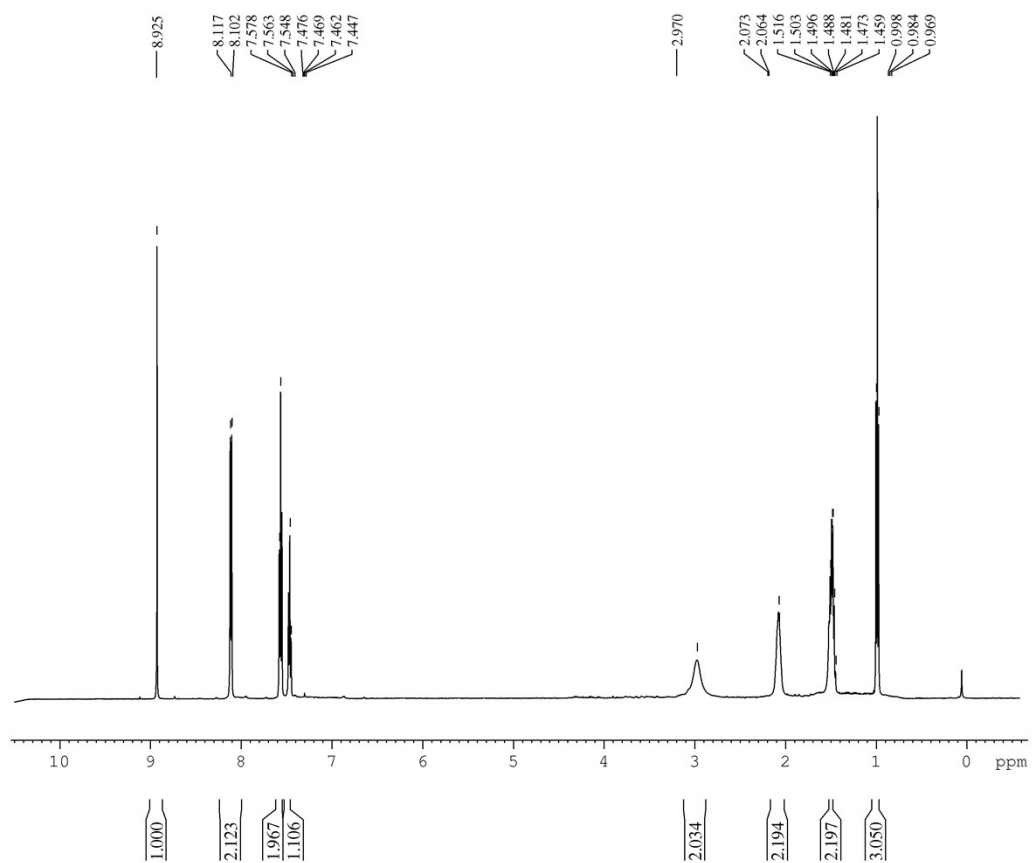


Figure S19. Copy of ^1H NMR spectra of compound **5**

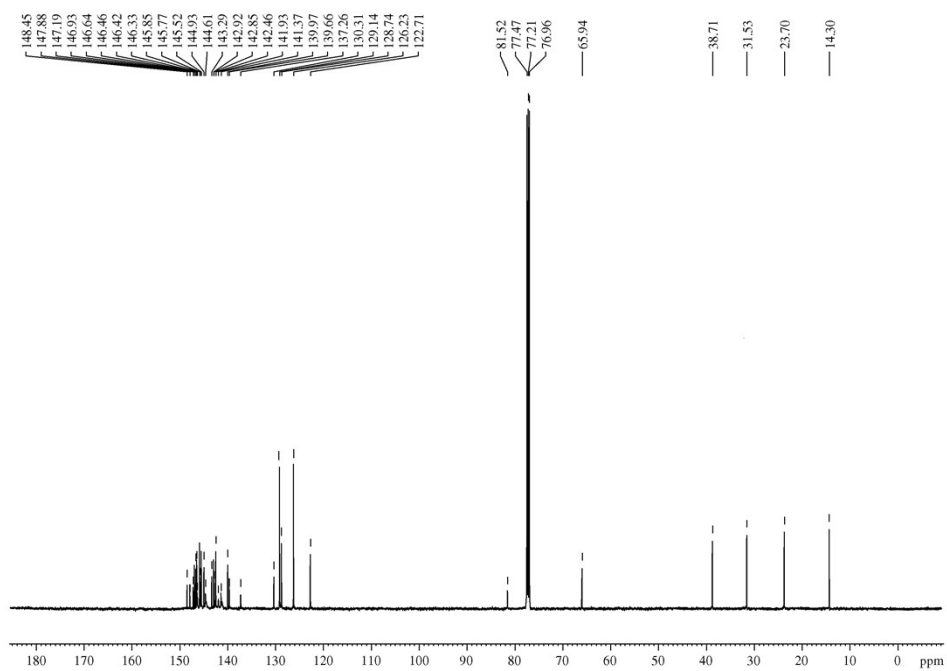


Figure S20. Copy of ^{13}C NMR spectra of compound **5**

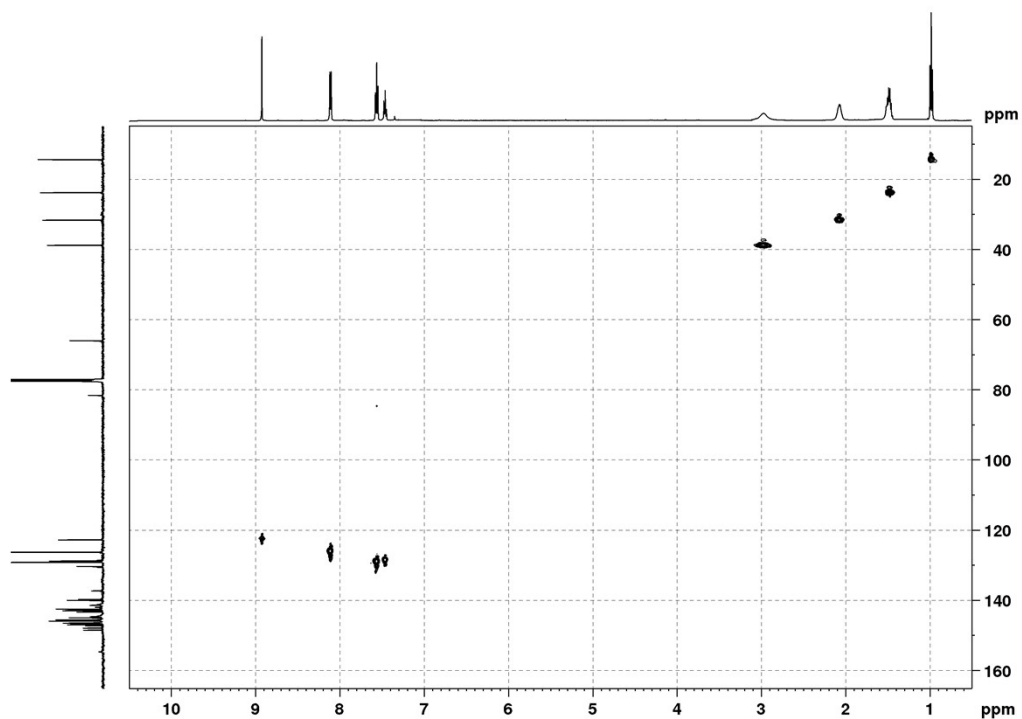


Figure S21. Copy of HSQC NMR spectra of compound **5**

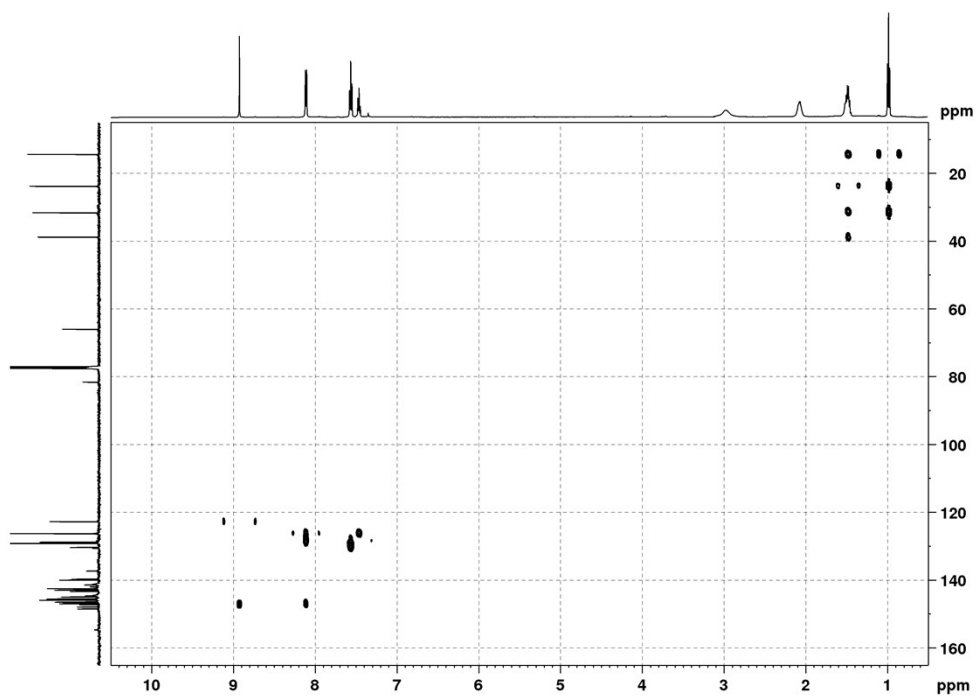


Figure S22. Copy of HMBC NMR spectra of compound **5**

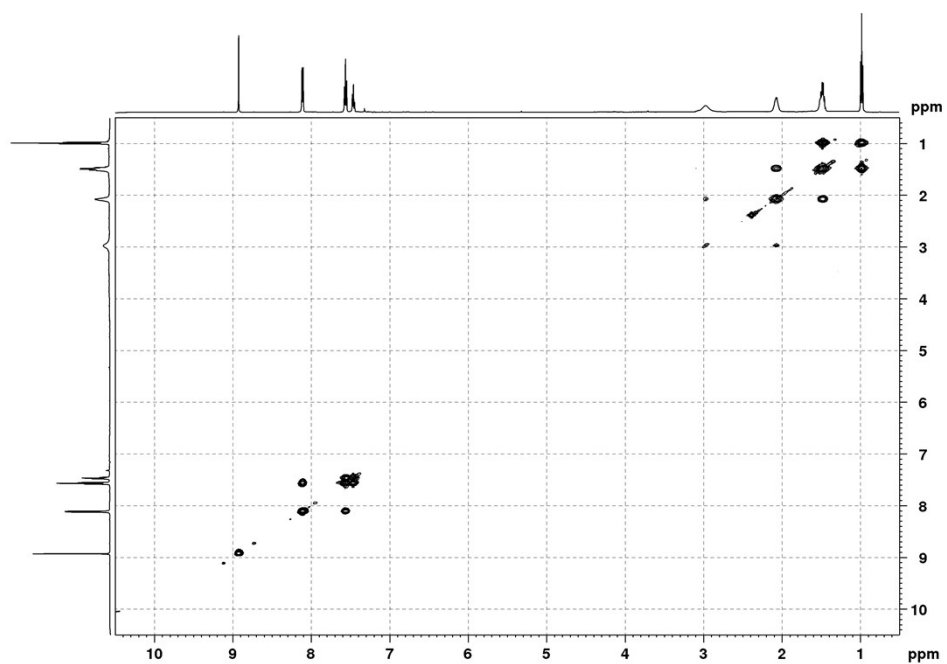


Figure S23. Copy of COSY NMR spectra of compound **5**

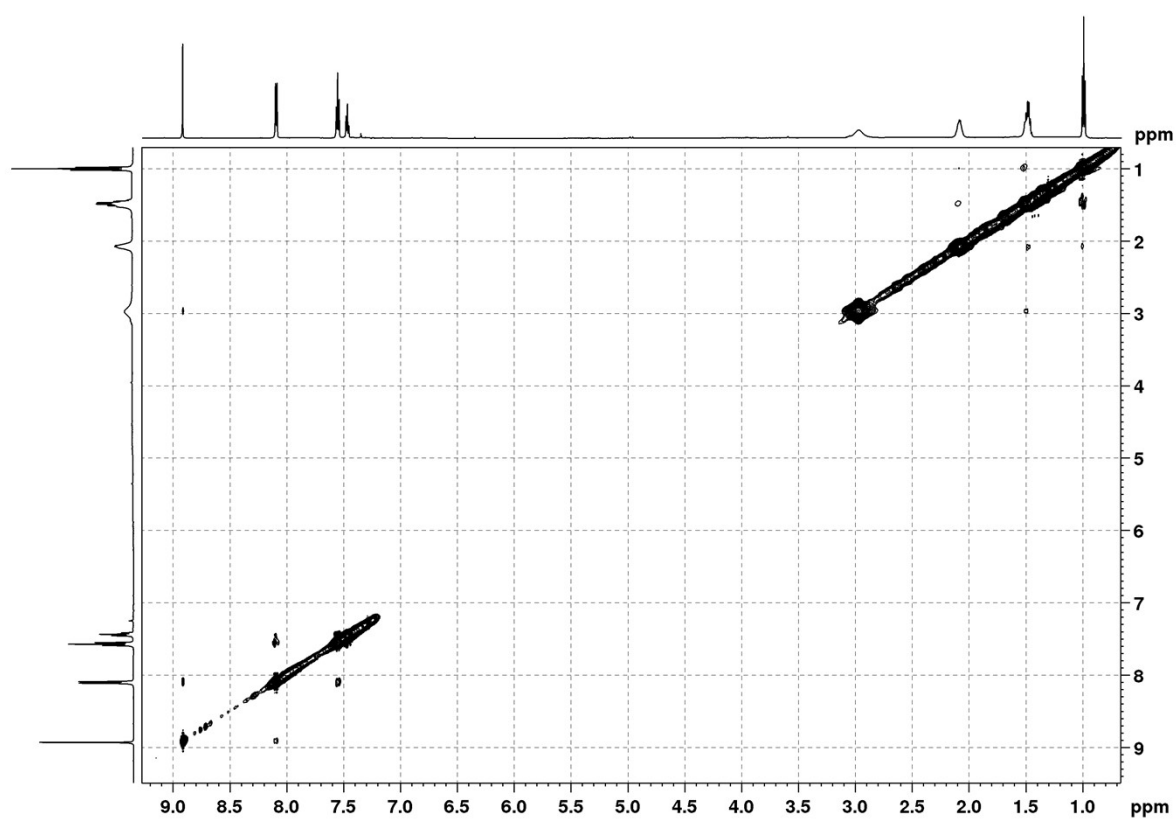


Figure S24. Copy of NOESY NMR spectra of compound **5**

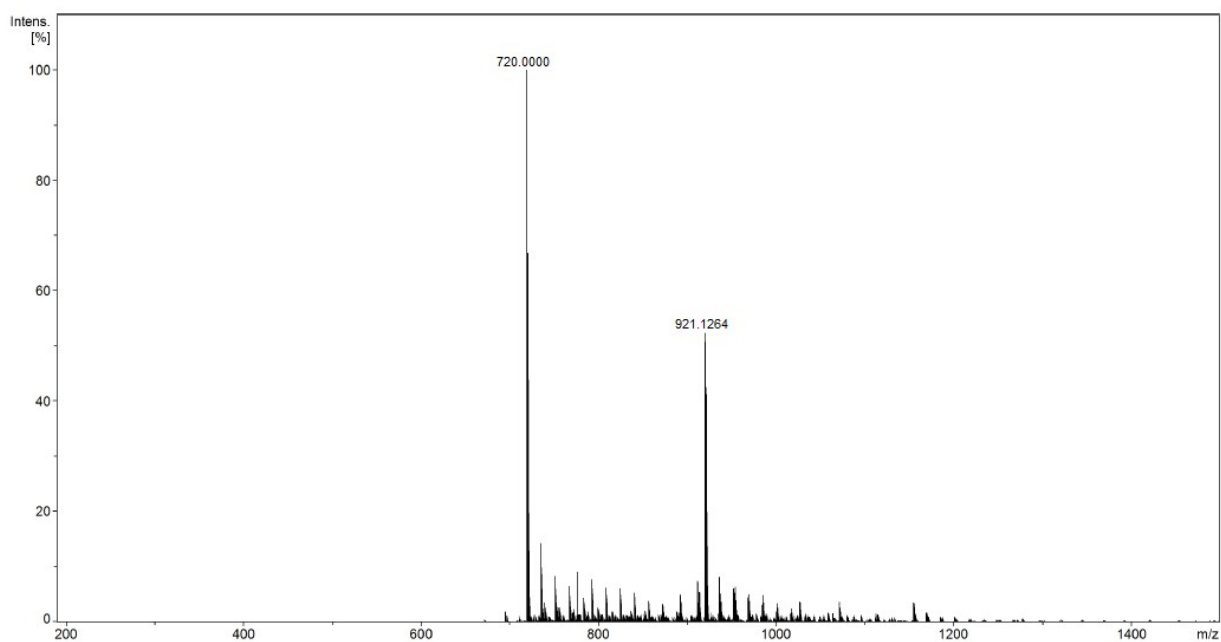


Figure S25. Copy of MALDI TOF spectra of compound **5**

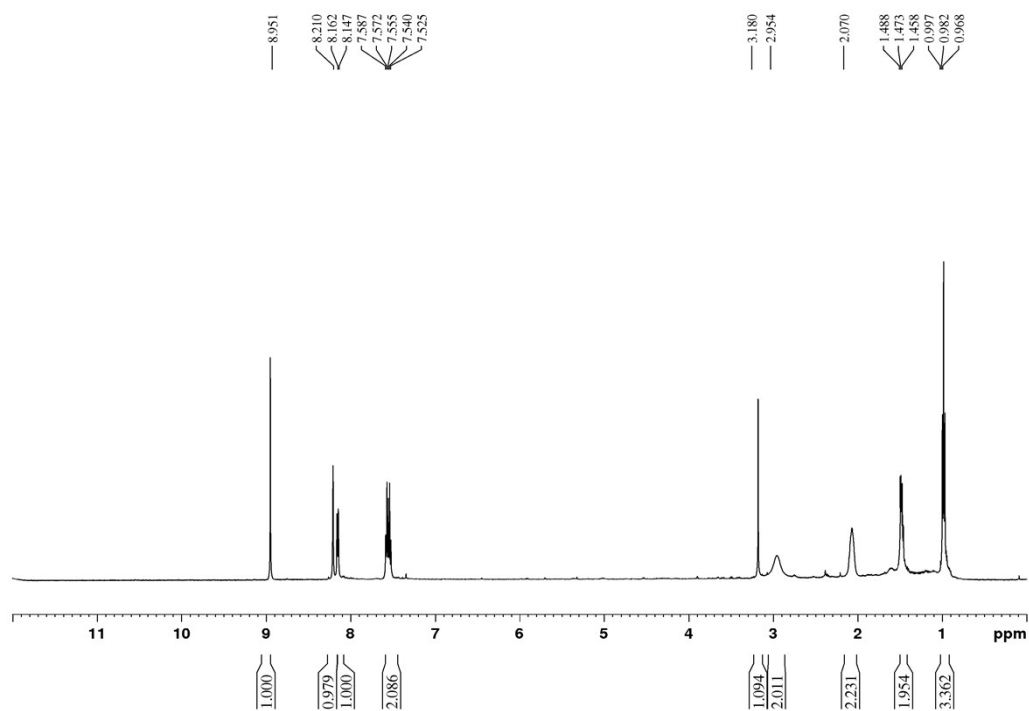


Figure S26. Copy of ¹H NMR spectra of compound **6**

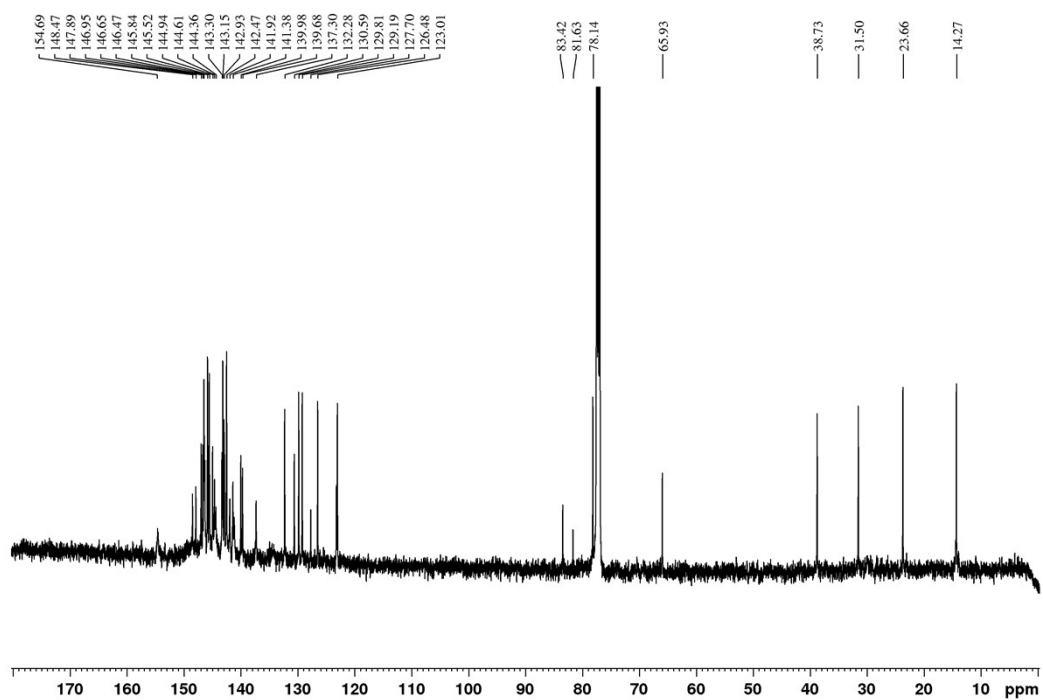


Figure S27. Copy of ^{13}C NMR spectra of compound 6

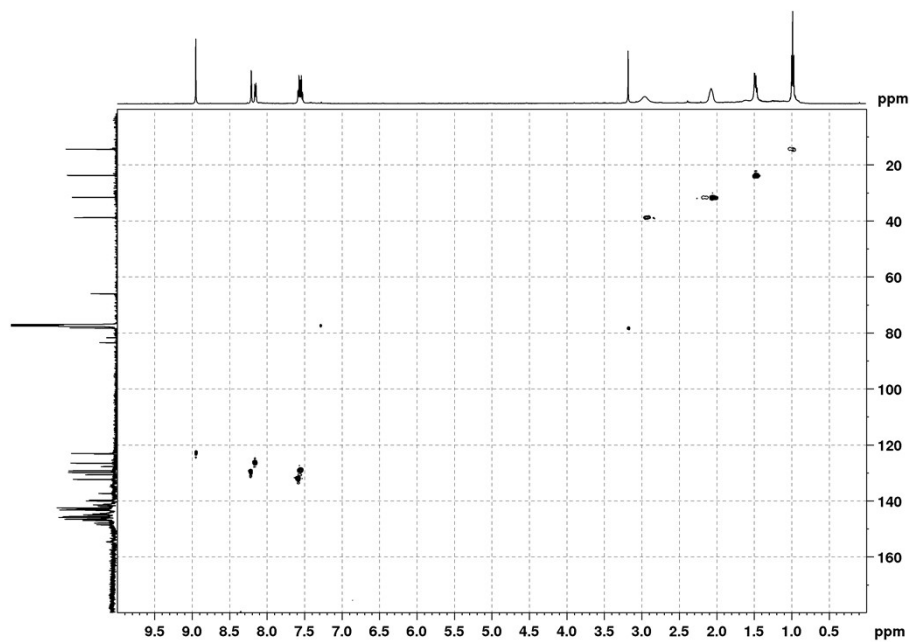


Figure S28. Copy of HSQC NMR spectra of compound 6

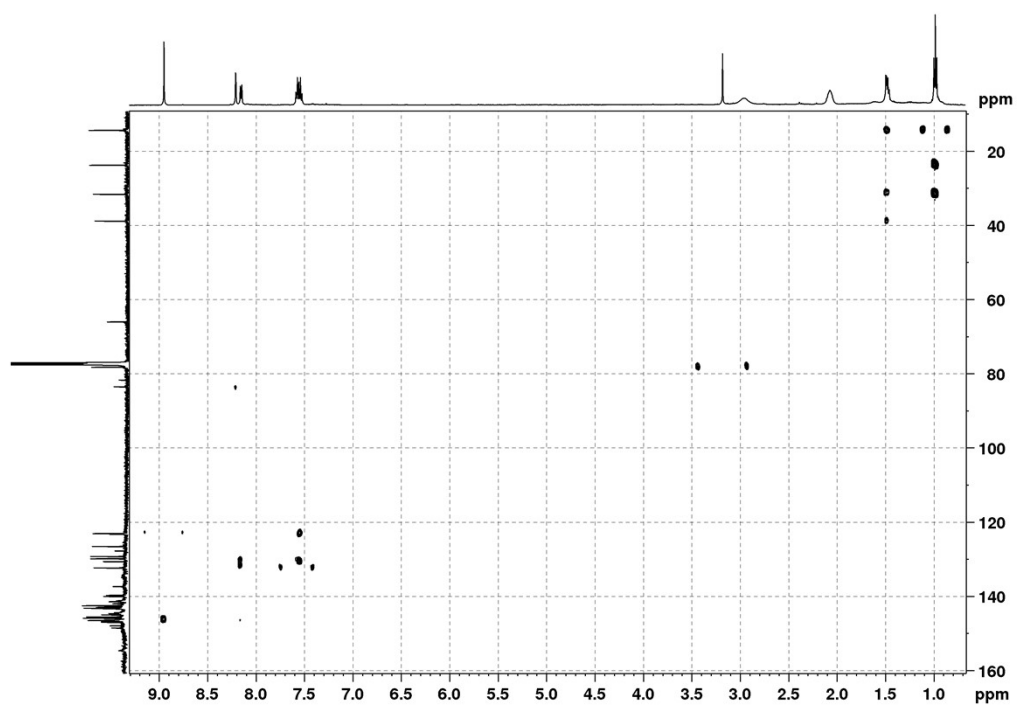


Figure S29. Copy of HMBC NMR spectra of compound **6**

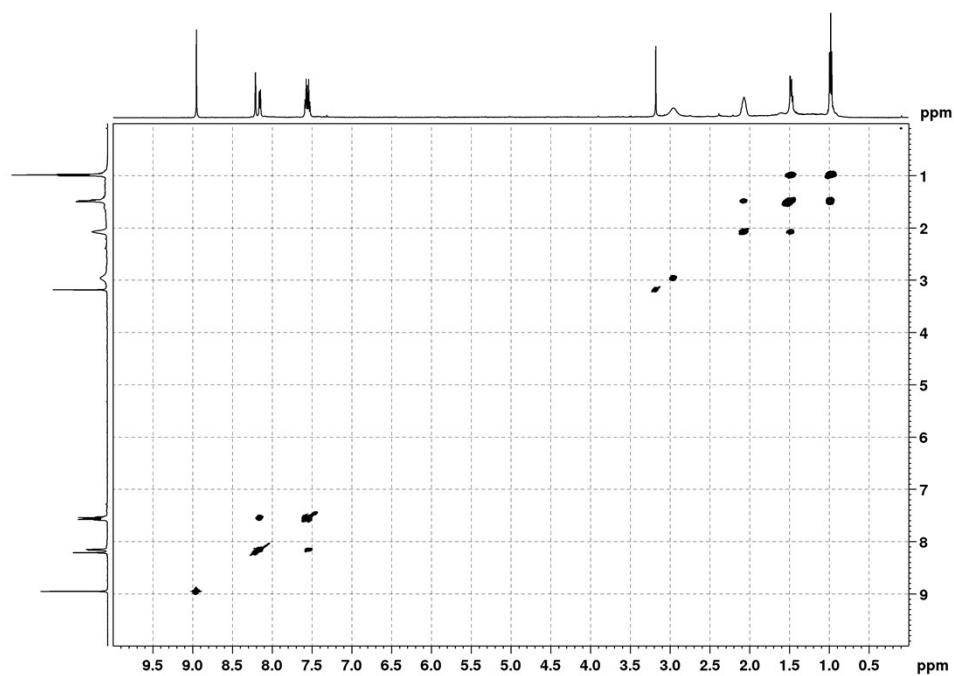


Figure S30. Copy of COSY NMR spectra of compound **6**

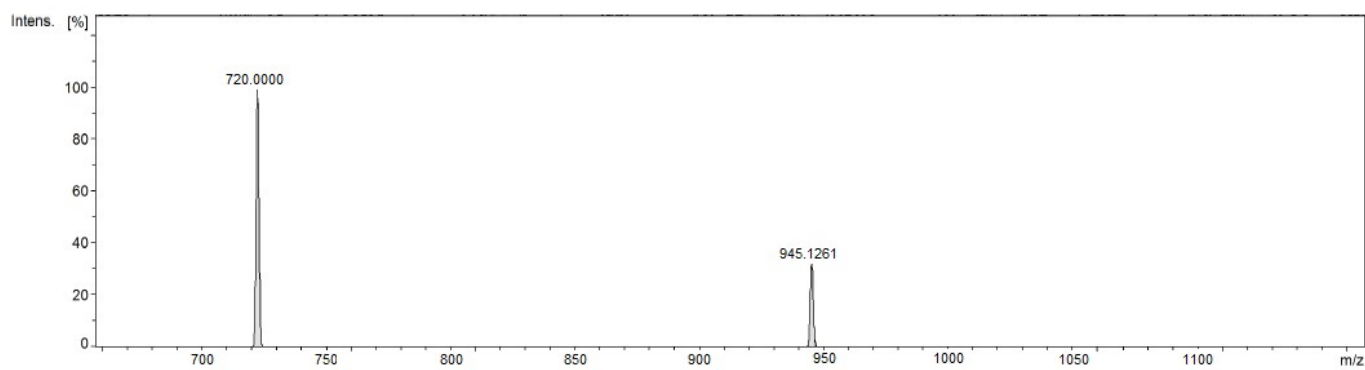


Figure S31. Copy of MALDI TOF spectra of compound 6

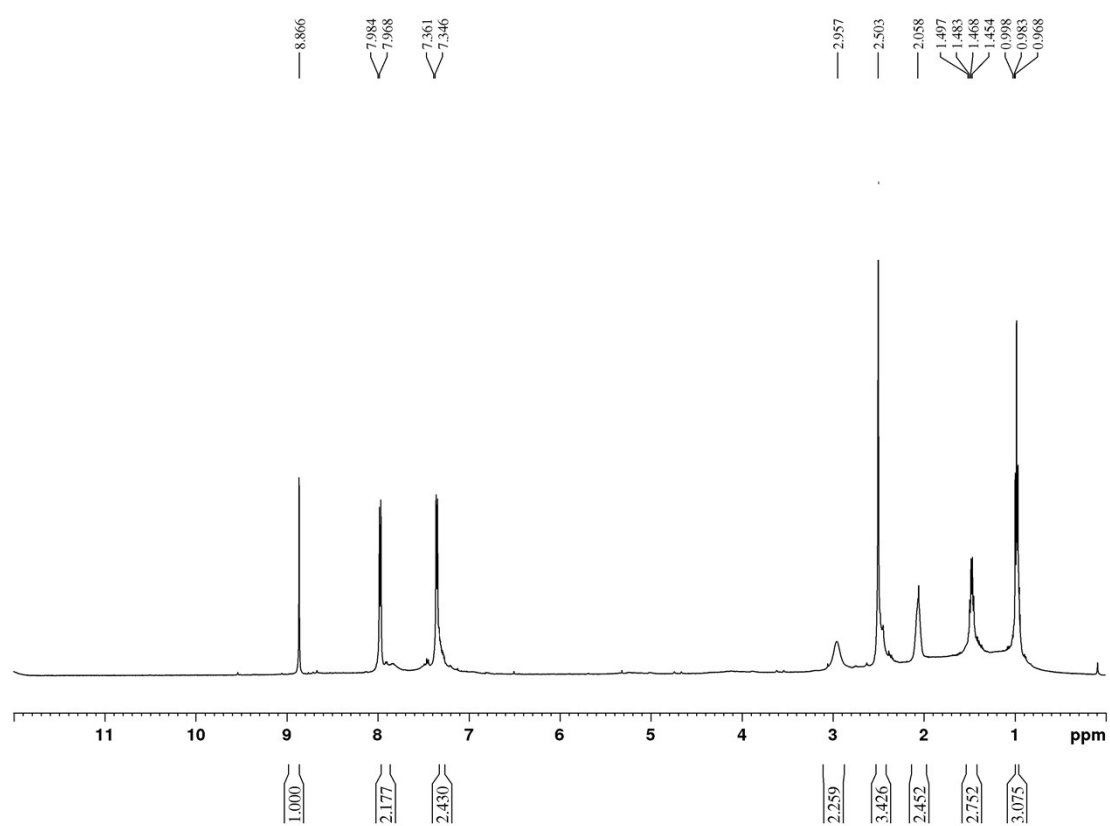


Figure S32. Copy of ¹H NMR spectra of compound 7

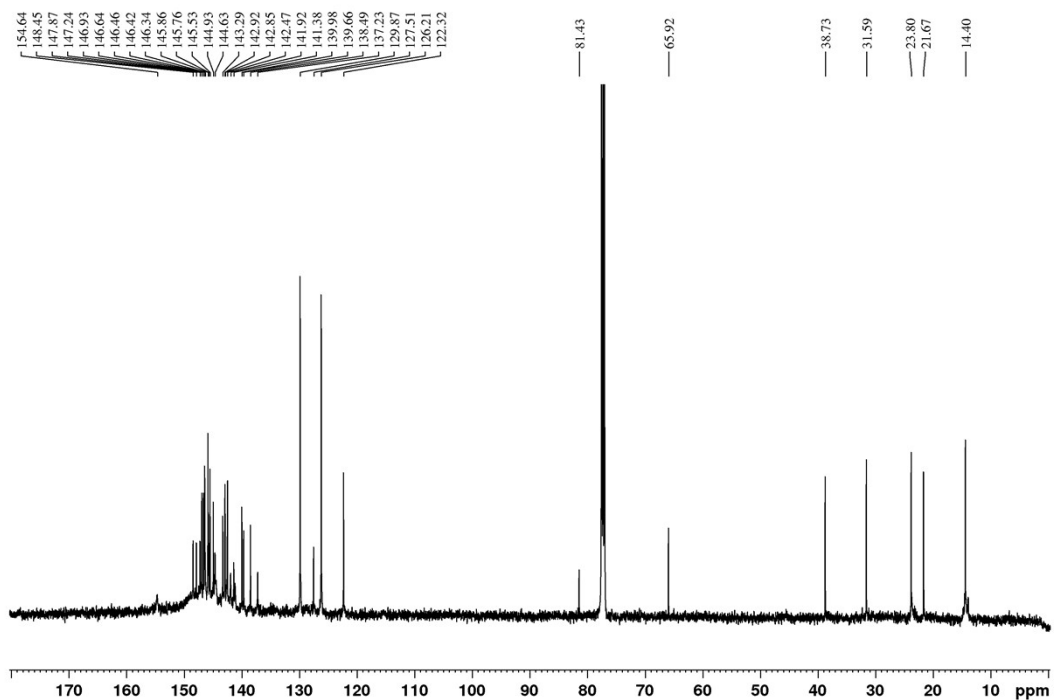


Figure S33. Copy of ^{13}C NMR spectra of compound 7

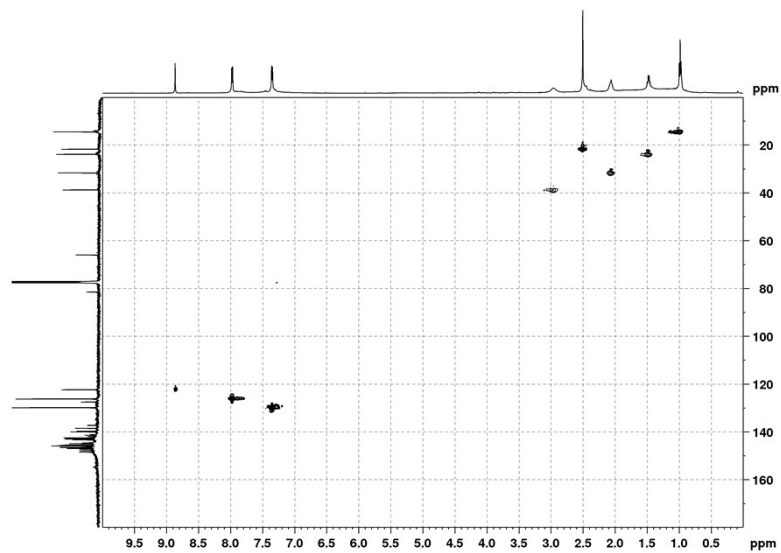


Figure S34. Copy of HSQC spectra of compound 7

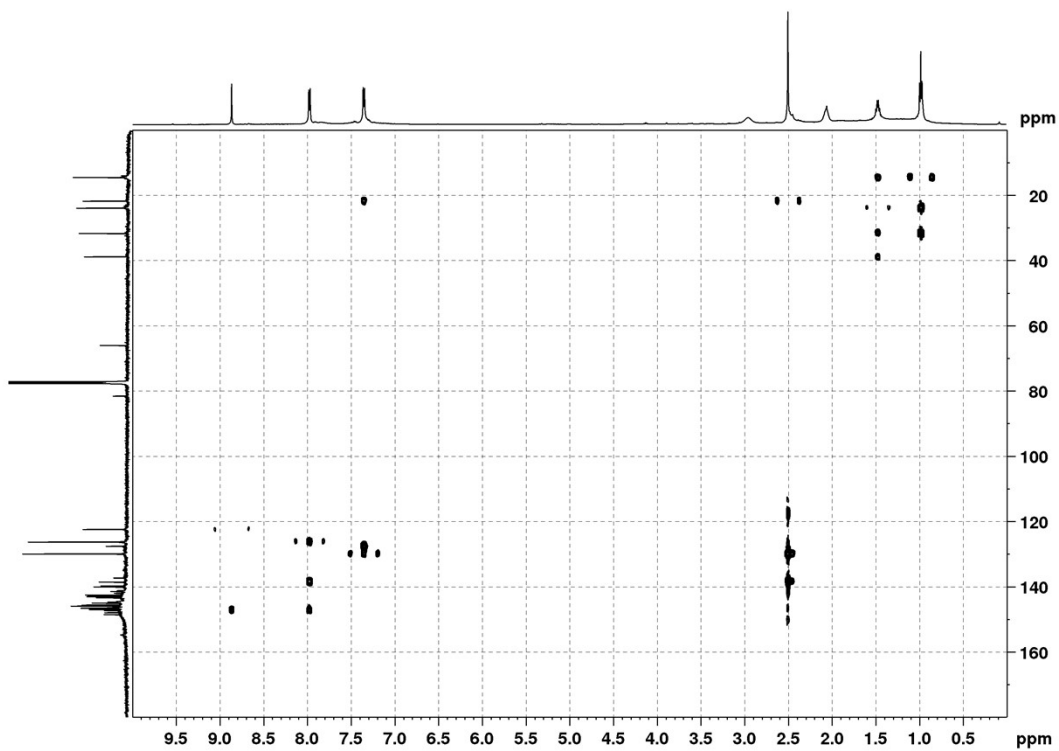


Figure S35. Copy of HMBC spectra of compound 7

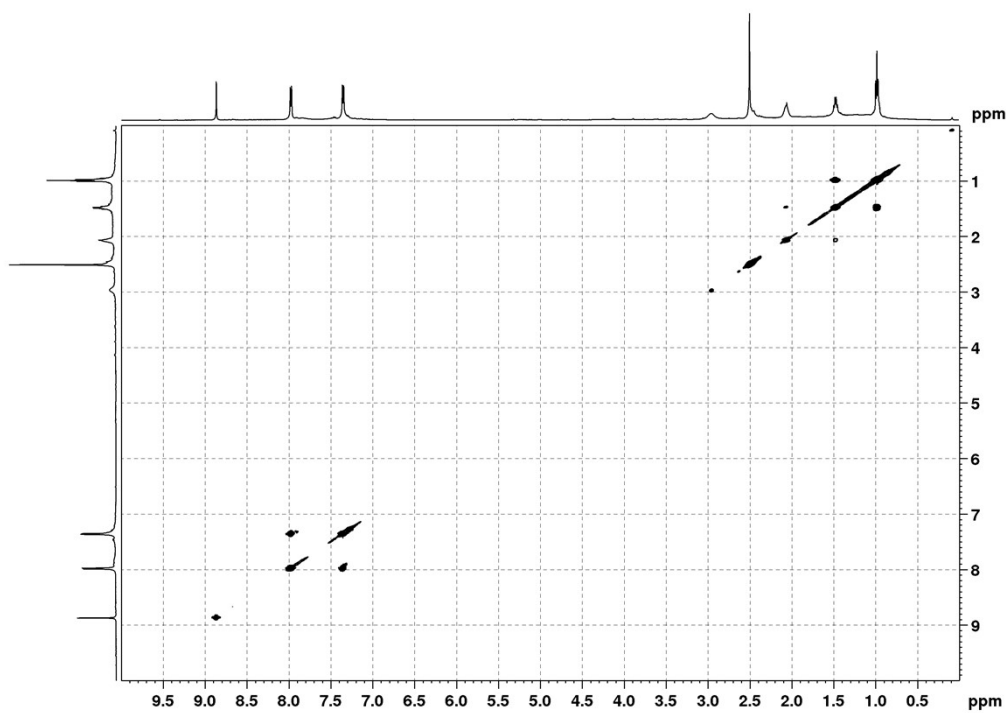


Figure S36. Copy of COSY spectra of compound 7

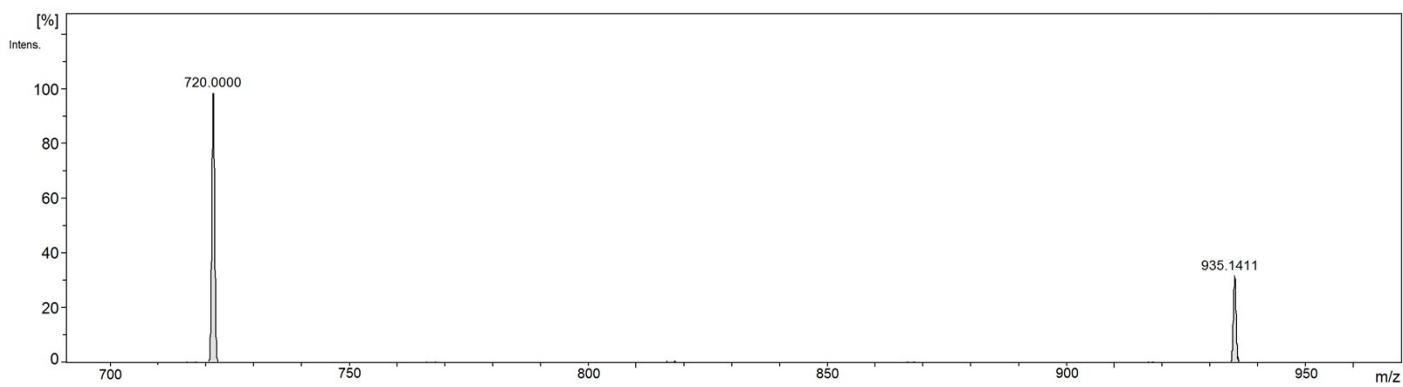


Figure S37. Copy of MALDI TOF spectra of compound **7**

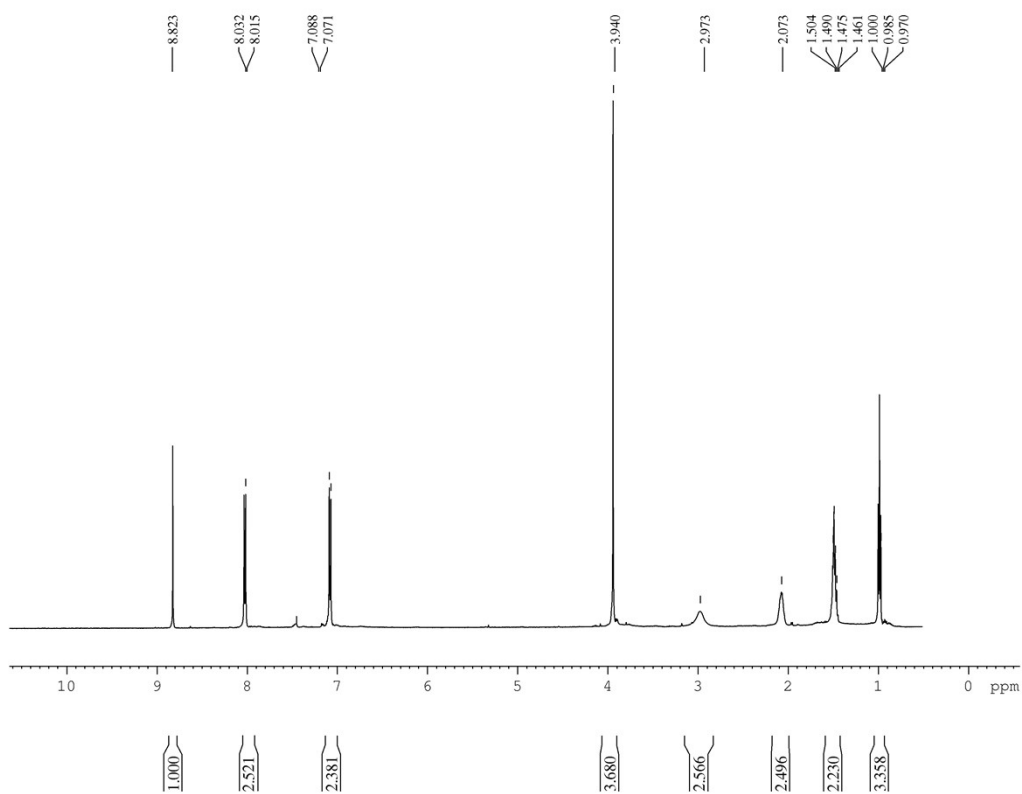


Figure S38. Copy of ¹H NMR spectra of compound **8**

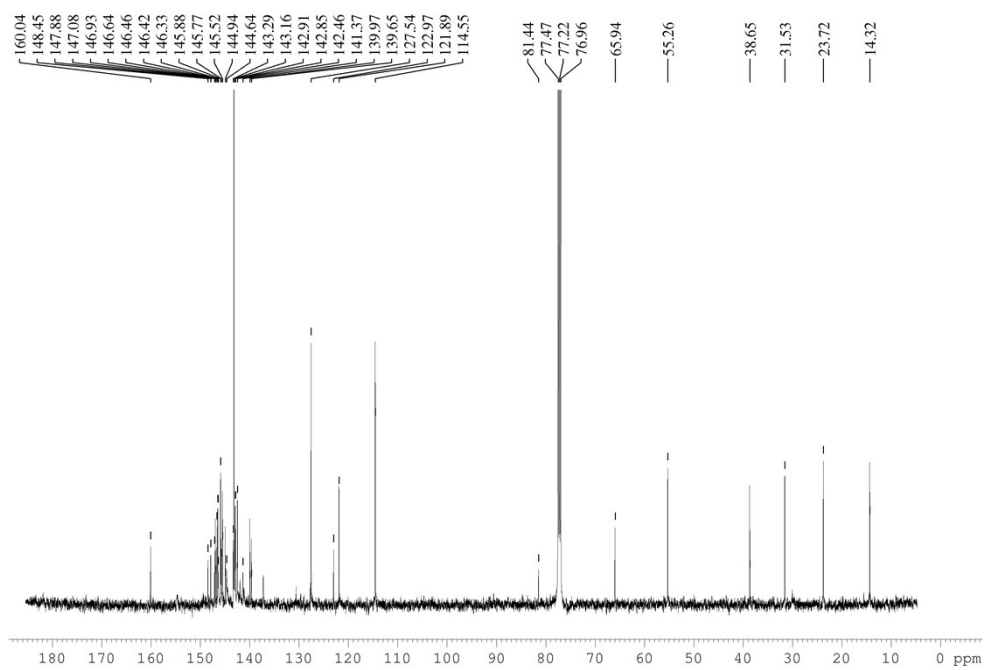


Figure S39. Copy of ^{13}C NMR spectra of compound 8

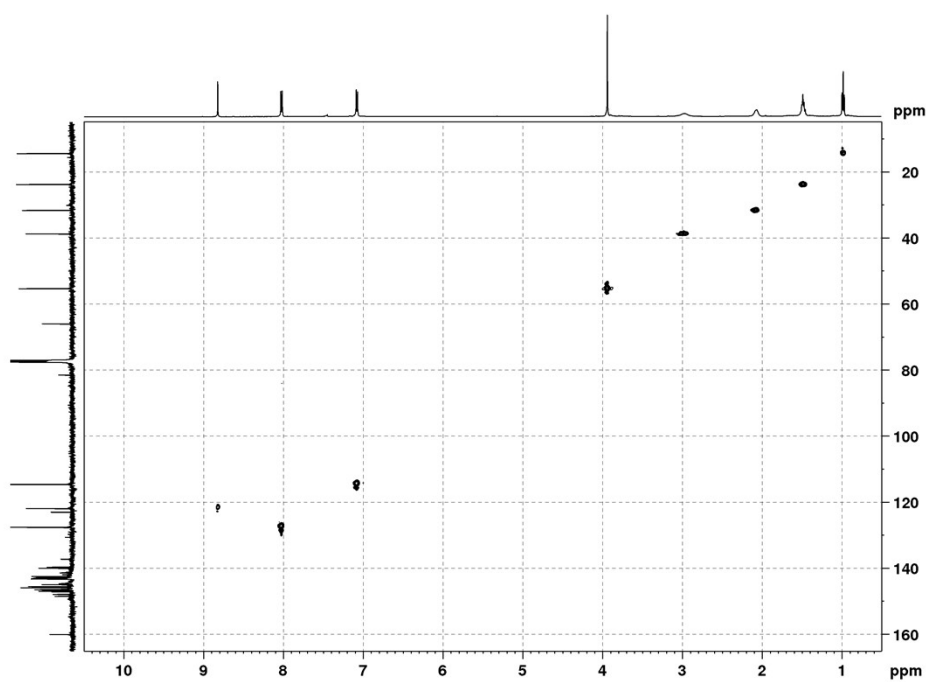


Figure S40. Copy of HSQC NMR spectra of compound 8

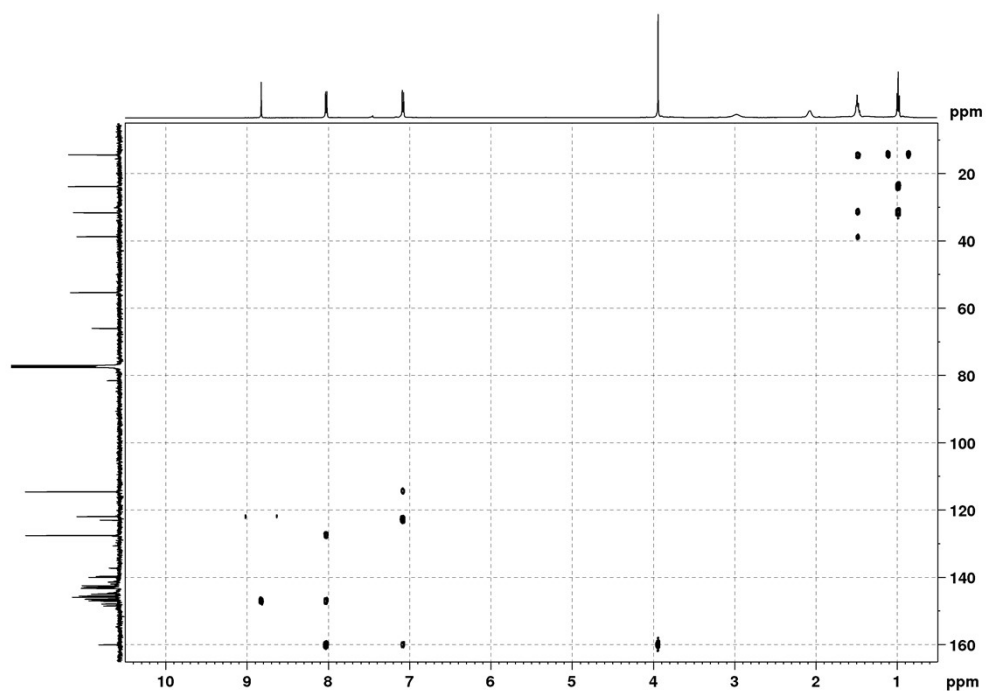


Figure S41. Copy of HMBC NMR spectra of compound 8

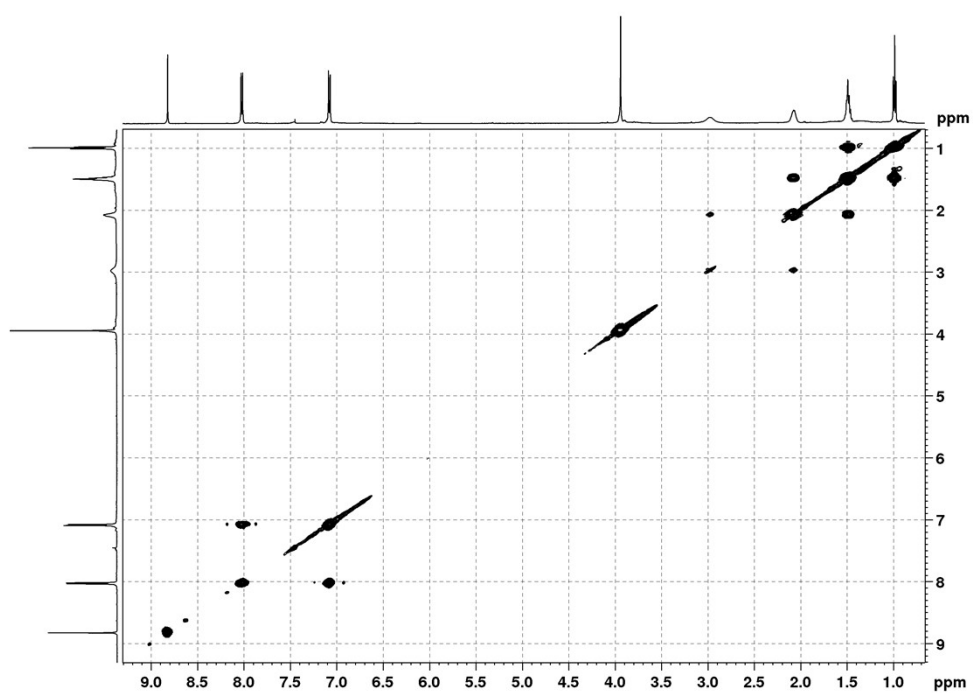


Figure S42. Copy of COSY spectra of compound 8

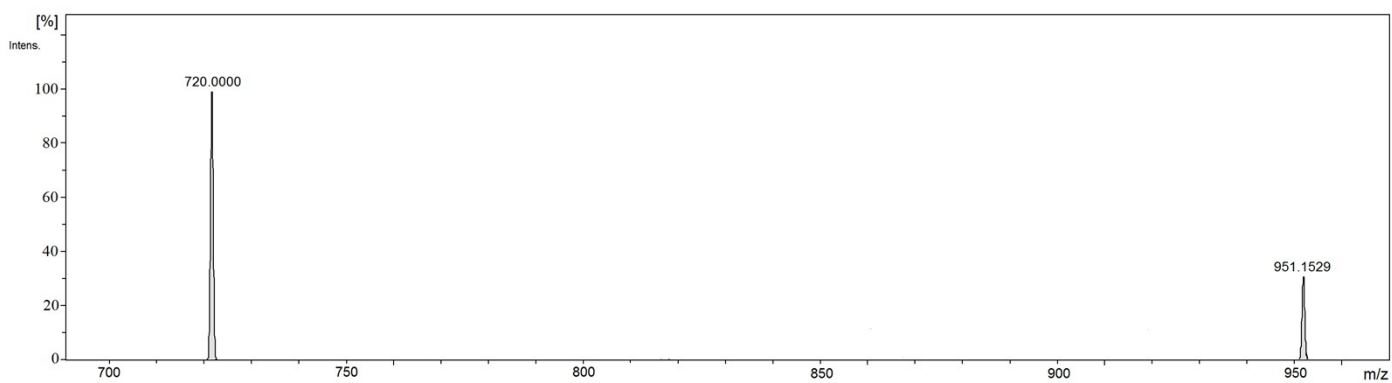


Figure S43. Copy of MALDI TOF spectra of compound 8

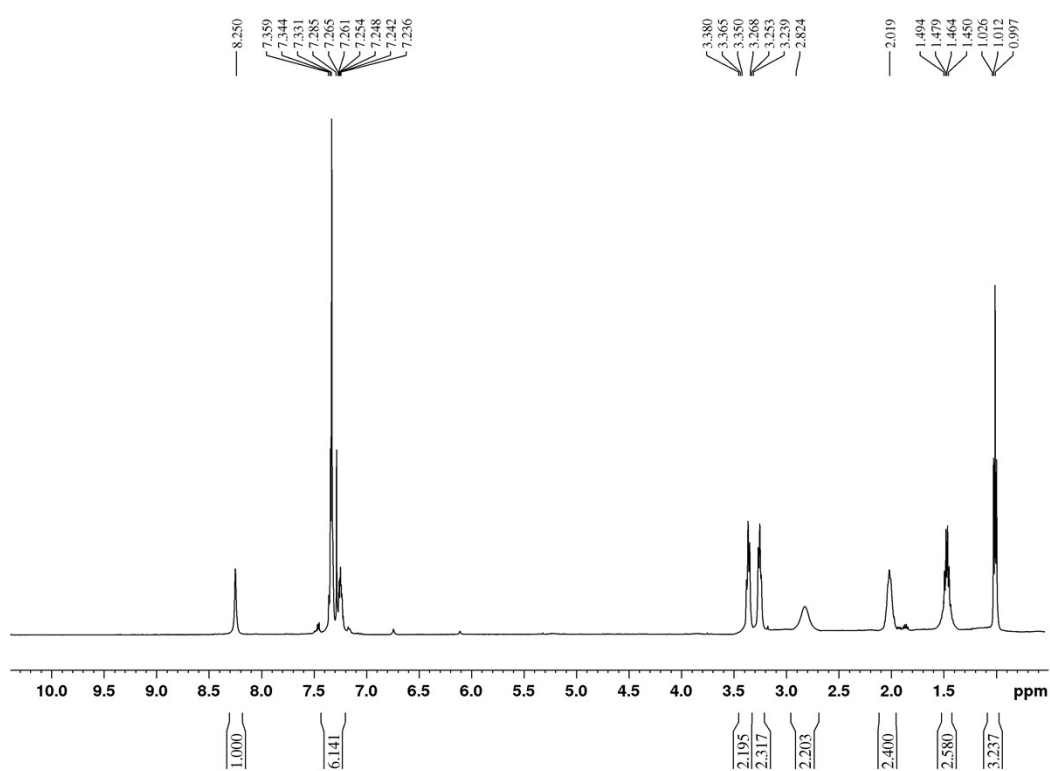


Figure S44. Copy of ^1H NMR spectra of compound 9

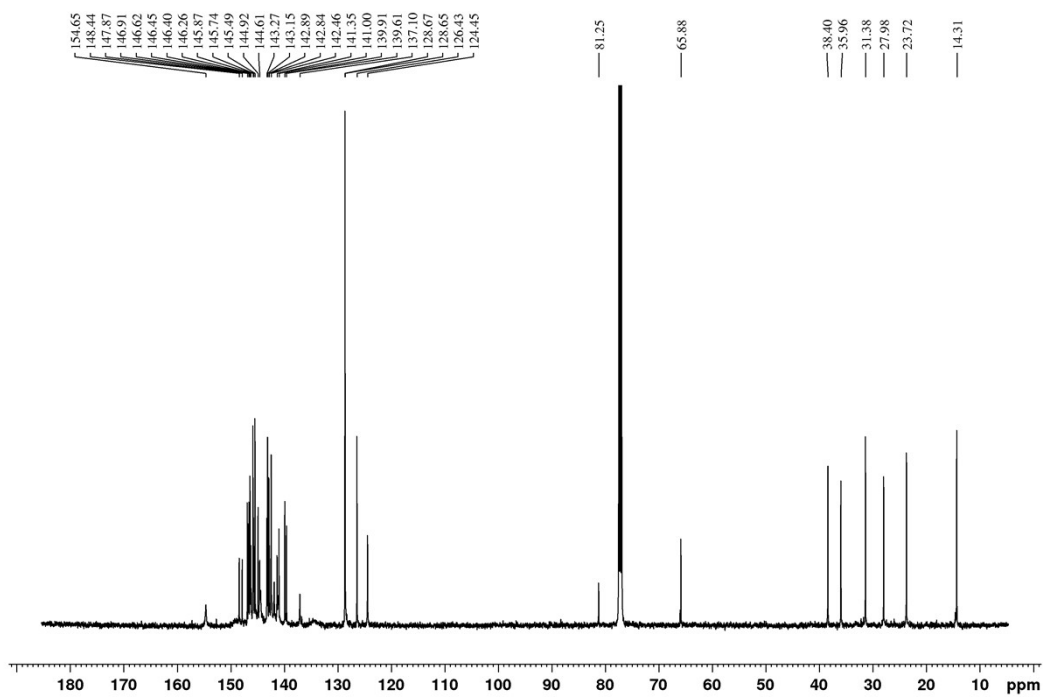


Figure S45. Copy of ^{13}C NMR spectra of compound **9**

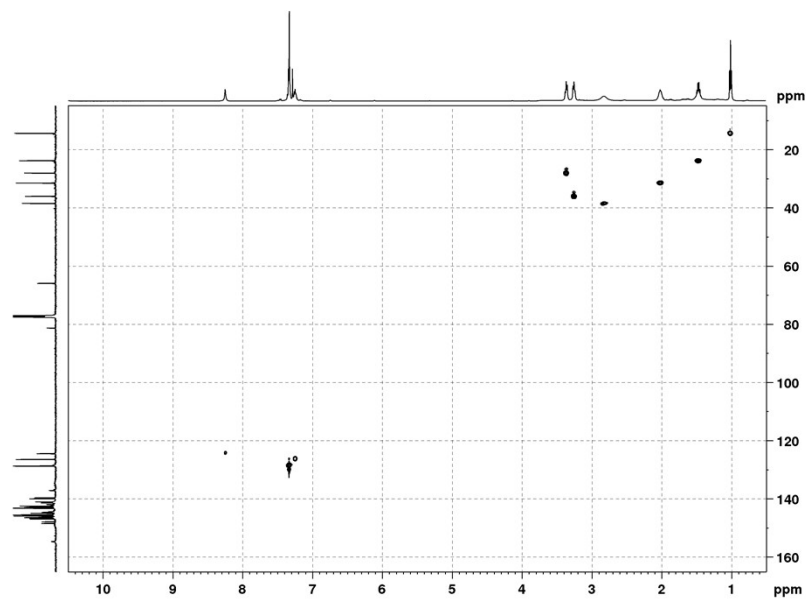


Figure S46. Copy of HSQC NMR spectra of compound **9**

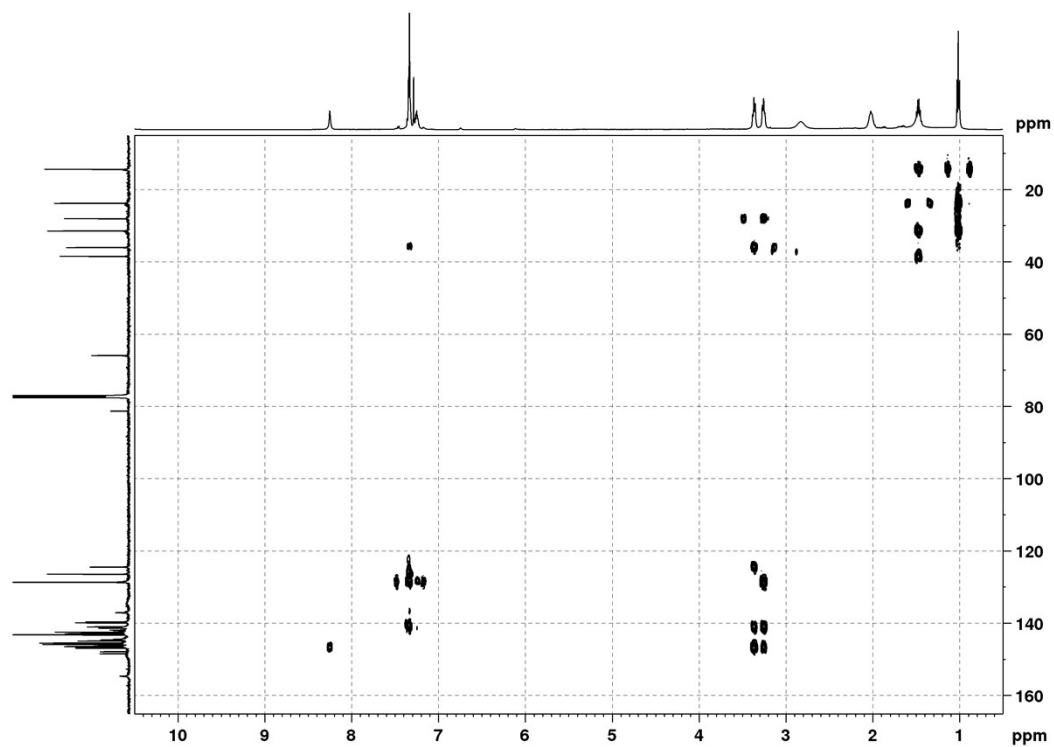


Figure S47. Copy of HMBC NMR spectra of compound 9

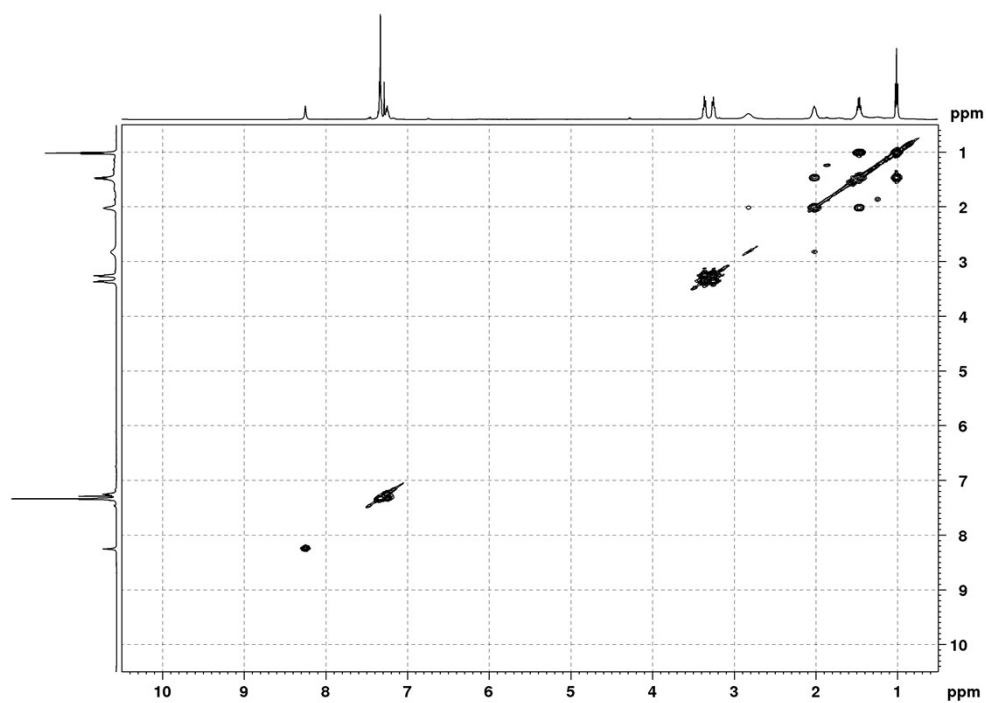


Figure S48. Copy of COSY NMR spectra of compound 9

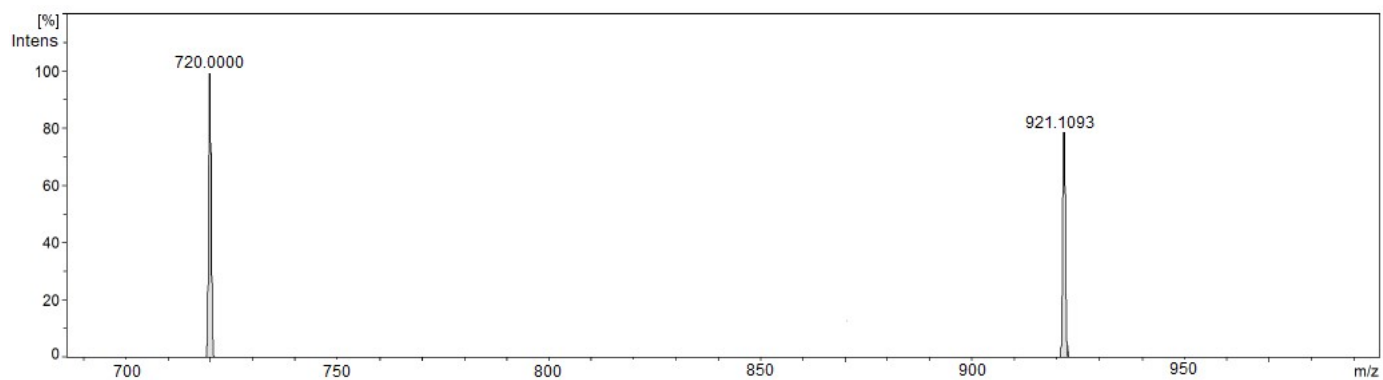


Figure S49. Copy of MALDI TOF spectra of compound **9**

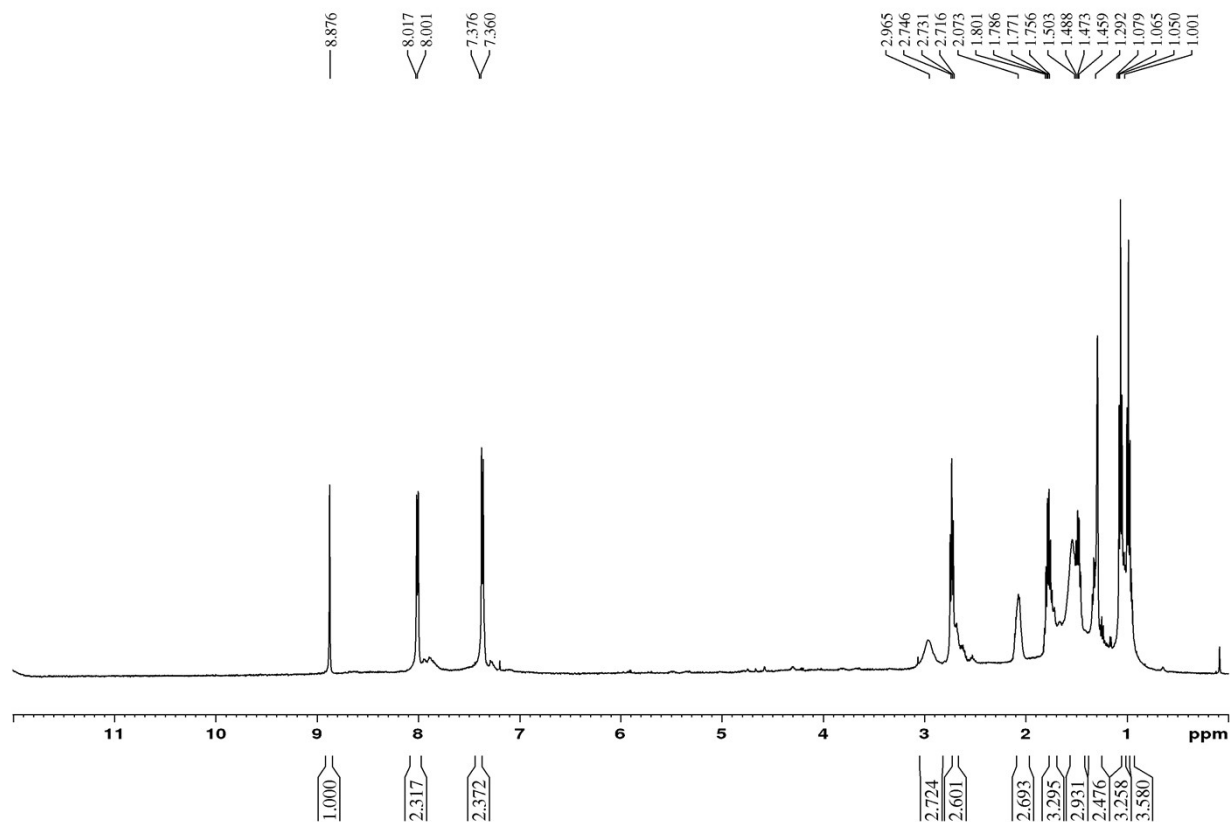


Figure S50. Copy of ¹H NMR spectra of compound **10**

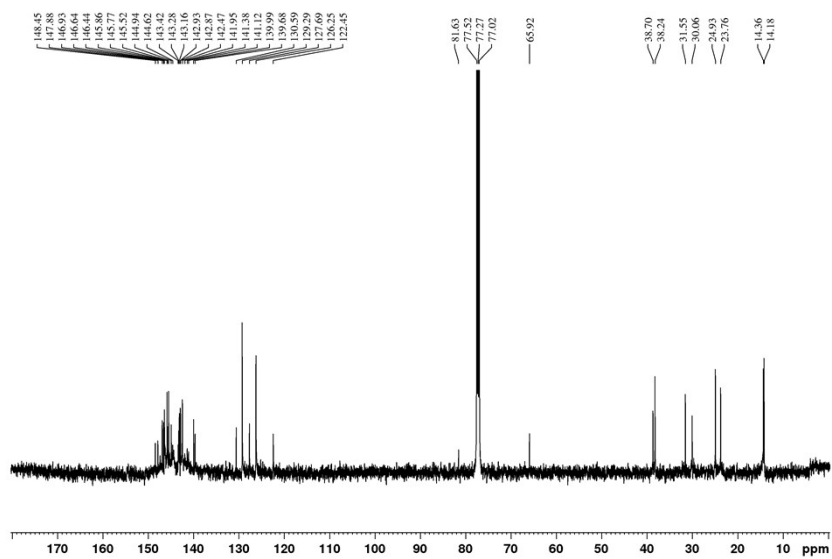


Figure S51. Copy of ^{13}C NMR spectra of compound 10

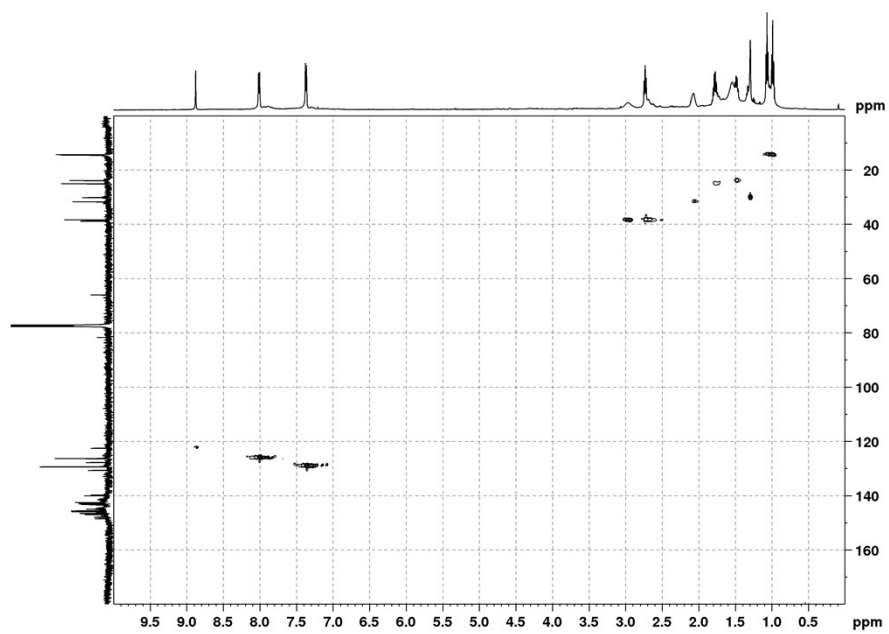


Figure S52. Copy of HSQC NMR spectra of compound 10

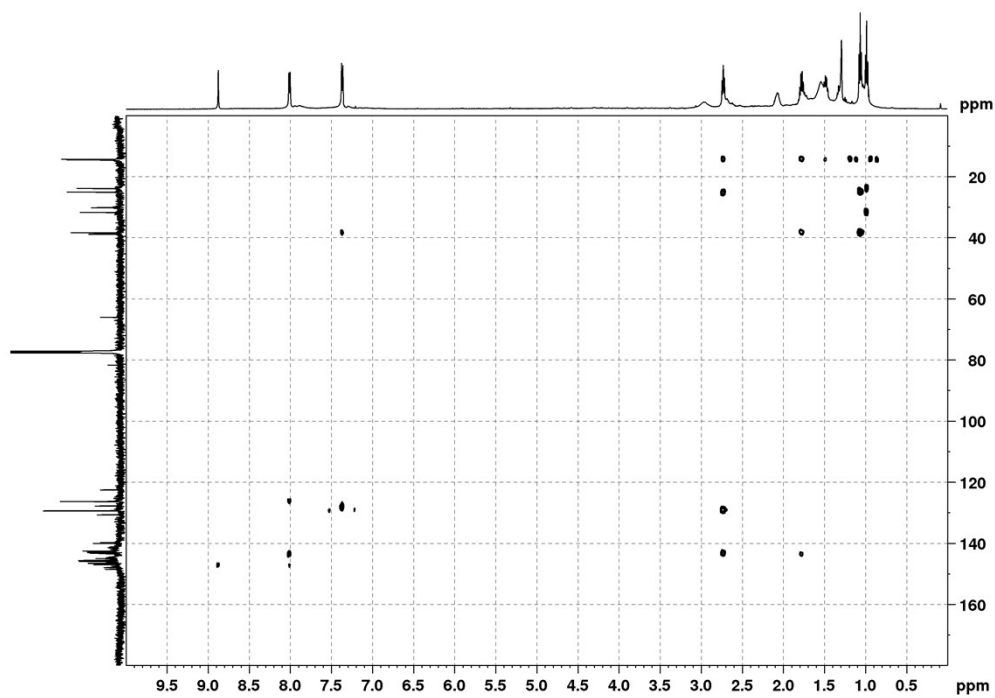


Figure S53. Copy of HMBC NMR spectra of compound **10**

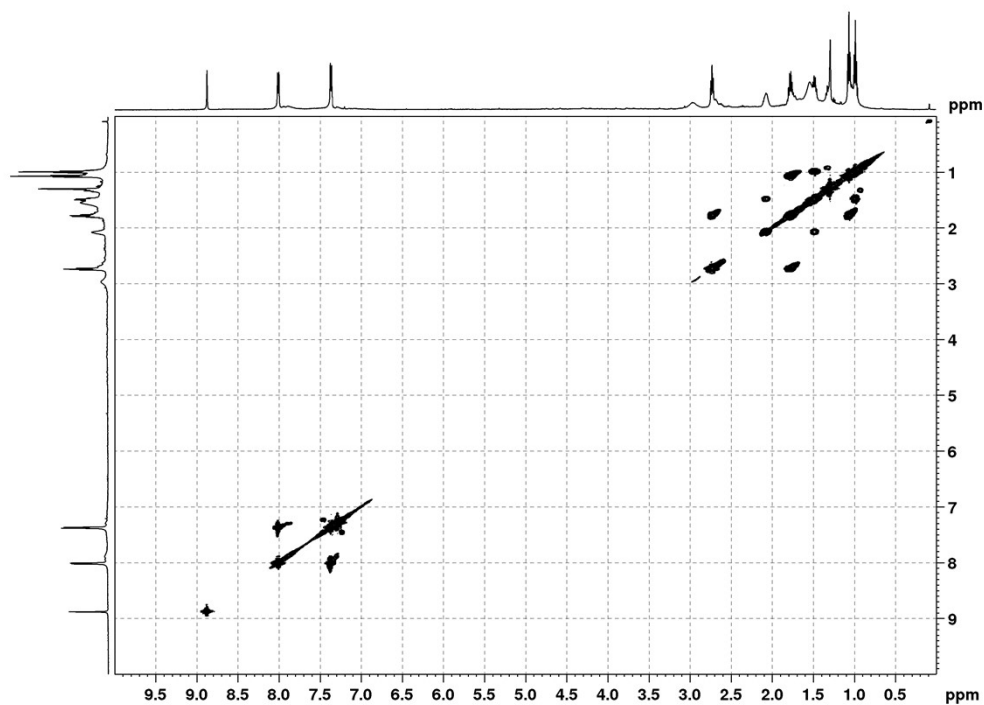


Figure S54. Copy of COSY NMR spectra of compound **10**

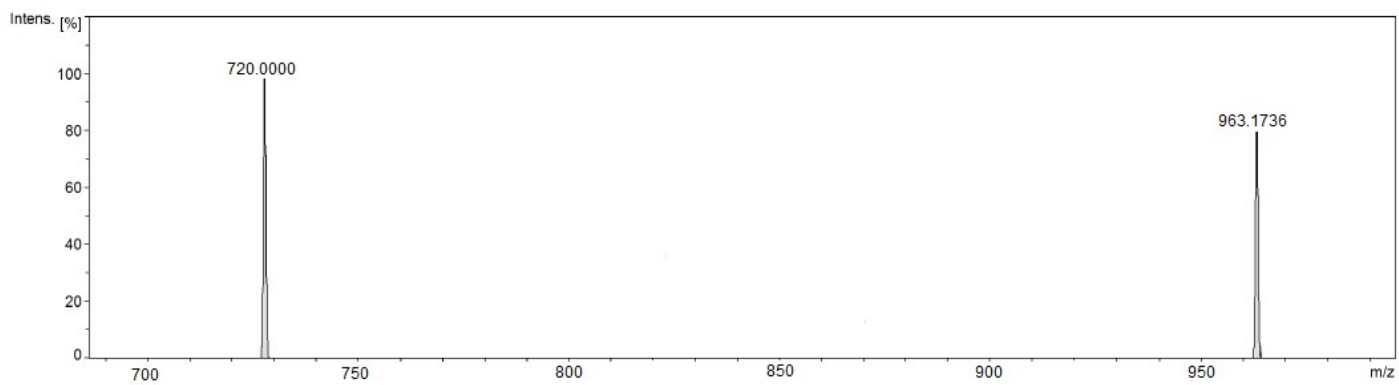


Figure S55. Copy of MALDI TOF spectra of compound 10

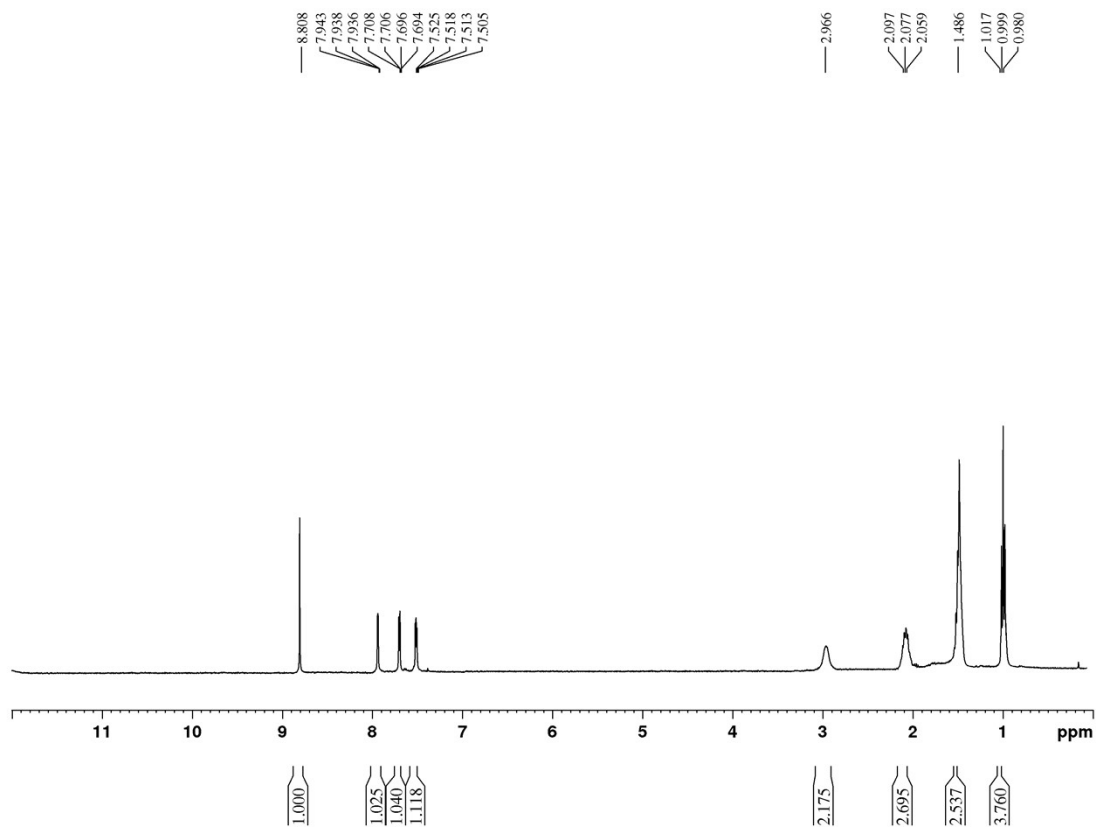


Figure S56. Copy of ¹H NMR spectra of compound 11

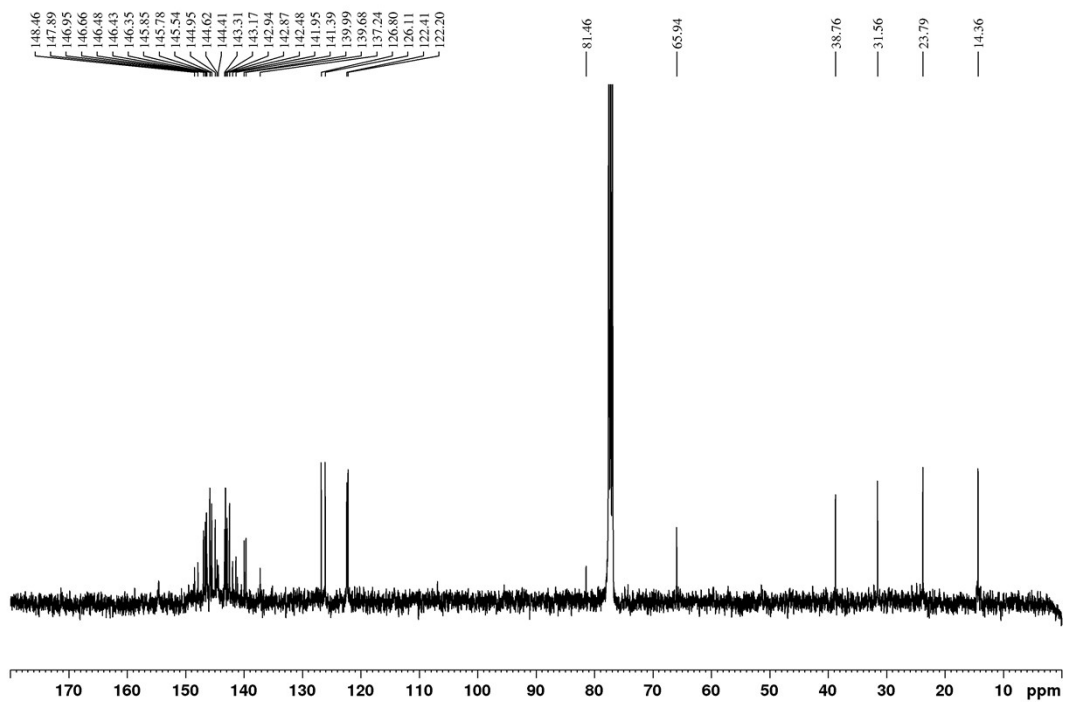


Figure S57. Copy of ^{13}C NMR spectra of compound 11

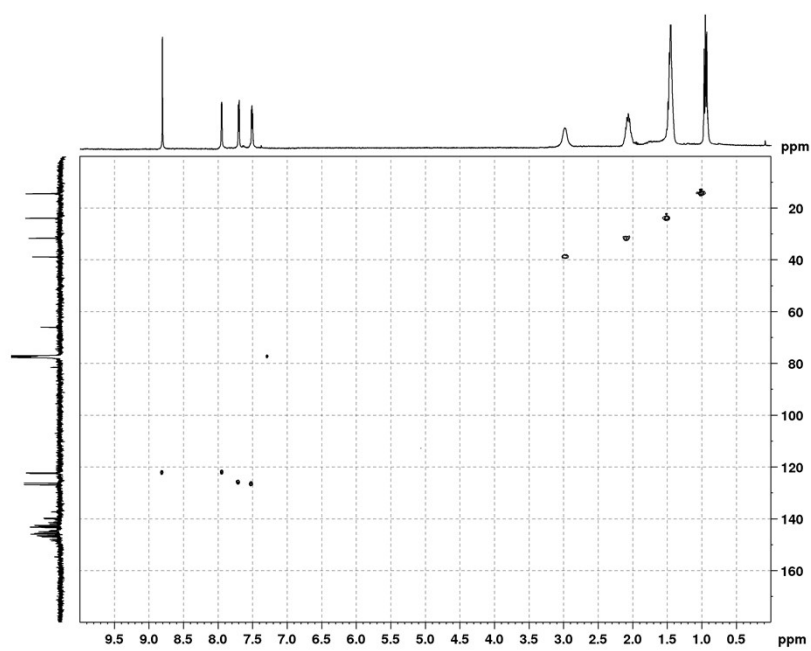


Figure S58. Copy of HSQC NMR spectra of compound 11

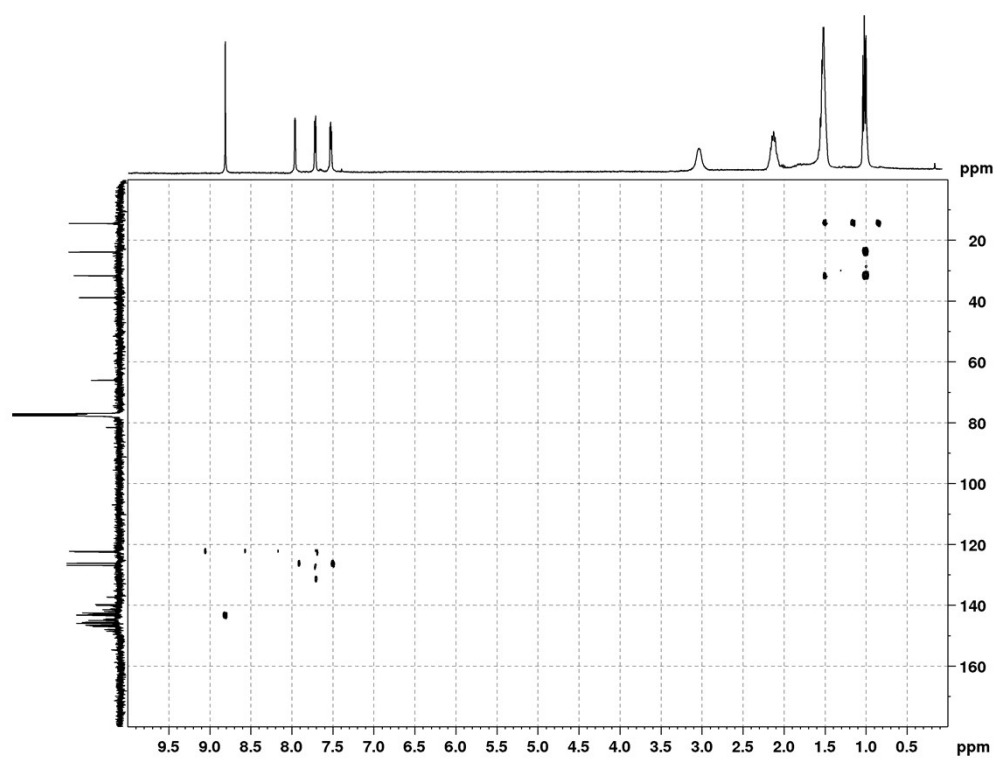


Figure S59. Copy of HMBC NMR spectra of compound **11**

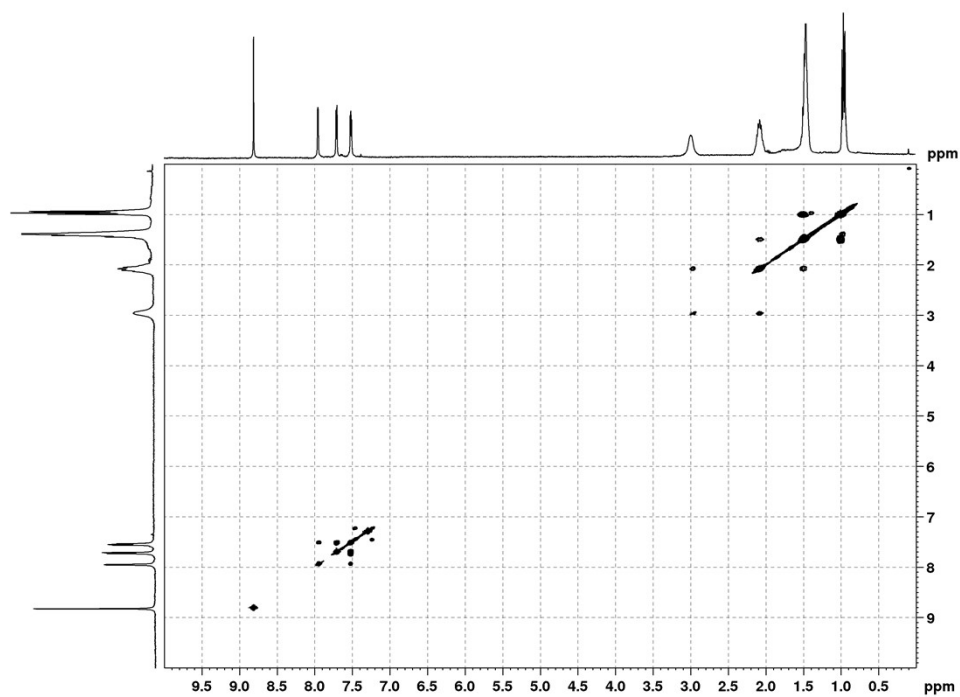


Figure S60. Copy of COSY NMR spectra of compound **11**

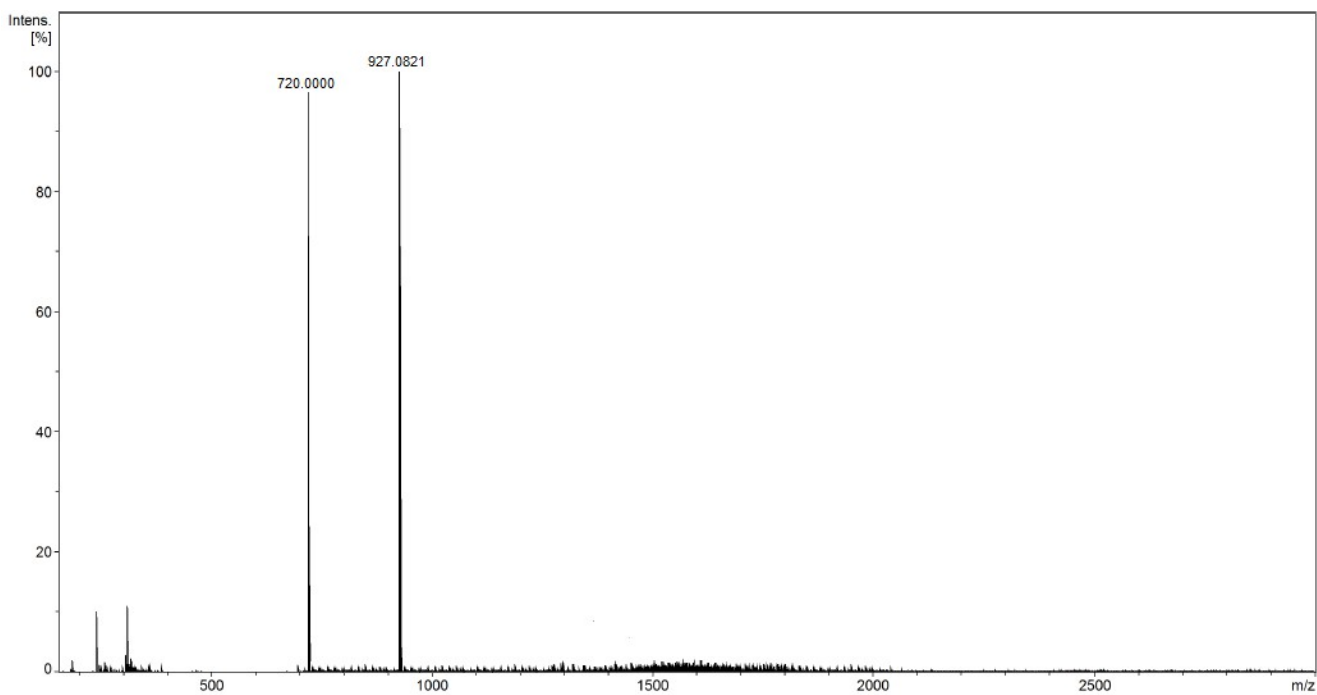


Figure S61. Copy of MALDI TOF spectra of compound 11

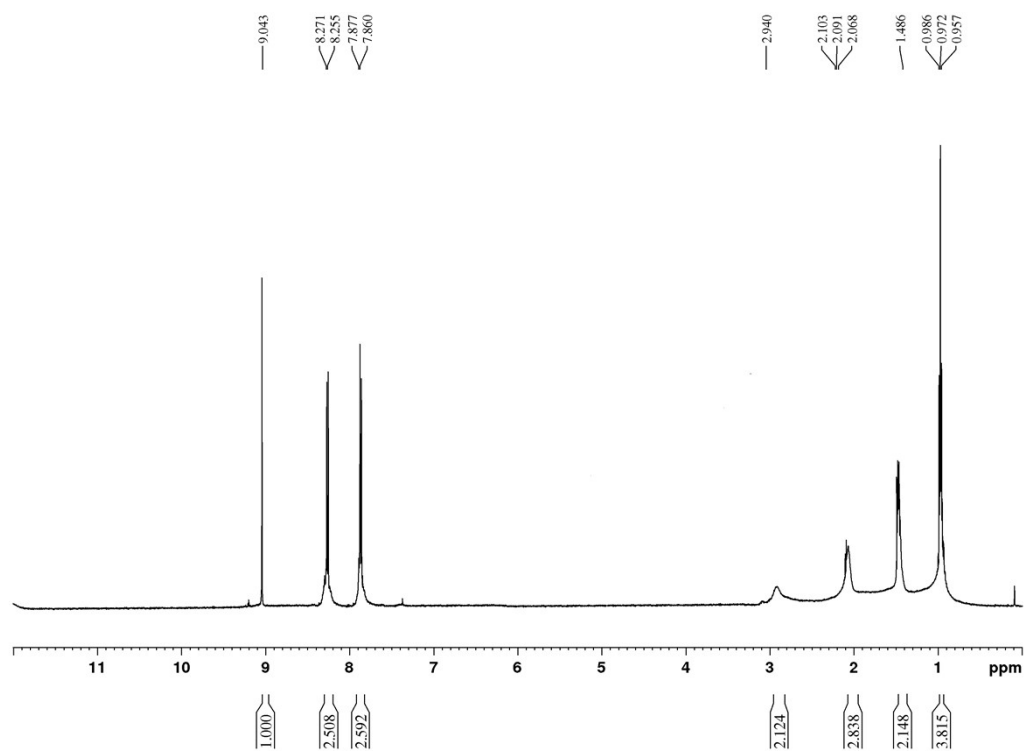


Figure S62. Copy of ¹H NMR spectra of compound 12

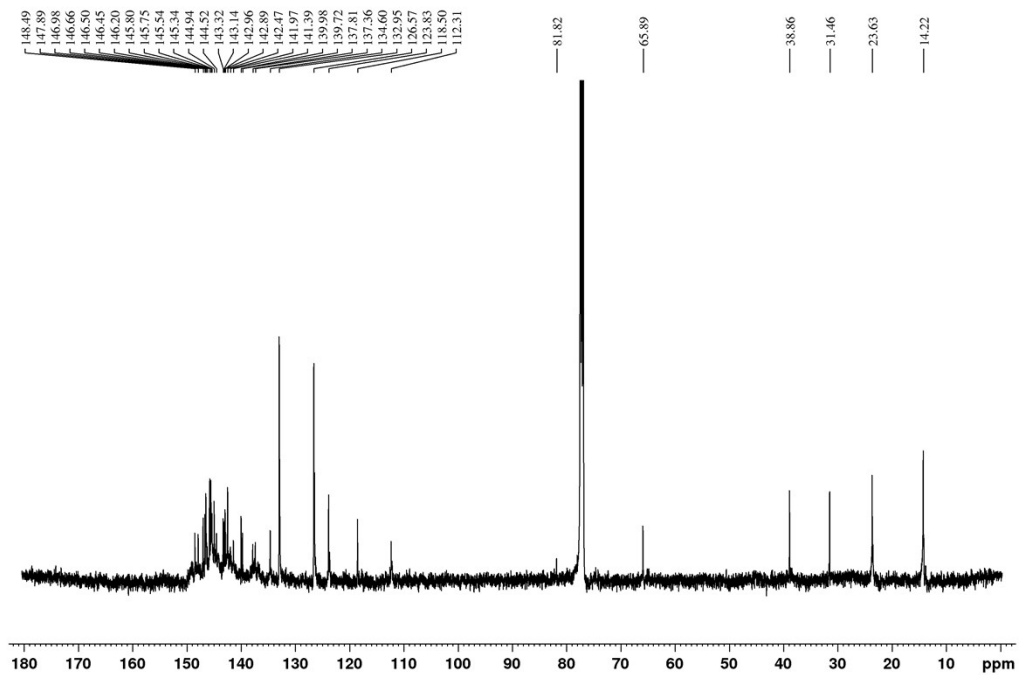


Figure S63. Copy of ^{13}C NMR spectra of compound 12

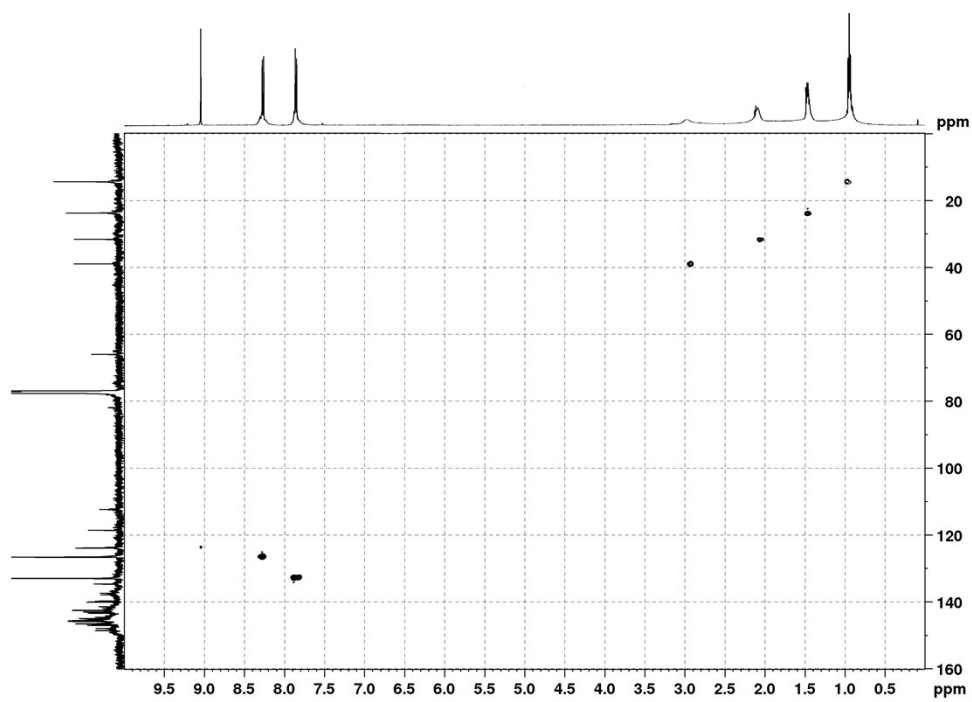


Figure S64. Copy of HSQC NMR spectra of compound 12

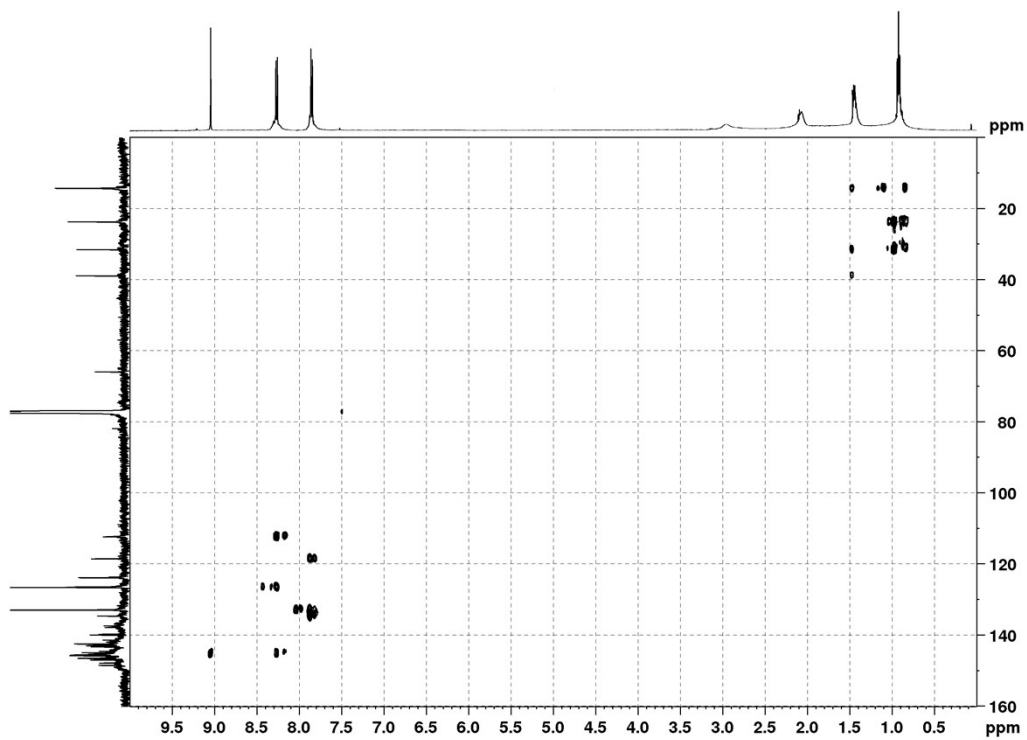


Figure S65. Copy of HMBC NMR spectra of compound 12

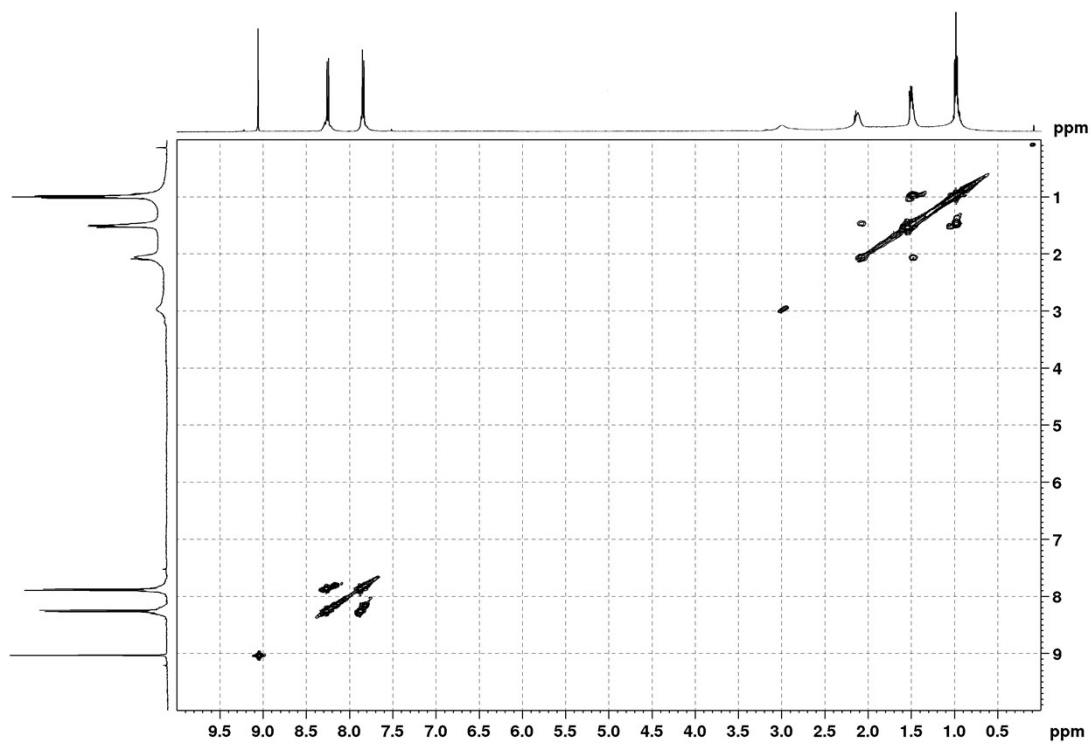


Figure S66. Copy of COSY NMR spectra of compound 12

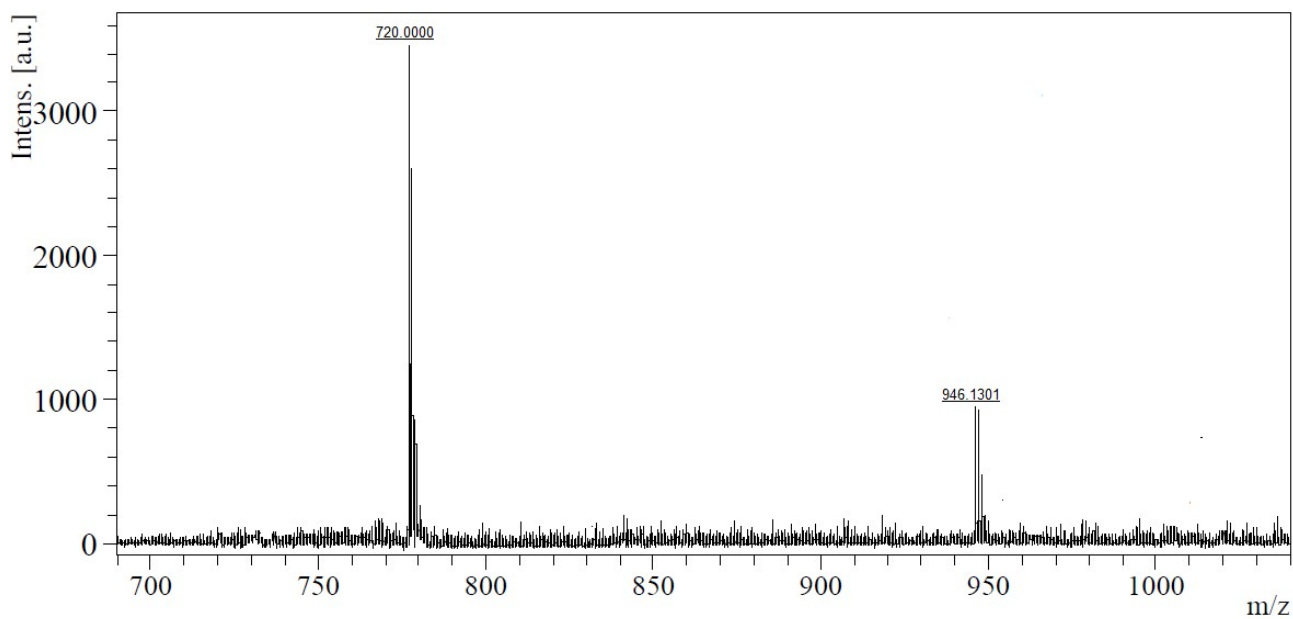


Figure S67. Copy of MALDI TOF spectra of compound 12

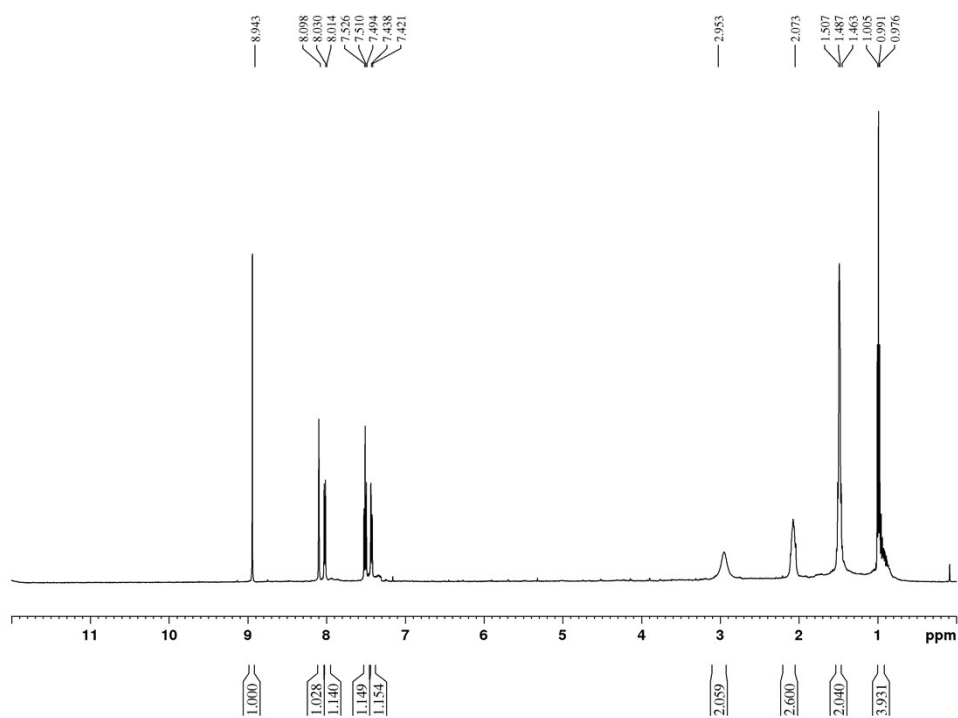


Figure S68. Copy of ¹H NMR spectra of compound 13

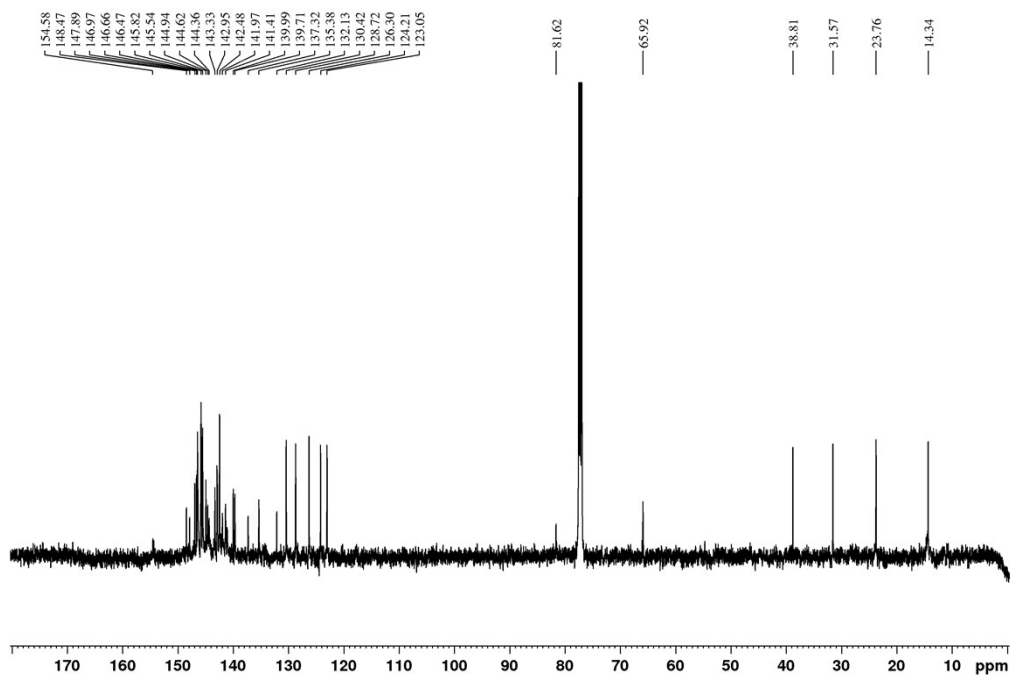


Figure S69. Copy of ^{13}C NMR spectra of compound **13**

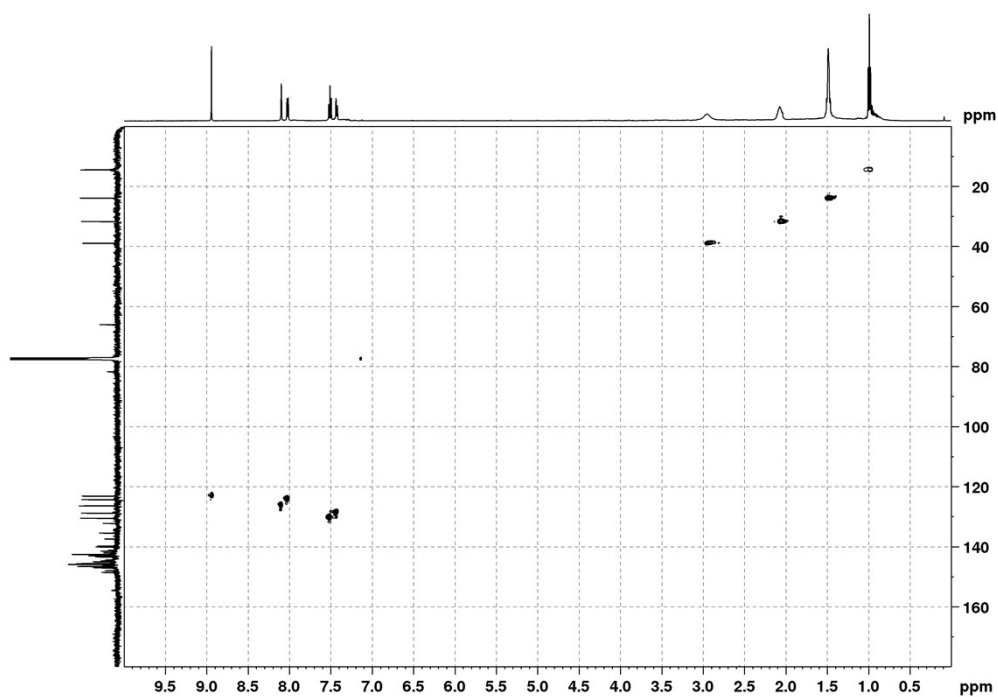


Figure S70. Copy of HSQC NMR spectra of compound **13**

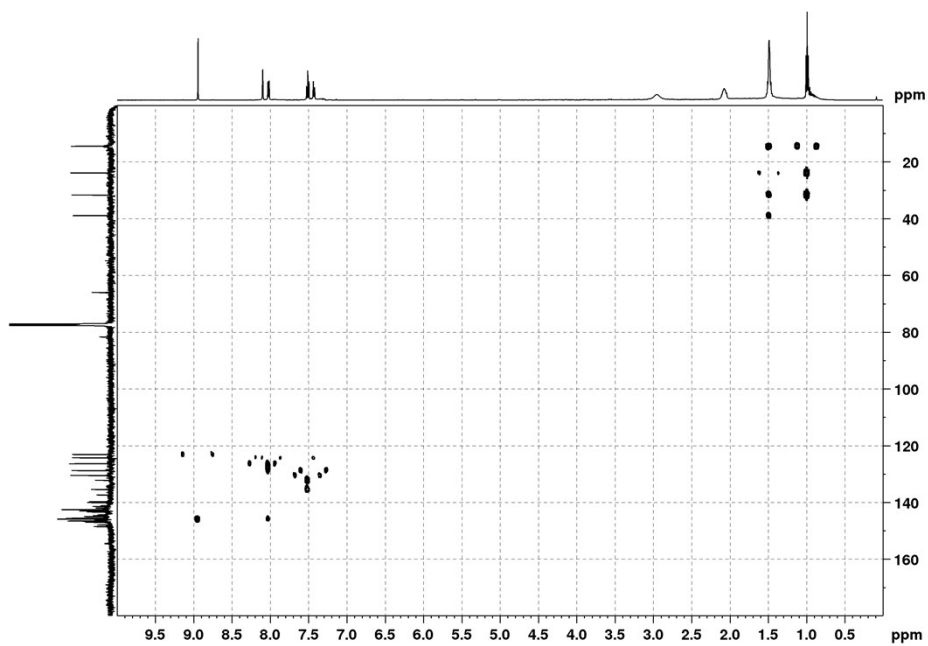


Figure S71. Copy of HMBC NMR spectra of compound **13**

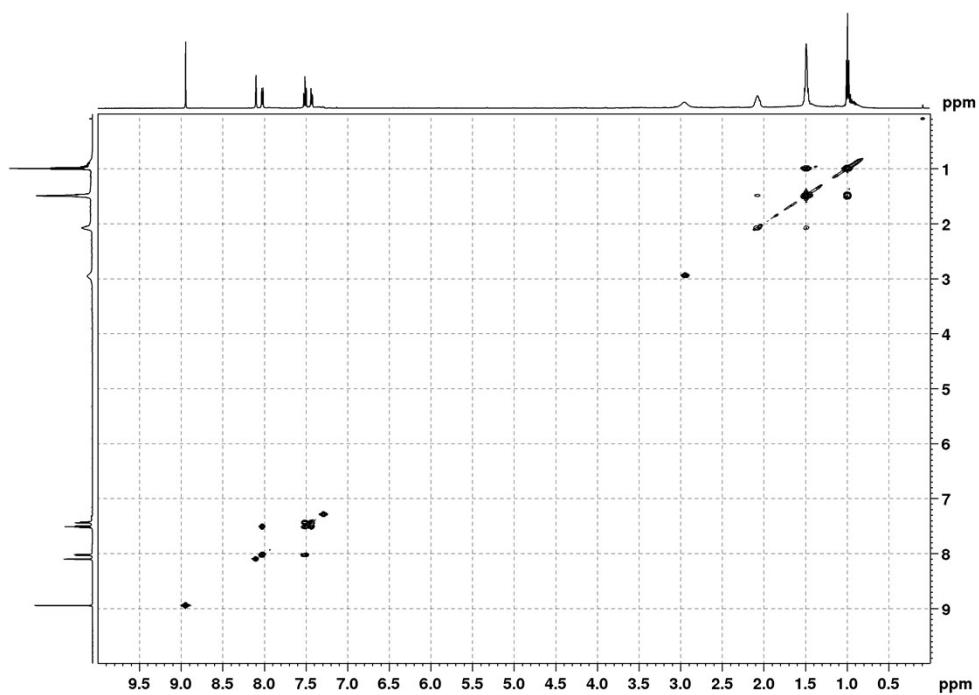


Figure S72. Copy of COSY NMR spectra of compound **13**

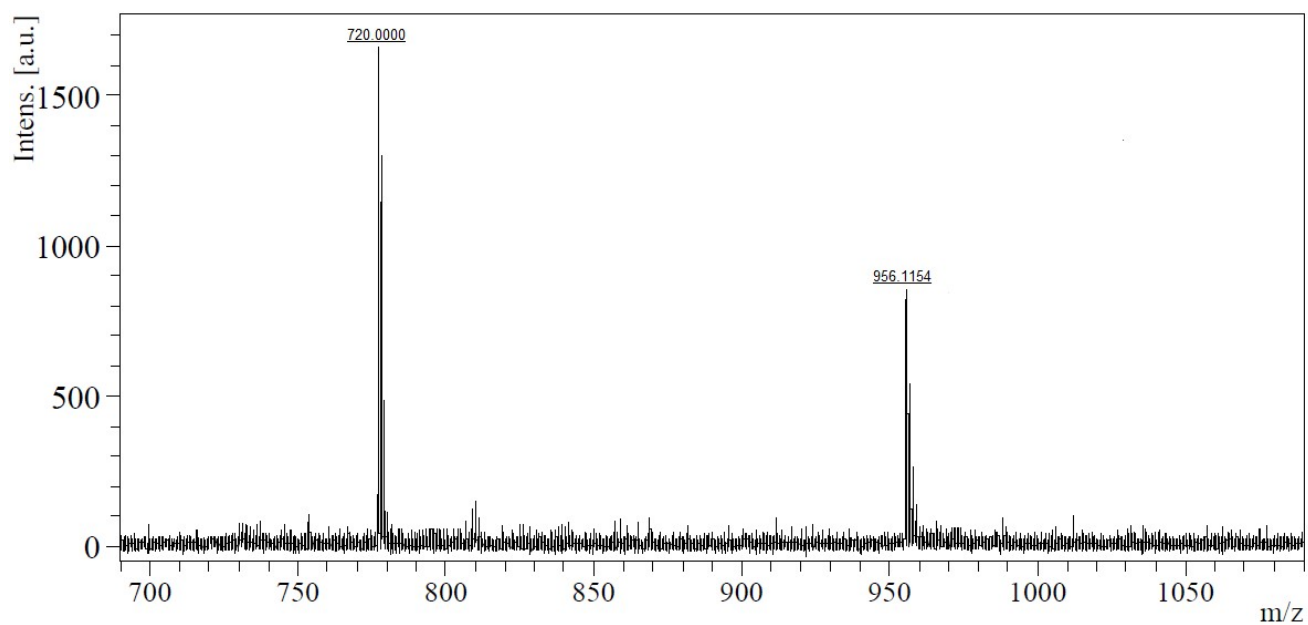


Figure S73. Copy of MALDI TOF spectra of compound 13

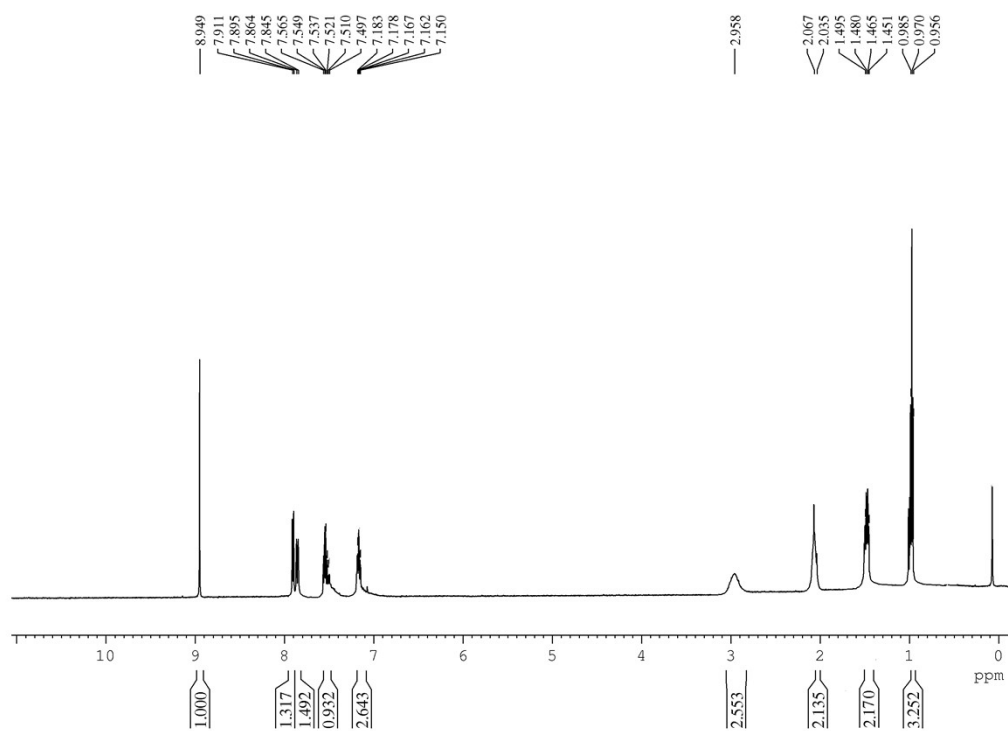


Figure S74. Copy of ¹H NMR spectra of compound 14

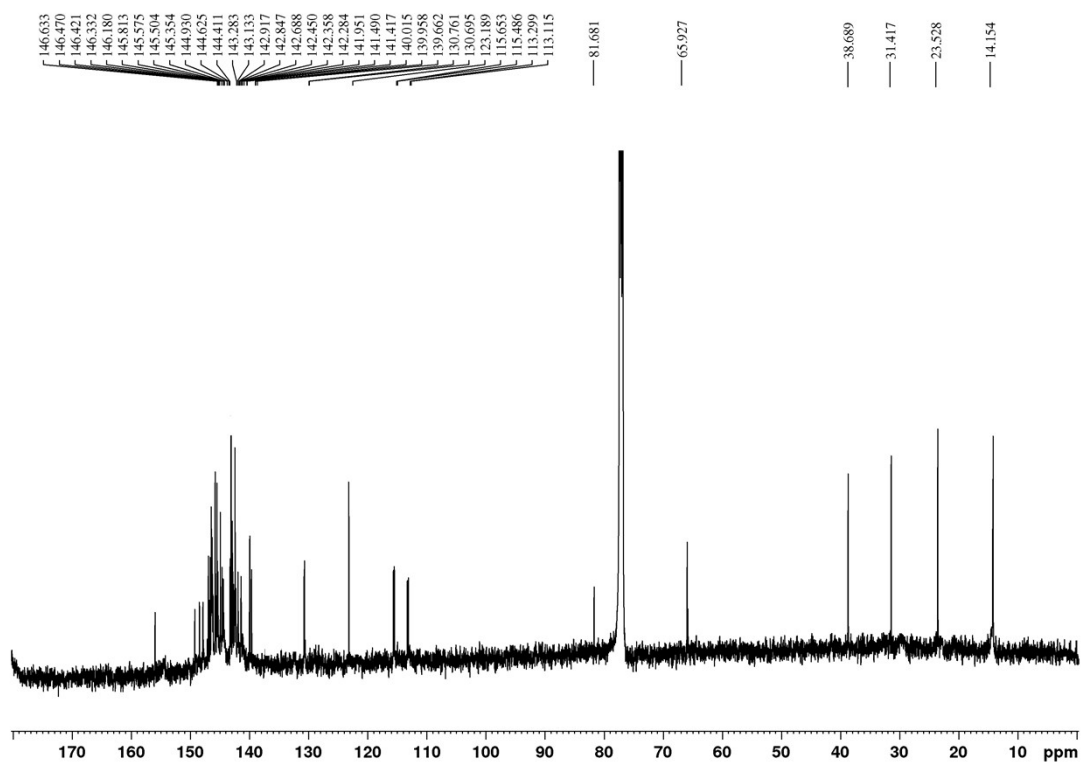


Figure S75. Copy of ^{13}C NMR spectra of compound 14

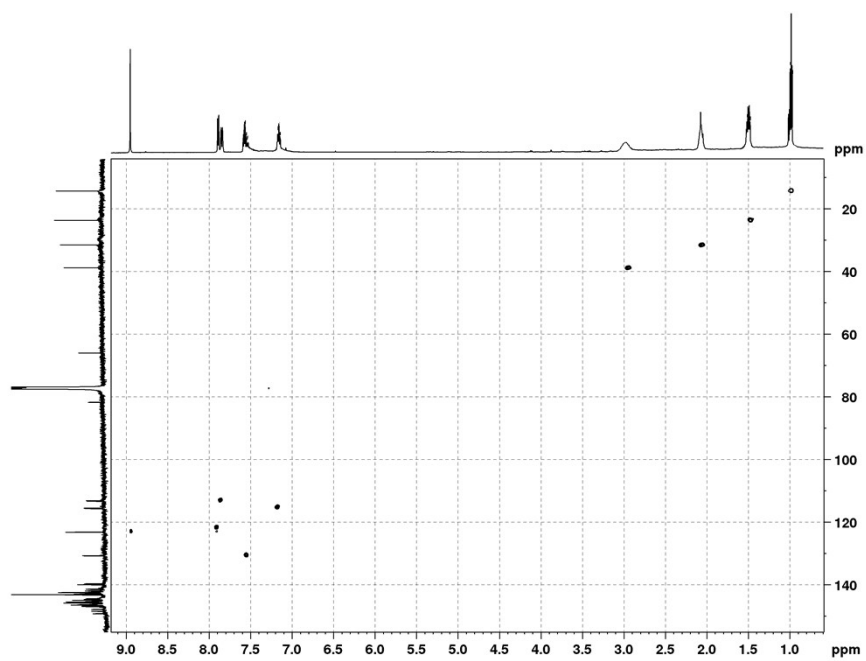


Figure S76. Copy of HSQC NMR spectra of compound 14

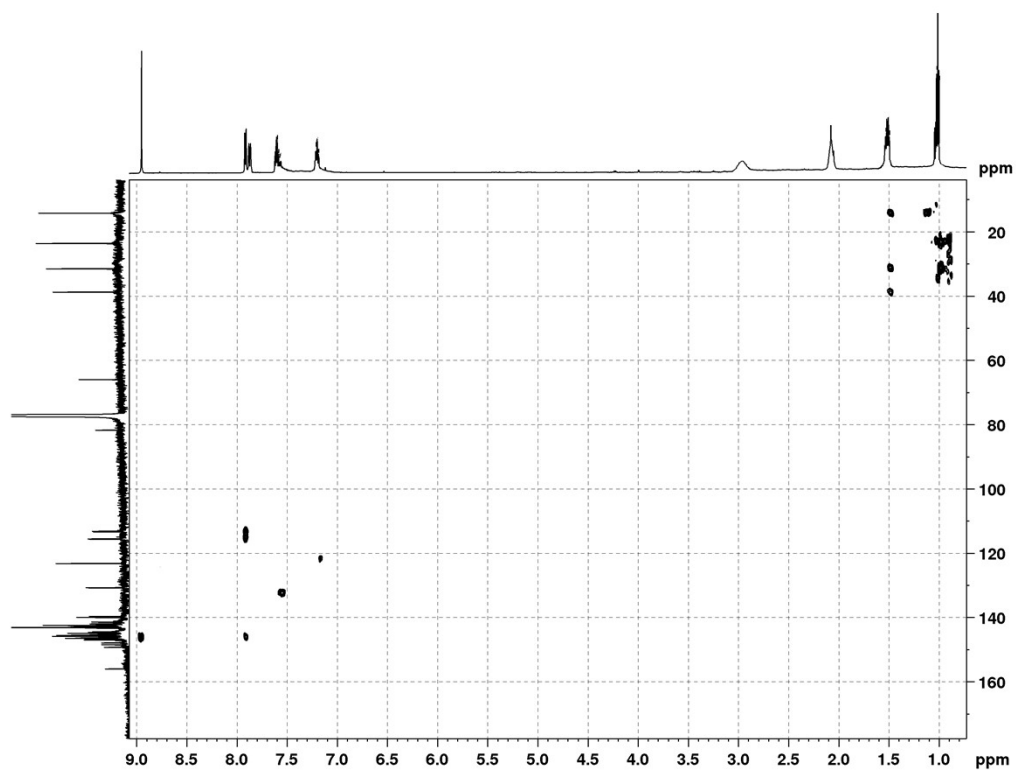


Figure S77. Copy of HMBC NMR spectra of compound 14

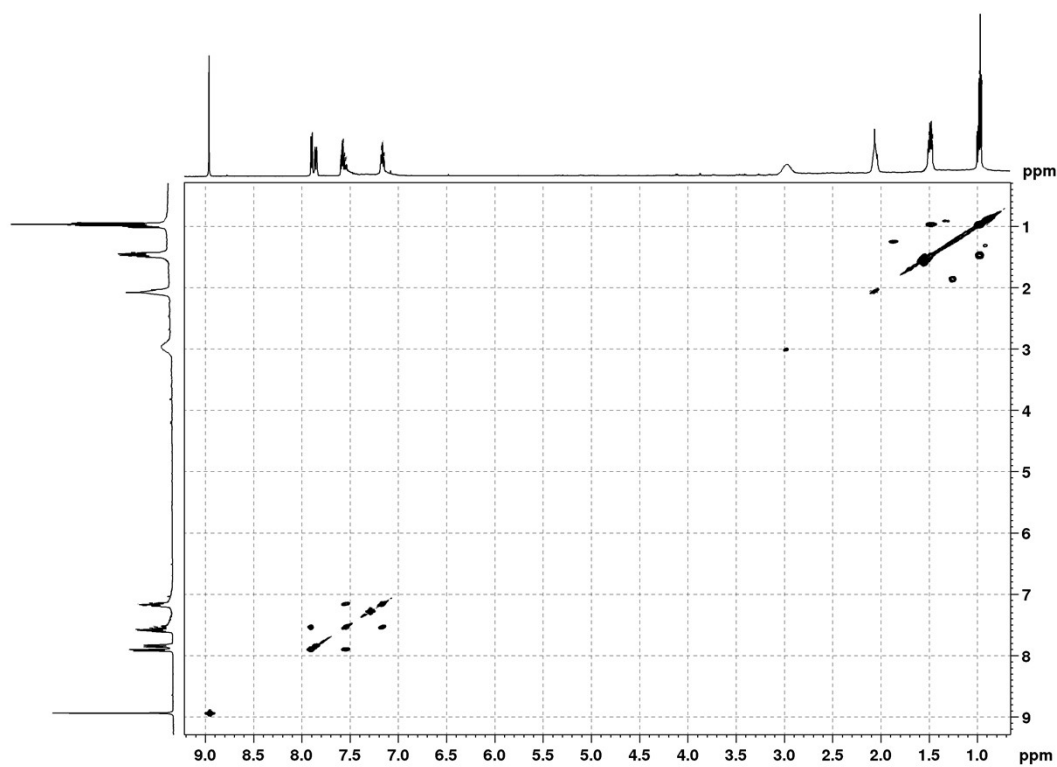


Figure S78. Copy of COSY NMR spectra of compound 14

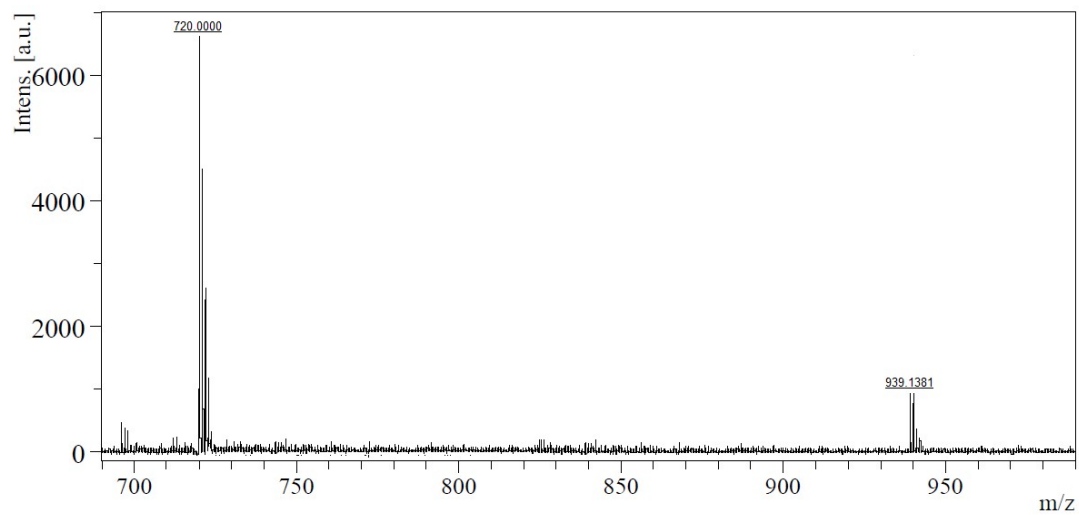


Figure S79. Copy of MALDI TOF spectra of compound 14

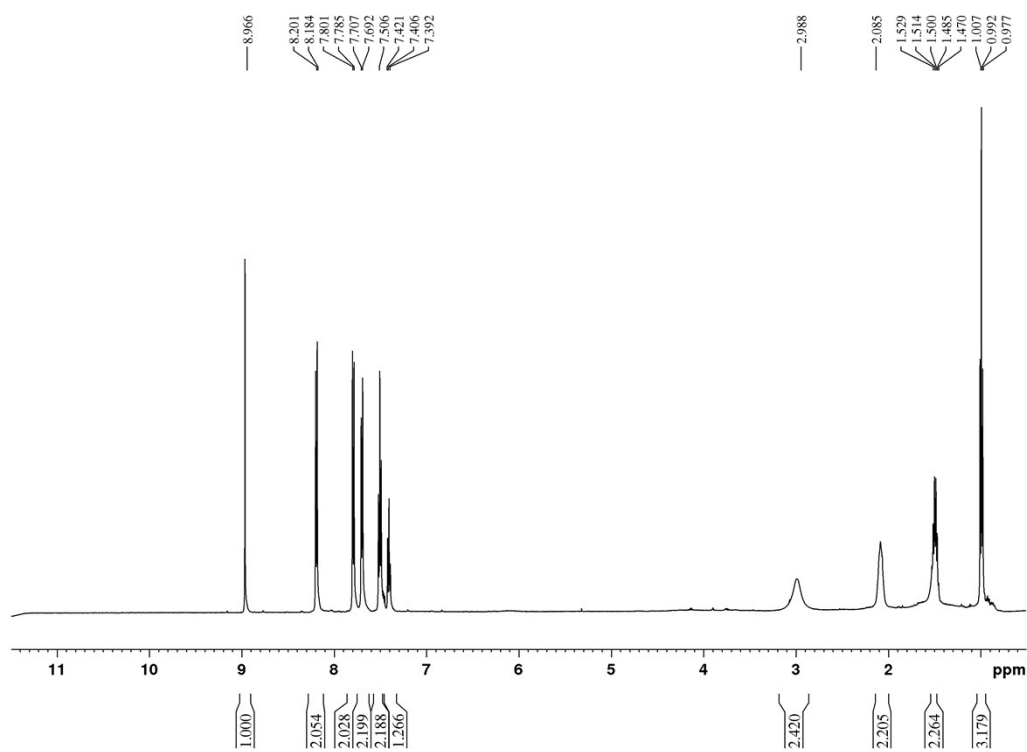


Figure S80. Copy of ¹H NMR spectra of compound 15

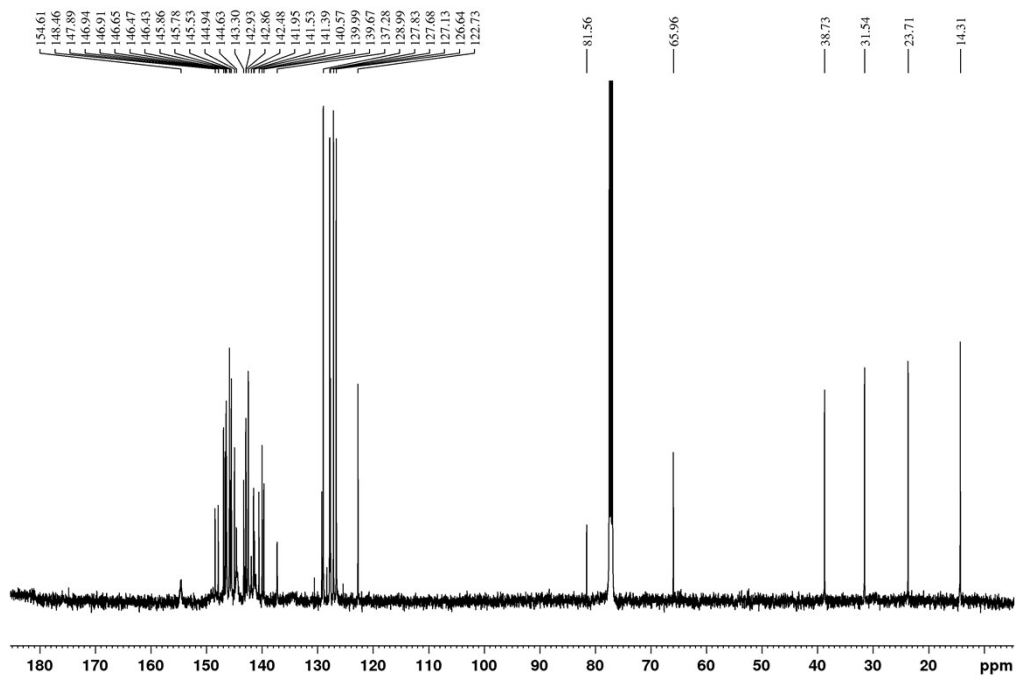


Figure S81. Copy of ^{13}C NMR spectra of compound **15**

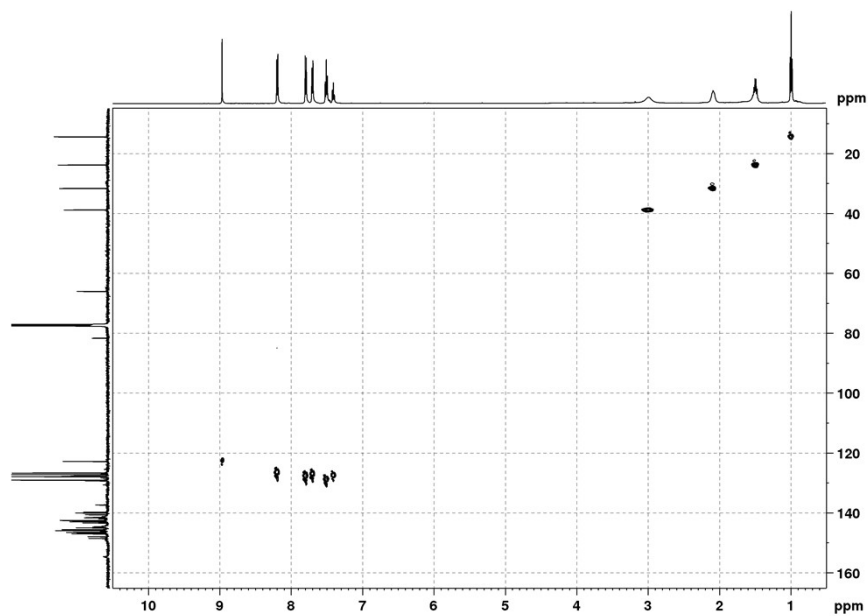


Figure S82. Copy of HSQC NMR spectra of compound **15**

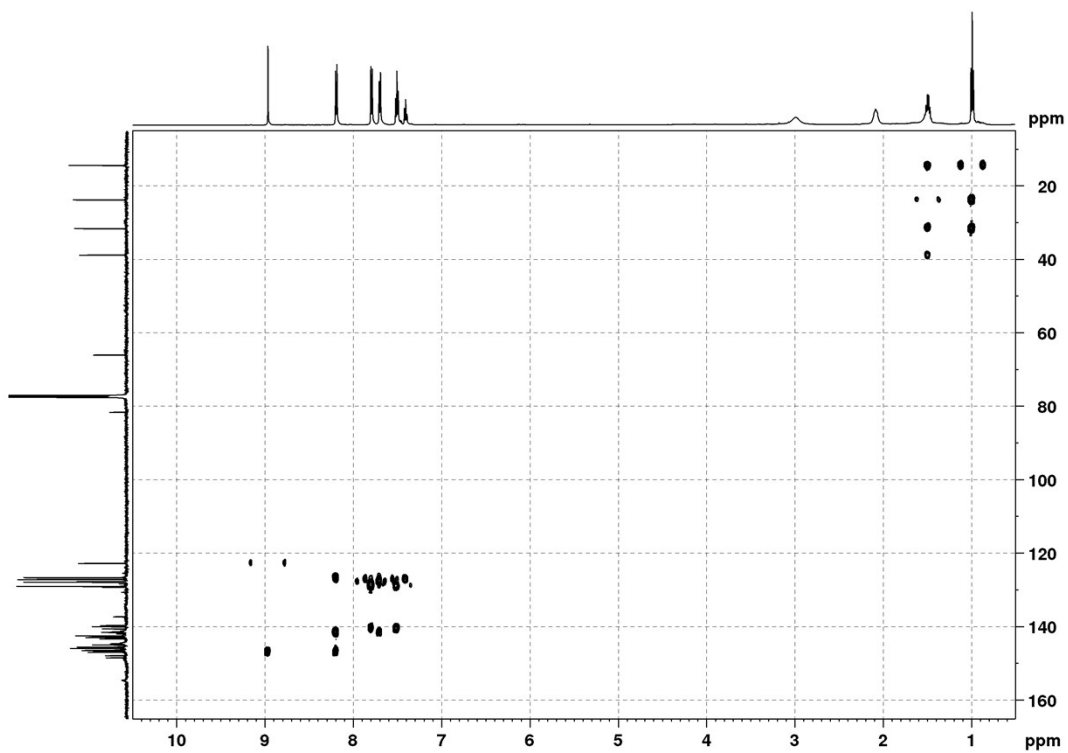


Figure S83. Copy of HMBC NMR spectra of compound 15

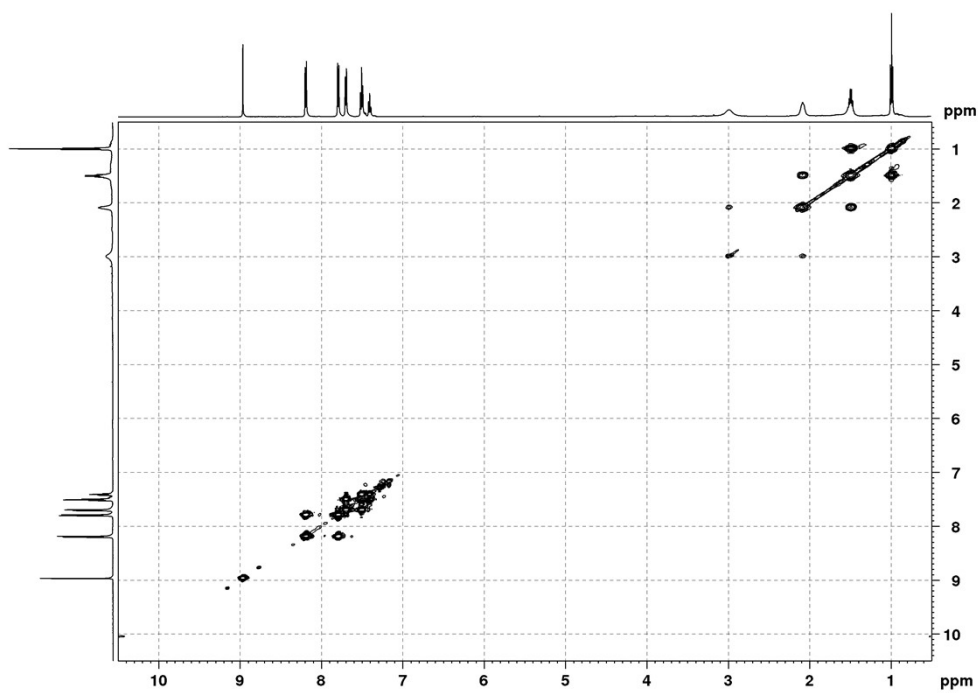


Figure S84. Copy of COSY NMR spectra of compound 15

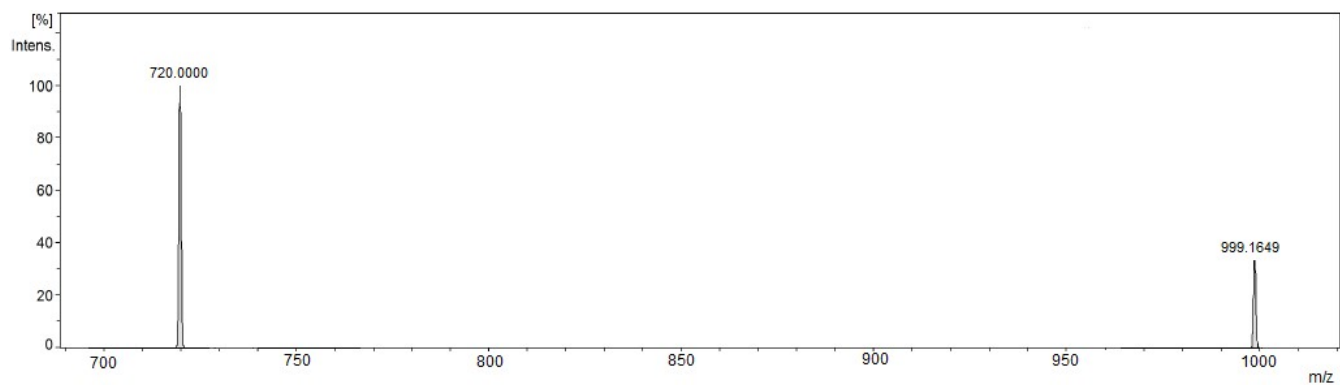


Figure S85. Copy of MALDI TOF spectra of compound **15**

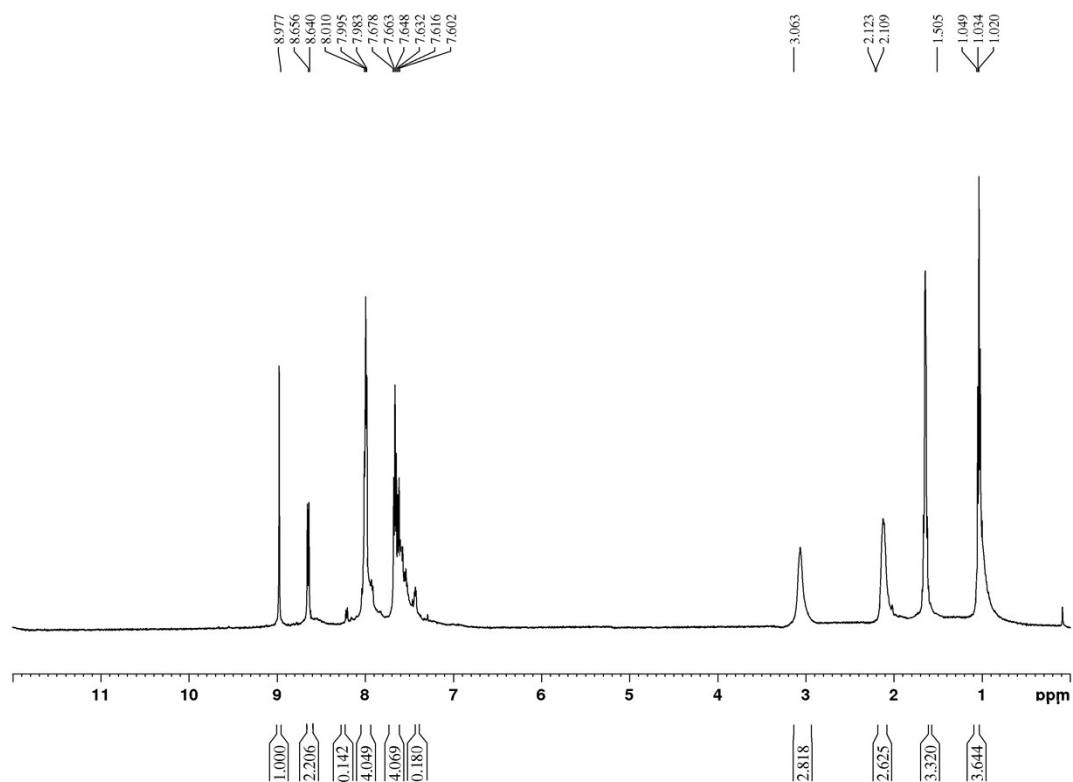


Figure S86. Copy of ¹H NMR spectra of compound **16**

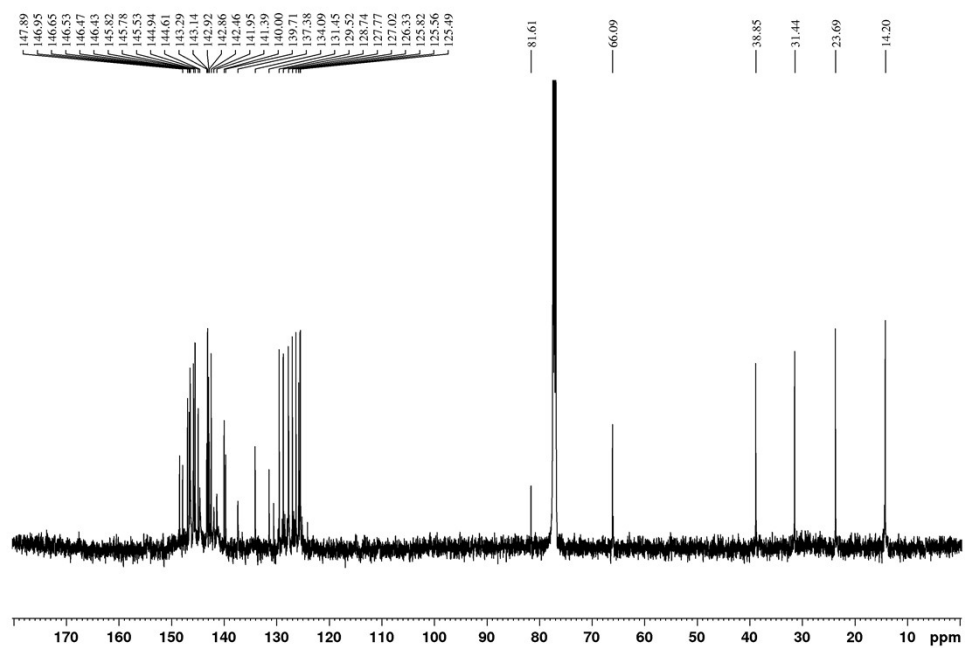


Figure S87. Copy of ^{13}C NMR spectra of compound 16

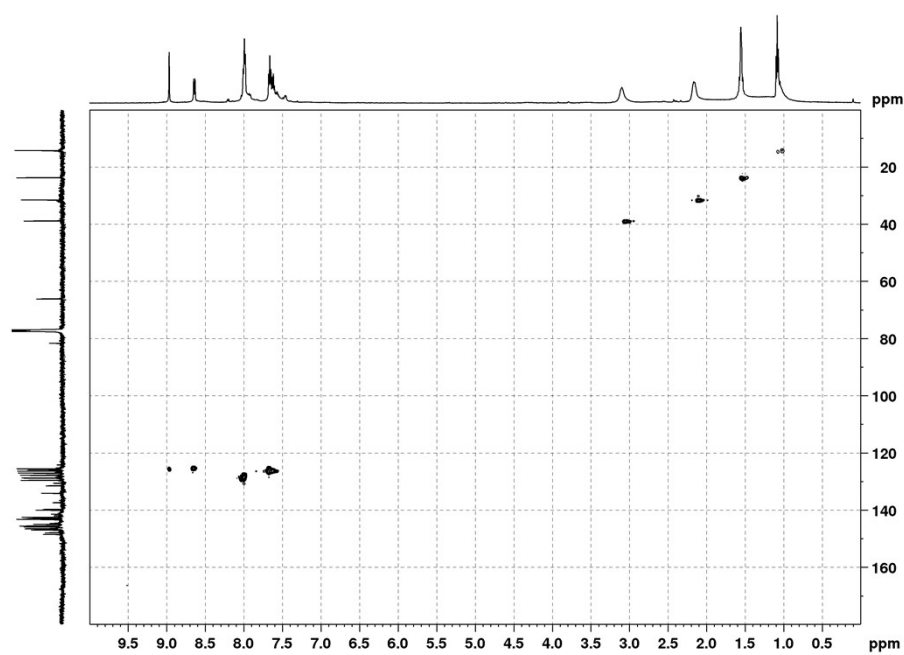


Figure S88. Copy of HSQC NMR spectra of compound 16

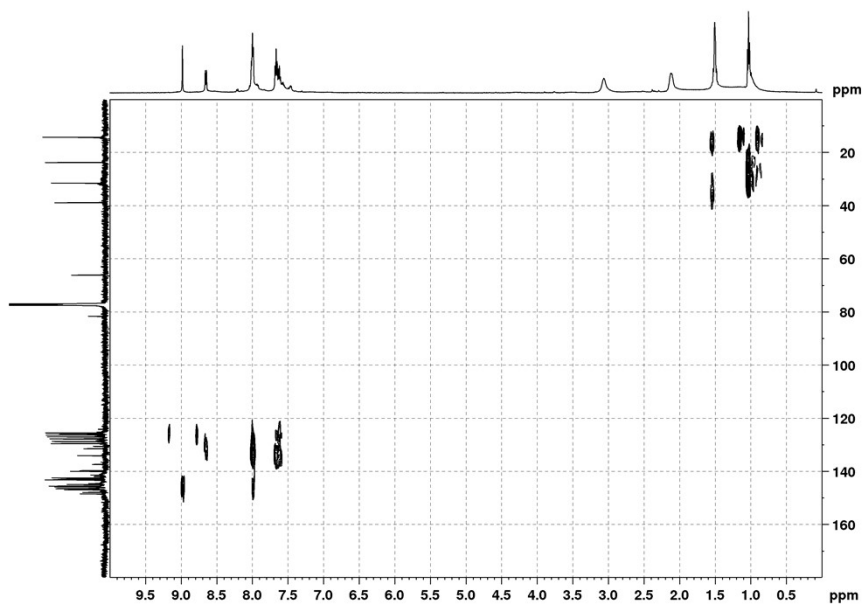


Figure S89. Copy of HMBC NMR spectra of compound **16**

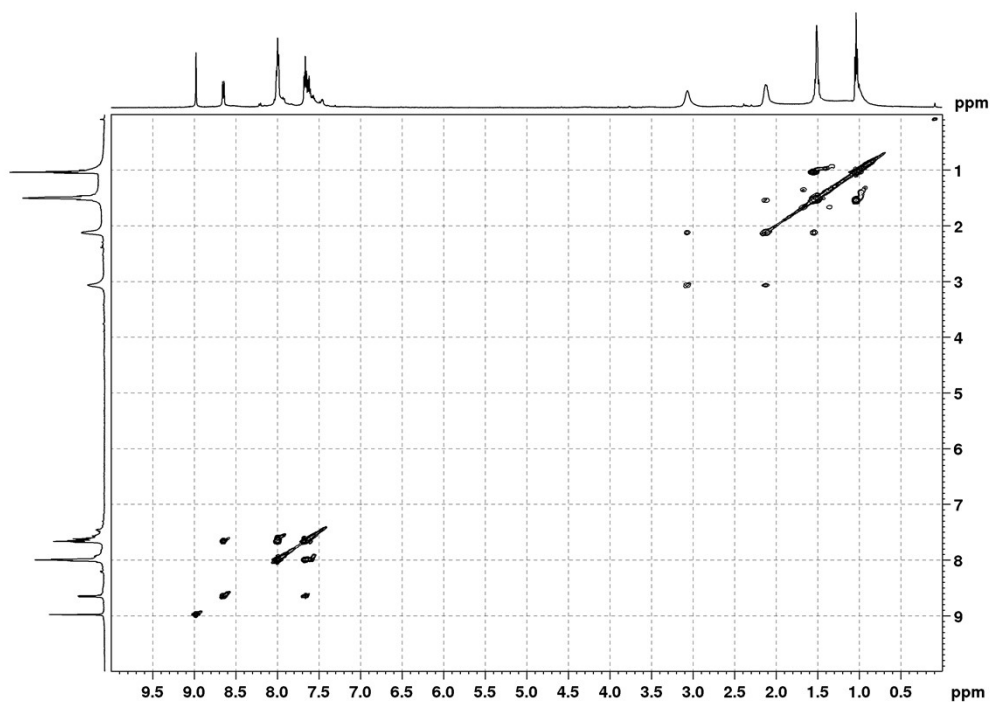


Figure S90. Copy of COSY NMR spectra of compound **16**

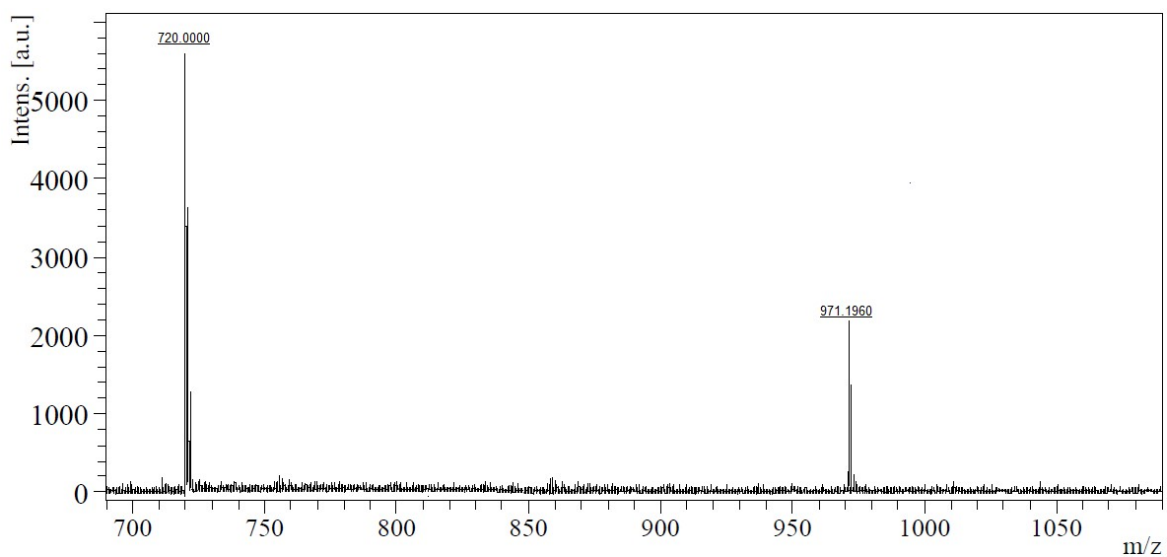


Figure S91. Copy of MALDI TOF spectra of compound **16**

Cartesian coordinates

Compound 5

| | | | |
|---|--------------|--------------|--------------|
| 6 | 1.821167000 | 1.449243000 | -0.105222000 |
| 6 | 2.117621000 | -0.124847000 | -0.392510000 |
| 6 | 1.621314000 | -1.083303000 | 0.706617000 |
| 6 | 1.175742000 | -0.674913000 | 1.948758000 |
| 6 | 0.891425000 | 0.750575000 | 2.215397000 |
| 6 | 1.057727000 | 1.685935000 | 1.210501000 |
| 6 | 0.052650000 | 2.698987000 | 1.027611000 |
| 6 | -0.101126000 | 2.929744000 | -0.396923000 |
| 6 | 0.809609000 | 2.059509000 | -1.093314000 |
| 6 | 0.403122000 | 1.475890000 | -2.278949000 |
| 6 | 0.689743000 | 0.051262000 | -2.540112000 |
| 6 | 1.373706000 | -0.707946000 | -1.613273000 |
| 6 | 0.919674000 | -2.039474000 | -1.315492000 |
| 6 | 1.072709000 | -2.271595000 | 0.109530000 |
| 6 | 0.140270000 | -3.064184000 | 0.798728000 |
| 6 | -0.310336000 | -2.648872000 | 2.107575000 |
| 6 | 0.196895000 | -1.464879000 | 2.667131000 |
| 6 | -0.693129000 | -0.554774000 | 3.365896000 |
| 6 | -0.265092000 | 0.805486000 | 3.085963000 |
| 6 | -1.224428000 | 1.820590000 | 2.936450000 |
| 6 | -1.059482000 | 2.792859000 | 1.881195000 |
| 6 | -2.370856000 | 3.098798000 | 1.331129000 |
| 6 | -2.519671000 | 3.320212000 | -0.043433000 |
| 6 | -1.364268000 | 3.247041000 | -0.923684000 |
| 6 | -1.779609000 | 2.647808000 | -2.169740000 |
| 6 | -0.908258000 | 1.761990000 | -2.824083000 |
| 6 | -1.431391000 | 0.544818000 | -3.420362000 |
| 6 | -0.445479000 | -0.506641000 | -3.243787000 |
| 6 | -0.864221000 | -1.823685000 | -2.993357000 |
| 6 | -0.163951000 | -2.609232000 | -2.004008000 |
| 6 | -1.140863000 | -3.413685000 | -1.286102000 |
| 6 | -0.991892000 | -3.637512000 | 0.087635000 |
| 6 | -2.147307000 | -3.569780000 | 0.966381000 |
| 6 | -1.723883000 | -2.958442000 | 2.217453000 |
| 6 | -2.581896000 | -2.076417000 | 2.890426000 |
| 6 | -2.055845000 | -0.856153000 | 3.484518000 |
| 6 | -3.048152000 | 0.194180000 | 3.312413000 |
| 6 | -2.638152000 | 1.508283000 | 3.042935000 |
| 6 | -3.349552000 | 2.300514000 | 2.050142000 |
| 6 | -4.441984000 | 1.750166000 | 1.365717000 |
| 6 | -4.597875000 | 1.982254000 | -0.062720000 |
| 6 | -3.654743000 | 2.755474000 | -0.754307000 |
| 6 | -3.194032000 | 2.336910000 | -2.070426000 |
| 6 | -3.696002000 | 1.159741000 | -2.644230000 |
| 6 | -2.798283000 | 0.250048000 | -3.340039000 |
| 6 | -3.230184000 | -1.111825000 | -3.062708000 |
| 6 | -2.279534000 | -2.129839000 | -2.894705000 |

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|---|--------------|--------------|--------------|
| 6 | -2.452336000 | -3.115440000 | -1.837486000 |
| 6 | -3.567557000 | -3.047256000 | -0.990666000 |
| 6 | -3.412531000 | -3.279192000 | 0.437660000 |
| 6 | -4.300575000 | -2.367141000 | 1.139192000 |
| 6 | -3.891671000 | -1.778535000 | 2.344899000 |
| 6 | -4.179235000 | -0.373919000 | 2.604658000 |
| 6 | -4.864492000 | 0.388685000 | 1.647836000 |
| 6 | -5.281248000 | -0.221275000 | 0.395926000 |
| 6 | -5.116030000 | 0.763460000 | -0.660492000 |
| 6 | -4.672920000 | 0.361323000 | -1.928911000 |
| 6 | -4.384513000 | -1.043728000 | -2.187761000 |
| 6 | -4.551744000 | -1.993057000 | -1.169227000 |
| 6 | -5.005552000 | -1.573192000 | 0.146349000 |
| 6 | 3.158464000 | 2.269859000 | -0.117096000 |
| 1 | 3.635751000 | 2.110493000 | -1.096699000 |
| 1 | 3.828921000 | 1.832722000 | 0.641632000 |
| 6 | 3.031896000 | 3.774296000 | 0.144381000 |
| 1 | 2.381144000 | 4.240781000 | -0.615707000 |
| 1 | 2.546976000 | 3.957254000 | 1.119466000 |
| 6 | 4.400781000 | 4.469214000 | 0.126497000 |
| 1 | 5.055057000 | 4.004219000 | 0.885534000 |
| 1 | 4.889062000 | 4.286963000 | -0.847251000 |
| 6 | 4.307500000 | 5.976513000 | 0.381608000 |
| 1 | 3.857670000 | 6.189047000 | 1.364999000 |
| 1 | 3.686271000 | 6.472549000 | -0.381522000 |
| 1 | 5.301190000 | 6.449075000 | 0.360685000 |
| 6 | 4.498734000 | -0.804106000 | 0.302663000 |
| 6 | 5.686247000 | -0.837921000 | -0.420112000 |
| 1 | 4.245552000 | -1.050436000 | 1.327536000 |
| 7 | 3.563701000 | -0.381480000 | -0.594302000 |
| 7 | 4.131364000 | -0.159549000 | -1.814733000 |
| 7 | 5.402024000 | -0.434018000 | -1.705794000 |
| 6 | 7.041241000 | -1.217430000 | -0.007019000 |
| 6 | 7.327588000 | -1.601292000 | 1.317353000 |
| 6 | 8.088415000 | -1.199659000 | -0.949186000 |
| 6 | 8.625234000 | -1.959123000 | 1.688832000 |
| 6 | 9.384198000 | -1.557627000 | -0.573377000 |
| 6 | 9.659520000 | -1.938960000 | 0.745439000 |
| 1 | 6.531641000 | -1.621001000 | 2.066358000 |
| 1 | 7.862997000 | -0.901334000 | -1.974496000 |
| 1 | 8.830538000 | -2.255135000 | 2.720255000 |
| 1 | 10.185597000 | -1.539575000 | -1.315775000 |
| 1 | 10.674131000 | -2.219198000 | 1.037360000 |

Compound 6

| | | | |
|---|-------------|--------------|--------------|
| 6 | 1.491215000 | 1.548221000 | -0.060078000 |
| 6 | 1.855400000 | -0.023683000 | -0.274063000 |

| | | | |
|---|--------------|--------------|--------------|
| 6 | 1.350920000 | -0.957630000 | 0.841942000 |
| 6 | 0.8444464000 | -0.519864000 | 2.050047000 |
| 6 | 0.498979000 | 0.902836000 | 2.250459000 |
| 6 | 0.669410000 | 1.805314000 | 1.216551000 |
| 6 | -0.364764000 | 2.771368000 | 0.957192000 |
| 6 | -0.472262000 | 2.941907000 | -0.480062000 |
| 6 | 0.495964000 | 2.081267000 | -1.107497000 |
| 6 | 0.157428000 | 1.438026000 | -2.283638000 |
| 6 | 0.506631000 | 0.016577000 | -2.478406000 |
| 6 | 1.183452000 | -0.680914000 | -1.499025000 |
| 6 | 0.766020000 | -2.016210000 | -1.165340000 |
| 6 | 0.871279000 | -2.187796000 | 0.272166000 |
| 6 | -0.056419000 | -2.989015000 | 0.957239000 |
| 6 | -0.571343000 | -2.542684000 | 2.231928000 |
| 6 | -0.130831000 | -1.319269000 | 2.762451000 |
| 6 | -1.079509000 | -0.418282000 | 3.391984000 |
| 6 | -0.691674000 | 0.945839000 | 3.074518000 |
| 6 | -1.681390000 | 1.916946000 | 2.850650000 |
| 6 | -1.512005000 | 2.853828000 | 1.764556000 |
| 6 | -2.811415000 | 3.088552000 | 1.154922000 |
| 6 | -2.915340000 | 3.251723000 | -0.231988000 |
| 6 | -1.725257000 | 3.189964000 | -1.065431000 |
| 6 | -2.069742000 | 2.528574000 | -2.301659000 |
| 6 | -1.141882000 | 1.652235000 | -2.887251000 |
| 6 | -1.596124000 | 0.394317000 | -3.454471000 |
| 6 | -0.579481000 | -0.610970000 | -3.200868000 |
| 6 | -0.958494000 | -1.932677000 | -2.914891000 |
| 6 | -0.268332000 | -2.653128000 | -1.870359000 |
| 6 | -1.241838000 | -3.467084000 | -1.158211000 |
| 6 | -1.137765000 | -3.632821000 | 0.228043000 |
| 6 | -2.327533000 | -3.576412000 | 1.060436000 |
| 6 | -1.975679000 | -2.902332000 | 2.301483000 |
| 6 | -2.890797000 | -2.028468000 | 2.906437000 |
| 6 | -2.433663000 | -0.767332000 | 3.471373000 |
| 6 | -3.456848000 | 0.236708000 | 3.221883000 |
| 6 | -3.085755000 | 1.554494000 | 2.916737000 |
| 6 | -3.786932000 | 2.280747000 | 1.867742000 |
| 6 | -4.830468000 | 1.662692000 | 1.165309000 |
| 6 | -4.939663000 | 1.834578000 | -0.275507000 |
| 6 | -4.000178000 | 2.616871000 | -0.961493000 |
| 6 | -3.474730000 | 2.167548000 | -2.242942000 |
| 6 | -3.909768000 | 0.950518000 | -2.787561000 |
| 6 | -2.953211000 | 0.050414000 | -3.413591000 |
| 6 | -3.344852000 | -1.315589000 | -3.099143000 |
| 6 | -2.364405000 | -2.289283000 | -2.856853000 |
| 6 | -2.541109000 | -3.240059000 | -1.768839000 |
| 6 | -3.689954000 | -3.183172000 | -0.967056000 |
| 6 | -3.581378000 | -3.354714000 | 0.474171000 |
| 6 | -4.528887000 | -2.451322000 | 1.106016000 |
| 6 | -4.189051000 | -1.802406000 | 2.302133000 |

| | | | |
|---|--------------|--------------|--------------|
| 6 | -4.538169000 | -0.401110000 | 2.495907000 |
| 6 | -5.213601000 | 0.297946000 | 1.485066000 |
| 6 | -5.558755000 | -0.374421000 | 0.243336000 |
| 6 | -5.389449000 | 0.575403000 | -0.843878000 |
| 6 | -4.883201000 | 0.142801000 | -2.078097000 |
| 6 | -4.534134000 | -1.259061000 | -2.271344000 |
| 6 | -4.704896000 | -2.175015000 | -1.223159000 |
| 6 | -5.223561000 | -1.723005000 | 0.057340000 |
| 6 | 2.797439000 | 2.416454000 | -0.056133000 |
| 1 | 3.315406000 | 2.240029000 | -1.011828000 |
| 1 | 3.455523000 | 2.032239000 | 0.741060000 |
| 6 | 2.607894000 | 3.923607000 | 0.145166000 |
| 1 | 1.964822000 | 4.337568000 | -0.651038000 |
| 1 | 2.086084000 | 4.122891000 | 1.097778000 |
| 6 | 3.949816000 | 4.669897000 | 0.142174000 |
| 1 | 4.596881000 | 4.259880000 | 0.938218000 |
| 1 | 4.475283000 | 4.470424000 | -0.808538000 |
| 6 | 3.791239000 | 6.180870000 | 0.335471000 |
| 1 | 3.303408000 | 6.412776000 | 1.296046000 |
| 1 | 3.175697000 | 6.622849000 | -0.464594000 |
| 1 | 4.766541000 | 6.690569000 | 0.325381000 |
| 6 | 4.223422000 | -0.591542000 | 0.548646000 |
| 6 | 5.442483000 | -0.612649000 | -0.119136000 |
| 1 | 3.931218000 | -0.808031000 | 1.569824000 |
| 7 | 3.317760000 | -0.234235000 | -0.404557000 |
| 7 | 3.933463000 | -0.039625000 | -1.606476000 |
| 7 | 5.205651000 | -0.267373000 | -1.430636000 |
| 6 | 6.787527000 | -0.934246000 | 0.369998000 |
| 6 | 7.022407000 | -1.255319000 | 1.721293000 |
| 6 | 7.869565000 | -0.922929000 | -0.525606000 |
| 6 | 8.312527000 | -1.559752000 | 2.161853000 |
| 6 | 9.172603000 | -1.228141000 | -0.086892000 |
| 6 | 9.387484000 | -1.549120000 | 1.272029000 |
| 1 | 6.195069000 | -1.267384000 | 2.434938000 |
| 1 | 7.689510000 | -0.674397000 | -1.572151000 |
| 1 | 8.481992000 | -1.807984000 | 3.211985000 |
| 1 | 10.396714000 | -1.786511000 | 1.612364000 |
| 6 | 10.263548000 | -1.213883000 | -1.005887000 |
| 6 | 11.196277000 | -1.202975000 | -1.785653000 |
| 1 | 12.014351000 | -1.192825000 | -2.475602000 |

Compound 15

| | | | |
|---|--------------|--------------|--------------|
| 6 | 0.554711000 | 1.857709000 | -0.118583000 |
| 6 | 1.077611000 | 0.374037000 | -0.531227000 |
| 6 | 0.801636000 | -0.718713000 | 0.518573000 |
| 6 | 0.368720000 | -0.467424000 | 1.805762000 |
| 6 | -0.120113000 | 0.873820000 | 2.187318000 |

| | | | |
|---|--------------|--------------|--------------|
| 6 | -0.160494000 | 1.885400000 | 1.244808000 |
| 6 | -1.323385000 | 2.730368000 | 1.179902000 |
| 6 | -1.591311000 | 3.023593000 | -0.215850000 |
| 6 | -0.595718000 | 2.356886000 | -1.012818000 |
| 6 | -0.970293000 | 1.793078000 | -2.218215000 |
| 6 | -0.476848000 | 0.452862000 | -2.594141000 |
| 6 | 0.367898000 | -0.243164000 | -1.754892000 |
| 6 | 0.148690000 | -1.646583000 | -1.532912000 |
| 6 | 0.415403000 | -1.939463000 | -0.136467000 |
| 6 | -0.337537000 | -2.915144000 | 0.535837000 |
| 6 | -0.773006000 | -2.662695000 | 1.890304000 |
| 6 | -0.429396000 | -1.449797000 | 2.510148000 |
| 6 | -1.411682000 | -0.741410000 | 3.311484000 |
| 6 | -1.221074000 | 0.685161000 | 3.110089000 |
| 6 | -2.336158000 | 1.538495000 | 3.077405000 |
| 6 | -2.386619000 | 2.589180000 | 2.087480000 |
| 6 | -3.758200000 | 2.712305000 | 1.619721000 |
| 6 | -4.017481000 | 2.994608000 | 0.273038000 |
| 6 | -2.916589000 | 3.166078000 | -0.661991000 |
| 6 | -3.301210000 | 2.587029000 | -1.927334000 |
| 6 | -2.338731000 | 1.897283000 | -2.682561000 |
| 6 | -2.694910000 | 0.651265000 | -3.339821000 |
| 6 | -1.546601000 | -0.235841000 | -3.284249000 |
| 6 | -1.736366000 | -1.617065000 | -3.110409000 |
| 6 | -0.866667000 | -2.340163000 | -2.211526000 |
| 6 | -1.661896000 | -3.334628000 | -1.508136000 |
| 6 | -1.401999000 | -3.619099000 | -0.162368000 |
| 6 | -2.501997000 | -3.795961000 | 0.770938000 |
| 6 | -2.111358000 | -3.203459000 | 2.041711000 |
| 6 | -3.059249000 | -2.516243000 | 2.814211000 |
| 6 | -2.700916000 | -1.266640000 | 3.469022000 |
| 6 | -3.855368000 | -0.382319000 | 3.418293000 |
| 6 | -3.674540000 | 0.995678000 | 3.225950000 |
| 6 | -4.556361000 | 1.723500000 | 2.324476000 |
| 6 | -5.583429000 | 1.047428000 | 1.651898000 |
| 6 | -5.852884000 | 1.340054000 | 0.252304000 |
| 6 | -5.086332000 | 2.298634000 | -0.424100000 |
| 6 | -4.640974000 | 2.045533000 | -1.786561000 |
| 6 | -4.981078000 | 0.840918000 | -2.420028000 |
| 6 | -3.991297000 | 0.134013000 | -3.218954000 |
| 6 | -4.185345000 | -1.294504000 | -3.020052000 |
| 6 | -3.077581000 | -2.153514000 | -2.968694000 |
| 6 | -3.032460000 | -3.219004000 | -1.977686000 |
| 6 | -4.094619000 | -3.385316000 | -1.078170000 |
| 6 | -3.825024000 | -3.679920000 | 0.321136000 |
| 6 | -4.804687000 | -2.968823000 | 1.125311000 |
| 6 | -4.428254000 | -2.400588000 | 2.350764000 |
| 6 | -4.920232000 | -1.080125000 | 2.723604000 |
| 6 | -5.769533000 | -0.379114000 | 1.855644000 |
| 6 | -6.154076000 | -0.968329000 | 0.583316000 |

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| 6 | -6.205005000 | 0.094489000 | -0.406973000 |
| 6 | -5.776274000 | -0.149152000 | -1.719522000 |
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| 6 | -5.242682000 | -2.496210000 | -1.136654000 |
| 6 | -5.681619000 | -2.238647000 | 0.225171000 |
| 6 | 1.745971000 | 2.877299000 | -0.136964000 |
| 1 | 2.178745000 | 2.860995000 | -1.149567000 |
| 1 | 2.522973000 | 2.498603000 | 0.548136000 |
| 6 | 1.412032000 | 4.323233000 | 0.244959000 |
| 1 | 0.638360000 | 4.728184000 | -0.430628000 |
| 1 | 0.987193000 | 4.367483000 | 1.263164000 |
| 6 | 2.655022000 | 5.222592000 | 0.178953000 |
| 1 | 3.431630000 | 4.820772000 | 0.854166000 |
| 1 | 3.083364000 | 5.175458000 | -0.837809000 |
| 6 | 2.358050000 | 6.679364000 | 0.546977000 |
| 1 | 1.959290000 | 6.759435000 | 1.571225000 |
| 1 | 1.612179000 | 7.119145000 | -0.134603000 |
| 1 | 3.265438000 | 7.299740000 | 0.492809000 |
| 6 | 3.568819000 | -0.016560000 | -0.021194000 |
| 6 | 4.700792000 | 0.155694000 | -0.810901000 |
| 1 | 3.415712000 | -0.378990000 | 0.988734000 |
| 7 | 2.532290000 | 0.360313000 | -0.821578000 |
| 7 | 2.986143000 | 0.749357000 | -2.048022000 |
| 7 | 4.284607000 | 0.627551000 | -2.036592000 |
| 6 | 6.112031000 | -0.103477000 | -0.517761000 |
| 6 | 6.537858000 | -0.546847000 | 0.749071000 |
| 6 | 7.083881000 | 0.081170000 | -1.520521000 |
| 6 | 7.884448000 | -0.801094000 | 1.001803000 |
| 6 | 8.428574000 | -0.175741000 | -1.263754000 |
| 6 | 8.861271000 | -0.624291000 | 0.000926000 |
| 1 | 5.809036000 | -0.706757000 | 1.548023000 |
| 1 | 6.762081000 | 0.434526000 | -2.501767000 |
| 1 | 8.184681000 | -1.172795000 | 1.984417000 |
| 1 | 9.165811000 | -0.001798000 | -2.051261000 |
| 6 | 10.291988000 | -0.904423000 | 0.268812000 |
| 6 | 10.873964000 | -0.584759000 | 1.512250000 |
| 6 | 11.108904000 | -1.500327000 | -0.713508000 |
| 6 | 12.222271000 | -0.850531000 | 1.764036000 |
| 6 | 12.456898000 | -1.766906000 | -0.461058000 |
| 6 | 13.020200000 | -1.443242000 | 0.778651000 |
| 1 | 10.266731000 | -0.095666000 | 2.277954000 |
| 1 | 10.671923000 | -1.782446000 | -1.674530000 |
| 1 | 12.654495000 | -0.584996000 | 2.731839000 |
| 1 | 13.068666000 | -2.238757000 | -1.233761000 |
| 1 | 14.074262000 | -1.651655000 | 0.975488000 |

Compound 16

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|---|--------------|--------------|--------------|
| 6 | 1.122096000 | 1.671634000 | -0.080077000 |
| 6 | 1.503647000 | 0.196786000 | -0.654374000 |
| 6 | 1.177916000 | -0.968355000 | 0.299475000 |
| 6 | 0.819539000 | -0.809587000 | 1.623876000 |
| 6 | 0.459583000 | 0.523298000 | 2.151362000 |
| 6 | 0.467783000 | 1.622895000 | 1.312573000 |
| 6 | -0.620228000 | 2.561840000 | 1.384429000 |
| 6 | -0.919510000 | 3.008830000 | 0.036767000 |
| 6 | -0.016949000 | 2.345533000 | -0.866463000 |
| 6 | -0.484921000 | 1.933148000 | -2.100021000 |
| 6 | -0.121590000 | 0.601012000 | -2.622573000 |
| 6 | 0.697117000 | -0.238966000 | -1.896323000 |
| 6 | 0.367766000 | -1.635322000 | -1.796859000 |
| 6 | 0.664860000 | -2.084692000 | -0.448774000 |
| 6 | -0.142602000 | -3.056429000 | 0.164504000 |
| 6 | -0.500750000 | -2.903132000 | 1.556126000 |
| 6 | -0.031572000 | -1.787879000 | 2.269488000 |
| 6 | -0.917416000 | -1.084612000 | 3.179347000 |
| 6 | -0.614111000 | 0.334670000 | 3.105244000 |
| 6 | -1.653195000 | 1.274395000 | 3.206762000 |
| 6 | -1.654346000 | 2.417720000 | 2.324575000 |
| 6 | -3.028657000 | 2.697357000 | 1.938614000 |
| 6 | -3.317287000 | 3.128693000 | 0.637939000 |
| 6 | -2.244179000 | 3.301246000 | -0.328797000 |
| 6 | -2.726596000 | 2.881815000 | -1.623464000 |
| 6 | -1.857035000 | 2.193359000 | -2.485544000 |
| 6 | -2.343420000 | 1.049713000 | -3.237821000 |
| 6 | -1.273390000 | 0.071744000 | -3.321066000 |
| 6 | -1.572275000 | -1.299492000 | -3.269271000 |
| 6 | -0.730575000 | -2.175012000 | -2.487387000 |
| 6 | -1.578721000 | -3.167322000 | -1.844256000 |
| 6 | -1.289943000 | -3.601112000 | -0.544854000 |
| 6 | -2.362816000 | -3.778512000 | 0.419722000 |
| 6 | -1.872744000 | -3.347391000 | 1.720671000 |
| 6 | -2.727301000 | -2.664472000 | 2.599179000 |
| 6 | -2.238388000 | -1.517269000 | 3.349630000 |
| 6 | -3.314393000 | -0.541776000 | 3.437713000 |
| 6 | -3.025537000 | 0.828969000 | 3.367266000 |
| 6 | -3.878861000 | 1.710589000 | 2.583824000 |
| 6 | -4.986258000 | 1.188189000 | 1.900562000 |
| 6 | -5.287014000 | 1.637806000 | 0.549616000 |
| 6 | -4.468100000 | 2.592287000 | -0.069684000 |
| 6 | -4.100361000 | 2.437978000 | -1.469705000 |
| 6 | -4.566259000 | 1.332330000 | -2.196431000 |
| 6 | -3.672608000 | 0.629748000 | -3.104207000 |
| 6 | -3.979729000 | -0.791109000 | -3.032624000 |
| 6 | -2.947353000 | -1.737634000 | -3.115317000 |
| 6 | -2.952750000 | -2.895146000 | -2.232862000 |
| 6 | -3.988202000 | -3.062891000 | -1.302908000 |

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|---|--------------|--------------|--------------|
| 6 | -3.687856000 | -3.511956000 | 0.048291000 |
| 6 | -4.571105000 | -2.806839000 | 0.962081000 |
| 6 | -4.099111000 | -2.392848000 | 2.215739000 |
| 6 | -4.461838000 | -1.080073000 | 2.733335000 |
| 6 | -5.283285000 | -0.231895000 | 1.976869000 |
| 6 | -5.767622000 | -0.661135000 | 0.674791000 |
| 6 | -5.769727000 | 0.494720000 | -0.206909000 |
| 6 | -5.415498000 | 0.346422000 | -1.555709000 |
| 6 | -5.051881000 | -0.967148000 | -2.072502000 |
| 6 | -5.057580000 | -2.082133000 | -1.221944000 |
| 6 | -5.418066000 | -1.924096000 | 0.177290000 |
| 6 | 2.389145000 | 2.595796000 | -0.062253000 |
| 1 | 2.783728000 | 2.635390000 | -1.089780000 |
| 1 | 3.157802000 | 2.105306000 | 0.557785000 |
| 6 | 2.180345000 | 4.024676000 | 0.451572000 |
| 1 | 1.412944000 | 4.539959000 | -0.152069000 |
| 1 | 1.800522000 | 4.011498000 | 1.488364000 |
| 6 | 3.481763000 | 4.838728000 | 0.405263000 |
| 1 | 4.254242000 | 4.326362000 | 1.006162000 |
| 1 | 3.864080000 | 4.854449000 | -0.630658000 |
| 6 | 3.303539000 | 6.273298000 | 0.911302000 |
| 1 | 2.953564000 | 6.287853000 | 1.956185000 |
| 1 | 2.563053000 | 6.820557000 | 0.305921000 |
| 1 | 4.249383000 | 6.834155000 | 0.868278000 |
| 6 | 3.981170000 | -0.339136000 | -0.239768000 |
| 6 | 5.104823000 | -0.147736000 | -1.036805000 |
| 1 | 3.835583000 | -0.751106000 | 0.752278000 |
| 7 | 2.941905000 | 0.103386000 | -1.001088000 |
| 7 | 3.384924000 | 0.550082000 | -2.211649000 |
| 7 | 4.680585000 | 0.395476000 | -2.229428000 |
| 1 | 6.241638000 | -1.077957000 | 1.270383000 |
| 6 | 6.955712000 | -0.896783000 | 0.461358000 |
| 6 | 6.519397000 | -0.424050000 | -0.771123000 |
| 6 | 7.477992000 | -0.191077000 | -1.802873000 |
| 6 | 8.817323000 | -0.429469000 | -1.584756000 |
| 6 | 9.287602000 | -0.912045000 | -0.331019000 |
| 6 | 8.328302000 | -1.150951000 | 0.715051000 |
| 6 | 8.790832000 | -1.630734000 | 1.973120000 |
| 6 | 10.135184000 | -1.864122000 | 2.190954000 |
| 6 | 11.079421000 | -1.628636000 | 1.159478000 |
| 6 | 10.662537000 | -1.163145000 | -0.073882000 |
| 1 | 7.120481000 | 0.181001000 | -2.764289000 |
| 1 | 9.542237000 | -0.247316000 | -2.383065000 |
| 1 | 11.388140000 | -0.980291000 | -0.871350000 |
| 1 | 12.139523000 | -1.816951000 | 1.344198000 |
| 1 | 10.476158000 | -2.231941000 | 3.161524000 |
| 1 | 8.061738000 | -1.812205000 | 2.767967000 |