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# Biradical *o*-Iminobenzosemiquinonato(1−) Complexes of Nickel(II): Catalytic Activity in Three-Component Coupling of Aldehydes, Amines and Alkynes

**Mina Nasibipour [a], Elham Safaei [a,*], Ali Moaddeli [a], Marziyeh Sadat Masoumpour [b], Andrzej Wojtczak [c]**

*[a] Department of Chemistry, College of Sciences, Shiraz University, 71454, Shiraz, Iran*
*[b] Department of Chemistry, Estahban Higher Education Center, Estahban 74519-44655, Iran*
*[c] Nicolaus Copernicus University, Faculty of Chemistry, 87-100 Torun, Poland*

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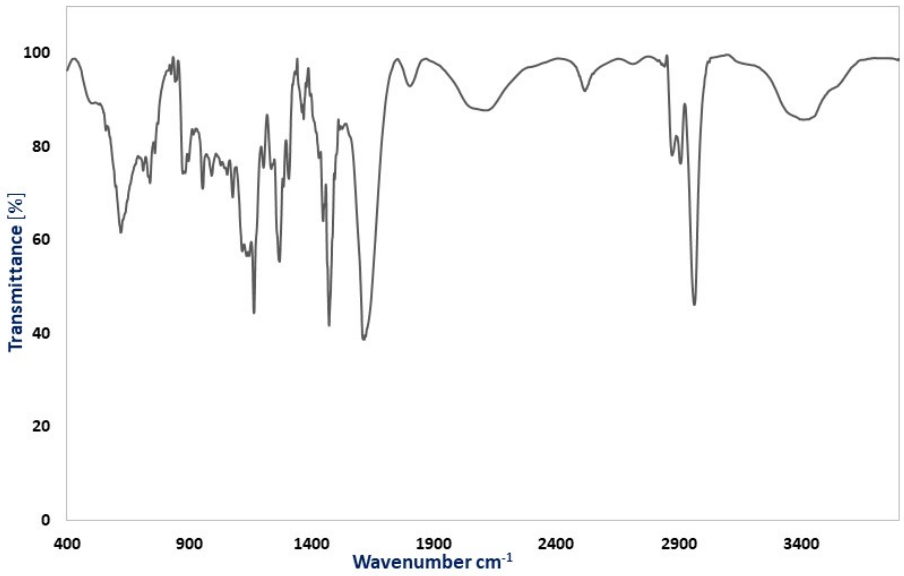


**Figure S1** IR spectrum of $Ni^{II}L_2^{BIS}$.

**Table S1** Crystal data and structure refinement for $Ni^{II}L_2^{BIS}$.

| | |
|---|---|
| Identification code | e1464a_sq |
| Empirical formula | C70 H88 N4 Ni O4 |
| Formula weight | 1108.15 |
| Temperature; K | 293(2) |
| Wavelength; Å | 0.71073 |
| Crystal system | Monoclinic |
| Space group | $P2_1/n$ |
| Unit cell dimensions; Å, ° | a = 18.1423(6) |
| | b = 17.5195(5) |
| | c = 23.9371(9) |
| | α = 90 |
| | β = 106.001(3) |
| | γ = 90 |
| Volume; $Å^3$ | 7313.5(4) |
| Z | 4 |
| Density (calculated); $Mg/m^3$ | 1.006 |
| Absorption coefficient; $mm^{-1}$ | 0.308 |
| F(000) | 2384 |
| Crystal size; mm | 0.793 x 0.564 x 0.517 |
| Theta range for data collection | 2.325 to 28.366°. |
| Index ranges | -22<=h<=21, -22<=k<=22, -31<=l<=29 |
| Reflections collected | 52213 |
| Independent reflections | 16548 [R(int) = 0.0442] |
| Completeness to theta = 25.242° | 99.9 % |
| Absorption correction | Analytical |
| Max. and min. transmission | 0.883 and 0.839 |
| Refinement method | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 16548 / 0 / 712 |
| Goodness-of-fit on $F^2$ | 1.040 |
| Final R indices [I>2sigma(I)] | R1 = 0.0614, wR2 = 0.1426 |
| R indices (all data) | R1 = 0.1017, wR2 = 0.1725 |
| Largest diff. peak and hole; $e.Å^{-3}$ | 0.649 and -0.271 |

**Table 2** Bond lengths [Å] and angles [°] for $Ni^{II}L_2^{BIS}$.

| | |
|---|---|
| Ni(1)-N(41) | 2.0193(19) |
| Ni(1)-N(1) | 2.027(2) |
| Ni(1)-O(41) | 2.0425(18) |
| Ni(1)-O(1) | 2.0466(19) |
| Ni(1)-N(2) | 2.143(2) |
| Ni(1)-N(42) | 2.153(2) |
| O(1)-C(1) | 1.286(3) |
| C(1)-C(2) | 1.446(4) |
| C(1)-C(6) | 1.466(4) |
| C(2)-C(3) | 1.375(4) |
| C(2)-C(20) | 1.536(5) |
| C(3)-C(4) | 1.427(5) |
| C(4)-C(5) | 1.368(5) |
| C(4)-C(24) | 1.547(4) |
| C(5)-C(6) | 1.428(4) |
| C(6)-N(1) | 1.355(4) |
| N(1)-C(7) | 1.398(4) |
| C(7)-C(8) | 1.412(4) |
| C(7)-C(12) | 1.414(4) |
| C(8)-C(9) | 1.376(5) |
| C(9)-C(10) | 1.371(6) |
| C(10)-C(11) | 1.388(5) |
| C(11)-C(12) | 1.395(4) |
| C(12)-C(13) | 1.469(4) |
| C(13)-N(2) | 1.302(3) |
| C(13)-O(2) | 1.372(3) |
| N(2)-C(14) | 1.411(3) |
| C(14)-C(19) | 1.381(4) |
| C(14)-C(15) | 1.396(4) |
| C(15)-C(16) | 1.395(4) |
| C(16)-C(17) | 1.405(4) |
| C(16)-C(28) | 1.548(4) |
| C(17)-C(18) | 1.397(4) |
| C(18)-C(19) | 1.400(4) |
| C(18)-C(32) | 1.521(4) |
| C(19)-O(2) | 1.392(3) |
| C(20)-C(21) | 1.530(6) |
| C(20)-C(23) | 1.551(5) |
| C(20)-C(22) | 1.556(5) |
| C(24)-C(25) | 1.461(7) |
| C(24)-C(27) | 1.474(8) |
| C(24)-C(26) | 1.575(8) |
| C(28)-C(29) | 1.448(7) |
| C(28)-C(30) | 1.463(6) |
| C(28)-C(31) | 1.527(8) |
| C(32)-C(35) | 1.513(5) |
| C(32)-C(33) | 1.523(6) |
| C(32)-C(34) | 1.551(5) |
| O(41)-C(41) | 1.283(3) |
| C(41)-C(42) | 1.452(4) |
| C(41)-C(46) | 1.465(3) |
| C(42)-C(43) | 1.369(4) |
| C(42)-C(60) | 1.546(4) |
| C(43)-C(44) | 1.430(4) |
| C(44)-C(45) | 1.375(4) |
| C(44)-C(64) | 1.536(4) |
| C(45)-C(46) | 1.420(3) |
| C(46)-N(41) | 1.363(3) |
| N(41)-C(47) | 1.394(3) |
| C(47)-C(48) | 1.401(4) |
| C(47)-C(52) | 1.418(3) |
| C(48)-C(49) | 1.386(4) |
| C(49)-C(50) | 1.384(5) |
| C(50)-C(51) | 1.377(4) |
| C(51)-C(52) | 1.405(4) |
| C(52)-C(53) | 1.465(3) |
| C(53)-N(42) | 1.306(3) |
| C(53)-O(42) | 1.371(3) |
| N(42)-C(54) | 1.415(3) |
| C(54)-C(59) | 1.382(4) |
| C(54)-C(55) | 1.392(4) |
| C(55)-C(56) | 1.396(4) |

| | |
|---|---|
| C(56)-C(57) | 1.405(4) |
| C(56)-C(68) | 1.547(4) |
| C(57)-C(58) | 1.396(4) |
| C(58)-C(59) | 1.397(4) |
| C(58)-C(72) | 1.535(4) |
| C(59)-O(42) | 1.392(3) |
| C(60)-C(62) | 1.536(6) |
| C(60)-C(61) | 1.543(6) |
| C(60)-C(63) | 1.546(5) |
| C(64)-C(65) | 1.536(5) |
| C(64)-C(67) | 1.538(5) |
| C(64)-C(66) | 1.542(5) |
| C(68)-C(69) | 1.504(6) |
| C(68)-C(70) | 1.509(7) |
| C(68)-C(71) | 1.517(7) |
| C(72)-C(74) | 1.525(6) |
| C(72)-C(75) | 1.527(6) |
| C(72)-C(73) | 1.540(5) |
| N(41)-Ni(1)-N(1) | 171.41(9) |
| N(41)-Ni(1)-O(41) | 80.73(7) |
| N(1)-Ni(1)-O(41) | 93.90(8) |
| N(41)-Ni(1)-O(1) | 94.40(8) |
| N(1)-Ni(1)-O(1) | 80.16(8) |
| O(41)-Ni(1)-O(1) | 102.55(8) |
| N(41)-Ni(1)-N(2) | 98.03(8) |
| N(1)-Ni(1)-N(2) | 88.61(9) |
| O(41)-Ni(1)-N(2) | 89.99(8) |
| O(1)-Ni(1)-N(2) | 163.62(8) |
| N(41)-Ni(1)-N(42) | 88.14(8) |
| N(1)-Ni(1)-N(42) | 98.28(8) |
| O(41)-Ni(1)-N(42) | 164.88(8) |
| O(1)-Ni(1)-N(42) | 88.40(8) |
| N(2)-Ni(1)-N(42) | 81.41(8) |
| C(1)-O(1)-Ni(1) | 111.03(17) |
| O(1)-C(1)-C(2) | 122.8(3) |
| O(1)-C(1)-C(6) | 117.5(2) |
| C(2)-C(1)-C(6) | 119.7(2) |
| C(3)-C(2)-C(1) | 116.8(3) |
| C(3)-C(2)-C(20) | 123.8(3) |
| C(1)-C(2)-C(20) | 119.4(3) |
| C(2)-C(3)-C(4) | 124.9(3) |
| C(5)-C(4)-C(3) | 118.6(3) |
| C(5)-C(4)-C(24) | 121.3(4) |
| C(3)-C(4)-C(24) | 120.1(4) |
| C(4)-C(5)-C(6) | 121.2(3) |
| N(1)-C(6)-C(5) | 126.6(3) |
| N(1)-C(6)-C(1) | 114.3(2) |
| C(5)-C(6)-C(1) | 118.8(3) |
| C(6)-N(1)-C(7) | 123.3(2) |
| C(6)-N(1)-Ni(1) | 111.56(17) |
| C(7)-N(1)-Ni(1) | 124.81(19) |
| N(1)-C(7)-C(8) | 122.6(3) |
| N(1)-C(7)-C(12) | 120.1(2) |
| C(8)-C(7)-C(12) | 117.1(3) |
| C(9)-C(8)-C(7) | 121.2(4) |
| C(10)-C(9)-C(8) | 121.3(3) |
| C(9)-C(10)-C(11) | 119.3(4) |
| C(10)-C(11)-C(12) | 120.7(4) |
| C(11)-C(12)-C(7) | 120.4(3) |
| C(11)-C(12)-C(13) | 118.0(3) |
| C(7)-C(12)-C(13) | 121.6(2) |
| N(2)-C(13)-O(2) | 114.4(2) |
| N(2)-C(13)-C(12) | 128.6(3) |
| O(2)-C(13)-C(12) | 117.0(2) |
| C(13)-N(2)-C(14) | 105.1(2) |
| C(13)-N(2)-Ni(1) | 119.78(18) |
| C(14)-N(2)-Ni(1) | 130.06(17) |
| C(19)-C(14)-C(15) | 121.0(3) |
| C(19)-C(14)-N(2) | 108.2(2) |
| C(15)-C(14)-N(2) | 130.8(3) |
| C(16)-C(15)-C(14) | 117.6(3) |
| C(15)-C(16)-C(17) | 119.0(3) |
| C(15)-C(16)-C(28) | 119.7(3) |

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|---|---|
| C(17)-C(16)-C(28) | 121.2(3) |
| C(18)-C(17)-C(16) | 125.4(3) |
| C(17)-C(18)-C(19) | 112.6(3) |
| C(17)-C(18)-C(32) | 124.3(3) |
| C(19)-C(18)-C(32) | 123.0(3) |
| C(14)-C(19)-O(2) | 107.8(2) |
| C(14)-C(19)-C(18) | 124.4(3) |
| O(2)-C(19)-C(18) | 127.8(3) |
| C(13)-O(2)-C(19) | 104.4(2) |
| C(21)-C(20)-C(2) | 110.4(3) |
| C(21)-C(20)-C(23) | 108.3(4) |
| C(2)-C(20)-C(23) | 111.8(3) |
| C(21)-C(20)-C(22) | 110.2(3) |
| C(2)-C(20)-C(22) | 108.7(3) |
| C(23)-C(20)-C(22) | 107.4(3) |
| C(25)-C(24)-C(27) | 116.8(6) |
| C(25)-C(24)-C(4) | 111.1(4) |
| C(27)-C(24)-C(4) | 110.1(4) |
| C(25)-C(24)-C(26) | 105.6(6) |
| C(27)-C(24)-C(26) | 101.7(5) |
| C(4)-C(24)-C(26) | 111.1(4) |
| C(29)-C(28)-C(30) | 113.5(6) |
| C(29)-C(28)-C(31) | 106.5(6) |
| C(30)-C(28)-C(31) | 103.9(5) |
| C(29)-C(28)-C(16) | 108.9(4) |
| C(30)-C(28)-C(16) | 113.1(3) |
| C(31)-C(28)-C(16) | 110.7(4) |
| C(35)-C(32)-C(18) | 112.2(3) |
| C(35)-C(32)-C(33) | 110.0(4) |
| C(18)-C(32)-C(33) | 111.0(3) |
| C(35)-C(32)-C(34) | 108.9(3) |
| C(18)-C(32)-C(34) | 107.6(3) |
| C(33)-C(32)-C(34) | 106.9(4) |
| C(41)-O(41)-Ni(1) | 111.27(15) |
| O(41)-C(41)-C(42) | 123.2(2) |
| O(41)-C(41)-C(46) | 118.6(2) |
| C(42)-C(41)-C(46) | 118.2(2) |
| C(43)-C(42)-C(41) | 117.8(3) |
| C(43)-C(42)-C(60) | 123.6(3) |
| C(41)-C(42)-C(60) | 118.6(3) |
| C(42)-C(43)-C(44) | 124.7(3) |
| C(45)-C(44)-C(43) | 118.1(2) |
| C(45)-C(44)-C(64) | 122.5(3) |
| C(43)-C(44)-C(64) | 119.4(2) |
| C(44)-C(45)-C(46) | 121.2(2) |
| N(41)-C(46)-C(45) | 126.3(2) |
| N(41)-C(46)-C(41) | 113.8(2) |
| C(45)-C(46)-C(41) | 119.9(2) |
| C(46)-N(41)-C(47) | 122.0(2) |
| C(46)-N(41)-Ni(1) | 111.79(15) |
| C(47)-N(41)-Ni(1) | 125.67(15) |
| N(41)-C(47)-C(48) | 122.1(2) |
| N(41)-C(47)-C(52) | 120.3(2) |
| C(48)-C(47)-C(52) | 117.5(2) |
| C(49)-C(48)-C(47) | 121.6(3) |
| C(50)-C(49)-C(48) | 120.6(3) |
| C(51)-C(50)-C(49) | 119.1(3) |
| C(50)-C(51)-C(52) | 121.4(3) |
| C(51)-C(52)-C(47) | 119.5(2) |
| C(51)-C(52)-C(53) | 118.3(2) |
| C(47)-C(52)-C(53) | 122.2(2) |
| N(42)-C(53)-O(42) | 114.2(2) |
| N(42)-C(53)-C(52) | 128.8(2) |
| O(42)-C(53)-C(52) | 116.9(2) |
| C(53)-N(42)-C(54) | 105.2(2) |
| C(53)-N(42)-Ni(1) | 120.77(16) |
| C(54)-N(42)-Ni(1) | 131.18(17) |
| C(59)-C(54)-C(55) | 121.0(2) |
| C(59)-C(54)-N(42) | 108.1(2) |
| C(55)-C(54)-N(42) | 130.9(2) |
| C(54)-C(55)-C(56) | 117.8(3) |
| C(55)-C(56)-C(57) | 118.8(3) |
| C(55)-C(56)-C(68) | 121.1(3) |

| | |
|---|---|
| C(57)-C(56)-C(68) | 120.1(3) |
| C(58)-C(57)-C(56) | 125.3(3) |
| C(57)-C(58)-C(59) | 112.9(3) |
| C(57)-C(58)-C(72) | 124.7(3) |
| C(59)-C(58)-C(72) | 122.4(3) |
| C(54)-C(59)-O(42) | 107.8(2) |
| C(54)-C(59)-C(58) | 124.2(3) |
| O(42)-C(59)-C(58) | 128.0(3) |
| C(62)-C(60)-C(61) | 110.8(4) |
| C(62)-C(60)-C(63) | 107.3(4) |
| C(61)-C(60)-C(63) | 108.7(4) |
| C(62)-C(60)-C(42) | 110.2(3) |
| C(61)-C(60)-C(42) | 108.6(3) |
| C(63)-C(60)-C(42) | 111.2(3) |
| C(44)-C(64)-C(65) | 111.9(3) |
| C(44)-C(64)-C(67) | 110.5(3) |
| C(65)-C(64)-C(67) | 108.7(3) |
| C(44)-C(64)-C(66) | 108.8(3) |
| C(65)-C(64)-C(66) | 107.9(3) |
| C(67)-C(64)-C(66) | 109.0(3) |
| C(69)-C(68)-C(70) | 108.5(4) |
| C(69)-C(68)-C(71) | 108.0(4) |
| C(70)-C(68)-C(71) | 109.0(5) |
| C(69)-C(68)-C(56) | 111.8(3) |
| C(70)-C(68)-C(56) | 111.7(3) |
| C(71)-C(68)-C(56) | 107.8(4) |
| C(74)-C(72)-C(75) | 109.0(4) |
| C(74)-C(72)-C(58) | 108.5(3) |
| C(75)-C(72)-C(58) | 109.7(3) |
| C(74)-C(72)-C(73) | 109.1(4) |
| C(75)-C(72)-C(73) | 108.8(4) |
| C(58)-C(72)-C(73) | 111.7(3) |

**Table 3** Torsion angles [°] for $Ni^{II}L_2^{BIS}$.

| | |
|---|---|
| Ni(1)-O(1)-C(1)-C(2) | 159.9(2) |
| Ni(1)-O(1)-C(1)-C(6) | -20.2(3) |
| O(1)-C(1)-C(2)-C(3) | -179.1(3) |
| C(6)-C(1)-C(2)-C(3) | 1.0(4) |
| O(1)-C(1)-C(2)-C(20) | -0.9(4) |
| C(6)-C(1)-C(2)-C(20) | 179.2(3) |
| C(1)-C(2)-C(3)-C(4) | -0.5(5) |
| C(20)-C(2)-C(3)-C(4) | -178.6(3) |
| C(2)-C(3)-C(4)-C(5) | -0.9(5) |
| C(2)-C(3)-C(4)-C(24) | 176.8(3) |
| C(3)-C(4)-C(5)-C(6) | 1.7(5) |
| C(24)-C(4)-C(5)-C(6) | -176.0(3) |
| C(4)-C(5)-C(6)-N(1) | 172.7(3) |
| C(4)-C(5)-C(6)-C(1) | -1.2(4) |
| O(1)-C(1)-C(6)-N(1) | 5.3(4) |
| C(2)-C(1)-C(6)-N(1) | -174.8(2) |
| O(1)-C(1)-C(6)-C(5) | 179.9(2) |
| C(2)-C(1)-C(6)-C(5) | -0.2(4) |
| C(5)-C(6)-N(1)-C(7) | 24.6(4) |
| C(1)-C(6)-N(1)-C(7) | -161.4(2) |
| C(5)-C(6)-N(1)-Ni(1) | -161.3(2) |
| C(1)-C(6)-N(1)-Ni(1) | 12.7(3) |
| C(6)-N(1)-C(7)-C(8) | 34.9(4) |
| Ni(1)-N(1)-C(7)-C(8) | -138.4(3) |
| C(6)-N(1)-C(7)-C(12) | -148.8(3) |
| Ni(1)-N(1)-C(7)-C(12) | 37.8(4) |
| N(1)-C(7)-C(8)-C(9) | 178.3(4) |
| C(12)-C(7)-C(8)-C(9) | 1.9(5) |
| C(7)-C(8)-C(9)-C(10) | 0.6(7) |
| C(8)-C(9)-C(10)-C(11) | -1.9(8) |
| C(9)-C(10)-C(11)-C(12) | 0.5(8) |
| C(10)-C(11)-C(12)-C(7) | 2.1(6) |
| C(10)-C(11)-C(12)-C(13) | -176.9(4) |

| | |
|---|---|
| N(1)-C(7)-C(12)-C(11) | -179.7(3) |
| C(8)-C(7)-C(12)-C(11) | -3.3(5) |
| N(1)-C(7)-C(12)-C(13) | -0.8(4) |
| C(8)-C(7)-C(12)-C(13) | 175.7(3) |
| C(11)-C(12)-C(13)-N(2) | 144.3(3) |
| C(7)-C(12)-C(13)-N(2) | -34.7(5) |
| C(11)-C(12)-C(13)-O(2) | -33.3(4) |
| C(7)-C(12)-C(13)-O(2) | 147.7(3) |
| O(2)-C(13)-N(2)-C(14) | 0.8(3) |
| C(12)-C(13)-N(2)-C(14) | -176.8(3) |
| O(2)-C(13)-N(2)-Ni(1) | -156.58(18) |
| C(12)-C(13)-N(2)-Ni(1) | 25.8(4) |
| C(13)-N(2)-C(14)-C(19) | -1.0(3) |
| Ni(1)-N(2)-C(14)-C(19) | 153.10(19) |
| C(13)-N(2)-C(14)-C(15) | 177.2(3) |
| Ni(1)-N(2)-C(14)-C(15) | -28.6(4) |
| C(19)-C(14)-C(15)-C(16) | -0.8(4) |
| N(2)-C(14)-C(15)-C(16) | -178.8(3) |
| C(14)-C(15)-C(16)-C(17) | -0.6(4) |
| C(14)-C(15)-C(16)-C(28) | 176.2(3) |
| C(15)-C(16)-C(17)-C(18) | 0.7(5) |
| C(28)-C(16)-C(17)-C(18) | -176.0(3) |
| C(16)-C(17)-C(18)-C(19) | 0.6(4) |
| C(16)-C(17)-C(18)-C(32) | -179.3(3) |
| C(15)-C(14)-C(19)-O(2) | -177.5(2) |
| N(2)-C(14)-C(19)-O(2) | 0.9(3) |
| C(15)-C(14)-C(19)-C(18) | 2.3(4) |
| N(2)-C(14)-C(19)-C(18) | -179.2(3) |
| C(17)-C(18)-C(19)-C(14) | -2.1(4) |
| C(32)-C(18)-C(19)-C(14) | 177.7(3) |
| C(17)-C(18)-C(19)-O(2) | 177.7(3) |
| C(32)-C(18)-C(19)-O(2) | -2.4(5) |
| N(2)-C(13)-O(2)-C(19) | -0.2(3) |
| C(12)-C(13)-O(2)-C(19) | 177.6(2) |
| C(14)-C(19)-O(2)-C(13) | -0.4(3) |
| C(18)-C(19)-O(2)-C(13) | 179.7(3) |
| C(3)-C(2)-C(20)-C(21) | -120.1(4) |
| C(1)-C(2)-C(20)-C(21) | 61.9(4) |
| C(3)-C(2)-C(20)-C(23) | 0.6(5) |
| C(1)-C(2)-C(20)-C(23) | -177.4(3) |
| C(3)-C(2)-C(20)-C(22) | 119.0(4) |
| C(1)-C(2)-C(20)-C(22) | -59.0(4) |
| C(5)-C(4)-C(24)-C(25) | -119.0(6) |
| C(3)-C(4)-C(24)-C(25) | 63.5(7) |
| C(5)-C(4)-C(24)-C(27) | 110.1(6) |
| C(3)-C(4)-C(24)-C(27) | -67.5(6) |
| C(5)-C(4)-C(24)-C(26) | -1.7(6) |
| C(3)-C(4)-C(24)-C(26) | -179.3(4) |
| C(15)-C(16)-C(28)-C(29) | -92.7(6) |
| C(17)-C(16)-C(28)-C(29) | 84.0(7) |
| C(15)-C(16)-C(28)-C(30) | 34.5(6) |
| C(17)-C(16)-C(28)-C(30) | -148.7(5) |
| C(15)-C(16)-C(28)-C(31) | 150.6(5) |
| C(17)-C(16)-C(28)-C(31) | -32.7(6) |
| C(17)-C(18)-C(32)-C(35) | -4.2(5) |
| C(19)-C(18)-C(32)-C(35) | 176.0(4) |
| C(17)-C(18)-C(32)-C(33) | -127.7(4) |
| C(19)-C(18)-C(32)-C(33) | 52.5(4) |
| C(17)-C(18)-C(32)-C(34) | 115.6(4) |
| C(19)-C(18)-C(32)-C(34) | -64.2(4) |
| Ni(1)-O(41)-C(41)-C(42) | 166.3(2) |
| Ni(1)-O(41)-C(41)-C(46) | -15.2(3) |
| O(41)-C(41)-C(42)-C(43) | -179.9(3) |
| C(46)-C(41)-C(42)-C(43) | 1.6(4) |

| | |
|---|---|
| O(41)-C(41)-C(42)-C(60) | 0.8(4) |
| C(46)-C(41)-C(42)-C(60) | -177.7(3) |
| C(41)-C(42)-C(43)-C(44) | 1.1(5) |
| C(60)-C(42)-C(43)-C(44) | -179.7(3) |
| C(42)-C(43)-C(44)-C(45) | -2.5(5) |
| C(42)-C(43)-C(44)-C(64) | 179.0(3) |
| C(43)-C(44)-C(45)-C(46) | 1.1(4) |
| C(64)-C(44)-C(45)-C(46) | 179.5(3) |
| C(44)-C(45)-C(46)-N(41) | 178.1(3) |
| C(44)-C(45)-C(46)-C(41) | 1.5(4) |
| O(41)-C(41)-C(46)-N(41) | 1.6(3) |
| C(42)-C(41)-C(46)-N(41) | -179.9(2) |
| O(41)-C(41)-C(46)-C(45) | 178.6(2) |
| C(42)-C(41)-C(46)-C(45) | -2.9(4) |
| C(45)-C(46)-N(41)-C(47) | 24.4(4) |
| C(41)-C(46)-N(41)-C(47) | -158.8(2) |
| C(45)-C(46)-N(41)-Ni(1) | -163.6(2) |
| C(41)-C(46)-N(41)-Ni(1) | 13.1(3) |
| C(46)-N(41)-C(47)-C(48) | 34.3(4) |
| Ni(1)-N(41)-C(47)-C(48) | -136.5(2) |
| C(46)-N(41)-C(47)-C(52) | -150.5(2) |
| Ni(1)-N(41)-C(47)-C(52) | 38.7(3) |
| N(41)-C(47)-C(48)-C(49) | 178.9(3) |
| C(52)-C(47)-C(48)-C(49) | 3.5(5) |
| C(47)-C(48)-C(49)-C(50) | 1.3(6) |
| C(48)-C(49)-C(50)-C(51) | -3.3(6) |
| C(49)-C(50)-C(51)-C(52) | 0.3(6) |
| C(50)-C(51)-C(52)-C(47) | 4.6(5) |
| C(50)-C(51)-C(52)-C(53) | -172.7(3) |
| N(41)-C(47)-C(52)-C(51) | 178.2(2) |
| C(48)-C(47)-C(52)-C(51) | -6.4(4) |
| N(41)-C(47)-C(52)-C(53) | -4.6(4) |
| C(48)-C(47)-C(52)-C(53) | 170.9(3) |
| C(51)-C(52)-C(53)-N(42) | 149.1(3) |
| C(47)-C(52)-C(53)-N(42) | -28.2(4) |
| C(51)-C(52)-C(53)-O(42) | -26.3(4) |
| C(47)-C(52)-C(53)-O(42) | 156.4(2) |
| O(42)-C(53)-N(42)-C(54) | 0.1(3) |
| C(52)-C(53)-N(42)-C(54) | -175.4(2) |
| O(42)-C(53)-N(42)-Ni(1) | -162.83(16) |
| C(52)-C(53)-N(42)-Ni(1) | 21.7(4) |
| C(53)-N(42)-C(54)-C(59) | -0.3(3) |
| Ni(1)-N(42)-C(54)-C(59) | 160.06(19) |
| C(53)-N(42)-C(54)-C(55) | 178.3(3) |
| Ni(1)-N(42)-C(54)-C(55) | -21.3(4) |
| C(59)-C(54)-C(55)-C(56) | -0.7(4) |
| N(42)-C(54)-C(55)-C(56) | -179.1(3) |
| C(54)-C(55)-C(56)-C(57) | -0.8(5) |
| C(54)-C(55)-C(56)-C(68) | 176.1(3) |
| C(55)-C(56)-C(57)-C(58) | 1.0(5) |
| C(68)-C(56)-C(57)-C(58) | -176.0(3) |
| C(56)-C(57)-C(58)-C(59) | 0.3(5) |
| C(56)-C(57)-C(58)-C(72) | -177.9(3) |
| C(55)-C(54)-C(59)-O(42) | -178.3(3) |
| N(42)-C(54)-C(59)-O(42) | 0.5(3) |
| C(55)-C(54)-C(59)-C(58) | 2.2(5) |
| N(42)-C(54)-C(59)-C(58) | -179.1(3) |
| C(57)-C(58)-C(59)-C(54) | -1.9(4) |
| C(72)-C(58)-C(59)-C(54) | 176.4(3) |
| C(57)-C(58)-C(59)-O(42) | 178.7(3) |
| C(72)-C(58)-C(59)-O(42) | -3.1(5) |
| N(42)-C(53)-O(42)-C(59) | 0.2(3) |
| C(52)-C(53)-O(42)-C(59) | 176.3(2) |
| C(54)-C(59)-O(42)-C(53) | -0.4(3) |

| | |
|---|---|
| C(58)-C(59)-O(42)-C(53) | 179.1(3) |
| C(43)-C(42)-C(60)-C(62) | 120.8(4) |
| C(41)-C(42)-C(60)-C(62) | -59.9(4) |
| C(43)-C(42)-C(60)-C(61) | -117.6(4) |
| C(41)-C(42)-C(60)-C(61) | 61.6(4) |
| C(43)-C(42)-C(60)-C(63) | 2.0(5) |
| C(41)-C(42)-C(60)-C(63) | -178.8(4) |
| C(45)-C(44)-C(64)-C(65) | 3.5(4) |
| C(43)-C(44)-C(64)-C(65) | -178.1(3) |
| C(45)-C(44)-C(64)-C(67) | 124.8(4) |
| C(43)-C(44)-C(64)-C(67) | -56.8(4) |
| C(45)-C(44)-C(64)-C(66) | -115.6(3) |
| C(43)-C(44)-C(64)-C(66) | 62.8(4) |
| C(55)-C(56)-C(68)-C(69) | 139.1(4) |
| C(57)-C(56)-C(68)-C(69) | -44.0(5) |
| C(55)-C(56)-C(68)-C(70) | 17.3(6) |
| C(57)-C(56)-C(68)-C(70) | -165.8(5) |
| C(55)-C(56)-C(68)-C(71) | -102.4(5) |
| C(57)-C(56)-C(68)-C(71) | 74.5(5) |
| C(57)-C(58)-C(72)-C(74) | 116.2(4) |
| C(59)-C(58)-C(72)-C(74) | -61.9(5) |
| C(57)-C(58)-C(72)-C(75) | -124.9(4) |
| C(59)-C(58)-C(72)-C(75) | 57.0(5) |
| C(57)-C(58)-C(72)-C(73) | -4.2(5) |
| C(59)-C(58)-C(72)-C(73) | 177.8(4) |

Symmetry transformations used to generate equivalent atoms

**Table S4** Selected bond lengths of optimized structure of $Ni^{II}L_2^{BIS}$.

| Ligand 1 | | | Ligand 2 | | |
|---|---|---|---|---|---|
| Bond | Experimental | Theoretical | Bond | Experimental | Theoretical |
| Ni1-O2 | 2.046 | 2.074 | Ni1-O85 | 2.043 | 2.071 |
| Ni1-N11 | 2.026 | 2.084 | Ni1-N94 | 2.019 | 2.075 |
| Ni1-N23 | 2.143 | 2.163 | Ni1-N106 | 2.153 | 2.160 |
| C3-O2 | 1.286 | 1.283 | C86-O85 | 1.283 | 1.284 |
| C10-N11 | 1.356 | 1.360 | C93-N94 | 1.364 | 1.362 |
| C3-C4 | 1.447 | 1.449 | C86-C87 | 1.451 | 1.449 |
| C4-C5 | 1.375 | 1.380 | C87-C88 | 1.370 | 1.381 |
| C5-C7 | 1.426 | 1.432 | C88-C90 | 1.430 | 1.431 |
| C7-C8 | 1.368 | 1.379 | C90-C91 | 1.374 | 1.380 |
| C8-C10 | 1.429 | 1.422 | C91-C93 | 1.420 | 1.422 |
| C10-C3 | 1.465 | 1.468 | C93-C86 | 1.465 | 1.465 |

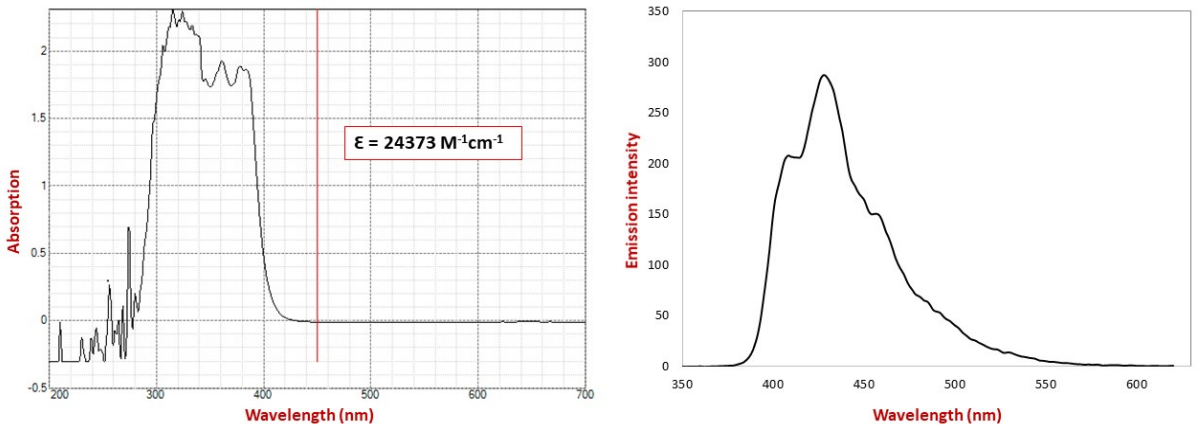


**Figure S2** Absorption and emission spectrums of the 0.1mM $CH_2Cl_2$ solutions of $H_2L^{BAP}$ ligand.

The extinction coefficient value of the $H_2L^{BAP}$ ligand which extracted by the plot of the absorption maxima at a selected wavelength 314 nm versus varied concentrations is 24373 $M^{-1}cm^{-1}$.

## Physical and spectroscopic data for selected compounds

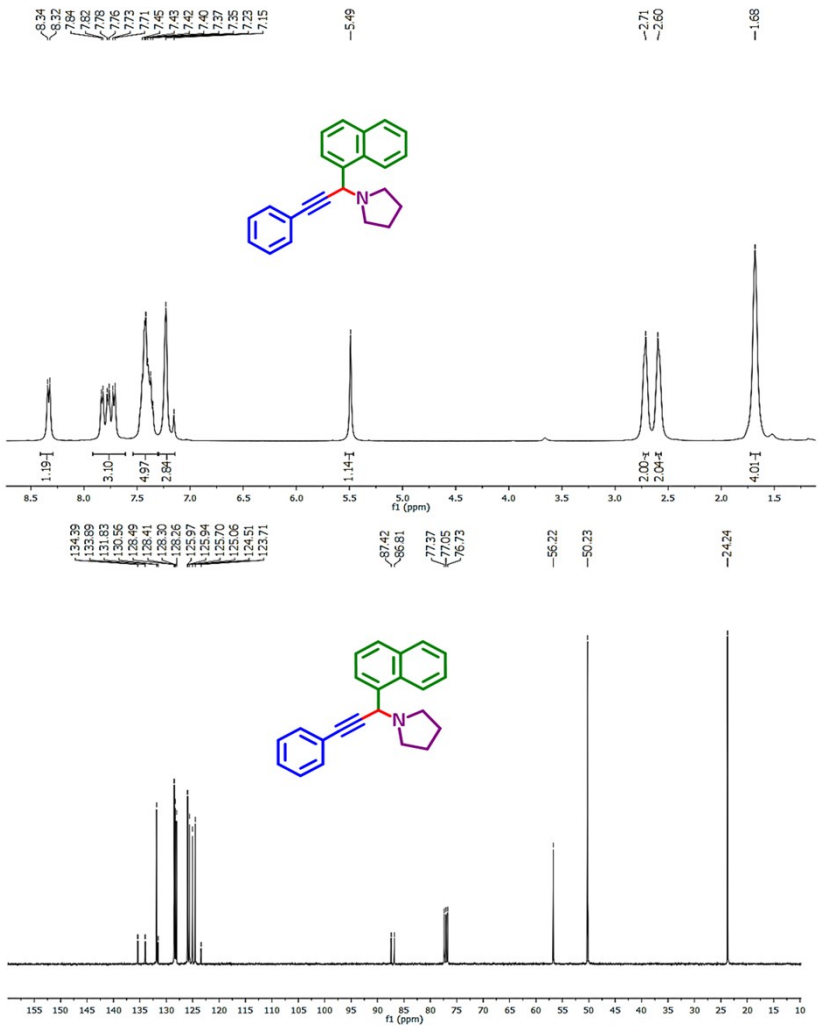

**Figure S3** $^{1}$H NMR and $^{13}$C NMR of 1-(1-(Naphthalen-1-yl)-3-phenylprop-2-yn-1-yl)pyrrolidine.

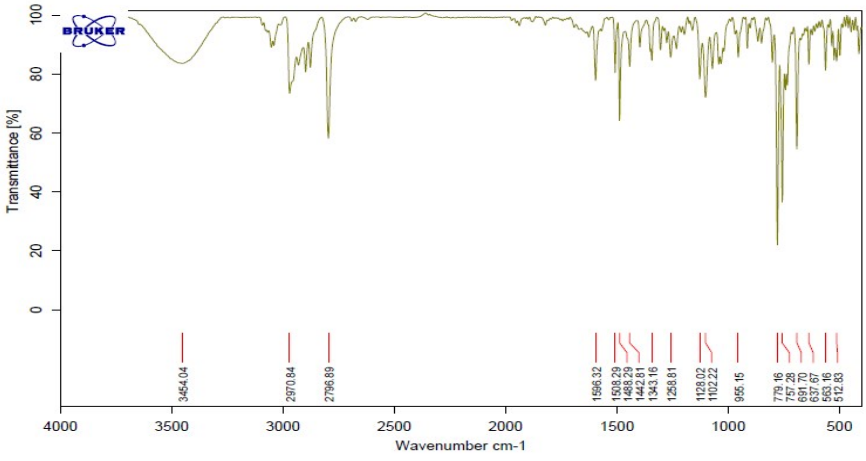


**Figure S4** IR spectrum of 2.5.1 1-(1-(Naphthalen-1-yl)-3-phenylprop-2-yn-1-yl)pyrrolidine.

*1-(1-(Naphthalen-1-yl)-3-phenylprop-2-yn-1-yl)pyrrolidine* **(4c)**
White solid, mp = 117–118 ˚C, $^{1}$H NMR (400 MHz, $CDCl_3$, ppm): δ 8.33 (d, 8.15 Hz, 1H), 7.83 (d, 1H), 7.77 (d, 1H), 7.72 (d, 1H), 7.57–7.35 (m, 5H), 7.23 (br.s, 3H), 5.49 (s, 1H), 2.71 (s, 2H), 2.61 (s, 2H), 1.68 (s, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm): 134.3, 133.8, 131.8, 130.5, 128.5, 128.4, 128.3, 128.1, 126.0, 126.0, 125.7, 125.0, 124.5, 123.7, 87.4, 86.8, 56.2, 50.2, 24.2; IR (neat) $\nu_{max}$: 3053, 2971, 2878, 2797, 1596, 1508, 1488, 1443, 1397, 1343, 1259, 1128, 1102, 1071, 1043, 955, 914, 851, 802, 779, 757, 692, 638, 563, 513 cm$^{-1}$.

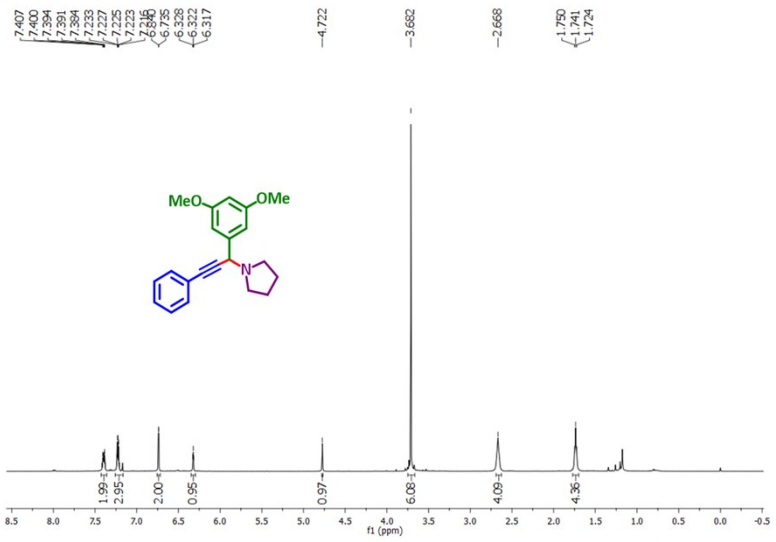


**Figure S5** $^{1}$H NMR of 1-(1-(3,5-Dimethoxyphenyl)-3-phenylprop-2-yn-1-yl)pyrrolidine.

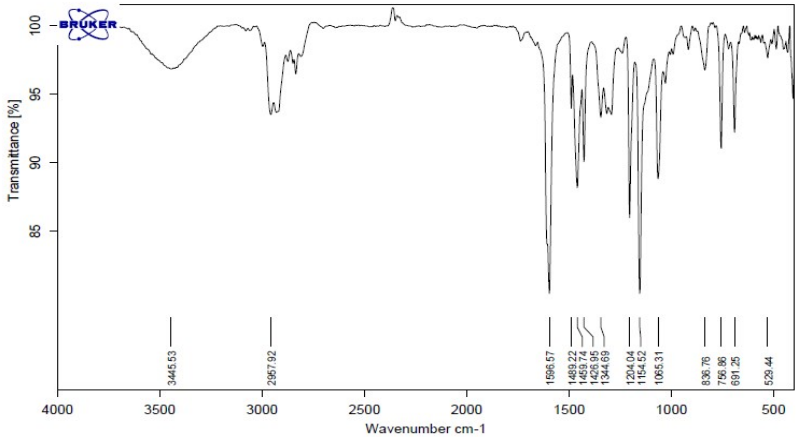


**Figure S6** IR spectrum of 1-(1-(3,5-Dimethoxyphenyl)-3-phenylprop-2-yn-1-yl)pyrrolidine.

*1-(1-(3,5-Dimethoxyphenyl)-3-phenylprop-2-yn-1-yl)pyrrolidine* **(4d)**

Yellowish oil, $^{1}$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.40–7.38 (m, 2H), 7.23–7.21 (m, 3H), 7.73 (d, 2H), 6.32 (t, 1H), 4.72 (s, 1H), 3.68 (s, 6H), 2.61–2.77 (m, 4H), 1.74 (t, 5.78 Hz, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) 160.7, 141.5, 131.8, 128.3, 128.2, 123.1, 106.4, 99.8, 87.0, 86.3, 59.3, 55.4, 50.4, 23.6, IR (neat) $\nu_{max}$: 3080, 2997, 2958, 2930, 2835, 1597, 1489, 1460, 1427, 1345, 1293, 1204, 1155, 1065, 1029, 917, 757, 691 cm$^{-1}$ (Figure S5 and Figure S6).

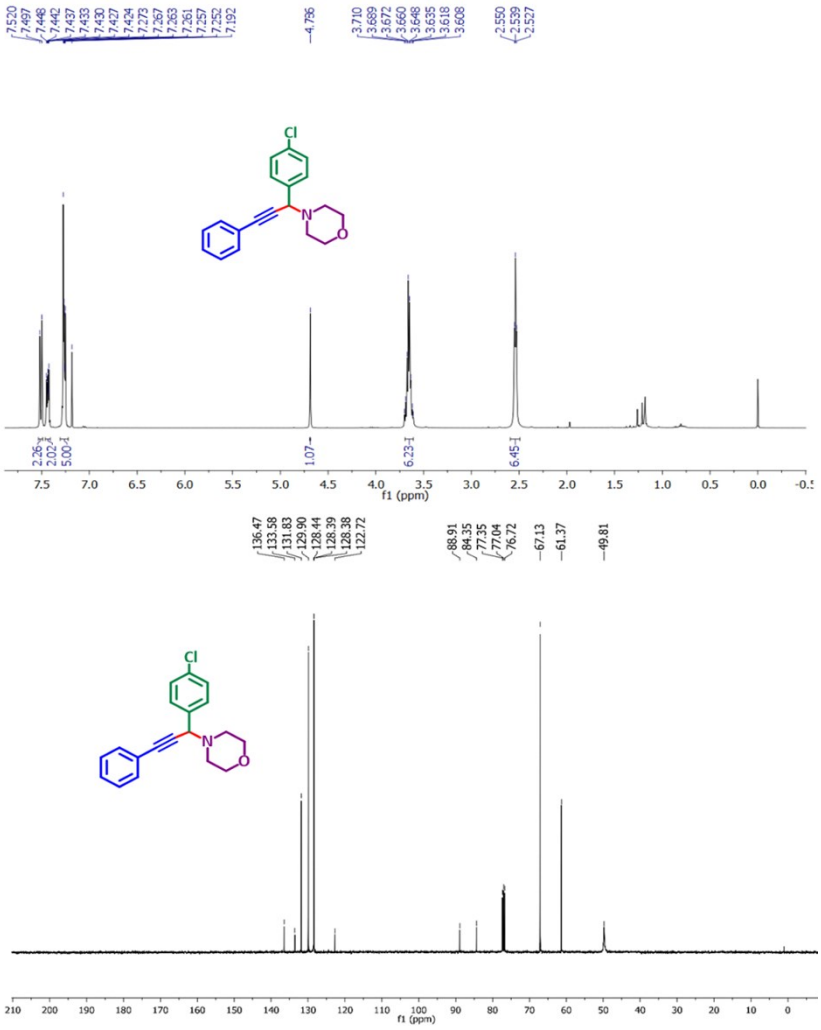

**Figure S7** $^{1}$H NMR and $^{13}$C NMR of 4-(1-(4-Chlorophenyl)-3-phenylprop-2-yn-1-yl)morpholine.

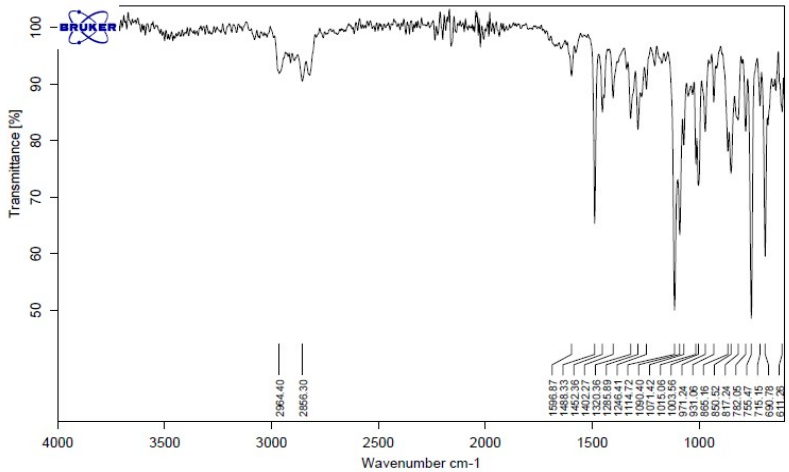


**Figure S8** IR spectrum of 4-(1-(4-Chlorophenyl)-3-phenylprop-2-yn-1-yl)morpholine.

*4-(1-(4-Chlorophenyl)-3-phenylprop-2-yn-1-yl) morpholine* **(4f)**

Yellowish liquid, $^{1}$H NMR (400 MHz, $CDCl_3$, ppm): δ 7.52 (d, 2H), 7.44–7.43 (m, 2H), 7.27–7.19 (m, 5H), 4.73 (s, 1H), 3.71–3.61 (m, 4H), 2.55–2.52 (t, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$, ppm) 136.5, 133.6, 131.9, 129.9, 128.44, 128.39, 128.38, 122.7, 88.9, 84.3, 67.1, 61.4, 49.8, IR (neat) $\nu_{max}$: 3080, 2964, 2856, 2822, 1597, 1488, 1452, 1402, 1320, 1286, 1115, 1096, 1004, 971, 851, 782, 755, 691 $cm^{-1}$ (Figure S7 and Figure S8).

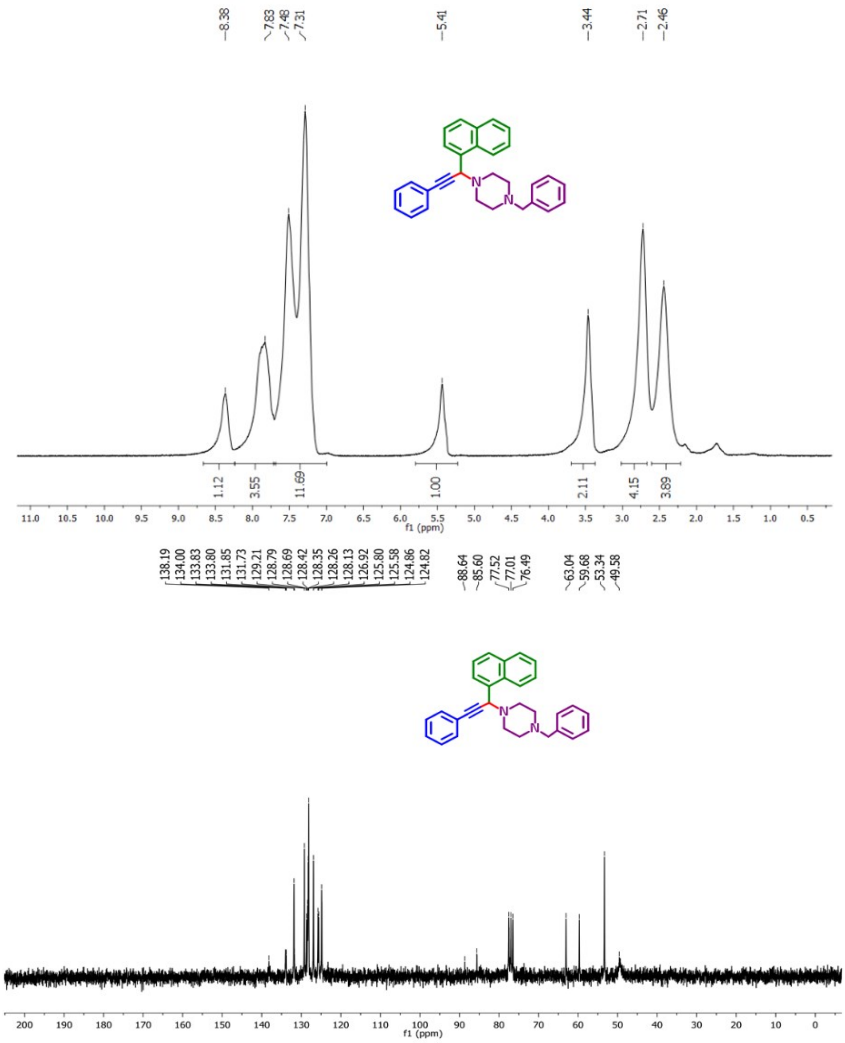

**Figure S9** $^{1}$H NMR and $^{13}$C NMR of 1-Benzyl-4-(1-(naphthalen-1-yl)-3-phenylprop-2-yn-1-yl) piperazine.

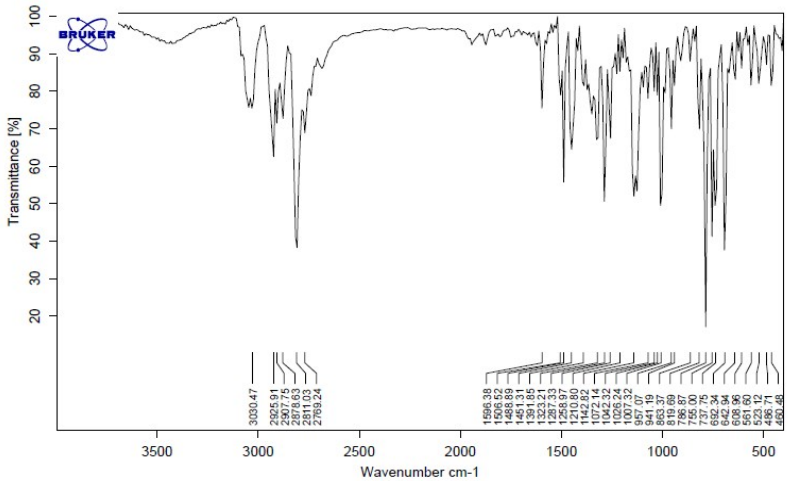


**Figure S10** IR spectrum of 1-Benzyl-4-(1-(naphthalen-1-yl)-3-phenylprop-2-yn-1-yl) piperazine.

*1-Benzyl-4-(1-(naphthalen-1-yl)-3-phenylprop-2-yn-1-yl) piperazine* **(4l)**

White solid, mp = 154–156 ˚C, $^{1}$H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.31–8.38 (m, 11H), 5.41 (s, 1H), 3.44 (br, 2H), 2.71 (br, 4H), 2.46 (br, 4H); $^{13}$C NMR (100 MHz, $CDCl_3$): 138.19, 134.00, 133.83, 133.80, 131.85, 131.73, 129.21, 128.79, 128.69, 128.42, 128.35, 128.26, 128.13, 126.92, 125.80, 125.58, 124.86, 124.82, 88.64, 85.60, 63.04, 59.68, 53.34, 49.58,; IR (neat) $\nu_{max}$: 3030, 2925, 2907, 2878, 2811, 2769, 1596, 1506, 1488, 1451, 1391, 1323, 1287, 1258, 1210, 1142, 1026, 1007, 957, 819, 786, 755, 692, 523 $cm^{-1}$ (Figure S9 and Figure S10).

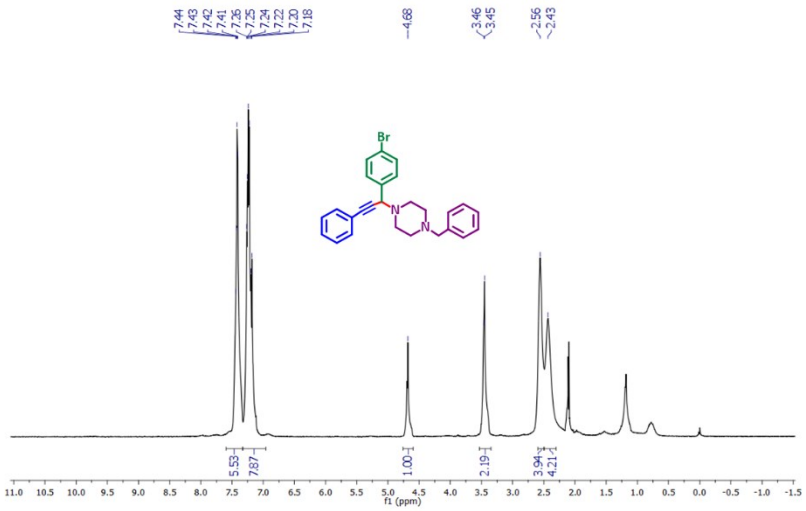


**Figure S11** $^{1}$H NMR of 1-benzyl-4-(1-(4-bromophenyl)-3-phenylprop-2-yn-1-yl)piperazine.

*1-benzyl-4-(1-(4-bromophenyl)-3-phenylprop-2-yn-1-yl)piperazine* **(4k)**
White solid, mp = 154–156 ˚C, $^{1}$H NMR (250 MHz, $CDCl_3$): δ (ppm) = 7.18–7.44 (m, 14H), 4.68 (s, 1H), 3.45 (br, 2H), 2.56 (br, 4H), 2.43 (br, 4H) (Figure S11).

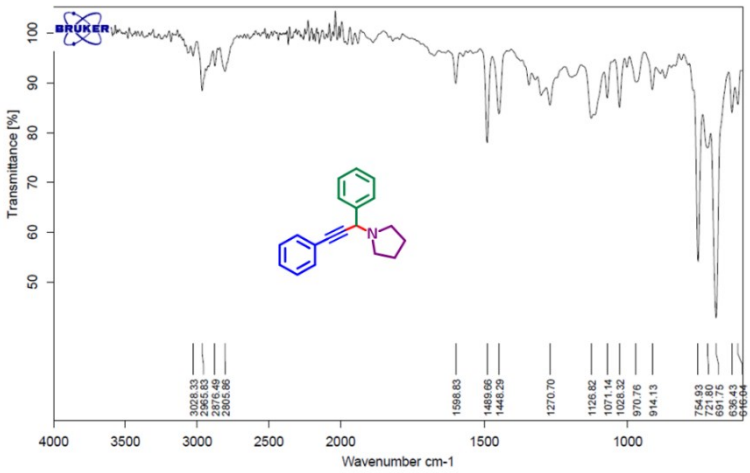


**Figure S12** IR spectrum of 1-(1,3-diphenylprop-2-yn-1-yl)pyrrolidine.

*1-(1,3-diphenylprop-2-yn-1-yl)pyrrolidine* **(4a)**
Yellowish oil, IR (neat) $\nu_{max}$: 3028, 2876, 2805, 1598, 1489, 1448, 1270, 1126, 1071, 1028, 970, 914, 754, 721, 691, 636, 616 $cm^{-1}$ (Figure S12).

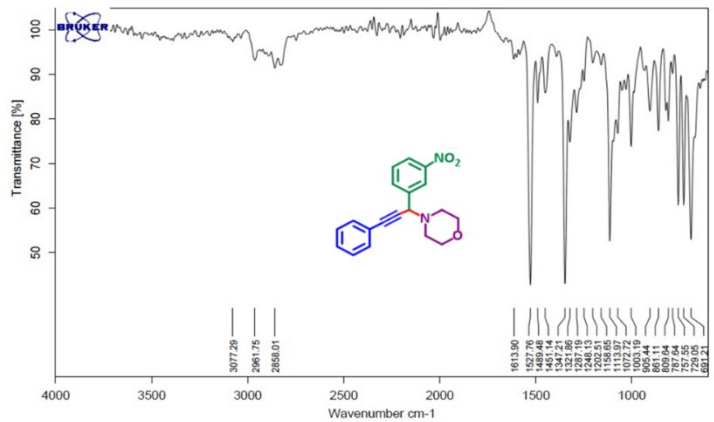


**Figure S13** IR spectrum of 1-(1-(3-nitrophenyl)-3-phenylprop-2-yn-1-yl)morpholine.

*1-(1-(3-nitrophenyl)-3-phenylprop-2-yn-1-yl)*morpholine **(4g)**
Yellowish oil, IR (neat) $\nu_{max}$: 3077, 2961, 2858, 1613, 1527, 1489, 1451, 1347, 1321, 1287, 1248, 1202, 1158, 1113, 1072, 1003, 905, 861, 809, 787, 757, 729, 691 $cm^{-1}$ (Figure S13).

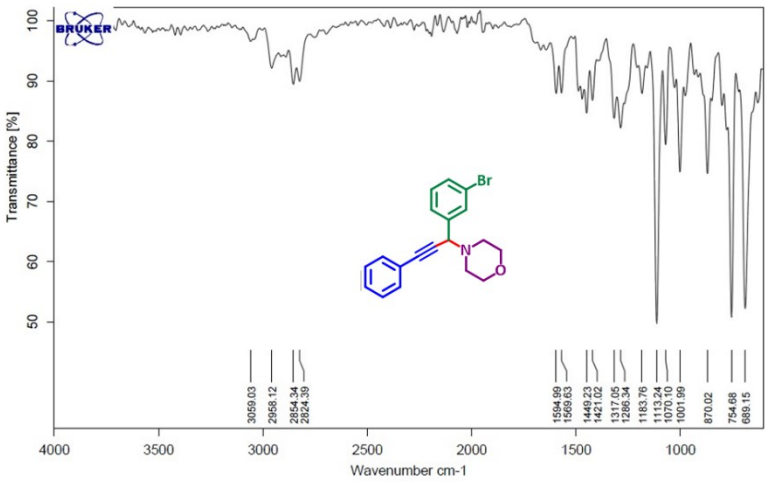


**Figure S14** IR spectrum of 4-(1-(4-Bromophenyl)-3-phenylprop-2-yn-1-yl)morpholine.

*4-(1-(4-Bromophenyl)-3-phenylprop-2-yn-1-yl)morpholine* **(4h)**
Yellowish oil, IR (neat) $\nu_{max}$: 1594, 1569, 1449, 1421, 1317, 1286, 1183, 1113, 1070, 1001, 870, 754, 689 $cm^{-1}$ (Figure S14).

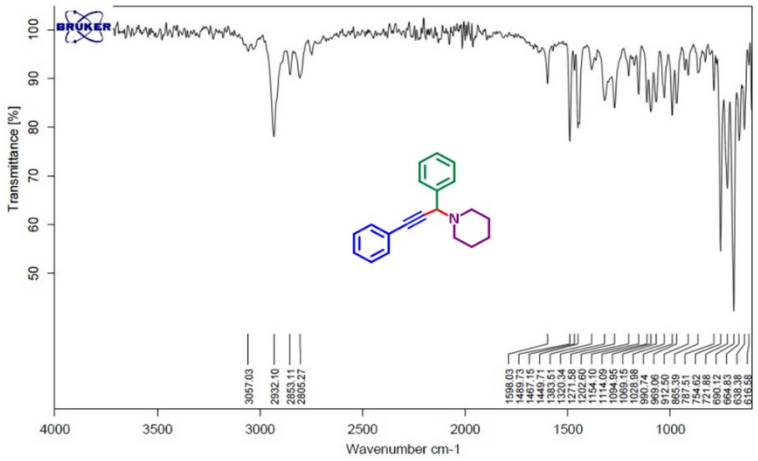


**Figure S15** IR spectrum of 1-(1,3-diphenylprop-2-yn-1-yl)Piperidine.

*1-(1,3-diphenylprop-2-yn-1-yl) Piperidine* **(4i)**
Yellowish oil, IR (neat) $\nu_{max}$: 1598, 1489, 1467, 1449, 1383, 1320, 1271, 1202, 1154, 1114, 1094, 1069, 1028, 990, 969, 912, 865, 787, 754, 721, 690, 664, 638, 616 $cm^{-1}$ (Figure S15).

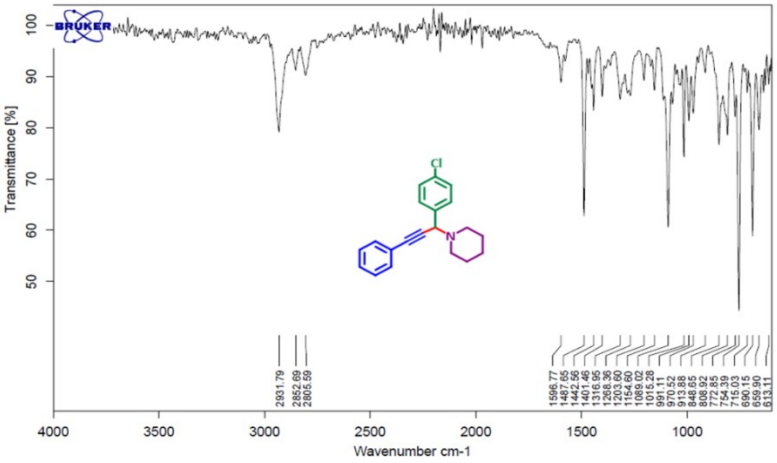


**Figure S16** IR spectrum of 4-(1-(4-Chlorophenyl)-3-phenylprop-2-yn-1-yl)Piperidine.

*4-(1-(4-Chlorophenyl)-3-phenylprop-2-yn-1-yl)Piperidine* **(4j)**
Yellowish oil, IR (neat) $\nu_{max}$: 1596, 1487, 1442, 1401, 1316, 1268, 1203, 1154, 1089, 1015, 991, 970, 913, 848, 808, 772, 754, 715, 690, 659, 613 $cm^{-1}$ (Figure S16).