# Supporting Information

# A Functional Molecular System of Bis(pyrazolyl)pyridine Derivatives: Photo-physics, Spectroscopy, Computation and Ion Sensing

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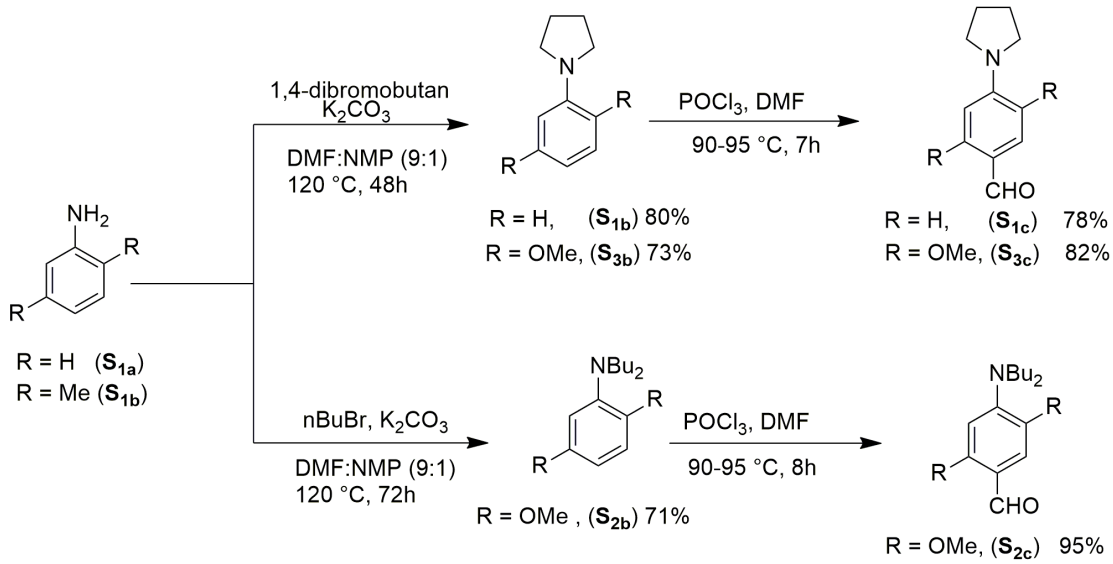
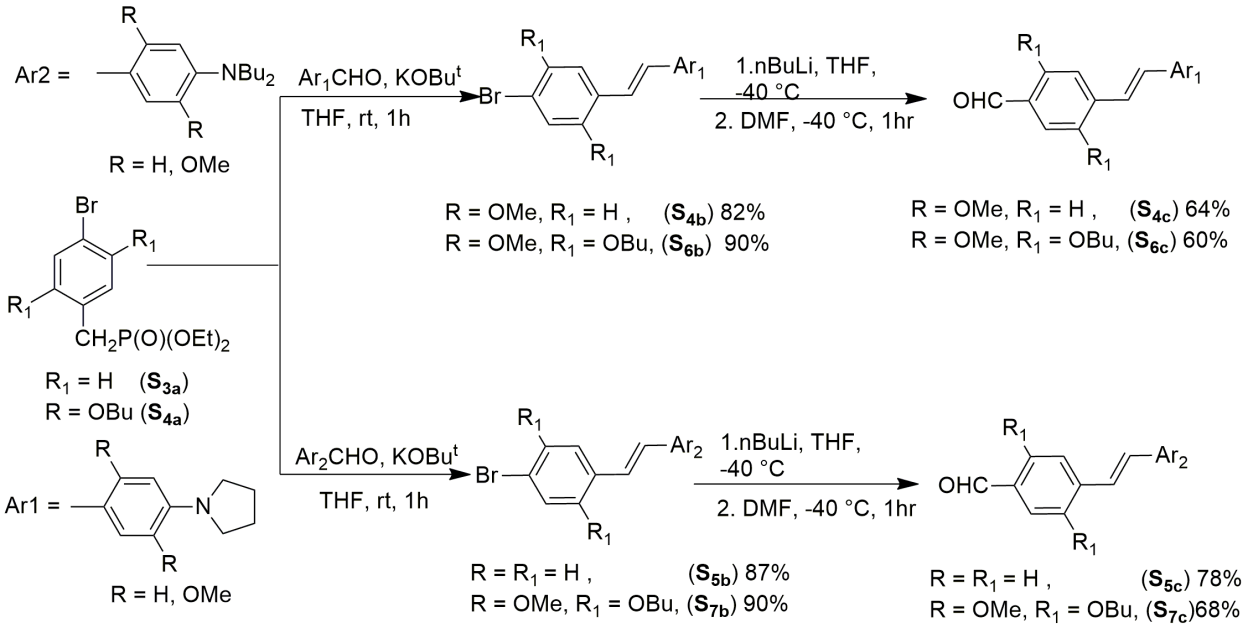
**Scheme S1.** Synthetic route of donor molecules and their staring materials ($S_{1c-7c}$)

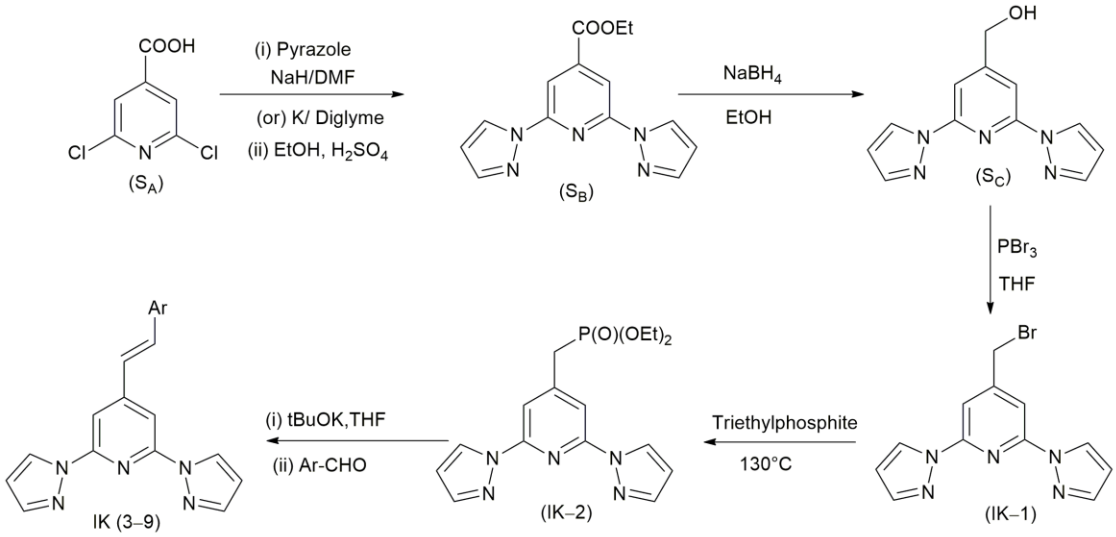
**A. Synthetic route of the alkylamino benzaldehydes**




**B. Synthetic route of 4-Styrylbenzaldehydes**



**Scheme S2.** Synthetic route of acceptor molecule including its staring materials and title compounds ($S_A$- $S_C$ and **IK-(1-9)**)



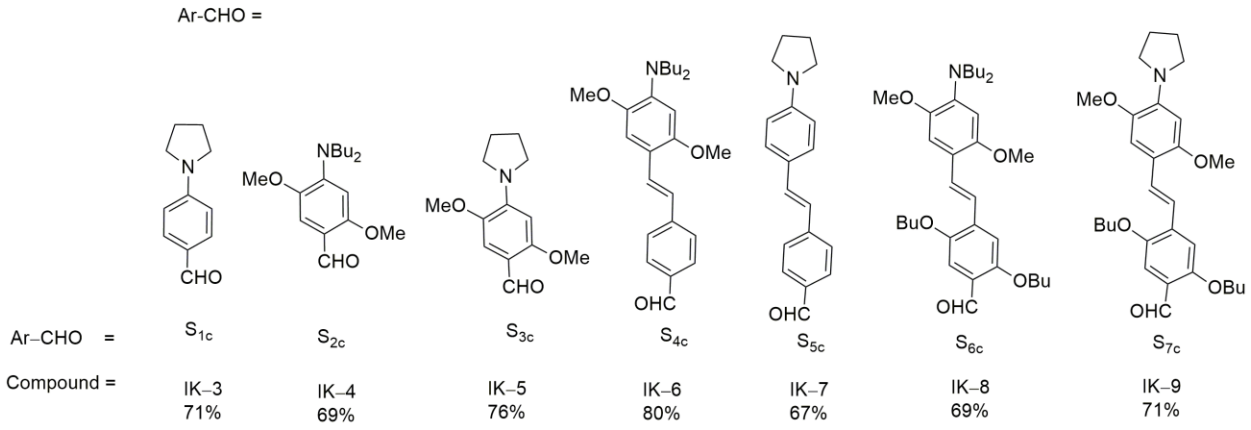



**Table S1.** Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound **IK–2**. $U_{eq}$ is defined as 1/3 of the trace of the orthogonalised $U_{IJ}$ tensor.

| Atom | x | y | z | U(eq) |
|---|---|---|---|---|
| O(3) | 2600(4) | 1573(3) | 2959(3) | 52(1) |
| O(1) | 2595(4) | 395(3) | 5131(3) | 53(1) |
| O(2) | 3307(5) | 2859(3) | 4349(3) | 61(1) |
| C(13) | 5086(13) | 2693(9) | 4940(9) | 122(3) |
| C(14) | 4740(20) | 3023(12) | 5985(11) | 199(7) |
| C(15) | 4383(7) | 1173(6) | 2634(5) | 64(1) |
| C(16) | 4215(9) | 599(8) | 1650(6) | 84(2) |
| P(1) | 2222(1) | 1660(1) | 4225(1) | 40(1) |
| N(2) | -2488(4) | 4216(3) | 172(3) | 35(1) |
| N(1) | -1551(4) | 5656(3) | 1187(3) | 32(1) |
| N(4) | -692(5) | 7198(3) | 2102(3) | 37(1) |
| C(4) | -396(5) | 4799(4) | 3131(3) | 35(1) |
| C(2) | -1295(5) | 3260(4) | 2119(3) | 33(1) |
| C(1) | -1739(5) | 4379(4) | 1194(3) | 31(1) |
| C(3) | -594(5) | 3483(4) | 3110(3) | 32(1) |
| C(5) | -870(5) | 5838(4) | 2143(3) | 32(1) |
| N(5) | -4(6) | 7539(4) | 3017(3) | 52(1) |
| C(12) | -82(5) | 2306(4) | 4140(3) | 37(1) |
| C(11) | -1119(7) | 8308(4) | 1217(4) | 53(1) |
| N(3) | -2945(6) | 5218(5) | -808(4) | 60(1) |
| C(8) | -2822(6) | 2985(4) | 85(3) | 41(1) |
| C(6) | -3622(7) | 4572(5) | -1555(4) | 53(1) |
| C(10) | -734(8) | 9411(5) | 1552(5) | 58(1) |
| C(9) | -53(8) | 8876(5) | 2665(5) | 59(1) |
| C(7) | -3507(8) | 3214(6) | -955(5) | 62(1) |

**Table S2.** Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound **IK–2.** The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

| **Atom** | **$U_{11}$** | **$U_{22}$** | **$U_{33}$** | **$U_{23}$** | **$U_{13}$** | **$U_{12}$** |
|---|---|---|---|---|---|---|
| O(3) | 39(2) | 64(2) | 48(2) | -11(2) | -4(1) | 11(1) |
| O(1) | 53(2) | 33(2) | 61(2) | 7(1) | -11(2) | 4(1) |
| O(2) | 59(2) | 40(2) | 76(2) | -1(2) | -27(2) | -12(2) |
| C(13) | 118(7) | 81(5) | 159(9) | -25(6) | 19(6) | 17(5) |
| C(14) | 320(20) | 121(9) | 155(11) | -55(8) | 24(12) | 42(11) |
| C(15) | 40(3) | 73(4) | 68(3) | -6(3) | -4(2) | 10(2) |
| C(16) | 69(4) | 101(5) | 92(5) | -46(4) | 16(3) | 1(3) |
| P(1) | 41(1) | 28(1) | 43(1) | 0(1) | -10(1) | -1(1) |
| N(2) | 35(2) | 35(2) | 35(2) | -8(1) | -3(1) | 0(1) |
| N(1) | 32(2) | 28(2) | 35(2) | -6(1) | -3(1) | 1(1) |
| N(4) | 44(2) | 26(2) | 40(2) | -6(1) | -4(1) | -2(1) |
| C(4) | 38(2) | 31(2) | 35(2) | -7(2) | -4(2) | 0(2) |
| C(2) | 32(2) | 23(2) | 43(2) | -7(2) | 0(2) | -1(1) |
| C(1) | 26(2) | 34(2) | 33(2) | -10(2) | 0(1) | 1(1) |
| C(3) | 28(2) | 28(2) | 37(2) | -3(2) | 2(1) | 1(1) |
| C(5) | 29(2) | 28(2) | 39(2) | -9(2) | 1(2) | -1(1) |
| N(5) | 81(3) | 36(2) | 43(2) | -12(2) | -4(2) | -14(2) |
| C(12) | 40(2) | 27(2) | 37(2) | -1(2) | -1(2) | -1(2) |
| C(11) | 72(3) | 30(2) | 50(3) | -3(2) | -16(2) | 2(2) |
| N(3) | 56(3) | 68(3) | 52(2) | -11(2) | -6(2) | 4(2) |
| C(8) | 63(3) | 27(2) | 35(2) | -10(2) | -7(2) | -7(2) |
| C(6) | 53(3) | 66(3) | 42(2) | -18(2) | -10(2) | 1(2) |
| C(10) | 80(4) | 28(2) | 63(3) | -7(2) | 1(3) | -4(2) |
| C(9) | 90(4) | 34(2) | 59(3) | -19(2) | 9(3) | -17(2) |
| C(7) | 77(4) | 61(3) | 56(3) | -25(3) | -5(3) | -15(3) |

**Table S3.** Bond lengths [Å] in the crystal structure of compound **IK–2**.

| | | | |
|---|---|---|---|
| O(3)-C(15) | 1.444(6) | N(4)-N(5) | 1.357(5) |
| O(3)-P(1) | 1.572(3) | N(4)-C(5) | 1.397(5) |
| O(1)-P(1) | 1.454(3) | C(4)-C(3) | 1.375(5) |
| O(2)-C(13) | 1.482(10) | C(4)-C(5) | 1.387(5) |
| O(2)-P(1) | 1.562(3) | C(2)-C(1) | 1.381(5) |
| C(13)-C(14) | 1.406(11) | C(2)-C(3) | 1.385(5) |
| C(15)-C(16) | 1.469(8) | C(3)-C(12) | 1.499(5) |
| P(1)-C(12) | 1.786(4) | N(5)-C(9) | 1.315(6) |
| N(2)-C(8) | 1.337(5) | C(11)-C(10) | 1.350(7) |
| N(2)-N(3) | 1.358(5) | N(3)-C(6) | 1.372(6) |
| N(2)-C(1) | 1.408(5) | C(8)-C(7) | 1.305(6) |
| N(1)-C(5) | 1.323(5) | C(6)-C(7) | 1.377(7) |
| N(1)-C(1) | 1.325(5) | C(10)-C(9) | 1.382(7) |
| N(4)-C(11) | 1.346(5) | | |

**Table S4.** Bond angles in the crystal structure of compound **IK–2**

| | | | |
|---|---|---|---|
| C(15)-O(3)-P(1) | 120.7(3) | N(1)-C(1)-C(2) | 124.7(3) |
| C(13)-O(2)-P(1) | 124.7(4) | N(1)-C(1)-N(2) | 114.9(3) |
| C(14)-C(13)-O(2) | 105.3(9) | C(2)-C(1)-N(2) | 120.4(3) |
| O(3)-C(15)-C(16) | 108.4(5) | C(4)-C(3)-C(2) | 118.8(3) |
| O(1)-P(1)-O(2) | 114.51(19) | C(4)-C(3)-C(12) | 121.0(4) |

| | | | |
|---|---|---|---|
| O(1)-P(1)-O(3) | 115.4(2) | C(2)-C(3)-C(12) | 120.2(3) |
| O(2)-P(1)-O(3) | 104.4(2) | N(1)-C(5)-C(4) | 124.6(3) |
| O(1)-P(1)-C(12) | 113.49(19) | N(1)-C(5)-N(4) | 114.4(3) |
| O(2)-P(1)-C(12) | 104.94(19) | C(4)-C(5)-N(4) | 121.0(4) |
| O(3)-P(1)-C(12) | 102.82(18) | C(9)-N(5)-N(4) | 103.6(4) |
| C(8)-N(2)-N(3) | 112.4(4) | C(3)-C(12)-P(1) | 115.5(3) |
| C(8)-N(2)-C(1) | 121.0(3) | N(4)-C(11)-C(10) | 107.8(4) |
| N(3)-N(2)-C(1) | 126.6(3) | N(2)-N(3)-C(6) | 105.4(4) |
| C(5)-N(1)-C(1) | 116.1(3) | C(7)-C(8)-N(2) | 104.4(4) |
| C(11)-N(4)-N(5) | 111.2(3) | N(3)-C(6)-C(7) | 105.0(4) |
| C(11)-N(4)-C(5) | 127.7(4) | C(11)-C(10)-C(9) | 104.1(4) |
| N(5)-N(4)-C(5) | 121.0(3) | N(5)-C(9)-C(10) | 113.2(4) |
| C(3)-C(4)-C(5) | 118.0(4) | C(8)-C(7)-C(6) | 112.8(5) |
| C(1)-C(2)-C(3) | 117.9(3) | | |

**Table S5.** Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for Compound **IK–3**. $U_{eq}$ is defined as 1/3 of of the trace of the orthogonalised $U_{IJ}$ tensor.

| **Atom** | **x** | **y** | **z** | **U(eq)** |
|---|---|---|---|---|
| N(1) | 1383(2) | 4309(7) | 4889(2) | 51(1) |
| N(5) | 1280(2) | 7693(7) | 3966(2) | 54(1) |
| N(6) | 1495(2) | 9341(9) | 3546(3) | 71(1) |
| N(3) | 1432(2) | 960(7) | 5800(3) | 54(1) |
| C(5) | 1649(2) | 5784(8) | 4525(3) | 51(1) |
| C(6) | 3240(2) | 3304(10) | 5375(3) | 61(1) |
| C(3) | 2604(2) | 3608(9) | 5218(3) | 53(1) |

| | | | | |
|---|---|---|---|---|
| C(1) | 1730(2) | 2507(8) | 5425(3) | 49(1) |
| C(10) | 5210(2) | -1098(10) | 6812(3) | 66(1) |
| N(2A) | 6100(2) | 65(10) | 6630(3) | 68(1) |
| C(2B) | 2327(2) | 2045(9) | 5614(3) | 55(1) |
| N(4C) | 1747(2) | -771(9) | 6394(3) | 72(1) |
| C(7D) | 3618(2) | 1403(10) | 5849(3) | 55(1) |
| C(8E) | 4252(2) | 1042(9) | 6017(3) | 53(1) |
| C(13F) | 4547(2) | 2490(13) | 5634(3) | 71(1) |
| C(11G) | 5493(2) | 399(9) | 6424(3) | 51(1) |
| C(22H) | 514(2) | 10203(10) | 3200(3) | 69(1) |
| C(21I) | 689(2) | 8211(10) | 3756(3) | 61(1) |
| C(12J) | 5153(2) | 2150(12) | 5832(3) | 70(2) |
| C(17K) | 6488(2) | -1245(13) | 7321(4) | 76(2) |
| C(9L) | 4601(2) | -756(10) | 6601(3) | 62(1) |
| C(19M) | 763(3) | -956(12) | 6144(4) | 83(2) |
| C(23N) | 1030(3) | 10814(11) | 3092(4) | 76(2) |
| C(20O) | 1331(3) | -1916(14) | 6589(4) | 80(2) |
| C(4P) | 2254(2) | 5550(10) | 4669(3) | 55(1) |
| C(18Q) | 836(2) | 888(10) | 5630(4) | 68(2) |
| C(14R) | 6419(2) | 1406(13) | 6236(4) | 77(2) |
| C(15S) | 7049(3) | 292(18) | 6653(5) | 119(3) |
| C(16T) | 7105(2) | -529(17) | 7385(5) | 100(2) |

**Table S6.** Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for compound **IK–3**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

| **Atom** | **$U_{11}$** | **$U_{22}$** | **$U_{33}$** | **$U_{23}$** | **$U_{13}$** | **$U_{12}$** |
|---|---|---|---|---|---|---|
| N(1) | 50(2) | 52(2) | 48(3) | -10(2) | 19(2) | 0(1) |
| N(5) | 61(2) | 53(2) | 47(3) | -5(2) | 20(2) | 3(2) |
| N(6) | 83(3) | 69(2) | 65(3) | 4(2) | 34(3) | 9(2) |
| N(3) | 50(2) | 58(2) | 55(3) | -3(2) | 21(2) | 0(1) |
| C(5) | 53(2) | 52(2) | 46(3) | -9(2) | 18(2) | 1(2) |
| C(6) | 57(3) | 65(3) | 64(4) | 3(2) | 29(3) | 0(2) |
| C(3) | 55(3) | 51(2) | 53(3) | -6(2) | 21(2) | -2(2) |
| C(1) | 52(2) | 43(2) | 53(3) | -7(2) | 21(2) | 0(2) |
| C(10) | 62(3) | 79(3) | 58(4) | 18(3) | 26(3) | 11(2) |
| N(2A) | 49(2) | 90(3) | 64(3) | 19(2) | 22(2) | 4(2) |
| C(2B) | 54(3) | 54(2) | 57(3) | -1(2) | 21(3) | 4(2) |
| N(4C) | 62(3) | 78(3) | 70(3) | 16(2) | 22(3) | -1(2) |
| C(7D) | 50(3) | 64(3) | 52(3) | -4(2) | 20(2) | -3(2) |
| C(8E) | 55(3) | 49(2) | 57(3) | -8(2) | 25(3) | -4(2) |
| C(13F) | 58(3) | 87(3) | 63(4) | 22(3) | 20(3) | 6(2) |
| C(11G) | 49(2) | 57(2) | 44(3) | -4(2) | 14(2) | 0(2) |
| C(22H) | 70(3) | 68(3) | 50(3) | -3(3) | 4(3) | 12(2) |
| C(21I) | 58(3) | 62(3) | 58(4) | -2(2) | 16(3) | 2(2) |
| C(12J) | 55(3) | 91(3) | 69(4) | 19(3) | 31(3) | 1(2) |
| C(17K) | 63(3) | 100(4) | 62(4) | 16(3) | 22(3) | 13(3) |
| C(9L) | 58(3) | 70(3) | 66(4) | 6(2) | 33(3) | 1(2) |
| C(19M) | 68(4) | 97(4) | 96(5) | 11(3) | 48(4) | 5(3) |
| C(23N) | 104(5) | 68(3) | 55(4) | 13(3) | 32(4) | 19(3) |
| C(20O) | 86(4) | 95(4) | 64(4) | 20(3) | 35(4) | -5(3) |
| C(4P) | 57(3) | 61(3) | 47(3) | -4(2) | 21(2) | 0(2) |
| C(18Q) | 50(3) | 83(3) | 72(4) | 6(3) | 24(3) | 5(2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C(14R) | 54(3) | 104(4) | 71(4) | 13(3) | 23(3) | -3(3) |
| C(15S) | 50(3) | 190(7) | 110(7) | 61(6) | 25(4) | 9(4) |
| C(16T) | 56(3) | 130(5) | 97(6) | 35(4) | 13(4) | 3(3) |

**Table S7.** Bond lengths in the crystal structure of compound **IK–3**.

| | | | |
|---|---|---|---|
| N(1)-C(1) | 1.329(6) | C(8E)-C(13F) | 1.397(6) |
| N(1)-C(5) | 1.324(6) | C(13F)-C(12J) | 1.384(6) |
| N(5)-N(6) | 1.362(5) | C(13F)-H(13F) | 0.95 |
| N(5)-C(21I) | 1.355(5) | C(11G)-C(12J) | 1.373(7) |
| N(5)-C(5) | 1.400(6) | C(22H)-C(21I) | 1.342(7) |
| N(6)-C(23N) | 1.308(7) | C(22H)-C(23N) | 1.390(6) |
| N(3)-N(4C) | 1.356(6) | C(22H)-H(22H) | 0.95 |
| N(3)-C(18Q) | 1.360(6) | C(21I)-H(21I) | 0.95 |
| N(3)-C(1) | 1.411(5) | C(12J)-H(12J) | 0.95 |
| C(5)-C(4P) | 1.394(6) | C(17K)-C(16T) | 1.498(7) |
| C(6)-C(7D) | 1.325(7) | C(17K)-H(17A) | 0.99 |
| C(6)-C(3) | 1.467(6) | C(17K)-H(17B) | 0.99 |
| C(6)-H(6) | 0.95 | C(9L)-H(9L) | 0.95 |
| C(3)-C(4P) | 1.384(7) | C(19M)-C(18Q) | 1.374(8) |
| C(3)-C(2B) | 1.408(6) | C(19M)-C(20O) | 1.382(8) |
| C(1)-C(2B) | 1.371(5) | C(19M)-H(19M) | 0.95 |
| C(10)-C(11G) | 1.392(6) | C(23N)-H(23N) | 0.95 |
| C(10)-C(9L) | 1.386(6) | C(20O)-H(20O) | 0.95 |
| C(10)-H(10) | 0.95 | C(4P)-H(4P) | 0.95 |
| N(2A)-C(11G) | 1.383(6) | C(18Q)-H(18Q) | 0.95 |
| N(2A)-C(14R) | 1.435(6) | C(14R)-C(15S) | 1.511(8) |
| N(2A)-C(17K) | 1.436(7) | C(14R)-H(14A) | 0.99 |

| | | | |
|---|---|---|---|
| C(2B)-H(2B) | 0.95 | C(14R)-H(14B) | 0.99 |
| N(4C)-C(20O) | 1.327(6) | C(15S)-C(16T) | 1.441(12) |
| C(7D)-C(8E) | 1.459(6) | C(15S)-H(15A) | 0.99 |
| C(7D)-H(7D) | 0.95 | C(15S)-H(15B) | 0.99 |
| C(8E)-C(9L) | 1.382(7) | C(16T)-H(16A) | 0.99 |
| C(16T)-H(16B) | 0.99 | | |

**Table S8.** Bond Angles in the crystal structure of compound **IK–3**.

| | | | |
|---|---|---|---|
| C(1)-N(1)-C(5) | 115.9(3) | N(2A)-C(17K)-C(16T) | 104.6(5) |
| N(6)-N(5)-C(21I) | 110.5(4) | C(8E)-C(9L)-C(10) | 123.0(4) |
| N(6)-N(5)-C(5) | 121.5(4) | C(18Q)-C(19M)-C(20O) | 104.9(4) |
| C(21I)-N(5)-C(5) | 128.1(4) | N(6)-C(23N)-C(22H) | 112.9(5) |
| C(23N)-N(6)-N(5) | 104.2(4) | N(4C)-C(20O)-C(19M) | 113.0(5) |
| N(4C)-N(3)-C(18Q) | 112.3(4) | C(3)-C(4P)-C(5) | 118.7(4) |
| N(4C)-N(3)-C(1) | 119.9(4) | C(20O)-N(4C)-N(3) | 103.6(4) |
| C(18Q)-N(3)-C(1) | 127.7(5) | C(6)-C(7D)-C(8E) | 127.5(4) |
| N(1)-C(5)-C(4P) | 124.5(4) | C(9L)-C(8E)-C(13F) | 116.0(4) |
| N(1)-C(5)-N(5) | 115.3(4) | C(9L)-C(8E)-C(7D) | 120.0(4) |
| C(4P)-C(5)-N(5) | 120.2(4) | C(13F)-C(8E)-C(7D) | 124.0(5) |
| C(7D)-C(6)-C(3) | 126.1(4) | C(12J)-C(13F)-C(8E) | 121.7(5) |
| C(4P)-C(3)-C(2B) | 117.4(4) | N(2A)-C(11G)-C(10) | 120.0(5) |
| C(4P)-C(3)-C(6) | 119.6(4) | N(2A)-C(11G)-C(12J) | 121.5(4) |
| C(2B)-C(3)-C(6) | 123.0(4) | C(10)-C(11G)-C(12J) | 118.5(4) |
| N(1)-C(1)-C(2B) | 125.4(4) | C(21I)-C(22H)-C(23N) | 104.2(4) |
| N(1)-C(1)-N(3) | 114.4(3) | C(1)-C(2B)-C(3) | 118.2(4) |
| C(2B)-C(1)-N(3) | 120.2(4) | C(11G)-C(10)-C(9L) | 119.7(5) |
| C(11G)-N(2A)-C(14R) | 123.5(5) | C(11G)-N(2A)-C(17K) | 123.1(4) |
| C(14R)-N(2A)-C(17K) | 112.7(4) | | |

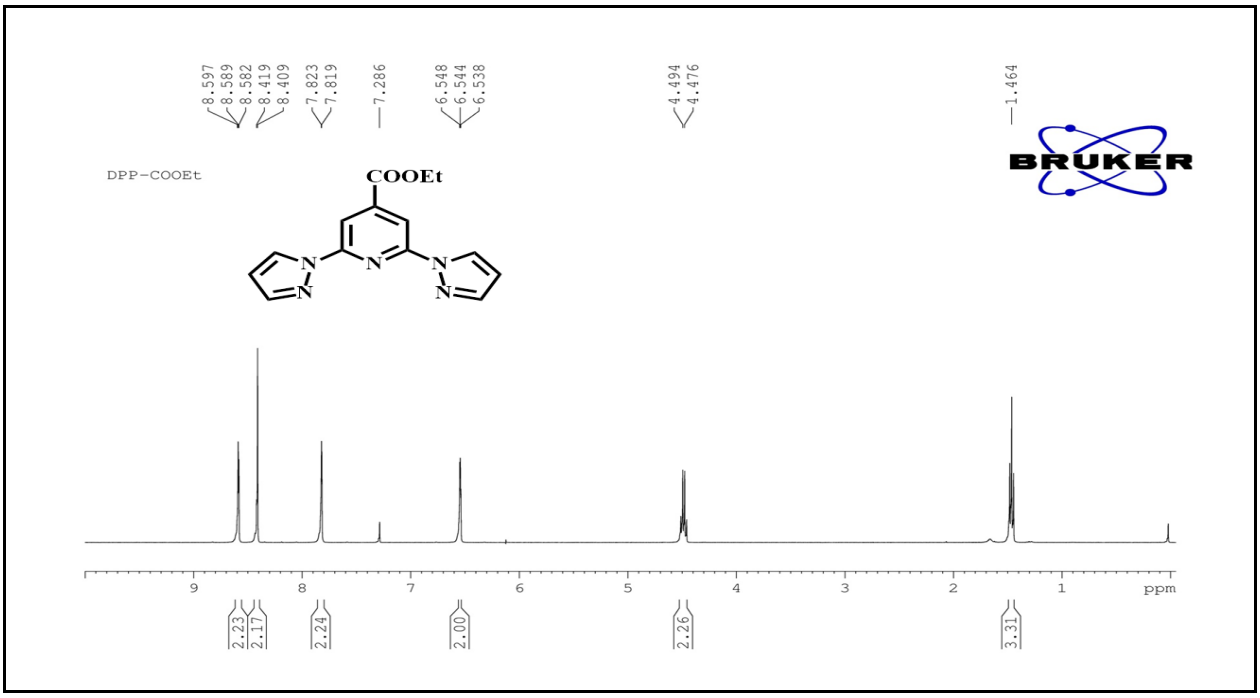



**Figure S1.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of $S_B$

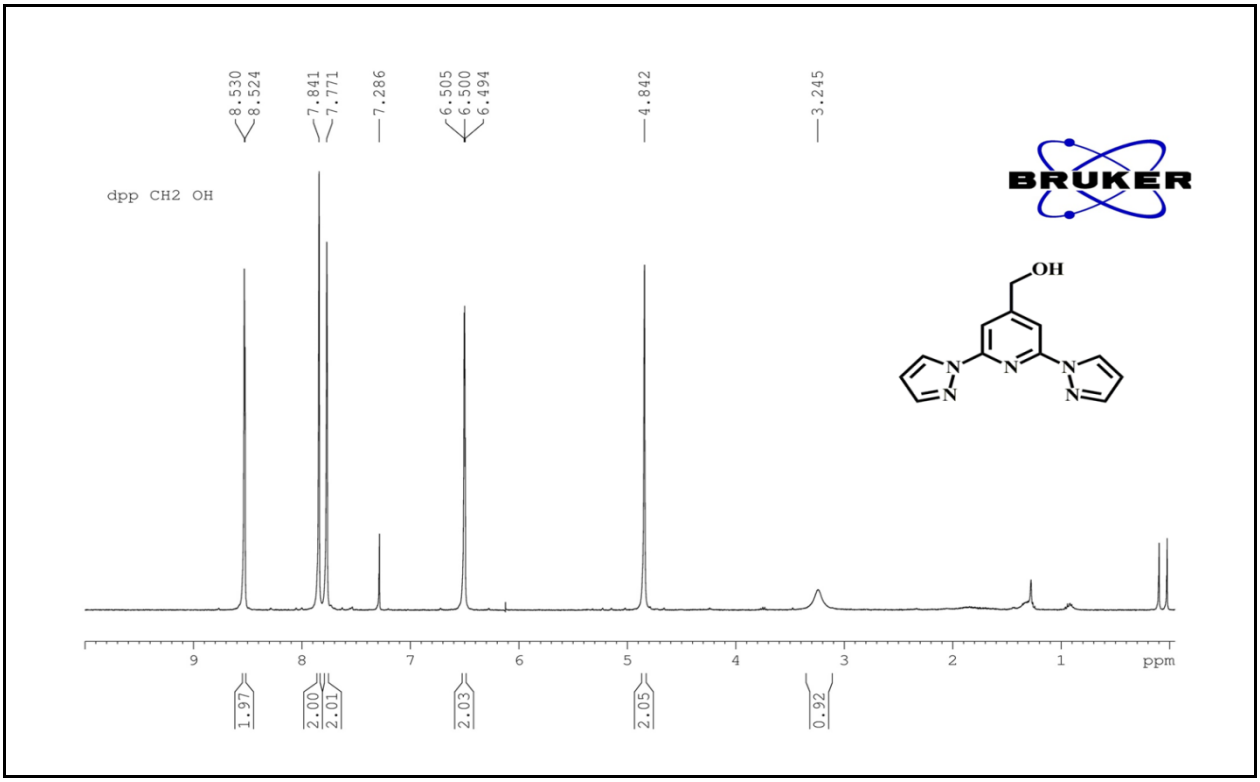



**Figure S2.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **S**C


**Figure S3.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **IK–1**

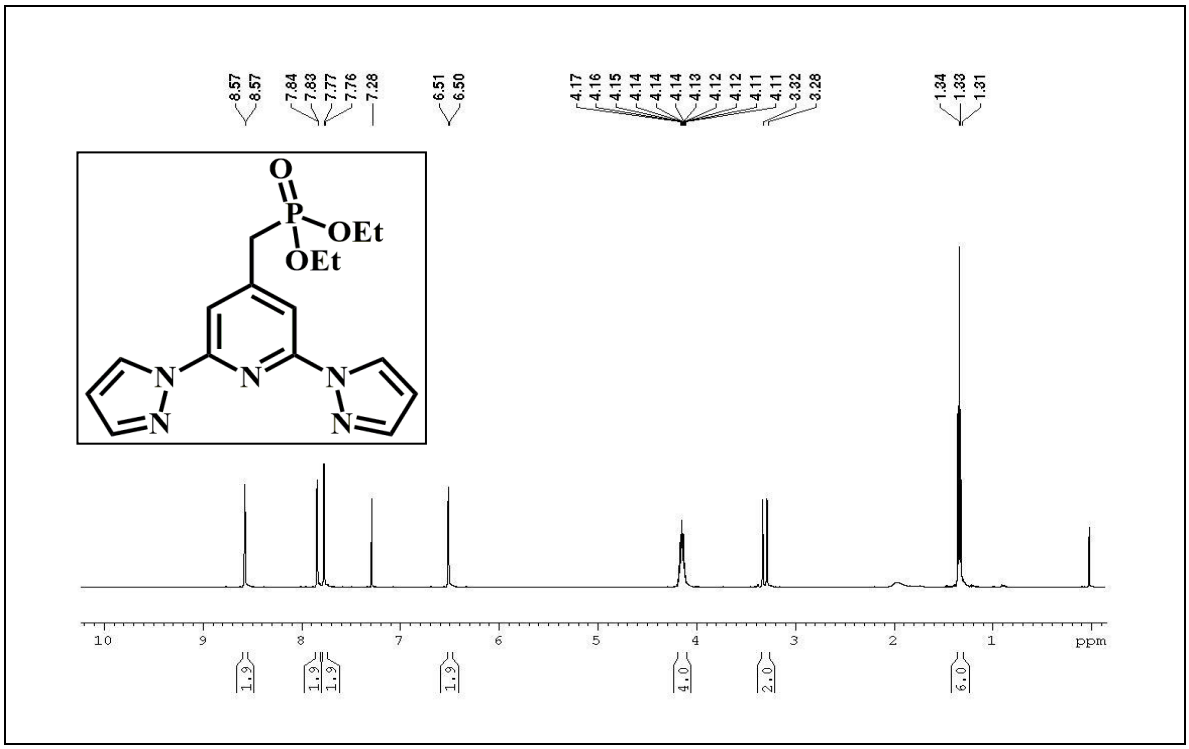



**Figure S4.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **IK–2**

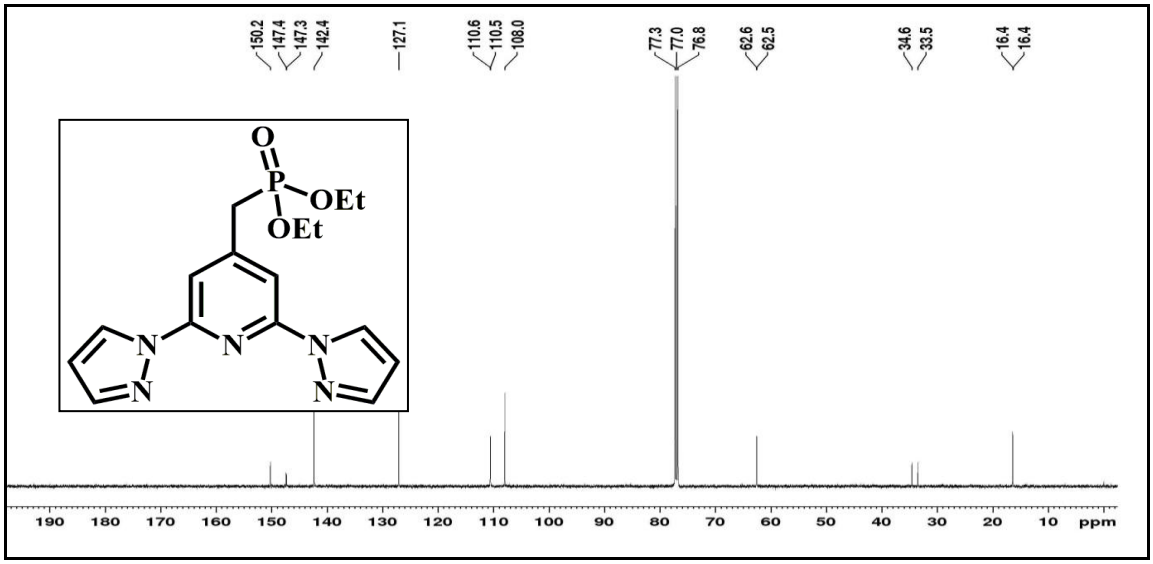



**Figure S5.**$^{13}$C NMR spectrum (100 MHz, $CDCl_3$) of **IK–2**

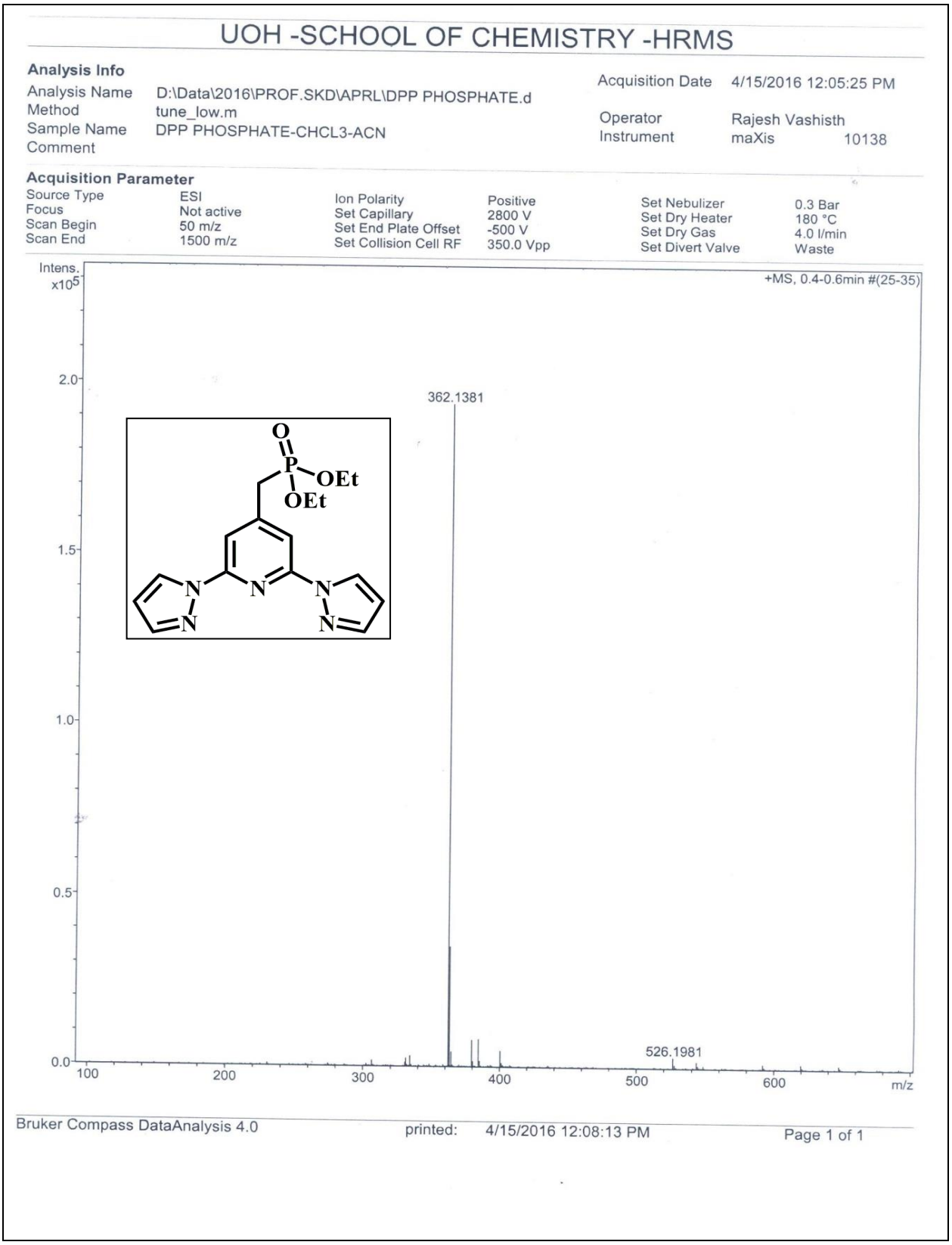



**Figure S6.** HRMS spectrum of compound **IK–2**

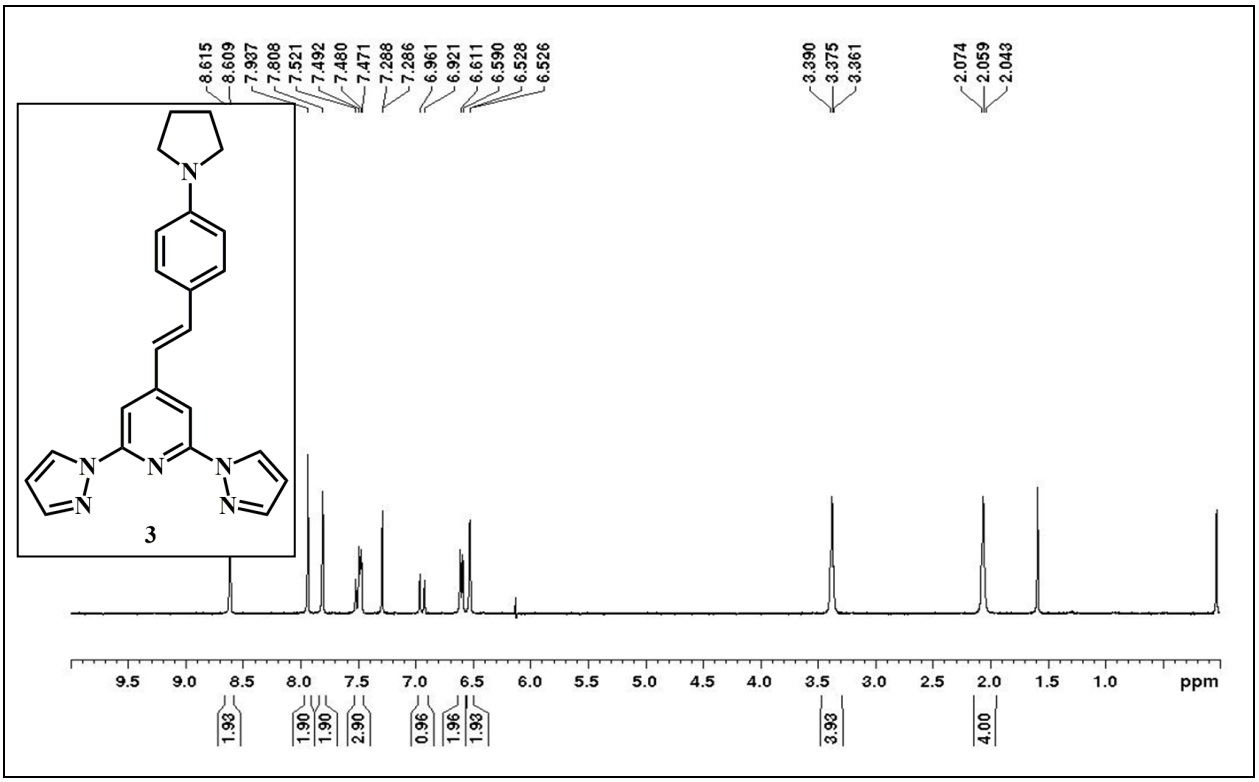



**Figure S7.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **IK–3**

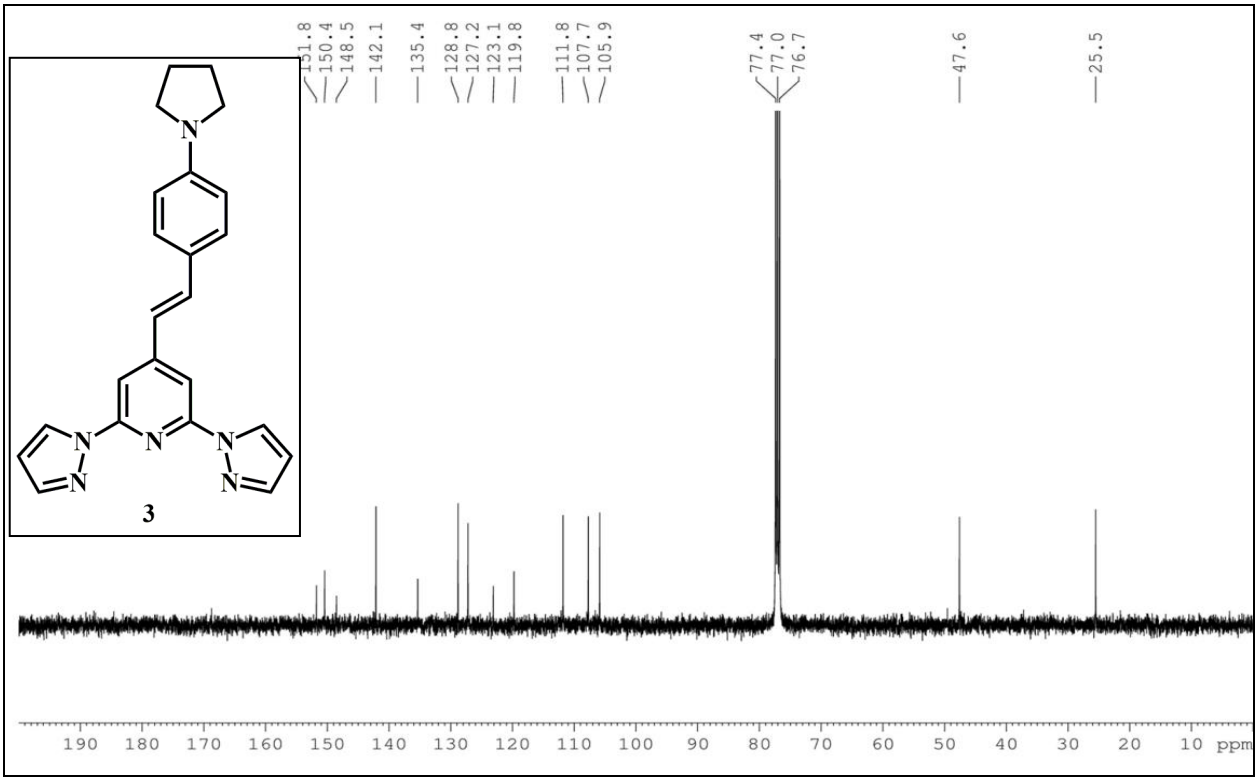



**Figure S8.** $^{13}$C NMR spectrum (100 MHz, $CDCl_3$) of **IK–3**

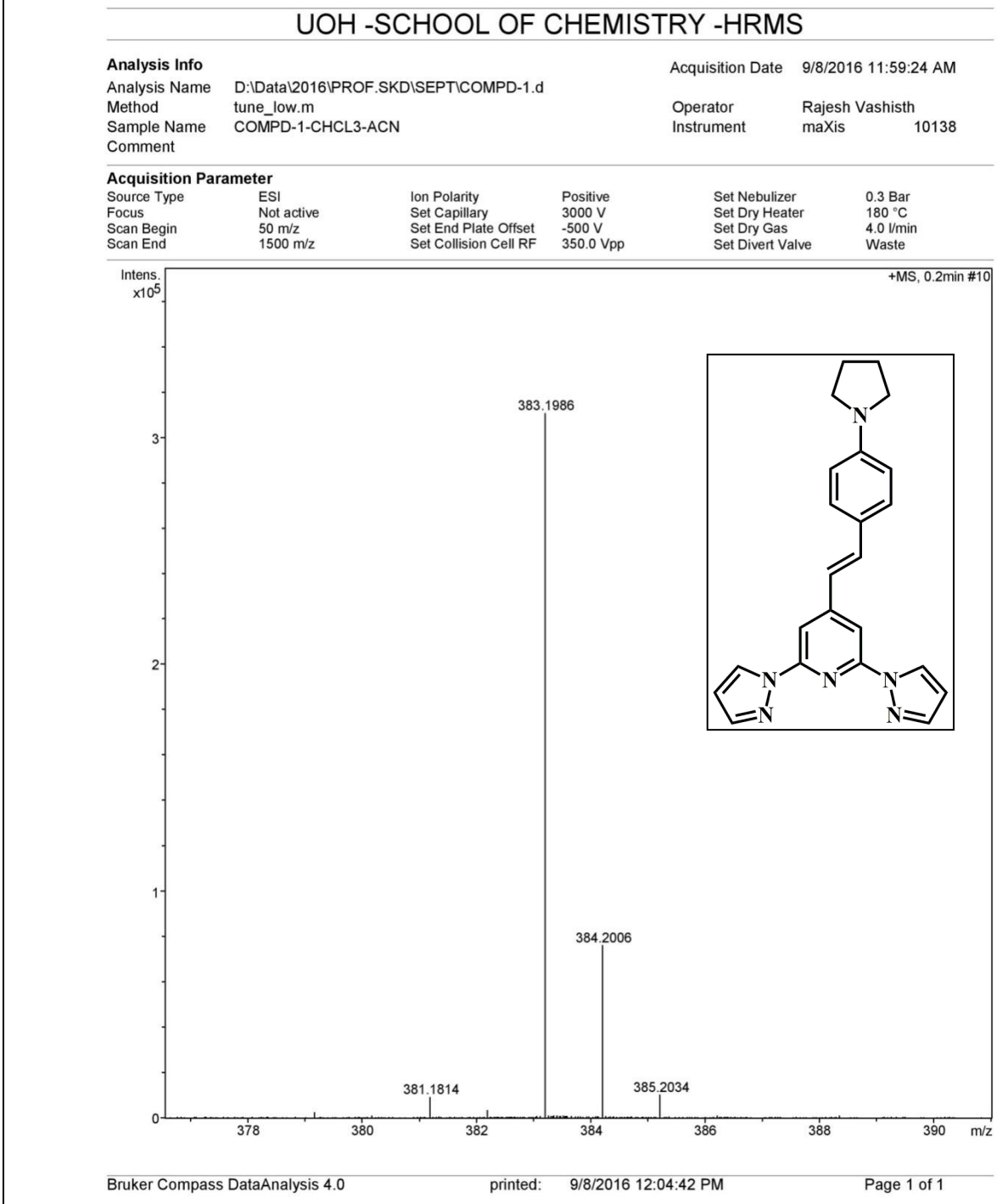
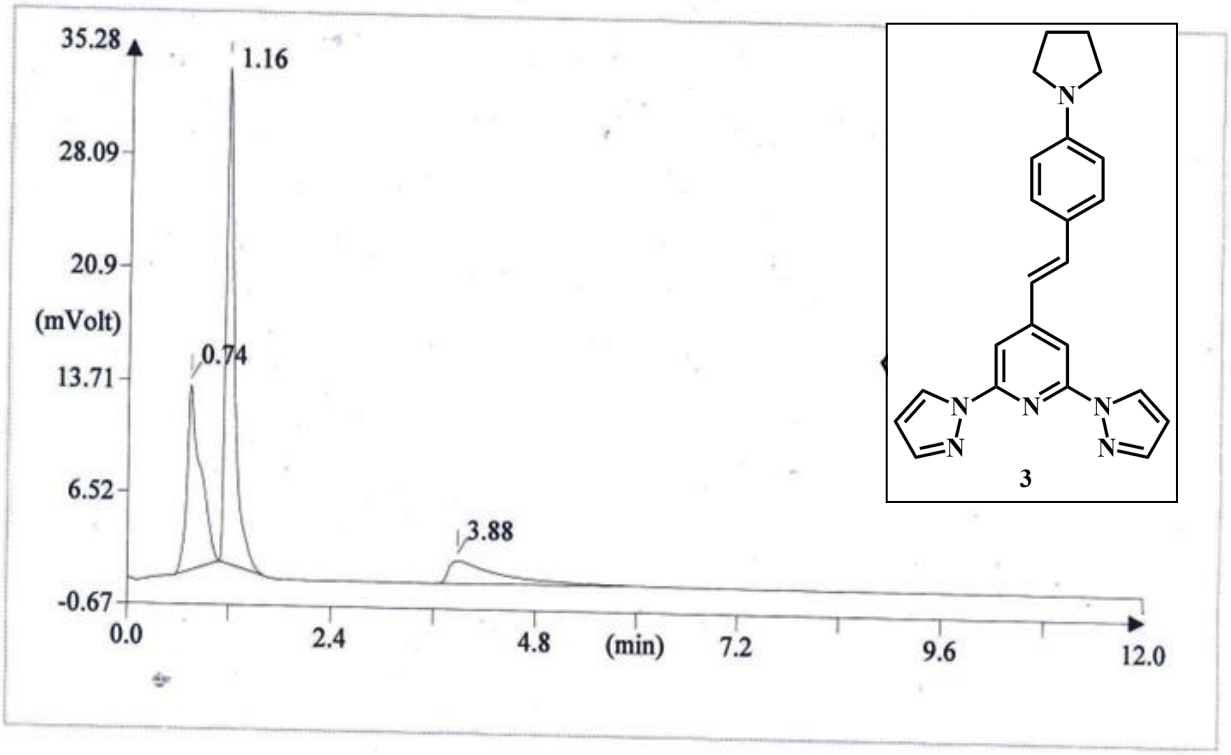



**Figure S9.** HRMS spectrum of compound **IK–3**

# FLASH EA 1112 SERIES CHN REPORT
# THERMO FINNIGAN

Method filename: C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID: COMPOUND-1 (# 4)
Analysis type: UnkNown
Chromatogram filename: UNK-03082016-4.dat
Sample weight: 1.113







3

| Element Name | Element % | Ret. Time |
|---|---|---|
| Nitrogen | 21. 82 | 0. 74 |
| Carbon | 72. 35 | 1. 16 |
| Hydrogen | 5. 72 | 3. 88 |

**Figure S10.** Elemental analysis of compound **IK–3**

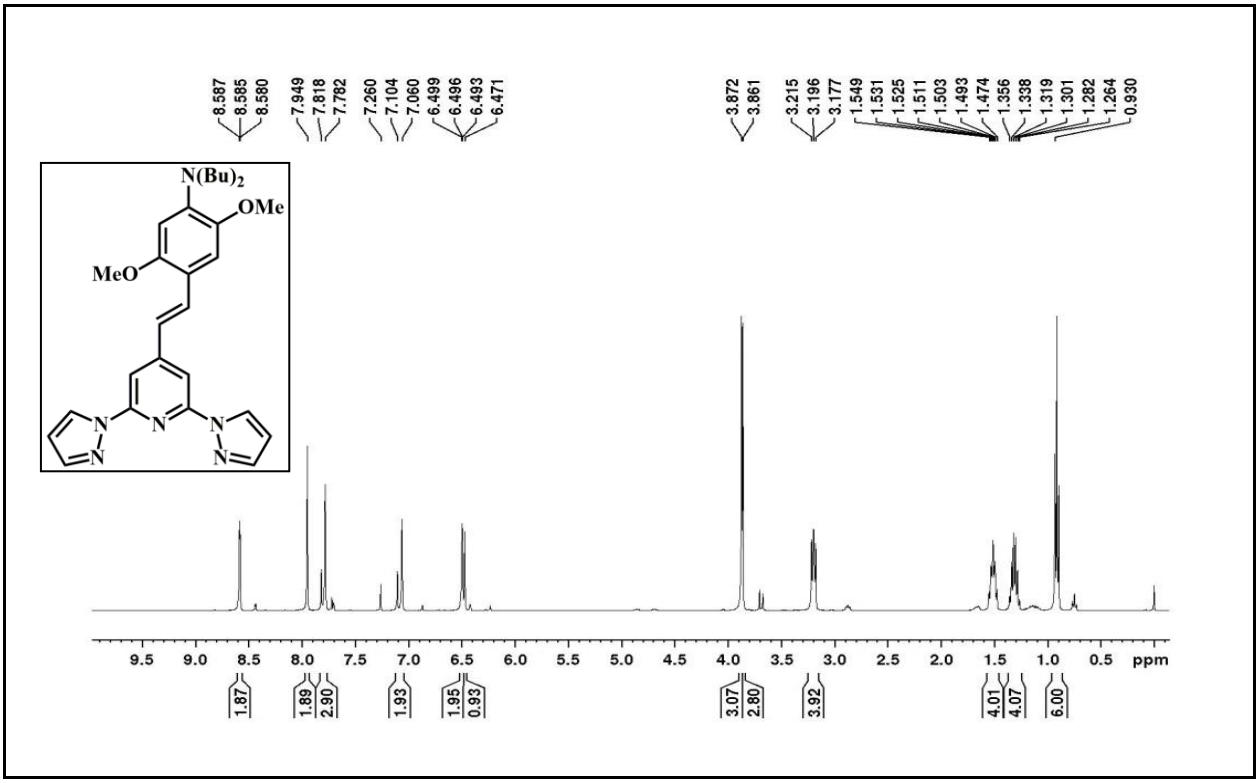



**Figure S11.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **IK–4**

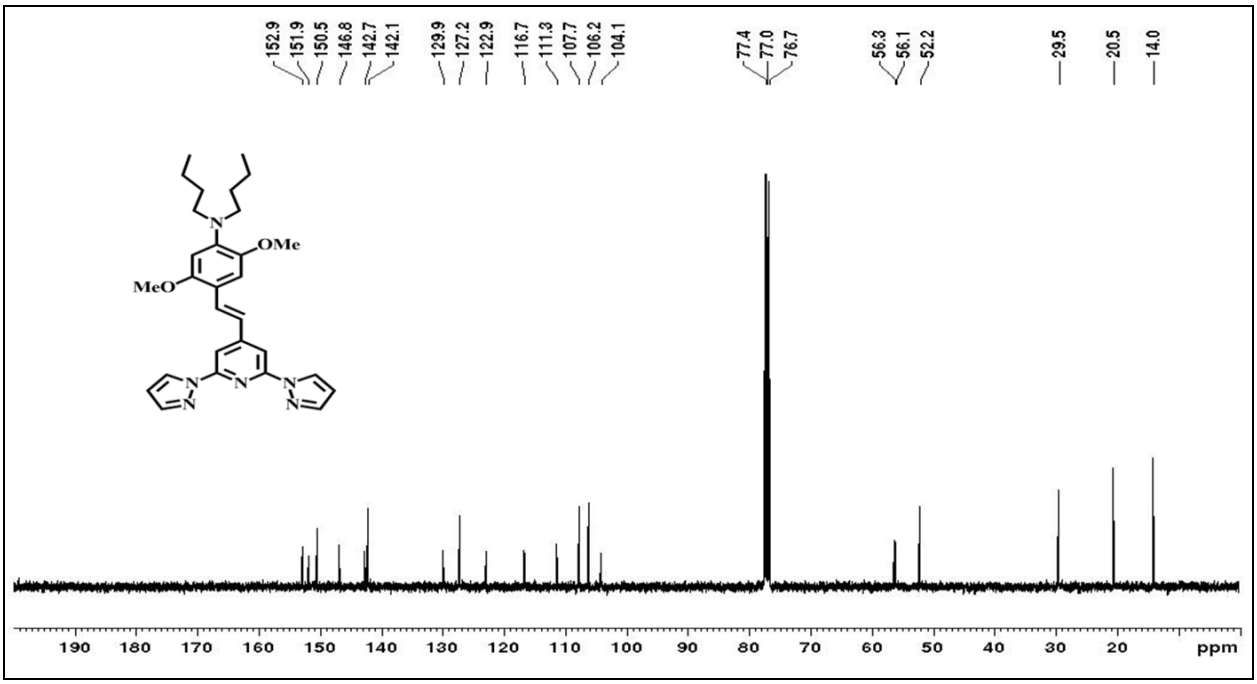



**Figure S12.** $^{13}$C NMR spectrum (400 MHz, $CDCl_3$) of **IK–4**

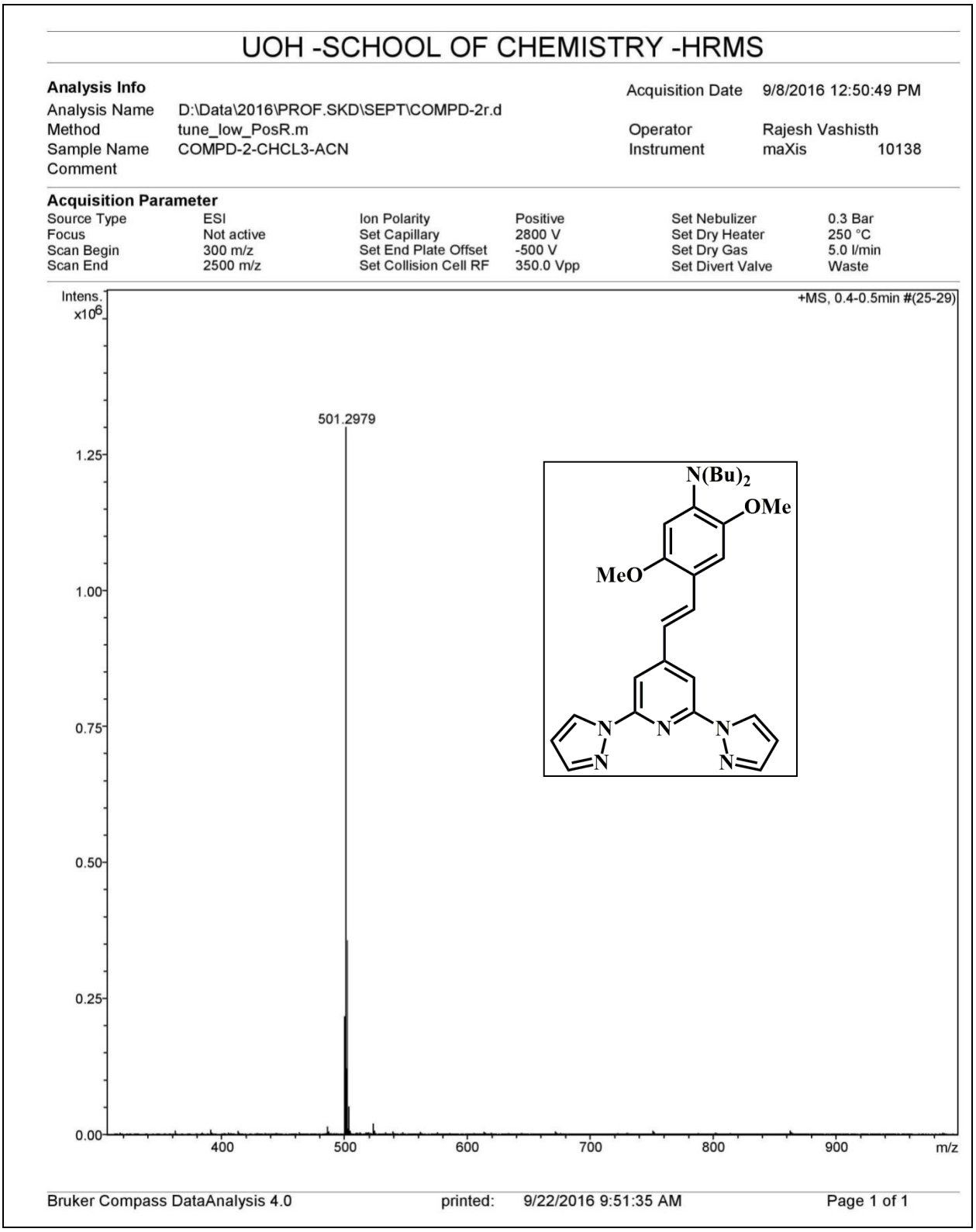
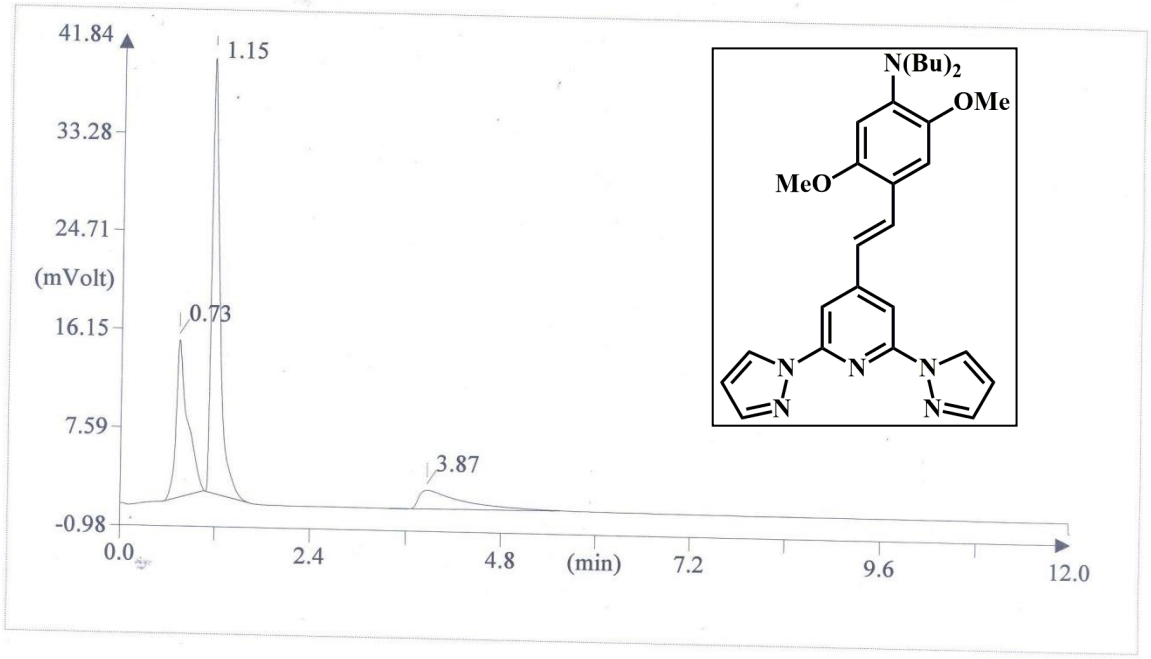



**Figure S13.** HRMS spectrum of compund **IK–4**

FLASH EA 1112 SERIES CHN REPORT
THERMO FINNIGAN

| | |
|---|---|
| Method filename: | C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex |
| Sample ID: | COMPOUND-4 (# 7) |
| Analysis type: | UnkNown |
| Chromatogram filename: | UNK-03082016-7.dat |
| Sample weight: | 1.205 |




| Element Name | Element % | Ret. Time |
|---|---|---|
| Nitrogen | 14. 07 | 0. 73 |
| Carbon | 73. 65 | 1. 15 |
| Hydrogen | 7. 14 | 3. 87 |

**Figure S14.** Elemental analysis of compound **IK–4**

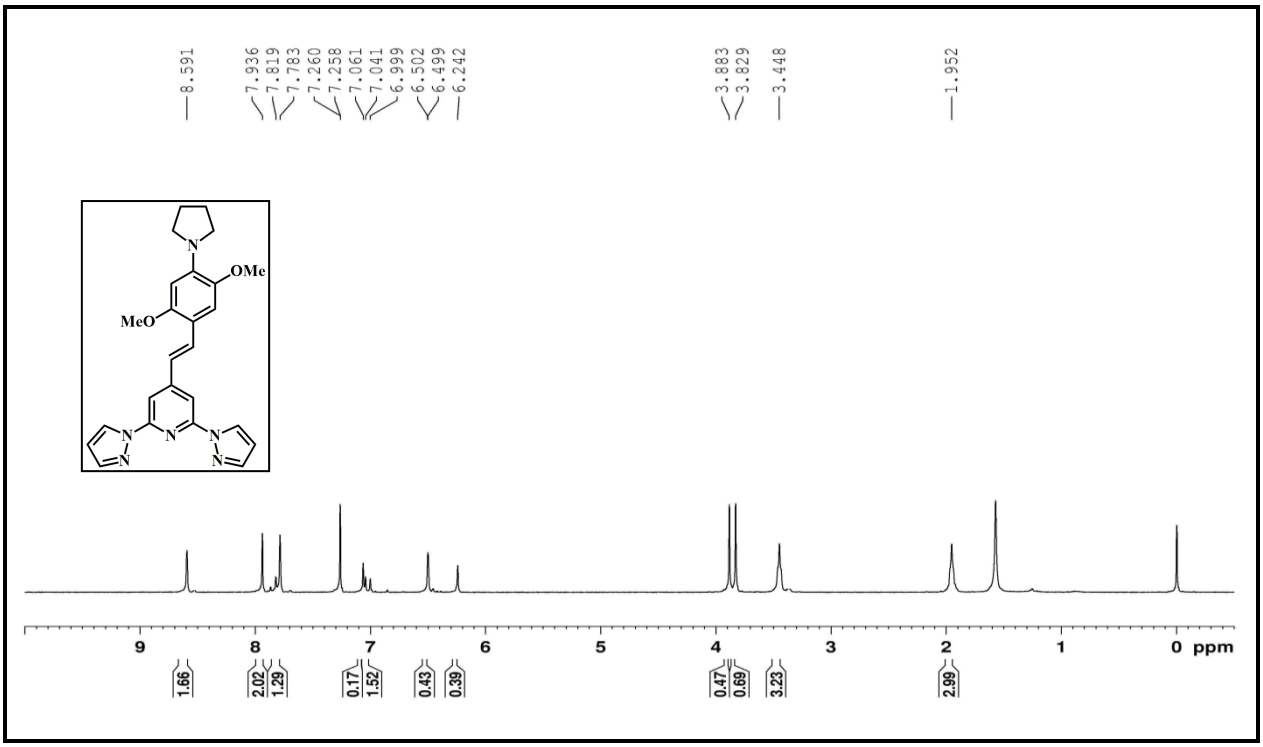



**Figure S15.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **IK–5**

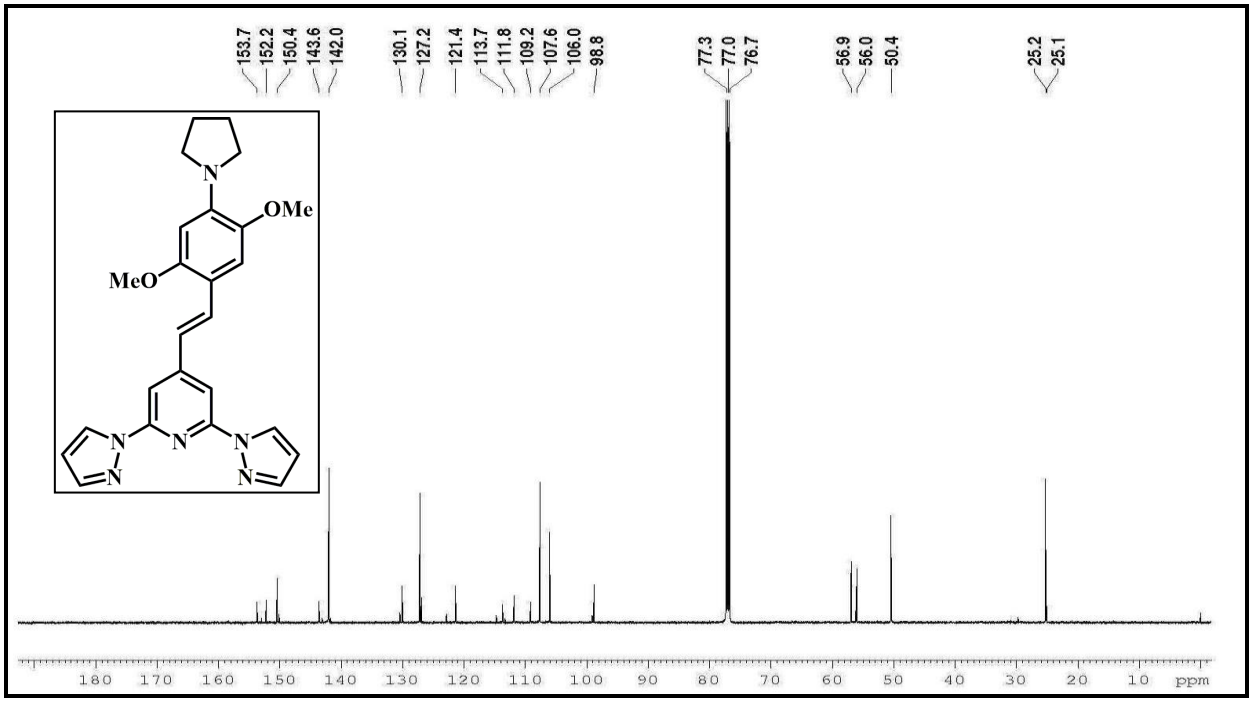



**Figure S16.** $^{13}$C NMR spectrum (100 MHz, $CDCl_3$) of **IK–5**

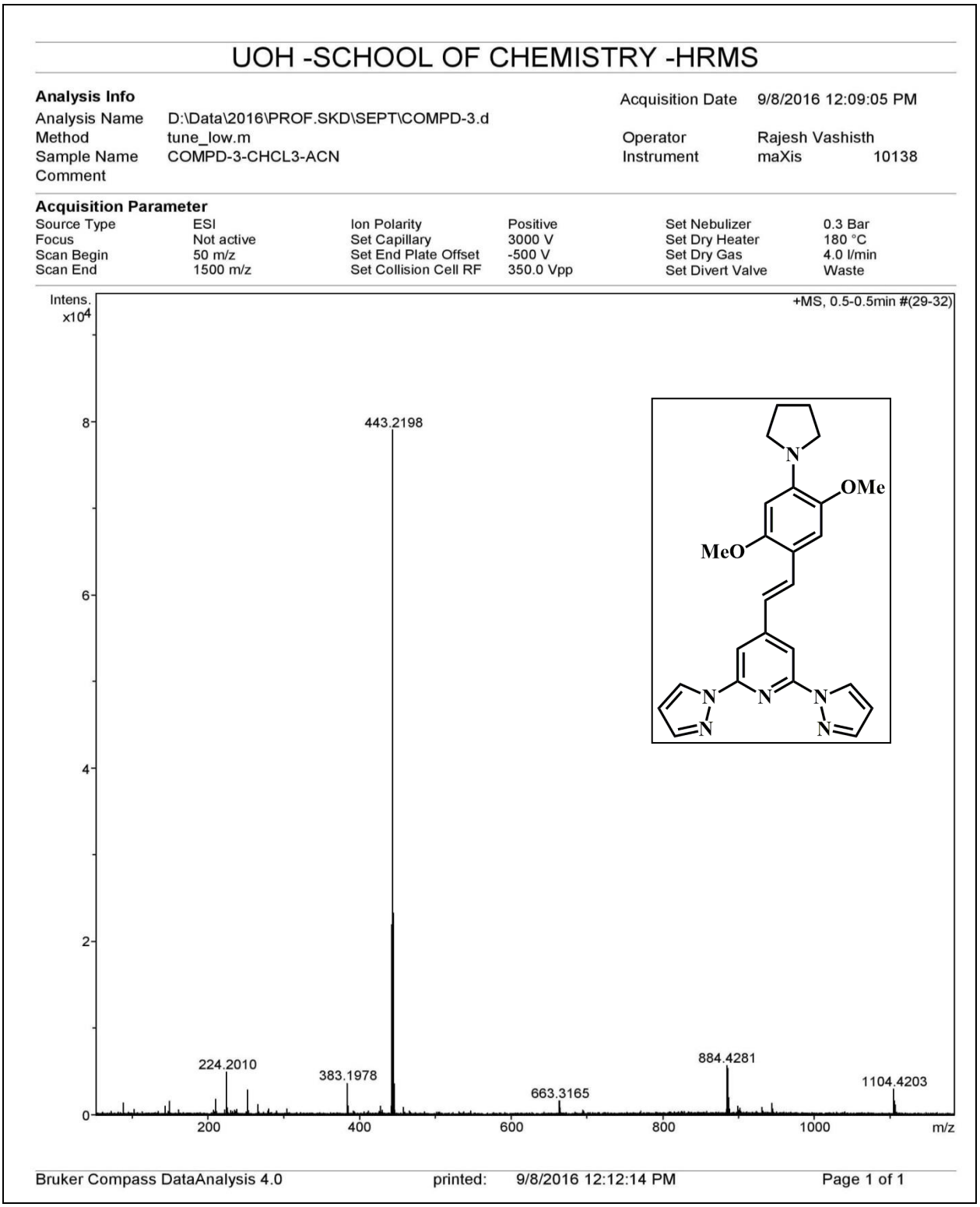



**Figure S17.** HRMS spectrum of compund **IK–5**

FLASH EA 1112 SERIES CHN REPORT
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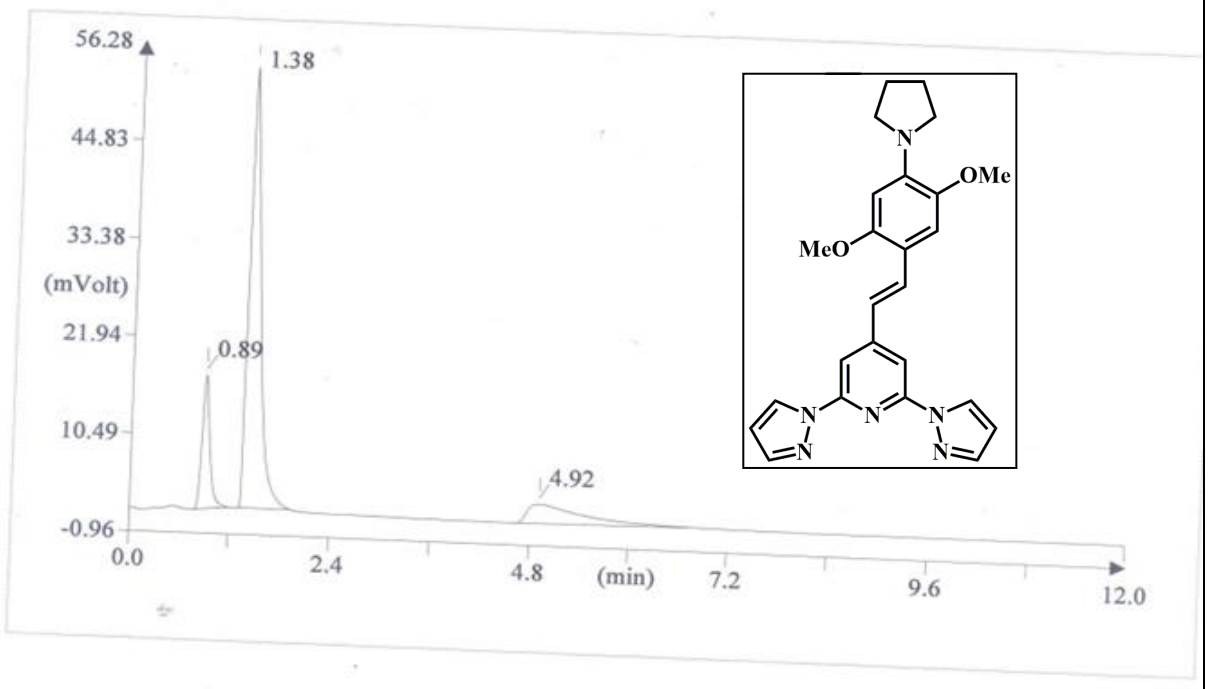
| | |
|---|---|
| Method filename: | C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex |
| Sample ID: | COMPOUND-3 (# 6) |
| Analysis type: | UnkNown |
| Chromatogram filename: | UNK-03082016-6.dat |
| Sample weight: | 1.614 |




| Element Name | Element % | Ret. Time |
|---|---|---|
| Nitrogen | 18. 82 | 0. 89 |
| Carbon | 67. 73 | 1. 38 |
| Hydrogen | 5. 98 | 4. 92 |

**Figure S18.** Elemental analysis of compound **IK–5**

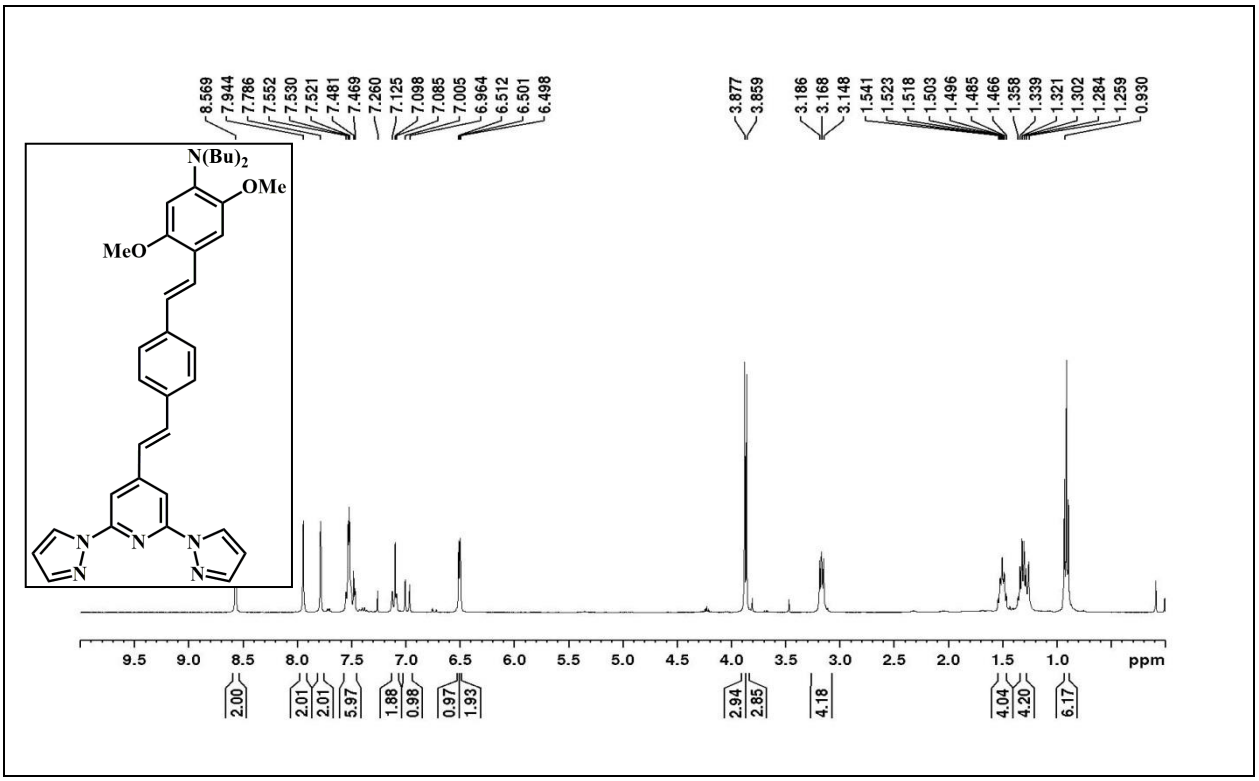



**Figure S19.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **IK–6**

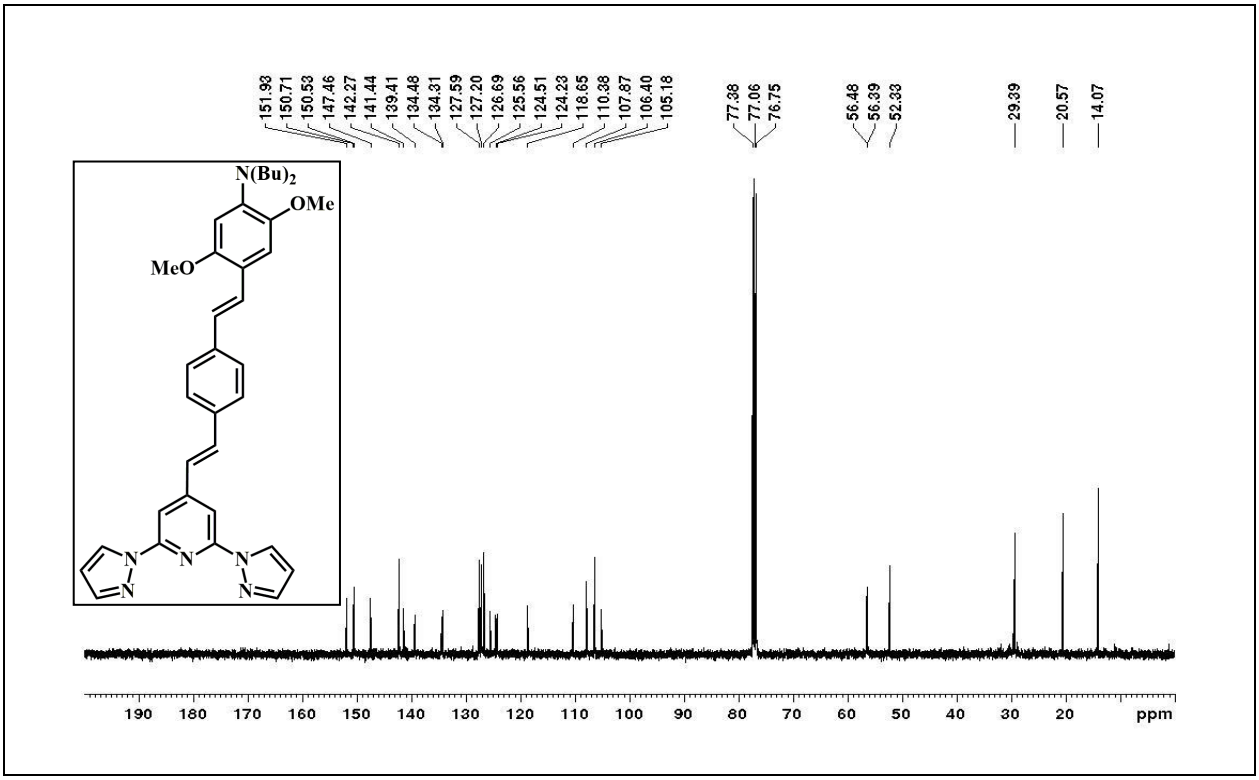



**Figure S20.** $^{13}$C NMR spectrum (400 MHz, $CDCl_3$) of **IK–6**

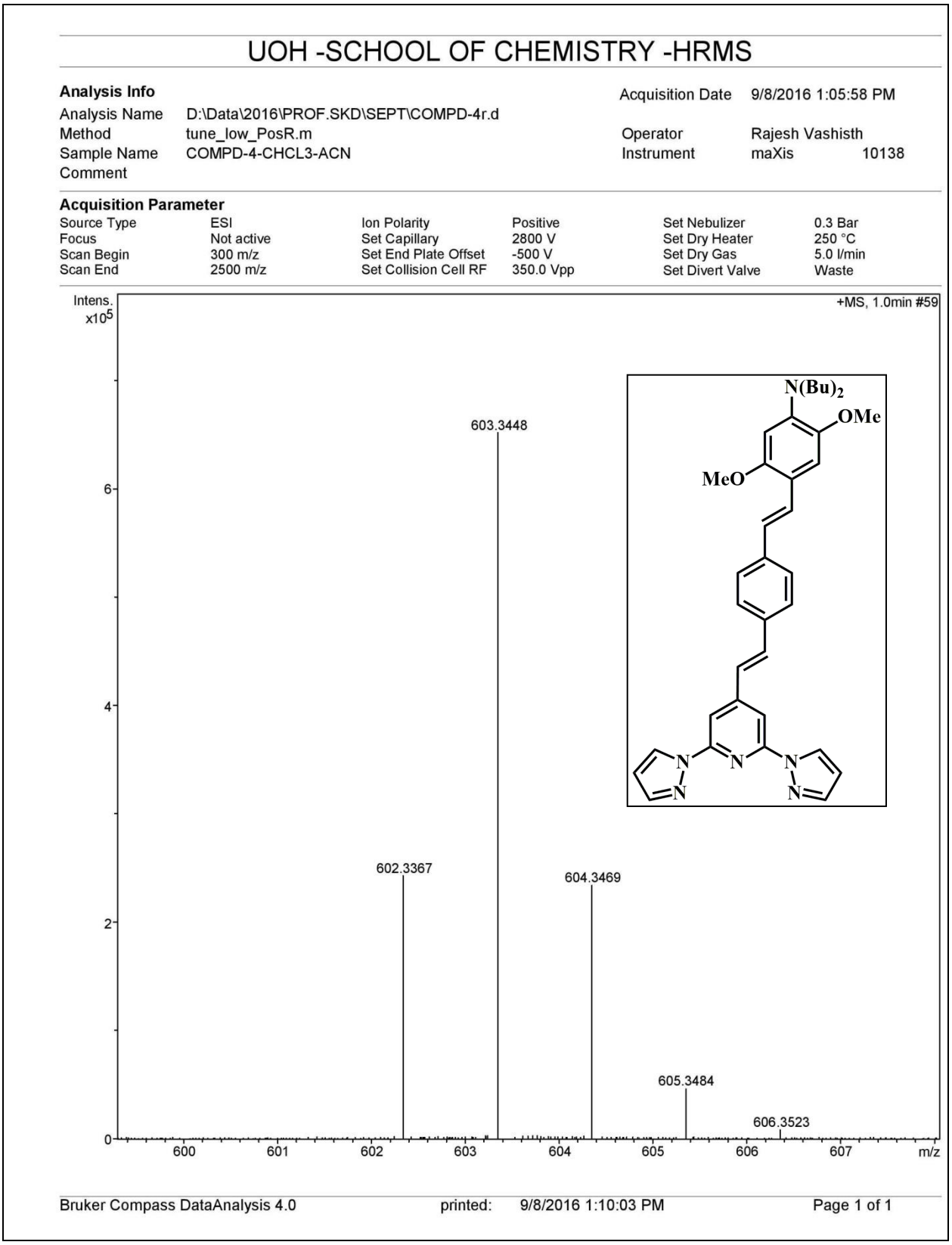



**Figure S21.** HRMS spectrum of compund **IK–6**

FLASH EA 1112 SERIES CHN REPORT
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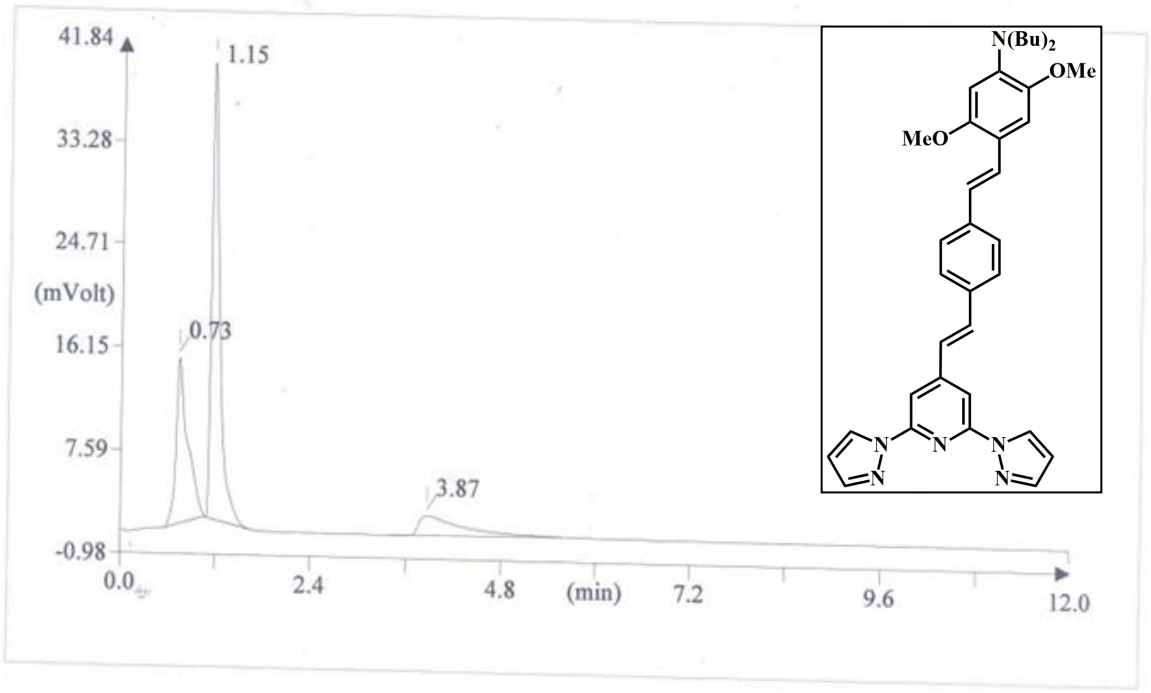
| | |
|---|---|
| Method filename: | C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex |
| Sample ID: | COMPOUND-4 (# 7) |
| Analysis type: | UnkNown |
| Chromatogram filename: | UNK-03082016-7.dat |
| Sample weight: | 1.205 |




| Element Name | Element % | Ret. Time |
|---|---|---|
| Nitrogen | 14. 07 | 0. 73 |
| Carbon | 73. 65 | 1. 15 |
| Hydrogen | 7. 14 | 3. 87 |

**Figure S22.** Elemental analysis of compound **IK–6**

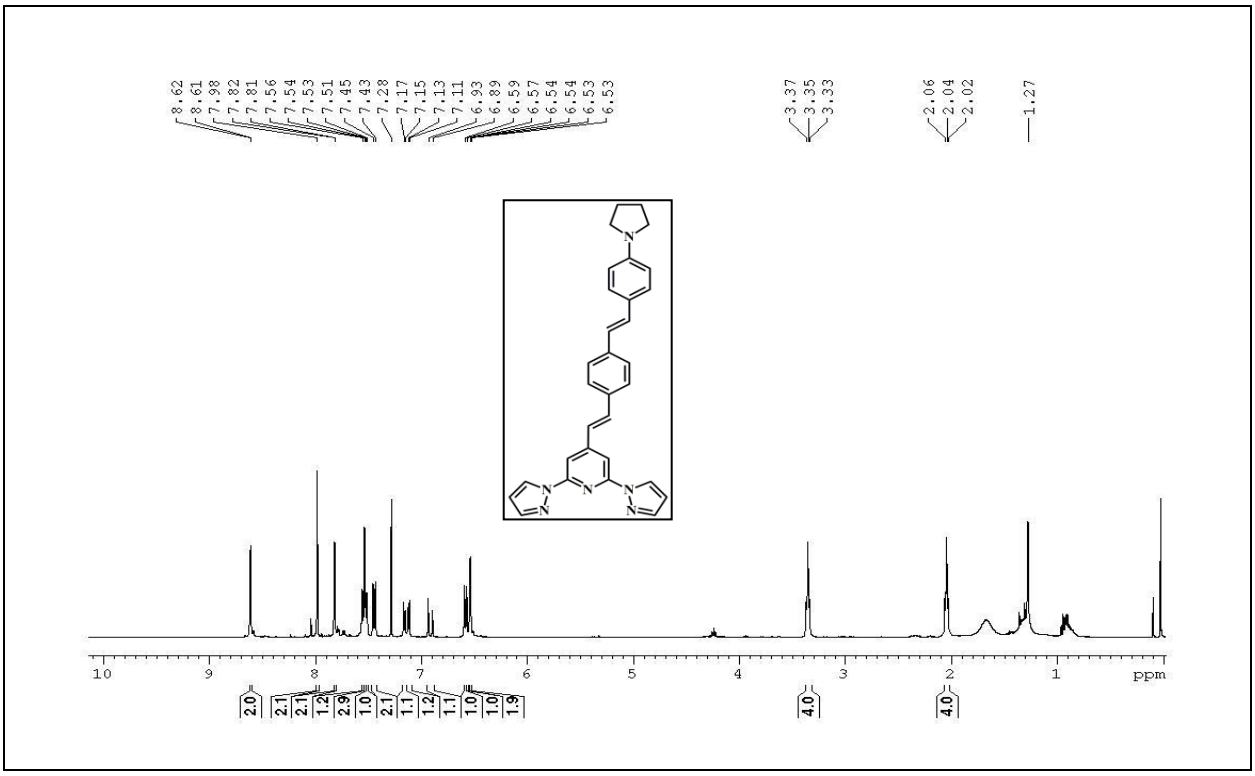



**Figure S23.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **IK–7**

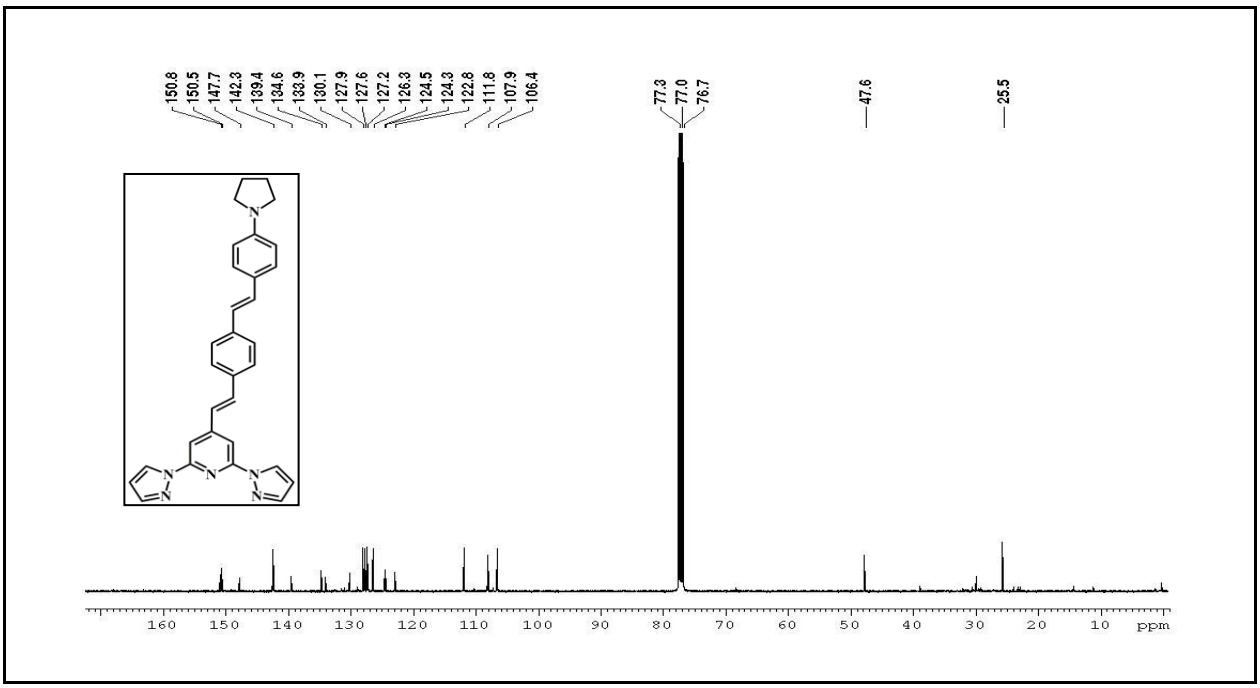



**Figure S24.** $^{13}$C NMR spectrum (100 MHz, $CDCl_3$) of **IK–7**

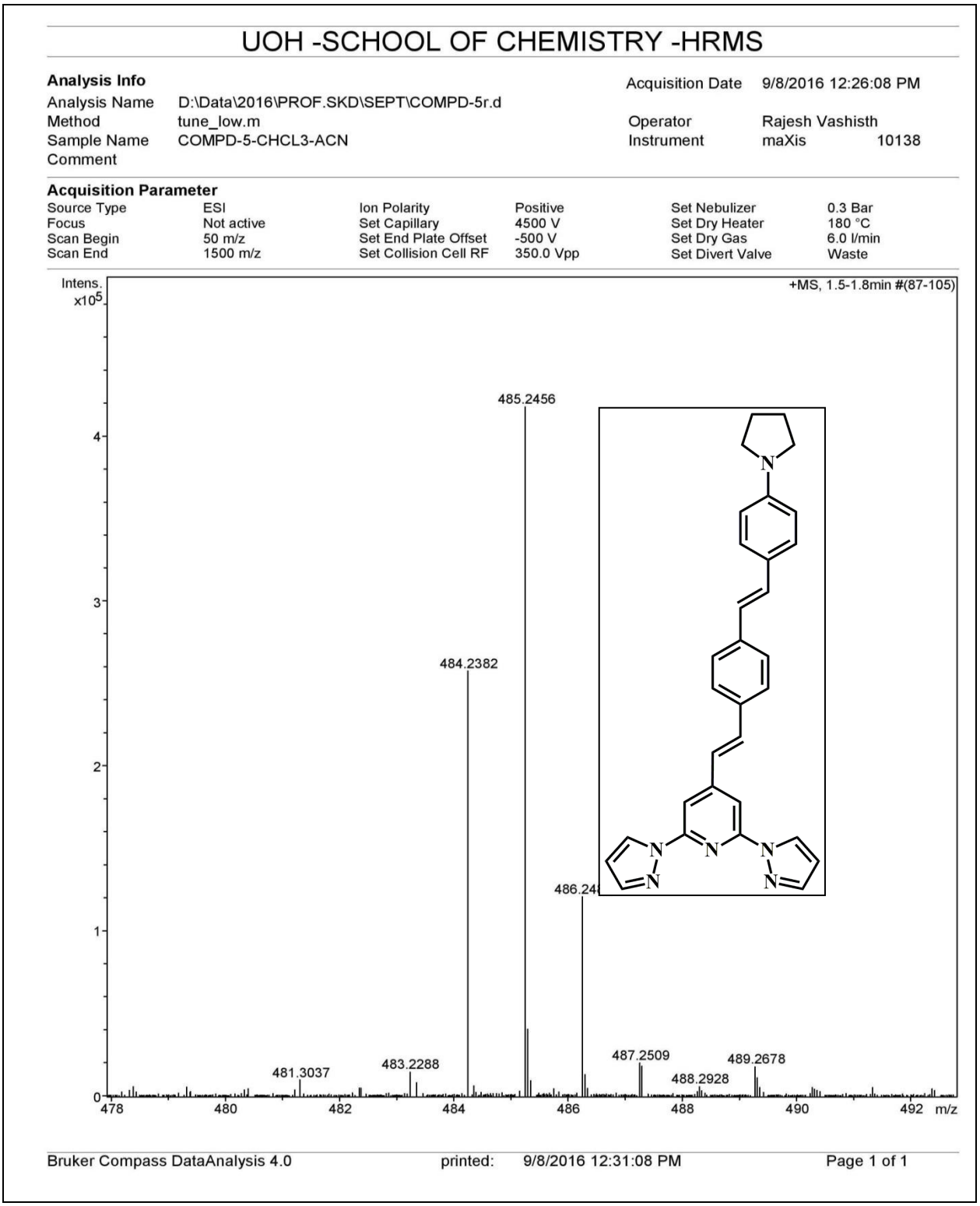



**Figure S25.** HRMS spectra of compund **IK–7**

FLASH EA 1112 SERIES CHN REPORT
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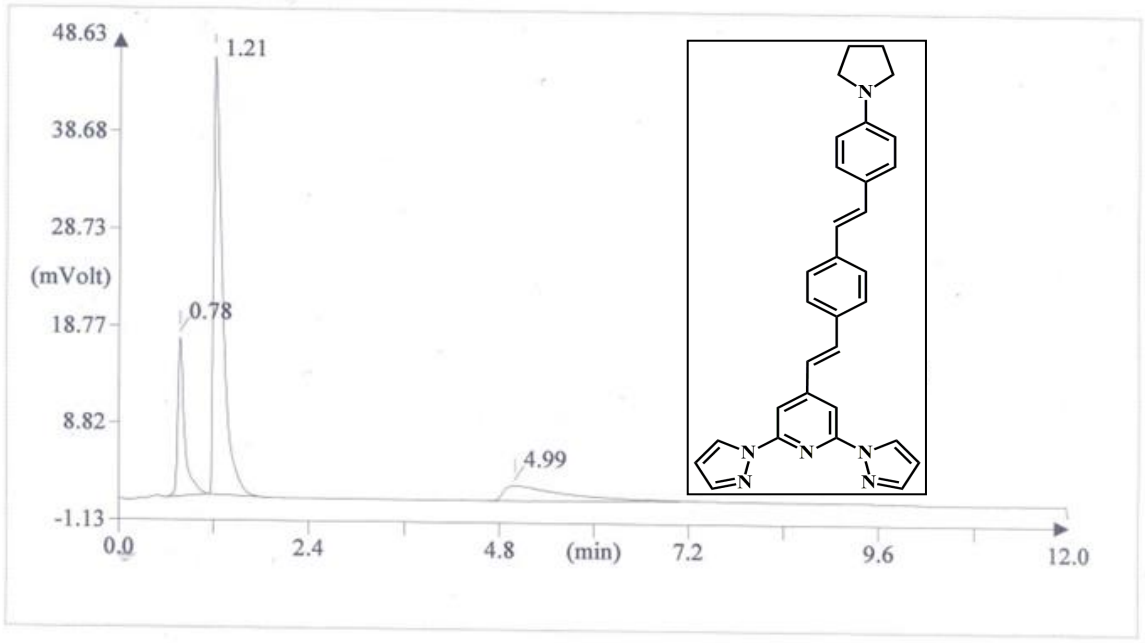
| | |
|---|---|
| Method filename: | C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex |
| Sample ID: | COMPOUND-5 (# 8) |
| Analysis type: | UnkNown |
| Chromatogram filename: | UNK-03082016-8.dat |
| Sample weight: | 1.211 |




| Element Name | Element % | Ret. Time |
|---|---|---|
| Nitrogen | 17. 25 | 0. 78 |
| Carbon | 76. 93 | 1. 21 |
| Hydrogen | 5. 75 | 4. 99 |

**Figure S26.** Elemental analysis of compound **IK–7**

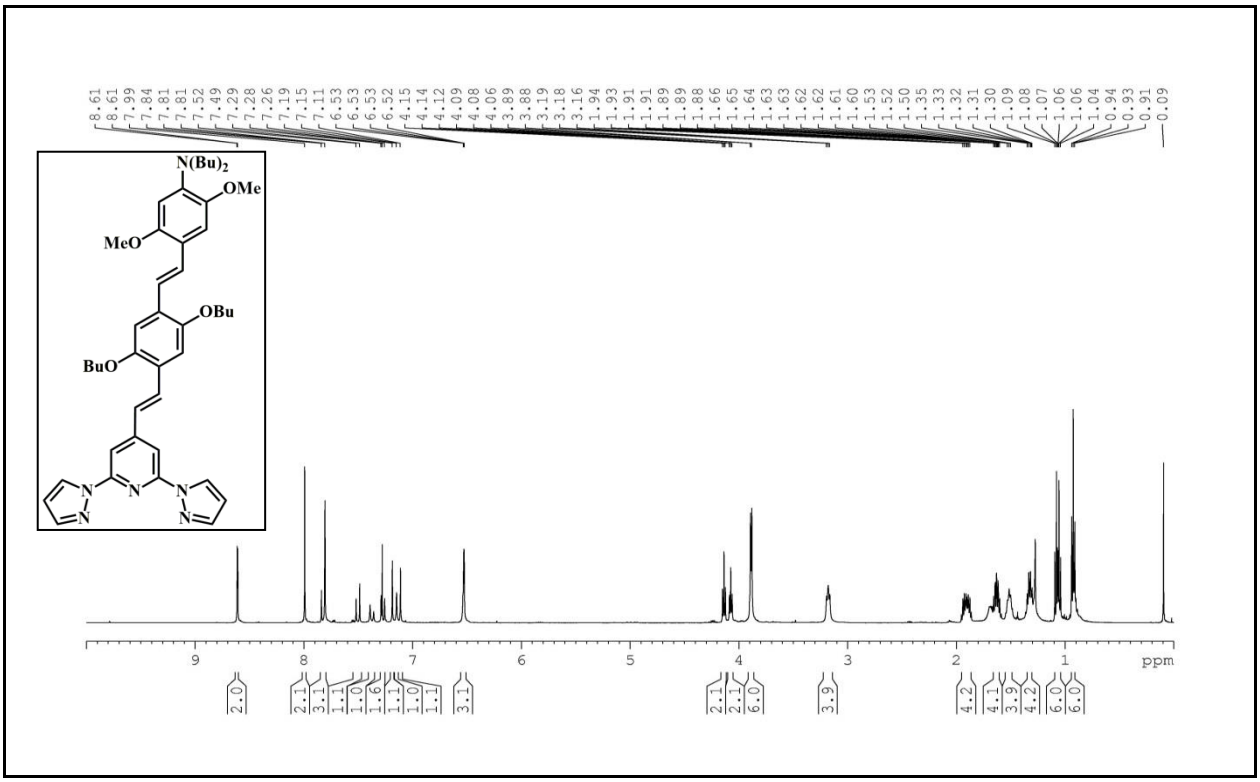



**Figure S27.** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **IK–8**

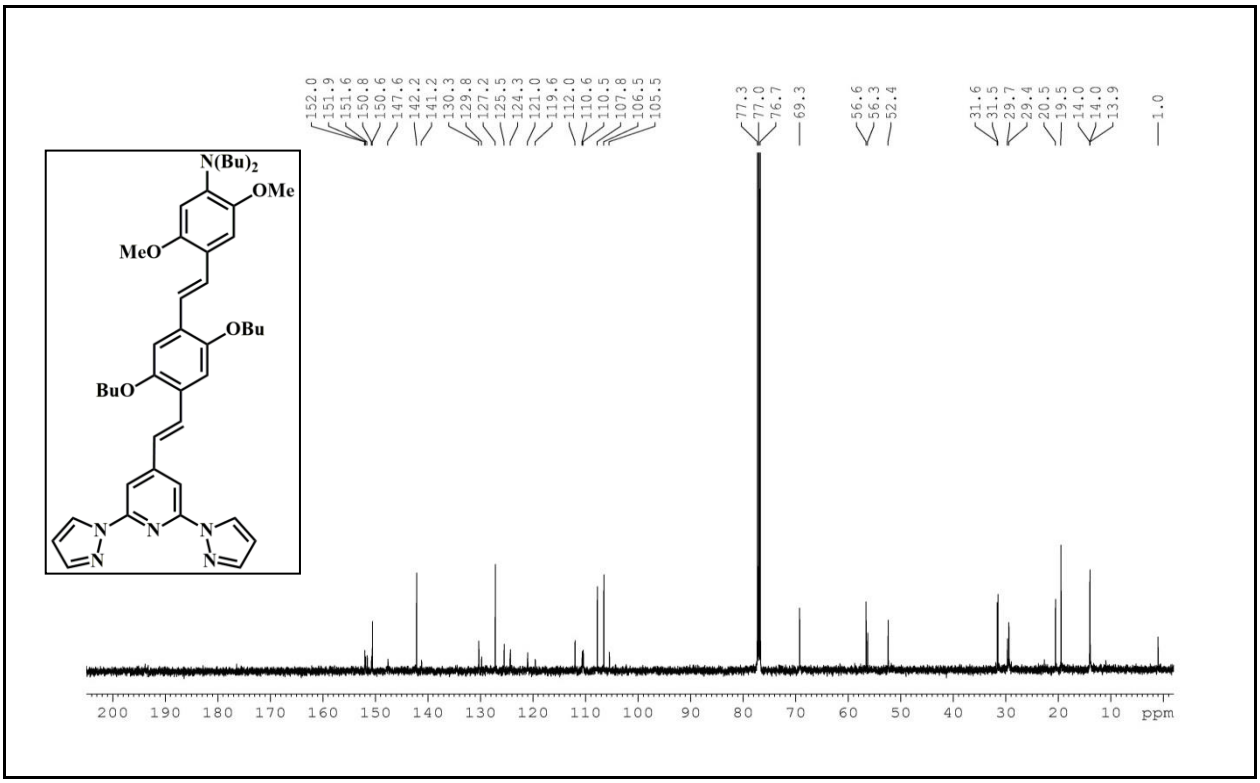



**Figure S28.** $^{13}$C NMR spectrum (100 MHz, $CDCl_3$) of **IK–8**

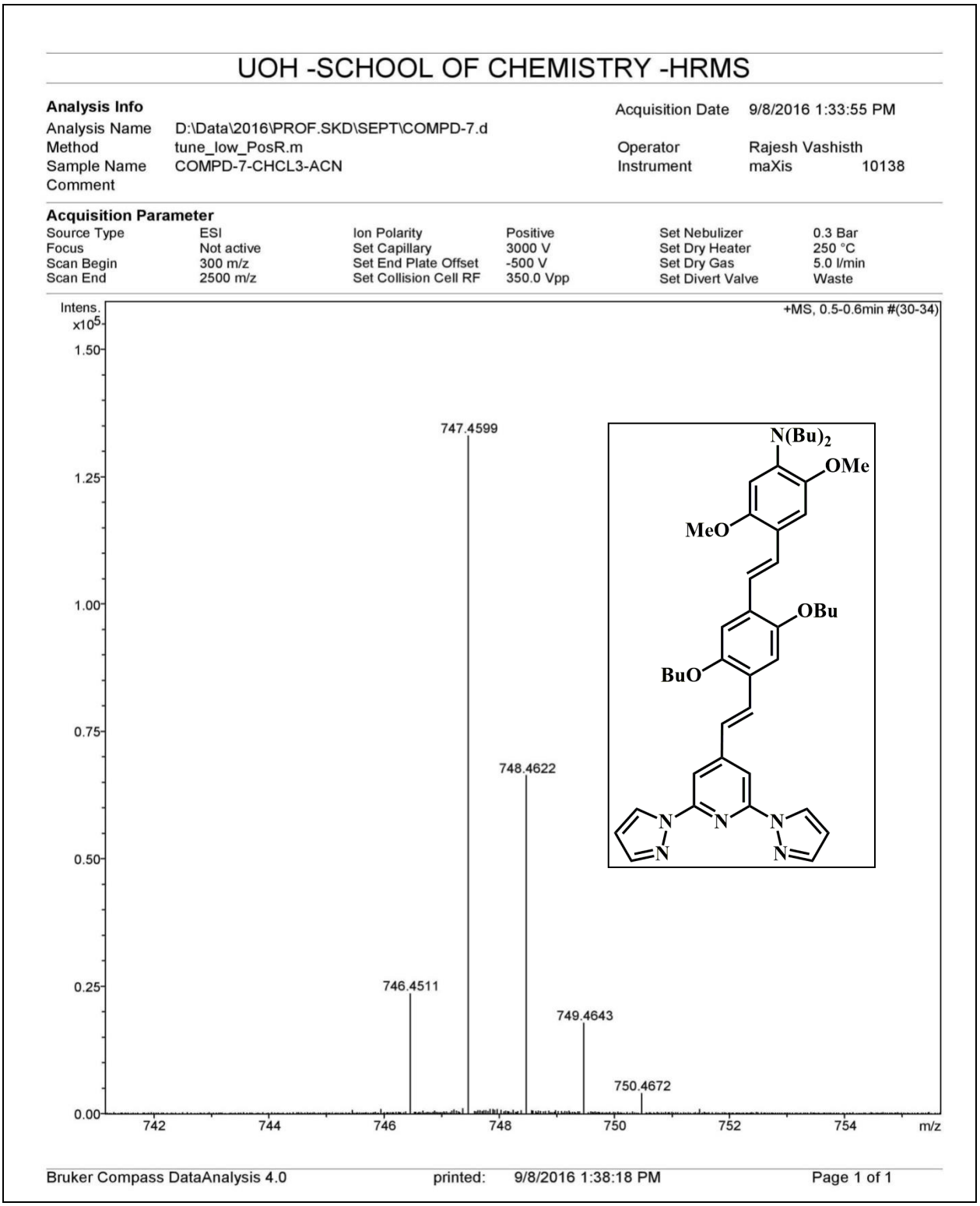
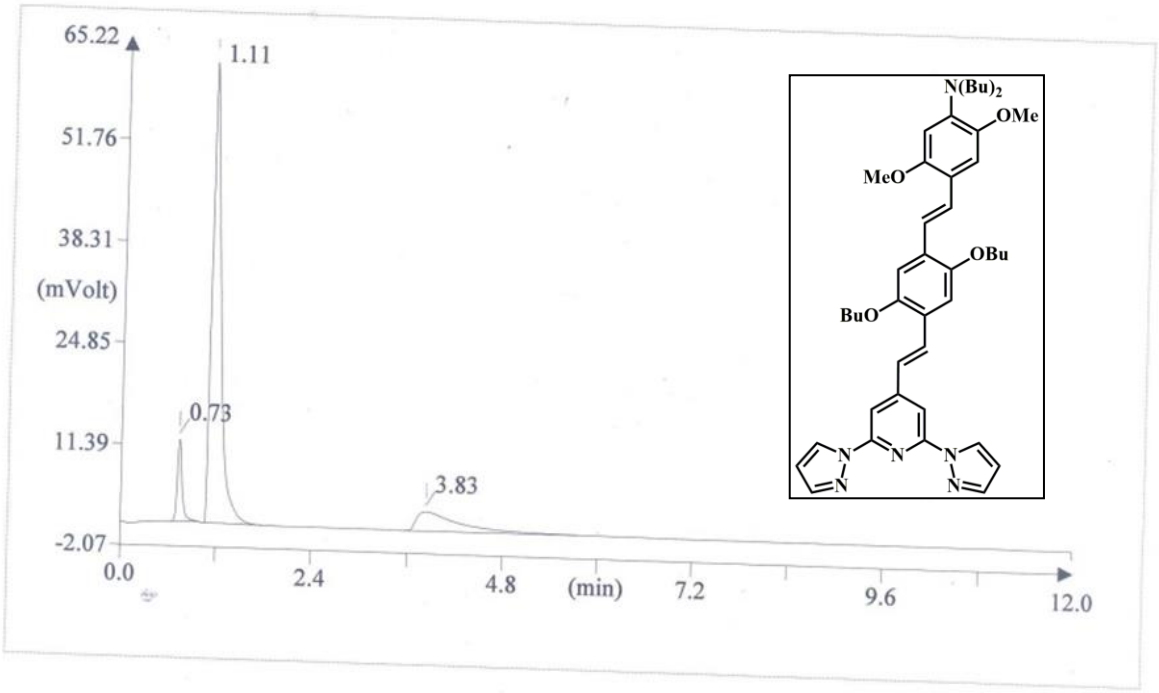



**Figure S29.** HRMS spectrum of compund **IK–8**

# FLASH EA 1112 SERIES CHN REPORT
# THERMO FINNIGAN

| | |
|---|---|
| Method filename: | C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex |
| Sample ID: | COMPOUND-7 (# 10) |
| Analysis type: | UnkNown |
| Chromatogram filename: | UNK-03082016-10.dat |
| Sample weight: | 1.703 |




| Element Name | Element % | Ret. Time |
|---|---|---|
| Nitrogen | 11. 36 | 0. 73 |
| Carbon | 72. 45 | 1. 11 |
| Hydrogen | 7. 76 | 3. 83 |

**Figure S30.** Elemental analysis of compound **IK–8**

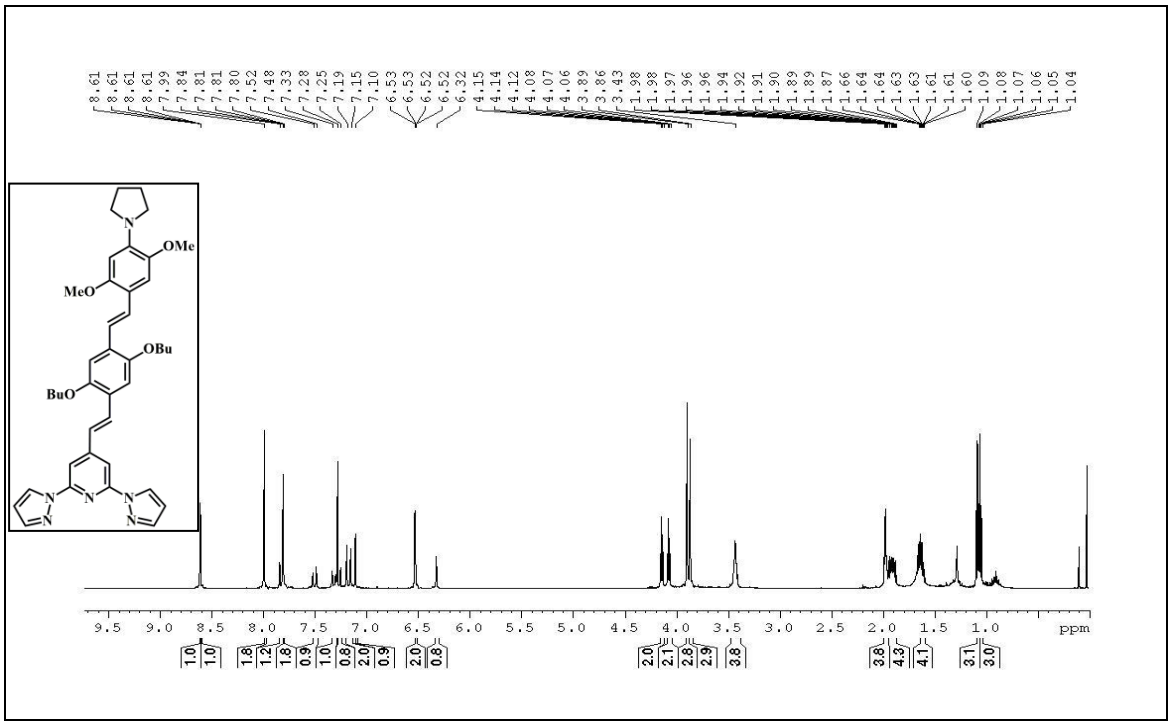



**Figure S31.** $^{1}H$ NMR spectrum (400 MHz, $CDCl_3$) of **IK–9**

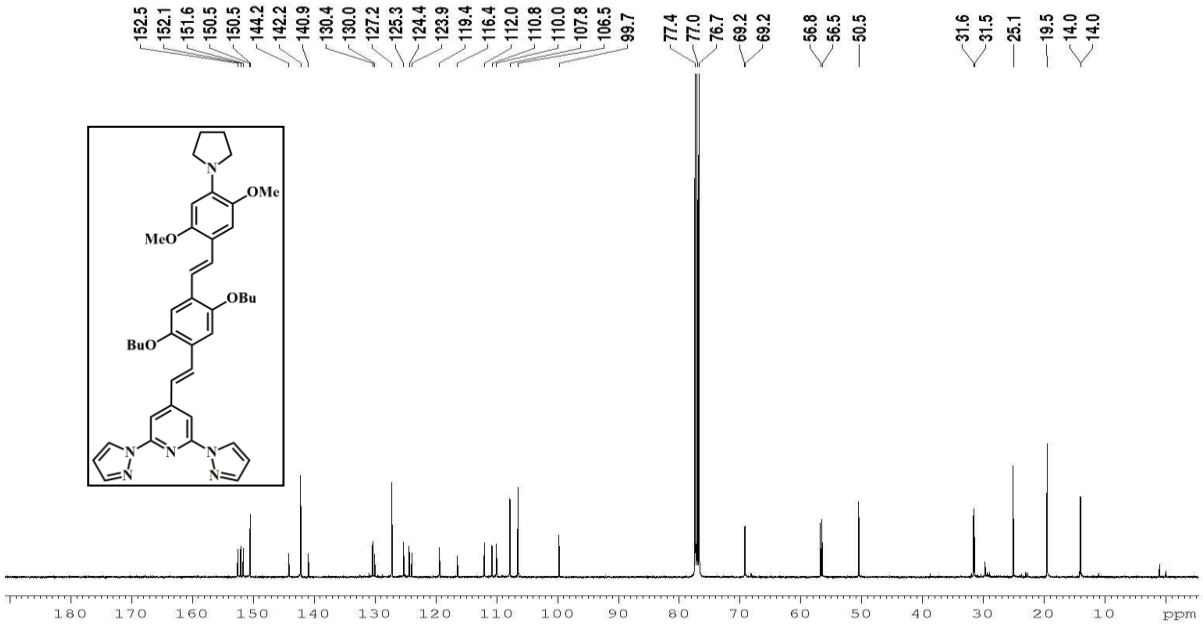



**Figure S32.** $^{13}C$ NMR spectrum (100 MHz, $CDCl_3$) of **IK–9**

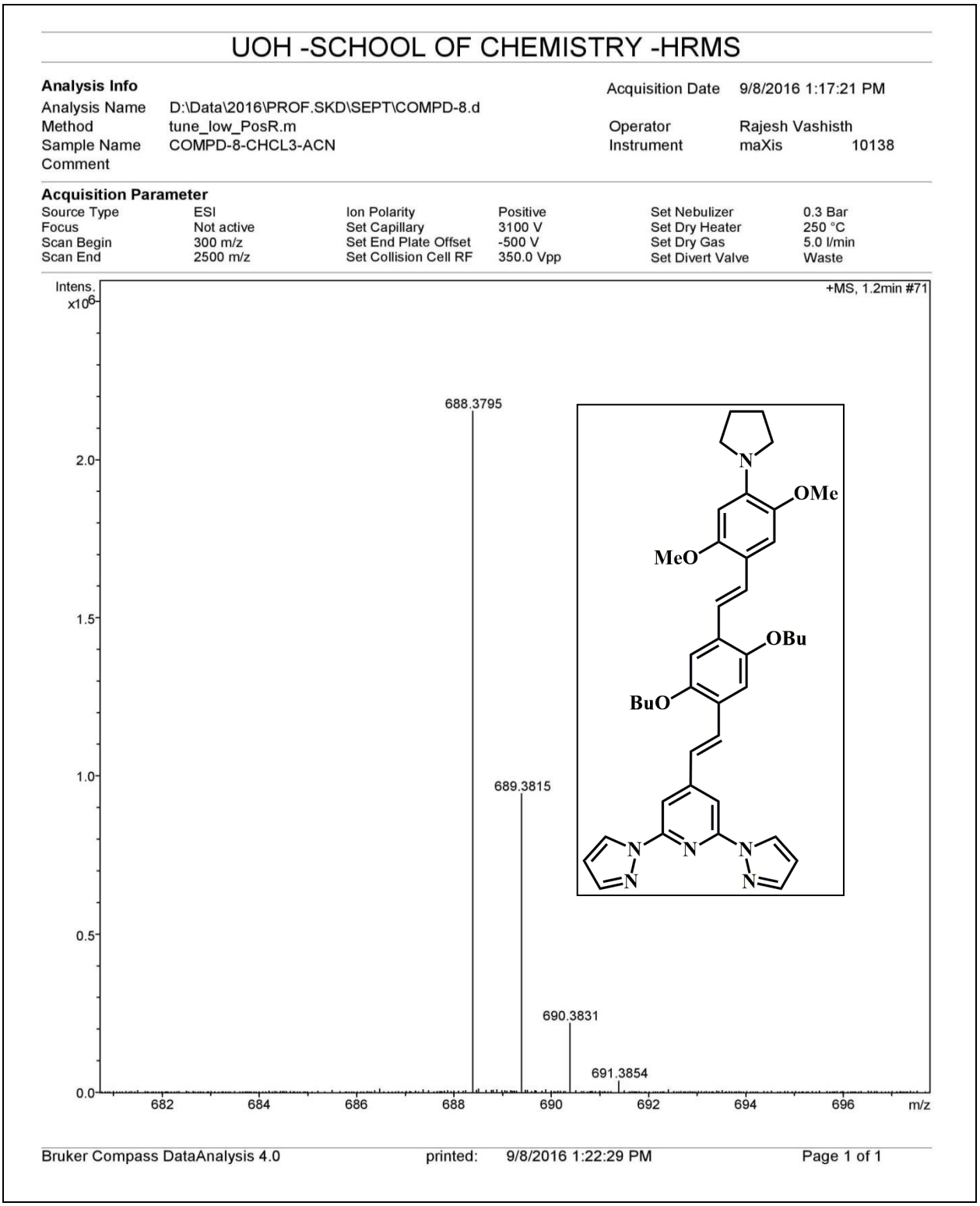
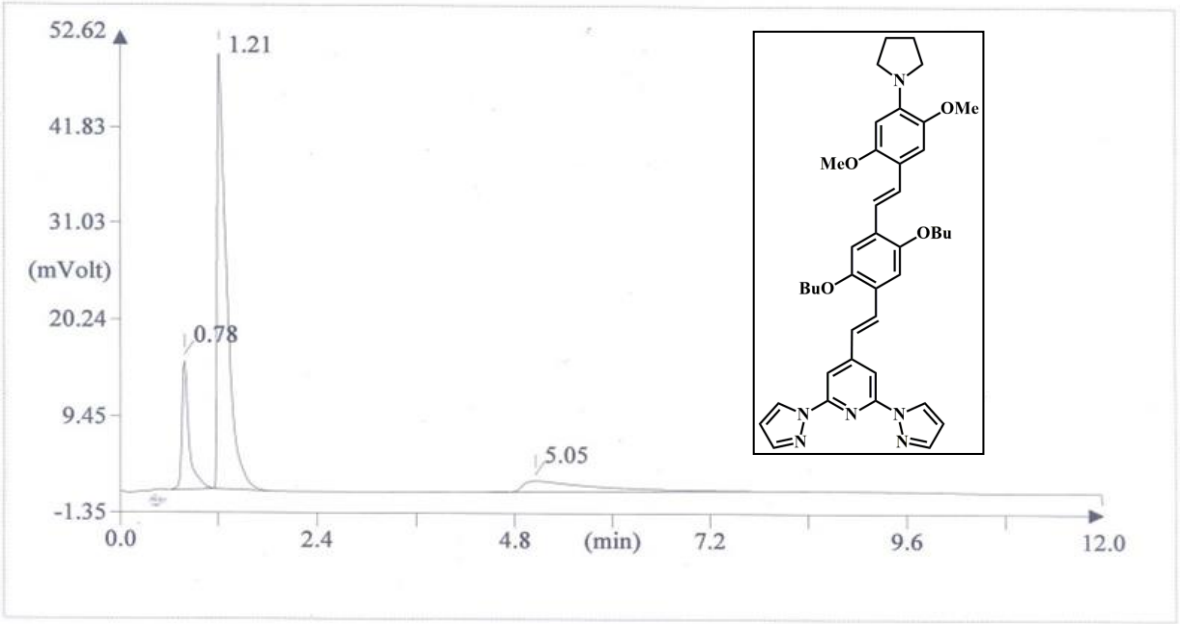



**Figure S33.** HRMS spectrum of compund **IK–9**

FLASH EA 1112 SERIES CHN REPORT
THERMO FINNIGAN

| | |
|---|---|
| Method filename: | C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex |
| Sample ID: | COMPOUND-8 (# 11) |
| Analysis type: | UnkNown |
| Chromatogram filename: | UNK-03082016-11.dat |
| Sample weight: | 1.476 |




| Element Name | Element % | Ret. Time |
|---|---|---|
| Nitrogen | 12. 36 | 0. 78 |
| Carbon | 71. 32 | 1. 21 |
| Hydrogen | 7. 08 | 5. 05 |

**Figure S34.** Elemental analysis of compound **IK–9**

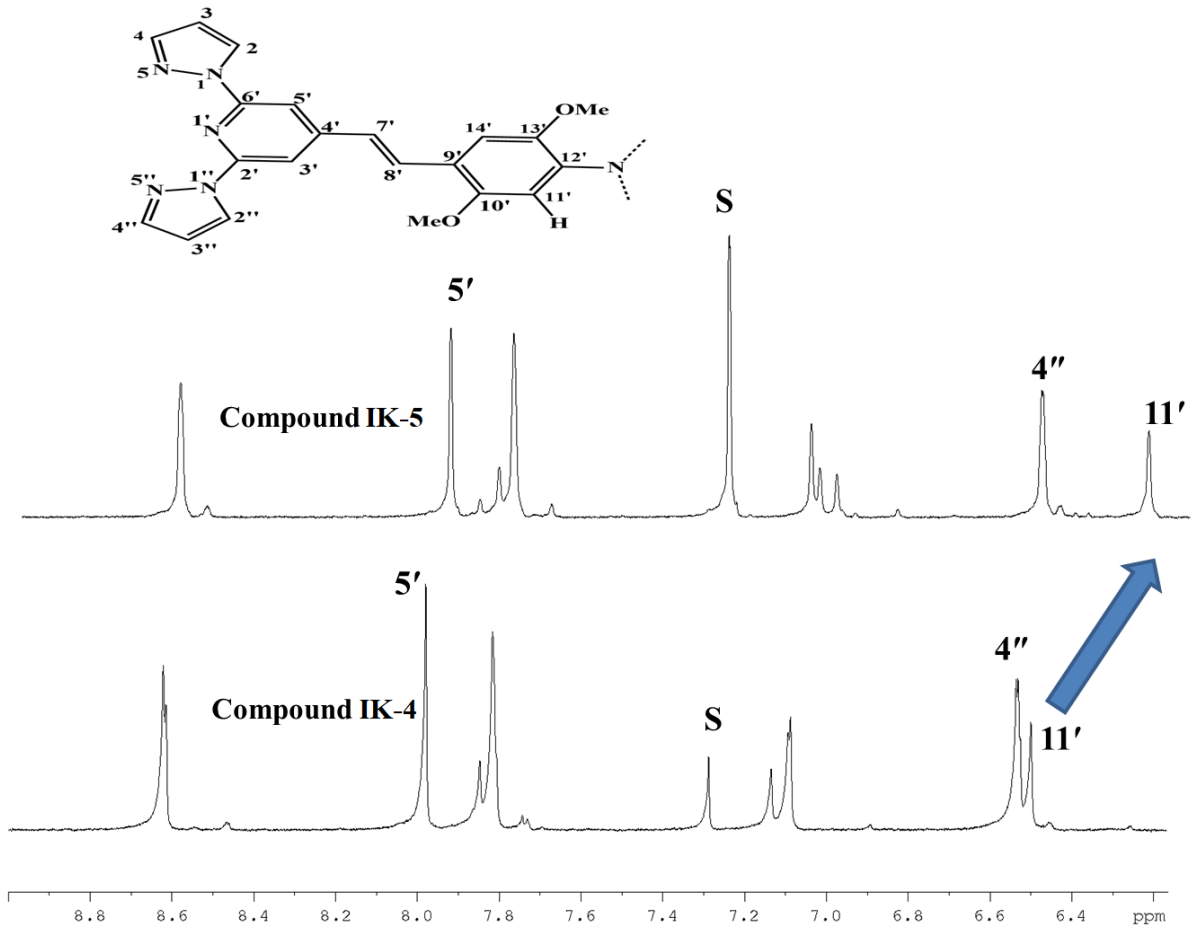



**Figure S35.** $^{1}$HNMR signals of compounds IK–4 and IK–5 in the aromatic region of the spectra (400 MHz, $CDCl_3$ , 298±2 K) showing the difference in chemical shift of the proton adjcent to the amino donor ($H^{11'}$). S= solvent signal

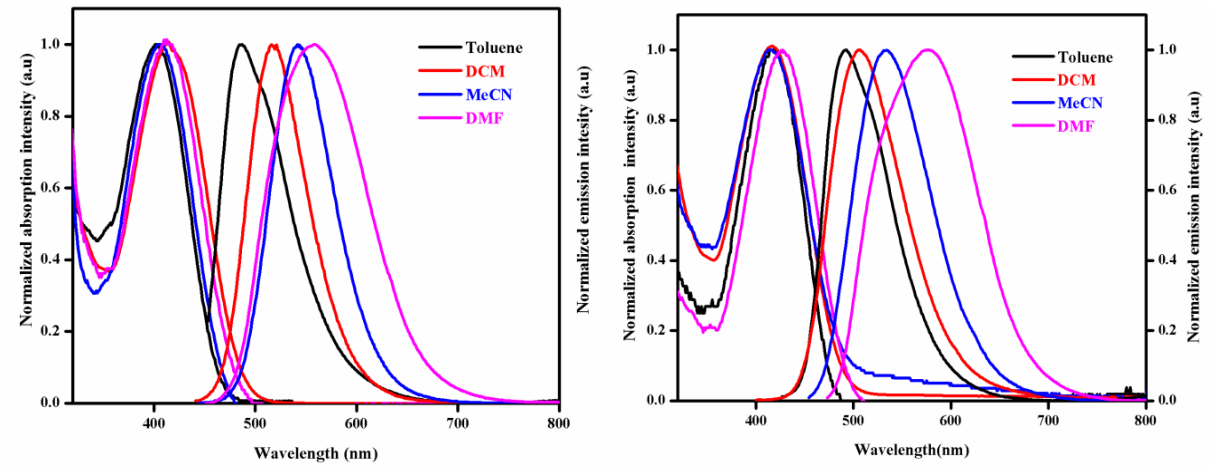



**Figure S36.** UV-visible and Fluorescence spectra of **IK–4** (left) and **IK–5** (right).

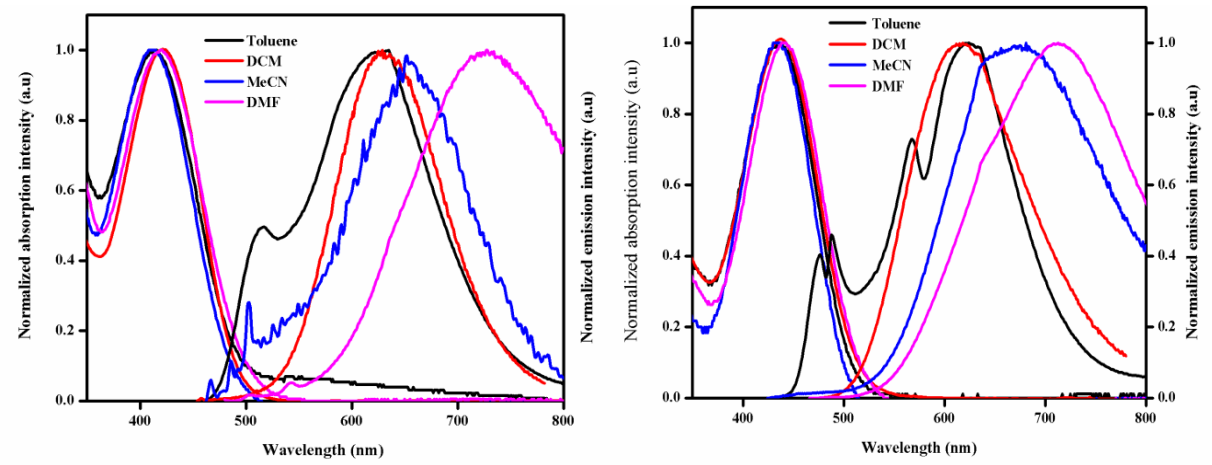



**Figure S37.** UV -visible and Fluorescence spectra of **IK–6** (left) and **IK–7** (right).

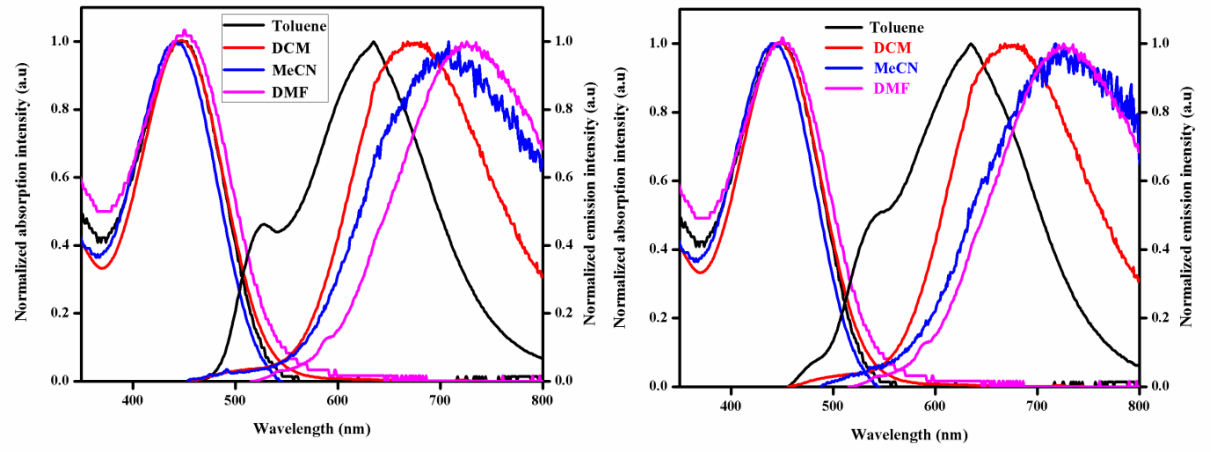



**Figure S38.** UV-visible and Fluorescence spectra of **IK–8** (left) and **IK–9** (right)

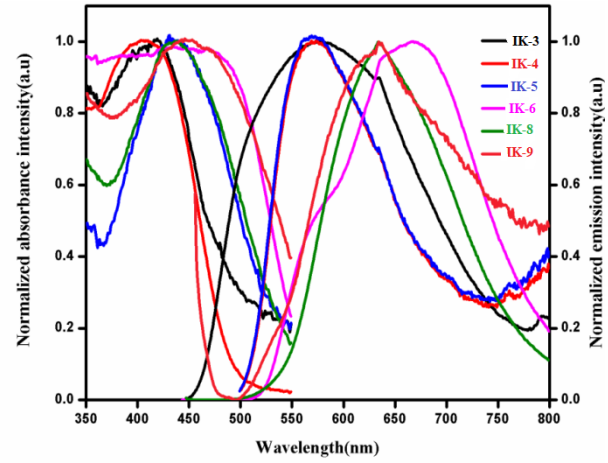



**Figure S39.** Solid-state absorption spectra (recorded in diffuse reflectance mode), and solid state emission spectra of the compounds (**IK–(3–6), IK– 8 and IK– 9**) at room temperature.

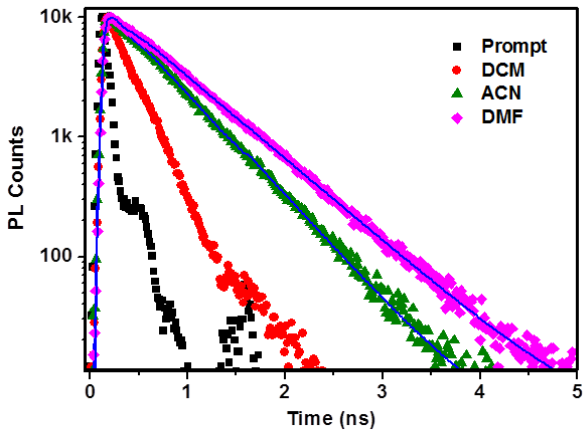



**Figure S40.** Fluorescence decay profiles of compound **IK–3** in DCM (red) , MeCN (green) and DMF (pink). In DCM solvent, the decay profile cannot be fitted properly as it is much closed to the instrument response function.

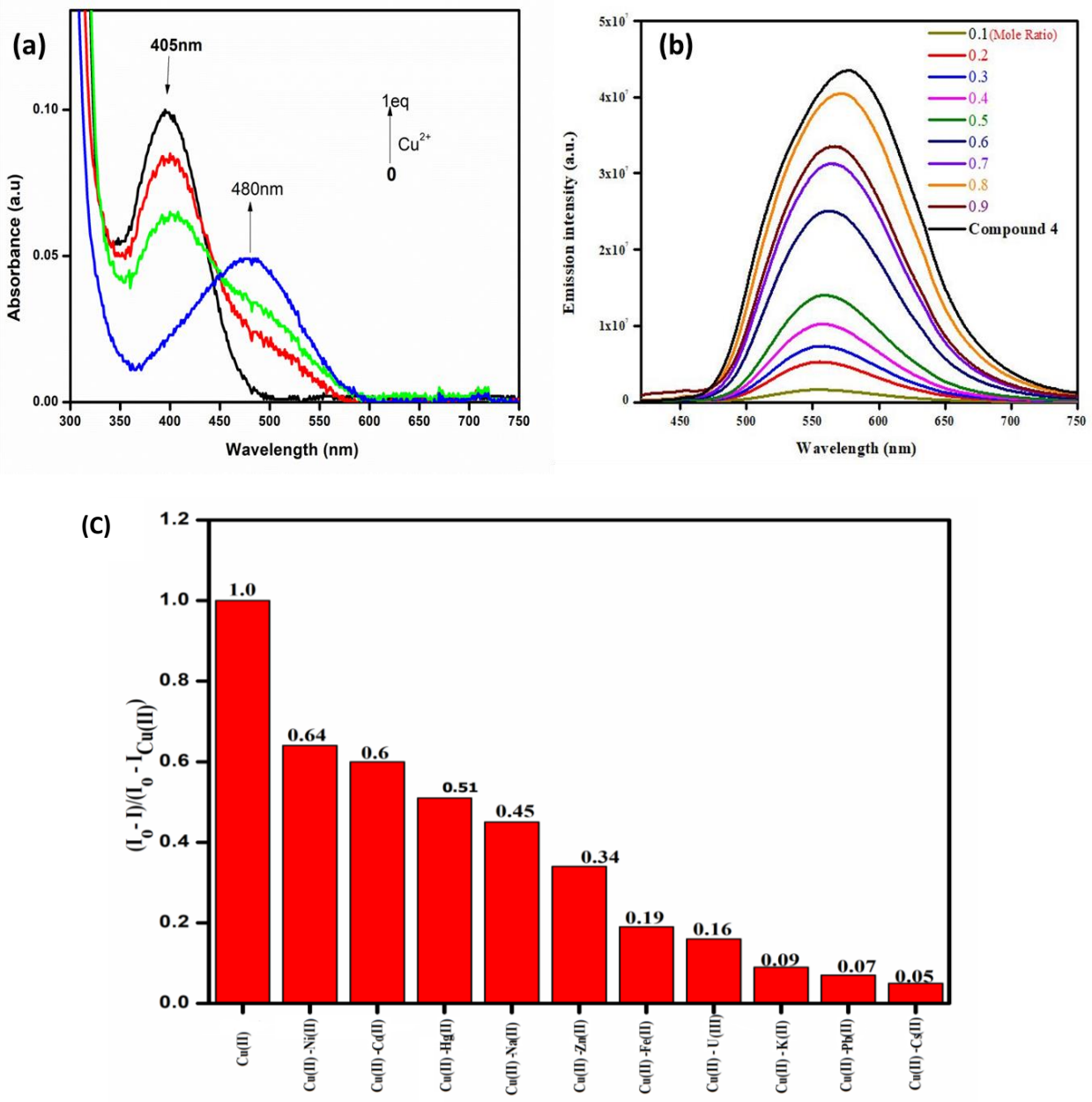



**Figure S41.** (a) UV-vis spectral changes of chromophore **IK–4** (10 μM) (black line) in MeOH with increasing amount of $Cu^{2+}$ (10 μM) (red, green and blue) (as its acetate salt). (b) Emission spectra of **IK–4** (10 μM) in MeOH upon the addition of $Cu^{2+}$ (Mole ratio method) = [**IK–4**]/{[**IK–4**]+[$Cu^{2+}$]}. (c) Competitive experiments in the [**IK-4**] =10 μM, [$Cu^{2+}$] = 10 μM, and [$M^{n+}$] =10 μM, $\lambda_{max}$ = 408 nm.

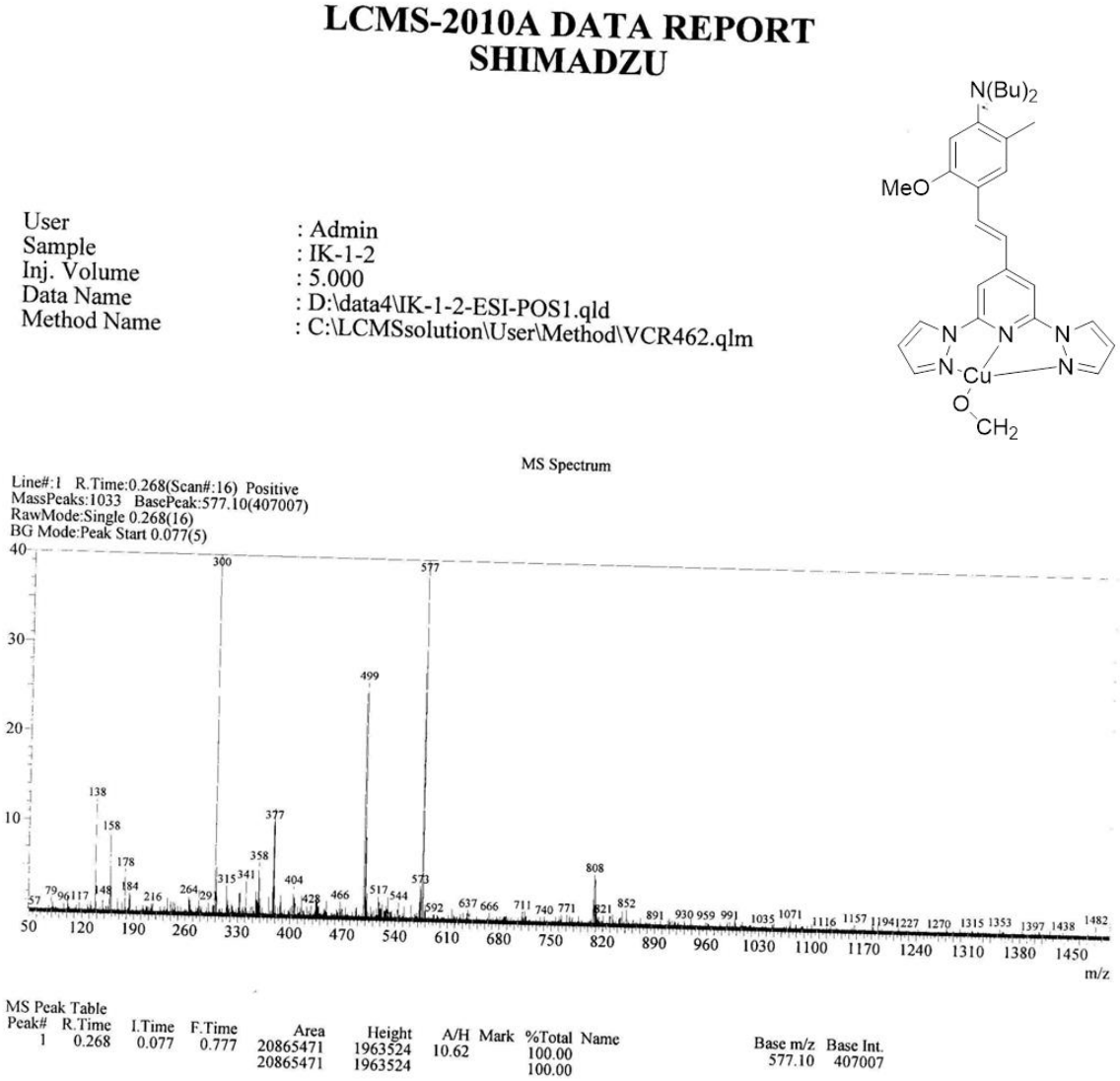



**Figure S42.** ESI-MS for [**IK-4** + $Cu^{2+}$ (as its acetate salt)] complex in methanol solution.

**Table S9**: Theoretical values of $\lambda_{max}$, computed in gas phase and solvent medium (toluene, DCM, MeCN and DMF) and compared with experimental values of compound **IK-**(**3-9**)

| **Compound IK-** | **$\lambda_{max}$ (Gas)(nm)** | **Solvent** | **Experimental (nm) $\lambda_{max}$** | **$\lambda_{max}$ (LR)calculation (nm)** | **$\lambda_{max}$ state-specific (SS)caculation (nm)** |
|---|---|---|---|---|---|
| 3 | 330 | | 398 | 350 | 368 |
| 4 | 346 | | 402 | 362 | 378 |
| 5 | 355 | | 419 | 376 | 392 |
| 6 | 361 | Toluene | 415 | 375 | 387 |
| 7 | 367 | | 424 | 385 | 414 |
| 8 | 369 | | 437 | 381 | 388 |
| 9 | 382 | | 449 | 398 | 420 |
| 3 | | | 391 | 354 | 376 |
| 4 | | | 403 | 364 | 382 |
| 5 | | | 419 | 380 | 401 |
| 6 | | DCM | 422 | 376 | 387 |
| 7 | | | 424 | 386 | 417 |
| 8 | | | 436 | 382 | 387 |
| 9 | | | 446 | 398 | 418 |
| 3 | | | 399 | 354 | 376 |
| 4 | | | 404 | 363 | 381 |
| 5 | | | 413 | 380 | 401 |
| 6 | | MeCN | 413 | 376 | 385 |
| 7 | | | 413 | 385 | 411 |
| 8 | | | 433 | 386 | 390 |
| 9 | | | 442 | 397 | 413 |
| 3 | | | 405 | 355 | 380 |
| 4 | | | 412 | 365 | 385 |
| 5 | | | 426 | 382 | 405 |
| 6 | | DMF | 421 | 378 | 390 |
| 7 | | | 419 | 387 | 419 |
| 8 | | | 442 | 388 | 393 |
| 9 | | | 451 | 399 | 420 |

**Table S10.** Computational outputs (coordinates of the G09 optimized structures at $S_0$ state in DCM Solution)

**Compound IK–3**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -4.287750 | 0.059672 | -0.000953 |
| 2 | 7 | 0 | -4.640717 | -2.226317 | -0.018352 |
| 3 | 7 | 0 | -4.197087 | -3.503692 | -0.025630 |
| 4 | 7 | 0 | -4.084047 | 2.363837 | 0.016833 |
| 5 | 6 | 0 | -3.732276 | -1.145025 | -0.008104 |
| 6 | 6 | 0 | -0.059483 | -0.514387 | 0.005275 |
| 7 | 6 | 0 | -1.502171 | -0.276002 | 0.003760 |
| 8 | 6 | 0 | -3.456918 | 1.097192 | 0.008905 |
| 9 | 6 | 0 | 4.551636 | 1.258385 | 0.001934 |
| 10 | 7 | 0 | 6.529184 | -0.134256 | 0.003025 |
| 11 | 6 | 0 | -2.076331 | 1.001800 | 0.011963 |
| 12 | 7 | 0 | -3.350905 | 3.499712 | 0.027016 |
| 13 | 6 | 0 | 0.889787 | 0.436101 | 0.003239 |
| 14 | 6 | 0 | 2.334553 | 0.244741 | 0.003698 |
| 15 | 6 | 0 | 2.957737 | -1.013161 | 0.006387 |
| 16 | 6 | 0 | 5.171555 | -0.008329 | 0.003753 |
| 17 | 6 | 0 | -6.461951 | -3.445542 | -0.032507 |
| 18 | 6 | 0 | -6.000882 | -2.155737 | -0.022280 |
| 19 | 6 | 0 | 4.331061 | -1.145128 | 0.005631 |
| 20 | 6 | 0 | 7.445125 | 0.995645 | -0.109879 |
| 21 | 6 | 0 | 3.173763 | 1.367062 | 0.000996 |
| 22 | 6 | 0 | -5.564834 | 3.979817 | 0.025395 |
| 23 | 6 | 0 | -5.293675 | -4.240350 | -0.034157 |

| | | | | | |
|---|---|---|---|---|---|
| 24 | 6 | 0 | -4.241887 | 4.475360 | 0.032219 |
| 25 | 6 | 0 | -2.365475 | -1.376634 | -0.006128 |
| 26 | 6 | 0 | -5.422015 | 2.617330 | 0.015577 |
| 27 | 6 | 0 | 7.225806 | -1.412304 | 0.106090 |
| 28 | 6 | 0 | 8.679329 | -1.007579 | 0.353955 |
| 29 | 6 | 0 | 8.798447 | 0.334267 | -0.371378 |
| 30 | 1 | 0 | 8.929257 | 0.170467 | -1.445378 |
| 31 | 1 | 0 | 9.633008 | 0.943450 | -0.019634 |
| 32 | 1 | 0 | -1.991069 | -2.390568 | -0.012585 |
| 33 | 1 | 0 | 0.580177 | 1.479157 | 0.000140 |
| 34 | 1 | 0 | -1.487718 | 1.906869 | 0.021135 |
| 35 | 1 | 0 | 0.226871 | -1.562338 | 0.006997 |
| 36 | 1 | 0 | 2.727897 | 2.358065 | 0.002111 |
| 37 | 1 | 0 | 7.122893 | -1.995135 | -0.820104 |
| 38 | 1 | 0 | 6.820113 | -2.017169 | 0.923404 |
| 39 | 1 | 0 | 8.847826 | -0.871136 | 1.426524 |
| 40 | 1 | 0 | 5.154295 | 2.157978 | 0.011877 |
| 41 | 1 | 0 | 7.147069 | 1.663649 | -0.924474 |
| 42 | 1 | 0 | 7.458674 | 1.588237 | 0.815814 |
| 43 | 1 | 0 | -6.486245 | 4.540805 | 0.027426 |
| 44 | 1 | 0 | -6.136573 | 1.811425 | 0.007864 |
| 45 | 1 | 0 | -5.215200 | -5.318937 | -0.041241 |
| 46 | 1 | 0 | -6.504351 | -1.203505 | -0.017419 |
| 47 | 1 | 0 | 4.765215 | -2.137192 | -0.004053 |
| 48 | 1 | 0 | -3.910111 | 5.504641 | 0.040687 |
| 49 | 1 | 0 | -7.489923 | -3.772583 | -0.038056 |
| 50 | 1 | 0 | 9.385901 | -1.757848 | -0.005394 |
| 51 | 1 | 0 | 2.355845 | -1.916165 | 0.004729 |

**Lowest three frequencies:**

| | 1 | 2 | 3 |
|---|---|---|---|
| | A | A | A |
| Frequencies -- | 6.3298 | 20.6623 | 29.9539 |
| Red. masses -- | 3.3125 | 4.7983 | 5.6924 |
| Frc consts -- | 0.0001 | 0.0012 | 0.0030 |
| IR Inten -- | 0.0326 | 1.7650 | 0.6829 |

**Thermochemical data:**

| | | |
|---|---|---|
| Zero-point correction | = | 0.421202 (Hartree/Particle) |
| Thermal correction to Energy | = | 0.444914 |
| Thermal correction to Enthalpy | = | 0.445858 |
| Thermal correction to Gibbs Free Energy | = | 0.362730 |
| Sum of electronic and zero-point Energies | = | -1217.138500 |
| Sum of electronic and thermal Energies | = | -1217.114788 |
| Sum of electronic and thermal Enthalpies | = | -1217.113844 |
| Sum of electronic and thermal Free Energies | = | -1217.196972 |

**Compound IK– 4**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -5.799695 | 0.108827 | 0.073834 |
| 2 | 7 | 0 | -6.190126 | -2.167825 | -0.052225 |
| 3 | 7 | 0 | -5.768212 | -3.447522 | -0.166890 |
| 4 | 7 | 0 | -5.559398 | 2.405734 | 0.204253 |
| 5 | 6 | 0 | -5.265952 | -1.100265 | -0.039280 |
| 6 | 6 | 0 | -1.589830 | -0.515630 | -0.224242 |
| 7 | 6 | 0 | -3.027044 | -0.260340 | -0.121819 |
| 8 | 6 | 0 | -4.954151 | 1.134281 | 0.086767 |
| 9 | 6 | 0 | 3.081148 | 1.016157 | -0.022050 |
| 10 | 7 | 0 | 5.000248 | -0.369731 | -0.650131 |
| 11 | 6 | 0 | -3.577822 | 1.022176 | -0.009052 |
| 12 | 7 | 0 | -4.808338 | 3.529382 | 0.238061 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 6 | 0 | -0.625950 | 0.414658 | -0.131716 |
| 14 | 6 | 0 | 0.809915 | 0.191352 | -0.253910 |
| 15 | 6 | 0 | 1.352321 | -1.013582 | -0.730751 |
| 16 | 6 | 0 | 3.618551 | -0.185926 | -0.486794 |
| 17 | 6 | 0 | -8.027067 | -3.362622 | -0.013560 |
| 18 | 6 | 0 | -7.546143 | -2.081324 | 0.042283 |
| 19 | 6 | 0 | 2.712419 | -1.211258 | -0.863398 |
| 20 | 6 | 0 | 5.816421 | 0.838011 | -0.756313 |
| 21 | 6 | 0 | 1.705520 | 1.214570 | 0.087976 |
| 22 | 6 | 0 | -7.010769 | 4.037535 | 0.390407 |
| 23 | 6 | 0 | -6.874327 | -4.169408 | -0.143844 |
| 24 | 6 | 0 | -5.681525 | 4.514518 | 0.350276 |
| 25 | 6 | 0 | -3.905525 | -1.348152 | -0.139765 |
| 26 | 6 | 0 | -6.891107 | 2.676261 | 0.293958 |
| 27 | 6 | 0 | 5.604688 | -1.476690 | 0.103427 |
| 28 | 6 | 0 | 5.851878 | -1.183321 | 1.584498 |
| 29 | 6 | 0 | 7.180037 | 0.573217 | -1.392361 |
| 30 | 1 | 0 | 7.027978 | -0.053376 | -2.277959 |
| 31 | 1 | 0 | -3.547816 | -2.364329 | -0.227402 |
| 32 | 1 | 0 | -0.903559 | 1.445108 | 0.063263 |
| 33 | 1 | 0 | -2.974697 | 1.917712 | 0.000035 |
| 34 | 1 | 0 | -1.325443 | -1.559022 | -0.371793 |
| 35 | 1 | 0 | 6.547363 | -1.747699 | -0.380778 |
| 36 | 1 | 0 | 4.950154 | -2.341894 | 0.004758 |
| 37 | 1 | 0 | 4.910200 | -0.868925 | 2.051735 |
| 38 | 1 | 0 | 3.757440 | 1.801798 | 0.279774 |
| 39 | 1 | 0 | 5.271291 | 1.541039 | -1.393766 |
| 40 | 1 | 0 | 5.952023 | 1.335583 | 0.216316 |
| 41 | 1 | 0 | -7.921285 | 4.609470 | 0.477322 |
| 42 | 1 | 0 | -7.618039 | 1.881586 | 0.280297 |
| 43 | 1 | 0 | -6.813658 | -5.246389 | -0.221197 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 1 | 0 | -8.032997 | -1.125405 | 0.139464 |
| 45 | 1 | 0 | -5.333045 | 5.537122 | 0.399236 |
| 46 | 1 | 0 | -9.058034 | -3.676785 | 0.032406 |
| 47 | 1 | 0 | 0.671793 | -1.792660 | -1.046104 |
| 48 | 8 | 0 | 3.262757 | -2.346131 | -1.387974 |
| 49 | 8 | 0 | 1.158851 | 2.374133 | 0.547867 |
| 50 | 6 | 0 | 2.392585 | -3.383040 | -1.798930 |
| 51 | 1 | 0 | 1.720628 | -3.050804 | -2.597976 |
| 52 | 1 | 0 | 3.030440 | -4.181481 | -2.176563 |
| 53 | 1 | 0 | 1.794869 | -3.763715 | -0.963491 |
| 54 | 6 | 0 | 2.015940 | 3.458334 | 0.855545 |
| 55 | 1 | 0 | 2.692815 | 3.213185 | 1.680727 |
| 56 | 1 | 0 | 2.604747 | 3.764580 | -0.015404 |
| 57 | 1 | 0 | 1.366940 | 4.279384 | 1.157748 |
| 58 | 6 | 0 | 6.410702 | -2.397026 | 2.324100 |
| 59 | 6 | 0 | 7.912932 | 1.855727 | -1.794878 |
| 60 | 1 | 0 | 5.711475 | -3.236076 | 2.221672 |
| 61 | 1 | 0 | 8.817725 | 1.576047 | -2.345251 |
| 62 | 1 | 0 | 7.291471 | 2.422513 | -2.499045 |
| 63 | 1 | 0 | 7.342495 | -2.717357 | 1.841520 |
| 64 | 6 | 0 | 6.669977 | -2.126146 | 3.802869 |
| 65 | 1 | 0 | 7.066280 | -3.010837 | 4.308751 |
| 66 | 1 | 0 | 7.393207 | -1.314981 | 3.933765 |
| 67 | 1 | 0 | 5.748775 | -1.832838 | 4.316166 |
| 68 | 6 | 0 | 8.303526 | 2.752445 | -0.621348 |
| 69 | 1 | 0 | 8.908360 | 2.202609 | 0.107194 |
| 70 | 1 | 0 | 8.891089 | 3.609264 | -0.962189 |
| 71 | 1 | 0 | 7.428311 | 3.144614 | -0.096181 |
| 72 | 1 | 0 | 7.818659 | 0.004036 | -0.707315 |
| 73 | 1 | 0 | 6.549738 | -0.344226 | 1.694257 |

**Lowest three frequencies:**

| | 1 | 2 | 3 |
|---|---|---|---|
| | A | A | A |
| Frequencies -- | 6.1577 | 12.3758 | 22.7985 |
| Red. masses -- | 5.1482 | 4.7098 | 5.2397 |
| Frc consts -- | 0.0001 | 0.0004 | 0.0016 |
| IR Inten -- | 0.0067 | 0.1890 | 0.4026 |

**Thermochemical data:**

| | | |
|---|---|---|
| Zero-point correction | = | 0.622558 (Hartree/Particle) |
| Thermal correction to Energy | = | 0.658733 |
| Thermal correction to Enthalpy | = | 0.659677 |
| Thermal correction to Gibbs Free Energy | = | 0.547590 |
| Sum of electronic and zero-point Energies | = | -1604.252235 |
| Sum of electronic and thermal Energies | = | -1604.216060 |
| Sum of electronic and thermal Enthalpies | = | -1604.215116 |
| Sum of electronic and thermal Free Energies | = | -1604.327203 |

**Compound IK– 5**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -4.795925 | -0.003279 | 0.023382 |
| 2 | 7 | 0 | -5.122782 | -2.291205 | 0.122589 |
| 3 | 7 | 0 | -4.665236 | -3.562835 | 0.165269 |
| 4 | 7 | 0 | -4.617880 | 2.300912 | -0.077632 |
| 5 | 6 | 0 | -4.226334 | -1.200836 | 0.065308 |
| 6 | 6 | 0 | -0.561435 | -0.530988 | -0.012689 |
| 7 | 6 | 0 | -2.005509 | -0.309118 | -0.003060 |
| 8 | 6 | 0 | -3.976253 | 1.041891 | -0.032836 |
| 9 | 6 | 0 | 4.047670 | 1.217584 | 0.038717 |
| 10 | 7 | 0 | 6.024439 | -0.155496 | -0.110158 |
| 11 | 6 | 0 | -2.595118 | 0.961374 | -0.050703 |
| 12 | 7 | 0 | -3.898127 | 3.443650 | -0.137753 |
| 13 | 6 | 0 | 0.374074 | 0.435201 | -0.031064 |

| | | | | | |
|---|---|---|---|---|---|
| 14 | 6 | 0 | 1.816237 | 0.256108 | -0.056340 |
| 15 | 6 | 0 | 2.429342 | -1.001661 | -0.208660 |
| 16 | 6 | 0 | 4.654702 | -0.040334 | -0.086684 |
| 17 | 6 | 0 | -6.930305 | -3.528529 | 0.198584 |
| 18 | 6 | 0 | -6.483354 | -2.234880 | 0.141205 |
| 19 | 6 | 0 | 3.796149 | -1.165692 | -0.242025 |
| 20 | 6 | 0 | 6.871233 | 1.035033 | -0.105500 |
| 21 | 6 | 0 | 2.663496 | 1.369358 | 0.051667 |
| 22 | 6 | 0 | -6.117130 | 3.899258 | -0.123359 |
| 23 | 6 | 0 | -5.753585 | -4.310466 | 0.211185 |
| 24 | 6 | 0 | -4.800240 | 4.408731 | -0.165465 |
| 25 | 6 | 0 | -2.857536 | -1.417769 | 0.055530 |
| 26 | 6 | 0 | -5.958465 | 2.539564 | -0.067314 |
| 27 | 6 | 0 | 6.776642 | -1.339626 | 0.348011 |
| 28 | 6 | 0 | 8.137649 | -0.775377 | 0.761284 |
| 29 | 6 | 0 | 8.285349 | 0.467610 | -0.114740 |
| 30 | 1 | 0 | 8.570872 | 0.186407 | -1.133180 |
| 31 | 1 | 0 | 9.020905 | 1.181321 | 0.260945 |
| 32 | 1 | 0 | -2.472088 | -2.426910 | 0.093300 |
| 33 | 1 | 0 | 0.055639 | 1.472275 | -0.020380 |
| 34 | 1 | 0 | -2.016116 | 1.871132 | -0.102812 |
| 35 | 1 | 0 | -0.264615 | -1.575947 | 0.004924 |
| 36 | 1 | 0 | 6.876280 | -2.069128 | -0.459725 |
| 37 | 1 | 0 | 6.263925 | -1.834822 | 1.174910 |
| 38 | 1 | 0 | 8.121087 | -0.484402 | 1.816425 |
| 39 | 1 | 0 | 4.675499 | 2.087680 | 0.147901 |
| 40 | 1 | 0 | 6.654634 | 1.668054 | -0.971743 |
| 41 | 1 | 0 | 6.710218 | 1.641542 | 0.799224 |
| 42 | 1 | 0 | -7.044918 | 4.449574 | -0.132845 |
| 43 | 1 | 0 | -6.663597 | 1.726681 | -0.021409 |
| 44 | 1 | 0 | -5.663207 | -5.387384 | 0.251872 |

| | | | | | |
|---|---|---|---|---|---|
| 45 | 1 | 0 | -6.997109 | -1.288614 | 0.111813 |
| 46 | 1 | 0 | -4.480385 | 5.440640 | -0.214804 |
| 47 | 1 | 0 | -7.954532 | -3.865951 | 0.227434 |
| 48 | 1 | 0 | 8.941170 | -1.502269 | 0.626489 |
| 49 | 1 | 0 | 1.795226 | -1.868032 | -0.338783 |
| 50 | 8 | 0 | 4.409870 | -2.368648 | -0.463652 |
| 51 | 8 | 0 | 2.059348 | 2.582182 | 0.185998 |
| 52 | 6 | 0 | 3.596701 | -3.513561 | -0.618073 |
| 53 | 1 | 0 | 2.936410 | -3.424876 | -1.488271 |
| 54 | 1 | 0 | 4.276936 | -4.351244 | -0.769371 |
| 55 | 1 | 0 | 2.988069 | -3.700146 | 0.273937 |
| 56 | 6 | 0 | 2.863067 | 3.744675 | 0.266674 |
| 57 | 1 | 0 | 3.506358 | 3.727715 | 1.152731 |
| 58 | 1 | 0 | 3.483428 | 3.867101 | -0.627292 |
| 59 | 1 | 0 | 2.172479 | 4.583804 | 0.342143 |

**Lowest three frequencies:**

| | 1 | 2 | 3 |
|---|---|---|---|
| | A | A | A |
| Frequencies -- | 8.5125 | 21.2961 | 26.9666 |
| Red. masses -- | 4.9587 | 4.9927 | 5.5816 |
| Frc consts -- | 0.0002 | 0.0013 | 0.0024 |
| IR Inten -- | 0.0237 | 1.1738 | 0.7312 |

**Thermochemical data:**

| | | |
|---|---|---|
| Zero-point correction | = | 0.487251 (Hartree/Particle) |
| Thermal correction to Energy | = | 0.516132 |
| Thermal correction to Enthalpy | = | 0.517076 |
| Thermal correction to Gibbs Free Energy | = | 0.423386 |
| Sum of electronic and zero-point Energies | = | -1446.025069 |
| Sum of electronic and thermal Energies | = | -1445.996188 |
| Sum of electronic and thermal Enthalpies | = | -1445.995244 |
| Sum of electronic and thermal Free Energies | = | -1446.088934 |

**Compound IK–6**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | -9.269610 | -0.035423 | 0.074597 |
| 2 | 7 | 0 | -9.614156 | -2.315927 | -0.102444 |
| 3 | 7 | 0 | -9.163097 | -3.587307 | -0.200193 |
| 4 | 7 | 0 | -9.077004 | 2.262457 | 0.257851 |
| 5 | 6 | 0 | -8.711455 | -1.234588 | -0.019415 |
| 6 | 6 | 0 | -5.041075 | -0.589058 | 0.025953 |
| 7 | 6 | 0 | -6.488143 | -0.357332 | 0.045982 |
| 8 | 6 | 0 | -8.445229 | 1.003651 | 0.156021 |
| 9 | 6 | 0 | -0.432079 | 1.159183 | -0.032478 |
| 10 | 6 | 0 | -7.063385 | 0.914035 | 0.148316 |
| 11 | 7 | 0 | -8.346975 | 3.397152 | 0.347862 |
| 12 | 6 | 0 | -4.097680 | 0.362837 | 0.037345 |
| 13 | 6 | 0 | -2.647896 | 0.159959 | 0.020540 |
| 14 | 6 | 0 | -2.041055 | -1.102487 | 0.044012 |
| 15 | 6 | 0 | 0.176582 | -0.103153 | -0.017102 |
| 16 | 6 | 0 | -11.428374 | -3.541743 | -0.195139 |
| 17 | 6 | 0 | -10.975079 | -2.253239 | -0.096672 |
| 18 | 6 | 0 | -0.663377 | -1.226096 | 0.026202 |
| 19 | 6 | 0 | -1.810150 | 1.283218 | -0.015404 |
| 20 | 6 | 0 | -10.562519 | 3.868472 | 0.388790 |
| 21 | 6 | 0 | -10.255400 | -4.327753 | -0.256228 |
| 22 | 6 | 0 | -9.240787 | 4.366627 | 0.426907 |
| 23 | 6 | 0 | -7.342551 | -1.459486 | -0.037995 |
| 24 | 6 | 0 | -10.416107 | 2.511003 | 0.279722 |
| 25 | 1 | 0 | -6.963039 | -2.468427 | -0.117087 |

| | | | | | |
|---|---|---|---|---|---|
| 26 | 1 | 0 | -4.403433 | 1.406141 | 0.055615 |
| 27 | 1 | 0 | -6.477412 | 1.817667 | 0.224910 |
| 28 | 1 | 0 | -4.751495 | -1.635444 | -0.006949 |
| 29 | 1 | 0 | -2.255357 | 2.273774 | -0.027061 |
| 30 | 1 | 0 | 0.175831 | 2.056929 | -0.051418 |
| 31 | 1 | 0 | -11.485449 | 4.425026 | 0.434858 |
| 32 | 1 | 0 | -11.128617 | 1.705730 | 0.216136 |
| 33 | 1 | 0 | -10.171064 | -5.402740 | -0.338709 |
| 34 | 1 | 0 | -11.484269 | -1.306835 | -0.023559 |
| 35 | 1 | 0 | -0.218123 | -2.21 6408 | 0.045497 |
| 36 | 1 | 0 | -8.912269 | 5.393697 | 0.508890 |
| 37 | 1 | 0 | -12.454397 | -3.873912 | -0.219916 |
| 38 | 1 | 0 | -2.647804 | -2.000666 | 0.080390 |
| 39 | 6 | 0 | 1.627749 | -0.305604 | -0.038847 |
| 40 | 1 | 0 | 1.937224 | -1.343602 | 0.059728 |
| 41 | 6 | 0 | 2.559238 | 0.648963 | -0.181372 |
| 42 | 1 | 0 | 2.252173 | 1.681770 | -0.311260 |
| 43 | 6 | 0 | 4.009126 | 0.456021 | -0.193018 |
| 44 | 6 | 0 | 4.625469 | -0.768705 | 0.123972 |
| 45 | 6 | 0 | 4.845283 | 1.522516 | -0.523886 |
| 46 | 6 | 0 | 5.997793 | -0.930237 | 0.087459 |
| 47 | 1 | 0 | 4.000714 | -1.611097 | 0.387656 |
| 48 | 6 | 0 | 6.230378 | 1.376425 | -0.533880 |
| 49 | 6 | 0 | 6.845239 | 0.164725 | -0.232800 |
| 50 | 1 | 0 | 6.830952 | 2.248837 | -0.761089 |
| 51 | 6 | 0 | 8.991314 | 0.896389 | -1.137490 |
| 52 | 6 | 0 | 8.883207 | -0.366989 | 0.991284 |
| 53 | 6 | 0 | 10.325162 | 0.339245 | -1.640130 |
| 54 | 1 | 0 | 9.179249 | 1.865740 | -0.648110 |
| 55 | 1 | 0 | 8.367087 | 1.106879 | -2.010521 |
| 56 | 6 | 0 | 9.016569 | 0.792720 | 1.983497 |

| | | | | | |
|---|---|---|---|---|---|
| 57 | 1 | 0 | 9.864753 | -0.788581 | 0.764216 |
| 58 | 1 | 0 | 8.302944 | -1.170843 | 1.446298 |
| 59 | 1 | 0 | 10.800505 | 1.158850 | -2.191196 |
| 60 | 1 | 0 | 8.030547 | 1.252869 | 2.116181 |
| 61 | 7 | 0 | 8.238451 | -0.014997 | -0.280056 |
| 62 | 8 | 0 | 6.621522 | -2.117535 | 0.332505 |
| 63 | 8 | 0 | 4.305198 | 2.761672 | -0.798197 |
| 64 | 6 | 0 | 5.823291 | -3.248813 | 0.627858 |
| 65 | 1 | 0 | 5.244764 | -3.104817 | 1.546637 |
| 66 | 1 | 0 | 5.138828 | -3.481893 | -0.194827 |
| 67 | 1 | 0 | 6.515242 | -4.078696 | 0.766056 |
| 68 | 6 | 0 | 4.240147 | 3.076662 | -2.184321 |
| 69 | 1 | 0 | 5.233926 | 3.054282 | -2.644408 |
| 70 | 1 | 0 | 3.585941 | 2.376719 | -2.716349 |
| 71 | 1 | 0 | 3.830679 | 4.084405 | -2.261331 |
| 72 | 6 | 0 | 10.231562 | -0.881684 | -2.562890 |
| 73 | 6 | 0 | 9.556421 | 0.357188 | 3.348232 |
| 74 | 1 | 0 | 10.997552 | 0.122513 | -0.801913 |
| 75 | 1 | 0 | 9.671281 | 1.570849 | 1.572530 |
| 76 | 1 | 0 | 9.449809 | -0.700133 | -3.311565 |
| 77 | 1 | 0 | 11.170844 | -0.957330 | -3.122956 |
| 78 | 1 | 0 | 9.493075 | 1.206504 | 4.037398 |
| 79 | 1 | 0 | 8.902526 | -0.420053 | 3.763355 |
| 80 | 6 | 0 | 9.970489 | -2.215487 | -1.864554 |
| 81 | 1 | 0 | 9.965491 | -3.037062 | -2.587464 |
| 82 | 1 | 0 | 10.754964 | -2.429901 | -1.130649 |
| 83 | 1 | 0 | 9.012996 | -2.208871 | -1.340932 |
| 84 | 6 | 0 | 10.996800 | -0.151425 | 3.317973 |
| 85 | 1 | 0 | 11.353003 | -0.383903 | 4.325342 |
| 86 | 1 | 0 | 11.097323 | -1.060145 | 2.718118 |
| 87 | 1 | 0 | 11.668600 | 0.601647 | 2.893010 |

**Lowest three frequencies:**

| | 1 | 2 | 3 |
|---|---|---|---|
| | A | A | A |
| Frequencies -- | 2.7911 | 9.5522 | 12.0621 |
| Red. masses -- | 4.9267 | 5.4086 | 3.6213 |
| Frc consts -- | 0.0000 | 0.0003 | 0.0003 |
| IR Inten -- | 0.0703 | 0.0681 | 0.7275 |

**Thermochemical data:**

| | | |
|---|---|---|
| Zero-point correction | = | 0.738025 (Hartree/Particle) |
| Thermal correction to Energy | = | 0.781261 |
| Thermal correction to Enthalpy | = | 0.782205 |
| Thermal correction to Gibbs Free Energy | = | 0.650558 |
| Sum of electronic and zero-point Energies | = | -1912.420040 |
| Sum of electronic and thermal Energies | = | -1912.376804 |
| Sum of electronic and thermal Enthalpies | = | -1912.375860 |
| Sum of electronic and thermal Free Energies | = | -1912.507507 |

**Compound IK–7**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 7.318921 | 0.055647 | 0.003822 |
| 2 | 7 | 0 | 7.703582 | -2.224390 | 0.067321 |
| 3 | 7 | 0 | 7.275495 | -3.507177 | 0.090487 |
| 4 | 7 | 0 | 7.086313 | 2.356048 | -0.064043 |
| 5 | 6 | 0 | 6.781855 | -1.156632 | 0.025611 |
| 6 | 6 | 0 | 3.101139 | -0.575023 | -0.043458 |
| 7 | 6 | 0 | 4.543546 | -0.317196 | -0.029703 |
| 8 | 6 | 0 | 6.476449 | 1.082521 | -0.037385 |
| 9 | 6 | 0 | -1.538797 | 1.085420 | 0.108240 |
| 10 | 6 | 0 | 5.096666 | 0.967881 | -0.057663 |

| | | | | | |
|---|---|---|---|---|---|
| 11 | 7 | 0 | 6.337145 | 3.481081 | -0.103392 |
| 12 | 6 | 0 | 2.140815 | 0.358808 | 0.008644 |
| 13 | 6 | 0 | 0.695170 | 0.131568 | -0.006432 |
| 14 | 6 | 0 | 0.109762 | -1.134209 | -0.140683 |
| 15 | 6 | 0 | -2.127219 | -0.180378 | -0.023762 |
| 16 | 6 | 0 | 9.539238 | -3.420003 | 0.127751 |
| 17 | 6 | 0 | 9.062936 | -2.136590 | 0.088907 |
| 18 | 6 | 0 | -1.265447 | -1.281490 | -0.148120 |
| 19 | 6 | 0 | -0.163021 | 1.233159 | 0.115456 |
| 20 | 6 | 0 | 8.544219 | 3.992204 | -0.091149 |
| 21 | 6 | 0 | 8.380737 | -4.229450 | 0.126926 |
| 22 | 6 | 0 | 7.214313 | 4.468728 | -0.119847 |
| 23 | 6 | 0 | 5.417396 | -1.406733 | 0.009793 |
| 24 | 6 | 0 | 8.420841 | 2.628508 | -0.055650 |
| 25 | 1 | 0 | 5.055492 | -2.424993 | 0.030059 |
| 26 | 1 | 0 | 2.428807 | 1.405277 | 0.075574 |
| 27 | 1 | 0 | 4.494873 | 1.863354 | -0.099792 |
| 28 | 1 | 0 | 2.830033 | -1.625779 | -0.091128 |
| 29 | 1 | 0 | 0.264573 | 2.226297 | 0.218276 |
| 30 | 1 | 0 | -2.160143 | 1.968859 | 0.205134 |
| 31 | 1 | 0 | 9.457505 | 4.566275 | -0.096001 |
| 32 | 1 | 0 | 9.146715 | 1.833281 | -0.025593 |
| 33 | 1 | 0 | 8.315658 | -5.308652 | 0.151574 |
| 34 | 1 | 0 | 9.555035 | -1.178500 | 0.074568 |
| 35 | 1 | 0 | -1.692974 | -2.274078 | -0.254832 |
| 36 | 1 | 0 | 6.868376 | 5.492855 | -0.151709 |
| 37 | 1 | 0 | 10.570902 | -3.734164 | 0.153257 |
| 38 | 1 | 0 | 0.732128 | -2.016352 | -0.245001 |
| 39 | 6 | 0 | -3.573320 | -0.410625 | -0.041968 |
| 40 | 1 | 0 | -3.860433 | -1.452699 | -0.161925 |
| 41 | 6 | 0 | -4.532119 | 0.522213 | 0.072571 |

| | | | | | |
|---|---|---|---|---|---|
| 42 | 1 | 0 | -4.236557 | 1.562498 | 0.194603 |
| 43 | 6 | 0 | -5.977892 | 0.311856 | 0.053026 |
| 44 | 6 | 0 | -6.585036 | -0.943663 | -0.101222 |
| 45 | 6 | 0 | -6.833811 | 1.411914 | 0.192485 |
| 46 | 6 | 0 | -7.957593 | -1.094293 | -0.115638 |
| 47 | 1 | 0 | -5.971547 | -1.832281 | -0.210313 |
| 48 | 6 | 0 | -8.211379 | 1.284724 | 0.178874 |
| 49 | 1 | 0 | -6.402505 | 2.402377 | 0.311459 |
| 50 | 6 | 0 | -8.813895 | 0.020489 | 0.023063 |
| 51 | 1 | 0 | -8.377393 | -2.086652 | -0.225791 |
| 52 | 1 | 0 | -8.826066 | 2.170791 | 0.278981 |
| 53 | 6 | 0 | -11.103963 | 0.971338 | 0.243545 |
| 54 | 6 | 0 | -10.848031 | -1.387243 | -0.266832 |
| 55 | 6 | 0 | -12.451588 | 0.266218 | 0.402085 |
| 56 | 1 | 0 | -11.114569 | 1.673743 | -0.602351 |
| 57 | 1 | 0 | -10.826397 | 1.538754 | 1.138081 |
| 58 | 6 | 0 | -12.304382 | -0.973810 | -0.482001 |
| 59 | 1 | 0 | -10.748282 | -2.083268 | 0.578357 |
| 60 | 1 | 0 | -10.424111 | -1.878419 | -1.148897 |
| 61 | 1 | 0 | -12.593257 | -0.031125 | 1.445652 |
| 62 | 1 | 0 | -13.290261 | 0.903951 | 0.116879 |
| 63 | 1 | 0 | -13.004539 | -1.771765 | -0.228103 |
| 64 | 1 | 0 | -12.462533 | -0.707497 | -1.531563 |
| 65 | 7 | 0 | -10.172035 | -0.124546 | 0.006913 |

**Lowest three frequencies:**

| | 1 | 2 | 3 |
|---|---|---|---|
| | A | A | A |
| Frequencies -- | 8.7766 | 10.2079 | 13.5772 |
| Red. masses -- | 3.8467 | 4.2616 | 3.8630 |
| Frc consts -- | 0.0002 | 0.0003 | 0.0004 |
| IR Inten -- | 0.0853 | 0.1163 | 0.3876 |

**Thermochemical data:**

| | | |
|---|---|---|
| Zero-point correction | = | 0.536843 (Hartree/Particle) |
| Thermal correction to Energy | = | 0.567651 |
| Thermal correction to Enthalpy | = | 0.568595 |
| Thermal correction to Gibbs Free Energy | = | 0.467002 |
| Sum of electronic and zero-point Energies | = | -1525.310704 |
| Sum of electronic and thermal Energies | = | -1525.279896 |
| Sum of electronic and thermal Enthalpies | = | -1525.278952 |
| Sum of electronic and thermal Free Energies | = | -1525.380545 |

**Compound IK–8**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 8.926507 | 0.226262 | 0.246903 |
| 2 | 7 | 0 | 9.233800 | 2.389106 | -0.514096 |
| 3 | 7 | 0 | 8.761664 | 3.584336 | -0.935706 |
| 4 | 7 | 0 | 8.771614 | -1.949434 | 1.017230 |
| 5 | 6 | 0 | 8.348859 | 1.353109 | -0.146802 |
| 6 | 6 | 0 | 4.689433 | 0.685778 | 0.094724 |
| 7 | 6 | 0 | 6.140498 | 0.491172 | 0.162355 |
| 8 | 6 | 0 | 8.119206 | -0.768252 | 0.600970 |
| 9 | 6 | 0 | 0.111489 | -1.088702 | 0.254731 |
| 10 | 6 | 0 | 6.736155 | -0.702231 | 0.584992 |
| 11 | 7 | 0 | 8.060374 | -3.036375 | 1.392997 |
| 12 | 6 | 0 | 3.768239 | -0.260155 | 0.325285 |

| | | | | | |
|---|---|---|---|---|---|
| 13 | 6 | 0 | 2.317440 | -0.085734 | 0.272110 |
| 14 | 6 | 0 | 1.702331 | 1.174780 | 0.227178 |
| 15 | 6 | 0 | -0.508893 | 0.156954 | 0.184185 |
| 16 | 6 | 0 | 11.027385 | 3.575759 | -0.935444 |
| 17 | 6 | 0 | 10.595524 | 2.350483 | -0.502176 |
| 18 | 6 | 0 | 0.323047 | 1.301659 | 0.176685 |
| 19 | 6 | 0 | 1.492666 | -1.217587 | 0.292561 |
| 20 | 6 | 0 | 10.283345 | -3.444090 | 1.550091 |
| 21 | 6 | 0 | 9.841516 | 4.301114 | -1.190227 |
| 22 | 6 | 0 | 8.969996 | -3.938658 | 1.714772 |
| 23 | 6 | 0 | 6.976517 | 1.546612 | -0.210099 |
| 24 | 6 | 0 | 10.114601 | -2.161493 | 1.100092 |
| 25 | 1 | 0 | 6.580481 | 2.495537 | -0.543396 |
| 26 | 1 | 0 | 4.083107 | -1.270511 | 0.565247 |
| 27 | 1 | 0 | 6.163252 | -1.561407 | 0.900426 |
| 28 | 1 | 0 | 4.379236 | 1.688662 | -0.185440 |
| 29 | 1 | 0 | -0.486816 | -1.991195 | 0.311001 |
| 30 | 1 | 0 | 11.215314 | -3.954885 | 1.735015 |
| 31 | 1 | 0 | 10.813743 | -1.386610 | 0.833769 |
| 32 | 1 | 0 | 9.739302 | 5.316252 | -1.548784 |
| 33 | 1 | 0 | 11.120273 | 1.463258 | -0.189559 |
| 34 | 1 | 0 | 8.658363 | -4.916759 | 2.054971 |
| 35 | 1 | 0 | 12.047757 | 3.905397 | -1.053155 |
| 36 | 1 | 0 | 2.322923 | 2.060109 | 0.244247 |
| 37 | 6 | 0 | -1.964192 | 0.317987 | 0.147926 |
| 38 | 1 | 0 | -2.322103 | 1.308935 | 0.406035 |
| 39 | 6 | 0 | -2.836329 | -0.640544 | -0.199217 |
| 40 | 1 | 0 | -2.466879 | -1.606919 | -0.528781 |
| 41 | 6 | 0 | -4.294913 | -0.523669 | -0.204659 |
| 42 | 6 | 0 | -4.981216 | 0.539706 | 0.409140 |
| 43 | 6 | 0 | -5.066306 | -1.505038 | -0.826971 |

| | | | | | |
|---|---|---|---|---|---|
| 44 | 6 | 0 | -6.360666 | 0.635646 | 0.380669 |
| 45 | 1 | 0 | -4.405406 | 1.306946 | 0.908513 |
| 46 | 6 | 0 | -6.456710 | -1.431471 | -0.834885 |
| 47 | 6 | 0 | -7.141461 | -0.376010 | -0.239386 |
| 48 | 1 | 0 | -7.003736 | -2.241066 | -1.302575 |
| 49 | 6 | 0 | -9.233846 | -0.954094 | -1.354045 |
| 50 | 6 | 0 | -9.210709 | -0.317065 | 1.039670 |
| 51 | 6 | 0 | -10.597865 | -0.363276 | -1.718355 |
| 52 | 1 | 0 | -9.362159 | -2.028907 | -1.146762 |
| 53 | 1 | 0 | -8.593461 | -0.884608 | -2.238022 |
| 54 | 6 | 0 | -9.256784 | -1.709498 | 1.676716 |
| 55 | 1 | 0 | -10.220902 | 0.079970 | 0.918273 |
| 56 | 1 | 0 | -8.688945 | 0.371380 | 1.706129 |
| 57 | 1 | 0 | -11.017367 | -1.031520 | -2.479169 |
| 58 | 1 | 0 | -8.240513 | -2.119822 | 1.689085 |
| 59 | 7 | 0 | -8.543842 | -0.263424 | -0.267941 |
| 60 | 8 | 0 | -7.052270 | 1.679518 | 0.920240 |
| 61 | 8 | 0 | -4.457320 | -2.598359 | -1.408003 |
| 62 | 6 | 0 | -6.320672 | 2.727396 | 1.529281 |
| 63 | 1 | 0 | -5.745417 | 2.369487 | 2.389861 |
| 64 | 1 | 0 | -5.640457 | 3.207443 | 0.817569 |
| 65 | 1 | 0 | -7.058483 | 3.453794 | 1.867836 |
| 66 | 6 | 0 | -4.282945 | -2.485098 | -2.815527 |
| 67 | 1 | 0 | -5.243635 | -2.349010 | -3.324159 |
| 68 | 1 | 0 | -3.626082 | -1.644003 | -3.064562 |
| 69 | 1 | 0 | -3.824289 | -3.414661 | -3.154465 |
| 70 | 6 | 0 | -10.576506 | 1.064356 | -2.277380 |
| 71 | 6 | 0 | -9.813396 | -1.702037 | 3.102807 |
| 72 | 1 | 0 | -11.287101 | -0.419946 | -0.867804 |
| 73 | 1 | 0 | -9.859959 | -2.388525 | 1.061912 |
| 74 | 1 | 0 | -9.776306 | 1.139487 | -3.024696 |

| | | | | | |
|---|---|---|---|---|---|
| 75 | 1 | 0 | -11.512802 | 1.230725 | -2.822609 |
| 76 | 1 | 0 | -9.682000 | -2.699983 | 3.535455 |
| 77 | 1 | 0 | -9.213303 | -1.021933 | 3.720414 |
| 78 | 6 | 0 | -10.411957 | 2.173022 | -1.238883 |
| 79 | 1 | 0 | -10.454503 | 3.158444 | -1.712961 |
| 80 | 1 | 0 | -11.216066 | 2.131689 | -0.496127 |
| 81 | 1 | 0 | -9.461274 | 2.083159 | -0.710663 |
| 82 | 6 | 0 | -11.286991 | -1.310070 | 3.198033 |
| 83 | 1 | 0 | -11.648636 | -1.387933 | 4.227058 |
| 84 | 1 | 0 | -11.459431 | -0.281794 | 2.868474 |
| 85 | 1 | 0 | -11.906907 | -1.965127 | 2.577049 |
| 86 | 8 | 0 | -0.320121 | 2.498481 | 0.121526 |
| 87 | 8 | 0 | 2.050255 | -2.471469 | 0.399427 |
| 88 | 6 | 0 | 0.445385 | 3.697762 | 0.141371 |
| 89 | 6 | 0 | -0.519878 | 4.864144 | 0.078669 |
| 90 | 1 | 0 | 1.131302 | 3.715433 | -0.715361 |
| 91 | 1 | 0 | 1.048263 | 3.740347 | 1.057683 |
| 92 | 6 | 0 | 0.197992 | 6.211832 | 0.089305 |
| 93 | 1 | 0 | -1.127062 | 4.770699 | -0.828722 |
| 94 | 1 | 0 | -1.207519 | 4.799684 | 0.929472 |
| 95 | 6 | 0 | -0.768752 | 7.390087 | 0.026524 |
| 96 | 1 | 0 | 0.812718 | 6.289837 | 0.994050 |
| 97 | 1 | 0 | 0.892103 | 6.261219 | -0.758209 |
| 98 | 1 | 0 | -0.234533 | 8.343694 | 0.036070 |
| 99 | 1 | 0 | -1.373622 | 7.354817 | -0.884846 |
| 100 | 1 | 0 | -1.454275 | 7.382278 | 0.879559 |
| 101 | 6 | 0 | 2.183186 | -3.174049 | -0.840589 |
| 102 | 6 | 0 | 2.781616 | -4.535350 | -0.554499 |
| 103 | 1 | 0 | 2.826018 | -2.597915 | -1.519695 |
| 104 | 1 | 0 | 1.197970 | -3.271074 | -1.314844 |
| 105 | 6 | 0 | 2.969226 | -5.366907 | -1.821360 |

| | | | | | |
|---|---|---|---|---|---|
| 106 | 1 | 0 | 3.745834 | -4.398738 | -0.051153 |
| 107 | 1 | 0 | 2.129499 | -5.065625 | 0.148928 |
| 108 | 6 | 0 | 3.569842 | -6.740255 | -1.537963 |
| 109 | 1 | 0 | 2.002230 | -5.486543 | -2.324675 |
| 110 | 1 | 0 | 3.613832 | -4.822357 | -2.521720 |
| 111 | 1 | 0 | 3.693744 | -7.318032 | -2.457686 |
| 112 | 1 | 0 | 4.552632 | -6.650063 | -1.065018 |
| 113 | 1 | 0 | 2.929824 | -7.318015 | -0.863938 |

**Lowest three frequencies:**

| | 1 | 2 | 3 |
|---|---|---|---|
| | A | A | A |
| Frequencies -- | 3.4096 | 5.0810 | 7.4956 |
| Red. masses -- | 5.9764 | 4.1023 | 5.2850 |
| Frc consts -- | 0.0000 | 0.0001 | 0.0002 |
| IR Inten -- | 0.0249 | 0.0828 | 0.0610 |

**Thermochemical data:**

| | | |
|---|---|---|
| Zero-point correction | = | 0.975508 (Hartree/Particle) |
| Thermal correction to Energy | = | 1.032462 |
| Thermal correction to Enthalpy | = | 1.033406 |
| Thermal correction to Gibbs Free Energy | = | 0.868267 |
| Sum of electronic and zero-point Energies | = | -2376.898800 |
| Sum of electronic and thermal Energies | = | -2376.841846 |
| Sum of electronic and thermal Enthalpies | = | -2376.840902 |
| Sum of electronic and thermal Free Energies | = | -2377.006040 |

**Compound IK– 9**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 7.995041 | 0.227252 | -0.208266 |
| 2 | 7 | 0 | 8.293592 | 2.485573 | 0.194750 |
| 3 | 7 | 0 | 7.817097 | 3.729719 | 0.427780 |
| 4 | 7 | 0 | 7.848116 | -2.044636 | -0.618097 |
| 5 | 6 | 0 | 7.412851 | 1.397561 | 0.015345 |
| 6 | 6 | 0 | 3.756630 | 0.675192 | -0.046230 |
| 7 | 6 | 0 | 5.207711 | 0.481329 | -0.108983 |
| 8 | 6 | 0 | 7.191363 | -0.816767 | -0.382743 |
| 9 | 6 | 0 | -0.816544 | -1.125692 | -0.056233 |
| 10 | 6 | 0 | 5.808404 | -0.759702 | -0.347879 |
| 11 | 7 | 0 | 7.141445 | -3.182959 | -0.800366 |
| 12 | 6 | 0 | 2.836641 | -0.289441 | -0.189025 |
| 13 | 6 | 0 | 1.385849 | -0.117161 | -0.144648 |
| 14 | 6 | 0 | 0.764616 | 1.141262 | -0.161234 |
| 15 | 6 | 0 | -1.444683 | 0.118574 | -0.072596 |
| 16 | 6 | 0 | 10.082425 | 3.737061 | 0.386069 |
| 17 | 6 | 0 | 9.655190 | 2.455113 | 0.163215 |
| 18 | 6 | 0 | -0.614843 | 1.265009 | -0.118726 |
| 19 | 6 | 0 | 0.564561 | -1.250867 | -0.098767 |
| 20 | 6 | 0 | 9.365205 | -3.594218 | -0.935103 |
| 21 | 6 | 0 | 8.894103 | 4.485617 | 0.543495 |
| 22 | 6 | 0 | 8.054300 | -4.118486 | -0.991670 |
| 23 | 6 | 0 | 6.040095 | 1.587938 | 0.077352 |
| 24 | 6 | 0 | 9.191412 | -2.257281 | -0.693093 |
| 25 | 1 | 0 | 5.640647 | 2.574590 | 0.265318 |
| 26 | 1 | 0 | 3.153431 | -1.314753 | -0.350134 |

| | | | | | |
|---|---|---|---|---|---|
| 27 | 1 | 0 | 5.239850 | -1.664010 | -0.505272 |
| 28 | 1 | 0 | 3.444801 | 1.698898 | 0.141172 |
| 29 | 1 | 0 | -1.407556 | -2.033115 | -0.002305 |
| 30 | 1 | 0 | 10.298858 | -4.121177 | -1.054649 |
| 31 | 1 | 0 | 9.887046 | -1.444429 | -0.568313 |
| 32 | 1 | 0 | 8.788104 | 5.544463 | 0.736195 |
| 33 | 1 | 0 | 10.183135 | 1.532898 | -0.013064 |
| 34 | 1 | 0 | 7.746663 | -5.140773 | -1.164321 |
| 35 | 1 | 0 | 11.101391 | 4.088434 | 0.429897 |
| 36 | 1 | 0 | 1.380437 | 2.027585 | -0.227411 |
| 37 | 6 | 0 | -2.899295 | 0.280177 | -0.039298 |
| 38 | 1 | 0 | -3.240255 | 1.282144 | 0.196707 |
| 39 | 6 | 0 | -3.792949 | -0.688202 | -0.297640 |
| 40 | 1 | 0 | -3.443693 | -1.673522 | -0.591336 |
| 41 | 6 | 0 | -5.247133 | -0.567336 | -0.242508 |
| 42 | 6 | 0 | -5.910249 | 0.568757 | 0.261807 |
| 43 | 6 | 0 | -6.052204 | -1.609067 | -0.701338 |
| 44 | 6 | 0 | -7.285724 | 0.669262 | 0.291740 |
| 45 | 1 | 0 | -5.315469 | 1.396522 | 0.623350 |
| 46 | 6 | 0 | -7.440957 | -1.534391 | -0.650862 |
| 47 | 6 | 0 | -8.103154 | -0.413894 | -0.142694 |
| 48 | 1 | 0 | -8.001350 | -2.391837 | -0.999317 |
| 49 | 6 | 0 | -10.276317 | -1.419390 | -0.703898 |
| 50 | 6 | 0 | -10.247899 | 0.352261 | 0.937962 |
| 51 | 6 | 0 | -11.710373 | -1.004233 | -0.402879 |
| 52 | 1 | 0 | -10.058218 | -2.393100 | -0.237079 |
| 53 | 1 | 0 | -10.066341 | -1.512168 | -1.774144 |
| 54 | 6 | 0 | -11.579159 | -0.403043 | 0.996188 |
| 55 | 1 | 0 | -10.395115 | 1.402141 | 0.672921 |
| 56 | 1 | 0 | -9.718418 | 0.328536 | 1.893586 |
| 57 | 1 | 0 | -12.039934 | -0.244247 | -1.118237 |

| | | | | | |
|---|---|---|---|---|---|
| 58 | 1 | 0 | -12.405930 | -1.844199 | -0.452232 |
| 59 | 1 | 0 | -12.410402 | 0.249979 | 1.269943 |
| 60 | 1 | 0 | -11.525635 | -1.205830 | 1.738360 |
| 61 | 7 | 0 | -9.482052 | -0.345987 | -0.113688 |
| 62 | 8 | 0 | -7.949953 | 1.787855 | 0.707811 |
| 63 | 8 | 0 | -5.474418 | -2.766781 | -1.182085 |
| 64 | 6 | 0 | -7.189865 | 2.890752 | 1.159772 |
| 65 | 1 | 0 | -6.584478 | 2.631861 | 2.035522 |
| 66 | 1 | 0 | -6.532529 | 3.275990 | 0.372350 |
| 67 | 1 | 0 | -7.908815 | 3.661441 | 1.436035 |
| 68 | 6 | 0 | -5.403668 | -2.834419 | -2.601276 |
| 69 | 1 | 0 | -6.399872 | -2.769067 | -3.052198 |
| 70 | 1 | 0 | -4.778045 | -2.029288 | -3.002983 |
| 71 | 1 | 0 | -4.957670 | -3.797699 | -2.851434 |
| 72 | 8 | 0 | -1.261216 | 2.461976 | -0.139318 |
| 73 | 8 | 0 | 1.126377 | -2.507798 | -0.115051 |
| 74 | 6 | 0 | -0.496681 | 3.661496 | -0.149727 |
| 75 | 6 | 0 | -1.463839 | 4.827757 | -0.124050 |
| 76 | 1 | 0 | 0.128901 | 3.696749 | -1.051060 |
| 77 | 1 | 0 | 0.168064 | 3.687837 | 0.723460 |
| 78 | 6 | 0 | -0.746802 | 6.175837 | -0.138667 |
| 79 | 1 | 0 | -2.132909 | 4.750409 | -0.988440 |
| 80 | 1 | 0 | -2.090498 | 4.746867 | 0.771303 |
| 81 | 6 | 0 | -1.715153 | 7.354105 | -0.111980 |
| 82 | 1 | 0 | -0.070104 | 6.237615 | 0.722045 |
| 83 | 1 | 0 | -0.113722 | 6.241686 | -1.031643 |
| 84 | 1 | 0 | -1.181332 | 8.307918 | -0.123643 |
| 85 | 1 | 0 | -2.383089 | 7.334141 | -0.978678 |
| 86 | 1 | 0 | -2.338610 | 7.330911 | 0.787189 |
| 87 | 6 | 0 | 1.284805 | -3.108424 | 1.174498 |
| 88 | 6 | 0 | 1.895763 | -4.481344 | 0.987718 |

| | | | | | |
|---|---|---|---|---|---|
| 89 | 1 | 0 | 0.307279 | -3.178272 | 1.669094 |
| 90 | 1 | 0 | 1.929747 | -2.473336 | 1.796684 |
| 91 | 6 | 0 | 2.103781 | -5.212502 | 2.312012 |
| 92 | 1 | 0 | 1.243263 | -5.070320 | 0.333030 |
| 93 | 1 | 0 | 2.853932 | -4.373659 | 0.466014 |
| 94 | 6 | 0 | 2.718725 | -6.596272 | 2.127439 |
| 95 | 1 | 0 | 2.747411 | -4.609381 | 2.963598 |
| 96 | 1 | 0 | 1.142428 | -5.304964 | 2.831532 |
| 97 | 1 | 0 | 2.857193 | -7.101485 | 3.086940 |
| 98 | 1 | 0 | 2.080321 | -7.230621 | 1.504707 |
| 99 | 1 | 0 | 3.696457 | -6.530691 | 1.640106 |

**Lowest three frequencies:**

| | 1<br>A | 2<br>A | 3<br>A |
|---|---|---|---|
| Frequencies -- | 4.2401 | 7.9381 | 8.5540 |
| Red. masses -- | 5.9850 | 4.6451 | 4.9845 |
| Frc consts -- | 0.0001 | 0.0002 | 0.0002 |
| IR Inten -- | 0.0458 | 0.2573 | 0.0426 |

**Thermochemical data:**

| | | |
|---|---|---|
| Zero-point correction | = | 0.839978 (Hartree/Particle) |
| Thermal correction to Energy | = | 0.889854 |
| Thermal correction to Enthalpy | = | 0.890798 |
| Thermal correction to Gibbs Free Energy | = | 0.743632 |
| Sum of electronic and zero-point Energies | = | -2218.673319 |
| Sum of electronic and thermal Energies | = | -2218.623444 |
| Sum of electronic and thermal Enthalpies | = | -2218.622499 |
| Sum of electronic and thermal Free Energies | = | -2218.769666 |

********** END **********