# Supporting Information

# Metallo-porphyrin Based Inclusion Materials: Exploiting Ligating Topologies and Hydrogen Bonding Backbone in Generating New Supramolecular Architectures

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## FT–IR for ~~10~~11–16 & 18-20

~~**[{(ZnTPP)$_2$4BPU} •X] 10:**~~
~~FT–IR (cm$^{-1}$): 3298b, 3022w, 2925m, 2342w, 1815m, 1724b, 1673s, 1654m, 1593vs, 1483s, 1385vs, 1284vs, 1253m, 1197b, 1174s, 1090m, 1064s, 991vs, 830s, 796vs, 750vs, 750vs, 718m, 702vs, 659vs, 527s, 429m~~

**[{(ZnTPP)$_2$4BPU}•{(ZnTPP)DMF}•4DMF •X] 11:**
FT–IR (cm$^{-1}$): 3399b, 3022w, 2923m, 2363m, 2343w, 1813, 1737m, 1673s, 1652vs, 1593vs, 1523vs, 1483m, 1384s, 1335vs, 1291m, 1252b, 1175b, 1088w, 991vs, 830m, 796vs, 750vs, 718m, 702vs, 659s, 527m, 428m

**[{(ZnTPP)4BPU}•Toluene •CHCl$_3$ •X] 12:**
FT–IR (cm$^{-1}$): 3374b, 3022w, 2923m, 2852w, 2360m, 1809b, 1732s, 1586vs, 1507s, 1439vs, 1422vs, 1335vs, 1283vs, 1246w, 1182vs, 1068vs, 991vs, 880w, 827s, 795vs, 749s, 701vs, 659m, 567w, 527b, 431s

**[{(ZnTPP)$_2$3BPU}•Br–benzene•H$_2$O] 13**:
FT–IR (cm$^{-1}$): 3358m, 3051w, 2337b, 1813m, 1713vs, 1594vs, 1549vs, 1482vs, 1439s, 1335s, 1291s, 1202s, 1175m, 1067vs, 990vs, 831w, 796vs, 740vs, 700vs, 638w, 568m, 457m, 432m

**[{(ZnTPP)$_2$3BPU}•Toluene•H$_2$O] 14:**
FT–IR (cm$^{-1}$): 3368b, 3051w, 3021m, 2362b, 1801b, 1722s, 1655m, 1595vs, 1546vs, 1482vs, 1439m, 1336s, 1291m, 1201vs, 1176m, 1129w, 1068vs, 993vs, 831w, 796vs, 751s, 732w, 718w, 700vs, 660m, 641w, 571w, 539b, 465m, 432m

**[{(ZnTPP)$_2$4PIN}•Toluene•X] 15:**
FT–IR (cm$^{-1}$): 3396b, 3024w, 2924w, 2358w, 1813m, 1690b, 1662m, 1593vs, 1518s, 1483s, 1439s, 1419m, 1334vs, 1291s, 1201s, 1174s, 1065vs, 991vs, 831m, 796vs, 751vs, 717w, 701vs, 659vs, 587m, 526b, 430s

**[{(ZnTPP)4PIN}•p–xylene•2–p–tolyl–ethenol] 16:**
FT–IR (cm$^{-1}$): 3908w, 3251w, 3046b, 2921m, 2852w, 2632m, 1815b, 1701vs, 1594vs, 1512vs, 1483vs, 1440s, 1421s, 1330s, 1290vs, 1206vs, 1175m, 1114m, 1065vs, 992vs, 836m, 797vs, 750vs, 719w, 701vs, 659m, 587s, 511w, 482m, 420m

~~**[{(MnTPP)4BPU}Cl•X]$_n$ 17:**~~
~~FT–IR (cm$^{-1}$): 3496b, 3139b, 3052w, 2960b, 2361m, 1829b, 1719vs, 1592vs, 1525vs, 1484w, 1439b, 1336s, 1289vs, 1185vs, 1075m, 1007vs, 955m, 831vs, 801vs, 756s, 704vs, 657b, 560w, 531s, 453m~~

**[{(MnTPP)3BPU}Cl•2Nitrobenzene.H$_2$O.X]$_n$ 18:**
FT–IR (cm$^{-1}$): 3435b, 3233b, 3056m, 2361m, 1818b, 1710vs, 1591s, 1550vs, 1523vs, 1478s, 1423s, 1343vs, 1273vs, 1199vs, 1129m, 1107w, 1071m, 1009vs, 924b, 849m, 802vs, 752vs, 701vs, 632m, 561w, 521m, 452m

**[{(MnTPP)(3BPU)$_2$}Cl•Toluene•CHCl$_3$] 19:**
FT–IR (cm$^{-1}$): 3232b, 3052m, 2361s, 1832b, 1708vs, 1583vs, 1544s, 1476s, 1441m, 1418vs, 1340m, 1259vs, 1201vs, 1128m, 1074m, 1010vs, 896m, 803vs, 752vs, 701vs, 663m, 631w, 563w, 536w, 456s, 419m

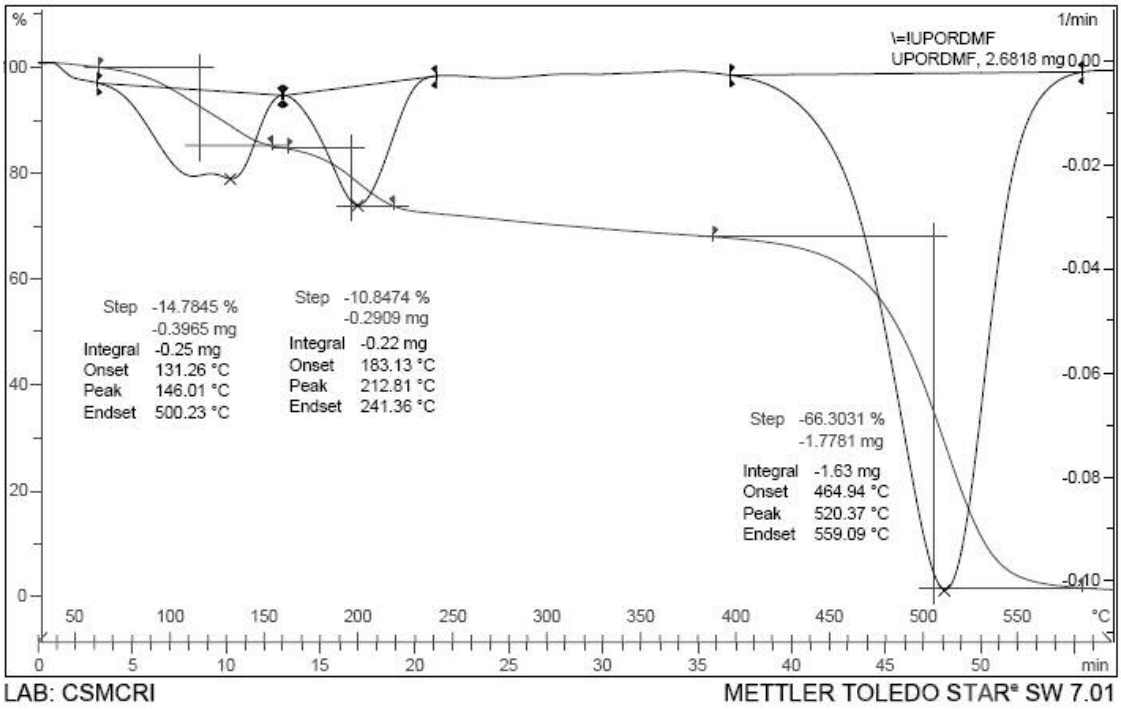
**[{(MnTPP)(3BPU)$_2$}Cl•p–xylene•H$_2$O] 20:** FT–IR (cm$^{-1}$): 3230b, 3053m, 2922m, 2360s, 814b, 1708vs, 1589b, 1542vs, 1474s, 1440w, 1424s, 1340vs, 1268vs, 1200vs, 1200vs, 1129m, 1072s, 1010vs, 928m, 799vs, 753vs, 702vs, 662m, 630w, 524m, 484s, 452s, 419m

## Hydrogen Bonding Parameters for 11–14 & 16–20

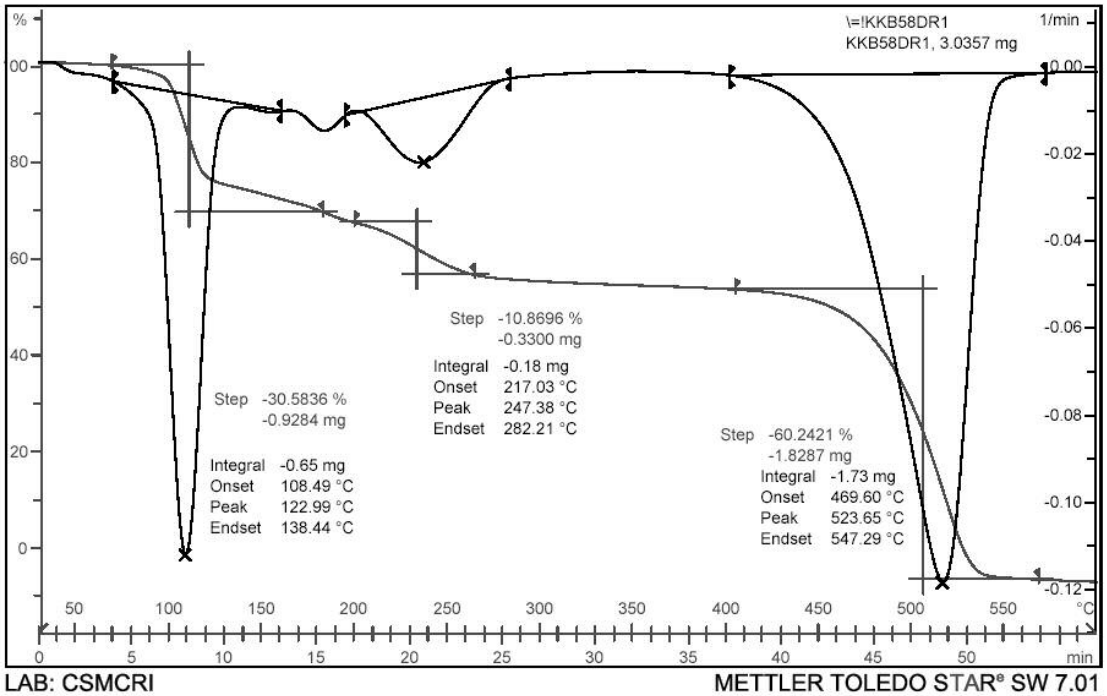
| D–H…A | D–H/Å | H…A/Å | D…A/Å | D–H…A/$^0$ | Symmetry operation for A |
|---|---|---|---|---|---|
| **11** | | | | | |
| N(55)–H(55···O(175) | 0.86 | 1.94 | 2.787(4) | 169 | x, y, z |
| N(58)–H(58)···O(175) | 0.86 | 2.37 | 3.122(4) | 146 | x, y, z |
| N(58)–H(58)···O(165) | 0.86 | 2.51 | 3.089(4) | 126 | 1–x, 1–y, 1–z |
| **12** | | | | | |
| N(55)–H(55)···N(62) | 0.88 | 2.53 | 3.283(5) | 145 | 2/3-y, 1/3+x-y,1 /3+z |
| N(58)–H(58)···N(62) | 0.88 | 2.05 | 2.901(5) | 164 | 2/3-y, 1/3+x-y, 1/3+z |
| **13** | | | | | |
| N(55)–H(55)···O(72) | 0.86 | 2.11 | 2.930(8) | 159 | x, y, z |
| **14** | | | | | |
| N(55)–H(55)···O(2) | 0.88 | 2.11 | 2.944(4) | 158 | x, y, z |
| **16** | | | | | |
| N(55)–H(55)···O(81) | 0.88 | 2.13 | 2.954(5) | 157 | 1–x, 1–y, 1–z |
| O(81)–H(81)···N(61) | 0.69(4) | 2.07(4) | 2.755(5) | 175(4) | x, 1+y, z |
| **18** | | | | | |
| N(31)–H(31)···Cl(3) | 0.88 | 2.36 | 3.191(5) | 159 | x, y, -1+z |
| N(34)–H(34)···Cl(3) | 0.88 | 2.33 | 3.177(5) | 163 | x, y, -1+z |
| **19** | | | | | |
| N(31)–H(31)···Cl(4) | 0.88 | 2.37 | 3.164(4) | 151 | 1+x, y, z |
| N(31')–H(31')···Cl(4) | 0.88 | 2.53 | 3.358(3) | 158 | x, y, z |
| N(34)–H(34)···Cl(4) | 0.88 | 2.42 | 3.236(4) | 154 | 1+x, y, z |
| N(34')–H(34')···Cl(4) | 0.88 | 2.37 | 3.219(3) | 164 | x, y, z |
| **20** | | | | | |
| N(31')–H(31')···Cl(53) | 0.84(4) | 2.37(3) | 3.201(3) | 169(3) | x, y, z |
| N(31)–H(31H)···Cl(53) | 0.92(4) | 2.33(4) | 3.212(3) | 161(3) | 1+x, y, z |
| N(34')–H(34')···Cl(53) | 0.77(4) | 2.59(4) | 3.300(3) | 154(3) | x, y, z |
| N(34)–H(34H)···Cl(53) | 0.94(4) | 2.34(4) | 3.227(3) | 159(3) | 1+x, y, z |

# Thermal Analyses Plot for ~~10–~~11, 13-14, 16, 18–20

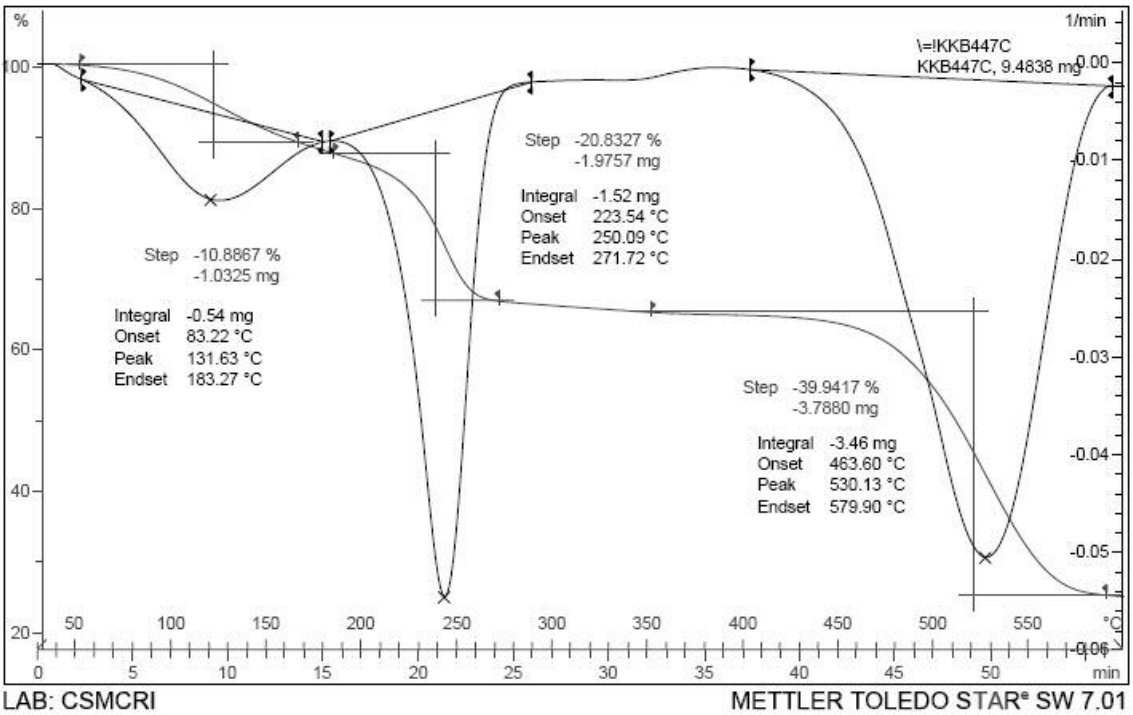
## Compound 11



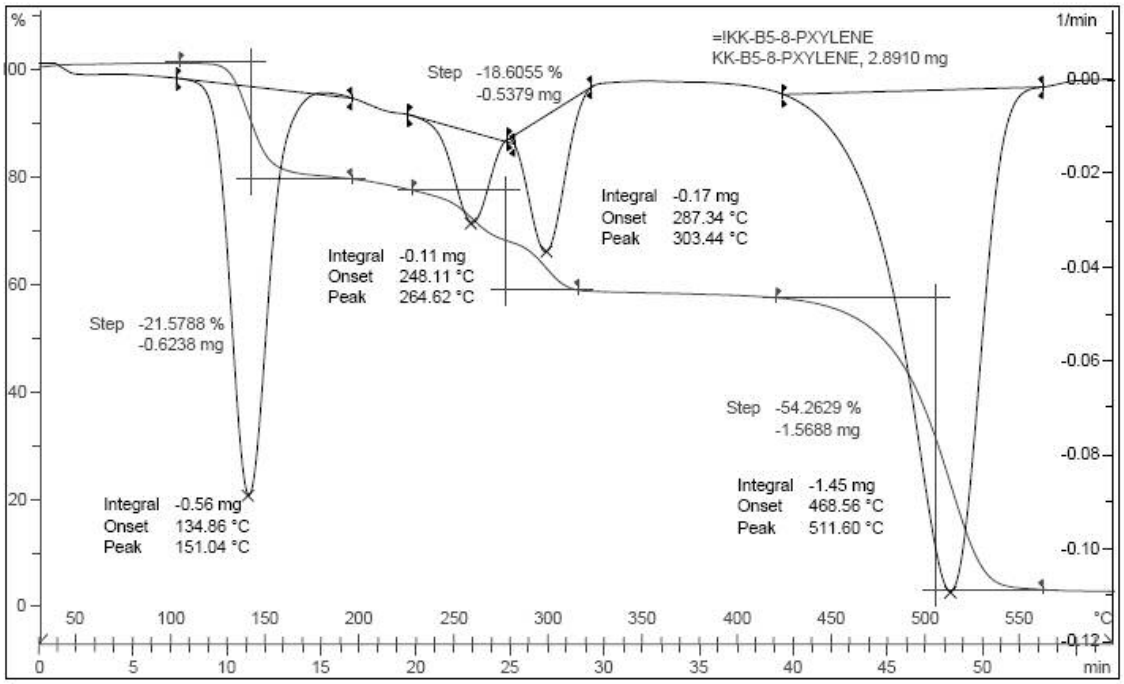
# Compound 13


\=!KKB58DR1
KKB58DR1, 3.0357 mg
Step -30.5836 %
-0.9284 mg
Integral -0.65 mg
Onset 108.49 °C
Peak 122.99 °C
Endset 138.44 °C
Step -10.8696 %
-0.3300 mg
Integral -0.18 mg
Onset 217.03 °C
Peak 247.38 °C
Endset 282.21 °C
Step -60.2421 %
-1.8287 mg
Integral -1.73 mg
Onset 469.60 °C
Peak 523.65 °C
Endset 547.29 °C
LAB: CSMCRI
METTLER TOLEDO STAR SW 7.01

# Compound 14


%
1/min
\=!KKB447C
KKB447C, 9.4838 mg
Step -20.8327 %
-1.9757 mg
Integral -1.52 mg
Onset 223.54 °C
Peak 250.09 °C
Endset 271.72 °C
Step -10.8867 %
-1.0325 mg
Integral -0.54 mg
Onset 83.22 °C
Peak 131.63 °C
Endset 183.27 °C
Step -39.9417 %
-3.7880 mg
Integral -3.46 mg
Onset 463.60 °C
Peak 530.13 °C
Endset 579.90 °C
°C
min
LAB: CSMCRI
METTLER TOLEDO STAR® SW 7.01

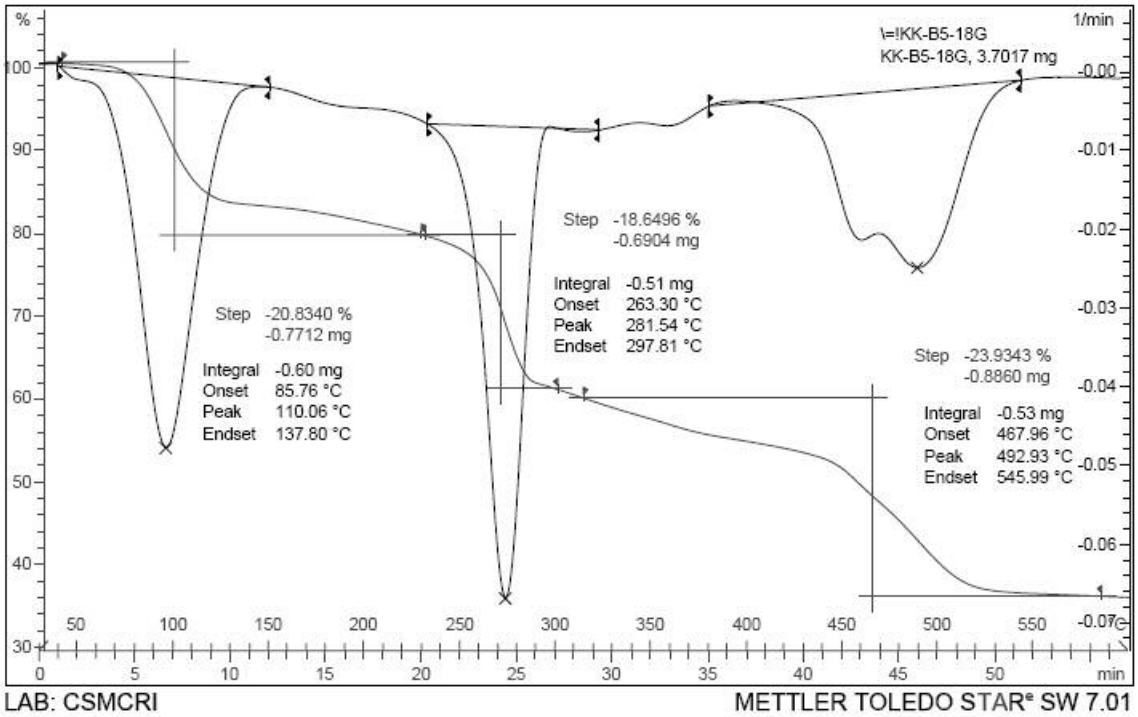
# Compound 16




LAB: CSMCRI

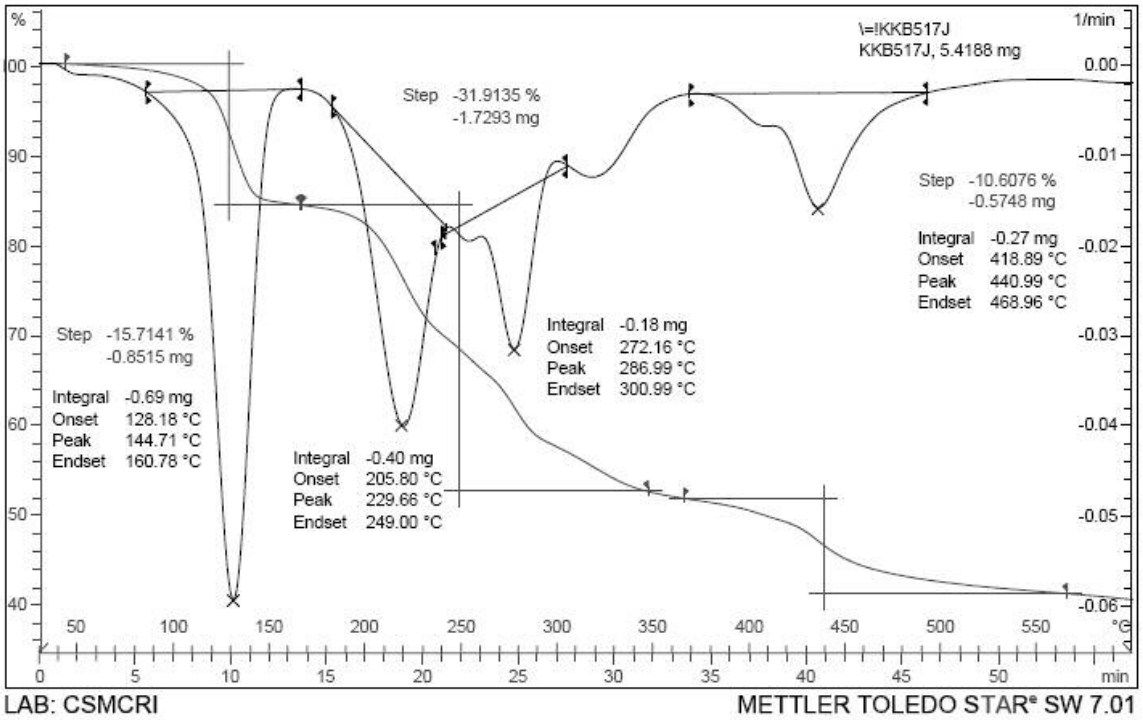
METTLER TOLEDO STAR® SW 7.01

# Compound 18

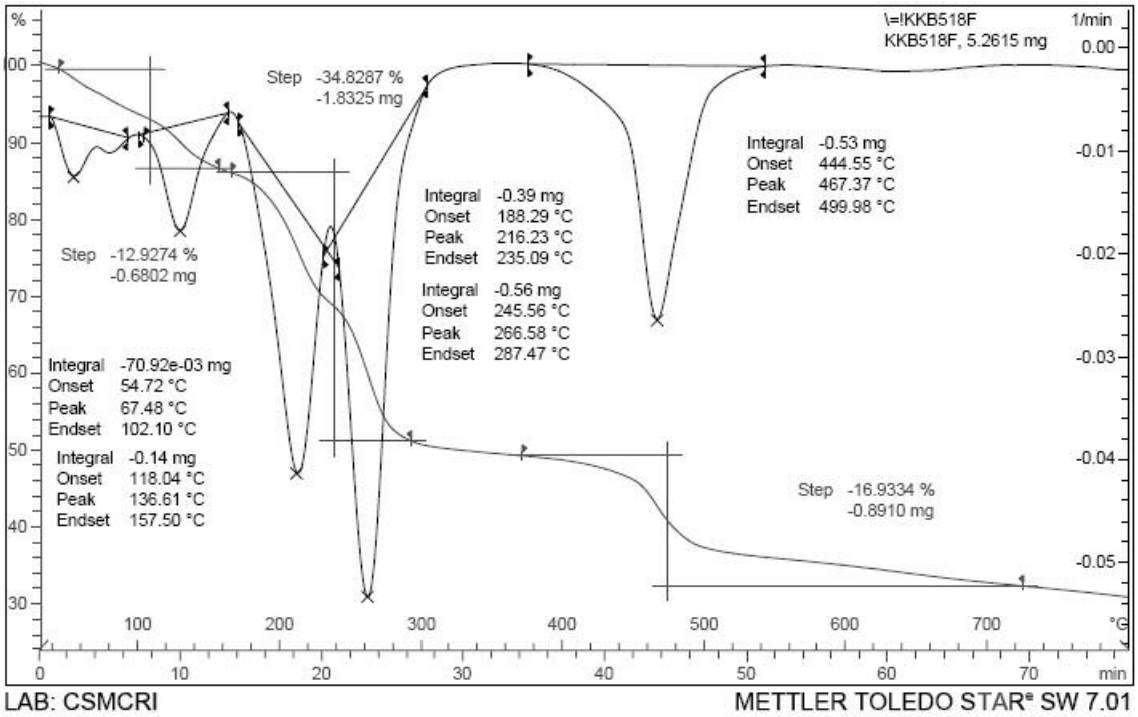



LAB: CSMCRI METTLER TOLEDO STAR$^e$ SW 7.01

# Compound 19


%
1/min
\=!KKB517J
KKB517J, 5.4188 mg
Step -31.9135 %
-1.7293 mg
Step -10.6076 %
-0.5748 mg
Integral -0.27 mg
Onset 418.89 °C
Peak 440.99 °C
Endset 468.96 °C
Integral -0.18 mg
Onset 272.16 °C
Peak 286.99 °C
Endset 300.99 °C
Step -15.7141 %
-0.8515 mg
Integral -0.69 mg
Onset 128.18 °C
Peak 144.71 °C
Endset 160.78 °C
Integral -0.40 mg
Onset 205.80 °C
Peak 229.66 °C
Endset 249.00 °C
°C
min
LAB: CSMCRI
METTLER TOLEDO STAR® SW 7.01

# Compound 20


\=!KKB518F
KKB518F, 5.2615 mg
1/min
Step -34.8287 %
-1.8325 mg
Integral -0.53 mg
Onset 444.55 °C
Peak 467.37 °C
Endset 499.98 °C
Integral -0.39 mg
Onset 188.29 °C
Peak 216.23 °C
Endset 235.09 °C
Step -12.9274 %
-0.6802 mg
Integral -0.56 mg
Onset 245.56 °C
Peak 266.58 °C
Endset 287.47 °C
Integral -70.92e-03 mg
Onset 54.72 °C
Peak 67.48 °C
Endset 102.10 °C
Integral -0.14 mg
Onset 118.04 °C
Peak 136.61 °C
Endset 157.50 °C
Step -16.9334 %
-0.8910 mg
%
°C
min
LAB: CSMCRI
METTLER TOLEDO STAR® SW 7.01