SUPPORTING INFORMATION

Supporting Information

Synthesis of Thiol-Derivatized Porphyrin Dimers and Trimers for Studies of Architectural Effects on Multibit Information Storage

Characterization of the porphyrins.

Porphyrins generally afford strong molecule ion peaks with very little fragmentation upon analysis by LD-MS (without a matrix). Indeed, in many cases the molecule ion peak is the most intense peak in the mass spectrum. However, the (*S*-acetylthio)- or thiocyanato-derivatized porphyrins exhibit characteristic fragmentation patterns. In this section we list the major peaks observed upon LD-MS analysis of the various (*S*-acetylthio)- or thiocyanato-derivatized porphyrins (rather than just the molecule ion peak as listed in the body of the paper).

ZnFb-3. LD-MS obsd 1600.5, 1615.5 [$M^+ + 15$], 1558.4 [$M^+ - CH_3CO$].

ZnZn-3. LD-MS obsd 1664.2, 1622.1 [$M^+ - CH_3CO$], 1636.0 [$M^+ - 15$].

ZnFb-5. LD-MS obsd 1737.8, 1751.8 [$M^+ + 15$], 1709.4 [$M^+ - 28$], 1695.2 [$M^+ - CH_3CO$].

ZnZn-5. LD-MS obsd 1815.1, 1772.9 [$M^+ - CH_3CO$], 1786.9 [$M^+ - 28$].

Zn(II)-5,15-Bis(3-iodophenyl)-10,20-bis[3-(thiocyanatomethyl)phenyl]porphyrin (Zn-6). LD-MS obsd 1071.3 [M^+], 1013.4 [$M^+ - SCN$], 955.3 [$M^+ - 2\ SCN$].

Zn(II)-5,15-Bis[3-(*S*-acetylthiomethyl)phenyl]-10,20-bis(3-iodophenyl)porphyrin (Zn-7). LD-MS obsd 1120.4 [$M^+ + 15$], 1105.4 [M^+], 1063.4 [$M^+ - COCH_3$], 1031.2 [$M^+ -$

$SCOCH_3$], 979.3 [M^+ – I], 955.5 [M^+ – 2 $SCOCH_3$], 936.1 [M^+ – I – $COCH_3$], 904.5 [M^+ – I – $SCOCH_3$].

Cu(II)- 5,15-Bis[3-(*S*-acetylthiomethyl)phenyl]-10,20-bis(3-iodophenyl)porphyrin (Cu-7). LD-MS obsd 1118.0 [M^+ + 15], 1103.0 [M^+], 1061.0 [M^+ – $COCH_3$], 1028.0 [M^+ – $SCOCH_3$], 977.0 [M^+ – I], 953.0 [M^+ – 2 $SCOCH_3$], 934.0 [M^+ – I – $COCH_3$], 902.1 [M^+ – I – $SCOCH_3$], 827.2 [M^+ – I – 2 $SCOCH_3$], 731.0 [M^+ – 2 I – $SCOCH_3$].

Ni(II)- 5,15-Bis[3-(*S*-acetylthiomethyl)phenyl]-10,20-bis(3-iodophenyl)porphyrin (Ni-7). LD-MS obsd 1114.8 [M^+ + 15], 1099.8 [M^+], 1058.6 [M^+ – $COCH_3$], 1024.7 [M^+ – $SCOCH_3$], 973.6 [M^+ – I], 949.5 [M^+ – 2 $SCOCH_3$].

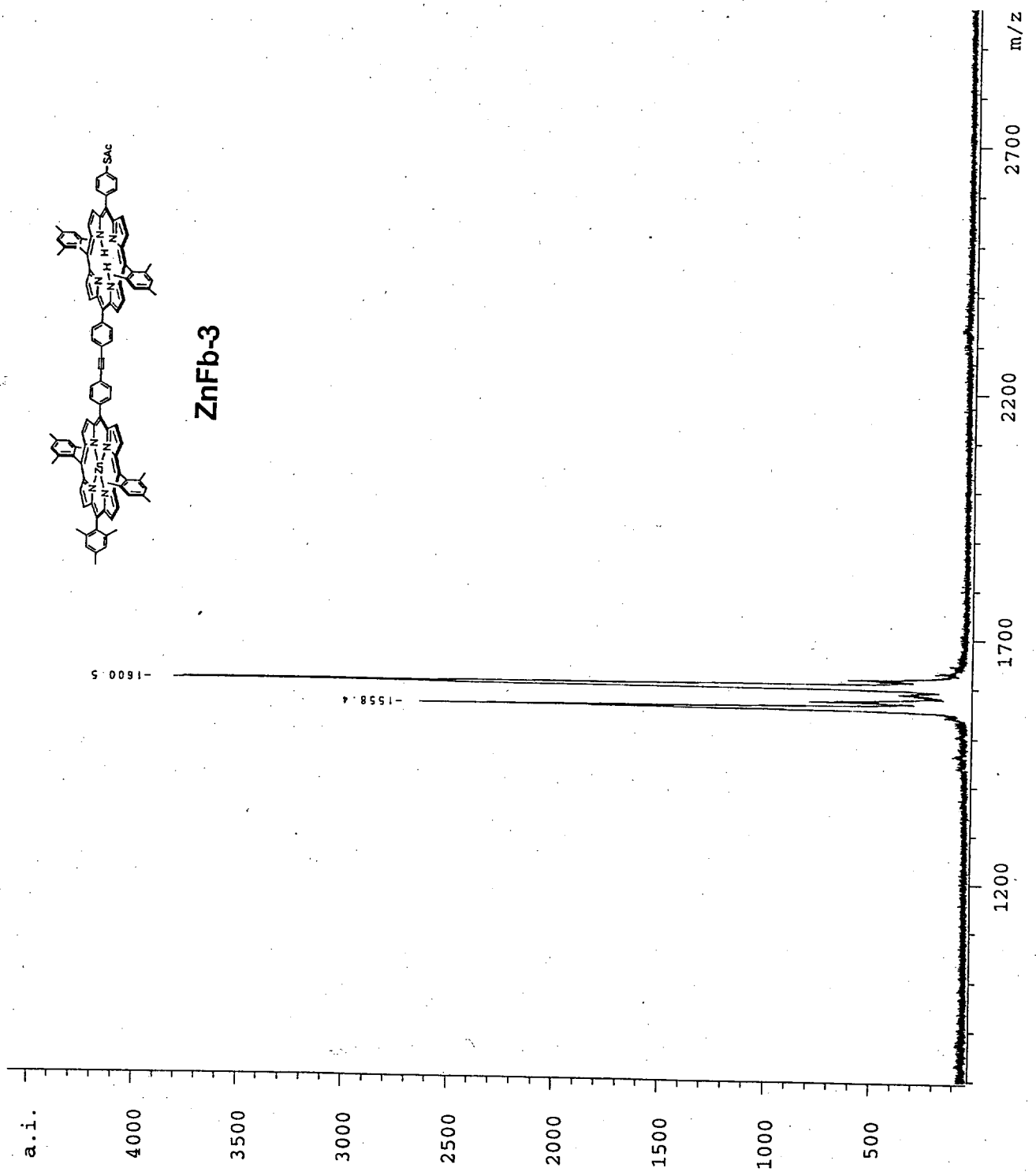
ZnZnZn-10. LD-MS obsd 2509.4 [M^+], 2463.4 [M^+ – $COCH_3$], 2435.2 [M^+ – $SCOCH_3$], 2360.3 [M^+ – 2 $SCOCH_3$].

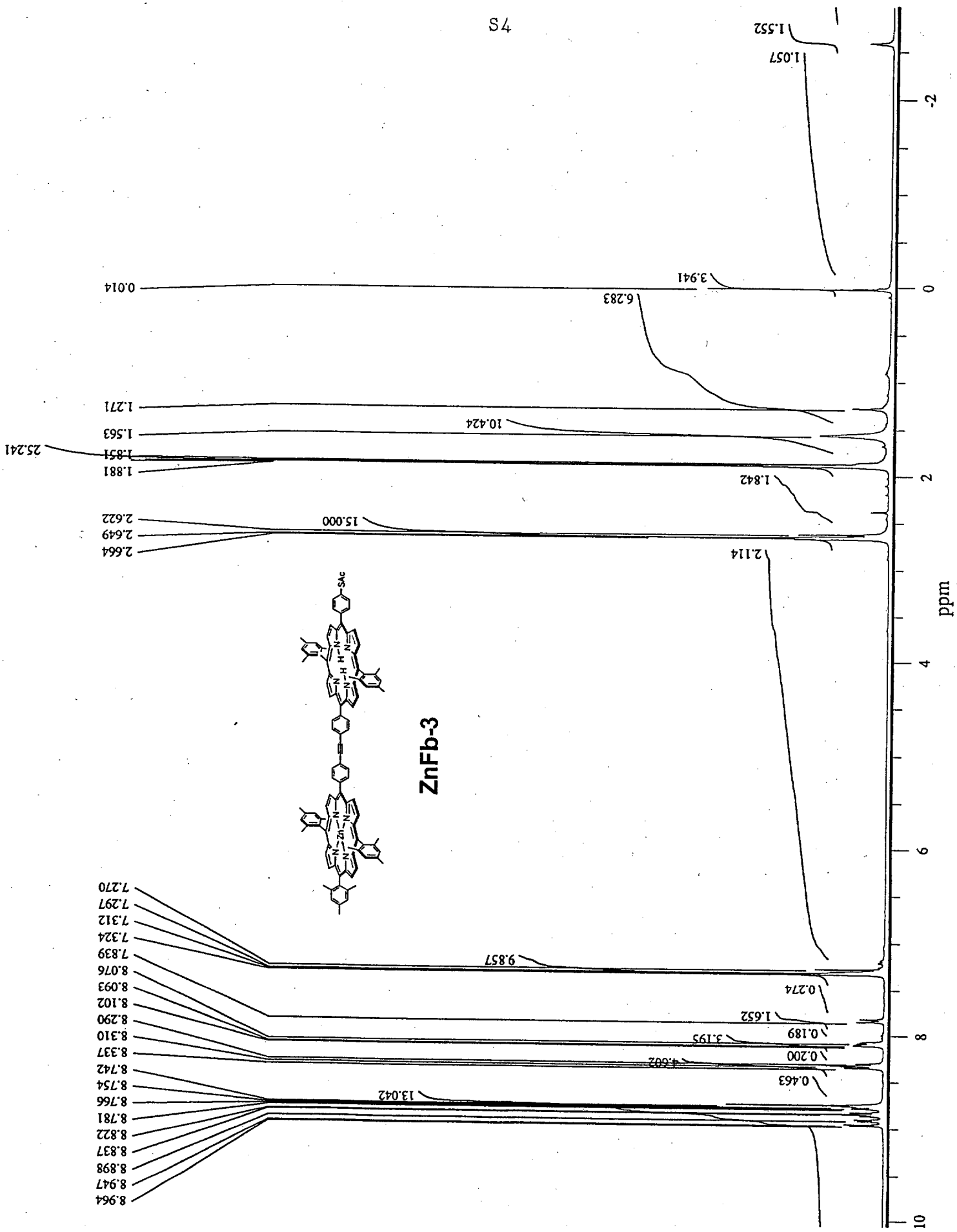
ZnNiZn-10. LD-MS obsd 2502.7 [M^+], 2476.0 [M^+ – CO], 2459.7 [M^+ – $COCH_3$], 2428.3 [M^+ – $SCOCH_3$], 2385.3 [M^+ – $SCOCH_3$ – $COCH_3$], 2355.3 [M^+ – 2 $SCOCH_3$].

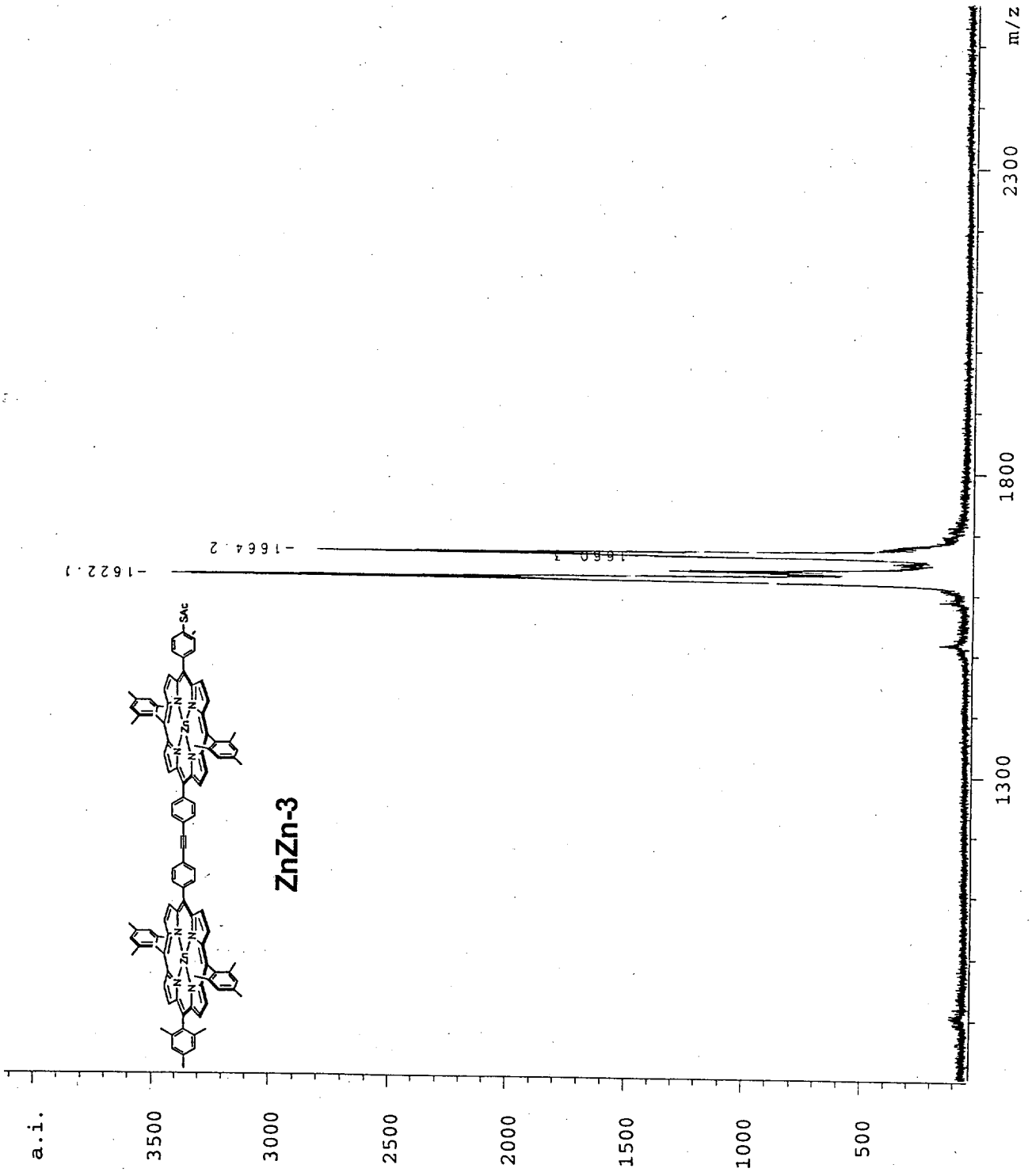
ZnCuZn-10. LD-MS obsd 2508.5 [M^+], 2480.8 [M^+ – CO], 2463.1 [M^+ – $COCH_3$], 2433.8 [M^+ – $SCOCH_3$], 2388.3 [M^+ – $SCOCH_3$ – $COCH_3$], 2358.0 [M^+ – 2 $SCOCH_3$], 2268.5 [M^+ – 2 $SCOCH_3$ – $PhCH_2$].

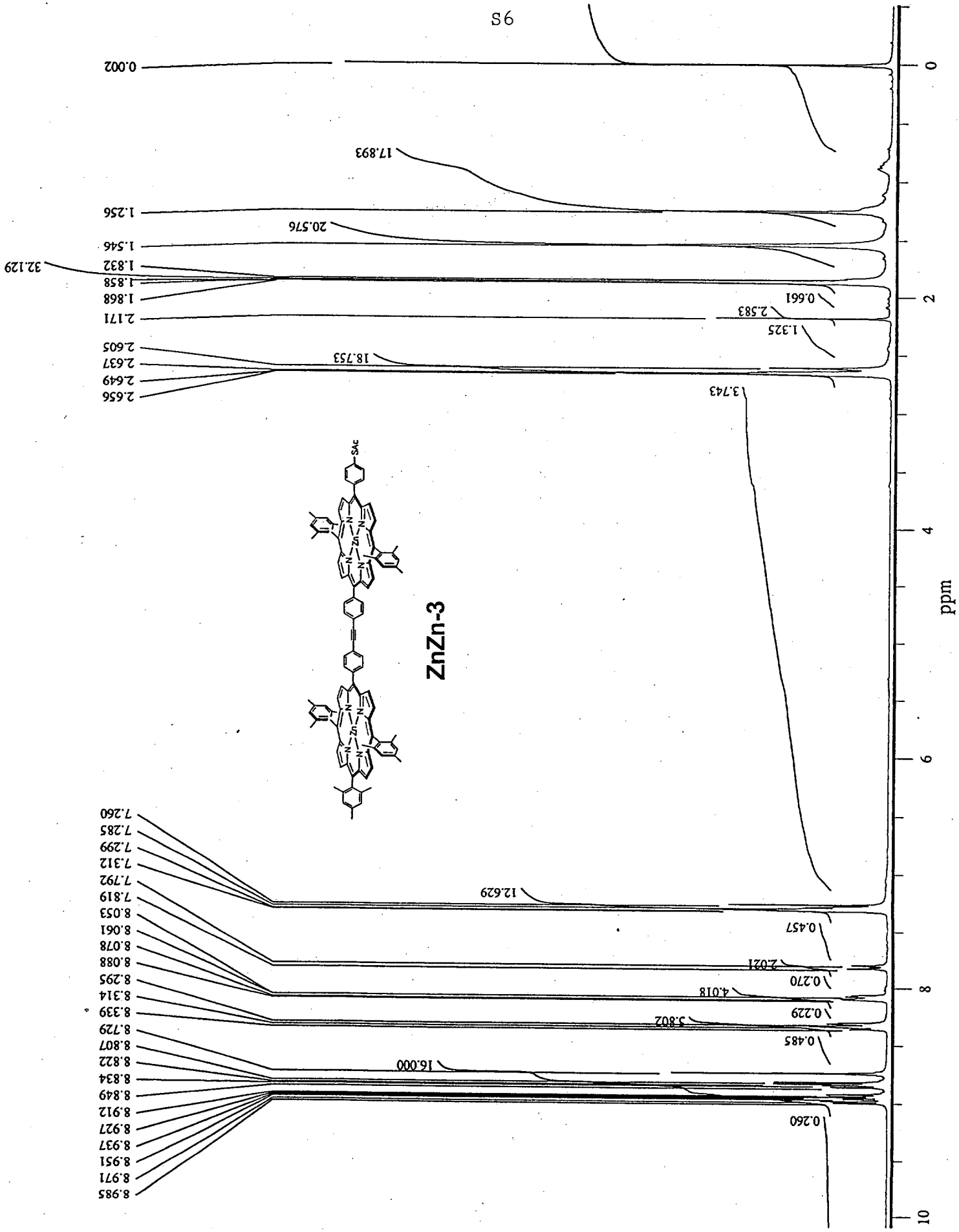
MgCuMg-10. LD-MS obsd 2425.9 [M^+], 2380.2 [M^+ – $COCH_3$], 2351.1 [M^+ – $SCOCH_3$], 2309.3 [M^+ – $SCOCH_3$ – $COCH_3$], 2275.2 [M^+ – 2 $SCOCH_3$].

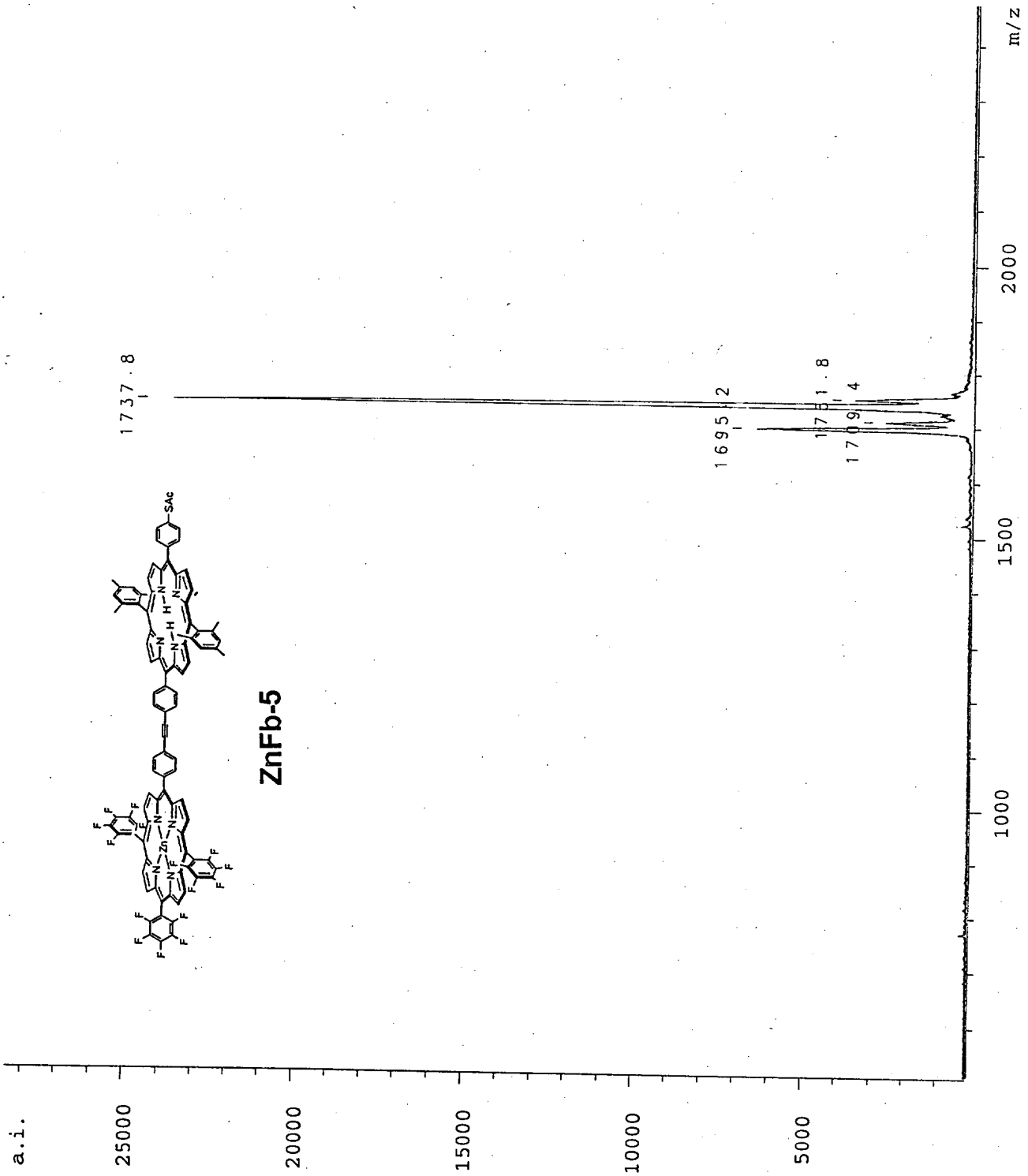
ZnZnZn-11. LD-MS obsd 2470.8 [M^+], 2396.2 [M^+ – $SCOCH_3$], 2352.1 [M^+ – $SCOCH_3$ – $COCH_3$], 2319.5 [M^+ – 2 $SCOCH_3$], 2331.2 [M^+ – 2 $SCOCH_3$ – $PhCH_2$].

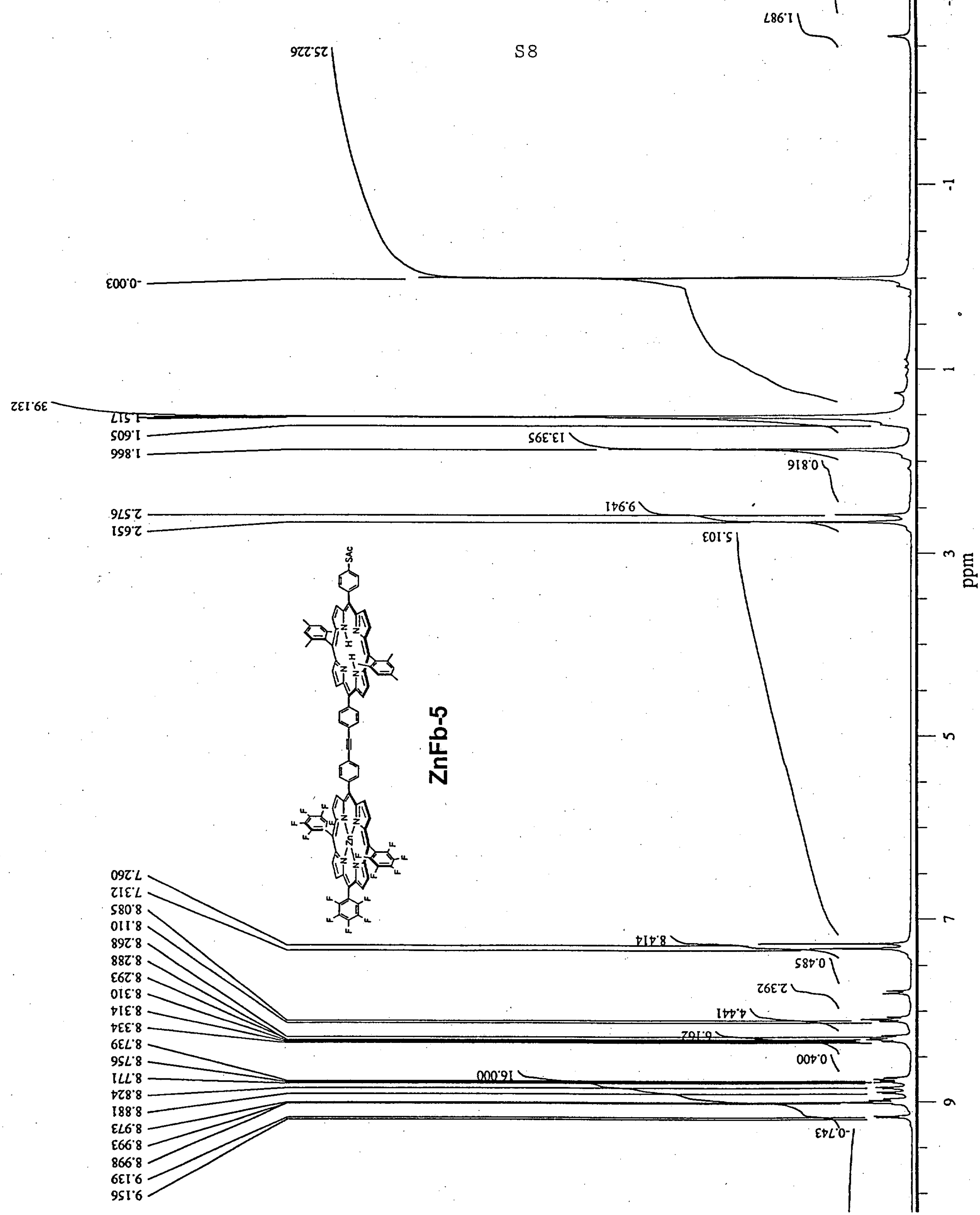


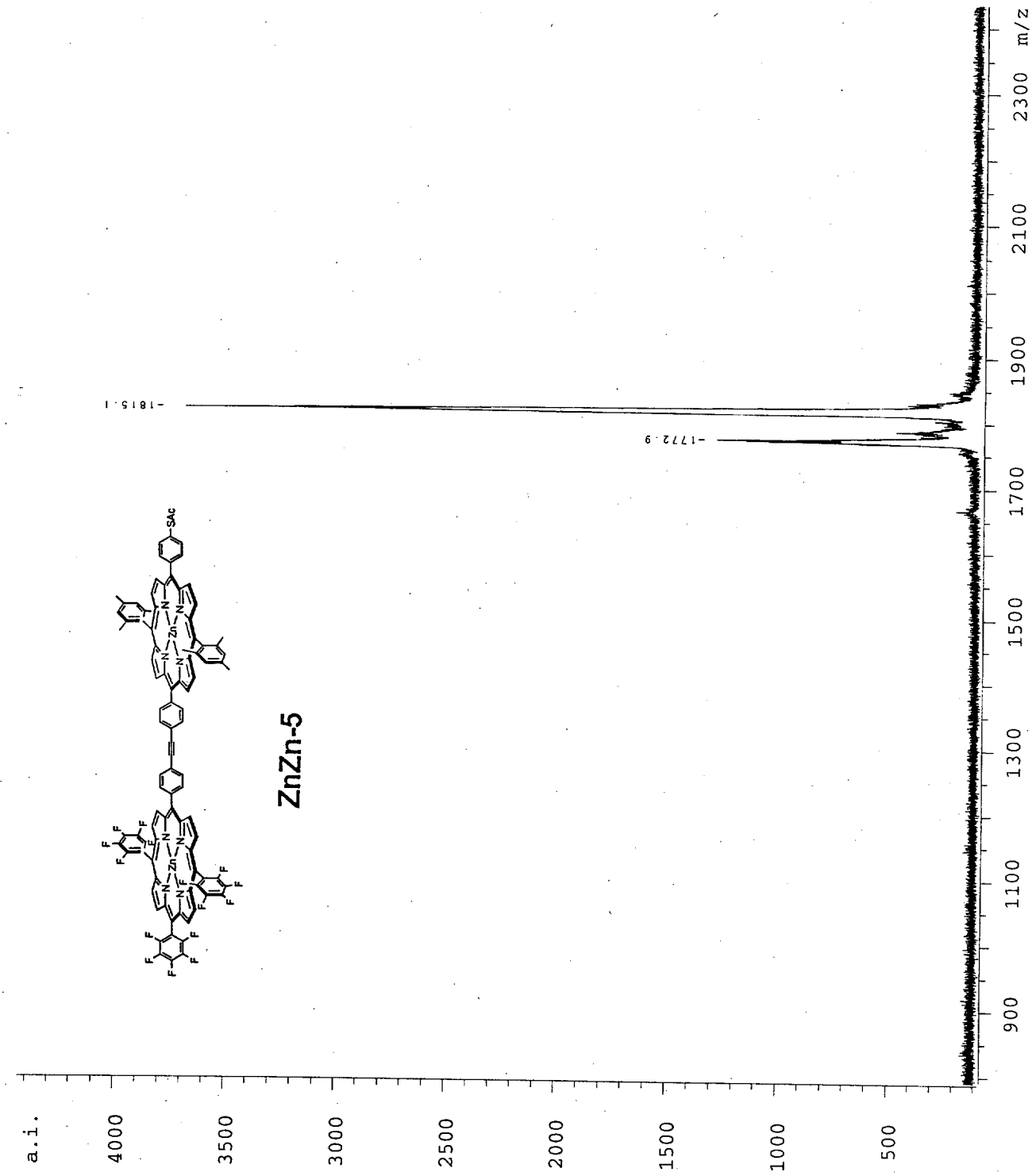


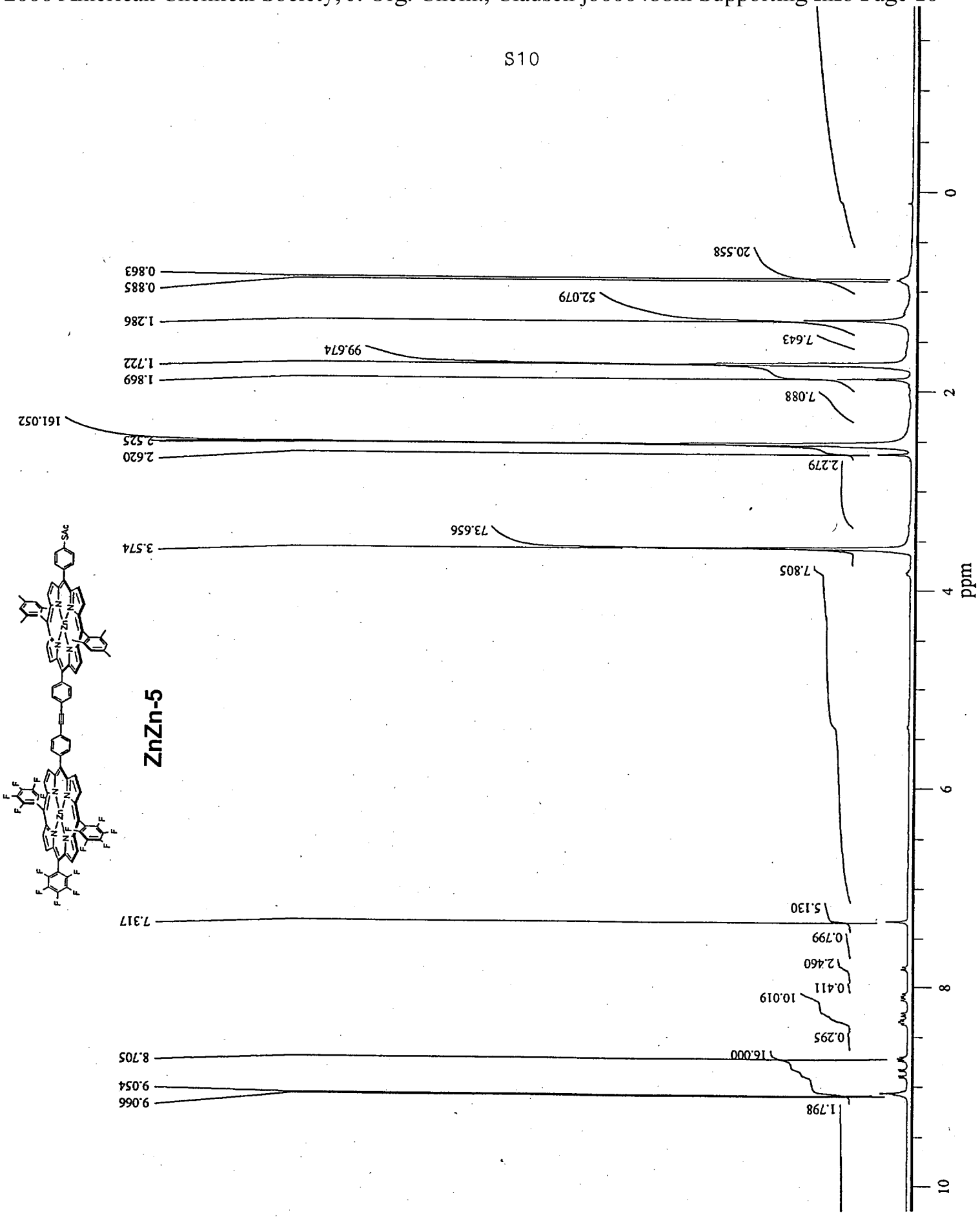


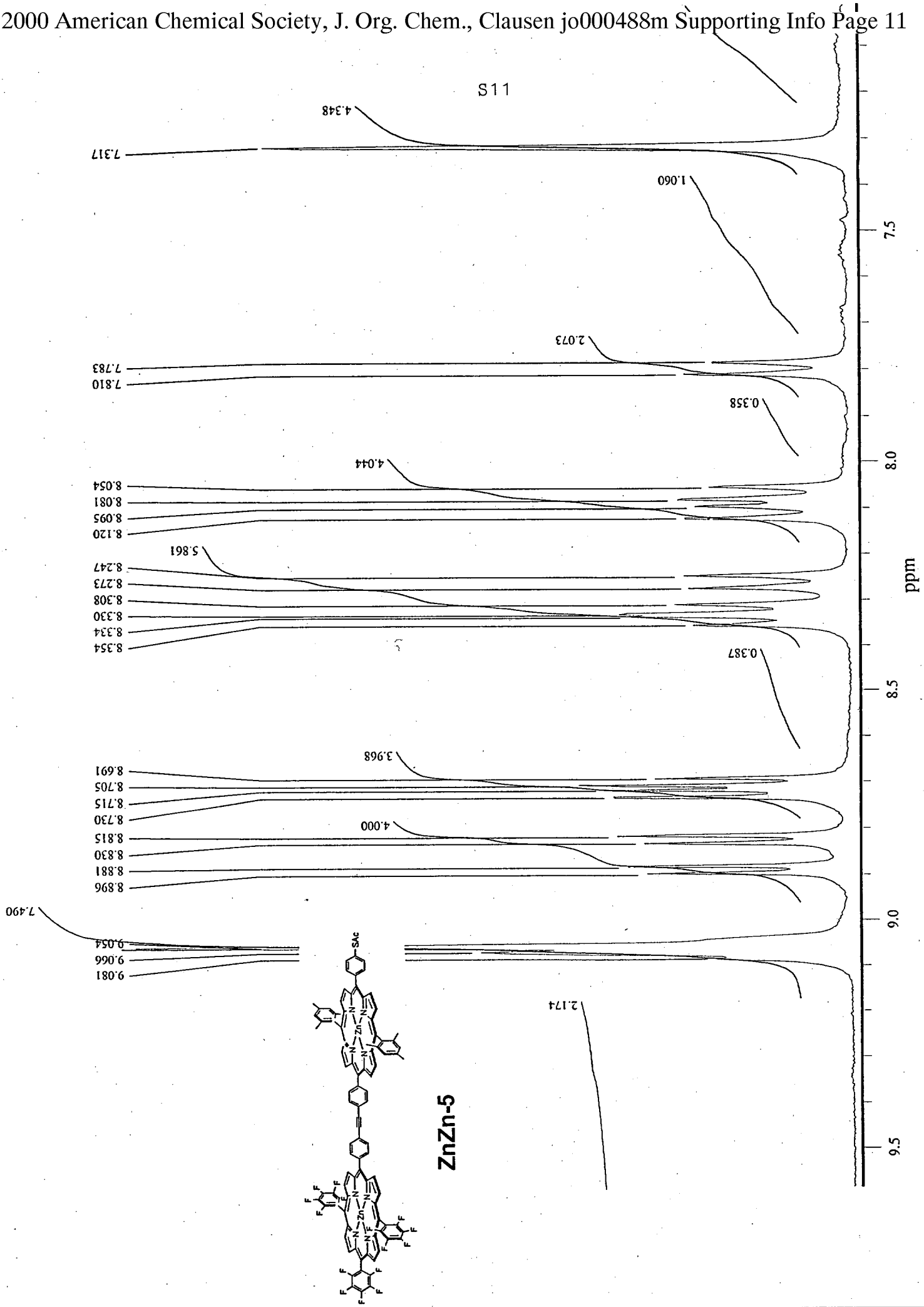


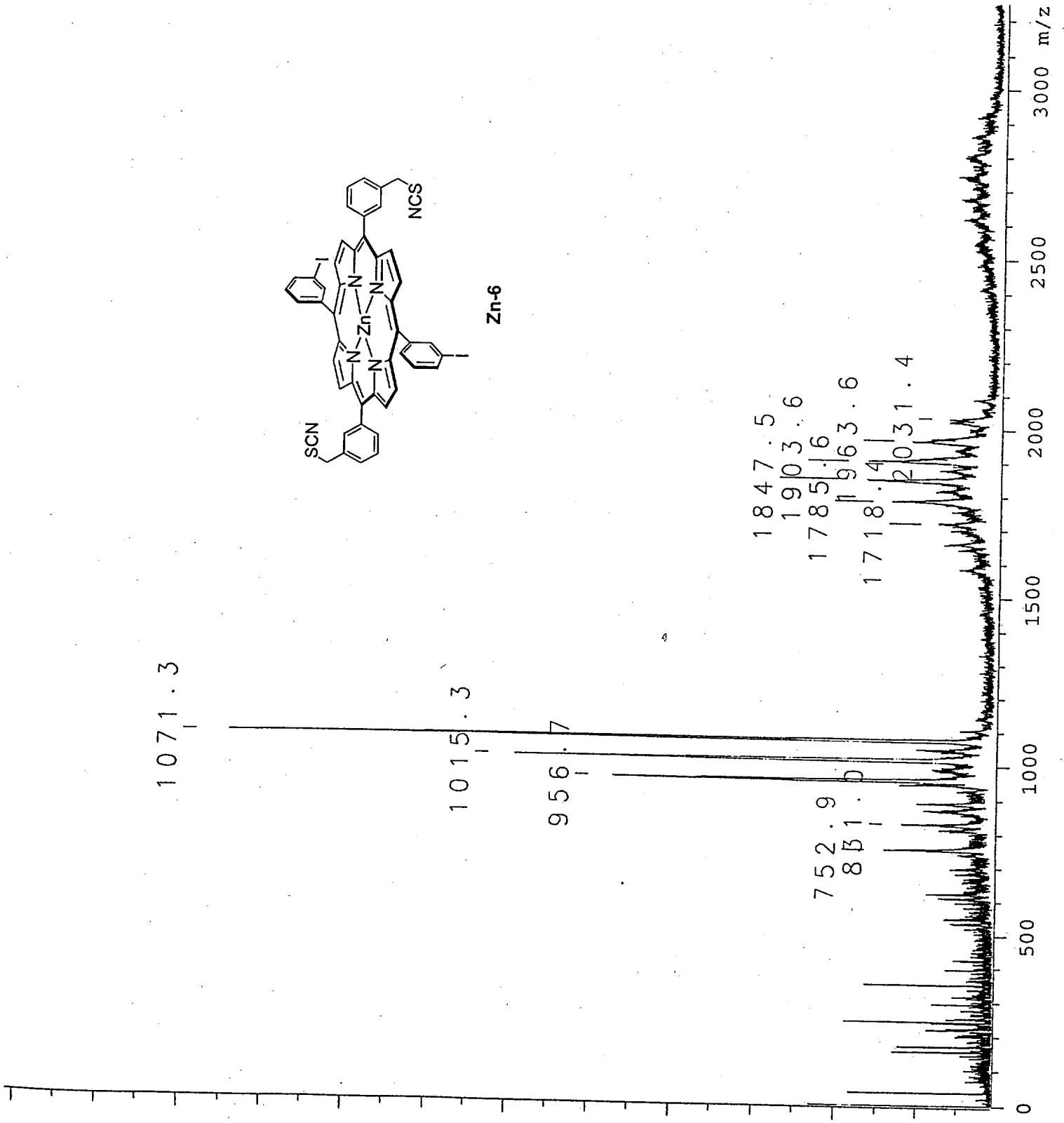



S8
ZnFb-5
ppm

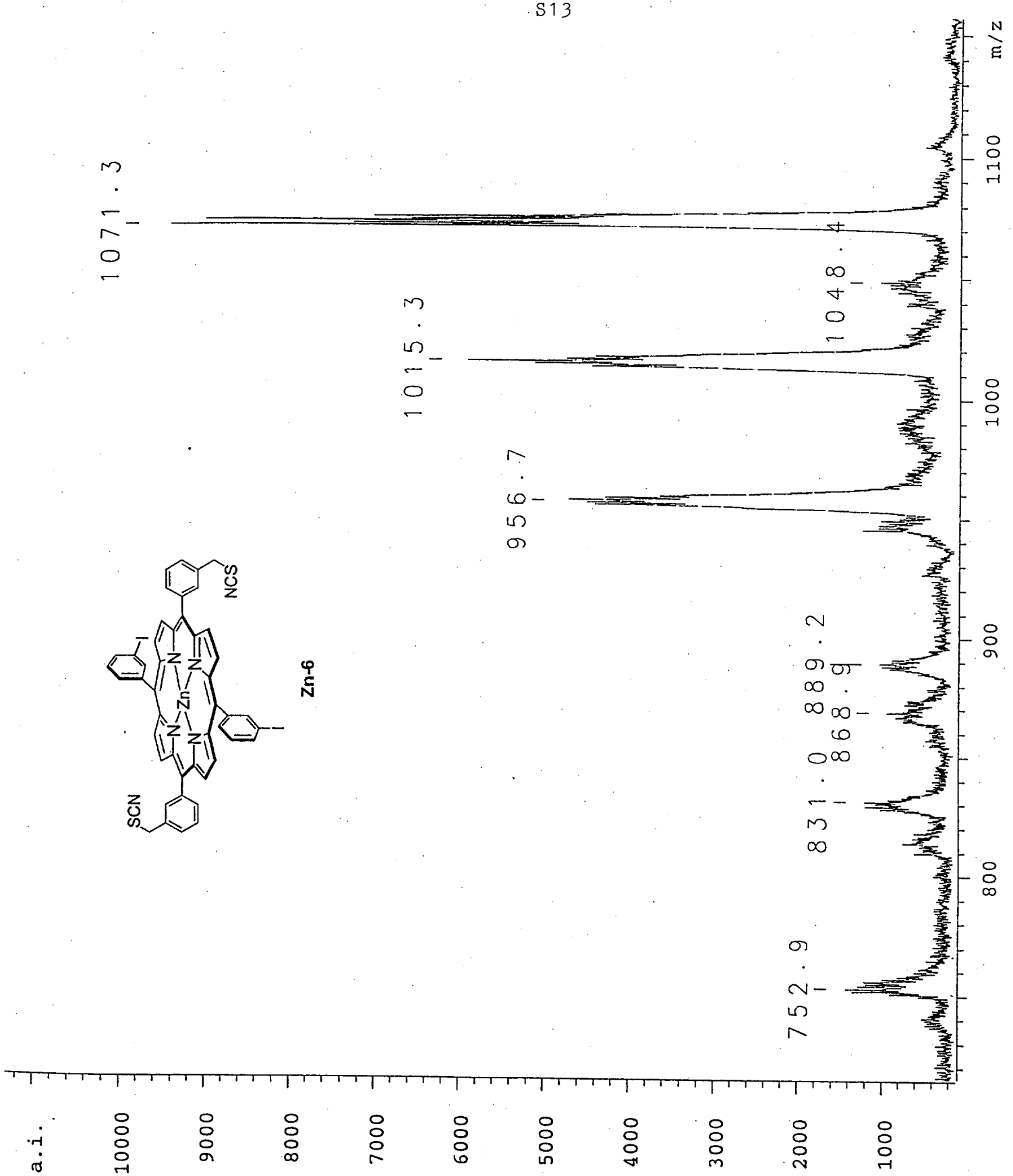




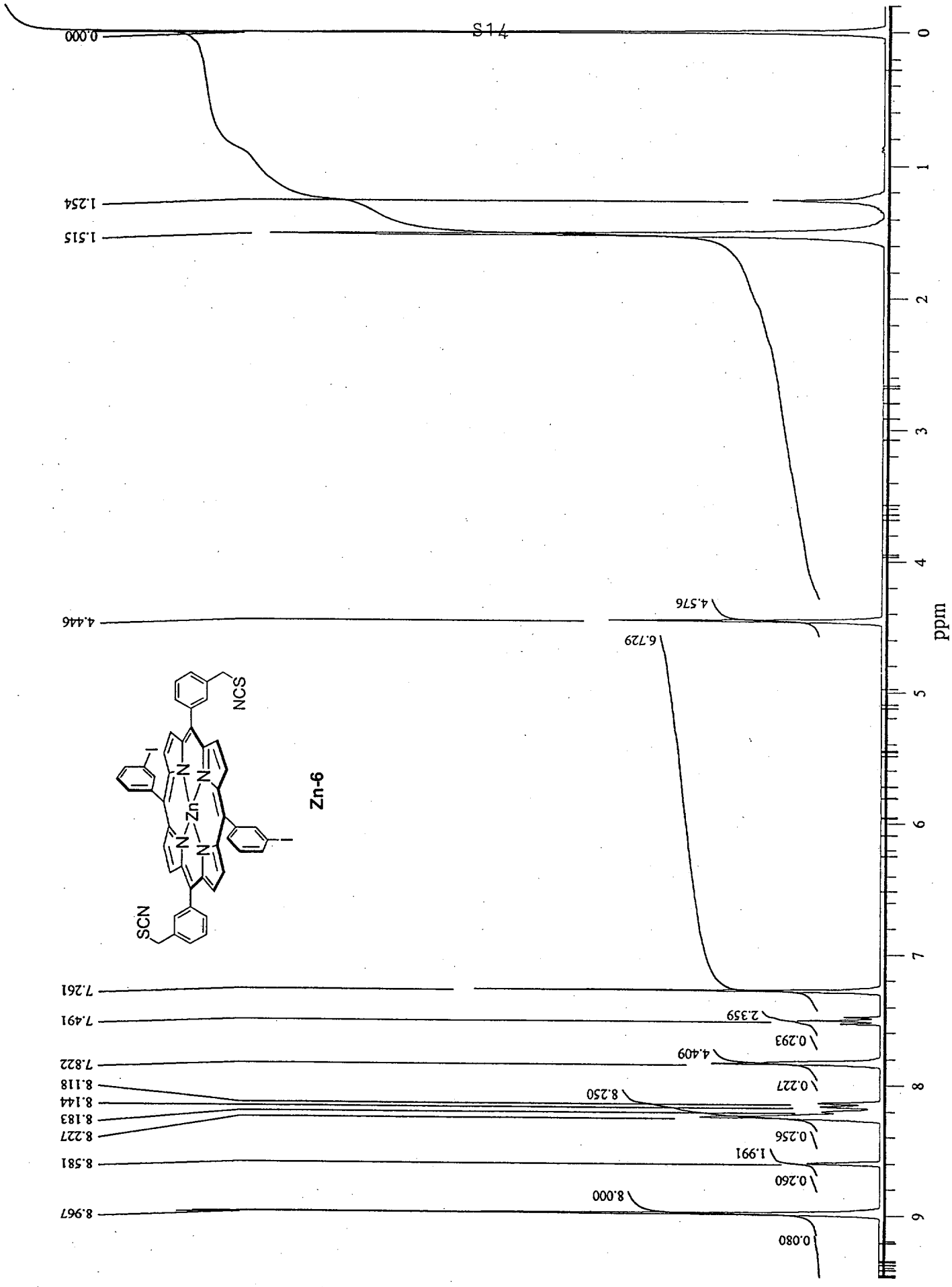


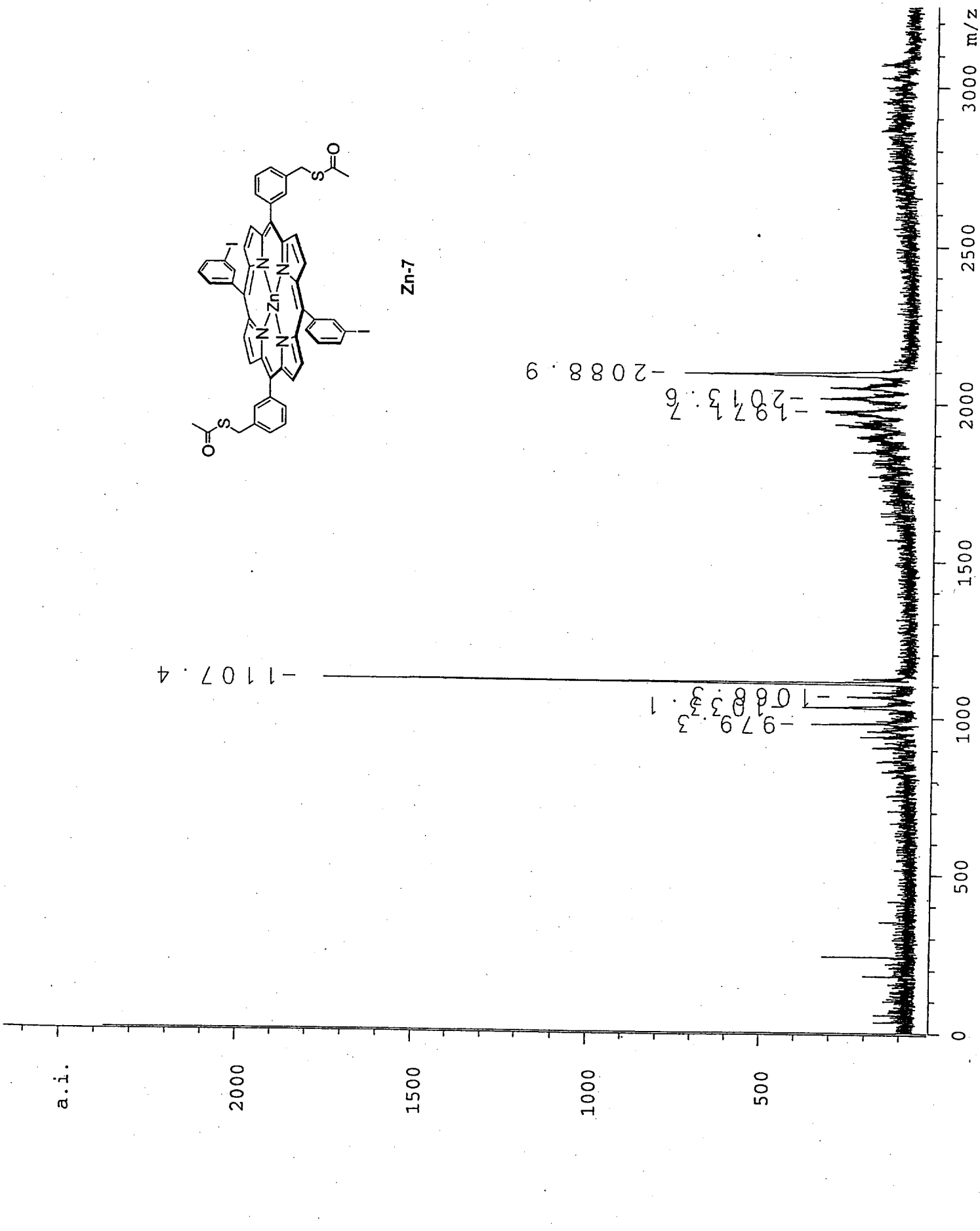


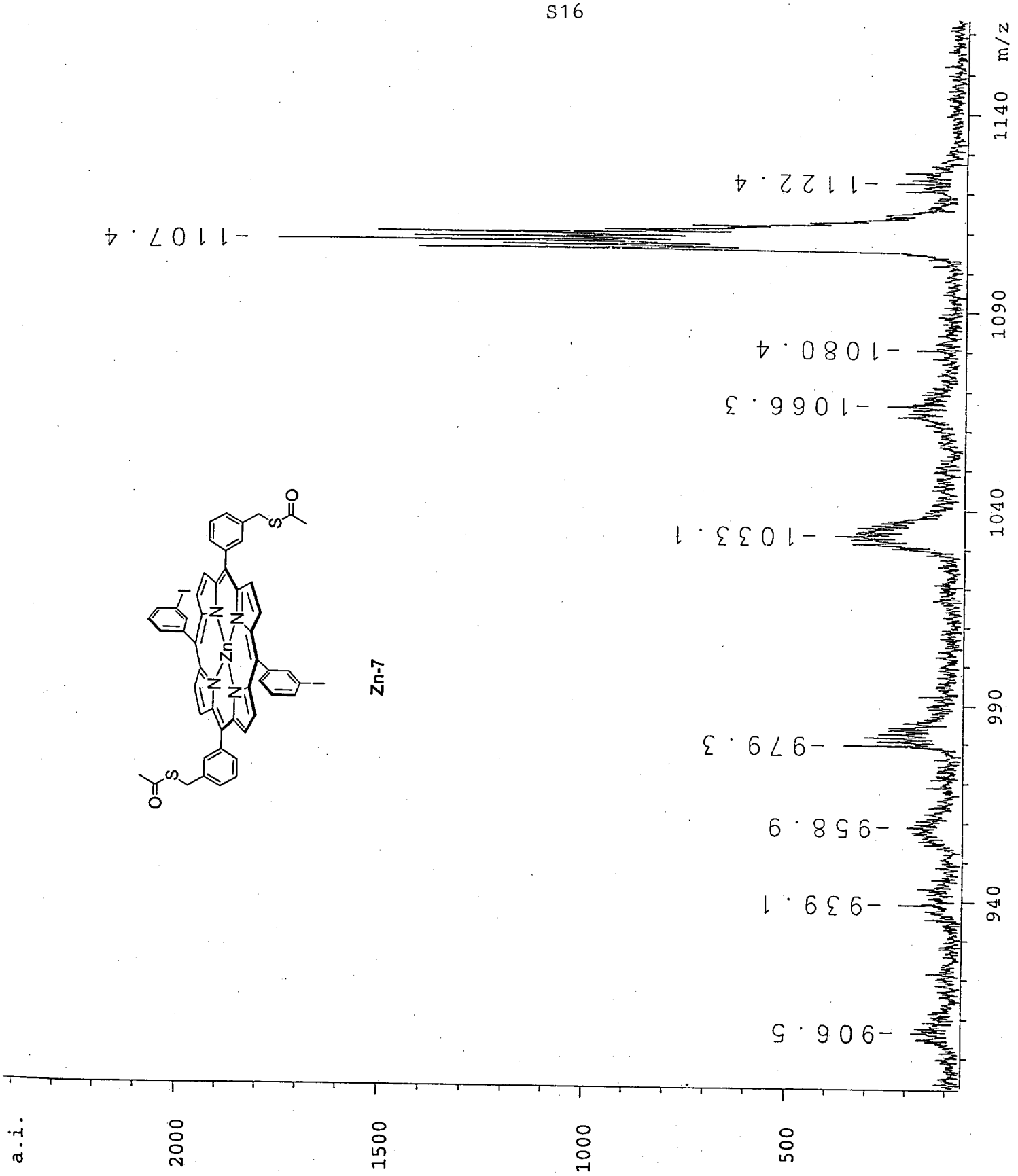
Zn-6

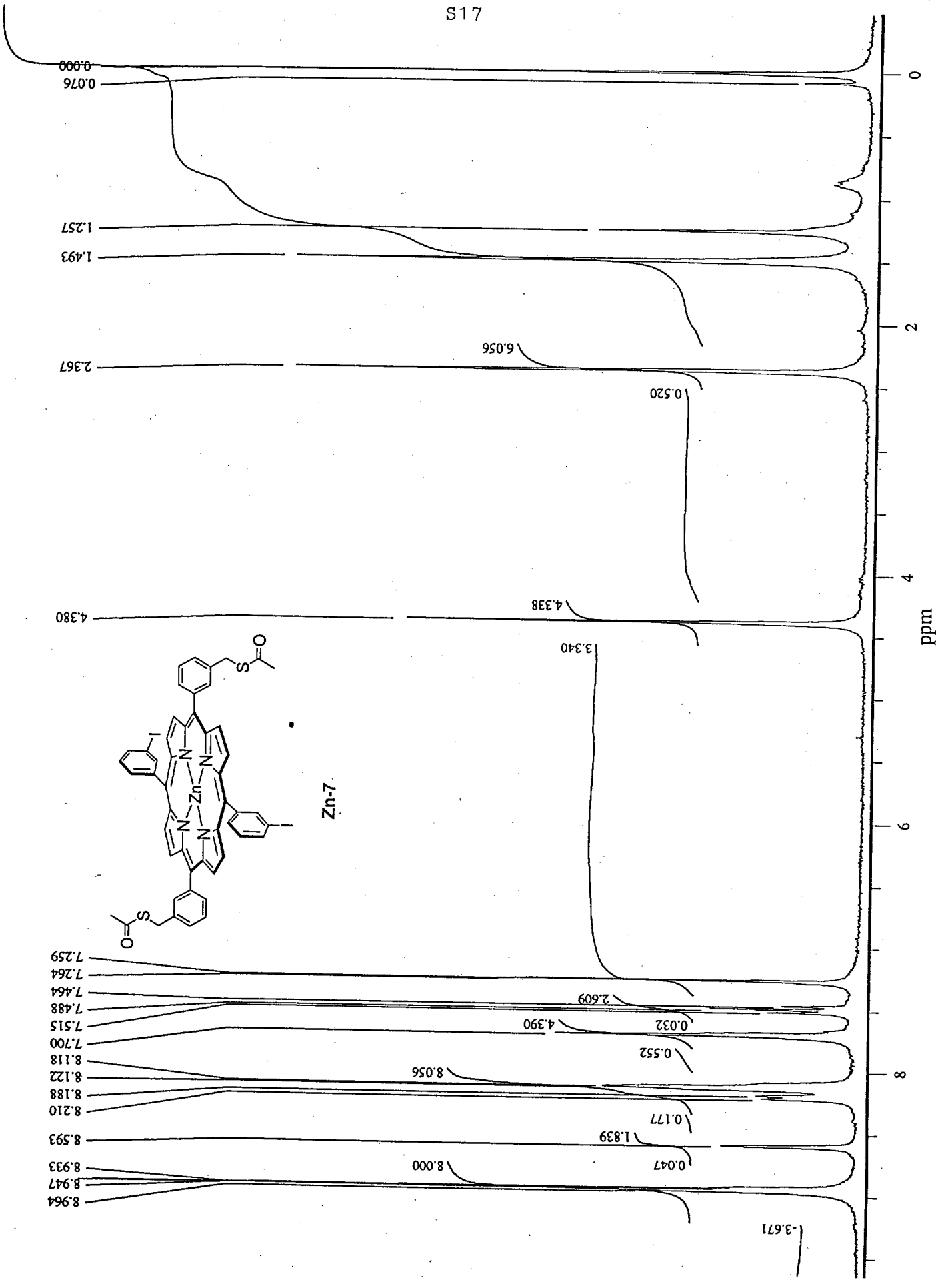


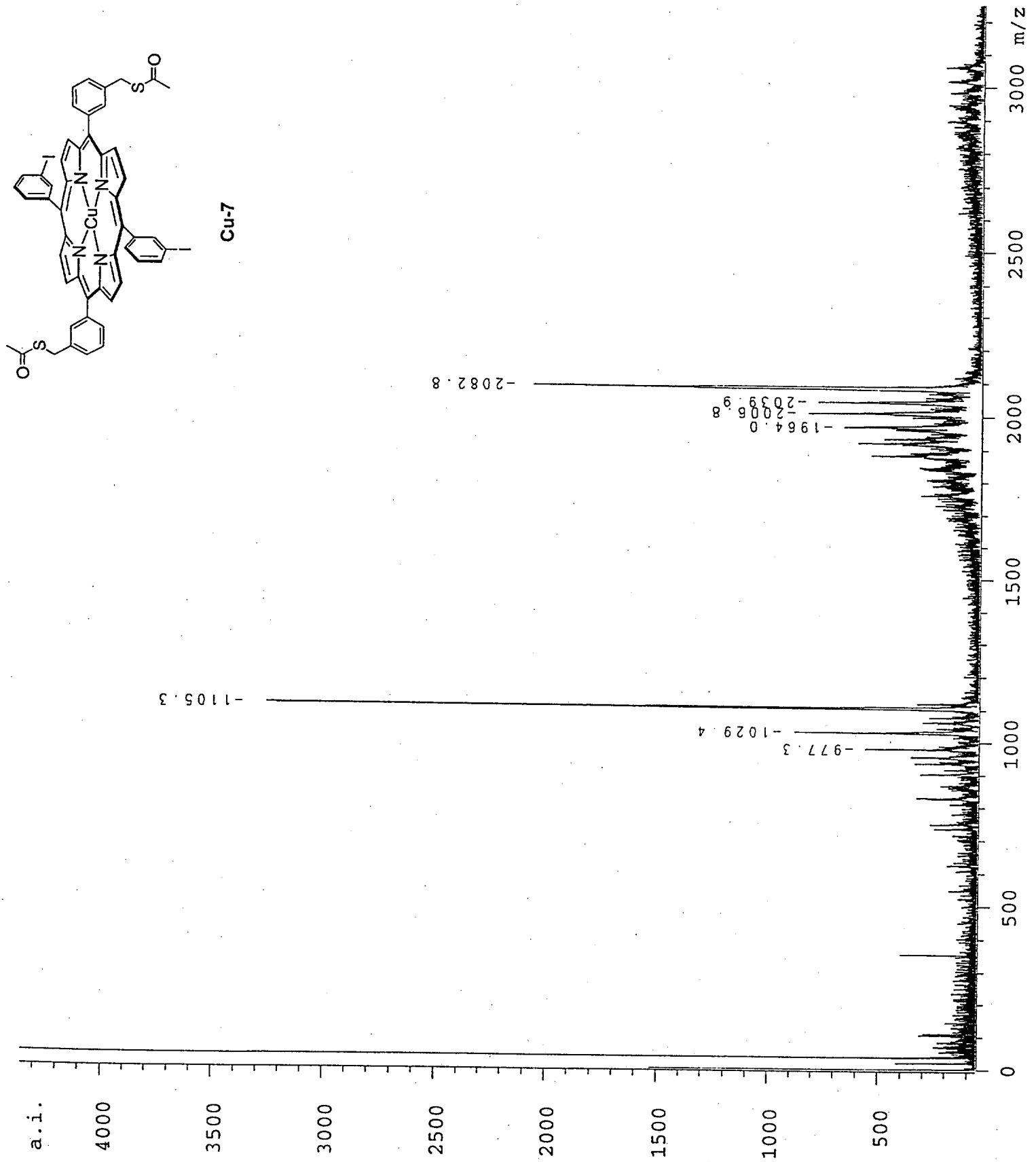
Zn-6

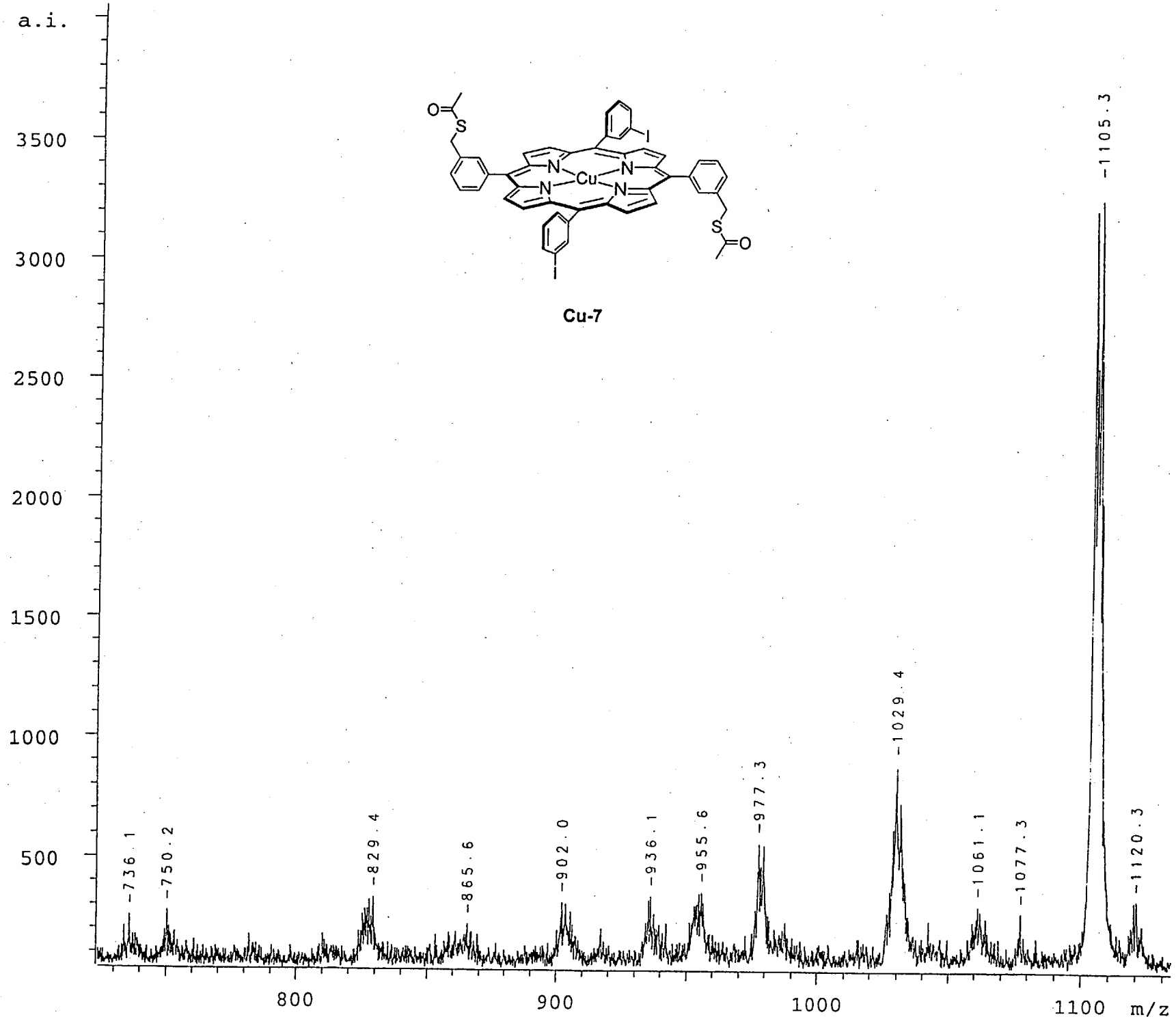


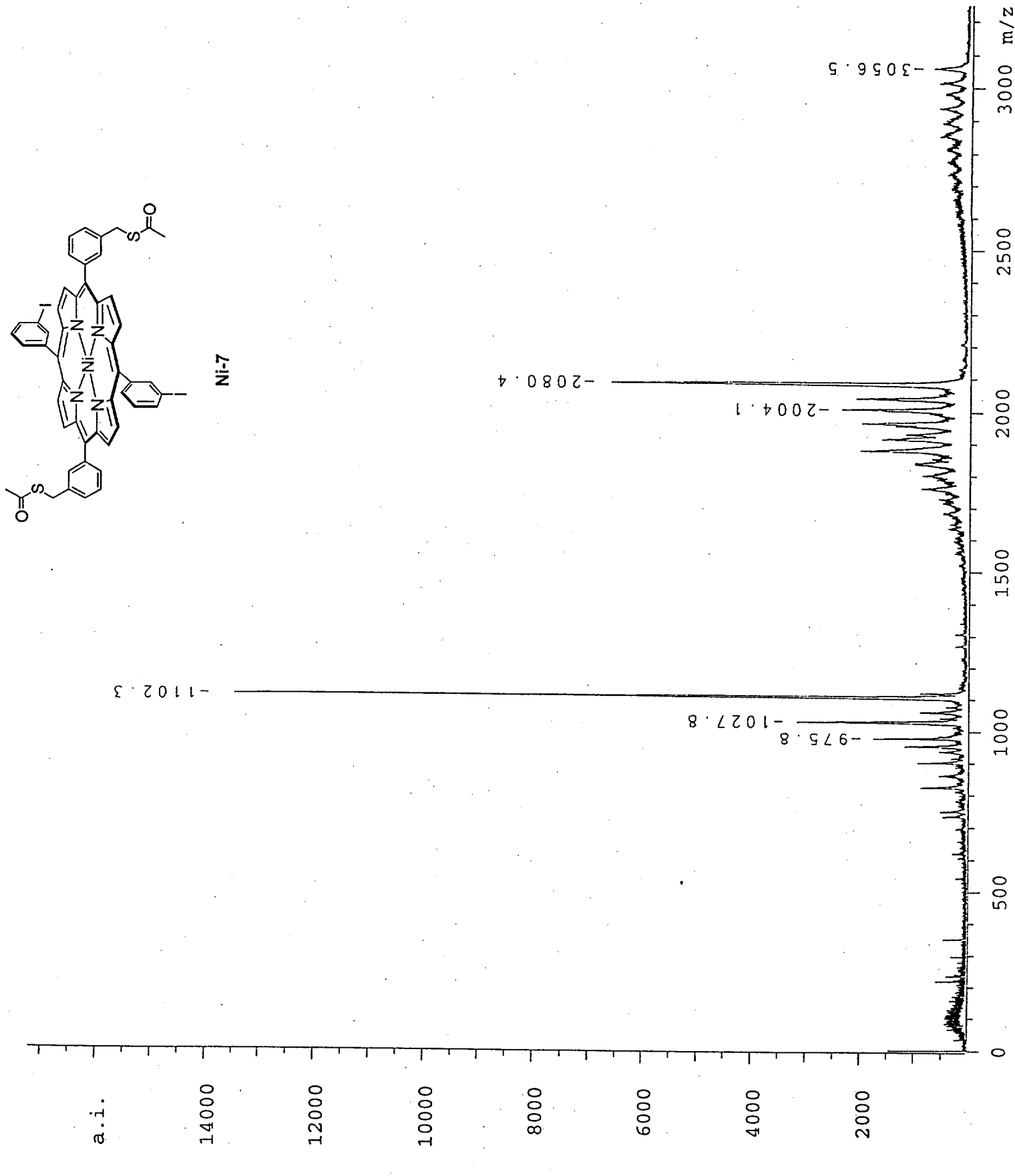


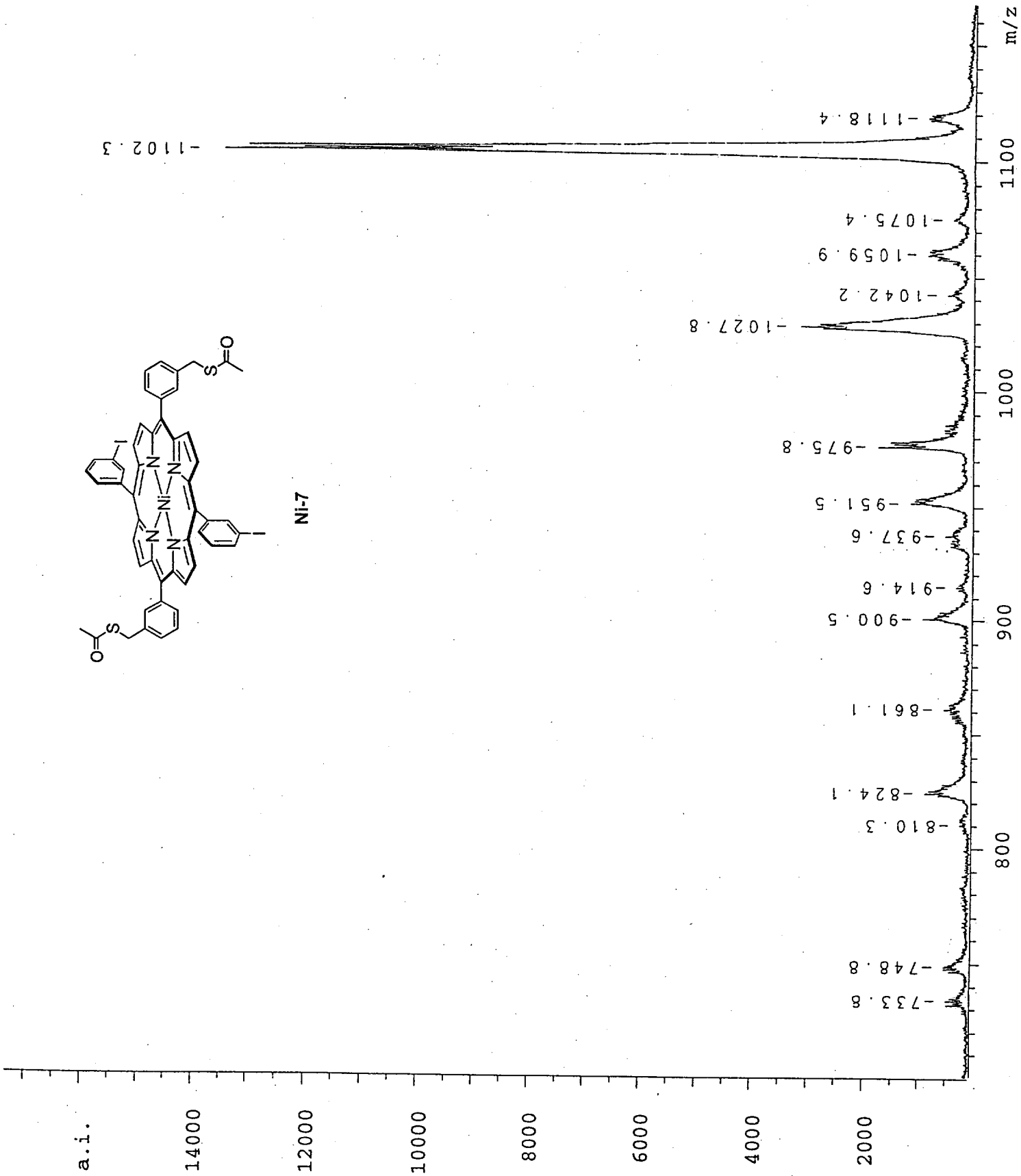


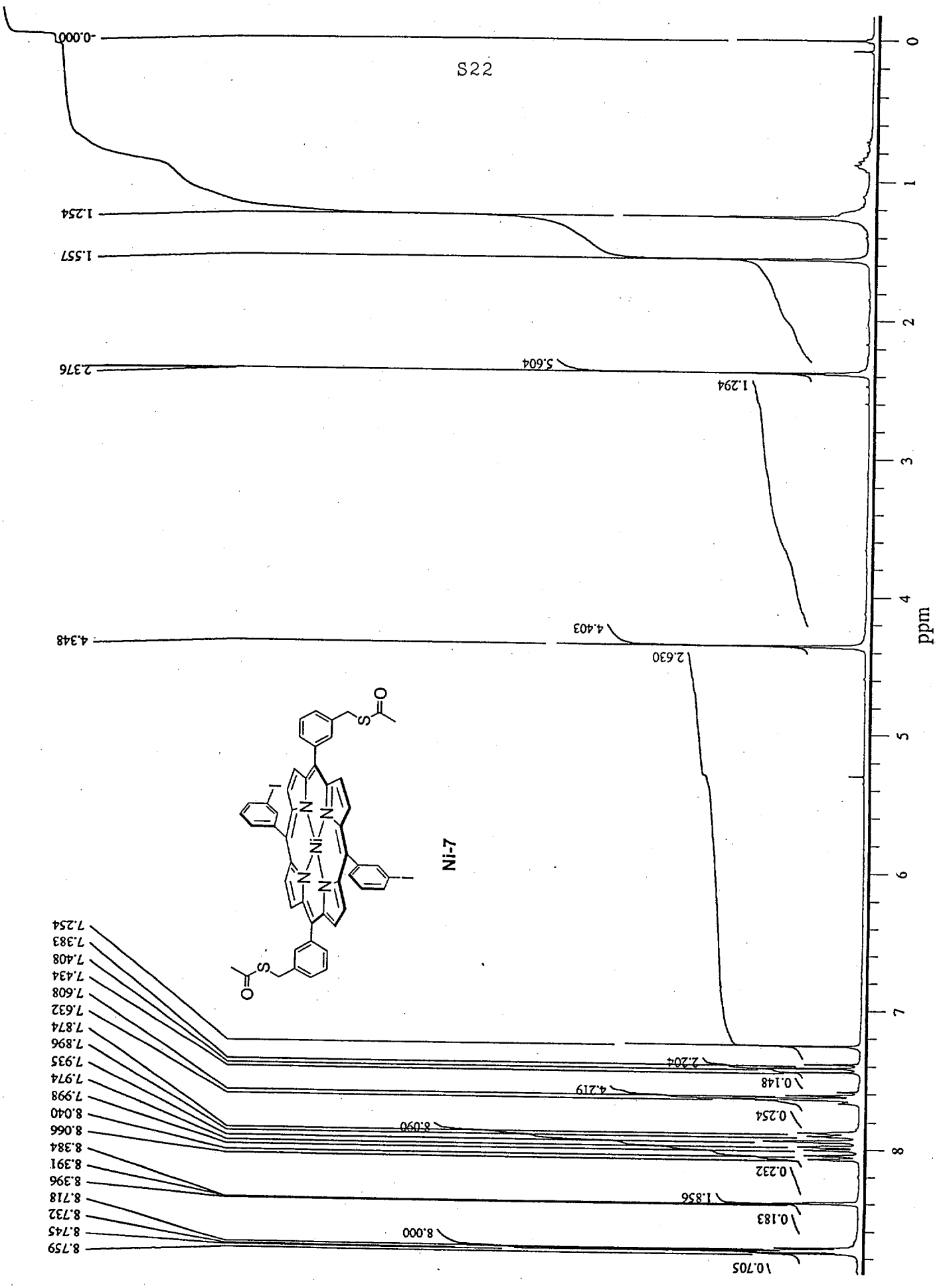


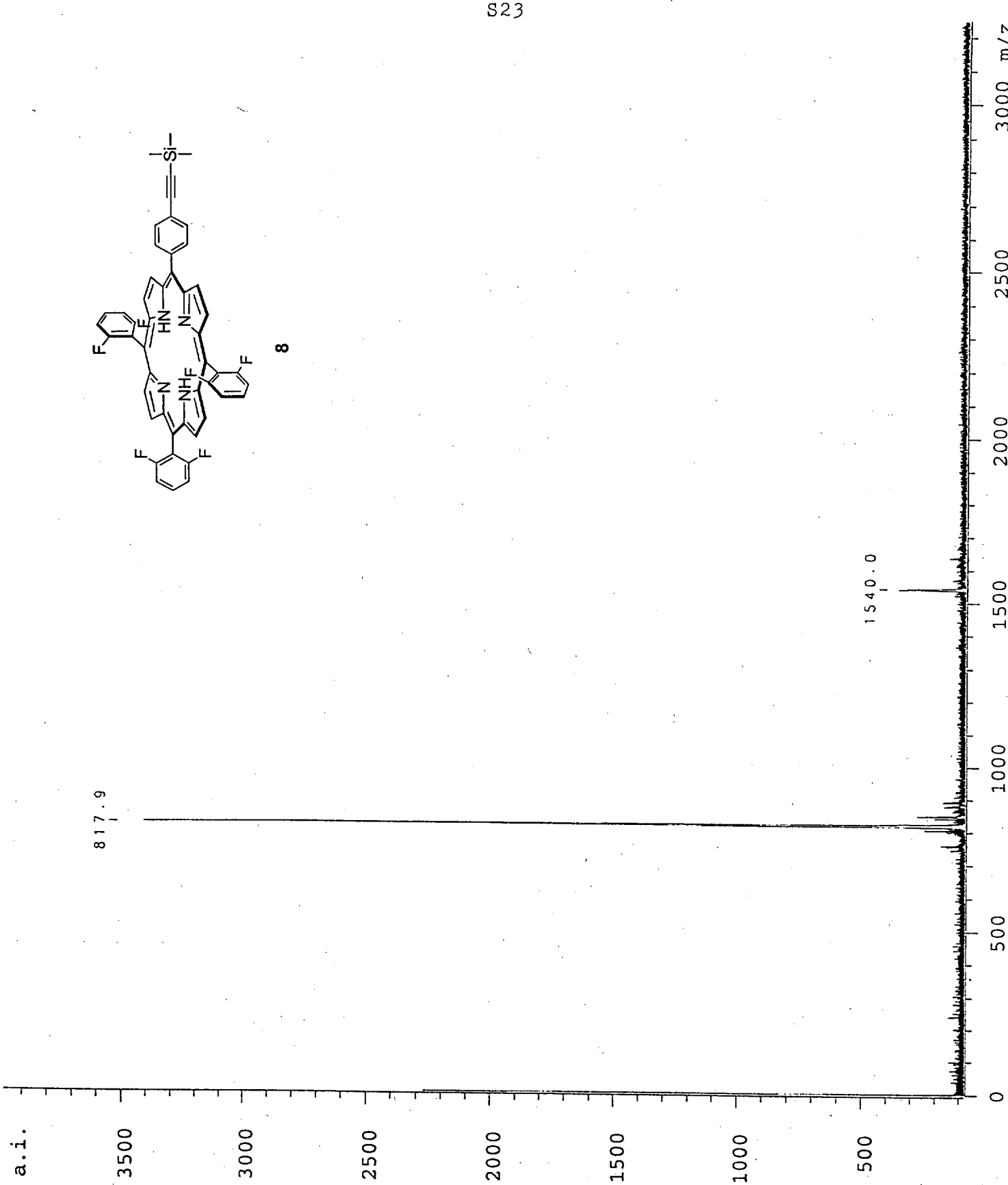












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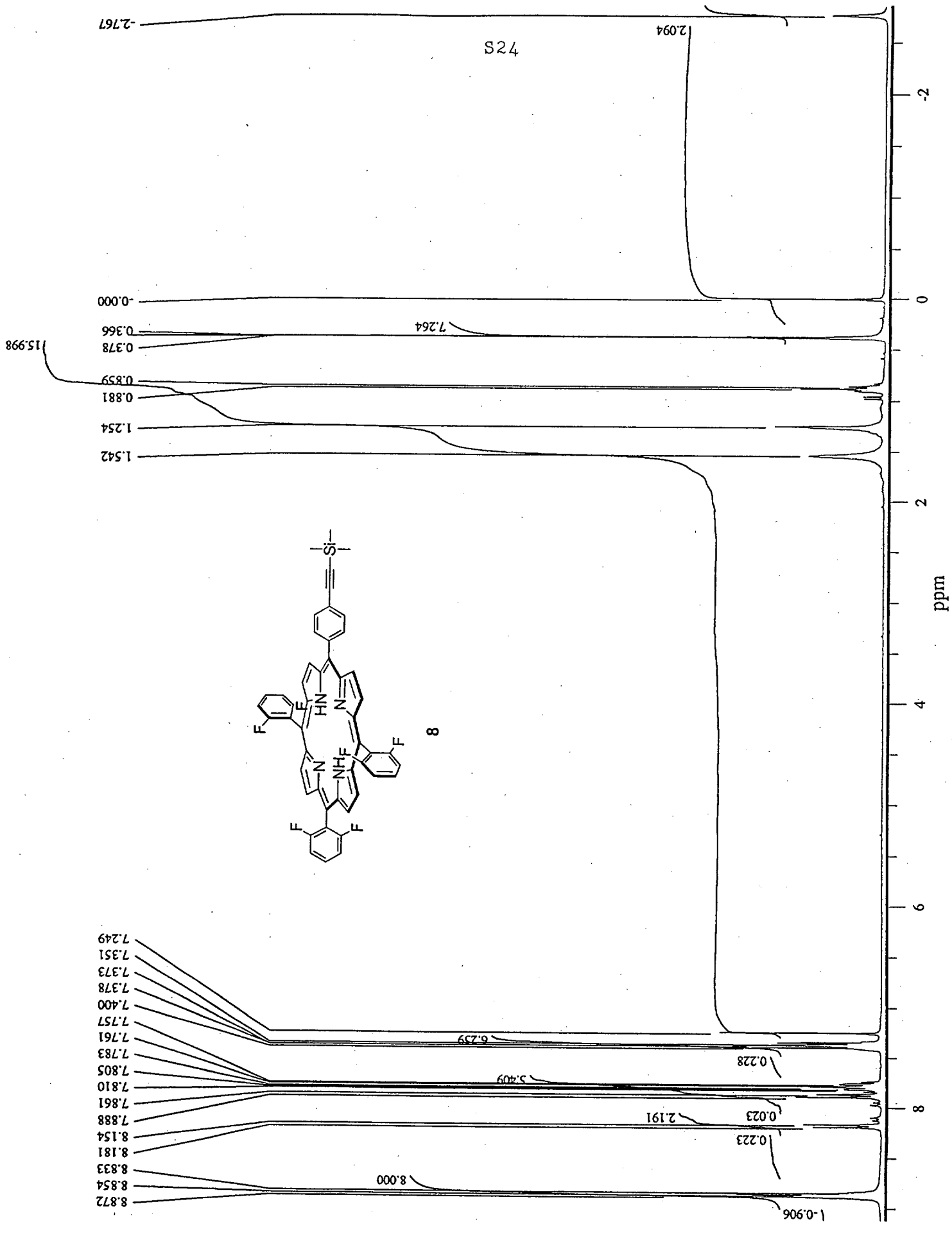
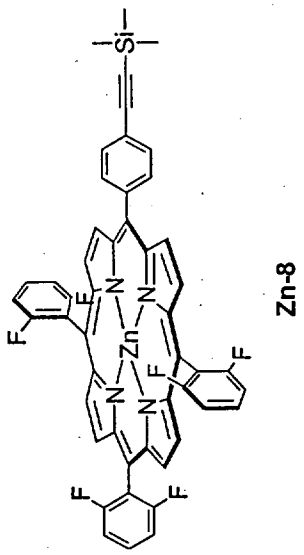
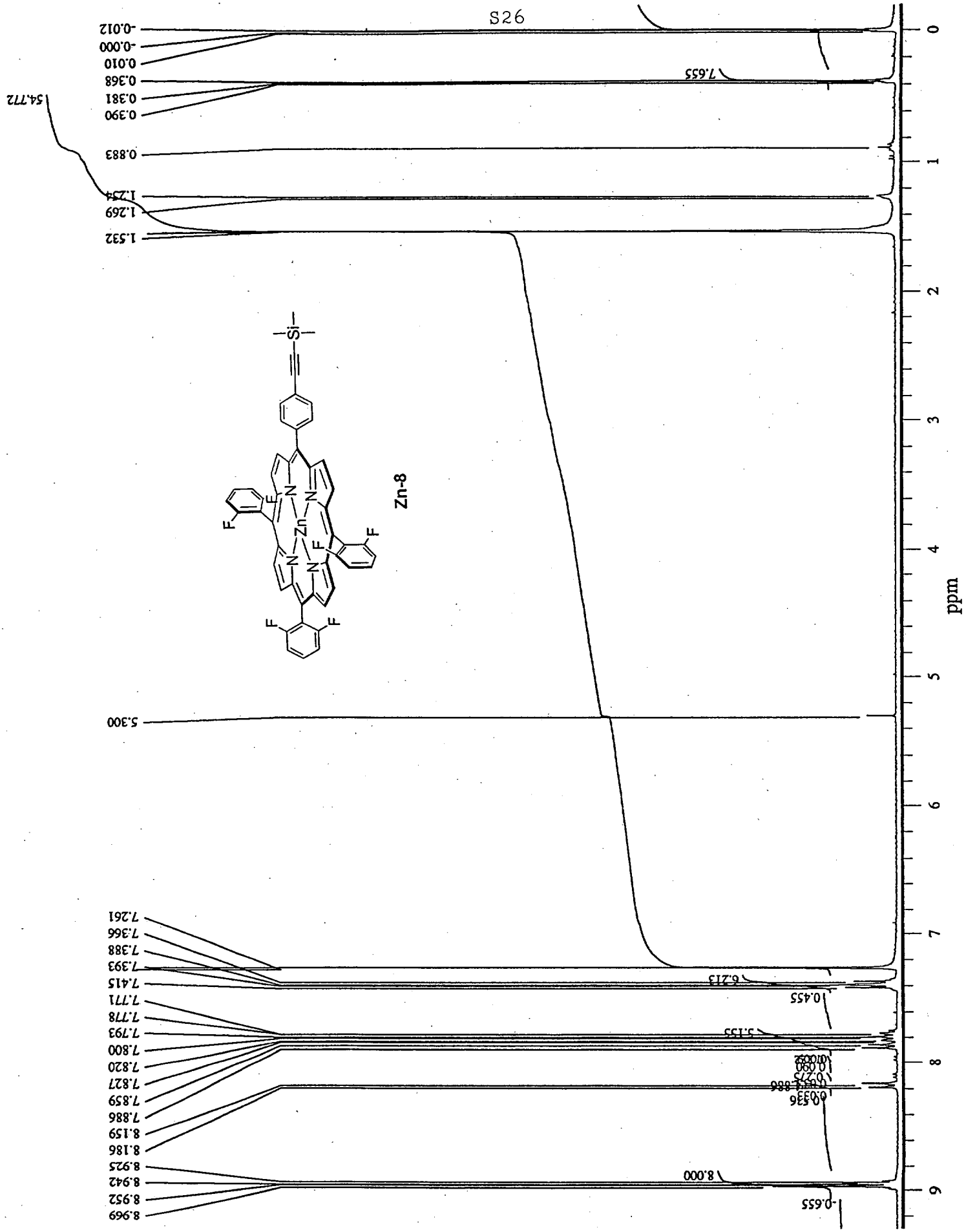
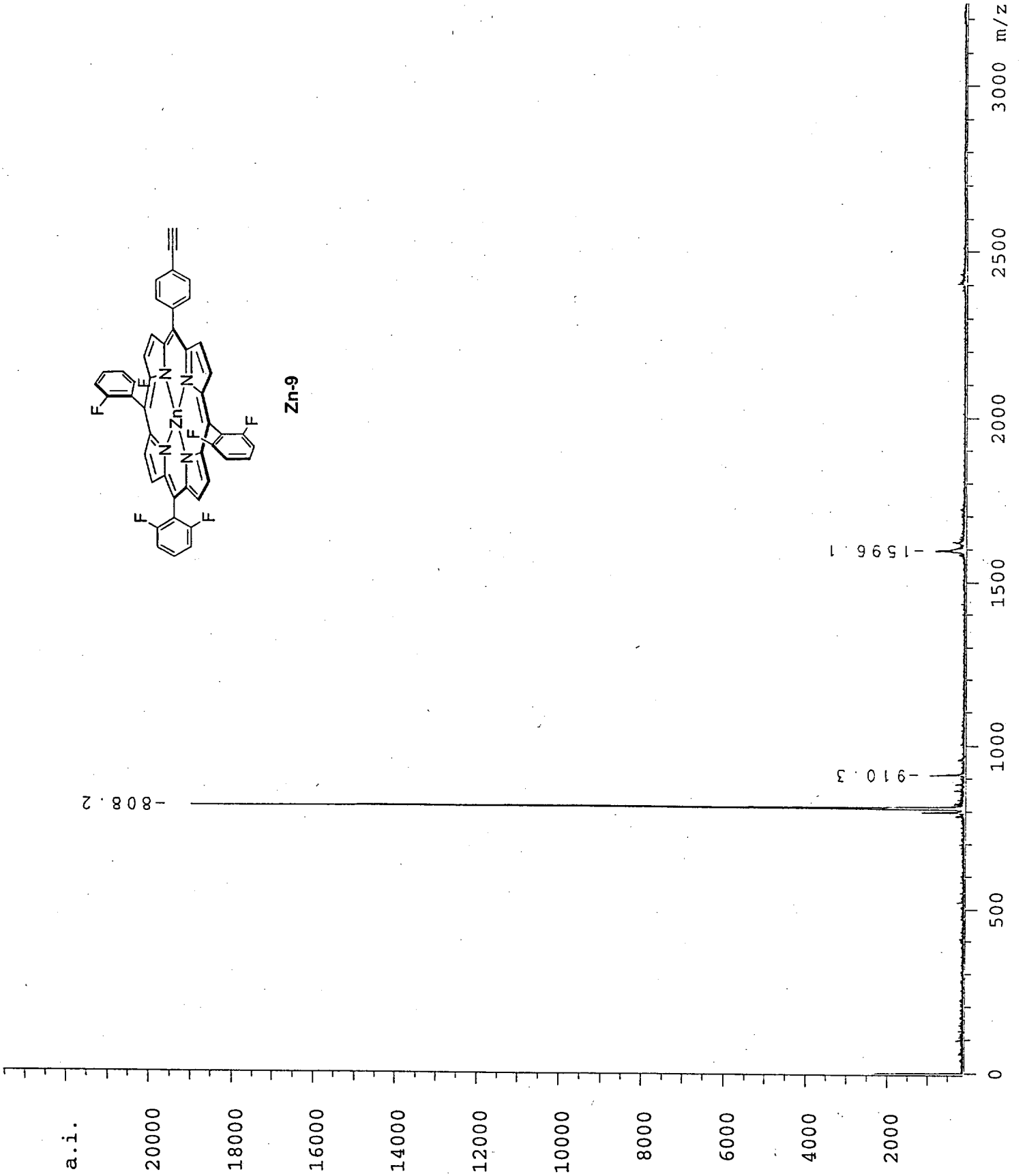
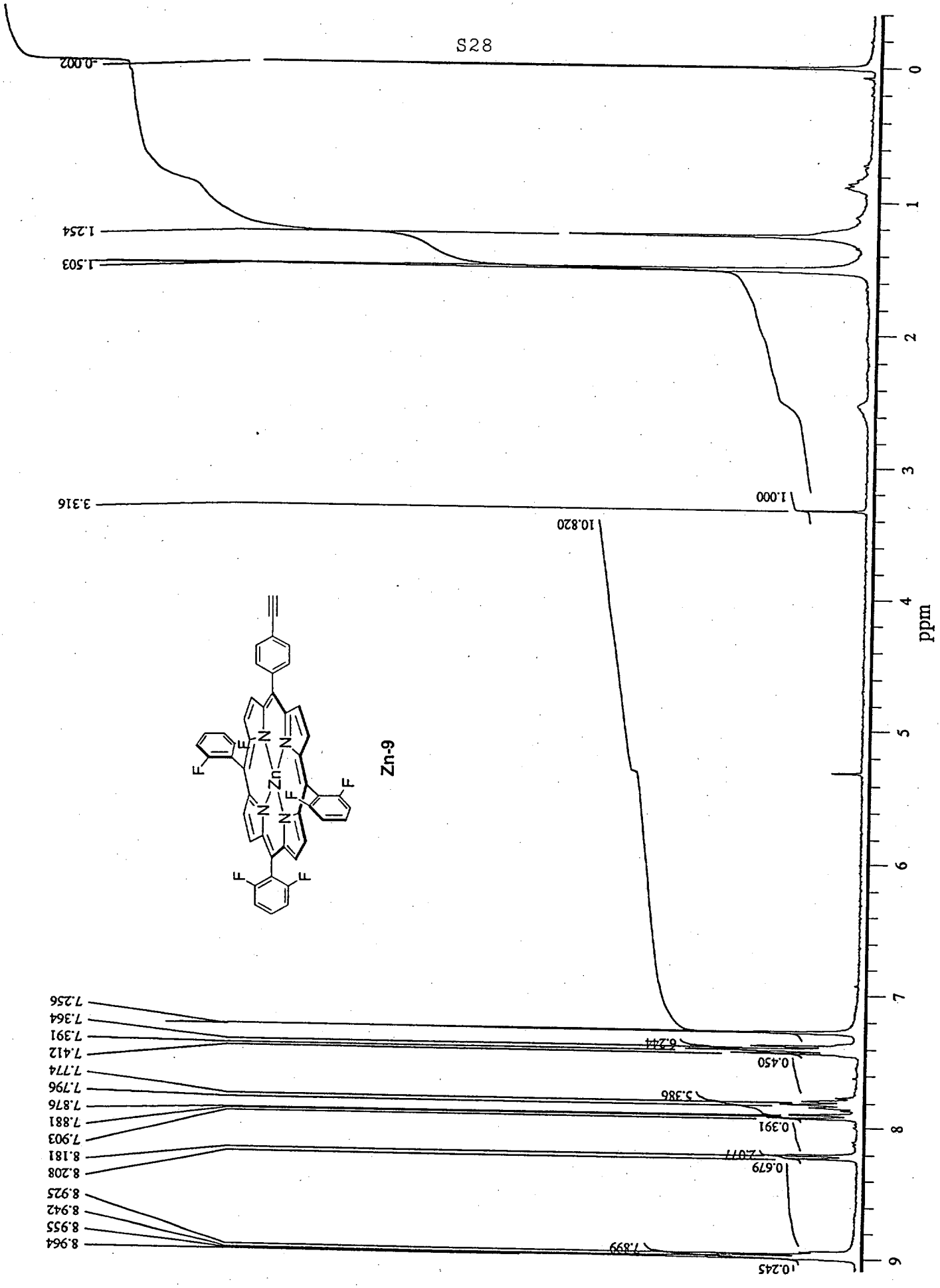


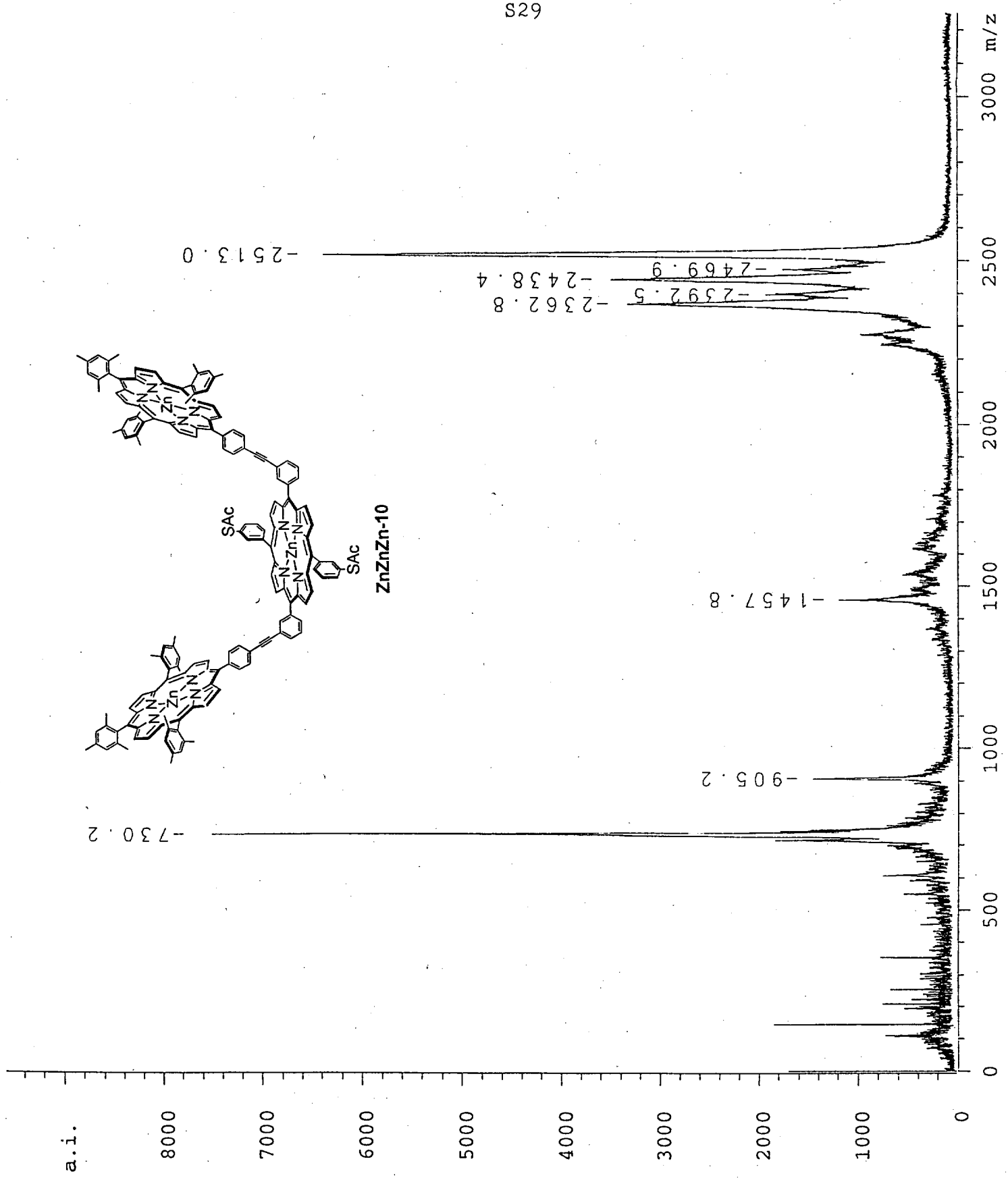


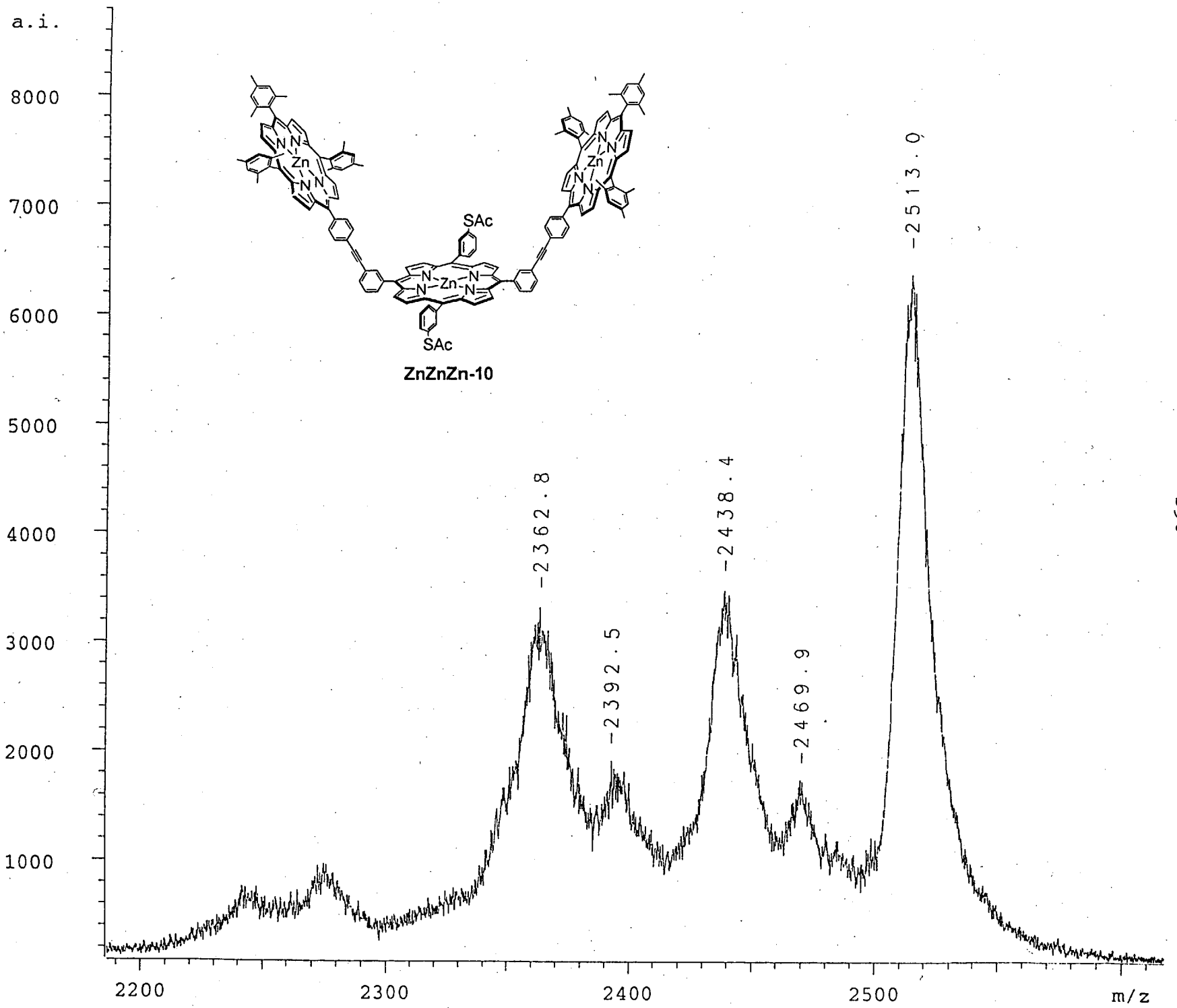
Zn-8

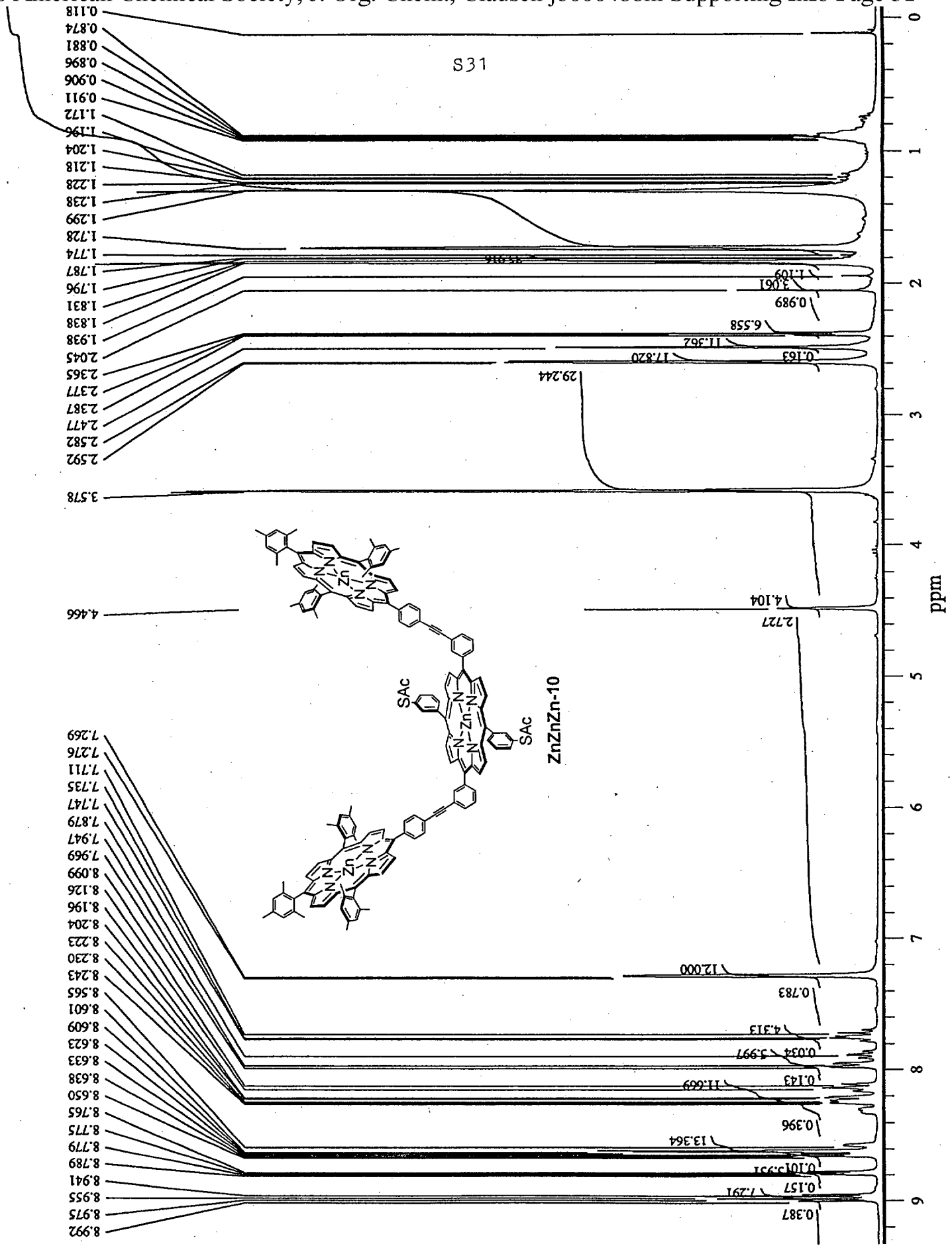


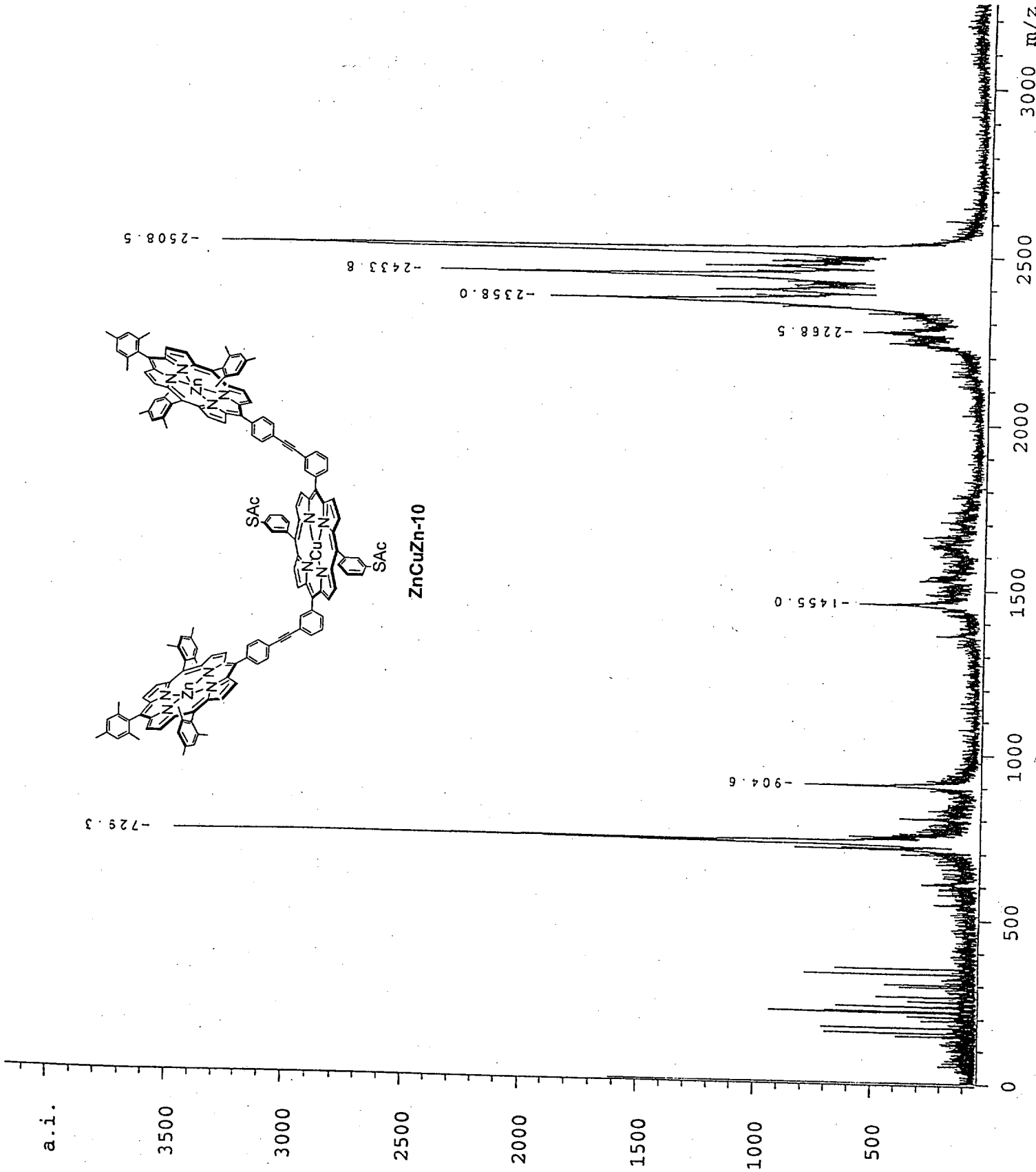


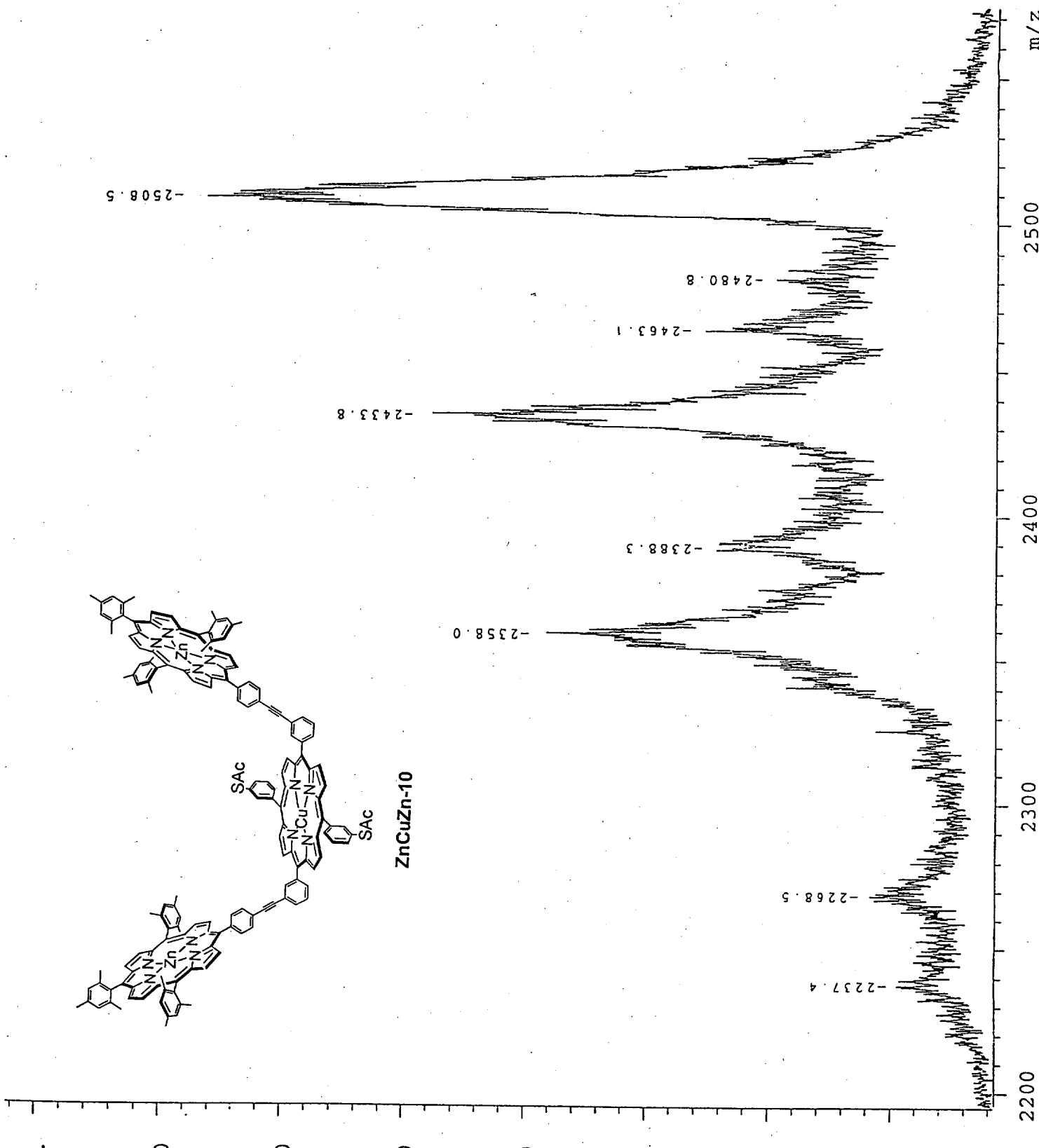


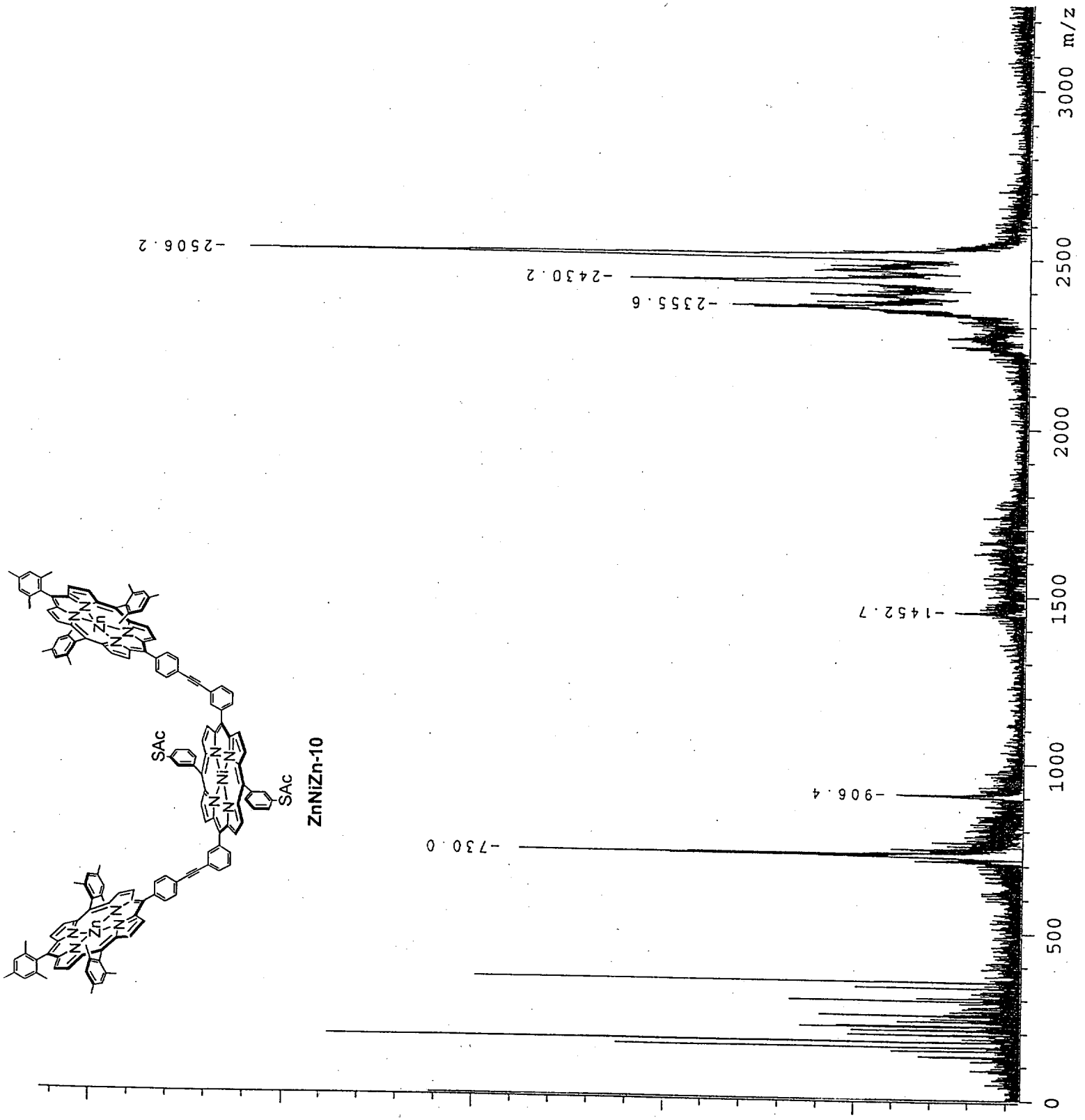


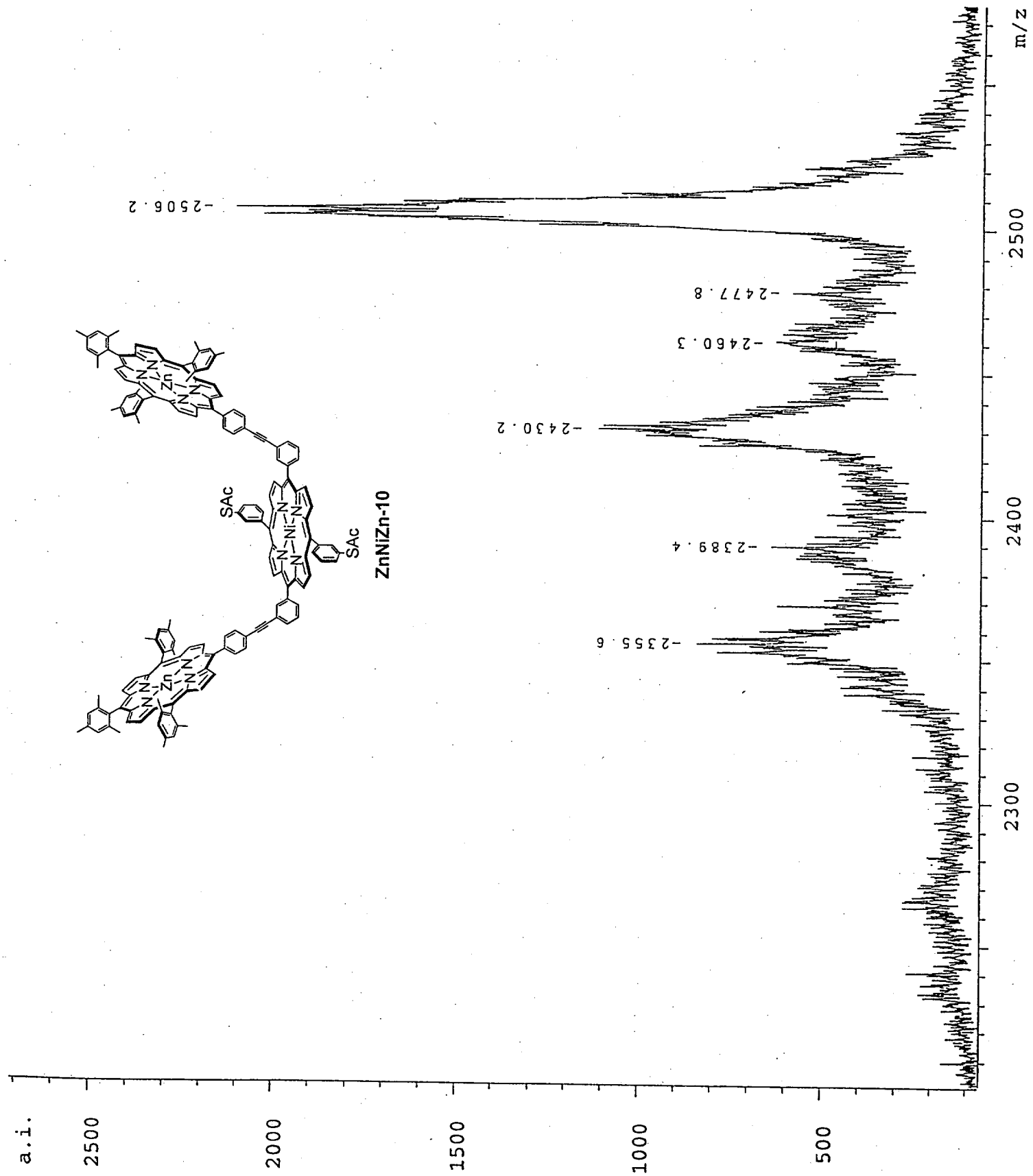


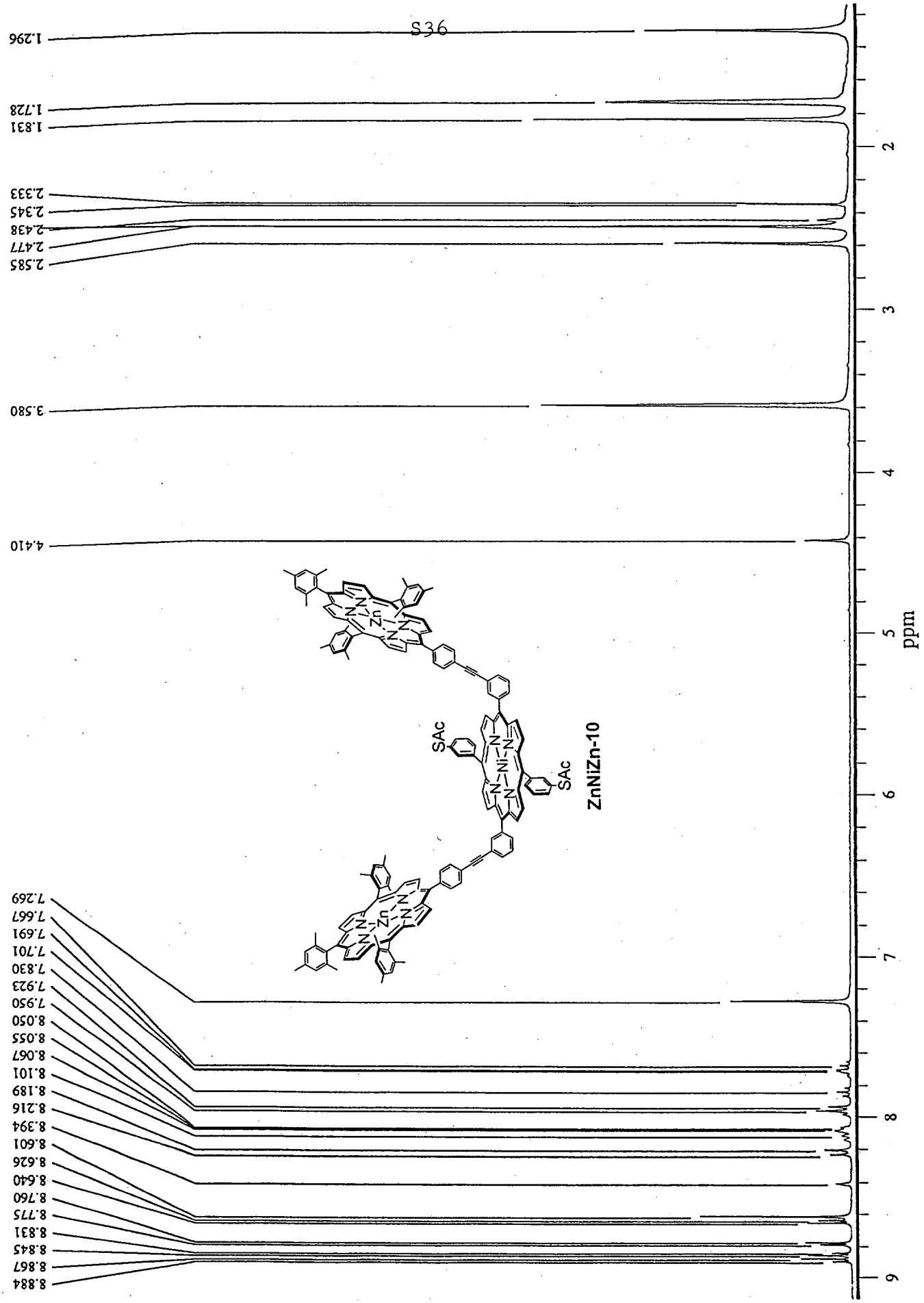


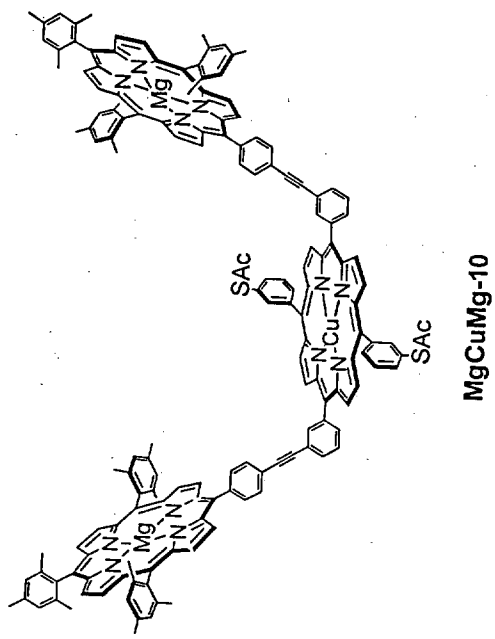












MgCuMg-10