Supplementary Material

Protecting-group-free synthesis of GF109203X

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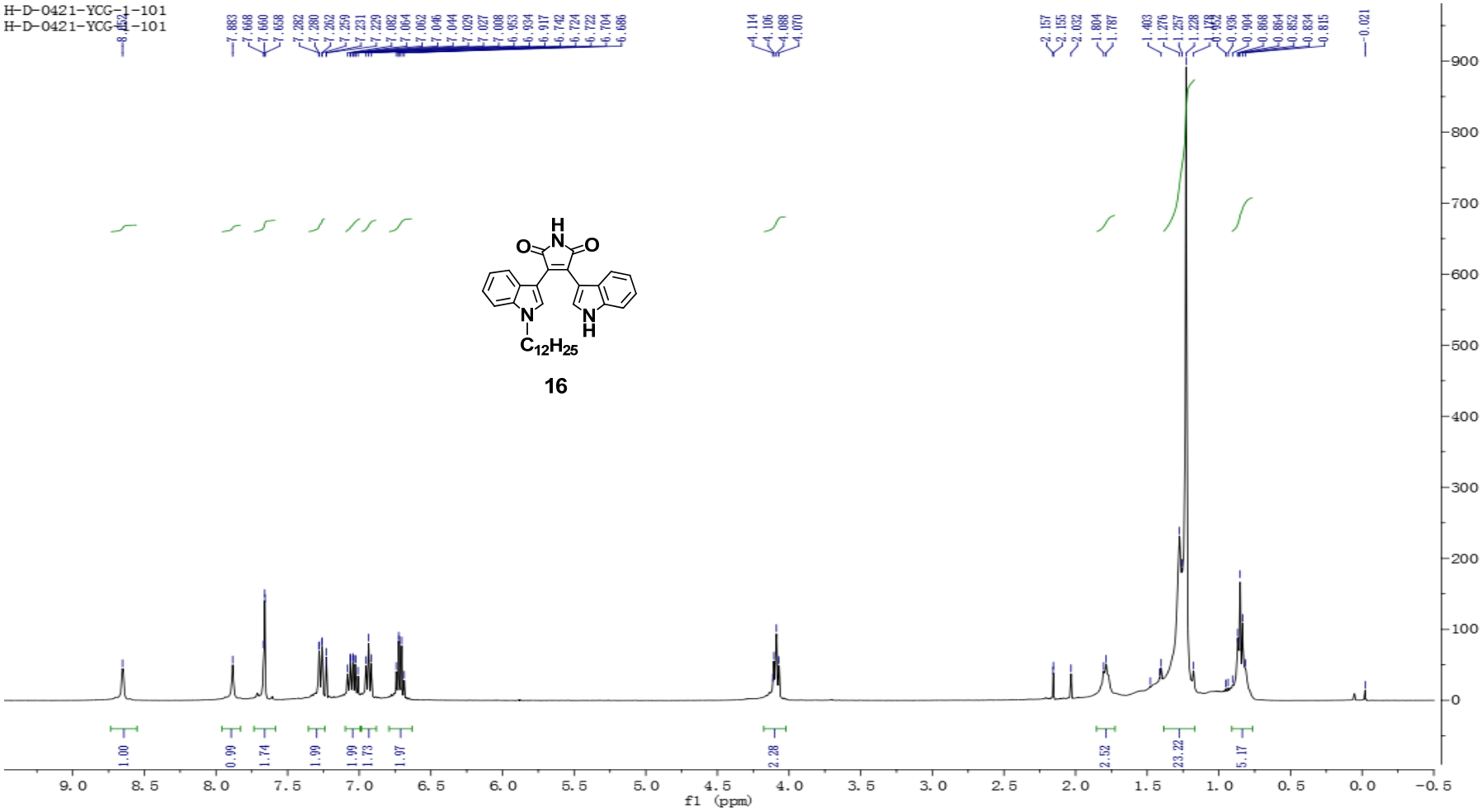
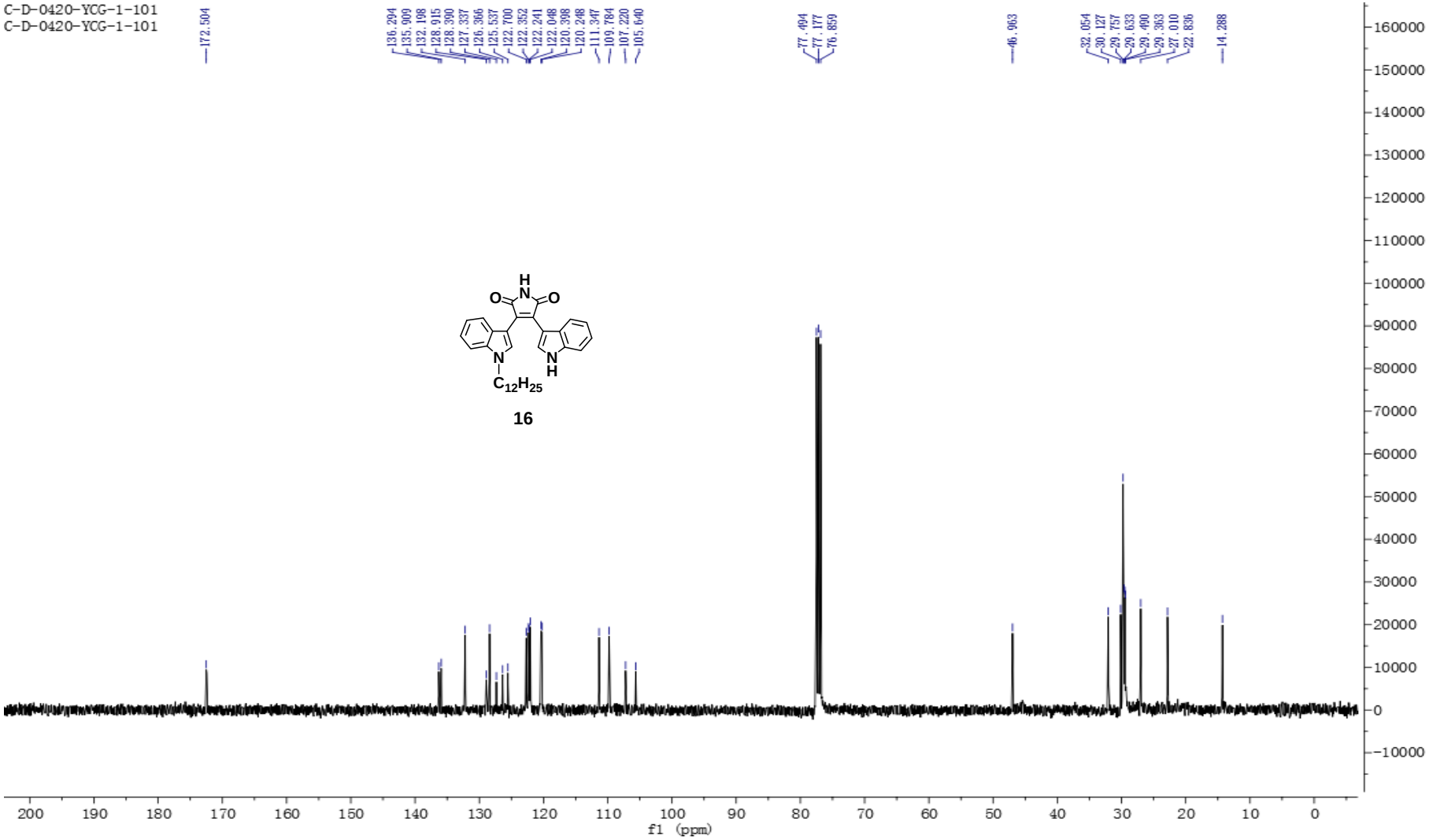
1. General Information

All reagents were used as received from commercial sources without further purification or prepared as described in the literature. Tetrahydrofuran was distilled from sodium and benzophenone immediately before use. Reactions were stirred using Teflon-coated magnetic stir bars. Analytical TLC was performed with 0.20 mm silica gel 60F plates. Chromatographic purification of products was carried out by flash chromatography on silica gel (230-400 mesh). Melting points were determined using a electrothermal melting point apparatus or DSC. Infrared spectra were recorded on a Nicolet 8700 Fourier transform spectrometer. NMR spectra were measured in $CDCl_3$ (with TMS as internal standard) or DMSO-d6 on a Bruker AV400 or Varian INOVA-400M (^1H at 400 MHz, ^{13}C at 100 MHz) magnetic resonance spectrometer. Chemical shifts (δ) are reported in ppm, and coupling constants (*J*) are in Hz. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High-resolution EI mass spectra (HR-EI-MS) were recorded on an GCT CA127 Micronass UK mass spectrometer.

2. ^{1}H, ^{13}C-NMR, IR and HR-MS Spectrum





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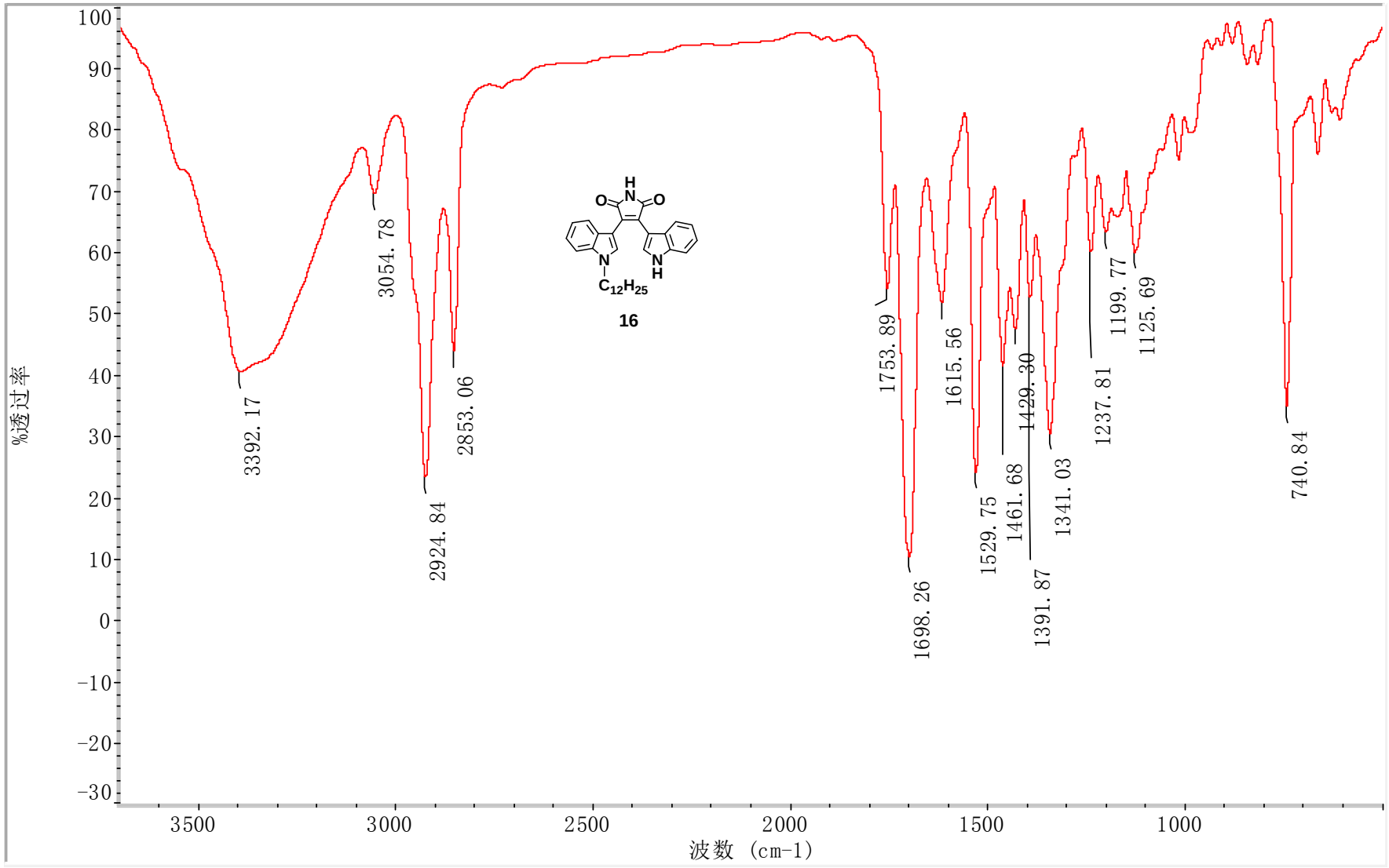

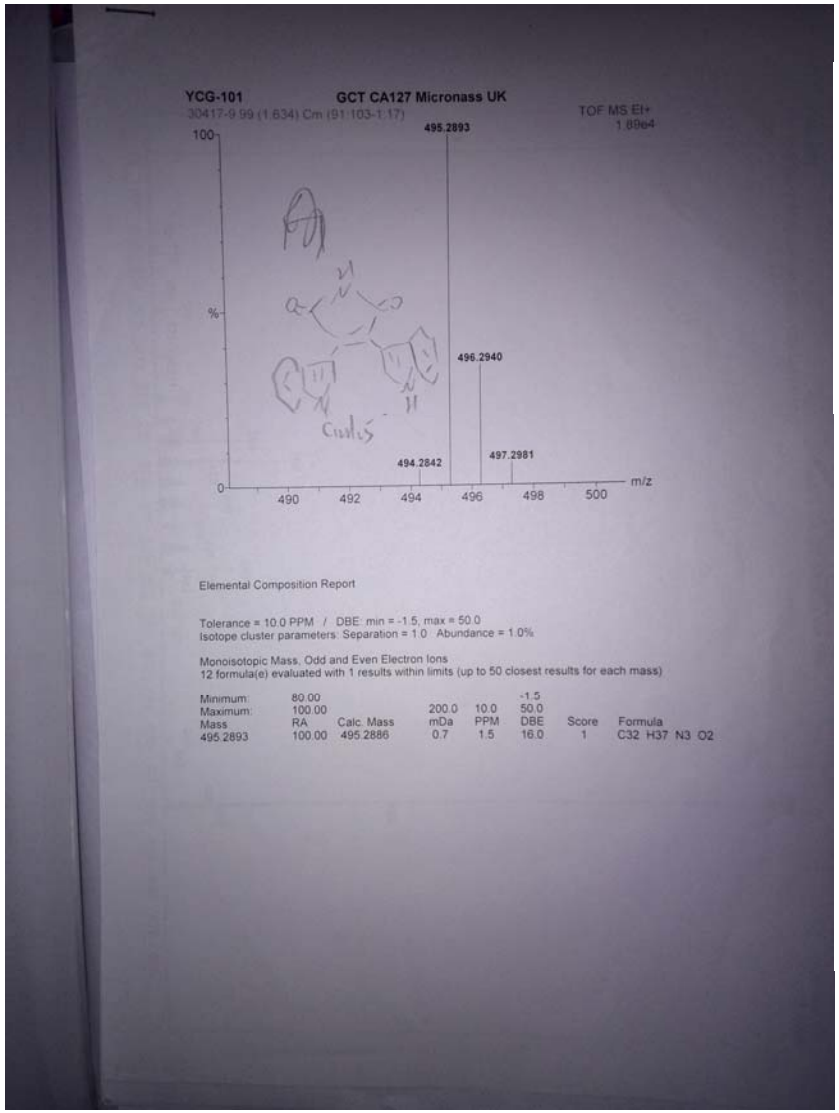

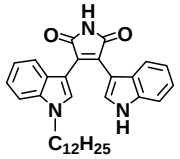

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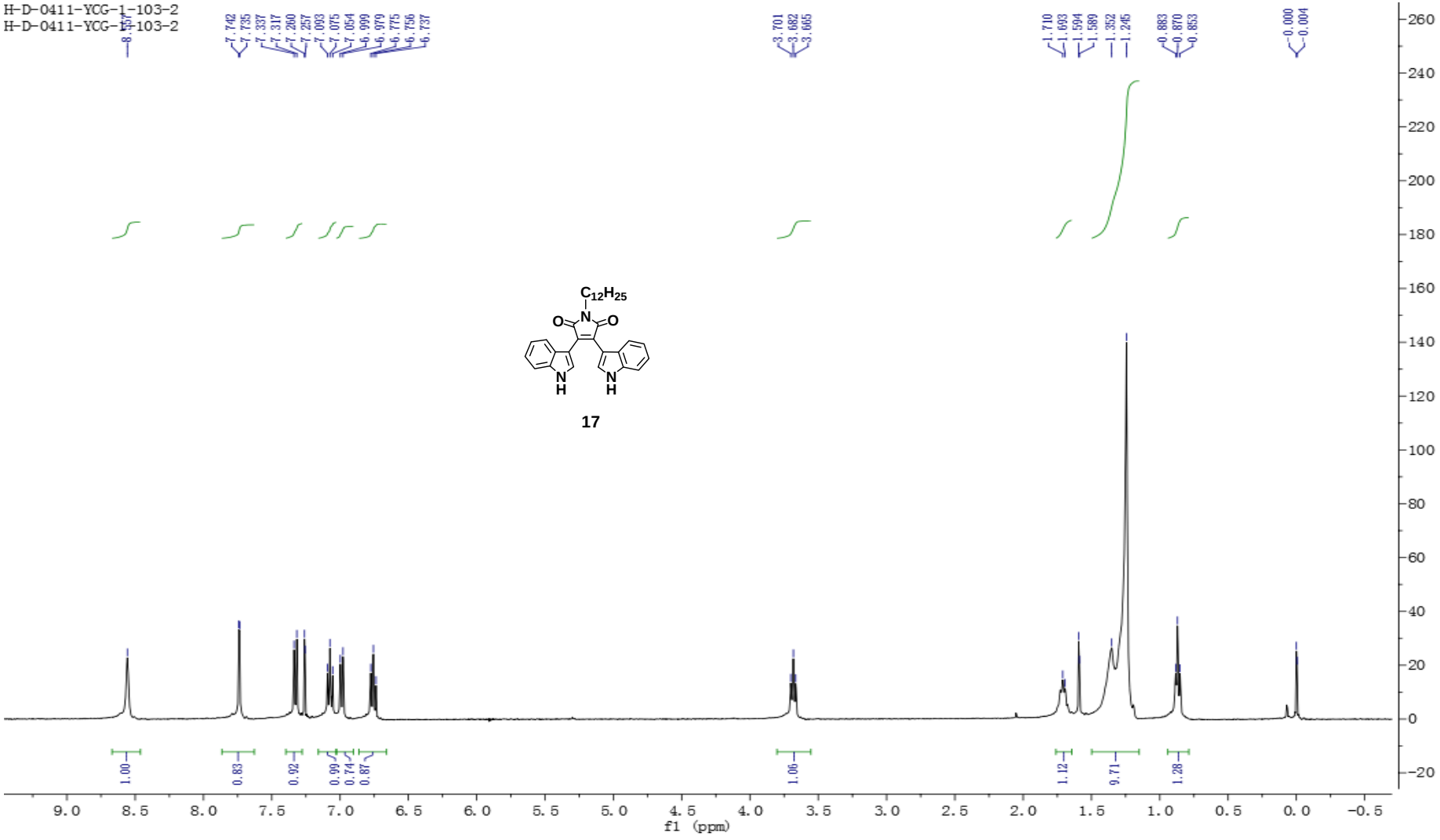

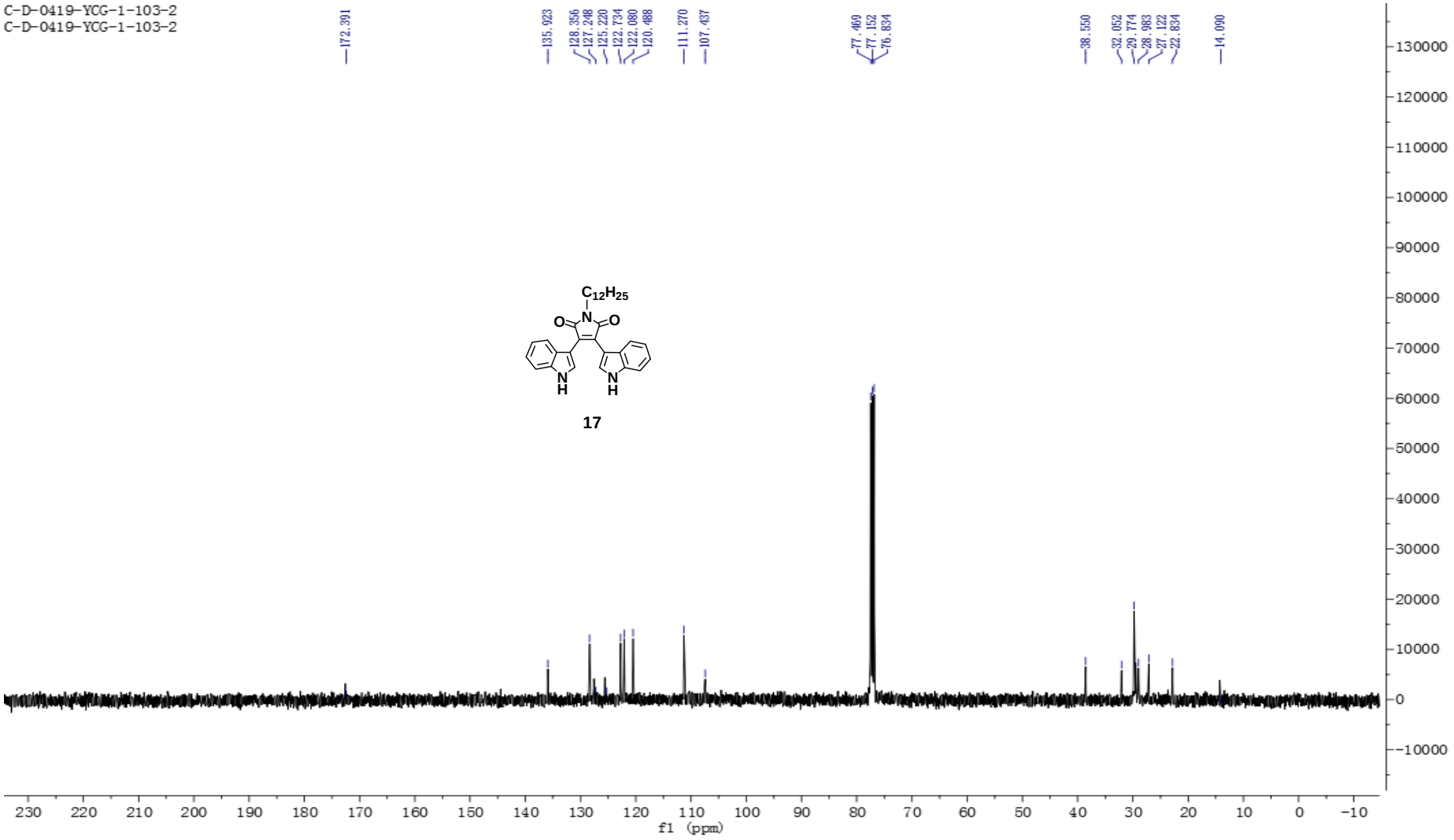

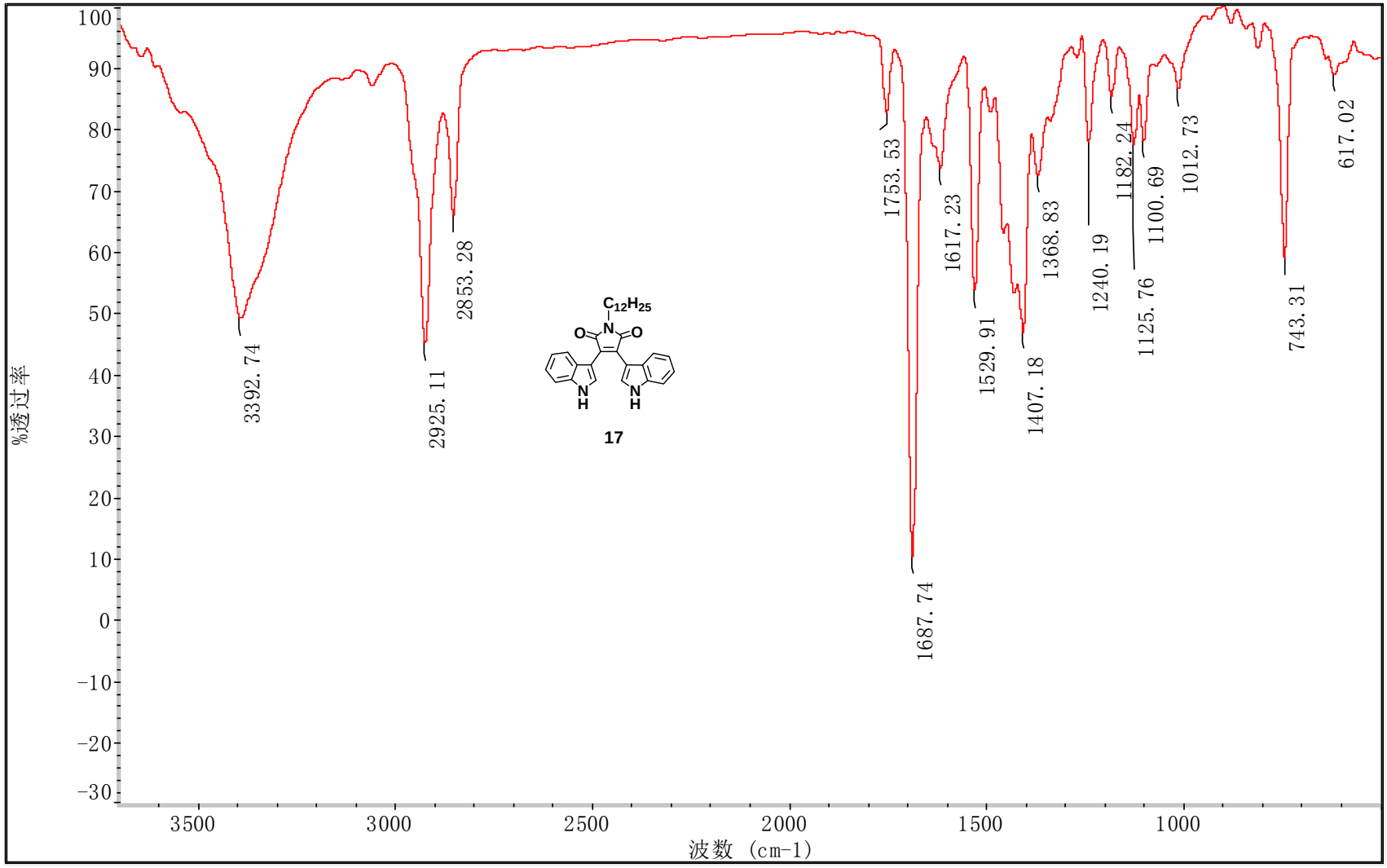

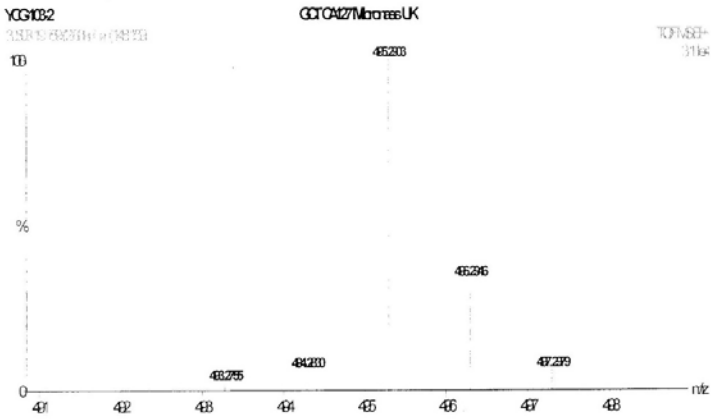

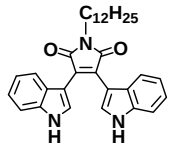

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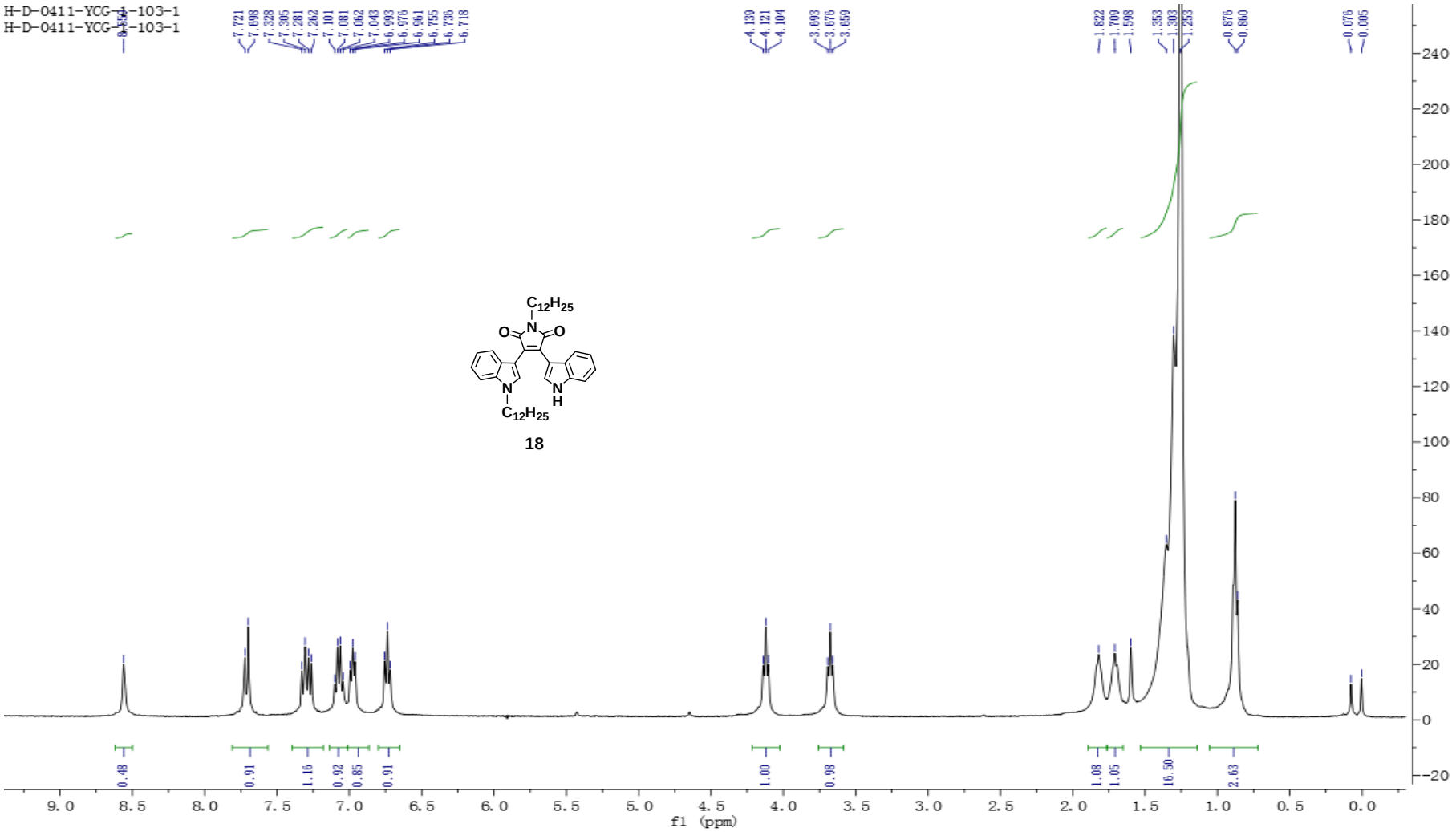
Elemental Composition Report

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
180 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Minimum:	80.00				-1.5		
Maximum:	100.00			200.0	10.0	50.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
495.2903	100.00	495.2886	1.7	3.5	16.0	1	C32 H37 N3 O2



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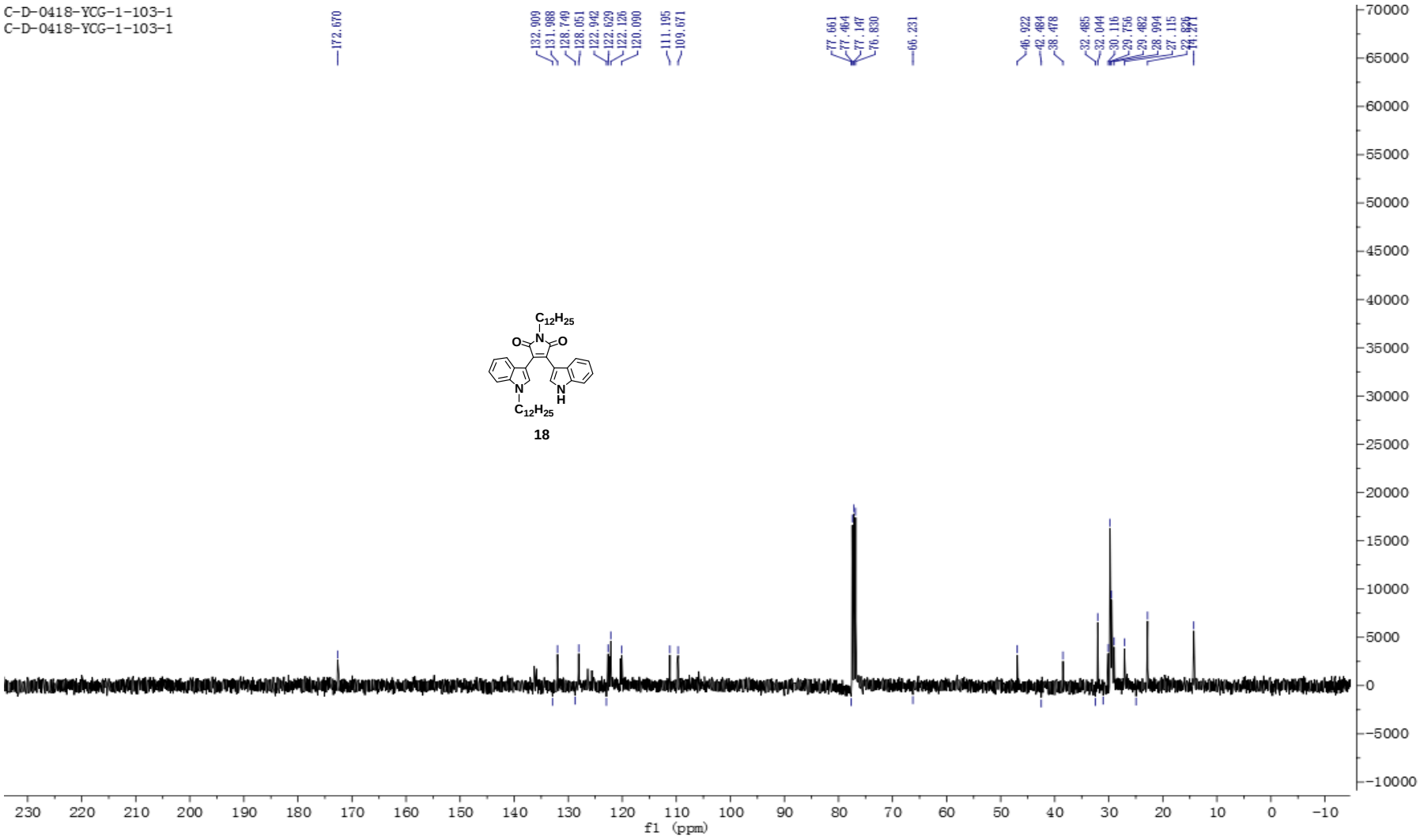

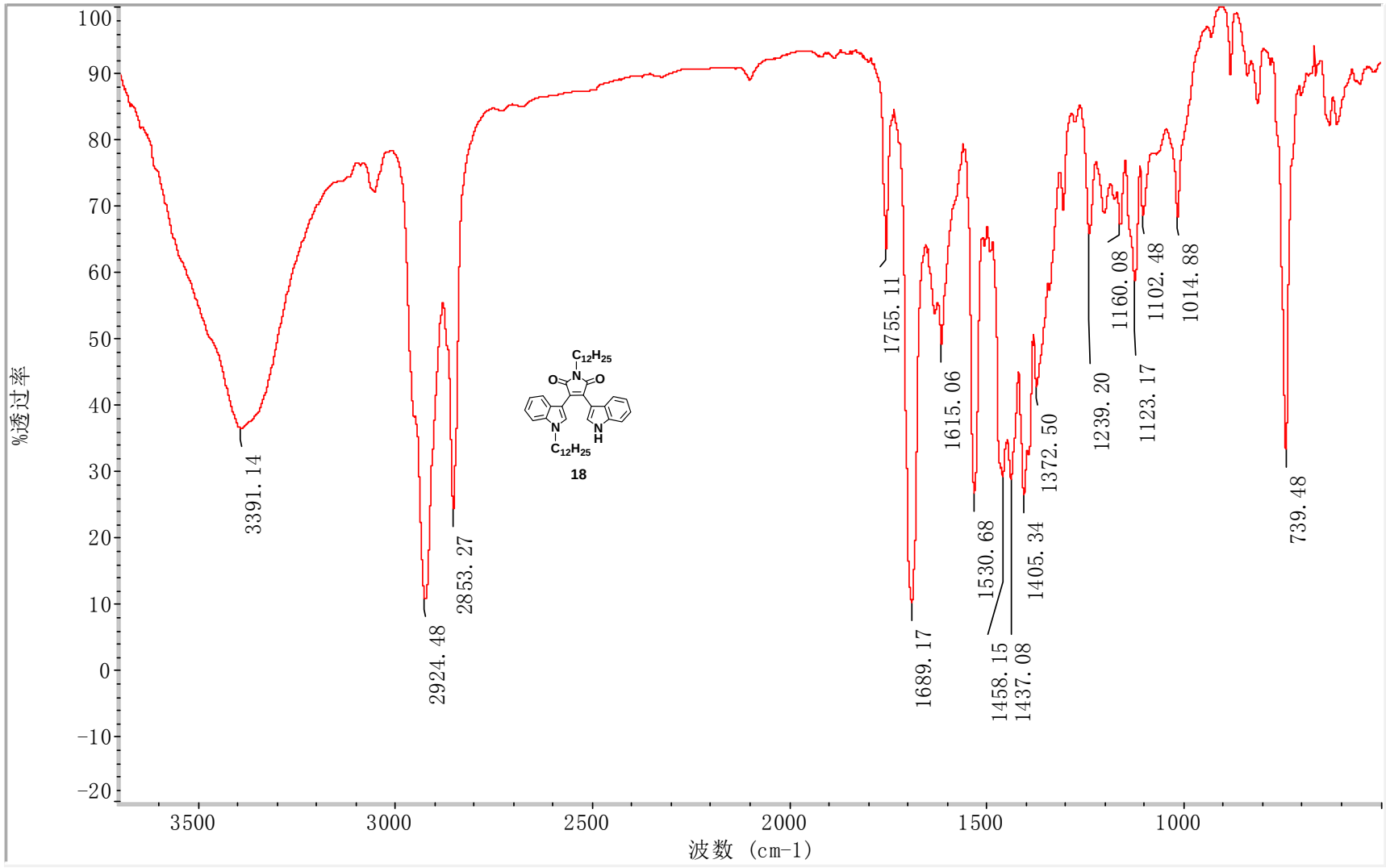

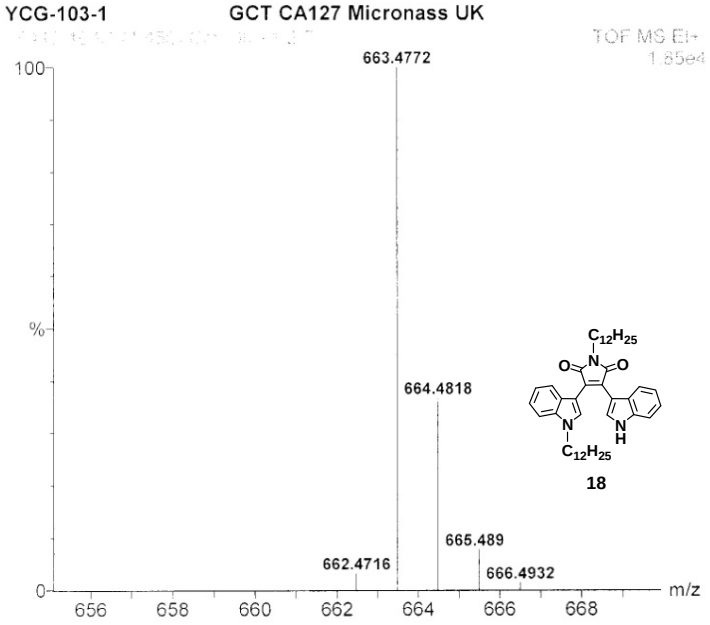

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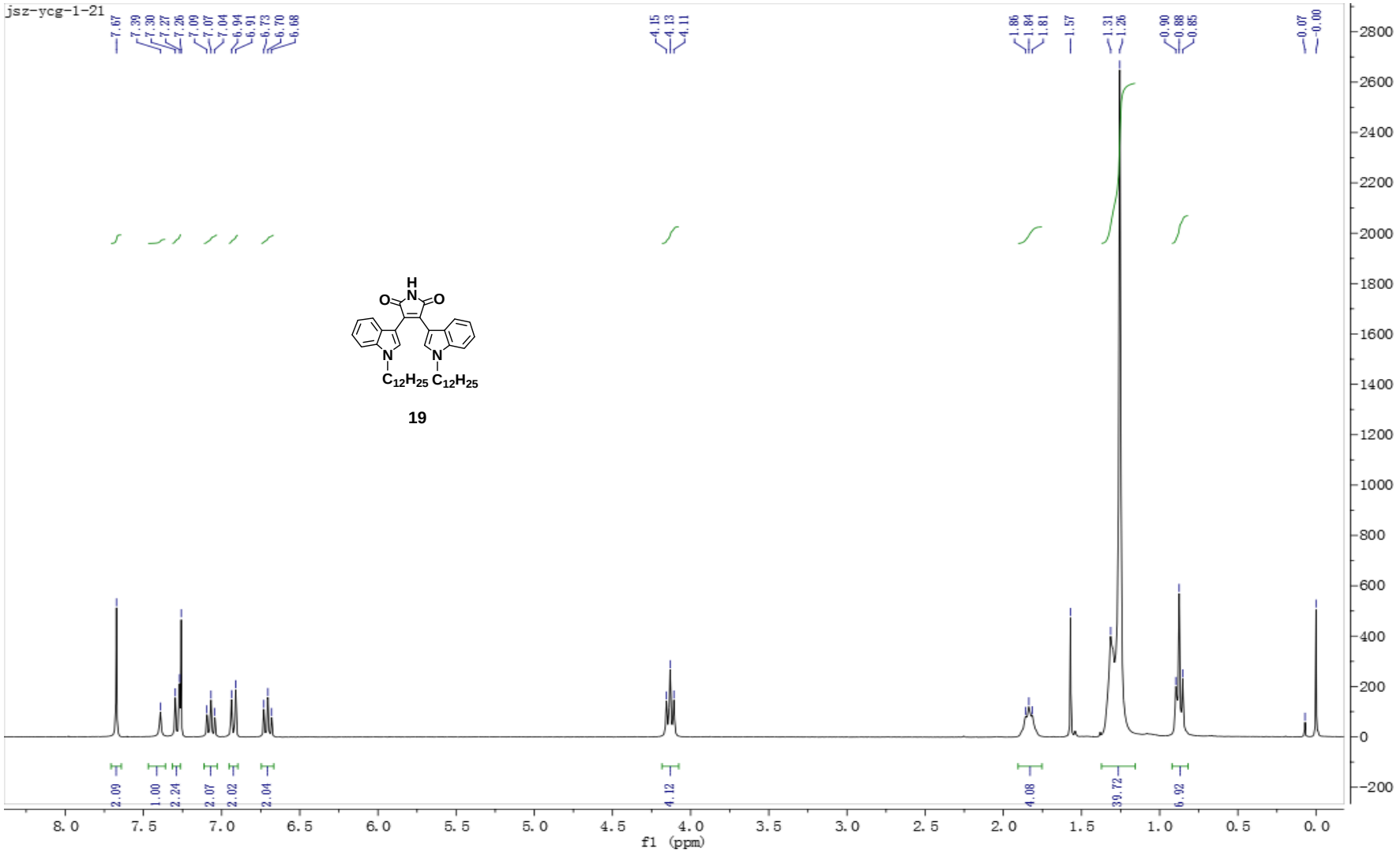
Elemental Composition Report

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Minimum:	80.00				-1.5		
Maximum:	100.00		200.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
663.4772	100.00	663.4764	0.8	1.2	16.0	1	C44 H61 N3 O2



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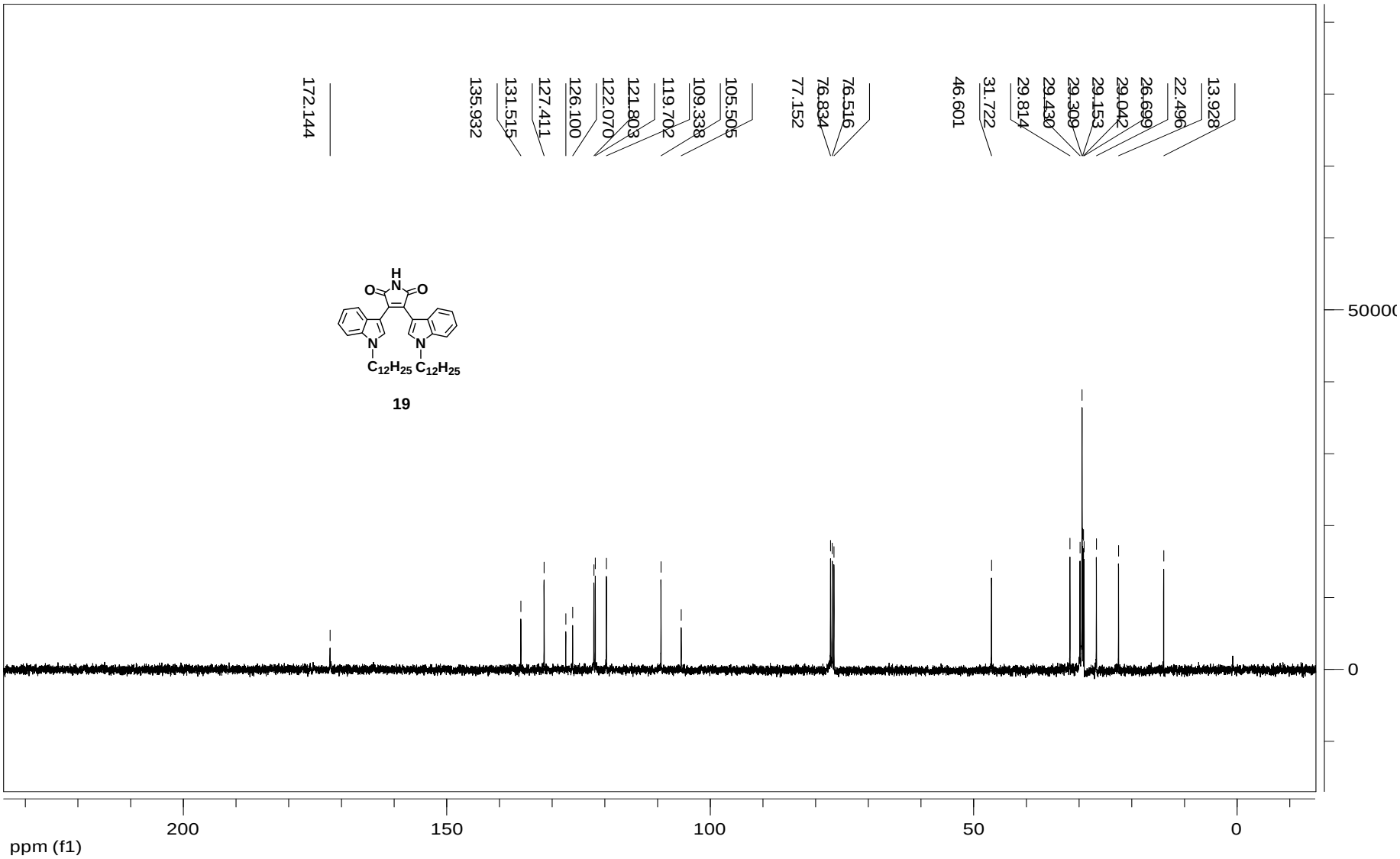

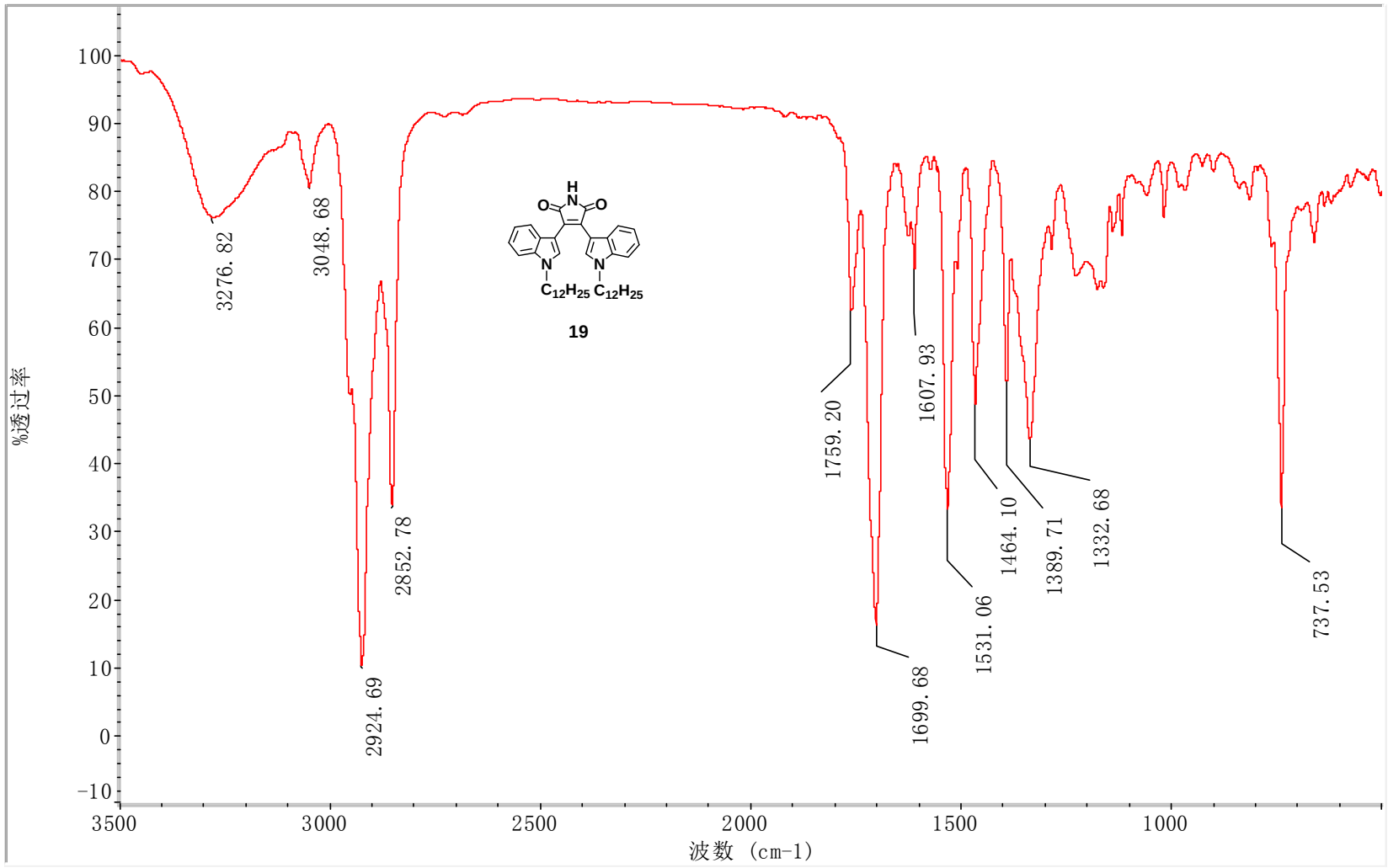

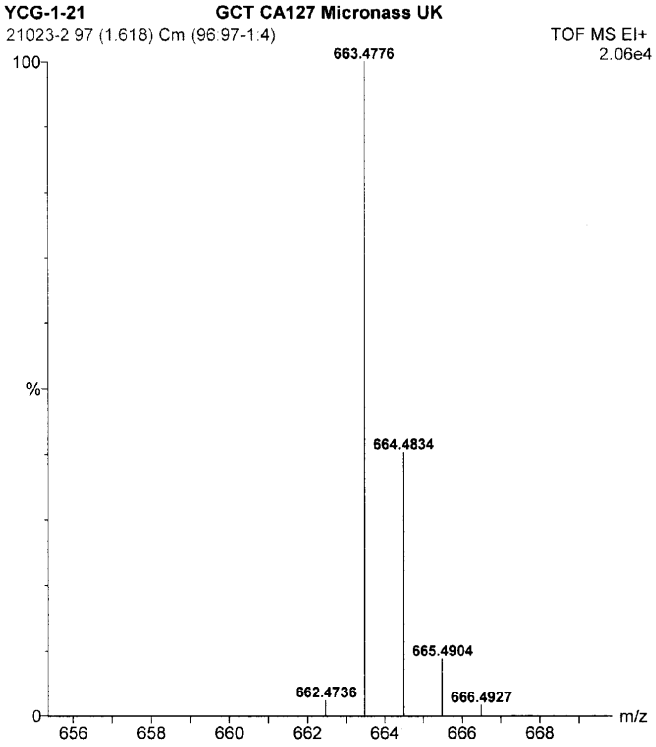

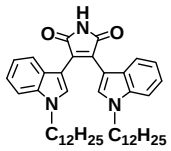

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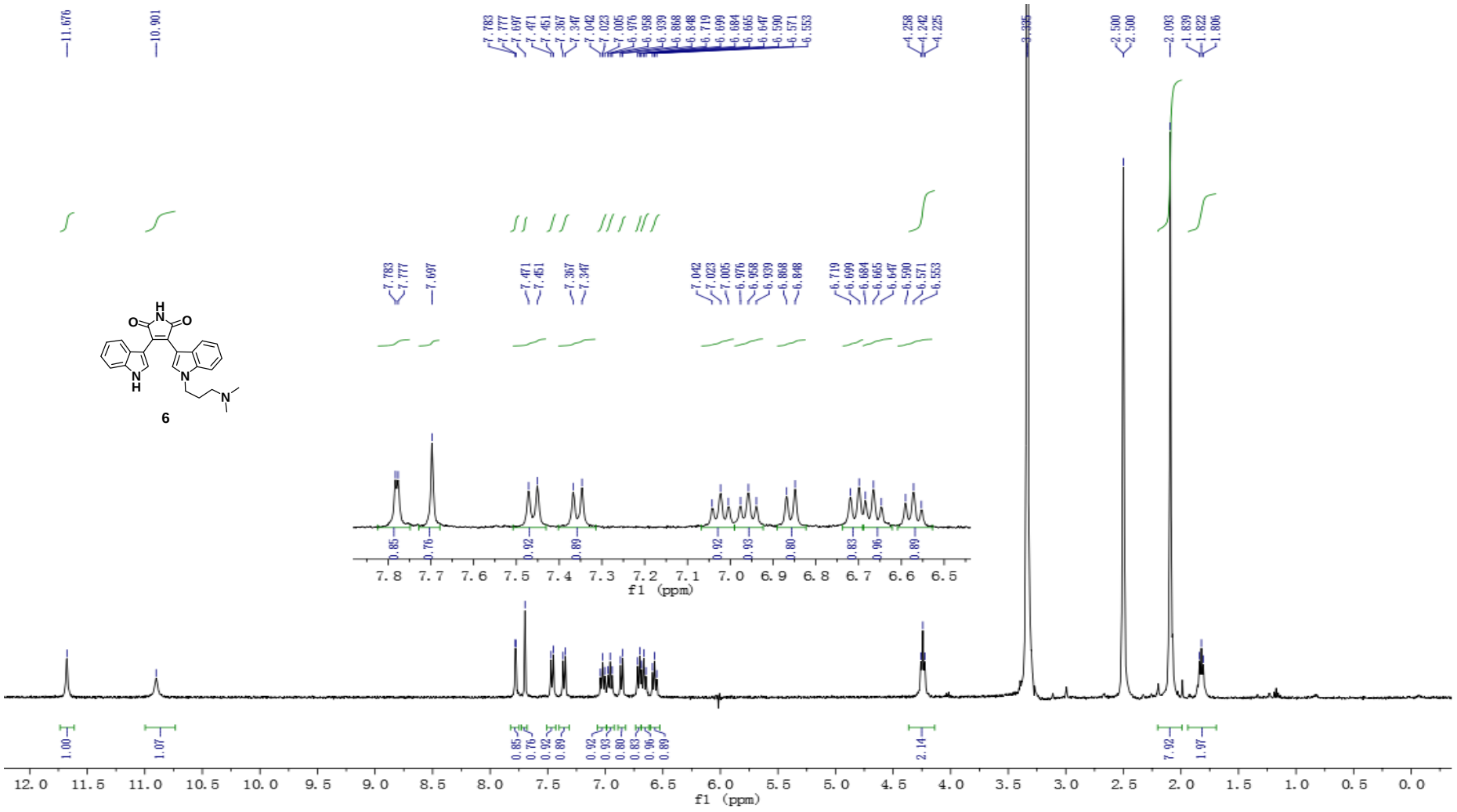
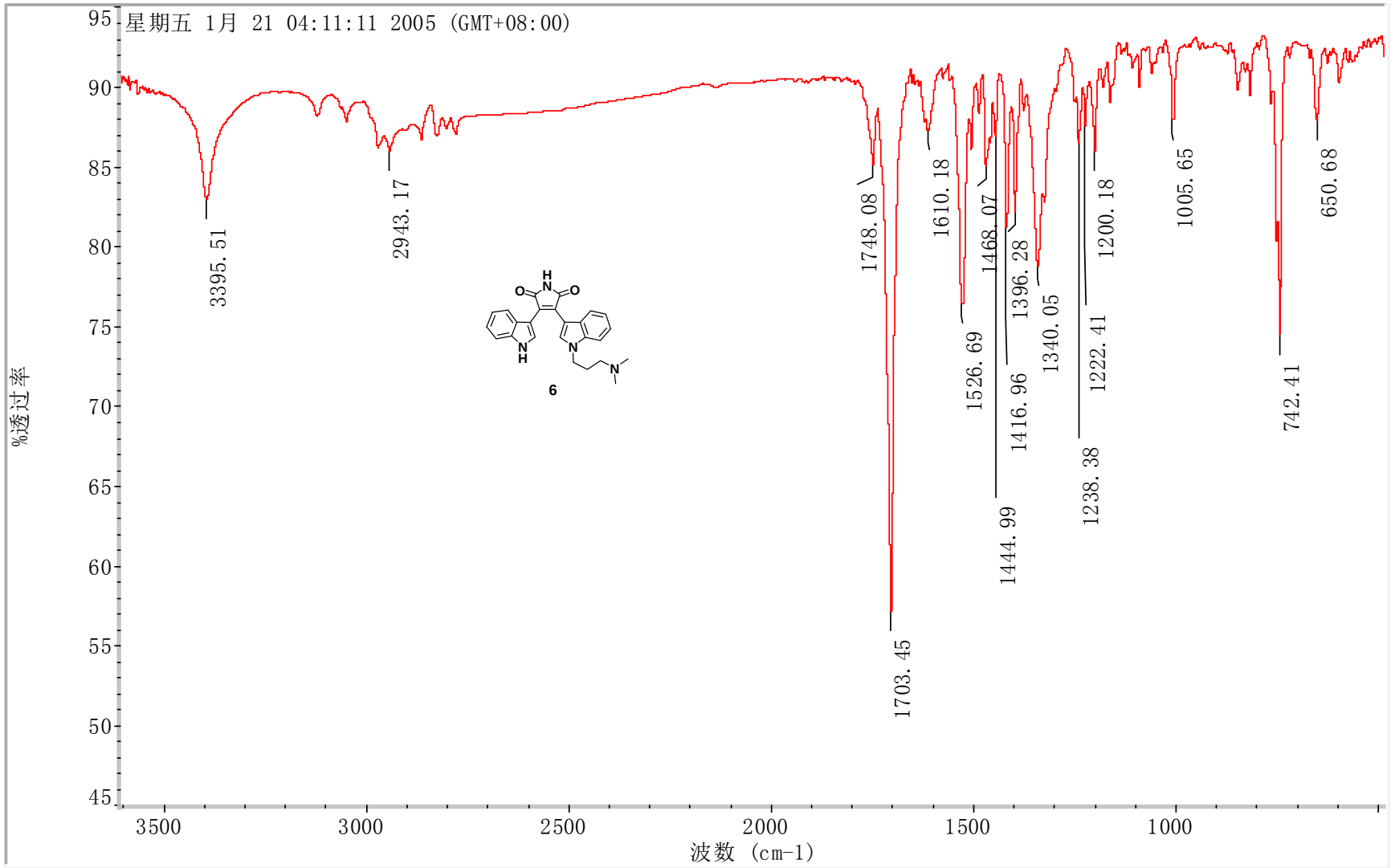
Elemental Composition Report

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Minimum:	80.00				-1.5		
Maximum:	100.00		200.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
663.4776	100.00	663.4764	1.2	1.8	16.0	1	C44 H61 N3 O2





YCG-2-115 GCT CA127 Micronass UK

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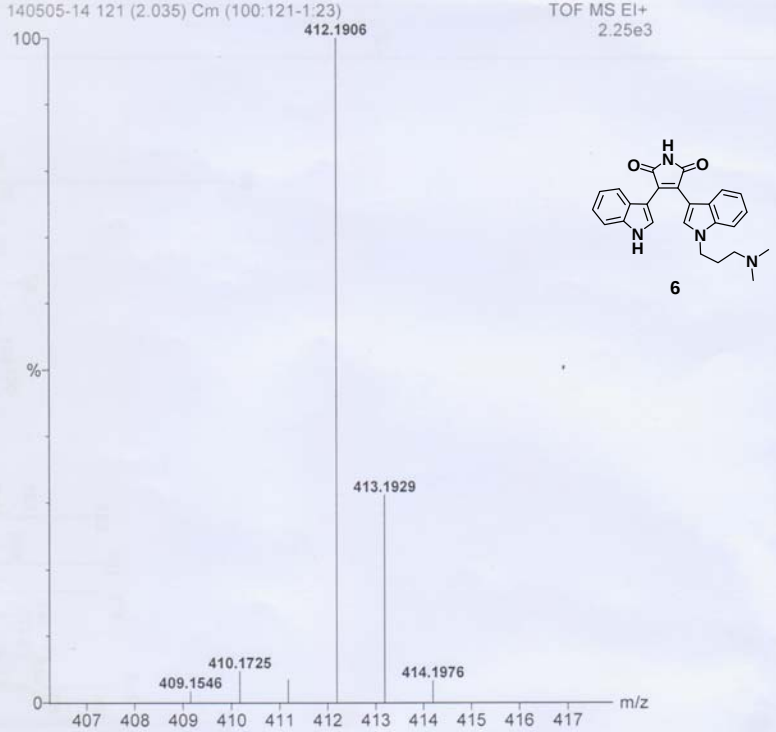

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Elemental Composition Report

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
27 formula(e) evaluated with 2 results within limits (up to 50 closest results for each mass)

Minimum:	80.00				-1.5		
Maximum:	100.00		200.0	10.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
412.1906	100.00	412.1899	0.7	1.6	16.0	1	C25 H24 N4 O2

3. Comparison of ^{1}H-NMR Spectra of GF109203X

Comparison of ^{1}H-NMR of our synthetic sample with the reported data of GF109203X (7)

Protons in **6**	Our Synthetic Sample	GF109203X by Faul[a]	GF109203X by Toullec[b]
$H_{N''}$	11.68 (s, 1H)	11.65 (bs, 1H)	11.66(s)
H_{N}	10.90 (s, 1H)	10.88 (s, 1H)	10.0-11.29 (bs)
$H_{2'}$	7.78 (d, *J* = 2.4 Hz, 1H)	7.75 (d, 1H, *J* = 2.58 Hz)	7.77 (bs)
$H_{2''}$	7.70 (s, 1H)	7.66 (s, 1H)	7.68(s)
$H_{4''}$	7.46 (d, *J* = 8.0 Hz, 1H)	7.37 (d, 1H, *J* = 8.22 Hz)	7.45 (d, J = 8.2 Hz)
$H_{4'}$	7.36 (d, *J* = 8.8 Hz, 1H)	7.16 (d, 1H, *J* = 8.12 Hz),	7.35 (d, J = 8.1 Hz)
H_{Ar}(3H)	7.03 (t, *J* = 7.6 Hz, 1H), 6.96 (t, *J* = 7.6 Hz, 2H), 6.86 (d, *J* = 8.0 Hz, 1H)	7.01-6.90 (m, 2H), 6.83 (d, 1H, *J* = 7.96 Hz)	7.01-6.83 (m)
$H_{Ar'}$ (3H)	6.70 (d, *J* = 8.0 Hz, 1H), 6.67 (t, *J* = 7.6 Hz, 1H), 6.57 (t, *J* = 7.6 Hz, 1H)	6.69-6.61 (m, 2H), 6.54 (t, 1H, *J* = 7.54 Hz)	6.72-6.56 (m)
$C\underline{H_2}(CH_2)_2N(CH_3)_2$	4.24 (t, *J* = 6.4 Hz, 2H)	4.21 (t, 2H, *J* = 6.48 Hz)	4.22 (t, *J* = 6.5 Hz),
$CH_2C\underline{H_2}$ $N(C\underline{H_3})_2$	2.09 (bs, 8H)	2.06-2.03 (bs, 8H),	2.06-2.03 (bs)
$CH_2C\underline{H_2}$ CH_2	1.82 (t, *J* = 6.8 Hz, 2H)	1.81-1.77 (m, 2H);	1.83 (t, J = 7.0 Hz)

[a] Faul, M. M.; Winneroski, L. L.; Krumrich, C. A. *J. Org. Chem.* **1998**, 63, 6053.

[b] Toullec, D.; Pianetti, P.; Coste, H.; Bellevergue, P.; Grand-Perret, T.; Ajakane, M.; Baudet, V.; Boissin, P.; Boursier, E.; Loriolle, F. *J. Biol. Chem.* **1991**, *266*, 15771.