

Naphthoquinone-thiazole hybrids bearing adamantane: Synthesis, antimicrobial, DNA cleavage, antioxidant activity, acid dissociation constant, and drug-likeness

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Copy of $^1\text{H}/^{13}\text{C}$ NMR, FT-IR and HRMS spectra of 6a

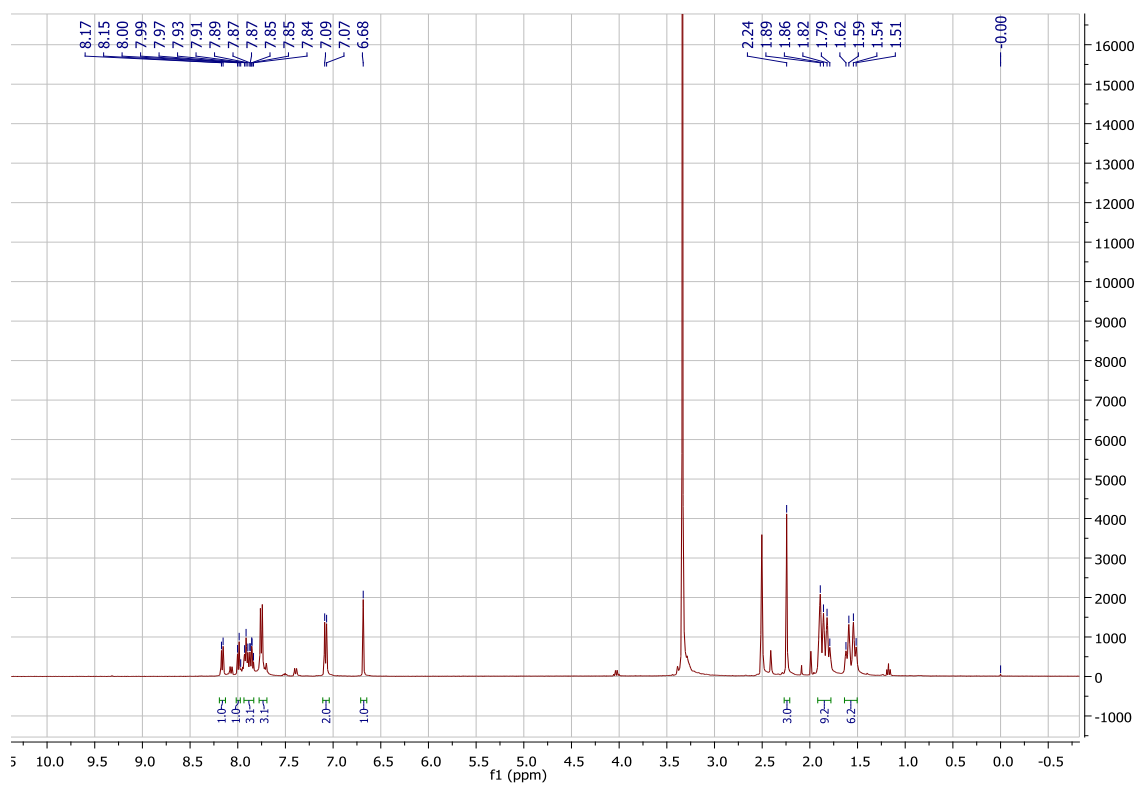


Figure S1. ^1H NMR Spectrum of 6a

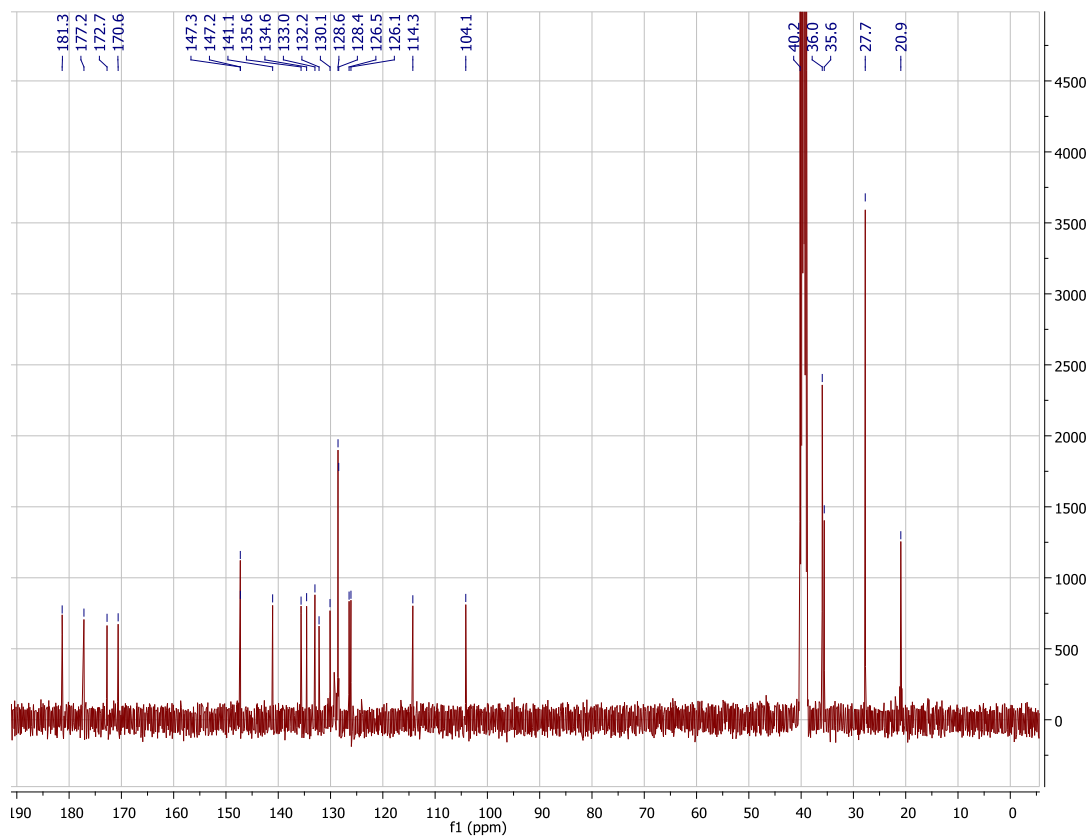


Figure S2. ^{13}C NMR Spectrum of 6a

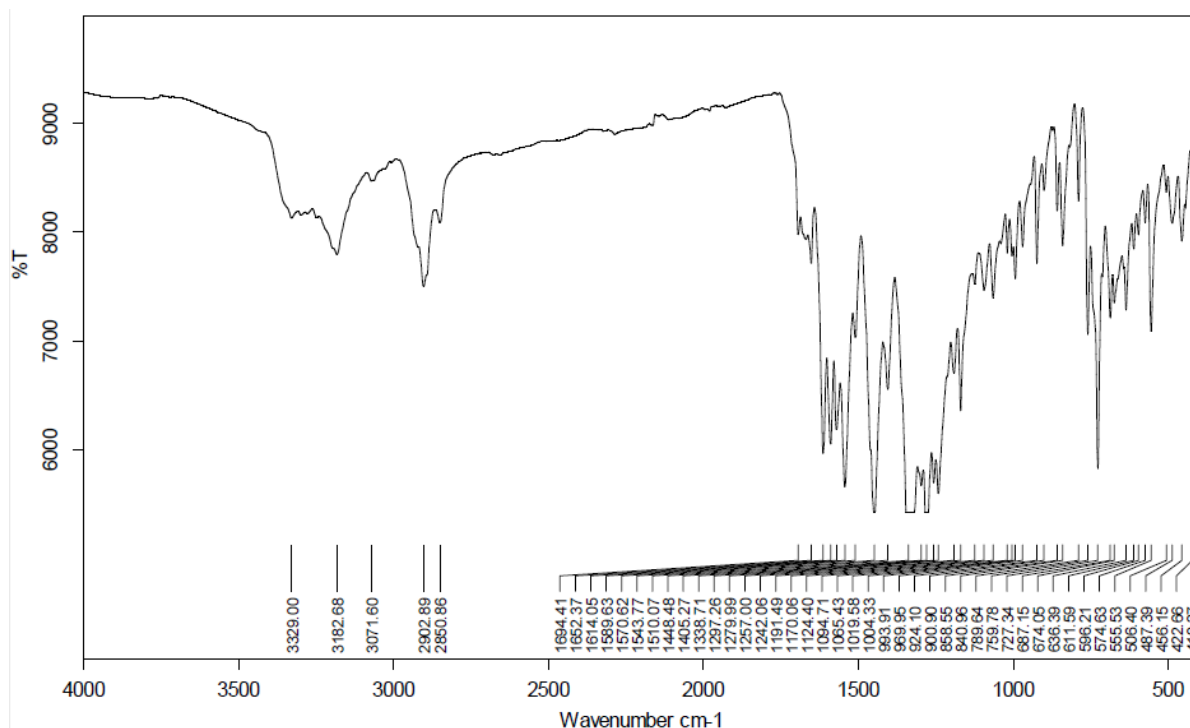


Figure S3. FT-IR Spectrum of 6a

Elemental Composition Report

Single Mass Analysis

Tolerance = 5000.0 PPM / DBE: min = -5.5, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

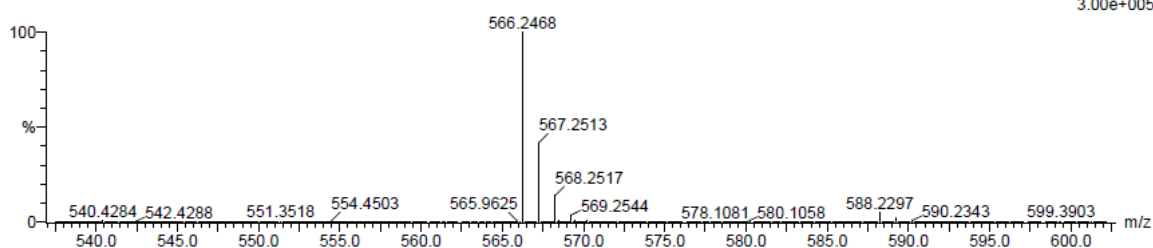
Elements Used:

C: 34-34 H: 34-36 N: 3-3 O: 3-3 Na: 0-1 S: 1-1

Yahya Nural

29812_20200619_02_02 4 (0.172) Cm (1:15)

1: TOF MS ES+
3.00e+005



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
566.2468	566.2477	-0.9	-1.6	18.5	498.0	0.0	C34 H36 N3 O3 S

Figure S4. HRMS Spectrum of 6a

Copy of $^1\text{H}/^{13}\text{C}$ NMR, FT-IR and HR-MS spectra of 6b

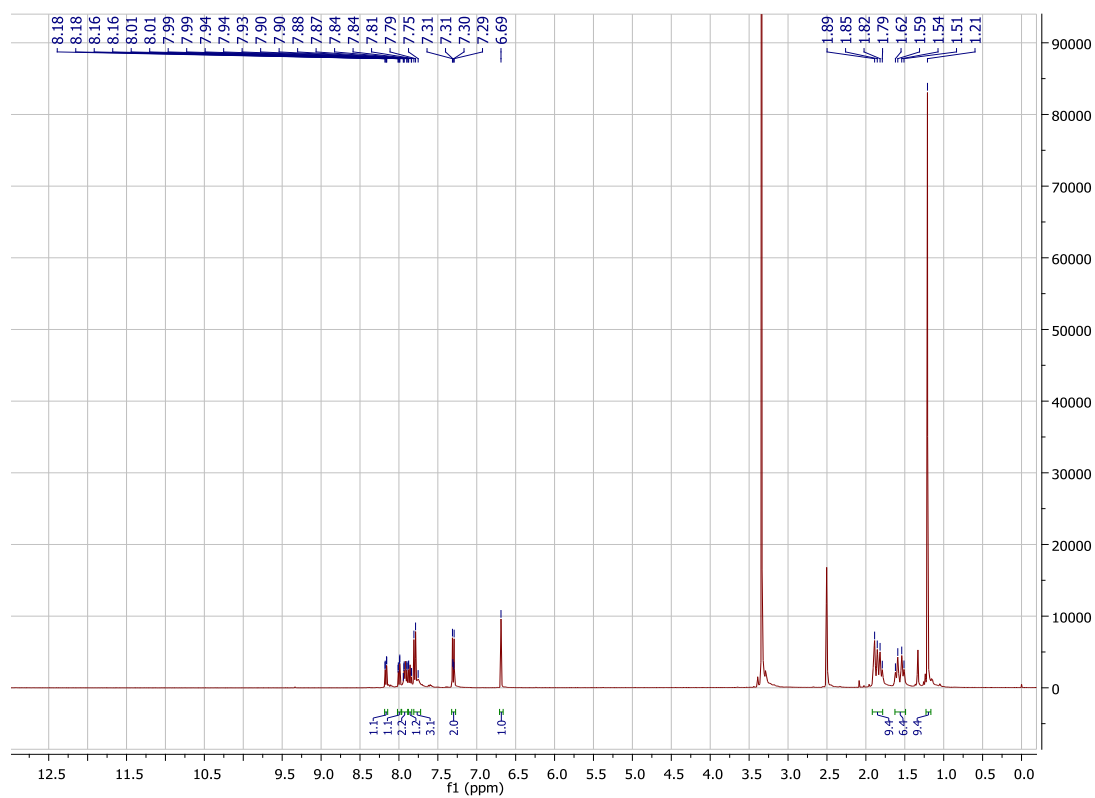


Figure S5. ^1H NMR Spectrum of 6b

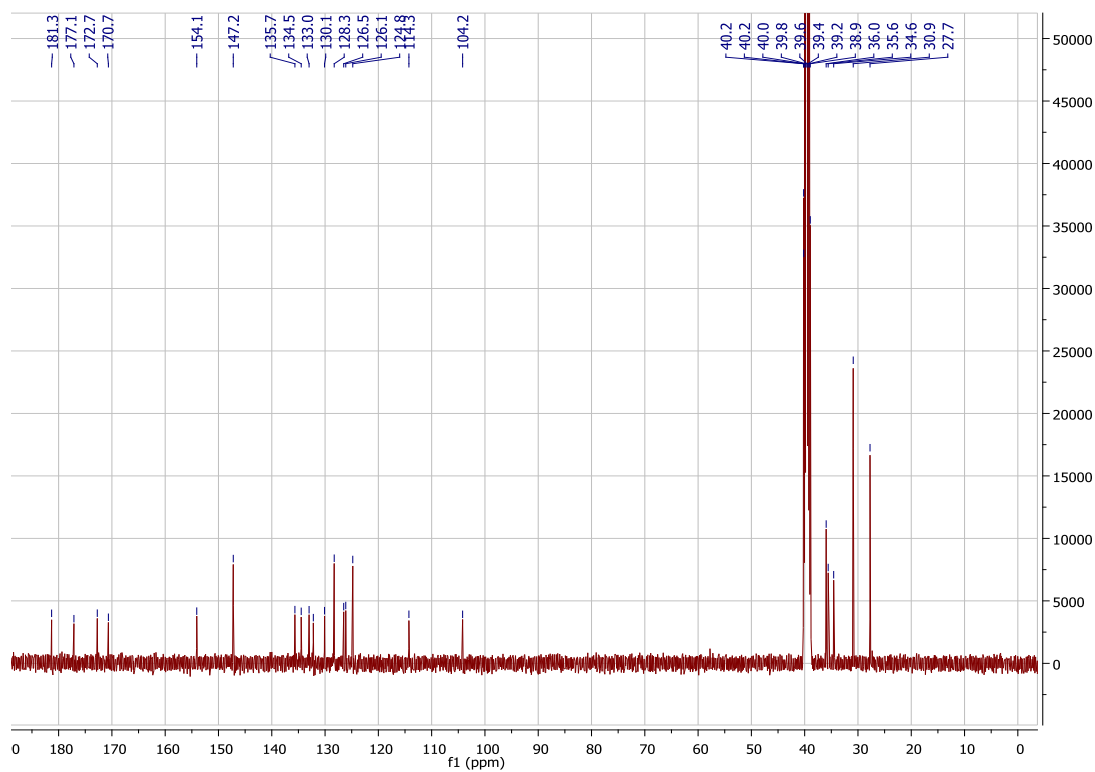


Figure S6. ^{13}C NMR Spectrum of 6b

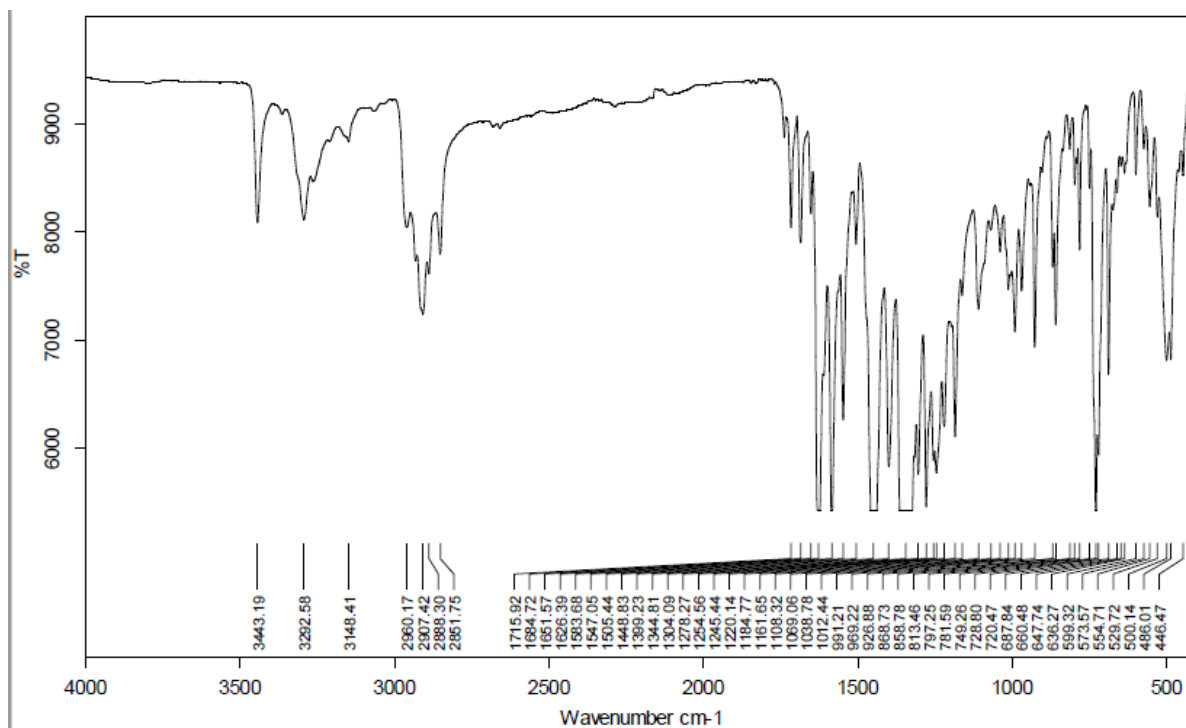


Figure S7. FT-IR Spectrum of 6b

Elemental Composition Report

Single Mass Analysis

Tolerance = 5000.0 PPM / DBE: min = -5.5, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

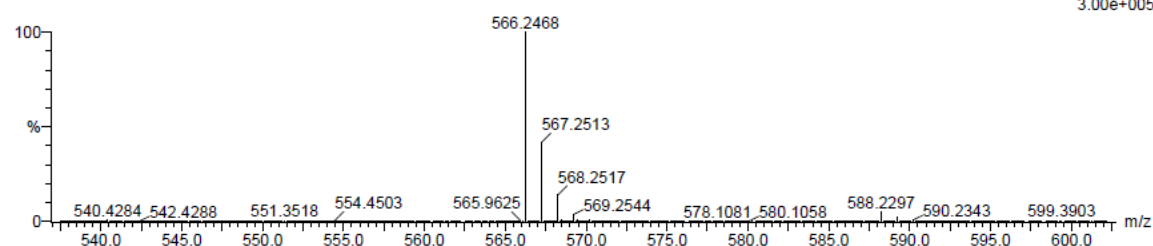
Elements Used:

C: 34-34 H: 34-36 N: 3-3 O: 3-3 Na: 0-1 S: 1-1

Yahya Nural

29812_20200619_02_02 4 (0.172) Cm (1:15)

1: TOF MS ES+
3.00e+005



Minimum: -5.5
Maximum: 1000.0 5000.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
566.2468	566.2477	-0.9	-1.6	18.5	498.0	0.0	C34 H36 N3 O3 S

Figure S8. HRMS Spectrum of 6b

Copy of $^1\text{H}/^{13}\text{C}$ NMR, FT-IR and HR-MS spectra of 6c

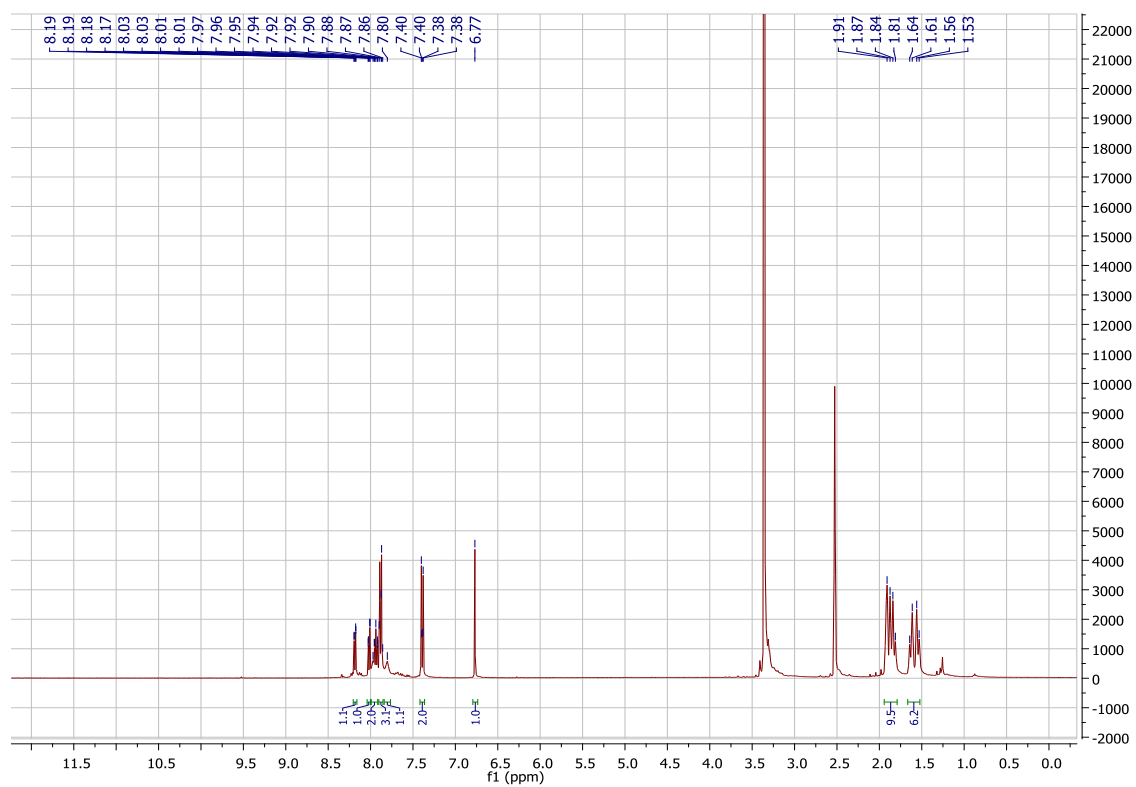


Figure S9. ^1H NMR Spectrum of 6c

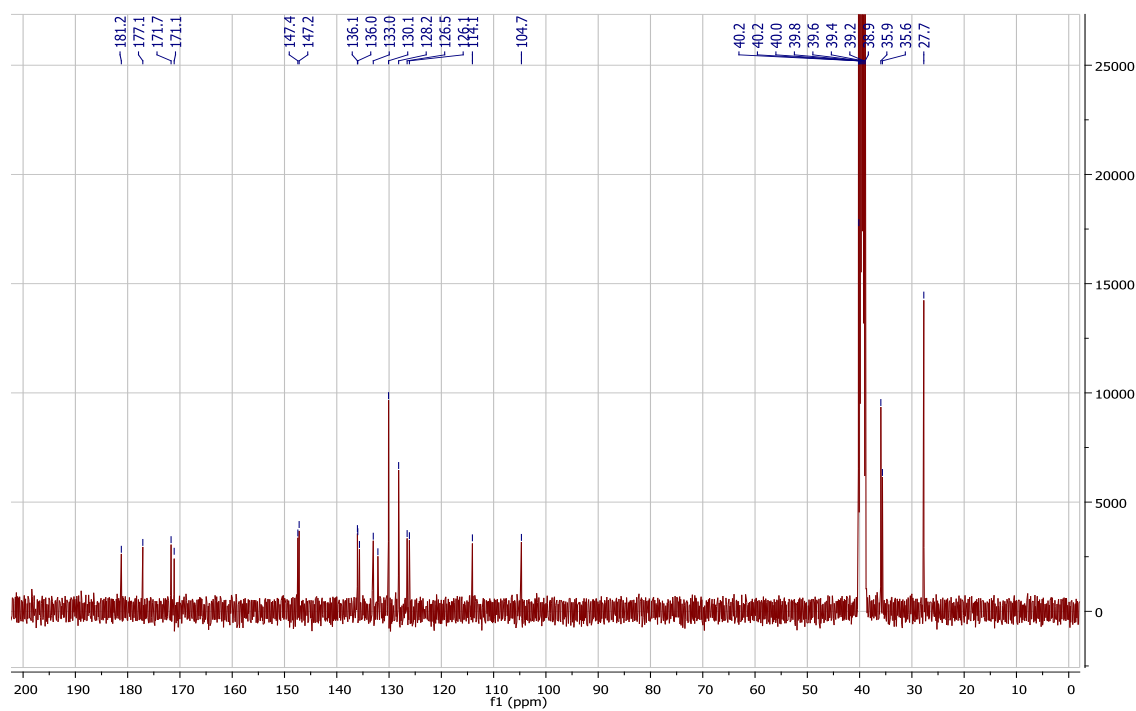


Figure S10. ^{13}C NMR Spectrum of 6c

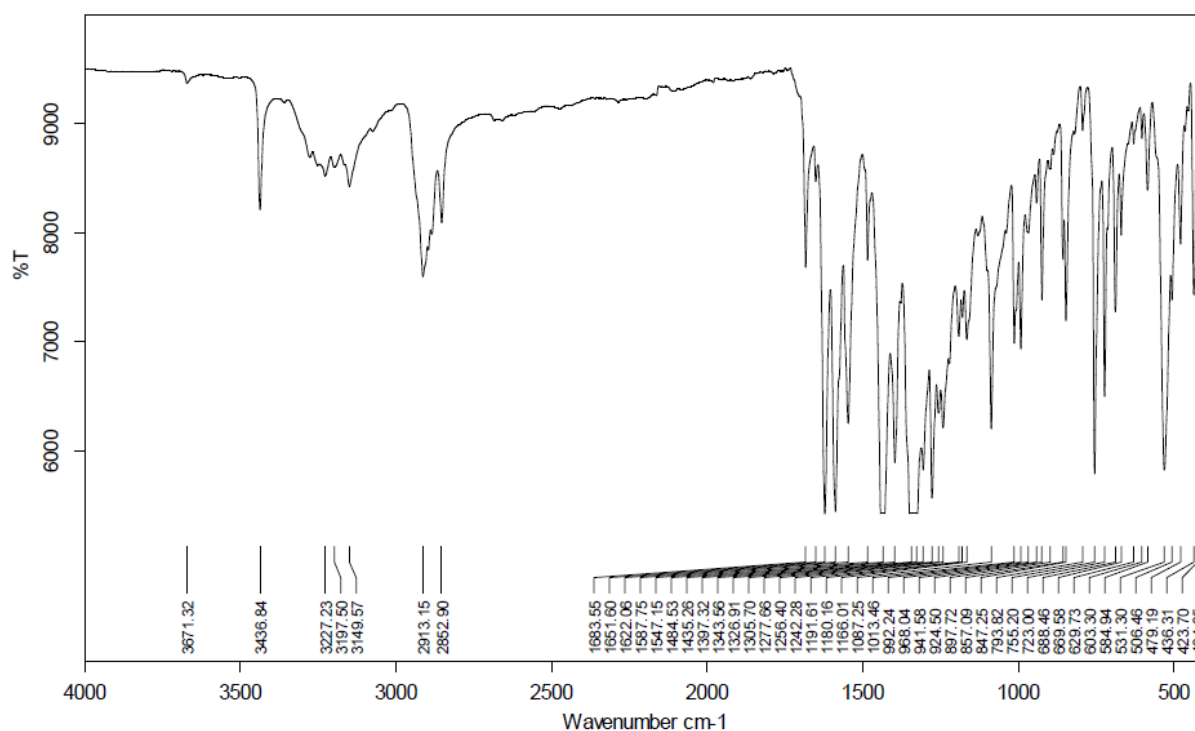


Figure S11. FT-IR Spectrum of 6c

Single Mass Analysis

Tolerance = 5000.0 PPM / DBE: min = -5.5, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

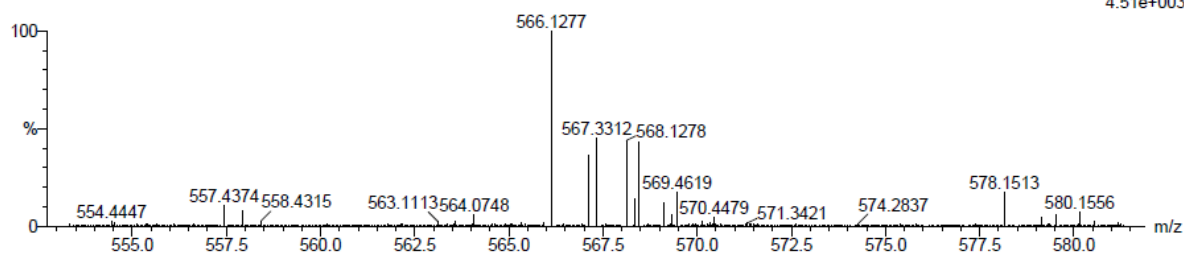
Elements Used:

C: 30-30 H: 26-27 N: 3-3 O: 3-3 Na: 0-1 S: 1-1 Cl: 1-1

Yahya Nural

29812_20200619_01_03 22 (0.863) Cm (1:25)

1: TOF MS ES+
4.51e+003



Minimum: -5.5
Maximum: 1000.0 5000.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	1-FIT	1-FIT (Norm)	Formula
566.1277	566.1281	-0.4	-0.7	18.5	227.6	0.0	C30 H26 N3 O3 Na S Cl

Figure S12. HRMS Spectrum of 6c

Copy of $^1\text{H}/^{13}\text{C}$ NMR, FT-IR and HR-MS spectra of 6d

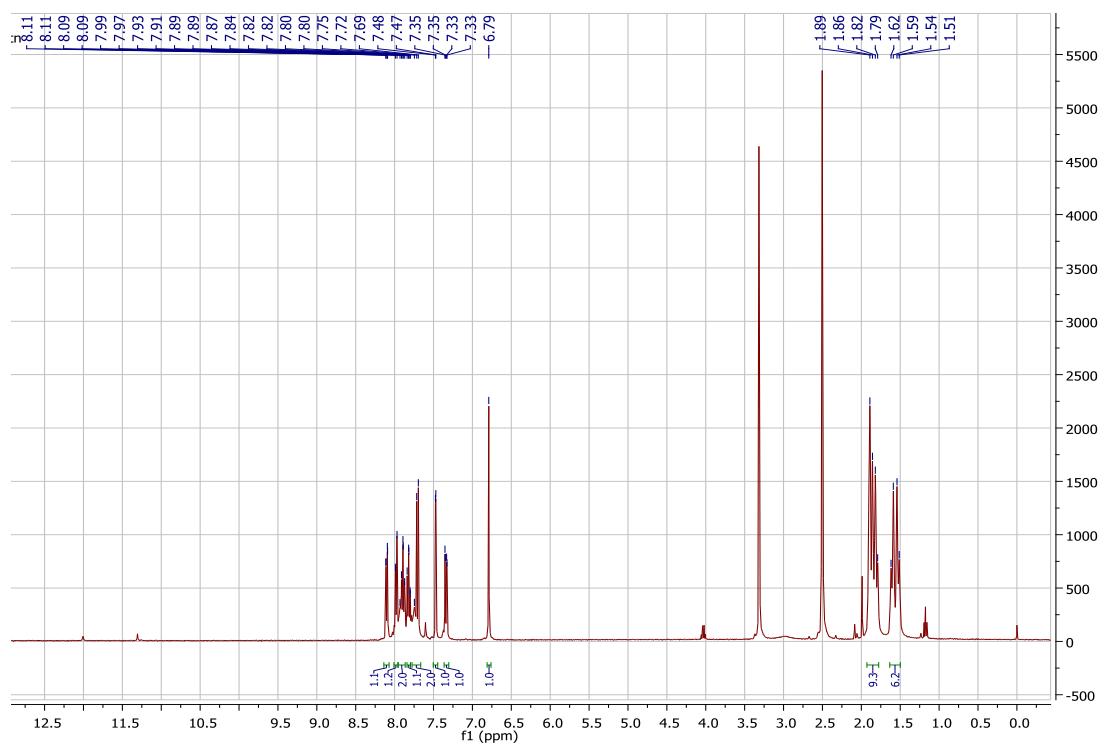


Figure S13. ^1H NMR Spectrum of 6d

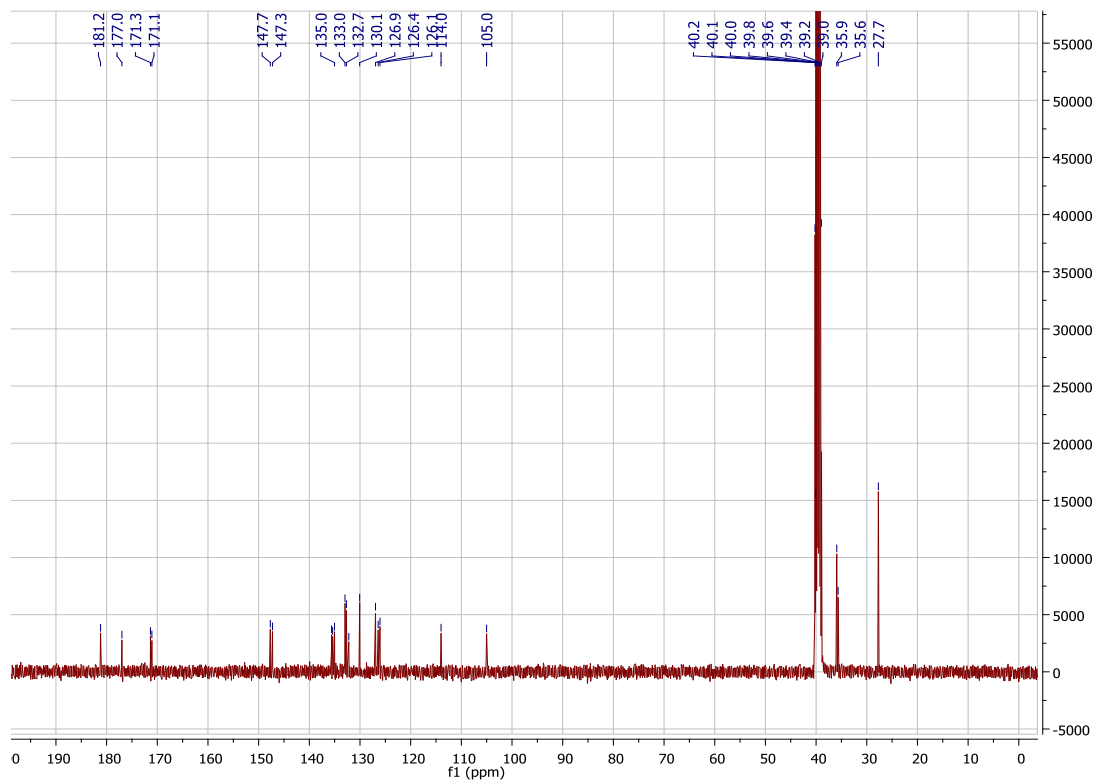


Figure S14. ^{13}C NMR Spectrum of 6d

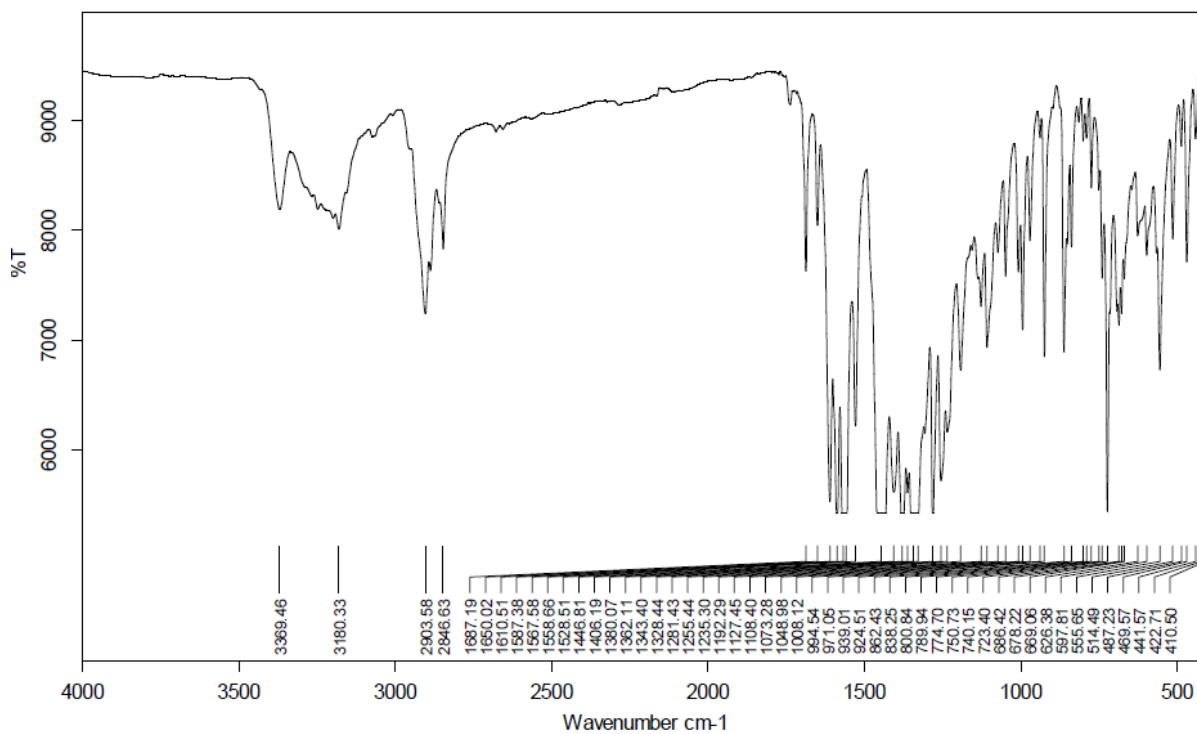


Figure S15. FT-IR Spectrum of 6d

Elemental Composition Report

Single Mass Analysis

Tolerance = 5000.0 PPM / DBE: min = -5.5, max = 1000.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

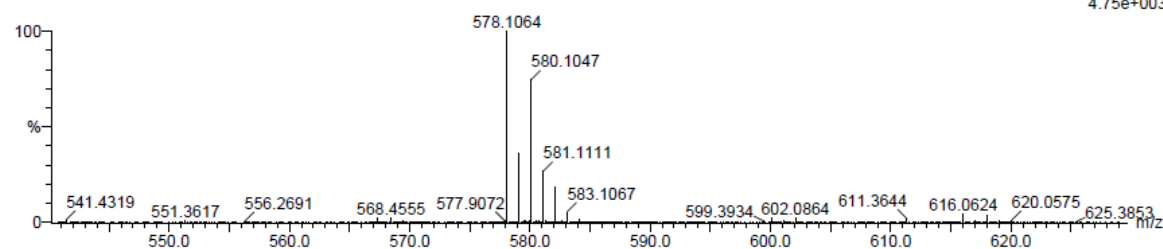
Elements Used:

C: 30-30 H: 25-26 N: 3-3 O: 3-3 Na: 0-1 S: 1-1 Cl: 1-2

Yahya Nural

29812_20200619_04_03 5 (0.206) Cm (2:7)

1: TOF MS ES+
4.75e+003



Minimum:

Maximum: 1000.0 5000.0 1000.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
578.1064	578.1072	-0.8	-1.4	18.5	160.8	0.0	C30 H26 N3 O3 S Cl2

Figure S16. HRMS Spectrum of 6d