

3-Hydroxy-2-iodophenyl-(4-ethylbenzenesulfonate)

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Supplementary Materials

Figure S1: ¹H NMR spectrum of compound 2, 2-iodo-1,3-phenylene bis(4-methylbenzene-sulfonate)

Figure S2: ¹³C NMR spectrum of compound 2

Figure S3: HRMS of spectrum compound 2

Figure S4: IR spectrum of compound 2

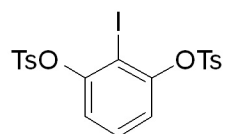
Figure S5: ¹H NMR spectrum of compound 3, 3-hydroxy-2-iodophenyl-(4-methylbenzene-sulfonate)

Figure S6: ¹³C NMR spectrum of compound 3

Figure S7: HRMS spectrum of compound 3

Figure S8: IR spectrum of compound 3

Figure S1



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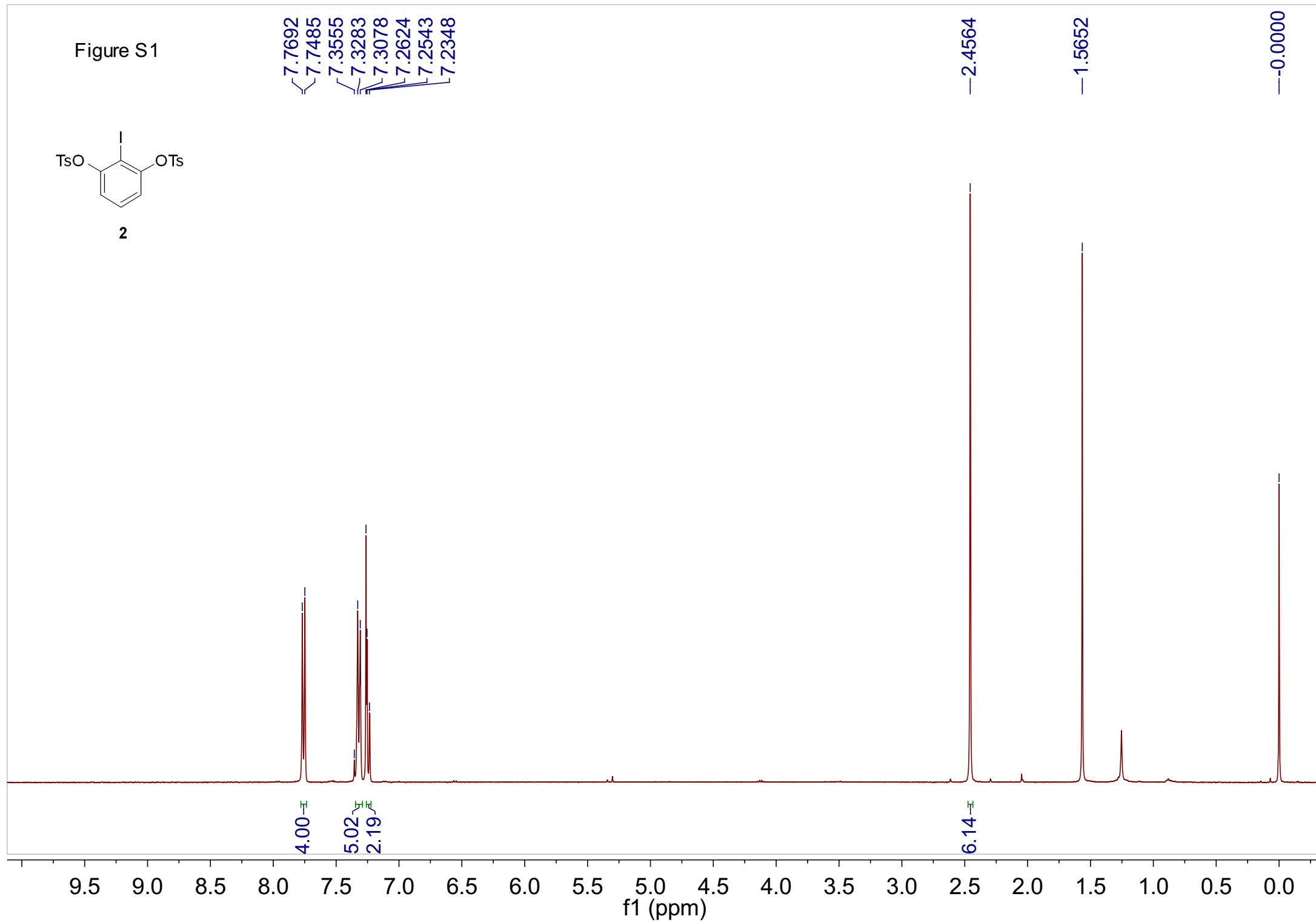
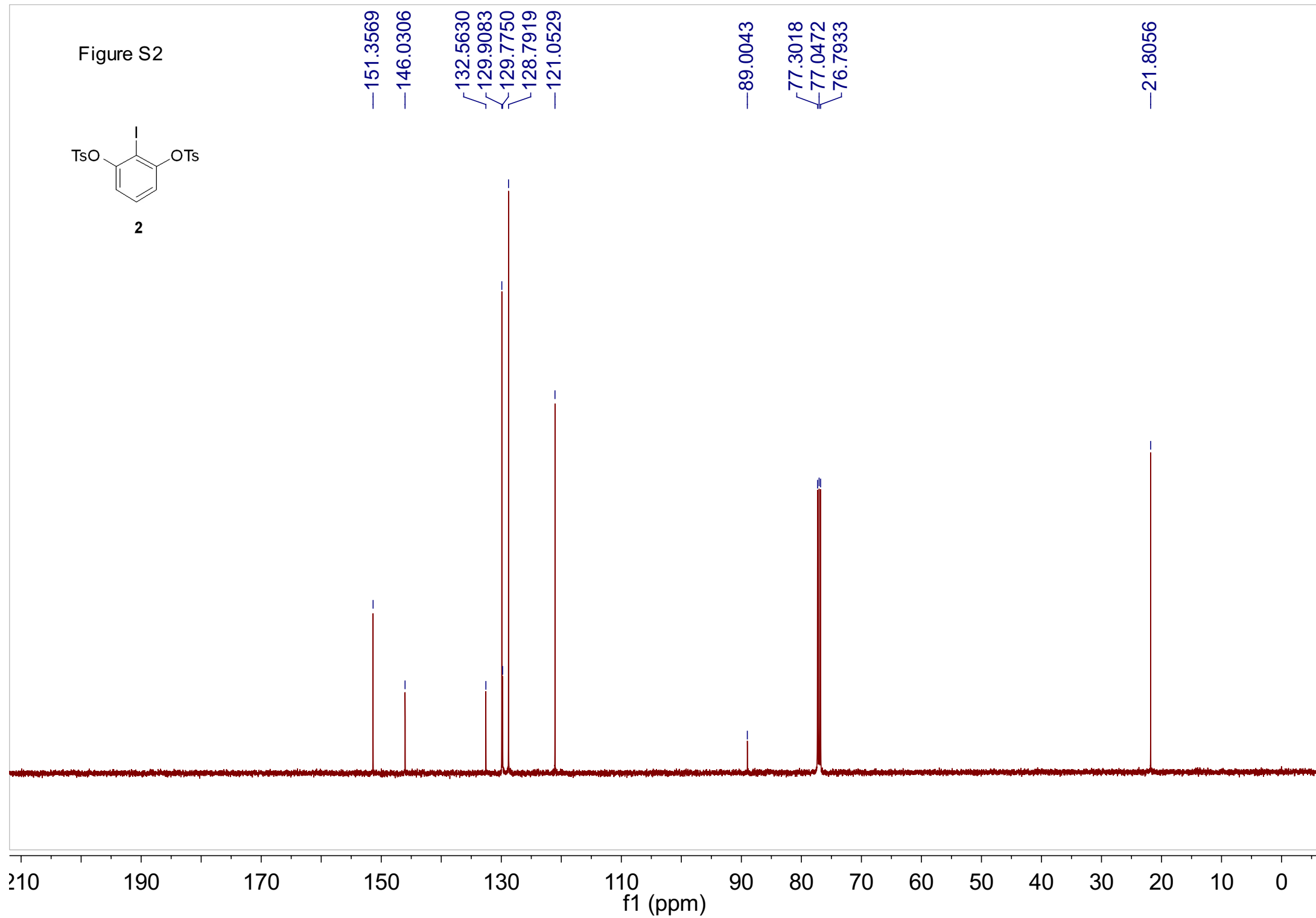
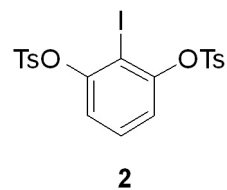


Figure S2



Tolerance = 0.4 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

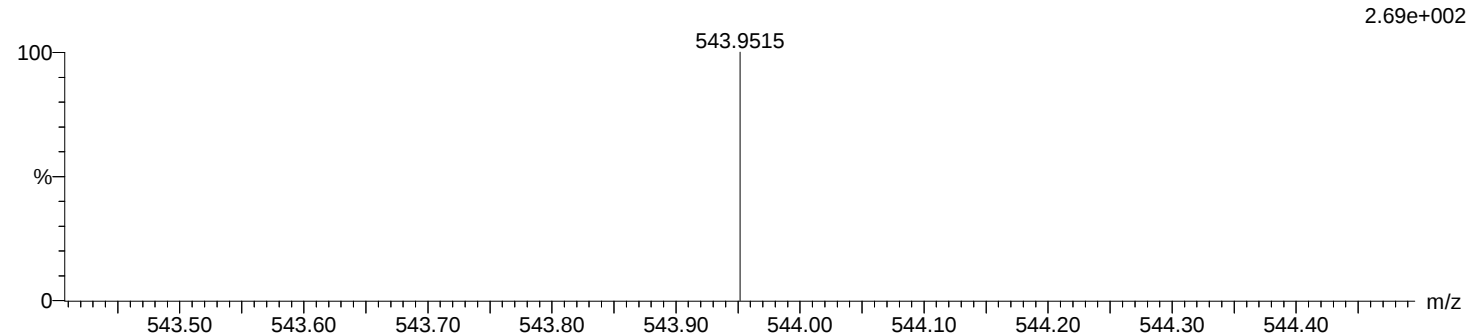
775 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)

Elements Used:

C: 0-50 H: 0-100 O: 0-6 S: 0-2 Br: 0-4 I: 0-1

F-T-7 1125 (6.954)

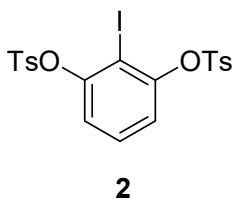
TOF MS EI+



Minimum: -1.5
Maximum: 0.4 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
543.9515	543.9511	0.4	0.7	12.0	5546148.5	C20 H17 O6 S2 I

Figure S3



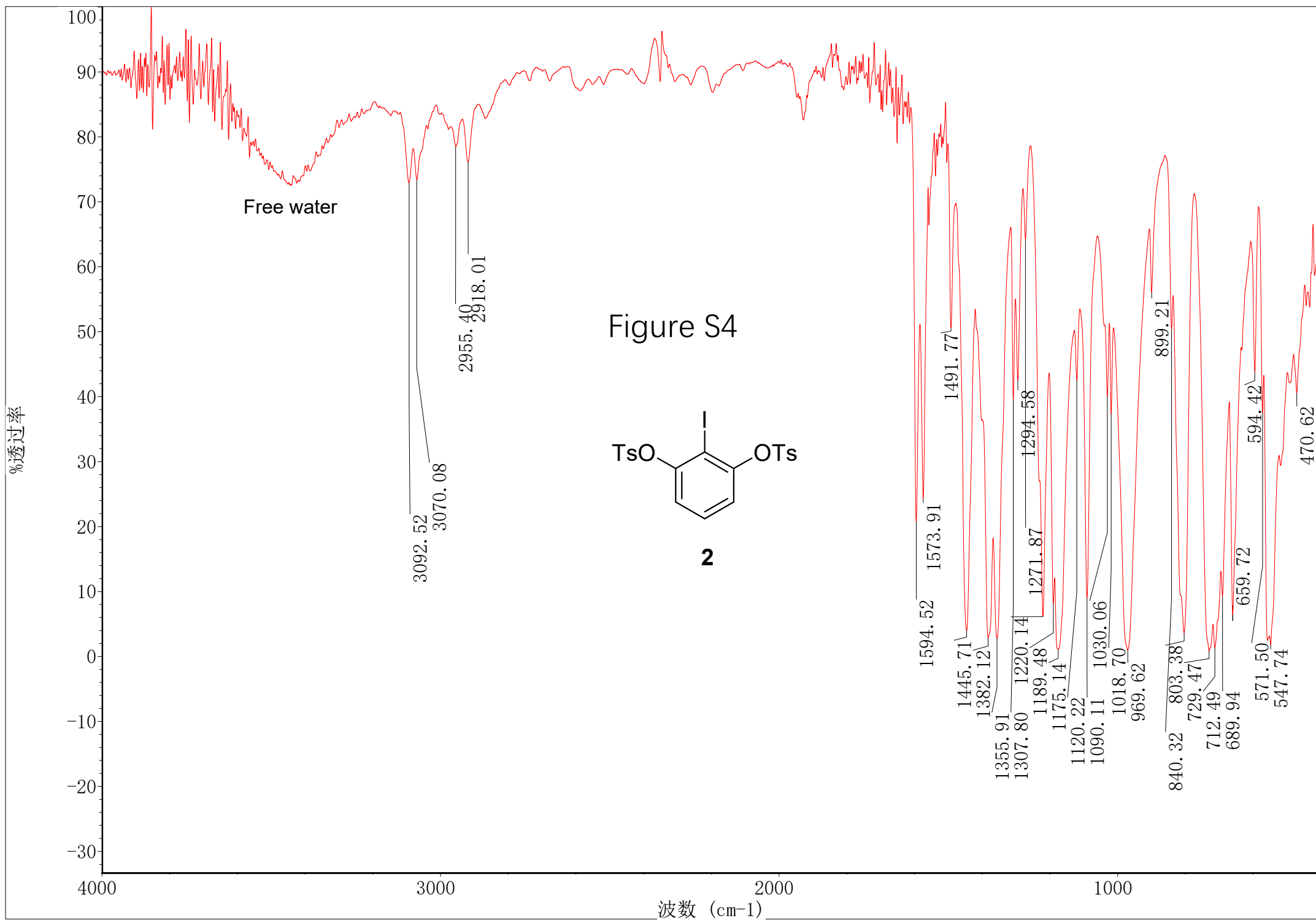
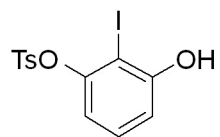


Figure S5



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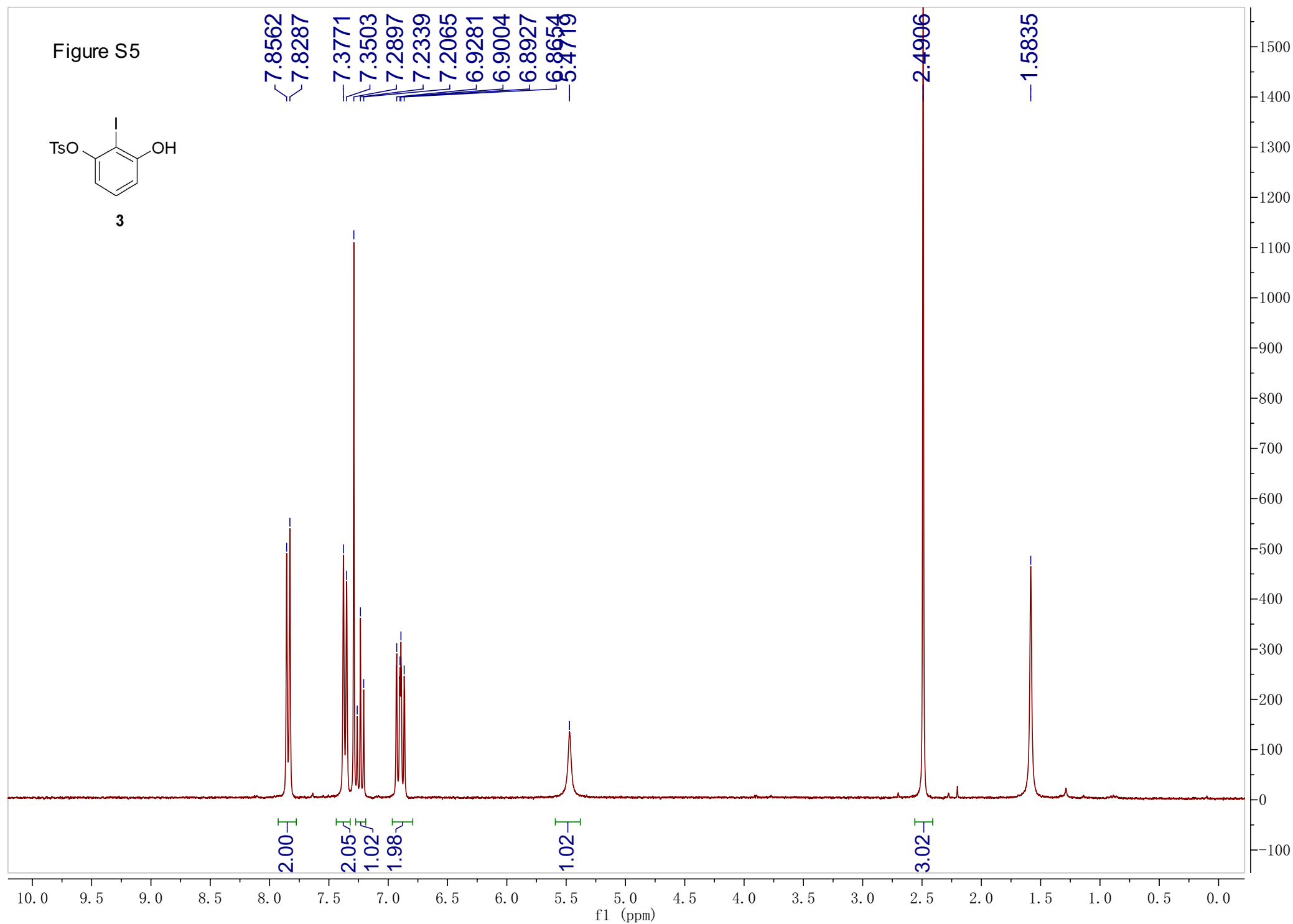
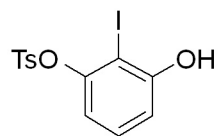
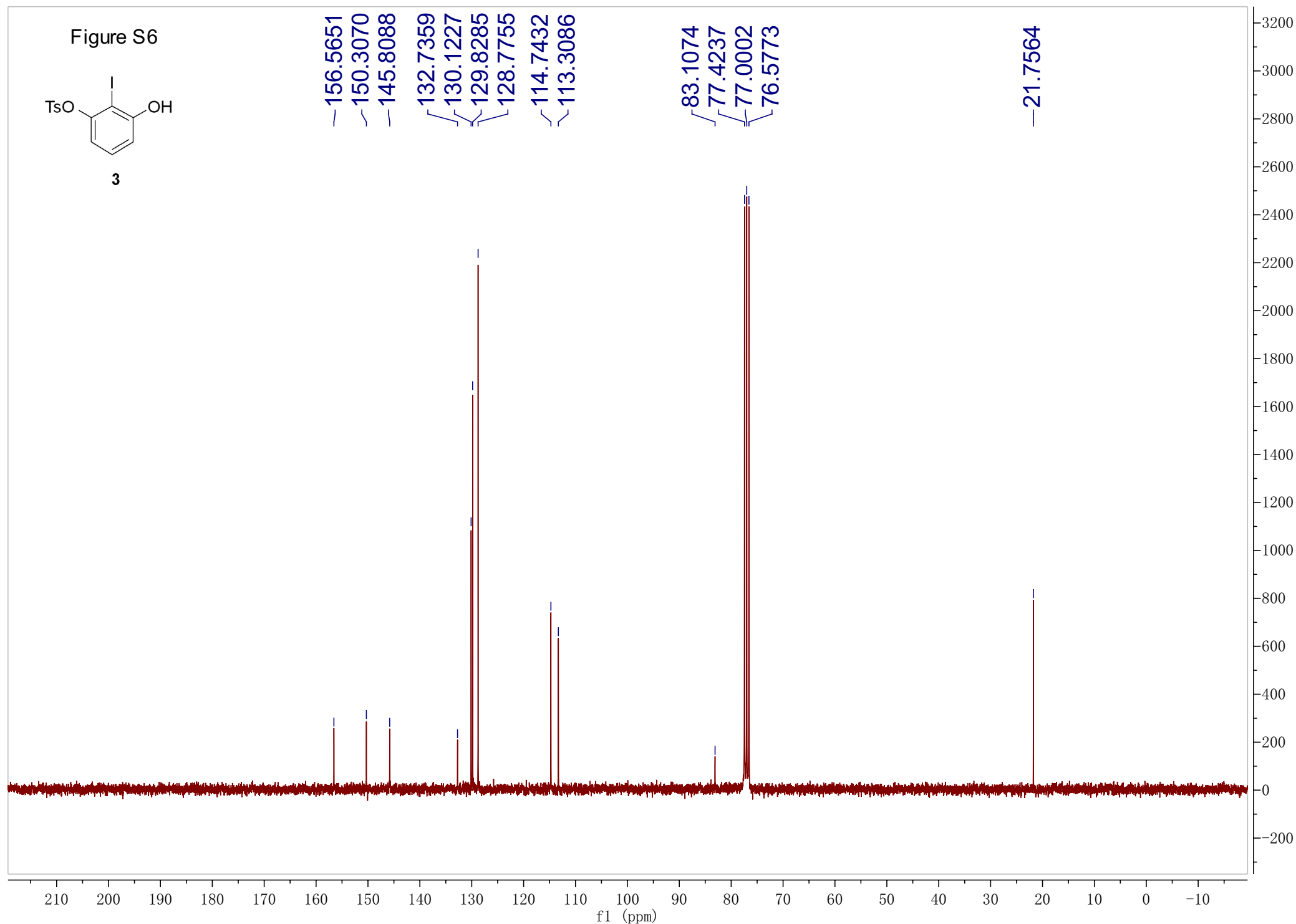


Figure S6



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Tolerance = 0.4 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Monoisotopic Mass, Odd and Even Electron Ions

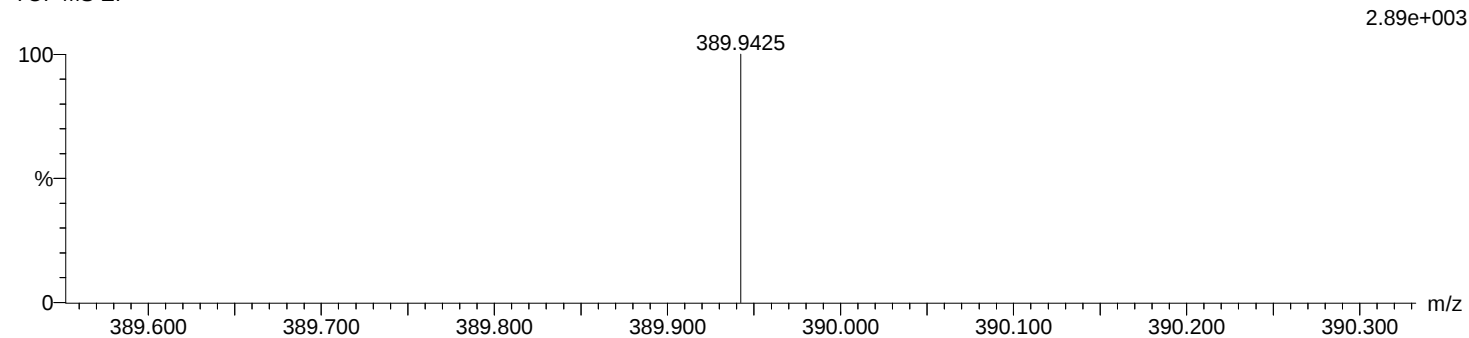
293 formula(e) evaluated with 1 results within limits (up to 70 best isotopic matches for each mass)

Elements Used:

C: 0-50 H: 0-100 O: 0-6 S: 0-1 Br: 0-4 I: 0-1

F-3 712 (4.750)

TOF MS EI+



Minimum: -1.5
Maximum: 0.4 10.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
389.9425	389.9423	0.2	0.5	8.0	5547446.0	C13 H11 O4 S I

Figure S7

