

Supporting Information

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Synthesis, characterization, antioxidant, in silico based virtual screening and anti- cancer potential of substituted 2-(4-acetyl-5-methyl-1h-1,2,3-triazol-1-yl)-n- phenylacetamide derivatives

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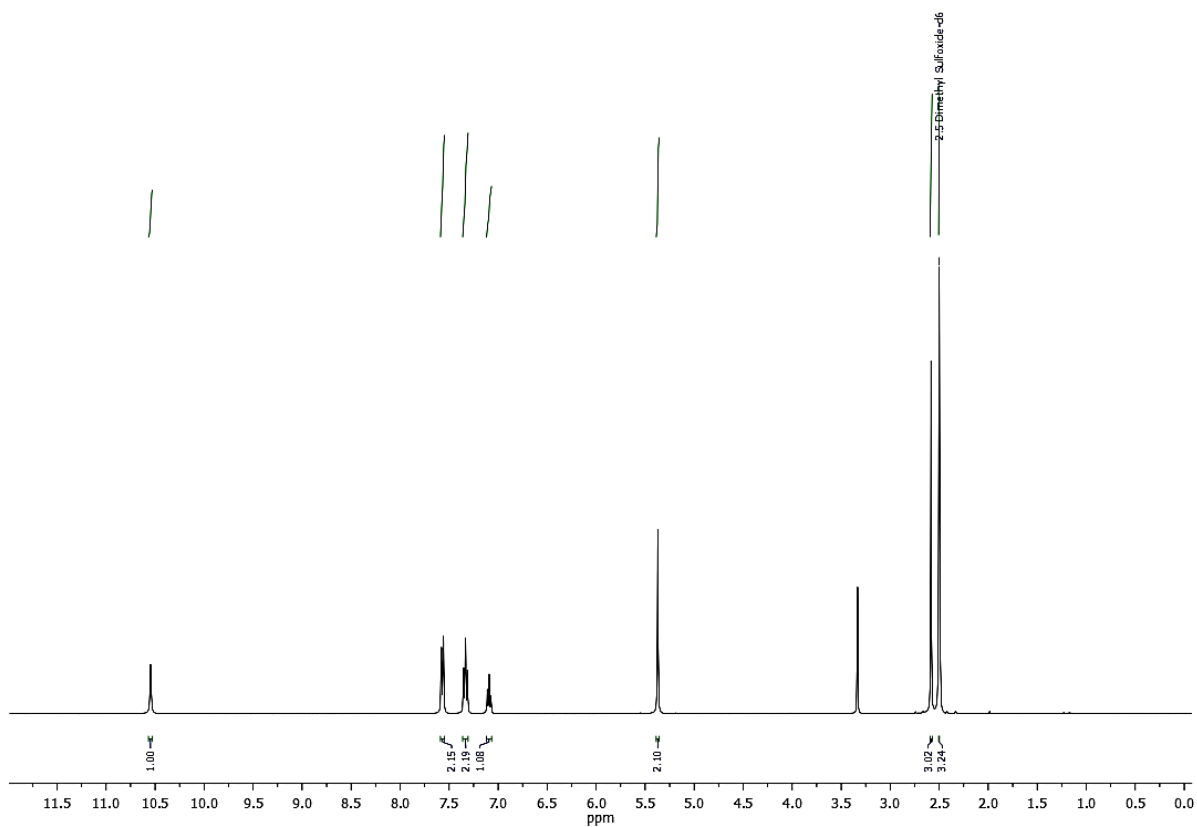


Figure S1: ^1H NMR of (**3a**)

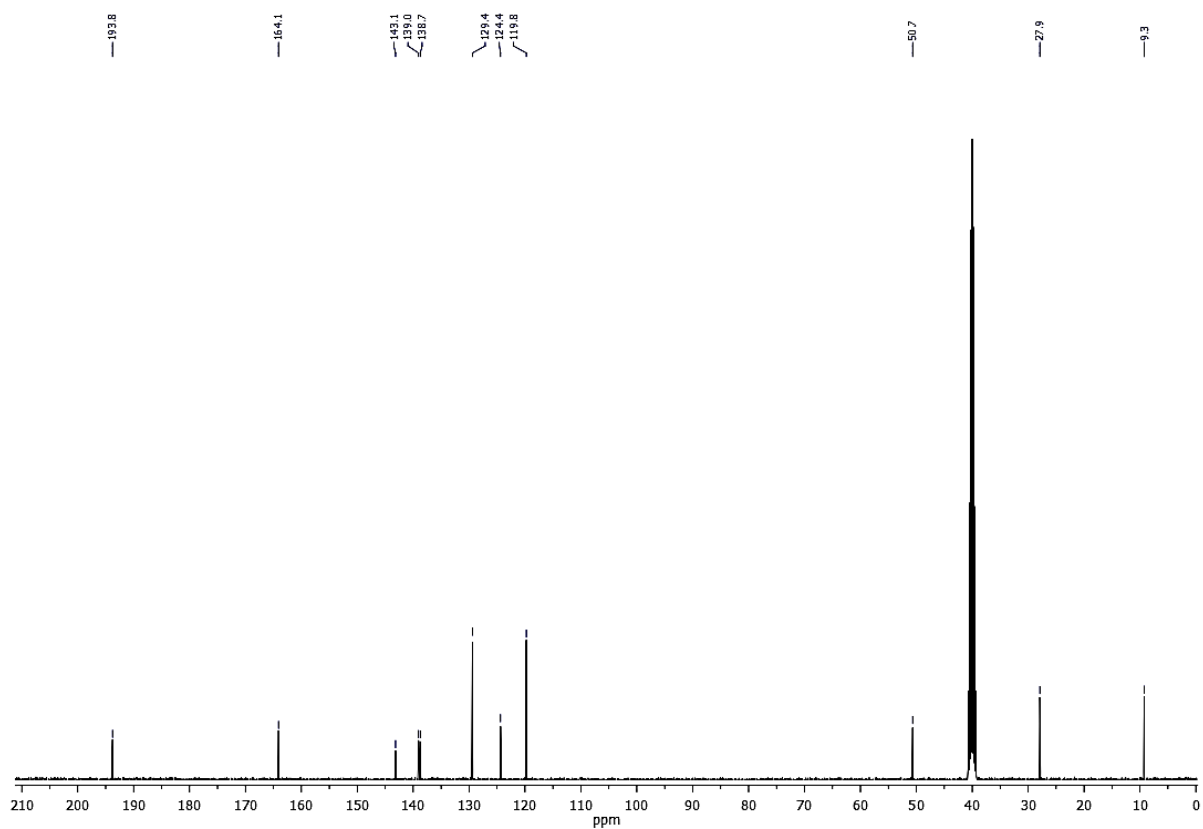


Figure S2: ^{13}C NMR of (3a)

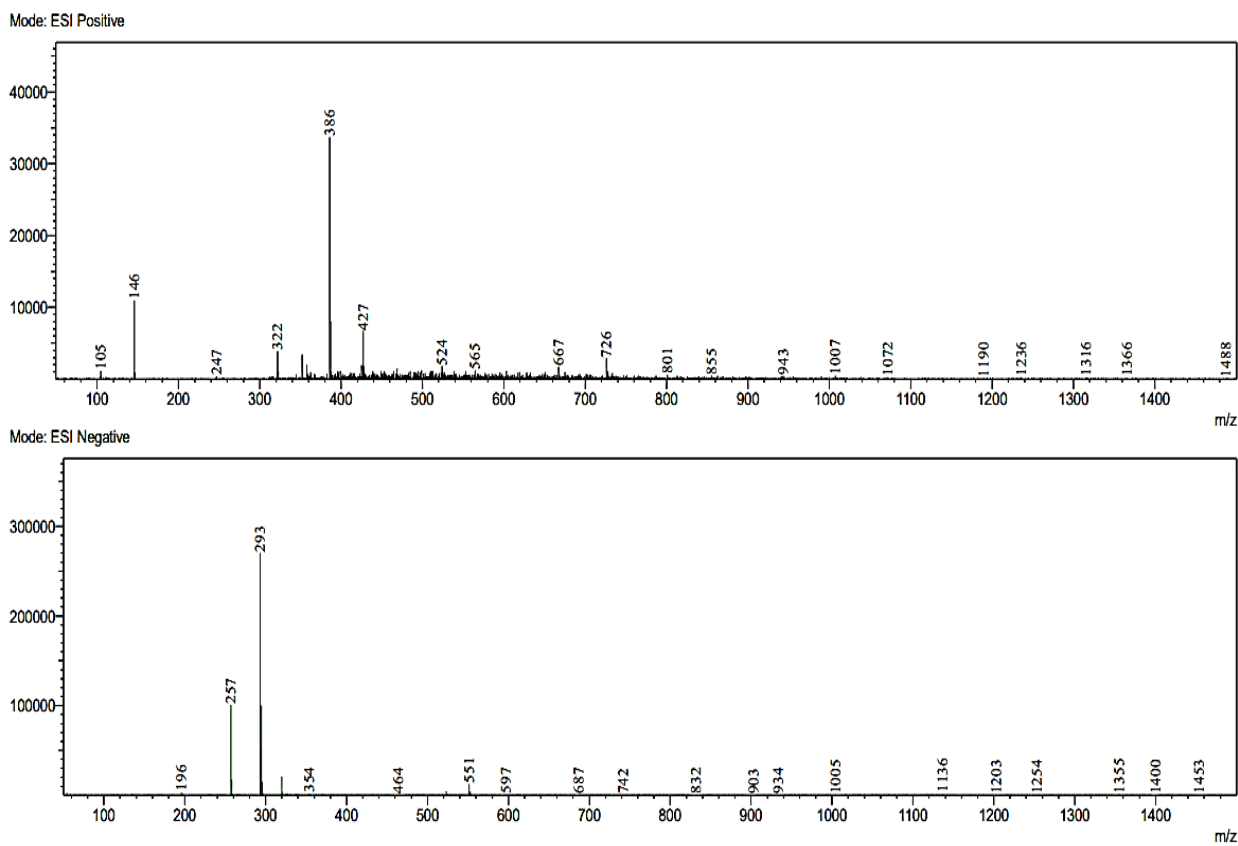


Figure S3: ESI-LCMS of (3a)

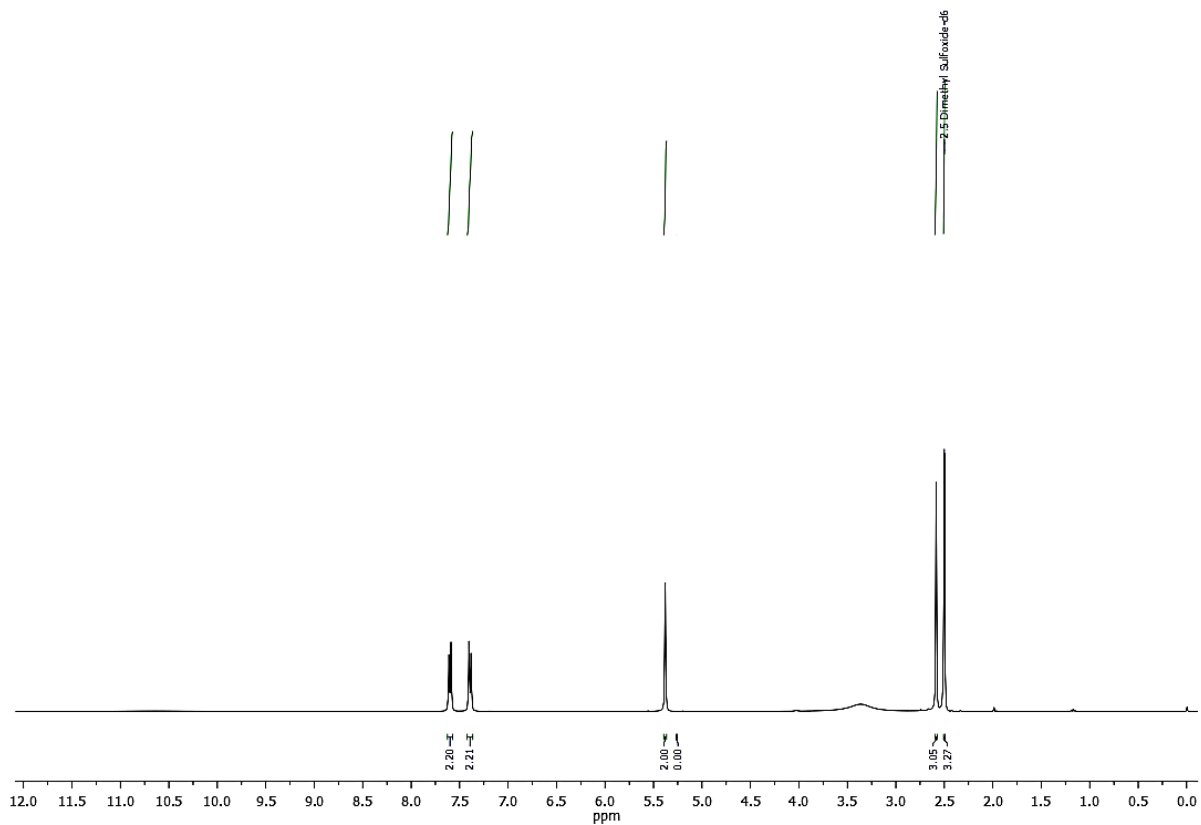


Figure S4: ^1H NMR of (**3b**)

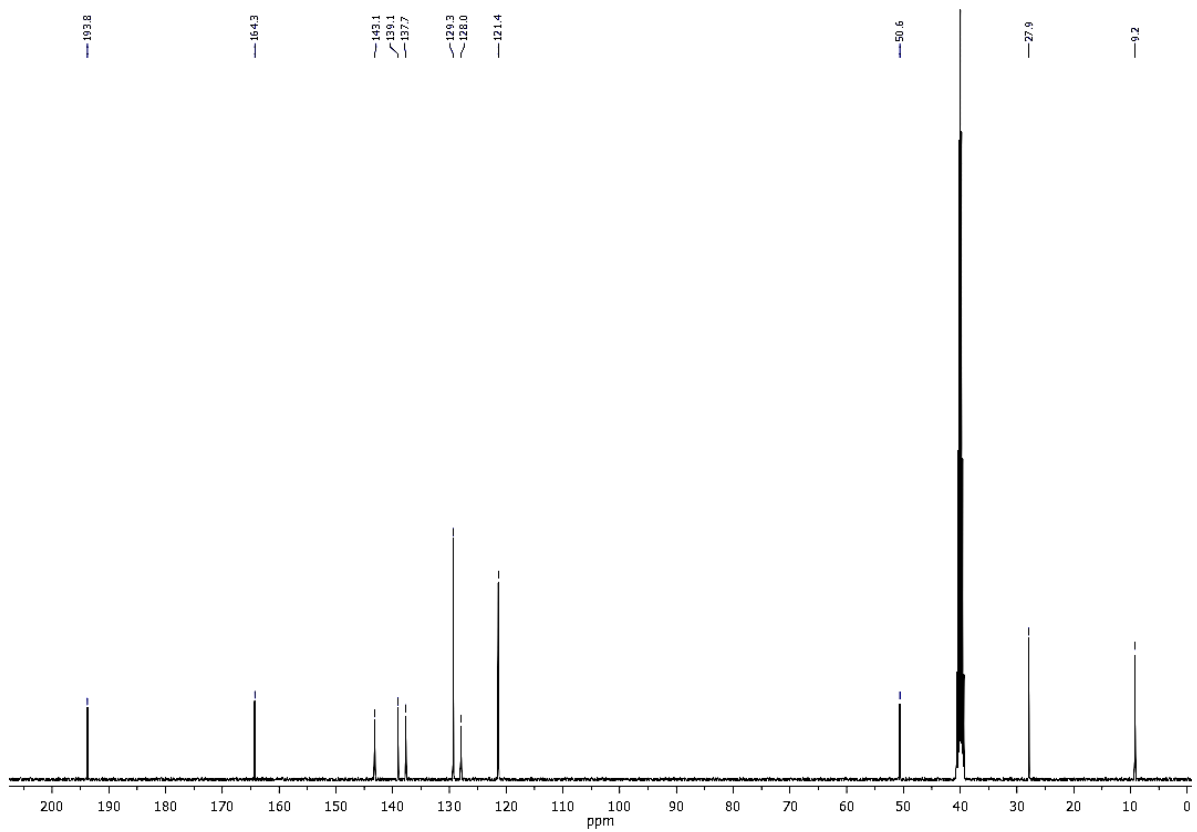


Figure S5: ^{13}C NMR of (3b)

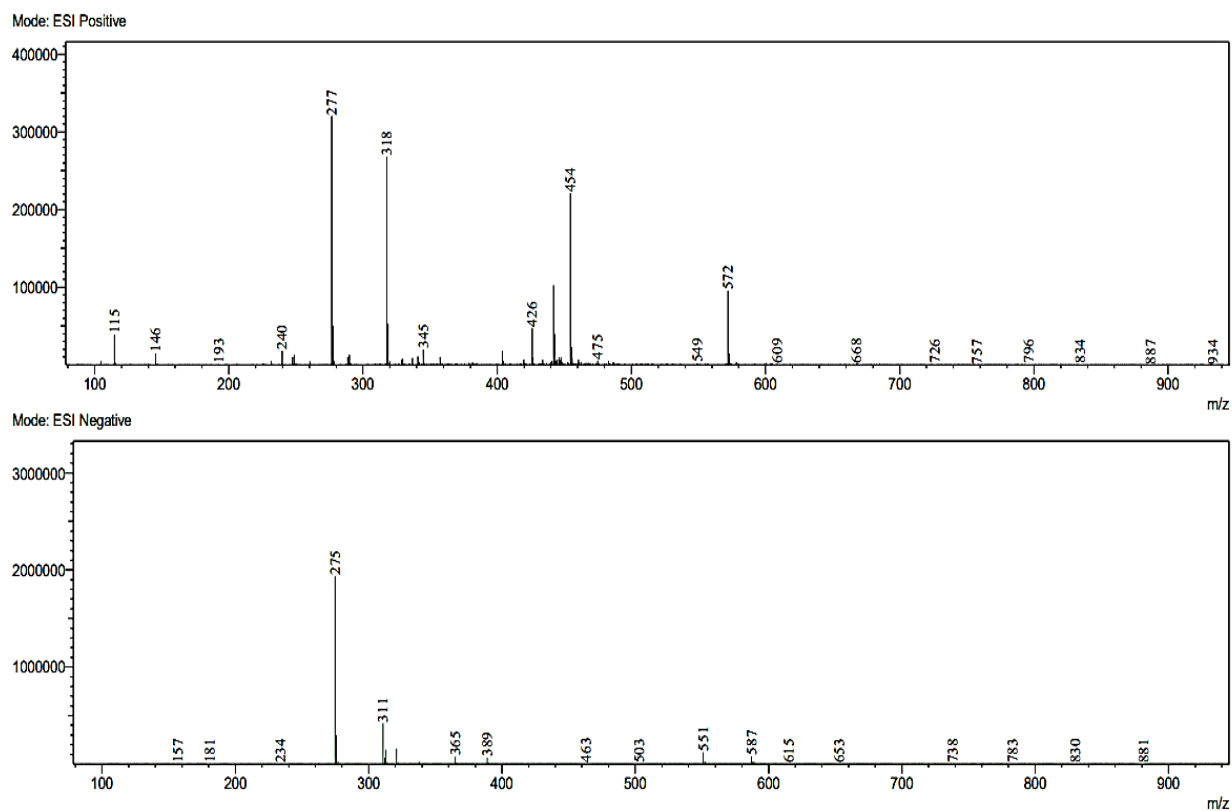


Figure S6: ESI-LCMS of (3b)

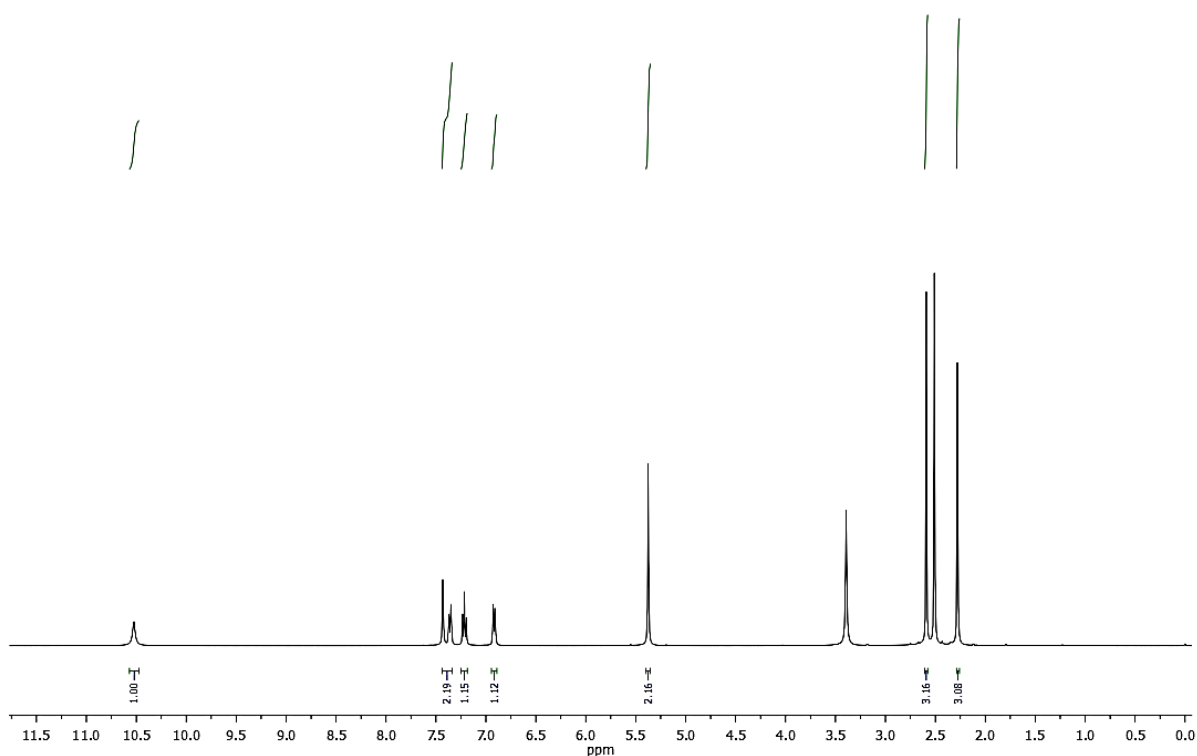


Figure S7: ^1H NMR of (**3c**)

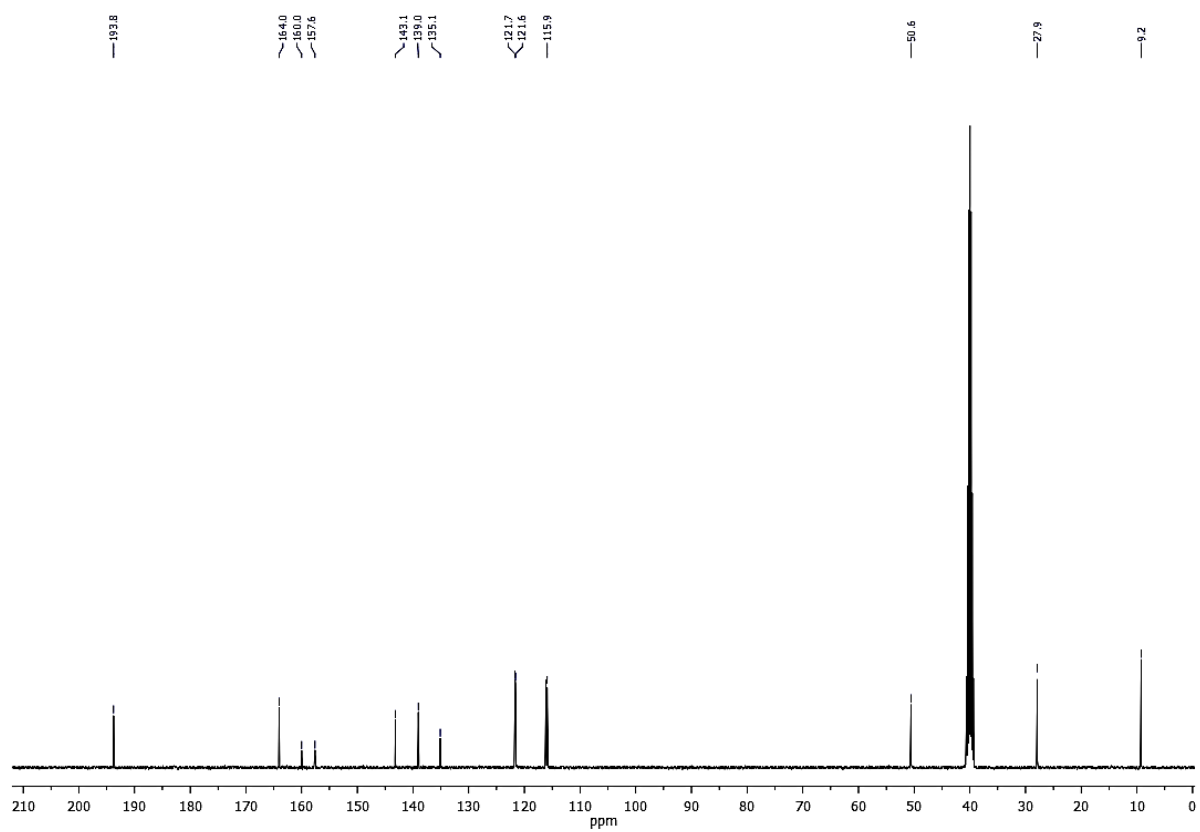


Figure S8: ^{13}C NMR of (3c)

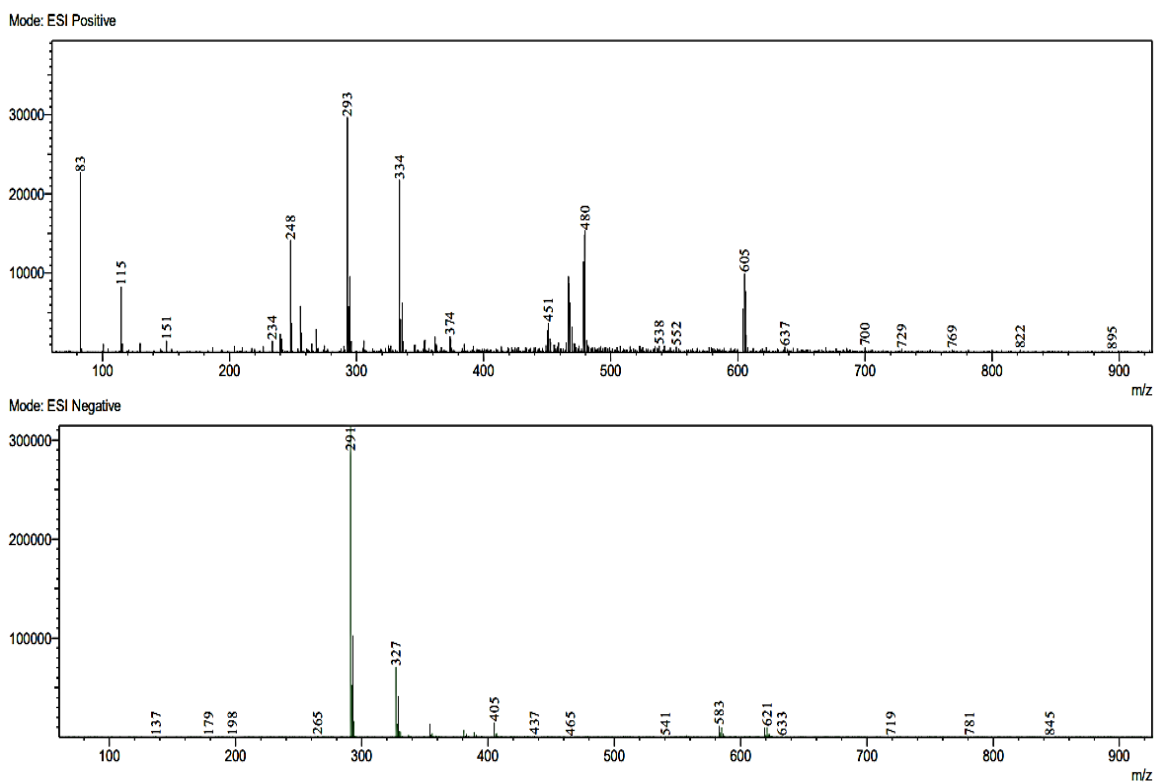


Figure S9: ESI-LCMS of (3c)

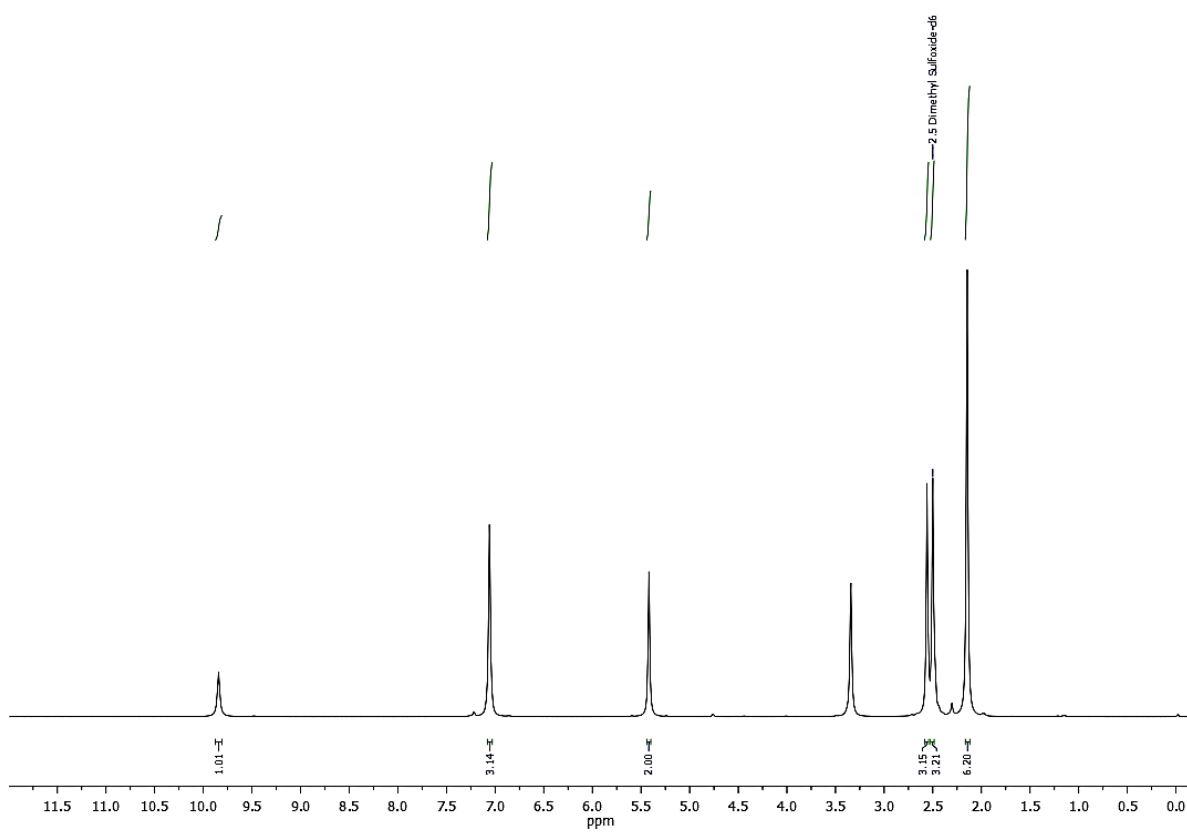


Figure S10: ^1H NMR of (**3d**)

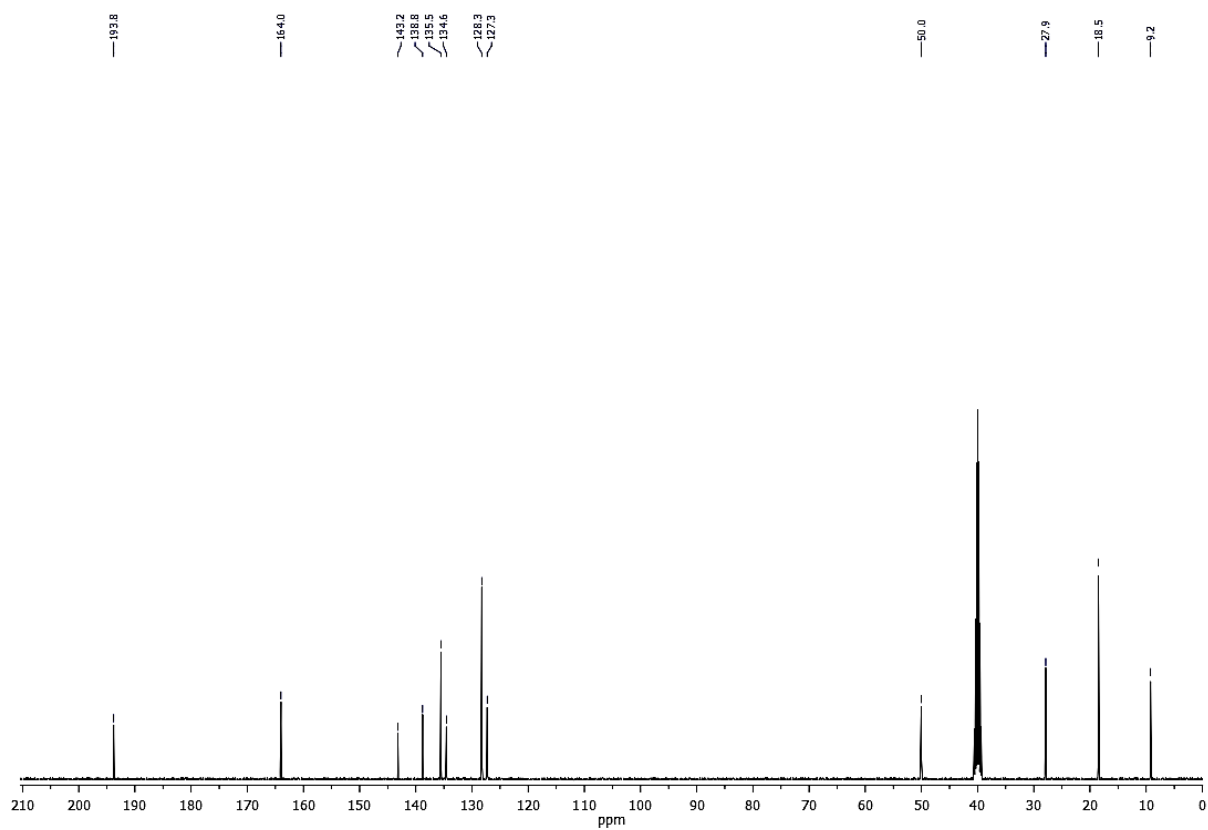


Figure S11: ^{13}C NMR of (3d)

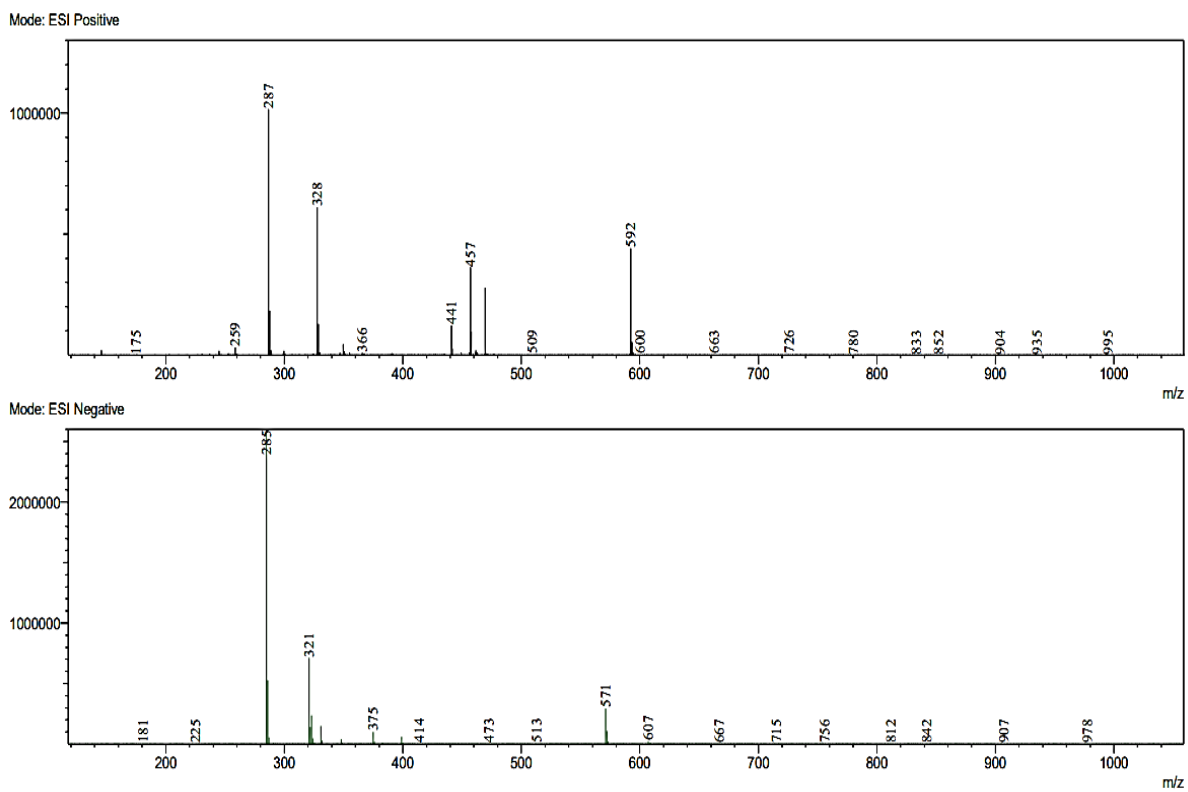


Figure S12: ESI-LCMS of (3d)

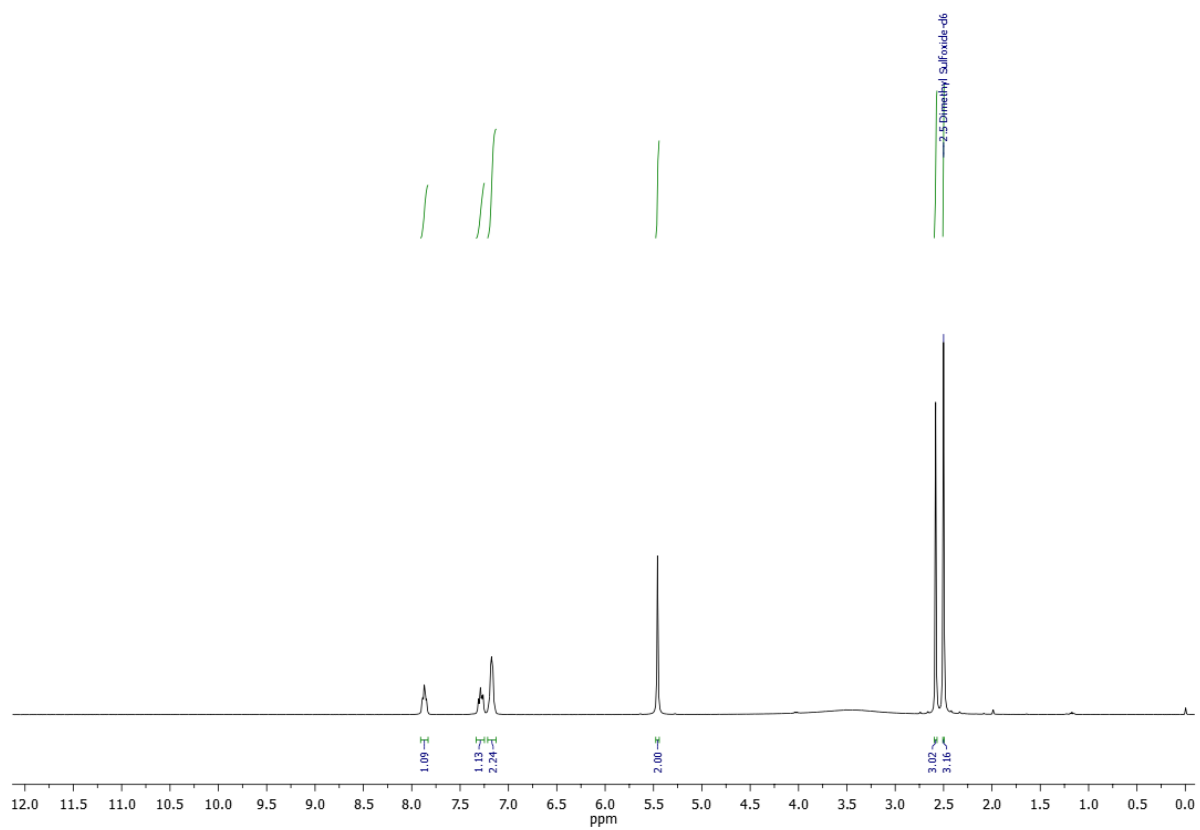


Figure S13: ^1H NMR of (3e)

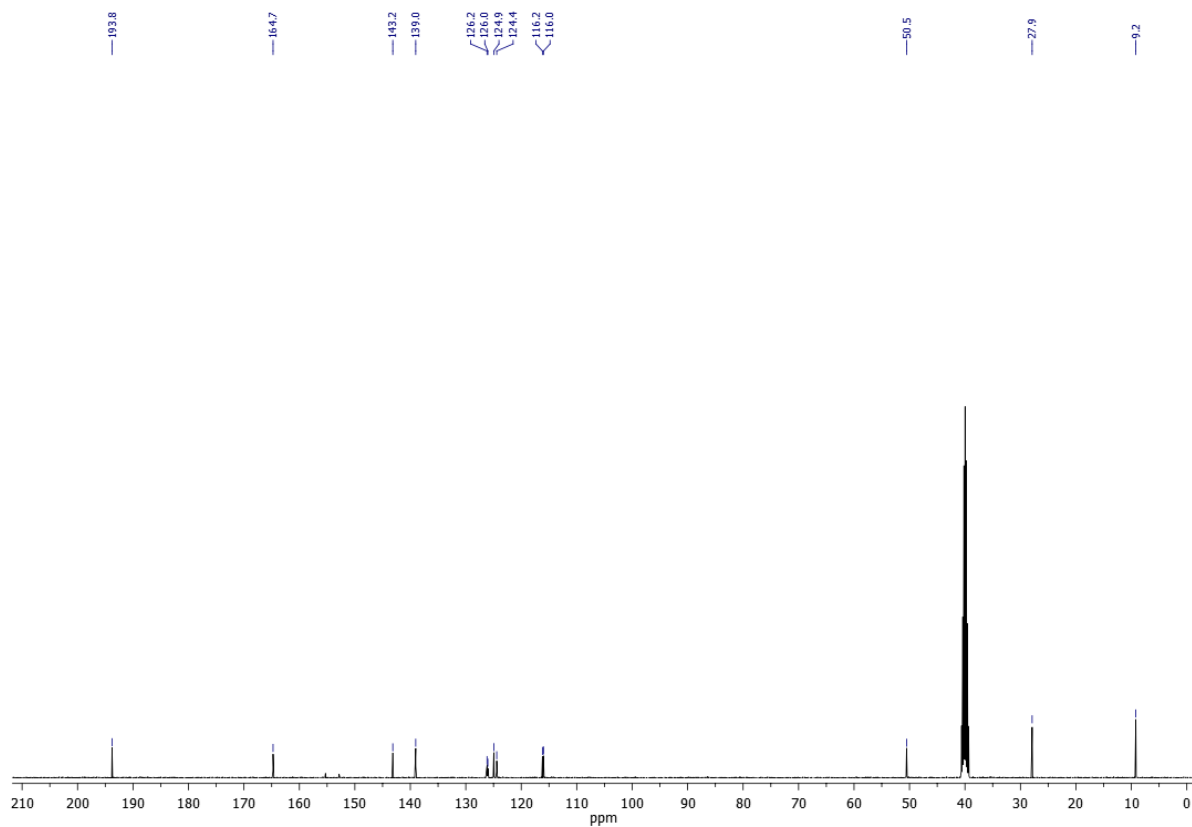


Figure S14: ^{13}C NMR of (3e)

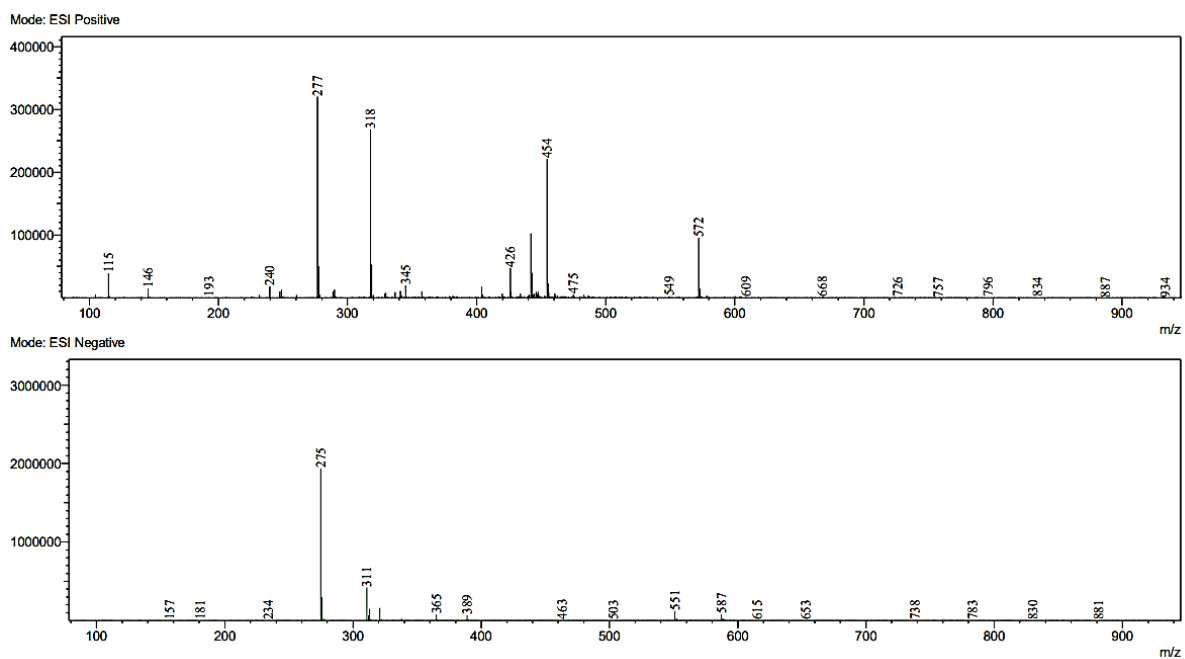


Figure S15: ESI-LCMS of (3e)

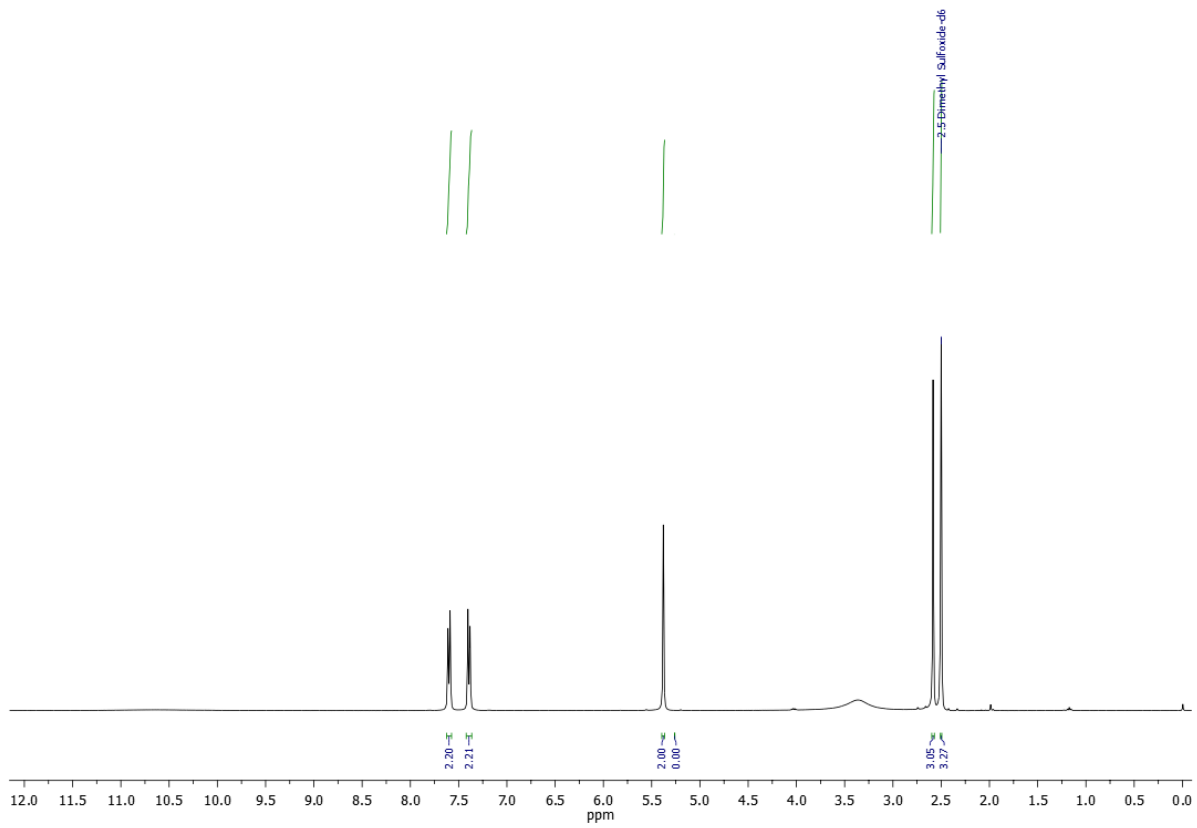


Figure S16: ^1H NMR of (**3f**)

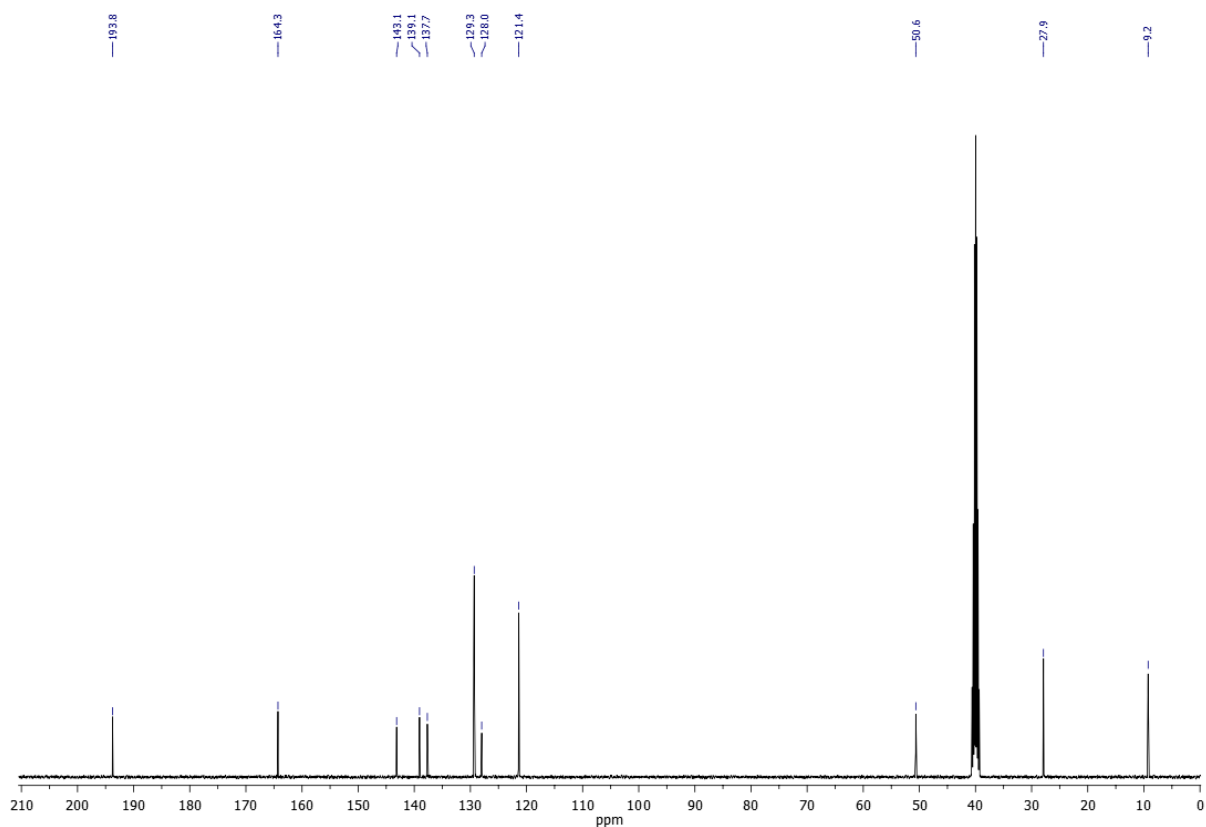


Figure S17: ^{13}C NMR of **(3f)**

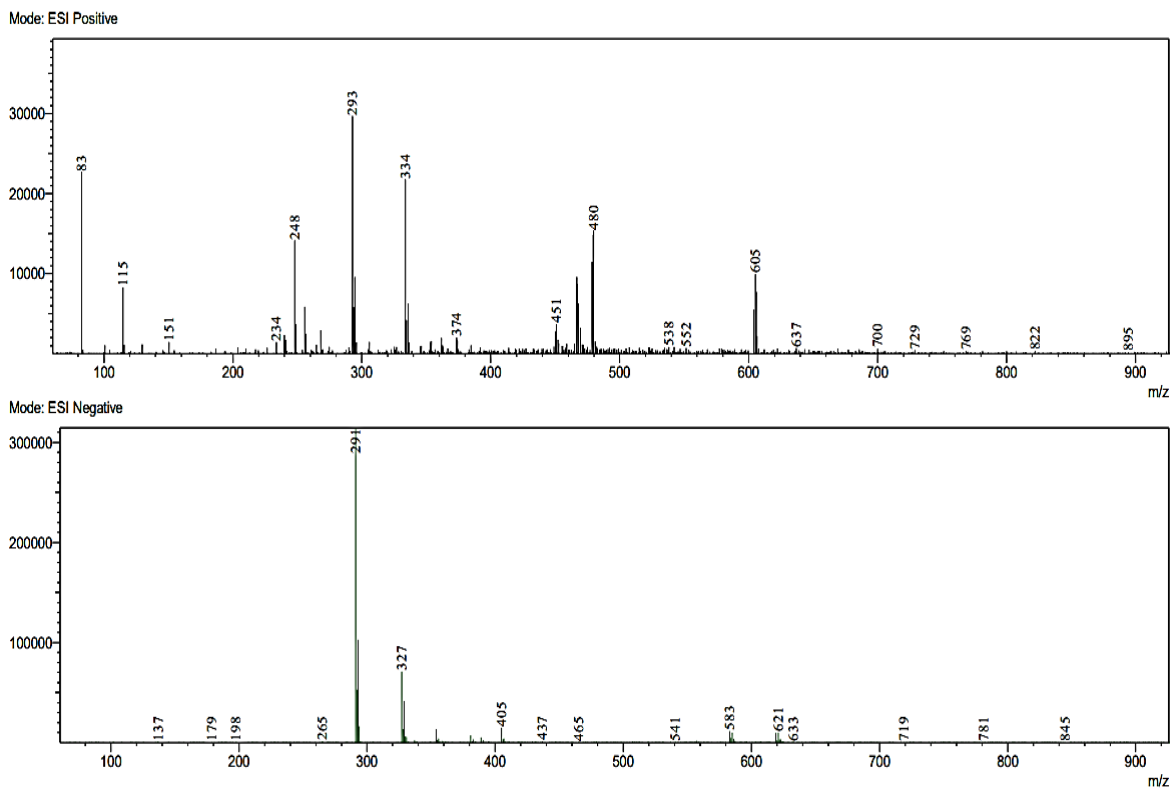


Figure S18: ESI-LCMS of (3f)

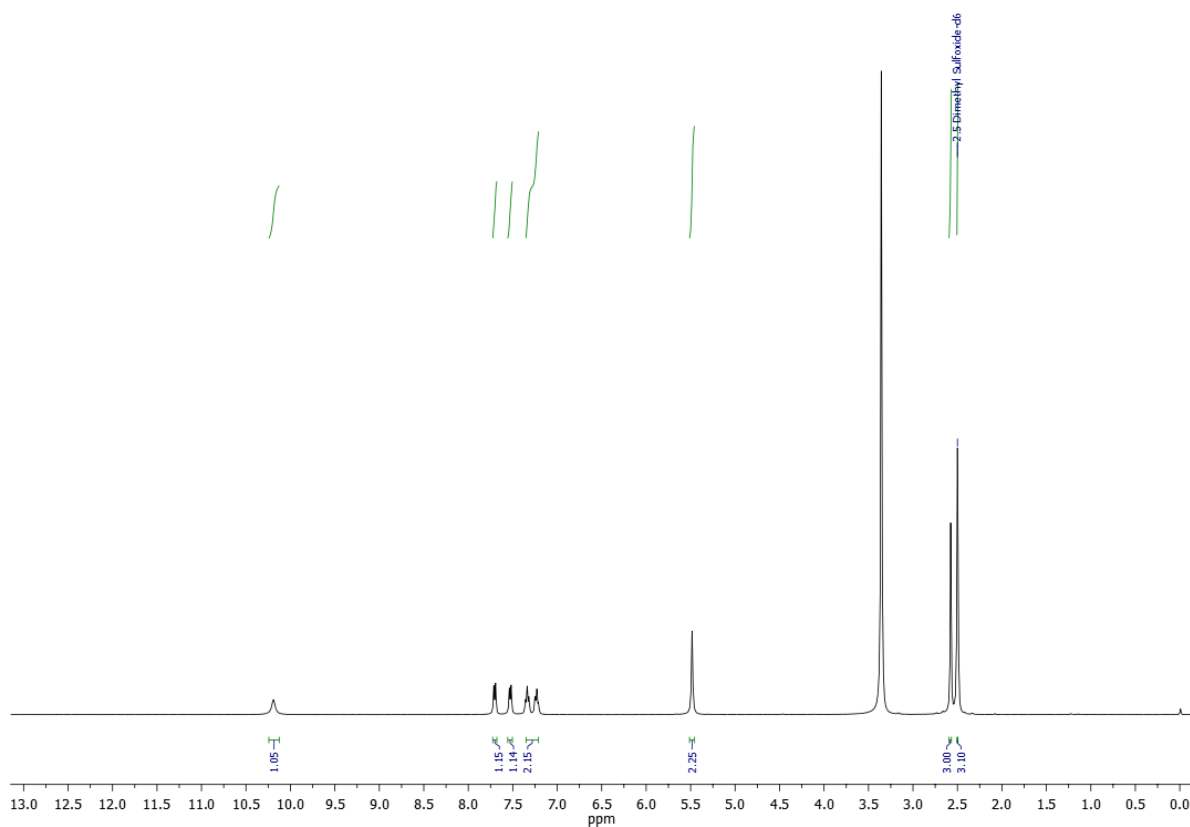


Figure S19: ^1H NMR of (**3g**)

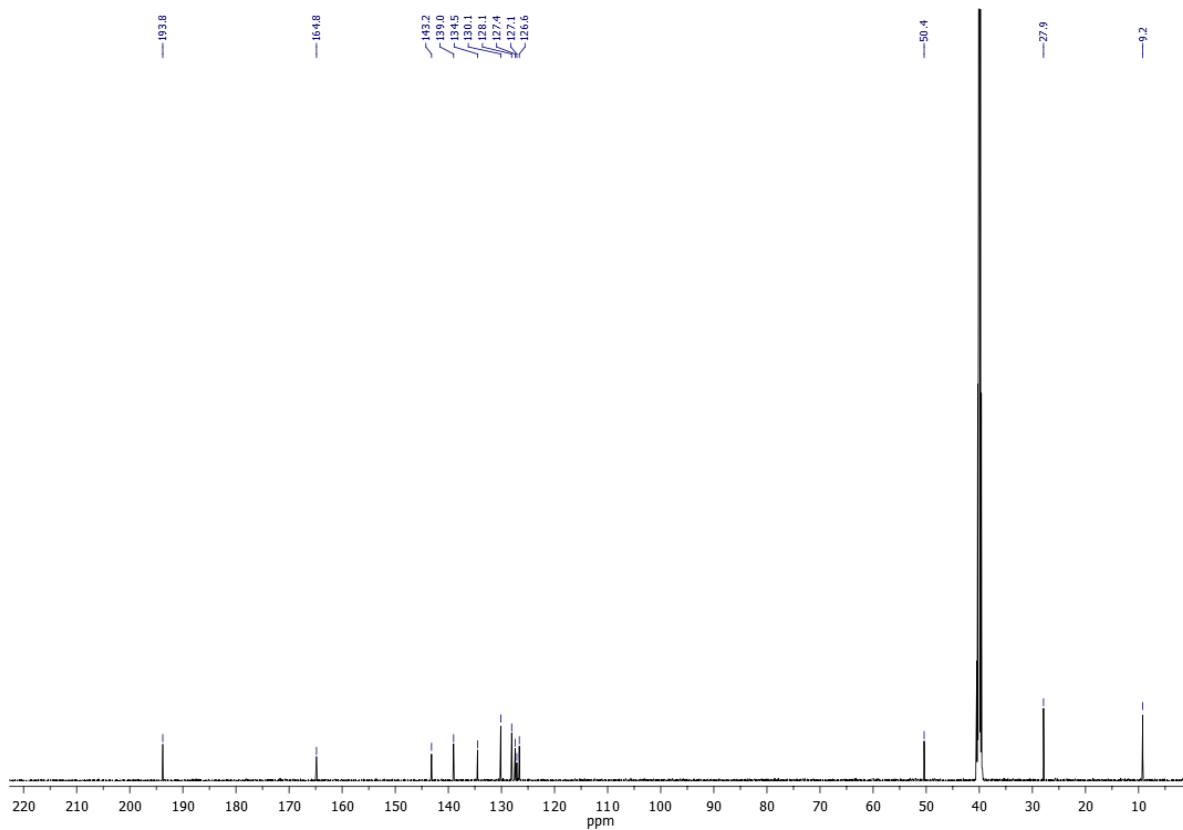


Figure S20: ^{13}C NMR of (3g)

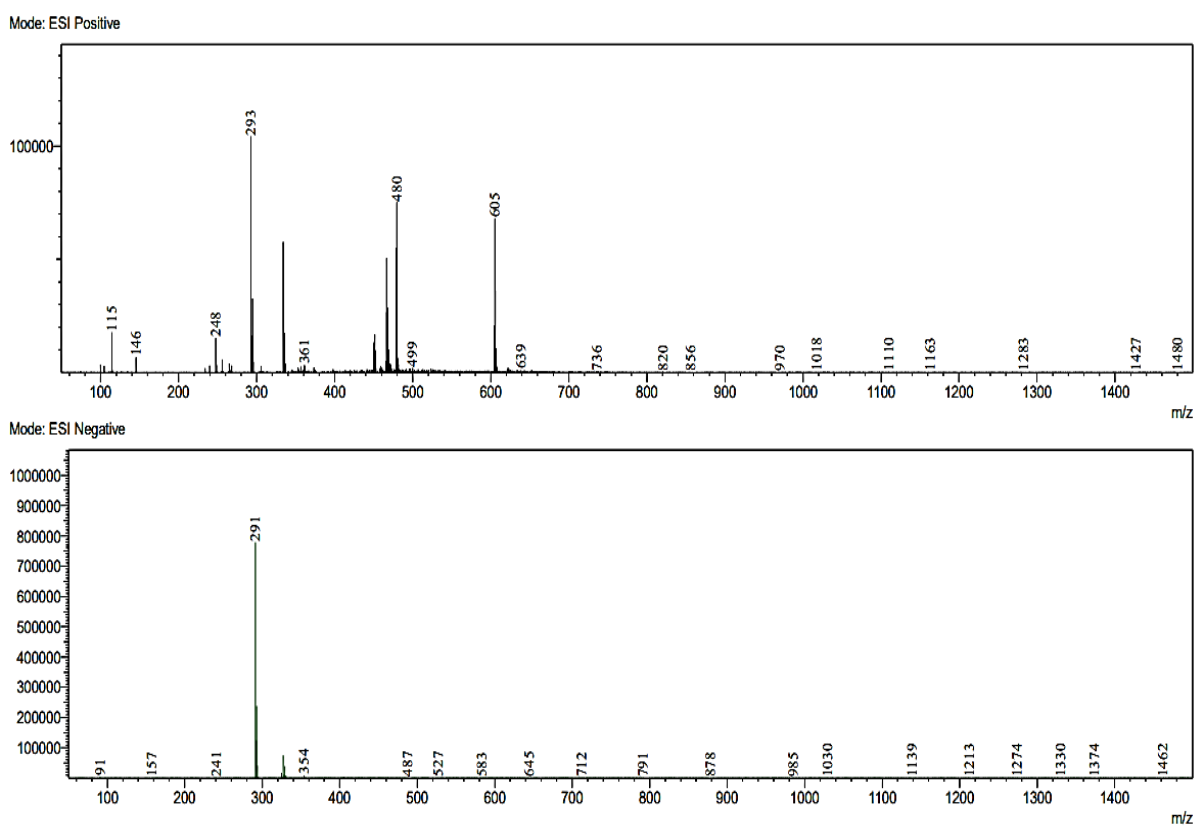


Figure S21: ESI-LCMS of (3g)

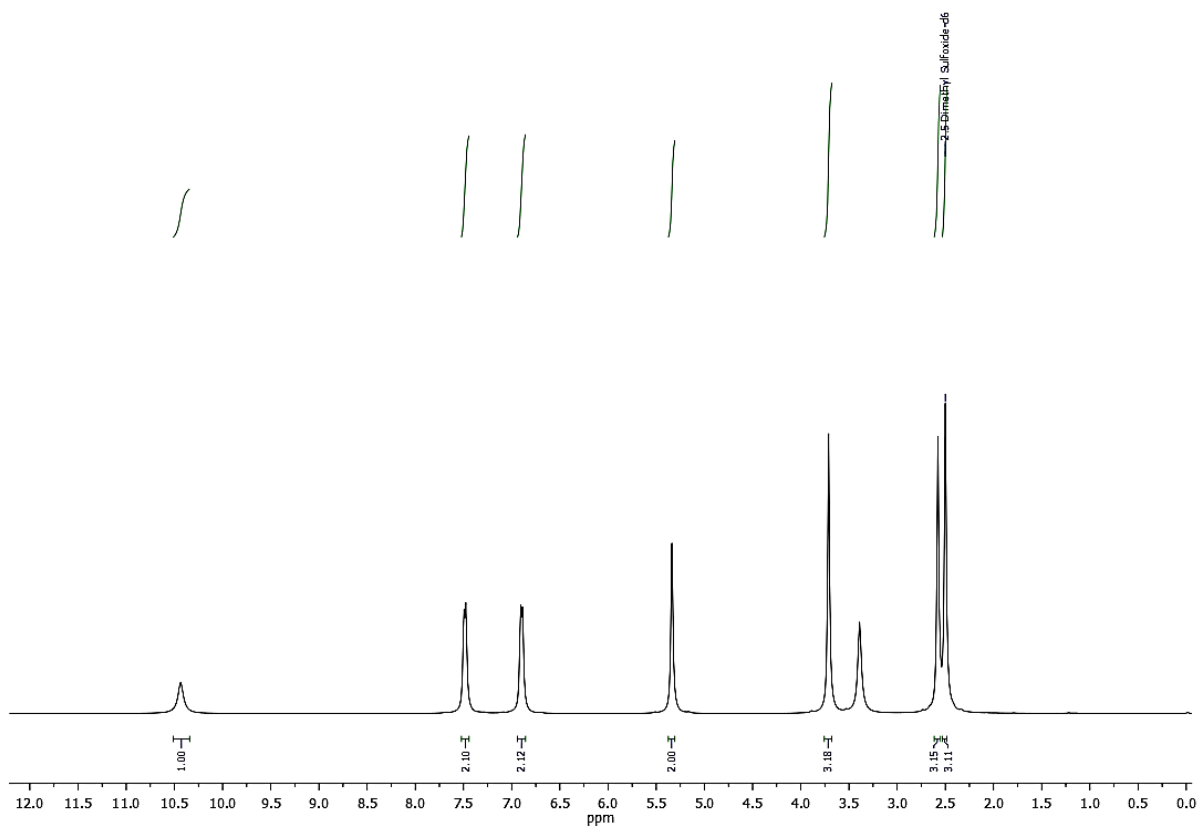


Figure S22: ^1H NMR of (3h)

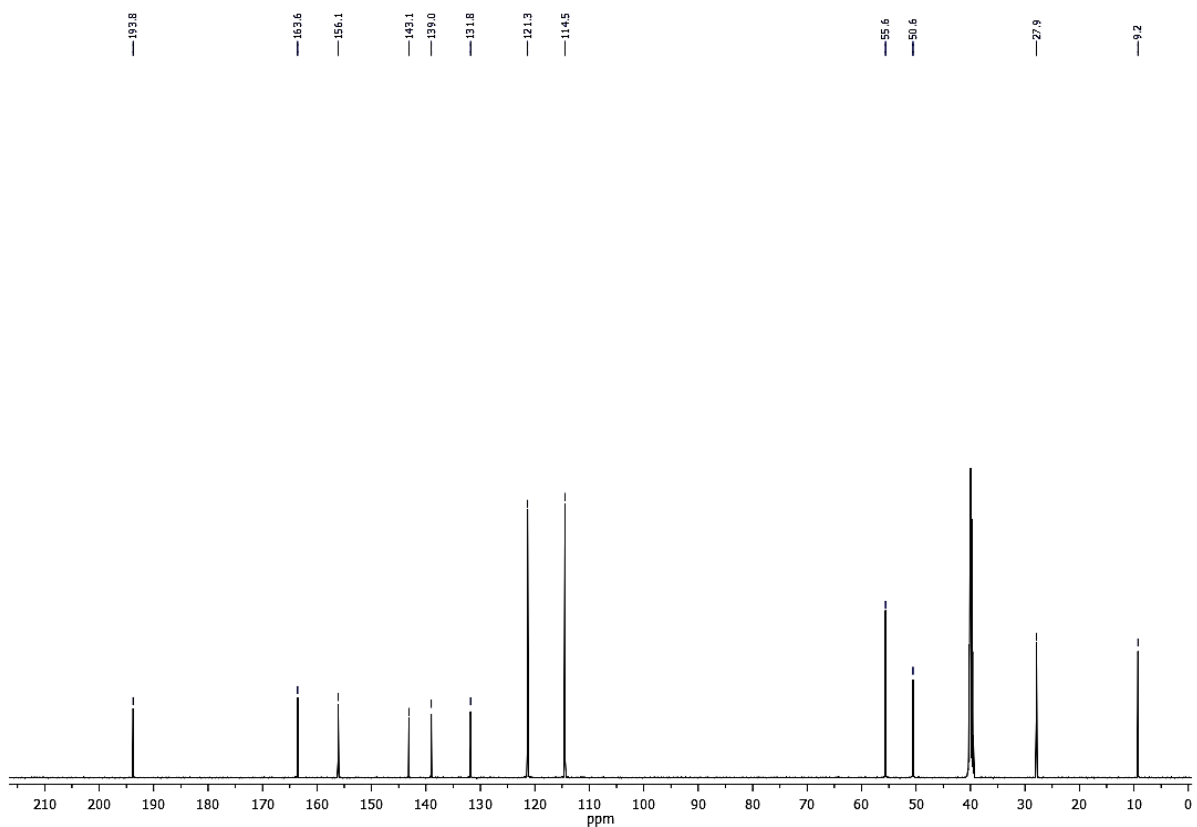


Figure S23: ^{13}C NMR of (3h)

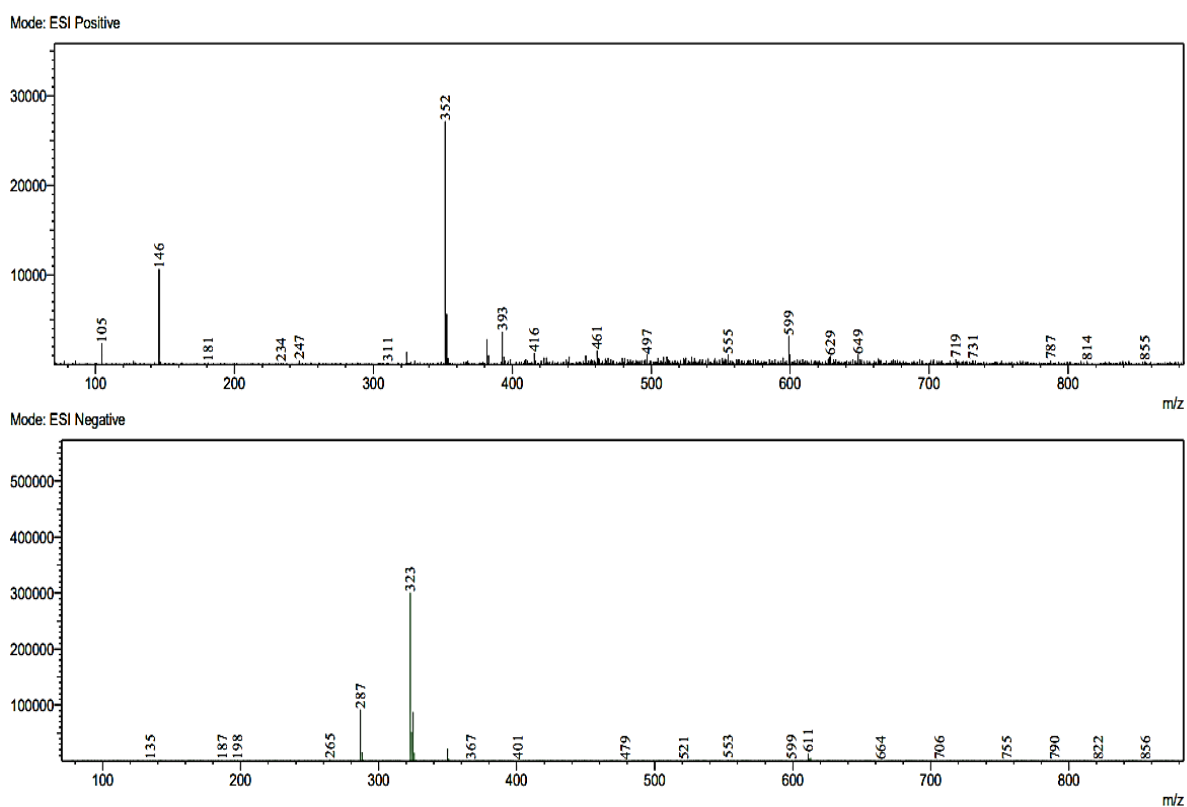


Figure S24: ESI-LCMS of (3h)

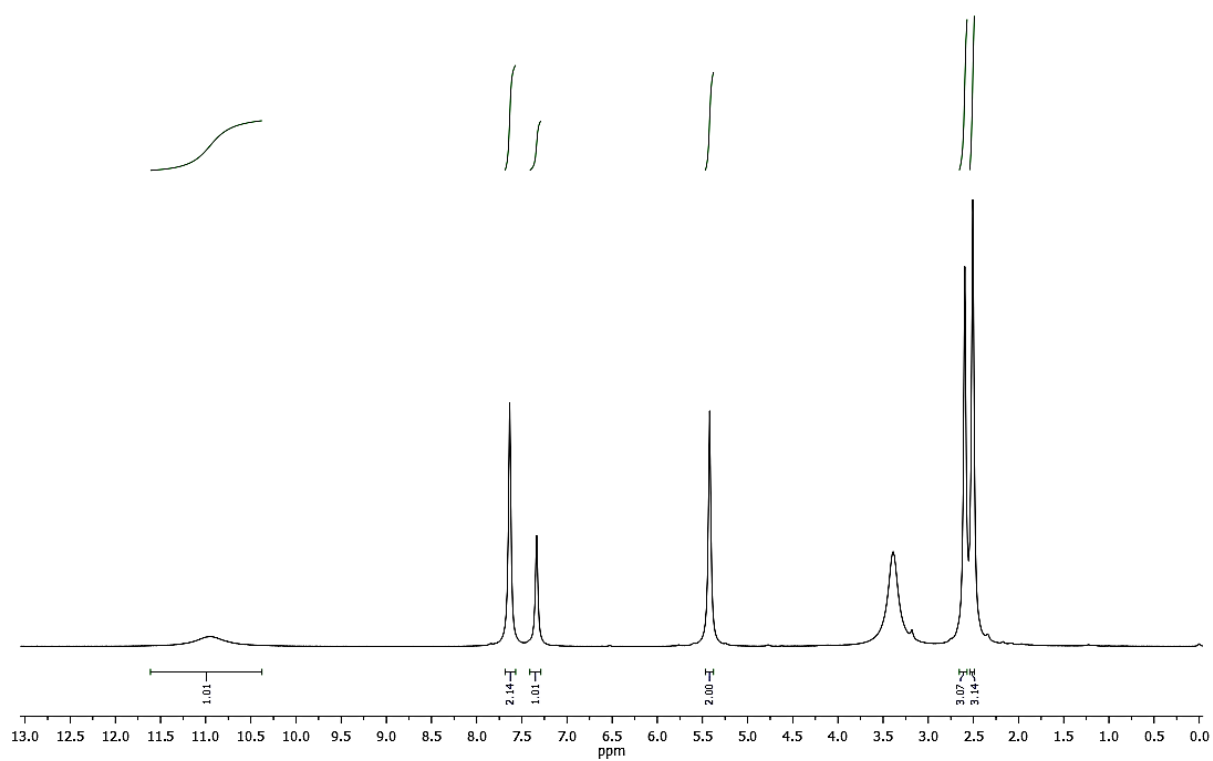


Figure S25: ^1H NMR of (3i)

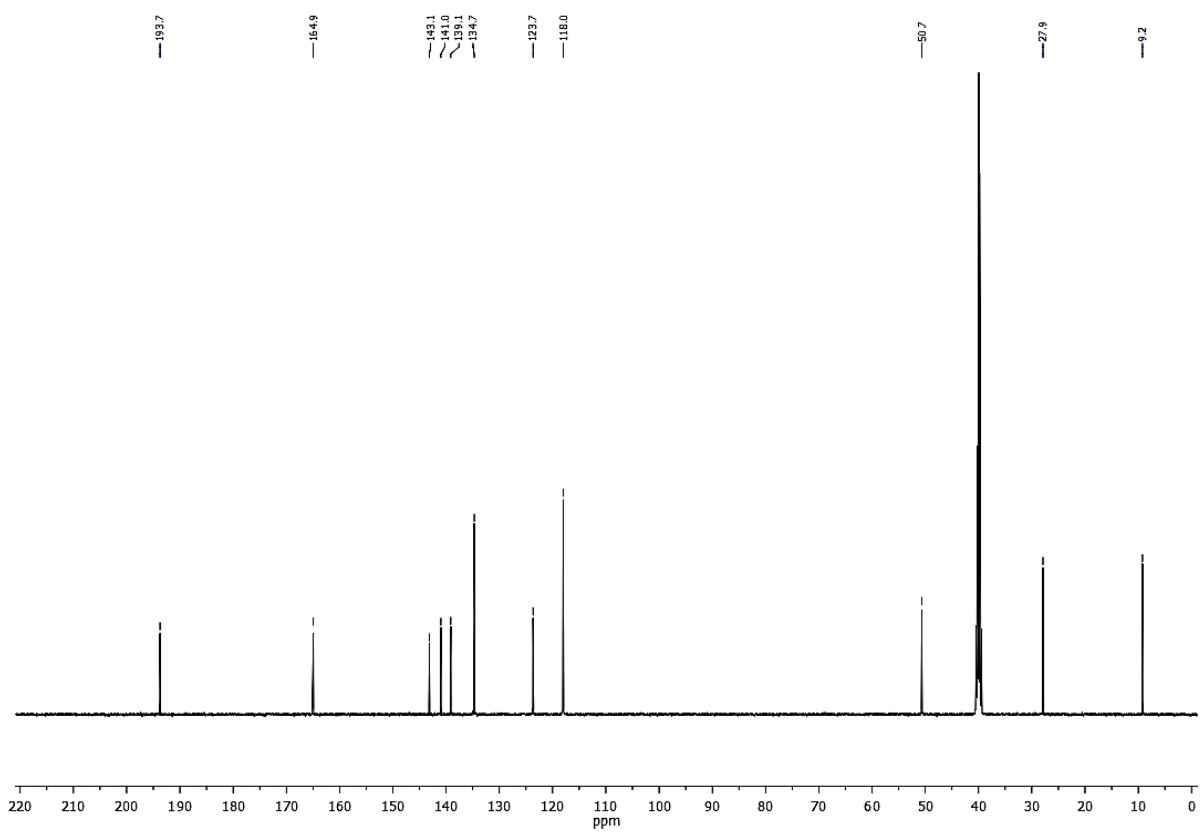


Figure S26: ^{13}C NMR of (3i)

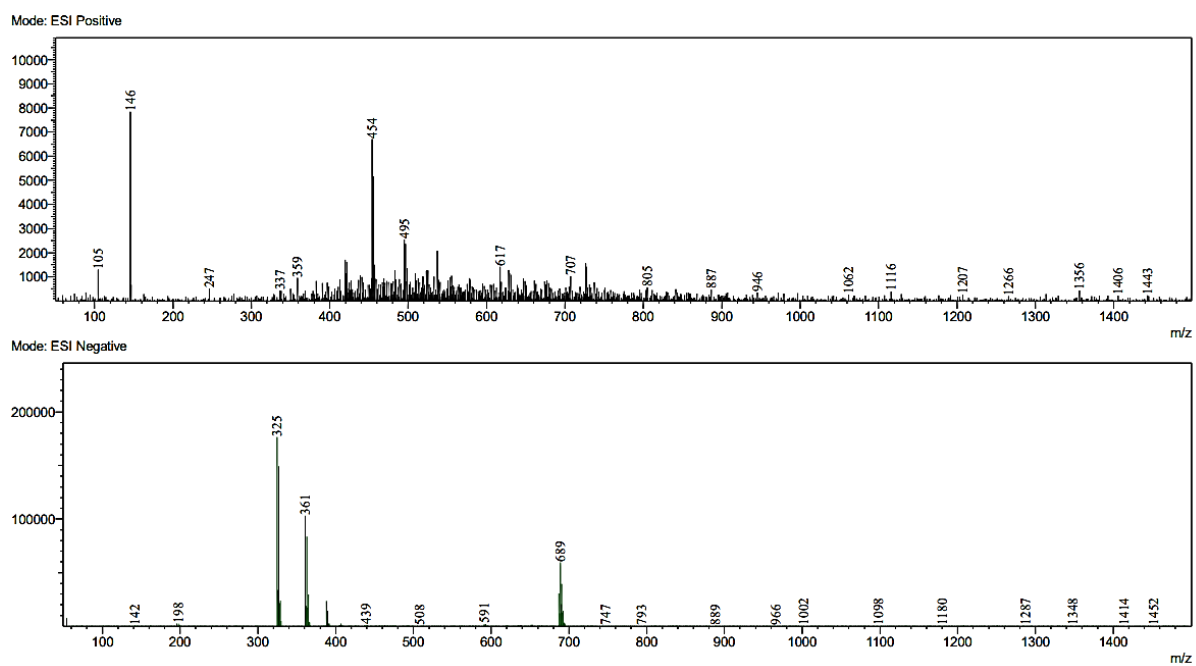


Figure S27: ESI-LCMS of (3i)

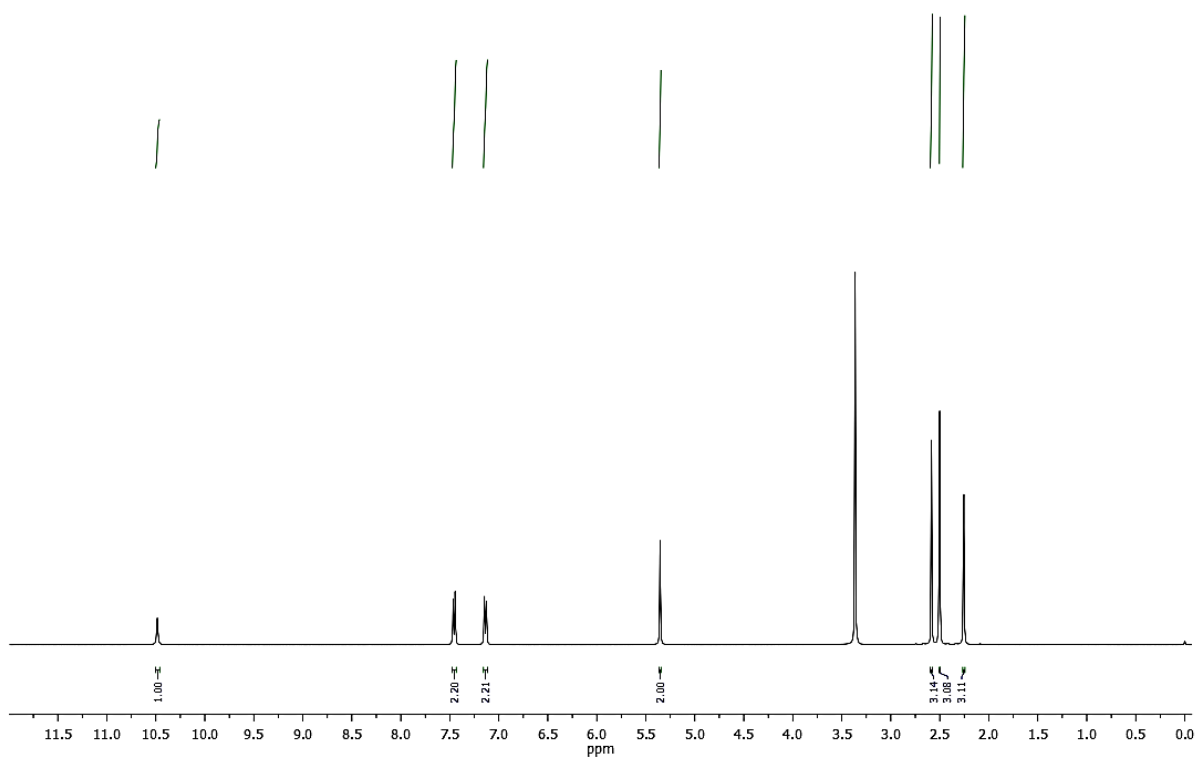


Figure S28: ^1H NMR of (3j)

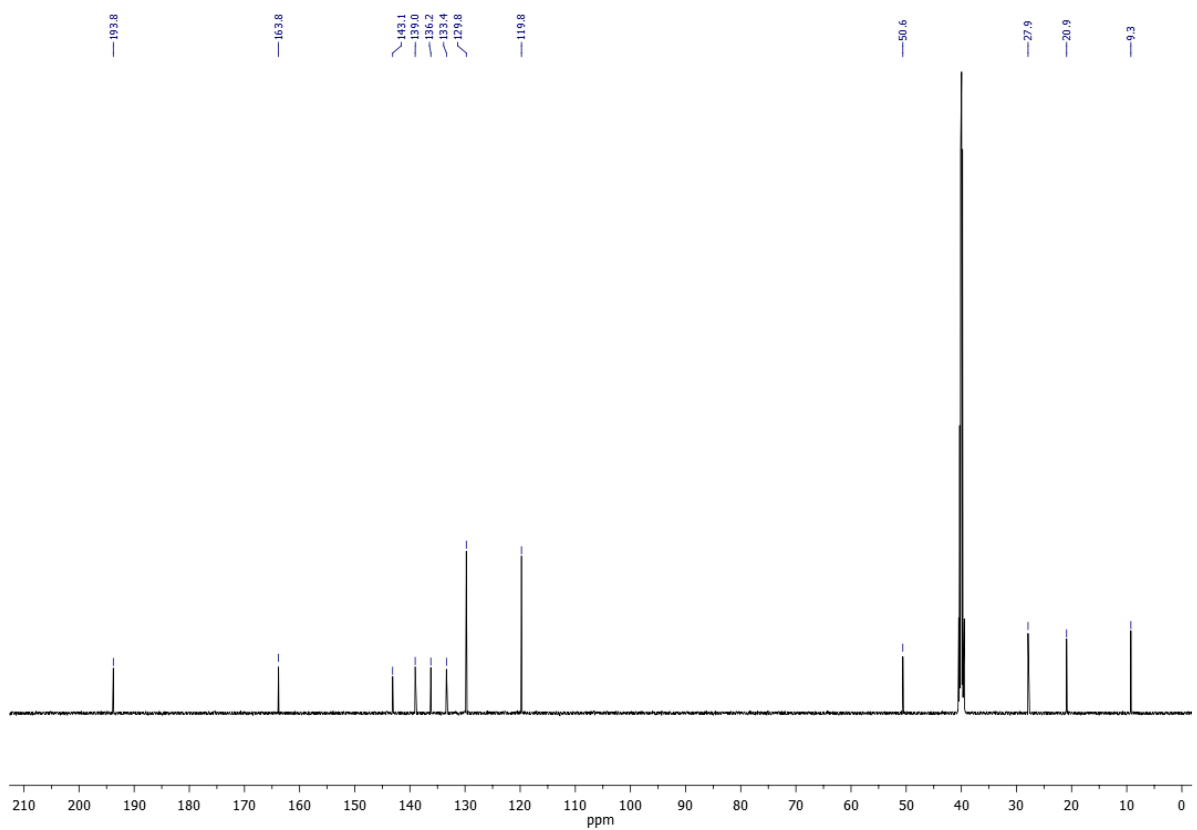


Figure S29: ^{13}C NMR of (3j)

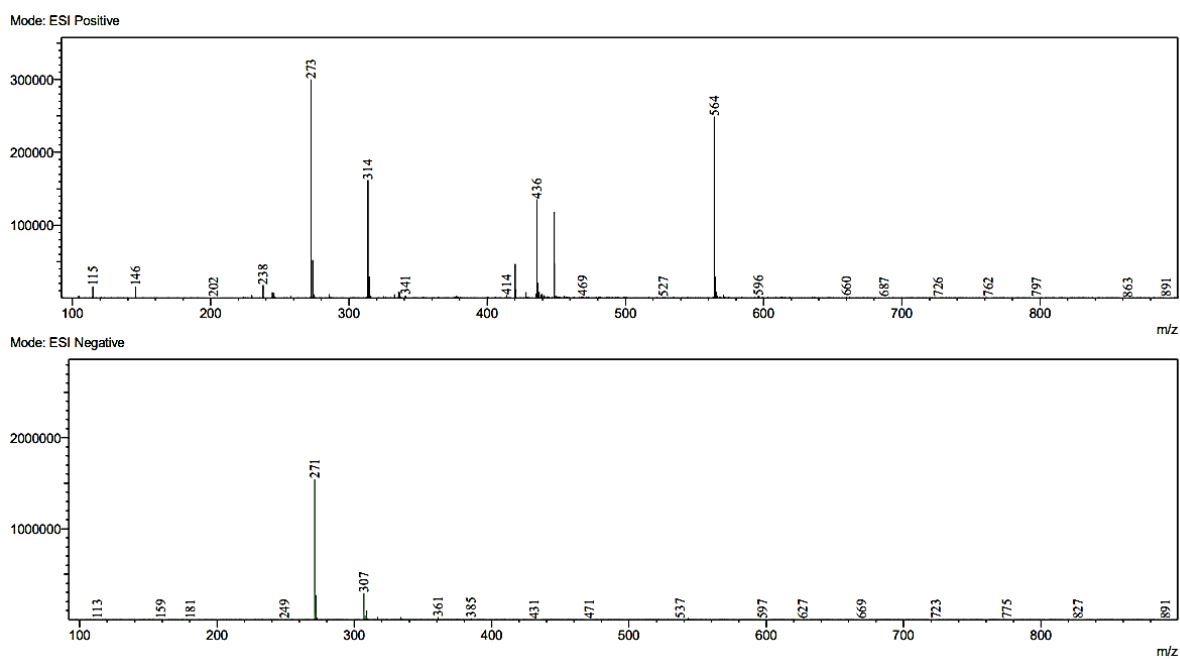


Figure S30: ESI-LCMS of (3j)

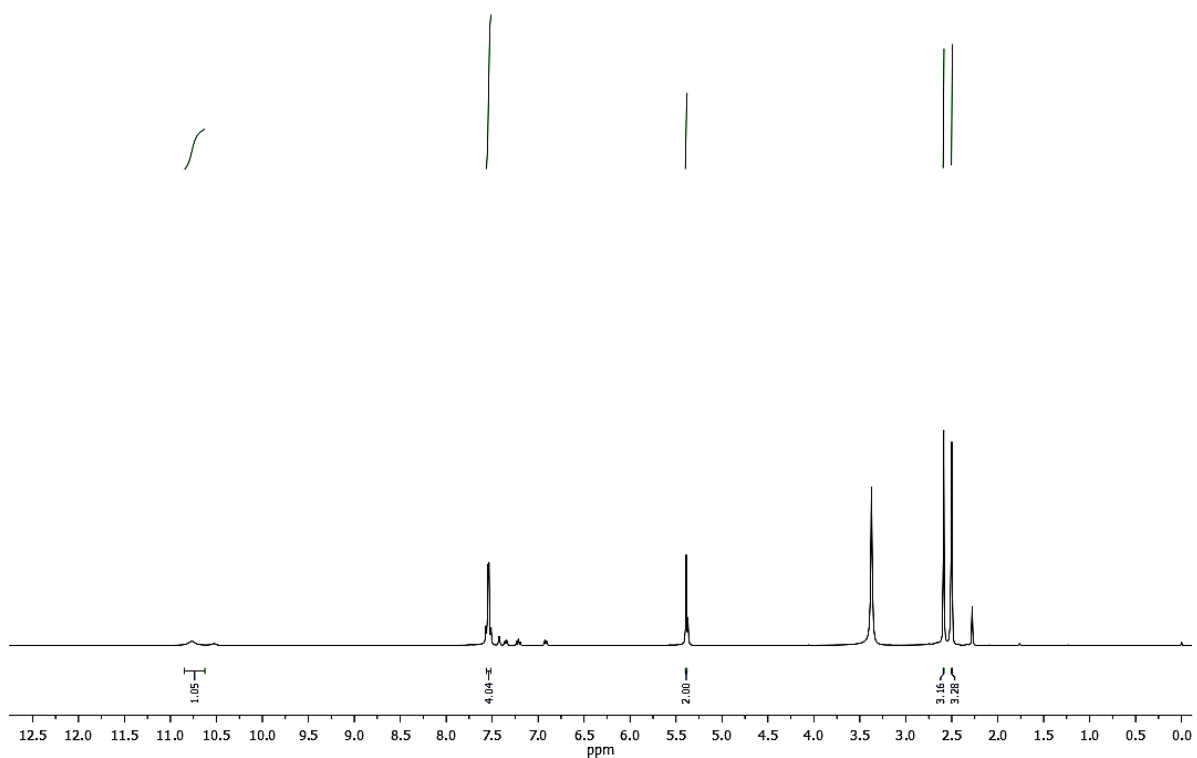


Figure S31: ^1H NMR of (**3k**)

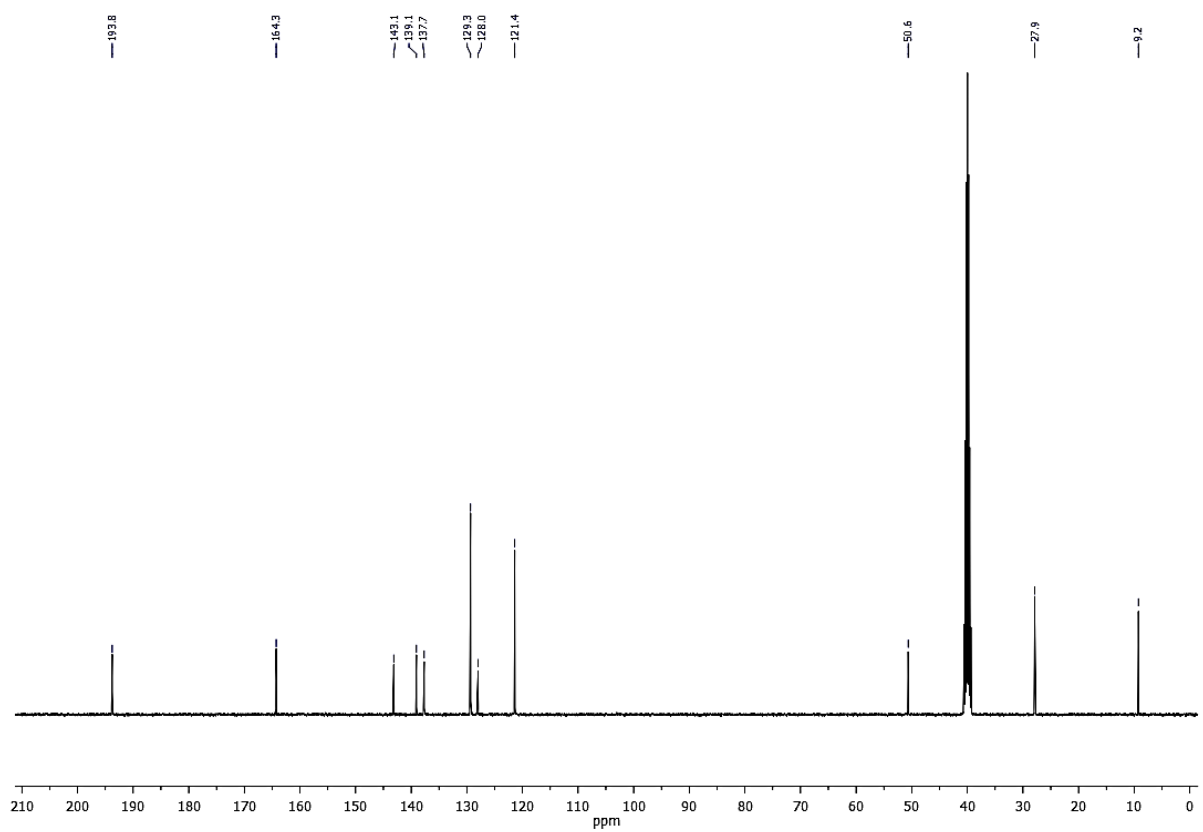


Figure S32: ^{13}C NMR of **(3k)**

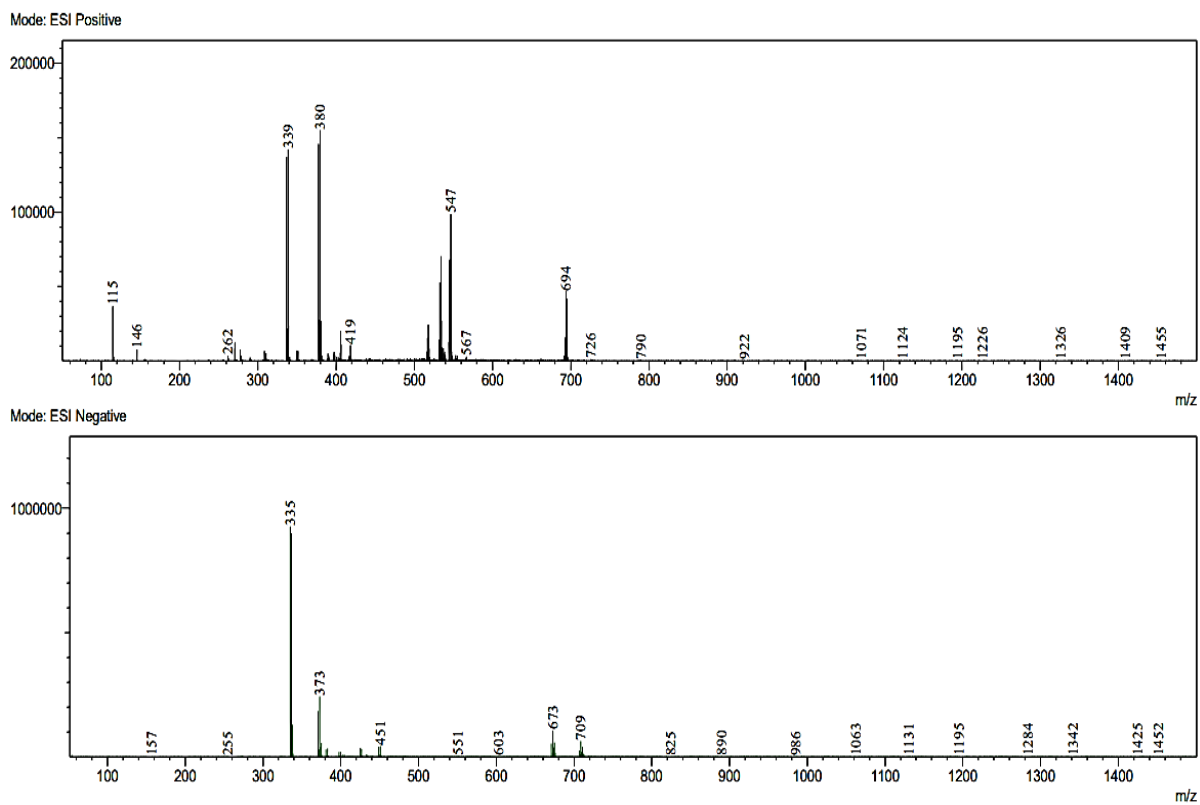


Figure S33: ESI-LCMS of (3k)

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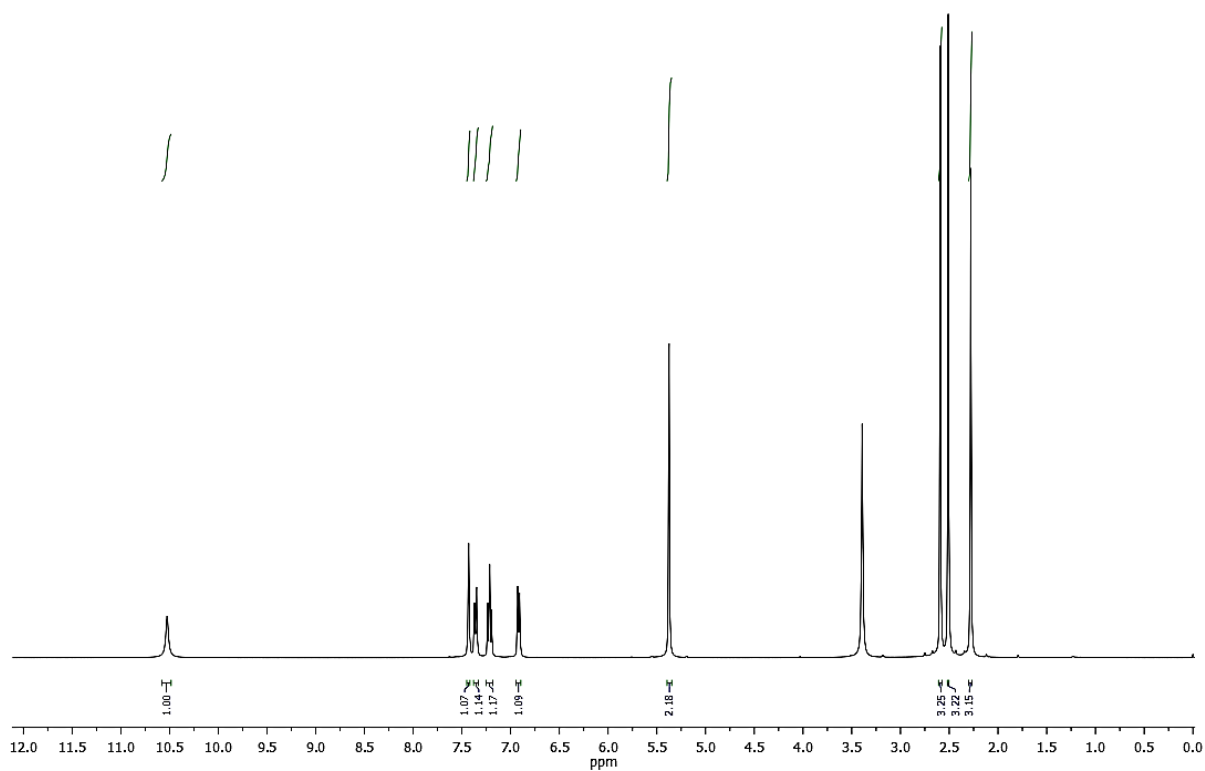


Figure S34: ^1H NMR of (31)

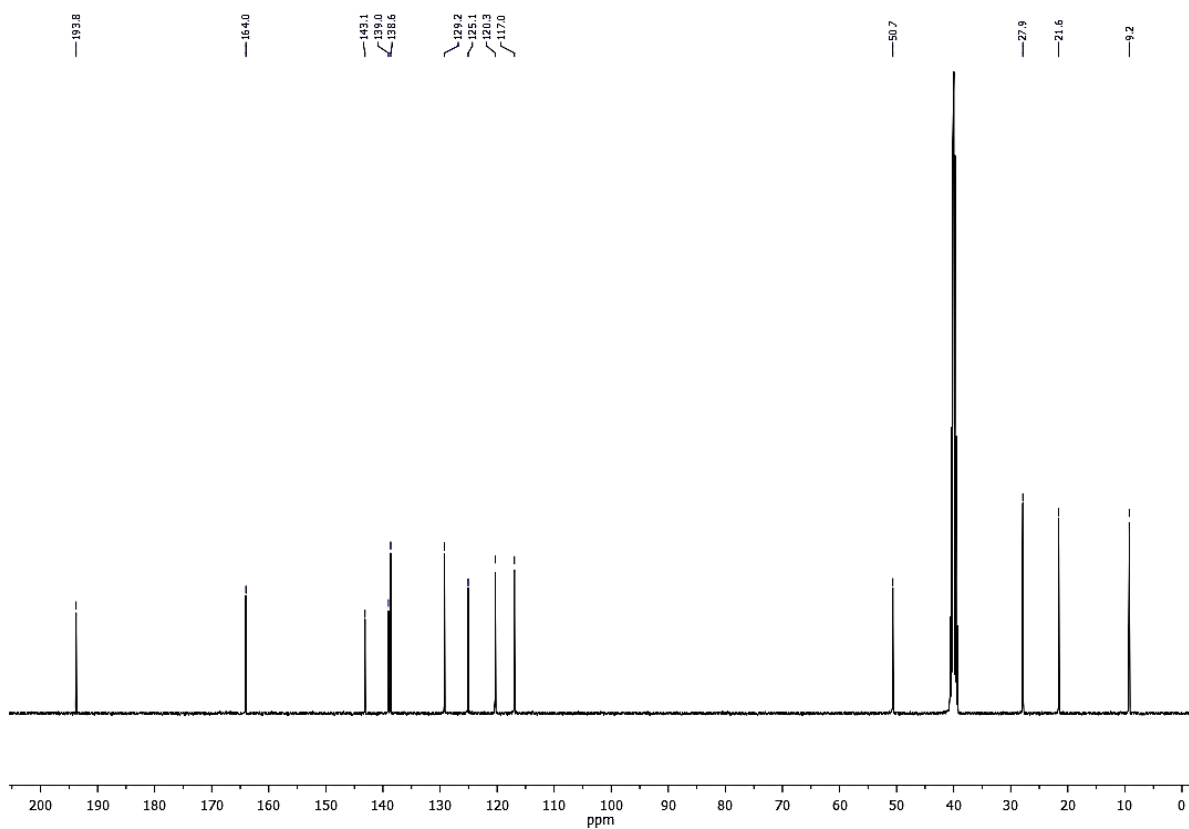


Figure S35: ^{13}C NMR of (31)

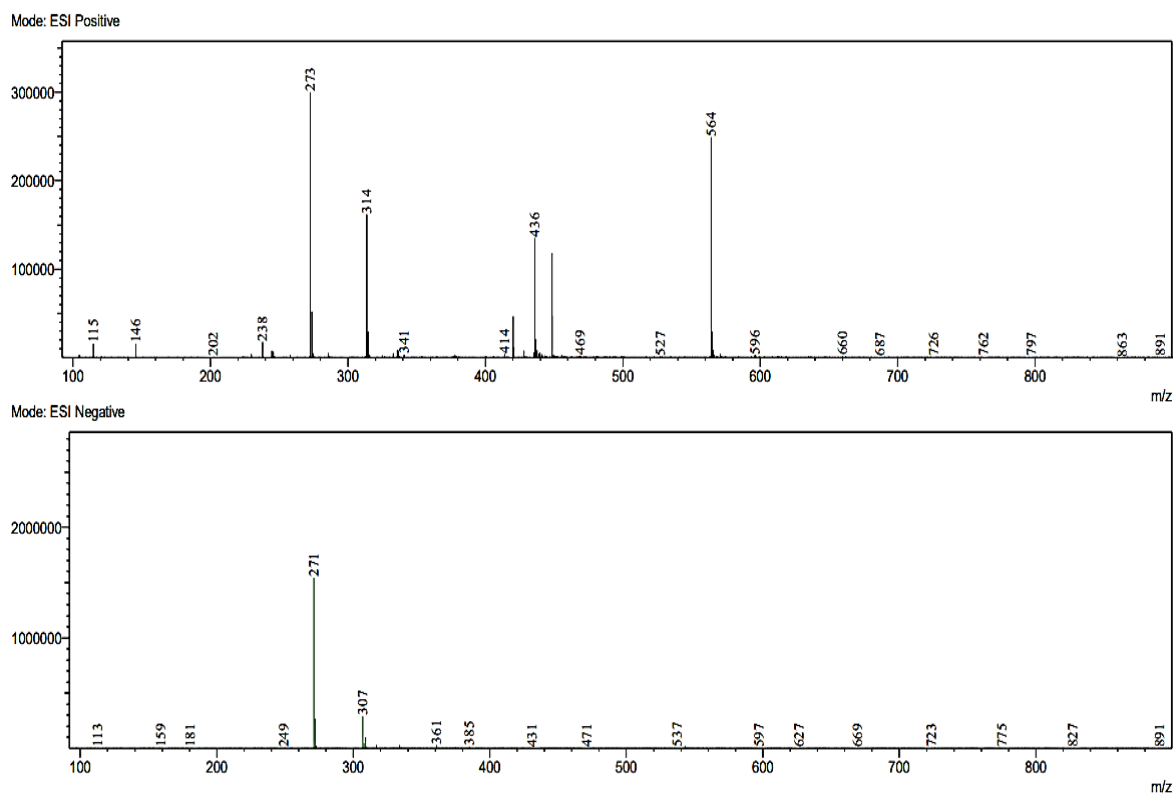


Figure S36: ESI-LCMS of (31)

VN-MS-13 1H
VN-MS-13 1H

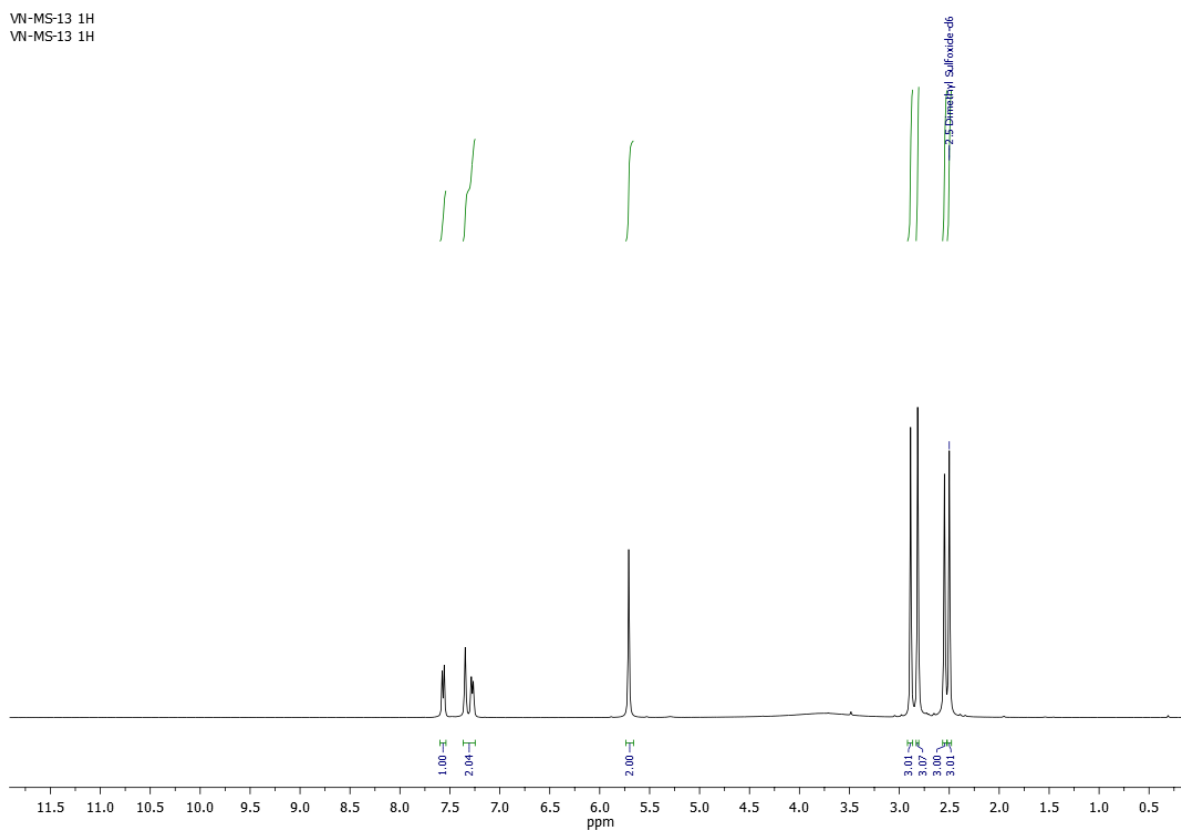


Figure S37: ^1H NMR of (**3m**)

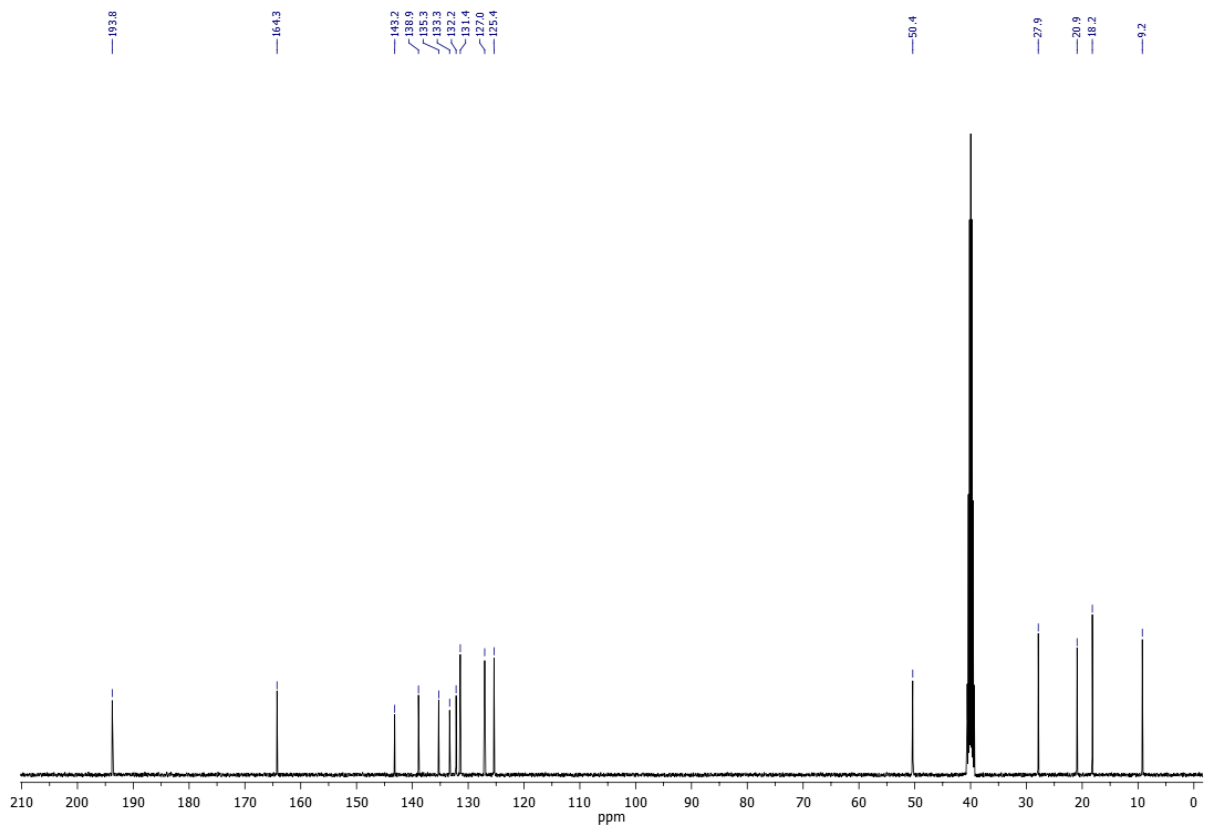


Figure S38: ^{13}C NMR of (3m)

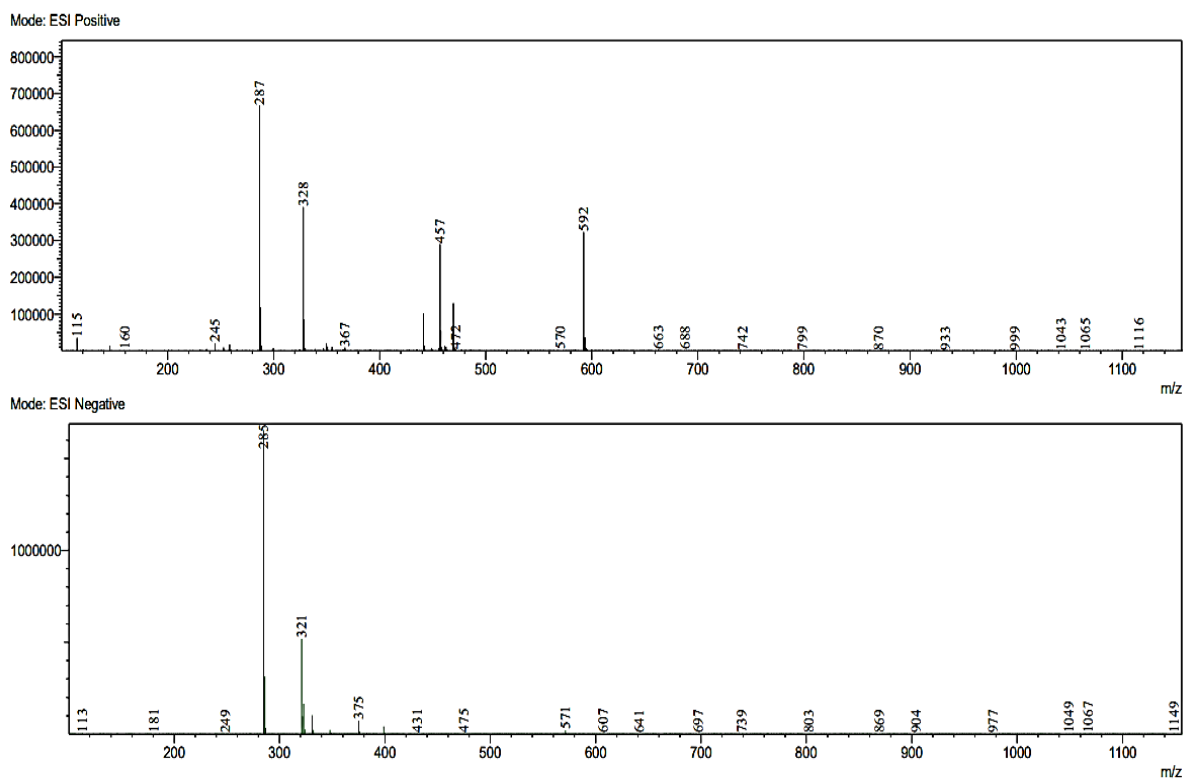


Figure S39: ESI-LCMS of (3m)

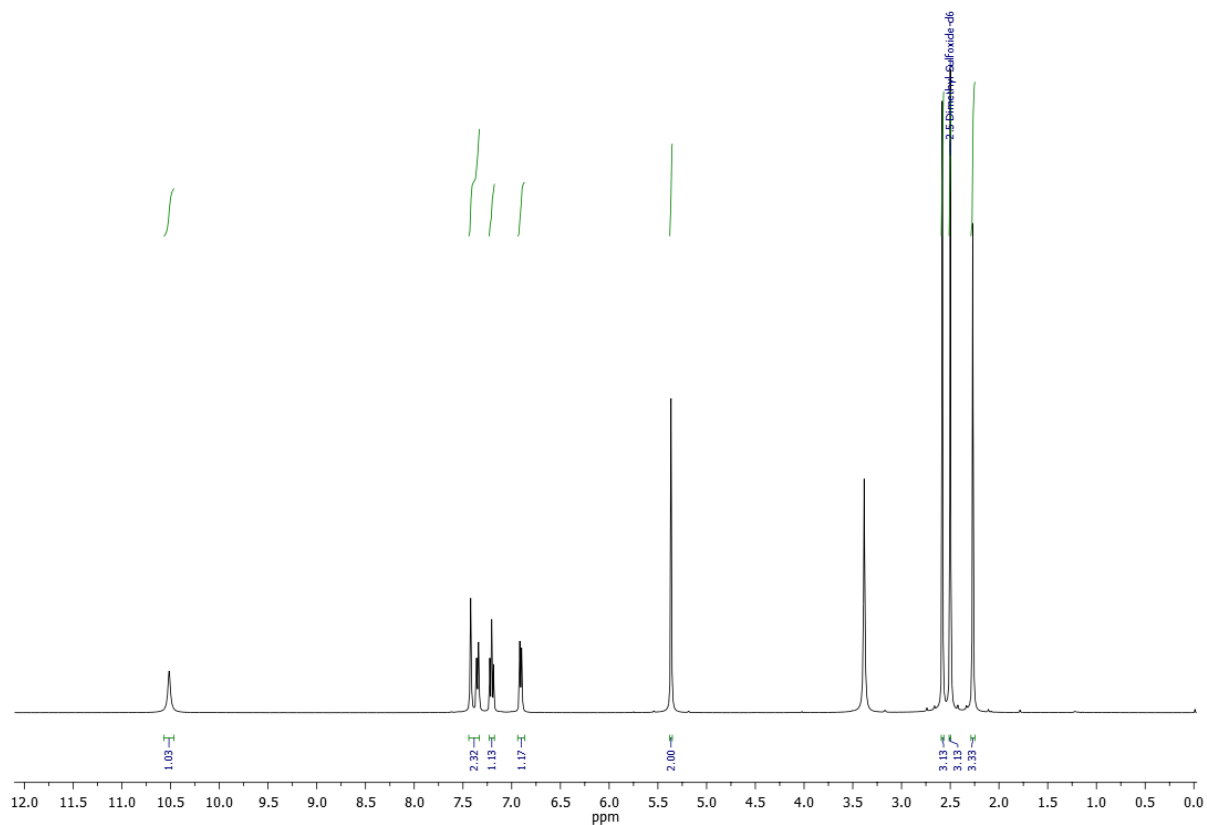


Figure S40: ^1H NMR of (3n)

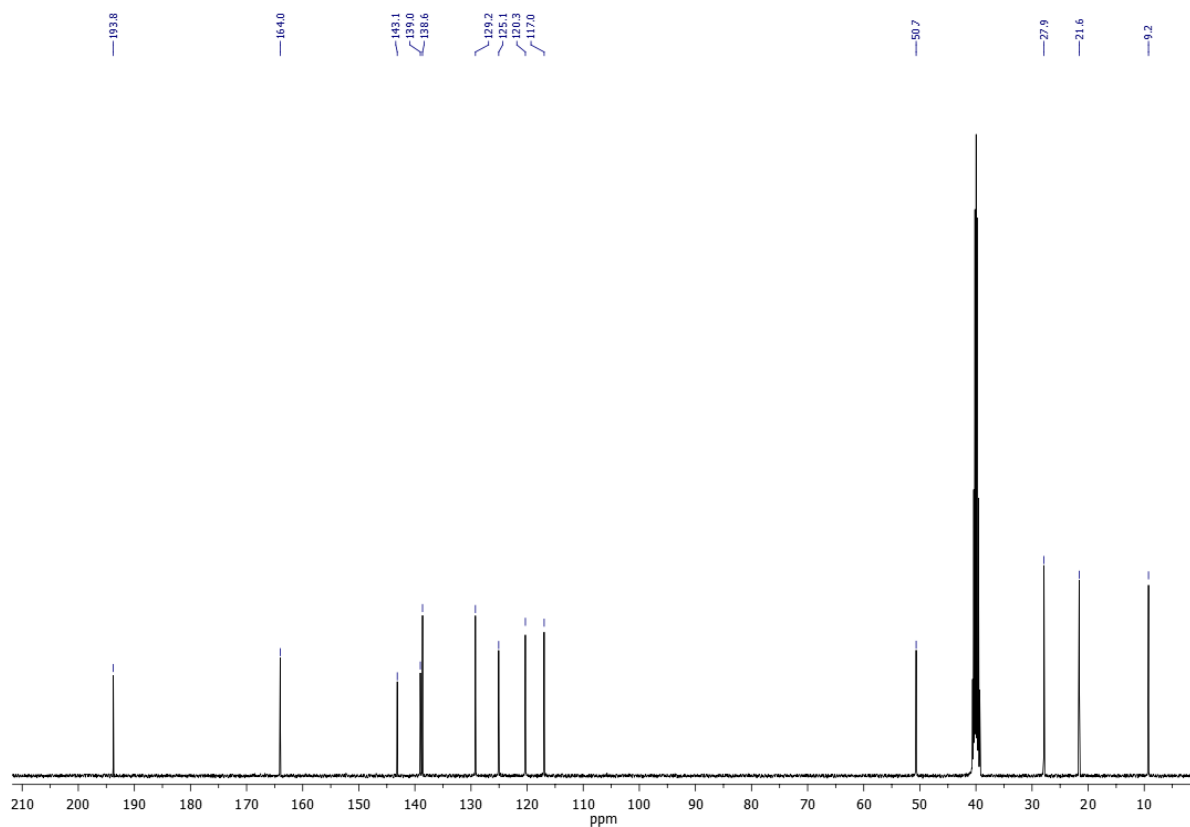


Figure S41: ^{13}C NMR of (**3n**)

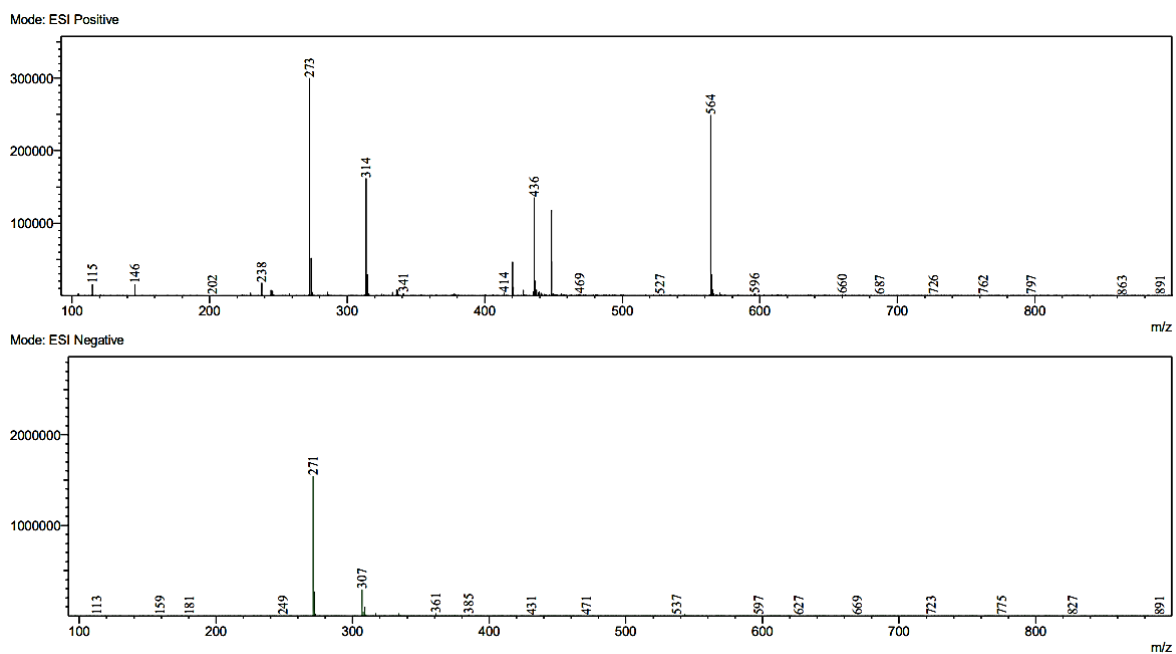


Figure S42: ESI-LCMS of (3n)

S1:DPPH and ABTS

Table S1: The radical scavenging activity of synthesized compounds using DPPH assay

Compounds	% Free RSA mean value \pm SD ($\mu\text{g/mL}$)				
	5 $\mu\text{g/mL}$	10 $\mu\text{g/mL}$	20 $\mu\text{g/mL}$	50 $\mu\text{g/mL}$	100 $\mu\text{g/mL}$
3a	13.80 \pm 0.24	56.80 \pm 2.2	73.10 \pm 1.4	76.10 \pm 1.4	79.60 \pm 1.7
3b	13.30 \pm 0.36	54.80 \pm 1.4	72.90 \pm 0.62	75.80 \pm 0.68	78.50 \pm 1.4
3c	18.30 \pm 0.54	56.02 \pm 0.64	73.50 \pm 1.34	76.30 \pm 1.42	79.30 \pm 2.4
3d	18.70 \pm 0.44	55.30 \pm 1.8	73.90 \pm 0.94	76.60 \pm 2.1	79.80 \pm 1.5
3e	21.10 \pm 1.54	57.10 \pm 0.78	73.90 \pm 0.74	78.80 \pm 2.4	80.20 \pm 2.4
3f	14.10 \pm 2.4	54.20 \pm 1.84	72.20 \pm 0.46	75.40 \pm 0.54	78.30 \pm 2.7
3g	15.30 \pm 1.4	54.80 \pm 0.6	71.90 \pm 1.7	75.10 \pm 0.4	77.90 \pm 1.8
3h	18.10 \pm 0.8	56.90 \pm 1.9	74.30 \pm 1.3	79.10 \pm 2.8	81.10 \pm 1.6
3i	18.1 \pm 1.4	56.30 \pm 2.8	73.50 \pm 2.4	76.20 \pm 2.0	79.40 \pm 2.0
3j	15.10 \pm 2.6	55.30 \pm 2.3	72.10 \pm 1.8	75.90 \pm 0.8	78.90 \pm 0.6
3k	16.80 \pm 2.5	58.90 \pm 0.8	72.10 \pm 1.6	75.90 \pm 2.8	78.10 \pm 0.8
3l	12.90 \pm 0.6	53.90 \pm 1.8	71.80 \pm 2.2	75.30 \pm 1.5	77.70 \pm 1.9
3m	16.60 \pm 0.4	58.10 \pm 1.4	72.50 \pm 2.8	76.20 \pm 1.7	78.70 \pm 2.8
3n	21.40 \pm 0.8	57.90 \pm 1.6	73.90 \pm 0.8	78.10 \pm 2.6	80.70 \pm 2.8
Ascorbic acid	2.10 \pm 1.26	23.80 \pm 0.5	51.10 \pm 1.8	85.20 \pm 0.9	87.10 \pm 3.2

Table S2: The radical scavenging activity of synthesized compounds using ABTS assay

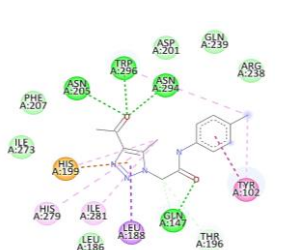
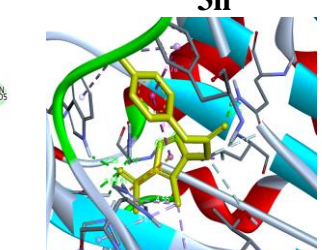
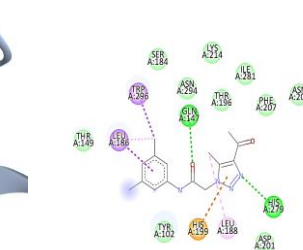
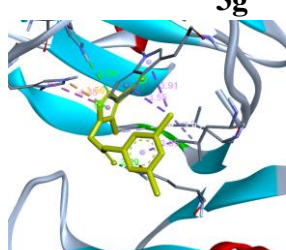
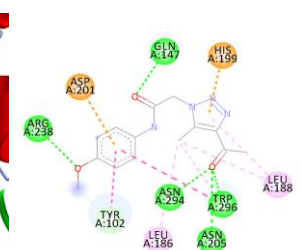
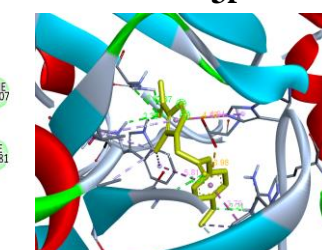
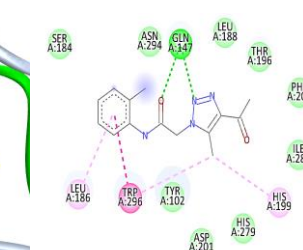
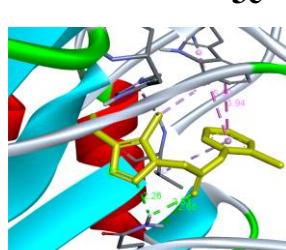
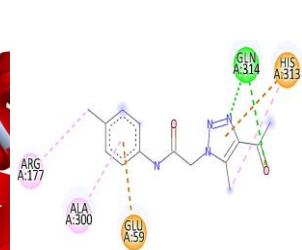
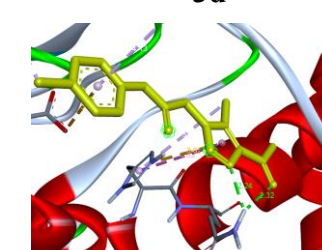
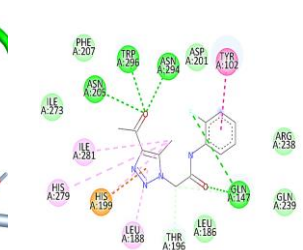
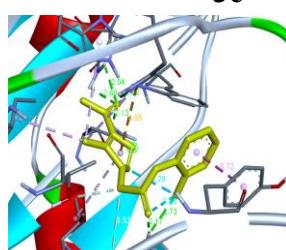
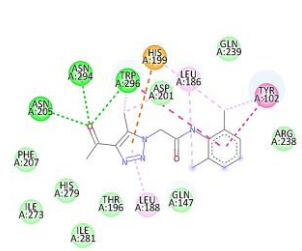
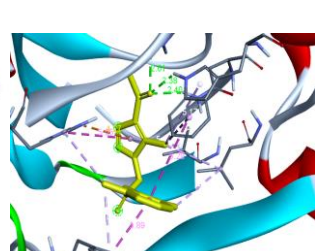
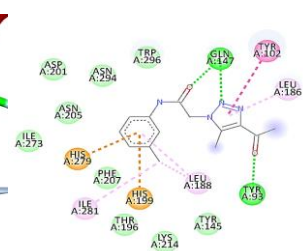
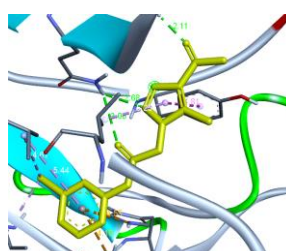
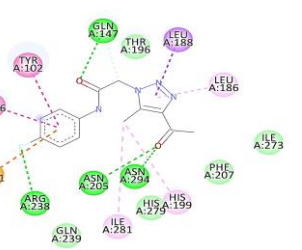
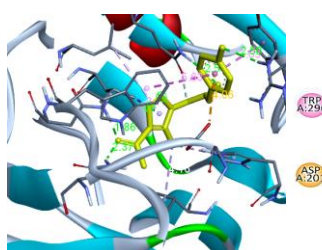
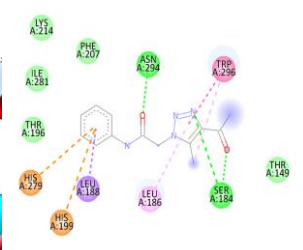
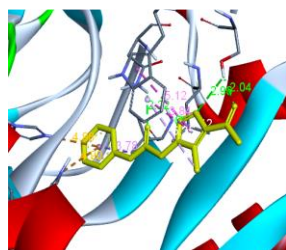
Compounds	% Free RSA mean value \pm SD ($\mu\text{g/mL}$)				
	5 $\mu\text{g/ml}$	10 $\mu\text{g/mL}$	5 $\mu\text{g/mL}$	50 $\mu\text{g/mL}$	5 $\mu\text{g/ml}$
3a	25.30 \pm 2.14	3a	25.30 \pm 2.14	3a	25.30 \pm 2.14
3b	28.40 \pm 0.6	3b	28.40 \pm 0.6	3b	28.40 \pm 0.6
3c	26.60 \pm 1.7	3c	26.60 \pm 1.7	3c	26.60 \pm 1.7
3d	21.60 \pm 1.8	3d	21.60 \pm 1.8	3d	21.60 \pm 1.8
3e	2.50 \pm 1.5	3e	2.50 \pm 1.5	3e	2.50 \pm 1.5
3f	7.70 \pm 1.6	3f	7.70 \pm 1.6	3f	7.70 \pm 1.6
3g	9.00 \pm 1.8	3g	9.00 \pm 1.8	3g	9.00 \pm 1.8
3h	10.90 \pm 1.5	3h	10.90 \pm 1.5	3h	10.90 \pm 1.5
3i	37.30 \pm 2.8	3i	37.30 \pm 2.8	3i	37.30 \pm 2.8
3j	25.10 \pm 1.5	3j	25.10 \pm 1.5	3j	25.10 \pm 1.5
3k	14.10 \pm 2.8	3k	14.10 \pm 2.8	3k	14.10 \pm 2.8
3l	3.10 \pm 0.4	3l	3.10 \pm 0.4	3l	3.10 \pm 0.4
3m	5.80 \pm 0.4	3m	5.80 \pm 0.4	3m	5.80 \pm 0.4
3n	4.40 \pm 0.9	3n	4.40 \pm 0.9	3n	4.40 \pm 0.9
Gallic acid	8.40 \pm 0.6	Gallic acid	8.40 \pm 0.6	Gallic acid	8.40 \pm 0.6

Table S3: Drug likeness properties of synthesized compounds with reference drug

Compounds	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
3a	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3b	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3c	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3d	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3e	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3f	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3g	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3h	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3i	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3j	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3k	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3l	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3m	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
3n	Yes; 0 violation	Yes	Yes	Yes	Yes	0.55
Cisplatin	Yes; 0 violation	No	Yes	Yes	No	0.56

S2: Molecular Docking

HIF-1 alpha



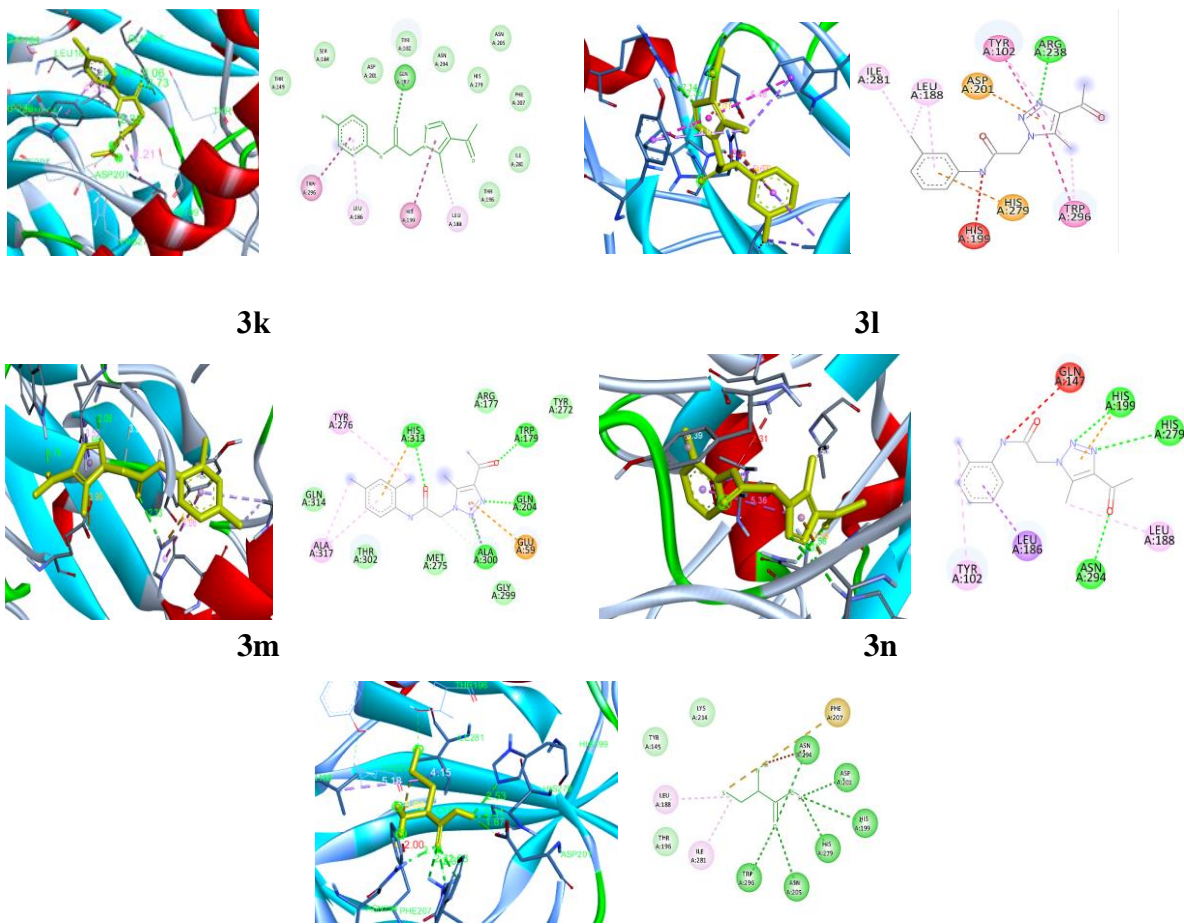
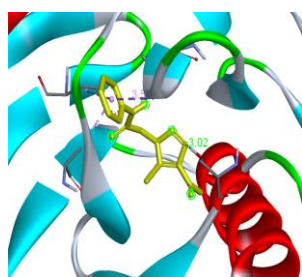
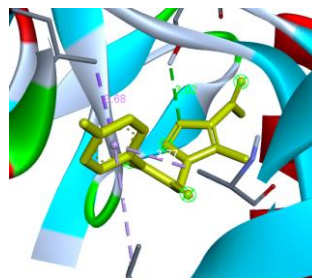
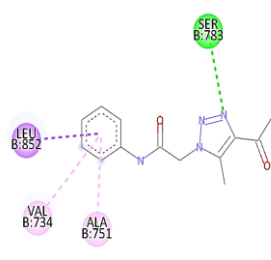


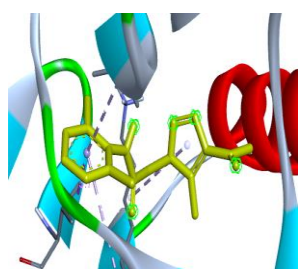
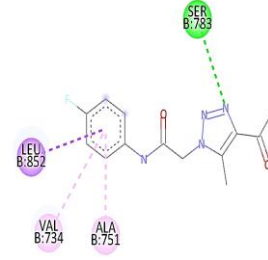
Figure S43: 2D and 3D poses of synthesized compounds and reference drug with their binding complex of protein HIF-1 α .



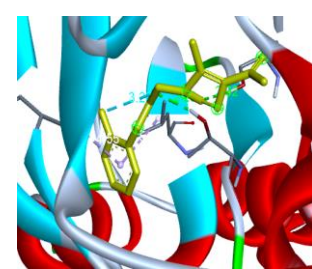
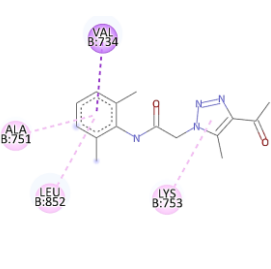
3a



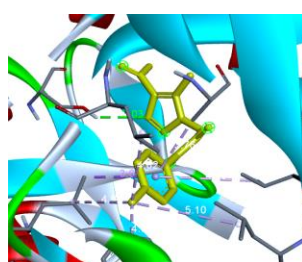
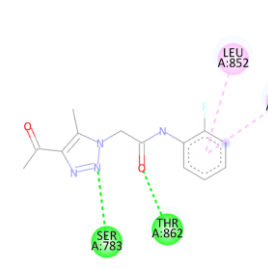
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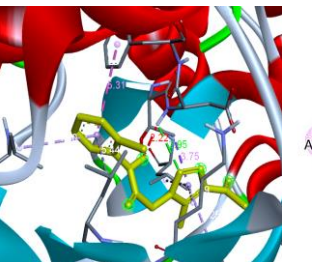
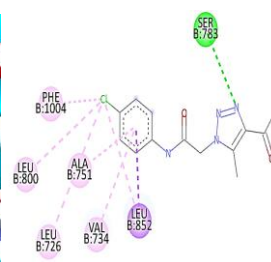
3c



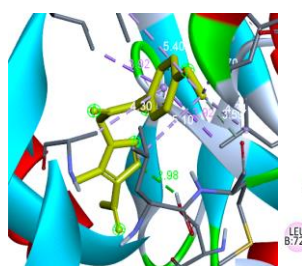
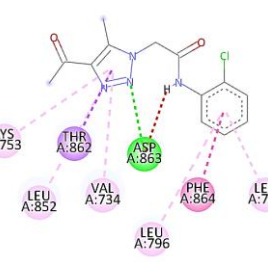
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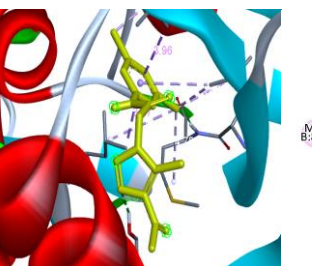
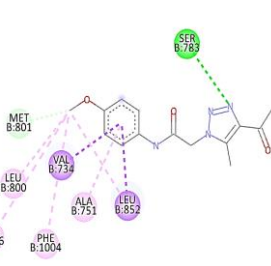
3e



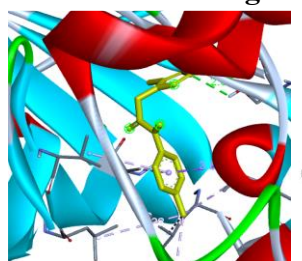
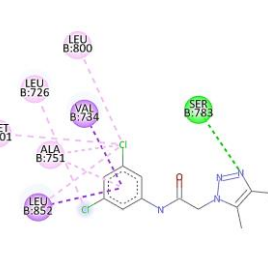
3f



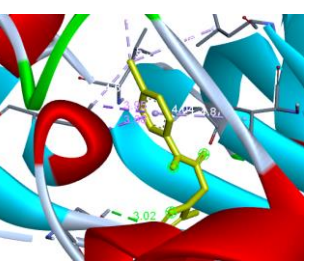
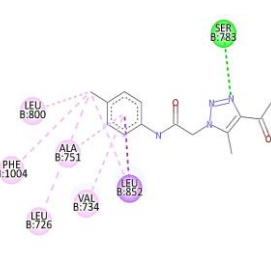
3g



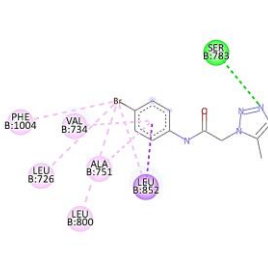
3h



3i



3j



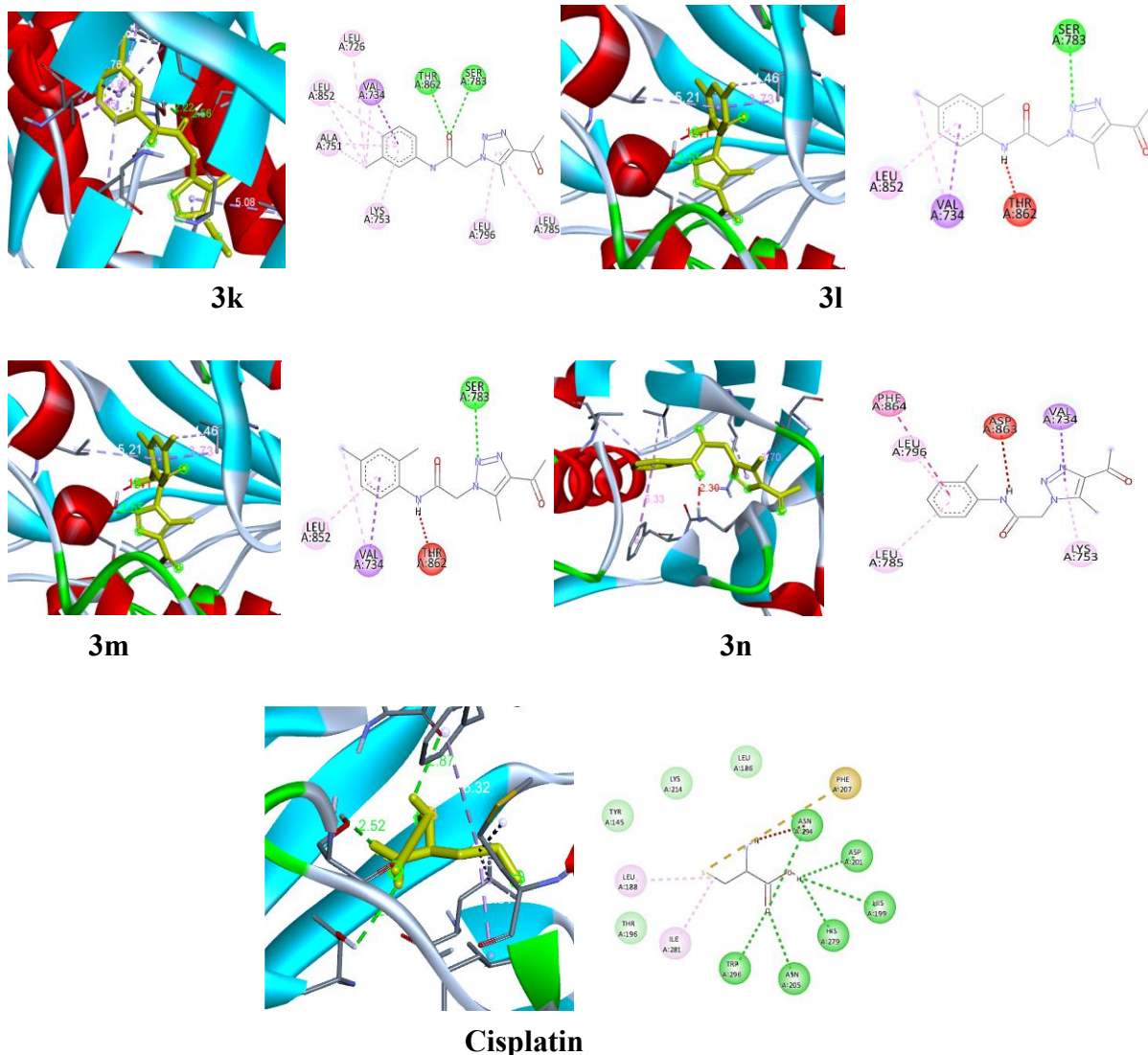


Figure S44: 2D and 3D poses of synthesized compounds and reference drug with their binding complex of protein HER2.