

CuO nanostructures of variable shapes as an efficient catalyst for [3+2] cycloaddition of azides with terminal alkyne

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1. Figure S1-6

Figure S-1. IR spectra of phenylacetylene

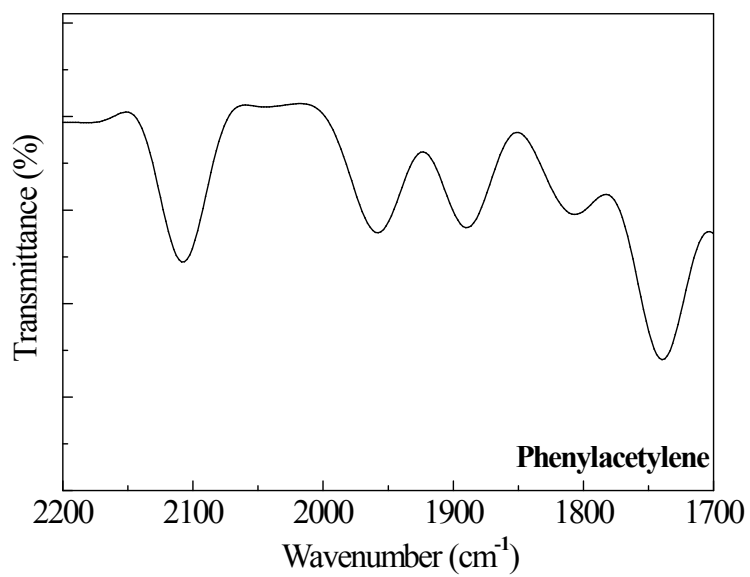
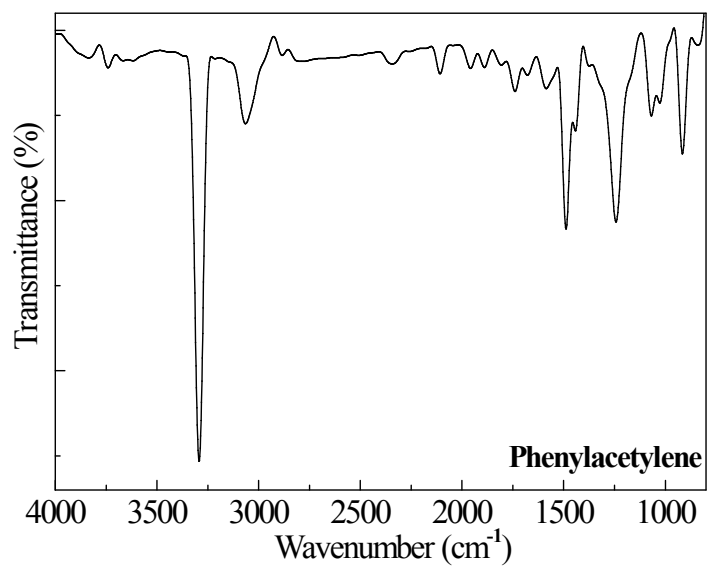


Figure S-2. IR spectra of the mixture of catalyst (CuO-NW), phenylacetylene with sodium L-ascorbate

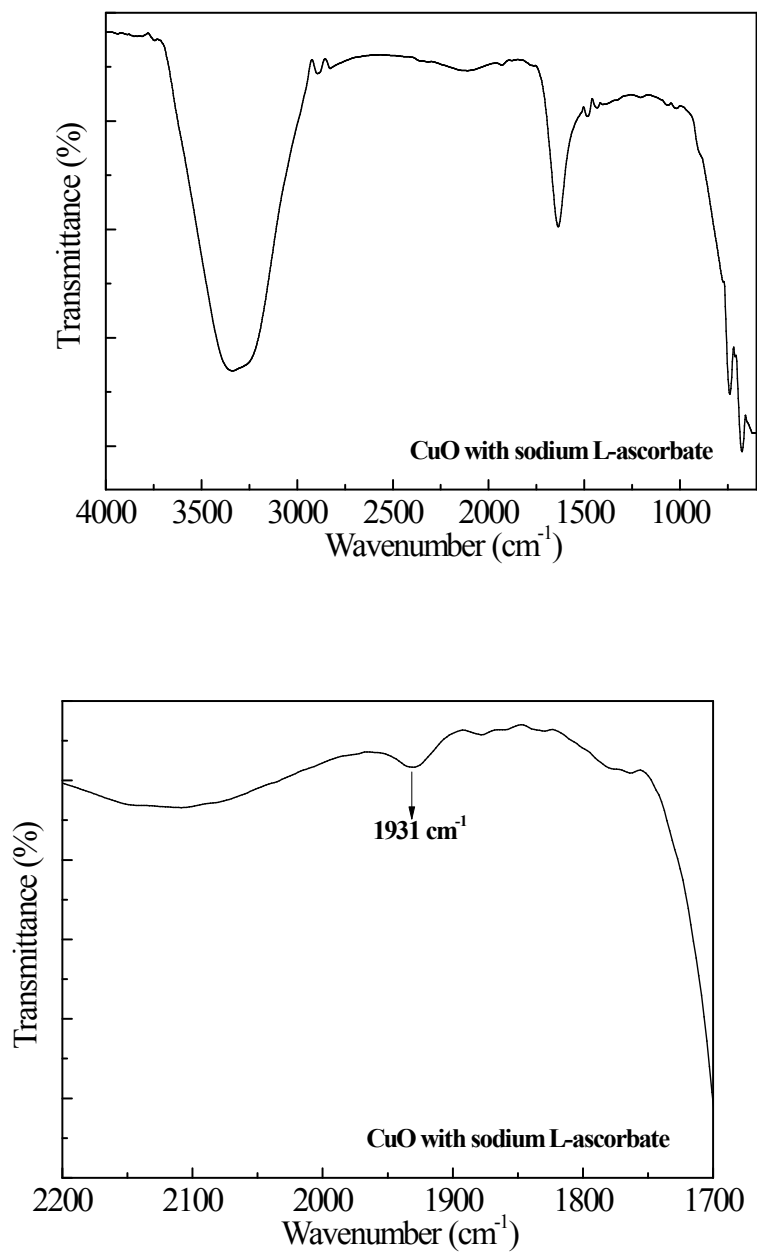


Figure S-3. IR spectra of the mixture of CuO-NW, phenylacetylene without sodium L-ascorbate

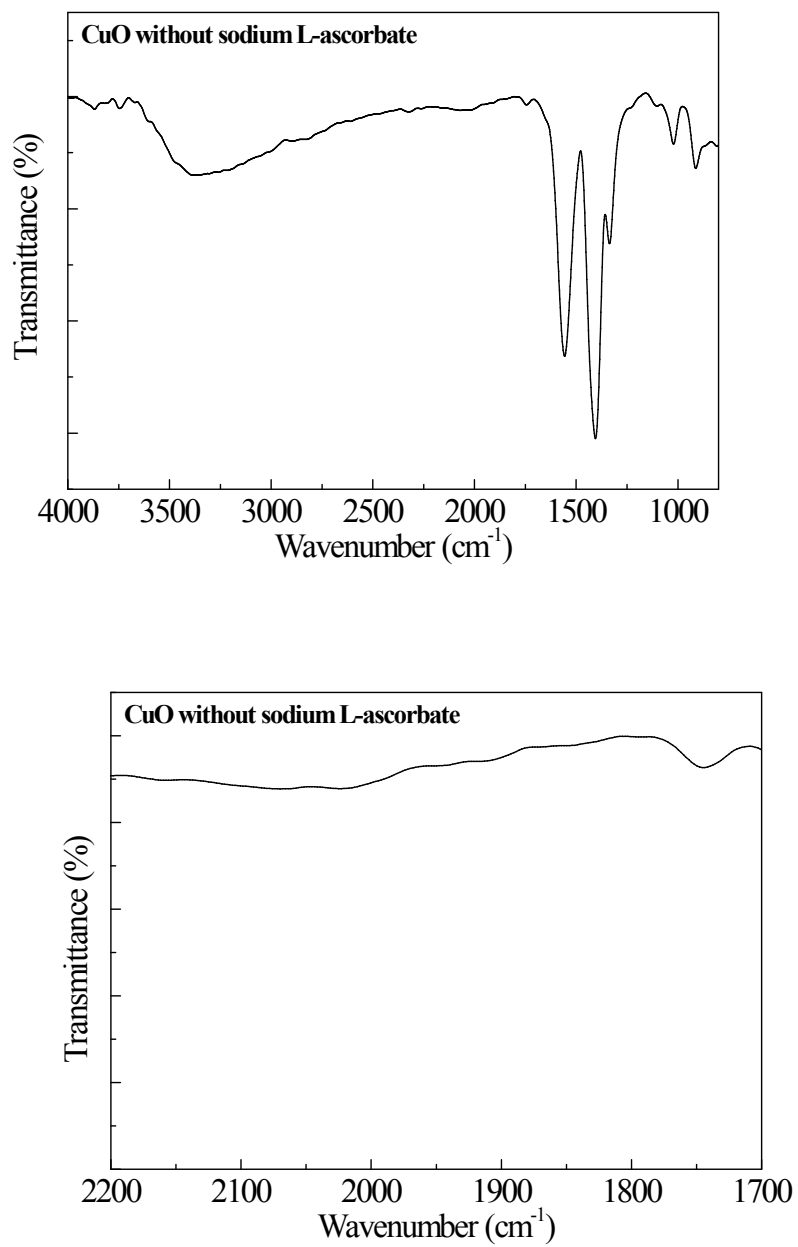


Fig. S-4. The XPS spectra of Cu(I)-acetylide complex (greenish yellow colour solid) and the *inset* shows the Cu 2p core level binding energy spectrum

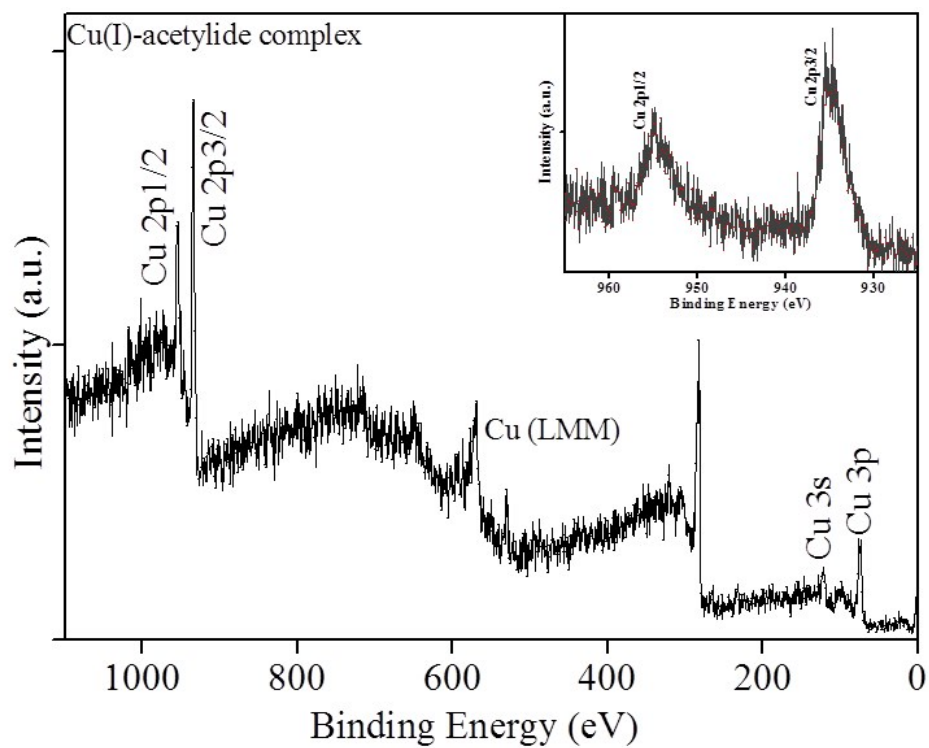


Fig. S-5. The XPS spectra of CuO-NW and Cu(I)-acetylide complex, showing the Cu 2p core level binding energy spectrum

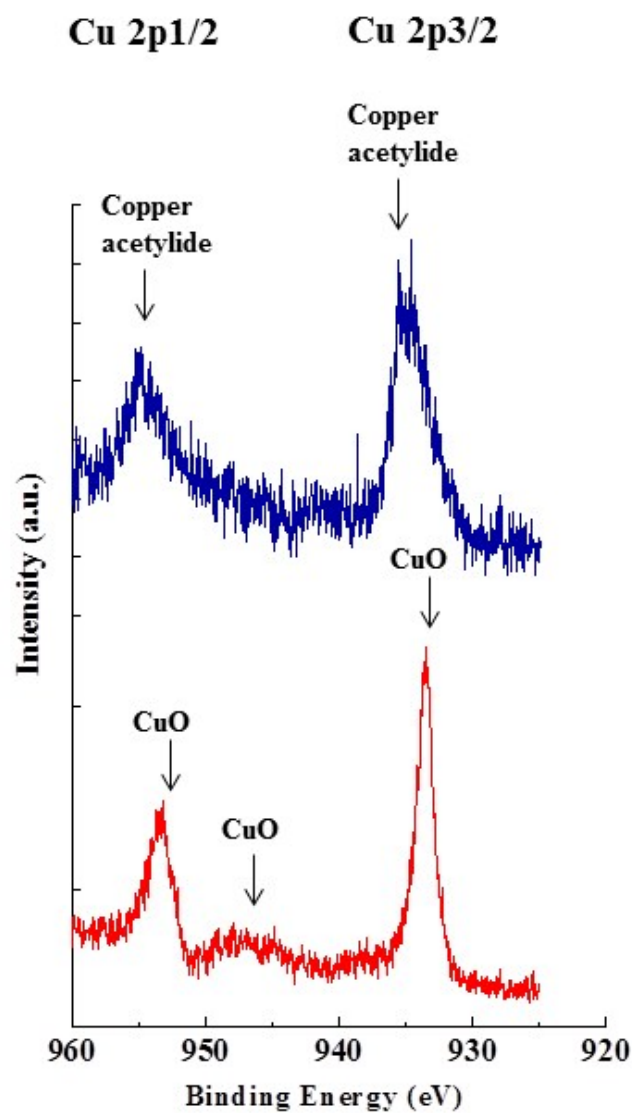
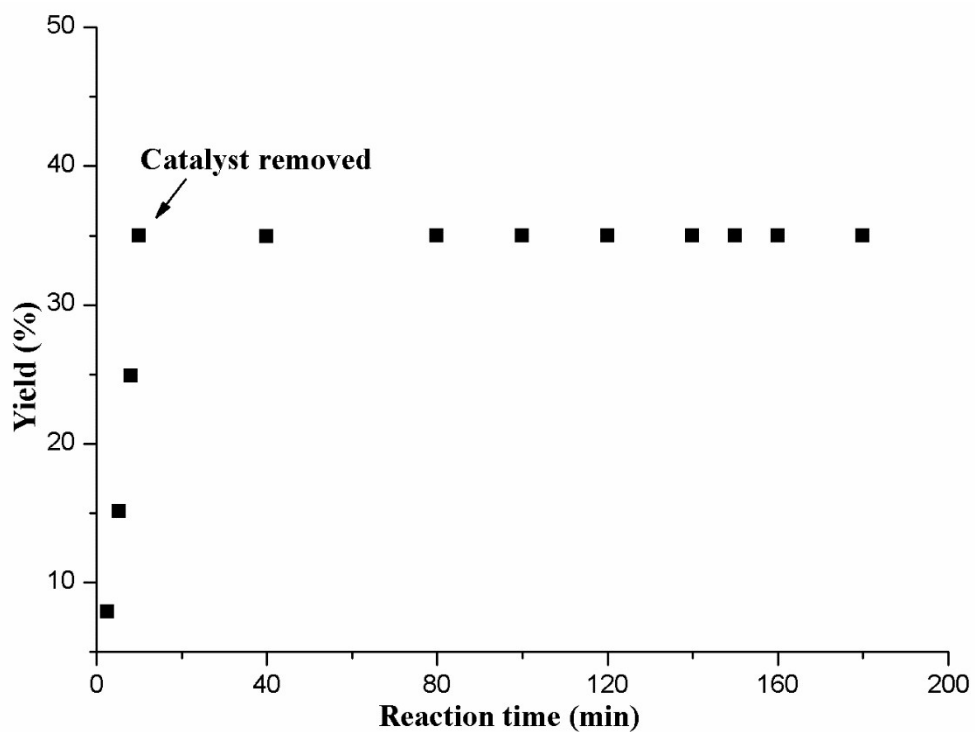
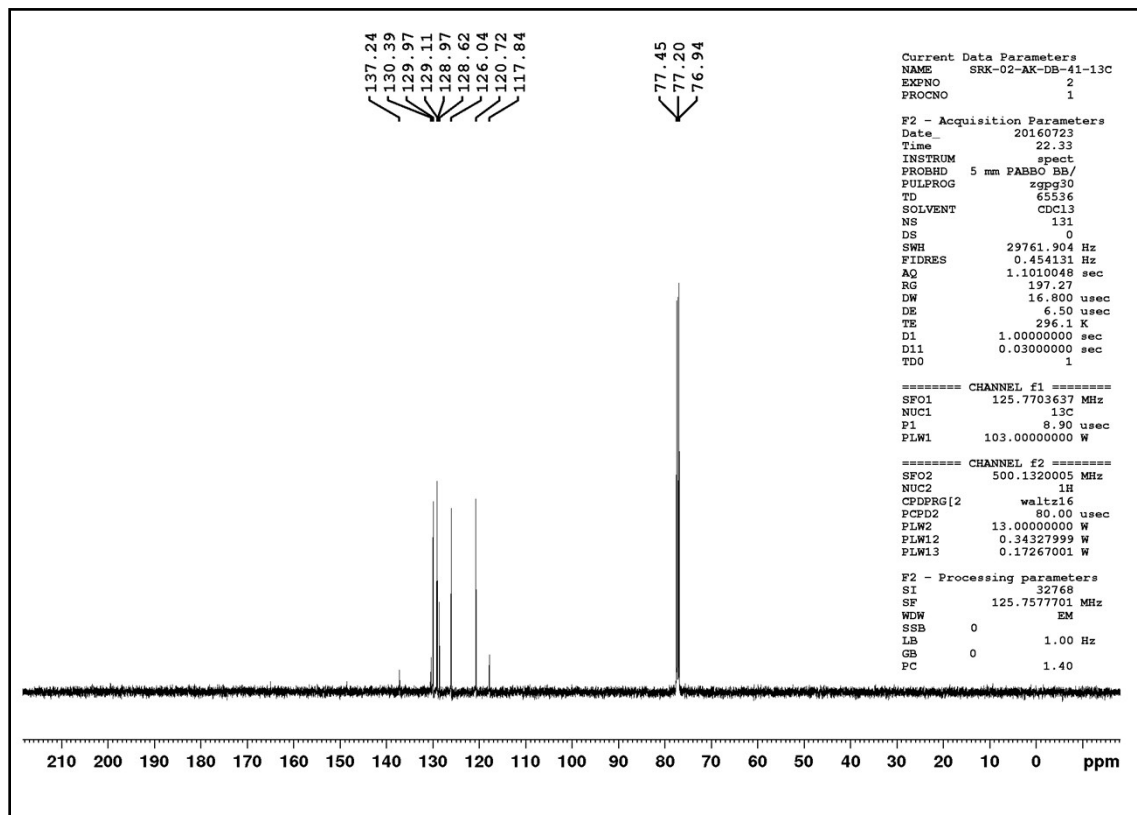
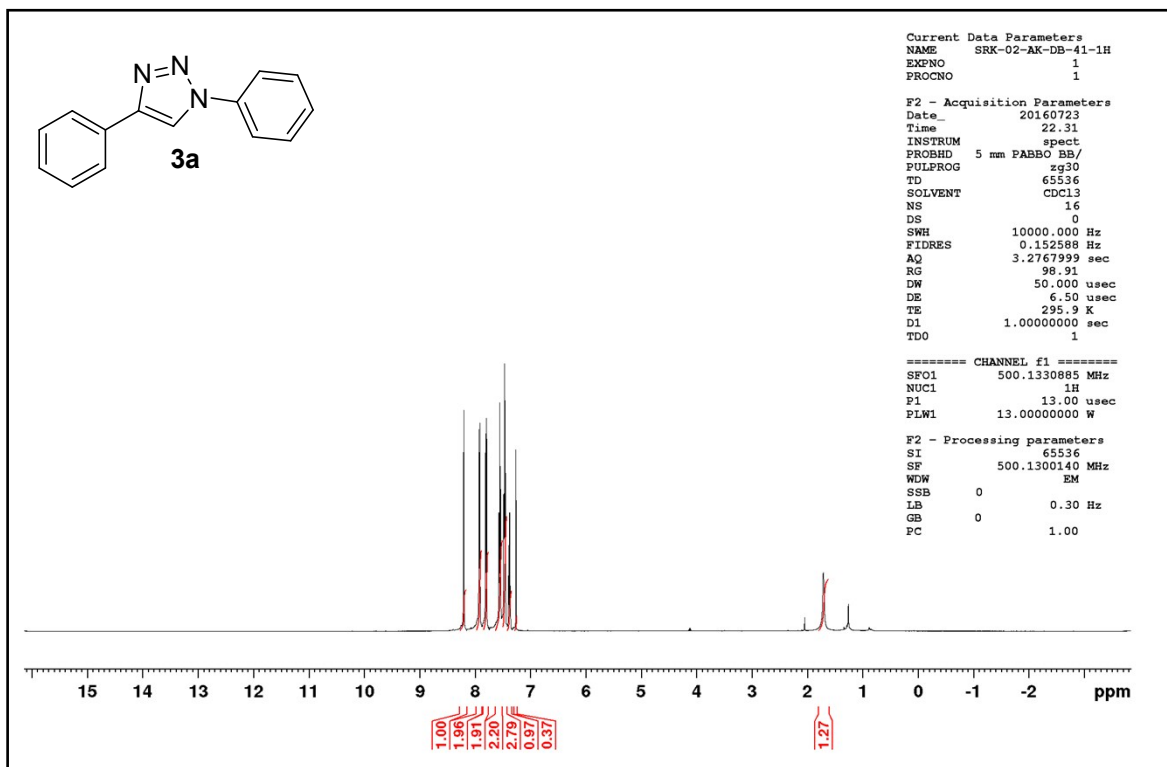


Fig. S-6. Leaching test of CuO-NW for the reaction of phenylacetylene and phenyl azide in the presence of sodium ascorbate in H₂O/*t*-BuOH (3:1) at room temperature



2. ^1H NMR, ^{13}C NMR and HRMS spectra of compounds 3a, 3b and 3c

^1H NMR (500 MHz, CDCl_3), ^{13}C NMR (125 MHz, CDCl_3) and HRMS of compound 3a



Analysis Info

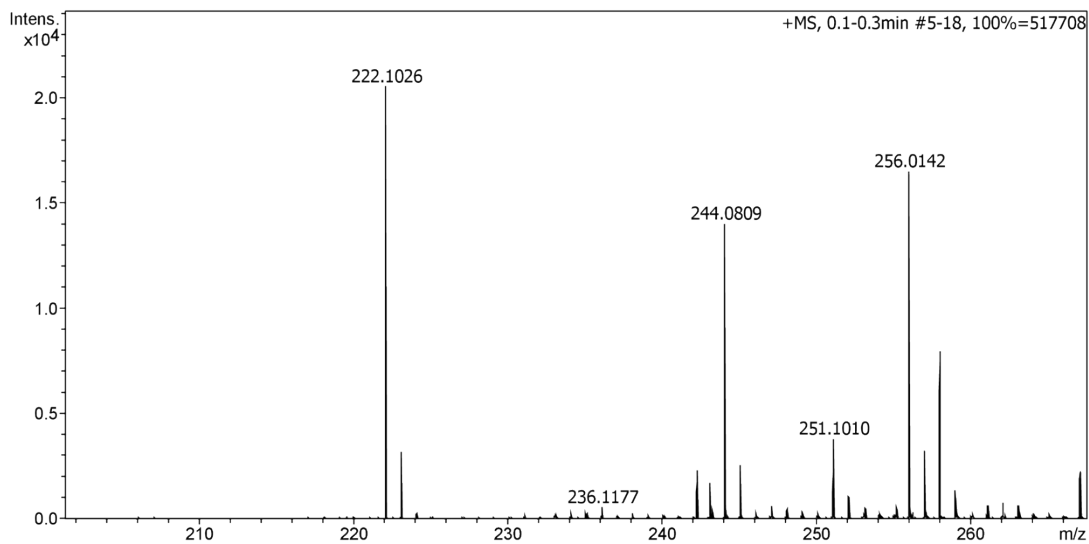
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Operator srkin
Instrument maXis impact 282001.00081

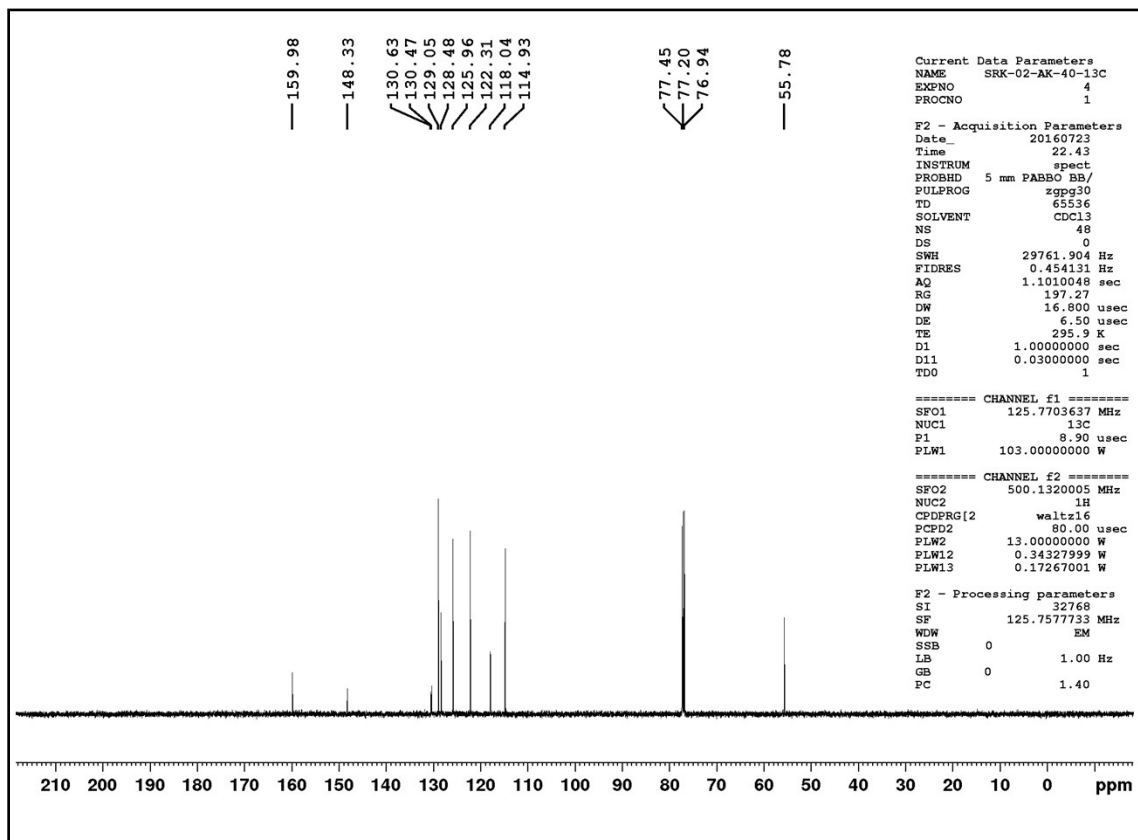
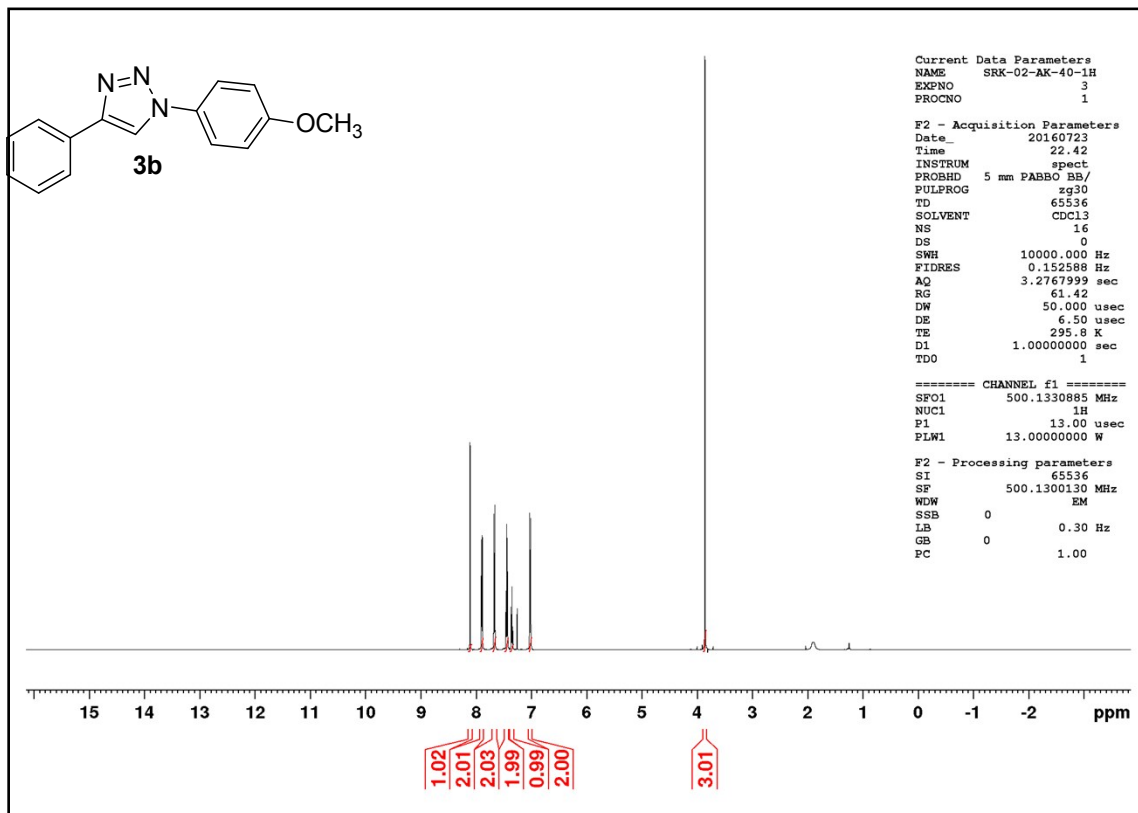
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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
222.1026	1	C14H12N3	222.1026	0.1	9.1	1	100.00	10.5	even	ok

^1H NMR (500 MHz, CDCl_3), ^{13}C NMR (125 MHz, CDCl_3) and HRMS of compound **3b**



Analysis Info

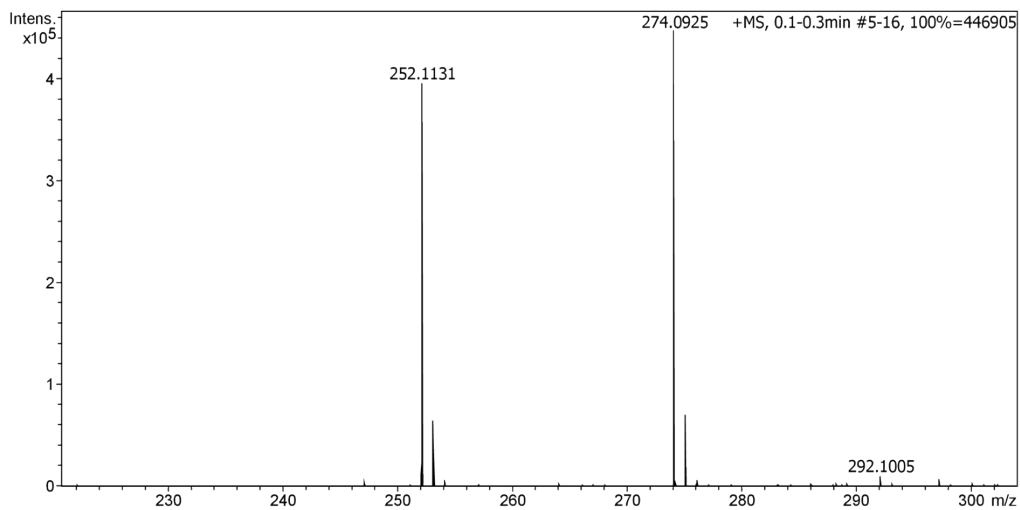
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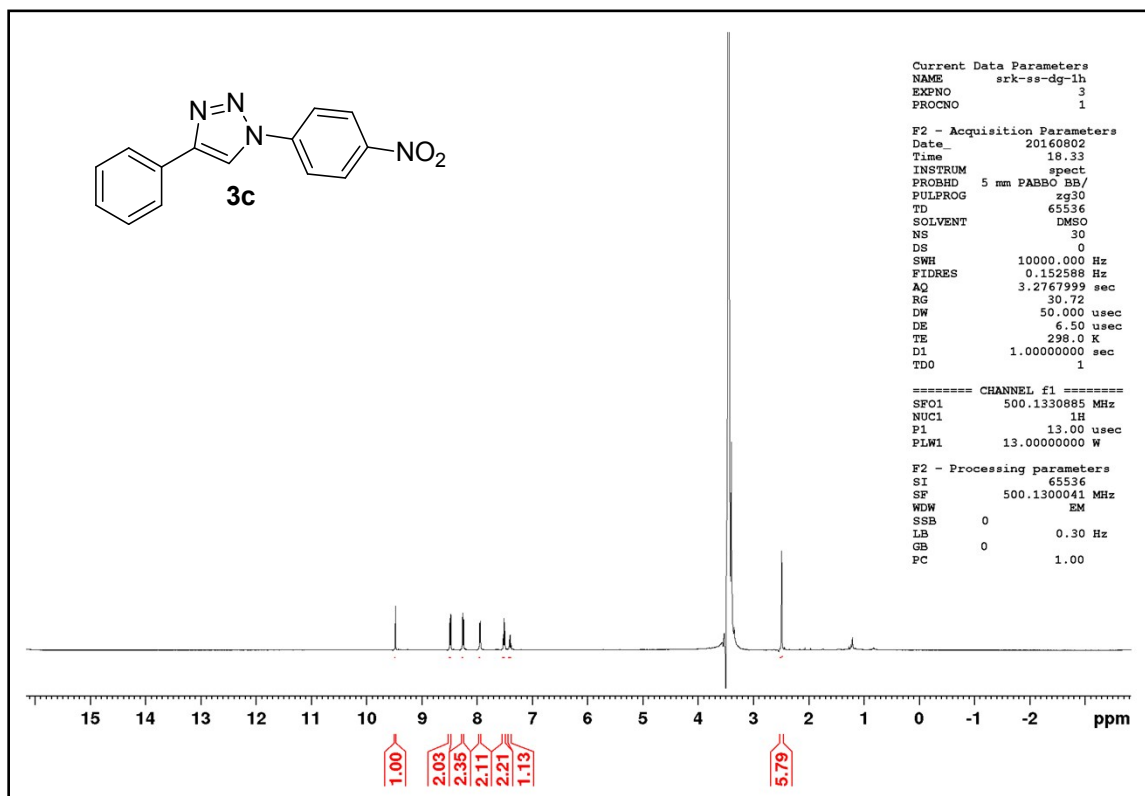
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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
252.1131	1	C15H14N3O	252.1131	-0.2	6.7	1	100.00	10.5	even	ok

^1H NMR (500 MHz, DMSO- d_6), ^{13}C NMR (125 MHz, DMSO- d_6) and HRMS of compound **3c**



Analysis Info

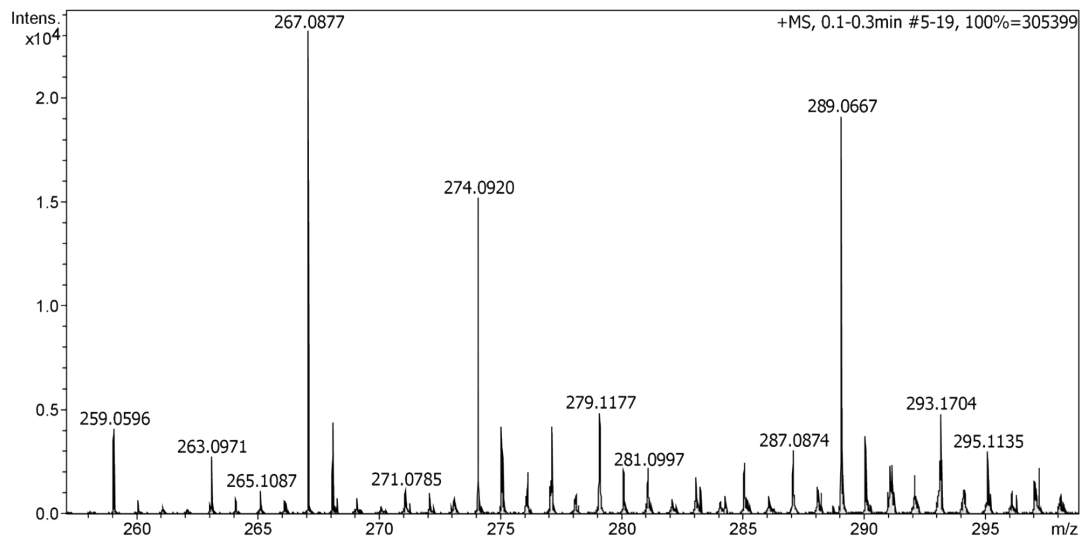
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Operator srkin
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Scan End	700 m/z	Set Collision Cell RF	900.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
267.0877	1	C14H11N4O2	267.0877	0.1	14.9	1	100.00	11.5	even	ok