Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Synthesis and evaluation of novel quinuclidinone derivatives as potential anti-proliferative agents

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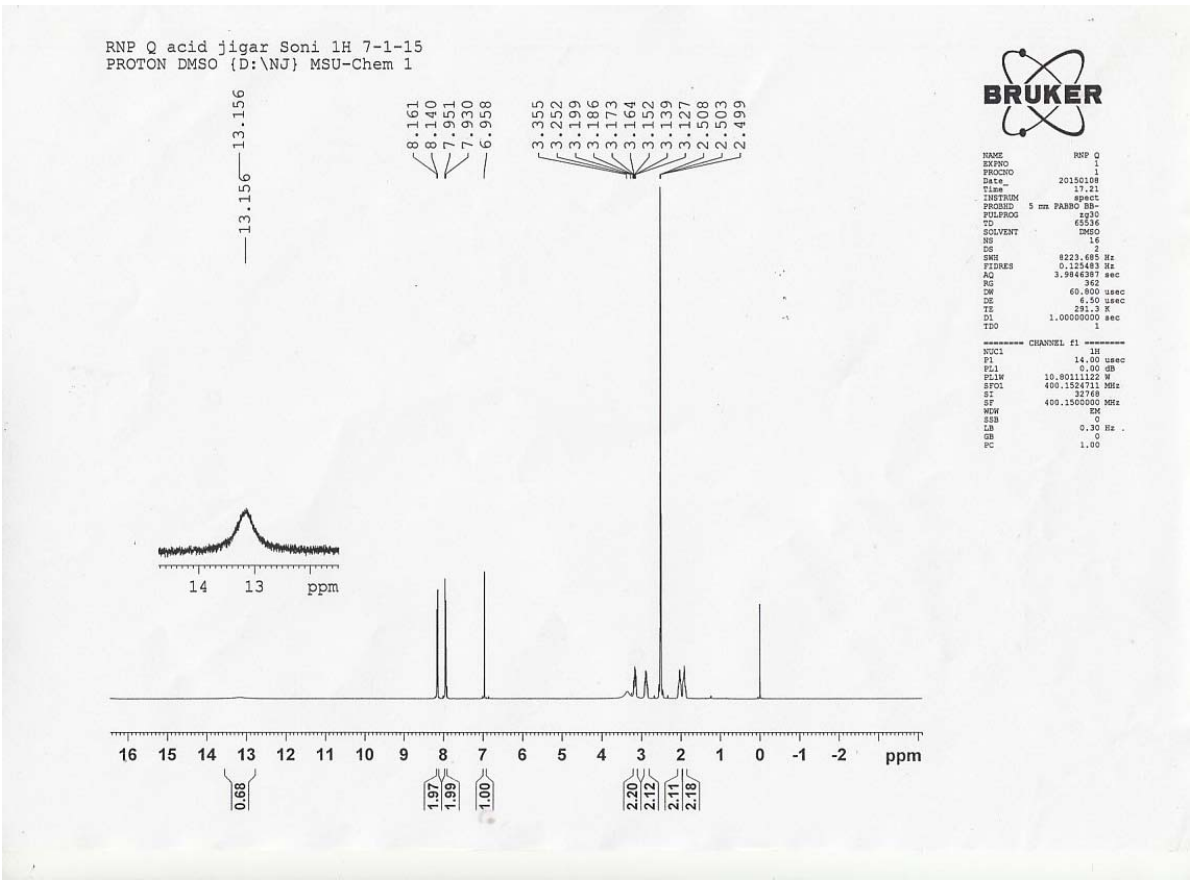
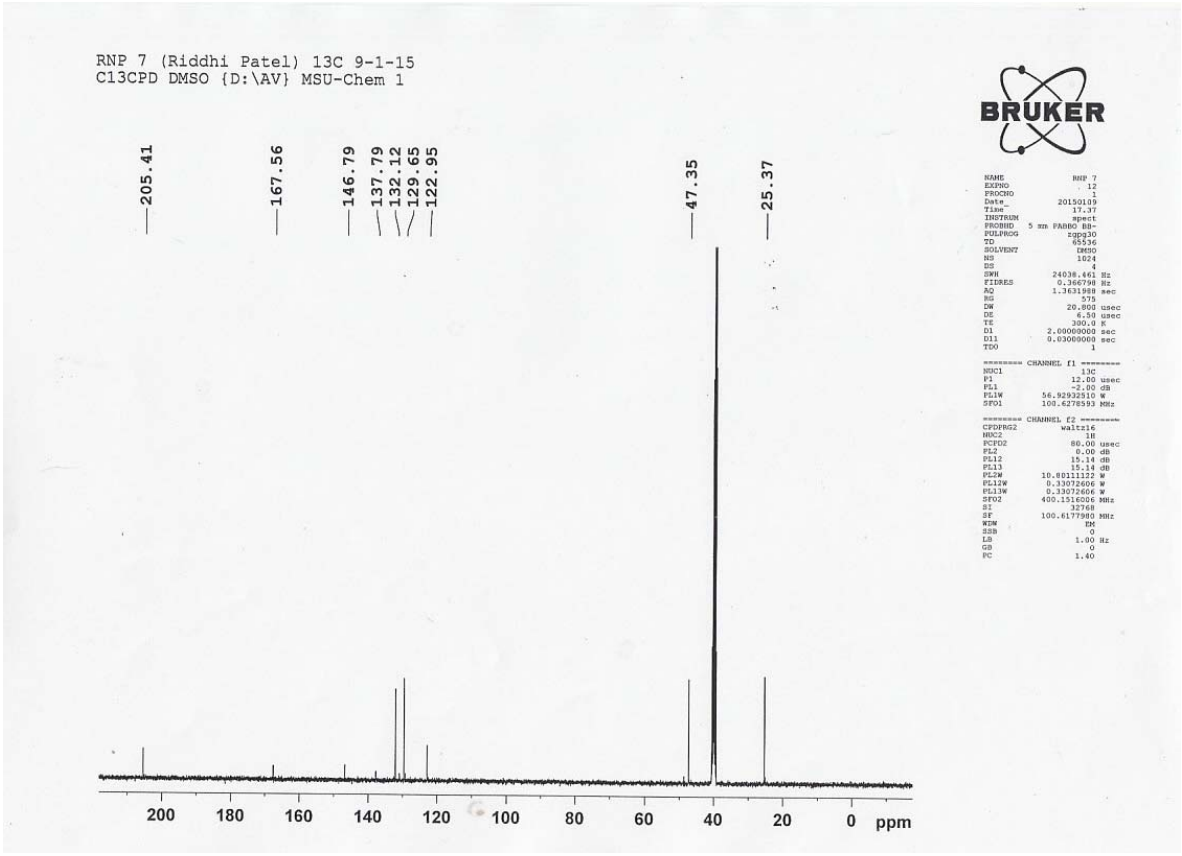
The M. S.University of Baroda, Vadodara, 390 001, India.

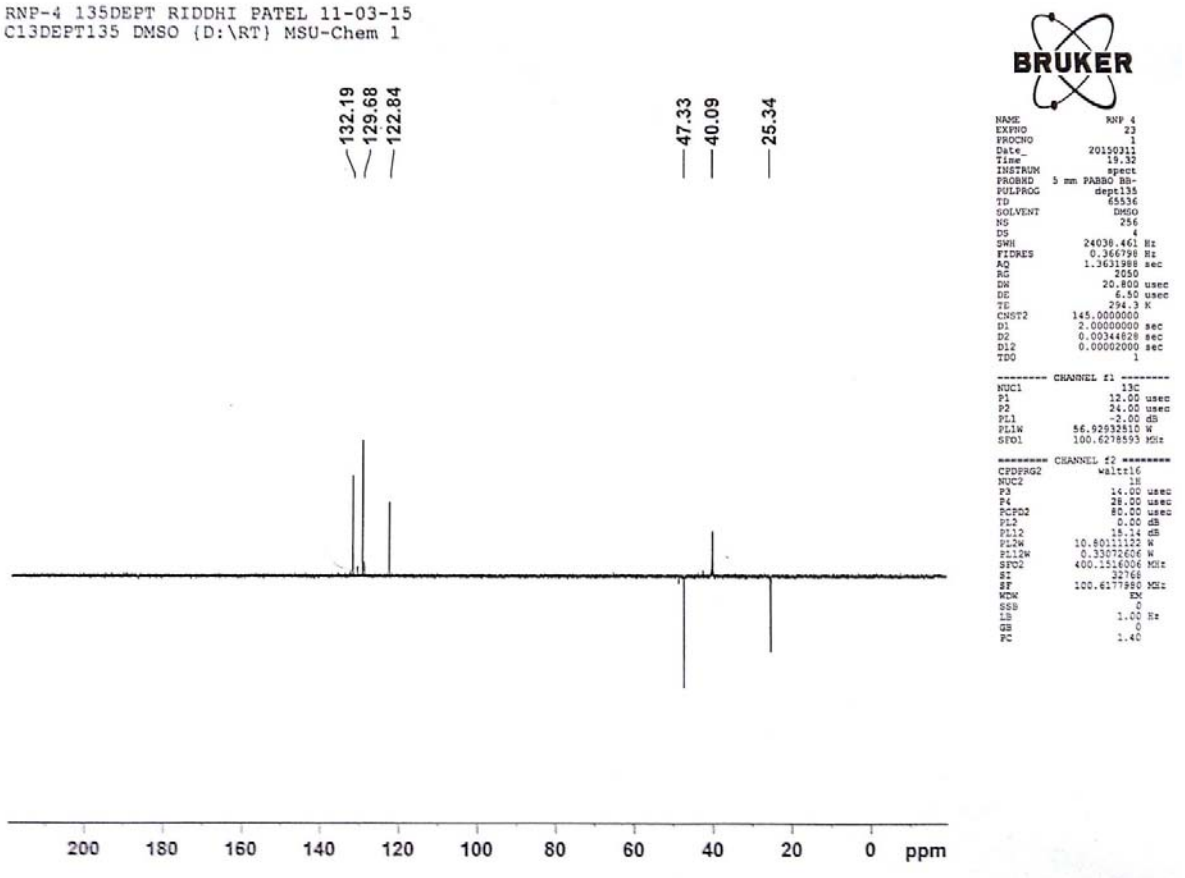
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoic acid ^{1}H NMR (3)



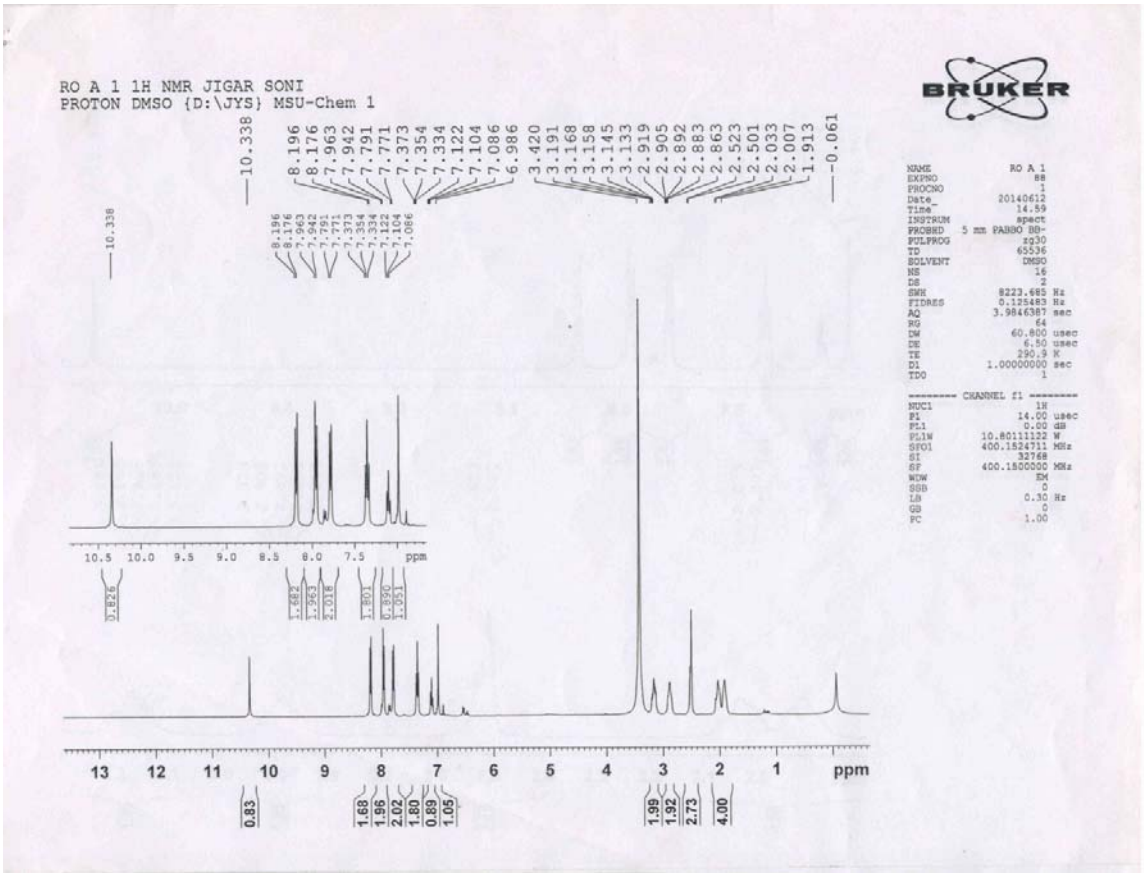
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoic acid ^{13}C NMR (3)



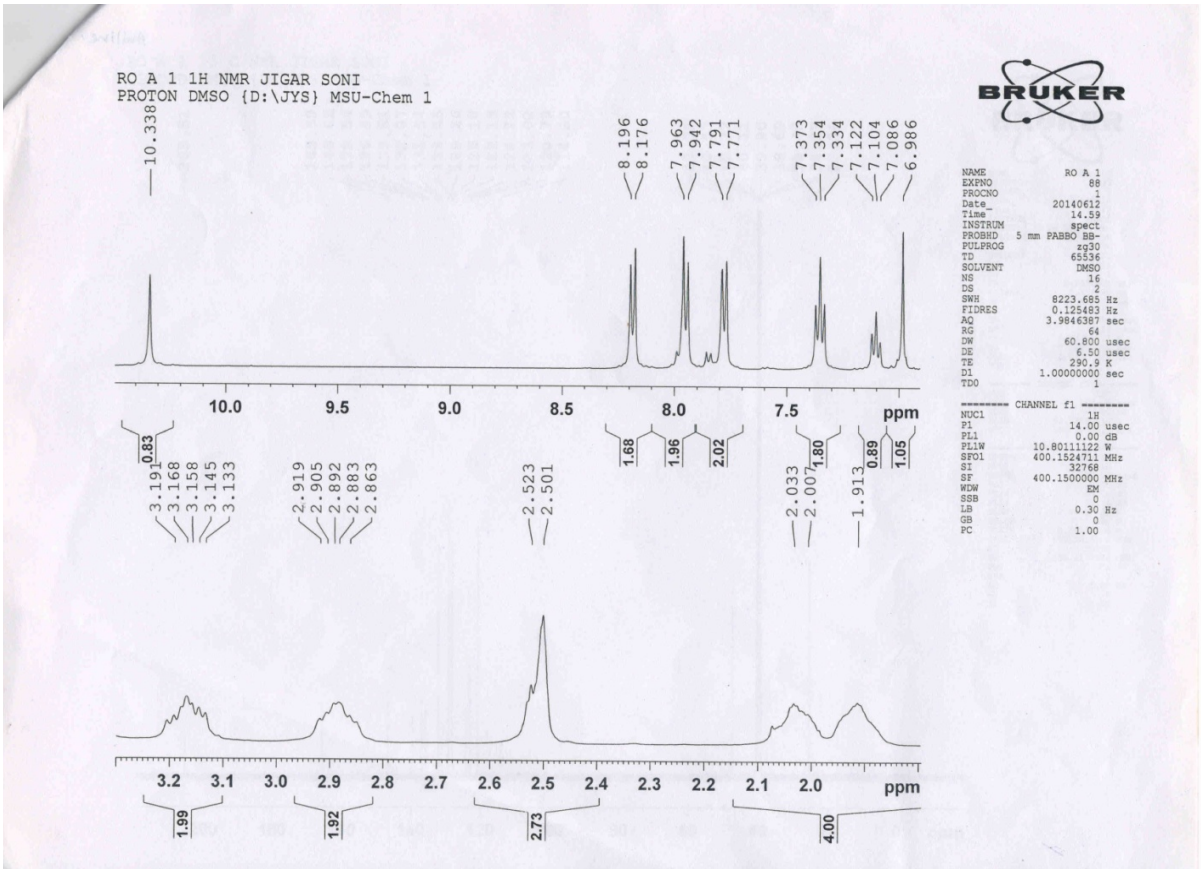
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoic acid DEPT-135 (3)



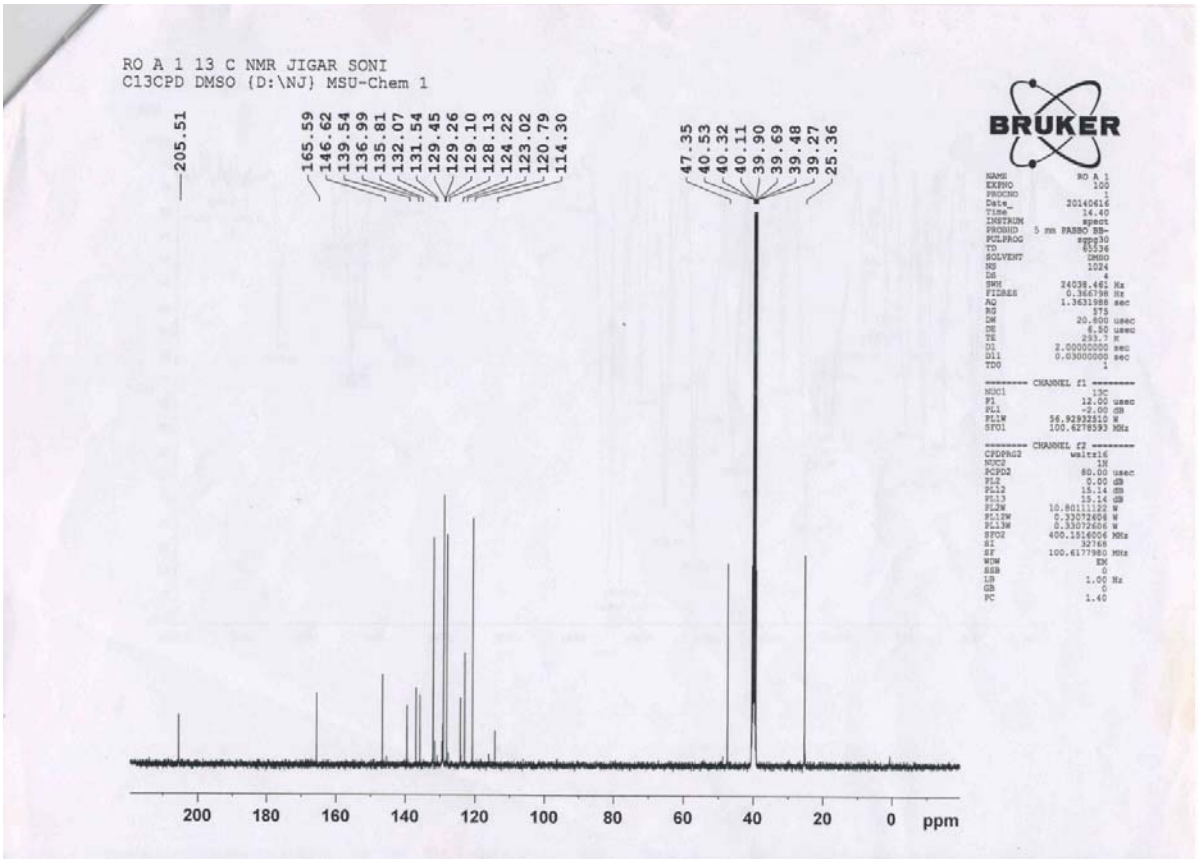
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-phenylbenzamide ^{1}H NMR (4a)



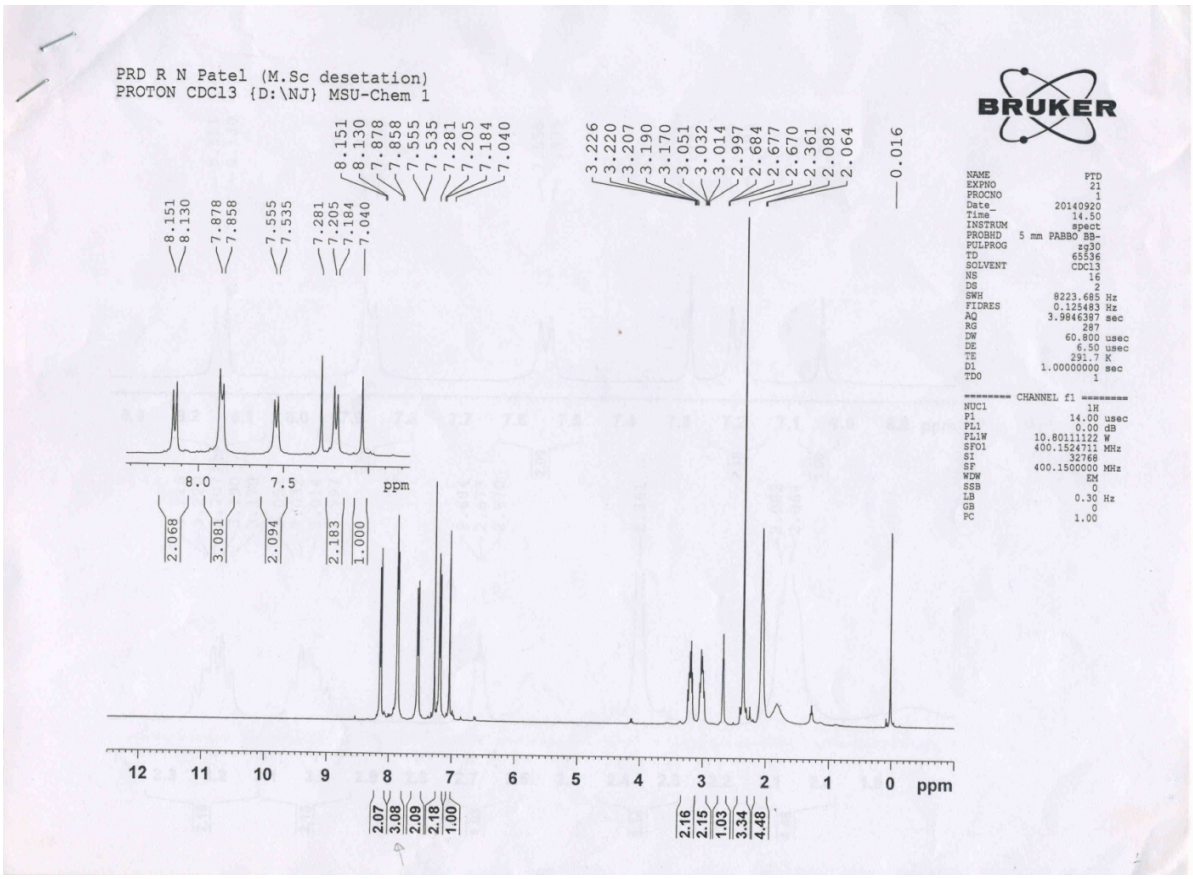
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-phenylbenzamide 1H NMR expansion (4a)



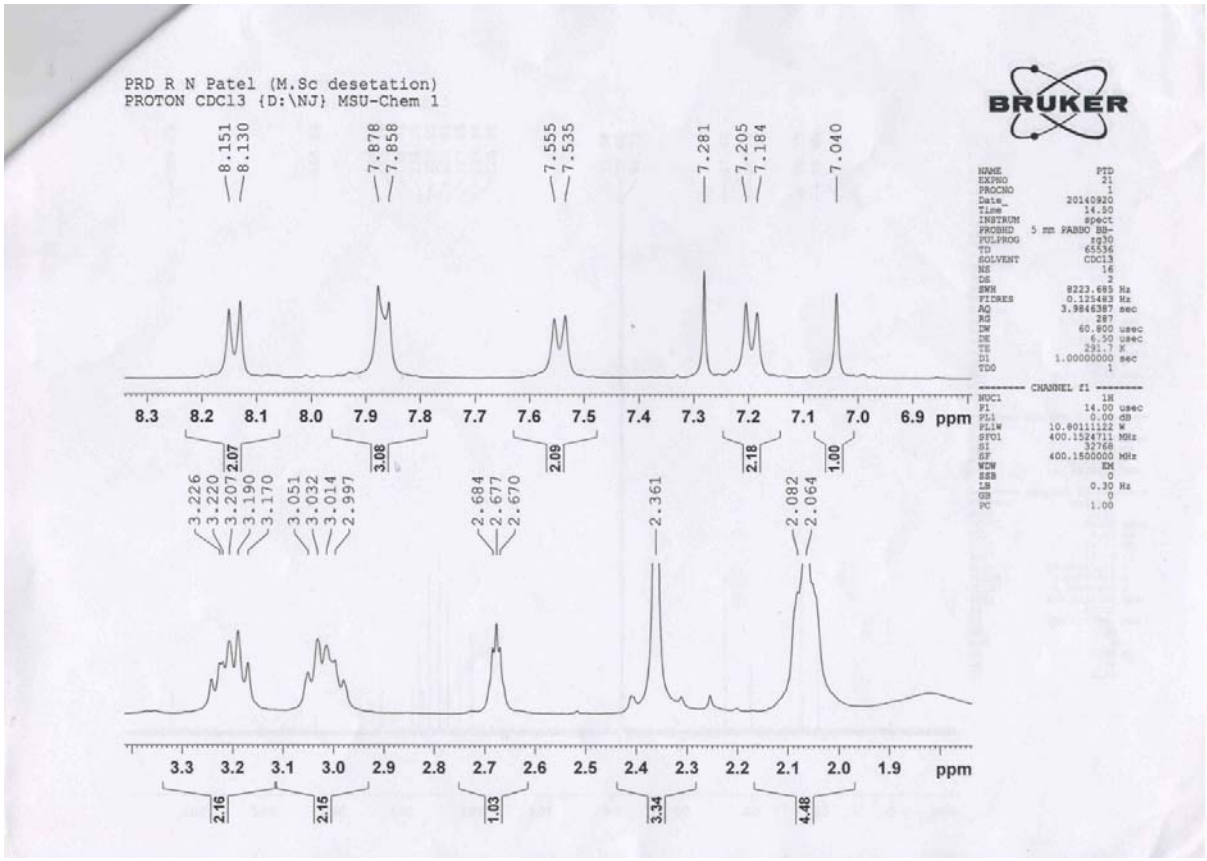
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-phenylbenzamide ^{13}C NMR (4a)



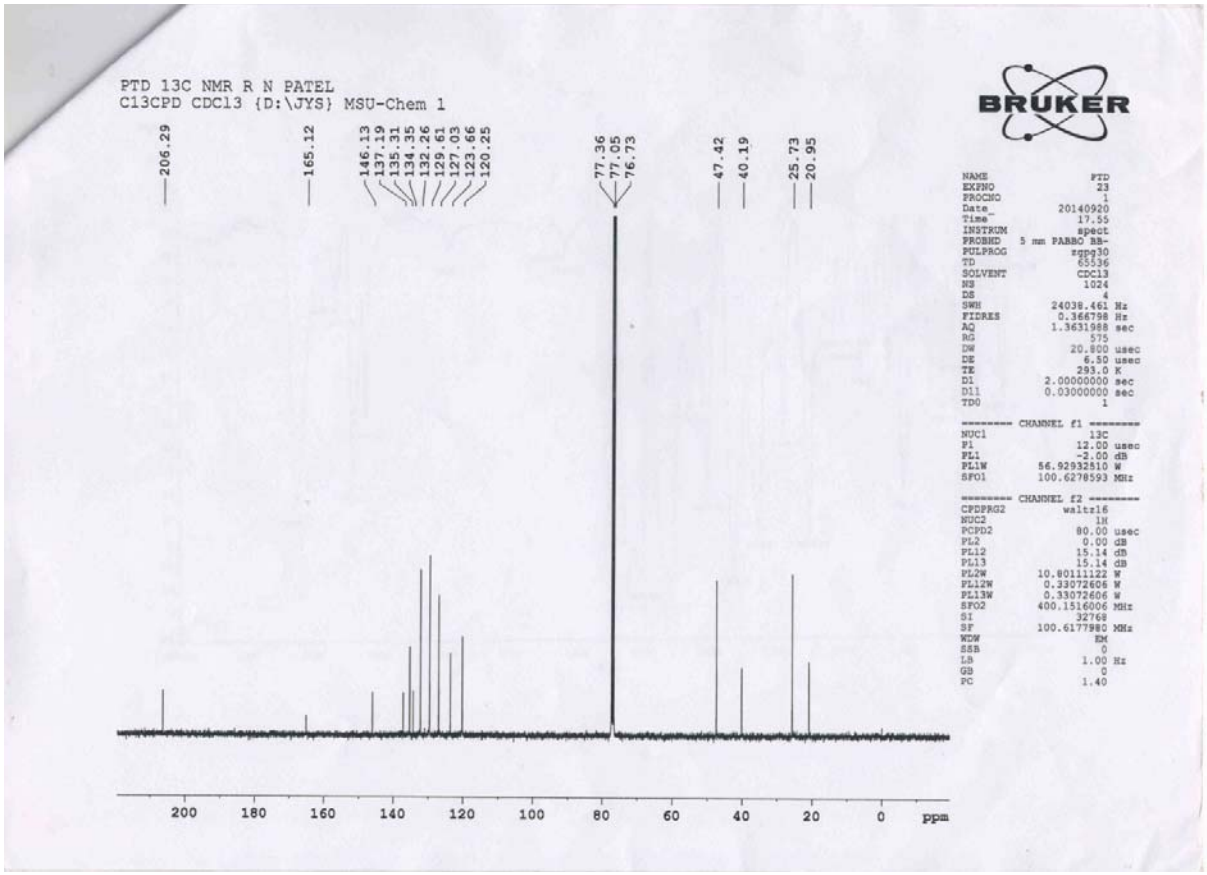
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-(p-tolyl)benzamide ^{1}H NMR(4b)



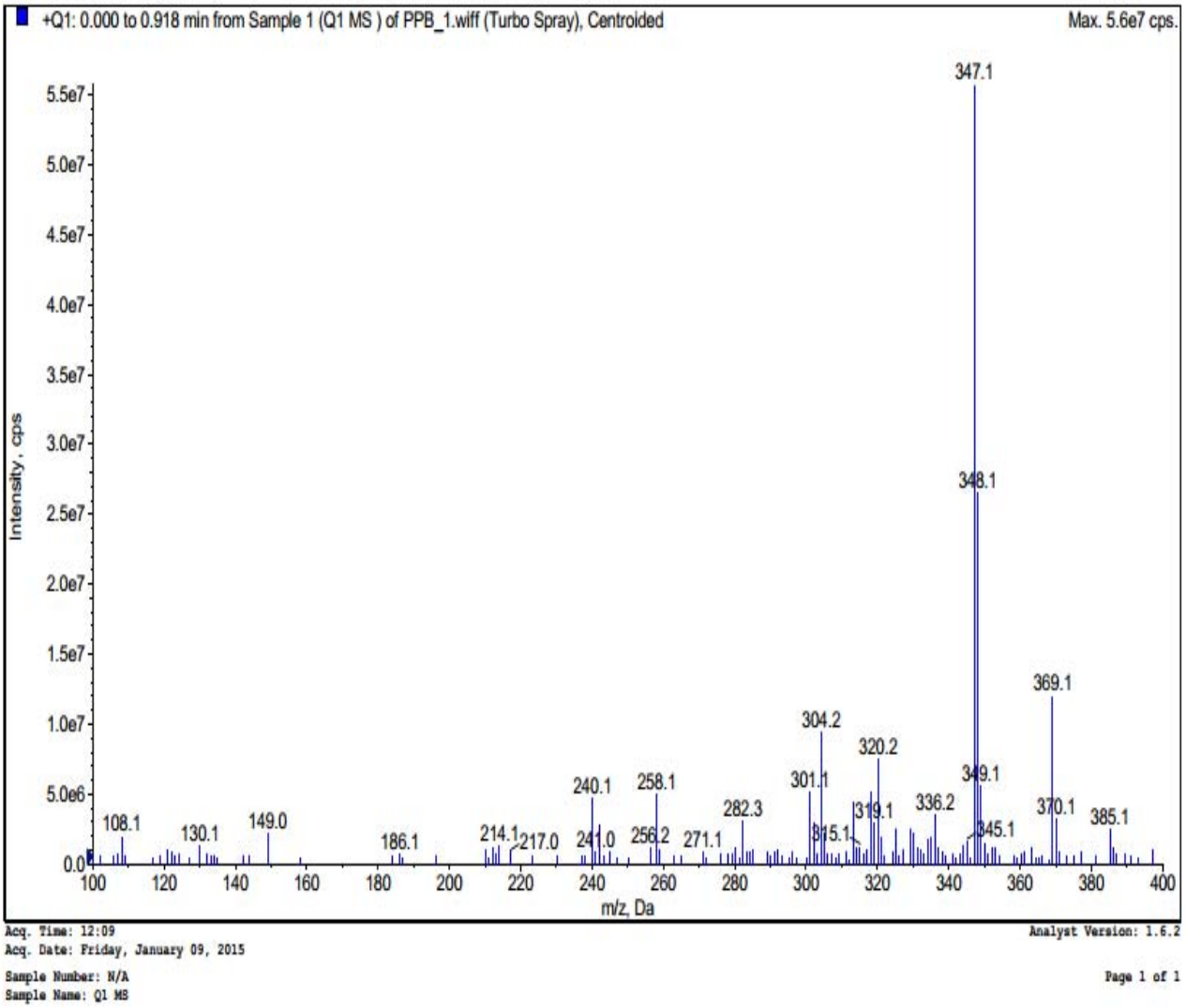
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-(p-tolyl)benzamide ^{1}H NMR (4b)



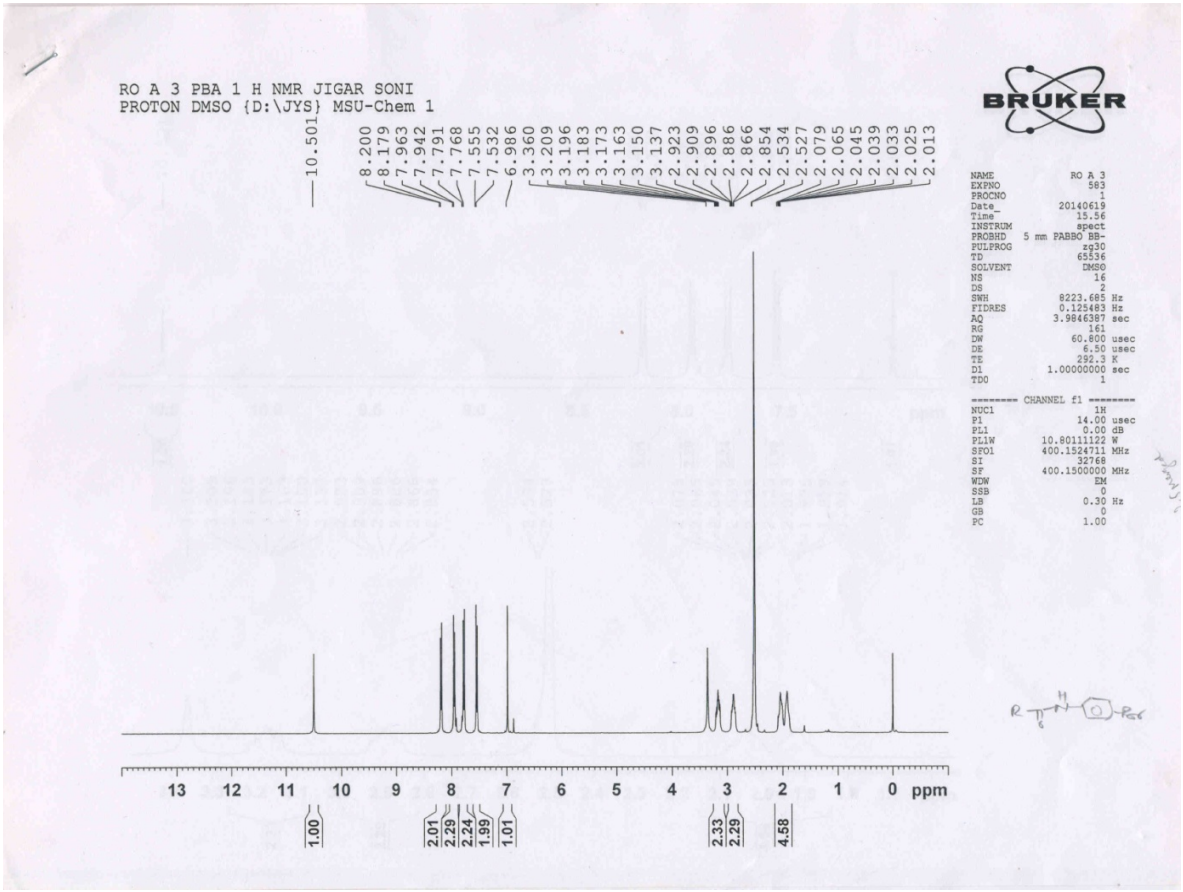
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-(p-tolyl)benzamide ^{13}C NMR (4b)



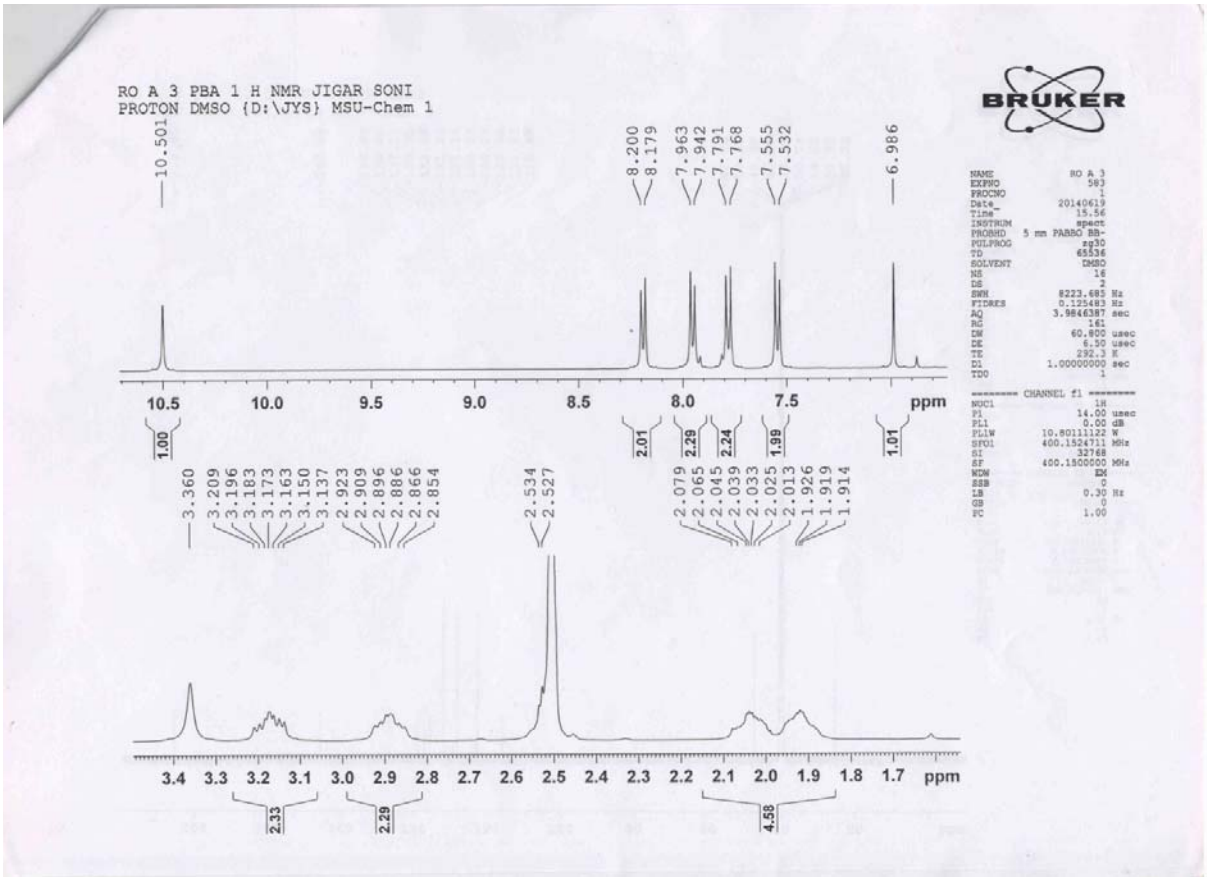
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-(p-tolyl)benzamide Mass Spectra



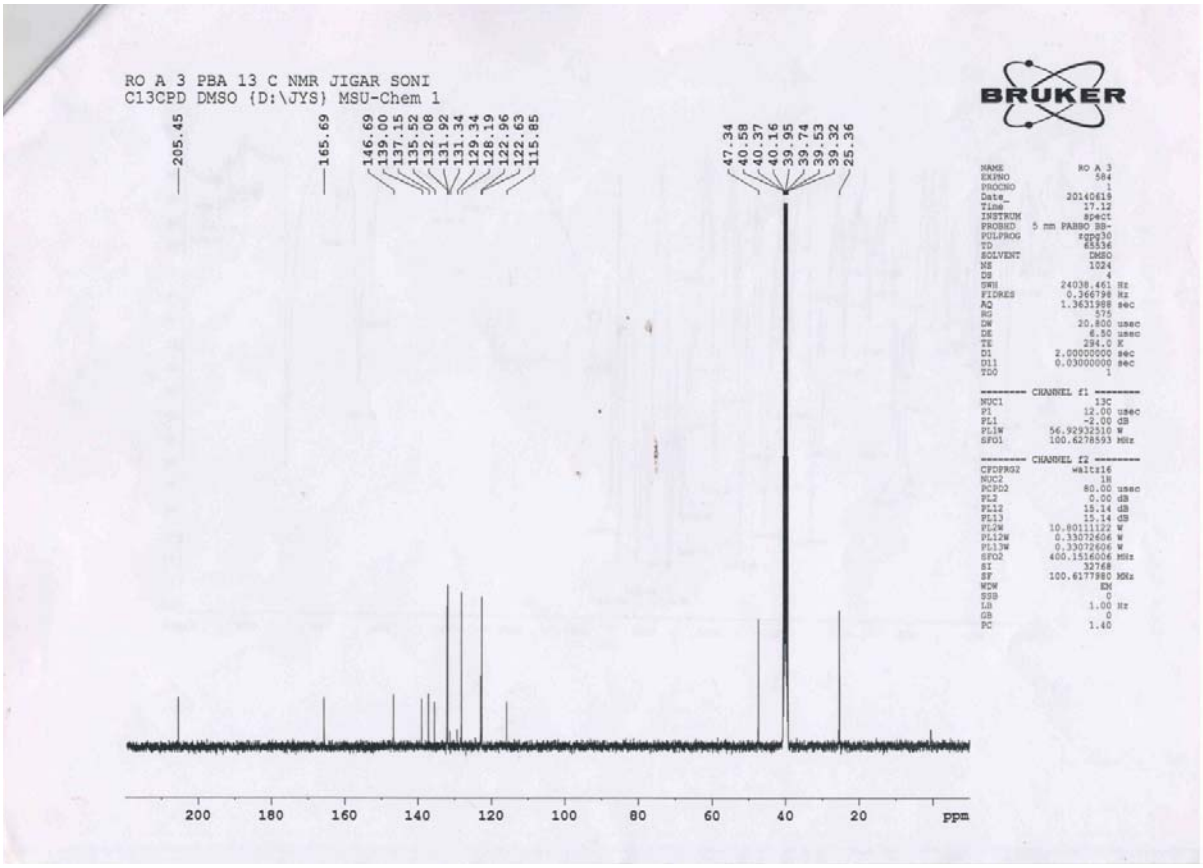
(Z)-N-(4bromophenyl)-4-((3-oxoquinuclidin-2-ylidene)methyl) benzamide ^{1}H NMR (4c)



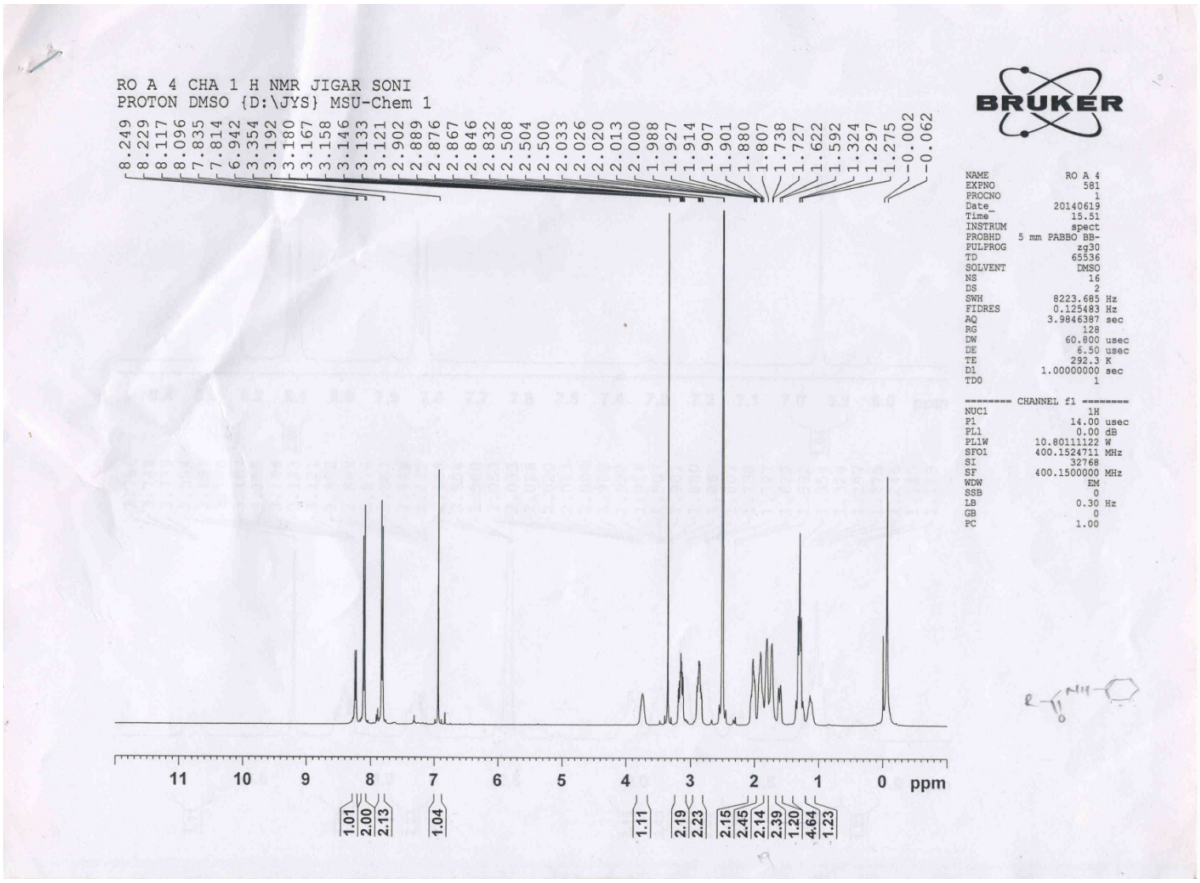
(Z)-N-(4bromophenyl)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzamide ^{1}H NMR Expansion (4c)



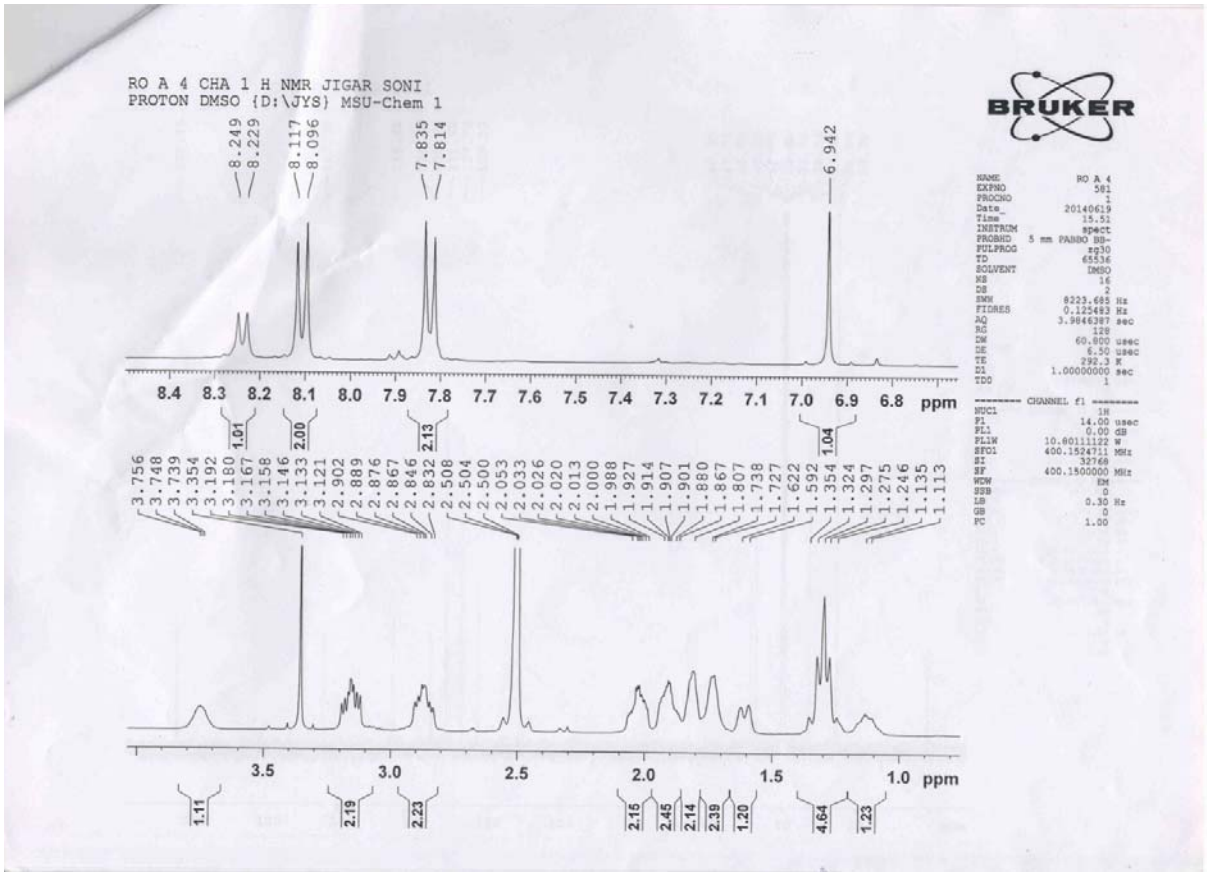
(Z)-N-(4bromophenyl)-4-((3-oxoquinuclidin-2-ylidene)methyl) benzamide ^{13}C NMR (4c)



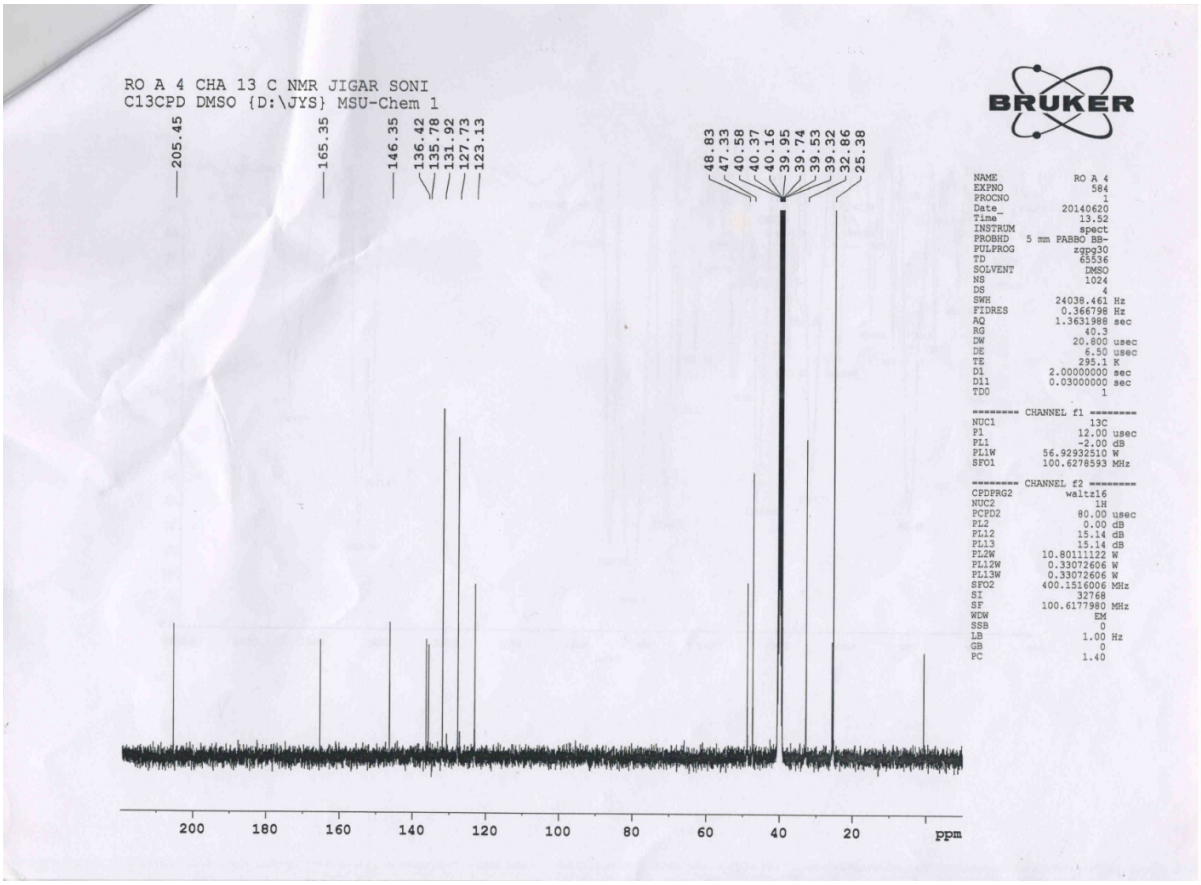
(Z)-N-cyclohexyl-4-((3-oxoquinuclidin-2-ylidene)methyl) benzamide ^{1}H NMR (4d)



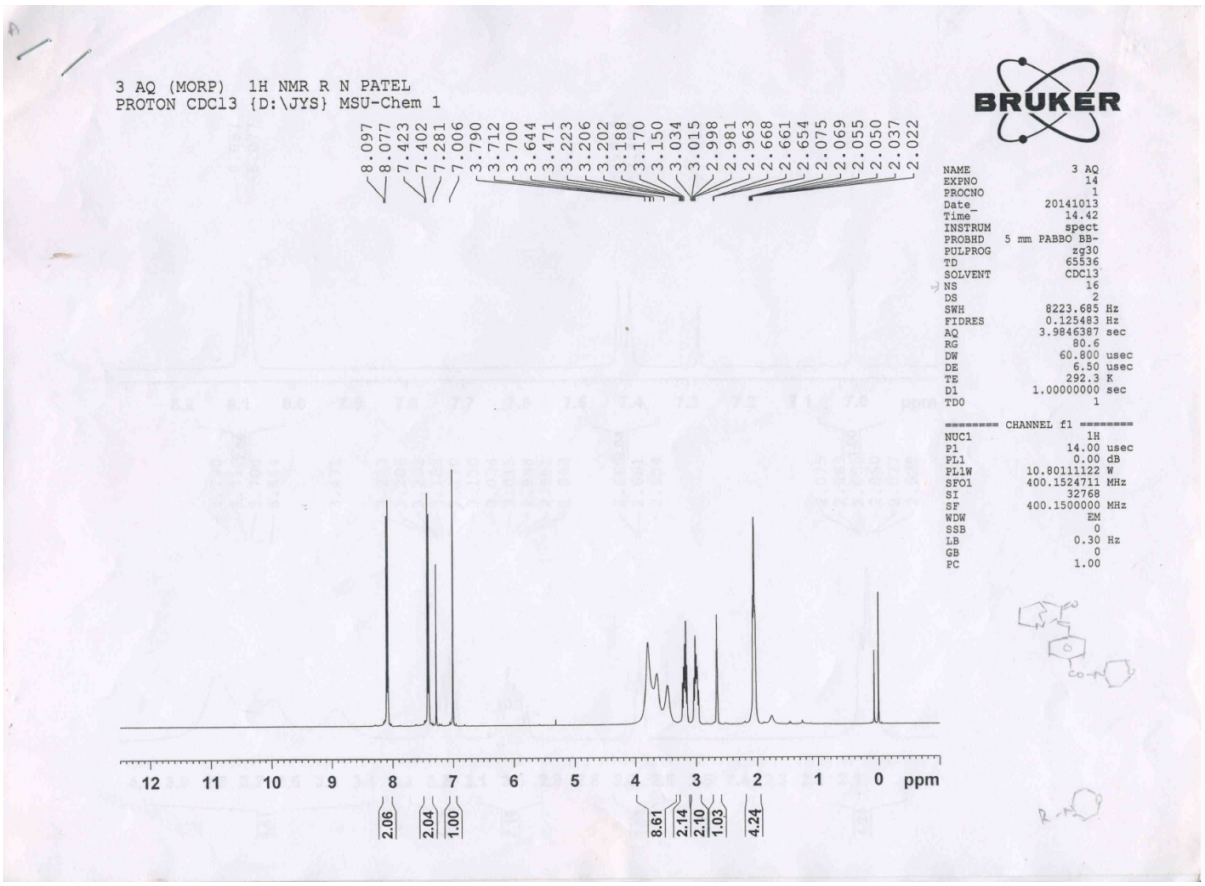
(Z)-N-cyclohexyl-4-((3-oxoquinuclidin-2-ylidene)methyl) benzamide ^{1}H NMR (4d)



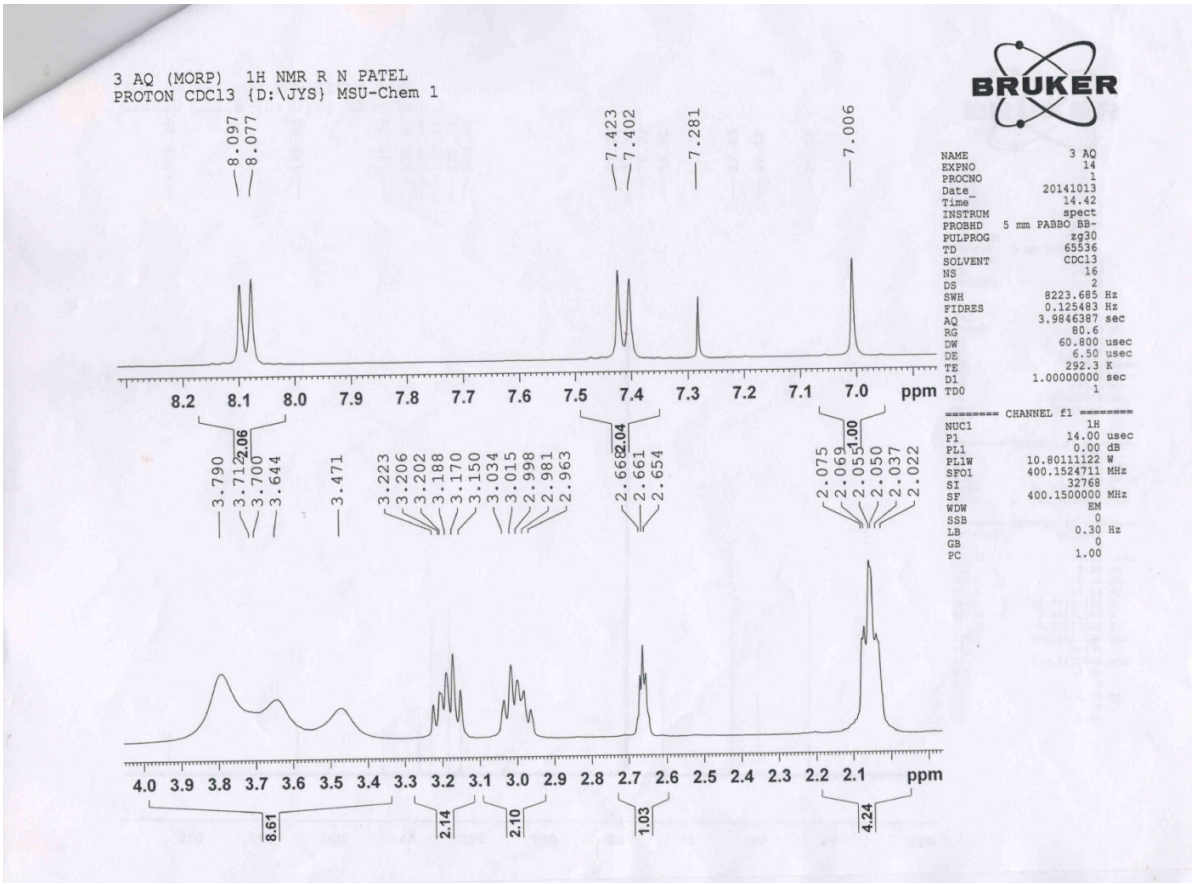
(Z)-N-cyclohexyl-4-((3-oxoquinuclidin-2-ylidene)methyl) benzamide^{13}C NMR (4d)



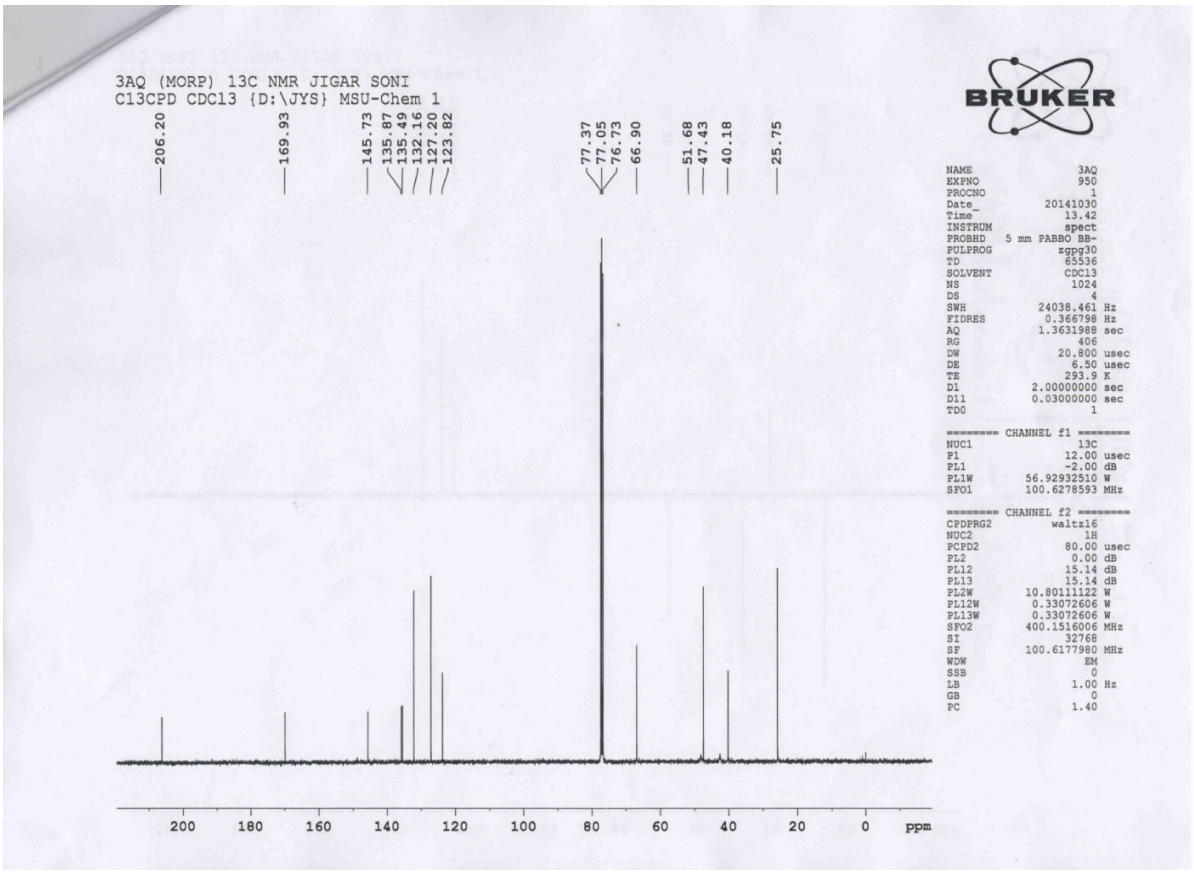
(Z)-2-(4-(morpholine-4-carbonyl)benzylidene)quinuclidin-3-one^{1}H NMR (4e)



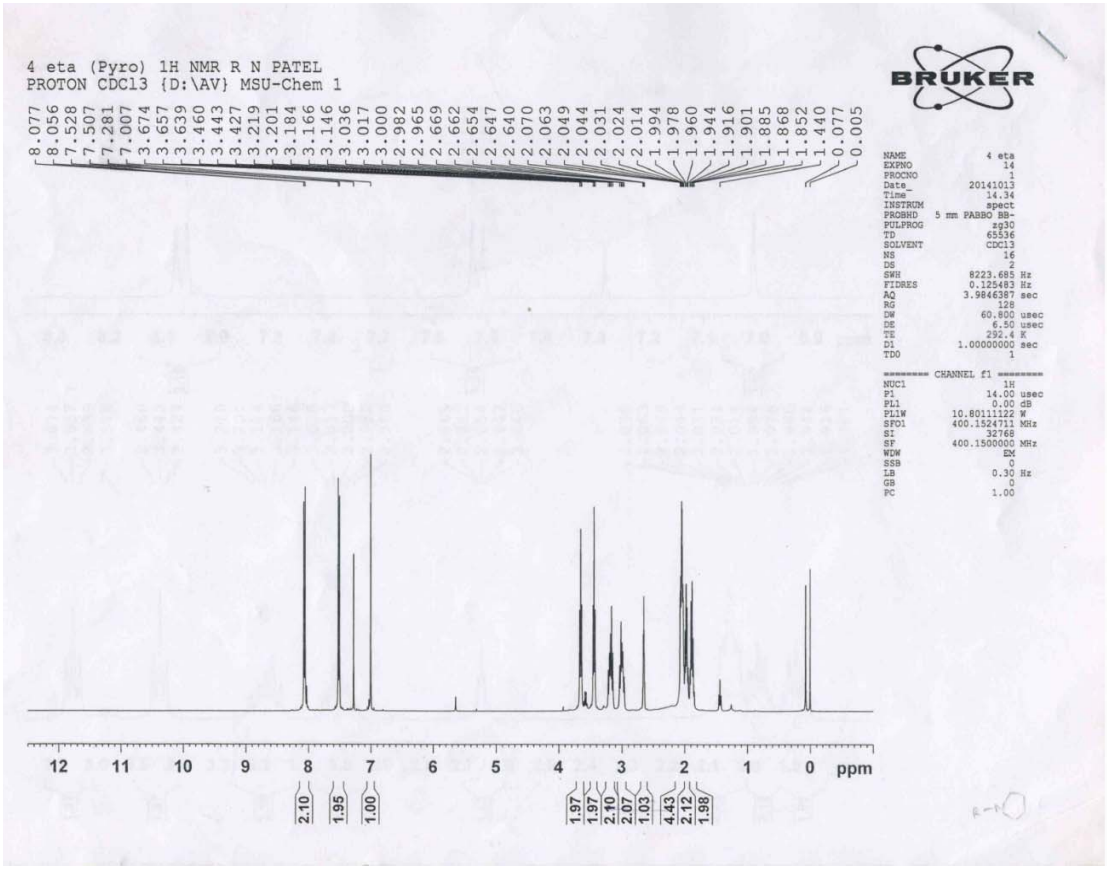
(Z)-2-(4-(morpholine-4-carbonyl)benzylidene)quinuclidin-3-one ^{1}H NMR Expansion (4e)



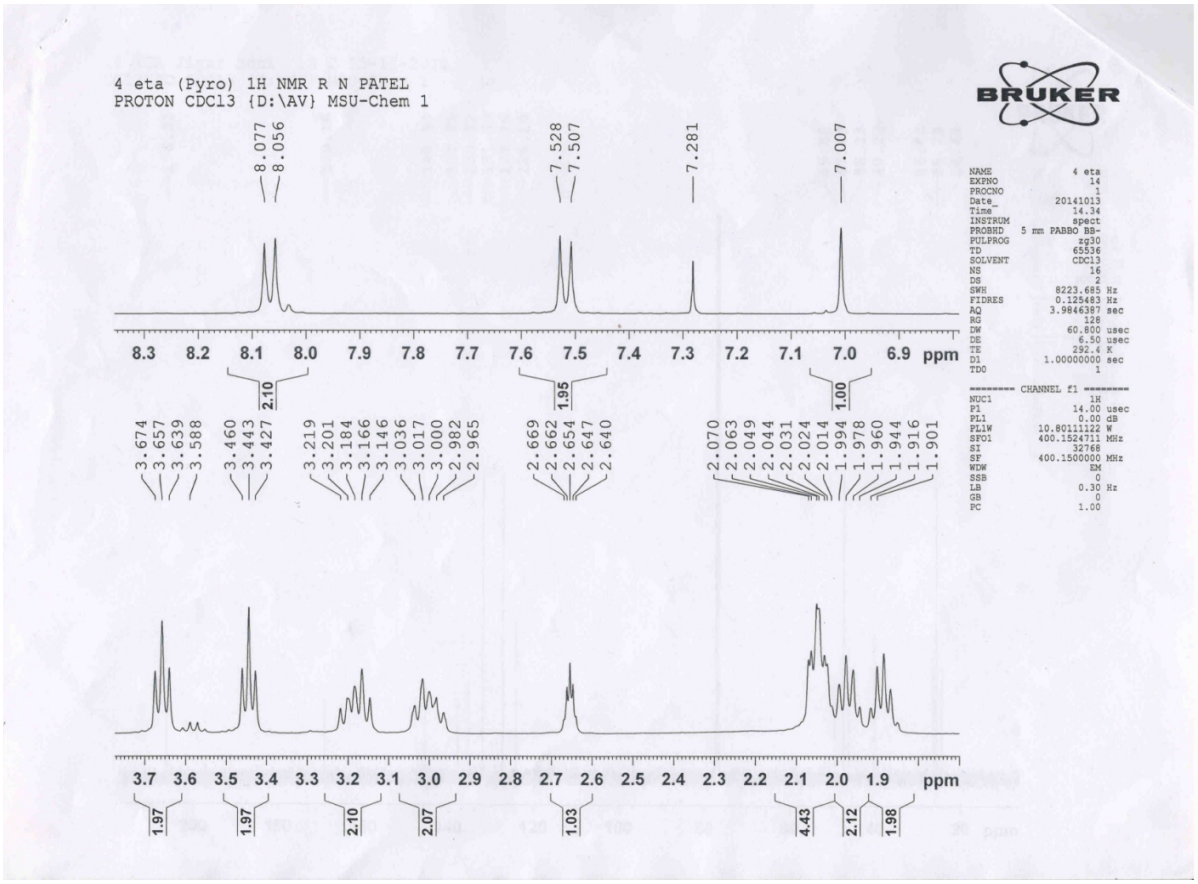
(Z)-2-(4-(morpholine-4-carbonyl)benzylidene)quinuclidin-3-one ^{13}C NMR (4e)



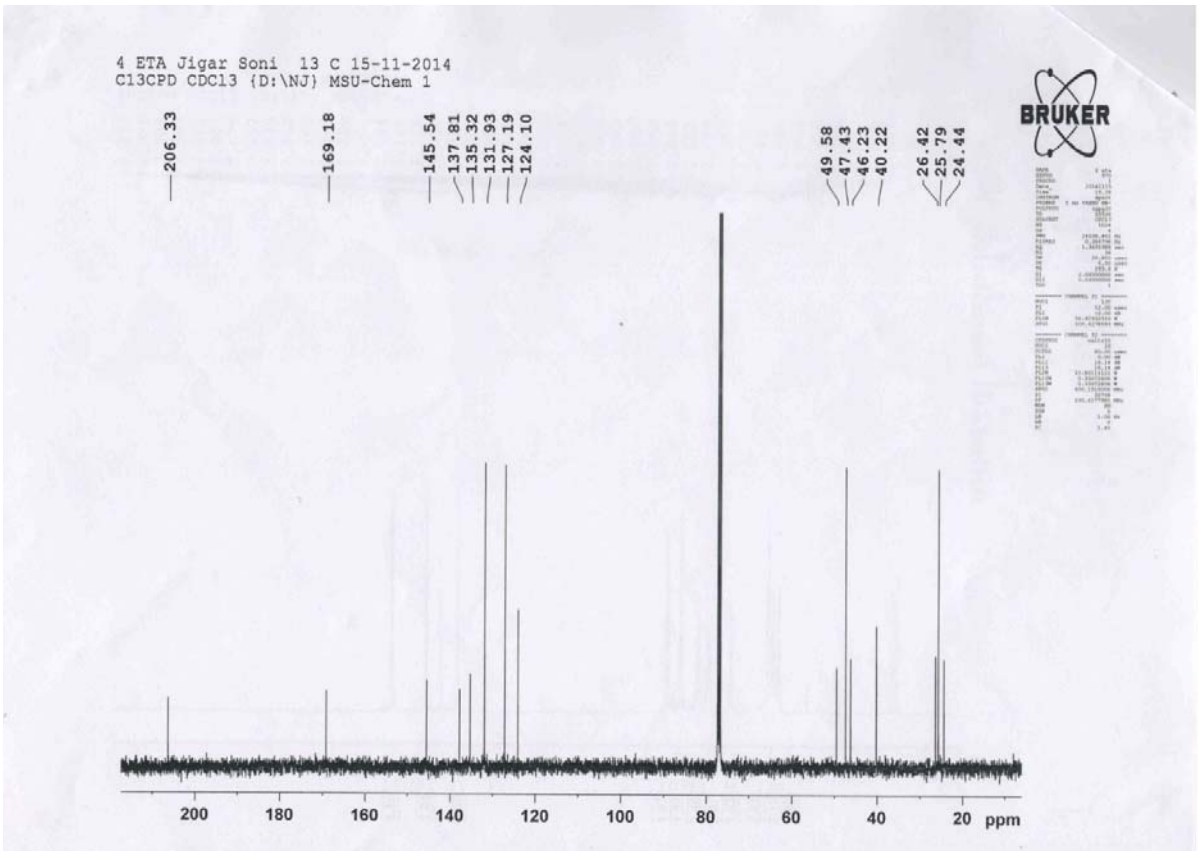
(Z)-2-(4-(pyrrolidine-1-carbonyl)benzylidene)quinuclidin-3-one ^{1}H NMR (4f)



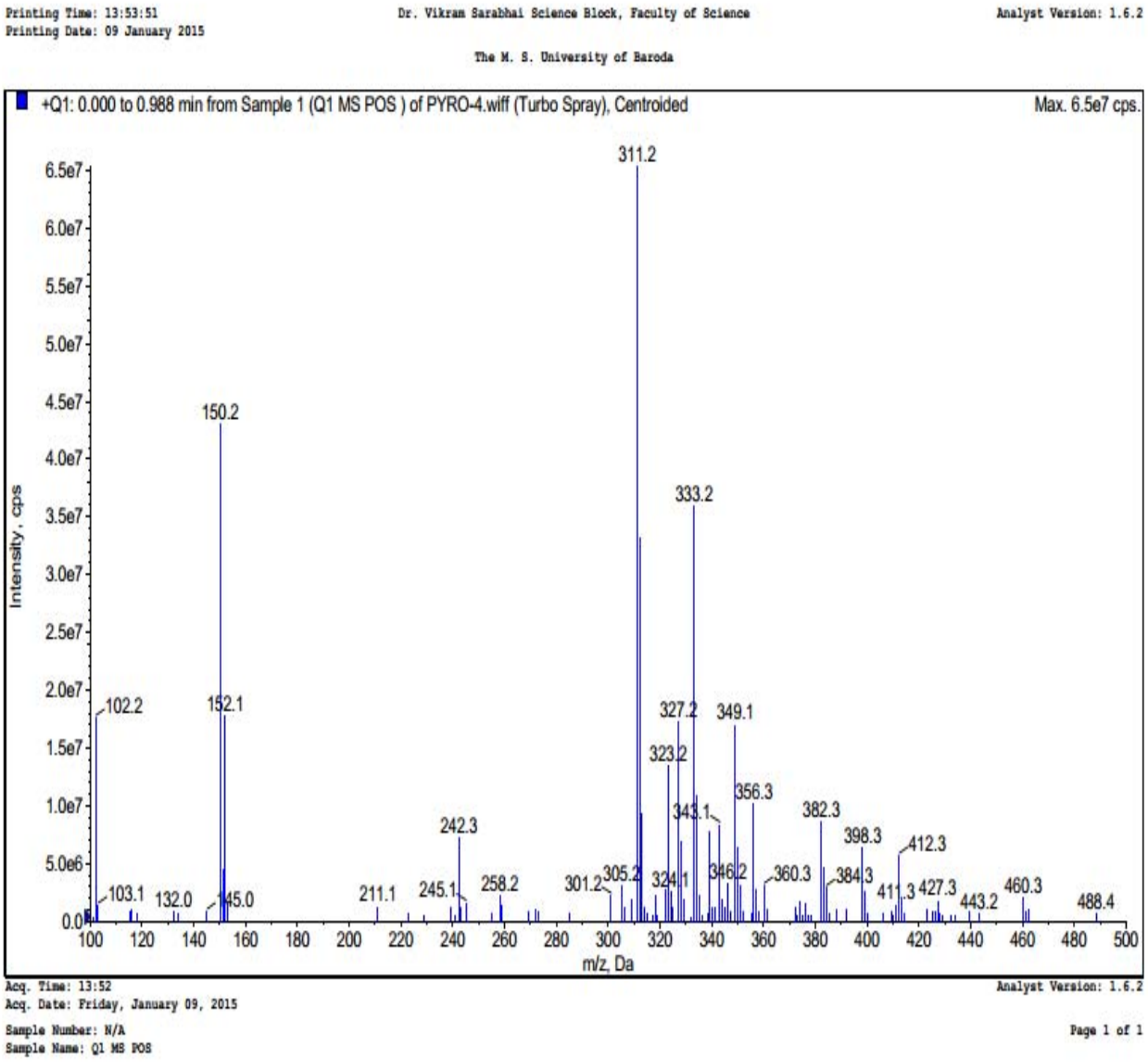
(Z)-2-(4-(pyrrolidine-1-carbonyl)benzylidene)quinuclidin-3-one ^{1}H NMR (4f)



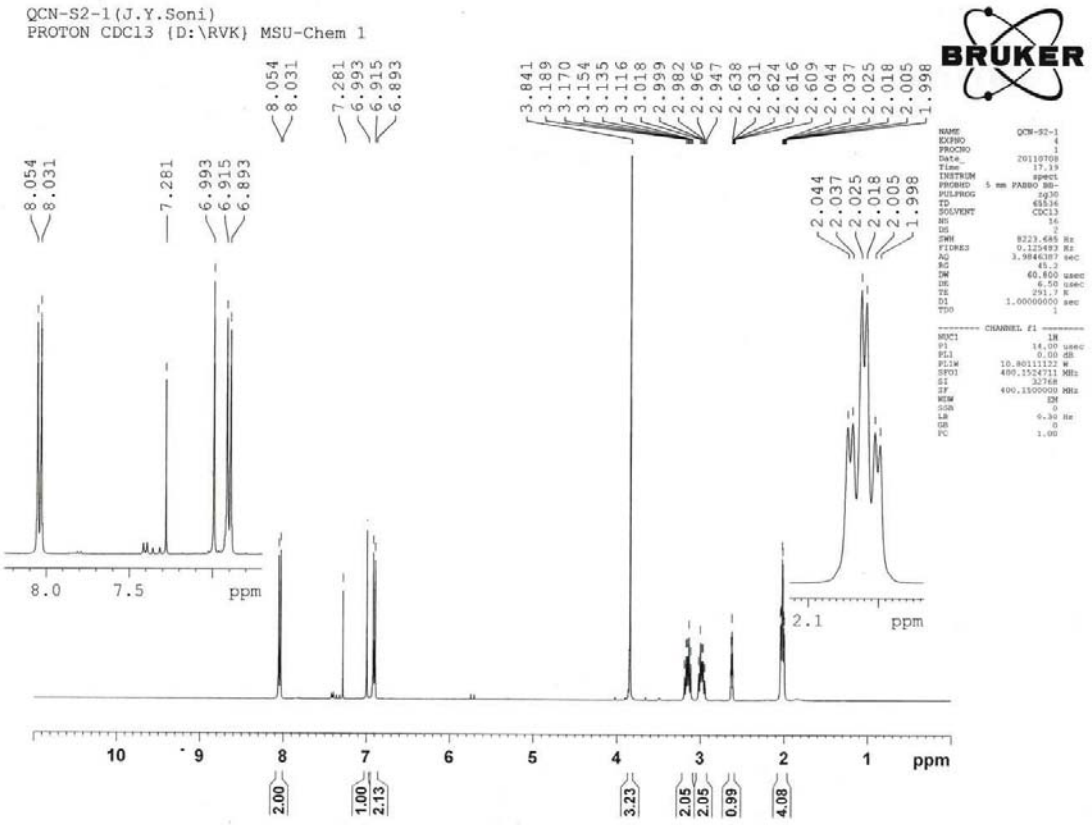
(Z)-2-(4-(pyrrolidine-1-carbonyl)benzylidene)quinuclidin-3-one ^{13}C NMR (4f)



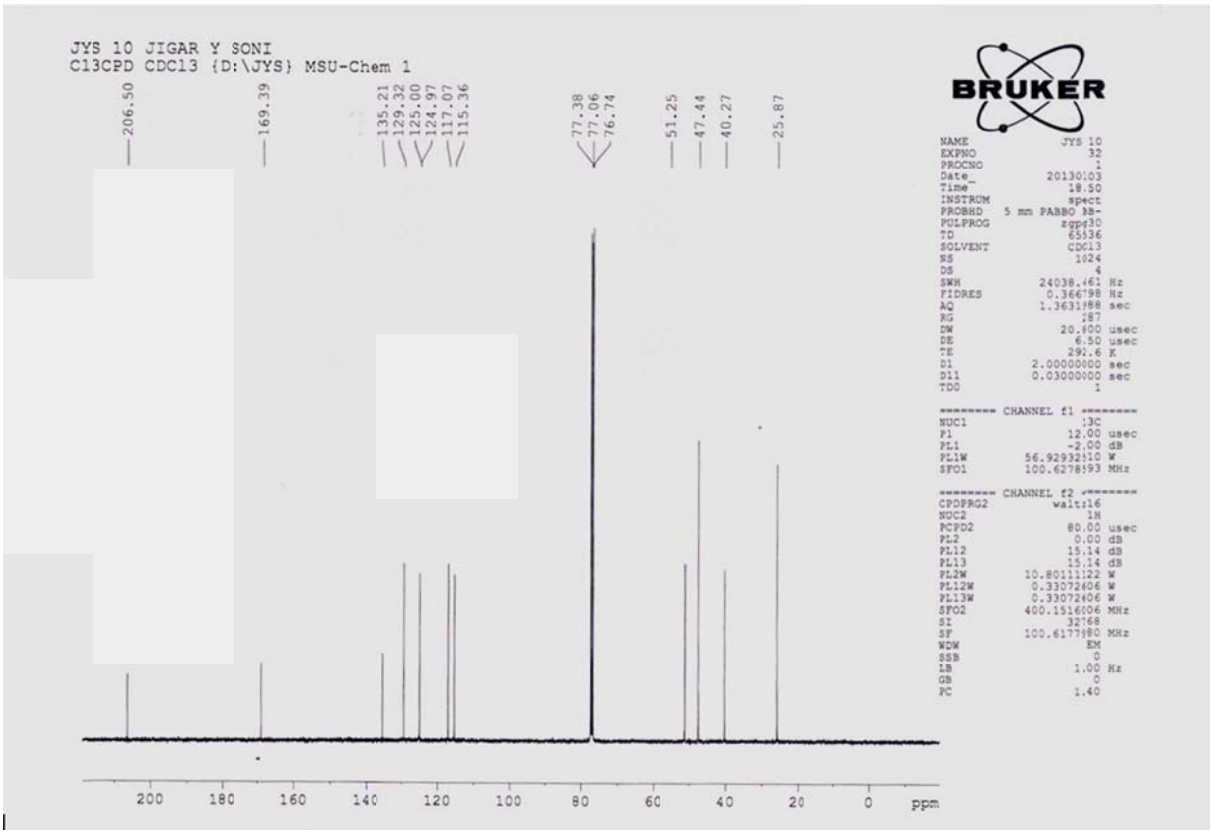
(Z)-2-(4-(pyrrolidine-1-carbonyl)benzylidene)quinuclidin-3-one Mass Spectra



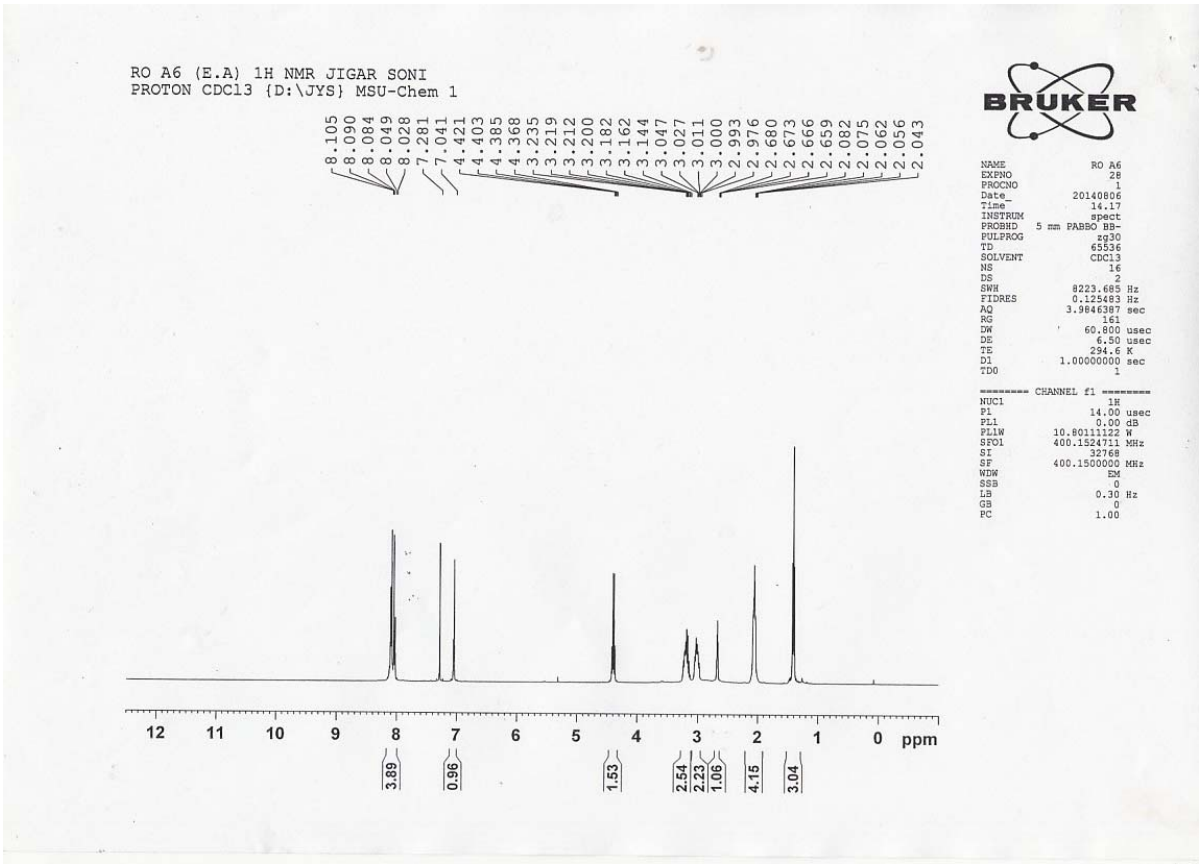
Methyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{1}H NMR (5a)



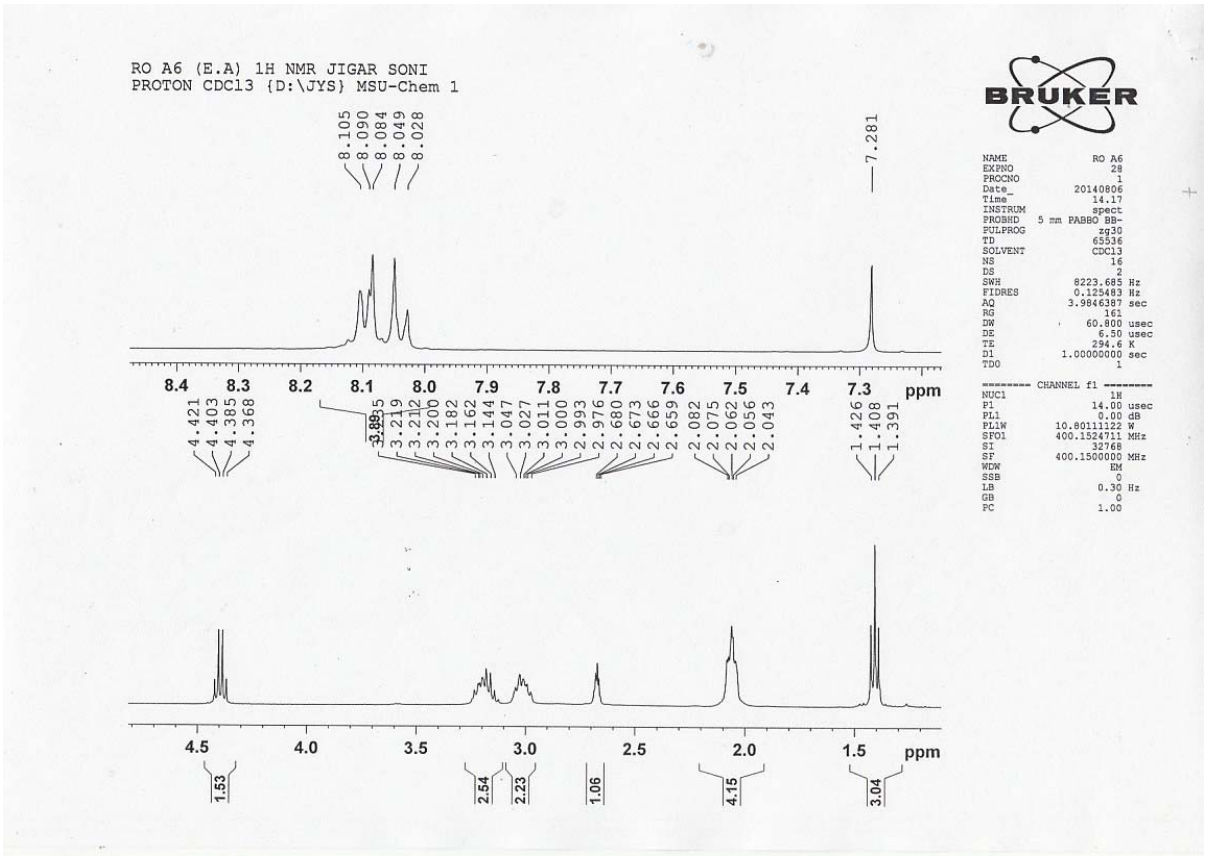
Methyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate^{13}C NMR (5a)



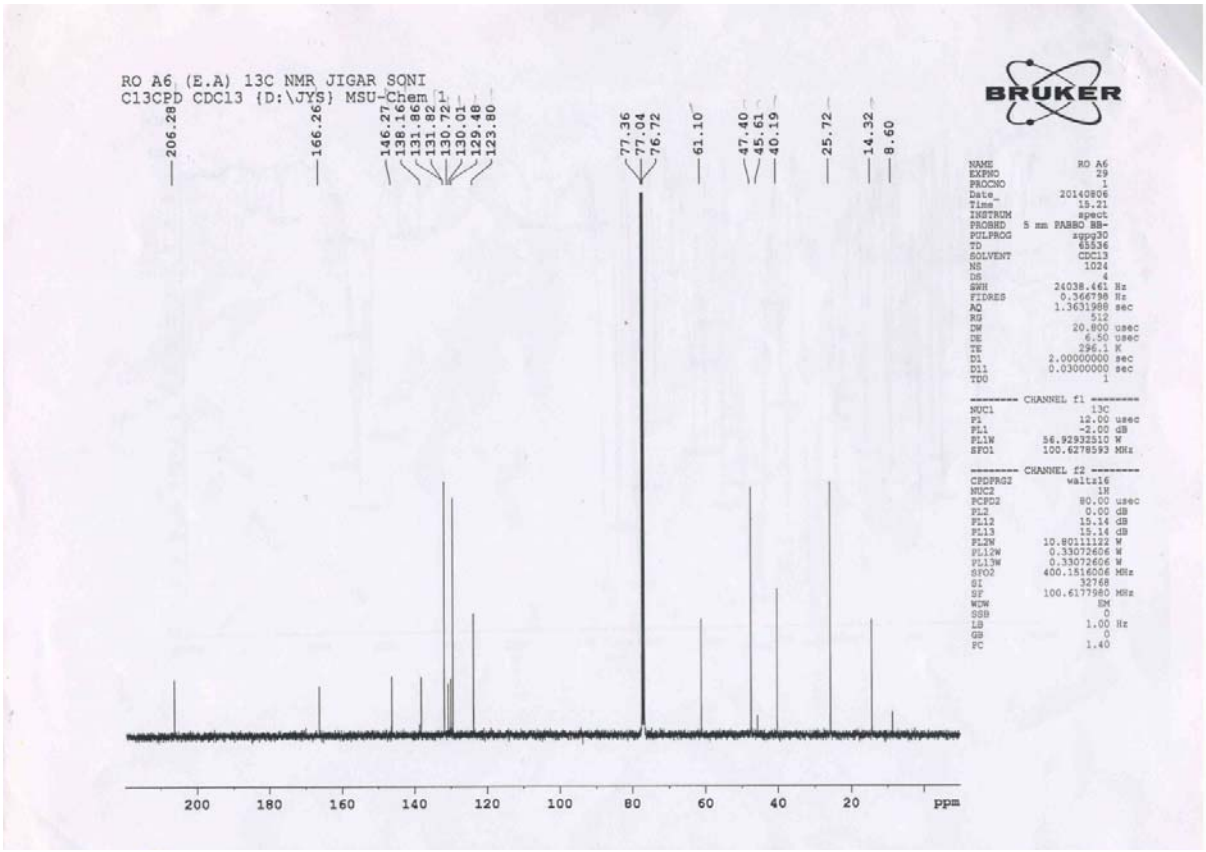
Ethyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{1}H NMR (5b)



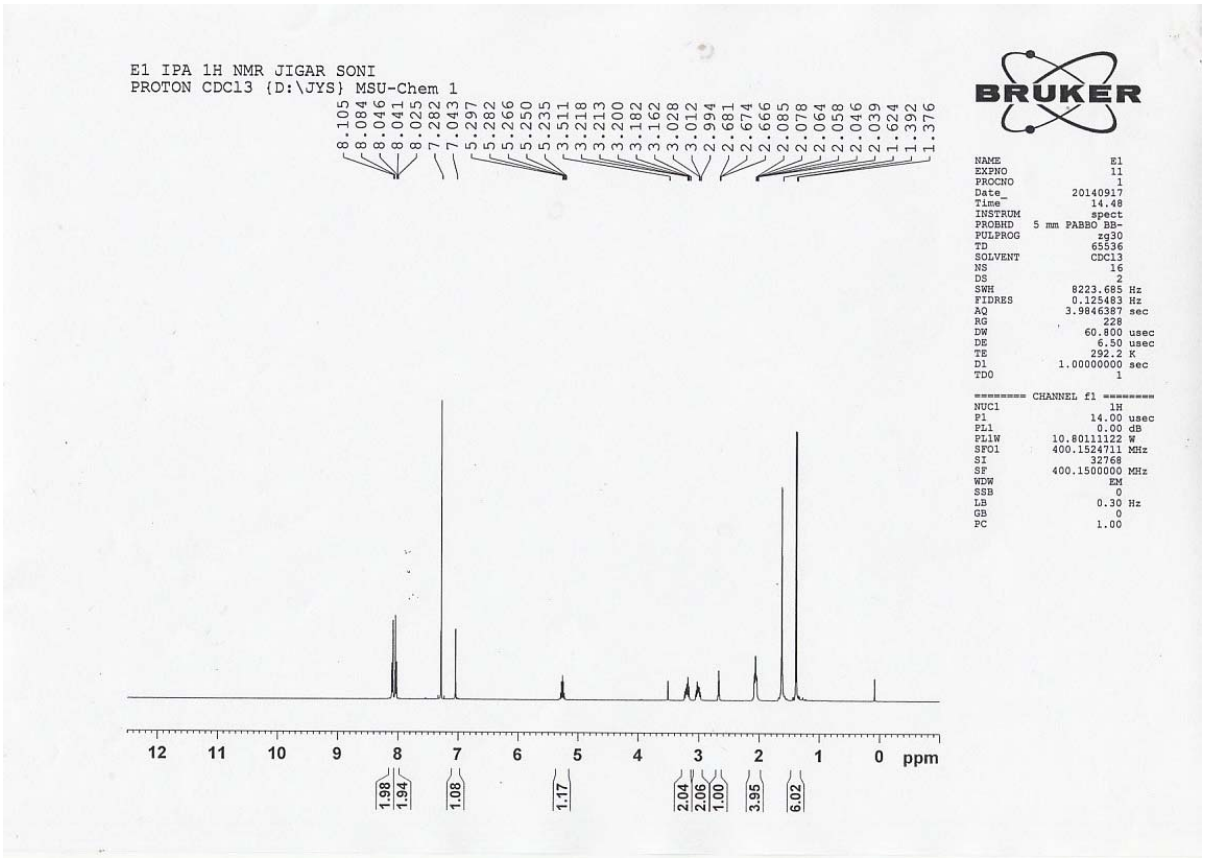
Ethyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{1}H NMR expansion (5b)



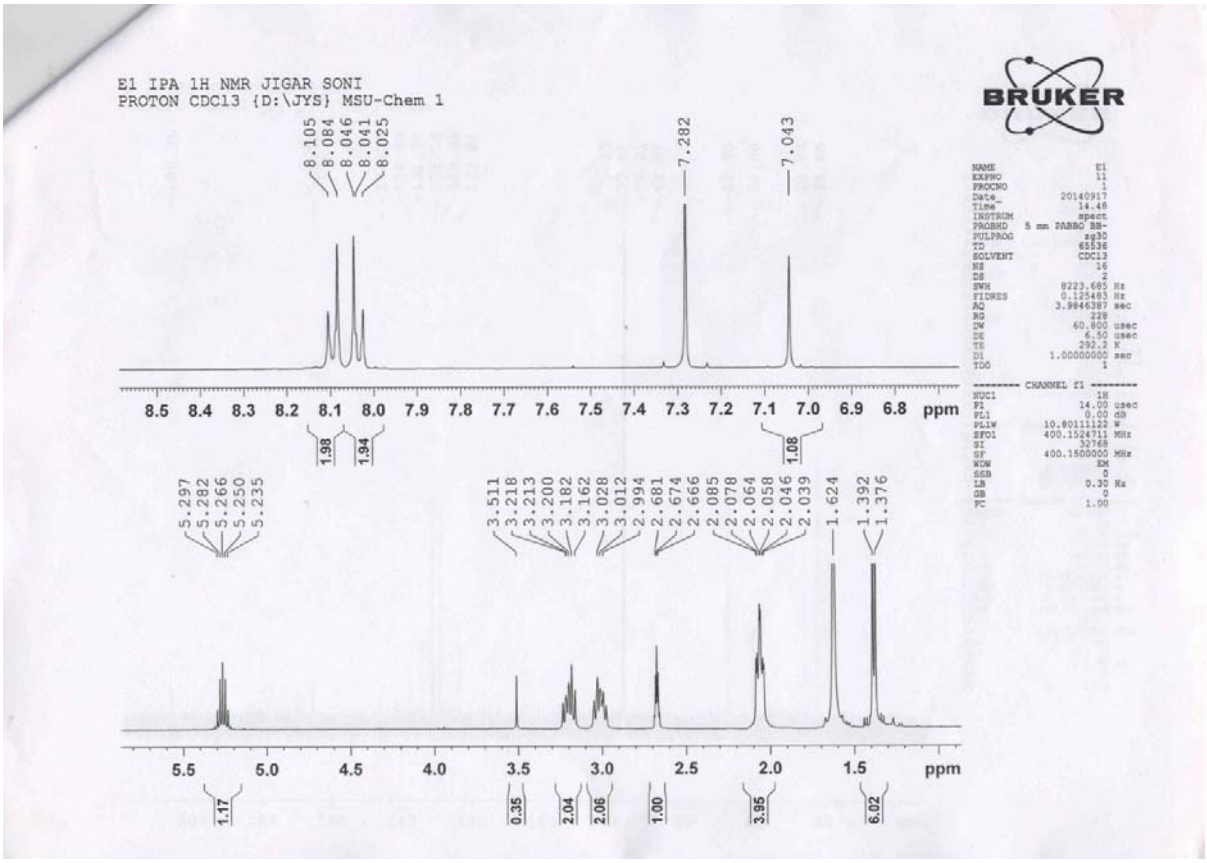
Ethyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{13}C NMR (5b)



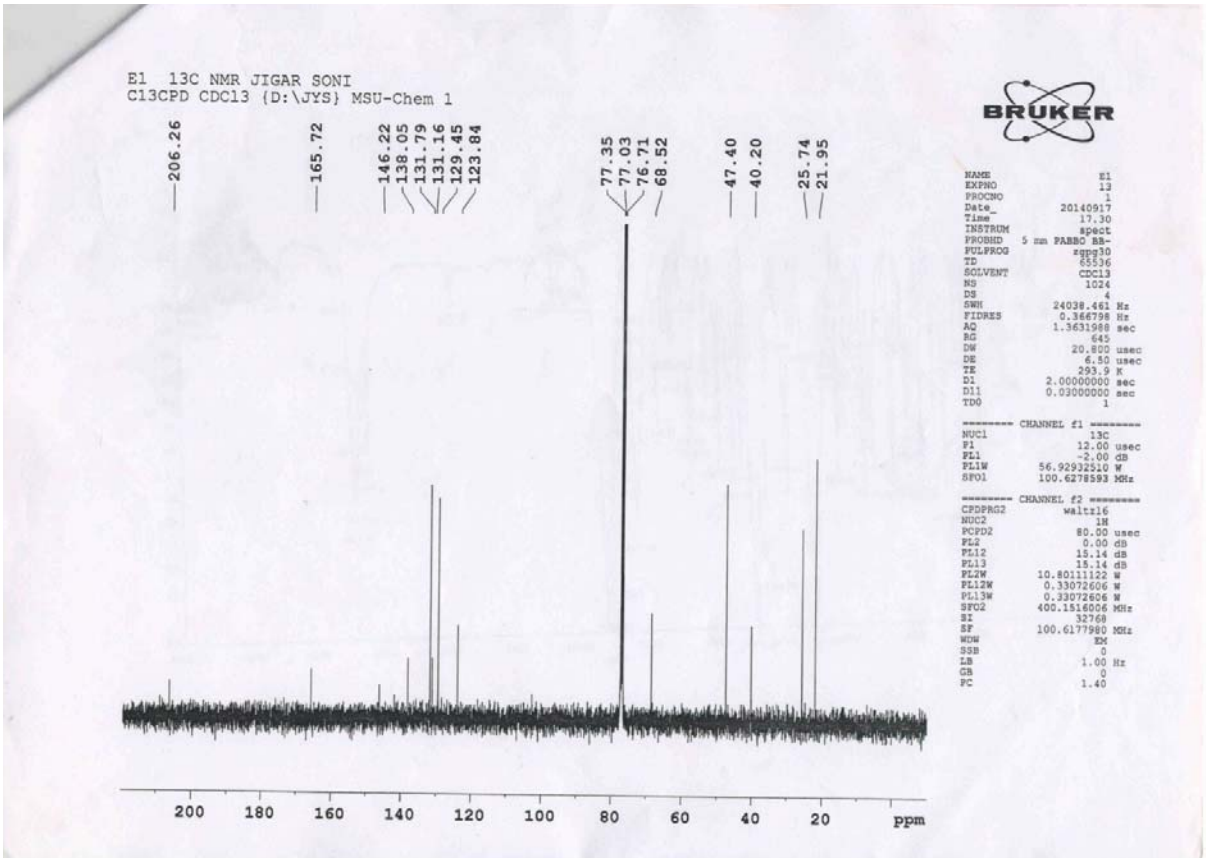
Isopropyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{1}H NMR (5c)



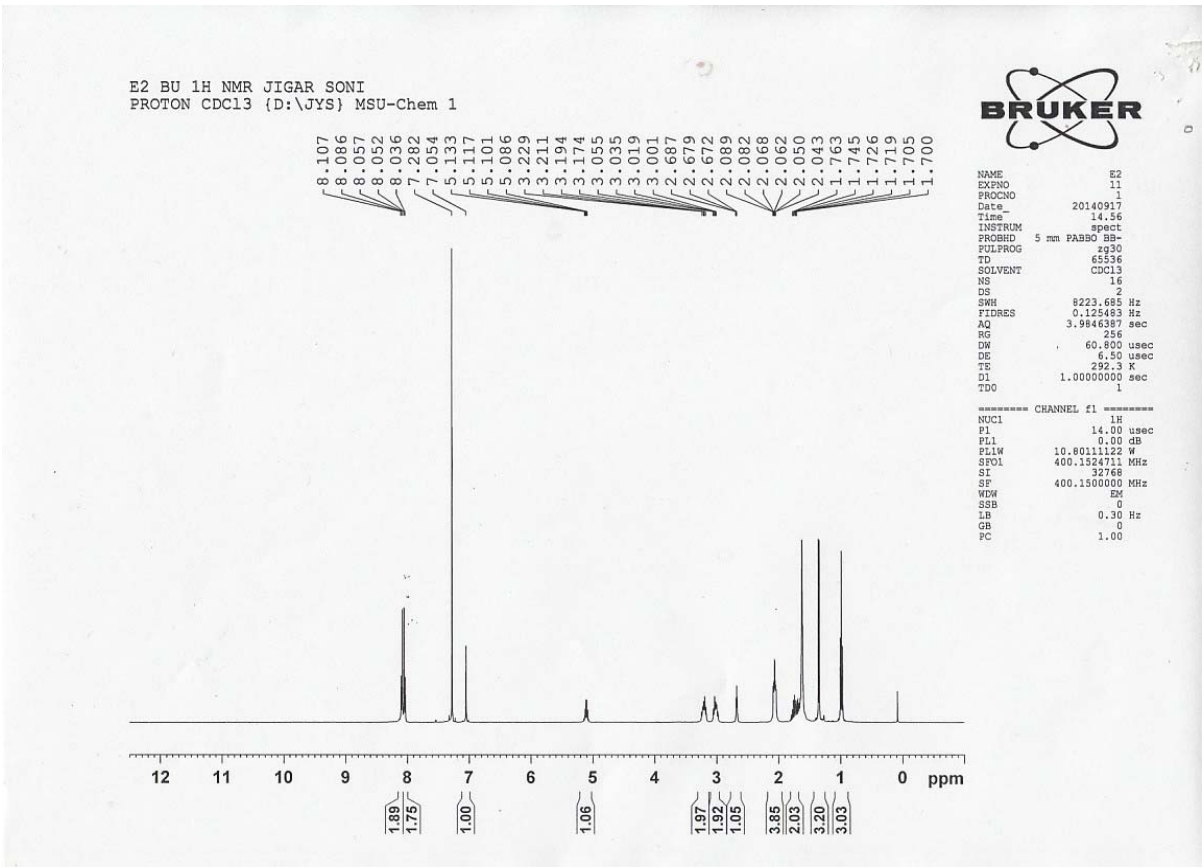
Isopropyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{1}H NMR Expansion (5c)



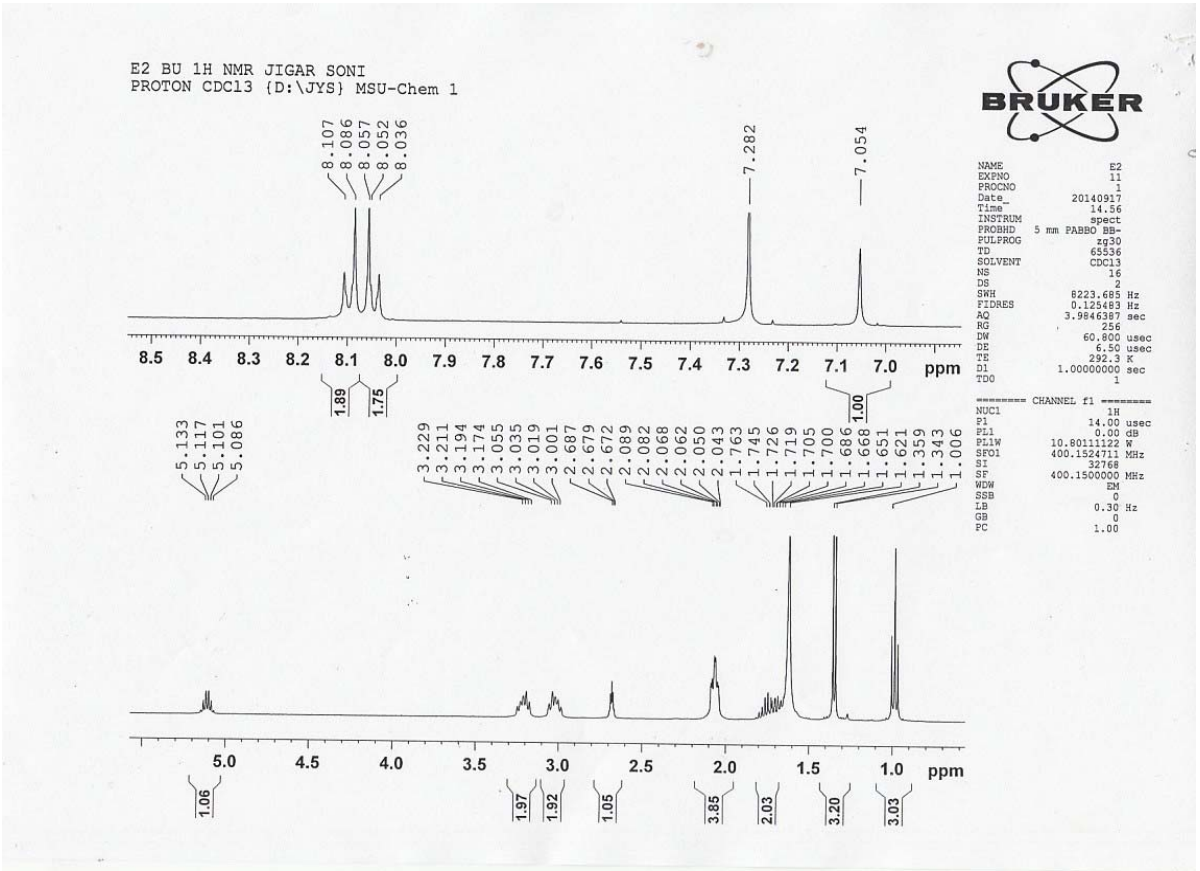
Isopropyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate (IPA) ^{13} C NMR (5c)



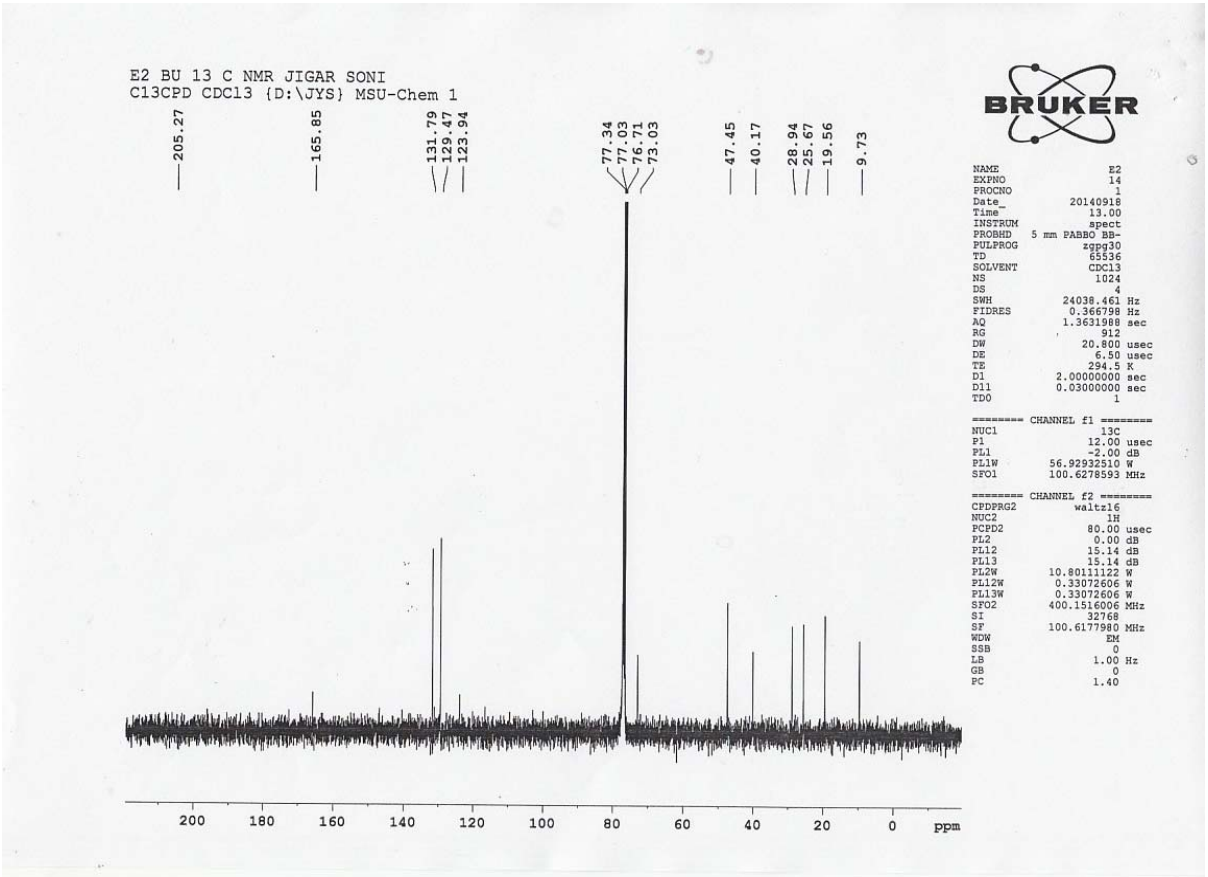
Sec-butyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{1}H NMR (5d)



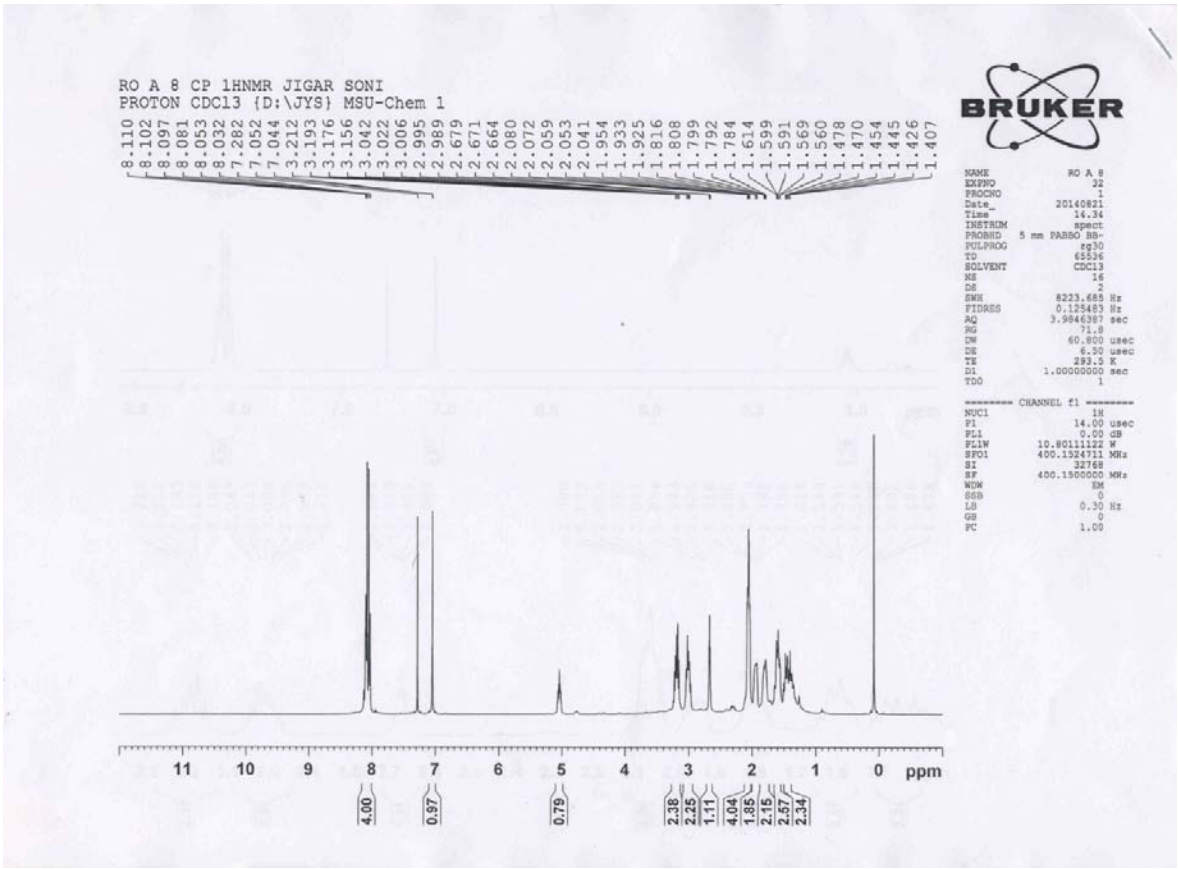
Sec-butyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{1}H NMR Expansion (5d)



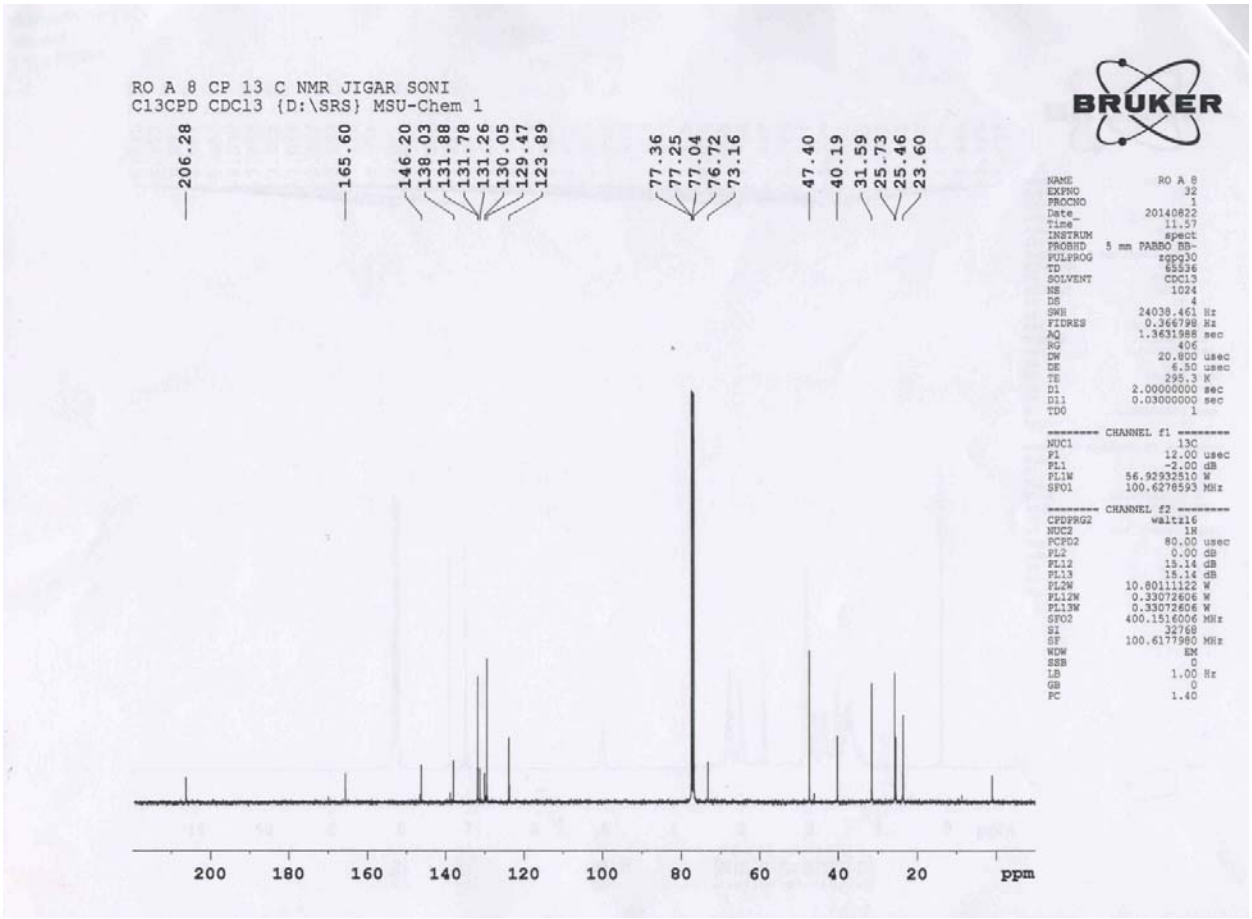
Sec-butyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{13}CNMR (5d)



Cyclopentyl(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{1}HNMR (5e)



Cyclopentyl(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ^{13}CNMR (5e)



Single crystal data of 4c

Table 1 Crystal data and structure refinement for exp_617.	
Identification code	exp_617
Empirical formula	$C_{16}H_{17}NO_3$
Formula weight	271.31
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	5.8724(3)
b/Å	8.1184(3)
c/Å	17.0501(10)
α/°	90.00
β/°	94.221(5)
γ/°	90.00
Volume/Å^3	810.64(7)
Z	2
ρ_{calc}g/cm^3	1.111
μ/mm^{-1}	0.625
F(000)	288.0
Crystal size/mm^3	0.32 × 0.25 × 0.23
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.4 to 146.2
Index ranges	$-7 \leq h \leq 6$, $-10 \leq k \leq 5$, $-21 \leq l \leq 18$
Reflections collected	3740
Independent reflections	2183 [R_{int} = 0.0305, R_{sigma} = 0.0336]
Data/restraints/parameters	2183/8/201
Goodness-of-fit on F^2	1.310
Final R indexes [I>=2σ (I)]	R_1 = 0.0850, wR_2 = 0.2430
Final R indexes [all data]	R_1 = 0.0878, wR_2 = 0.2507
Largest diff. peak/hole / e Å^{-3}	0.86/-0.24
Flack parameter	-0.2(7)

Single crystal data of 5c

Table 1 Crystal data and structure refinement for exp_592.	
Identification code	exp_592
Empirical formula	$C_{21}H_{19}BrN_2O_2$
Formula weight	411.29
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	9.1410(4)
b/Å	9.6496(7)
c/Å	11.1631(8)
α/°	75.954(6)
β/°	80.580(5)
γ/°	74.016(5)
Volume/Å^3	913.33(10)
Z	2
ρ_{calc}mg/mm^3	1.496
m/mm^{-1}	3.209
F(000)	420.0
Crystal size/mm^3	0.30 × 0.28 × 0.25
2Θ range for data collection	8.2 to 150.86°
Index ranges	$-8 \le h \le 11$, $-12 \le k \le 12$, $-13 \le l \le 13$
Reflections collected	6973
Independent reflections	3753[R(int) = 0.0313]
Data/restraints/parameters	3753/0/235
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0435, wR_2 = 0.1206
Final R indexes [all data]	R_1 = 0.0483, wR_2 = 0.1275
Largest diff. peak/hole / e Å^{-3}	0.72/-0.53