

Supporting information

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

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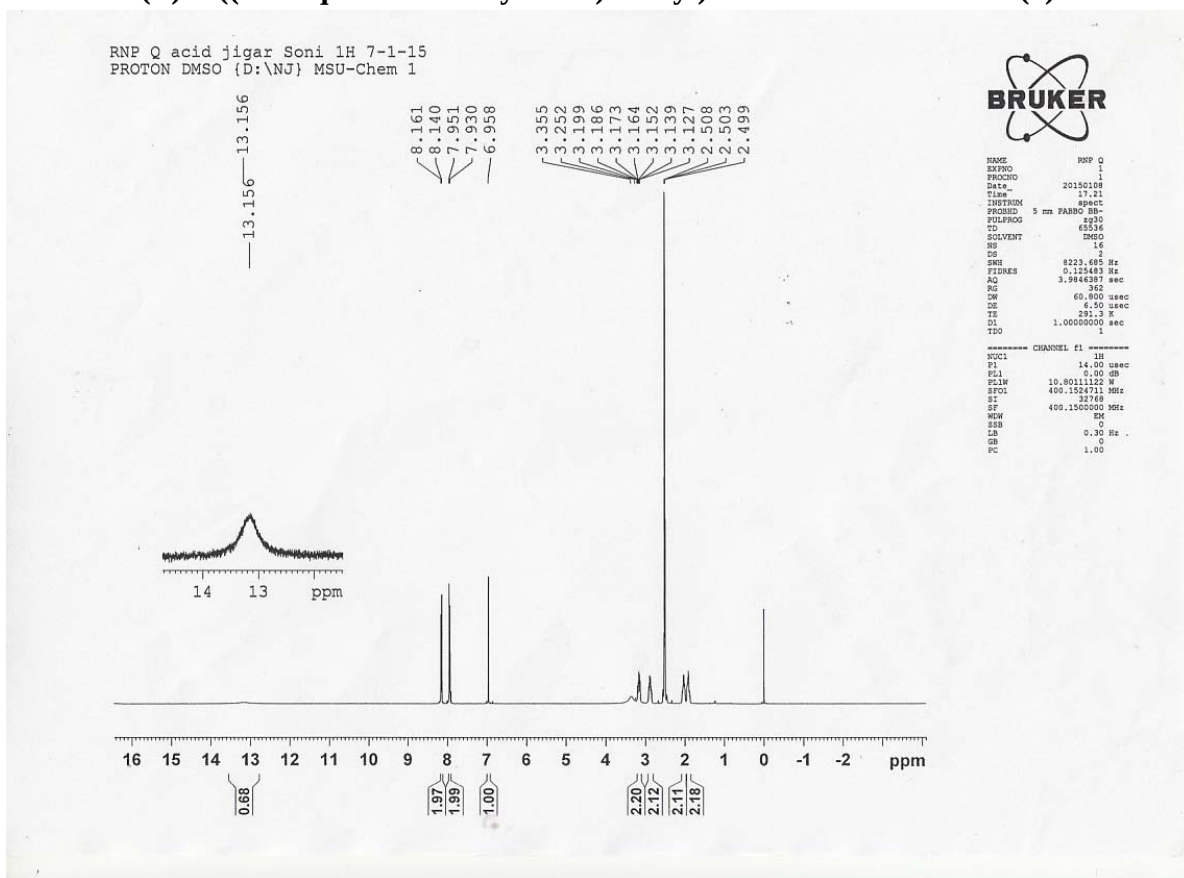
^aDepartment of Chemistry, Faculty of Science,

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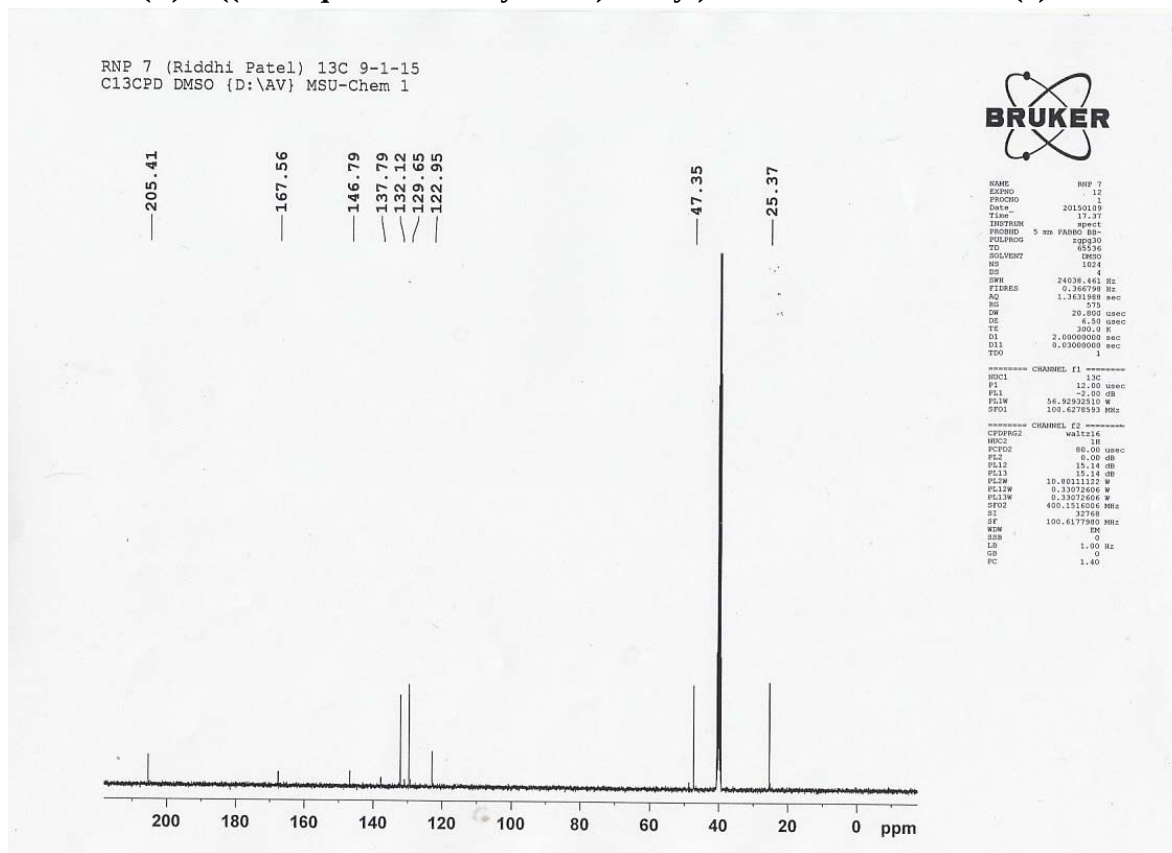
^bDepartment of Zoology, Faculty of Science

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

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

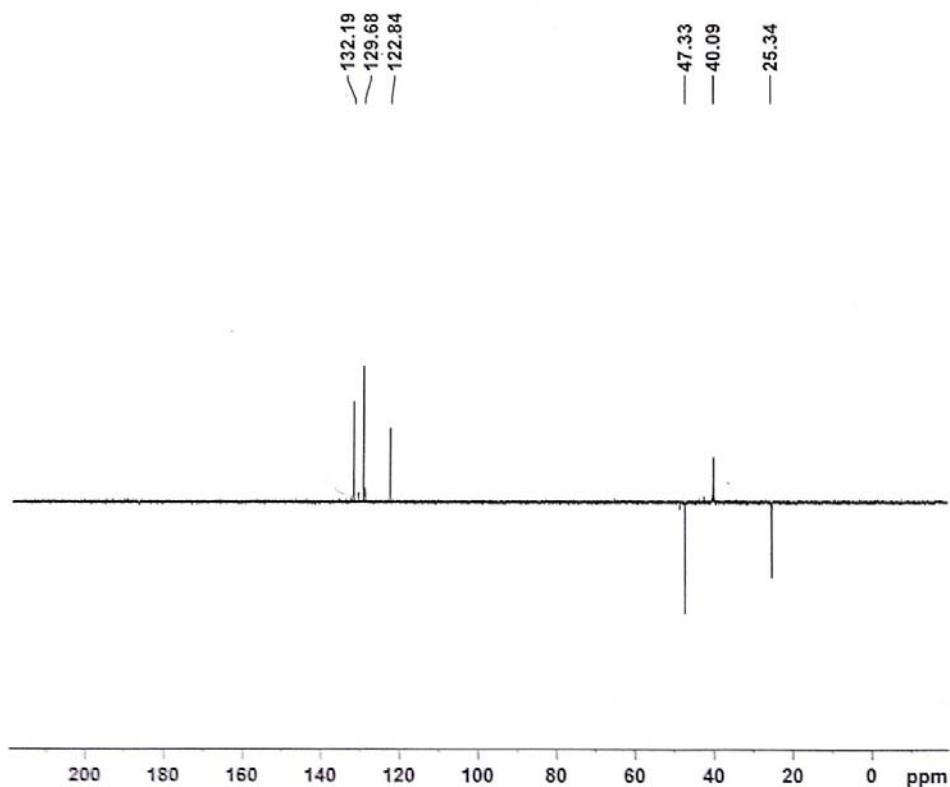


(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoic acid ¹³C NMR (3)



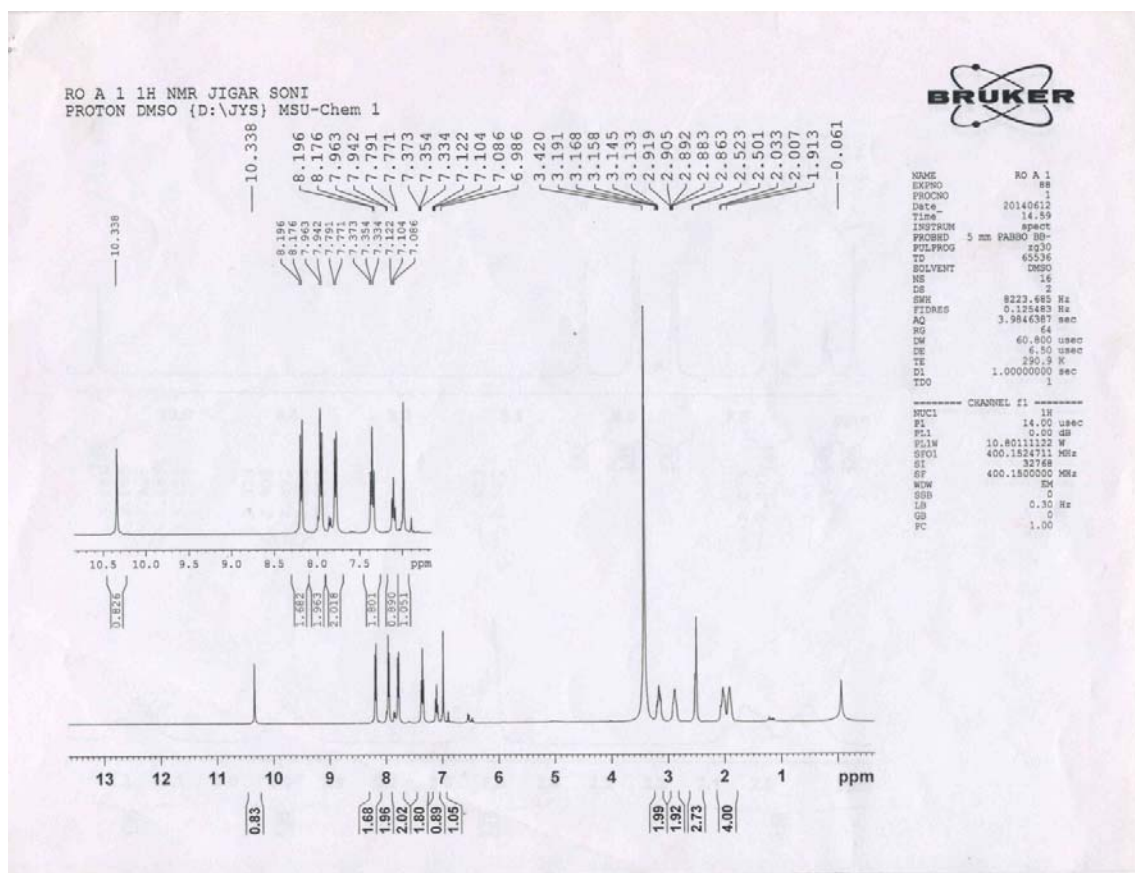
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoic acid DEPT-135 (3)

RNP-4 135DEPT RIDDHI PATEL 11-03-15
C13DEPT135 DMSO {D:\RT} MSU-Chem 1

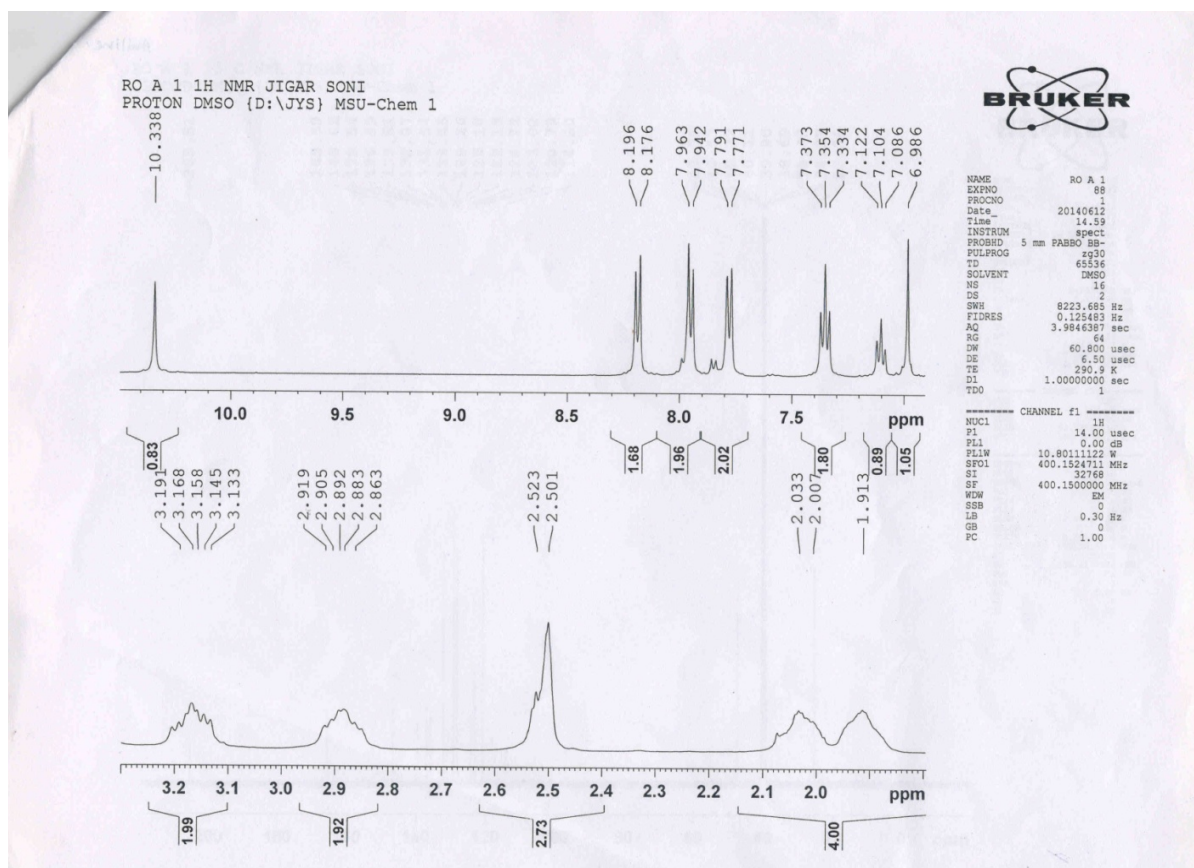


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PROCNO 1
Date_ 20150311
Time 19.32
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TD 65536
SOLVENT DMSO
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DS 4
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FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
SW 20.800 usec
DE 6.50 usec
TE 294.3 K
CHST2 145.000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00000000 sec
TD0 1
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P2 24.00 usec
PL1 -2.00 dB
PL1W 56.92932810 W
SFO1 100.6278593 MHz
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CPDPRG2 waltz16
NUC2 1H
P3 14.00 usec
P4 28.00 usec
PCPD2 80.00 usec
PL3 0.00 dB
PL12 18.14 dB
PL1W 10.80111122 W
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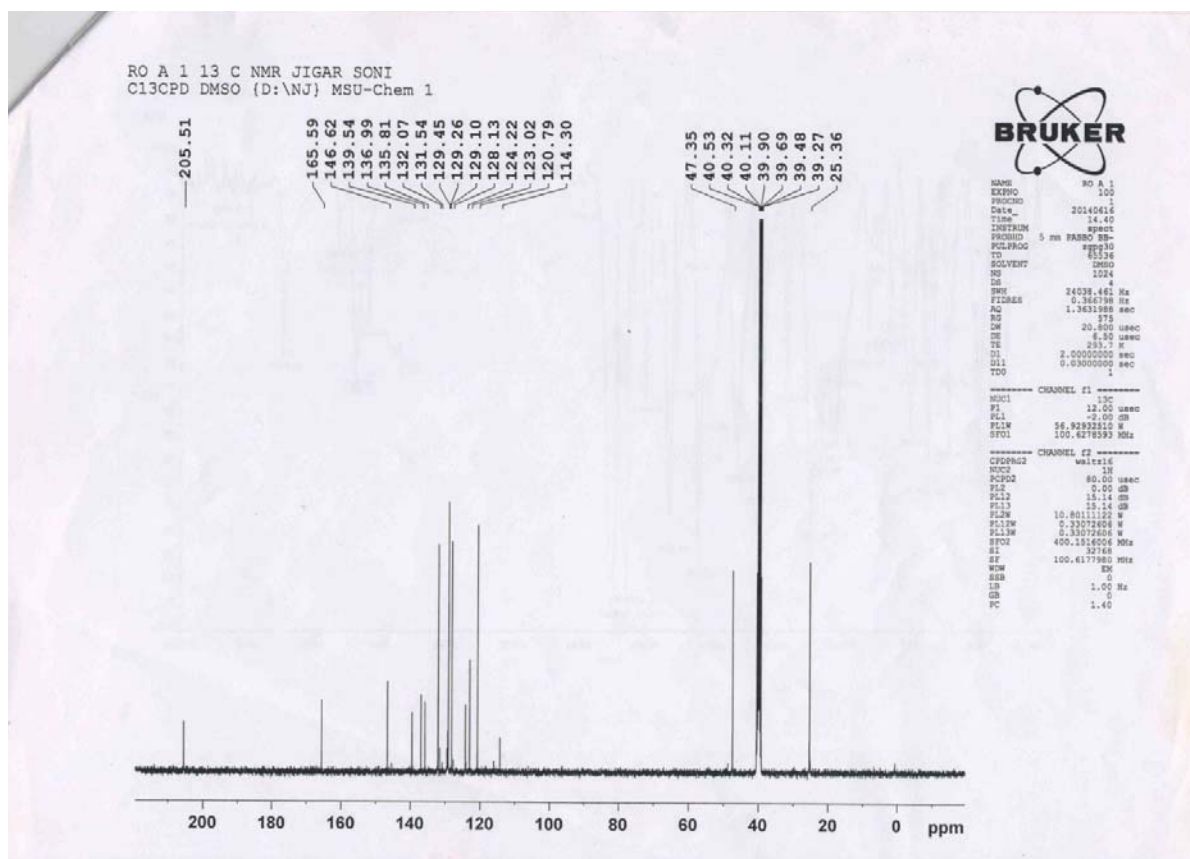
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-phenylbenzamide ¹H NMR (4a)



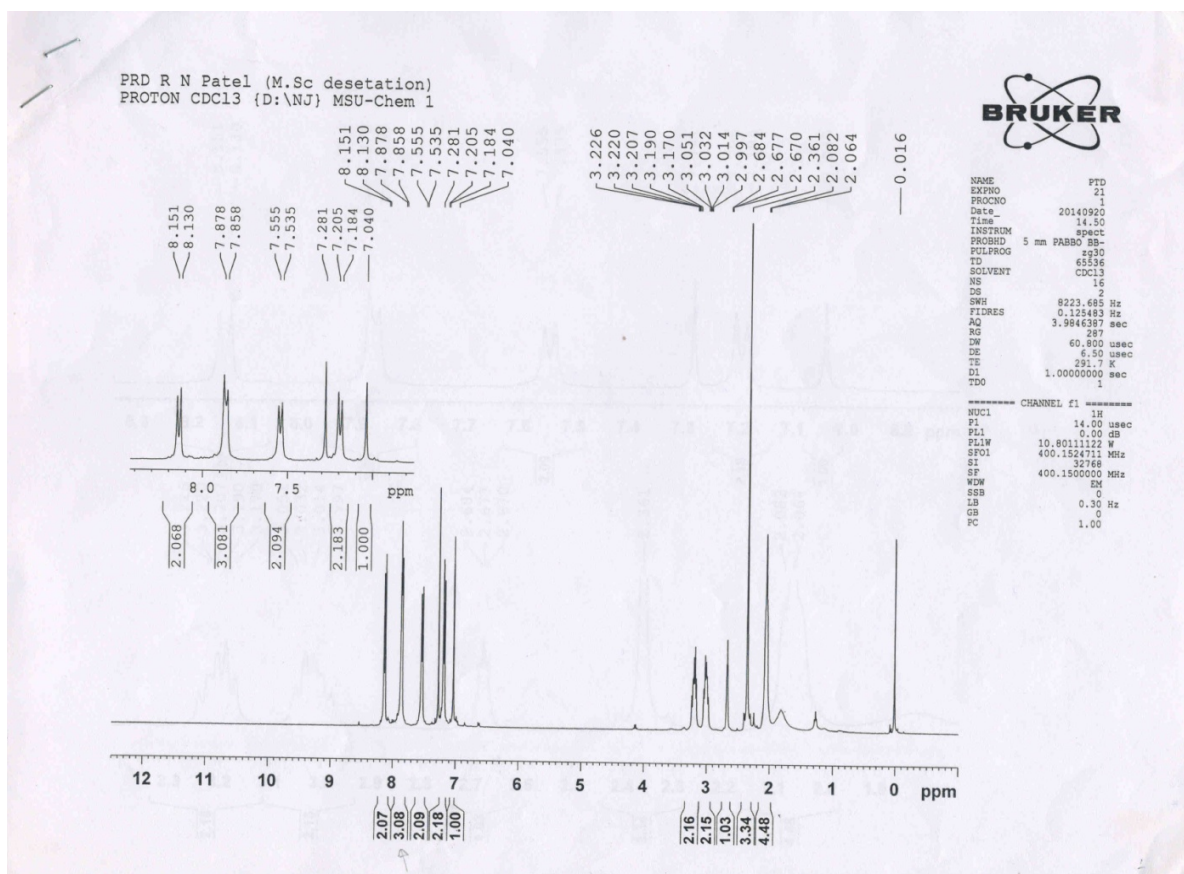
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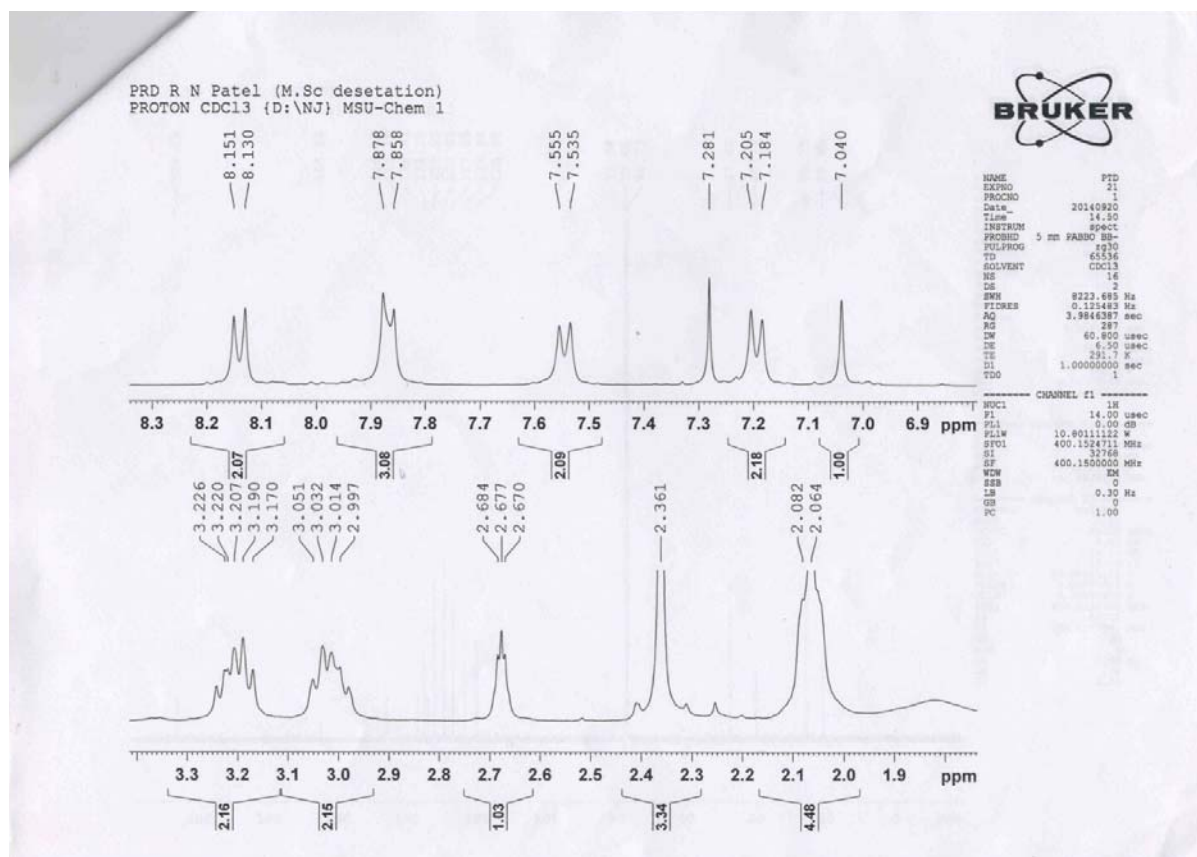
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-phenylbenzamide ¹³C NMR (4a)



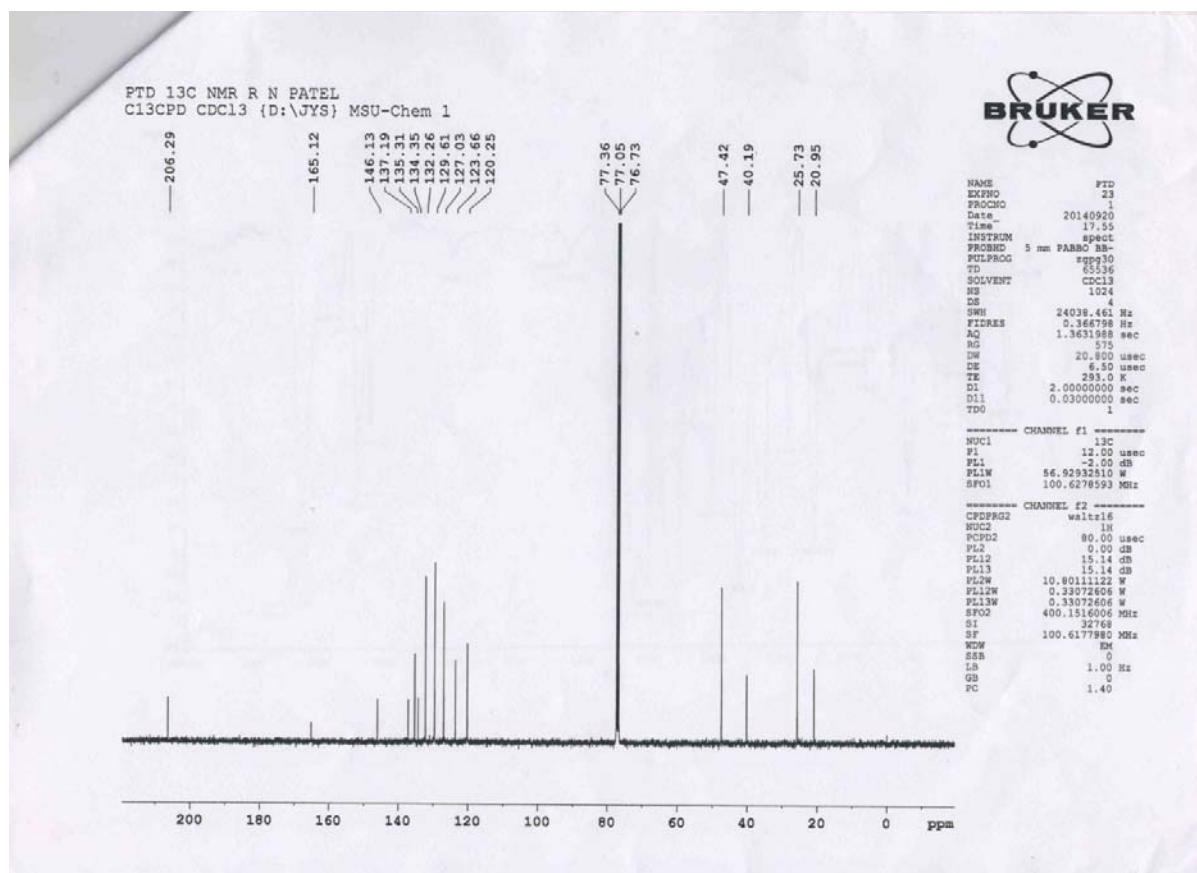
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-(p-tolyl)benzamide ¹H NMR(4b)



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



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



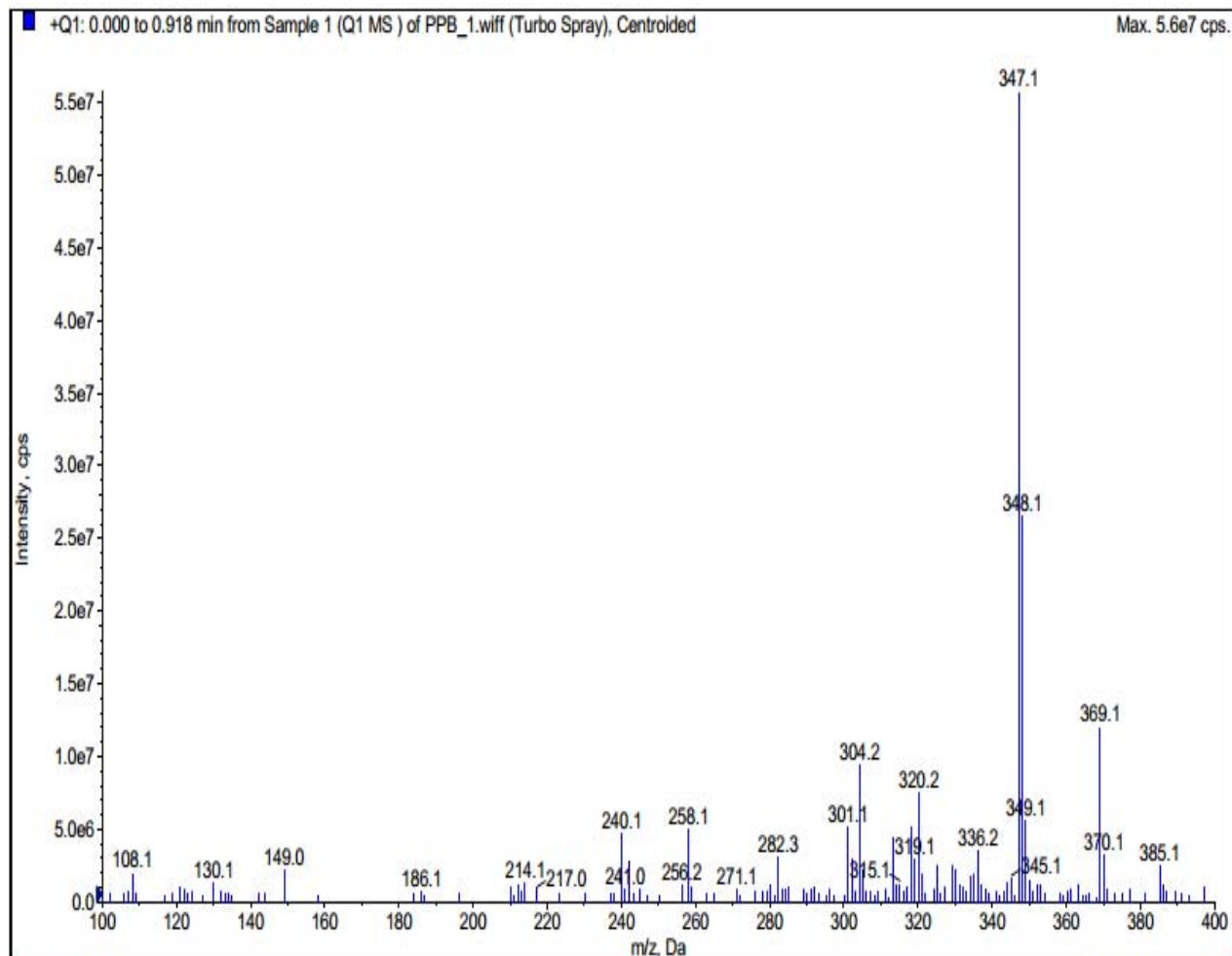
(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)-N-(p-tolyl)benzamide Mass Spectra

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Analyst Version: 1.6.2

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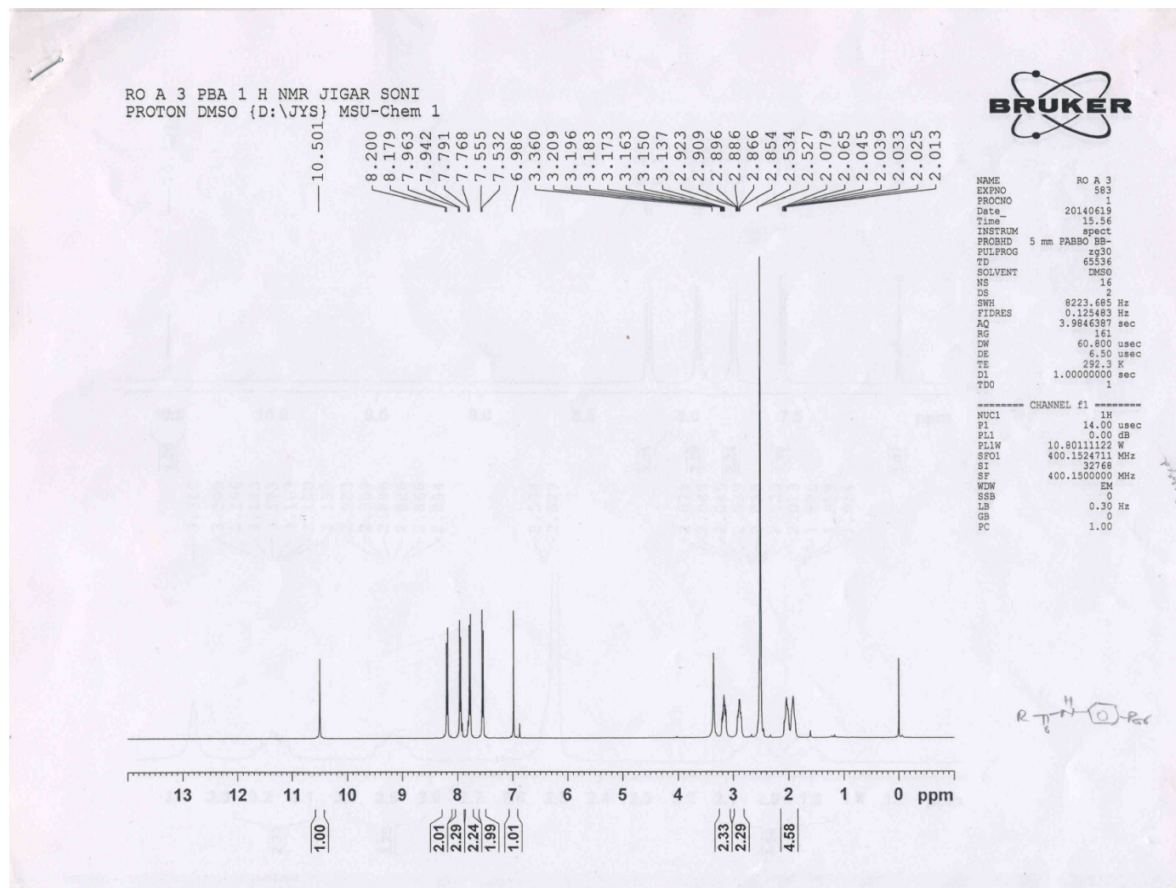
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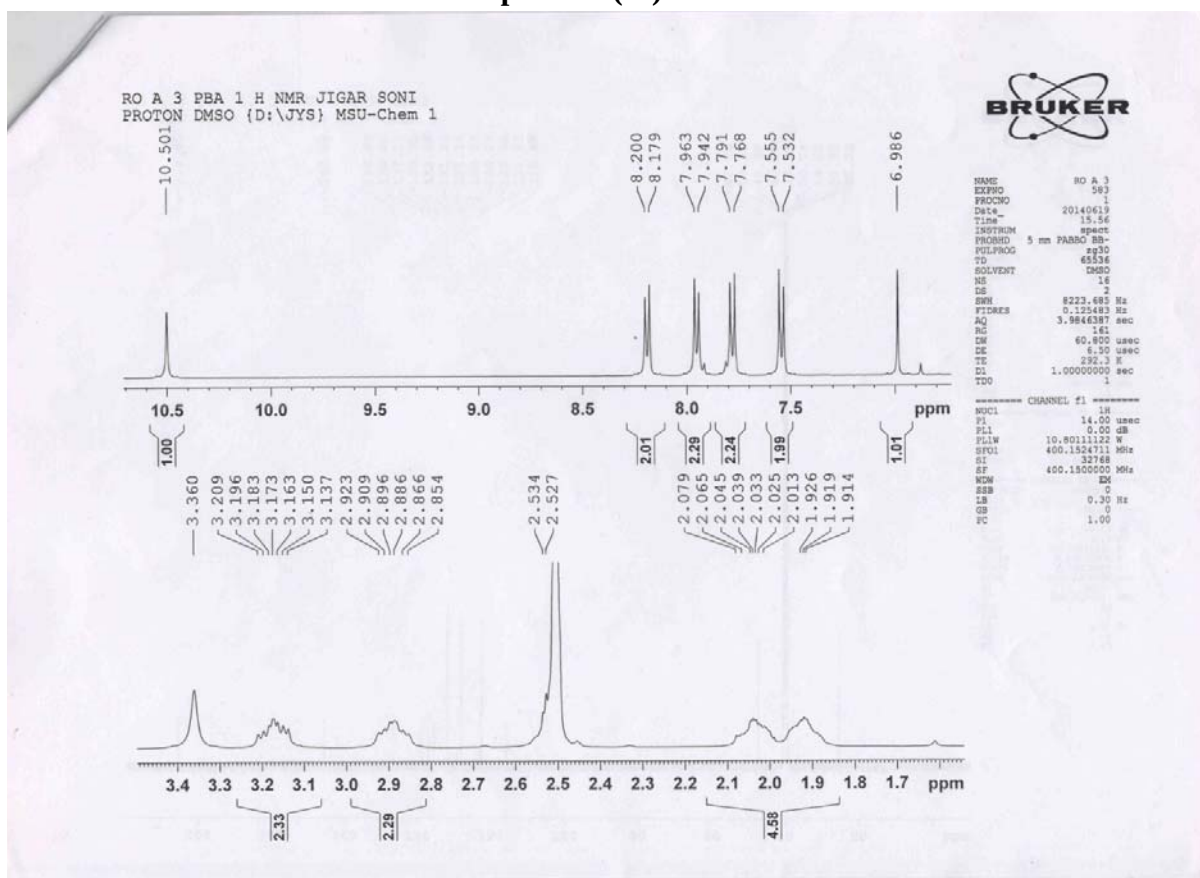
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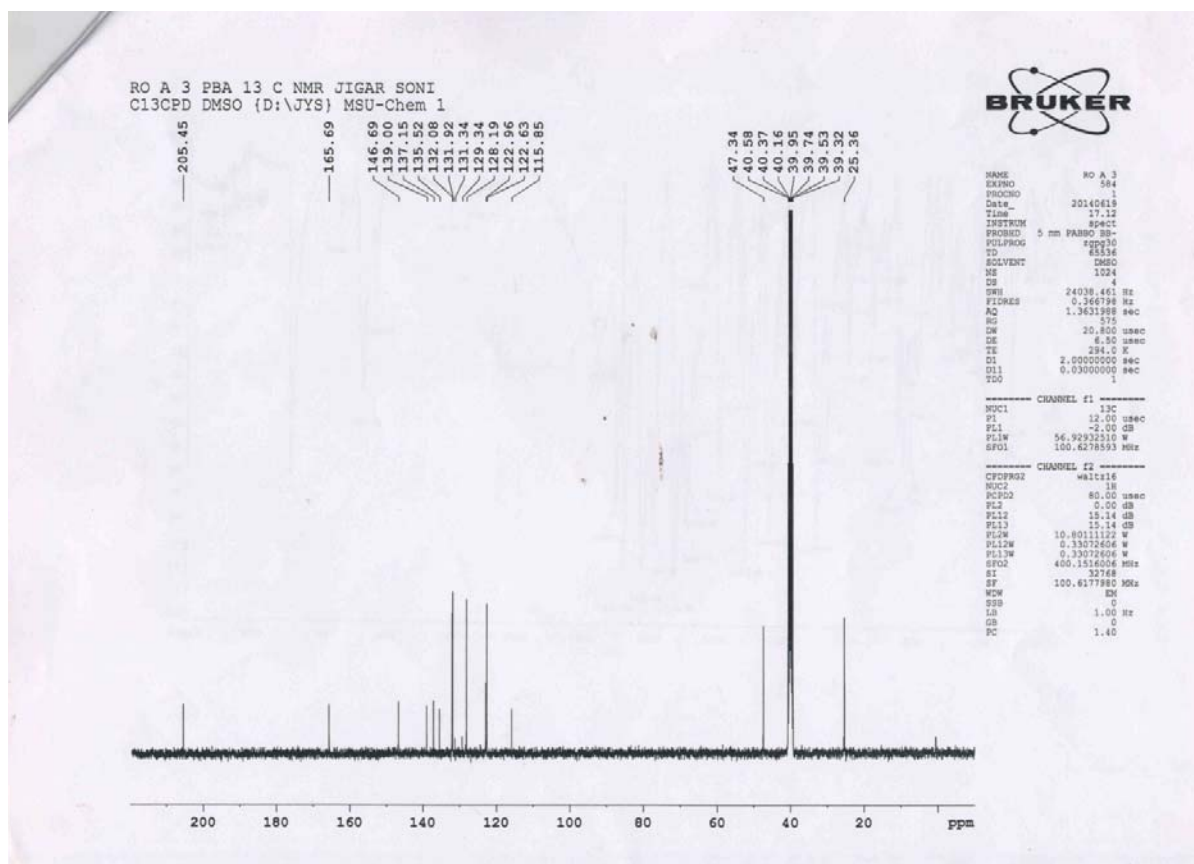
**(Z)-N-(4bromophenyl)-4-((3-oxoquinuclidin-2-ylidene)methyl) benzamide ¹H NMR
(4c)**



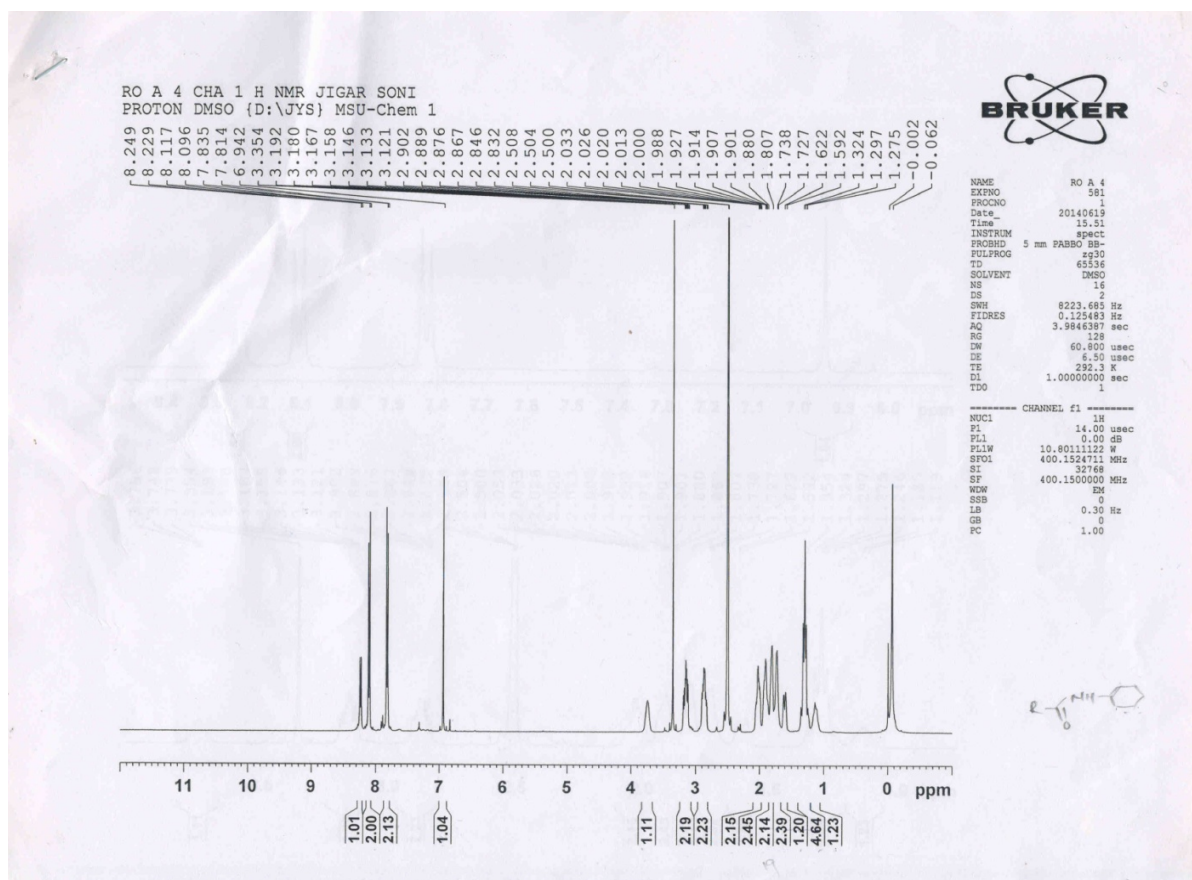
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Expansion (4c)



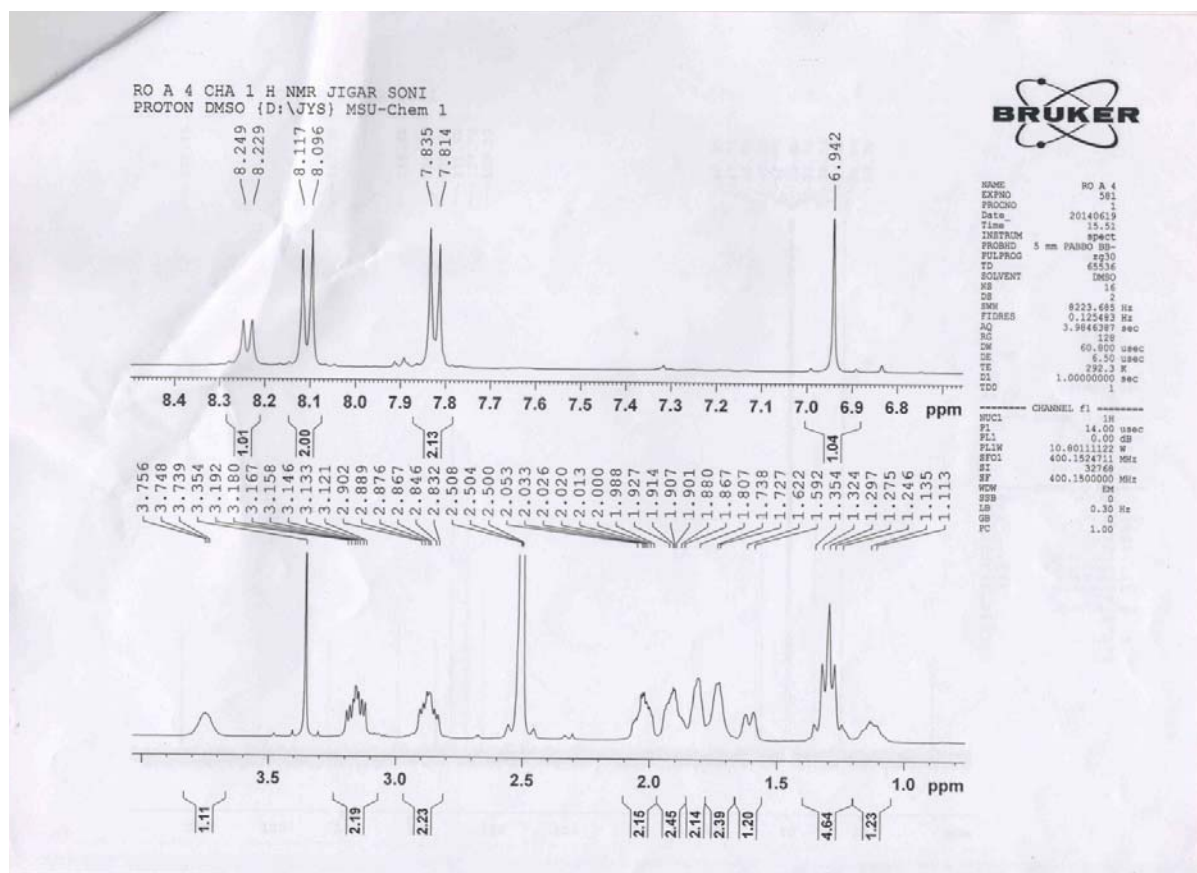
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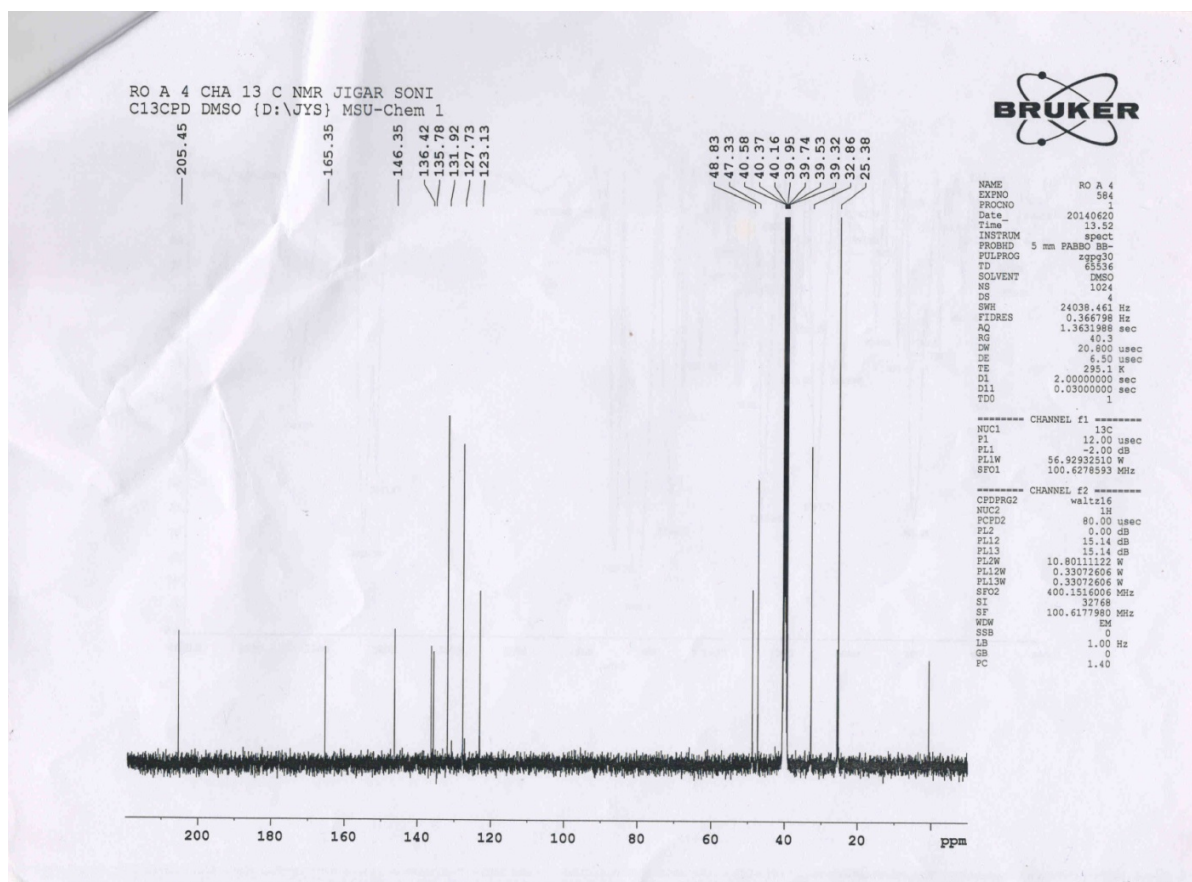
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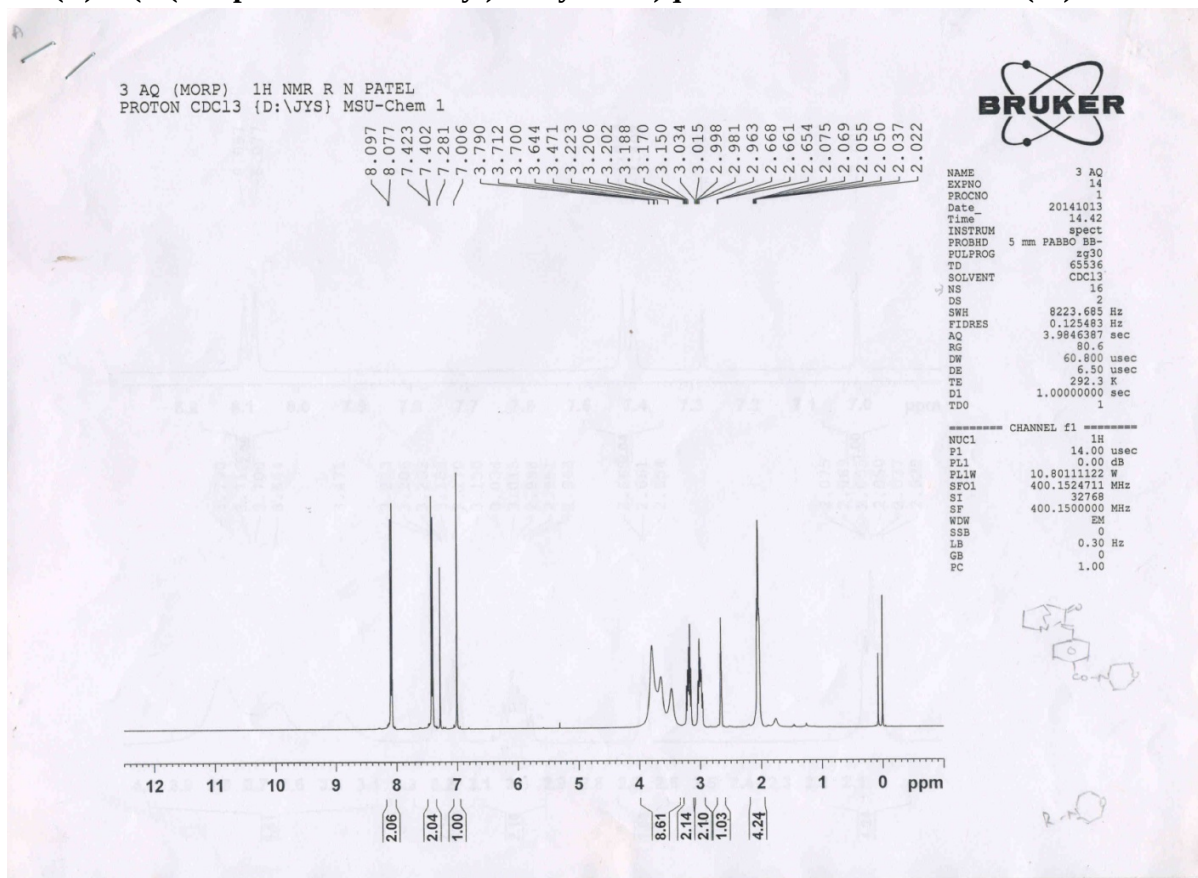
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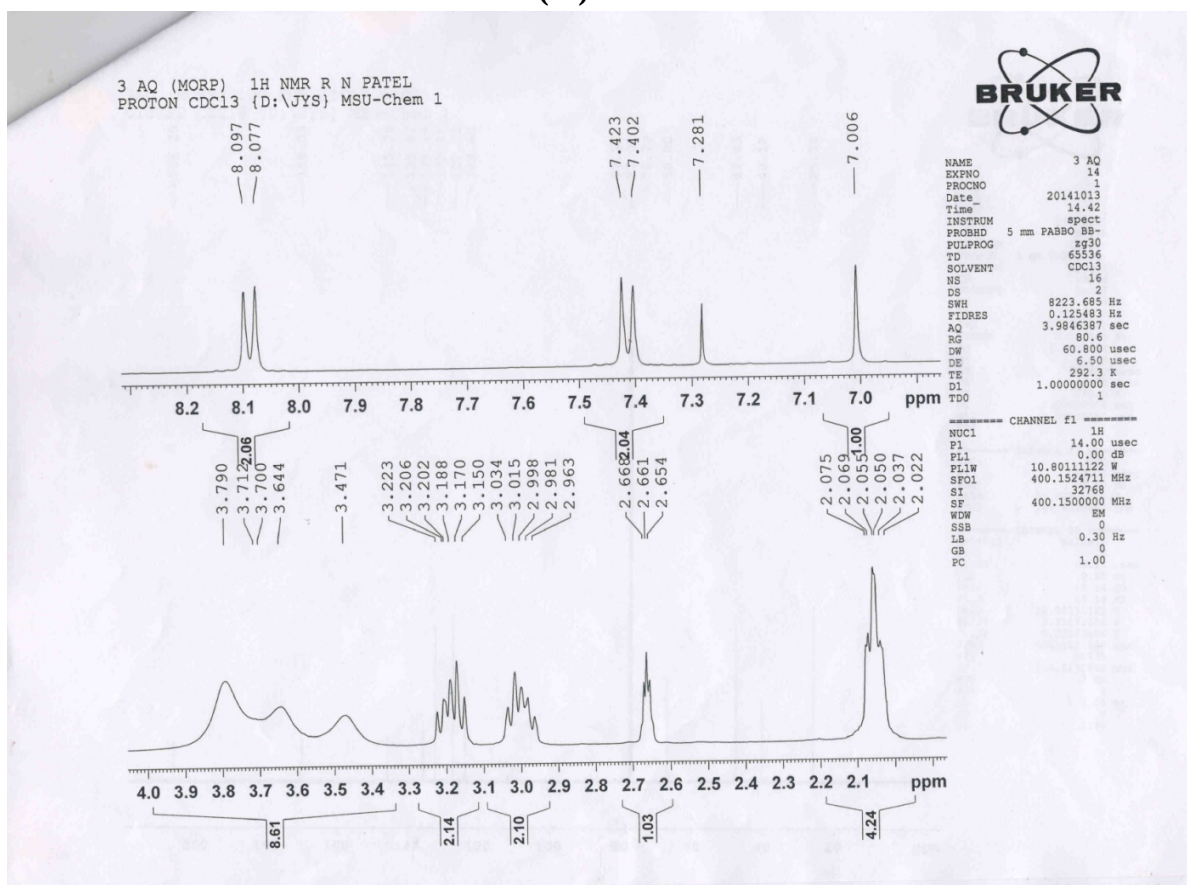
(Z)-N-cyclohexyl-4-((3-oxoquinuclidin-2-ylidene)methyl) benzamide ¹³C NMR (4d)



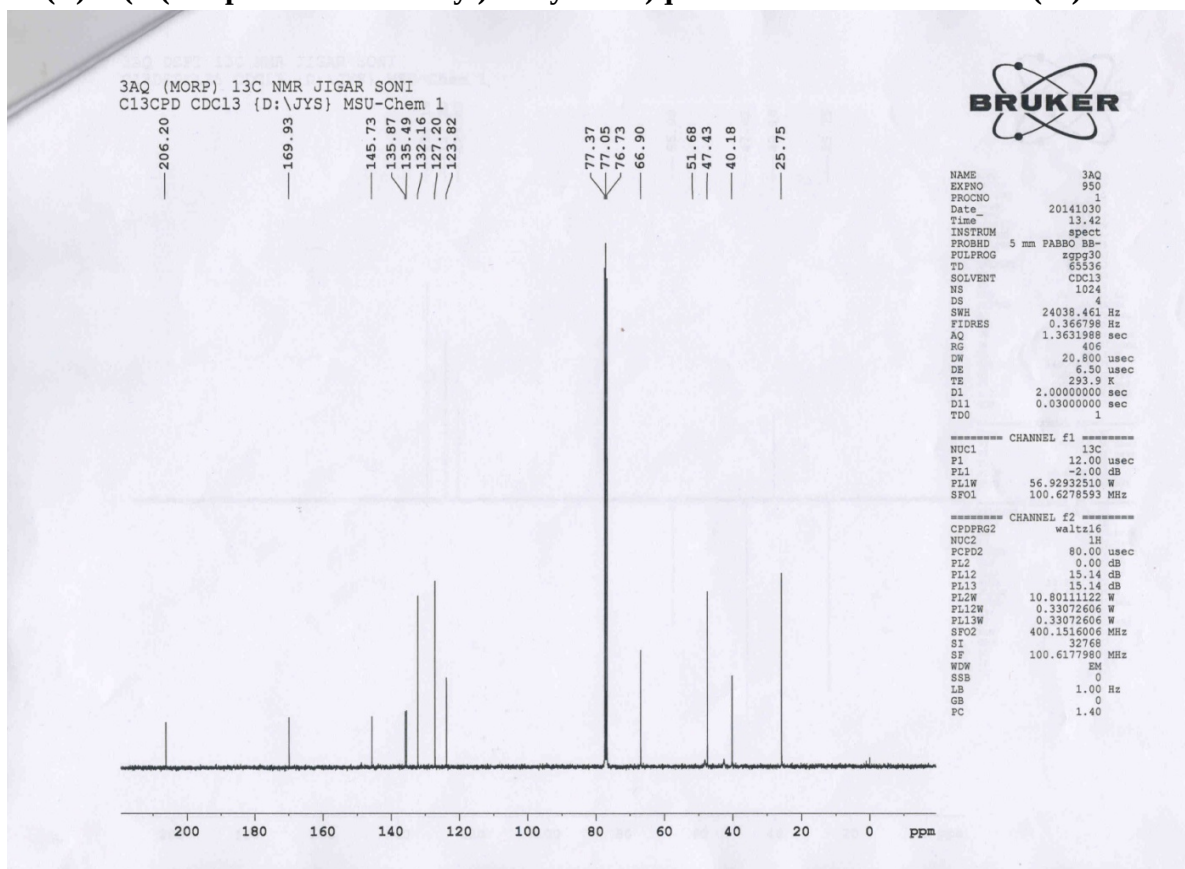
(Z)-2-(4-(morpholine-4-carbonyl)benzylidene)quinuclidin-3-one ¹H NMR (4e)



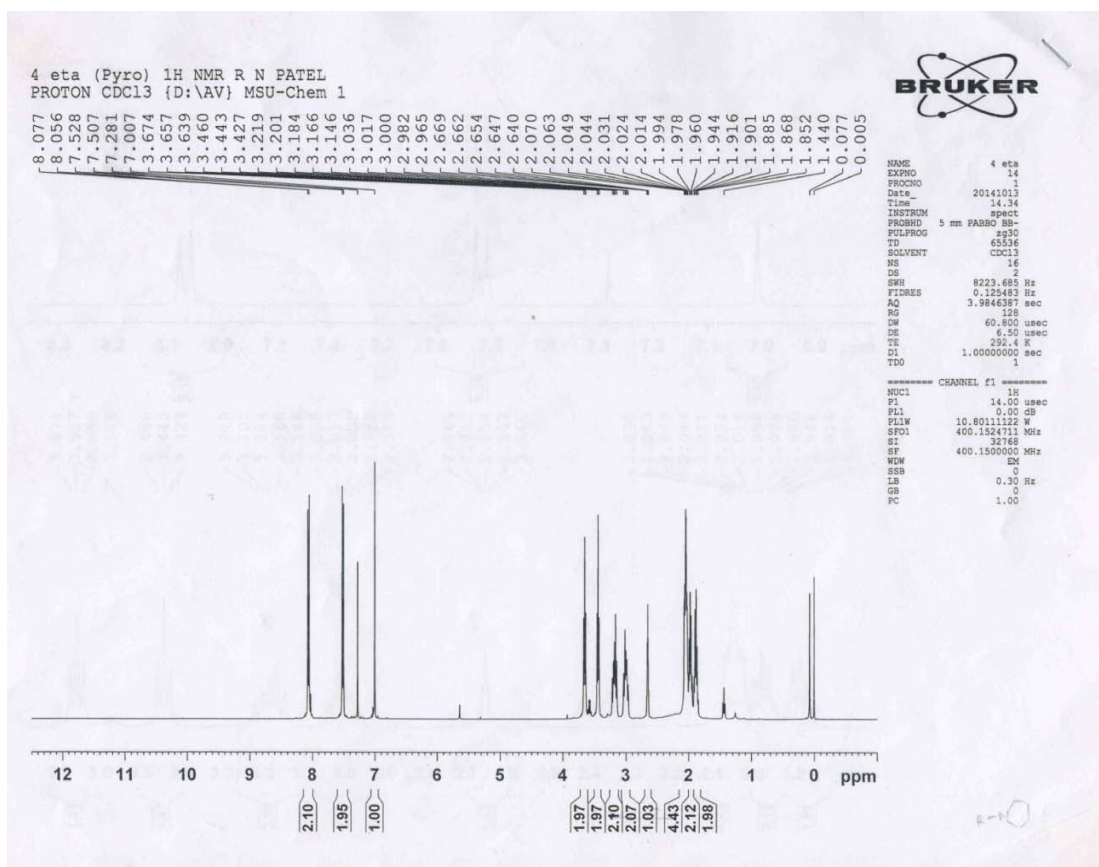
**(Z)-2-(4-(morpholine-4-carbonyl)benzylidene)quinuclidin-3-one ¹H NMR Expansion
(4e)**



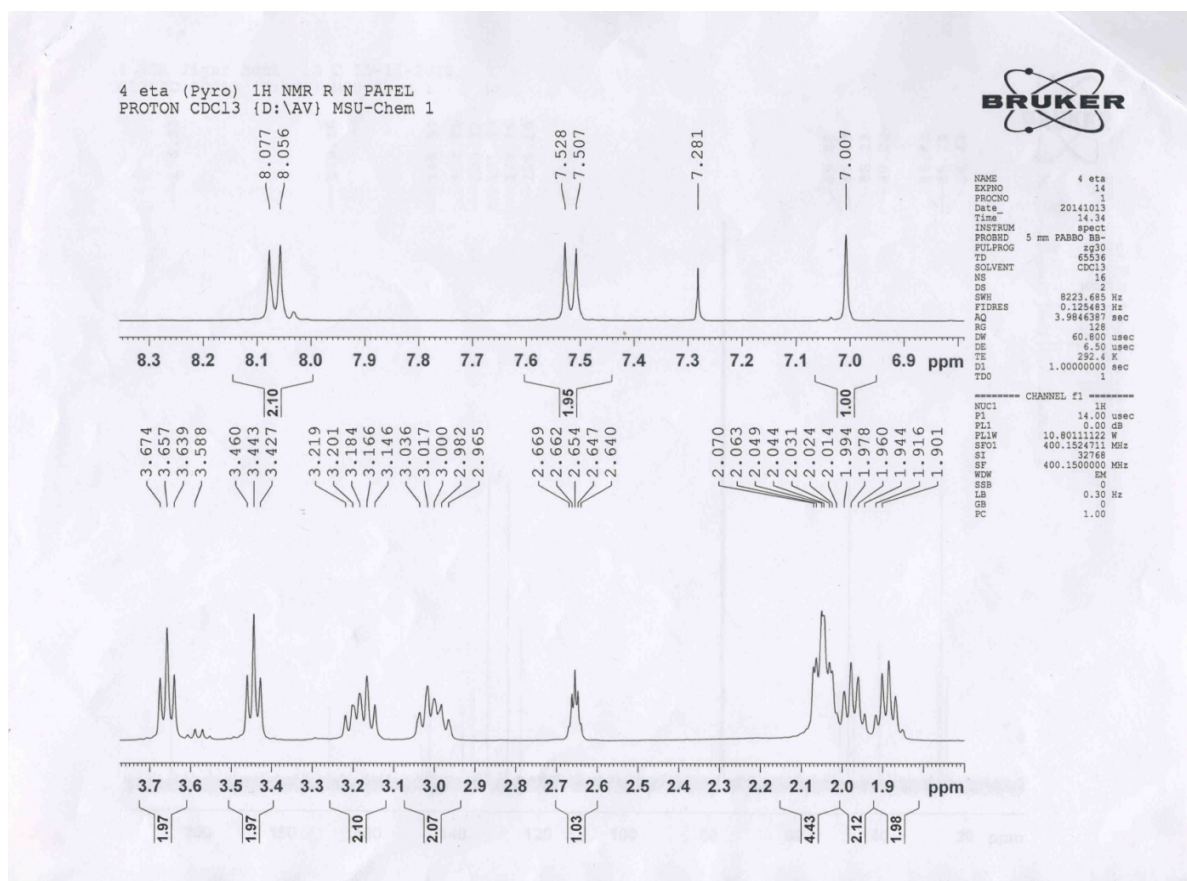
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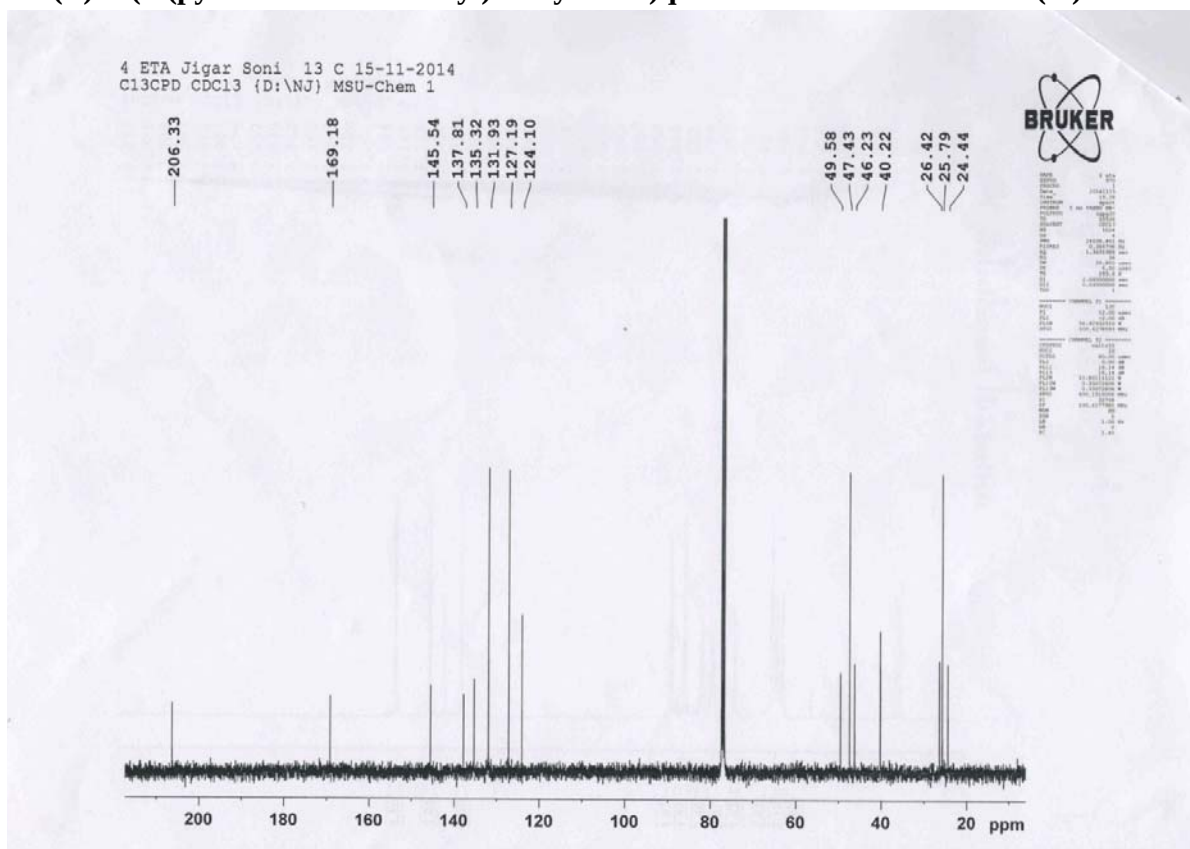
(Z)-2-(4-(pyrrolidine-1-carbonyl)benzylidene)quinuclidin-3-one ¹H NMR (4f)



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



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



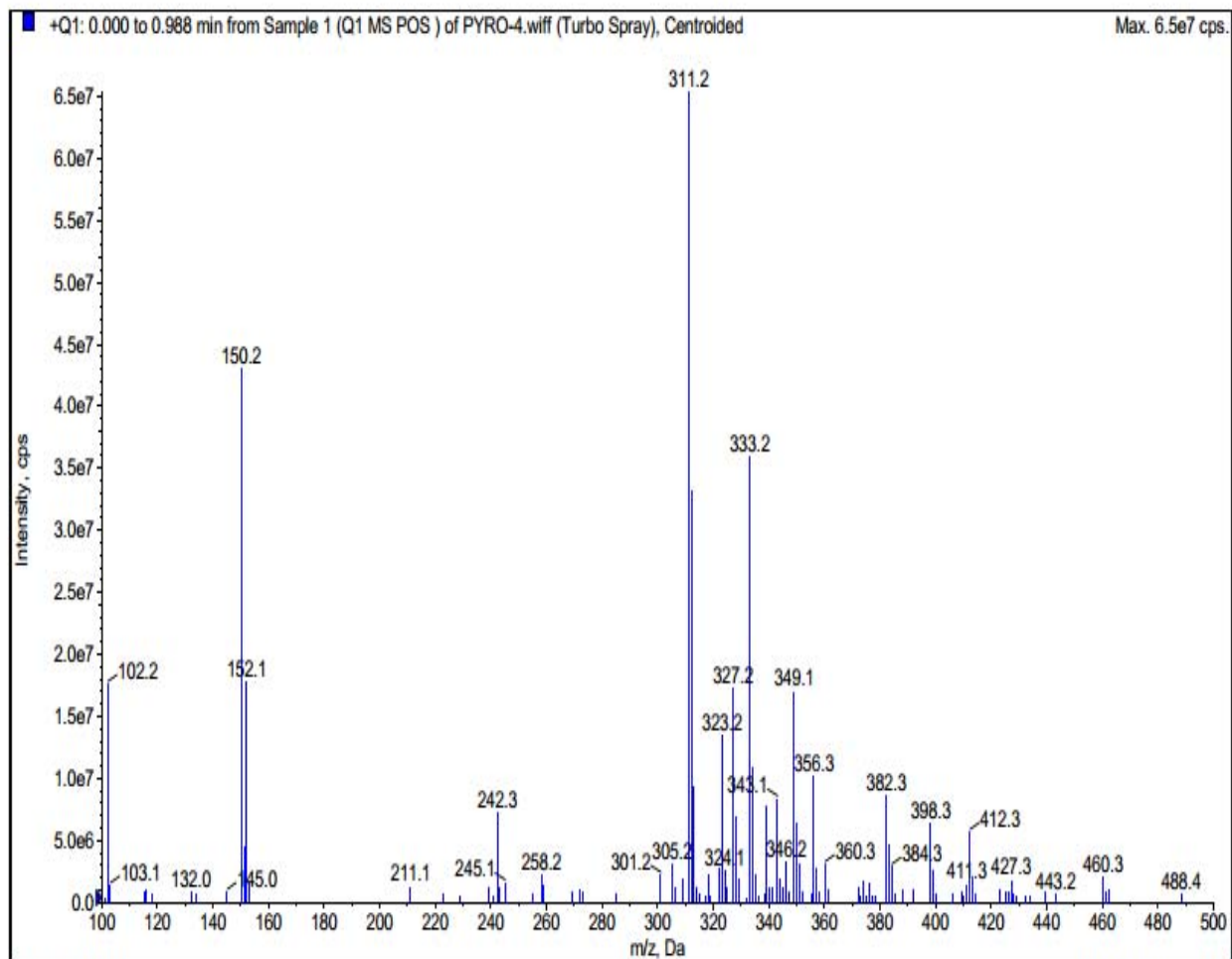
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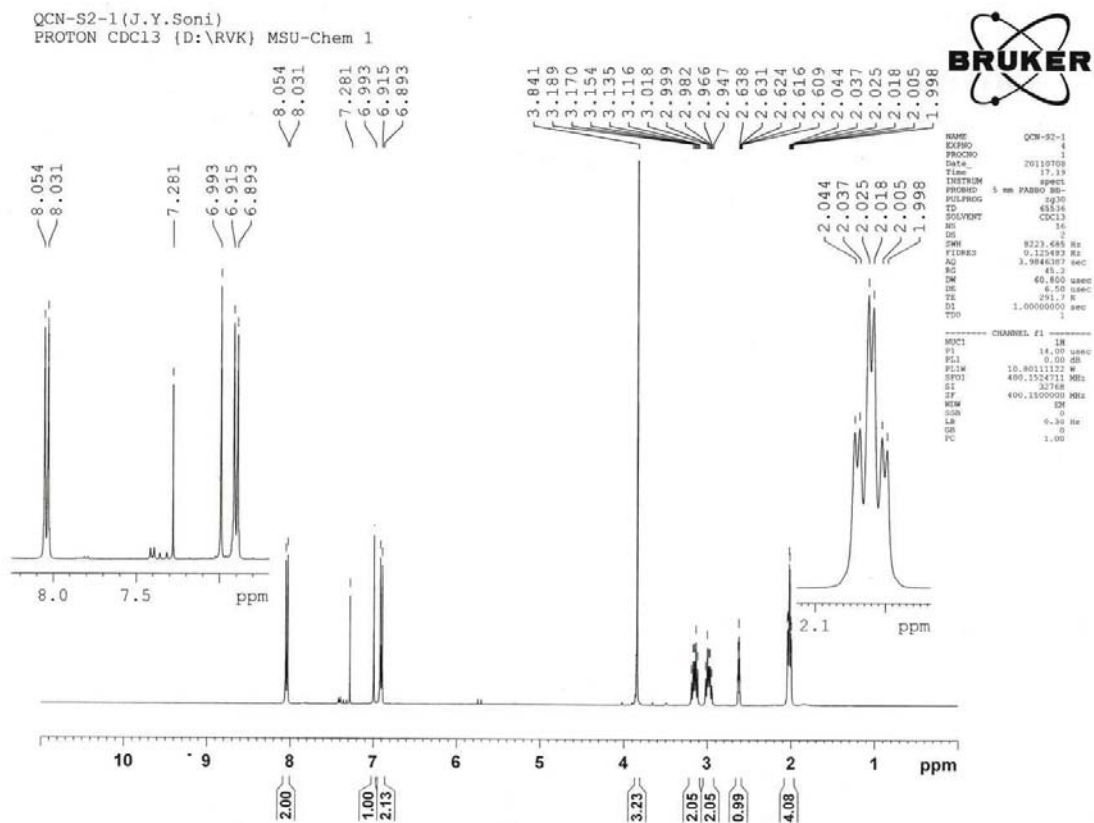
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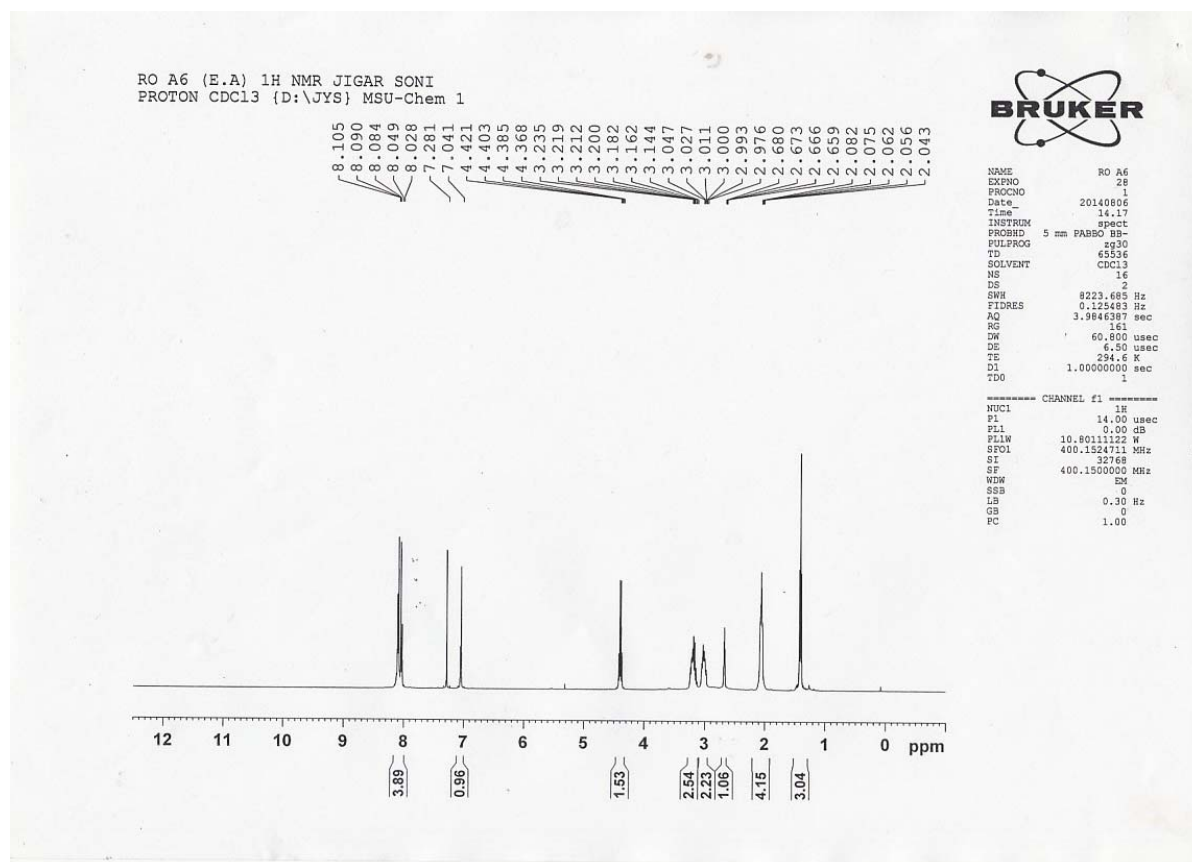
Methyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ¹H NMR (5a)



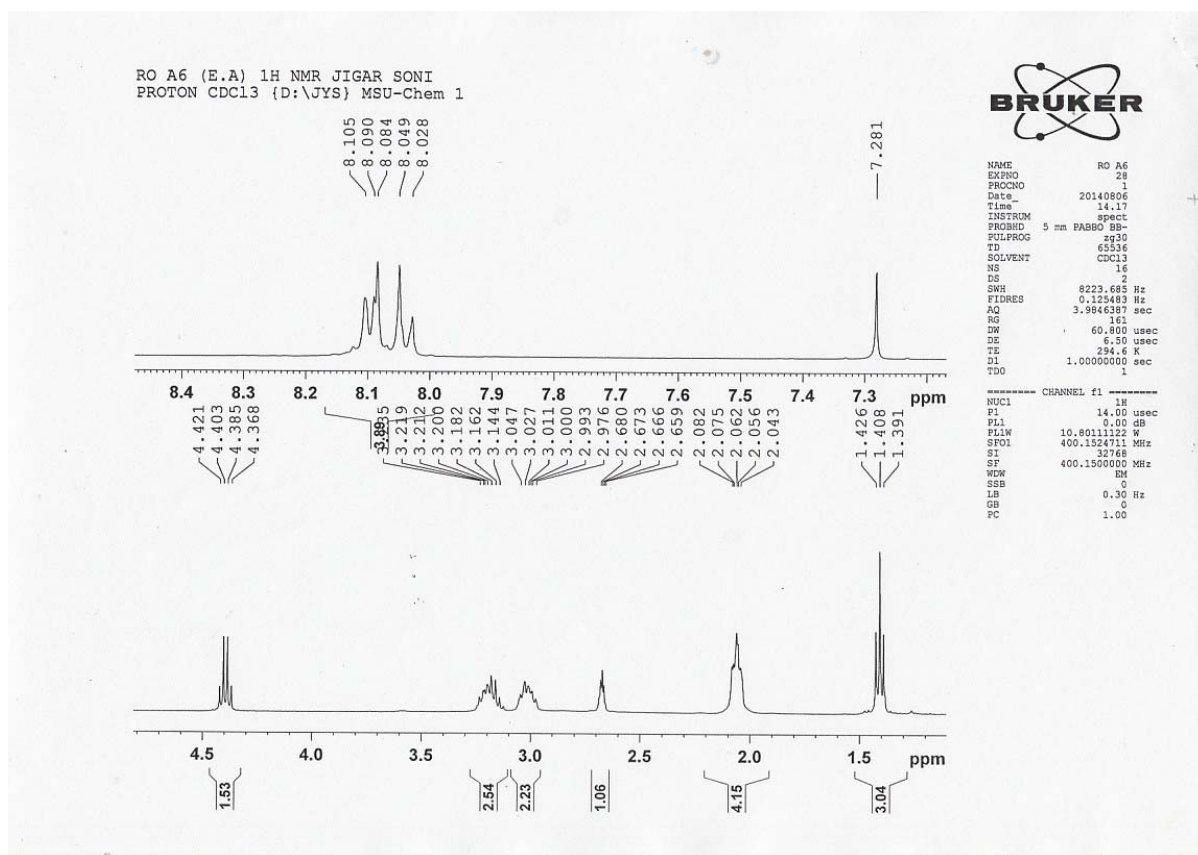
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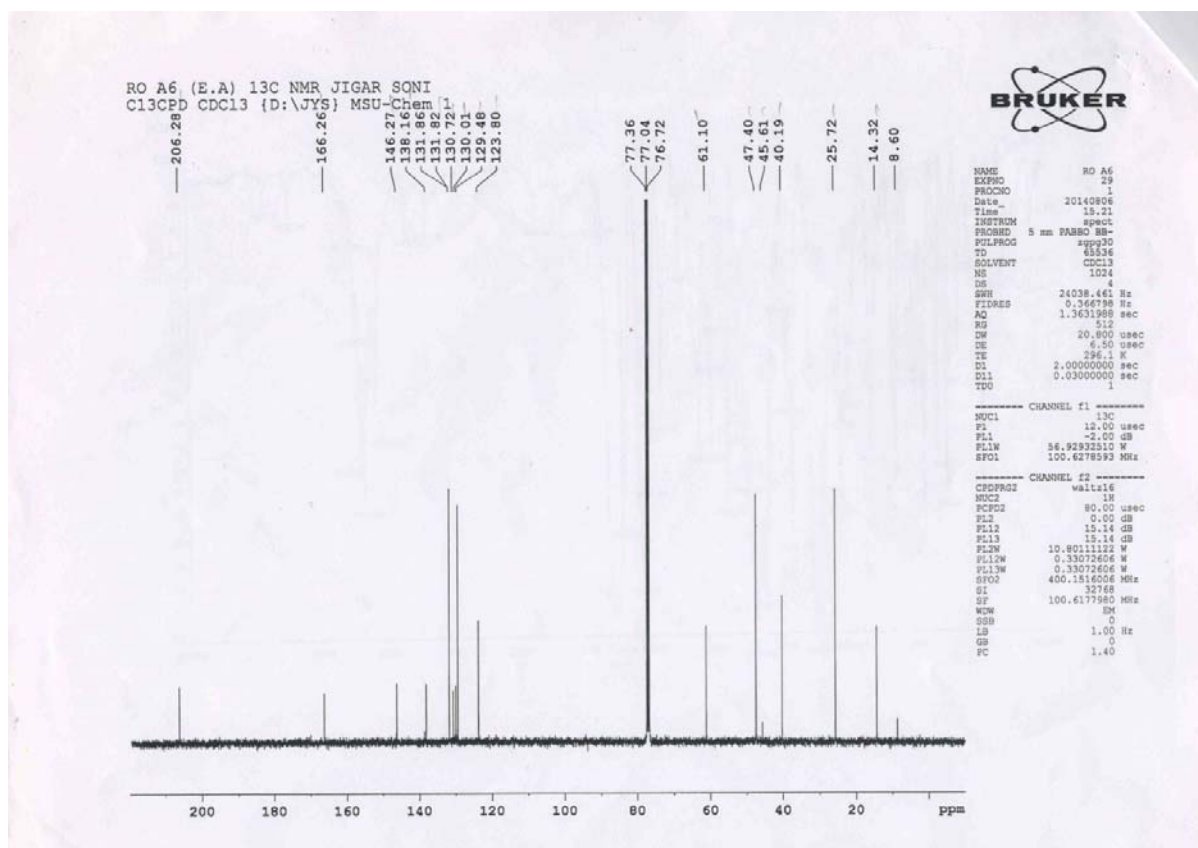
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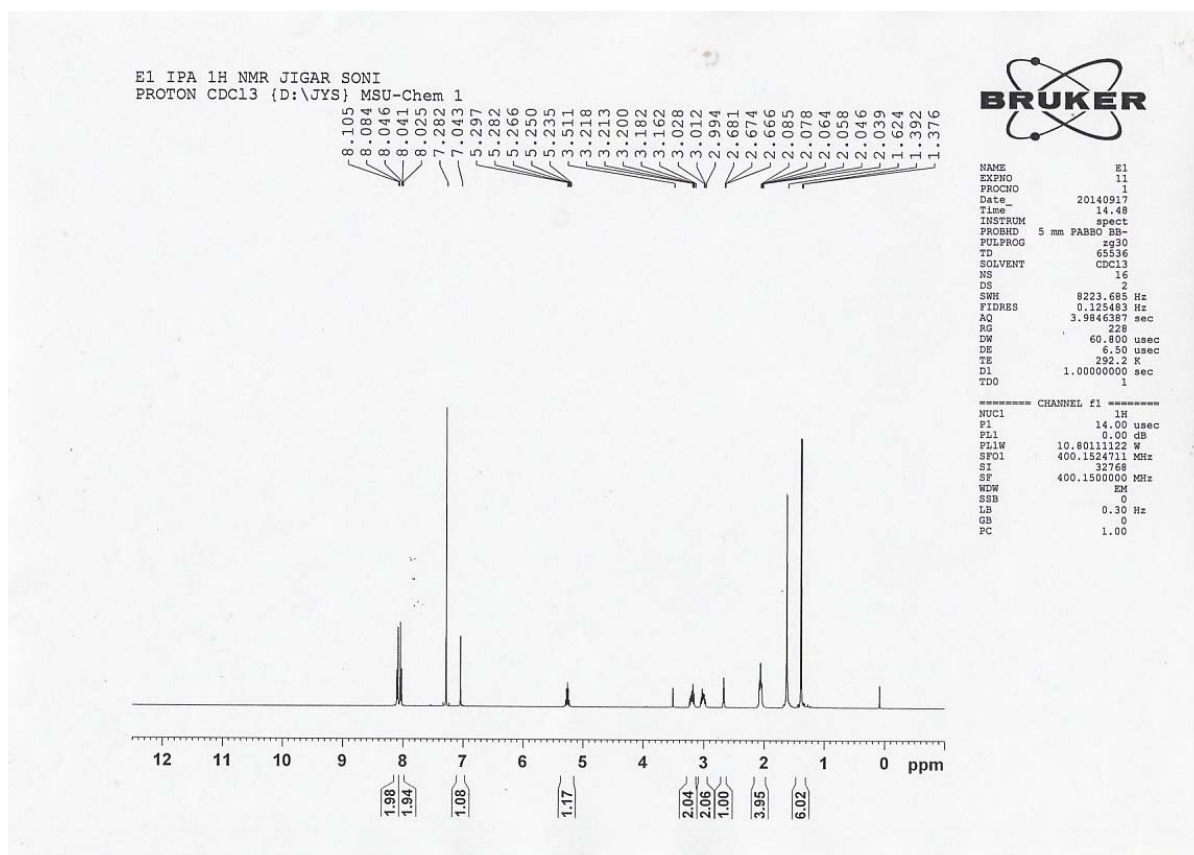
Ethyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ¹H NMR expansion (5b)



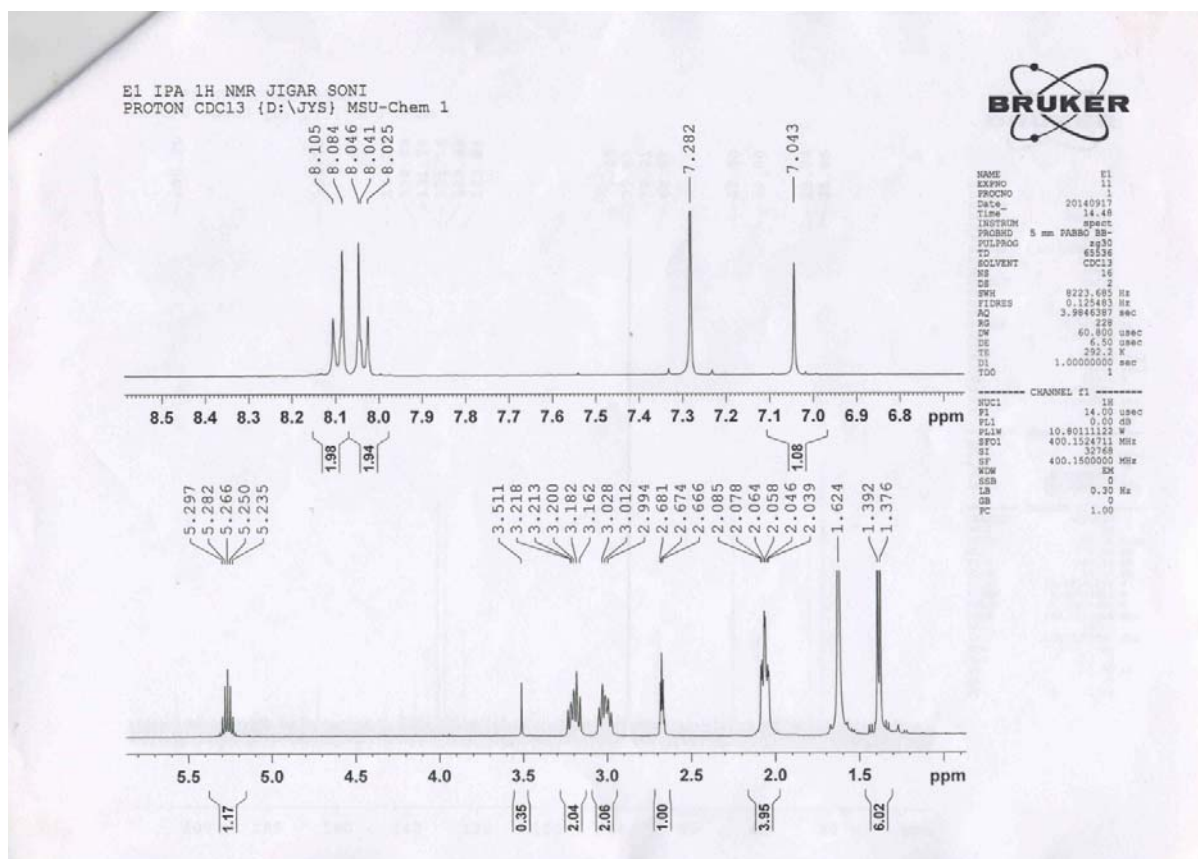
Ethyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ¹³C NMR (5b)



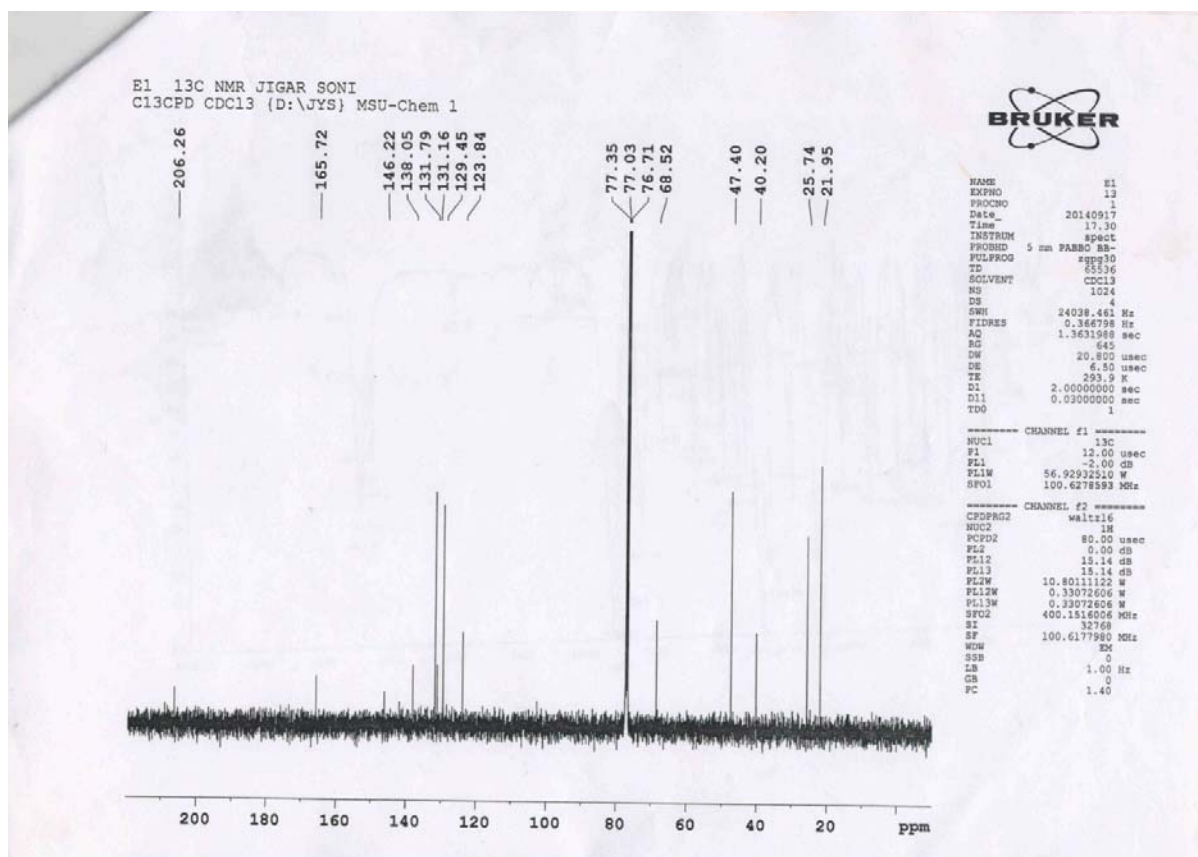
Isopropyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ¹H NMR (5c)



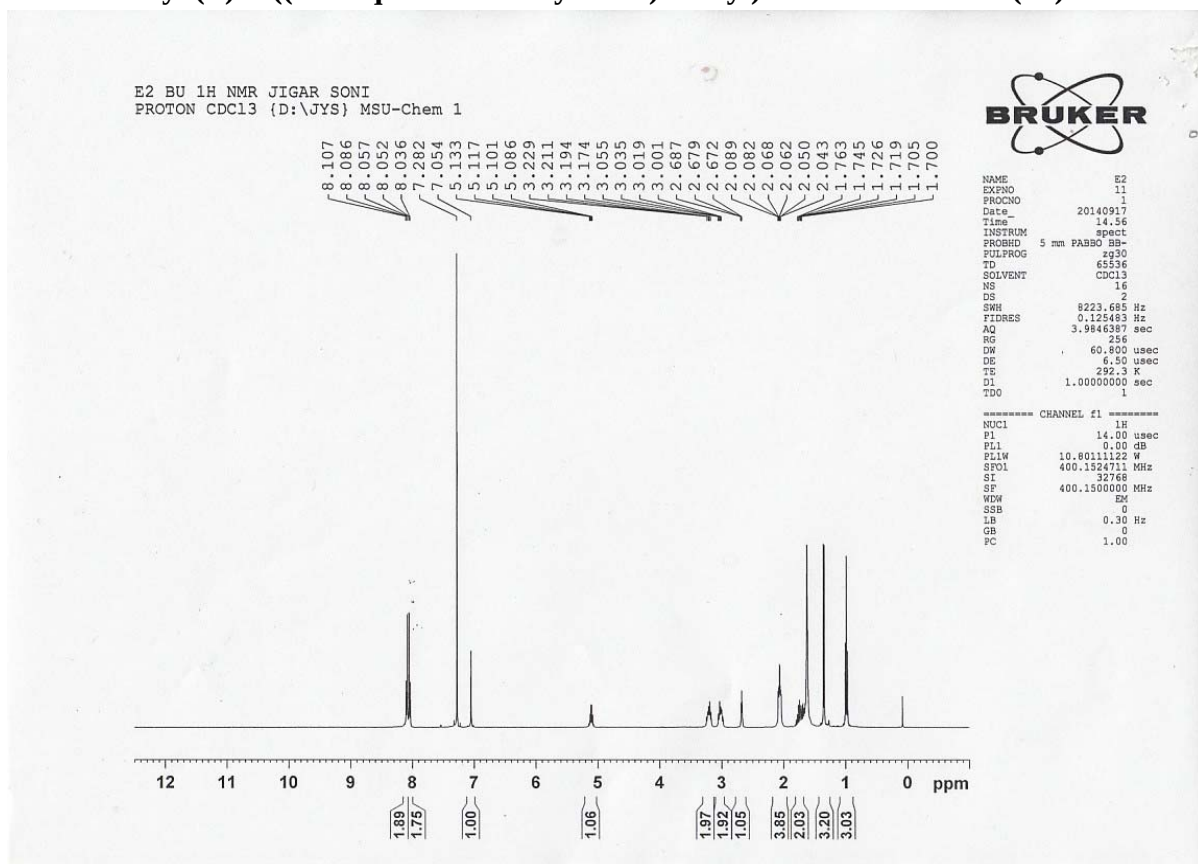
Isopropyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ¹H NMR Expansion (5c)



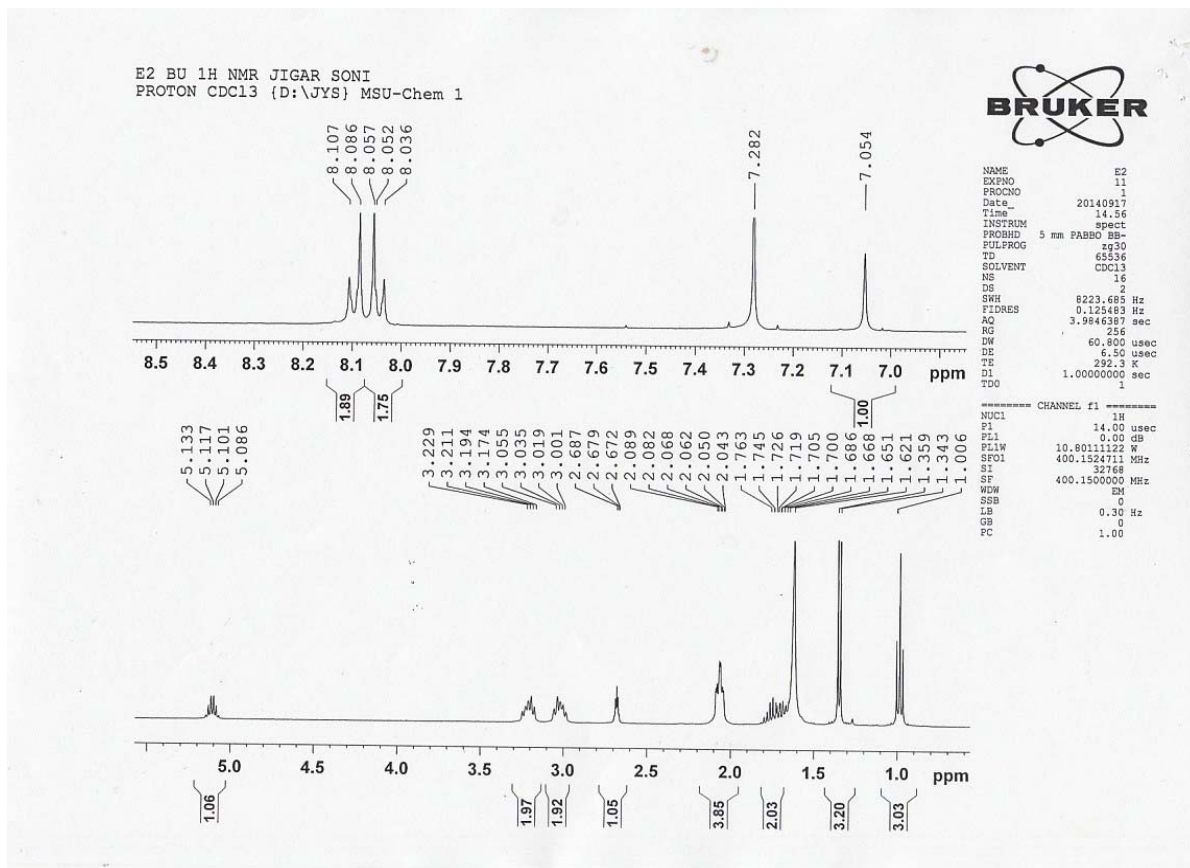
Isopropyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate (IPA) ¹³ C NMR (5c)



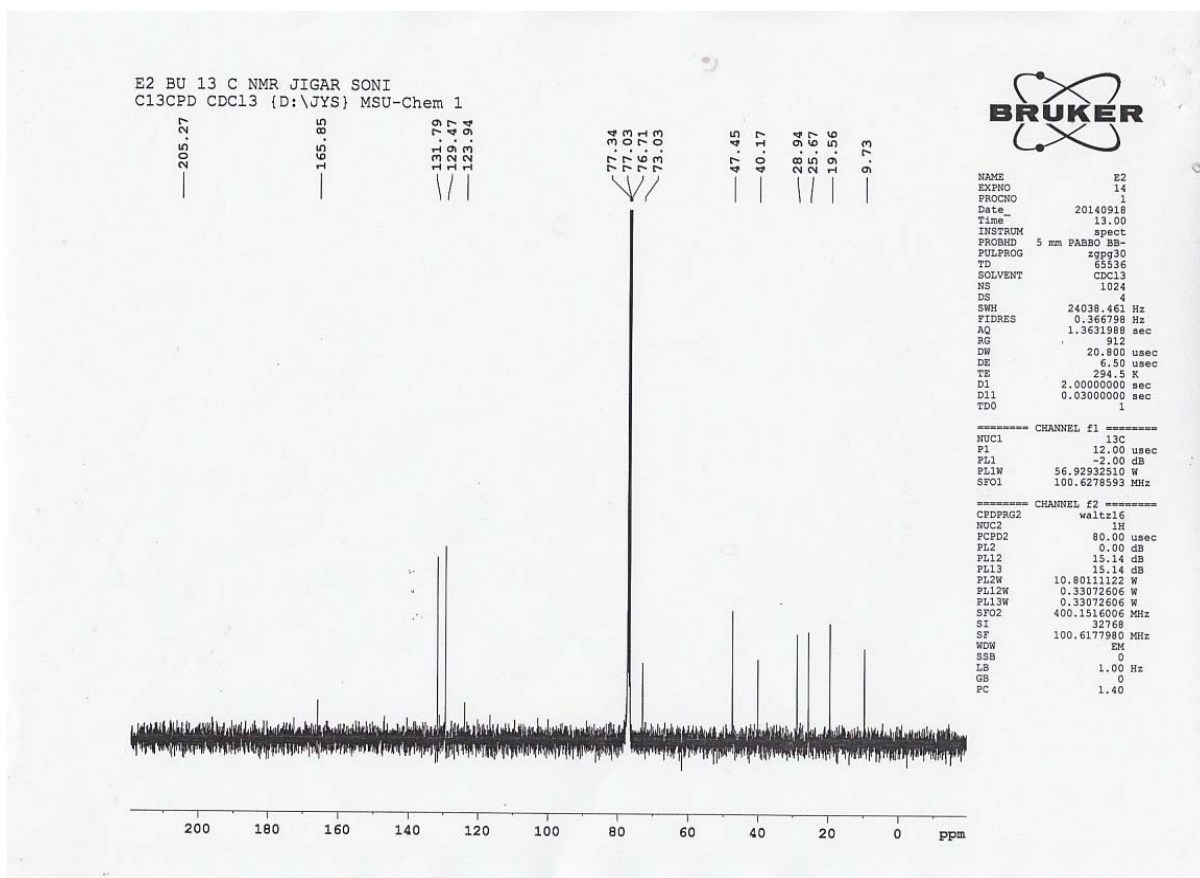
Sec-butyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ¹H NMR (5d)



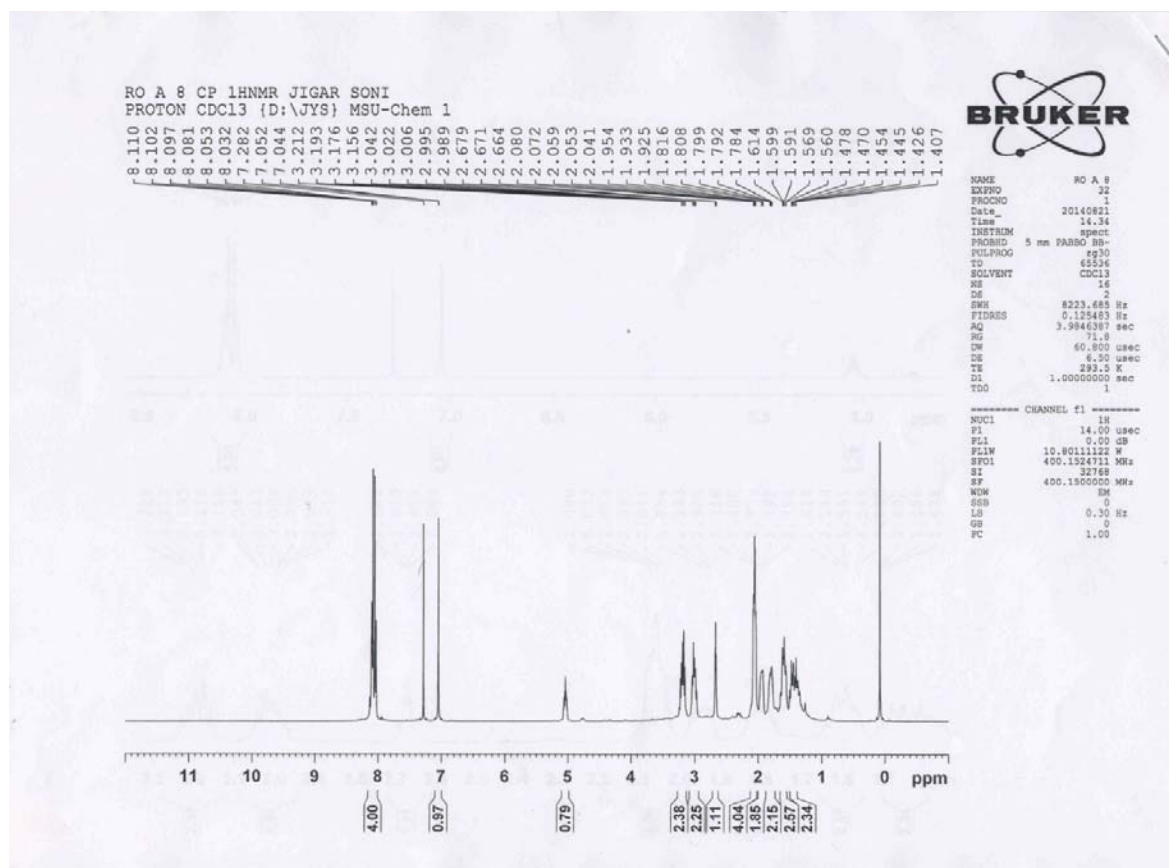
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(5d)



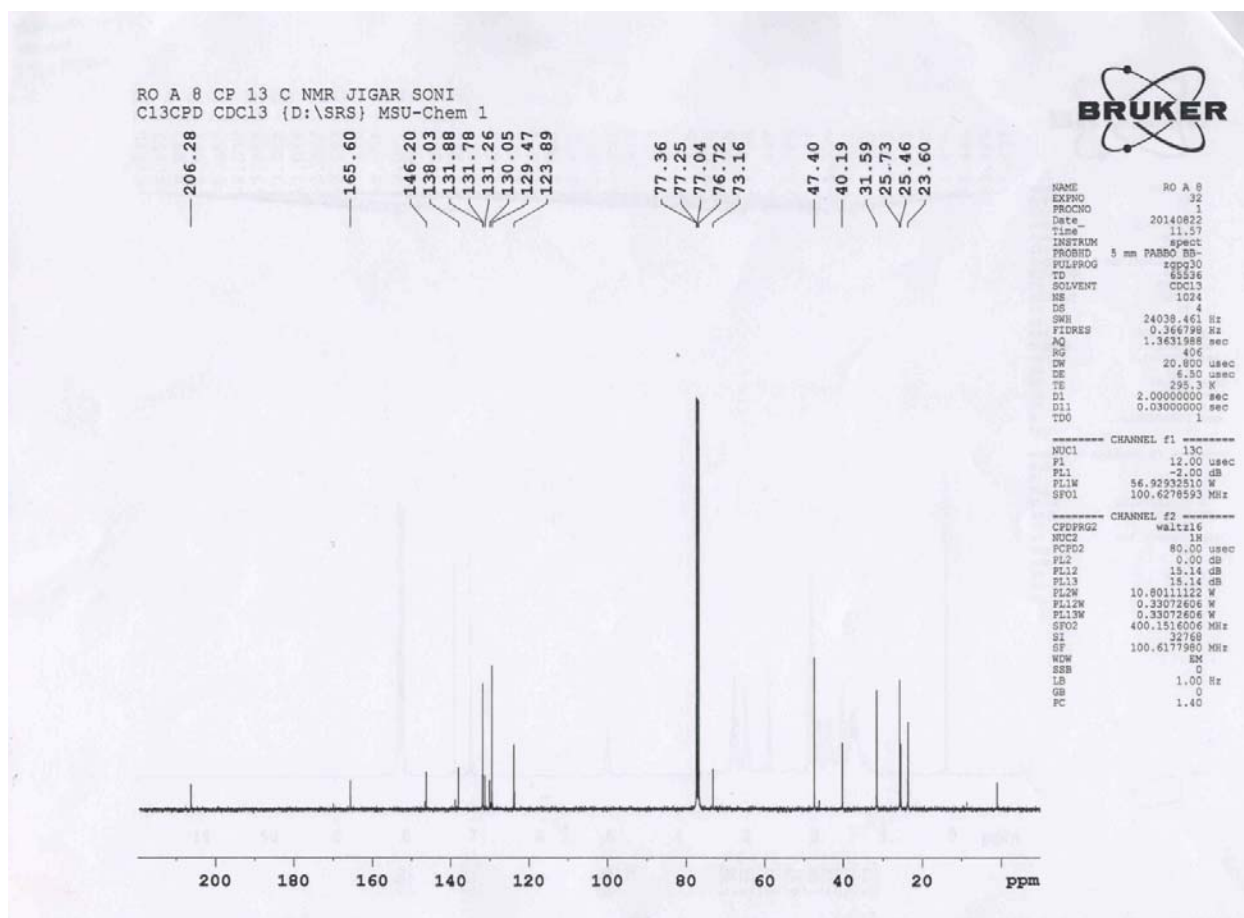
Sec-butyl (Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ¹³CNMR (5d)



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



Cyclopentyl(Z)-4-((3-oxoquinuclidin-2-ylidene)methyl)benzoate ¹³CNMR (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 ≤ h ≤ 6, -10 ≤ k ≤ 5, -21 ≤ l ≤ 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 ₂ O 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 ≤ h ≤ 11, -12 ≤ k ≤ 12, -13 ≤ l ≤ 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