SUPPORTING INFORMATION

Synthesis of 6-methyl-3,4-dihydropyrazinones using a Ugi 4-CR/allenamide cycloisomerization protocol

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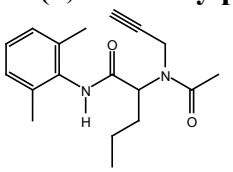
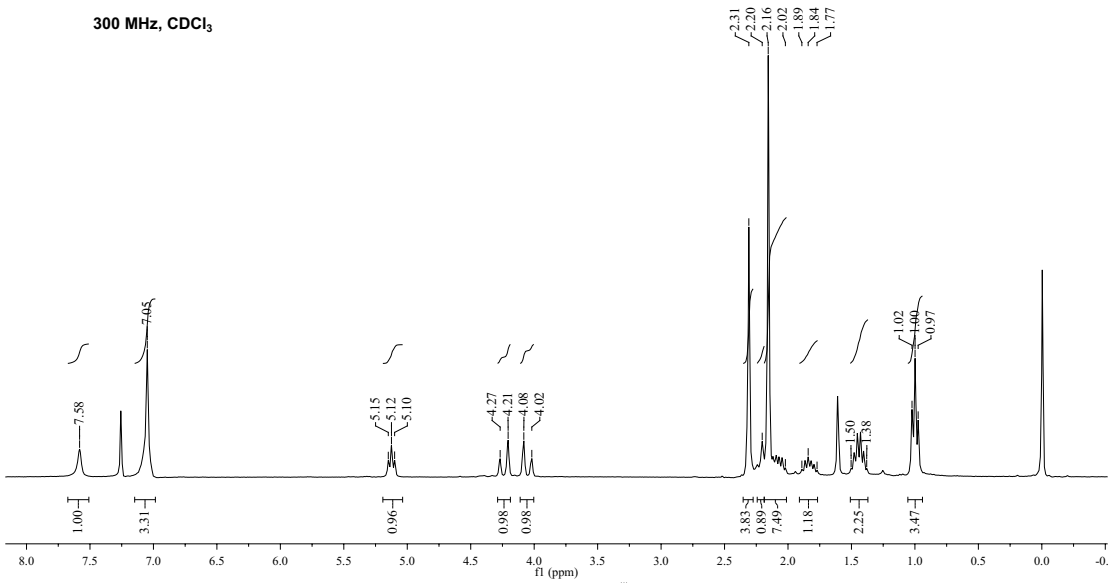
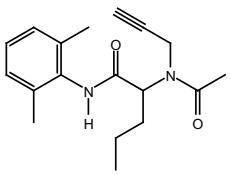
Ugi Adducts spectra

N-(2,6-dimethylphenyl)-2-(*N*-(prop-2-yn-1-yl)acetamido)pentanamide (11a)



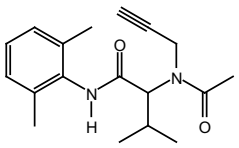
300 MHz, $CDCl_3$



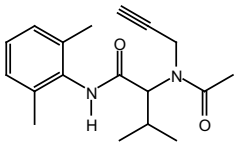


75 MHz, $CDCl_3$

_N_-(2,6-dimethylphenyl)-3-methyl-2-(_N_-(prop-2-yn-1-yl)acetamido)butanamide (11b).

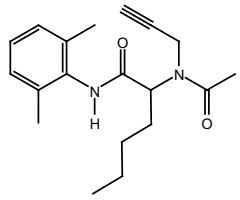


300 Mhz, $CDCl_3$



75 MHz, $CDCl_3$

N-(2,6-dimethylphenyl)-2-(*N*-(prop-2-yn-1-yl)acetamido)hexanamide (11c)



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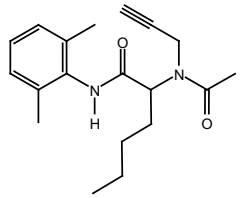
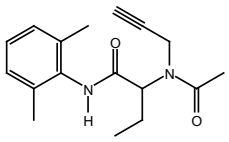


75 MHz, $CDCl_3$

N-(2,6-dimethylphenyl)-2-(*N*-(prop-2-yn-1-yl)acetamido)butanamide (11d)



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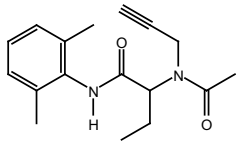
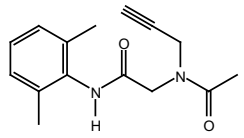


75 MHz, $CDCl_3$

N-(2,6-dimethylphenyl)-2-(*N*-(prop-2-yn-1-yl)acetamido)acetamide (11e)



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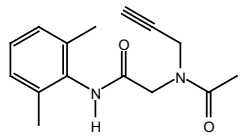

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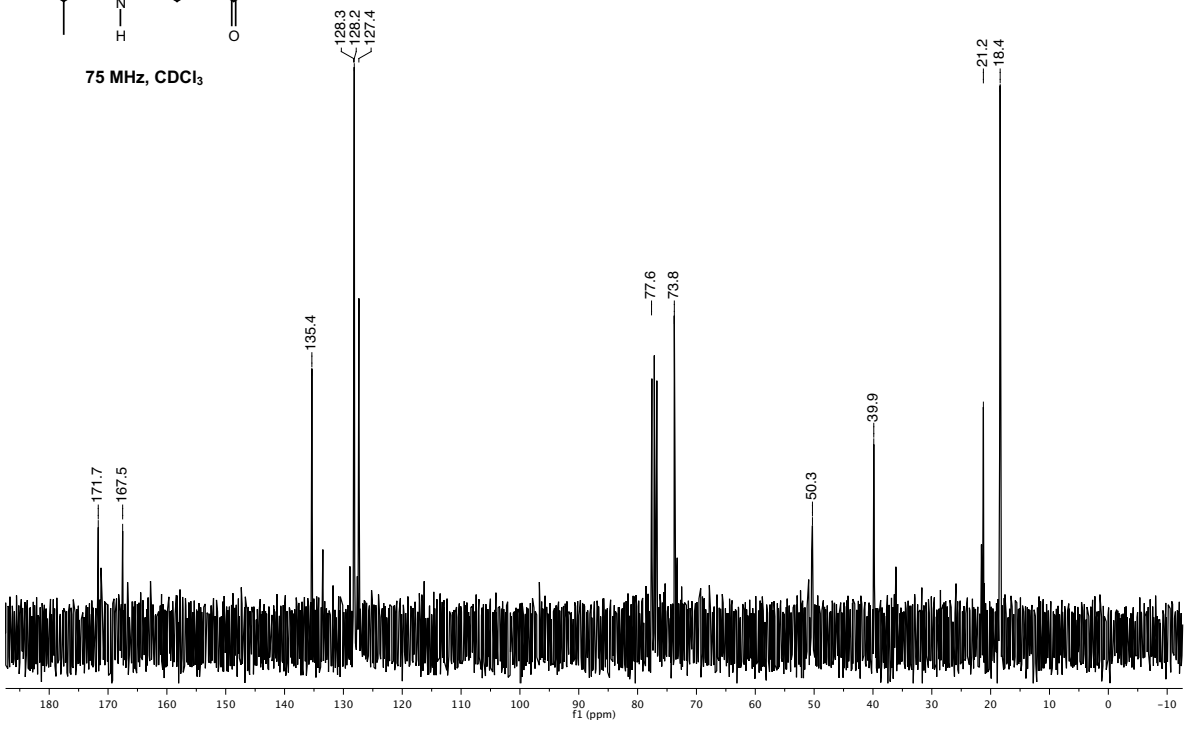
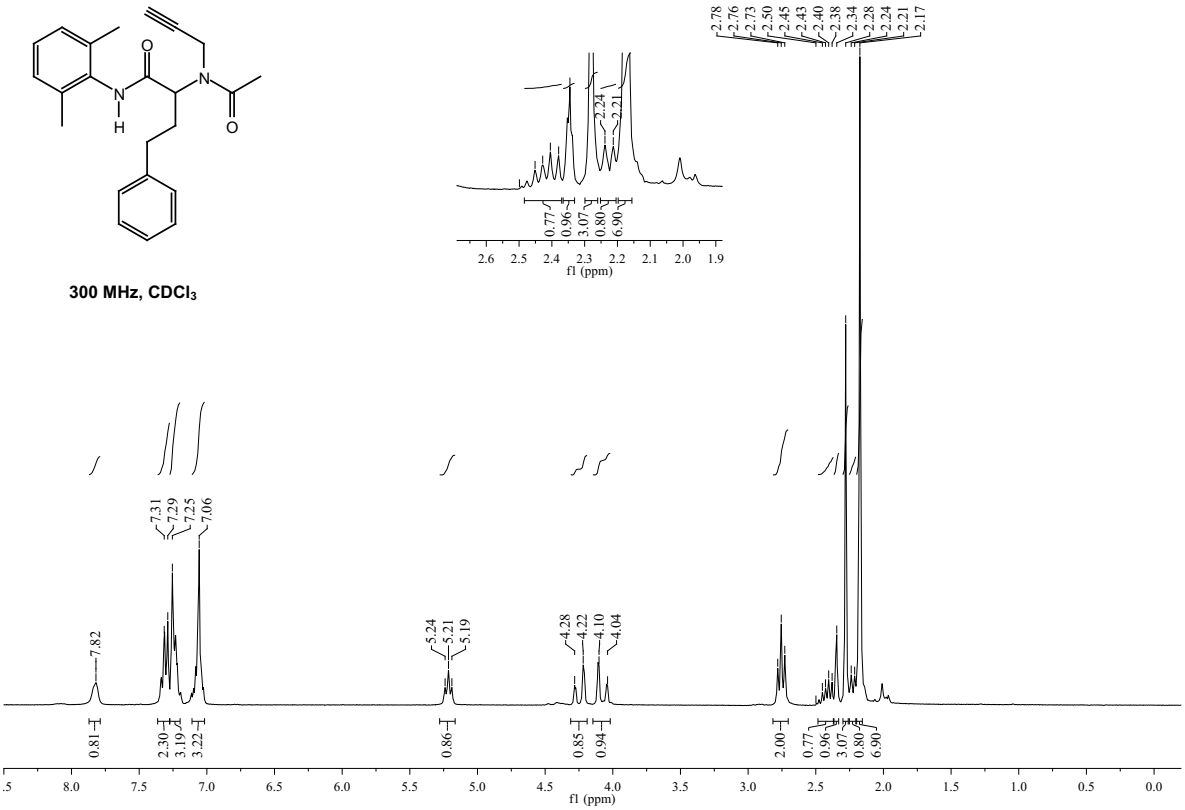
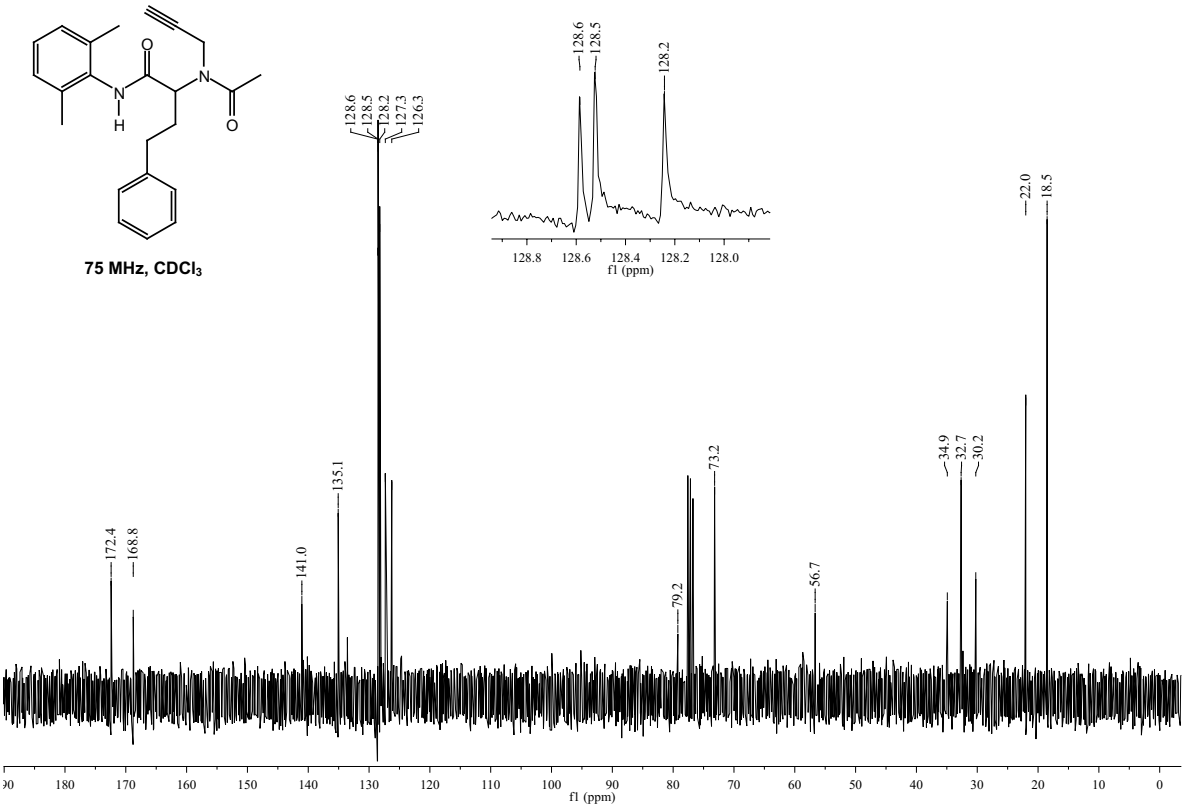
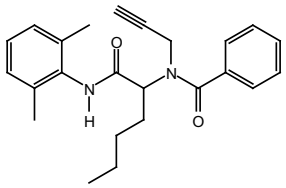


N-(2,6-dimethylphenyl)-4-phenyl-2-(*N*-(prop-2-yn-1-yl)acetamido)butanamide (11f)

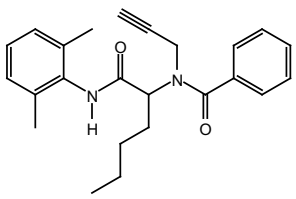




N-(1-((2,6-dimethylphenyl)amino)-1-oxohexan-2-yl)-*N*-(prop-2-yn-1-yl)benzamide (11g)

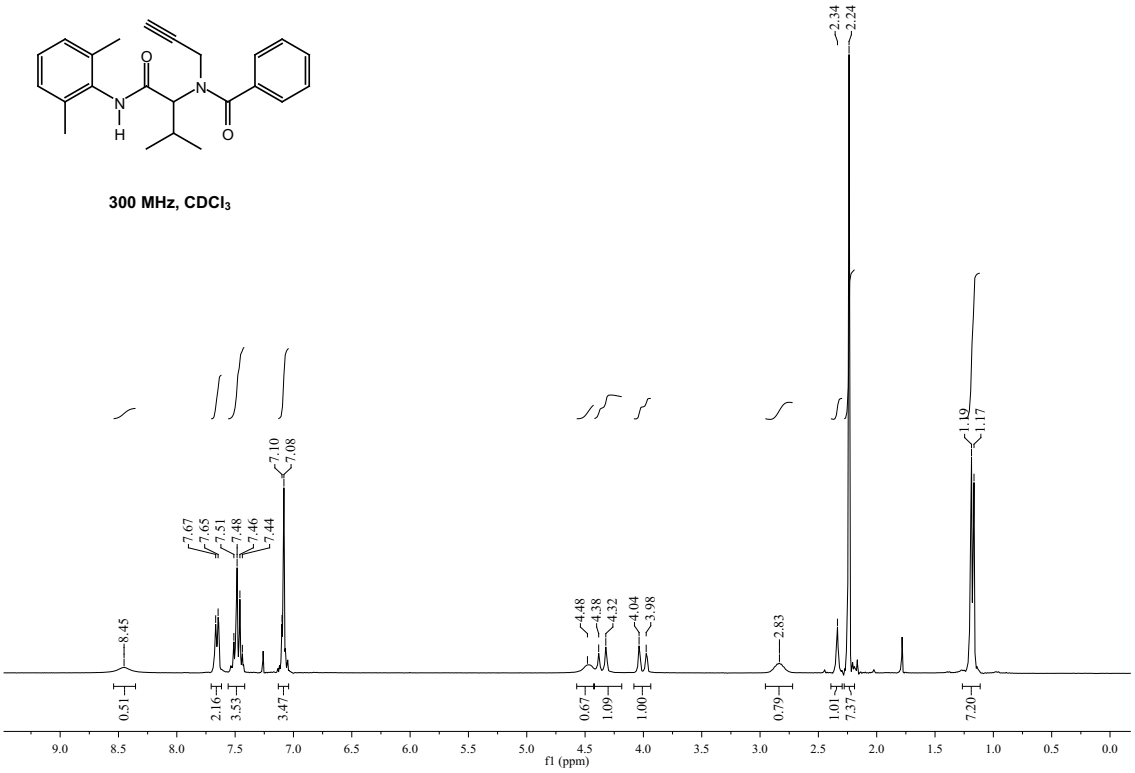


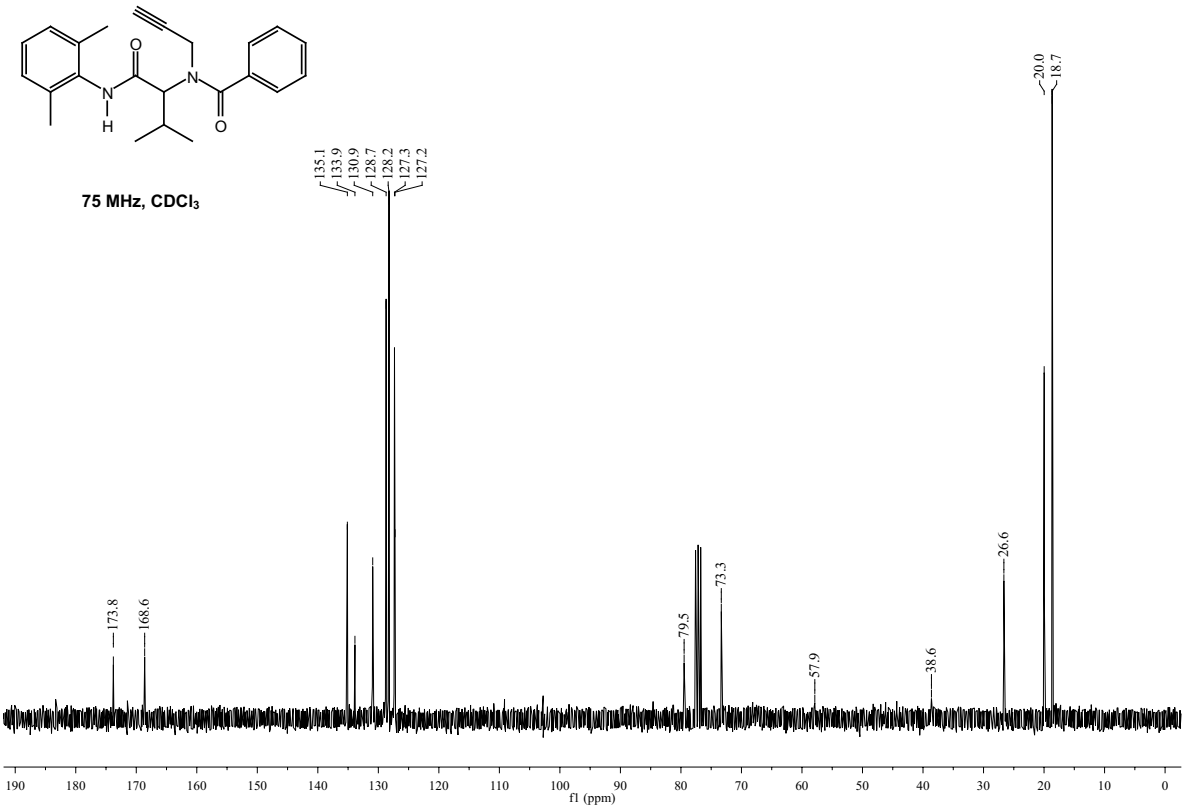
300 MHz, $CDCl_3$



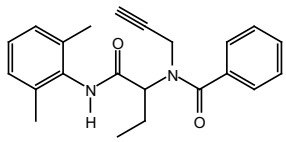
75 MHz, $CDCl_3$

_N_-(1-((2,6-dimethylphenyl)amino)-3-methyl-1-oxobutan-2-yl)-_N_-(prop-2-yn-1-yl) benzamide (11h)

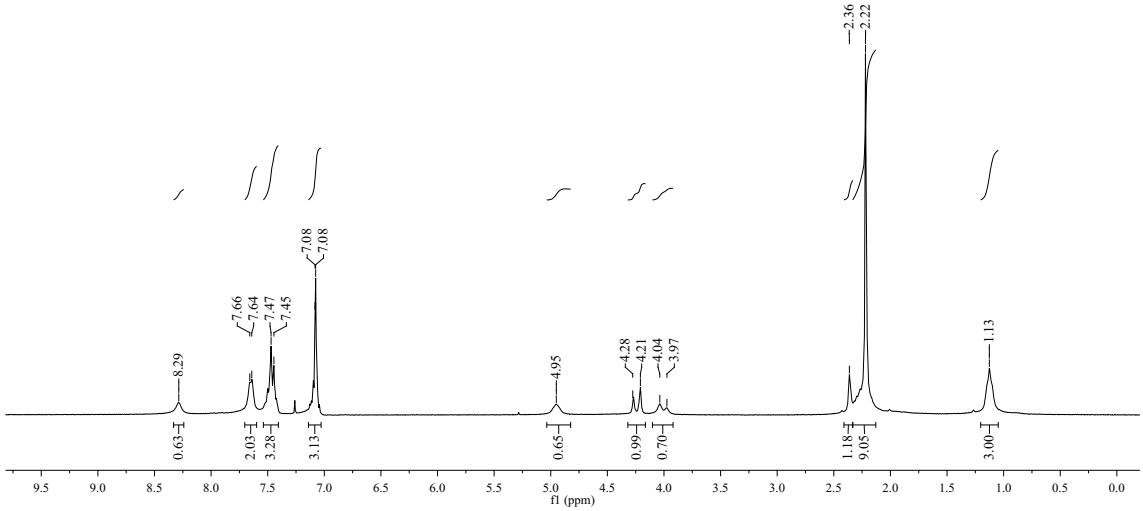


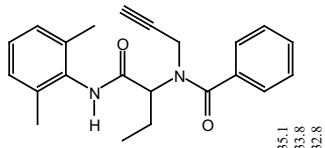


N-(1-((2,6-dimethylphenyl)amino)-1-oxobutan-2-yl)-*N*-(prop-2-yn-1-yl)benzamide (11i)



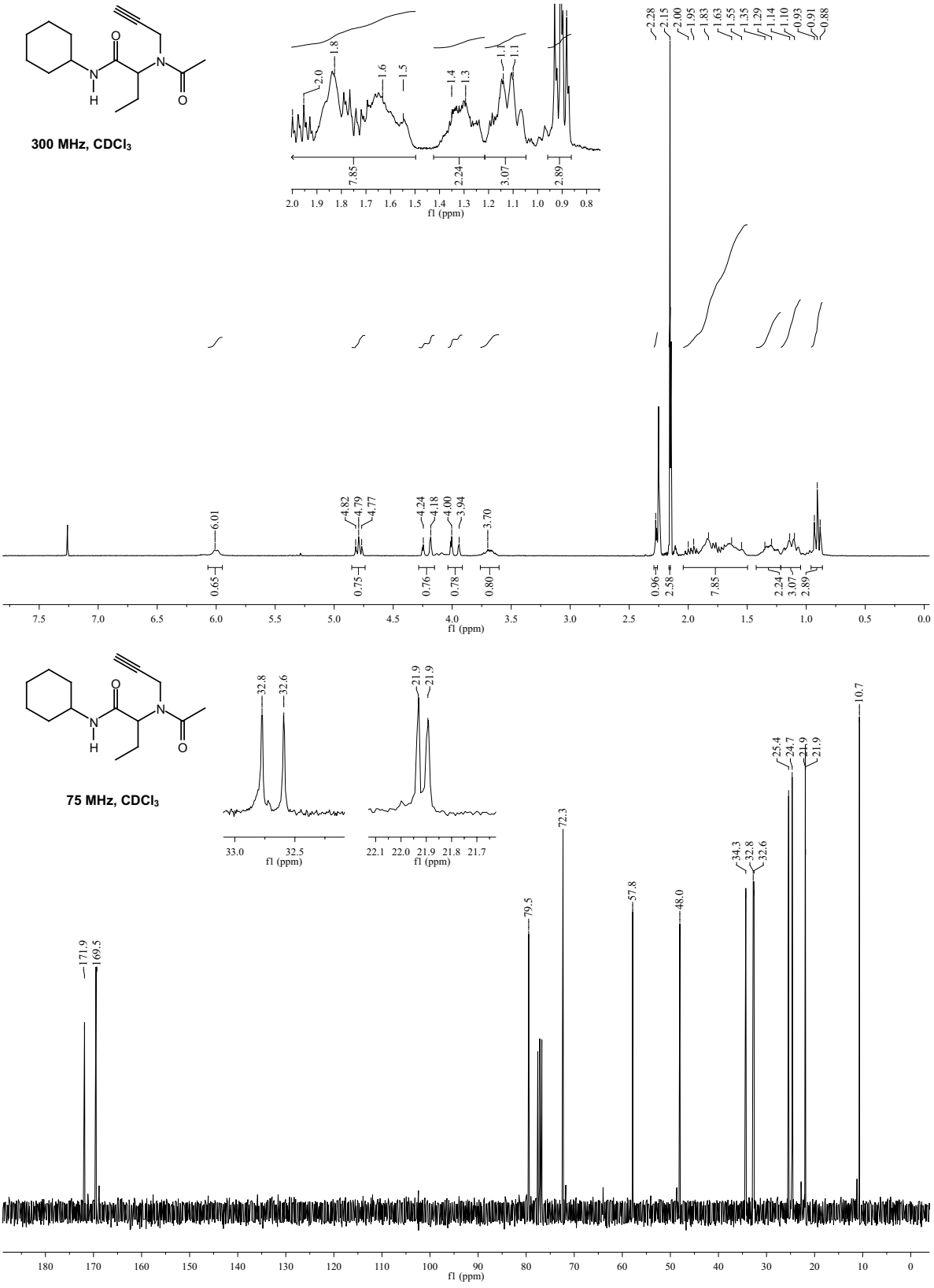
300 MHz, $CDCl_3$



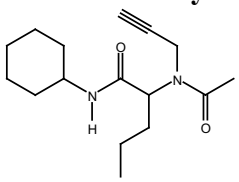


75 MHz, $CDCl_3$

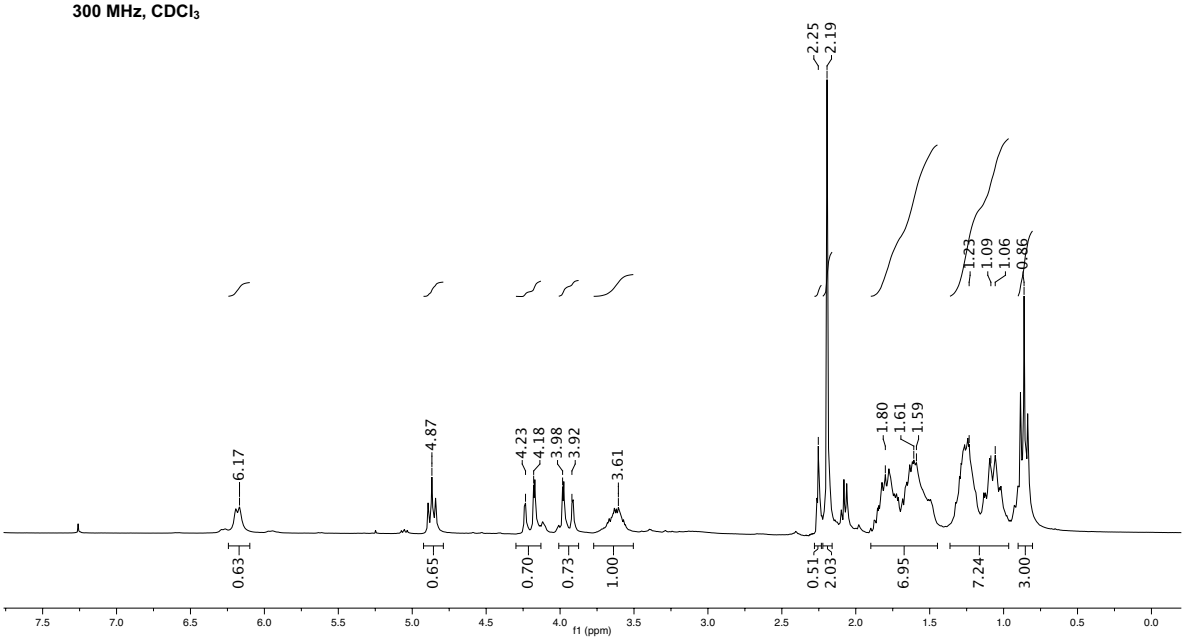
N-cyclohexyl-2-(*N*-(prop-2-yn-1-yl)acetamido)butanamide (11j)

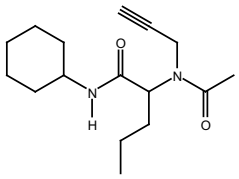


N-cyclohexyl-2-(*N*-(prop-2-yn-1-yl)acetamido)pentanamide (11k).

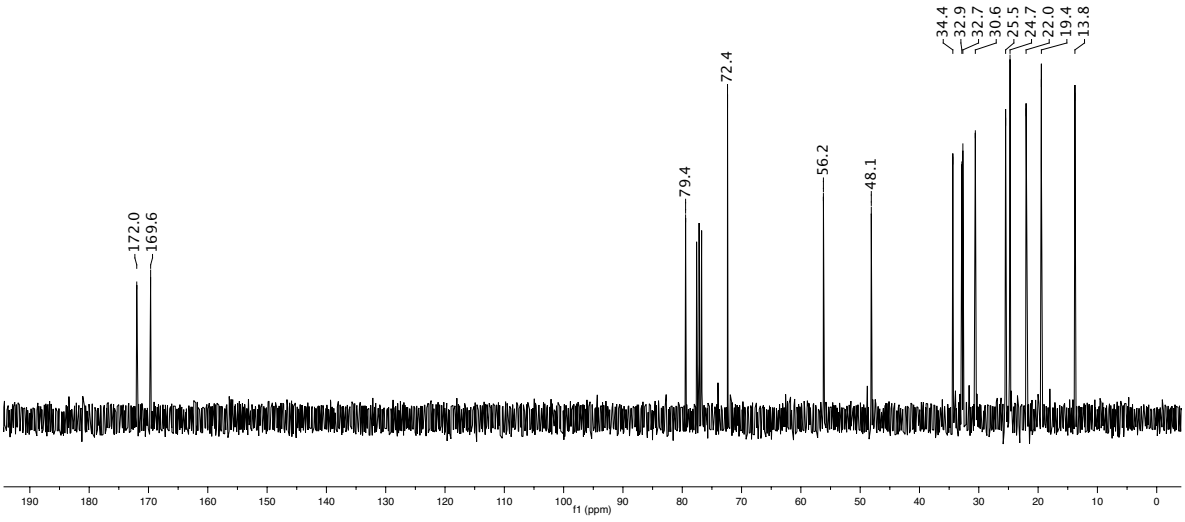


300 MHz, $CDCl_3$

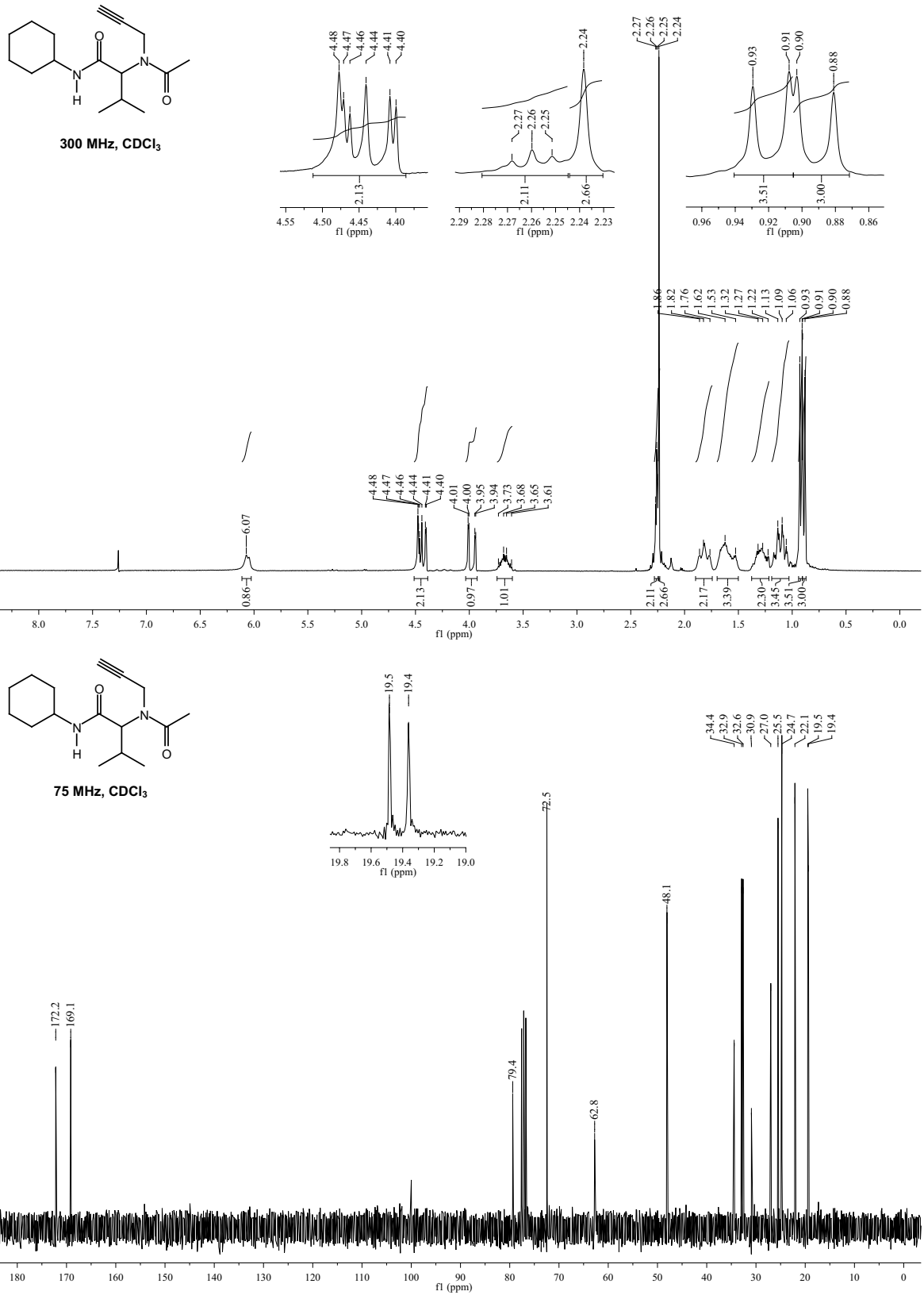




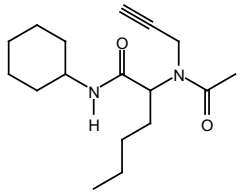
75 MHz, $CDCl_3$



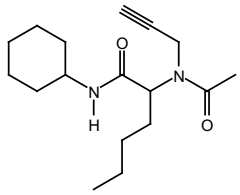
N-cyclohexyl-3-methyl-2-(*N*-(prop-2-yn-1-yl)acetamido)butanamide (11l)



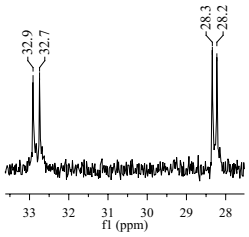
N-cyclohexyl-2-(*N*-(prop-2-yn-1-yl)acetamido)hexanamide (11m)

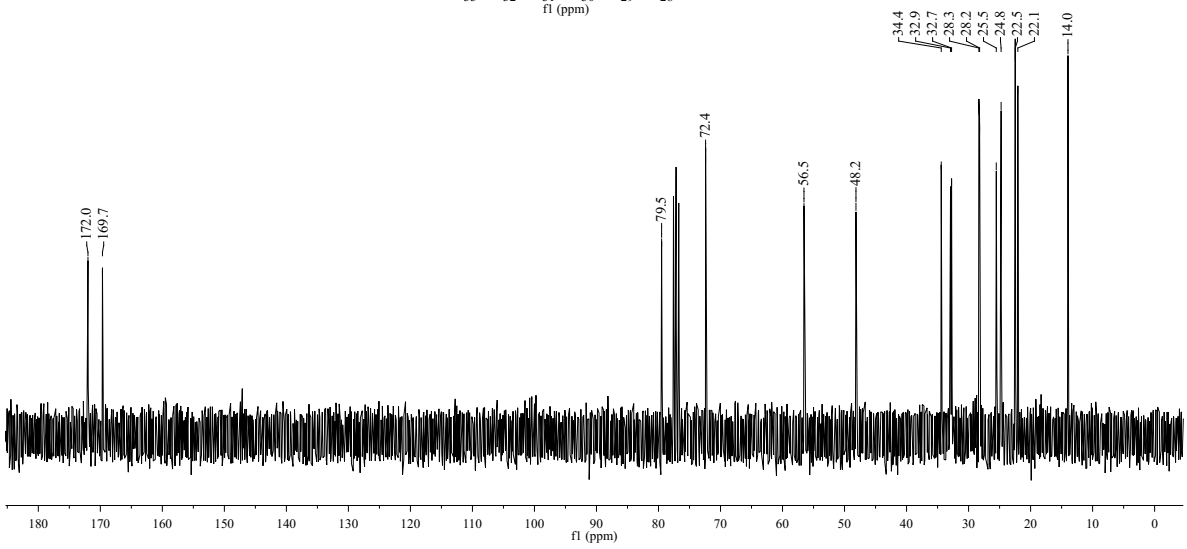


300 MHz, $CDCl_3$

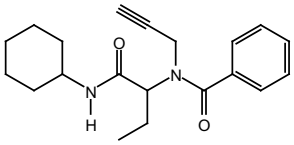


75 MHz, $CDCl_3$

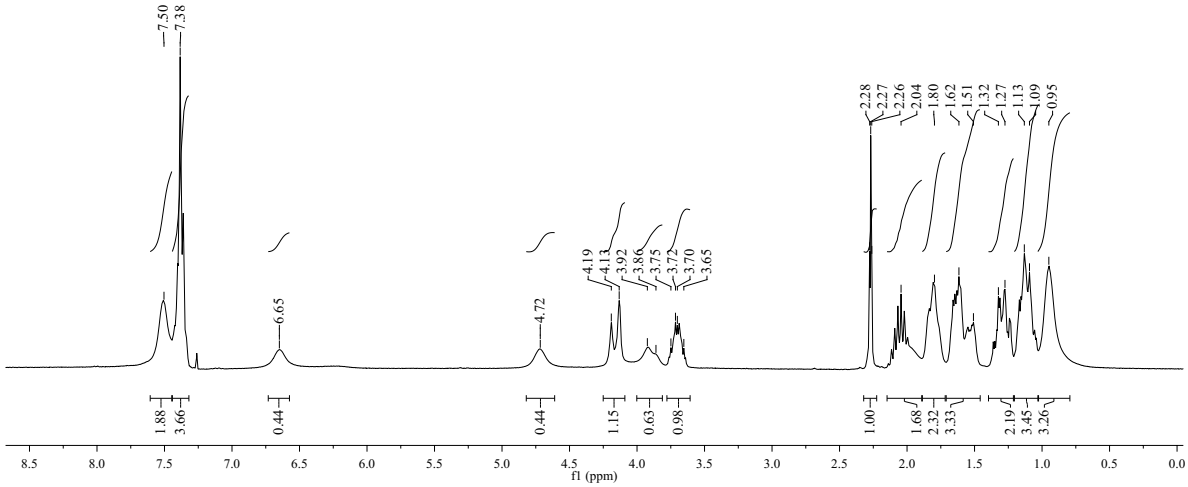


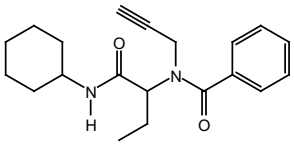


N-(1-(cyclohexylamino)-1-oxobutan-2-yl)-*N*-(prop-2-yn-1-yl)benzamide (11n)



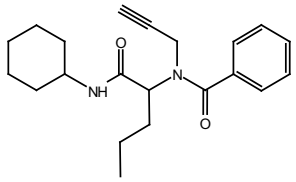
300 MHz, $CDCl_3$



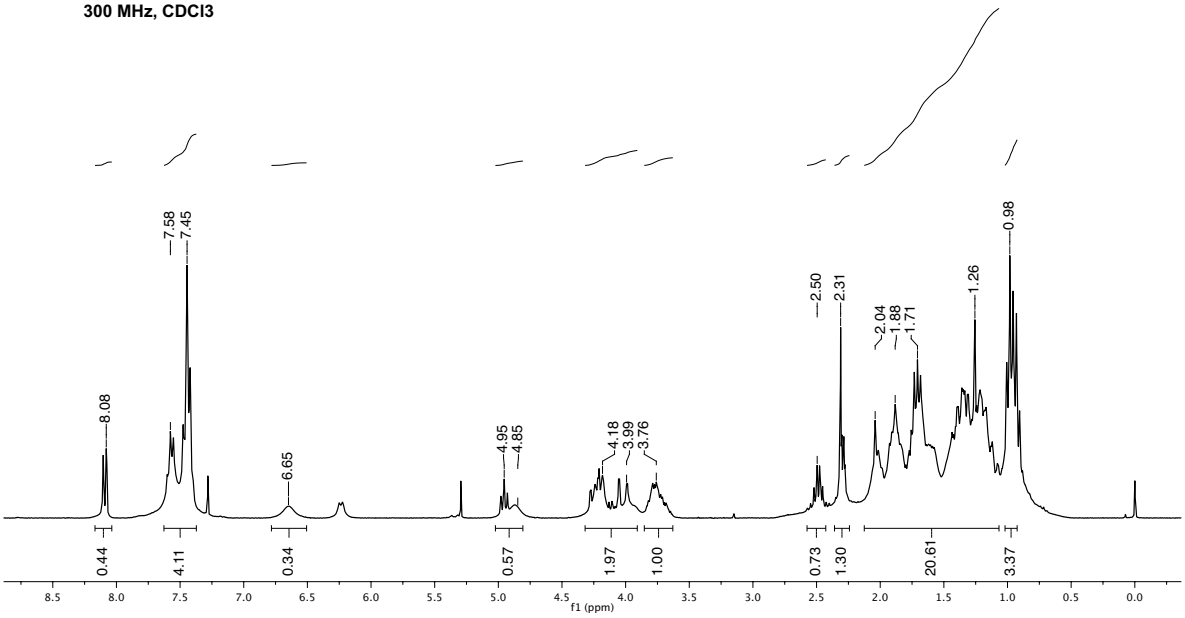


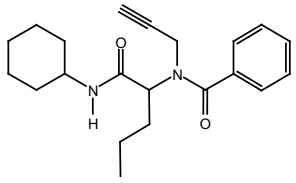
75 MHz, $CDCl_3$

N-(1-(cyclohexylamino)-1-oxopentan-2-yl)-*N*-(prop-2-yn-1-yl)benzamide (11o)

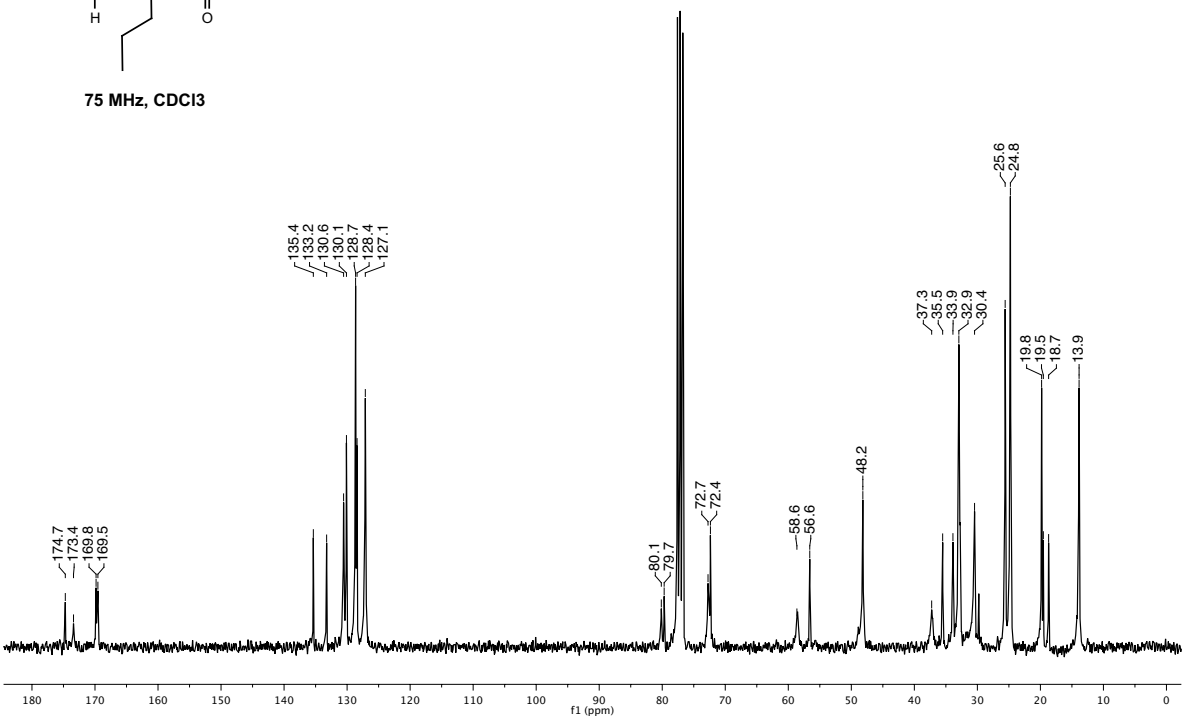


300 MHz, CDCl3

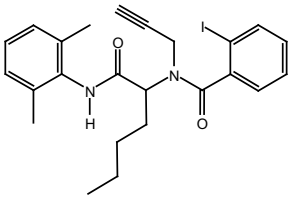




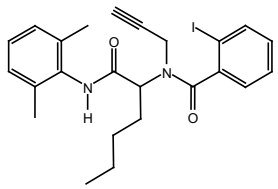
75 MHz, CDCl3



N-(1-((2,6-dimethylphenyl)amino)-1-oxohexan-2-yl)-2-iodo-*N*-(prop-2-yn-1-yl)benzamide (11p)

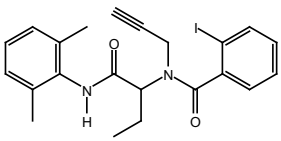


300 MHz, $CDCl_3$

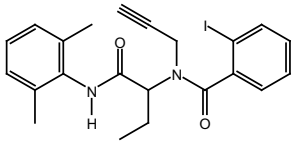


75 MHz, $CDCl_3$

N-(1-((2,6-dimethylphenyl)amino)-1-oxobutan-2-yl)-2-iodo-*N*-(prop-2-yn-1-yl)-benzamide (11q)

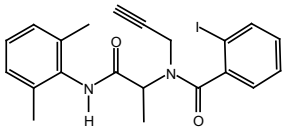


400 MHz, $CDCl_3$

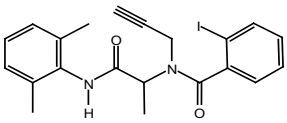


100 MHz, $CDCl_3$

_N_-(1-((2,6-dimethylphenyl)amino)-1-oxopropan-2-yl)-2-iodo-_N_-(prop-2-yn-1-yl)benzamide (11r)

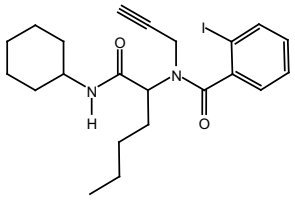


400 MHz, $CDCl_3$

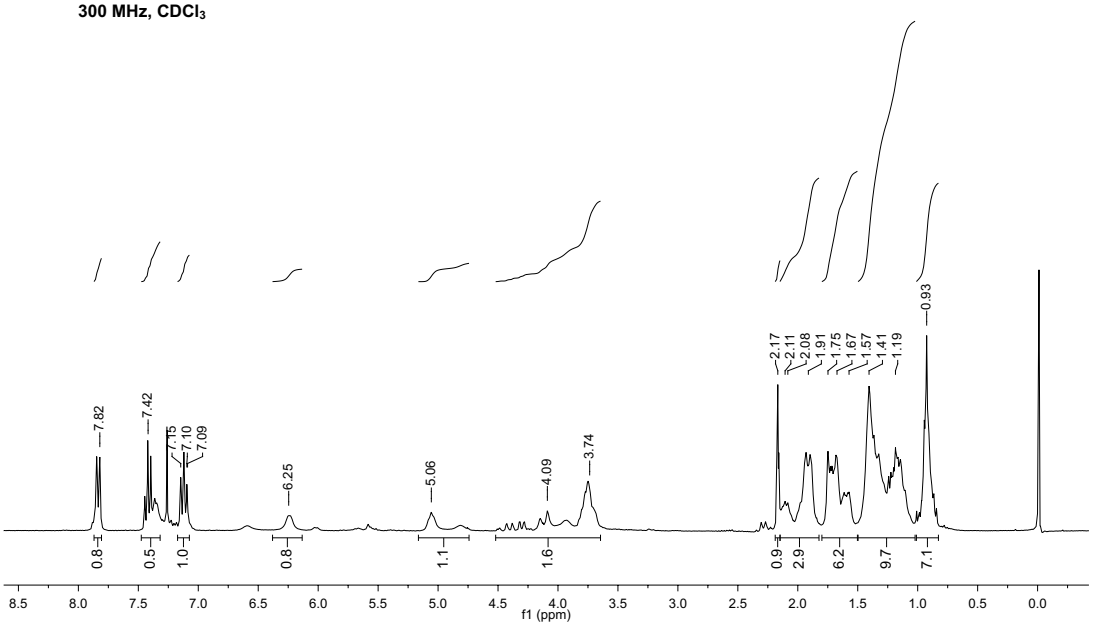


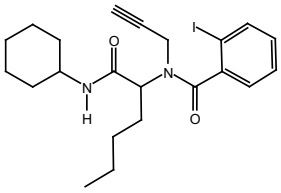
100 MHz, $CDCl_3$

N-(1-(cyclohexylamino)-1-oxohexan-2-yl)-2-iodo-*N*-(prop-2-yn-1-yl)benzamide (11s)



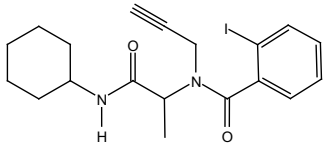
300 MHz, $CDCl_3$



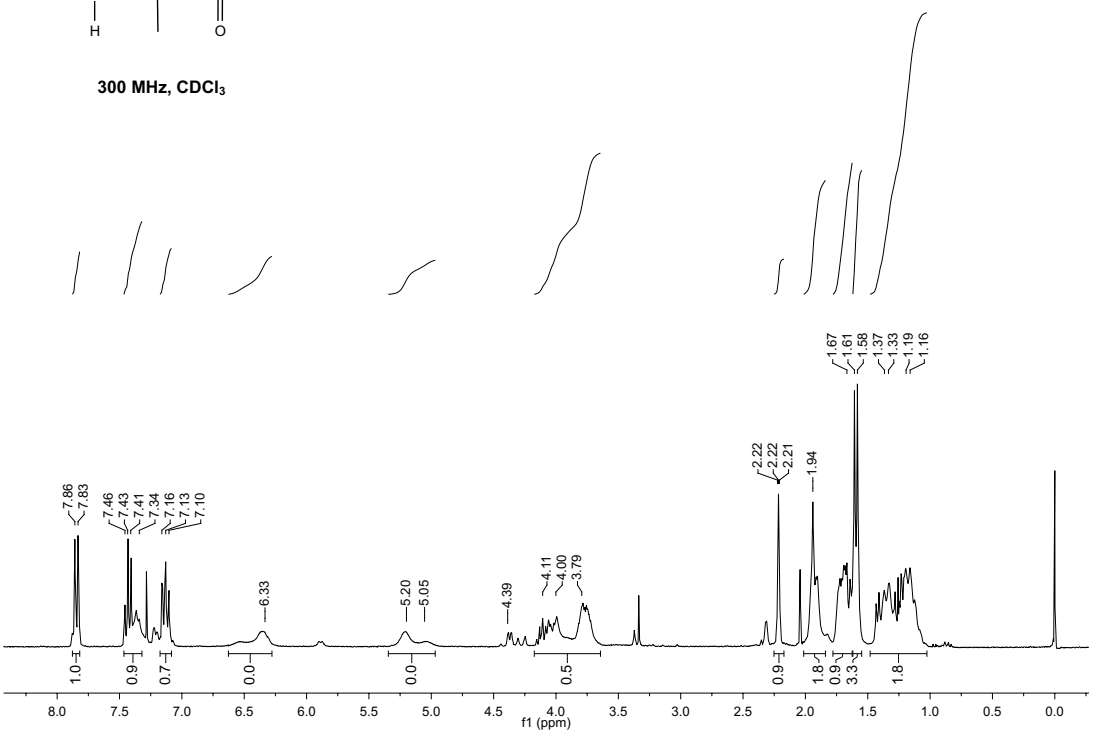


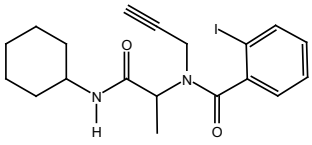
75 MHz, $CDCl_3$

N-(1-(cyclohexylamino)-1-oxopropan-2-yl)-2-iodo-*N*-(prop-2-yn-1-yl)benzamide (11t)

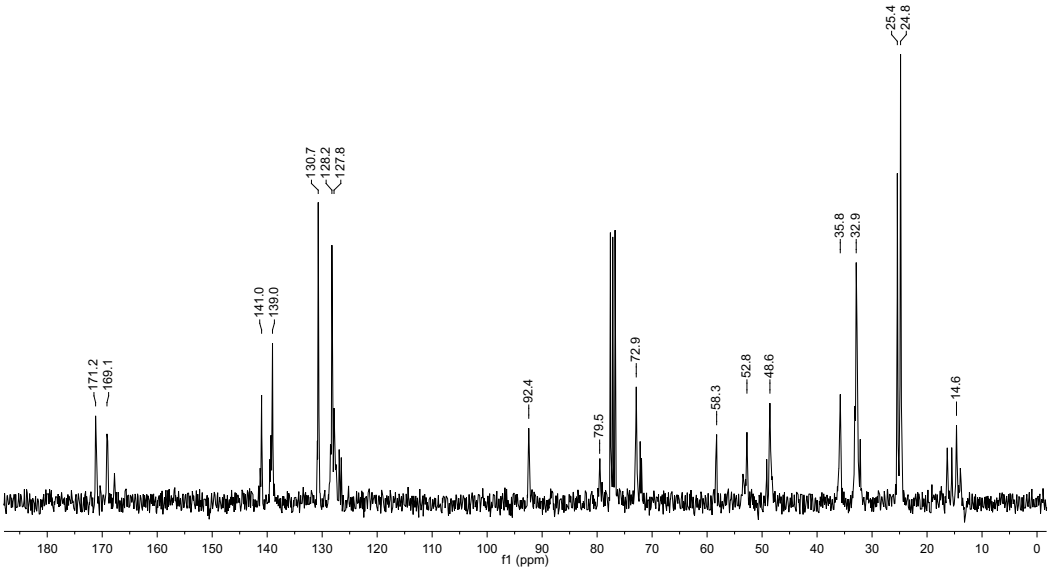


300 MHz, $CDCl_3$

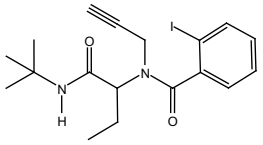




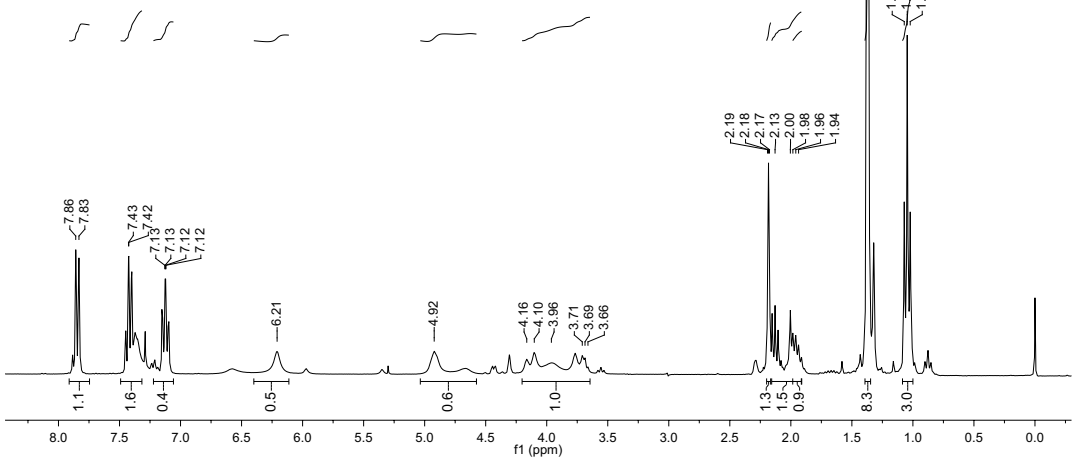
75 MHz, $CDCl_3$

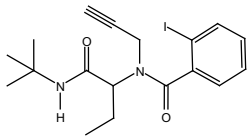


N-(1-(*tert*-butylamino)-1-oxobutan-2-yl)-2-iodo-*N*-(prop-2-yn-1-yl)benzamide (11u)

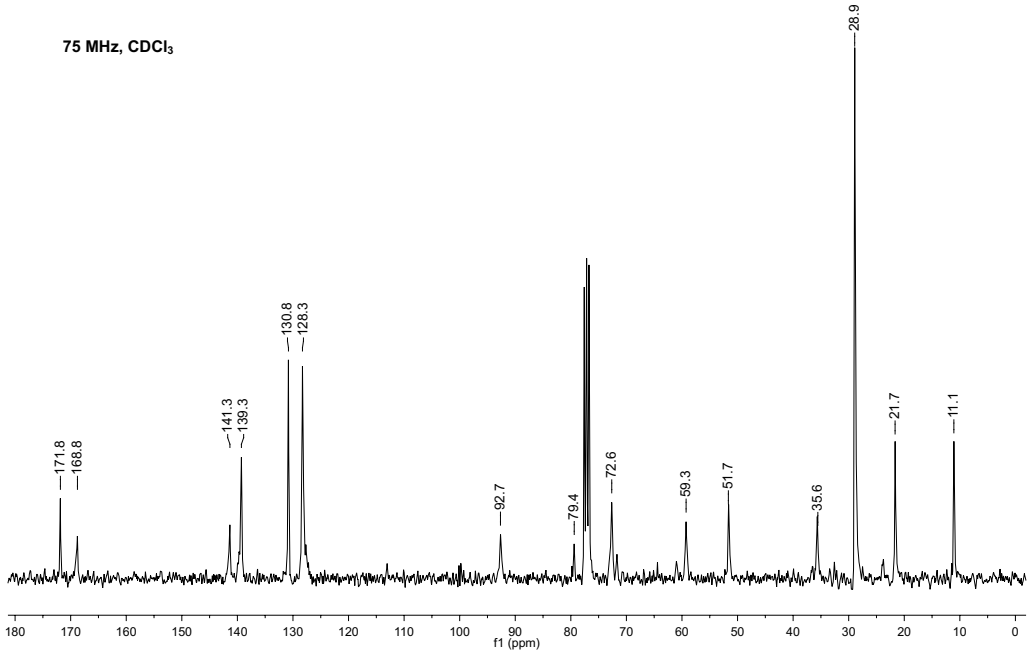


300 MHz, $CDCl_3$

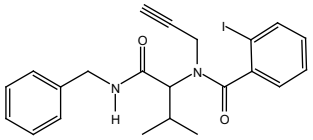




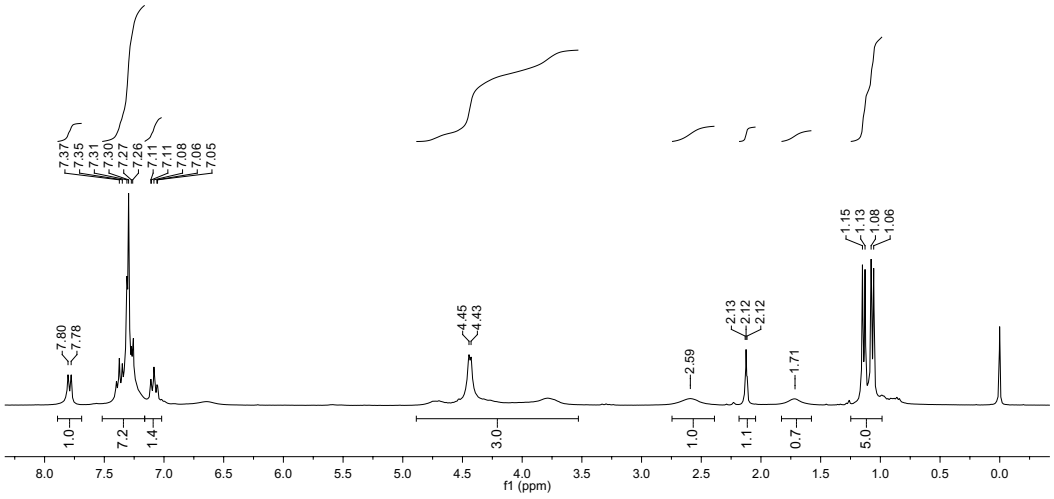
75 MHz, $CDCl_3$

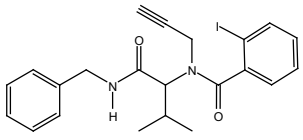


N-(1-(benzylamino)-3-methyl-1-oxobutan-2-yl)-2-iodo-*N*-(prop-2-yn-1-yl)benzamide (11v)



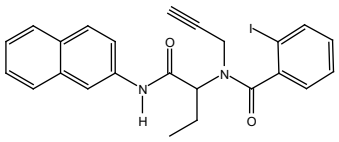
300 MHz, $CDCl_3$



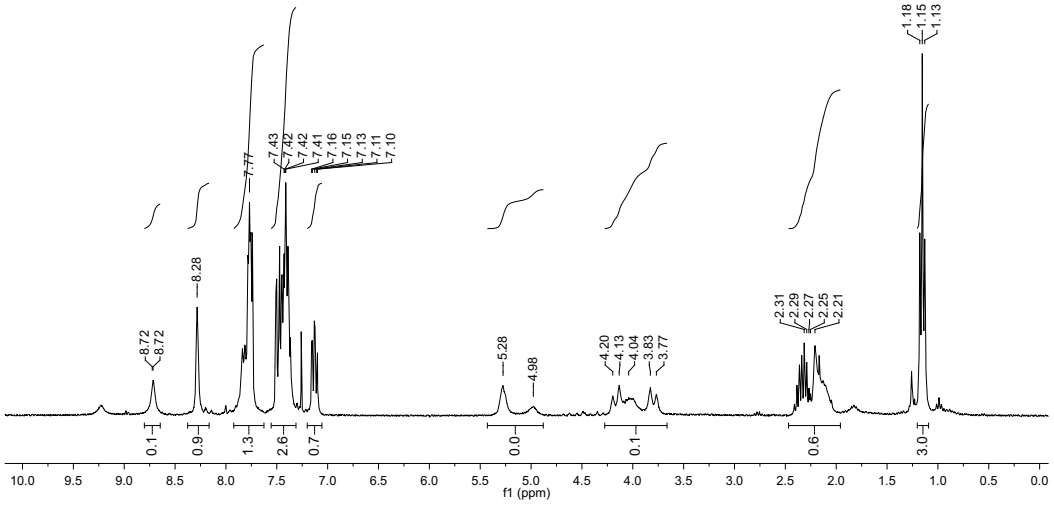


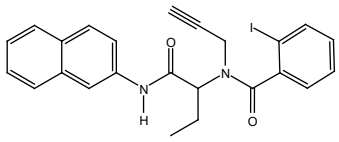
75 MHz, $CDCl_3$

2-iodo-*N*-(1-(naphthalen-2-ylamino)-1-oxobutan-2-yl)-*N*-(prop-2-yn-1-yl)benzamide (11w)

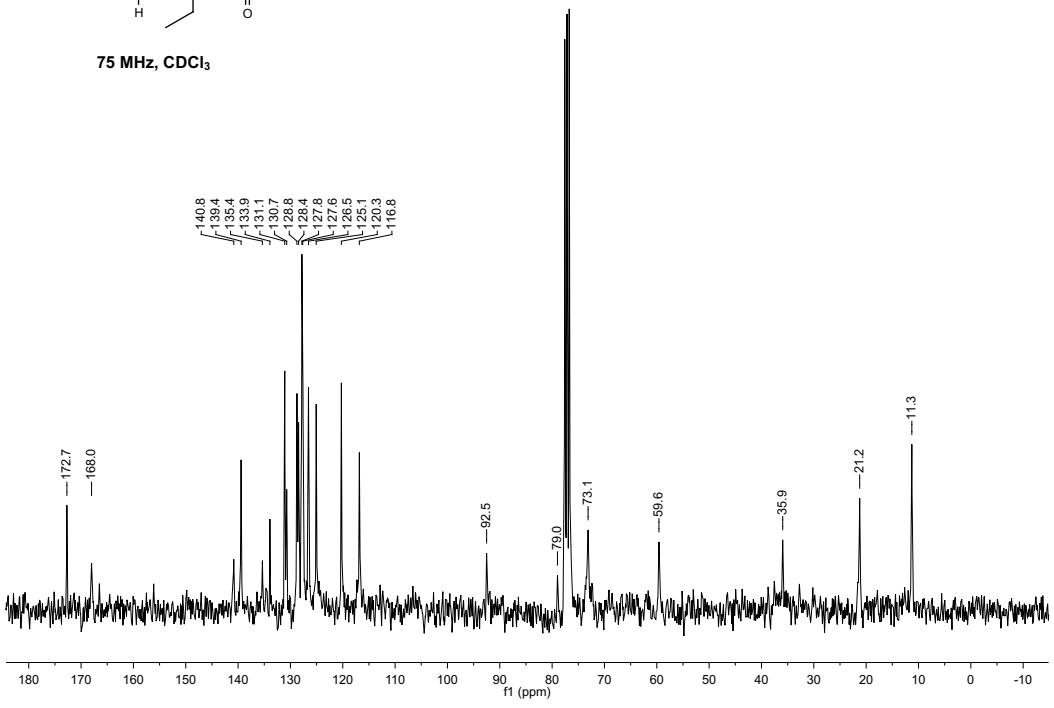


300 MHz, $CDCl_3$

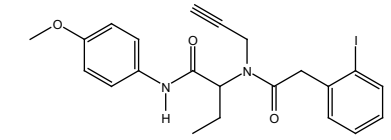




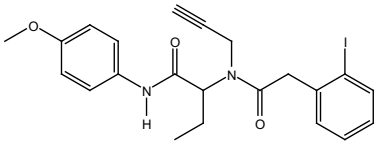
75 MHz, $CDCl_3$



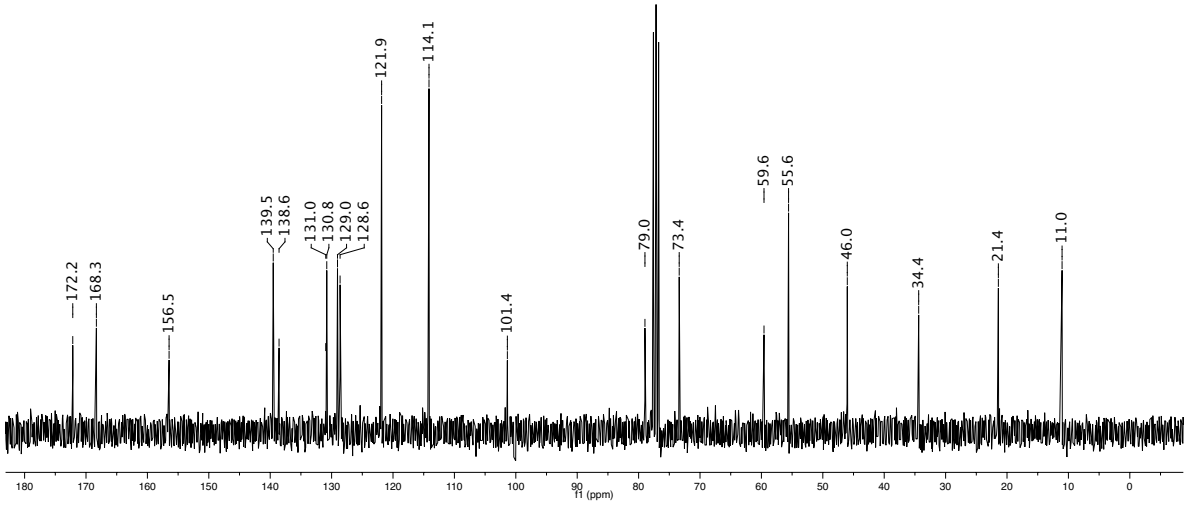
2-(2-(2-iodophenyl)-*N*-(prop-2-yn-1-yl)acetamido)-*N*-(4-methoxyphenyl)butanamide (11x)



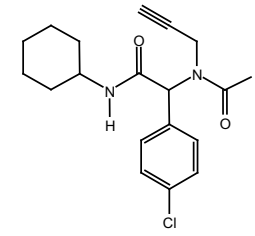
300 MHz, $CDCl_3$



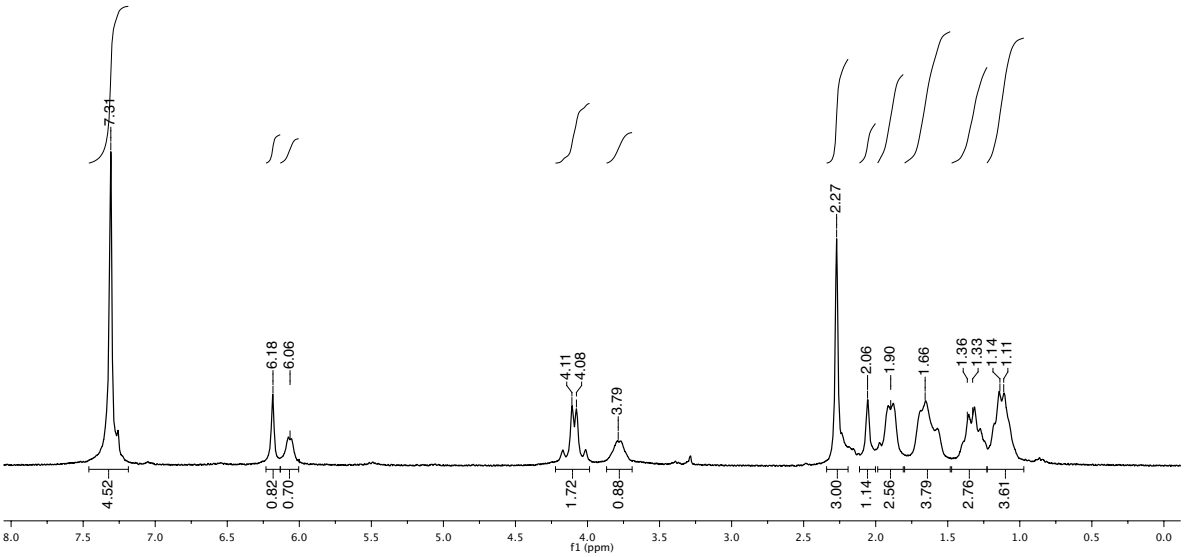
75 MHz, $CDCl_3$

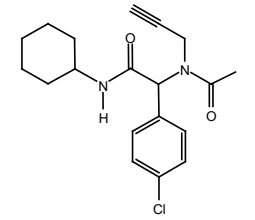


2-(4-chlorophenyl)-*N*-cyclohexyl-2-(*N*-(prop-2-yn-1-yl)acetamido)acetamide (11y)



300 MHz, $CDCl_3$

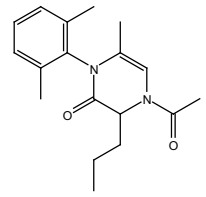




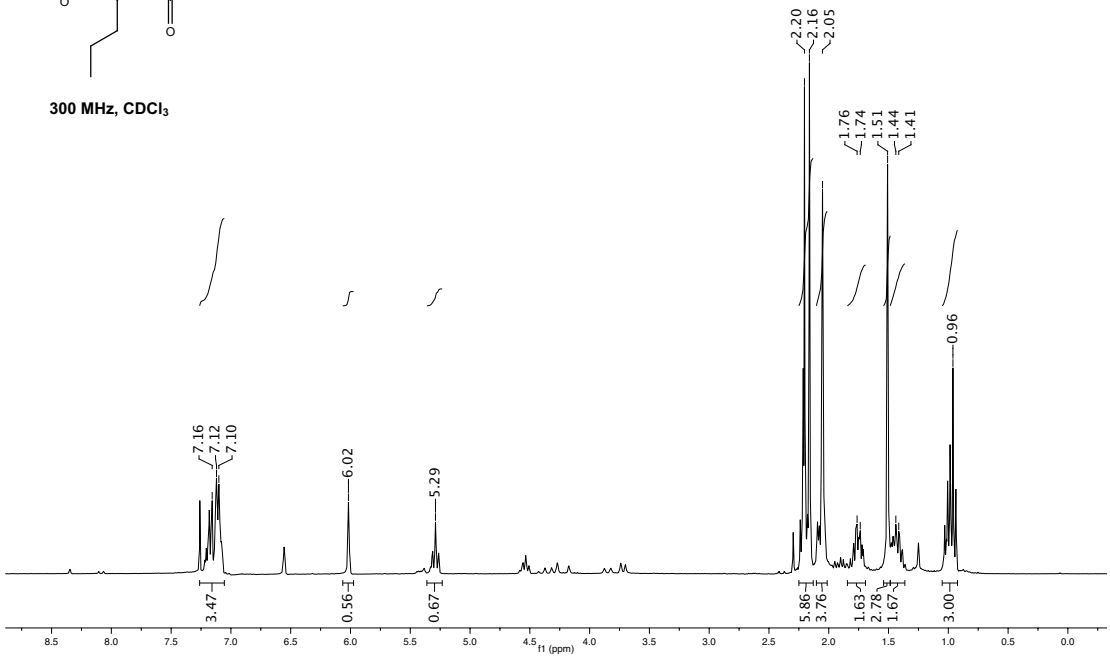
75 MHz, $CDCl_3$

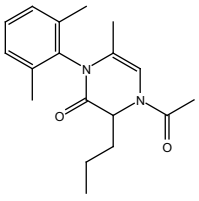
Dihydropyrazinone spectra

4-Acetyl-1-(2,6-dimethylphenyl)-6-methyl-3-propyl-3,4-dihydropyrazin-2(1*H*)-one (13a)

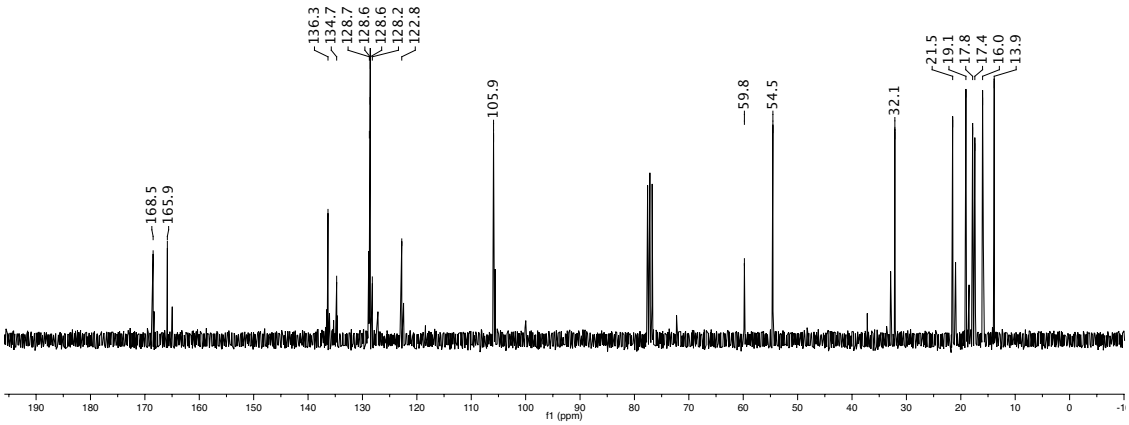


300 MHz, $CDCl_3$

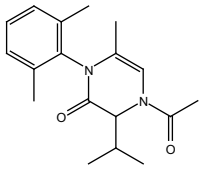




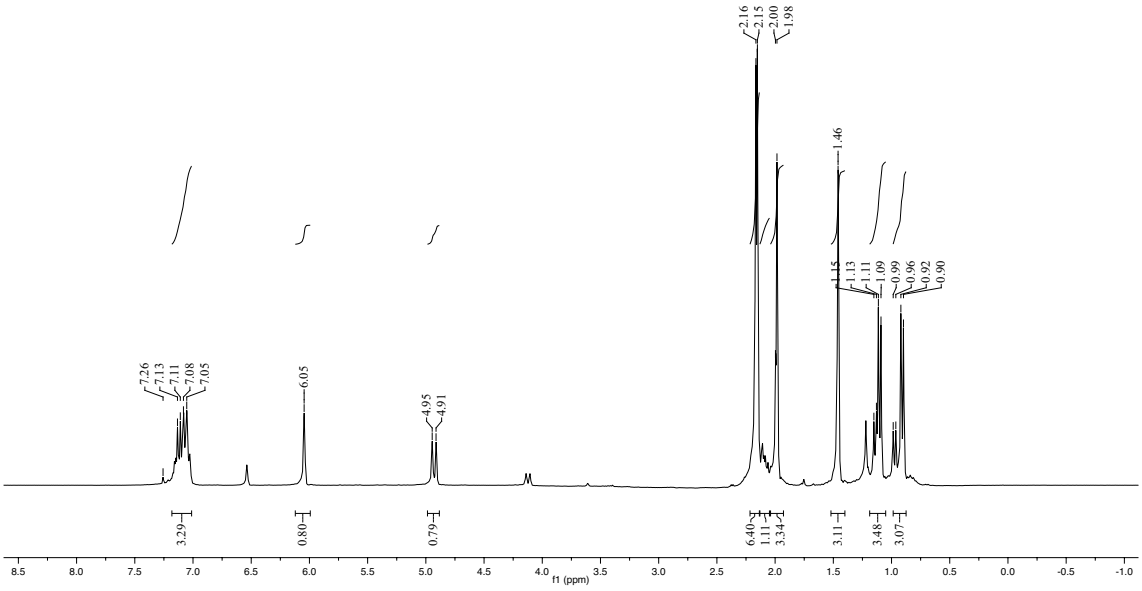
75 MHz, $CDCl_3$

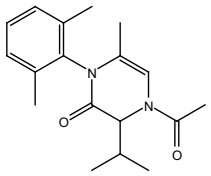


4-Acetyl-1-(2,6-dimethylphenyl)-3-isopropyl-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13b)

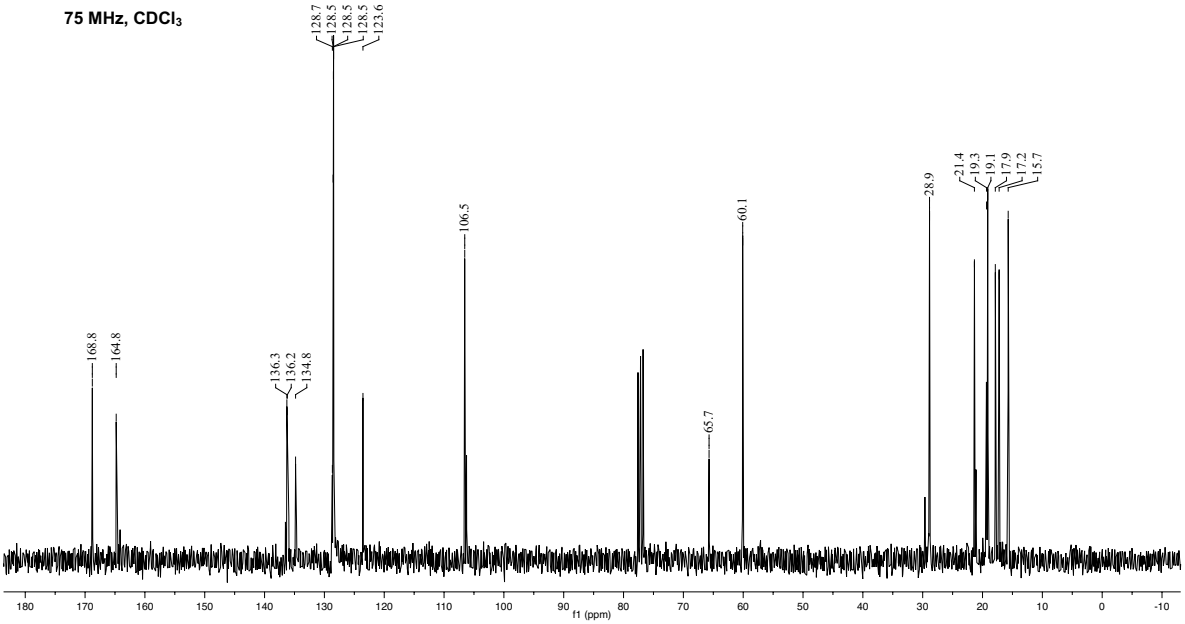


300 MHz, $CDCl_3$

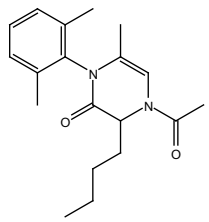




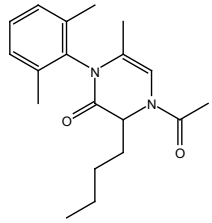
75 MHz, $CDCl_3$



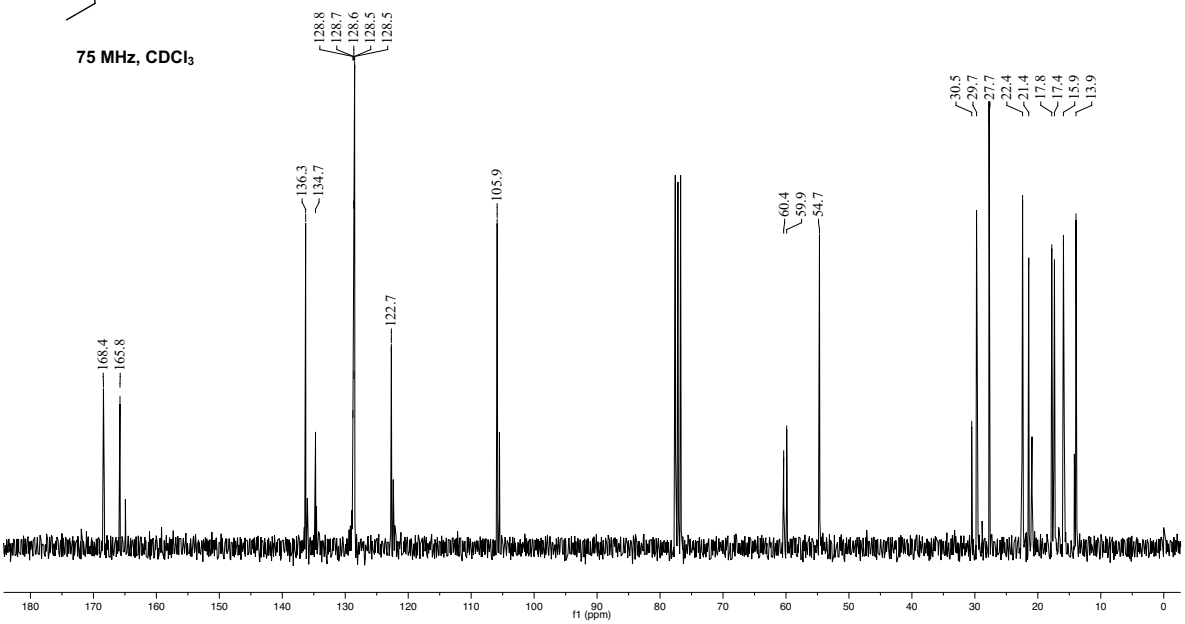
4-Acetyl-3-butyl-1-(2,6-dimethylphenyl)-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13c)



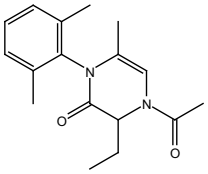
300 MhZ, $CDCl_3$



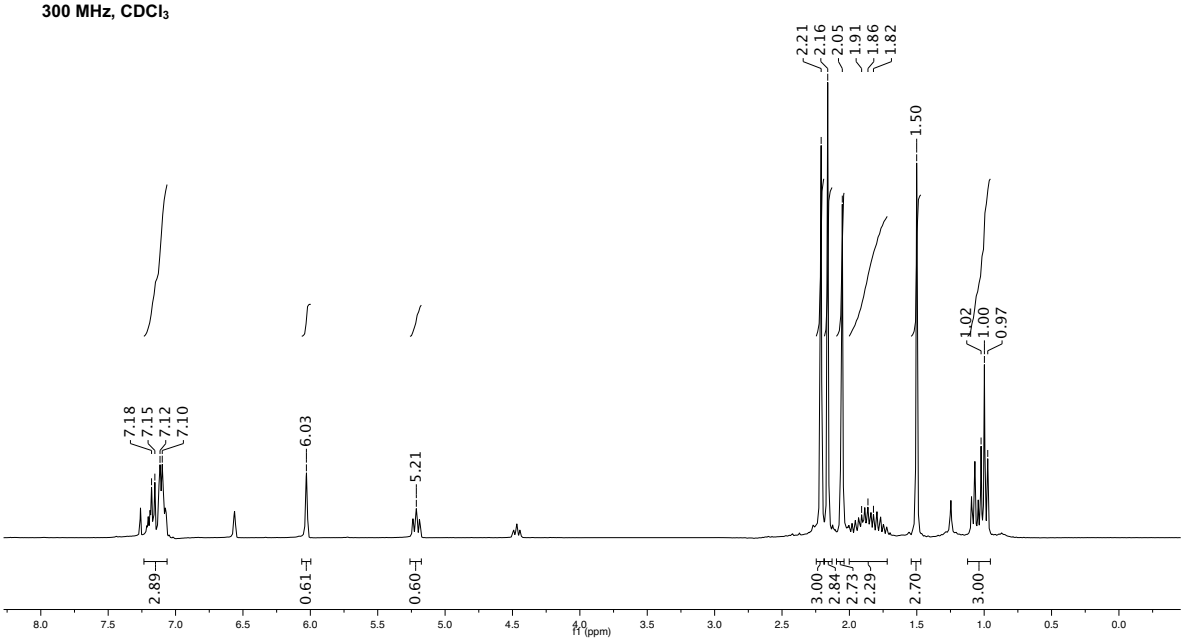
75 MHz, $CDCl_3$

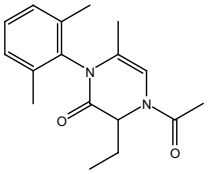


4-Acetyl-1-(2,6-dimethylphenyl)-3-ethyl-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13d)

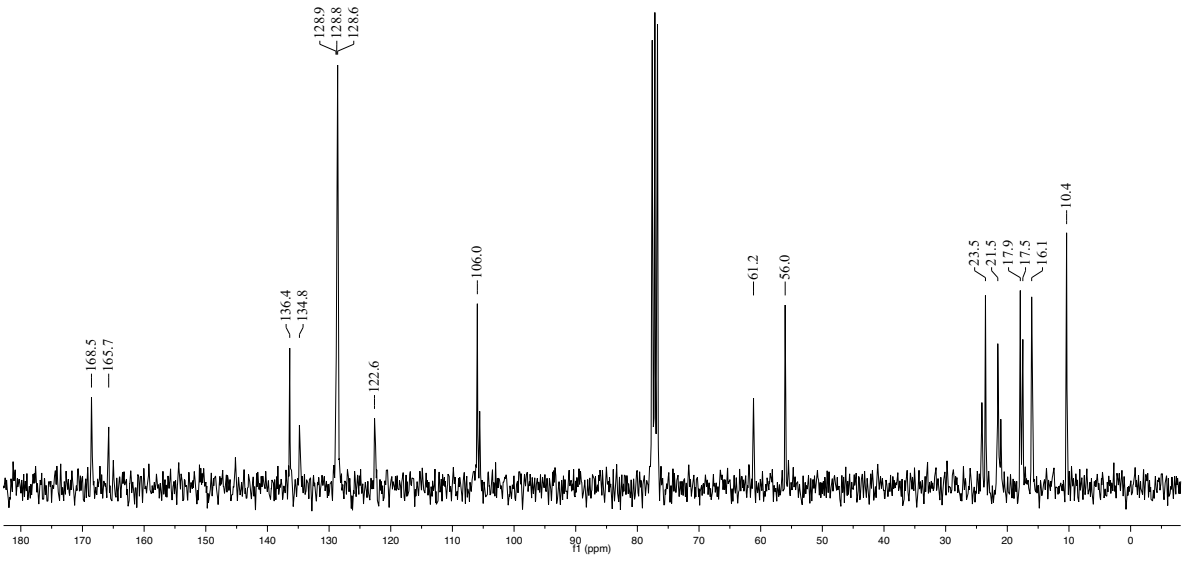


300 MHz, $CDCl_3$

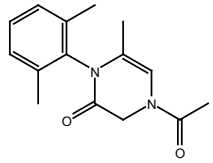




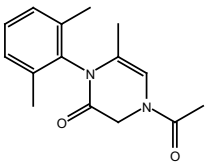
75MHz, $CDCl_3$



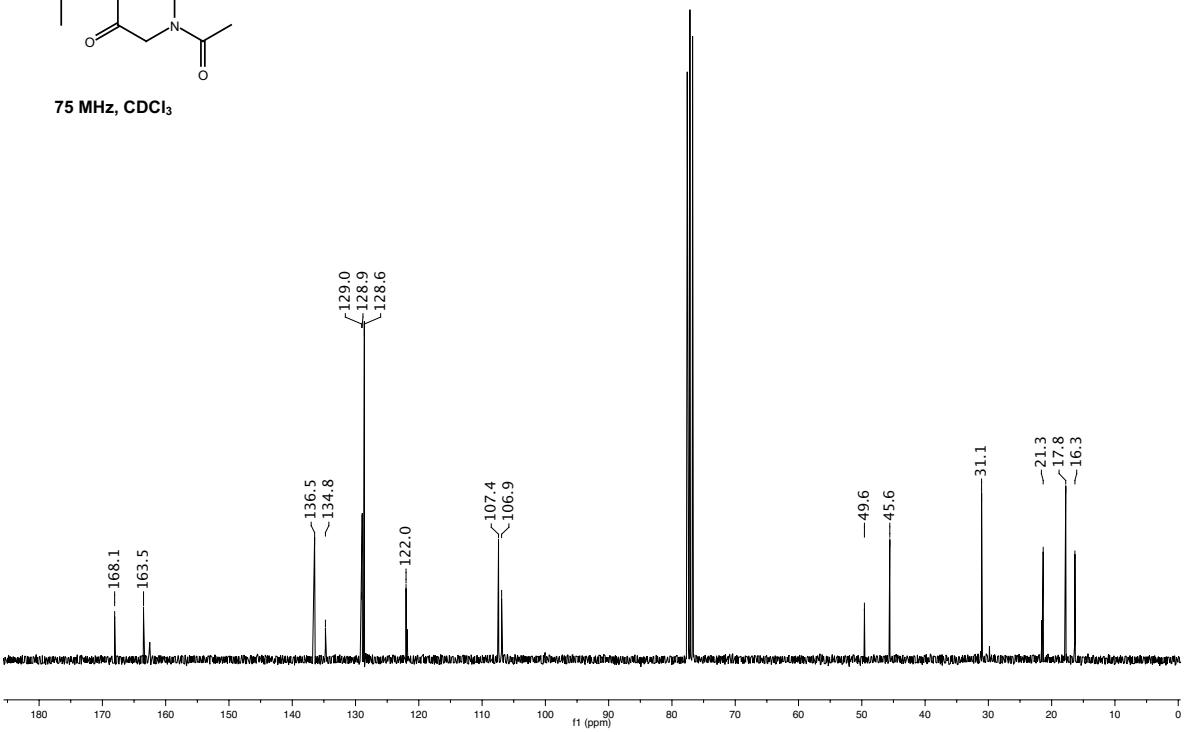
4-Acetyl-1-(2,6-dimethylphenyl)-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13e).



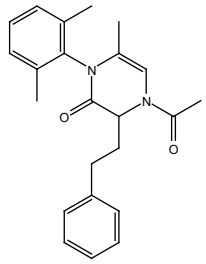
300 MHz, $CDCl_3$



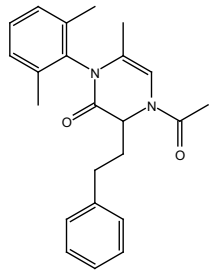
75 MHz, $CDCl_3$



4-Acetyl-1-(2,6-dimethylphenyl)-6-methyl-3-phenethyl-3,4-dihydropyrazin-2(1*H*)-one (13f)

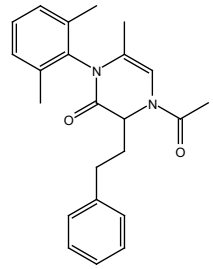


300 MHz, $CDCl_3$

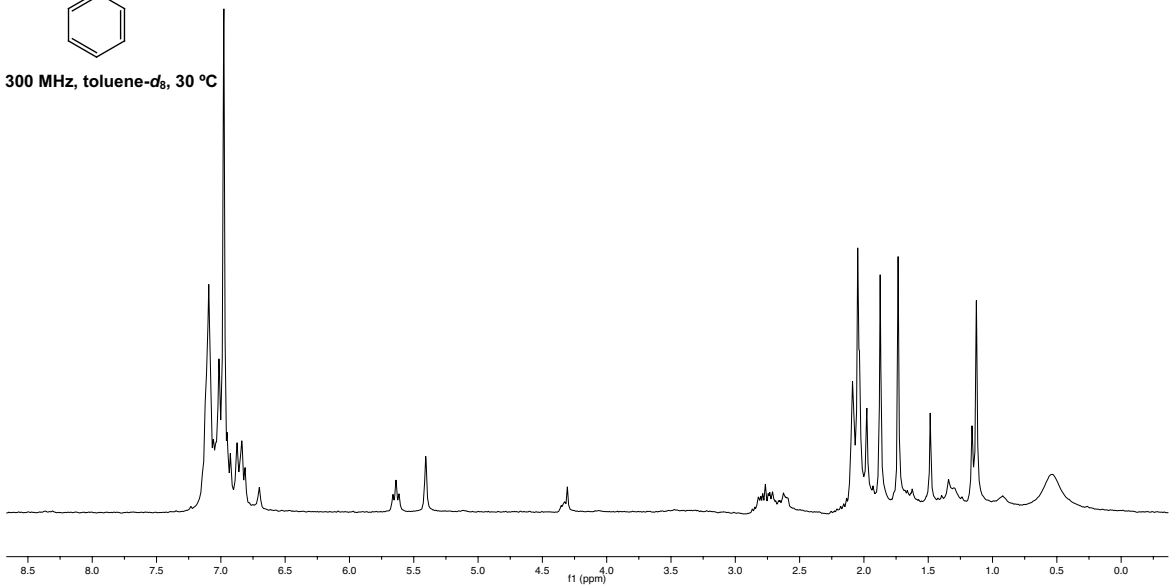


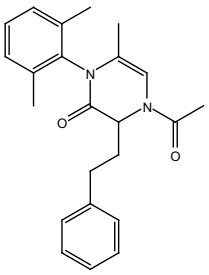
75 MHz, $CDCl_3$

(Variable-temperature ^{1}H NMR studies for compound 13f)

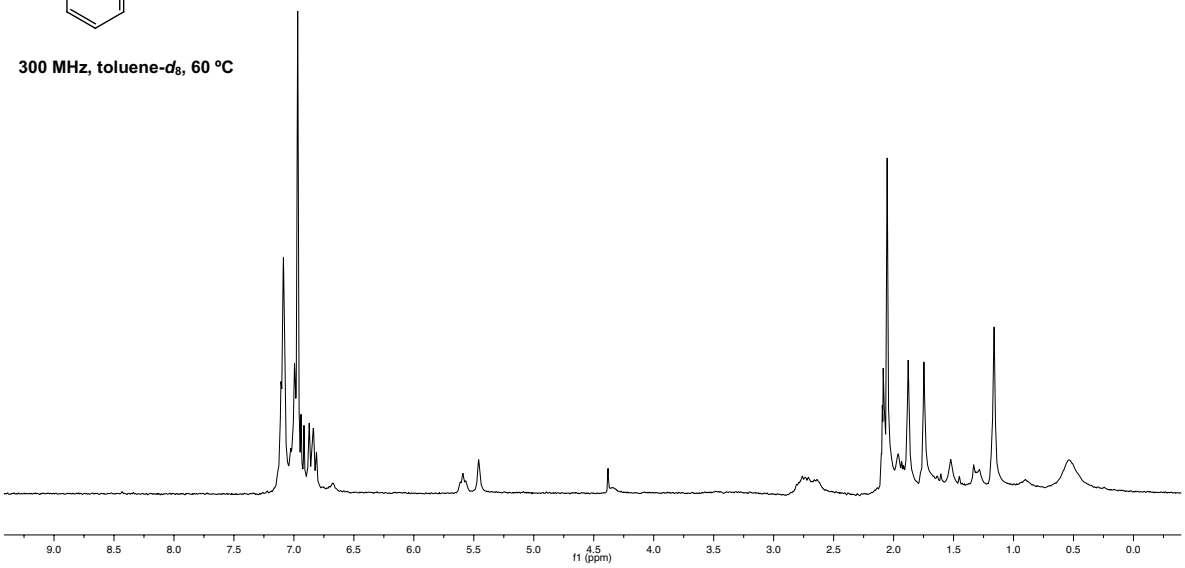


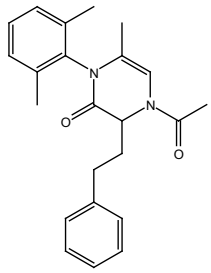
300 MHz, toluene-d_8, 30 ºC



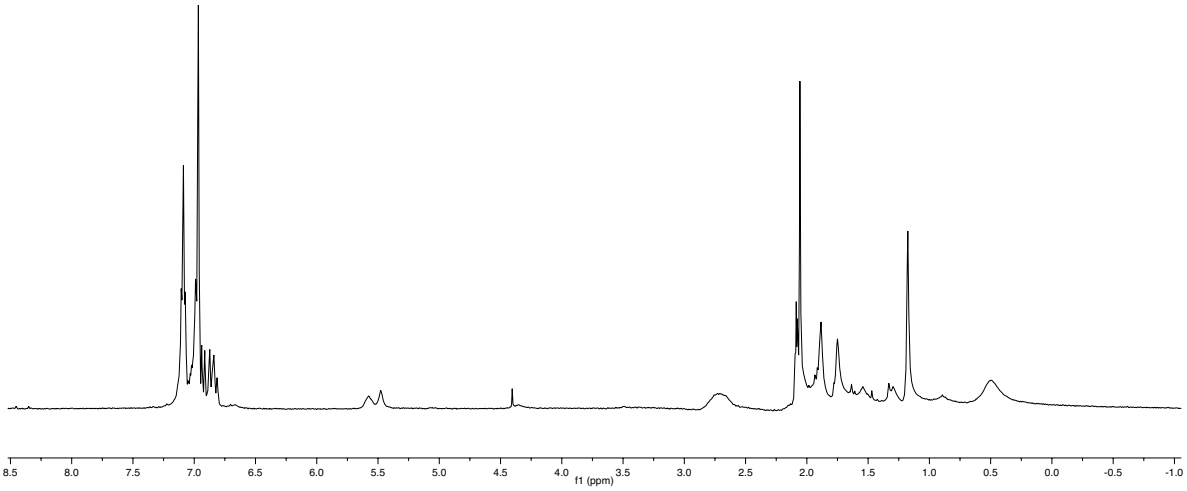


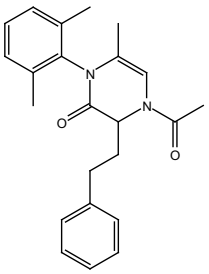
300 MHz, toluene-d_8, 60 ºC



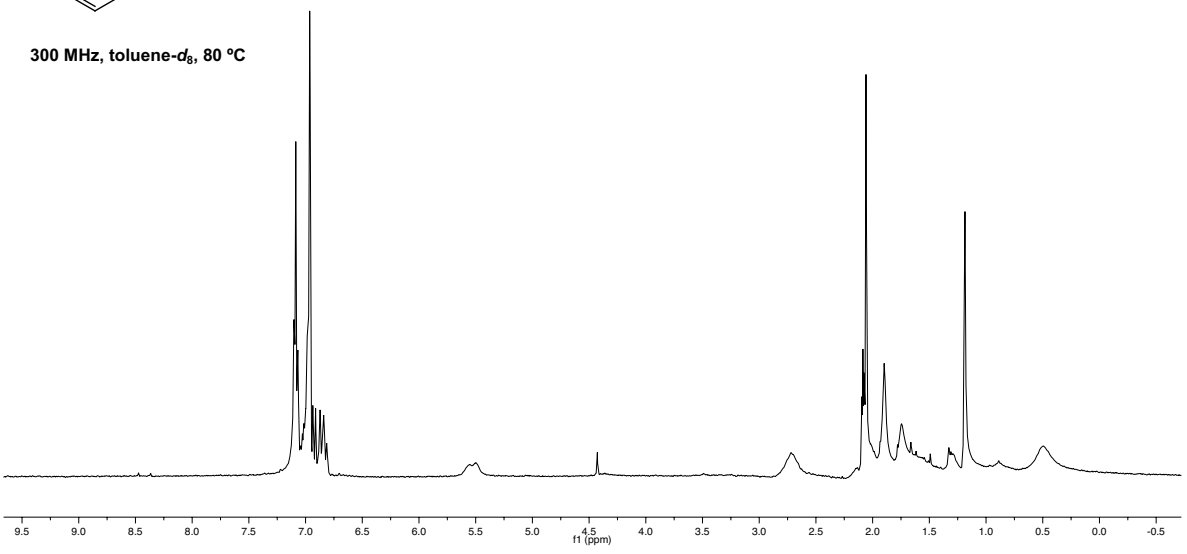


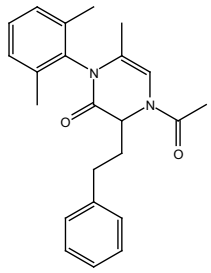
300 MHz, toluene-d_8, 70 ºC



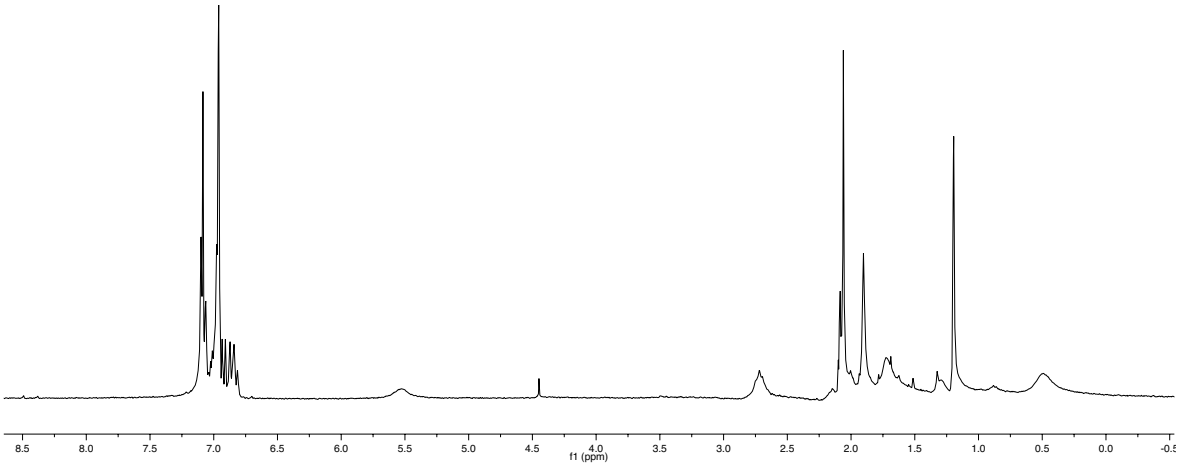


300 MHz, toluene-d_8, 80 ºC

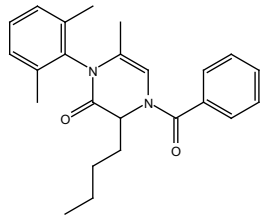




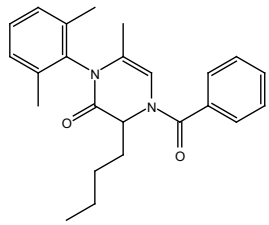
300 MHz, toluene-d_8, 90 ºC



4-Benzoyl-3-butyl-1-(2,6-dimethylphenyl)-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13g)

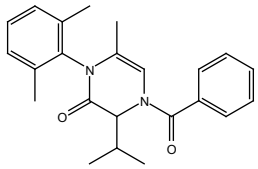


300 MHz, $CDCl_3$

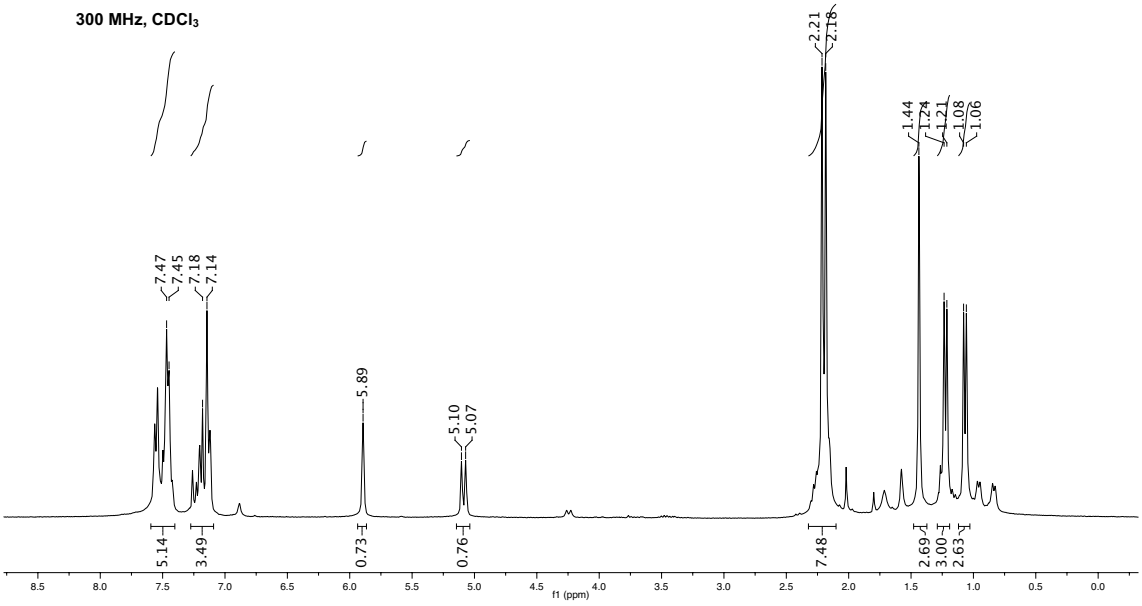


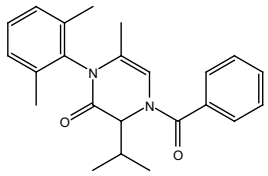
75 MHz, $CDCl_3$

4-Benzoyl-1-(2,6-dimethylphenyl)-3-isopropyl-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13h)

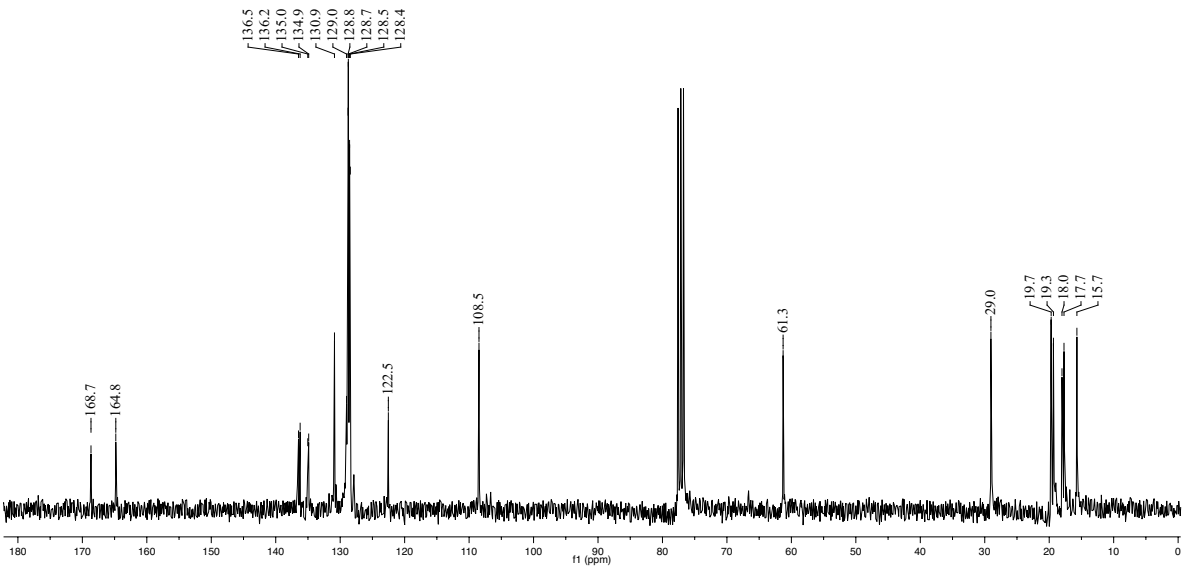


300 MHz, $CDCl_3$

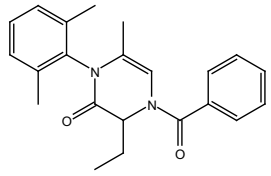




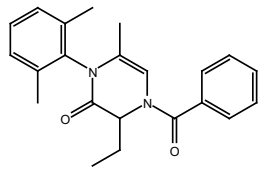
75 MHz, $CDCl_3$



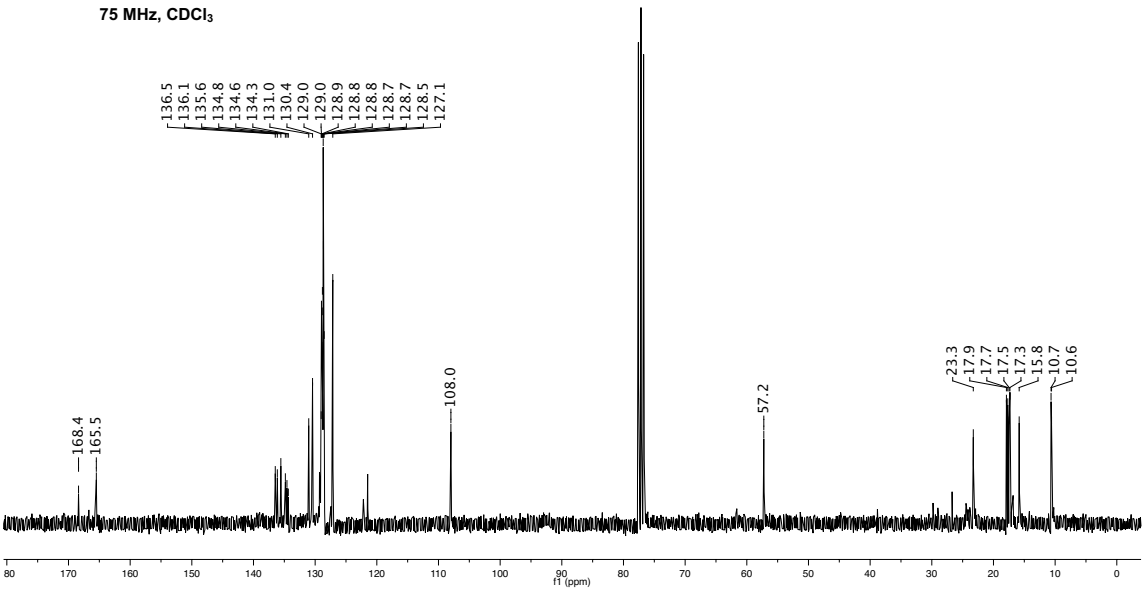
4-benzoyl-1-(2,6-dimethylphenyl)-3-ethyl-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13i).



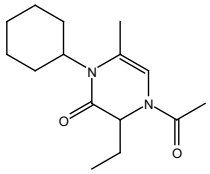
300 MHz, $CDCl_3$



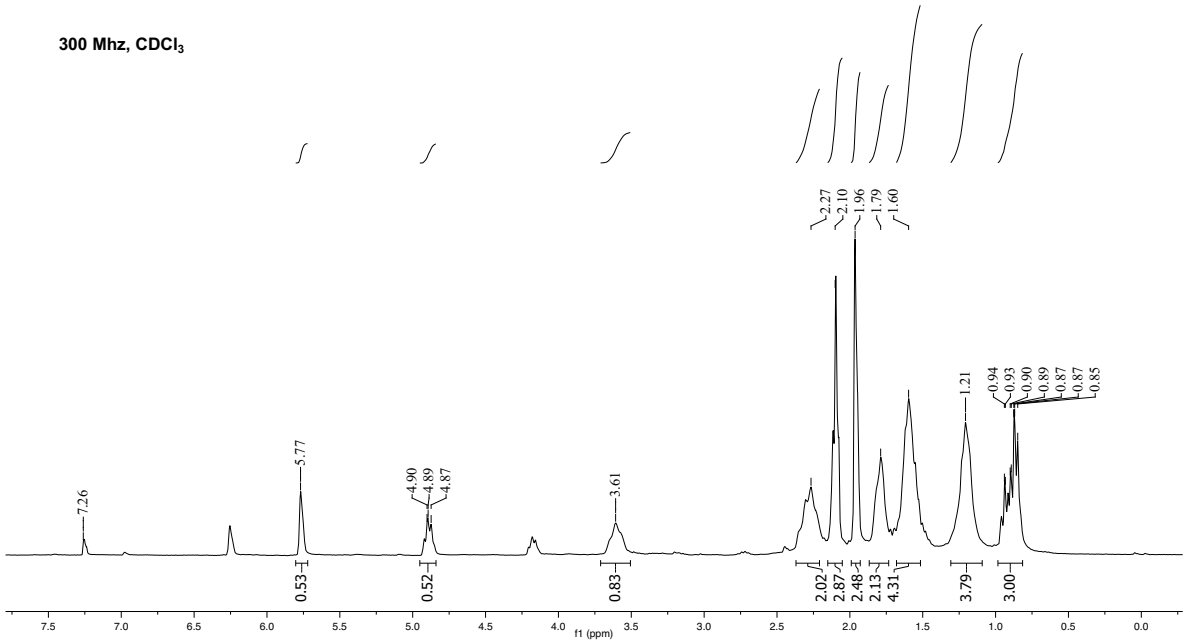
75 MHz, $CDCl_3$

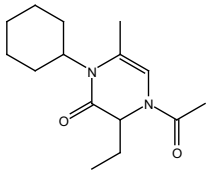


4-Acetyl-1-cyclohexyl-3-ethyl-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13j)

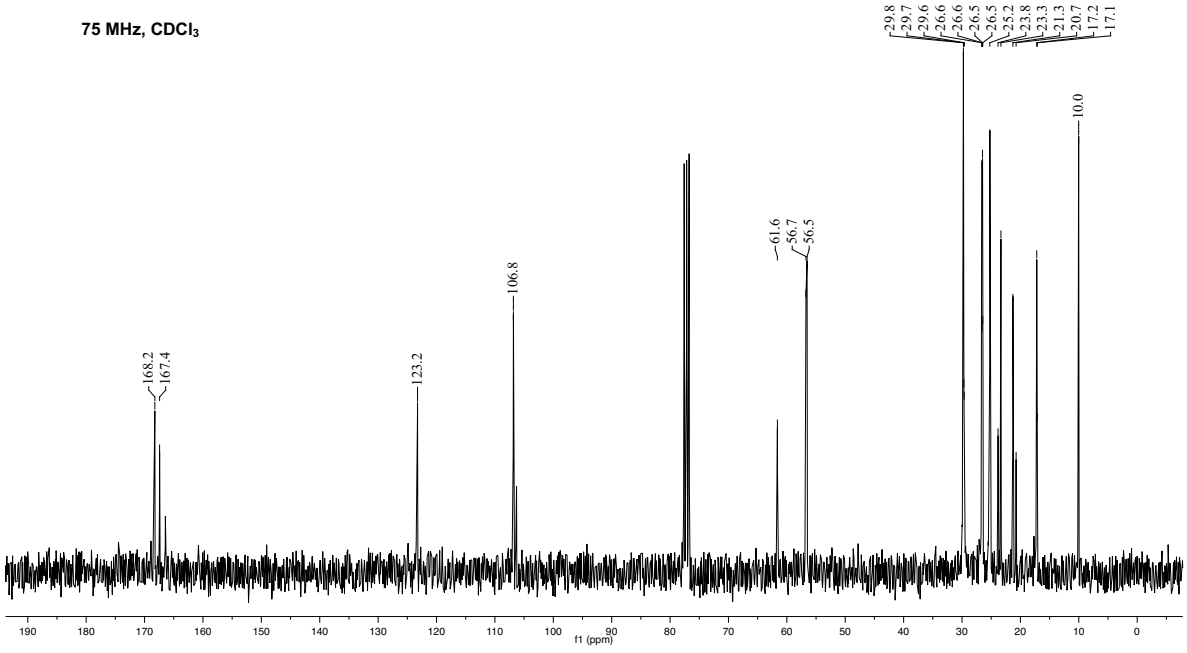


300 Mhz, $CDCl_3$

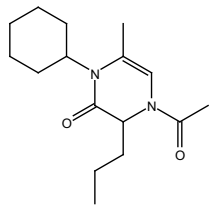




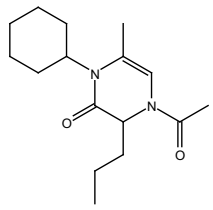
75 MHz, $CDCl_3$



4-Acetyl-1-cyclohexyl-6-methyl-3-propyl-3,4-dihydropyrazin-2(1*H*)-one (13k)

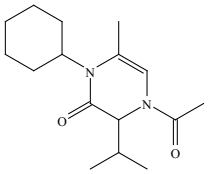


300 MHz, $CDCl_3$

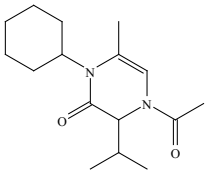


75 MHz, $CDCl_3$

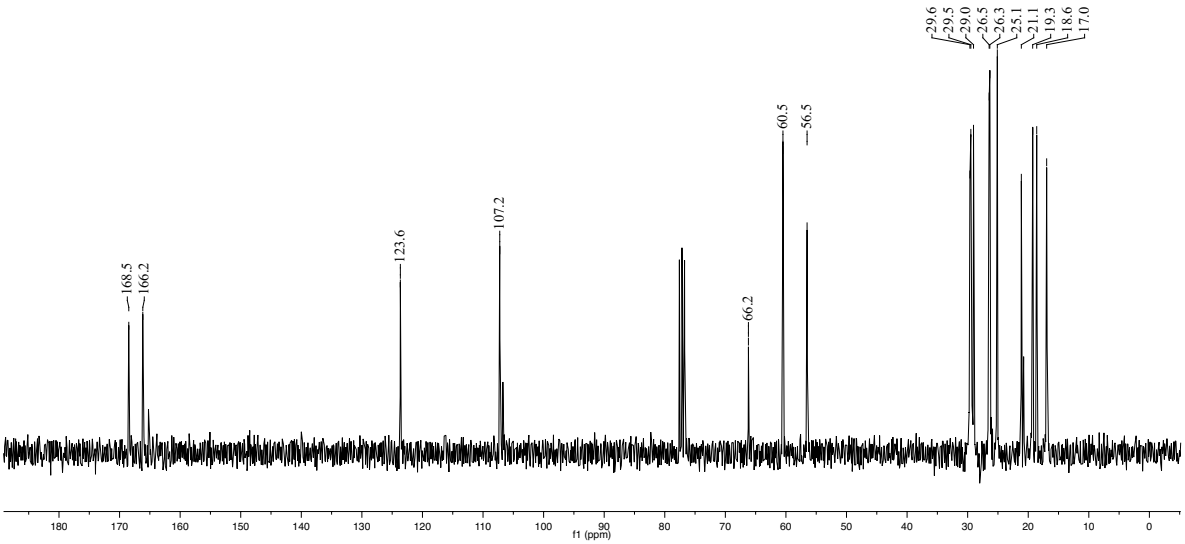
4-Acetyl-1-cyclohexyl-3-isopropyl-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13l)



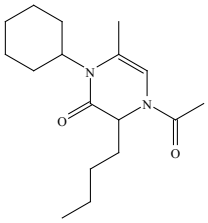
300 MHz, $CDCl_3$



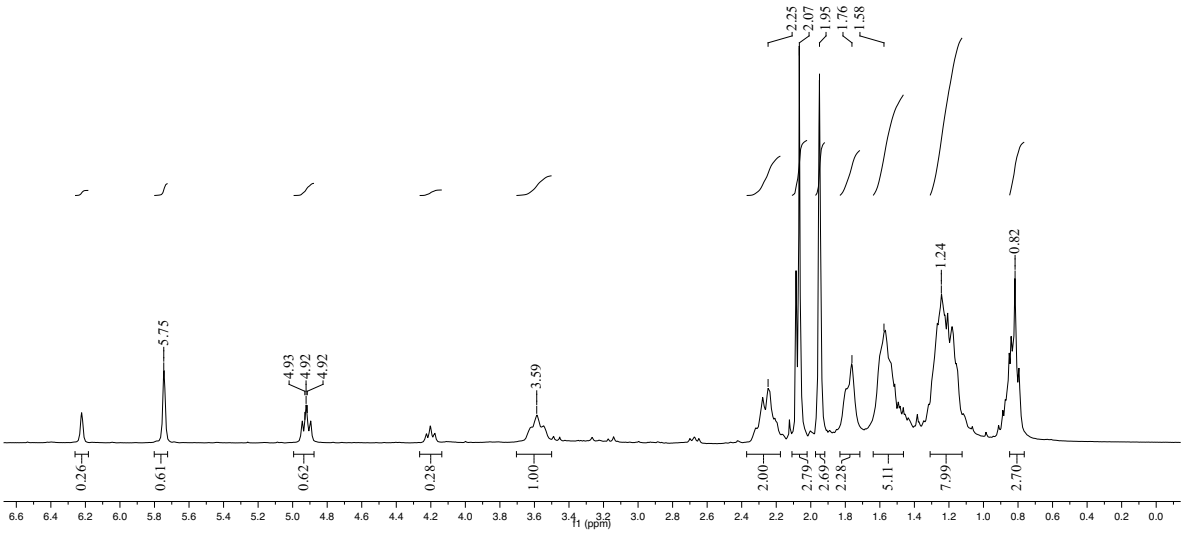
75 MHz, $CDCl_3$

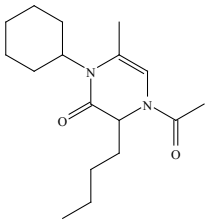


4-Acetyl-3-butyl-1-cyclohexyl-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13m)

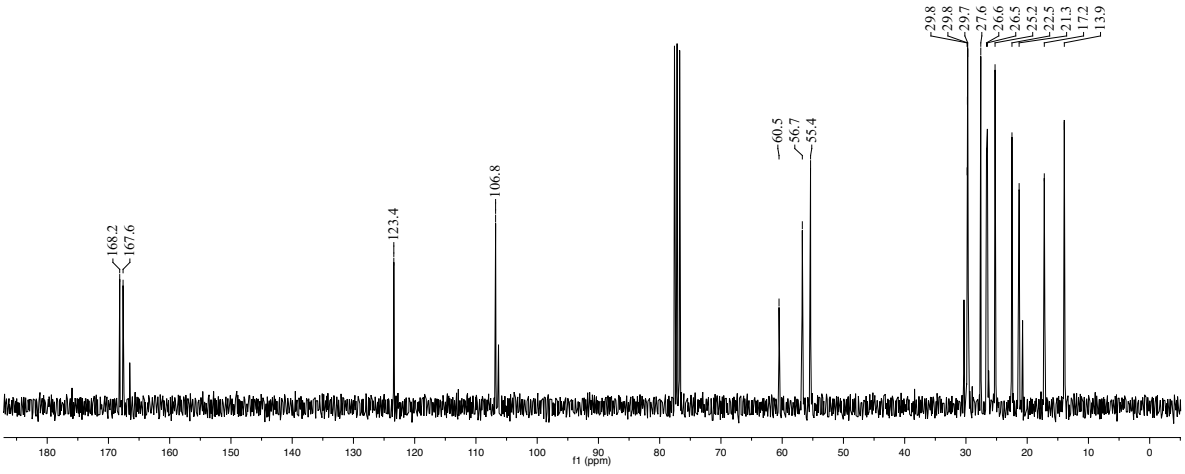


300 MHz, $CDCl_3$

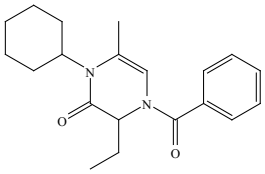




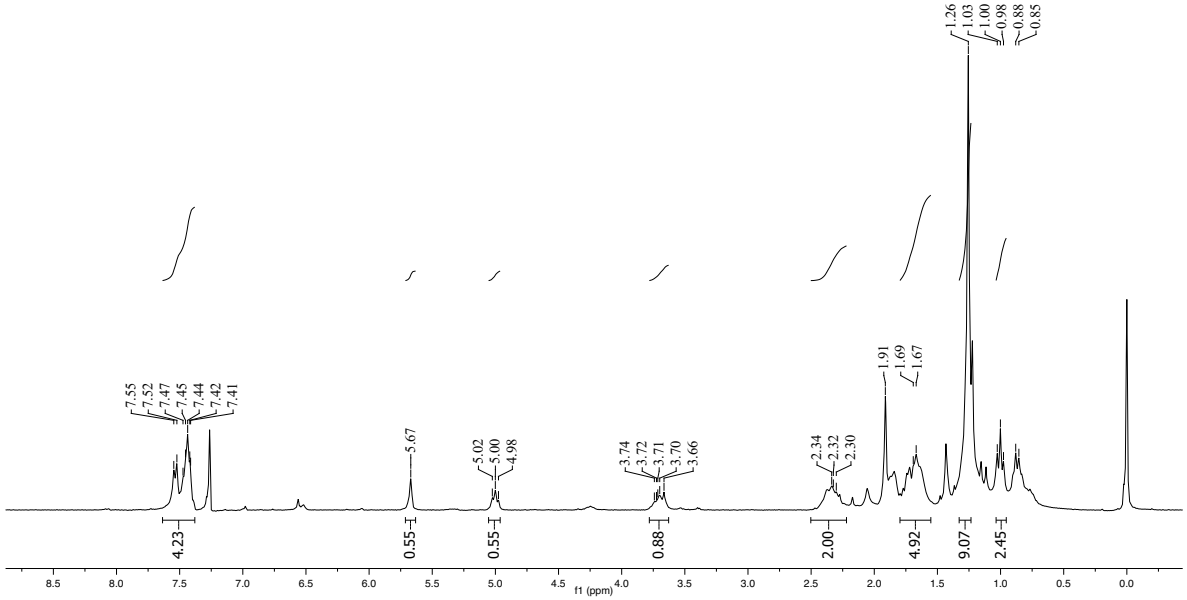
75 MHz, $CDCl_3$

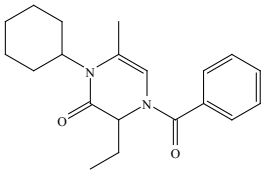


4-Benzoyl-1-cyclohexyl-3-ethyl-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13n)

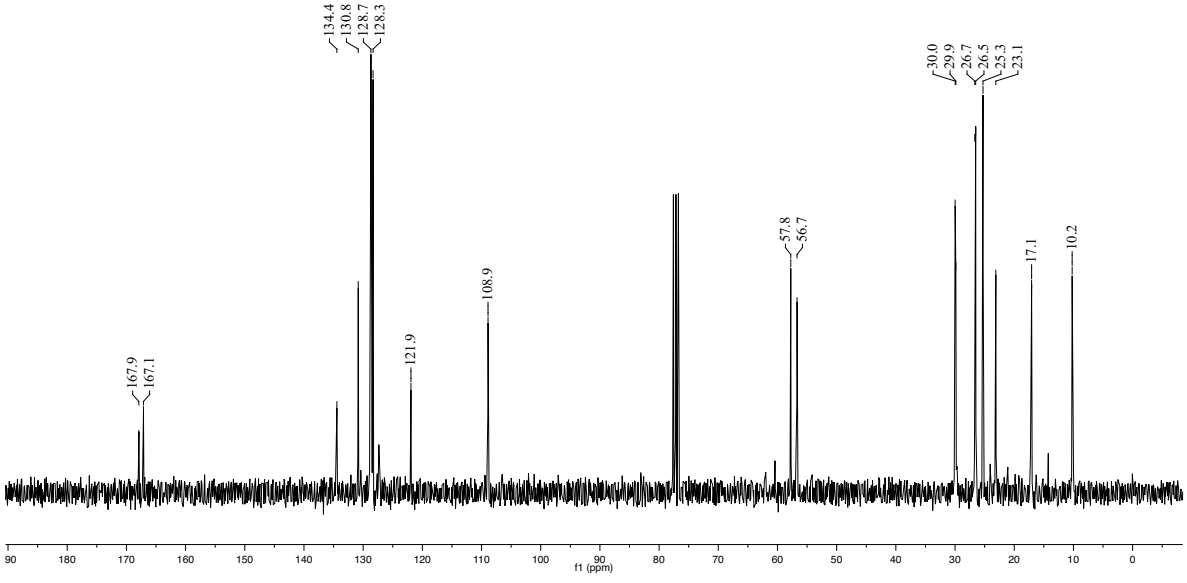


300 MHz, $CDCl_3$

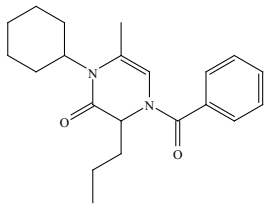




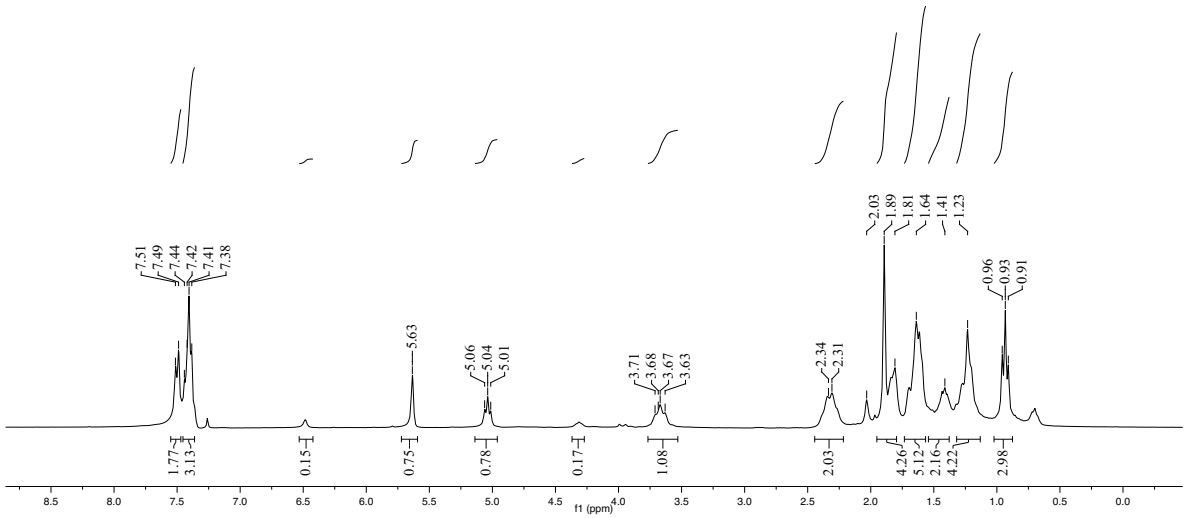
75 MHz, $CDCl_3$

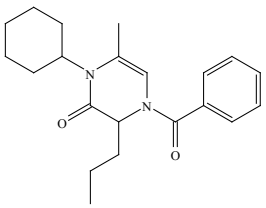


4-Benzoyl-1-cyclohexyl-6-methyl-3-propyl-3,4-dihydropyrazin-2(1*H*)-one (13o)

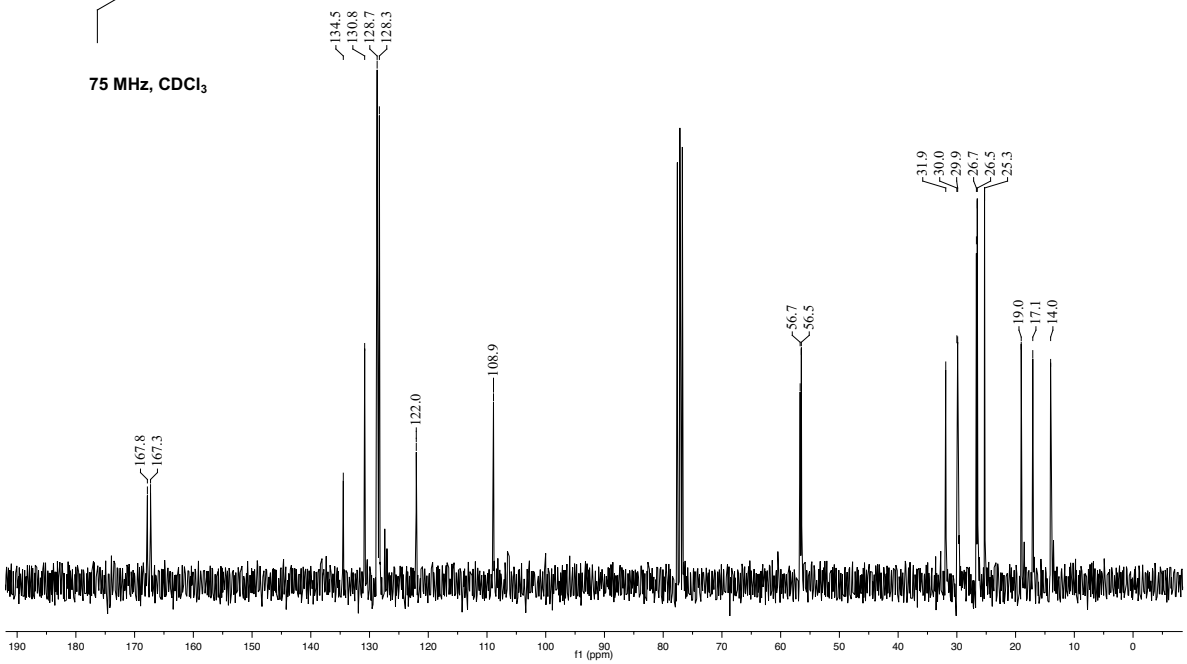


300 MHz, $CDCl_3$

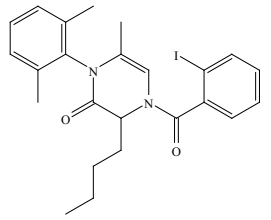


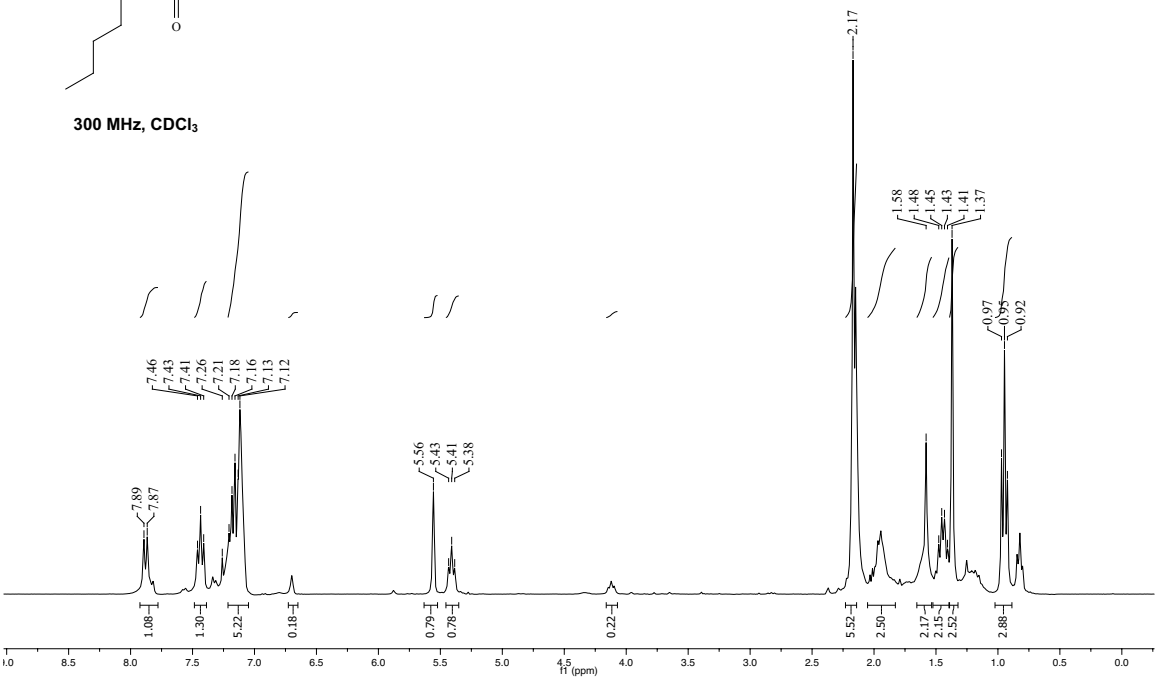


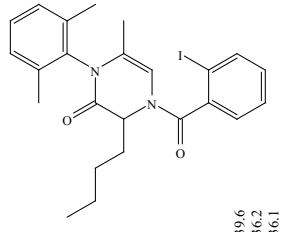
75 MHz, $CDCl_3$

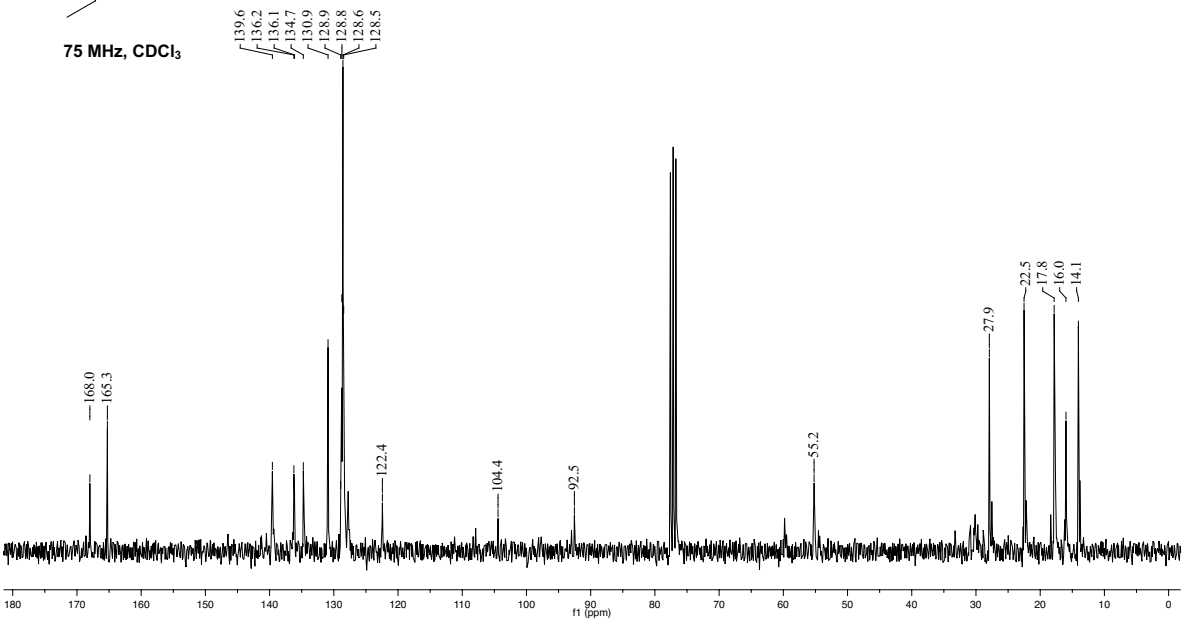


3-Butyl-1-(2,6-dimethylphenyl)-4-(2-iodobenzoyl)-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13p)

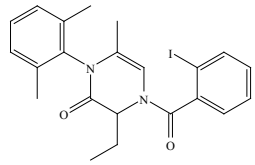


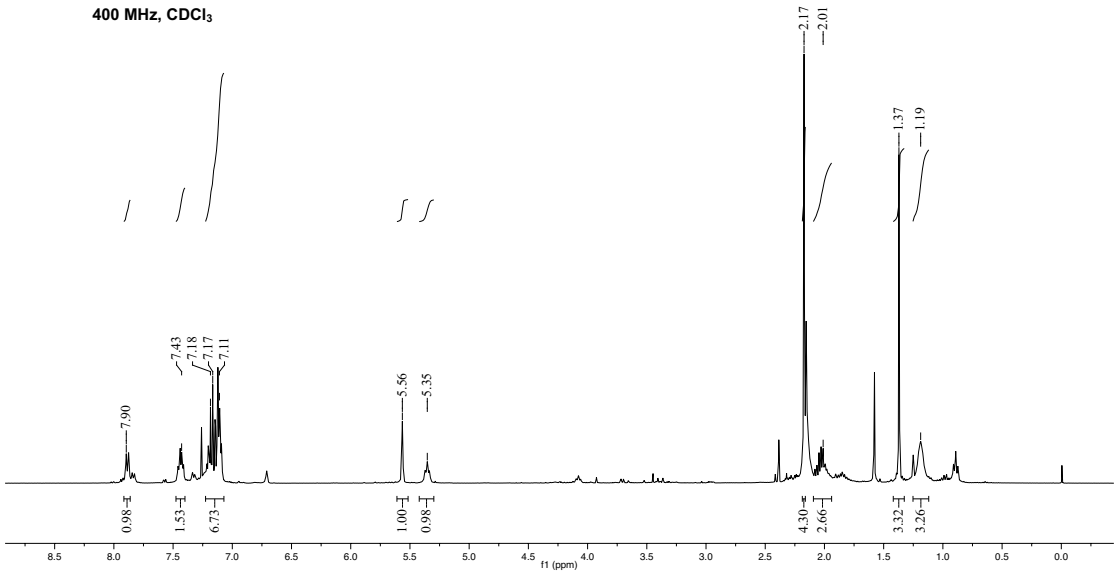


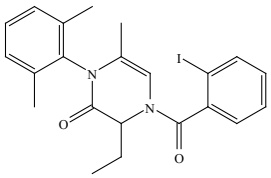


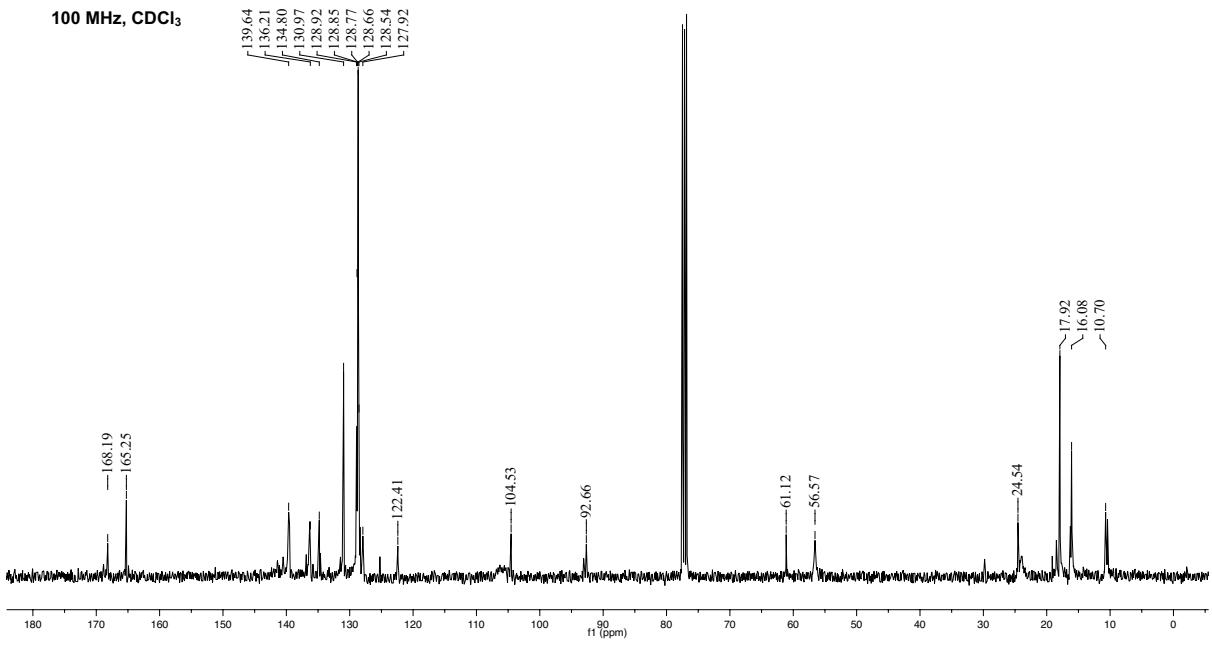


1-(2,6-Dimethylphenyl)-3-ethyl-4-(2-iodobenzoyl)-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13q)

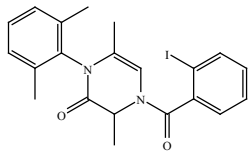




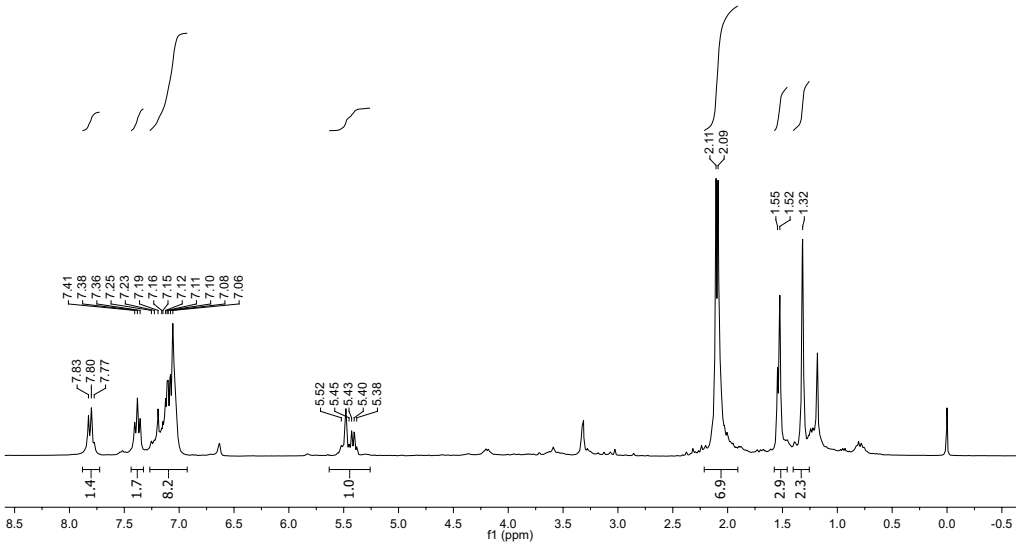


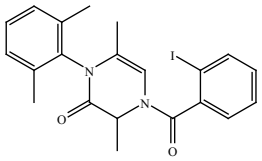


1-(2,6-Dimethylphenyl)-4-(2-iodobenzoyl)-3,6-dimethyl-3,4-dihydropyrazin-2(1*H*)-one (13r).

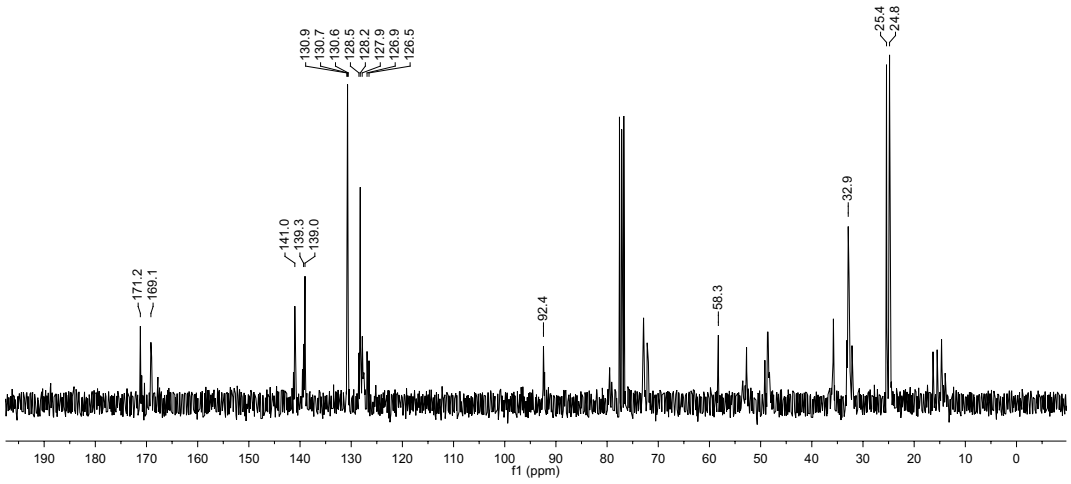


300 MHz, $CDCl_3$

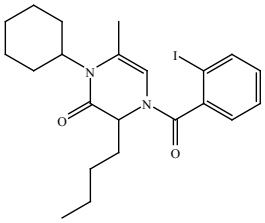




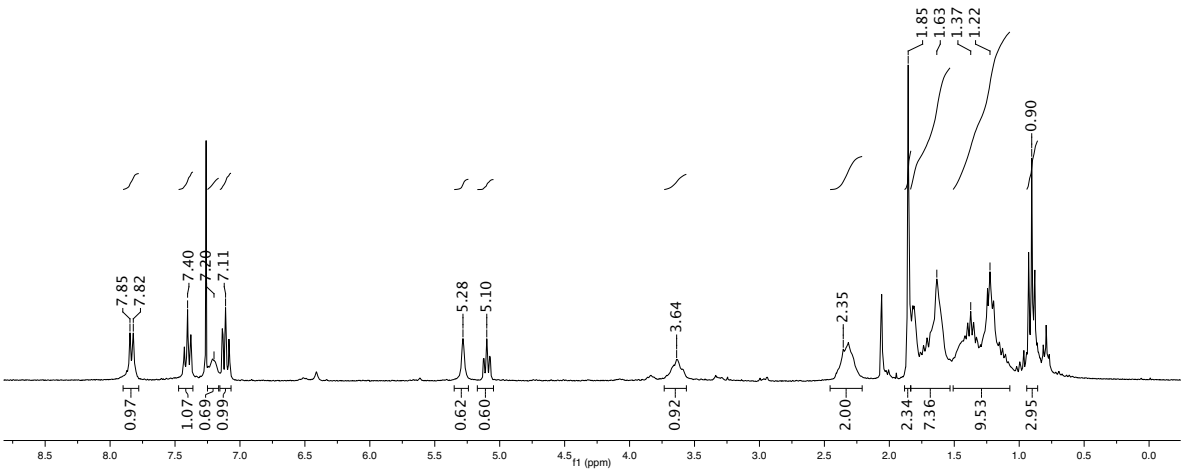
75 MHz, $CDCl_3$

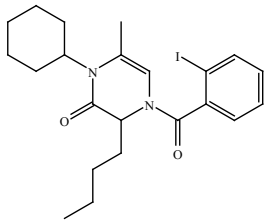


3-Butyl-1-cyclohexyl-4-(2-iodobenzoyl)-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13s)



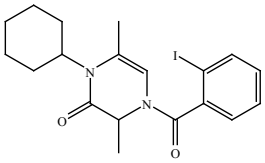
300 MHz, $CDCl_3$



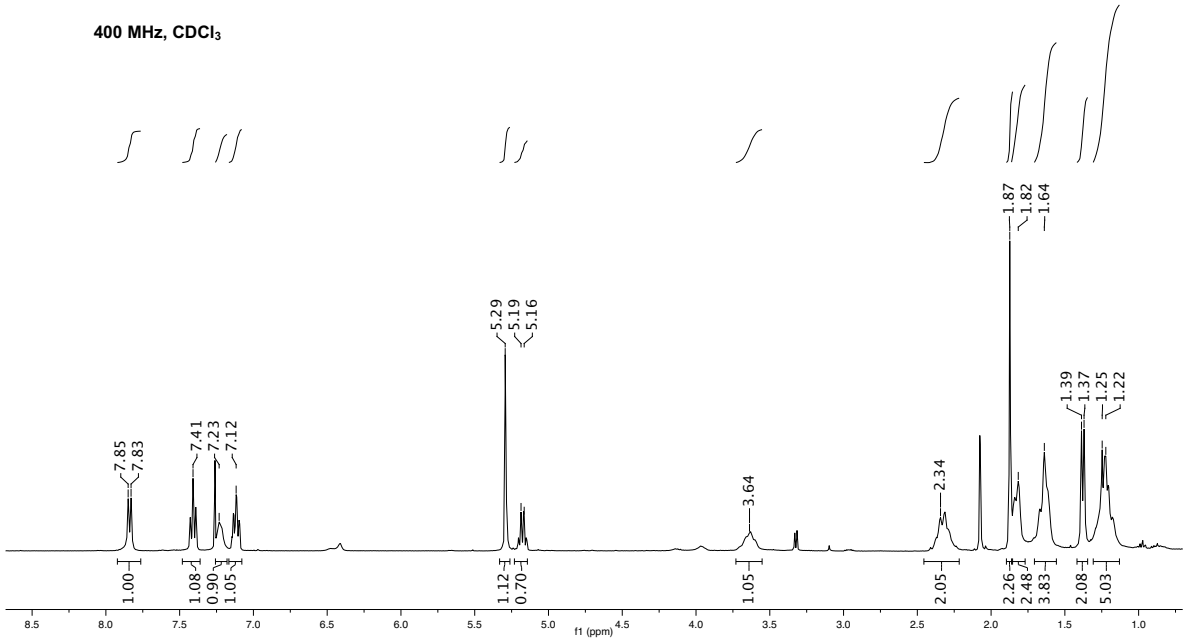


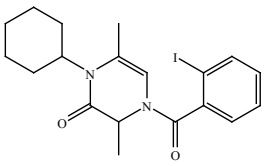
75 MHz, $CDCl_3$

1-Cyclohexyl-4-(2-iodobenzoyl)-3,6-dimethyl-3,4-dihydropyrazin-2(1*H*)-one (13t)

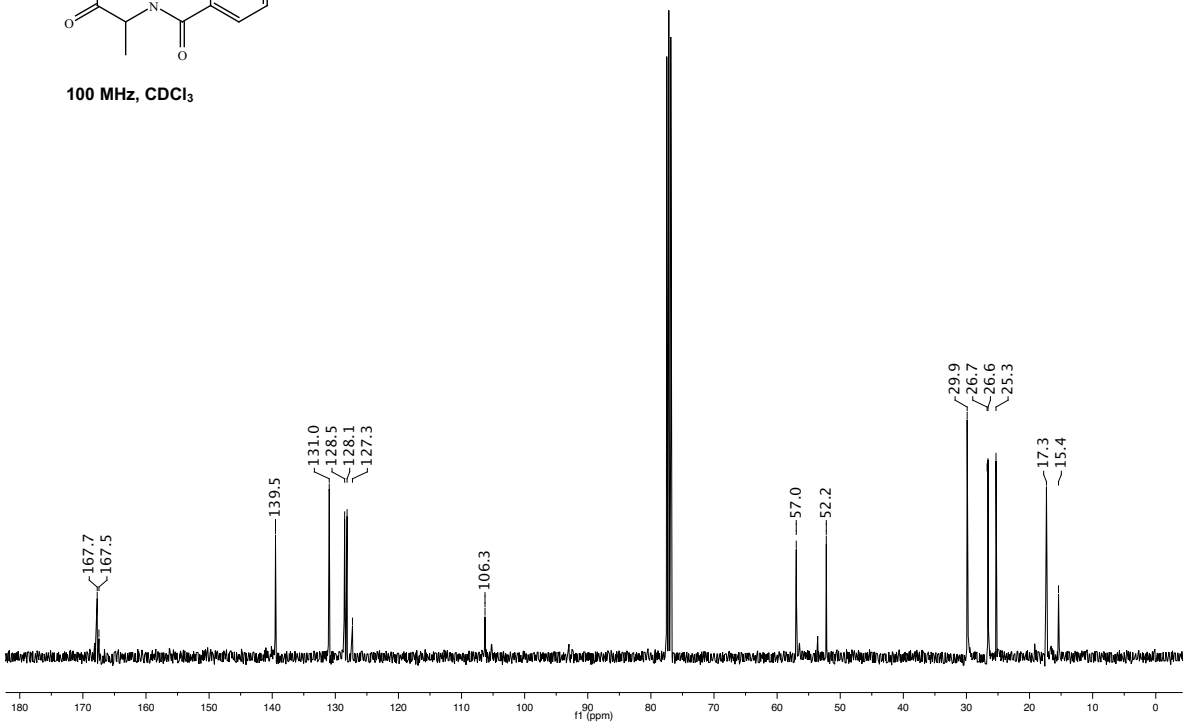


400 MHz, $CDCl_3$

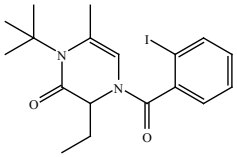




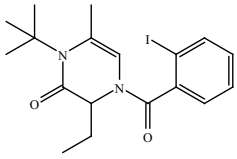
100 MHz, $CDCl_3$



1-(*Tert*-butyl)-3-ethyl-4-(2-iodobenzoyl)-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13u)

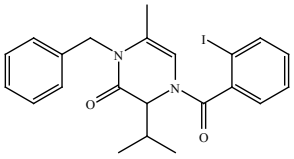


300 MHz, $CDCl_3$

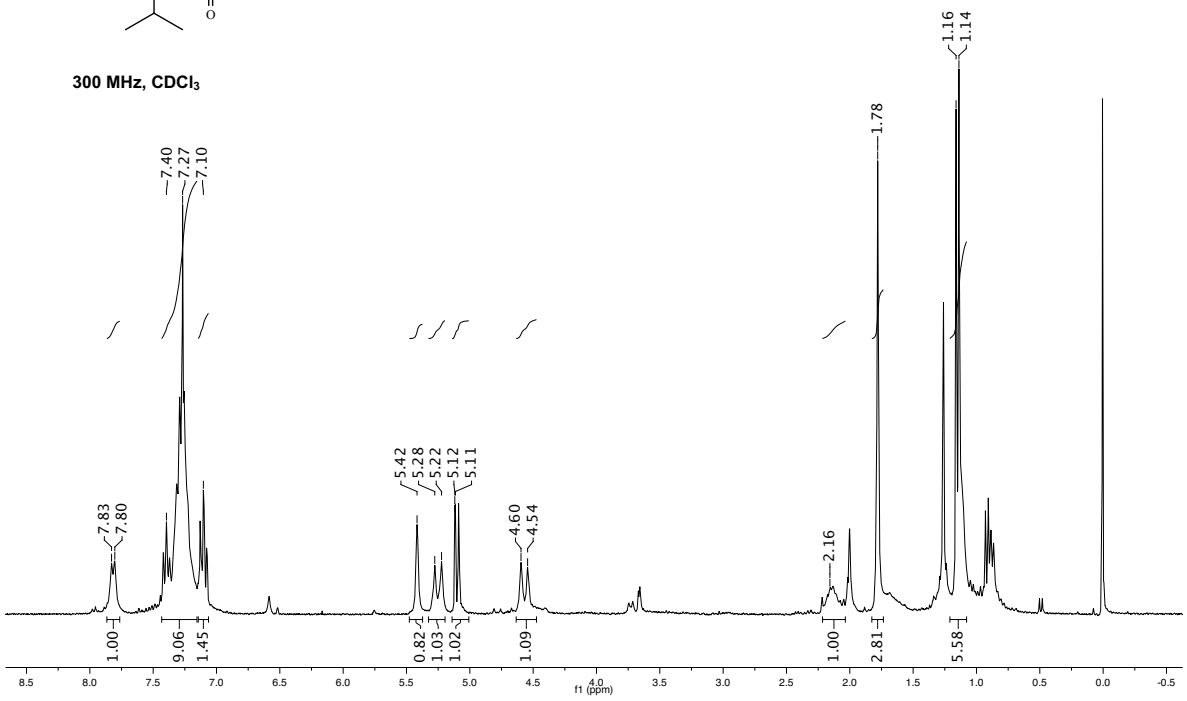


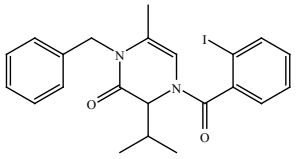
75 MHz, $CDCl_3$

1-Benzyl-4-(2-iodobenzoyl)-3-isopropyl-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13v)

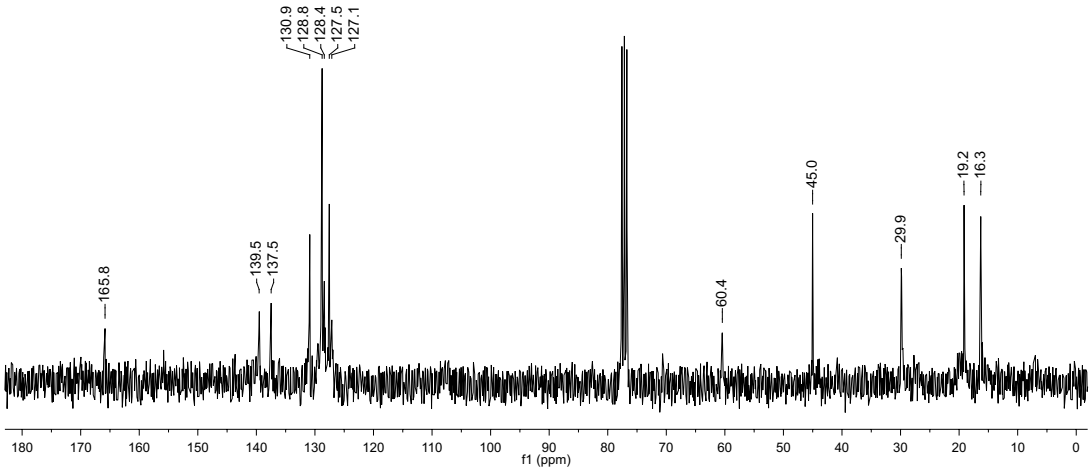


300 MHz, $CDCl_3$

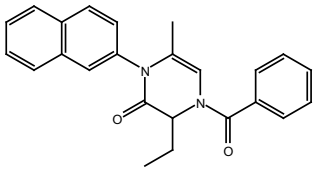




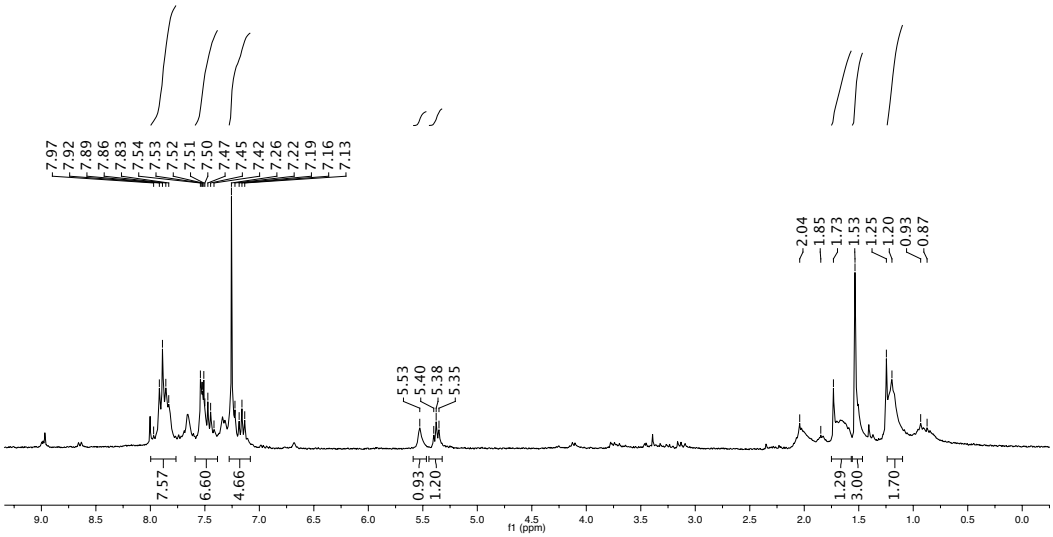
75 MHz, $CDCl_3$

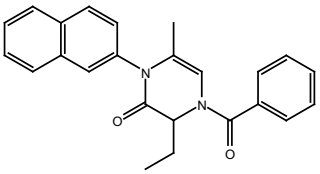


3-Ethyl-4-(2-iodobenzoyl)-6-methyl-1-(naphthalen-2-yl)-3,4-dihydropyrazin-2(1*H*)-one (13w)

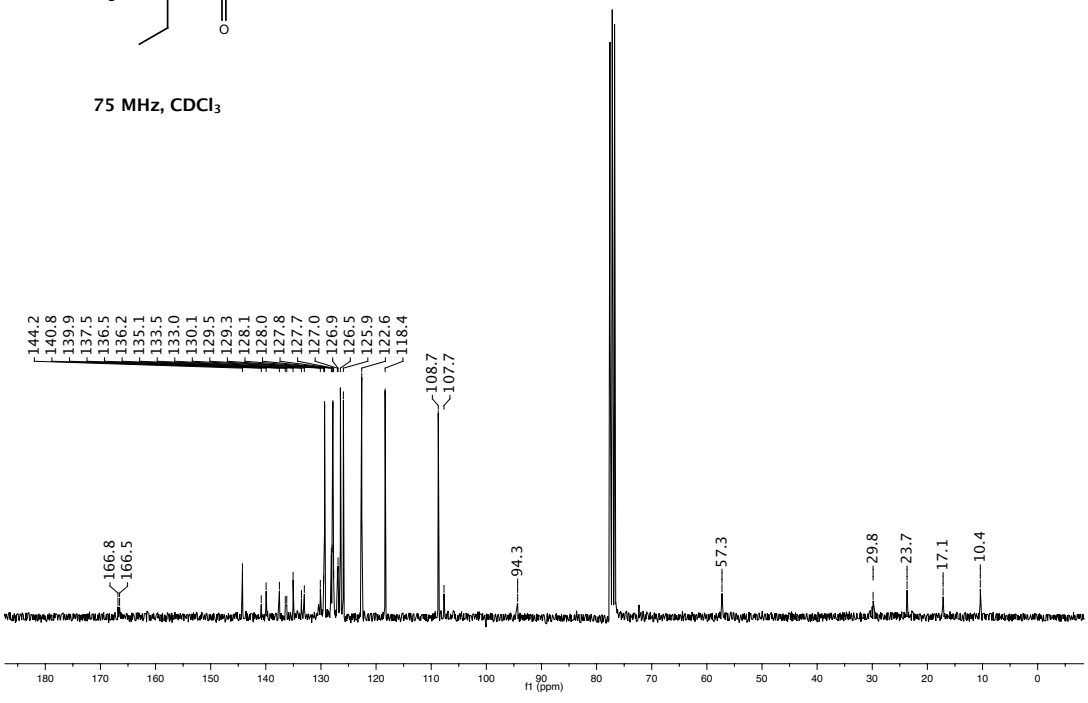


300 MHz, $CDCl_3$

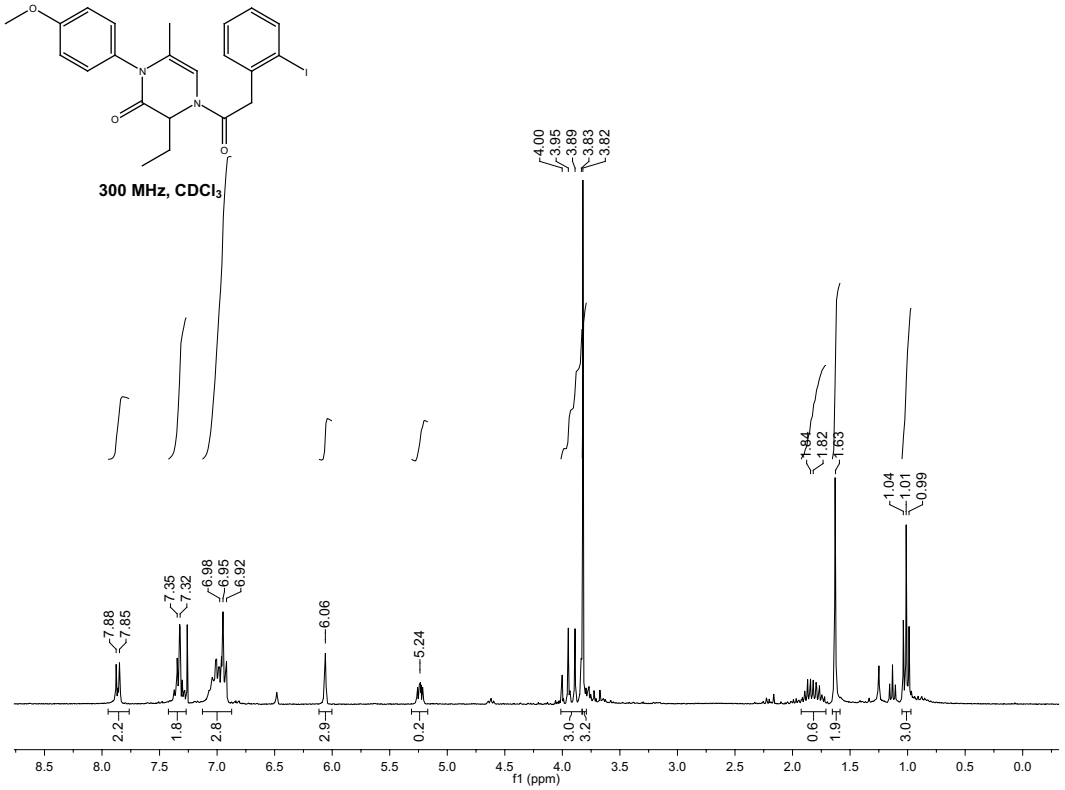


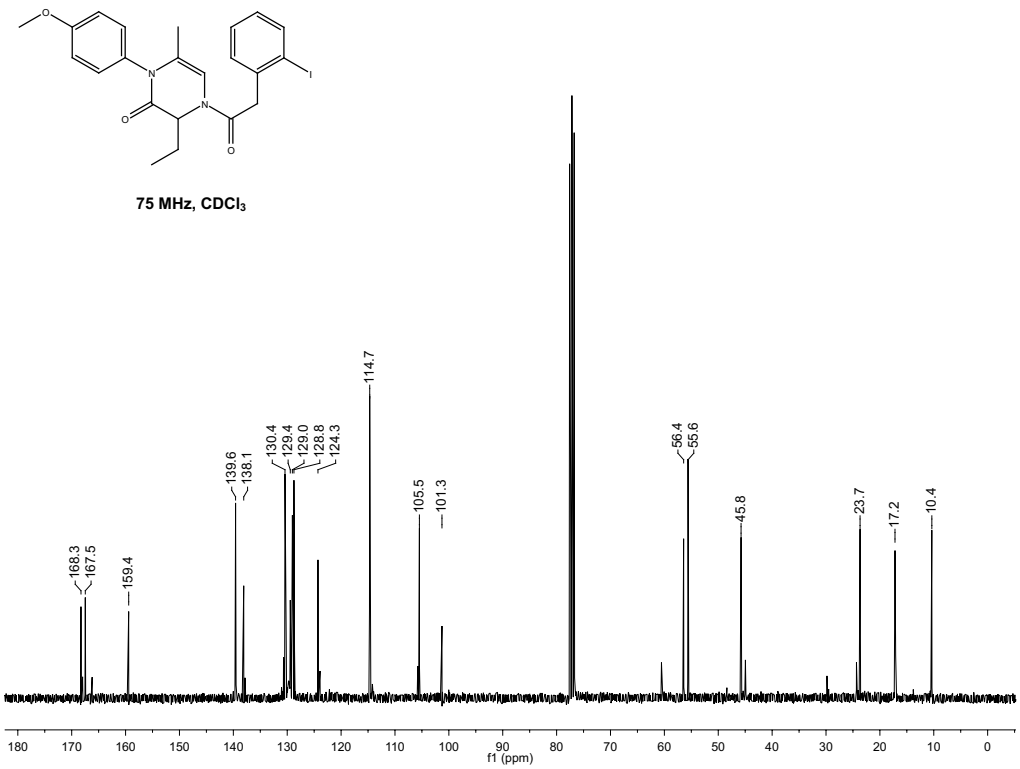


75 MHz, $CDCl_3$

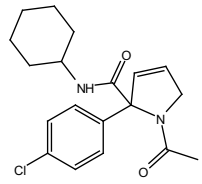


3-Ethyl-4-(2-(2-iodophenyl)acetyl)-1-(4-methoxyphenyl)-6-methyl-3,4-dihydropyrazin-2(1*H*)-one (13x)

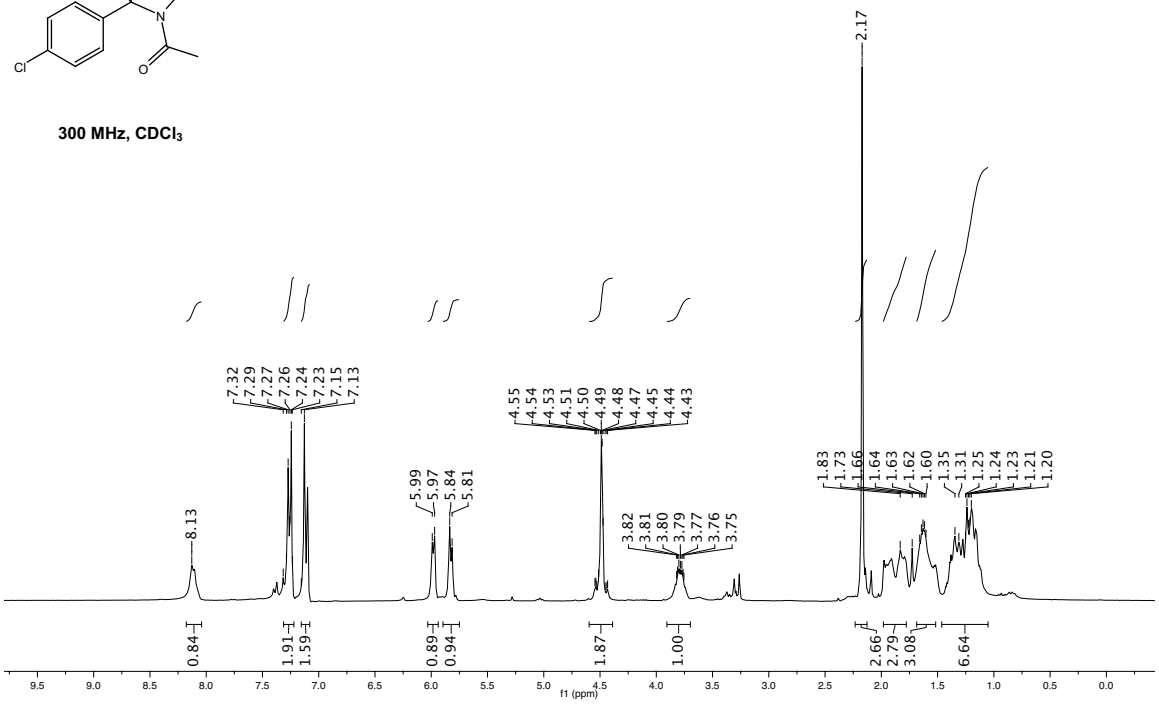


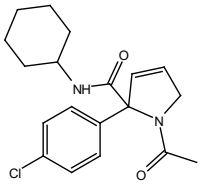


1-Acetyl-2-(4-chlorophenyl)-*N*-cyclohexyl-2,5-dihydro-1*H*-pyrrole-2-carboxamide (12y)

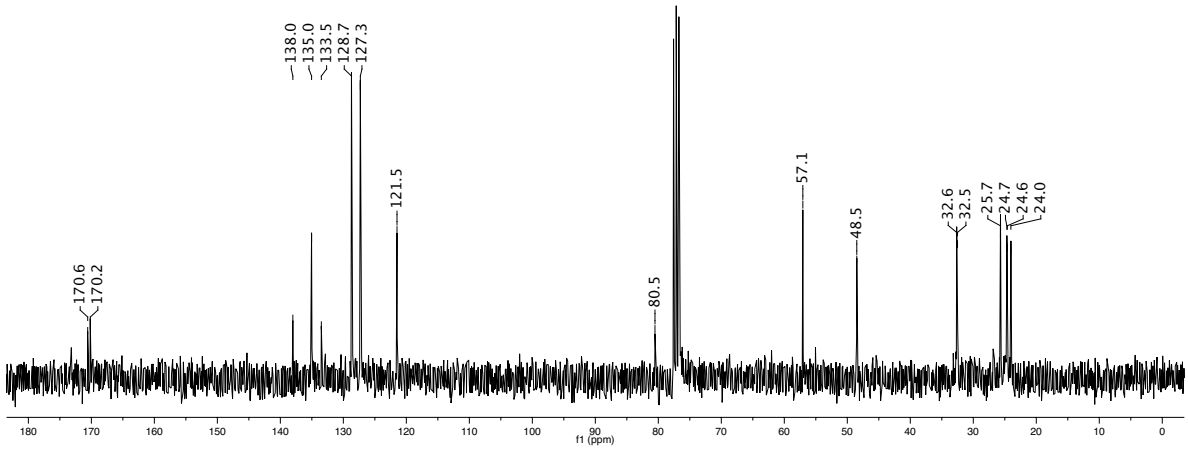


300 MHz, $CDCl_3$



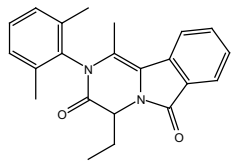


75 MHz, $CDCl_3$

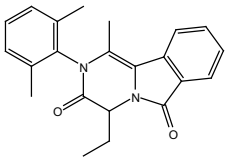


Tricyclic pyrazinone spectra

2-(2,6-Dimethylphenyl)-4-ethyl-1-methylpyrazino[2,1-*a*]isoindole-3,6(2*H*,4*H*)-dione (14q)

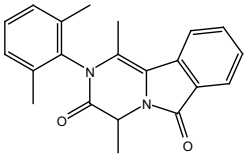


400 MHz, $CDCl_3$

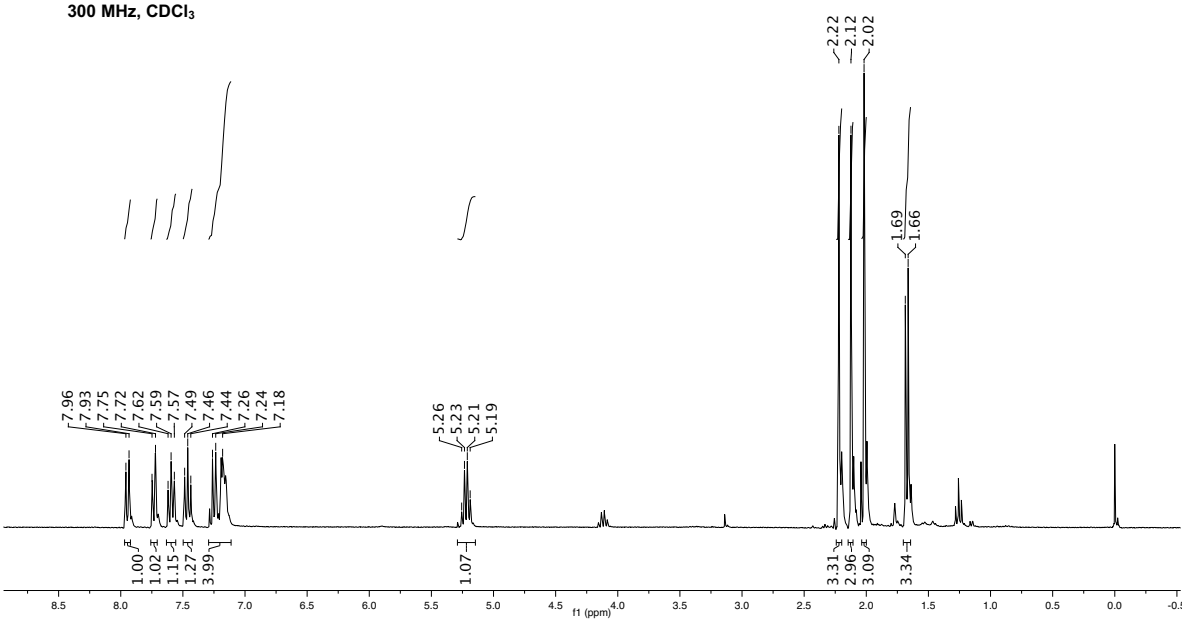


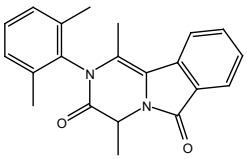
100 MHz, $CDCl_3$

2-(2,6-Dimethylphenyl)-1,4-dimethylpyrazino[2,1-*a*]isoindole-3,6(2*H*,4*H*)-dione (14r)

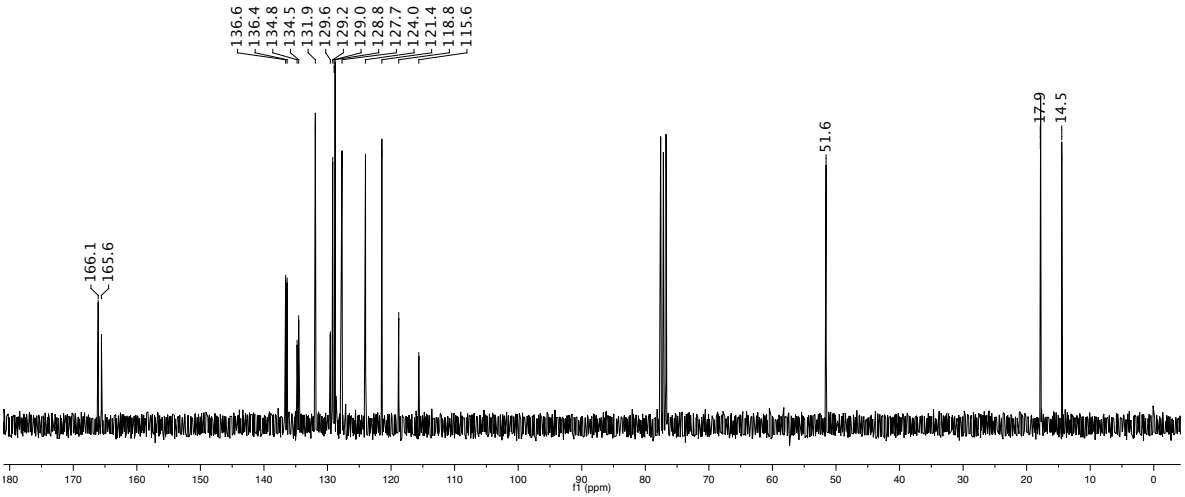


300 MHz, $CDCl_3$

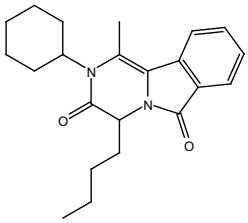




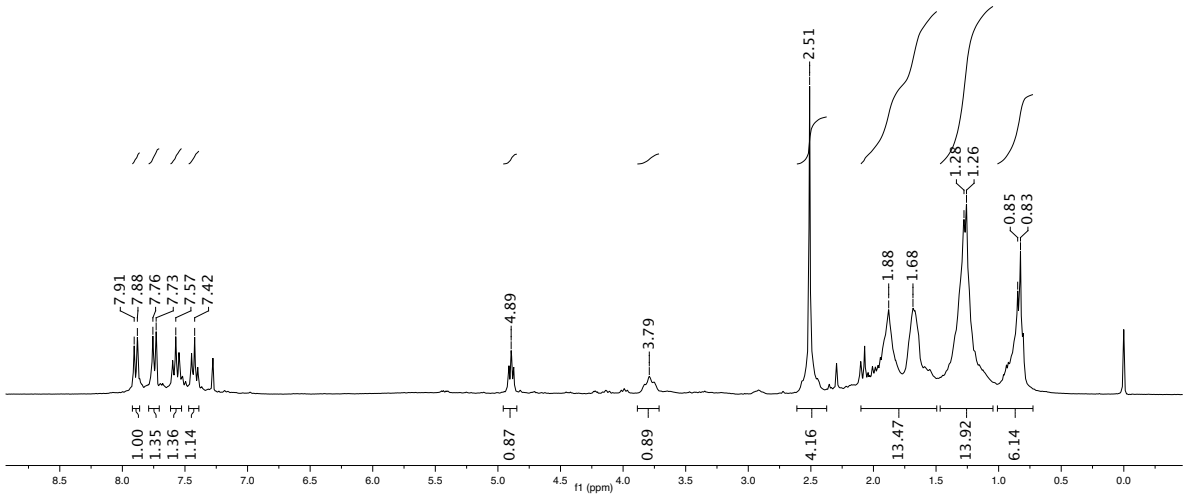
75 MHz, $CDCl_3$

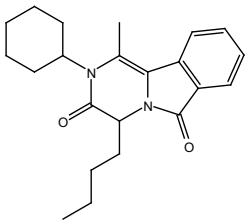


4-Butyl-2-cyclohexyl-1-methylpyrazino[2,1-*a*]isoindole-3,6(2*H*,4*H*)-dione (14s)

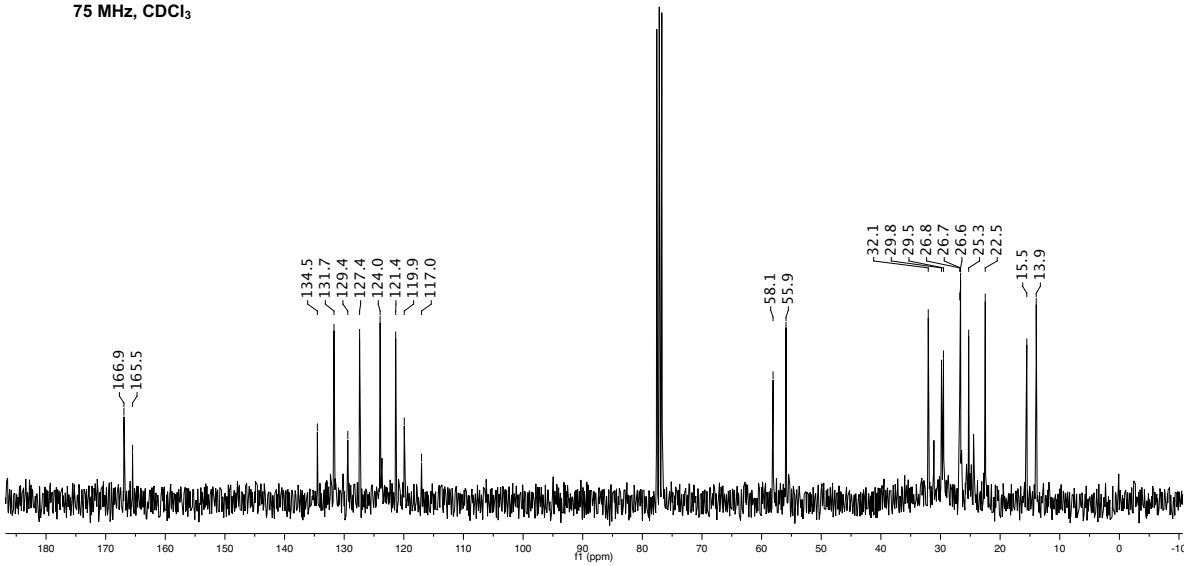


300 MHz, $CDCl_3$

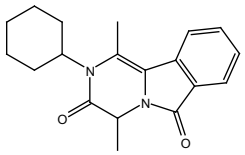




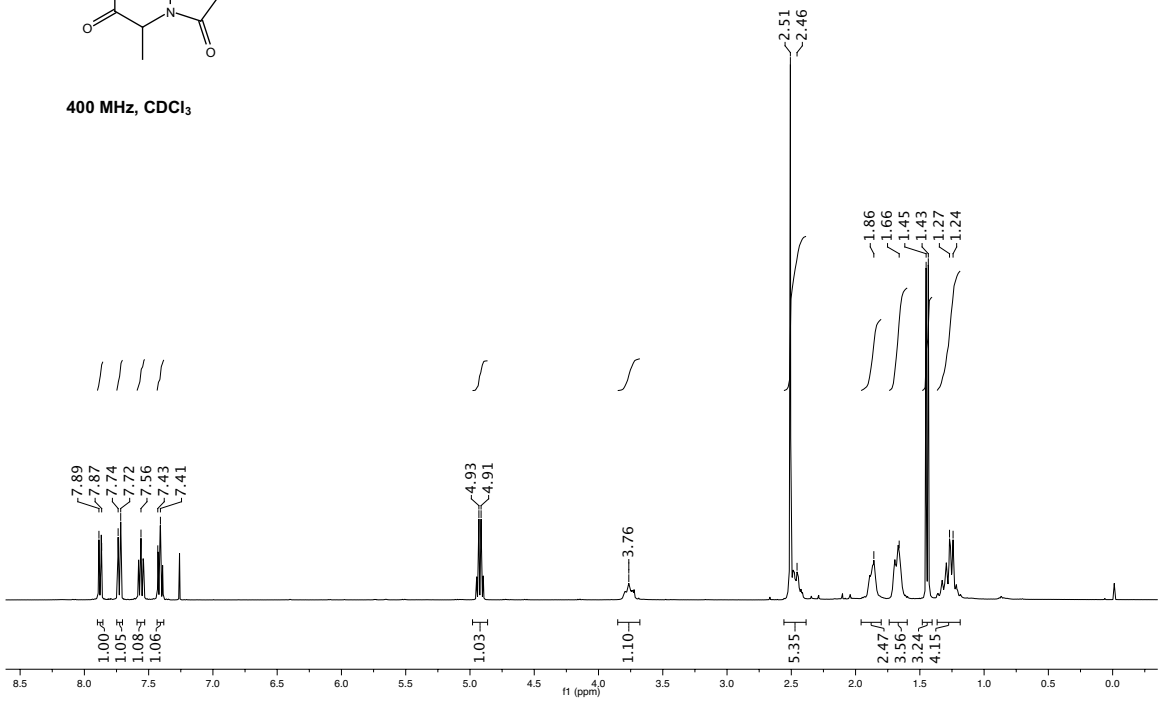
75 MHz, $CDCl_3$

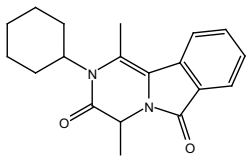


2-Cyclohexyl-1,4-dimethylpyrazino[2,1-*a*]isoindole-3,6(2*H*,4*H*)-dione (14t)

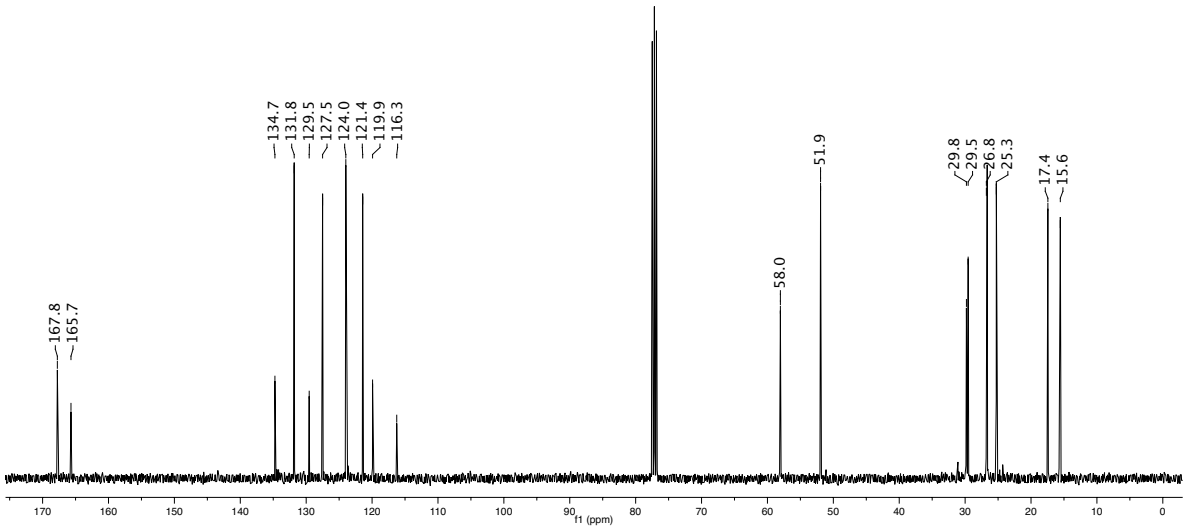


400 MHz, $CDCl_3$

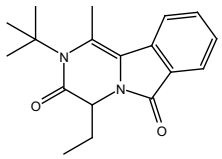




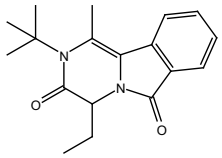
100 MHz, $CDCl_3$



2-(*Tert*-butyl)-4-ethyl-1-methylpyrazino[2,1-*a*]isoindole-3,6(2*H*,4*H*)-dione (14u)

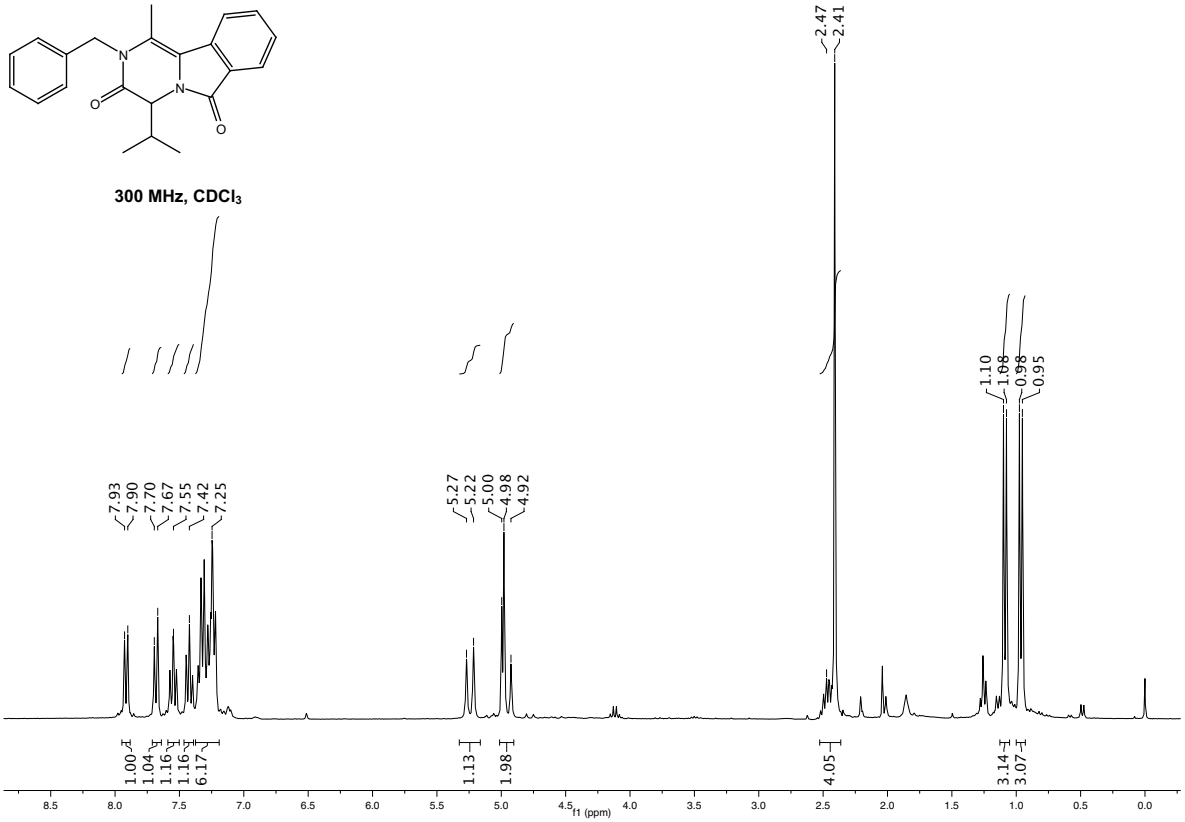


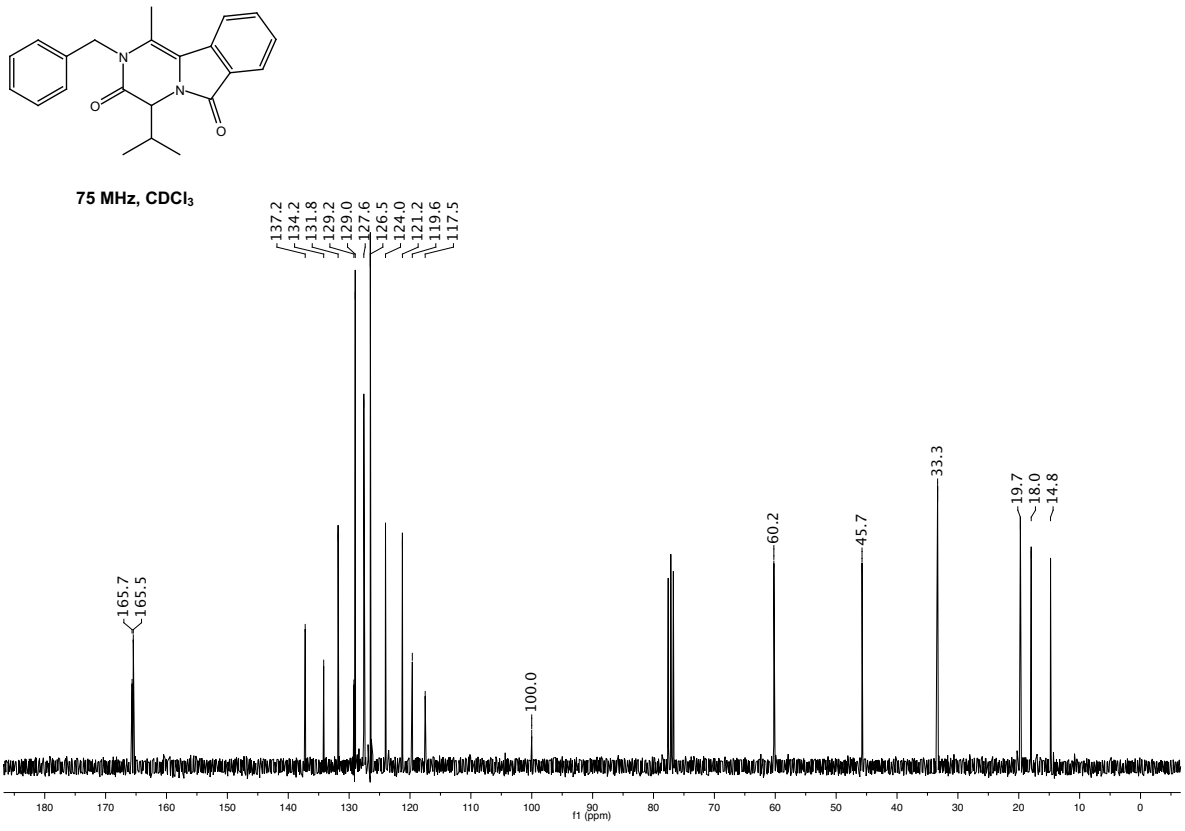
300 MHz, $CDCl_3$



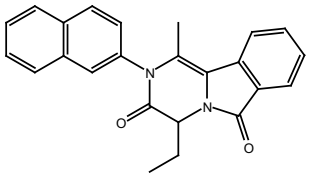
75 MHz, $CDCl_3$

2-Benzyl-4-isopropyl-1-methylpyrazino[2,1-*a*]isoindole-3,6(2*H*,4*H*)-dione (14v)

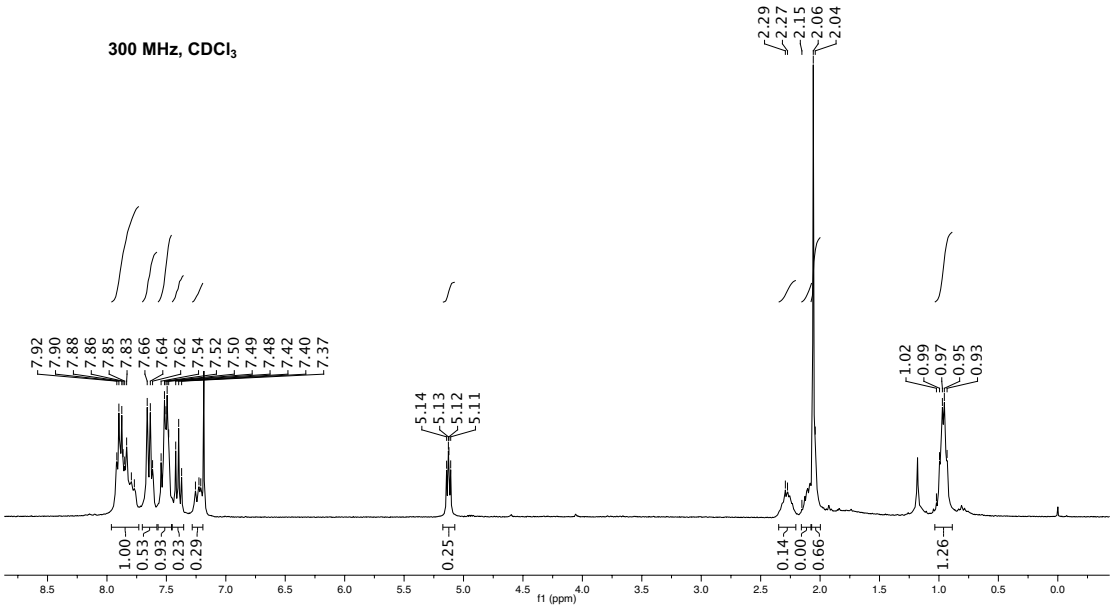


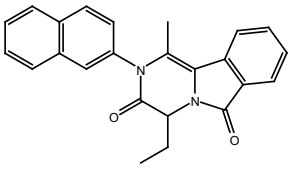


4-Ethyl-1-methyl-2-(naphthalen-2-yl)pyrazino[2,1-*a*]isoindole-3,6(2*H*,4*H*)-dione (14w)



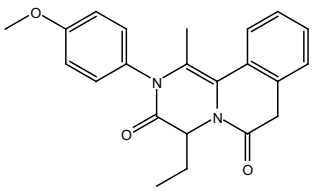
300 MHz, $CDCl_3$



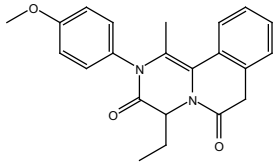


75 MHz, $CDCl_3$

4-Ethyl-2-(4-methoxyphenyl)-1-methyl-2*H*-pyrazino[2,1-*a*]isoquinoline-3,6(4*H*,7*H*)-dione (14x)



300 MHz, $CDCl_3$



75 MHz, $CDCl_3$

X-Ray Crystallographic Data

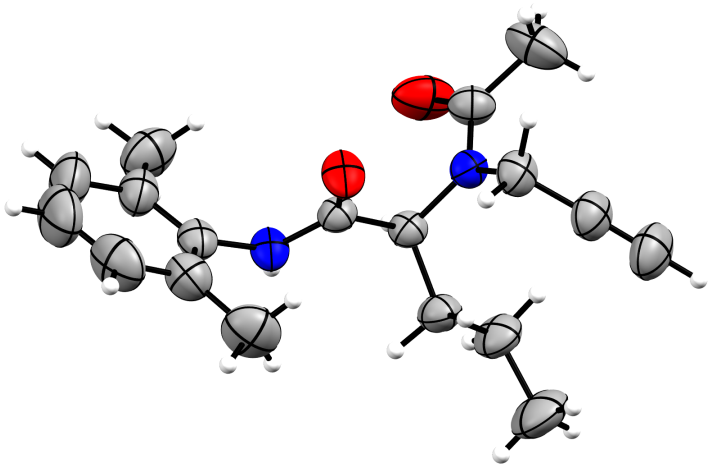


Figure 1. Molecular structure for compound **11a**, thermal ellipsoids are drawn at 30 % probability for all atoms except than hydrogen.

Table 1. Crystal data and structure refinement for **11a**. Identification code 376MGL14 (Solved by: R. A. Toscano)

Compound	**11a**
Empirical formula	$C_{18}H_{24}N_2O_2$
Formula weight	300.39
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	*P* b c a
Unit cell dimensions	*a* = 9.344(3) Å α= 90° *b* = 22.993(7) Å β= 90° *c* = 16.649(5) Å γ = 90°
Volume	3576.9(19) $Å^3$
Z	8
Density (calculated)	1.116 Mg/m^3

Absorption coefficient	0.073 mm^{-1}
$F(000)$	1296
Crystal size / colour / shape	0.380 x 0.132 x 0.058 mm / colourless / prism
Theta range for data collection	2.153 to 27.610°
Index ranges	$-11 \leq h \leq 12$, $-29 \leq h \leq 29$, $-21 \leq h \leq 14$
Reflections collected	22418
Independent reflections	4111 [R(int) = 0.1461]
Completeness to theta = 25.242°	99.9 %
Measurement device	Bruker Smart Apex CCD diffractometer 01-670-01
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9958 and 0.9728
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4111 / 0 / 207
Goodness-of-fit on F^2	1.001
Final R indices [$I>2\sigma(I)$]	$R1$ = 0.0763, $wR2$ = 0.1767
R indices (all data)	$R1$ = 0.1588, $wR2$ = 0.2355
Extinction coefficient	0.0077(16)
Largest diff. peak and hole	0.302 and -0.226 e.$Å^{-3}$

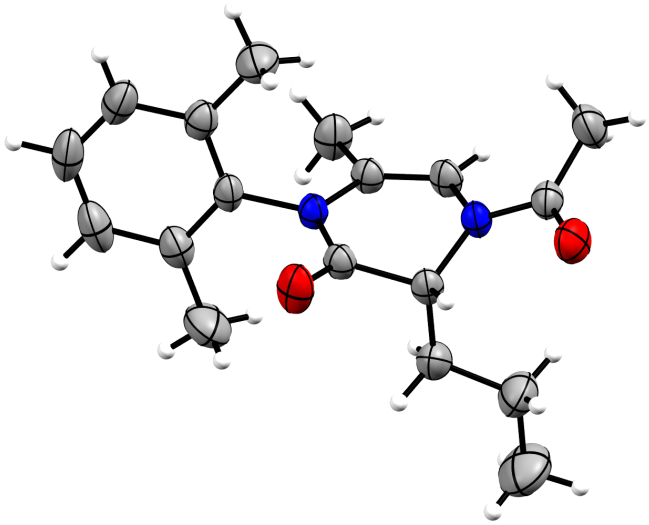


Figure 2. Molecular structure for compound **13a**, thermal ellipsoids are drawn at 30 % probability for all atoms except than hydrogen.

Table 2. Crystal data and structure refinement for **13a**. Identification code 361MGL14 (Solved by: R. A. Toscano)

Compound	**13a**
Empirical formula	$C_{18}H_{24}N_2O_2$
Formula weight	300.39
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P* 2_1/n
Unit cell dimensions	*a* = 7.2997(3) Å α= 90° *b* = 8.7192(7) Å β= 90° *c* = 27.1071(5) Å γ = 90°
Volume	1710.00(12) $Å^3$
Z	4
Density (calculated)	1.167 Mg/m^3
Absorption coefficient	0.076 mm^{-1}

$F(000)$	648
Crystal size / colour / shape	0.491 x 0.305 x 0.279 mm / colourless / prism
Theta range for data collection	2.456 to 27.518°
Index ranges	$-9 \leq h \leq 9$, $-11 \leq k \leq 11$, $-34 \leq l \leq 35$
Reflections collected	16910
Independent reflections	3930 [R(int) = 0.0343]
Completeness to theta = 25.242°	99.8 %
Measurement device	Bruker Smart Apex CCD diffractometer 01-670-01
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9790 and 0.9635
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3930 / 0 / 204
Goodness-of-fit on F^2	1.035
Final R indices [$I>2\sigma(I)$]	$R1$ = 0.0472, $wR2$ = 0.1161
R indices (all data)	$R1$ = 0.0708, $wR2$ = 0.1310
Largest diff. peak and hole	0.201 and -0.180 e.Å^{-3}

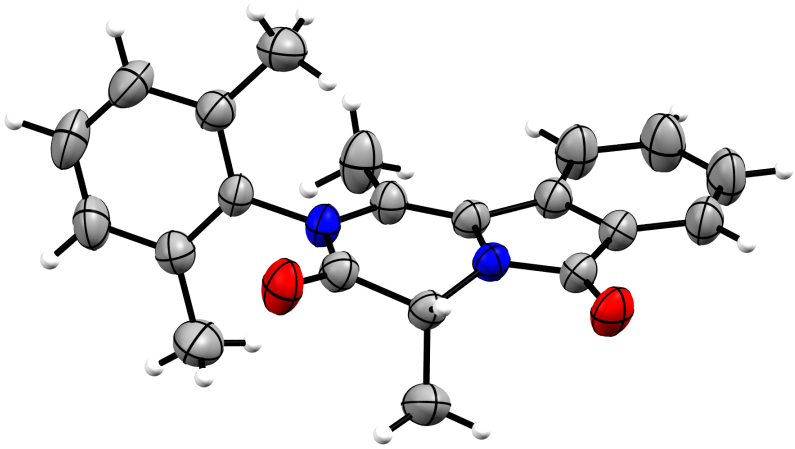


Figure 3. Molecular structure for compound **14r**, thermal ellipsoids are drawn at 30 % probability for all atoms except than hydrogen.

Table 3. Crystal data and structure refinement for **14r**. Identification code 364MGL15 (Solved by: R. A. Toscano)

Compound	**14r**
Empirical formula	$C_{21}H_{20}N_2O_2$
Formula weight	332.39
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P* 2_1/n
Unit cell dimensions	*a* = 8.2348(7) Å α= 90° *b* = 26.914(2) Å β= 90° *c* = 8.2642(3) Å γ = 90°
Volume	1733.3(3) $Å^3$
Z	4
Density (calculated)	1.274 Mg/m^3
Absorption coefficient	0.083 mm^{-1}
F(000)	704

Crystal size	0.360 x 0.280 x 0.200 mm
Theta range for data collection	2.712 to 25.319°
Index ranges	$-9 \leq h \leq 9$, $-32 \leq k \leq 31$, $-9 \leq l \leq 9$
Reflections collected	19869
Independent reflections	3138 [R(int) = 0.0826]
Completeness to theta = 25.242°	100.0 %
Measurement device	Bruker Smart Apex CCD diffractometer 01-670-01
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3138 / 0 / 231
Goodness-of-fit on F^2	1.070
Final R indices [$I>2\sigma(I)$]	$R1$ = 0.0532, $wR2$ = 0.1406
R indices (all data)	$R1$ = 0.0664, $wR2$ = 0.1508
Extinction coefficient	0.018(3)
Largest diff. peak and hole	0.250 and -0.209 e.Å^{-3}

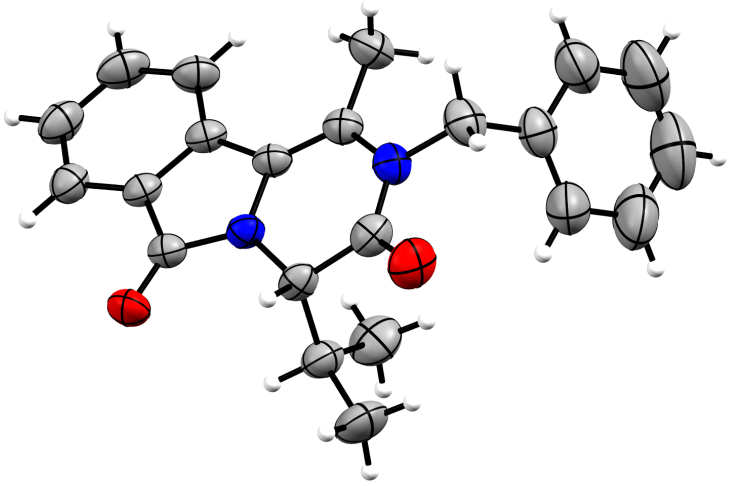


Figure 4. Molecular structure for compound **14v**, thermal ellipsoids are drawn at 30 % probability for all atoms except than hydrogen.

Table 4. Crystal data and structure refinement for **14v**. Identification code 364MGL15 (Solved by: R. A. Toscano)

Compound	**14v**
Empirical formula	$C_{22}H_{22}N_2O_2$
Formula weight	346.41
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*P* 2_1/n
Unit cell dimensions	*a* = 14.0741(7) Å α= 90° *b* = 8.4735(2) Å β= 90° *c* = 16.5267(3) Å γ = 90°
Volume	1785.99(11) $Å^3$
Z	4
Density (calculated)	1.288 Mg/m^3
Absorption coefficient	0.083 mm^{-1}

$F(000)$	736
Crystal size	0.256 x 0.176 x 0.087 mm
Theta range for data collection	2.497 to 25.390°
Index ranges	$-16 \leq h \leq 16$, $-10 \leq k \leq 8$, $-19 \leq l \leq 19$
Reflections collected	13978
Independent reflections	3275 [R(int) = 0.0317]
Completeness to theta = 25.242°	99.6 %
Measurement device	Bruker Smart Apex CCD diffractometer 01-670-01
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3275 / 0 / 238
Goodness-of-fit on F^2	1.040
Final R indices [$I>2\sigma(I)$]	$R1$ = 0.0409, $wR2$ = 0.1019
R indices (all data)	$R1$ = 0.0499, $wR2$ = 0.1081
Largest diff. peak and hole	0.139 and -0.151 e.Å^{-3}