Contents

1 General info

Unless otherwise stated, all reactions were performed in oven-dried glassware, using a magnetically-stirred Teflon stir bar under argon atmosphere. All the reagents and solvents (HPLC grade) were used as without any further purification, with the exception of dichloromethane and triethylamine that have been distilled over CaH_2 prior to use, toluene which was distilled from sodium prior to use and THF which was distilled over sodium prior to use. $NaHCO_3$ that was used for quenching refers to a saturated solution in H_2O. Synthesized products and intermediates were stored under argon atmosphere and protected from light at -20 °C.

Where useful, reactions were monitored by thin layer chromatography (TLC), with SIL G25 UV254 TLC plates with silica gel of 0.25 mm in thickness. Visualisation was obtained by irradiation with UV light (254 nm) and by staining with an anisaldehyde solution (5% para-anisaldehyde and 1% sulfuric acid in ethanol), and/or a ceric ammonium molybdate solution (2.5% $(NH_4)_6Mo_7O_{24} \cdot {}_4H_2O$, 1% $Ce(NH_4)_4(SO_4)_4 \cdot {}_2H_2O$ and 10% sulfuric acid in water). Column chromatography was performed with ROCC N.V. silica (particle size of from 0.060 to 0.200 mm). Technical grade pentane was used as the standard apolar mobile phase, typically enriched with a gradient of ethyl acetate.

^1H Nuclear Magnetic Resonance (NMR) spectra were recorded with a resolution of 700, 500, 400 or 300 MHz. The 300 MHz measurements were performed on a 300 MHz Avance I (Bruker) with a 5 mm dual channel probe head - ^1H and Broadband (BBO-type) equiped with an ultrashield type magnet. Measurements with 400 MHz resolution were carried out on a 400 MHz Avance II (Bruker) with a 5 mm dual channel probe head - ^1H and Broadband (BBO-type) and an ultrashield type magnet. Samples measured with 500 MHz resolution were realised with the 500 MHz Avance II (Bruker) with a 5 mm triple channel probe head - ^1H ^{13}C ^{19}F (TXO type) provided with an Oxford type magnet. Measurements with 700 MHz resolution were caried out on the 700 MHz Avance II (Bruker) with a 5 mm triple channel

probe head - ^{1}H ^{13}C ^{19}F (TXI type) and equipped with an Ultrashield + type magnet. The chemical shifts (δ) are expressed in ppm and the residual solvent peak was used as the internal standard ($CDCl_3$: δH = 7.26 ppm; δC = 77.16 ppm, C_6D_6: δH = 7.16 ppm; δC = 128.06 ppm, Acetone-d_6: δH = 2.05 ppm; δC = 29.84 ppm,DCM-d_2: δH = 5.32 ppm; δC = 53.84 ppm,). Scalar couplings (J) are reported in Hertz (Hz). The multiplicity of the signals were designated by the following abbreviations: s, singlet; d, doublet; t, triplet; q, quadruplet; p, quintuplet; sx, sextet; sept, septuplet; m, multiplet; br broadened; band, several overlapping signals; AB, AB system with strongly skewed signals; app., apparent multiplicity of a signal.

LC-MS analysis was performed on an Agilent 1100 series HPLC connected to an Agilent G1956B single quadrupole MS, using an ESI-ionization source. A Phenomenex Kinetex C18 column (150 x 4.6 mm, particle size 5 μm) was used at 35 °C with a linear solvent gradient 100% A to 100%B in 6 min or 75% B to 100% B in 6 min (A: 5 mM NH_4OH in H_2O; B: MeCN). For all compounds with a urazole motive inside, the linear solvent gradient consists of A: 0.1%(v/v) HCOOH in H_2O. HRMS was recorded with direct injection by an Agilent 1100 Series HPLC on an Agilent 6220A time of flight HRMS using ESI/APCI-multimode ionization source. GCMS spectra were recorded on an Agilent 6890GC connected to an Agilent 5973 single quadrupole MS using EI ionization. The column used for the GCMS is an Agilent DB-5 (60 m x 0.25 mm, film thickness 0.25 μm) with He as carrier gas and going from 70 °C to 320 °C with a 17.5 °C/min gradient. Chiral analysis was performed using an Agilent 1100 series HPLC equipped with a DAD-UV detector. The column used was a Phenomenex Lux Amylose-2 column (150 x 4.6 mm, particle size 5 m) at 35 °C. The eluent was Hexane/Ethanol(abs.) in an 80:20 ratio, with a flow of 1 mL/min for 30 min.

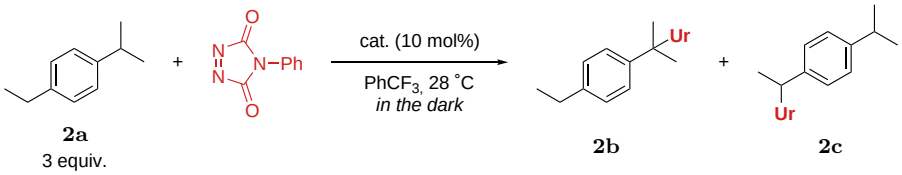
Infrared (IR) spectra were obtained with a Perkin-Elmer 1000 FT-IR spectrometer equipped with a HATR module. The intensity of the peaks were designated by the following abbreviations: s: strong (> 50% absorption); m: medium (between 20% and 50% absorption); w: weak (less then 20% absorption); br: broadened.

2 Synthetic protocols

2.1 General procedure for the metal screening

Different metals were screened in a qualitative manner to determine which showed activity towards promoting the C-H amination (see table S1). The catalysts were chosen as they were reported in the context of azodicarboxilates to catalyse amination reactions ($LiClO_4$[1] and $Cu(OTf)_2$[2]), activate the N=N bond (Pd[3]) or complexate with them (Au[4;5], V[6] and Ti[7]). The reactions were stirred in absence of light and were checked for colour change every 24 h. $PhCF_3$ was chosen as solvent as it should be stable in the presence of PTAD and could be heated to higher temperatures if needed. As only a quick qualitative answer was desired on the question if the catalyst was promoting the C-H amination, the crude reaction mixture was put in the LCMS to check whether the mass could be found of the amination product or not. This quickly showed that the combination of [AuCl(IPr)] and $AgSbF_6$ promoted fast full conversion of the TAD, giving the correct mass in the MS. The reaction without catalyst was still bright red after 3 days at room temperature, so it was decided to heat this mixture to 60 °C for another day, after which the colour had disappeared.

For the reaction with $LiClO_4$, it was concluded that the $LiClO_4$ did nothing as it behaved in the same way as the blanc reaction and gave the same spectra. The use of $V(acac)_3$ showed quick conversion, but the mass found in the MS was the adduct of TAD onto the acetylacetonate ligand. Using $Ti(Cp)_2(CO)_2$ gave an intractable mixture without indication of the correct mass, just as the reaction with $Cu(OTf)_2$. Finally, although the reaction with $Pd(PPh_3)_4$ gave a peak with the correct mass, the crude NMR indicated a complex mixture of different products and side products. As this reaction took 3 days to complete while the reaction with the cationic gold was considerably faster, this was not investigated further.



2a
3 equiv.

2b **2c**

The catalyst (25 μmol, 10 mol%) was brought into a 4 ml screwcap vial and was dissolved in 2.5 ml of α,α,α-trifluorotoluene. The vial was then shielded from light with aluminum foil, then PTAD (45.1 mg, 0.25 mmol, 1 equiv.) was added to the mixture after which 1-ethyl-4-isopropylbenzene (0.13 ml, 0.75 mmol, 3 equiv.) was added in one portion. The reaction mixture was then stirred in a metal heating block at 28 °C untill the red colour of the PTAD had dissapeared and the mixture was yellow to light orange of colour (for reaction times, see table underneath). The colour of the reaction was checked every 24 h. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then filtered over celite (with EtOAc) and concentrated *in vacuo*. The reactions were then qualitatively judged by crude NMR and LCMS.

catalyst	time	temp.	mass found on LCMS?
[AuCl(IPr)] + AgSbF$_6$	1 day	RT	✓
[V(acac)$_3$]	1 day	RT	x
[Ti(Cp)$_2$(CO)$_2$]	2 days	RT	x
[Cu(OTf)$_2$]	3 days	RT	x
[Pd(PPh$_3$)$_4$]	3 days	RT	✓
_[a]	3 days	RT	✓
	1 day	65 °C	
LiClO$_4$[a,b]	3 days	RT	✓
	1 day	65 °C	

Unless stated otherwise: 1 equiv. PTAD, 3 equiv. 1-ethyl-4-isopropylbenzene, cat. 10 mol%, $PhCF_3$ (0.1 M), performed in the dark on RT.

[a]Reaction was heated to 65 °C after 3 days.

[b]1 equivalent of $LiClO_4$ was used.

Table S1: Data per reaction.

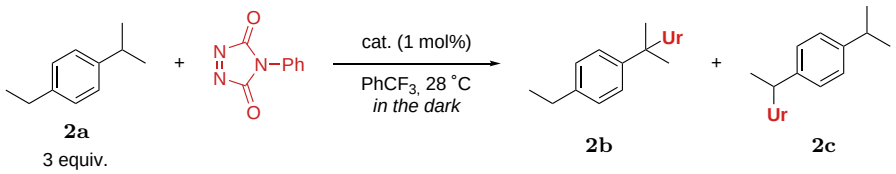
Other, more classical lewis acids ($Zn(OTf)_2$, $Sc(OTf)_3$ and $Ga(OTf)_3$) were also tested to determine if they could activate PTAD (**1**) towards C-H amination (see table S2). The same reaction conditions as above were used, with the only difference that after concentration *in vacuo* an internal standard (1,3,5-trimethoxybenzene) was added, the mixture was then made homogeneous in $CDCl_3$ and an NMR was taken to determine yield and ratio of the two regio-isomers. It could be concluded that these lewis acids accelerate the decomposition pathways of PTAD **1** instead of promoting the C-H amination.

catalyst	time	yield[a] (%)	**2b** : **2c**[a]
$\mathbf{Zn(OTf)_2}$	4 days	14	62:38
$\mathbf{Sc(OTf)_3}$	3 days	20	73:27
$\mathbf{Ga(OTf)_3}$	3 days	12	53:47

1 equiv. PTAD (0.5 mmol), 3 equiv. 1-ethyl-4-isopropylbenzene, cat. 10 mol%, $PhCF_3$ (0.1 M), performed in the dark on RT.
[a]Determined on NMR vs 1,3,5-trimethoxybenzene.

Table S2: Data per reaction of the more classical lewis acids.

2.2 General procedure for the Au(I) screening



Most of these reactions were performed in triplicate (see table underneath for amount of repetitions).

The catalyst (5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of α,α,α-trifluorotoluene. The flask was then shielded from light with aluminum foil, then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which 1-ethyl-4-isopropylbenzene (0.26ml, 1.5 mmol, 3 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared and the mixture was yellow to light orange of colour (see table underneath for reaction times). The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo*. 5 ml of EtOAc was added to the remaining orange oil, 1 ml was then again concentrated *in vacuo*, dissolved in $DCCl_3$ and added to an NMR tube where a carefully weighed amount of 1,3,5-trimethoxybenzene was present (usually between 10 to 18 mg). The yield and ratios of **2b** and **2c** (see table underneath) were then determined on NMR versus 1,3,5-trimethoxybenzene as internal standard. This rudimental procedure would explain the rather high standard deviation on the yield while the standard deviation on the ratio remains small.

The confidence interval of the yield was calculated as follows:

$$\bar{y} = (\sum_{i=1}^{n} y_i)/n \tag{1}$$

$$\sigma^2 = \sum_{i=1}^{n} (\bar{y} - y_i)^2 \tag{2}$$

$$yield = \bar{y} \pm 1.96 * \sigma \tag{3}$$

with:
$\bar{y}$ the mean yield,
n the amount of repetitions of the reaction,
y_i the yield of the i'th iteration of the reaction
The confidence interval of the ratio was calculated as follows:

$$b = \frac{2b}{2b + 2c} \tag{4}$$

$$\bar{b} = (\sum_{i=1}^{n} b_i)/n \tag{5}$$

$$\sigma^2 = \sum_{i=1}^{n} (\bar{b} - b_i)^2 \tag{6}$$

$$ratio = \bar{b} \pm 1.96 * \sigma : (1 - \bar{b}) \mp 1.96 * \sigma \tag{7}$$

with:
b the percentage of **2b** compared to the total of **2b** and **2c** together
$\bar{b}$ the mean percentage of **2b**,
n the amount of repetitions of the reaction,
b_i the percentage of **2b** of the i'th iteration of the reaction

Catalyst	n[a]	time[b]	yield[c](%)	ratio **2b** : **2c**[c]
_	2	30 min[d]	2.1±0.5	_[e]
_	3	5 days	47.2±1.0	85.1±0.8 : 14.9∓0.8
_[f]	1	2.5 h	46	81 : 19
$AgSbF_6$	1	30 min[d]	2	_[e]
[AuCl(IPr)]	1	30 min[d]	2	_[e]
[AuCl(IPr)] + $AgSbF_6$	3	30 min	72.0±7.9	76.4±3.0 : 23.6 ∓3.0
[AuCl(IPr)] + NaBARF	3	30 min	79.6±5.6	79.6±0.5 : 20.4∓0.5
[Au(IPr)(MeCN)]BF_4	**3**	**2 h**	**81.9±4.8**	**79.5±0.5 : 20.5∓0.5**
[Au(NTf_2)(IPr)]	3	5 h	76.6±4.5	79.7±0.8 : 20.3∓0.8
[Au$(IPr)_2(\mu$−OH)]BF_4	3	2 h	82.2±5.6	79.7±0.2 : 20.3∓0.2
[Au(OTf)(IPr*)]	3	2 h	73.3±1.5	62.2±1.6 : 37.8∓1.6
[Au(NTf_2)(PPh_3)]	3	3 days	36.0±4.0	72.0±2.7 : 28.0∓2.7
[Au(JohnPhos)(MeCN)]SbF_6	3	4 h	53±9.4	67±1.3 : 33∓1.3
[AuCl(SIPr)] + NaBARF	3	30 min	76.6±2.3	76.1±0.9 : 23.9∓0.9
[AuCl(IAd)] + NaBARF	3	2.5 h	69.7±6.4	80.1±0.4 : 19.9∓0.4
[Au(NTf_2)(IMes)]	3	2.5h	67.0±9.7	80.8±1.4 : 19.2∓1.4
[AuCl(IPr^{Me})] + NaBARF	3	30 min	77.8±9.1	78.5±0.9 : 21.5∓0.9
[Au(IPr^{Cl})(MeCN)]BF_4	3	5h	72.7±14.2	78.5±0.8 : 21.5∓0.8

[a]Amount of repetitions of the reaction.

[b]Reaction was stopped once the red colour of the PTAD was gone and the reaction was yellow to orange of colour.

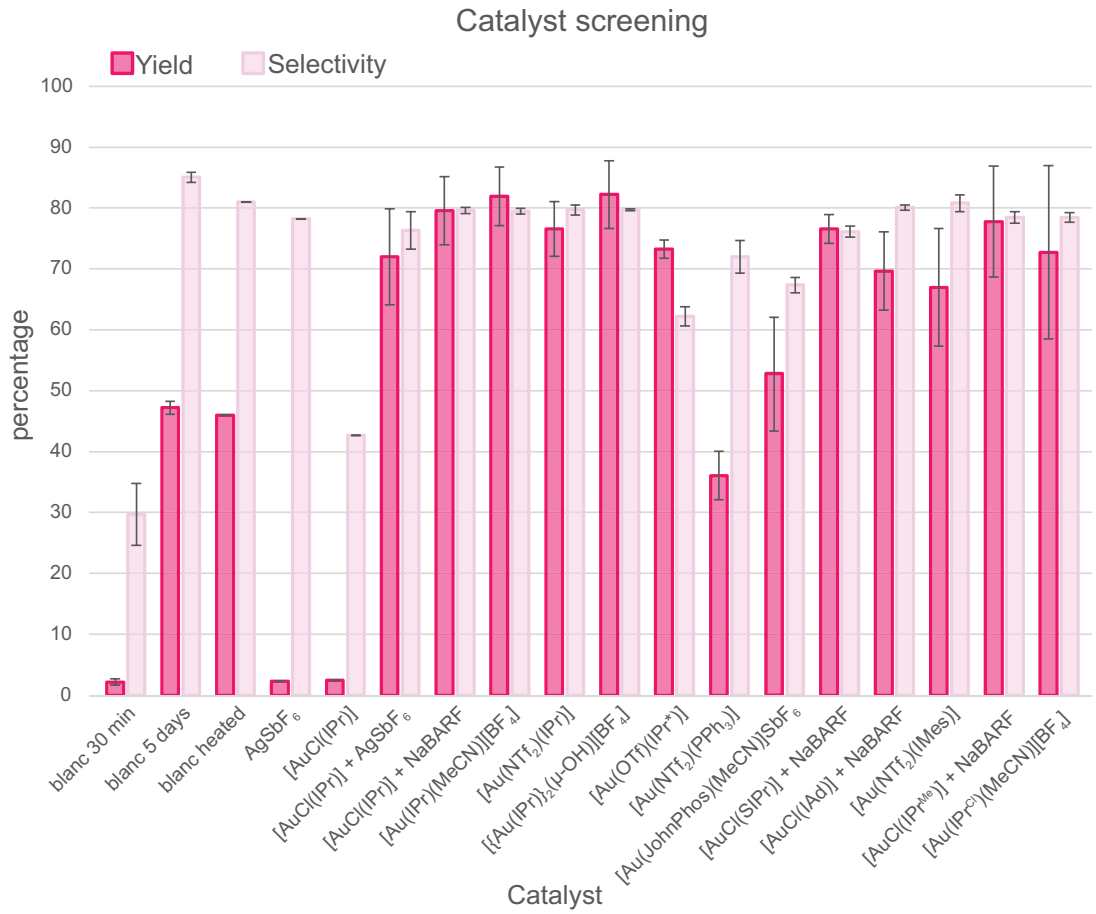
[c]Average with 95% confidence interval determined on NMR versus 1,3,5-trimethoxybenzene as internal standard.

[d]Reaction was stopped after 30 minutes to compare to the [AuCl(IPr)] + $AgSbF_6$ system.

[e]Integration on the NMR was not reliable due to low conversion.

[f]Was heated to 80 °C.

Table S3: Data per reaction.



2.3 Determination of the influence of light

Light (being UV or visible) can play an important role in activating TADs towards different reactions.[8;9] That's why the catalyst screening was done by covering the flask in aluminium foil to shield the reaction mixture from external light. As the disappearance of the red PTAD colour is indicative of the reaction being finished or not, it is desirable to leave the flask unwrapped and not shielded from light as it's more convenient to check whether the reaction is finished or not. In order to check if wrapping the flask in aluminium foil had an influence, it was decided to run a reaction without wrapping it. The blanc reaction (without catalyst) shown in figure S1a was chosen to be a good test as this reaction takes 5 days to complete. In this way, the reaction is exposed for 5 days to ambient light during the day and night. This

would give the greatest change in reaction outcome if wrapping the reaction flask in aluminium foil would make a difference. The result of both reactions (wrapped in aluminium foil or not) is the same, as can be seen in figure S1. Hence it was decided to not wrap the reaction flasks in aluminium foil for all further reactions.

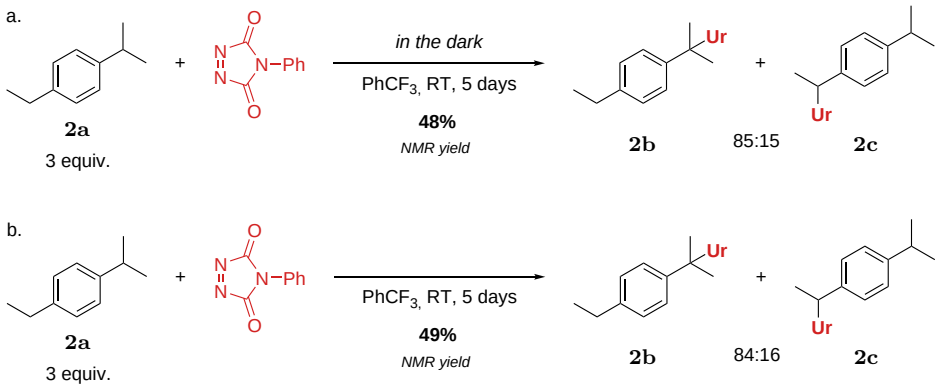


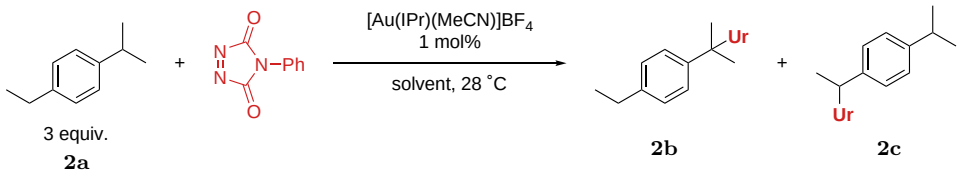
Figure S1: Influence of light on the blanc reaction. **a.** Performed with flask wrapped in aluminium foil, result is average of 3 replicates. **b.** Performed without wrapping the flask in aluminium foil, result of only 1 replicate.

5 ml of α,α,α-trifluorotoluene was brought into a 10 ml roundbottom flask (wrapped in aluminium foil or not) after which PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added, followed by 1-ethyl-4-isopropylbenzene (0.26 ml, 1.5 mmol, 3 equiv.) in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared after 5 days and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was concentrated *in vacuo* after which the yield and ratios were determined on NMR versus 1,3,5-trimethoxybenzene as internal standard. (see figure S1 for the results)

2.4 Solvent screening

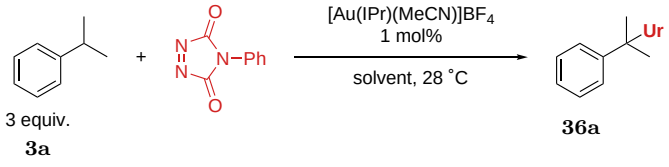
First the amination reaction on model substrate **2a** was performed in different solvents to check which would give the best result. As there are few solvents that would not give background reactivity towards PTAD, there were hardly

any viable options left. $PhCF_3$, DCM, DCE, *n*-hexane and $MeNO_2$ were tested. Nitromethane and *n*-hexane could be excluded for further tests as PTAD dissolved insufficiently and the reaction wasn't even finished after a week. $PhCF_3$, DCM and DCE performed practically equally good (see table S4), although reactions in $PhCF_3$ were slower, which is probably attributed to the lower solubility of PTAD in $PhCF_3$. DCM was then adopted as solvent of choice for testing other substrates, while DCE was kept for slow reacting substrates, in order to heat the reaction to higher temperatures. The reaction on cumene was also tested with both DCM en $PhCF_3$ to confirm DCM to be the superior solvent choice (see Table S5).



Solvent	time	yield (%)	**2b**:**2c**
DCM	30 min	94	80:20
$PhCF_3$	2 h	88	81:19
DCE	30 min	94	79:21
Yields are isolated yields, ratios determined on NMR.			

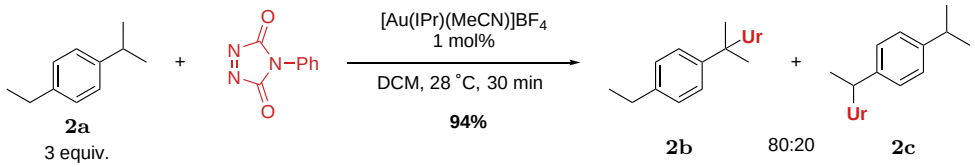
Table S4: Solvent screening on model substrate.



Solvent	time	yield (%)
DCM	10 h	85
$PhCF_3$	4 days	71
Yields are isolated yields.		

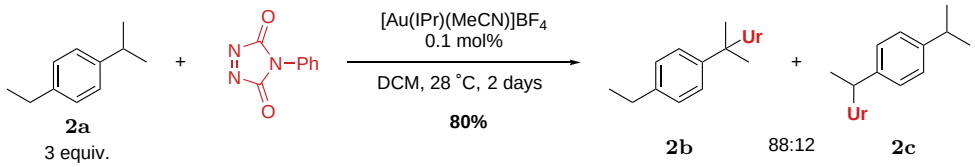
Table S5: Confirmation of solvent choice.

2.5 Optimised reaction conditions on model substrate 2a



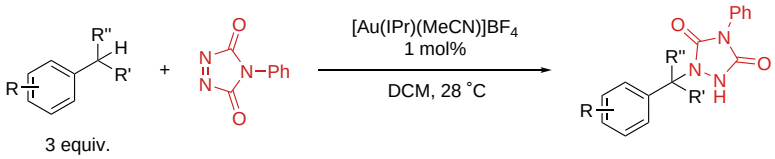
$[Au(IPr)(MeCN)]BF_4$ (3.6 mg, 5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which 1-ethyl-4-isopropylbenzene (0.26 ml, 1.5 mmol, 3 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared after 30 minutes and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo* after which it was subjected to column chromatography over silica using 20% EtOAc in pentane, yielding 151.8 mg of both regioisomers (94% yield). A fraction of which was pure **2b**. Even after several attempts, **2c** was not obtained analitically pure. The ratios of both regioisomers was determined on NMR. Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.6 Optimised reaction conditions on model substrate 2a with 0.1 mol% of catalyst loading



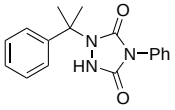
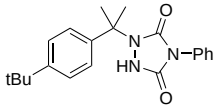
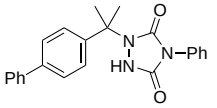
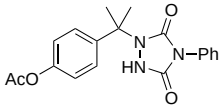
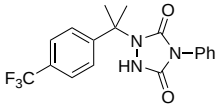
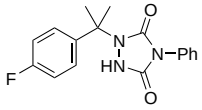
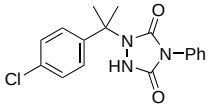
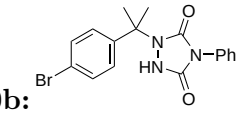
[Au(IPr)(MeCN)]BF_4 (3.6 mg, 5 μmol, 1 mol%) was brought into a 100 ml roundbottom flask and was dissolved in 50 ml of DCM. 5 ml of this solution was then brought into a 10 ml roundbottom flask (giving 0.36 mg, 0.5 μmol, 0.1 mol% of catalyst loading). Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which 1-ethyl-4-isopropylbenzene (0.26 ml, 1.5 mmol, 3 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared after 2 days and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo* after which it was subjected to column chromatography over silica using 20% EtOAc in pentane, yielding 129.9 mg of both regioisomers (80% yield). A fraction of which was pure **2b**. Even after several attempts, **2c** was not obtained analitically pure. The ratios of both regioisomers was determined on NMR. Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

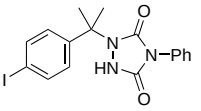
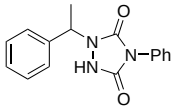
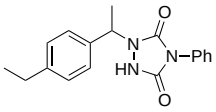
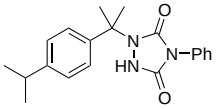
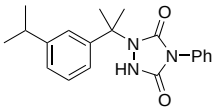
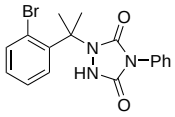
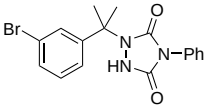
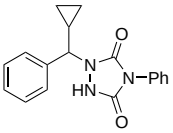
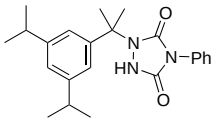
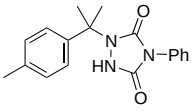
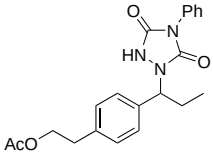
2.7 General procedure for the substrate scope

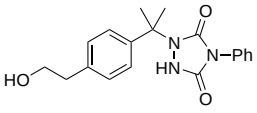
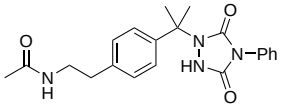
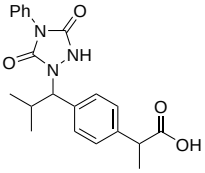
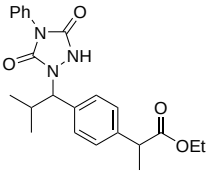


[Au(IPr)(MeCN)]BF_4 (3.6 mg, 5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (90.3

mg, 0.5 mmol, 1 equiv.) was added to the mixture after which the substrate (1.5 mmol, 3 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared and the mixture was yellow to light orange of colour (see table underneath for reaction times). The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo* after which column chromatography over silica was performed (see table underneath for column eluens and yield). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

compound	duration	FC eluens	Yield (%)
3b: 	10 h	7:3 pentane:EtOAc	85
4b: 	30 min	[a]8:2 to 3:1 pentane:EtOAc	89
5b: 	1.5 h	[a]8:2 to 7:3 pentane:EtOAc	85
6b: 	12 h	[a]70:30 to 60:40 pentane:EtOAc	84
7b: 	7 days	[a]85:15 to 75:25 pentane:EtOAc	12
8b: 	16 h	75:25 pentane:EtOAc	65
9b: 	3 days	[a]75:25 to 70:30 pentane:EtOAc	17
10b: 	19 h	75:25 pentane:EtOAc	33

11b: 	3 days	[a]75:25 to 70:30 pentane:EtOAc	52
12b: 	3 days	3:1 pentane:EtOAc	80
13b: 	3 h	7:3 pentane:EtOAc	90
14b: 	20 min	3:1 pentane:EtOAc	94
15b: 	3.5 h	[a]9:1 to 85:15 pentane:EtOAc	90
16b: 	7 days[b]	[a]90:10 to 75:25 pentane:EtOAc	<5[c]
17b: 	5 days	[a]90:10 to 75:25 pentane:EtOAc	60
18b: 	5 days	75:25 pentane:EtOAc	44
19b: 	9 h	9:1 pentane:EtOAc	59
24b: 	1 h	8:2 pentane:EtOAc	86
26b: 	24 h	[a]75:25 to 70:30 pentane:EtOAc	95

27b: 	5 h	[a]60:40 to 40:60 pentane:EtOAc	73
28b: 	24 h	[a]20:80 to 0:100 pentane:EtOAc	45
29b: 	3 days	[a]70:30:1 to 60:40:1 pentane:EtOAc:HOAc	78
30b: 	3 days	[a]80:20 to 60:40 pentane:EtOAc	74

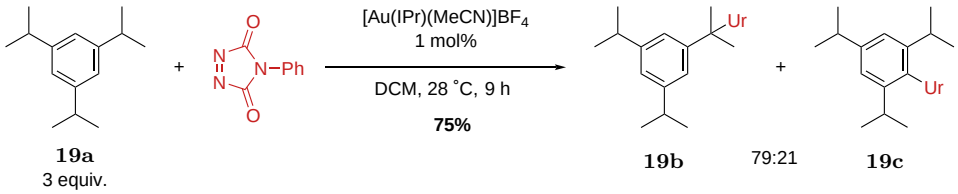
[a] stepwise gradient was used

[b] reaction was stopped after 7 days, which meant 90% consumption of PTAD (**1**)

[c] determined on NMR

Table S6: Data per compound.

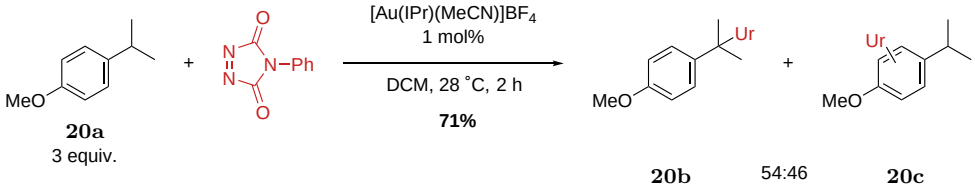
2.8 C-H amination on 1,3,5-triisopropylbenzene (19a) giving 19b and 19c



$[Au(IPr)(MeCN)]BF_4$ (3.6 mg, 5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which 1,3,5-triisopropylbenzene (0.38ml, 1.5 mmol, 3 equiv.) was added in one portion. The

reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared after 9 h and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo* after which column chromatography over silica was performed using 15% EtOAc in pentane. This yielded 17.4 mg of **19b** as white solid and 124.3 mg of a mixture of **19b** and **19c** as an off white oil, both adding up to 75% yield. Determining the ratio on NMR gives then a 79:21 ratio of **19b** vs. **19c**. Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.9 C-H amination on 4-isopropylanisole (20a) giving 20b and 20c



$[Au(IPr)(MeCN)]BF_4$ (3.6 mg, 5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which 4-isopropylanisole (0.25ml, 1.5 mmol, 3 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared after 2 h and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo* after which column chromatography over silica was performed using 25% EtOAc in pentane. This yielded 116.2 mg of a mixture of **20b** and **20c** as an off white oil, adding up to 71% yield. **20c** is a mixture of products with the same mass as **20b**. Determining the ratio on NMR gives then a 54:46 ratio of **20b** vs. **20c**. Compound analysis of the mixture can be found in section 3 and NMR

spectra of the mixture can be found in section 4.

2.10 General procedure for the substrate scope on elevated temperatures

$[Au(IPr)(MeCN)]BF_4$ (3.6 mg, 5 μmol, 1 mol%) was brought into a pressure tube and was dissolved in 5 ml of DCE. Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which the substrate (1.5 mmol, 3 equiv.) was added in one portion. The reaction mixture was then heated to 80 °C untill the red colour of the PTAD had dissapeared and the mixture was yellow to light orange of colour (see table underneath for reaction times). The reaction was then cooled to room temperature after which it was quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo* after which column chromatography over silica was performed (see table underneath for eluens and yield). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

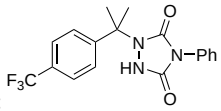
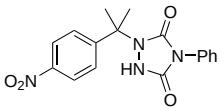
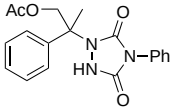
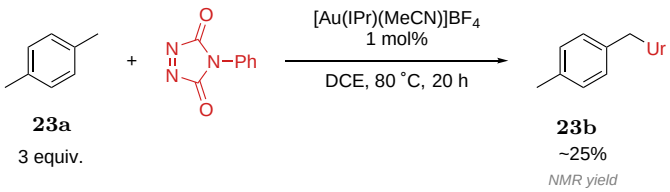
compound	duration	FC eluens	Yield (%)
7b: 	2 days	[a]80:20 to 70:30 pentane:EtOAc	74
21b: 	5 days	7:3 pentane:EtOAc	39
22b: 	9 days	75:25 pentane:EtOAc	32

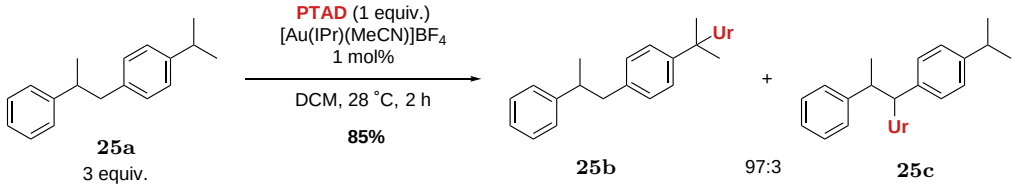
Table S7: Data per compound.

2.11 C-H amination on p-xylene (23a) giving 23b



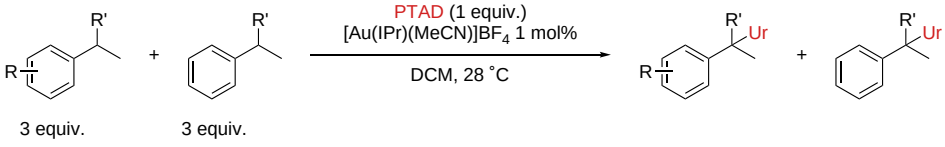
[Au(IPr)(MeCN)]BF_4 (3.6 mg, 5 μmol, 1 mol%) was brought into a pressure tube and was dissolved in 5 ml of DCE. Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which p-xylene (0.19 ml, 1.5 mmol, 3 equiv.) was added in one portion. The reaction mixture was then heated to 80 °C untill the red colour of the PTAD had dissapeared and the mixture was yellow to light orange of colour (20 h). The reaction was then cooled to room temperature after which it was quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo*. To the remaining solids, 15 ml of $CDCl_3$ was added, toghether with 43.0 mg of 1,3,5-trimethoxybenzene as internal standard. This mixture was then sonicated to dissolve as much of the solids as possible. The mixture was then filtered over a syringe filter and analysed via NMR. The filter was washed twice again with fresh $CDCl_3$ to see if all of the target molecule (**23b**) was dissolved the first time to check if the estimate made by reference to the internal standard was justified. The NMR spectra of the washes dind't show a significant loss in **23b** compared to the internal standard, leading to conclude that the estimate of the yield is a good estimate. There was an attempt made to purify the C-H aminated product from the mixture (by column chromatography over silica with 25% EtOAc in pentane), but this only resulted in an enriched fraction of the target **23b**. Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.12 C-H amination on 25a giving 25b



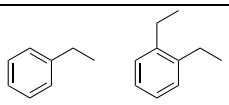
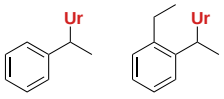
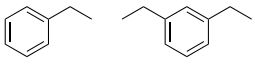
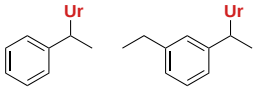
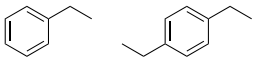
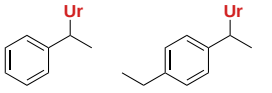
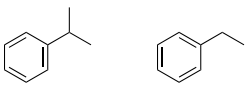
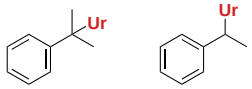
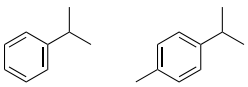
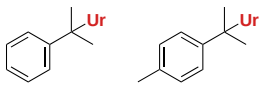
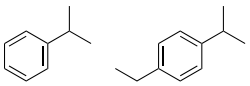
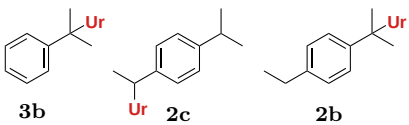
[Au(IPr)(MeCN)]BF_4 (3.6 mg, 5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which 1-isopropyl-4-(2-phenylpropyl)benzene (**25a**) (361.2 mg, 1.5 mmol, 3 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared after 2 hours and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo* after which column chromatography over silica was performed using 20% EtOAc in pentane, yielding 176.4 mg of both regioisomers (85% yield). A fraction of which was pure **37**. Even after several attempts, **25c** was not obtained analitically pure. The ratios of both regioisomers was determined on NMR. Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.13 General procedure for the intermolecular competition reactions



[Au(IPr)(MeCN)]BF_4 (3.6 mg, 5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (90.3 mg,

0.5 mmol, 1 equiv.) was added to the mixture after which both substrates (both 1.5 mmol, 3 equiv.) at once were added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared and the mixture was yellow to light orange of colour. Generally, the reactions were stirred longer as the timeframe of the reaction didn't really matter here (see table underneath for reaction times). The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo* after which column chromatography was performed over silica. All C-H aminated products were collected together from the column to determine the yield. Ratios of the different products were determined by NMR (see table underneath for yields and ratios). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

starting materials	time	Yield[a] (%)	result[b]
 **12a** **13a**	20 h	65	 **12b** 51:49 **32b**
 **12a** **31a**	20 h	76	 **12b** 18:82 **31b**
 **12a** **32a**	2 h	87	 **12b** 2:98 **13b** c
 **3a** **12a**	10 h	87	 **3b** 87:13 **12b**
 **3a** **24a**	3 h	81	 **3b** 12:88 **24b**
 **3a** **2a**	45 min	89	 **3b** **2c** 73:18:9 **2b**

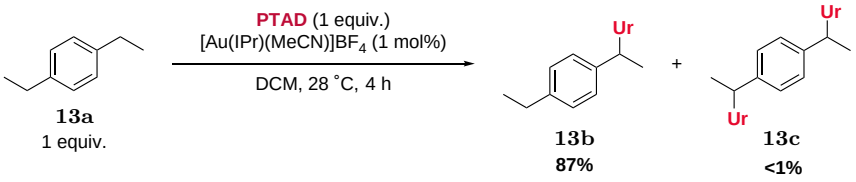
[a] isolated yields

[b] Determined on NMR

[c] Ratio determined by deconvolution of the NMR spectrum

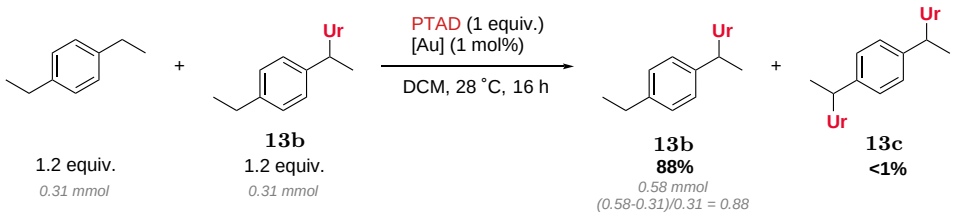
Table S8: Data per reaction.

2.14 C-H amination using 1 equivalent of substrate (13a)



$[Au(IPr)(MeCN)]BF_4$ (3.6 mg, 5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which 1,4-diethylbenzene (0.08 ml, 0.5 mmol, 1 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared after 4 h and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated to dryness *in vacuo*. The C-H aminated product was then purified by precipitation by adding 1 ml of EtOAc, sonication to let everything dissolve, and then adding 9 ml of n-pentane under stirring. Filtration and washing with pentane then led to 135.5 mg of a white solid (87% yield). In the NMR spectra, no trace of double addition could be observed. In the LCMS spectra, there was only a small trace of double addition present, integrating for less than 1% on 214 nm. These observations were made in the spectra of the crude reaction mixture after work-up, the spectra of the filtrate and the spectra of the precipitate.

2.15 C-H amination using a 1:1 mixture of substrate (13a) and aminated product (13b)

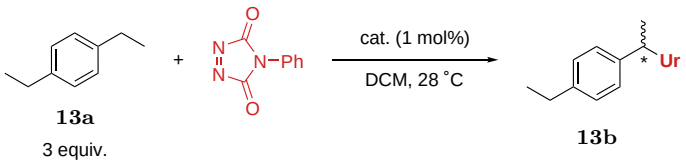


$[Au(IPr)(MeCN)]BF_4$ (1.8 mg, 2.5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (45.1 mg, 0.25 mmol, 1 equiv.) was added to the mixture after which 1,4-diethylbenzene (0.05 ml, 0.31 mmol, 1.2 equiv.) and 1-(1-(4-ethylphenyl)ethyl)-4-phenyl-1,2,4-triazolidine-3,5-dione (**13b**) (95.8 mg, 0.31 mmol, 1.2 equiv.) were added together in one portion. The reaction mixture was then stirred in a water bath at 28 °C overnight (16 h) after which the red colour of the PTAD had dissapeared and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated to dryness *in vacuo*. The C-H aminated product was then purified by precipitation by adding 1 ml of EtOAc, sonication to let everything dissolve, and then adding 9 ml of n-pentane under stirring. Filtration and washing with pentane then led to 179.5 mg of a white solid (88% yield). In the NMR spectra, no trace of double addition could be observed. In the LCMS spectra, there was only a small trace of double addition present, integrating for less than 1% on 214 nm. These observations were made in the spectra of the crude reaction mixture after work-up, the spectra of the filtrate and the spectra of the precipitate.

2.16 General procedure for chiral amination of 13a

Enantioselective C-H amination was attempted with 1,4-diethylbenzene (**13a**) as substrate and various chiral gold(I) complexes (see table S9). Two blanc reactions with achiral catalysts were performed (both with IPr as ancillary

ligand, and one being a well-defined cationic gold complex) giving evidently an ee of 0%. Taking a chiral counterion (+-CSA in this case) also didn't induce any chirality in the reaction. Then, two chiral NHC ligands were tested, both resulting in modest enantioselectivity (14% and 10%). As last, a chiral phosphine was tested as well, which gave good enantioselectivity as an ee of 62% was achieved.



The catalyst (5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which 1-ethyl-4-isopropylbenzene (0.26 ml, 1.5 mmol, 3 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared and the mixture was yellow to light orange of colour (see table underneath for reaction times). The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo* and then column chromatography over silica was performed using a 7:3 pentane:EtOAc mixture as eluens to yield both enantiomers of **13b** (see table underneath for yields). The enantiomeric ratio was then determined by chiral LCMS (see table underneath for er).

catalyst	time	yield (%)[a]	er[b]
[AuCl(IPr)] + $AgSbF_6$	30 min	n.d.[c]	50:50
[Au(IPr)(MeCN)]BF_4	3h	90	50:50
[Au(+-CSA)(IPr)]	48h	66	50:50
[AuCl((R,R)−SINpEt)] + $AgSbF_6$	30 min	85	57:43
[AuCl((S,S)−SINnPent)] + $AgSbF_6$	23 h	76	45:55

[AuCl((R)−DTBM−SEGPHOS)] + $AgSbF_6$	25 h	79	81:19

[a]Isolated yield.

[b]Determined by chiral LCMS.

[c]Yield was not determined.

Table S9: Data per reaction.

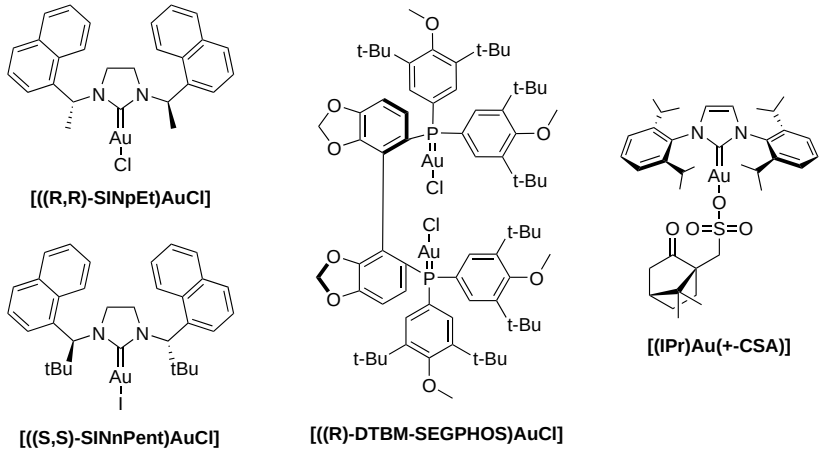
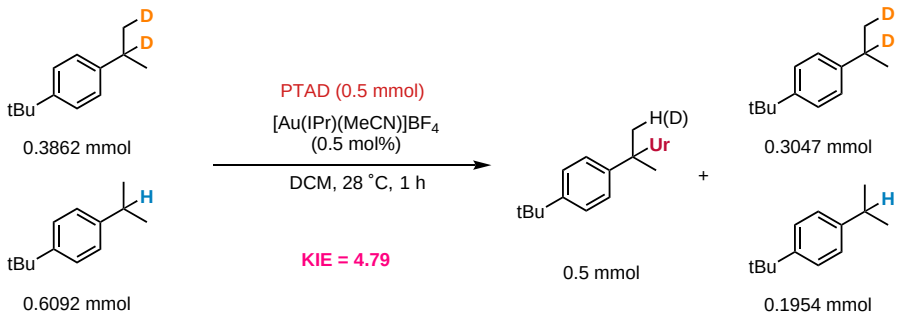


Figure S2: Used chiral catalysts.

2.17 Determination of the KIE

The KIE was determined by performing the C-H amination reaction on a mixture of deuterated and non-deuterated 4-tert-butylcumene. By performing integrations on the NMR, the relative ratio of deuterated and non-deuterated 4-tert-butylcumene could be determined before and after the reaction.

$$KIE = \frac{ln([S_H]/[S_H]^0)}{ln([S_D]/[S_D]^0)} = \frac{ln(0.1954/0.6092)}{ln(0.3047/0.3862)} = 4.79 \qquad (8)$$



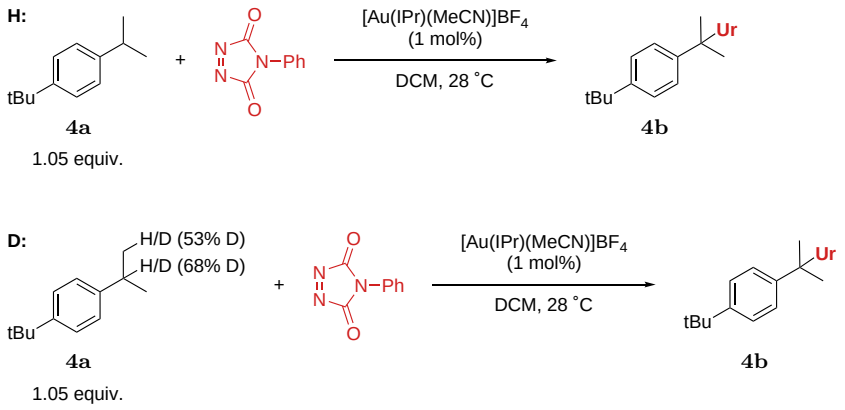
The deuterated version of 4-tert-butylcumene was diluted with 4-tert-butylcumene (**20a**) with the aim to create a mixture close to 1:1 of deuterated and non deuterated benzylic position. The ratio of deuterated and non deuterated benzylic position was determined by NMR.

[Au(IPr)(MeCN)]BF_4 (3.6 mg, 5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 5 ml of DCM. Then PTAD (90.3 mg, 0.5 mmol, 1 equiv.) was added to the mixture after which the mixture of deuterated and non-deuterated 4-tert-butylcumene (178.5 mg, 1 mmol, 2 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C untill the red colour of the PTAD had dissapeared after 1 h and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then carefully concentrated *in vacuo*. The KIE was then calculated by doing integrations on the NMR.

As this experiment doesn't necessarily proves that the C-H bond is being broken during the rate determining step, but maybe the product determining step[10], a second experiment was envisioned. Here, in two different reaction vessels the same experiment should be performed, once using the normal substrate, and once using the deuterated substrate, both in near 1 equivalence. If there would be a rate difference between these two, one could conclude that indeed the C-H bond is being broken during the rate determining step.

Unfortunately, obtaining pure deuterated 4-tert-butylcumene (with near 100% D on the benzylic position) was not an easy task. It was then decided to still proceed with this experiment, but using 4-tert-butylcumene that was only deuterated for 68%. Still, if there would be a rate determining C-H bond

breakage, there should be a difference in reaction rate between the reaction vessel with only hydrogen at the benzylic position and the vessel with the mixture of both deuterated and non deuterated substrate.



[Au(IPr)(MeCN)]BF_4 (7.2 mg, 10 μmol, 1 mol%) was brought into a 20 ml roundbottom flask and was dissolved in 10 ml of DCM. Then PTAD (180.6 mg, 1.0 mmol, 1 equiv.) was added to the mixture after which the substrate (1.05 mmol, 1.05 equiv.) was added in one portion. The reaction mixture was then stirred in a water bath at 28 °C. At distinct time intervals, a 0.25 ml sample was taken from the reaction vessel and quenched with isoprene. This sample was then concentrated *in vacuo* after which an NMR was taken to determine the conversion of the reaction (see fig. S3).

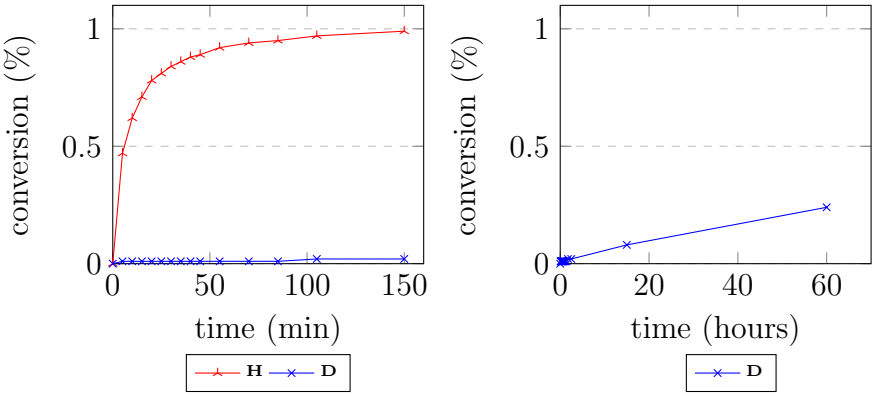
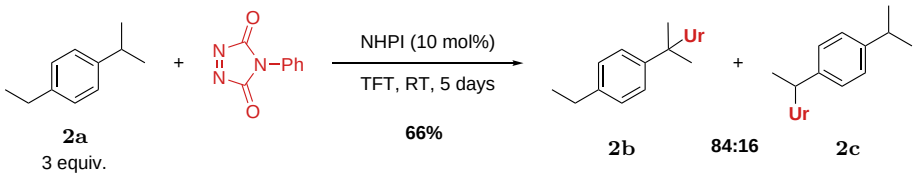


Figure S3: **left:** Comparison of the conversion of the two reaction vessels with the normal (**H**) and with the partly deuterated substrate (**D**). **right:** Conversion of the partly deuterated substrate over a longer timespan.

From these results, it can clearly been stated that the C-H bond breakage is part of the rate determining step and not only of the product determining step.

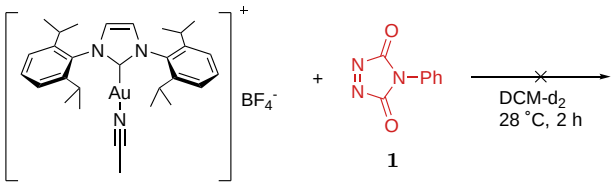
2.18 Control experiment with model substrate 2a using NHPI



N-hydroxyphthalimide (4.2 mg, 25 μmol, 10 mol%) was brought into a 4 ml screwcap vial and was dissolved in 2.5 ml of α,α,α-trifluorotoluene. Then PTAD (45.1 mg, 0.25 mmol, 1 equiv.) was added to the mixture after which 1-ethyl-4-isopropylbenzene (0.13 ml, 0.75 mmol, 3 equiv.) was added in one portion. The reaction mixture was then stirred in a metal heating block at 28 °C untill the red colour of the PTAD had dissapeared (after 5 days) and the mixture was yellow to light orange of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo*. 1,3,5-trimethoxybenzene was then added as internal standard after which everything was disolved in $CDCl_3$ to measure a ^{1}H-NMR spectrum. On this spectrum, it was determined that the yield was 66% and the ratio of **2b**:**2c** was 84:16.

2.19 Complexation of PTAD (1) with gold

In a first attempt to provide experimental support for the computationally identified intermediate **I** (the PTAD-gold complex), PTAD was left to stir with 1 equivalent of [Au(IPr)(MeCN)]BF_4 under Schlenk conditions:



[Au(IPr)(MeCN)]BF_4 (61.7 mg, 90 μmol, 1 equiv.) was dissolved in 2 ml of DCM-d_2 after which PTAD (**1**) (15.0 mg, 90 μmol, 1 equiv.) was added. The mixture was left to stir for 2 h at 28 °C while shielded from light. 0.55 ml was then taken out of the reaction mixture by means of a syringe and a needle, then filtered directly into an NMR tube after which the NMR was taken immediately.

No complexation of the PTAD **1** to the gold was observed as only the starting materials were visible in the NMR spectra.

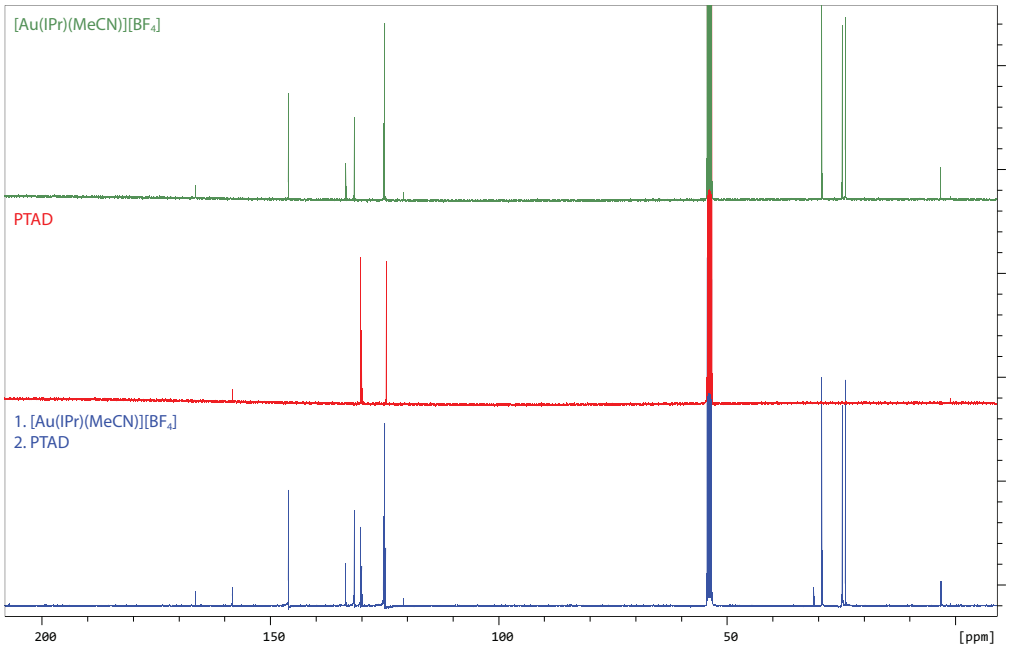


Figure S4: $^{13}C\{^1H\}$-NMR (100 MHz, DCM-d_2) of the mixture compared to PTAD and [Au(IPr)(MeCN)]BF_4.

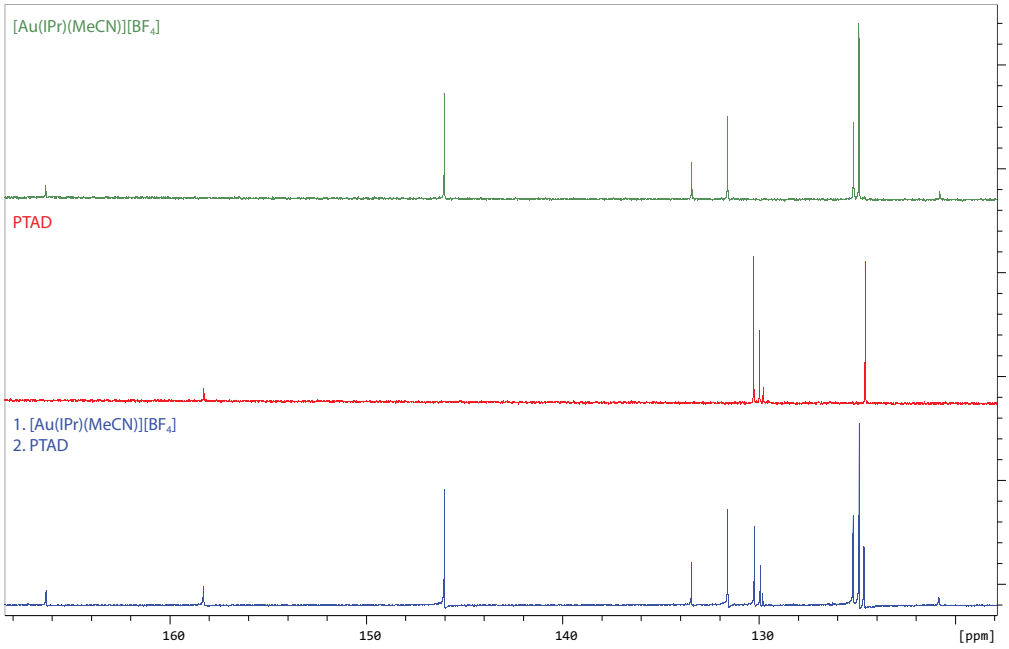
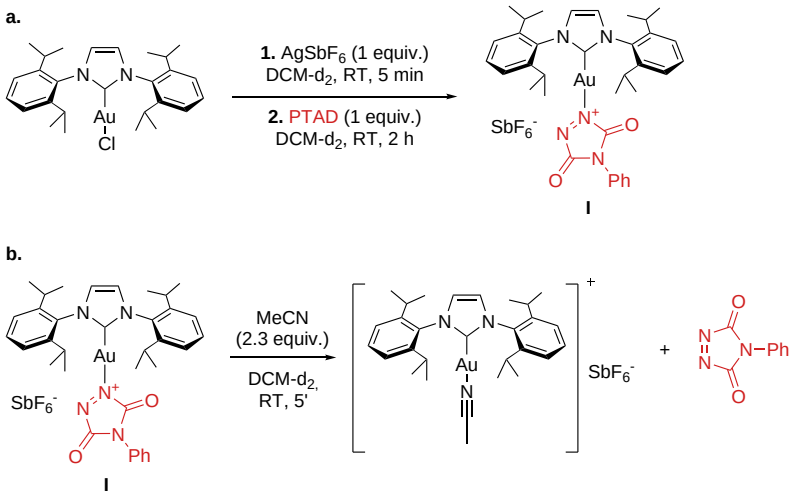


Figure S5: Zoomed in area of the $^{13}C\{^1H\}$-NMR (100 MHz, DCM-d_2) of the mixture compared to PTAD and [Au(IPr)(MeCN)]BF_4 (full spectra in S4).

One possible explanation for the lack of observation of a gold-TAD complex, is the fact that acetonitrile might be a better ligand then PTAD (which is quite electron poor). We thus decided to generate cationic cold first, and the combine it with PTAD. Instead, now in the glovebox, cationic gold was generated first from [AuCl(IPr)] and $AgSbF_6$ after which 1 equivalent of PTAD (**1**) was added to see if now coordination would be observed. $^{13}C\{^1H\}$-NMR (100 MHz, DCM-d_2) clearly showed that the peaks of the PTAD had not only shifted, but also that the PTAD had been desymmetrised. This would mean that the PTAD is coordinated to the gold with the nitrogen on the 1 position or with its oxygen (as any other logical option would leave the TAD symmetrical). DFT calculations showed that the coordination of the cationic $Au(IPr)^+$ is favoured on the N instead of the O by a difference of 10.6 kcal/mol, leaving nitrogen 1 as most likely option for the coordination.

As it was unexpected that PTAD (**1**) didn't show coordination with [Au(IPr)(MeCN)]BF_4 under Schlenk conditions, it was thought that MeCN had a stronger binding to the cationic gold than PTAD (**1**) itself. As to con-

firm this, the experiment above (creating cationic gold *in situ* and adding PTAD) was repeated again, but after the complexation of PTAD (**1**) with gold, MeCN was added to see if the gold-acetonitrile complex would be reformed:



$AgSbF_6$ (60.7 mg, 0.17 mmol, 1 equiv.) and [AuCl(IPr)] (107.4 mg, 0.17 mmol, 1 equiv.) were dissolved in 4 ml of DCM-d_2 after which this mixture was stirred for 5 minutes, shielding it from light. Then, PTAD (**1**) (30.0 mg, 0.17 mmol, 1 equiv.) was added to this mixture and stirred for 2 h shielded from light. Then, an NMR sample was taken. Afterwards, MeCN (18 μl, 0.34 mmol, 2.3 equiv.) was added to the reaction mixture. The colour of the reaction turned from brown/bordeaux to bright red (the colour of PTAD) in less than a second upon addition of MeCN, indicating the release of PTAD (**1**) from the gold. After that, the DCM-d_2 was concentrated *in vacuo* (leaving approximately 1 ml) and 15 ml of C_6D_6 was added in an attempt to precipitate the [Au(IPr)(MeCN)]SbF_6 complex. As precipitation was incomplete, the vial was taken outside of the glovebox and concentrated *in vacuo* (leaving approximately 5 ml). This gave a white precipitate at the side of the vial, which was then decantated, washed with C_6D_6, dissolved in DCM-d_2 and measured in the NMR to show indeed the [Au(IPr)(MeCN)]SbF_6 complex. Copies of the $^{13}C\{^1H\}$-NMR (100 MHz, DCM-d_2) spectra are given underneath in Figure S6-S13.

In Figure S10 the complexation of PTAD with Au can be seen as the peaks of the PTAD have clearly shifted, have splitted (desymmetrisation) and formed a single product (complex) with the gold. Figure S11 then shows the spectrum after addition of MeCN, clearly showing the return of the PTAD peaks. Figure S12 also distinctly shows that the [Au(IPr)(MeCN)]SbF_6 complex is formed. The NMR samples were taken in the following way: 0.55 ml was taken out of the reaction mixture by means of a syringe and a needle, then filtered directly into an amber NMR tube.

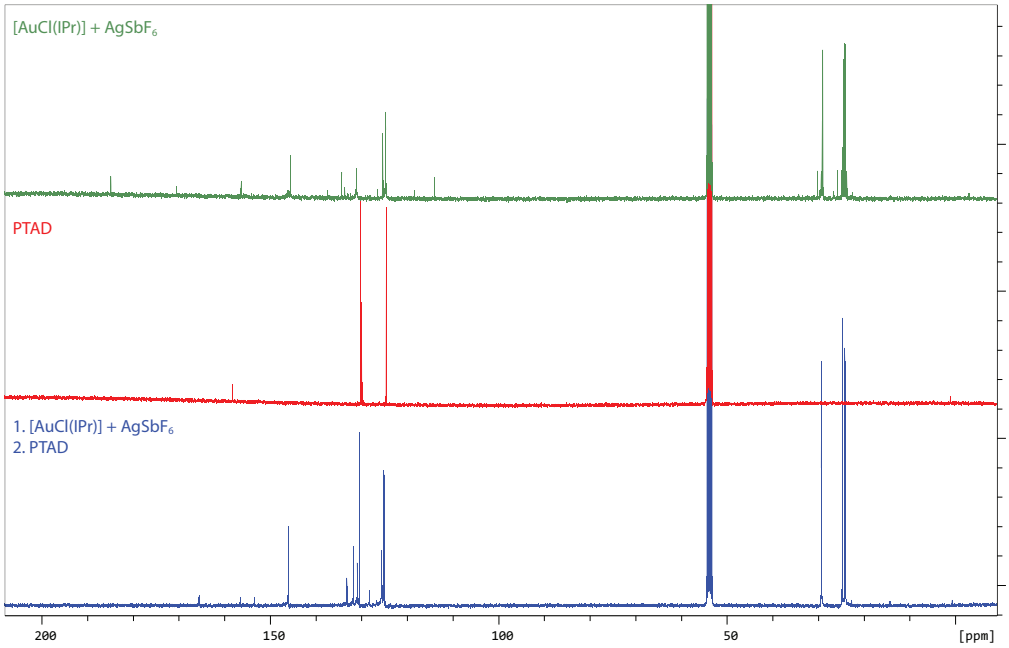


Figure S6: $^{13}C\{^1H\}$-NMR (100 MHz, DCM-d_2) of the PTAD-Au complex compared to PTAD and the *in situ* cationic gold made from [AuCl(IPr)] and $AgSbF_6$.

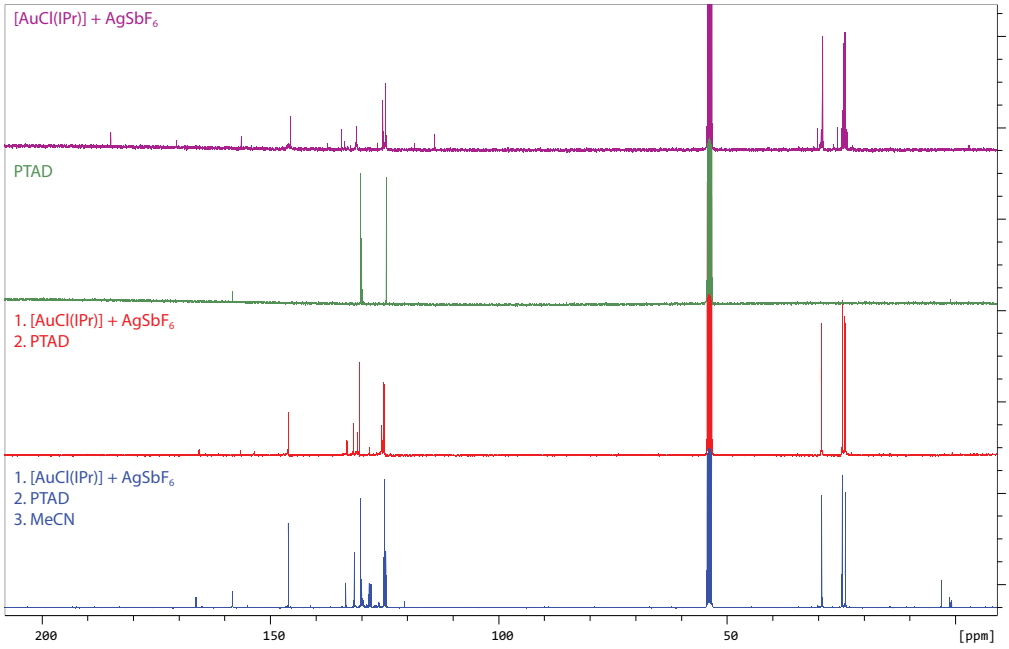


Figure S7: $^{13}C\{^{1}H\}$-NMR (100 MHz, DCM-d_2) after the addition of MeCN complex compared to the PTAD-Au complex, PTAD and the *in situ* cationic gold made from [AuCl(IPr)] and $AgSbF_6$.

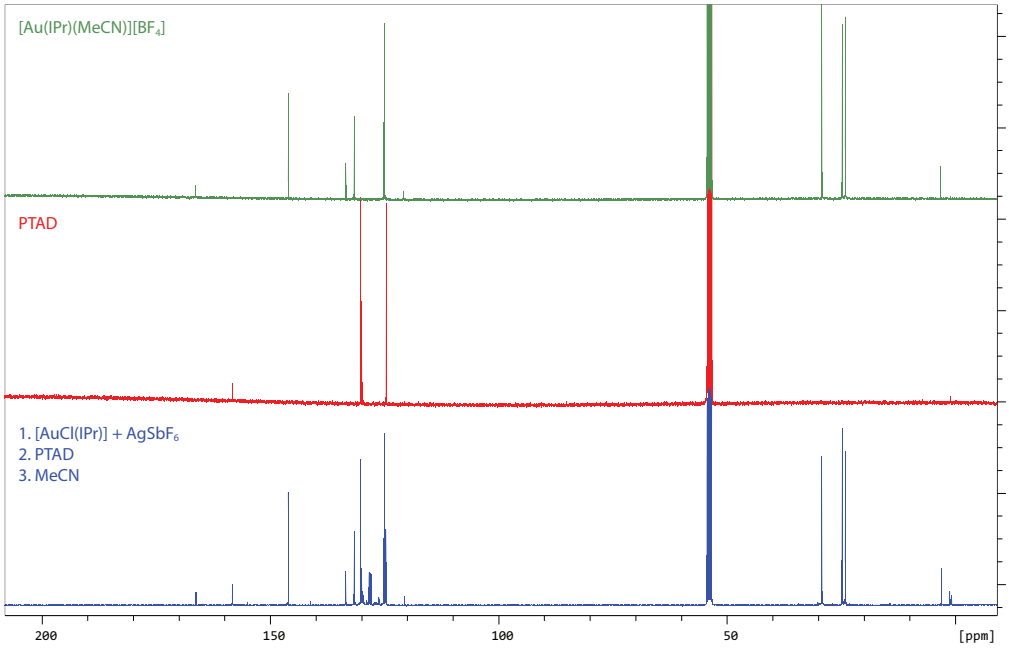


Figure S8: $^{13}C\{^{1}H\}$-NMR (100 MHz, DCM-d_2) after the addition of MeCN complex compared to PTAD and the [Au(IPr)(MeCN)]BF_4 complex.

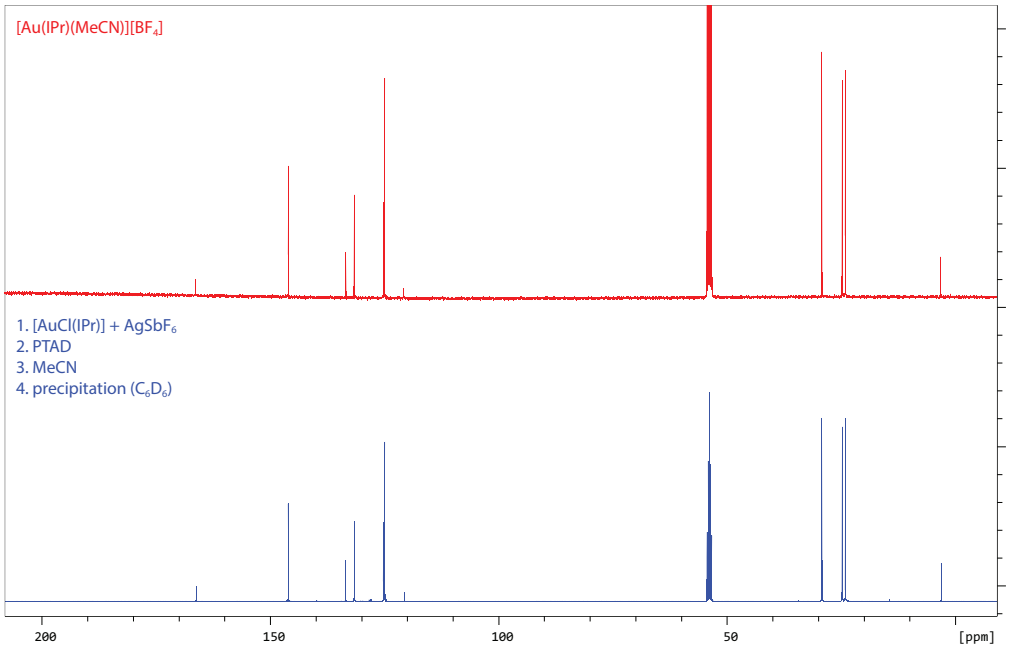


Figure S9: $^{13}C\{^{1}H\}$-NMR (100 MHz, DCM-d_2) of the white precipitate compared to the [Au(IPr)(MeCN)]BF_4 complex.

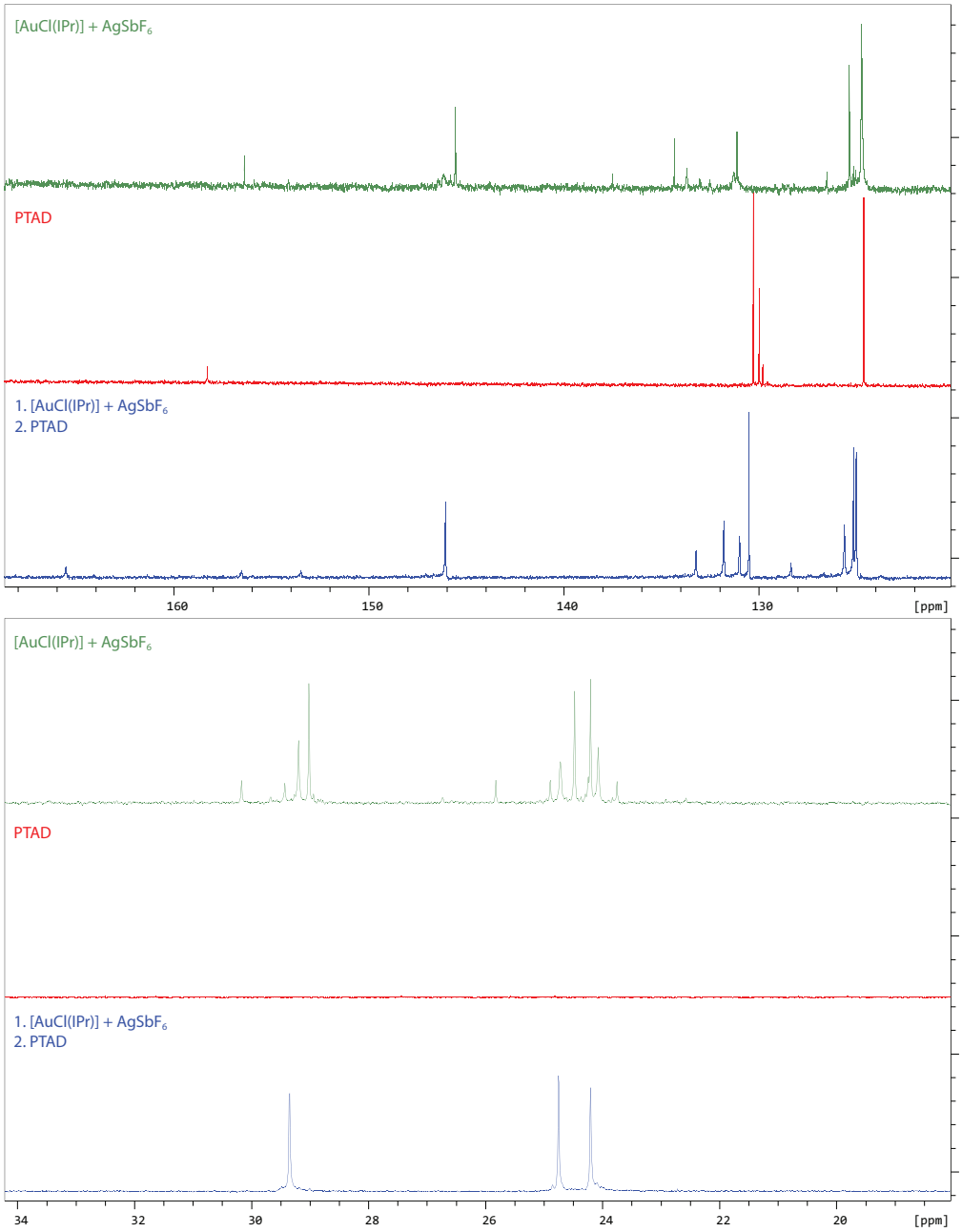


Figure S10: Zoomed in areas of the $^{13}C\{^{1}H\}$-NMR (100 MHz, DCM-d_2) of the PTAD-Au complex compared to PTAD and the *in situ* cationic gold made from [AuCl(IPr)] and $AgSbF_6$ (full spectra in S6).

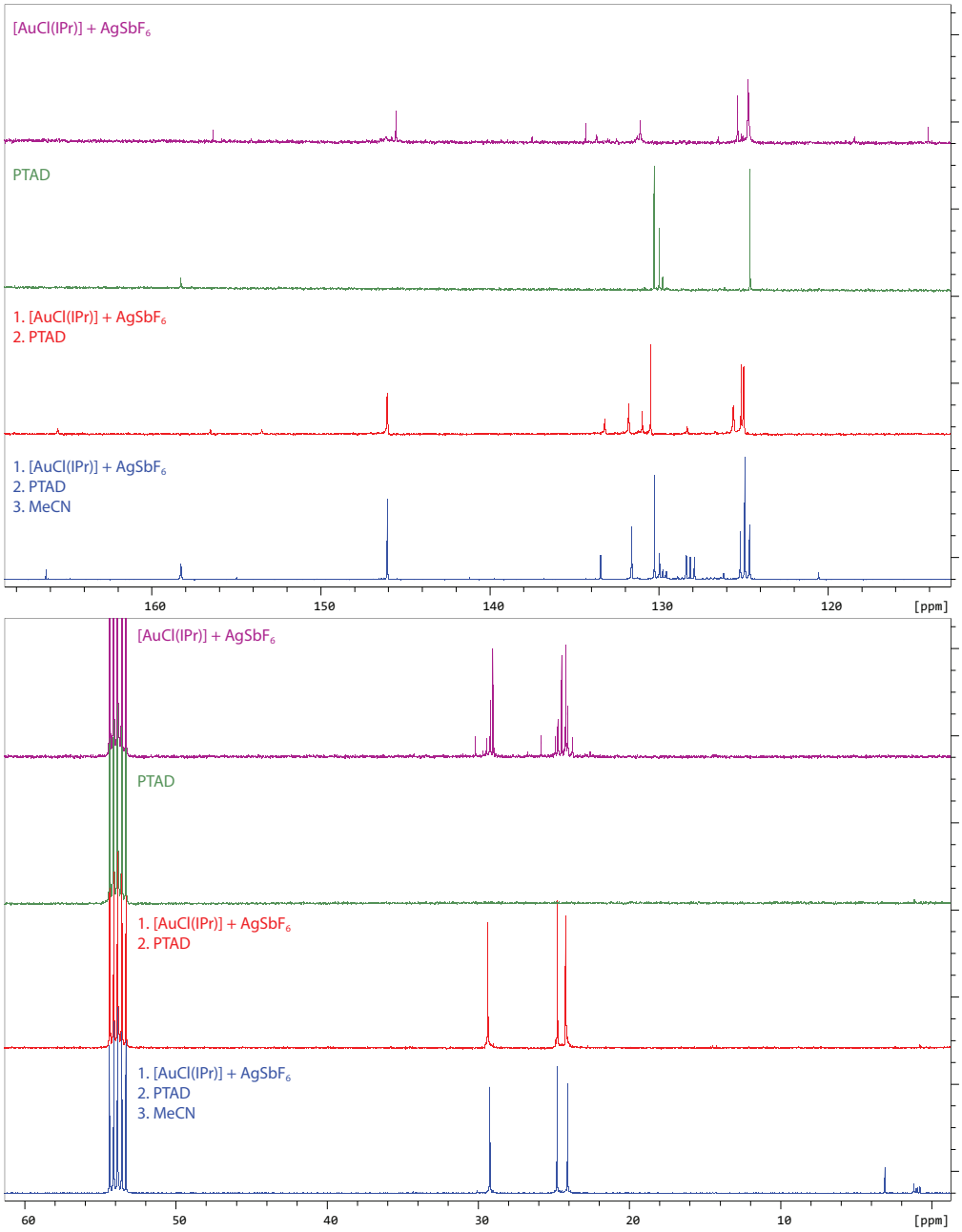


Figure S11: Zoomed in areas of the $^{13}C\{^{1}H\}$-NMR (100 MHz, DCM-d_2) after the addition of MeCN complex compared to the PTAD-Au complex, PTAD and the *in situ* cationic gold made from [AuCl(IPr)] and $AgSbF_6$ (full spectra in S7).

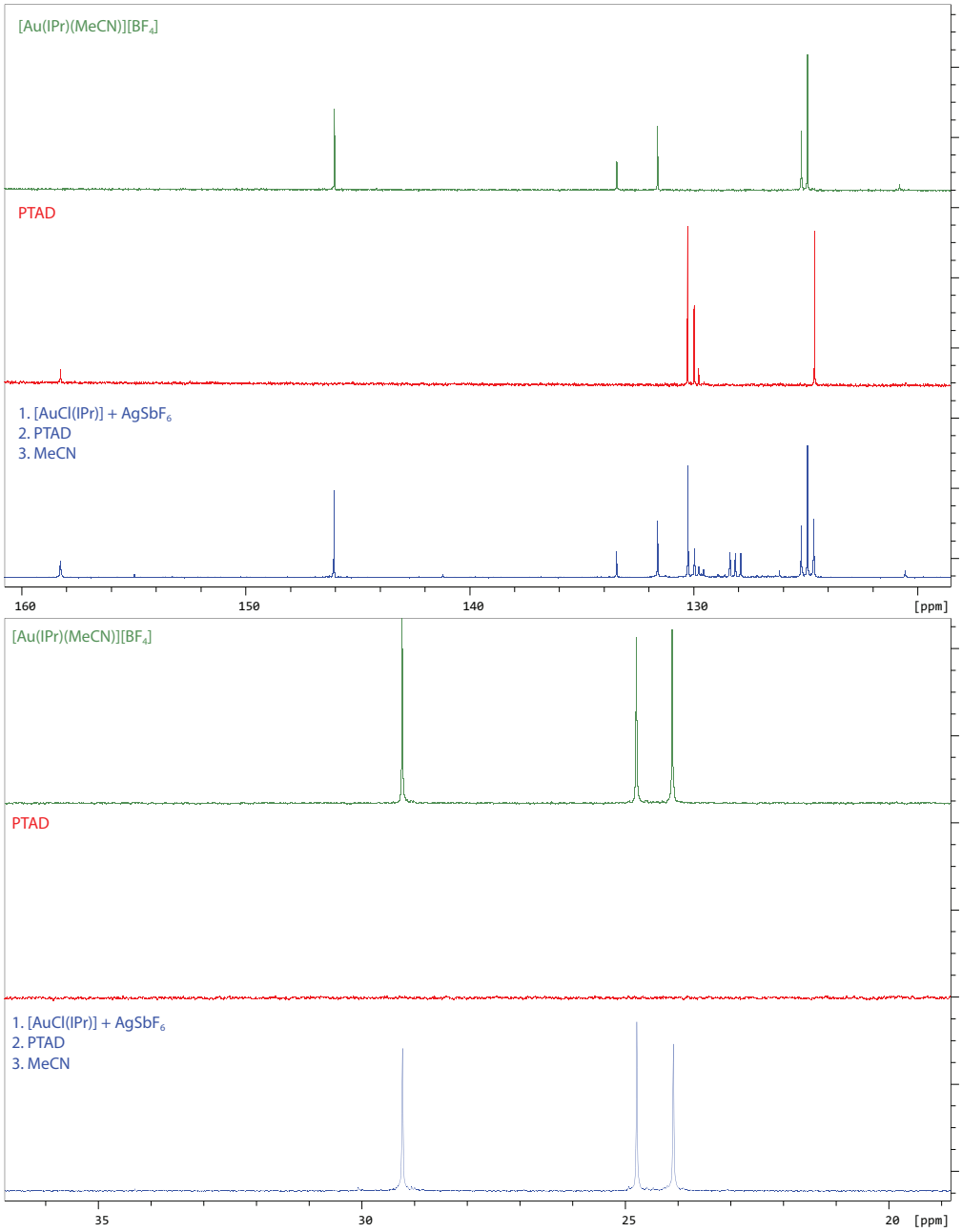


Figure S12: Zoomed in areas of the $^{13}C\{^{1}H\}$-NMR (100 MHz, DCM-d_2) after the addition of MeCN complex compared to PTAD and the [Au(IPr)(MeCN)]BF_4 complex (full spectra in S8).

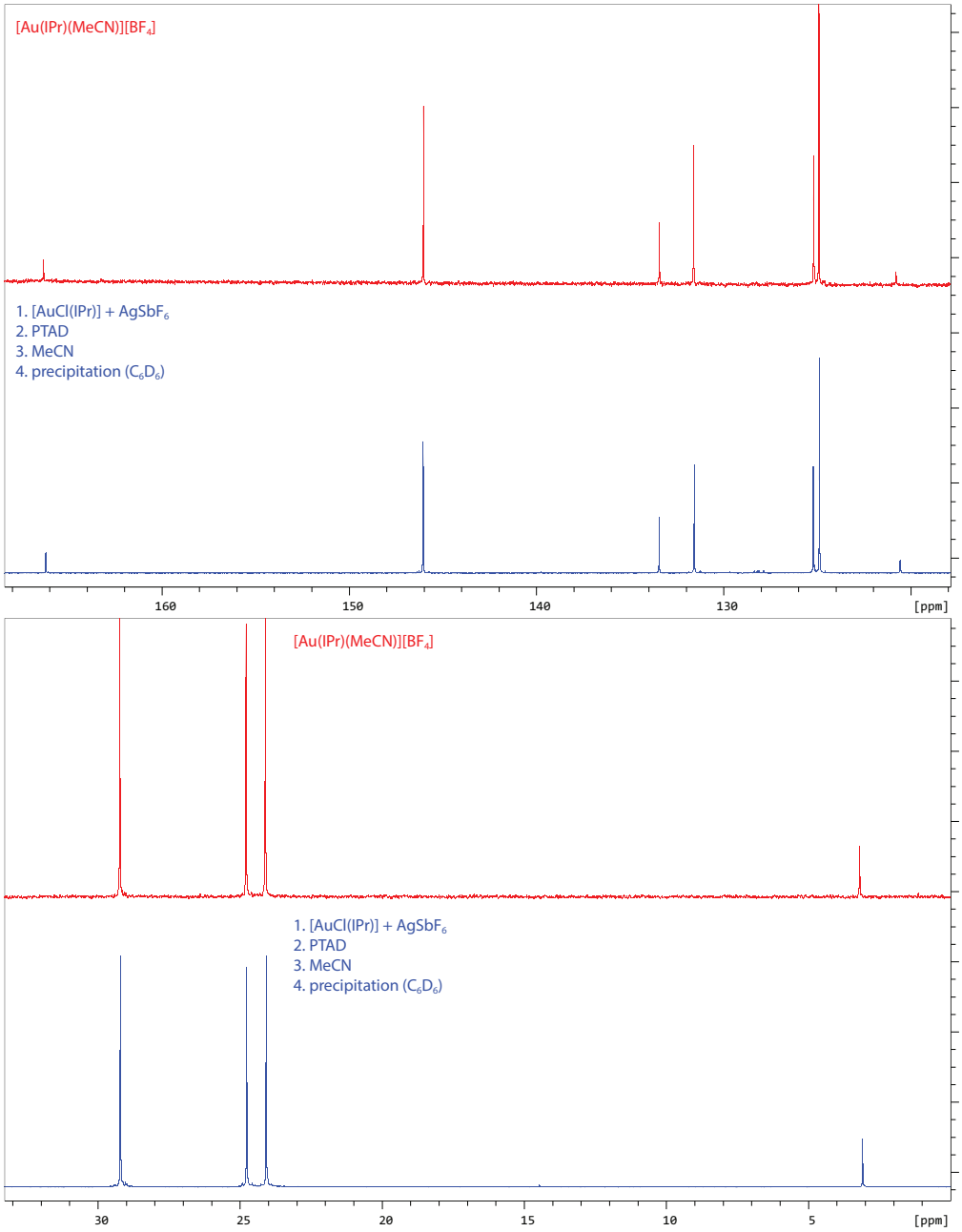
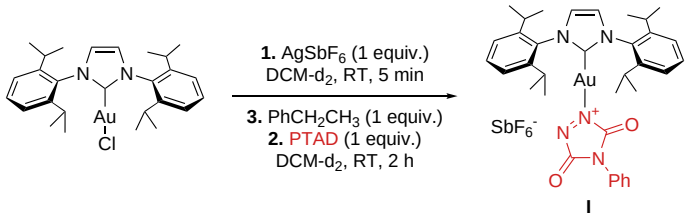


Figure S13: Zoomed in areas of the $^{13}C\{^{1}H\}$-NMR (100 MHz, DCM-d_2) of the white precipitate compared to the [Au(IPr)(MeCN)]BF_4 complex (full spectra in S9).

The calculations identified a pathway in which the rate determining step is a hydride transfer from the alkylarene substrate, without complexation of the gold to the aryl ring involved at this stage, nor a direct complexation of the

gold to the substrate prior to the hydride transfer. The coordination sphere of the gold cation is only involved with the activation of the PTAD electrophile, and then in guiding the collapse of the ion pair into the formed product (together with decomplexation of the nucleophilic nitrogen) as it combines with the tightly associated carbocation. The gold cation can also act as a pi-acid for the arene ring before the hydride transfer. but this is not found in our calculations, and would likely also not be a contributing factor to a nucleophilic transfer of hydride from the substrate to PTAD, as it would make the aryl substrate likely more electrophilic, and not more nucleophilic. This pathway, where the gold first complexes the aryl, was also investigated. This was done to see if the Au-TAD complex is favoured to form in the presence of the aryl starting materials, in accordance with the proposed and calculated mechanism. Therefore, to provide experimental support for the complexation of PTAD to the gold in the presence of the substrate, another experiment was performed in the glovebox where the substrate (ethylbenzene) is added to the *in situ* generated cationic gold after which the PTAD is added. Ethylbenzene is chosen as this substrate needs 3 days to reach full conversion under the optimised reaction conditions, so here there is a chance to see intermediates or pre-reactive complex formation before the reaction is done (as with 1 equivalent of gold, the reaction should go significantly faster).



$AgSbF_6$ (30.3 mg, 90 μmol, 1 equiv.) and [AuCl(IPr)] (33.7 mg, 90 μmol, 1 equiv.) were dissolved in 4 ml of DCM-d_2 after which this mixture was stirred for 5 minutes, shielding it from light. Ethylbenzene (11 μl, 90 μmol, 1 equiv.) was added to the mixture and left to stir for 30 minutes at room temperature shielded from light. An NMR sample was taken at this point, after which PTAD (**1**) (11.5 mg, 60 μmol, 1 equiv.) was added to this mixture and stirred for 2 h shielded from light. Then an NMR sample was

taken. Afterwards, MeCN (18 μl, 0.34 mmol, 2.3 equiv.) was added to the reaction mixture, and after 5 minutes of stirring, an NMR sample was taken. The NMR samples were taken in the following way: 0.55 ml was taken out of the reaction mixture by means of a syringe and a needle, then filtered directly into an amber NMR tube.

The corresponding NMR spectra are given in Figure S14 and Figure S15. They show that indeed again the PTAD (**1**) peaks have shifted and that a complex with gold is made even in the presence of ethylbenzene (with similar peaks to the ones observed in the absence of ethylbenzene, see Figure S6). As expected, the C-H amination is already occurring significantly by the time the NMR is measured after PTAD (**1**) addition. The NMR spectrum of the sample after MeCN addition was measured significantly later (a couple of hours) after the previous mentioned spectrum, so this shows only a small amount of PTAD and starting material and almost full conversion towards the expected C-H aminated product. No shifts in the resonances for the ethyl benzene substrate can be seen, showing that - in contrast to acetonitrile - it is not a competitive ligand for the gold cation. These data thus confirm the calculated pathway.

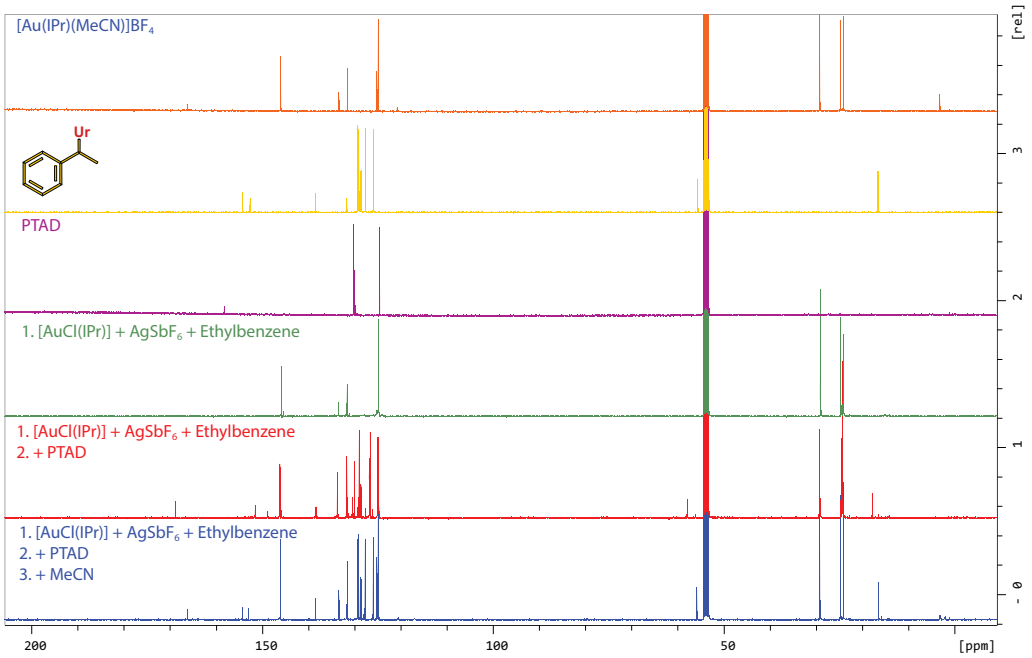


Figure S14: $^{13}C\{^{1}H\}$-NMR (100 MHz, DCM-d_2) of the PTAD complexation in presence of ethylbenzene.

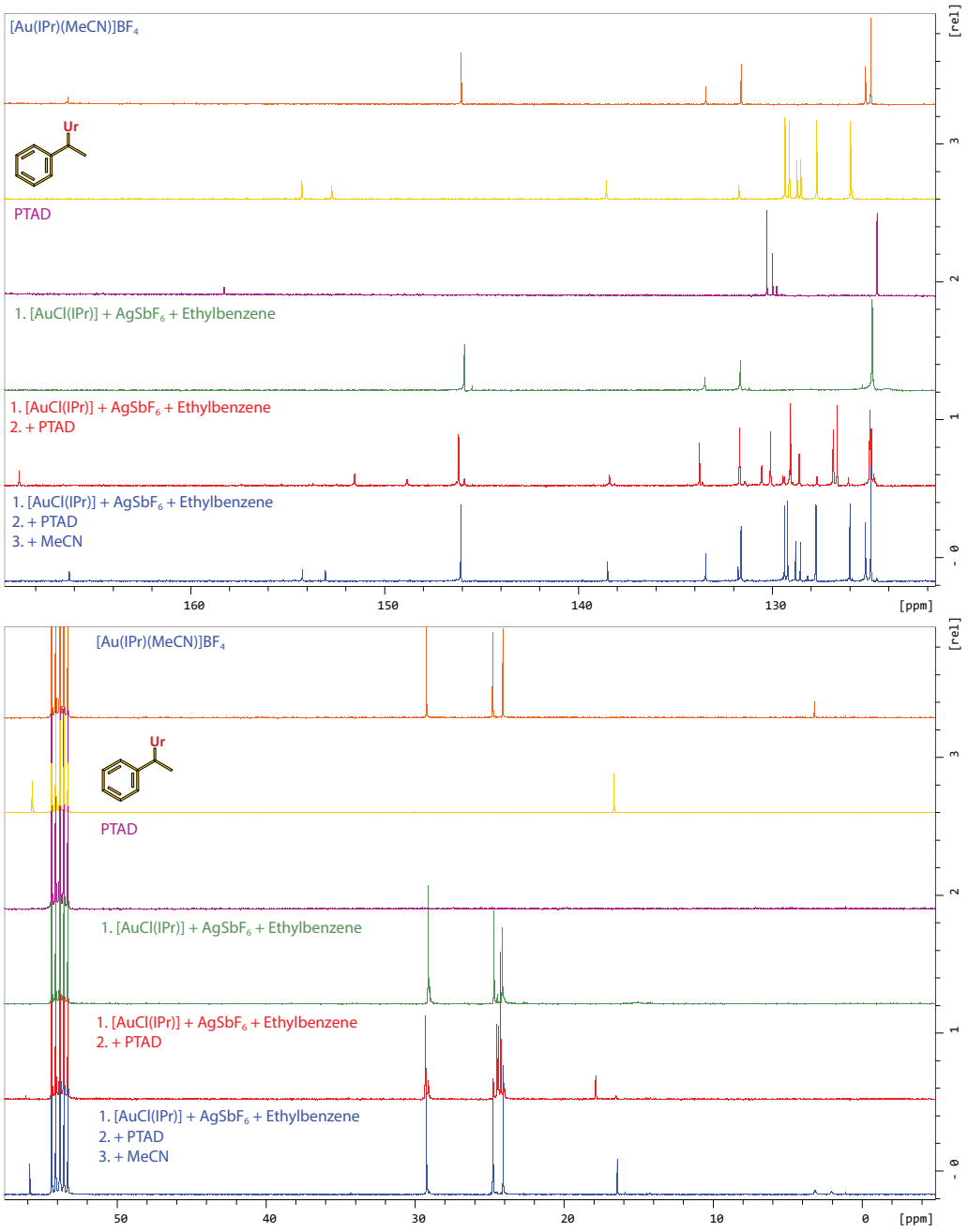
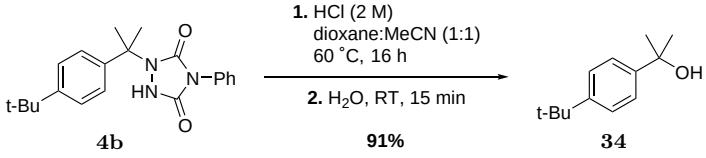


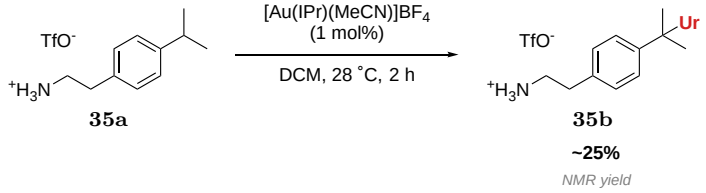
Figure S15: Zoomed in areas of the $^{13}C\{^1H\}$-NMR (100 MHz, DCM-d_2) of the PTAD complexation in presence of ethylbenzene (full spectra in S14).

2.20 Hydrolysis of 4b to 2-(4-(tert-butyl)phenyl)propan-2-ol (34)



4b (50.0 mg, 0.14 mmol, 1 equiv.) was brought into a pressure tube and dissolved in 1.4 ml acetonitrile after which 1.4 ml of HCl in dioxane (4M) was added. The mixture was then stirred at 60 °C overnight (16 h) after which it was cooled down, quenched with 5 ml of H_2O and stirred for 15 minutes. Then an extraction was done with DCM (3 x 7 ml) after which the organic phase was dried with Na_2SO_4, filtered over a cotton plug and concentrated *in vacuo*. This resulted in a white solid which was subjected to column chromatography over silica with 5% EtOAc in pentane, which resulted in 24.5 mg of the title compound as white solid (91% yield). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.21 C-H amination on ammonium salt 35a giving 35b



$[Au(IPr)(MeCN)]BF_4$ (1.8 mg, 2.5 μmol, 1 mol%) was brought into a 10 ml roundbottom flask and was dissolved in 2.5 ml of DCM. Then PTAD (45.1 mg, 0.25 mmol, 1 equiv.) was added to the mixture after which 2--(4-isopropylphenyl)ethan-1-aminium trifluoromethanesulfonate (**35a**) (361.2 mg, 1.5 mmol, 3 equiv.) was added in one portion. The colour of the reaction changed from dark red to bright red. The reaction mixture was then stirred

in a water bath at 28 °C untill the red colour of the PTAD had dissapeared after 2 hours and the mixture was yellowish of colour. The reaction was then quenched with isoprene and left to stir for 5 minutes. The mixture was then concentrated *in vacuo*. The crude NMR and LCMS show the presence of the expected aminated product **35b**, so an attempt was made to purify this via column chromatography over silica using a gradient starting with 99:1:1 DCM:MeOH:HOAc to 90:10:1 DCM:MeOH:HOAc. The effort was fruitless and the target **35b** was not recovered. Integrations on the crude NMR give an estimate of 25% yield, which is mainly due to a low conversion.

Compound analysis on the crude mixture can be found in section 3 and NMR spectra of this mixture can be found in section 4.

The LCMS (see Figure S16) clearly shows two peaks at 7.03 min and 7.27 min (integrating 2:1 relatively on 214 nm) having the correct $[M]^+$ for the expected aminated product next to the peak (at 7.80) of the substrate. There are also smaller peaks eluting at 5.30 and 5.95 showing an m/z of 355.1, which corresponds to the expected aminated product +16 D.

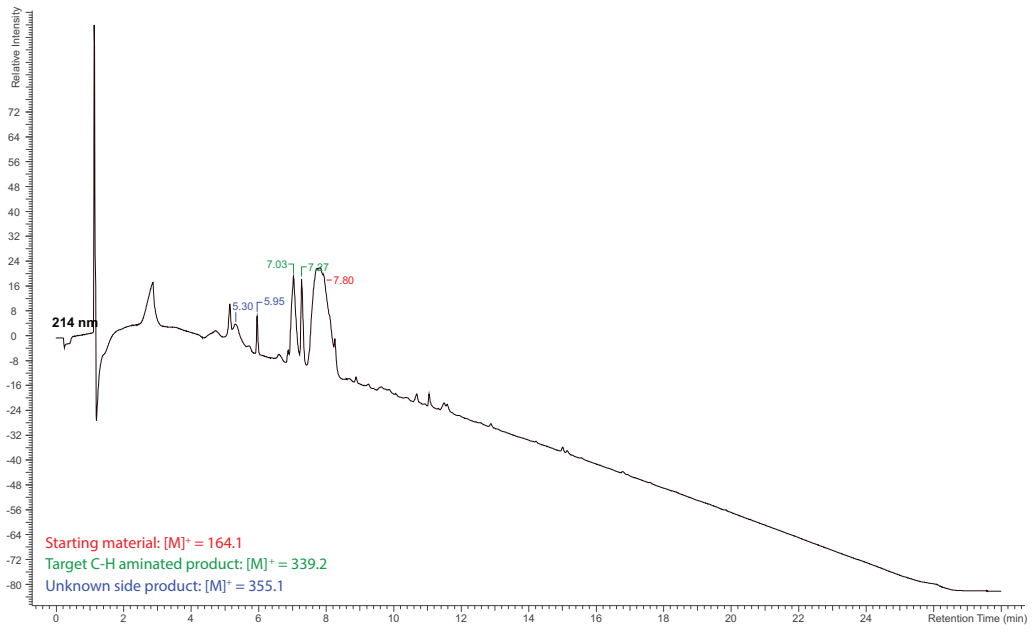
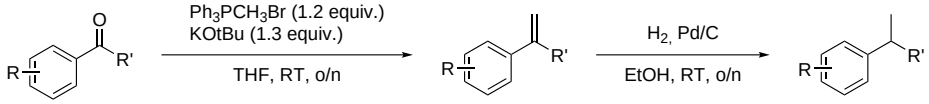


Figure S16: 214 nm spectrum of the LCMS of the crude reaction mixture after work-up. Linear solvent gradient 100% A to 50:50 A:B in 24 min (A: 0.1%(v/v) HCOOH in H_2O, B: MeCN)

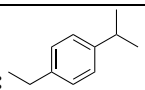
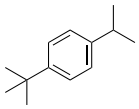
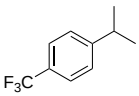
2.22 Synthesis of model substrate 2a, 4-tert-butylcumene (4a) and 4-trifluoromethylcumene (7a)



The phosphonium salt (Ph_3PCH_3Br, 1.2 equiv.) was brought in a round bottom flask onto which dry THF (2 ml per mmol substrate) was added. The stirring mixture was then cooled to 0 °C onto which KOtBu (1.3 equiv.) was added. The mixture became bright yellow and was stirred for 30 minutes at 0 °C. The substrate (1 equiv.) was then added to the mixture which was then stirred for 30 minutes on 0 °C before it was allowed to warm to room temperature. The mixture was then stirred overnight (16 h) at room temperature after which it became red to brownish. TLC never showed full consumption of the starting material. A glass filter was prepared with celite packed with pentane onto which the reaction mixture was poured. The filter was washed with pentane. In the filtrate precipitation occured, so before evaporation the mixture was filtered over a cotton plug to remove these solids. After evaporation pentane was added and again filtered over a cotton plug to get rid of the solids after which it was again concentrated *in vacuo*. The resulting mixture was then filtered over silica with pentane to yield the alkene. The alkene was then used in the next step without any further purification.

The alkene was solubilized in denaturated ethanol in a non-dried round bottom flask after which the flask was flushed with Argon. Pd/C (5%) was added untill the sollution became fully black. A hydrogen balloon was then bubbled trough the mixture after which a hydrogen atmosphere was kept on the flask by means of a balloon. This mixture was stirred at room temperature until crude NMR showed full conversion of the starting material (see table underneath for reaction times), after which it was filtered over a glass filter loaded with packed celite (packed with pentane) and washed with pentane. The filtrate was then evaporated after which the resulting yellowish

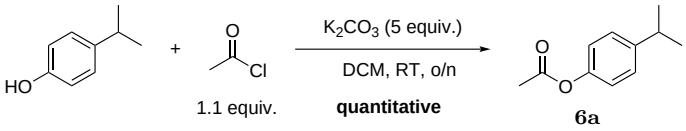
liquid was subjected to column chromatography with pentane to yield the pure alkane. Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

compound	time	yield (%)[a]	isolated mass
2a: 	3 days	83	28.7 g
4a: 	16 h	75	2.34 g
7a: 	16 h	39	1.98 g

[a] isolated yield over the two steps

Table S10: Data per compound.

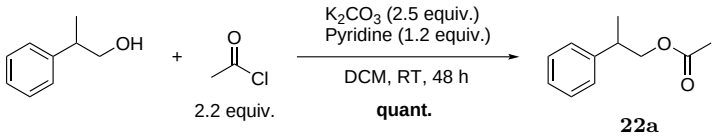
2.23 Synthesis of 4-isopropylphenyl acetate (6a)



4-isopropylphenol (1.3897 g, 10 mmol, 1 equiv.) was brought into a round bottom flask and was dissolved in 5 ml DCM. Then, K_2CO_3 (7.0 g, 50 mmol, 5 equiv.) was added after which the mixture was cooled down to 0 °C. Acetyl chloride (0.80 ml, 11 mmol, 1.1 equiv.) was then added to the stirring mixture after which it was allowed to warm to room temperature. The reaction was left stirring at room temperature overnight (16 h) after which it was quenched with a saturated aqueous $NaHCO_3$ sollution (5 ml). This mixture was then extracted with chloroform (3 x 10 ml), dried on Na_2SO_4, filtered of over cotton and concentrated *in vacuo*. The resulting yellow oil was then subjected to column chromatography over silica with 5% ether in n-hexane yielding the title compound as a clear liquid in quantitative yield

(1.8 g). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

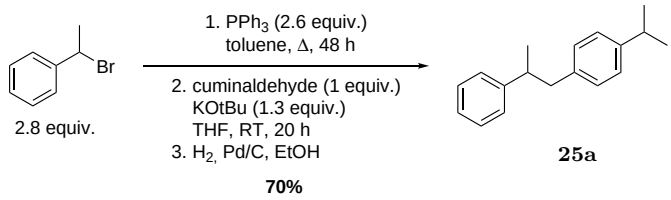
2.24 Synthesis of 2-phenylpropyl acetate (22a)



22a

K_2CO_3 (3.5g, 25 mmol, 2.5 equiv.) was brought into a 25 ml round bottom flask onto which 12.5 ml DCM was added. Then, 2-phenyl-1-propanol (1.44 ml, 10 mmol, 1 equiv.) was added after which the mixture was cooled down to 0 °C. Acetylchloride (0.8 ml, 11 mmol, 1.1 equiv.) was then added dropwise while stirring at 0 °C. The reaction was then stirred for 24 h after which TLC indicated no full conversion of the starting material. It was then decided to add another 1.1 equiv. of acetylchloride (0.8 ml, 11 mmol) and 1 ml of dry pyridine (12 mmol, 1.2 equiv.). This mixture was then again stirred for 24 h, this time showing full conversion of the starting material on TLC. The reaction was quenched with 10 ml $NaHCO_3$ and extracted with DCM (3 x 15 ml). The organic phase was dried with Na_2SO_4, filtered over a cotton plug and concentrated *in vacuo*. The resulting yellowish liquid was then subjected to column chromatography over silica with 10% ether in pentane yielding 1.78 g of the title compound **22a** (quantitative yield). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.25 Synthesis of 1-isopropyl-4-(2-phenylpropyl)benzene (25a)

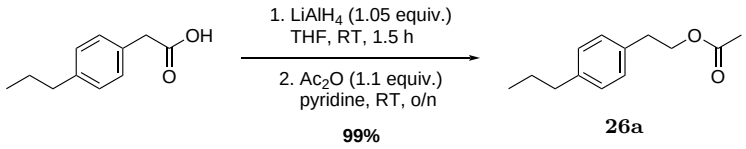


PPh_3 (14.6 g, 54.5 mmol, 2.6 equiv.) was brought into a 500 ml round bottom flask, onto which 240 ml toluene was added. (1-bromoetyl)benzene (8.62 ml, 60 mmol, 2.8 equiv.) was then added at once after which the mixture was heated to reflux for 48 h. After cooling down the mixture, a sticky solid was present in the flask. The supernatant was first decanted out using a cannula and then 100 ml of THF was added. The mixture was then stirred at 0 °C and KOtBu (3.176 g, 27.7 mmol, 1.3 equiv.) was added, resulting in a bright red colour of the mixture. This mixture was then stirred at 0 °C for another 15 minutes after which cuminaldehyde (3.13 ml, 21.3 mmol, 1 equiv.) was added dropwise. This was then stirred at 0 °C for 30 minutes before it was allowed to warm up to room temperature where it was allowed to react for 20 h. A glass filter was prepared with celite, which was packed with pentane, onto which the reaction mixture was poured and which was then washed with pentane. In the filtrate precipitation occured, so before evaporation the mixture was filtered over a cotton plug to remove these solids. After evaporation pentane was added and again filtered over a cotton plug to get rid of the solids. The resulting mixture was first concentrated *in vacuo* and then filtered over silica with pentane to yield 3.8616 g of the alkene. The alkene was then used in the next step without any further purification.

The alkene was dissolved in 10 ml denaturated ethanol in a non-dried round bottom flask after which the flask was flushed with Argon. Pd/C (5%) was added untill the sollution became fully black. A hydrogen balloon was then bubbled trough the mixture after which a hydrogen atmosphere was kept on the flask by means of a balloon. This mixture was stirred 48 h

at room temperature after which it was filtered over a glass filter loaded with packed celite (packed with pentane) and washed with pentane. The filtrate was then evaporated after which the resulting yellow oil was subjected to column chromatography with pentane to yield 3.5477 g of the title compound **25a** (70% yield over two steps). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.26 Synthesis of 4-propylphenethyl acetate (26a)



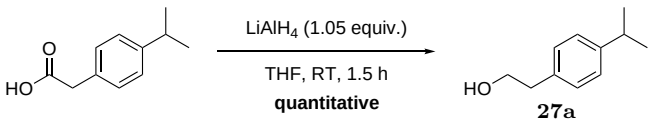
26a

$LiAlH_4$ (597.7 mg, 15.75 mmol, 1.05 equiv.) was brought into a round bottom flask onto which 20 ml of THF was added. The mixture was cooled to 0 °C and a solution of 4-propylphenylacetic acid (2.6735 g, 15 mmol, 1 equiv.) in 10 ml THF was then added dropwise under stirring. The reaction was then stirred for 1.5 h on room temperature after which it was cooled down to 0 °C again. Then, 30 ml of diethylether was added and 0.7 ml of H_2O was added carefully. After that, 0.7 ml of a 15% NaOH in H_2O solution was added, followed again by 2.1 ml of H_2O. Then the mixture was allowed again to stir at room temperature for 20 minutes after which some anhydrous magnesium sulfate was added and the mixture was again stirred for 15 minutes at room temperature. The mixture was then filtered over a cotton plug and concentrated *in vacuo*. The alcohol was then used in the next step without any further purification.

The alcohol was dissolved in 25 ml of pyridine, and the resulting mixture was cooled down to 0 °C. Then, acetic anhydride (1.56 ml, 16.5 mmol, 1.1 equiv.) was added dropwise and afterwards the reaction was allowed to warm to room temperature and was stirred overnight (16 h). The mixture was then evaporated and subjected to columned chromatography over silica using 5% ether in pentane, yielding 3.0515 g of 4-propylphenethyl acetate **26a** (99%

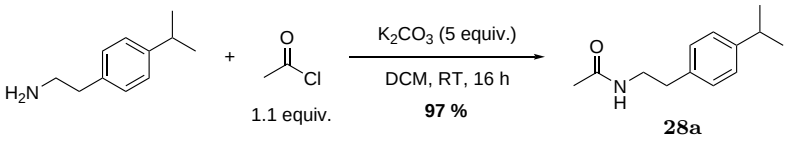
yield over 2 steps). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.27 Synthesis of 2-(4-isopropylphenyl)ethan-1-ol (27a)



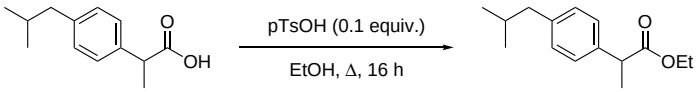
$LiAlH_4$ (251.7 mg, 6.3 mmol, 1.05 equiv.) was brought into a round bottom flask onto which 8 ml of THF was added. The mixture was cooled to 0 °C and a solution of 2-(4-isopropylphenyl)acetic acid (1.08 g, 6.0 mmol, 1 equiv.) in 4 ml THF was then added dropwise under stirring. The reaction was then stirred for 1.5 h on room temperature after which it was cooled down to 0 °C again. Then, 12 ml of diethylether was added and 0.25 ml of H_2O was added carefully. After that, 0.25 ml of a 15% NaOH in H_2O solution was added, followed again by 0.76 ml of H_2O. Then the mixture was allowed again to stir at room temperature for 20 minutes after which some anhydrous magnesium sulfate was added and the mixture was again stirred for 15 minutes at room temperature. The mixture was then filtered over a cotton plug and concentrated *in vacuo* after which it was subjected to column chromatography over silica using 10% EtOAc in pentane. This yielded the title compound as a yellowish transparent liquid in quantitative yield (985.5 mg). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.28 Synthesis of N-(4-isopropylphenethyl)acetamide (28a)



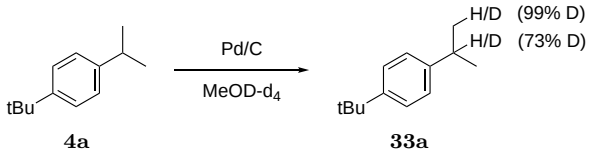
2-(4-isopropylphenyl)ethan-1-amine (500 mg, 2.91 mmol, 1 equiv.) was brought into a round bottom flask and was dissolved in 7.8 ml DCM. Then, K_2CO_3 (2.03 g, 14.55 mmol, 5 equiv.) was added after which the mixture was cooled down to 0 °C. Acetyl chloride (0.23 ml, 3.20 mmol, 1.1 equiv.) was then added to the stirring mixture after which it was allowed to warm to room temperature. The reaction was left stirring at room temperature overnight (16 h) after which it was quenched with a saturated aqueous $NaHCO_3$ sollution (5 ml). This mixture was then extracted with DCM (3 x 10 ml), washed with NH_4Cl (30 ml), dried on Na_2SO_4, filtered of over cotton and concentrated *in vacuo*. The resulting yellowish solid was then subjected to column chromatography over silica with 50% EtOAc in n-pentane yielding 579.3 mg of the title compound as a white solid (97% yield). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.29 Synthesis of ibuprofen ethyl ester (30a)



ibuprofen (2.1049 g, 10 mmol, 1 equiv.) was brought into a non-dry round bottom flask where it was dissolved in 60 ml of non-dry ethanol. pTsOH (194.1 mg, 1 mmol, 0.1 equiv.) was then added, after which the mixture was refluxed overnight (16 h). After cooling down and concentrating *in vacuo*, the mixture was redissolved in EtOAc (20 ml) and washed with $NaHCO_3$ (2 x 15 ml). The organic phase was then dried on Na_2SO_4, filtered over a cotton plug and conentrated invacuo. This yielded the title compound pure in quantitative yield as a clear liquid (2.3433 g). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

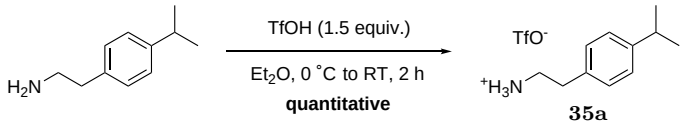
2.30 Deuteration of 4-tert-butylcumene



4a **33a**

4-tert-butylcumene (311.6 mg, 1.77 mmol) was brought into a round bottom flask and was dissolved in deuterated methanol (MeOD−d_4). Pd/C (5%) was added untill the sollution became fully black. A hydrogen balloon was then bubbled trough the mixture and then an argon atmosphere was kept on the reaction while it was stirring at room temperature over the weekend (72h). The mixture was then filtered over a glass filter loaded with packed celite (packed with pentane) and washed with pentane. The filtrate was then evaporated after which the resulting colourless liquid was subjected to column chromatography with pentane to yield 315 mg of the deuterated product **33a**. The amount of deuteration was determined by integration on H-NMR by subtracting the integral from the amount of protons in the starting material (so 6 for the methyls and 1 for the CH of the isopropyl). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.31 Synthesis of 2-(4-isopropylphenyl)ethan-1-aminium trifluoromethanesulfonate (35a)



35a

2-(4-isopropylphenyl)ethan-1-amine (271.2 mg, 1.58 mmol, 1 equiv.) was brought into a round bottom flask and dissolved in 8 ml of Et_2O after which the mixture was cooled down to 0 °C. Triflic acid (0.22 ml, 2.37 mmol, 1.5

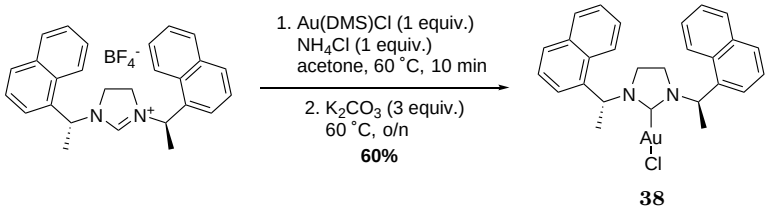
equiv.) was then added dropwise. While adding the triflic acid, white precipitation was forming. The reaction was then stirred 15 minutes on 0 °C after which it was stirred at room temperature for 2 more hours. Then 10 ml of pentane was added, after which the mixture was filtered over a glass filter, washing the solid with pentane. After drying this solid under reduced pressure, this yielded 494.5 mg of the title compound as a white solid (quantitative yield). Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.32 Synthesis of achiral the Au(I) complexes.

All complexes were synthesised via previously reported methods:

catalyst	doi	ref
[AuCl(IPr)]	10.1038/s41596-020-00461-6	[11]
[Au(IPr)(MeCN)]BF_4	10.1002/chem.202000876	[12]
[Au(NTf_2)(IPr)]	10.1039/C0CC00018C	[13]
[$Au(IPr)_2(\mu-OH)]BF_4$	10.1038/s41596-020-00461-6	[11]
[Au(OTf)(IPr^*)]	10.1039/D0GC00498G	[14]
[AuCl(SIPr)]	10.1039/D2CC03056J	[15]
[AuCl(IAd)]	10.1021/om050111c	[16]
[Au(NTf_2)(IMes)]	10.1021/acs.organomet.7b00622	[17]
[AuCl(IPr^{Me})]	10.1039/c3cc43076f	[18]
[Au(IPr^{Cl})(MeCN)]BF_4	10.1021/acs.organomet.7b00622	[17]

2.33 Synthesis of [((R,R)-SINpEt)AuCl]

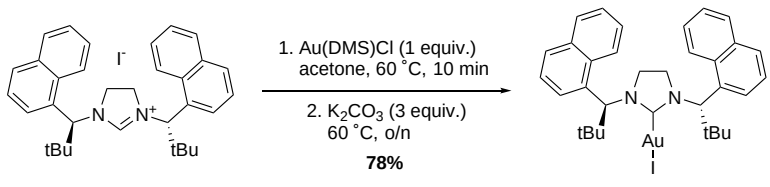


38

This is an adapted procedure from Nahra F. *et al.*, Nature Protocols, 16, **2021**, 1476-1493 (doi: 10.1038/s41596-020-00461-6).[11]

(R,R)−SINpEt · HBF_4 (98.2 mg, 0.2 mmol, 1 equiv.) and Au(DMS)Cl (60.7 mg, 0.2 mmol, 1 equiv.) were added to a 4 ml screwcap vial after which 1.07 ml of non dry HPLC acetone was added. NH_4Cl (10.8 mg, 0.2 mmol, 1 equiv.) was then added to this mixture which was first stirred at room temperature for 30 minutes. After this, the yellow solution was heated to 60 °C where it was stirred for 10 minutes before cooling down again to room temperature. Once cooled down, freshly grinded K_2CO_3 (83.8 mg, 0.6 mmol, 3 equiv.) was added. The reaction was then heated up to 60 °C and left to stir at this temperature overnight (16h). The mixture that now contained some black percipitate was concentrated *in vacuo* after which it was filtered over a plug of silica using DCM to wash everything of the silica. The filtrate was again concentrated *in vacuo* after which the titel compound was percipitated by adding a small amount of DCM and adding pentane onto it. The solid was retrieved by decantation and dried using the oil pump, which delivered 73.9 mg (60% yield) of the title compound. Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

2.34 Synthesis of [((R,R)-SINnPent)AuI]



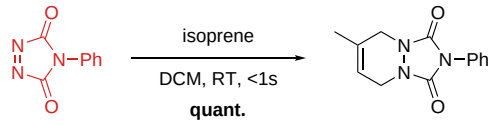
39

This is an adapted procedure from Nahra F. *et al.*, Nature Protocols, 16, **2021**, 1476-1493 (doi: 10.1038/s41596-020-00461-6).[11]

(R,R)−SINnPent · I (101.1 mg, 0.17 mmol, 1 equiv.) and Au(DMS)Cl (52.0 mg, 0.17 mmol, 1 equiv.) were added to a 4 ml screwcap vial after which 0.92 ml of non dry HPLC acetone was added. The mixture was first stirred at room temperature for 30 minutes, after which the orange solution

was heated to 60 °C where it was stirred for 10 minutes before cooling down again to room temperature. Once cooled down, freshly grinded K_2CO_3 (83.8 mg, 0.6 mmol, 3 equiv.) was added. The reaction was then heated up to 60 °C and left to stir at this temperature overnight (16 h). The brown mixture was concentrated *in vacuo* after which it was filtered over a plug of silica using DCM to wash everything of the silica. The filtrate was again concentrated *in vacuo* after which the title compound was percipitated by adding a small amount of DCM and adding pentane onto it. The solid was retrieved by decantation and dried using the oil pump, which delivered 104.4 mg (78% yield) of the title compound. Compound analysis can be found in section 3 and NMR spectra can be found in section 4.

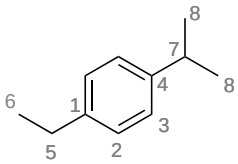
2.35 Adduct (40) formation of PTAD (1) with isoprene



PTAD (9.0 mg, 0.05 mmol) was added to a 4 ml screwcap vial onto which 1 ml of DCM was added. One drop of isoprene was then added, discolouring the mixture. The mixture was then concentrated *in vacuo* yielding 12.2 mg of a white solid (quantitative).

3 Compound analysis

3.1 2a: 1-ethyl-4-isopropylbenzene



Formula: $C_{11}H_{16}$
Molecular weight: 148.249 g/mol
Exact mass: 148.1252 D

appearance: colourless liquid

Product didn't ionize for HRMS analysis.
GCMS m/z: $[M]^{\bullet}$ Calcd for $C_{11}H_{16}$ 148.1; Found 148.1

$\mathbf{R}_f$: 0.75 (pentane)

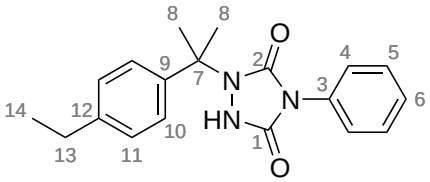
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.17 (4H, m, *C2-H and C3-H*), 2.90 (1H, sept, J = 6.9 Hz, *C7-H*), 2.65 (2H, q, J = 7.6 Hz, *C5-*H_2), 1.27 (6H, d, J = 6.9 Hz, *C8-*H_3), 1.26 (3H, t, J = 7.6 Hz, *C6-*H_3)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 146.2 (Ar−Cq, *C4*), 141.7 (Ar−Cq, *C1*), 127.9 (Ar−CH, *C2*), 126.7 (Ar−CH, *C3*), 33.8 (CH, *C7*), 28.5 (CH_2, *C5*), 24.2 (CH_3, *C8*), 15.7 (CH_3, *C6*)

HSQC : 7.17 x 127.9, 7.17 x 126.7, 2.90 x 33.8, 2.65 x 28.5, 1.27 x 24.2, 1.26 x 15.7

IR: $\nu_{max}(cm^{-1})$: 3034(w), 2959(m), 2930(w), 2870(w), 1515(w), 1461(w), 827(s)

3.2 2b: 1-(2-(4-ethylphenyl)propan-2-yl)-4-phenyl-urazole



Formula: $C_{19}H_{21}N_3O_2$
Molecular weight: 323.396 g/mol
Exact mass: 323.16338 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{22}N_3O_2$ 324.1712; found 324.1720 (Δ = 4.2 ppm)

$\mathbf{R}_f$: 0.33 (7:3 pentane: EtOAc)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.50-7.43 (4H, band, *C5-H*

and C4-H), 7.42-7.34 (3H, band, *C6-H and C10-H*), 7.24 (2H, m, *C11-H*), 6.82 (1H, s(br), *NH*), 2.66 (2H, q, J = 7.6 Hz, *C13-*H_2), 1.89 (6H, s, *C8-*H_3), 1.25 (3H, t, J = 7.6 Hz, *C14-*H_3)

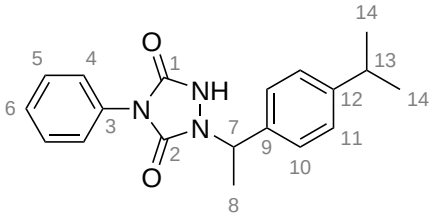
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.1 (C=O, *C1 or C2*), 153.1 (C=O, *C1 or C2*), 144.4 (Ar−Cq, *C12*), 140.6 (Ar−Cq, *C9*), 131.3 (Ar−Cq, *C3*), 129.2 (Ar−H, *C5*), 128.7 (Ar−H, *C11*), 128.3 (Ar−H, *C6*), 125.8 (Ar−H, *C4*), 125.5 (Ar−H, *C10*), 64.5 (Cq, *C7*), 28.5 (CH_2, *C13*), 26.1 (CH_3, *C8*), 15.6 (CH_3, *C14*)

HSQC : 7.50-7.44 x 125.8, 7.48-7.43 x 129.2, 7.42-7.37 x 125.5, 7.39-7.34 x 128.3, 7.24 x 128.7, 2.66 x 28.5, 1.89 x 26.1, 1.25 x 15.6

IR: $\nu_{max}(cm^{-1})$: 3056(w), 2960(w), 1766(w), 1690(s), 1414(s), 767(s), 691(s)

3.3 2c: 1-(1-(4-isopropylphenyl)ethyl)-4-phenyl-urazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **2b** and **2c** in a 71:29 ratio*



Formula: $C_{19}H_{21}N_3O_2$
Molecular weight: 323.396 g/mol
Exact mass: 323.16338 D

appearance: white solid

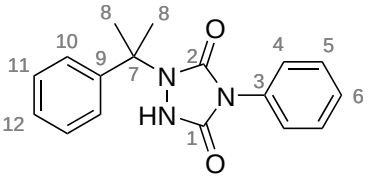
$\mathbf{R}_f$: 0.25 (7:3 pentane: EtOAc)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 29%, only clear resonances are given]*: δ(ppm) = 8.83 (1H, s(br), *NH*), 7.50-7.43 (4H, band, *C4-H and C6-H*), 7.38 (1H, m, *C5-H*), 7.33 (2H, m, *C10-H*), 7.20 (2H, m, *C11-H*), 5.43 (1H, q, J = 7.1 Hz, *C7-H*), 2.90 (1H, sept, J = 6.9 Hz, *C13-H*), 1.65 (3H, d, J = 7.1 Hz, *C8-*H_3), 1.24 (6H, d, J = 6.9 Hz, *C14-*H_3)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 29%, only clear resonances are given]*: δ(ppm) = 153.8 (C=O, *1*), 152.2 (C=O, *2*), 149.2 (Ar−Cq, *C12*), 135.4 (Ar−Cq, *C9*), 131.3 (Ar−Cq, *C3*), 129.1 (Ar−H, *C6*), 128.1 (Ar−H, *C5*), 127.5 (Ar−H, *C10*), 126.9 (Ar−H, *C11*), 125.5 (Ar−H, *C4*), 55.1 (CH, *C7*), 33.8 (CH, *C13*), 24.0 (CH_3, *C14*), 16.7 (CH_3, *C8*)

HSQC *[minor, integrating for 29%, only clear resonances are given]*: 7.50-7.43 x 129.1, 7.50-7.43 x 125.5, 7.38 x 128.1, 7.33 x 127.5, 7.20 x 126.9, 5.43 x 55.1, 2.90 x 33.8, 1.65 x 16.7, 1.24 x 24.0

3.4 3b: 4-phenyl-1-(2-phenylpropan-2-yl)-urazole



Formula: $C_{17}H_{17}N_3O_2$
Molecular weight: 295.342 g/mol
Exact mass: 295.13208 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{17}H_{16}N_3O_2$ 294.1243; found 294.1244 (Δ = -1.4 ppm)

$\mathbf{R}_f$: 0.29 (7:3 pentane: EtOAc)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.52-7.39 (8H, m, *C4-H, C5-H, C10-H and C11-H*), 7.39-7.31 (2H, m, *C6-H and C12-H*), 6.70 (1H, s(br), *NH*), 1.91 (6H, s, *CH3*)

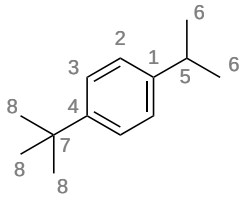
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.3 (C=O, *C1 or C2*), 153.2 (C=O, *C1 or C2*), 143.4 (Cq, *C9*), 131.2 (Cq, *C3*), 129.3 (Ar−H, *C4, C5, C10 or C11*), 129.2 (Ar−H, *C4, C5, C10 or C11*), 128.4 (Ar−H, *C6 or C12*), 128.3 (Ar−H, *C6 or C12*), 125.8 (Ar−H, *C4, C5, C10 or C11*), 125.5

(Ar−H, *C4, C5, C10 or C11*), 64.8 (Cq, *C7*), 26.1 (CH_3, *C8*)

HSQC : 7.52-7.45 x 125.8, 7.52-7.45 x 125.5, 7.49-7.39 x 129.3, 7.49-7.39 x 129.2, 7.39-7.31 x 128.4, 7.39-7.31 x 128.3, 1.91 x 26.1

IR: $\nu_{max}(cm^{-1})$: 3073(w), 2862(w), 1770(w), 1698(s), 1424(m), 771(s), 720(m), 701(s)

3.5 4a: 1-(tert-butyl)-4-isopropylbenzene



Formula: $C_{13}H_{20}$
Molecular weight: 176.303 g/mol
Exact mass: 176.1565 D

appearance: colourless liquid

Product didn't ionize for HRMS analysis.
GCMS m/z: $[M]^{\bullet}$ Calcd for $C_{13}H_{20}$ 176.2; Found 176.1

$\mathbf{R}_f$: 0.81 (pentane)

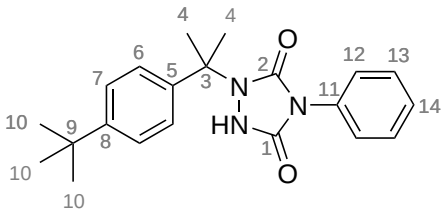
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.35 (2H, m, *C3-H*), 7.20 (2H, m, *C2-H*), 2.92 (1H, sept, J = 6.9 Hz, *C5-H*), 1.35 (9H, s, *C8-*H_3), 1.28 (6H, d, J = 6.9 Hz, *C6-*H_3)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 148.6 (Ar−Cq, *C4*), 145.9 (Ar−Cq, *C1*), 126.2 (Ar−H, *C2*), 125.3 (Ar−H, *C3*), 34.5 (Cq, *C7*), 33.7 (CH, *C5*), 31.6 (CH_3, *C8*), 24.2 (CH_3, *C6*)

HSQC : 7.35 x 125.3, 7.20 x 126.2, 2.92 x 33.7, 1.35 x 31.6, 1.28 x 24.2

IR: $\nu_{max}(cm^{-1})$: 2957(m), 1508(w), 1461(w), 1362(s), 828(s)

3.6 4b: 1-(2-(4-(tert-butyl)phenyl)propan-2-yl)-4-phenyl-urazole



Formula: $C_{21}H_{25}N_3O_2$
Molecular weight: 351.45 g/mol
Exact mass: 351.19468 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M\text{-}H]^-$ Calcd for $C_{21}H_{24}N_3O_2$ 350.1869; found 350.1863 (Δ = -3.1 ppm)

$\mathbf{R}_f$: 0.14 (20% EtOAc in pentane)

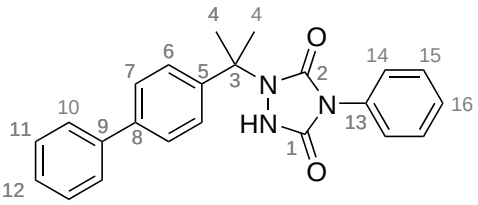
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.51-7.34 (9H, band, *C6-H, C7-H, C12-H, C13-H and C14-H*), 6.44 (1H, s(br), *NH*), 1.91 (6H, s, *C4-H*$_3$), 1.34 (9H, s, *C10-H*$_3$)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.1 (C=O, *C1 or C2*), 153.0 (C=O, *C1 or C2*), 151.4 (Ar−Cq, *C8*), 140.2 (Ar−Cq, *C5*), 131.2 (Ar−Cq, *C11*), 129.2 (Ar−H, *C13*), 128.4 (Ar−H, *C14*), 126.3 (Ar−H, *C7*), 125.8 (Ar−H, *C12*), 125.3 (Ar−H, *C6*), 64.6 (Cq, *C3*), 34.7 (Cq, *C9*), 31.4 (CH_3, *C10*), 25.9 (CH_3, *C4*)

HSQC : 7.50-7.47 x 129.2, 7.49-7.46 x 125.8, 7.46-7.40 x 126.3, 7.44-7.41 x 125.3, 7.40-7.34 x 128.4, 1.91 x 25.9, 1.34 x 31.4

IR: $\nu_{max}(cm^{-1})$: 3044(w), 2959(w), 1769(w), 1698(s), 1430(s), 825(m), 769(s), 686(m)

3.7 5b: 1-(2-([1,1'-biphenyl]-4-yl)propan-2-yl)-4-phenyl-urazole



Formula: $C_{23}H_{21}N_3O_2$
Molecular weight: 371.44 g/mol
Exact mass: 371.16338 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M\text{-}H]^-$ Calcd for $C_{23}H_{20}N_3O_2$ 370.1556; found 370.1557 (Δ = -1.1 ppm)

$\mathbf{R}_f$: 0.15 (20% EtOAc in pentane)

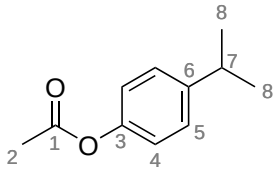
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.64 (2H, m, *C7-H*), 7.59 (2H, m, *C10-H*), 7.56 (2H, m, *C6-H*), 7.51 - 7.42 (6H, band, *C11-H, C14-H and C15-H*), 7.41 - 7.33 (2H, band, *C12-H and C16-H*), 6.68 (1H, s(br), *NH*), 1.95 (6H, s, *C4-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.3 (C=O, *C1 or C2*), 153.2 (C=O, *C1 or C2*), 142.3 (Ar−Cq, *C5*), 141.3 (Ar−Cq, *C8*), 140.4 (Ar−Cq, *C9*), 131.2 (Ar−Cq, *C13*), 129.2 (Ar−CH, *C15*), 129.0 (Ar−CH, *C11*), 128.4 (Ar−CH, *C12*), 128.0 (Ar−CH, *C7*), 127.8 (Ar−CH, *C16*), 127.3 (Ar−CH, *C10*), 126.0 (Ar−CH, *C6*), 125.8 (Ar−CH, *C14*), 64.6 (Cq, *C3*), 26.1 (CH_3, *C4*)

HSQC : 7.64 x 128.0, 7.59 x 127.3, 7.56 x 126.0, 7.51 - 7.42 x 129.2, 7.51 - 7.42 x 129.0, 7.51 - 7.42 x 125.8, 7.41 - 7.33 x 128.4, 7.41 - 7.33 x 127.8, 1.95 x 26.1

IR: $\nu_{max}(cm^{-1})$: 3179(w), 3077(w), 2978(w), 1769(m), 1695(s), 1420(s), 868(m), 768(s), 735(s), 692(s) 682(s)

3.8 6a: 4-isopropylphenyl acetate



Formula: $C_{11}H_{14}O_2$
Molecular weight: 178.231 g/mol
Exact mass: 178.09938 D

appearance: clear liquid

Product didn't ionize for HRMS analysis.
GCMS m/z: $[M]^{\bullet}$ Calcd for $C_{11}H_{14}O_2$ 178.1; Found 178.0

$\mathbf{R}_f$: 0.5 (10% EtOAc in pentane)

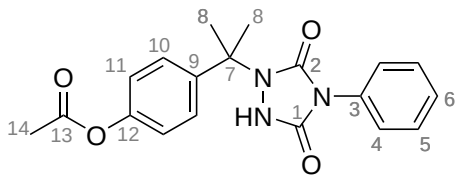
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.23 (2H, m, *C5-H*), 7.00 (2H, m, *C4-H*), 2.91 (1H, sept, J = 6.9 Hz, *C7-H*), 2.29 (3H, s, *C2-*H_3), 1.25 (6H, d, J = 6.9 Hz, *C8-*H_3)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 169.9 (C=O, *C1*), 148.7 (Ar−Cq, *C3*), 146.5 (Ar−Cq, *C6*), 127.5 (Ar−H, *C5*), 121.3 (Ar−H, *C4*), 33.7 (CH, *C7*), 24.2 (CH_3, *C8*), 21.3 (CH_3, *C2*)

HSQC : 7.23 x 127.5, 7.00 x 121.3, 2.91 x 33.7, 2.29 x 21.3, 1.25 x 24.2

IR: $\nu_{max}(cm^{-1})$: 2959(w), 2869(w), 1764(s), 1508(m), 1190(s), 1430(s), 845(s)

3.9 6b: 4-(2-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-propan-2-yl)phenyl acetate



Formula: $C_{19}H_{19}N_3O_4$
Molecular weight: 353.378 g/mol
Exact mass: 353.13756 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M\text{-}H]^-$ Calcd for $C_{19}H_{18}N_3O_4$ 352.1297; found 352.1308 (Δ = 1.5 ppm)

$\mathbf{R}_f$: 0.21 (40% EtOAc in pentane)

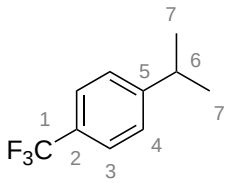
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.51 (2H, m, *C11-H*), 7.49-7.43 (4H, band, *C4-H and C5-H*), 7.37 (1H, m, *C6-H*), 7.14 (2H, m, *C10-H*), 6.72 (1H, s(br), *NH*), 2.32 (3H, s, *C14-H_3*), 1.90 (6H, s, *C8-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 169.5 (C=O, *C13*), 153.4 (C=O, *C1 or C2*), 153.2 (C=O, *C1 or C2*), 150.4 (Ar−Cq, *C12*), 140.9 (Ar−Cq, *C9*), 131.2 (Ar−Cq, *C3*), 129.2 (Ar−H, *C5*), 128.4 (Ar−H, *C6*), 126.9 (Ar−H, *C11*), 125.7 (Ar−H, *C4*), 122.3 (Ar−H, *C10*), 64.4 (Cq, *C7*), 26.2 (CH_3, *C8*), 21.3 (CH_3, *C14*)

HSQC : 7.51 x 126.9, 7.49-7.43 x 125.7, 7.48-7.45 x 129.2, 7.37 x 128.4, 7.14 x 122.3, 2.32 x 21.3, 1.90 x 26.2

IR: $\nu_{max}(cm^{-1})$: 3210(w), 2993(w), 1767(s), 1698(s), 1435(s), 1197(s), 866(m)

3.10 7a: 4-trifluoromethylcumene



Formula: $C_{10}H_{11}F_3$
Molecular weight: 188.19321 g/mol
Exact mass: 188.08128 D

appearance: colourless liquid

$\mathbf{R}_f$: 0.86 (pentane)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.55 (2H, d, J = 8.1 Hz, *C3-H*), 7.33 (2H, d, J = 8.1 Hz, *C4-H*), 2.97 (1H, sept, J = 6.9 Hz, *C6-H*),

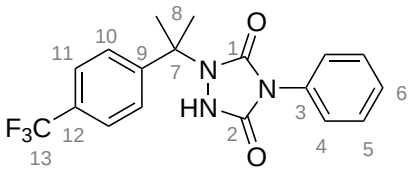
1.27 (6H, d, J = 6.9 Hz, *C7-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.0 (Ar−Cq, *C5*), 128.2 (q, 32Hz) (Ar−Cq, *C2*), 126.9 (Ar−H, *C4*), 125.4 (q, 4Hz) (Ar−H, *C3*), 124.5 (q, 271Hz) (CF_3, *C1*), 34.2 (CH, *C6*), 23.9 (CH_3, *C7*)

HSQC : 7.55 x 125.4, 7.33 x 126.9, 2.97 x 34.2, 1.27 x 23.9

IR: $\nu_{max}(cm^{-1})$: 2964(w), 2874(m), 1322(s), 1116(s), 1000(s), 836(s), 724(w)

3.11 7b: 1-(2-(4-trifluoromethylphenyl)propan-2-yl)--4-phenyl-urazole



Formula: $C_{18}H_{16}F_3N_3O_2$
Molecular weight: 363.34021 g/mol
Exact mass: 363.11946 D

appearance: white solid

$[M]^+$ Calcd for $C_{18}H_{16}F_3N_3O_2$ 364.1; found 364.1

$\mathbf{R}_f$: 0.19 (25% EtOAc in pentane)

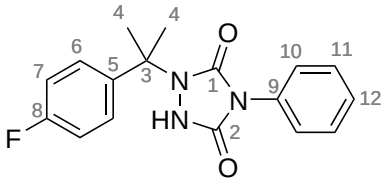
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.65 (2H, m, *C11-H*), 7.60 (2H, m, *C10-H*), 7.45 (4H, band, *C4-H, C5-H*), 7.37 (1H, m, *C6-H*), 1.87 (6H, s, *C8-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.8 (C=O, *C1/C2*), 153.3 (C=O, *C1/C2*), 147.6 (Ar−Cq, *C9*), 130.9 (Ar−Cq, *C3*), 130.2 (q, 32Hz) (Ar−Cq, *C12*), 129.3 (Ar−CH, *C4*), 128.5 (Ar−CH, *C6*), 126.1 (q, 4Hz) (Ar−CH, *C11*), 125.9 (Ar−CH, *C10*), 125.6 (Ar−CH, *C5*), 123.8 (q, 272Hz) (CF_3, *C13*), 64.1 (Cq, *C7*), 26.3 (CH_3, *C8*)

HSQC : 7.65 x 126.1, 7.60 x 125.9, 7.49-7.43 x 129.3, 7.47-7.40 x 125.6, 7.37 x 128.5, 1.87 x 26.3

IR: $\nu_{max}(cm^{-1})$: 3062(w), 2859(w), 1768(w), 1698(s), 1326(s), 1123(s), 768(m), 727(m)

3.12 8b: 1-(2-(4-fluorophenyl)propan-2-yl)-4-phenyl--urazole



Formula: $C_{17}H_{16}FN_3O_2$
Molecular weight: 313.3324 g/mol
Exact mass: 313.12265 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{17}H_{15}FN_3O_2$ 312.1148; found 312.1151 (Δ = -0.9 ppm)

$\mathbf{R}_f$: 0.27 (30% EtOAc in pentane)

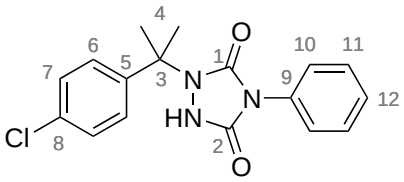
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.49-7.43 (6H, band, *C6-H, C10-H and C11-H*), 7.37 (1H, m, *C12-H*), 7.19 (1H, s(br), *NH*), 7.08 (2H, m, *C7-H*), 1.88 (6H, s, *C4-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 162.4 [d, 247 Hz] (Ar−Cq, *C8*), 153.4 (C=O, *C1 or C2*), 153.2 (C=O, *C1 or C2*), 139.3 [d, 4Hz] (Ar−Cq, *C5*), 131.1 (Ar−Cq, *C9*), 129.2 (Ar−H, *C11*), 128.4 (Ar−H, *C12*), 127.5 [d, 8Hz] (Ar−H, *C6*), 125.6 (Ar−H, *C10*), 116.0 [d, 22Hz] (Ar−H, *C7*), 64.1 (Cq, *C3*), 26.3 (CH_3, *C4*)

HSQC : 7.49-7.43 x 129.2, 7.49-7.43 x 127.5, 7.49-7.43 x 125.6, 7.37 x 128.4, 7.08 x 116.0, 1.88 x 26.3

IR: $\nu_{max}(cm^{-1})$: 3067(w), 2984(w), 1767(w), 1693(s), 1424(s), 830(m), 767(s), 728(s), 687(s)

3.13 9b: 1-(2-(4-chlorophenyl)propan-2-yl)-4-phenyl--urazole



Formula: $C_{17}H_{16}ClN_3O_2$
Molecular weight: 329.784 g/mol
Exact mass: 329.0931 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{17}H_{15}ClN_3O_2$ 328.0853; found 328.0854 (Δ = -1.3 ppm)

$\mathbf{R}_f$: 0.14 (25% EtOAc in pentane)

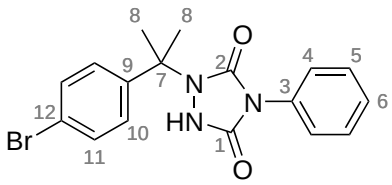
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.55-7.42 (4H, band, *C10-H and C11-H*), 7.42-7.31 (5H, band, *C6-H, C7-H and C12-H*), 1.84 (3H, s, *C4-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.7 (C=O, *C1 or C2*), 153.0 (C=O, *C1 or C2*), 142.1 (Ar−Cq, *C5*), 133.9 (Ar−Cq, *C8*), 131.1 (Ar−Cq, *C9*), 129.2 (Ar−CH, *C11*), 129.2 (Ar−CH, *C7*), 128.4 (Ar−CH, *C12*), 127.0 (Ar−CH, *C6*), 125.6 (Ar−CH, *C10*), 63.9 (Cq, *C3*), 26.4 (CH_3, *C4*)

HSQC : 7.55-7.43 x 129.2, 7.46-7.42 x 125.6, 7.42-7.38 x 127.0, 7.38-7.34 x 128.4, 7.39-7.31 x 129.2, 1.84 x 26.4

IR: $\nu_{max}(cm^{-1})$: 3064(w), 2925(w), 1769(w), 1689(s), 1421(s), 763(s), 700(s)

3.14 10b: 1-(2-(4-bromophenyl)propan-2-yl)-4-phenyl-urazole



Formula: $C_{17}H_{16}BrN_3O_2$
Molecular weight: 374.238 g/mol
Exact mass: 373.04259 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{17}H_{15}BrN_3O_2$ 372.0348; found 372.0365 (Δ = 3.2 ppm)

$\mathbf{R}_f$: 0.23 (30% EtOAc in pentane)

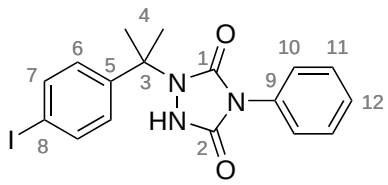
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.73 (1H, s(br), *NH*), 7.51 (2H, m, *C11-H*), 7.49-7.41 (4H, band, *C4-H and C5-H*), 7.40-7.32 (3H, band, *C6-H and C10-H*), 1.84 (6H, s, *C8-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.6 (C=O, *C1 or C2*), 153.1 (C=O, *C1 or C2*), 142.7 (Ar−Cq, *C9*), 132.2 (Ar−H, *C11*), 131.1 (Ar−Cq, *C3*), 129.2 (Ar−H, *C5*), 128.4 (Ar−H, *C6*), 127.3 (Ar−H, *C10*), 125.6 (Ar−H, *C4*), 122.2 (Ar−Cq, *C12*), 64.1 (Cq, *C7*), 26.3 (CH_3, *C8*)

HSQC : 7.51 x 132.2, 7.49-7.43 x 129.2, 7.48-7.41 x 125.6, 7.40-7.34 x 128.4, 7.36-7.32 x 127.3, 1.84 x 26.3

IR: $\nu_{max}(cm^{-1})$: 3068(w), 2953(w), 1770(w), 1698(s), 1428(s), 816(m), 724(s), 688(m)

3.15 11b: 1-(2-(4-iodophenyl)propan-2-yl)-4-phenyl-urazole



Formula: $C_{17}H_{16}IN_3O_2$
Molecular weight: 421.23847 g/mol
Exact mass: 421.02872 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{17}H_{15}IN_3O_2$ 420.0209; found 420.0222 (Δ = 1.8 ppm)

$\mathbf{R}_f$: 0.15 (25% EtOAc in pentane)

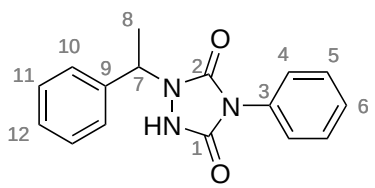
^{1}**H-NMR** (300 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.72 (2H, m, *C7-H*), 7.50-7.42 (4H, band, *C10-H and C11-H*), 7.37 (1H, m, *C12-H*), 7.22 (2H, m, *C6-H*), 1.84 (6H, s, *C4-H_3*)

^{13}**C-NMR** (75 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.6 (C=O, *C1 or C2*), 153.2 (C=O, *C1 or C2*), 143.4 (Ar−Cq, *C5*), 138.2 (Ar−H, *C7*), 131.1 (Ar−Cq, *C9*), 129.2 (Ar−H, *C11*), 128.4 (Ar−H, *C12*), 127.5 (Ar−H, *C6*), 125.7 (Ar−H, *C10*), 93.8 (Ar−Cq, *C8*), 64.2 (Cq, *C3*), 26.2 (CH_3, *C4*)

HSQC : 7.72 x 138.2, 7.50-7.44 x 129.2, 7.49-7.42 x 125.7, 7.37 x 128.4, 7.22 x 127.5, 1.84 x 26.2

IR: $\nu_{max}(cm^{-1})$: 3064(w), 2979(w), 1772(w), 1692(s), 1426(s), 775(s), 645(s)

3.16 12b: 4-phenyl-1-(1-phenylethyl)-urazole



Formula: $C_{16}H_{15}N_3O_2$
Molecular weight: 281.315 g/mol
Exact mass: 281.11643 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M\text{-}H]^-$ Calcd for $C_{16}H_{14}N_3O_2$ 280.1086; found 280.1090 (Δ = -0.5 ppm)

$\mathbf{R}_f$: 0.25 (35% EtOAc in pentane)

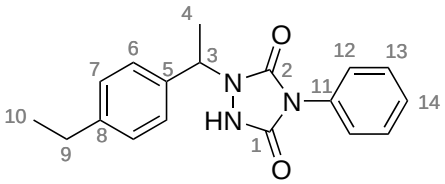
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.51-7.32 (10H, band, *Ar-H*), 7.24 (1H, s(br), *NH*), 5.46 (1H, q, J = 7.0 Hz, *C7-H*), 1.69 (3H, d, J = 7.0 Hz, *C8-*H_3)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 154.0 (C=O, *C1 or C2*), 152.9 (C=O, *C1 or C2*), 137.8 (Ar−Cq, *C9*), 131.3 (Ar−Cq, *C3*), 129.3 (Ar−CH, *C4, C5, C6, C11 or C12*), 129.2 (Ar−CH, *C4, C5, C6, C11 or C12*), 128.8 (Ar−CH, *C4, C5, C6, C11 or C12*), 128.4 (Ar−CH, *C4, C5, C6, C11 or C12*), 127.6 (Ar−CH, *C10*), 125.6 (Ar−CH, *C4, C5, C6, C11 or C12*), 55.7 (CH, *C7*), 16.1 (CH_3, *C8*)

HSQC : 7.51-7.46 x 125.6, 7.51-7.46 x 129.3, 7.46-7.39 x 127.6, 7.42-7.41 x 129.2, 7.41-7.33 x 128.4, 7.40-7.32 x 128.8, 5.46 x 55.7, 1.69 x 16.1

IR: $\nu_{max}(cm^{-1})$: 3167(w), 3058(w), 2864(w), 1760(w), 1679(s), 1436(m), 715(s), 702(s)

3.17 13b: 1-(1-(4-ethylphenyl)ethyl)-4-phenyl-urazole



Formula: $C_{18}H_{19}N_3O_2$
Molecular weight: 309.369 g/mol
Exact mass: 309.14773 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{20}N_3O_2$ 310.1556; found

310.1536 (Δ = -4.5 ppm)

R$_f$: 0.25 (30% EtOAc in pentane)

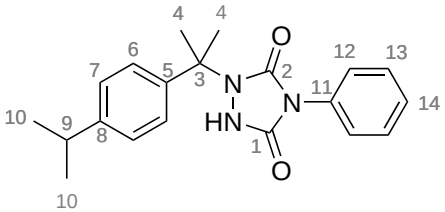
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.50-7.44 (4H, band, *C12-H and C13-H*), 7.41-7.36 (1H, m, *C14-H*), 7.34 (2H, m, *C6-H*), 7.21 (2H, m, *C7-H*), 5.44 (1H, q, J = 7.0 Hz, *C3-H*), 2.65 (2H, q, J = 7.6 Hz, *C9-H*$_2$), 1.67 (3H, t, J = 7.0 Hz, *C4-H*$_3$), 1.23 (3H, t, J = 7.6 Hz, *C10-H*$_3$)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.9 (C=O, *C1*), 152.7 (C=O, *C2*), 144.9 (Ar−Cq, *C8*), 135.0 (Ar−Cq, *C5*), 131.4 (Ar−Cq, *C11*), 129.2 (Ar−H, *C13*), 128.6 (Ar−H, *C7*), 128.3 (Ar−H, *C14*), 127.6 (Ar−H, *C6*), 125.6 (Ar−H, *C12*), 55.4 (CH, *C3*), 28.6 (CH_2, *C9*), 16.3 (CH_3, *C4*), 15.6 (CH_3, *C10*)

HSQC : 7.50-7.44 x 129.2, 7.50-7.44 x 125.6, 7.41-7.36 x 128.3, 7.34 x 127.6, 7.21 x 128.6, 5.44 x 55.4, 2.65 x 28.6, 1.67 x 16.3, 1.23 x 15.6

IR: $\nu_{max}(cm^{-1})$: 3060(w), 2956(w), 2868(w), 1761(w), 1681(s), 1433(m), 831(m), 764(m), 698(s)

3.18 14b: 1-(2-(4-isopropylphenyl)propan-2-yl)-4-phenyl-urazole



Formula: $C_{20}H_{23}N_3O_2$
Molecular weight: 337.423 g/mol
Exact mass: 337.17903 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{20}H_{22}N_3O_2$ 336.1712; found 336.1710 (Δ = -2.2 ppm)

$\mathbf{R}_f$: 0.28 (30% EtOAc in pentane)

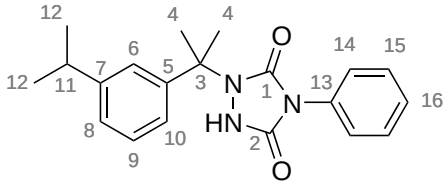
^{1}H-NMR (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.50-7.43 (4H, band, *C12-H and C13-H*), 7.40 (2H, m, *C6-H*), 7.38-7.24 (1H, m, *C14-H*), 7.27 (2H, m, *C7-H*), 6.67 (1H, s(br), *NH*), 2.92 (1H, sept, J = 6.9 Hz, *C9-H*), 1.90 (6H, s, *C4-*H_3), 1.26 (6H, d, J = 6.9 Hz, *C10-*H_3)

^{13}C-NMR (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.1 (C=O, *C1 or C2*), 153.1 (C=O, *C1 or C2*), 149.1 (Ar−Cq, *C8*), 140.6 (Ar−Cq, *C5*), 131.2 (Ar−Cq, *C11*), 129.2 (Ar−H, *C13*), 128.3 (Ar−H, *C14*), 127.3 (Ar−H, *C7*), 125.8 (Ar−H, *C12*), 125.6 (Ar−H, *C6*), 64.6 (Cq, *C3*), 33.8 (CH, *C9*), 26.0 (CH_3, *C4*), 24.0 (CH_3, *C10*)

HSQC : 7.50-7.43 x 129.2, 7.50-7.43 x 125.8, 7.40 x 125.6, 7.38-7.24 x 128.3, 7.27 x 127.3, 2.92 x 33.8, 1.90 x 26.0, 1.26 x 24.0

IR: $\nu_{max}(cm^{-1})$: 3040(w), 2962(w), 1763(w), 1685(s), 1430(m), 826(m), 768(s), 687(s)

3.19 15b: 1-(2-(3-isopropylphenyl)propan-2-yl)-4-phenylurazole



Formula: $C_{20}H_{23}N_3O_2$
Molecular weight: 337.423 g/mol
Exact mass: 337.17903 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{20}H_{22}N_3O_2$ 336.1712; found 336.1716 (Δ = -0.5 ppm)

$\mathbf{R}_f$: 0.17 (20% EtOAc in pentane)

^{1}H-NMR (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.51-7.43 (4H, band, *C14-H and C15-H*), 7.41-7.27 (4H, band, *C6-H, C7-H, C9-H and C16-H*), 7.21 (1H, dt, J = 7.4 Hz, 1.4 Hz, *C8-H*), 6.63 (1H, s(br), *NH*), 2.93 (1H, sept, J = 6.9 Hz, *C11-H*), 1.91 (6H, s, *C4-*H_3), 1.27 (6H, d, J = 6.9 Hz, *C12-*H_3)

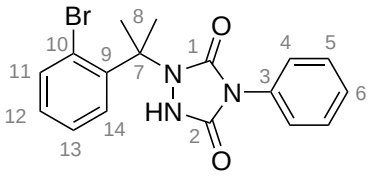
^{13}C-NMR (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.2 (C=O, *C1 or C2*), 153.0 (C=O, *C1 or C2*), 150.1 (Ar−Cq, *C7*), 143.3 (Ar−Cq, *C5*), 131.2 (Ar−Cq, *C13*), 129.3 (Ar−H, *C9*), 129.2 (Ar−H, *C15*), 128.4 (Ar−H, *C16*), 126.3 (Ar−H, *C8*), 125.8 (Ar−H, *C14*), 123.7 (Ar−H, *C6*), 123.0 (Ar−H, *C10*), 64.9 (Cq, *C3*), 34.4 (CH, *C11*), 26.1 (CH_3, *C4*), 24.2 (CH_3, *C12*)

HSQC : 7.51-7.43 x 129.2, 7.51-7.43 x 125.8, 7.41-7.27 x 129.3, 7.41-7.27 x 128.4, 7.41-7.27 x 123.7, 7.41-7.27 x 123.0, 7.21 x 126.3, 2.93 x 34.4, 1.91 x 26.1, 1.27 x 24.2

IR: $\nu_{max}(cm^{-1})$: 3054(w), 2960(w), 1770(w), 1703(s), 1423(s), 870(m), 769(s), 724(s), 700(s), 686(s)

3.20 16b: 1-(2-(2-bromophenyl)propan-2-yl)-4-phenylurazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **17b** and the PTAD-isoprene adduct **40** in a 22:78 ratio*



Formula: $C_{17}H_{16}BrN_3O_2$
Molecular weight: 374.238 g/mol
Exact mass: 373.04259 D

$[M]^+$ Calcd for $C_{17}H_{16}N_3O_2$ 374.0; found 374.0

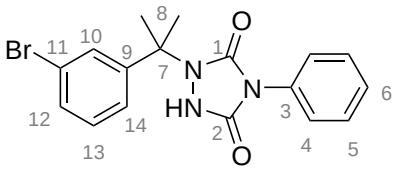
$\mathbf{R}_f$: 0.26 (30% EtOAc in pentane)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 22%, only clear resonances are given]*: δ(ppm) = 1.81 (6H, s, *C8-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 22%, only clear resonances are given]*: δ(ppm) = 153.6 (C=O, *C1/C2*), 153.3 (C=O, *C1/C2*), 142.8 (Ar−Cq, *C9*), 132.1 (Ar−CH, *C11*), 127.3 (Ar−CH, *C14*), 122.5 (Ar−Cq, *C10*), 64.0 (Cq, *C7*), 26.2 (CH_3, *C8*)

HSQC *[minor, integrating for 22%, only clear resonances are given]*: 7.52-7.47 x 132.1, 7.34-7.30 x 127.3, 1.81 x 26.2

3.21 17b: 1-(2-(3-bromophenyl)propan-2-yl)-4-phenylurazole



Formula: $C_{17}H_{16}BrN_3O_2$
Molecular weight: 374.238 g/mol
Exact mass: 373.04259 D

appearance: white solid

$[M]^+$ Calcd for $C_{17}H_{16}N_3O_2$ 374.0; found 374.0

$\mathbf{R}_f$: 0.13 (20% EtOAc in pentane)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.90 (1H, s(br), *NH*), 7.60 (1H, t, J = 1.8 Hz, *C10-H*), 7.50-7.35 (7H, band, *Ar-H*), 7.23 (1H, t, J = 7.9 Hz, *C13-H*), 1.84 (6H, s, *C8-H_3*)

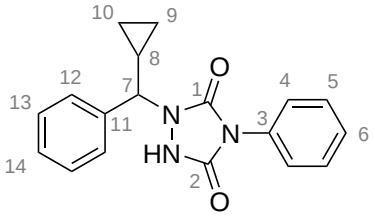
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.6 (C=O, *C1/C2*), 153.1 (C=O, *C1/C2*), 145.9 (Cq, *C9*), 131.2 (Ar−H, *C12*), 131.0 (Ar−Cq, *C3*), 130.6 (Ar−H, *C13*), 129.2 (Ar−H, *C5*), 128.9 (Ar−H, *C10*), 128.4 (Ar−H,

C6), 125.7 (Ar−H, *C4*), 124.1 (Ar−H, *C14*), 123.3 (Ar−Cq, *C11*), 64.1 (Cq, *C7*), 26.2 (CH_3, *C8*)

HSQC : 7.60 x 128.9, 7.50-7.44 x 129.2, 7.48-7.42 x 125.7, 7.45-7.40 x 131.2, 7.43-7.38 x 124.1, 7.40-7.35 x 128.4, 7.23 x 130.6, 1.84 x 26.2

IR: $\nu_{max}(cm^{-1})$: 3067(m), 2853(w), 1767(w), 1695(s), 1420(s), 869(w), 767(m), 691(m)

3.22 18b: 1-(cyclopropyl(phenyl)methyl)-4-phenyl-urazole



Formula: $C_{18}H_{17}N_3O_2$
Molecular weight: 307.353 g/mol
Exact mass: 307.13208 D

appearance: yellowish solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{18}N_3O_2$ 308.1399; found 308.1381 (Δ = -4.1 ppm)

$\mathbf{R}_f$: 0.23 (30% EtOAc in pentane)

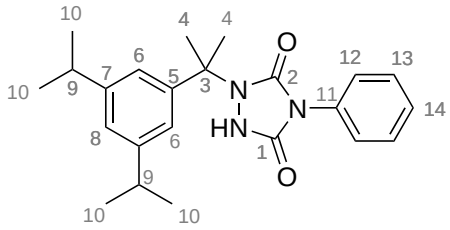
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 8.46 (1H, s(br), *NH*), 7.52-7.44 (6H, band, *C12-H, C4-H and C5-H*), 7.41-7.31 (4H, band, *C13-H, C14-H and C6-H*), 4.54 (1H, d, J = 10.1 Hz, *C7-H*), 1.58 (1H, m, *C8-H*), 0.77 (1H, m, *C9-H**H***), 0.69 (2H, m, *C10-*H_2), 0.44 (1H, m, *C9-**H**H*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 154.0 (C=O, *C2*), 152.8 (C=O, *C1*), 137.5 (Ar−Cq, *C11*), 131.4 (Ar−Cq, *C3*), 129.2 (Ar−H, *C5*), 128.9 (Ar−H, *C13*), 128.5 (Ar−H, *C6*), 128.3 (Ar−H, *C14*), 127.8 (Ar−H, *C12*), 125.5 (Ar−H, *C4*), 65.0 (CH, *C7*), 12.8 (CH, *C8*), 5.1 (CH_2, *C9*), 4.3 (CH_2, *C10*)

HSQC : 7.52-7.47 x 127.8, 7.51-7.46 x 125.5, 7.50-7.44 x 129.2, 7.41-7.35 x 128.9, 7.41-7.34 x 128.5, 7.35-7.31 x 128.4, 4.54 x 65.0, 1.58 x 12.8, 0.77 x 5.1, 0.69 x 4.3, 0.44 x 5.1

IR: $\nu_{max}(cm^{-1})$: 3096(w), 2958(w), 1769(w), 1681(s), 1430(m), 760(m), 704(s)

3.23 19b: 1-(2-(3,5-diisopropylphenyl)propan-2-yl)-4-phenyl-urazole



Formula: $C_{23}H_{29}N_3O_2$
Molecular weight: 379.504 g/mol
Exact mass: 379.22598 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{30}N_3O_2$ 380.2338; found 380.2315 (Δ = -4.6 ppm)

$\mathbf{R}_f$: 0.38 (30% EtOAc in pentane)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.52-7.44 (4H, band, *C12-H and C13-H*), 7.37 (1H, m, *C14-H*), 7.13 (2H, d, J = 1.5 Hz, *C6-H*), 7.07 (1H, t, J = 1.5 Hz, *C8-H*), 6.27 (1H, s(br), *NH*), 2.92 (2H, sept, J = 6.9 Hz, *C9-H*), 1.92 (6H, s, *C4-H_3*), 1.27 (12H, d, J = 6.9 Hz, *C10-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.3 (C=O, *C1 or C2*), 152.9 (C=O, *C1 or C2*), 150.2 (Ar−Cq, *C7*), 143.1 (Ar−Cq, *C5*), 131.3 (Ar−Cq, *C11*), 129.3 (Ar−H, *C13*), 128.4 (Ar−H, *C14*), 125.8 (Ar−H, *C12*), 124.6 (Ar−H, *C8*), 121.2 (Ar−H, *C6*), 65.1 (Cq, *C3*), 34.5 (CH, *C9*), 25.9

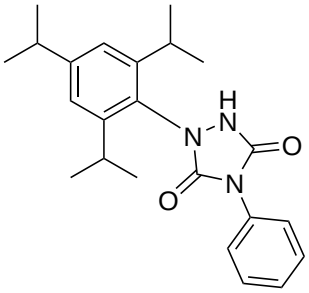
(CH_3, *C4*), 24.3 (CH_3, *C10*)

HSQC : 7.52-7.44 x 125.8, 7.52-7.44 x 129.3, 7.37 x 128.4, 7.13 x 121.2, 7.07 x 124.6, 2.92 x 34.5, 1.92 x 25.9, 1.27 x 24.3

IR: $\nu_{max}(cm^{-1})$: 3047(w), 2960(w), 1772(m), 1704(s), 1430(s), 867(s), 768(s), 708(s), 687(s)

3.24 19c: 4-phenyl-1-(2,4,6-triisopropylphenyl)-urazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **19b** and **19c** in a 79:21 ratio*



Formula: $C_{23}H_{29}N_3O_2$
Molecular weight: 379.504 g/mol
Exact mass: 379.22598 D

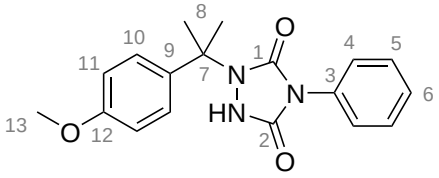
^{1}**H-NMR** (300 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 21%, only clear resonances are given]*: δ(ppm) = 7.64-7.58 (2H, band, *Ar-H*), 7.54-7.34 (3H, band, *Ar-H*), 7.08 (2H, m, *Ar-H*), 3.02-2.8 (3H, band, *CH*), 1.30-1.24 (18H, band, *CH3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 21%, only clear resonances are given]*: δ(ppm) = 153.2 (Cq, *Ar-Cq or C=O*), 151.9 (Cq, *Ar-Cq or C=O*), 150.7 (Cq, *Ar-Cq or C=O*), 148.8 (Ar−Cq), 131.6 (Ar−Cq), 128.3 (Ar−H), 126.9 (Ar−H), 125.7 (Ar−H), 122.6 (Ar−H), 34.5 (CH), 29.2 (CH), 24.04 (CH_3), 24.02 (CH_3)

HSQC *[minor, integrating for 21%, only clear resonances are given]*: 7.64-7.58 x 125.7, 7.54-7.34 x 128.3, 7.54-7.34 x 126.9, 7.08 x 122.6, 3.02-2.8 x 34.5, 3.02-2.8 x 29.2, 1.30-1.24 x 24.04, 1.30-1.24 x 24.02

3.25 20b: 1-(2-(4-methoxyphenyl)propan-2-yl)-4-phenyl-urazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **20b** and **20c** in a 54:46 ratio*



Formula: $C_{18}H_{19}N_3O_3$
Molecular weight: 325.368 g/mol
Exact mass: 325.14264 D

Three peaks were found on the LCMS all giving $[M+H]^+$ Calcd for $C_{18}H_{19}N_3O_3$ 326.1; found 326.1

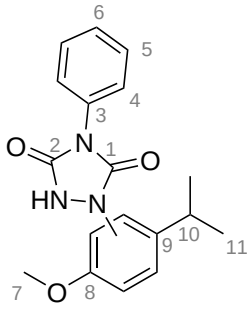
^{1}H-NMR (400 MHz, $CDCl_3$, 21 °C)*[major, integrating for 54%, only clear resonances are given]*: δ(ppm) = 7.62-5.57 (2H, m, *Ar-H*), 7.54-7.34 (5H, band, *Ar-H*), 6.94 (2H, m, *Ar-H*), 3.83 (3H, s, *C13-H$_3$*), 1.90 (6H, s, *C8-H$_3$*)

^{13}C-NMR (100 MHz, $CDCl_3$, 21 °C)*[major, integrating for 54%, only clear resonances are given]*: δ(ppm) = 159.3 (Ar−Cq, *C12*), 135.4 (Ar−Cq, *C9*), 131.2 (Ar−Cq, *C3*), 129.3 (Ar−H), 126.9 (Ar−H), 125.9 (Ar−H), 125.7 (Ar−H), 114.3 (Ar−H), 64.1 (Cq, *C7*), 55.4 (CH_3, *C13*), 26.4 (CH_3, *C8*)

HSQC *[major, integrating for 54%, only clear resonances are given]*: 7.62-5.57 x 125.9, 7.54-7.45 x 129.3, 7.50-7.46 x 125.7, 7.45-7.40 x 126.9, 6.94 x 114.3, 3.83 x 55.4, 1.90 x 26.4

3.26 20c: Side products of amination on 4-isopropylanisole

*These compounds were not obtained analytically pure and the assignments were made on a sample containing a mixture of **20b** and **20c** in a 54:(24:16:6) ratio*



Formula: $C_{18}H_{19}N_3O_3$
Molecular weight: 325.368 g/mol
Exact mass: 325.14264 D

appearance: yellowish oil

Three peaks were found on the LCMS all giving $[M+H]^+$ Calcd for $C_{18}H_{19}N_3O_3$ 326.1; found 326.1

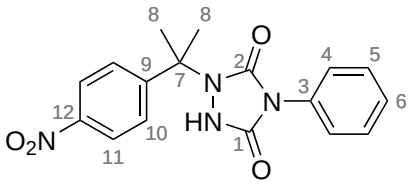
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 24%, only clear resonances are given]*: δ(ppm) = 7.54-7.51 (1H, m, *Ar-H*), 7.33-7.29 (1H, m, *Ar-H*), 6.92-6.90 (1H, m, *Ar-H*), 3.16 (1H, sept, J = 6.9 Hz, *C10-H*), 3.84 (3H, s, *C7-*H_3), 1.29-1.21 (3H, m, *C11-*H_3),
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 24%, only clear resonances are given]*: δ(ppm) = 160.8 (Ar−Cq, *C8*), 149.4 (Ar−Cq, *C9*), 128.9 (Ar−CH), 125.8 (Ar−CH), 112.7 (Ar−CH), 55.6 (CH_3, *C7*), 28.7 (CH, *C10*), 23.8 (CH_3, *C11*),
HSQC *[minor, integrating for 24%, only clear resonances are given]*: 7.54-7.51 x 125.8, 7.33-7.29 x 128.9, 6.92-6.90 x 112.7, 3.84 x 55.6, 3.16 x 28.7, 1.29-1.21 x 23.8,

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 16%, only clear resonances are given]*: δ(ppm) = 7.63-7.58 (1H, m, *Ar-H*), 7.19 (1H, m, *Ar-H*), 6.98-6.94 (1H, m, *Ar-H*), 3.92 (3H, s, *C7-*H_3), 2.89 (1H, sept, J = 6.9 Hz, *C10-H*), 1.29-1.21 (3H, m, *C11-*H_3),
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 16%, only clear resonances are given]*: δ(ppm) = 151.2 (Ar−Cq, *C8*), 142.1 (Ar−Cq, *C9*), 127.3 (Ar−CH), 123.8 (Ar−CH), 112.0 (Ar−CH), 56.1 (CH_3, *C7*), 33.5 (CH, *C10*), 24.1 (CH_3, *C11*),
HSQC *[minor, integrating for 16%, only clear resonances are given]*: 7.63-

7.58 x 123.8, 7.19 x 127.3, 6.98-6.94 x 112.0, 3.92 x 56.1, 2.89 x 33.5, 1.29-1.21 x 24.1,

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 6%, only clear resonances are given]*: δ(ppm) = 7.61-7.56 (1H, m, *Ar-H*), 6.92 (1H, m, *Ar-H*), 6.87 (1H, m, *Ar-H*), 3.94 (3H, s, *C7-*H_3), 2.93 (1H, m, *C10-H*), 1.29-1.21 (3H, m, *C11-*H_3)
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C)*[minor, integrating for 6%, only clear resonances are given]*: δ(ppm) = 153.5 (Ar−Cq, *C8*), 151.5 (Ar−Cq, *C9*), 129.2 (Ar−CH), 119.3 (Ar−CH), 110.2 (Ar−CH), 55.9 (CH_3, *C7*), 34.5 (CH, *C10*), 24.0 (CH_3)
HSQC *[minor, integrating for 6%, only clear resonances are given]*: 7.61-7.56 x 129.2, 6.92 x 119.3, 6.87 x 110.2, 3.94 x 55.9, 2.93 x 34.5, 1.29-1.21 x 24.0

3.27 21b: 1-(2-(4-nitrophenyl)propan-2-yl)-4-phenyl--urazole



Formula: $C_{17}H_{16}N_4O_4$
Molecular weight: 340.339 g/mol
Exact mass: 340.11716 D

appearance: Yellow solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{17}H_{15}N_4O_4$ 339.1093; found 339.1100 (Δ = 0.3 ppm)

$\mathbf{R}_f$: 0.22 (50% EtOAc in pentane)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 8.23 (2H, m, *C11-H*), 7.93

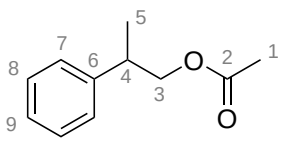
(1H, s(br), *NH*), 7.65 (2H, m, *C10-H*), 7.49-7.35 (5H, band, *C4-H, C5-H and C6-H*), 1.86 (6H, s, *C8-H*$_3$)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 154.0 (C=O, *C1 or C2*), 153.4 (C=O, *C1 or C2*), 150.9 (Ar−Cq, *C9*), 147.4 (Ar−Cq, *C12*), 130.8 (Ar−Cq, *C3*), 129.3 (Ar−H, *C5*), 128.6 (Ar−H, *C6*), 126.5 (Ar−H, *C10*), 125.5 (Ar−H, *C4*), 124.2 (Ar−H, *C11*), 64.0 (Cq, *C7*), 26.2 (CH_3, *C8*)

HSQC : 8.23 x 124.2, 7.65 x 126.5, 7.49-7.40 x 129.3, 7.41-7.35 x 128.6, 7.45-7.41 x 125.5, 1.86 x 26.2

IR: $\nu_{max}(cm^{-1})$: 3048(w), 2987(w), 1767(w), 1695(s), 1504(s), 1430(s), 1345(s), 850(m), 724(s), 688(s)

3.28 22a: 2-phenylpropyl acetate



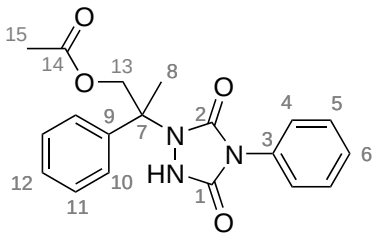
Formula: $C_{11}H_{14}O_2$
Molecular weight: 178.231 g/mol
Exact mass: 178.09938 D

appearance: colourless liquid

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.32 (2H, m, *Ar-H*), 7.26-7.21 (3H, band, *Ar-H*), 4.20 (1H, dd, J = 10.8 Hz, 7.0 Hz, *C3-**H**H*), 4.14 (1H, dd, J = 10.8 Hz, 7.0 Hz, *C3-H**H***), 3.10 (1H, sx, J = 7.0 Hz, *C4-H*), 2.02 (3H, s, *C1-H*$_3$), 1.31 (3H, d, J = 7.0 Hz, *C5-H*$_3$)

^{1}H-NMR data is consistent with literature.[19]

3.29 22b: 2-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-phenylpropyl acetate



Formula: $C_{19}H_{19}N_3O_4$
Molecular weight: 353.378 g/mol
Exact mass: 353.13756 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{19}H_{20}N_3O_4$ 354.1454; found 354.1436 (Δ = -3.5 ppm)

$\mathbf{R}_f$: 0.16 (30% EtOAc in pentane)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 8.54 (1H, s(br), *NH*), 7.47-7.29 (10H, band, *Ar-H*), 4.68 (1H, d, J = 11.8 Hz, *C13-**H**H*), 4.62 (1H, d, J = 11.8 Hz, *13-H**H***), 1.97 (3H, s, *C15-*H_3), 1.94 (3H, s, *C8-*H_3)

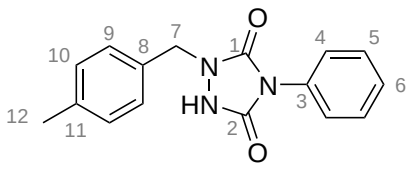
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 170.7 (C=O, *C14*), 153.9 (C=O, *C1 or C2*), 153.0 (C=O, *C1 or C2*), 139.7 (Ar−Cq, *C9*), 131.1 (Ar−Cq, *C3*), 129.1 (Ar−H, *C4-6 or C10-12*), 129.0 (Ar−H, *C4-6 or C10-12*), 128.5 (Ar−H, *C4-6 or C10-12*), 128.3 (Ar−H, *C4-6 or C10-12*), 125.8 (Ar−H, *C4-6 or C10-12*), 125.7 (Ar−H, *C4-6 or C10-12*), 67.9 (CH_2, *C13*), 65.8 (Cq, *C7*), 21.9 (CH_3, *C15*), 20.8 (CH_3, *C8*)

HSQC : 7.47-7.41 x 129.1, 7.47-7.41 x 129.0, 7.46-7.41 x 125.7, 7.46-7.41 x 125.8, 7.40-7.29 x 128.5, 7.40-7.29 x 128.3, 4.68 x 67.9, 4.62 x 67.9, 1.97 x 20.8, 1.94 x 21.9

IR: $\nu_{max}(cm^{-1})$: 3058(w), 2991(w), 1770(m), 1741(s), 1695(s), 1424(s), 1226(s), 767(s), 698(s)

3.30 23b: 1-(4-Methylbenzyl)-4-phenylurazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **23** together with unidentified side-products*



Formula: $C_{16}H_{15}N_3O_2$
Molecular weight: 281.315 g/mol
Exact mass: 281.11643 D

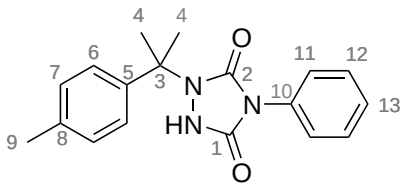
Low resolution mass from the LCMS giving $[M+H]^+$ Calcd for $C_{16}H_{15}N_3O_2$ 281.1; found 281.2

^{1}H-NMR (400 MHz, $CDCl_3$, 21 °C)*[only clear resonances are given]*: δ(ppm) = 7.25 (1H, m, *C9-H*), 7.19 (2H, m, *C10-H*), 4.70 (2H, s, *C7-H_2*), 2.36 (3H, s, *C12-H_3*)

^{13}C-NMR (100 MHz, $CDCl_3$, 21 °C)*[only clear resonances are given]*: δ(ppm) = 153.6 (C=O, *C2*), 153.3 (C=O, *C1*), 138.8 (Ar−Cq, *C11*), 130.7 (Ar−Cq, *C8*), 129.9 (Ar−CH, *C10*), 128.9 (Ar−CH, *C9*), 51.0 (CH_2, *C7*), 21.3 (CH_3, *C12*)

HSQC *[only clear resonances are given]*: 7.25 x 128.9, 7.19 x 129.9, 4.70 x 51.0, 2.36 x 21.3

3.31 24b: 4-phenyl-1-(2-(p-tolyl)propan-2-yl)-urazole



Formula: $C_{18}H_{19}N_3O_2$
Molecular weight: 309.369 g/mol
Exact mass: 309.14773 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M\text{-}H]^-$ Calcd for $C_{18}H_{18}N_3O_2$ 308.1399; found 308.1395 (Δ = -3.1 ppm)

$\mathbf{R}_f$: 0.13 (20% EtOAc in pentane)

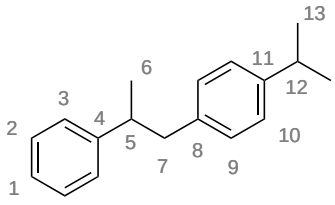
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.50-7.43 (4H, band, *C11-H and C12-H*), 7.40-7.34 (3H, band, *C6-H and C13-H*), 7.21 (2H, m, *C7-H*), 6.87 (1H, s(br), *NH*), 2.35 (3H, s, *C9-H*$_3$), 1.88 (6H, s, *C4-H*$_3$)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.1 (C=O, *C1 or C2*), 153.1 (C=O, *C1 or C2*), 140.4 (Ar−Cq, *C5*), 138.1 (Ar−Cq, *C8*), 131.3 (Ar−Cq, *C10*), 129.9 (Ar−H, *C7*), 129.2 (Ar−H, *C12*), 128.3 (Ar−H, *C13*), 125.8 (Ar−H, *C11*), 125.5 (Ar−H, *C6*), 64.5 (Cq, *C3*), 26.1 (CH_3, *C4*), 21.1 (CH_3, *C9*)

HSQC : 7.50-7.43 x 129.2, 7.50-7.43 x 125.8, 7.40-7.34 x 128.3, 7.40-7.34 x 125.5, 7.21 x 129.9, 2.35 x 21.1, 1.88 x 26.1

IR: $\nu_{max}(cm^{-1})$: 3056(w), 2848(w), 1770(w), 1700(s), 1429(s), 813(m), 772(s), 690(m)

3.32 25a: 1-isopropyl-4-(2-phenylpropyl)benzene



Formula: $C_{18}H_{22}$
Molecular weight: 238.374 g/mol
Exact mass: 238.17215 D

appearance: clear liquid

Product didn't ionize for HRMS analysis.
GCMS m/z: $[M]^\bullet$ Calcd for $C_{18}H_{22}$ 238.2; Found 238.1

$\mathbf{R}_f$: 0.30 (pentane)

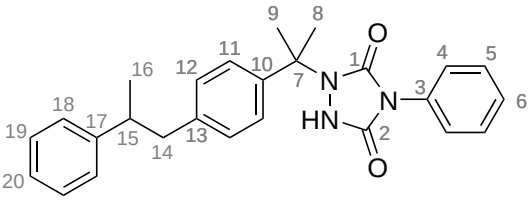
^{1}H-NMR (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.31 (2H, m, *C2-H*), 7.25-7.18 (3H, band, *C3-H and C1-H*), 7.13 (2H, m, *C10-H*), 7.05 (2H, m, *C9-H*), 3.06-2.93 (2H, band, *C5-H and C7-**H**H*), 2.89 (1H, sept, J = 7.0 Hz, *C12-H*), 2.74 (1H, dd, J = 12.9 Hz, 8.3 Hz, *C7-H**H***), 1.26 (6H, d, J = 7.0 Hz, *C13-H_3*), 1.25 (3H, d, J = 6.9 Hz, *C6-H_3*)

^{13}C-NMR (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 147.5 (Ar−Cq, *C4*), 146.5 (Ar−Cq, *C8*), 138.3 (Ar−Cq, *C11*), 129.2 (Ar−H, *C9*), 128.4 (Ar−H, *C2*), 127.2 (Ar−H, *C3*), 126.3 (Ar−H, *C10*), 126.1 (Ar−H, *C1*), 44.7 (CH_2, *C7*), 41.9 (CH, *C5*), 33.8 (CH, *C12*), 24.2 (CH_3, *C13*), 21.3 (CH_3, *C6*)

HSQC : 7.31 x 128.4, 7.25-7.23 x 127.2, 7.24-7.18 x 126.1, 7.13 x 126.3, 7.05 x 129.2, 3.06-2.97 x 41.9, 3.00-2.93 x 44.7, 2.89 x 33.8, 2.74 x 44.7, 1.26 x 24.2, 1.25 x 21.3

IR: $\nu_{max}(cm^{-1})$: 3025(w), 2958(m), 1452(w), 809(m), 759(m), 697(s)

3.33 25b: 4-phenyl-1-(2-(4-(2-phenylpropyl)phenyl)propan-2-yl)-urazole



Formula: $C_{26}H_{27}N_3O_2$
Molecular weight: 413.521 g/mol
Exact mass: 413.21033 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{26}H_{28}N_3O_2$ 414.2182; found 414.2172 (Δ = -1.0 ppm)

$\mathbf{R}_f$: 0.13 (20% EtOAc in pentane)

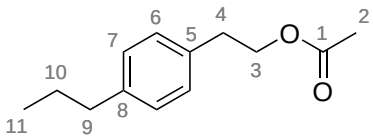
^{1}H-NMR (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.49-7.43 (4H, band, *C4-H and C5-H*), 7.39-7.32 (3H, band, *C11-H and C6-H*), 7.29 (2H, m, *C19-H*), 7.22-7.17 (3H, band, *C18-H and C20-H*), 7.12 (2H, m, *C12-H*), 6.42 (1H, s(br), *NH*), 3.06-2.91 (2H, band, *C14-**H**H and C15-H*), 2.80 (1H, dd, J = 13.0 Hz, 7.9 Hz, *C14-H**H***), 1.88 (3H, s, *C8-H_3 or C9-H_3*), 1.88 (3H, s, *C8-H_3 or C9-H_3*), 1.27 (3H, d, J = 6.8 Hz, *C16-H_3*)

^{13}C-NMR (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.2 (C=O, *C1 or C2*), 153.0 (C=O, *C1 or C2*), 146.8 (Ar−Cq, *C17*), 141.1 (Ar−Cq, *C13*), 140.8 (Ar−Cq, *C10*), 131.2 (Ar−Cq, *C3*), 130.0 (Ar−H, *C12*), 129.2 (Ar−H, *C5*), 128.5 (Ar−H, *C19*), 128.4 (Ar−H, *C6*), 127.2 (Ar−H, *C18*), 126.3 (Ar−H, *C20*), 125.8 (Ar−H, *C4*), 125.4 (Ar−H, *C11*), 64.7 (Cq, *C7*), 44.6 (CH_2, *C14*), 41.9 (CH, *C15*), 26.1 (CH_3, *C8 or C9*), 25.9 (CH_3, *C8 or C9*), 21.5 (CH_3, *C16*)

HSQC : 7.49-7.43 x 129.2, 7.48-7.45 x 125.8, 7.39-7.7.34 x 128.4, 7.36-7.32 x 125.4, 7.29 x 128.5, 7.22-7.19 x 126.3, 7.20-7.17 x 127.2, 7.12 x 130.0, 3.06-2.95 x 41.9, 2.99-2.91 x 44.6, 2.80 x 44.6, 1.88 x 26.1, 1.88 x 25.9, 1.27 x 21.5

IR: $\nu_{max}(cm^{-1})$: 3061(w), 2966(w), 1770(w), 1690(s), 1423(s), 765(s), 691(s)

3.34 26a: 4-propylphenethyl acetate



Formula: $C_{13}H_{18}O_2$
Molecular weight: 206.285 g/mol
Exact mass: 206.13068 D

appearance: colourless liquid

Product didn't ionize for HRMS analysis.
GCMS m/z: $[M]^\bullet$ Calcd for $C_{13}H_{18}O_2$ 206.1; Found $[M]^\bullet$ not found; $[M-OAc]^\bullet$ Calcd for $C_{11}H_{14}$ 146.1; found 146.1

$\mathbf{R}_f$: 0.29 (5% Et_2O in pentane)

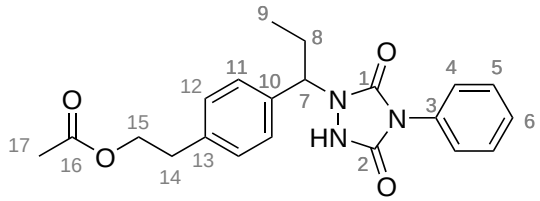
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.14 (4H, m, *C6-H and C7-H*), 4.28 (2H, t, J = 7.2 Hz, *C3-*H_2), 2.92 (2H, t, J = 7.2 Hz, *C4-*H_2), 2.58 (2H, m, *C9-*H_2), 2.05 (3H, s, *C2-*H_3), 1.65 (2H, m, *C10-*H_2), 0.95 (3H, t, J = 7.3 Hz, *C11-*H_3)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 171.1 (C=O, *C2*), 141.0 (Ar−Cq, *C8*), 135.0 (Ar−Cq, *C5*), 128.8 (Ar−H, *C7*), 128.7 (Ar−H, *C6*), 65.2 (CH_2, *C3*), 37.8 (CH_2, *C9*), 34.8 (CH_2, *C4*), 24.7 (CH_2, *C10*), 21.1 (CH_3, *C2*), 13.9 (CH_3, *C11*)

HSQC : 7.14 x 128.8, 7.14 x 128.7, 4.28 x 65.2, 2.92 x 34.8, 2.58 x 37.8, 2.05 x 21.1, 1.65 x 24.7, 0.95 x 13.9

IR: $\nu_{max}(cm^{-1})$: 3011(w), 2958(m), 1737(s), 1363(m), 1232(s), 1031(s), 799(m)

3.35 26b: 4-(1-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)propyl)phenethyl acetate



Formula: $C_{21}H_{23}N_3O_4$
Molecular weight: 381.432 g/mol
Exact mass: 381.16886 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{21}H_{24}N_3O_4$ 382.1767; found 382.1754 (Δ = -1.9 ppm)

$\mathbf{R}_f$: 0.12 (30% EtOAc in pentane)

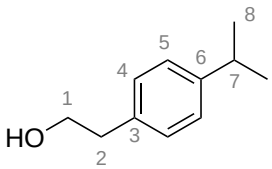
^{1}**H-NMR** (300 MHz, $CDCl_3$, 21 °C): δ(ppm) = 8.16 (1H, s(br), *NH*), 7.51-7.41 (4H, band, *C4-H and C5-H*), 7.41-7.31 (3H, band, *C6-H and C11-H*), 7.20 (2H, m, *C12-H*), 5.15 (1H, t, J = 7.9 Hz, *C7-H*), 4.26 (2H, t, J = 6.9 Hz, *C15-*H_2), 2.92 (2H, t, J = 6.9 Hz, *C14-*H_2), 2.13 (2H, m, *C8-*H_2), 2.03 (3H, s, *C17-*H_3), 0.98 (3H, t, J = 7.3 Hz, *C9-*H_3)

^{13}**C-NMR** (75 MHz, $CDCl_3$, 21 °C): δ(ppm) = 171.2 (C=O, *C16*), 154.0 (C=O, *C1 or C2*), 152.6 (C=O, *C1 or C2*), 138.5 (Ar−Cq, *C13*), 135.4 (Ar−Cq, *C10*), 131.4 (Ar−Cq, *C3*), 129.5 (Ar−CH, *C12*), 129.2 (Ar−CH, *C5*), 128.3 (Ar−CH, *C6*), 128.2 (Ar−CH, *C11*), 125.6 (Ar−CH, *C4*), 64.8 (CH_2, *C15*), 61.5 (CH, *C7*), 34.8 (CH_2, *C14*), 24.5 (CH_2, *C8*), 21.1 (CH_3, *C17*), 11.2 (CH_3, *C9*)

HSQC : 7.51-7.41 x 125.6, 7.51-7.41 x 129.2, 7.41-7.31 x 128.3, 7.41-7.31 x 128.2, 7.20 x 129.5, 5.15 x 61.5, 4.26 x 64.8, 2.92 x 34.8, 2.13 x 24.5, 2.03 x 21.1, 0.98 x 11.2

IR: $\nu_{max}(cm^{-1})$: 3084(w), 2942(w), 1770(w), 1752(w), 1738(s), 1677(s), 1415(s), 1235(s), 766(s), 760(s)

3.36 27a: 2-(4-isopropylphenyl)ethan-1-ol



Formula: $C_{11}H_{16}O$
Molecular weight: 164.248 g/mol
Exact mass: 164.12012 D

appearance: yellowish transparent liquid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{11}H_{17}O$ 165.1279; found 165.1270 (Δ = -2.4 ppm)

$\mathbf{R}_f$: 0.24 (15% EtOAc in pentane)

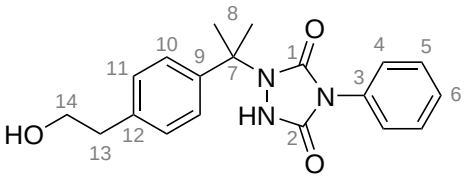
^{1}H-NMR (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.18 (4H, band, *Ar-H*), 3.85 (2H, t, J = 6.6 Hz, *C1-H*$_2$), 2.90 (1H, sept, J = 6.9 Hz, *C7-H*), 2.85 (2H, t, J = 6.6 Hz, *C2-H*$_2$), 1.25 (6H, d, J = 6.9 Hz, *C8-H*$_3$)

^{13}C-NMR (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 147.2 (Ar−Cq, *C6*), 135.8 (Ar−Cq, *C3*), 129.1 (Ar−H, *C4*), 126.8 (Ar−H, *C5*), 63.8 (CH_2, *C1*), 38.9 (CH_2, *C2*), 33.8 (CH, *C7*), 24.2 (CH_3, *C8*)

HSQC : 7.18 x 129.1, 7.18 x 126.8, 3.85 x 63.8, 2.90 x 33.8, 2.85 x 38.9, 1.25 x 24.2

IR: $\nu_{max}(cm^{-1})$: 3314(m,br), 3011(w), 2956(m), 1460(w), 1043(s), 818(s)

3.37 27b: 1-(2-(4-(2-hydroxyethyl)phenyl)propan-2-yl)-4-phenyl-urazole



Formula: $C_{19}H_{21}N_3O_3$
Molecular weight: 339.395 g/mol
Exact mass: 339.15829 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{19}H_{20}N_3O_3$ 338.1505; found 338.1512 (Δ = -0.5 ppm)

R$_f$: 0.12 (50% EtOAc in pentane)

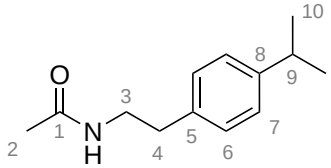
^{1}H-NMR (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.49-7.45 (4H, band, *C4-H, C5-H*), 7.43 (2H, m, *C10-H*), 7.37 (1H, m, *C6-H*), 7.27 (2H, m, *C11-H*), 6.86 (1H, s(br), *NH*), 3.85 (2H, t, J = 6.5 Hz, *C14-H*$_2$), 2.86 (2H, t, J = 6.5 Hz, *C13-H*$_2$), 1.89 (6H, s, *C8-H*$_3$)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.2 (C=O, *C1/C2*), 153.2 (C=O, *C1/C2*), 141.5 (Ar−Cq, *C9*), 138.8 (Ar−Cq, *C12*), 131.1 (Ar−Cq, *C3*), 129.9 (Ar−CH, *C11*), 129.2 (Ar−CH, *C5*), 128.4 (Ar−CH, *C6*), 125.8 (Ar−CH, *C10*), 125.8 (Ar−CH, *C4*), 64.5 (Cq, *C7*), 63.5 (CH_2, *C12*), 38.7 (CH_2, *C13*), 26.1 (CH_3, *C8*)

HSQC : 7.49-7.45 x 129.2, 7.49-7.45 x 125.8, 7.43 x 125.8, 7.37 x 128.4, 7.27 x 129.9, 3.85 x 63.5, 2.86 x 38.7, 1.89 x 26.1

IR: $\nu_{max}(cm^{-1})$: 3452(w, br), 3068(w), 2930(w), 1768(w), 1688(s), 1424(m), 769(m), 694(m)

3.38 28a: N-(4-isopropylphenethyl)acetamide



Formula: $C_{13}H_{19}NO$
Molecular weight: 205.301 g/mol
Exact mass: 205.14666 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{13}H_{20}NO$ 206.1545; found 206.1530 (Δ = -4.6 ppm)

$\mathbf{R}_f$: 0.33 (EtOAc)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.18 (2H, m, *C6-H*), 7.12 (2H, m, *C7-H*), 5.73 (1H, s(br), *NH*), 3.51 (2H, q, J = 6.8 Hz, *C3-*H_2), 2.89 (1H, sept, J = 6.9 Hz, *C9-H*), 2.79 (2H, t, J = 6.8 Hz, *C4-*H_2), 1.97 (3H, s, *C2-*H_3), 1.24 (6H, d, J = 6.9 Hz, *C10-*H_3)

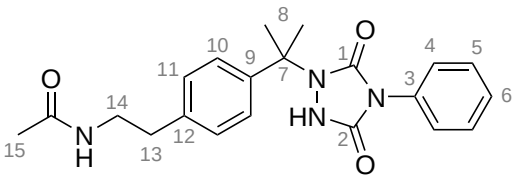
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 170.4 (C=O, *C1*), 147.3 (Ar−Cq, *C8*), 136.2 (Ar−Cq, *C5*), 128.8 (Ar−CH, *C7*), 126.8 (Ar−CH, *C6*), 40.9 (CH, *C3*), 35.2 (CH_2, *C4*), 33.8 (CH_2, *C9*), 24.2 (CH_3, *C10*), 23.4

(CH_3, *C2*)

HSQC : 7.18 x 126.8, 7.12 x 128.8, 3.51 x 40.9, 2.89 x 33.8, 2.79 x 35.2, 1.97 x 23.4, 1.24 x 24.2

IR: $\nu_{max}(cm^{-1})$: 3250(m), 3078(w), 2956(m), 1631(s), 1564(s), 1360(s), 1298(s), 1100(m), 815(m), 743(m)

3.39 28b: N-(4-(2-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)propan-2-yl)phenethyl)acetamide



Formula: $C_{21}H_{24}N_4O_3$
Molecular weight: 380.448 g/mol
Exact mass: 380.18484 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M-H]^-$ Calcd for $C_{21}H_{23}N_4O_3$ 379.177; found 379.1770 (Δ = -1.5 ppm)

$\mathbf{R}_f$: 0.19 (EtOAc)

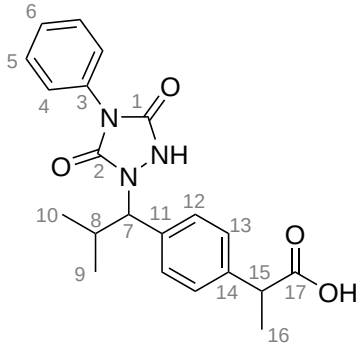
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.48-7.45 (4H, band, *C4-H, C5-H*), 7.43 (2H, m, *C10-H*), 7.37 (1H, m, *C6-H*), 7.23 (2H, m, *C11-H*), 5.88 (1H, s(br), *NH*), 3.50 (2H, app q, J = 6.6 Hz, *C14-*H_2), 2.82 (2H, t, J = 6.6 Hz, *C13-*H_2), 1.98 (3H, s, *C15-*H_3), 1.89 (6H, s, *C8-*H_3)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 170.7 (C=O, *C15*), 153.3 (C=O, *C1/C2*), 153.2 (C=O, *C1/C2*), 141.7 (Ar−Cq, *C9*), 139.0 (Ar−Cq, *C12*), 131.1 (Ar−Cq, *C3*), 129.6 (Ar−CH, *C11*), 129.3 (Ar−CH, *C5*), 128.4 (Ar−CH, *C6*), 125.9 (Ar−CH, *C10*), 125.8 (Ar−CH, *C4*), 64.5 (Cq, *C7*), 40.9 (CH_2, *C14*), 35.3 (CH_2, *C13*), 26.1 (CH_3, *C8*), 23.2 (CH_3, *C15*)

HSQC : 7.48-7.45 x 129.3, 7.48-7.45 x 125.8, 7.43 x 125.9, 7.37 x 128.4, 7.23 x 129.6, 3.50 x 40.9, 2.82 x 35.3, 1.98 x 23.2, 1.89 x 26.1

IR: $\nu_{max}(cm^{-1})$: 3340(m), 3059(w), 2987(w), 1769(w), 1703(s), 1427(m), 772(m), 723(m)

3.40 29b: 2-(4-(1-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-methylpropyl)phenyl)propanoic acid



Formula: $C_{21}H_{23}N_3O_4$
Molecular weight: 381.432 g/mol
Exact mass: 381.16886 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{21}H_{24}N_3O_4$ 382.1767; found 382.1769 (Δ = 2.0 ppm)

$\mathbf{R}_f$: 0.15 (35% EtOAc, 1% HOAc in pentane)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 11.4-9.7 (1H, m(br), *COOH*), 7.56-7.32 (9H, band, *C4-H, C5-H, C6-H, C12-H, C13-H*), 4.89 (0.5H, d, J = 11.4 Hz, *C7-H*), 4.84 (0.5H, d, J = 11.4 Hz, *C7-H*), 3.79 (0.5H, q, J = 7.1 Hz, *C15-H*), 3.76 (0.5H, q, J = 7.1 Hz, *C15-H*), 2.59 (1H, m, *C8-H*), 1.56 (3H, d, J = 7.1 Hz, *C16-H*$_3$), 1.13 (1.5H, d, J = 6.6 Hz, *C9-H*$_3$), 1.11 (1.5H, d, J = 6.6 Hz, *C9-H*$_3$), 0.86 (1.5H, d, J = 6.6 Hz, *C10-H*$_3$), 0.83 (1.5H, d, J = 6.6 Hz, *C10-H*$_3$)

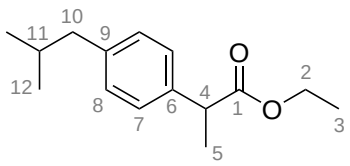
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 179.6 and 179.2 (C=O,

C17), 154.1 and 153.9 (C=O, *C1*), 151.0 and 150.6 C=O (C_2), 140.7 and 140.3 (Ar−Cq, *C14*), 135.9 and 135.8 (Ar−Cq, *C11*), 131.1 and 129.6 (Ar−Cq, *C3*), 129.5 and 129.3 (Ar−CH, *C5*), 129.3 and 128.7 (Ar−CH, *C6*), 128.7 and 128.5 Ar-CH (C_{12}), 128.4 and 128.2 (Ar−CH, *C13*), 125.8 and 125.7 (Ar−CH, *C4*), 66.2 and 65.7 (CH, *C7*), 45.4 and 45.0 (CH, *C15*), 29.8 and 29.6 (CH, *C8*), 20.2 (CH_3, *C10*), 20.0 and 19.9 (CH_3, *C9*), 18.7 and 17.7 (CH_3, *C16*)

HSQC : 7.45-7.34 x 129.7-128.2, 7.44-7.40 x 125.8 and 125.7, 4.89 x 65.7, 4.84 x 66.2, 3.79 x 45.4, 3.76 x 45.0, 2.59 x 29.8 and 29.6, 1.56 x 18.7 and 17.7, 1.13 x 20.0, 1.11 x 20.0, 0.86 x 20.2, 0.83 x 20.2

IR: $\nu_{max}(cm^{-1})$: 3061(w, br), 2964(w), 1762(w), 1685(s), 1426(m), 767(m), 704(m)

3.41 30a: ibuprofen ethyl ester



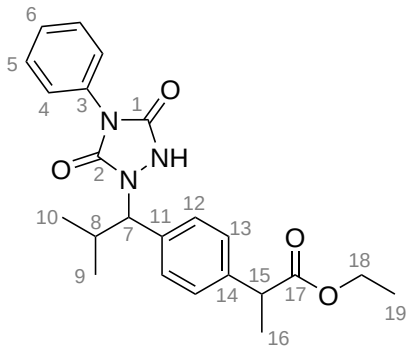
Formula: $C_{15}H_{22}O_2$
Molecular weight: 234.339 g/mol
Exact mass: 234.16198 D

appearance: clear liquid

^{1}**H-NMR** (300 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.21 (2H, m, *C7-H*), 7.09 (2H, m, *C8-H*), 4.12 (2H, m, *C2-*H_2), 3.68 (1H, q, J = 7.2 Hz, *C4-H*), 2.45 (2H, d, J = 6.7 Hz, *C10-*H_2), 1.85 (1H, n, J = 6.7 Hz, *C11-H*), 1.49 (3H, d, J = 7.2 Hz, *C5-*H_3), 1.21 (3H, t, J = 7.1 Hz, *C3-*H_3), 0.90 (6H, d, J = 6.7 Hz, *C12-*H_3)

^{1}H-NMR data is consistent with literature.[20]

3.42 30b: ethyl 2-(4-(1-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-methylpropyl)phenyl)propanoate



Formula: $C_{23}H_{27}N_3O_4$
Molecular weight: 409.486 g/mol
Exact mass: 409.20016 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{23}H_{28}N_3O_4$ 410.208; found 410.2058 (Δ = -4.0 ppm)

$\mathbf{R}_f$: 0.15 (30% EtOAc in pentane)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 8.65 (1H, s(br), *NH*), 7.46 (4H, band, *C4-H, C5-H*), 7.38 (1H, m, *C6-H*), 7.34 (2H, m, *C12-H*), 7.27 (2H, m, *C13-H*), 4.79 (1H, d, J = 11.3 Hz, *C7-H*), 4.12 (2H, m, *C18-*H_2), 3.69 (1H, q, J = 7.2 Hz, *C15-H*), 2.52 (1H, m, *C8-H*), 1.47 (3H, d, J = 7.2 Hz, *C16-*H_3), 1.20 (3H, td, J = 7.2 Hz, 0.9 Hz, *C19-*H_3), 1.11 (3H, d, J = 6.5 Hz, *C9-*H_3), 0.81 (3H, d, J = 6.6 Hz, *C10-*H_3)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 174.5 and 174.4 (C=O, *C17*), 154.0 (C=O, *C1*), 152.1 (C=O, *C2*), 141.1 and 141.0 (Ar−Cq, *C11*), 135.4 (Ar−Cq, *C14*), 131.3 (Ar−Cq, *C3*), 129.2 (Ar−H, *C5*), 128.7 (Ar−H, *C12*), 128.3 (Ar−H, *C6*), 128.2 (Ar−H, *C13*), 125.6 (Ar−H, *C4*), 66.6 (CH, *C7*), 61.0 (CH_2, *C18*), 45.4 and 45.3 (CH, *C15*), 29.5 (CH, *C8*), 20.3 (CH_3, *C10*), 20.1 (CH_3, *C9*), 18.7 and 18.6 (CH_3, *C16*), 14.3 (CH_3, *C19*)

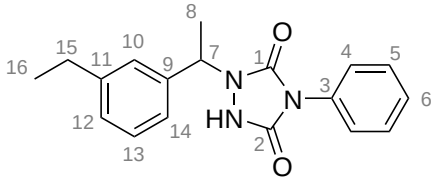
HSQC : 7.47-7.42 x 125.6, 7.50-7.44 x 129.2, 7.38 x 128.3, 7.34 x 128.7,

7.27 x 128.2, 4.79 x 66.6, 4.12 x 61.0, 3.69 x 45.4 and 45.3, 2.52 x 29.5, 1.47 x 18.7 and 18.6, 1.20 x 14.3, 1.11 x 20.1, 0.81 x 20.3

IR: $\nu_{max}(cm^{-1})$: 3198(w), 2968(w), 1769(w), 1727(m), 1682(s), 1445(m), 771(m), 705(m)

3.43 31b: 1-(1-(3-ethylphenyl)ethyl)-4-phenyl-urazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **31b** and **12b** in a 82:18 ratio*



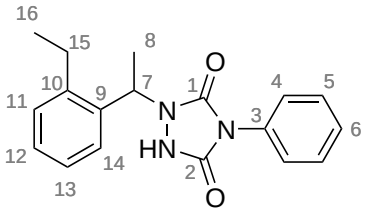
Formula: $C_{18}H_{19}N_3O_2$
Molecular weight: 309.369 g/mol
Exact mass: 309.14773 D

^{1}H-NMR (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.29-7.23 (1H, m, *Ar-H*), 7.27-7.20 (1H, m, *Ar-H*), 7.20-7.15 (1H, m, *Ar-H*), 5.44 (1H, q, J = 7.0 Hz, *C7-H*), 2.63 (2H, q, J = 7.6 Hz, *C15-H*), 1.67 (3H, d, J = 7.0 Hz, *C8-H$_3$*), 1.22 (3H, t, J = 7.6 Hz, *C16-H$_3$*)

^{13}C-NMR (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 154.0 (C=O, *C2*), 152.2 (C=O, *C1*), 145.1 (Ar−Cq, *C11*), 138.0 (Ar−Cq, *C9*), 128.2 (Ar−CH), 127.5 (Ar−CH), 127.1 (Ar−CH, *C10*), 124.6 (Ar−CH), 55.4 (CH, *C7*), 28.8 (CH_2, *C15*), 16.7 (CH_3, *C8*), 15.6 (CH_3, *C16*)

HSQC : 7.29-7.23 x 127.1, 7.27-7.20 x 124.6, 7.20-7.15 x 128.2, 5.44 x 55.4, 28.8 x 2.63, 1.67 x 16.7, 1.22 x 15.6

3.44 32b: 1-(1-(2-ethylphenyl)ethyl)-4-phenyl-urazole



Formula: $C_{18}H_{19}N_3O_2$
Molecular weight: 309.369 g/mol
Exact mass: 309.14773 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+H]^+$ Calcd for $C_{18}H_{20}N_3O_2$ 310.1556; found 310.1546 (Δ = -1.3 ppm)

$\mathbf{R}_f$: 0.28 (30% EtOAc in pentane)

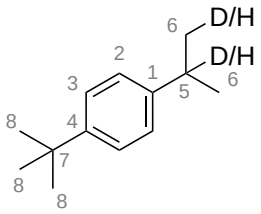
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.85 (1H, s(br), *NH*), 7.52-7.44 (5H, band, *C4-H, C5-H and C14-H*), 7.38 (1H, m, *C6-H*), 7.31-7.24 (2H, band, *C13-H and C11-H*), 7.20 (1H, m, *C12-H*), 5.72 (1H, q, J = 6.9 Hz, *C7-H*), 2.88 (1H, dq, J = 14.8 Hz, 7.6 Hz, *C15-**H**H*), 2.73 (1H, dq, J = 14.8 Hz, 7.6 Hz, *C15-H**H***), 1.67 (3H, d, J = 6.9 Hz, *C8-H_3*), 1.25 (3H, t, J = 7.6 Hz, *C16-H_3*)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 153.9 (C=O, *C2*), 151.9 (C=O, *C1*), 143.1 (Ar−Cq, *C9*), 135.0 (Ar−Cq, *C10*), 131.4 (Ar−Cq, *C3*), 129.4 (Ar−H, *C11*), 129.2 (Ar−H, *C5*), 129.0 (Ar−H, *C13*), 128.2 (Ar−H, *C6*), 126.6 (Ar−H, *C14*), 126.4 (Ar−H, *C12*), 125.4 (Ar−H, *C4*), 51.2 (CH, *C7*), 25.3 (CH_2, *C15*), 16.4 (CH_3, *C8*), 15.5 (CH_3, *C16*)

HSQC : 7.52-7.46 x 125.4, 7.51-7.44 x 129.2, 7.49-7.44 x 126.6, 7.38 x 128.2, 7.31-7.25 x 129.0, 7.30-7.24 x 129.4, 7.20 x 126.4, 5.72 x 51.2, 2.88 x 25.3, 2.73 x 25.3, 1.67 x 16.4, 1.25 x 15.5

IR: $\nu_{max}(cm^{-1})$: 3073(w), 2966(w), 1765(m), 1691(s), 1427(s), 765(s)

3.45 33a: Deuterated 1-(tert-butyl)-4-isopropylbenzene



Formula: $C_{13}H_{19}D$
Molecular weight: 177.3091 g/mol
Exact mass: 177.16278 D

appearance: colourless liquid

Product didn't ionize for HRMS analysis.
GCMS m/z: $[M]^{\bullet}$ Calcd for $C_{13}H_{19}D$ 177.2; Found 177.1

$\mathbf{R}_f$: 0.81 (pentane)

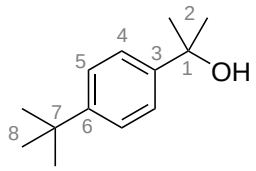
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.34 (2H, m, *C3-H*), 7.19 (2H, m, *C2-H*), 2.91 (1H[28% H, 72% D], m, *C5-H*), 1.34 (9H, s, *C8-*H_3), 1.26 (6H[86% H, 14% D], m, *C6-*H_3)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 148.6 (Ar−Cq, *C4*), 145.6 (m,Ar−Cq, *C1*), 126.2 (Ar−CH, *C2*), 125.3 (Ar−CH, *C3*), 34.5 (Cq, *C7*), 33.3 (m,CH, *C5*), 31.6 (CH_3, *C8*), 24.1 (m,CH_3, *C6*)

HSQC : 7.34 x 125.3, 7.19 x 126.2, 2.91 x 33.3, 1.34 x 31.6, 1.26 x 1.26

IR: $\nu_{max}(cm^{-1})$: 2956(m), 1507(w), 1460(w), 1362(s), 828(s)

3.46 34: 2-(4-(tert-butyl)phenyl)propan-2-ol



Formula: $C_{13}H_{20}O$
Molecular weight: 192.302 g/mol
Exact mass: 192.15142 D

appearance: white solid

Product didn't ionize for HRMS analysis.
GCMS m/z: $[M]^{\bullet}$ Calcd for $C_{13}H_{20}O$ 192.2; Found 192.2

$\mathbf{R}_f$: 0.16 (10% EtOAc in pentane)

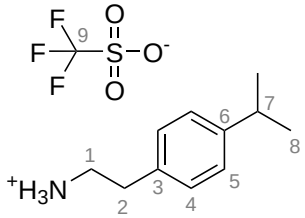
^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.43 (2H, m, *C4-H*), 7.37 (2H, m, *C5-H*), 1.72 (1H, s(br), *OH*), 1.59 (6H, s, *C2-H*$_3$), 1.33 (9H, s, *C8-H*$_3$)

^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 149.7 (Ar−Cq, *C6*), 146.2 (Ar−Cq, *C3*), 125.2 (Ar−CH, *C5*), 124.2 (Ar−CH, *C4*), 72.5 (Cq, *C1*), 34.5 (Cq, *C7*), 31.8 (CH_3, *C2*), 31.5 (CH_3, *C8*)

HSQC : 7.43 x 124.2, 7.37 x 125.2, 1.59 x 31.8, 1.33 x 31.5

IR: $\nu_{max}(cm^{-1})$: 3330(w, br), 2963(w), 1128(s), 830(m), 671(m)

3.47 35a: 2-(4-isopropylphenyl)ethan-1-aminium trifluoromethanesulfonate



Formula: $C_{12}H_{18}F_3NO_3S$
Molecular weight: 313.33521 g/mol
Exact mass: 313.09595 D

appearance: white solid

$[M]^+$ Calcd for $C_{11}H_{18}N$ 164,1; found 164,2

$[OTf]^-$ Calcd for CF_3O_3S 149,0; found 149,0

$\mathbf{R}_f$: 0.17 (5% MeOH 1% HOAc in pentane)

^{1}**H-NMR** (400 MHz, Acetone, 21 °C): δ(ppm) = 7.71 (3H, s(br), *NH*$_3$),

7.25 (2H, m, *C4-H*), 7.21 (2H, m, *C5-H*), 3.48 (2H, m, *C1-H_2*), 3.12 (2H, m, *C2-H_2*), 2.89 (1H, sept, J = 6.9 Hz, *C7-H*), 1.21 (6H, d, J = 6.9 Hz, *C8-H_3*)

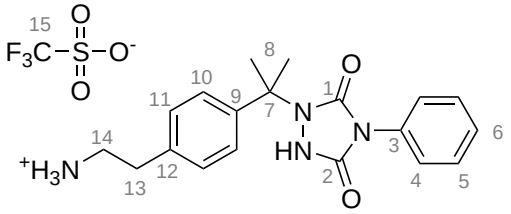
^{13}C-NMR (100 MHz, Acetone, 21 °C): δ(ppm) = 148.3 (Ar−Cq, *C6*), 135.1 (Ar−Cq, *C3*), 129.7 (Ar−CH, *C4-H*), 127.6 (Ar−CH, *C5-H*), 42.7 (CH_2, *C1*), 34.4 (CH, *C7*), 33.6 (CH_2, *C2*), 24.3 (CH_3, *C8*)

HSQC : 7.25 x 129.7, 7.21 x 127.6, 3.48 x 42.7, 3.12 x 33.6, 2.89 x 34.4, 1.21 x 24.3

IR: $\nu_{max}(cm^{-1})$: 3171(w), 2965(w), 1239(s), 1166(s), 1029(s), 820(m), 632(s)

3.48 35b: 1-(2-(4-(2-amino-ethyl)phenyl)propan-2-yl)-4-phenyl-urazole triflic acid salt

*This compound was not obtained analytically pure and the assignments were made on a sample from the crude mixture of the reaction after workup, containing a mixture of **35a** and **35b** in a 91:9 ratio*



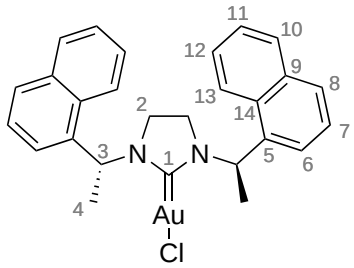
Formula: $C_{20}H_{23}F_3N_4O_5S$
Molecular weight: 488.48221 g/mol
Exact mass: 488.13413 D

^{1}H-NMR (400 MHz, Acetone−d_6, 21 °C): δ(ppm) = 3.16 (2H, m, *C13-H_2*), 1.85 (6H, s, *C8-H_3*)

^{13}C-NMR (100 MHz, Acetone−d_6, 21 °C): δ(ppm) = 144.5 (Cq, *C9*), 136.5 (Cq, *C12*), 129.4 (Ar−CH, *C11*), 126.4 (Ar−CH, *C10*), 64.0 (Cq, *C7*), 42.4 (CH_2, *C14*), 33.4 (CH_2, *C13*), 27.3 (CH_3, *C8*)

HSQC : 3.16 x 33.4, 1.85 x 27.3

3.49 38: (1,3-bis((R)-1-(naphthalen-1-yl)ethyl)imidazolidin-2-ylidene)gold(I) chloride



Formula: $C_{27}H_{26}AuClN_2$
Molecular weight: 610.93557 g/mol
Exact mass: 610.145 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+NH4]^+$ Calcd for $C_{27}H_{30}AuClN_3$ 628.1794; found 628.178 (Δ = -1.4 ppm)

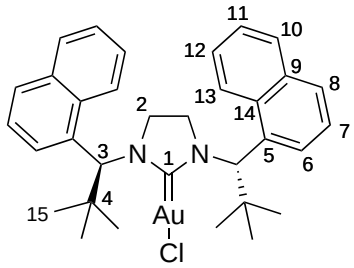
^{1}**H-NMR** (400 MHz, DCM−d_2, 21 °C): δ(ppm) = 8.45 (2H, d, J = 8.6 Hz, *C13-H*), 7.92 (2H, m, *C10-H*), 7.87 (2H, dd, J = 7.5 Hz, 1.4 Hz, *C8-H*), 7.66 (2H, ddd, J = 8.6 Hz, 6.9 Hz, 1.4 Hz, *C12-H*), 7.57 (2H, ddd, J = 8.1 Hz, 6.9 Hz, 1.1 Hz, *C11-H*), 7.51-7.44 (4H, band(AB), *C7-H and C6-H*), 6.51 (2H, q, J = 6.9 Hz, *C3-H*), 3.15 (2H, m, *C2-**H**H*), 2.60 (2H, m, *C2-H**H***), 1.80 (6H, d, J = 6.9 Hz, *C4-H_3*)

^{13}**C-NMR** (100 MHz, DCM−d_2, 21 °C): δ(ppm) = 192.8 (Cq, *C1*), 134.4 (Ar−Cq, *C9*), 133.9 (Ar−Cq, *C5*), 132.0 (Ar−Cq, *C14*), 129.7 (Ar−H, *C8*), 129.3 (Ar−H, *C10*), 127.4 (Ar−H, *C12*), 126.5 (Ar−H, *C11*), 125.3 (Ar−H, *C7*), 125.0 (Ar−H, *C6*), 124.0 (Ar−H, *C13*), 55.3 (CH, *C3*), 43.9 (CH_2, *C2*), 18.1 (CH_3, *C4*)

HSQC : 8.45 x 124.0, 7.92 x 129.3, 7.87 x 129.7, 7.66 x 127.4, 7.57 x 126.5, 7.50 x 125.3, 7.48 x 125.0, 6.51 x 55.3, 3.15 x 43.9, 2.60 x 43.9, 1.80 x 18.1

IR: $\nu_{max}(cm^{-1})$: 3047.0(w), 2970.3(w), 1598.3(w), 1494.5(m), 1448.3(m), 1271.1(s), 801.06(m), 773.0(s), 722.4(m)

3.50 39: (1,3-bis((S)-2,2-dimethyl-1-(naphthalen-1-yl)-propyl)imidazolidin-2-ylidene)gold(I) iodide



Formula: $C_{33}H_{38}AuIN_2$
Molecular weight: 786.55204 g/mol
Exact mass: 786.17452 D

appearance: white solid

HRMS (Q-TOF) m/z: $[M+NH4]^+$ Calcd for $C_{33}H_{42}AuIN_3$ 804.2089; found 804.2071 (Δ = -1.6 ppm)

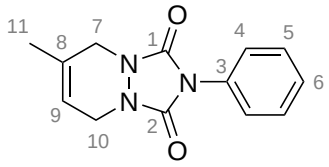
^{1}**H-NMR** (400 MHz, DCM−d_2, 21 °C): δ(ppm) = 8.89 (2H, d, J = 8.7 Hz, *C13-H*), 7.92 (2H, m, *C10-H*), 7.89 (2H, m, *C8-H*), 7.72 (2H, dd, J = 7.4 Hz, 1.0 Hz, *C6-H*), 7.66 (2H, ddd, J = 8.7 Hz, 6.9 Hz, 1.4 Hz, *C12-H*), 7.56 (2H, ddd, J = 8.0 Hz, 6.9 Hz, 1.0 Hz, *C11-H*), 7.49 (2H, dd, J = 8.0 Hz, 7.4 Hz, *C7-H*), 6.65 (2H, s, *C3-H*), 3.68 (2H, m, *C2-**H**H*), 3.13 (2H, m, *C2-H**H***), 1.12 (18H, s, *C15-H_3*)

^{13}**C-NMR** (100 MHz, DCM−d_2, 21 °C): δ(ppm) = 206.1 (Cq, *C1*), 134.8 (Ar−Cq, *C9*), 132.8 (Ar−Cq, *C14*), 132.1 (Ar−Cq, *C5*), 129.4 (Ar−H, *C10*), 129.3 (Ar−H, *C8*), 127.6 (Ar−H, *C12*), 127.2 (Ar−H, *C6*), 126.4 (Ar−H, *C11*), 124.6 (Ar−H, *C13*), 124.5 (Ar−H, *C7*), 65.7 (CH, *C3*), 48.1 (CH_2, *C2*), 37.5 (Cq, *C4*), 29.1 (CH_3, *C15*)

HSQC : 8.89 x 124.6, 7.92 x 129.4, 7.89 x 129.3, 7.72 x 127.2, 7.66 x 127.6, 7.56 x 126.4, 7.49 x 124.5, 6.65 x 65.7, 3.68 x 48.1, 3.13 x 48.1, 1.12 x 29.1

IR: $\nu_{max}(cm^{-1})$: 3043.6(w), 2956.5(w), 1598.1(w), 1486.3(m), 1447.6(m), 1269.1(s), 803.9(m), 782.3(s), 736.6(m)

3.51 40: PTAD-isoprene adduct



Formula: $C_{13}H_{13}N_3O_2$
Molecular weight: 243.266 g/mol
Exact mass: 243.10078 D

appearance: white solid

$[M]^+$ Calcd for $C_{13}H_{13}N_3O_2$ 243.1; found 243.1

$\mathbf{R}_f$: 0.26 (30% EtOAc in pentane)

^{1}**H-NMR** (400 MHz, $CDCl_3$, 21 °C): δ(ppm) = 7.52 (2H, m, *C4-H*), 7.47 (2H, m, *C5-H*), 7.36 (1H, m, *C6-H*), 5.63 (1H, oct, J = 1.6 Hz, *C9-H*), 4.13 (2H, m, *C10-*H_2), 4.04 (2H, m, *C7-*H_2), 1.86 (3H, s(br), *C11-*H_3)

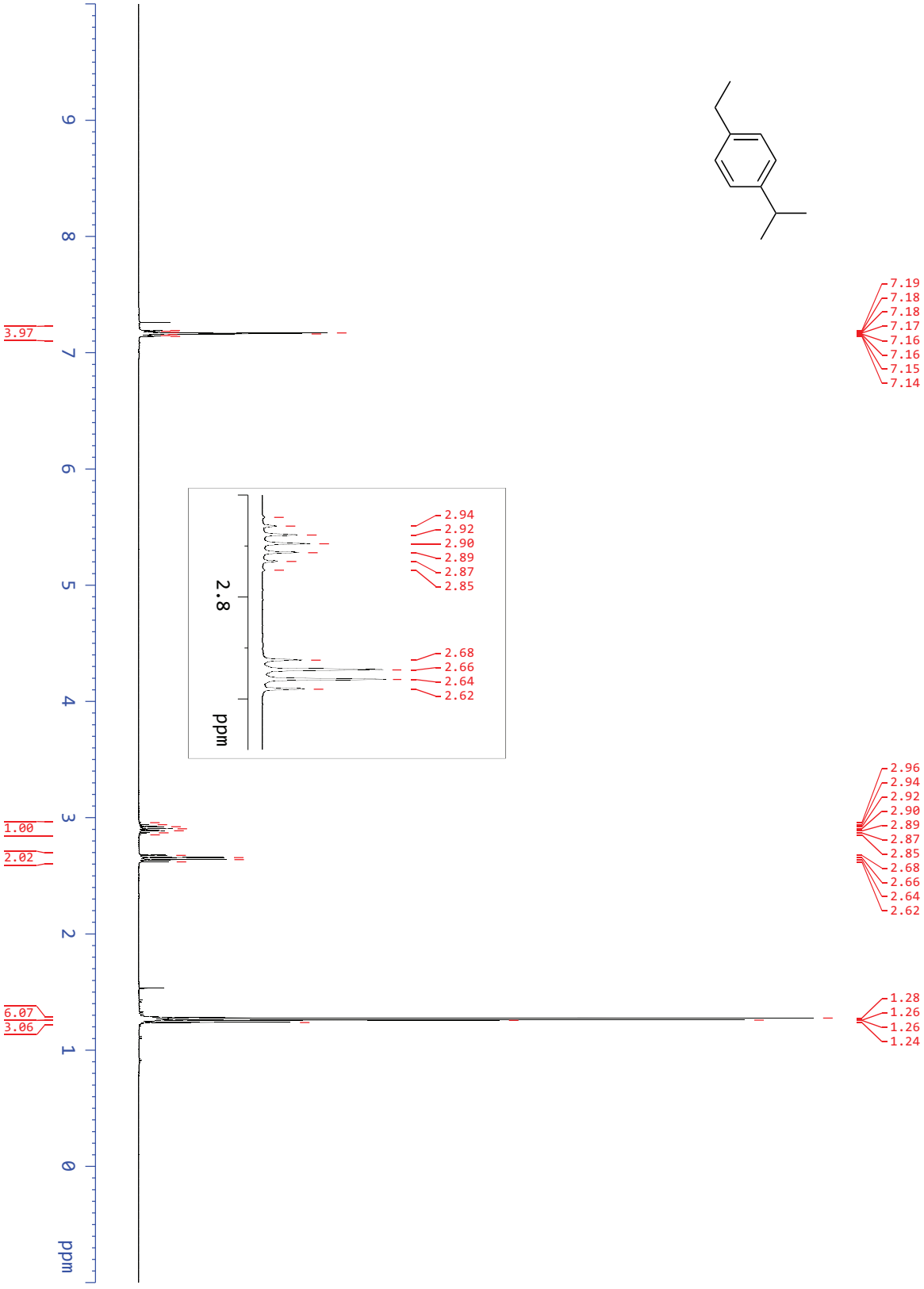
^{13}**C-NMR** (100 MHz, $CDCl_3$, 21 °C): δ(ppm) = 152.5 (C=O, *C1/C2*), 152.3 (C=O, *C1/C2*), 131.3 (Ar−Cq, *C3*), 129.3 (Ar−CH, *C5*), 129.0 (Cq, *C8*), 128.2 (Ar−CH, *C6*), 125.5 (Ar−CH, *C4*), 115.1 (CH, *C9*), 46.7 (CH_2, *C7*), 43.3 (CH_2, *C10*), 20.3 (CH_3, *C11*)

HSQC : 7.52 x 125.5, 7.47 x 129.3, 7.36 x 128.2, 5.63 x 115.1, 4.13 x 43.3, 4.04 x 46.7, 1.86 x 20.3

4 Copies of NMR spectra

4.1 2a: 1-ethyl-4-isopropylbenzene

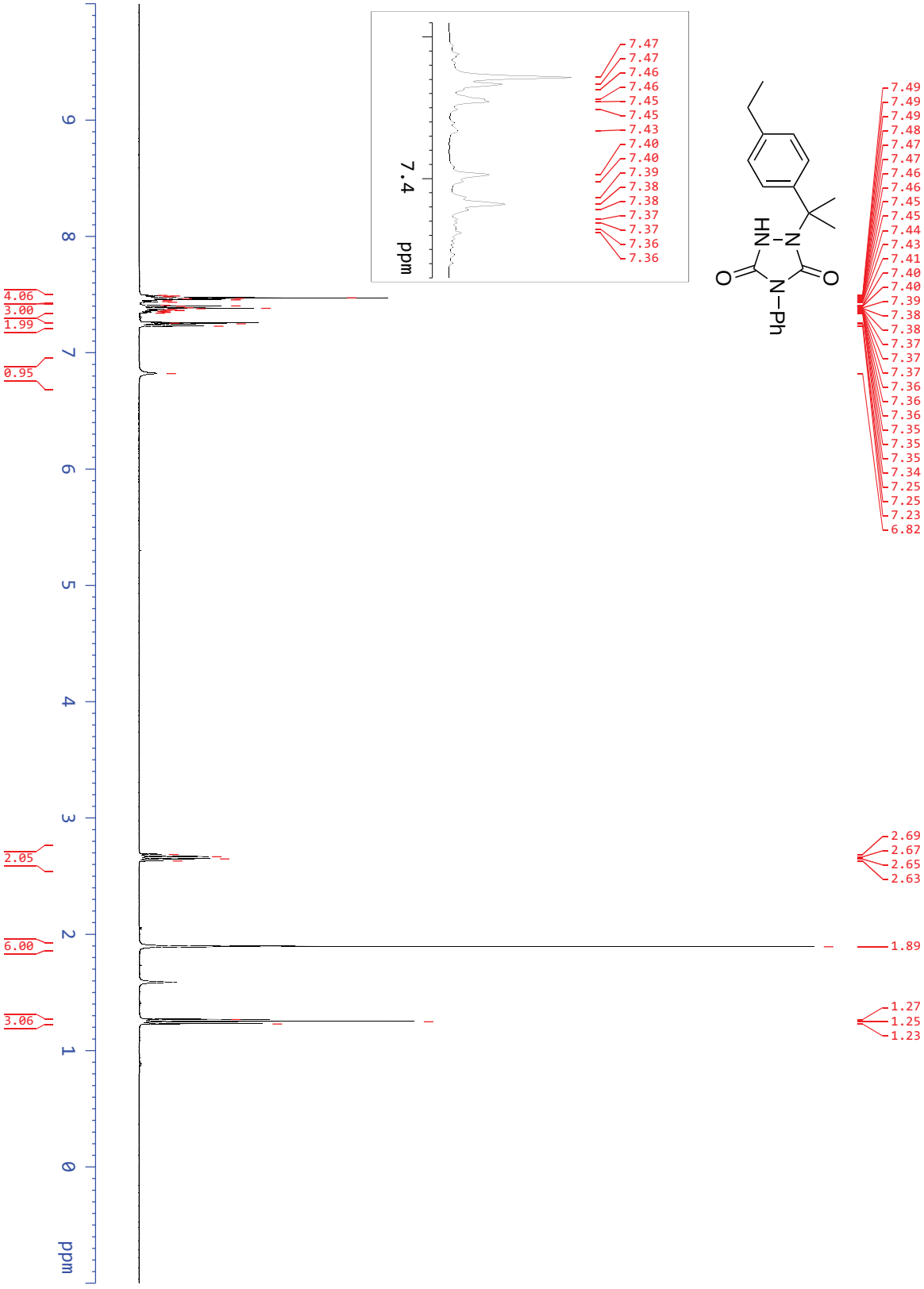
^{1}H-NMR (400 MHz, $CDCl_3$)



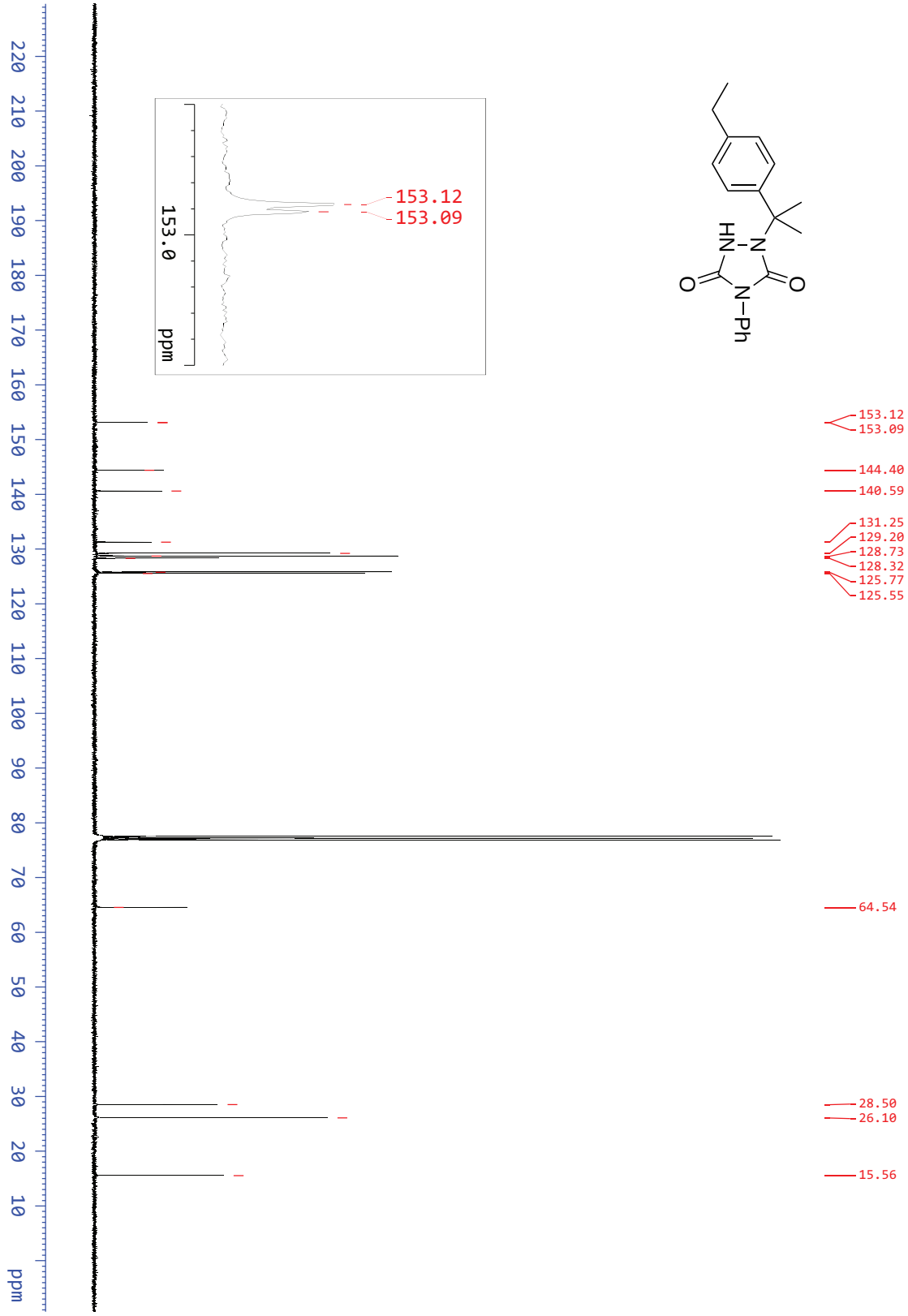
$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

4.2 2b: 1-(2-(4-ethylphenyl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)



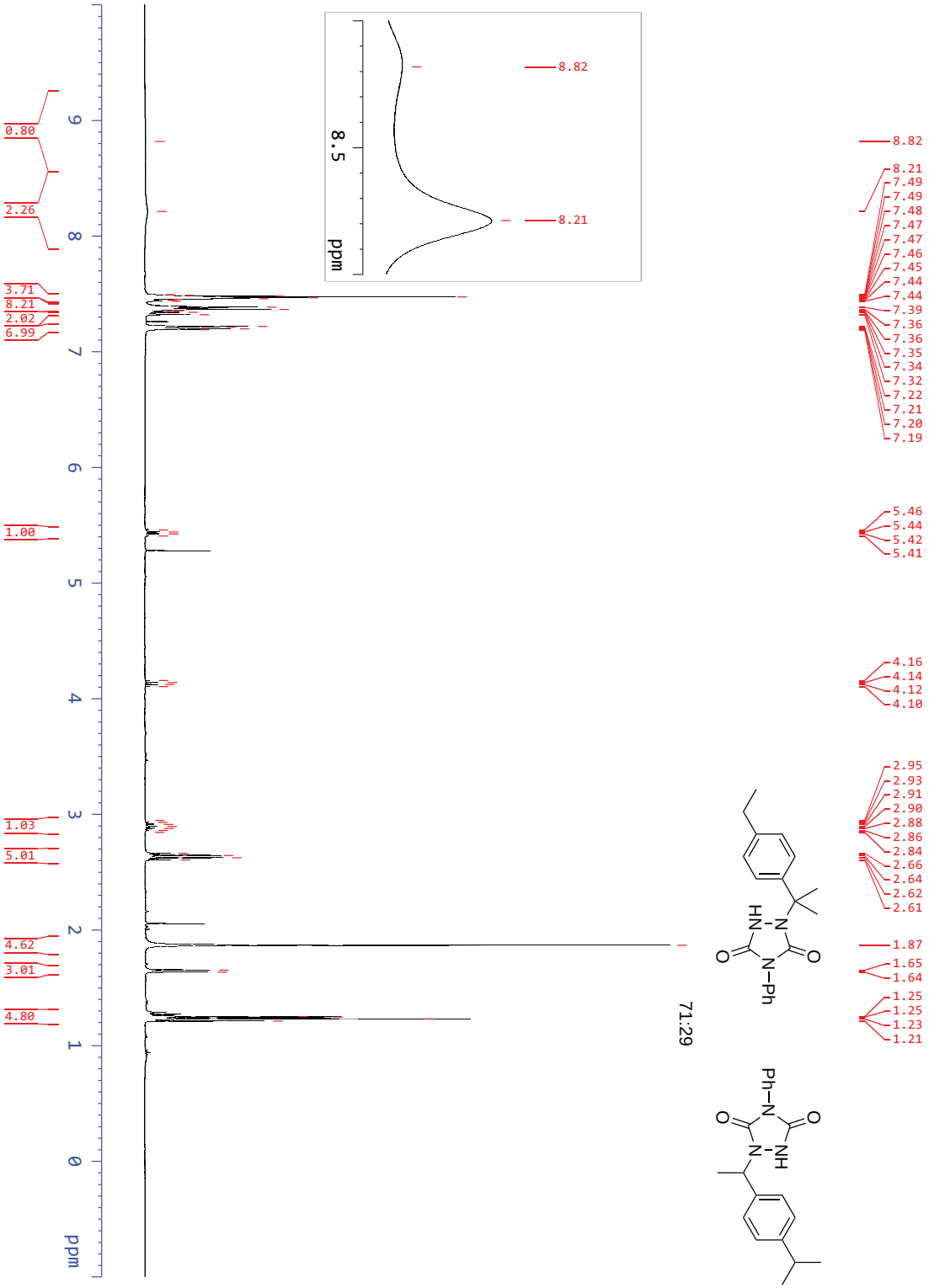
$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)



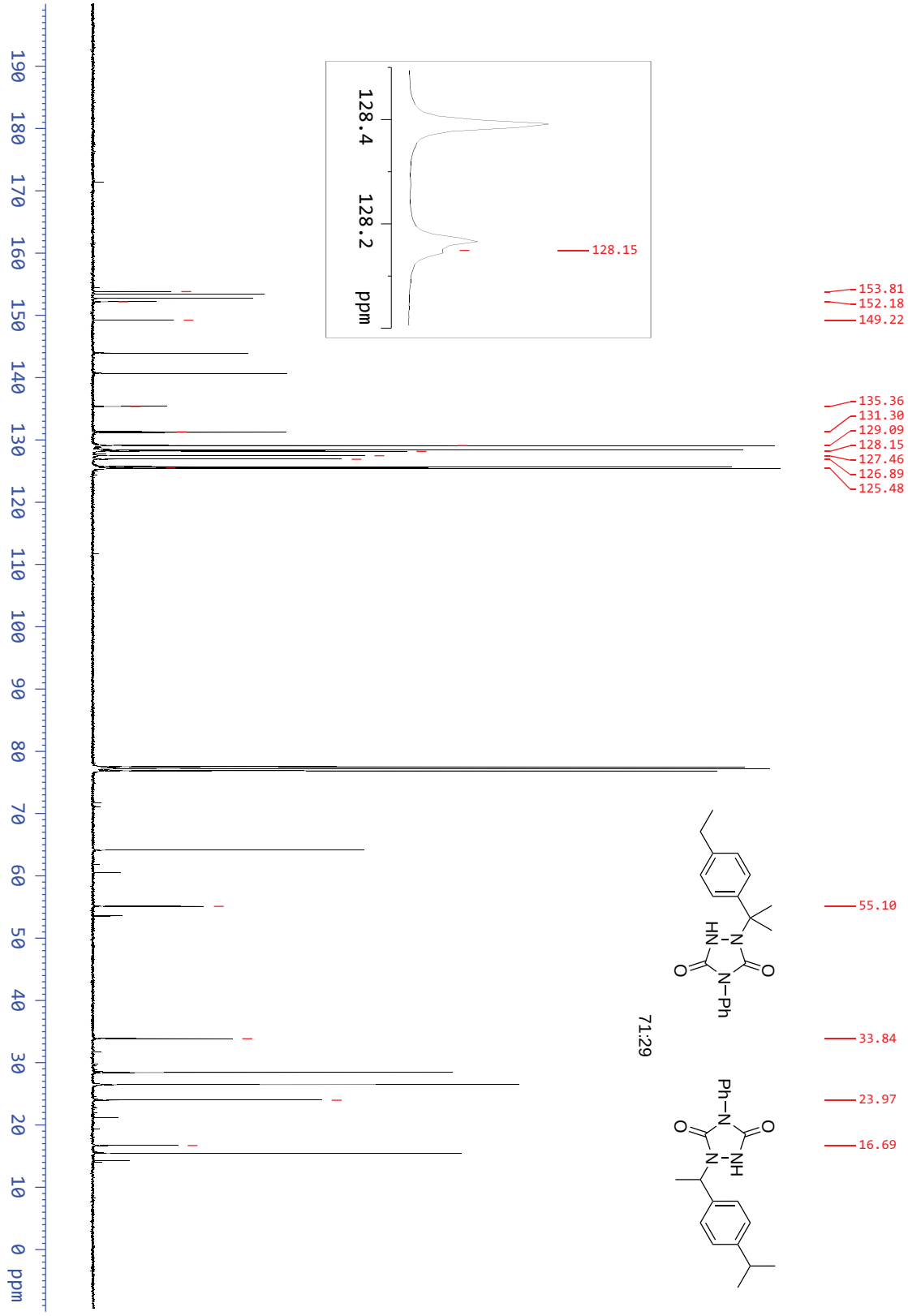
4.3 2c: 1-(1-(4-isopropylphenyl)ethyl)-4-phenyl-urazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **2b** and **2c** in a 71:29 ratio*

^{1}H-NMR (400 MHz, $CDCl_3$ + residual DCM)

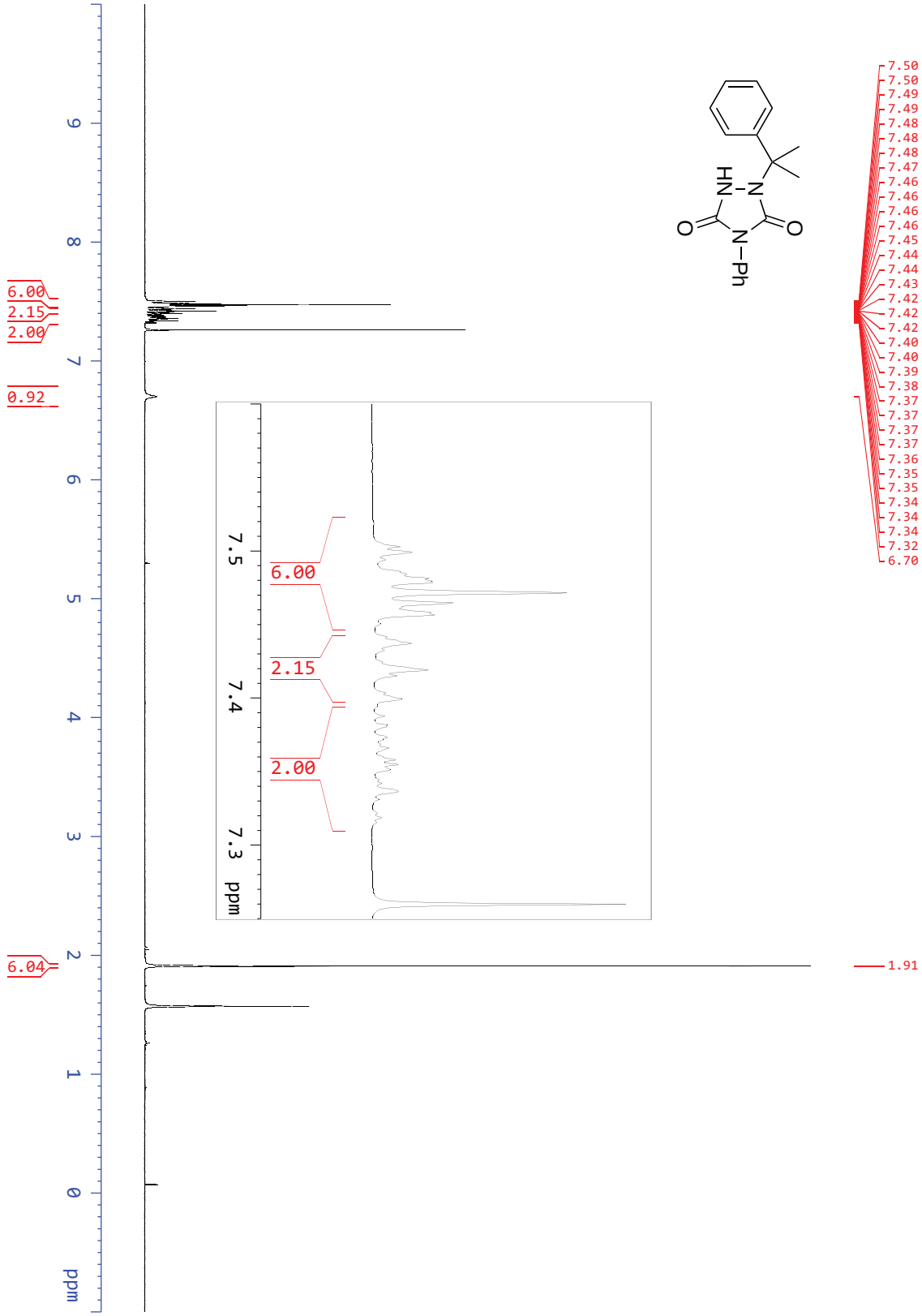


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

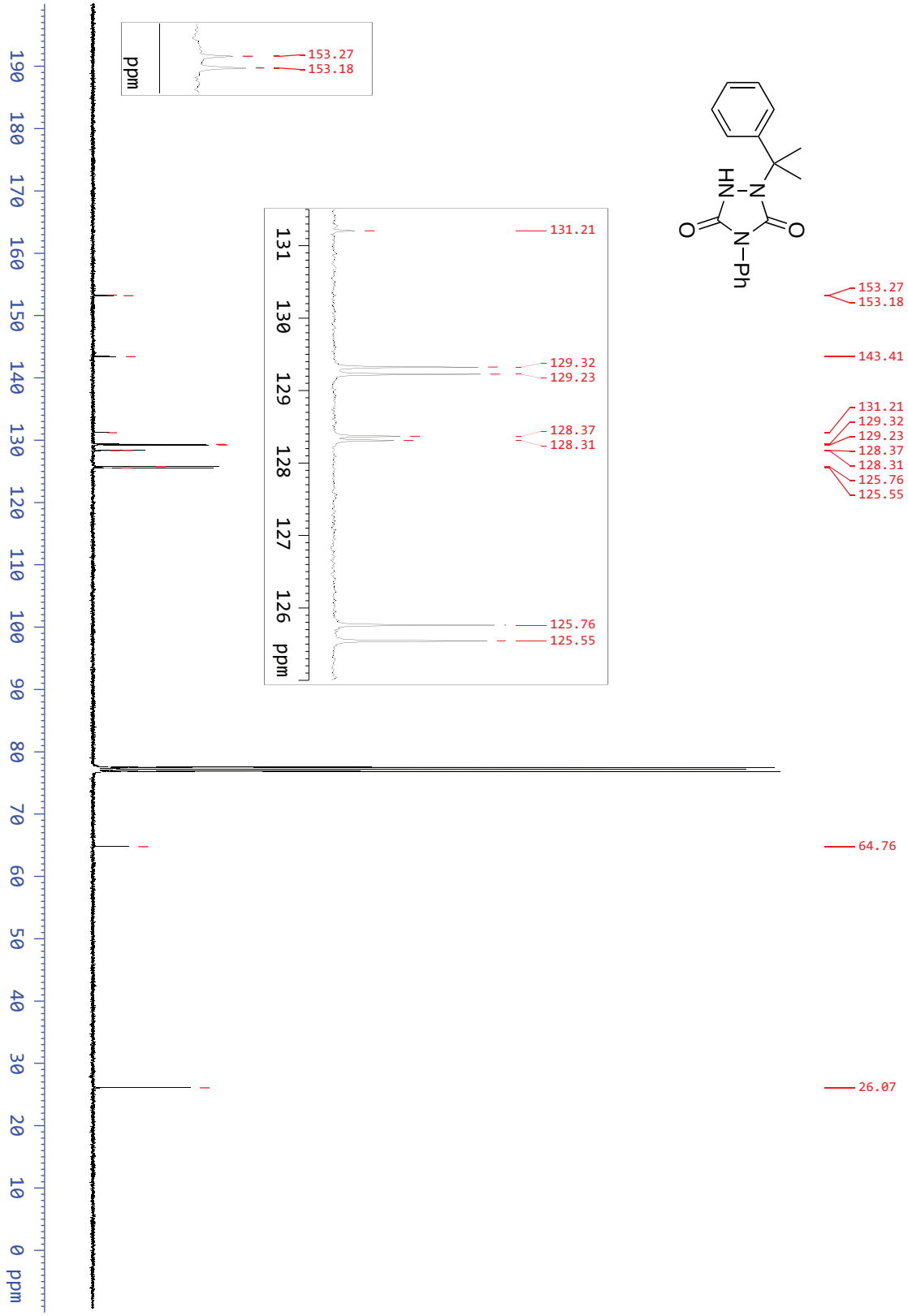


4.4 3b: 4-phenyl-1-(2-phenylpropan-2-yl)-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

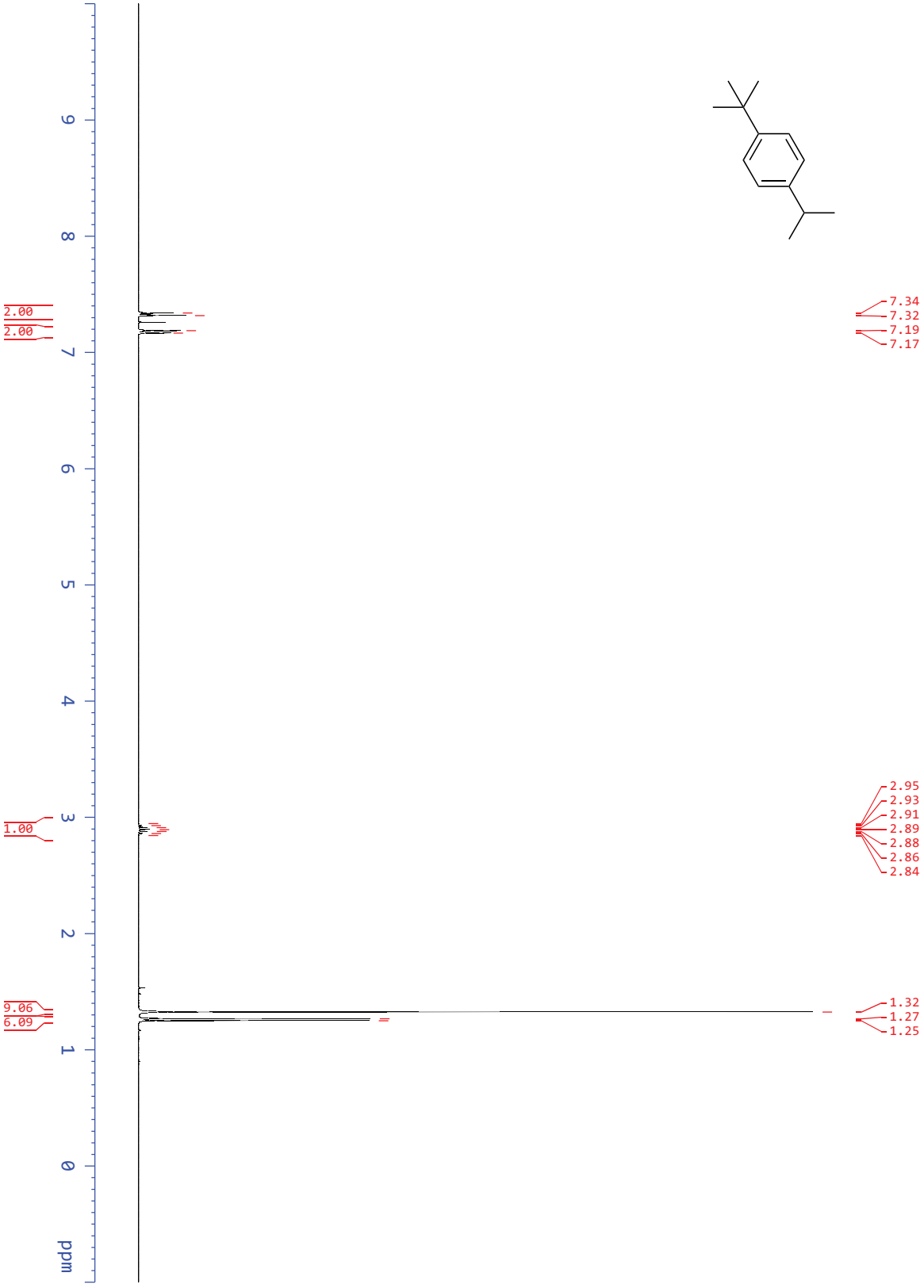


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

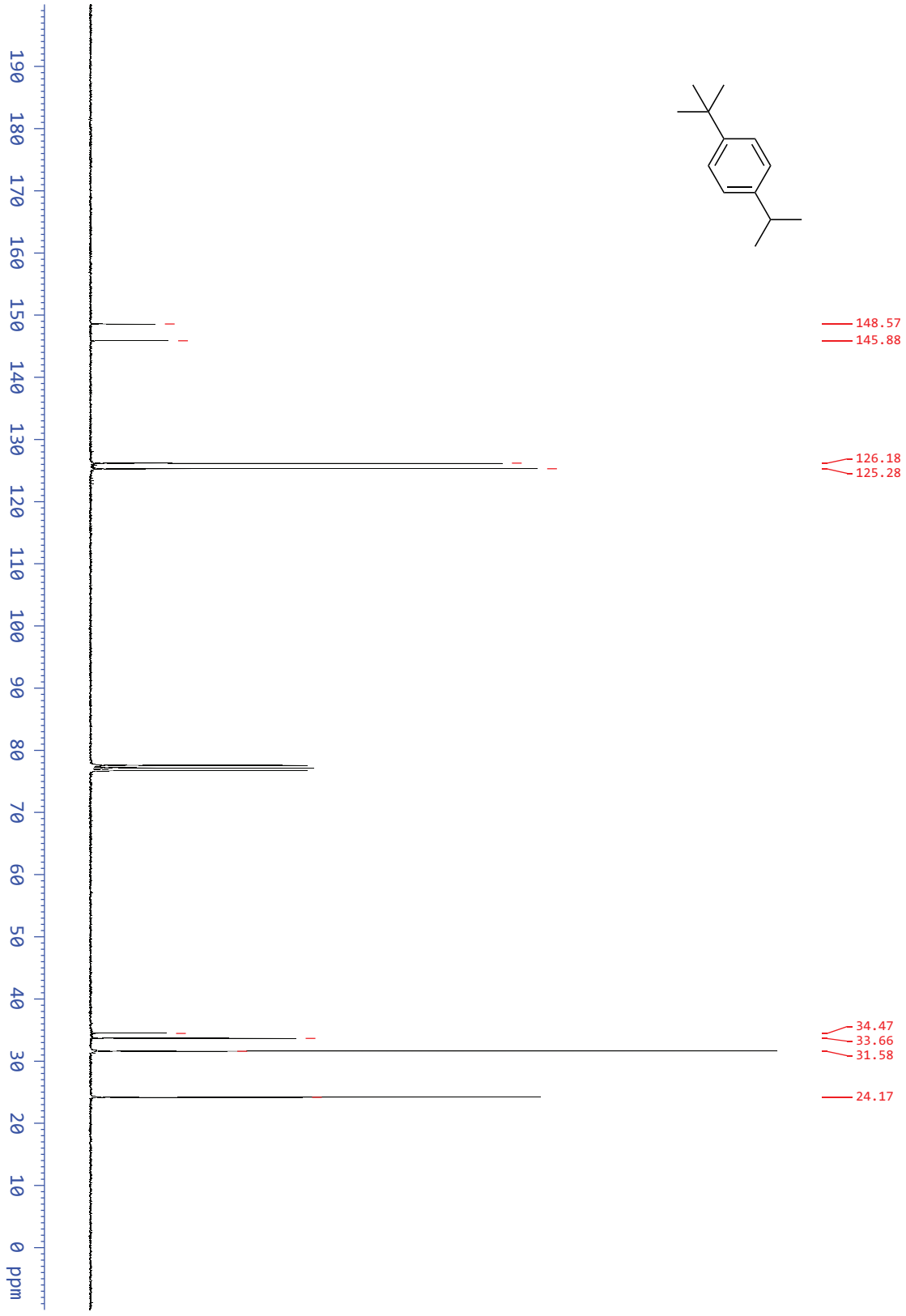


4.5 4a: 1-(tert-butyl)-4-isopropylbenzene

^{1}H-NMR (400 MHz, $CDCl_3$)

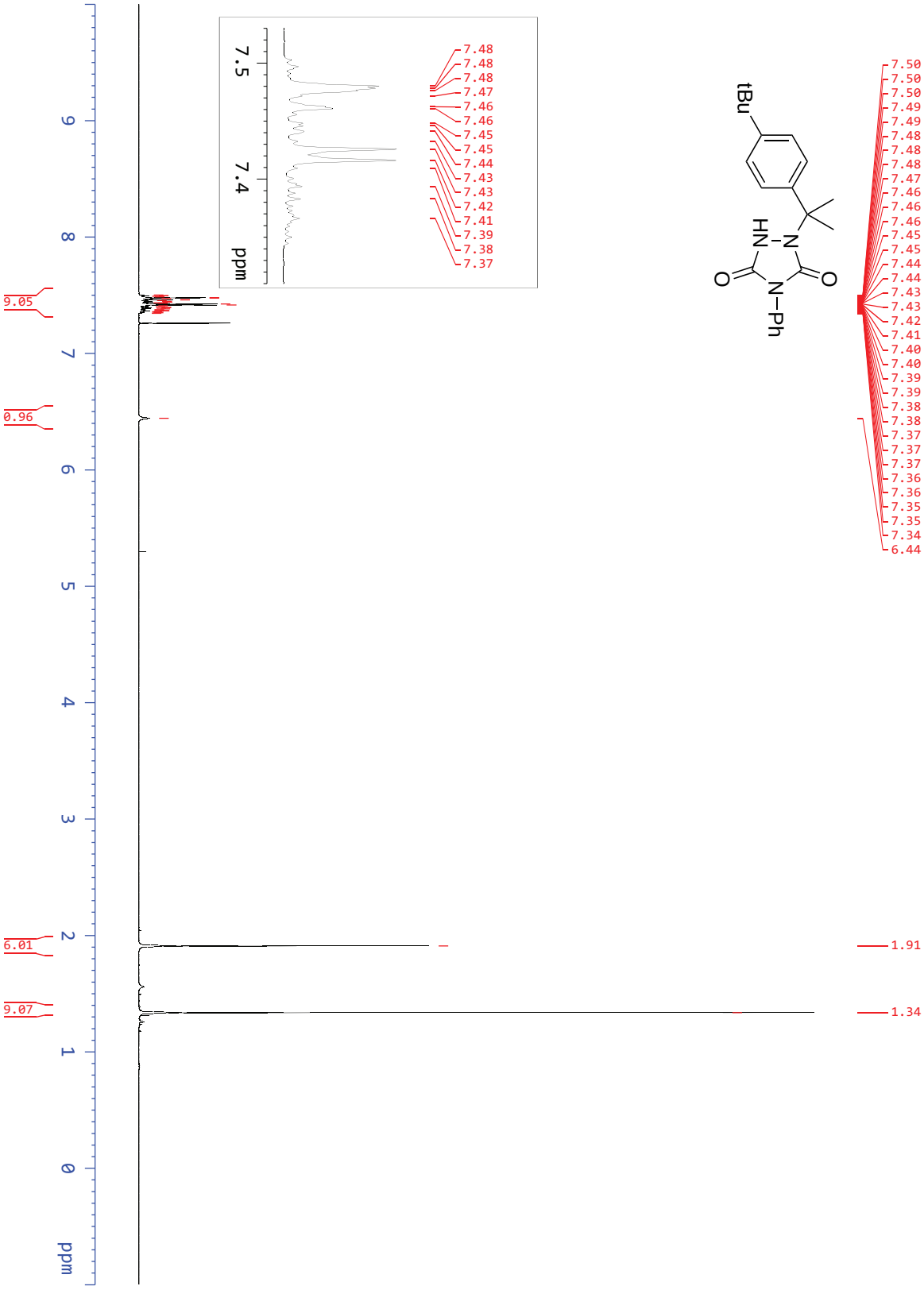


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

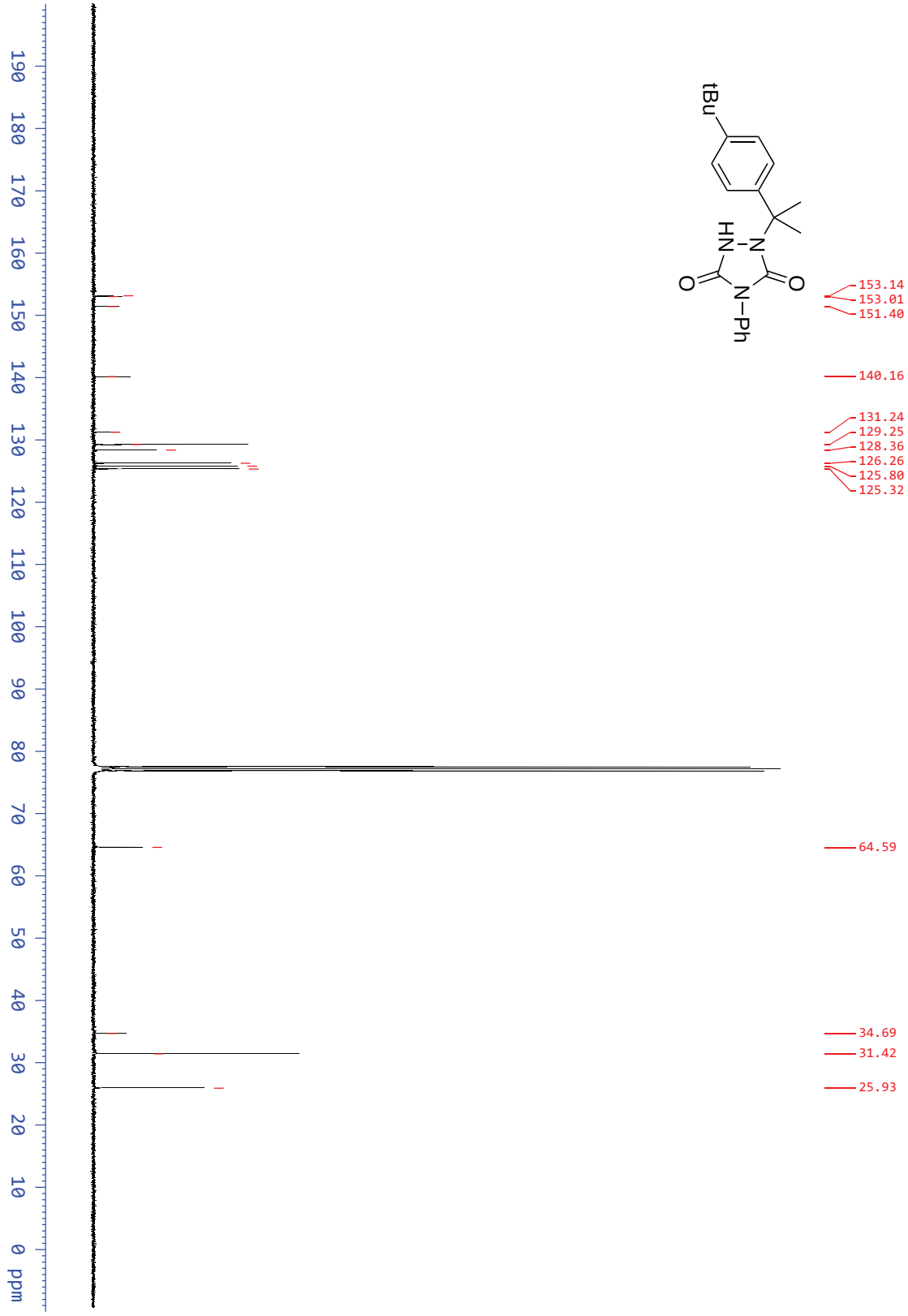


4.6 4b: 1-(2-(4-(tert-butyl)phenyl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

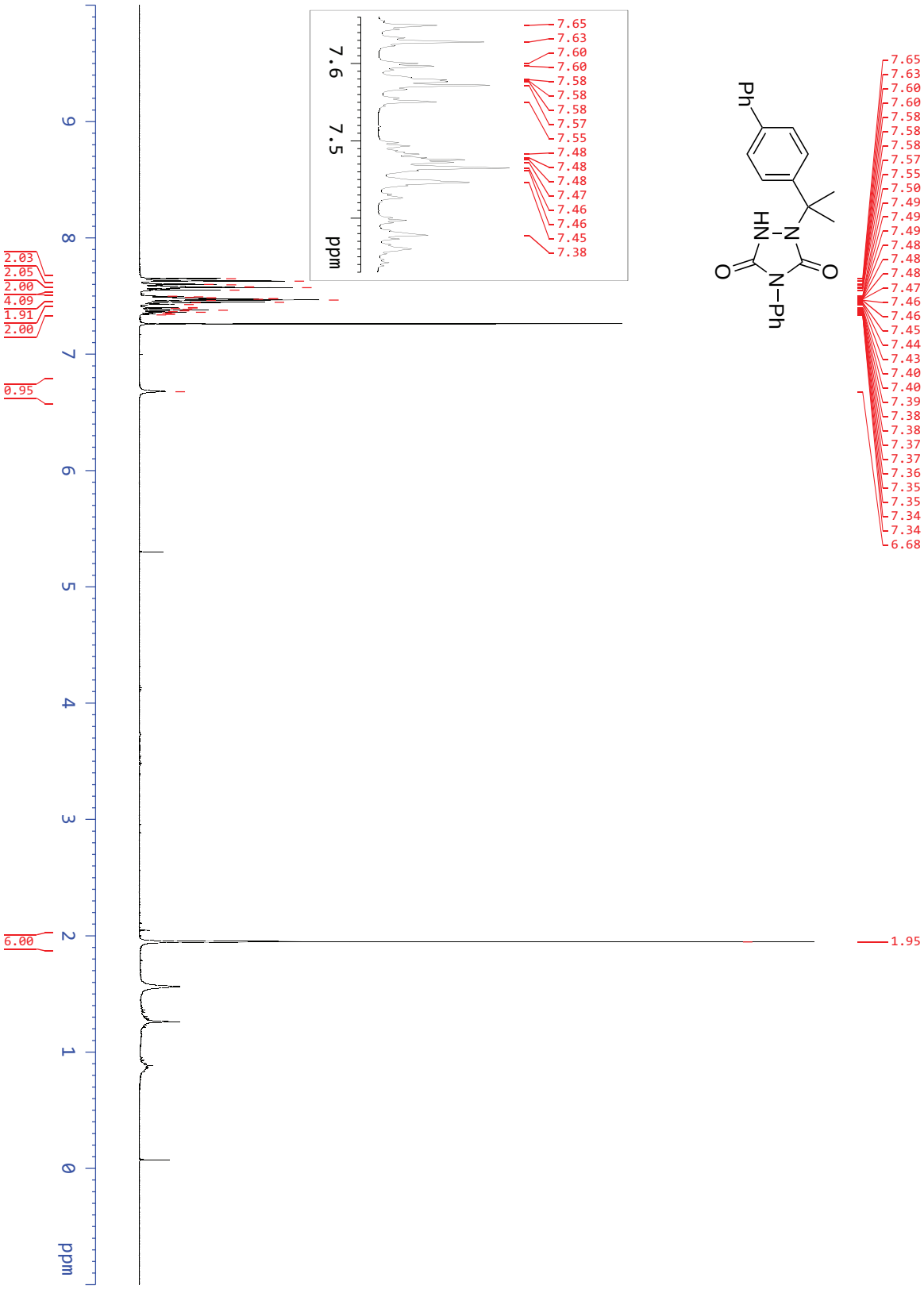


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

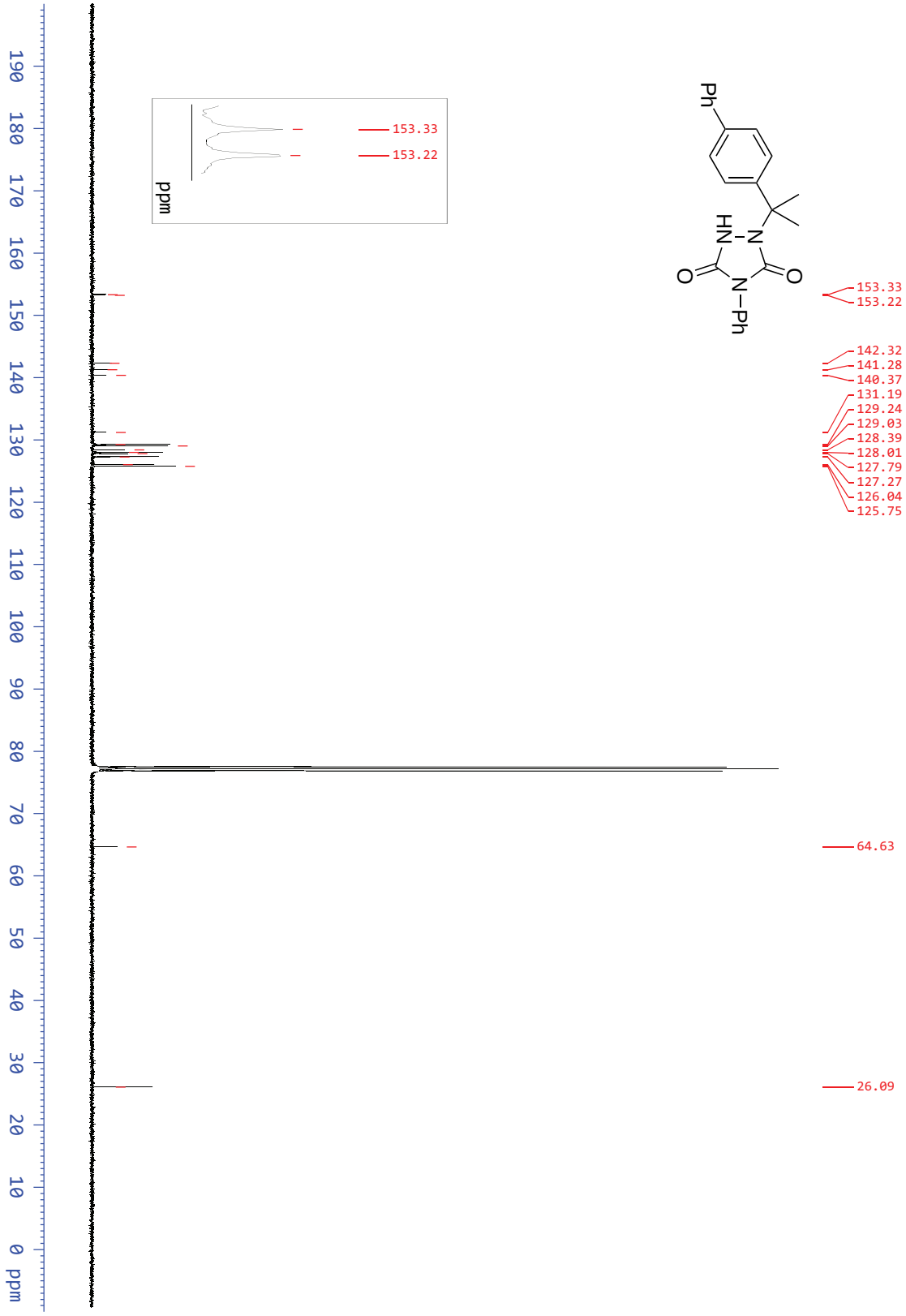


4.7 5b: 1-(2-([1,1'-biphenyl]-4-yl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$ + residual DCM)

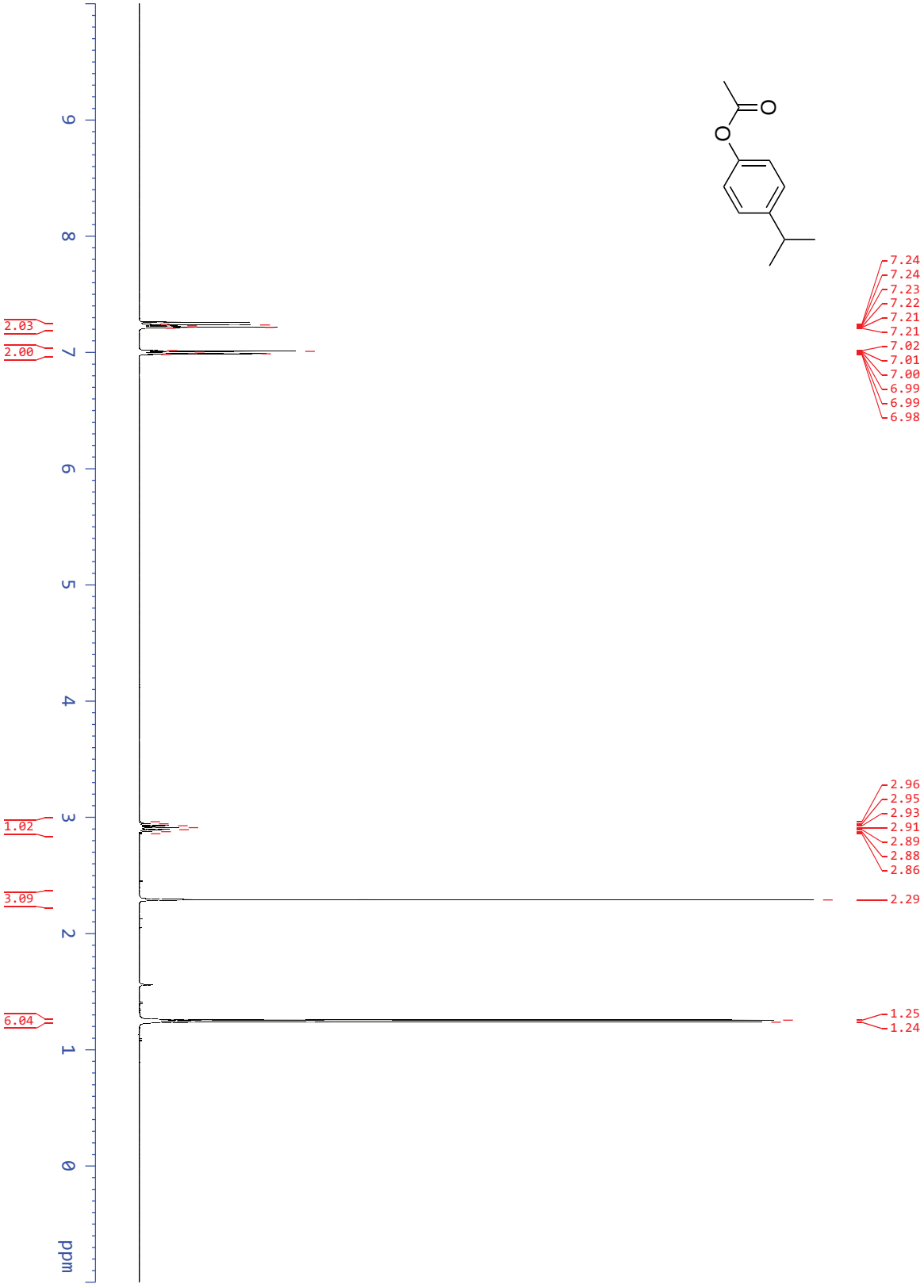


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

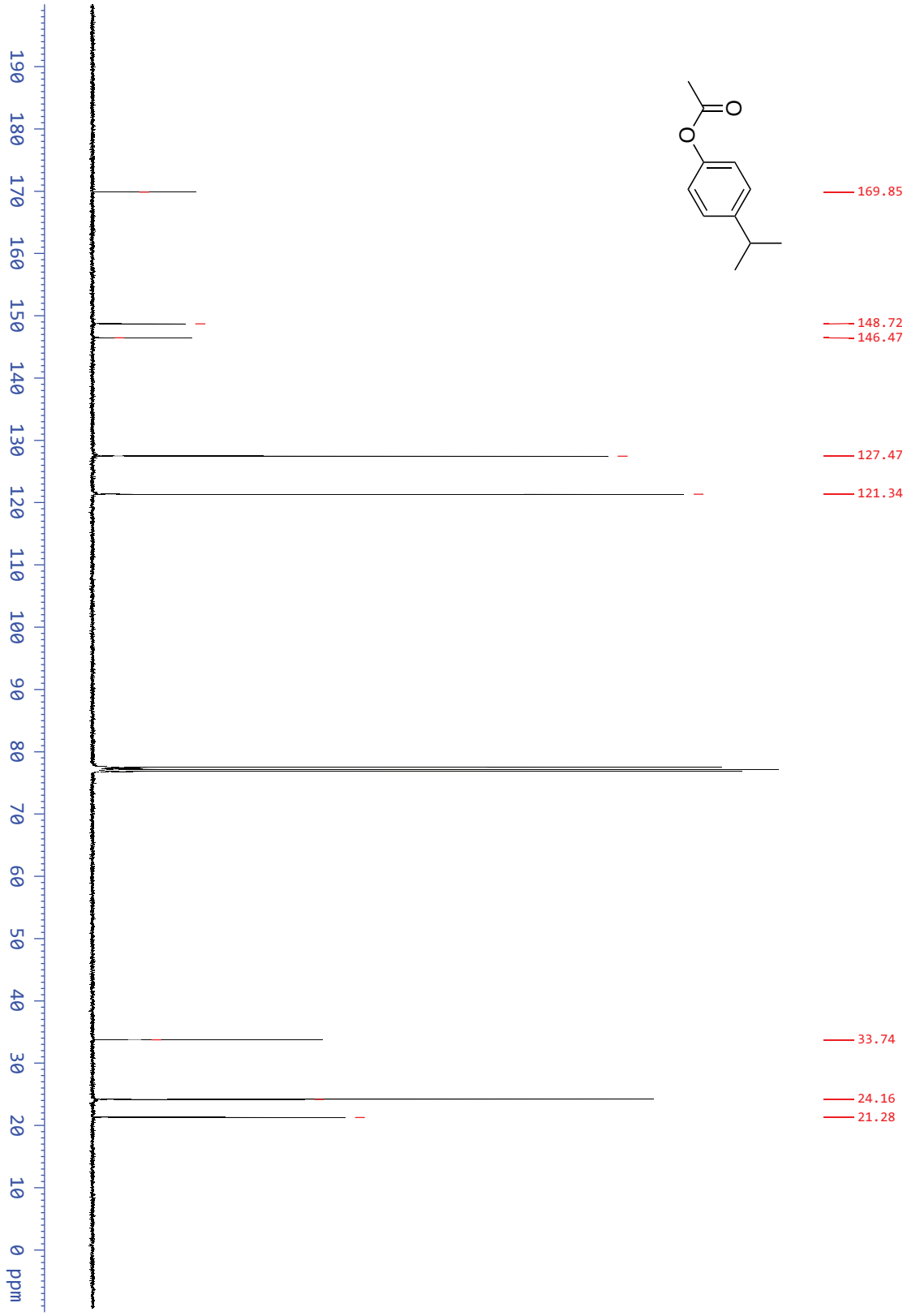


4.8 6a: 4-isopropylphenyl acetate

^{1}H-NMR (400 MHz, $CDCl_3$)

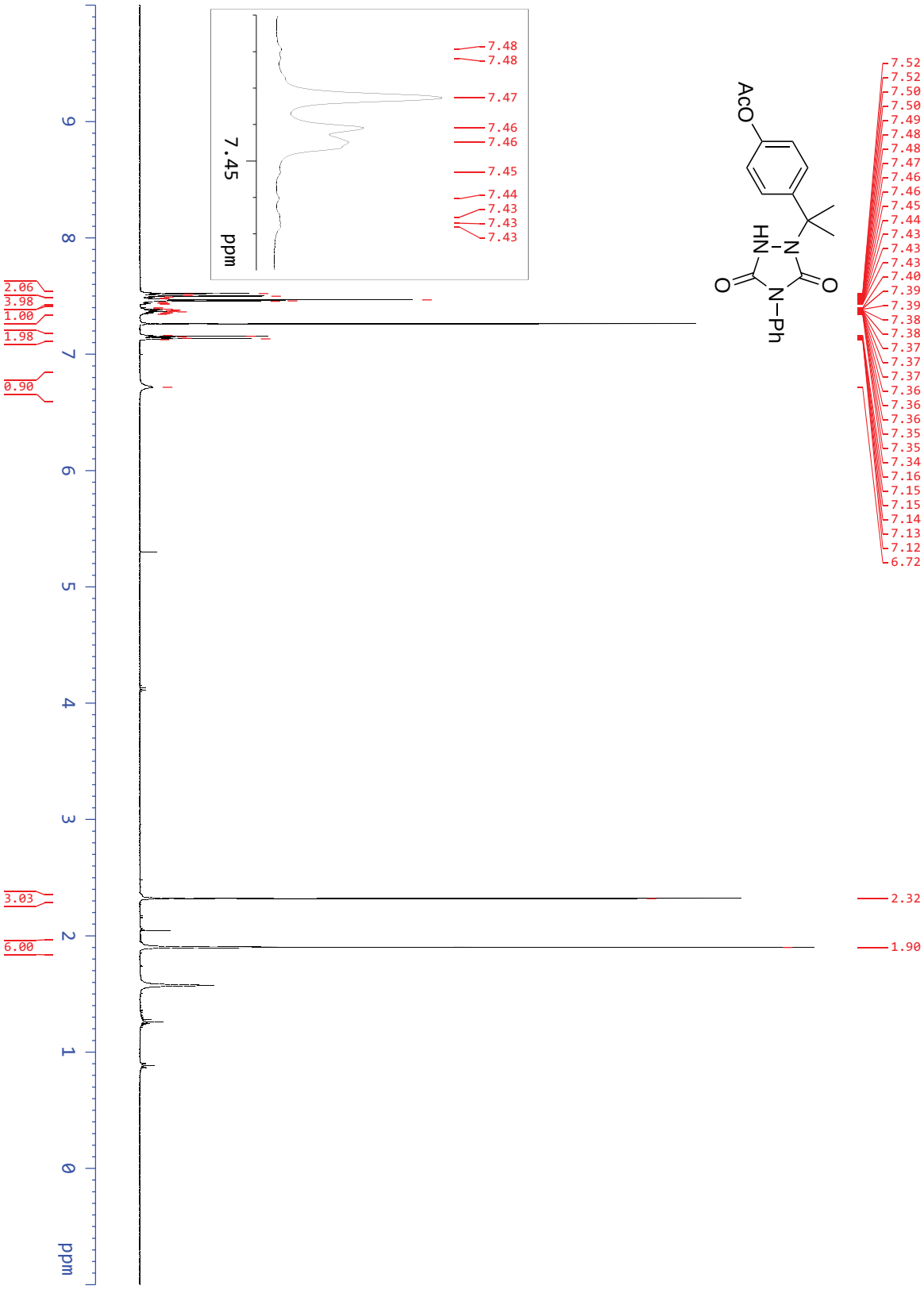


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

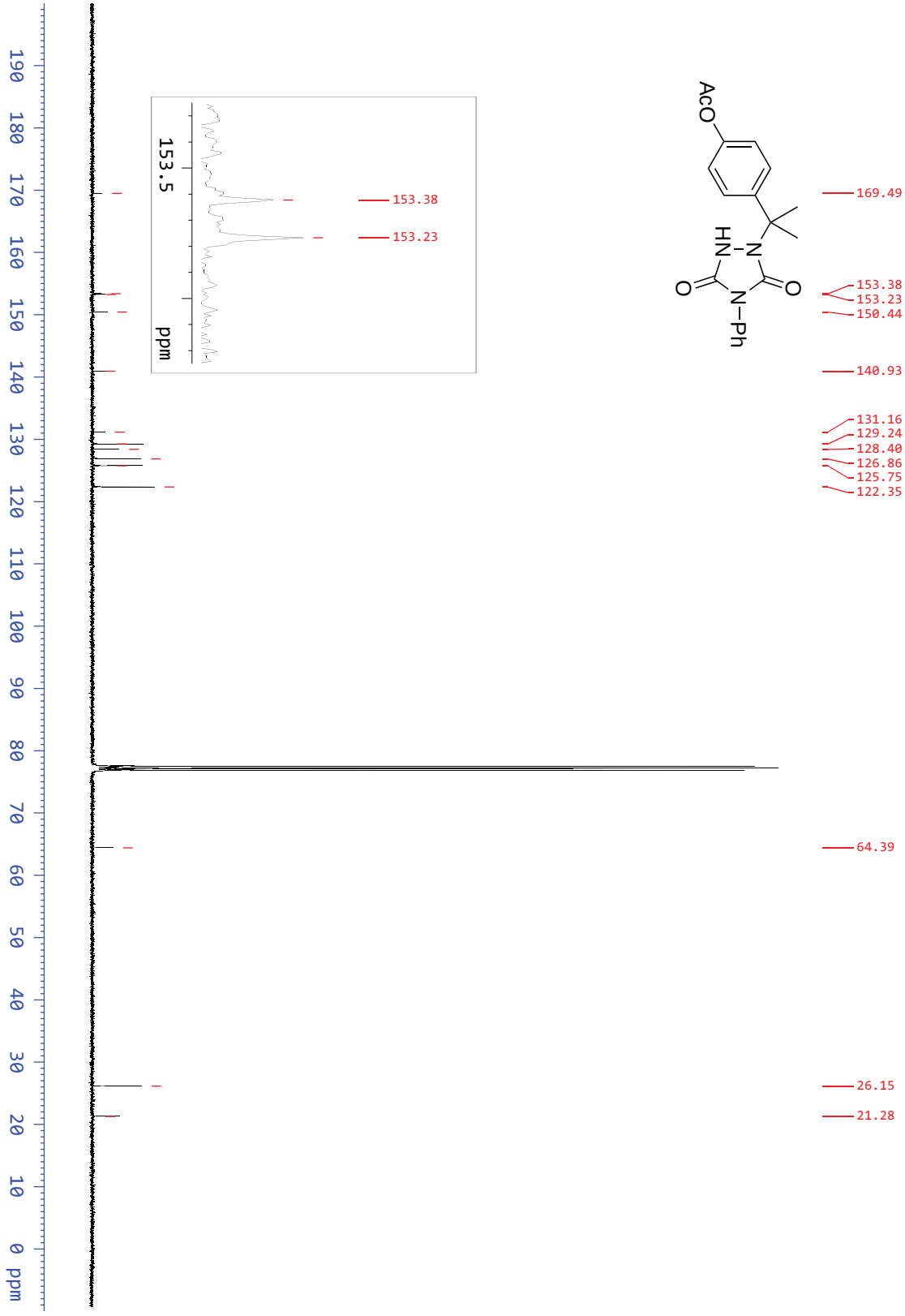


4.9 6b: 4-(2-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-propan-2-yl)phenyl acetate

^{1}H-NMR (400 MHz, $CDCl_3$)

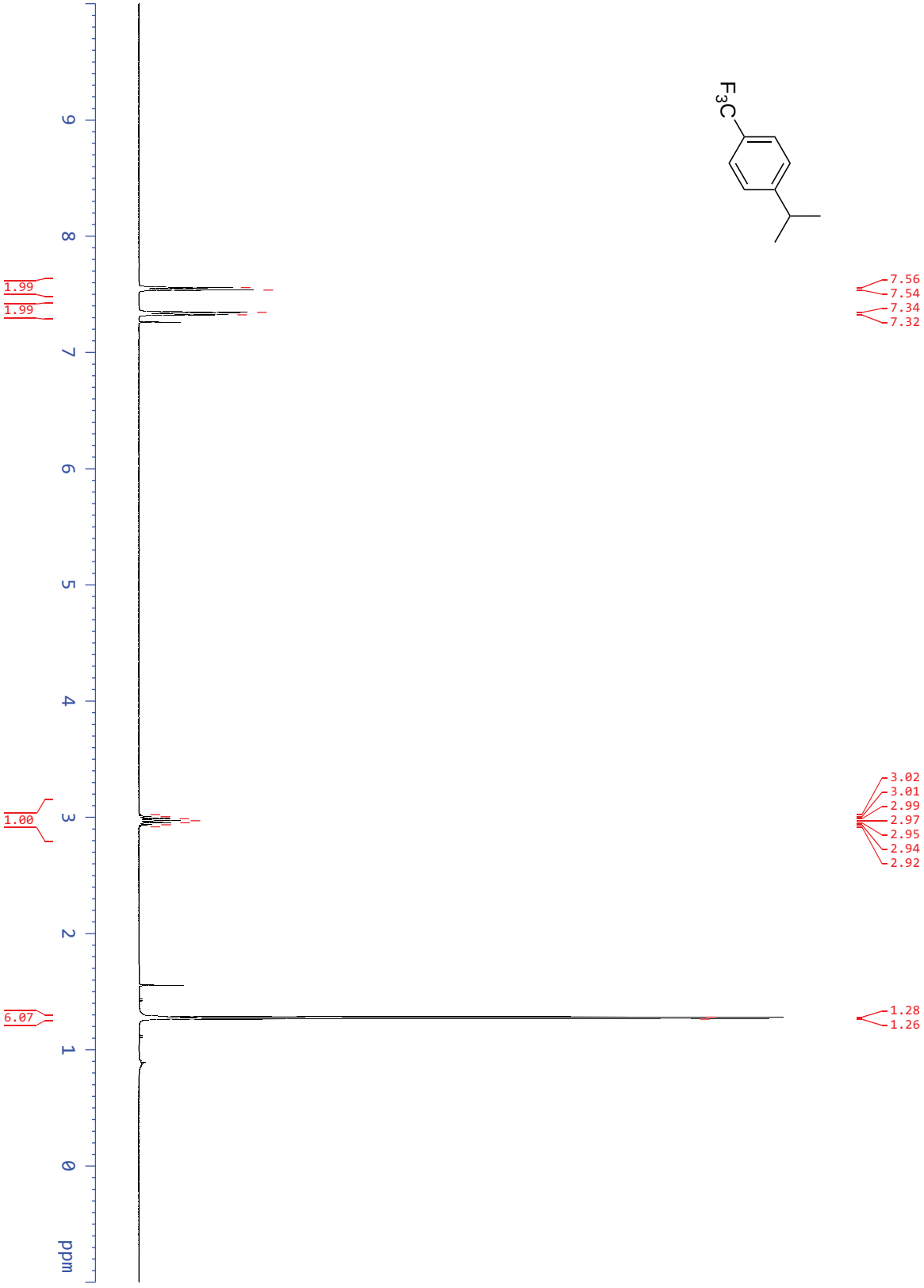


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

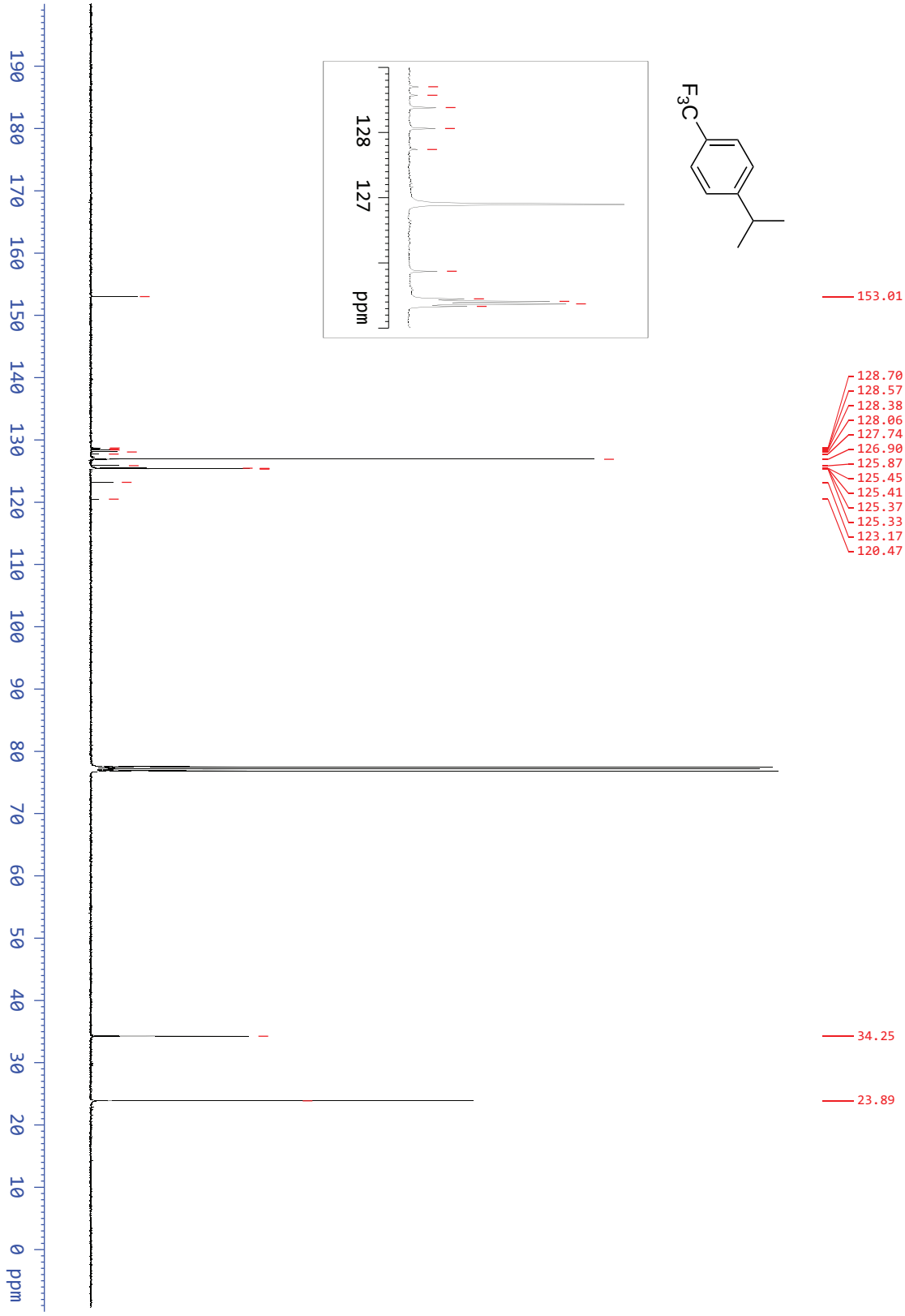


4.10 7a: 4-trifluoromethylcumene

^{1}H-NMR (400 MHz, $CDCl_3$)

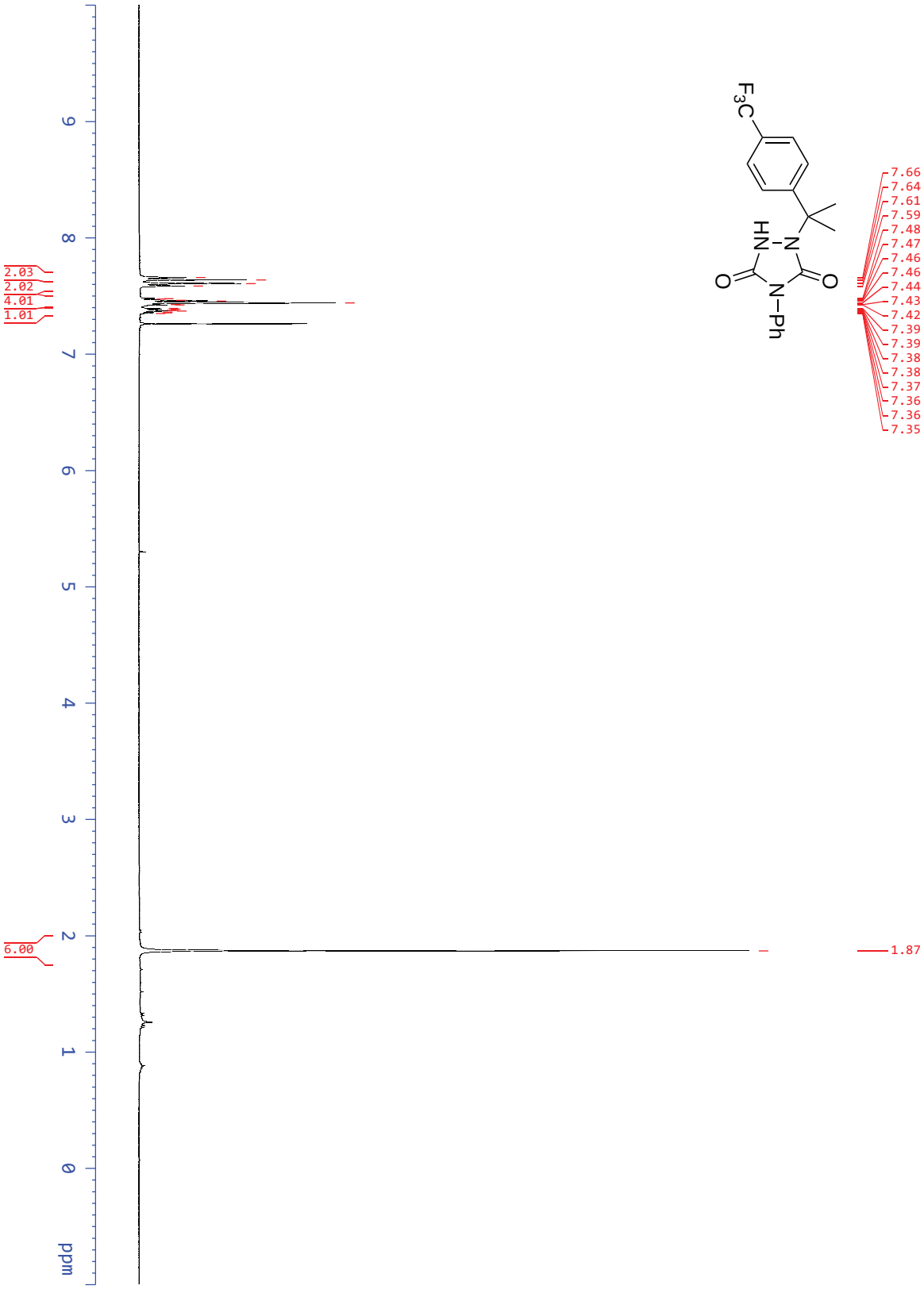


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

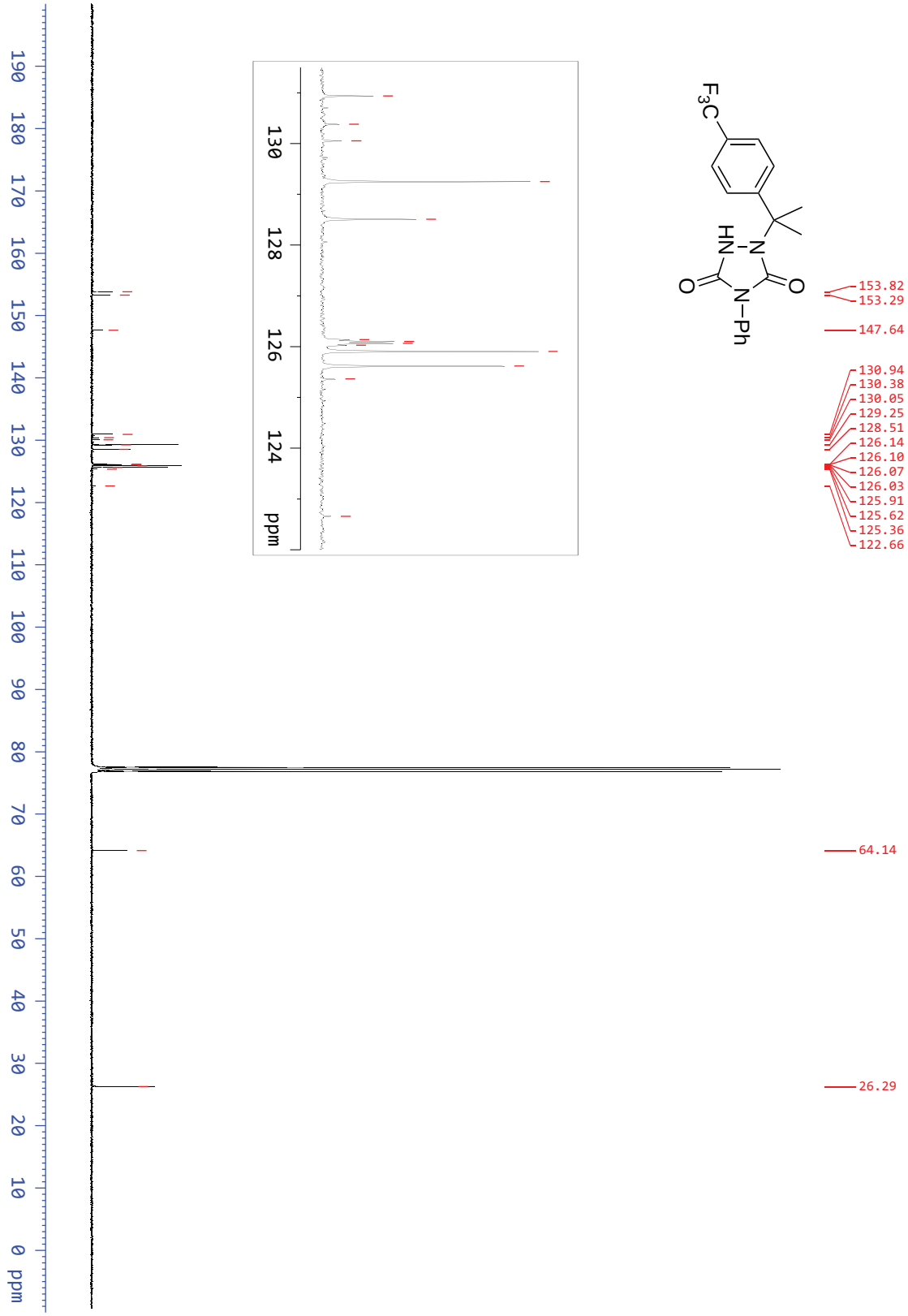


4.11 7b: 1-(2-(4-trifluoromethylphenyl)propan-2-yl)--4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

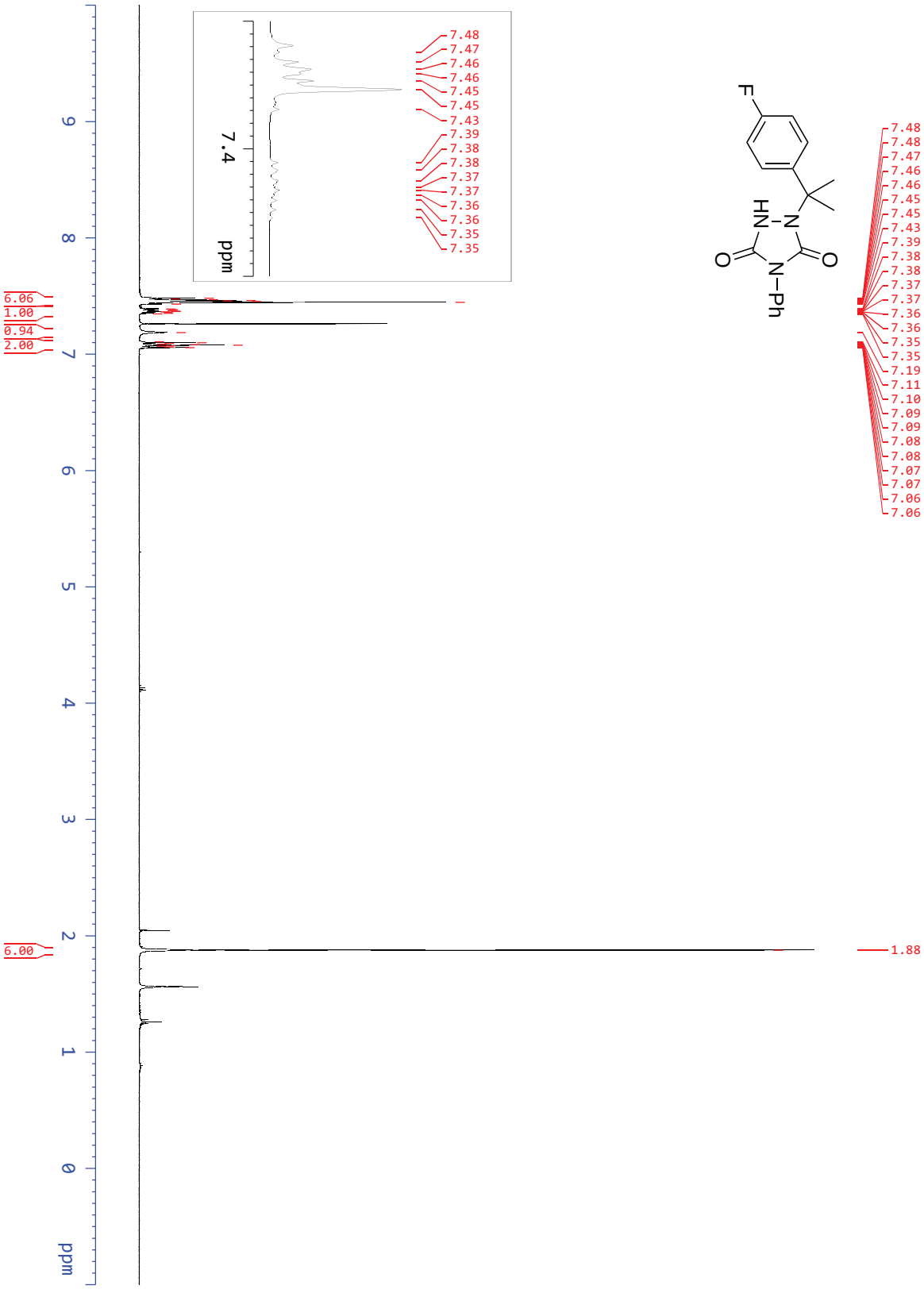


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

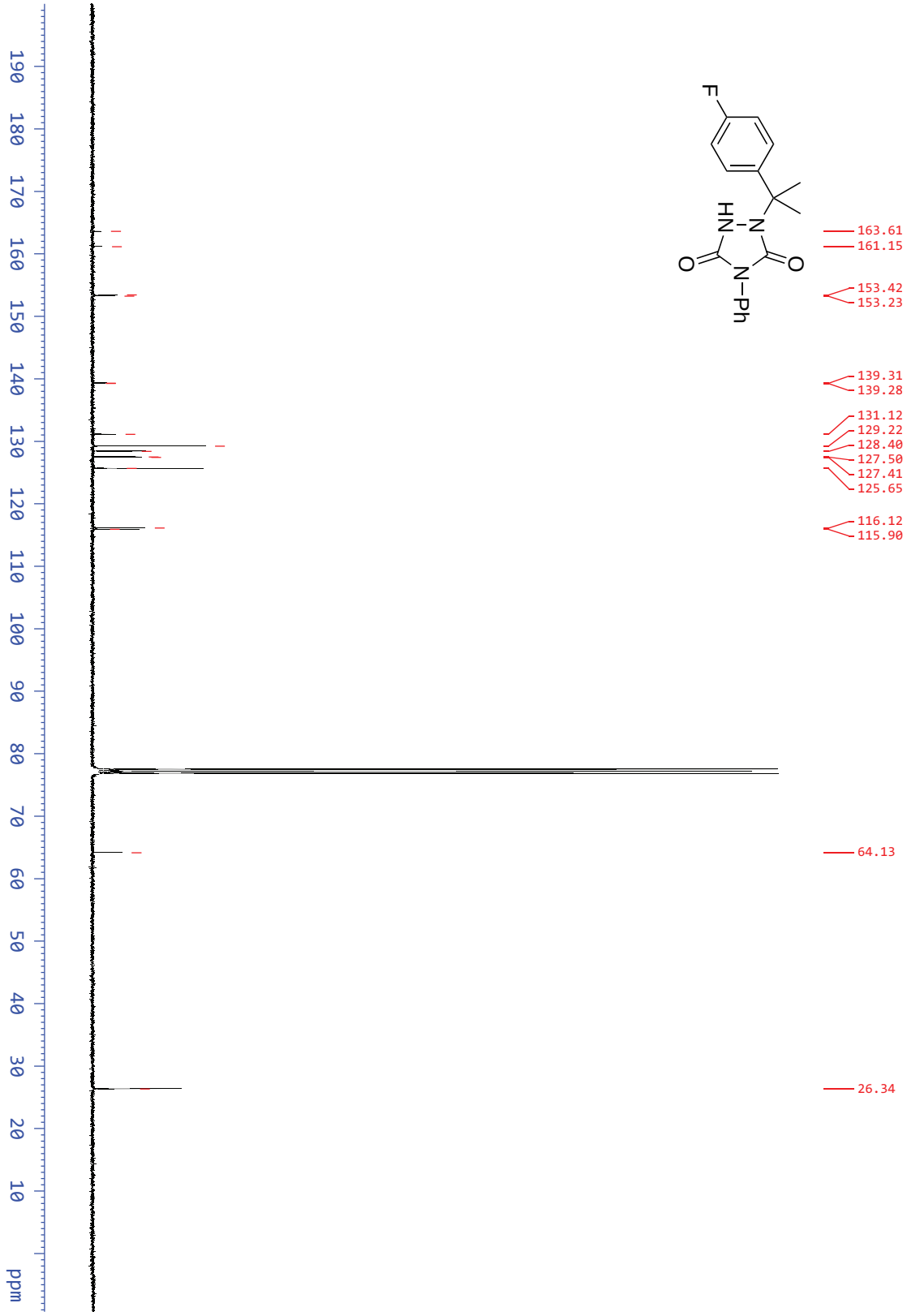


4.12 8b: 1-(2-(4-fluorophenyl)propan-2-yl)-4-phenyl--urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

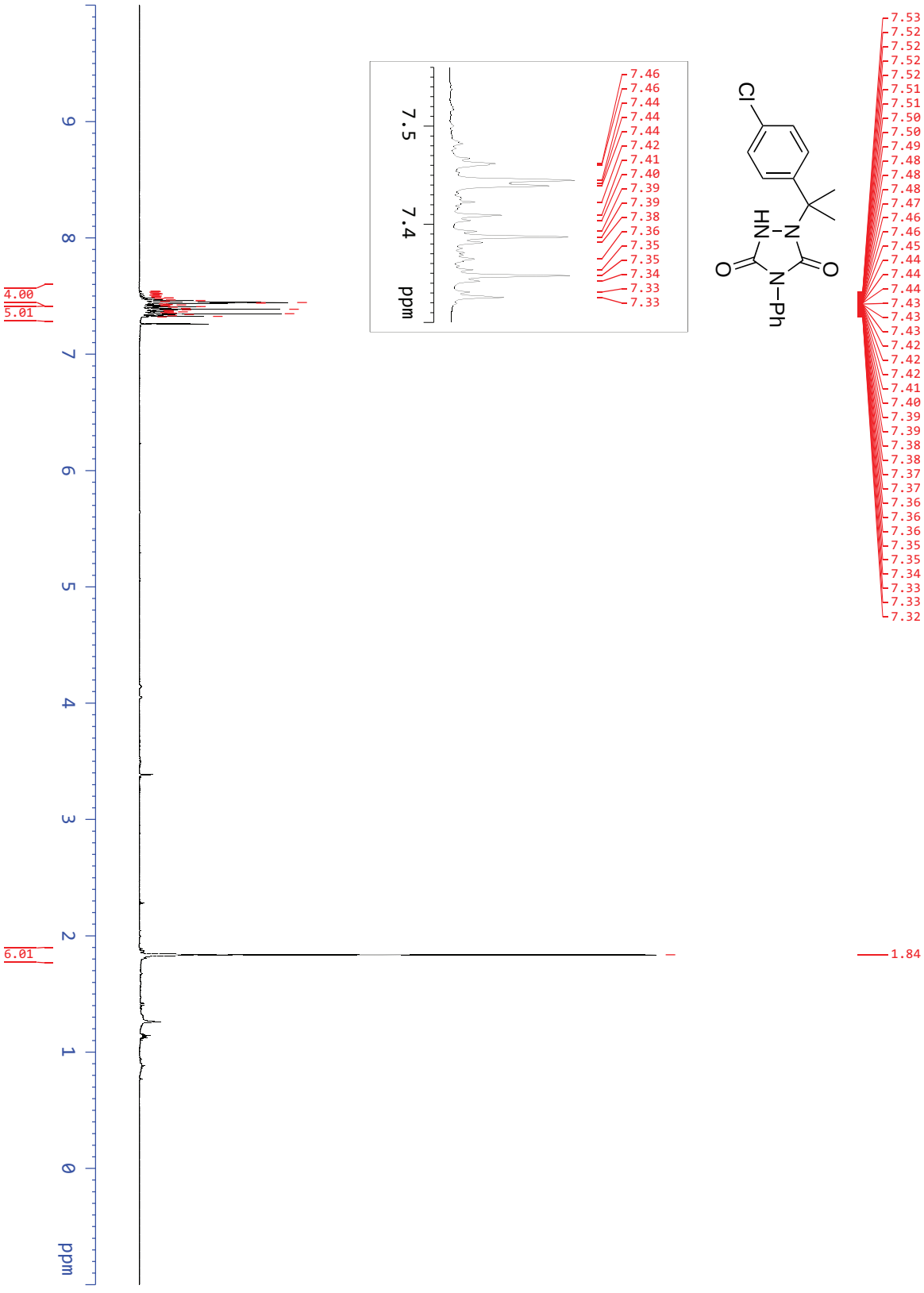


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

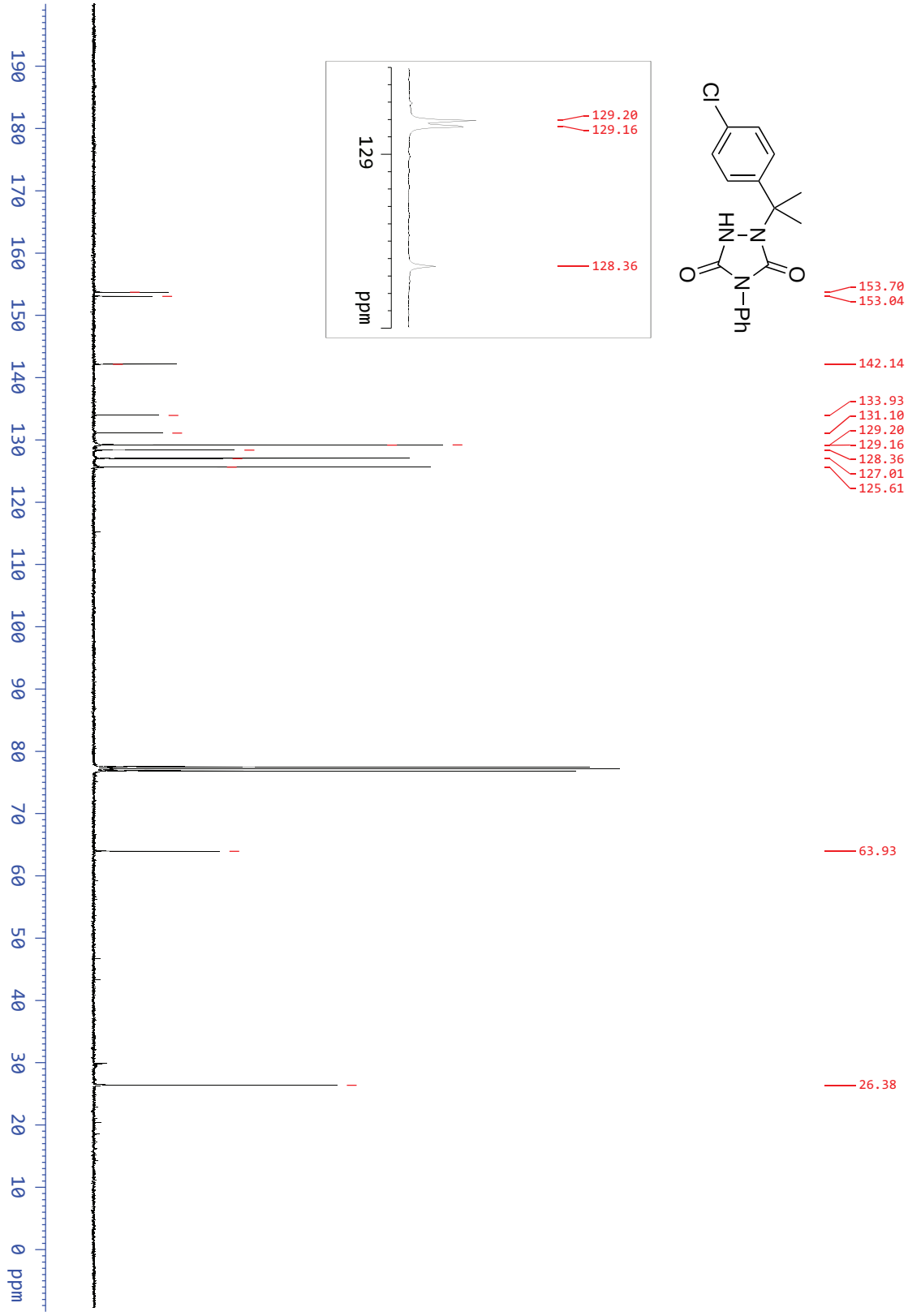


4.13 9b: 1-(2-(4-chlorophenyl)propan-2-yl)-4-phenyl--urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

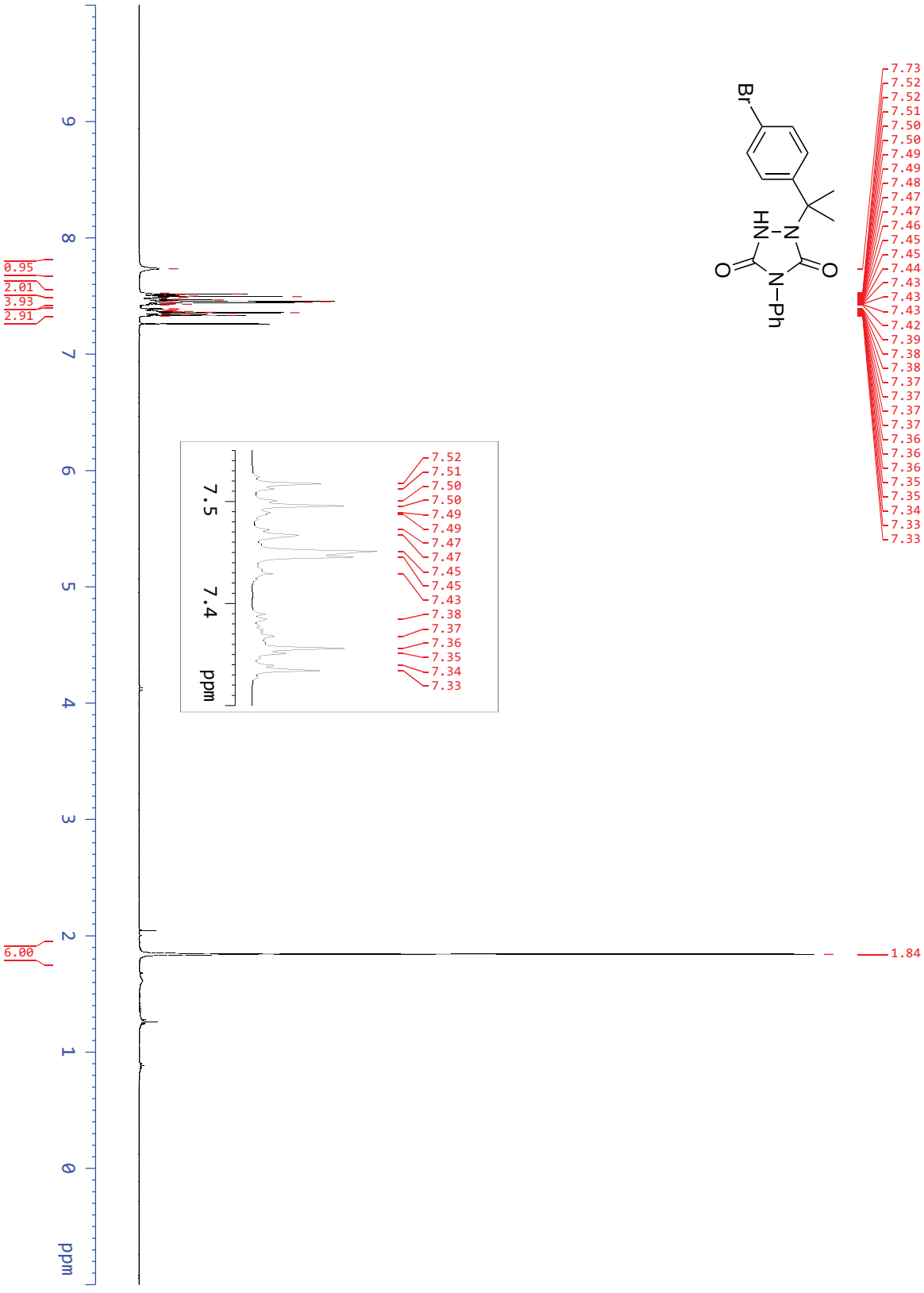


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

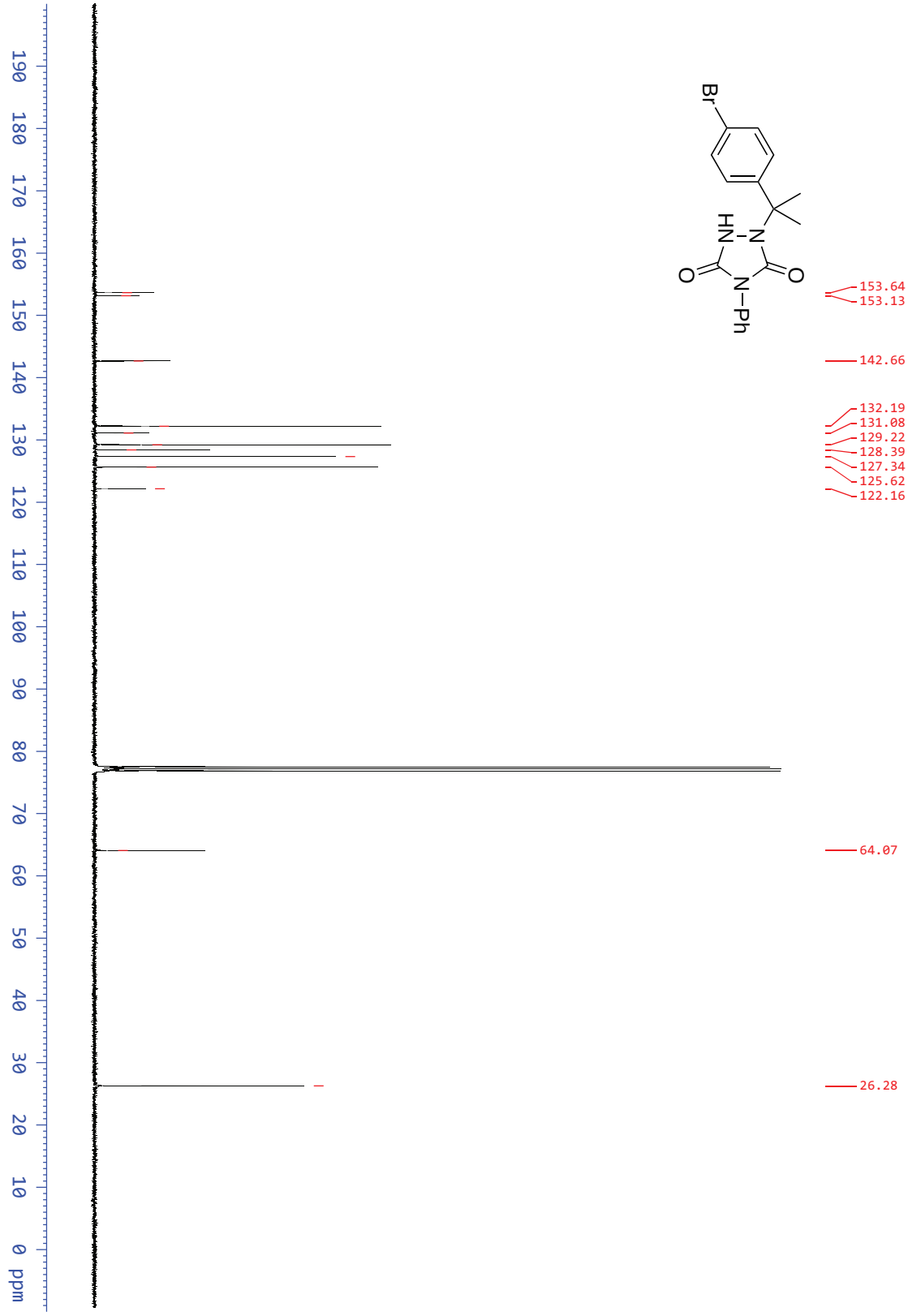


4.14 10b: 1-(2-(4-bromophenyl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

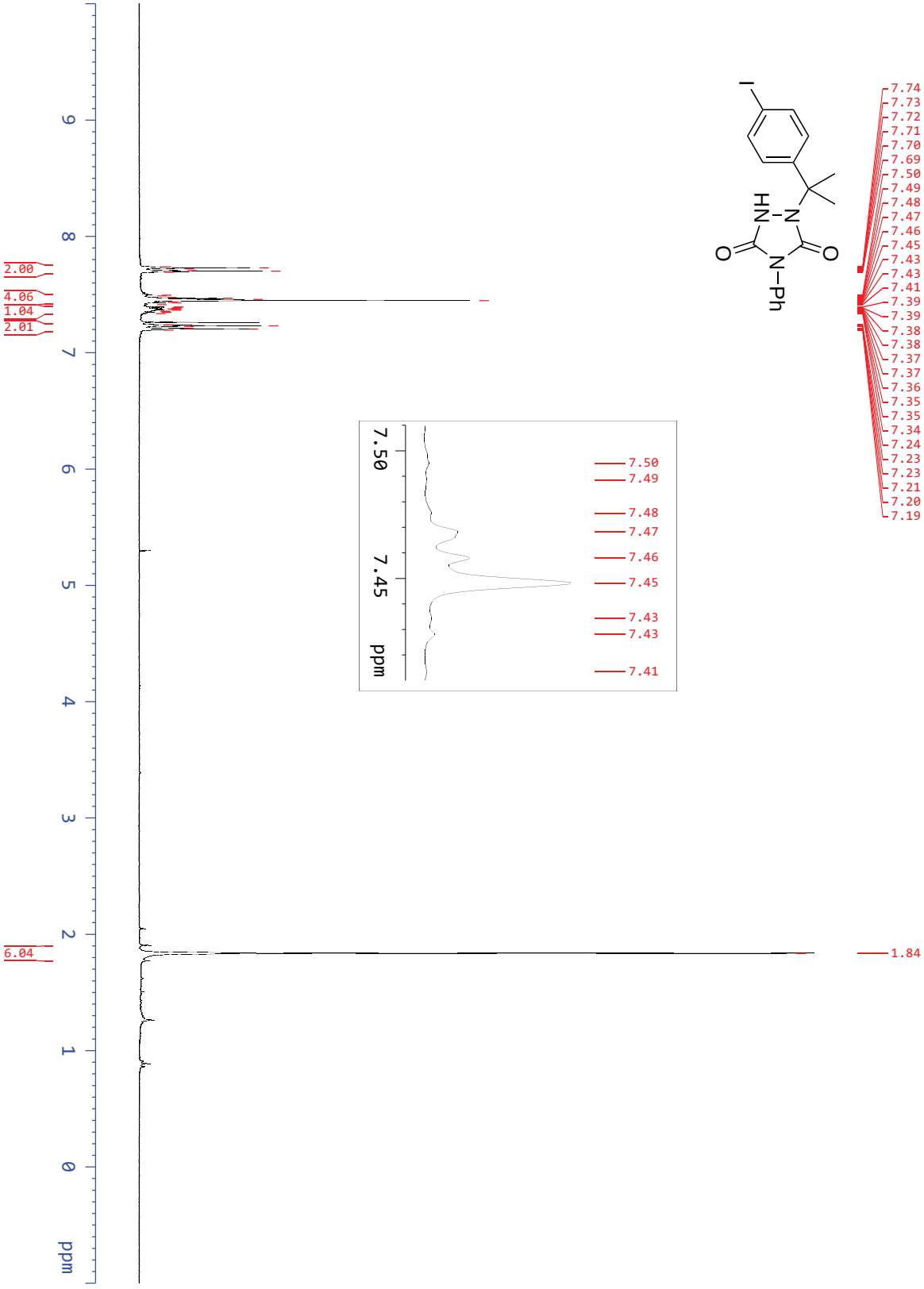


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

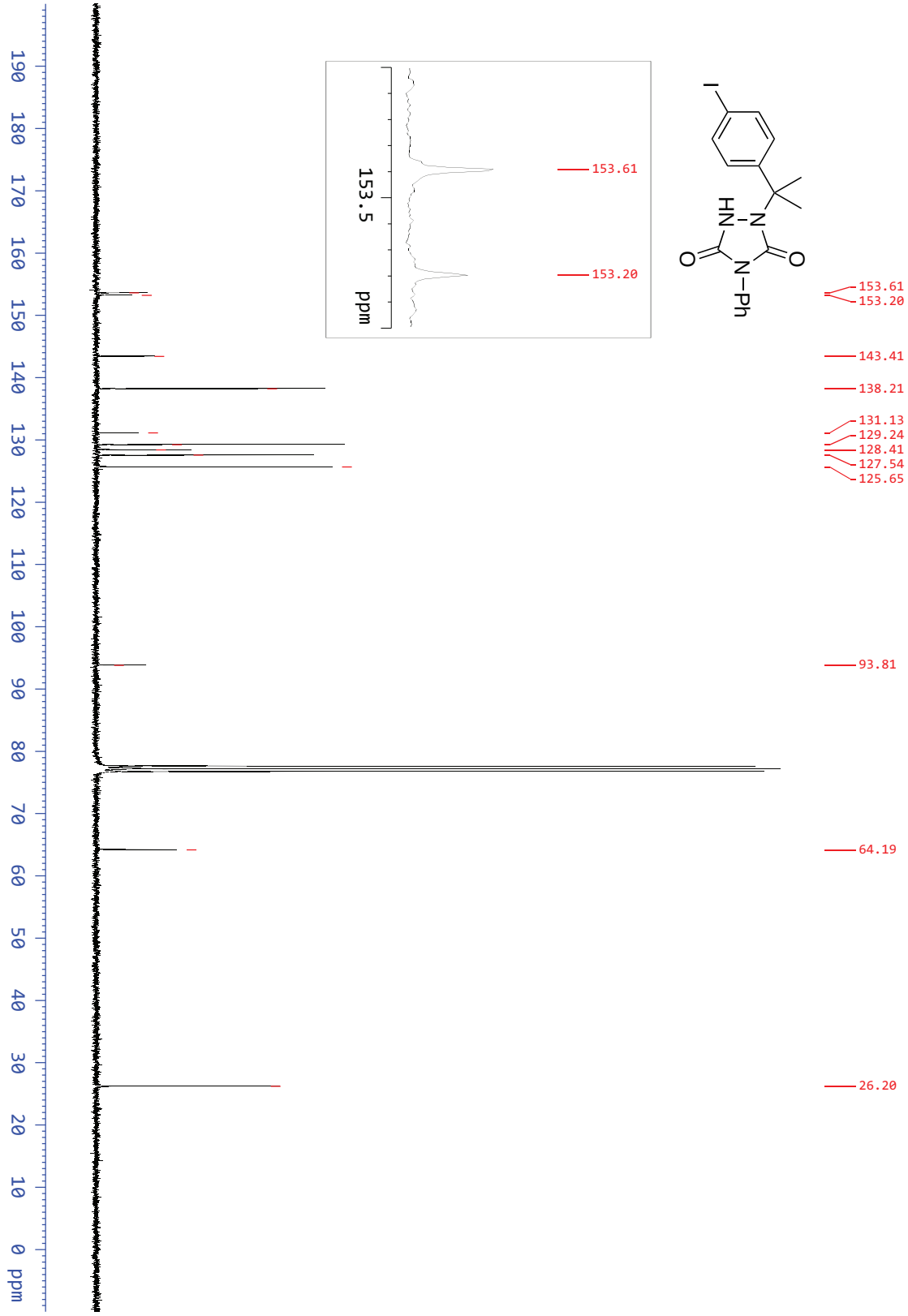


4.15 11b: 1-(2-(4-iodophenyl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (300 MHz, $CDCl_3$)

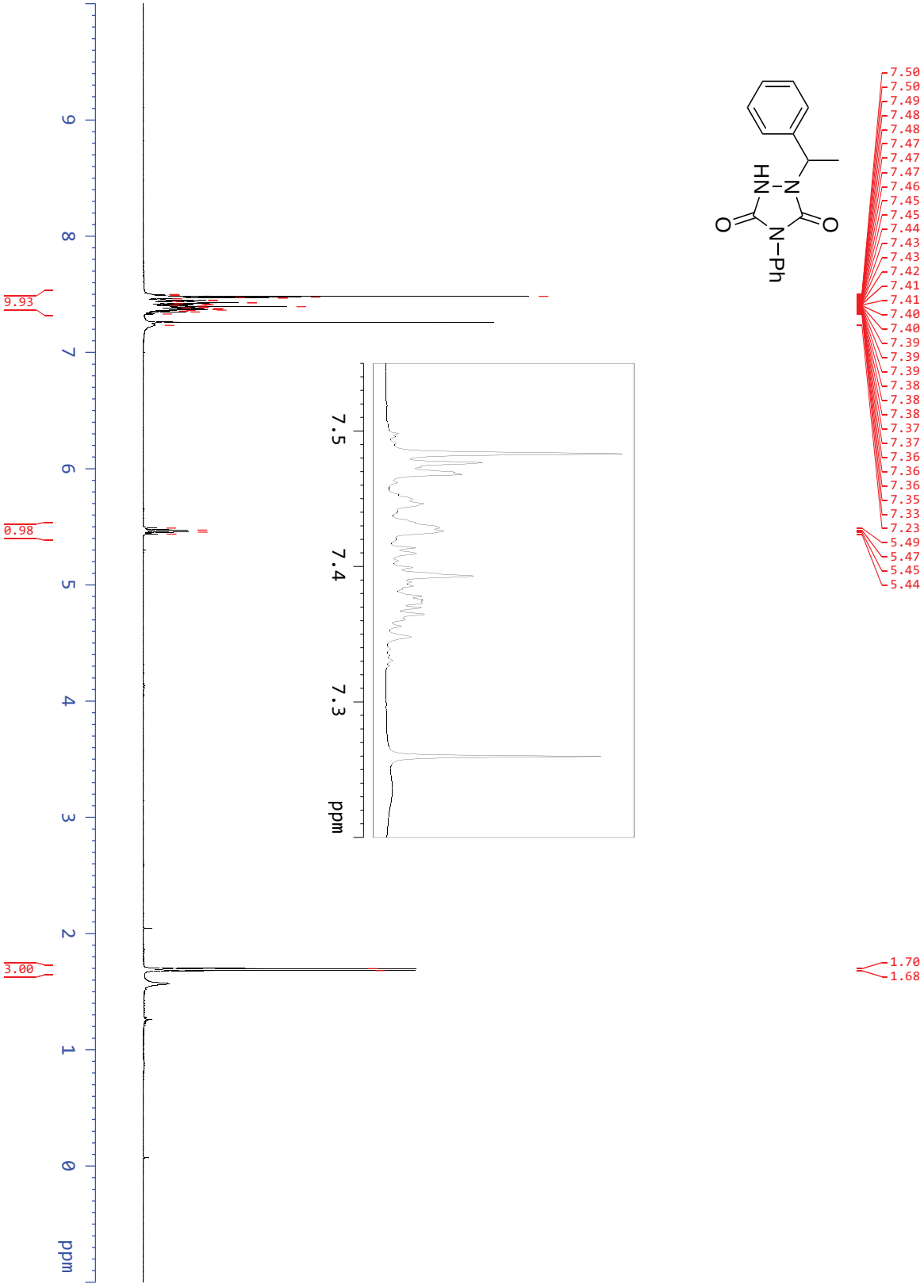


$^{13}C\{^{1}H\}$-NMR (75 MHz, $CDCl_3$)

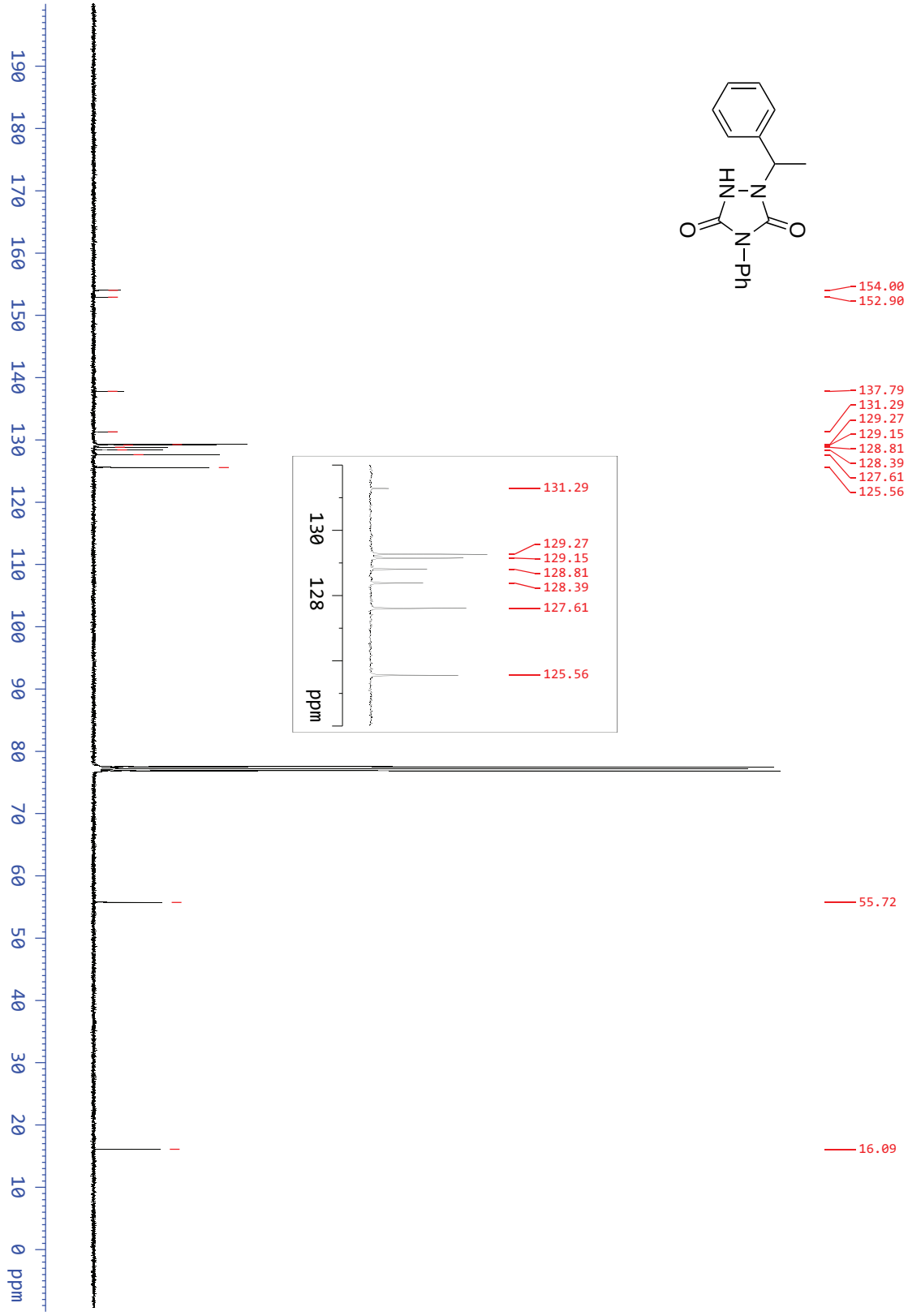


4.16 12b: 4-phenyl-1-(1-phenylethyl)-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

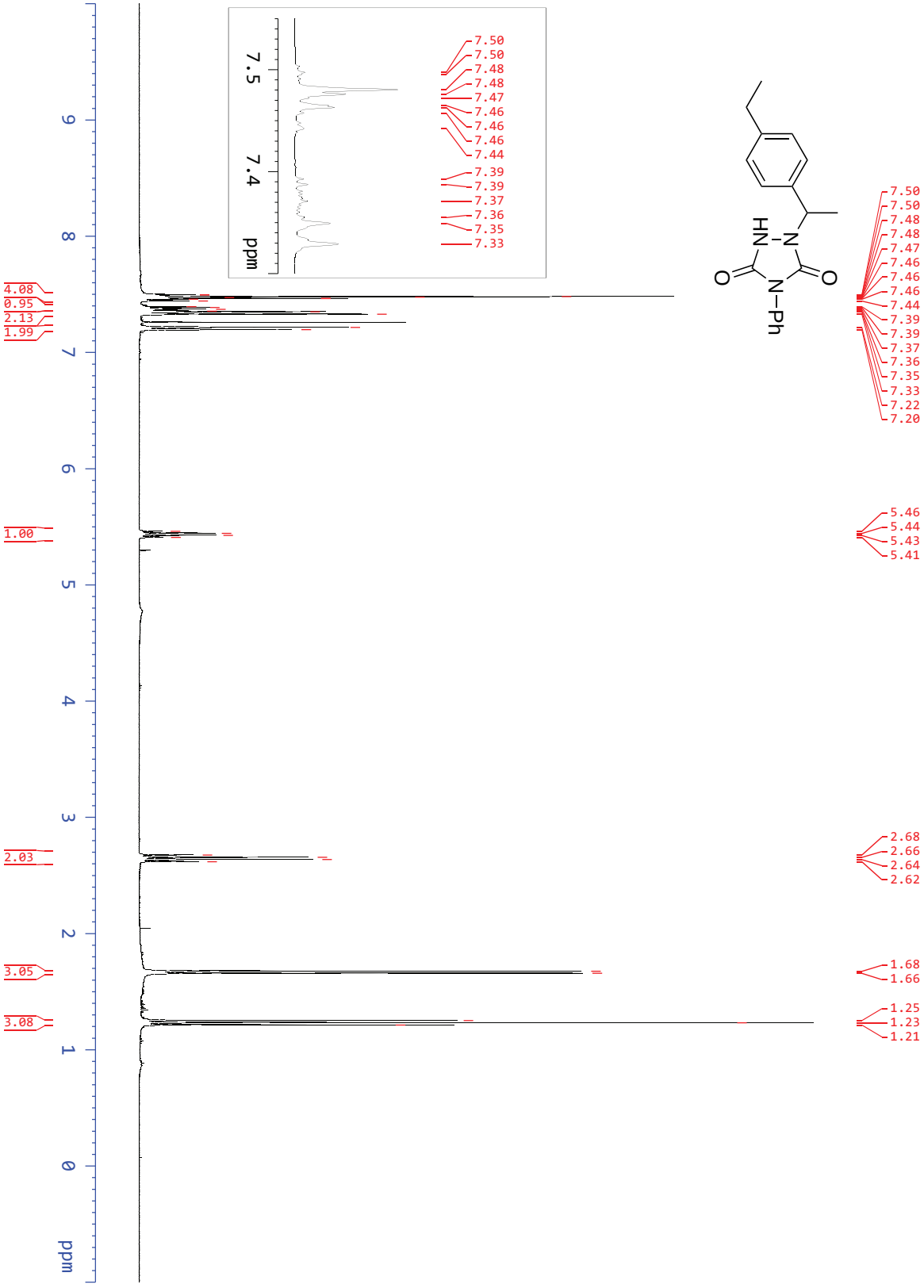


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

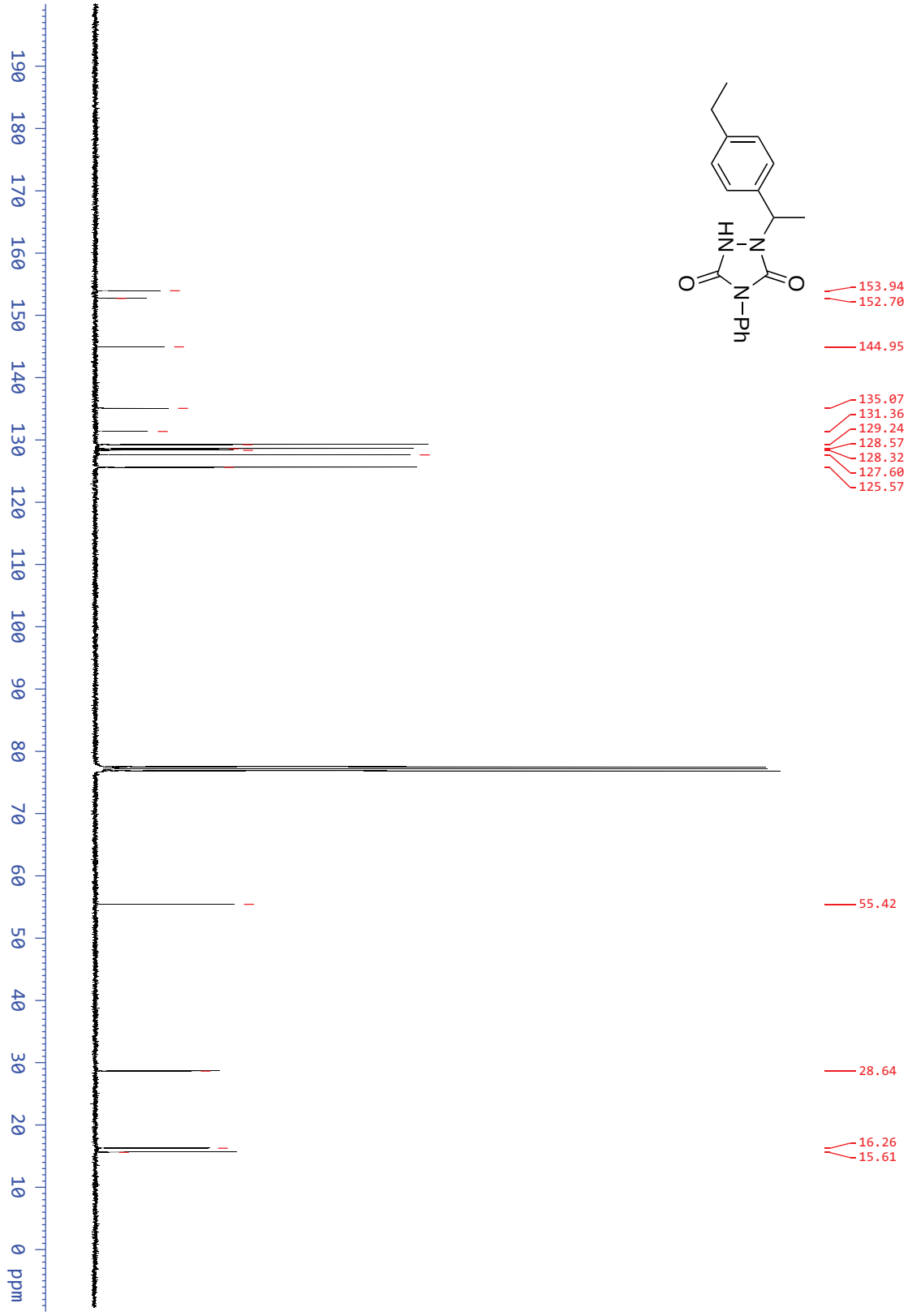


4.17 13b: 1-(1-(4-ethylphenyl)ethyl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

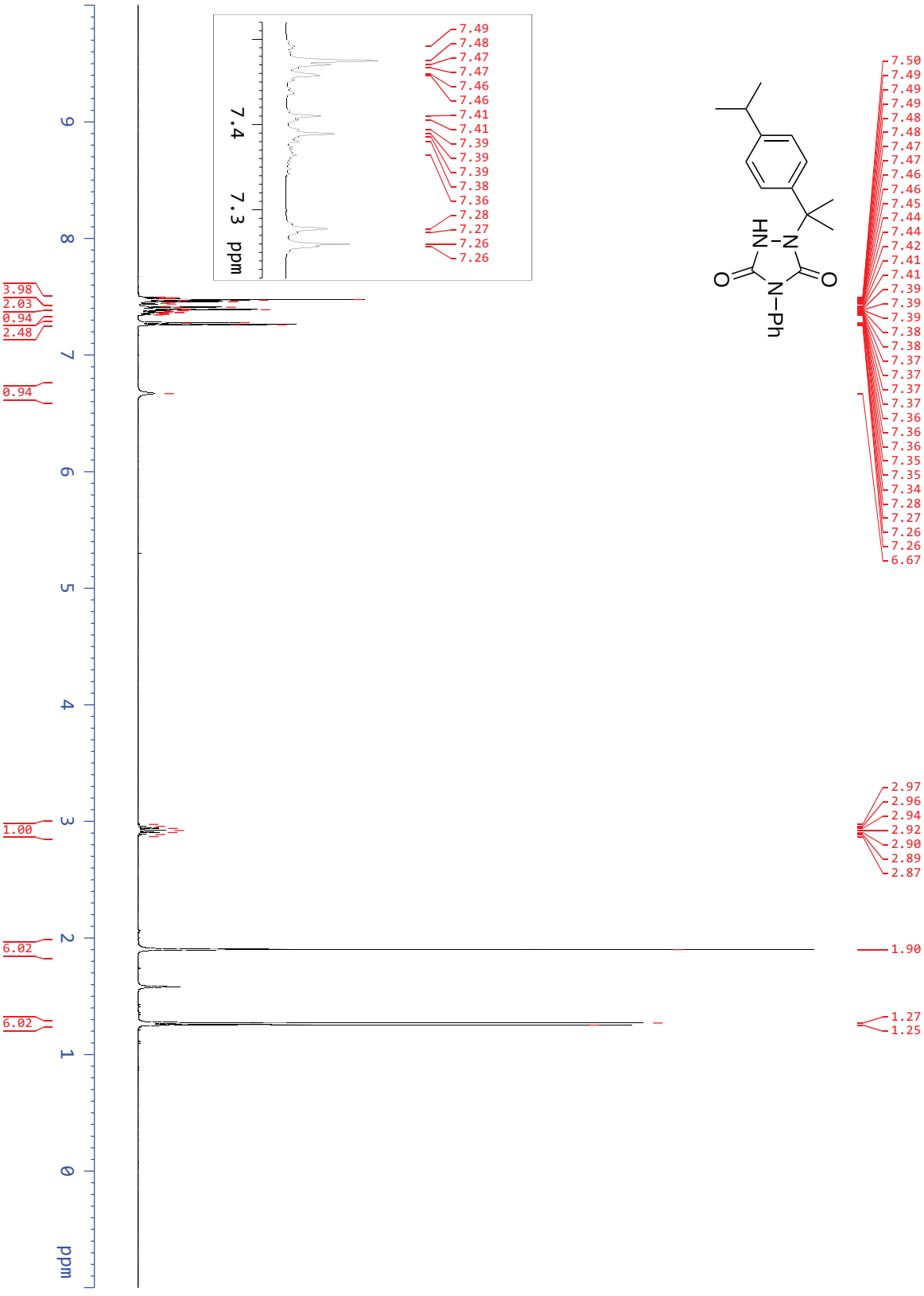


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

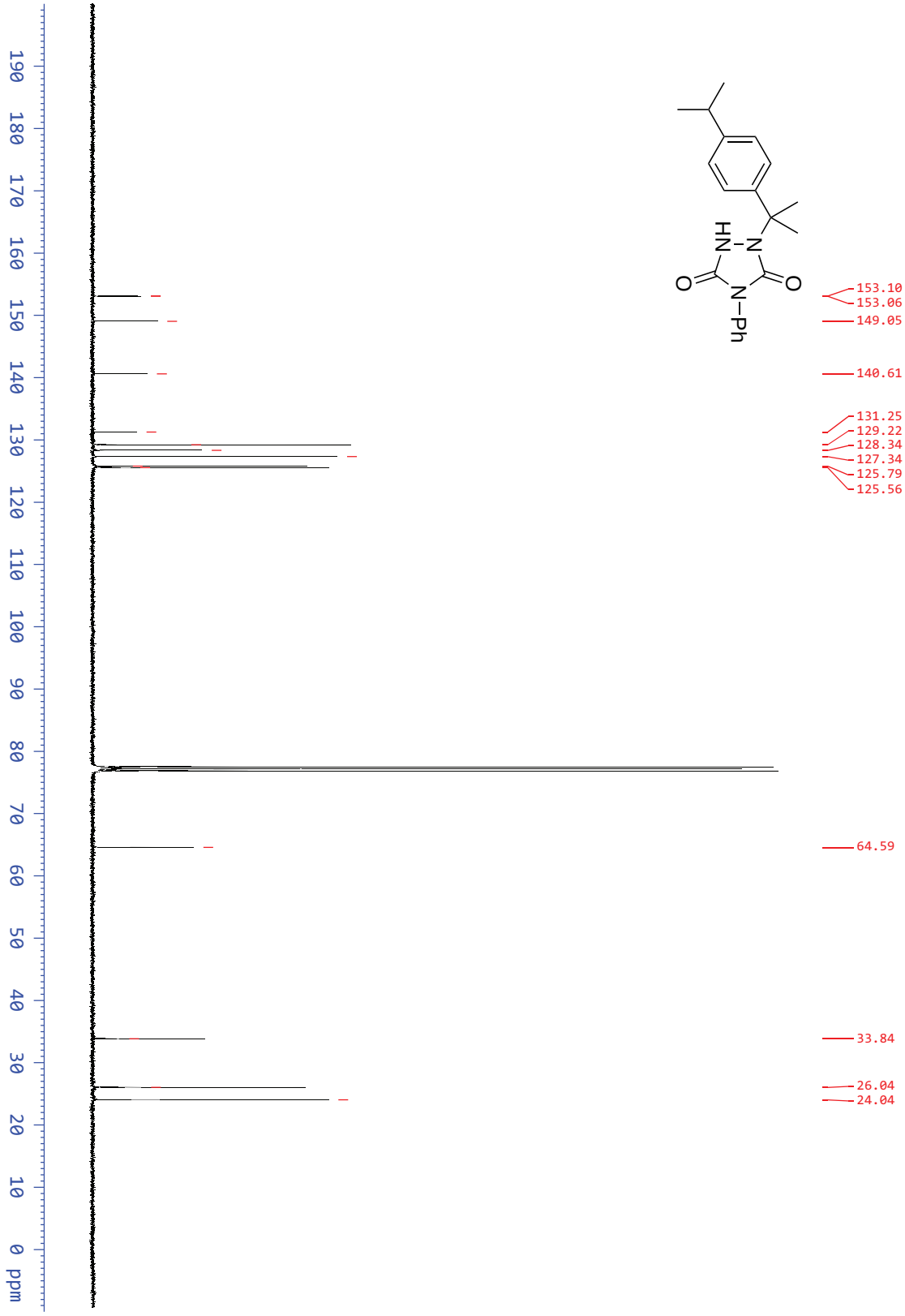


4.18 14b: 1-(2-(4-isopropylphenyl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

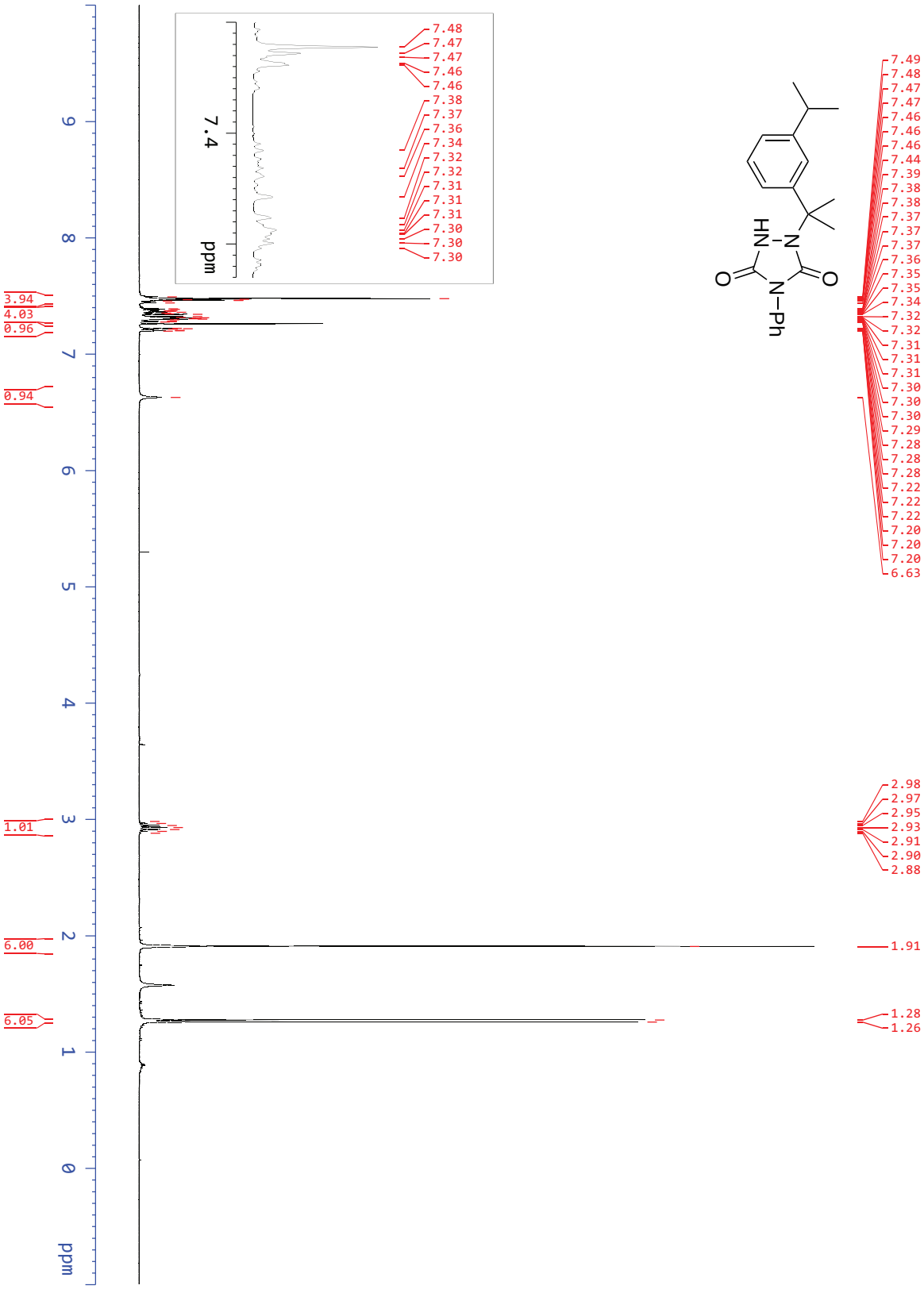


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

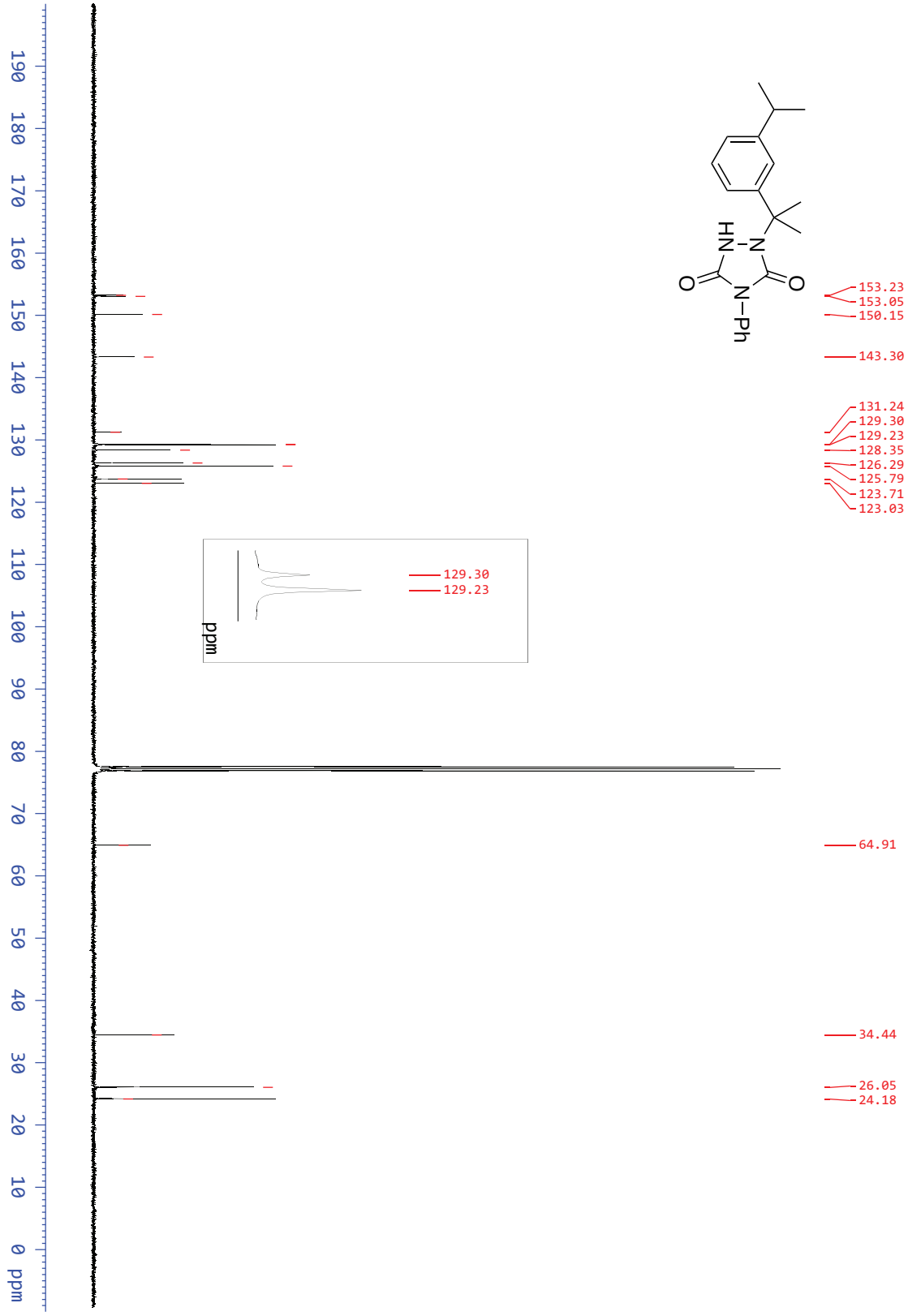


4.19 15b: 1-(2-(3-isopropylphenyl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)



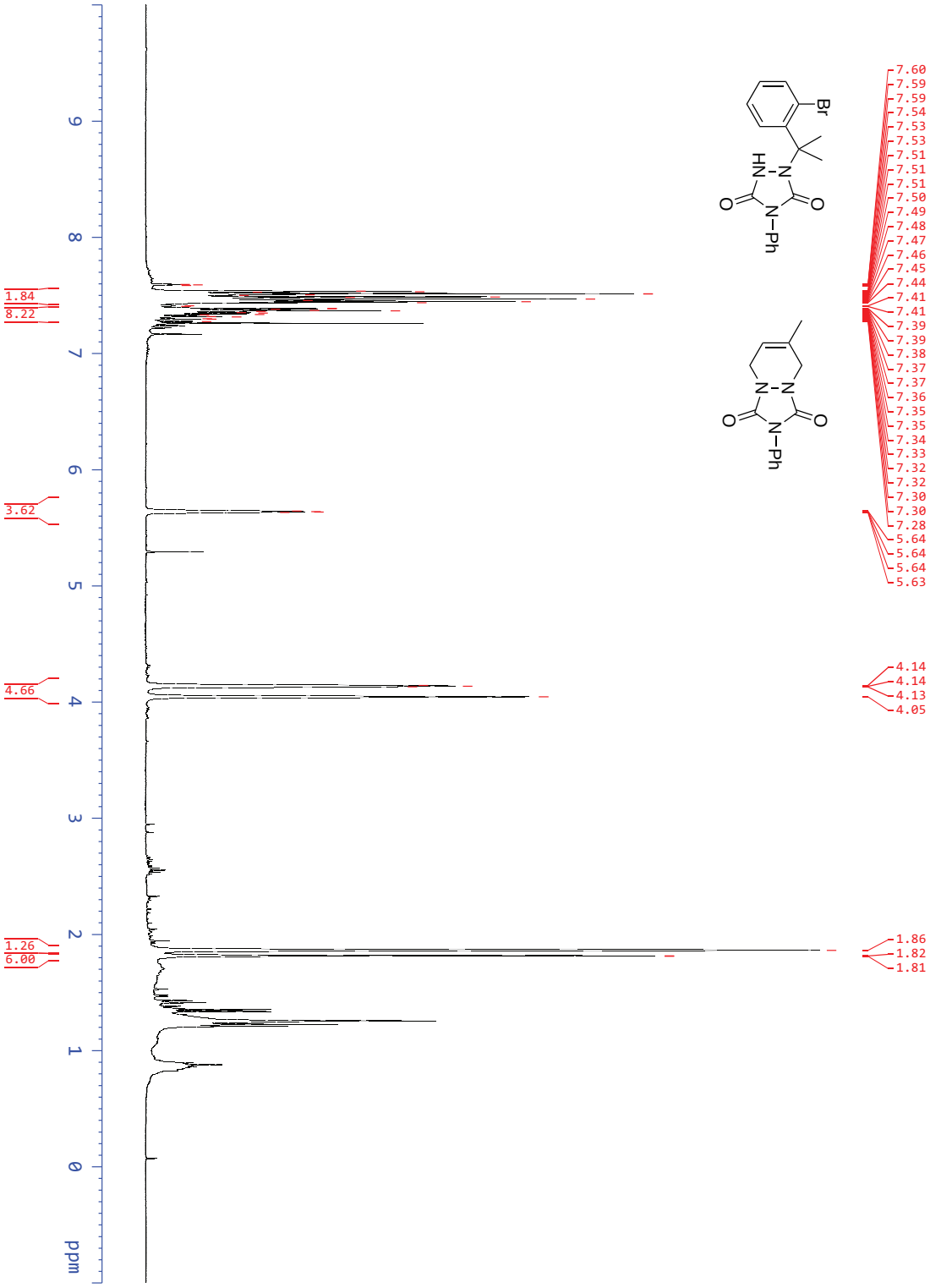
$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)



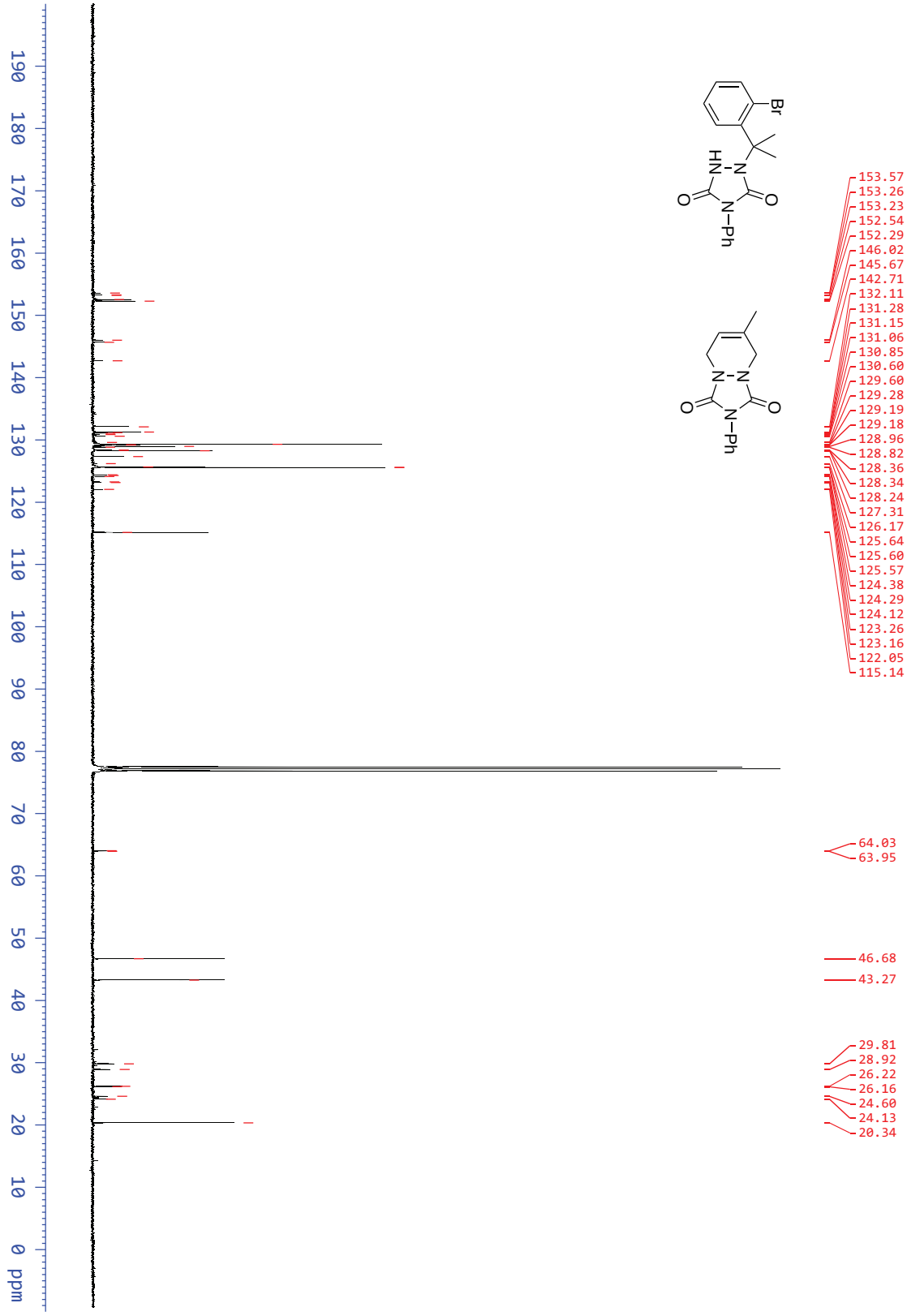
4.20 16b: 1-(2-(2-bromophenyl)propan-2-yl)-4-phenyl-urazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **17b** and the PTAD-isoprene adduct **40** in a 22:78 ratio*

^{1}H-NMR (400 MHz, $CDCl_3$ + residual DCM)

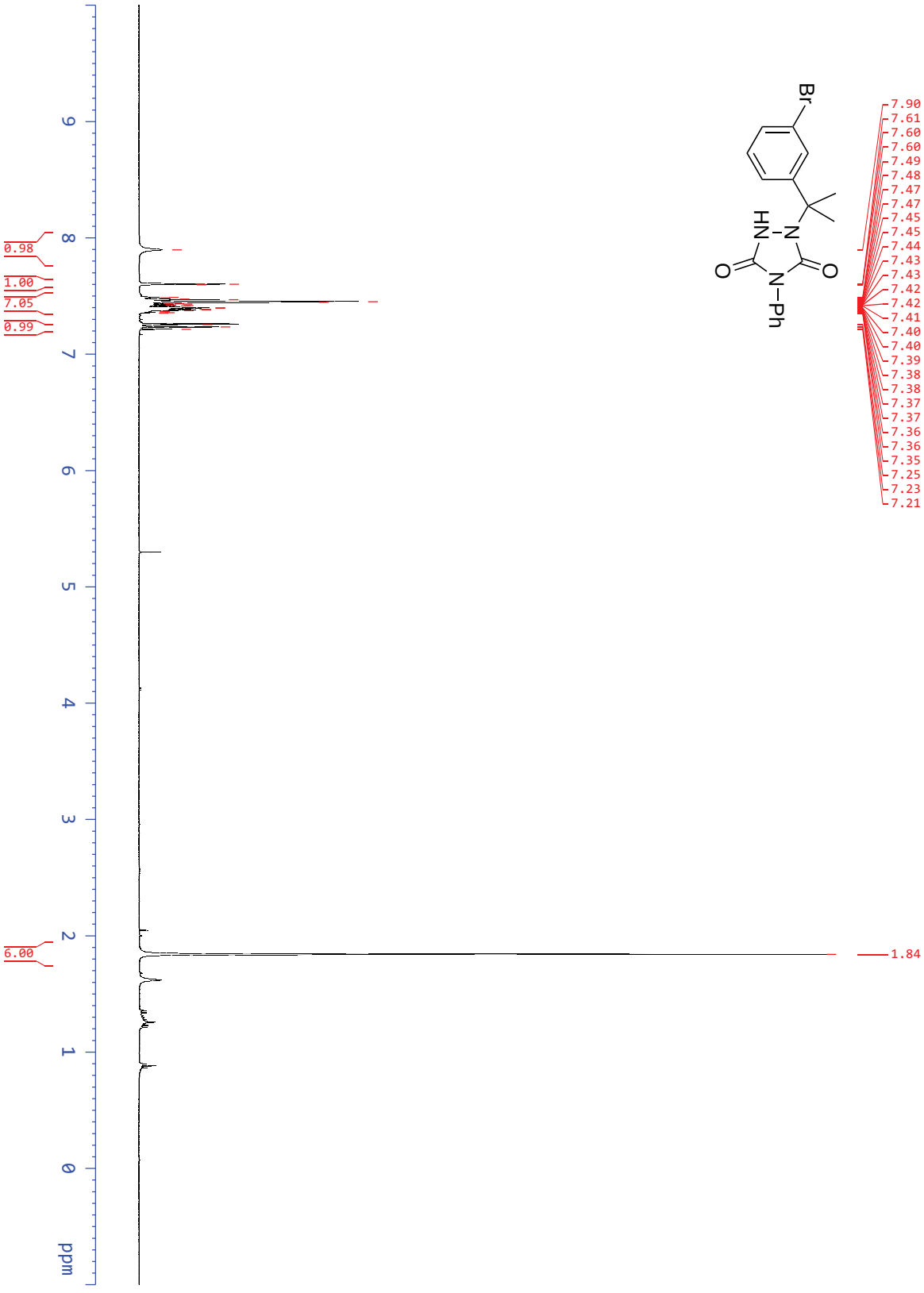


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

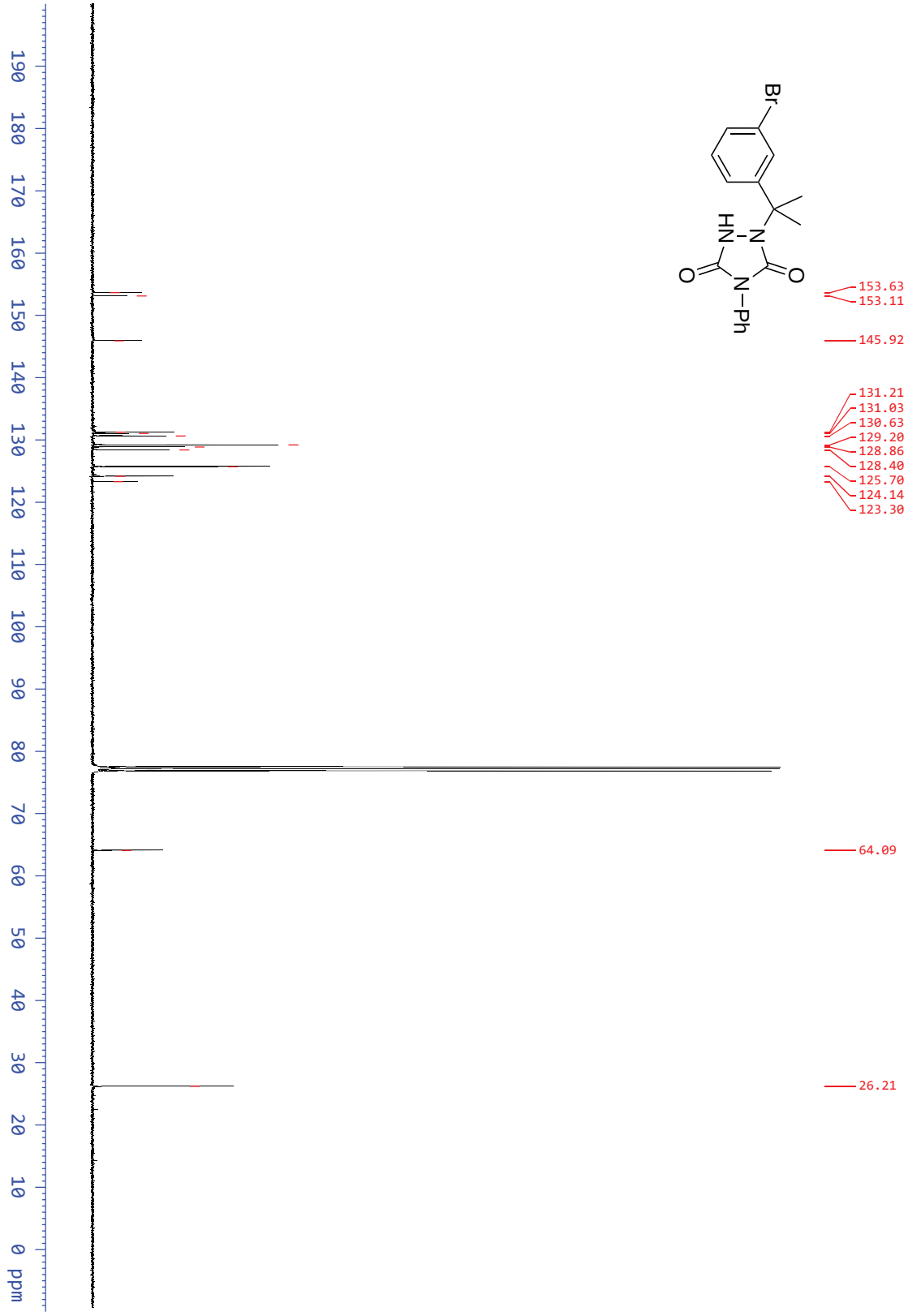


4.21 17b: 1-(2-(3-bromophenyl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$ + residual DCM)

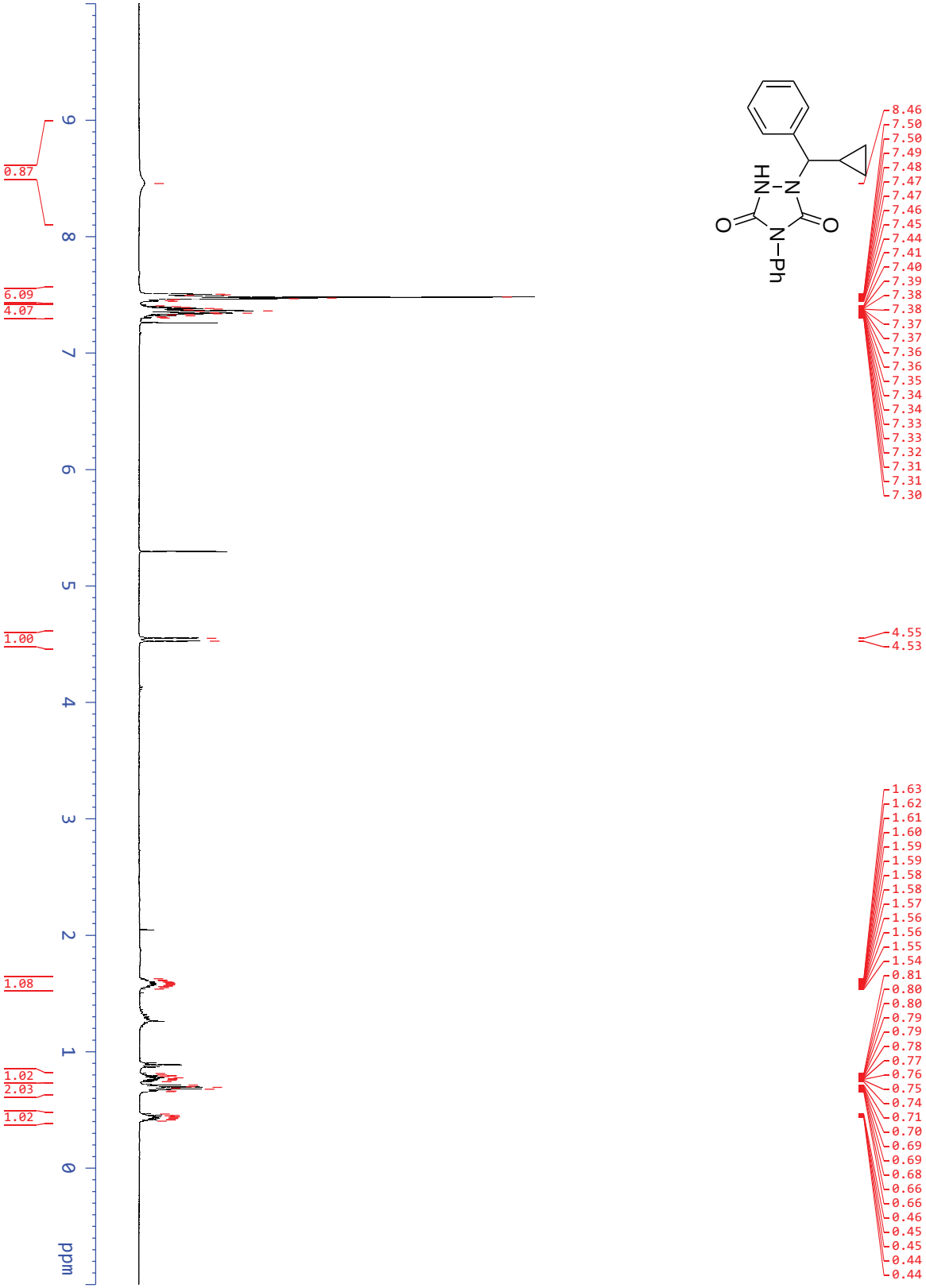


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

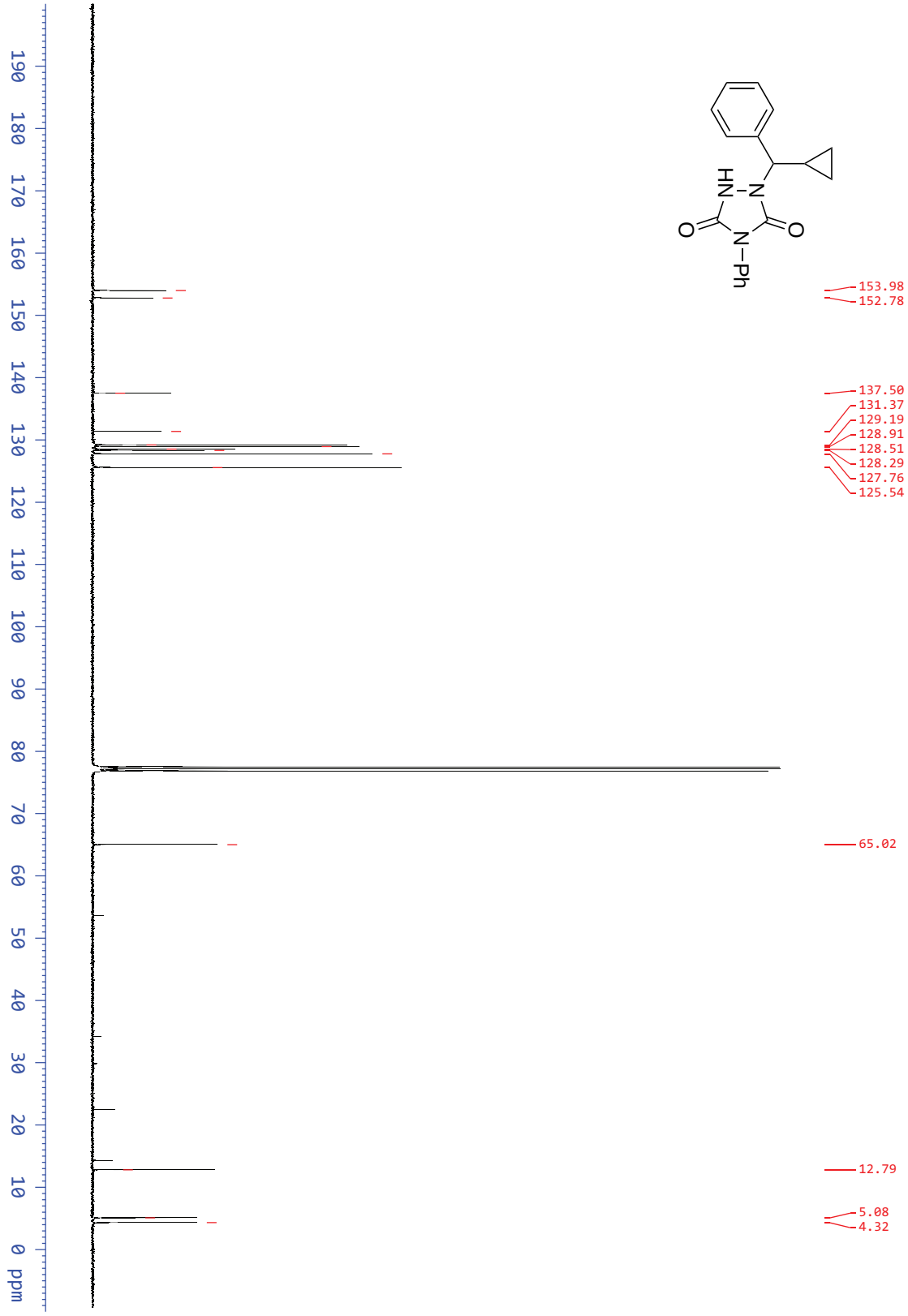


4.22 18b: 1-(cyclopropyl(phenyl)methyl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$ + residual DCM)

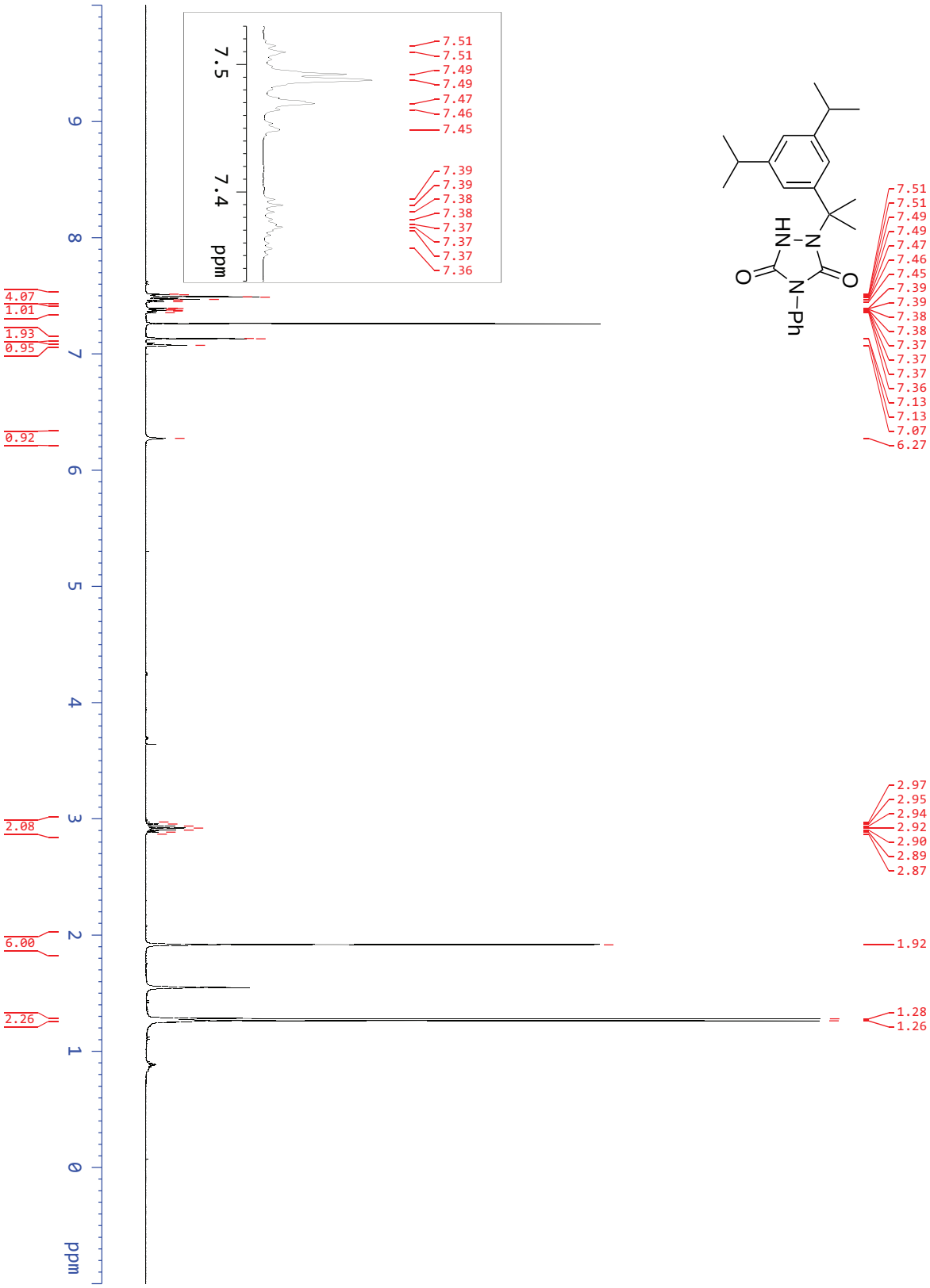


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

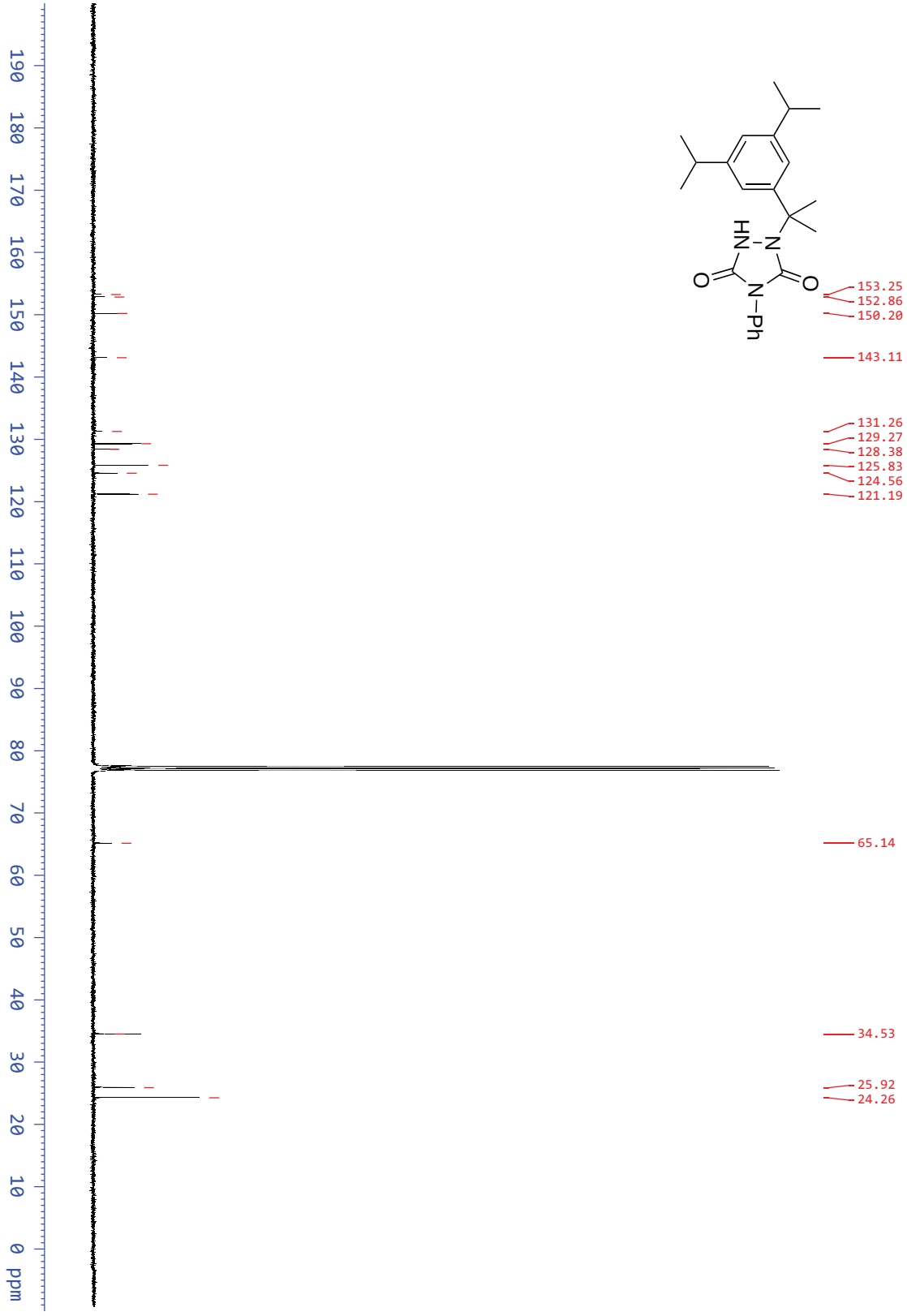


4.23 19b: 1-(2-(3,5-diisopropylphenyl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)



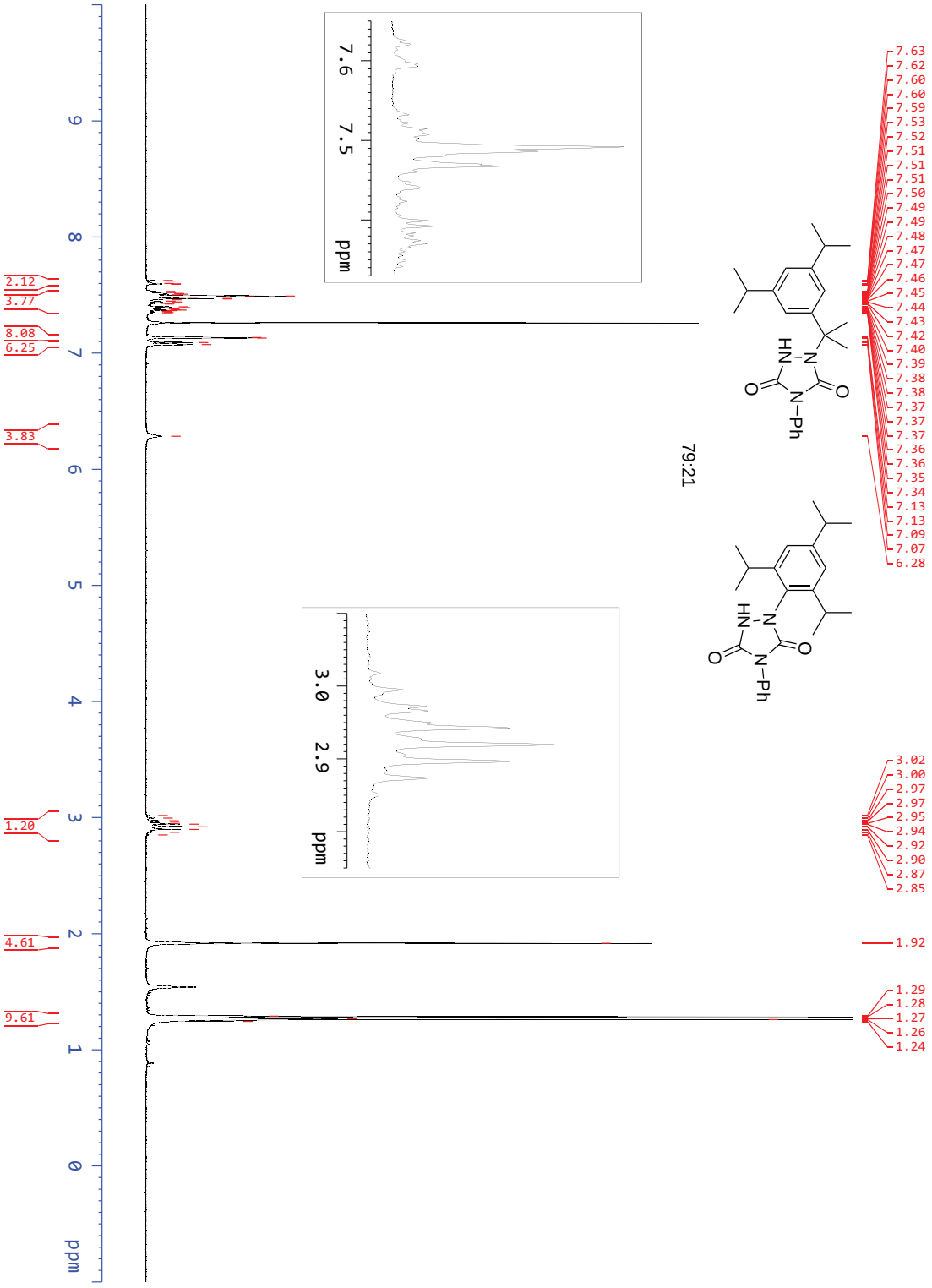
$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)



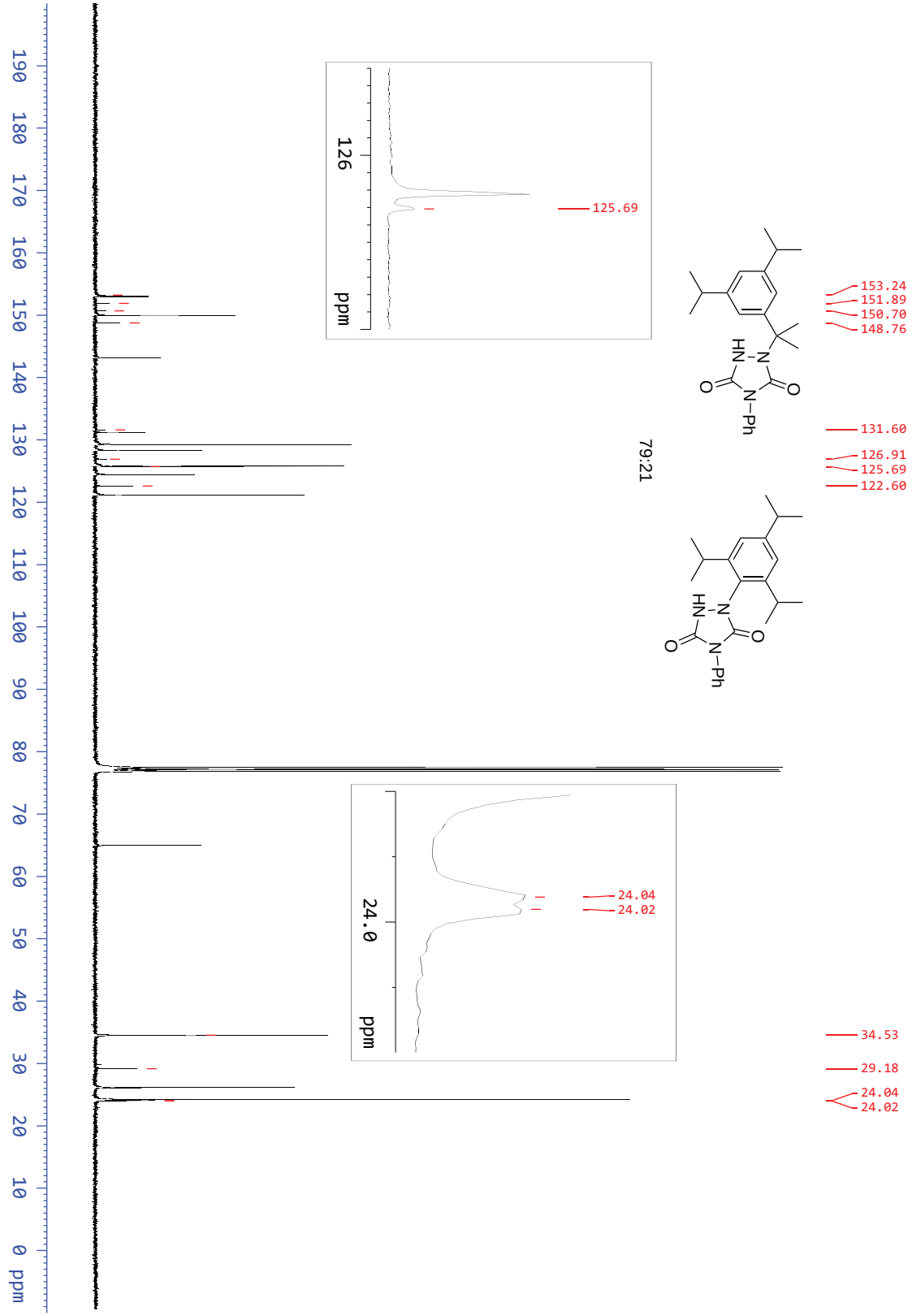
4.24 19c: 4-phenyl-1-(2,4,6-triisopropylphenyl)-urazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **19b** and **19c** in a 79:21 ratio*

^{1}H-NMR (300 MHz, $CDCl_3$)



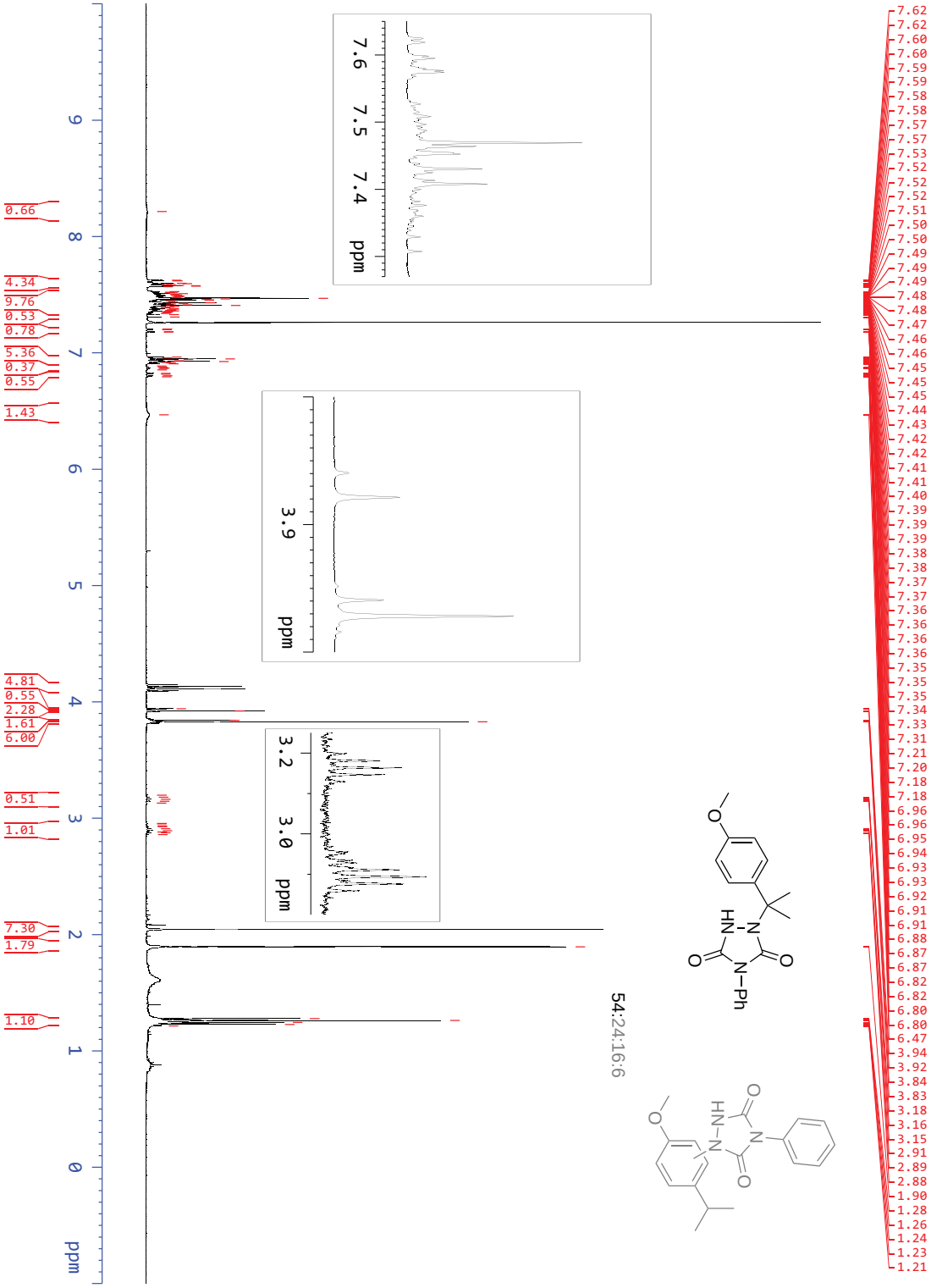
$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)



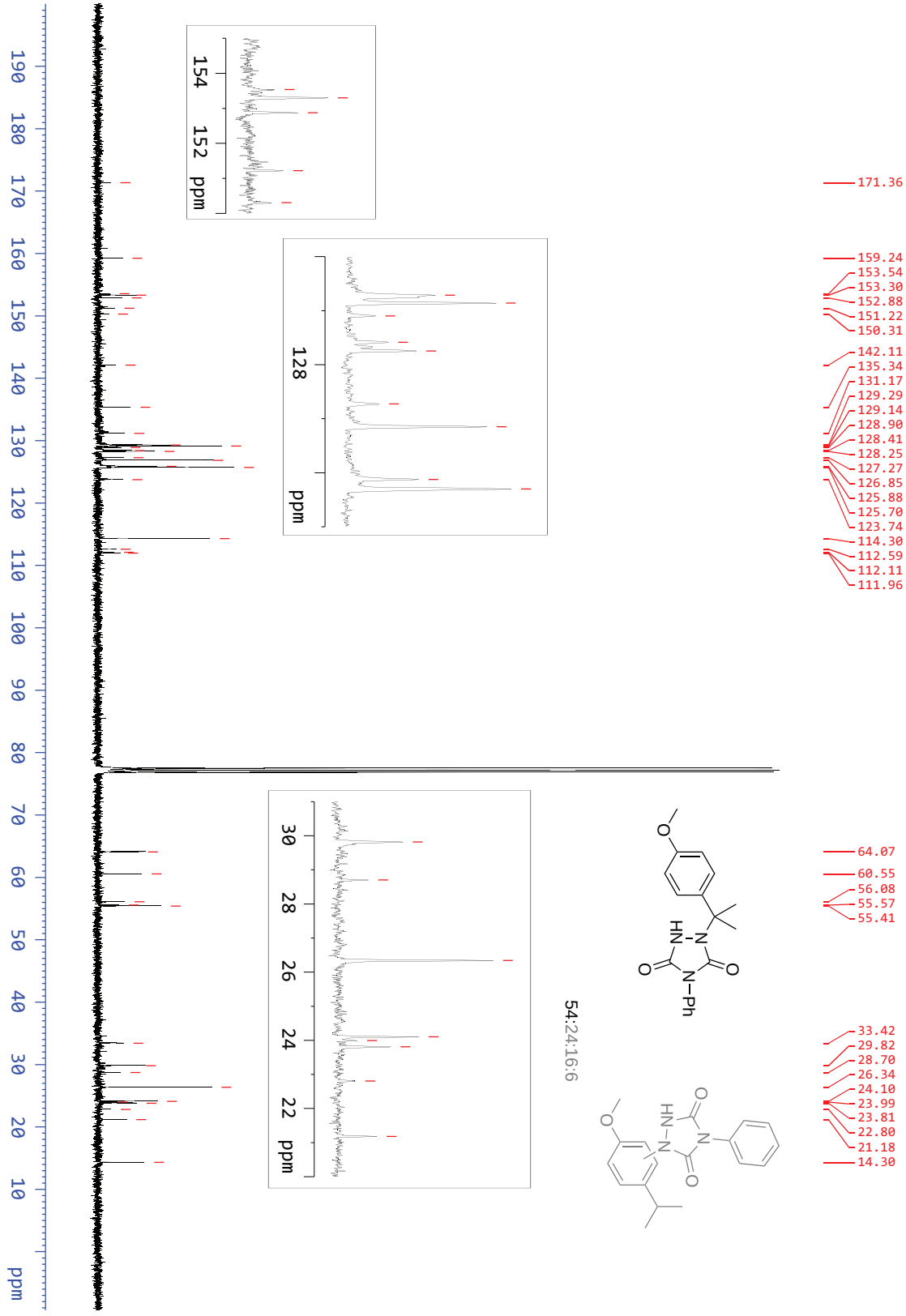
4.25 20b: 1-(2-(4-methoxyphenyl)propan-2-yl)-4-phenyl-urazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **20b** and **20c** in a 54:46 ratio*

^{1}H-NMR (400 MHz, $CDCl_3$ + residual EtOAc)



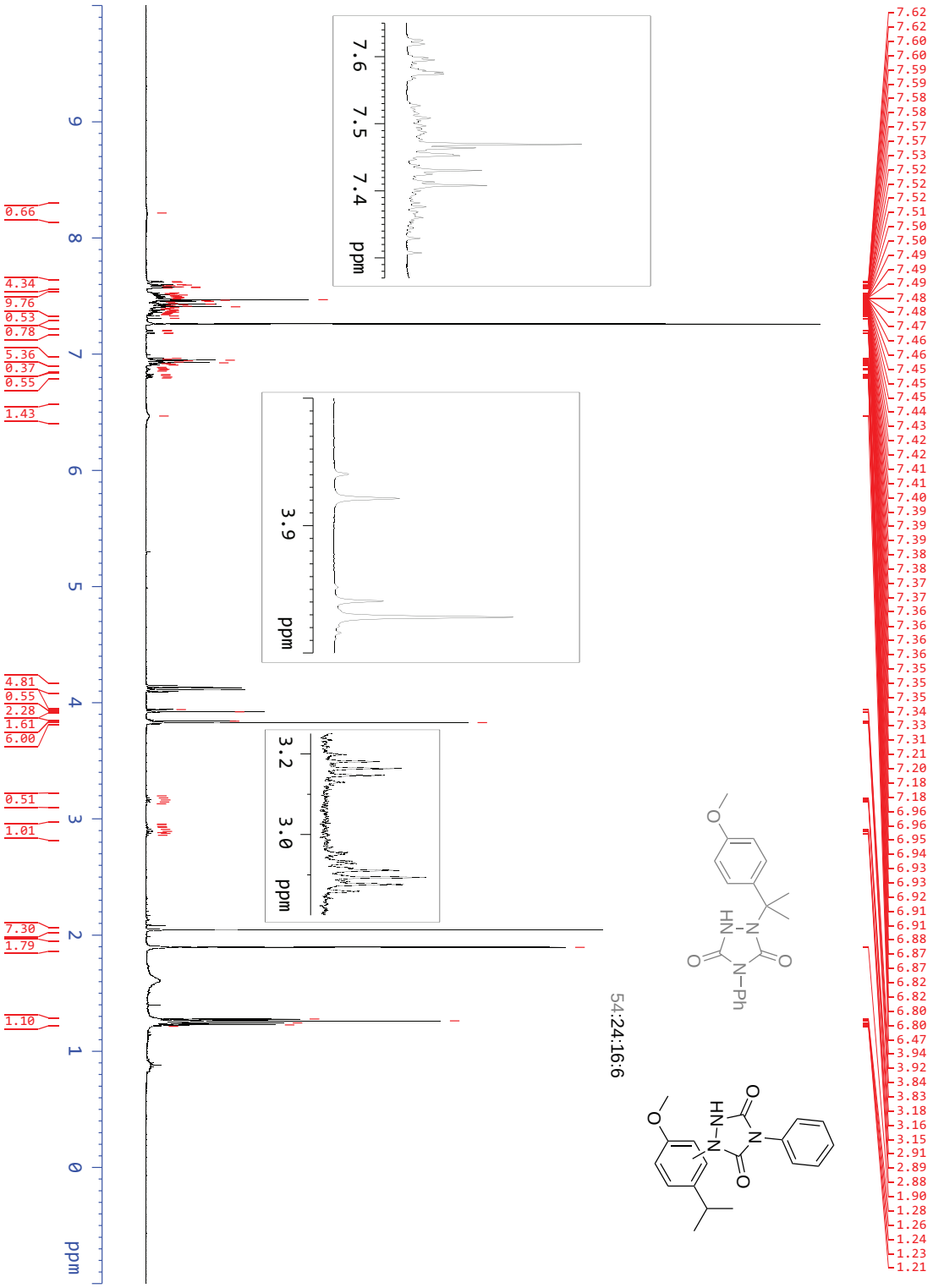
$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$ + residual EtOAc)



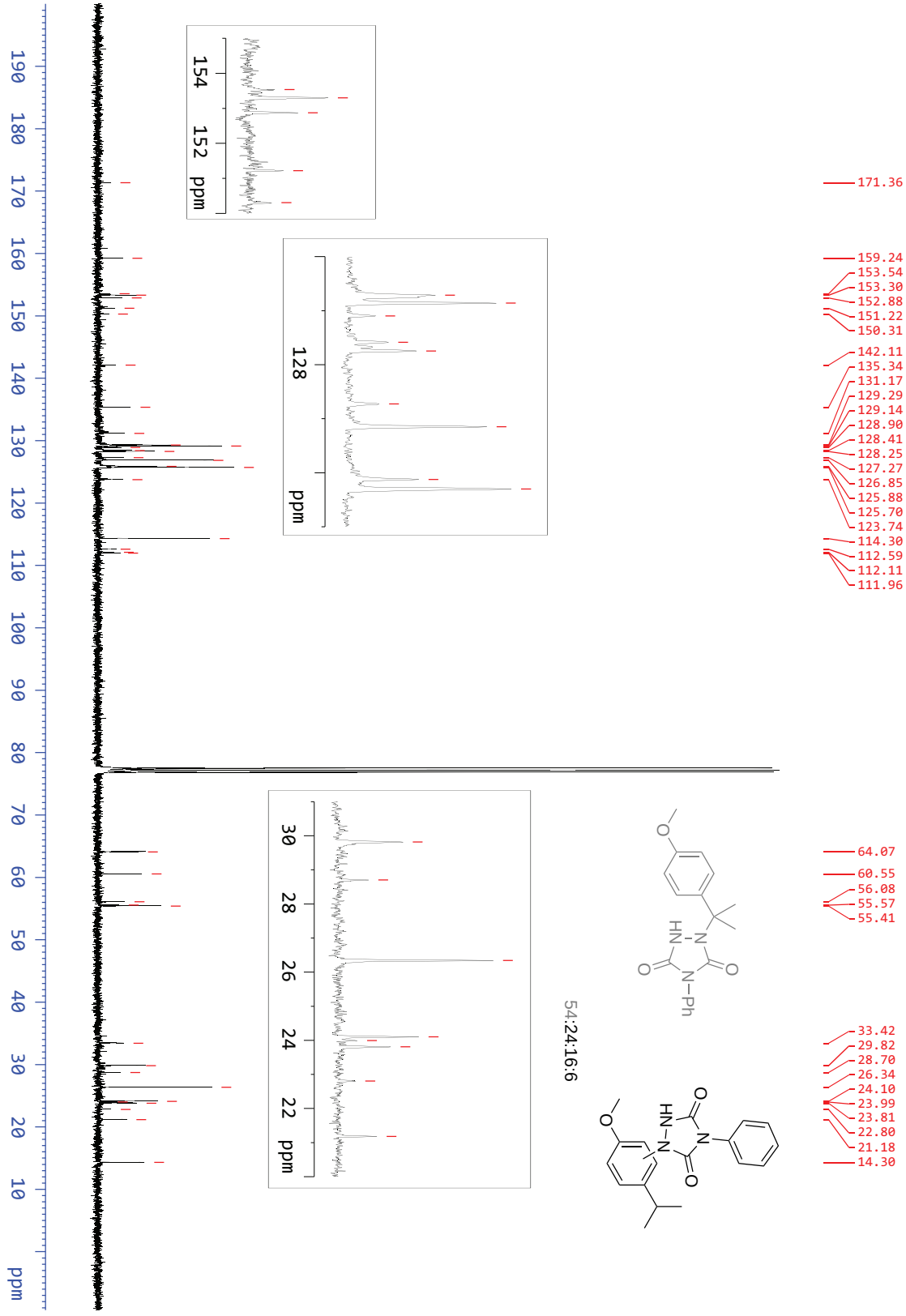
4.26 20c: Side products of amination on 4-isopropylanisole

*These compounds were not obtained analytically pure and the assignments were made on a sample containing a mixture of **20b** and **20c** in a 54:(24:16:6) ratio*

^{1}H-NMR (400 MHz, $CDCl_3$)

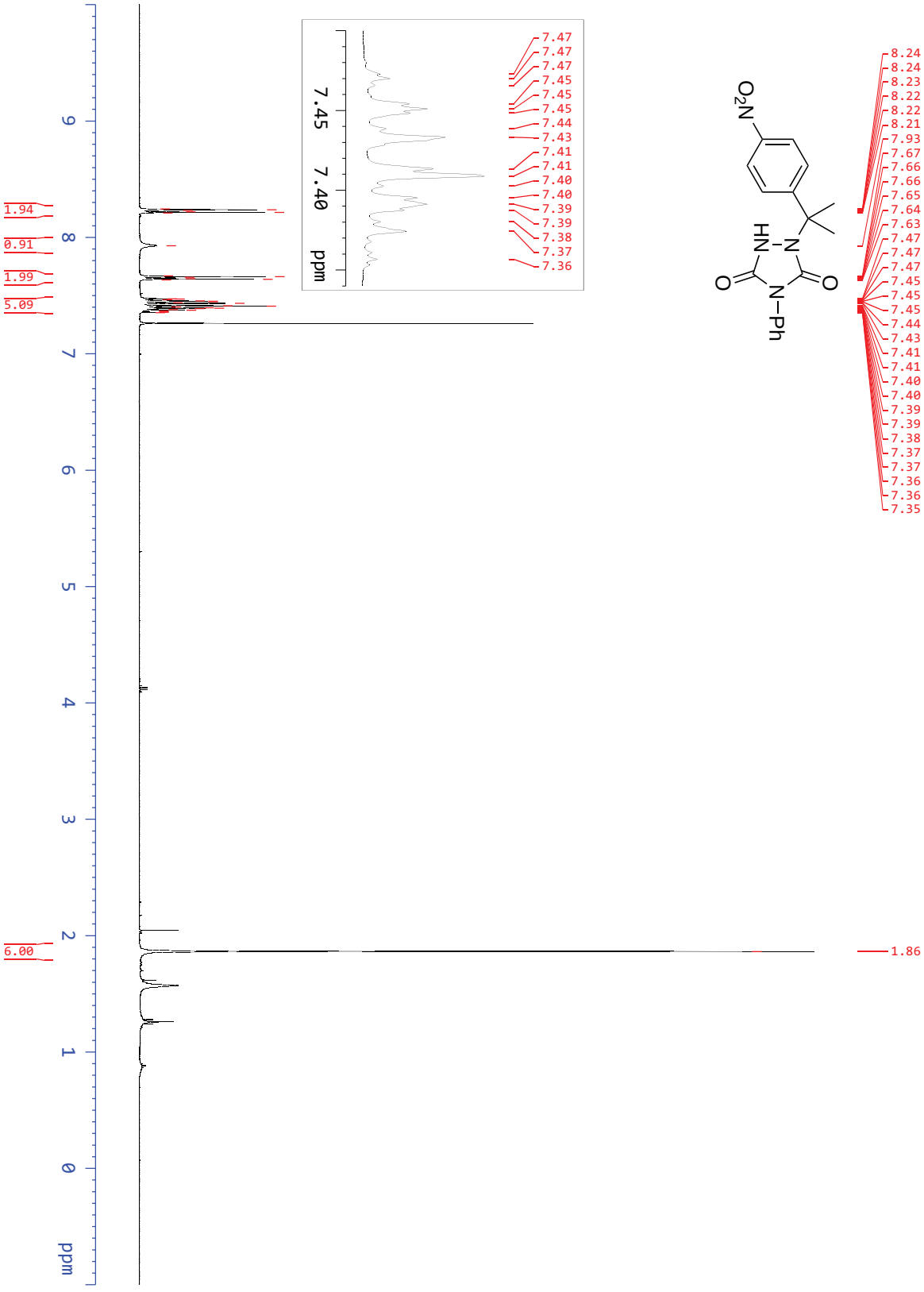


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

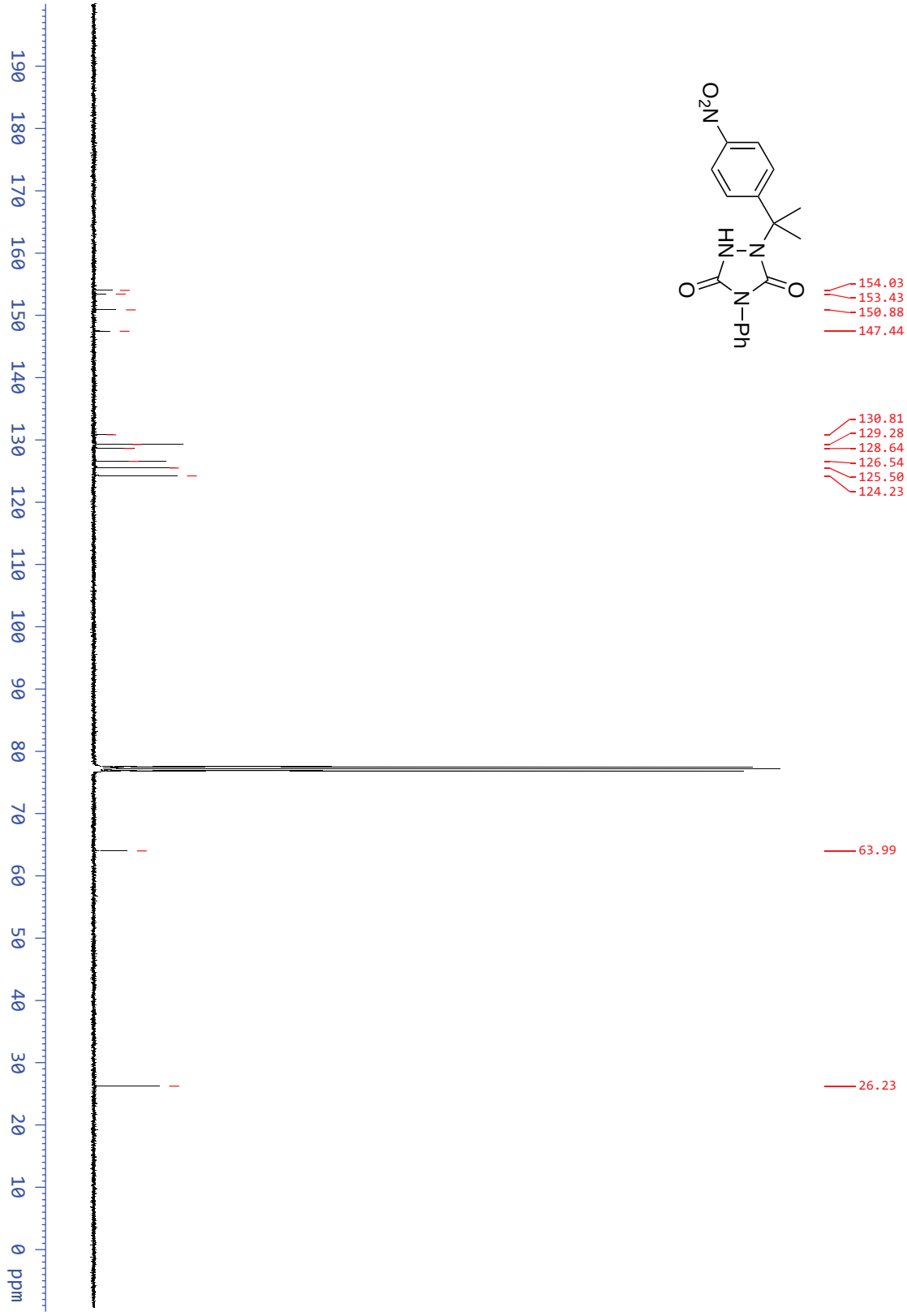


4.27 21b: 1-(2-(4-nitrophenyl)propan-2-yl)-4-phenyl--urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

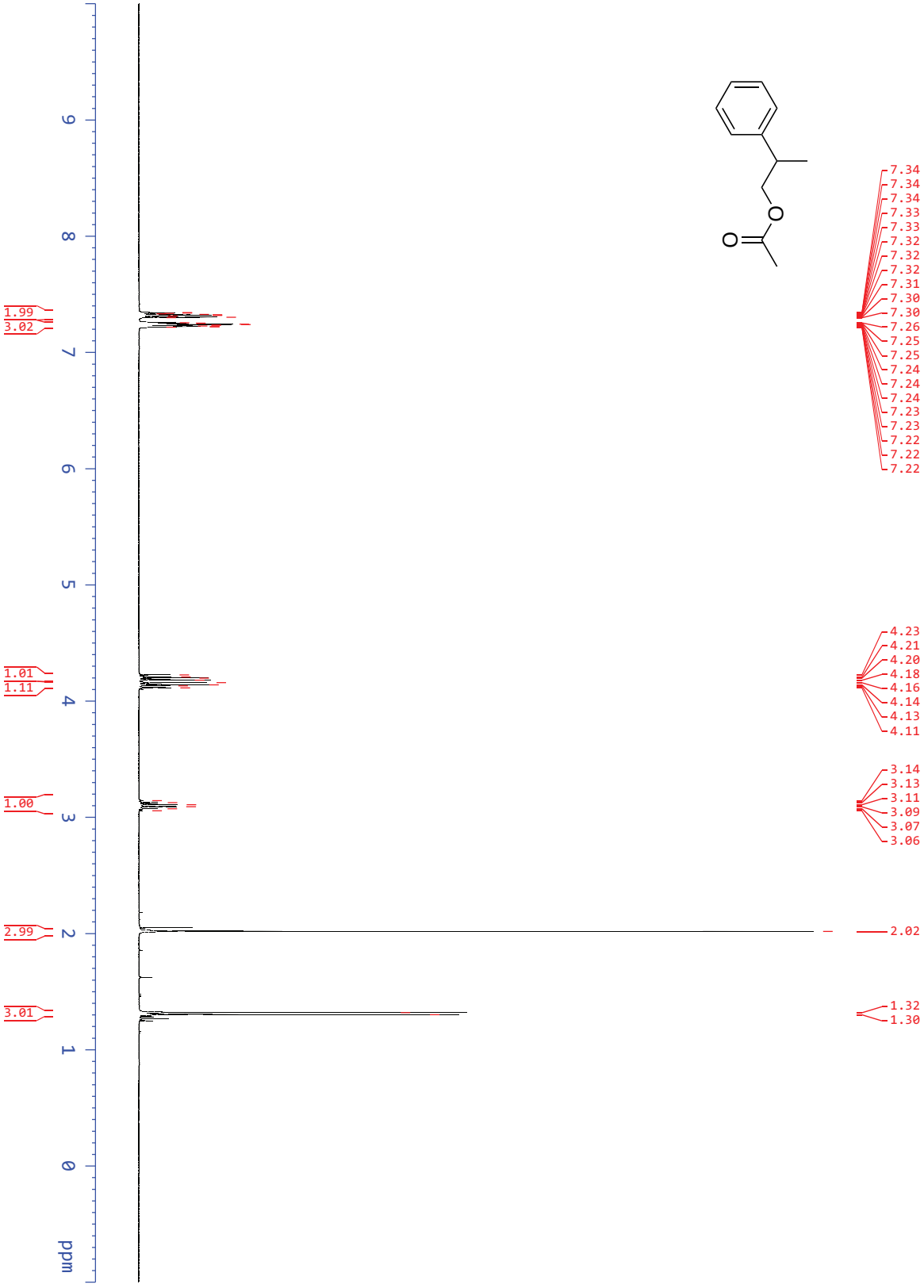


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)



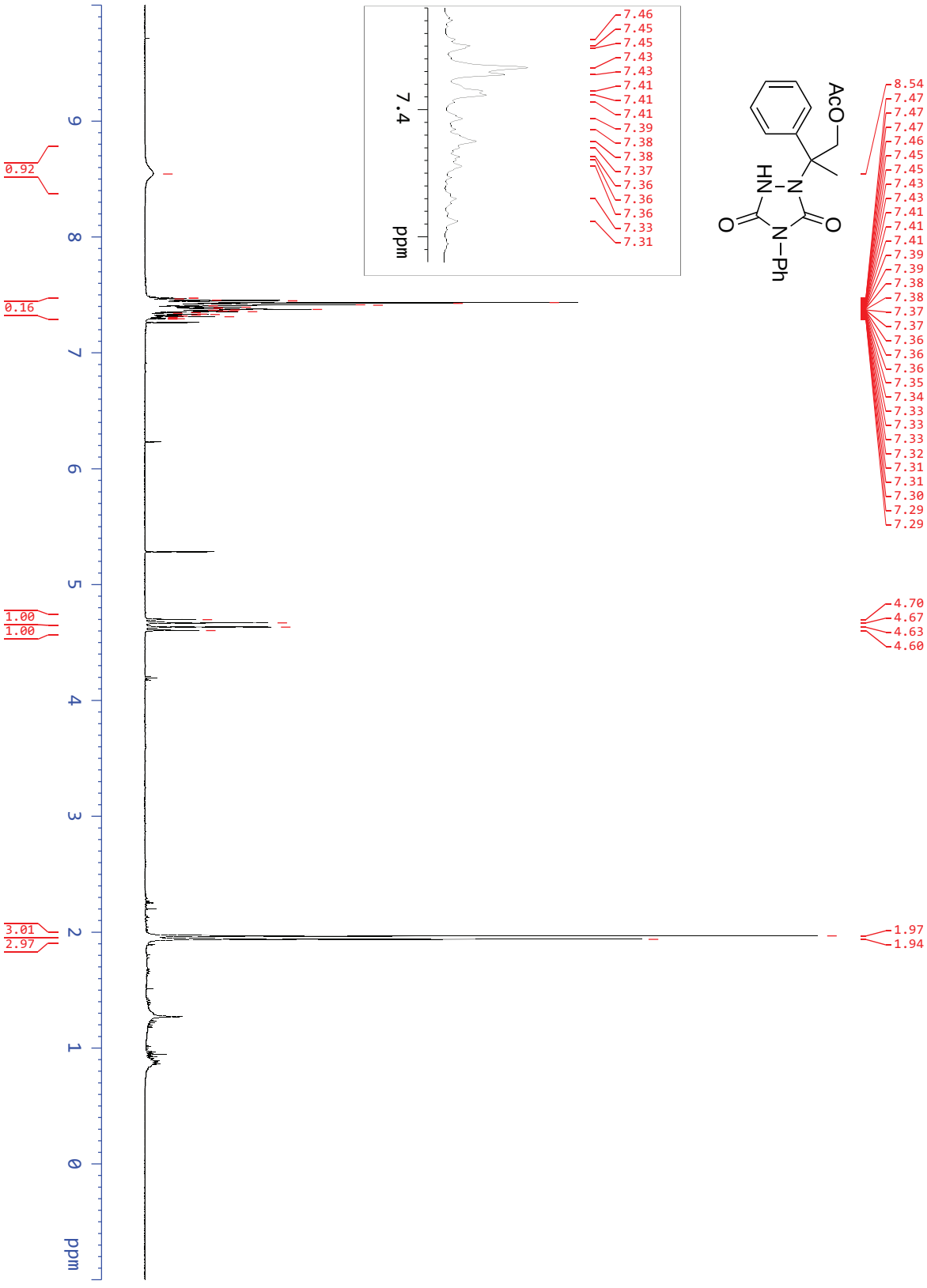
4.28 22a: 2-phenylpropyl acetate

^{1}H-NMR (400 MHz, $CDCl_3$)

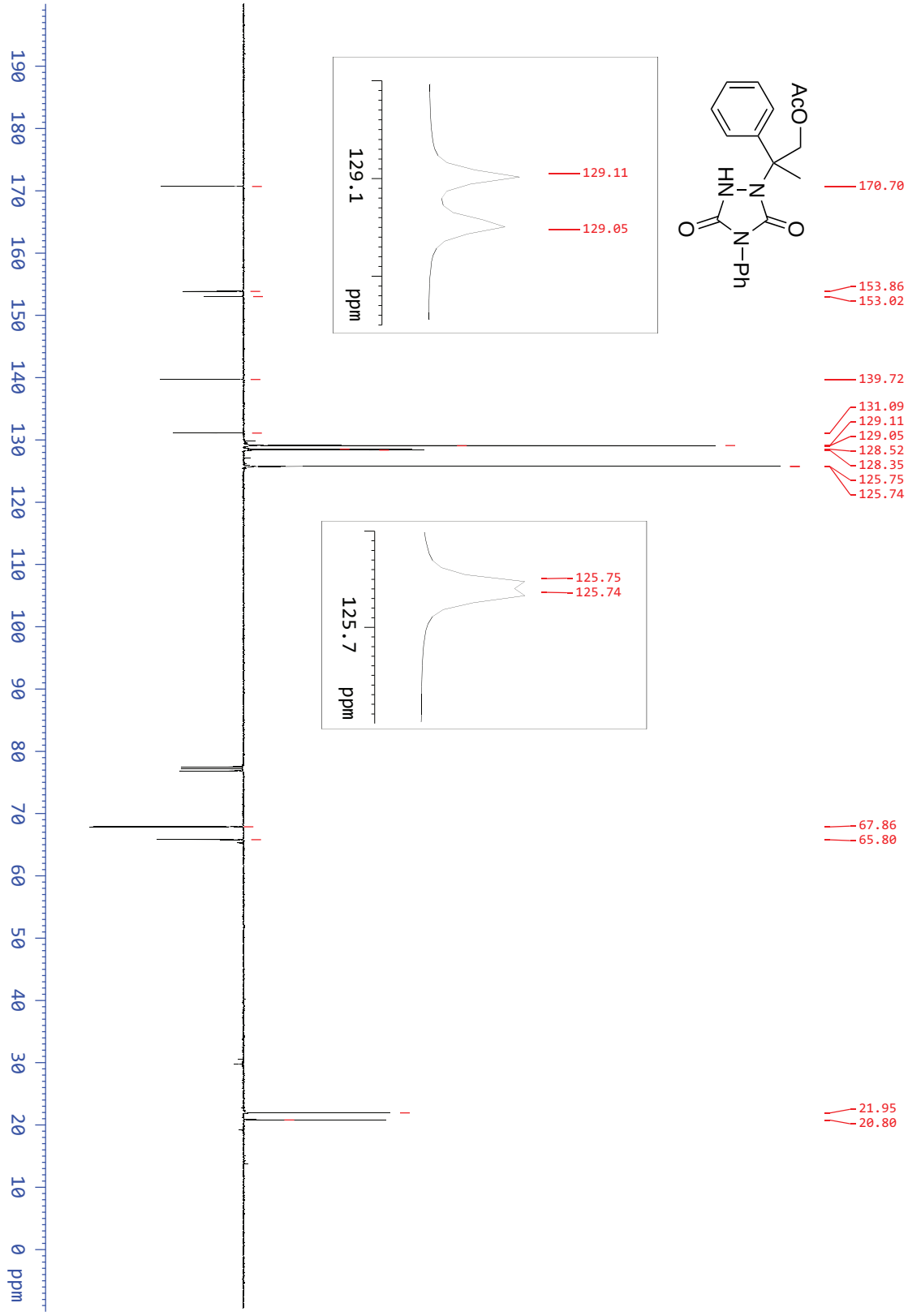


4.29 22b: 2-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-phenylpropyl acetate

^{1}H-NMR (400 MHz, $CDCl_3$ + residual DCM)



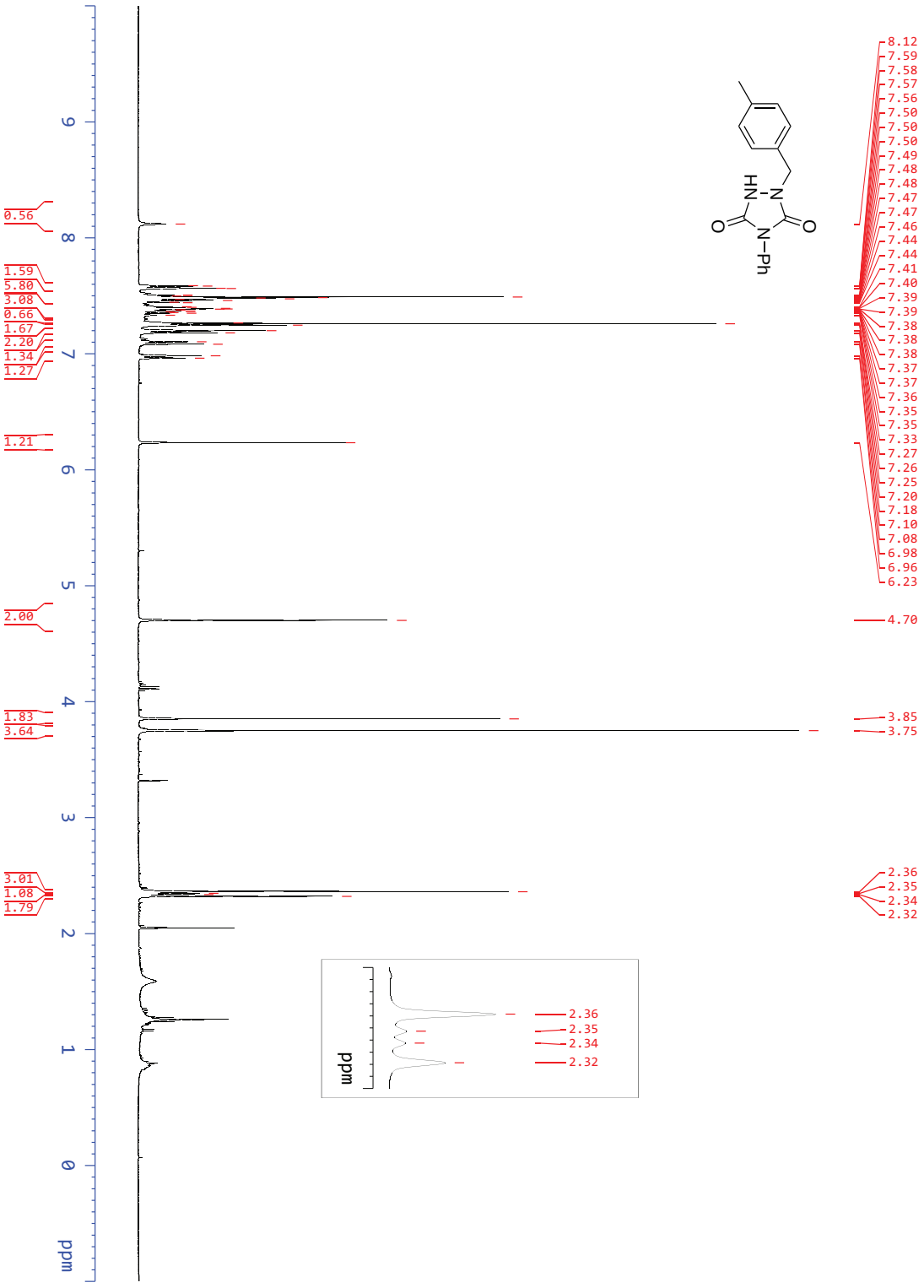
$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)



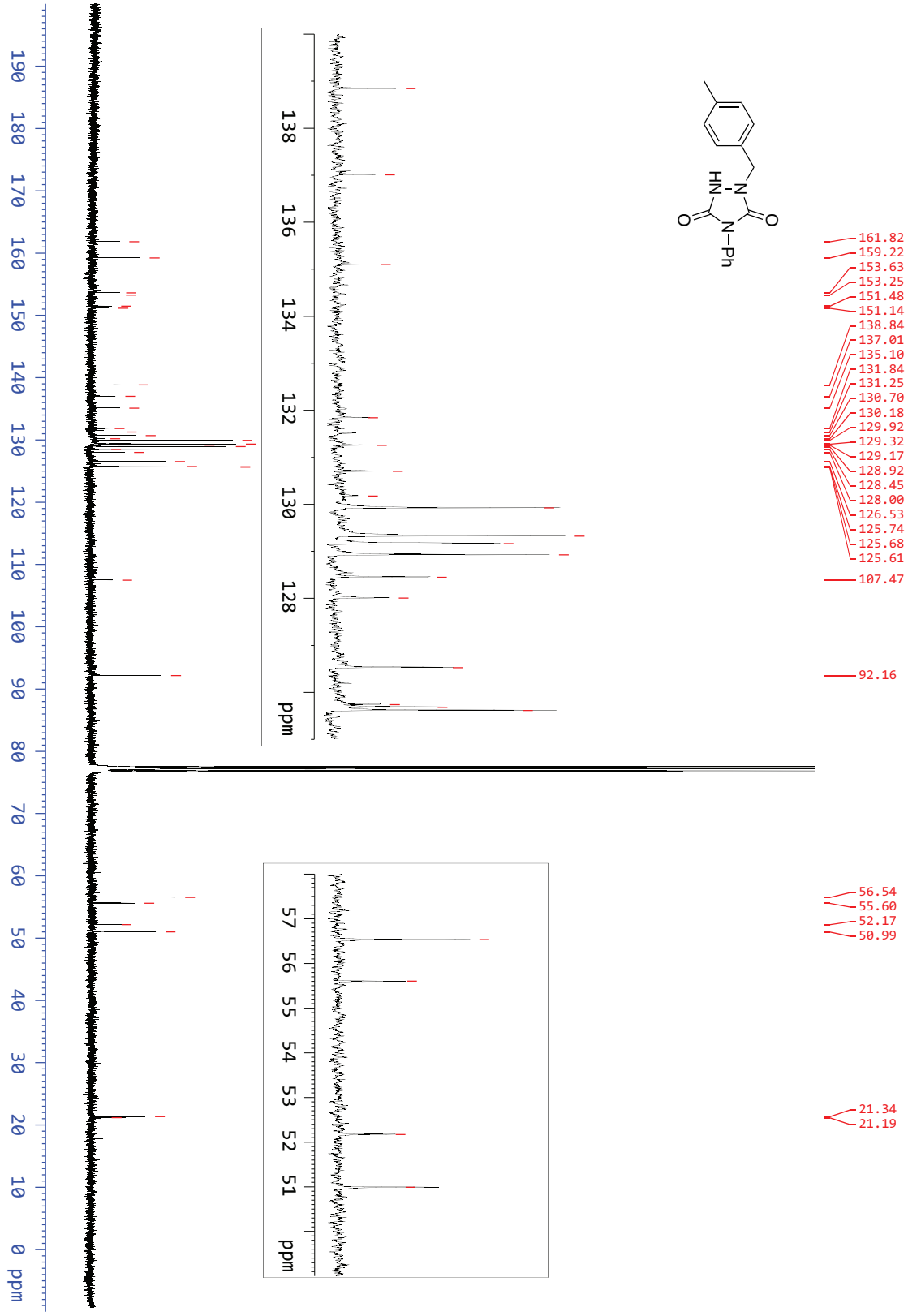
4.30 23b: 1-(4-Methylbenzyl)-4-phenylurazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **23** together with unidentified side-products*

^{1}H-NMR (400 MHz, $CDCl_3$ + residual EtOAc)

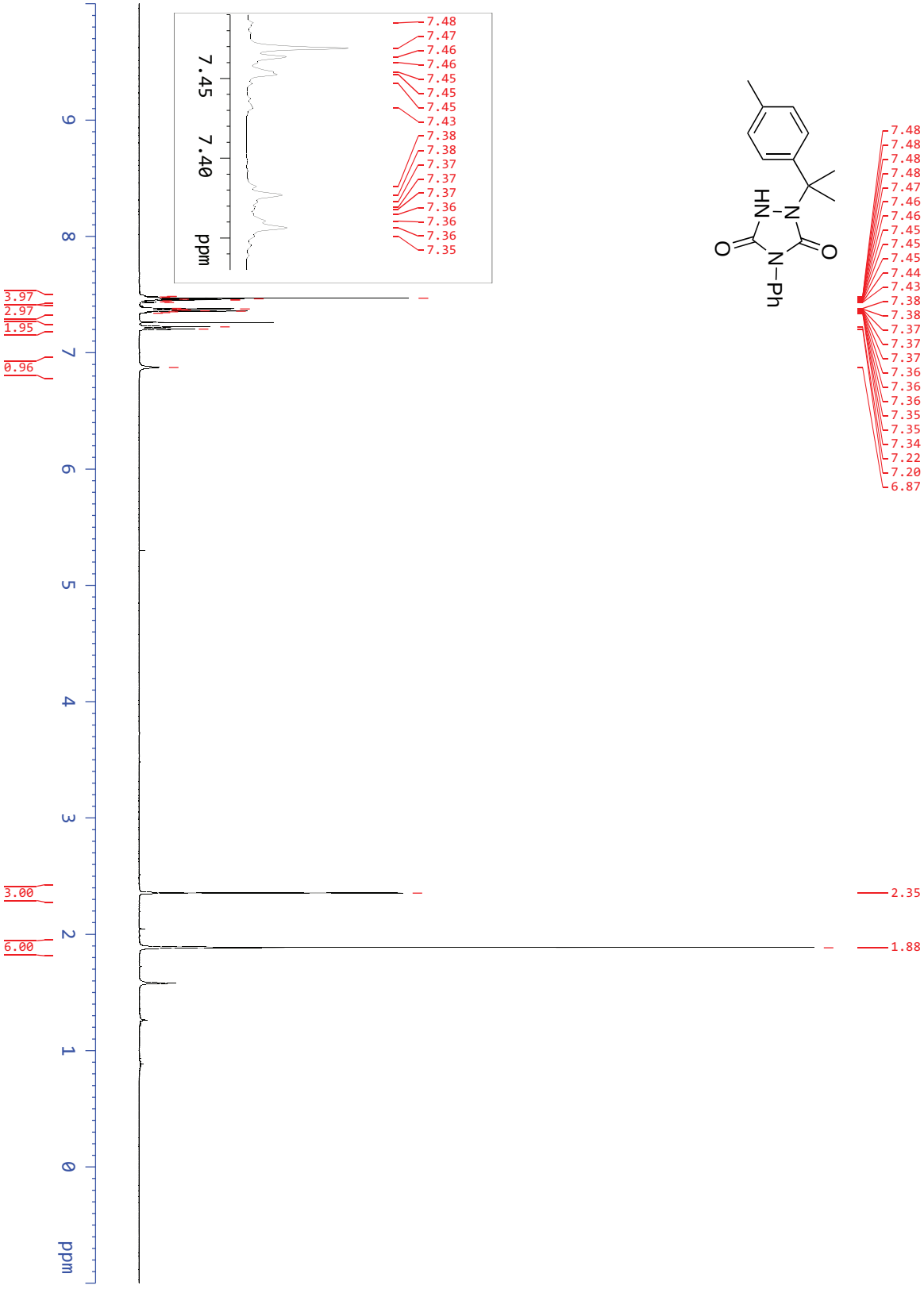


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$ + residual EtOAc)

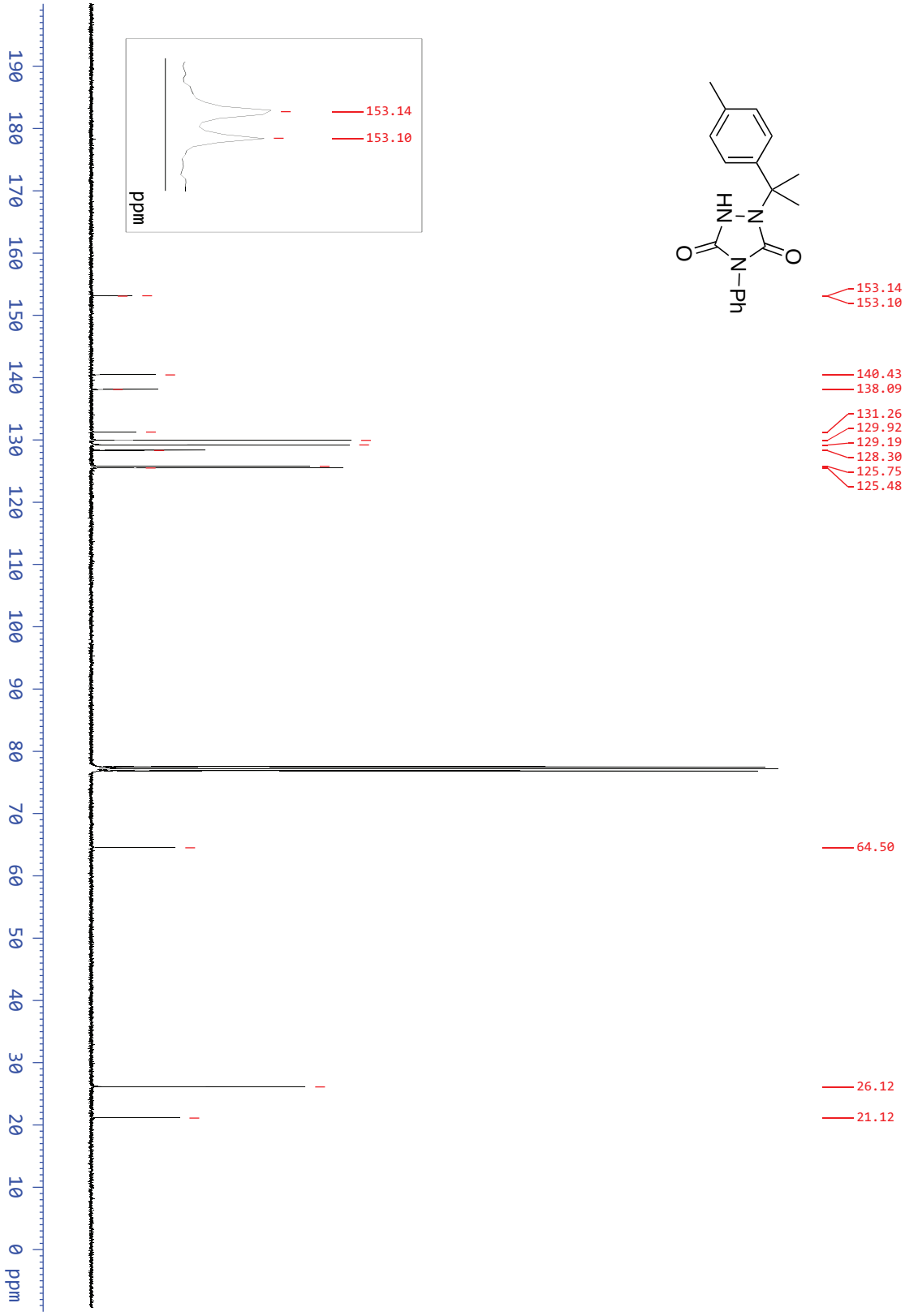


4.31 24b: 4-phenyl-1-(2-(p-tolyl)propan-2-yl)-urazole

^{1}H-NMR (400 MHz, $CDCl_3$)

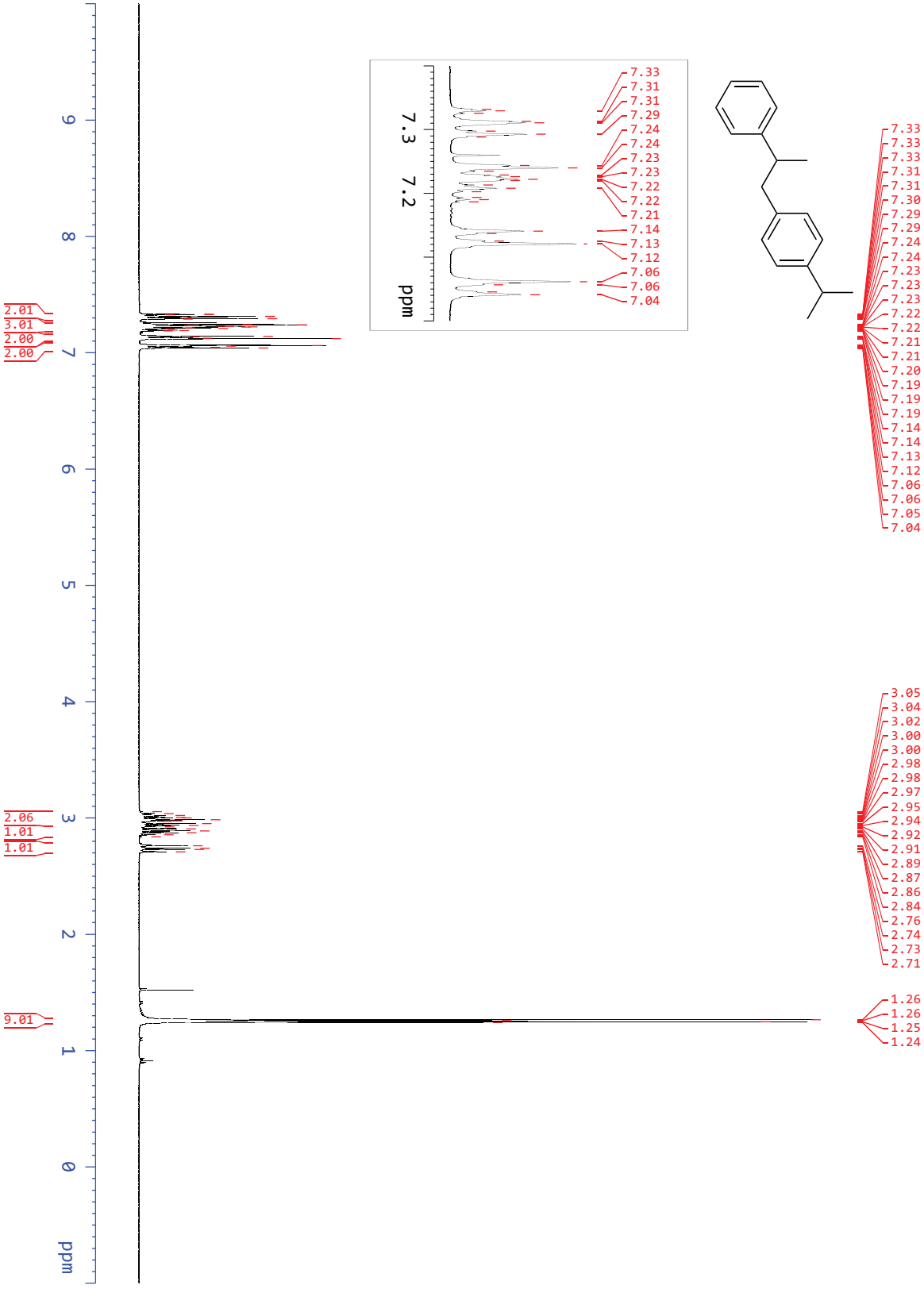


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

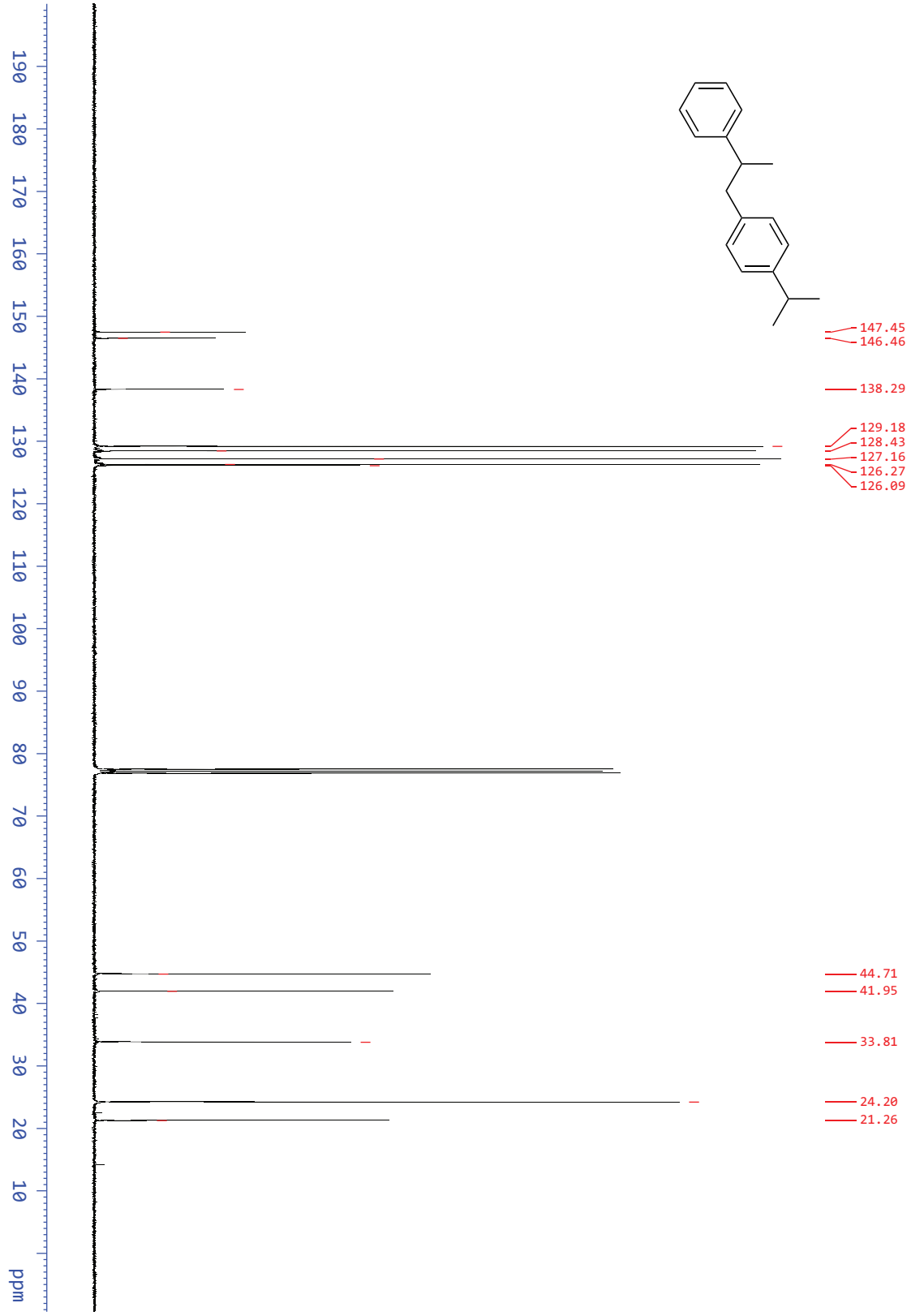


4.32 25a: 1-isopropyl-4-(2-phenylpropyl)benzene

^{1}H-NMR (400 MHz, $CDCl_3$)

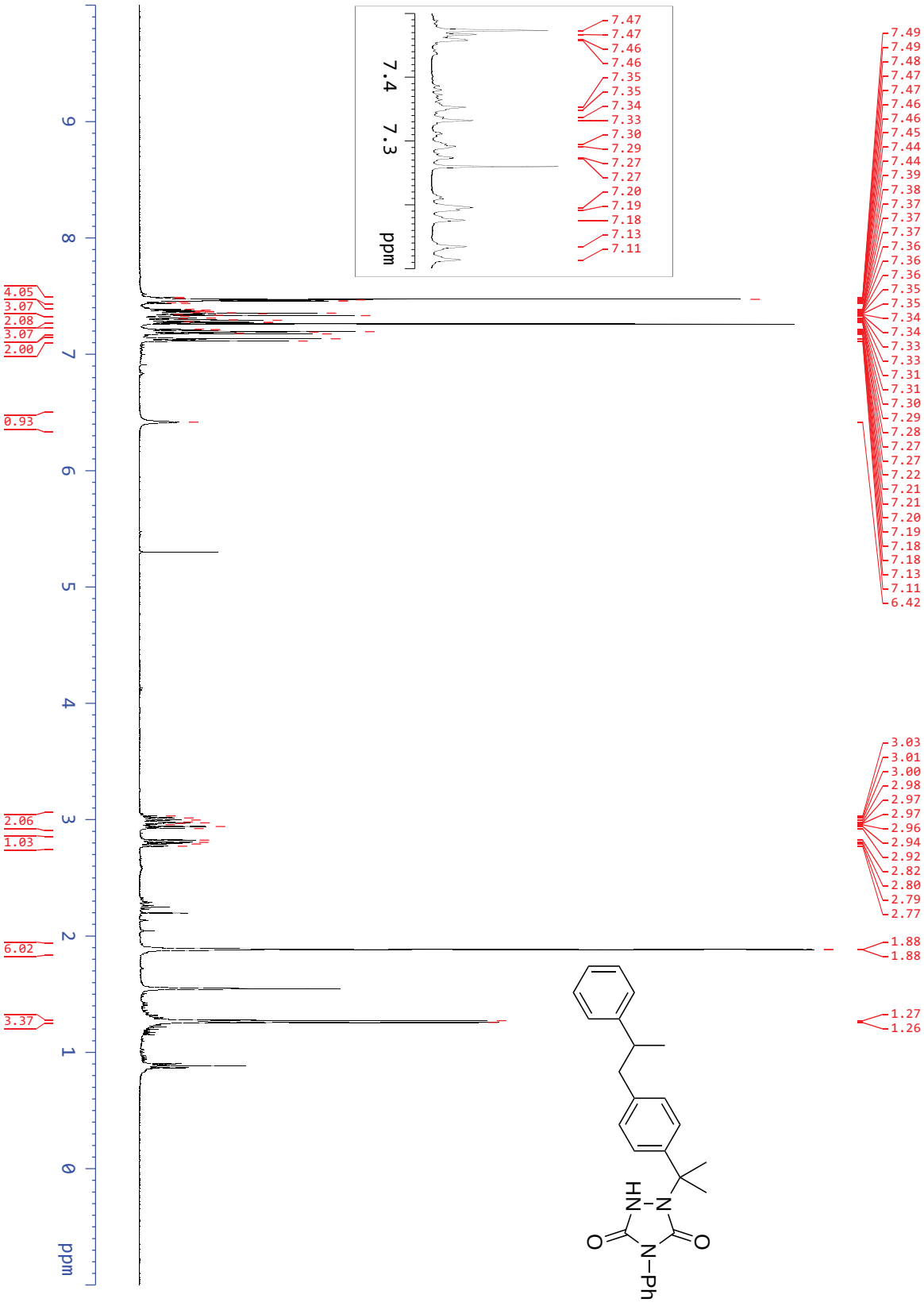


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

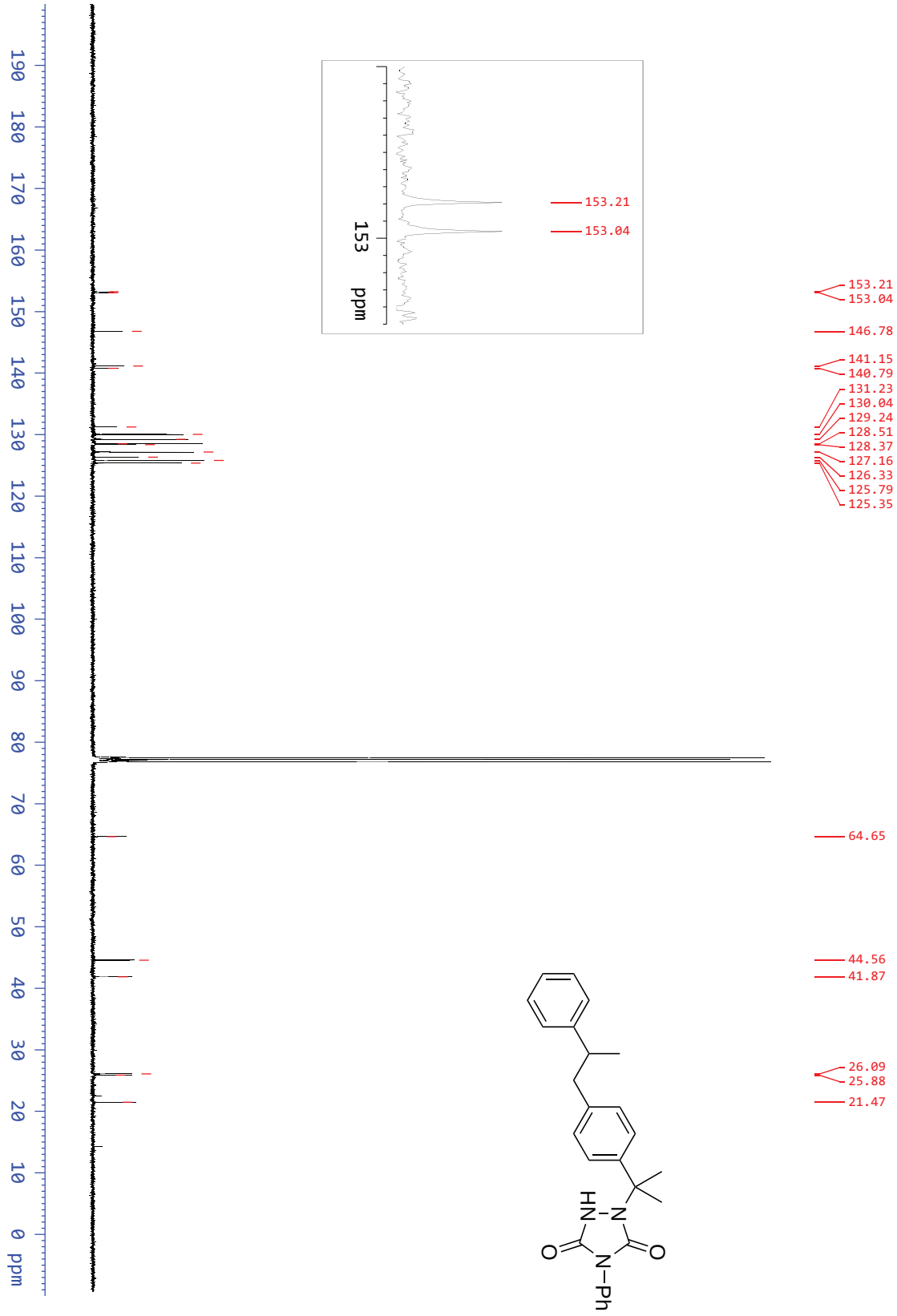


4.33 25b: 4-phenyl-1-(2-(4-(2-phenylpropyl)phenyl)propan-2-yl)-urazole

^{1}H-NMR (400 MHz, $CDCl_3$ + residual DCM)

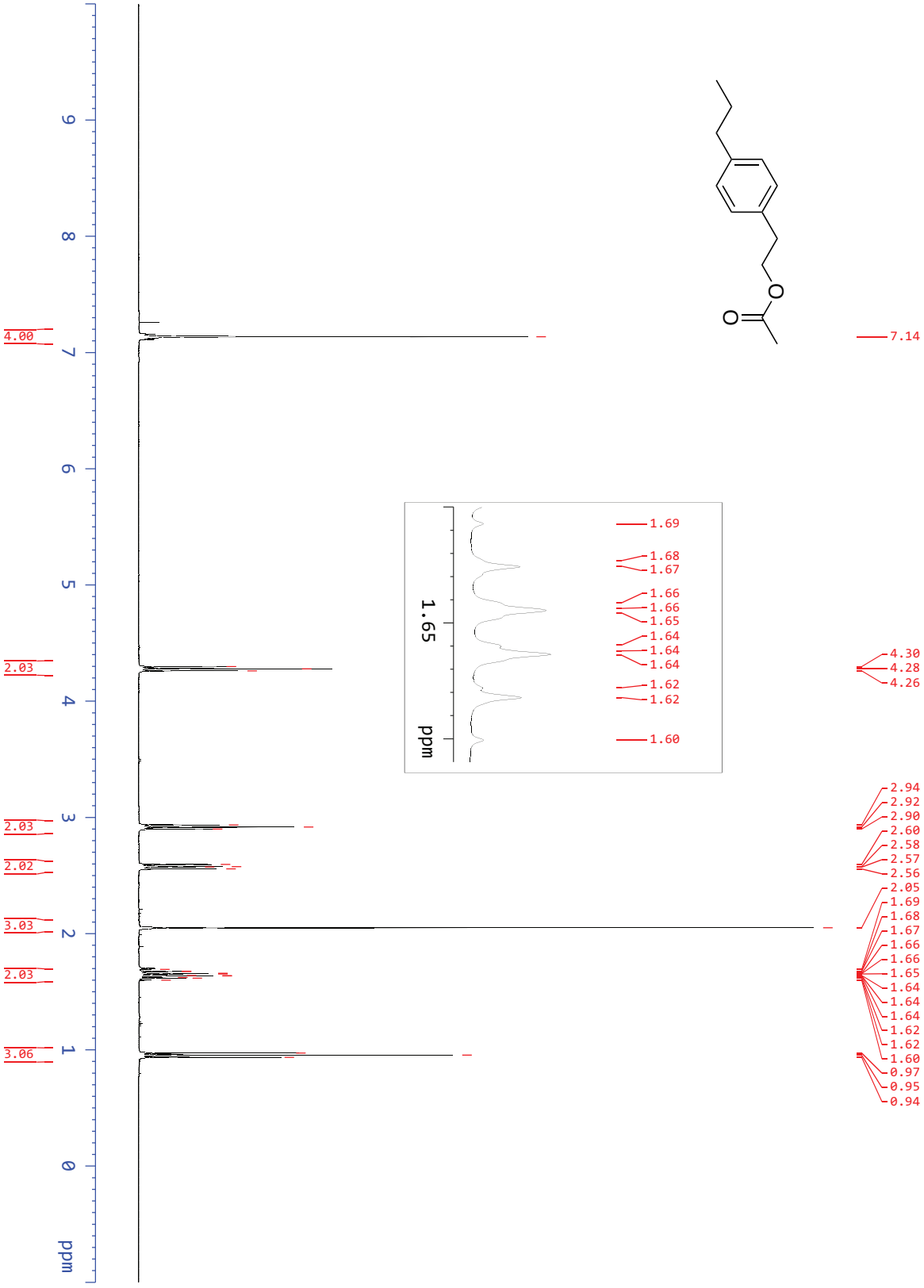


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

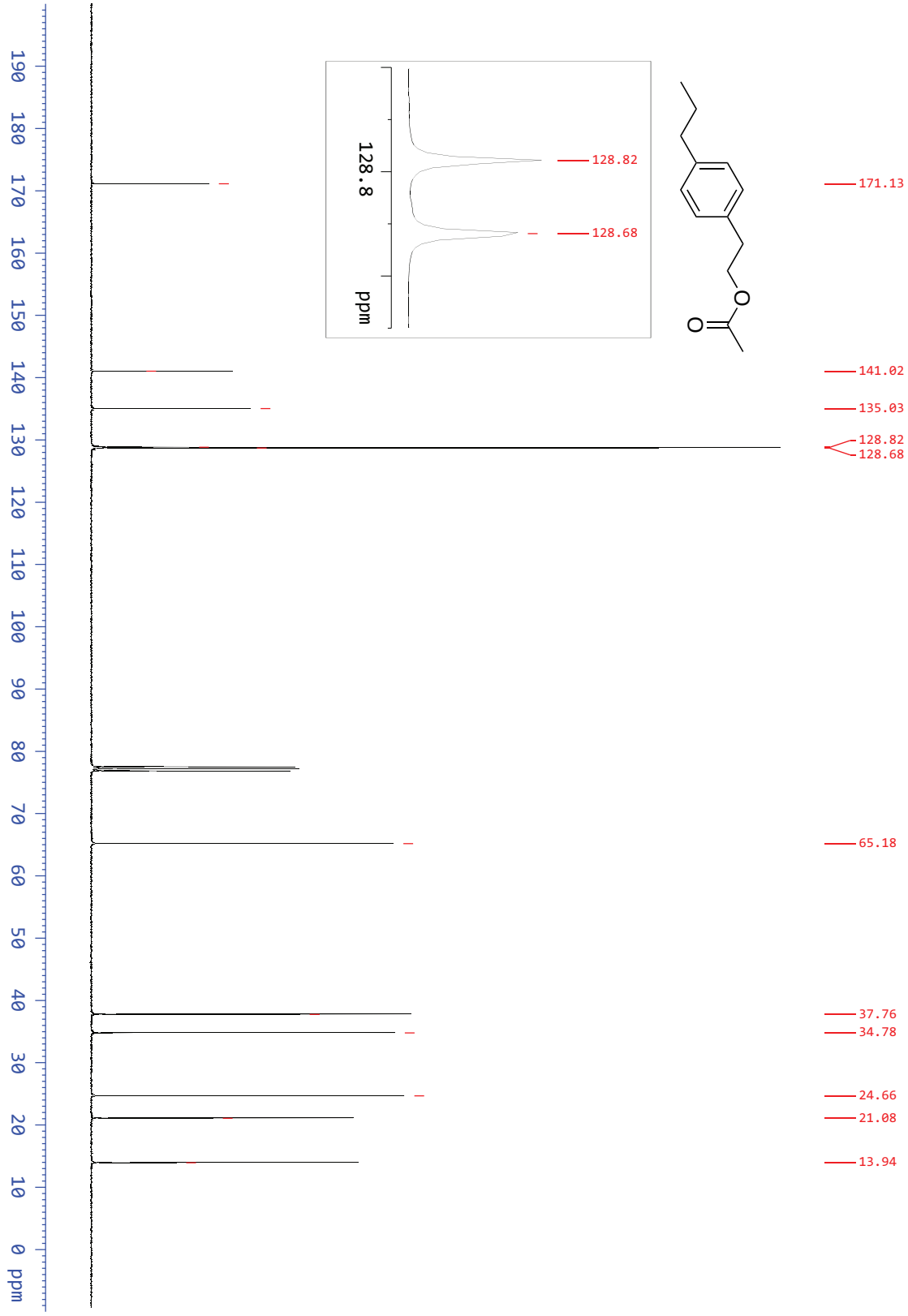


4.34 26a: 4-propylphenethyl acetate

^{1}H-NMR (400 MHz, $CDCl_3$)

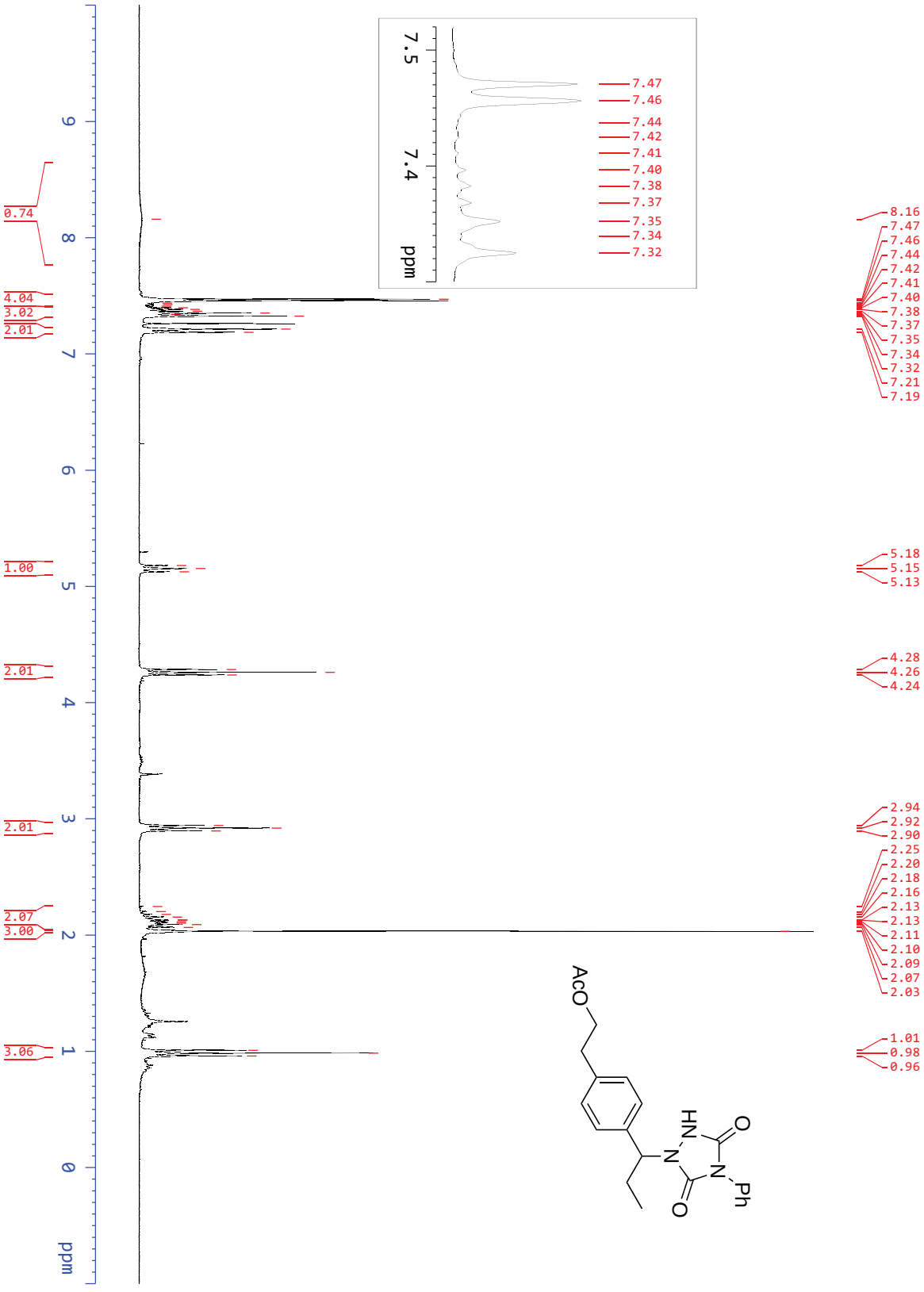


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

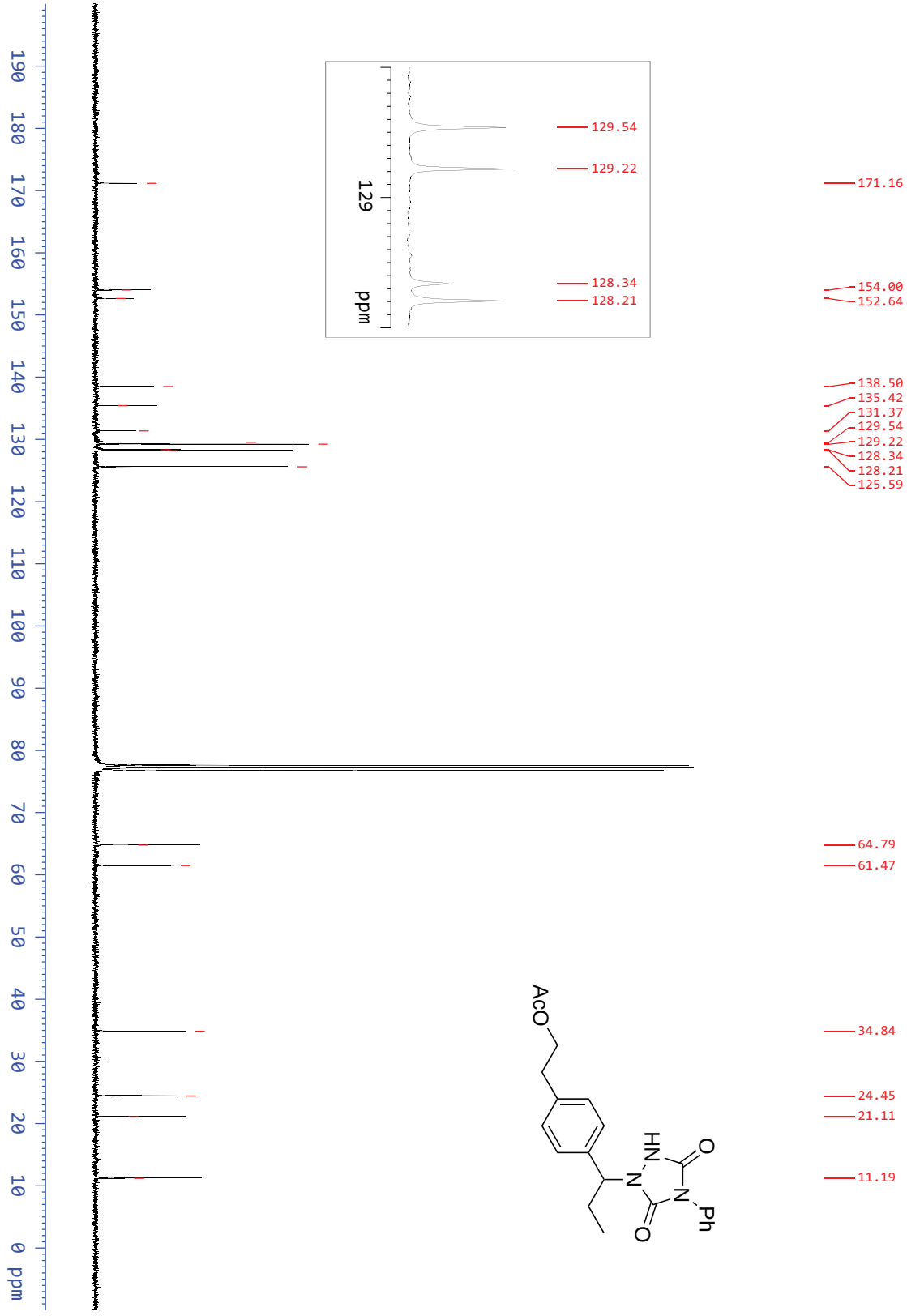


4.35 26b: 4-(1-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)propyl)phenethyl acetate

^{1}H-NMR (300 MHz, $CDCl_3$)

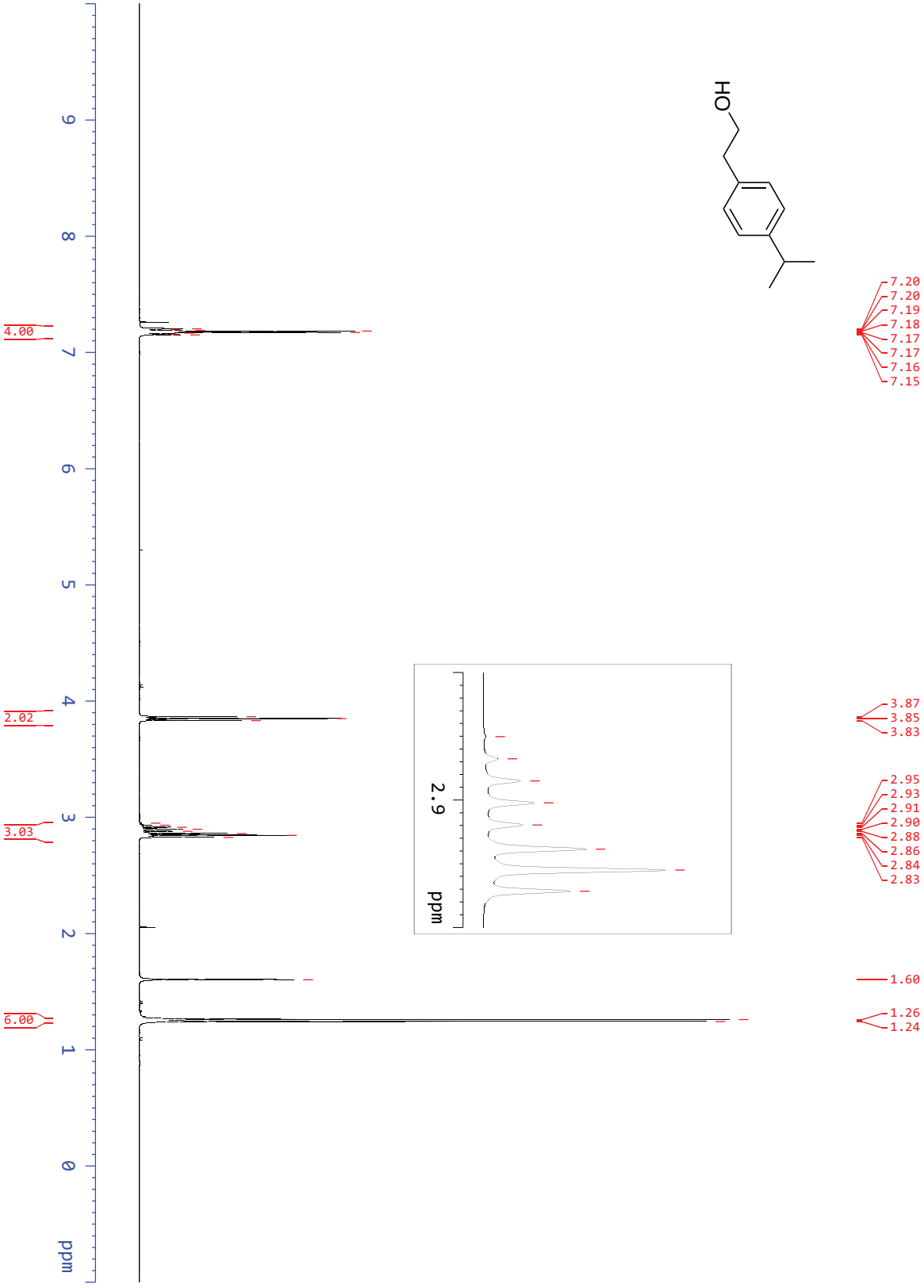


$^{13}C\{^{1}H\}$-NMR (75 MHz, $CDCl_3$)

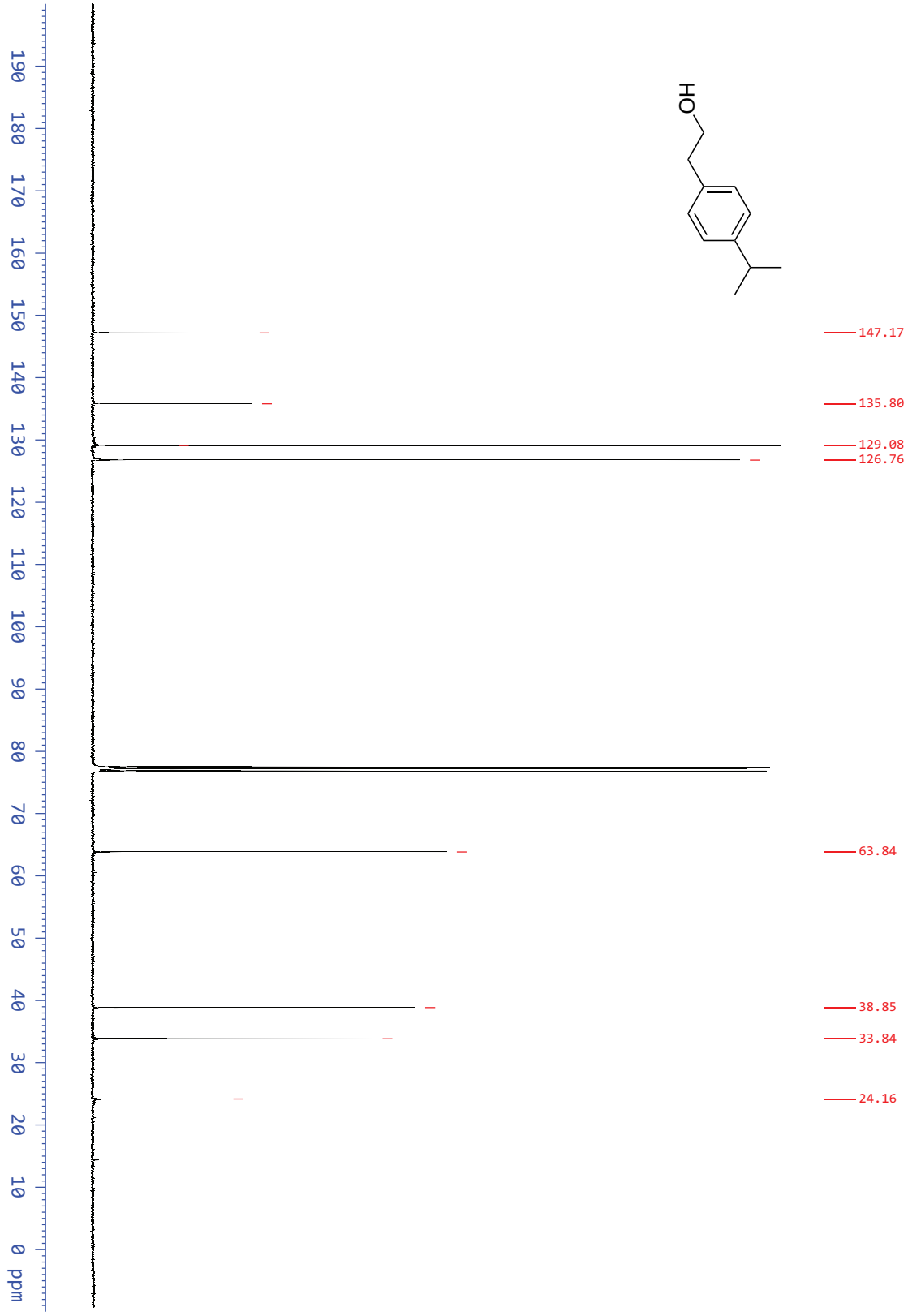


4.36 27a: 2-(4-isopropylphenyl)ethan-1-ol

^{1}H-NMR (400 MHz, $CDCl_3$)

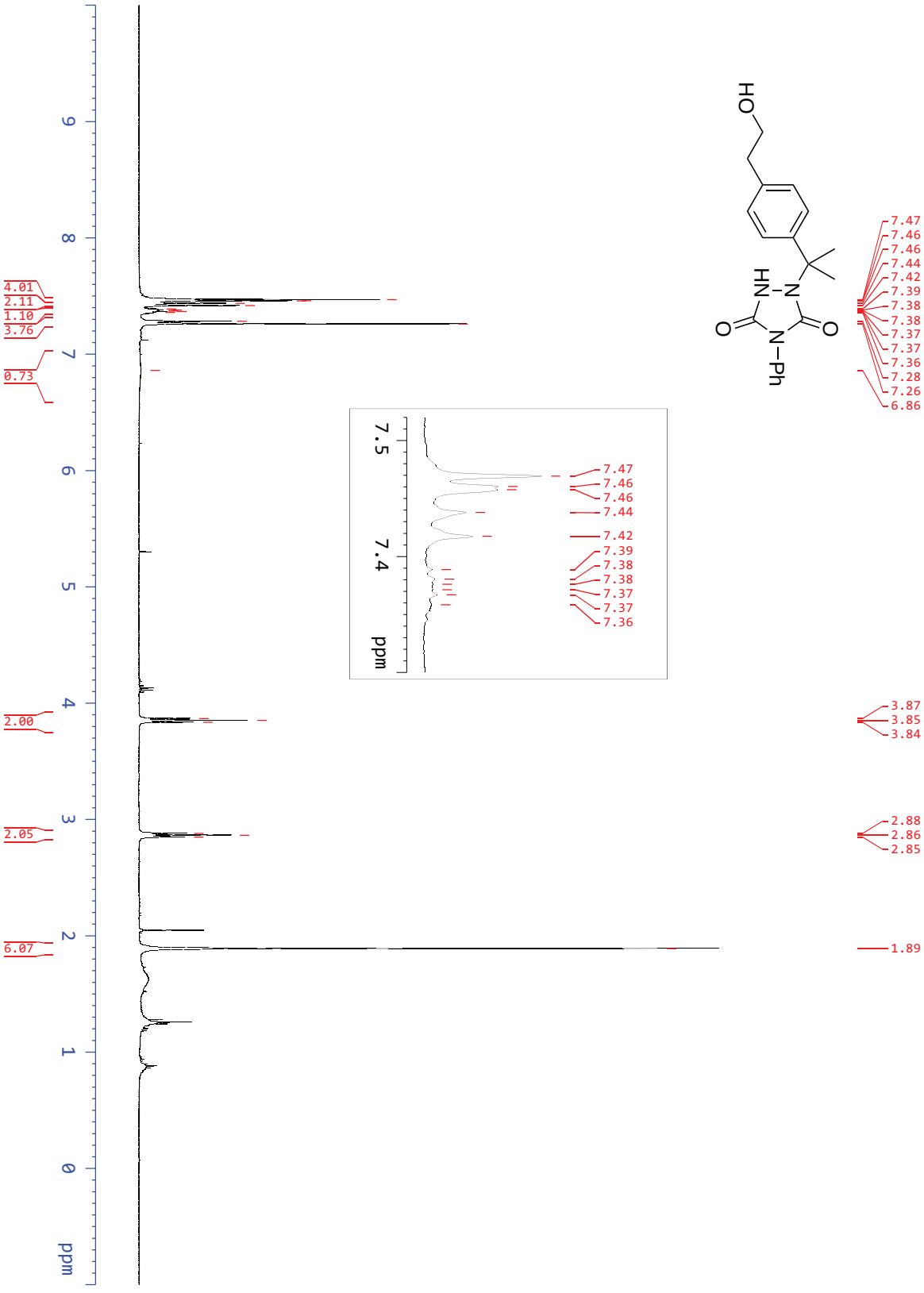


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

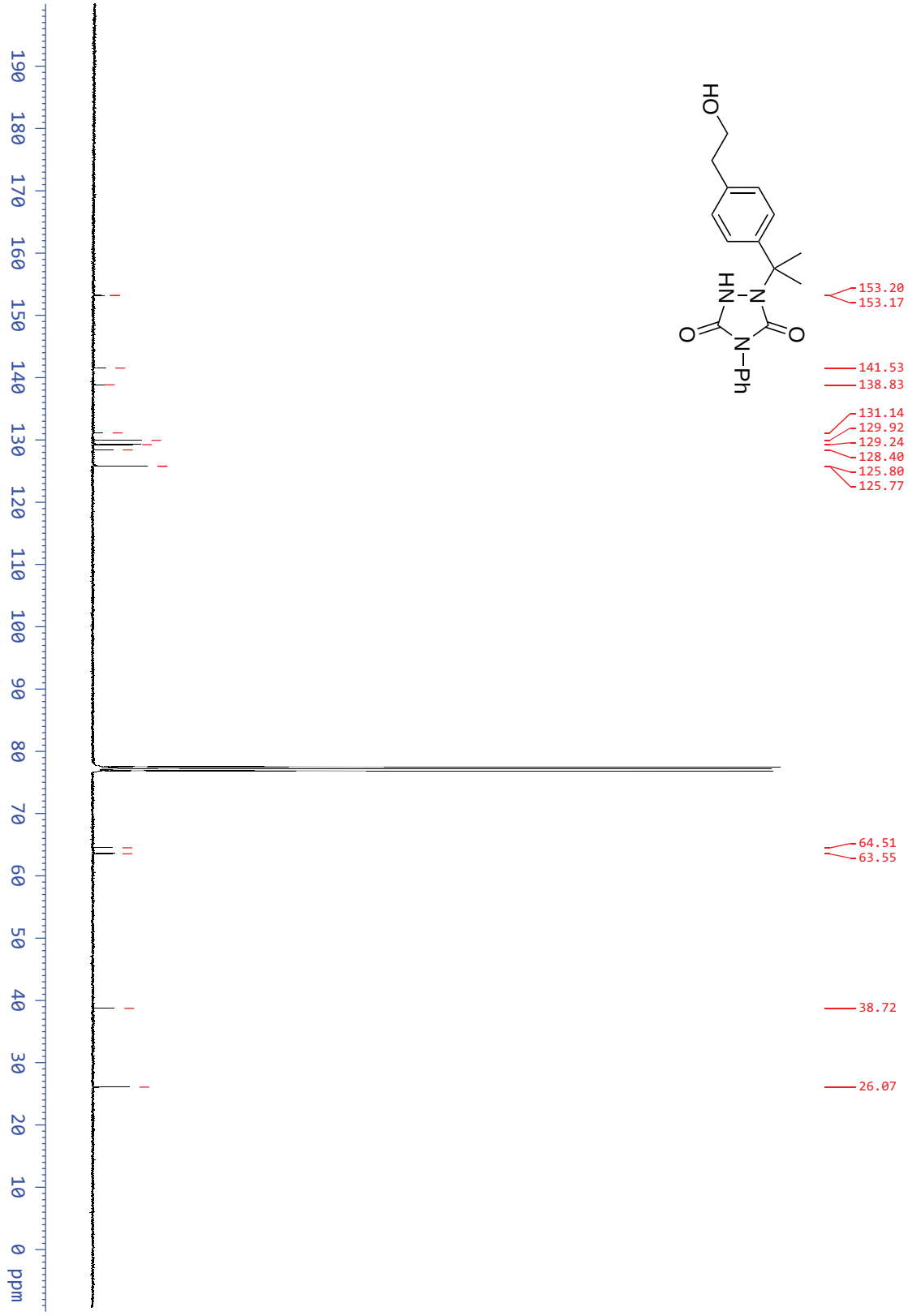


4.37 27b: 1-(2-(4-(2-hydroxyethyl)phenyl)propan-2-yl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$ + residual EtOAc)

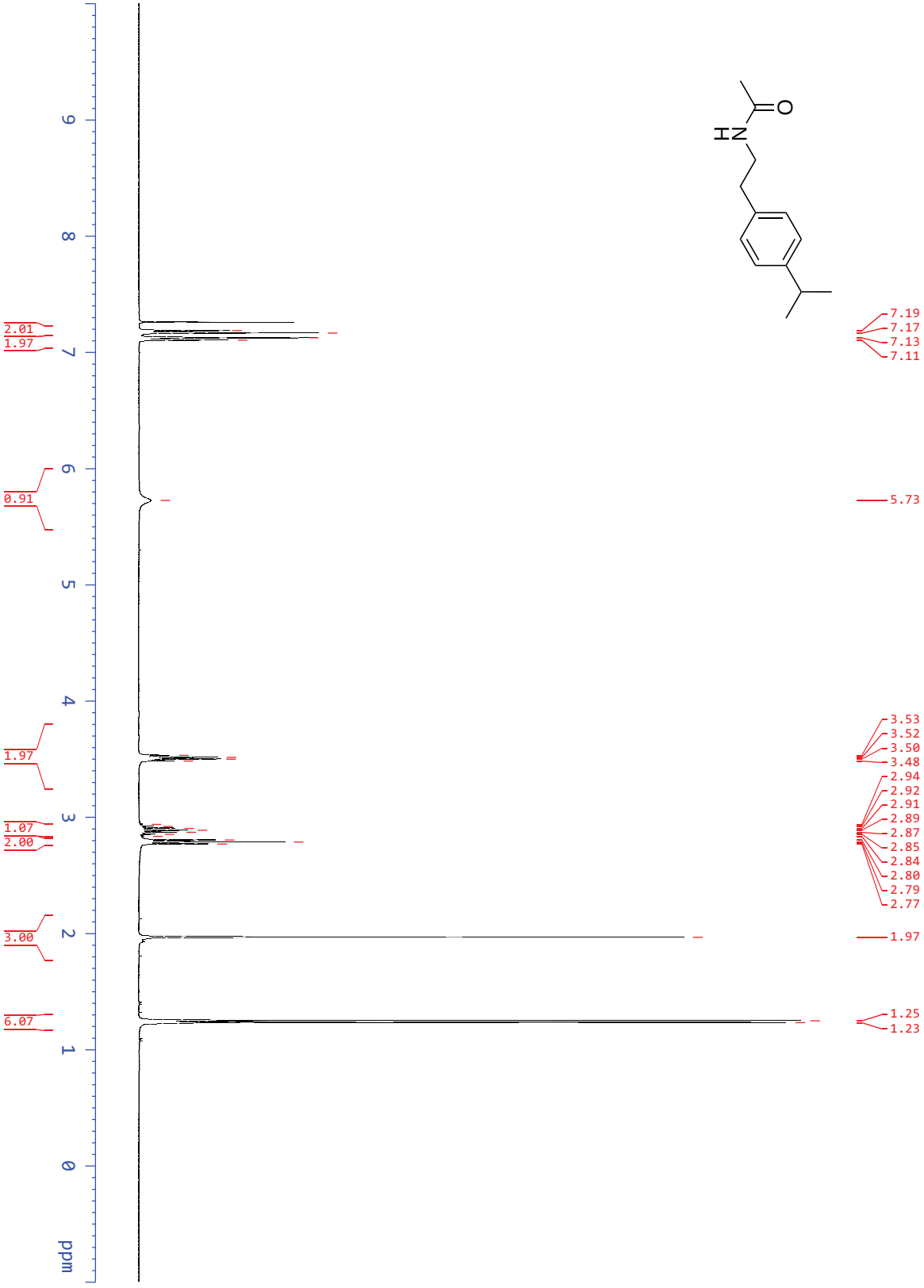


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

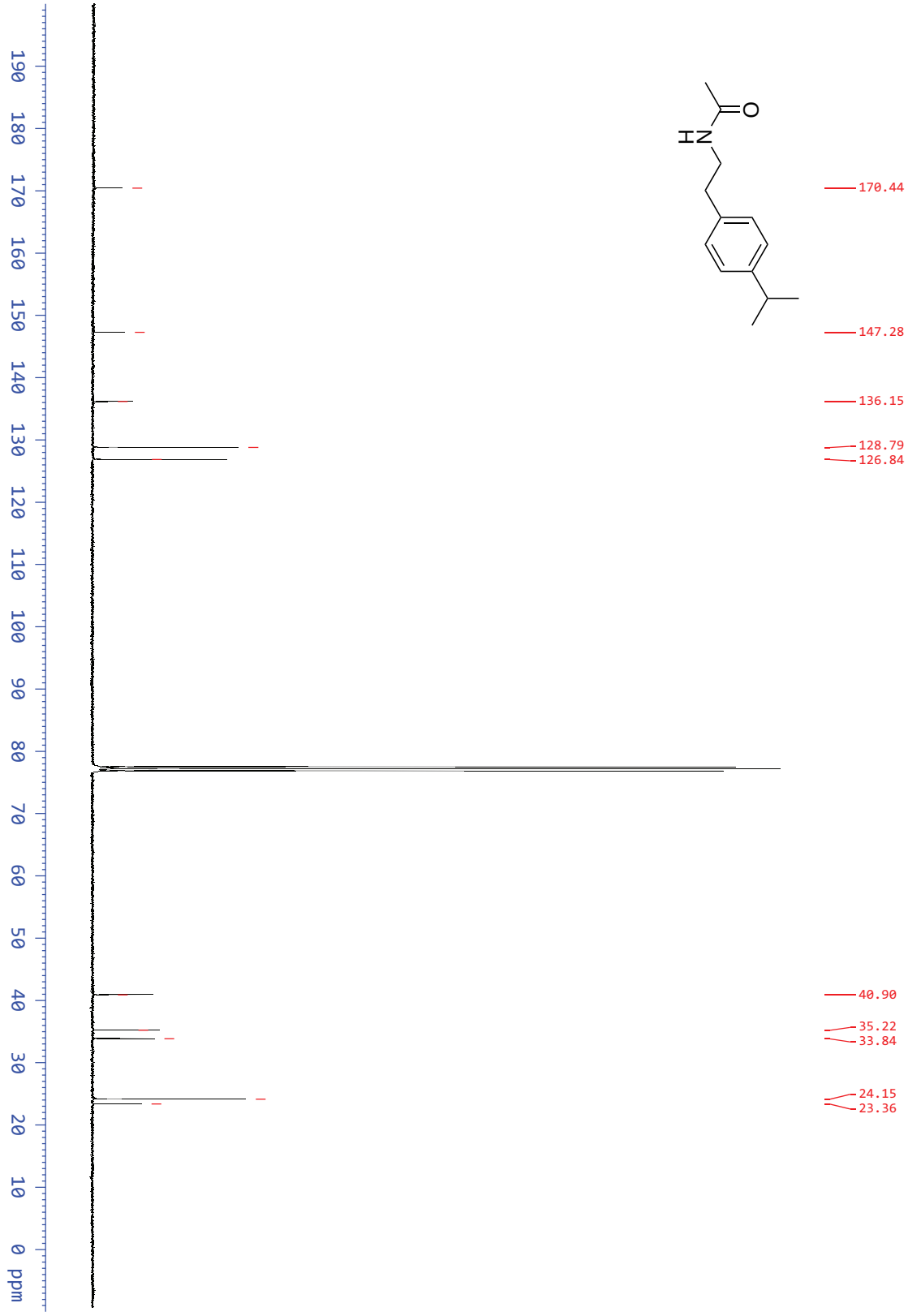


4.38 28a: N-(4-isopropylphenethyl)acetamide

^{1}H-NMR (400 MHz, $CDCl_3$)

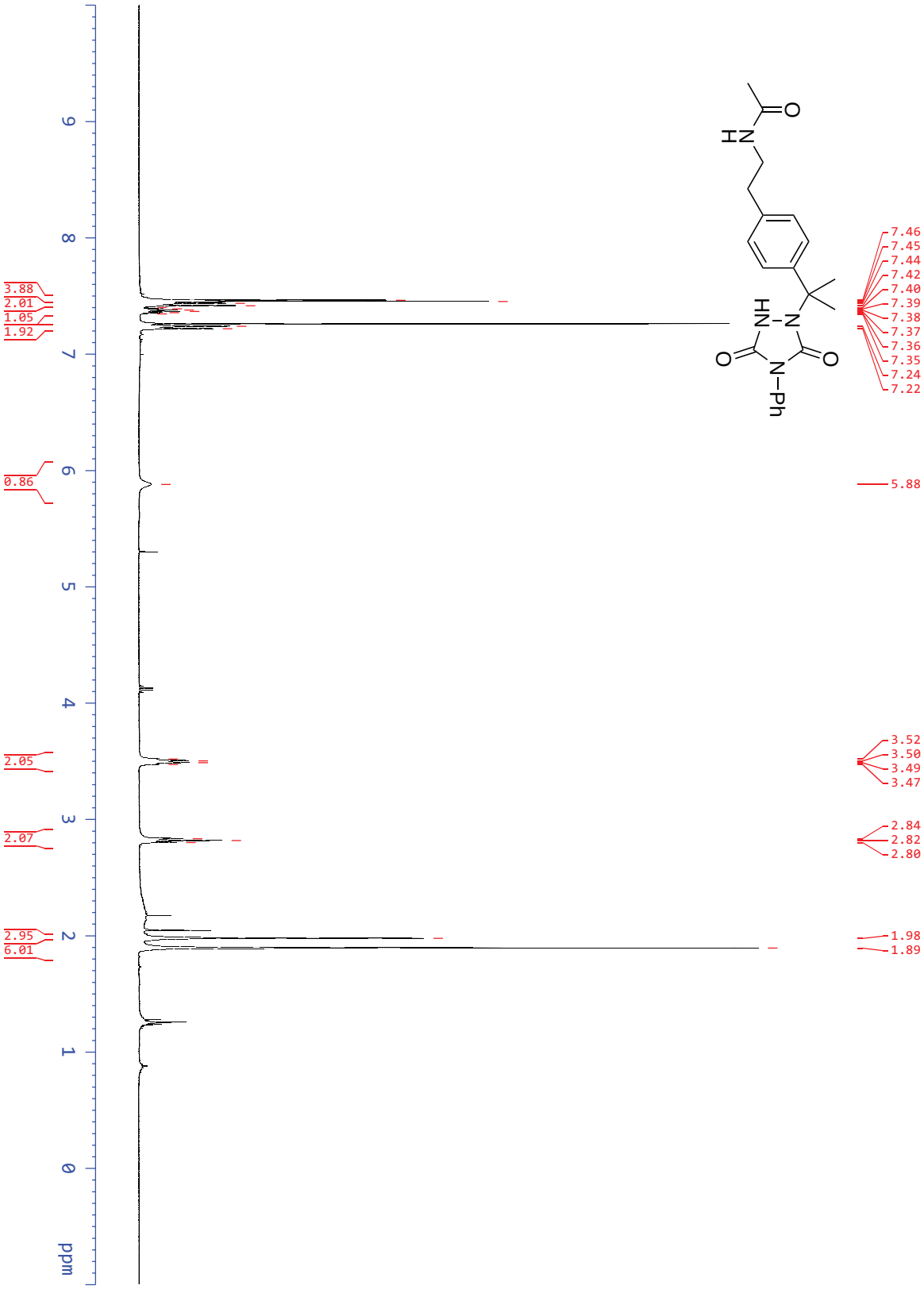


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

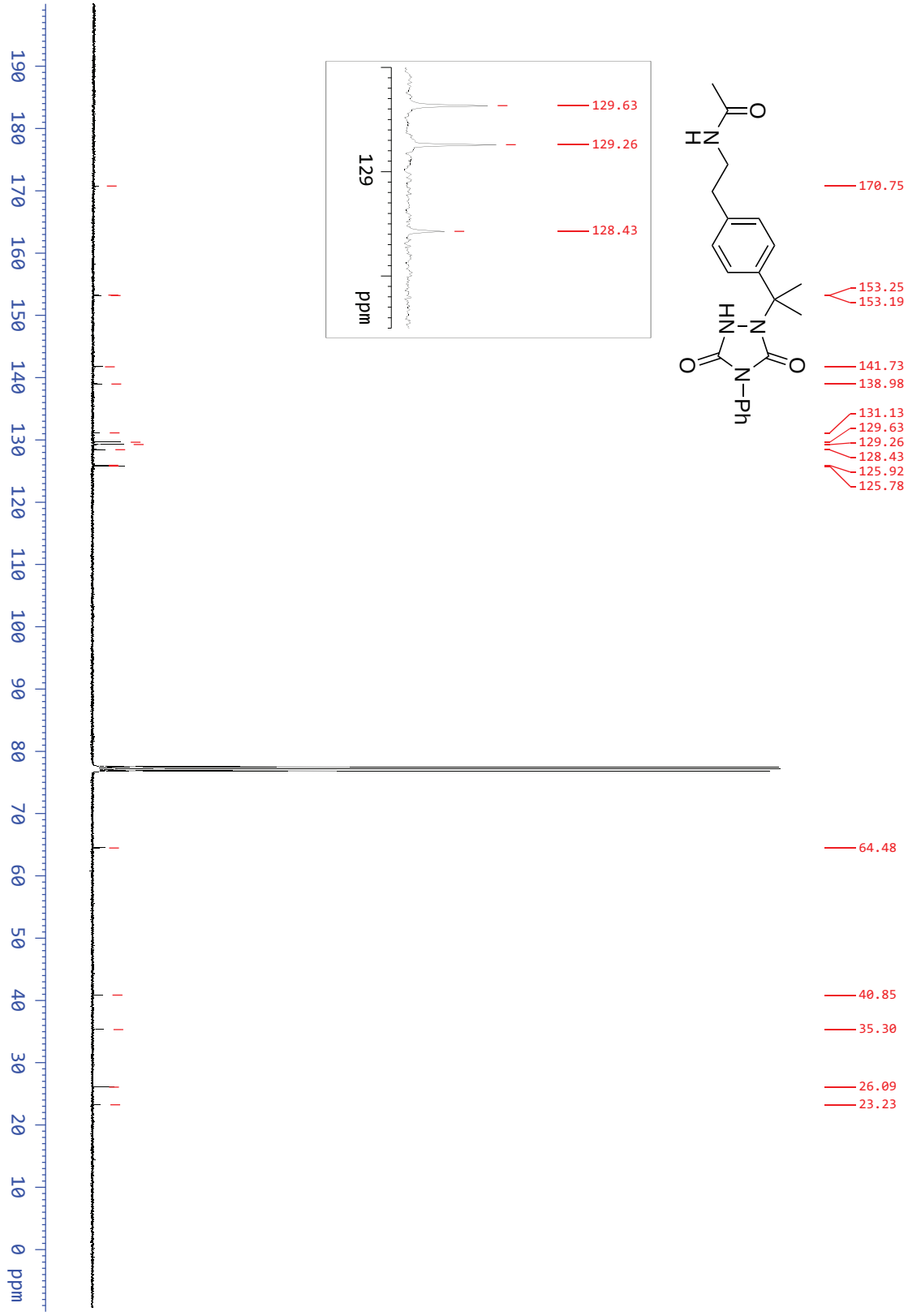


4.39 28b: N-(4-(2-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)propan-2-yl)phenethyl)acetamide

^{1}H-NMR (400 MHz, $CDCl_3$ + residual EtOAc)

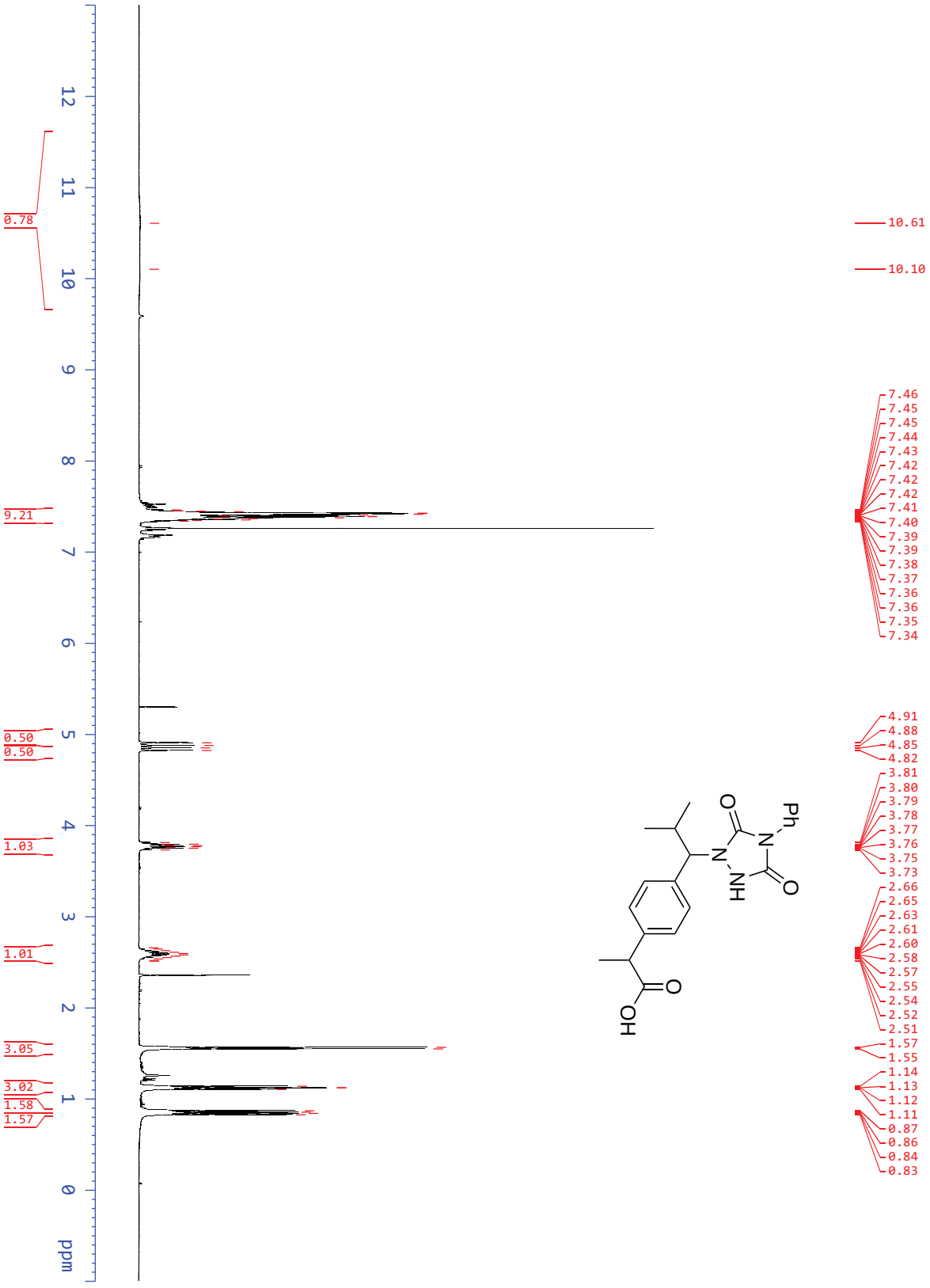


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$ + residual EtOAc)



4.40 29b: 2-(4-(1-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-methylpropyl)phenyl)propanoic acid

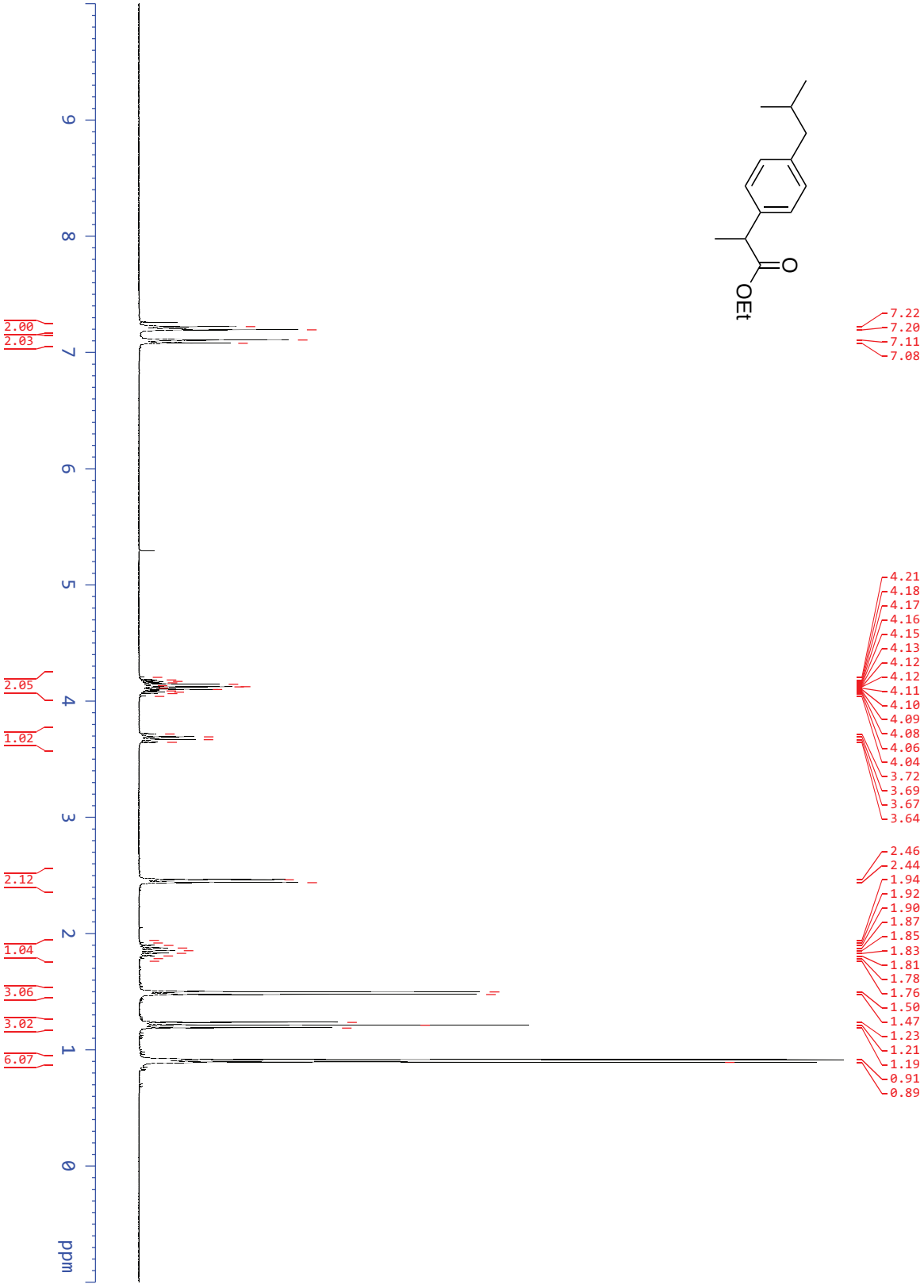
^{1}H-NMR (400 MHz, $CDCl_3$ + residual toluene)



$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

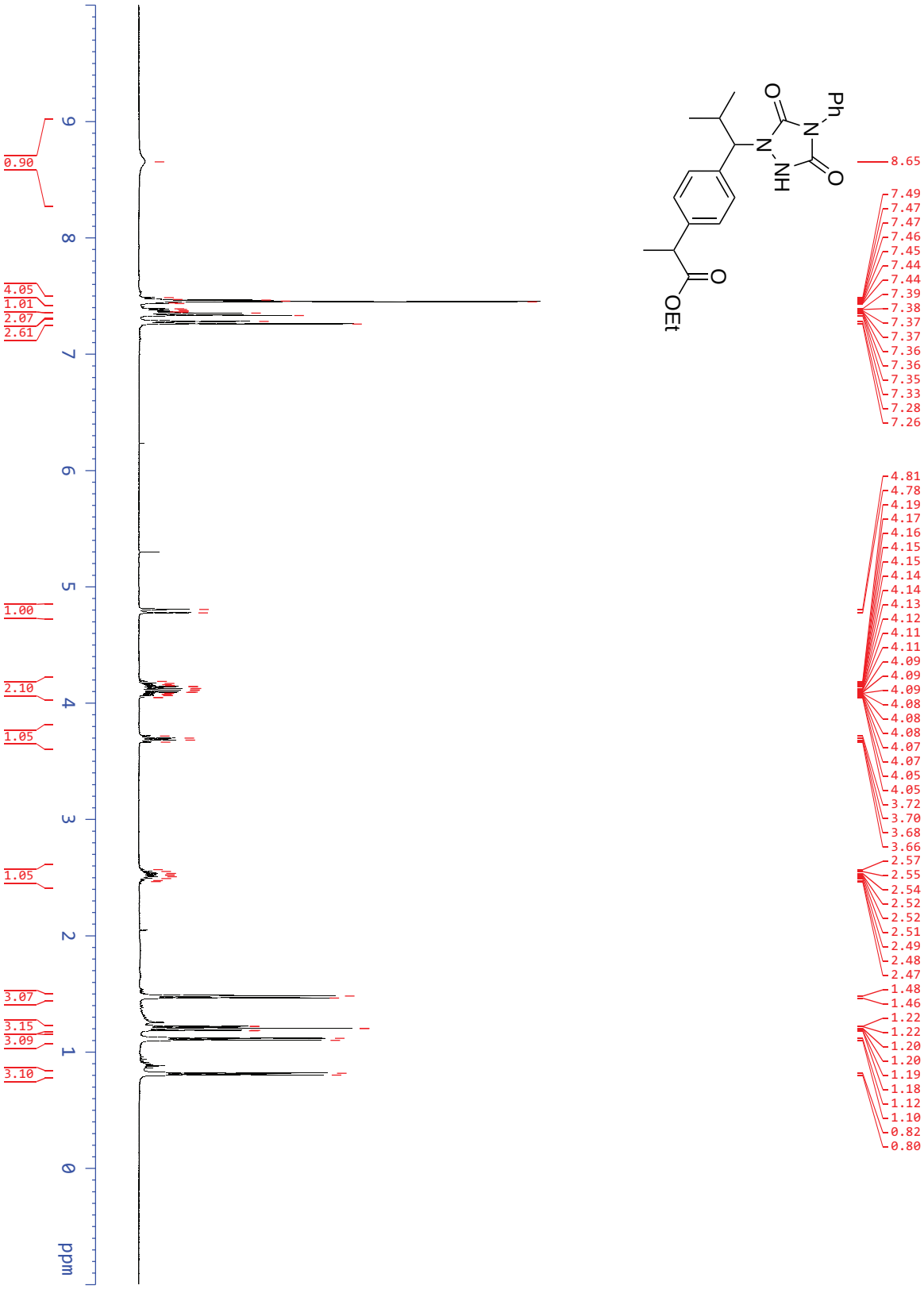
4.41 30a: ibuprofen ethyl ester

^{1}H-NMR (300 MHz, $CDCl_3$)

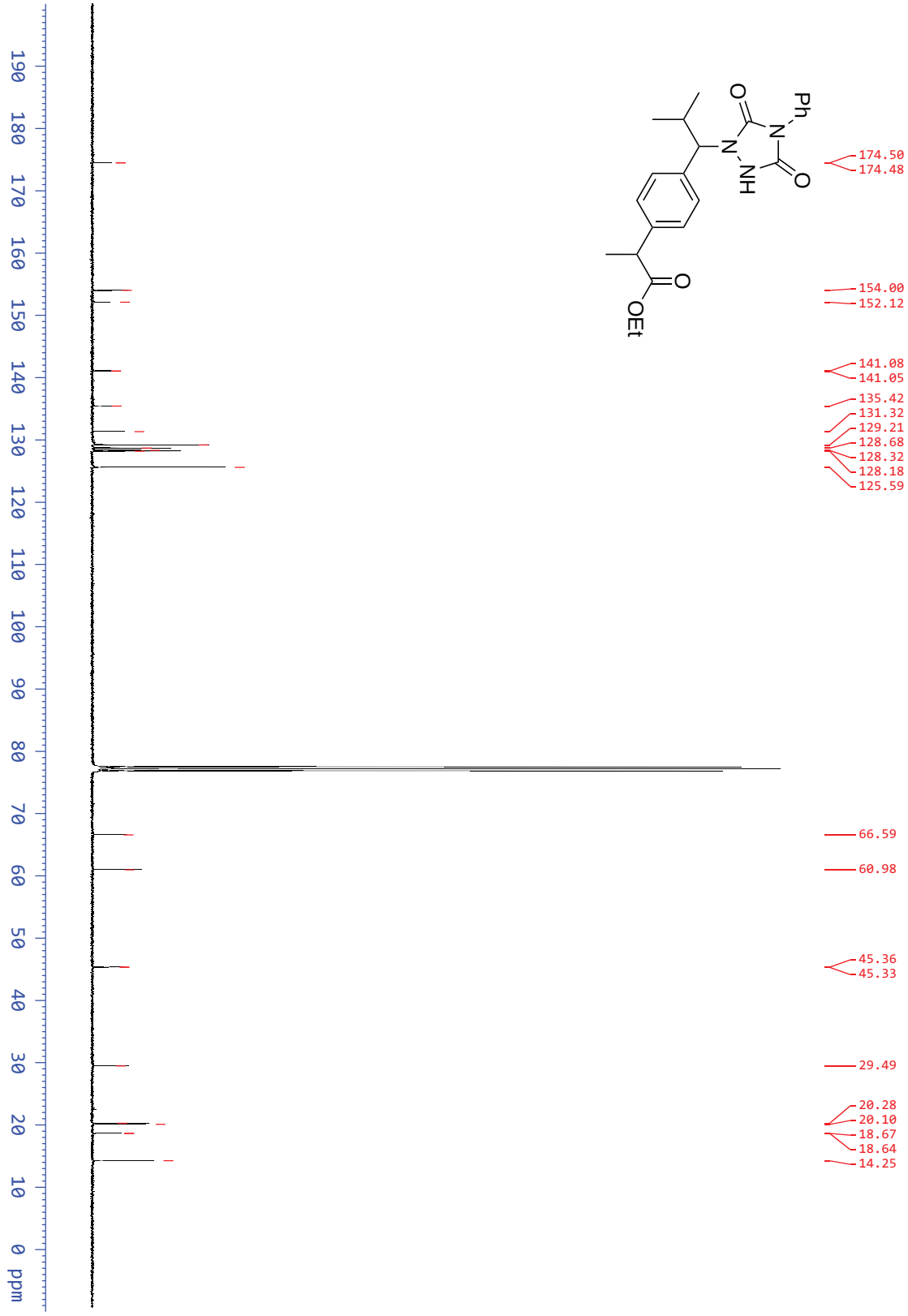


4.42 30b: ethyl 2-(4-(1-(3,5-dioxo-4-phenyl-1,2,4-triazolidin-1-yl)-2-methylpropyl)phenyl)propanoate

^{1}H-NMR (400 MHz, $CDCl_3$)



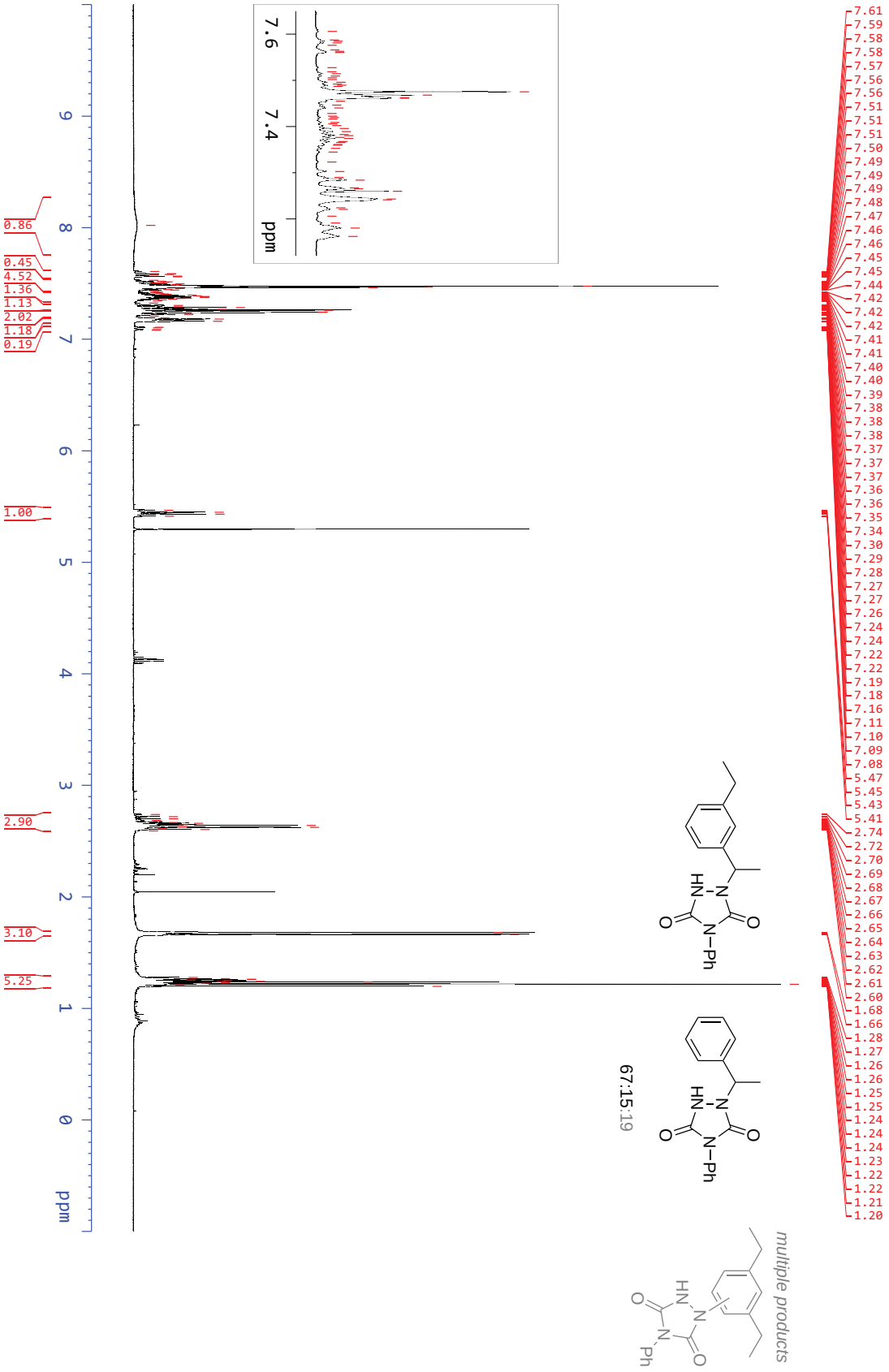
$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)



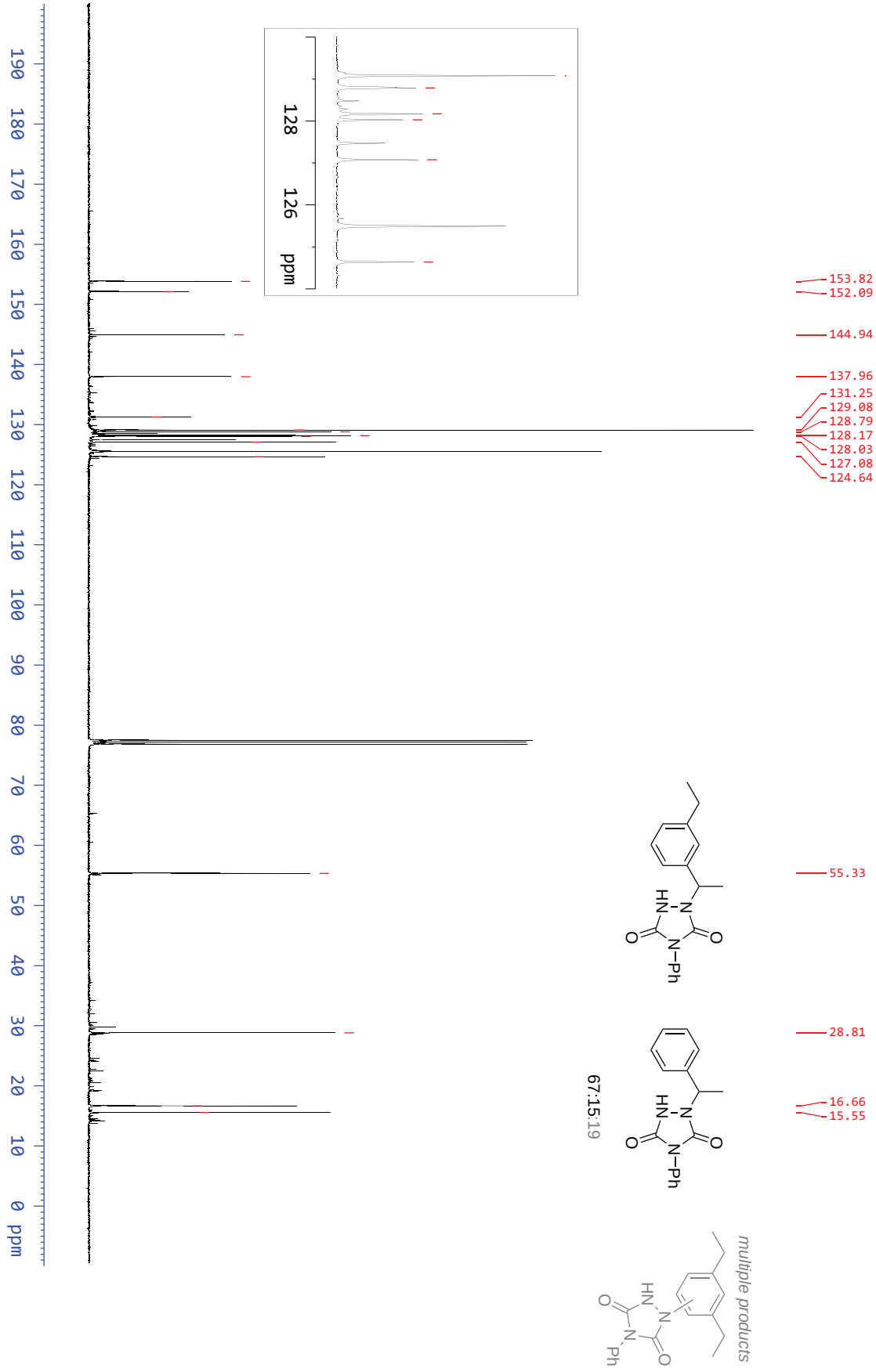
4.43 31b: 1-(1-(3-ethylphenyl)ethyl)-4-phenyl-urazole

*This compound was not obtained analytically pure and the assignments were made on a sample containing a mixture of **31b** and **12b** in a 82:18 ratio*

^{1}H-NMR (400 MHz, $CDCl_3$ + residual EtOAc)

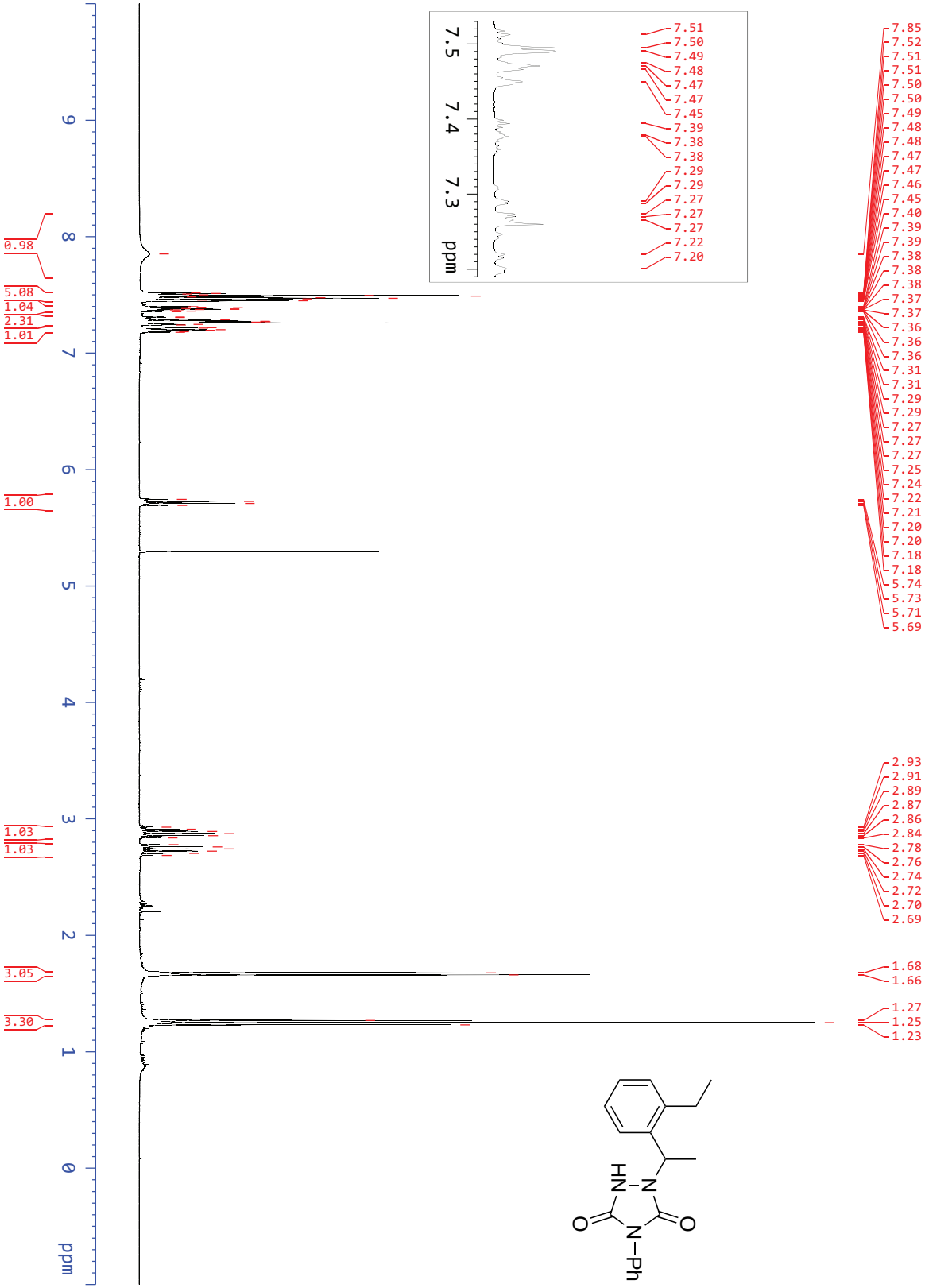


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$ + residual EtOAc)

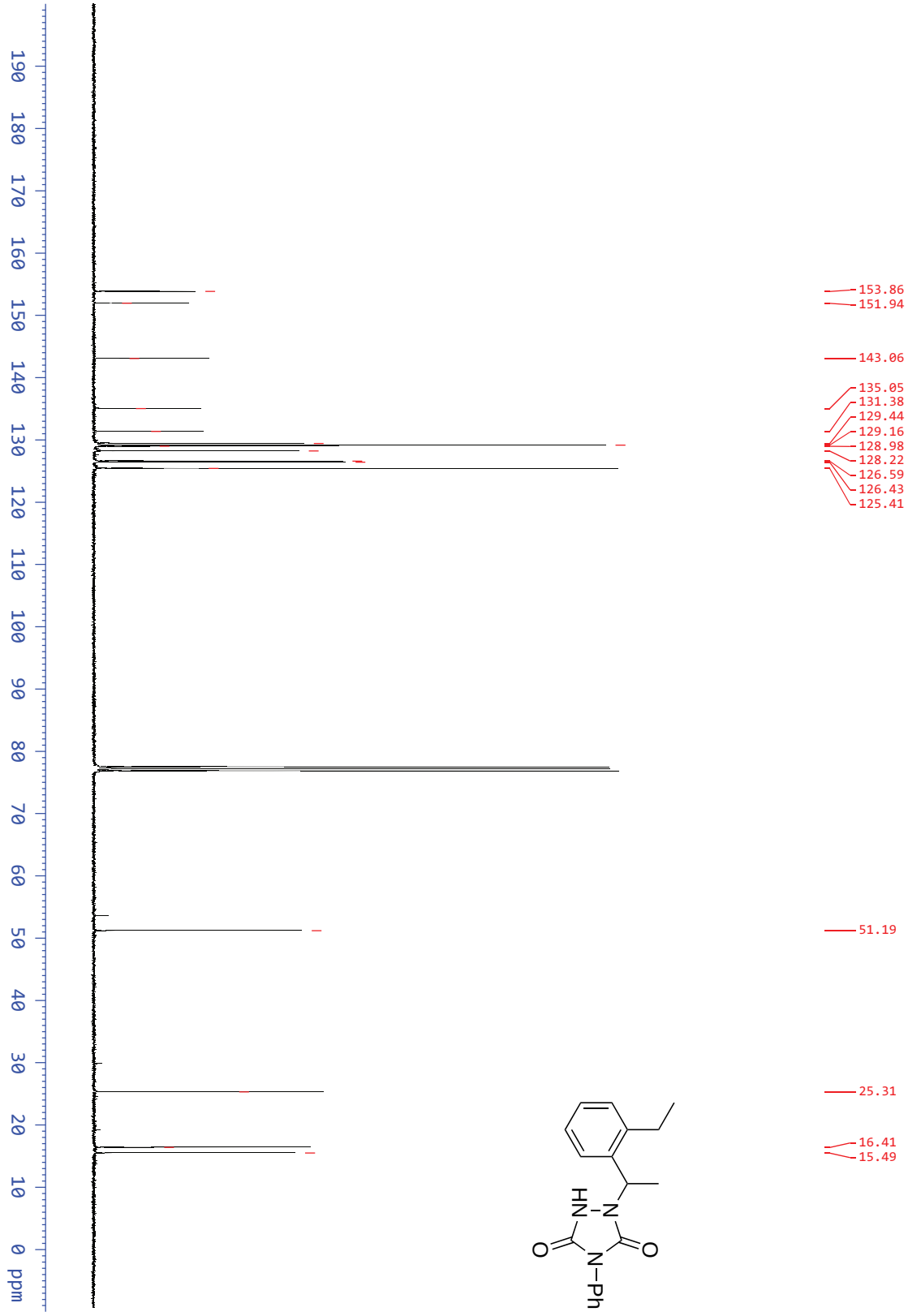


4.44 32b: 1-(1-(2-ethylphenyl)ethyl)-4-phenyl-urazole

^{1}H-NMR (400 MHz, $CDCl_3$ + residual DCM)

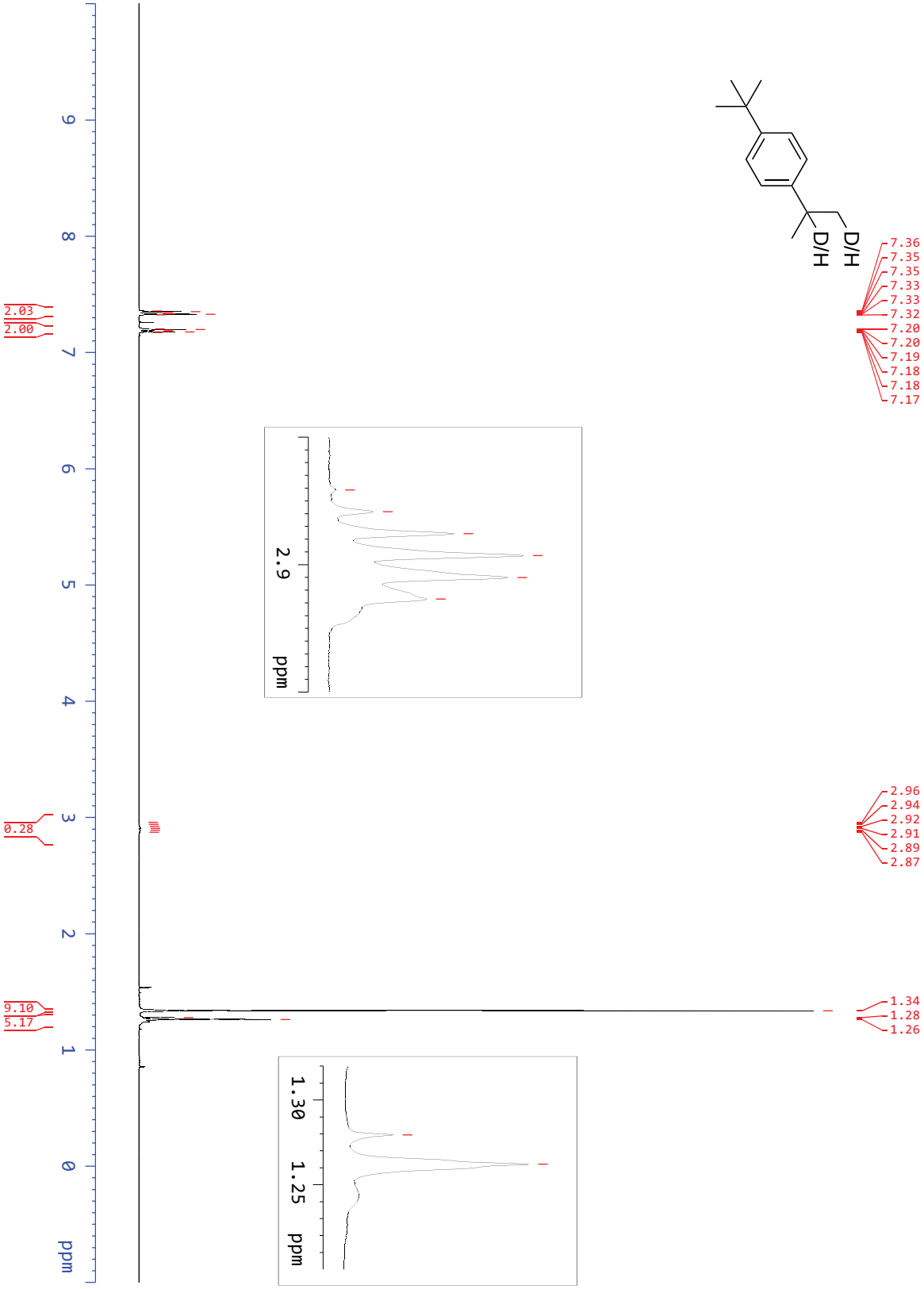


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

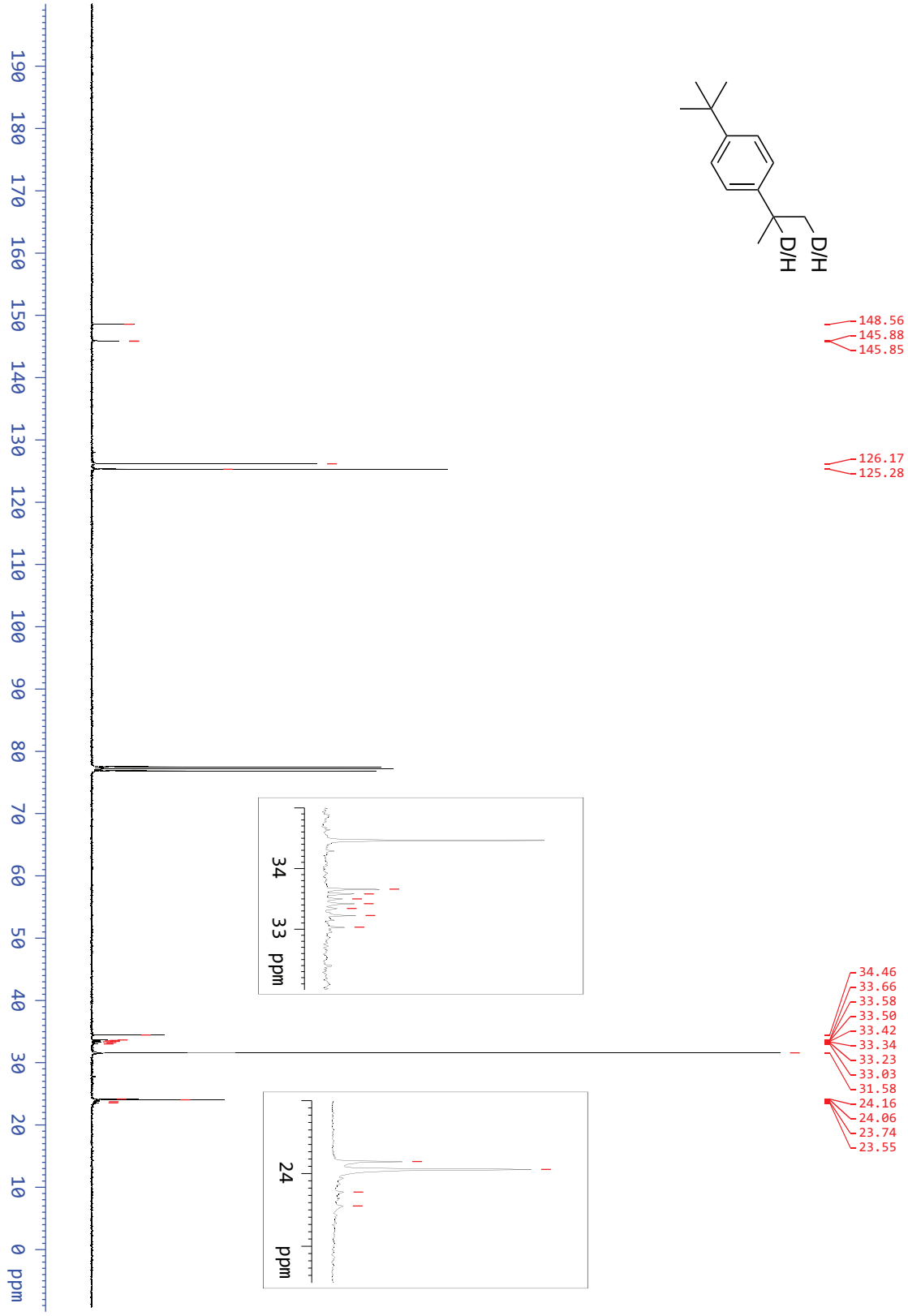


4.45 33a: Deuterated 1-(tert-butyl)-4-isopropylbenzene

^{1}H-NMR (400 MHz, $CDCl_3$)

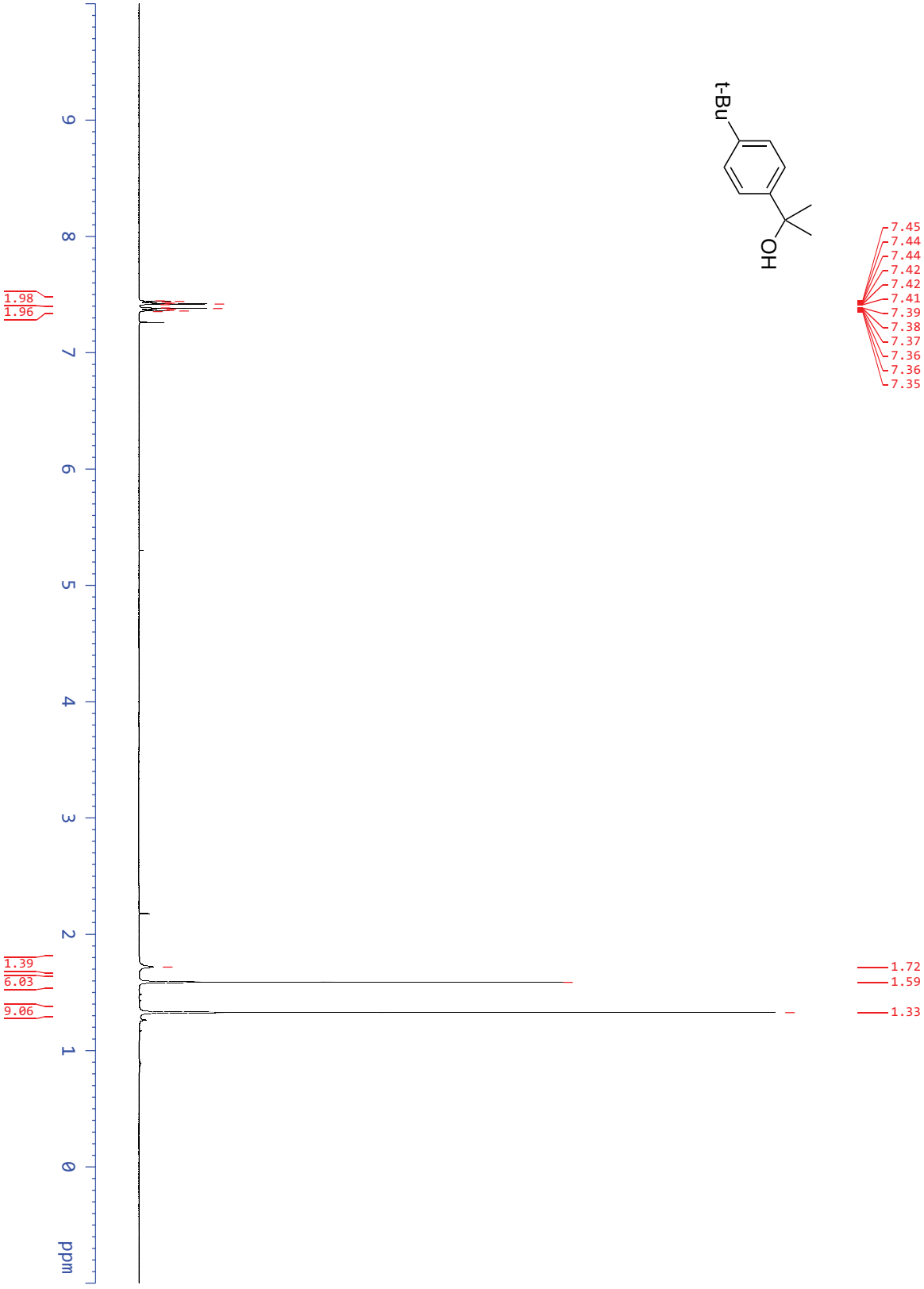


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

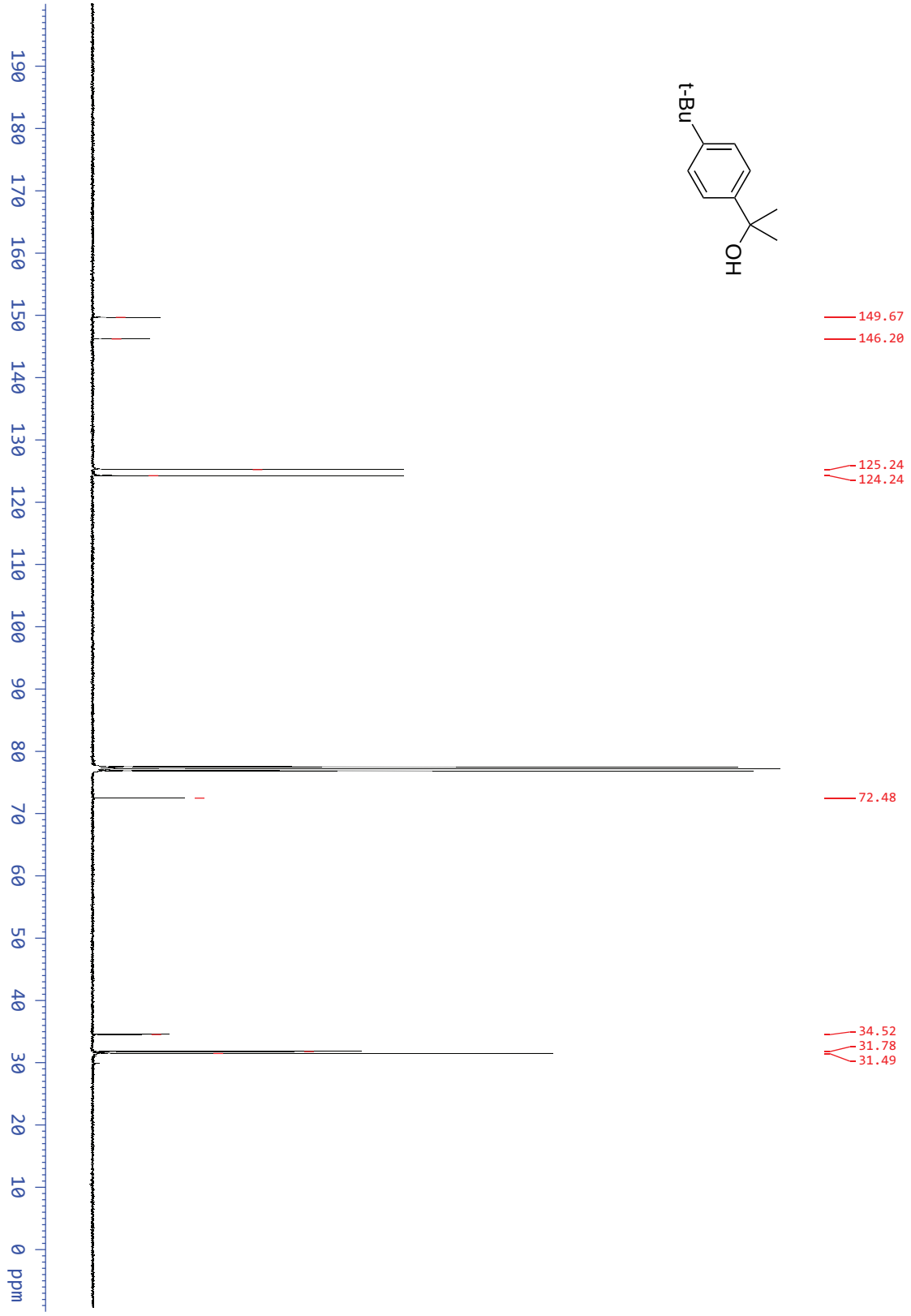


4.46 34: 2-(4-(tert-butyl)phenyl)propan-2-ol

^{1}H-NMR (400 MHz, $CDCl_3$)

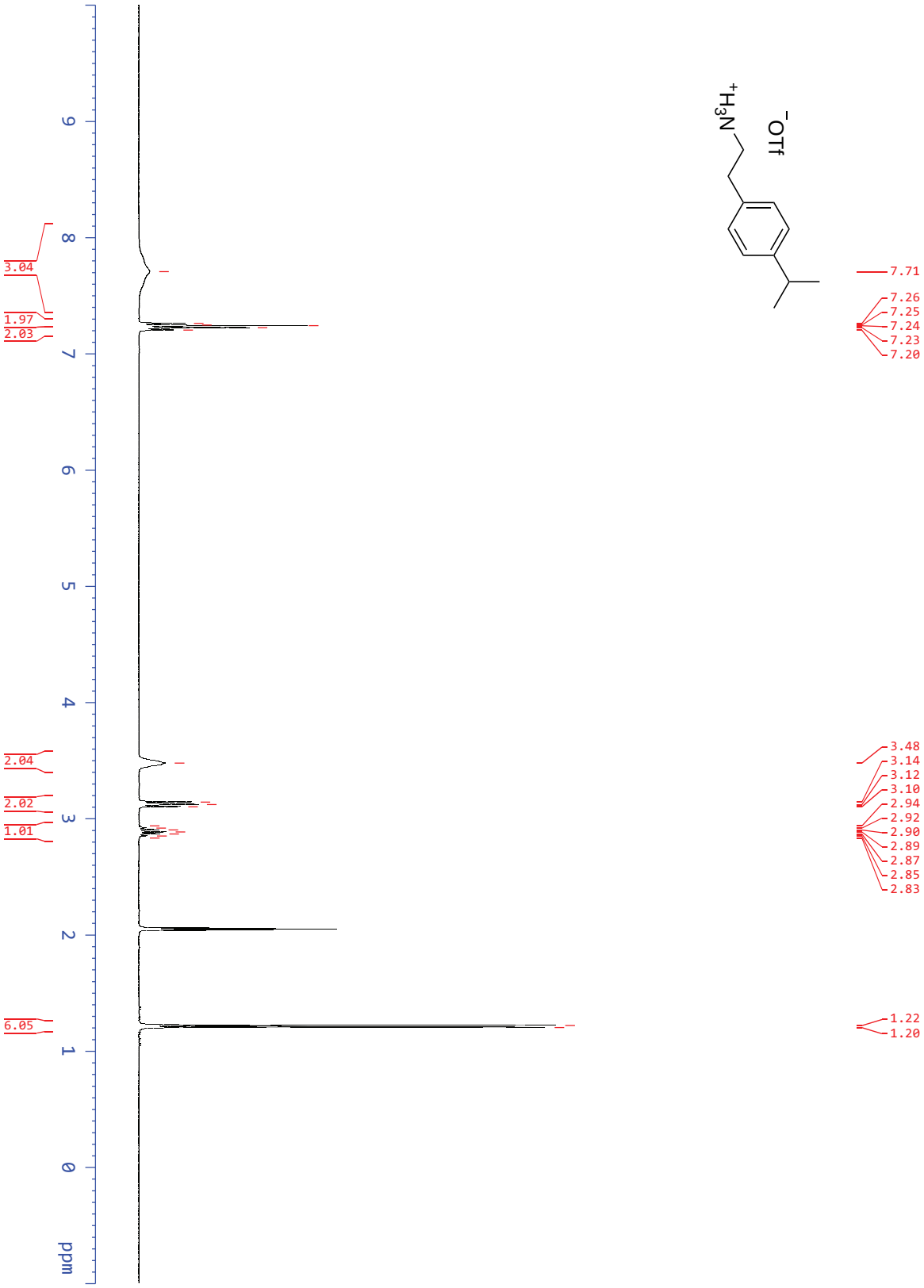


$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)

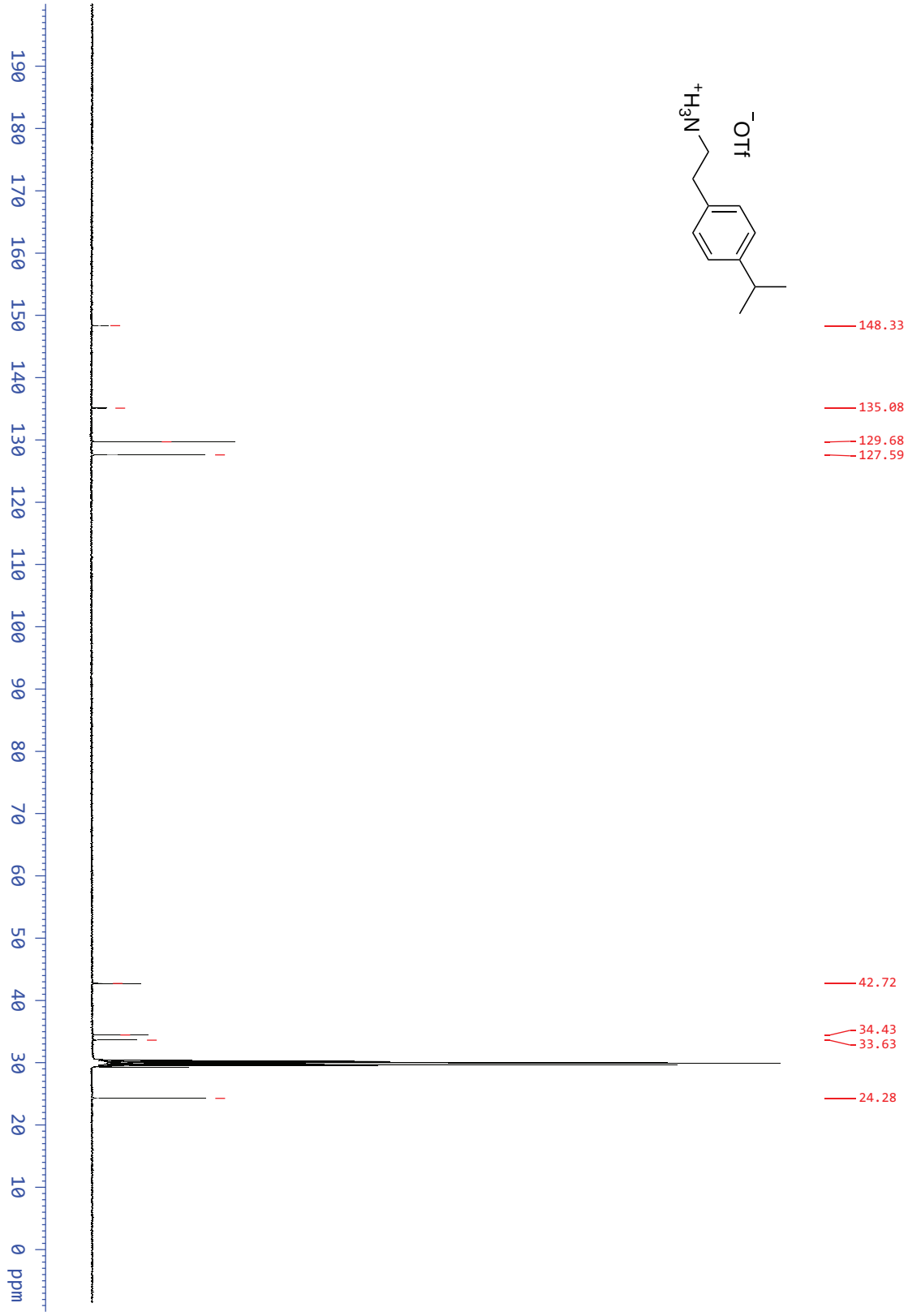


4.47 35a: 2-(4-isopropylphenyl)ethan-1-aminium trifluoromethanesulfonate

^{1}H-NMR (400 MHz, Acetone)



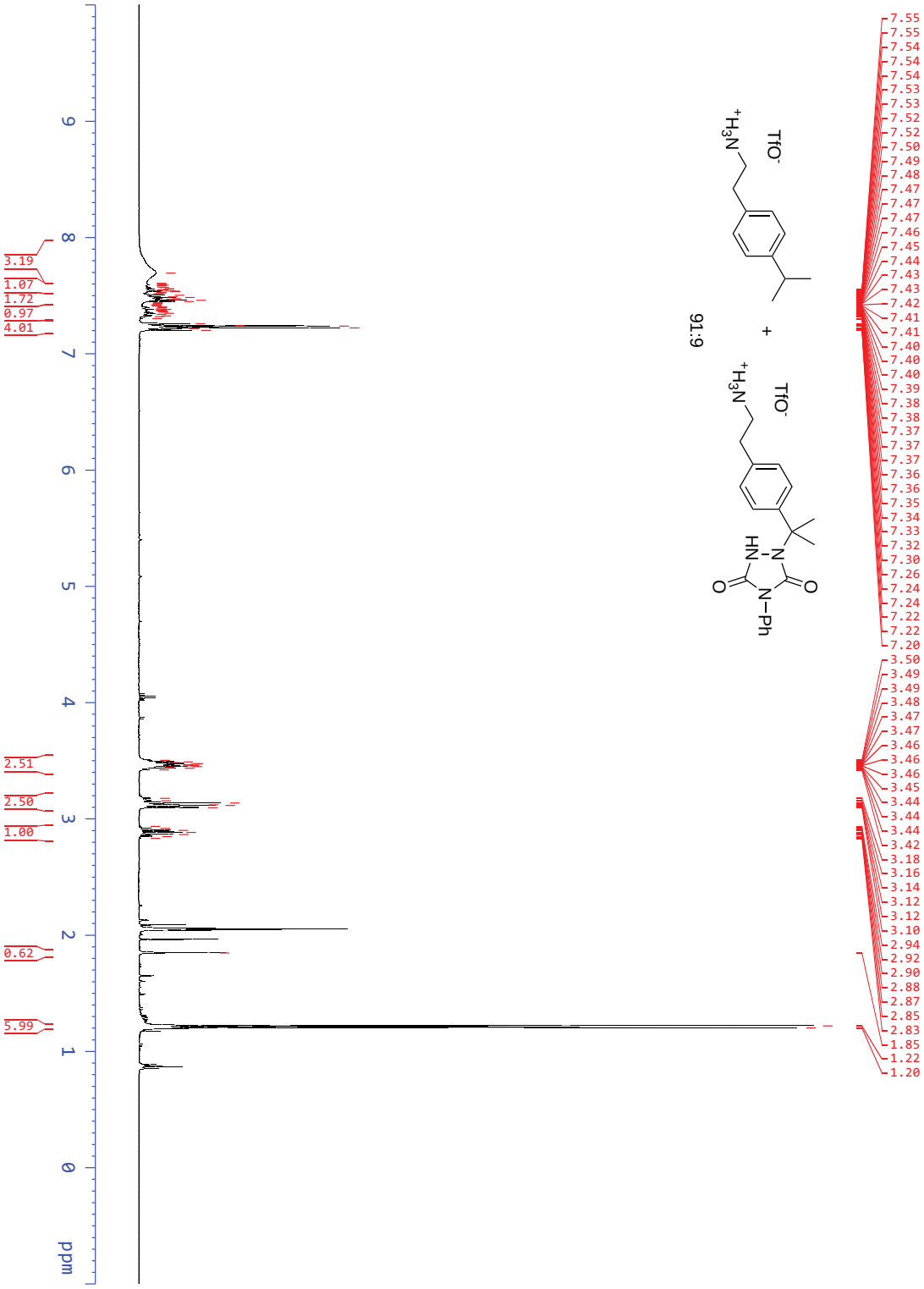
$^{13}C\{^{1}H\}$-NMR (100 MHz, Acetone)



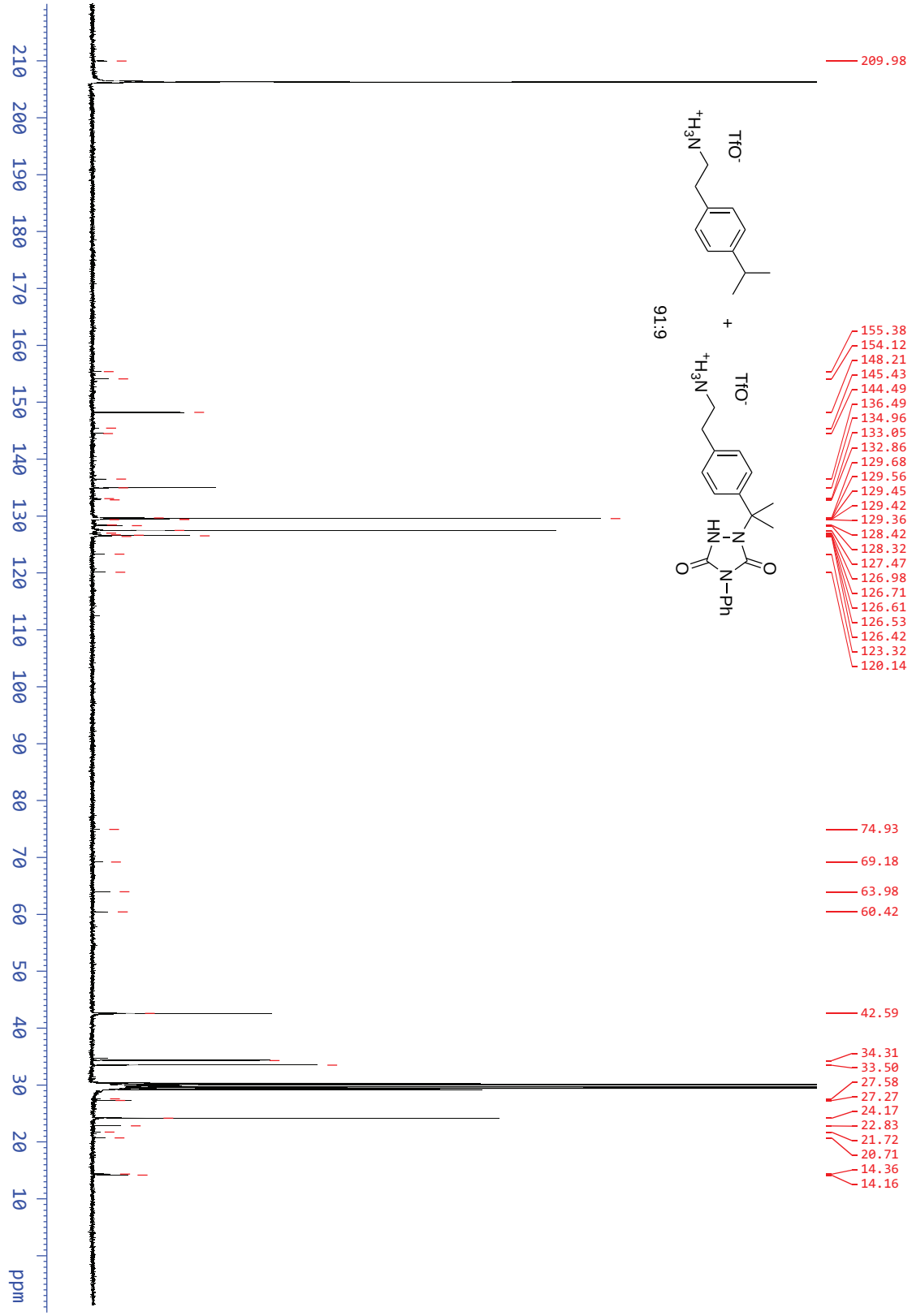
4.48 35b: 1-(2-(4-(2-amino-ethyl)phenyl)propan-2-yl)-4-phenyl-urazole triflic acid salt

*This compound was not obtained analytically pure and the assignments were made on a sample from the crude mixture of the reaction after workup, containing a mixture of **35a** and **35b** in a 91:9 ratio*

^{1}H-NMR (400 MHz, Acetone−d_6 + residual EtOAc)

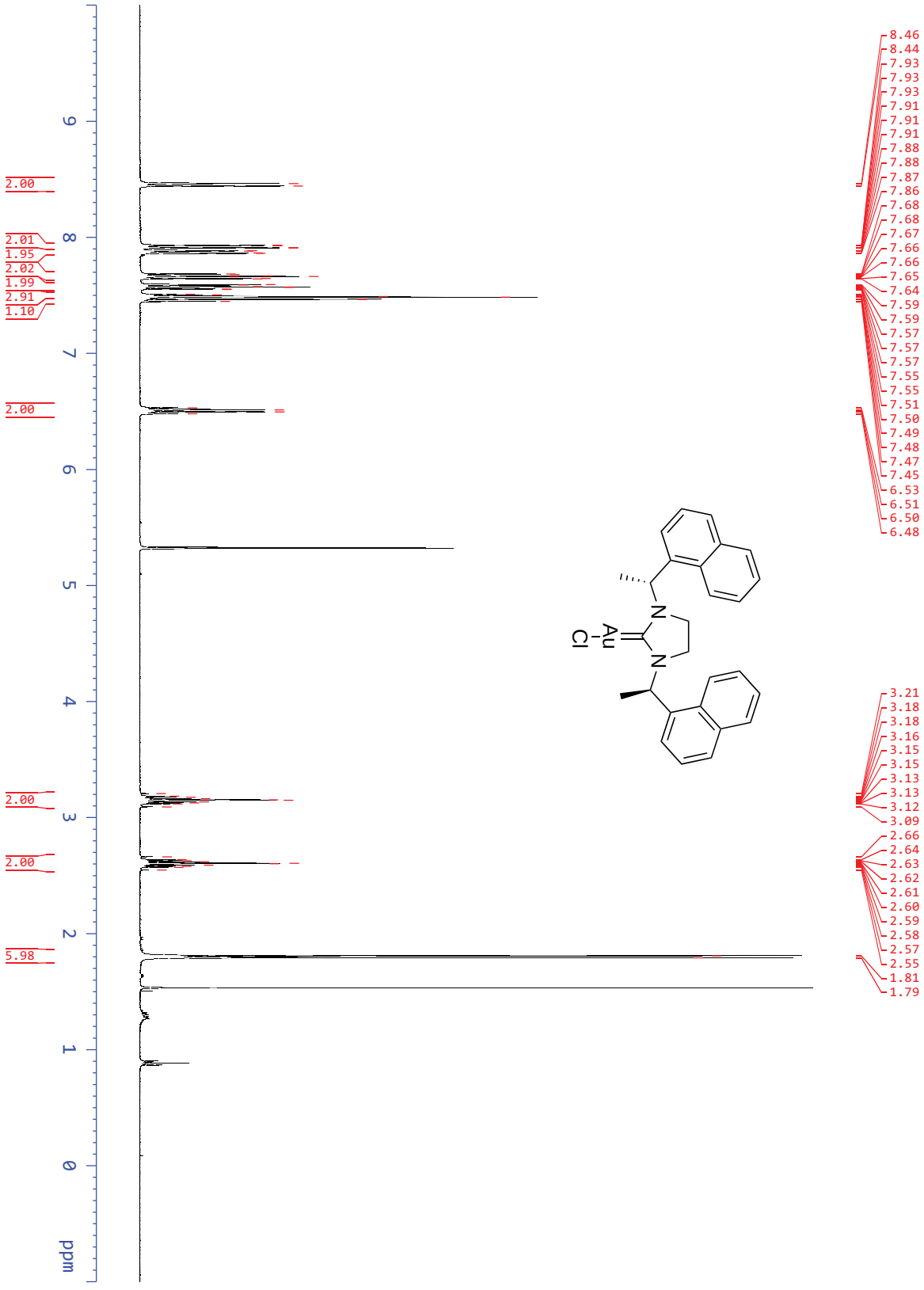


$^{13}C\{^{1}H\}$-NMR (100 MHz, Acetone−d_6 + residual EtOAc)

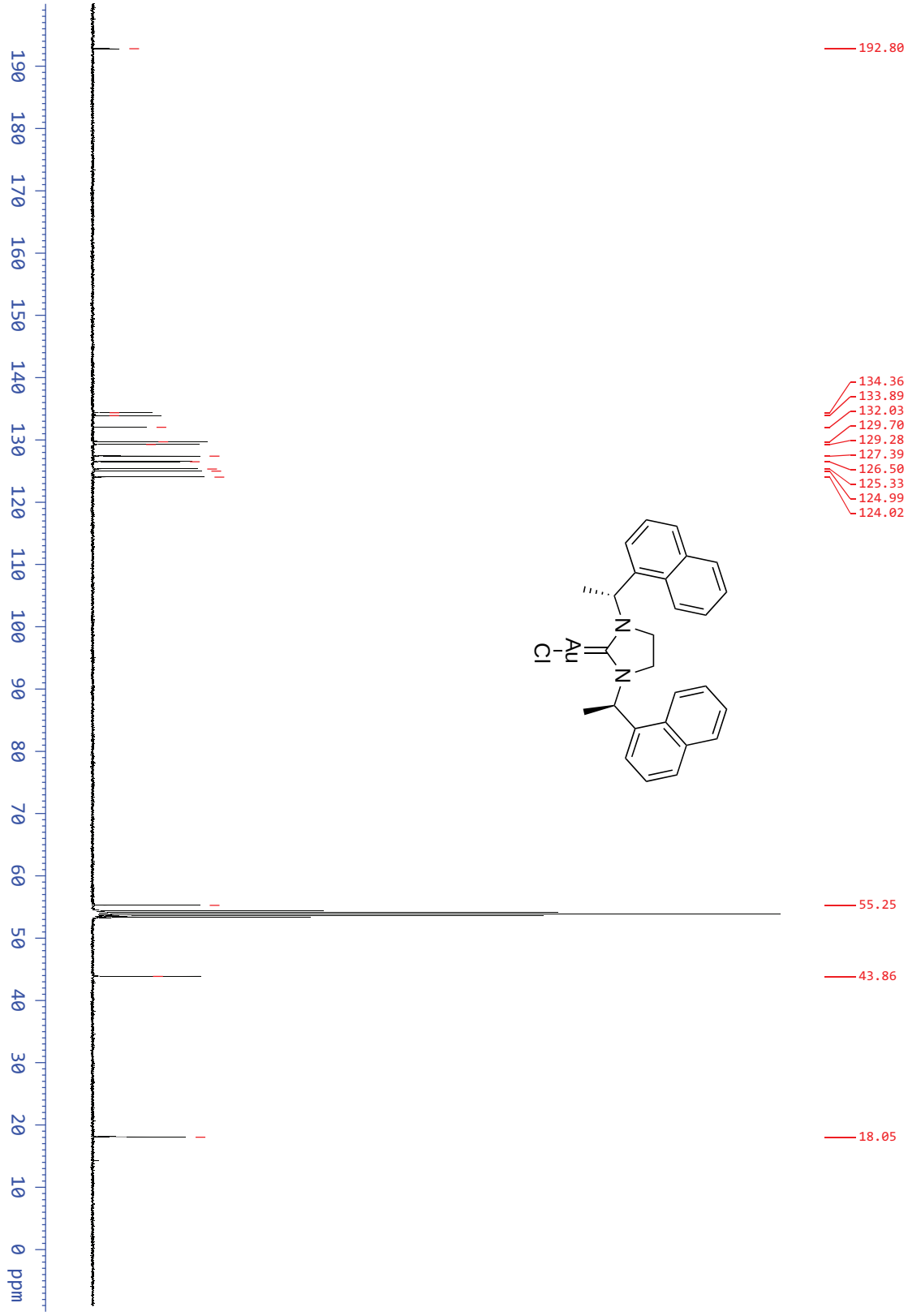


4.49 38: (1,3-bis((R)-1-(naphthalen-1-yl)ethyl)imidazolidin-2-ylidene)gold(I) chloride

^{1}H-NMR (400 MHz, DCM−d_2)

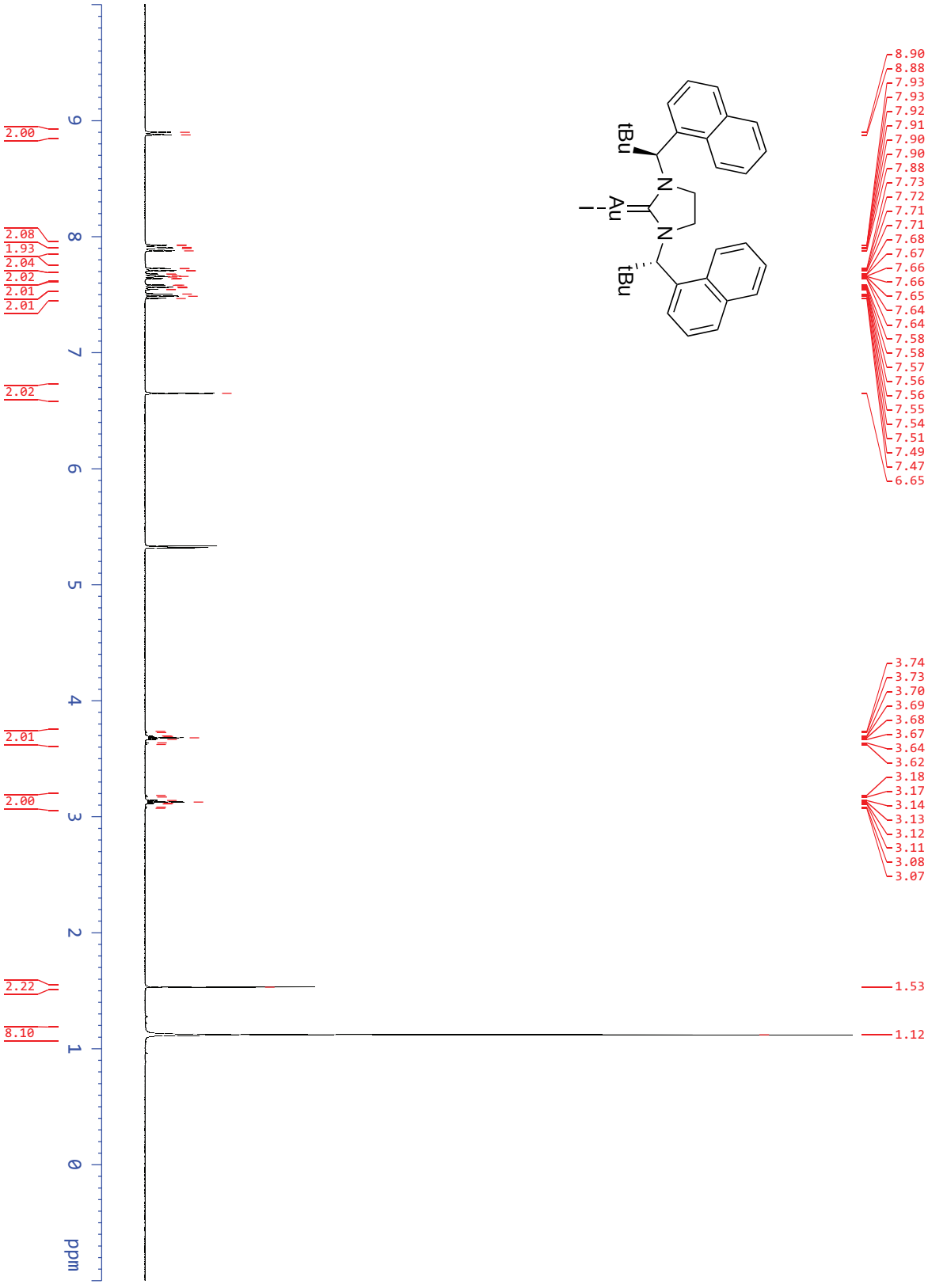


$^{13}C\{^{1}H\}$-NMR (100 MHz, DCM−d_2)

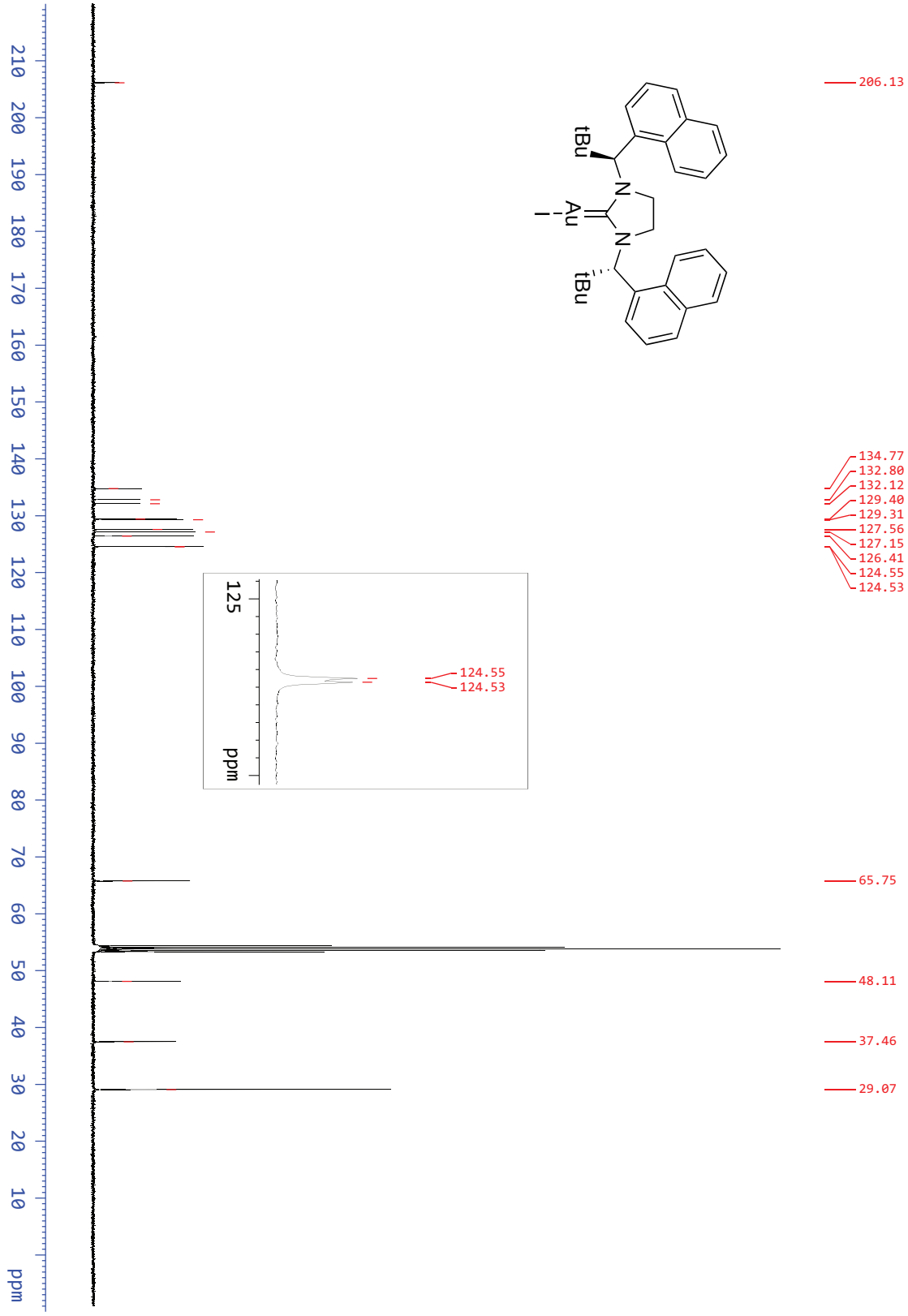


4.50 39: (1,3-bis((S)-2,2-dimethyl-1-(naphthalen-1-yl)-propyl)imidazolidin-2-ylidene)gold(I) iodide

^{1}H-NMR (400 MHz, DCM−d_2)

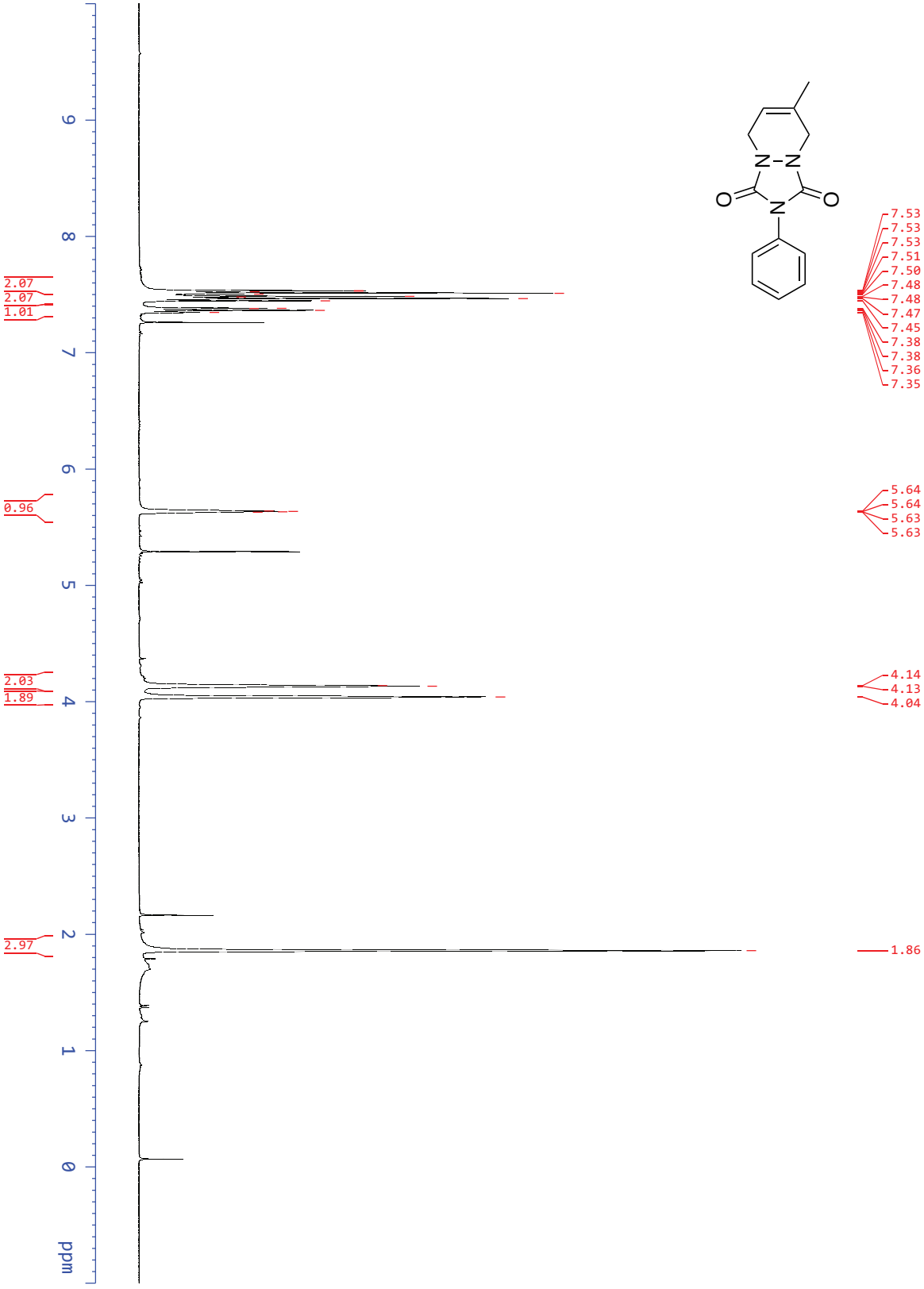


$^{13}C\{^{1}H\}$-NMR (100 MHz, DCM−d_2)

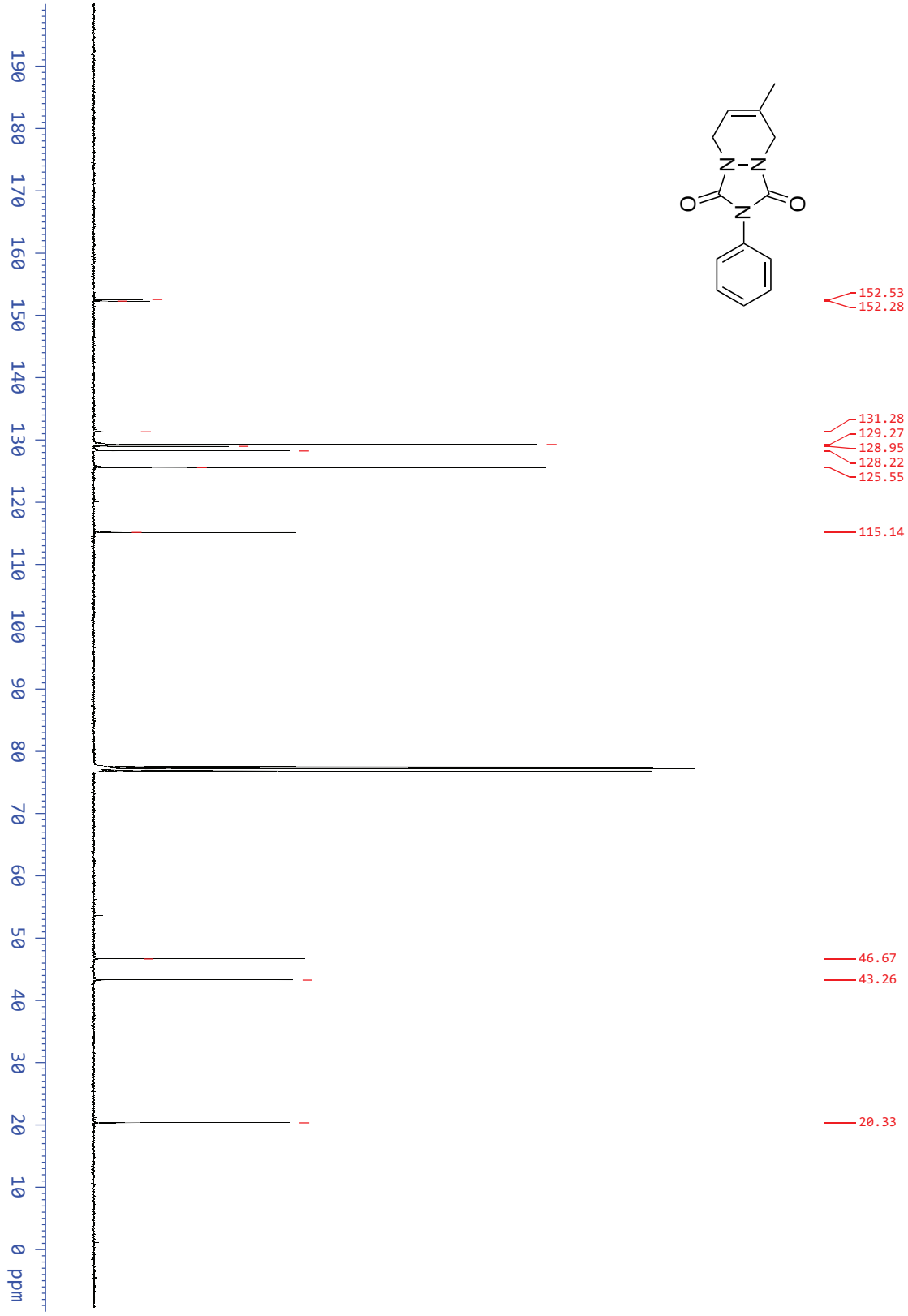


4.51 40: PTAD-isoprene adduct

^{1}H-NMR (400 MHz, $CDCl_3$ + residual DCM)



$^{13}C\{^{1}H\}$-NMR (100 MHz, $CDCl_3$)



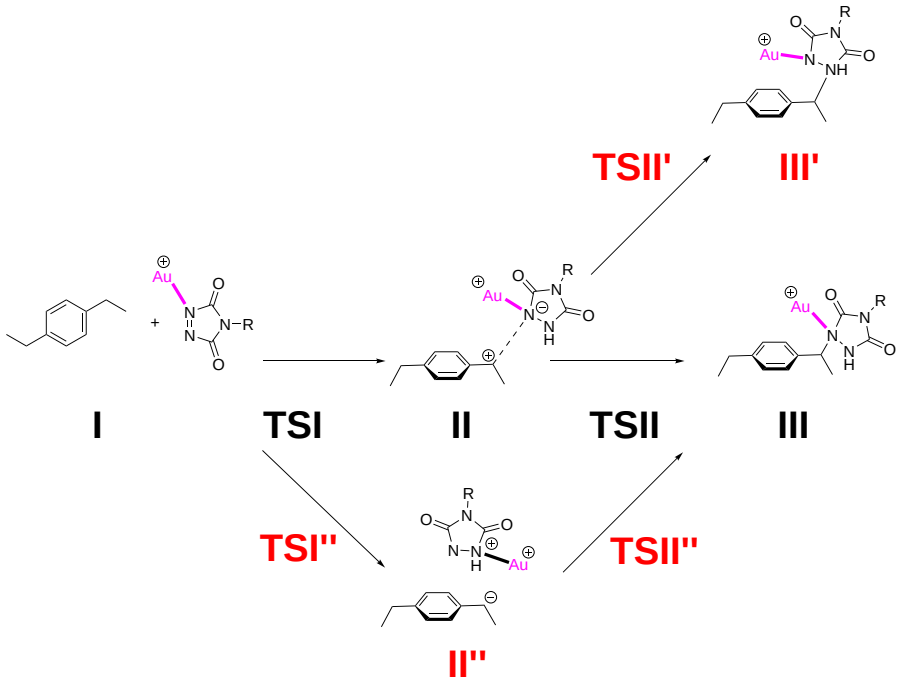
5 Computational chemistry summary

Computational Details Gaussian 16 package was applied to perform all the DFT calculations. The geometry optimizations were performed using the pure GGA BP86 functional of Becke and Perdew.[21;22] In the case of non-metal atoms the split-valence basis set (Def2SVP keyword in Gaussian)[23;24] was used, while for Au the small core quasi-relativistic Stuttgart/Dresden effective core potential, with an associated valence basis set (standard SDD keyword in Gaussian16) was adopted,[25–27] to address relativistic effects. The geometry optimizations were carried out without symmetry constraints, and analytical frequency calculations were performed to prove the nature of the stationary points, either minima or transition states. In addition, single-point energy calculations using the hybrid M06 functional of Truhlar and coworkers,[28] and def2-TZVP basis set for the non-metal atoms were performed,[29] a solvation contribution evaluated by means of the SMD continuum solvation model based on the quantum mechanical charge density of the solute interacting with a continuum description of the solvent (dichloromethane).[30] The reported Gibbs energies in this work include energies obtained at the M06/Def2-TZVP~sdd(SMD-DCM)//BP86/Def2-SVP~sdd level of theory corrected with zero-point energies, thermal corrections, and entropy effects evaluated with the BP86/Def2SVP~SDD method.

		E_{gas}	G_{gas}	E_{solv}	G_{solv}
BP86	**I**	-50.4	-25.7	-24.8	-0.2
	TS-I	-46.5	-19.6	-13.0	13.9
	II	-60.8	-32.9	-42.3	-14.4
	TS-II	-60.7	-31.5	-42.8	-13.6
	III	-74.3	-43.1	-64.8	-33.5
TPSSh[a]	**I**	-49.3	-25.7	-27.7	-4.1
	TS-I	-40.9	-17.5	-14.6	8.8
	III	-76.0	-45.3	-64.7	-33.9
PBEH1PBE[a]	**I**	-50.9	-27.1	-31.0	-7.1
	TS-I	-41.7	-18.4	-15.4	8.1
	III	-85.7	-54.7	-64.8	-33.8
PBEPBE	**I**	-55.4	-31.3	-26.1	-2.0
	TS-I	-51.5	-28.1	-15.1	8.3
	II	-66.8	-39.3	-43.7	-16.3
	TS-II	-66.6	-38.0	-44.2	-15.6
	III	-80.7	-50.7	-65.5	-35.5

[a]For hybrid funcionals species II and TS-II do not exist.

Table S12: Relative energies (in kcal/mol) with respect to Au(IPr)$(CH_3CN)^+$ with BP86, TPSSh, PBEPBE and PBEh1PBE.



	With [**Au(IPr)**]$^+$					
Substituents on the aryl	Et/-	Et/iPr	Et/Et	iPr/-	iPr/Et	iPr/Me
[**Au(IPr)**]$^+$	0.0	0.0	0.0	0.0	0.0	0.0
I	-0.2	1.1	-0.1	-0.9	-0.9	0.0
TSI	13.8	9.6	9.3	10.3	9.4	8.4
II	-14.5	-16.8	-17.0	-20.3	-22.1	-22.5
TSII	-13.7	-16.2	-17.3	-16.9	-19.3	-19.0
III	-33.6	-35.1	-34.8	-33.3	-33.2	-34.6
TSI"	15.8	12.9	12.7	12.7	10.0	10.7
II"	-11.5	-11.9	-12.9	-13.3	-14.1	-13.8
TSII"	7.6	4.9	4.3	-0.2	-1.5	-1.8
	Without [**Au(IPr)**]$^+$					
I	0.0	-0.5	-0.5	-0.5	0.0	1.3
TSI	21.1	19.6	19.3	19.6	17.8	18.9
II	6.4	3.6	3.3	2.7	0.3	0.7
TSII	Not located[a]	Not located[a]	Not located[a]	Not located[a]	Not located[a]	Not located[a]

III	-31.7	-31.9	-32.5	-31.1	-31.6	-31.3
TSII'	-	-	-	3.7	2.5	2.6
III'	-10.3	-11.0	-11.4	-8.7	-9.2	-9.0

[a]TS not located and barrierless according to linear transit calculations.

Table S13: Catalytic cycle calculated at the M06/Def2-TZVP~sdd(SMD-DCM)//BP86/Def2-SVP~sdd level of theory (Gibbs energies in kcal/mol referenced to the cationic complex Au(IPr)$^+$ (= [Au]$^+$)), with alternative steps (in red), and also without the presence of the metal catalyst.

5.1 xyz coordinates and absolute energies (in a.u.) of all computed DFT species.

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AuIPrUrN2+ SCF Done: -1917.05829672 A.U.

N	2.981224	-0.292060	-0.009576
N	2.174017	1.736369	-0.065850
C	1.808328	0.416735	-0.020648
C	4.065112	0.572077	-0.047348
H	5.096794	0.206137	-0.045640
C	3.556126	1.851248	-0.082760
H	4.054656	2.825158	-0.118252
C	3.085061	-1.742494	0.033927
C	3.157739	-2.375357	1.303088
C	3.113971	-1.606601	2.624647
H	3.051731	-0.522697	2.389318
C	3.270643	-3.781119	1.310515
H	3.328061	-4.312014	2.273536
C	3.313376	-4.513785	0.116208
C	3.245266	-3.855355	-1.119455
H	3.283276	-4.444064	-2.049256
C	3.131157	-2.451746	-1.195505
C	3.056932	-1.765241	-2.560316
H	3.002832	-0.668698	-2.390503

C	1.255445	2.863875	-0.093132
C	0.827761	3.354419	-1.355155
C	1.270111	2.740402	-2.684349
H	1.977279	1.913019	-2.461771
C	-0.049596	4.458463	-1.347401
H	-0.406955	4.869560	-2.304378
C	-0.472403	5.043072	-0.145682
C	-0.024875	4.536683	1.082382
H	-0.362492	5.008935	2.018080
C	0.853058	3.434796	1.143184
C	1.320419	2.905003	2.499832
H	2.034967	2.074467	2.316251
Au	-0.042715	-0.335321	0.020165
C	4.322048	-2.033300	-3.404075
H	4.428101	-3.109990	-3.651939
H	4.273987	-1.476480	-4.362725
H	5.244314	-1.720505	-2.872802
C	1.774941	-2.170047	-3.320202
H	1.706628	-1.627972	-4.286138
H	1.760374	-3.256824	-3.545528
H	0.864207	-1.937497	-2.728965
C	0.073559	2.122952	-3.440373
H	-0.675144	2.894078	-3.717582
H	0.413941	1.635775	-4.377569
H	-0.444180	1.359719	-2.822200
C	2.026373	3.761628	-3.561576
H	1.372262	4.606497	-3.862062
H	2.902350	4.189370	-3.032039
H	2.391272	3.278879	-4.491734
C	2.074614	3.983449	3.307306
H	2.937113	4.391995	2.741774
H	1.413628	4.835415	3.570447
H	2.459149	3.558149	4.257366
C	0.140961	2.318060	3.305663
H	-0.615242	3.094907	3.544062

H	-0.372143	1.511666	2.740479
H	0.498056	1.892806	4.266507
C	4.400514	-1.819788	3.451574
H	5.308264	-1.537858	2.879537
H	4.373998	-1.205670	4.375449
H	4.516624	-2.879163	3.761734
C	1.852529	-1.966627	3.439364
H	0.926795	-1.773375	2.857444
H	1.847567	-3.037337	3.731897
H	1.805829	-1.365984	4.371337
H	-1.156405	5.905825	-0.166618
H	3.403538	-5.610794	0.148799
N	-1.934022	-1.137127	0.058220
C	-3.180843	-0.254279	0.023397
N	-4.223095	-1.158173	0.052239
C	-3.713147	-2.471243	0.104290
N	-2.227550	-2.358512	0.099885
C	-5.626105	-0.815120	0.041411
C	-6.497387	-1.510908	-0.816699
C	-6.092145	0.205293	0.890636
H	-6.119957	-2.307721	-1.473412
H	-5.399802	0.737967	1.558541
C	-7.860936	-1.176410	-0.814981
C	-7.456592	0.535114	0.870094
H	-8.550701	-1.718966	-1.479360
H	-7.829634	1.334052	1.528991
C	-8.341249	-0.154629	0.022626
H	-9.411039	0.104741	0.015817
O	-4.296652	-3.520073	0.141160
O	-3.133102	0.945833	-0.017067

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AuIPrUrN2+ISOMER (though O) SCF Done: -1917.03650263 A.U.

N	-2.618972	-1.010117	0.310785
N	-2.625358	1.151269	-0.002796

C	-1.799600	0.064936	0.100109
C	-3.947922	-0.600208	0.340255
H	-4.765721	-1.309676	0.500245
C	-3.952194	0.758982	0.142137
H	-4.774596	1.479332	0.091410
C	-2.178964	-2.384619	0.484568
C	-2.102228	-3.218336	-0.662461
C	-2.454216	-2.735202	-2.070127
H	-2.684422	-1.650093	-2.010850
C	-1.690449	-4.551624	-0.457884
H	-1.617777	-5.231318	-1.321151
C	-1.374199	-5.026885	0.822417
C	-1.465594	-4.177453	1.934026
H	-1.219805	-4.566425	2.934561
C	-1.873648	-2.834426	1.796650
C	-1.971074	-1.936592	3.031100
H	-2.337695	-0.940980	2.702271
C	-2.194248	2.519661	-0.235602
C	-1.912613	3.339523	0.889062
C	-2.017650	2.842422	2.331500
H	-2.363753	1.787309	2.305309
C	-1.516161	4.668026	0.629833
H	-1.289510	5.337156	1.474587
C	-1.410628	5.152785	-0.681315
C	-1.700247	4.316889	-1.768876
H	-1.617066	4.712479	-2.793257
C	-2.101854	2.978649	-1.576378
C	-2.411037	2.093658	-2.784887
H	-2.729227	1.098414	-2.408242
Au	0.169828	0.057589	-0.022844
C	-2.991380	-2.482288	4.053696
H	-2.676017	-3.464937	4.462440
H	-3.092788	-1.784550	4.910642
H	-3.995247	-2.615512	3.600787
C	-0.585687	-1.718589	3.677131

H	-0.663111	-1.028750	4.542999
H	-0.153824	-2.671751	4.047820
H	0.132738	-1.280575	2.952272
C	-0.638999	2.850414	3.026949
H	-0.231832	3.879543	3.113632
H	-0.718107	2.436249	4.053499
H	0.100324	2.241354	2.465455
C	-3.062128	3.645222	3.137007
H	-2.768706	4.710804	3.239894
H	-4.061213	3.618823	2.655539
H	-3.165127	3.229970	4.160923
C	-3.578660	2.658991	-3.622314
H	-4.493698	2.797020	-3.010490
H	-3.323627	3.642741	-4.068781
H	-3.826199	1.970908	-4.456985
C	-1.151983	1.868792	-3.650164
H	-0.779205	2.820592	-4.083198
H	-0.328156	1.422567	-3.054294
H	-1.376113	1.183778	-4.493993
C	-3.718460	-3.443657	-2.605376
H	-4.588303	-3.300208	-1.931674
H	-3.992212	-3.048443	-3.605618
H	-3.556159	-4.536702	-2.711630
C	-1.265194	-2.893542	-3.041576
H	-0.360194	-2.374052	-2.664880
H	-1.000492	-3.960548	-3.195072
H	-1.520037	-2.471637	-4.035890
H	-1.103348	6.195573	-0.857557
H	-1.057302	-6.073104	0.956100
N	2.601536	-1.883478	-1.327994
C	3.076914	-0.689348	-0.585233
N	4.433950	-0.710229	-0.568555
C	4.850075	-1.882371	-1.282469
N	3.577127	-2.559626	-1.718856
C	5.326326	0.255158	0.023024

C	6.380441	-0.197812	0.838402
C	5.135369	1.625100	-0.238650
H	6.518361	-1.271453	1.031661
H	4.315311	1.961686	-0.889719
C	7.256289	0.745173	1.399052
C	6.015256	2.554242	0.337815
H	8.085586	0.400721	2.035472
H	5.875133	3.627705	0.138869
C	7.074723	2.117489	1.153173
H	7.764896	2.851197	1.597108
O	5.958711	-2.269969	-1.502477
O	2.310490	0.146411	-0.088916

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AuUrN2BF4 SCF Done: -2341.37460667 A.U.

N	-3.213495	0.352588	0.164057
N	-2.414226	-1.662590	0.372020
C	-2.040179	-0.351788	0.237487
C	-4.306526	-0.504310	0.257431
H	-5.335610	-0.134719	0.218200
C	-3.801441	-1.773946	0.390032
H	-4.299550	-2.742635	0.492012
C	-3.300622	1.789994	-0.010225
C	-3.356500	2.610534	1.147107
C	-3.298097	2.043550	2.566352
H	-3.345825	0.936738	2.492064
C	-3.435130	4.003680	0.945656
H	-3.474466	4.673783	1.818850
C	-3.455932	4.549751	-0.345618
C	-3.401326	3.711427	-1.467244
H	-3.413348	4.153137	-2.475937
C	-3.324606	2.309351	-1.331346
C	-3.265814	1.424742	-2.577518
H	-3.260527	0.365616	-2.244200
C	-1.500420	-2.789672	0.445199

C	-1.226303	-3.510057	-0.748051
C	-1.866146	-3.166276	-2.094656
H	-2.359080	-2.175963	-1.992559
C	-0.346202	-4.606483	-0.644875
H	-0.097545	-5.181416	-1.549941
C	0.228845	-4.965225	0.581442
C	-0.064921	-4.234025	1.740180
H	0.398675	-4.522460	2.696446
C	-0.936523	-3.126632	1.703475
C	-1.251119	-2.360169	2.988763
H	-1.845129	-1.463841	2.712513
Au	-0.197950	0.413776	0.174024
C	-4.518571	1.615745	-3.460703
H	-4.573659	2.643874	-3.876817
H	-4.494382	0.913644	-4.320004
H	-5.455740	1.432772	-2.894458
C	-1.965915	1.654382	-3.378984
H	-1.955908	1.012099	-4.283898
H	-1.876689	2.708865	-3.715477
H	-1.061774	1.401509	-2.789022
C	-0.831520	-3.037233	-3.230660
H	-0.308467	-3.997058	-3.424200
H	-1.343805	-2.750620	-4.173141
H	-0.068806	-2.265683	-3.008487
C	-2.964487	-4.195561	-2.449470
H	-2.531989	-5.210225	-2.580344
H	-3.743673	-4.267016	-1.661524
H	-3.465261	-3.918946	-3.401080
C	-2.119131	-3.210373	3.943146
H	-3.065314	-3.534001	3.461334
H	-1.580983	-4.125785	4.268726
H	-2.379654	-2.632603	4.855088
C	0.028900	-1.855178	3.686328
H	0.647895	-2.695921	4.064679
H	0.660545	-1.257675	2.997914

H	-0.233273	-1.221592	4.559692
C	-4.500487	2.493360	3.422468
H	-5.466344	2.225999	2.945900
H	-4.466464	2.010467	4.421452
H	-4.500959	3.591334	3.587975
C	-1.955033	2.394485	3.243637
H	-1.098778	2.016941	2.646026
H	-1.834176	3.492614	3.357103
H	-1.896525	1.941214	4.255471
H	0.921313	-5.820171	0.632751
H	-3.512467	5.641740	-0.478940
N	1.688028	1.255398	0.096041
C	2.864289	0.668146	0.854826
N	3.954684	1.305151	0.292703
C	3.525195	2.250315	-0.656651
N	2.040475	2.146895	-0.710104
C	5.328776	0.969905	0.532728
C	6.118646	0.570808	-0.561573
C	5.855329	1.029147	1.834886
H	5.660876	0.506970	-1.560017
H	5.215932	1.337622	2.674944
C	7.466063	0.245268	-0.341569
C	7.201486	0.684830	2.040878
H	8.093017	-0.066152	-1.191541
H	7.622562	0.723721	3.057724
C	8.008149	0.299934	0.955384
H	9.064633	0.036898	1.121986
O	4.165923	3.066274	-1.262098
O	2.757347	-0.066284	1.801354
B	2.303763	-0.655853	-2.293253
F	2.662512	-1.724360	-3.090475
F	0.974516	-0.227754	-2.559110
F	2.373167	-1.027814	-0.897170
F	3.195267	0.450077	-2.467192

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AuUrN2BF4isomer SCF Done: -2341.37155308 A.U.

N	3.072455	-0.782510	0.270882
N	2.594469	1.322617	0.558009
C	2.027097	0.106292	0.283948
C	4.273985	-0.131901	0.535526
H	5.226883	-0.668591	0.568325
C	3.970626	1.194318	0.717342
H	4.604557	2.056952	0.942973
C	2.950651	-2.204616	0.014845
C	2.784799	-3.078878	1.121337
C	2.680003	-2.576476	2.562076
H	2.915786	-1.491513	2.561293
C	2.677182	-4.456979	0.843636
H	2.541496	-5.165785	1.675643
C	2.733376	-4.938690	-0.471972
C	2.899027	-4.049132	-1.542169
H	2.935759	-4.439146	-2.571421
C	3.013715	-2.659521	-1.328273
C	3.174895	-1.714567	-2.519398
H	3.307726	-0.686306	-2.122485
C	1.886740	2.589042	0.646053
C	1.855917	3.421542	-0.502788
C	2.534693	3.046902	-1.821552
H	2.859947	1.987124	-1.746583
C	1.182340	4.652931	-0.381951
H	1.121314	5.319536	-1.255778
C	0.571861	5.032613	0.820052
C	0.622013	4.186729	1.935399
H	0.129655	4.492929	2.871795
C	1.280441	2.942038	1.878520
C	1.316338	2.042038	3.114139
H	1.855641	1.110249	2.841672
Au	0.106951	-0.351079	-0.041305
C	4.434410	-2.048262	-3.347512

H	4.362146	-3.050845	-3.819579
H	4.565137	-1.308491	-4.164570
H	5.352878	-2.036255	-2.724361
C	1.904197	-1.701406	-3.396769
H	2.019053	-0.982811	-4.234435
H	1.702570	-2.701870	-3.834552
H	1.010475	-1.397081	-2.814158
C	1.574068	3.136886	-3.024887
H	1.227420	4.177392	-3.196956
H	2.095045	2.808451	-3.949119
H	0.679844	2.498910	-2.881467
C	3.802357	3.902685	-2.046396
H	3.545087	4.978903	-2.142476
H	4.524996	3.808578	-1.208438
H	4.320056	3.597160	-2.980156
C	2.101408	2.700762	4.269532
H	3.137386	2.960847	3.967293
H	1.609682	3.635495	4.612702
H	2.160434	2.016437	5.142238
C	-0.103975	1.630284	3.555544
H	-0.696455	2.508354	3.888466
H	-0.664176	1.146970	2.729449
H	-0.054197	0.920207	4.408030
C	3.699219	-3.261704	3.495875
H	4.738787	-3.143950	3.125835
H	3.646600	-2.822390	4.513923
H	3.500421	-4.349450	3.597349
C	1.235805	-2.725264	3.089608
H	0.519213	-2.177053	2.442733
H	0.924784	-3.791102	3.119129
H	1.151235	-2.318917	4.119289
H	0.039949	5.994854	0.884359
H	2.644169	-6.019508	-0.665244
N	-1.820163	-1.049729	-0.327247
C	-2.994748	-0.562419	0.505340

N	-4.087155	-1.186592	-0.079997
C	-3.663661	-1.976862	-1.152953
N	-2.180045	-1.863951	-1.208905
C	-5.456559	-0.882380	0.232813
C	-5.898105	0.446428	0.093184
C	-6.324528	-1.906287	0.650049
H	-5.192359	1.209463	-0.268749
H	-5.955267	-2.938248	0.745371
C	-7.234032	0.750097	0.399825
C	-7.661985	-1.588751	0.938129
H	-7.590180	1.786954	0.296923
H	-8.351985	-2.383586	1.261794
C	-8.115255	-0.262773	0.819662
H	-9.163777	-0.018412	1.052023
O	-4.308627	-2.657004	-1.908759
O	-2.884416	0.087961	1.507642
B	-1.887694	1.837556	-1.692403
F	-1.281231	2.156860	-0.450665
F	-0.993553	1.005168	-2.433227
F	-3.073437	1.044476	-1.405402
F	-2.233654	2.967739	-2.406054

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AuIMesCH3CN+

N	1.061727	-1.777597	0.005808
N	-1.123399	-1.749332	0.007051
C	-0.020410	-0.937218	0.003237
C	0.640955	-3.100144	0.011342
H	1.351520	-3.933342	0.014544
C	-0.735955	-3.082396	0.011957
H	-1.467862	-3.896894	0.015876
C	2.450041	-1.352069	0.003944
C	3.102132	-1.170718	-1.240194
C	2.383494	-1.384597	-2.552892
H	1.956664	-2.406764	-2.634306

C	4.454060	-0.779186	-1.209316
H	4.981889	-0.636220	-2.166520
C	5.149900	-0.572538	0.000401
C	4.456124	-0.774036	1.211315
H	4.985498	-0.627229	2.166993
C	3.103567	-1.165655	1.245814
C	2.387584	-1.374607	2.560752
H	1.968526	-2.399338	2.650353
C	-2.502157	-1.294097	0.004124
C	-3.147528	-1.075912	1.246050
C	-2.426725	-1.267660	2.560910
H	-1.982572	-2.281419	2.651542
C	-4.491418	-0.659582	1.210536
H	-5.012206	-0.482442	2.165934
C	-5.187292	-0.466516	-0.001648
C	-4.498436	-0.696586	-1.209675
H	-5.024584	-0.549142	-2.167019
C	-3.153388	-1.114560	-1.239407
C	-2.441044	-1.349802	-2.551850
H	-1.585529	-0.652574	-2.683050
Au	0.022949	1.058946	-0.002833
H	3.075786	-1.219681	3.413221
H	1.538903	-0.667251	2.681320
H	-1.595769	-0.538950	2.679741
H	-3.117873	-1.127333	3.413550
H	-2.032083	-2.379673	-2.627385
H	-3.128556	-1.200364	-3.405885
H	3.071956	-1.240962	-3.407128
H	1.540080	-0.671688	-2.677965
C	-6.639583	-0.050749	0.001993
H	-6.954150	0.354901	-0.979476
H	-7.296680	-0.918701	0.228324
H	-6.841397	0.716585	0.776747
C	6.592872	-0.125764	-0.004486
H	7.111838	-0.402175	0.934436

H	7.153585	-0.563749	-0.854481
H	6.660993	0.979679	-0.105404
N	0.072462	3.338397	-0.009764
C	0.104384	4.808044	-0.014233
C	0.137827	6.347674	-0.018915
H	0.134781	6.749956	1.000530
H	1.036059	6.725754	-0.520254
H	-0.731365	6.764083	-0.540660

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AuIMesUrN2+ SCF Done: -1681.38098312 A.U.

N	3.327076	0.247943	-0.023354
N	2.258024	2.153753	-0.047687
C	2.071780	0.797024	-0.020734
C	4.287686	1.249257	-0.051789
H	5.359105	1.023111	-0.058934
C	3.614102	2.450195	-0.066955
H	3.979770	3.482117	-0.090059
C	3.616744	-1.174755	-0.000657
C	3.777863	-1.814156	1.252818
C	3.631600	-1.059646	2.554618
H	4.326077	-0.195111	2.617226
C	4.079773	-3.189180	1.241915
H	4.213198	-3.705710	2.206631
C	4.222221	-3.918555	0.042735
C	4.059115	-3.232380	-1.178249
H	4.176374	-3.782864	-2.126050
C	3.756517	-1.857813	-1.232721
C	3.588610	-1.150245	-2.558054
H	4.287843	-0.294063	-2.666386
C	1.199294	3.147373	-0.053251
C	0.690450	3.590039	-1.298889
C	1.194034	3.027371	-2.608465
H	2.296128	3.120083	-2.708398
C	-0.317213	4.572142	-1.272037

H	-0.728441	4.929595	-2.230423
C	-0.810768	5.110633	-0.064835
C	-0.270944	4.634904	1.147211
H	-0.645119	5.042011	2.100802
C	0.739178	3.653619	1.185584
C	1.295508	3.161409	2.502211
H	1.092820	2.078984	2.652275
Au	0.339113	-0.194579	0.013543
H	3.775367	-1.842457	-3.400843
H	2.560853	-0.744655	-2.677894
H	0.950187	1.947457	-2.708220
H	0.734459	3.553700	-3.466450
H	2.396113	3.295402	2.567816
H	0.841739	3.707638	3.350802
H	3.840471	-1.719246	3.418117
H	2.603220	-0.657385	2.680515
N	-1.427077	-1.242734	0.046703
C	-2.780942	-0.535791	0.007442
N	-3.692140	-1.571809	0.035925
C	-3.010208	-2.804133	0.091253
N	-1.553414	-2.492524	0.089531
C	-5.128610	-1.421190	0.021763
C	-5.896175	-2.230577	-0.835775
C	-5.729923	-0.471009	0.867451
H	-5.413257	-2.970701	-1.489710
H	-5.117215	0.152027	1.534988
C	-7.292428	-2.083618	-0.837026
C	-7.126418	-0.328868	0.843935
H	-7.901223	-2.716185	-1.500931
H	-7.605366	0.413787	1.500203
C	-7.908073	-1.134117	-0.002925
H	-9.003114	-1.021968	-0.011947
O	-3.447135	-3.922020	0.129087
O	-2.894646	0.659805	-0.035507
C	-1.870016	6.187591	-0.078305

H	-2.369720	6.285889	0.905269
H	-1.423217	7.175762	-0.323726
H	-2.645963	5.985824	-0.844444
C	4.519368	-5.399363	0.069337
H	5.003527	-5.738255	-0.867704
H	5.178056	-5.668968	0.919140
H	3.581614	-5.985672	0.186335

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AuIMes+ SCF Done: -1059.21301894 A.U.

N	-1.099330	1.296611	0.001039
N	1.099351	1.296616	0.001073
C	0.000013	0.492821	0.000368
C	-0.687114	2.627396	0.002179
H	-1.410318	3.449713	0.002842
C	0.687129	2.627398	0.002197
H	1.410334	3.449714	0.002932
C	-2.482337	0.849734	0.000693
C	-3.129821	0.655794	-1.244072
C	-2.417673	0.882277	-2.558256
H	-2.022943	1.916793	-2.646013
C	-4.473883	0.237257	-1.210599
H	-4.997951	0.076816	-2.166935
C	-5.165936	0.023295	0.000078
C	-4.473826	0.235270	1.211081
H	-4.997854	0.073262	2.167177
C	-3.129773	0.653753	1.245176
C	-2.417566	0.878132	2.559690
H	-2.022933	1.912543	2.649112
C	2.482356	0.849729	0.000739
C	3.129722	0.653575	1.245221
C	2.417455	0.877776	2.559732
H	2.022712	1.912138	2.649230
C	4.473783	0.235081	1.211137
H	4.997757	0.072935	2.167236

C	5.165947	0.023265	0.000148
C	4.473948	0.237388	-1.210543
H	4.998055	0.077050	-2.166876
C	3.129901	0.655941	-1.244026
C	2.417832	0.882653	-2.558213
H	1.553600	0.195121	-2.683746
Au	-0.000018	-1.474915	-0.001303
H	-3.102260	0.708525	3.412044
H	-1.553566	0.190096	2.684085
H	1.553521	0.189641	2.684046
H	3.102141	0.708165	3.412092
H	2.023566	1.917344	-2.646013
H	3.102513	0.714167	-3.410801
H	-3.102434	0.714125	-3.410845
H	-1.553749	0.194358	-2.683822
C	6.618742	-0.388503	-0.000189
H	6.876820	-0.983222	-0.898748
H	7.277844	0.507328	-0.001074
H	6.877591	-0.982110	0.898869
C	-6.618726	-0.388492	-0.000195
H	-6.876915	-0.984114	0.897733
H	-7.277850	0.507317	0.001453
H	-6.877418	-0.981231	-0.899875

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I-EtEt SCF Done: -2306.27983102 A.U.

N	-3.993041	0.509725	0.149281
N	-3.505238	-1.615201	0.124383
C	-2.945299	-0.367159	0.054277
C	-5.192580	-0.180621	0.276703
H	-6.151384	0.339767	0.364540
C	-4.885425	-1.519906	0.262258
H	-5.520840	-2.407771	0.338370
C	-3.883382	1.958793	0.112997
C	-3.725321	2.654924	1.340328

C	-3.640264	1.949907	2.694575
H	-3.698027	0.855475	2.513764
C	-3.646150	4.061364	1.273094
H	-3.522081	4.638721	2.202462
C	-3.722225	4.736339	0.047053
C	-3.880462	4.017788	-1.146239
H	-3.941656	4.561493	-2.101983
C	-3.968124	2.610261	-1.146110
C	-4.142822	1.856994	-2.465897
H	-4.223479	0.773769	-2.233919
C	-2.773161	-2.869489	0.082929
C	-2.525957	-3.468464	-1.180520
C	-2.974324	-2.843243	-2.502054
H	-3.521481	-1.905599	-2.267663
C	-1.830388	-4.695581	-1.182772
H	-1.618689	-5.192700	-2.142307
C	-1.410068	-5.295598	0.012340
C	-1.676060	-4.679743	1.243591
H	-1.345843	-5.165731	2.175090
C	-2.365873	-3.451446	1.312838
C	-2.642557	-2.806930	2.672238
H	-3.214619	-1.871291	2.497500
Au	-1.011442	0.093564	-0.174716
C	-5.444124	2.265985	-3.189341
H	-5.426295	3.333899	-3.491683
H	-5.581542	1.663532	-4.111152
H	-6.335862	2.115714	-2.546711
C	-2.909607	2.033960	-3.378195
H	-3.026955	1.445439	-4.311774
H	-2.766491	3.095805	-3.668754
H	-1.981829	1.694015	-2.871647
C	-1.762219	-2.455441	-3.376525
H	-1.172404	-3.347472	-3.674662
H	-2.098459	-1.952450	-4.306858
H	-1.079555	-1.764932	-2.838151

C	-3.952091	-3.762944	-3.265248
H	-3.466866	-4.713681	-3.570067
H	-4.838071	-4.021920	-2.649814
H	-4.311677	-3.264341	-4.189145
C	-3.514449	-3.714156	3.567184
H	-4.471157	-3.981378	3.073189
H	-2.993828	-4.661120	3.821128
H	-3.754352	-3.201957	4.521944
C	-1.330219	-2.407540	3.380720
H	-0.705292	-3.295576	3.611806
H	-0.725976	-1.720688	2.752037
H	-1.546103	-1.893901	4.340512
C	-4.829925	2.326314	3.604575
H	-5.804074	2.097228	3.125376
H	-4.779746	1.766412	4.561515
H	-4.826234	3.408402	3.852484
C	-2.288134	2.224540	3.387374
H	-1.434290	1.947965	2.735227
H	-2.174280	3.297381	3.648753
H	-2.210923	1.644286	4.330336
H	-0.873999	-6.257300	-0.015675
H	-3.659975	5.835581	0.021354
N	0.966680	0.599705	-0.464635
C	1.542997	1.850189	0.101395
N	2.844199	1.876302	-0.380708
C	3.061018	0.737366	-1.182726
N	1.816693	-0.038413	-1.173213
C	3.810537	2.912276	-0.123612
C	5.142031	2.558210	0.165771
C	3.407938	4.260630	-0.168383
H	5.444407	1.501685	0.197464
H	2.364777	4.523365	-0.394409
C	6.078742	3.576176	0.406169
C	4.355334	5.264575	0.087020
H	7.122698	3.306817	0.628378

H	4.045357	6.320465	0.056954
C	5.690033	4.926604	0.370720
H	6.429670	5.718671	0.564546
O	4.055203	0.407687	-1.786715
O	0.929347	2.616939	0.804793
C	7.759532	-1.222884	-0.095146
C	7.025185	-1.680255	-1.213733
C	7.079925	-1.131011	1.147611
H	7.522397	-1.754579	-2.194567
H	7.630720	-0.781333	2.036669
C	5.678114	-2.036326	-1.095781
C	5.729873	-1.484212	1.270371
H	5.129140	-2.389452	-1.983173
H	5.245153	-1.409814	2.255709
C	4.998080	-1.958604	0.153736
C	3.555569	-2.379845	0.239584
H	2.930740	-1.635194	-0.339631
H	3.419469	-3.305764	-0.363994
C	2.948869	-2.558254	1.632827
H	2.950279	-1.614505	2.217670
H	3.504234	-3.315936	2.224237
H	1.896776	-2.898517	1.556507
C	9.231823	-0.894940	-0.204223
H	9.444509	-0.490071	-1.216959
H	9.485641	-0.091075	0.520257
C	10.138799	-2.117858	0.056466
H	9.936621	-2.930217	-0.671574
H	9.976970	-2.530501	1.073625
H	11.208107	-1.836971	-0.032405

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I-EtiPr SCF Done: -2345.56195489 A.U.

N	-4.191090	0.414630	-0.172708
N	-3.627194	-1.636926	0.300029
C	-3.109140	-0.403637	0.010160

C	-5.372689	-0.298264	0.000401
H	-6.353505	0.175374	-0.106416
C	-5.017768	-1.590791	0.299932
H	-5.624662	-2.476253	0.513029
C	-4.127146	1.826468	-0.511830
C	-4.122537	2.775631	0.544401
C	-4.172986	2.381129	2.021020
H	-4.123263	1.273063	2.079907
C	-4.082078	4.137801	0.180803
H	-4.077575	4.905477	0.970220
C	-4.049209	4.531091	-1.164255
C	-4.057751	3.567440	-2.182436
H	-4.035559	3.891050	-3.234848
C	-4.100116	2.189581	-1.884695
C	-4.114321	1.164415	-3.019739
H	-4.180096	0.152697	-2.566158
C	-2.848616	-2.829313	0.586199
C	-2.495196	-3.681590	-0.493186
C	-2.874321	-3.388274	-1.945412
H	-3.467863	-2.449732	-1.960234
C	-1.757354	-4.841891	-0.178813
H	-1.465039	-5.529851	-0.987547
C	-1.395745	-5.137652	1.143014
C	-1.764711	-4.276180	2.186034
H	-1.478880	-4.523909	3.220332
C	-2.503228	-3.100542	1.936876
C	-2.891530	-2.182133	3.096751
H	-3.506172	-1.353536	2.685608
Au	-1.179883	0.113890	-0.132850
C	-5.350723	1.337228	-3.928504
H	-5.340131	2.315713	-4.452593
H	-5.374421	0.545761	-4.706066
H	-6.296217	1.277724	-3.351217
C	-2.803425	1.211339	-3.834373

H	-2.806943	0.431650	-4.624152
H	-2.669315	2.192829	-4.335517
H	-1.918898	1.039003	-3.185734
C	-1.620009	-3.145331	-2.812660
H	-0.980300	-4.051184	-2.866617
H	-1.909941	-2.880905	-3.850750
H	-1.001210	-2.317746	-2.406921
C	-3.765577	-4.501181	-2.538127
H	-3.228333	-5.471118	-2.592138
H	-4.681807	-4.659910	-1.933058
H	-4.078682	-4.238650	-3.569883
C	-3.758369	-2.915849	4.142708
H	-4.667968	-3.356967	3.685813
H	-3.199001	-3.738262	4.635635
H	-4.081947	-2.213410	4.938494
C	-1.644199	-1.542297	3.744356
H	-0.979880	-2.310083	4.193648
H	-1.050226	-0.972329	2.999406
H	-1.940476	-0.842615	4.553177
C	-5.506209	2.815223	2.669764
H	-6.382044	2.389086	2.138198
H	-5.552052	2.480451	3.726929
H	-5.618383	3.919734	2.664451
C	-2.959660	2.931105	2.800683
H	-2.000436	2.614681	2.342420
H	-2.965757	4.040654	2.837094
H	-2.979337	2.568884	3.849558
H	-0.824978	-6.053384	1.363846
H	-4.020368	5.601388	-1.422305
N	0.794749	0.687733	-0.319352
C	1.346836	1.840966	0.438585
N	2.656155	1.952023	-0.009465
C	2.898592	0.951310	-0.972969
N	1.662583	0.172830	-1.103152
C	3.605534	2.945472	0.420250

C	4.941111	2.567710	0.656660
C	3.183415	4.277228	0.595251
H	5.259648	1.525216	0.513636
H	2.137544	4.559237	0.408881
C	5.861415	3.544893	1.068523
C	4.114701	5.238378	1.019169
H	6.908082	3.256835	1.250896
H	3.788955	6.280321	1.161111
C	5.452903	4.877183	1.253248
H	6.179575	5.636687	1.580475
O	3.905985	0.724678	-1.602065
O	0.713594	2.486941	1.239943
C	7.611390	-1.340689	-0.643773
C	6.748353	-1.677691	-1.712017
C	7.053547	-1.293145	0.661611
H	7.151178	-1.717399	-2.737166
H	7.697706	-1.043355	1.520166
C	5.397769	-1.962895	-1.490616
C	5.701338	-1.575822	0.888603
H	4.750030	-2.223738	-2.343001
H	5.314929	-1.546586	1.918848
C	4.840682	-1.931959	-0.180825
C	3.392669	-2.288931	0.015730
H	2.761030	-1.500504	-0.495743
H	3.162592	-3.189953	-0.597475
C	2.891454	-2.477690	1.448690
H	2.994001	-1.554098	2.056397
H	3.448719	-3.282236	1.972529
H	1.819433	-2.759464	1.450974
C	9.086683	-1.056390	-0.886680
H	9.248303	-1.119341	-1.985460
C	9.983160	-2.126194	-0.222201
H	9.724943	-3.146905	-0.570474
H	9.884939	-2.109959	0.883969
H	11.049962	-1.940561	-0.465497

C	9.483756	0.367274	-0.438763
H	8.861065	1.138774	-0.936308
H	9.377451	0.495124	0.659558
H	10.545077	0.569038	-0.692585

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AuIPrUrN2H–PhEt1+ISOMERpre SCF Done: -2227.70834732 A.U.

N	3.549936	0.846761	-0.216596
N	3.318200	-1.319524	-0.117093
C	2.615972	-0.144519	-0.072055
C	4.819889	0.298931	-0.349462
H	5.708877	0.925299	-0.473011
C	4.674003	-1.066479	-0.288352
H	5.408830	-1.875076	-0.352630
C	3.269915	2.273379	-0.221002
C	3.028167	2.909810	-1.467091
C	3.031482	2.161654	-2.800821
H	3.168075	1.080554	-2.585245
C	2.786408	4.298919	-1.439999
H	2.594039	4.830451	-2.384935
C	2.786290	5.013824	-0.234375
C	3.030181	4.353980	0.978225
H	3.030265	4.929103	1.917363
C	3.281974	2.966947	1.018339
C	3.548662	2.278642	2.358011
H	3.762265	1.207441	2.156327
C	2.739703	-2.649321	-0.024296
C	2.594134	-3.236689	1.260161
C	3.002982	-2.528919	2.552599
H	3.420087	-1.536030	2.280863
C	2.045601	-4.535170	1.311958
H	1.916418	-5.026708	2.288886
C	1.668826	-5.212611	0.143981
C	1.832825	-4.605393	-1.109273
H	1.539181	-5.152289	-2.018938

C	2.374667	-3.308603	-1.228108
C	2.540067	-2.673111	-2.609713
H	3.034936	-1.687799	-2.476555
Au	0.646271	0.090622	0.192516
C	4.789924	2.864477	3.065240
H	4.640674	3.929559	3.339900
H	5.001267	2.308106	4.001871
H	5.692830	2.808367	2.423132
C	2.303208	2.328281	3.269516
H	2.492012	1.785576	4.218965
H	2.030052	3.372282	3.530009
H	1.424456	1.861987	2.775832
C	1.782490	-2.274923	3.463614
H	1.319929	-3.225940	3.801180
H	2.084897	-1.712015	4.370931
H	1.000099	-1.688162	2.938177
C	4.113404	-3.302142	3.296801
H	3.761391	-4.299200	3.634668
H	5.004074	-3.462048	2.654983
H	4.437923	-2.742608	4.198513
C	3.450824	-3.519203	-3.525224
H	4.445195	-3.695245	-3.066003
H	3.003972	-4.511087	-3.745730
H	3.608792	-3.005293	-4.495950
C	1.169336	-2.404553	-3.268096
H	0.613375	-3.348302	-3.449126
H	0.535848	-1.754623	-2.628680
H	1.299436	-1.900383	-4.248173
C	4.214448	2.605282	-3.689776
H	5.189685	2.463026	-3.180058
H	4.233577	2.020938	-4.633130
H	4.135214	3.678212	-3.963604
C	1.684111	2.309387	-3.539470
H	0.834056	1.987663	-2.903622
H	1.496331	3.360579	-3.842519

H	1.680830	1.695019	-4.463690
H	1.248349	-6.228360	0.210612
H	2.596649	6.098647	-0.240114
N	-1.369613	0.369434	0.521921
C	-2.095885	1.551040	-0.043832
N	-3.378602	1.436615	0.467509
C	-3.451719	0.289956	1.282676
N	-2.127497	-0.349445	1.248133
C	-4.461929	2.355344	0.224684
C	-5.744387	1.849146	-0.058446
C	-4.217866	3.740599	0.278367
H	-5.922973	0.764990	-0.099220
H	-3.210876	4.121517	0.500911
C	-6.795150	2.752854	-0.283702
C	-5.277838	4.629013	0.037876
H	-7.801964	2.364662	-0.501053
H	-5.093304	5.713631	0.074849
C	-6.566045	4.139051	-0.239371
H	-7.394615	4.840726	-0.421305
O	-4.386109	-0.136833	1.917847
O	-1.581529	2.369340	-0.765908
C	-7.868534	-1.759767	-0.266119
C	-7.282949	-2.095214	0.966451
C	-7.094201	-1.816347	-1.444904
H	-7.878564	-2.058035	1.891733
H	-7.551888	-1.565188	-2.414927
C	-5.936398	-2.487012	1.018882
C	-5.746482	-2.205759	-1.391684
H	-5.484745	-2.758983	1.985751
H	-5.165801	-2.256818	-2.325141
C	-5.141793	-2.555552	-0.161082
H	-8.928134	-1.463401	-0.315104
C	-3.699017	-2.986580	-0.054510
H	-3.117346	-2.160777	0.448273

H	-3.630673	-3.811387	0.689891
C	-2.983337	-3.380161	-1.348803
H	-2.916114	-2.536602	-2.067393
H	-3.505661	-4.214003	-1.862847
H	-1.948298	-3.712934	-1.133200

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II-EtEt SCF Done: -2306.29887025 A.U.

N	3.456301	-1.079683	-0.176140
N	3.541498	1.062373	0.213187
C	2.668973	0.027359	0.000841
C	4.803067	-0.741686	-0.072557
H	5.595773	-1.488316	-0.181341
C	4.856759	0.607923	0.171500
H	5.705855	1.282163	0.320083
C	2.968270	-2.421531	-0.440632
C	2.657730	-3.260716	0.662230
C	2.817283	-2.818604	2.117137
H	3.091230	-1.742385	2.117032
C	2.206265	-4.564623	0.368193
H	1.957445	-5.246528	1.196155
C	2.075526	-5.008940	-0.954922
C	2.394587	-4.155621	-2.021334
H	2.295393	-4.520406	-3.055912
C	2.851352	-2.840887	-1.792751
C	3.196064	-1.936385	-2.977423
H	3.561886	-0.969040	-2.573414
C	3.156807	2.440971	0.458604
C	3.058192	3.322737	-0.650447
C	3.330027	2.882762	-2.090083
H	3.629028	1.813527	-2.069703
C	2.689261	4.657043	-0.380673
H	2.603790	5.372490	-1.213687
C	2.435578	5.090182	0.928542
C	2.549883	4.195906	2.001982

H	2.354396	4.551223	3.025838
C	2.916366	2.849125	1.797479
C	3.040006	1.903369	2.992886
H	3.352487	0.908831	2.610313
Au	0.676801	0.110465	0.057016
C	4.331003	-2.530292	-3.839451
H	4.028119	-3.487278	-4.313499
H	4.607552	-1.829771	-4.654569
H	5.241018	-2.729690	-3.237287
C	1.946008	-1.625543	-3.828581
H	2.198974	-0.930672	-4.656236
H	1.522225	-2.545297	-4.283754
H	1.152470	-1.151719	-3.213131
C	2.055274	2.979193	-2.955958
H	1.694532	4.026182	-3.036203
H	2.253688	2.615312	-3.985620
H	1.234083	2.367045	-2.527025
C	4.498933	3.672399	-2.717869
H	4.261508	4.752921	-2.809313
H	5.424311	3.584279	-2.112556
H	4.720458	3.294385	-3.737525
C	4.130214	2.375783	3.979434
H	5.114764	2.488899	3.480720
H	3.872509	3.353886	4.436851
H	4.247626	1.644601	4.805899
C	1.681556	1.710779	3.700877
H	1.305133	2.663251	4.129408
H	0.912060	1.325728	2.999183
H	1.776919	0.984908	4.534755
C	3.969539	-3.585139	2.804729
H	4.930566	-3.459037	2.264432
H	4.111611	-3.222304	3.843890
H	3.756620	-4.673535	2.857558
C	1.498359	-2.951156	2.907479
H	0.667163	-2.396406	2.425195

H	1.184654	-4.011749	3.005190
H	1.627084	-2.554111	3.935775
H	2.152021	6.137958	1.114930
H	1.728514	-6.034528	-1.157523
N	-1.394419	0.225011	0.201394
C	-2.145091	-0.501345	1.129571
N	-3.375590	0.180511	1.290744
C	-3.383618	1.355928	0.496470
N	-2.138429	1.324372	-0.133875
C	-4.450213	-0.226382	2.150162
C	-5.287659	0.748944	2.732981
C	-4.665970	-1.596153	2.413667
H	-5.123356	1.813380	2.521530
H	-3.994158	-2.350504	1.985009
C	-6.342333	0.344661	3.567024
C	-5.719058	-1.980905	3.259077
H	-6.993581	1.110240	4.017030
H	-5.876597	-3.050575	3.468538
C	-6.563497	-1.016869	3.835472
H	-7.388539	-1.325539	4.495907
O	-4.245671	2.207743	0.360574
O	-1.784667	-1.553082	1.660441
C	-5.635959	0.887124	-2.390543
C	-4.368443	1.258788	-2.900487
C	-5.751442	-0.358600	-1.707976
H	-4.265905	2.211014	-3.444789
H	-6.733498	-0.663149	-1.312577
C	-3.250284	0.451299	-2.695647
C	-4.650832	-1.182125	-1.513958
H	-2.270320	0.750427	-3.101582
H	-4.773776	-2.129762	-0.968647
C	-3.352694	-0.795909	-1.991159
C	-2.177934	-1.543933	-1.730570
H	-1.737175	2.104385	-0.655891
H	-1.243726	-1.139881	-2.156615

C	-2.088542	-2.857978	-1.065553
H	-1.806276	-2.706867	0.016458
H	-1.276227	-3.473192	-1.502259
H	-3.039273	-3.425352	-1.069668
C	-6.849844	1.754541	-2.609162
H	-7.486921	1.717239	-1.699748
H	-6.529447	2.810163	-2.731836
C	-7.681173	1.317317	-3.836756
H	-8.044328	0.274300	-3.731383
H	-7.084521	1.374702	-4.770152
H	-8.565751	1.975129	-3.954837

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II-EtiPr SCF Done: -2345.58191082 A.U.

N	3.618767	-0.850720	-0.446109
N	3.581754	1.150678	0.414358
C	2.769523	0.132763	-0.012015
C	4.944286	-0.453869	-0.290120
H	5.778338	-1.101693	-0.577024
C	4.921059	0.807377	0.250749
H	5.730493	1.487487	0.533516
C	3.208494	-2.128017	-1.001929
C	2.980875	-3.213632	-0.114818
C	3.155503	-3.102395	1.400143
H	3.337025	-2.034111	1.643266
C	2.605700	-4.444986	-0.692152
H	2.422626	-5.311511	-0.037990
C	2.469088	-4.587115	-2.080083
C	2.705116	-3.495565	-2.928473
H	2.602353	-3.623329	-4.017689
C	3.082786	-2.238333	-2.412523
C	3.340741	-1.069447	-3.365211
H	3.638288	-0.190789	-2.755062
C	3.119032	2.410839	0.968040
C	2.919952	3.504405	0.083891

C	3.153666	3.406481	-1.424720
H	3.571101	2.400401	-1.640783
C	2.475275	4.717037	0.650362
H	2.310196	5.589130	-0.001727
C	2.245800	4.833824	2.028740
C	2.459974	3.737030	2.875003
H	2.281639	3.844655	3.956361
C	2.905116	2.497621	2.369277
C	3.131160	1.322579	3.321610
H	3.511049	0.467182	2.724027
Au	0.778969	0.067465	0.096085
C	4.505493	-1.369372	-4.333582
H	4.269387	-2.219407	-5.007402
H	4.716595	-0.487533	-4.973477
H	5.436473	-1.625546	-3.787540
C	2.059932	-0.673979	-4.130998
H	2.249061	0.205105	-4.781595
H	1.701298	-1.498525	-4.782258
H	1.240243	-0.411629	-3.429554
C	1.823196	3.520332	-2.200668
H	1.341283	4.507320	-2.037563
H	1.994836	3.407688	-3.291518
H	1.107875	2.732756	-1.881399
C	4.185254	4.443352	-1.917971
H	3.822061	5.483248	-1.780677
H	5.148835	4.351536	-1.376218
H	4.387391	4.304855	-3.000340
C	4.203311	1.648289	4.384067
H	5.163733	1.952030	3.919134
H	3.880063	2.472494	5.053728
H	4.397742	0.761366	5.022019
C	1.807527	0.867763	3.973846
H	1.366165	1.668847	4.603182
H	1.056540	0.585153	3.206261
H	1.977500	-0.013761	4.626085

C	4.394065	-3.897653	1.871572
H	5.320166	-3.563325	1.359749
H	4.543470	-3.772463	2.964155
H	4.276342	-4.983632	1.672622
C	1.884722	-3.531826	2.163119
H	0.990623	-2.962413	1.835581
H	1.668317	-4.611873	2.023739
H	2.018872	-3.365916	3.252171
H	1.902098	5.792172	2.448770
H	2.182988	-5.561713	-2.506221
N	-1.289217	0.008135	0.301883
C	-1.960794	-0.958373	1.053909
N	-3.222439	-0.413106	1.395696
C	-3.327123	0.910368	0.897781
N	-2.108438	1.105063	0.247708
C	-4.237490	-1.075380	2.163464
C	-5.090886	-0.319299	2.995113
C	-4.377851	-2.477683	2.089254
H	-4.983915	0.771906	3.047240
H	-3.692377	-3.066258	1.466318
C	-6.087463	-0.972173	3.738053
C	-5.372764	-3.114752	2.848148
H	-6.752247	-0.376815	4.383278
H	-5.471803	-4.210228	2.793581
C	-6.233568	-2.368218	3.670647
H	-7.013149	-2.873697	4.261313
O	-4.240703	1.713976	0.989678
O	-1.521249	-2.078028	1.320736
C	-5.620638	1.005395	-2.046013
C	-4.382320	1.545501	-2.475773
C	-5.655714	-0.362666	-1.652489
H	-4.331184	2.594712	-2.804840
H	-6.613806	-0.797757	-1.326446
C	-3.222350	0.773884	-2.462586
C	-4.511246	-1.150078	-1.653163

H	-2.267482	1.206384	-2.803370
H	-4.576699	-2.199406	-1.328915
C	-3.245175	-0.600558	-2.045725
C	-2.029412	-1.324240	-1.971882
H	-1.775698	2.006567	-0.096321
H	-1.126267	-0.786257	-2.307281
C	-1.859111	-2.746359	-1.619245
H	-1.539653	-2.824093	-0.539680
H	-1.038729	-3.207889	-2.205233
H	-2.783880	-3.346095	-1.722357
C	-6.887787	1.841330	-2.033250
H	-7.648683	1.257179	-1.470554
C	-7.422934	2.036896	-3.473206
H	-7.608545	1.067575	-3.979074
H	-6.705765	2.614392	-4.094040
H	-8.378786	2.599666	-3.449488
C	-6.695399	3.189419	-1.307379
H	-7.672579	3.702956	-1.198836
H	-6.257282	3.043726	-0.300069
H	-6.030213	3.872379	-1.877169

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AuIPrUrN2H–PhEt1+ISOMERpre1 SCF Done: -2227.72493716 A.U.

N	-3.144909	1.106058	0.428026
N	-3.262543	-1.064529	0.275091
C	-2.386846	-0.013311	0.208318
C	-4.477531	0.758651	0.632733
H	-5.246999	1.511676	0.828982
C	-4.551869	-0.608547	0.535272
H	-5.399478	-1.294610	0.627920
C	-2.641716	2.468162	0.443783
C	-2.148341	2.995143	1.666963
C	-2.128971	2.197522	2.971395
H	-2.447268	1.159149	2.739631
C	-1.686177	4.328022	1.650284

H	-1.297847	4.773717	2.579247
C	-1.719716	5.095844	0.477880
C	-2.218377	4.546329	-0.712323
H	-2.248041	5.164107	-1.623727
C	-2.693662	3.219190	-0.760942
C	-3.249756	2.655608	-2.070005
H	-3.529402	1.595566	-1.893702
C	-2.902168	-2.461692	0.110027
C	-2.968950	-3.027821	-1.190797
C	-3.387692	-2.227494	-2.425331
H	-3.690904	-1.213707	-2.088410
C	-2.617233	-4.387607	-1.319147
H	-2.657438	-4.864340	-2.311181
C	-2.224275	-5.144534	-0.206093
C	-2.177539	-4.557071	1.065808
H	-1.873473	-5.165091	1.932171
C	-2.517635	-3.201749	1.259513
C	-2.460184	-2.594228	2.661798
H	-2.790635	-1.536446	2.589585
Au	-0.412163	-0.117469	-0.054042
C	-4.529896	3.401994	-2.505991
H	-4.322962	4.469804	-2.728142
H	-4.953545	2.946257	-3.424975
H	-5.310750	3.371207	-1.718670
C	-2.188113	2.661703	-3.190259
H	-2.594047	2.200360	-4.114386
H	-1.868296	3.692892	-3.448588
H	-1.284771	2.090236	-2.890501
C	-2.201340	-2.045199	-3.397146
H	-1.839968	-3.020891	-3.784964
H	-2.500555	-1.428066	-4.269874
H	-1.349624	-1.539831	-2.893814
C	-4.606474	-2.855584	-3.134425
H	-4.371625	-3.859805	-3.544868
H	-5.467459	-2.969474	-2.444421

H	-4.931307	-2.219716	-3.983942
C	-3.426889	-3.308770	3.631116
H	-4.470241	-3.297031	3.254158
H	-3.139803	-4.369484	3.788320
H	-3.416438	-2.812825	4.623756
C	-1.016515	-2.582049	3.209344
H	-0.615221	-3.610568	3.326123
H	-0.333538	-2.025173	2.533906
H	-0.982348	-2.095717	4.206173
C	-3.143577	2.772510	3.985441
H	-4.172935	2.796959	3.571782
H	-3.160868	2.157076	4.908796
H	-2.877709	3.809309	4.280472
C	-0.711466	2.113865	3.575830
H	0.021302	1.688296	2.859548
H	-0.339302	3.112640	3.886754
H	-0.718928	1.472965	4.481757
H	-1.957666	-6.205851	-0.330477
H	-1.361033	6.137173	0.493544
N	1.655008	-0.281283	-0.268269
C	2.561040	0.123680	0.723999
N	3.746274	-0.619986	0.531334
C	3.573520	-1.537673	-0.537422
N	2.270361	-1.278016	-0.975029
C	4.940573	-0.506625	1.320569
C	5.753985	-1.641247	1.525289
C	5.295412	0.735197	1.888990
H	5.480954	-2.604369	1.075125
H	4.645741	1.609135	1.752667
C	6.925033	-1.521213	2.290572
C	6.464182	0.833580	2.660807
H	7.558334	-2.408810	2.444393
H	6.732164	1.802789	3.109790
C	7.285312	-0.288977	2.861900
H	8.201953	-0.204434	3.465810

O	4.340981	-2.364238	-0.994942
O	2.335651	0.993817	1.564397
C	5.440423	-0.203439	-3.542366
C	4.116168	-0.467343	-3.937022
C	5.715075	0.783756	-2.566826
H	3.911815	-1.225937	-4.707718
H	6.755588	0.986869	-2.271586
C	3.062415	0.228516	-3.335733
C	4.673105	1.493381	-1.974590
H	2.023110	0.041885	-3.650748
H	4.898315	2.254520	-1.212779
C	3.311822	1.228087	-2.338127
H	6.270561	-0.762572	-4.001303
C	2.205066	1.859475	-1.702732
H	1.749363	-1.881883	-1.612756
H	1.209279	1.588696	-2.091767
C	2.258559	2.960711	-0.721902
H	2.162649	2.539817	0.320321
H	1.398814	3.649191	-0.846278
H	3.208295	3.529537	-0.746243

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III-EtEt SCF Done: -2306.31745148 A.U.

N	3.456759	-0.945306	0.476532
N	3.301347	1.105325	-0.249540
C	2.562547	-0.012419	0.027893
C	4.744319	-0.416401	0.481578
H	5.607904	-1.003569	0.809125
C	4.646509	0.874563	0.024215
H	5.407207	1.646254	-0.129613
C	3.118979	-2.295425	0.893584
C	2.786409	-2.518295	2.256205
C	2.764220	-1.404381	3.303895
H	3.055826	-0.457450	2.802120
C	2.470964	-3.841614	2.629815

H	2.207619	-4.056923	3.677165
C	2.492878	-4.886519	1.695520
C	2.834321	-4.632618	0.359368
H	2.854451	-5.464656	-0.361801
C	3.159560	-3.331528	-0.077256
C	3.525247	-3.086189	-1.542177
H	3.807924	-2.017528	-1.649589
C	2.763665	2.360117	-0.746805
C	2.669476	2.546019	-2.151723
C	3.109168	1.485872	-3.163060
H	3.553324	0.638604	-2.598845
C	2.139414	3.772754	-2.602420
H	2.047885	3.956848	-3.684295
C	1.733266	4.764618	-1.698382
C	1.852858	4.553494	-0.317640
H	1.539060	5.345197	0.380570
C	2.373505	3.347362	0.196425
C	2.496003	3.151031	1.708297
H	2.964457	2.160078	1.887470
Au	0.590002	-0.232291	-0.169043
C	4.745062	-3.925509	-1.979124
H	4.529075	-5.013689	-1.944569
H	5.031211	-3.678999	-3.022545
H	5.625057	-3.738319	-1.330278
C	2.312466	-3.329328	-2.466746
H	2.573223	-3.104920	-3.521885
H	1.972361	-4.385215	-2.423574
H	1.454755	-2.684666	-2.179151
C	1.902155	0.925873	-3.946641
H	1.396690	1.716405	-4.539765
H	2.224558	0.131063	-4.650780
H	1.152218	0.484971	-3.254752
C	4.199690	2.019505	-4.116867
H	3.819986	2.844188	-4.755333
H	5.077441	2.405134	-3.559067

H	4.551732	1.213349	-4.793297
C	3.418314	4.212259	2.346913
H	4.424303	4.218036	1.879262
H	2.997302	5.234508	2.247496
H	3.546151	4.011731	3.430770
C	1.109159	3.126112	2.386148
H	0.574300	4.090334	2.258656
H	0.466522	2.324464	1.966026
H	1.211208	2.943553	3.475871
C	3.795203	-1.662284	4.424689
H	4.820934	-1.785680	4.020318
H	3.809319	-0.814196	5.140165
H	3.550863	-2.578306	5.002082
C	1.345771	-1.196584	3.877066
H	0.611449	-0.961070	3.078742
H	0.985623	-2.100044	4.412328
H	1.340089	-0.357530	4.603166
H	1.325271	5.715561	-2.075205
H	2.247063	-5.911908	2.013441
N	-1.564307	-0.404584	-0.457644
C	-2.213460	0.342557	0.675421
N	-2.828351	1.445474	0.116402
C	-2.612276	1.515666	-1.294614
N	-1.961474	0.327217	-1.623704
C	-3.565767	2.429121	0.865212
C	-3.351447	3.797834	0.612339
C	-4.496485	2.007797	1.833979
H	-2.632552	4.112135	-0.156397
H	-4.660547	0.936201	2.013166
C	-4.083459	4.749470	1.340594
C	-5.209650	2.972072	2.563113
H	-3.925903	5.820689	1.140902
H	-5.935911	2.647051	3.324027
C	-5.007959	4.341688	2.317741
H	-5.575731	5.093342	2.887670

O	-2.912556	2.411770	-2.049323
O	-2.155400	-0.021503	1.827366
C	-6.447024	-2.030654	-0.843772
C	-5.635393	-1.946531	-1.996543
C	-5.801396	-2.075887	0.412349
H	-6.108309	-1.915169	-2.991765
H	-6.408938	-2.150616	1.329401
C	-4.237112	-1.902511	-1.897081
C	-4.402887	-2.032434	0.518780
H	-3.631555	-1.844607	-2.816128
H	-3.940814	-2.074579	1.516441
C	-3.595019	-1.939598	-0.638648
C	-2.079753	-1.891150	-0.564483
H	-1.290132	0.340742	-2.398949
H	-1.670266	-2.187748	-1.552162
C	-1.441997	-2.759740	0.517236
H	-1.746364	-2.458854	1.536089
H	-0.333487	-2.717391	0.462483
H	-1.754259	-3.809939	0.350518
C	-7.955551	-2.126404	-0.953087
H	-8.418356	-1.643151	-0.065826
H	-8.295723	-1.547463	-1.838448
C	-8.460220	-3.579422	-1.066135
H	-8.166070	-4.178780	-0.179653
H	-8.043087	-4.082424	-1.963083
H	-9.566342	-3.607223	-1.144001

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III-EtiPr SCF Done: -2345.59964328 A.U.

N	3.618377	-0.976565	0.371451
N	3.451043	1.072910	-0.355135
C	2.713812	-0.034806	-0.036266
C	4.910751	-0.463134	0.309931
H	5.782591	-1.059362	0.596711
C	4.805381	0.827134	-0.147565

H	5.566292	1.589362	-0.342096
C	3.286319	-2.320352	0.812891
C	3.033385	-2.534126	2.193908
C	3.084444	-1.414983	3.234996
H	3.385314	-0.479793	2.716841
C	2.720733	-3.851235	2.590995
H	2.517576	-4.059388	3.653081
C	2.669877	-4.898994	1.660976
C	2.933580	-4.654246	0.305647
H	2.897204	-5.488577	-0.412244
C	3.251936	-3.359667	-0.154762
C	3.531852	-3.124053	-1.639984
H	3.827399	-2.061124	-1.767554
C	2.905479	2.332593	-0.831090
C	2.752732	2.517577	-2.231014
C	3.130714	1.448770	-3.258174
H	3.599257	0.601637	-2.713877
C	2.218930	3.750134	-2.660876
H	2.082803	3.933643	-3.738133
C	1.864067	4.748108	-1.742099
C	2.039799	4.537229	-0.367373
H	1.765496	5.333386	0.342286
C	2.567615	3.325643	0.126148
C	2.750915	3.129716	1.631891
H	3.217635	2.134831	1.792967
Au	0.731755	-0.235261	-0.139824
C	4.706554	-3.986989	-2.148554
H	4.472775	-5.070847	-2.098000
H	4.932828	-3.747508	-3.208185
H	5.627928	-3.815336	-1.555253
C	2.260080	-3.346039	-2.487469
H	2.459471	-3.129174	-3.557460
H	1.903175	-4.395048	-2.419346
H	1.434202	-2.684100	-2.149605
C	1.878187	0.892686	-3.969923

H	1.345182	1.683697	-4.537748
H	2.155317	0.091809	-4.686386
H	1.165982	0.461190	-3.233644
C	4.170737	1.967769	-4.274201
H	3.762255	2.789813	-4.898085
H	5.080183	2.351583	-3.768352
H	4.479963	1.153889	-4.962181
C	3.707854	4.183195	2.231083
H	4.694012	4.179501	1.722923
H	3.292310	5.209115	2.147870
H	3.877842	3.982368	3.309078
C	1.392529	3.117655	2.365517
H	0.861492	4.086519	2.258667
H	0.726225	2.321578	1.972485
H	1.536957	2.934883	3.450400
C	4.146580	-1.695549	4.320328
H	5.152723	-1.854080	3.880583
H	4.212454	-0.842022	5.026332
H	3.895538	-2.597950	4.915958
C	1.693392	-1.162962	3.856019
H	0.940016	-0.908171	3.081612
H	1.325330	-2.054429	4.405848
H	1.737079	-0.321981	4.578605
H	1.452149	5.703572	-2.102901
H	2.427910	-5.919497	1.997048
N	-1.433727	-0.393797	-0.335637
C	-2.032027	0.404151	0.790708
N	-2.656181	1.491815	0.212158
C	-2.494179	1.503847	-1.207732
N	-1.869051	0.295878	-1.513709
C	-3.354846	2.512131	0.948791
C	-3.137869	3.867442	0.633668
C	-4.251175	2.139342	1.968577
H	-2.446229	4.143540	-0.173762
H	-4.417568	1.077425	2.196507

C	-3.832372	4.854812	1.351013
C	-4.926675	3.139174	2.685601
H	-3.672709	5.915585	1.103048
H	-5.625684	2.852174	3.486299
C	-4.722063	4.495824	2.378343
H	-5.260305	5.275420	2.939327
O	-2.814596	2.372946	-1.985506
O	-1.933777	0.084969	1.953108
C	-6.342768	-1.992145	-0.498452
C	-5.565977	-1.962358	-1.679074
C	-5.655801	-1.989265	0.735091
H	-6.061363	-1.974892	-2.663047
H	-6.235022	-2.026385	1.672541
C	-4.165820	-1.925133	-1.624840
C	-4.253403	-1.952688	0.797003
H	-3.589588	-1.915103	-2.564406
H	-3.761486	-1.961797	1.781220
C	-3.482450	-1.914026	-0.387044
C	-1.965328	-1.878176	-0.364401
H	-1.230385	0.269077	-2.315720
H	-1.591321	-2.218630	-1.352051
C	-1.299670	-2.708920	0.730189
H	-1.570796	-2.367003	1.745454
H	-0.193054	-2.677219	0.640076
H	-1.623612	-3.762346	0.613699
C	-7.866905	-2.038945	-0.548685
H	-8.220335	-2.048411	0.506492
C	-8.375724	-3.332770	-1.219887
H	-7.980608	-4.237315	-0.713818
H	-8.074147	-3.383169	-2.287755
H	-9.484036	-3.378556	-1.185737
C	-8.454996	-0.781971	-1.224706
H	-8.159123	-0.717568	-2.293384
H	-9.563978	-0.804361	-1.188957
H	-8.115539	0.147769	-0.723779

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AuIPrUrN2H–PhEt1+ISOMERpost1 SCF Done: -2227.74654574 A.U.

N	3.309205	-0.220451	0.508009
N	2.613950	1.766772	-0.061407
C	2.202564	0.471911	0.099337
C	4.404457	0.633229	0.603323
H	5.389899	0.274647	0.916606
C	3.966622	1.884353	0.245071
H	4.491314	2.842679	0.181050
C	3.343222	-1.641428	0.808682
C	3.076837	-2.056110	2.140688
C	2.751488	-1.077987	3.270572
H	2.793367	-0.049024	2.854523
C	3.124929	-3.441769	2.401268
H	2.924845	-3.805004	3.421389
C	3.428826	-4.362608	1.388792
C	3.695695	-3.917865	0.085978
H	3.940911	-4.652177	-0.697270
C	3.663553	-2.545739	-0.238831
C	3.959209	-2.092183	-1.669469
H	3.942507	-0.981846	-1.686481
C	1.764511	2.869550	-0.477765
C	1.642366	3.142509	-1.866309
C	2.359167	2.324446	-2.942102
H	3.005897	1.579837	-2.431523
C	0.813114	4.221112	-2.237575
H	0.689716	4.465583	-3.304214
C	0.148917	4.992324	-1.273131
C	0.301428	4.703046	0.090059
H	-0.219036	5.322798	0.836926
C	1.113862	3.635208	0.525788
C	1.268995	3.355720	2.021595
H	1.931147	2.471638	2.137736
Au	0.368959	-0.254145	-0.196890
C	5.363978	-2.533325	-2.133593

H	5.450827	-3.638539	-2.187393
H	5.580069	-2.135545	-3.146728
H	6.155506	-2.168570	-1.447427
C	2.864444	-2.577078	-2.644693
H	3.061363	-2.204416	-3.671334
H	2.823496	-3.685417	-2.693298
H	1.861952	-2.214021	-2.332463
C	1.353078	1.533835	-3.806505
H	0.660964	2.209423	-4.351199
H	1.882860	0.915082	-4.560127
H	0.740623	0.853631	-3.175618
C	3.279781	3.204394	-3.814995
H	2.702188	3.950259	-4.399651
H	4.017419	3.759503	-3.200161
H	3.840660	2.578973	-4.539983
C	1.952275	4.536507	2.746229
H	2.938971	4.778045	2.300179
H	1.331885	5.455971	2.701845
H	2.111273	4.294640	3.817495
C	-0.082294	2.998261	2.676511
H	-0.801336	3.841968	2.620948
H	-0.552962	2.120192	2.187798
H	0.059257	2.754429	3.749682
C	3.797673	-1.153621	4.404129
H	4.825935	-0.974382	4.028126
H	3.580555	-0.392871	5.182215
H	3.791464	-2.146064	4.901288
C	1.319707	-1.292533	3.807280
H	0.561271	-1.184735	3.004064
H	1.198618	-2.301340	4.254624
H	1.086218	-0.549427	4.597553
H	-0.489392	5.832617	-1.588173
H	3.464730	-5.439003	1.619002
N	-1.651085	-0.975592	-0.596501
C	-2.519131	-0.453504	0.516656

N	-3.370522	0.472628	-0.052351
C	-3.120044	0.636795	-1.449590
N	-2.174903	-0.338525	-1.768849
C	-4.365295	1.214971	0.677185
C	-4.492603	2.600868	0.462443
C	-5.201496	0.542346	1.588487
H	-3.842246	3.110460	-0.261393
H	-5.096950	-0.541088	1.738697
C	-5.473457	3.313936	1.170438
C	-6.167417	1.272288	2.298534
H	-5.583140	4.396131	1.000132
H	-6.821364	0.750895	3.014454
C	-6.307842	2.655641	2.090361
H	-7.072495	3.221592	2.644573
O	-3.606423	1.448900	-2.202011
O	-2.419408	-0.825112	1.663166
C	-5.877663	-3.816445	-1.264919
C	-5.085081	-3.500520	-2.381693
C	-5.331418	-3.723068	0.027338
H	-5.502010	-3.581548	-3.397538
H	-5.943650	-3.983249	0.905034
C	-3.754646	-3.087781	-2.203584
C	-4.000377	-3.310490	0.206218
H	-3.135888	-2.853892	-3.084938
H	-3.587336	-3.252400	1.224192
C	-3.195180	-2.981604	-0.909758
H	-6.919781	-4.144900	-1.402065
C	-1.749649	-2.537722	-0.753965
H	-1.495307	-0.127044	-2.507671
H	-1.231791	-2.689007	-1.723474
C	-0.957403	-3.243579	0.344191
H	-1.376211	-3.064953	1.351149
H	0.102573	-2.911909	0.347649
H	-0.975229	-4.333103	0.141900

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III-iPrEt180 SCF Done: -2345.59774945 A.U.

N	3.536244	-0.614292	0.637053
N	3.206580	1.406165	-0.114386
C	2.577130	0.213571	0.120136
C	4.753442	0.054675	0.728386
H	5.650897	-0.431943	1.122631
C	4.546350	1.326383	0.254351
H	5.226168	2.177336	0.147185
C	3.325412	-1.994671	1.037867
C	2.866860	-2.253557	2.356818
C	2.599254	-1.149629	3.380936
H	2.797326	-0.173060	2.890526
C	2.679787	-3.605221	2.715157
H	2.324689	-3.848968	3.728633
C	2.946505	-4.641912	1.810103
C	3.411614	-4.351130	0.519503
H	3.627546	-5.176434	-0.176868
C	3.614816	-3.020552	0.098490
C	4.155410	-2.736194	-1.304197
H	4.143133	-1.636344	-1.458289
C	2.571027	2.594263	-0.657155
C	2.540249	2.760897	-2.067428
C	3.140187	1.742869	-3.039060
H	3.656204	0.962235	-2.440870
C	1.915275	3.924163	-2.562753
H	1.868506	4.090962	-3.650286
C	1.359599	4.875866	-1.695792
C	1.420152	4.687060	-0.308068
H	0.988576	5.447761	0.361134
C	2.028423	3.542914	0.249656
C	2.090996	3.375312	1.768740
H	2.588261	2.406329	1.985833
Au	0.652204	-0.202958	-0.201695
C	5.622058	-3.203782	-1.439692

H	5.708334	-4.303760	-1.317307
H	6.023395	-2.945645	-2.441664
H	6.276709	-2.732619	-0.678021
C	3.268407	-3.355570	-2.404029
H	3.649527	-3.081607	-3.409491
H	3.254117	-4.463977	-2.348800
H	2.220169	-3.000173	-2.326112
C	2.036401	1.034005	-3.853845
H	1.464904	1.752667	-4.477973
H	2.474336	0.272845	-4.532417
H	1.319523	0.516514	-3.179780
C	4.199113	2.381389	-3.963213
H	3.753340	3.142498	-4.636867
H	5.002715	2.877972	-3.381960
H	4.669424	1.608142	-4.605252
C	2.945619	4.484005	2.421967
H	3.971262	4.515650	2.000193
H	2.493346	5.487072	2.274954
H	3.030792	4.314873	3.515384
C	0.681095	3.309585	2.393277
H	0.119653	4.254745	2.240344
H	0.080741	2.484624	1.956919
H	0.748787	3.138527	3.487499
C	3.562964	-1.258587	4.583648
H	4.625128	-1.236333	4.263797
H	3.400046	-0.416664	5.287998
H	3.404027	-2.200231	5.149636
C	1.125010	-1.137744	3.837418
H	0.429979	-1.007990	2.981916
H	0.850062	-2.079339	4.357271
H	0.947294	-0.304719	4.548584
H	0.879775	5.777798	-2.106859
H	2.797915	-5.689319	2.116359
N	-1.466767	-0.542816	-0.601702
C	-2.216582	0.006800	0.583418

N	-2.946961	1.086705	0.124529
C	-2.689442	1.350060	-1.252763
N	-1.890858	0.291490	-1.685122
C	-3.819168	1.881297	0.948709
C	-3.778146	3.285804	0.853555
C	-4.707192	1.240206	1.833716
H	-3.091229	3.772258	0.147953
H	-4.734735	0.143047	1.889650
C	-4.641264	4.050031	1.655495
C	-5.552640	2.019373	2.638791
H	-4.618910	5.148140	1.578825
H	-6.245222	1.522354	3.335530
C	-5.524488	3.422392	2.550768
H	-6.195122	4.027982	3.179819
O	-3.060386	2.292559	-1.915035
O	-2.138966	-0.455207	1.698490
C	-6.248527	-2.415903	-0.967945
C	-5.527980	-1.953243	-2.090150
C	-5.506057	-2.763917	0.181074
H	-6.071774	-1.681958	-3.009894
H	-6.032811	-3.144523	1.071761
C	-4.129353	-1.847848	-2.068681
C	-4.107043	-2.656134	0.210351
H	-3.620191	-1.496229	-2.976961
H	-3.579453	-2.951146	1.127966
C	-3.383726	-2.194157	-0.915570
C	-1.853615	-2.080747	-0.889600
H	-1.189237	0.488350	-2.406075
C	-1.190513	-2.929258	0.204830
H	-1.513832	-2.653732	1.223143
H	-0.085856	-2.825900	0.158322
H	-1.441120	-3.993824	0.025747
C	-7.761107	-2.503601	-0.986784
H	-8.098120	-2.784851	-2.007714
H	-8.088943	-3.323239	-0.311992

C	-8.447449	-1.187800	-0.567294
H	-8.167296	-0.352993	-1.242735
H	-8.160130	-0.894023	0.463599
H	-9.551342	-1.292743	-0.596035
C	-1.208265	-2.428637	-2.239465
H	-0.107176	-2.291859	-2.190513
H	-1.410799	-3.494739	-2.462824
H	-1.603830	-1.834487	-3.083917

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III-iPrX SCF Done: -2267.02693007 A.U.

N	3.225310	-0.374047	0.818044
N	2.787093	1.621000	0.053601
C	2.245243	0.376189	0.227610
C	4.368741	0.394749	1.014820
H	5.269037	-0.019310	1.479203
C	4.093409	1.650523	0.532785
H	4.704465	2.557337	0.487697
C	3.102834	-1.773273	1.190024
C	2.561748	-2.090039	2.464248
C	2.112193	-1.028190	3.468773
H	2.232845	-0.033074	2.990543
C	2.469533	-3.457638	2.798147
H	2.055828	-3.745668	3.777139
C	2.901954	-4.454026	1.912151
C	3.441585	-4.105533	0.665629
H	3.786291	-4.898905	-0.015842
C	3.557869	-2.756617	0.270784
C	4.182173	-2.406908	-1.081543
H	4.078278	-1.311429	-1.232710
C	2.099929	2.755519	-0.538503
C	2.187809	2.940547	-1.944019
C	2.974465	2.001470	-2.860346
H	3.475617	1.242132	-2.223389
C	1.507295	4.049367	-2.488966

H	1.549311	4.228608	-3.574769
C	0.785713	4.932265	-1.672922
C	0.731979	4.728374	-0.286973
H	0.169615	5.435686	0.342442
C	1.388085	3.636279	0.318591
C	1.322539	3.451118	1.835404
H	1.872464	2.520641	2.090603
Au	0.392991	-0.193867	-0.245855
C	5.692813	-2.732446	-1.096380
H	5.872508	-3.820465	-0.968717
H	6.148777	-2.428324	-2.061407
H	6.235184	-2.208691	-0.282595
C	3.452027	-3.095415	-2.253436
H	3.885389	-2.773028	-3.222761
H	3.542550	-4.200539	-2.205039
H	2.370884	-2.845747	-2.261062
C	2.035526	1.239207	-3.820105
H	1.491371	1.932021	-4.495730
H	2.611063	0.534980	-4.456050
H	1.282599	0.649015	-3.254662
C	4.082159	2.750073	-3.632746
H	3.660025	3.501833	-4.331737
H	4.771524	3.282195	-2.945772
H	4.682781	2.038403	-4.236195
C	2.022262	4.613467	2.574115
H	3.077656	4.729353	2.252419
H	1.509292	5.580537	2.389849
H	2.016415	4.436961	3.669674
C	-0.129494	3.266209	2.324298
H	-0.745158	4.169827	2.133478
H	-0.621188	2.408401	1.820151
H	-0.150859	3.076205	3.417230
C	3.006416	-1.040593	4.728800
H	4.077237	-0.897416	4.476040
H	2.707729	-0.229219	5.424504

H	2.918817	-2.000247	5.279943
C	0.620233	-1.178540	3.833708
H	-0.031182	-1.133937	2.936363
H	0.419239	-2.141356	4.348437
H	0.307957	-0.366649	4.522693
H	0.264880	5.792484	-2.121707
H	2.824308	-5.514528	2.198907
N	-1.661245	-0.690173	-0.796370
C	-2.512368	-0.410271	0.416236
N	-3.339779	0.645011	0.083258
C	-3.059938	1.144205	-1.222313
N	-2.133346	0.252913	-1.765330
C	-4.334401	1.202012	0.962423
C	-4.436791	2.599584	1.100179
C	-5.198475	0.338409	1.662272
H	-3.766603	3.261553	0.535211
H	-5.114102	-0.749915	1.534203
C	-5.419701	3.131416	1.950498
C	-6.166176	0.885722	2.518885
H	-5.509537	4.223636	2.056002
H	-6.842089	0.214419	3.070753
C	-6.280911	2.279635	2.663550
H	-7.046735	2.703272	3.331544
O	-3.506778	2.134695	-1.754261
O	-2.428040	-1.029760	1.451369
C	-6.164038	-2.966270	-1.623936
C	-5.501063	-2.249006	-2.633319
C	-5.433603	-3.439160	-0.520995
H	-6.059317	-1.877757	-3.506805
H	-5.938026	-4.013458	0.271894
C	-4.120193	-2.008353	-2.541107
C	-4.053798	-3.192557	-0.424980
H	-3.630338	-1.452905	-3.352870
H	-3.510977	-3.577537	0.449054
C	-3.369059	-2.470753	-1.432707

H	-7.244942	-3.162211	-1.700350
C	-1.860624	-2.195814	-1.325061
H	-1.427170	0.634416	-2.403274
C	-1.134172	-3.122868	-0.339849
H	-1.507714	-3.034098	0.694650
H	-0.047111	-2.897238	-0.328347
H	-1.261216	-4.170157	-0.679208
C	-1.147230	-2.265346	-2.683746
H	-0.071633	-2.012565	-2.571033
H	-1.216609	-3.302991	-3.066016
H	-1.590374	-1.601804	-3.449150

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IIImetal-EtX SCF Done: -2227.74365370 A.U.

N	-2.290815	1.557739	-0.926188
C	-3.622784	1.216115	-0.747325
N	-3.706372	-0.198216	-1.054213
C	-2.526190	-0.686050	-1.552352
N	-1.552921	0.464964	-1.480493
C	-4.918234	-0.963678	-0.919191
C	-5.280169	-1.887609	-1.918911
C	-5.728149	-0.771062	0.217255
H	-4.640339	-2.033705	-2.800158
H	-5.442685	-0.039055	0.985060
C	-6.462637	-2.629280	-1.769059
C	-6.913452	-1.512160	0.344776
H	-6.746653	-3.354890	-2.546795
H	-7.552381	-1.359422	1.228214
C	-7.282174	-2.442561	-0.642345
H	-8.211800	-3.022378	-0.534356
O	-2.210321	-1.763984	-1.998720
O	-4.531498	1.928784	-0.388891
C	-2.757017	5.067585	2.691129
C	-3.147098	5.587627	1.446849
C	-2.041532	3.857344	2.745006

H	-3.710444	6.532315	1.394900
H	-1.730144	3.442453	3.716473
C	-2.829650	4.903694	0.259592
C	-1.720437	3.179104	1.559550
H	-3.157168	5.325832	-0.701519
H	-1.159804	2.229766	1.607185
C	-2.113928	3.692429	0.304091
H	-3.009788	5.603384	3.619335
C	-1.718227	2.924984	-0.961102
H	-1.292004	0.680080	-2.464888
H	-0.619598	2.743764	-0.896267
C	-2.026372	3.622447	-2.293823
H	-1.667711	3.018807	-3.154255
H	-1.511761	4.602060	-2.347230
H	-3.114598	3.789440	-2.419250
N	3.254448	-0.110292	0.137022
N	2.225773	-1.765886	1.117451
C	2.021088	-0.676972	0.314845
C	4.222397	-0.839578	0.821176
H	5.278929	-0.555049	0.803670
C	3.574520	-1.880953	1.438430
H	3.949009	-2.690173	2.072907
C	3.527339	1.074119	-0.659039
C	3.742681	0.916131	-2.054065
C	3.716960	-0.443192	-2.755377
H	3.524516	-1.221735	-1.987221
C	4.006591	2.085069	-2.798554
H	4.180176	2.005594	-3.883201
C	4.064924	3.342437	-2.181529
C	3.864794	3.460620	-0.798726
H	3.926342	4.453094	-0.326041
C	3.591990	2.330962	0.000593
C	3.425818	2.484631	1.513564
H	3.053053	1.518260	1.915273
C	1.194933	-2.687253	1.566935

C	0.561364	-2.434232	2.812558
C	0.915829	-1.239972	3.700028
H	1.638352	-0.604239	3.145345
C	-0.418616	-3.357457	3.232210
H	-0.932924	-3.198909	4.192932
C	-0.745823	-4.474758	2.451250
C	-0.096122	-4.697676	1.229367
H	-0.360458	-5.581714	0.628885
C	0.893394	-3.812298	0.753852
C	1.612104	-4.105051	-0.563932
H	2.235507	-3.220569	-0.815495
Au	0.296779	-0.106034	-0.510524
C	4.787766	2.770696	2.187171
H	5.212463	3.735351	1.838542
H	4.673330	2.832040	3.289330
H	5.534172	1.980430	1.965389
C	2.386428	3.561124	1.886273
H	2.244198	3.593259	2.986162
H	2.708280	4.575491	1.571297
H	1.399249	3.360310	1.422110
C	-0.317593	-0.363909	4.003795
H	-1.075587	-0.912213	4.601036
H	-0.021853	0.531022	4.589660
H	-0.810380	-0.019735	3.070878
C	1.612086	-1.698410	5.000912
H	0.938719	-2.327334	5.620106
H	2.524004	-2.294463	4.791364
H	1.909993	-0.822689	5.614240
C	2.566356	-5.311645	-0.413532
H	3.311230	-5.152402	0.393369
H	2.006295	-6.239085	-0.171202
H	3.119781	-5.491535	-1.358605
C	0.625079	-4.310656	-1.731865
H	0.010438	-5.224662	-1.594209
H	-0.069121	-3.452534	-1.840462

H	1.179865	-4.433191	-2.685193
C	5.079878	-0.770787	-3.403869
H	5.904865	-0.735700	-2.663196
H	5.062878	-1.787202	-3.848793
H	5.329352	-0.057268	-4.216740
C	2.568871	-0.528597	-3.783473
H	1.584915	-0.353541	-3.297700
H	2.687863	0.220016	-4.594588
H	2.540241	-1.532284	-4.255617
H	-1.513535	-5.182592	2.801063
H	4.279013	4.239651	-2.783322

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IIImetal-iPrEt180 SCF Done: -2345.59362793 A.U.

N	2.317177	-0.273042	-1.472898
C	3.369546	0.600021	-1.216596
N	2.817173	1.934600	-1.294732
C	1.525856	1.922735	-1.754072
N	1.137046	0.472296	-1.816084
C	3.586659	3.122397	-1.032164
C	3.458777	4.244897	-1.873548
C	4.464530	3.139428	0.069644
H	2.769355	4.223807	-2.728619
H	4.566385	2.253853	0.711606
C	4.214404	5.395716	-1.598119
C	5.221162	4.294213	0.323003
H	4.114327	6.275681	-2.252148
H	5.913435	4.308141	1.178962
C	5.097457	5.423566	-0.504900
H	5.692627	6.326647	-0.299224
O	0.764278	2.807010	-2.072834
O	4.520268	0.317886	-0.970516
C	4.486288	-3.949580	1.278523
C	4.942232	-4.044767	-0.052457
C	3.399984	-3.083230	1.533952

H	5.788693	-4.710343	-0.288983
H	3.019220	-2.982604	2.563888
C	4.344579	-3.307488	-1.088403
C	2.796190	-2.350044	0.502380
H	4.744645	-3.414588	-2.106995
H	1.954897	-1.677103	0.739035
C	3.260300	-2.447816	-0.826968
C	2.527800	-1.688793	-1.951474
H	0.855107	0.275380	-2.795998
C	3.310078	-1.639272	-3.281073
H	2.764930	-1.022894	-4.027330
H	3.413490	-2.652516	-3.715812
H	4.321415	-1.212344	-3.138023
N	-3.249855	-0.934277	0.443288
N	-2.691939	0.882586	1.514298
C	-2.270807	0.017759	0.540913
C	-4.274785	-0.665788	1.346068
H	-5.158364	-1.306735	1.423087
C	-3.922682	0.476916	2.020438
H	-4.433484	1.035631	2.810693
C	-3.237600	-2.063791	-0.469987
C	-3.718000	-1.870562	-1.792572
C	-4.257614	-0.531423	-2.298106
H	-4.234592	0.187859	-1.452427
C	-3.695928	-2.988896	-2.652366
H	-4.060065	-2.881227	-3.686134
C	-3.232989	-4.236362	-2.211230
C	-2.782490	-4.396969	-0.893085
H	-2.433992	-5.385885	-0.557135
C	-2.772733	-3.316626	0.013601
C	-2.319622	-3.532415	1.458959
H	-2.228342	-2.534935	1.939306
C	-1.973457	2.065139	1.959772
C	-1.072973	1.935849	3.050207
C	-0.823966	0.611158	3.773136

H	-1.399600	-0.179457	3.246531
C	-0.407651	3.104895	3.474005
H	0.298183	3.048191	4.317410
C	-0.632969	4.337369	2.845159
C	-1.533892	4.430534	1.775274
H	-1.703566	5.405804	1.293624
C	-2.230454	3.298558	1.303702
C	-3.236241	3.440010	0.160359
H	-3.546158	2.418756	-0.148131
Au	-0.624403	0.190426	-0.569682
C	-3.379339	-4.332283	2.251220
H	-3.509907	-5.351154	1.830066
H	-3.072595	-4.443339	3.311983
H	-4.371825	-3.836866	2.233679
C	-0.935564	-4.206526	1.550831
H	-0.615647	-4.281873	2.610588
H	-0.948255	-5.238200	1.141889
H	-0.159624	-3.635012	1.001794
C	0.662608	0.200639	3.717957
H	1.309486	0.924228	4.256458
H	0.809041	-0.790857	4.194558
H	1.026770	0.137810	2.671497
C	-1.339701	0.661291	5.228502
H	-0.791124	1.417995	5.827513
H	-2.417811	0.918986	5.273808
H	-1.202175	-0.321524	5.725447
C	-4.506608	4.182100	0.634651
H	-4.986671	3.673384	1.496089
H	-4.270890	5.220050	0.950430
H	-5.252359	4.242166	-0.185163
C	-2.618413	4.119845	-1.079171
H	-2.351008	5.178042	-0.876859
H	-1.699925	3.599788	-1.419325
H	-3.347186	4.124063	-1.916144
C	-5.727892	-0.647890	-2.755934

H	-6.377561	-1.046097	-1.949837
H	-6.120831	0.346800	-3.051733
H	-5.833176	-1.319356	-3.633504
C	-3.364420	0.052941	-3.413252
H	-2.322224	0.195551	-3.054232
H	-3.332834	-0.610653	-4.302766
H	-3.747020	1.040439	-3.744294
H	-0.103024	5.236948	3.195439
H	-3.232642	-5.096214	-2.899451
C	1.154843	-2.359233	-2.182784
H	0.520245	-2.336554	-1.274062
H	0.589973	-1.908533	-3.027352
H	1.331875	-3.420914	-2.441002
C	5.169557	-4.706658	2.400546
H	4.420639	-4.959698	3.182141
H	5.551244	-5.674565	2.009926
C	6.331460	-3.920540	3.040593
H	5.979014	-2.960599	3.472192
H	7.115020	-3.680684	2.292309
H	6.805630	-4.506758	3.854485

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N	-2.247035	1.593920	-0.883054
C	-3.539512	1.145545	-0.621160
N	-3.562631	-0.255587	-0.974816
C	-2.407513	-0.638329	-1.606339
N	-1.485734	0.544650	-1.505509
C	-4.715762	-1.096699	-0.786361
C	-5.100788	-2.000831	-1.795564
C	-5.446775	-0.996301	0.413792
H	-4.522987	-2.074574	-2.727014
H	-5.145619	-0.278417	1.188868
C	-6.225523	-2.815830	-1.590629
C	-6.575600	-1.810237	0.596625

H	-6.527252	-3.525674	-2.376234
H	-7.153290	-1.729038	1.530301
C	-6.966192	-2.721754	-0.399753
H	-7.851596	-3.358445	-0.248917
O	-2.080440	-1.663340	-2.158897
O	-4.466435	1.785703	-0.179694
C	-2.688794	5.263903	2.561618
C	-3.146240	5.768976	1.334509
C	-2.011738	4.031791	2.591909
H	-3.684090	6.729189	1.297685
H	-1.655538	3.620731	3.549594
C	-2.931787	5.050613	0.144493
C	-1.793322	3.318349	1.403176
H	-3.312098	5.467694	-0.798946
H	-1.273351	2.346903	1.440843
C	-2.251674	3.816994	0.164139
H	-2.863879	5.824742	3.492867
C	-1.928148	3.046714	-1.133393
H	-1.228254	0.810444	-2.476043
C	-2.740773	3.518637	-2.357704
H	-2.516328	2.881296	-3.239651
H	-2.470370	4.555695	-2.636463
H	-3.829227	3.479235	-2.159009
N	3.262018	-0.243858	0.280161
N	2.133132	-1.933056	1.074528
C	2.003955	-0.779601	0.349847
C	4.169626	-1.056618	0.953478
H	5.233769	-0.808209	1.011419
C	3.458567	-2.118727	1.454202
H	3.773245	-2.985135	2.044069
C	3.616520	0.990324	-0.398836
C	3.898395	0.940823	-1.789964
C	3.852365	-0.352135	-2.606102
H	3.605340	-1.184943	-1.914372
C	4.246951	2.155591	-2.417101

H	4.474054	2.160036	-3.494733
C	4.322944	3.352750	-1.691765
C	4.054706	3.363228	-0.315423
H	4.130918	4.308759	0.243515
C	3.695442	2.183506	0.369051
C	3.457055	2.215273	1.880044
H	3.018879	1.238230	2.175836
C	1.051555	-2.846705	1.403780
C	0.341920	-2.641326	2.616502
C	0.653064	-1.495783	3.581015
H	1.514035	-0.926658	3.170409
C	-0.690462	-3.553819	2.917373
H	-1.265903	-3.429707	3.848113
C	-0.992706	-4.618142	2.056510
C	-0.265989	-4.796630	0.871167
H	-0.511996	-5.639477	0.207041
C	0.776580	-3.917456	0.511935
C	1.574631	-4.158985	-0.770019
H	2.229723	-3.276782	-0.933757
Au	0.338415	-0.101241	-0.510117
C	4.793491	2.372834	2.641382
H	5.280204	3.341060	2.400200
H	4.624429	2.344783	3.737861
H	5.513181	1.567808	2.386993
C	2.451179	3.307049	2.297859
H	2.253811	3.249368	3.388187
H	2.836256	4.327331	2.091758
H	1.481464	3.199330	1.770377
C	-0.532611	-0.512503	3.684248
H	-1.434827	-1.003517	4.105204
H	-0.276460	0.339375	4.347944
H	-0.804832	-0.104925	2.687952
C	1.074639	-2.018951	4.971296
H	0.249755	-2.570642	5.468592
H	1.943185	-2.705833	4.904933

H	1.355906	-1.175191	5.635058
C	2.493549	-5.393024	-0.621948
H	3.187582	-5.292217	0.237980
H	1.900664	-6.318323	-0.464185
H	3.103511	-5.537561	-1.537848
C	0.663121	-4.282485	-2.008752
H	0.026783	-5.190810	-1.961667
H	-0.008699	-3.406482	-2.113819
H	1.277406	-4.364236	-2.929415
C	5.224904	-0.675395	-3.235793
H	6.024158	-0.732734	-2.468763
H	5.188111	-1.650203	-3.764667
H	5.527412	0.092541	-3.977988
C	2.738695	-0.306235	-3.673952
H	1.745842	-0.134293	-3.205210
H	2.913095	0.503202	-4.413479
H	2.690057	-1.264821	-4.230613
H	-1.801697	-5.319437	2.314361
H	4.604435	4.286964	-2.202647
C	-0.417370	3.196171	-1.422856
H	0.207054	2.779391	-0.607327
H	-0.113219	2.727222	-2.383397
H	-0.188232	4.276219	-1.502219

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N	3.625861	-0.699739	0.337836
N	3.410056	1.387201	-0.245710
C	2.694476	0.242057	-0.013012
C	4.905407	-0.149840	0.326835
H	5.790623	-0.740193	0.582778
C	4.768847	1.165113	-0.041921
H	5.510411	1.958794	-0.175542
C	3.331170	-2.078705	0.679368
C	3.007910	-2.388308	2.027376

C	2.973258	-1.338261	3.138616
H	3.210550	-0.353642	2.683664
C	2.735155	-3.740057	2.327169
H	2.484640	-4.021168	3.362131
C	2.793273	-4.731428	1.337247
C	3.128840	-4.393379	0.018041
H	3.184627	-5.184179	-0.746642
C	3.408414	-3.059380	-0.345572
C	3.794913	-2.725488	-1.787718
H	3.946936	-1.627754	-1.854130
C	2.835400	2.662854	-0.636108
C	2.704219	2.949580	-2.020819
C	3.123651	1.966967	-3.115640
H	3.628148	1.106805	-2.626642
C	2.144028	4.195960	-2.368980
H	2.023881	4.455885	-3.432380
C	1.741847	5.111442	-1.386002
C	1.895031	4.801154	-0.027761
H	1.580271	5.531836	0.733633
C	2.448062	3.570705	0.384636
C	2.608234	3.268842	1.875314
H	3.069139	2.263031	1.972457
Au	0.706868	0.056847	-0.092461
C	5.127907	-3.398564	-2.182669
H	5.045513	-4.505601	-2.169684
H	5.426558	-3.098785	-3.208609
H	5.949652	-3.117787	-1.492371
C	2.668558	-3.084514	-2.779854
H	2.952364	-2.792014	-3.812102
H	2.462369	-4.175424	-2.790443
H	1.725111	-2.559937	-2.522210
C	1.890077	1.406747	-3.857327
H	1.327838	2.212247	-4.374906
H	2.196226	0.663998	-4.623394
H	1.195924	0.906845	-3.148372

C	4.137758	2.590738	-4.097692
H	3.693988	3.432132	-4.669649
H	5.032306	2.979951	-3.569733
H	4.478247	1.834842	-4.835461
C	3.561806	4.275110	2.556184
H	4.555617	4.299086	2.063399
H	3.152105	5.306589	2.532634
H	3.714663	4.004054	3.621419
C	1.241105	3.212141	2.590302
H	0.716040	4.189322	2.546388
H	0.575762	2.447913	2.137551
H	1.374098	2.954826	3.661535
C	4.053863	-1.620667	4.206160
H	5.068372	-1.678971	3.760722
H	4.061729	-0.815995	4.970260
H	3.865273	-2.578392	4.735146
C	1.570675	-1.217968	3.771156
H	0.800435	-0.947914	3.019058
H	1.259934	-2.165953	4.259012
H	1.567094	-0.430175	4.552552
H	1.308873	6.079759	-1.682296
H	2.586963	-5.781327	1.599115
N	-1.376880	-0.029853	-0.141822
C	-2.133107	0.279435	0.984244
N	-3.353282	0.839507	0.531505
C	-3.357099	0.897343	-0.887630
N	-2.120357	0.365349	-1.230893
C	-4.418670	1.311612	1.366363
C	-5.239058	2.371323	0.921723
C	-4.643638	0.725937	2.631192
H	-5.066176	2.823845	-0.063131
H	-3.983016	-0.073143	2.990224
C	-6.284894	2.827679	1.740120
C	-5.687973	1.202369	3.440242
H	-6.921277	3.653770	1.385869

H	-5.851426	0.746897	4.429608
C	-6.515541	2.249155	2.999911
H	-7.333618	2.616634	3.638572
O	-4.219900	1.299870	-1.653268
O	-1.789101	0.060622	2.150711
C	-5.771700	-1.714160	-1.990168
C	-4.565003	-1.981981	-2.680343
C	-5.765268	-1.832366	-0.572347
H	-4.547322	-1.905205	-3.779053
H	-6.692358	-1.637560	-0.010470
C	-3.401882	-2.335623	-1.997010
C	-4.615232	-2.192235	0.118170
H	-2.493536	-2.547379	-2.578557
H	-4.661946	-2.270462	1.213382
C	-3.381024	-2.460366	-0.567362
C	-2.186283	-2.808963	0.145654
H	-1.746866	0.330848	-2.179417
C	-2.157228	-2.940438	1.626863
H	-1.910214	-1.934816	2.075240
H	-1.356513	-3.631379	1.955451
H	-3.120362	-3.253918	2.071628
C	-7.024492	-1.307306	-2.724194
H	-6.909862	-1.540445	-3.803396
H	-7.871345	-1.926522	-2.352330
C	-7.374693	0.187525	-2.547531
H	-6.544939	0.833317	-2.894881
H	-7.562602	0.436782	-1.483370
H	-8.289647	0.433593	-3.123297
C	-0.930630	-3.223888	-0.555934
H	-0.897489	-4.339029	-0.576692
H	-0.836997	-2.867251	-1.596406
H	-0.035947	-2.900855	0.014838

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N	3.339379	-0.631886	0.561260
N	3.115125	1.466348	0.022104
C	2.416880	0.294674	0.151520
C	4.596352	-0.046067	0.689250
H	5.471108	-0.619426	1.011245
C	4.454668	1.275890	0.348452
H	5.180545	2.094051	0.310126
C	3.057859	-2.030485	0.826438
C	2.610997	-2.397782	2.123677
C	2.431450	-1.390414	3.260243
H	2.689148	-0.384533	2.867122
C	2.352569	-3.766755	2.349061
H	2.008406	-4.092304	3.343285
C	2.541708	-4.719536	1.337882
C	2.998401	-4.324643	0.071865
H	3.157412	-5.085543	-0.708450
C	3.270186	-2.970976	-0.217192
C	3.796454	-2.575232	-1.598241
H	3.893295	-1.469444	-1.621836
C	2.541756	2.736939	-0.386975
C	2.535685	3.061392	-1.769671
C	3.084921	2.122188	-2.845043
H	3.582571	1.271477	-2.332967
C	1.973218	4.301420	-2.136258
H	1.948060	4.590076	-3.198696
C	1.449383	5.174699	-1.172294
C	1.480702	4.828152	0.185449
H	1.071370	5.526307	0.932235
C	2.030106	3.602213	0.615877
C	2.052992	3.258211	2.105784
H	2.555836	2.274656	2.221386
Au	0.452371	0.055932	-0.125763
C	5.201443	-3.165595	-1.851612
H	5.179363	-4.275421	-1.869078
H	5.596949	-2.824060	-2.830666

H	5.923223	-2.859650	-1.066748
C	2.813783	-2.965165	-2.722307
H	3.195312	-2.623808	-3.706901
H	2.675648	-4.064923	-2.785790
H	1.817319	-2.503682	-2.562578
C	1.939398	1.531025	-3.696116
H	1.388389	2.325904	-4.241477
H	2.336260	0.818302	-4.448980
H	1.211703	0.988502	-3.055148
C	4.149416	2.806214	-3.728428
H	3.720007	3.640272	-4.321631
H	4.980486	3.220037	-3.121420
H	4.580511	2.079520	-4.447867
C	2.874146	4.286887	2.913472
H	3.909692	4.381935	2.526697
H	2.411544	5.295492	2.882459
H	2.933453	3.983541	3.979281
C	0.623623	3.106518	2.669504
H	0.052976	4.055957	2.595557
H	0.053210	2.324095	2.126679
H	0.656792	2.820932	3.741310
C	3.400593	-1.686670	4.426405
H	4.457479	-1.706516	4.089380
H	3.307172	-0.909616	5.213072
H	3.182176	-2.666324	4.900879
C	0.967149	-1.326497	3.743499
H	0.273392	-1.046881	2.923409
H	0.632553	-2.299320	4.161692
H	0.859408	-0.569058	4.547161
H	1.016858	6.138763	-1.482742
H	2.343669	-5.783664	1.542391
N	-1.614914	-0.089235	-0.389134
C	-2.491038	0.143254	0.671285
N	-3.672724	0.699268	0.128448
C	-3.537172	0.831118	-1.280627

N	-2.250245	0.358761	-1.520956
C	-4.835540	1.092965	0.871266
C	-5.659727	2.129669	0.381626
C	-5.153474	0.450970	2.088106
H	-5.417652	2.623463	-0.568055
H	-4.493779	-0.330606	2.485122
C	-6.800808	2.507439	1.107228
C	-6.293620	0.849530	2.804639
H	-7.440131	3.314936	0.717375
H	-6.530297	0.350336	3.757396
C	-7.124246	1.873400	2.318827
H	-8.017776	2.179240	2.884677
O	-4.331042	1.242948	-2.110556
O	-2.255174	-0.134669	1.851353
C	-5.631362	-1.683877	-2.796311
C	-4.374310	-1.923585	-3.381624
C	-5.812151	-1.876324	-1.409200
H	-4.236948	-1.787229	-4.465076
H	-6.796596	-1.695829	-0.952159
C	-3.294545	-2.317342	-2.586310
C	-4.743113	-2.280927	-0.612734
H	-2.323888	-2.505139	-3.066686
H	-4.907990	-2.412640	0.465785
C	-3.441090	-2.509133	-1.171952
H	-6.475799	-1.353662	-3.420513
C	-2.323558	-2.870770	-0.339822
H	-1.793327	0.359309	-2.433195
C	-2.467521	-3.094745	1.122594
H	-2.313150	-2.113976	1.659667
H	-1.686966	-3.781322	1.504448
H	-3.465372	-3.463990	1.425927
C	-0.986078	-3.222278	-0.911739
H	-0.927296	-4.333327	-0.998768
H	-0.777653	-2.797139	-1.908920
H	-0.171546	-2.925513	-0.219521

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TSImetal-EtXpre SCF Done: -2227.71835672 A.U.

N	-1.781792	0.548413	-1.753878
C	-2.756611	-0.293223	-1.526122
N	-2.407431	-1.649204	-1.658035
C	-1.078725	-1.712222	-2.069770
N	-0.641894	-0.292285	-2.017122
C	-3.269341	-2.789709	-1.489822
C	-3.276712	-3.801315	-2.469122
C	-4.078985	-2.886896	-0.341585
H	-2.635096	-3.718323	-3.357628
H	-4.061418	-2.092235	0.417770
C	-4.105228	-4.920684	-2.290108
C	-4.913095	-4.004886	-0.184811
H	-4.111440	-5.715377	-3.051940
H	-5.553396	-4.081144	0.707546
C	-4.926380	-5.023528	-1.153908
H	-5.578818	-5.900560	-1.022883
O	-0.389643	-2.649730	-2.395561
O	-3.994566	0.006211	-1.209521
C	-9.061982	2.320924	0.883271
C	-8.765141	2.230747	-0.491260
C	-8.038819	2.614782	1.800763
H	-9.565864	2.005893	-1.213130
H	-8.265038	2.691779	2.875748
C	-7.456279	2.432533	-0.946235
C	-6.726733	2.814525	1.345224
H	-7.245230	2.366559	-2.025088
H	-5.926164	3.049421	2.066153
C	-6.410466	2.726763	-0.033745
H	-10.093649	2.165521	1.235934
C	-5.018886	2.955022	-0.455458
H	-0.208094	-0.020404	-2.917627
H	-4.324927	3.202552	0.369822
C	-4.502145	2.897738	-1.713508

H	-3.443089	3.137083	-1.897673
H	-5.128007	2.699400	-2.599943
H	-4.138679	1.009627	-1.225411
N	3.659231	0.858116	0.421225
N	2.550842	-0.184075	1.983551
C	2.468440	0.238619	0.685250
C	4.480643	0.824450	1.544385
H	5.481228	1.267823	1.540921
C	3.782981	0.168015	2.528011
H	4.049020	-0.079139	3.560401
C	4.021649	1.460273	-0.850394
C	4.680156	0.653497	-1.816052
C	5.013756	-0.821019	-1.584068
H	4.700077	-1.084249	-0.551660
C	5.023436	1.268698	-3.038072
H	5.534883	0.677431	-3.813689
C	4.729862	2.617873	-3.280983
C	4.084745	3.387536	-2.302668
H	3.864914	4.447438	-2.505298
C	3.715136	2.830948	-1.060554
C	3.011212	3.697177	-0.014937
H	2.851441	3.075566	0.891510
C	1.509059	-0.898750	2.700493
C	0.553456	-0.143362	3.430532
C	0.561611	1.385357	3.479377
H	1.442894	1.740896	2.904839
C	-0.437038	-0.864909	4.128622
H	-1.195761	-0.316135	4.708413
C	-0.468408	-2.266391	4.103207
C	0.493776	-2.981388	3.376505
H	0.460082	-4.081995	3.369485
C	1.509425	-2.318287	2.656406
C	2.557633	-3.128906	1.892968
H	3.208031	-2.414787	1.344839
Au	0.958468	-0.016499	-0.587097

C	3.879502	4.902358	0.406660
H	4.053114	5.598953	-0.439989
H	3.377945	5.478954	1.211366
H	4.872027	4.581247	0.784115
C	1.618813	4.148304	-0.507483
H	1.101384	4.739199	0.276767
H	1.694472	4.788520	-1.411324
H	0.977295	3.278300	-0.761466
C	-0.691704	1.973001	2.794991
H	-1.620685	1.671629	3.323376
H	-0.651356	3.082211	2.795950
H	-0.773417	1.632580	1.741375
C	0.716727	1.910936	4.922771
H	-0.150321	1.630907	5.556923
H	1.629525	1.510224	5.409413
H	0.785612	3.018550	4.927007
C	3.462370	-3.921777	2.862688
H	3.960527	-3.257268	3.598482
H	2.881576	-4.675903	3.434144
H	4.252194	-4.463734	2.302273
C	1.913188	-4.054772	0.839704
H	1.271651	-4.828829	1.310413
H	1.286925	-3.487427	0.120957
H	2.697750	-4.585787	0.261998
C	6.532244	-1.084491	-1.679457
H	7.105005	-0.448595	-0.973498
H	6.756489	-2.145319	-1.443353
H	6.919906	-0.884356	-2.700167
C	4.220143	-1.732179	-2.545574
H	3.125470	-1.583366	-2.434312
H	4.484322	-1.534368	-3.605590
H	4.440040	-2.800420	-2.340876
H	-1.248461	-2.808129	4.660973
H	5.011398	3.076141	-4.242060

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IImetal-iPrEt180 SCF Done: -2345.57544243 A.U.

N	2.011720	-0.081541	0.230743
C	2.625355	1.061721	0.062994
N	2.255979	1.760653	-1.102570
C	1.350344	0.973720	-1.807769
N	1.103017	-0.164011	-0.884173
C	2.771795	3.024303	-1.557458
C	3.192073	3.159800	-2.894445
C	2.832073	4.113040	-0.665993
H	3.133312	2.305413	-3.583316
H	2.495822	3.995653	0.373998
C	3.675565	4.401320	-3.337633
C	3.332199	5.343487	-1.120110
H	4.001557	4.511990	-4.383339
H	3.387146	6.195233	-0.424604
C	3.751319	5.491903	-2.454056
H	4.137286	6.461002	-2.806109
O	0.844515	1.120964	-2.895524
O	3.526736	1.592792	0.851900
C	7.309652	-2.791787	-0.241119
C	6.152365	-3.165620	0.480809
C	7.856232	-1.516515	0.018313
H	5.717667	-4.166817	0.323244
H	8.765129	-1.197543	-0.518163
C	5.565408	-2.303460	1.414343
C	7.275954	-0.651285	0.956955
H	4.690224	-2.650180	1.985076
H	7.742251	0.330627	1.127095
C	6.107295	-1.017591	1.670460
C	5.491814	-0.097578	2.666570
H	1.239728	-1.061938	-1.381889
C	4.183803	-0.211391	3.053201
H	3.779648	0.429264	3.854273
H	3.522022	-1.001643	2.664549

H	3.791276	0.943104	1.595802
N	-3.722850	-1.389608	0.113391
N	-3.627783	0.646071	0.889062
C	-2.879268	-0.326199	0.284549
C	-4.988766	-1.086388	0.606473
H	-5.811975	-1.806326	0.564505
C	-4.928943	0.195326	1.094926
H	-5.689164	0.824840	1.567634
C	-3.356302	-2.654958	-0.499207
C	-3.520675	-2.798458	-1.902585
C	-4.051738	-1.679358	-2.799739
H	-4.313395	-0.816471	-2.151345
C	-3.161889	-4.040912	-2.465854
H	-3.273773	-4.192650	-3.550814
C	-2.670686	-5.085549	-1.670400
C	-2.527004	-4.912081	-0.286590
H	-2.144611	-5.743071	0.326623
C	-2.867485	-3.693652	0.336911
C	-2.695731	-3.535557	1.848512
H	-3.061595	-2.525464	2.130011
C	-3.146192	1.964785	1.261725
C	-2.592456	2.139953	2.557584
C	-2.463898	1.000324	3.569545
H	-2.906085	0.088621	3.115083
C	-2.147956	3.435180	2.895329
H	-1.713949	3.613248	3.891749
C	-2.255502	4.499711	1.989236
C	-2.812276	4.292979	0.719380
H	-2.895084	5.139145	0.019505
C	-3.274608	3.021237	0.321163
C	-3.892895	2.834113	-1.065138
H	-4.151826	1.760442	-1.181452
Au	-0.967460	-0.229057	-0.262269
C	-3.544030	-4.561382	2.630810
H	-3.212216	-5.602469	2.435219

H	-3.454703	-4.385868	3.722946
H	-4.618173	-4.496703	2.361111
C	-1.206939	-3.607363	2.252453
H	-1.091770	-3.448407	3.344849
H	-0.767177	-4.597870	2.011353
H	-0.607720	-2.833351	1.728277
C	-0.982969	0.683126	3.870465
H	-0.470712	1.547089	4.343828
H	-0.903404	-0.175214	4.569585
H	-0.428222	0.424484	2.944217
C	-3.253942	1.293663	4.863283
H	-2.845926	2.174227	5.402216
H	-4.324248	1.496689	4.653730
H	-3.199523	0.427996	5.555543
C	-5.203925	3.638850	-1.207035
H	-5.940710	3.367598	-0.423066
H	-5.021386	4.731193	-1.129756
H	-5.671177	3.448917	-2.195550
C	-2.892608	3.182961	-2.187802
H	-2.600327	4.253507	-2.158574
H	-1.966247	2.576821	-2.114582
H	-3.345959	2.991999	-3.182463
C	-5.341231	-2.101981	-3.536523
H	-6.130173	-2.430592	-2.829113
H	-5.744074	-1.254114	-4.128347
H	-5.155199	-2.938181	-4.242507
C	-2.968998	-1.192900	-3.787476
H	-2.064069	-0.833125	-3.254171
H	-2.656078	-2.002329	-4.479926
H	-3.353883	-0.355677	-4.405836
H	-1.906739	5.503672	2.278266
H	-2.401225	-6.047734	-2.133627
C	6.355288	1.001955	3.244331
H	7.285525	0.583332	3.682554
H	6.671526	1.725691	2.462781

H	5.819748	1.567107	4.031181
C	7.922355	-3.715139	-1.274635
H	9.019486	-3.544009	-1.315634
H	7.782124	-4.769847	-0.953406
C	7.323768	-3.526780	-2.683487
H	7.477673	-2.490766	-3.050868
H	6.231318	-3.724359	-2.686539
H	7.796305	-4.219076	-3.410357

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IImetal-iPrX SCF Done: -2267.00495517 A.U.

N	2.263402	-0.542181	-0.010643
C	3.037943	0.509635	-0.078130
N	2.724445	1.404905	-1.117917
C	1.672619	0.862121	-1.850544
N	1.298729	-0.340830	-1.061455
C	3.407774	2.627609	-1.446929
C	3.784022	2.872844	-2.781351
C	3.674428	3.569757	-0.434597
H	3.563876	2.133534	-3.564307
H	3.370046	3.368666	0.602460
C	4.433040	4.076696	-3.099259
C	4.337642	4.761765	-0.765719
H	4.725531	4.273712	-4.142155
H	4.553936	5.498136	0.023693
C	4.715104	5.019427	-2.095480
H	5.229877	5.958661	-2.350242
O	1.141731	1.227660	-2.872671
O	4.050572	0.790523	0.706254
C	6.565451	-4.058388	-1.315772
C	5.476318	-4.324174	-0.465049
C	7.398220	-2.958306	-1.050274
H	4.832933	-5.199043	-0.649712
H	8.258503	-2.745606	-1.704191
C	5.218519	-3.492625	0.633541

C	7.144120	-2.129406	0.054160
H	4.384772	-3.736938	1.309404
H	7.811131	-1.274504	0.240443
C	6.041240	-2.370718	0.911711
H	6.772244	-4.716189	-2.174563
C	5.768781	-1.483573	2.079546
H	1.271533	-1.174285	-1.675863
C	4.522369	-1.377316	2.631934
H	4.362491	-0.776305	3.542310
H	3.661552	-1.951282	2.253436
H	4.244523	0.014892	1.339069
N	-3.601949	-0.981713	0.097333
N	-3.167802	0.902450	1.105609
C	-2.601901	-0.080423	0.340987
C	-4.784111	-0.567362	0.704143
H	-5.706901	-1.150876	0.628573
C	-4.510778	0.618886	1.339129
H	-5.145714	1.283780	1.932800
C	-3.456718	-2.195324	-0.688050
C	-3.702768	-2.128596	-2.085214
C	-4.102819	-0.837834	-2.801575
H	-4.199548	-0.038407	-2.036641
C	-3.558198	-3.324577	-2.818959
H	-3.739325	-3.315258	-3.905146
C	-3.193269	-4.523674	-2.190980
C	-2.964566	-4.555595	-0.808110
H	-2.683835	-5.505820	-0.327340
C	-3.091592	-3.393573	-0.018874
C	-2.834383	-3.462367	1.487269
H	-3.017453	-2.452604	1.911719
C	-2.477577	2.079779	1.602999
C	-1.840378	2.003824	2.869804
C	-1.834999	0.735884	3.725115
H	-2.418754	-0.041090	3.187708
C	-1.192159	3.167856	3.332482

H	-0.687627	3.150800	4.311313
C	-1.185510	4.346418	2.573122
C	-1.829110	4.388463	1.328394
H	-1.820102	5.322312	0.744883
C	-2.493496	3.257565	0.809405
C	-3.202084	3.342716	-0.543297
H	-3.605225	2.335644	-0.781426
Au	-0.724933	-0.187932	-0.314043
C	-3.807905	-4.434722	2.188008
H	-3.661110	-5.479966	1.844295
H	-3.646226	-4.421622	3.285856
H	-4.866700	-4.165371	1.995357
C	-1.362873	-3.820401	1.788844
H	-1.179898	-3.824144	2.883541
H	-1.101763	-4.828509	1.403967
H	-0.666044	-3.089746	1.327020
C	-0.403722	0.184639	3.902653
H	0.242690	0.901335	4.451622
H	-0.420702	-0.760743	4.483853
H	0.074490	-0.022905	2.922500
C	-2.526015	0.964699	5.086937
H	-1.978212	1.706701	5.704764
H	-3.564492	1.334793	4.963284
H	-2.567160	0.018327	5.665109
C	-4.401861	4.314421	-0.484872
H	-5.126371	4.027817	0.305070
H	-4.072948	5.353709	-0.274514
H	-4.940682	4.325487	-1.454992
C	-2.226564	3.719686	-1.678437
H	-1.798560	4.733466	-1.532323
H	-1.382988	3.002701	-1.749675
H	-2.753479	3.722670	-2.654988
C	-5.476181	-0.973012	-3.494463
H	-6.269451	-1.274538	-2.779871
H	-5.776044	-0.006962	-3.950796

H	-5.452803	-1.728848	-4.307100
C	-3.010108	-0.386221	-3.794833
H	-2.035546	-0.232393	-3.285629
H	-2.858018	-1.134222	-4.601009
H	-3.295151	0.571083	-4.278307
H	-0.677884	5.244687	2.958532
H	-3.090798	-5.445131	-2.785450
C	6.918886	-0.677829	2.641200
H	7.778232	-1.336450	2.886946
H	7.291922	0.068082	1.906948
H	6.621735	-0.130552	3.556326

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I-iPrEt180 SCF Done: -2345.56125262 A.U.

N	-4.061927	0.479374	-0.219458
N	-3.527940	-1.576361	0.269975
C	-2.991970	-0.350181	-0.017494
C	-5.253718	-0.219561	-0.060642
H	-6.227556	0.264359	-0.183979
C	-4.917673	-1.514655	0.249561
H	-5.537490	-2.392358	0.457507
C	-3.977751	1.889165	-0.563123
C	-3.981875	2.842583	0.489272
C	-4.062142	2.454713	1.966327
H	-4.020901	1.346595	2.030594
C	-3.921946	4.202749	0.120944
H	-3.923421	4.973642	0.907216
C	-3.862435	4.590120	-1.224928
C	-3.863009	3.622393	-2.239282
H	-3.819900	3.941415	-3.292442
C	-3.923832	2.246252	-1.936801
C	-3.927757	1.216400	-3.067659
H	-4.015941	0.207628	-2.611289
C	-2.767355	-2.776209	0.573007
C	-2.409101	-3.637994	-0.497105

C	-2.765956	-3.348434	-1.955717
H	-3.349739	-2.404062	-1.983121
C	-1.689188	-4.805156	-0.166517
H	-1.394238	-5.501035	-0.967458
C	-1.349352	-5.098065	1.161867
C	-1.722969	-4.227114	2.195255
H	-1.454646	-4.472840	3.234701
C	-2.444472	-3.044588	1.929845
C	-2.841163	-2.117484	3.079949
H	-3.434334	-1.280176	2.655161
Au	-1.055529	0.146900	-0.133816
C	-5.142355	1.400617	-4.003135
H	-5.107953	2.376055	-4.531839
H	-5.159957	0.605497	-4.777106
H	-6.100497	1.356347	-3.445687
C	-2.599440	1.243340	-3.854577
H	-2.596089	0.460590	-4.641317
H	-2.442319	2.221137	-4.356266
H	-1.731089	1.062432	-3.186606
C	-1.498121	-3.122697	-2.807791
H	-0.866765	-4.035021	-2.848604
H	-1.772016	-2.861069	-3.850937
H	-0.876363	-2.299125	-2.398509
C	-3.660683	-4.455313	-2.554473
H	-3.132548	-5.430795	-2.597065
H	-4.586154	-4.601967	-1.960530
H	-3.957845	-4.194663	-3.591402
C	-3.740468	-2.836107	4.108976
H	-4.647620	-3.263220	3.634251
H	-3.204164	-3.666922	4.613347
H	-4.068765	-2.127821	4.897619
C	-1.597865	-1.495808	3.752291
H	-0.954753	-2.272688	4.216557
H	-0.980153	-0.935820	3.019173
H	-1.899979	-0.790340	4.553883

C	-5.404308	2.900381	2.588303
H	-6.272948	2.477662	2.042410
H	-5.471999	2.570680	3.645885
H	-5.508961	4.005572	2.575983
C	-2.859994	2.999867	2.766378
H	-1.894567	2.676116	2.326708
H	-2.859889	4.109534	2.799301
H	-2.901178	2.641218	3.815843
H	-0.792612	-6.019270	1.395254
H	-3.818904	5.659017	-1.486693
N	0.926231	0.704770	-0.292817
C	1.468678	1.867695	0.462809
N	2.785510	1.968871	0.037675
C	3.042300	0.956190	-0.909899
N	1.805944	0.177652	-1.051818
C	3.731420	2.962825	0.474828
C	5.060308	2.581200	0.740879
C	3.312298	4.298135	0.627955
H	5.376561	1.536077	0.613379
H	2.271699	4.583220	0.418134
C	5.977241	3.558003	1.160965
C	4.239898	5.259053	1.060445
H	7.018817	3.267086	1.366595
H	3.916639	6.303919	1.185521
C	5.571470	4.893894	1.324414
H	6.295258	5.653249	1.658281
O	4.058676	0.722138	-1.520447
O	0.821695	2.523356	1.244525
C	7.757874	-1.614846	-0.660909
C	6.780630	-1.869242	-1.651139
C	7.318499	-1.499590	0.682853
H	7.088457	-1.953374	-2.706151
H	8.060387	-1.312942	1.477090
C	5.432276	-2.017449	-1.313214
C	5.967263	-1.641391	1.025027

H	4.695414	-2.207926	-2.109495
H	5.676020	-1.564407	2.083244
C	4.990683	-1.923439	0.037516
C	3.530096	-2.163886	0.365017
H	2.941766	-1.499930	-0.335674
C	3.114752	-1.796244	1.796423
H	3.393476	-0.755865	2.065238
H	3.584031	-2.470116	2.544266
H	2.016580	-1.898560	1.917224
C	9.213643	-1.426733	-1.024312
H	9.850943	-1.820649	-0.203291
H	9.447817	-2.032210	-1.925885
C	9.583160	0.048667	-1.291919
H	9.398856	0.678974	-0.397314
H	8.985764	0.467824	-2.127649
H	10.656084	0.140868	-1.557659
C	3.089070	-3.605551	0.011710
H	3.605861	-4.336385	0.669051
H	1.995091	-3.724036	0.152708
H	3.329906	-3.869404	-1.037275

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I-iPrX SCF Done: -2266.99004064 A.U.

N	-3.648297	0.777789	0.207999
N	-3.345652	-1.379162	0.095307
C	-2.681978	-0.181519	0.060633
C	-4.900114	0.188078	0.332507
H	-5.809455	0.784330	0.456953
C	-4.709520	-1.171471	0.263043
H	-5.417885	-2.003952	0.318981
C	-3.414165	2.212588	0.222460
C	-3.196167	2.848164	1.473357
C	-3.180745	2.091832	2.802401
H	-3.287899	1.008778	2.580080
C	-2.997255	4.244197	1.455729

H	-2.823961	4.775371	2.404544
C	-3.015965	4.966508	0.254667
C	-3.236258	4.307330	-0.962798
H	-3.252013	4.888285	-1.898227
C	-3.444529	2.913404	-1.012470
C	-3.687158	2.225946	-2.357137
H	-3.862687	1.146410	-2.163325
C	-2.723711	-2.688951	-0.002829
C	-2.540300	-3.257648	-1.290870
C	-2.953083	-2.550138	-2.582208
H	-3.416308	-1.579092	-2.306370
C	-1.948420	-4.536744	-1.347491
H	-1.788531	-5.013262	-2.327303
C	-1.567347	-5.214226	-0.180867
C	-1.770217	-4.626328	1.075847
H	-1.472461	-5.173134	1.984255
C	-2.355544	-3.349123	1.199577
C	-2.566471	-2.736904	2.585496
H	-3.068479	-1.755056	2.453808
Au	-0.721214	0.121602	-0.201423
C	-4.948864	2.773047	-3.059311
H	-4.837446	3.844959	-3.325212
H	-5.140968	2.217118	-4.000339
H	-5.848845	2.679909	-2.417406
C	-2.445122	2.326299	-3.269066
H	-2.615461	1.783831	-4.222130
H	-2.209623	3.381111	-3.522657
H	-1.549745	1.888225	-2.779457
C	-1.726379	-2.233895	-3.465001
H	-1.216728	-3.160461	-3.802731
H	-2.033922	-1.673599	-4.372215
H	-0.980556	-1.620645	-2.916876
C	-4.015835	-3.357875	-3.358556
H	-3.616216	-4.334138	-3.704054
H	-4.910856	-3.564207	-2.736360

H	-4.346475	-2.798791	-4.258314
C	-3.493696	-3.608927	3.459590
H	-4.473189	-3.785873	2.969700
H	-3.042759	-4.600645	3.672470
H	-3.683694	-3.115583	4.435252
C	-1.219462	-2.463805	3.288902
H	-0.657481	-3.403503	3.472431
H	-0.575203	-1.795681	2.679924
H	-1.384689	-1.977125	4.272474
C	-4.376215	2.497652	3.692673
H	-5.346627	2.333102	3.180472
H	-4.380980	1.906313	4.631837
H	-4.325951	3.570295	3.974330
C	-1.838592	2.271203	3.543557
H	-0.979834	1.974571	2.907183
H	-1.678535	3.325532	3.851550
H	-1.820256	1.652751	4.464869
H	-1.113106	-6.215037	-0.251497
H	-2.859956	6.056609	0.267888
N	1.282222	0.474000	-0.535658
C	1.966836	1.682955	0.030533
N	3.251914	1.613618	-0.481301
C	3.364200	0.473135	-1.301087
N	2.063745	-0.215634	-1.262503
C	4.303672	2.568581	-0.237953
C	5.600262	2.104802	0.053285
C	4.015129	3.944822	-0.298945
H	5.812435	1.026861	0.100460
H	2.997398	4.291973	-0.528051
C	6.620516	3.042652	0.279205
C	5.044961	4.867839	-0.057571
H	7.638200	2.687813	0.502780
H	4.825999	5.945826	-0.100100
C	6.346942	4.420550	0.227539
H	7.151676	5.149317	0.409990

O	4.310606	0.084008	-1.941464
O	1.423425	2.480961	0.753509
C	7.981737	-1.634690	-0.032978
C	7.194989	-1.996468	-1.139180
C	7.387881	-1.546582	1.243203
H	7.644666	-2.061026	-2.142161
H	8.000822	-1.272931	2.116746
C	5.830042	-2.275523	-0.968033
C	6.019589	-1.817129	1.412046
H	5.222650	-2.555088	-1.842889
H	5.583236	-1.747179	2.419445
C	5.214853	-2.199605	0.313770
H	9.055181	-1.423558	-0.159408
C	3.739930	-2.544763	0.451841
H	3.203528	-1.955354	-0.344476
C	3.111303	-2.163972	1.799675
H	3.269270	-1.094738	2.053851
H	3.530132	-2.768655	2.631847
H	2.018459	-2.353488	1.781500
C	3.469010	-4.031398	0.114653
H	3.951466	-4.690184	0.867326
H	2.379360	-4.239910	0.117322
H	3.867964	-4.311374	-0.880617

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TSI-EtEt SCF Done: -2306.27542328 A.U.

N	3.155023	-1.846611	0.329191
N	3.848056	0.060559	-0.463118
C	2.722509	-0.605813	-0.057647
C	4.534101	-1.954054	0.168490
H	5.075753	-2.870119	0.423654
C	4.969782	-0.751960	-0.331062
H	5.970357	-0.402958	-0.604349
C	2.307147	-2.907154	0.841791
C	2.084031	-2.977245	2.242611

C	2.682046	-1.974700	3.230841
H	3.345760	-1.290017	2.661979
C	1.265206	-4.025988	2.711106
H	1.069913	-4.115561	3.791262
C	0.704882	-4.960603	1.828753
C	0.953304	-4.868569	0.451820
H	0.516030	-5.615702	-0.229139
C	1.762597	-3.841809	-0.078169
C	2.017758	-3.771034	-1.584544
H	2.708325	-2.922386	-1.773524
C	3.878363	1.422744	-0.968887
C	3.731219	1.626889	-2.366562
C	3.514949	0.482892	-3.358458
H	3.536094	-0.470903	-2.789801
C	3.785536	2.957748	-2.829779
H	3.674341	3.158680	-3.906869
C	3.981374	4.027589	-1.945302
C	4.125816	3.790400	-0.571423
H	4.278423	4.640139	0.111919
C	4.078049	2.482760	-0.045385
C	4.252309	2.257071	1.456918
H	4.082821	1.178284	1.660081
Au	0.858874	0.119495	-0.031387
C	2.710165	-5.048053	-2.107615
H	2.063422	-5.942906	-1.991790
H	2.944362	-4.947064	-3.187628
H	3.659299	-5.249911	-1.569997
C	0.715525	-3.475599	-2.359858
H	0.921628	-3.381920	-3.446320
H	-0.027694	-4.290683	-2.231324
H	0.248684	-2.528485	-2.017093
C	2.127511	0.579748	-4.029250
H	2.031074	1.505691	-4.634047
H	1.962153	-0.281479	-4.709653
H	1.314296	0.583412	-3.273509

C	4.646462	0.413711	-4.406713
H	4.669022	1.321410	-5.045349
H	5.643158	0.316598	-3.929207
H	4.502001	-0.458849	-5.077190
C	5.692518	2.588725	1.907336
H	6.446773	1.994240	1.351396
H	5.929249	3.661417	1.746136
H	5.821060	2.377464	2.989392
C	3.208303	3.042742	2.278649
H	3.351958	4.139232	2.180906
H	2.172703	2.809817	1.956902
H	3.302973	2.795740	3.356639
C	3.552958	-2.670354	4.298880
H	4.357357	-3.280262	3.838899
H	4.030615	-1.916787	4.958672
H	2.952000	-3.342135	4.946936
C	1.581284	-1.105220	3.876467
H	0.996516	-0.561366	3.104797
H	0.874977	-1.720836	4.472536
H	2.028091	-0.353050	4.559202
H	4.023034	5.058162	-2.331392
H	0.075587	-5.775718	2.219797
N	-1.049149	0.921389	-0.027895
C	-1.334795	2.216801	0.524443
N	-2.663952	2.502299	0.150610
C	-3.178981	1.422521	-0.572718
N	-2.091158	0.438909	-0.676048
C	-3.372754	3.714180	0.457818
C	-4.238366	4.273425	-0.503074
C	-3.193029	4.329100	1.712672
H	-4.375808	3.785387	-1.477796
H	-2.508565	3.891884	2.452536
C	-4.931807	5.454606	-0.195194
C	-3.885202	5.516639	1.999076
H	-5.610831	5.891480	-0.943712

H	-3.741165	6.002208	2.976684
C	-4.756674	6.080398	1.051282
H	-5.299013	7.009838	1.283730
O	-4.282943	1.253533	-1.042770
O	-0.545331	2.908781	1.131709
C	-7.222070	-2.002772	-0.962853
C	-6.089467	-2.687514	-1.478532
C	-7.027531	-1.120438	0.128880
H	-6.217674	-3.375825	-2.329610
H	-7.891835	-0.574948	0.540764
C	-4.823754	-2.497902	-0.929612
C	-5.762176	-0.918611	0.681700
H	-3.958143	-3.037575	-1.347260
H	-5.650233	-0.221702	1.525435
C	-4.624954	-1.616848	0.176900
C	-3.278331	-1.442413	0.718562
H	-2.691354	-0.627228	-0.112109
H	-2.600469	-2.285591	0.462354
C	-3.020512	-0.865281	2.092205
H	-1.955358	-0.572907	2.206882
H	-3.222431	-1.627451	2.877093
H	-3.651050	0.017564	2.319324
C	-8.599125	-2.243167	-1.533450
H	-9.207811	-1.320108	-1.426249
H	-8.514828	-2.447314	-2.622365
C	-9.330748	-3.420176	-0.848847
H	-9.463351	-3.235725	0.237009
H	-8.766399	-4.368417	-0.963678
H	-10.334955	-3.563702	-1.296686

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N	3.230592	-1.930137	0.304435
N	3.967785	-0.093406	-0.605637
C	2.836726	-0.685475	-0.110540

C	4.591415	-2.113211	0.072363
H	5.102201	-3.044465	0.336047
C	5.055014	-0.955431	-0.501260
H	6.053869	-0.668304	-0.844028
C	2.363801	-2.925271	0.908431
C	2.223097	-2.931308	2.321650
C	2.927419	-1.923911	3.231772
H	3.581424	-1.289928	2.596779
C	1.384850	-3.919076	2.879778
H	1.251658	-3.958051	3.972317
C	0.727303	-4.856539	2.070636
C	0.894483	-4.828064	0.678730
H	0.380279	-5.576691	0.055618
C	1.718174	-3.863896	0.060669
C	1.885233	-3.863986	-1.459619
H	2.583072	-3.042431	-1.725629
C	4.033489	1.243989	-1.170476
C	3.814192	1.398678	-2.565059
C	3.484367	0.227627	-3.492130
H	3.520505	-0.705225	-2.890331
C	3.900825	2.705858	-3.086966
H	3.735353	2.868703	-4.163504
C	4.196191	3.799821	-2.261497
C	4.410838	3.611214	-0.889312
H	4.641365	4.479491	-0.252597
C	4.335321	2.329329	-0.306028
C	4.582020	2.157686	1.193245
H	4.403441	1.091325	1.447616
Au	1.012633	0.128819	-0.017163
C	2.515800	-5.180656	-1.962837
H	1.857125	-6.052346	-1.765725
H	2.686275	-5.135272	-3.058478
H	3.491046	-5.381798	-1.473862
C	0.547766	-3.568927	-2.172128

H	0.694060	-3.523228	-3.271270
H	-0.204506	-4.360397	-1.970001
H	0.121597	-2.598152	-1.842978
C	2.051158	0.349370	-4.054340
H	1.935903	1.258959	-4.680355
H	1.805186	-0.526897	-4.689736
H	1.301411	0.404180	-3.237123
C	4.525115	0.079908	-4.622781
H	4.523474	0.959740	-5.299627
H	5.553585	-0.031362	-4.221939
H	4.301003	-0.813277	-5.242241
C	6.048370	2.476902	1.559890
H	6.763036	1.848088	0.989619
H	6.296740	3.538304	1.349281
H	6.226415	2.301499	2.641316
C	3.593618	2.995809	2.032118
H	3.748122	4.084283	1.877722
H	2.539207	2.767294	1.774129
H	3.739842	2.794250	3.113817
C	3.835352	-2.621932	4.267006
H	4.581944	-3.281946	3.779528
H	4.385975	-1.868918	4.867965
H	3.249359	-3.244500	4.975121
C	1.910131	-0.983635	3.914024
H	1.297970	-0.442475	3.162141
H	1.220266	-1.545004	4.578894
H	2.433295	-0.228172	4.536174
H	4.261066	4.811001	-2.692993
H	0.084743	-5.623788	2.530829
N	-0.857770	1.011294	0.050659
C	-1.068434	2.330815	0.578892
N	-2.404380	2.654431	0.264936
C	-2.993689	1.574943	-0.399890
N	-1.947958	0.550100	-0.530118
C	-3.053661	3.898737	0.573700

C	-3.946834	4.464408	-0.357731
C	-2.788929	4.538540	1.800725
H	-4.150514	3.956906	-1.310683
H	-2.083731	4.095446	2.517258
C	-4.581850	5.677561	-0.048100
C	-3.423469	5.757473	2.088702
H	-5.282300	6.119660	-0.773454
H	-3.213029	6.262272	3.044280
C	-4.321662	6.328214	1.170484
H	-4.818507	7.282444	1.404181
O	-4.125933	1.433715	-0.807996
O	-0.224732	3.009686	1.124947
C	-7.161286	-1.740757	-0.506154
C	-6.071296	-2.470631	-1.054473
C	-6.888531	-0.836887	0.549393
H	-6.249801	-3.182807	-1.875424
H	-7.718645	-0.260646	0.988813
C	-4.777519	-2.303083	-0.569329
C	-5.593224	-0.655720	1.038440
H	-3.948469	-2.881789	-1.008502
H	-5.424708	0.057244	1.859082
C	-4.500967	-1.398801	0.501808
C	-3.126184	-1.250595	0.976254
H	-2.557169	-0.479313	0.096158
H	-2.486007	-2.121433	0.715363
C	-2.788468	-0.642488	2.319070
H	-1.711143	-0.379275	2.376522
H	-2.975959	-1.375310	3.134828
H	-3.382093	0.265203	2.547688
C	-8.574978	-1.918881	-1.035472
H	-9.228306	-1.241782	-0.442382
C	-9.083854	-3.362996	-0.824168
H	-9.036374	-3.661251	0.242941
H	-8.490253	-4.095964	-1.410293
H	-10.139002	-3.448277	-1.156599

C	-8.682347	-1.492628	-2.517334
H	-8.072168	-2.145986	-3.176067
H	-9.735172	-1.565061	-2.860063
H	-8.343795	-0.447273	-2.666709

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AuIPrUrN2–H–PhEt1+ISOMER SCF Done: -2227.70209192 A.U.

N	-3.318317	-0.479080	0.953809
N	-3.328732	0.698850	-0.879258
C	-2.494837	0.069512	0.006672
C	-4.649726	-0.196518	0.663651
H	-5.466618	-0.546994	1.302012
C	-4.656365	0.545428	-0.491566
H	-5.480123	0.974255	-1.070566
C	-2.877178	-1.247906	2.104434
C	-2.734723	-2.653930	1.965431
C	-3.034338	-3.397717	0.663432
H	-3.252815	-2.640004	-0.118592
C	-2.319711	-3.371571	3.106796
H	-2.197810	-4.463866	3.040067
C	-2.064734	-2.721985	4.322437
C	-2.222615	-1.332722	4.427341
H	-2.026553	-0.836363	5.390830
C	-2.635265	-0.559273	3.322700
C	-2.806216	0.953582	3.471480
H	-3.154258	1.355742	2.496677
C	-2.900277	1.414842	-2.068333
C	-2.650513	2.808785	-1.964577
C	-2.791234	3.583702	-0.653537
H	-3.160088	2.879083	0.121581
C	-2.246918	3.478496	-3.138129
H	-2.042670	4.559977	-3.099024
C	-2.104127	2.793490	-4.352933
C	-2.365807	1.418159	-4.422488
H	-2.254351	0.893729	-5.384398

C	-2.773727	0.691985	-3.284146
C	-3.052844	-0.807507	-3.396021
H	-3.394585	-1.166659	-2.402253
Au	-0.503545	-0.079262	-0.113744
C	-3.882034	1.305617	4.521580
H	-3.589539	0.966128	5.537220
H	-4.034203	2.403920	4.569850
H	-4.857935	0.836082	4.281385
C	-1.461480	1.642054	3.789109
H	-1.590255	2.743160	3.844850
H	-1.050902	1.304513	4.763890
H	-0.706224	1.420923	3.006049
C	-1.422862	4.112303	-0.170916
H	-0.992571	4.841257	-0.889385
H	-1.526807	4.627472	0.806939
H	-0.693504	3.283635	-0.052610
C	-3.828805	4.721117	-0.766983
H	-3.512925	5.493288	-1.499277
H	-4.819974	4.341124	-1.089139
H	-3.958966	5.227406	0.212032
C	-4.186487	-1.103468	-4.401722
H	-5.118992	-0.561874	-4.141013
H	-3.905819	-0.808576	-5.434455
H	-4.415137	-2.189244	-4.418823
C	-1.768625	-1.591018	-3.743931
H	-1.368013	-1.297051	-4.736718
H	-0.972433	-1.414530	-2.990511
H	-1.973654	-2.681155	-3.775548
C	-4.292613	-4.282892	0.809092
H	-5.179395	-3.693011	1.120541
H	-4.533130	-4.778288	-0.154487
H	-4.140498	-5.080927	1.565913
C	-1.821182	-4.216565	0.174580
H	-0.919436	-3.583213	0.048632
H	-1.566422	-5.033376	0.882102

H	-2.047742	-4.690701	-0.802931
H	-1.789516	3.338598	-5.256684
H	-1.745394	-3.305882	5.200014
N	1.550101	-0.274666	-0.302517
C	2.182950	-1.551409	-0.498811
N	3.524928	-1.264343	-0.821372
C	3.717314	0.118952	-0.801648
N	2.406367	0.711226	-0.482145
C	4.532132	-2.241909	-1.133311
C	5.467027	-1.972527	-2.152260
C	4.570308	-3.455710	-0.419244
H	5.432413	-1.021623	-2.701670
H	3.831407	-3.661198	0.367551
C	6.450603	-2.929374	-2.448788
C	5.553208	-4.406481	-0.737510
H	7.184231	-2.719900	-3.242536
H	5.581253	-5.358637	-0.185436
C	6.495722	-4.146761	-1.747407
H	7.266012	-4.895139	-1.989398
O	4.719088	0.772356	-0.990464
O	1.621564	-2.624726	-0.450560
C	6.707776	3.989460	1.197063
C	5.444759	4.588053	0.999859
C	6.797700	2.641513	1.595833
H	5.377275	5.642099	0.689544
H	7.784027	2.177049	1.747745
C	4.282177	3.842936	1.202421
C	5.636053	1.888414	1.794784
H	3.295173	4.309989	1.052365
H	5.722191	0.837298	2.107242
C	4.349365	2.478093	1.617538
H	7.625070	4.577598	1.037308
C	3.103756	1.736377	1.817667
H	2.717059	1.405105	0.600880

H	2.226969	2.403450	1.966401
C	3.026754	0.457252	2.615933
H	2.086941	-0.094128	2.396958
H	3.007310	0.682280	3.705559
H	3.882188	-0.223366	2.434282

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TSII-EtiPrDelEtEt180 SCF Done: -2306.29827759 A.U.

N	3.475084	-1.038867	0.334109
N	3.539018	1.070675	-0.208097
C	2.679348	0.025009	0.001344
C	4.815599	-0.662554	0.335337
H	5.613906	-1.370533	0.578500
C	4.855997	0.666029	-0.007255
H	5.696670	1.356812	-0.124727
C	2.998329	-2.375856	0.640506
C	2.654379	-2.682167	1.983980
C	2.769362	-1.671212	3.125366
H	3.046273	-0.690535	2.683890
C	2.211225	-3.995176	2.248536
H	1.936877	-4.272638	3.278172
C	2.119379	-4.952143	1.228303
C	2.471392	-4.617811	-0.087554
H	2.402590	-5.381981	-0.877784
C	2.922830	-3.322427	-0.415946
C	3.306523	-2.991407	-1.859389
H	3.652739	-1.936793	-1.887358
C	3.140967	2.416887	-0.580179
C	3.072816	2.743922	-1.960622
C	3.382773	1.737165	-3.069808
H	3.730301	0.797567	-2.590655
C	2.687992	4.059825	-2.291459
H	2.624312	4.353404	-3.351045
C	2.390933	5.001816	-1.296205
C	2.476004	4.648536	0.057694

H	2.245478	5.400155	0.828812
C	2.855991	3.348750	0.452887
C	2.938889	2.997009	1.938826
H	3.295258	1.948500	2.022047
Au	0.686479	0.077597	-0.067017
C	4.475796	-3.869802	-2.354872
H	4.195023	-4.943157	-2.391823
H	4.779296	-3.571156	-3.379718
H	5.363657	-3.779758	-1.696012
C	2.088063	-3.091655	-2.802145
H	2.369079	-2.803123	-3.836352
H	1.686234	-4.125842	-2.842760
H	1.268970	-2.420048	-2.469017
C	2.112100	1.390876	-3.876517
H	1.702773	2.284185	-4.393612
H	2.335748	0.628738	-4.651838
H	1.318006	0.984897	-3.214255
C	4.520260	2.226246	-3.991637
H	4.234137	3.143524	-4.547390
H	5.441440	2.456504	-3.418193
H	4.771159	1.449690	-4.743668
C	3.961106	3.885680	2.680056
H	4.968061	3.826626	2.218161
H	3.654295	4.952496	2.679241
H	4.051953	3.569213	3.739771
C	1.547382	3.057866	2.605475
H	1.125236	4.084236	2.575220
H	0.828551	2.379401	2.099335
H	1.611611	2.754097	3.670816
C	3.896965	-2.068241	4.104598
H	4.874758	-2.170119	3.589966
H	4.007760	-1.302504	4.900238
H	3.678973	-3.036740	4.601790
C	1.425920	-1.475687	3.859360
H	0.613196	-1.177497	3.165378

H	1.104112	-2.403097	4.378088
H	1.524094	-0.686914	4.633790
H	2.095575	6.024438	-1.578972
H	1.776375	-5.972348	1.462207
N	-1.403672	0.188148	-0.091696
C	-2.149048	0.055471	1.101796
N	-3.300769	0.854982	0.965036
C	-3.260827	1.557861	-0.270540
N	-2.079142	1.107554	-0.860276
C	-4.337844	0.996050	1.948068
C	-5.030472	2.220036	2.064917
C	-4.658110	-0.085737	2.795623
H	-4.786226	3.057419	1.398807
H	-4.099000	-1.027061	2.721903
C	-6.047771	2.348103	3.024158
C	-5.670607	0.064493	3.756580
H	-6.587461	3.304252	3.108751
H	-5.910488	-0.780037	4.421460
C	-6.372026	1.276622	3.873469
H	-7.166645	1.387123	4.627487
O	-4.044122	2.366410	-0.731389
O	-1.830897	-0.663786	2.044679
C	-5.943573	-0.611719	-2.265847
C	-4.788295	-0.307804	-3.024170
C	-5.796389	-1.427009	-1.108234
H	-4.884854	0.314042	-3.928233
H	-6.687821	-1.673791	-0.509640
C	-3.531607	-0.773796	-2.632995
C	-4.550891	-1.901650	-0.710957
H	-2.645319	-0.546274	-3.246542
H	-4.468980	-2.518225	0.197100
C	-3.374475	-1.580917	-1.461705
C	-2.065400	-1.972063	-1.051908
H	-1.638388	1.554336	-1.665732
H	-1.253260	-1.714095	-1.750814

C	-1.750857	-2.944728	0.025043
H	-1.796514	-2.451516	1.030704
H	-0.729554	-3.356143	-0.083233
H	-2.483900	-3.778194	0.051423
C	-7.308185	-0.133176	-2.699135
H	-7.916384	0.095069	-1.797782
H	-7.201632	0.817686	-3.262412
C	-8.053351	-1.169565	-3.570190
H	-8.204590	-2.124003	-3.025103
H	-7.489851	-1.396584	-4.498399
H	-9.050471	-0.782016	-3.861440

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TSII-EtiPrFllqst3 SCF Done: -2345.58131693 A.U.

N	3.654083	-0.652746	-0.513654
N	3.480317	1.152297	0.694470
C	2.739438	0.195599	0.052023
C	4.950208	-0.233105	-0.226222
H	5.827077	-0.779268	-0.587369
C	4.840913	0.904513	0.533828
H	5.602417	1.556222	0.973215
C	3.332974	-1.825109	-1.308376
C	3.137287	-3.064081	-0.642186
C	3.251012	-3.221511	0.874455
H	3.359999	-2.207249	1.313565
C	2.852989	-4.186702	-1.447900
H	2.696569	-5.165831	-0.969232
C	2.772309	-4.080008	-2.843301
C	2.973624	-2.841688	-3.469746
H	2.914015	-2.773475	-4.567493
C	3.260647	-1.682267	-2.719749
C	3.480823	-0.347243	-3.433640
H	3.703972	0.419888	-2.662547
C	2.933348	2.268803	1.444795
C	2.710078	3.495160	0.764084

C	3.002117	3.684087	-0.725517
H	3.466404	2.748842	-1.103535
C	2.186441	4.564416	1.519993
H	2.000483	5.532533	1.028892
C	1.904601	4.418939	2.885831
C	2.144205	3.196886	3.529325
H	1.923763	3.098380	4.603768
C	2.667394	2.090223	2.828245
C	2.920333	0.772926	3.562744
H	3.351883	0.053559	2.835098
Au	0.751560	0.024386	0.044645
C	4.693840	-0.403698	-4.387420
H	4.532491	-1.128693	-5.212474
H	4.873124	0.589638	-4.848767
H	5.619394	-0.704991	-3.855324
C	2.205511	0.113319	-4.171838
H	2.363078	1.106171	-4.642249
H	1.920957	-0.595092	-4.977927
H	1.347125	0.196702	-3.472456
C	1.698063	3.896870	-1.525017
H	1.172769	4.822120	-1.207191
H	1.914601	3.990687	-2.609642
H	1.001747	3.042871	-1.384922
C	4.009776	4.826546	-0.975033
H	3.601558	5.810656	-0.663519
H	4.956087	4.666198	-0.418961
H	4.256032	4.898079	-2.054773
C	3.950475	0.944734	4.700239
H	4.908747	1.361372	4.327432
H	3.575656	1.625287	5.493157
H	4.165943	-0.033208	5.178415
C	1.602419	0.157855	4.081282
H	1.112821	0.813768	4.831349
H	0.881837	-0.008069	3.253044
H	1.794593	-0.820514	4.568377

C	4.516418	-4.024444	1.252036
H	5.439054	-3.555209	0.852092
H	4.618613	-4.093101	2.355035
H	4.470237	-5.060482	0.855435
C	1.980898	-3.847464	1.488041
H	1.067324	-3.275935	1.224261
H	1.834864	-4.894377	1.148343
H	2.064200	-3.873960	2.594362
H	1.499274	5.269334	3.456352
H	2.555896	-4.973383	-3.450123
N	-1.332040	-0.163979	0.115203
C	-1.925689	-1.300122	0.719690
N	-3.171331	-0.886176	1.235131
C	-3.339255	0.511935	1.040837
N	-2.140109	0.899052	0.443632
C	-4.117389	-1.734866	1.900741
C	-4.922456	-1.211449	2.934372
C	-4.236853	-3.088461	1.520823
H	-4.832647	-0.155979	3.222673
H	-3.588409	-3.498936	0.735826
C	-5.852001	-2.046797	3.574267
C	-5.163903	-3.911880	2.179375
H	-6.480976	-1.633399	4.378071
H	-5.248271	-4.969753	1.885240
C	-5.976891	-3.396567	3.203417
H	-6.703882	-4.046818	3.714076
O	-4.275669	1.232306	1.337101
O	-1.423620	-2.416918	0.747315
C	-5.655992	1.422732	-1.909279
C	-4.435260	2.074117	-2.222880
C	-5.640010	0.010261	-1.763126
H	-4.421414	3.165747	-2.367154
H	-6.581588	-0.512068	-1.530570
C	-3.247620	1.353519	-2.335219
C	-4.462577	-0.722641	-1.886496

H	-2.309152	1.875429	-2.587917
H	-4.491366	-1.813840	-1.748644
C	-3.220198	-0.068799	-2.161086
C	-1.969134	-0.752849	-2.184353
H	-1.975707	1.831390	0.060351
H	-1.090145	-0.136052	-2.437133
C	-1.767578	-2.220323	-2.261619
H	-1.078796	-2.572454	-1.459012
H	-1.266494	-2.466269	-3.224783
H	-2.701986	-2.806361	-2.188024
C	-6.944882	2.206587	-1.732379
H	-7.731077	1.471065	-1.454110
C	-7.382638	2.884391	-3.050869
H	-7.503560	2.147975	-3.871288
H	-6.646639	3.647308	-3.381923
H	-8.354626	3.399880	-2.908446
C	-6.825405	3.225719	-0.576433
H	-6.477980	2.738884	0.356447
H	-6.109627	4.038332	-0.823362
H	-7.810102	3.699285	-0.384346

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AuIPrUrN2H–PhEt1+ISOMERFll SCF Done: -2227.72482072 A.U.

N	3.170411	-1.003217	0.537394
N	3.217592	1.153305	0.227068
C	2.381101	0.068837	0.216517
C	4.484309	-0.593901	0.748464
H	5.273596	-1.302563	1.017735
C	4.514223	0.764368	0.552067
H	5.334927	1.485668	0.614634
C	2.712249	-2.377204	0.642884
C	2.217932	-2.832903	1.893993
C	2.154228	-1.946605	3.138433
H	2.451874	-0.919201	2.839773
C	1.796443	-4.177416	1.965016

H	1.408948	-4.569686	2.918121
C	1.868380	-5.022990	0.849159
C	2.367462	-4.542413	-0.370357
H	2.427437	-5.220467	-1.236280
C	2.805214	-3.208291	-0.505324
C	3.354871	-2.717820	-1.846099
H	3.651743	-1.654733	-1.725257
C	2.815065	2.520582	-0.052298
C	2.909637	2.992964	-1.388428
C	3.401763	2.122041	-2.545721
H	3.721040	1.144719	-2.126042
C	2.515540	4.325667	-1.628573
H	2.574960	4.730355	-2.651147
C	2.055723	5.146015	-0.588498
C	1.983095	4.651073	0.720991
H	1.626287	5.308558	1.529133
C	2.363136	3.327157	1.025734
C	2.274014	2.821107	2.466130
H	2.648270	1.775714	2.484738
Au	0.412663	0.077469	-0.105950
C	4.618270	-3.501123	-2.264207
H	4.394995	-4.574027	-2.441101
H	5.037102	-3.089782	-3.206000
H	5.408537	-3.448613	-1.487540
C	2.274769	-2.762028	-2.948195
H	2.673146	-2.358777	-3.902347
H	1.930922	-3.799425	-3.143477
H	1.388580	-2.156625	-2.663365
C	2.262599	1.833935	-3.547841
H	1.888973	2.767628	-4.018464
H	2.615796	1.167168	-4.361864
H	1.405702	1.337836	-3.044327
C	4.629608	2.738579	-3.249523
H	4.382069	3.703900	-3.738351
H	5.457906	2.927805	-2.536416

H	5.007597	2.056283	-4.038900
C	3.172205	3.643518	3.415538
H	4.229437	3.648627	3.079340
H	2.837604	4.699715	3.484182
H	3.141538	3.219930	4.440738
C	0.810939	2.788007	2.958433
H	0.365312	3.804516	2.983094
H	0.178658	2.155444	2.300321
H	0.754800	2.373881	3.986371
C	3.161953	-2.422780	4.208871
H	4.199510	-2.450803	3.816474
H	3.146636	-1.743106	5.086040
H	2.915055	-3.442283	4.572630
C	0.723256	-1.856819	3.709473
H	-0.003835	-1.497267	2.952425
H	0.367496	-2.841360	4.079369
H	0.697611	-1.156863	4.570233
H	1.756638	6.184644	-0.799971
H	1.539554	-6.070893	0.932716
N	-1.660237	0.140125	-0.397171
C	-2.554020	-0.117599	0.667741
N	-3.712678	0.646567	0.433067
C	-3.536998	1.452840	-0.724629
N	-2.262022	1.098251	-1.173613
C	-4.882762	0.663069	1.266244
C	-5.637823	1.848567	1.389001
C	-5.270243	-0.503158	1.959320
H	-5.339856	2.752085	0.841659
H	-4.665779	-1.416063	1.883756
C	-6.784726	1.854243	2.198954
C	-6.413568	-0.475495	2.773652
H	-7.373342	2.780544	2.288456
H	-6.707531	-1.385743	3.319321
C	-7.177193	0.698067	2.894469
H	-8.074508	0.712331	3.532213

O	-4.284753	2.268787	-1.227527
O	-2.329760	-0.899947	1.587235
C	-5.655658	-0.481576	-3.415115
C	-4.394457	-0.128909	-3.928058
C	-5.760800	-1.366605	-2.317370
H	-4.320276	0.549801	-4.791145
H	-6.752915	-1.641354	-1.928157
C	-3.236093	-0.639761	-3.331531
C	-4.611595	-1.887040	-1.723650
H	-2.245513	-0.389364	-3.743797
H	-4.703711	-2.569956	-0.865666
C	-3.315257	-1.529709	-2.213702
H	-6.568387	-0.072272	-3.875521
C	-2.105324	-1.969775	-1.590798
H	-1.739573	1.620191	-1.878871
H	-1.174812	-1.671765	-2.100549
C	-1.996144	-3.018670	-0.549263
H	-2.082281	-2.565150	0.475011
H	-1.010706	-3.521776	-0.585431
H	-2.804886	-3.773678	-0.624736

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N	3.534226	-0.850585	0.538779
N	3.431448	1.306386	0.245119
C	2.675308	0.163895	0.205897
C	4.808476	-0.347012	0.787453
H	5.639979	-0.997562	1.075236
C	4.744634	1.011084	0.600383
H	5.508671	1.789602	0.688645
C	3.183660	-2.257747	0.619640
C	2.619100	-2.749857	1.826587
C	2.386537	-1.870953	3.056154
H	2.533485	-0.813586	2.750213
C	2.312860	-4.126079	1.875814

H	1.874316	-4.546062	2.794106
C	2.563618	-4.967738	0.783492
C	3.129922	-4.451284	-0.390845
H	3.330787	-5.126233	-1.237552
C	3.454946	-3.083609	-0.504459
C	4.106942	-2.556549	-1.784619
H	4.145376	-1.448673	-1.716106
C	2.936167	2.642357	-0.034110
C	3.011681	3.126113	-1.367387
C	3.584132	2.300125	-2.520569
H	3.946354	1.336880	-2.103442
C	2.525443	4.428059	-1.608089
H	2.568030	4.840147	-2.628629
C	1.995977	5.209152	-0.570896
C	1.945016	4.705166	0.736268
H	1.533459	5.332343	1.542510
C	2.416294	3.410888	1.041060
C	2.351423	2.895249	2.479424
H	2.793523	1.876776	2.497545
Au	0.709053	0.063308	-0.124572
C	5.561335	-3.062955	-1.914702
H	5.595529	-4.169117	-2.002978
H	6.045110	-2.638151	-2.818803
H	6.176267	-2.781769	-1.035289
C	3.286075	-2.901924	-3.044149
H	3.746906	-2.444573	-3.944103
H	3.239207	-3.996667	-3.221156
H	2.244844	-2.527301	-2.965006
C	2.494071	1.961570	-3.560509
H	2.085358	2.878219	-4.035512
H	2.909122	1.324055	-4.368790
H	1.649608	1.414746	-3.089994
C	4.794705	2.996808	-3.178391
H	4.506257	3.955747	-3.657362
H	5.590749	3.219172	-2.438576

H	5.232658	2.351342	-3.967813
C	3.188076	3.772497	3.436066
H	4.244752	3.847390	3.106478
H	2.784777	4.804500	3.504085
H	3.179070	3.345557	4.460305
C	0.891349	2.764015	2.963855
H	0.378315	3.748253	2.988175
H	0.306850	2.091595	2.301126
H	0.857887	2.344844	3.990773
C	3.431451	-2.182585	4.152210
H	4.470074	-2.051821	3.783878
H	3.291688	-1.511726	5.025313
H	3.334898	-3.228056	4.513497
C	0.947756	-1.988603	3.599839
H	0.188877	-1.768968	2.820851
H	0.740462	-3.003805	3.998758
H	0.798566	-1.276305	4.437677
H	1.625417	6.224502	-0.782416
H	2.321604	-6.040165	0.850298
N	-1.372764	0.051551	-0.371359
C	-2.178823	-0.416337	0.680608
N	-3.317737	0.415873	0.745829
C	-3.222099	1.441847	-0.233116
N	-2.030609	1.150685	-0.894642
C	-4.377960	0.301630	1.705822
C	-5.065611	1.458918	2.132073
C	-4.724381	-0.961653	2.232103
H	-4.800182	2.439944	1.718037
H	-4.167814	-1.854995	1.923476
C	-6.101929	1.340990	3.072297
C	-5.756311	-1.058726	3.179435
H	-6.635056	2.247707	3.398524
H	-6.014788	-2.046288	3.592902
C	-6.452549	0.086969	3.600953
H	-7.261661	0.003516	4.342974

O	-3.982345	2.364805	-0.468494
O	-1.923736	-1.398697	1.376357
C	-6.058347	-0.474468	-2.276296
C	-5.047882	0.136907	-3.054888
C	-5.691238	-1.572595	-1.451178
H	-5.310111	0.982587	-3.709940
H	-6.464057	-2.072961	-0.846316
C	-3.726107	-0.308418	-3.004292
C	-4.376852	-2.023712	-1.390821
H	-2.980512	0.187619	-3.640223
H	-4.134971	-2.873746	-0.736882
C	-3.341372	-1.401490	-2.163339
C	-1.972865	-1.839025	-2.065077
H	-1.536183	1.827046	-1.479008
C	-1.603957	-3.026645	-1.235005
H	-1.752766	-2.812731	-0.147581
H	-0.545611	-3.313176	-1.377676
H	-2.244763	-3.901339	-1.478107
C	-7.471628	0.052419	-2.281917
H	-7.676076	0.547318	-3.254786
H	-8.182210	-0.797879	-2.196113
C	-7.726215	1.052726	-1.130442
H	-7.024281	1.909255	-1.182360
H	-7.590180	0.571344	-0.140599
H	-8.762738	1.442945	-1.183697
C	-0.929975	-1.349730	-3.021537
H	0.076940	-1.389647	-2.559791
H	-0.910158	-2.044597	-3.894736
H	-1.105295	-0.332789	-3.416666

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N	3.221055	-0.912361	0.644044
N	3.167757	1.253431	0.406091
C	2.397106	0.125442	0.294914

C	4.487884	-0.437235	0.973426
H	5.292613	-1.109379	1.286564
C	4.455391	0.926364	0.821416
H	5.225743	1.689038	0.971586
C	2.845763	-2.315390	0.669905
C	2.210171	-2.828018	1.832260
C	1.927192	-1.976721	3.070771
H	2.093214	-0.913268	2.797157
C	1.882139	-4.200095	1.830002
H	1.388885	-4.635693	2.712507
C	2.179841	-5.018589	0.731890
C	2.816338	-4.482563	-0.396783
H	3.053562	-5.139787	-1.247953
C	3.166005	-3.117687	-0.458456
C	3.896440	-2.569803	-1.686512
H	3.931148	-1.463254	-1.596616
C	2.706623	2.604830	0.142451
C	2.850894	3.123943	-1.171731
C	3.459037	2.318242	-2.321023
H	3.822645	1.354245	-1.906729
C	2.392995	4.438663	-1.397904
H	2.488179	4.878121	-2.403296
C	1.825926	5.198302	-0.364574
C	1.707891	4.659559	0.924239
H	1.267678	5.270319	1.727928
C	2.147662	3.350774	1.213932
C	2.008648	2.796133	2.632469
H	2.444000	1.774599	2.644129
Au	0.448545	0.076520	-0.137997
C	5.355747	-3.076978	-1.734123
H	5.393588	-4.181670	-1.838043
H	5.895405	-2.638601	-2.599274
H	5.915323	-2.811715	-0.813785
C	3.156998	-2.892258	-3.001206

H	3.671458	-2.416008	-3.861368
H	3.125658	-3.983306	-3.202656
H	2.111472	-2.522125	-2.980141
C	2.393008	1.980017	-3.386093
H	1.982054	2.898895	-3.855049
H	2.830603	1.358575	-4.195053
H	1.547322	1.416347	-2.937416
C	4.675608	3.032806	-2.947081
H	4.387981	3.990500	-3.428936
H	5.451881	3.260095	-2.188066
H	5.138698	2.396294	-3.729327
C	2.801359	3.640725	3.653710
H	3.873049	3.719412	3.377913
H	2.399439	4.672457	3.732755
H	2.740903	3.184156	4.663297
C	0.525522	2.661403	3.040233
H	0.016373	3.647698	3.062430
H	-0.028528	2.007928	2.333626
H	0.439101	2.218329	4.053947
C	2.921062	-2.321225	4.203986
H	3.975607	-2.188123	3.885069
H	2.746425	-1.670850	5.086255
H	2.803127	-3.374595	4.534691
C	0.465499	-2.097861	3.548258
H	-0.256965	-1.856520	2.741735
H	0.235753	-3.120065	3.915642
H	0.283203	-1.403089	4.394185
H	1.478756	6.224245	-0.564337
H	1.919635	-6.088500	0.758674
N	-1.618126	0.128240	-0.481322
C	-2.489927	-0.375256	0.495458
N	-3.628402	0.458751	0.522055
C	-3.468950	1.517072	-0.414597
N	-2.230437	1.249968	-0.996683
C	-4.764381	0.300839	1.386566

C	-5.527431	1.430621	1.754746
C	-5.114889	-0.978154	1.871828
H	-5.261267	2.423559	1.371322
H	-4.502014	-1.850302	1.613281
C	-6.640372	1.269488	2.595456
C	-6.225720	-1.117450	2.719428
H	-7.231857	2.155229	2.875378
H	-6.487301	-2.116999	3.100873
C	-6.995944	0.000348	3.082208
H	-7.866938	-0.116570	3.745415
O	-4.213096	2.444435	-0.678845
O	-2.277987	-1.390016	1.162060
C	-6.020340	0.145118	-2.865660
C	-4.886087	0.624748	-3.544054
C	-5.916177	-0.983905	-2.023304
H	-4.968772	1.500274	-4.205388
H	-6.805407	-1.361809	-1.496746
C	-3.647672	-0.002188	-3.369241
C	-4.686384	-1.616584	-1.848988
H	-2.779342	0.381423	-3.921963
H	-4.625799	-2.488287	-1.182129
C	-3.507790	-1.142442	-2.513435
C	-2.226072	-1.766341	-2.289422
H	-1.714154	1.922858	-1.565430
C	-2.094828	-2.987718	-1.444372
H	-2.141833	-2.708730	-0.356721
H	-1.125393	-3.494778	-1.607306
H	-2.917263	-3.711680	-1.615625
C	-1.023247	-1.397391	-3.099697
H	-0.094736	-1.555937	-2.514884
H	-0.970433	-2.091348	-3.972466
H	-1.025036	-0.366500	-3.496131
H	-6.991971	0.646708	-2.994551

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N	-1.977623	1.888565	0.312894
C	-3.187878	1.312966	0.429055
N	-3.450661	0.410159	-0.670844
C	-2.389587	0.444490	-1.550716
N	-1.378664	1.269330	-0.835618
C	-4.662213	-0.334171	-0.863256
C	-5.177796	-0.519524	-2.162658
C	-5.325536	-0.878656	0.255928
H	-4.650380	-0.103984	-3.031875
H	-4.921954	-0.722457	1.265234
C	-6.360523	-1.256791	-2.334734
C	-6.513129	-1.602280	0.066094
H	-6.759780	-1.404404	-3.350277
H	-7.034083	-2.021241	0.941140
C	-7.033660	-1.796386	-1.225359
H	-7.964097	-2.367731	-1.366934
O	-2.217612	-0.052178	-2.644590
O	-4.032593	1.569196	1.320715
C	0.720360	6.348441	0.484760
C	-0.106019	6.146225	1.610431
C	0.315505	5.895099	-0.786518
H	0.216468	6.504911	2.599963
H	0.957901	6.064487	-1.664247
C	-1.337281	5.500804	1.471130
C	-0.910931	5.238842	-0.929428
H	-1.976684	5.349134	2.353454
H	-1.241499	4.899238	-1.925309
C	-1.764264	5.031527	0.195063
H	1.683554	6.870189	0.599555
C	-3.039673	4.395906	-0.012825
H	-0.961201	1.974617	-1.467778
H	-3.241001	4.083554	-1.054365
C	-4.115184	4.246808	0.921035

H	-5.118045	4.325029	0.455801
H	-4.035015	4.817297	1.863814
H	-4.120901	3.086383	1.240060
N	3.106181	-1.039919	0.011567
N	1.664474	-2.438496	0.859065
C	1.769681	-1.221482	0.242640
C	3.831039	-2.132990	0.479655
H	4.920556	-2.183756	0.389992
C	2.922831	-3.013053	1.013439
H	3.056183	-3.990493	1.487221
C	3.696231	0.122124	-0.628343
C	3.837693	0.118160	-2.041358
C	3.383556	-1.047059	-2.921676
H	2.997426	-1.847356	-2.255634
C	4.427392	1.256698	-2.629612
H	4.556211	1.292253	-3.722744
C	4.860019	2.337428	-1.848411
C	4.712117	2.305311	-0.454492
H	5.063440	3.157624	0.148068
C	4.128170	1.196883	0.193181
C	3.975917	1.193316	1.715086
H	3.554252	0.210431	2.013588
C	0.421352	-3.055452	1.289179
C	-0.048723	-2.783319	2.601248
C	0.680854	-1.854015	3.572462
H	1.609279	-1.501513	3.075148
C	-1.248226	-3.411668	2.995534
H	-1.646753	-3.226399	4.005303
C	-1.938362	-4.269667	2.127846
C	-1.444222	-4.519195	0.839910
H	-1.995993	-5.196601	0.169744
C	-0.251263	-3.919987	0.384968
C	0.271544	-4.229512	-1.018673
H	1.165727	-3.595276	-1.197162
Au	0.273338	-0.007004	-0.259834

C	5.336989	1.340163	2.428621
H	5.808763	2.322510	2.216640
H	5.207733	1.266536	3.528344
H	6.051934	0.551851	2.115481
C	2.974556	2.274086	2.177339
H	2.838103	2.232757	3.278067
H	3.333220	3.293644	1.922777
H	1.980735	2.134970	1.702881
C	-0.165582	-0.602823	3.892694
H	-1.110528	-0.871690	4.409689
H	0.394602	0.085132	4.559720
H	-0.432559	-0.045978	2.970226
C	1.106696	-2.594249	4.858904
H	0.228151	-2.948249	5.437796
H	1.737348	-3.478964	4.634357
H	1.688078	-1.919033	5.520559
C	0.724141	-5.702682	-1.130853
H	1.496450	-5.956067	-0.375486
H	-0.127243	-6.399822	-0.983411
H	1.150030	-5.903804	-2.135803
C	-0.760806	-3.873808	-2.109428
H	-1.676980	-4.494965	-2.025963
H	-1.068569	-2.809433	-2.055902
H	-0.333028	-4.054304	-3.117365
C	4.559140	-1.648411	-3.722119
H	5.386584	-1.971254	-3.057346
H	4.220558	-2.532709	-4.300677
H	4.977266	-0.919639	-4.447635
C	2.222050	-0.629319	-3.849406
H	1.353717	-0.254359	-3.267764
H	2.531454	0.169863	-4.555376
H	1.876604	-1.493209	-4.454061
H	-2.870969	-4.752095	2.460124
H	5.325054	3.211422	-2.331262

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N	-1.942494	-0.249976	1.688351
C	-2.698836	-1.361342	1.538937
N	-2.854959	-1.692062	0.131698
C	-2.256260	-0.719445	-0.635618
N	-1.574000	0.152525	0.362212
C	-3.583076	-2.818091	-0.375786
C	-4.277801	-2.719825	-1.599827
C	-3.591283	-4.024793	0.355457
H	-4.254908	-1.783445	-2.172841
H	-3.058546	-4.092056	1.313113
C	-4.976937	-3.835844	-2.087241
C	-4.304369	-5.126479	-0.142189
H	-5.513876	-3.758105	-3.045611
H	-4.313638	-6.065226	0.433431
C	-4.997136	-5.039553	-1.362316
H	-5.551708	-5.909139	-1.747677
O	-2.217698	-0.531375	-1.834927
O	-3.272182	-1.978400	2.458669
C	-4.719257	3.076055	-1.043531
C	-3.613131	3.565362	-0.308872
C	-5.469029	2.015257	-0.474707
H	-3.012313	4.391380	-0.722684
H	-6.331607	1.608402	-1.026778
C	-3.266034	3.021727	0.933357
C	-5.138011	1.472589	0.767226
H	-2.408215	3.448102	1.473982
H	-5.747622	0.646933	1.161681
C	-4.024632	1.960904	1.516980
C	-3.671295	1.394158	2.812927
H	-1.865661	1.140902	0.197986
C	-2.549809	1.956117	3.629816
H	-2.974476	2.754846	4.283455
H	-1.723829	2.393000	3.042376

H	-2.134611	1.178329	4.298324
N	3.296874	-1.125184	-0.250492
N	3.406513	1.050379	-0.324054
C	2.533258	0.007510	-0.170925
C	4.634327	-0.795339	-0.450917
H	5.410245	-1.561797	-0.541093
C	4.704137	0.574774	-0.497602
H	5.553064	1.251104	-0.637524
C	2.790661	-2.483109	-0.146961
C	2.725891	-3.083828	1.138185
C	3.144676	-2.360585	2.419031
H	3.504976	-1.348515	2.137112
C	2.245815	-4.408368	1.203224
H	2.179197	-4.909930	2.181351
C	1.855049	-5.097427	0.046629
C	1.934186	-4.475171	-1.207023
H	1.624815	-5.028908	-2.107150
C	2.404190	-3.151957	-1.338802
C	2.492299	-2.507961	-2.723296
H	2.825712	-1.456940	-2.589955
C	3.040883	2.455035	-0.310338
C	2.690729	3.075132	-1.538812
C	2.669381	2.327547	-2.872789
H	3.005526	1.285997	-2.685350
C	2.349700	4.443227	-1.492737
H	2.075279	4.961230	-2.425100
C	2.362042	5.155562	-0.285274
C	2.718965	4.514059	0.909470
H	2.732431	5.087697	1.849523
C	3.070593	3.148299	0.928816
C	3.450270	2.474603	2.248508
H	3.768664	1.435393	2.021484
Au	0.559856	0.096544	0.085347
C	3.548081	-3.215553	-3.601746
H	3.269584	-4.272074	-3.798662

H	3.641465	-2.707049	-4.583842
H	4.548623	-3.218823	-3.122029
C	1.117029	-2.461477	-3.422621
H	1.199361	-1.942705	-4.400258
H	0.724201	-3.480213	-3.622978
H	0.362578	-1.922726	-2.813288
C	1.238089	2.245255	-3.446349
H	0.832168	3.253644	-3.673208
H	1.230682	1.663043	-4.390998
H	0.544448	1.748680	-2.735887
C	3.652331	2.947804	-3.889320
H	3.360670	3.983402	-4.163090
H	4.686695	2.986155	-3.490041
H	3.669077	2.351135	-4.824804
C	4.642625	3.176820	2.932458
H	5.525222	3.231750	2.262714
H	4.390008	4.213326	3.239351
H	4.942465	2.626151	3.848031
C	2.232354	2.377909	3.193298
H	1.854704	3.384847	3.470629
H	1.399782	1.816148	2.719235
H	2.507477	1.853609	4.132034
C	4.315086	-3.081501	3.122527
H	5.189750	-3.198319	2.450037
H	4.643777	-2.508992	4.014706
H	4.022272	-4.094682	3.469026
C	1.944883	-2.166260	3.371595
H	1.119354	-1.611567	2.878480
H	1.537520	-3.139286	3.717601
H	2.253363	-1.596361	4.272800
H	2.098913	6.225147	-0.276295
H	1.486340	-6.132399	0.122810
C	-4.491279	0.368916	3.460668
H	-5.554895	0.330421	3.167575
H	-3.993984	-0.588596	3.051937

H	-4.361184	0.324794	4.557288
C	-5.119724	3.692563	-2.363222
H	-4.218133	4.102354	-2.866119
H	-5.523908	2.900054	-3.028776
C	-6.172587	4.811655	-2.202051
H	-5.789833	5.638699	-1.569450
H	-7.101287	4.429013	-1.731073
H	-6.441549	5.233991	-3.191270

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N	-2.242628	1.352381	0.459188
C	-3.307953	0.536161	0.552479
N	-3.392250	-0.347085	-0.599383
C	-2.373447	-0.049778	-1.476580
N	-1.546522	0.931449	-0.723473
C	-4.423836	-1.316851	-0.827543
C	-4.888189	-1.560278	-2.137341
C	-4.963951	-2.025785	0.266079
H	-4.453630	-1.017444	-2.987481
H	-4.604656	-1.823115	1.283627
C	-5.893461	-2.518613	-2.345170
C	-5.976049	-2.971716	0.040548
H	-6.250766	-2.710281	-3.369018
H	-6.400736	-3.519588	0.896244
C	-6.443348	-3.223946	-1.261206
H	-7.235452	-3.969698	-1.430509
O	-2.114835	-0.444056	-2.596016
O	-4.174031	0.556457	1.455265
C	-0.470956	6.148182	0.764427
C	-1.058796	5.507595	1.874265
C	-1.003927	5.953692	-0.524039
H	-0.638700	5.653387	2.881215
H	-0.553397	6.460961	-1.391002
C	-2.179073	4.691332	1.701728

C	-2.115007	5.122058	-0.704357
H	-2.616849	4.188079	2.575323
H	-2.526943	5.000806	-1.716918
C	-2.737537	4.478425	0.406581
H	0.402417	6.804101	0.905682
C	-3.931257	3.665008	0.224886
H	-1.303066	1.740567	-1.321759
C	-4.777514	3.252435	1.326362
H	-5.849512	3.207436	1.045743
H	-4.627929	3.779738	2.283983
H	-4.545148	2.111758	1.523563
N	3.337182	-0.456701	-0.093083
N	2.232087	-2.098116	0.821186
C	2.072252	-0.889731	0.199301
C	4.279674	-1.384965	0.342193
H	5.353327	-1.226021	0.202067
C	3.583276	-2.418182	0.918127
H	3.923786	-3.347087	1.385900
C	3.661796	0.790435	-0.761377
C	3.729439	0.801119	-2.179804
C	3.466383	-0.437956	-3.036789
H	3.273525	-1.291315	-2.352872
C	4.057432	2.026645	-2.796650
H	4.120426	2.076507	-3.894981
C	4.312535	3.177609	-2.038037
C	4.245752	3.129936	-0.638329
H	4.456519	4.039485	-0.054077
C	3.920023	1.935708	0.037472
C	3.854959	1.915329	1.565471
H	3.615392	0.878791	1.883275
C	1.151354	-2.938435	1.307441
C	0.696498	-2.750141	2.639385
C	1.278800	-1.691809	3.577445
H	2.092246	-1.165329	3.034580
C	-0.342158	-3.592560	3.087258

H	-0.723916	-3.478354	4.113906
C	-0.893821	-4.573297	2.251113
C	-0.418551	-4.734763	0.942202
H	-0.860136	-5.510450	0.297334
C	0.617172	-3.923192	0.434397
C	1.126240	-4.138678	-0.991761
H	1.889104	-3.359611	-1.203101
Au	0.347045	0.007152	-0.233081
C	5.213316	2.284672	2.199783
H	5.508280	3.327596	1.959248
H	5.160867	2.201851	3.305237
H	6.026465	1.618140	1.845958
C	2.720502	2.821597	2.090172
H	2.654186	2.759501	3.196410
H	2.896528	3.885483	1.825364
H	1.737441	2.524005	1.669631
C	0.221654	-0.630206	3.951483
H	-0.622317	-1.077494	4.517271
H	0.671894	0.156280	4.592485
H	-0.199821	-0.140170	3.049059
C	1.909047	-2.330428	4.834184
H	1.148777	-2.849654	5.454437
H	2.689094	-3.073904	4.570239
H	2.379703	-1.552357	5.470494
C	1.821768	-5.511073	-1.133582
H	2.656349	-5.627270	-0.411638
H	1.111036	-6.345805	-0.958451
H	2.234862	-5.634108	-2.156305
C	0.002444	-3.967059	-2.035772
H	-0.792325	-4.732212	-1.912899
H	-0.476402	-2.968753	-1.967283
H	0.410124	-4.078600	-3.061892
C	4.697068	-0.809486	-3.892375
H	5.601598	-0.960512	-3.267969
H	4.508480	-1.748023	-4.453603

H	4.932298	-0.020915	-4.637487
C	2.203870	-0.260837	-3.907829
H	1.307048	-0.057409	-3.285734
H	2.318807	0.577512	-4.626708
H	2.005441	-1.180163	-4.496679
H	-1.701913	-5.221584	2.624804
H	4.573989	4.120680	-2.543489
C	-4.430966	3.343643	-1.153786
H	-3.629457	3.183474	-1.899625
H	-5.102477	2.463031	-1.138662
H	-5.045895	4.199462	-1.519300

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N	-3.784995	0.355929	-0.666814
N	-3.497708	-1.299600	0.720986
C	-2.822808	-0.326442	0.030838
C	-5.042886	-0.182723	-0.415895
H	-5.947187	0.221467	-0.881144
C	-4.862274	-1.225072	0.459159
H	-5.576844	-1.914789	0.918757
C	-3.544474	1.485361	-1.548585
C	-3.573352	2.793651	-0.996715
C	-3.851105	3.066469	0.482073
H	-3.827577	2.093067	1.016617
C	-3.361972	3.868380	-1.885178
H	-3.376558	4.898249	-1.496329
C	-3.135348	3.650010	-3.251075
C	-3.116933	2.345449	-3.764005
H	-2.942395	2.188822	-4.840130
C	-3.323840	1.228951	-2.927680
C	-3.303178	-0.181334	-3.519593
H	-3.511776	-0.899868	-2.698986
C	-2.892117	-2.272466	1.613196
C	-2.566964	-3.553554	1.093347

C	-2.822556	-3.949884	-0.361774
H	-3.193800	-3.052126	-0.899811
C	-1.999833	-4.485223	1.987190
H	-1.736146	-5.490591	1.623094
C	-1.768754	-4.156031	3.330171
C	-2.107228	-2.884442	3.812916
H	-1.927011	-2.641751	4.871865
C	-2.682640	-1.910441	2.970399
C	-3.059855	-0.540972	3.537183
H	-3.503323	0.058947	2.714637
Au	-0.869617	0.094764	0.122855
C	-4.405541	-0.370964	-4.583845
H	-4.246633	0.291248	-5.460478
H	-4.412203	-1.416801	-4.955325
H	-5.412327	-0.147329	-4.175214
C	-1.909068	-0.531405	-4.082636
H	-1.891471	-1.574421	-4.462100
H	-1.630528	0.135263	-4.925599
H	-1.127098	-0.433502	-3.300733
C	-1.525912	-4.395479	-1.069741
H	-1.107096	-5.318963	-0.617878
H	-1.723683	-4.612921	-2.140009
H	-0.746554	-3.607902	-1.014716
C	-3.918615	-5.033736	-0.463593
H	-3.607021	-5.973463	0.038782
H	-4.867761	-4.704492	0.007067
H	-4.130826	-5.276536	-1.525620
C	-4.131732	-0.661864	4.642447
H	-5.039262	-1.186165	4.278697
H	-3.751341	-1.222568	5.521794
H	-4.437394	0.344099	4.997705
C	-1.816316	0.224959	4.037136
H	-1.321519	-0.303020	4.879131
H	-1.067488	0.347295	3.226315
H	-2.100304	1.235510	4.397146

C	-5.263091	3.664543	0.675626
H	-6.053199	3.003854	0.262525
H	-5.476866	3.819184	1.753743
H	-5.354898	4.649187	0.170755
C	-2.768685	3.960437	1.122114
H	-1.751458	3.544701	0.973528
H	-2.779940	4.986386	0.698039
H	-2.949938	4.058682	2.212625
H	-1.325257	-4.900825	4.009516
H	-2.975011	4.506751	-3.924324
N	1.130577	0.594710	0.321699
C	1.545089	1.961151	0.528844
N	2.910257	1.893070	0.860890
C	3.320246	0.555129	0.839209
N	2.130618	-0.239726	0.492417
C	3.745020	3.017538	1.184142
C	4.705015	2.897228	2.208315
C	3.591945	4.225612	0.475593
H	4.820632	1.949986	2.752821
H	2.834255	4.313427	-0.315270
C	5.519775	3.998443	2.515623
C	4.407012	5.320548	0.804347
H	6.272590	3.905751	3.313670
H	4.284874	6.267568	0.256203
C	5.372825	5.210882	1.819662
H	6.011078	6.072244	2.070063
O	4.412422	0.073890	1.042585
O	0.815013	2.927583	0.476898
C	7.149050	-2.430865	-1.113823
C	6.034663	-3.226015	-0.743147
C	6.890925	-1.175978	-1.715526
H	6.205695	-4.204608	-0.265844
H	7.736977	-0.538779	-2.020061
C	4.729021	-2.794292	-0.972106
C	5.585372	-0.730985	-1.936150

H	3.894734	-3.438827	-0.657819
H	5.435869	0.246174	-2.417141
C	4.461542	-1.537467	-1.592083
C	3.067046	-1.094948	-1.843655
H	2.644847	-0.833424	-0.676227
C	2.847577	0.209938	-2.598903
H	1.792633	0.543242	-2.501918
H	3.036911	0.070720	-3.686141
H	3.500698	1.033692	-2.249954
C	2.044875	-2.171202	-2.221353
H	2.098443	-3.070979	-1.579943
H	1.012491	-1.770331	-2.163428
H	2.221484	-2.496370	-3.270579
C	8.560539	-2.884664	-0.825168
H	8.615542	-3.991196	-0.910768
H	9.245183	-2.469795	-1.595489
C	9.048742	-2.456386	0.576972
H	8.404665	-2.879731	1.374919
H	9.038095	-1.352581	0.687066
H	10.085793	-2.808735	0.750635

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N	-3.371225	-0.756443	0.699618
N	-3.342444	0.855065	-0.767310
C	-2.525877	0.030466	-0.038062
C	-4.696910	-0.428578	0.434510
H	-5.528171	-0.944072	0.925239
C	-4.679070	0.585992	-0.490247
H	-5.491298	1.135638	-0.975795
C	-2.960477	-1.793206	1.630986
C	-2.775962	-3.112224	1.137784
C	-3.001004	-3.491306	-0.326478
H	-3.123767	-2.551023	-0.904925
C	-2.403201	-4.099429	2.073612

H	-2.249942	-5.134424	1.731093
C	-2.228338	-3.788499	3.429176
C	-2.424645	-2.476993	3.883960
H	-2.290822	-2.248731	4.953042
C	-2.797074	-1.444916	2.998032
C	-3.030028	-0.029600	3.529673
H	-3.237658	0.631519	2.661766
C	-2.894213	1.864906	-1.710277
C	-2.761196	3.202969	-1.253092
C	-3.065828	3.624495	0.185369
H	-3.295806	2.707598	0.768251
C	-2.344735	4.165944	-2.195350
H	-2.231909	5.215219	-1.880518
C	-2.075720	3.812692	-3.525108
C	-2.223629	2.483815	-3.945521
H	-2.015993	2.221609	-4.994738
C	-2.641366	1.475161	-3.052339
C	-2.810181	0.039353	-3.551427
H	-3.162129	-0.579840	-2.699461
Au	-0.530980	-0.085283	-0.129138
C	-4.265757	0.024444	4.455232
H	-4.121144	-0.601074	5.360929
H	-4.456079	1.064290	4.793545
H	-5.179340	-0.340018	3.942149
C	-1.777305	0.531615	4.234362
H	-1.948411	1.580774	4.553543
H	-1.520006	-0.051755	5.143054
H	-0.895525	0.514288	3.560878
C	-1.847080	4.291550	0.856732
H	-1.572653	5.244207	0.357267
H	-2.070361	4.528274	1.917857
H	-0.959299	3.626783	0.829413
C	-4.311412	4.536002	0.250462
H	-4.146299	5.487378	-0.297395
H	-5.202528	4.047127	-0.194190

H	-4.552963	4.793410	1.302730
C	-3.884341	-0.053844	-4.657073
H	-4.860698	0.347532	-4.315879
H	-3.588263	0.512962	-5.564477
H	-4.036511	-1.110145	-4.961405
C	-1.464719	-0.556204	-4.018497
H	-1.049748	0.000328	-4.884848
H	-0.710089	-0.528803	-3.204238
H	-1.593957	-1.613197	-4.330729
C	-4.304976	-4.305509	-0.487745
H	-5.187983	-3.754777	-0.102496
H	-4.488754	-4.539845	-1.556960
H	-4.247394	-5.268517	0.061890
C	-1.793234	-4.238521	-0.928774
H	-0.852460	-3.663997	-0.808954
H	-1.646767	-5.231998	-0.455372
H	-1.956278	-4.417122	-2.011908
H	-1.752783	4.582794	-4.243119
H	-1.940592	-4.578624	4.140437
N	1.523961	-0.266120	-0.324200
C	2.151249	-1.547541	-0.548012
N	3.489333	-1.260218	-0.873131
C	3.685468	0.123582	-0.830736
N	2.380425	0.717169	-0.477647
C	4.491408	-2.235262	-1.209753
C	5.419565	-1.951207	-2.230753
C	4.531209	-3.460891	-0.516323
H	5.384267	-0.990813	-2.763261
H	3.797710	-3.677428	0.272612
C	6.398148	-2.905748	-2.550416
C	5.509062	-4.408879	-0.857540
H	7.126872	-2.684807	-3.345557
H	5.538666	-5.370065	-0.321428
C	6.444894	-4.134807	-1.869864
H	7.211469	-4.880979	-2.129789

O	4.686016	0.775057	-1.024685
O	1.582827	-2.617059	-0.513318
C	6.918231	3.652950	1.223255
C	5.714738	4.268892	0.824459
C	6.886644	2.379332	1.820779
H	5.735245	5.259595	0.344781
H	7.823273	1.893571	2.135058
C	4.493610	3.621982	1.030603
C	5.665575	1.723701	2.017580
H	3.567644	4.112689	0.695957
H	5.666769	0.733472	2.494919
C	4.434119	2.337593	1.647756
H	7.880206	4.164162	1.062142
C	3.126222	1.667234	1.872296
H	2.765528	1.362846	0.680990
C	3.109599	0.328181	2.594521
H	2.127375	-0.173687	2.461747
H	3.243324	0.472081	3.689589
H	3.900824	-0.366375	2.250607
C	1.934876	2.552822	2.242777
H	1.854127	3.463496	1.619961
H	0.982890	1.990250	2.155962
H	2.036450	2.880394	3.301463

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N	-2.213207	-0.644538	-1.367497
C	-3.461829	-0.039735	-1.204743
N	-3.607522	0.357902	0.190411
C	-2.522816	-0.074013	0.904317
N	-1.632604	-0.723649	-0.132931
C	-4.741883	1.048710	0.733861
C	-5.184179	0.757868	2.041156
C	-5.401390	2.021158	-0.046179
H	-4.656119	0.013157	2.651946

H	-5.056626	2.238624	-1.065521
C	-6.290200	1.446726	2.563815
C	-6.512138	2.692604	0.488794
H	-6.630347	1.223327	3.586998
H	-7.028647	3.448945	-0.122396
C	-6.959665	2.411374	1.791216
H	-7.828546	2.945839	2.205312
O	-2.231078	-0.018514	2.079972
O	-4.284495	0.157637	-2.078639
C	-5.329626	-2.736005	-2.299156
C	-5.599400	-2.841389	-0.904820
C	-4.024156	-2.866586	-2.783226
H	-6.634925	-2.746764	-0.543869
H	-3.818617	-2.783295	-3.860263
C	-4.568481	-3.061439	-0.002862
C	-2.964869	-3.054107	-1.880096
H	-4.789719	-3.151834	1.071029
H	-1.939856	-3.185427	-2.256707
C	-3.213337	-3.197385	-0.466399
H	-6.160372	-2.559286	-2.999520
C	-2.100120	-3.331923	0.412616
H	-1.648846	-1.837647	0.206363
H	-1.147306	-3.624492	-0.072339
C	-2.170325	-3.557825	1.893592
H	-1.226221	-3.258230	2.389969
H	-2.303696	-4.646352	2.096521
H	-3.006575	-3.022902	2.383537
N	3.437340	-0.278614	0.244702
N	2.776345	1.741250	-0.240572
C	2.321668	0.471418	-0.011295
C	4.580071	0.514389	0.175415
H	5.579401	0.103381	0.349037
C	4.163041	1.786252	-0.130072
H	4.723761	2.714335	-0.278137
C	3.437326	-1.697940	0.549866

C	3.345451	-2.096180	1.909974
C	3.233236	-1.098774	3.064076
H	3.300162	-0.075485	2.638183
C	3.356024	-3.481774	2.174819
H	3.290154	-3.831379	3.217112
C	3.457975	-4.419720	1.137583
C	3.553913	-3.992068	-0.194395
H	3.642217	-4.739475	-0.998475
C	3.549363	-2.620490	-0.524059
C	3.654052	-2.185561	-1.986724
H	3.699053	-1.076351	-2.010555
C	1.935728	2.885742	-0.549162
C	1.638464	3.158645	-1.910755
C	2.153489	2.299065	-3.066087
H	2.766285	1.479315	-2.634778
C	0.828851	4.282403	-2.176977
H	0.574419	4.528126	-3.219855
C	0.345257	5.092294	-1.139911
C	0.662012	4.796833	0.193379
H	0.278044	5.443540	0.997777
C	1.466433	3.686954	0.525561
C	1.803102	3.400232	1.989701
H	2.413087	2.472713	2.024511
Au	0.423933	-0.138037	-0.051473
C	4.946183	-2.708231	-2.650412
H	4.959510	-3.816669	-2.709192
H	5.032218	-2.321895	-3.687087
H	5.850879	-2.391814	-2.091887
C	2.399328	-2.604269	-2.783834
H	2.466381	-2.247939	-3.832696
H	2.286125	-3.708602	-2.812422
H	1.477690	-2.175523	-2.336096
C	0.990924	1.638738	-3.838400
H	0.340693	2.396385	-4.323747
H	1.383040	0.977164	-4.638689

H	0.352175	1.027117	-3.167486
C	3.071990	3.107619	-4.008249
H	2.521137	3.932450	-4.506725
H	3.926331	3.558545	-3.462625
H	3.482284	2.453882	-4.805743
C	2.657328	4.532603	2.601436
H	3.589673	4.702852	2.024527
H	2.101184	5.493052	2.627260
H	2.941473	4.284840	3.645261
C	0.531903	3.137950	2.825309
H	-0.125284	4.031872	2.862555
H	-0.063285	2.297306	2.412909
H	0.802225	2.883714	3.871218
C	4.397102	-1.251592	4.067069
H	5.383801	-1.152175	3.569832
H	4.332063	-0.473924	4.855944
H	4.375763	-2.238743	4.574426
C	1.862417	-1.207824	3.766702
H	1.027208	-1.035676	3.055618
H	1.721261	-2.207980	4.228191
H	1.778796	-0.453549	4.576336
H	-0.282944	5.966140	-1.373791
H	3.471584	-5.496204	1.370512

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N	2.086900	-0.461529	1.054732
C	3.282753	0.247201	0.892374
N	3.281525	0.851915	-0.432583
C	2.160184	0.455309	-1.110364
N	1.418834	-0.414657	-0.119991
C	4.309857	1.706940	-0.950362
C	4.666930	1.634460	-2.312644
C	4.949285	2.623185	-0.089875
H	4.153009	0.932341	-2.983193

H	4.668853	2.671907	0.970540
C	5.667786	2.484425	-2.809432
C	5.955497	3.458273	-0.600919
H	5.941041	2.431303	-3.874806
H	6.456478	4.171143	0.072347
C	6.317471	3.394534	-1.957676
H	7.103799	4.056447	-2.352244
O	1.754399	0.674633	-2.232214
O	4.160003	0.383983	1.722600
C	5.566034	-2.572515	1.289353
C	5.598272	-2.408584	-0.129805
C	4.323666	-2.848449	1.891176
H	6.562344	-2.209956	-0.625039
H	4.266648	-2.973762	2.983377
C	4.447654	-2.506263	-0.898915
C	3.151526	-2.938863	1.129933
H	4.524607	-2.389676	-1.989366
H	2.209289	-3.166306	1.643913
C	3.175647	-2.800618	-0.299871
C	1.954013	-2.839881	-1.084490
H	1.542760	-1.516455	-0.663042
C	2.013004	-2.738717	-2.597641
H	1.007553	-2.538460	-3.016437
H	2.358502	-3.707580	-3.024931
H	2.693563	-1.948703	-2.967003
N	-3.695233	-0.452510	-0.007325
N	-3.144539	1.597568	0.485558
C	-2.618782	0.374571	0.167516
C	-4.882534	0.245767	0.199844
H	-5.860127	-0.237539	0.108061
C	-4.534702	1.536930	0.510109
H	-5.146524	2.413238	0.745492
C	-3.620985	-1.858238	-0.360301
C	-3.630232	-2.210506	-1.736256
C	-3.705708	-1.175476	-2.859949

H	-3.808497	-0.173004	-2.393774
C	-3.565171	-3.585130	-2.047222
H	-3.573619	-3.899836	-3.102626
C	-3.502321	-4.556717	-1.037962
C	-3.504482	-4.174787	0.311248
H	-3.464710	-4.948888	1.093637
C	-3.566983	-2.816324	0.686585
C	-3.573161	-2.431855	2.166987
H	-3.678951	-1.328492	2.232045
C	-2.366503	2.794086	0.759083
C	-1.959727	3.044279	2.096548
C	-2.292484	2.108191	3.259308
H	-2.893298	1.264895	2.857421
C	-1.214360	4.218532	2.330639
H	-0.878877	4.448622	3.353992
C	-0.896511	5.098158	1.286392
C	-1.318313	4.823166	-0.021954
H	-1.063890	5.524429	-0.831953
C	-2.064739	3.664671	-0.321763
C	-2.522913	3.402250	-1.757096
H	-3.031528	2.415071	-1.777290
Au	-0.679251	-0.064803	0.001695
C	-4.775510	-3.049999	2.912768
H	-4.721651	-4.158634	2.931991
H	-4.797643	-2.702204	3.966291
H	-5.739449	-2.770073	2.440458
C	-2.236407	-2.798697	2.847318
H	-2.238736	-2.477130	3.909416
H	-2.059338	-3.894853	2.831491
H	-1.379335	-2.304260	2.343509
C	-1.013413	1.501701	3.876111
H	-0.365332	2.284721	4.322529
H	-1.273121	0.786052	4.683735
H	-0.412359	0.959812	3.116197
C	-3.156296	2.814071	4.327174

H	-2.610147	3.654102	4.805019
H	-4.090379	3.226726	3.893422
H	-3.437637	2.102538	5.131082
C	-3.553169	4.458124	-2.216078
H	-4.432263	4.497771	-1.540194
H	-3.107420	5.474561	-2.242752
H	-3.918150	4.227395	-3.238505
C	-1.329820	3.317234	-2.732660
H	-0.786724	4.283020	-2.800865
H	-0.600651	2.540330	-2.423764
H	-1.684226	3.067334	-3.754252
C	-4.946291	-1.391966	-3.753310
H	-5.884624	-1.385439	-3.161604
H	-5.017927	-0.589479	-4.516330
H	-4.899014	-2.359530	-4.295458
C	-2.405575	-1.155434	-3.692818
H	-1.522406	-0.934393	-3.057084
H	-2.232360	-2.128417	-4.199374
H	-2.459097	-0.375304	-4.480121
H	-0.316062	6.010544	1.495164
H	-3.461037	-5.624313	-1.305927
C	0.728324	-3.573703	-0.567482
H	-0.203497	-3.153360	-0.999272
H	0.782083	-4.636209	-0.897426
H	0.629359	-3.572821	0.533118
C	6.829801	-2.441710	2.102864
H	6.650478	-2.838222	3.123755
H	7.615309	-3.084480	1.645052
C	7.350105	-0.990201	2.190951
H	6.583849	-0.324052	2.633467
H	7.604169	-0.586587	1.189239
H	8.265849	-0.949456	2.814560

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N	2.188612	-0.612956	1.373867
C	3.454833	-0.024473	1.252005
N	3.613177	0.444828	-0.118389
C	2.521175	0.073310	-0.853781
N	1.624511	-0.630336	0.144133
C	4.758469	1.148598	-0.620603
C	5.199192	0.924734	-1.941460
C	5.430225	2.066424	0.213232
H	4.662000	0.222843	-2.593587
H	5.086760	2.231579	1.242767
C	6.316096	1.625345	-2.423652
C	6.551614	2.750465	-0.282156
H	6.655221	1.454178	-3.457180
H	7.077804	3.463887	0.370931
C	6.997693	2.535754	-1.597641
H	7.875071	3.079755	-1.980202
O	2.226626	0.207342	-2.022605
O	4.272241	0.115226	2.139285
C	5.376937	-2.883112	2.092575
C	5.573424	-2.886425	0.687363
C	4.088407	-3.021211	2.620336
H	6.590719	-2.792934	0.277427
H	3.930034	-3.014039	3.708676
C	4.489274	-3.007239	-0.175035
C	2.984467	-3.125959	1.758989
H	4.666981	-3.018428	-1.259743
H	1.984688	-3.238560	2.196344
C	3.153281	-3.151704	0.331795
H	6.241565	-2.776448	2.765531
C	2.004776	-3.182985	-0.557347
H	1.677519	-1.770389	-0.278206
C	2.199413	-3.223540	-2.060275
H	1.250873	-2.998421	-2.585518
H	2.508744	-4.248460	-2.368640
H	2.966053	-2.518011	-2.432023

N	-3.459811	-0.198879	-0.219338
N	-2.767400	1.820511	0.219554
C	-2.331525	0.539696	0.014328
C	-4.590899	0.611731	-0.160177
H	-5.597049	0.211533	-0.319027
C	-4.153810	1.883382	0.116307
H	-4.700391	2.822157	0.248959
C	-3.483786	-1.624413	-0.490775
C	-3.396253	-2.056919	-1.840796
C	-3.271671	-1.089136	-3.018662
H	-3.322189	-0.055228	-2.617074
C	-3.428390	-3.448366	-2.072174
H	-3.366735	-3.824151	-3.105611
C	-3.550118	-4.359025	-1.012714
C	-3.644072	-3.897545	0.308171
H	-3.749566	-4.623511	1.129609
C	-3.616414	-2.518599	0.604651
C	-3.722235	-2.045978	2.055564
H	-3.746856	-0.935926	2.051506
C	-1.908844	2.958801	0.501073
C	-1.594222	3.249450	1.855108
C	-2.109506	2.416259	3.029534
H	-2.737525	1.597929	2.617779
C	-0.767713	4.366843	2.095058
H	-0.499256	4.625725	3.131214
C	-0.285471	5.154455	1.040381
C	-0.620105	4.842287	-0.284731
H	-0.237158	5.471789	-1.103067
C	-1.440824	3.736982	-0.591095
C	-1.801239	3.434294	-2.046320
H	-2.390813	2.493129	-2.062782
Au	-0.435573	-0.081535	0.053868
C	-5.028864	-2.528179	2.721711
H	-5.062879	-3.634336	2.808673
H	-5.115478	-2.113998	3.747501

H	-5.923503	-2.209819	2.148275
C	-2.481728	-2.467295	2.873145
H	-2.551748	-2.085152	3.912628
H	-2.388624	-3.572459	2.929642
H	-1.548800	-2.065267	2.424524
C	-0.948766	1.753210	3.802213
H	-0.283199	2.509922	4.267812
H	-1.341945	1.111363	4.617858
H	-0.325372	1.120601	3.136317
C	-3.007996	3.253154	3.966269
H	-2.441209	4.078595	4.445450
H	-3.861258	3.706531	3.420983
H	-3.419451	2.618694	4.778593
C	-2.694357	4.545267	-2.642290
H	-3.618972	4.694768	-2.047397
H	-2.160826	5.518175	-2.678515
H	-2.993171	4.290001	-3.680232
C	-0.544908	3.196891	-2.910936
H	0.085432	4.108244	-2.977497
H	0.084750	2.378903	-2.504683
H	-0.835552	2.922751	-3.946324
C	-4.440953	-1.248782	-4.014410
H	-5.424369	-1.123619	-3.516547
H	-4.367503	-0.490612	-4.821289
H	-4.435438	-2.247695	-4.498632
C	-1.905157	-1.234411	-3.722868
H	-1.066009	-1.053102	-3.018586
H	-1.778203	-2.247984	-4.158576
H	-1.814434	-0.502477	-4.551916
H	0.355719	6.024073	1.253862
H	-3.582414	-5.440420	-1.219667
C	0.677455	-3.754093	-0.094779
H	-0.171970	-3.286922	-0.635333
H	0.651879	-4.839762	-0.343718
H	0.492338	-3.658124	0.990150

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N	-1.951636	0.690581	0.927623
N	-0.088747	1.813823	1.076212
C	-0.660009	0.725267	0.475062
C	-2.185902	1.745889	1.803836
H	-3.160460	1.896806	2.278508
C	-1.012986	2.453438	1.897301
H	-0.753129	3.349357	2.469733
C	-2.942626	-0.306058	0.559224
C	-3.742758	-0.072165	-0.590627
C	-3.607180	1.177940	-1.461409
H	-2.833826	1.830892	-1.004165
C	-4.699112	-1.056237	-0.917234
H	-5.339603	-0.913147	-1.801573
C	-4.854964	-2.207682	-0.132818
C	-4.056499	-2.401374	1.003233
H	-4.196668	-3.306107	1.615288
C	-3.080204	-1.456201	1.381245
C	-2.240281	-1.687982	2.638544
H	-1.509410	-0.855678	2.719817
C	1.282581	2.255648	0.891161
C	2.275865	1.761515	1.777505
C	1.968201	0.777866	2.907599
H	0.874190	0.586739	2.906052
C	3.595584	2.218543	1.580783
H	4.395351	1.860320	2.247790
C	3.905731	3.126117	0.558128
C	2.898375	3.602695	-0.292581
H	3.155054	4.322950	-1.085157
C	1.559343	3.183756	-0.147465
C	0.481646	3.734480	-1.082721
H	-0.490831	3.289707	-0.782875
Au	0.175575	-0.534563	-0.853053
C	-3.115910	-1.656062	3.910892

H	-3.858368	-2.481301	3.913973
H	-2.488022	-1.769029	4.818951
H	-3.677061	-0.703241	4.000185
C	-1.426164	-2.996256	2.549376
H	-0.787100	-3.116766	3.448643
H	-2.085298	-3.887519	2.491347
H	-0.767548	-3.001897	1.656201
C	2.665094	-0.579809	2.673284
H	3.770354	-0.475132	2.677350
H	2.395356	-1.299122	3.474329
H	2.368956	-1.020343	1.698058
C	2.326445	1.365609	4.289728
H	3.416811	1.549249	4.387291
H	1.807784	2.328930	4.472843
H	2.035930	0.662300	5.097446
C	0.343379	5.266858	-0.949843
H	0.130702	5.570882	0.095588
H	1.268899	5.790351	-1.268409
H	-0.484191	5.638647	-1.588843
C	0.738663	3.316059	-2.546319
H	1.691201	3.736860	-2.930994
H	0.791489	2.211397	-2.644502
H	-0.076134	3.681576	-3.205106
C	-4.920840	1.988455	-1.504038
H	-5.263694	2.267637	-0.486691
H	-4.780938	2.922794	-2.086112
H	-5.739953	1.416868	-1.988147
C	-3.117907	0.821199	-2.881617
H	-2.146656	0.283158	-2.847008
H	-3.845172	0.173148	-3.413989
H	-2.980748	1.739147	-3.489958
H	4.943040	3.472423	0.427740
H	-5.612297	-2.959176	-0.405859
C	1.180992	-1.493944	-2.703424
C	0.648380	-2.613807	-1.988406

C	2.572312	-1.205311	-2.578595
H	-0.387187	-2.944118	-2.170203
H	3.003204	-0.363707	-3.142393
C	1.502022	-3.408417	-1.182972
C	3.393845	-2.009850	-1.784145
H	1.081075	-4.283921	-0.662584
H	4.466925	-1.776411	-1.722529
C	2.879475	-3.131120	-1.077459
H	0.587211	-0.999296	-3.489872
C	3.761346	-4.034106	-0.230954
H	3.540139	-5.086379	-0.517835
C	5.271159	-3.787249	-0.295354
H	5.547012	-2.778521	0.076307
H	5.663924	-3.891169	-1.328169
H	5.805845	-4.524418	0.335939
H	3.413504	-3.952326	0.824414

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AuIPrPhEt2+ SCF Done: -1684.16183335 A.U.

N	1.584486	1.632970	0.587191
N	-0.540442	1.929790	0.970891
C	0.351049	1.075946	0.379517
C	1.465851	2.822418	1.300013
H	2.339659	3.424183	1.568562
C	0.127685	3.009205	1.542095
H	-0.407460	3.807256	2.066056
C	2.846657	1.063867	0.147813
C	3.575181	0.257213	1.062472
C	3.098945	-0.022430	2.489201
H	2.097106	0.440633	2.612313
C	4.800303	-0.276951	0.611703
H	5.397400	-0.904986	1.291330
C	5.274691	-0.017360	-0.681967
C	4.535967	0.793165	-1.555354
H	4.926876	0.998571	-2.564201

C	3.305430	1.360480	-1.163066
C	2.535281	2.257181	-2.133796
H	1.627240	2.625532	-1.611132
C	-1.982185	1.756986	1.000103
C	-2.753416	2.347218	-0.036454
C	-2.134552	3.153229	-1.179779
H	-1.030744	3.121071	-1.061916
C	-4.152589	2.181310	0.031589
H	-4.787234	2.627810	-0.749924
C	-4.749981	1.468745	1.081203
C	-3.959060	0.904925	2.092247
H	-4.442657	0.355750	2.915279
C	-2.554607	1.036393	2.081522
C	-1.721456	0.422355	3.207503
H	-0.654977	0.663457	3.013020
Au	-0.051154	-0.609723	-0.647585
C	3.361741	3.496727	-2.540343
H	4.272718	3.214202	-3.108098
H	2.761506	4.166399	-3.190482
H	3.686846	4.081031	-1.655262
C	2.057524	1.466914	-3.370886
H	1.463093	2.117816	-4.045045
H	2.911913	1.069657	-3.957869
H	1.420472	0.606448	-3.073787
C	-2.459765	2.535348	-2.556134
H	-3.549302	2.552370	-2.767866
H	-1.957717	3.104234	-3.365905
H	-2.118297	1.480783	-2.616004
C	-2.559898	4.636962	-1.114655
H	-3.655241	4.752641	-1.252939
H	-2.296763	5.097559	-0.140341
H	-2.059437	5.220925	-1.914668
C	-2.084353	1.031674	4.579319
H	-1.972094	2.135314	4.581179
H	-3.131972	0.801720	4.865337

H	-1.426742	0.619994	5.372742
C	-1.842541	-1.116712	3.223017
H	-2.883441	-1.441638	3.431575
H	-1.538732	-1.556109	2.249781
H	-1.195139	-1.549214	4.013930
C	4.037392	0.629568	3.529083
H	4.134223	1.722934	3.368001
H	3.651573	0.468740	4.557095
H	5.057926	0.195106	3.483647
C	2.931892	-1.533356	2.754156
H	2.223452	-1.993460	2.034652
H	3.897829	-2.074504	2.675251
H	2.540331	-1.706202	3.777998
H	-5.845288	1.359041	1.116099
H	6.235550	-0.443999	-1.009999
C	0.235593	-3.721816	-0.669930
C	0.188797	-2.709442	-1.684416
C	-0.986841	-4.112198	-0.105576
H	1.101664	-2.500834	-2.268924
H	-1.002356	-4.894422	0.668155
C	-1.055107	-2.147855	-2.107075
C	-2.219792	-3.553114	-0.521617
H	-1.083366	-1.522878	-3.016693
H	-3.145015	-3.921927	-0.054168
C	-2.294261	-2.576912	-1.524636
C	-3.598923	-2.008608	-2.052271
H	-3.623530	-2.185755	-3.152062
C	-4.883847	-2.547028	-1.417922
H	-4.927732	-2.334691	-0.329549
H	-4.987570	-3.642988	-1.557972
H	-5.770063	-2.071541	-1.883219
C	1.569156	-4.353625	-0.313864
H	1.997312	-4.783791	-1.248454
H	2.274790	-3.540735	-0.030124
C	1.546963	-5.426453	0.778016

H	0.911410	-6.291333	0.496201
H	1.171808	-5.028225	1.743868
H	2.569189	-5.815725	0.955308
H	-3.563720	-0.901279	-1.943082

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AuIPrBF4 SCF Done: -1719.25652305 A.U.

N	-1.090124	1.190433	1.147124
N	1.090236	1.190395	1.147137
C	0.000050	0.676267	0.494125
C	-0.686022	2.015056	2.194964
H	-1.409413	2.523055	2.839738
C	0.686152	2.015039	2.194962
H	1.409557	2.522994	2.839757
C	-2.471930	0.902900	0.810008
C	-3.132970	1.752995	-0.115133
C	-2.430697	2.916129	-0.816722
H	-1.429797	3.038631	-0.351386
C	-4.480210	1.460330	-0.409913
H	-5.024791	2.092790	-1.128443
C	-5.134061	0.373858	0.187872
C	-4.450788	-0.450121	1.092237
H	-4.971659	-1.307871	1.545428
C	-3.101743	-0.210235	1.426253
C	-2.385945	-1.128136	2.417635
H	-1.318642	-0.823707	2.451277
C	2.472022	0.902785	0.810004
C	3.101750	-0.210415	1.426206
C	2.385875	-1.128288	2.417559
H	1.318616	-0.823711	2.451268
C	4.450792	-0.450365	1.092215
H	4.971609	-1.308156	1.545389
C	5.134133	0.373620	0.187908
C	4.480358	1.460156	-0.409846
H	5.025005	2.092628	-1.128315

C	3.133126	1.752878	-0.115096
C	2.430930	2.916094	-0.816618
H	1.430068	3.038685	-0.351221
Au	-0.000082	-0.586971	-0.996900
C	-2.957487	-0.956083	3.842897
H	-4.025224	-1.258614	3.888687
H	-2.399980	-1.589269	4.564567
H	-2.893741	0.096298	4.190700
C	-2.421245	-2.603916	1.966832
H	-1.841902	-3.231395	2.676059
H	-3.458317	-3.000901	1.951059
H	-1.987781	-2.742862	0.955586
C	2.420937	-2.604036	1.966624
H	3.457935	-3.001210	1.950904
H	1.841409	-3.231475	2.675735
H	1.987548	-2.742788	0.955316
C	2.957499	-0.956411	3.842807
H	4.025197	-1.259092	3.888538
H	2.893914	0.095955	4.190684
H	2.399936	-1.589570	4.564458
C	3.183153	4.250583	-0.633267
H	3.334954	4.492646	0.439092
H	4.182154	4.230762	-1.117454
H	2.611941	5.083116	-1.094731
C	2.201843	2.592660	-2.309777
H	3.165097	2.462646	-2.846666
H	1.619009	1.655616	-2.430698
H	1.645081	3.414093	-2.807760
C	-3.182795	4.250681	-0.633325
H	-3.334488	4.492757	0.439047
H	-2.611559	5.083172	-1.094835
H	-4.181843	4.230933	-1.117419
C	-2.201696	2.592642	-2.309878
H	-1.618913	1.655564	-2.430777
H	-3.164964	2.462666	-2.846750

H	-1.644900	3.414027	-2.807903
H	6.186191	0.161904	-0.060354
H	-6.186123	0.162183	-0.060408
B	-0.000036	-3.432613	-2.007467
F	1.155711	-3.492172	-1.235287
F	0.000016	-4.248998	-3.101203
F	-1.155560	-3.492577	-1.235042
F	-0.000332	-1.962314	-2.584551

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AuIPrCH3CNBF4 SCF Done: -1851.92535277 A.U.

N	0.145757	-1.873947	-0.586308
N	-1.902774	-1.136558	-0.640376
C	-0.630961	-0.795168	-0.250837
C	-0.629433	-2.873049	-1.167342
H	-0.191627	-3.820006	-1.496199
C	-1.920013	-2.409755	-1.205540
H	-2.842457	-2.862929	-1.580724
C	1.581983	-1.978418	-0.385140
C	2.439384	-1.647018	-1.467315
C	1.912446	-1.205955	-2.834181
H	0.854522	-0.893076	-2.698641
C	3.824769	-1.767418	-1.245402
H	4.523180	-1.486498	-2.046664
C	4.327700	-2.202129	-0.012952
C	3.454350	-2.527065	1.032002
H	3.864314	-2.854718	2.000469
C	2.058058	-2.421626	0.874871
C	1.132335	-2.757929	2.044487
H	0.084443	-2.639590	1.695451
C	-3.071926	-0.291799	-0.502562
C	-3.863861	-0.414364	0.669372
C	-3.501601	-1.361087	1.814310
H	-2.650481	-1.989309	1.477696
C	-5.003566	0.410114	0.768235

H	-5.638996	0.346248	1.665609
C	-5.337767	1.311808	-0.251974
C	-4.535710	1.408835	-1.397382
H	-4.805939	2.123900	-2.190260
C	-3.384249	0.609403	-1.554202
C	-2.514943	0.756803	-2.803504
H	-1.732980	-0.030257	-2.768051
Au	-0.074632	0.901348	0.624041
C	1.294681	-4.222788	2.503383
H	2.315744	-4.416869	2.894381
H	0.577657	-4.459338	3.317955
H	1.115513	-4.935343	1.671409
C	1.333981	-1.770819	3.214196
H	0.609689	-1.977265	4.030625
H	2.356170	-1.851243	3.639909
H	1.197879	-0.723058	2.875530
C	-3.017624	-0.566688	3.047440
H	-3.819783	0.091044	3.444497
H	-2.711797	-1.256962	3.861512
H	-2.147007	0.072097	2.789562
C	-4.659379	-2.316308	2.171213
H	-5.539491	-1.768454	2.569277
H	-4.997714	-2.898856	1.289321
H	-4.339409	-3.035662	2.953790
C	-3.322799	0.536890	-4.099892
H	-3.833813	-0.448355	-4.104230
H	-4.098956	1.318661	-4.240477
H	-2.651734	0.578114	-4.983006
C	-1.785807	2.118337	-2.810929
H	-2.506708	2.962866	-2.842624
H	-1.152252	2.239281	-1.907758
H	-1.125424	2.201566	-3.698885
C	1.926485	-2.387313	-3.832071
H	1.333071	-3.253675	-3.471373
H	1.511217	-2.075789	-4.814070

H	2.964255	-2.744798	-4.002940
C	2.670516	0.009847	-3.403236
H	2.712254	0.833251	-2.664808
H	3.712095	-0.252306	-3.685072
H	2.165208	0.370135	-4.324361
H	-6.232333	1.947013	-0.152333
H	5.416102	-2.269254	0.140037
N	0.417637	2.655137	1.550702
C	1.017662	3.588325	1.909763
C	1.856990	4.705317	2.292511
H	1.411105	5.663271	1.958603
H	2.006922	4.724825	3.390305
H	2.824839	4.524799	1.769687
B	3.261552	1.917243	-0.053451
F	3.652621	3.191209	0.454679
F	4.297812	1.342631	-0.789675
F	2.886173	1.076675	1.034066
F	2.109649	2.101426	-0.895423

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BF4- SCF Done: -424.180119353 A.U.

B	0.000000	0.000000	0.000000
F	0.819664	0.819664	0.819664
F	-0.819664	-0.819664	0.819664
F	-0.819664	0.819664	-0.819664
F	0.819664	-0.819664	-0.819664

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CH3CN SCF Done: -132.652040075 A.U.

N	1.449344	0.000006	-0.000006
C	0.277910	-0.000014	0.000013
C	-1.183297	0.000002	-0.000002
H	-1.571050	-0.906258	0.508190
H	-1.571018	0.893261	0.530738
H	-1.571020	0.013028	-1.038955

5.2 xyz coordinates and absolute energies (in a.u.) of all the computed species for the benchmark study.

5.2.1 TPSSh

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AuIPrCH3CN+ SCF Done: -1427.59819183 A.U.

N	-1.083178	0.099634	-1.467872
N	1.082721	0.099610	-1.468069
C	-0.000156	0.045645	-0.648169
C	-0.682296	0.186861	-2.791172
H	-1.399994	0.240115	-3.603939
C	0.681602	0.186828	-2.791297
H	1.399152	0.240054	-3.604195
C	-2.462903	0.067696	-1.024207
C	-3.100449	-1.186703	-0.907413
C	-2.402942	-2.504586	-1.227279
H	-1.368108	-2.277165	-1.527503
C	-4.438353	-1.185262	-0.483601
H	-4.968607	-2.134834	-0.381296
C	-5.103682	0.007022	-0.196355
C	-4.445473	1.230065	-0.329175
H	-4.981274	2.155765	-0.107178
C	-3.107700	1.293323	-0.748711
C	-2.418382	2.645182	-0.899941
H	-1.379727	2.463248	-1.217525
C	2.462528	0.067681	-1.024656
C	3.107393	1.293322	-0.749368
C	2.418062	2.645180	-0.900546
H	1.379191	2.463213	-1.217405
C	4.445272	1.230083	-0.330165
H	4.981132	2.155796	-0.108366
C	5.103509	0.007042	-0.197444
C	4.438093	-1.185258	-0.484426
H	4.968361	-2.134830	-0.382190

C	3.100084	-1.186718	-0.907908
C	2.402499	-2.504616	-1.227532
H	1.367512	-2.277225	-1.527255
Au	0.000119	-0.086452	1.344922
C	-3.089003	3.496239	-1.994360
H	-4.130500	3.740155	-1.731385
H	-2.545978	4.445245	-2.126598
H	-3.101490	2.970746	-2.961837
C	-2.357584	3.401471	0.439364
H	-1.808195	4.348421	0.318081
H	-3.365401	3.645659	0.810963
H	-1.847099	2.803566	1.210889
C	2.358179	3.401918	0.438544
H	3.366237	3.646296	0.809359
H	1.808679	4.348809	0.317308
H	1.848265	2.804288	1.210656
C	3.088054	3.495830	-1.995673
H	4.129760	3.739672	-1.733457
H	3.099828	2.970053	-2.963005
H	2.545068	4.444869	-2.127828
C	3.074796	-3.221805	-2.412956
H	3.098273	-2.582640	-3.309177
H	4.112433	-3.504842	-2.175144
H	2.525598	-4.143097	-2.663090
C	2.326730	-3.417111	0.009854
H	3.330312	-3.710378	0.356592
H	1.813049	-2.913643	0.844208
H	1.773369	-4.339045	-0.229118
C	-3.075743	-3.221921	-2.412326
H	-3.099697	-2.582823	-3.308581
H	-2.526581	-4.143182	-2.662651
H	-4.113242	-3.505035	-2.174007
C	-2.326545	-3.416965	0.010155
H	-1.812436	-2.913387	0.844182
H	-3.329960	-3.710178	0.357426

H	-1.773298	-4.338921	-0.228997
H	6.146244	-0.016785	0.127168
H	-6.146326	-0.016820	0.128549
N	0.000615	-0.221354	3.376692
C	0.001018	-0.298314	4.531629
C	0.001629	-0.395073	5.980930
H	1.036506	-0.481149	6.344337
H	-0.462079	0.505080	6.411258
H	-0.568877	-1.282952	6.291856

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AuIPr+ SCF Done: -1294.85653608 A.U.

N	1.089661	-0.000229	1.103171
N	-1.089846	-0.000222	1.102986
C	-0.000025	-0.000161	0.301301
C	0.682361	-0.000494	2.427871
H	1.399905	-0.000632	3.242795
C	-0.682770	-0.000466	2.427756
H	-1.400452	-0.000581	3.242558
C	2.469237	-0.000092	0.648936
C	3.105451	-1.244694	0.448144
C	2.414577	-2.582504	0.690072
H	1.378072	-2.380133	1.004194
C	4.439763	-1.210625	0.014614
H	4.971965	-2.149510	-0.153318
C	5.098941	0.000162	-0.200753
C	4.439642	1.210822	0.014959
H	4.971750	2.149808	-0.152707
C	3.105328	1.244633	0.448503
C	2.414317	2.582307	0.690798
H	1.377847	2.379747	1.004910
C	-2.469345	-0.000073	0.648518
C	-3.105383	1.244658	0.447955
C	-2.414394	2.582325	0.690353
H	-1.377973	2.379753	1.004622

C	-4.439622	1.210860	0.014181
H	-4.971686	2.149851	-0.153593
C	-5.098903	0.000207	-0.201625
C	-4.439781	-1.210587	0.013877
H	-4.971969	-2.149466	-0.154131
C	-3.105544	-1.244669	0.447636
C	-2.414733	-2.582487	0.689704
H	-1.378282	-2.380129	1.004011
Au	0.000141	0.000171	-1.673755
C	3.092239	3.362946	1.832563
H	4.130946	3.625015	1.577002
H	2.548849	4.300407	2.028613
H	3.113399	2.777039	2.764490
C	2.343138	3.423110	-0.596753
H	1.793060	4.358936	-0.411459
H	3.347440	3.692608	-0.959330
H	1.829262	2.876897	-1.404130
C	-2.343012	3.423131	-0.597184
H	-3.347255	3.692643	-0.959911
H	-1.792950	4.358950	-0.411804
H	-1.829021	2.876915	-1.404487
C	-3.092481	3.362967	1.832018
H	-4.131148	3.625043	1.576301
H	-3.113785	2.777059	2.763941
H	-2.549114	4.300424	2.028151
C	-3.092911	-3.363315	1.831188
H	-3.114128	-2.777629	2.763252
H	-4.131616	-3.625193	1.575418
H	-2.549666	-4.300892	2.027089
C	-2.343478	-3.422993	-0.598037
H	-3.347762	-3.692288	-0.960814
H	-1.829428	-2.876651	-1.405216
H	-1.793536	-4.358928	-0.412889
C	3.092539	-3.363352	1.831671

H	3.113595	-2.777675	2.763745
H	2.549247	-4.300924	2.027465
H	4.131286	-3.625240	1.576086
C	2.343540	-3.422997	-0.597689
H	1.829644	-2.876639	-1.404956
H	3.347884	-3.692305	-0.960289
H	1.793549	-4.358924	-0.412649
H	-6.138342	0.000318	-0.536977
H	6.138438	0.000262	-0.535926

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CH3CN SCF Done: -132.662455280 A.U.

N	1.441420	0.000004	0.000005
C	0.279338	-0.000010	-0.000011
C	-1.180861	0.000002	0.000003
H	-1.560273	-0.686304	-0.771540
H	-1.560268	-0.325018	0.980136
H	-1.560257	1.011337	-0.208584

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I-EtX SCF Done: -2227.73102576 A.U.

N	3.552028	0.785250	-0.270042
N	3.236832	-1.358088	-0.251872
C	2.594293	-0.167491	-0.119947
C	4.785037	0.197045	-0.493700
H	5.683944	0.788647	-0.637021
C	4.586466	-1.153199	-0.483594
H	5.275868	-1.980669	-0.620019
C	3.320446	2.214944	-0.194144
C	3.022133	2.910015	-1.386333
C	2.935205	2.224333	-2.745463
H	3.026188	1.138723	-2.583315
C	2.820021	4.294818	-1.282473
H	2.588716	4.870454	-2.181371
C	2.911291	4.948041	-0.053058

C	3.209753	4.230213	1.105585
H	3.282805	4.756086	2.060286
C	3.425144	2.844061	1.065727
C	3.765536	2.087930	2.345682
H	3.884489	1.023268	2.090507
C	2.601382	-2.659193	-0.177922
C	2.490020	-3.282012	1.084295
C	3.007317	-2.648153	2.370983
H	3.406858	-1.652575	2.122095
C	1.883112	-4.547075	1.119292
H	1.778872	-5.064243	2.075762
C	1.418001	-5.157690	-0.045838
C	1.548813	-4.515627	-1.277964
H	1.185384	-5.008529	-2.182579
C	2.145158	-3.248987	-1.377136
C	2.285846	-2.575814	-2.738460
H	2.763700	-1.595551	-2.585490
Au	0.646533	0.132790	0.249042
C	5.102422	2.566720	2.941639
H	5.050320	3.623618	3.247526
H	5.357687	1.972532	3.833116
H	5.924790	2.467455	2.216278
C	2.626769	2.182413	3.377112
H	2.871230	1.588250	4.271750
H	2.461320	3.222037	3.701390
H	1.680389	1.802077	2.960639
C	1.877040	-2.441459	3.395205
H	1.448863	-3.401713	3.723564
H	2.263016	-1.926426	4.289006
H	1.060870	-1.834274	2.972930
C	4.164587	-3.468913	2.970546
H	3.830775	-4.476680	3.264420
H	4.990732	-3.585168	2.251936
H	4.559897	-2.971217	3.869983
C	3.199589	-3.388867	-3.674203

H	4.194144	-3.546629	-3.228877
H	2.769812	-4.378844	-3.894643
H	3.332407	-2.860850	-4.631512
C	0.913164	-2.314121	-3.384089
H	0.379991	-3.254974	-3.593865
H	0.274904	-1.701463	-2.728188
H	1.036944	-1.780234	-4.339483
C	4.101822	2.652275	-3.656049
H	5.077109	2.435700	-3.192716
H	4.053087	2.117667	-4.617796
H	4.064642	3.732436	-3.869221
C	1.575913	2.469635	-3.424406
H	0.740951	2.166643	-2.774314
H	1.437141	3.532462	-3.678240
H	1.513023	1.895597	-4.362396
H	0.954482	-6.145511	0.006013
H	2.752373	6.027376	0.002008
N	-1.348023	0.465229	0.669869
C	-2.129222	1.542425	-0.027711
N	-3.373408	1.481033	0.549781
C	-3.389668	0.469896	1.513860
N	-2.044076	-0.137980	1.515609
C	-4.492594	2.326525	0.217102
C	-5.744267	1.742418	-0.004136
C	-4.299710	3.709442	0.125991
H	-5.877878	0.662171	0.067277
H	-3.315641	4.145686	0.303160
C	-6.824318	2.571993	-0.316831
C	-5.388359	4.521502	-0.200537
H	-7.806623	2.127092	-0.487148
H	-5.248893	5.601586	-0.277916
C	-6.649488	3.956089	-0.418049
H	-7.498080	4.596634	-0.666969
O	-4.275349	0.109958	2.229564
O	-1.661057	2.240231	-0.877551

C	-7.738215	-1.694729	-0.361143
C	-7.249304	-1.979704	0.919342
C	-6.884728	-1.807615	-1.465459
H	-7.905869	-1.897665	1.788590
H	-7.259165	-1.594715	-2.469729
C	-5.921719	-2.379696	1.088584
C	-5.553233	-2.204733	-1.292979
H	-5.551388	-2.608391	2.091332
H	-4.910637	-2.296986	-2.170931
C	-5.049688	-2.503926	-0.015560
H	-8.779849	-1.395342	-0.499204
C	-3.624056	-2.958541	0.220472
H	-3.132287	-2.237654	0.907255
H	-3.653389	-3.897511	0.801369
C	-2.747926	-3.152475	-1.014948
H	-2.631993	-2.217857	-1.588977
H	-3.170460	-3.908673	-1.695175
H	-1.742607	-3.490170	-0.720604

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III-EtX SCF Done: -2227.77353359 A.U.

N	3.293011	-0.151629	0.528208
N	2.537759	1.806963	-0.008369
C	2.176872	0.503041	0.115651
C	4.348934	0.736436	0.662580
H	5.333214	0.410787	0.984593
C	3.873415	1.969456	0.324763
H	4.357848	2.940420	0.291464
C	3.362490	-1.574569	0.794904
C	3.075644	-2.026815	2.101605
C	2.710827	-1.085573	3.244704
H	2.692357	-0.059066	2.846423
C	3.150604	-3.410215	2.327633
H	2.937901	-3.801405	3.325080
C	3.497626	-4.292293	1.303704

C	3.781419	-3.810397	0.025099
H	4.058944	-4.512358	-0.764610
C	3.723278	-2.437975	-0.262754
C	4.048746	-1.937655	-1.666213
H	3.941011	-0.841724	-1.669520
C	1.644203	2.871256	-0.420776
C	1.536384	3.160577	-1.798807
C	2.333581	2.417930	-2.866152
H	2.962195	1.668122	-2.360987
C	0.654360	4.187456	-2.168719
H	0.540723	4.442811	-3.224735
C	-0.075448	4.891978	-1.210365
C	0.063594	4.587602	0.144266
H	-0.506479	5.154076	0.884133
C	0.928090	3.569331	0.576114
C	1.075267	3.273725	2.065066
H	1.762620	2.420458	2.175746
Au	0.369395	-0.276309	-0.218616
C	5.505033	-2.255154	-2.053136
H	5.681860	-3.341438	-2.097034
H	5.735920	-1.838212	-3.045991
H	6.215429	-1.828355	-1.328408
C	3.059320	-2.494657	-2.705686
H	3.276625	-2.079273	-3.702399
H	3.125909	-3.591713	-2.778967
H	2.021247	-2.234424	-2.442910
C	1.408731	1.657863	-3.833633
H	0.750618	2.344394	-4.389080
H	2.002308	1.091845	-4.568676
H	0.771710	0.943960	-3.286042
C	3.277331	3.368263	-3.626238
H	2.714648	4.133198	-4.184205
H	3.960831	3.889145	-2.938154
H	3.884617	2.804158	-4.351415
C	1.705357	4.467857	2.806825

H	2.681347	4.740840	2.376218
H	1.056712	5.356866	2.758237
H	1.856172	4.220536	3.869338
C	-0.264228	2.863059	2.702158
H	-1.004928	3.676565	2.649205
H	-0.693580	1.980544	2.203141
H	-0.118728	2.614956	3.765215
C	3.774187	-1.124398	4.358372
H	4.774526	-0.877690	3.969871
H	3.524588	-0.399324	5.148797
H	3.831139	-2.120887	4.824335
C	1.306167	-1.383177	3.799822
H	0.538218	-1.310801	3.013941
H	1.251622	-2.392473	4.237923
H	1.050972	-0.662670	4.592692
H	-0.752933	5.690019	-1.522373
H	3.553534	-5.364434	1.505384
N	-1.624352	-1.034904	-0.635264
C	-2.481578	-0.507613	0.461414
N	-3.317041	0.421440	-0.106340
C	-3.073414	0.570992	-1.493556
N	-2.150044	-0.417001	-1.811143
C	-4.288043	1.188279	0.624978
C	-4.346160	2.575355	0.443177
C	-5.161816	0.534135	1.501169
H	-3.665363	3.066954	-0.251888
H	-5.107878	-0.547884	1.623390
C	-5.299575	3.311876	1.151020
C	-6.099600	1.286396	2.212424
H	-5.357764	4.392962	1.008032
H	-6.782216	0.783109	2.900250
C	-6.172591	2.672422	2.037352
H	-6.913231	3.254391	2.589934
O	-3.548979	1.380961	-2.242182
O	-2.388877	-0.872791	1.602618

C	-5.836433	-3.857378	-1.177947
C	-5.078383	-3.538497	-2.309018
C	-5.257683	-3.773284	0.093020
H	-5.520060	-3.612131	-3.305107
H	-5.841354	-4.034855	0.978579
C	-3.749129	-3.131647	-2.166336
C	-3.927786	-3.366642	0.236823
H	-3.159281	-2.894617	-3.055434
H	-3.490609	-3.313394	1.235268
C	-3.158165	-3.034494	-0.893888
H	-6.874273	-4.179970	-1.287150
C	-1.713905	-2.588920	-0.776250
H	-1.473571	-0.216198	-2.545714
H	-1.219638	-2.747417	-1.745759
C	-0.897457	-3.275089	0.312068
H	-1.292406	-3.079795	1.316428
H	0.153233	-2.943805	0.280950
H	-0.921406	-4.358876	0.126127

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PhEt1 SCF Done: -310.689771291 A.U.

C	-0.234268	-2.330947	0.000000
C	-0.235092	-1.625902	1.208316
C	-0.235092	-1.625902	-1.208316
H	-0.240055	-2.167150	2.158003
H	-0.240055	-2.167150	-2.158003
C	-0.235092	-0.227369	1.205426
C	-0.235092	-0.227369	-1.205426
H	-0.241110	0.315201	2.155694
H	-0.241110	0.315201	-2.155694
C	-0.234744	0.495079	0.000000
H	-0.237437	-3.423728	0.000000
C	-0.191024	2.008793	0.000000
H	-0.730205	2.389125	-0.883773
H	-0.730205	2.389125	0.883773

C	1.239762	2.569375	0.000000
H	1.796250	2.231780	-0.888760
H	1.796250	2.231780	0.888760
H	1.231537	3.671256	0.000000

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TSI-EtX SCF Done: -2227.71751593 A.U.

N	-3.040743	1.399933	0.436783
N	-3.499713	-0.578750	-0.309648
C	-2.465445	0.237840	0.024052
C	-4.422734	1.310964	0.362907
H	-5.066852	2.136177	0.650307
C	-4.710850	0.063966	-0.107269
H	-5.658593	-0.422581	-0.315846
C	-2.309052	2.560688	0.898360
C	-2.018064	2.666662	2.276067
C	-2.447599	1.616770	3.295161
H	-2.993413	0.826372	2.757413
C	-1.306393	3.802060	2.694426
H	-1.065727	3.922685	3.753257
C	-0.911066	4.782805	1.783758
C	-1.221134	4.650831	0.429260
H	-0.916494	5.432217	-0.271091
C	-1.929703	3.537053	-0.048544
C	-2.265823	3.425131	-1.531742
H	-2.816014	2.483913	-1.683937
C	-3.356855	-1.930806	-0.813082
C	-3.279137	-2.120204	-2.210039
C	-3.330398	-0.967574	-3.207289
H	-3.422962	-0.029666	-2.637608
C	-3.153038	-3.440097	-2.669340
H	-3.089646	-3.629752	-3.743298
C	-3.109897	-4.513120	-1.778632
C	-3.191990	-4.290451	-0.403934
H	-3.158170	-5.140202	0.281383

C	-3.317622	-2.993040	0.116019
C	-3.424014	-2.780612	1.622103
H	-3.418124	-1.695652	1.811423
Au	-0.510213	-0.185463	-0.061455
C	-3.185658	4.572839	-1.987599
H	-2.688348	5.551001	-1.889911
H	-3.462547	4.442490	-3.045550
H	-4.111542	4.606104	-1.392828
C	-0.992744	3.349594	-2.393825
H	-1.256830	3.219608	-3.455172
H	-0.395168	4.271903	-2.309787
H	-0.360185	2.499468	-2.092562
C	-2.030573	-0.874316	-4.026790
H	-1.879869	-1.772513	-4.646432
H	-2.066714	-0.004903	-4.702462
H	-1.153549	-0.764612	-3.369709
C	-4.564673	-1.070241	-4.122246
H	-4.528646	-1.978190	-4.744934
H	-5.497417	-1.101210	-3.537852
H	-4.612433	-0.202387	-4.798877
C	-4.755138	-3.334351	2.165071
H	-5.620146	-2.874226	1.662077
H	-4.822501	-4.424073	2.017840
H	-4.840792	-3.135266	3.245090
C	-2.220162	-3.379283	2.371247
H	-2.191154	-4.476365	2.275964
H	-1.267546	-2.981740	1.989413
H	-2.289734	-3.143765	3.445243
C	-3.411277	2.208821	4.340106
H	-4.296940	2.656070	3.862808
H	-3.754395	1.422159	5.030197
H	-2.922436	2.991371	4.941961
C	-1.231625	0.952068	3.965474
H	-0.570677	0.488256	3.216272
H	-0.640509	1.681953	4.541730

H	-1.562417	0.165653	4.661975
H	-3.013361	-5.532384	-2.159437
H	-0.366255	5.662715	2.134128
N	1.509646	-0.614928	-0.150325
C	2.091522	-1.764199	0.452312
N	3.428838	-1.783642	0.026246
C	3.666873	-0.682877	-0.780474
N	2.391543	0.027368	-0.884026
C	4.395754	-2.787209	0.368856
C	5.307868	-3.222549	-0.601333
C	4.413643	-3.316828	1.665682
H	5.287566	-2.801234	-1.606412
H	3.692843	-2.978303	2.409848
C	6.251138	-4.194789	-0.259860
C	5.355419	-4.297814	1.986429
H	6.965977	-4.534191	-1.012390
H	5.368260	-4.718214	2.994220
C	6.276386	-4.736207	1.029548
H	7.012301	-5.500451	1.287953
O	4.679082	-0.311717	-1.314202
O	1.506604	-2.562010	1.139178
C	6.671942	3.552917	-1.618524
C	5.406862	3.940754	-2.089738
C	6.782930	2.714481	-0.500966
H	5.325038	4.594541	-2.960349
H	7.768272	2.413750	-0.139783
C	4.261717	3.492942	-1.444665
C	5.638982	2.258378	0.146852
H	3.275345	3.794203	-1.807249
H	5.739657	1.604888	1.014534
C	4.351305	2.650974	-0.303225
H	7.572705	3.905104	-2.126204
C	3.123553	2.200133	0.332866
H	2.717513	1.185970	-0.449695

H	2.244543	2.807731	0.064176
C	3.066381	1.648921	1.730931
H	2.141870	1.066857	1.882429
H	3.033887	2.478887	2.458635
H	3.929021	1.015187	1.980790

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UrN2 SCF Done: -622.106088168 A.U.

N	0.000000	-0.619875	2.986983
C	0.004346	-1.128052	1.583966
N	0.000000	0.000000	0.766046
C	-0.004346	1.128052	1.583966
N	0.000000	0.619875	2.986983
C	0.000000	0.000000	-0.665466
C	-0.711155	0.989759	-1.358088
C	0.711155	-0.989759	-1.358088
H	-1.254319	1.760477	-0.812137
H	1.254319	-1.760477	-0.812137
C	-0.700865	0.985516	-2.755038
C	0.700865	-0.985516	-2.755038
H	-1.250878	1.759274	-3.295166
H	1.250878	-1.759274	-3.295166
C	0.000000	0.000000	-3.457338
H	0.000000	0.000000	-4.549513
O	-0.016885	2.288284	1.291923
O	0.016885	-2.288284	1.291923

5.2.2 PBEPBE

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AuIPrCH3CN+ SCF Done: -1425.85811749 A.U.

N	-1.088400	0.000169	-1.495442
N	1.087754	0.000173	-1.495766
C	-0.000200	-0.000023	-0.670017
C	-0.686627	0.000282	-2.824335
H	-1.409816	0.000384	-3.645270

C	0.685588	0.000285	-2.824539
H	1.408533	0.000390	-3.645690
C	-2.468562	0.000171	-1.053020
C	-3.112131	-1.247779	-0.854934
C	-2.410019	-2.586538	-1.069060
H	-1.396729	-2.380881	-1.472822
C	-4.454267	-1.214365	-0.428747
H	-4.990495	-2.161031	-0.262936
C	-5.118215	0.000169	-0.216773
C	-4.454166	1.214706	-0.428420
H	-4.990317	2.161370	-0.262358
C	-3.112030	1.248121	-0.854608
C	-2.409793	2.586874	-1.068362
H	-1.396589	2.381234	-1.472349
C	2.468050	0.000195	-1.053761
C	3.111558	1.248156	-0.855540
C	2.409231	2.586904	-1.069009
H	1.395691	2.381242	-1.472140
C	4.453864	1.214761	-0.429882
H	4.990054	2.161438	-0.264011
C	5.118027	0.000233	-0.218538
C	4.454012	-1.214313	-0.430244
H	4.990318	-2.160974	-0.264655
C	3.111708	-1.247746	-0.855903
C	2.409561	-2.586523	-1.069795
H	1.395930	-2.380868	-1.472700
Au	0.000202	-0.000277	1.322398
C	-3.141168	3.460284	-2.104580
H	-4.154018	3.749199	-1.756918
H	-2.576786	4.396851	-2.288139
H	-3.257379	2.935514	-3.074035
C	-2.221080	3.332872	0.266830
H	-1.663340	4.278670	0.109736
H	-3.196189	3.591807	0.728262
H	-1.655009	2.716748	0.996160

C	2.221634	3.333235	0.266152
H	3.197111	3.592343	0.726704
H	1.663743	4.278978	0.109277
H	1.656212	2.717310	0.996149
C	3.139863	3.460004	-2.106019
H	4.153049	3.748820	-1.759254
H	3.255187	2.935026	-3.075468
H	2.575472	4.396622	-2.289291
C	3.140197	-3.459082	-2.107259
H	3.255282	-2.933699	-3.076517
H	4.153489	-3.747845	-1.760758
H	2.575951	-4.395732	-2.290817
C	2.222281	-3.333422	0.265089
H	3.197864	-3.592565	0.725396
H	1.656863	-2.717885	0.995416
H	1.664519	-4.279191	0.107913
C	-3.141359	-3.459472	-2.105706
H	-3.257342	-2.934337	-3.074990
H	-2.577087	-4.396057	-2.289513
H	-4.154307	-3.748357	-1.758305
C	-2.221599	-3.333052	0.265882
H	-1.655560	-2.717267	0.995523
H	-3.196807	-3.592043	0.727074
H	-1.663952	-4.278859	0.108522
H	6.168153	0.000248	0.110828
H	-6.168198	0.000168	0.113045
N	0.000814	-0.000525	3.354288
C	0.001185	-0.000707	4.520741
C	0.001703	-0.000968	5.968601
H	1.043044	-0.044464	6.346711
H	-0.480993	0.922244	6.348069
H	-0.556180	-0.880943	6.347700

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AuIPr+ SCF Done: -1293.29283509 A.U.

N	1.095792	-0.000125	1.133807
N	-1.095978	-0.000126	1.133628
C	-0.000027	0.000028	0.329436
C	0.686462	-0.000262	2.461275
H	1.409727	-0.000368	3.282514
C	-0.686865	-0.000264	2.461163
H	-1.410265	-0.000371	3.282283
C	2.475914	-0.000108	0.682970
C	3.114440	-1.250139	0.480812
C	2.411608	-2.588950	0.691727
H	1.404001	-2.386735	1.112550
C	4.453913	-1.215148	0.046707
H	4.989220	-2.161186	-0.124494
C	5.116066	-0.000065	-0.167914
C	4.453979	1.214996	0.047036
H	4.989336	2.161051	-0.123911
C	3.114506	1.249942	0.481147
C	2.411740	2.588733	0.692406
H	1.404112	2.386455	1.113148
C	-2.476026	-0.000105	0.682564
C	-3.114579	1.249947	0.480626
C	-2.411843	2.588737	0.691997
H	-1.404284	2.386457	1.112903
C	-4.453978	1.215005	0.046289
H	-4.989302	2.161061	-0.124754
C	-5.116035	-0.000055	-0.168763
C	-4.453925	-1.215140	0.045978
H	-4.989208	-2.161176	-0.125306
C	-3.114524	-1.250134	0.480307
C	-2.411730	-2.588947	0.691340
H	-1.404206	-2.386735	1.112362
Au	0.000131	0.000272	-1.638969
C	3.154535	3.475013	1.709660
H	4.160361	3.765285	1.343876
H	2.588644	4.410726	1.891797

H	3.287442	2.960402	2.682305
C	2.204975	3.321126	-0.647937
H	1.647652	4.267500	-0.494466
H	3.173170	3.575782	-1.125354
H	1.631305	2.698411	-1.366700
C	-2.204857	3.321128	-0.648312
H	-3.172974	3.575788	-1.125887
H	-1.647557	4.267501	-0.494751
H	-1.631073	2.698411	-1.366982
C	-3.154801	3.475018	1.709129
H	-4.160569	3.765289	1.343182
H	-3.287866	2.960409	2.681754
H	-2.588940	4.410732	1.891356
C	-3.154699	-3.475560	1.708175
H	-3.287850	-2.961237	2.680939
H	-4.160429	-3.765784	1.342086
H	-2.588796	-4.411294	1.890167
C	-2.204628	-3.320945	-0.649167
H	-3.172704	-3.575505	-1.126877
H	-1.630821	-2.697999	-1.367621
H	-1.647300	-4.267341	-0.495842
C	3.154384	-3.475542	1.708722
H	3.287338	-2.961202	2.681505
H	2.588452	-4.411278	1.890617
H	4.160188	-3.765761	1.342836
C	2.204768	-3.320973	-0.648806
H	1.631102	-2.698040	-1.367384
H	3.172937	-3.575542	-1.126323
H	1.647410	-4.267365	-0.495573
H	-6.163539	-0.000035	-0.505952
H	6.163626	-0.000048	-0.504926

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CH3CN SCF Done: -132.484301916 A.U.

N	1.447707	-0.000015	0.000038

C	0.276834	0.000033	-0.000087
C	-1.181405	-0.000007	0.000020
H	-1.568765	-0.393583	0.960822
H	-1.568877	1.028822	-0.139506
H	-1.568877	-0.635293	-0.821180

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I-EtX SCF Done: -2224.99512025 A.U.

N	3.564881	0.751183	-0.249354
N	3.193465	-1.391630	-0.323951
C	2.578747	-0.186554	-0.132829
C	4.783373	0.141370	-0.510113
H	5.703264	0.720325	-0.635128
C	4.549257	-1.210855	-0.558407
H	5.221719	-2.054803	-0.738808
C	3.372238	2.181057	-0.107216
C	3.049438	2.935769	-1.263095
C	2.884572	2.309211	-2.645135
H	2.994981	1.210049	-2.536799
C	2.884245	4.324271	-1.093205
H	2.634266	4.946919	-1.965460
C	3.032027	4.924486	0.163024
C	3.349604	4.148088	1.284426
H	3.462575	4.633911	2.265428
C	3.530721	2.755334	1.179757
C	3.862869	1.931115	2.421482
H	4.041869	0.883834	2.099982
C	2.523793	-2.676561	-0.304617
C	2.405673	-3.357620	0.933318
C	2.937682	-2.790517	2.246863
H	3.445974	-1.829547	2.023111
C	1.754093	-4.606624	0.916205
H	1.642497	-5.168253	1.856052
C	1.252420	-5.147067	-0.274190
C	1.390314	-4.448866	-1.480719

H	0.995122	-4.888027	-2.409231
C	2.031113	-3.195379	-1.529247
C	2.151860	-2.447050	-2.854856
H	2.776221	-1.545650	-2.683396
Au	0.642535	0.141592	0.244069
C	5.151583	2.418935	3.108920
H	5.042067	3.449821	3.503225
H	5.403736	1.763821	3.967193
H	6.013812	2.417199	2.412222
C	2.674442	1.905310	3.402372
H	2.904388	1.263979	4.277648
H	2.441010	2.920767	3.783278
H	1.759004	1.507921	2.916666
C	1.787911	-2.477451	3.223861
H	1.245201	-3.398014	3.521818
H	2.180590	-2.008086	4.148824
H	1.049755	-1.782786	2.772075
C	3.986262	-3.719896	2.886436
H	3.546812	-4.696645	3.174896
H	4.829663	-3.923339	2.196374
H	4.400456	-3.260230	3.806519
C	2.860613	-3.288903	-3.931726
H	3.860358	-3.628647	-3.594408
H	2.274074	-4.190567	-4.202316
H	2.995841	-2.695303	-4.858328
C	0.773556	-1.955046	-3.338584
H	0.090207	-2.804649	-3.544598
H	0.288378	-1.305737	-2.580389
H	0.874841	-1.370672	-4.275847
C	3.987075	2.785204	-3.610730
H	5.000671	2.560160	-3.221602
H	3.881413	2.288943	-4.596817
H	3.931105	3.879904	-3.781461
C	1.478736	2.566769	-3.219747
H	0.683288	2.231156	-2.523907

H	1.311953	3.644614	-3.422333
H	1.351204	2.028638	-4.181231
H	0.752800	-6.127738	-0.262752
H	2.899899	6.011905	0.269486
N	-1.347872	0.486128	0.647583
C	-2.114374	1.561656	-0.049648
N	-3.378254	1.495077	0.509493
C	-3.406112	0.465358	1.465942
N	-2.065243	-0.136211	1.489628
C	-4.488208	2.342809	0.167670
C	-5.763303	1.774552	0.001339
C	-4.277546	3.723684	0.007642
H	-5.916608	0.693844	0.125512
H	-3.275142	4.153858	0.139467
C	-6.840172	2.611785	-0.323344
C	-5.364104	4.543180	-0.328648
H	-7.841542	2.174285	-0.450682
H	-5.205828	5.624095	-0.458129
C	-6.645092	3.991811	-0.490948
H	-7.494840	4.641142	-0.749157
O	-4.320454	0.088058	2.156188
O	-1.639744	2.282321	-0.891812
C	-7.576207	-1.783747	-0.200609
C	-7.060784	-2.066069	1.074487
C	-6.724786	-1.830385	-1.322197
H	-7.717184	-2.034098	1.956982
H	-7.126198	-1.618732	-2.325091
C	-5.707298	-2.397238	1.224688
C	-5.369213	-2.156800	-1.170984
H	-5.309250	-2.624972	2.225509
H	-4.725272	-2.198708	-2.061594
C	-4.835390	-2.454901	0.102674
H	-8.641137	-1.535399	-0.325837
C	-3.389001	-2.815904	0.316709
H	-2.909074	-2.001635	0.932270

H	-3.339526	-3.686043	1.008941
C	-2.527708	-3.068230	-0.916935
H	-2.450645	-2.171460	-1.566942
H	-2.937988	-3.890286	-1.538915
H	-1.497788	-3.352205	-0.623066

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II-EtX SCF Done: -2225.01321395 A.U.

N	-3.092719	1.177191	0.489090
N	-3.357799	-0.950709	0.128407
C	-2.412210	0.034737	0.171930
C	-4.447374	0.909957	0.644662
H	-5.165482	1.693700	0.903411
C	-4.614486	-0.432263	0.415676
H	-5.508746	-1.062213	0.432829
C	-2.479935	2.478629	0.655096
C	-1.989446	2.834681	1.937141
C	-2.096266	1.916532	3.151770
H	-2.542078	0.957630	2.815434
C	-1.395912	4.106521	2.064378
H	-1.007342	4.422243	3.044456
C	-1.298465	4.975472	0.970354
C	-1.797532	4.593522	-0.282225
H	-1.722478	5.290414	-1.130780
C	-2.405245	3.336892	-0.471849
C	-2.930800	2.938483	-1.849396
H	-3.484584	1.983113	-1.739453
C	-3.083667	-2.345054	-0.153414
C	-3.145807	-2.786510	-1.499505
C	-3.468878	-1.850152	-2.661621
H	-3.773307	-0.871135	-2.236445
C	-2.867514	-4.145666	-1.742038
H	-2.904921	-4.528667	-2.773121
C	-2.548144	-5.018318	-0.694130
C	-2.502248	-4.550799	0.624792

H	-2.253662	-5.248833	1.438490
C	-2.770775	-3.202325	0.931757
C	-2.701455	-2.719158	2.378444
H	-3.022294	-1.656846	2.399806
Au	-0.446692	-0.158142	-0.091010
C	-3.920711	3.972455	-2.415940
H	-3.432054	4.948371	-2.613548
H	-4.342181	3.616593	-3.377708
H	-4.763940	4.154784	-1.720172
C	-1.769137	2.675589	-2.827888
H	-2.154608	2.351146	-3.816151
H	-1.161117	3.590095	-2.988165
H	-1.099413	1.877754	-2.443291
C	-2.217777	-1.597684	-3.526192
H	-1.854766	-2.536047	-3.994148
H	-2.442469	-0.879676	-4.341507
H	-1.391504	-1.177670	-2.914276
C	-4.646737	-2.360757	-3.511117
H	-4.405661	-3.316828	-4.018973
H	-5.552501	-2.528317	-2.894707
H	-4.901829	-1.625312	-4.300747
C	-3.665952	-3.500675	3.289972
H	-4.710356	-3.450502	2.921652
H	-3.386959	-4.571811	3.361299
H	-3.645368	-3.086817	4.318388
C	-1.256292	-2.766101	2.911923
H	-0.864161	-3.803741	2.930538
H	-0.572663	-2.155805	2.285775
H	-1.211052	-2.372593	3.947853
C	-3.042157	2.510912	4.213741
H	-4.051857	2.710532	3.801261
H	-3.153543	1.812111	5.067440
H	-2.650749	3.467702	4.616463
C	-0.713505	1.587550	3.744988
H	-0.035241	1.133687	2.993995

H	-0.215811	2.493572	4.148215
H	-0.818639	0.871971	4.585769
H	-2.336901	-6.077075	-0.907850
H	-0.837714	5.967175	1.097222
N	1.608578	-0.375168	-0.314855
C	2.511864	-0.276642	0.747140
N	3.701449	-0.914332	0.335928
C	3.534137	-1.455988	-0.962167
N	2.225176	-1.096648	-1.290807
C	4.902475	-1.021238	1.108802
C	5.740990	-2.142190	0.945149
C	5.244132	-0.007690	2.027110
H	5.478725	-2.926229	0.224109
H	4.575744	0.849437	2.174749
C	6.921895	-2.235218	1.695397
C	6.423678	-0.123237	2.776497
H	7.574161	-3.111285	1.561323
H	6.681040	0.666389	3.498557
C	7.268886	-1.231532	2.612717
H	8.194175	-1.314813	3.202057
O	4.310643	-2.081935	-1.659091
O	2.281732	0.296296	1.811625
C	5.414610	0.613446	-3.341377
C	4.095368	0.535499	-3.819086
C	5.696045	1.257010	-2.115025
H	3.887057	0.047831	-4.782652
H	6.733472	1.318563	-1.755024
C	3.051286	1.062783	-3.056095
C	4.665099	1.802365	-1.357586
H	2.014763	1.017905	-3.426241
H	4.895121	2.291395	-0.399930
C	3.306630	1.709289	-1.802716
H	6.236390	0.178676	-3.929959
C	2.206619	2.155325	-1.022239
H	1.715096	-1.457136	-2.097482

H	1.211552	2.038924	-1.483037
C	2.263533	2.885967	0.253764
H	2.149312	2.154492	1.105331
H	1.413170	3.589802	0.352228
H	3.222109	3.412796	0.422330

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III-EtX SCF Done: -2225.03537686 A.U.

N	3.317396	-0.059508	0.548115
N	2.498432	1.877405	-0.015738
C	2.178712	0.557324	0.119573
C	4.344931	0.866158	0.681209
H	5.344747	0.574306	1.016138
C	3.828638	2.087220	0.325667
H	4.285166	3.080710	0.286344
C	3.426695	-1.476263	0.831800
C	3.133539	-1.924263	2.144954
C	2.709062	-0.982930	3.269535
H	2.735557	0.054496	2.875828
C	3.240255	-3.308269	2.386193
H	3.022057	-3.697459	3.392213
C	3.622304	-4.194977	1.371983
C	3.909131	-3.717468	0.086854
H	4.212376	-4.425813	-0.698988
C	3.820811	-2.345030	-0.217628
C	4.121539	-1.853104	-1.631462
H	4.075465	-0.744147	-1.624705
C	1.569228	2.904296	-0.442968
C	1.456658	3.176615	-1.830435
C	2.274671	2.439245	-2.888420
H	3.011484	1.795509	-2.364299
C	0.526327	4.160940	-2.216524
H	0.406239	4.401637	-3.283619
C	-0.246258	4.840747	-1.266439
C	-0.102658	4.553908	0.096632

H	-0.710804	5.101138	0.832782
C	0.810119	3.579203	0.546497
C	0.937215	3.282480	2.038965
H	1.757273	2.546527	2.173145
Au	0.403664	-0.275129	-0.217815
C	5.538522	-2.244425	-2.089704
H	5.656697	-3.344453	-2.167525
H	5.752631	-1.819087	-3.090993
H	6.312303	-1.873505	-1.388135
C	3.051318	-2.344423	-2.625891
H	3.243491	-1.938534	-3.640074
H	3.046800	-3.451133	-2.703010
H	2.035821	-2.022327	-2.312532
C	1.378981	1.509043	-3.730154
H	0.610256	2.081343	-4.288971
H	1.983039	0.943617	-4.468747
H	0.856152	0.773212	-3.082074
C	3.073377	3.407201	-3.780661
H	2.407033	4.057485	-4.383232
H	3.731560	4.066540	-3.180309
H	3.710721	2.842179	-4.490441
C	1.324047	4.540151	2.839660
H	2.258411	4.998608	2.458072
H	0.530212	5.313688	2.798579
H	1.479059	4.284948	3.907386
C	-0.347274	2.634564	2.591597
H	-1.222293	3.308830	2.488942
H	-0.587068	1.688465	2.063723
H	-0.231802	2.399271	3.669189
C	3.687538	-1.040770	4.457928
H	4.727049	-0.815355	4.145568
H	3.396186	-0.304802	5.234316
H	3.691569	-2.041078	4.937147
C	1.260475	-1.260601	3.716035
H	0.545241	-1.167900	2.872730

H	1.154086	-2.280607	4.139237
H	0.952675	-0.541435	4.502116
H	-0.964636	5.607799	-1.593243
H	3.702260	-5.271431	1.586828
N	-1.578159	-1.074483	-0.644840
C	-2.443580	-0.562488	0.470268
N	-3.286952	0.371159	-0.091922
C	-3.041221	0.538942	-1.486507
N	-2.109340	-0.444371	-1.812053
C	-4.260419	1.125826	0.645374
C	-4.324223	2.520939	0.479550
C	-5.137888	0.457721	1.517128
H	-3.638659	3.025875	-0.214413
H	-5.082164	-0.634167	1.625828
C	-5.283704	3.249017	1.197819
C	-6.082004	1.201706	2.238379
H	-5.345505	4.339655	1.066298
H	-6.769435	0.684549	2.924204
C	-6.159037	2.594655	2.079201
H	-6.907435	3.172349	2.641974
O	-3.521474	1.360261	-2.230885
O	-2.345744	-0.940487	1.613902
C	-5.757712	-3.959640	-1.217861
C	-4.996222	-3.630605	-2.349993
C	-5.182424	-3.867679	0.059863
H	-5.436149	-3.710684	-3.355352
H	-5.770500	-4.138338	0.949947
C	-3.667899	-3.205634	-2.201568
C	-3.853332	-3.443435	0.209194
H	-3.073179	-2.959415	-3.095192
H	-3.417832	-3.383690	1.216858
C	-3.079710	-3.100640	-0.922559
H	-6.798861	-4.297457	-1.331845
C	-1.641863	-2.629101	-0.798285
H	-1.435418	-0.237002	-2.556204

H	-1.142568	-2.773469	-1.778074
C	-0.810477	-3.315084	0.280173
H	-1.203098	-3.135410	1.296896
H	0.244095	-2.969431	0.251519
H	-0.818753	-4.405435	0.086682

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PhEt1 SCF Done: -310.235076446 A.U.

C	-0.235490	-2.336787	0.000000
C	-0.236205	-1.629340	1.212672
C	-0.236205	-1.629340	-1.212672
H	-0.241121	-2.174634	2.169343
H	-0.241121	-2.174634	-2.169343
C	-0.236205	-0.226054	1.209670
C	-0.236205	-0.226054	-1.209670
H	-0.241778	0.321581	2.166462
H	-0.241778	0.321581	-2.166462
C	-0.236917	0.499048	0.000000
H	-0.238786	-3.437622	0.000000
C	-0.189479	2.012789	0.000000
H	-0.733489	2.397332	-0.888976
H	-0.733489	2.397332	0.888976
C	1.243269	2.570684	0.000000
H	1.805087	2.229730	-0.893537
H	1.805087	2.229730	0.893537
H	1.241996	3.679940	0.000000

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TSI-EtX SCF Done: -2224.98894230 A.U.

N	-2.927626	1.524897	0.520861
N	-3.565933	-0.408809	-0.241633
C	-2.456428	0.325917	0.063308
C	-4.316999	1.540178	0.503012
H	-4.890416	2.411565	0.832733
C	-4.718764	0.319540	0.022060

H	-5.715690	-0.094284	-0.156138
C	-2.090165	2.615940	0.972748
C	-1.743484	2.674853	2.346842
C	-2.206253	1.632997	3.362514
H	-2.919816	0.952978	2.852959
C	-0.919094	3.741888	2.755375
H	-0.630820	3.824504	3.814349
C	-0.468642	4.702260	1.840716
C	-0.834702	4.617975	0.491143
H	-0.483155	5.385840	-0.214896
C	-1.656460	3.574020	0.021444
C	-2.031635	3.502333	-1.456670
H	-2.725861	2.647235	-1.590838
C	-3.544043	-1.758244	-0.770313
C	-3.540603	-1.928633	-2.178087
C	-3.523749	-0.754909	-3.154632
H	-3.649309	0.179381	-2.568427
C	-3.525022	-3.250967	-2.662216
H	-3.519365	-3.427293	-3.748500
C	-3.516752	-4.343767	-1.786463
C	-3.521630	-4.139132	-0.401563
H	-3.513440	-5.007305	0.274660
C	-3.534903	-2.840839	0.144755
C	-3.537043	-2.648947	1.659005
H	-3.519486	-1.558244	1.864541
Au	-0.544203	-0.223593	-0.104901
C	-2.774670	4.768347	-1.922022
H	-2.131451	5.669930	-1.858777
H	-3.091976	4.663574	-2.979227
H	-3.679630	4.959683	-1.311229
C	-0.794392	3.218609	-2.330635
H	-1.084390	3.116143	-3.396216
H	-0.054435	4.043671	-2.265319
H	-0.290591	2.278652	-2.022661
C	-2.163854	-0.658550	-3.873960

H	-1.970520	-1.557770	-4.494279
H	-2.138617	0.224130	-4.545495
H	-1.329560	-0.563950	-3.148033
C	-4.690136	-0.818380	-4.157513
H	-4.614510	-1.703580	-4.821478
H	-5.670761	-0.868734	-3.643062
H	-4.690374	0.079851	-4.807683
C	-4.823001	-3.210677	2.295197
H	-5.732775	-2.749218	1.860679
H	-4.903004	-4.307437	2.149179
H	-4.831192	-3.020311	3.387704
C	-2.275113	-3.251782	2.305442
H	-2.245984	-4.354666	2.189430
H	-1.346438	-2.844686	1.856139
H	-2.258570	-3.034856	3.393247
C	-2.956853	2.272742	4.544925
H	-3.818361	2.880681	4.203013
H	-3.341746	1.487754	5.226713
H	-2.297171	2.933058	5.144295
C	-1.024755	0.768081	3.843861
H	-0.523289	0.262591	2.992298
H	-0.266522	1.379082	4.376194
H	-1.375689	-0.015792	4.545586
H	-3.506727	-5.368068	-2.188846
H	0.166633	5.532443	2.185722
N	1.447727	-0.742231	-0.259139
C	2.015699	-1.915877	0.341915
N	3.364475	-1.928596	-0.059436
C	3.620440	-0.803663	-0.844170
N	2.341304	-0.087195	-0.962821
C	4.324925	-2.936963	0.285095
C	5.281299	-3.335816	-0.667104
C	4.299624	-3.514673	1.568006
H	5.297603	-2.876713	-1.664430
H	3.544239	-3.204742	2.302177

C	6.220856	-4.317567	-0.322532
C	5.239663	-4.503456	1.891349
H	6.971085	-4.628792	-1.064682
H	5.217799	-4.960966	2.891718
C	6.202339	-4.905259	0.952174
H	6.939105	-5.679278	1.213728
O	4.650374	-0.421750	-1.350893
O	1.404032	-2.724028	1.004914
C	6.629671	3.500996	-1.604473
C	5.360903	3.872607	-2.093371
C	6.736032	2.657799	-0.483559
H	5.280669	4.532552	-2.969940
H	7.727608	2.368315	-0.105294
C	4.208887	3.404502	-1.463145
C	5.584857	2.181614	0.148617
H	3.215703	3.694020	-1.842030
H	5.682939	1.522871	1.023231
C	4.293419	2.557608	-0.319217
H	7.539188	3.870029	-2.102372
C	3.057606	2.080333	0.299914
H	2.676258	1.110818	-0.483327
H	2.176240	2.708450	0.045852
C	3.003119	1.519299	1.697656
H	2.048511	0.979649	1.871508
H	3.031530	2.342565	2.444528
H	3.842500	0.834198	1.928559

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TSII-EtX SCF Done: -2225.01294982 A.U.

N	3.179824	-0.990291	0.549529
N	3.266267	1.132103	0.083243
C	2.408918	0.071871	0.168309
C	4.504445	-0.599532	0.702967
H	5.283483	-1.304604	1.007687
C	4.558878	0.739093	0.407672

H	5.395481	1.444010	0.400976
C	2.678171	-2.329238	0.779089
C	2.210244	-2.659935	2.076249
C	2.221217	-1.672695	3.240320
H	2.622541	-0.708407	2.865438
C	1.725526	-3.969403	2.266829
H	1.356425	-4.266452	3.260205
C	1.710744	-4.898161	1.218773
C	2.184866	-4.539470	-0.050125
H	2.174489	-5.282155	-0.862322
C	2.684396	-3.246750	-0.302590
C	3.181432	-2.875310	-1.697896
H	3.639143	-1.866057	-1.639277
C	2.875673	2.480800	-0.273371
C	2.916915	2.856379	-1.640053
C	3.336741	1.894311	-2.749087
H	3.713361	0.965980	-2.271296
C	2.524010	4.171522	-1.955687
H	2.541754	4.503060	-3.004981
C	2.114805	5.064956	-0.957738
C	2.091864	4.663237	0.383320
H	1.771600	5.377304	1.157044
C	2.473974	3.361471	0.762859
C	2.429198	2.949270	2.232334
H	2.842421	1.922247	2.312052
Au	0.440426	0.081982	-0.136043
C	4.271528	-3.838266	-2.202307
H	3.881695	-4.867141	-2.342591
H	4.662592	-3.499352	-3.182866
H	5.123895	-3.896432	-1.496256
C	2.007997	-2.780962	-2.692980
H	2.367267	-2.467453	-3.694519
H	1.497432	-3.759303	-2.810111
H	1.256347	-2.038758	-2.350537
C	2.126752	1.496773	-3.617496

H	1.696002	2.377485	-4.137107
H	2.424504	0.760819	-4.392350
H	1.326927	1.039750	-2.996951
C	4.483725	2.459525	-3.606340
H	4.174078	3.367138	-4.163531
H	5.361555	2.730686	-2.986381
H	4.812280	1.710873	-4.355355
C	3.309415	3.859539	3.109085
H	4.358525	3.884008	2.751719
H	2.935571	4.903726	3.122355
H	3.313232	3.498778	4.157502
C	0.979235	2.894972	2.751870
H	0.495751	3.892640	2.710904
H	0.360229	2.192585	2.155786
H	0.956796	2.555488	3.807461
C	3.158826	-2.148179	4.367052
H	4.192598	-2.312060	4.001263
H	3.199002	-1.395304	5.180096
H	2.807749	-3.100584	4.814671
C	0.799301	-1.396570	3.764773
H	0.127099	-1.020532	2.966619
H	0.338300	-2.310446	4.193152
H	0.828985	-0.635830	4.571281
H	1.814245	6.088517	-1.228361
H	1.333060	-5.917045	1.394527
N	-1.631058	0.109288	-0.424382
C	-2.515361	0.158045	0.676251
N	-3.678243	0.815888	0.243616
C	-3.517310	1.255120	-1.097121
N	-2.235897	0.814548	-1.426094
C	-4.849013	1.046843	1.036574
C	-5.624921	2.202667	0.817602
C	-5.221073	0.119089	2.030203
H	-5.339526	2.919177	0.037518
H	-4.601120	-0.766206	2.217835

C	-6.775576	2.416159	1.589903
C	-6.368885	0.354724	2.800092
H	-7.380114	3.318343	1.412549
H	-6.650606	-0.368346	3.580380
C	-7.152472	1.498559	2.582451
H	-8.053620	1.676235	3.188087
O	-4.281792	1.872681	-1.810889
O	-2.277366	-0.328947	1.776678
C	-5.685514	-1.263416	-3.000184
C	-4.449585	-1.097429	-3.646794
C	-5.744853	-1.807968	-1.698646
H	-4.411843	-0.686973	-4.666389
H	-6.718330	-1.940367	-1.204014
C	-3.269582	-1.446073	-2.983813
C	-4.573962	-2.167948	-1.036091
H	-2.297784	-1.339186	-3.491063
H	-4.628934	-2.579874	-0.017621
C	-3.301769	-1.983898	-1.660322
H	-6.615114	-0.975234	-3.513785
C	-2.068096	-2.234097	-0.983791
H	-1.740249	1.071966	-2.279676
H	-1.159452	-2.095926	-1.591590
C	-1.914782	-2.957862	0.298777
H	-2.047825	-2.260628	1.167075
H	-0.904218	-3.397230	0.398515
H	-2.680564	-3.750710	0.420425

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UrN2 SCF Done: -621.378894071 A.U.

N	0.000000	-0.623139	3.001402
C	0.005845	-1.134260	1.588168
N	0.000000	0.000000	0.766370
C	-0.005845	1.134260	1.588168
N	0.000000	0.623139	3.001402
C	0.000000	0.000000	-0.664621

C	-0.676111	1.019243	-1.363007
C	0.676111	-1.019243	-1.363007
H	-1.192250	1.817288	-0.814118
H	1.192250	-1.817288	-0.814118
C	-0.666517	1.013770	-2.764848
C	0.666517	-1.013770	-2.764848
H	-1.191914	1.813356	-3.308529
H	1.191914	-1.813356	-3.308529
C	0.000000	0.000000	-3.470509
H	0.000000	0.000000	-4.570829
O	-0.021451	2.301827	1.294932
O	0.021451	-2.301827	1.294932

5.2.3 PBEH1PBE

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AuIPrCH3CN+ SCF Done: -1426.11043844 A.U.

N	-1.076710	0.000224	-1.486649
N	1.076094	0.000226	-1.486938
C	-0.000199	0.000041	-0.671323
C	-0.680375	0.000504	-2.806890
H	-1.398035	0.000727	-3.622419
C	0.679407	0.000511	-2.807072
H	1.396847	0.000740	-3.622794
C	-2.445444	0.000200	-1.044148
C	-3.084153	-1.237144	-0.844647
C	-2.388301	-2.567647	-1.067725
H	-1.376040	-2.361347	-1.450010
C	-4.414574	-1.206048	-0.415960
H	-4.946229	-2.145830	-0.249704
C	-5.072837	0.000193	-0.202433
C	-4.414427	1.206439	-0.415467
H	-4.945967	2.146224	-0.248840
C	-3.083985	1.237539	-0.844085
C	-2.387982	2.568051	-1.066634
H	-1.375638	2.361795	-1.448716

C	2.444950	0.000212	-1.044815
C	3.083540	1.237557	-0.844939
C	2.387472	2.568069	-1.067265
H	1.374790	2.361799	-1.448442
C	4.414141	1.206467	-0.416810
H	4.945726	2.146261	-0.250372
C	5.072648	0.000227	-0.204044
C	4.414311	-1.206021	-0.417312
H	4.946031	-2.145803	-0.251257
C	3.083731	-1.237129	-0.845509
C	2.387841	-2.567645	-1.068379
H	1.375239	-2.361349	-1.449760
Au	0.000165	-0.000347	1.323459
C	-3.105903	3.411554	-2.121940
H	-4.118627	3.694318	-1.795422
H	-2.550566	4.342410	-2.312963
H	-3.202873	2.871623	-3.075801
C	-2.226478	3.333704	0.248447
H	-1.674951	4.272269	0.084272
H	-3.203267	3.594446	0.685011
H	-1.674124	2.738489	0.992608
C	2.227143	3.334145	0.247710
H	3.204305	3.595071	0.683324
H	1.675469	4.272654	0.083710
H	1.675473	2.739201	0.992589
C	3.104620	3.411164	-2.123429
H	4.117682	3.693812	-1.797858
H	3.200664	2.870963	-3.077231
H	2.549291	4.342074	-2.314217
C	3.105292	-3.410421	-2.124582
H	3.201729	-2.869879	-3.078151
H	4.118206	-3.693306	-1.798761
H	2.549935	-4.341202	-2.315911
C	2.227237	-3.334074	0.246364
H	3.204317	-3.594961	0.682192

H	1.675264	-2.739390	0.991228
H	1.675742	-4.272621	0.081977
C	-3.106503	-3.410855	-2.123067
H	-3.203872	-2.870593	-3.076699
H	-2.551117	-4.341573	-2.314620
H	-4.119073	-3.693874	-1.796301
C	-2.226511	-3.333639	0.247129
H	-1.673869	-2.738668	0.991273
H	-3.203213	-3.594362	0.683905
H	-1.675143	-4.272233	0.082577
H	6.113608	0.000233	0.127270
H	-6.113662	0.000191	0.129303
N	0.000769	-0.000752	3.362024
C	0.001225	-0.000974	4.513955
C	0.001776	-0.000964	5.958744
H	1.036323	-0.043732	6.329194
H	-0.478195	0.916146	6.330121
H	-0.552266	-0.875324	6.330112

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AuIPr+ SCF Done: -1293.52360762 A.U.

N	1.082272	-0.000137	1.127677
N	-1.082455	-0.000154	1.127503
C	-0.000028	-0.000038	0.329949
C	0.680404	-0.000302	2.446416
H	1.398002	-0.000401	3.262333
C	-0.680799	-0.000310	2.446307
H	-1.398529	-0.000415	3.262108
C	2.450273	-0.000081	0.675119
C	3.083650	-1.239304	0.469403
C	2.389499	-2.570085	0.696133
H	1.381862	-2.366669	1.093299
C	4.409554	-1.206802	0.027249
H	4.939882	-2.145917	-0.146039
C	5.064979	0.000027	-0.192090

C	4.409570	1.206802	0.027598
H	4.939910	2.145959	-0.145422
C	3.083665	1.239193	0.469757
C	2.389506	2.569915	0.696811
H	1.381949	2.366401	1.094129
C	-2.450383	-0.000092	0.674724
C	-3.083721	1.239186	0.469223
C	-2.389601	2.569906	0.696405
H	-1.382026	2.366384	1.093674
C	-4.409553	1.206803	0.026843
H	-4.939849	2.145966	-0.146290
C	-5.064945	0.000034	-0.192918
C	-4.409578	-1.206800	0.026567
H	-4.939893	-2.145911	-0.146784
C	-3.083747	-1.239312	0.468939
C	-2.389629	-2.570094	0.695761
H	-1.382161	-2.366687	1.093360
Au	0.000129	0.000207	-1.648147
C	3.121089	3.418109	1.739187
H	4.128194	3.701527	1.396831
H	2.566932	4.348632	1.934292
H	3.232786	2.881934	2.693473
C	2.211661	3.331100	-0.618945
H	1.663170	4.270703	-0.451990
H	3.182220	3.588709	-1.070342
H	1.649549	2.735709	-1.356443
C	-2.211808	3.331269	-0.619251
H	-3.182377	3.588934	-1.070593
H	-1.663329	4.270857	-0.452178
H	-1.649705	2.735989	-1.356844
C	-3.121208	3.417926	1.738909
H	-4.128351	3.701290	1.396619
H	-3.232829	2.881632	2.693138
H	-2.567121	4.348472	1.934103
C	-3.121431	-3.418601	1.737728

H	-3.233352	-2.882702	2.692143
H	-4.128453	-3.701941	1.395065
H	-2.567300	-4.349169	1.932690
C	-2.211490	-3.330894	-0.620178
H	-3.181949	-3.588367	-1.071868
H	-1.649212	-2.735286	-1.357376
H	-1.663036	-4.270545	-0.453378
C	3.120948	-3.418373	1.738530
H	3.232422	-2.882325	2.692914
H	2.566831	-4.348970	1.933399
H	4.128143	-3.701648	1.396321
C	2.211912	-3.331109	-0.619747
H	1.649922	-2.735640	-1.357274
H	3.182552	-3.588655	-1.071005
H	1.663409	-4.270741	-0.453003
H	-6.101775	0.000084	-0.536624
H	6.101865	0.000070	-0.535624

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CH3CN SCF Done: -132.505987823 A.U.

N	1.434873	0.000002	0.000000
C	0.278422	-0.000004	0.000001
C	-1.174624	0.000001	-0.000001
H	-1.555637	0.065839	1.029106
H	-1.555632	0.858316	-0.571570
H	-1.555635	-0.924150	-0.457537

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I-EtX SCF Done: -2225.35949517 A.U.

N	3.582721	0.653414	-0.215771
N	3.100358	-1.433498	-0.434657
C	2.561785	-0.226985	-0.160616
C	4.759410	0.005023	-0.523048
H	5.702195	0.536970	-0.614286
C	4.454961	-1.313319	-0.661547

H	5.076140	-2.171859	-0.900698
C	3.458763	2.067676	0.018126
C	3.191326	2.905918	-1.079344
C	3.033070	2.384047	-2.495807
H	3.133298	1.287456	-2.466450
C	3.078037	4.275425	-0.821239
H	2.872400	4.960534	-1.646912
C	3.225865	4.779042	0.466519
C	3.492944	3.922625	1.529345
H	3.610729	4.333279	2.534828
C	3.618760	2.544274	1.332122
C	3.908594	1.631203	2.509837
H	4.020471	0.605127	2.124916
C	2.366733	-2.669632	-0.490961
C	2.219209	-3.415748	0.692458
C	2.791905	-2.968418	2.025045
H	3.337608	-2.025833	1.860447
C	1.507216	-4.616167	0.604094
H	1.371782	-5.225876	1.500405
C	0.976815	-5.049793	-0.606177
C	1.144303	-4.289832	-1.758997
H	0.724569	-4.644662	-2.703058
C	1.844546	-3.079985	-1.731396
C	2.001167	-2.262002	-3.000724
H	2.656397	-1.405933	-2.774485
Au	0.649015	0.185305	0.261727
C	5.223457	1.999993	3.199654
H	5.178101	3.003906	3.649332
H	5.446090	1.287652	4.008573
H	6.068334	1.989310	2.494786
C	2.741426	1.617269	3.499490
H	2.941636	0.916312	4.324396
H	2.576634	2.612156	3.941828
H	1.804137	1.307705	3.010441
C	1.680976	-2.676808	3.036211

H	1.101725	-3.583239	3.271704
H	2.106246	-2.301639	3.979703
H	0.977746	-1.919594	2.654924
C	3.797552	-3.982784	2.573702
H	3.317801	-4.947650	2.799726
H	4.611239	-4.175449	1.858435
H	4.246428	-3.612101	3.507748
C	2.676370	-3.063562	-4.114922
H	3.651287	-3.461441	-3.795602
H	2.057798	-3.915795	-4.436096
H	2.841152	-2.427977	-4.998131
C	0.655602	-1.692072	-3.456322
H	-0.054411	-2.494737	-3.710490
H	0.194940	-1.071586	-2.671517
H	0.784216	-1.065257	-4.352101
C	4.139387	2.916134	-3.409813
H	5.140097	2.665238	-3.026652
H	4.044446	2.487909	-4.419334
H	4.087267	4.011509	-3.509352
C	1.643933	2.694597	-3.056754
H	0.845504	2.293727	-2.413732
H	1.481381	3.779274	-3.154939
H	1.528230	2.254118	-4.059013
H	0.429871	-5.994343	-0.652506
H	3.136292	5.853296	0.643648
N	-1.319711	0.633225	0.731846
C	-2.174106	1.474539	-0.170104
N	-3.370057	1.553084	0.484162
C	-3.299851	0.842203	1.673612
N	-1.932264	0.277749	1.740647
C	-4.525597	2.260376	0.017390
C	-5.748265	1.594845	-0.041800
C	-4.397816	3.595425	-0.363626
H	-5.829419	0.546939	0.253412
H	-3.430588	4.098208	-0.307779

C	-6.867272	2.293528	-0.487601
C	-5.523793	4.274911	-0.819700
H	-7.830944	1.782504	-0.534315
H	-5.435908	5.319598	-1.124621
C	-6.757425	3.627210	-0.877945
H	-7.639036	4.166748	-1.230516
O	-4.112885	0.672863	2.516439
O	-1.780080	1.921374	-1.195145
C	-7.465535	-1.770646	-0.107146
C	-6.979424	-1.872335	1.197744
C	-6.587553	-1.922096	-1.178152
H	-7.656910	-1.753139	2.046528
H	-6.956495	-1.845283	-2.203758
C	-5.630200	-2.132539	1.422457
C	-5.234625	-2.180567	-0.949306
H	-5.261530	-2.214943	2.448956
H	-4.568546	-2.304609	-1.805730
C	-4.734986	-2.298948	0.353105
H	-8.526108	-1.578976	-0.286356
C	-3.290721	-2.630972	0.645427
H	-2.934434	-1.976986	1.464787
H	-3.252663	-3.643112	1.086907
C	-2.324517	-2.566940	-0.524294
H	-2.325828	-1.577569	-1.013017
H	-2.575530	-3.303490	-1.302511
H	-1.296223	-2.781892	-0.196824

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III-EtX SCF Done: -2225.41498758 A.U.

N	3.293924	-0.131243	0.550583
N	2.542843	1.818828	0.028012
C	2.189653	0.520839	0.132797
C	4.340596	0.752742	0.709221
H	5.322639	0.428212	1.041562
C	3.866218	1.984223	0.379415

H	4.348454	2.957572	0.364401
C	3.354762	-1.545876	0.803489
C	3.042502	-2.008231	2.094962
C	2.655137	-1.080226	3.232063
H	2.700959	-0.045661	2.856694
C	3.098036	-3.389363	2.307496
H	2.863803	-3.788557	3.297028
C	3.450227	-4.261292	1.283006
C	3.757693	-3.770853	0.018159
H	4.037693	-4.467543	-0.775397
C	3.719550	-2.399873	-0.253481
C	4.048898	-1.890768	-1.645145
H	4.023053	-0.789892	-1.618679
C	1.651049	2.871709	-0.379383
C	1.562258	3.181417	-1.749055
C	2.373256	2.457452	-2.809002
H	3.083855	1.790178	-2.295936
C	0.667573	4.189914	-2.118602
H	0.566967	4.459394	-3.172415
C	-0.094498	4.858368	-1.166068
C	0.024807	4.535072	0.181160
H	-0.573841	5.073930	0.919223
C	0.902284	3.533977	0.610231
C	1.010534	3.201766	2.087623
H	1.788429	2.430878	2.206316
Au	0.393742	-0.262710	-0.226856
C	5.457131	-2.299168	-2.081232
H	5.553455	-3.391981	-2.173402
H	5.696367	-1.864729	-3.063747
H	6.218274	-1.957438	-1.364006
C	2.995468	-2.343338	-2.658961
H	3.210157	-1.926036	-3.654816
H	2.974622	-3.440136	-2.755171
H	1.987872	-2.012537	-2.359358
C	1.474178	1.576607	-3.680155

H	0.729836	2.177225	-4.225972
H	2.070295	1.024567	-4.423003
H	0.932364	0.839822	-3.064446
C	3.197507	3.425811	-3.658987
H	2.556236	4.098287	-4.249215
H	3.853565	4.052279	-3.036492
H	3.829980	2.870848	-4.368336
C	1.452659	4.417560	2.904878
H	2.401724	4.833248	2.534283
H	0.701975	5.222330	2.873610
H	1.591763	4.139766	3.960662
C	-0.295857	2.611757	2.623391
H	-1.128870	3.326807	2.537466
H	-0.581577	1.697706	2.079771
H	-0.193134	2.349640	3.687512
C	3.642116	-1.181884	4.397125
H	4.674354	-0.977990	4.074812
H	3.382208	-0.458295	5.184609
H	3.627930	-2.183735	4.853566
C	1.217136	-1.330803	3.691640
H	0.497795	-1.210370	2.866552
H	1.095409	-2.346959	4.098273
H	0.938711	-0.622444	4.486811
H	-0.784964	5.645249	-1.478204
H	3.490693	-5.336176	1.473812
N	-1.591874	-1.023244	-0.665893
C	-2.443539	-0.509207	0.425930
N	-3.282903	0.409989	-0.135950
C	-3.041239	0.563390	-1.514534
N	-2.104313	-0.402781	-1.825738
C	-4.254318	1.159851	0.592805
C	-4.301655	2.546458	0.445878
C	-5.143833	0.492974	1.434915
H	-3.606995	3.049457	-0.227905
H	-5.098582	-0.593027	1.527833

C	-5.257721	3.269733	1.154253
C	-6.084700	1.230282	2.148362
H	-5.308037	4.354340	1.037258
H	-6.781834	0.714982	2.812333
C	-6.145199	2.616028	2.007836
H	-6.890753	3.188996	2.563351
O	-3.521545	1.365269	-2.257328
O	-2.349523	-0.872683	1.560087
C	-5.782133	-3.826710	-1.168444
C	-5.040930	-3.499315	-2.302184
C	-5.189301	-3.753698	0.091401
H	-5.495109	-3.564540	-3.293233
H	-5.761547	-4.023414	0.981990
C	-3.714391	-3.094821	-2.173030
C	-3.862183	-3.349249	0.220928
H	-3.136454	-2.849716	-3.067795
H	-3.412621	-3.303310	1.214362
C	-3.109627	-3.008353	-0.912254
H	-6.821322	-4.148418	-1.267365
C	-1.671300	-2.555096	-0.805547
H	-1.440785	-0.205975	-2.568564
H	-1.187038	-2.719930	-1.779894
C	-0.849270	-3.245956	0.265220
H	-1.219270	-3.039156	1.276568
H	0.207670	-2.938134	0.215942
H	-0.894387	-4.330186	0.090508

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PhEt1 SCF Done: -310.312975930 A.U.

C	-0.234817	-2.320749	0.000000
C	-0.235399	-1.618169	1.204161
C	-0.235399	-1.618169	-1.204161
H	-0.240032	-2.159411	2.153627
H	-0.240032	-2.159411	-2.153627
C	-0.235399	-0.224410	1.201164

C	-0.235399	-0.224410	-1.201164
H	-0.240696	0.319076	2.150780
H	-0.240696	0.319076	-2.150780
C	-0.235438	0.495194	0.000000
H	-0.238047	-3.413329	0.000000
C	-0.187533	2.001313	0.000000
H	-0.727526	2.382919	-0.881968
H	-0.727526	2.382919	0.881968
C	1.237419	2.551679	0.000000
H	1.793308	2.210946	-0.887006
H	1.793308	2.210946	0.887006
H	1.239732	3.652603	0.000000

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TSI-EtX SCF Done: -2225.34492513 A.U.

N	-2.985740	1.432365	0.561763
N	-3.552654	-0.474765	-0.256891
C	-2.481656	0.278973	0.069562
C	-4.365012	1.403486	0.545096
H	-4.963666	2.237192	0.900862
C	-4.722298	0.197664	0.028470
H	-5.698111	-0.240261	-0.161436
C	-2.188751	2.527085	1.042702
C	-1.836137	2.551335	2.404516
C	-2.260952	1.470328	3.381902
H	-2.937108	0.781507	2.851834
C	-1.049633	3.621672	2.842434
H	-0.758601	3.677122	3.894026
C	-0.641059	4.620093	1.964380
C	-1.012140	4.570579	0.624545
H	-0.694421	5.367659	-0.051981
C	-1.796638	3.523467	0.130277
C	-2.184585	3.492293	-1.336875
H	-2.829140	2.614147	-1.497774
C	-3.482082	-1.795145	-0.823883

C	-3.470693	-1.920668	-2.224951
C	-3.506377	-0.723378	-3.157545
H	-3.646912	0.180454	-2.543596
C	-3.403157	-3.214847	-2.748801
H	-3.390225	-3.355018	-3.832125
C	-3.352961	-4.325936	-1.913819
C	-3.368169	-4.167181	-0.532680
H	-3.328432	-5.048941	0.110919
C	-3.432857	-2.897127	0.048486
C	-3.452842	-2.754054	1.559249
H	-3.465531	-1.678581	1.797329
Au	-0.550623	-0.203836	-0.109377
C	-2.994763	4.728136	-1.733021
H	-2.402397	5.651247	-1.635614
H	-3.319195	4.654817	-2.782181
H	-3.892545	4.841798	-1.107161
C	-0.954770	3.316892	-2.230472
H	-1.251769	3.242513	-3.287859
H	-0.267284	4.173113	-2.139875
H	-0.399346	2.401953	-1.969794
C	-2.175314	-0.565470	-3.896629
H	-1.972391	-1.431542	-4.545845
H	-2.190113	0.332144	-4.534234
H	-1.334515	-0.471303	-3.191411
C	-4.683691	-0.793845	-4.131440
H	-4.594638	-1.651554	-4.815896
H	-5.643437	-0.889271	-3.601705
H	-4.725348	0.115500	-4.750226
C	-4.722402	-3.365777	2.156408
H	-5.631472	-2.918604	1.726224
H	-4.768951	-4.450978	1.975497
H	-4.749758	-3.210986	3.245939
C	-2.192151	-3.342371	2.196041
H	-2.131609	-4.430716	2.039961
H	-1.276045	-2.895205	1.780769

H	-2.196319	-3.167945	3.283192
C	-3.041125	2.048066	4.564064
H	-3.916199	2.625332	4.229784
H	-3.397871	1.238885	5.219137
H	-2.416571	2.715103	5.178389
C	-1.057882	0.648648	3.850818
H	-0.531943	0.187706	2.999728
H	-0.336047	1.272553	4.401451
H	-1.380625	-0.159478	4.524991
H	-3.302607	-5.328265	-2.345248
H	-0.035395	5.452442	2.330829
N	1.455666	-0.663331	-0.268457
C	2.065737	-1.755343	0.403053
N	3.387811	-1.777311	-0.040226
C	3.587304	-0.736208	-0.923120
N	2.303218	-0.056606	-1.039776
C	4.376968	-2.726195	0.353534
C	5.285812	-3.203715	-0.592621
C	4.424532	-3.164299	1.678362
H	5.244366	-2.852214	-1.623876
H	3.702499	-2.795267	2.407155
C	6.254308	-4.123569	-0.200084
C	5.391210	-4.094151	2.052007
H	6.968779	-4.496094	-0.937153
H	5.426344	-4.444483	3.085741
C	6.308531	-4.572805	1.118262
H	7.066606	-5.299320	1.418278
O	4.573470	-0.385909	-1.498044
O	1.509352	-2.502812	1.152546
C	6.744899	3.275041	-1.630592
C	5.527548	3.702811	-2.171537
C	6.762365	2.454223	-0.501761
H	5.517139	4.345065	-3.054517
H	7.713916	2.120599	-0.083151
C	4.336550	3.312071	-1.583391

C	5.570913	2.055341	0.087908
H	3.383956	3.646843	-2.003001
H	5.600835	1.413448	0.969981
C	4.332227	2.488735	-0.433741
H	7.684731	3.583831	-2.093995
C	3.055715	2.092666	0.139714
H	2.647357	1.129662	-0.641611
H	2.222997	2.748825	-0.163966
C	2.909220	1.556495	1.527685
H	1.960689	1.002872	1.635476
H	2.855458	2.387536	2.251242
H	3.736973	0.900468	1.831307

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UrN2 SCF Done: -621.441771445 A.U.

N	0.000000	-0.615132	2.969292
C	0.004826	-1.121928	1.577607
N	0.000000	0.000000	0.763259
C	-0.004826	1.121928	1.577607
N	0.000000	0.615132	2.969292
C	0.000000	0.000000	-0.659614
C	-0.691946	0.997341	-1.351598
C	0.691946	-0.997341	-1.351598
H	-1.220828	1.778502	-0.805902
H	1.220828	-1.778502	-0.805902
C	-0.682007	0.993430	-2.743847
C	0.682007	-0.993430	-2.743847
H	-1.218955	1.776383	-3.283890
H	1.218955	-1.776383	-3.283890
C	0.000000	0.000000	-3.444041
H	0.000000	0.000000	-4.536218
O	-0.018924	2.275099	1.289931
O	0.018924	-2.275099	1.289931

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