Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry


# - Supporting Information -

## *$^{15}$N NMR Spectroscopic and Theoretical GIAO-DFT Studies for the Unambiguous Characterization of Disubstituted 1,2,3-Triazoles*

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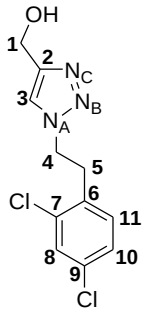
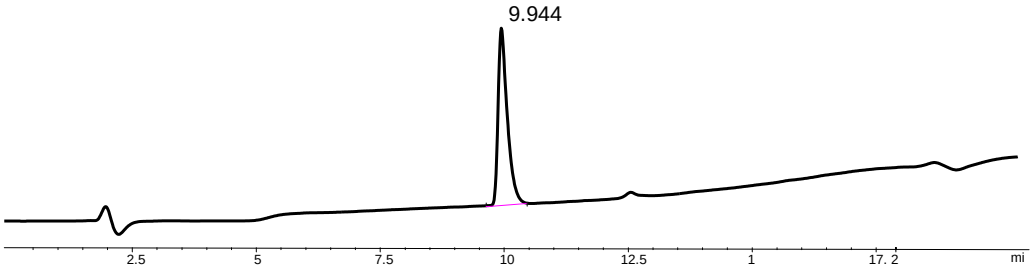
# 1. Data for the 1,4-disbustituted-1,2,3-triazoles (1,4-TAs)

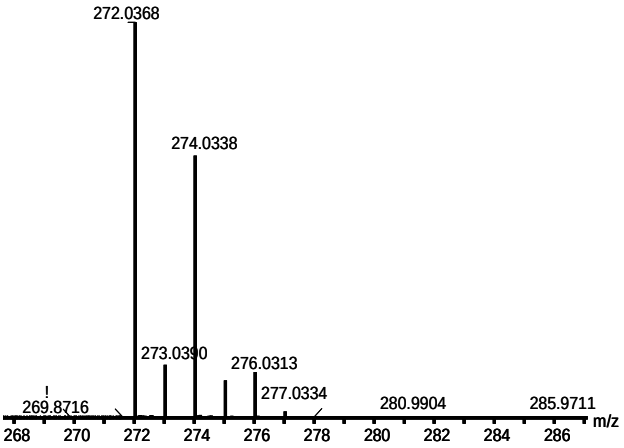
### 1-(2,4-Dichlorophenethyl)-4-hydroxymethyl-*1H*-1,2,3-triazole (1a)



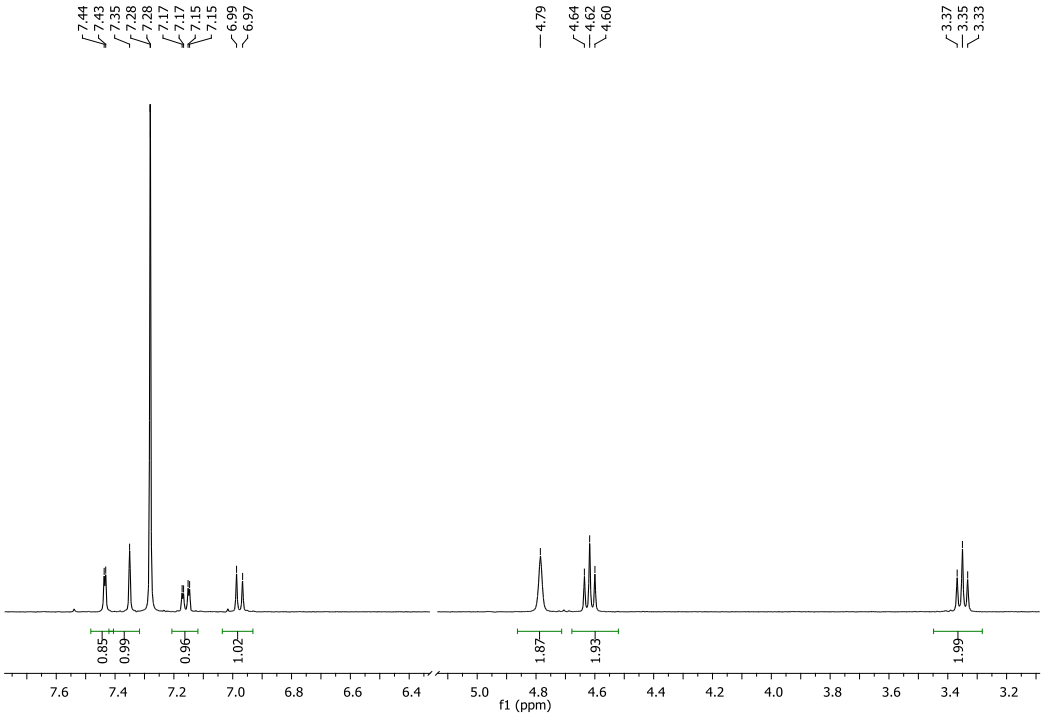

## HPLC



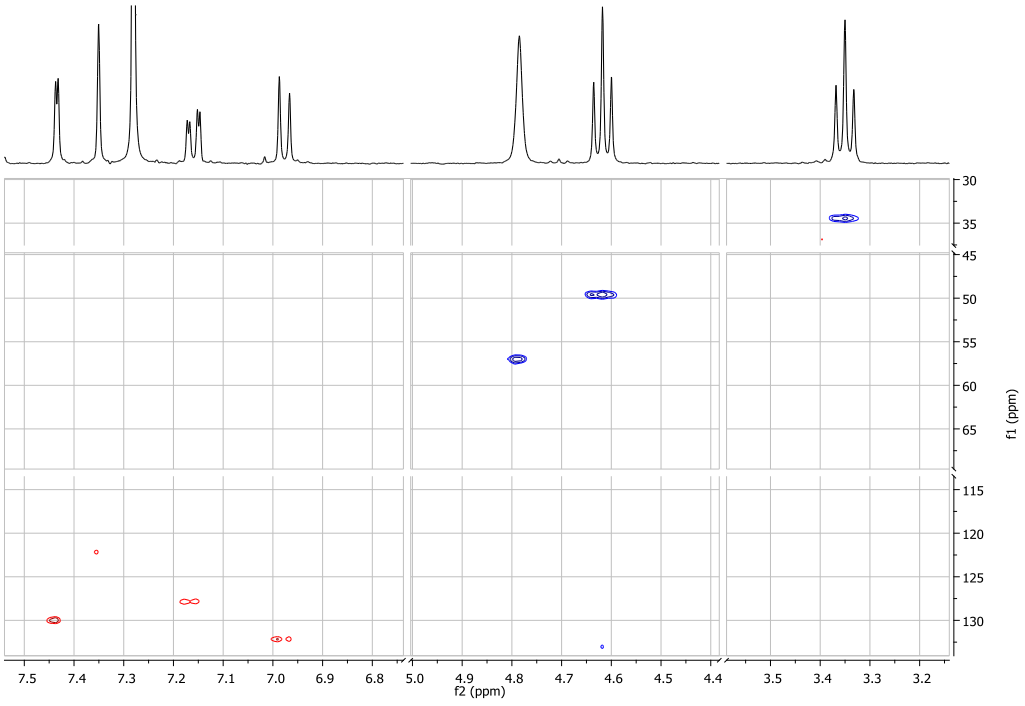

## HRMS



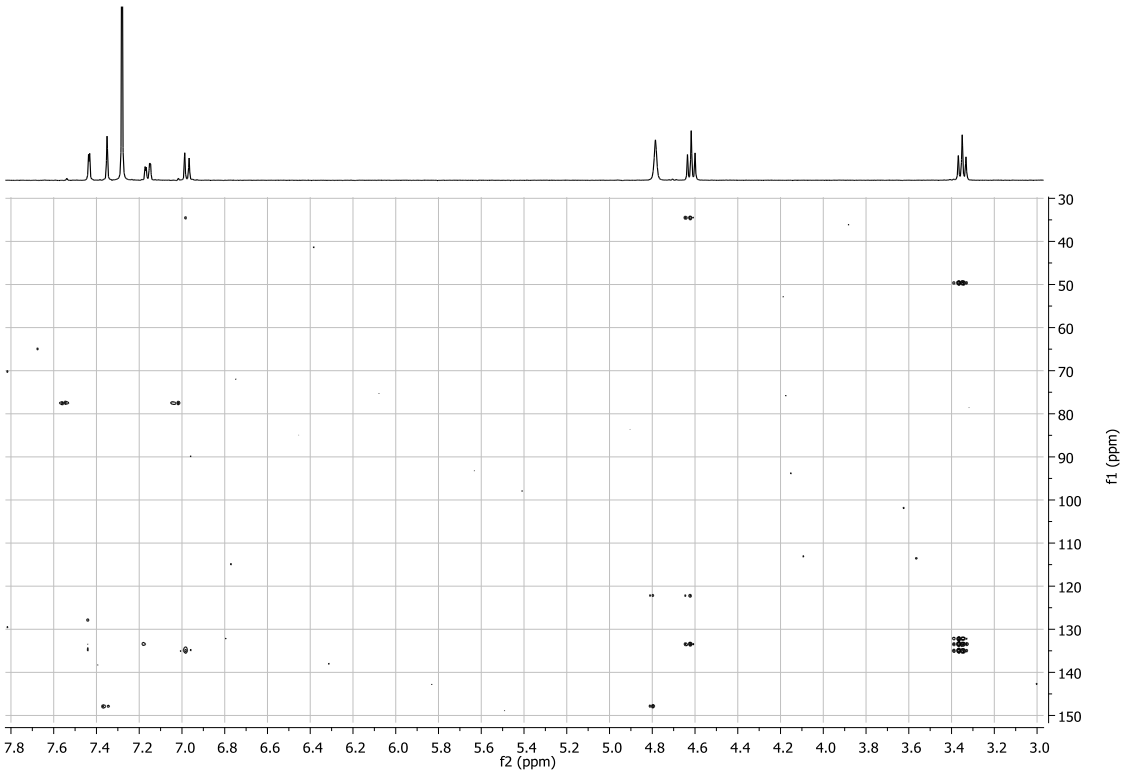
## $^{1}$H NMR



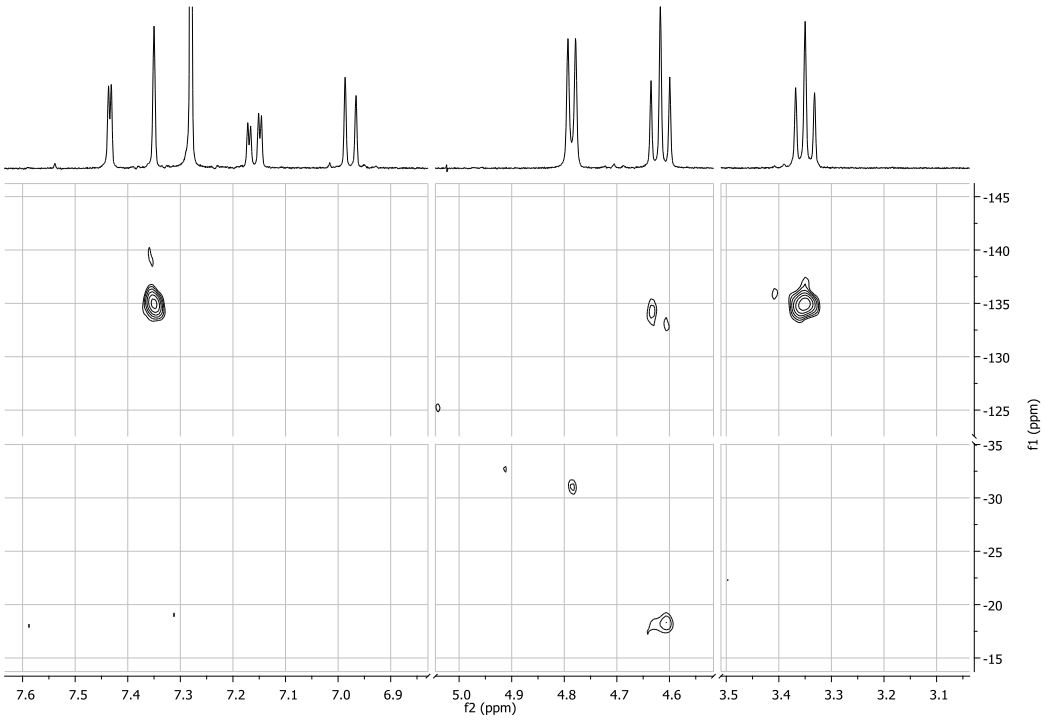

## $^{1}$H-$^{13}$C gHSQC



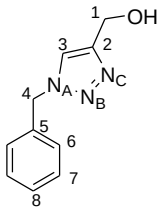
## $^{1}H$-$^{13}C$-gHMBC



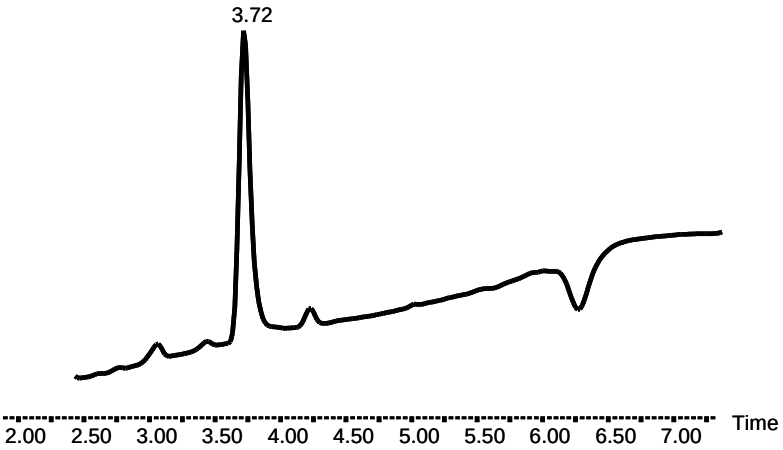

## $^{1}H$-$^{15}N$-gHMBC



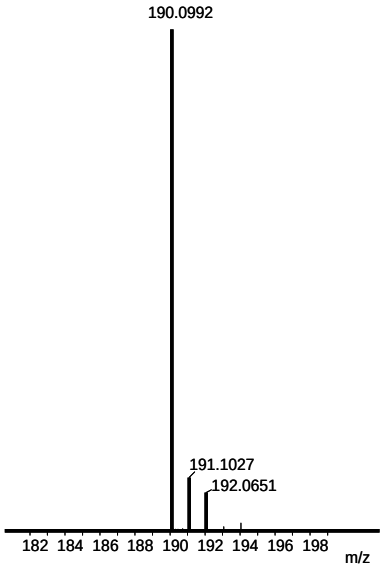
## 1-benzyl-4-hydroxymethyl-1*H*-1,2,3-triazole (1b)



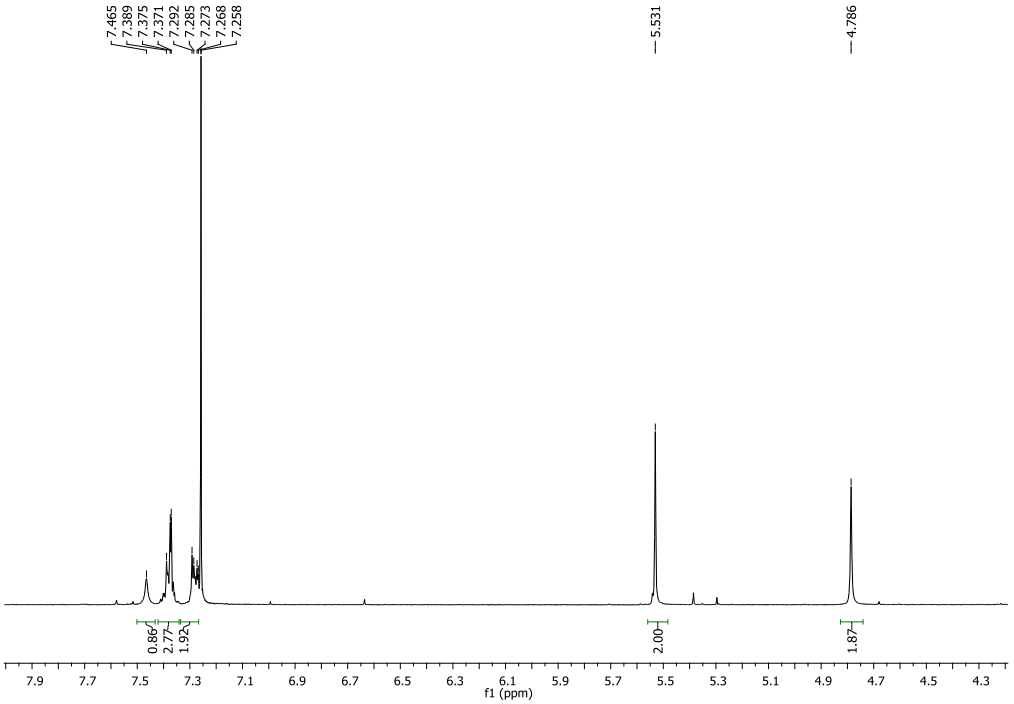

### HPLC



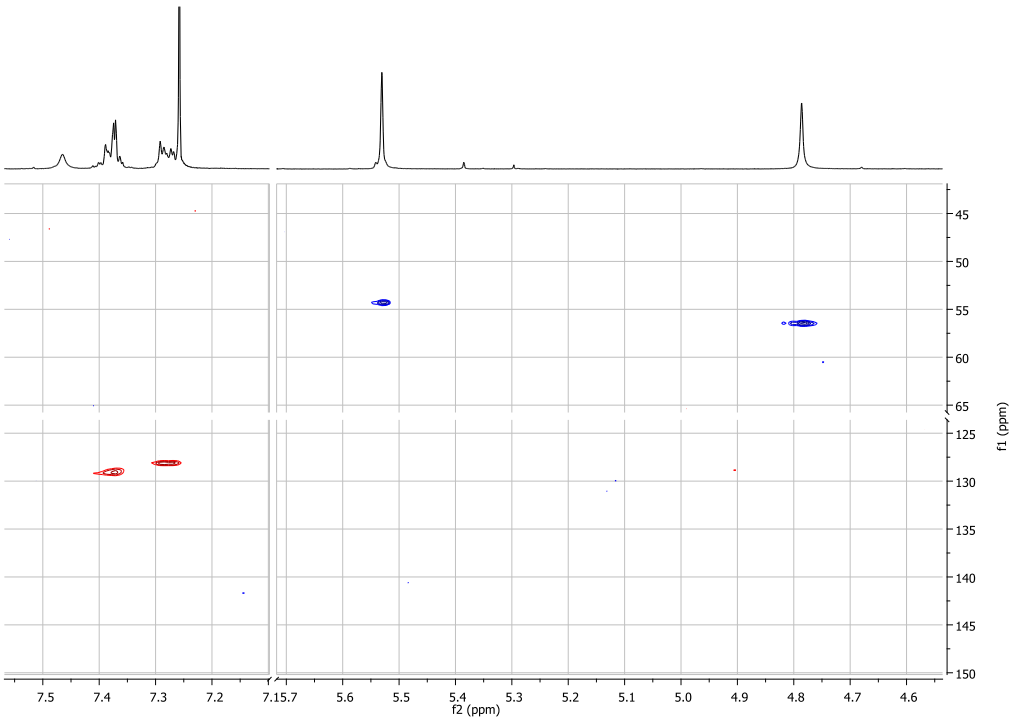

### HRMS



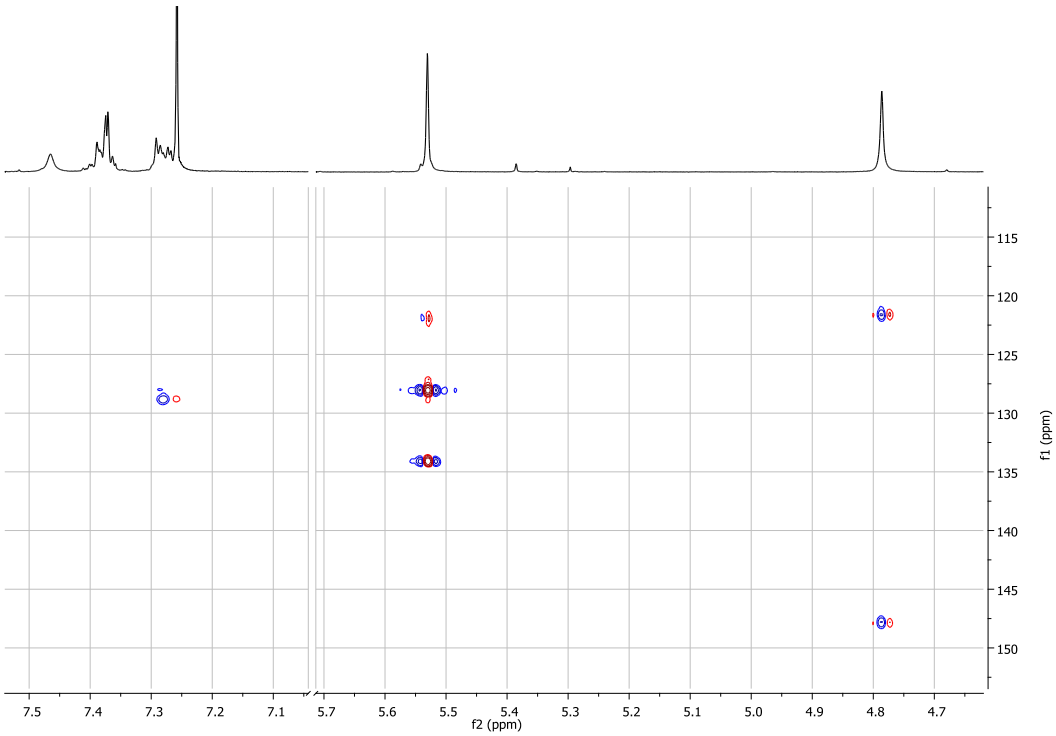
## $^{1}$H-NMR



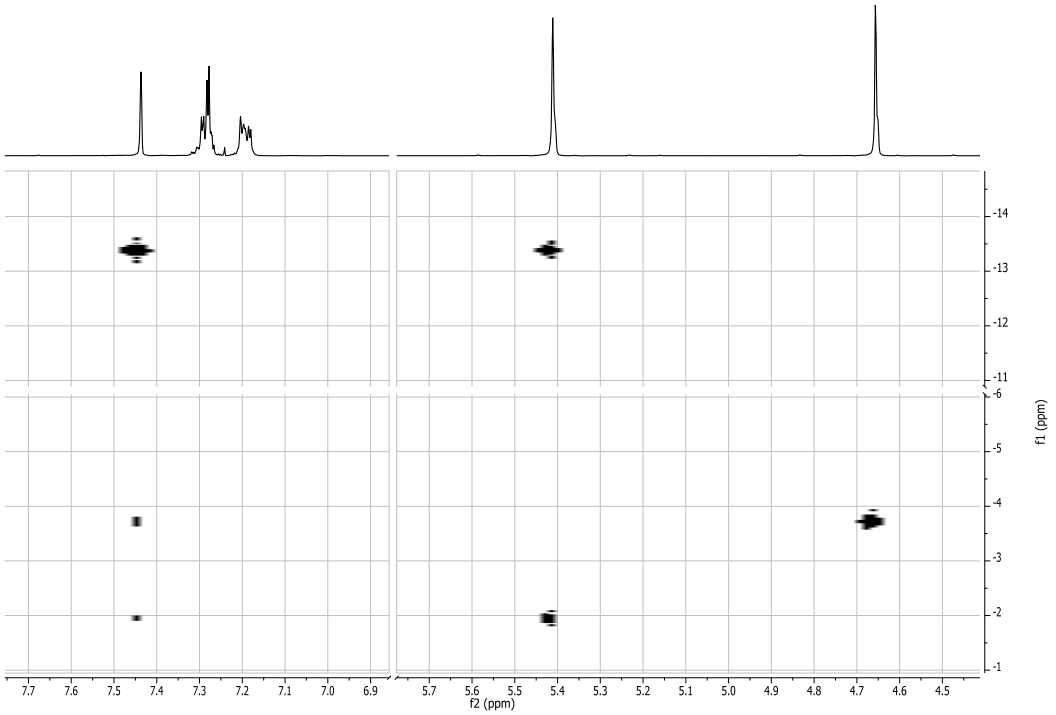

## $^{1}$H-$^{13}$C-HSQC



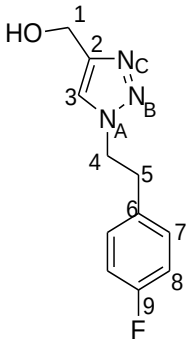
## $^{1}H$-$^{13}C$-HMBC



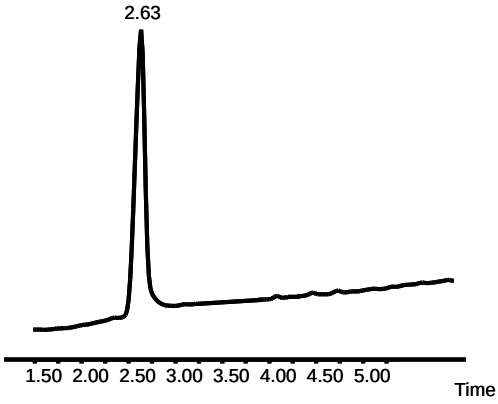

## $^{1}H$-$^{15}N$ HMBC



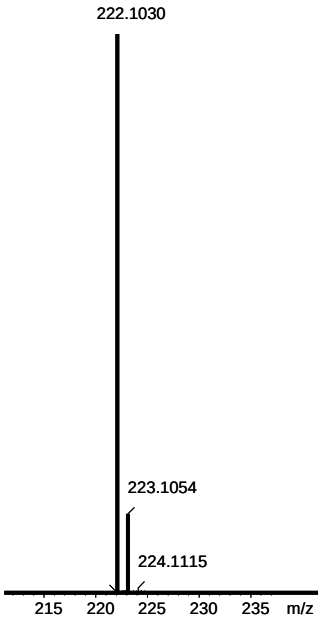
## 1-(4-Fluorophenethyl)-4-hydroxymethyl-1*H*-1,2,3-triazole (1c)



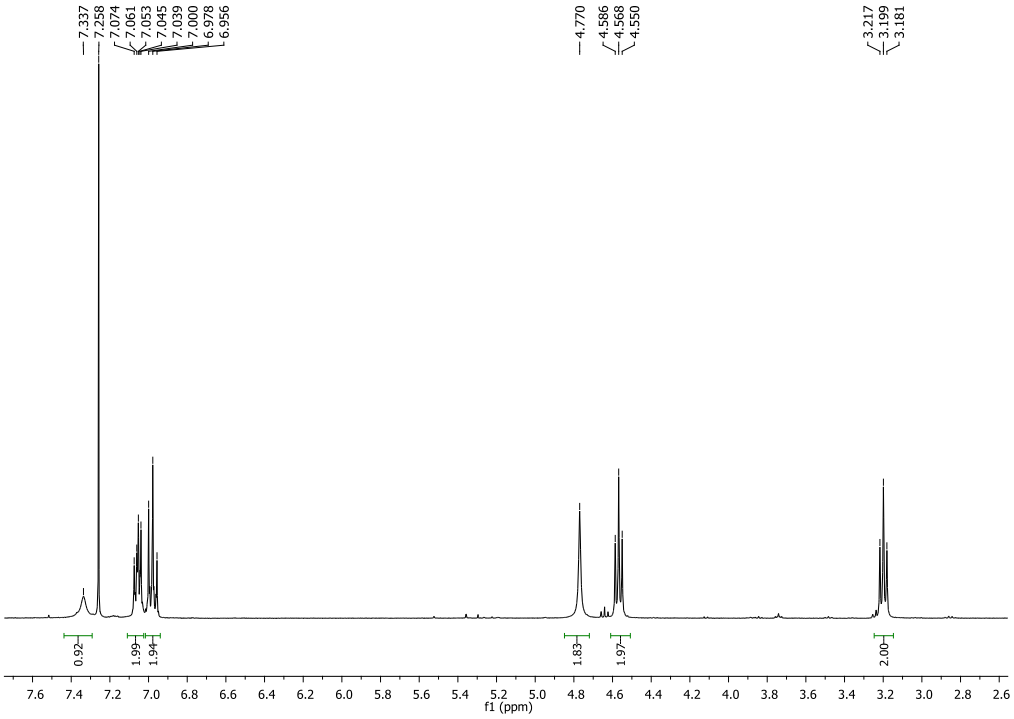

### HPLC



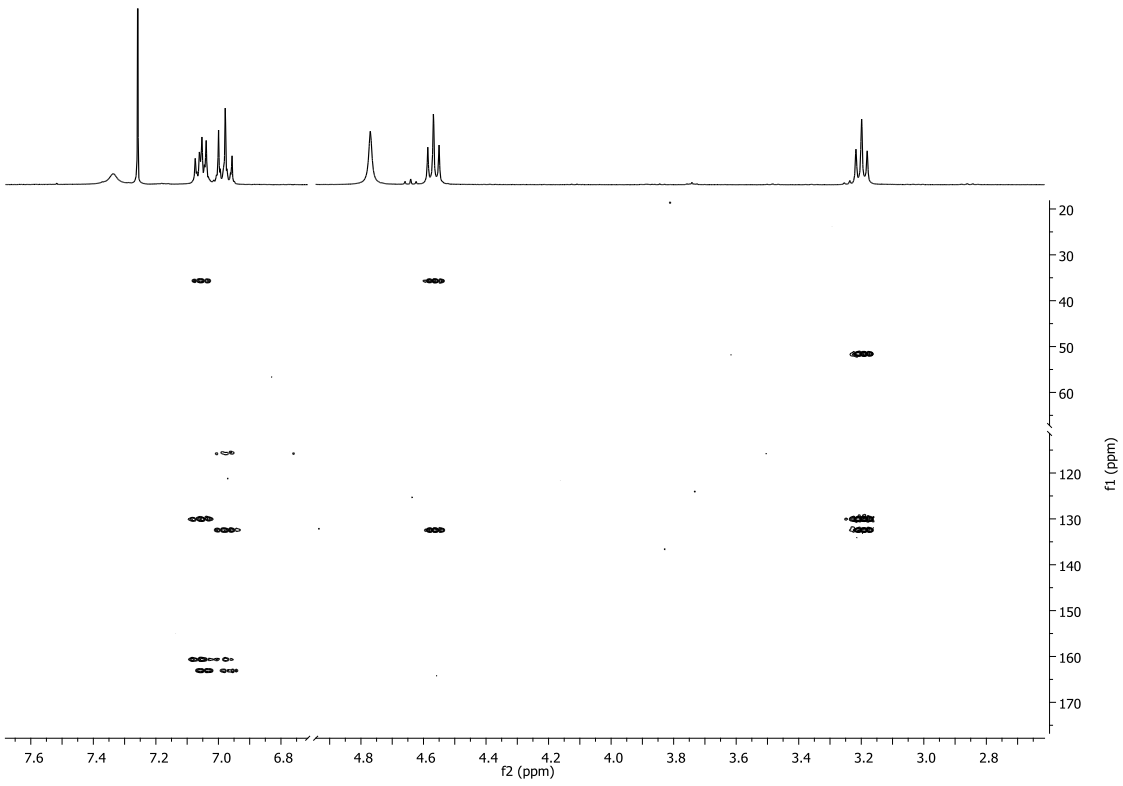

### HRMS



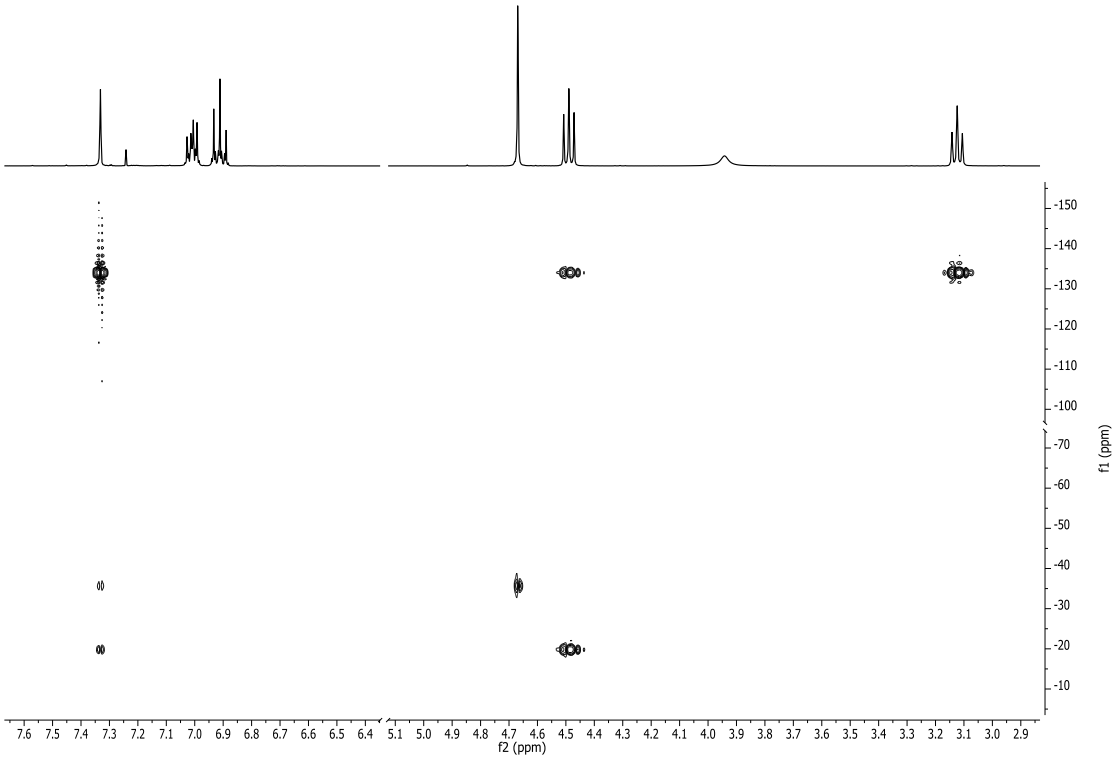
## $^{1}$H-NMR



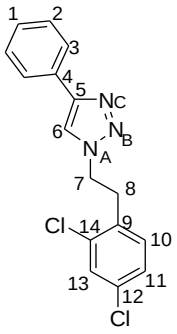

## $^{1}$H-$^{13}$C-gHMBC



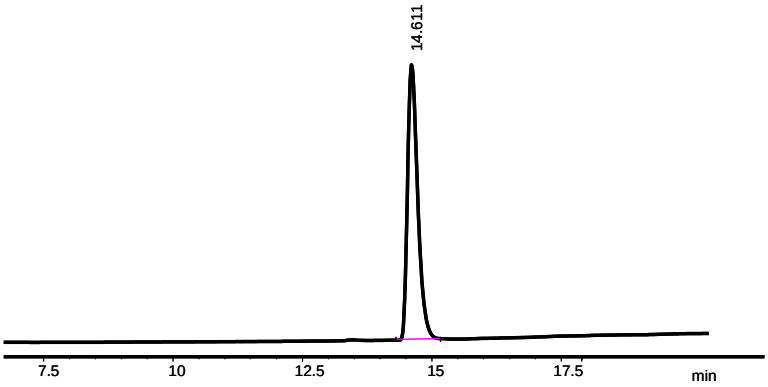
## $^{1}H$-$^{15}N$-gHMBC



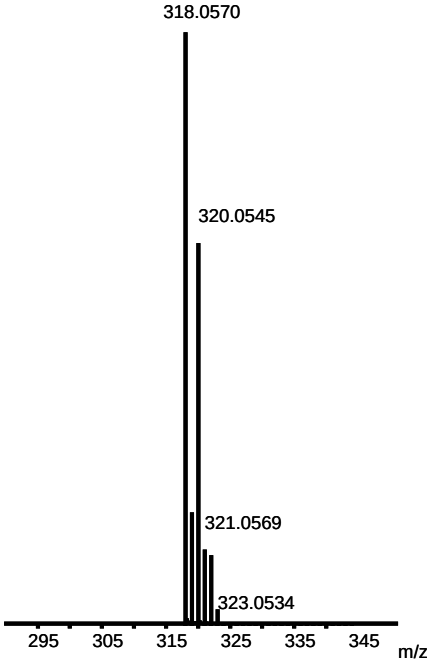
## 1-(*2,4*-dichlorophenethyl)-4-phenyl-1,2,3-triazole (1d)



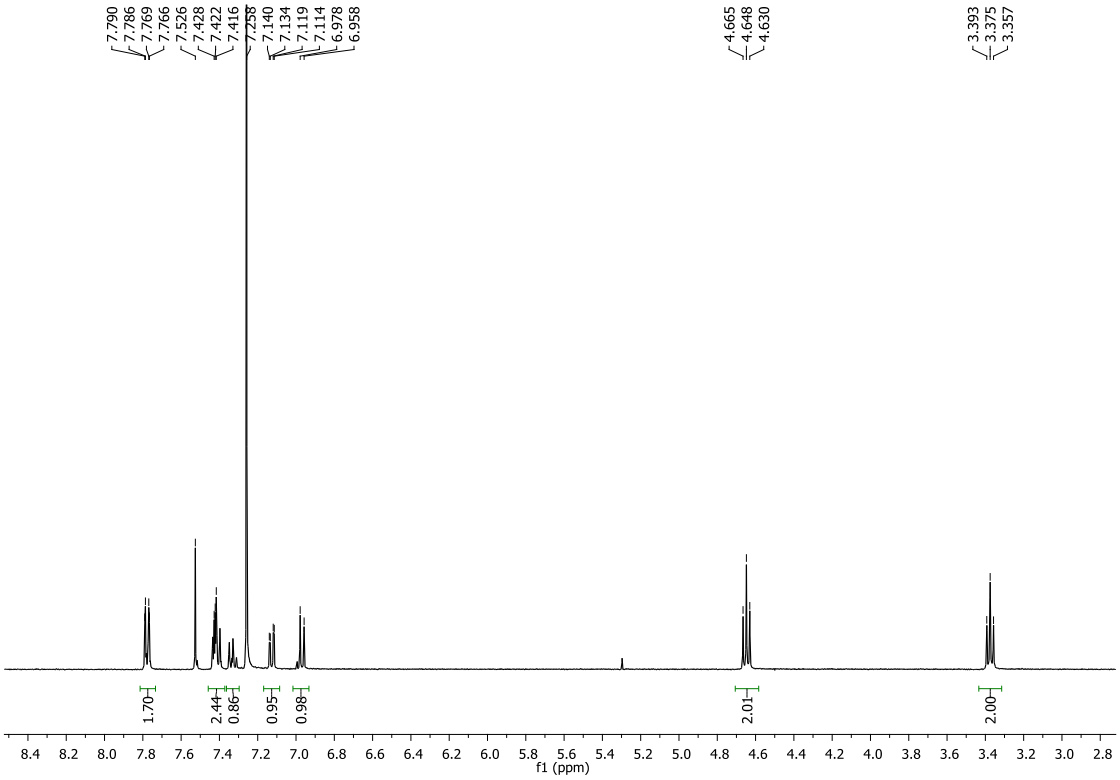

### HPLC




### HRMS



## $^{1}$H-NMR

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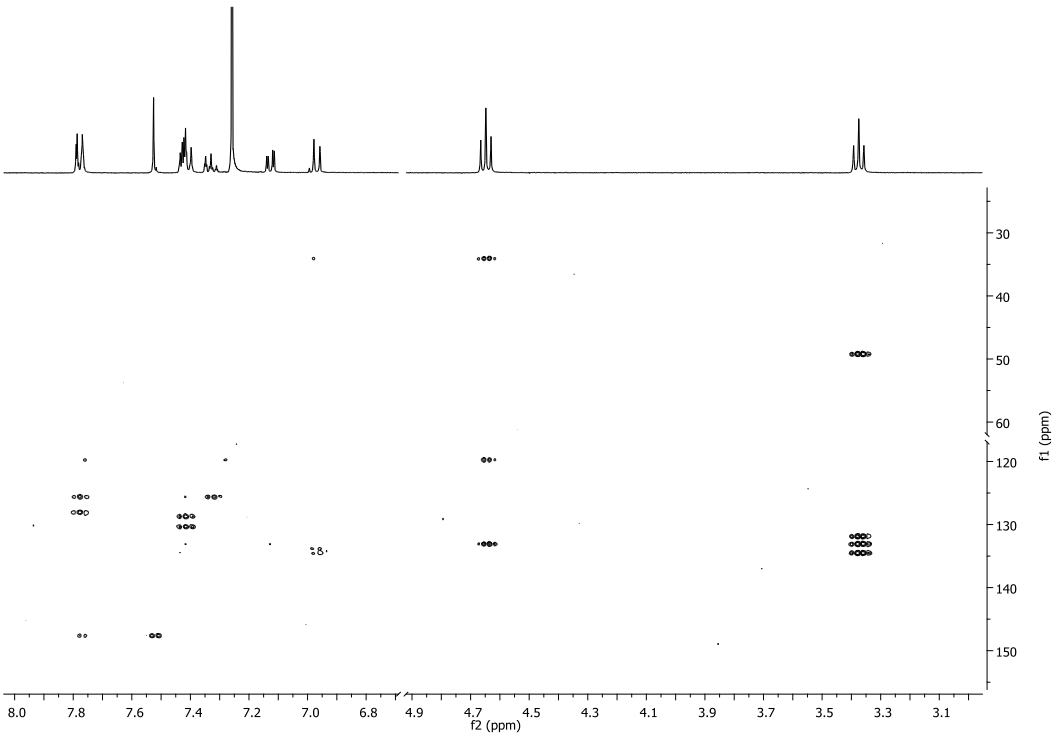
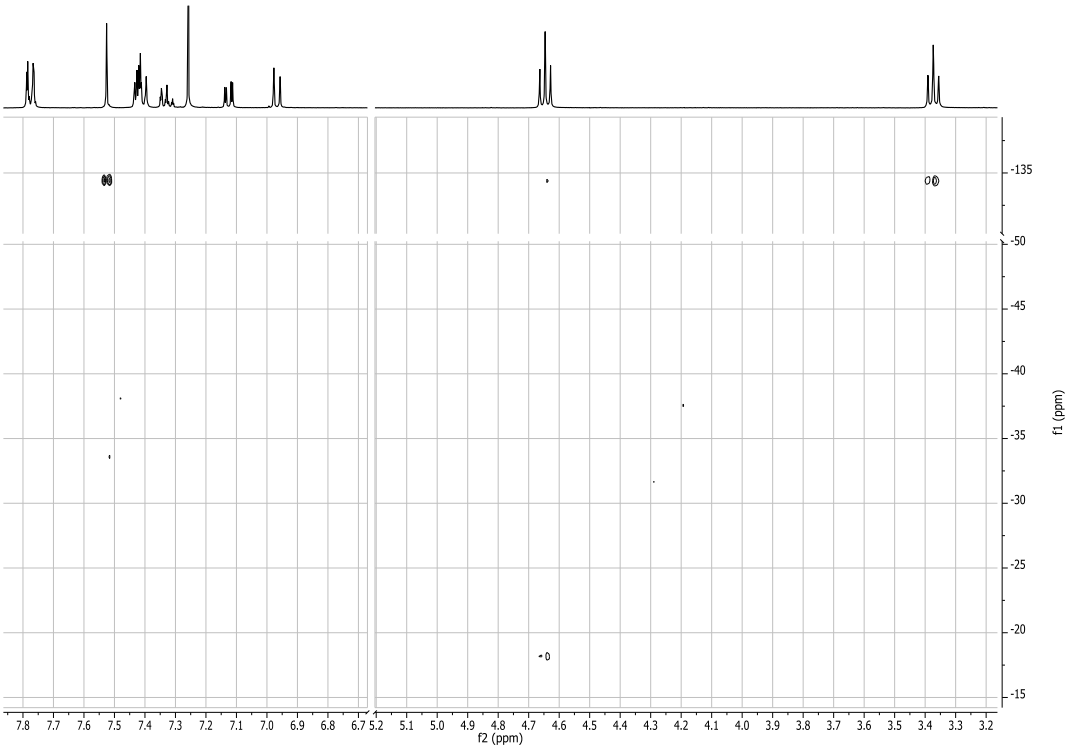
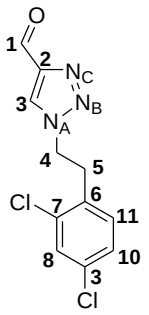


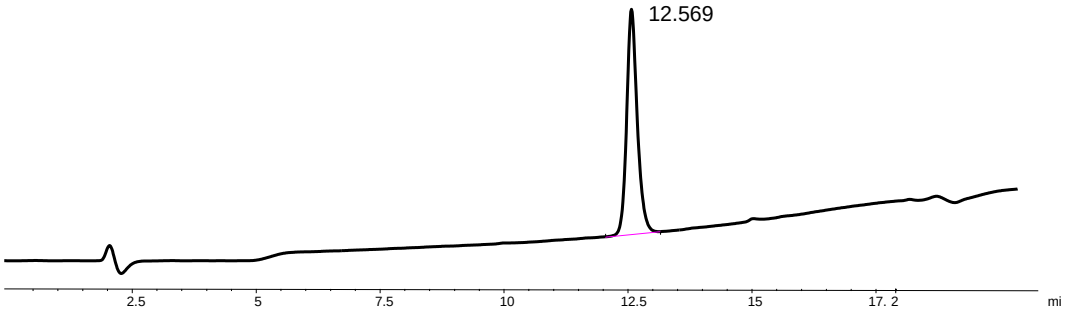
## $^{1}H$-$^{15}N$-gHMBC



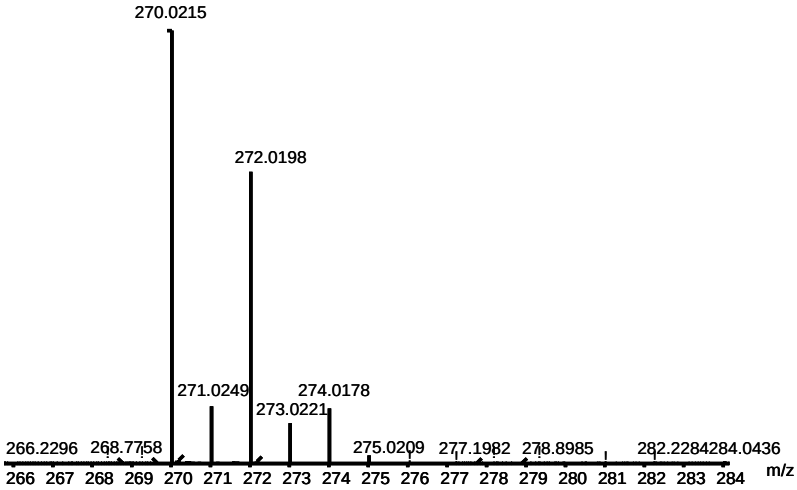
## 1-(2,4-Dichlorophenethyl)-4-formyl-*1H*-1,2,3-triazole (4a)



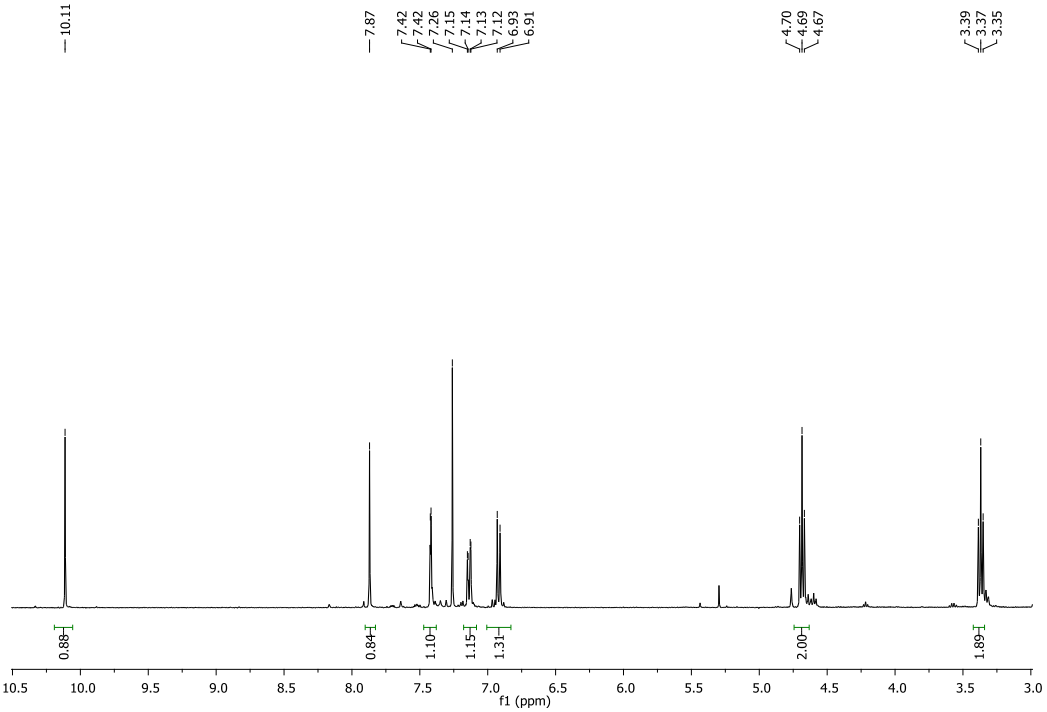

### HPLC



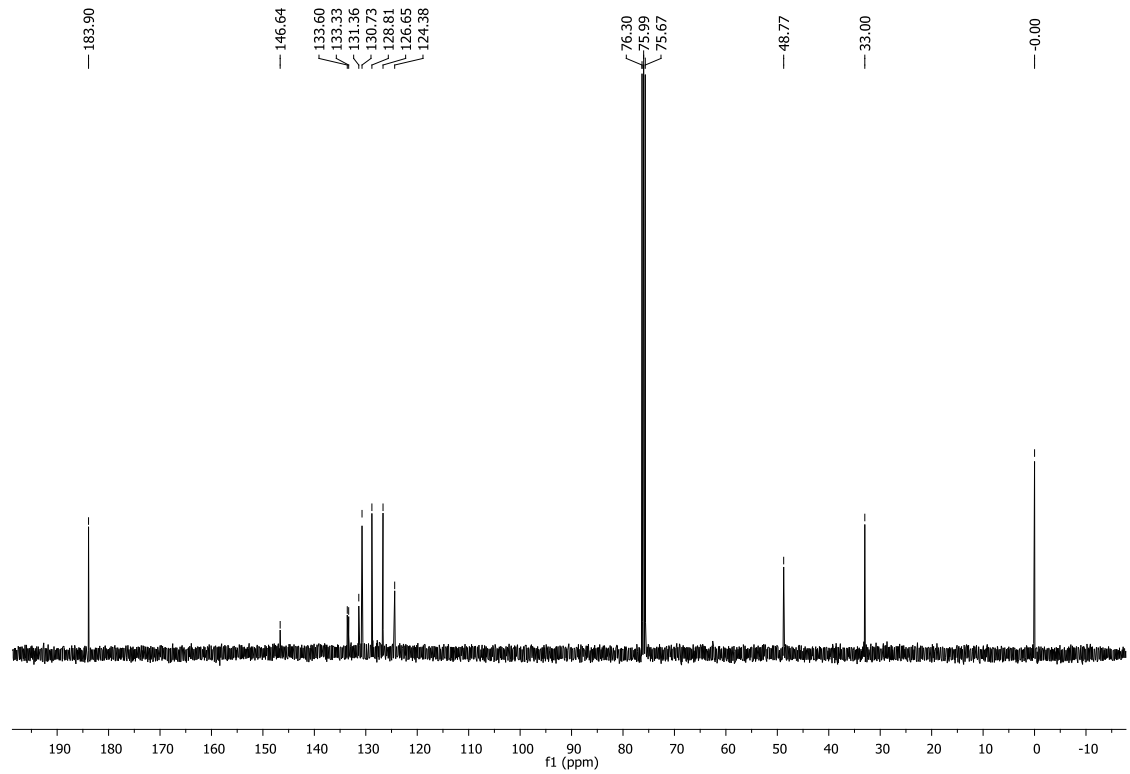

### HMRS



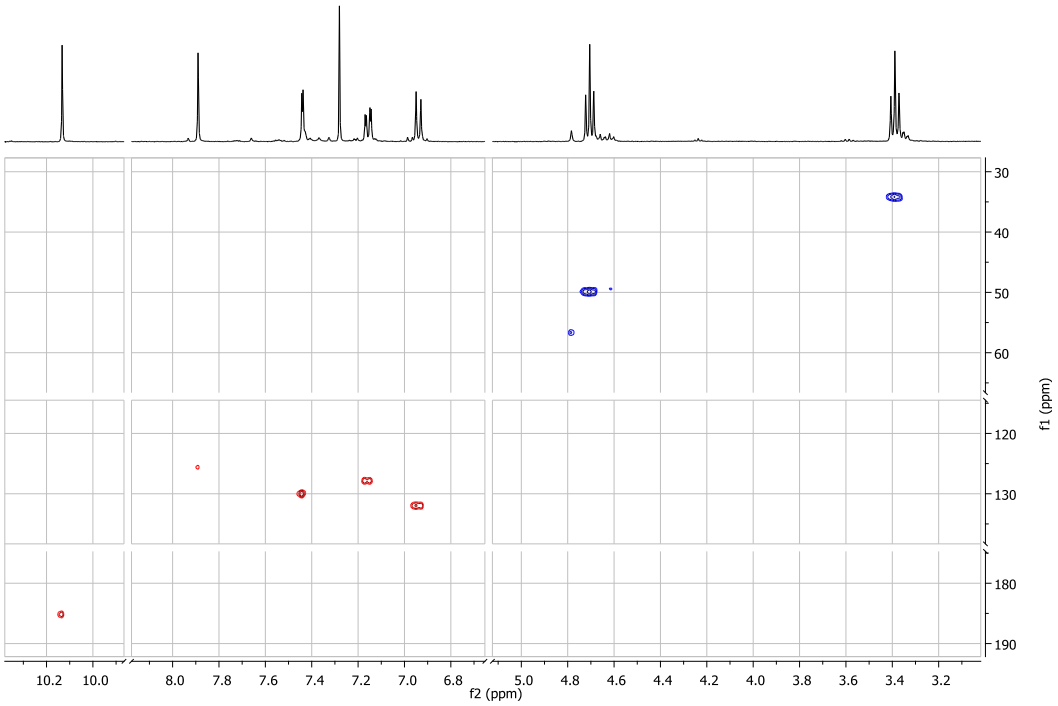
## $^{1}$H-NMR



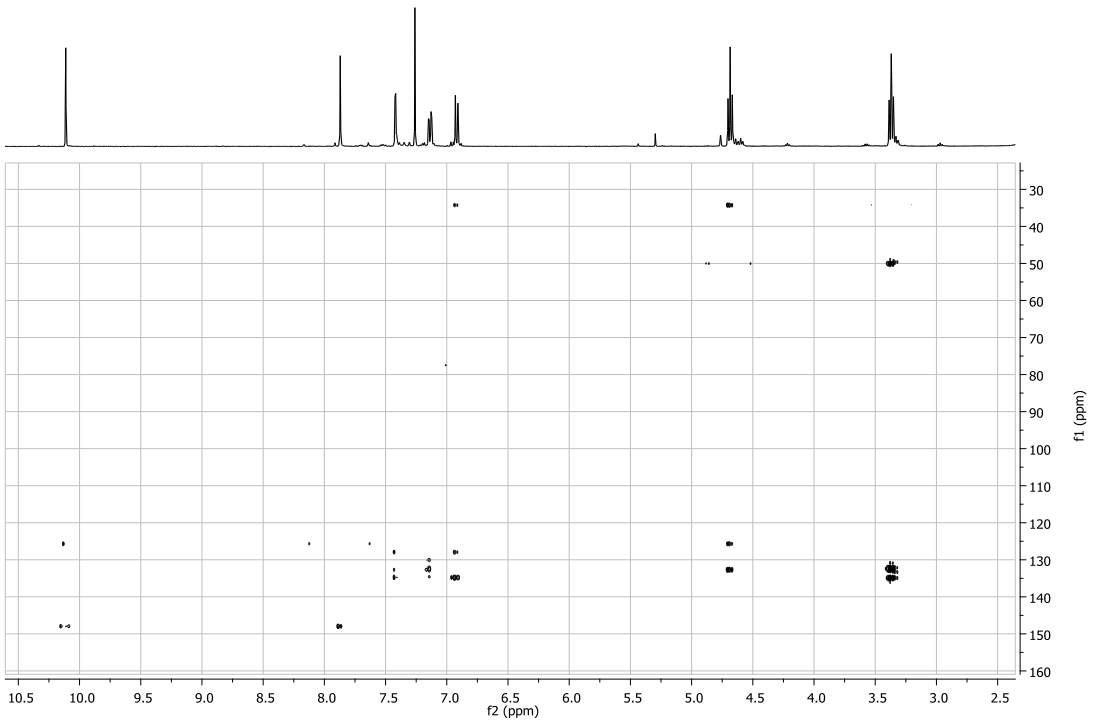

## $^{13}$C-NMR



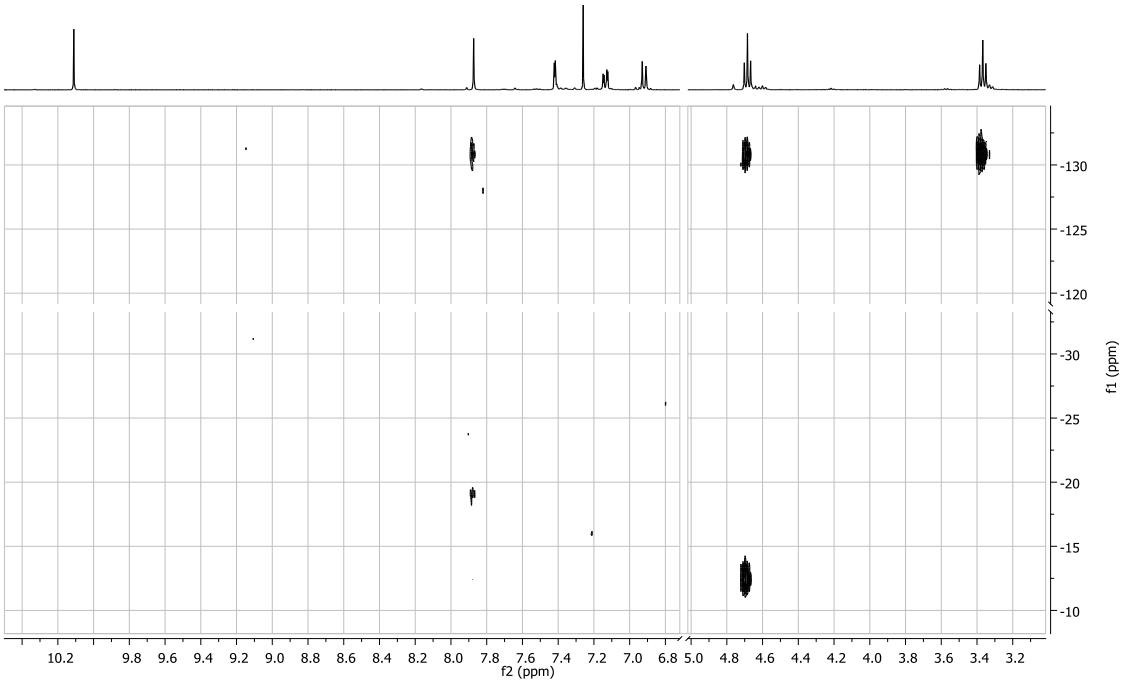
## $^{1}H$-$^{13}C$-gHSQC



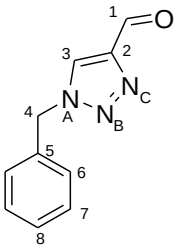

## $^{1}H$-$^{13}C$-gHMBC



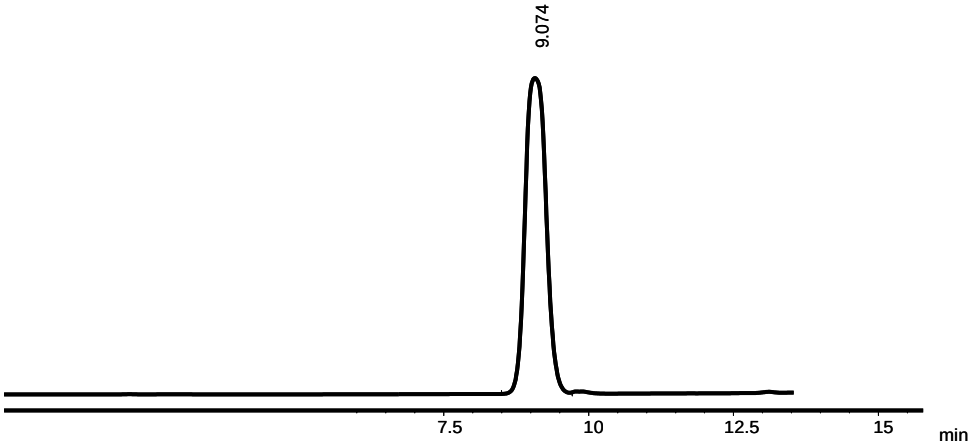
## $^{1}H$-$^{15}N$-HMBC



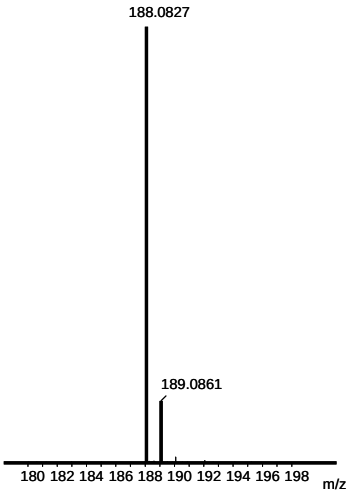
## 1-benzyl-4-formyl-1H-1,2,3-triazole (4b)



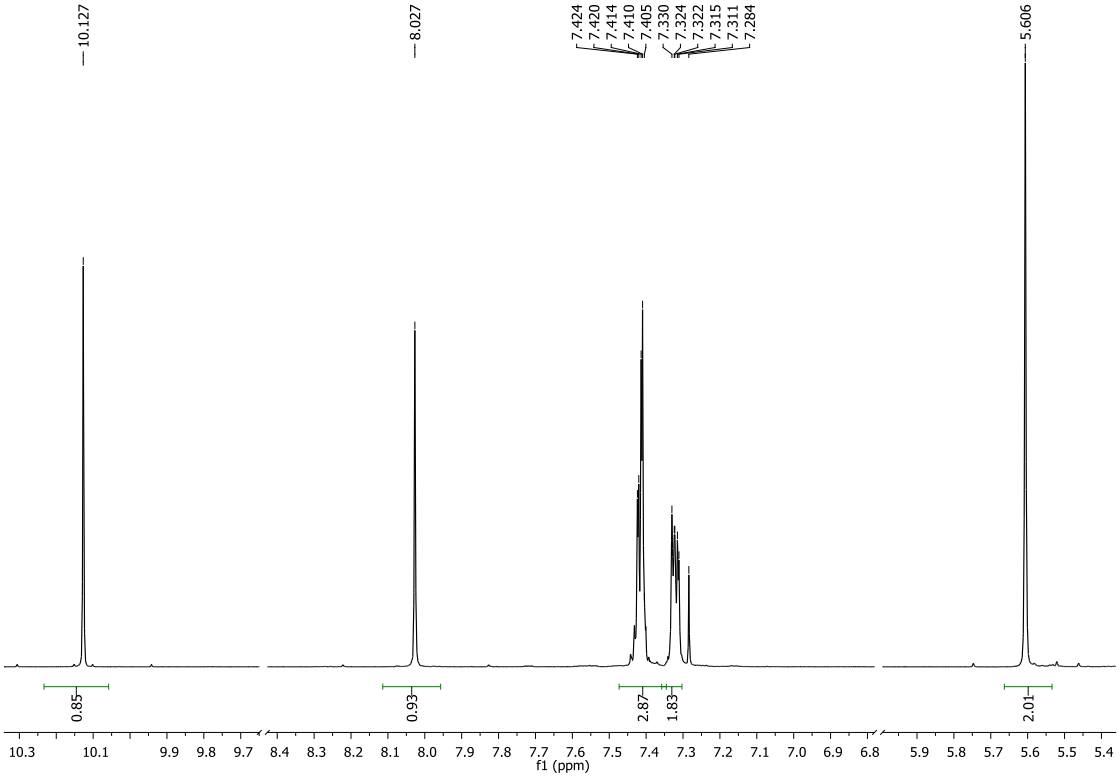

## HPLC



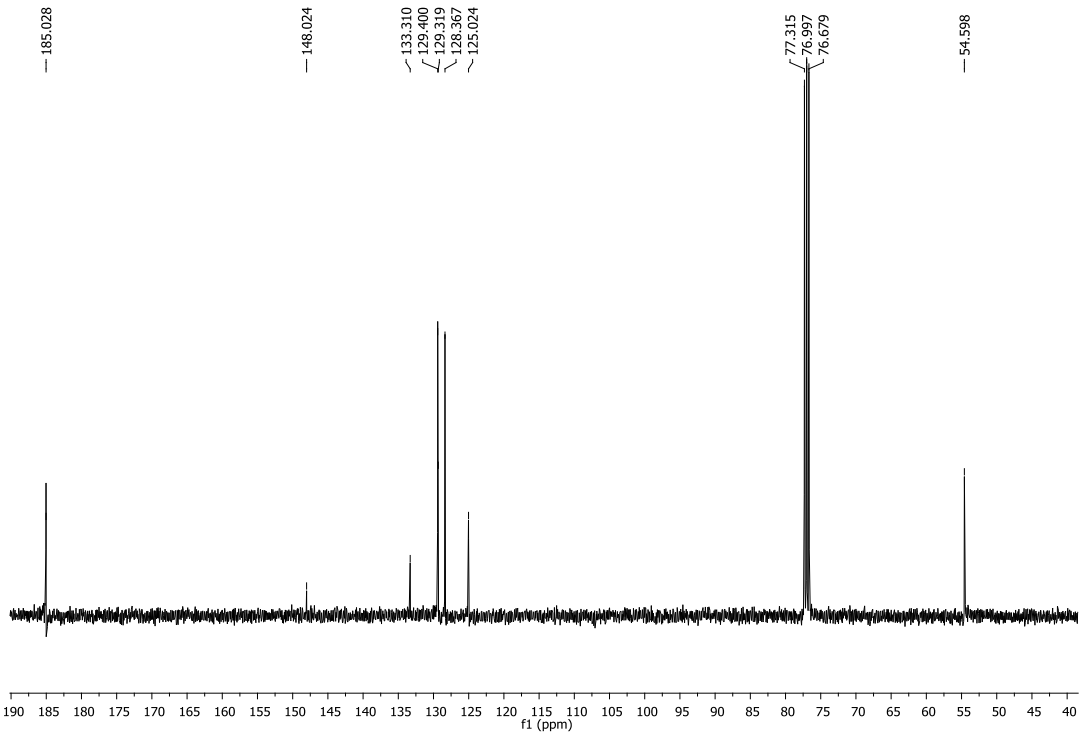

## HRMS



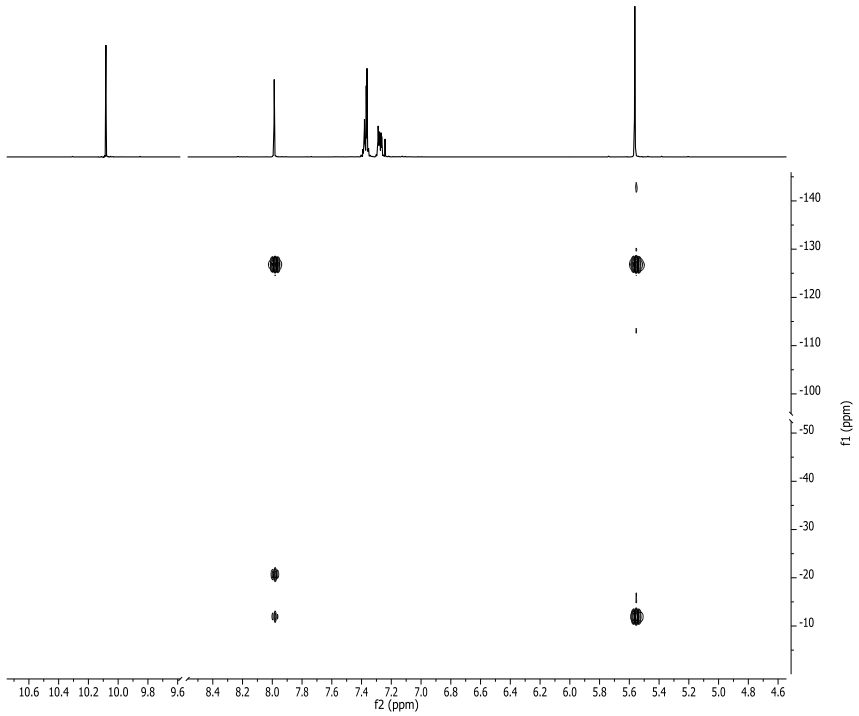
## $^{1}$H-NMR



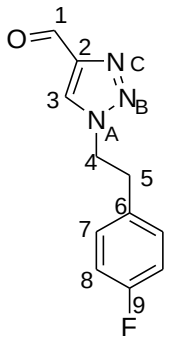

## $^{13}$C-NMR



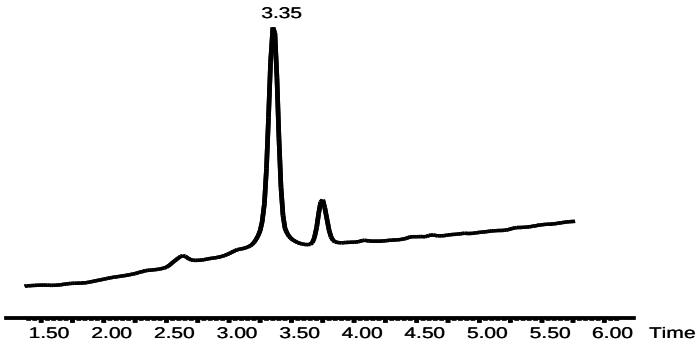
**$^{1}$H-$^{15}$N HMBC**



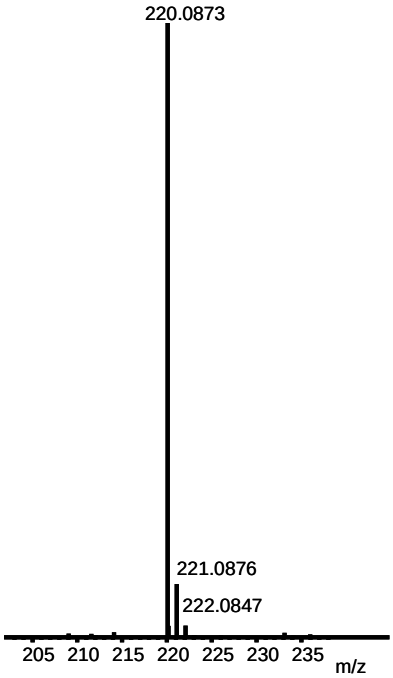
**1-(4-Fluorophenethyl)-4-formyl-1*H*-1,2,3-triazole (4b)**



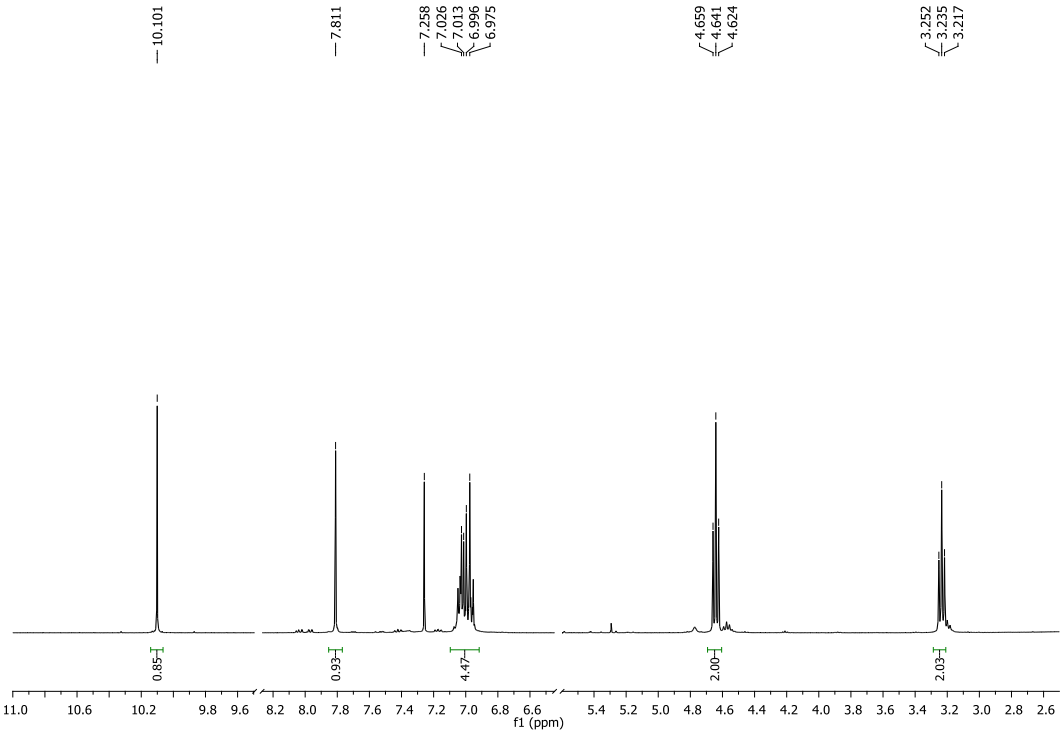

**HPLC**



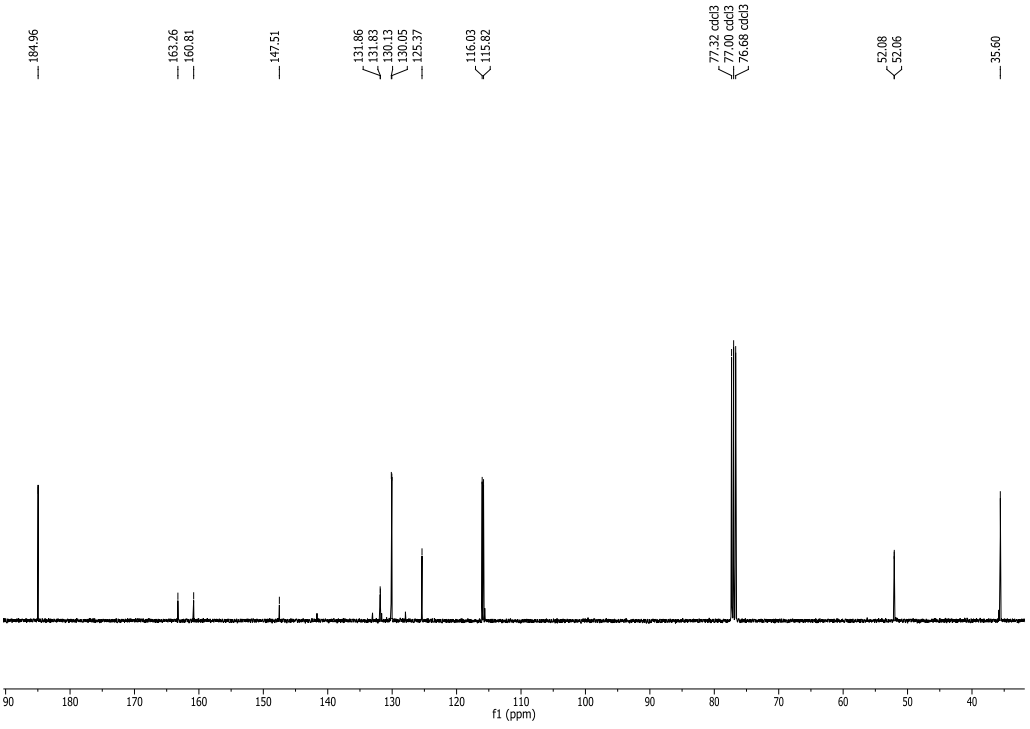

**HRMS**



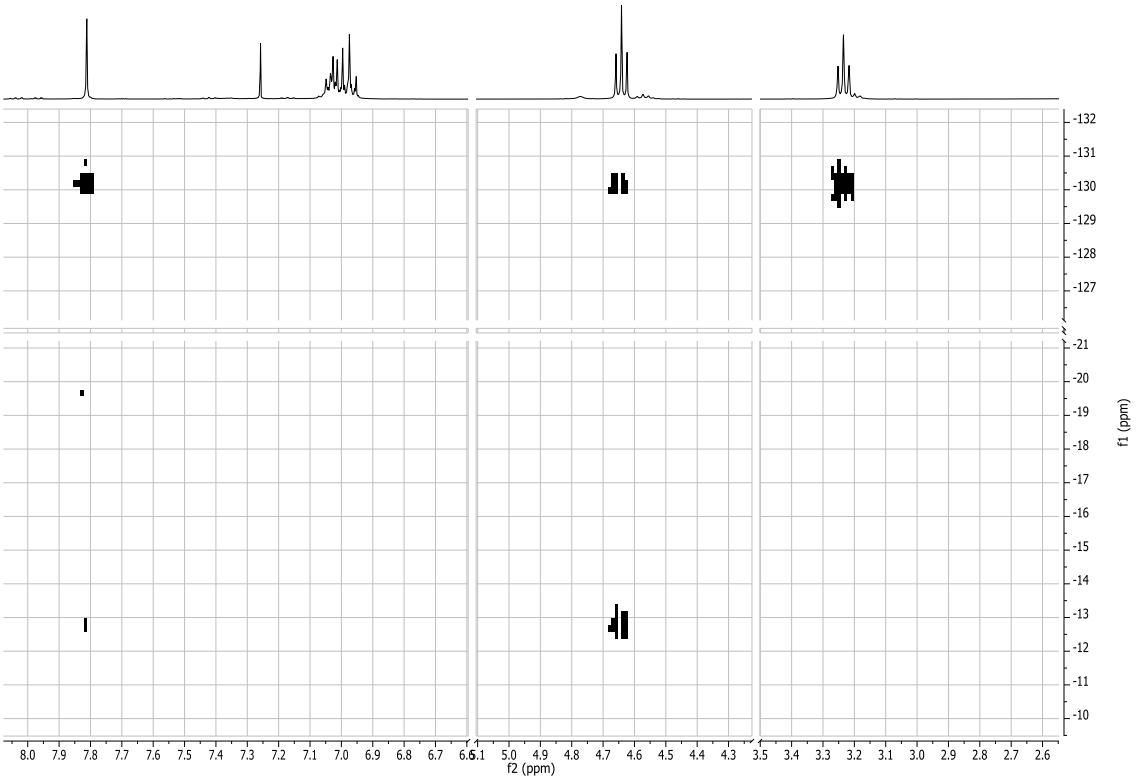
## $^{1}$H-NMR




## $^{13}$C-NMR

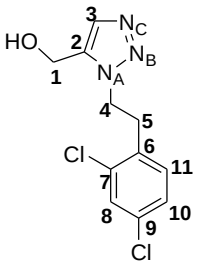


## $^{1}H$-$^{15}N$-gHMBC

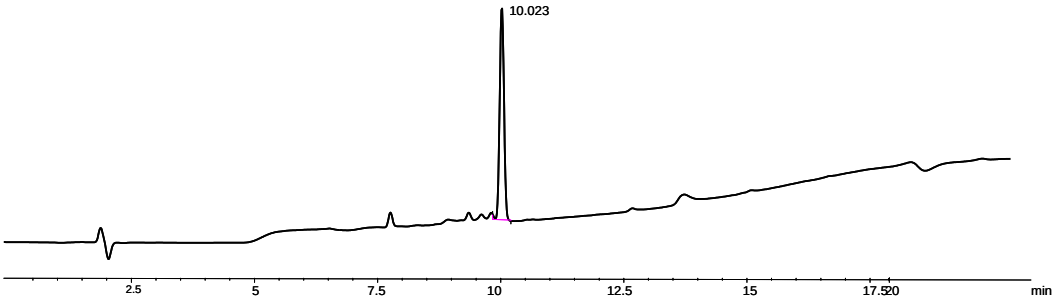


## 2. 1,5-Disubstituted-1,2,3-triazoles (1,5-TAs)

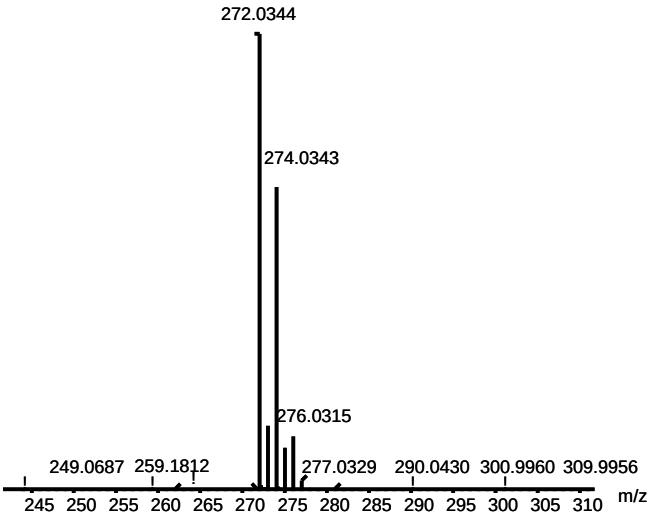
### 1-(2',4'-Dichlorophenethyl)-5-hydroxymethyl-1*H*-1,2,3-triazole (2a)



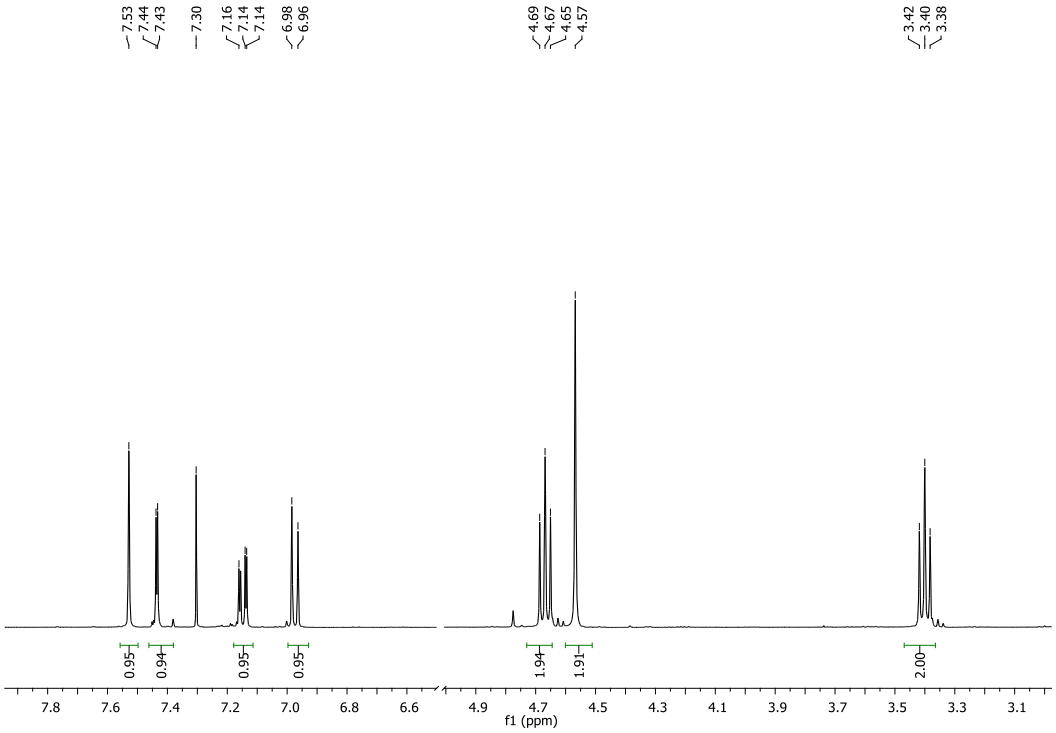

**HPLC**



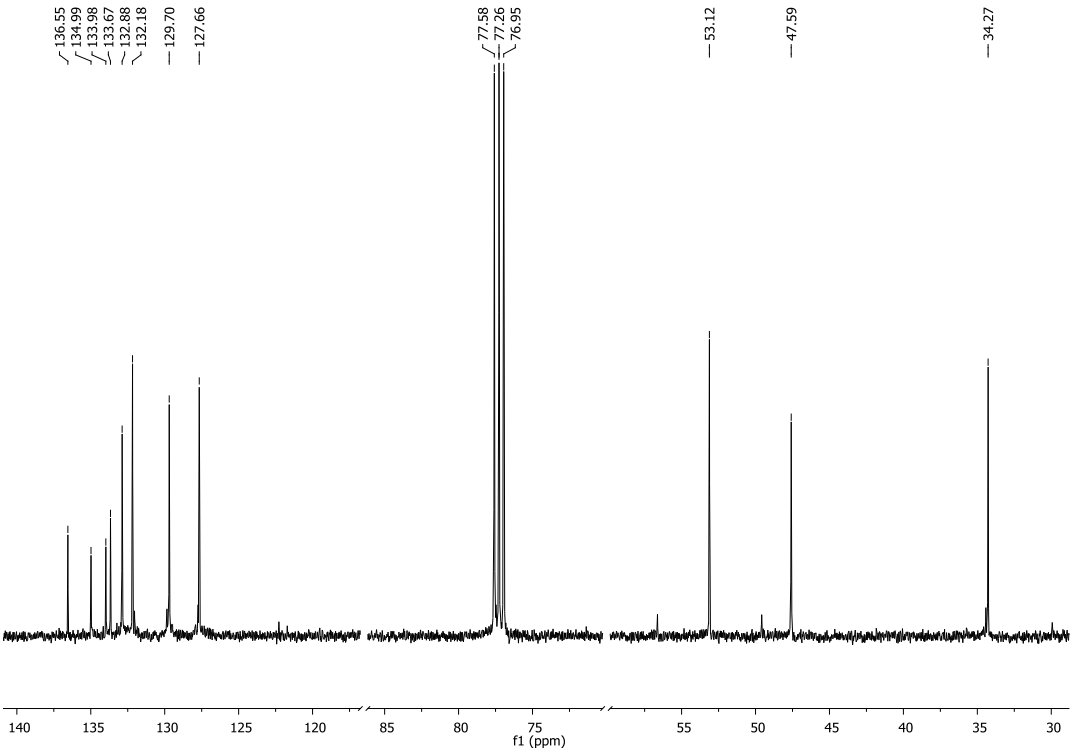

**HRMS**



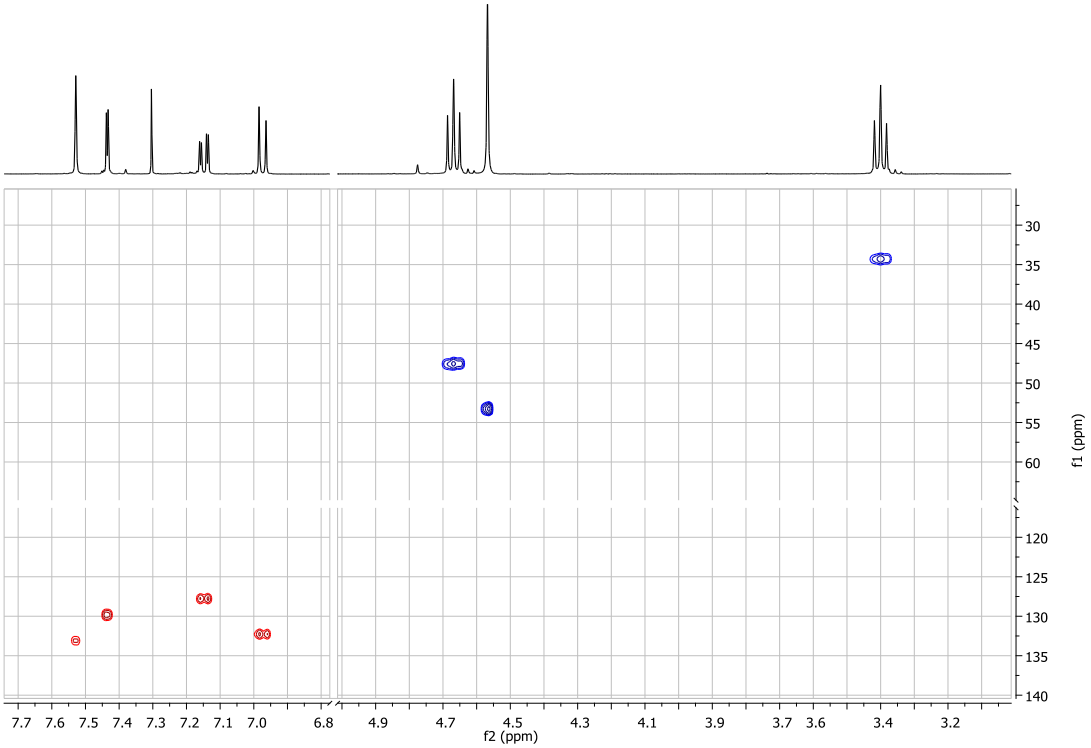
## $^{1}$H-NMR



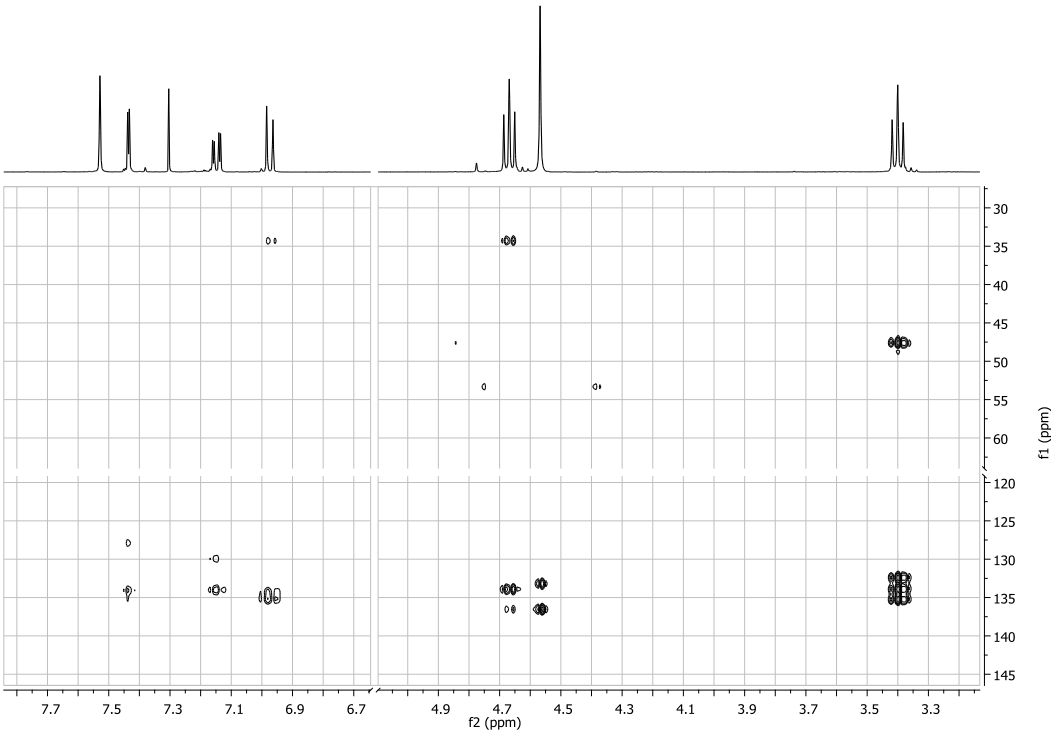

## $^{13}$C-NMR



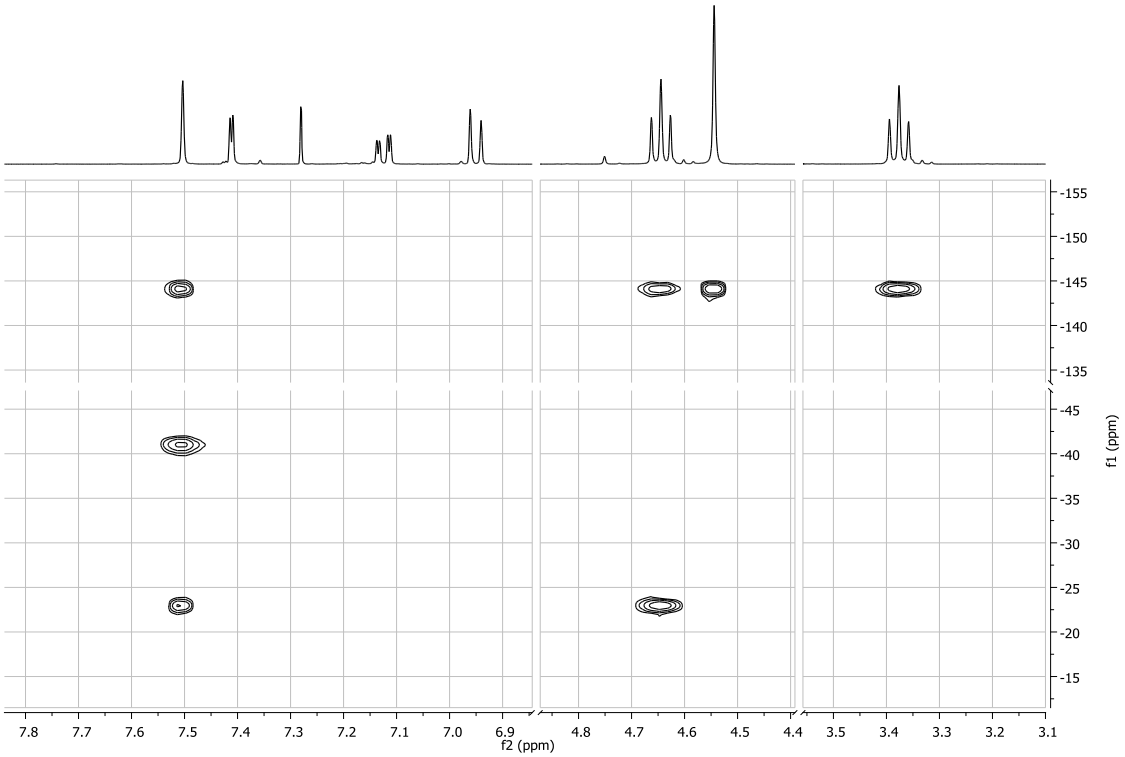
## $^{1}H$-$^{13}C$-gHSQC



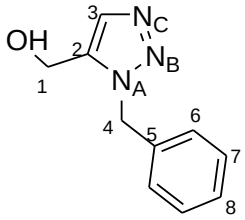

## $^{1}H$-$^{13}C$-gHMBC



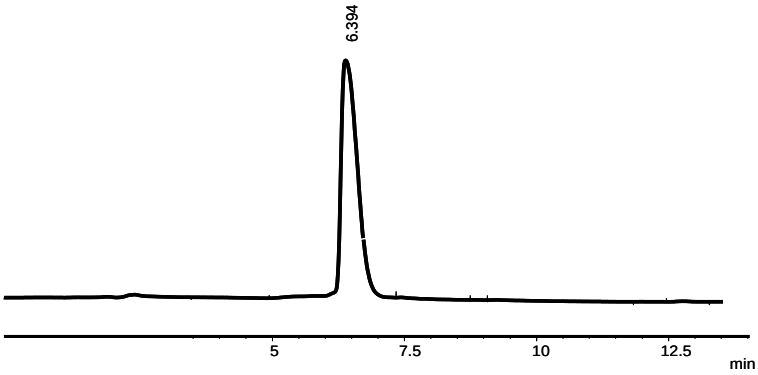
## $^{1}H$-$^{15}N$-gHMBC



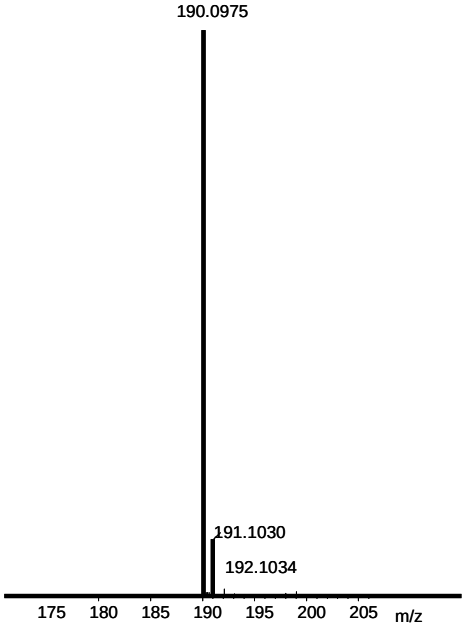
## 1-(benzyl)-5-hydroxymethyl-1*H*-1,2,3-triazole (2b)



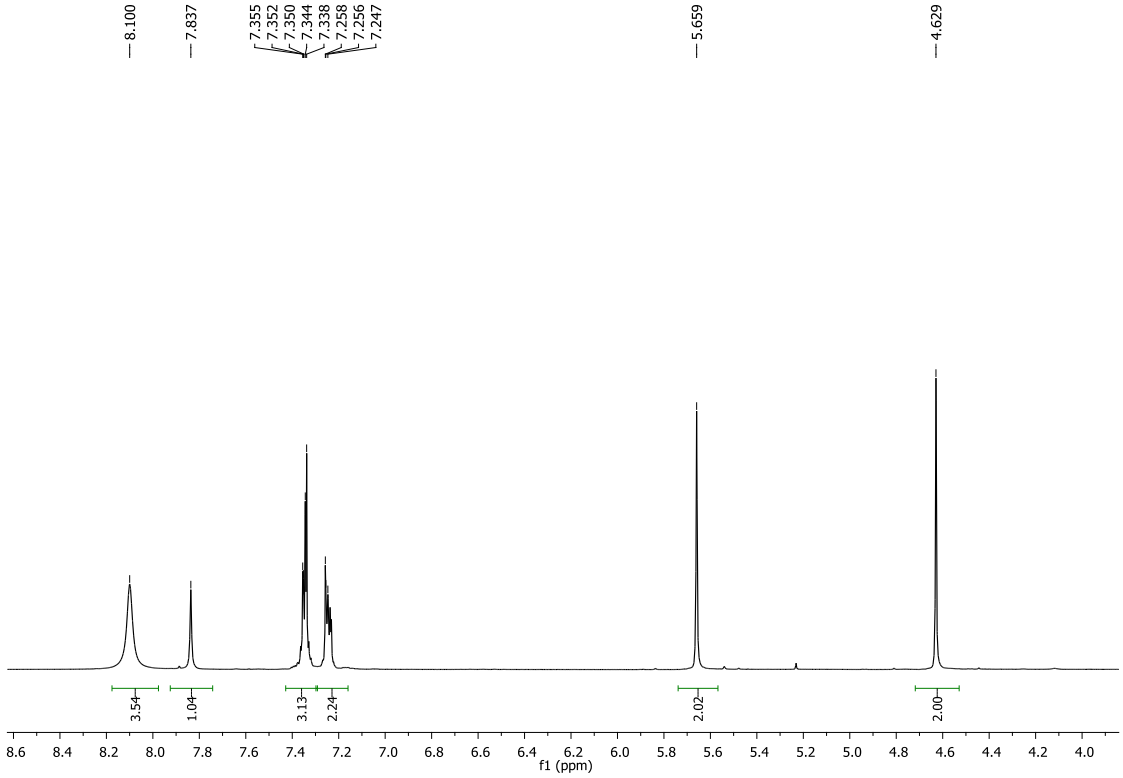

### HPLC



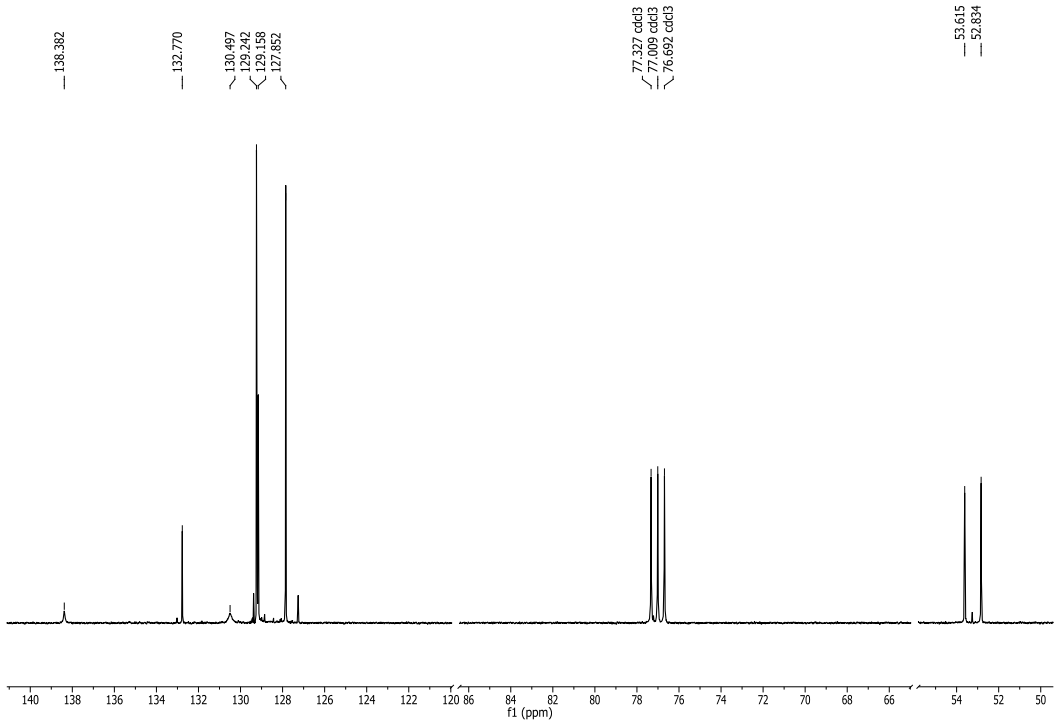

### HRMS



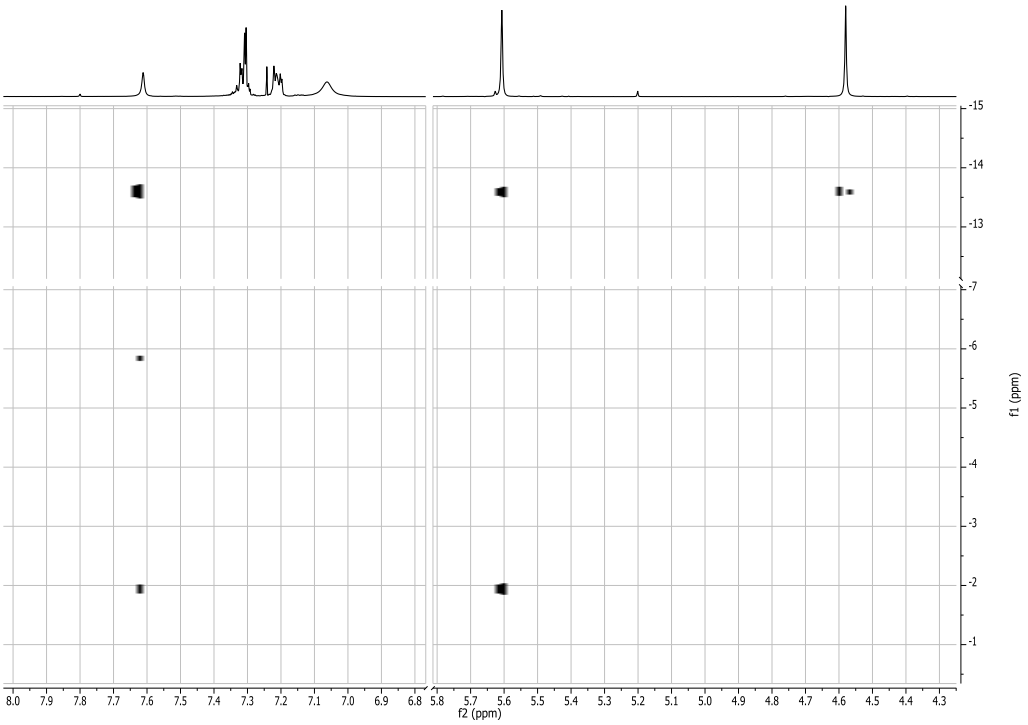
## $^{1}$H-NMR



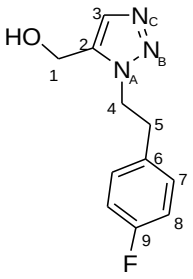

## $^{13}$C-NMR



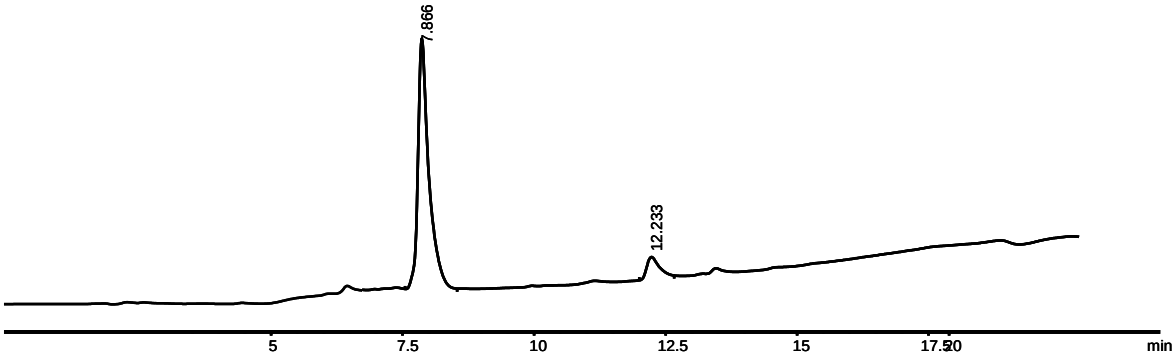
## $^{1}H$-$^{15}N$-gHMBC



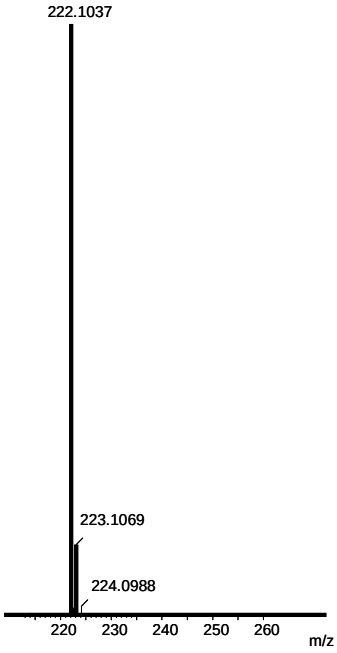
## 1-(4-Fluorophenethyl)-5-hydroxymethyl-*1H*-1,2,3-triazole (2c)



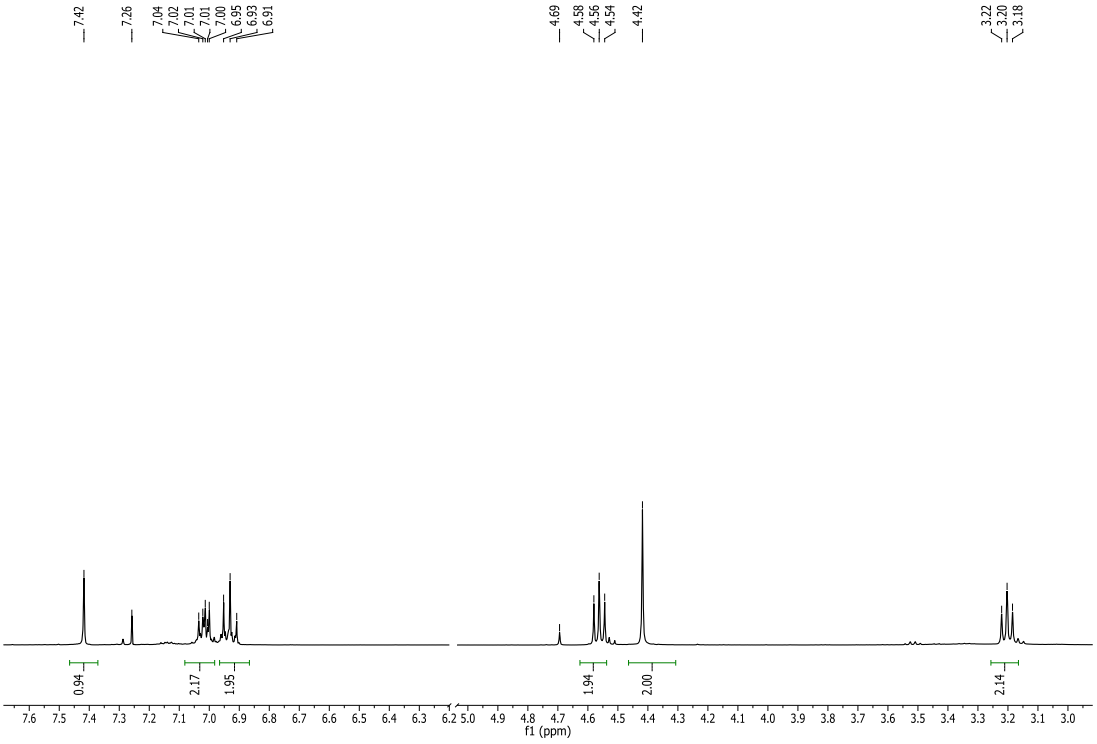

### HPLC



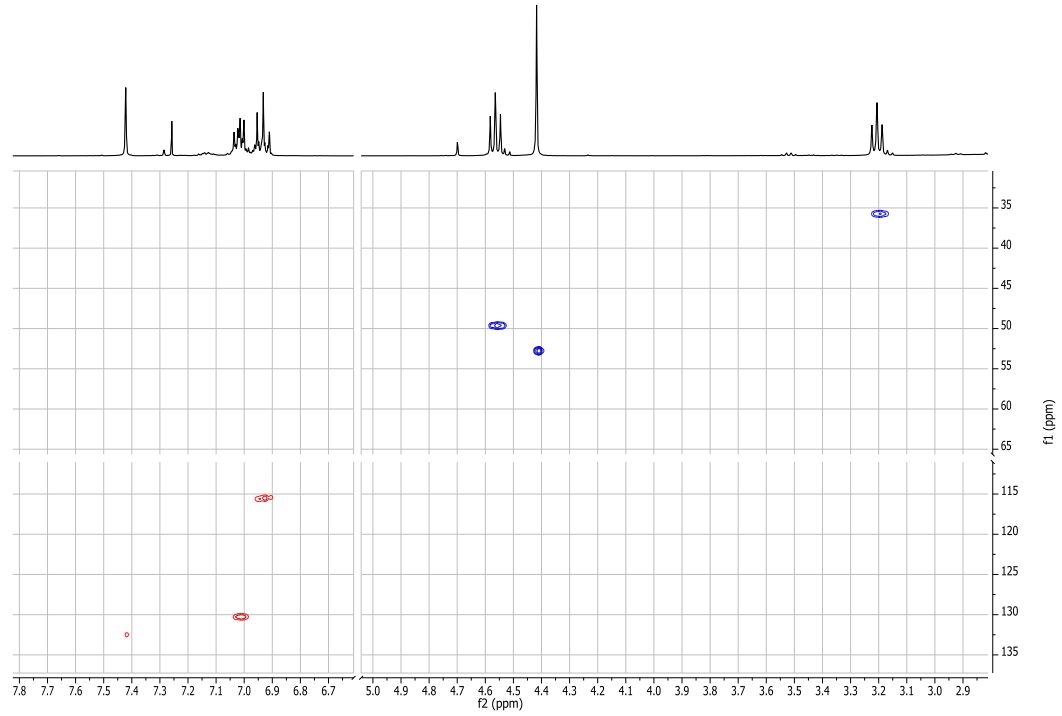

### HRMS



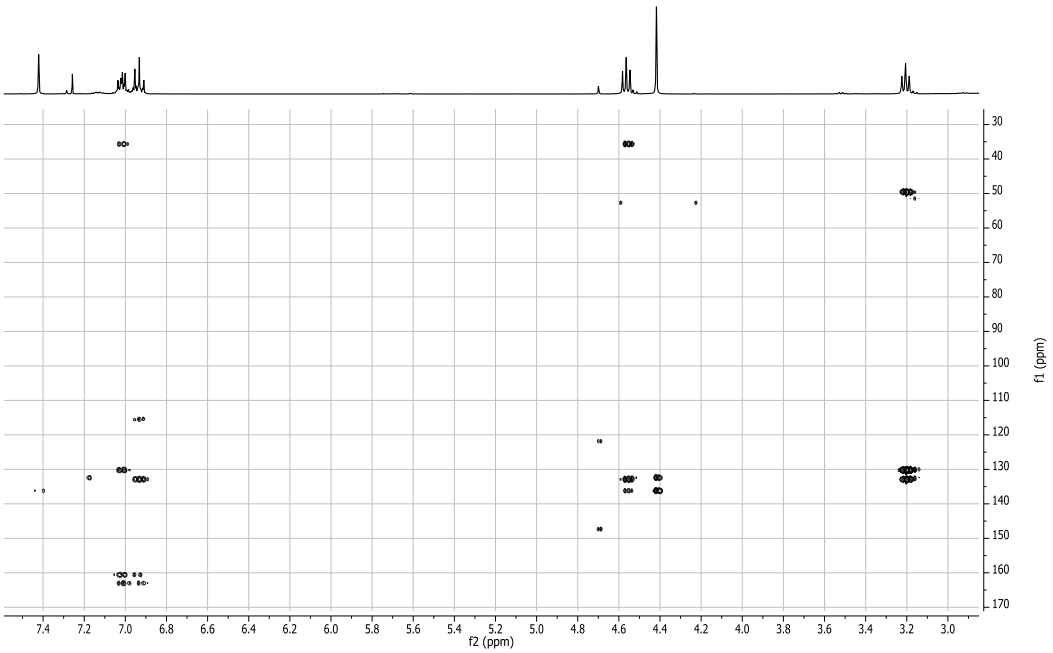
## $^{1}$H-NMR



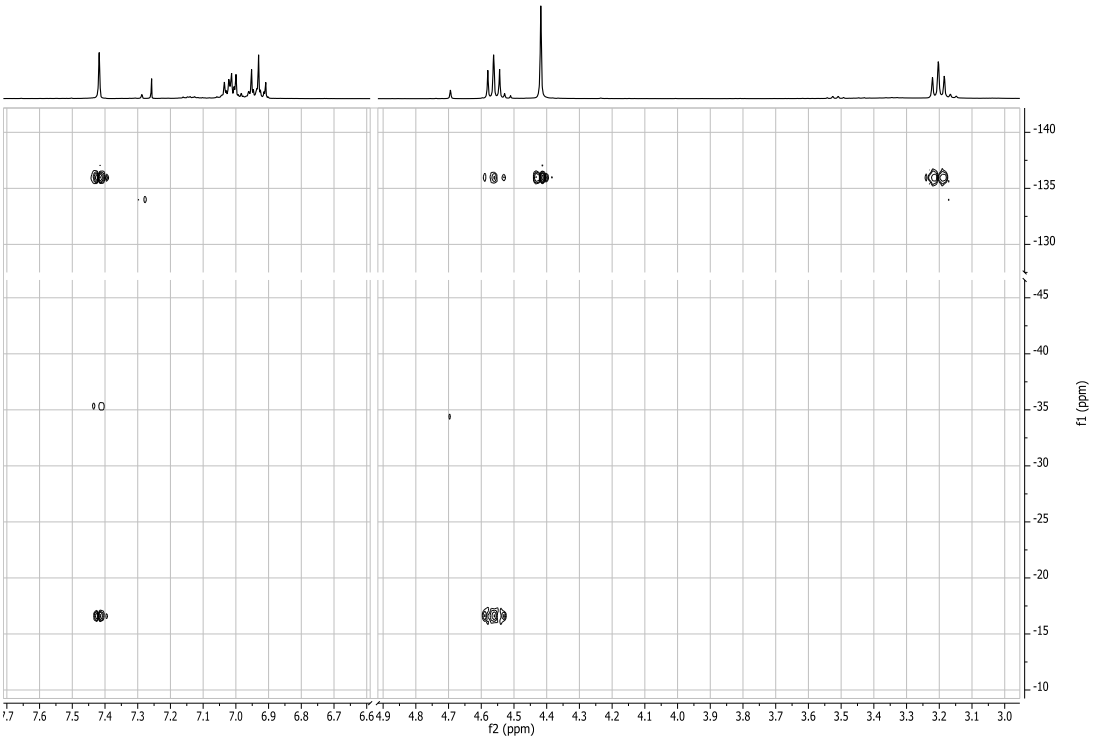

## $^{1}$H-$^{13}$C-gHSQC



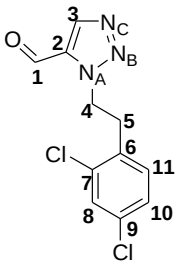
## $^{1}H$-$^{13}C$-gHMBC



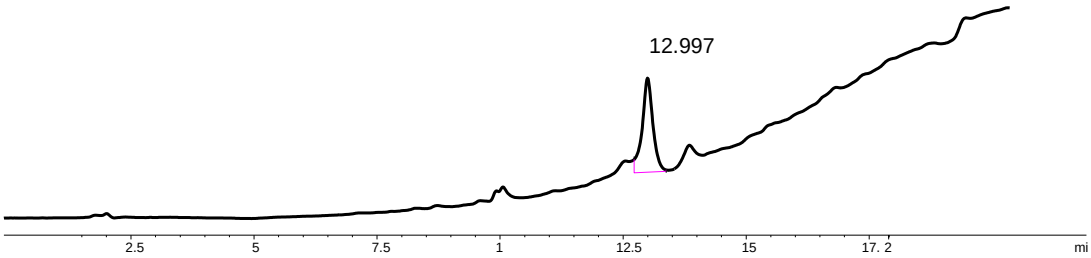

## $^{1}H$-$^{15}N$-gHMBC



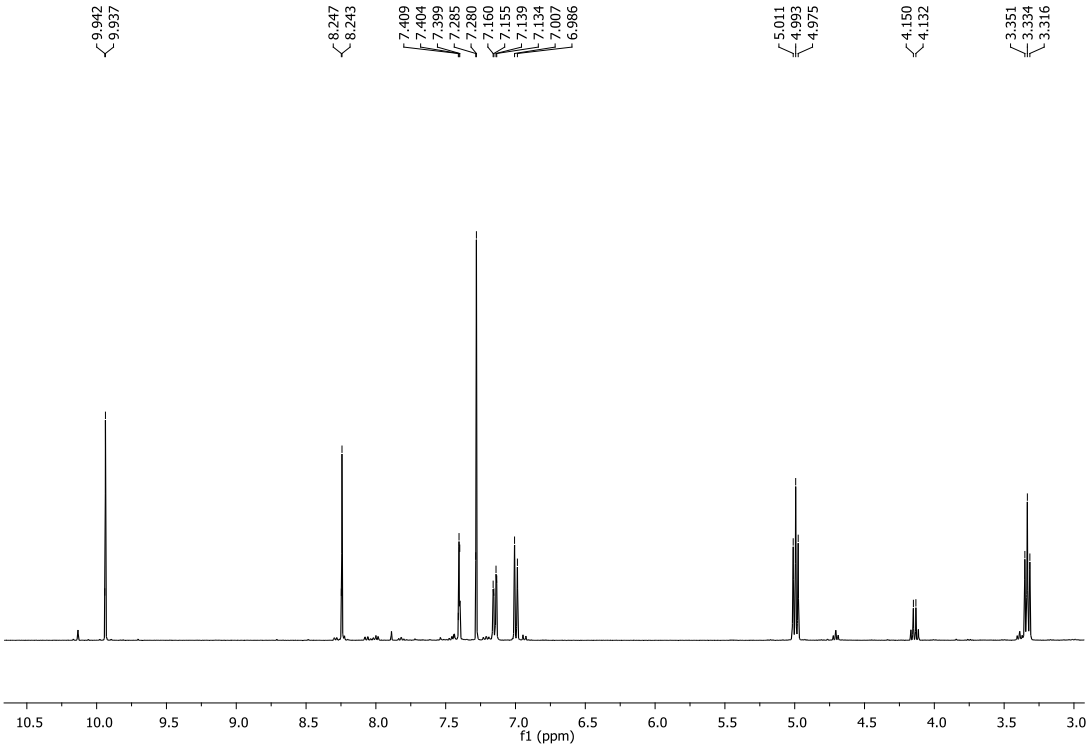
## 1-(2',4'-Dichlorophenethyl)-5-formyl-*1H*-1,2,3-triazole (5a)



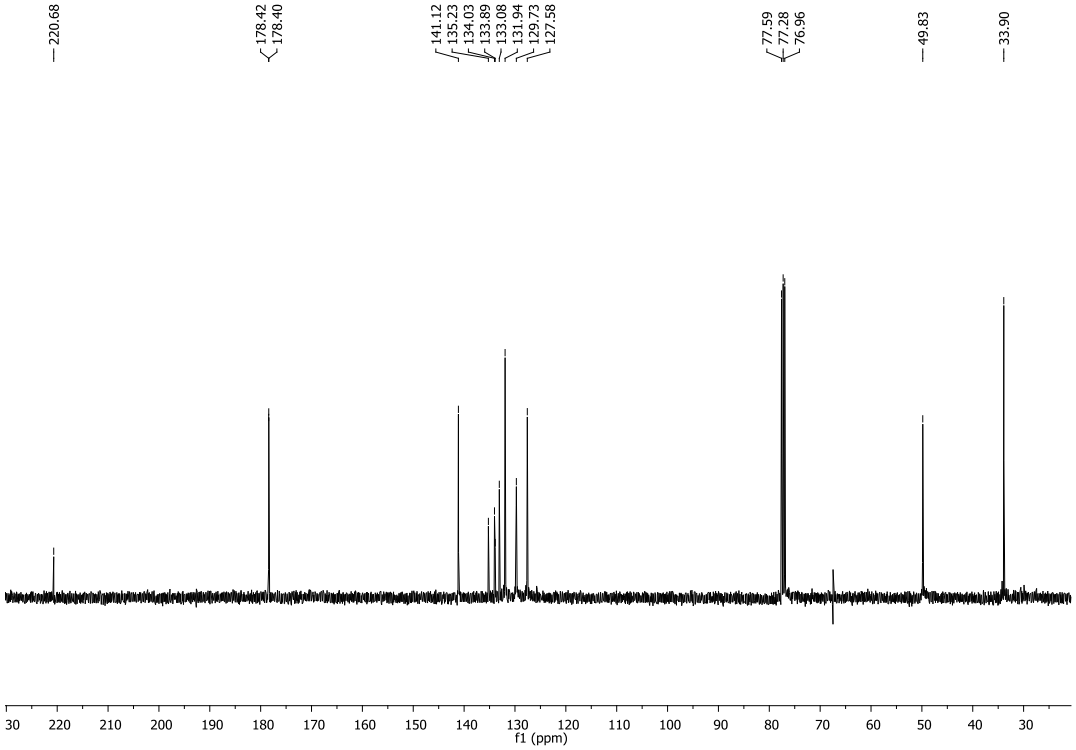

**HPLC:**



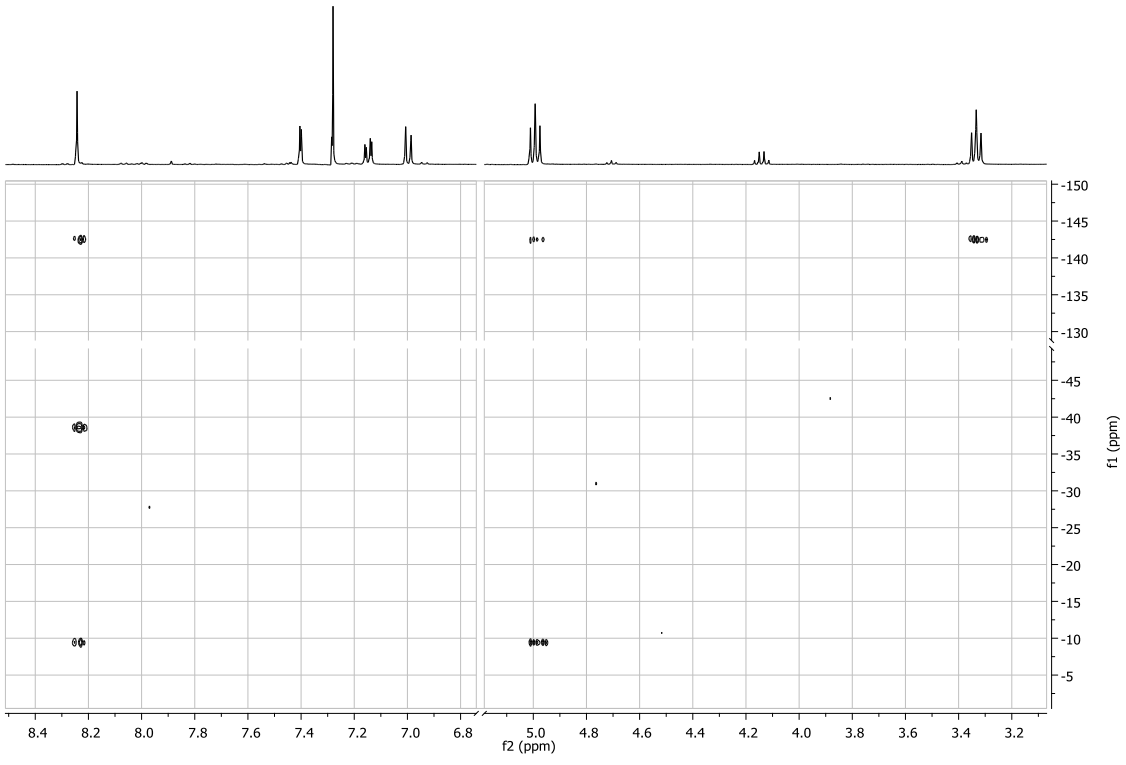

**$^{1}$H-NMR**



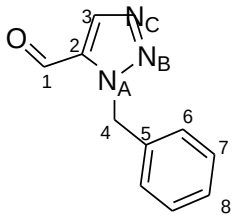
## $^{13}$C-NMR



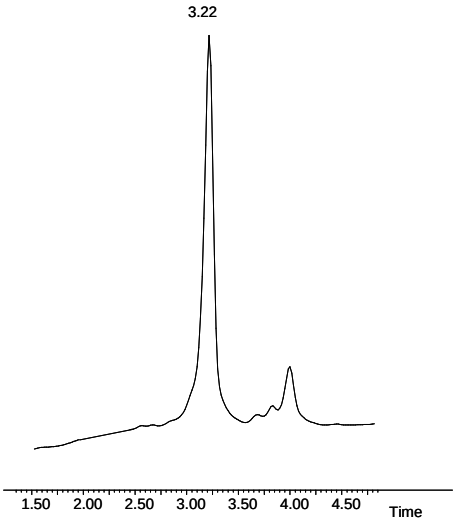

## $^{1}$H-$^{15}$N-gHMBC



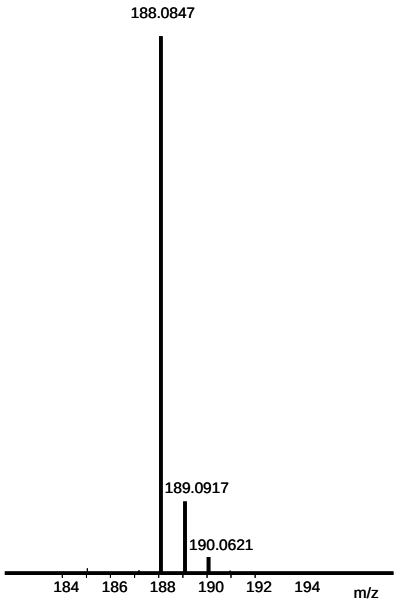
## 1-benzyl-5-formyl-1H-1,2,3-triazole (5b)



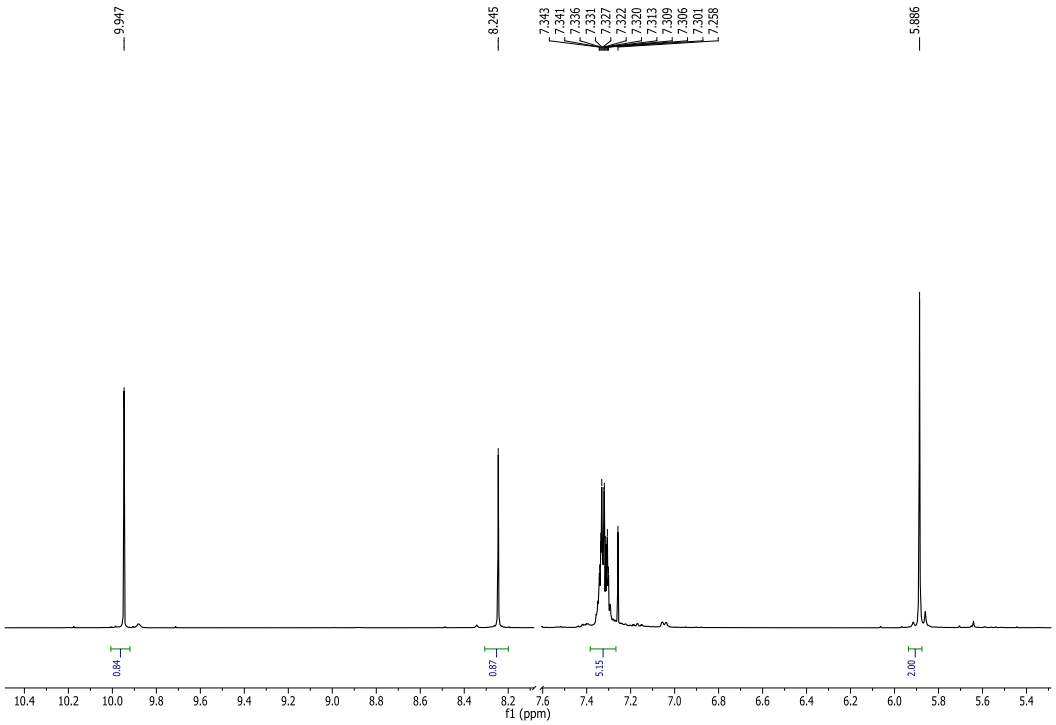

## HPLC



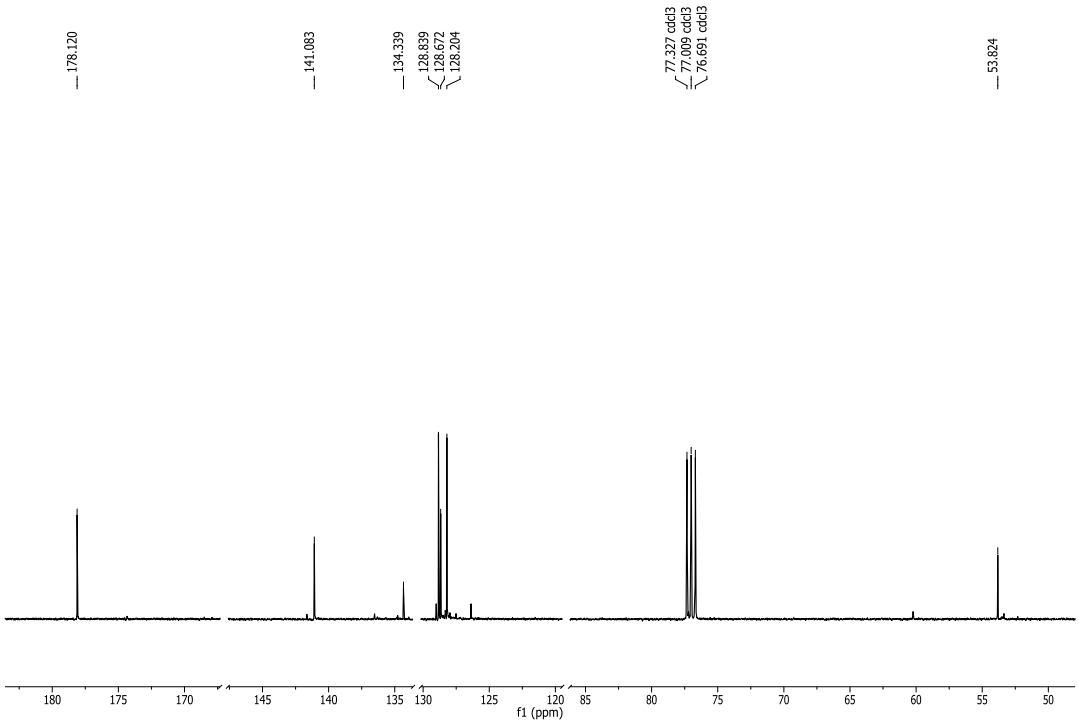

## HRMS



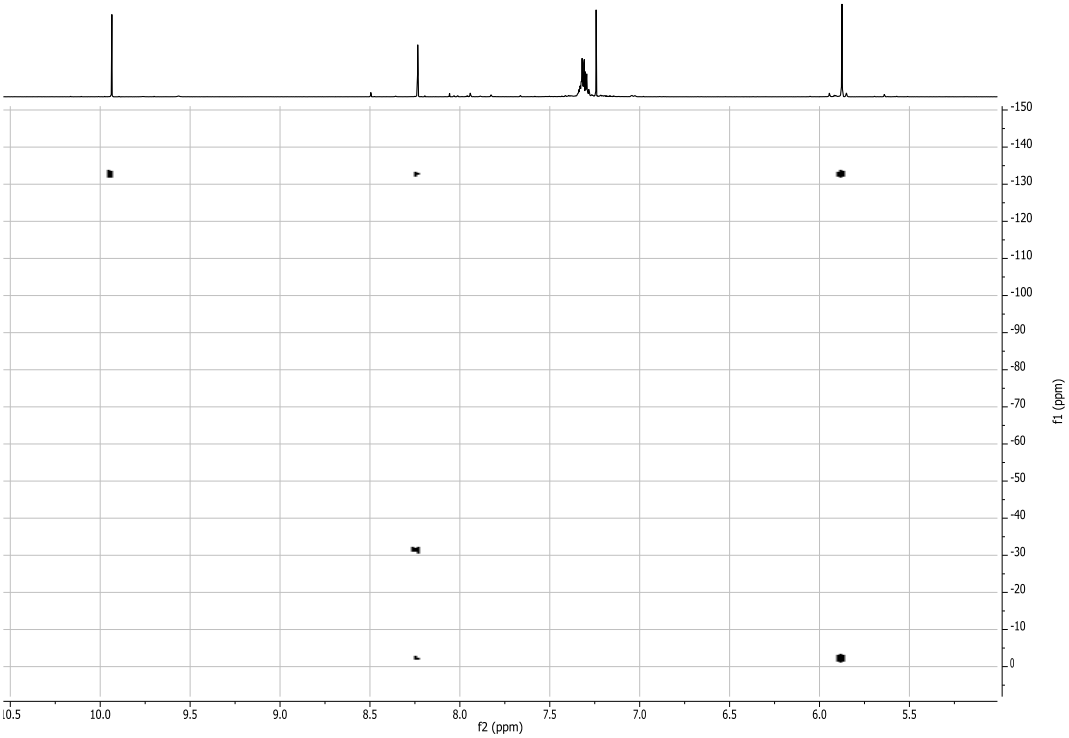
## $^{1}$H-NMR




## $^{13}$C-NMR

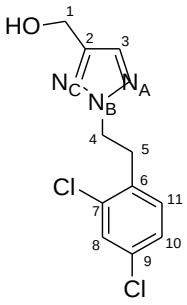


## $^{1}H$-$^{15}N$-gHMBC

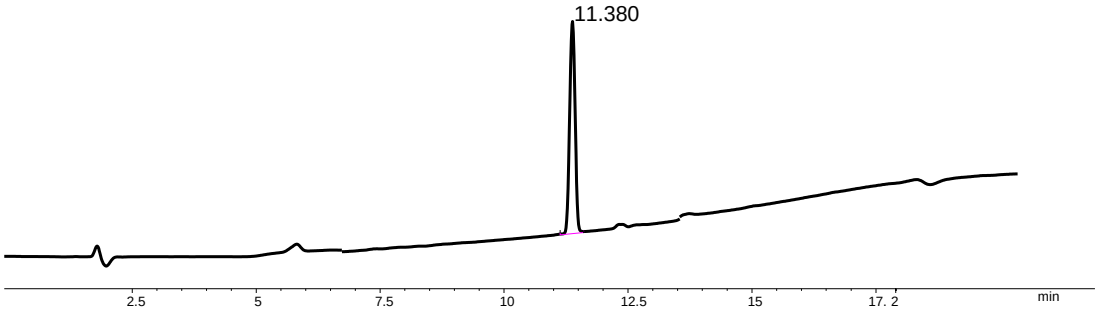


## 3. 2,4-Disubstituted-1,2,3-triazole derivatives (2,4-TA)

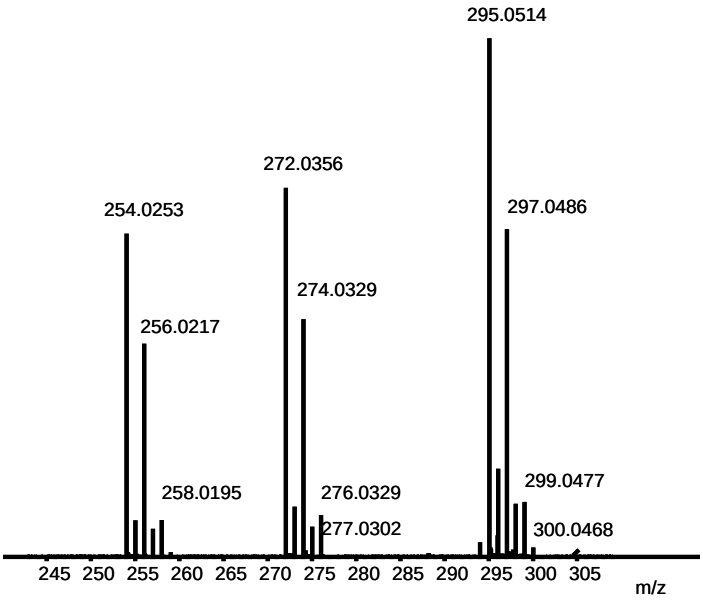
### 2-(2,4-Dichlorophenethyl)-4-hydroxymethyl-1*H*-1,2,3-triazole (3a)



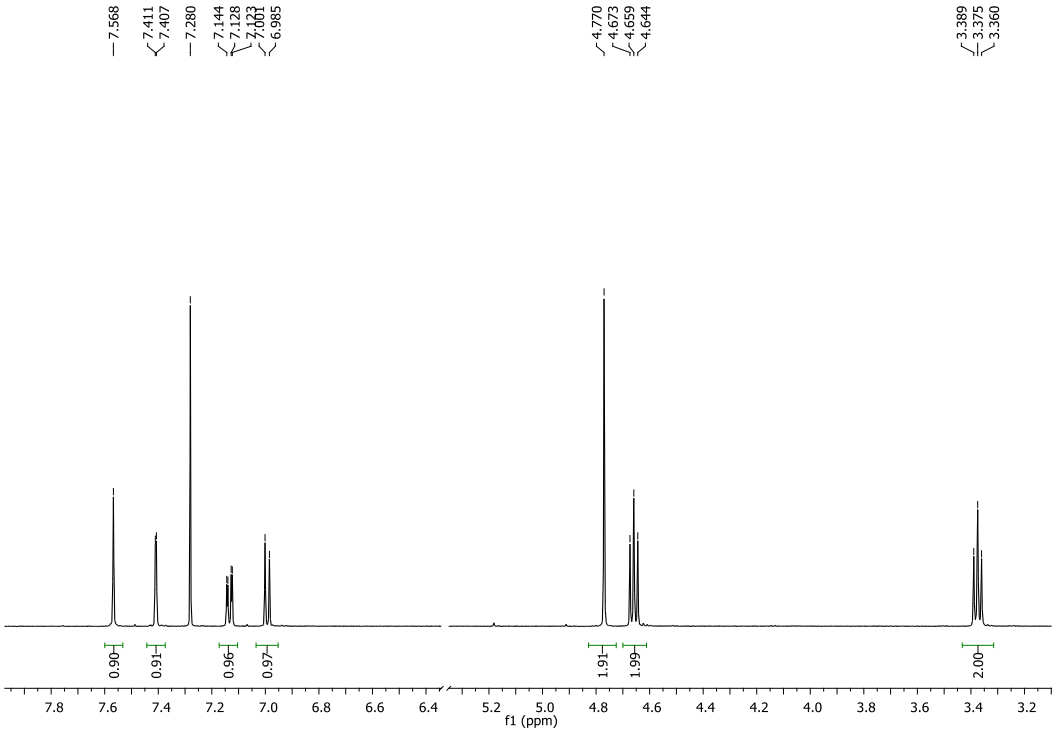

**HPLC:**



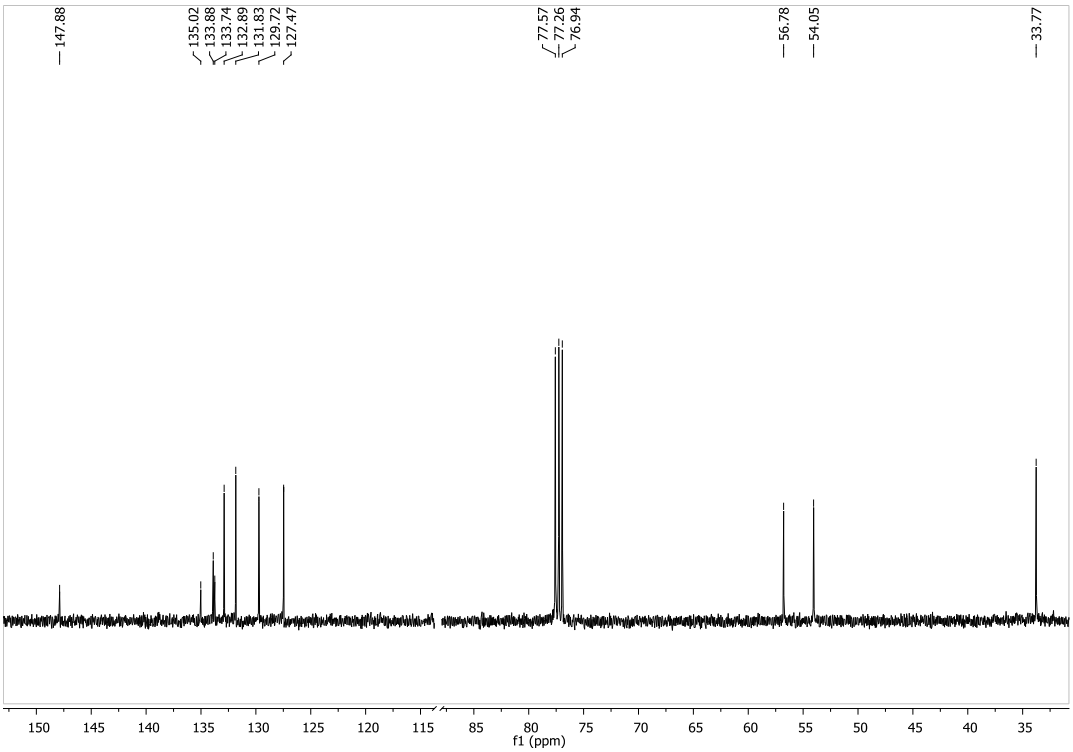

**HRMS:**



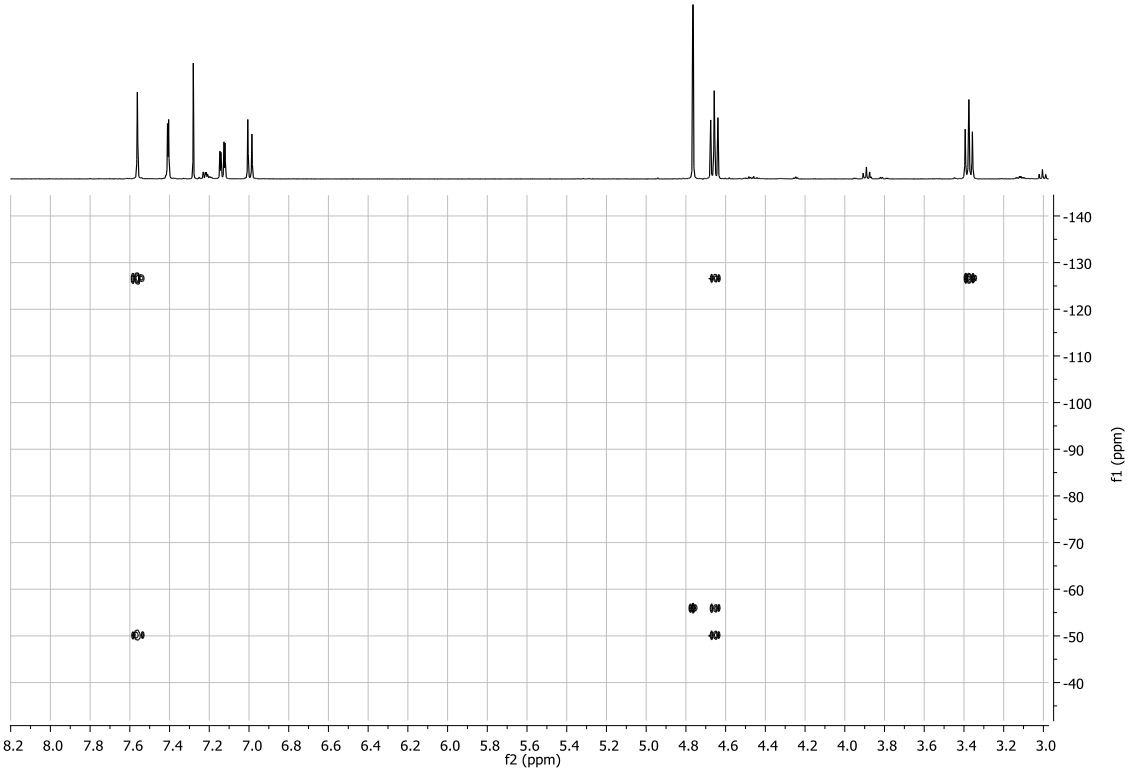
## $^{1}$H-NMR



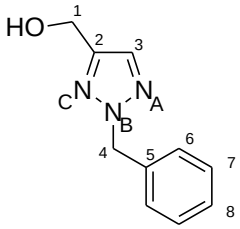

## $^{13}$C-NMR



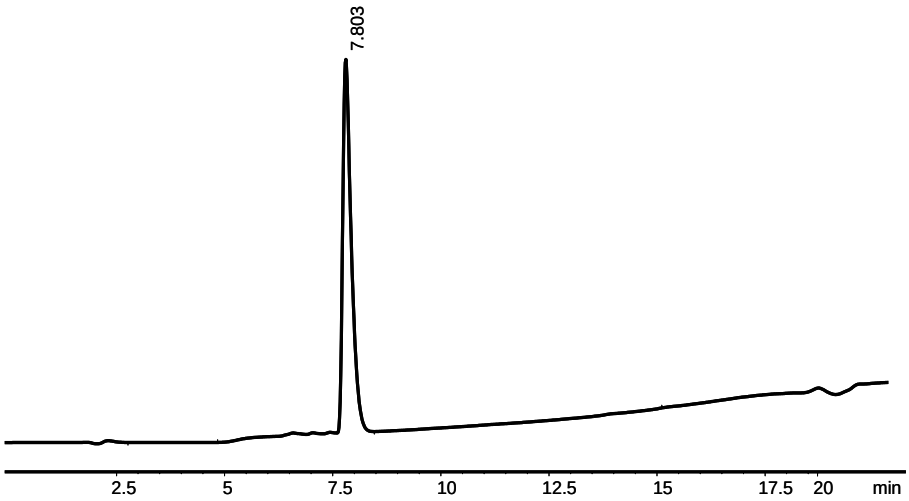
## $^{1}H$-$^{15}N$-gHMBC



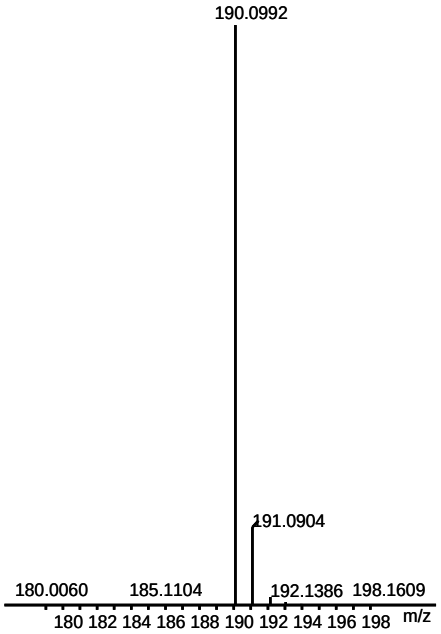
## 2-Benzyl-4-hydroxymethyl-1*H*-1,2,3-triazole (3b)



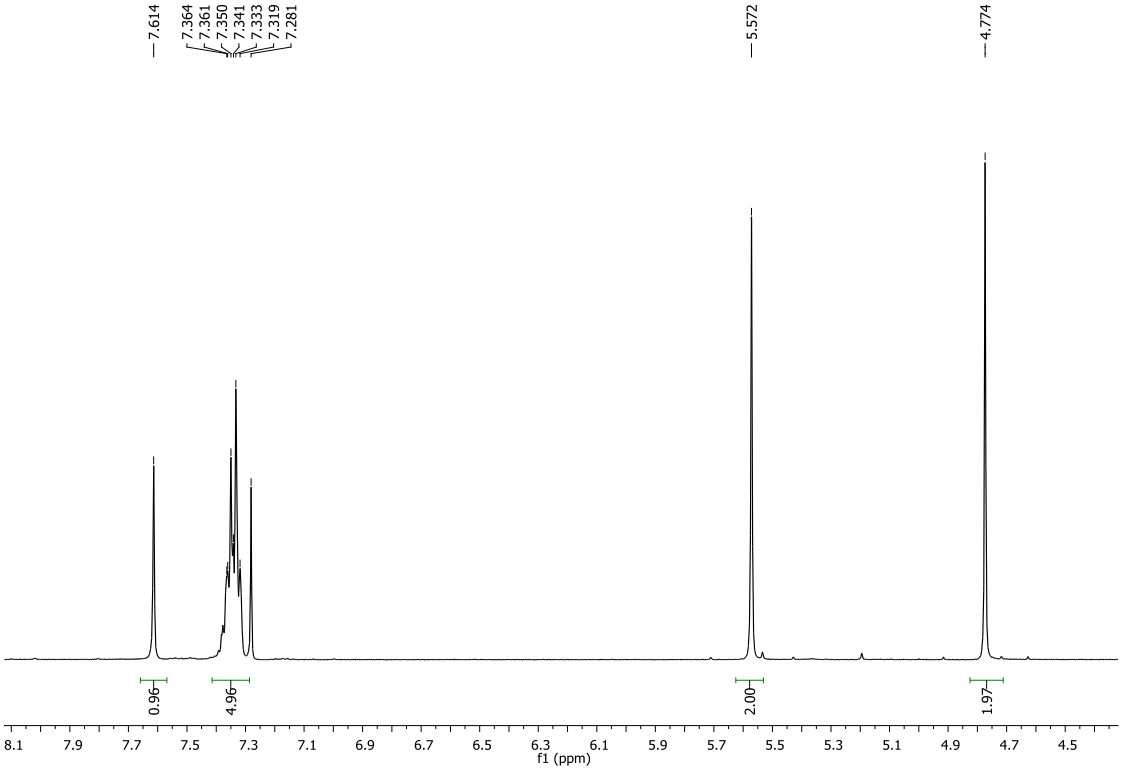

## HPLC



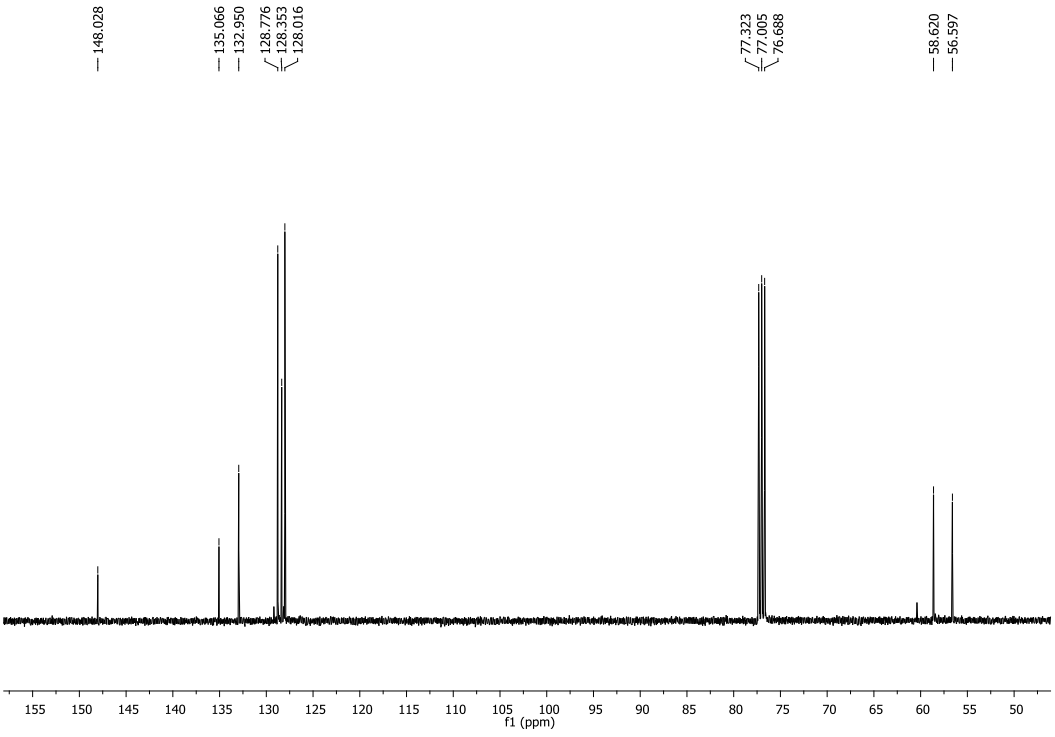

## HRMS



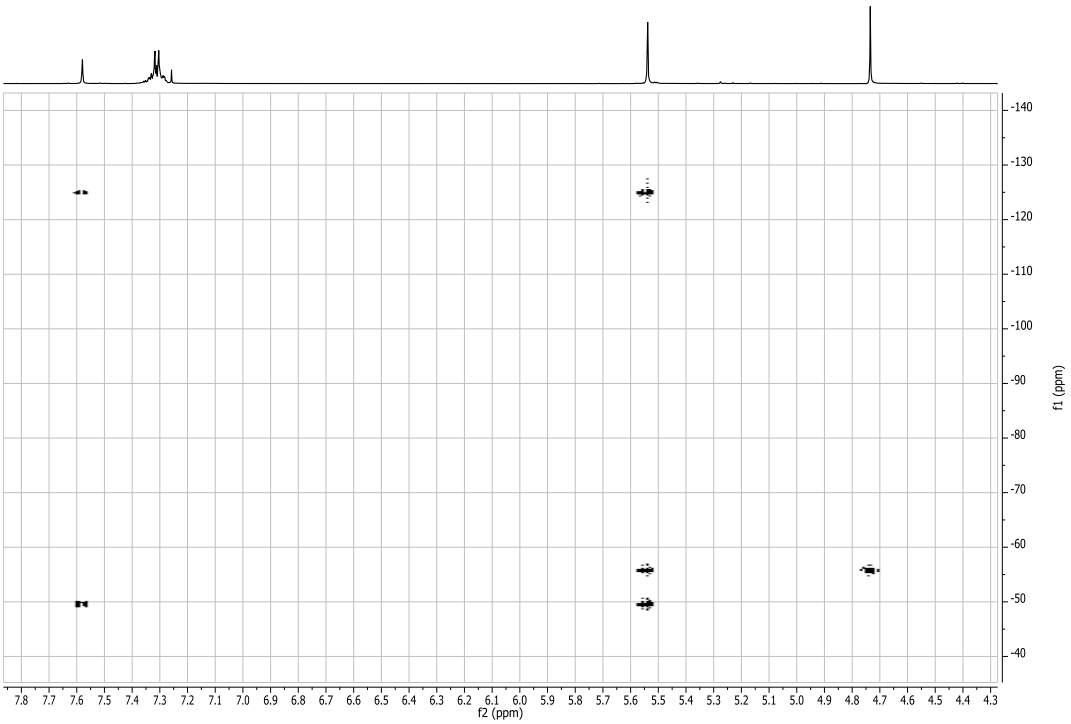
**$^{1}$H-NMR:**



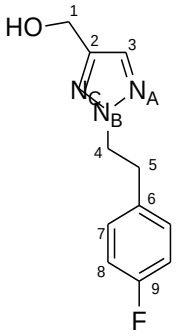

**$^{13}$C-NMR:**



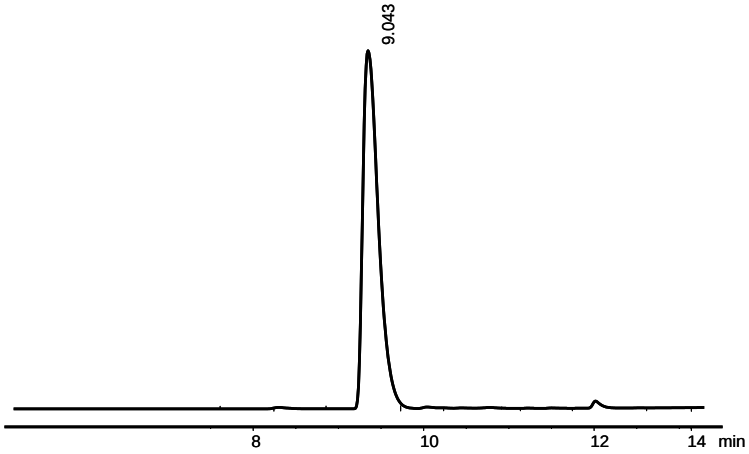
## $^{1}H$-$^{15}N$-gHMBC



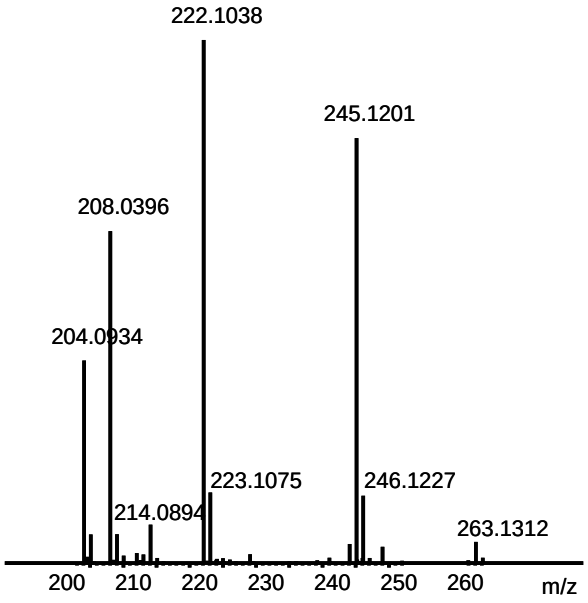
## 2-(4-Fluorophenethyl)-4-hydroxymethyl-1*H*-1,2,3-triazole (3c)



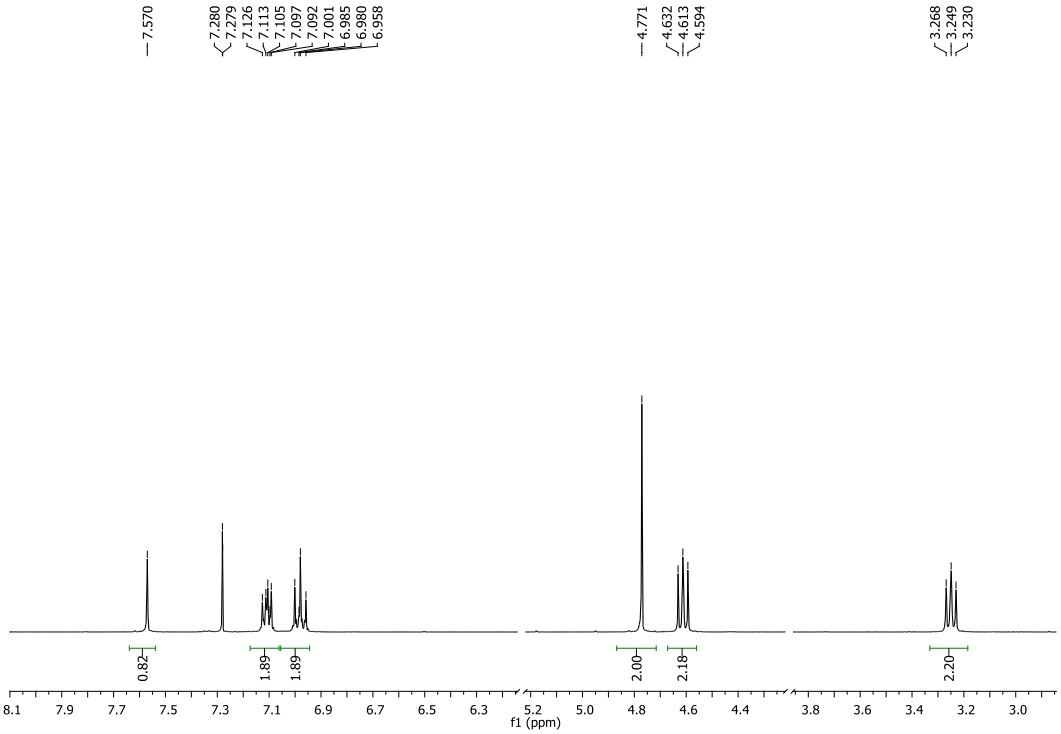

### HPLC



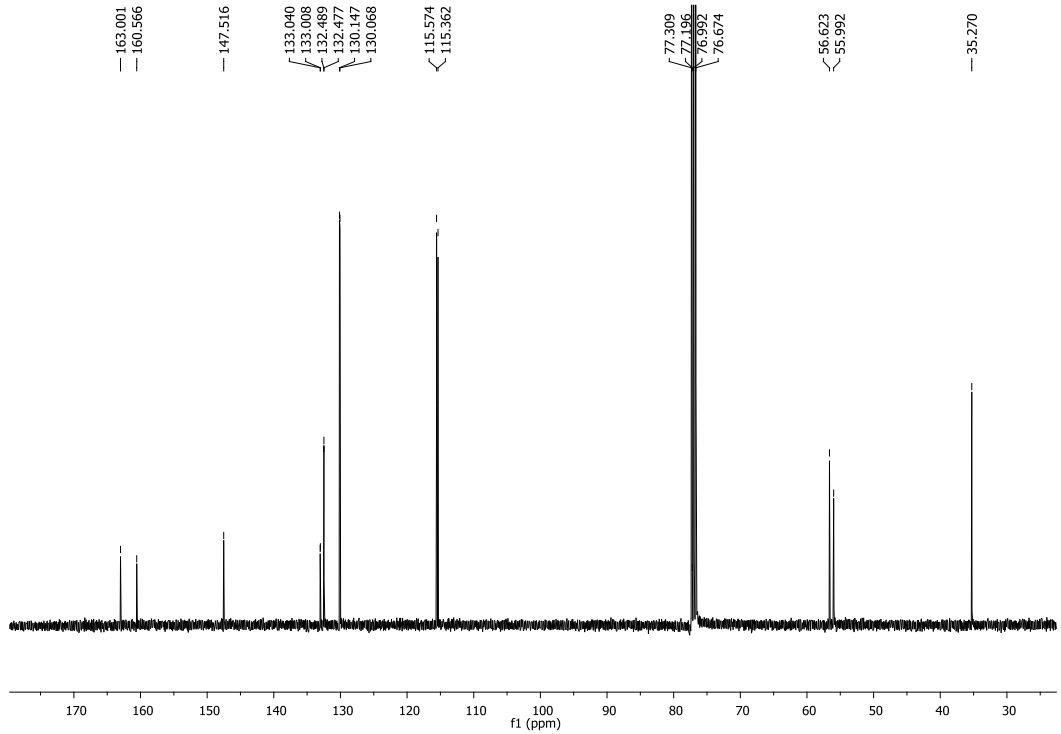

### HRMS



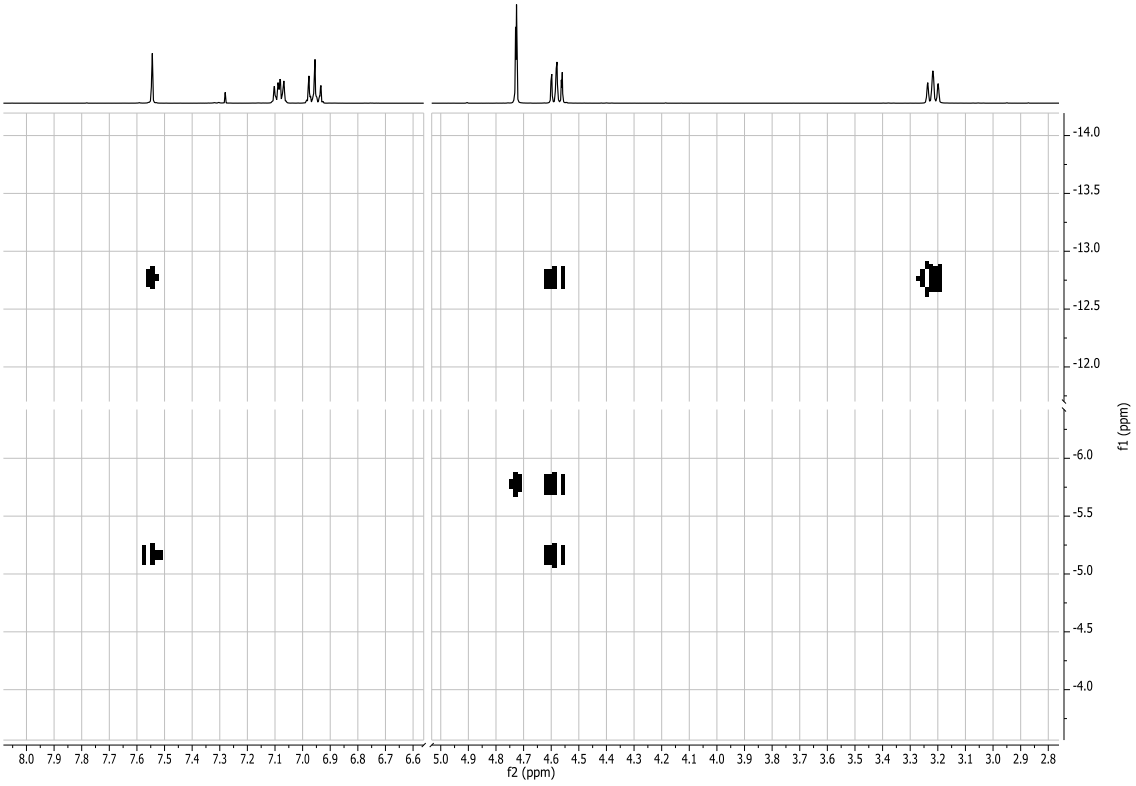
## $^{1}$H-NMR



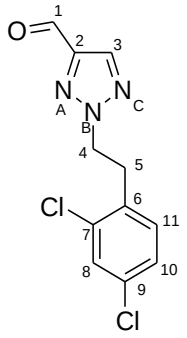

## $^{13}$C-NMR



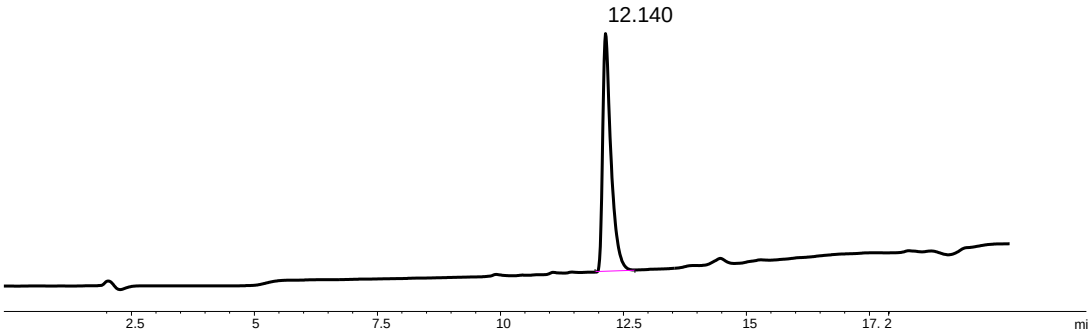
## $^{1}H$-$^{15}N$-gHMBC


-14.0
-13.5
-13.0
-12.5
-12.0
-6.0
-5.5
-5.0
-4.5
-4.0
f1 (ppm)
8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6
5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 2.9 2.8
f2 (ppm)

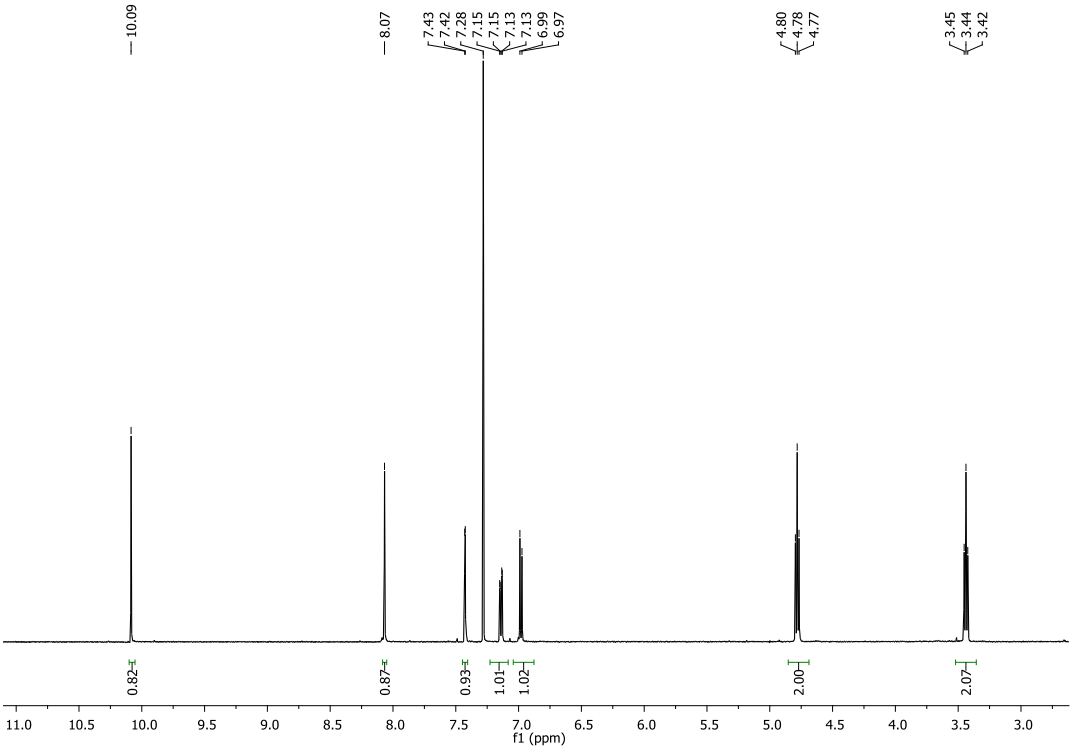
**2-(2',4'-Dichlorophenethyl)-4-formyl-1*H*-1,2,3-triazole (6a)**



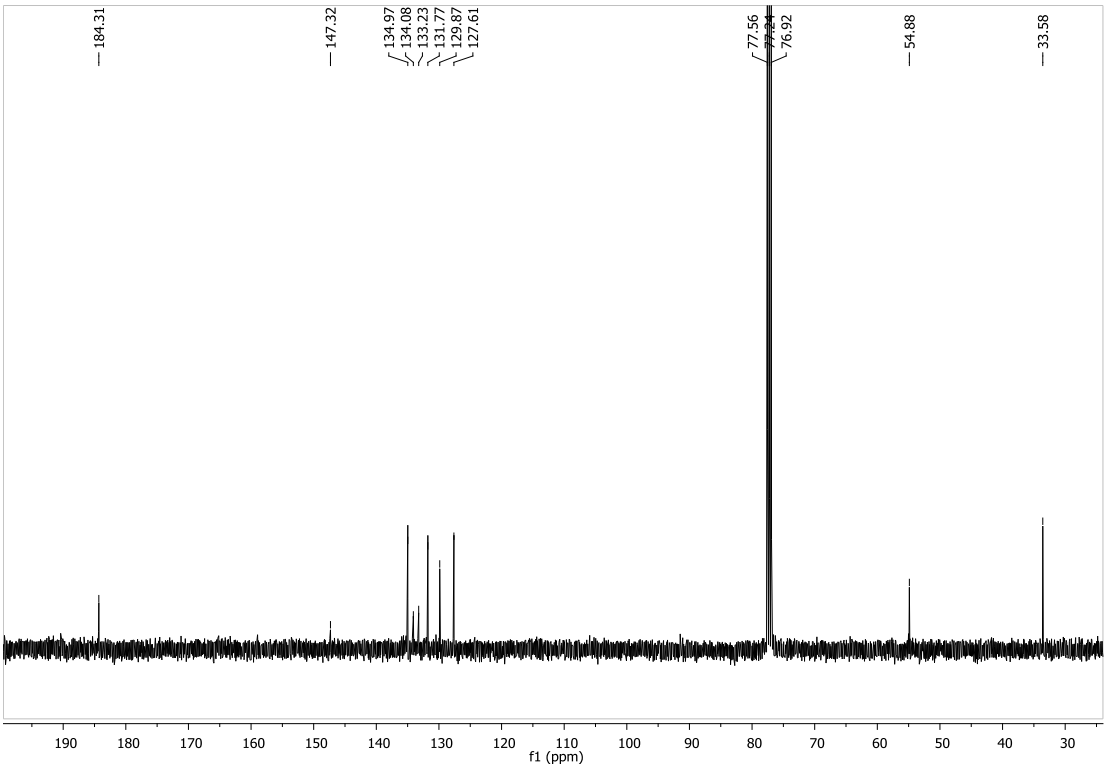

**HPLC**



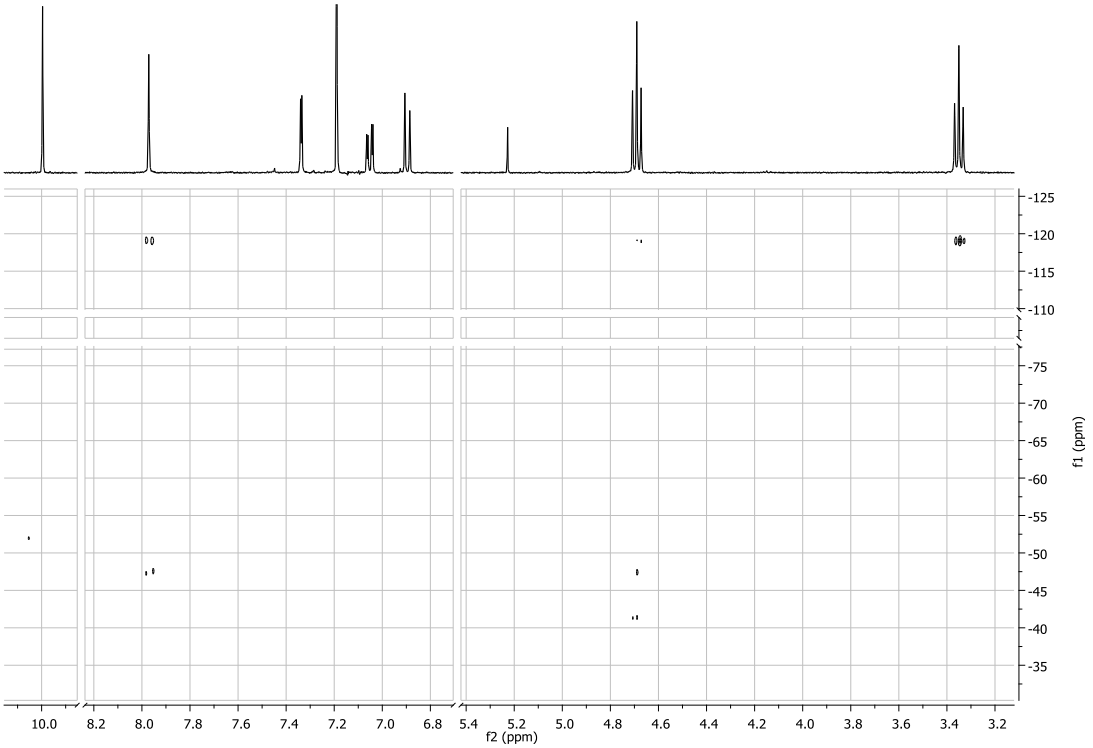
## $^{1}$H-NMR



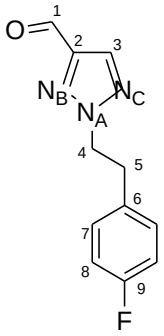

## $^{13}$C-NMR



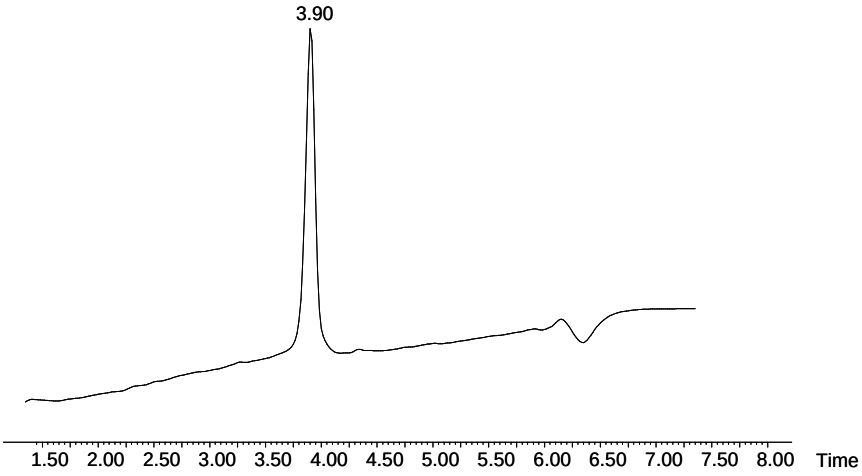
## $^{1}H$-$^{15}N$-gHMBC



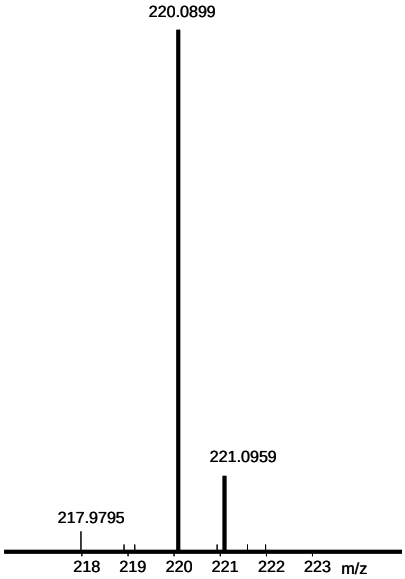
## 2-(4-Fluorophenethyl)-4-formyl-1*H*-1,2,3-triazole (6c)



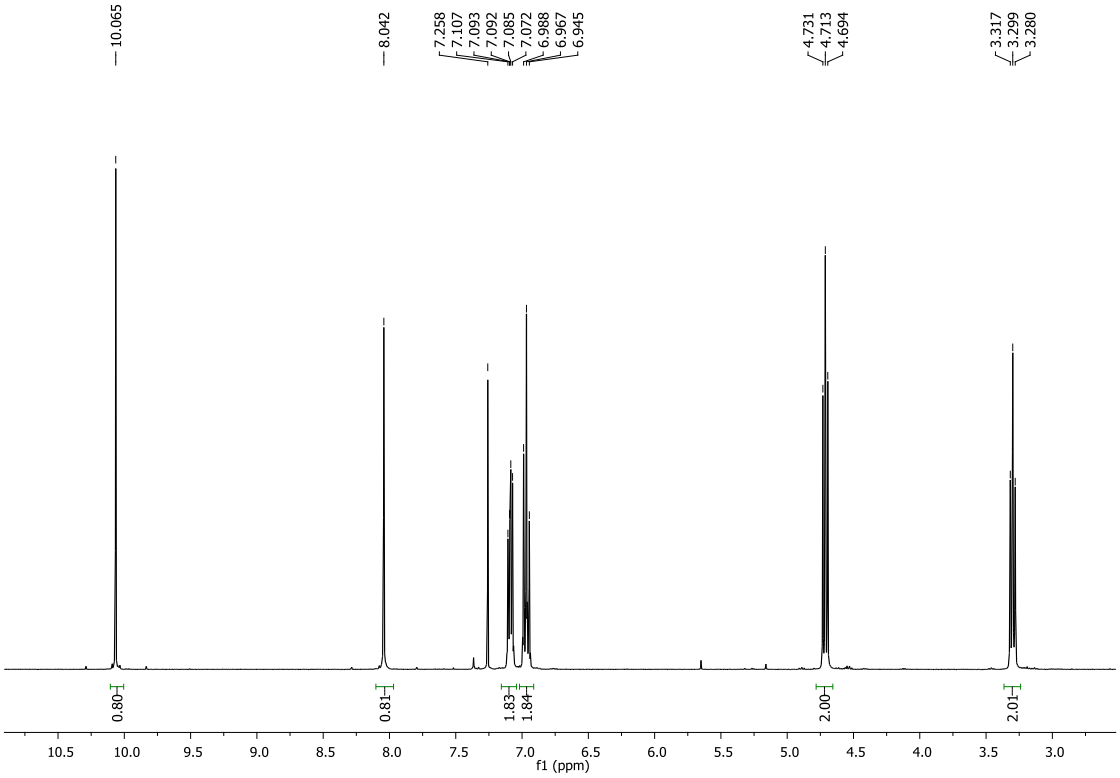

### HPLC



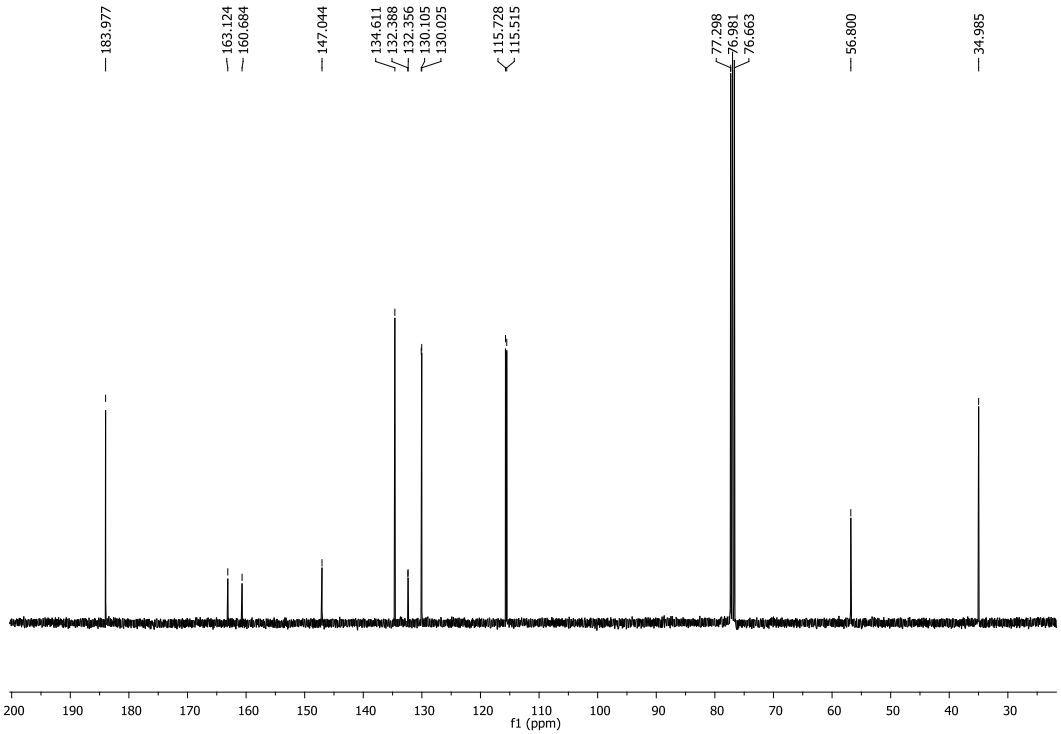

### HRMS



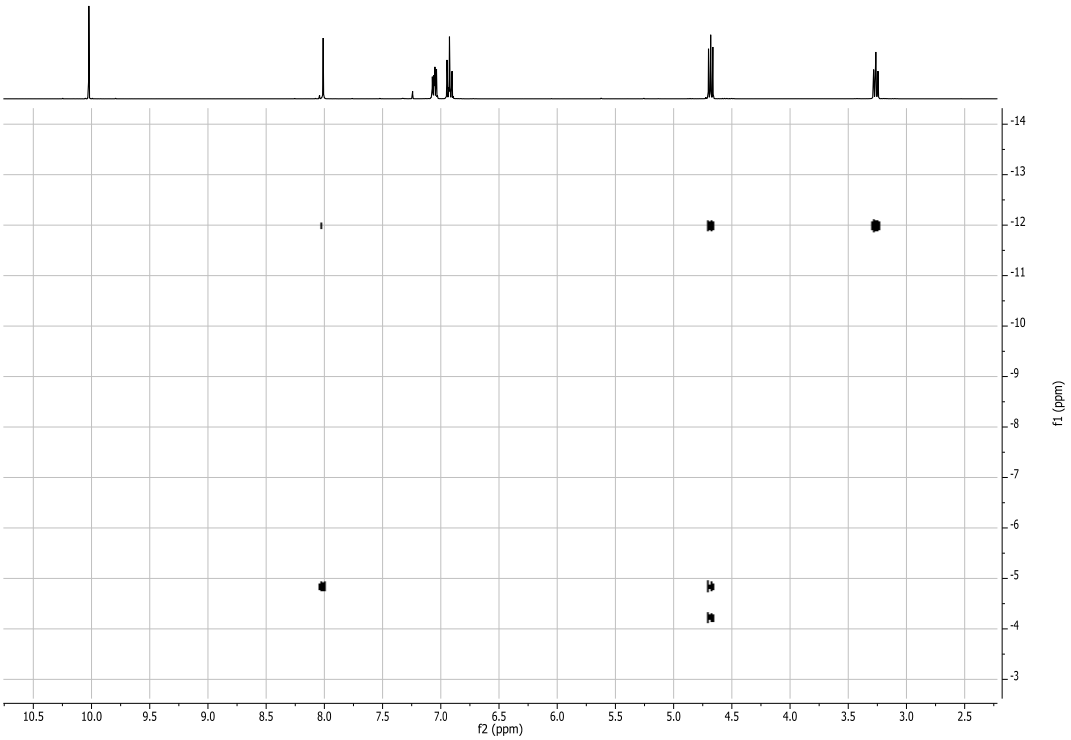
## $^{1}$H-NMR




## $^{13}$C-NMR

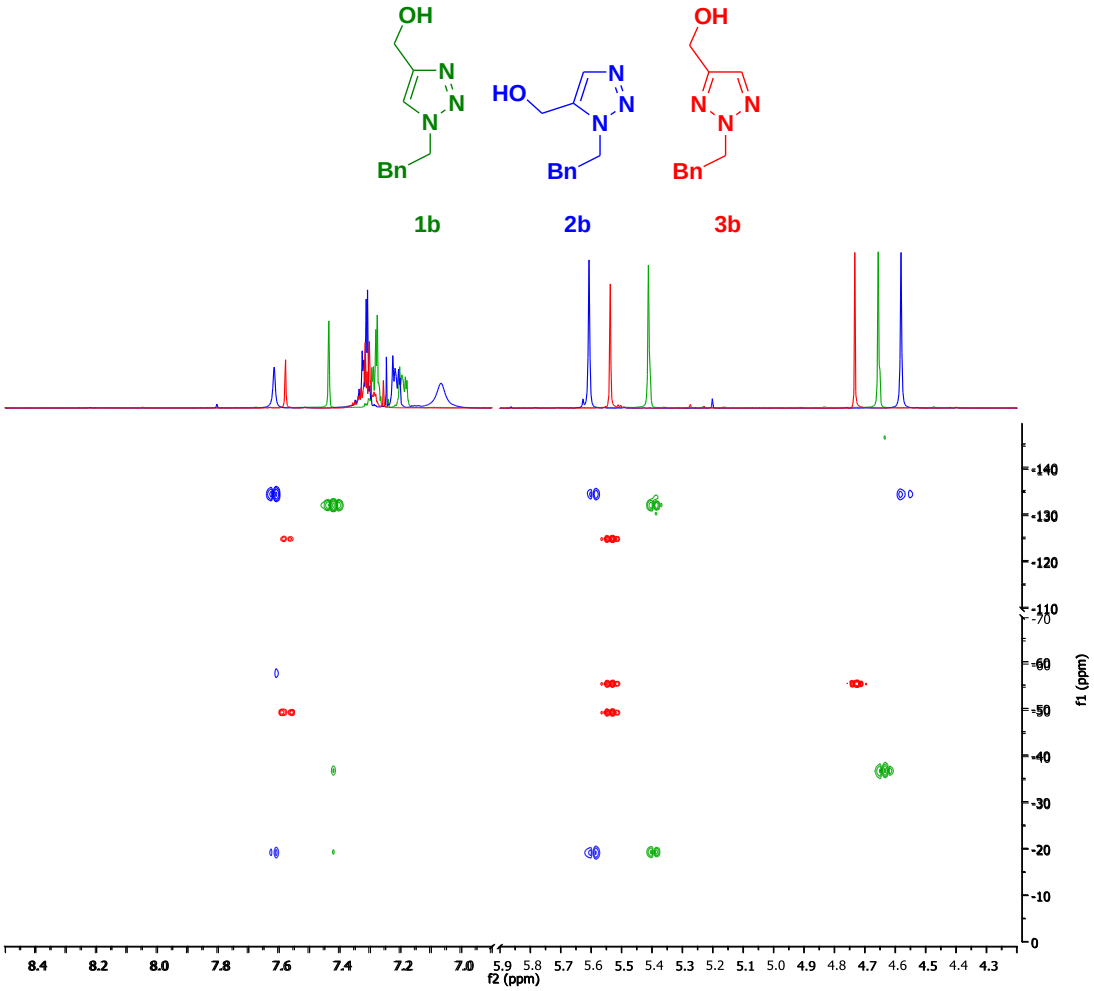


## $^{1}H$-$^{15}N$-gHMBC

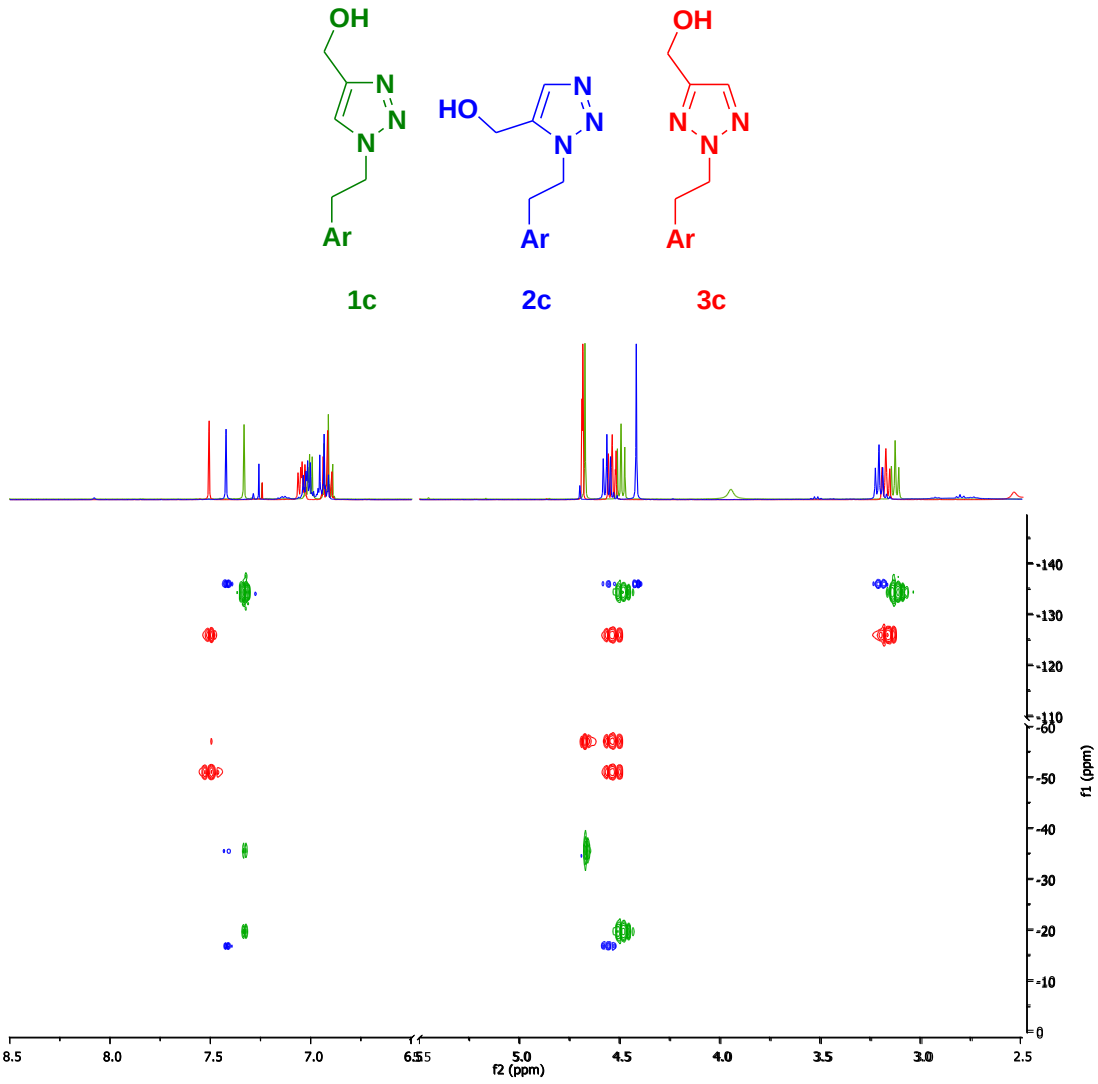


## 4. $^{1}H$ $^{15}N$ HMBC comparisons

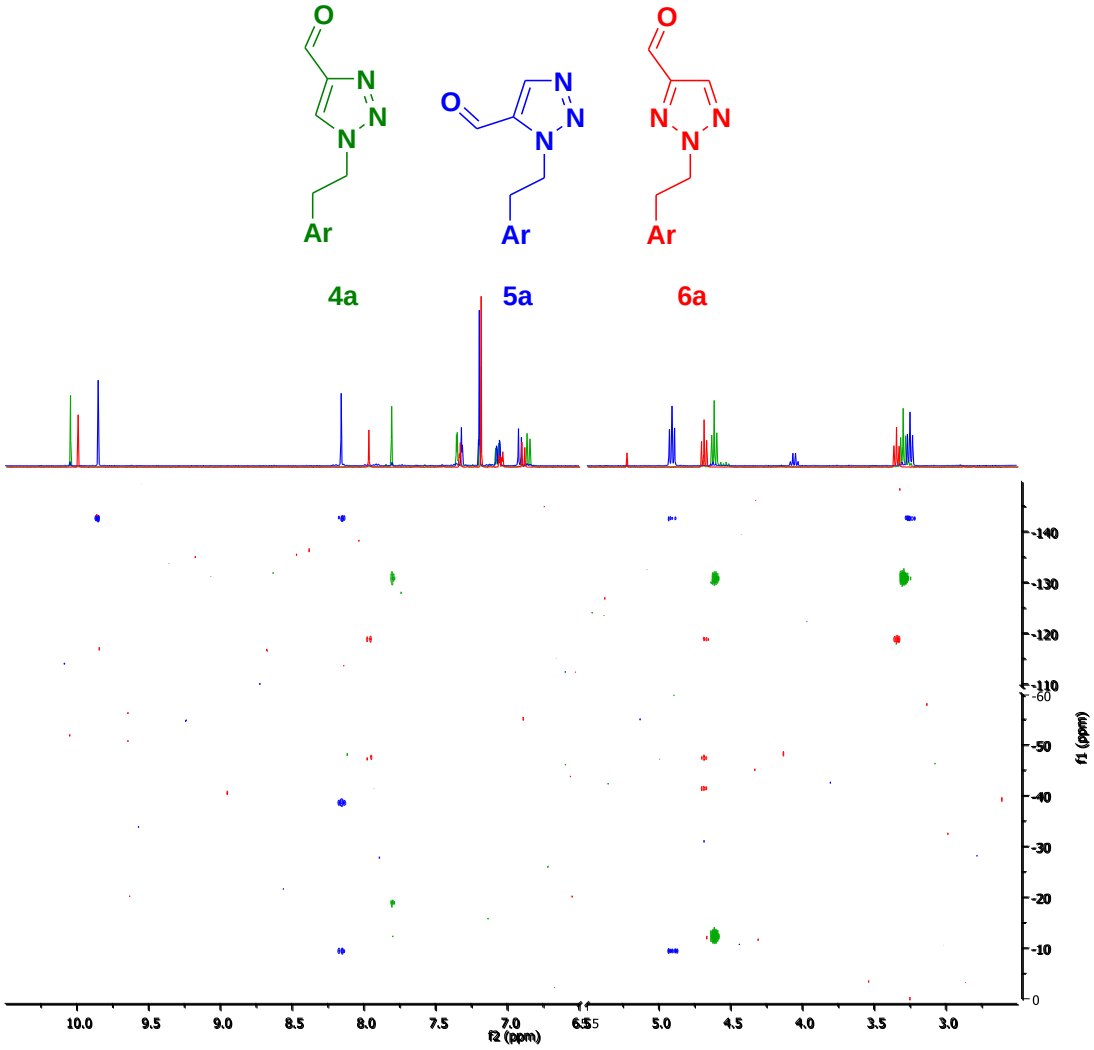
Superposition of the $^{1}H$ $^{15}N$ gHMBC spectra of the isomers (**1b** in green, **2b** in blue and **3b** in red), with the benzyl substituent.



Superposition of the $^{1}H$ $^{15}N$ gHMBC spectra of the isomers (**1c** in green, **2c** in blue and **3c** in red), where Ar = aryl and in this case *p*-fluorophenyl.



Superposition of the $^{1}H$ $^{15}N$ gHMBC spectra of the isomers (**4a** in green, **5a** in blue and **6a** in red) with the aldehyde moiety and where Ar = aryl is in this case 2,4-dichlorophenyl.



## 5. Theoretical Calculations

**Table S1**. Gas phase energy ($E^{gp}$, hartrees), zero point energy (ZPE, kcal $mol^{-1}$), enthalpic ($\Delta H$, kcal $mol^{-1}$) and entropic ($\Delta S$, cal $K^{-1}$ $mol^{-1}$) corrections at 298.15 K, total Gibbs free energy ($G^{gp}$, hartrees), and relative Boltzmann population ($P_i$, %), determined through density functional theory calculations at B3LYP/6-311++G** level for the lowest free energy minima of compounds **1a**, **2a**, **3a**, **4a**, **5a** and **6a** detected in gas phase.

| Compound | $E^{gp}$ | ZPE | $\Delta H$ | $\Delta S$ | $G^{gp}$ | $P_i$ [a] |
|---|---|---|---|---|---|---|
| **1a** | -1585.860862 | 141.68 | 9.72 | 126.62 | -1585.679742 | 9.0 |
| **2a** | -1585.859133 | 132.22 | 10.38 | 131.88 | -1585.694535 | 9.1 |
| **3a** | -1585.868018 | 141.49 | 9.72 | 126.66 | -1585.687220 | 7.3 |
| **4a** | -1584.651048 | 126.69 | 9.40 | 124.44 | -1584.493290 | 24.3 |
| **5a** | -1584.648800 | 117.29 | 10.00 | 128.38 | -1584.506953 | 22.0 |
| **6a** | -1584.657498 | 126.46 | 9.42 | 124.54 | -1584.500131 | 14.4 |

[a] The $P_i$ values shown correspond to the Boltzmann population of the lowest energy conformer, however it should be kept in mind that most conformers detected had a degeneracy of 2, that is, they had the same energetic, shielding parameters and relative population as their symmetry related counterpart.

**Table S2**. Gas phase energy ($E^{gp}$, hartrees), zero point energy (ZPE, kcal $mol_{-1}$), enthalpic ($\Delta H$, kcal $mol_{-1}$) and entropic ($\Delta S$, cal $K^{-1}$ $mol^{-1}$) corrections at 298.15 K, solvation energy ($E^{sol}$, kcal $mol^{-1}$), total Gibbs free energy in solution ($G^{sol}$, hartrees), and relative Boltzmann population ($P_i$, %), determined through density functional theory calculations at B3LYP/6-311++G** level for the lowest free energy minima of compounds **1a**, **2a**, **3a**, **4a**, **5a** and **6a** detected under implicit $CHCl_3$ solvation conditions.

| Compound | $E^{gp}$ | ZPE | $\Delta H$ | $\Delta S$ | $E^{sol}$ | $G^{sol}$ | $P_i$ [a] |
|---|---|---|---|---|---|---|---|
| **1a** | -1585.859981 | 141.32 | 9.79 | 126.87 | -11.51 | -1585.697805 | 9.4 |
| **2a** | -1585.858576 | 132.32 | 10.31 | 130.33 | -10.79 | -1585.710399 | 9.8 |
| **3a** | -1585.866775 | 141.12 | 9.79 | 127.00 | -9.68 | -1585.702040 | 7.4 |
| **4a** | -1584.650699 | 126.48 | 9.42 | 124.62 | -10.32 | -1584.509782 | 19.9 |
| **5a** | -1584.648783 | 117.27 | 10.02 | 128.77 | -8.58 | -1584.520801 | 31.2 |
| **6a** | -1584.656786 | 126.16 | 9.48 | 124.81 | -8.80 | -1584.513968 | 15.9 |

[a] The $P_i$ values shown correspond to the Boltzmann population of the lowest energy conformer, however it should be kept in mind that most conformers detected had a degeneracy of 2, that is, they had the same energetic, shielding parameters and relative population as their symmetry related counterpart.

- **Coordinates of lowest free energy minima detected in the gas phase.**

**1a:**

| | | | |
|---|---|---|---|
| C | -0.34200 | 1.69160 | 0.55570 |
| C | -0.21440 | 3.02760 | 0.86990 |
| H | -1.19760 | 1.04630 | 0.45200 |
| N | 1.80240 | 2.27060 | 0.55030 |
| N | 1.11520 | 3.33410 | 0.85460 |
| N | 0.92800 | 1.26090 | 0.36510 |
| C | -1.25200 | 4.07160 | 1.13160 |
| H | -2.17470 | 3.61220 | 1.48830 |
| H | -0.88390 | 4.75100 | 1.90880 |
| C | 1.41260 | -0.07930 | 0.04600 |
| H | 2.08310 | 0.00570 | -0.81110 |
| H | 0.54910 | -0.67290 | -0.25320 |
| O | -1.61710 | 4.80210 | -0.04380 |
| H | -0.82200 | 5.22340 | -0.38850 |
| C | 2.15970 | -0.73810 | 1.22060 |
| H | 2.53340 | -1.70280 | 0.86740 |
| H | 3.02660 | -0.12110 | 1.46290 |
| C | -0.22850 | -1.20400 | 4.78980 |
| C | 0.68460 | -0.16040 | 4.69560 |
| C | 1.44430 | -0.03610 | 3.53740 |
| C | 1.32020 | -0.92420 | 2.46180 |
| C | 0.38490 | -1.95600 | 2.60520 |
| C | -0.38830 | -2.11320 | 3.75110 |
| Cl | -1.19790 | -1.38720 | 6.24090 |
| H | 0.80070 | 0.54010 | 5.51200 |
| H | 2.15710 | 0.77700 | 3.45930 |
| Cl | 0.15380 | -3.13150 | 1.30910 |
| H | -1.09580 | -2.92680 | 3.82960 |

**2a:**

| | | | |
|---|---|---|---|
| C | 0.47770 | 0.21720 | 1.51870 |
| C | 1.66170 | -0.17630 | 0.93020 |
| H | 0.29690 | 0.54710 | 2.52930 |
| N | -0.52490 | 0.12630 | 0.60600 |
| C | 3.05590 | -0.25610 | 1.46390 |
| H | 3.47740 | -1.25170 | 1.31270 |
| H | 3.02370 | -0.07370 | 2.54330 |
| N | -0.02690 | -0.29480 | -0.52140 |
| N | 1.29670 | -0.48450 | -0.34610 |
| C | 2.10820 | -0.97630 | -1.45910 |
| H | 3.15360 | -0.82200 | -1.19650 |
| H | 1.88200 | -0.35240 | -2.32550 |
| C | 1.81200 | -2.45010 | -1.79610 |
| H | 0.75290 | -2.53820 | -2.04440 |
| H | 2.38100 | -2.69950 | -2.69480 |
| C | 2.70930 | -5.16920 | 1.43810 |

| | | | |
|---|---|---|---|
| C | 3.73980 | -4.75510 | 0.60270 |
| C | 3.44200 | -3.88210 | -0.43980 |
| C | 2.14480 | -3.41240 | -0.68130 |
| C | 1.14170 | -3.86360 | 0.18570 |
| C | 1.40490 | -4.73170 | 1.24000 |
| Cl | 3.07060 | -6.26500 | 2.76070 |
| H | 4.75210 | -5.10230 | 0.75600 |
| Cl | 4.77580 | -3.37880 | -1.47690 |
| H | 0.12560 | -3.52000 | 0.02730 |
| H | 0.61090 | -5.06390 | 1.89560 |
| O | 3.96290 | 0.63750 | 0.81210 |
| H | 3.65400 | 1.54020 | 0.94700 |

**3a:**

| | | | |
|---|---|---|---|
| C | -0.27690 | 2.87140 | 0.95340 |
| C | -0.37050 | 1.56150 | 0.44930 |
| H | -1.04020 | 3.50870 | 1.37070 |
| N | 0.85120 | 1.19090 | 0.04770 |
| N | 0.98660 | 3.28240 | 0.85340 |
| C | -1.54040 | 0.63140 | 0.36520 |
| H | -1.32310 | -0.14440 | -0.37690 |
| H | -2.43240 | 1.17100 | 0.04350 |
| N | 1.61640 | 2.24440 | 0.30970 |
| C | 3.04140 | 2.27840 | -0.00560 |
| H | 3.21150 | 3.08500 | -0.72280 |
| H | 3.26230 | 1.32810 | -0.48770 |
| O | -1.88750 | 0.05420 | 1.62800 |
| H | -1.13190 | -0.45290 | 1.94420 |
| C | 3.91690 | 2.50300 | 1.23920 |
| H | 4.94740 | 2.61690 | 0.89350 |
| H | 3.62290 | 3.44650 | 1.70220 |
| C | 3.59980 | -0.64110 | 4.18320 |
| C | 2.88930 | 0.54150 | 4.35150 |
| C | 3.01390 | 1.54040 | 3.39170 |
| C | 3.82770 | 1.39560 | 2.26180 |
| C | 4.52250 | 0.18650 | 2.13910 |
| C | 4.42430 | -0.83240 | 3.08140 |
| Cl | 3.46360 | -1.91850 | 5.37980 |
| H | 2.25390 | 0.67940 | 5.21640 |
| H | 2.46170 | 2.46480 | 3.51740 |
| Cl | 5.58340 | -0.09160 | 0.75830 |
| H | 4.97980 | -1.75130 | 2.95690 |

**4a:**

| | | | |
|---|---|---|---|
| C | -0.50430 | 1.61700 | 0.46430 |
| C | -0.40510 | 2.97350 | 0.72190 |

| | | | |
|---|---|---|---|
| H | -1.35360 | 0.96030 | 0.38540 |
| N | 1.62700 | 2.25810 | 0.46380 |
| N | 0.91900 | 3.31220 | 0.71200 |
| N | 0.76850 | 1.21260 | 0.30840 |
| C | -1.45670 | 3.96180 | 0.97030 |
| C | 1.29320 | -0.12410 | 0.03100 |
| H | 1.93680 | -0.04870 | -0.84720 |
| H | 0.44330 | -0.75830 | -0.21890 |
| O | -2.64140 | 3.70280 | 0.98280 |
| C | 2.09390 | -0.70220 | 1.21200 |
| H | 2.93490 | -0.03680 | 1.41400 |
| H | 2.50700 | -1.65870 | 0.88160 |
| C | -0.18760 | -1.17580 | 4.84940 |
| C | 0.67150 | -0.09280 | 4.70400 |
| C | 1.39680 | 0.03500 | 3.52440 |
| C | 1.28970 | -0.88790 | 2.47670 |
| C | 0.40820 | -1.95820 | 2.67030 |
| C | -0.32860 | -2.11980 | 3.83900 |
| Cl | -1.10940 | -1.36550 | 6.32870 |
| H | 0.77270 | 0.63500 | 5.49820 |
| H | 2.07020 | 0.87690 | 3.40870 |
| Cl | 0.20470 | -3.17880 | 1.41210 |
| H | -0.99460 | -2.96310 | 3.95700 |
| H | -1.08050 | 4.98660 | 1.14960 |

**5a:**

| | | | |
|---|---|---|---|
| C | -0.89620 | 0.85180 | 1.87080 |
| C | -0.21420 | 1.49810 | 0.85000 |
| H | -1.66570 | 1.23500 | 2.52230 |
| N | -0.44930 | -0.41810 | 1.96270 |
| C | -0.34160 | 2.86740 | 0.36920 |
| N | 0.47420 | -0.60150 | 1.04890 |
| N | 0.63160 | 0.53560 | 0.36720 |
| C | 1.62730 | 0.60820 | -0.70630 |
| H | 1.18530 | 1.15550 | -1.53800 |
| H | 1.81350 | -0.42260 | -1.00510 |
| C | 2.92550 | 1.29370 | -0.24240 |
| H | 2.68840 | 2.30490 | 0.09190 |
| H | 3.33350 | 0.74040 | 0.60580 |
| C | 5.76030 | 1.57310 | -3.48600 |
| C | 5.72380 | 0.41110 | -2.72560 |
| C | 4.80940 | 0.32720 | -1.67920 |
| C | 3.93430 | 1.37320 | -1.36310 |
| C | 4.00880 | 2.52260 | -2.15980 |
| C | 4.90720 | 2.63710 | -3.21480 |
| Cl | 6.90740 | 1.69220 | -4.80890 |
| H | 6.39000 | -0.41300 | -2.93950 |
| Cl | 4.78710 | -1.16230 | -0.74030 |
| H | 3.34110 | 3.34910 | -1.94170 |

| | | | |
|---|---|---|---|
| H | 4.94760 | 3.53690 | -3.81440 |
| O | 0.32690 | 3.36570 | -0.51510 |
| H | -1.12480 | 3.44930 | 0.89090 |

**6a:**

| | | | |
|---|---|---|---|
| C | -0.24290 | 2.98870 | 0.93580 |
| C | -0.36830 | 1.63860 | 0.55190 |
| H | -0.98890 | 3.66830 | 1.31400 |
| N | 0.83570 | 1.20970 | 0.13950 |
| N | 1.01960 | 3.36150 | 0.75660 |
| C | -1.53160 | 0.74480 | 0.55220 |
| N | 1.61550 | 2.26170 | 0.27900 |
| C | 3.04030 | 2.23700 | -0.04650 |
| H | 3.22880 | 3.03080 | -0.77230 |
| H | 3.22040 | 1.27380 | -0.51920 |
| O | -2.63650 | 1.07950 | 0.91920 |
| C | 3.93110 | 2.44100 | 1.19160 |
| H | 4.96450 | 2.48560 | 0.83820 |
| H | 3.69610 | 3.41210 | 1.63110 |
| C | 3.44310 | -0.60190 | 4.21780 |
| C | 2.83450 | 0.63780 | 4.37530 |
| C | 3.01320 | 1.60210 | 3.38910 |
| C | 3.78170 | 1.36700 | 2.24280 |
| C | 4.37500 | 0.10380 | 2.13210 |
| C | 4.22020 | -0.88280 | 3.10030 |
| Cl | 3.23730 | -1.83680 | 5.44700 |
| H | 2.23500 | 0.84520 | 5.25190 |
| H | 2.54190 | 2.57120 | 3.50860 |
| Cl | 5.37650 | -0.28650 | 0.73420 |
| H | 4.69620 | -1.84630 | 2.98390 |
| H | -1.32270 | -0.27860 | 0.18660 |

**Coordinates of lowest free energy minima detected in solution phase.**

**1a:**

| | | | |
|---|---|---|---|
| C | -0.51690 | 1.69440 | 0.63050 |
| C | -0.24880 | 3.03010 | 0.86080 |
| H | -1.43900 | 1.13520 | 0.58580 |
| N | 1.67300 | 2.04410 | 0.57960 |
| N | 1.10400 | 3.19510 | 0.82310 |
| N | 0.70080 | 1.12360 | 0.46740 |
| C | -1.16060 | 4.19320 | 1.09100 |
| H | -2.15550 | 3.84550 | 1.37370 |
| H | -0.76560 | 4.80220 | 1.91140 |
| C | 1.05620 | -0.25680 | 0.13320 |
| H | 0.30730 | -0.91190 | 0.57790 |
| H | 2.01540 | -0.45510 | 0.61250 |
| O | -1.34270 | 5.00370 | -0.08520 |
| H | -0.48950 | 5.38990 | -0.33240 |
| C | 1.15580 | -0.44880 | -1.39460 |
| H | 0.17030 | -0.29550 | -1.84210 |
| H | 1.81700 | 0.32300 | -1.79410 |
| C | 2.77800 | -4.28910 | -2.51190 |
| C | 3.58960 | -3.16070 | -2.54040 |
| C | 3.04030 | -1.93570 | -2.17340 |
| C | 1.70200 | -1.80350 | -1.77950 |
| C | 0.93160 | -2.97230 | -1.76860 |
| C | 1.44430 | -4.21520 | -2.12880 |
| Cl | 3.44290 | -5.85060 | -2.97500 |
| H | 4.62580 | -3.23320 | -2.84690 |
| H | 3.66700 | -1.05020 | -2.20240 |
| Cl | -0.77030 | -2.90530 | -1.30370 |
| H | 0.81780 | -5.09730 | -2.11290 |

**2a:**

| | | | |
|---|---|---|---|
| C | 0.65320 | 1.84510 | 0.53820 |
| C | 1.74310 | 1.00370 | 0.43230 |
| H | 0.61480 | 2.86980 | 0.87520 |
| N | -0.45750 | 1.18050 | 0.13350 |
| C | 3.19170 | 1.28060 | 0.68920 |
| H | 3.69010 | 0.42220 | 1.14100 |
| H | 3.26070 | 2.10790 | 1.40230 |
| N | -0.11580 | -0.03500 | -0.21610 |
| N | 1.20920 | -0.15860 | -0.04420 |
| C | 1.82690 | -1.47000 | -0.27750 |
| H | 2.90840 | -1.34380 | -0.22960 |
| H | 1.57110 | -1.77920 | -1.29290 |
| C | 1.31820 | -2.49910 | 0.75560 |
| H | 1.50050 | -2.11210 | 1.76140 |
| H | 0.23730 | -2.59640 | 0.63940 |

| | | | |
|---|---|---|---|
| C | 3.05930 | -6.42850 | 0.35160 |
| C | 3.75700 | -5.45740 | 1.05940 |
| C | 3.19190 | -4.19000 | 1.16630 |
| C | 1.95190 | -3.86230 | 0.60380 |
| C | 1.29250 | -4.87900 | -0.10030 |
| C | 1.82970 | -6.15620 | -0.23680 |
| Cl | 3.75480 | -8.03830 | 0.20830 |
| H | 4.71150 | -5.67840 | 1.51870 |
| Cl | 4.10020 | -2.97570 | 2.07120 |
| H | 0.32390 | -4.66850 | -0.54290 |
| H | 1.29750 | -6.92580 | -0.78260 |
| O | 3.92690 | 1.57480 | -0.50880 |
| H | 3.59310 | 2.39710 | -0.89580 |

**3a:**

| | | | |
|---|---|---|---|
| C | -0.33230 | 2.95730 | 0.84790 |
| C | -0.33190 | 1.59560 | 0.50410 |
| H | -1.14210 | 3.59060 | 1.17960 |
| N | 0.91890 | 1.26230 | 0.15900 |
| N | 0.90940 | 3.43350 | 0.70880 |
| C | -1.43800 | 0.58460 | 0.49720 |
| H | -1.46750 | 0.07110 | -0.47050 |
| H | -2.39420 | 1.09050 | 0.63830 |
| N | 1.61630 | 2.38090 | 0.30800 |
| C | 3.03540 | 2.45010 | -0.03500 |
| H | 3.50530 | 1.55220 | 0.36840 |
| H | 3.44130 | 3.32000 | 0.47950 |
| O | -1.33310 | -0.37230 | 1.56540 |
| H | -0.53260 | -0.90090 | 1.43530 |
| C | 3.23800 | 2.53750 | -1.56280 |
| H | 2.65000 | 1.74570 | -2.03150 |
| H | 2.84770 | 3.49240 | -1.92270 |
| C | 7.35500 | 1.96150 | -2.72570 |
| C | 6.47040 | 0.88880 | -2.75220 |
| C | 5.14920 | 1.10670 | -2.37370 |
| C | 4.68350 | 2.36480 | -1.96670 |
| C | 5.61800 | 3.40730 | -1.95480 |
| C | 6.94700 | 3.22970 | -2.33070 |
| Cl | 9.03020 | 1.71850 | -3.20600 |
| H | 6.80200 | -0.09350 | -3.06660 |
| H | 4.45190 | 0.27500 | -2.40280 |
| Cl | 5.12900 | 5.02960 | -1.46370 |
| H | 7.64080 | 4.06040 | -2.31640 |

**4a:**

| | | | |
|---|---|---|---|
| C | -0.40590 | 1.49920 | 0.77820 |
| C | -0.42100 | 2.88770 | 0.78420 |
| H | -1.12730 | 0.76620 | 1.10600 |
| N | 1.49060 | 2.29920 | -0.06010 |
| N | 0.76400 | 3.32420 | 0.25990 |
| N | 0.78750 | 1.18050 | 0.24980 |
| C | -1.43590 | 3.83520 | 1.23700 |
| C | 1.36420 | -0.14050 | -0.02690 |
| H | 0.70040 | -0.87520 | 0.42730 |
| H | 2.32850 | -0.18950 | 0.48300 |
| O | -2.50860 | 3.51460 | 1.72080 |
| C | 1.56150 | -0.39110 | -1.53600 |
| H | 2.01010 | -1.38360 | -1.63650 |
| H | 2.29140 | 0.32680 | -1.91340 |
| C | -2.01880 | -0.03470 | -3.92850 |
| C | -1.06460 | 0.97450 | -3.95800 |
| C | 0.08230 | 0.83250 | -3.18120 |
| C | 0.30360 | -0.28940 | -2.36990 |
| C | -0.68760 | -1.27810 | -2.38550 |
| C | -1.84520 | -1.17290 | -3.15050 |
| Cl | -3.47800 | 0.11710 | -4.89790 |
| H | -1.20990 | 1.85240 | -4.57500 |
| H | 0.83320 | 1.61470 | -3.21250 |
| Cl | -0.49070 | -2.74620 | -1.42510 |
| H | -2.58720 | -1.95980 | -3.13950 |
| H | -1.15520 | 4.89650 | 1.10620 |

**5a:**

| | | | |
|---|---|---|---|
| C | -1.09660 | 0.74910 | 1.58080 |
| C | -0.05150 | 1.54350 | 1.13530 |
| H | -2.05080 | 1.04420 | 1.98900 |
| N | -0.74780 | -0.54520 | 1.43420 |
| C | 0.03160 | 2.99850 | 1.10620 |
| N | 0.46440 | -0.59550 | 0.92130 |
| N | 0.90250 | 0.64590 | 0.73710 |
| C | 2.23320 | 0.85440 | 0.14880 |
| H | 2.78210 | -0.06620 | 0.34320 |
| H | 2.71300 | 1.67430 | 0.68110 |
| C | 2.14720 | 1.13820 | -1.36540 |
| H | 1.58700 | 2.06050 | -1.52790 |
| H | 1.59600 | 0.32590 | -1.84420 |
| C | 6.06140 | 1.61140 | -3.12580 |
| C | 5.54140 | 0.33040 | -2.99000 |
| C | 4.28030 | 0.18800 | -2.41710 |
| C | 3.51780 | 1.28160 | -1.98720 |
| C | 4.08990 | 2.55100 | -2.14860 |
| C | 5.35090 | 2.73180 | -2.70880 |

| | | | |
|---|---|---|---|
| Cl | 7.65430 | 1.81010 | -3.84580 |
| H | 6.09920 | -0.53660 | -3.32020 |
| Cl | 3.65130 | -1.45110 | -2.25410 |
| H | 3.52810 | 3.42340 | -1.83100 |
| H | 5.76920 | 3.72460 | -2.82290 |
| O | 0.98420 | 3.63530 | 0.69100 |
| H | -0.86720 | 3.50180 | 1.50260 |

**6a:**

| | | | |
|---|---|---|---|
| C | -0.39050 | 3.07120 | 0.66980 |
| C | -0.37470 | 1.66370 | 0.58670 |
| H | -1.21130 | 3.74780 | 0.85630 |
| N | 0.89150 | 1.27700 | 0.34280 |
| N | 0.84900 | 3.51350 | 0.47830 |
| C | -1.43850 | 0.66830 | 0.72030 |
| N | 1.57230 | 2.40030 | 0.29270 |
| C | 2.99930 | 2.43170 | -0.03710 |
| H | 3.43920 | 1.53200 | 0.39410 |
| H | 3.41920 | 3.30510 | 0.46020 |
| O | -2.60460 | 0.94880 | 0.93340 |
| C | 3.21360 | 2.48370 | -1.56440 |
| H | 2.64940 | 1.66770 | -2.02190 |
| H | 2.80460 | 3.42100 | -1.94900 |
| C | 7.35710 | 2.00680 | -2.67900 |
| C | 6.49740 | 0.91490 | -2.72550 |
| C | 5.16710 | 1.09890 | -2.36040 |
| C | 4.66830 | 2.34250 | -1.94900 |
| C | 5.57810 | 3.40660 | -1.91860 |
| C | 6.91540 | 3.26220 | -2.27890 |
| Cl | 9.04280 | 1.80630 | -3.14020 |
| H | 6.85520 | -0.05640 | -3.04480 |
| H | 4.48950 | 0.25190 | -2.40550 |
| Cl | 5.04520 | 5.01430 | -1.42630 |
| H | 7.58960 | 4.10820 | -2.24910 |
| H | -1.10900 | -0.38120 | 0.61240 |

**Table S3.** Isotropic shieldings calculated for the reference compounds TMS and nitromethane at the B3LYP/6-311++G** level, in gas phase ($\sigma^{gp}$) and in $CHCl_3$ solution phase ($\sigma^{sol}$).

| | $\sigma^{gp}$ | | | $\sigma^{sol}$ | | |
|---|---|---|---|---|---|---|
| | **H** | **C** | **N** | **H** | **C** | **N** |
| **TMS** | 31.97 | 184.11 | | 31.93 | 183.92 | |
| **nitromethane** | | | -151.99 | | | -168.33 |

**Table S4.** Summary of results obtained at B3LYP/6-311++G** level in gas phase for the triazole system of compounds **1a**, **2a**, **3a**, **4a**, **5a** and **6a**. $^{1}$H, $^{13}$C and $^{15}$N isotropic shieldings of the lowest free energy minima and Boltzmann averaged shieldings ($\sigma^{min}$ and $\overline{\sigma}$), chemical shifts calculated from each set of shieldings ($\delta^{min}$ and $\overline{\delta}$[a]), residuals ($res^{min}$ and $\overline{res}$ [b]) relative to the experimental values ($\delta^{exp}$), and RMS of the residuals.

| | 1a | | | 2a | | | 3a | | | 4a | | | 5a | | | 6a | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $H^5$ | | | $H^4$ | | | $H^5$ | | | $H^5$ | | | $H^4$ | | | $H^5$ | | | RMS |
| $\delta^{exp}$ | 7.36 | | | 7.52 | | | 7.57 | | | 7.89 | | | 8.23 | | | 8.07 | | | |
| $\sigma^{min}$ | 25.13 | | | 24.71 | | | 24.18 | | | 24.50 | | | 23.81 | | | 23.76 | | | |
| $\overline{\sigma}$ | 24.74 | | | 24.51 | | | 24.25 | | | 24.19 | | | 23.88 | | | 23.81 | | | |
| $\delta^{min}$ | 6.84 | | | 7.26 | | | 7.79 | | | 7.47 | | | 8.16 | | | 8.21 | | | |
| $\overline{\delta}$ | 7.23 | | | 7.46 | | | 7.72 | | | 7.78 | | | 8.09 | | | 8.16 | | | |
| $res^{min}$ | -0.52 | | | -0.26 | | | 0.22 | | | -0.42 | | | -0.07 | | | 0.14 | | | 0.31 |
| $\overline{res}$ | -0.13 | | | -0.06 | | | 0.15 | | | -0.11 | | | -0.14 | | | 0.09 | | | 0.12 |
| | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | |
| $\delta^{exp}$ | 147.90 | 122.10 | | 132.90 | 136.50 | | 147.80 | 129.70 | | 146.60 | 125.70 | | 141.10 | 133.90 | | 146.90 | 135.10 | | |
| $\sigma^{min}$ | 29.05 | 54.86 | | 46.65 | 40.35 | | 29.19 | 42.61 | | 29.03 | 52.26 | | 35.94 | 43.85 | | 30.11 | 42.57 | | |
| $\overline{\sigma}$ | 28.61 | 57.01 | | 45.86 | 41.77 | | 27.95 | 43.51 | | 28.52 | 53.33 | | 36.25 | 43.61 | | 29.00 | 43.32 | | |
| $\delta^{min}$ | 155.06 | 129.25 | | 137.46 | 143.76 | | 154.92 | 141.50 | | 155.07 | 131.85 | | 148.17 | 140.26 | | 154.00 | 141.54 | | |
| $\overline{\delta}$ | 155.50 | 127.10 | | 138.25 | 142.34 | | 156.16 | 140.60 | | 155.59 | 130.78 | | 147.86 | 140.50 | | 155.10 | 140.79 | | |
| $res^{min}$ | 7.16 | 7.15 | | 4.56 | 7.26 | | 7.12 | 11.80 | | 8.47 | 6.15 | | 7.07 | 6.36 | | 7.10 | 6.44 | | 7.40 |
| $\overline{res}$ | 7.60 | 5.00 | | 5.35 | 5.84 | | 8.36 | 10.90 | | 8.99 | 5.08 | | 6.76 | 6.60 | | 8.20 | 5.69 | | 7.24 |
| | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | |
| $\delta^{exp}$ | -134.80 | -18.30 | -31.50 | -144.10 | -22.90 | -40.90 | -50.10 | -126.70 | -55.90 | -130.90 | -12.80 | -18.90 | -142.40 | -9.30 | -38.60 | -41.40 | -119.00 | -47.40 | |
| $\sigma^{min}$ | -14.96 | -147.45 | -142.47 | -15.55 | -154.71 | -139.54 | -106.38 | -22.90 | -109.86 | -19.36 | -149.27 | -153.12 | -20.80 | -170.05 | -136.23 | -106.46 | -31.40 | -124.65 | |
| $\overline{\sigma}$ | -15.37 | -149.24 | -138.07 | -16.08 | -155.18 | -138.55 | -110.57 | -24.15 | -104.59 | -20.72 | -151.10 | -151.88 | -19.39 | -168.76 | -136.74 | -110.64 | -32.68 | -120.35 | |
| $\delta^{min}$ | -137.04 | -4.54 | -9.53 | -136.45 | 2.72 | -12.46 | -45.61 | -129.09 | -42.13 | -132.63 | -2.73 | 1.13 | -131.19 | 18.06 | -15.77 | -45.54 | -120.59 | -27.34 | |
| $\overline{\delta}$ | -136.62 | -2.75 | -13.92 | -135.92 | 3.18 | -13.44 | -41.43 | -127.84 | -47.41 | -131.27 | -0.89 | -0.12 | -132.60 | 16.77 | -15.25 | -41.35 | -119.32 | -31.64 | |
| $res^{min}$ | -2.24 | 13.76 | 21.97 | 7.65 | 25.62 | 28.44 | 4.49 | -2.39 | 13.77 | -1.73 | 10.07 | 20.03 | 11.21 | 27.36 | 22.83 | -4.14 | -1.59 | 20.06 | 16.23 |
| $\overline{res}$ | -1.82 | 15.55 | 17.58 | 8.18 | 26.08 | 27.46 | 8.67 | -1.14 | 8.49 | -0.37 | 11.91 | 18.78 | 9.80 | 26.07 | 23.35 | 0.05 | -0.32 | 15.76 | 15.40 |

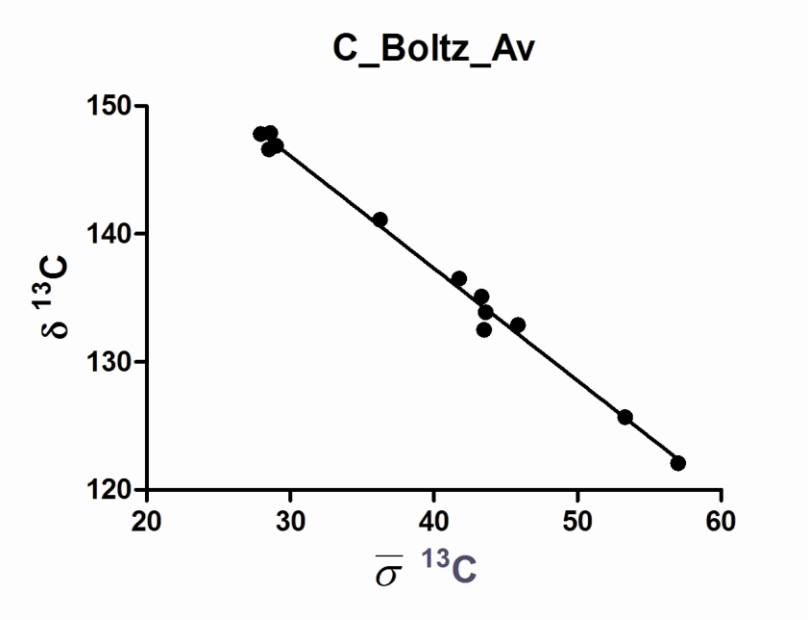
[a] Chemical shifts calculated by subtraction of calculated shieldings from values for reference compounds (Table S3). [b] Residuals calculated as the difference between calculated and experimental δ values.

**Table S5.** Summary of results obtained at B3LYP/6-311++G** level under implicit $CHCl_3$ solvation for the triazole system of compounds **1a**, **2a**, **3a**, **4a**, **5a** and **6a**. $^{1}H$, $^{13}C$ and $^{15}N$ isotropic shieldings of the lowest free energy minima and Boltzmann averaged shieldings ($\sigma^{min}$ and $\overline{\sigma}$), chemical shifts calculated from each set of shieldings ($\delta^{min}$ and $\overline{\delta}$[a]), residuals ($res^{min}$ and $\overline{res}$[b]) relative to the experimental values ($\delta^{exp}$), and RMS of the residuals.

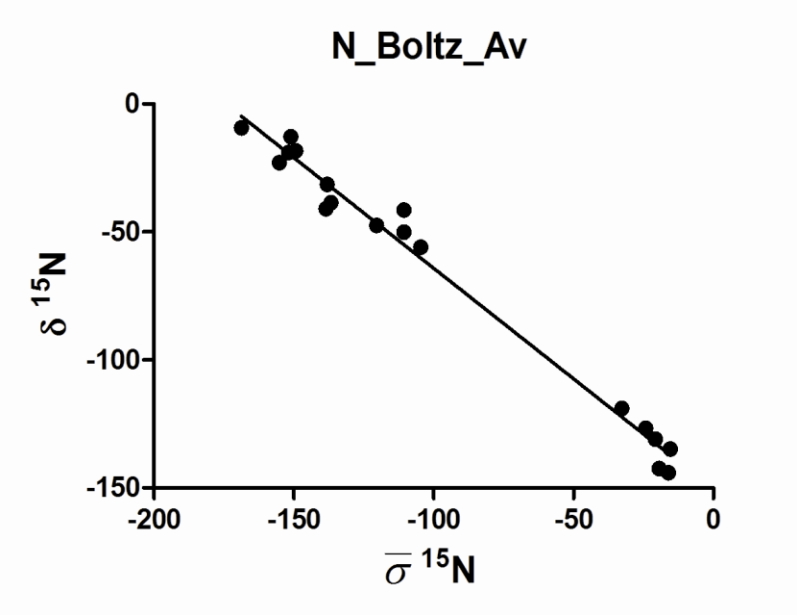
| | 1a | | | 2a | | | 3a | | | 4a | | | 5a | | | 6a | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $H^5$ | | | $H^4$ | | | $H^5$ | | | $H^5$ | | | $H^4$ | | | $H^5$ | | | RMS |
| $\delta^{exp}$ | 7.36 | | | 7.52 | | | 7.57 | | | 7.89 | | | 8.23 | | | 8.07 | | | |
| $\sigma^{min}$ | 23.66 | | | 23.35 | | | 23.64 | | | 23.56 | | | 22.89 | | | 22.86 | | | |
| $\overline{\sigma}$ | 23.90 | | | 23.17 | | | 23.50 | | | 23.19 | | | 22.99 | | | 22.94 | | | |
| $\delta^{min}$ | 8.27 | | | 8.58 | | | 8.29 | | | 8.37 | | | 9.04 | | | 9.07 | | | |
| $\overline{\delta}$ | 8.03 | | | 8.76 | | | 8.43 | | | 8.74 | | | 8.94 | | | 8.99 | | | |
| $res^{min}$ | 0.91 | | | 1.06 | | | 0.72 | | | 0.48 | | | 0.81 | | | 1.00 | | | 0.85 |
| $\overline{res}$ | 0.67 | | | 1.24 | | | 0.86 | | | 0.85 | | | 0.71 | | | 0.92 | | | 0.90 |
| | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | $C^4$ | $C^5$ | | |
| $\delta^{exp}$ | 147.90 | 122.10 | | 132.90 | 136.50 | | 147.80 | 129.70 | | 146.60 | 125.70 | | 141.10 | 133.90 | | 146.90 | 135.10 | | |
| $\sigma^{min}$ | 22.38 | 58.52 | | 44.77 | 42.59 | | 24.54 | 43.03 | | 24.30 | 51.70 | | 40.57 | 51.16 | | 28.39 | 43.43 | | |
| $\overline{\sigma}$ | 21.12 | 57.60 | | 40.71 | 41.24 | | 24.09 | 40.17 | | 24.20 | 53.12 | | 40.12 | 49.87 | | 28.49 | 43.38 | | |
| $\delta^{min}$ | 161.54 | 125.40 | | 139.15 | 141.33 | | 159.38 | 140.89 | | 159.62 | 132.22 | | 143.35 | 132.76 | | 155.53 | 140.49 | | |
| $\overline{\delta}$ | 162.80 | 126.32 | | 143.21 | 142.68 | | 159.83 | 143.75 | | 159.72 | 130.80 | | 143.80 | 134.05 | | 155.43 | 140.54 | | |
| $res^{min}$ | 13.64 | 3.30 | | 6.25 | 4.83 | | 11.58 | 11.19 | | 13.02 | 6.52 | | 2.25 | -1.14 | | 8.63 | 5.39 | | 8.37 |
| $\overline{res}$ | 14.90 | 4.22 | | 10.31 | 6.18 | | 12.03 | 14.05 | | 13.12 | 5.10 | | 2.70 | 0.15 | | 8.53 | 5.44 | | 9.28 |
| | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | $N^1$ | $N^2$ | $N^3$ | |
| $\delta^{exp}$ | -134.80 | -18.30 | -31.50 | -144.10 | -22.90 | -40.90 | -50.10 | -126.70 | -55.90 | -130.90 | -12.80 | -18.90 | -142.40 | -9.30 | -38.60 | -41.40 | -119.00 | -47.40 | |
| $\sigma^{min}$ | -24.80 | -152.14 | -171.11 | -22.31 | -153.16 | -158.25 | -118.87 | -35.71 | -104.77 | -22.56 | -153.19 | -179.17 | -19.00 | -168.28 | -148.26 | -116.41 | -38.79 | -118.77 | |
| $\overline{\sigma}$ | -22.21 | -151.61 | -173.10 | -22.42 | -155.42 | -159.19 | -119.43 | -31.36 | -106.15 | -23.91 | -154.91 | -180.46 | -20.35 | -168.70 | -150.40 | -115.85 | -37.26 | -119.85 | |
| $\delta^{min}$ | -143.53 | -16.19 | 2.78 | -146.02 | -15.17 | -10.08 | -49.46 | -132.62 | -63.56 | -145.77 | -15.14 | 10.84 | -149.33 | -0.05 | -20.07 | -51.92 | -129.54 | -49.56 | |
| $\overline{\delta}$ | -146.12 | -16.72 | 4.77 | -145.91 | -12.91 | -9.14 | -48.90 | -136.97 | -62.18 | -144.42 | -13.42 | 12.13 | -147.98 | 0.37 | -17.93 | -52.48 | -131.07 | -48.48 | |
| $res^{min}$ | -8.73 | 2.11 | 34.28 | -1.92 | 7.73 | 30.82 | 0.64 | -5.92 | -7.66 | -14.87 | -2.34 | 29.74 | -6.93 | 9.25 | 18.53 | -10.52 | -10.54 | -2.16 | 15.23 |
| $\overline{res}$ | -11.32 | 1.58 | 36.27 | -1.81 | 9.99 | 31.76 | 1.20 | -10.27 | -6.28 | -13.52 | -0.62 | 31.03 | -5.58 | 9.67 | 20.67 | -11.08 | -12.07 | -1.08 | 16.11 |

[a] Chemical shifts calculated by subtraction of calculated shieldings from values for reference compounds (Table S3). [b] Residuals calculated as the difference between calculated and experimental δ values.

**Figure S1.** Linear fits of the gas phase calculated Boltzmann averaged shieldings ( $\overline{\sigma}$ ) to the experimental $^{13}$C and $^{15}$N-chemical shifts.




$$\delta^{13}\mathrm{C} = (172.4 \pm 1.0) - (0.878 \pm 0.023)\ \sigma^{13}\mathrm{C} \qquad n = 12,\ r^2 = 0.993 \qquad (1)$$




$$\delta^{15}\mathrm{N} = -(150.0 \pm 3.0) - (0.864 \pm 0.027)\ \sigma^{15}\mathrm{N} \qquad n = 18,\ r^2 = 0.985 \qquad (2)$$

**Table S6.** $^{13}$C and $^{15}$N-chemical shifts ($\delta^{min}$ and $\overline{\delta}$) recalculated with equations (1) and (2) from the $^{13}$C and $^{15}$N isotropic shieldings of the lowest free energy minima and Boltzmann averaged shieldings ($\sigma^{min}$ and $\overline{\sigma}$), residuals ($res^{min}$ and $\overline{res}$ [a]) relative to the experimental values ($\delta^{exp}$), and RMS of the residuals.

| | **1a** | | | **2a** | | | **3a** | | | **4a** | | | **5a** | | | **6a** | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | **C$^4$** | **C$^5$** | | **C$^4$** | **C$^5$** | | **C$^4$** | **C$^5$** | | **C$^4$** | **C$^5$** | | **C$^4$** | **C$^5$** | | **C$^4$** | **C$^5$** | | **RMS** |
| $\delta^{exp}$ | 147.90 | 122.10 | | 132.90 | 136.50 | | 147.80 | 129.70 | | 146.60 | 125.70 | | 133.90 | 141.10 | | 147.70 | 135.10 | | |
| $\sigma^{min}$ | 29.05 | 54.86 | | 46.65 | 40.35 | | 29.19 | 42.61 | | 29.03 | 52.26 | | 35.94 | 43.85 | | 30.11 | 42.57 | | |
| $\overline{\sigma}$ | 28.61 | 57.01 | | 45.86 | 41.77 | | 27.95 | 43.51 | | 28.52 | 53.33 | | 36.25 | 43.61 | | 29.00 | 43.32 | | |
| $\delta^{min}$ | 147.56 | 122.99 | | 130.80 | 136.80 | | 147.43 | 134.65 | | 147.58 | 125.46 | | 141.00 | 133.47 | | 146.55 | 134.68 | | |
| $\overline{\delta}$ | 147.33 | 122.39 | | 132.18 | 135.77 | | 147.91 | 134.25 | | 147.40 | 125.62 | | 140.62 | 134.16 | | 146.98 | 134.41 | | |
| $res^{min}$ | -0.34 | 0.89 | | -2.10 | 0.30 | | -0.37 | 2.15 | | 0.98 | -0.24 | | -0.10 | -0.43 | | -0.35 | -0.42 | | 0.99 |
| $\overline{res}$ | -0.57 | 0.29 | | -0.72 | -0.73 | | 0.11 | 1.75 | | 0.80 | -0.08 | | -0.48 | 0.26 | | 0.08 | -0.69 | | 0.70 |
| | **N$^1$** | **N$^2$** | **N$^3$** | **N$^1$** | **N$^2$** | **N$^3$** | **N$^1$** | **N$^2$** | **N$^3$** | **N$^1$** | **N$^2$** | **N$^3$** | **N$^1$** | **N$^2$** | **N$^3$** | **N$^1$** | **N$^2$** | **N$^3$** | |
| $\delta^{exp}$ | -134.80 | -18.30 | -31.50 | -144.10 | -22.90 | -40.90 | -50.10 | -126.70 | -55.90 | -130.90 | -12.80 | -18.90 | -142.40 | -9.30 | -38.60 | -41.40 | -119.00 | -47.40 | |
| $\sigma^{min}$ | -14.96 | -147.45 | -142.47 | -15.55 | -154.71 | -139.54 | -106.38 | -22.90 | -109.86 | -19.36 | -149.27 | -153.12 | -20.80 | -170.05 | -136.23 | -106.46 | -31.40 | -124.65 | |
| $\overline{\sigma}$ | -15.37 | -149.24 | -138.07 | -16.08 | -155.18 | -138.55 | -110.57 | -24.15 | -104.59 | -20.72 | -151.10 | -151.88 | -19.39 | -168.76 | -136.74 | -110.64 | -32.68 | -120.35 | |
| $\delta^{min}$ | -136.86 | -23.71 | -27.96 | -136.35 | -17.51 | -30.46 | -58.78 | -130.07 | -55.81 | -133.09 | -22.16 | -18.86 | -131.87 | -4.41 | -33.29 | -58.72 | -122.81 | -43.18 | |
| $\overline{\delta}$ | -137.25 | -21.63 | -31.28 | -136.64 | -16.51 | -30.87 | -55.03 | -129.66 | -60.20 | -132.63 | -20.03 | -19.36 | -133.77 | -4.78 | -32.43 | -54.97 | -122.30 | -46.58 | |
| $res^{min}$ | -2.06 | -5.41 | 3.54 | 7.75 | 5.39 | 10.44 | -8.68 | -3.37 | 0.09 | -2.19 | -9.36 | 0.04 | 10.53 | 4.89 | 5.31 | -17.32 | -3.81 | 4.22 | 7.14 |
| $\overline{res}$ | -2.45 | -3.33 | 0.22 | 7.46 | 6.39 | 10.03 | -4.93 | -2.96 | -4.30 | -1.73 | -7.23 | -0.46 | 8.63 | 4.52 | 6.17 | -13.57 | -3.30 | 0.82 | 6.01 |

[a] Residuals calculated as the difference between calculated and experimental δ values.