

# Pushing on the boundaries of pterin chemistry

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## Supporting Information

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## NMR Spectra

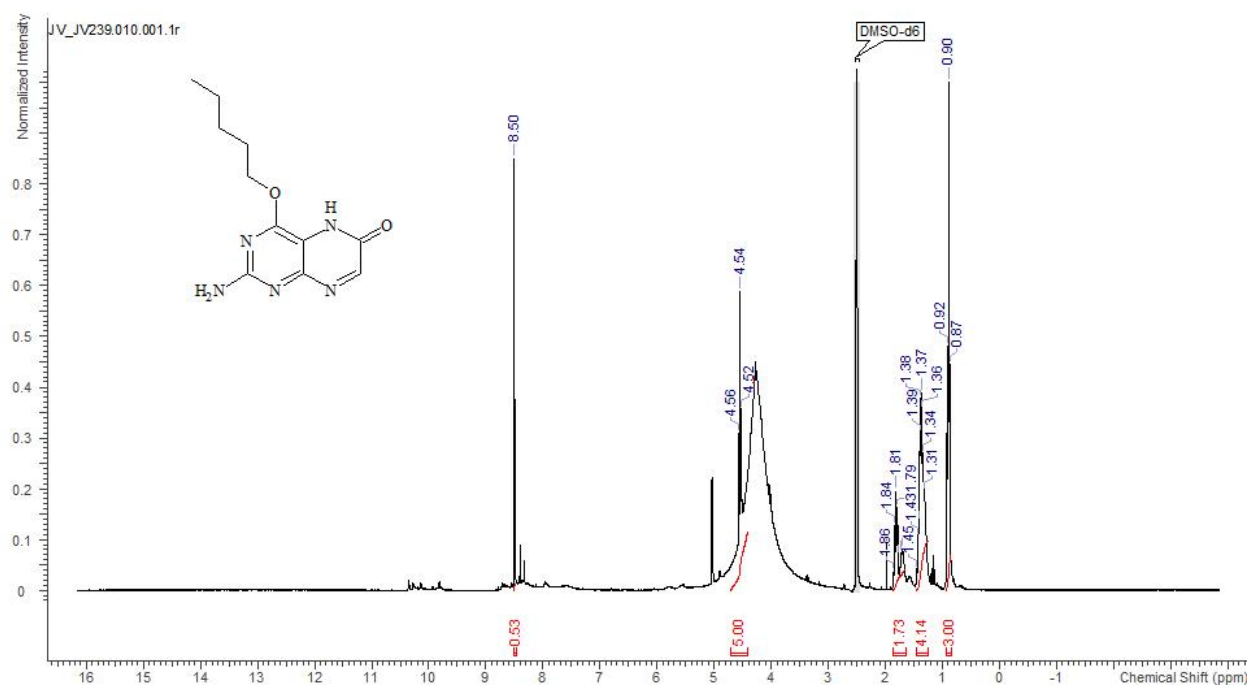


Figure 1: <sup>1</sup>H NMR (300 MHz, DMSO-d<sub>6</sub>) spectrum of compound 1

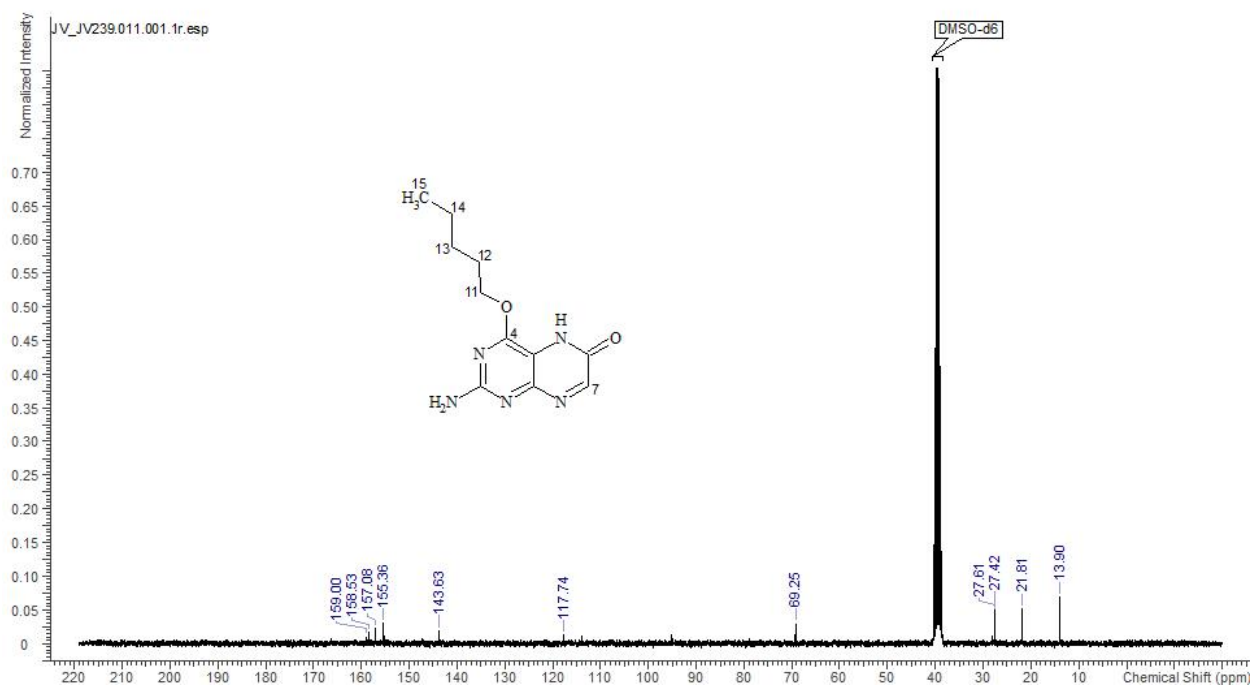


Figure 2:  $^{13}\text{C}$  NMR (300 MHz, DMSO- $d_6$ ) spectrum of compound 1

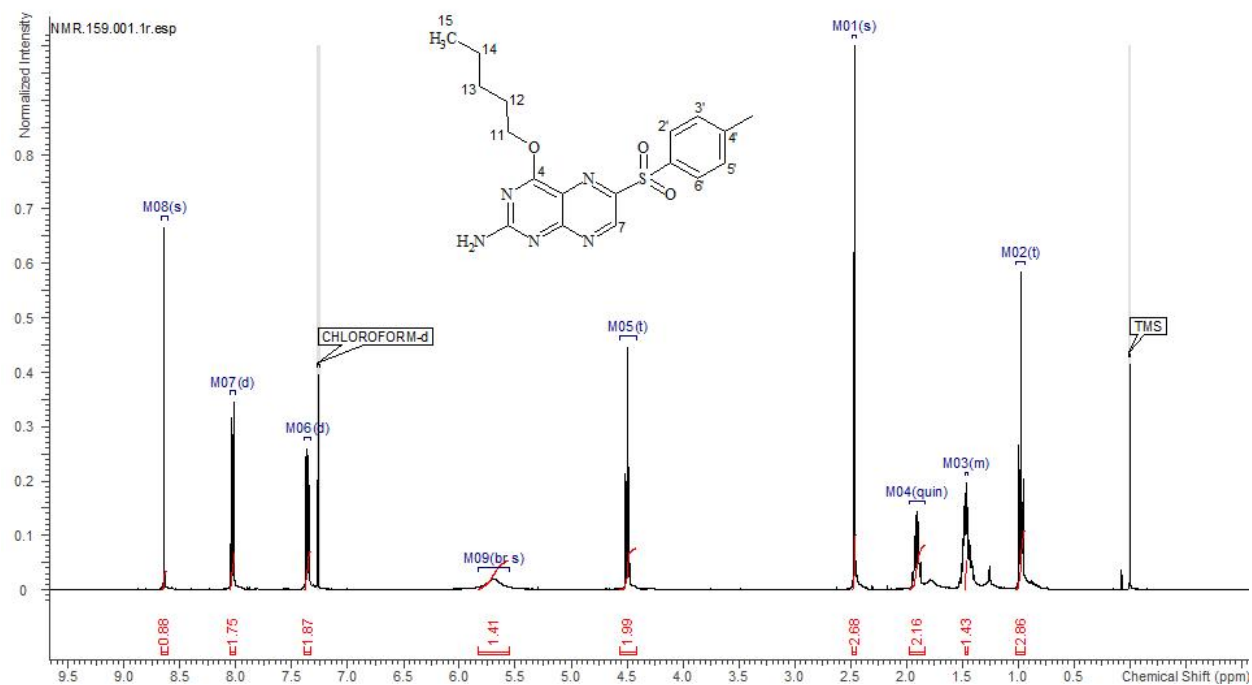


Figure 3:  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of compound 2

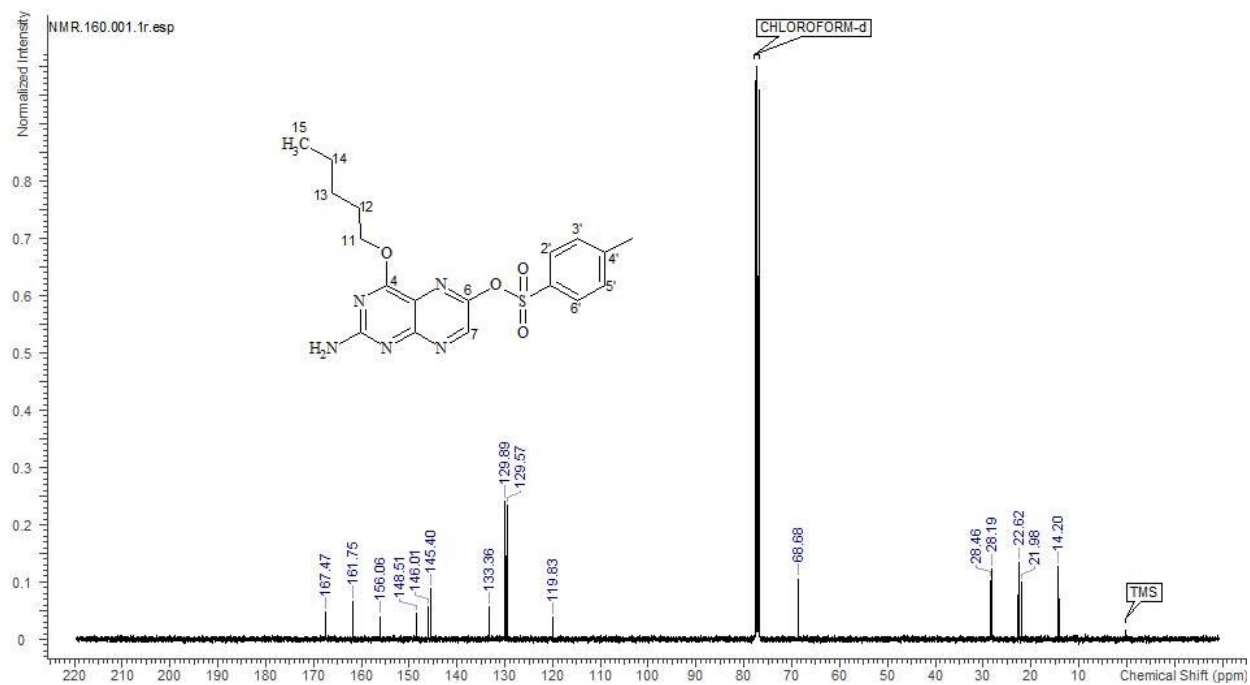


Figure 4:  $^{13}\text{C}$  NMR (400 MHz,  $\text{CDCl}_3$ ) spectrum of compound 2

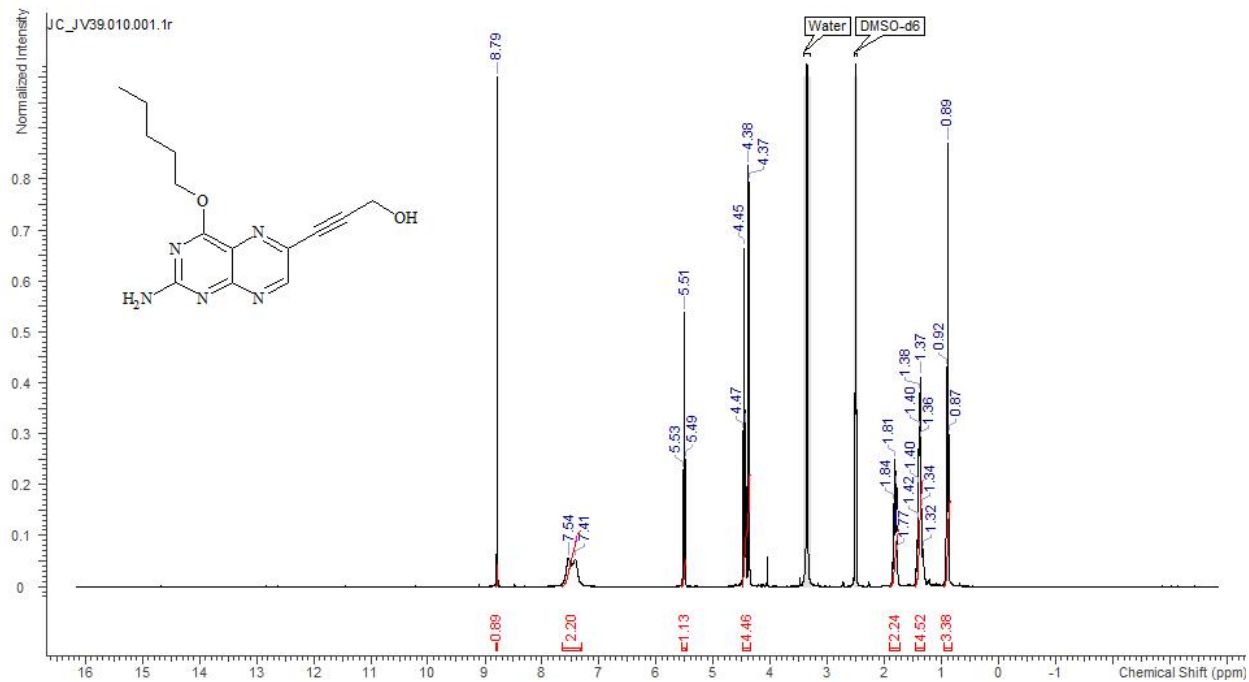


Figure 1:  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of compound **3**

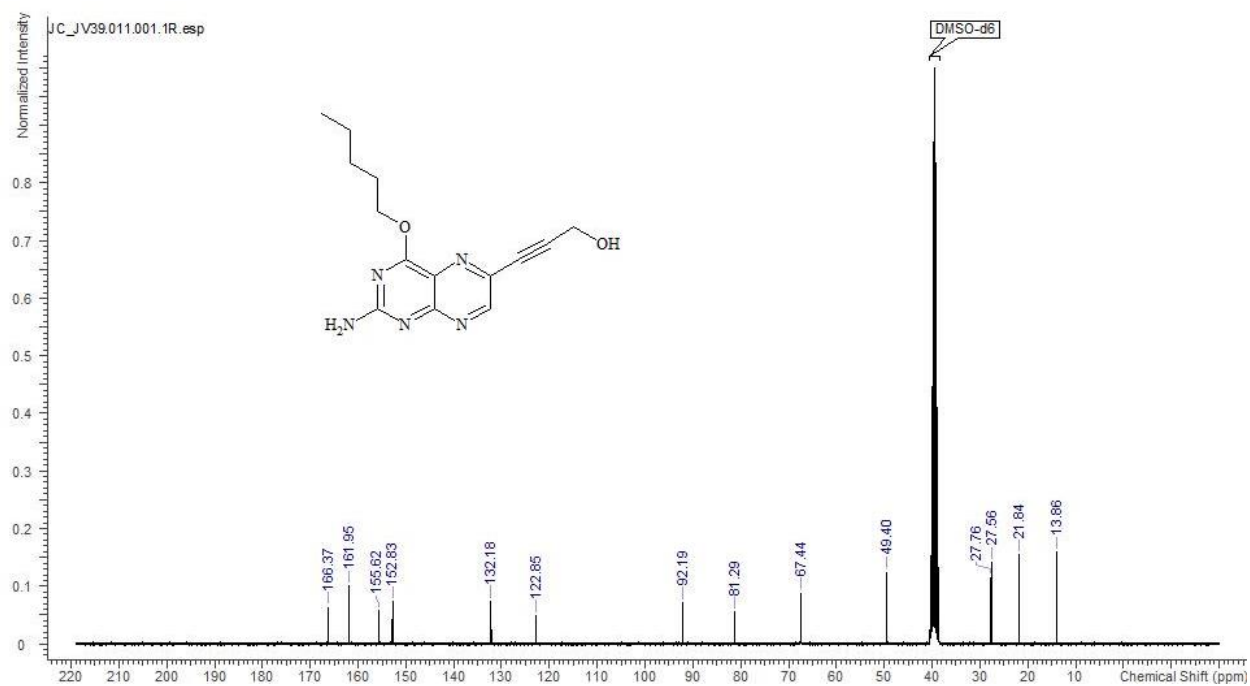


Figure 2:  $^{13}\text{C}$  NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of compound **3**

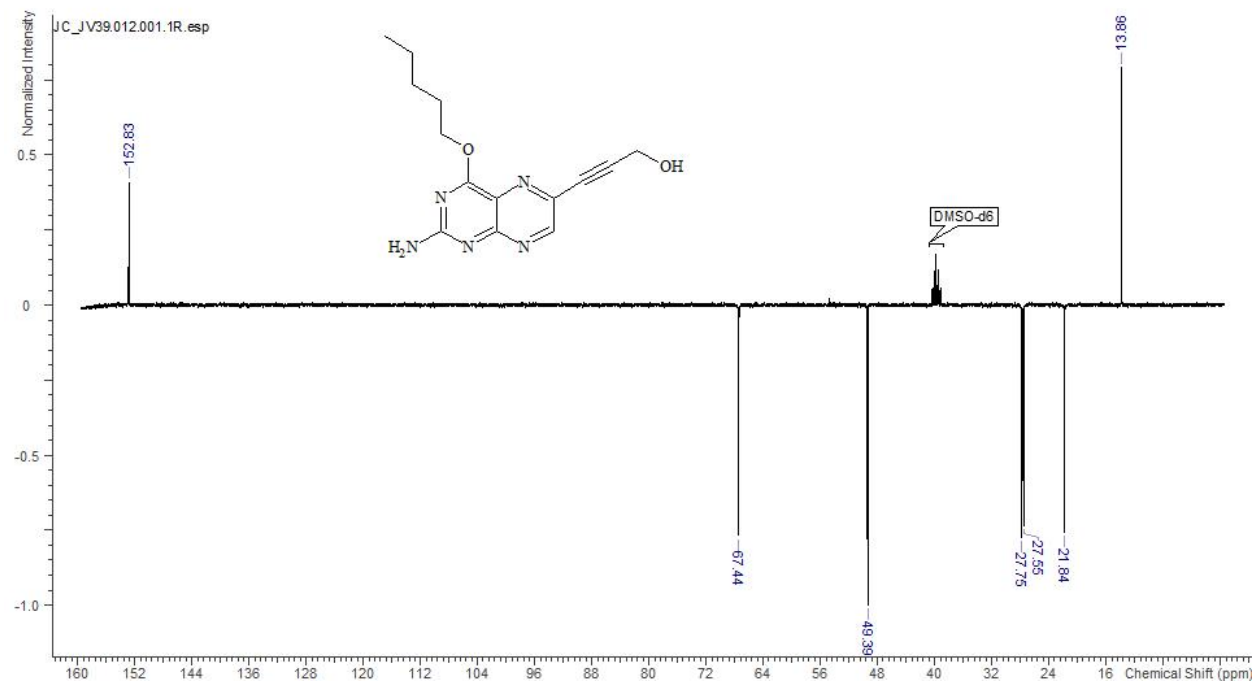


Figure 3:  $^{13}\text{C}$  DEPT135 NMR (300 MHz,  $\text{CDCl}_3$ ) spectrum of compound **3**



# Compound 4

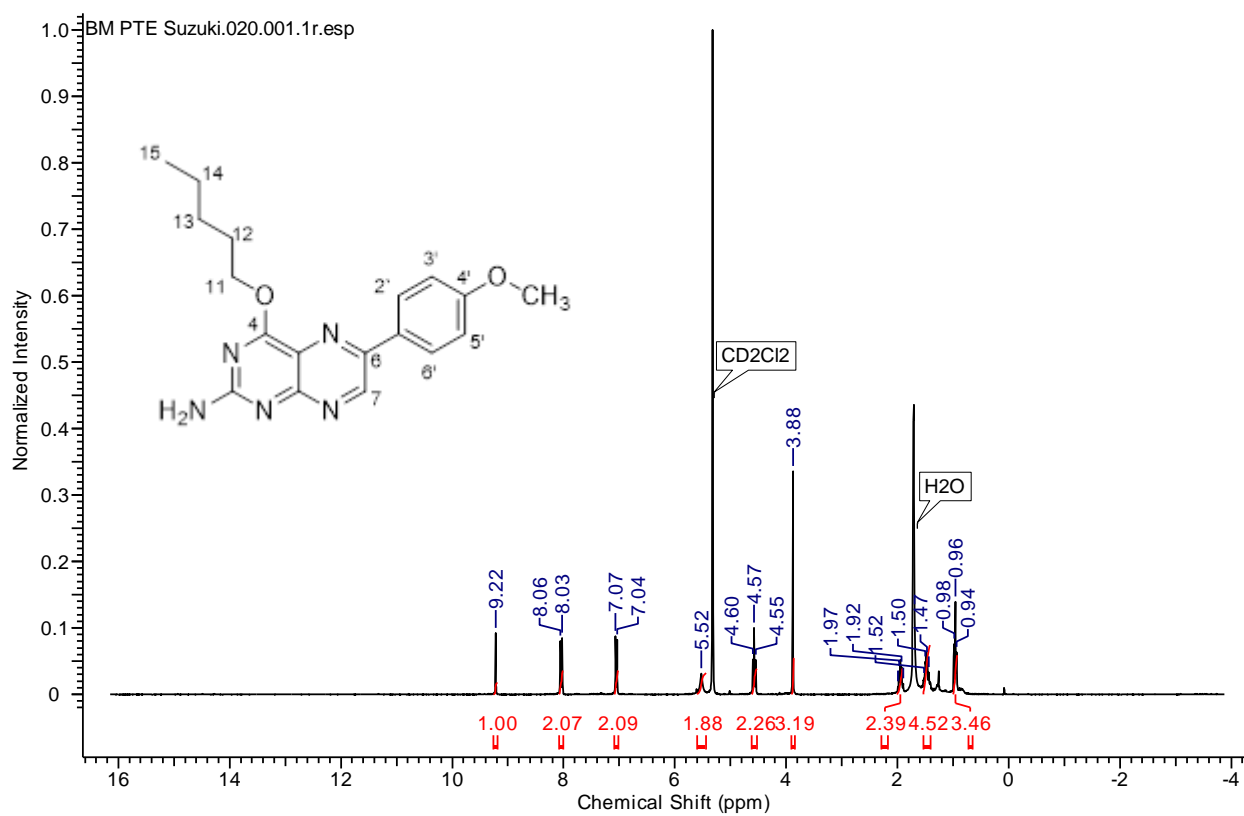


Figure 4:  $^1\text{H}$  NMR (300 MHz,  $\text{CD}_2\text{Cl}_2$ ) spectrum of compound 4

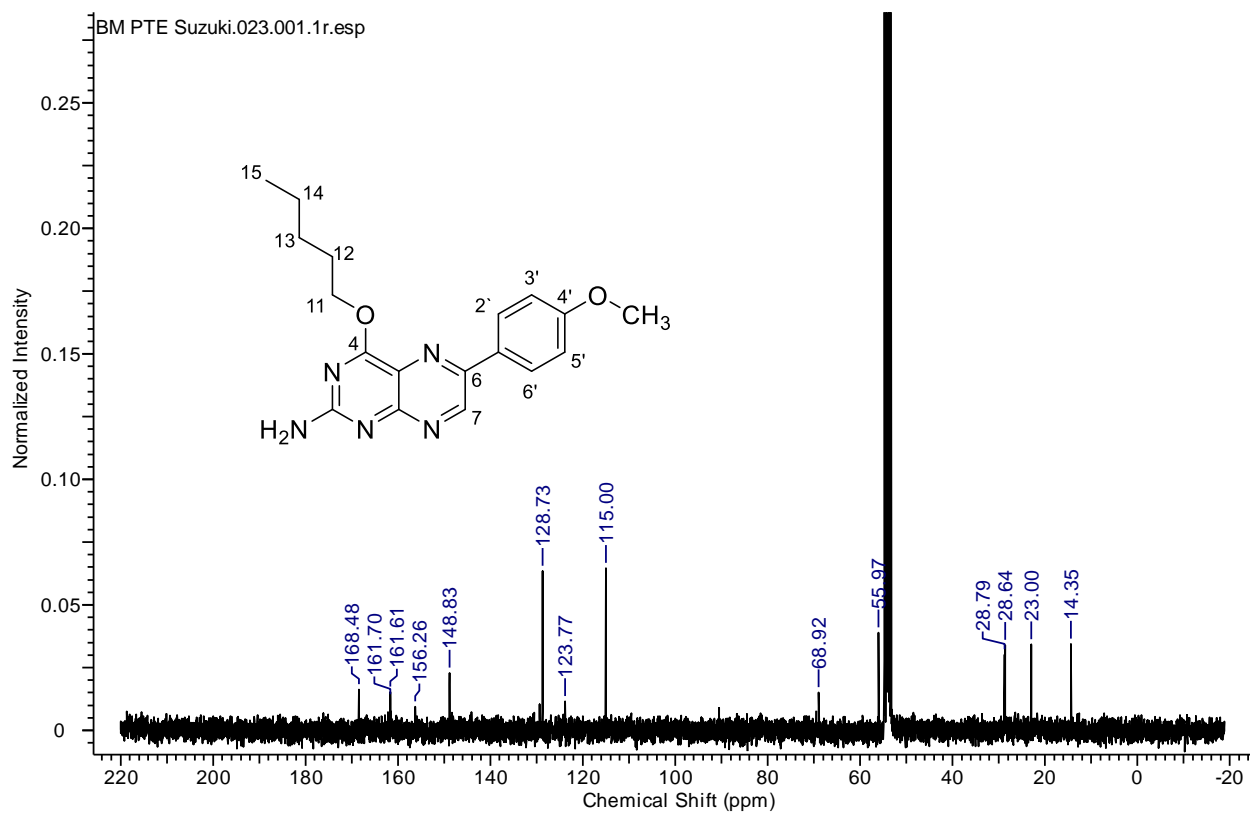


Figure 5:  $^{13}\text{C}$  NMR (300 MHz,  $\text{CD}_2\text{Cl}_2$ ) spectrum of compound **4**

# Compound 5'

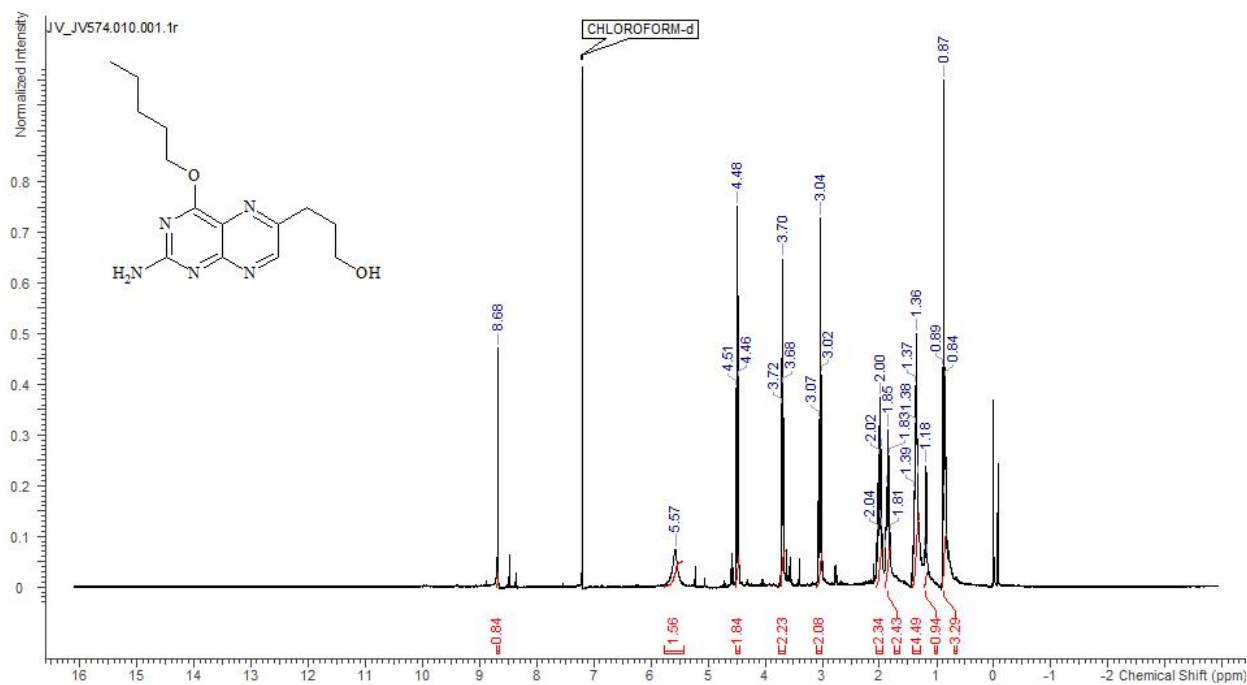


Figure 6: <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) spectrum of compound 5'

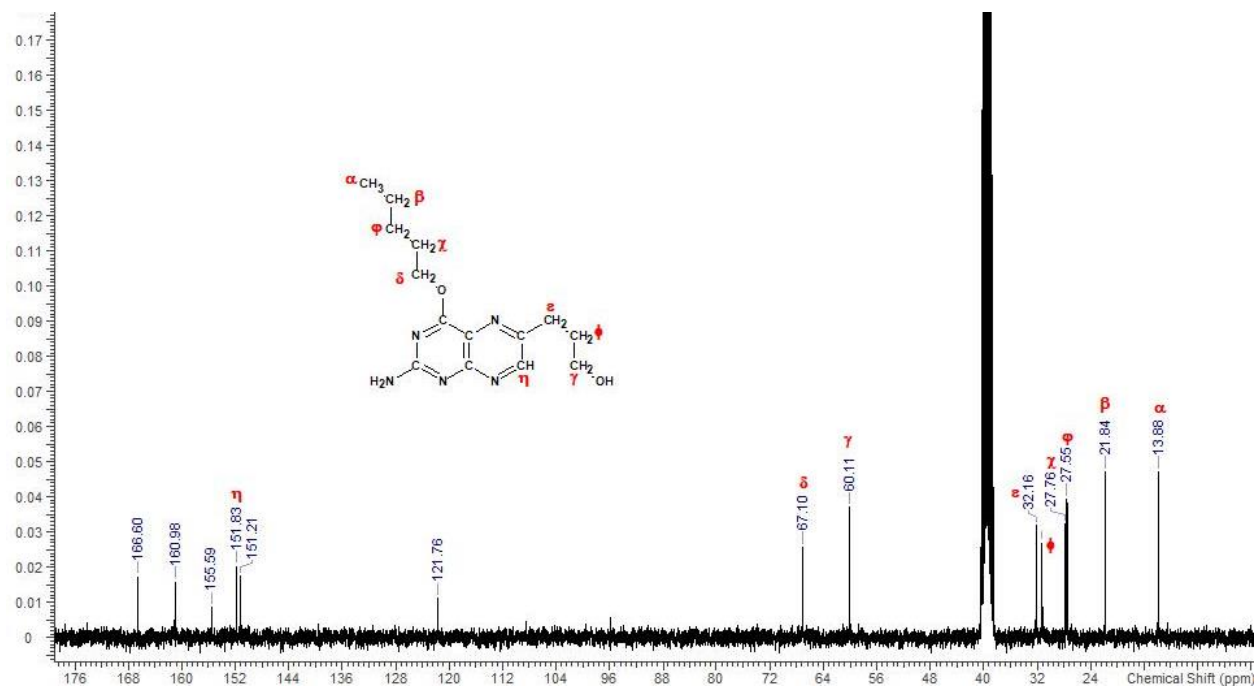


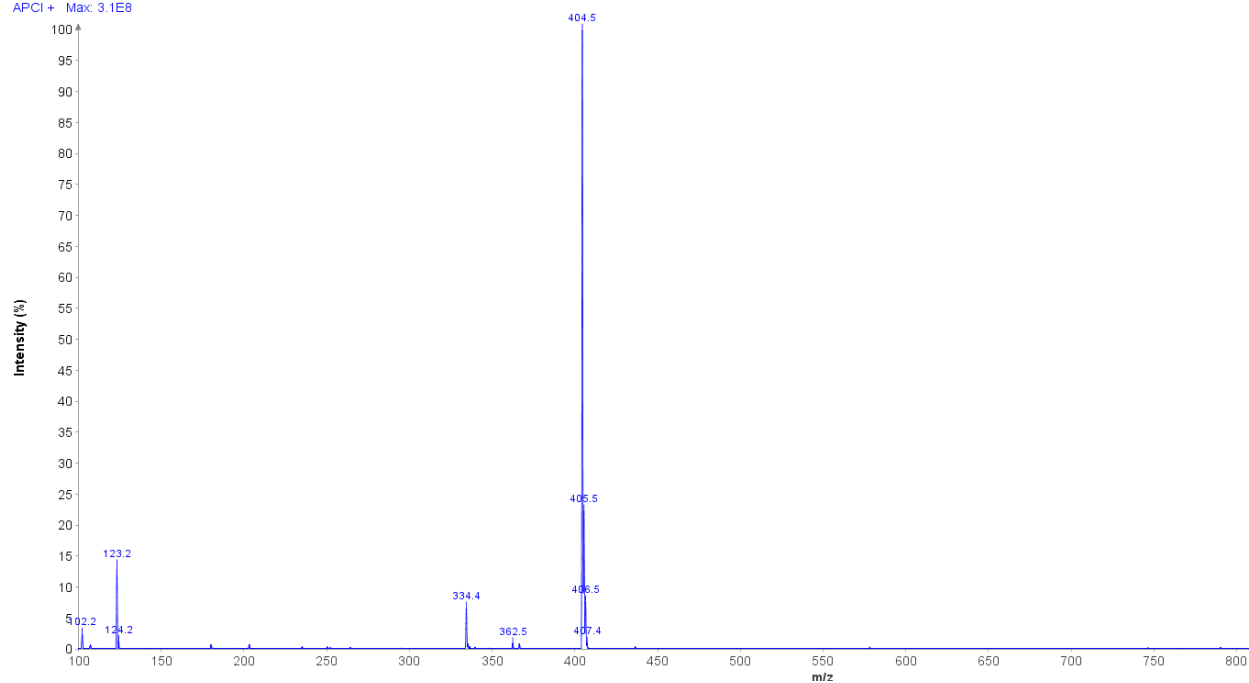
Figure 7: <sup>13</sup>C NMR (300 MHz, CDCl<sub>3</sub>) spectrum of compound 5'

## Mass Spectra

### Compound 1

Spectrum RT 3.68 - 3.98 (22 scans) - Background Subtracted 2.69 - 2.98  
JV252\_Scan1\_1s1.dabx  
APCI+ Max 3.1E8

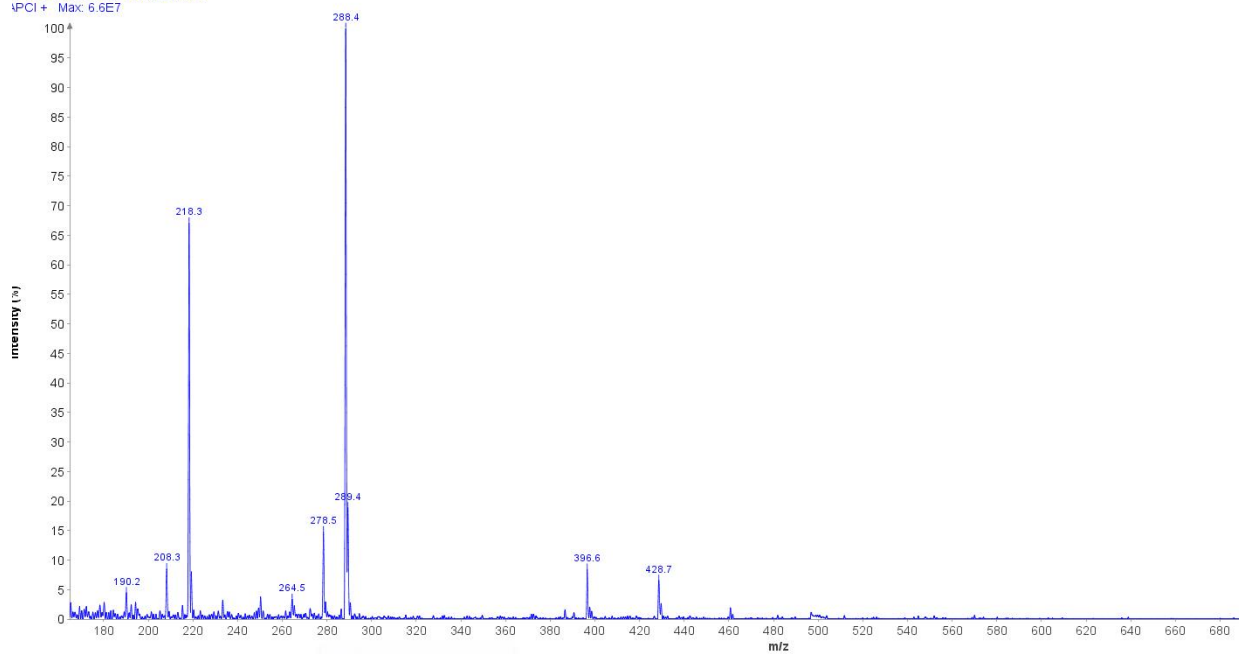
# 11 P



### Compound 3

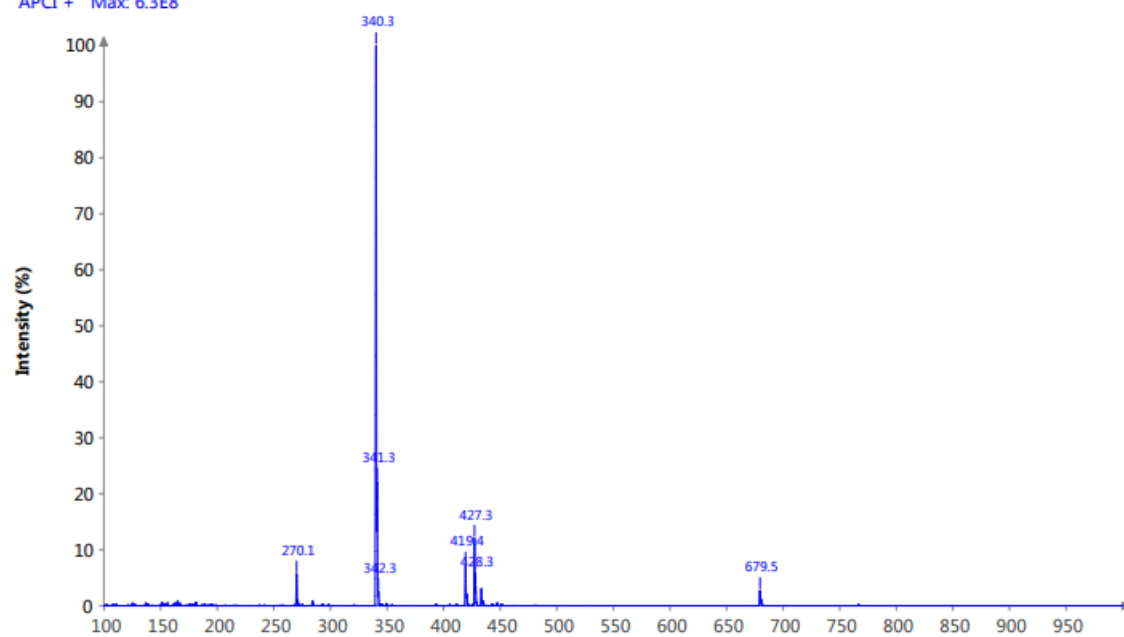
spectrum F1 4.70 - 4.76 (9 scans) - Background Subtracted 0.07 - 4.00  
IV472-Slurry-TLC\_Scan1\_is1.dabx  
PCI+ Max: 6.6E7

# 5 1 8 0 0



## Compound 4

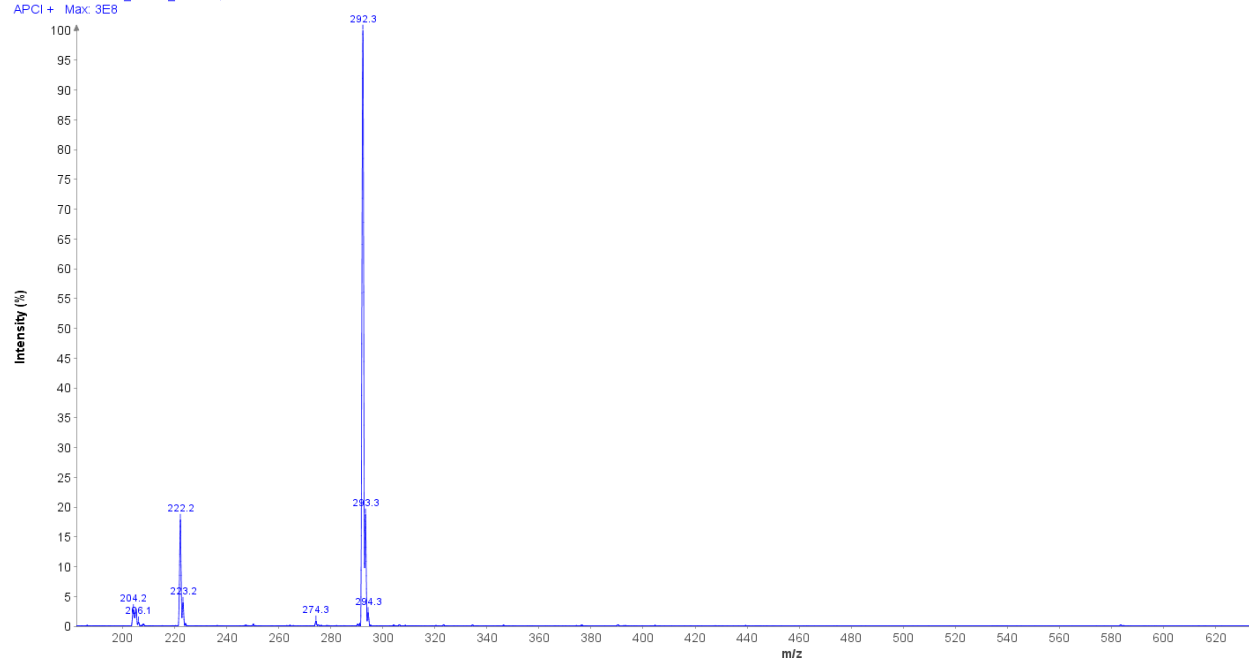
Spectrum RT 4.82 - 5.12 (47 scans) - Background Subtracted 0.19 - 4.73  
2024\_7\_23\_16\_51\_56;  
APCI + Max: 6.3E8



## Compound 5'

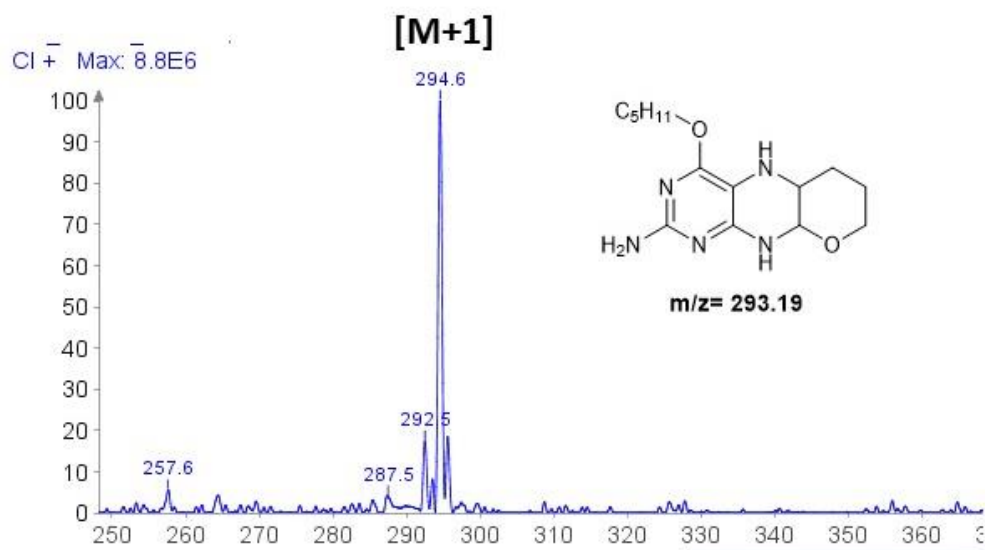
Spectrum RT 3.29 - 3.41 (9 scans) - Background Subtracted 0.00 - 7.05  
JV574 after column\_Scan1\_is1.dab;  
APCI+ Max: 3E8

# 25 P 8 X 1

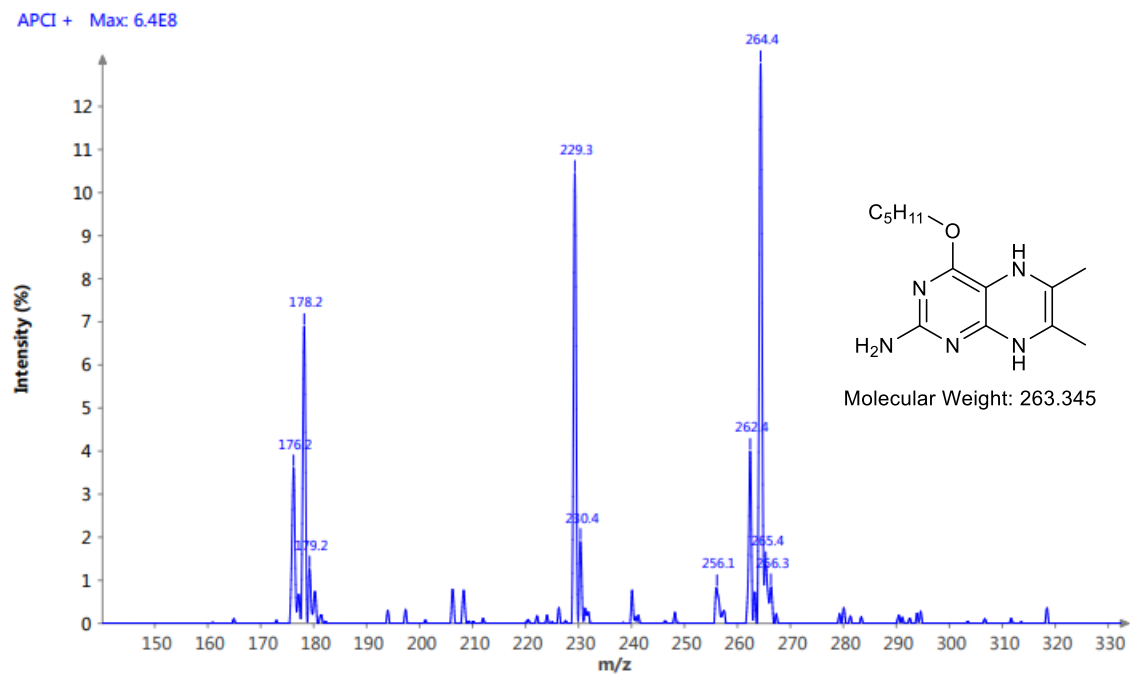


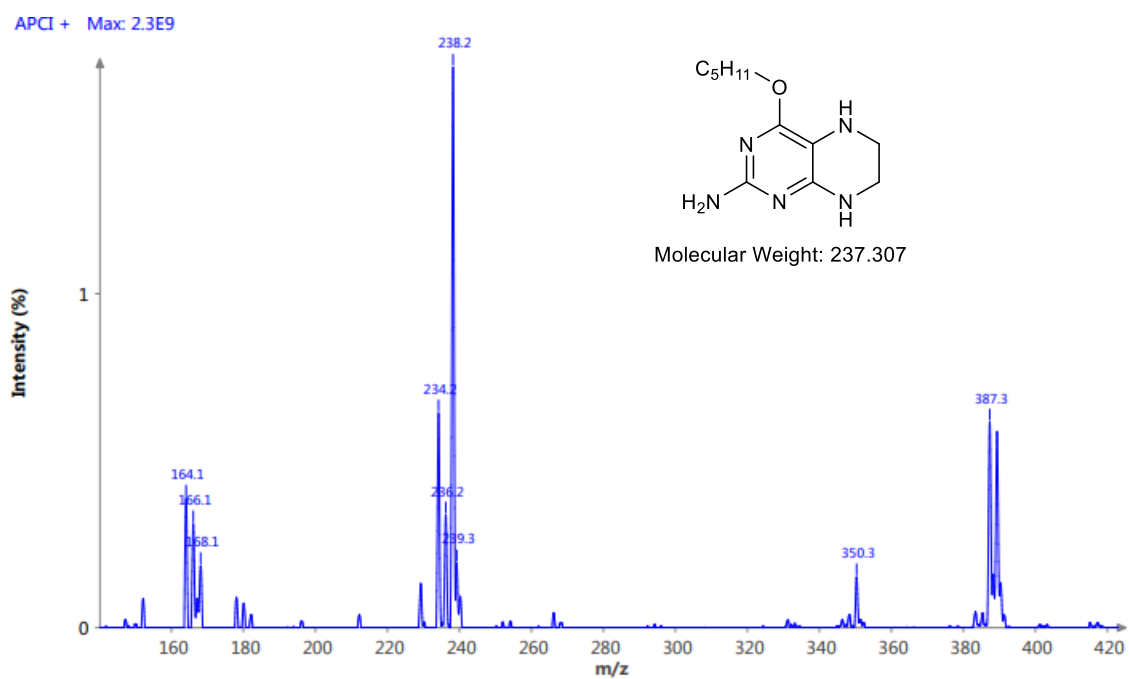


Compound 5



## APCI-MS spectra of reduction reactions

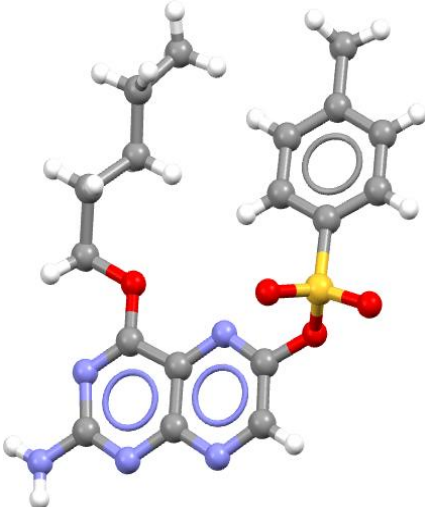




## Crystallographic data

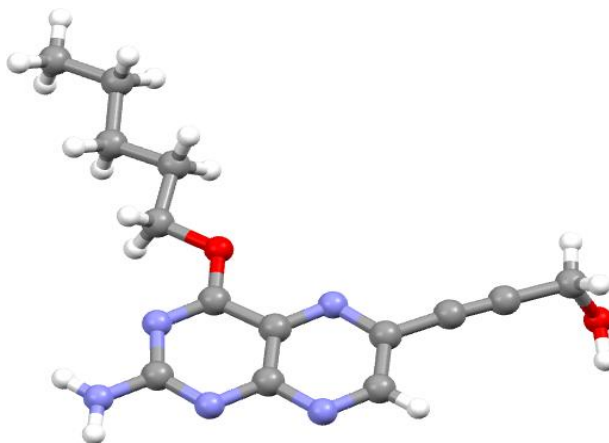
### Compound 2

Identification code	JV272B
Empirical formula	C <sub>18</sub> H <sub>21</sub> N <sub>5</sub> O <sub>4</sub> S
Formula weight	403.46
Temperature	170(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic,
Space group	P $\bar{1}$
Unit cell dimensions	a = 9.2429(18) Å $\alpha$ = 86.51(3) deg. b = 14.052(3) Å $\beta$ = 85.22(3) deg. c = 15.617(3) Å $\gamma$ = 73.11(3) deg
Volume	1932.7(7) Å <sup>3</sup>
Z, Calculated density	4, 1.387 Mg/m <sup>3</sup>
Absorption coefficient	0.203 mm <sup>-1</sup>
F(000)	848
Crystal size	0.119 x 0.109 x 0.031 mm
Theta range for data collection	2.041 to 29.466 deg.
Limiting indices	-12 ≤ h ≤ 12, -18 ≤ k ≤ 19, -21 ≤ l ≤ 21
Reflections collected / unique	22364 / 10627 [R(int) = 0.0517]
Completeness to theta = 25.000	99.8 %
Absorption correction	Numerical
Max. and min. transmission	0.9742 and 0.8575
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	10627 / 362 / 608
Goodness-of-fit on F <sup>2</sup>	1.019
Final R indices [I > 2σ(I)]	R <sub>1</sub> = 0.0470, wR <sub>2</sub> = 0.1272
R indices (all data)	R <sub>1</sub> = 0.0916, wR <sub>2</sub> = 0.1509
Extinction coefficient	n/a
Largest diff. peak and hole	0.363 and -0.595 e.Å <sup>-3</sup>



### Compound 3

Identification code	JV39
Empirical formula	C <sub>14</sub> H <sub>17</sub> N <sub>5</sub> O <sub>2</sub>
Formula weight	287.32
Temperature	170(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic,
Space group	P $\bar{1}$
Unit cell dimensions	a=4.9121(10) Å alpha = 91.32(3) deg. b=11.649(2) Å beta = 96.91(3) deg. c = 12.858(3) Å gamma = 101.82(3)
Volume	714.1(3) Å <sup>3</sup>
Z, Calculated density	2, 1.336 Mg/m <sup>3</sup>
Absorption coefficient	0.094 mm <sup>-1</sup>
F(000)	304
Crystal size	0.501 x 0.123 x 0.041 mm
Theta range for data collection	3.196 to 26.368 deg.
Limiting indices	-12<=h<=12, -18<=k<=19, -21<=l<=21
Reflections collected / unique	5910 / 2890 [R(int) = 0.0503]
Completeness to theta = 25.222	99.5 %
Absorption correction	Numerical
Max. and min. transmission	0.9774 and 0.6221
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	2890 / 96 / 232
Goodness-of-fit on F <sup>2</sup>	0.955
Final R indices [I>2sigma(I)]	R1 = 0.0452, wR2 = 0.1076
R indices (all data)	R1 = 0.0931, wR2 = 0.1268
Extinction coefficient	n/a
Largest diff. peak and hole	0.222 and -0.221 e.Å <sup>-3</sup>



## Compound 4

Identification code	SIV-BMSU
Empirical formula	C <sub>37</sub> H <sub>42</sub> Cl <sub>2</sub> D <sub>2</sub> N <sub>10</sub> O <sub>4</sub>
Formula weight	765.73
Temperature	299(2) K
Wavelength	1.54184 Å
Crystal system	Triclinic,
Space group	P $\bar{1}$
Unit cell dimensions	a = 8.3036(2) Å alpha = 89.677(2) deg. b = 12.7600(3) Å beta = 79.653(2) deg. c = 18.8608(4) Å gamma = 79.304(2) deg.
Volume	1930.93(8) Å <sup>3</sup>
Z, Calculated density	2, 1.317 Mg/m <sup>3</sup>
Absorption coefficient	1.945 mm <sup>-1</sup>
F(000)	804
Crystal size	0.290 x 0.200 x 0.120 mm
Theta range for data collection	3.527 to 65.518 deg.
Limiting indices	-9 <= h <= 9, -14 <= k <= 15, -22 <= l <= 22
Reflections collected / unique	60235 / 6618 [R(int) = 0.1254]
Completeness to theta = 25.023	0.0 %
Absorption correction	Numerical
Max. and min. transmission	1.000 and 0.481
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	6618 / 409 / 606
Goodness-of-fit on F <sup>2</sup>	1.058
Final R indices [I > 2sigma(I)]	R1 = 0.0995, wR2 = 0.2342
R indices (all data)	R1 = 0.1223, wR2 = 0.2532
Extinction coefficient	0.0013(3)
Largest diff. peak and hole	0.288 and -0.215 e.Å <sup>-3</sup>

