

Supporting information for:

S_NAr reactions on 2-amino-4,6-dichloropyrimidine-5-carbaldehyde

Jorge Trilleras ^{1,*}, Alfredo Pérez-Gamboa ¹ and Jairo Quiroga ²

¹ Grupo de Investigación en Compuestos Heterocíclicos, Universidad del Atlántico, Puerto Colombia 081007, Colombia; jorgetrilleras@mail.uniatlantico.edu.co; alfredoperez@mail.uniatlantico.edu.co

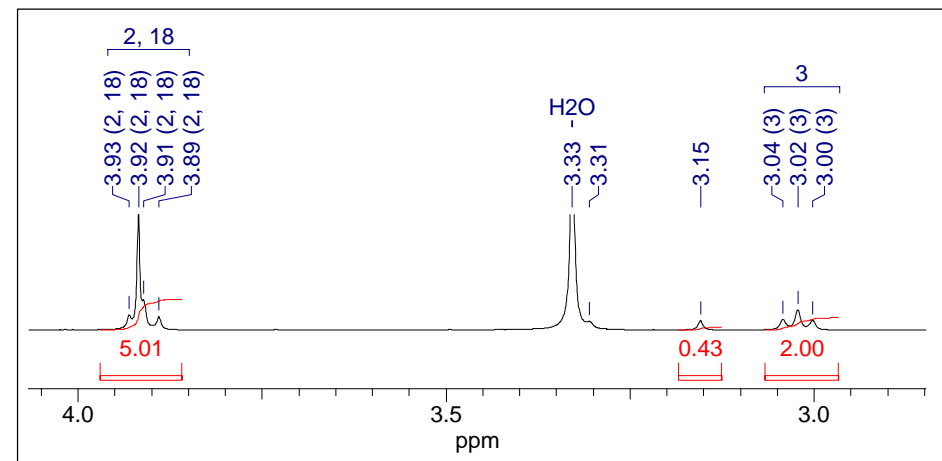
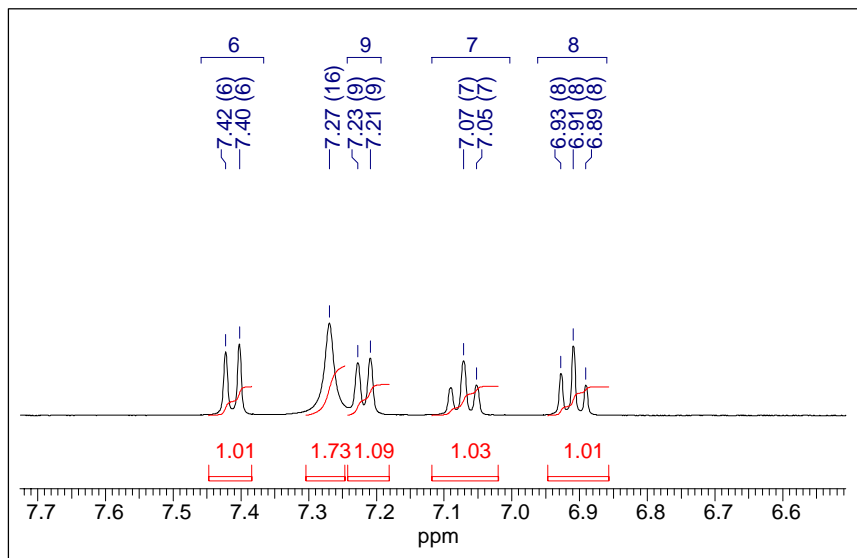
² Heterocyclic Compounds Research Group, Department of Chemistry, Universidad del Valle, Cali 760032, Colombia; jairo.quiroga@correounivalle.edu.co

* Correspondence: jorgetrilleras@mail.uniatlantico.edu.co

Table of Contents

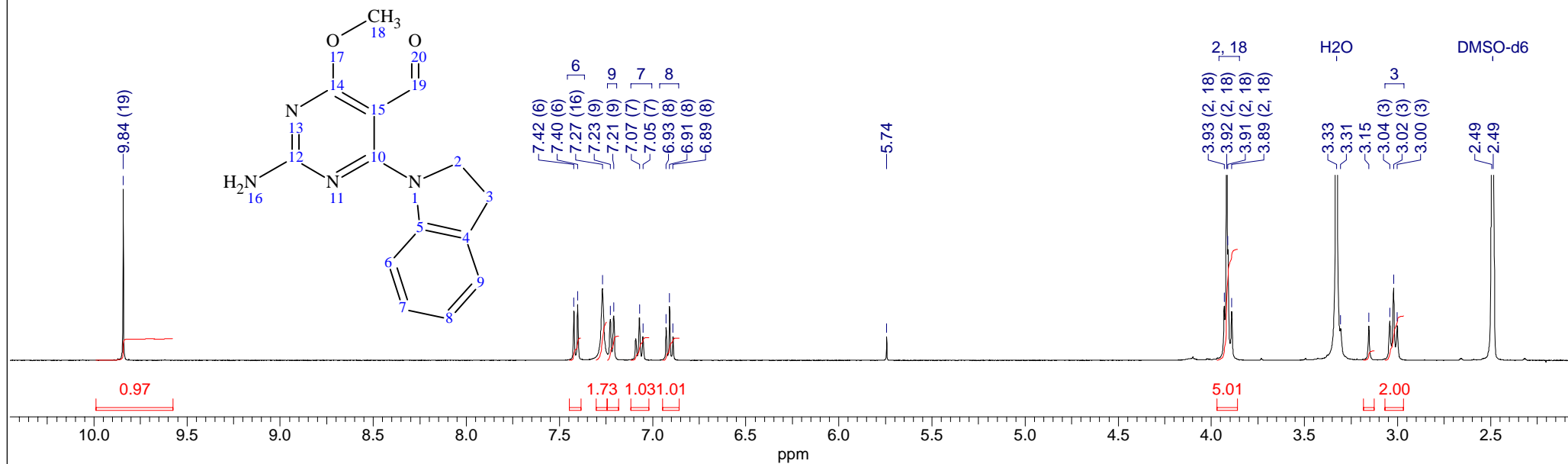
¹ H-NMR and ¹³ C-NMR data for compound I	Page 1 – 2
¹ H-NMR and ¹³ C-NMR data for compound II	Page 3 – 4
HR-MS data for compound I	Page 5
¹ H-NMR and ¹³ C-NMR data for compound III	Page 6 – 7
¹ H-NMR and ¹³ C-NMR data for compound IV	Page 8 – 9
HR-MS data for compound IV	Page 10

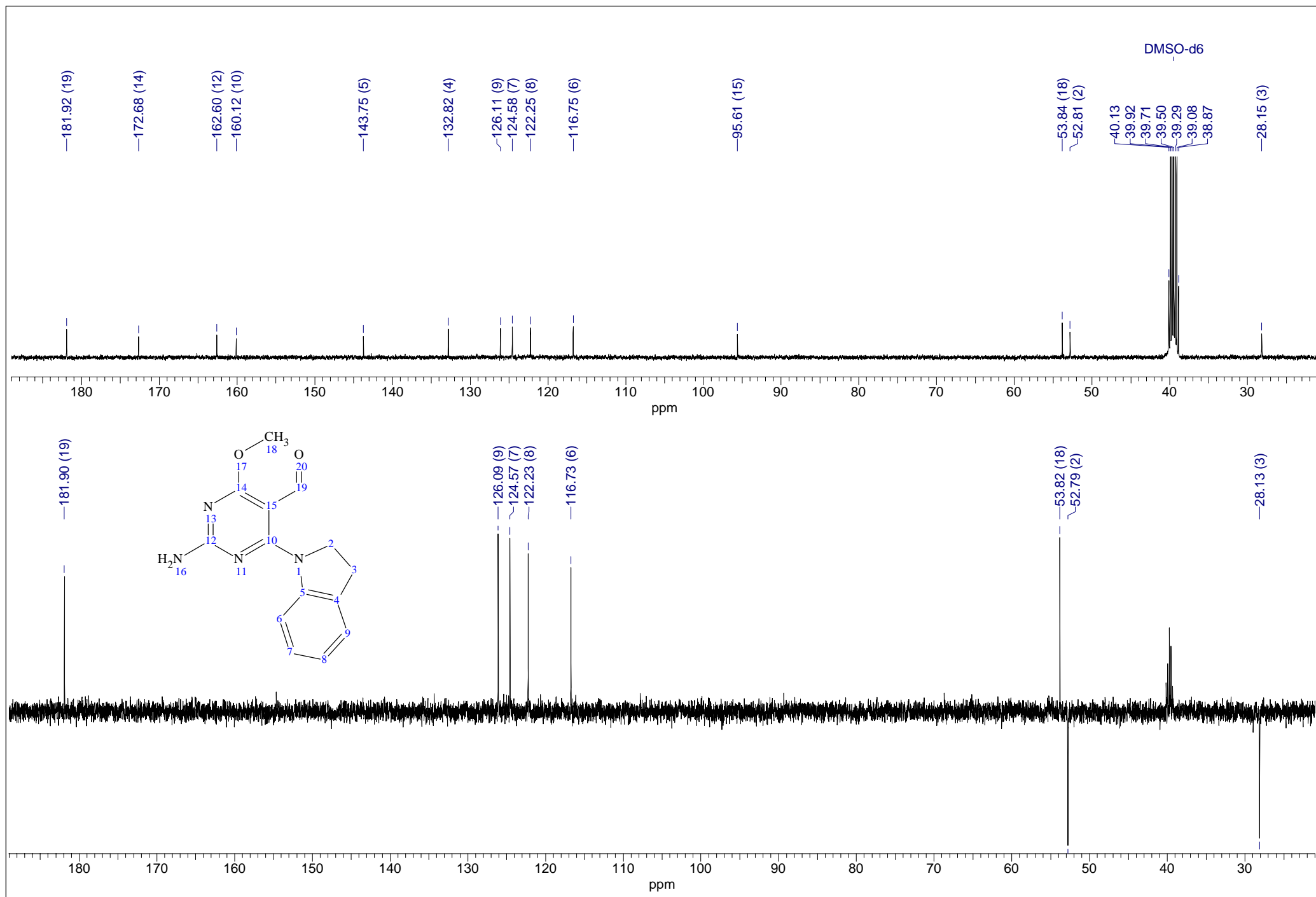
Compound I



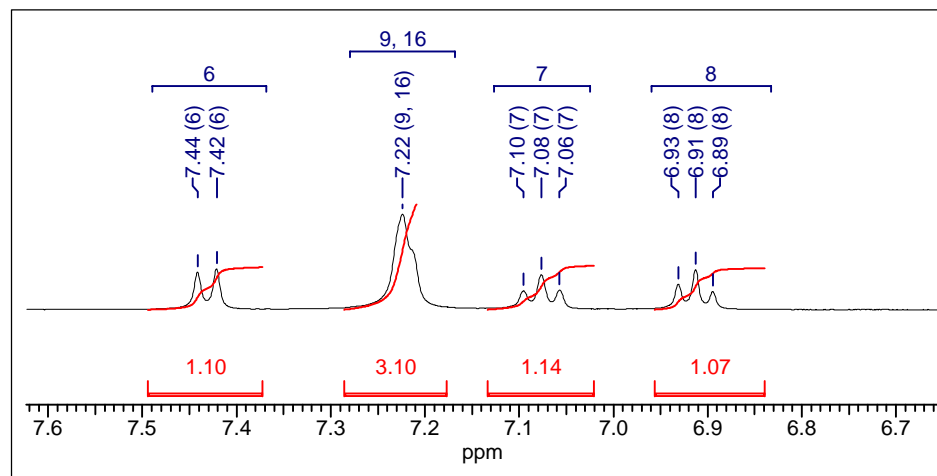
2-amino-4-(2,3-dihydro-1*H*-indol-1-yl)-6-methoxypyrimidine-5-carbaldehyde

Molecular Formula = C₁₄H₁₄N₄O₂

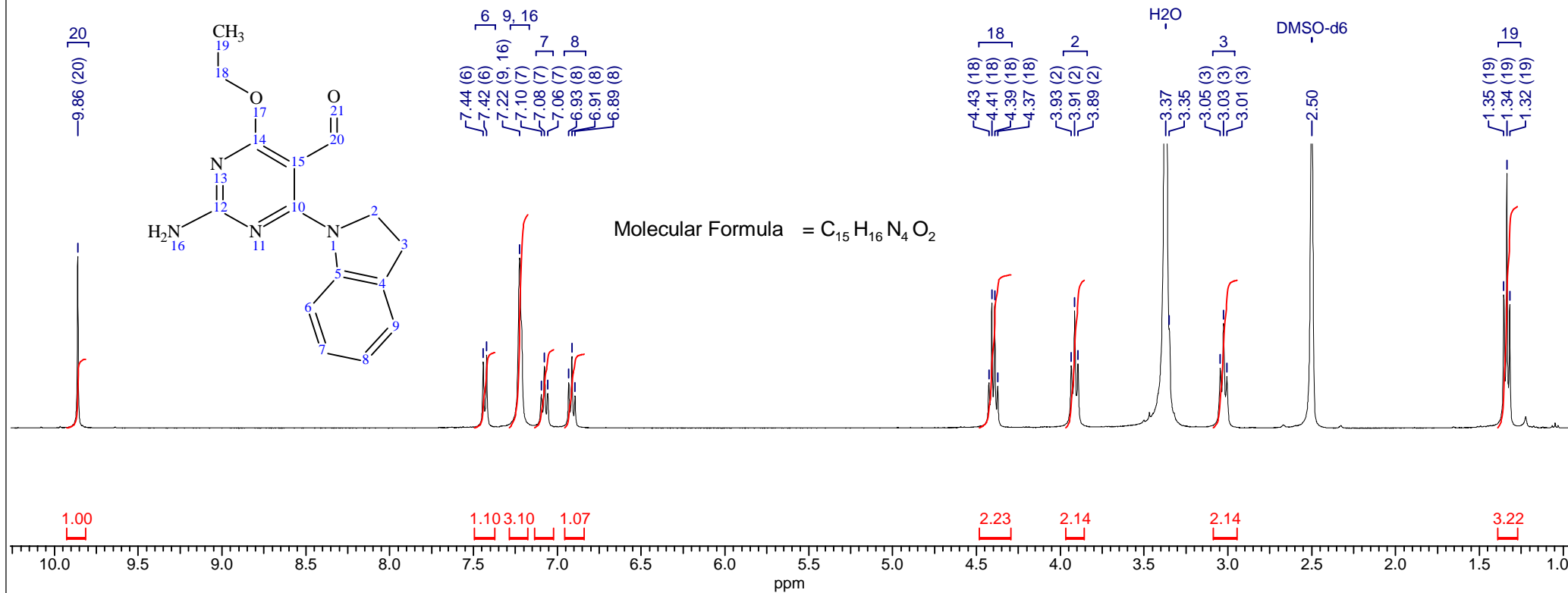
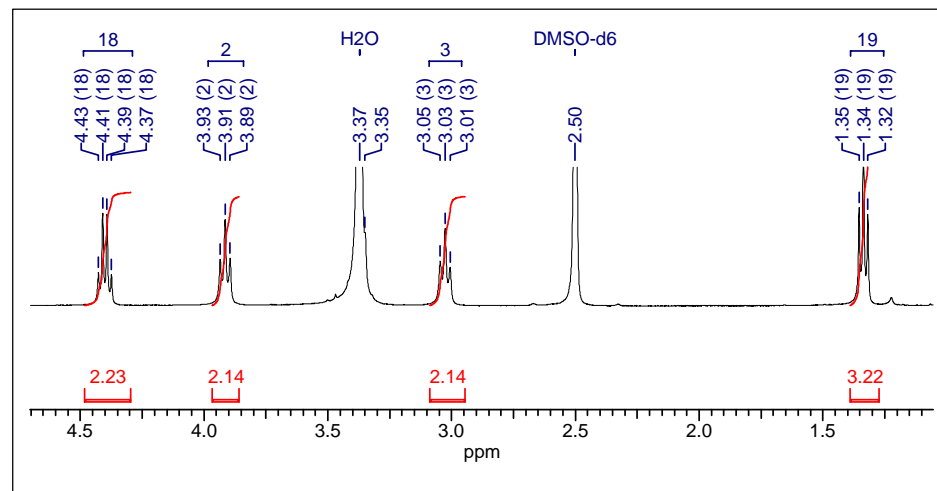




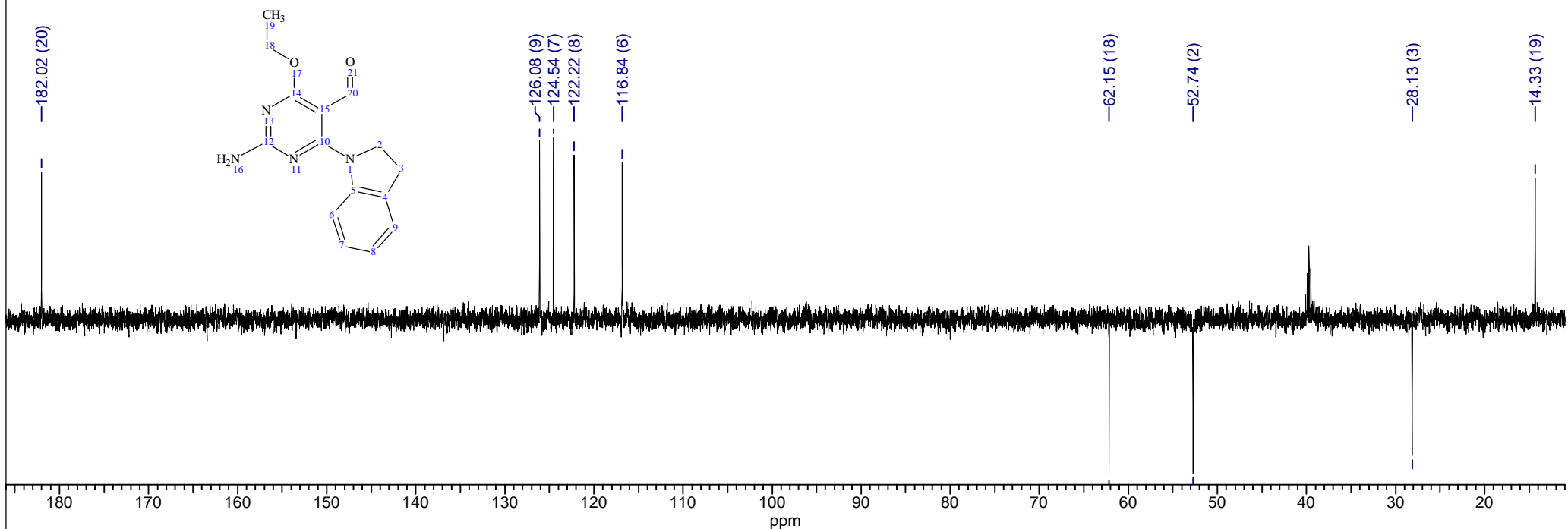
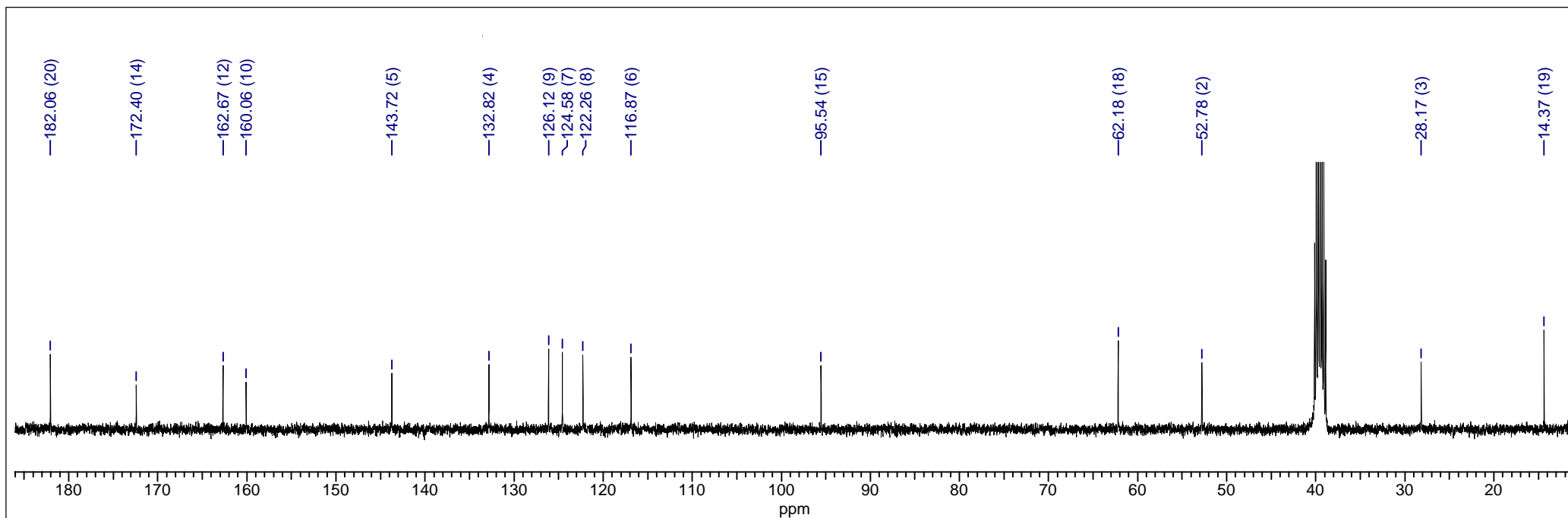
Compound II



2-amino-4-(2,3-dihydro-1H-indol-1-yl)-6-ethoxypyrimidine-5-carbaldehyde



Molecular Formula = C₁₅H₁₆N₄O₂



Single Mass Analysis (displaying only valid results)

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

513 formula(e) evaluated with 145 results within limits (up to 10 closest results for each mass)

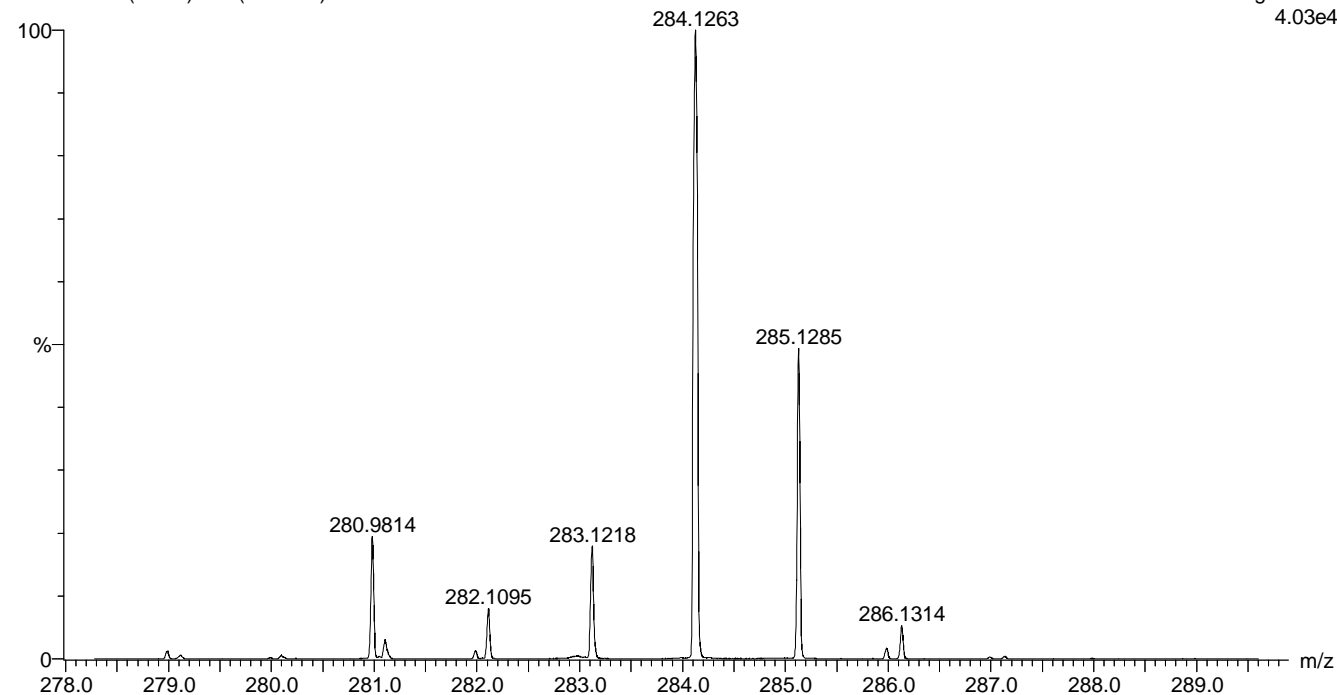
Elements Used:

C: 0-500 H: 0-1000 N: 0-20 O: 0-20

JT-E36

284

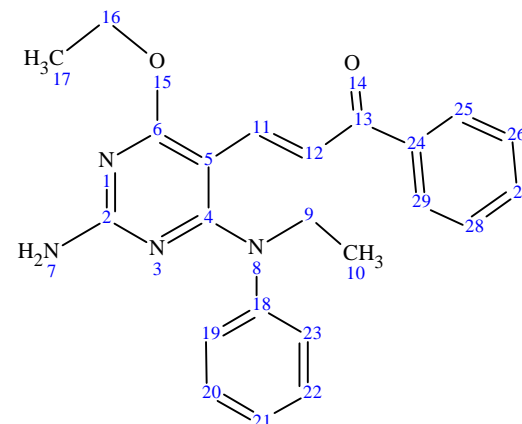
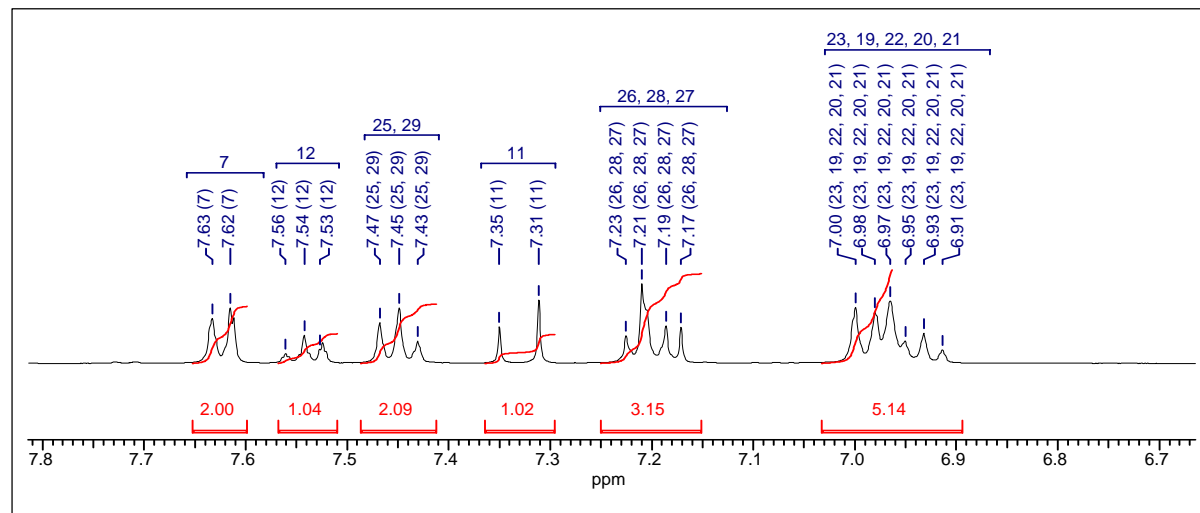
JT-E36 151 (2.613) Cm (137:164)

C₁₅H₁₆N₄O₂Magnet EI+
4.03e4

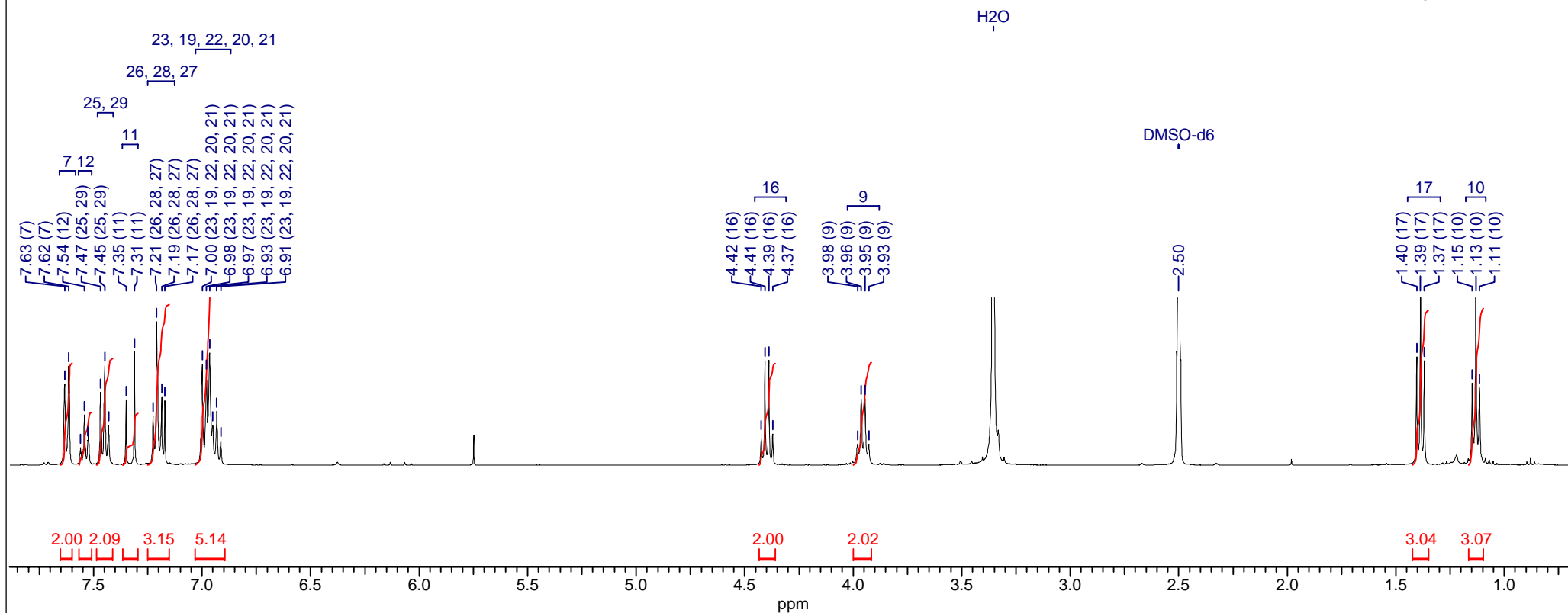
Minimum: -1.5
Maximum: 50.0 10.0 50.0

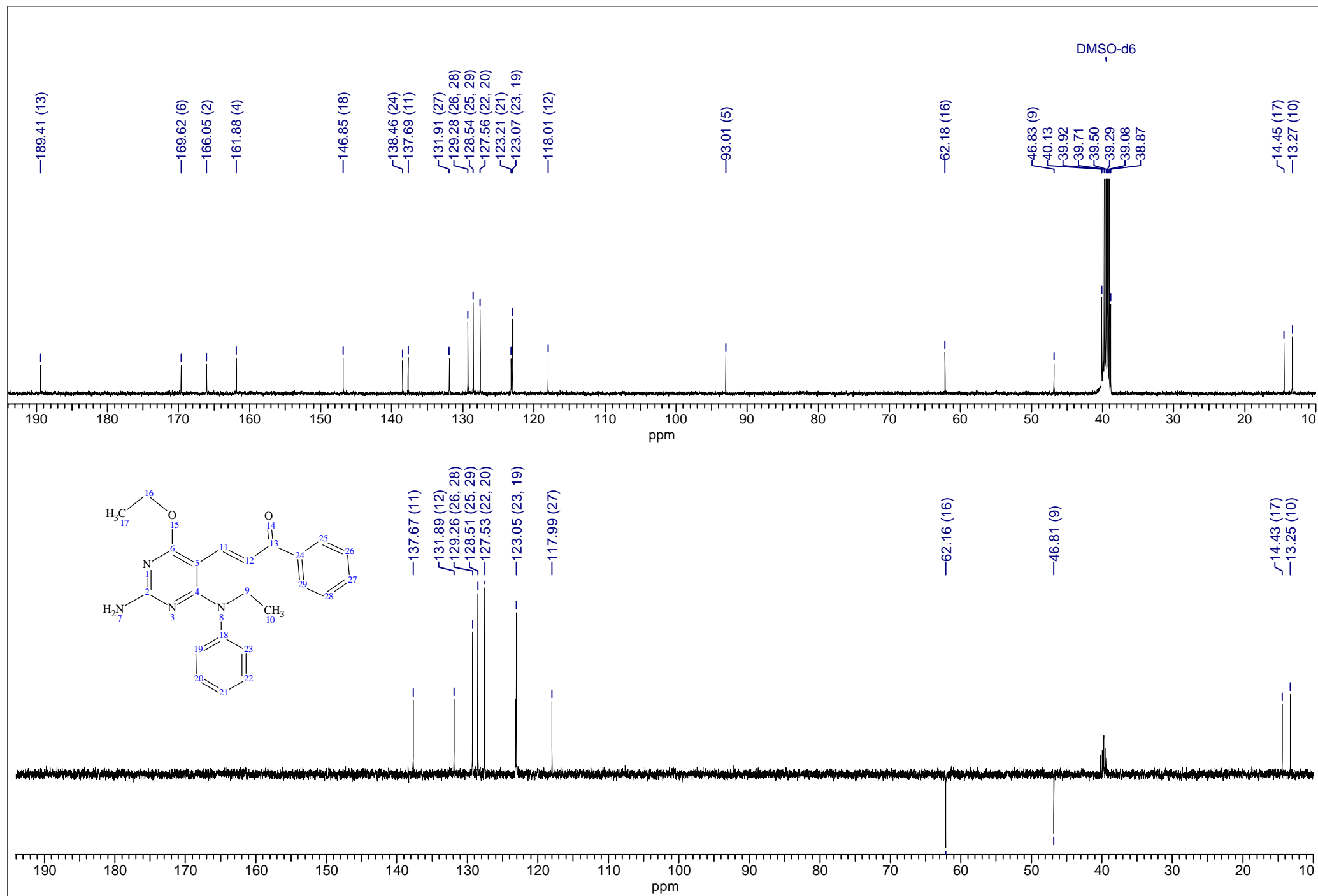
Mass	Calc. Mass	mDa	PPM	DBE	Formula			
284.1263	284.1260	0.3	1.1	10.5	C13	H14	N7	O
	284.1260	0.3	1.1	5.0	C14	H20	O6	
	284.1273	-1.0	-3.5	10.0	C15	H16	N4	O2
	284.1278	-1.5	-5.3	3.0	H12	N16	O3	
	284.1246	1.7	6.0	11.0	C11	H12	N10	
	284.1246	1.7	6.0	5.5	C12	H18	N3	O5
	284.1287	-2.4	-8.4	9.5	C17	H18	N	O3
	284.1292	-2.9	-10.2	2.5	C2	H14	N13	O4
	284.1233	3.0	10.6	6.0	C10	H16	N6	O4
	284.1305	-4.2	-14.8	2.0	C4	H16	N10	O5

Compound III

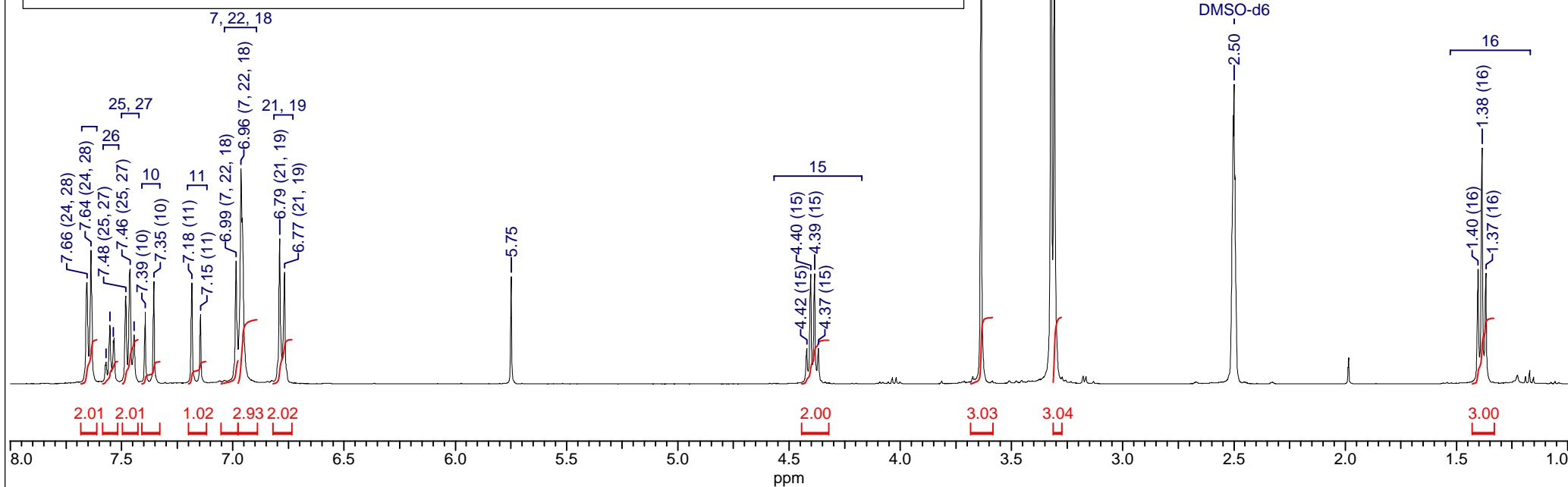
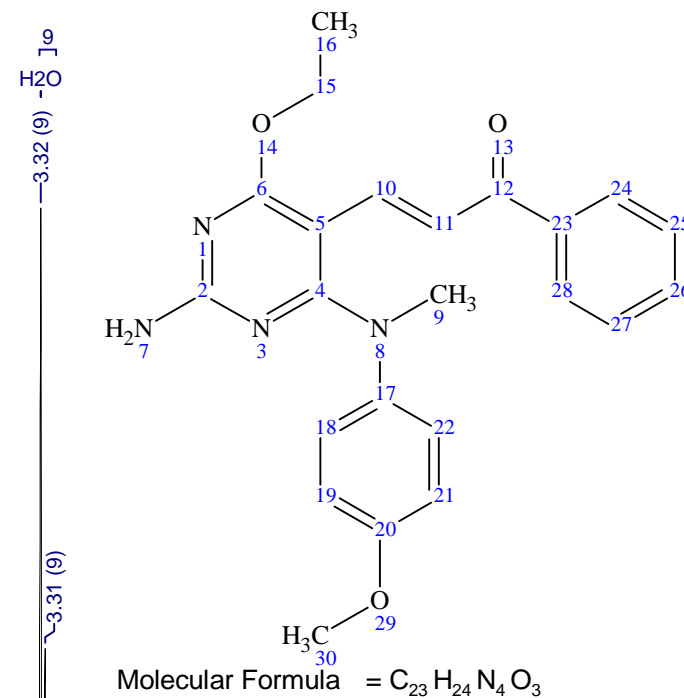
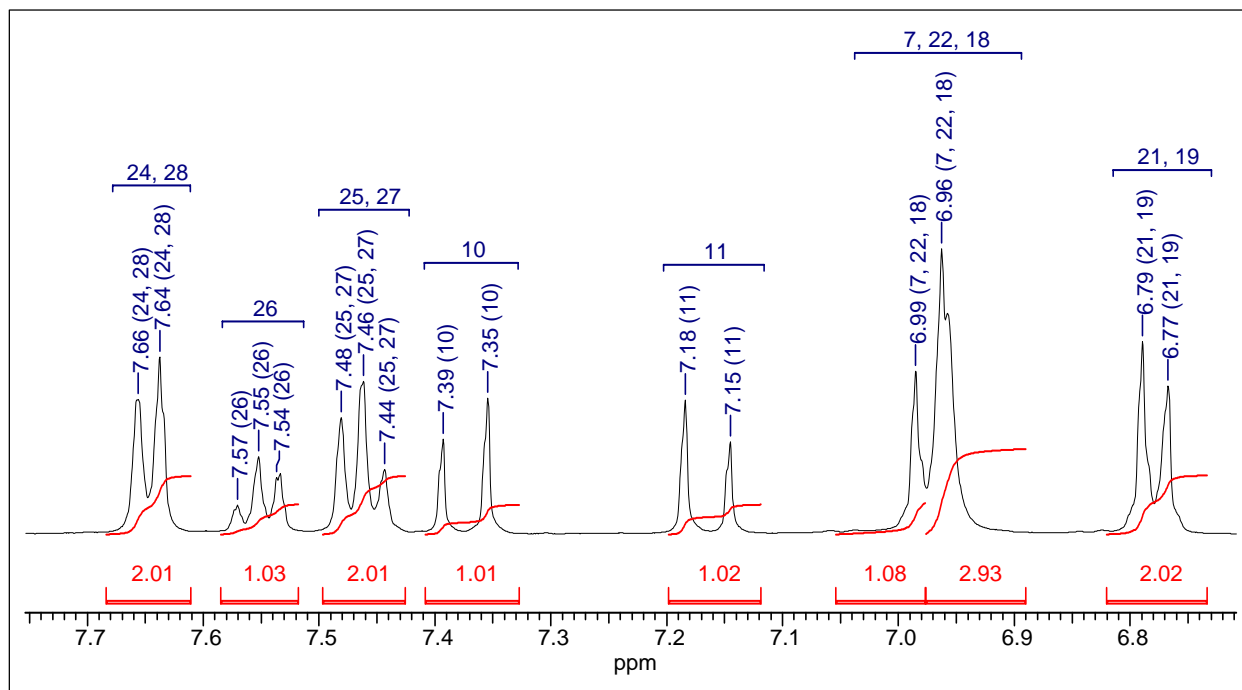


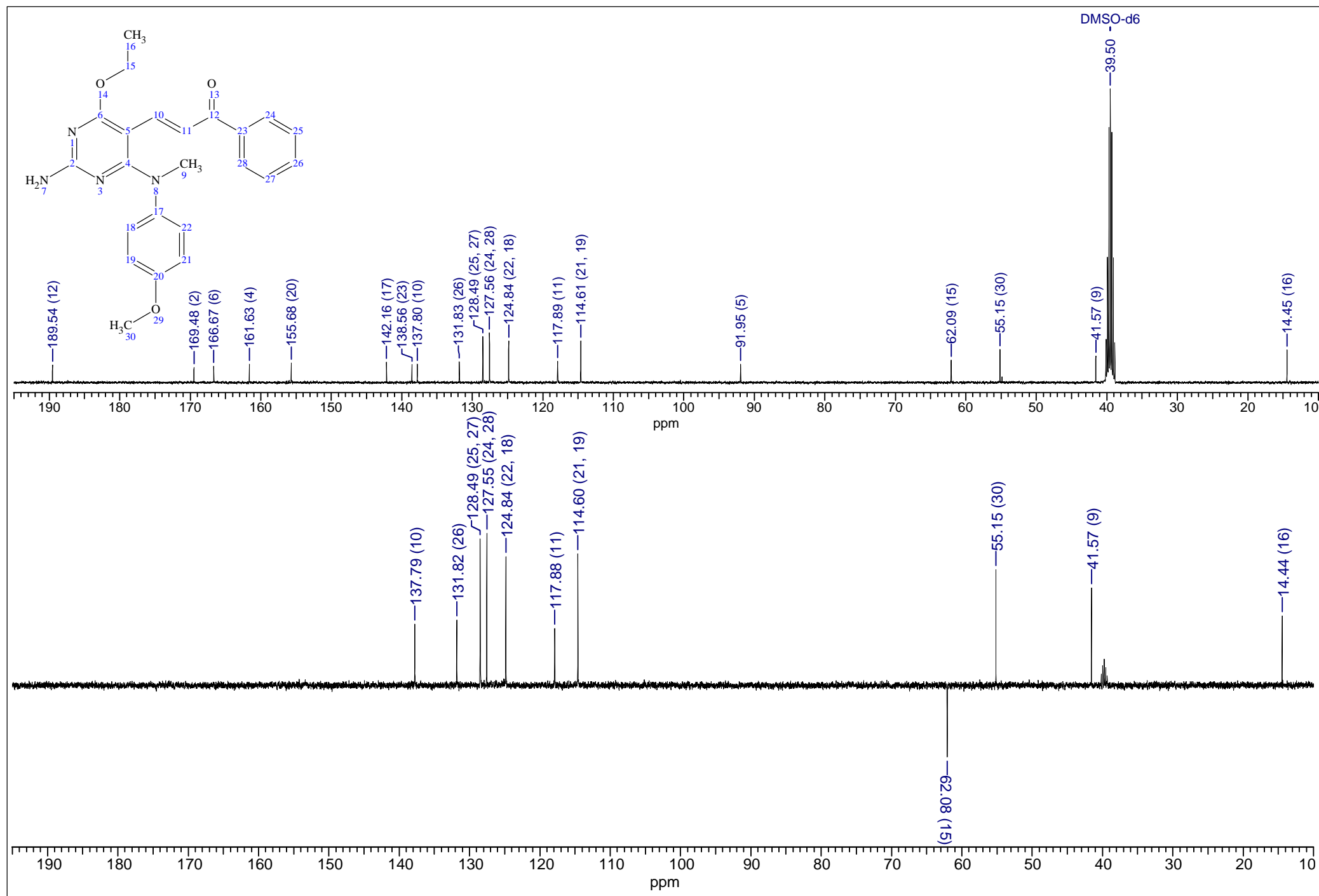
Molecular Formula = C₂₃H₂₄N₄O₂





Compound IV





Single Mass Analysis (displaying only valid results)

Tolerance = 50.0 mDa / DBE: min = -1.5, max = 50.0

Selected filters: Carbon;

Monoisotopic Mass, Odd and Even Electron Ions

1153 formula(e) evaluated with 116 results within limits (up to 10 closest results for each mass)

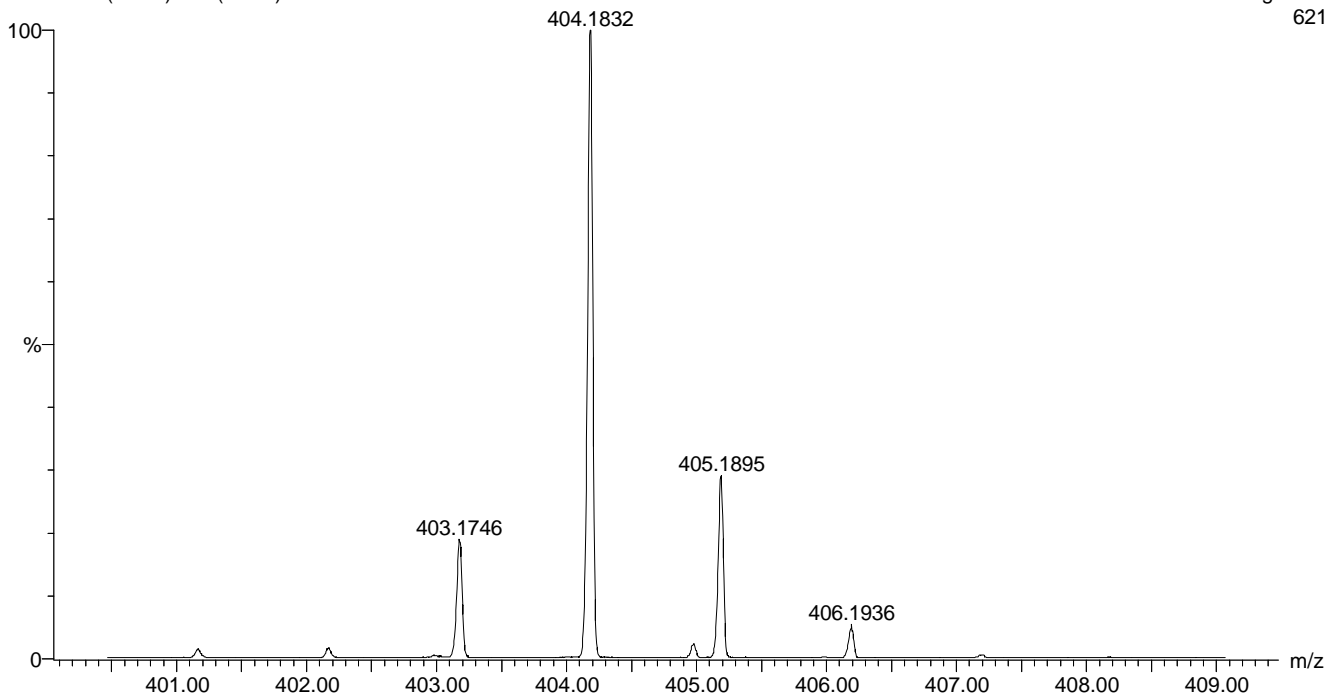
Elements Used:

C: 0-500 H: 0-1000 N: 0-20 O: 0-20

JT-E48

404

JT-E48 46 (4.067) Cm (46:52)

C₂₃H₂₄N₄O₃Voltage EI+
621

Minimum:

Maximum:

50.0

10.0

-1.5

50.0

Mass	Calc. Mass	mDa	PPM	DBE	Formula			
404.1832	404.1835	-0.3	-0.7	9.0	C22	H28	O7	
	404.1835	-0.3	-0.7	14.5	C21	H22	N7	O2
	404.1822	1.0	2.5	15.0	C19	H20	N10	O
	404.1822	1.0	2.5	9.5	C20	H26	N3	O6
	404.1848	-1.6	-4.0	14.0	C23	H24	N4	O3
	404.1808	2.4	5.9	10.0	C18	H24	N6	O5
	404.1808	2.4	5.9	15.5	C17	H18	N13	
	404.1862	-3.0	-7.4	13.5	C25	H26	N	O4
	404.1795	3.7	9.2	5.0	C17	H28	N2	O9
	404.1795	3.7	9.2	10.5	C16	H22	N9	O4