

Supplementary Materials

1-(2,5-Dimethoxy-4-nitrophenyl)piperidine

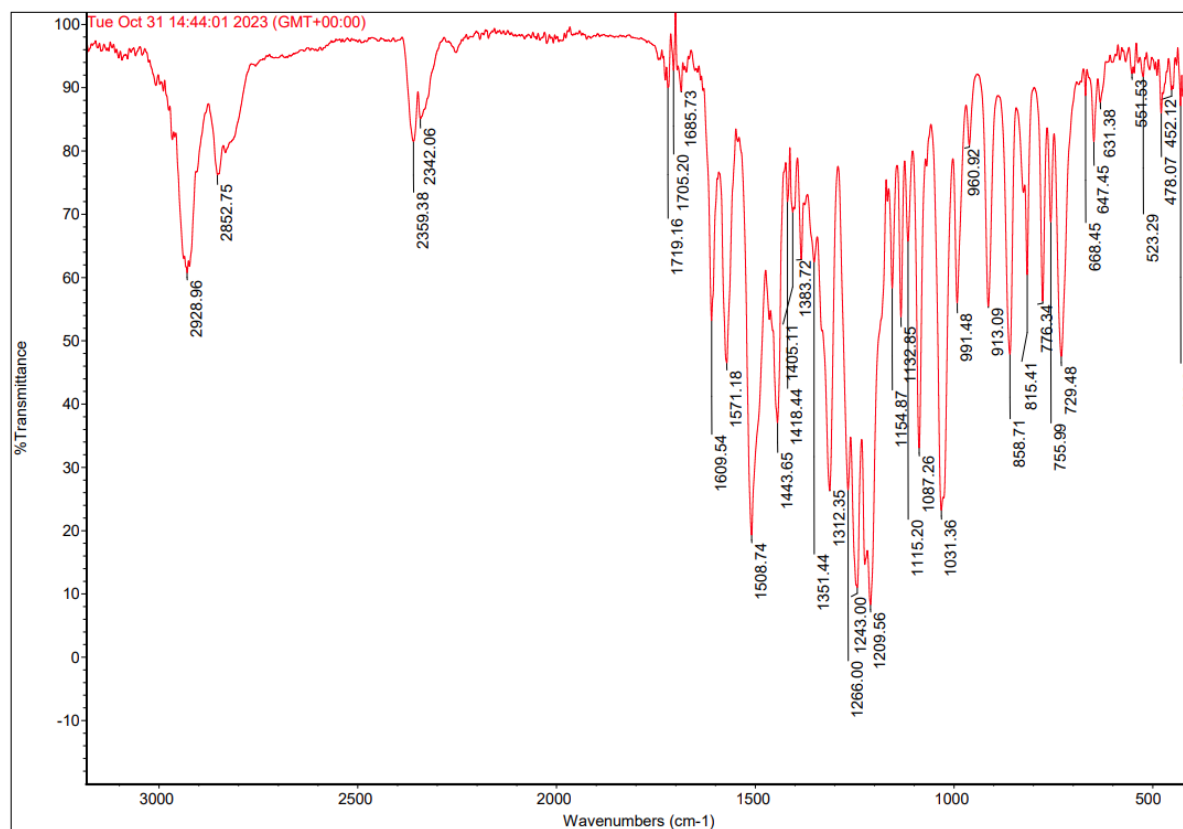
Tanjia M. Syeda, Muadh R. Al-Shaidi, Ibtihal Basri, Mahboub Merzouk and
Fawaz Aldabbagh*

Department of Pharmacy, School of Life Sciences, Pharmacy and Chemistry,
Kingston University, Penrhyn Road, Kingston upon Thames KT1 2EE, UK

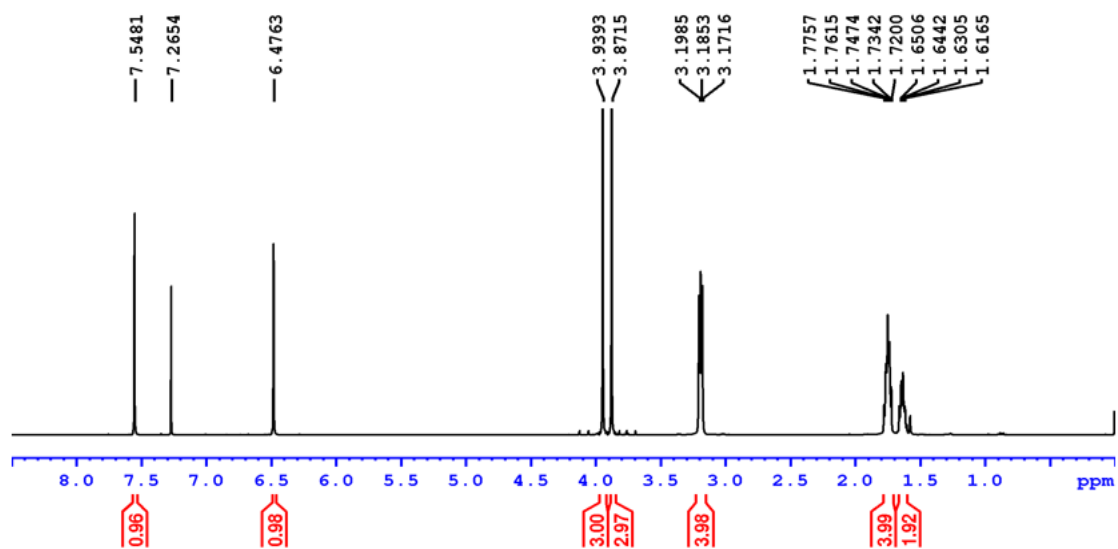
*Correspondence: f.aldeabbagh@kingston.ac.uk

Spectroscopic Data for compounds (**2b**) and (**3b**)

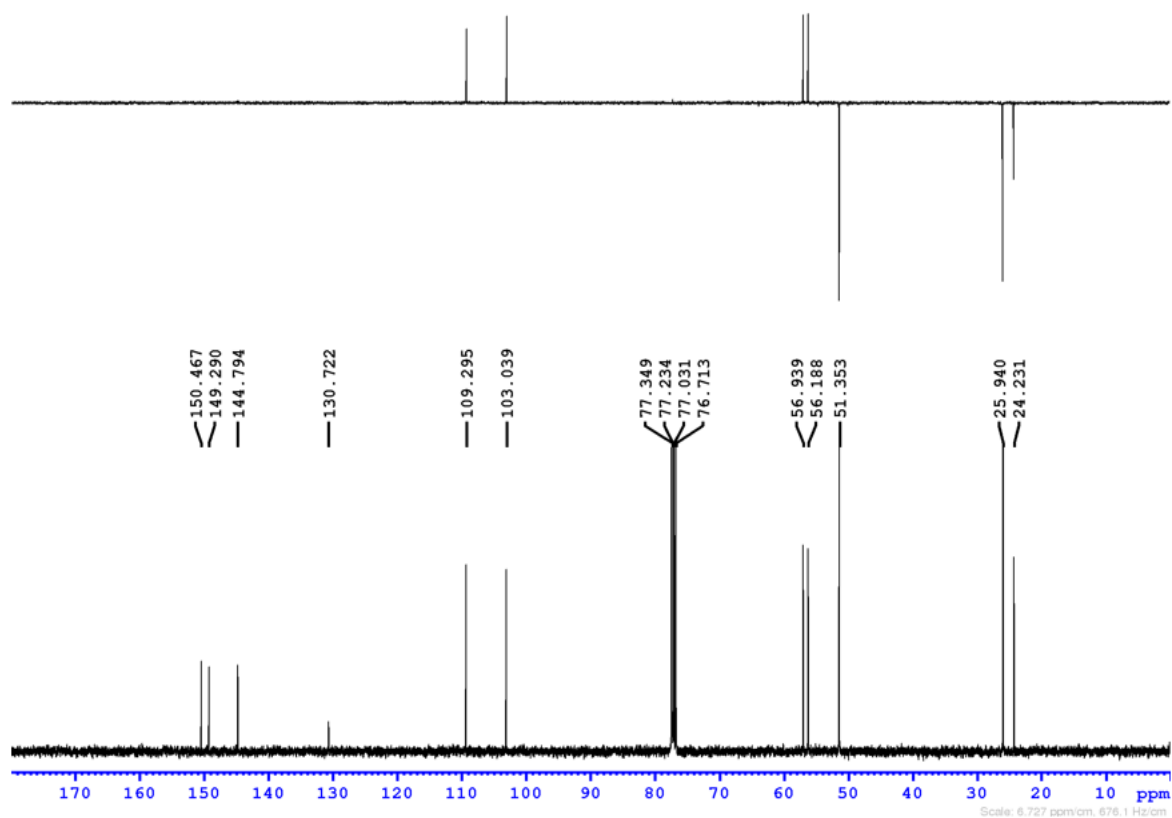
IR of 1-(2,5-dimethoxy-4-nitrophenyl)piperidine (2b)



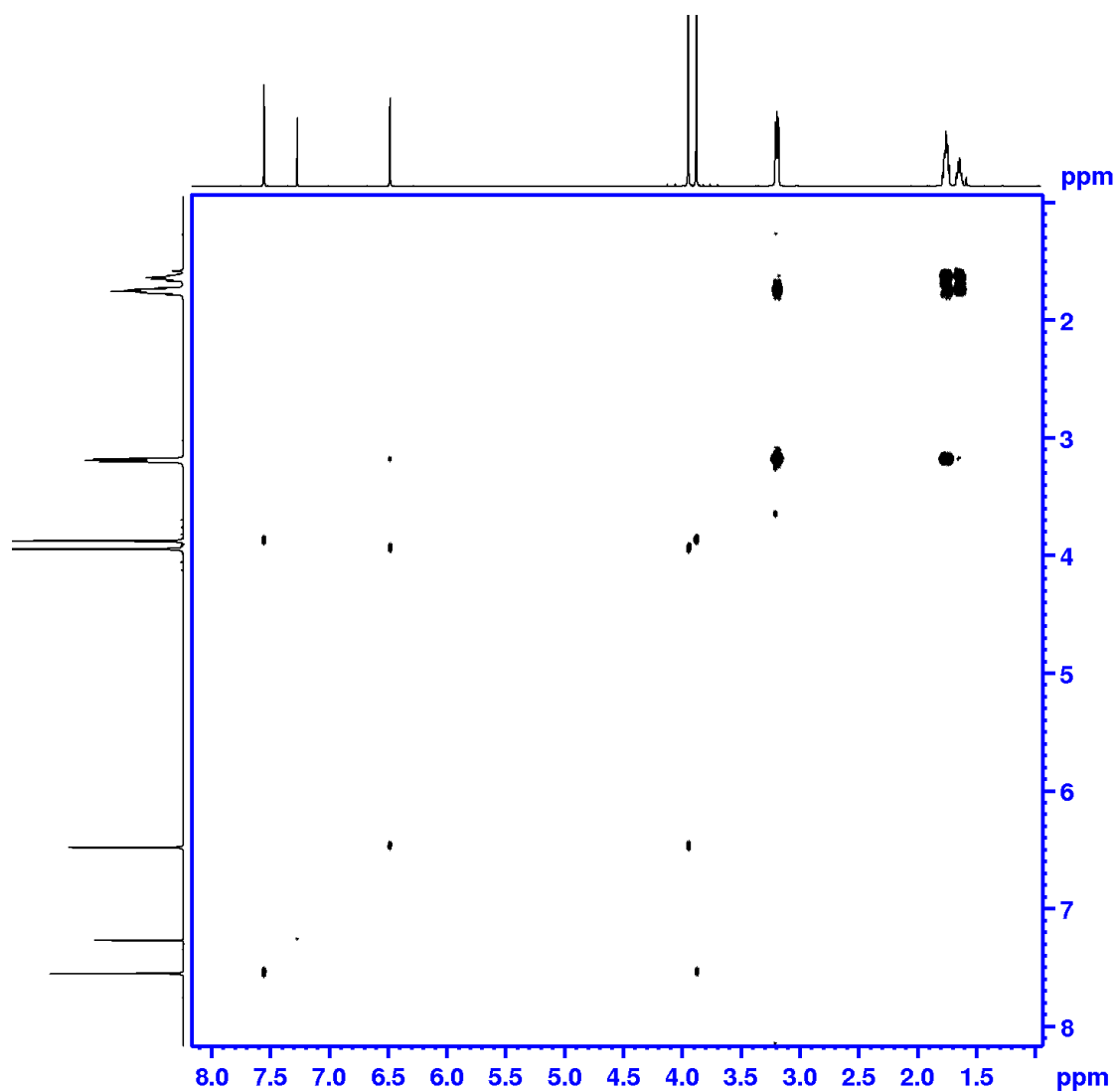
^1H NMR (400 MHz) of 1-(2,5-dimethoxy-4-nitrophenyl)piperidine (2b) in CDCl_3



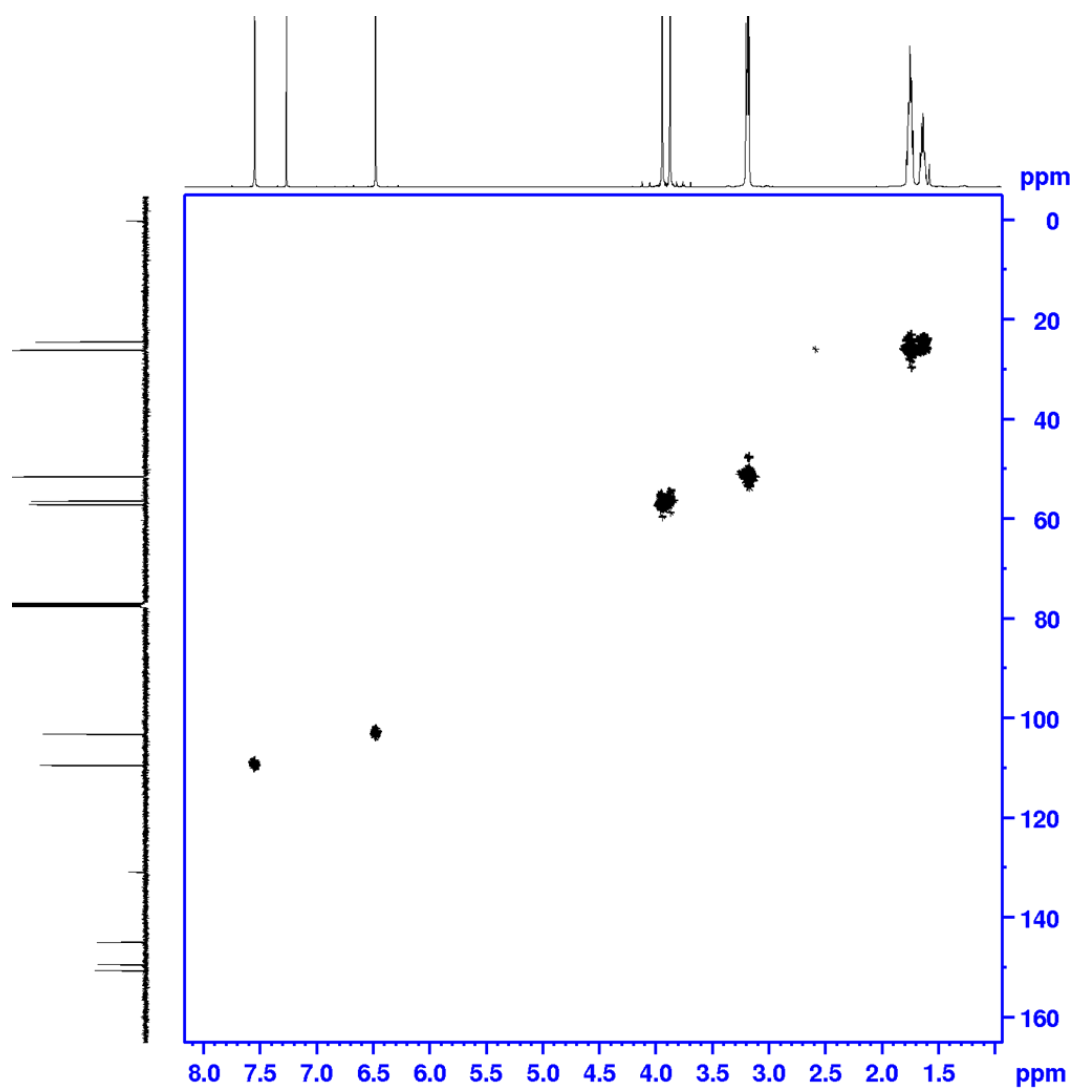
^{13}C NMR (100 MHz) and DEPT of 1-(2,5-dimethoxy-4-nitrophenyl)piperidine (2b) in CDCl_3



COSY of 1-(2,5-dimethoxy-4-nitrophenyl)piperidine (2b) in CDCl₃



HSQC of 1-(2,5-dimethoxy-4-nitrophenyl)piperidine (2b) in CDCl₃



HRMS of 1-(2,5-dimethoxy-4-nitrophenyl)piperidine (2b)

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

517 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-10 O: 0-14

TS26 MW=266? C13H18N2O4

National Mass Spectrometry Facility, Swansea

Fawaz Al-Dabbagh

ASAP (SOLID)

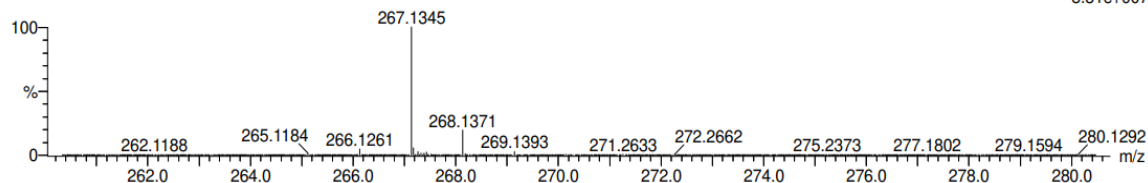
Xevo G2-S

12-Oct-2023

KINALD_NDD2D_WA_A 47 (0.454) AM (Cen,1, 80.00, Ar,10000.0,0.00,0.00); Cm (38:55)

1: TOF MS ASAP+

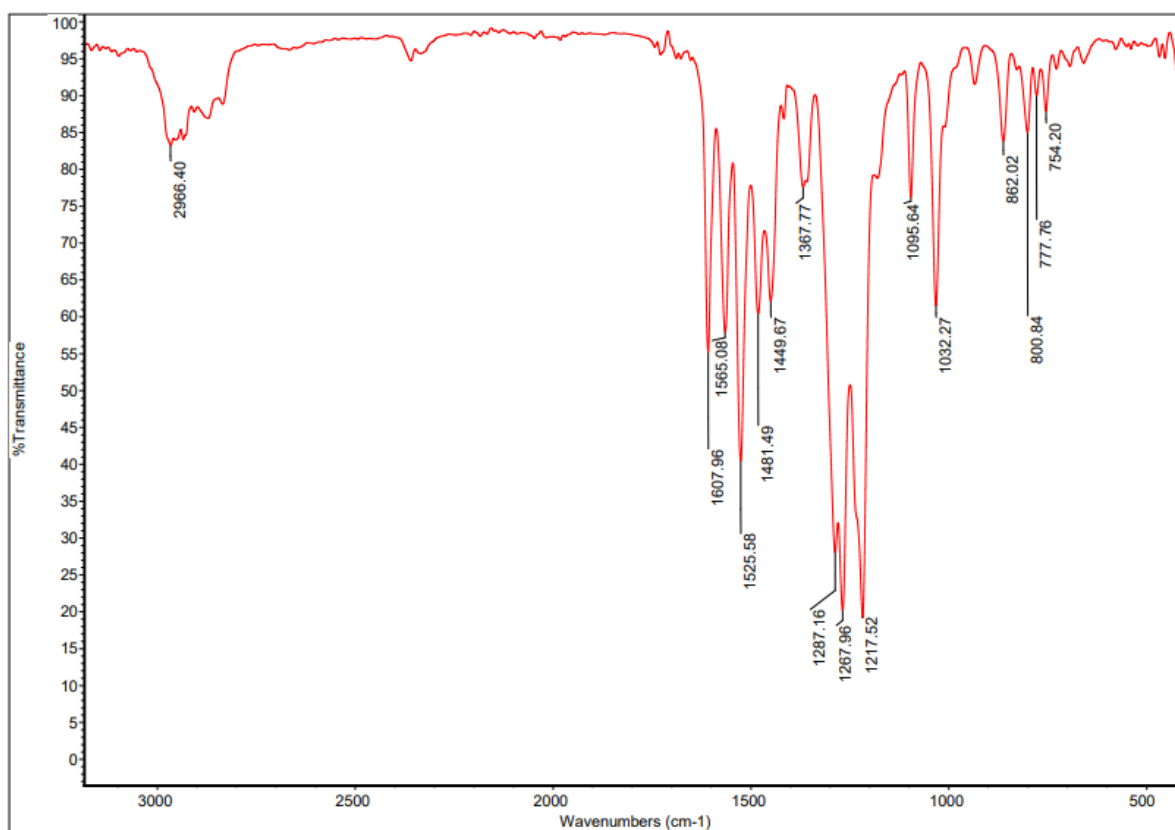
3.31e+007



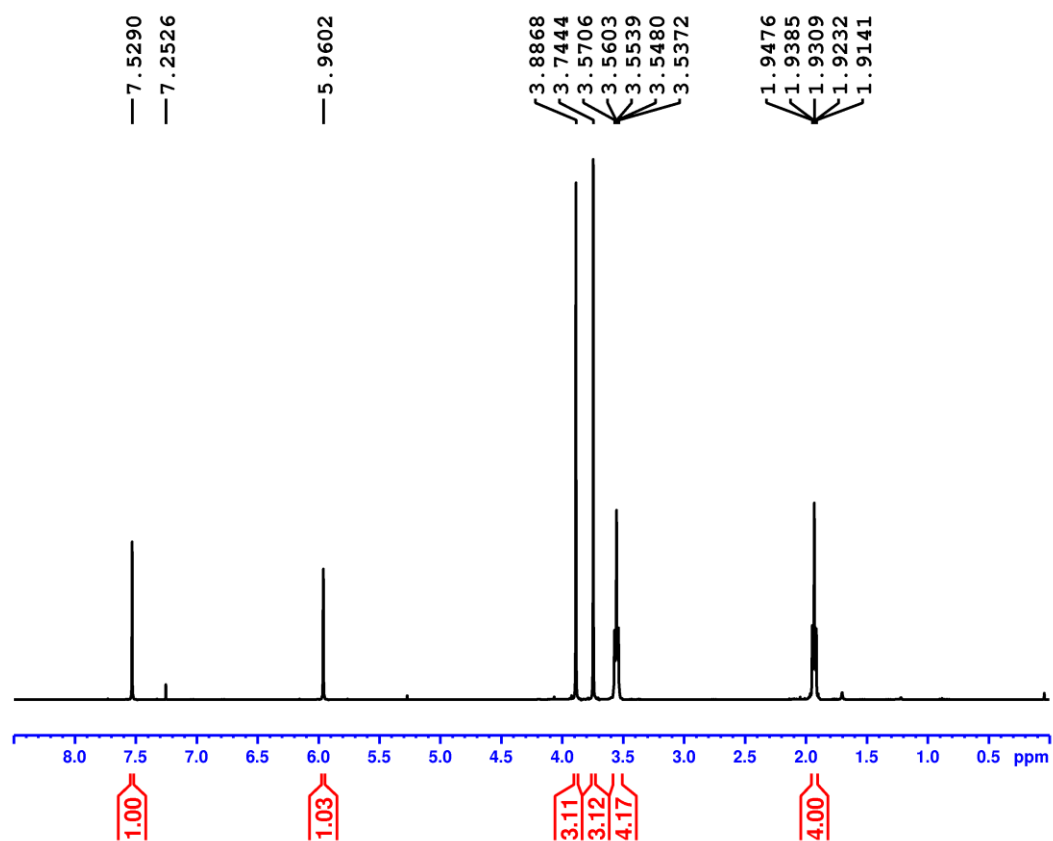
Minimum: -10.0
Maximum: 5.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
267.1345	267.1345	0.0	0.0	5.5	2271.7	1.439	23.72	C13 H19 N2 O4
	267.1358	-1.3	-4.9	10.5	2271.0	0.728	48.28	C14 H15 N6
	267.1331	1.4	5.2	6.0	2272.5	2.235	10.70	C11 H17 N5 O3
	267.1363	-1.8	-6.7	-7.5	2281.4	11.109	0.00	C H23 N4 O11
	267.1372	-2.7	-10.1	10.0	2272.0	1.755	17.30	C16 H17 N3 O

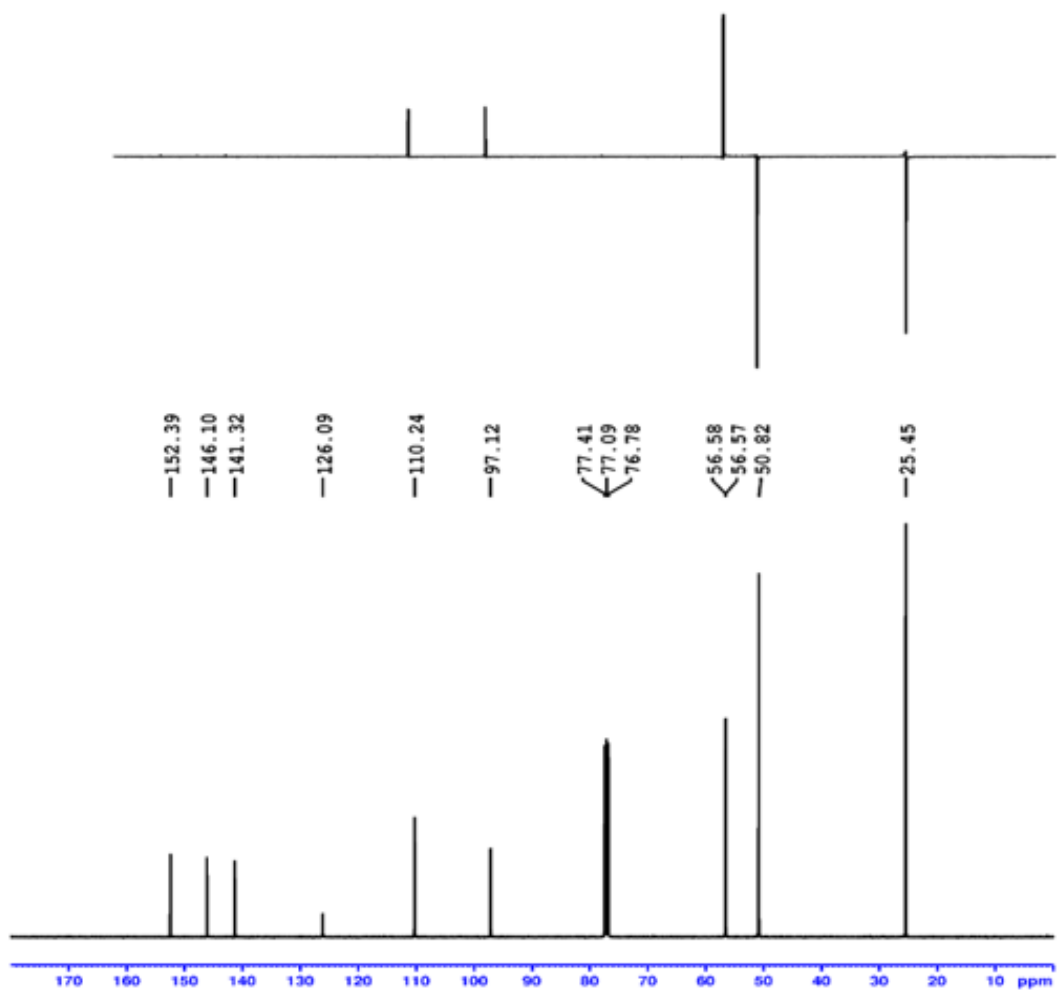
IR of 1-(2,5-dimethoxy-4-nitrophenyl)pyrrolidine (3b)



^1H NMR (400 MHz) of 1-(2,5-dimethoxy-4-nitrophenyl)pyrrolidine (3b) in CDCl_3



^{13}C NMR (100 MHz) and DEPT of 1-(2,5-dimethoxy-4-nitrophenyl)pyrrolidine (3b) in CDCl_3



HRMS of 1-(2,5-dimethoxy-4-nitrophenyl)pyrrolidine (3b)

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -10.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Odd and Even Electron Ions

473 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-60 H: 0-80 N: 0-10 O: 0-14

IB32 MW=252? C₁₂H₁₆N₂O₄

National Mass Spectrometry Facility, Swansea

Fawaz Al-Dabbagh

ASAP (SOLID)

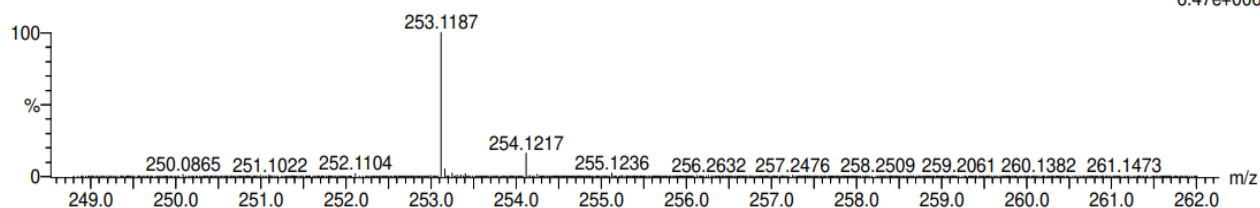
Xevo G2-S

12-Oct-2023

KINALD_NDER2_WA_A 218 (2.035) AM (Cen,1, 80.00, Ar,10000.0,0.00,0.00); Cm (216:222)

1: TOF MS ASAP+

6.47e+006



Minimum: -10.0
Maximum: 5.0 10.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
253.1187	253.1188	-0.1	-0.4	5.5	2405.9	0.138	87.08	C12 H17 N2 O4
	253.1175	1.2	4.7	6.0	2409.7	3.973	1.88	C10 H15 N5 O3
	253.1202	-1.5	-5.9	10.5	2408.0	2.204	11.04	C13 H13 N6
	253.1207	-2.0	-7.9	-7.5	2421.9	16.139	0.00	H21 N4 O11