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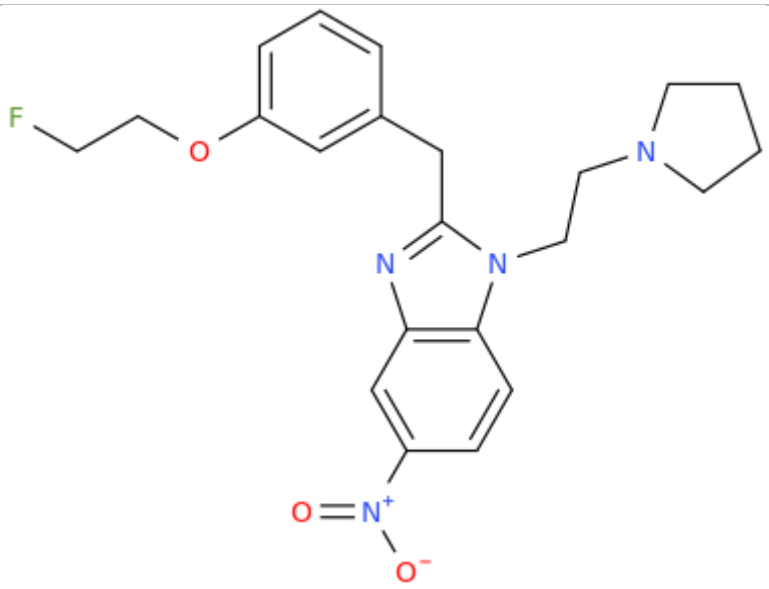
ANALYTICAL REPORT

Fluetonitazepyne (C22H25FN4O3)

2-{[3-(2-fluoroethoxy)phenyl]methyl}-5-nitro-1-[2-(pyrrolidin-1-yl)ethyl]-1H-1,3-benzodiazole

Remark – other NPS detected: none

Sample ID:	3325-25
Sample description:	powder
Sample type:	test purchase /NFL- purchasing
Date of entry (DD/MM/YYYY) into NFL database:	07/08/2025
Report updates (if any) will be published here:	http://www.policija.si/apps/nfl_response_web/seznam.php

Substance identified - structure[1] (base form)	
Systematic name	2-{[3-(2-fluoroethoxy)phenyl]methyl}-5-nitro-1-[2-(pyrrolidin-1-yl)ethyl]-1H-1,3-benzodiazole
Other names	2-[[4-(2-fluoroethoxy)phenyl]methyl]-5-nitro-1-(2-pyrrolidin-1-ylethyl)benzimidazole; 2-(4-(2-fluoroethoxy)benzyl)-5-nitro-1-(2-(pyrrolidin-1-yl)ethyl)-1H-benzo[d]imidazole; 2-{[4-(2-32.fluoroethoxy)phenyl]methyl}-5-nitro-1-[2-(pyrrolidin-1-yl)ethyl]-1H-
Formula (per base form)	C22H25FN4O3
M_w (g/mol)	412,47
Salt form/anions detected	base
StdInChIKey (per base form)	JRVLNWBHMCWJBL-UHFFFAOYSA-N
Other NPS detected	none
Additional info (purity..)	94% purity of a sample based on 1H NMR spectrum

[1] Created by OPSIN free tool: http://opsin.ch.cam.ac.uk/ **DOI:** 10.1021/ci100384d

Report updates

date	comments (explanation)

Instrumental methods (if applied) in NFL

1. GC-MS (Agilent): GC-method is RT locked to tetracosane (9.258 min). Injection volume 1 µl and split mode (1:50). Injector temperature: 280 0C. Chromatographic separation: on column HP1-MS (100% dimethylpolysiloxane), length 30 m, internal diameter 0.25 mm, film thickens 0.25 µm. Carrier gas He: flow-rate 1.2 ml/min. GC oven program: 170 ^{0}C for 1 min, followed by heating up to 190 ^{0}C at rate 8 ^{0}C/min, then heating up to 293 0C at a rate of 18 ^{0}C/min, hold for 6.1 min, then heating at 50 ^{0}C/min up to 325 ^{0}C and finally 9.1 min isothermal. MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300 until 6 min) amu.

2. HPLC-TOF (Agilent): 6230B TOF with Agilent 1260 Infinity HPLC with binary pump, column: Zorbax Eclipse XDB-C18, 50 x 4.6 mm, 1.8 micron. Mobile phases (A) 0.1% formic acid and 1mM ammonium formate in water; (B) 0.1% formic acid in methanol (B). Gradient: starting at 5% B, changing to 40% B over 4 min, then to 70% over 2 min and in 5 min to 100%, hold 1 min and back to 5%, equilibration for 1.7 min. The flow rate: 1.0 ml/min; Injection volume 1 µl. MS parameters: 2GHz, Extended Dynamic range mode to a maximum of 1700 amu, acquisition rate 1.30 spectra/sec. Sample ionisation: by Agilent Jet Stream technology (Dual AJS ESI). Ion source: positive ion scan mode with mass scanning from 82 to 1000 amu. Other TOF parameters: drying gas (N2) and sheath temperature 325 °C; drying gas flow rate 6 l/min; sheath gas flow rate 8 l/min; nebulizer 25 psig; Vcap. 4000 V; nozzle 2000 V; skimmer 65 V; fragmentor 175 V and Octopole RF 750 V.

3.FTIR-ATR (Perkin Elmer): scan range 4000-400 cm-1; resolution 4cm-1

4. GC- (MS)-IR solid phase (GC-MS (Agilent) & IR (Spectra analyses-Danny)
GC-method: Injection volume 1 µl and split mode (1:5). Injector temperature 280 ^{0}C. Chromatographic separation as above **(1).** Split MS : IR = 1: 9.
MSD source EI = 70 eV. GC-MS transfer line T= 235^{0}C, source and quadropole temperatures 280^{0}C and 180^{0}C, respectively. Scan range m/z scan range: from 50 (30 until 6 min.) to 550 (300) amu.
IR (condesed (solid) phase): IR scan range 4000 to 650, resolution 4 cm^{-1}.

5. **IC** (anions) (Thermo Scientific, Dionex ICS 2100), Column: IonPac AS19, 2 x 250mm; Eluent: 10mM KOH from 0 to 10 min, 10-58 mM from 10 to 40min; Flow rate: 0.25 ml/min; Temperature: 30˚C; Suppressor: AERS 500 2mm, suppressor current 13mA; Inj. Volume: 25 µl

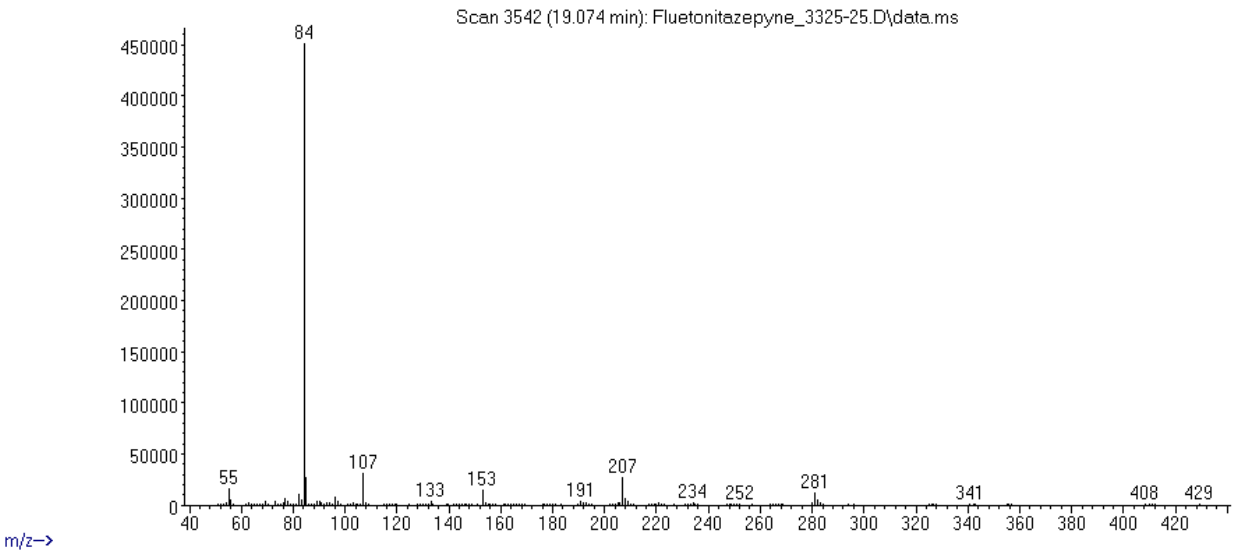
Supporting information

Solubility in	result/remark
CH_2Cl_2	/
MeOH	soluble
H_2O	/

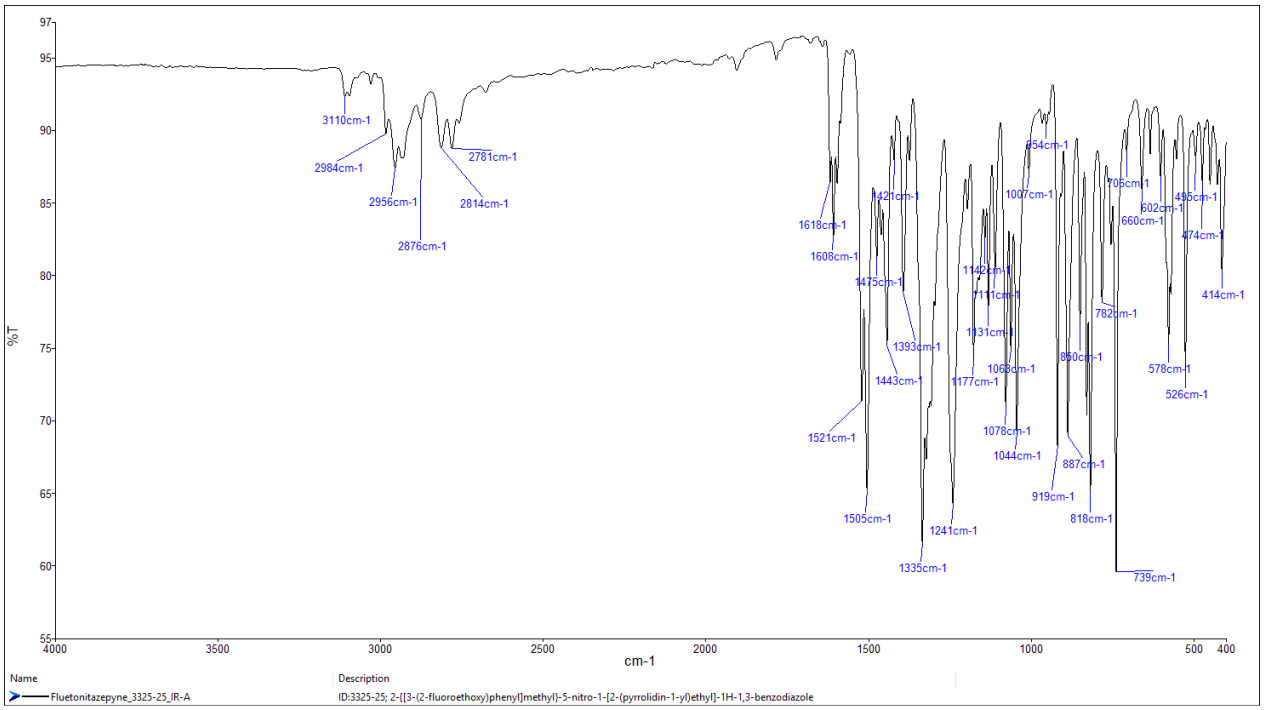
Analytical technique:	applied	remarks
GC-MS (EI ionization)	+	NFL GC-RT (min): 19,07 BP(1): 84; BP(2): 107,BP(3) :85,
HPLC-TOF	+	Exact mass (theoretical): 412,1911; measured value Δppm:-0,69; formula:C22H25FN4O3
FTIR-ATR	+	direct measurement (sample as received)
FTIR (solid phase) always as base form	+	
IC (anions)	/	
NMR (in FKKT)	+	
validation		
other		

ANALYTICAL RESULTS

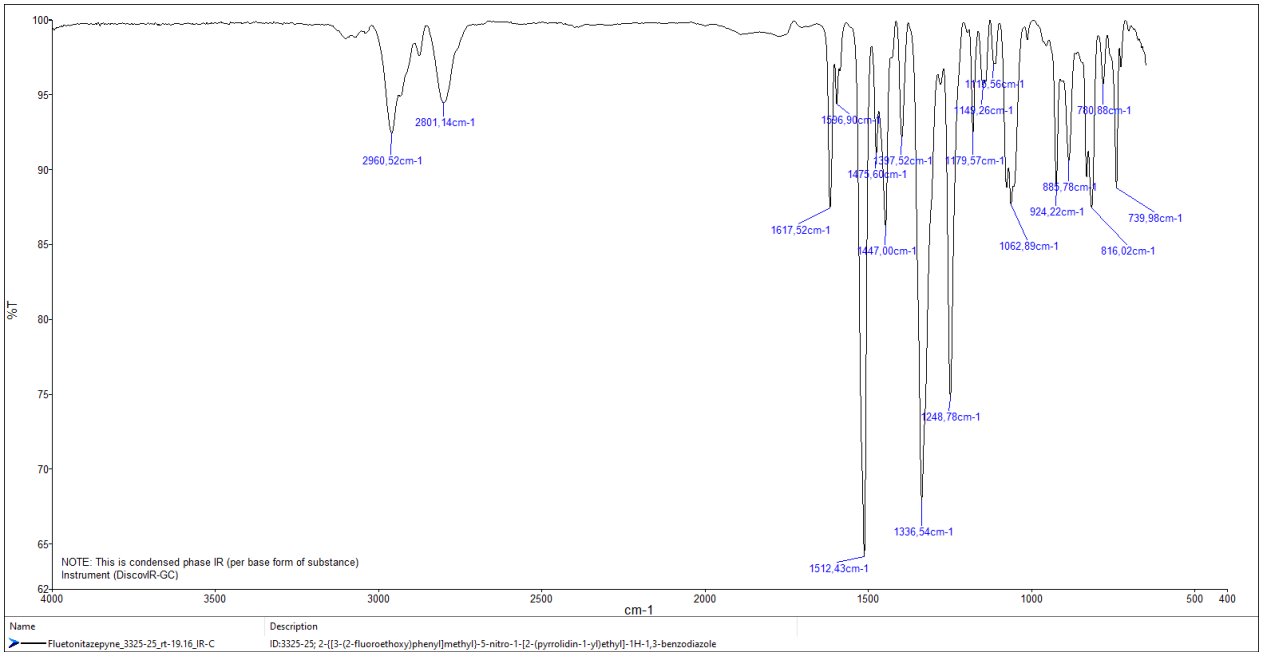
MS (EI)



FTIR-ATR - direct measurement (sample as received)



IR (solid phase – after chromatographic separation)



TOF REPORT

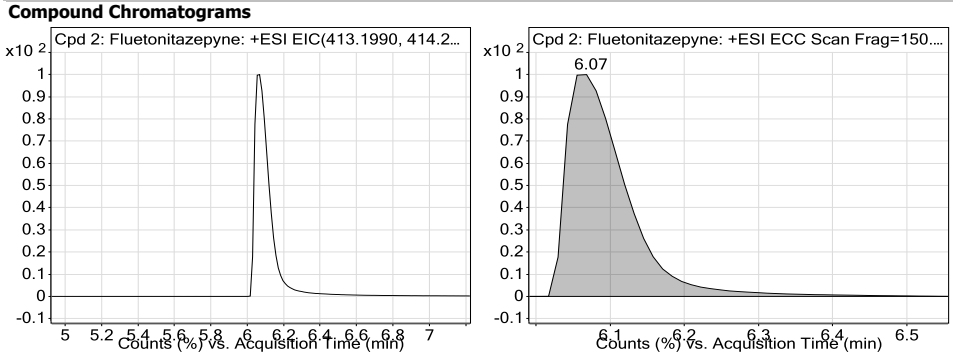
Data File	Fluetonitazepyne_3325-25.d	**Sample Name**	NLZOH_ST-466
Sample Type	Sample	**Position**	P1-A7
Instrument Name	6230B TOF LC-MS	**User Name**	TG
Acq Method	general-01_08_2024-XDB-C18-ESI+.m	**Acquired Time**	8/8/2024 11:41:38 AM
IRM Calibration Status	Success	**DA Method**	0-NPS in sorodne snovi.m
Comment	extract in MeOH		

Compound Table

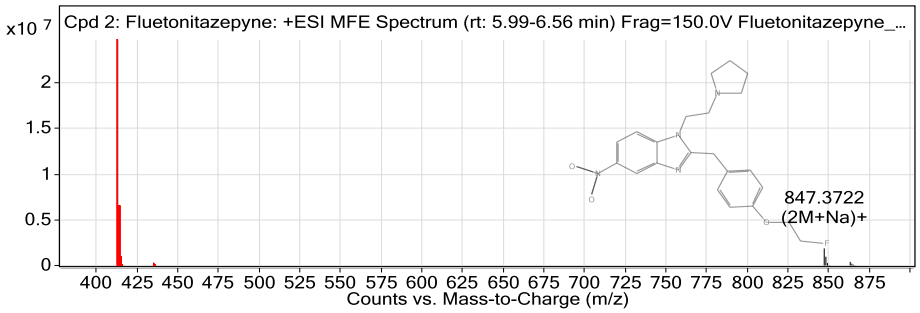
Label	Compound Name	MFG Formula	Obs. RT	Obs. Mass
Cpd 2: Fluetonitazepyne	Fluetonitazepyne	C22 H25 F N4 O3	6.07	412.1914

Name	*Obs. m/z*	Obs. RT	Obs. Mass	DB RT	DB Formula	DB Mass	DB Mass Error (ppm)
Fluetonitazepyne	413.1986	6.07	412.1914	6.07	C22 H25 F N4 O3	412.1911	-0.69

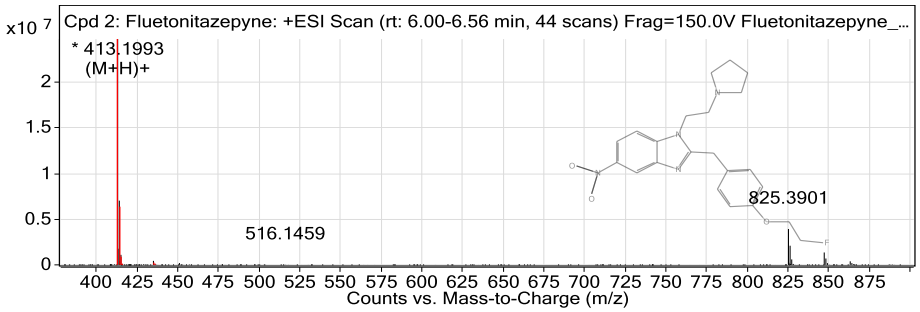
Compound Chromatograms



MFE MS Zoomed Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Obs. m/z	Charge	Abund	Formula	Ion/Isotope
413.1986	1	24744188	C22 H25 F N4 O3	(M+H)+
414.2018	1	6630847.46	C22 H25 F N4 O3	(M+H)+
415.2046	1	923283.67	C22 H25 F N4 O3	(M+H)+
416.207	1	84999.72	C22 H25 F N4 O3	(M+H)+
435.1805	1	312463.44	C22 H25 F N4 O3	(M+Na)+
847.3722	1	1869745.25		(2M+Na)+
848.3759	1	959673.85		(2M+Na)+
849.3779	1	256389.16		(2M+Na)+
863.346	1	397502.31		(2M+K)+
864.3488	1	196137.68		(2M+K)+

--- End Of Report ---

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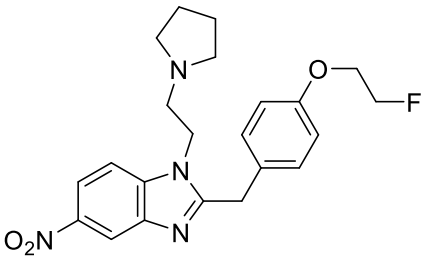
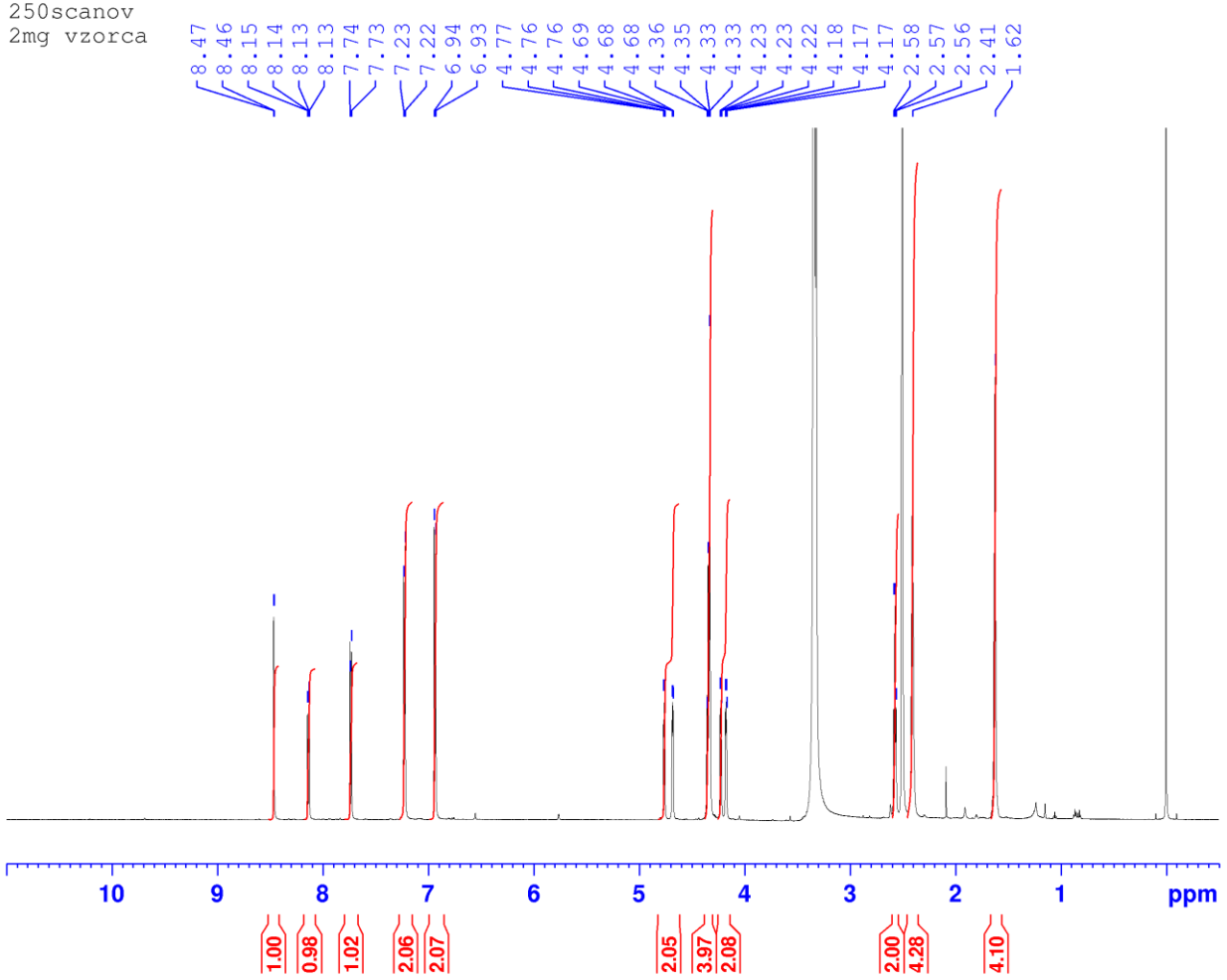
University
of Ljubljana

Faculty *of Chemistry*
and Chemical Technology

R E P O R T

Contract No.	C1714-21-460153 (Republic of Slovenia, Ministry of the Interior, POLICE)
Sample ID:	**3325-25**
Received date:	April 15, 2025
Our notebook code:	ST466
NMR sample preparation:	2 mg dissolved in 0.6 mL DMSO-d_6
NMR experiments:	^{1}H, ^{13}C, ^{19}F, ^{1}H–^{1}H *gs*-COSY, ^{1}H–^{1}H *gs*-NOESY, ^{1}H–^{19}F *gs*-HOESY, ^{1}H–^{13}C *gs*-HSQC, ^{1}H–^{13}C *gs*-HMBC, ^{13}C DEPT-45, ^{13}C DEPT-90, ^{13}C DEPT-135
Proposed structure with formula, exact mass, molecular weight:	 Chemical Formula: $C_{22}H_{25}FN_4O_3$ Exact Mass: 412,1911 Molecular Weight: 412,4654
Chemical name:	2-(4-(2-fluoroethoxy)benzyl)-5-nitro-1-((2-pyrrolidin-1-yl)ethyl)-1*H*-benzo[*d*]imidazole
Comments:	- Structure elucidation based on 1D and 2D NMR spectra and HRMS. - The sample consists of accompanying impurities, stereoisomers, etc. - The sample is 94% pure based on ^{1}H NMR spectrum.
Supporting information:	Copies of ^{1}H and ^{13}C NMR spectra, ^{1}H and ^{13}C FIDs.
Principal investigator:	Prof. Dr. Janez Košmrlj
Date of report:	May 6, 2025

ST466
DMSOd-6
1H
250scanov
2mg vzorca



Current Data Parameters

NAME	ST466
EXPNO	10
PROCNO	1

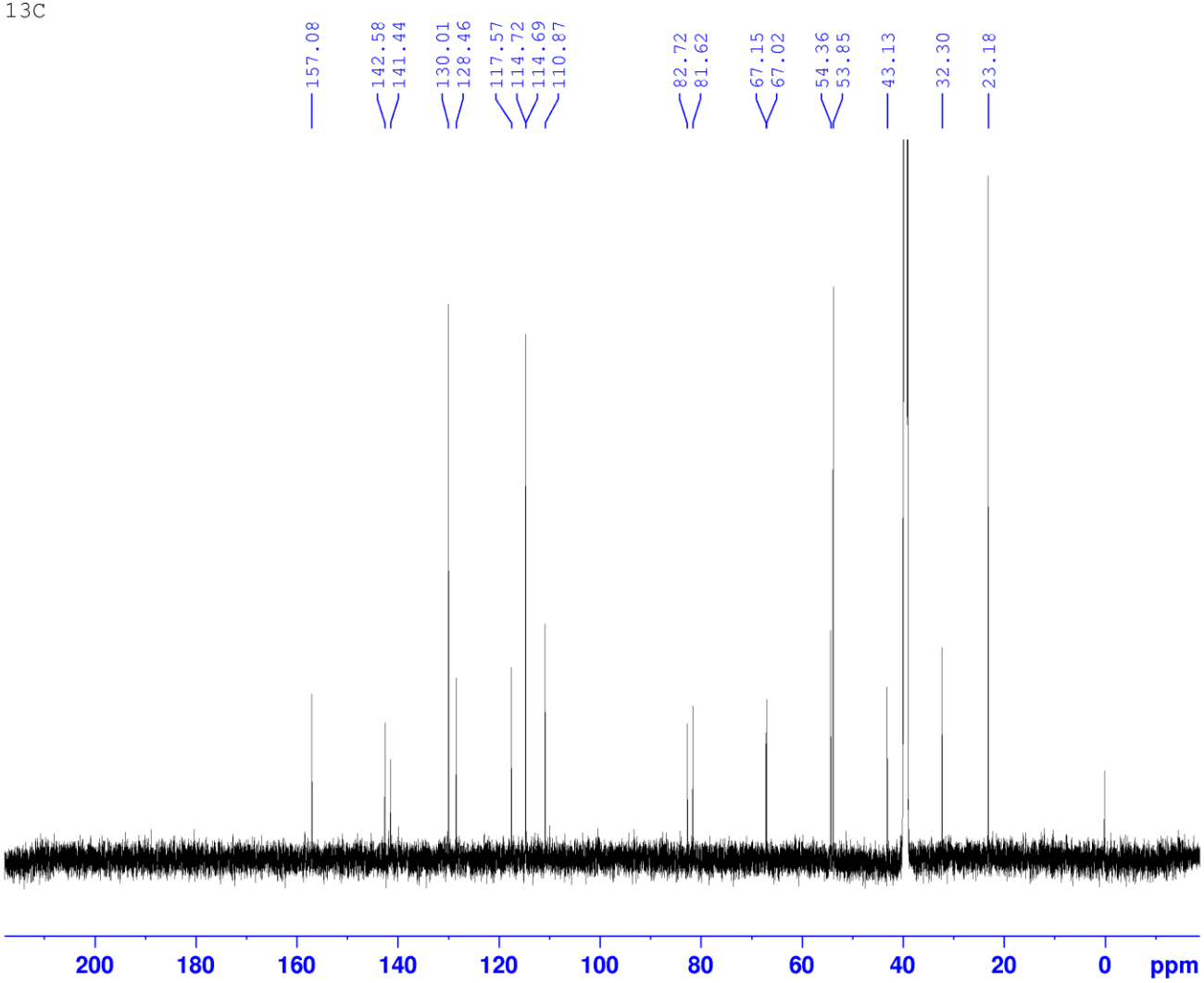
F2 - Acquisition Parameters

Date_	20250417
Time	2.16 h
INSTRUM	AV600 NEO
PROBHD	Z176567_0002 (
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	200
DS	2
SWH	11904.762 Hz
FIDRES	0.363304 Hz
AQ	2.7525120 sec
RG	101
DW	42.000 usec
DE	8.79 usec
TE	296.1 K
D1	1.00000000 sec
TD0	1
SFO1	600.1337058 MHz
NUC1	1H
P0	3.33 usec
P1	10.00 usec
PLW1	19.82900047 W

F2 - Processing parameters

SI	65536
SF	600.1300027 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

ST466
11k
13C



Current Data Parameters

NAME	ST466
EXPNO	21
PROCNO	1

F2 - Acquisition Parameters

Date_	20250418
Time	5.43 h
INSTRUM	AV600 NEO
PROBHD	Z176567_0002 (
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	11264
DS	4
SWH	35714.285 Hz
FIDRES	1.089913 Hz
AQ	0.9175040 sec
RG	101
DW	14.000 usec
DE	6.50 usec
TE	296.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	150.9178988 MHz
NUC1	13C
P0	4.00 usec
P1	12.00 usec
PLW1	112.23999786 W
SFO2	600.1324005 MHz
NUC2	1H
CPDPRG[2	waltz65
PCPD2	70.00 usec
PLW2	19.82900047 W
PLW12	0.40495440 W
PLW13	0.20296310 W

F2 - Processing parameters

SI	32768
SF	150.9028762 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40