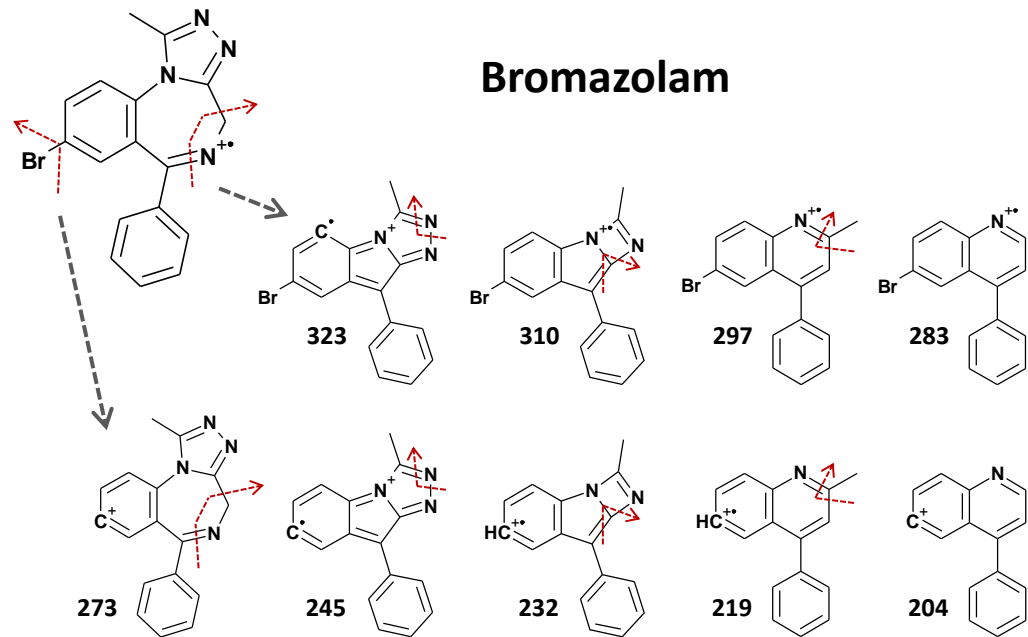


Bromazepam



Abundance

240000

220000

200000

180000

160000

140000

120000

100000

80000

60000

40000

20000

0

100

200

300

360

m/z

further aromatic
breakdown



204

323

273

352

245

219

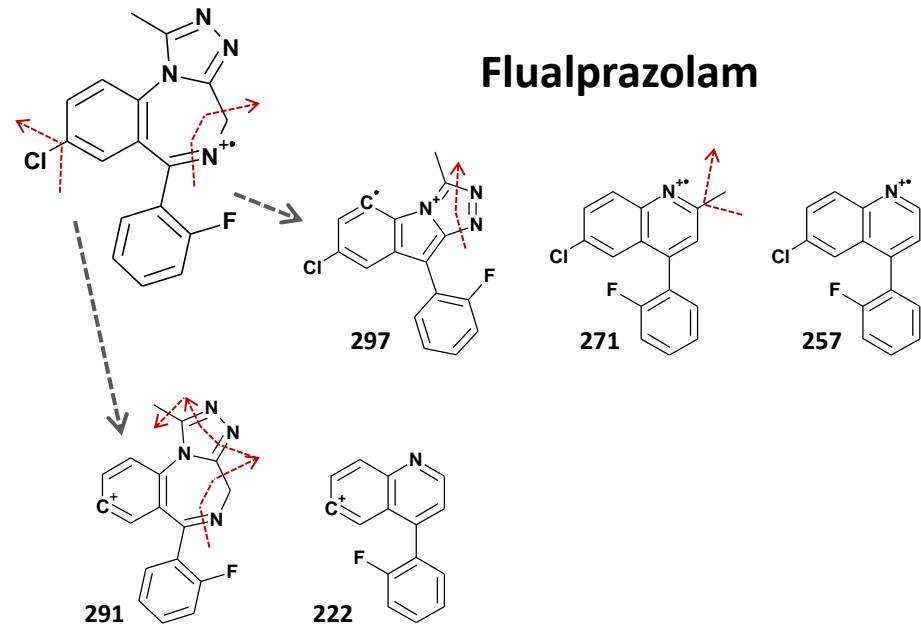
232

283

297

310

Flualprazolam



Abundance

10000

9000

8000

7000

6000

5000

4000

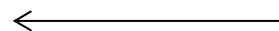
3000

2000

1000

0

further aromatic
breakdown



222

257

271

291

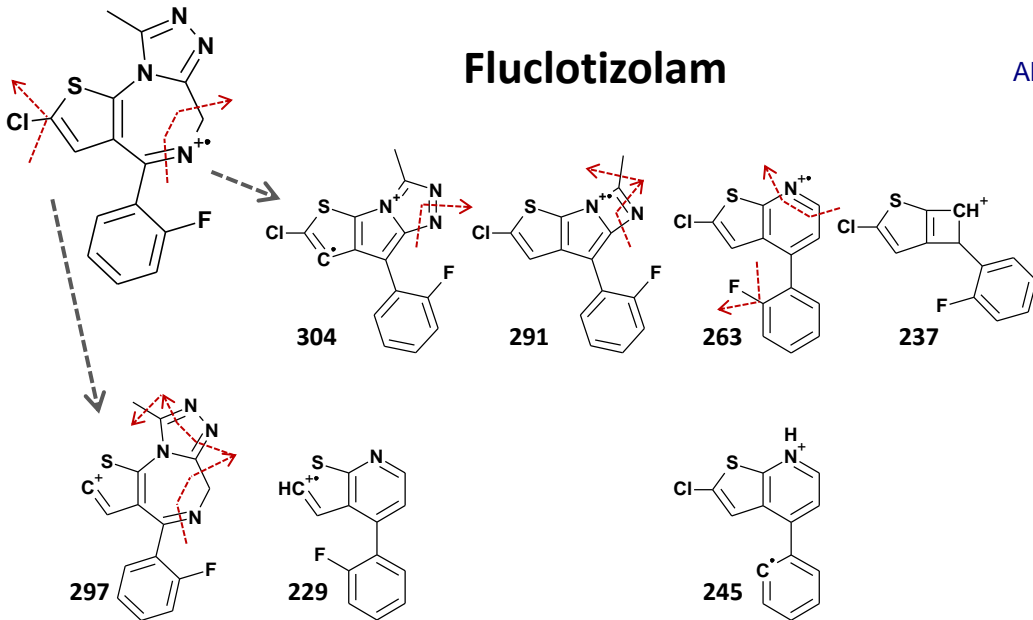
297

326

360

m/z

Fluclozotizolam



Abundance

40000

35000

30000

25000

20000

15000

10000

5000

0

100

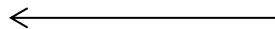
200

300

340

332

further aromatic
breakdown



229

263

237

245

291

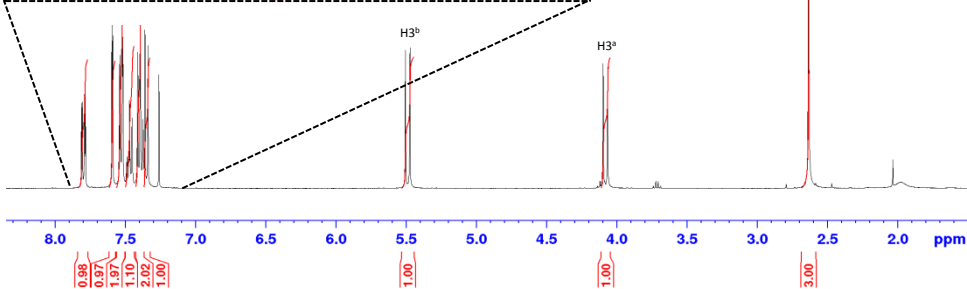
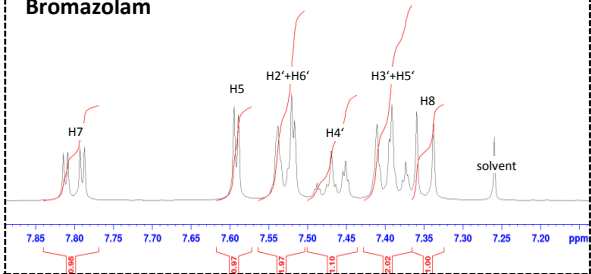
297

304

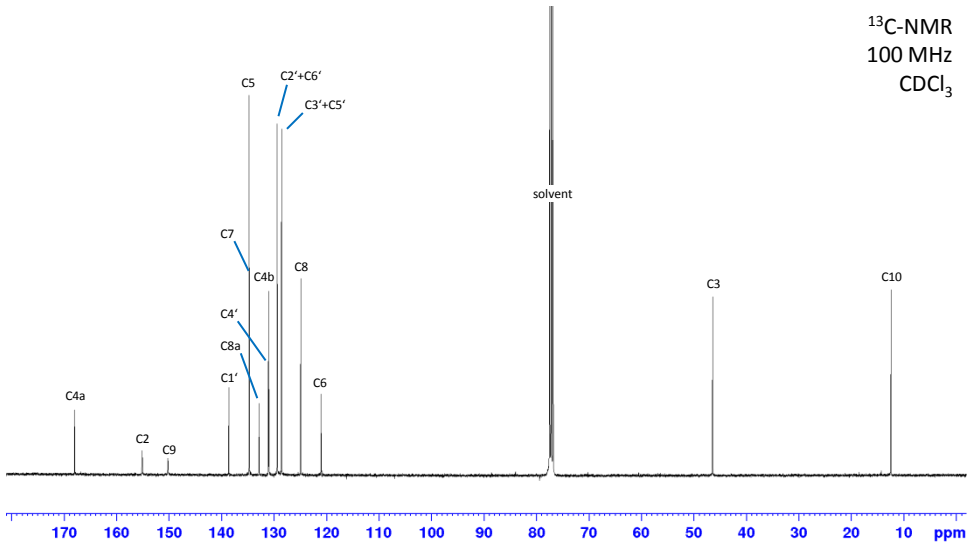
m/z

Bromazolam

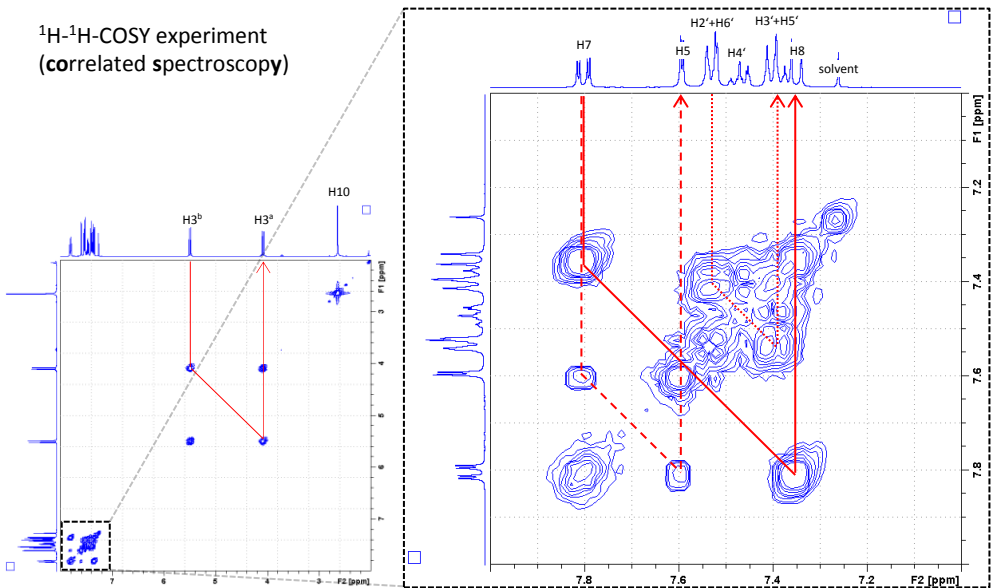
$^1\text{H-NMR}$
400 MHz
 CDCl_3



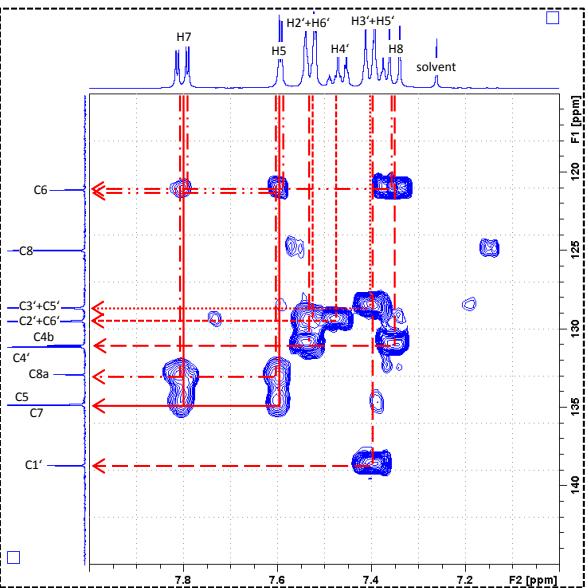
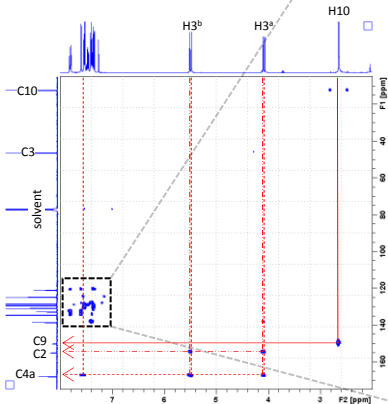
^{13}C -NMR
100 MHz
 CDCl_3



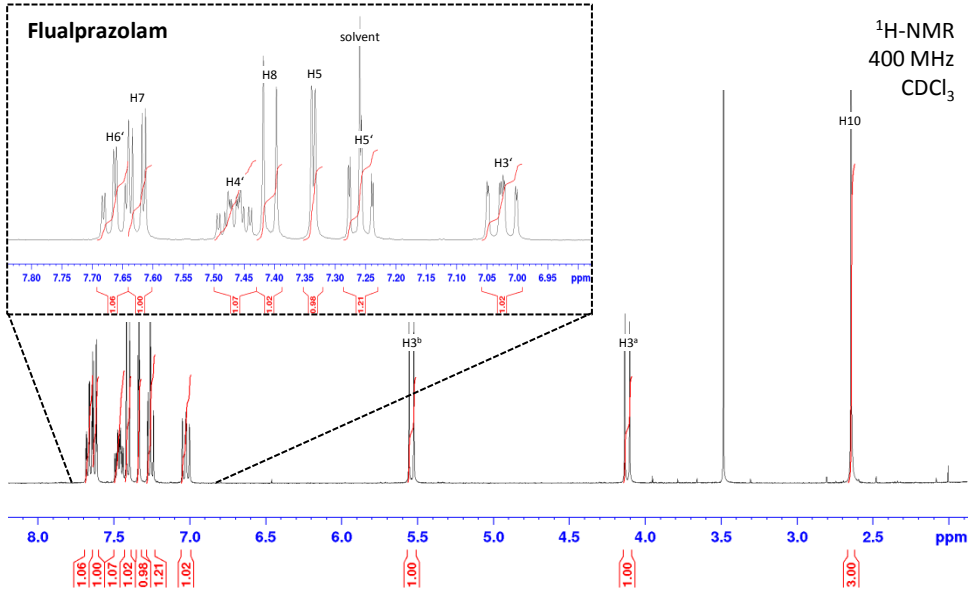
^1H - ^1H -COSY experiment
(correlated spectroscopy)



^{13}C - ^1H -HMBC experiment
(heteronuclear multiple bond correlation)

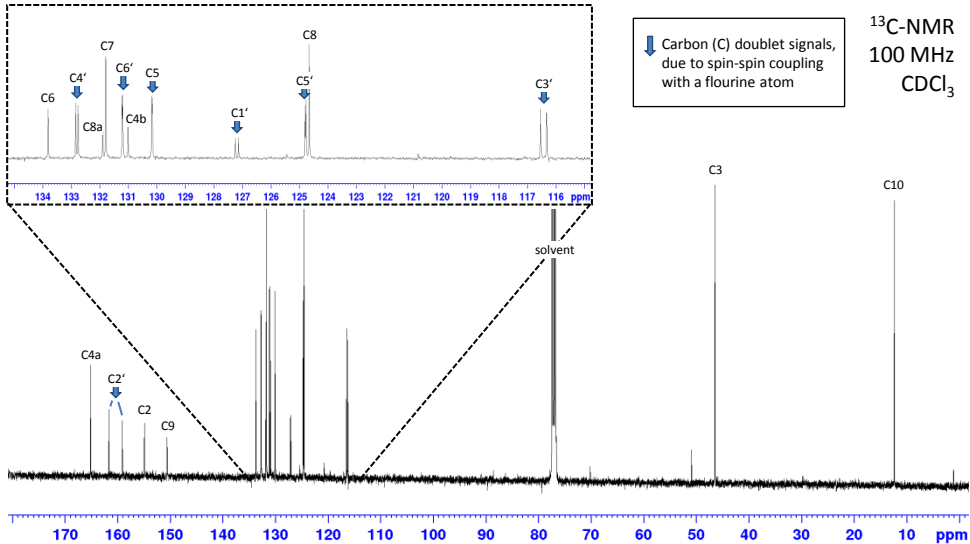


Flualprazolam

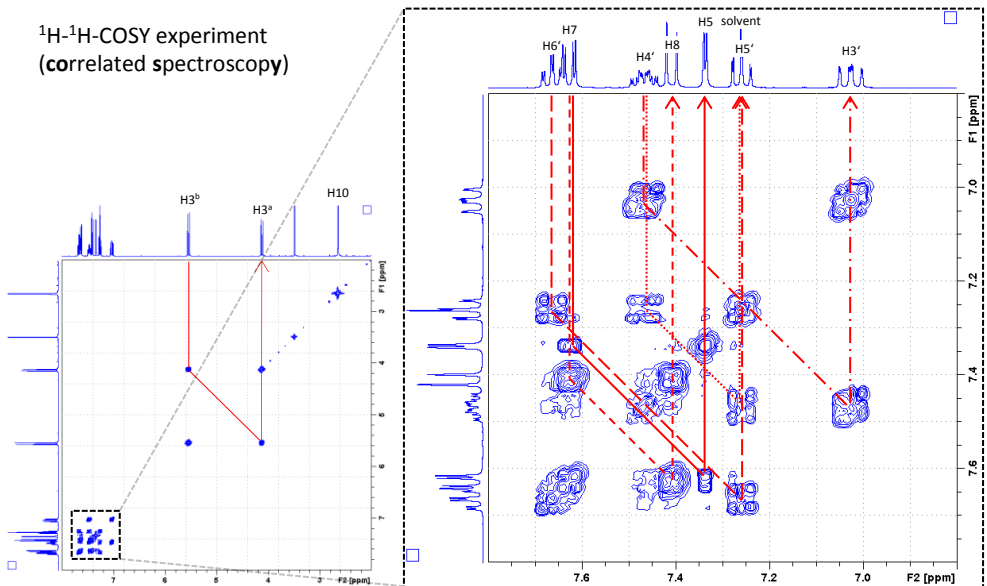


^{13}C -NMR
100 MHz
 CDCl_3

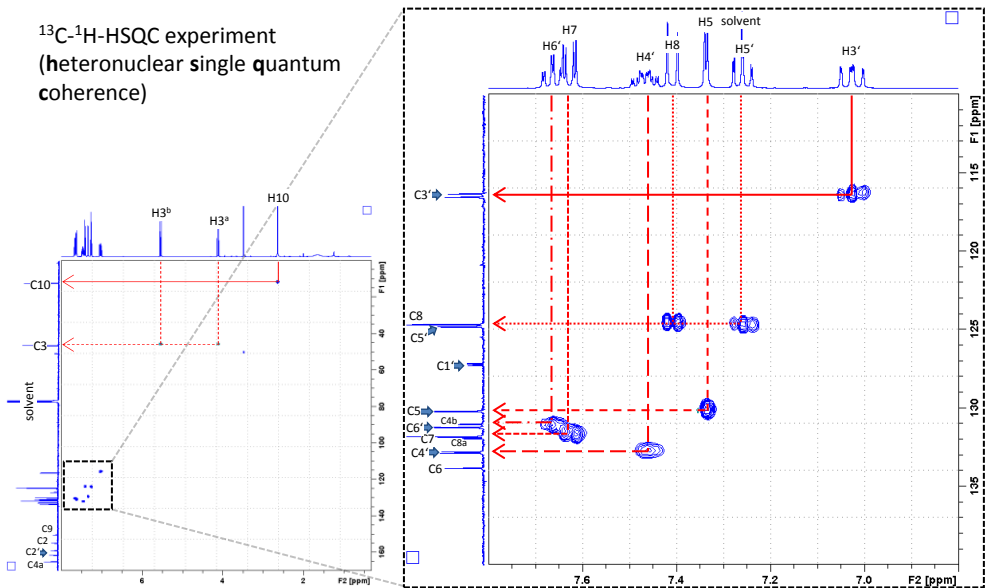
↓ Carbon (C) doublet signals,
due to spin-spin coupling
with a fluorine atom



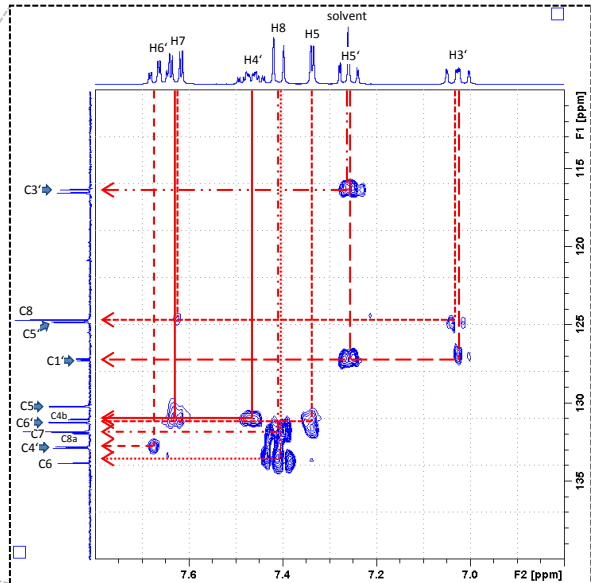
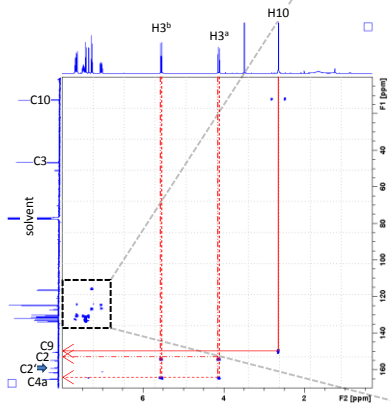
^1H - ^1H -COSY experiment
(correlated spectroscopy)



^{13}C - ^1H -HSQC experiment
(heteronuclear single quantum coherence)

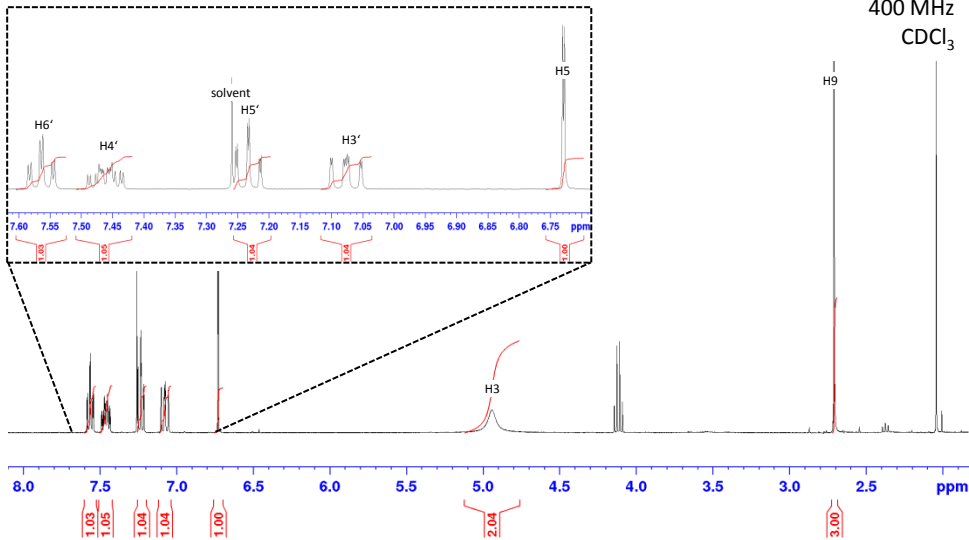


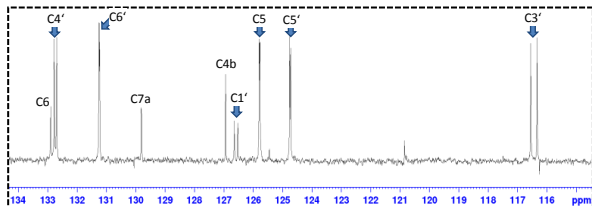
^{13}C - ^1H -HMBC experiment
(heteronuclear multiple bond correlation)



Fluclozotizolam

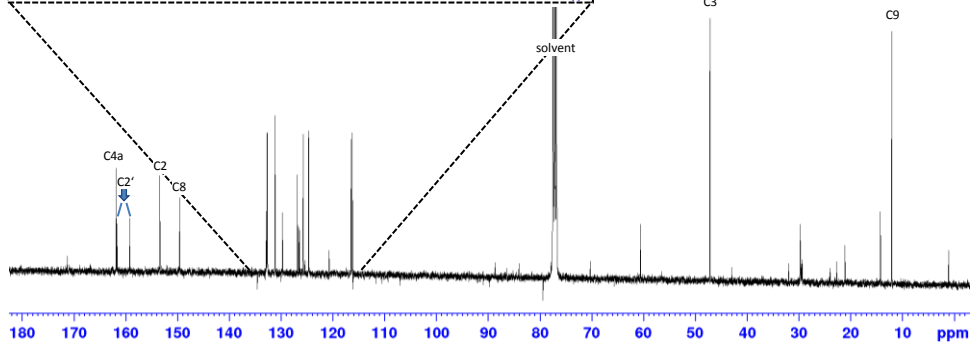
$^1\text{H-NMR}$
400 MHz
 CDCl_3



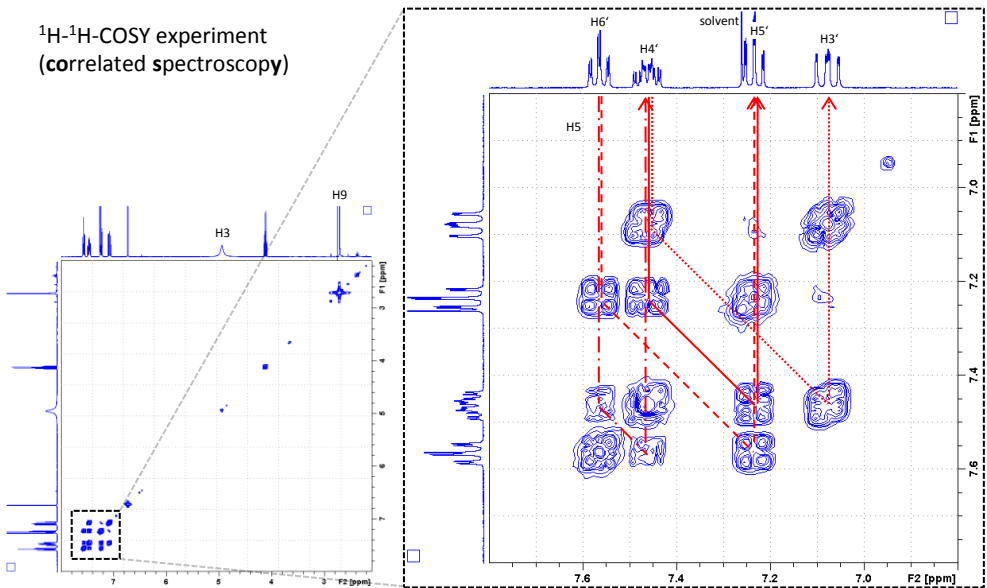


↓ Carbon (C) doublet signals,
due to spin-spin coupling
with a fluorine atom

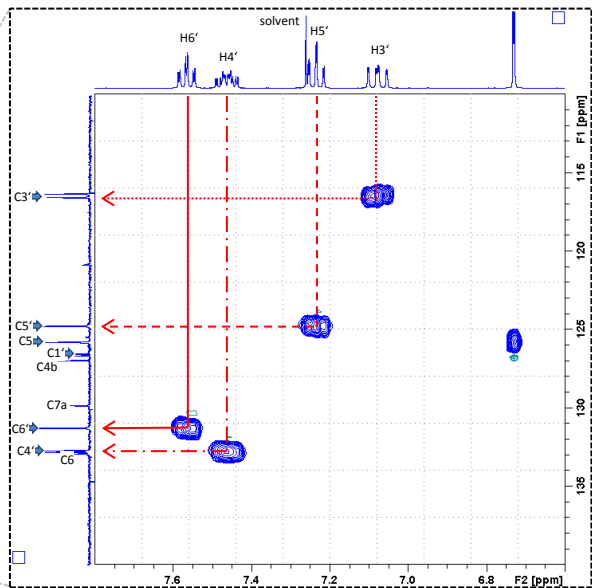
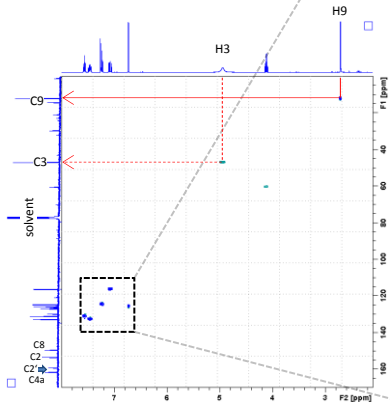
^{13}C -NMR
100 MHz
 CDCl_3



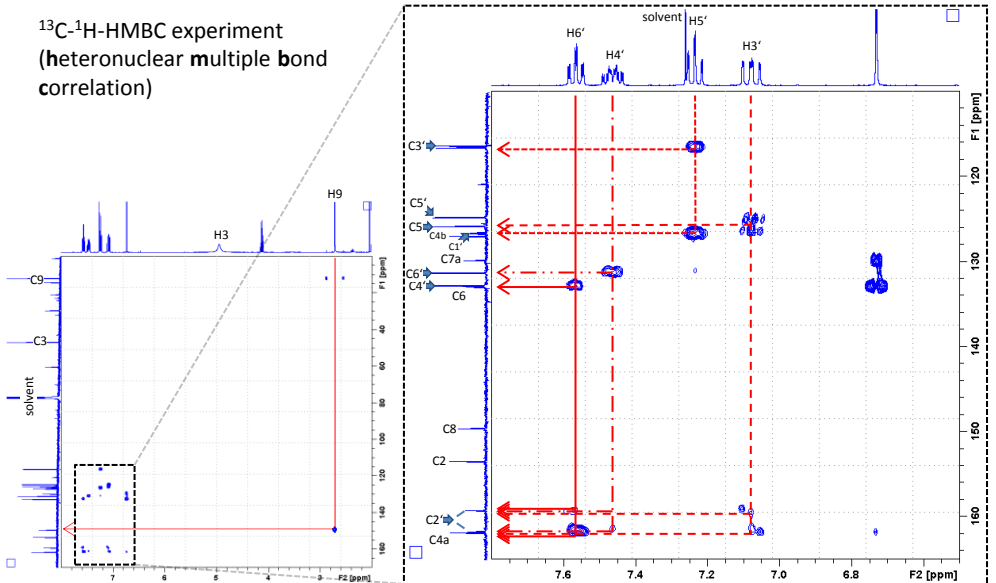
^1H - ^1H -COSY experiment
(correlated spectroscopy)



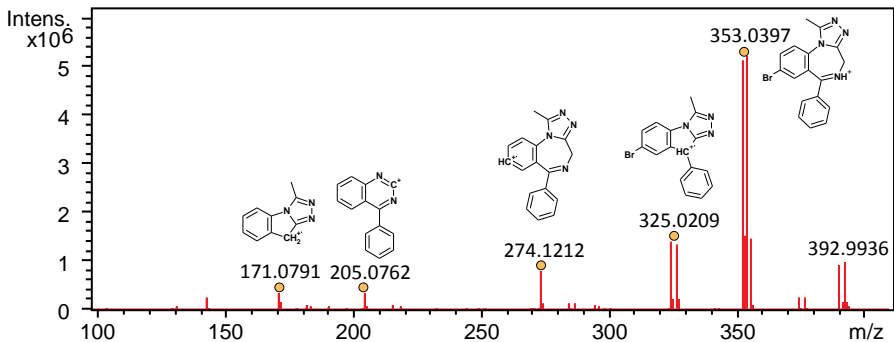
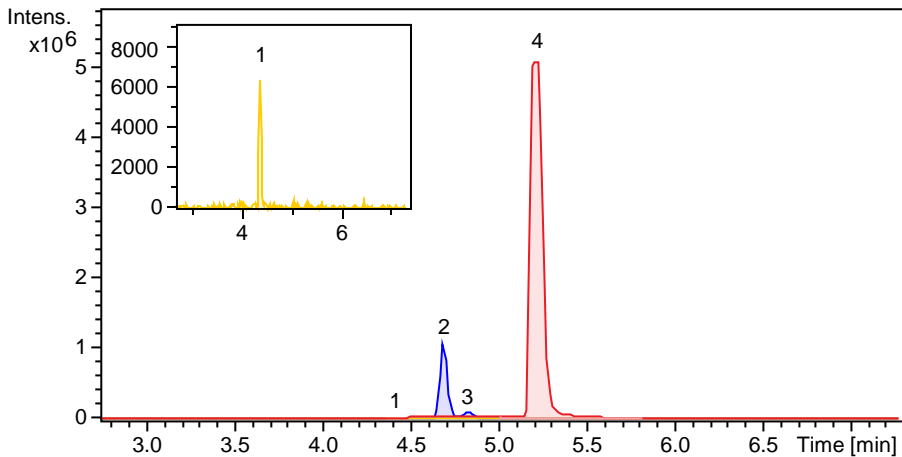
^{13}C - ^1H -HSQC experiment
(heteronuclear single quantum coherence)



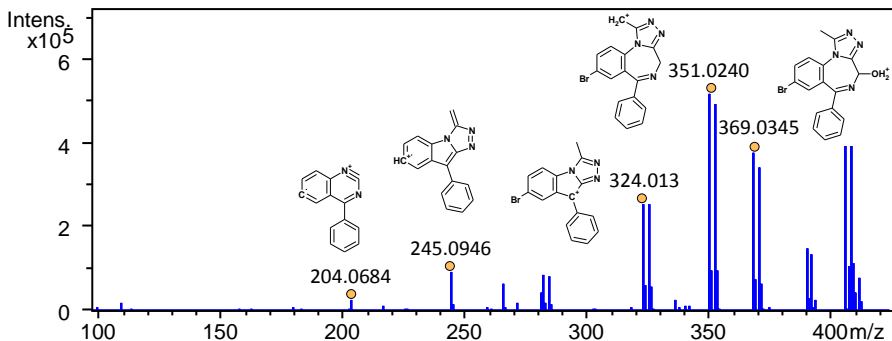
^{13}C - ^1H -HMBC experiment
(heteronuclear multiple bond correlation)



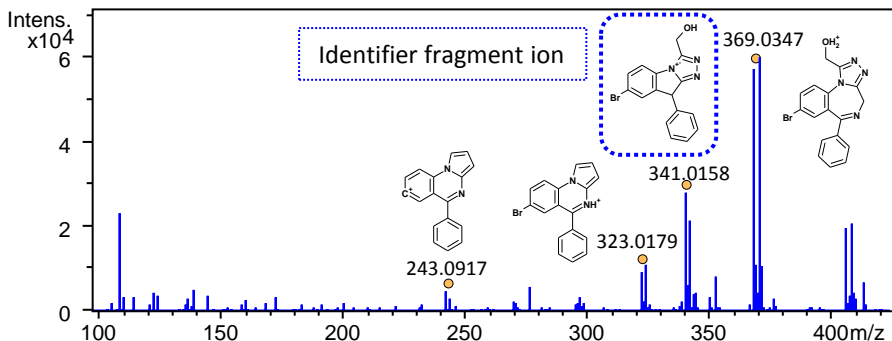
Bromazolam



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻	Conf
353.0397	C17H14BrN4	353.0396	-0.1	58.9	13		even
325.0209	C16H12BrN3	325.0209	0	18.8	12.5		odd
274.1212	C17H14N4	274.1213	0.5	9.3	13.5		odd
205.0762	C14H9N2	205.076	-1	15.6	12		even
171.0791	C10H9N3	171.0791	0.2	206.9	8.5		odd

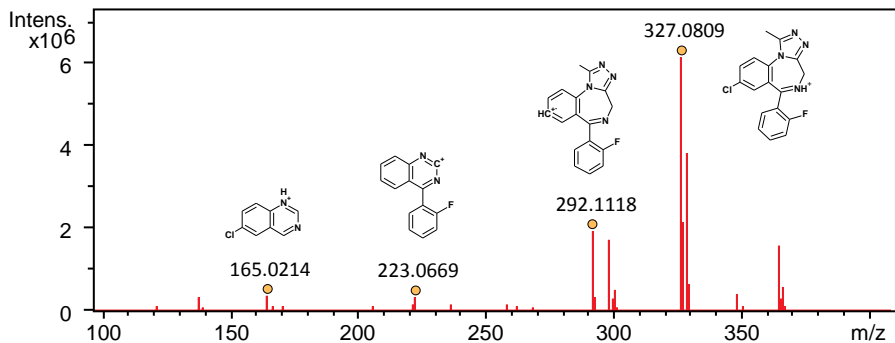
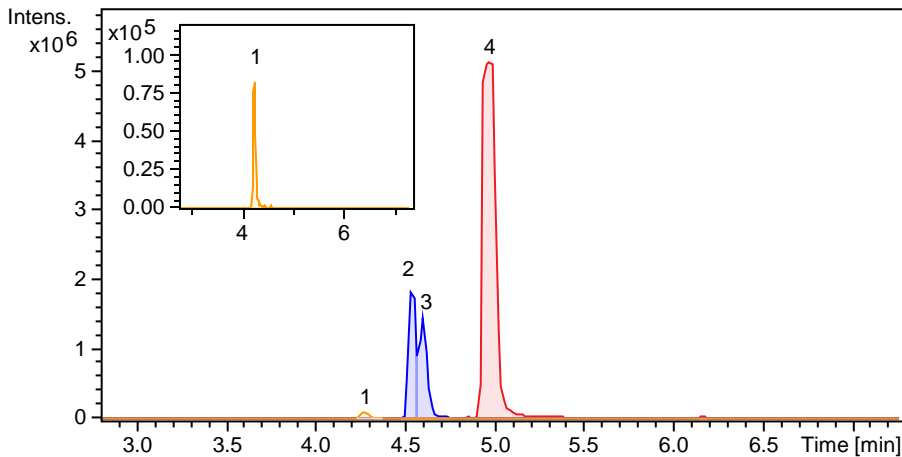


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
369.0345	C17H14BrN4O	369.0345	0	38.6	13	even
351.024	C17H12BrN4	351.024	0	20.4	14	even
324.013	C16H11BrN3	324.0131	0.1	33.9	13	even
245.0946	C16H11N3	245.0947	0.5	11.7	13.5	odd
204.0684	C14H8N2	204.0682	-1	n.a.	12.5	odd

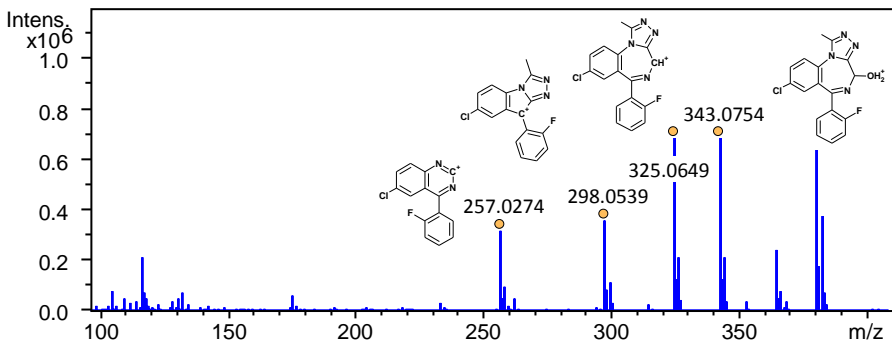


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
369.0347	C17H14BrN4O	369.0345	-0.3	22.5	13	even
341.0158	C16H12BrN3O	341.0158	0.1	119.4	12.5	odd
323.0179	C17H12BrN2	323.0178	-0.2	79	13	even
243.0917	C17H11N2	243.0917	0	260.7	14	even

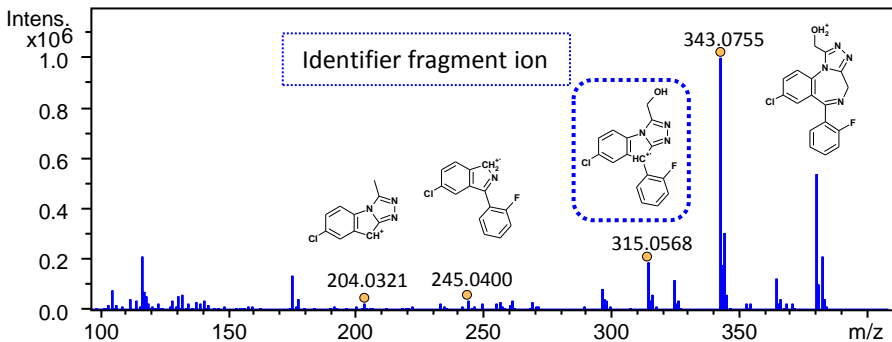
Flualprazolam



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻	Conf
327.0809	C17H13ClFN4	327.0807	-0.4	162	13	even	
292.1118	C17H13FN4	292.1119	0.2	15.3	13.5	odd	
223.0669	C14H8FN2	223.0666	-1.3	n.a.	12	even	
165.0214	C8H6ClN2	165.0214	0.3	49.8	7	even	

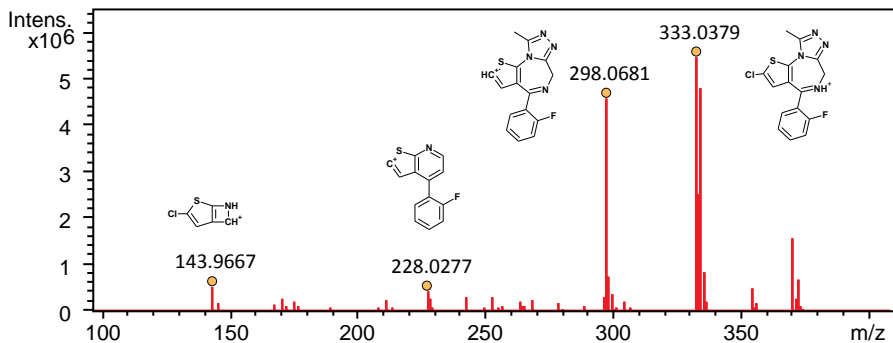
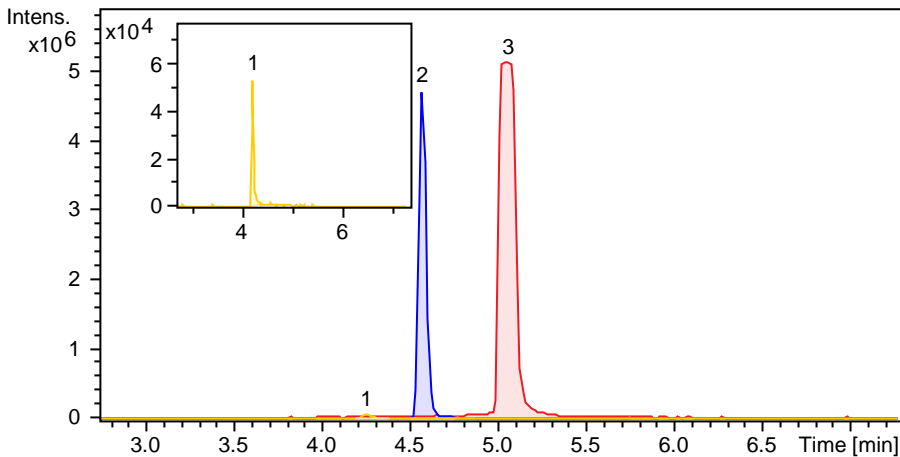


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻	Conf
343.0754	C17H13ClFN4O	343.0756	0.6	16.9	13	even	
325.0649	C17H11ClFN4	325.0651	0.6	18.3	14	even	
298.0539	C16H10ClFN3	298.0542	0.9	32.7	13	even	
257.0274	C14H7ClFN2	257.0276	0.7	17.1	12	even	

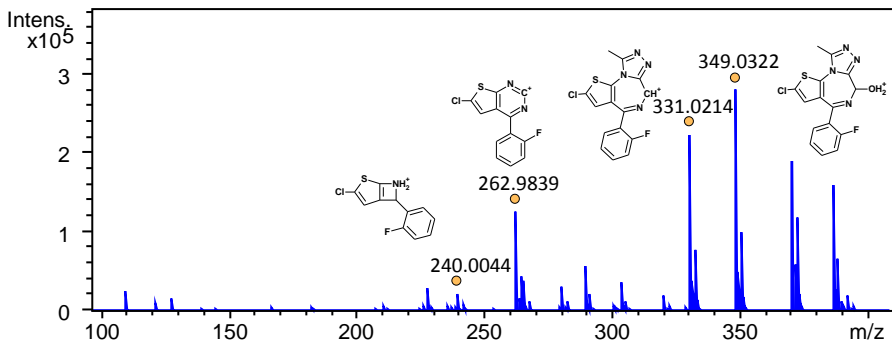


Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻	Conf
343.0755	C17H13ClFN4O	343.0756	0.5	21.6	13	even	
315.0568	C16H11ClFN3O	315.0569	0.4	12.4	12.5	odd	
245.04	C14H9ClFN	245.0402	1	8.5	10.5	odd	
204.0321	C10H7ClN3	204.0323	0.8	27.2	9	even	

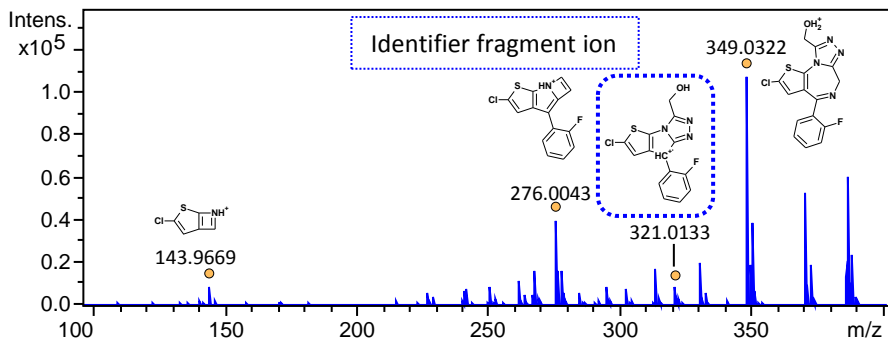
Fluclozotizolam



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻	Conf
333.0379	C15H11ClFN4S	333.0371	-2.3	256.5	12	even	
298.0681	C15H11FN4S	298.0683	0.5	16	12.5	odd	
228.0277	C13H7FNS	228.0278	0.3	198.3	11	even	
143.9667	C5H3ClNS	143.9669	1.7	24.8	5	even	



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
349.0322	C15H11ClF2N4OS	349.0321	-0.3	13	12	even
331.0214	C15H9ClF2N4S	331.0215	0.3	14.8	13	even
262.9839	C12H5ClF2N2S	262.9841	0.5	115.7	11	even
240.0044	C11H8ClFNS	240.0045	0.2	17.1	8	even



Meas. m/z	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
349.0322	C15H11ClF2N4OS	349.0321	-0.3	11.7	12	even
321.0133	C14H9ClF3N3OS	321.0133	0.1	98.2	11.5	odd
276.0043	C14H8ClFNS	276.0045	0.5	119.8	11	even
143.9669	C5H3ClNS	143.9669	-0.1	37.4	5	even