

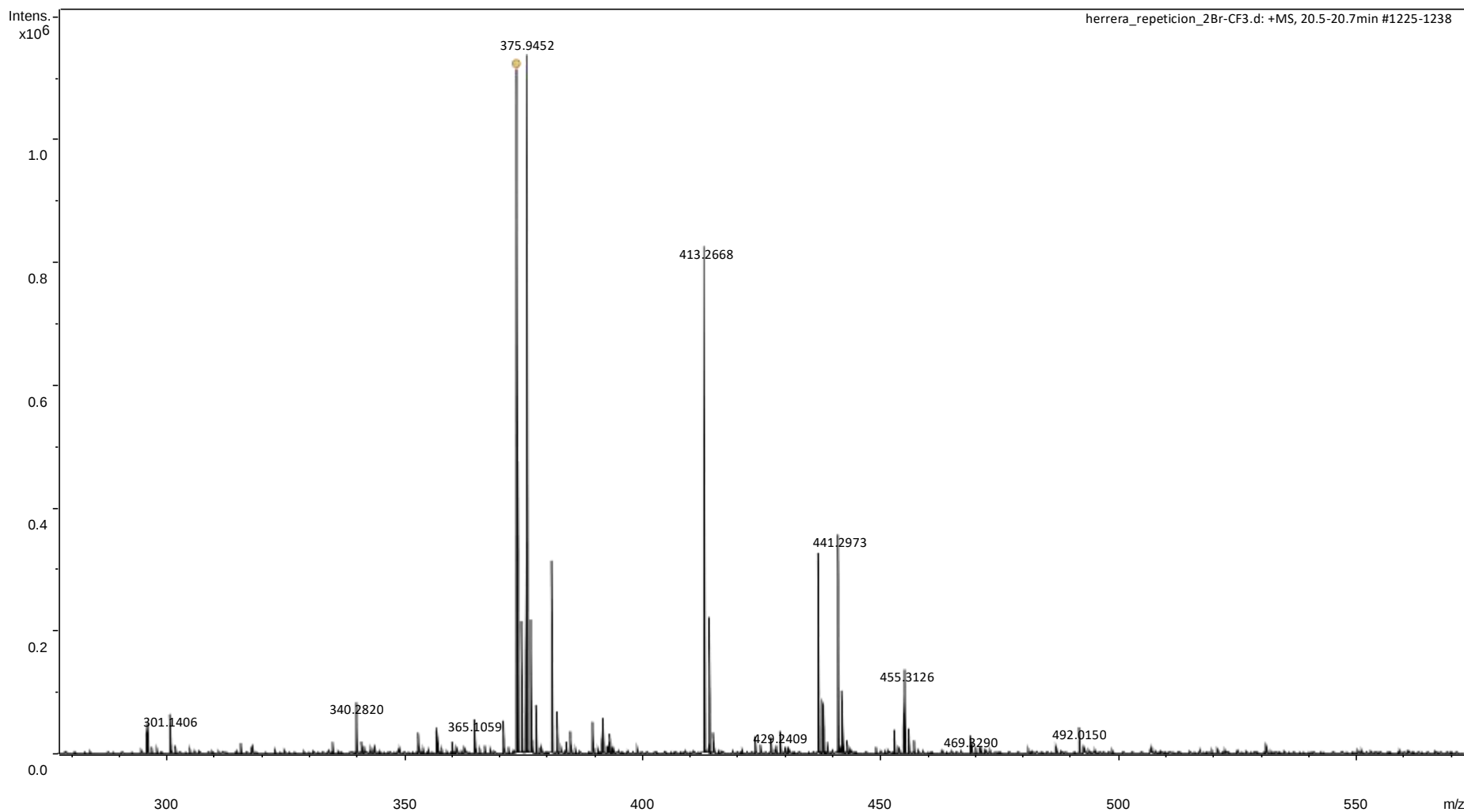


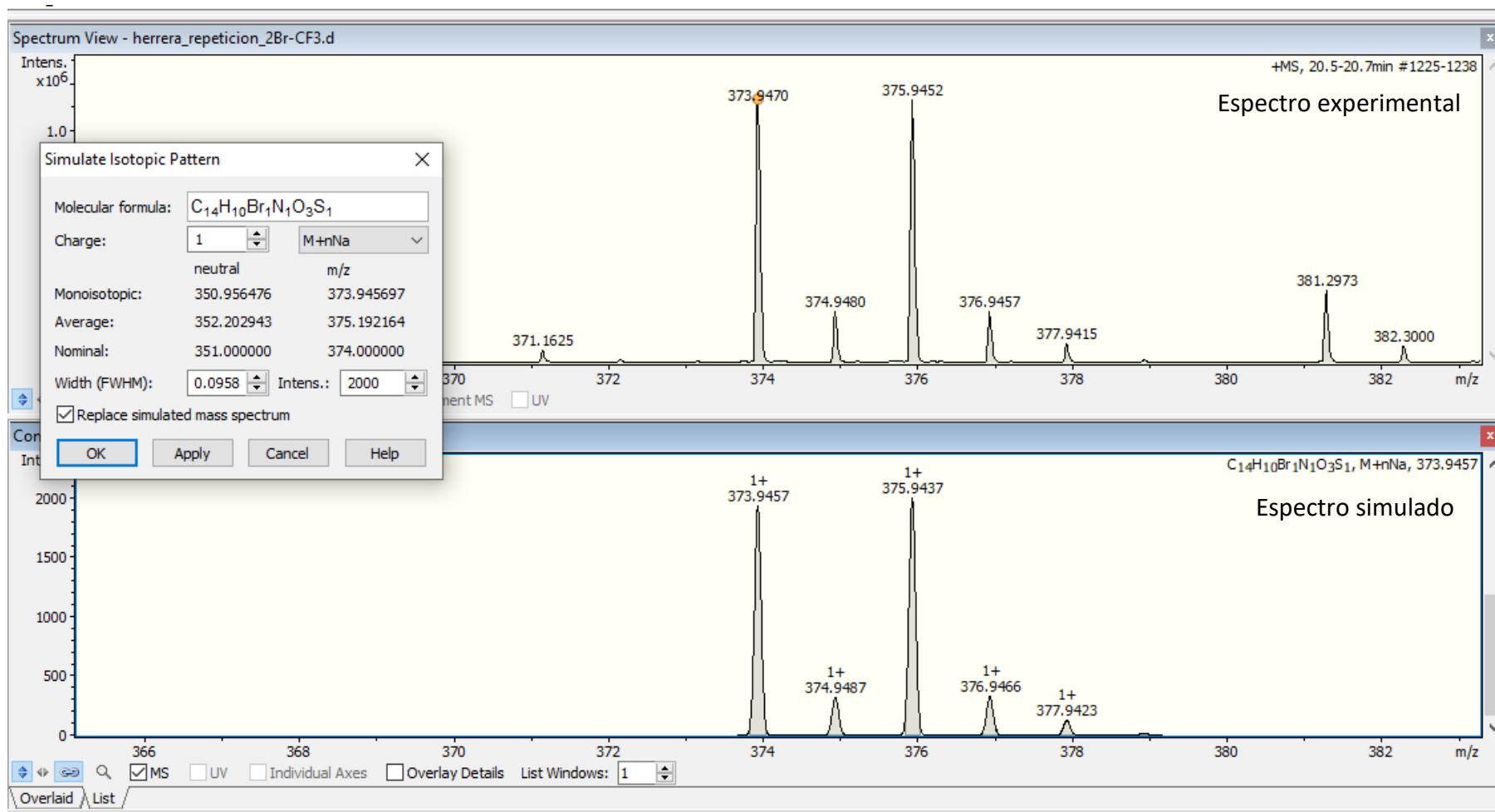
SUPPORTING INFORMATION FOR EDITOR

HRMS Spectra	Page
2-((4-bromobenzyl)sulfonyl)benzo[d]oxazole, 6h	2
2-((4-(trifluoromethyl)benzyl)sulfonyl)benzo[d]oxazole, 6c	5

HRMS spectrum of 2-((4-bromobenzyl)sulfonyl)benzo[d]oxazole, 6h

Espectro experimental





Spectrum View - herrera_repeticion_2Br-CF3.d

SmartFormula Manually

Lower formula:

Upper formula:

Note: for m < 2000 the elements C, H, N, and O are considered implicitly.

Adducts, pos. ☐ Collect adducts

Adducts, neg.

Measured m/z Tolerance: ppm Charge:

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score
373.9470	1	C ₁₄ H ₁₀ BrNNaO ₃ S	373.9457	3.6	18.5	1	100.00
	2	C ₁₁ H ₁₄ BrNNaO ₃ S ₂	373.9491	5.4	40.4	2	36.81
	3	C ₇ H ₁₀ BrN ₇ NaO ₅ S ₂	373.9464	1.8	49.2	3	67.71
	4	C ₉ H ₁₅ BrNNa ₂ O ₃ S ₂	373.9467	-1.0	49.6	4	76.41
	5	C ₇ H ₁₃ BrN ₃ Na ₄ O ₂ S	373.9497	-7.1	55.9	5	13.51
	6	C ₅ H ₈ BrN ₉ Na ₃ S	373.9494	-6.4	56.6	6	16.81

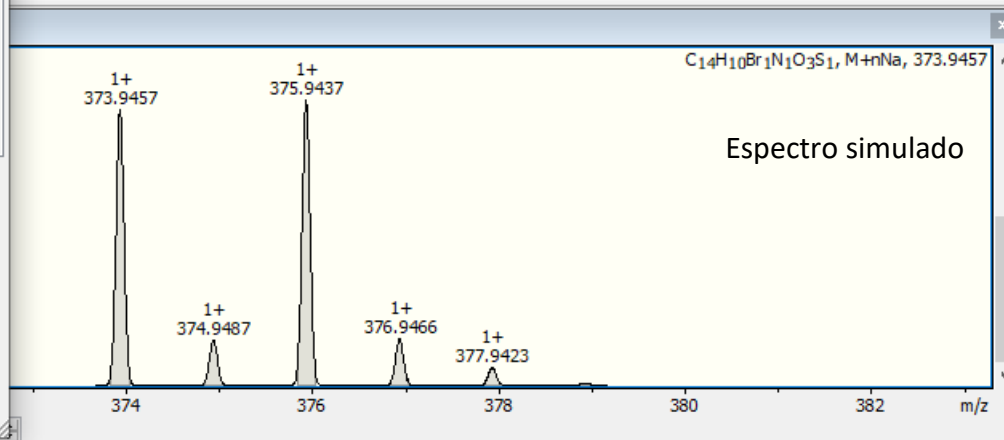
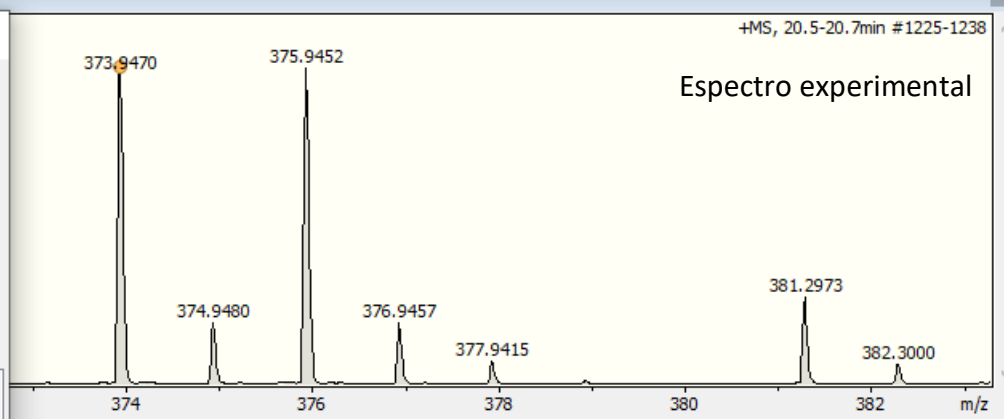
☐ Automatically locate monoisotopic peak Maximum number of formulae

☒ Check rings plus double bonds Minimum Maximum

Electron configuration

☒ Filter H/C element ratio Minimum H/C: Maximum H/C:

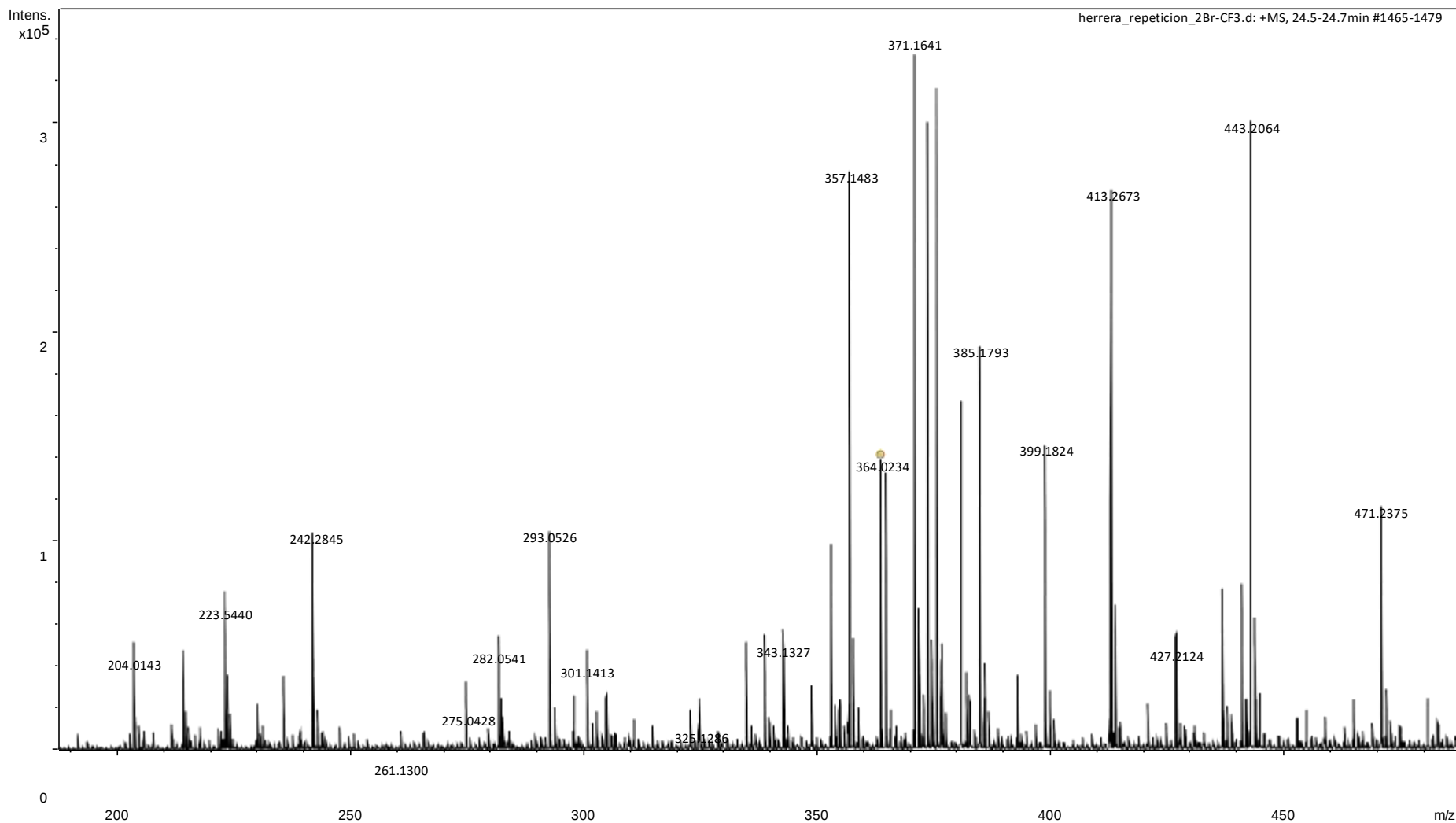
☒ Estimate carbon number ☒ Generate immediately

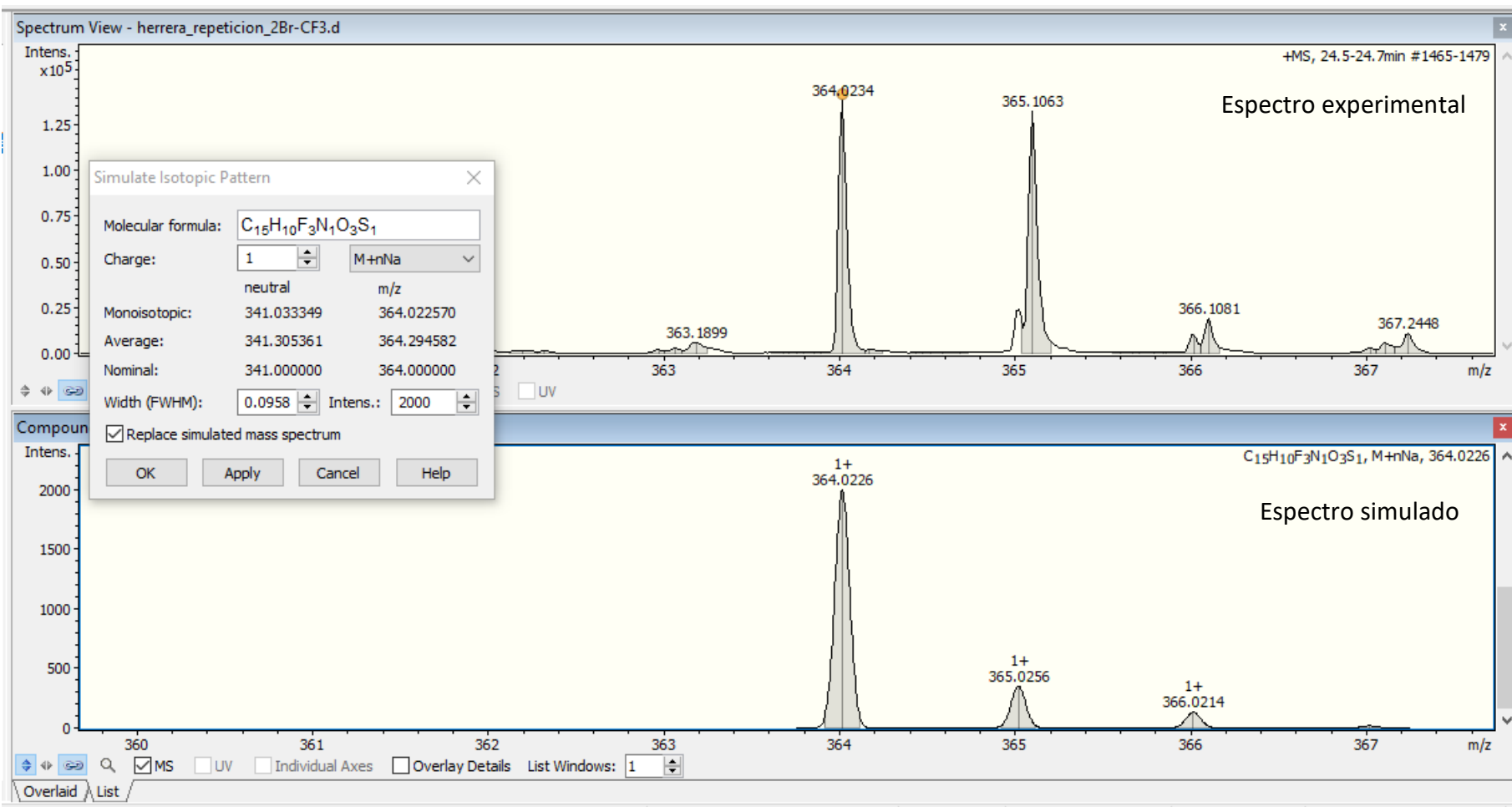


Overlaid List

HRMS spectrum of 2-((4-(trifluoromethyl)benzyl)sulfonyl)benzo[d]oxazole, 6c

Espectro experimental





Spectrum View - herrera_repeticion_2Br-CF3.d

SmartFormula Manually

Lower formula: $F_1Na_1S_1N_1$

Upper formula: S_1Na_1

F 1-n, N 1-n, Na 1-1, S 1-1

Note: for $m < 2000$ the elements C, H, N, and O are considered implicitly.

Adducts, pos. $M+H$

☐ Collect adducts

Adducts, neg. $M-H$

Measured m/z 364.0234

Tolerance: 5 ppm

Charge: 1

cas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB
364.0234	4	CH2F3N17NaS	364.0244	-2.8	48.8	4	38.74	7.5
	2	C3H5F2N13NaO3S	364.0219	-4.0	46.4	2	46.83	6.5
	5	C3H5F6N11NaS	364.0247	-3.4	48.8	5	33.53	3.5
	3	C5H8F5N7NaO3S	364.0222	-3.4	46.4	3	54.52	2.5
	6	C5H8F9N5NaS	364.0249	4.1	48.9	6	28.71	-0.5
	1	C6H13F2N3NaO9S	364.0233	0.3	45.2	1	100.00	0.5
	7	C7H9F2N7NaO5S	364.0246	-3.3	56.9	7	39.92	5.5
	9	C9H12FN3NaO8S	364.0221	-3.5	60.8	9	33.87	4.5
	8	C9H12F5NNaO5S	364.0249	4.0	56.9	8	34.25	1.5
	10	C10H8FN7NaO4S	364.0235	-0.2	72.5	10	41.03	9.5
	12	C11H4FN11NaS	364.0248	-3.9	84.3	12	12.69	14.5
	11	C12H11F4NNaO4S	364.0237	0.9	72.5	11	36.96	5.5
	13	C13H7F4N5NaS	364.0250	4.5	84.4	13	10.78	10.5
	14	C15H10F3NNaO3S	364.0226	2.3	88.3	14	15.05	9.5

☐ Automatically locate monoisotopic peak

Maximum number of formulae

500

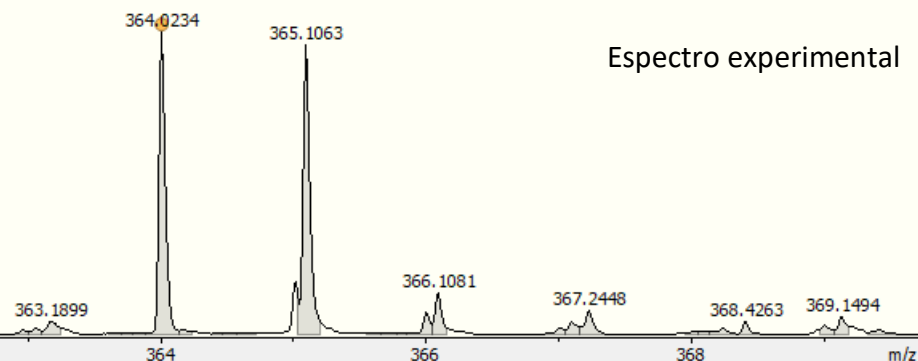
☒ Check rings plus double bonds

Minimum -0.5

Maximum 40

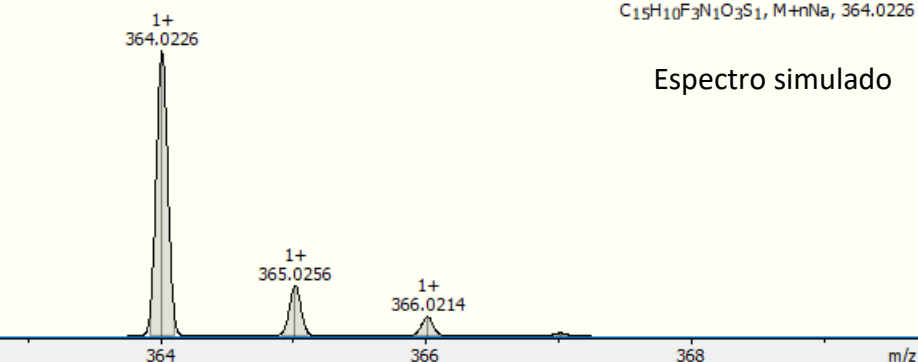
+MS, 24.5-24.7min #1465-1479

Espectro experimental



$C_{15}H_{10}F_3N_1O_3S_1$, $M+nNa$, 364.0226

Espectro simulado



Calibration