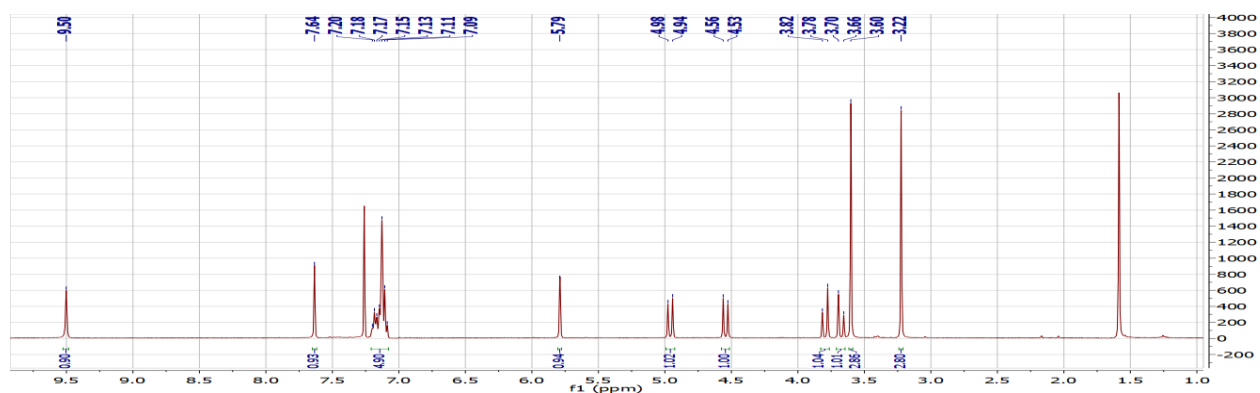
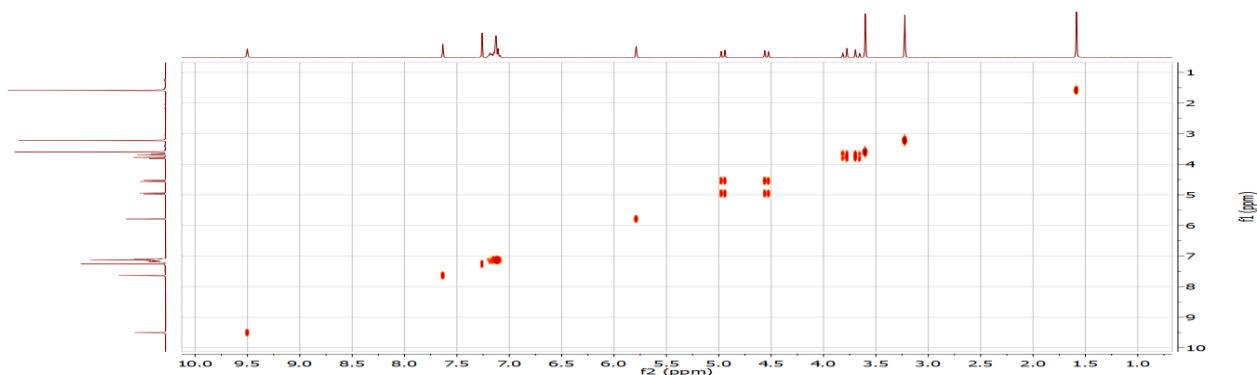


NMR AND HRMS SPECTRA FOR THIAZOLIDINE-4-ONE DERIVATIVES (6a-k)

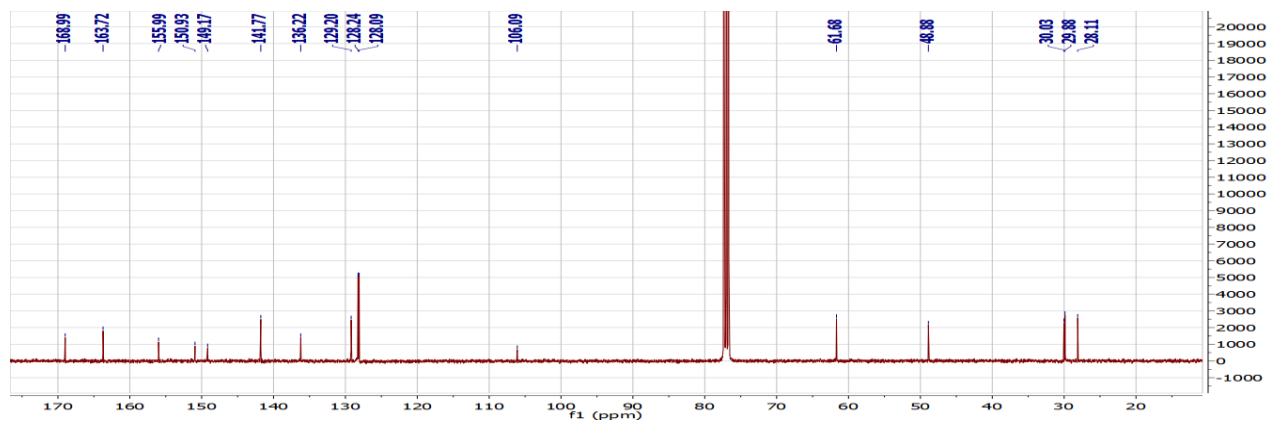
2-Phenyl-3-[(1,3-dimethylxanthin-7-yl)acetamido]thiazolidine-4-one (6a)



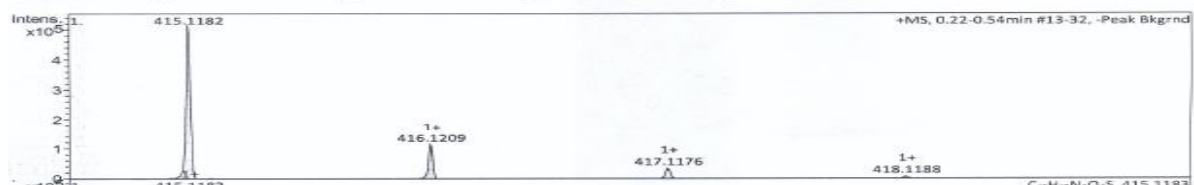
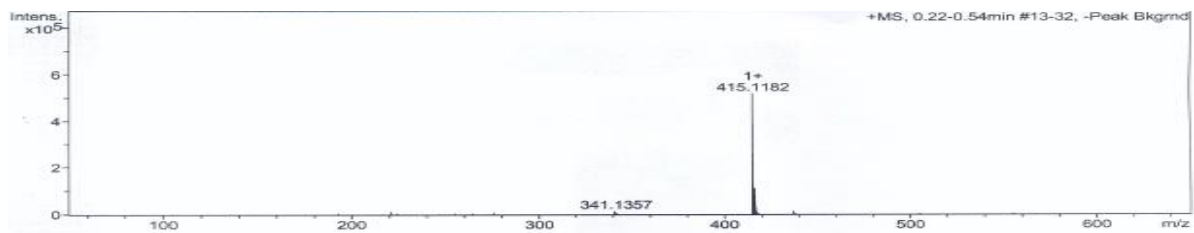
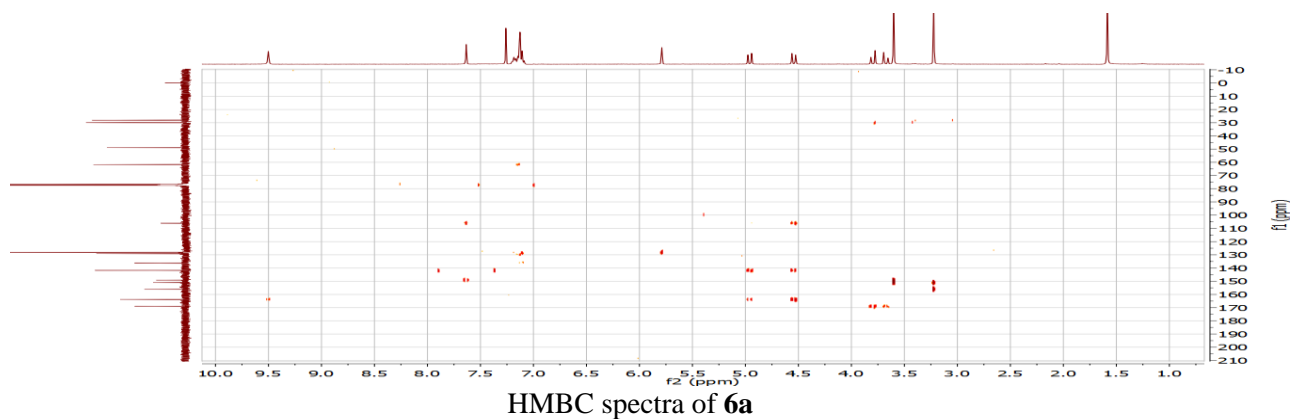
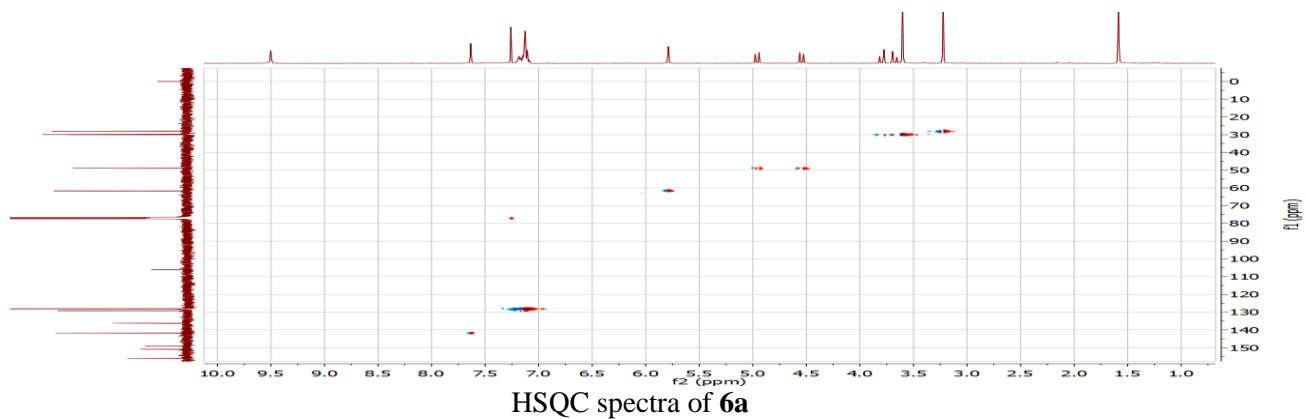
¹H-RMN spectra of **6a**



2D-COSY spectra of **6a**



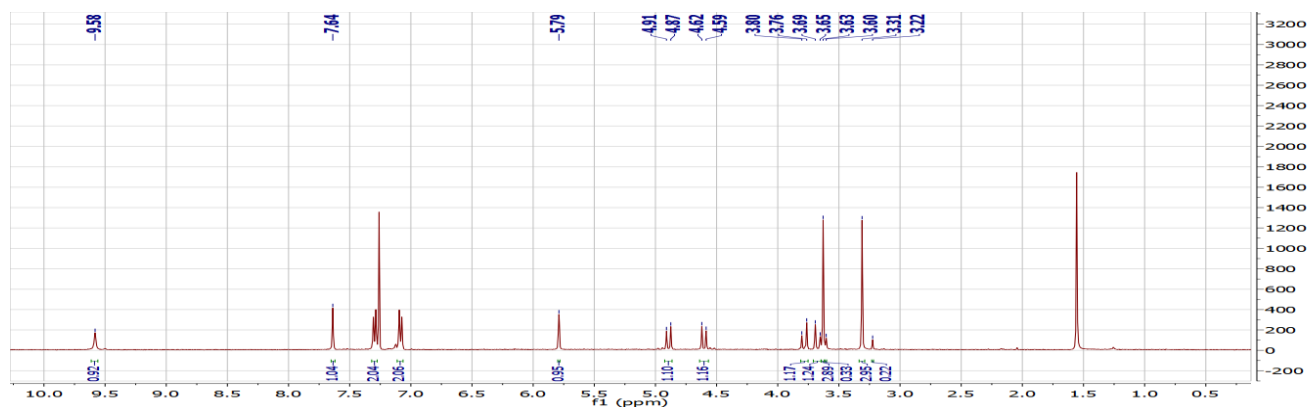
¹³C-RMN spectra of **6a**



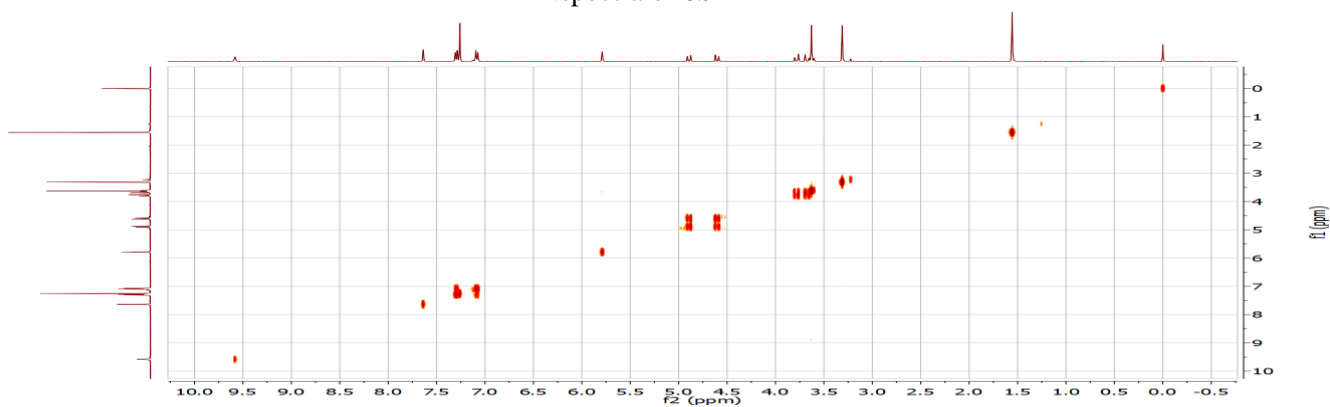
Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
415.118172	1+	1	C ₁₈ H ₁₉ N ₆ O ₄ S	415.118301	0.3	8.1	12.5	even

HRMS spectra of **6a**

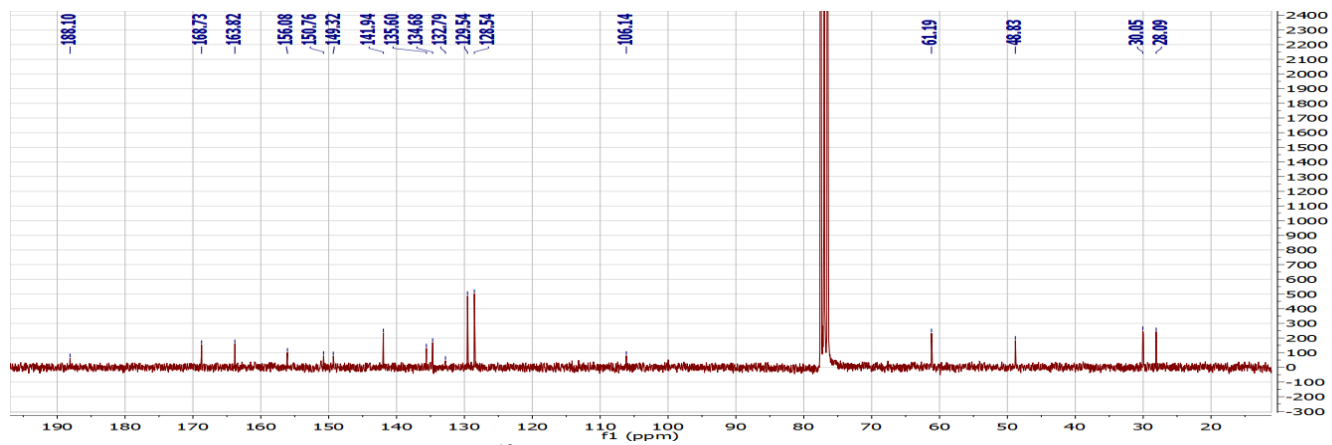
2-(4-Bromophenyl)-3-[(1,3-dimethylxanthin-7-yl)acethamido]thiazolidine-4-one (6b)



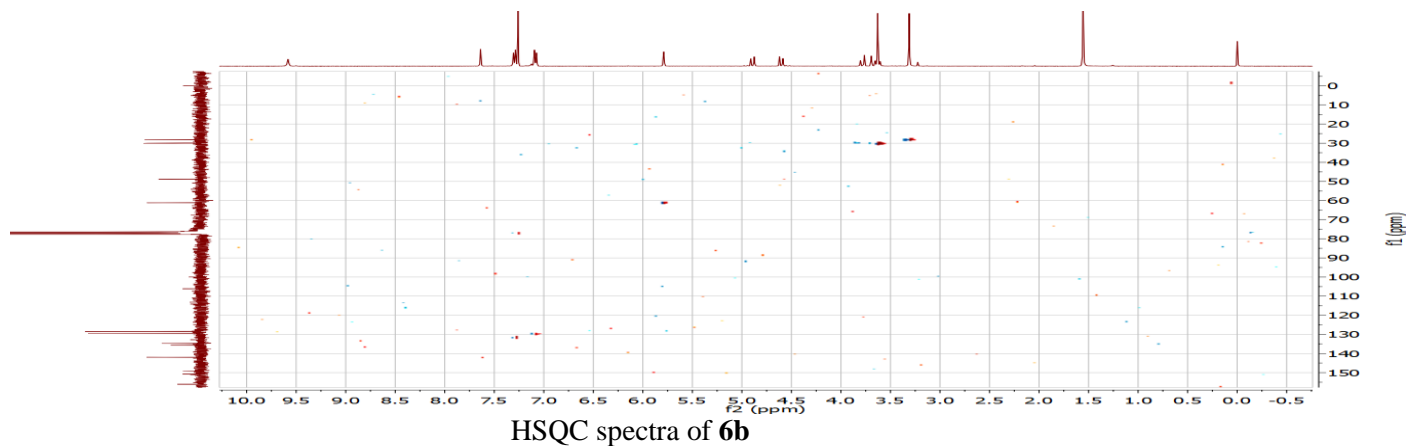
¹H-RMN spectra of **6b**



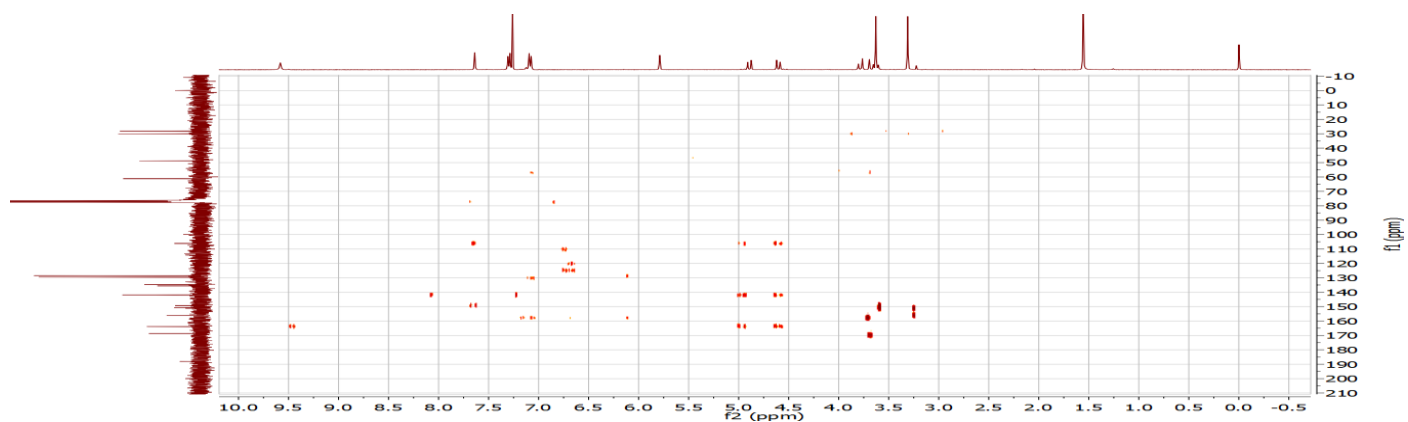
2D-COSY spectra of **6b**



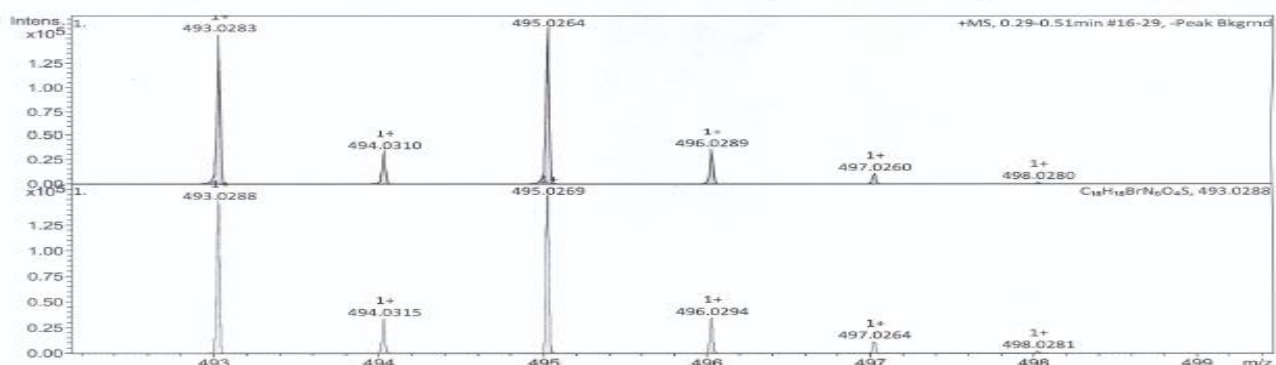
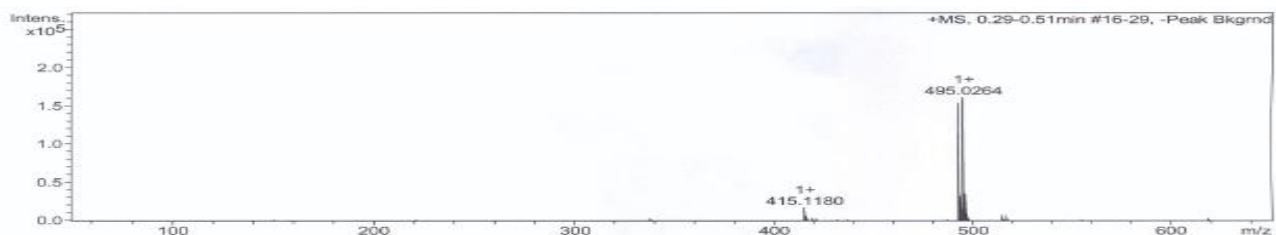
¹³C-RMN spectra of **6b**



HSQC spectra of **6b**



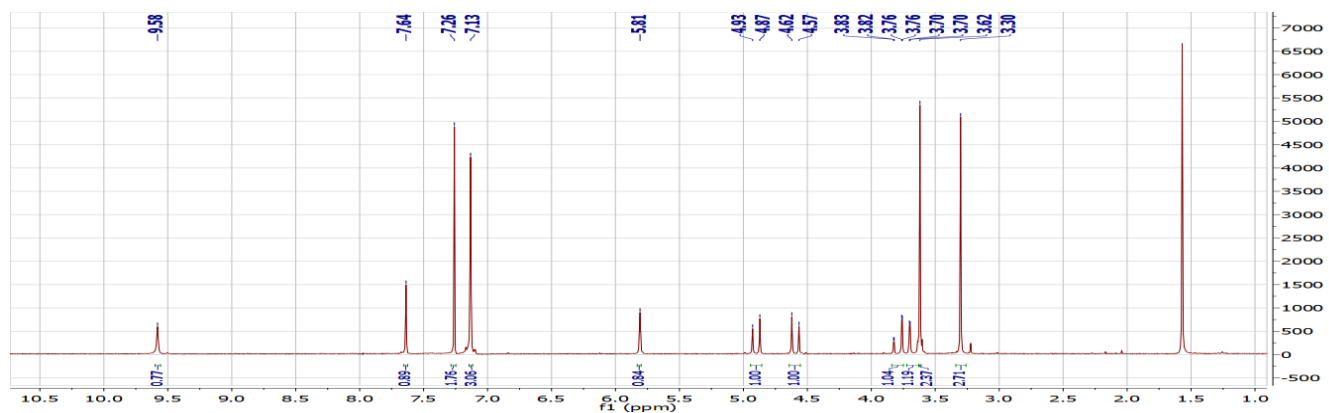
HMBC spectra of **6b**



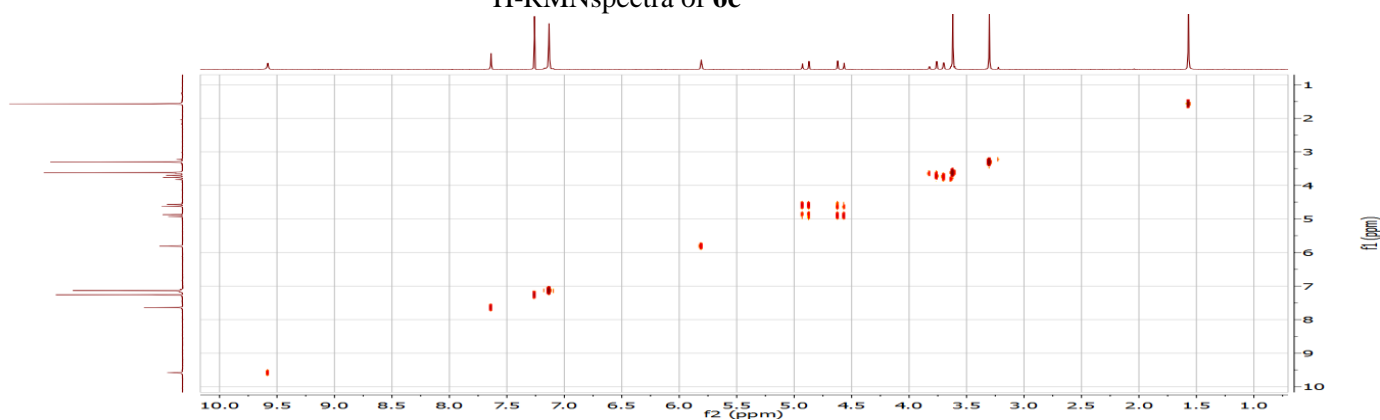
Meas. m/z	Z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
493.028312	1+	1	C18H18BrN6O4S	493.028813	1.0	7.9	12.5	even
	1+	2	C17H22BrN2O8S	493.027475	1.7	9.7	7.5	even

HRMS spectra of **6b**

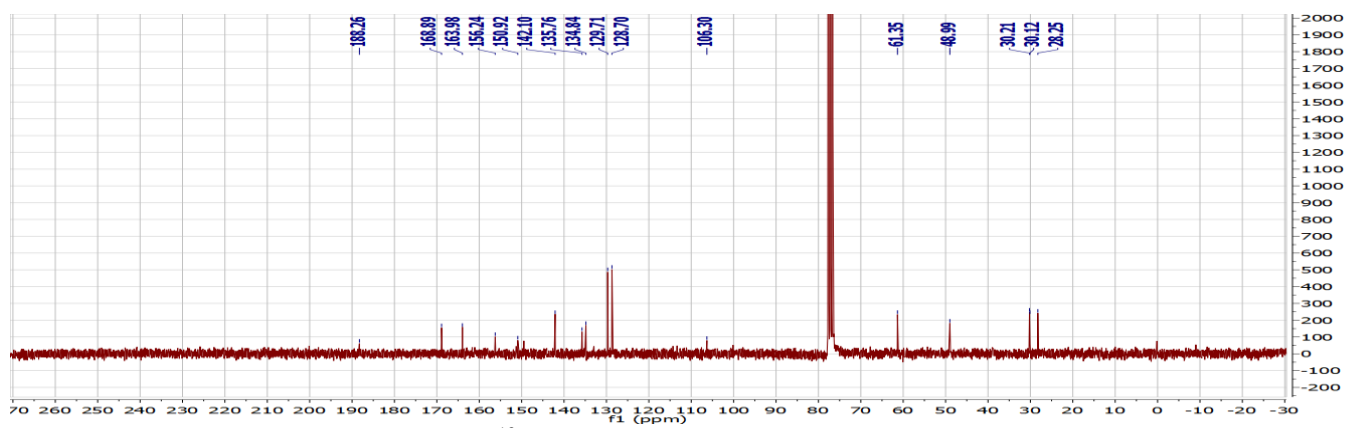
2-(4-Chlorophenyl)-3-[(1,3-dimethylxanthin-7-yl)acetamido]thiazolidine-4-one (6c)



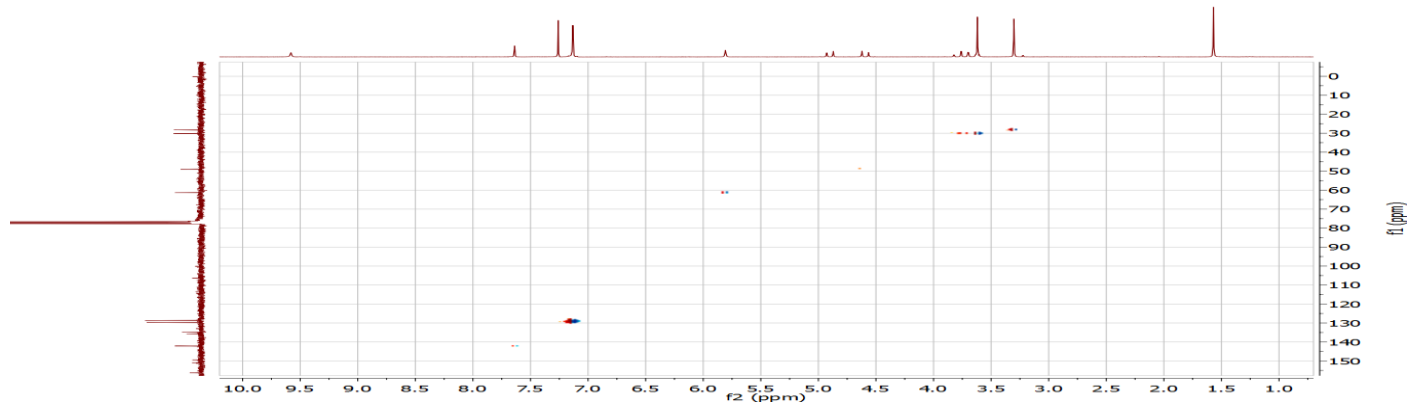
¹H-RMN spectra of **6c**



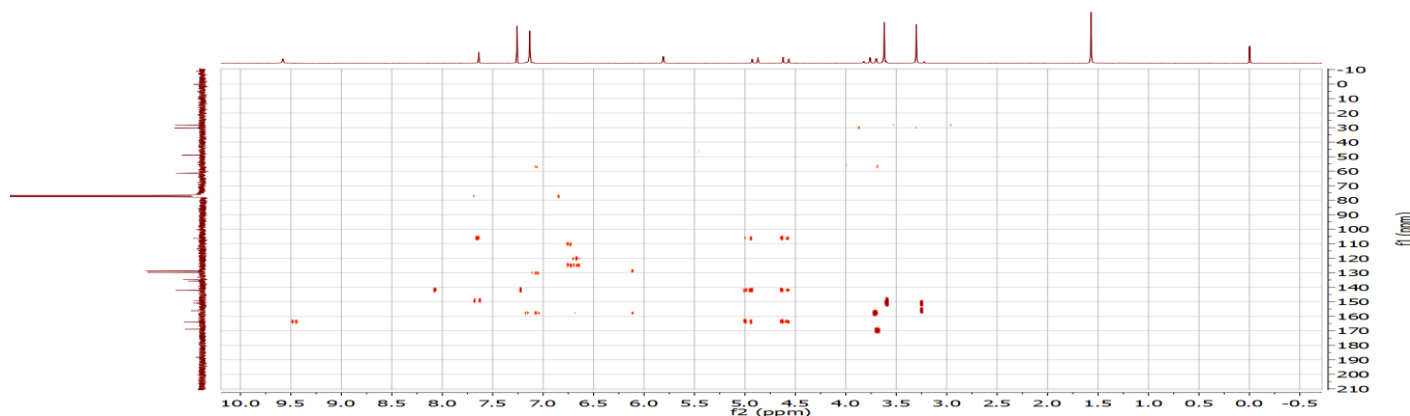
2D-COSY spectra of **6c**



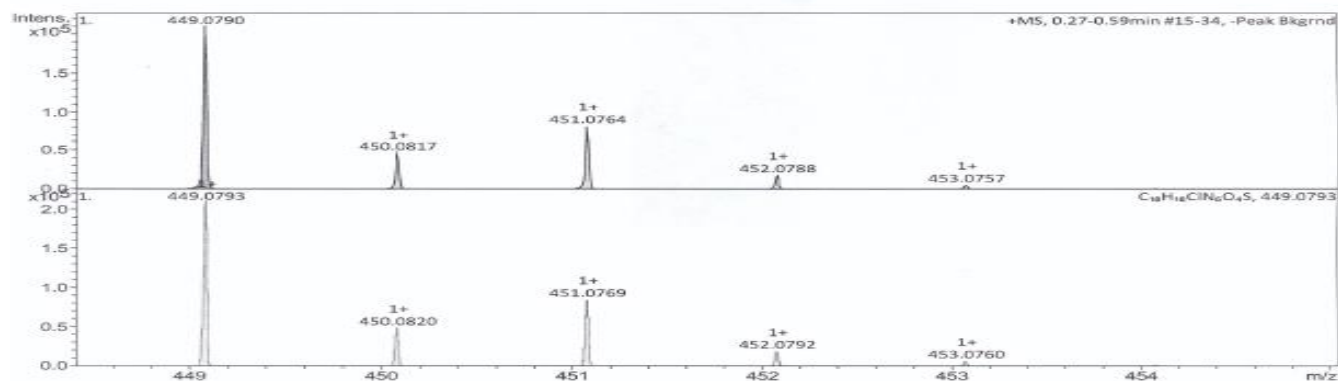
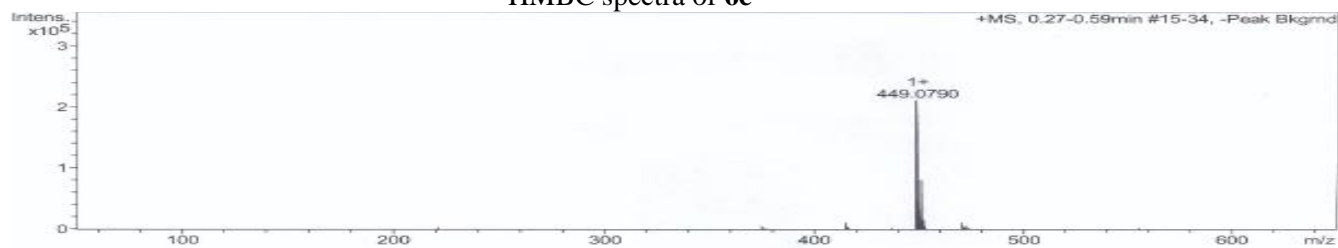
¹³C-RMN spectra of **6c**



HSQC spectra of **6c**



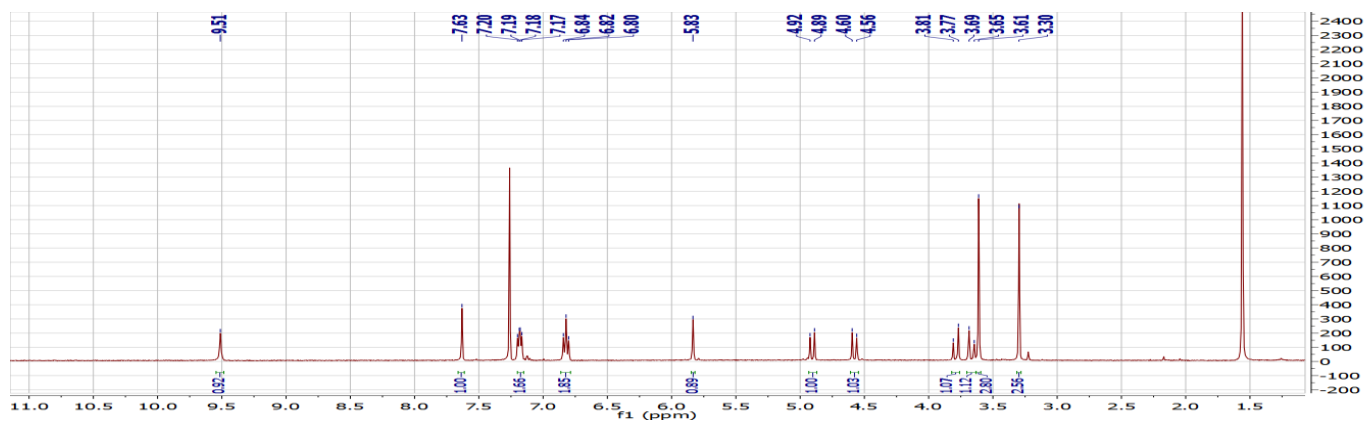
HMBC spectra of **6c**



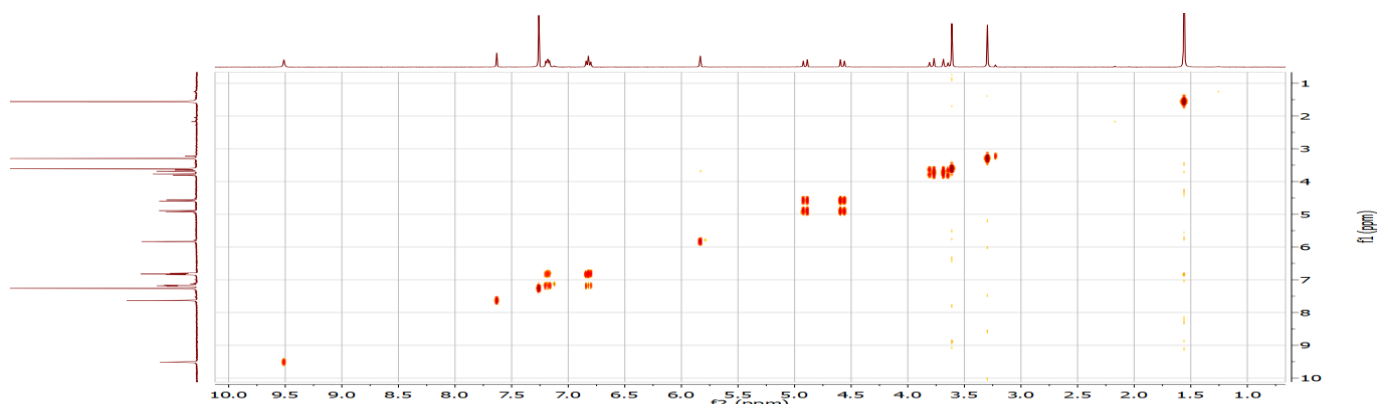
Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
415.117995	1+	1	C18H19N6O4S	415.118301	0.7	13.1	12.5	even
449.079004	1+	1	C18H18ClN6O4S	449.079328	-0.7	7.8	12.5	even

HRMS spectra of **6c**

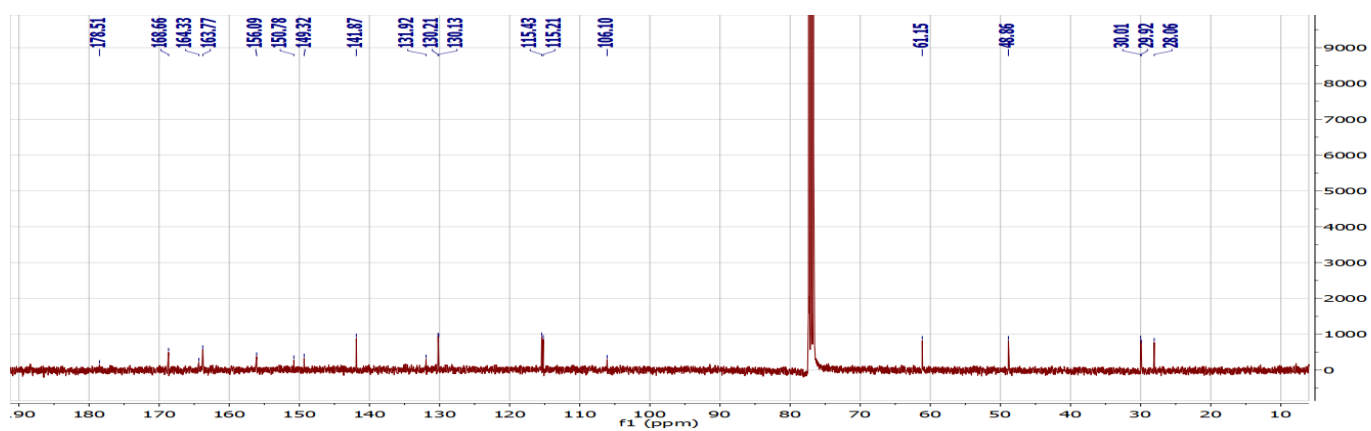
2-(4-Fluorophenyl)-3-[(1,3-dimethylxanthin-7-yl)acethamido]thiazolidine-4-one (6d)



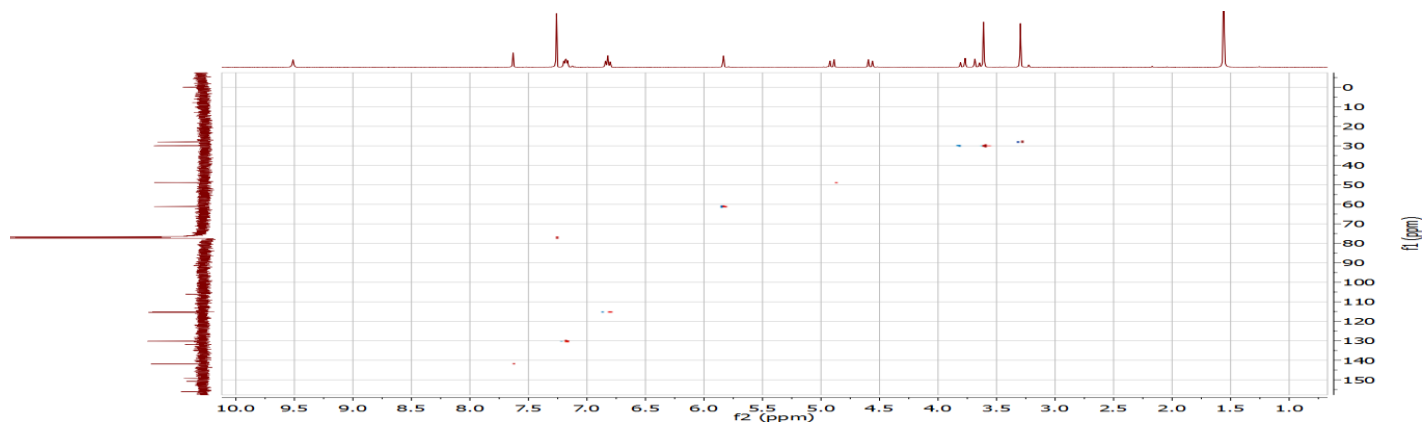
¹H-RMN spectra of **6d**



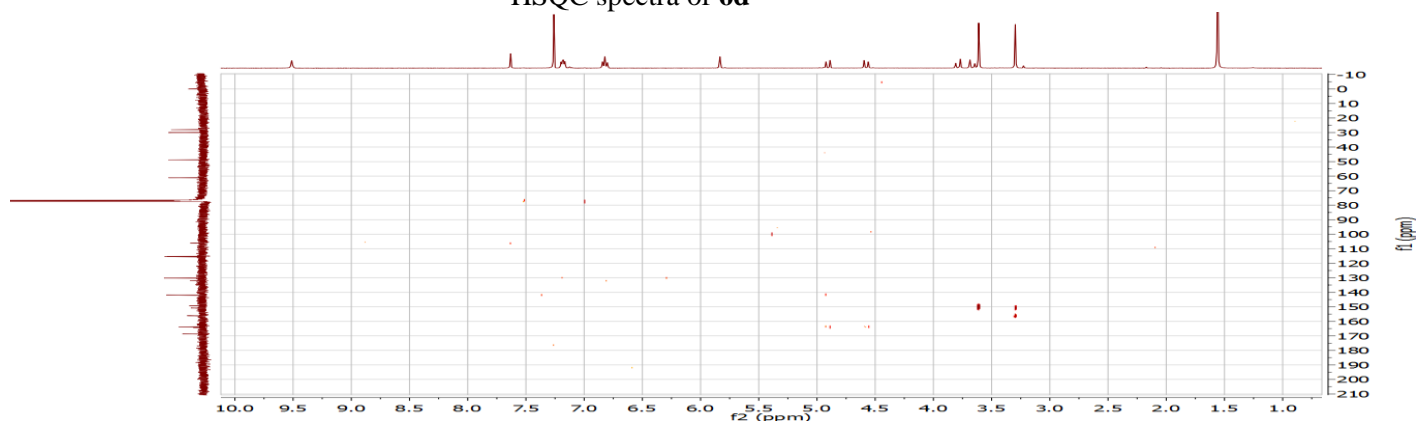
2D-COSY spectra of **6d**



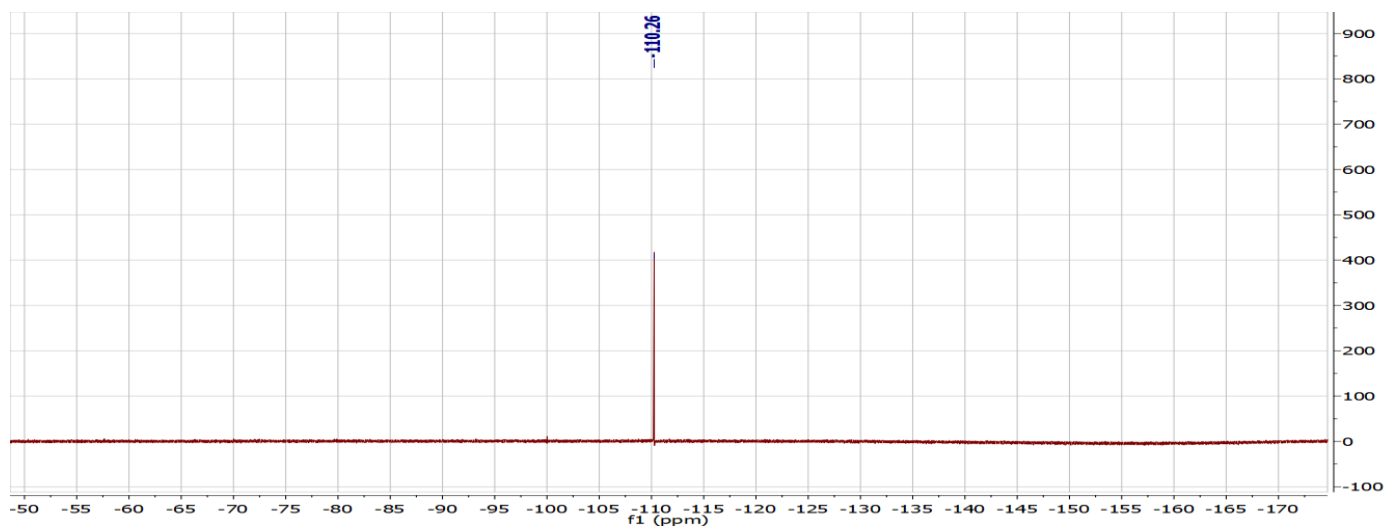
¹³C-RMN spectra of **6d**



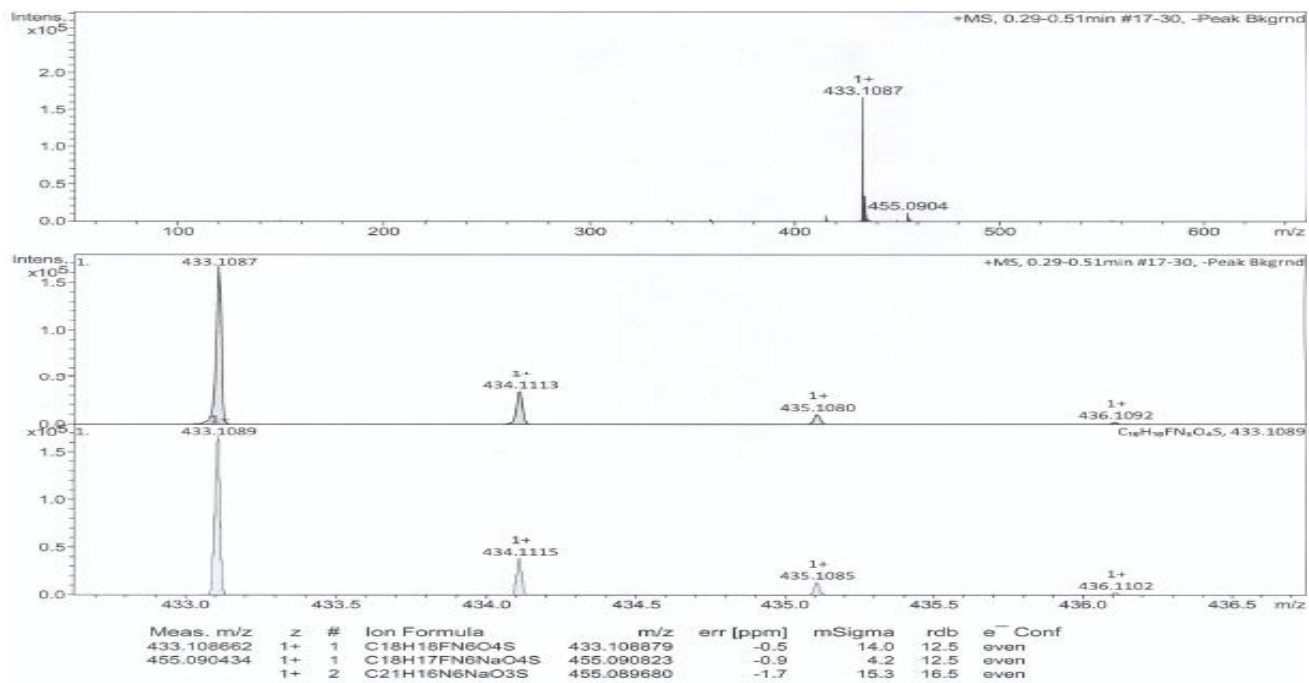
HSQC spectra of **6d**



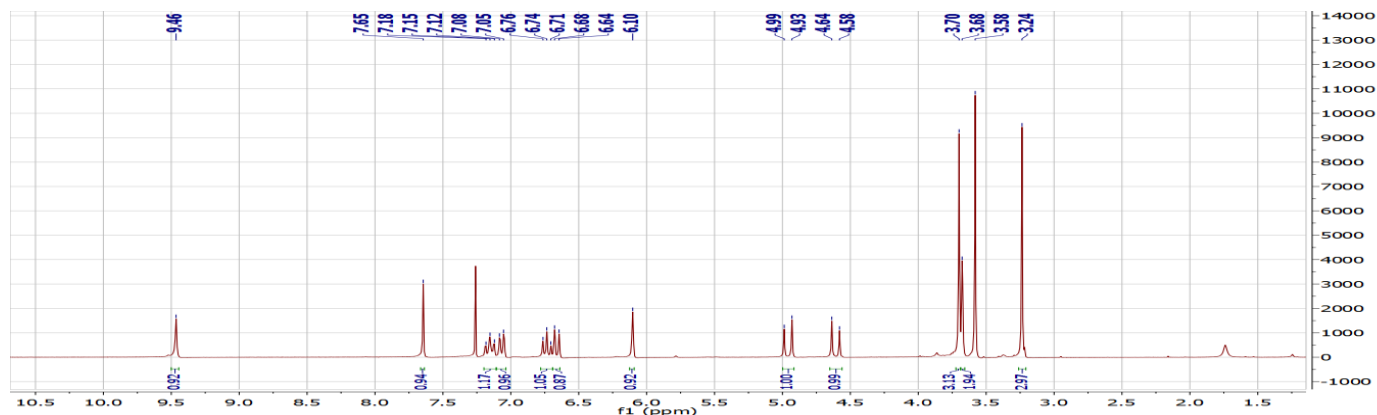
HMBC spectra of **6d**



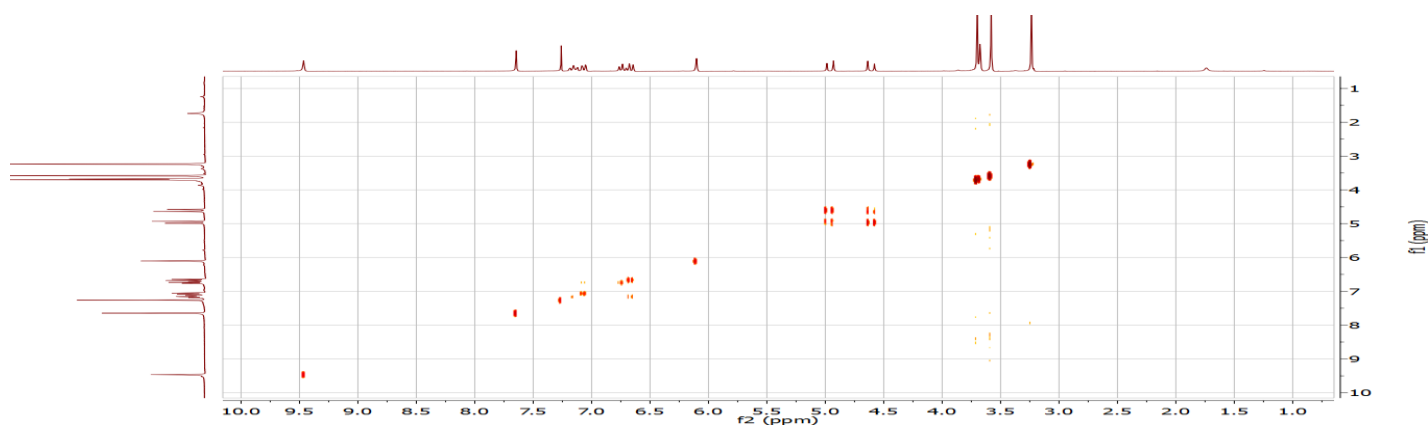
^{19}F -RMN spectra of **6f**



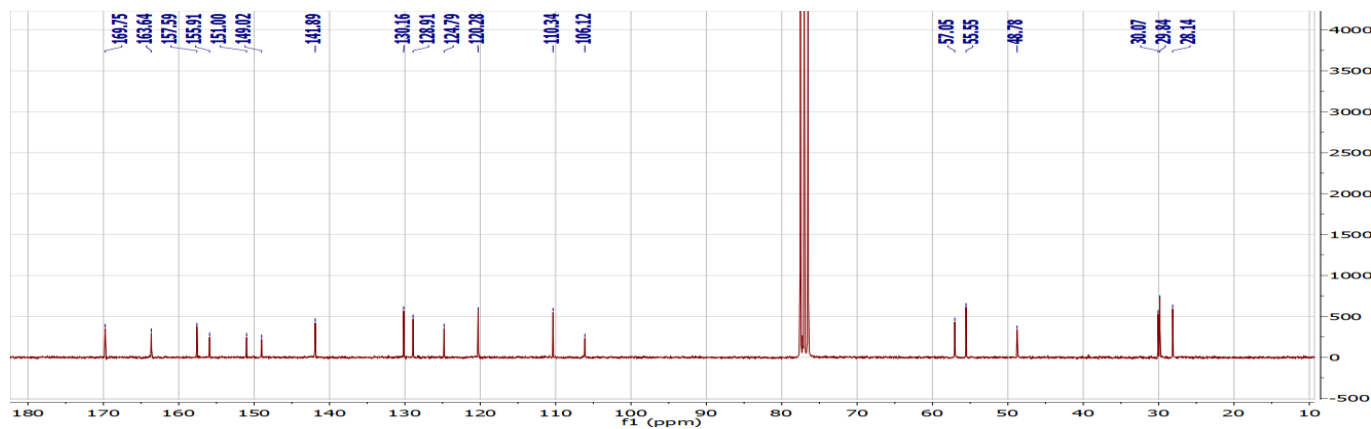
2-(2-Methoxyphenyl)-3-[(1,3-dimethylxanthin-7-yl)acetamido]thiazolidine-4-one (6e)



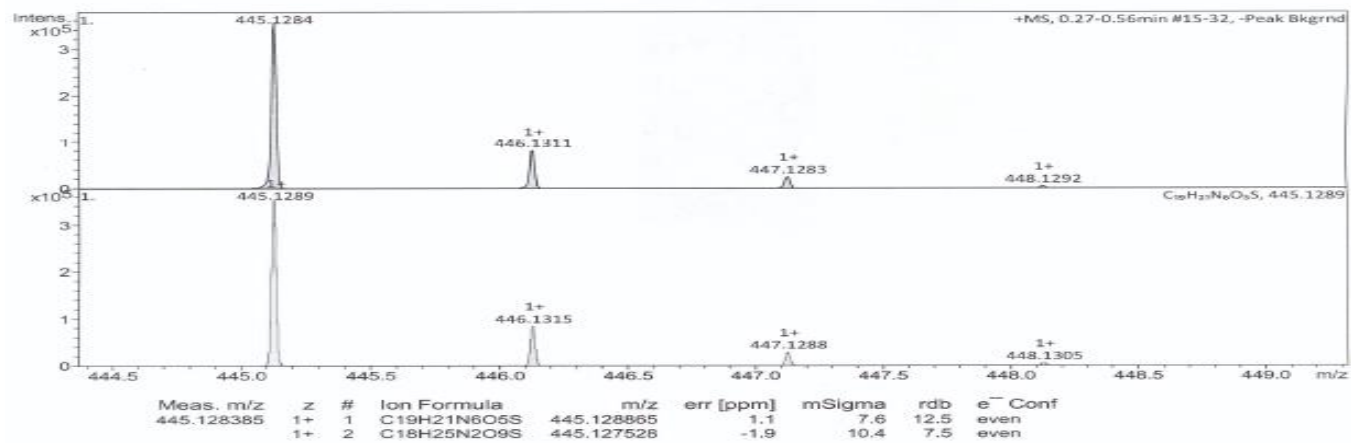
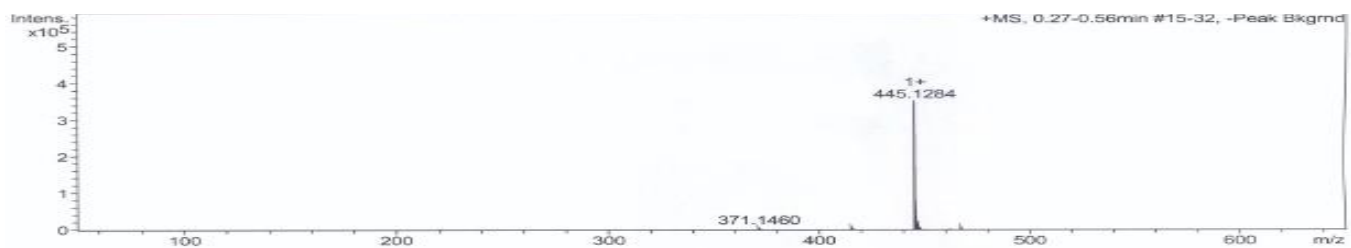
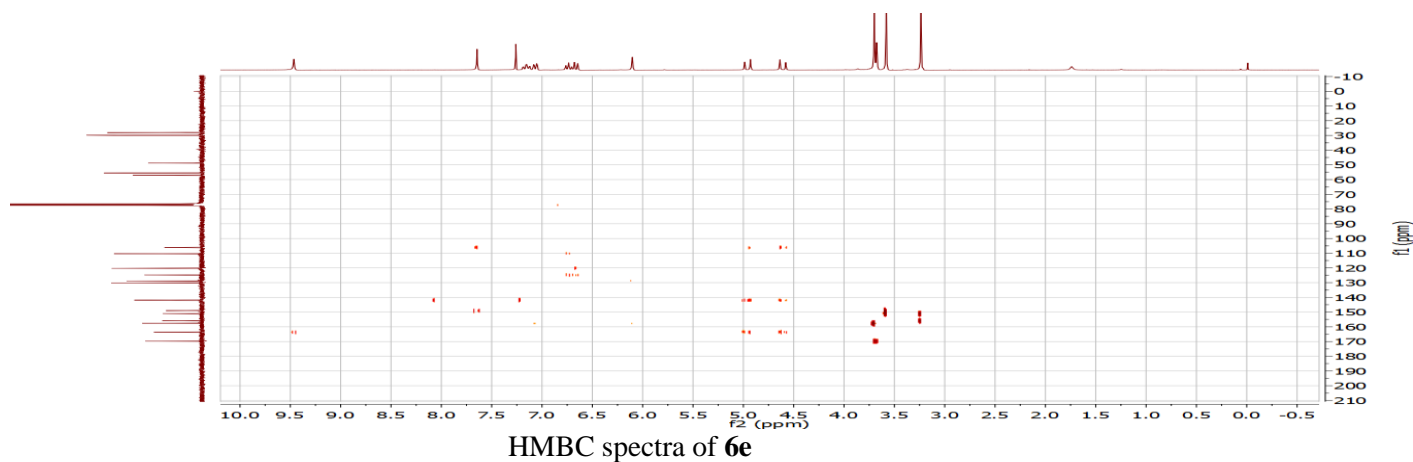
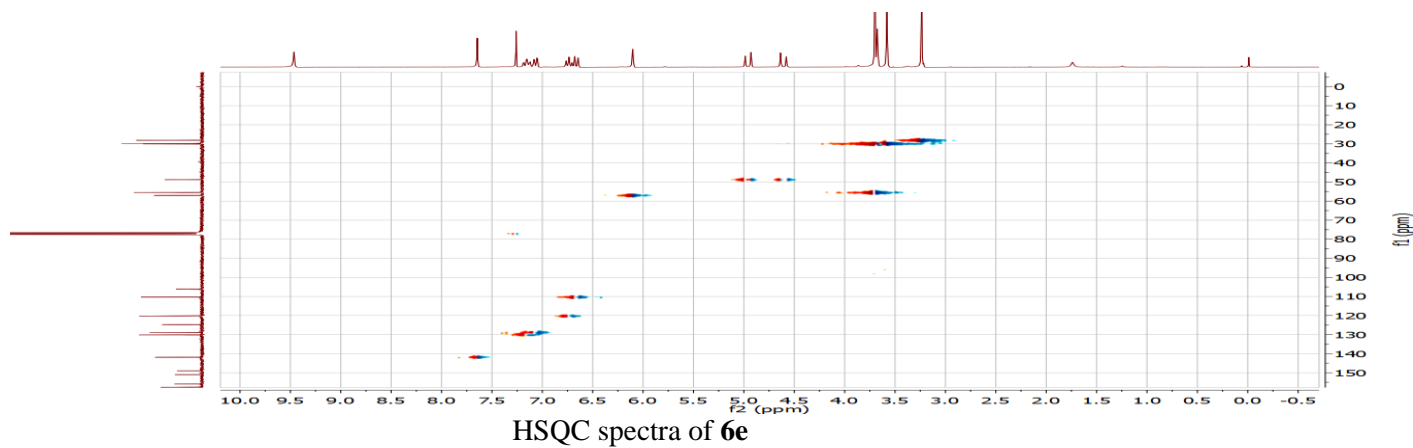
¹H-RMN spectra of **6e**



2D-COSY spectra of **6e**

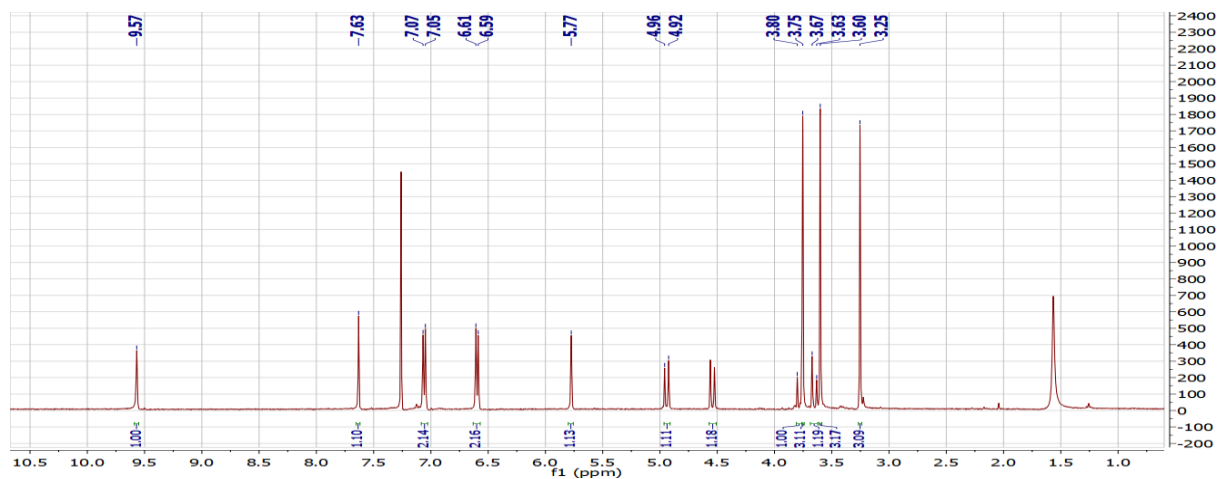


¹³C-RMN spectra of **6e**

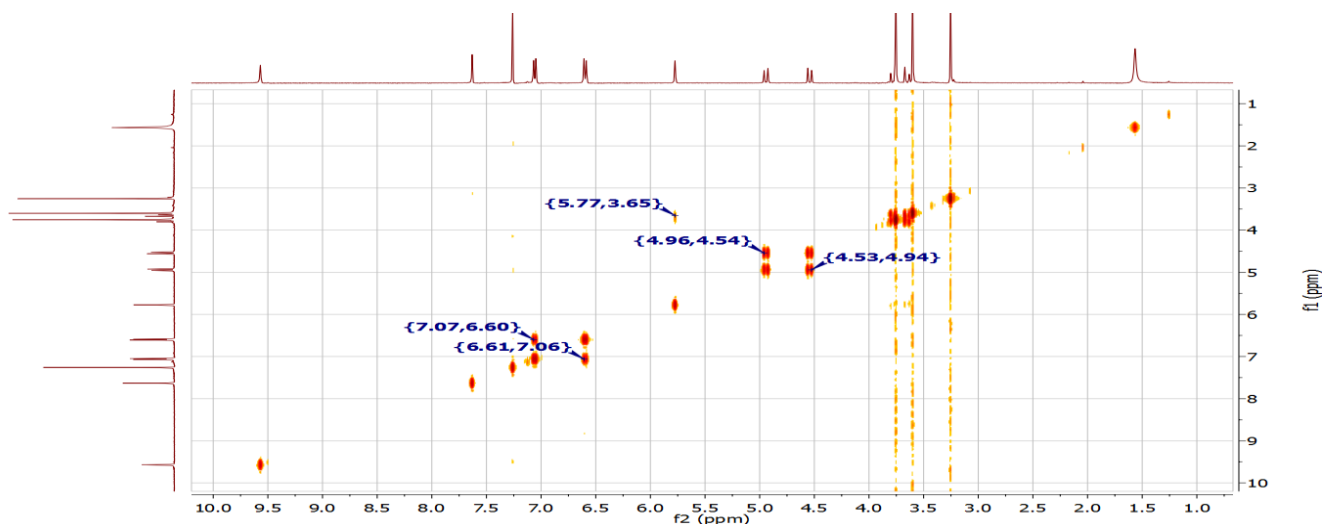


HRMS spectra of **6e**

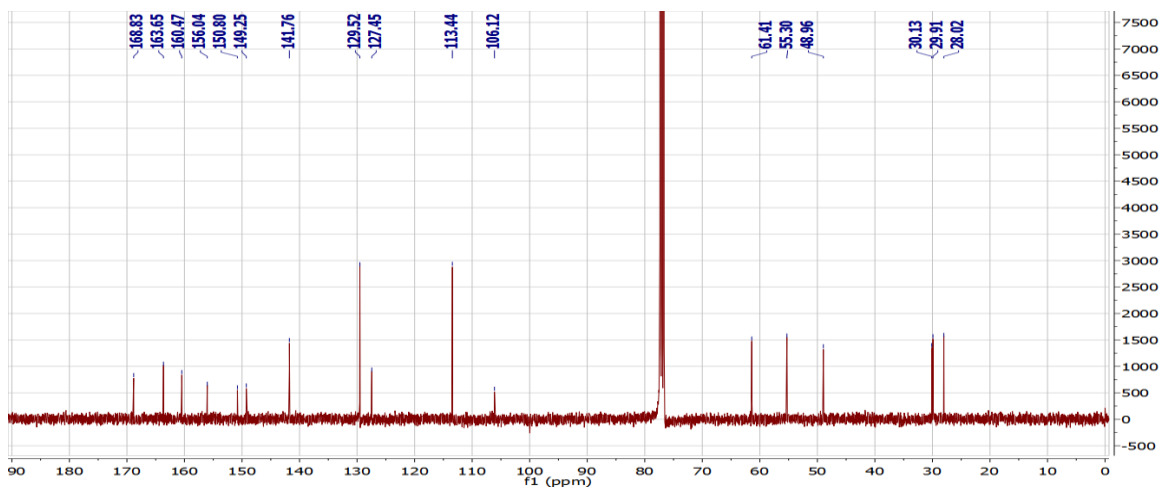
2-(4-Methoxyphenyl)-3-[(1,3-dimethylxanthin-7-yl)acethamido]thiazolidine-4-one (6f)



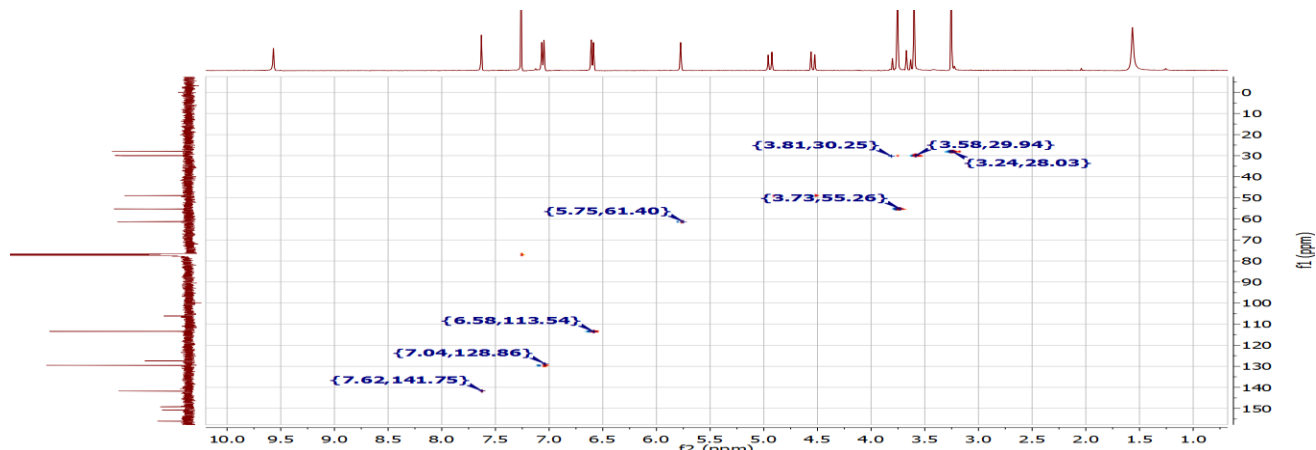
¹H-RMN spectra of **6f**



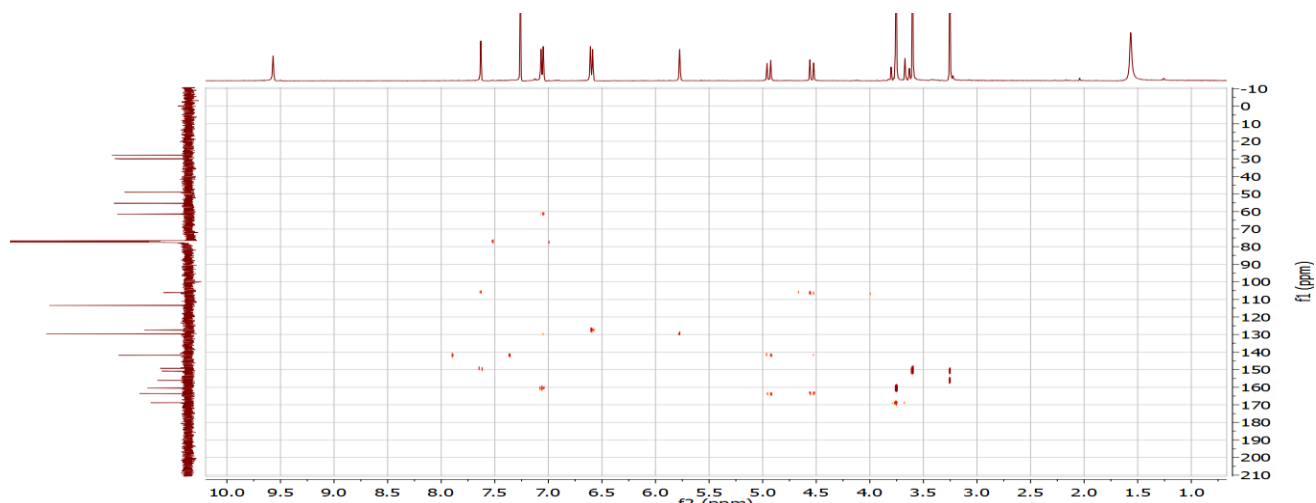
2D-COSY spectra of **6f**



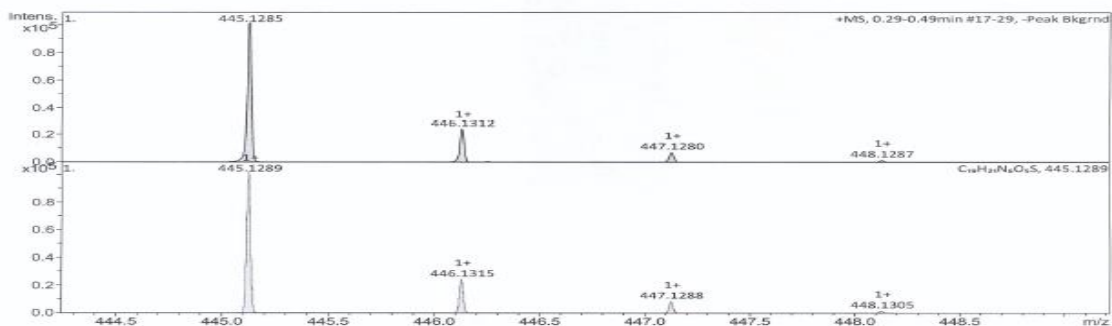
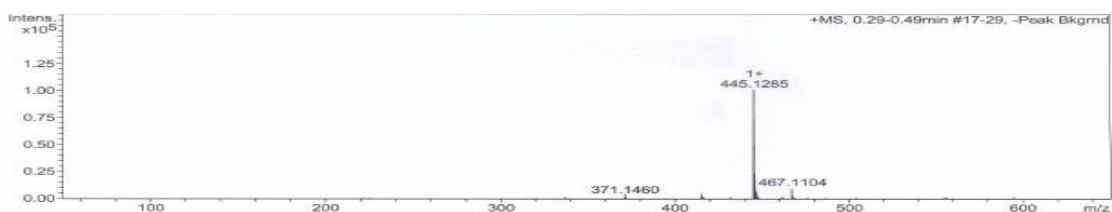
¹³C-RMN spectra of **6f**



HSQC spectra of **6f**



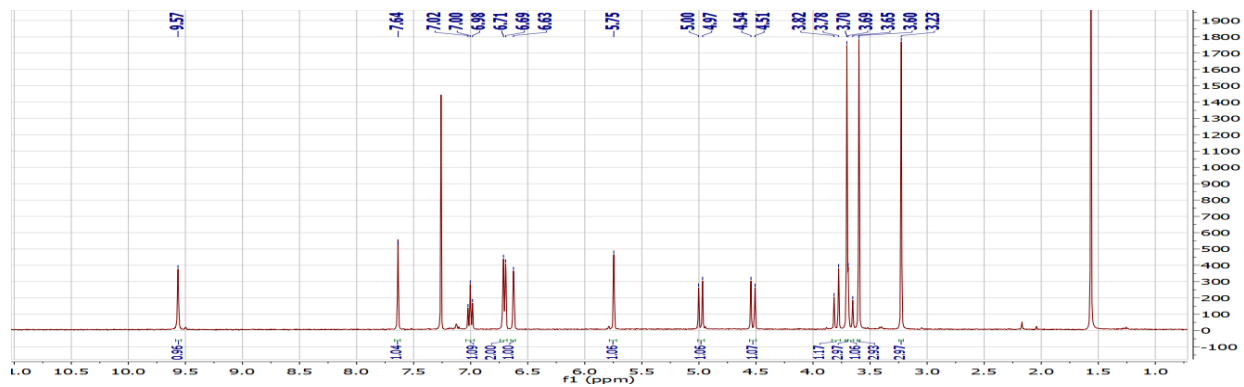
HMBC spectra of **6f**



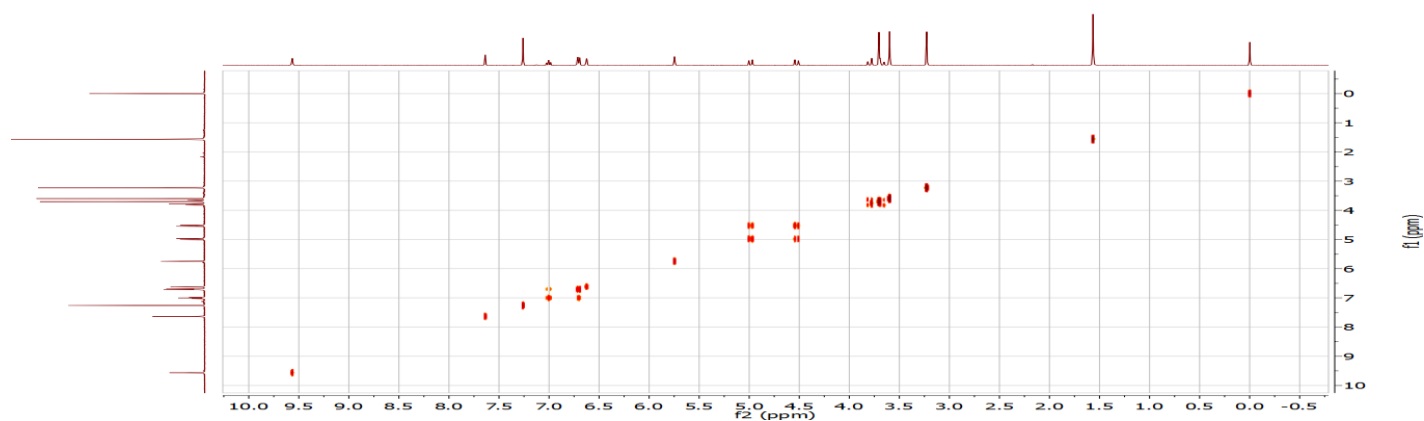
Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
445.128533	1+	1	C ₁₉ H ₂₁ N ₆ O ₅ S	445.128865	0.7	7.8	12.5	even
467.110416	1+	1	C ₁₉ H ₂₀ N ₆ NaO ₅ S	467.110609	-0.8	4.3	12.5	even

HRMS spectra for **6f**

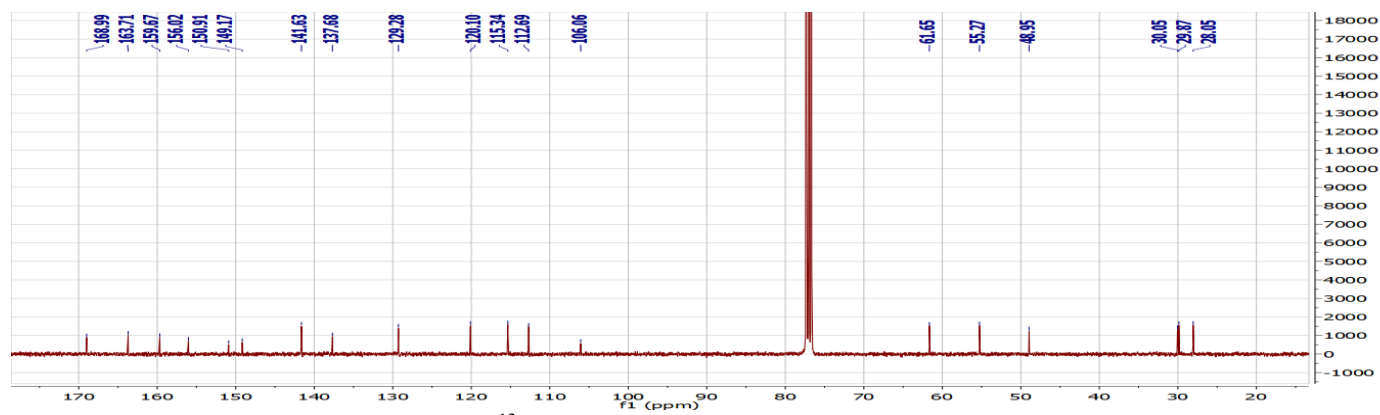
2-(3-Methoxyphenyl)-3-[(1,3-dimethylxanthin-7-yl)acetamido]thiazolidine-4-one (6g)



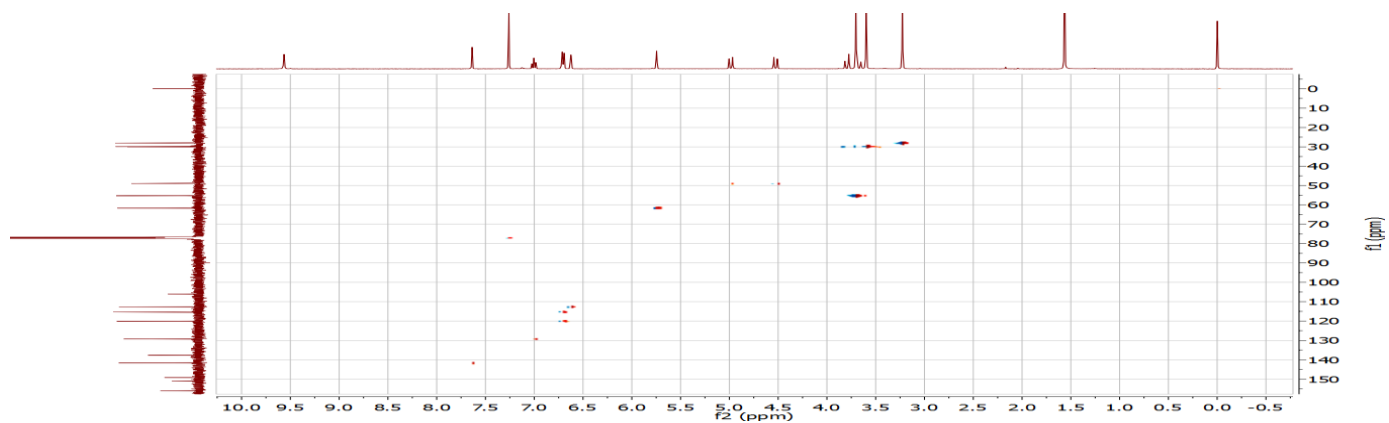
¹H-RMN spectra of 6g



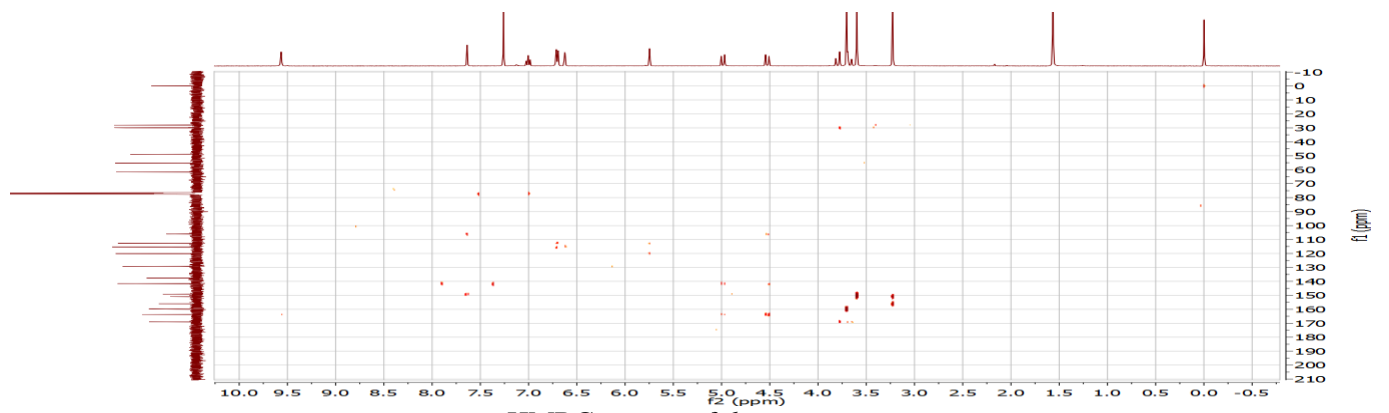
2D-COSY spectra of 6g



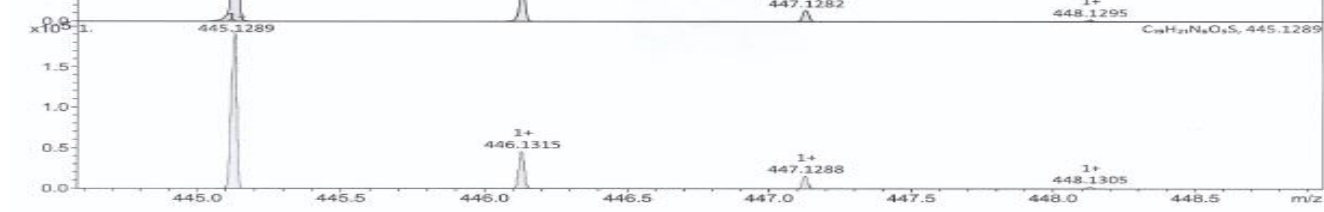
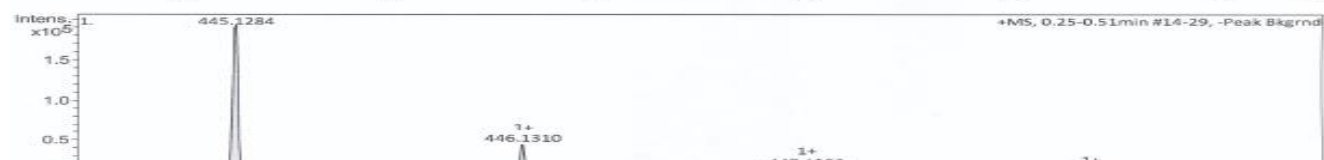
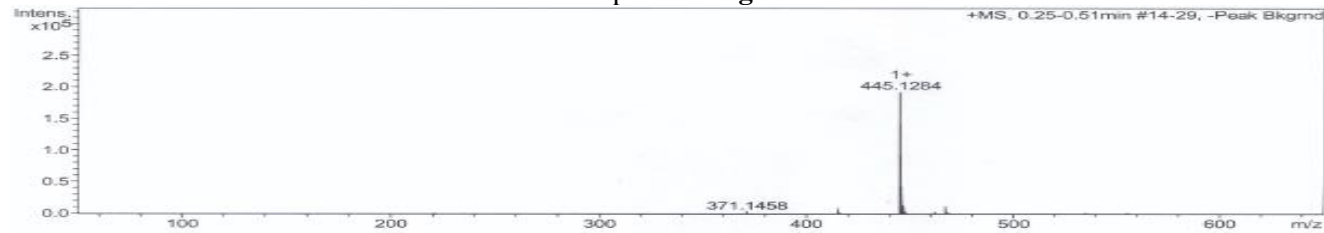
¹³C-RMN spectra of 6g



HSQC spectra of **6g**



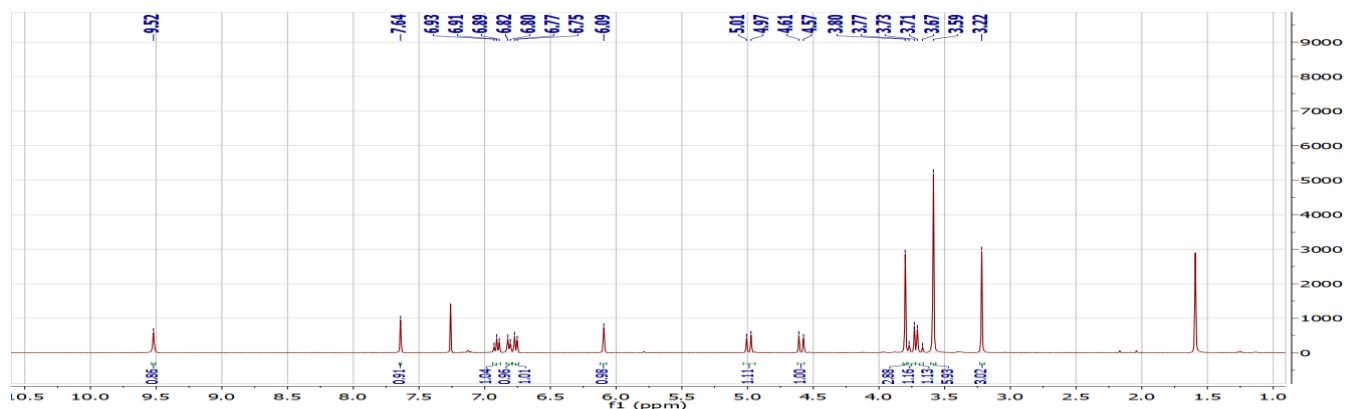
HMBC spectra of **6g**



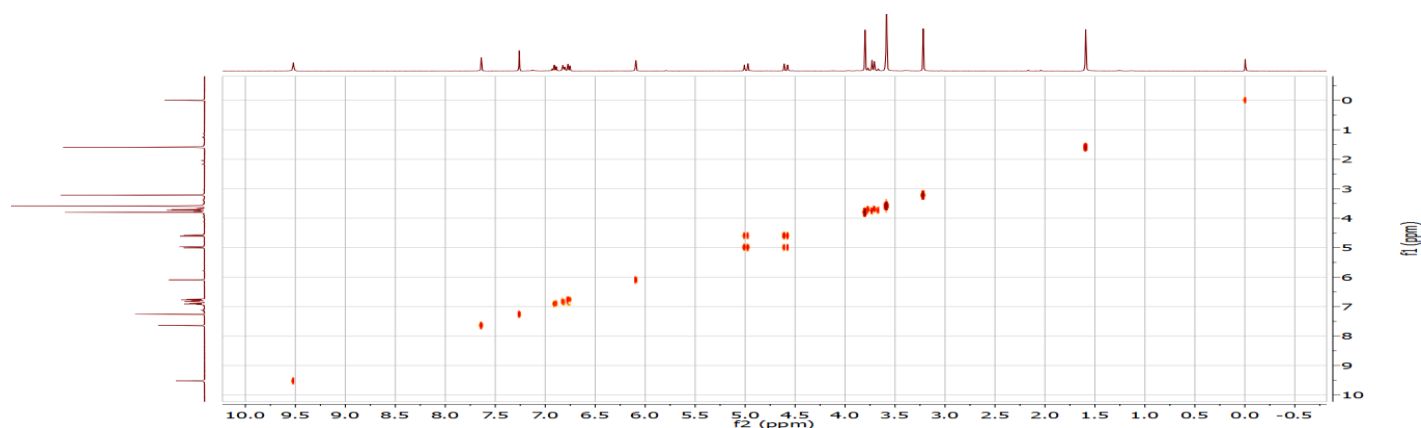
Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
445.128366	1+	1	C ₁₉ H ₂₁ N ₆ O ₅ S	445.128865	-1.1	7.5	12.5	even
467.110205	1+	2	C ₁₈ H ₂₅ N ₂ O ₉ S	445.127528	-1.9	10.0	7.5	even
	1+	1	C ₁₈ H ₂₄ N ₂ NaO ₉ S	467.109472	1.6	12.2	7.5	even
	1+	2	C ₁₉ H ₂₀ N ₆ NaO ₅ S	467.110809	1.3	16.0	12.5	even

HRMS spectra of **6g**

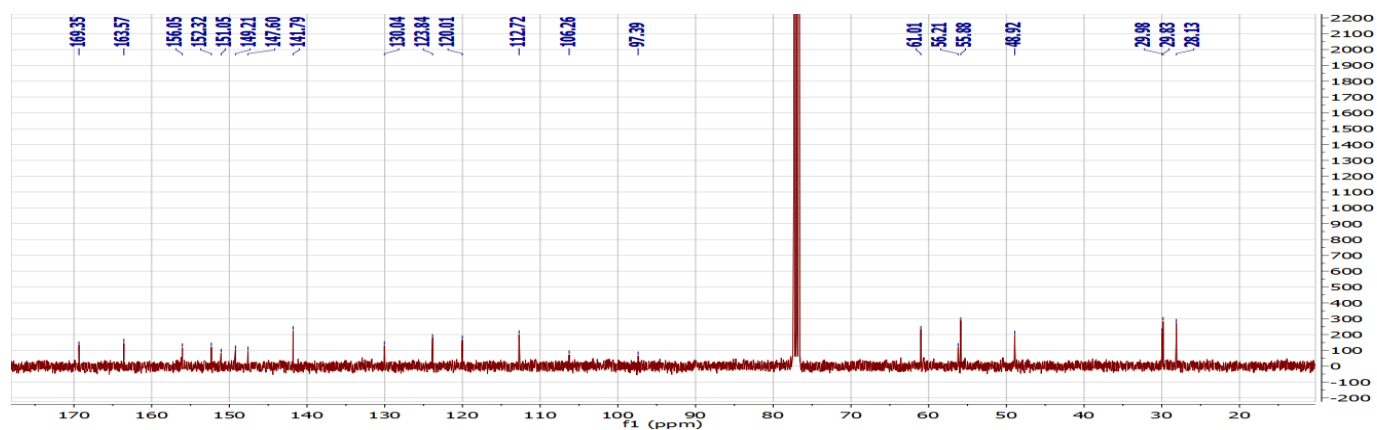
2-(2,3-Dimethoxyphenyl)-3-[(1,3-dimethylxanthin-7-yl)acetamido]thiazolidine-4-one (6h)



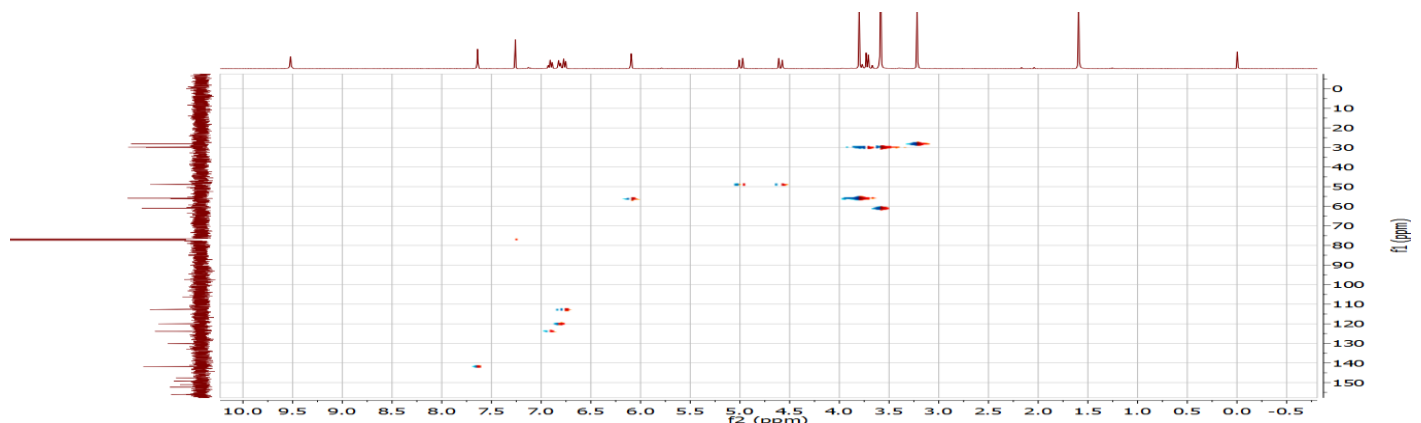
¹H-RMN spectra of **6h**



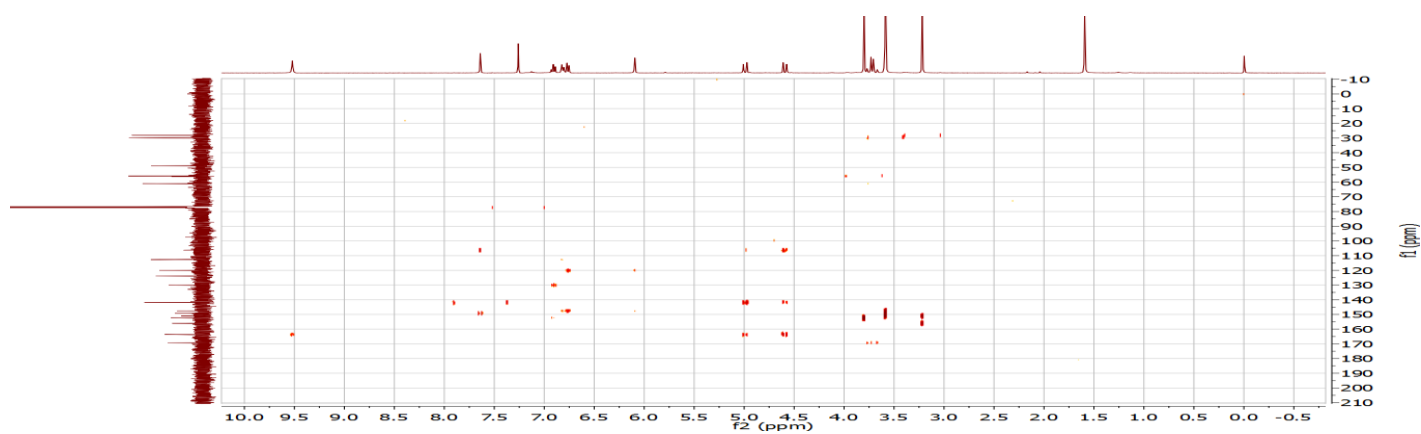
2D-COSY spectra of **6h**



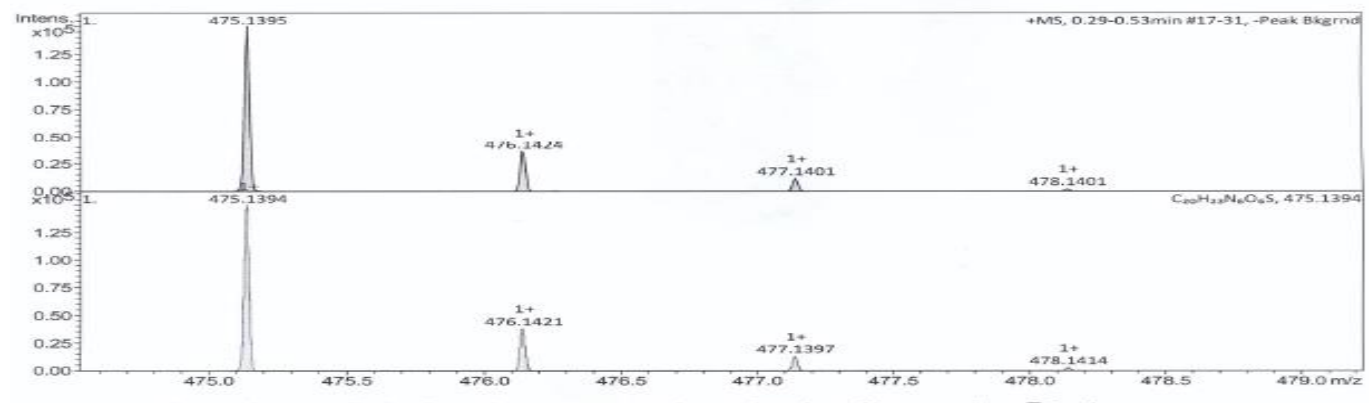
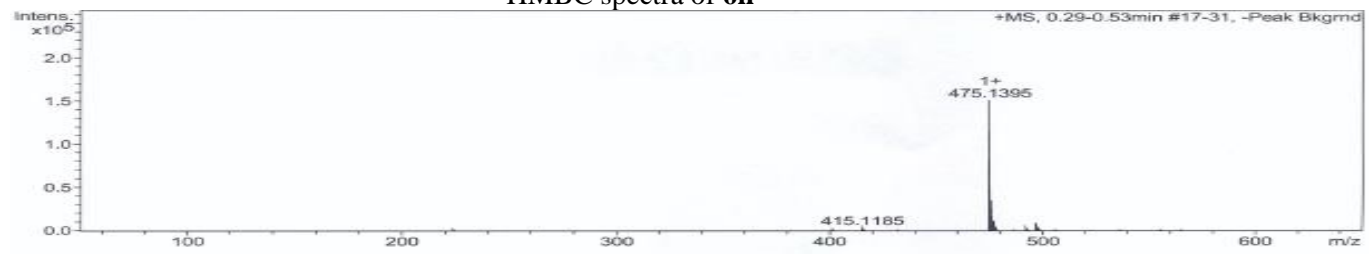
¹³C-RMN spectra of **6h**



HSQC spectra of **6h**



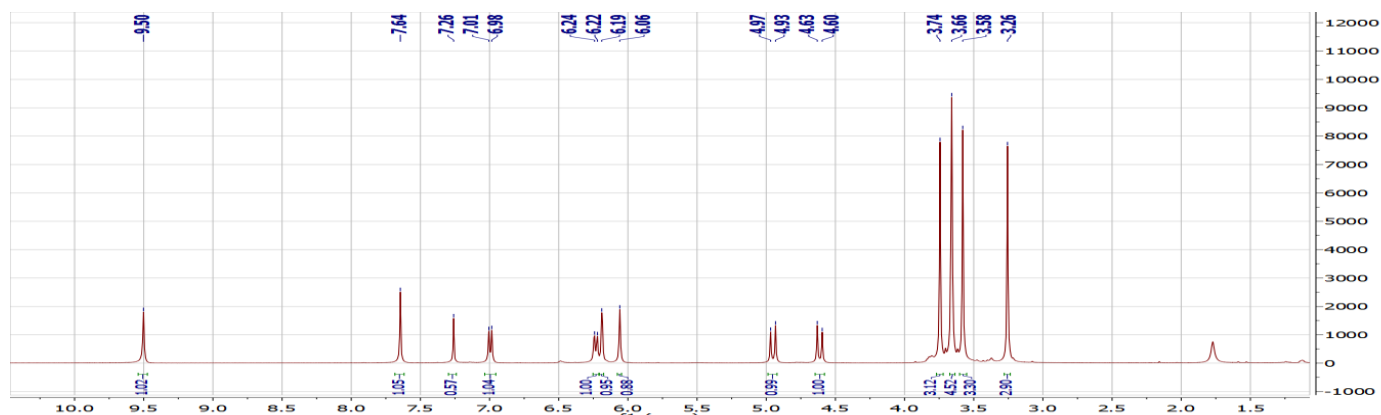
HMBC spectra of **6h**



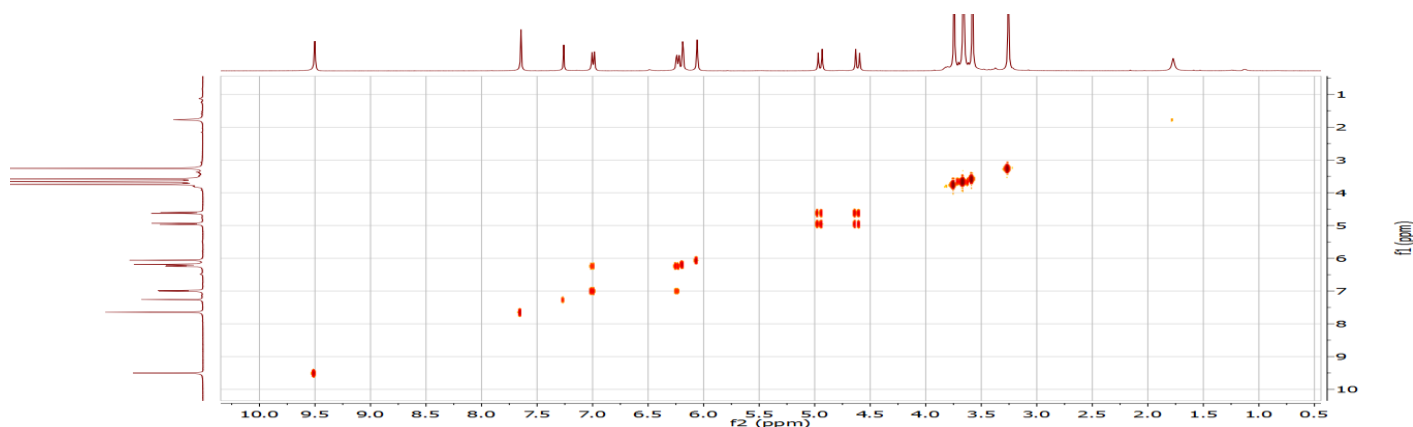
Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
415.118514	1+	1	C18H19N6O4S	415.118301	0.5	12.7	12.5	even
475.139544	1+	1	C20H23N6O6S	475.139430	-0.2	9.5	12.5	even
497.121583	1+	1	C20H22N6NaO6S	497.121374	-0.4	11.9	12.5	even

HRMS spectra of **6h**

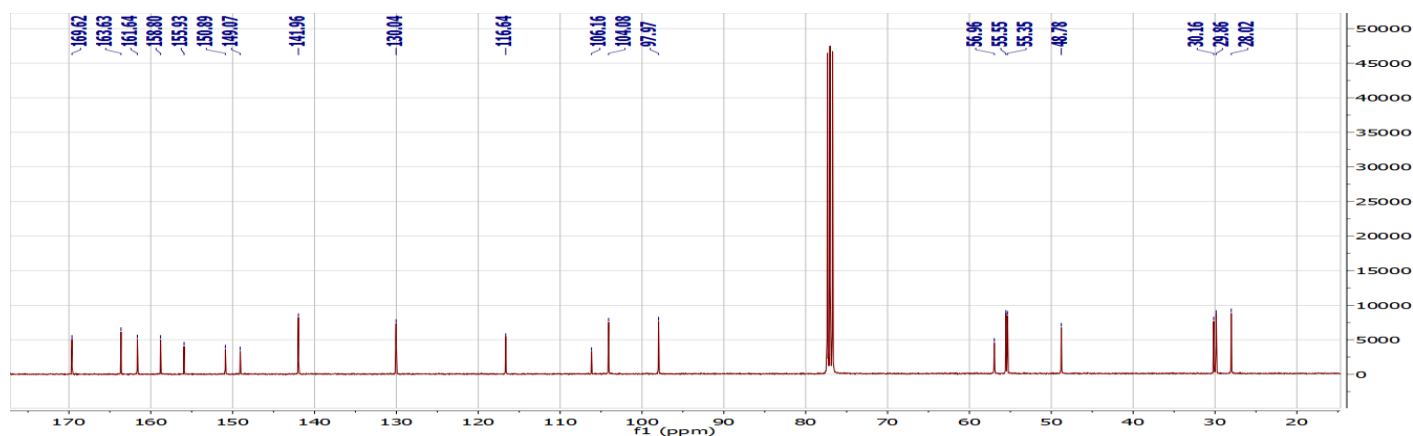
2-(2,4-Dimethoxyphenyl)-3-[(1,3-dimethylxanthin-7-yl)acethamido]thiazolidine-4-one (6i)



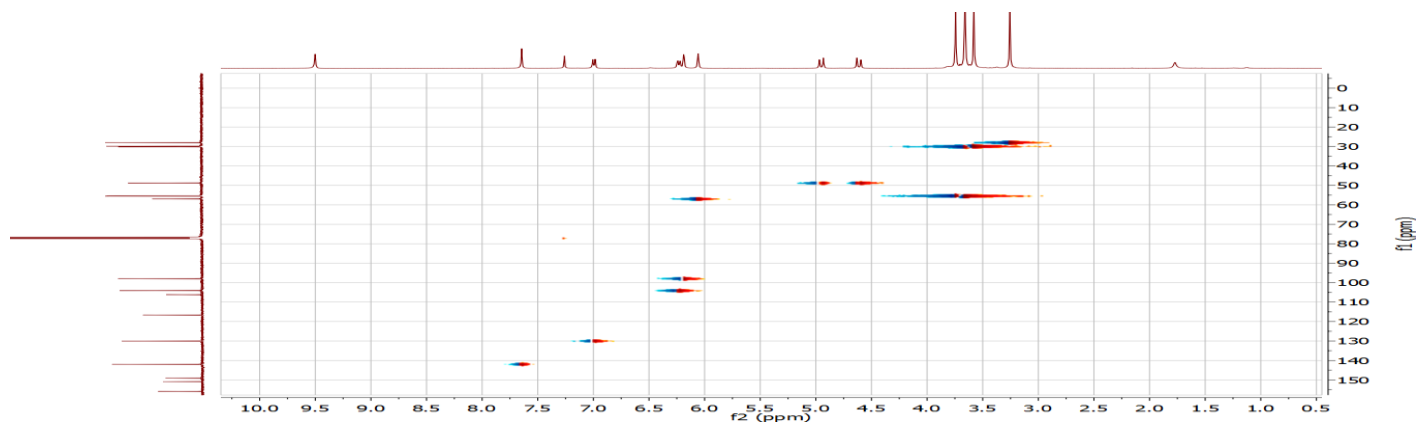
¹H-RMN spectra of **6i**



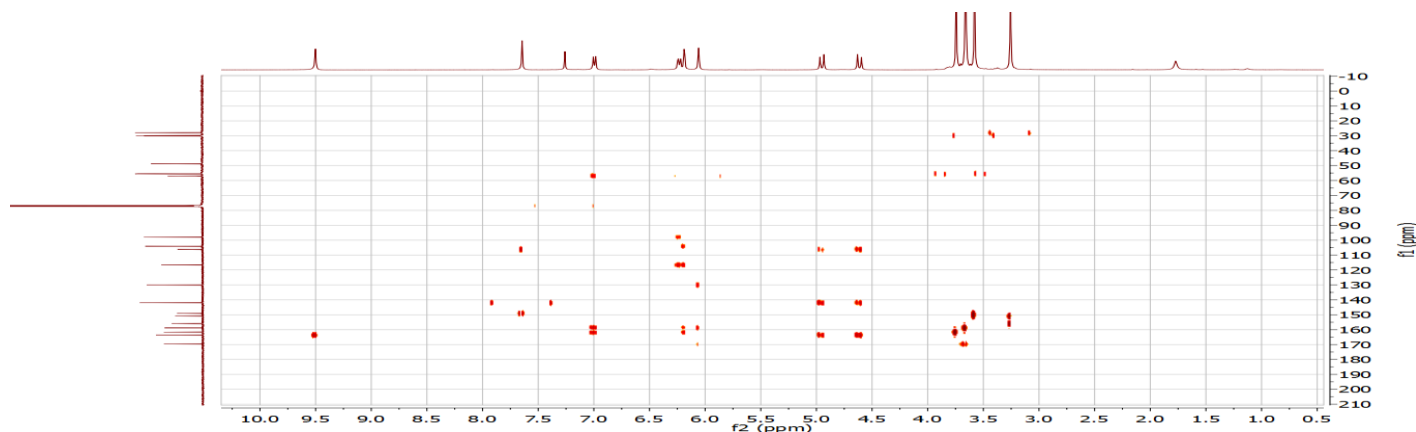
2D-COSY spectra of **6i**



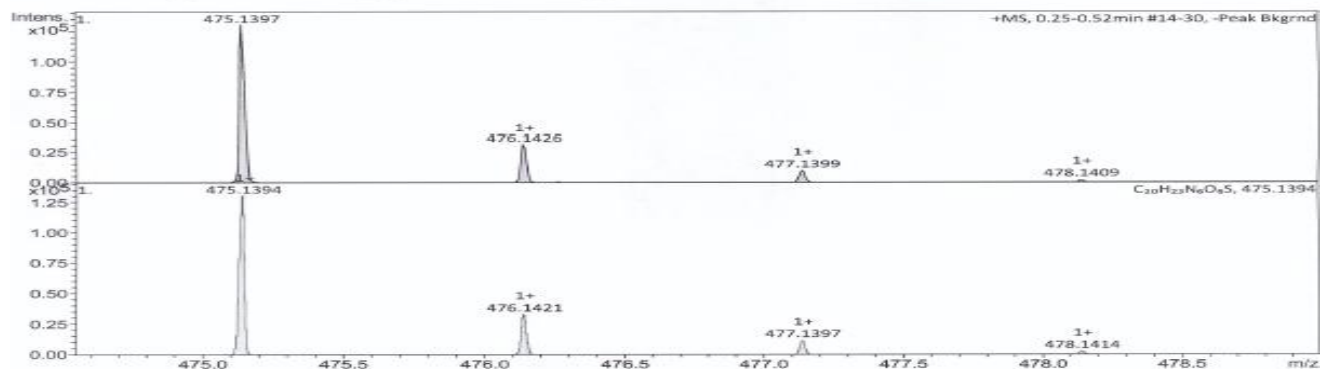
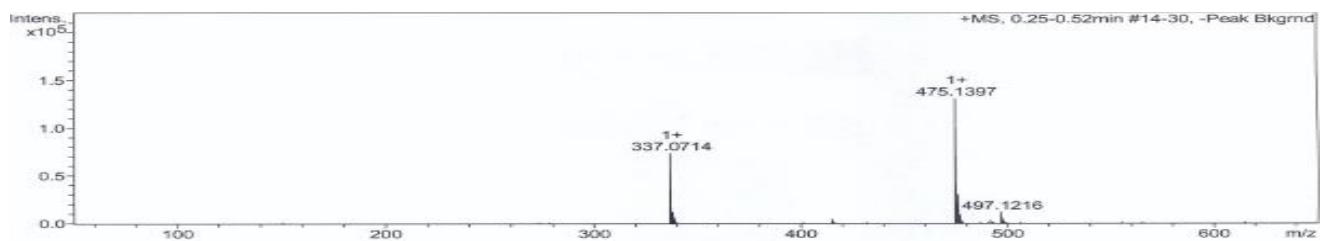
¹³C-RMN spectra of **6i**



HSQC spectra of **6i**



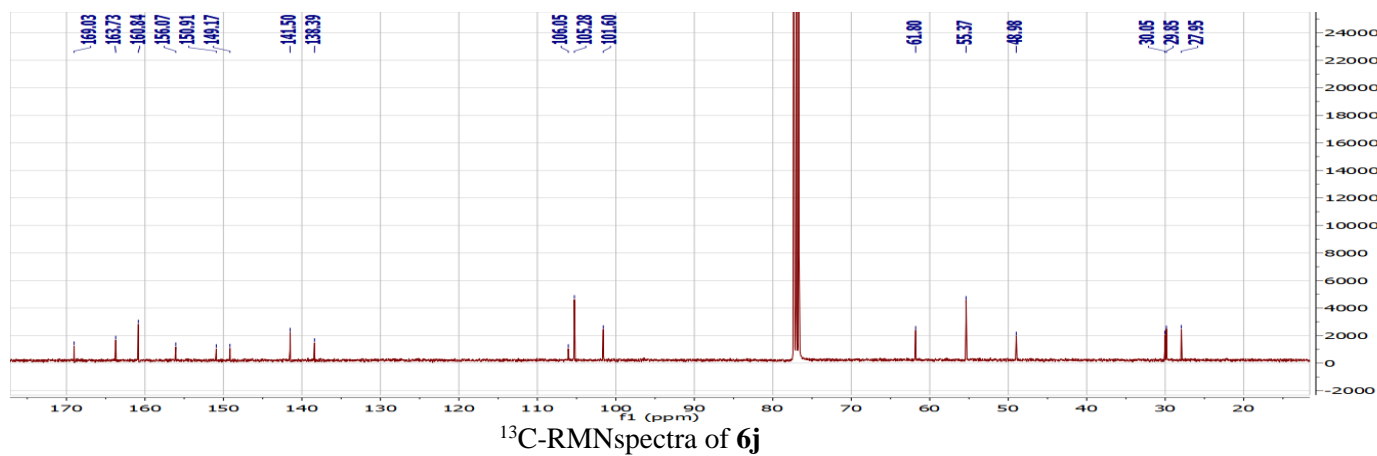
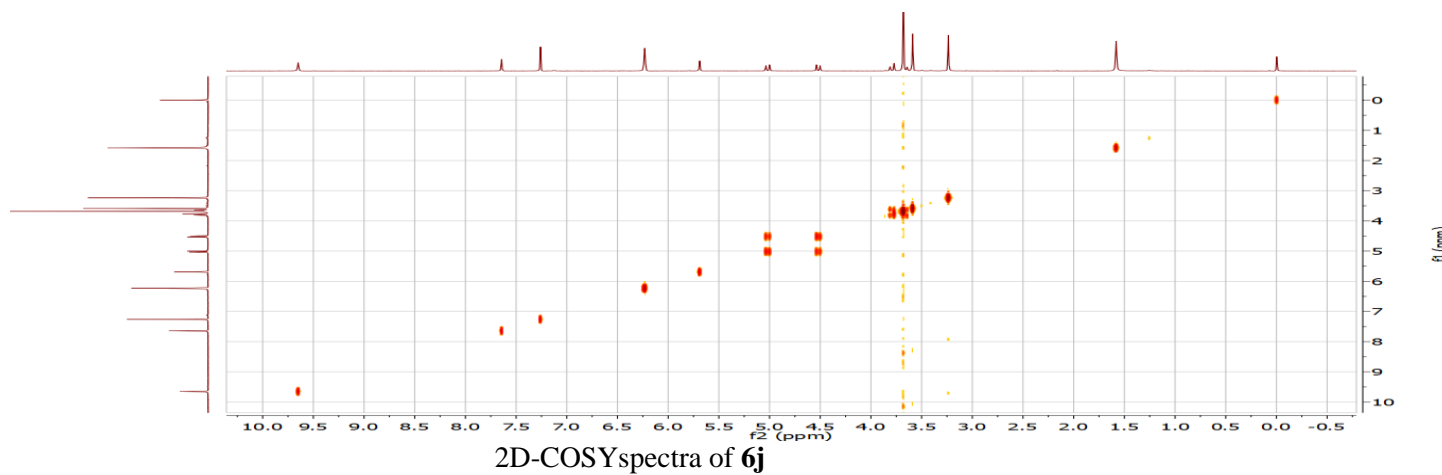
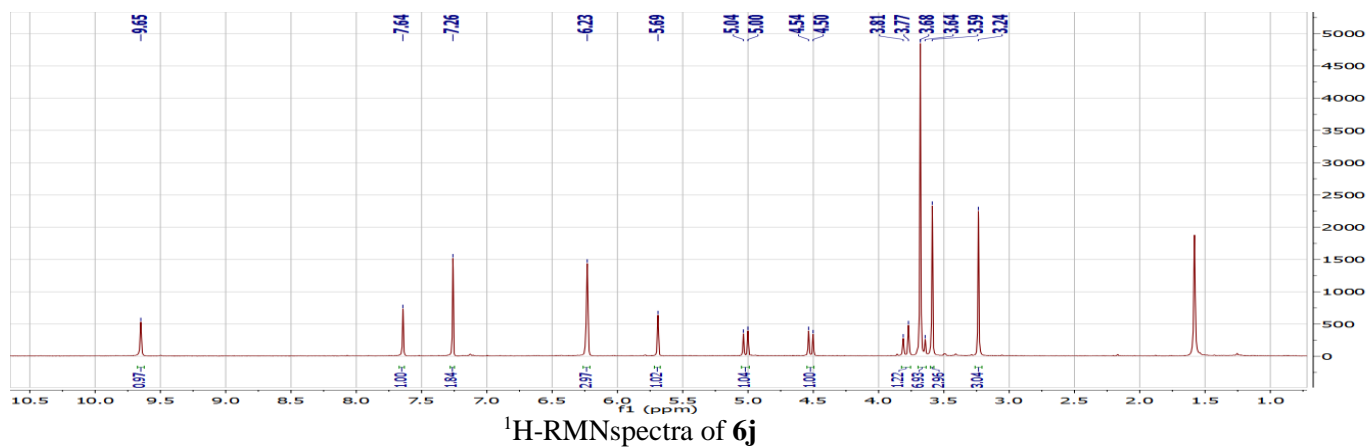
HMBC spectra of **6i**

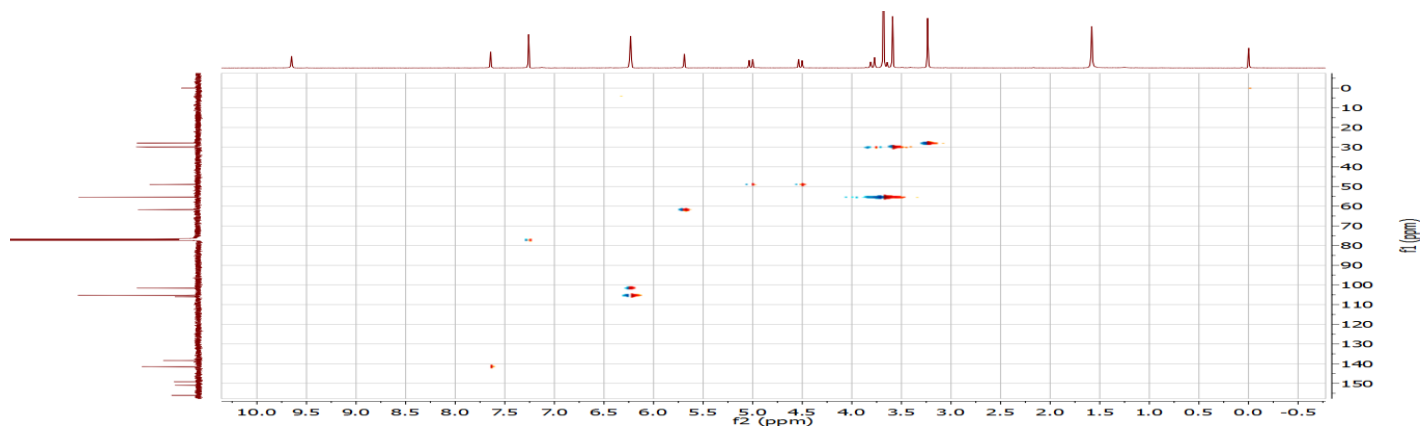


Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdB	e ⁻ Conf
337.071445	1+	1	C ₁₂ H ₁₃ N ₆ O ₄ S	337.071350	-0.3	6.0	9.5	even
475.139685	1+	1	C ₂₀ H ₂₃ N ₆ O ₆ S	475.139430	0.5	12.0	12.5	even
497.121569	1+	1	C ₂₀ H ₂₂ N ₆ NaO ₆ S	497.121374	-0.4	7.5	12.5	even

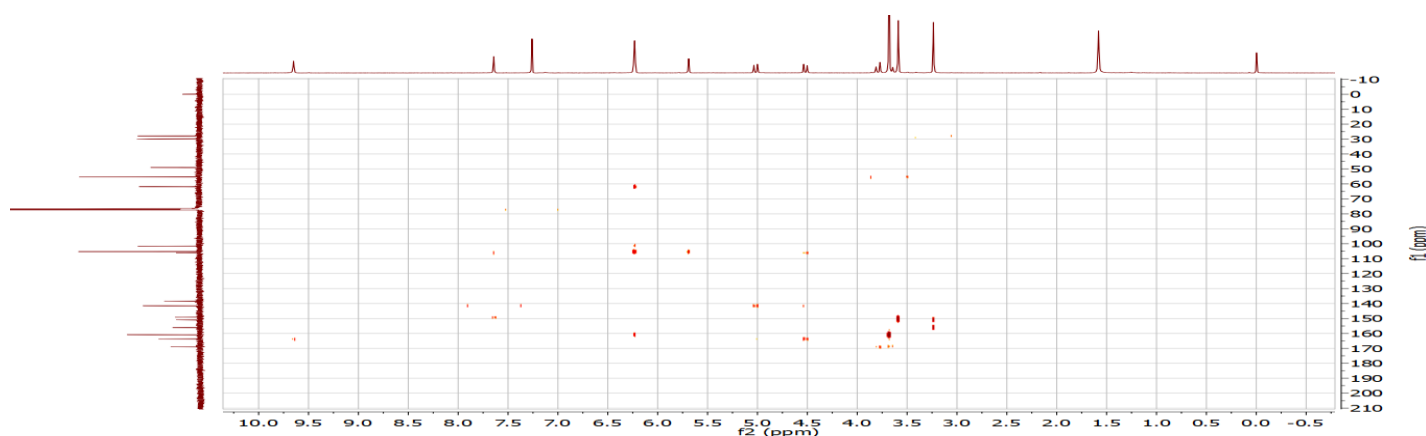
HRMS spectra of **6i**

2-(3,5-Dimethoxyphenyl)-3-[(1,3-dimethylxanthin-7-yl)acetamido]thiazolidine-4-one (6j)

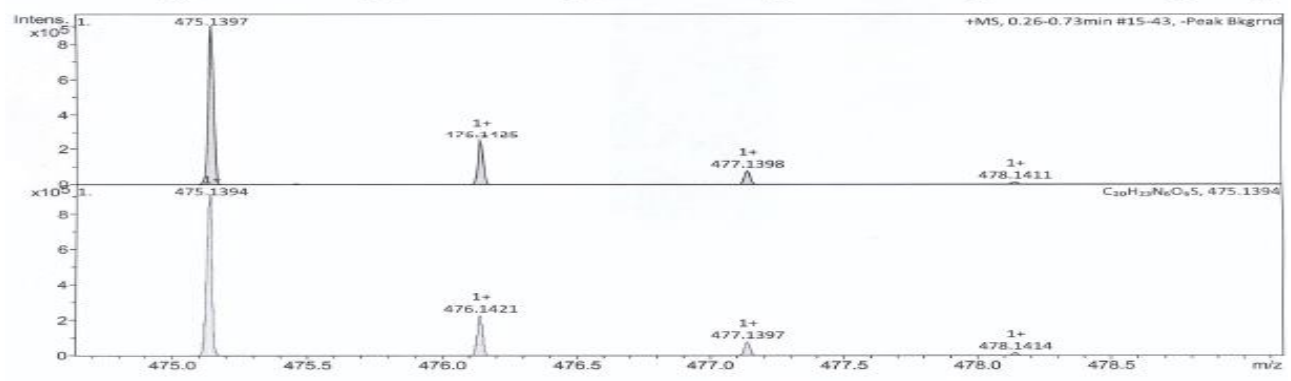
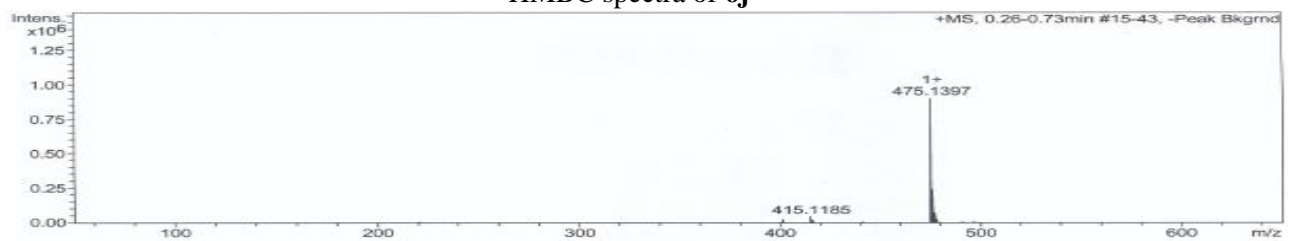




HSQC spectra of **6j**



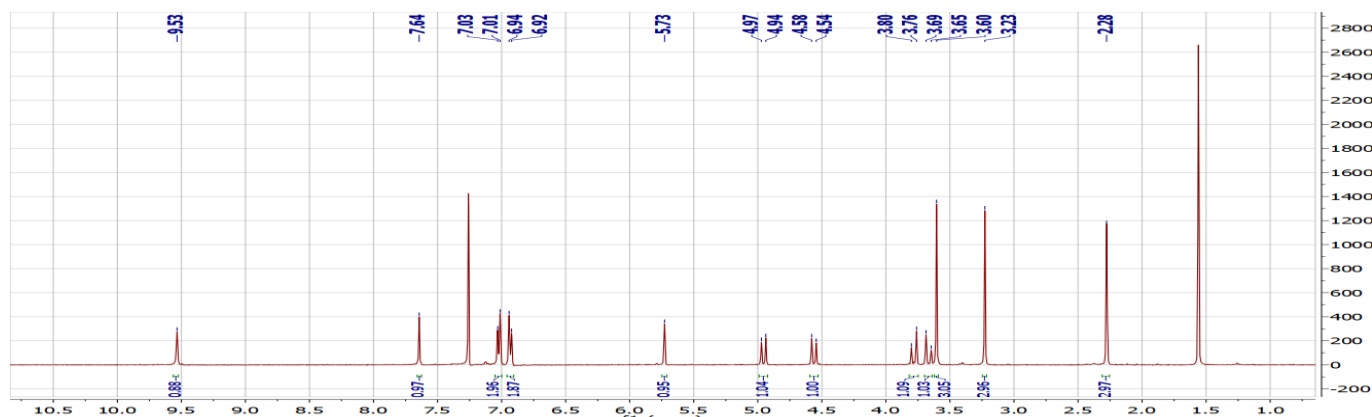
HMBC spectra of **6j**



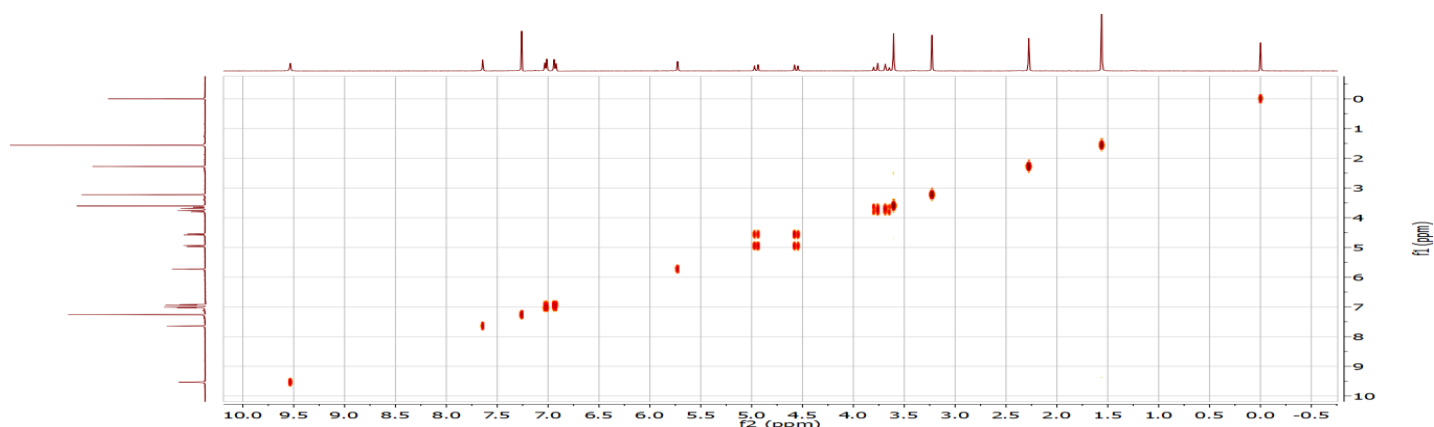
Meas. m/z	z	#	Ion Formula	m/z	err [ppm]	mSigma	rdb	e ⁻ Conf
415.118528	1+	1	C18H19N6O4S	415.118301	-0.5	11.0	12.5	even
475.139671	1+	1	C20H23N6O4S	475.139430	-0.5	11.3	12.5	even

HRMS spectra of **6j**

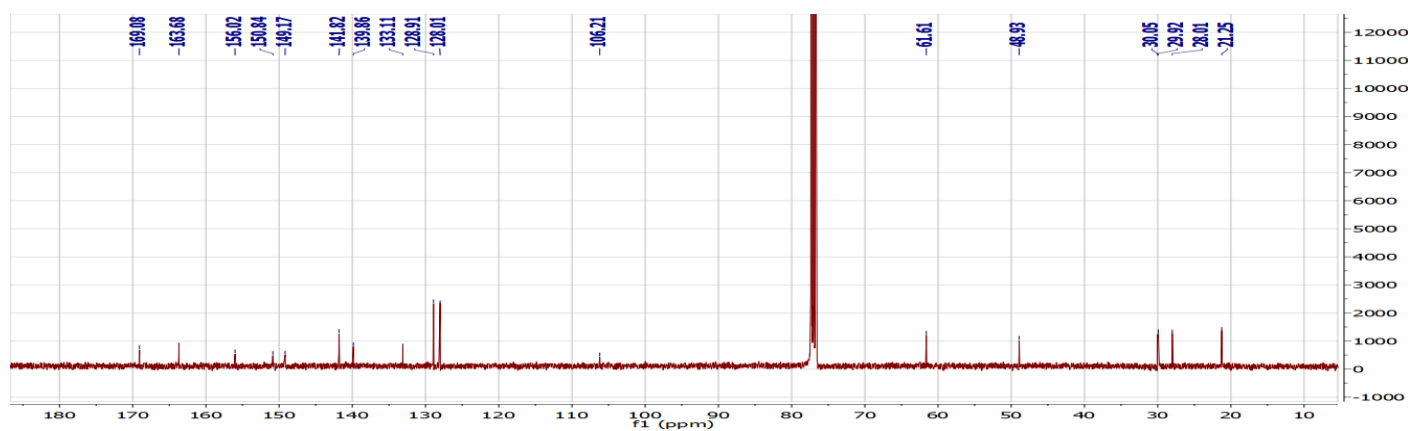
2-(4-Methylphenyl)-3-[(1,3-dimethylxanthin-7-yl)acethamido]thiazolidine-4-one (6k)



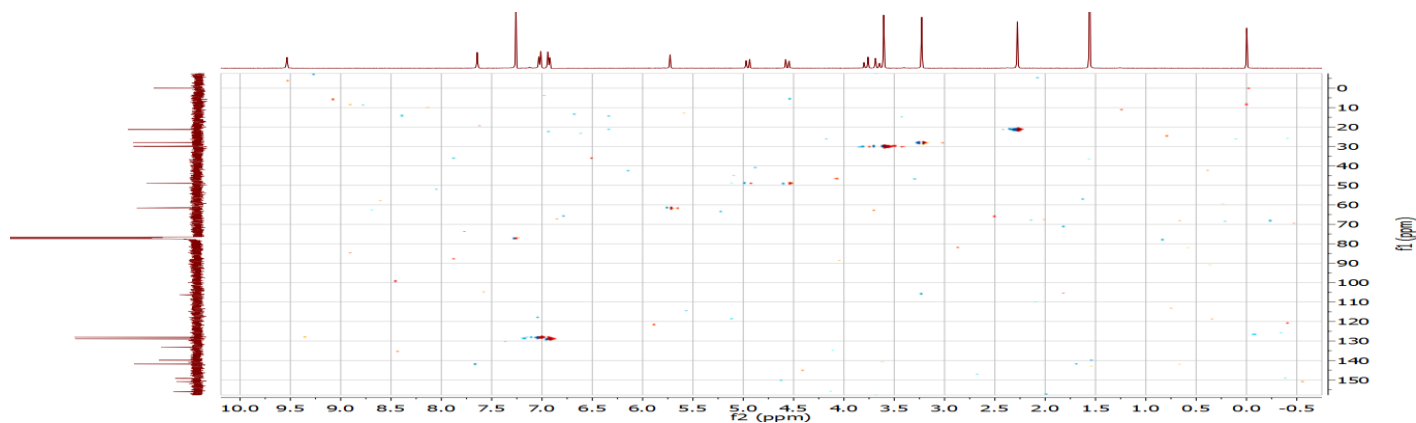
¹H-RMN spectra of **6k**



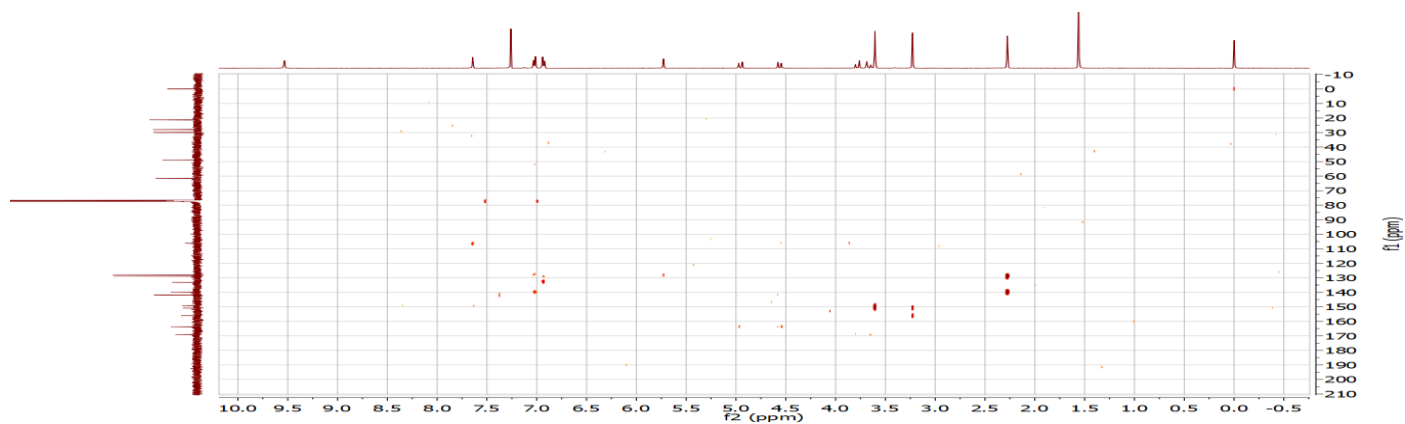
2D-COSY spectra of **6k**



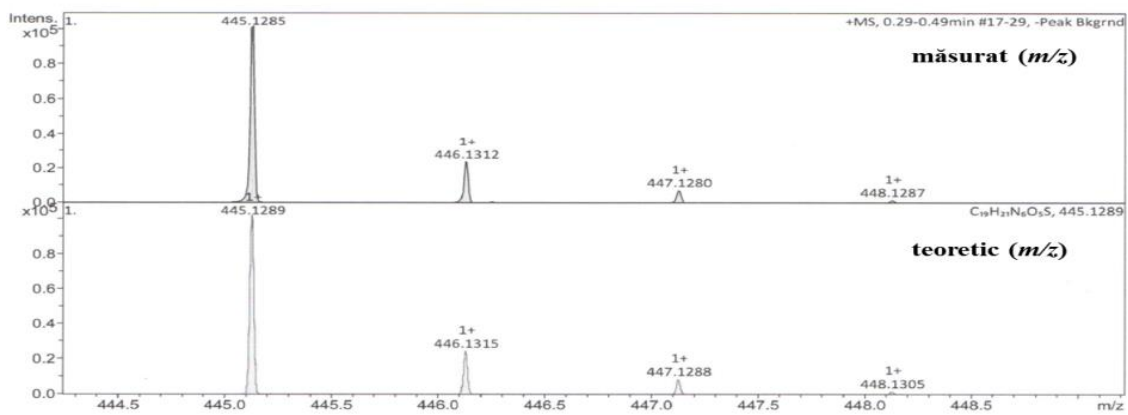
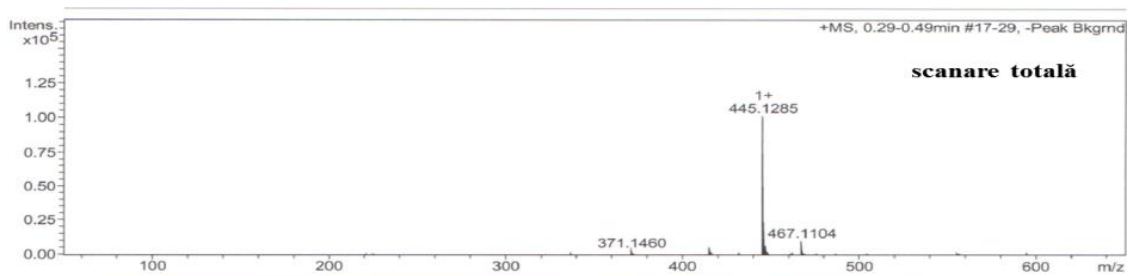
¹³C-RMN spectra of **6k**



HSQC spectra of **6k**



HMBC spectra of **6k**



HRMS spectra of **6k**