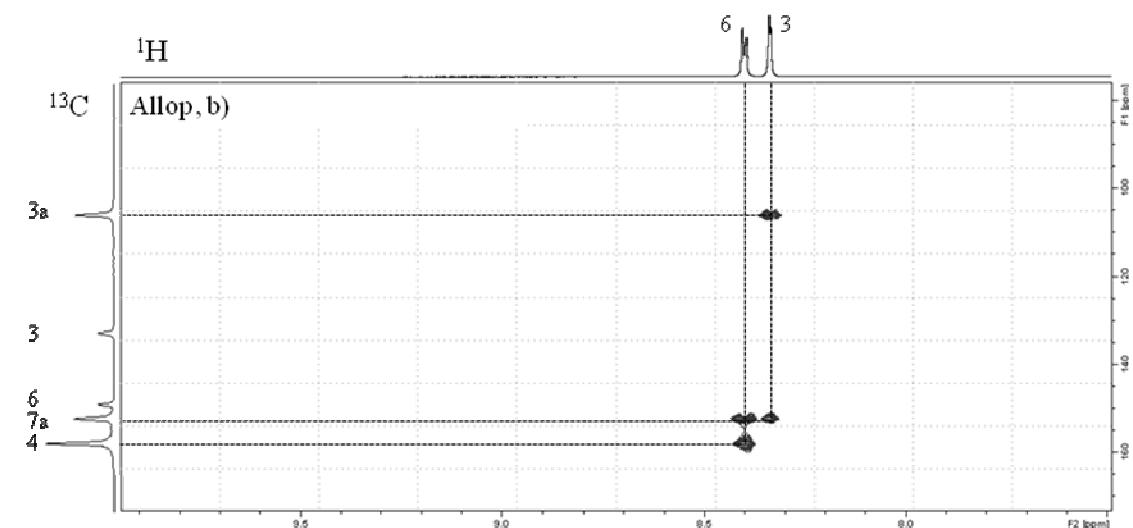
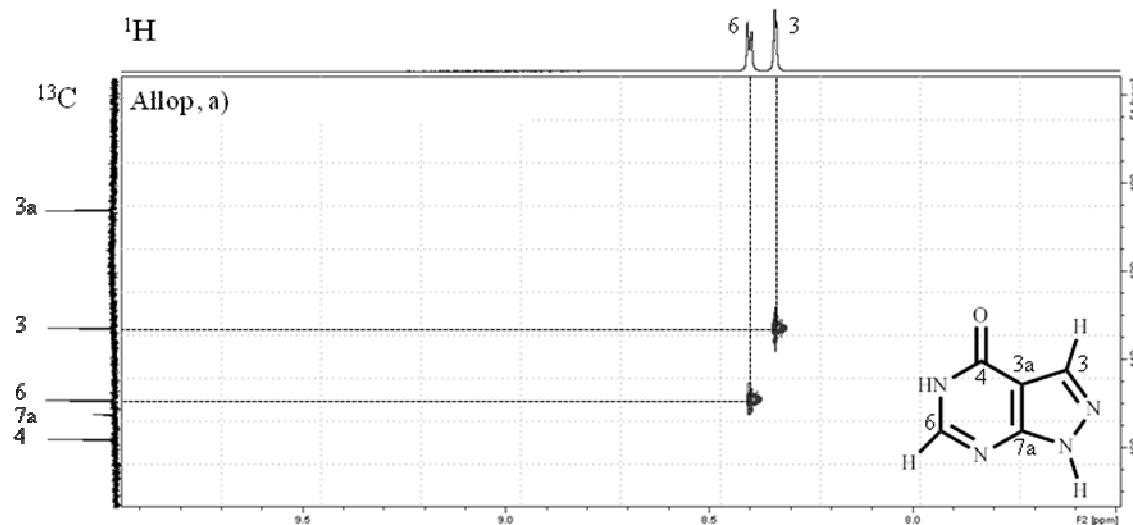


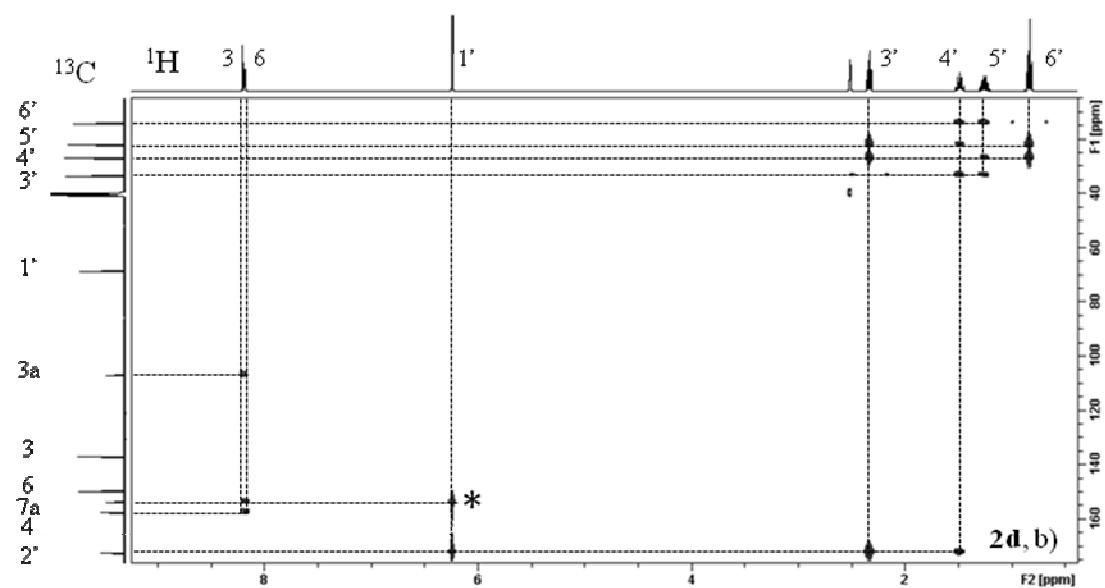
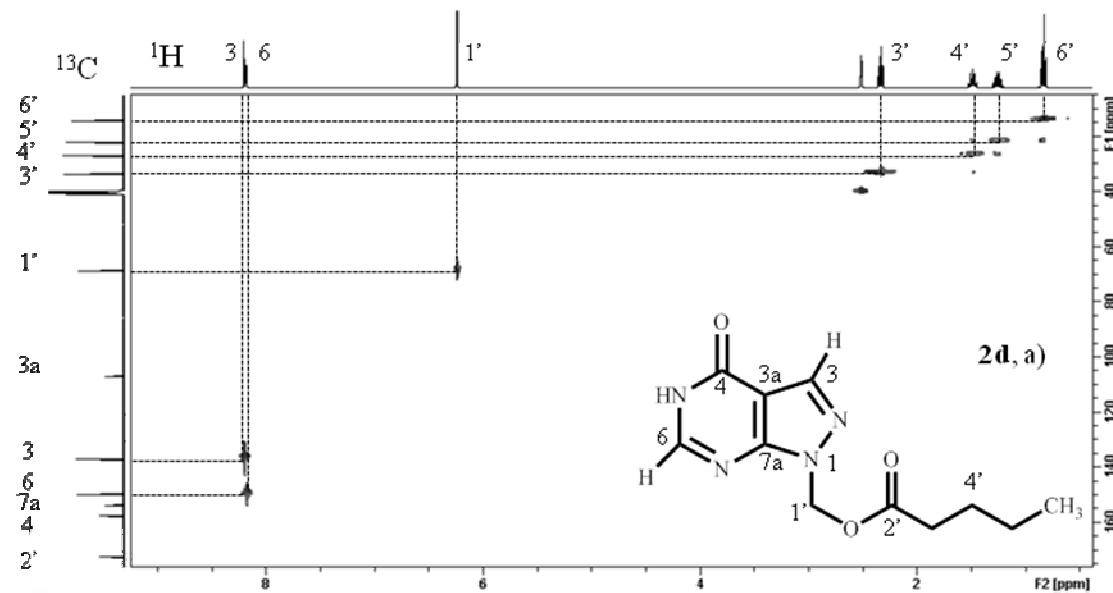
Supplementary Material.

a) HSQC-DEPT and b) HMBC of Allop (**1**) (DMSO-d₆)



a) HSQC-DEPT and b) HMBC of **2d** (DMSO-d₆)

* Indicates replacement in N1



a) HSQC-DEPT and b) HMBC of **2f** (DMSO-d₆)

* Indicates replacement in N2

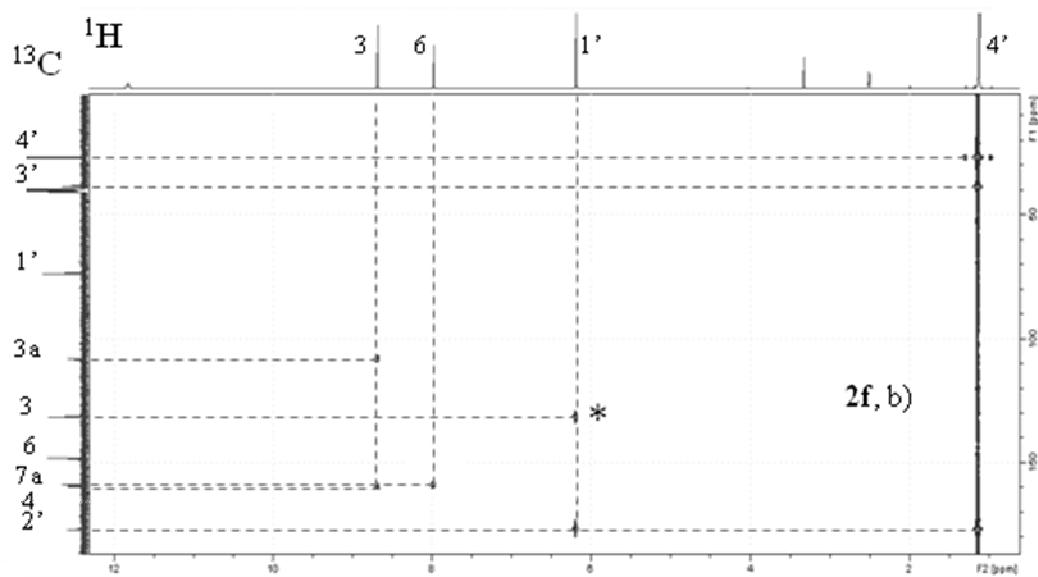
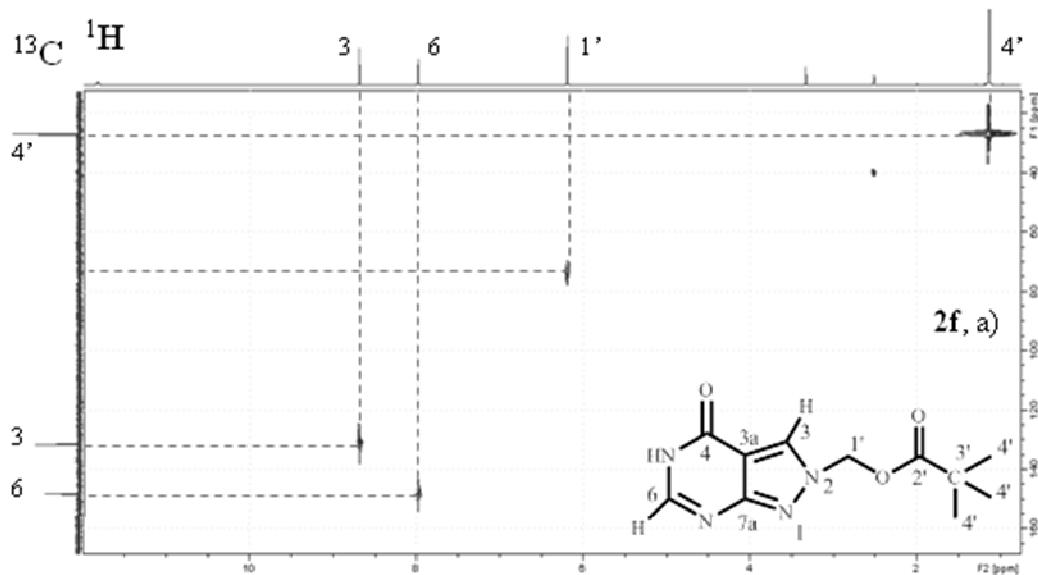


Table S1. Calibration parameters for Allop and its derivatives

Comp	Slope (10^7)	Intercept	r^2	LOD	LOQ
Allop	971±1	17±13	0.9998	0.20	0.68
2a	891±5	1±1	0.9998	0.36	1.2
2b	802±4	19±9	0.9999	0.17	0.56
2c	790±4	2±8	0.9999	0.40	1.3
2d	812±4	4±9	0.9999	0.22	0.74
2e	621±9	21±20	0.9998	0.25	0.84
2f	793±4	5±10	0.9999	0.23	0.76

r^2 : regression coefficients

LOD: limit of detection (10^{-9} mol mL $^{-1}$)

LOQ: limit of quantification (10^{-9} mol mL $^{-1}$)

Table S2. Intra- and inter-day precision (RSD) and recovery, corresponding to the studies of Allop derivatives and to their only degradation product Allop

Comp	Intra-day			Inter-day ± SD			Recovery [*] ± SD		
	RSD			c ₁	c ₂	c ₃	c ₁	c ₂	c ₃
	c ₁	c ₂	c ₃						
Allop	1.1	0.23	0.10	1.2±0.4	0.4±0.7	0.2±0.4	102±4	99±3	98±2
2^a	1.6	0.23	0.08	2±1	0.6±0.4	0.2±0.1	102±4	100±3	101±2
2^b	1.3	0.34	0.28	1.5±0.3	0.5±0.2	0.6±0.3	99±7	102±5	101±2
2^c	2.0	0.27	0.28	2.2±0.4	0.7±0.4	0.8±0.4	101±5	103±3	101±1
2^d	1.3	0.32	0.21	1.5±0.1	0.8±0.5	0.8±0.5	98±5	97±5	97±2
2^e	1.7	0.87	0.69	2.0±0.7	0.6±0.7	0.3±0.3	103±3	100±2	100±2
2^f	1.5	0.75	0.32	1.0±0.2	0.7±0.3	0.2±0.1	102±3	100±3	99±2

c₁ = 7.5 x 10⁻⁹, c₂ = 6.0 x 10⁻⁸ and c₃ = 3.5 x 10⁻⁷ mol mL⁻¹

^{*}Average Recovery Percentage in buffers and all matrices

Table S3. Robustness evaluation of the MLC method

Chromatographic changes	Level	Allop		2a		2b		2c		2d		2e		2f	
		t _R	Area	t _R	Area	t _R	Area	t _R	Area	t _R	Area	t _R	Area	t _R	Area
SDS conc. (M)															
0.09	-0.01	2.42	355	3.16	217.5	3.97	117.6	4.86	207	5.86	337	6.9	203	8.0	246
0.1	0	2.37	357	3.08	216.6	3.93	118.0	4.77	208	5.72	345	6.7	202	7.8	251
0.11	+0.01	2.41	358	3.19	218.5	3.89	118.2	4.77	202	5.72	340	6.7	204	7.8	248
Mean ± SD		2.40±0.03	357±2	3.14±0.06	217.5±0.9	3.93±0.04	117.9±0.3	4.80±0.05	206±3	5.77±0.08	341±5	6.8±0.1	203±1	7.8±0.1	248±3
RSD		1.1	0.43	1.8	0.42	1.0	0.26	1.0	1.5	1.4	1.3	1.6	0.49	1.7	1.1
% of propanol (v/v)															
7.4	-0.1	2.41	358	3.12	219	3.96	115	4.81	204	5.78	347	6.81	204	7.87	246
7.5	0	2.45	355	3.15	215	3.93	118	4.80	207	5.77	341	6.79	203	7.84	249
7.6	+0.1	2.39	360	3.09	216	3.91	119	4.75	204	5.71	341	6.71	205	7.74	251
Mean ± SD		2.42±0.03	357±3	3.12±0.03	217±2	3.94±0.02	117±2	4.79±0.03	205±2	5.75±0.04	343±3	6.77±0.05	204±1	7.82±0.06	249±2
RSD		1.3	0.70	0.96	0.91	0.59	1.9	0.70	0.93	0.66	1.0	0.75	0.54	0.82	0.98
pH of mobile phase															
2.9	-0.1	2.35	354	3.15	217	3.97	117	4.83	205	5.82	339	6.9	203.2	7.9	246
3.0	0	2.42	355	3.12	217	3.93	118	4.77	208	5.72	345	6.7	202.1	7.8	251
3.1	+0.1	2.38	352	3.14	216	3.99	115	4.88	206	5.88	334	7.0	202.3	8.0	244
Mean ± SD		2.38±0.04	354±2	3.14±0.02	217±1	3.96±0.03	117±2	4.83±0.05	206±1	5.81±0.08	340±6	6.9±0.1	202.5±0.6	7.9±0.2	247±4
RSD		1.5	0.42	0.49	0.43	0.73	1.3	1.1	0.58	1.4	1.7	1.7	0.27	1.8	1.4
Flow rate (mL min ⁻¹)															
0.9	-0.1	2.39	354	3.12	217	4.03	118.2	4.90	209	5.87	346	7.0	205	8.0	251
1	0	2.37	352	3.15	215	3.93	118.0	4.80	207	5.77	341	6.8	202	7.8	249
1.1	+0.1	2.40	357	3.18	217	3.87	117.9	4.75	208	5.69	345	6.7	203	7.8	250
Mean ± SD		2.39±0.02	354±2	3.15±0.03	216±1	3.94±0.08	118.0±0.2	4.82±0.08	208±1	5.78±0.09	344±3	6.8±0.1	204±1	7.9±0.1	250±1
RSD		0.64	0.66	0.95	0.48	2.0	0.13	1.6	0.50	1.6	0.78	2.0	0.68	1.7	0.50

Retention time expressed in minutes