

Supplementary Material

**LC and NMR Studies for Identification and Characterization of Degradation
Byproducts of Olmesartan, Elucidation of Their Degradation Pathway and
Ecotoxicity Assessment**

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Table S1. ^1H , ^{13}C and 2D NMR data of Olmesartan medoximil in CD_3OD .

Position	Residue	$^{13}\text{C}^a$	$^1\text{H}^a$, multiplicity (J in Hz)	^1H - ^1H COSY	^1H - ^{13}C HMBC
1	C	142.99	-		7.66, 7.63, 7.58, 7.07
2	C	124.80	-		7.63, 7.58, 7.54
3	CH	131.78	7.63, d (7.2)	7.66, 7.54	7.66, 7.54
4	CH	129.02	7.54, dd (7.0, 1.3)	7.66, 7.63, 7.58	7.66, 7.63, 7.58
5	CH	132.34	7.66, dd (8.5, 1.3)	7.63, 7.58, 7.54,	7.63, 7.58, 7.54
6	CH	131.49	7.58, d (8.3)	7.66, 7.54	7.66, 7.54
7	C	140.21	-		7.58, 7.07, 6.87
8/12	CH	130.55	7.07, d (8.2)	6.87	6.87
9/11	CH	126.56	6.87, d (8.2)	7.07, 5.51	7.07, 5.51
10	C	137.87	-		7.07, 6.87, 5.51
13	C	157.05	-		7.63
18	CH_2	50.12	5.51, s	6.87	6.87
20	C	153.52	-		5.51, 2.74, 1.61
22	C	158.33	-		1.59
23	C	118.42	-		5.51
24	CH_2	29.60	2.74, t (7.7)	1.61, 0.93	1.61, 0.93
25	CH_2	22.42	1.61, q (6.8)	2.74, 0.93	2.74, 0.93
26	CH_3	14.00	0.93, t (7.0)	2.74, 1.61	2.74, 1.61
27	C	71.63	-		1.59
28/29	CH_3	29.60	1.59, s		
31	C	162.24	-		5.02
34	CH_2	55.63	5.02, s		
35	C	142.23	-		5.02, 2.06
36	C	134.36	-		5.02, 2.06
38	C	153.43	-		
41	CH_3	9.10	2.06, s		

^aChemical shifts in ppm.

Table S2. ^1H , ^{13}C and 2D NMR data of **DP-1** in CD_3OD .

Position	Residue	$^{13}\text{C}^a$	$^1\text{H}^a$, multiplicity (J in Hz)	^1H - ^1H COSY	^1H - ^{13}C HMBC
1	C	141.02	-		7.63, 7.61, 7.54, 7.16
2	C	126.35	-		7.63, 7.56, 7.54
3	CH	131.69	7.63, dd (8.5, 1.6)	7.61, 7.56	7.61, 7.56
4	CH	128.86	7.56, m	7.63, 7.61, 7.54	7.63, 7.61, 7.54
5	CH	131.76	7.61, m	7.63, 7.56, 7.54	7.63, 7.56, 7.54
6	CH	131.81	7.54, m	7.61, 7.56	7.61, 7.56
7	C	140.78	-		7.54, 7.16, 7.06
8/12	CH	130.71	7.16, d (8.3)	7.06	7.06
9/11	CH	126.49	7.06, d (8.3)	7.16, 5.25	7.16, 5.25
10	C	136.39	-		7.16, 7.06, 5.25
13	C	158.58	-		7.63
18	CH_2	47.69	5.25, m	7.06	7.06
20	C	148.37	-		5.25, 2.63, 1.58
22	C	140.87	-		1.61
23	C	113.63	-		5.25
24	CH_2	29.83	2.63, m	1.58, 0.95,	1.58, 0.95
25	CH_2	22.65	1.58, sest (7.9)	2.63, 0.95	2.63, 0.95
26	CH_3	13.99	0.95, t (7.9)	2.63, 1.58	2.63, 1.58
27	C	70.28	-		1.61
28/29	CH_3	29.92	1.61, s		
31	C	158.45	-		

^aChemical shifts in ppm.

Table S3. ^1H , ^{13}C and 2D NMR data of **DP-2** in CD_3OD .

Position	Residue	$^{13}\text{C}^a$	$^1\text{H}^a$, multiplicity (J in Hz)	^1H - ^1H COSY	^1H - ^{13}C HMBC
1	C	142.82	-		7.57, 7.55, 7.12
2	C	127.80	-		7.47, 7.45
3	CH	131.72	7.55, d (7.4)	7.47	7.57, 7.47
4	CH	128.65	7.47, d (7.4)	7.57, 7.55	7.45
5	CH	131.26	7.57, m	7.47, 7.45	7.55, 7.47
6	CH	131.44	7.45, m	7.57	7.47
7	C	141.45	-		7.45, 6.97
8/12	CH	130.74	7.12, d (8.3)	6.97	7.12, 6.97
9/11	CH	127.04	6.97, d (8.3)	7.12	7.12, 6.97
10	C	135.97	-		7.12, 5.38, 5.31
13	C	159.79	-		7.55
18	CH_2	49.01	5.38, d (16.8) 5.31, d (16.8)	5.31 5.38	6.97
20	C	147.64	-		5.38, 5.31, 4.24, 1.80, 1.64
22	C	125.62	-		
23	C	115.76	-		5.38, 5.31
24	CH_2	79.51	4.24, t (7.2)	1.80, 1.64	1.80, 1.64, 0.82
25	CH_2	27.84	1.80, m 1.64, m	4.24, 1.64, 0.82 4.24, 1.80, 0.82	4.24, 0.82
26	CH_3	10.29	0.82, t (7.4)	1.80, 1.64	4.24, 1.80, 1.64
27	OCH_3	57.06	3.08, s		4.24

^aChemical shifts in ppm.

Table S4. ^1H , ^{13}C and 2D NMR data of **DP-3** in CD_3OD .

Position	Residue	$^{13}\text{C}^a$	$^1\text{H}^a$, multiplicity (J in Hz)	^1H - ^1H COSY	^1H - ^{13}C HMBC
1	C	142.96	-		7.52, 7.49, 7.11
2	C	128.27	-		7.43
3	CH	131.79	7.52, dd (7.8, 1.6)	7.49, 7.43	7.49, 7.43
4	CH	130.26	7.43, dd (7.9, 1.5)	7.52, 7.49	7.52, 7.43
5	CH	131.16	7.49, t (7.8)	7.52, 7.43	7.52, 7.43
6	CH	128.27	7.43, d (8.0)	7.49	7.43
7	C	142.35	-		7.43, 7.11
8/12	CH	129.85	7.11, d (8.1)	7.29	7.29, 7.11
9/11	CH	130.54	7.29, d (8.1)	7.11	7.29, 7.11
10	C	135.74	-		7.11, 4.52, 4.43
13	C	162.08	-		7.52
18	CH_2	43.67	4.52, d (15.0) 4.43, d (15.0)	4.43 4.52	7.29
20	C	98.91	-		2.75, 1.87, 1.14, 0.90
22	C	161.38	-		
23	C	160.68	-		
24	CH_2	39.62	1.87, m	1.14, 0.90	1.14, 0.90, 0.72
25	CH_2	17.18	1.14, m 0.90, m	1.87, 0.90, 0.72 1.87, 1.14, 0.72	1.87, 0.72
26	CH_3	13.66	0.72, t (8.0)	1.14, 0.90	1.87, 1.14, 0.90
27	OCH_3	48.67	2.75, s		

^aChemical shifts in ppm.

Table S5. ^1H , ^{13}C and 2D NMR data of **DP-4** in CD_3OD .

Position	Residue	$^{13}\text{C}^{\text{a}}$	$^1\text{H}^{\text{a}}$, multiplicity (J in Hz)	^1H - ^1H COSY	^1H - ^{13}C HMBC
1	C	143.02	-		7.52, 7.49, 7.08
2	C	128.17	-		7.43, 7.42
3	CH	131.68	7.52, d (7.7)	7.42	7.49
4	CH	128.17	7.42, dt (7.5, 1.6)	7.52, 7.49	7.52, 7.49
5	CH	130.08	7.49, dt (7.5, 1.7)	7.43, 7.42	7.43, 7.42
6	CH	130.96	7.43, d (7.3)	7.49	7.49
7	C	142.39	-		7.43, 7.29
8/12	CH	130.96	7.08, d (8.3)	7.29	7.29, 7.08
9/11	CH	130.08	7.29, d (8.3)	7.08	7.29, 7.08
10	C	135.28	-		7.08
13	C	162.31	-		7.52
18	CH_2	43.90	4.84, overlapped 4.18, d (15.4)	4.18 4.84	7.29
20	C	100.16	-		4.84, 4.42, 4.18
22	C	160.01	-		
23	C	160.70	-		4.84, 4.18
24	CH_2	66.46	4.42, dd (11.2, 2.6)	2.16, 1.58	2.16, 1.58, 1.12
25	CH_2	26.67	2.16, dsest (7.5, 2.5) 1.58, m	4.42, 1.12	4.42, 1.12
26	CH_3	12.02	1.12, t (7.5)	2.16, 1.58	4.42, 2.16, 1.58

^aChemical shifts in ppm.

Table S6. ^1H , ^{13}C and 2D NMR data of **DP-5** in CD_3OD .

Position	Residue	$^{13}\text{C}^a$	$^1\text{H}^a$, multiplicity (J in Hz)	^1H - ^1H COSY	^1H - ^{13}C HMBC
1	C	142.86	-		7.61, 7.60
2	C	126.97	-		7.52, 7.48
3	CH	131.61	7.61, m	7.60, 7.52	7.60
4	CH	128.81	7.52, dt (8.1, 1.3)	7.61, 7.60	7.61, 7.48
5	CH	130.60	7.60, m	7.52, 7.48	7.61, 7.52
6	CH	131.69	7.48, dd (7.0, 1.8)	7.60, 7.52	7.52
7	C	141.69	-		7.48, 7.37
8/12	CH	130.66	7.13, d (8.1)	7.37	7.37, 7.13
9/11	CH	130.31	7.37, d (8.1)	7.13	7.37, 7.13
10	C	136.07	-		7.13, 4.65, 4.43
13	C	158.81	-		7.61
18	CH_2	44.08	4.65, x (xx) 4.43, x (xx)	4.43 4.65	7.37
20	C	99.30	-		4.07, 2.92, 1.45, 1.26
22	C	128.68	-		
23	C	160.68	-		
24	CH_2	66.88	4.07, x (xx)		1.45, 1.26, 0.74
25	CH_2	26.18	1.45, x (xx) 1.26, x (xx)	4.07, 1.26, 0.74 4.07, 1.45, 0.74	4.07, 0.74
26	CH_3	11.05	0.74, x (xx)	1.45, 1.26	4.07, 1.45, 1.26
27	OCH_3	48.80	2.92, s		

^aChemical shifts in ppm.

Table S7. ^1H , ^{13}C and 2D NMR data of **DP-6** in CD_3OD .

Position	Residue	$^{13}\text{C}^a$	$^1\text{H}^a$, multiplicity (J in Hz)	^1H - ^1H COSY	^1H - ^{13}C HMBC
1	C	142.90	-		7.20, 7.59, 7.51
2	C	128.72	-		7.51, 7.49, 7.59
3	CH	131.73	7.59, dd (7.6, 1.5)	7.49, 7.59	7.49, 7.59
4	CH	131.61	7.49, dt (7.6, 1.4)	7.59, 7.51	7.51, 7.59
5	CH	132.52	7.59, dt (8.4, 2.2)	7.49, 7.59, 7.51	7.59, 7.49, 7.51
6	CH	131.61	7.51, d (7.4)	7.49, 7.59	7.49, 7.59
7	C	141.35	-		7.26, 7.51, 7.20
8/12	CH	130.51	7.20, d (8.3)	7.26	7.26
9/11	CH	129.21	7.26, d (8.3)	4.62, 4.63, 7.20	4.62, 4.63, 7.20
10	C	135.84	-		7.20, 7.26, 4.62, 4.63
13	C	159.25	-		7.59
18	CH_2	44.00	4.63, d (14.7) 4.62, d (14.7)	7.26	7.26
20	C	174.25	-		4.62, 4.63, 1.84, 1.98, 4.91
21	CH	82.06	4.93, dd (6.5, 4.7)	1.84, 1.98, 0.93	1.84, 1.98, 0.93
23	C	157.25	-		4.91, 4.62, 4.63
25	CH_2	25.09	1.98, m 1.84, m	4.91, 0.93	4.91, 0.93
26	CH_3	8.39	0.93, t (7.5)	4.91, 1.84, 1.98	4.91, 1.84, 1.98

^aChemical shifts in ppm

Table S8. ^1H , ^{13}C and 2D NMR data of **DP-7** in CD_3OD .

Position	Residue	$^{13}\text{C}^{\text{a}}$	$^1\text{H}^{\text{a}}$, multiplicity (J in Hz)	^1H - ^1H COSY	^1H - ^{13}C HMBC
1	C	144.14	-		7.11, 7.66, 7.56
2	C	127.00	-		7.56, 7.66
3	CH	132.54	7.66, m	7.66, 7.56	7.66, 7.56
4	CH	129.02	7.56, m	7.56, 7.66	7.56, 7.66
5	CH	131.63	7.66, m	7.66, 7.56	7.66, 7.56
6	CH	131.84	7.56, m	7.56, 7.66	7.56, 7.66
7	C	139.14	-		7.16, 7.56, 7.11
8/12	CH	130.51	7.11, d (8.4)	7.16	7.16
9/11	CH	127.26	7.16, d (8.4)	5.05, 7.11	5.05, 7.11
10	C	139.20	-		7.11, 5.05, 7.16
13	C	160.00	-		7.66
18	CH_2	47.01	5.05, s	7.16	7.16
20	C	178.71	-		5.05, 1.57, 2.48
21	CH_2	39.13	2.48, t (7.4)	0.86, 1.57	0.86, 1.57
22	CH_2	18.98	1.57, sest (7.2)	0.86, 2.48	0.86, 2.48
23	CH_3	13.79	0.86, t (7.6)	2.48, 1.57	2.48, 1.57
24	C	158.1	-		5.05

^aChemical shifts in ppm.

Table S9. ^1H , ^{13}C and 2D NMR data of **DP-8** in CD_3OD .

Position	Residue	$^{13}\text{C}^a$	$^1\text{H}^a$, multiplicity (J in Hz)	^1H - ^1H COSY	^1H - ^{13}C HMBC
1	C	141.75	-		7.06, 7.60, 7.62, 7.52
2	C	127.18	-		7.50, 7.52, 7.62
3	CH	130.32	7.62, d (7.5)	7.60, 7.50	7.60, 7.50
4	CH	130.22	7.50, dt (7.5, 1.4)	7.52, 7.60, 7.62	7.52, 7.60, 7.62
5	CH	130.19	7.60, dt (7.6, 1.5)	7.62, 7.50, 7.52	7.62, 7.50, 7.52
6	CH	130.32	7.52, dd (7.6, 2.0)	7.50, 7.60	7.50, 7.60
7	C	138.83	-		7.52, 7.18, 7.06
8/12	CH	128.85	7.06, d (8.4)	7.18	7.18
9/11	CH	126.84	7.18, d (8.4)	4.36, 7.06	4.36, 7.06
10	C	137.18	-		7.06, 4.36, 7.18
13	C	157.42	-		7.62
18	CH_2	41.63	4.36, s	7.18	7.18
20	C	160.96	-		4.36

^aChemical shifts in ppm.