Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY TABLE

Table S1. Optimized parameters of the developed HRMS, LC-HRMS and MS^n methods.

HRMS parameters		**MS^n parameters (Direct MS^n and LC-MS^n)**	
End plate offset (V)	-500	Spray voltage (kV)	5
Capillary (V)	4500	Sheath gas flow rate	40
Nebuliser (Bar)	1.2	Auxiliary gas flow rate	15
Dry gas (L/min)	6.0	Sweep gas flow rate	5
Dry temperature (°C)	220	Capillary temperature (°C)	271
Funnel 1 RF (Vpp)	250	Capillary voltage (V)	3
Funnel 2 RF (Vpp)	280	Tube lens (V)	15
ISCID energy (eV)	0		
Hexapole RF (Vpp)	280		
Ion energy	4.0		
Low Mass (m/z)	80		
Collision energy(eV/z)	10		
Transfer time (µs)	45		
Collision RF (Vpp)	250		
Pre pulse storage (µs)	10		

SUPPLEMENTARY FIGURES

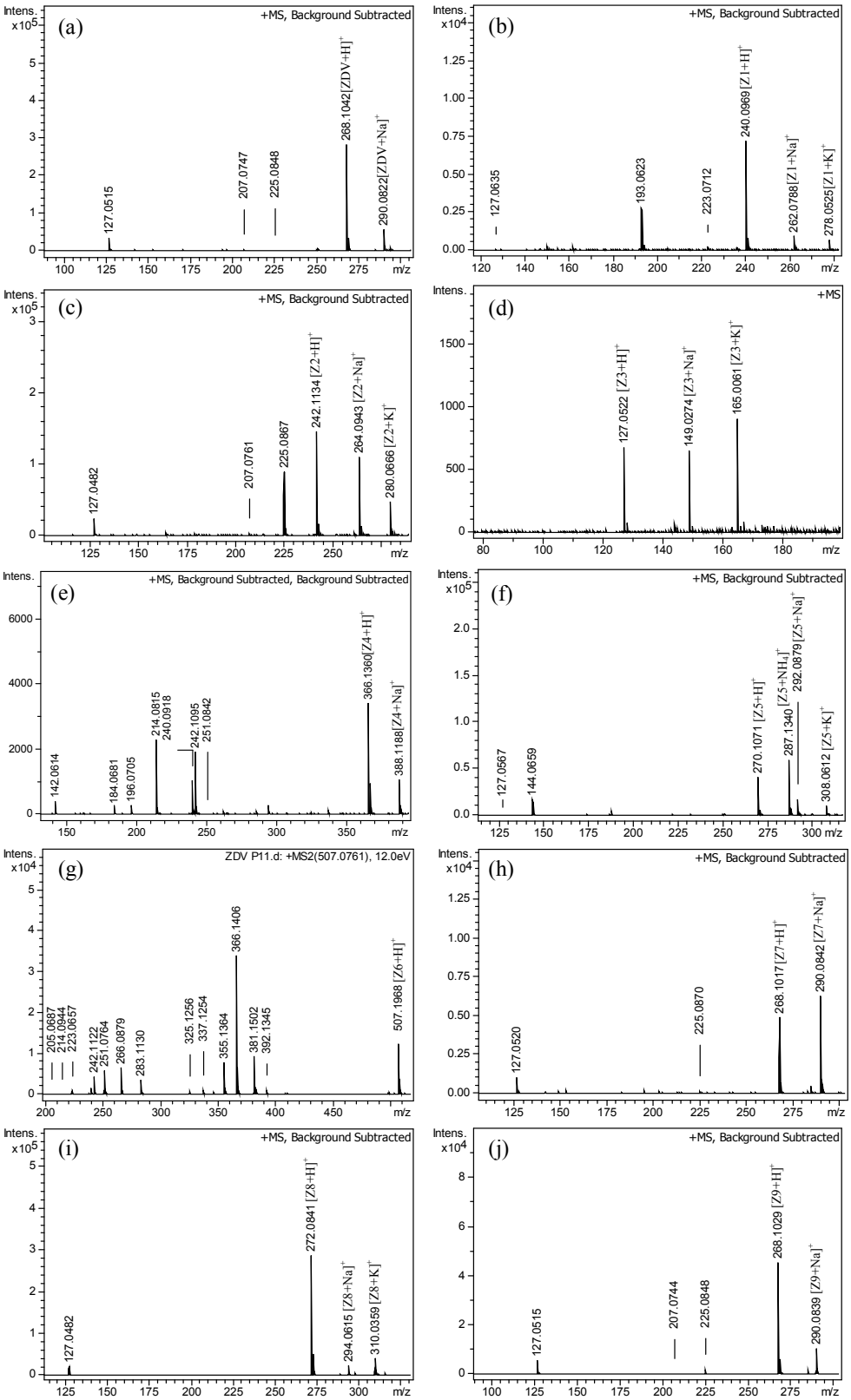
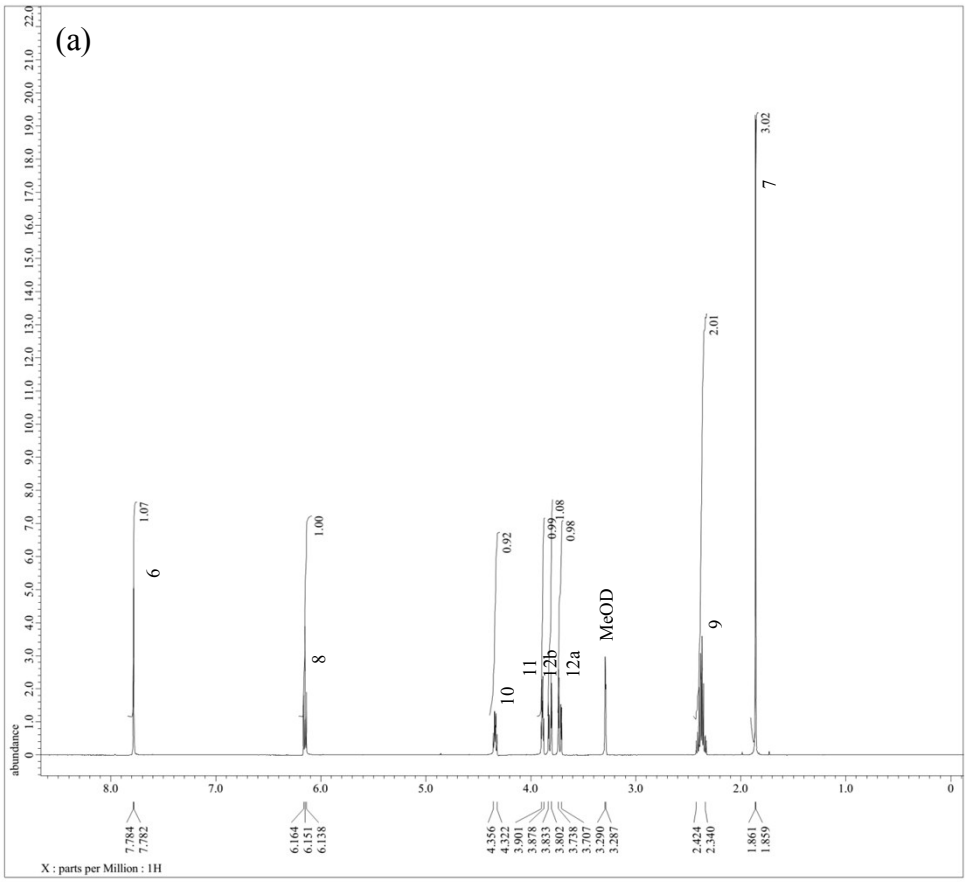
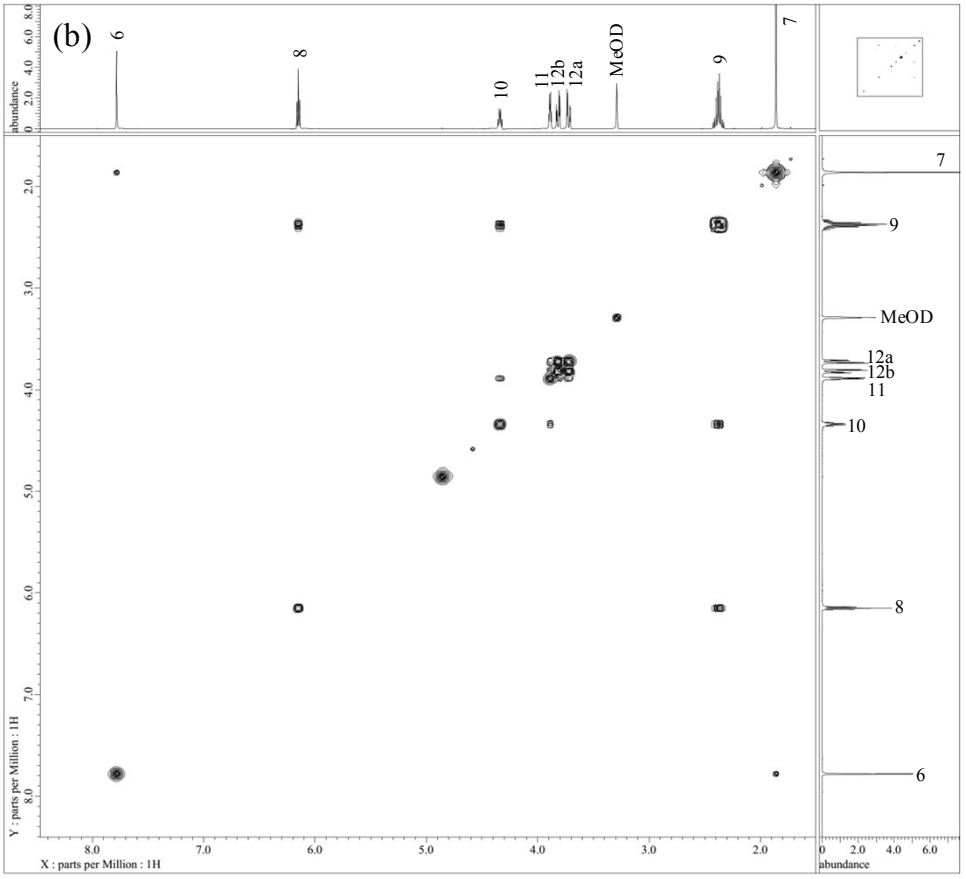
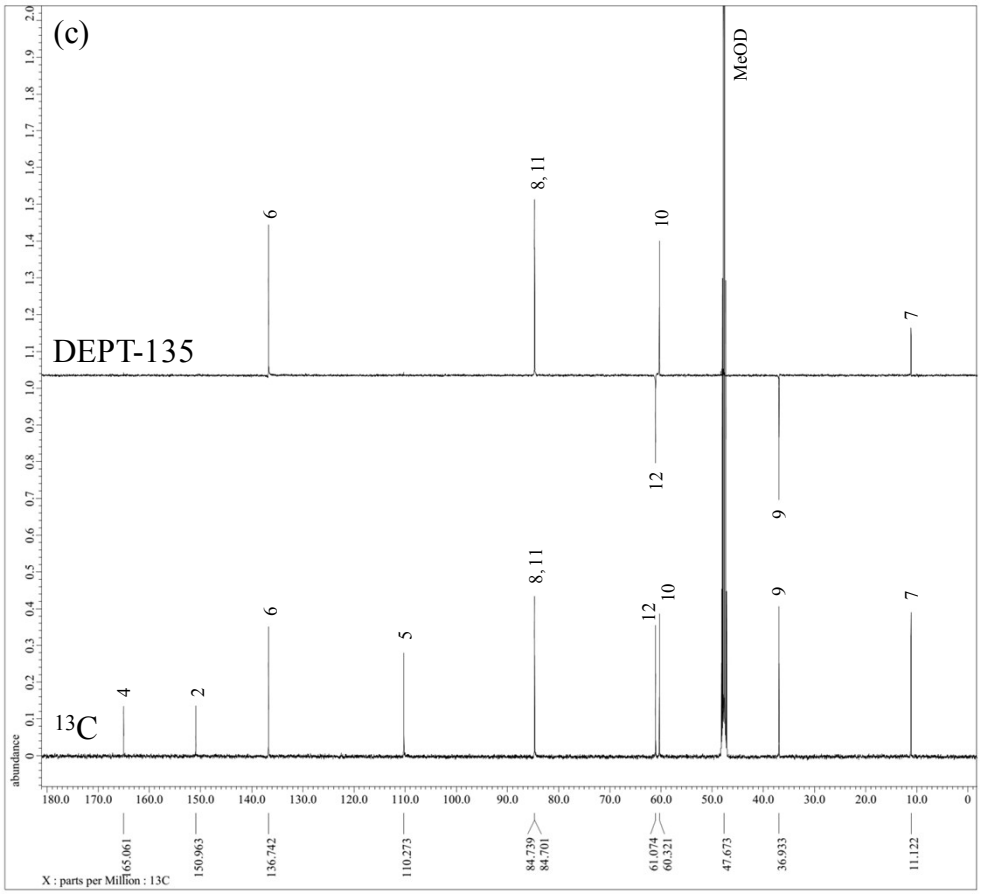
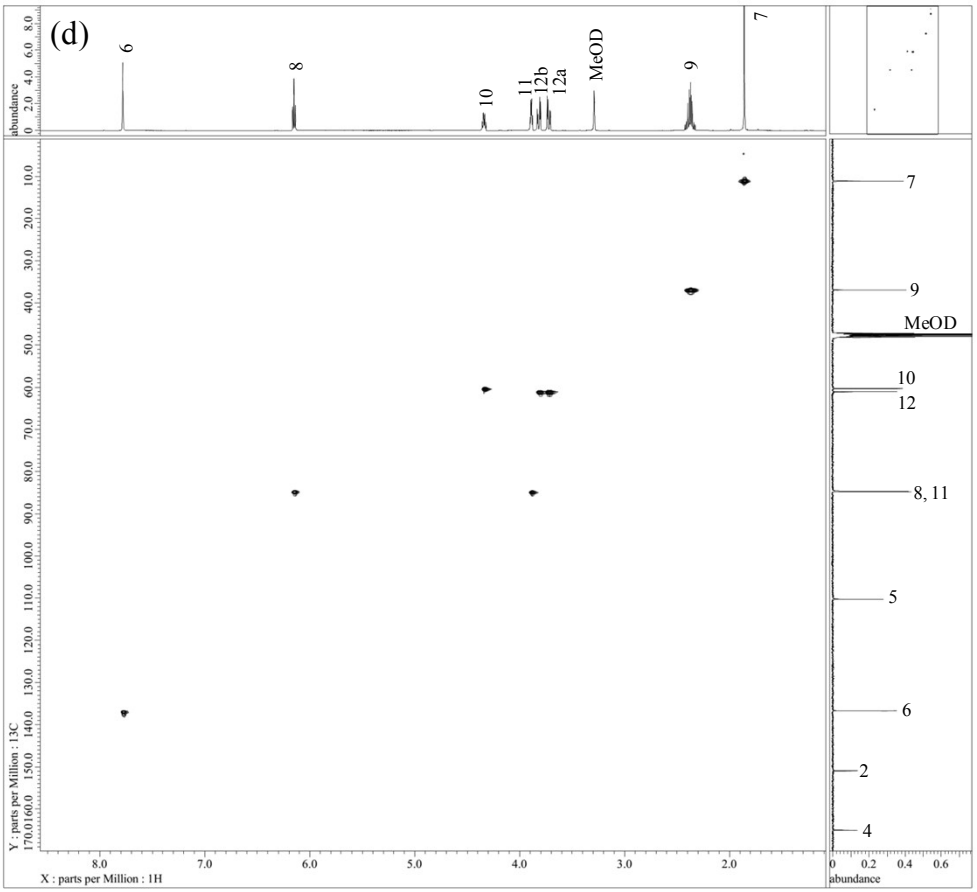


Fig. S1. HRMS line spectra of zidovudine (ZDV) (a) and its degradation products Z1-Z9 (b-j, respectively) under ESI +ve mode.


(a)
abundance
X : parts per Million : 1H
6
8
10
11
12b
12a
MeOD
9
7
1.07
1.00
0.92
0.99
1.08
0.98
2.01
3.02


(b)
abundance
X : parts per Million : 1H
Y : parts per Million : 1H
6
8
10
11
12b
12a
MeOD
9
7


(c)
DEPT-135
^{13}C
MeOD
6
8, 11
10
7
12
9
4
2
5
abundance
X : parts per Million : 13C
65.061
150.963
136.742
110.273
84.739
84.701
61.074
60.321
47.673
36.933
11.122


(d)
6
8
10
11
12b
12a
MeOD
9
7
abundance
Y : parts per Million : 13C
X : parts per Million : 1H
MeOD
10
12
8, 11
5
6
2
4

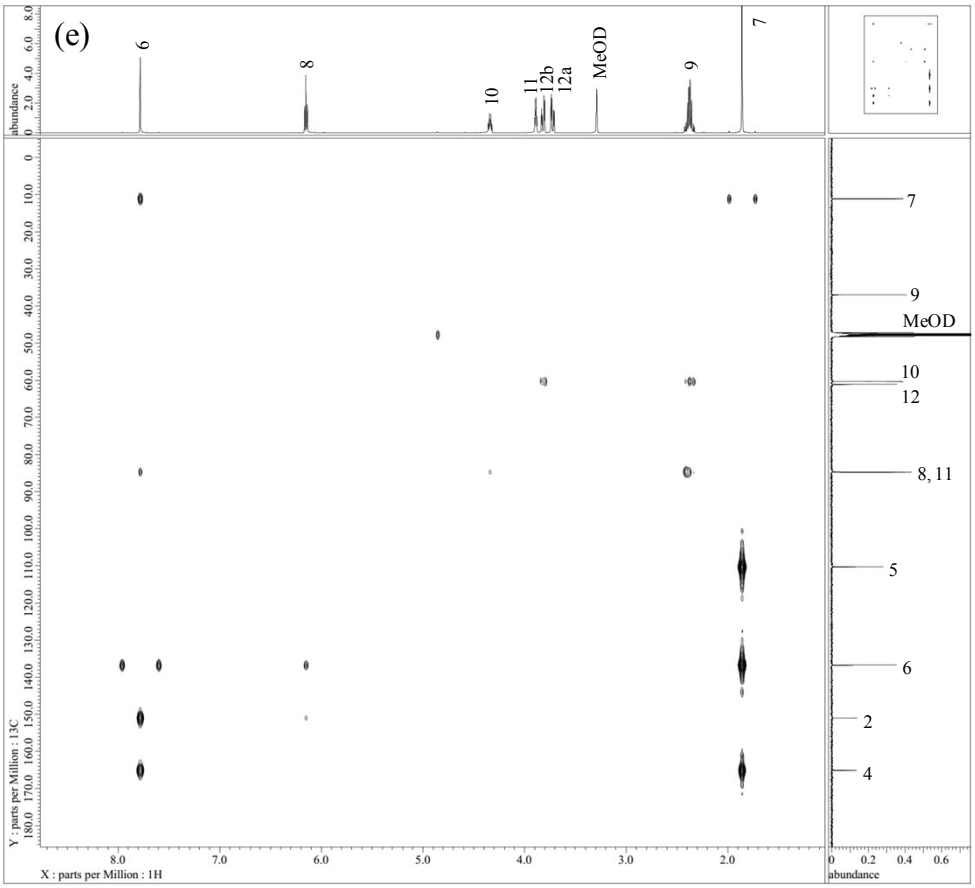


Fig. S2. NMR spectra of zidovudine (ZDV), ^{1}H (a); COSY (b); ^{13}C and DEPT-135 (c); HSQC (d), and HMBC (e).

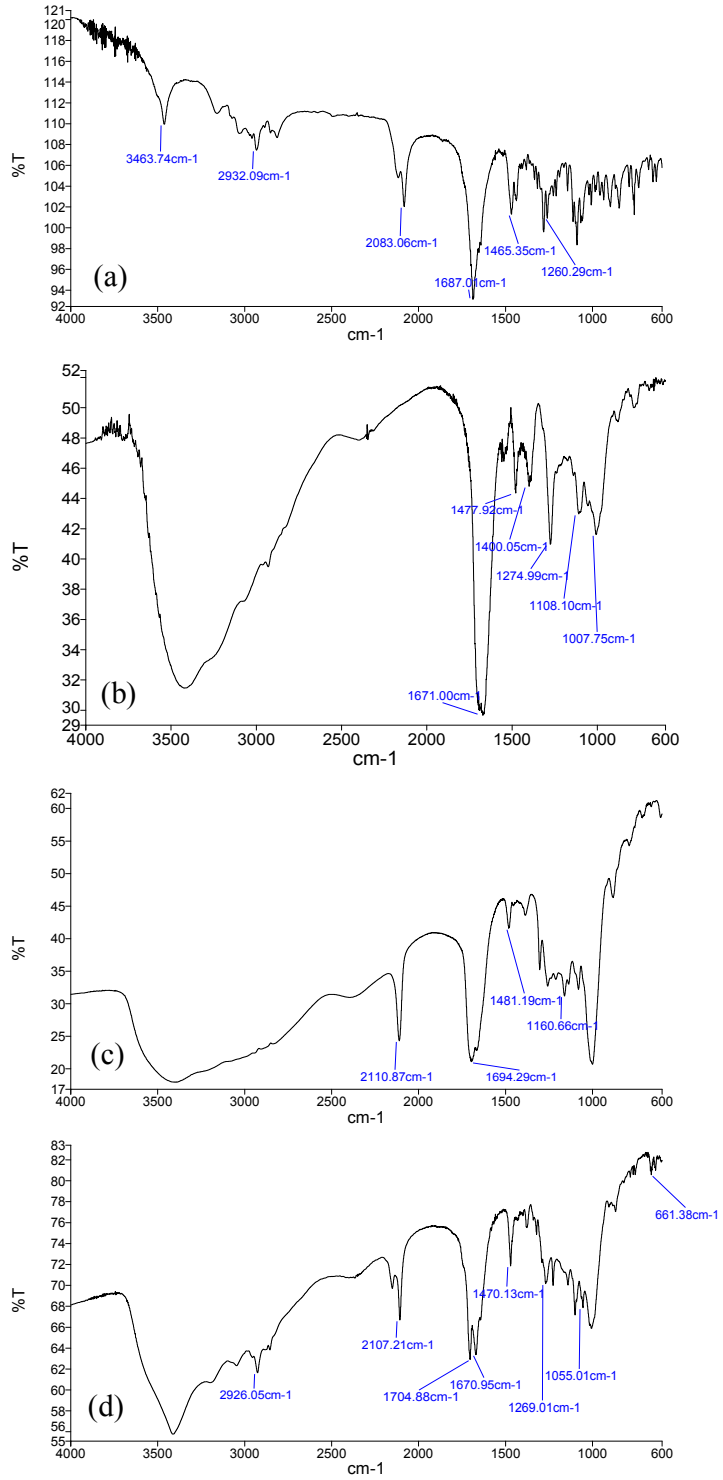
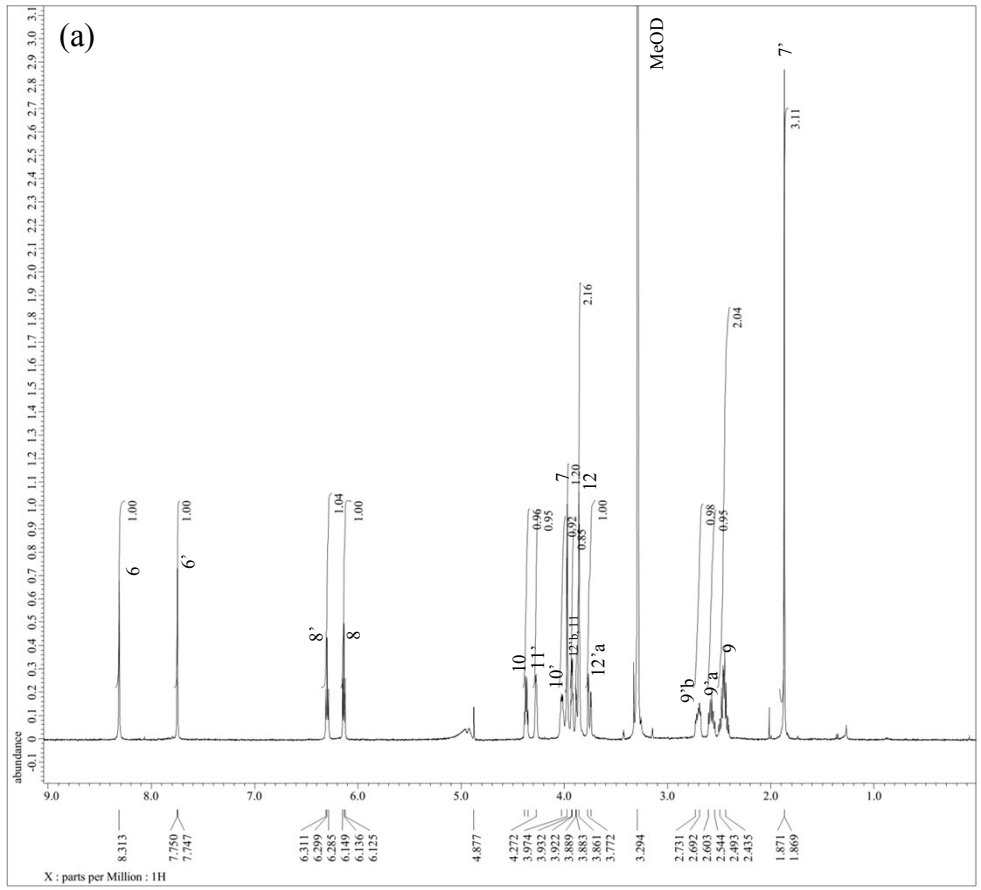
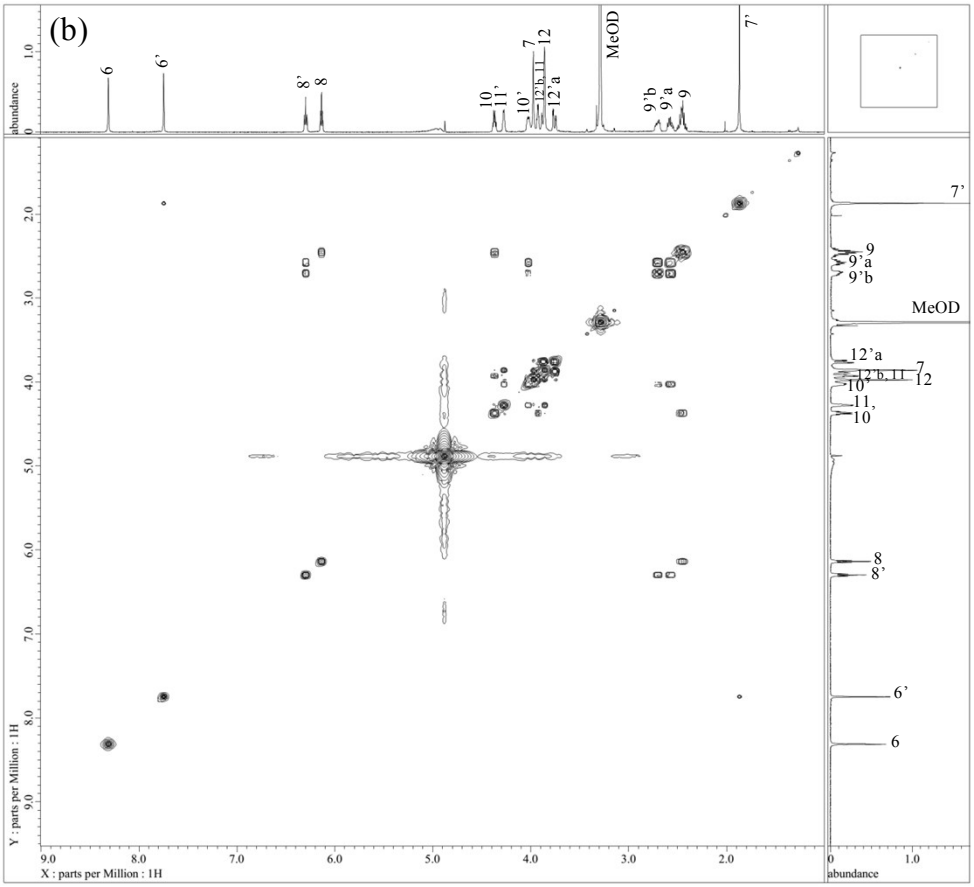
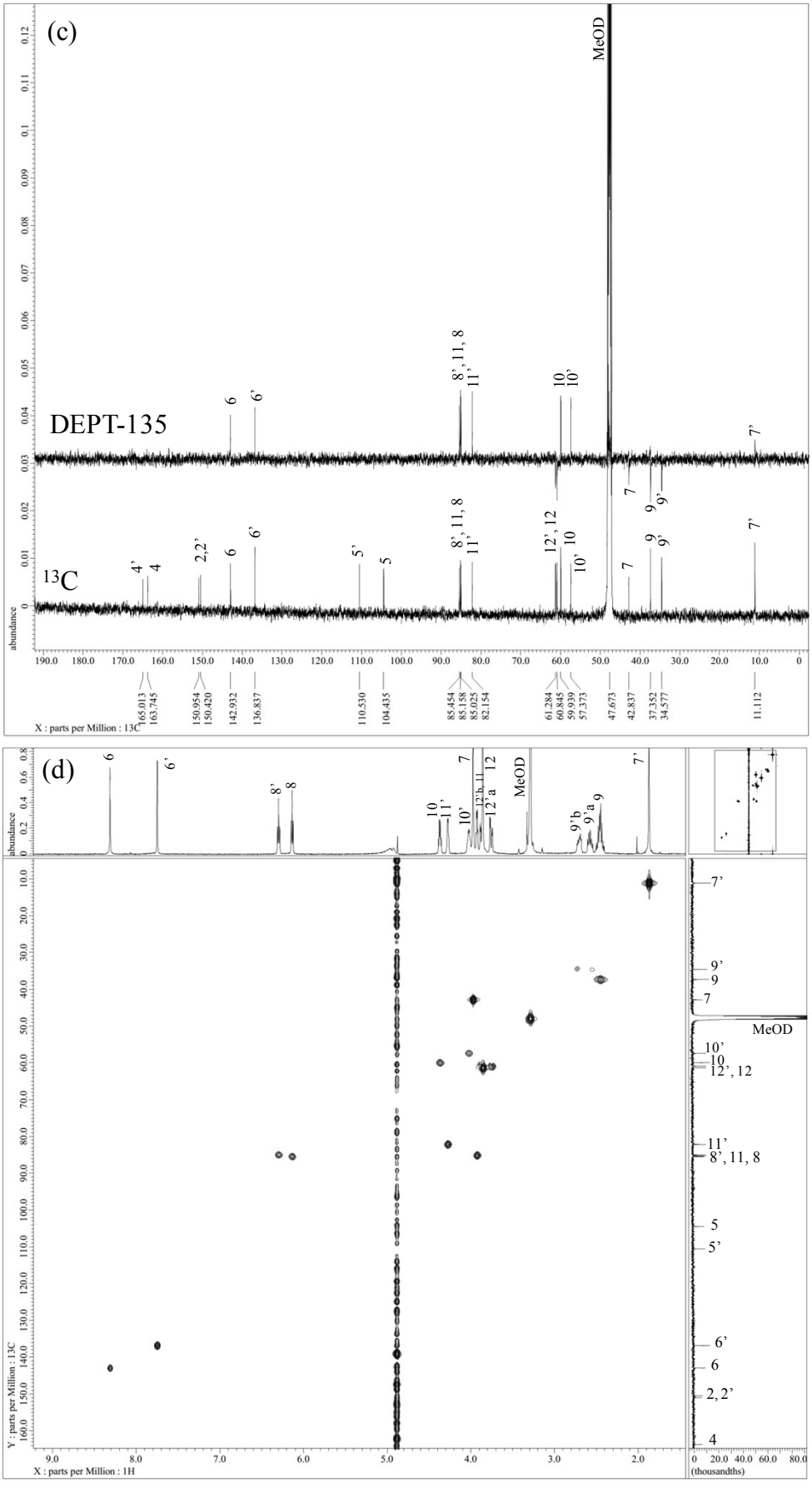


Fig. S3. IR spectra of zidovudine (ZDV, a) and its degradation products Z5, Z7 and Z9 (b-d, respectively).


(a)
MeOD
7'
6
6'
8'
8
10
11'
10'
12'b, 11
7
12
12'a
9'b
9'a
9
X : parts per Million : 1H
abundance


(b)
MeOD
7'
6
6'
8'
8
10'
11'
10'
12'b, 11
12'a
7
12
9'b
9'a
9
X : parts per Million : 1H
Y : parts per Million : 1H
abundance


(c)
DEPT-135
13C
MeOD
6
6'
8', 11, 8
11'
10
10'
7'
7
9
9'
4'
4
2,2'
5'
5
12', 12
abundance
X : parts per Million : 13C
(d)
MeOD
9'b
9'a
12'a
12'b, 11'
Y : parts per Million : 13C
X : parts per Million : 1H
(thousandths)

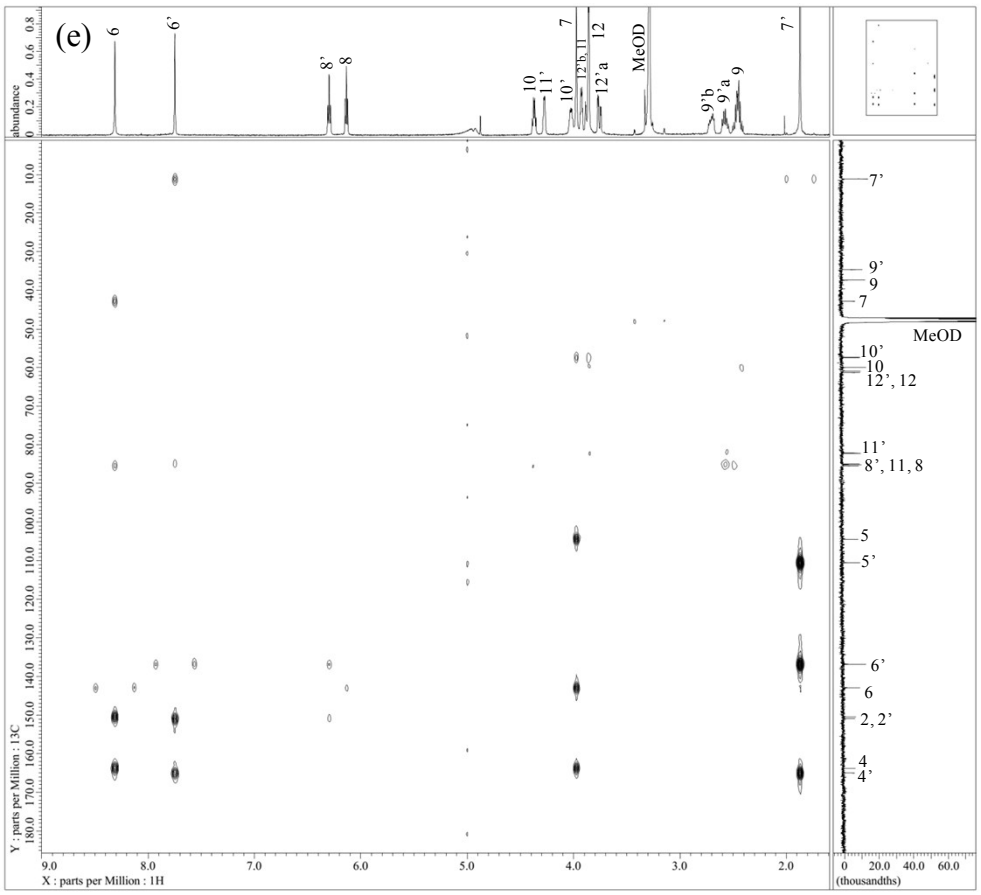
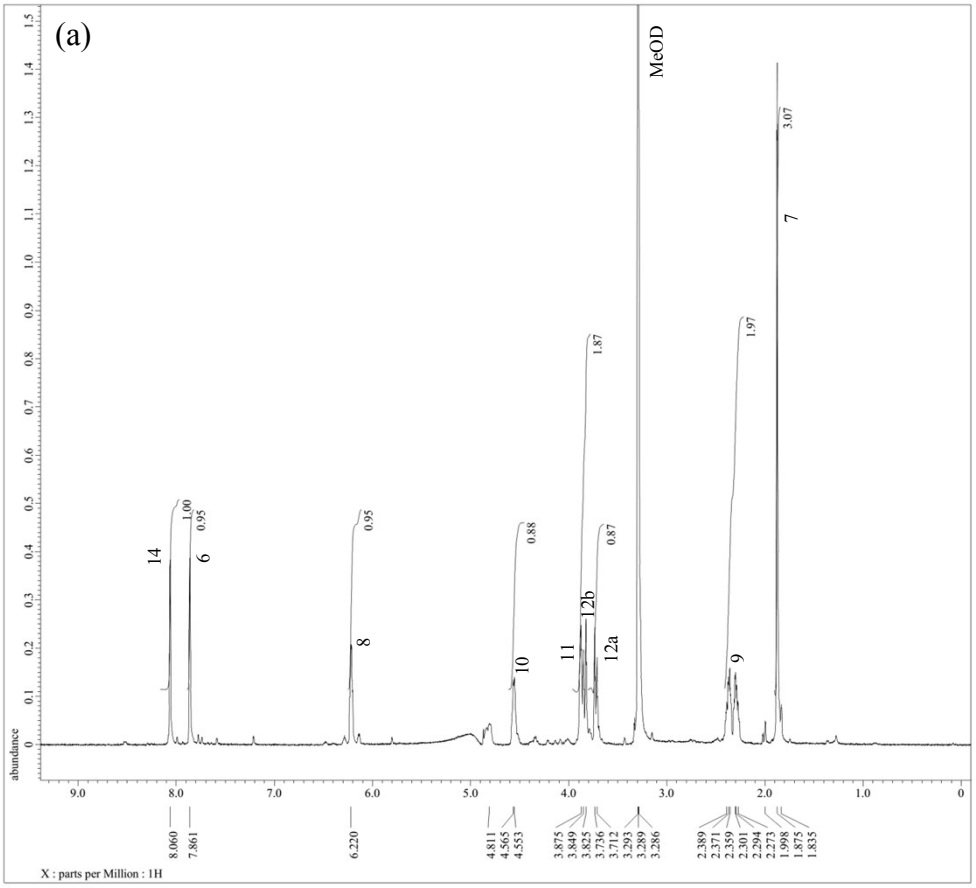
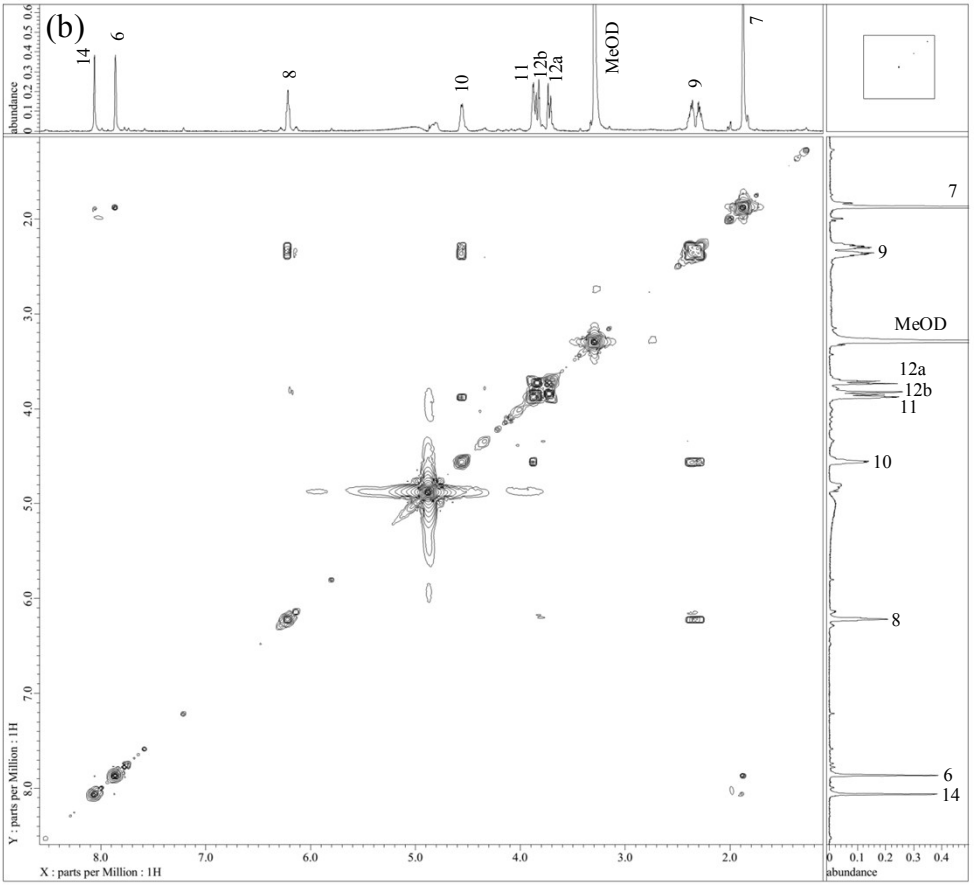
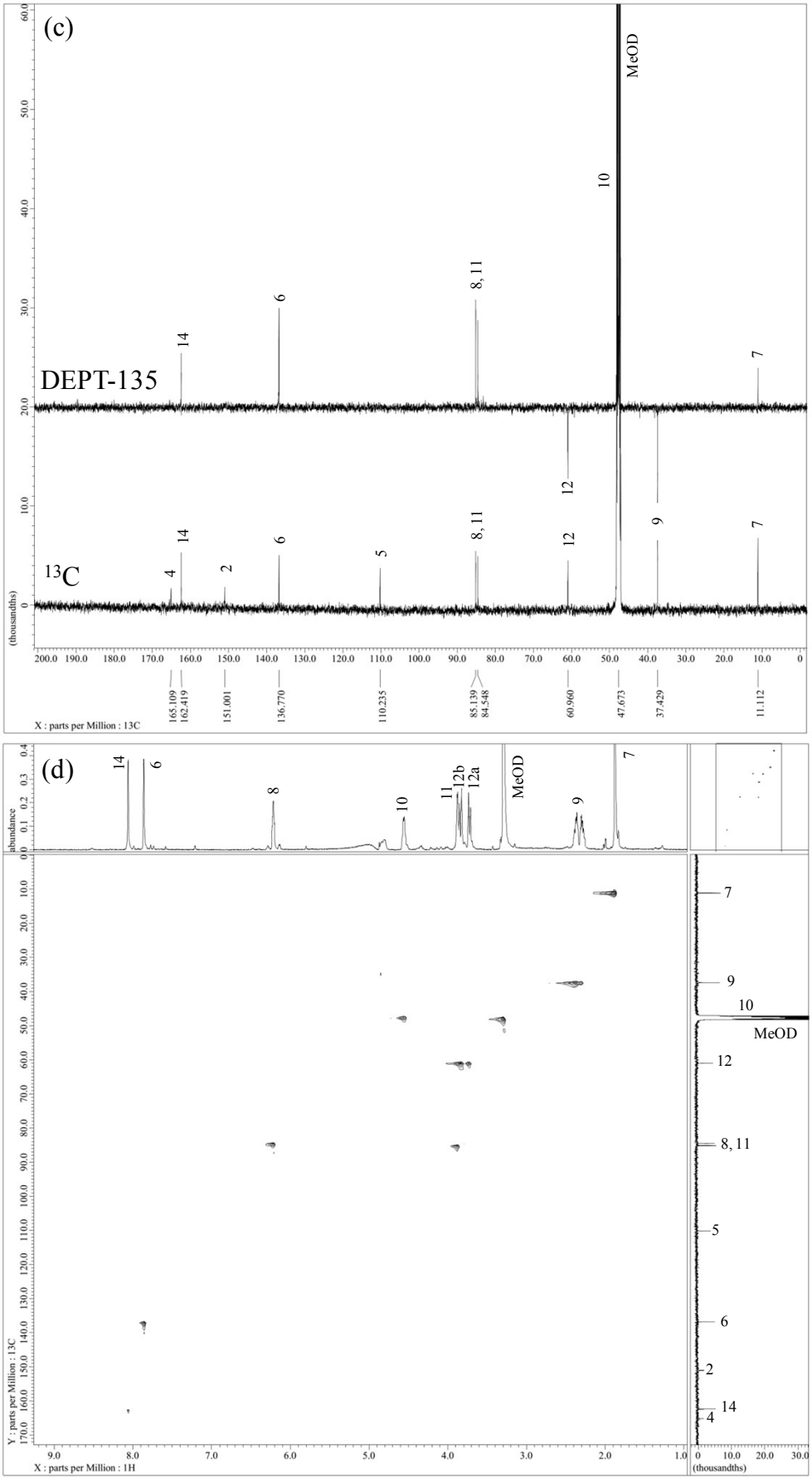


Fig. S4. NMR spectra of degradation product Z6, ^{1}H (a); COSY (b); ^{13}C and DEPT-135 (c); HSQC (d), and HMBC (e).


(a)
MeOD
14
6
8
10
11
12b
12a
9
7
abundance
X : parts per Million : 1H


(b)
14
6
8
10
11
12b
12a
MeOD
9
7
MeOD
12a
12b
11
10
8
6
14
Y : parts per Million : 1H
X : parts per Million : 1H
abundance


(c)
DEPT-135
^{13}C
MeOD
14
6
8, 11
10
7
12
9
5
4
2
(thousandths)
X : parts per Million : 13C
(d)
abundance
12b
12a
11
Y : parts per Million : 13C
X : parts per Million : 1H
(thousandths)

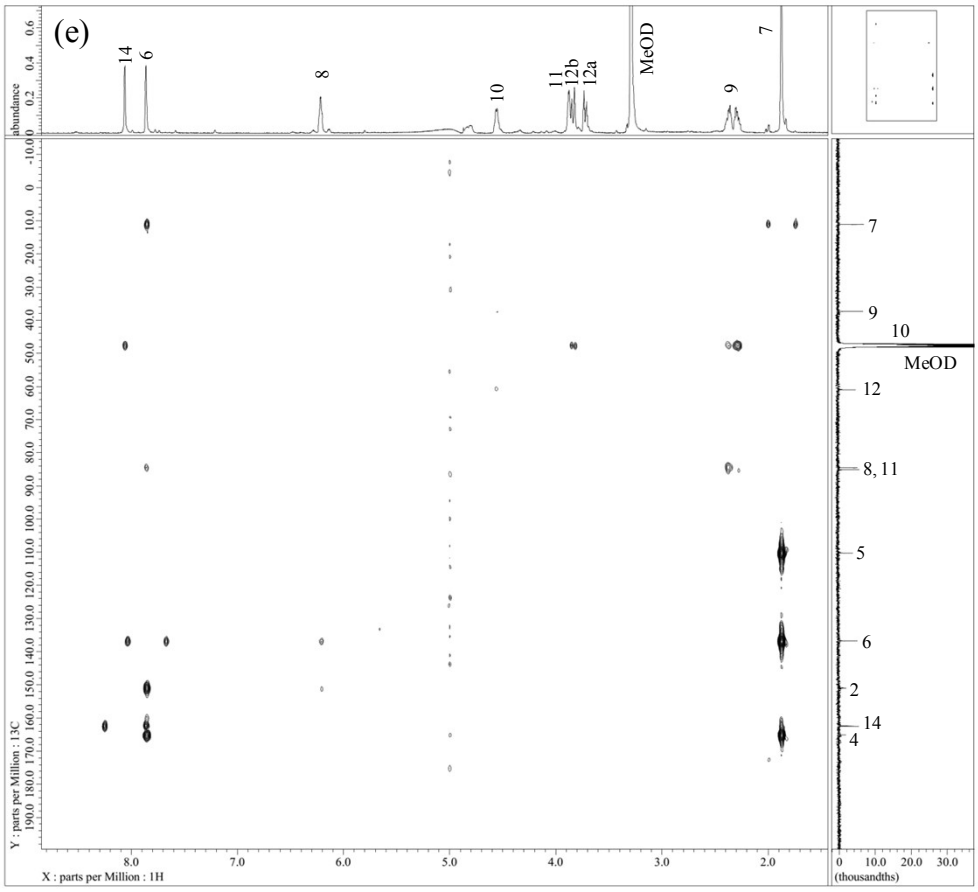
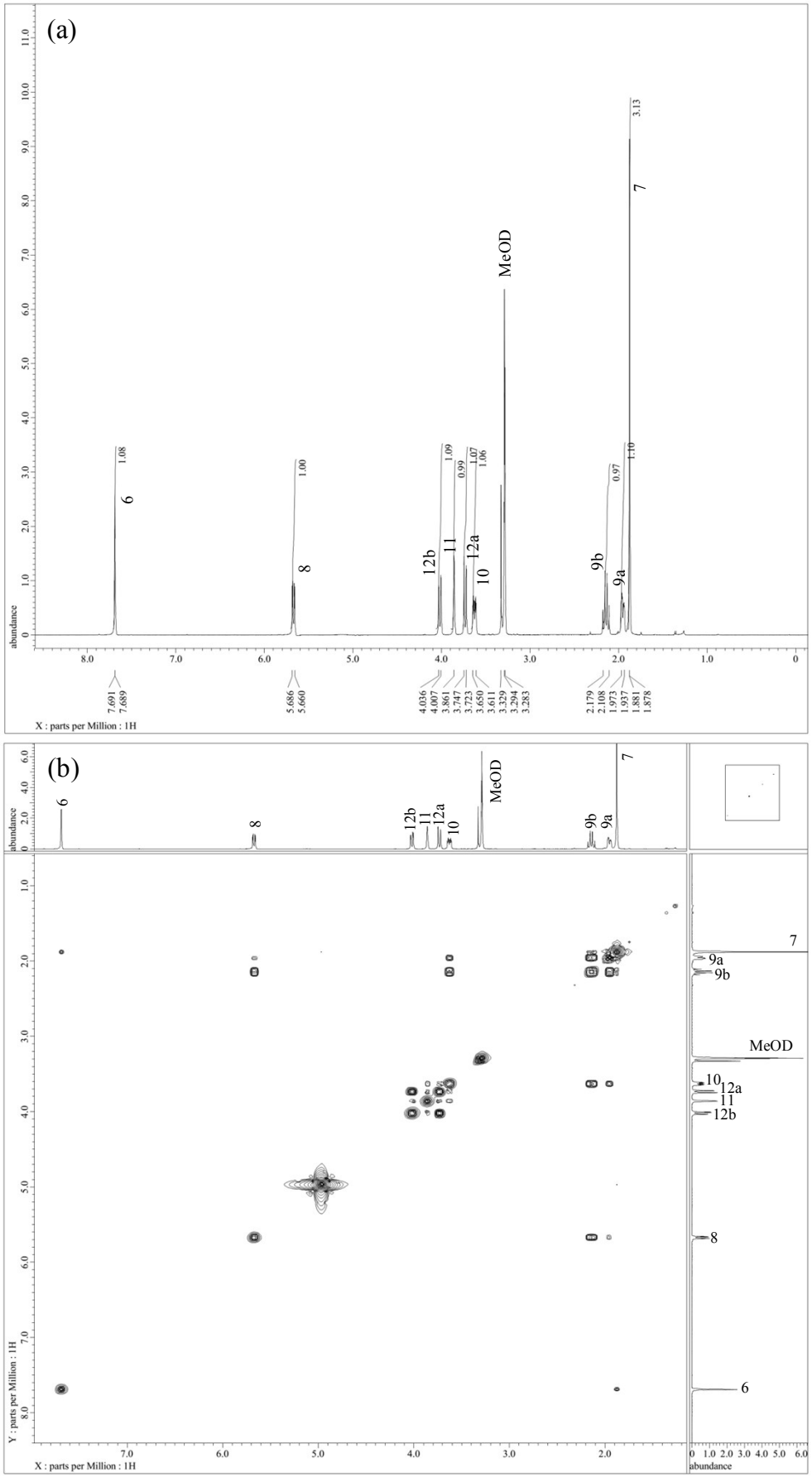
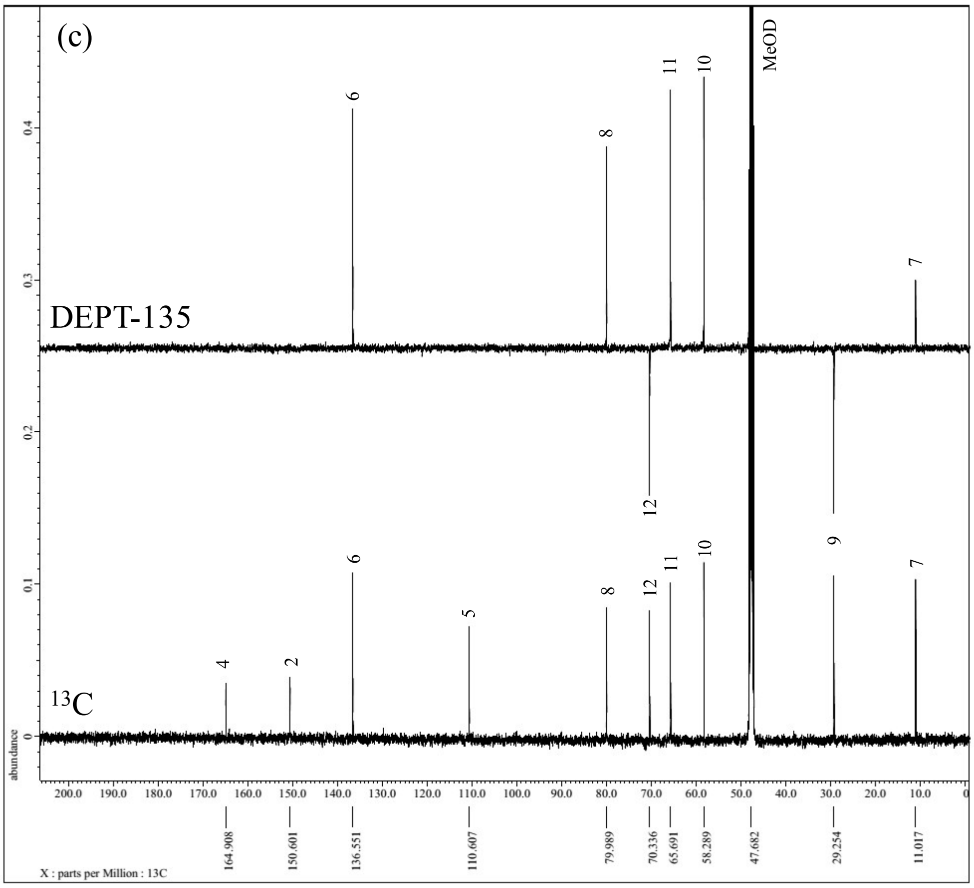
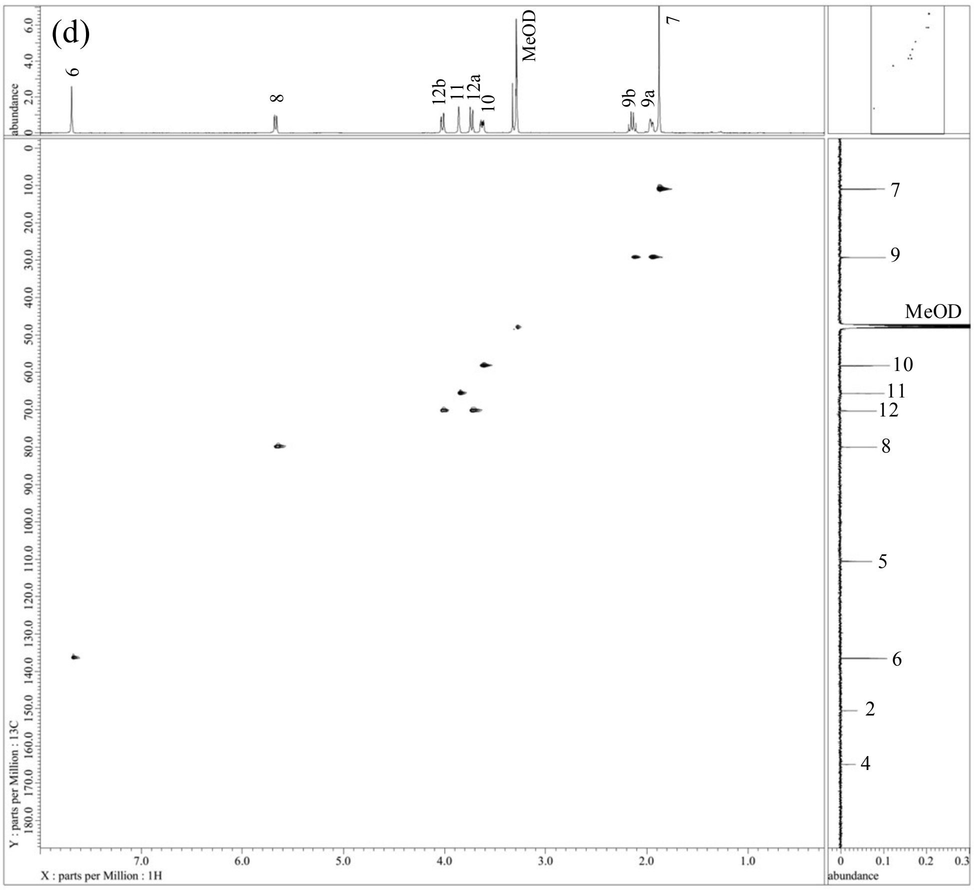


Fig. S5. NMR spectra of degradation product Z5, ^{1}H (a); COSY (b); ^{13}C and DEPT-135 (c); HSQC (d), and HMBC (e).


(a)
abundance
X : parts per Million : 1H
6
8
12b
11
12a
10
MeOD
9b
9a
7
1.08
1.00
1.09
0.99
1.07
1.06
0.97
1.10
3.13
7.691
7.689
5.686
5.660
4.036
4.007
3.861
3.747
3.723
3.650
3.611
3.329
3.294
3.283
2.179
2.108
1.973
1.937
1.881
1.878
(b)
Y : parts per Million : 1H
X : parts per Million : 1H
abundance


(c)
DEPT-135
13C
MeOD
6
8
11
10
7
12
9
4
2
5
164.908
150.601
136.551
110.607
79.989
70.336
65.691
58.289
47.682
29.254
11.017
X : parts per Million : 13C


(d)
6
8
12b
11
12a
10
MeOD
9b
9a
7
X : parts per Million : 1H
Y : parts per Million : 13C
10
11
12
8
5
6
2
4

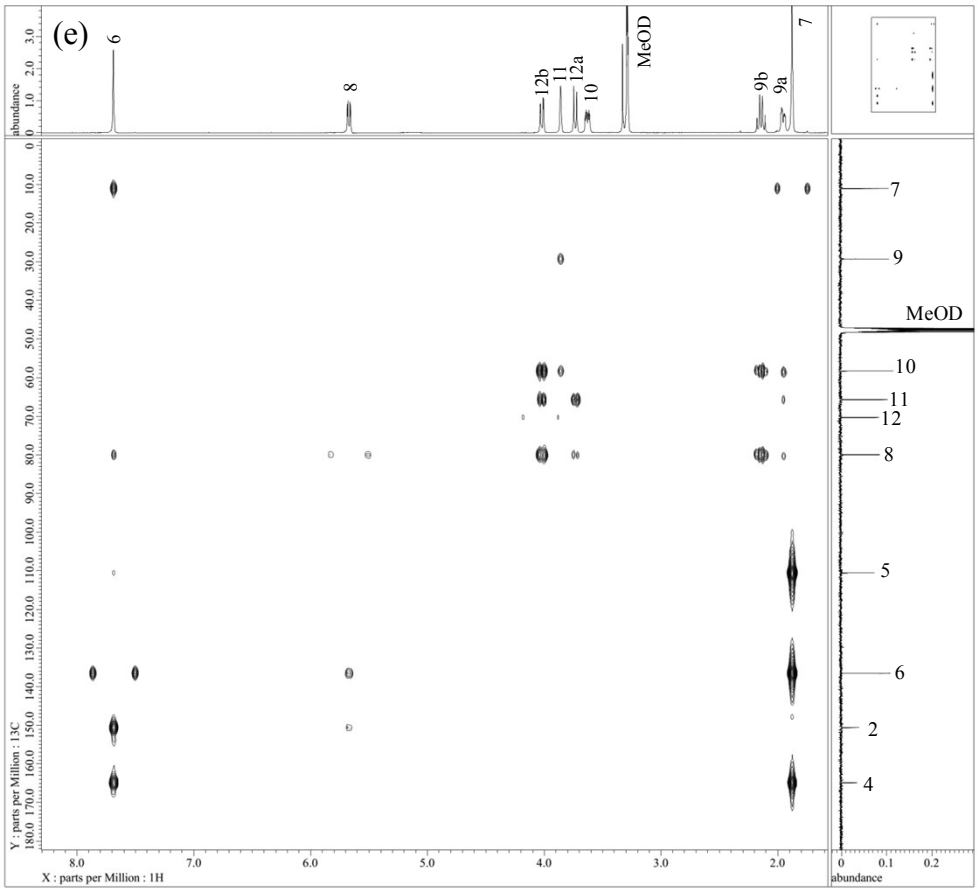
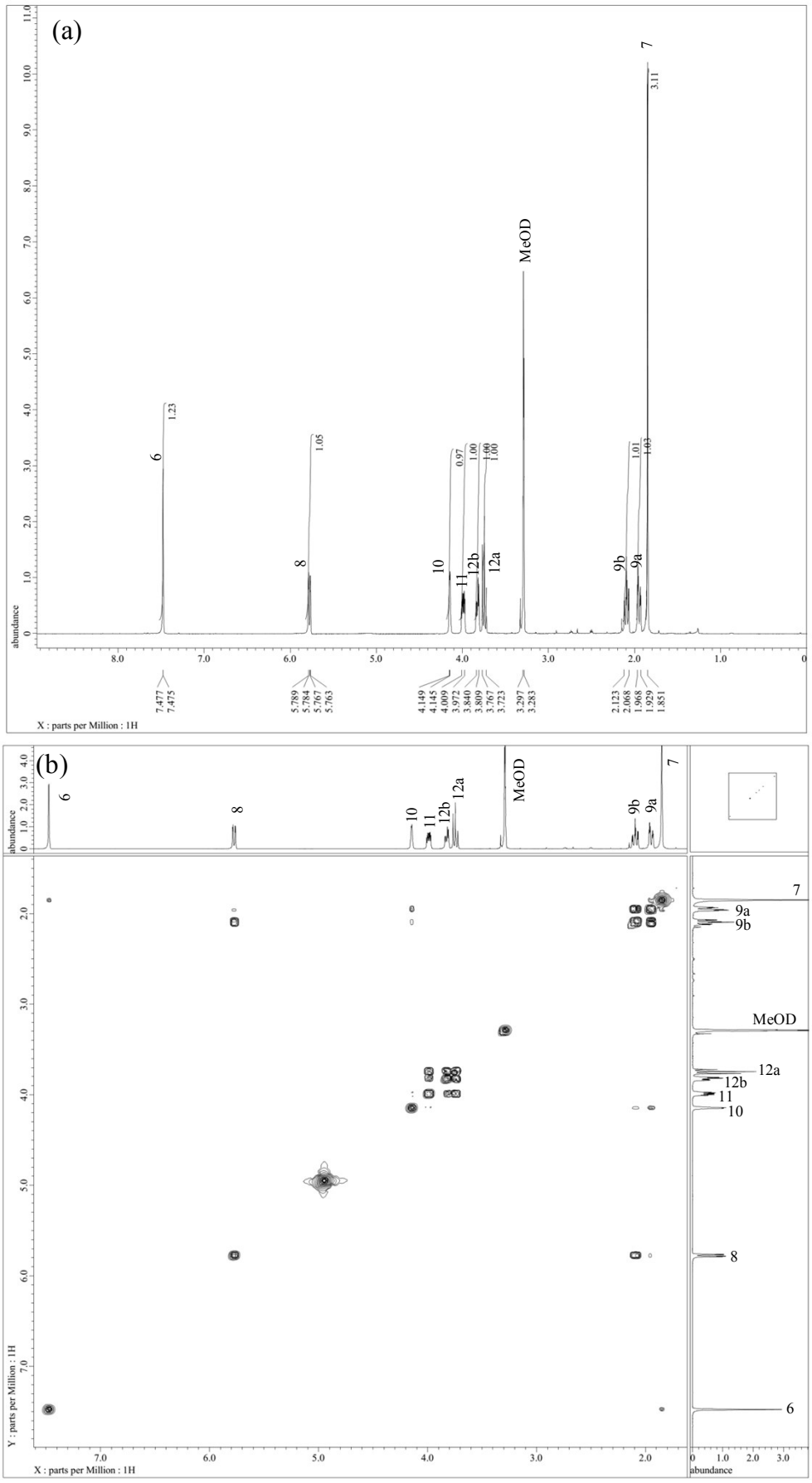
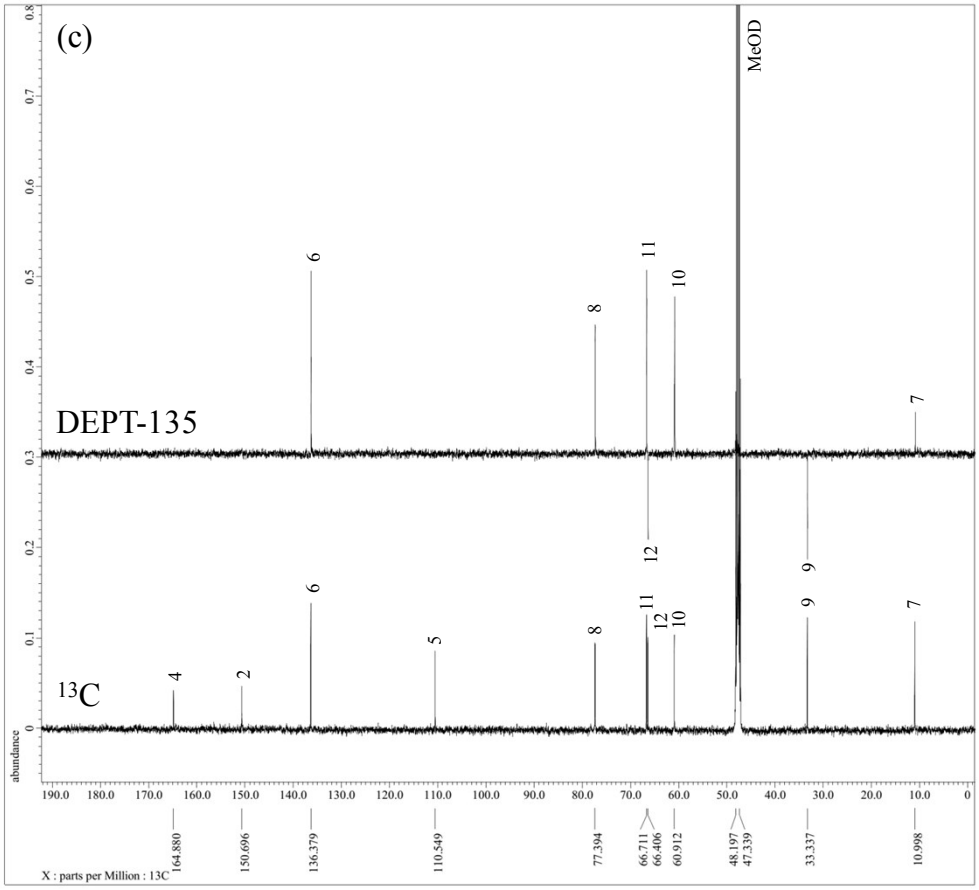
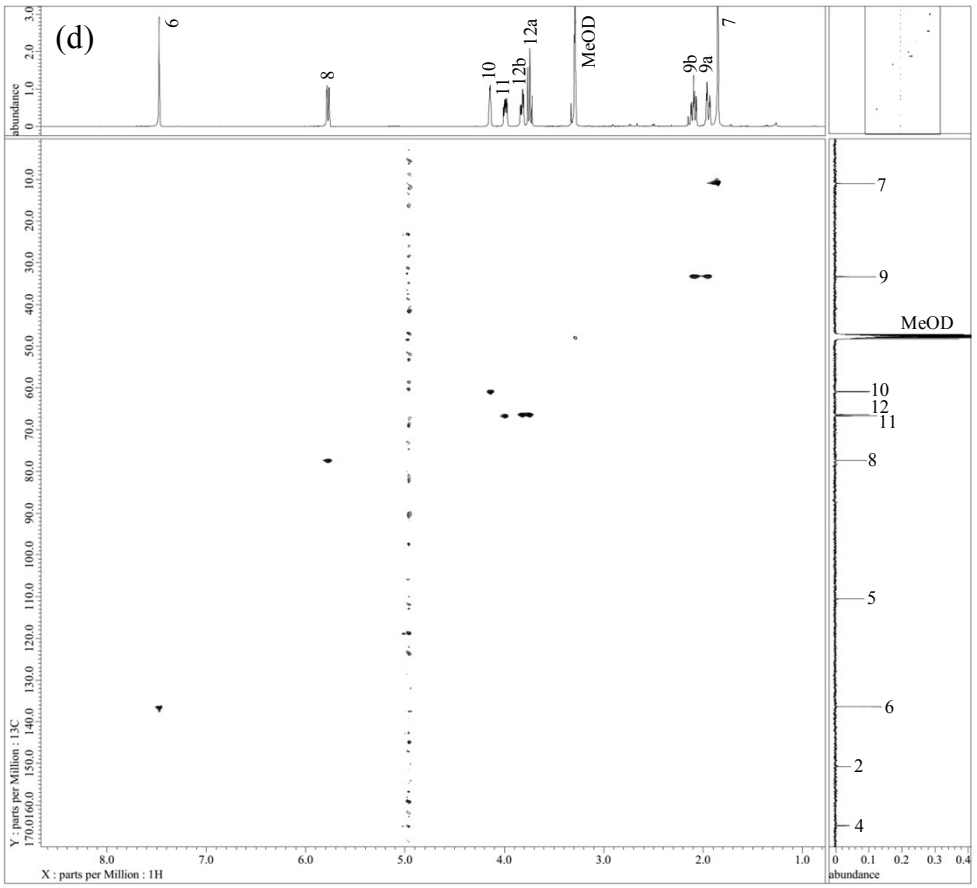


Fig. S6. NMR spectra of degradation product Z7, ^{1}H (a); COSY (b); ^{13}C and DEPT-135 (c); HSQC (d), and HMBC (e).


(a)
7
3.11
MeOD
6
1.23
8
1.05
10
11
12b
12a
9b
9a
abundance
X : parts per Million : 1H
(b)
Y : parts per Million : 1H
X : parts per Million : 1H
abundance


(c)
DEPT-135
^{13}C
MeOD
6
11
10
8
7
12
9
5
4
2
abundance
X : parts per Million : 13C
164.880
150.696
136.379
110.549
77.394
66.711
66.406
60.912
48.197
47.339
33.337
10.998


(d)
6
8
10
11
12b
12a
MeOD
9b
9a
7
abundance
Y : parts per Million : 13C
X : parts per Million : 1H
MeOD
10
12
11
8
5
6
2
4

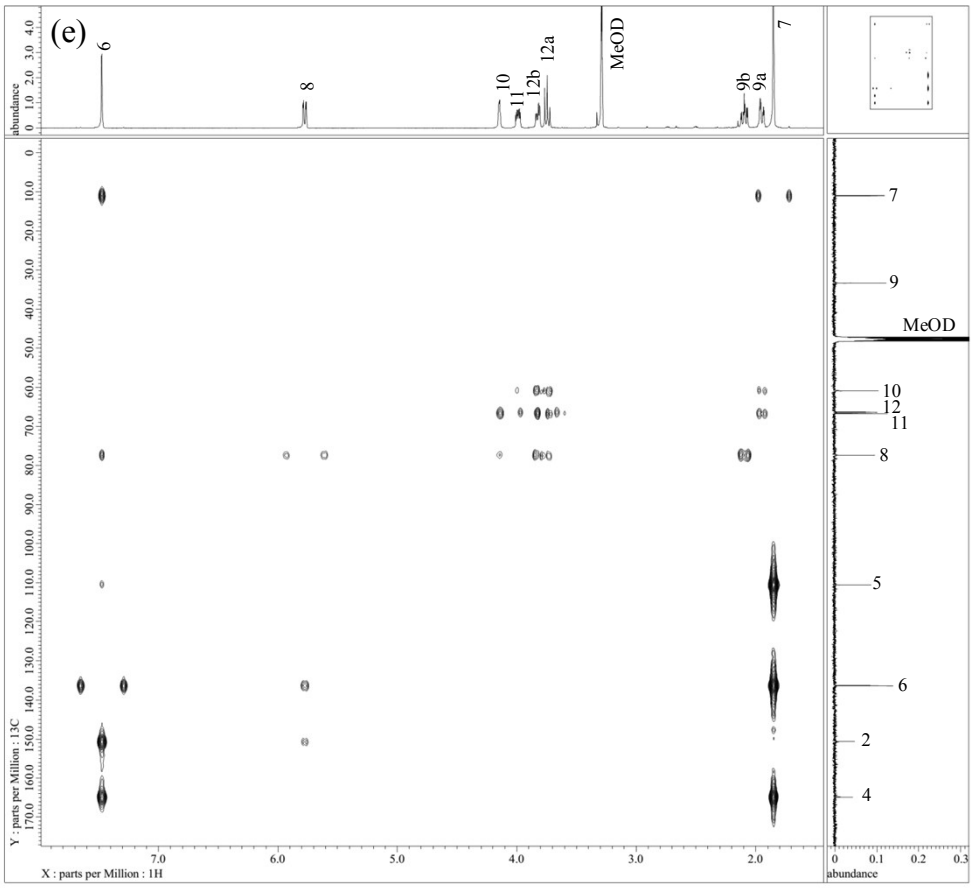
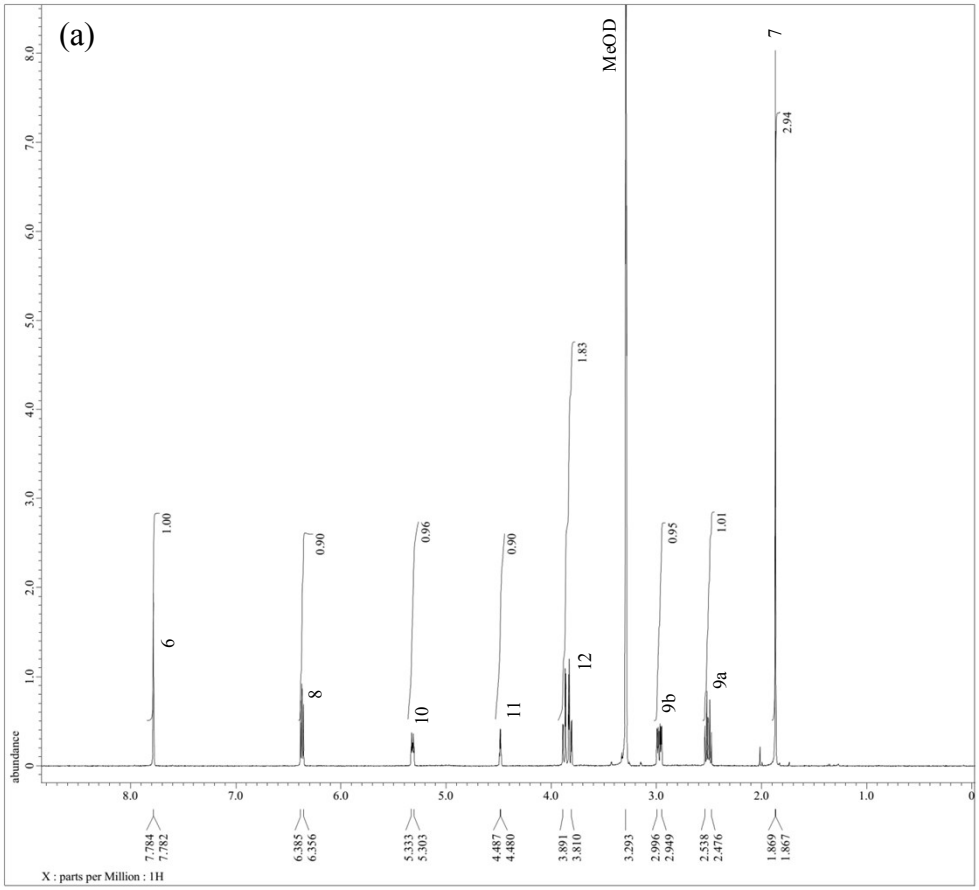
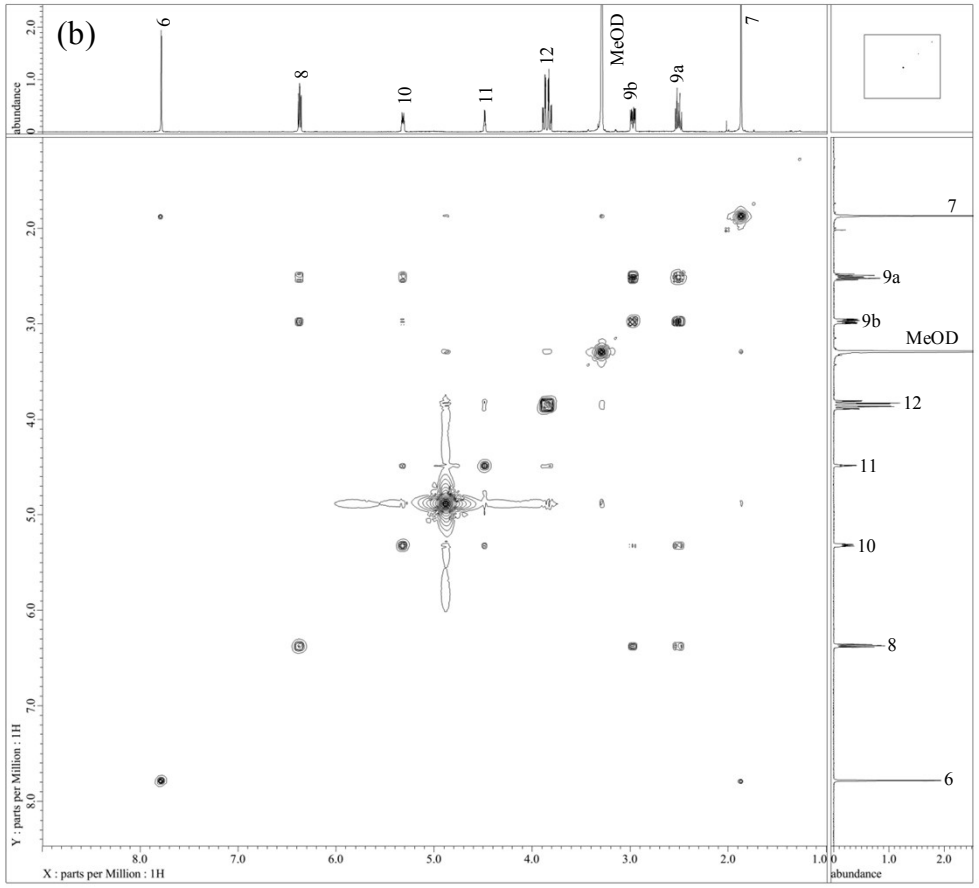
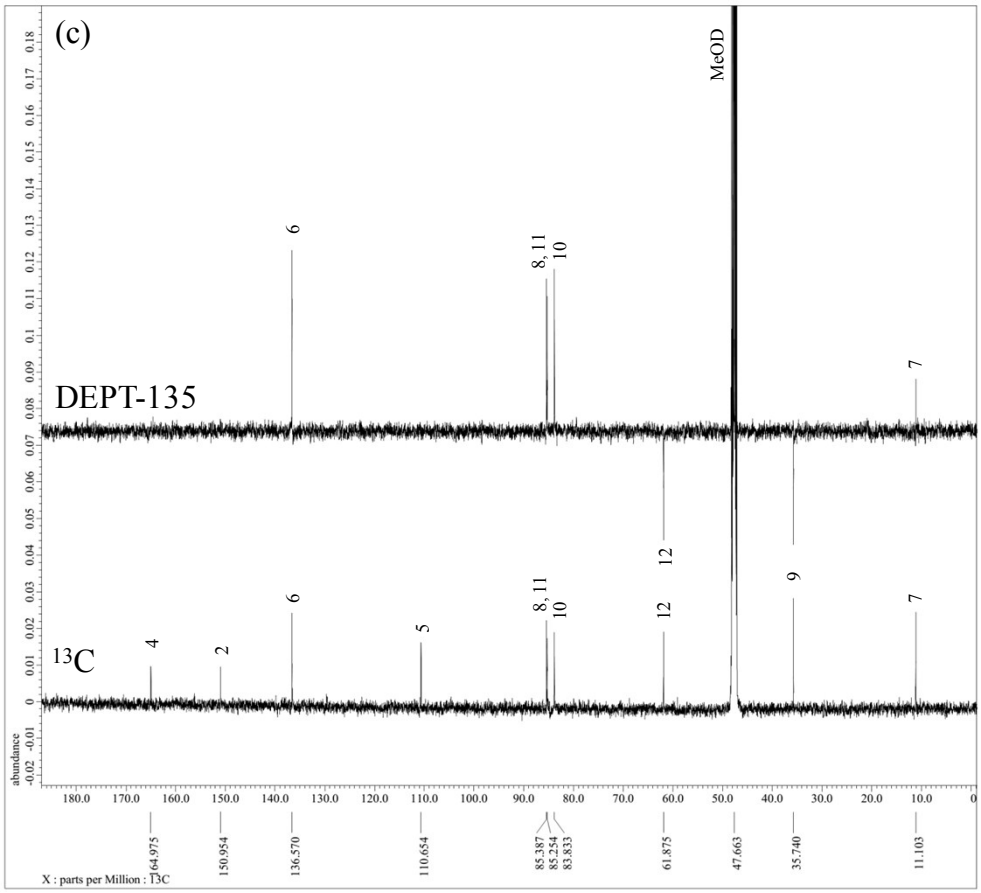
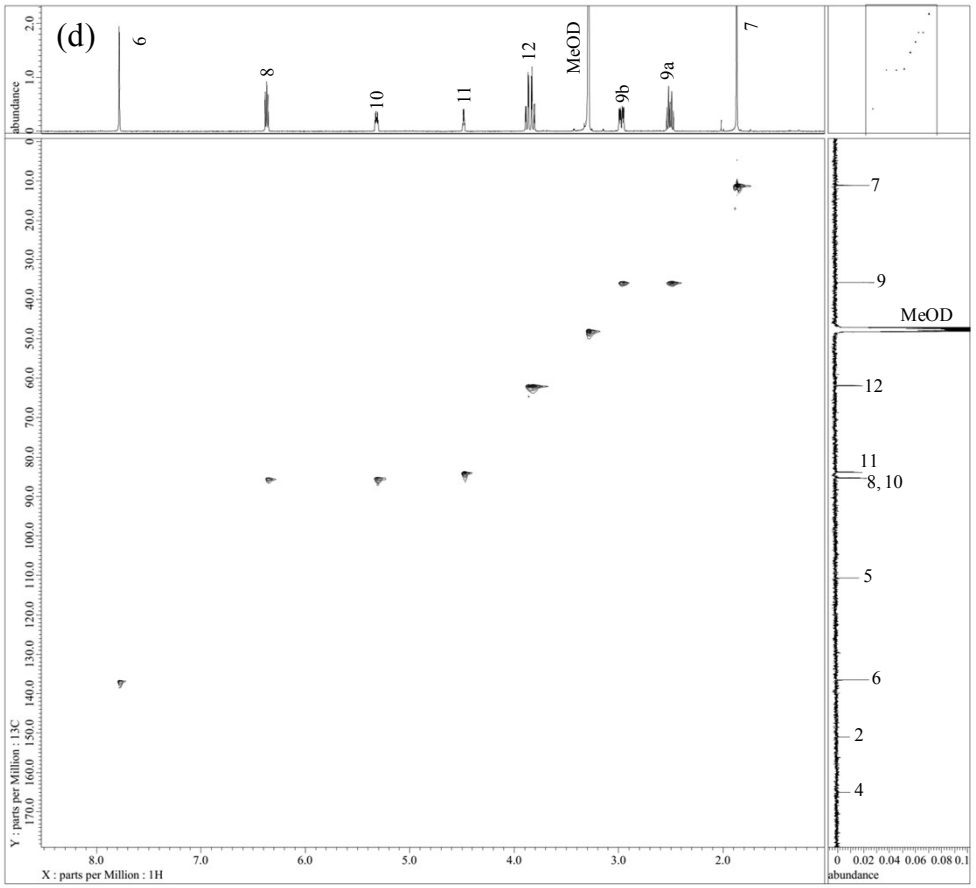


Fig. S7. NMR spectra of degradation product Z9, ^{1}H (a); COSY (b); ^{13}C and DEPT-135 (c); HSQC (d), and HMBC (e).


(a)
MeOD
7
2.94
1.83
1.00
0.90
0.96
0.90
0.95
1.01
6
8
10
11
12
9b
9a
abundance
X : parts per Million : 1H
7.784
7.782
6.385
6.356
5.333
5.303
4.487
4.480
3.891
3.810
3.293
2.996
2.949
2.538
2.476
1.869
1.867


(b)
6
8
10
11
12
MeOD
9b
9a
7
abundance
Y : parts per Million : 1H
X : parts per Million : 1H


(c)
DEPT-135
^{13}C
MeOD
6
8, 11
10
7
12
9
4
2
5
64.975
150.954
136.570
110.654
85.387
85.254
83.833
61.875
47.663
35.740
11.103
X : parts per Million : 13C
abundance


(d)
6
8
10
11
12
MeOD
9b
9a
7
9
12
11
8, 10
5
2
4
Y : parts per Million : 13C
X : parts per Million : 1H
abundance

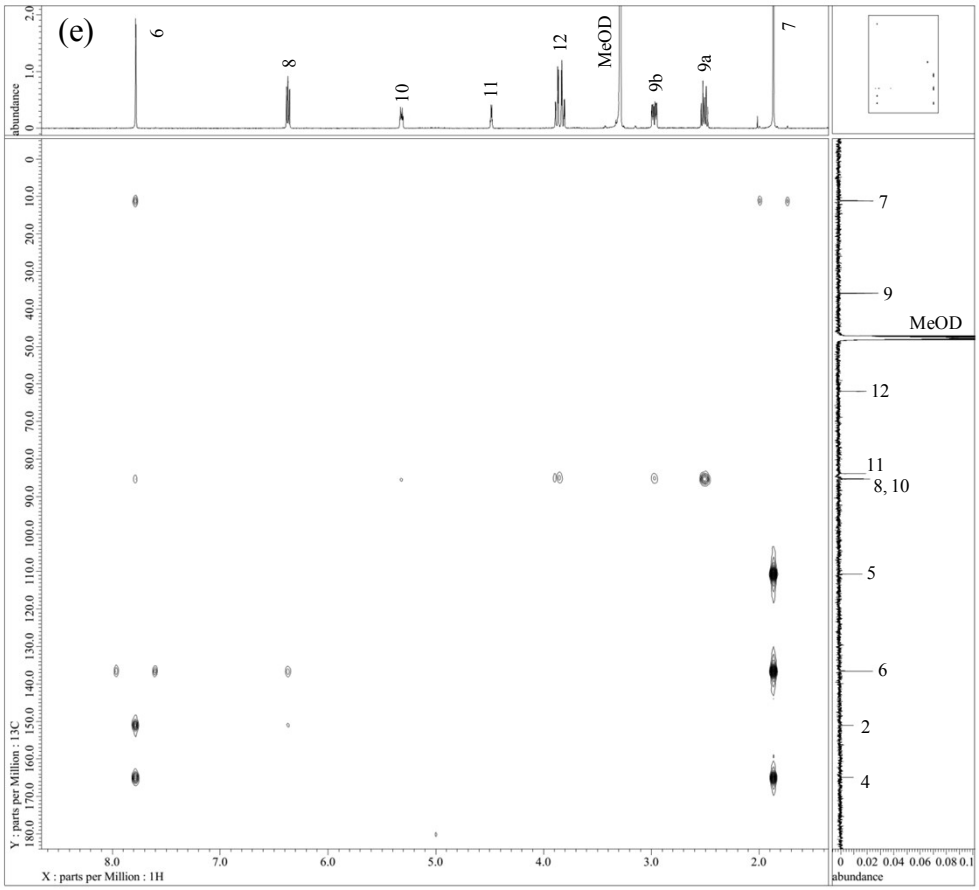


Fig. S8. NMR spectra of degradation product Z8, ^{1}H (a); COSY (b); ^{13}C and DEPT-135 (c); HSQC (d), and HMBC (e).