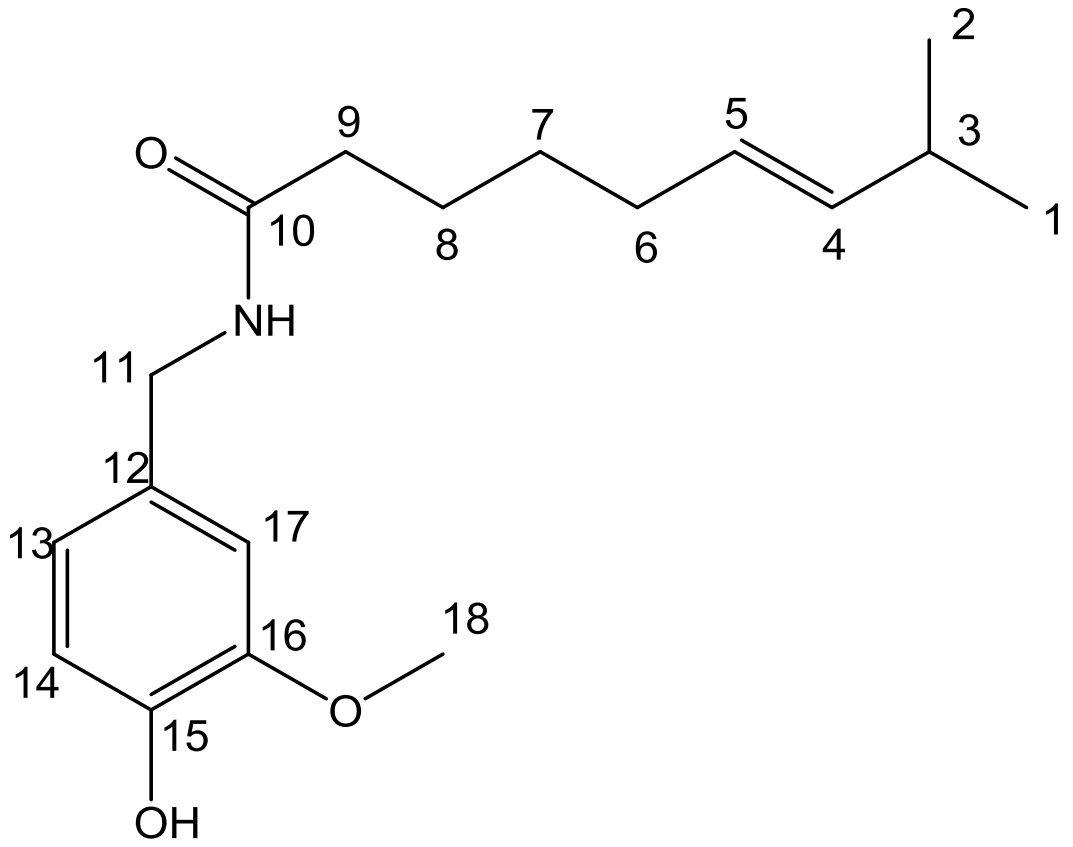
W5 (backwards)



(*E*)-*N*-(4-hydroxy-3-methoxybenzyl)-8-methylnon-6-enamide

Chemical Formula: $C_{18}H_{27}NO_3$

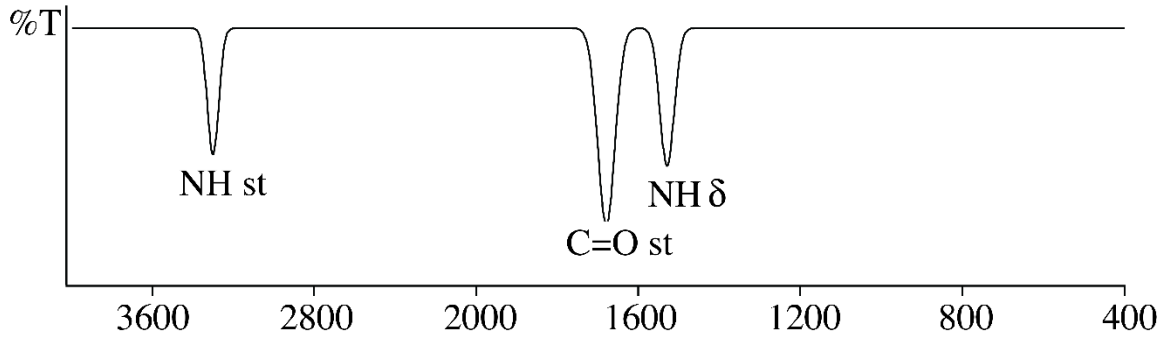
Molecular Weight: 305.42

Capsaicin is an active component of chili peppers

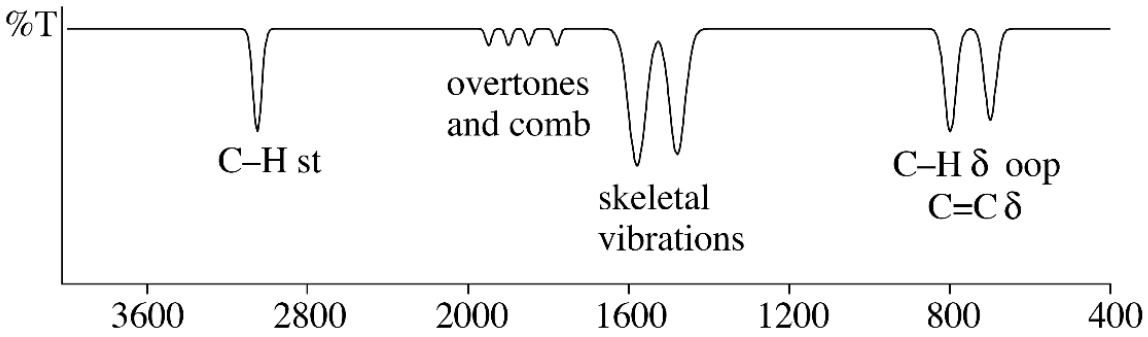
IR

3550 cm^{-1}	O–H free
3450 cm^{-1}	N–H free
≈ 3000 cm^{-1}	C–H str
1660 cm^{-1}	C=O str. – Amid I + C=C
1510 cm^{-1}	N–C=O st sy – Amid II
1620,1450,1430 cm^{-1}	Skeletal vibrations

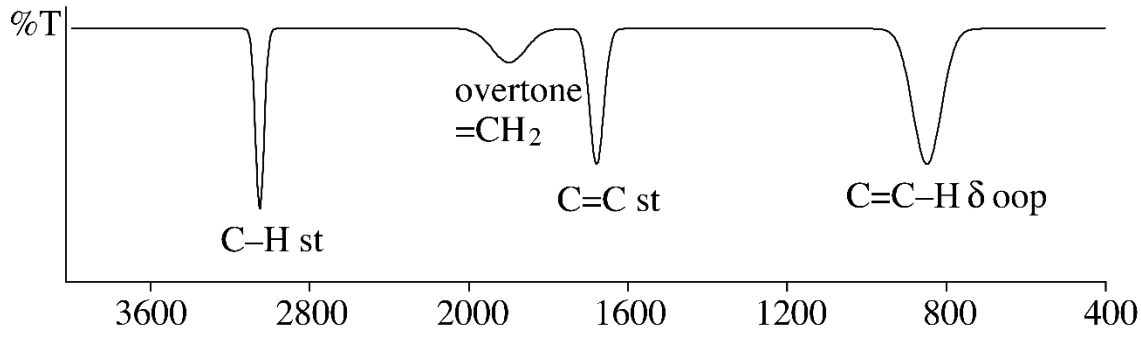
Secondary Amides



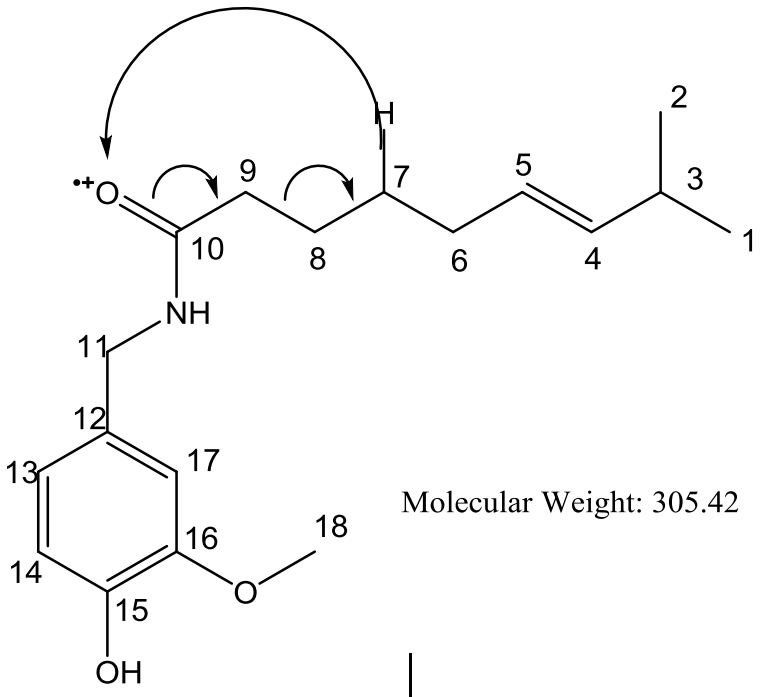
7.5 Aromatic Hydrocarbons



7.2.1 Monoenes

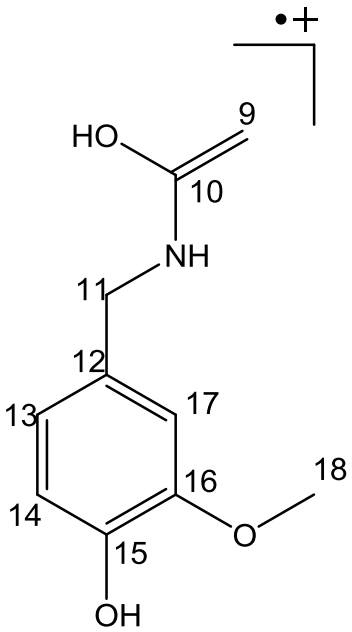


MS



Molecular Weight: 305.42

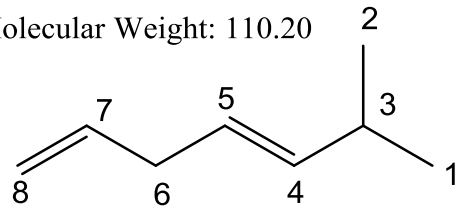
McLafferty rearrangement

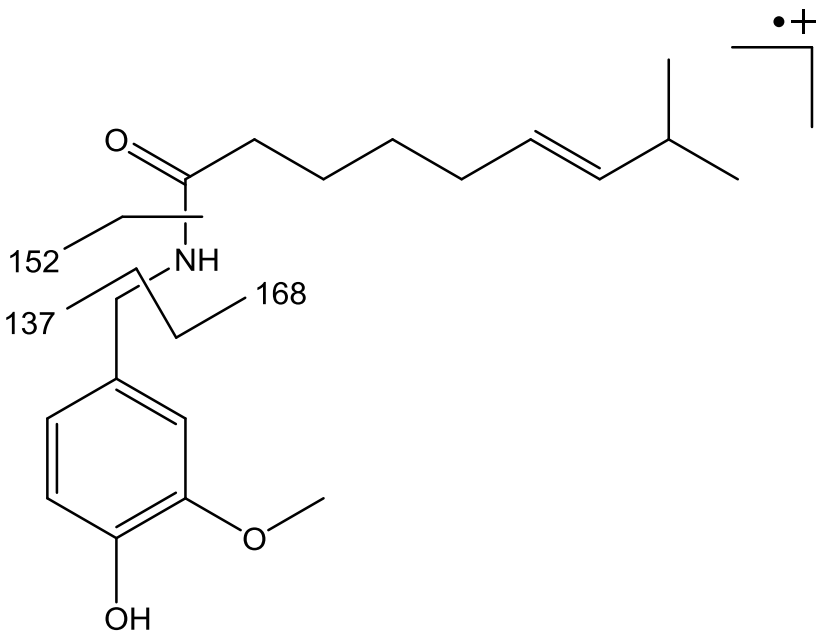


Molecular Weight: 195.22

+

Molecular Weight: 110.20




•+
O
NH
152
168
137
O
OH

^{13}C NMR-Spectrum

δ (ppm)	DEPT	Assignment	Group
172	C	10	C=O (amide)
146	C	15/16	Aromatic & C=C
145	C		
138	CH	13/14/17/4/5	
130	C	12	
126	CH	13/14/17/4/5	
120	CH		
114	CH		
110	CH		
55	CH_3	18	CH_3-O
43	CH_2	11	CH_2-N
36	CH_2	6/7/8/9	Aliphatic
32	CH_2		
30	CH	3	
29	CH_2	6/7/8/9	
25	CH_2		
22	CH_3	1/2	

^{1}H NMR-Spectrum

δ (ppm)	Int.	Couppl.	**Assignment**	Group
6.85	1	D	14	1x o-coupling
6.80	1	d	17	1x m- coupling
6.75	1	Dxd	13	o & m- coupling
5.67	1	S, broad	NH	
5.65	1	S	OH	
5.35	2	> 9L	4/5	-CH=CH-
4.35	2	d	11	$NH\text{-}CH_2$
3.87	3	S	18	$O\text{-}CH_3$
2.2	3	≥ 7L	3,6-9	Aliphatic
2.0	2	≈ Q		
1.65	~2	≈ 5L		
1.4	2	≈ 5L		
0.95	6	d	1/2	

HSQC

^{13}C NMR		^{1}H NMR				
δ (ppm)	**DEPT**	δ (ppm)	Int.	Couppl.	**Assignment**	Group
138	CH	6.85	1	D	14	1x o-coupling
110	CH	6.80	1	d	17	1x m-coupling
120	CH	6.75	1	Dxd	13	o & m-coupling
-		5.67	1	S, broad	NH	
-		5.65	1	S	OH	
126 & 138	2x CH	5.35	2	> 9L	4/5	-CH=CH-
43	CH_2	11	2	d	11	NH-CH_2
55	CH_3	3.87	3	S	18	O-CH_3
30	CH	2.2	3	≥ 7L	3	Aliphatic
36	CH_2				6-9	
32	CH_2	2.0	2	≈ Q		
25	CH_2	1.65	~2	≈ 5L		
29	CH_2	1.4	2	≈ 5L		
22	2xCH_3	0.95	6	d	1/2	

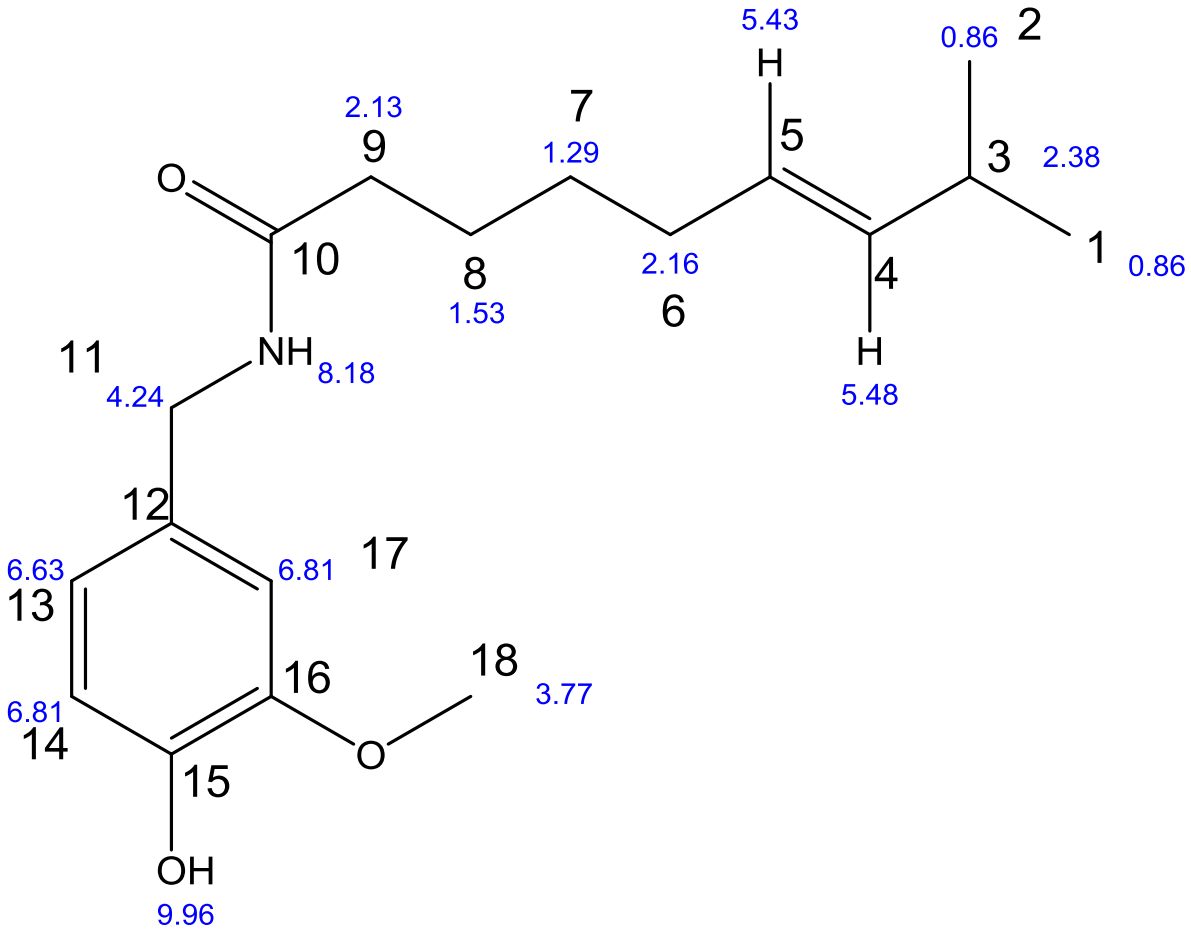
COSY

	#	14	17	13	NH	OH	4/5	11	18	3	9	6	8	7	1/2
#	δ (ppm)	6.85	6.8	6.75	5.67	5.65	5.35	4.35	3.87	2.2	2.2	2	1.65	1.4	0.95
14	6.85	x													
17	6.8	x	x												
13	6.75	x	x	x											
NH	5.67				x										
OH	5.65					x									
4/5	5.35						x								
11	4.35				x			x							
18	3.87								x						
3	2.2						x			x					
9	2.2										x				
6	2						x					x			
8	1.65										x		x		
7	1.4											x	x	x	
1/2	0.95									x					x

NOE

Protons sitting on #18 are next to #17 and –OH group

ChemNMR ^{1}H Estimation



ChemNMR ^{13}C Estimation