Synthesis, structural and antimicrobial studies of some 1-[2-(1*H*-benzimidazol-1-yl)acetyl]-2,6-diarylpiperidin-4-ones

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Table S1. Mass spectral data [*m/z* (relative intensity %)] of compounds **21-30**

Entry	**A**	**B**	**C**	**D/S**	**E**	**F**	**G**	**J**	**K**	**L**	**O**	**P**	**R**	**U**	**V**
21	423 (5.3)	159 (2.9)	264 (3.8)	104 (24.8)	249 (3.1)	-	176 (5.2)	119 (22.7)	132 (100)	131 (51.5)	160 (2.61)	132 (100)	119 (22.7)	104 (24.8)	77 (32.0)
22	437 (22.6)	159 (6.5)	278 (14.4)	104 (20.8)	249 (8.5)	-	176 (15.7)	119 (30.3)	132 (100)	-	-	-	119 (30.3)	104 (20.8)	77 (23.4)
23	437 (8.6)	159 (1.7)	278 (1.9)	104 (15.0)	263 (6.4)	262 (6.8)	176 (11.9)	119 (30.5)	132 (100)	131 (48.5)	160 (4.8)	132 (100)	119 (30.5)	104 (15.0)	77 (24.1)
24	459 (14.9)	159 (2.7)	-	122 (21.6)	-	-	176 (13.5)	119 (46.6)	132 (68.2)	131 (99.2)	178 (4.9)	150 (100)	137 (4.2)	104 (18.6)	77 (27.2)
25	473 (11.3)	159 (7.1)	-	122 (14.1)	-	298 (31.5)	176 (18.0)	119 (33.9)	132 (35.3)	131 (100)	178 (6.9)	150 (61.3)	137 (5.4)	104 (16.6)	77 (27.4)
26	491 (2.59)	159 (3.2)	333 (0.8)	138 (12.1)	-	-	176 (9.3)	119 (39.7)	132 (52.2)	131 (100)	194 (2.4)	166 (40.5)	153 (2.6)	104 (17.7)	77 (4.9)
27	505 (5.8)	159 (4.4)	-	138 (5.3)	-	331 (2.3)	176 (33.4)	119 (75.4)	132 (51.9)	131 (100)	194 (5.1)	166 (76.9)	153 (7.3)	104 (17.8)	77 (27.2)
28	579 (1.5)	159 (4.2)	-	-	-	406 (4.5)	176 (11.0)	119 (36.8)	132 (46.7)	131 (100)	-	211 (16.1)	-	104 (17.1)	77 (29.0)
29	593 (0.7)	159 (6.4)	-	-	-	-	176 (20.5)	119 (57.8)	132 (45.3)	131 (100)	-	211 (4.4)	-	104 (21.7)	77 (39.0)
30	465 (59.7)	159 (13.3)	306 (21.5)	118 (14.0)	-	290 (59.5)	176 (26.8)	119 (65.4)	132 (74.9)	131 (80.2)	174 (13.1)	146 (100)	133 (31.8)	104 (14.1)	77 (20.9)

A – Molecular ion-radical: **B** to **V** – Fragmented ions

Table S2. Crystal data and structure refinement of 1-Chloroacetyl-3,5-dimethyl-2,6-bis (*p*-methylphenyl)piperidin-4-one **20**

Empirical formula	$C_{23}H_{26}ClNO_2$
Formula weight	383.90
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.9590(4) A alpha = 95.483(2) deg. b = 14.3697(5) A beta = 113.333(2) deg. c = 14.7369(5) A gamma = 110.028(2) deg.
Volume	2104.84(12) A^3
Z, Calculated density	4, 1.211 Mg/m^3
Absorption coefficient	0.198 mm^{-1}
F(000)	816
Crystal size	0.26 x 0.20 x 0.20 mm
Theta range for data collection	1.56 to 24.54 deg.
Limiting indices	$-13 \leq h \leq 13$, $-16 \leq k \leq 16$, $-17 \leq l \leq 17$
Reflections collected / unique	36212 / 6958 [R(int.) = 0.0331]
Completeness to theta = 25.00	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9614 and 0.9503
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6958 / 0 / 528
Goodness-of-fit on F^2	1.028
Final R indices [I>2sigma(I)]	R1 = 0.0507, wR2 = 0.1411
R indices (all data)	R1 = 0.0740, wR2 = 0.1649
Extinction coefficient	0.0066(15)
Largest diff. peak and hole	0.746 and -0.473 $e.A^{-3}$

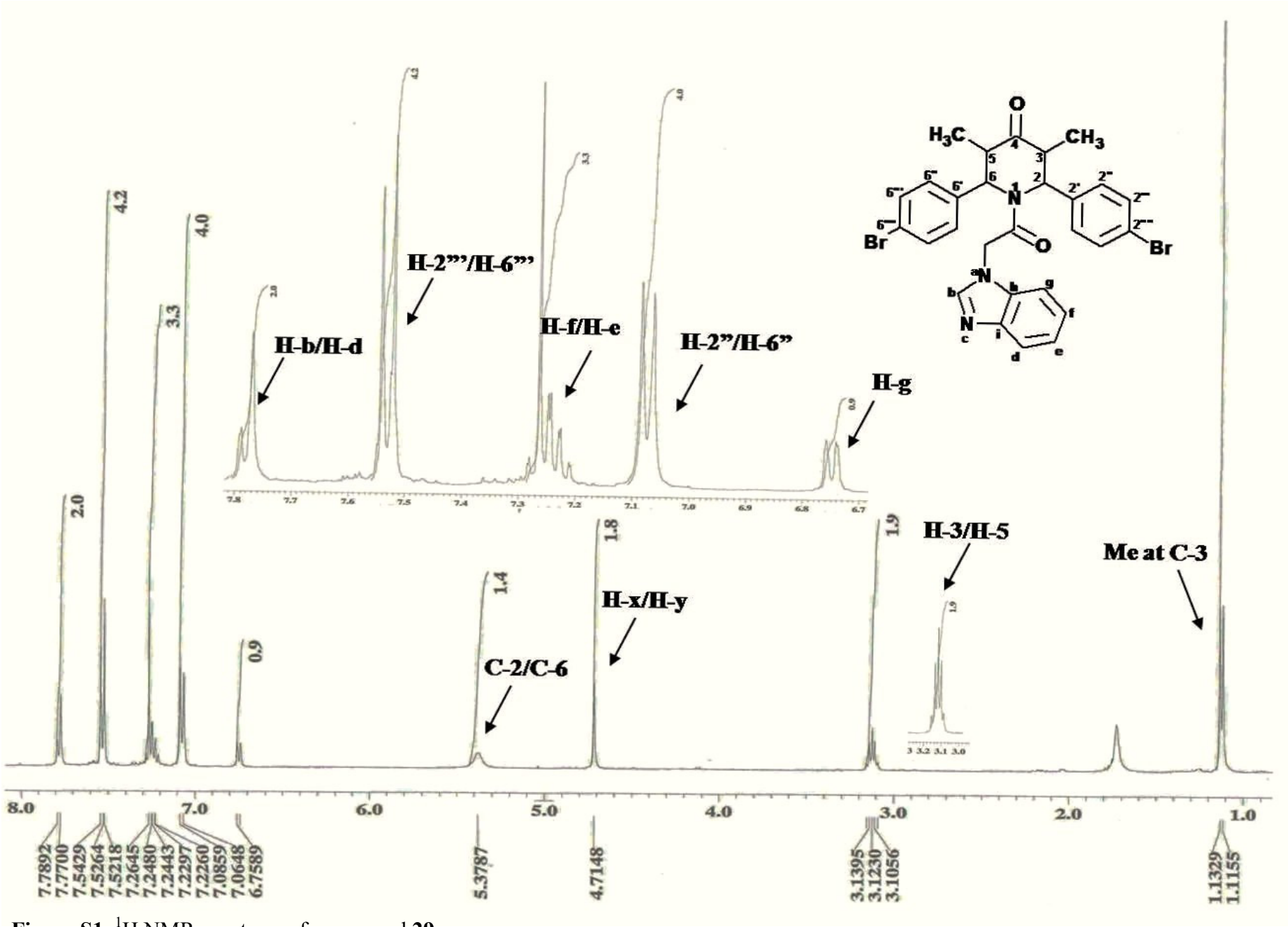

Figure S1. [1]H NMR spectrum of compound **29**

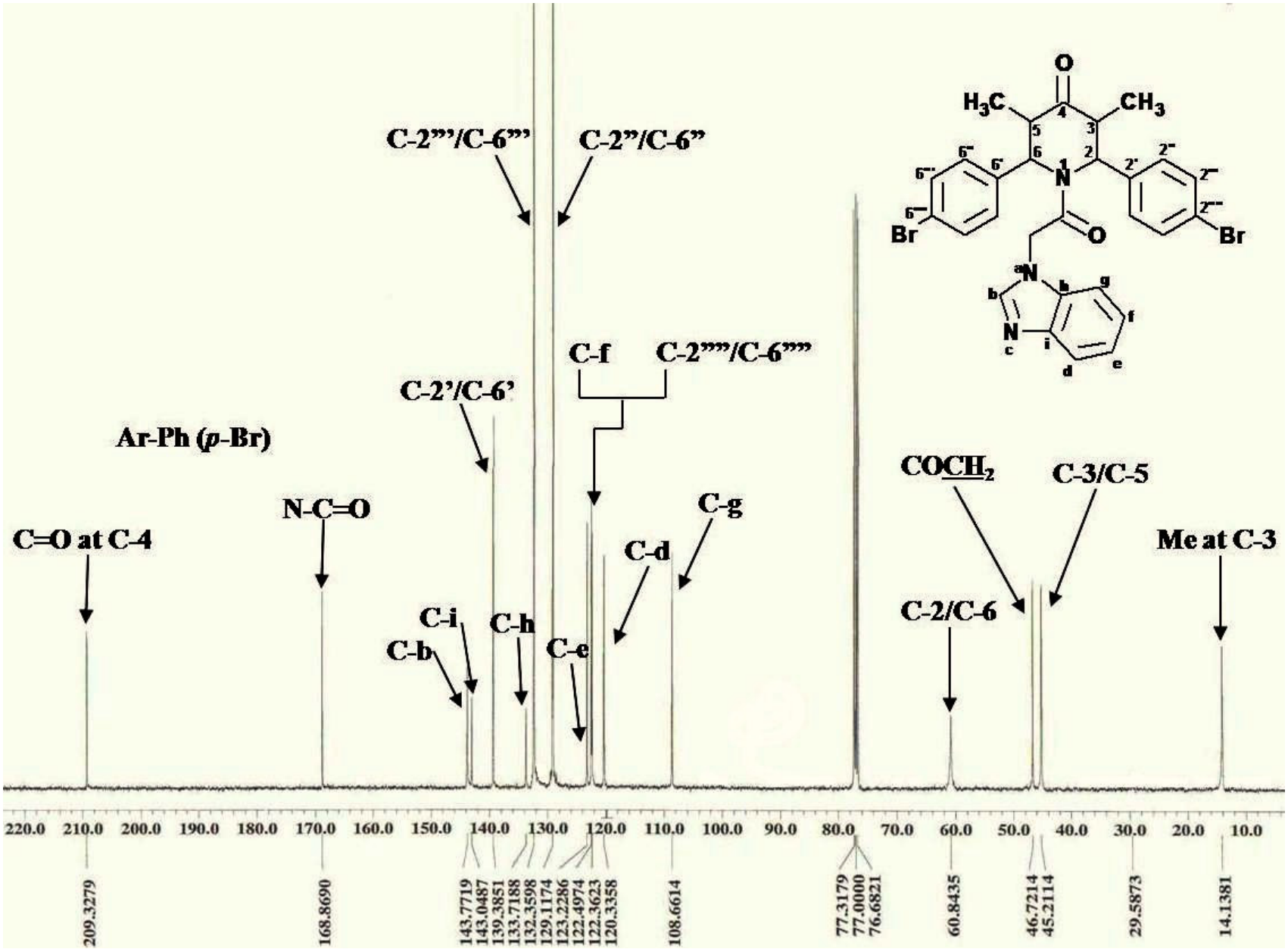

Figure S2. ^{13}C NMR spectrum of compound **29**

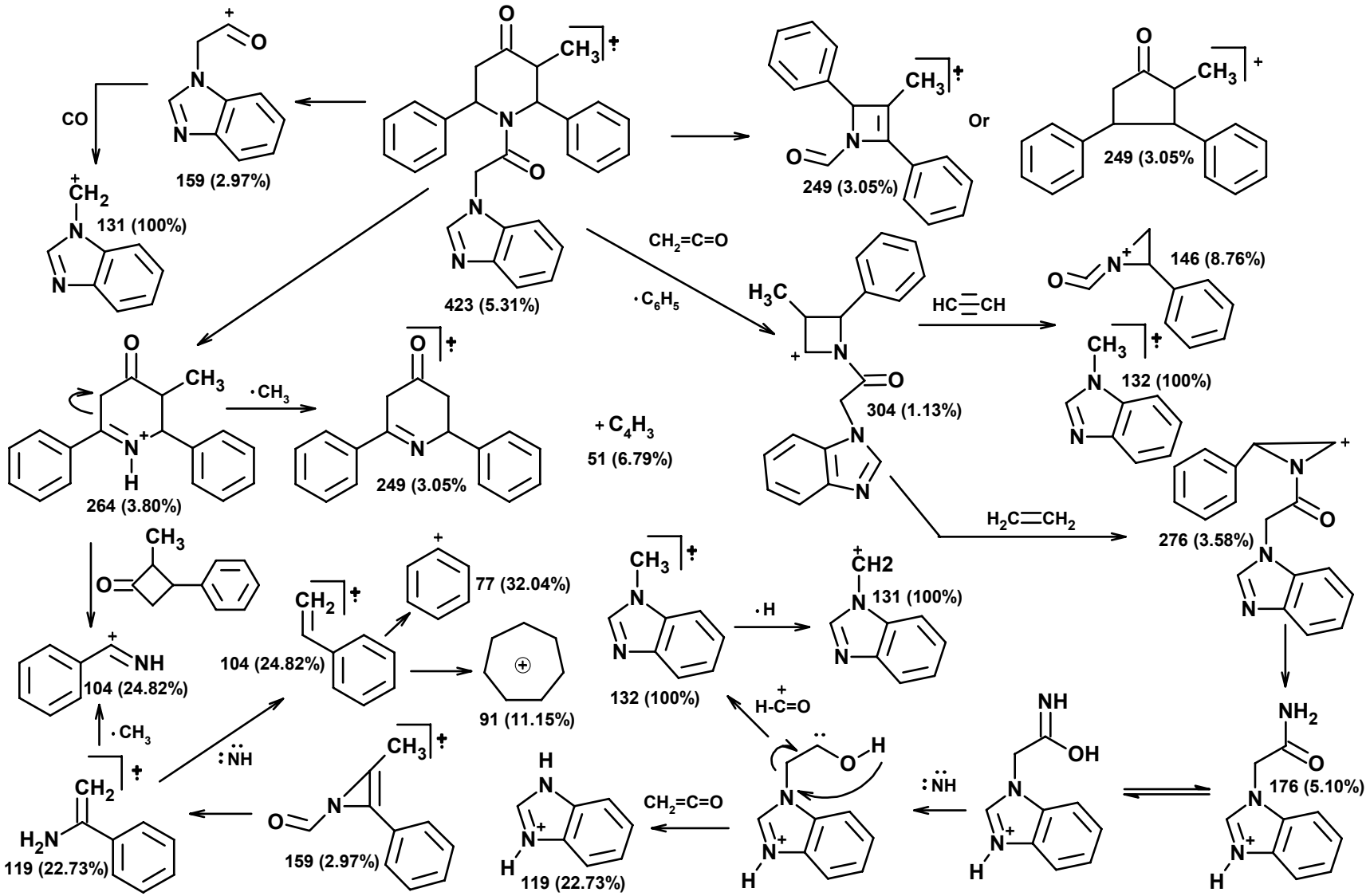

Figure S3. Mass fragmentation pattern for **21**

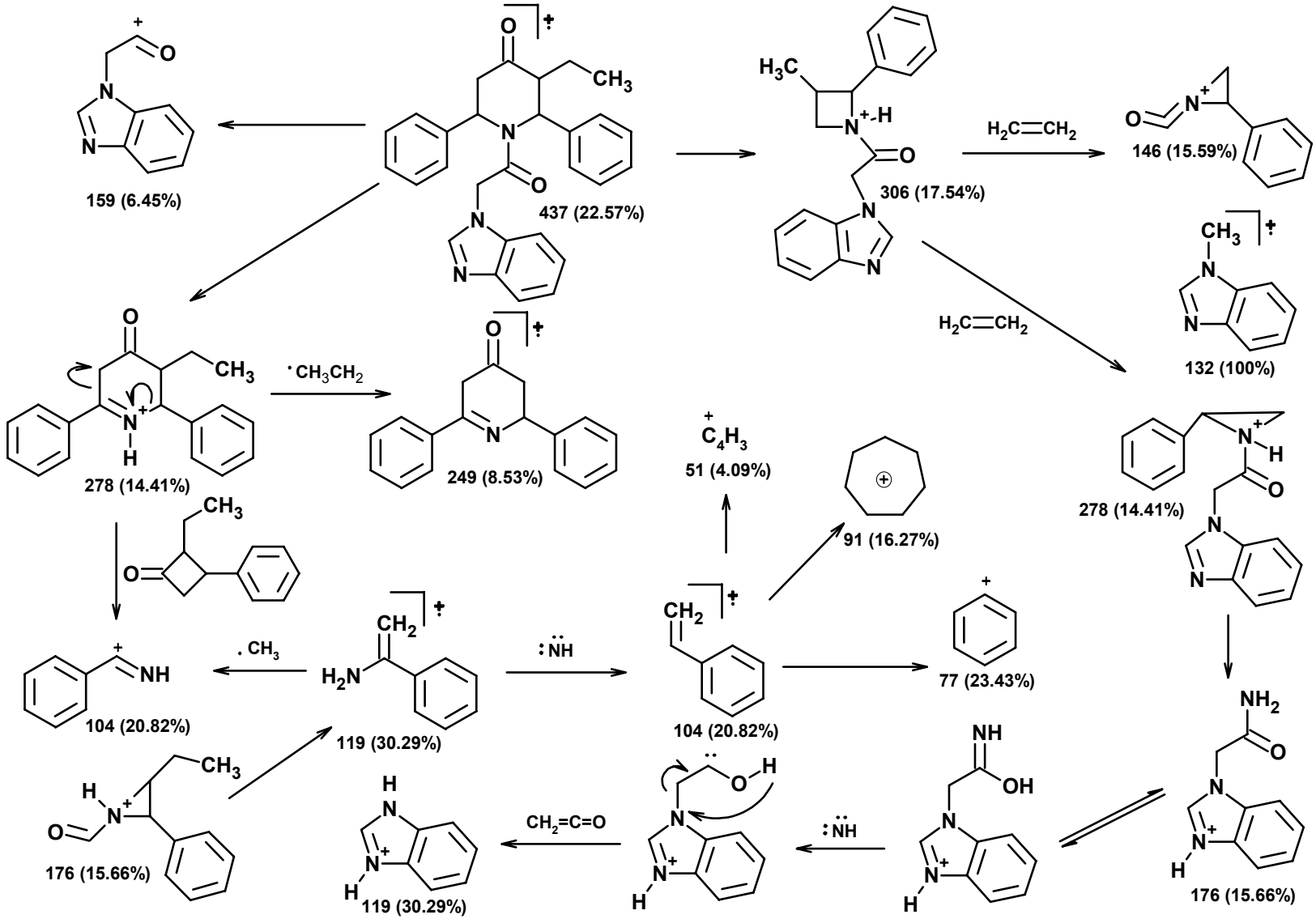

Figure S4. Mass fragmentation pattern for **22**

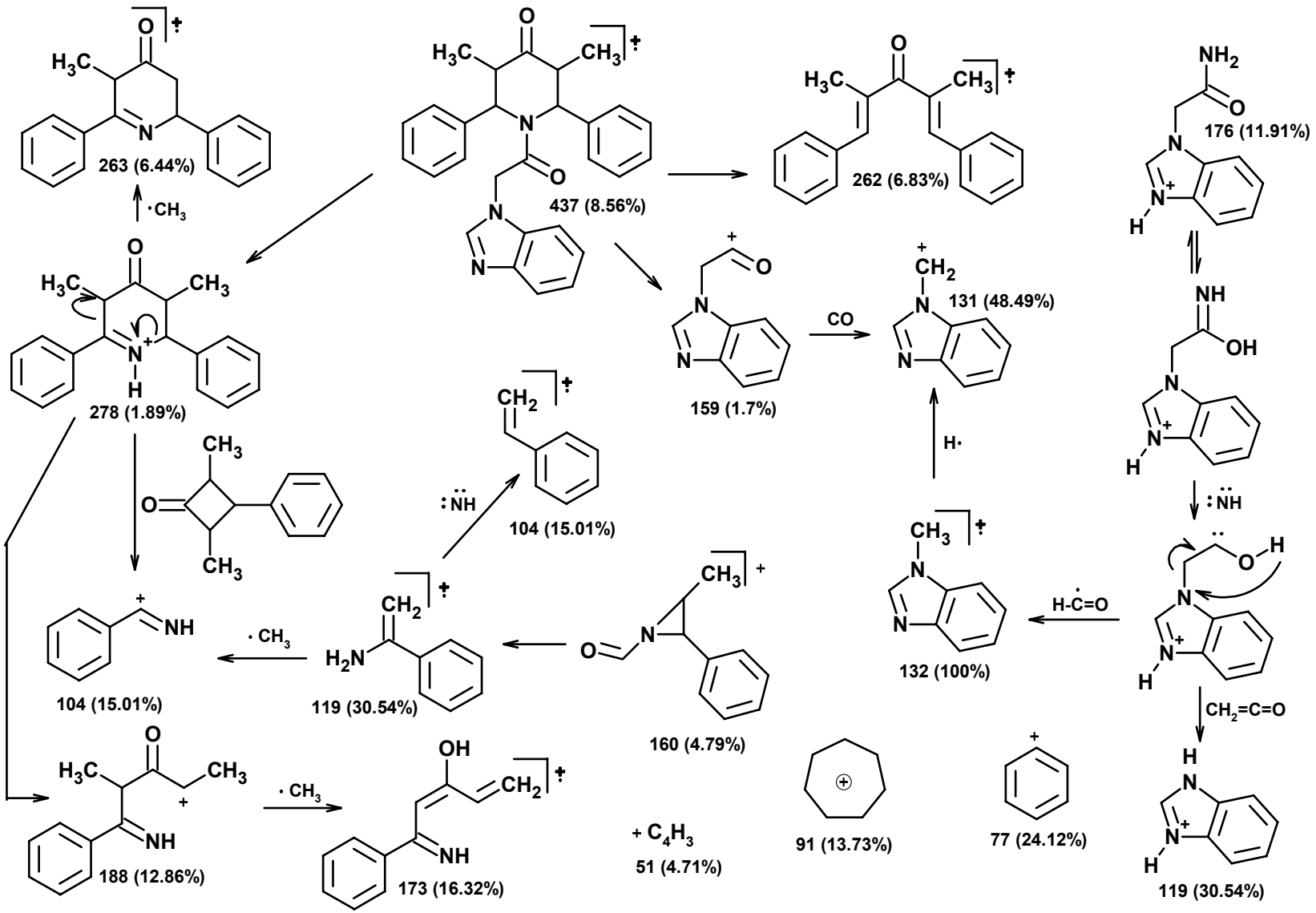

Figure S5. Mass fragmentation pattern for **23**

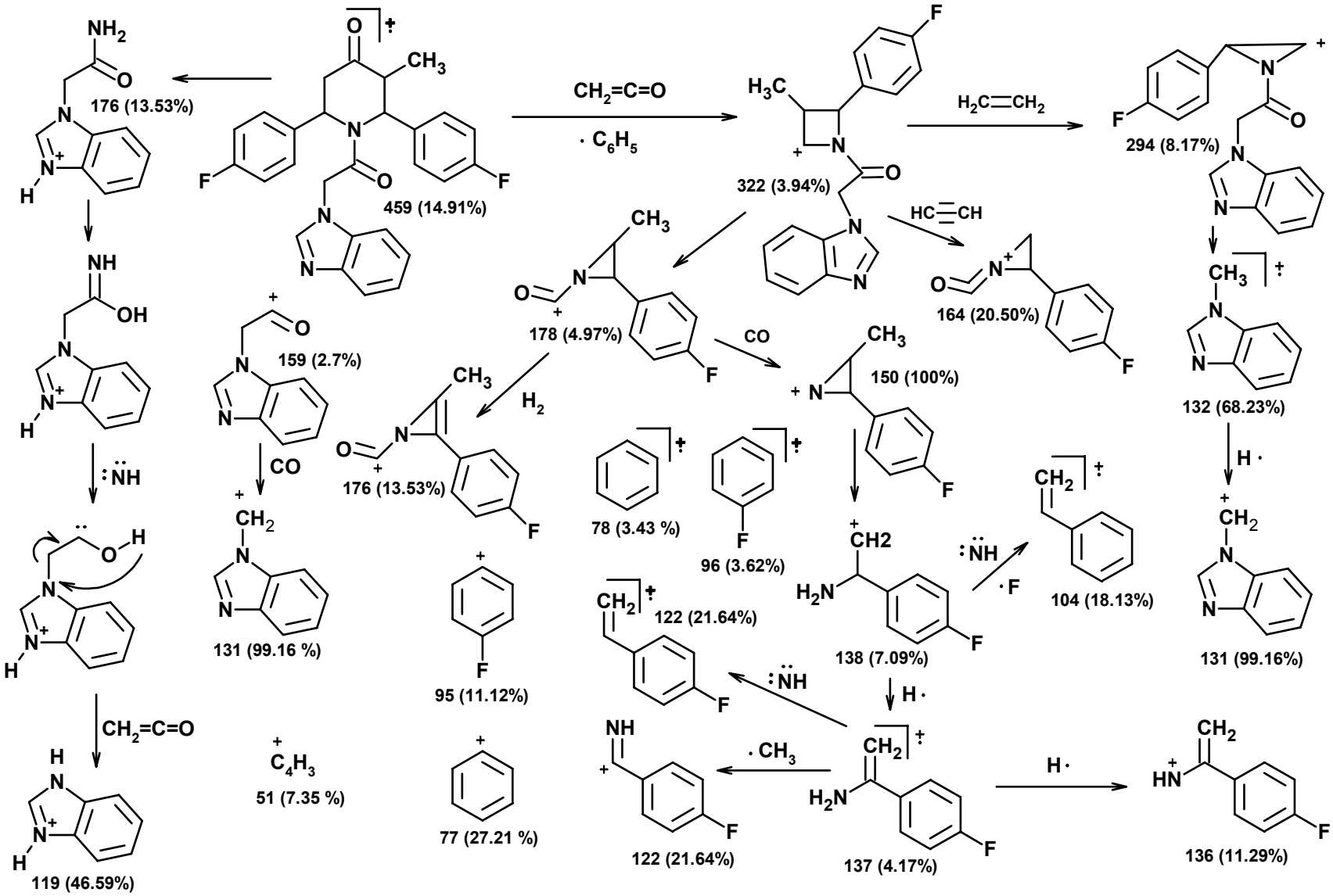

Figure S6. Mass fragmentation pattern for **24**

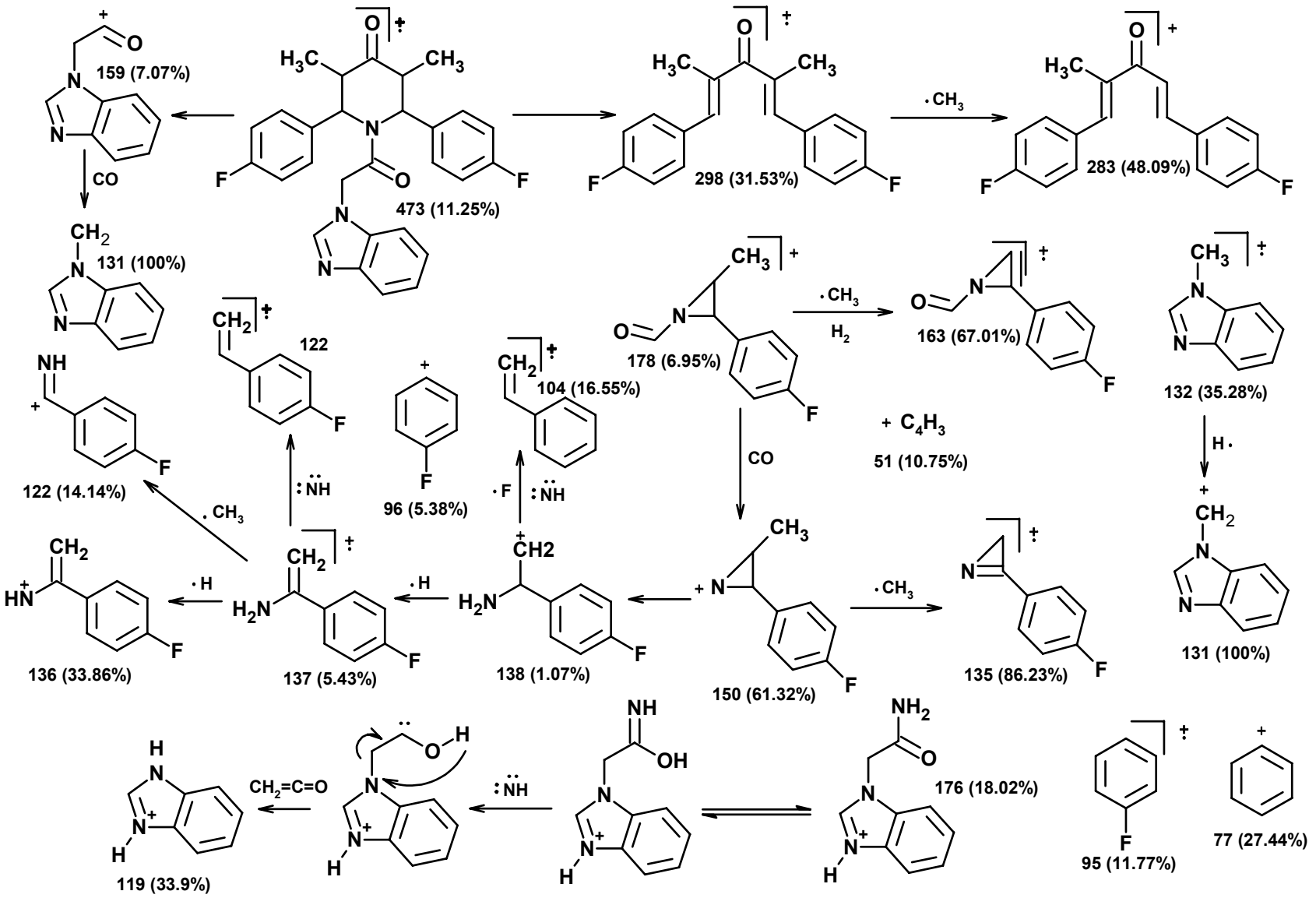

Figure S7. Mass fragmentation pattern for **25**

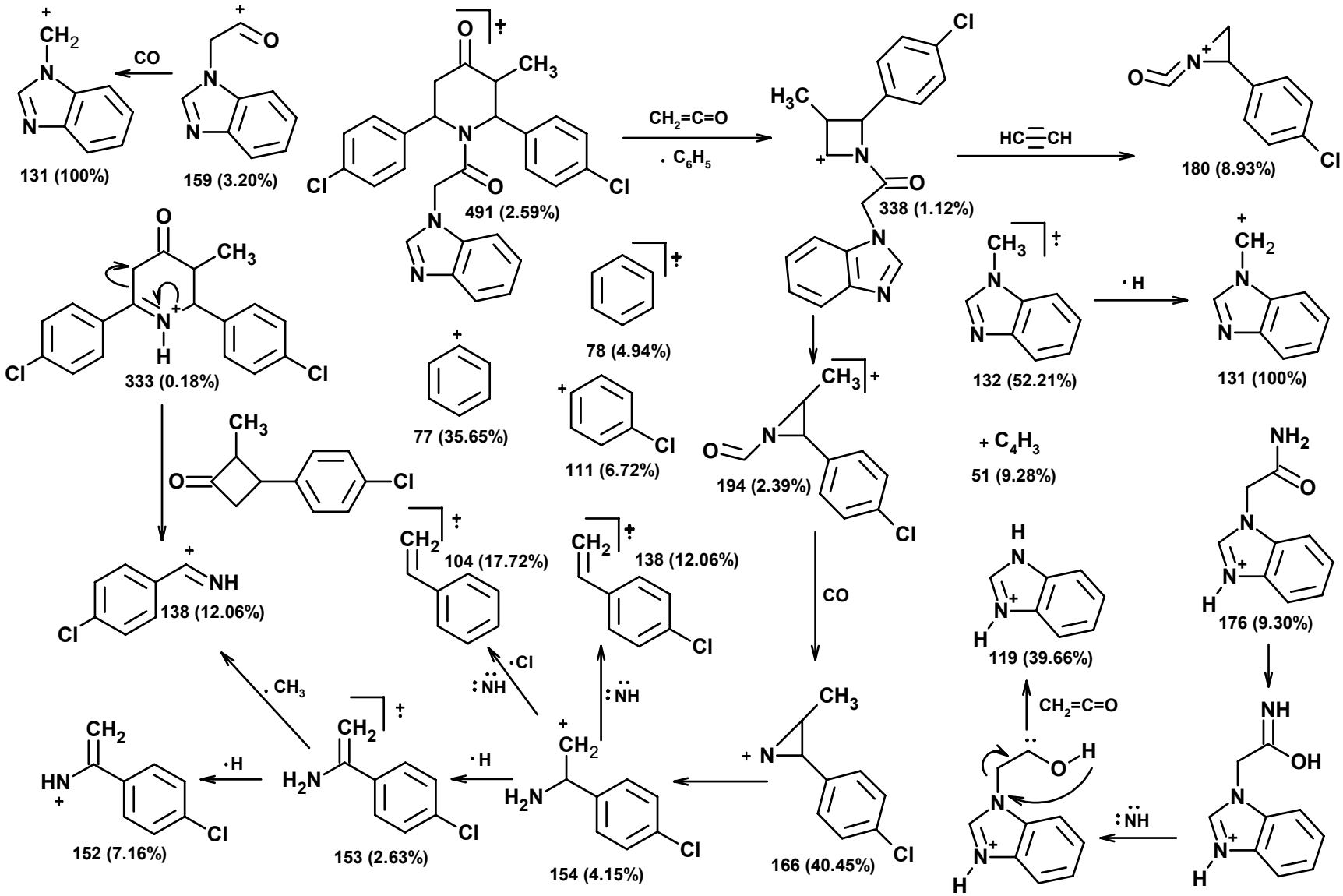

Figure S8. Mass fragmentation pattern for **26**

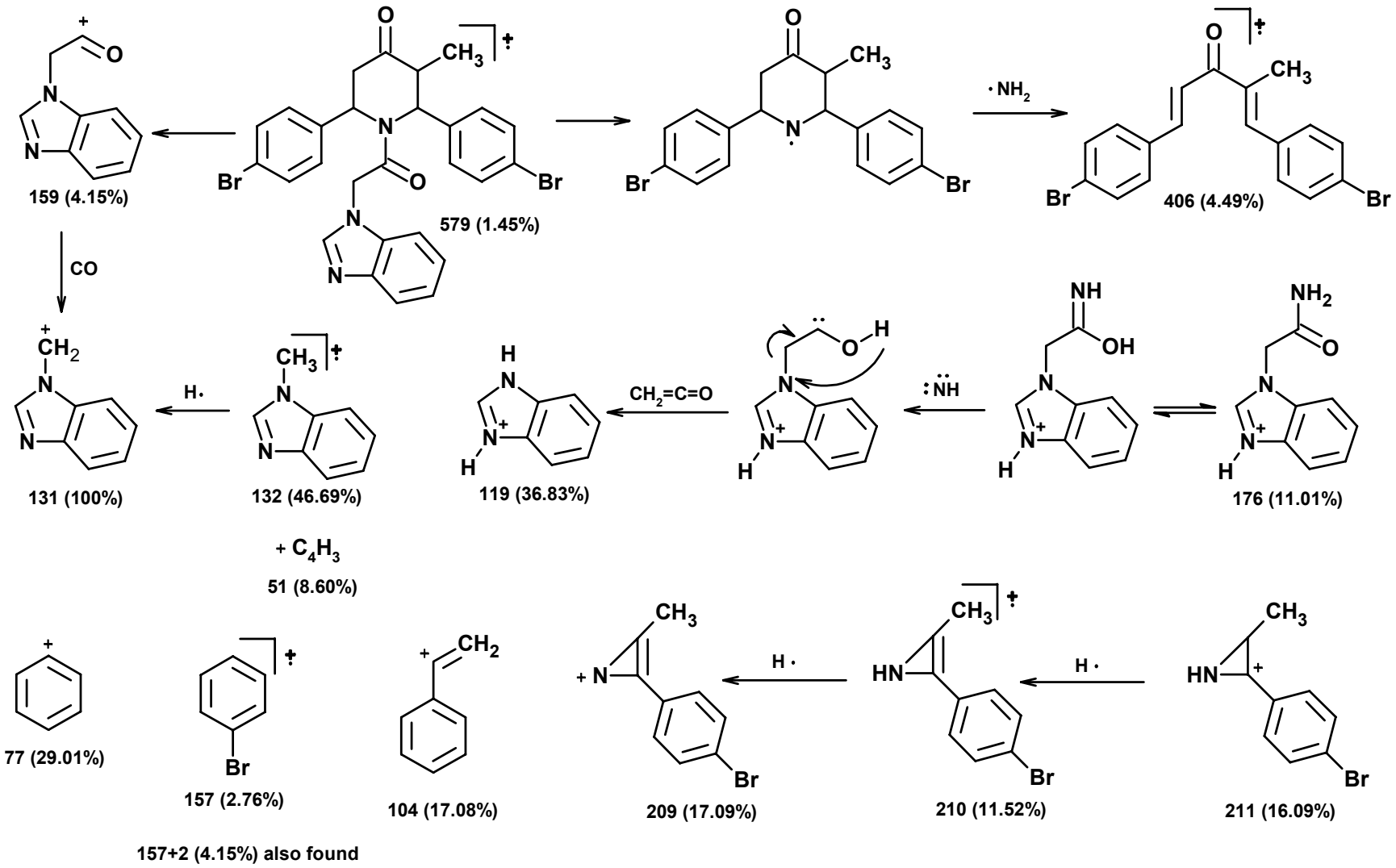

Figure S9: Mass fragmentation pattern for **28**

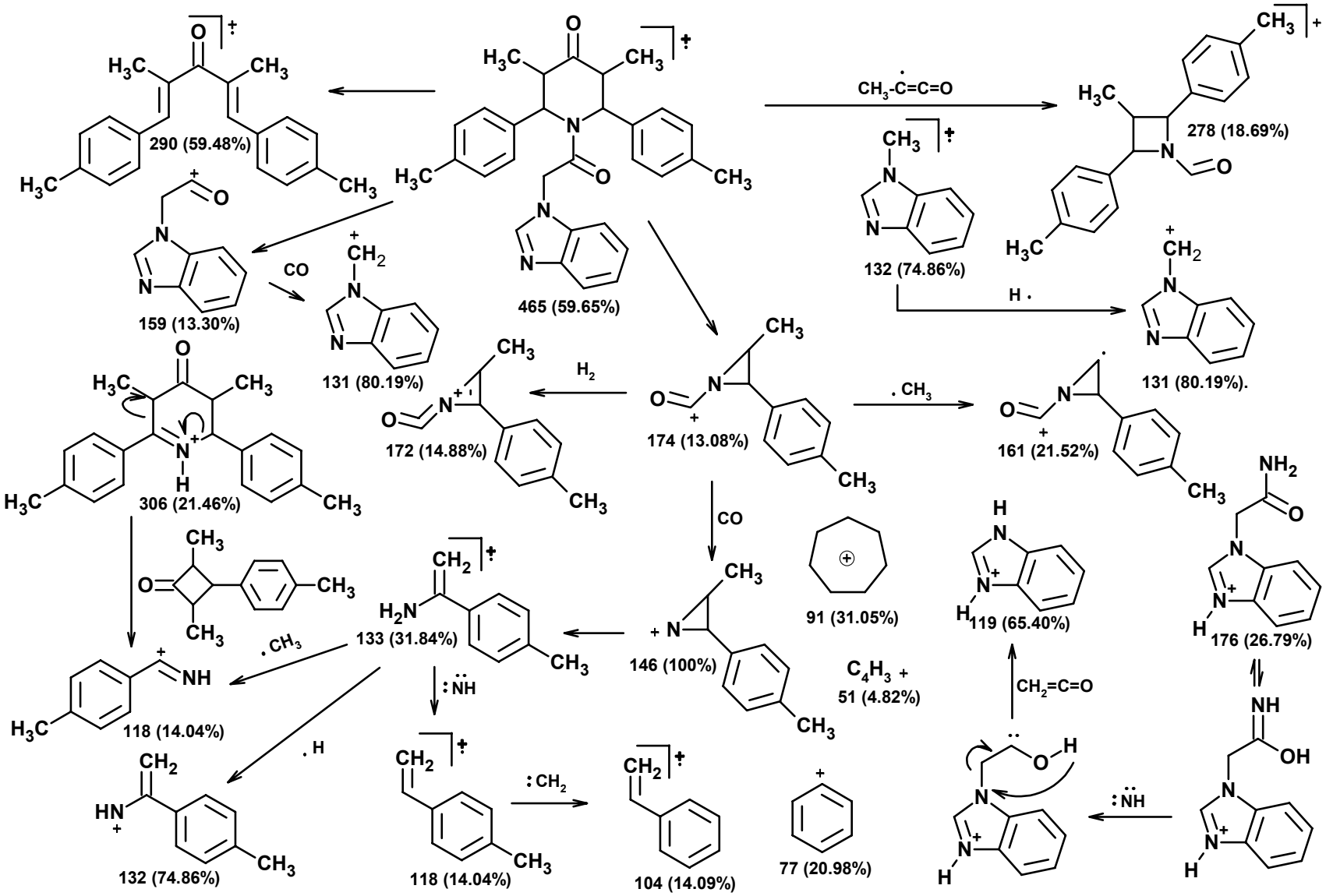

Figure S10. Mass fragmentation pattern for **30**