

## 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
<b>21</b>	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)
<b>22</b>	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)
<b>23</b>	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)
<b>24</b>	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)
<b>25</b>	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)
<b>26</b>	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)
<b>27</b>	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)
<b>28</b>	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)
<b>29</b>	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)
<b>30</b>	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 <sub>23</sub> H <sub>26</sub> ClNO <sub>2</sub>
Formula weight	383.90
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 11.9590(4) Å alpha = 95.483(2) deg. b = 14.3697(5) Å beta = 113.333(2) deg. c = 14.7369(5) Å gamma = 110.028(2) deg.
Volume	2104.84(12) Å <sup>3</sup>
Z, Calculated density	4, 1.211 Mg/m <sup>3</sup>
Absorption coefficient	0.198 mm <sup>-1</sup>
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 ≤ h ≤ 13, -16 ≤ k ≤ 16, -17 ≤ l ≤ 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 <sup>2</sup>
Data / restraints / parameters	6958 / 0 / 528
Goodness-of-fit on F <sup>2</sup>	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.Å <sup>-3</sup>

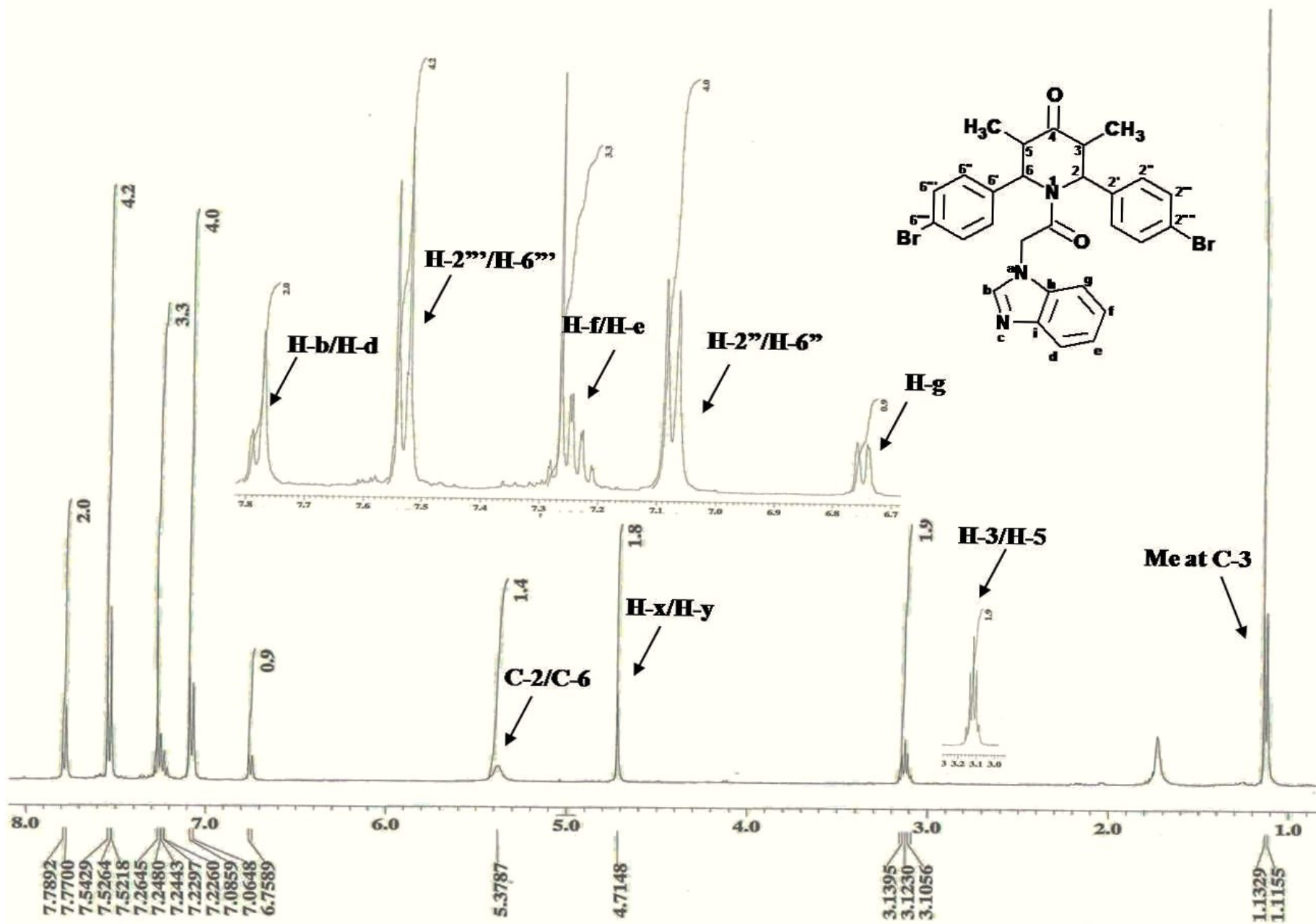


Figure S1. <sup>1</sup>H NMR spectrum of compound 29

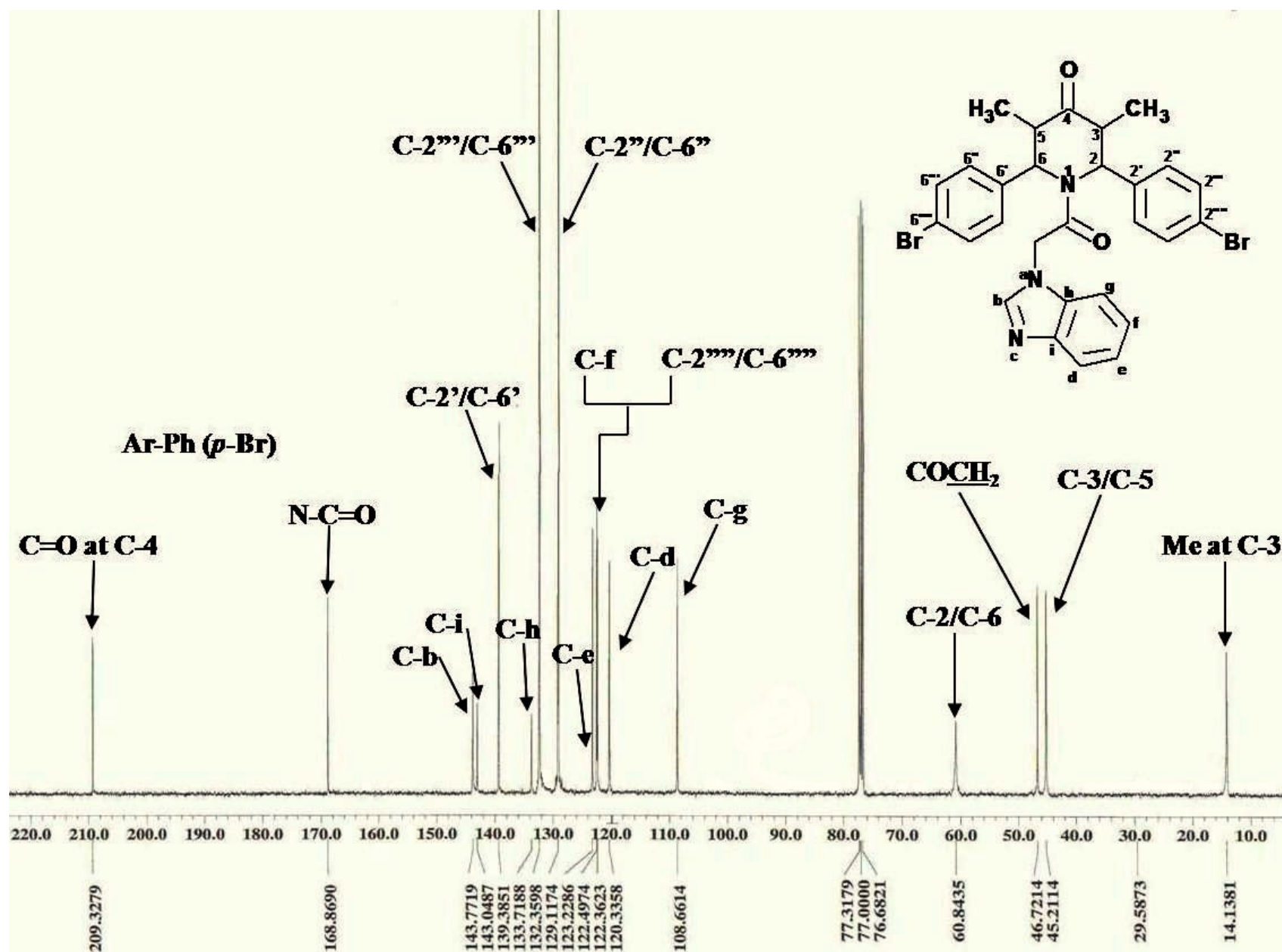


Figure S2.  $^{13}\text{C}$  NMR spectrum of compound 29

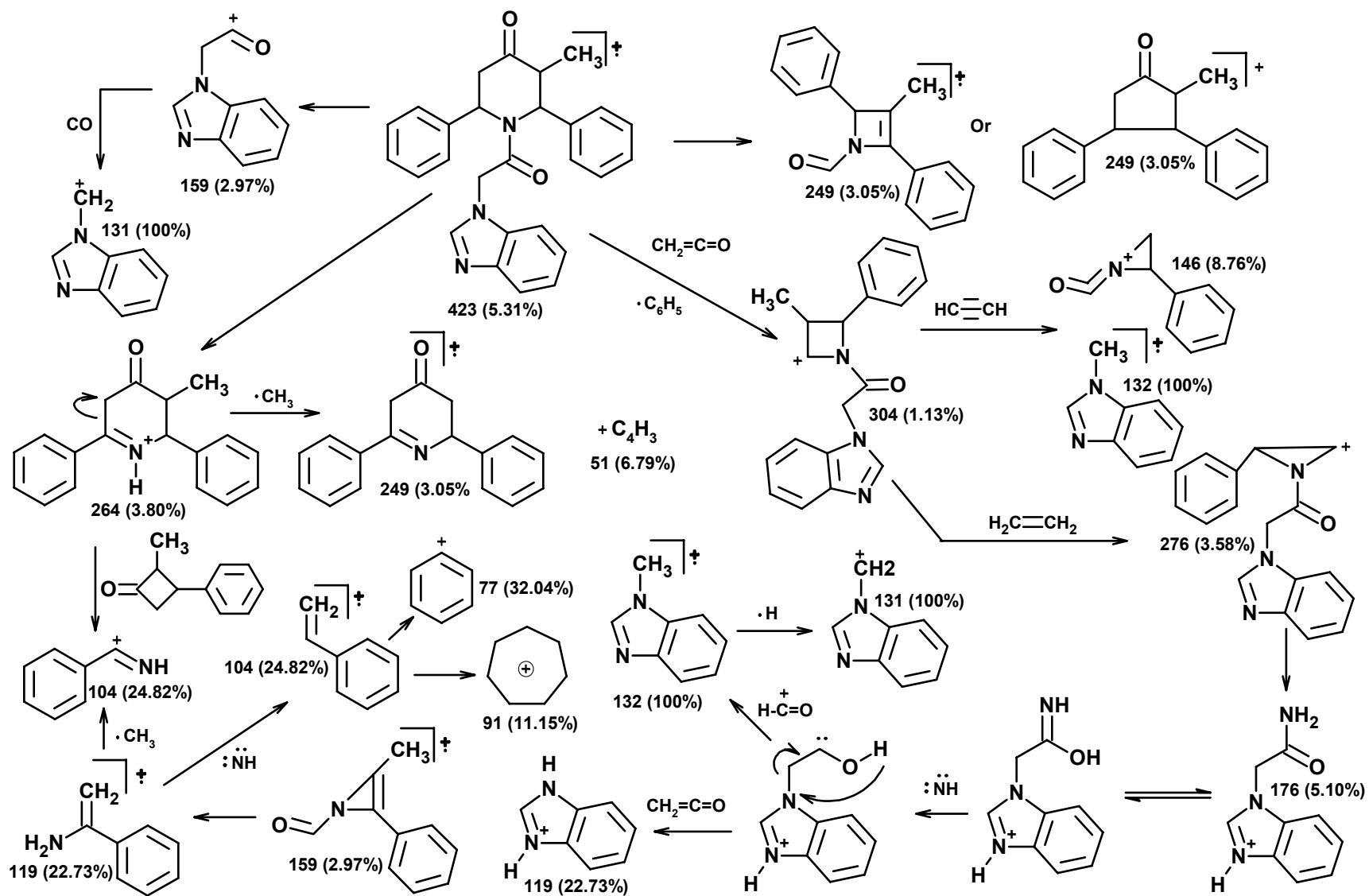


Figure S3. Mass fragmentation pattern for 21

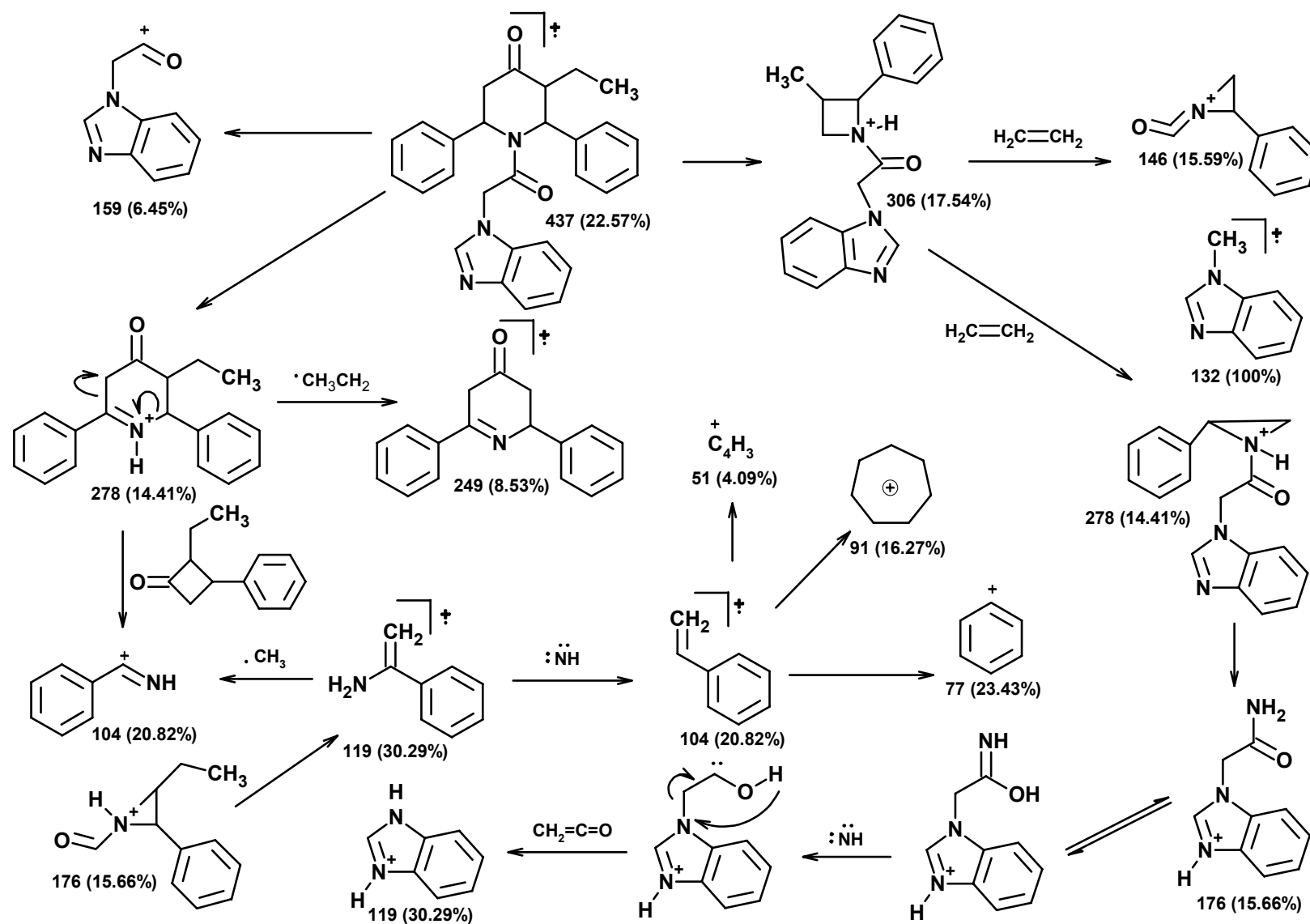


Figure S4. Mass fragmentation pattern for 22

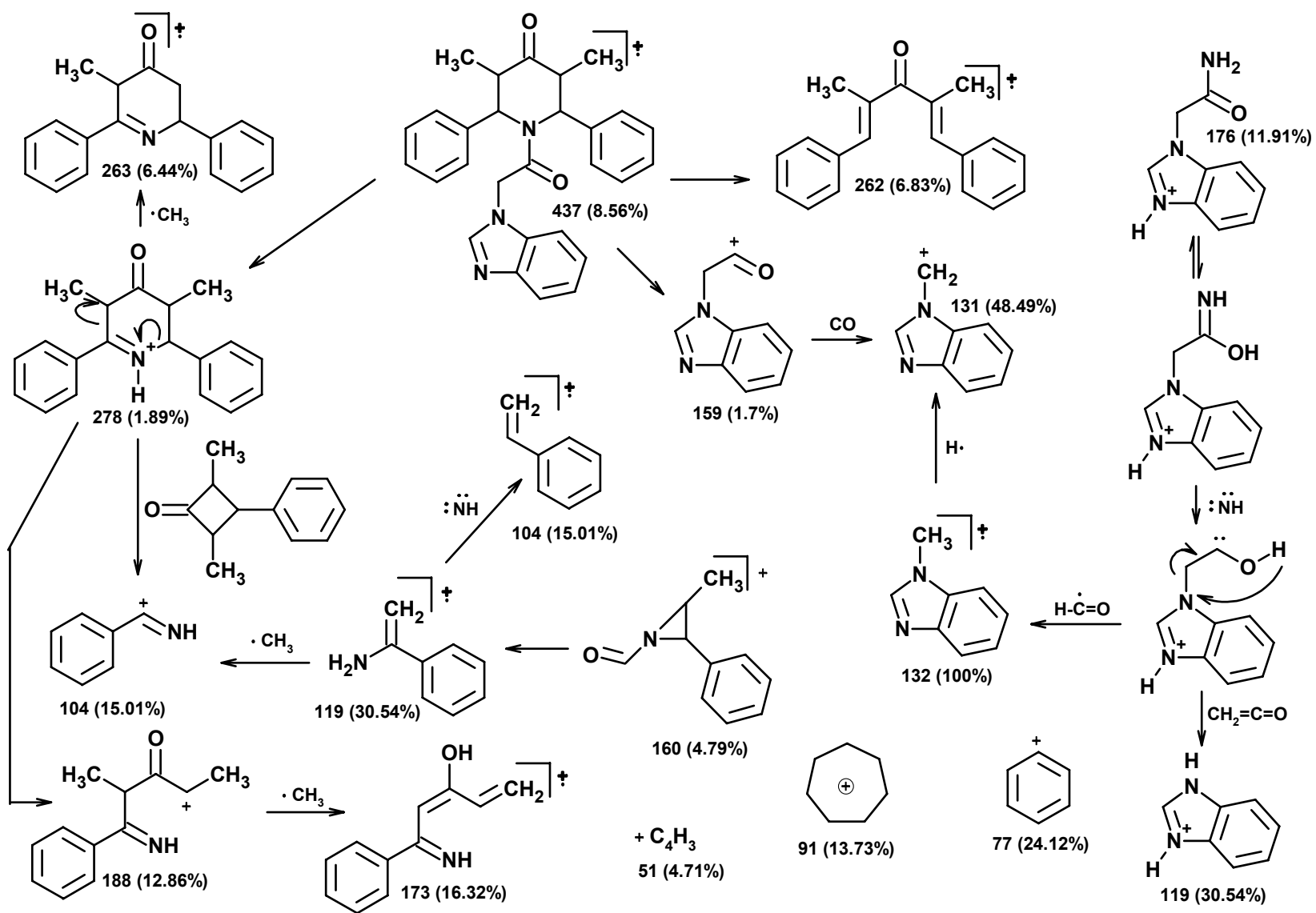


Figure S5. Mass fragmentation pattern for 23



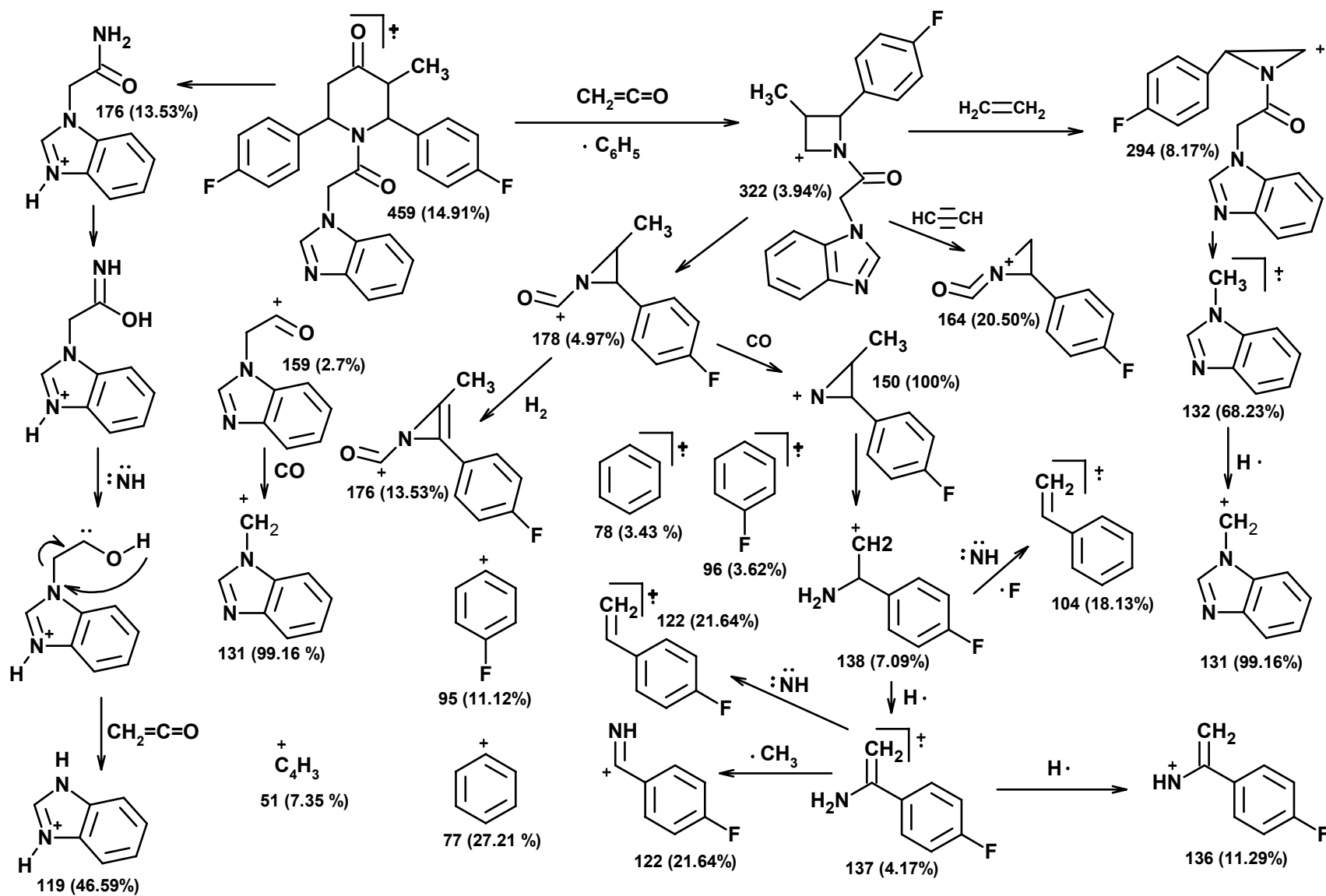


Figure S6. Mass fragmentation pattern for 24



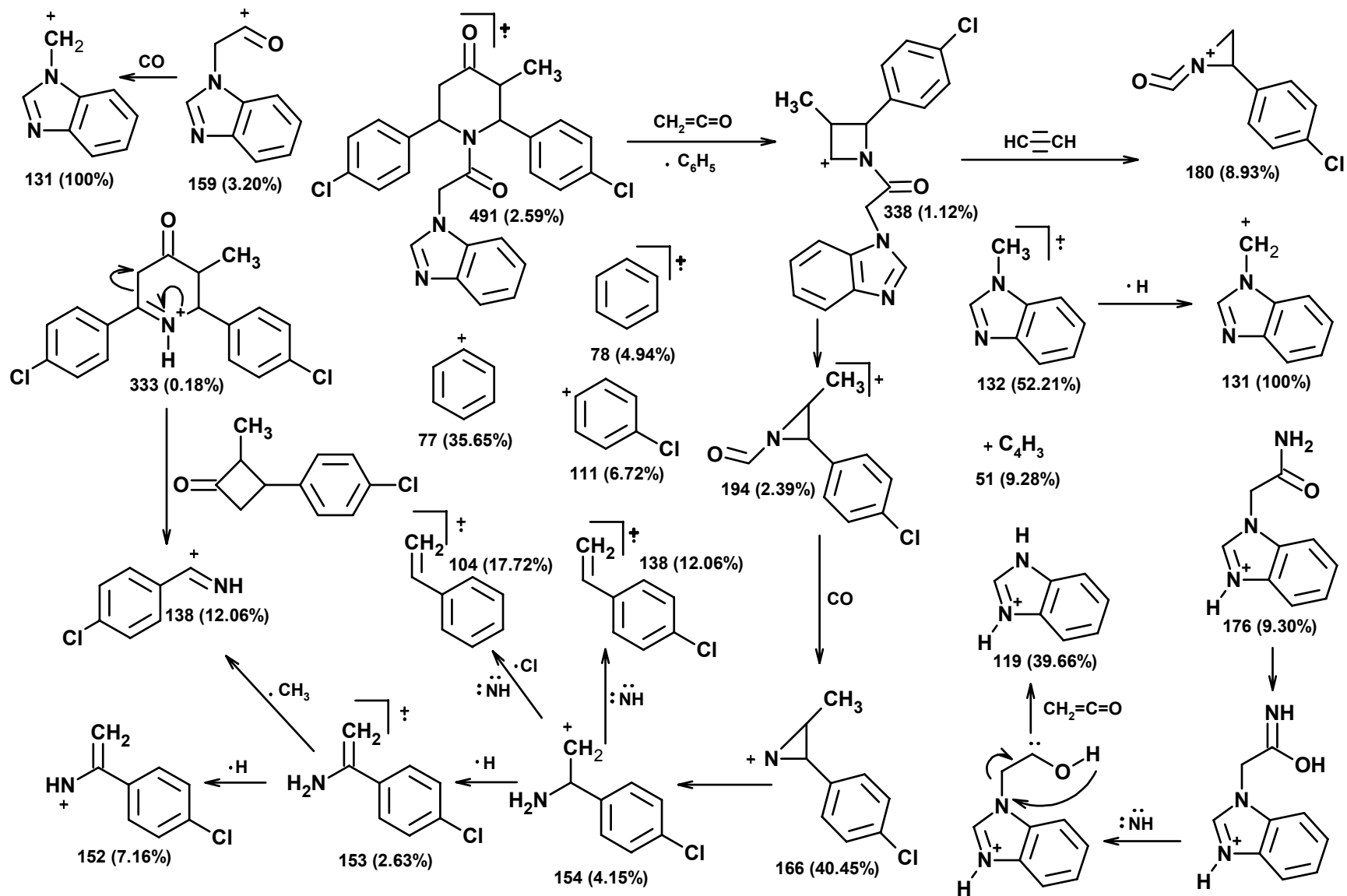
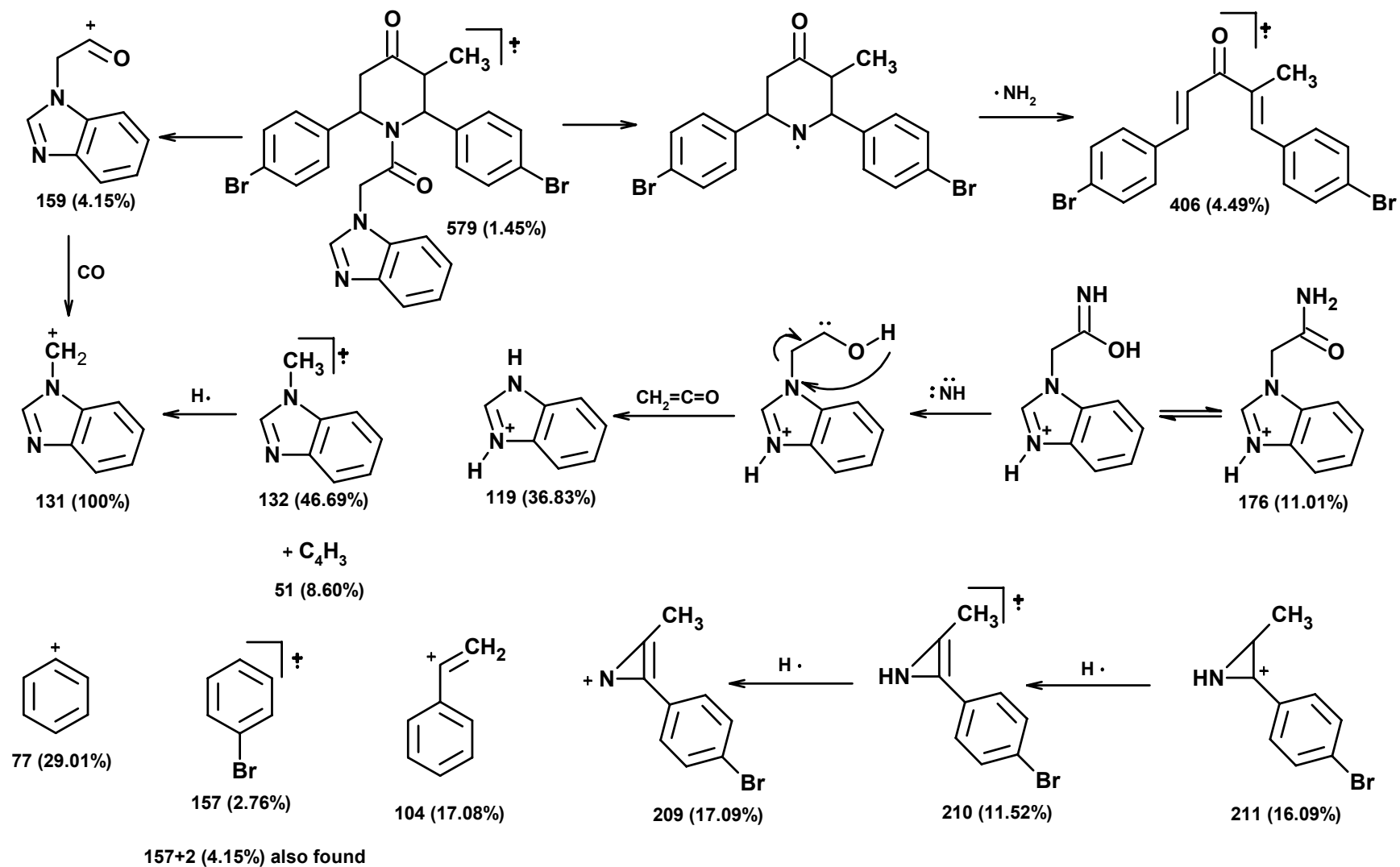


Figure S8. Mass fragmentation pattern for 26



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

