

Supplementary Material

A new and efficient synthesis of unsaturated benzoxazepines, using sodium metabisulfite and potassium permanganate as oxidative reagents

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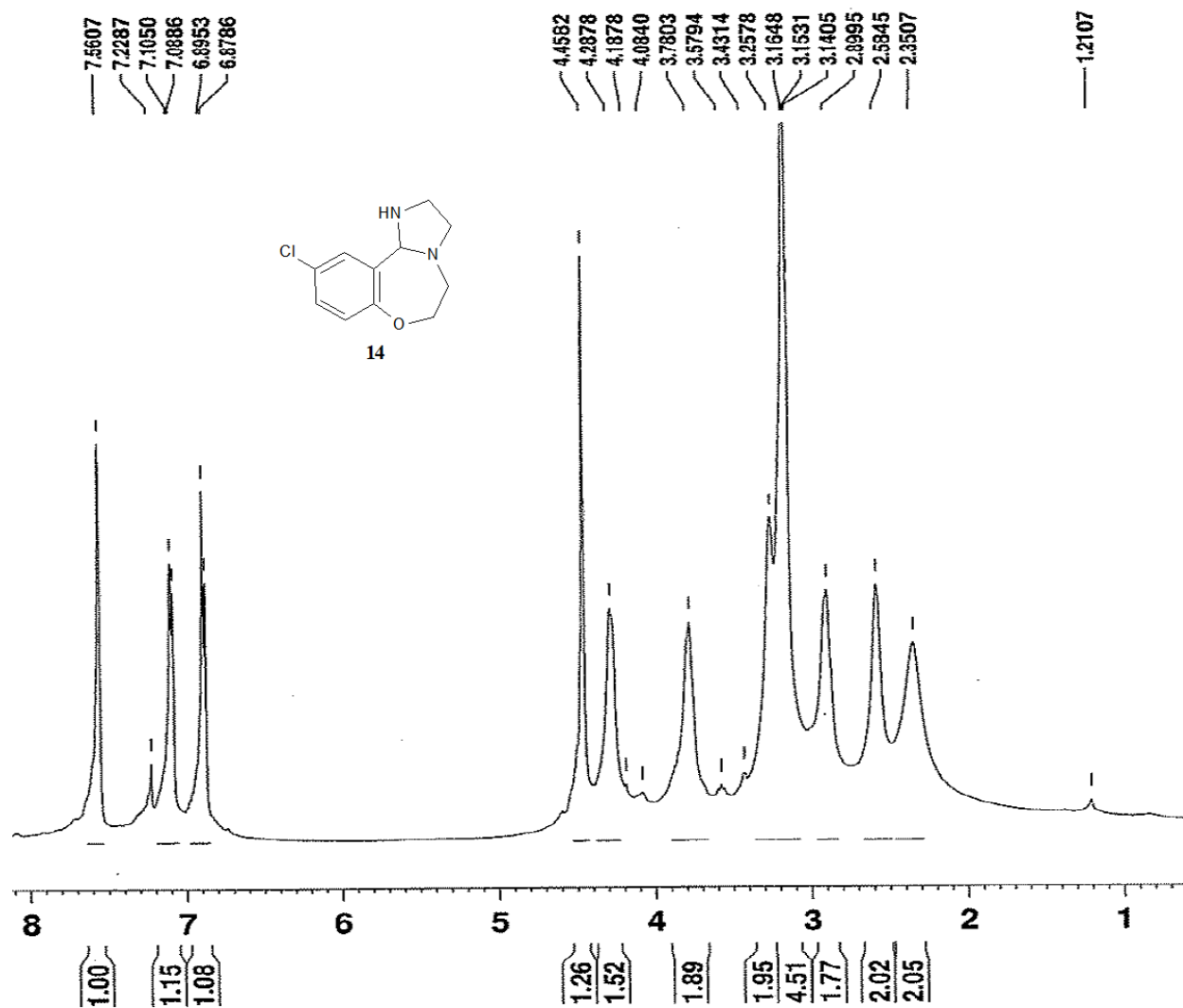
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| 1. Crystal data for structure 16, 29 and 36 | S2 |
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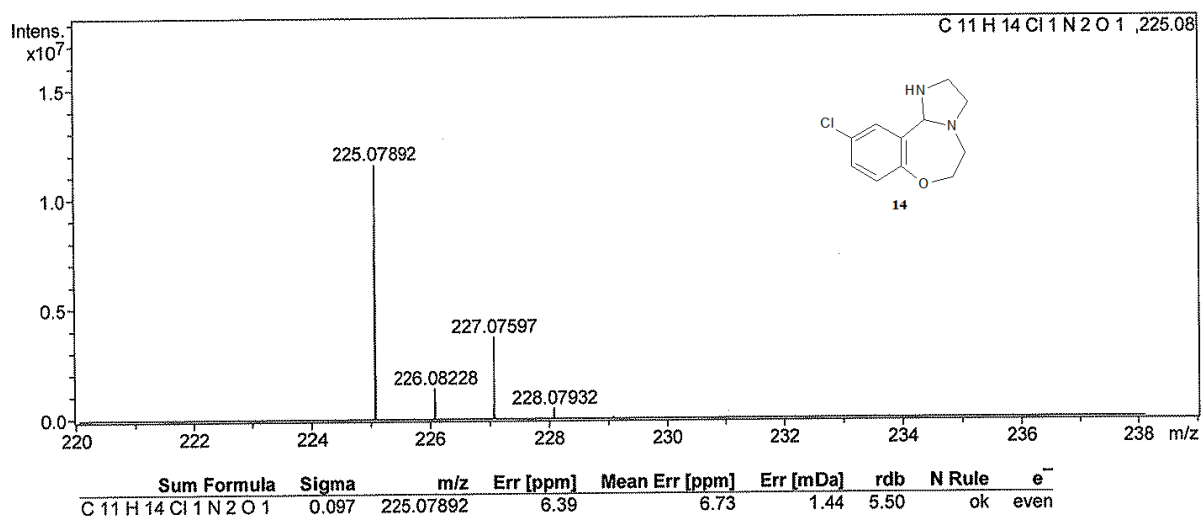
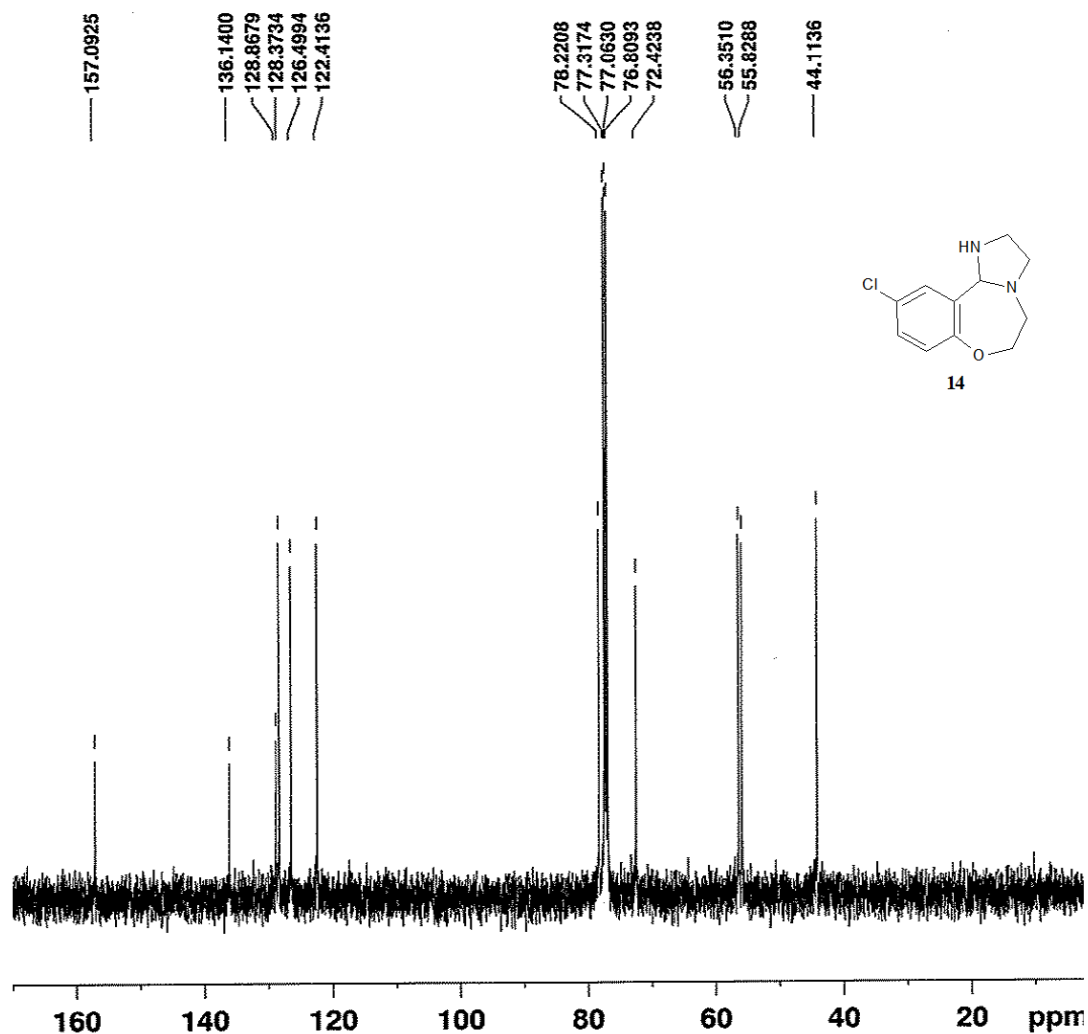
Table 1. Summary of data collection and refinement parameters for compounds **16**, **29** and **36**.

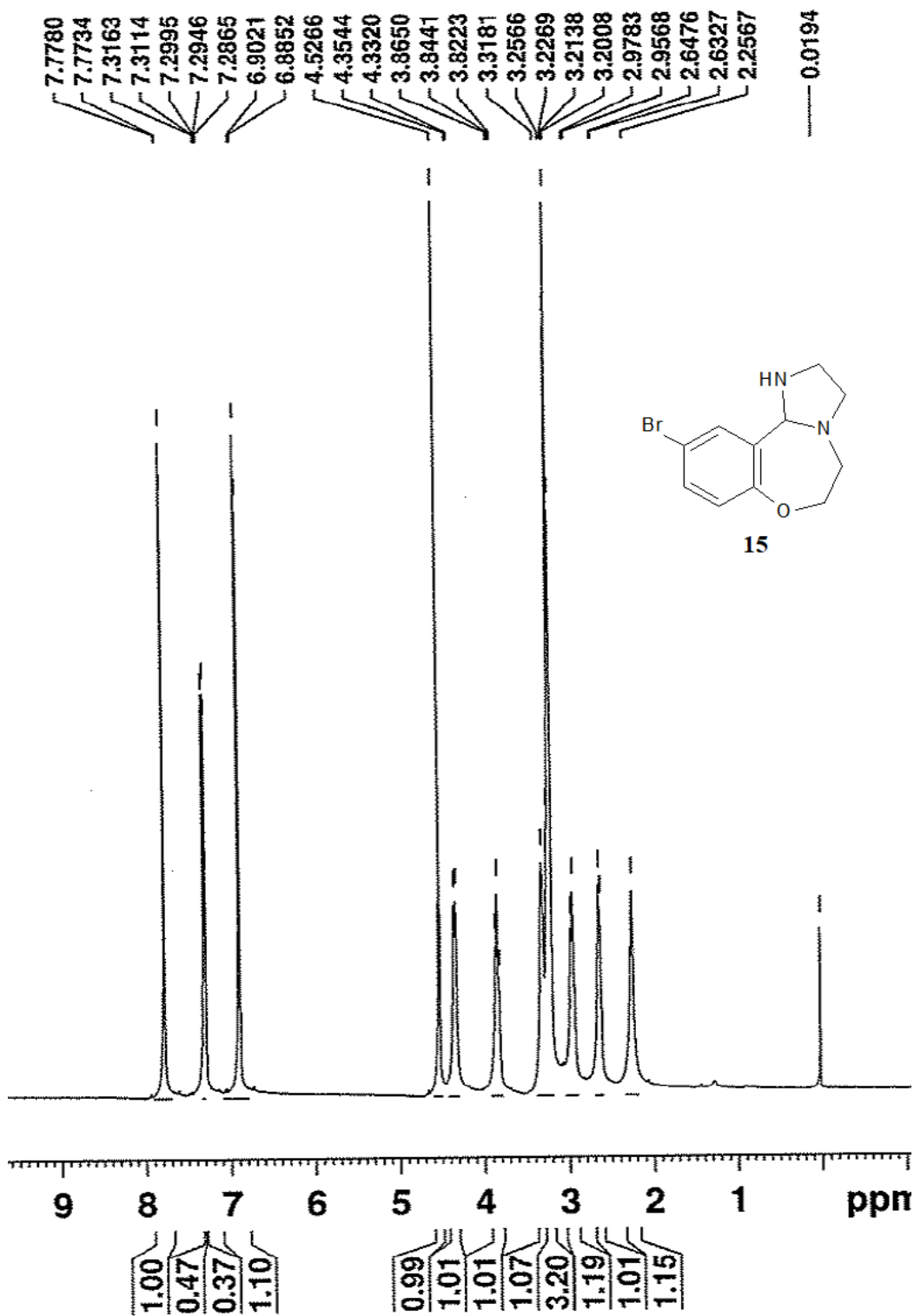
Crystal	16	29	36
Molecular formula	C ₁₂ H ₁₆ N ₂ O	C ₁₁ H ₁₁ BrN ₂ O	C ₁₅ H ₁₁ BrN ₂ O
Formula weight, M _r	204.27	267.13	315.17
Crystal system	Orthorhombic	Triclinic	Orthorhombic
Space group	Pna2 ₁	P-1	Pbca
<i>a</i> (Å)	13.6149(7)	7.3577(7)	8.9526(6)
<i>b</i> (Å)	10.7361(6)	8.8681(8)	15.2031(13)
<i>c</i> (Å)	7.5693(5)	9.2732(10)	18.7081(11)
α (°)	90	99.895(8)	90
β (°)	90	111.643(10)	90
γ (°)	90	103.274(8)	90
Volume (Å ³)	1106.41(11)	524.91(9)	2546.3(3)
<i>Z</i>	4	2	8
Independent reflections	1949	2122	2575
ρ _{calc} (Mg / m ³)	1.226	1.690	1.644
Reflections collected	4807	4109	12529
<i>R</i> _{int}	0.0278	0.0518	0.0312
Index ranges <i>hkl</i>	-12<= <i>h</i> <=16, -13<= <i>k</i> <=13, -9<= <i>l</i> <=9	-8<= <i>h</i> <=9 -10<= <i>k</i> <=11 -11<= <i>l</i> <=10	-11<= <i>h</i> <=11 -18<= <i>k</i> <=16 -21<= <i>l</i> <=23
Goodness- of- fit on <i>F</i> ²	0.957	1.012	1.044
Final <i>R</i> indices [<i>I</i> > 2σ (<i>I</i>)]	^a R1 = 0.0440, ^b wR2 = 0.0911	^a R1 = 0.0469, ^b wR2 = 0.0930	^a R1 = 0.0403, ^b wR2 = 0.0941
μ, mm ⁻¹	0.079	3.888	3.221
Δρ _{min} and _{max} (e / Å ³)	0.144 and -0.129	0.546 and -0.506	0.543 and -0.710
CCDC number	1897620	1897621	1897622

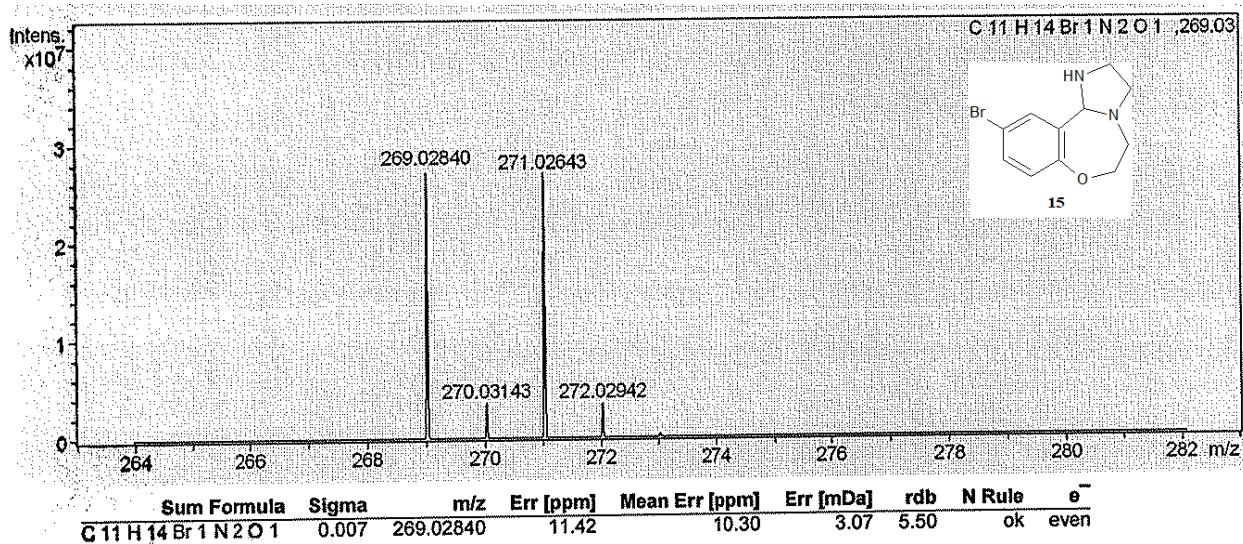
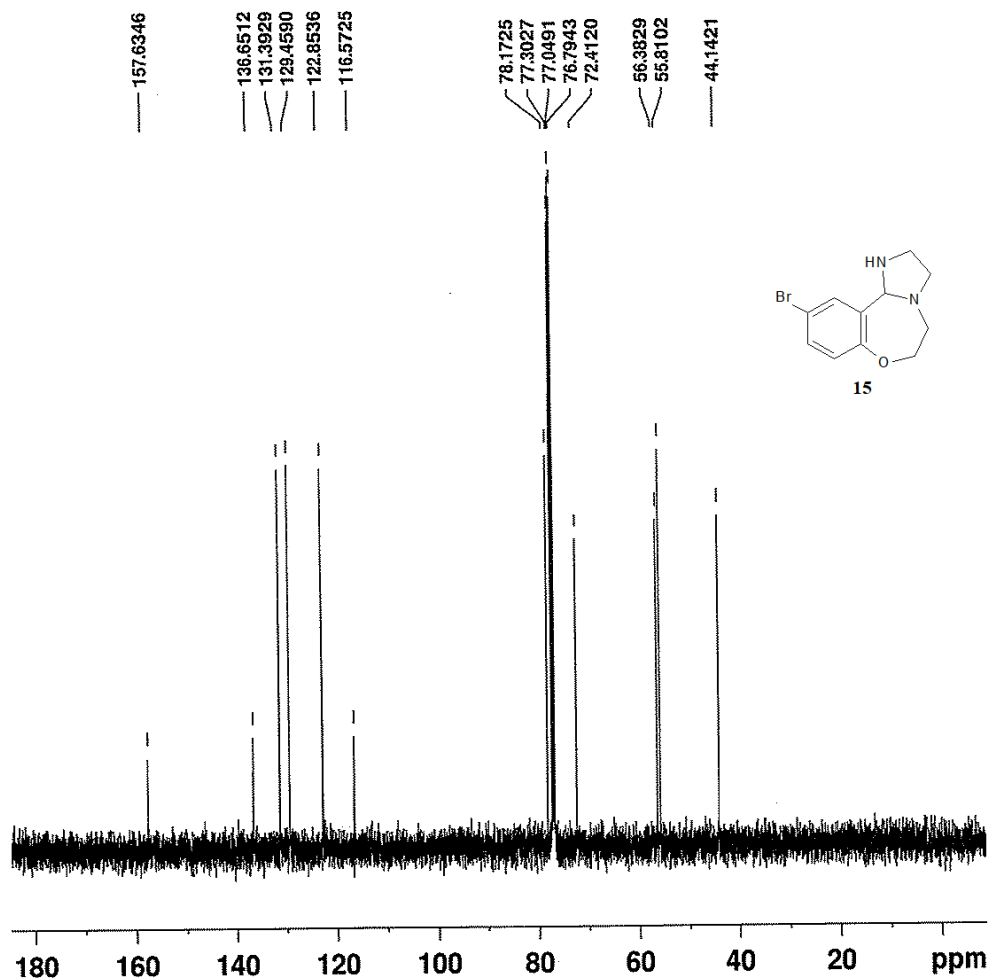
^a $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$.

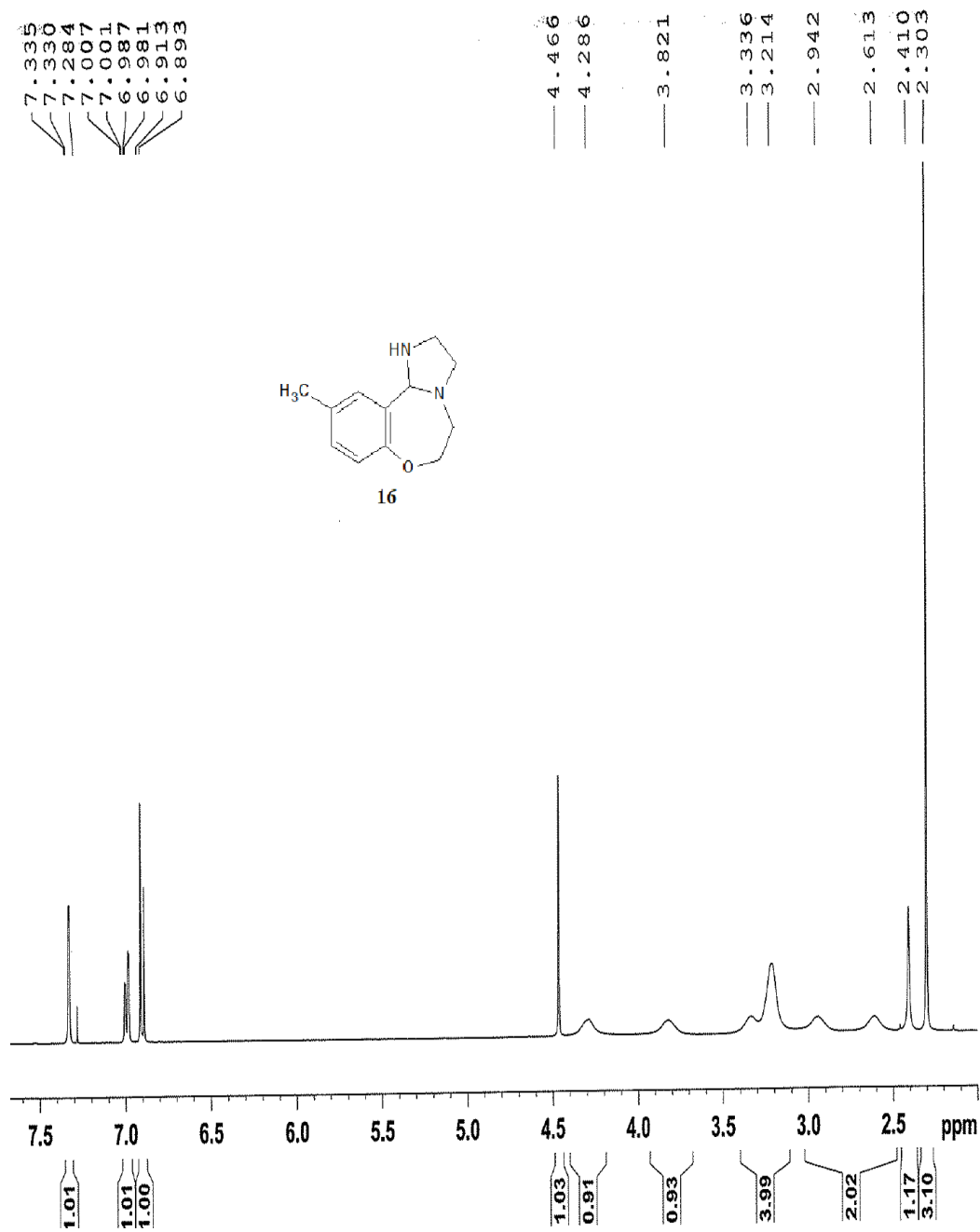
^b $wR_2 = \{ \sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2 \}^{1/2}$.

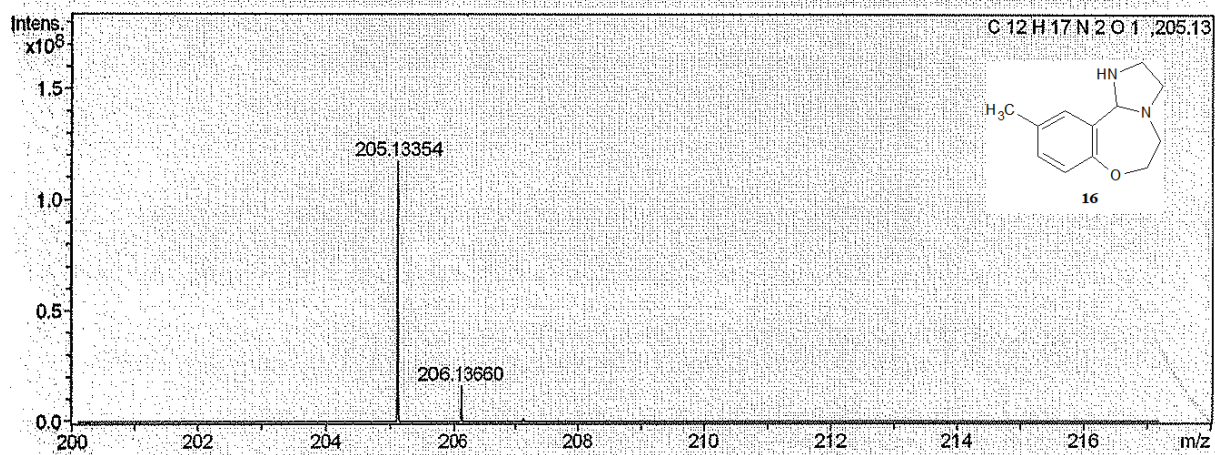
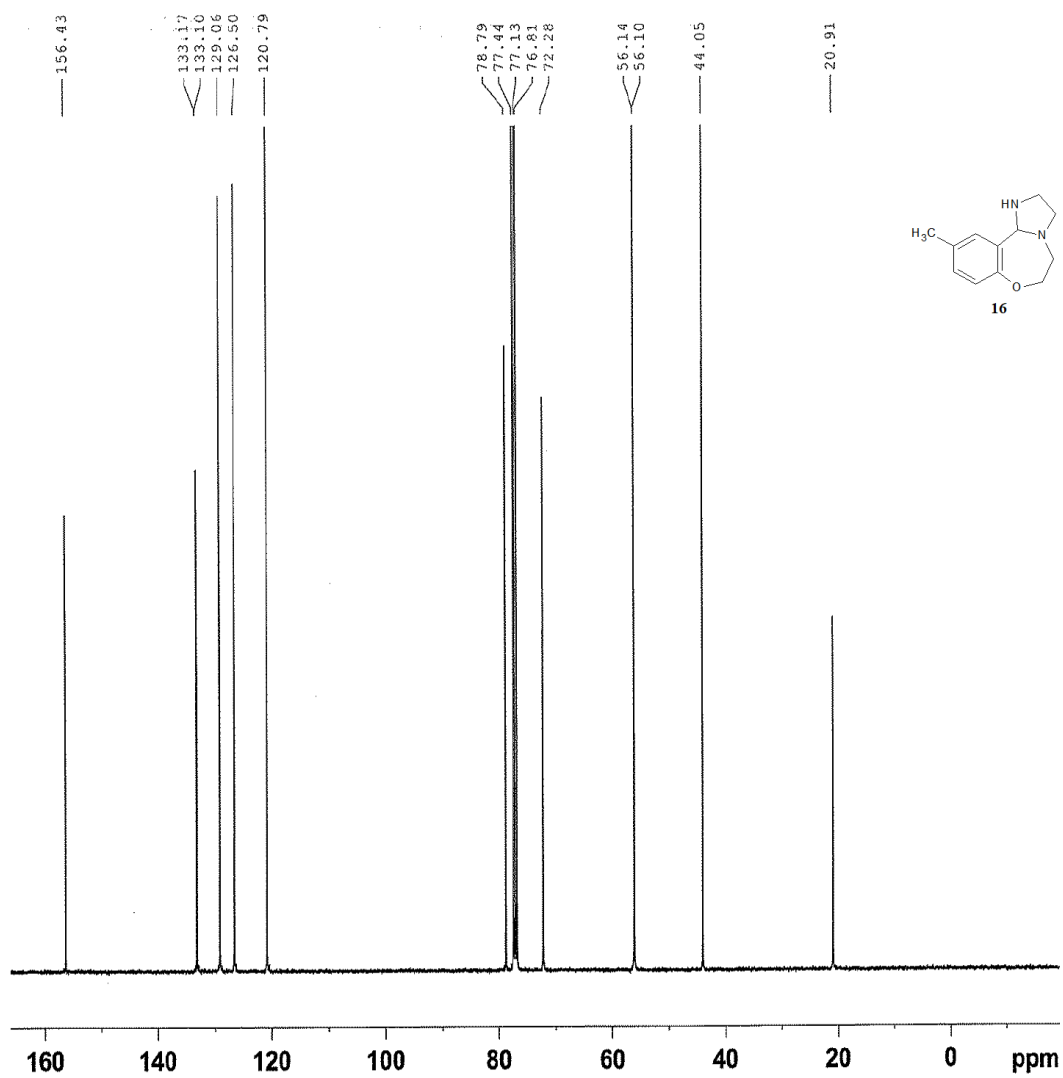


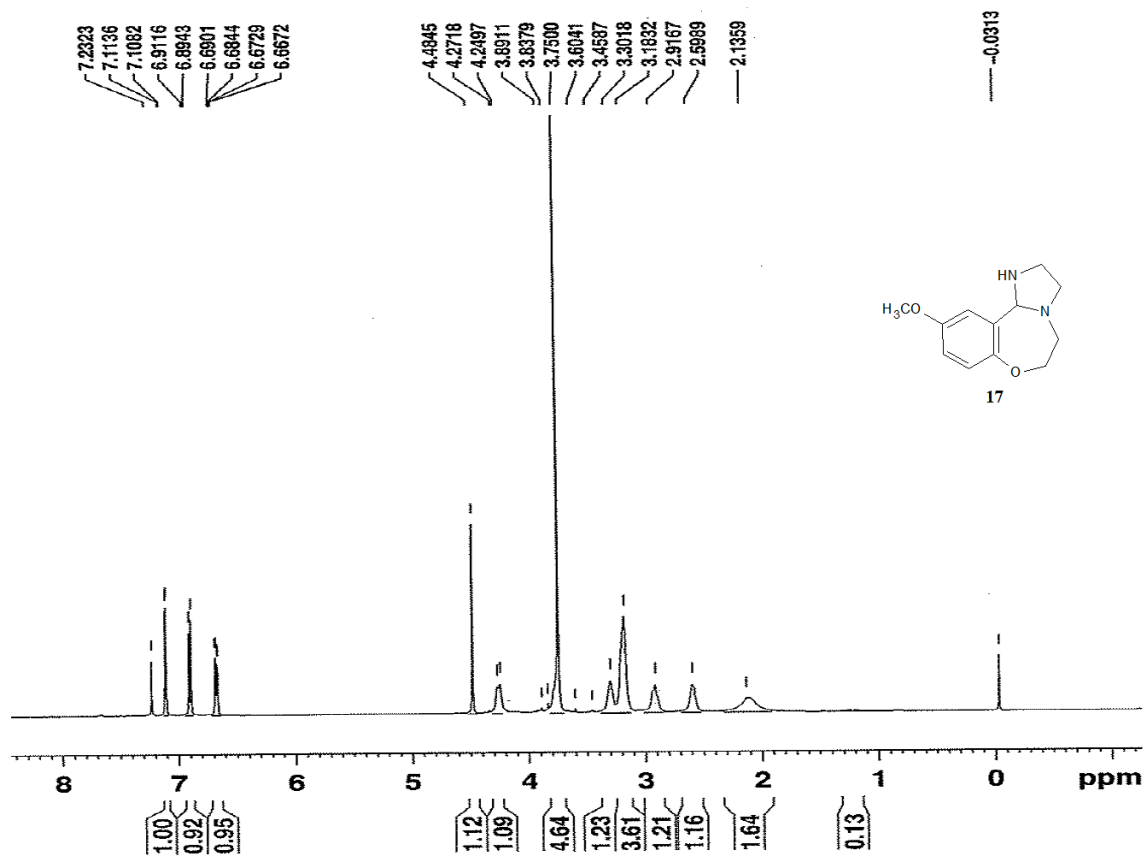


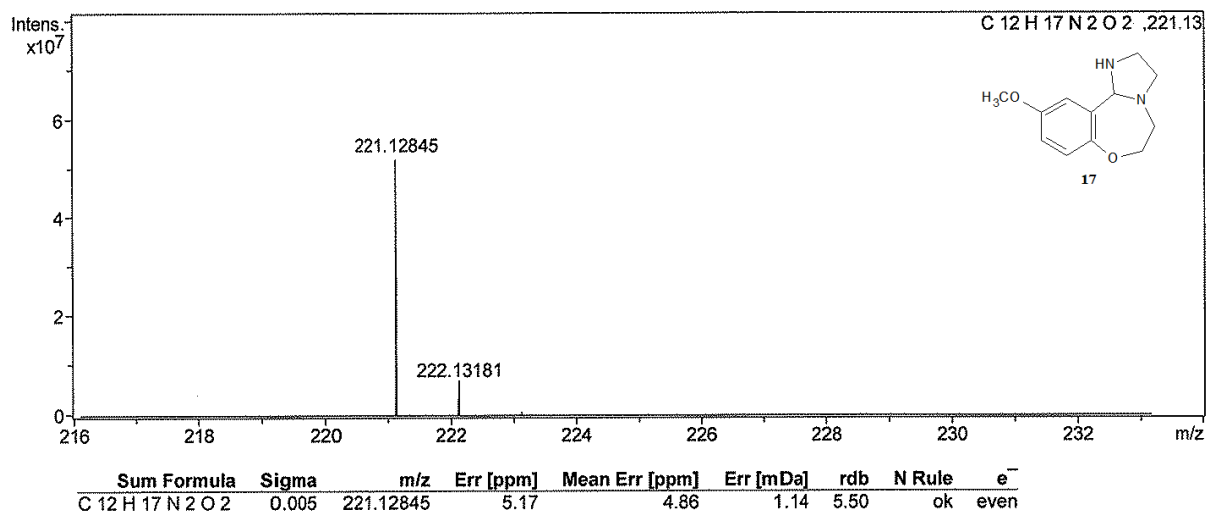
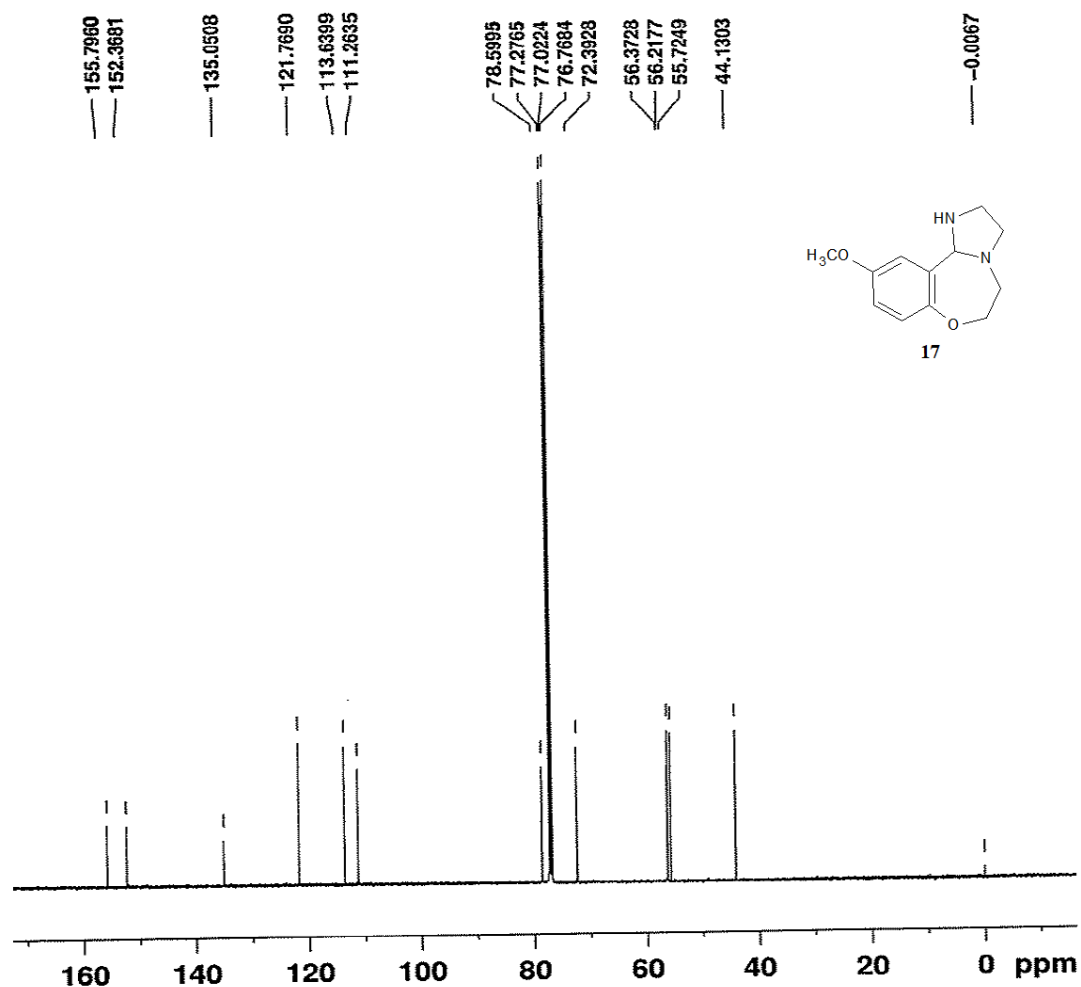


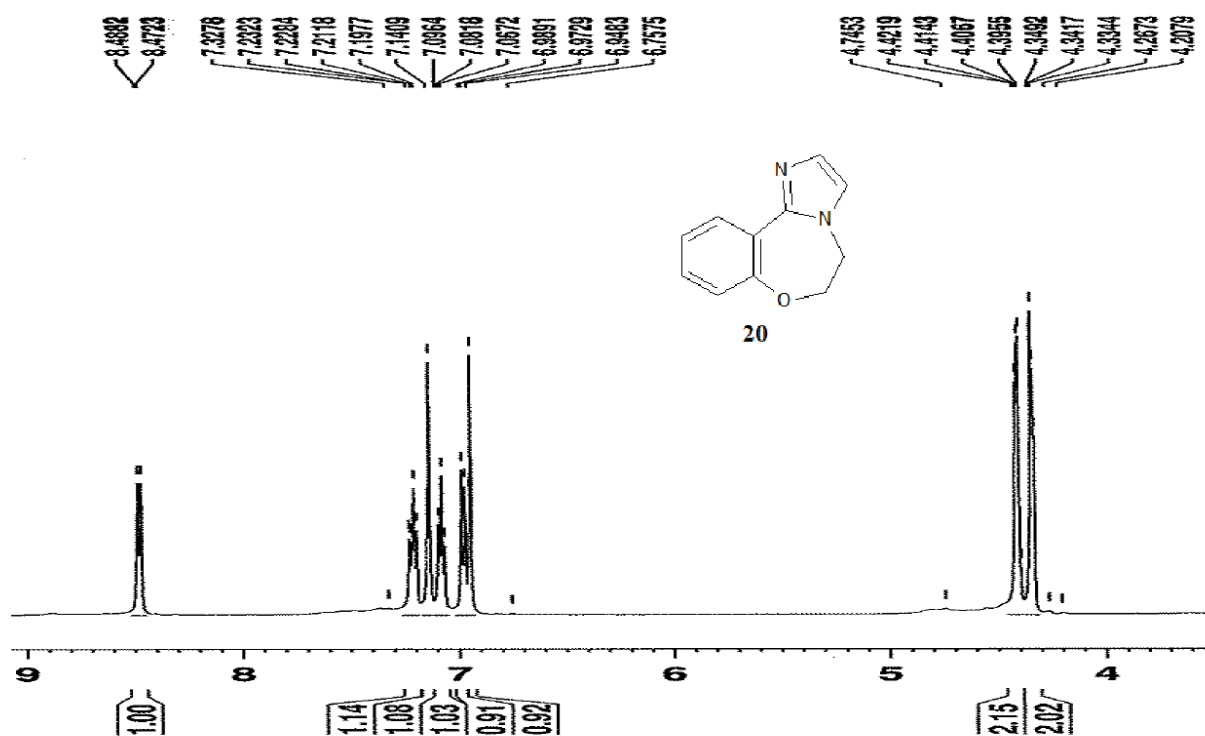


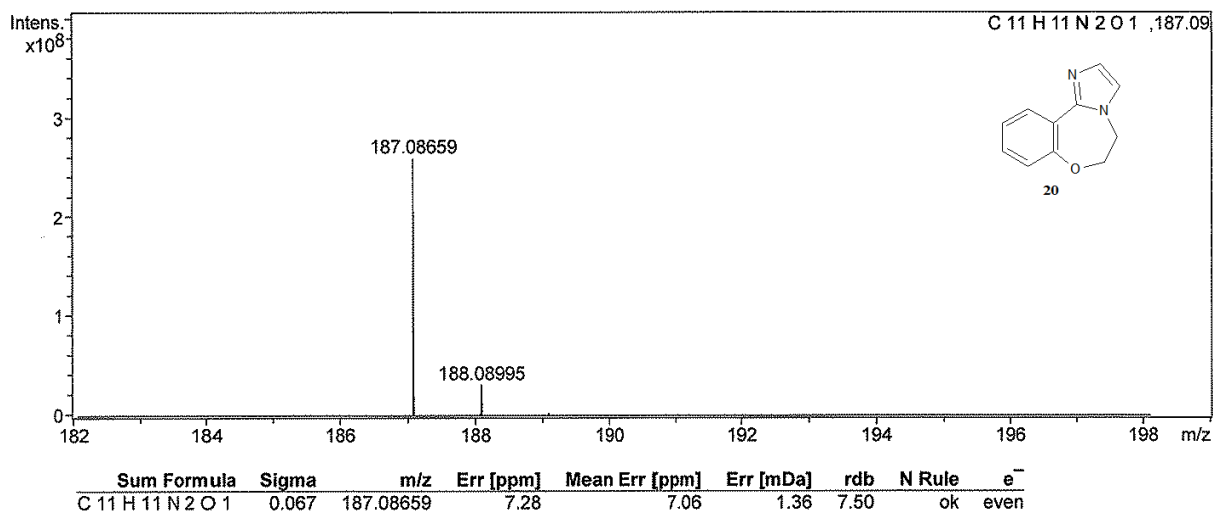
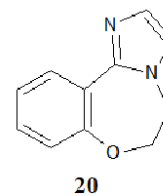
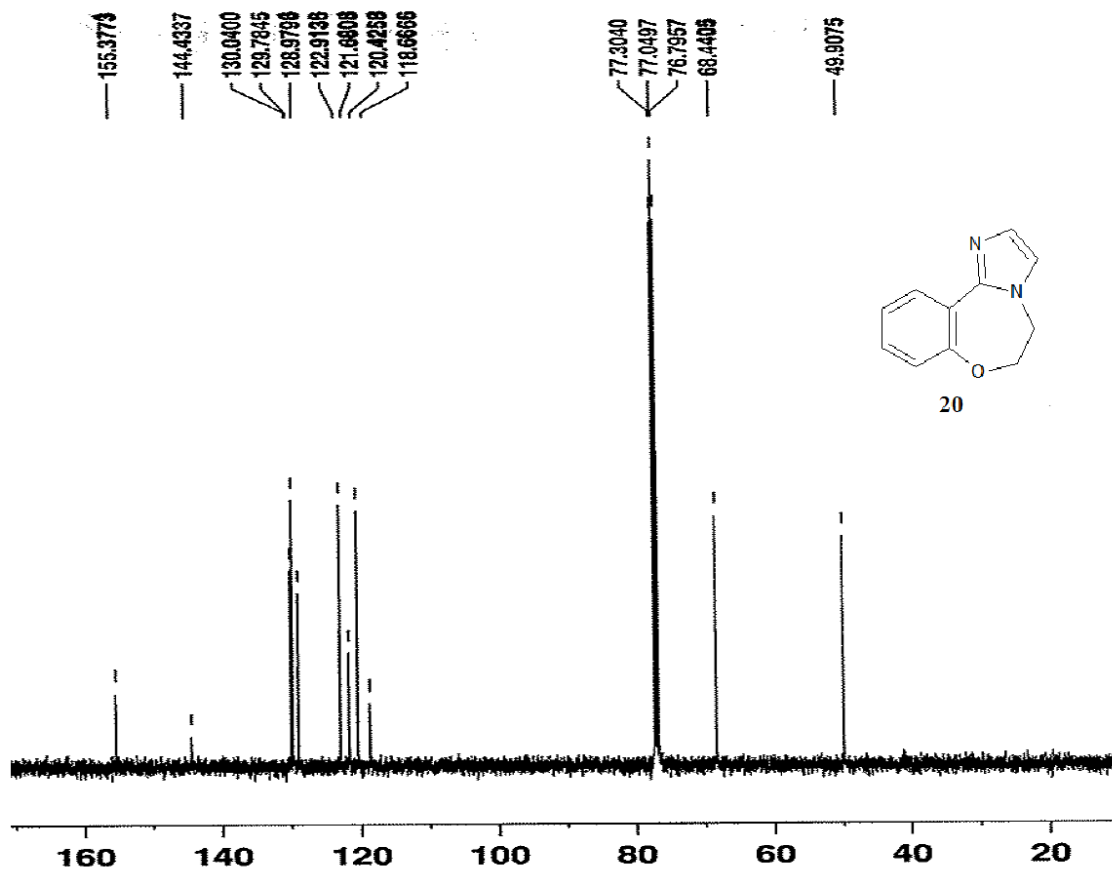


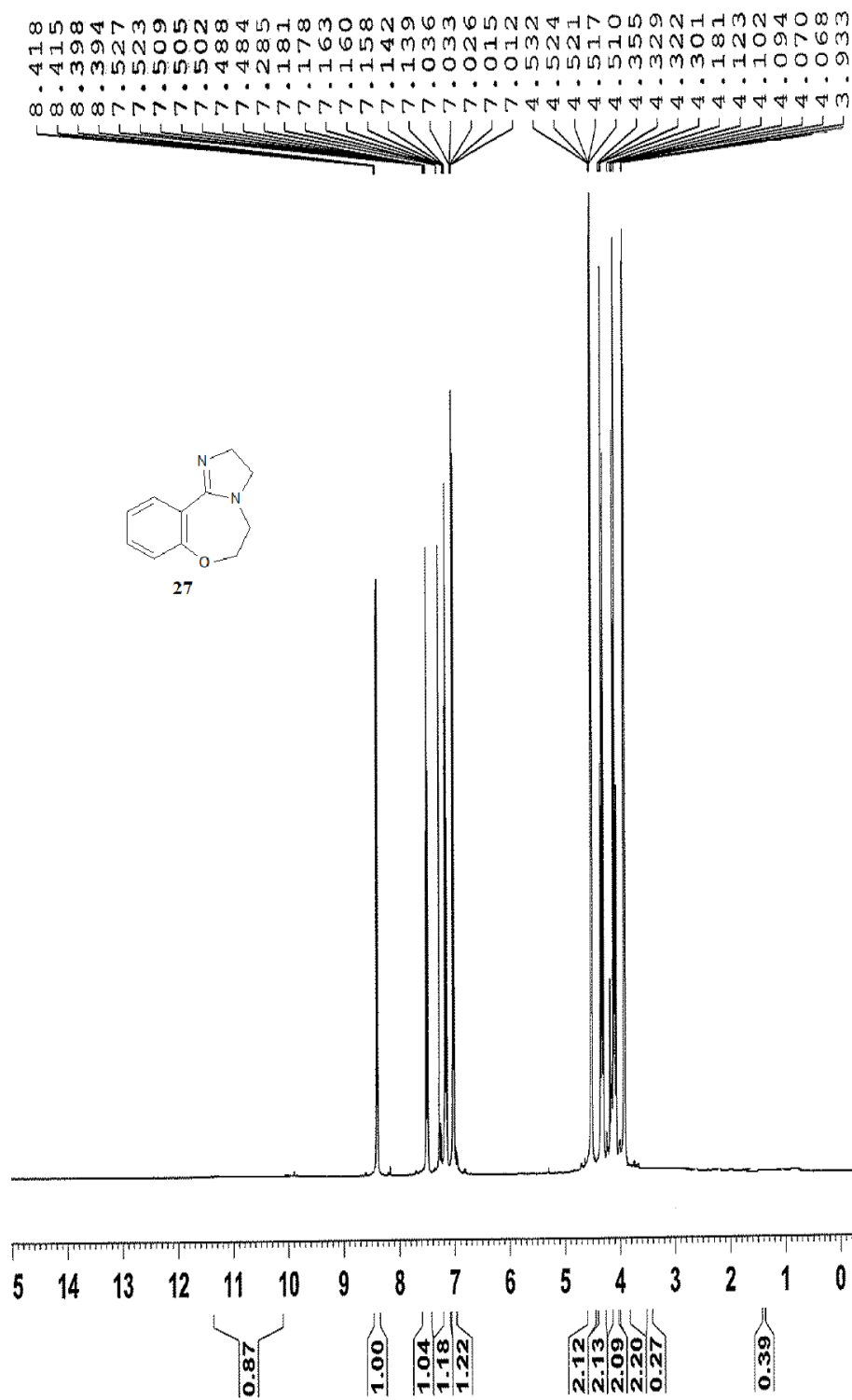


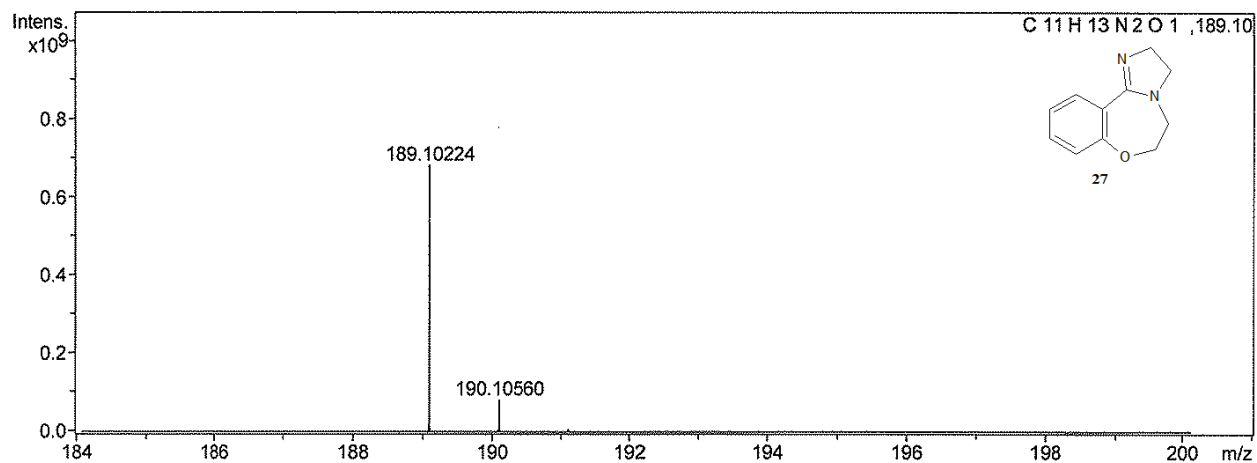
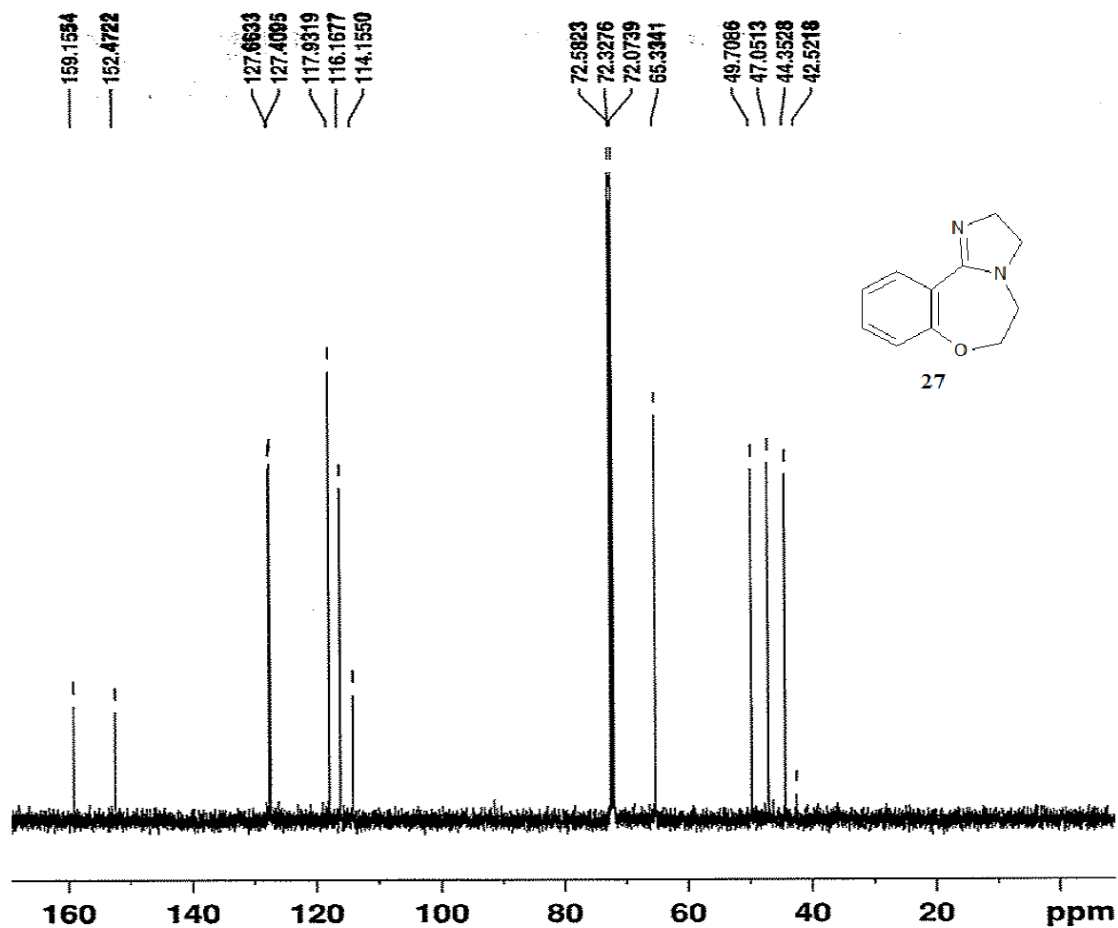




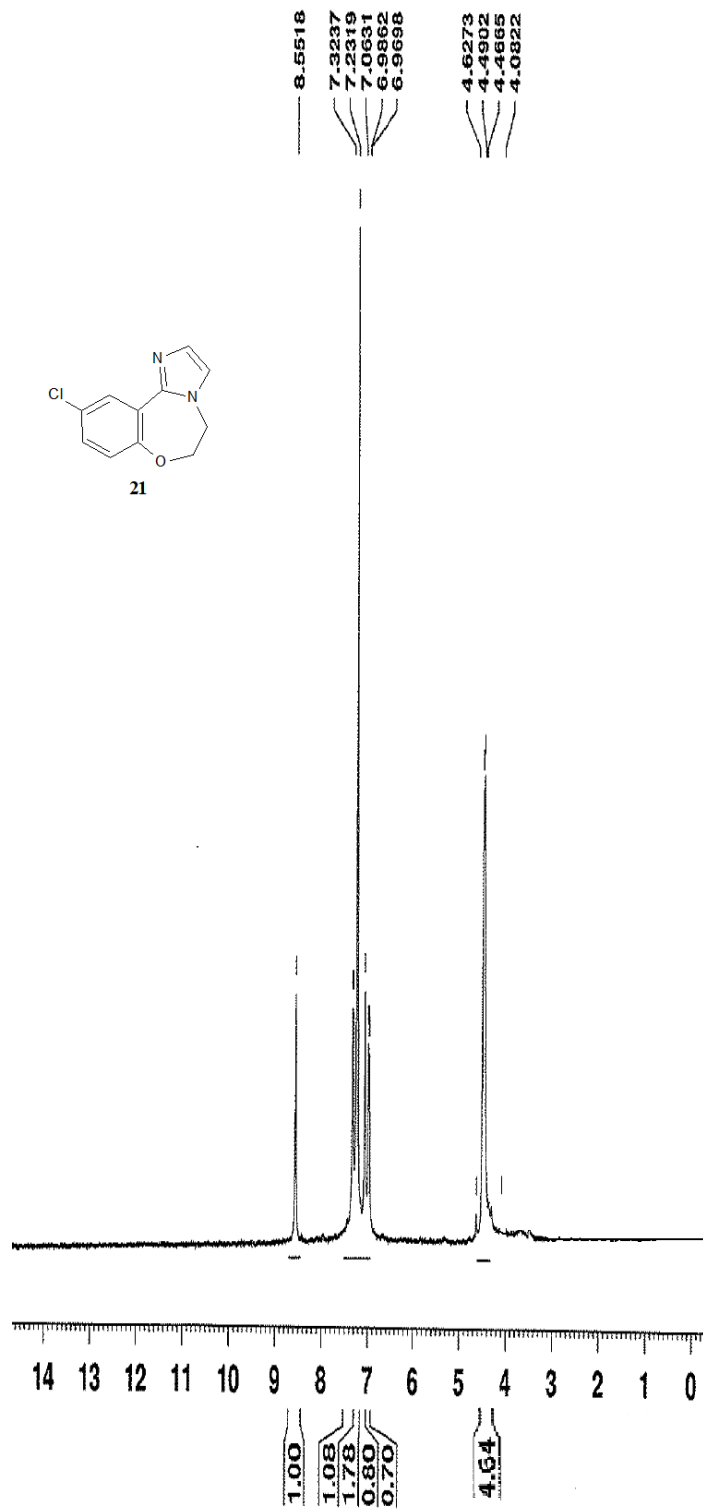


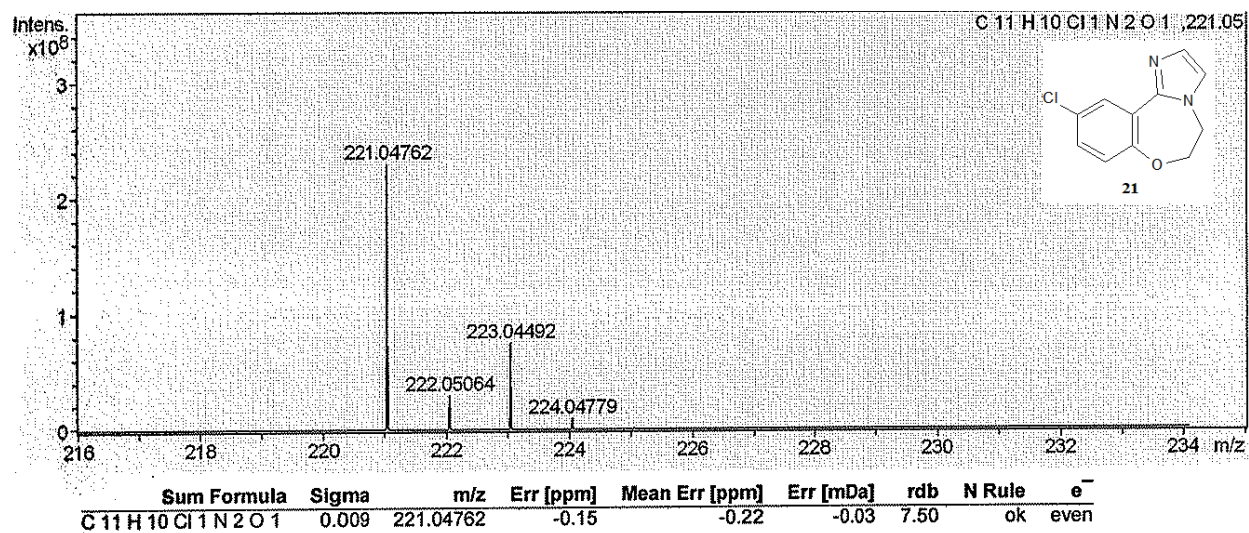
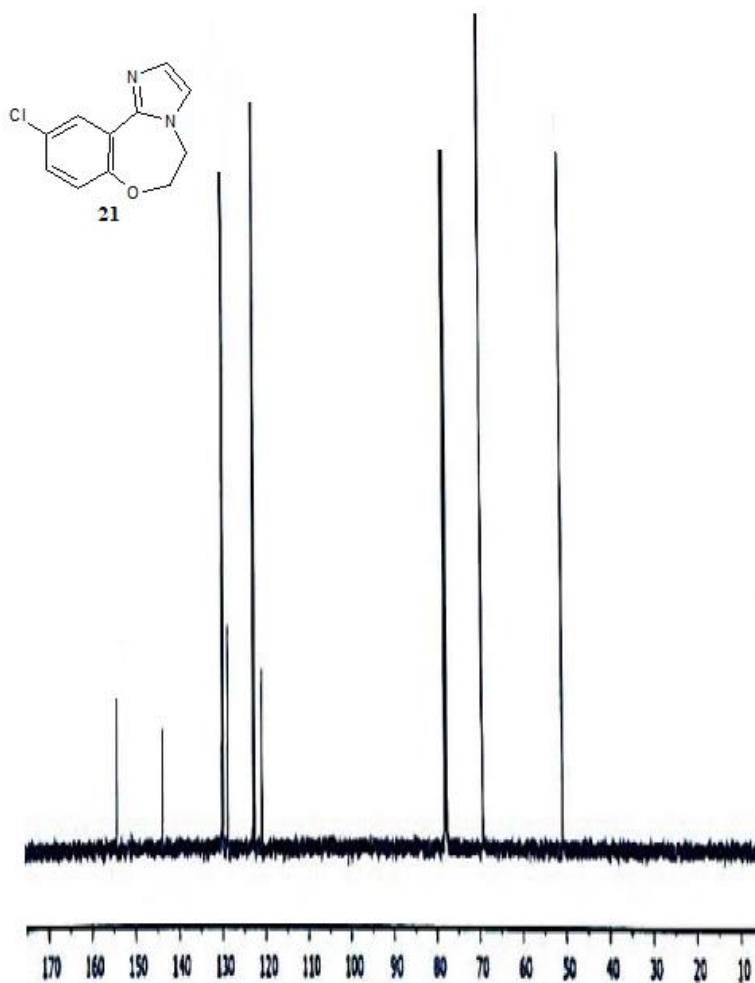


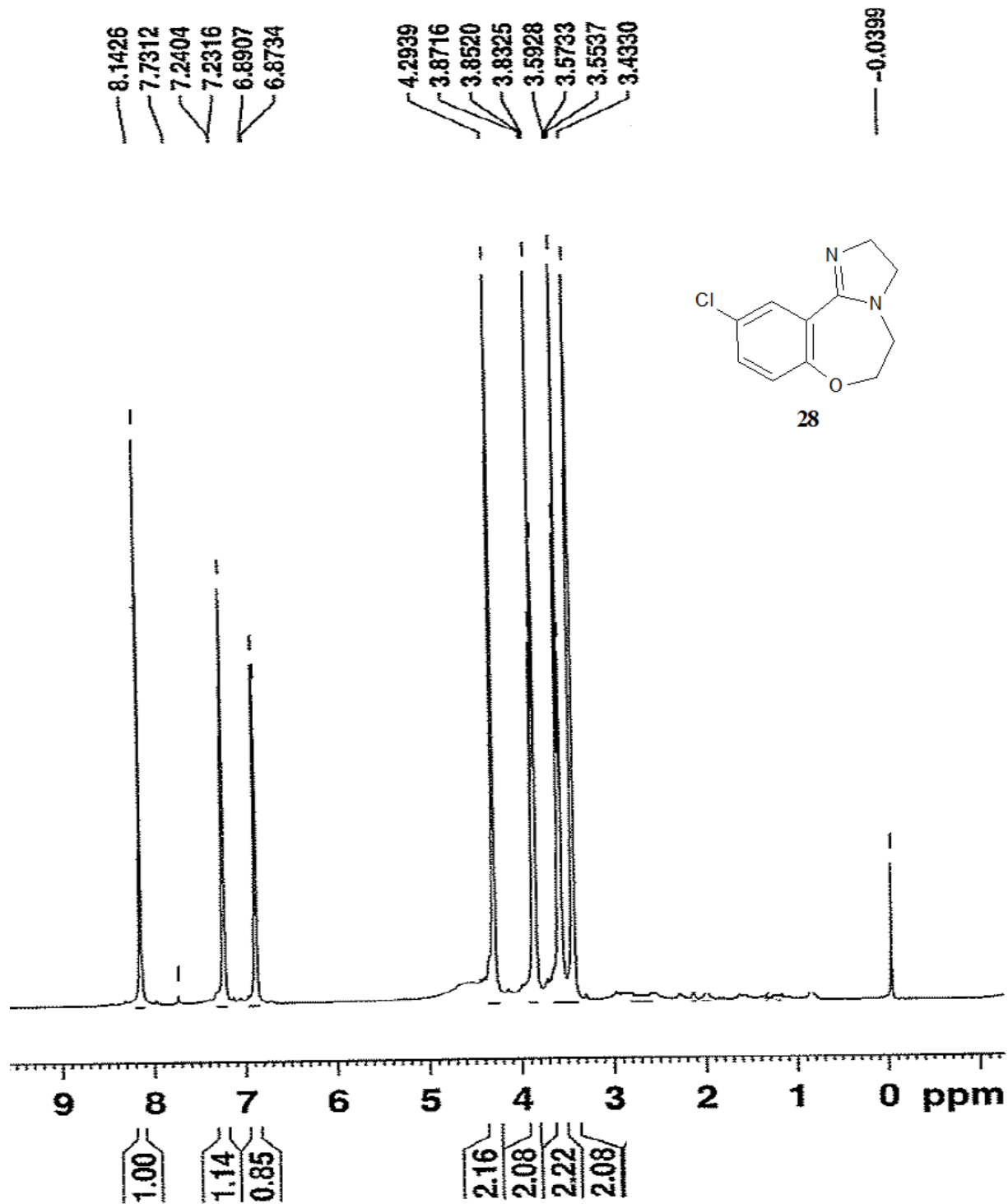


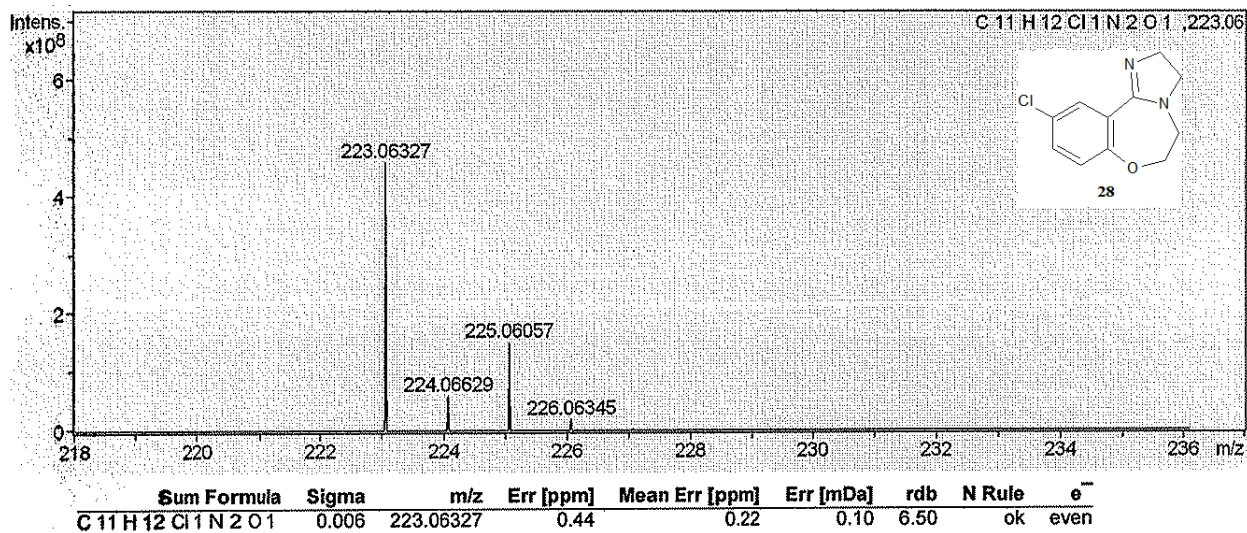
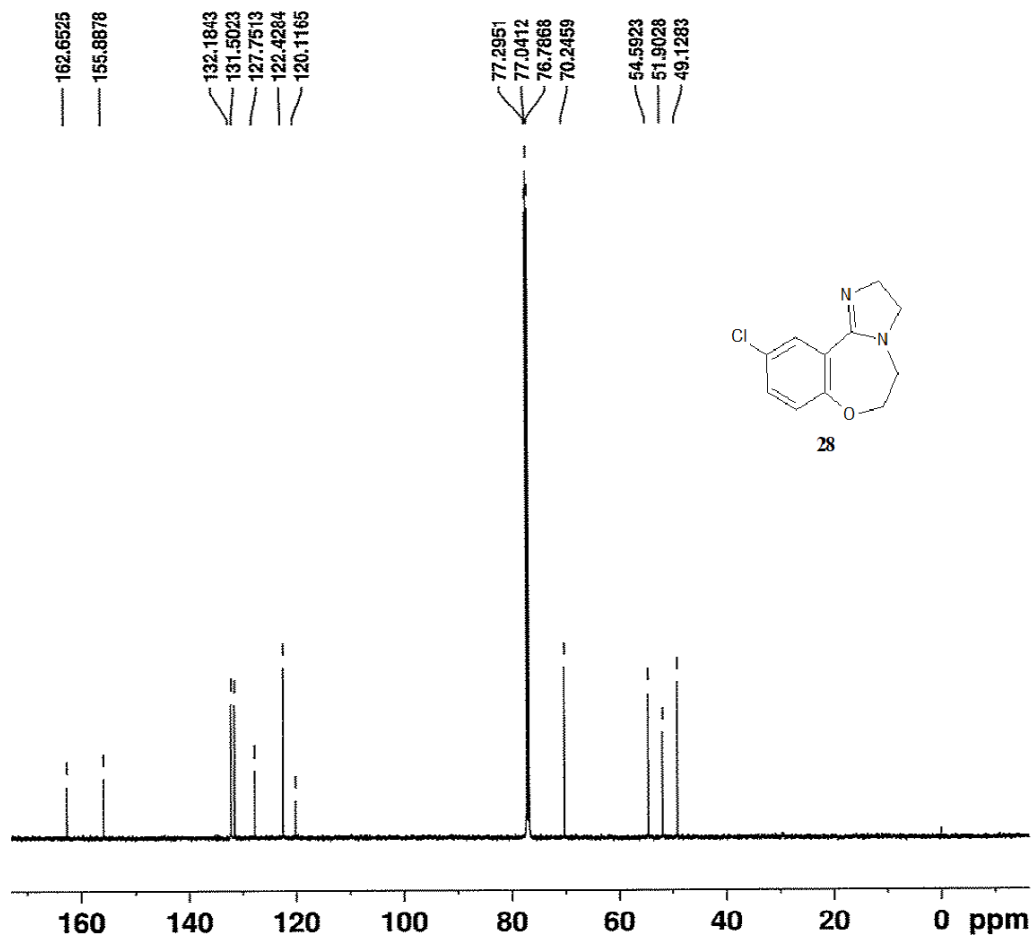


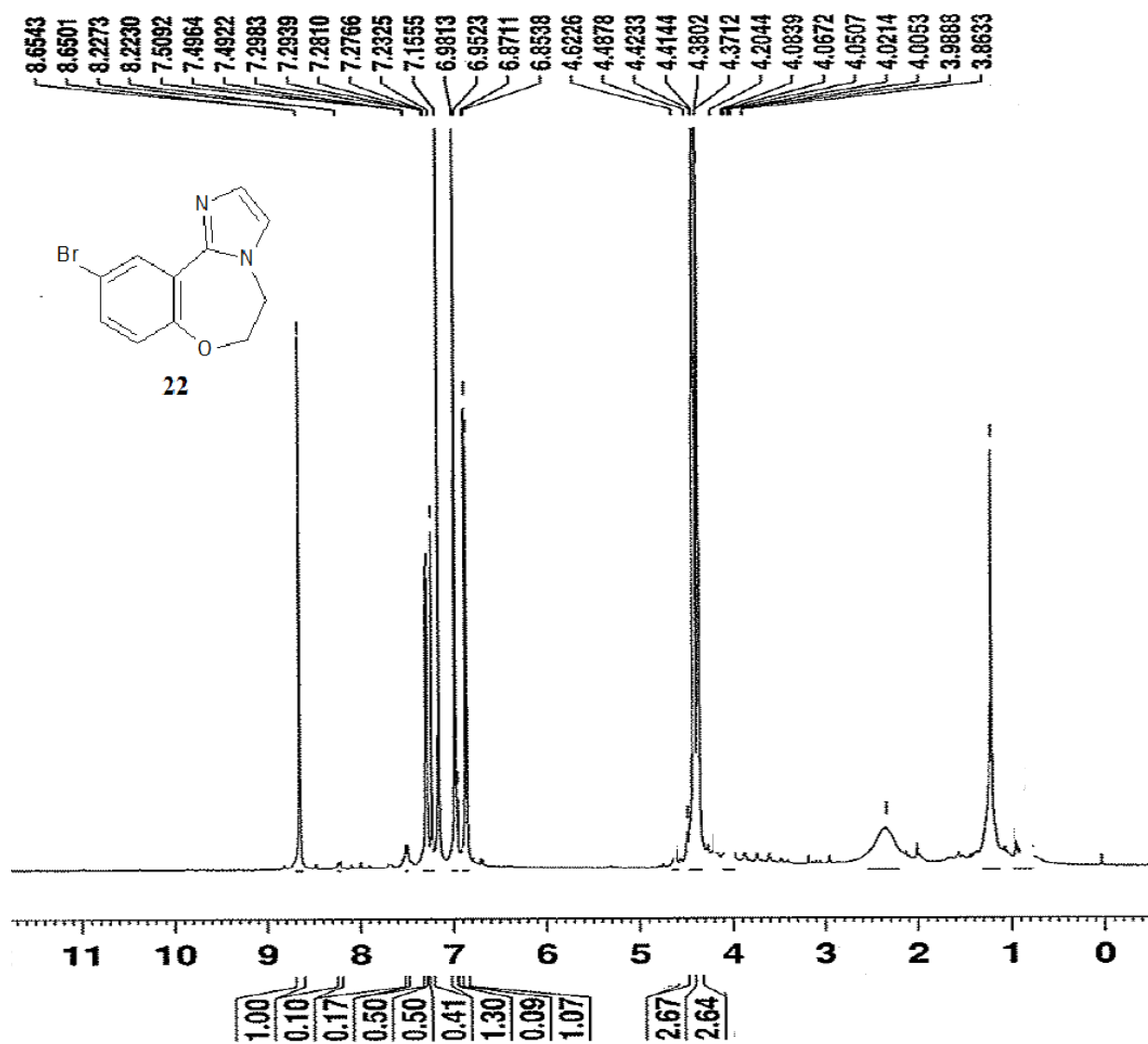
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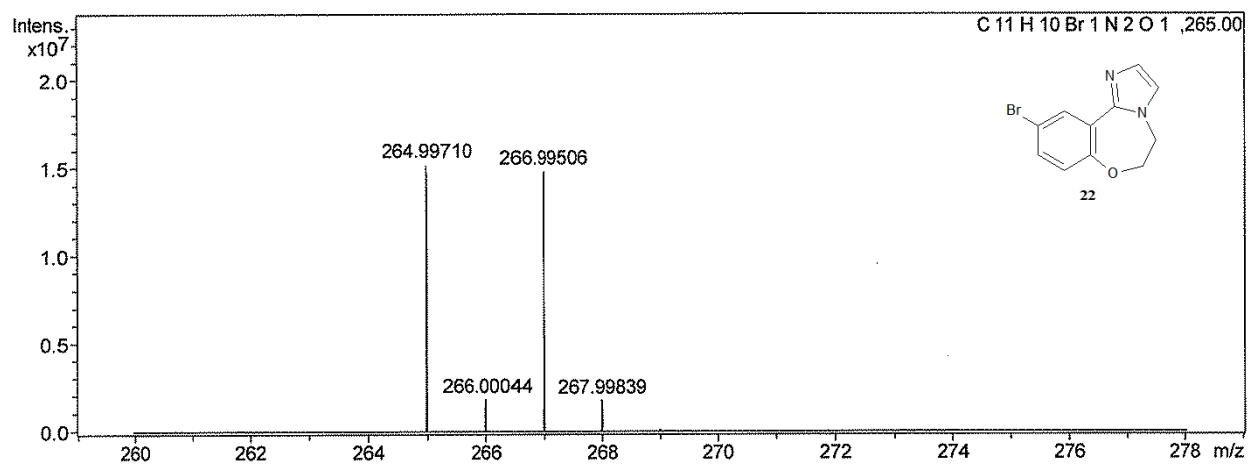
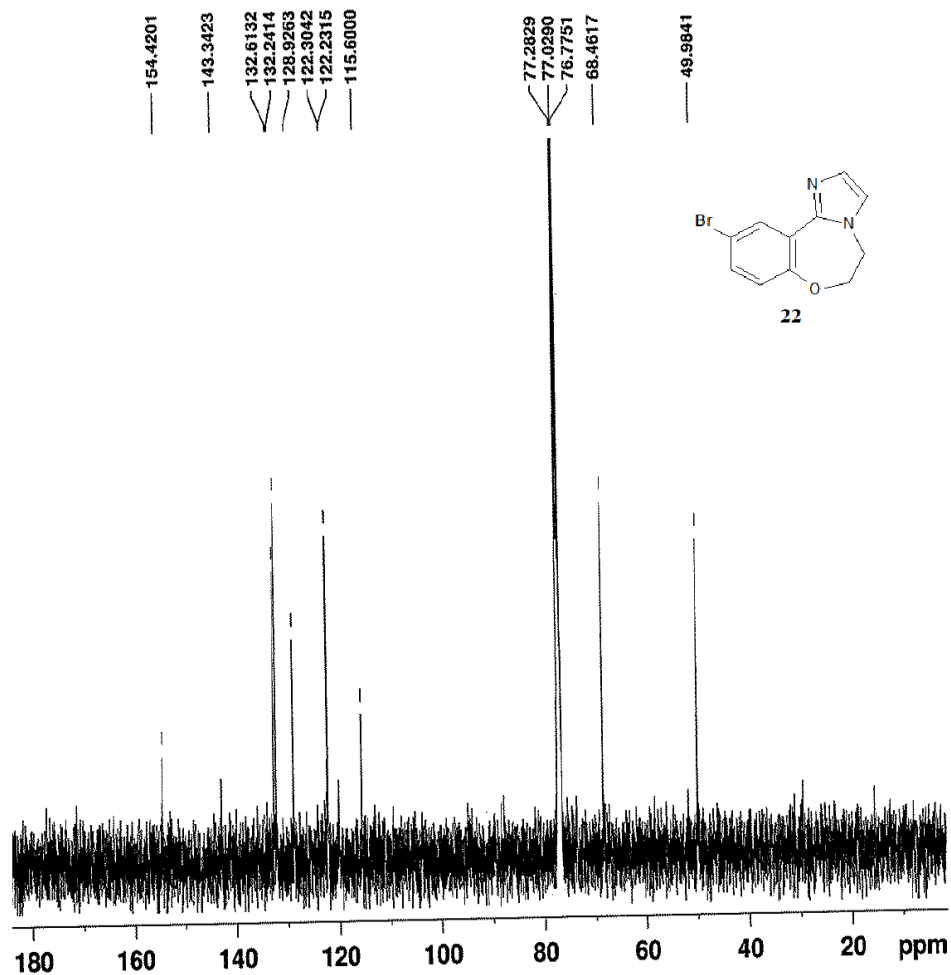




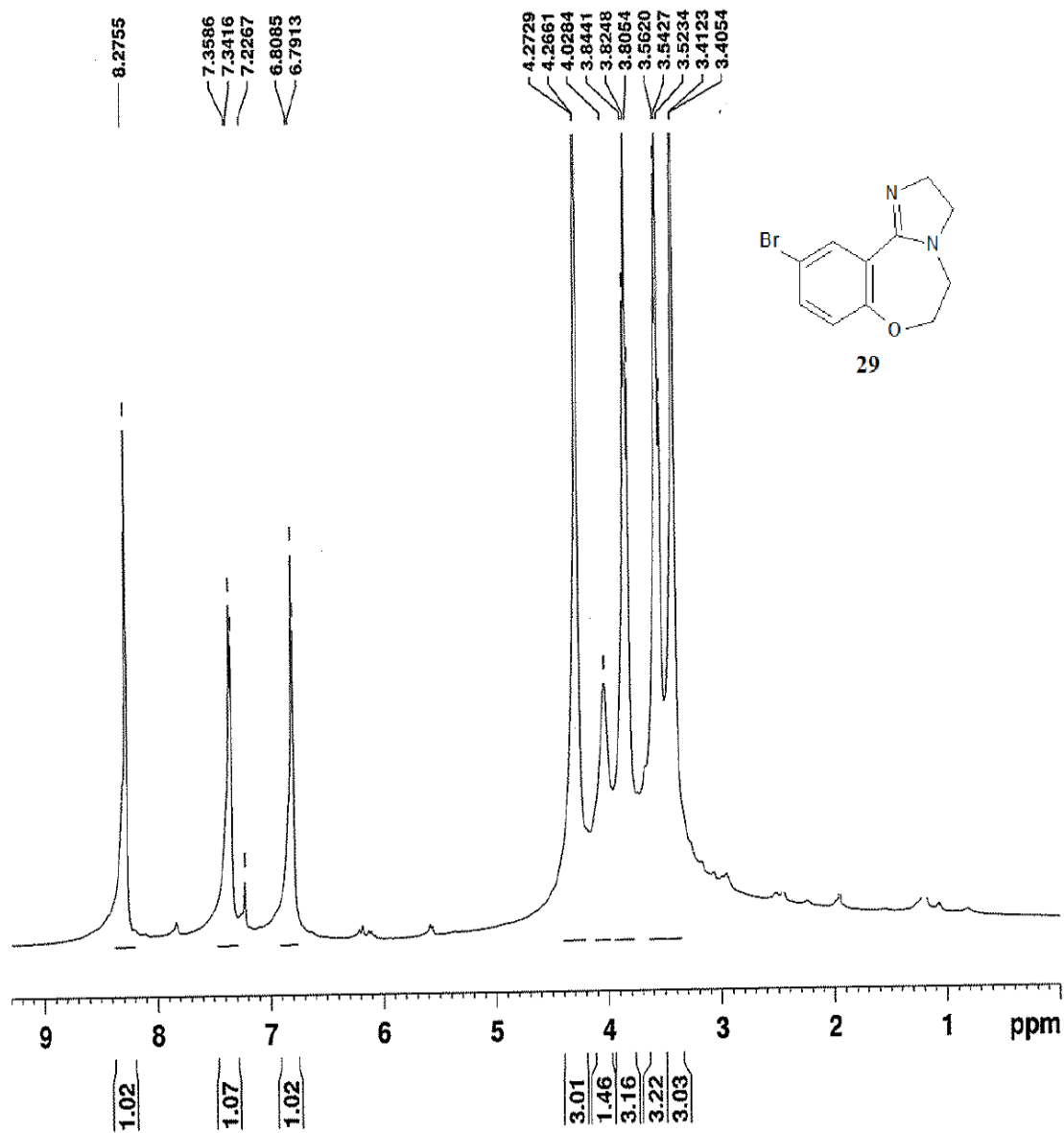


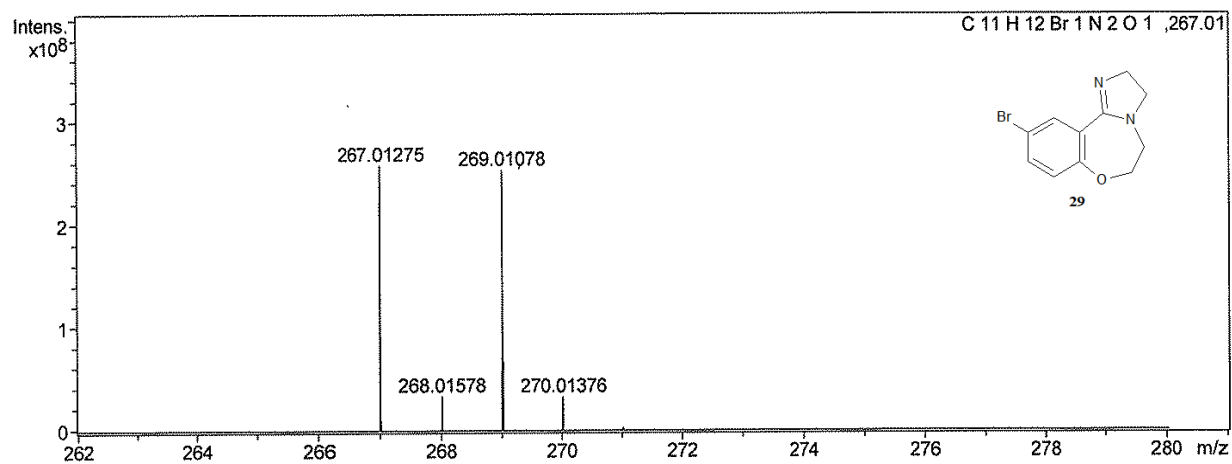
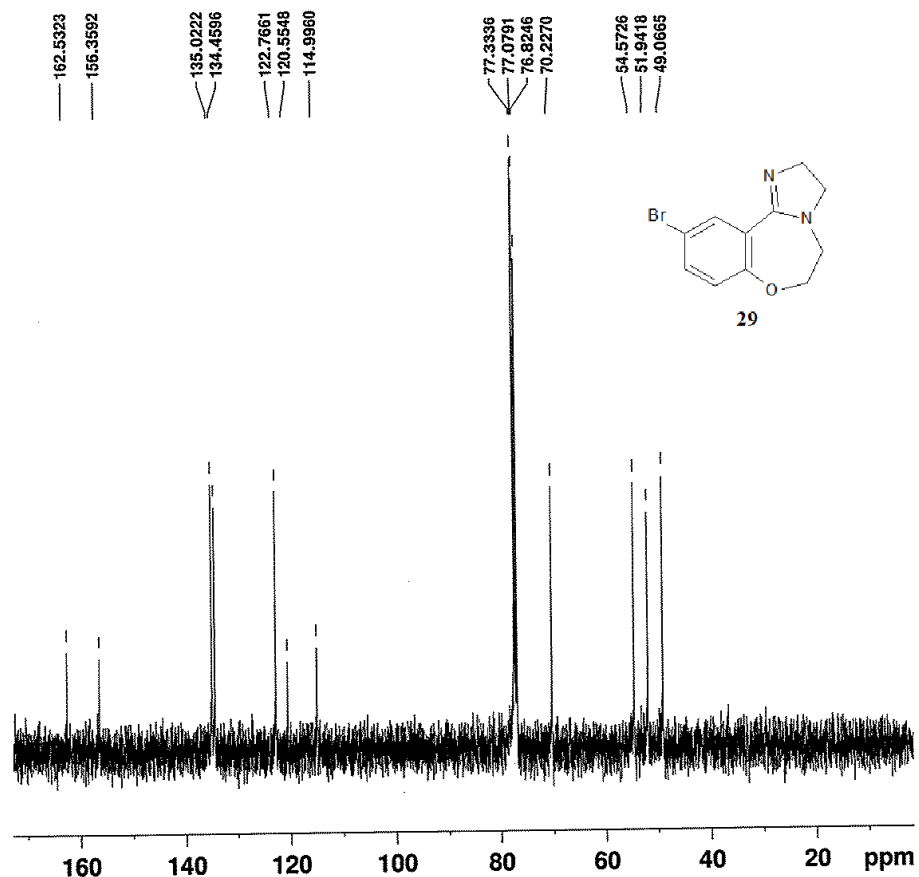




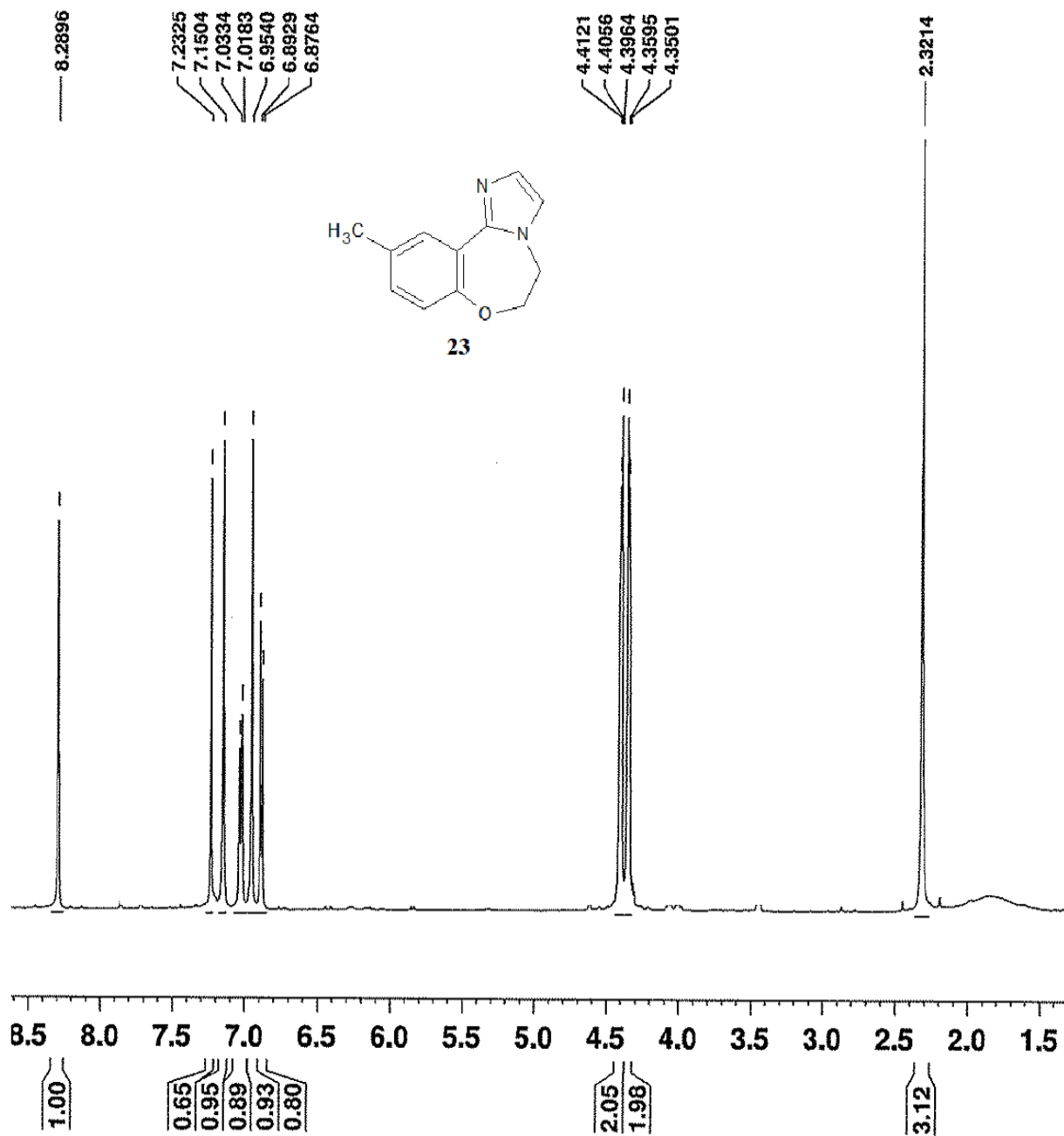


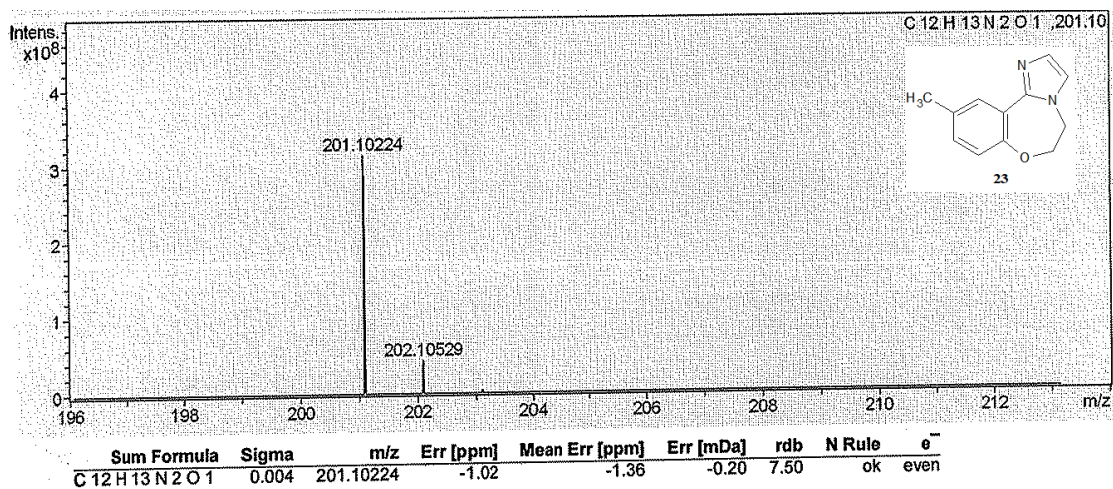
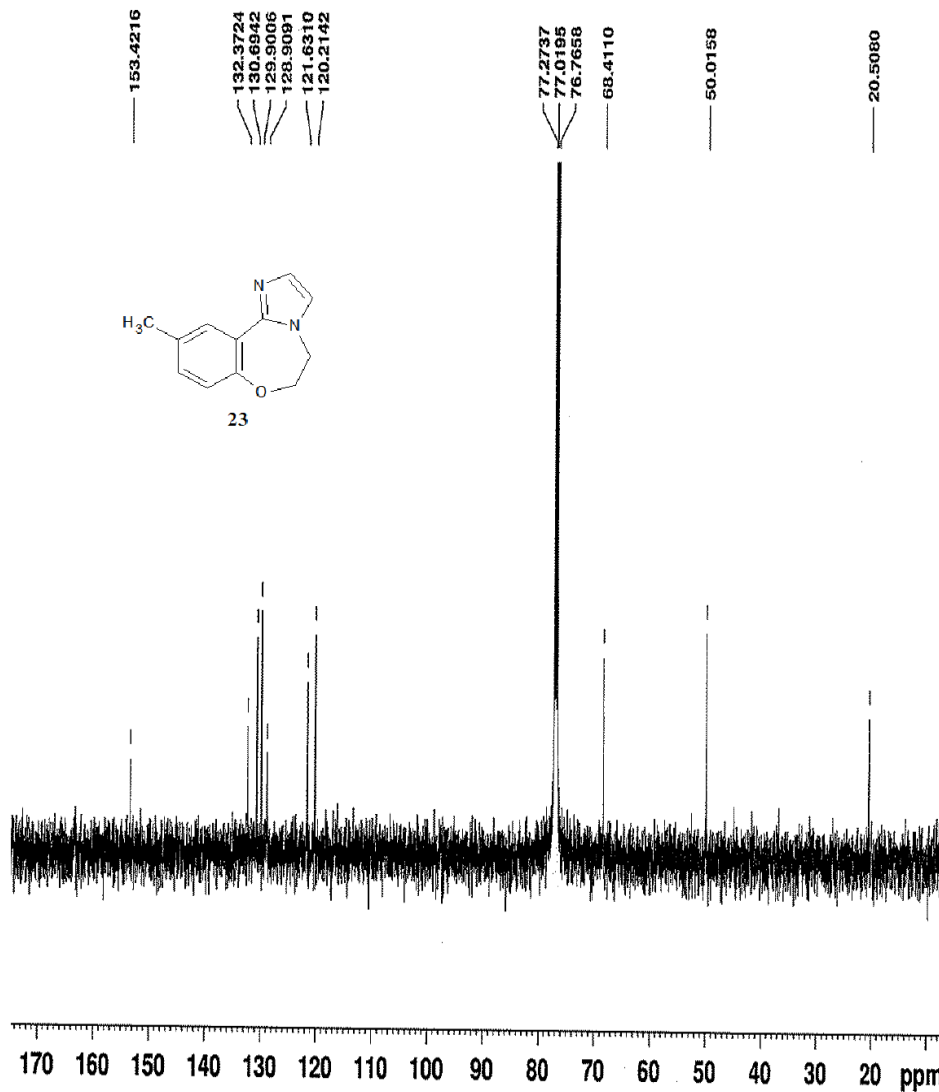
Sum	Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
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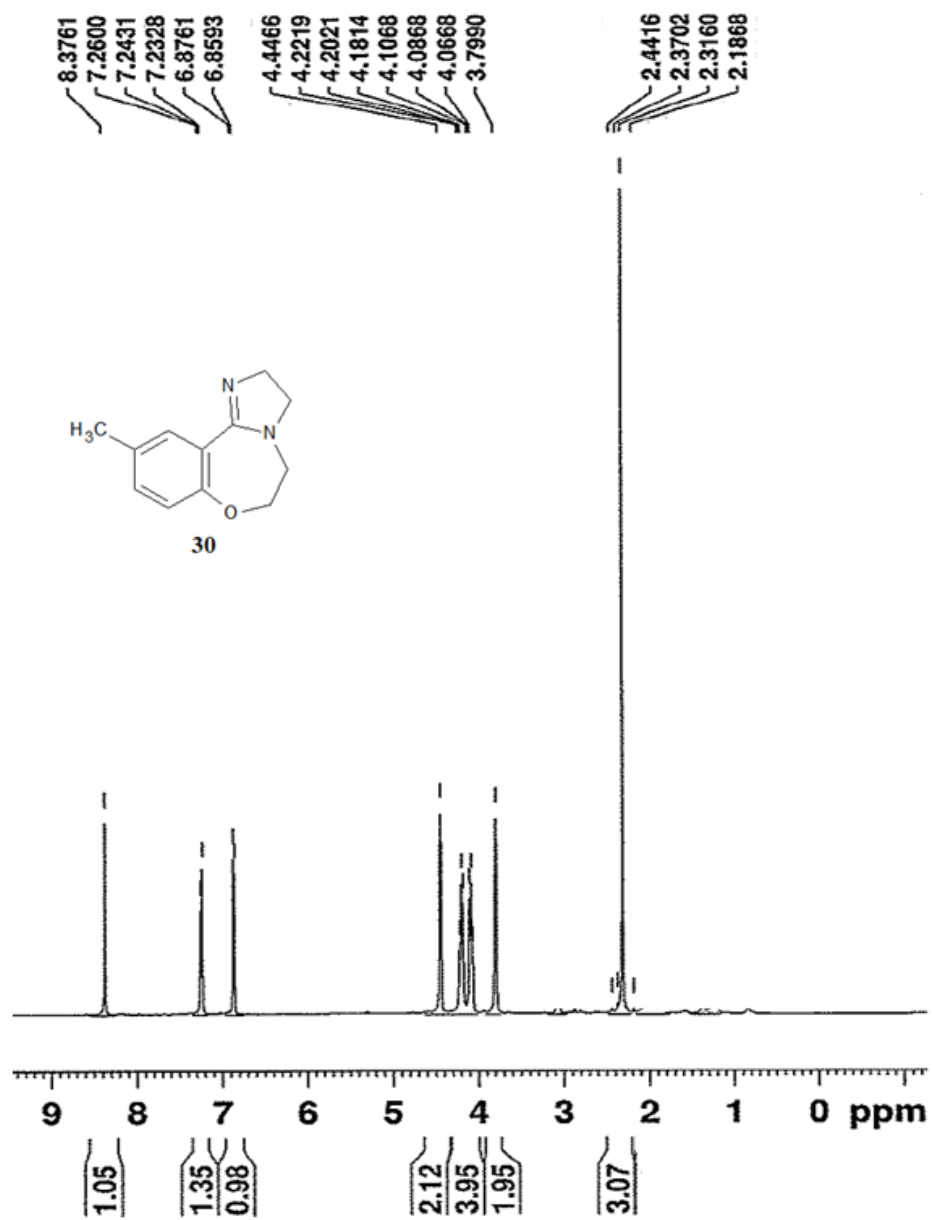


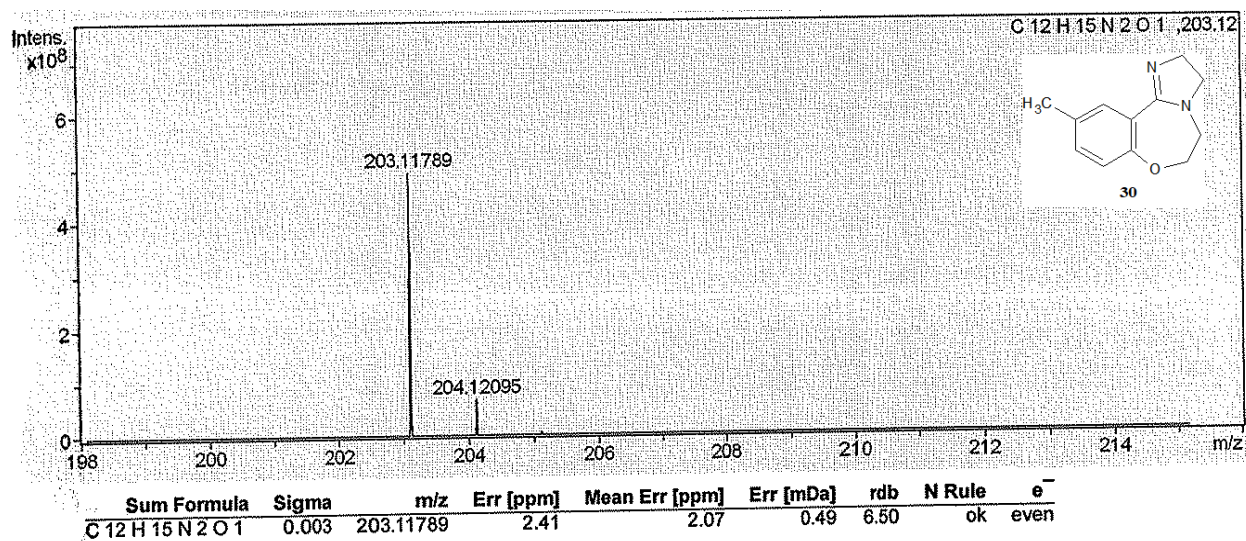
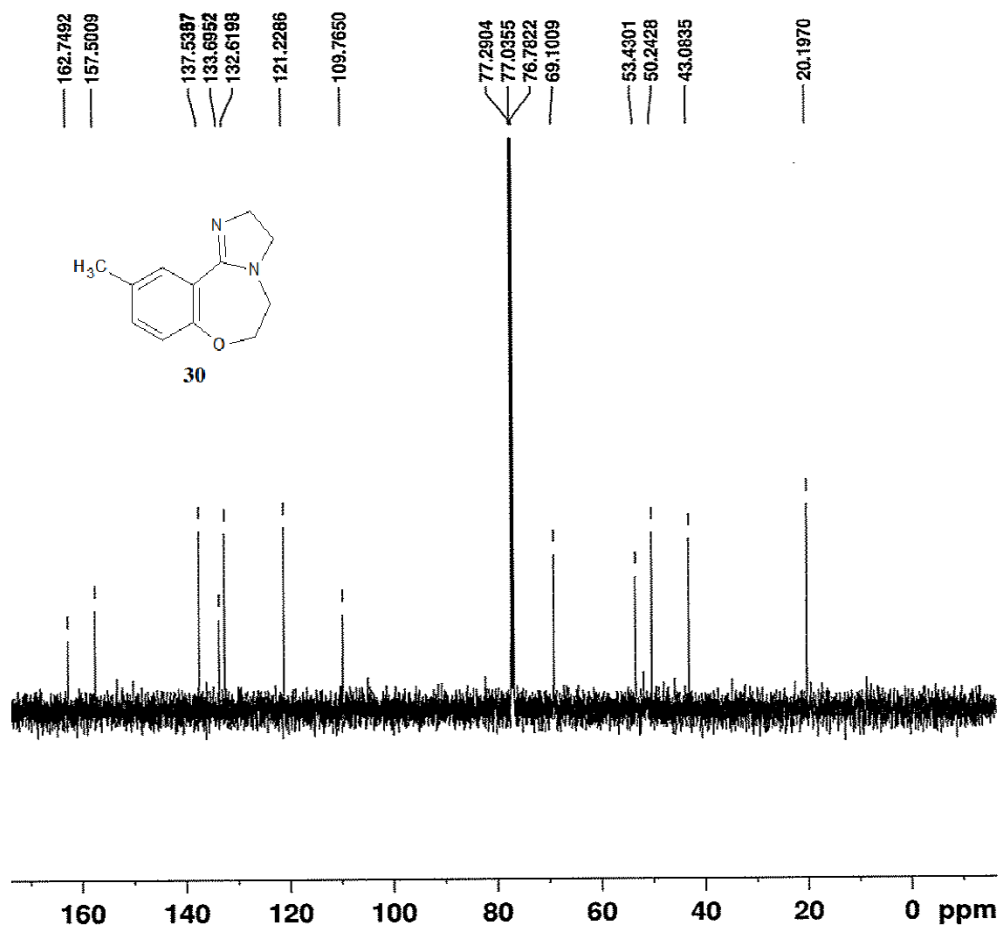


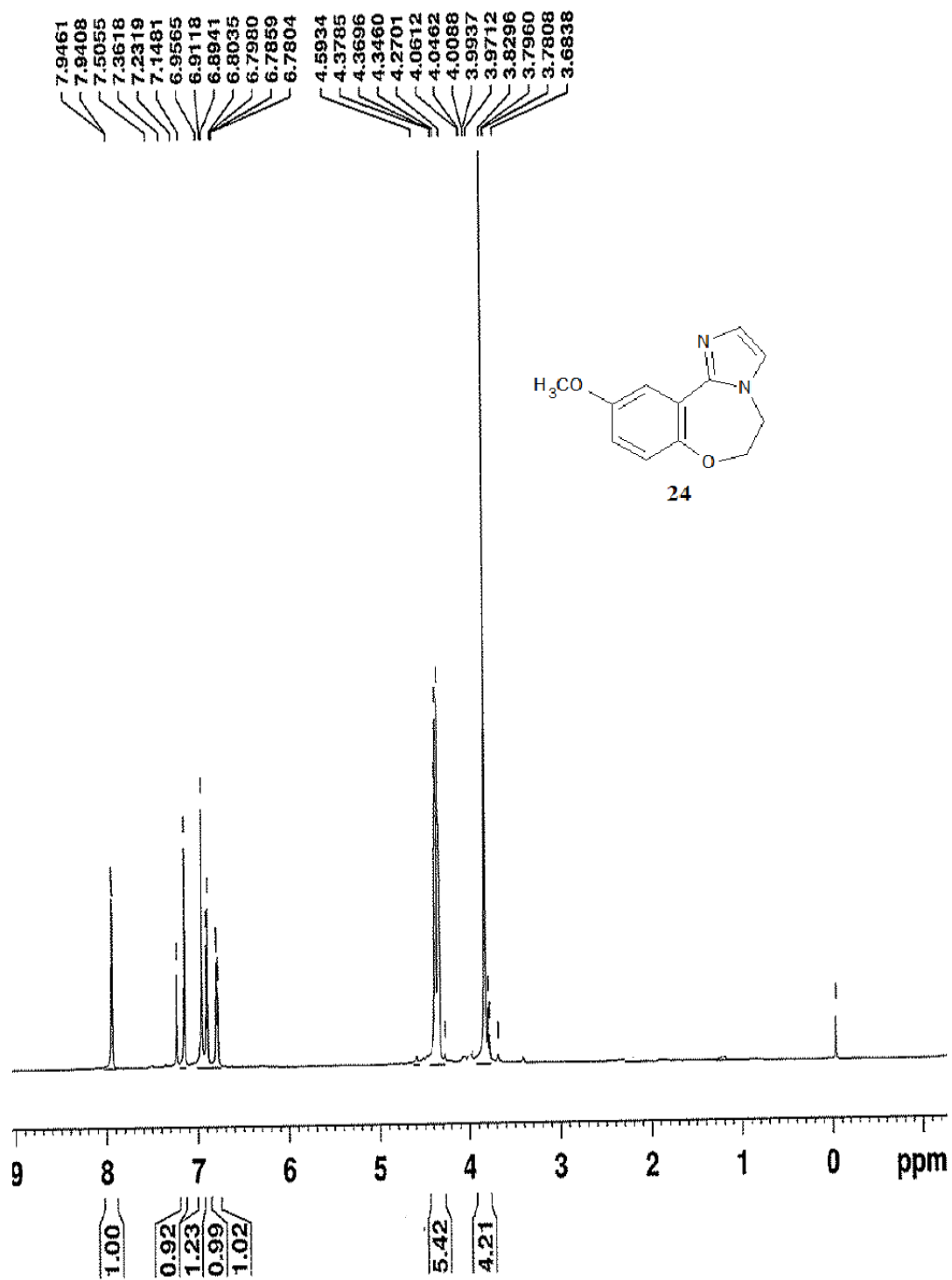
Sum	Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 11 H 12 Br 1 N 2 O 1		0.011	267.01275	4.62	3.15	1.23	6.50	ok	even

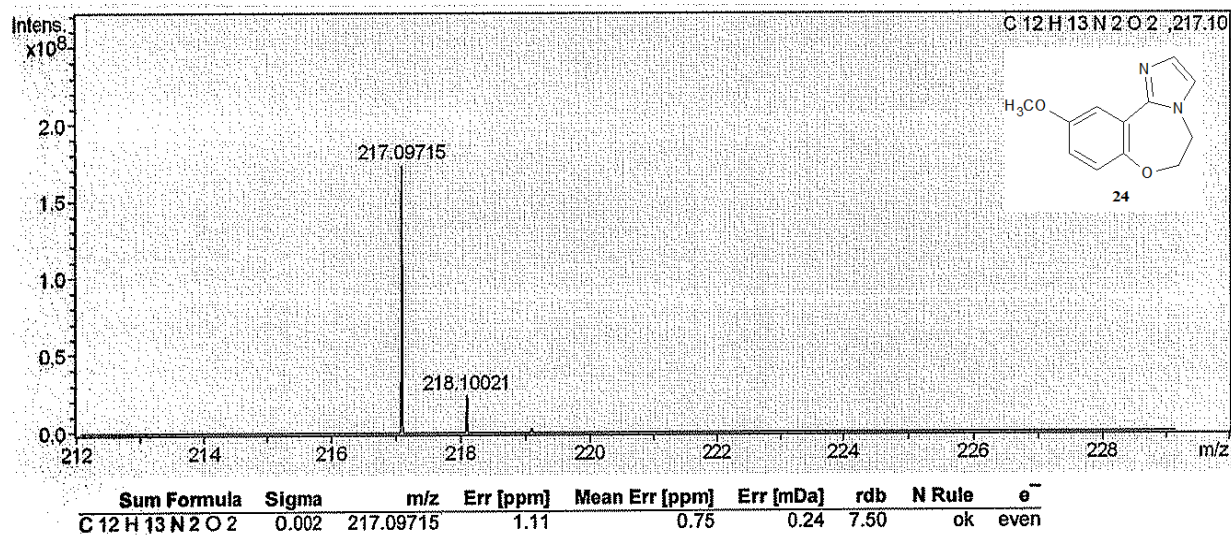
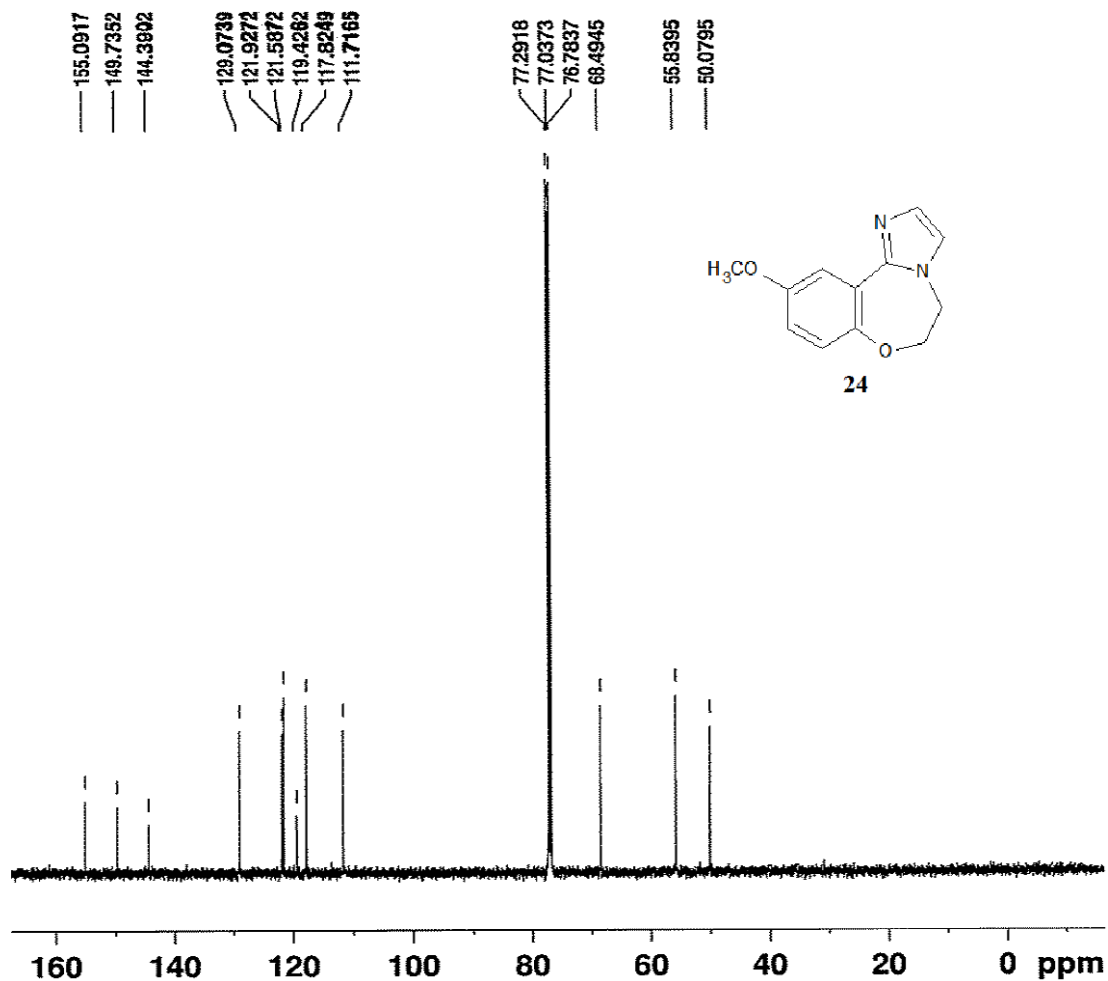


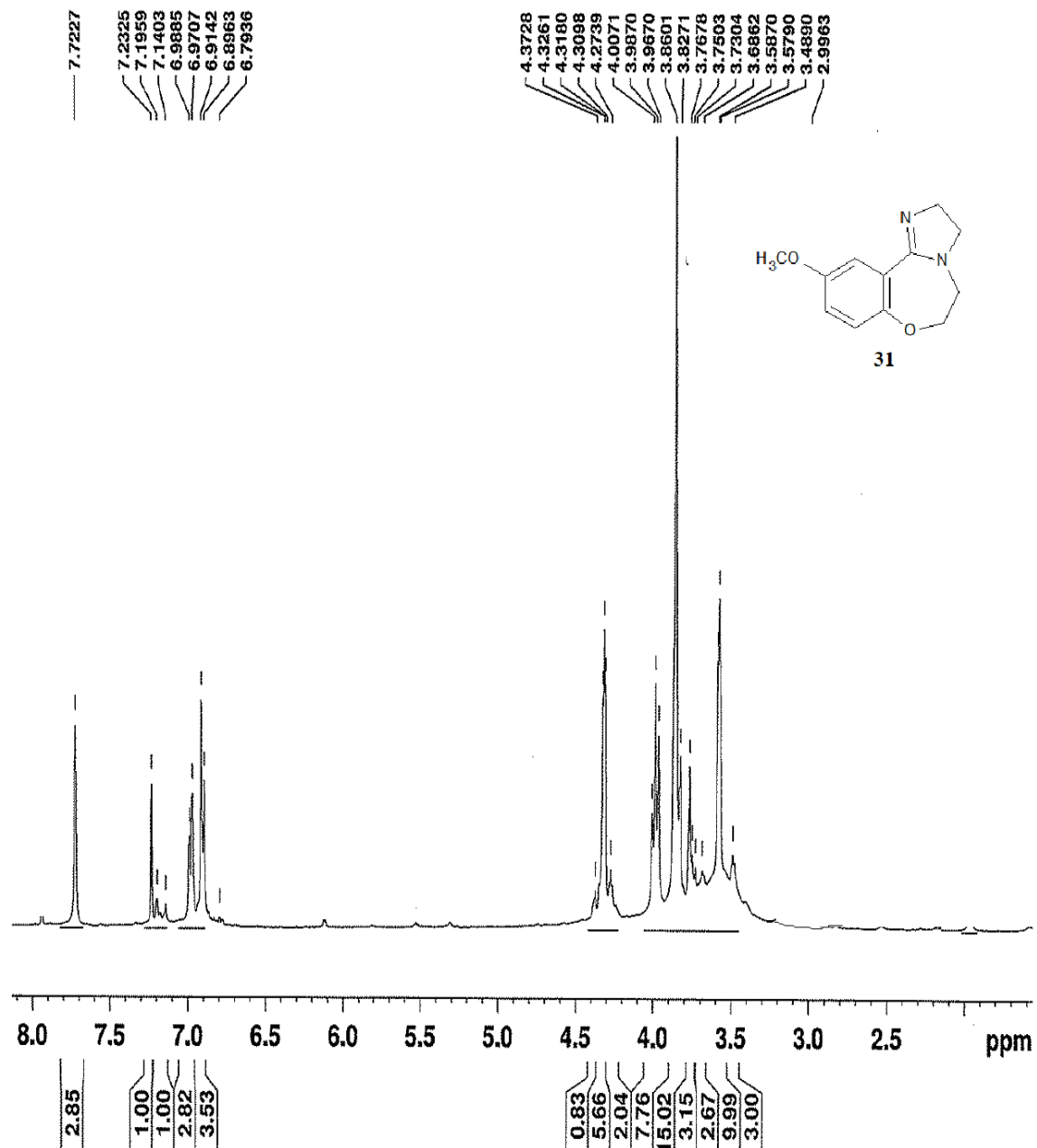


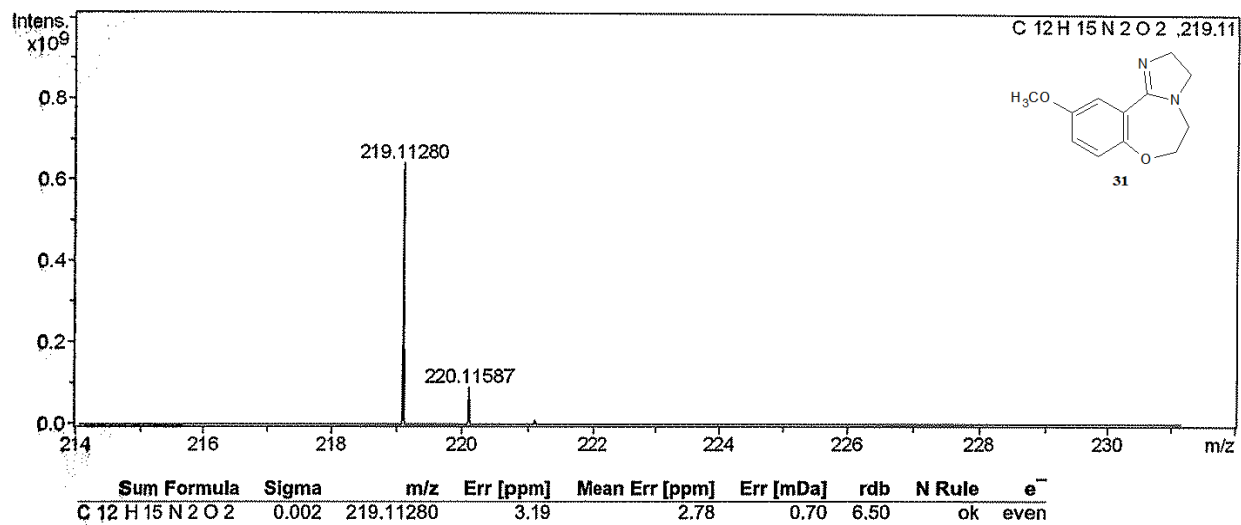
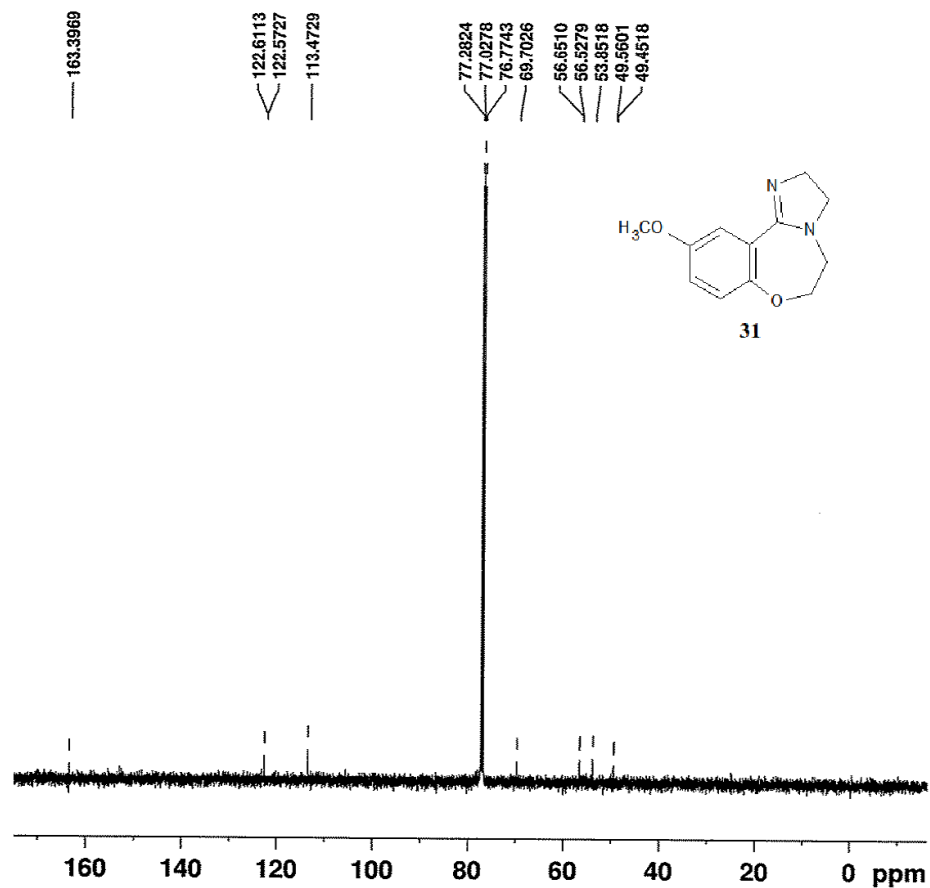


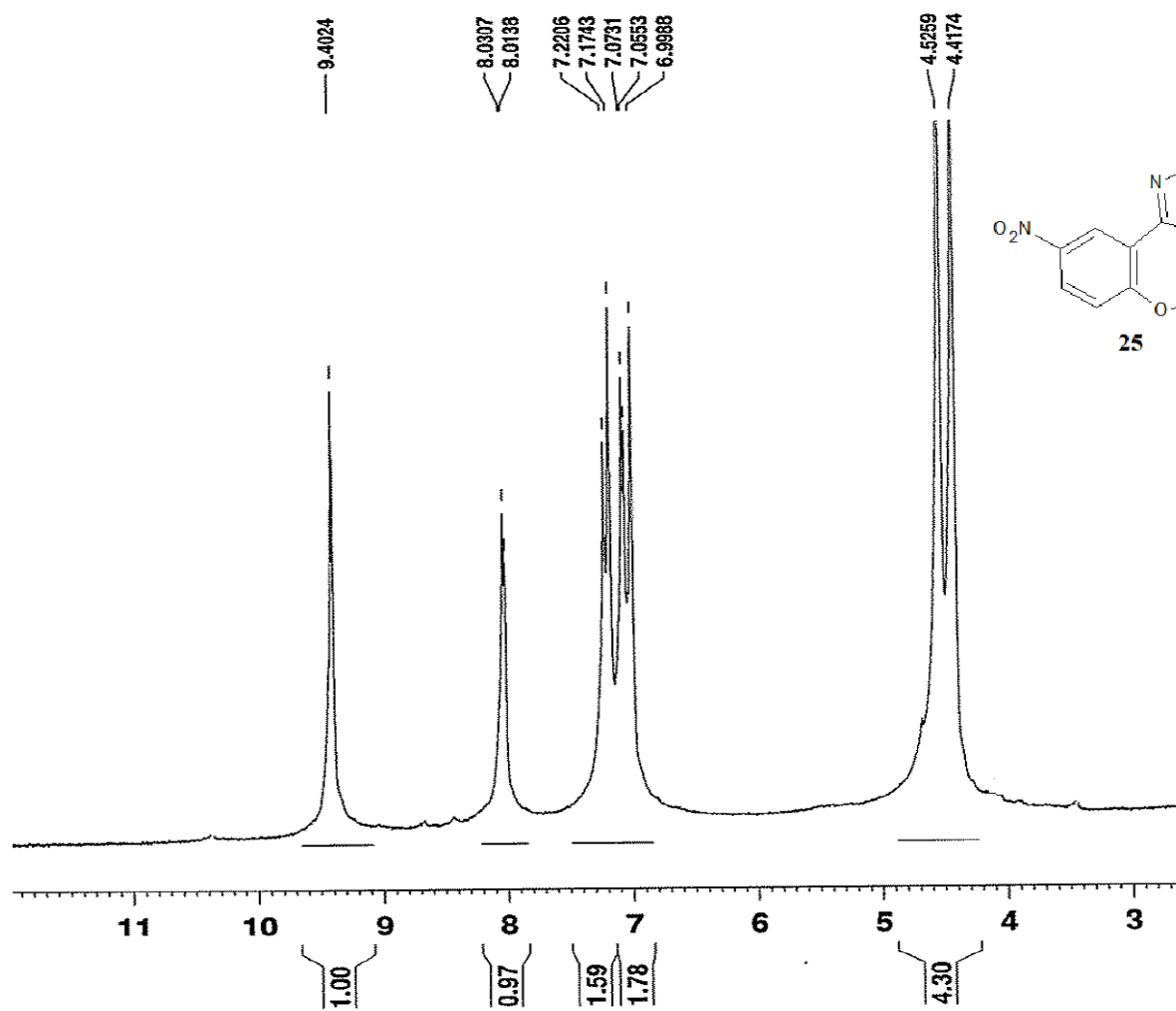


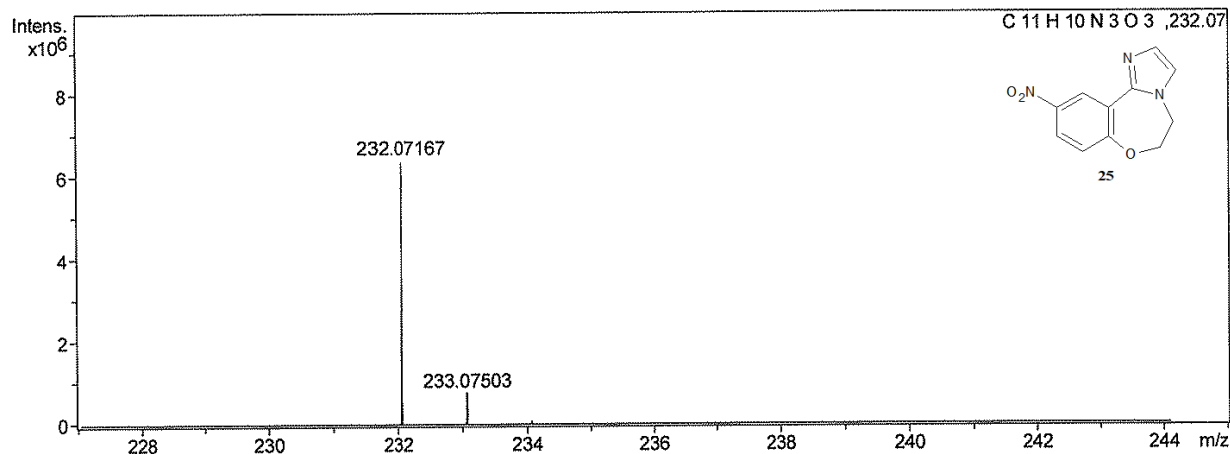
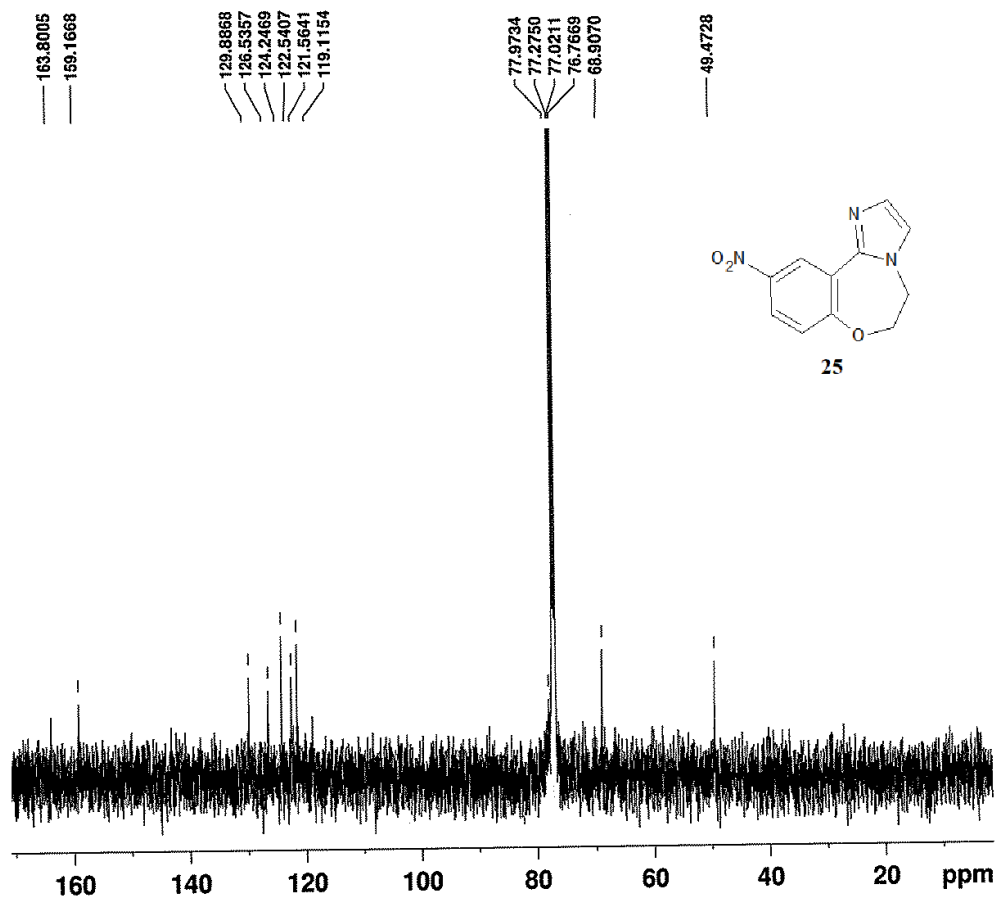




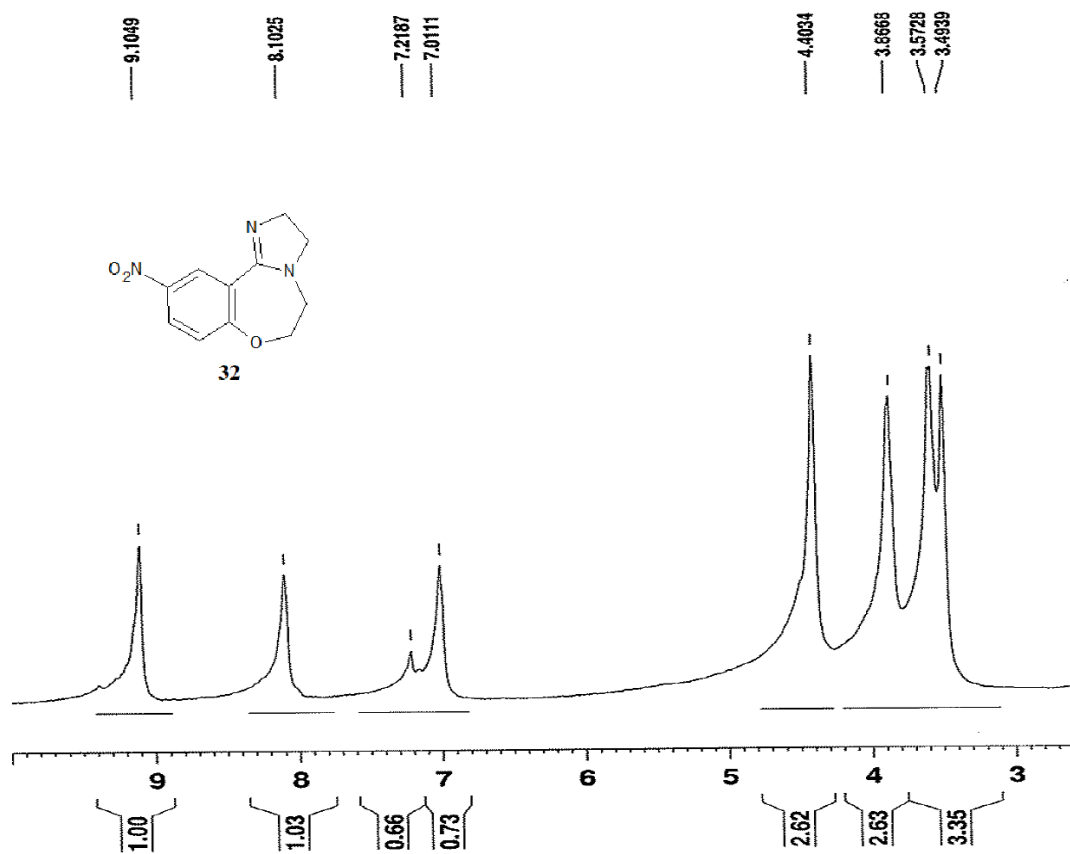


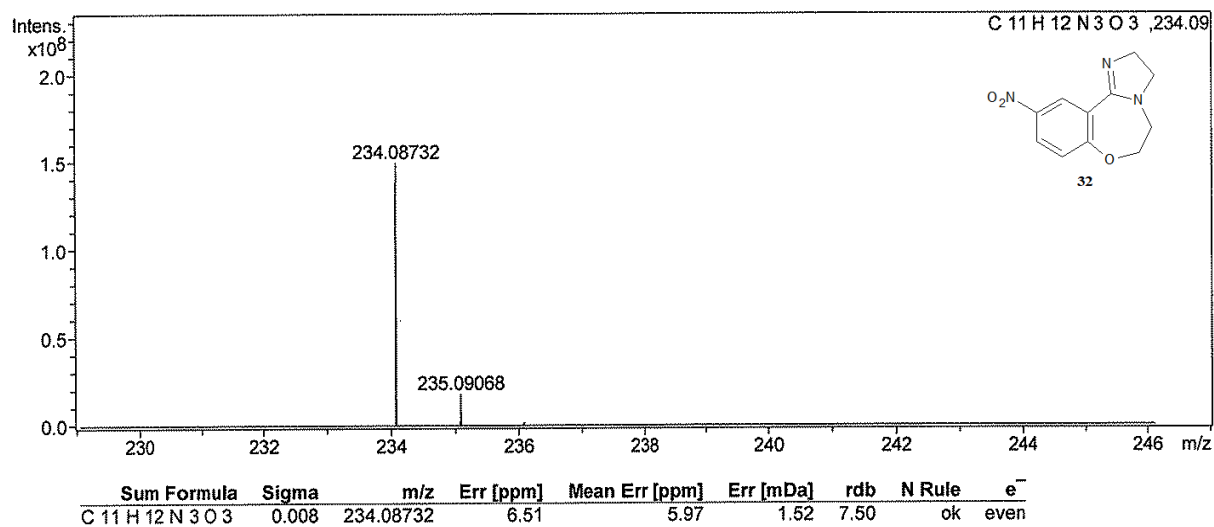
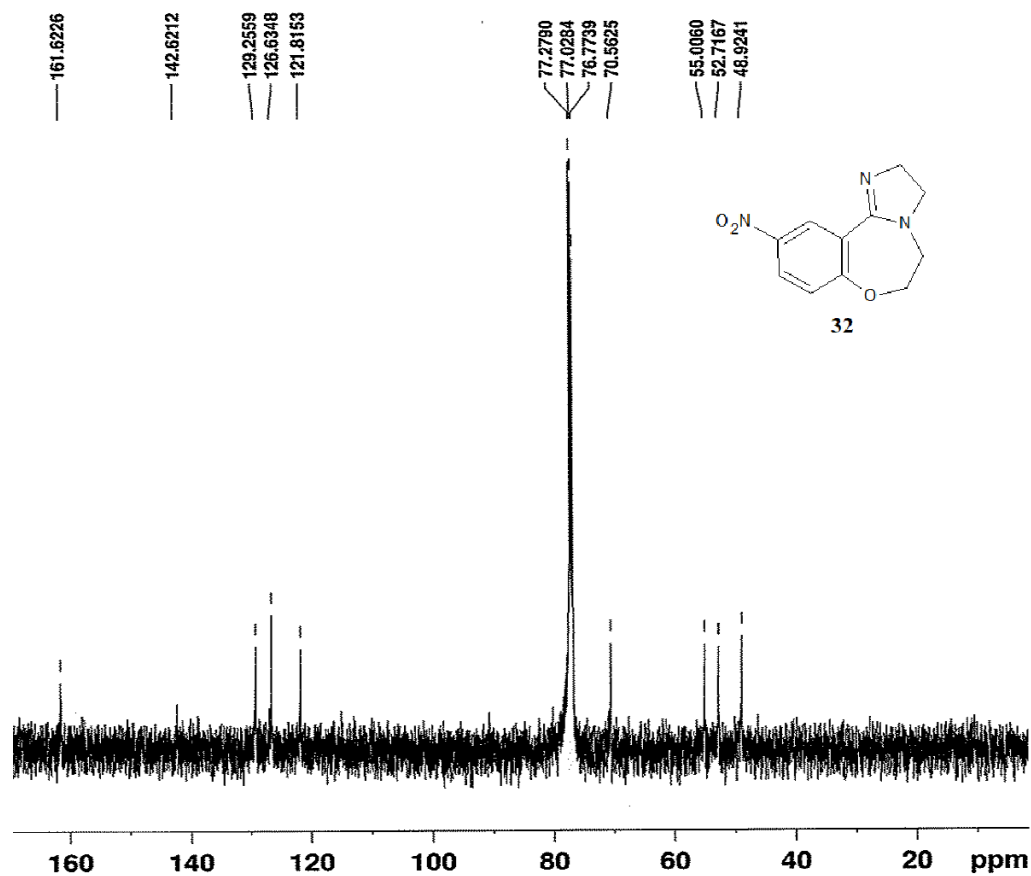


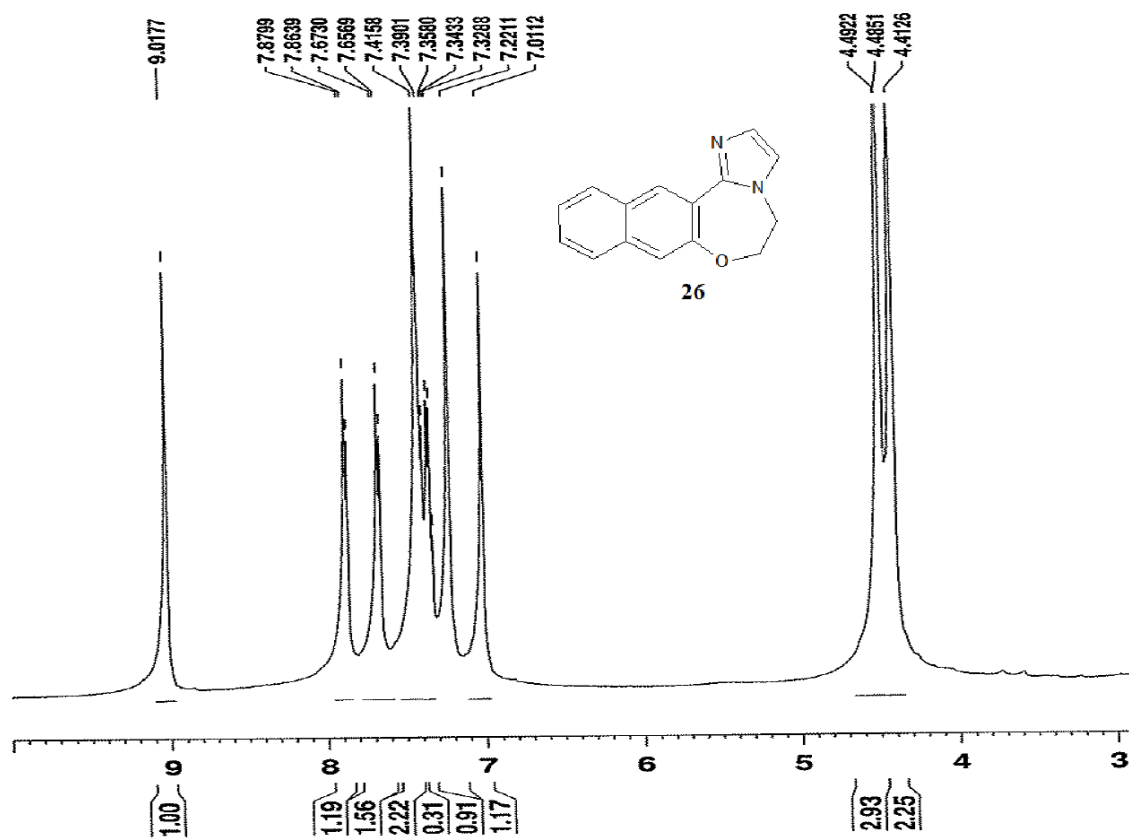


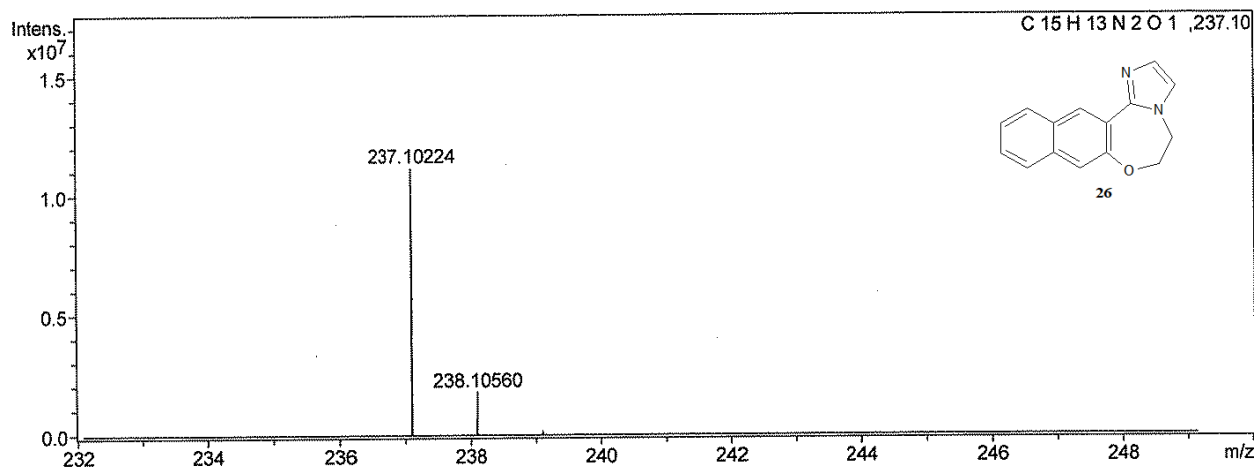
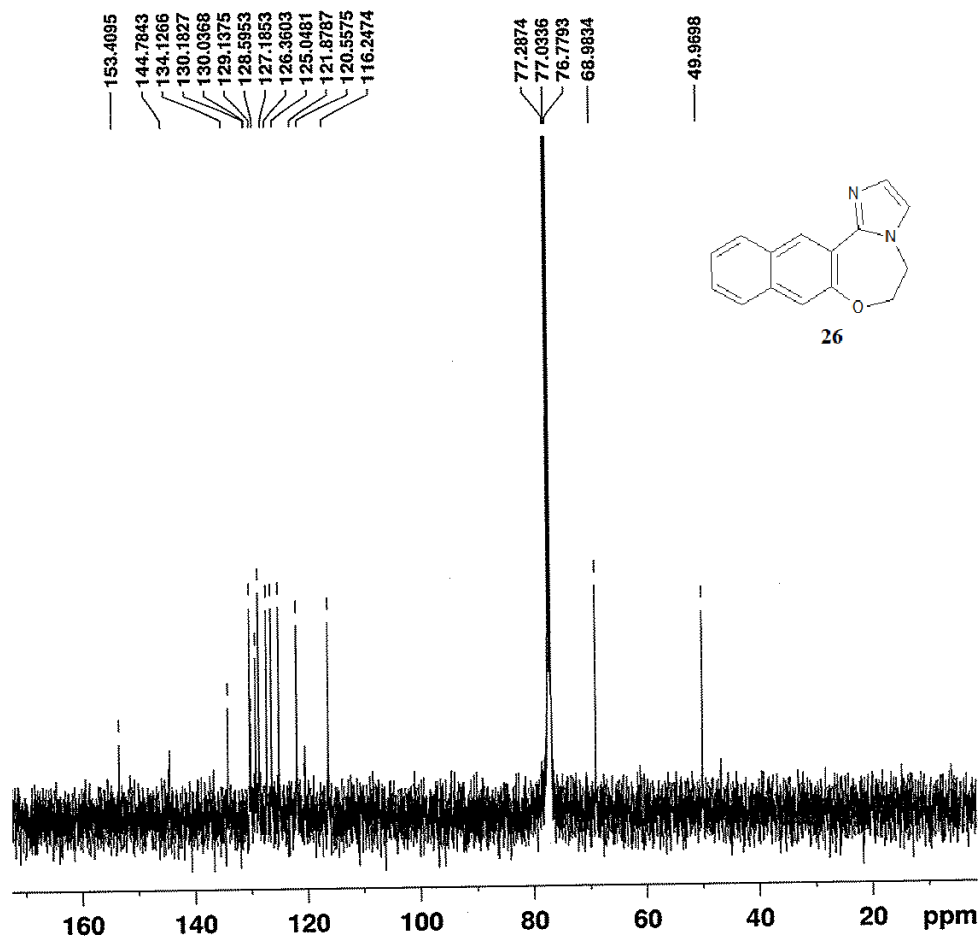


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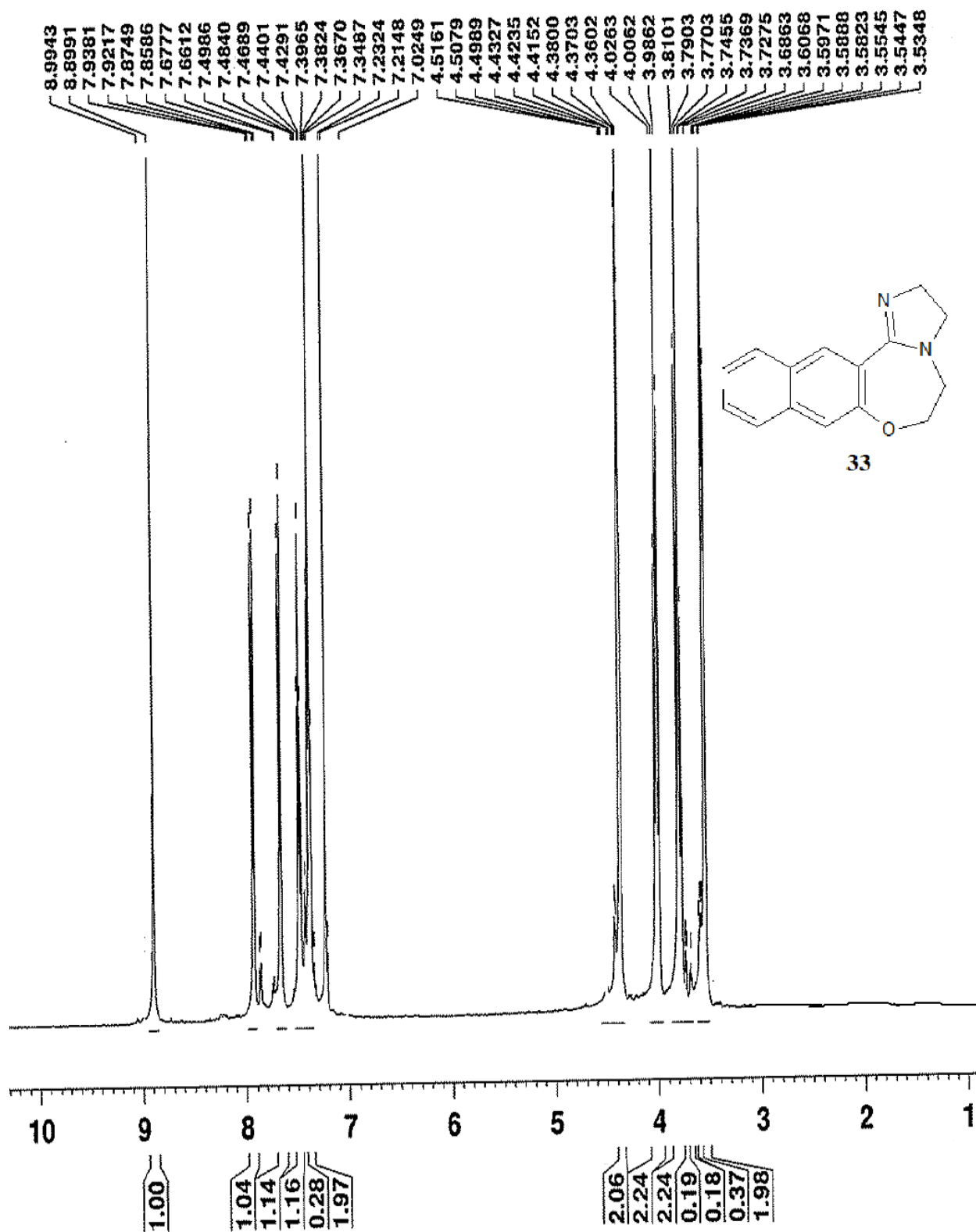


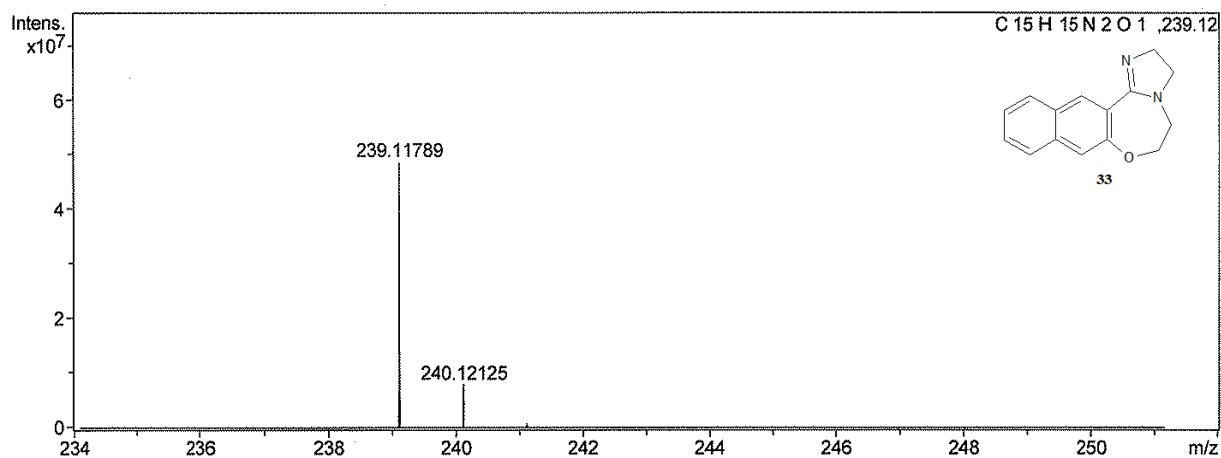
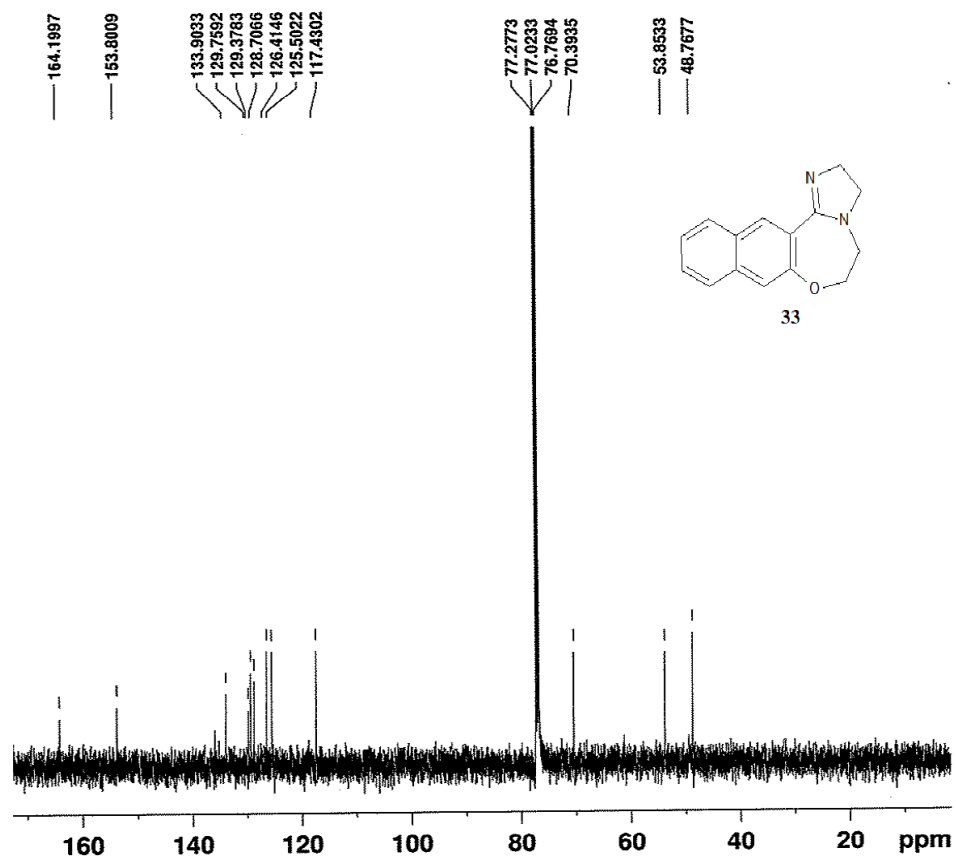






Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C ₁₅ H ₁₃ N ₂ O ₁	0.023	237.10224	8.27	8.13	1.96	10.50	ok	even





Sum	Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e ⁻
C 15	H 15	N 2	O 1	239.11789	3.80	3.53	0.91	9.50	ok even



