

Supplementary Information

Greener synthesis, spectroscopical relationships, molecular docking analysis, antimicrobial, antimalarial activities of aryl *E*-imines and X-ray crystal structure of (*E*)-*N*-(4-nitrobenzylidene)-2-(trifluoromethyl)aniline

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Table S1. Results of statistical analysis of infrared frequencies ($\nu_{\text{C=N}}$, cm^{-1}), NMR chemical shifts (δ , ppm) of CH=N of (*E*)-imines (**1-11**) with Hammett substituent constants (σ , σ^+ , σ_{I} , σ_{R}) and F and R parameters

Table S2. The antibacterial and antifungal activities by means of MICs of (*E*)-N-(substituted benzylidene)-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amines (**1-11**) and (*E*)-N-(substituted benzylidene)-2-(trifluoromethyl)anilines (**24-27**) using serial dilution method

Figures **S1-S30** NMR spectra of compounds **1-11** and **24-27** are shown in.

Figures **S31-S60** Mass spectra and mass fragments of compounds **1-11** and **24-27** as in

Table S1. Results of statistical analysis of infrared frequencies ($\nu_{\text{C=N}}$, cm^{-1}), NMR chemical shifts (δ , ppm) of CH=N of (*E*)-imines (**1-11**) with Hammett substituent constants (σ , σ^+ , σ_{I} , σ_{R}) and F and R parameters

Freq.	Constt.	r	I	ρ	s	n	Correlated derivatives
C=N	σ	0.832	1584.7	-3.307	3.541	11	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 4-
	σ^+	0.810	1584.12	-0.751	3.723		OH, 3-OCH ₃ , 2-CH ₃ , 3-NO ₂ , 4-
	σ_{I}	0.806	1584.35	-0.967	3.736		NO ₂
	σ_{R}	0.906	1582.16	-10.777	2.828		
	F	0.791	1583.30	1.696	3.719		
	R	0.906	1581.98	-8.458	2.789		
CH=N	σ	0.807	8.440	-0.002	0.121		H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 4-
	σ^+	0.802	8.440	-0.006	0.121	11	OH, 3-OCH ₃ , 2-CH ₃ , 3-NO ₂ , 4-
	σ_{I}	0.832	8.502	-0.164	0.114		NO ₂
	σ_{R}	0.900	8.478	0.228	0.109	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-OH, 3-OCH ₃ , 3-NO ₂ , 4-NO ₂
	F	0.833	8.503	-0.160	0.114	11	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 4- OH, 3-OCH ₃ , 2-CH ₃ , 3-NO ₂ , 4- NO ₂
	R	0.904	8.483	0.185	0.108	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-OH, 3- OCH ₃ , 3-NO ₂ , 4-NO ₂
CH=N	σ	0.928	157.77	-2.747	0.622	11	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 4-OH, 3-OCH ₃ , 2-CH ₃ , 3-NO ₂ , 4-

						NO ₂
σ^+	0.906	157.44	-1.432	0.924	9	3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 4-OH, 2-CH ₃ , 3-NO ₂ , 4-NO ₂
σ_I	0.918	158.72	-4.055	0.656	10	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 4-OH, 3-OCH ₃ , 3-NO ₂ , 4-NO ₂
σ_R	0.905	156.65	-3.097	0.951	9	3-Br, 4-Br, 3-Cl, 4-Cl, 4-OH, 3-OCH ₃ , 2-CH ₃ , 3-NO ₂ , 4-NO ₂
F	0.917	158.55	-3.450	0.800	9	H, 3-Br, 4-Br, 3-Cl, 4-Cl, 4-OH, 3-OCH ₃ , 3-NO ₂ , 4-NO ₂
R	0.950	156.65	-2.220	0.986	10	3-Br, 4-Br, 3-Cl, 4-Cl, 4-F, 4-OH, 3-OCH ₃ , 2-CH ₃ , 3-NO ₂ , 4-NO ₂

r=Correlation coefficient; I=intercept; ρ =slope; s=standard deviation; n=number of substituents.

Table S2. The antibacterial and antifungal activities by means of MICs of (*E*)-*N*-(substituted benzylidene)-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amines (**1-11**) and (*E*)-*N*-(substituted benzylidene)-2-(trifluoromethyl)anilines (**24-27**) using serial dilution method

Entry	X	MIC (µg/mL)							
		Antibacterial activity					Antifungal activity		
		<i>B. subtilis</i>	<i>S. aureus</i>	<i>S. pyogenes</i>	<i>E. coli</i>	<i>P. aeruginosa</i>	<i>A. niger</i>	<i>F. oxysporum</i>	<i>P. chrysogenum</i>
(<i>E</i>)- <i>N</i> -(substituted benzylidene)-2,3-dihydrobenzo(<i>b</i>)[1,4]-dioxin-6-amines									
1	H	20	35	30	40	40	70	70	80
2	3-Br	6	7	8.5	9.5	7.75	11.5	16	16
3	4-Br	6.5	8.5	9	9.5	9	12	5	19.5
4	3-Cl	7.0	9	9.5	9	9.5	15	25	18
5	4-Cl	6.5	8	9	9.5	10	16.5	18	15.75
6	4-F	9.0	5.5	7.5	7	60	20	30	14
7	4-OH	40	4.5	50	5.5	50	10	45.5	35
8	3-OCH ₃	6	6.25	110	12	11	11.5	85.5	95
9	2-CH ₃	12	9	100	100	9.5	17.5	75	80

10	3-NO ₂	35	35	30	25	30	25	20	25
11	4-NO ₂	30	35	30	20	40	30	25	30
<i>(E)</i> -N-(substituted benzylidene)-2-(trifluoromethyl)anilines									
24	2-Br	7.25	8.5	9.5	10	10	13.5	19	95
25	4-Cl	6.15	9.5	10	9	11	9.5	8.5	90
26	3-NO ₂	40	35	35	30	25	20	30	20
27	4-NO ₂	45	35	30	35	30	20	30	25
Standard			Ciprofloxacin					Clotrimazole	
		5.50	6.15	7.0	7.25	6.00	10.5	14.25	13.25

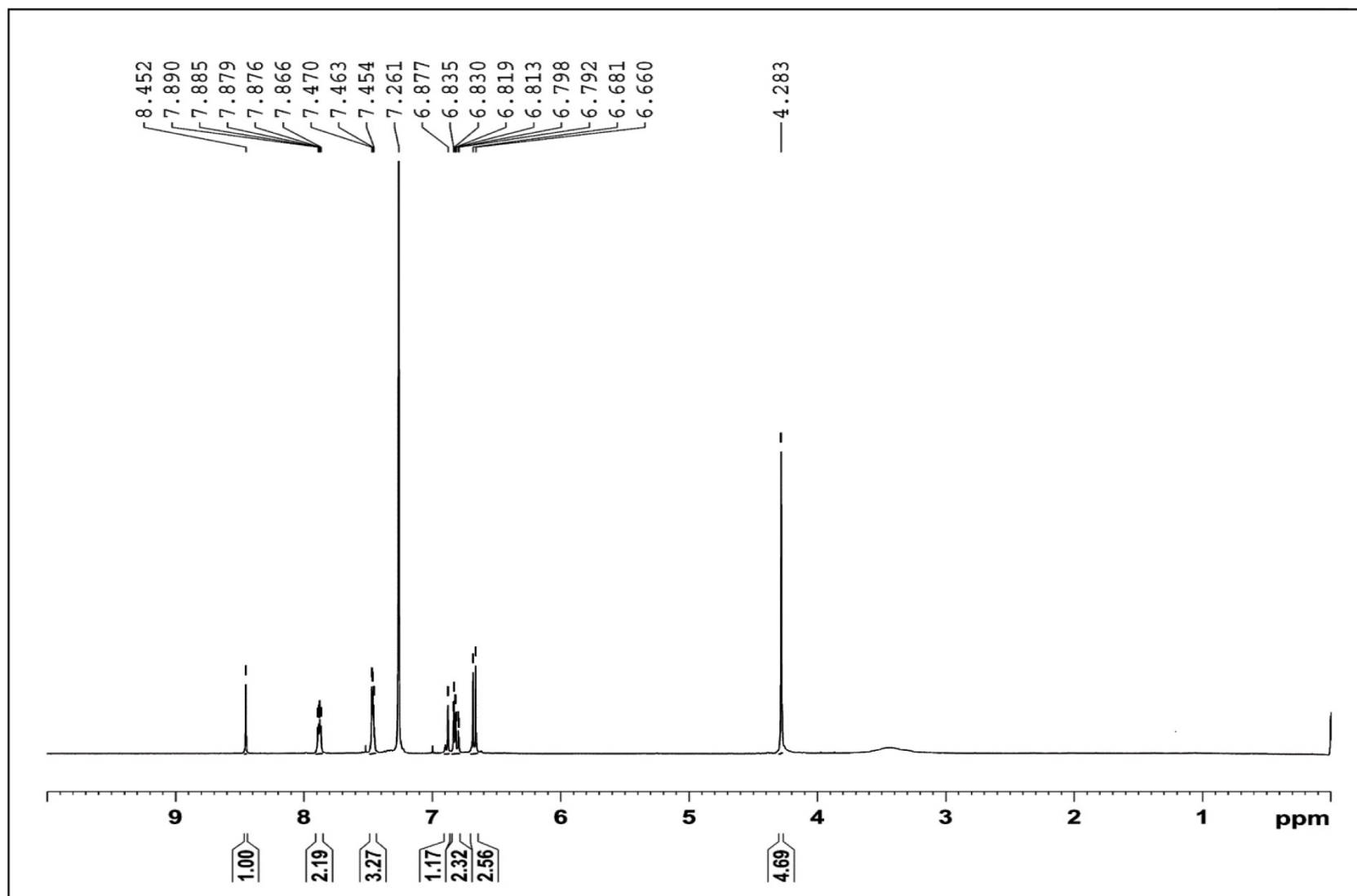


Figure S1. ^1H NMR spectrum of *(E)*-N-Benzylidene-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amine (1)

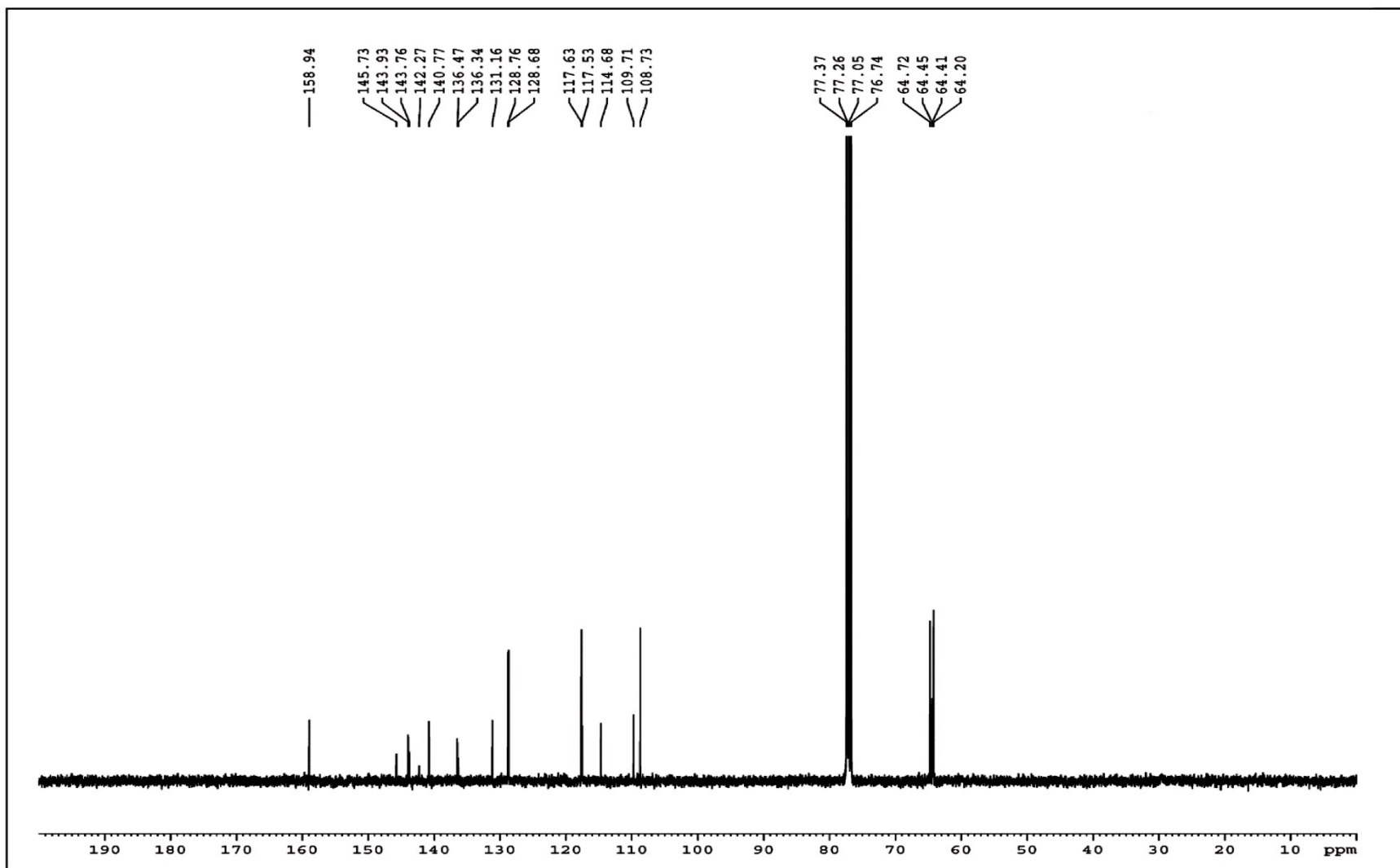


Figure S2. ^{13}C NMR spectrum of (*E*)-*N*-benzylidene-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amine (**1**)

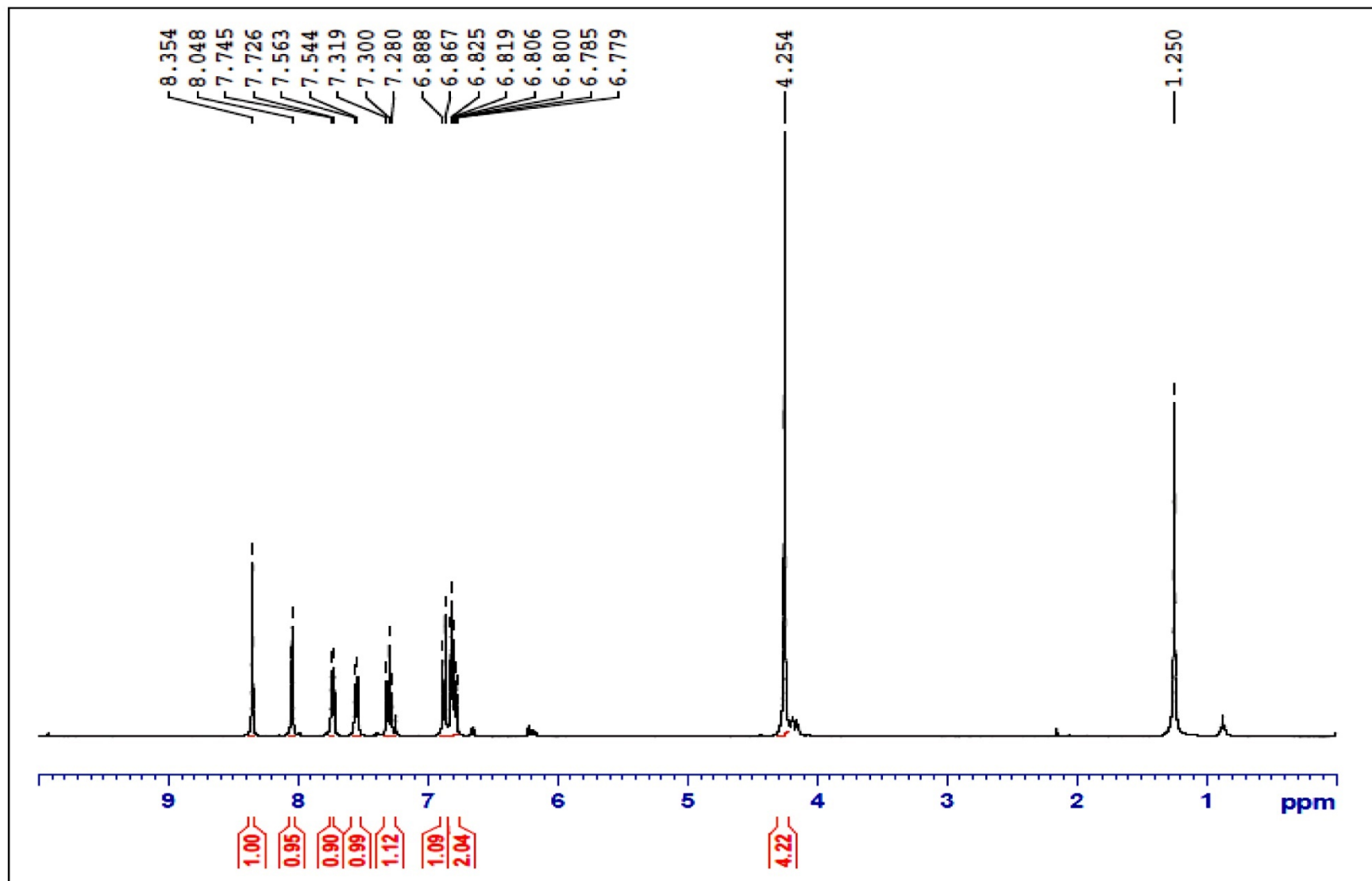


Figure S3. ¹H NMR spectrum of (*E*)-*N*-(3-Bromobenzylidene)-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amine (**2**)

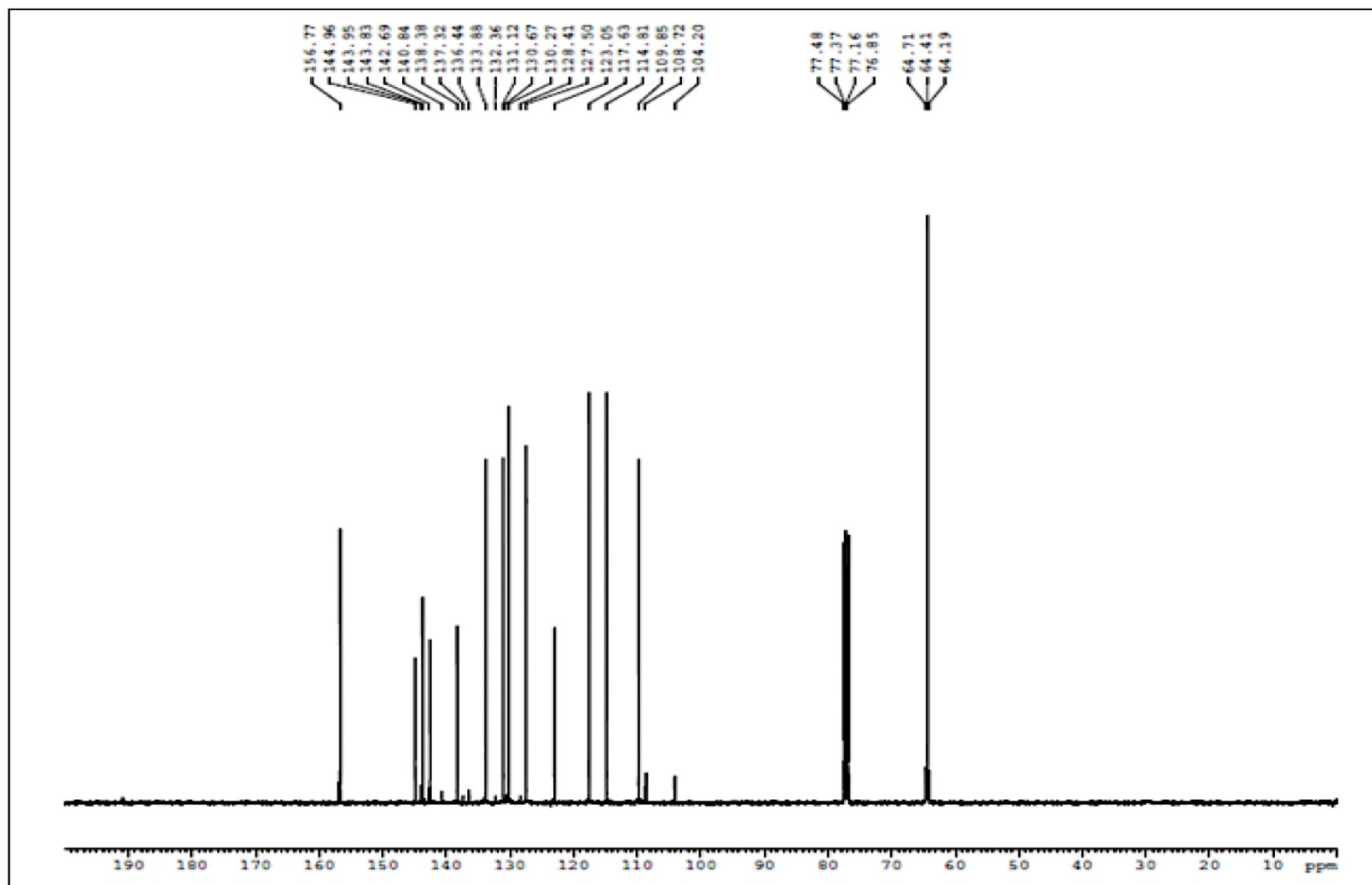


Figure S4. ¹³C NMR spectrum of (*E*)-*N*-(3-Bromobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**2**)

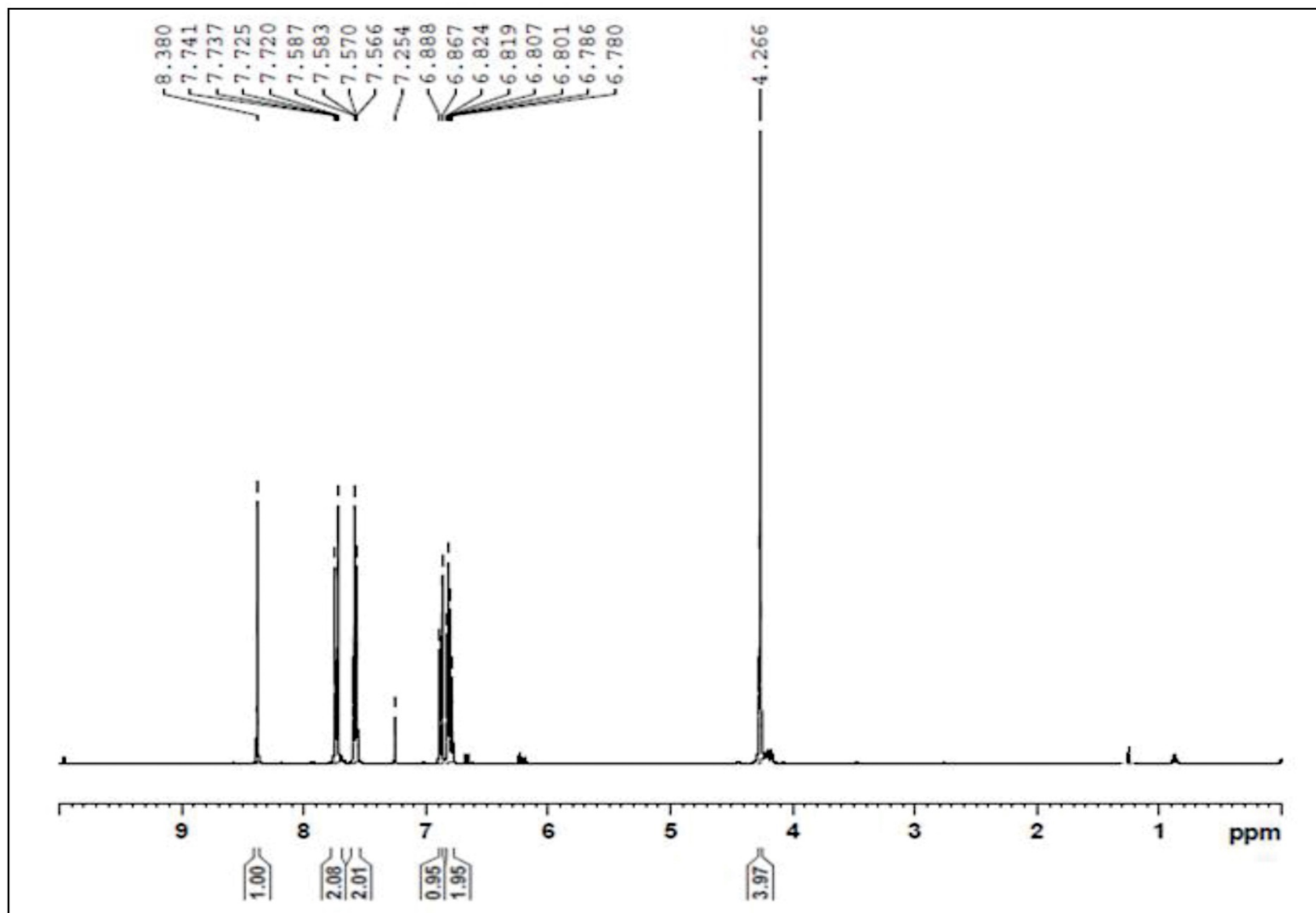


Figure S5. ^1H NMR spectrum of *(E)*-N-(4-Bromobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**3**)

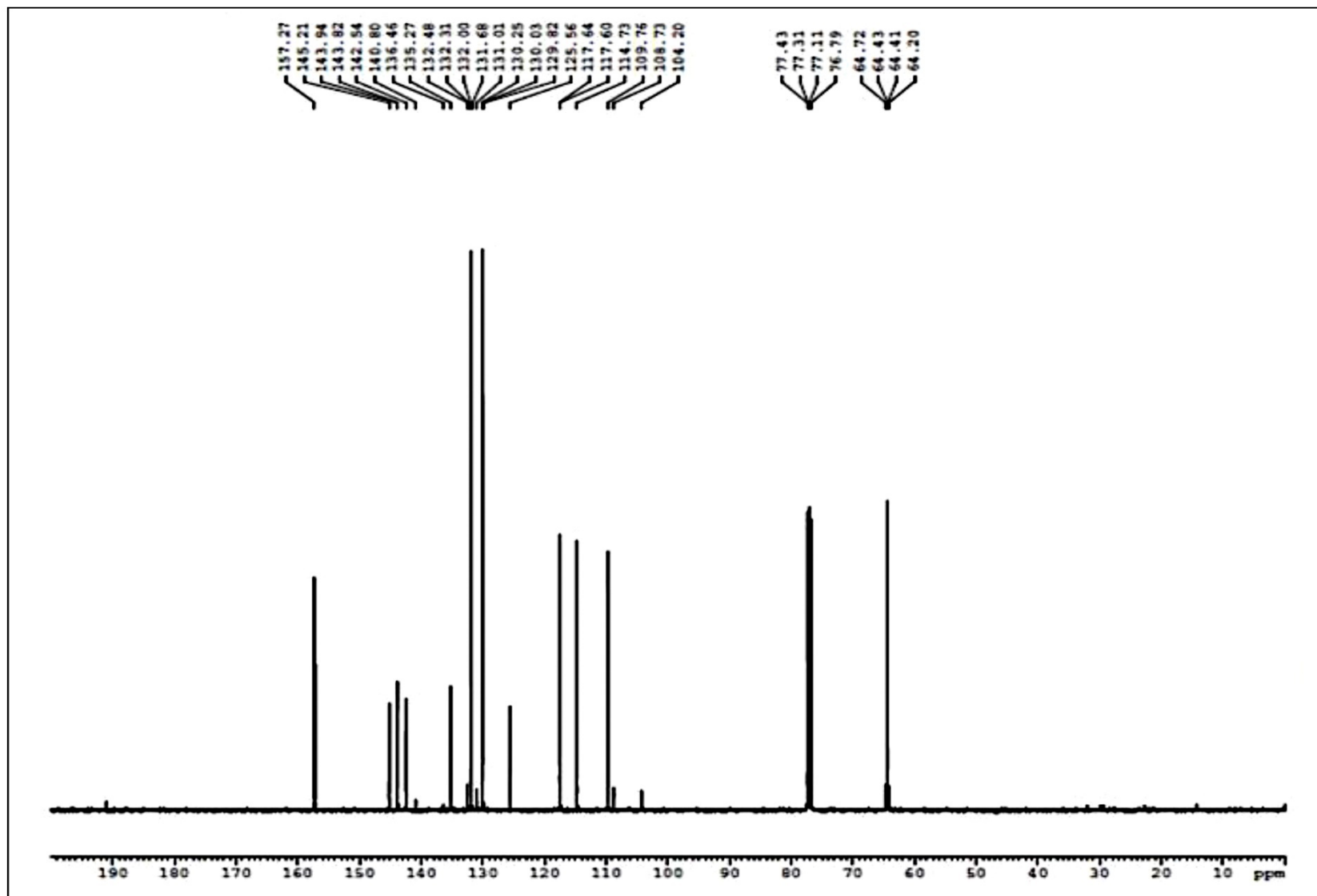


Figure S6. ^{13}C NMR spectrum of (*E*)-*N*-(4-Bromobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**3**)

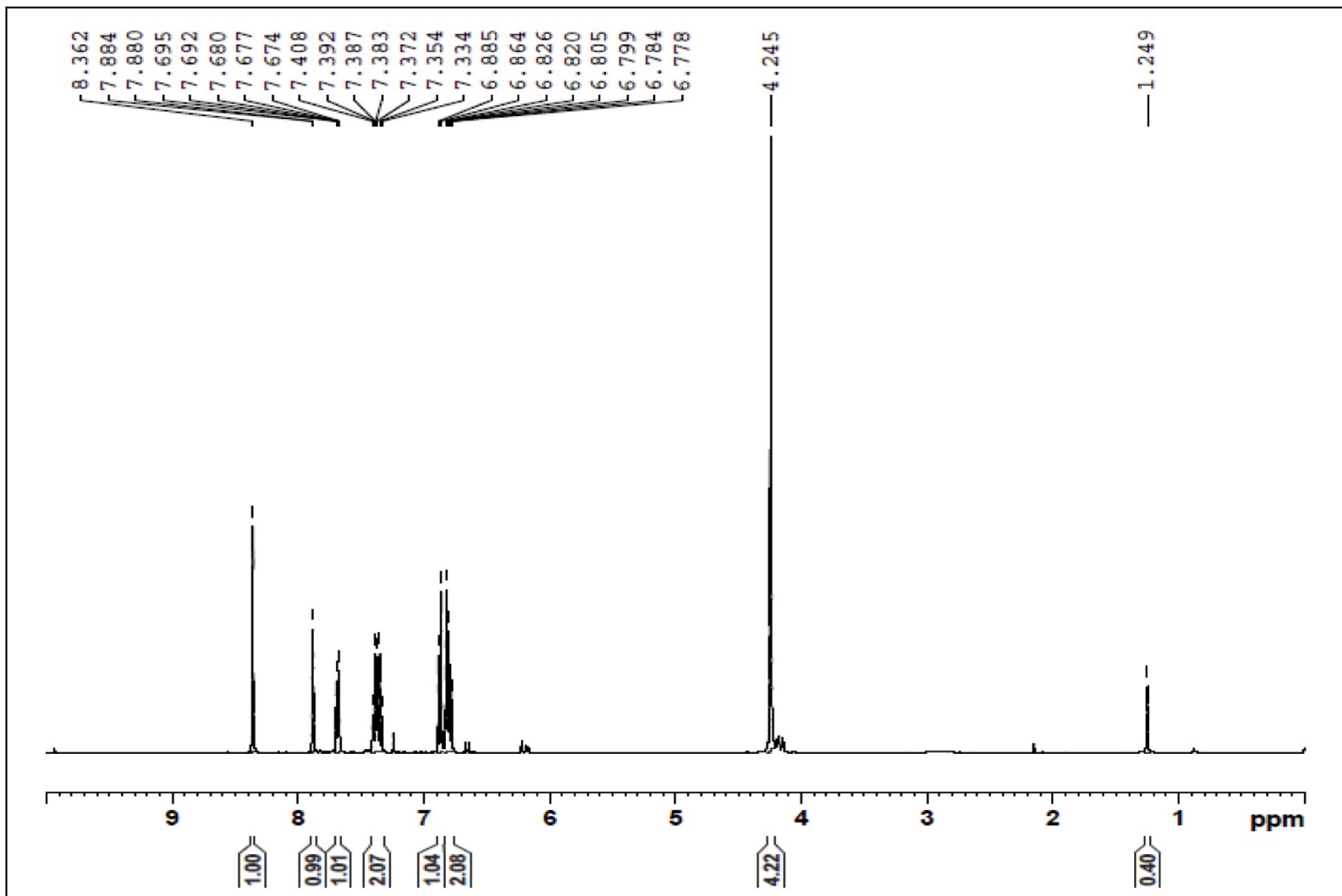


Figure S7. ¹H NMR spectrum of (E)-N-(3-Chlorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (4)

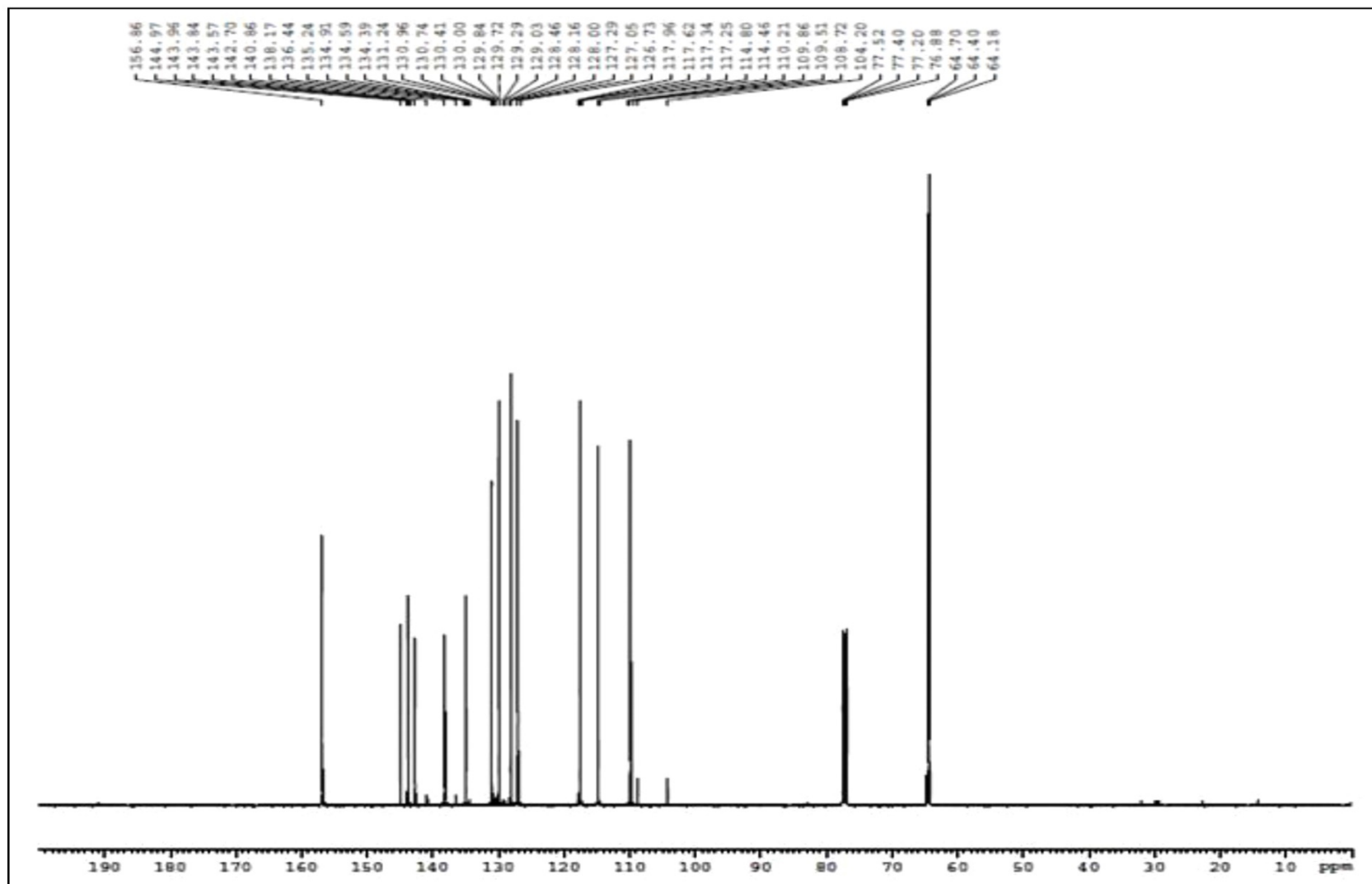


Figure S8. ^{13}C NMR spectrum of (*E*)-*N*-(3-Chlorobenzylidene)-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amine (**4**)

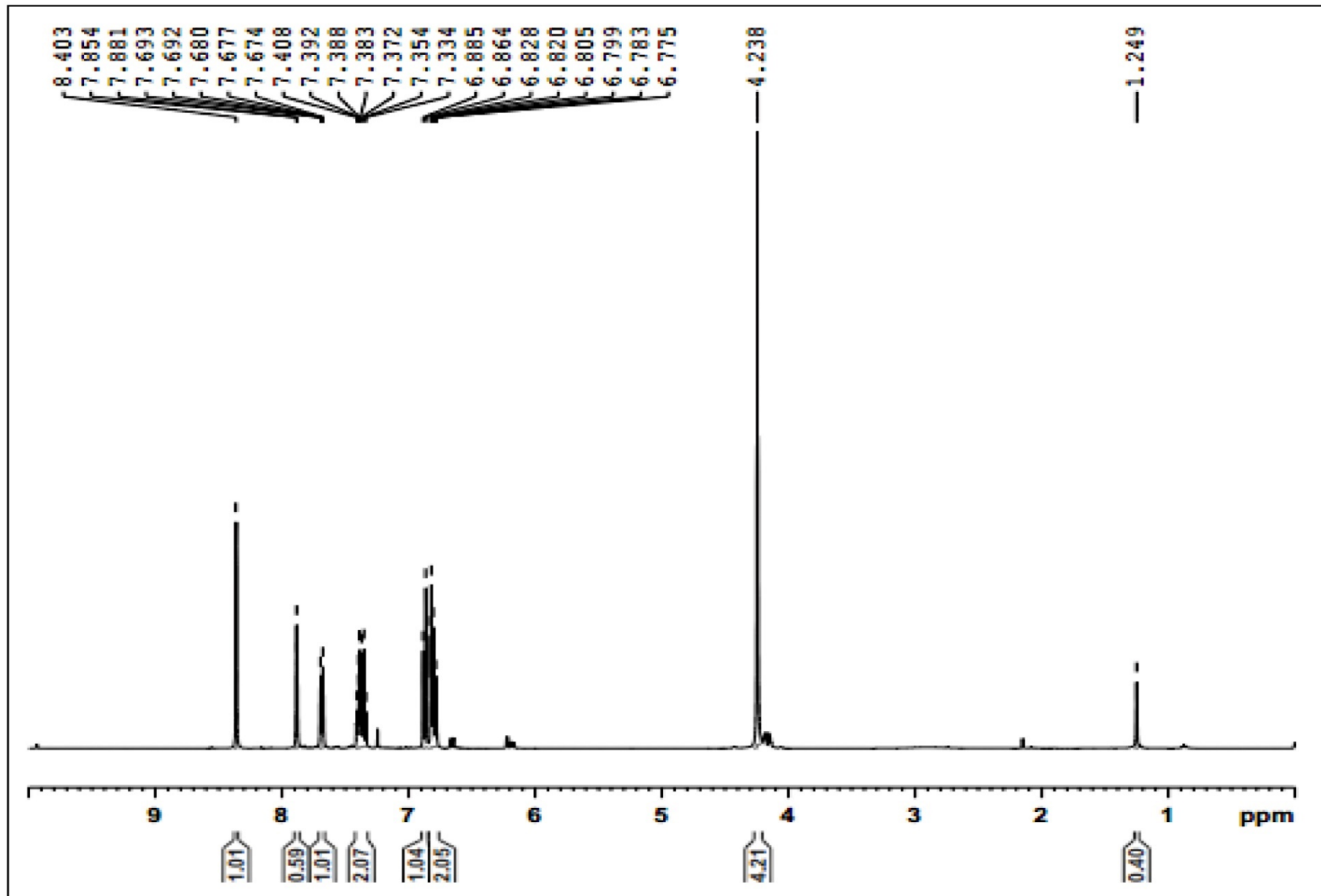


Figure S9. ¹H NMR spectrum of (*E*)-N-(4-Chlorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**5**)

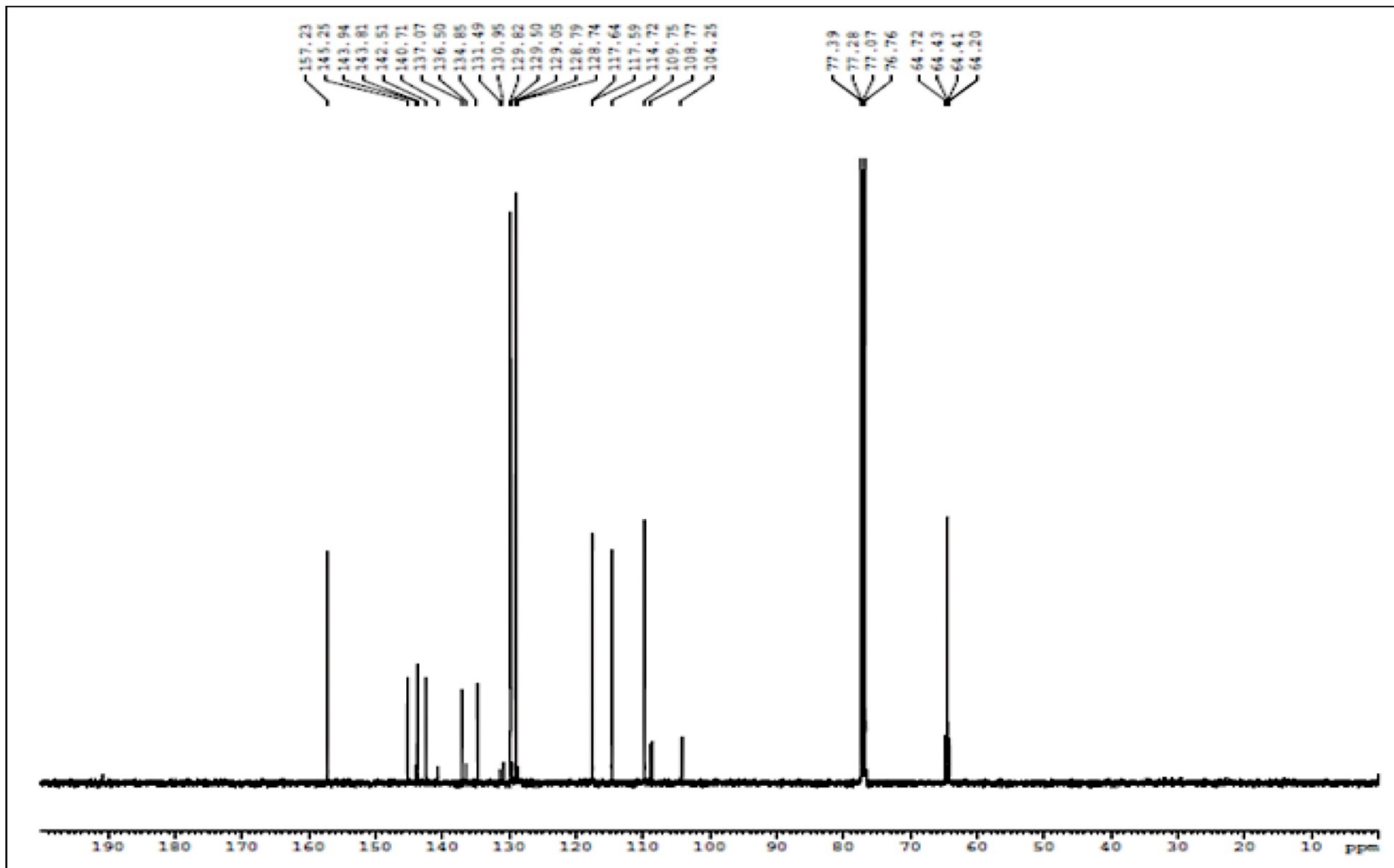


Figure S10. ^{13}C NMR spectrum of (*E*)-*N*-(4-Chlorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**5**)

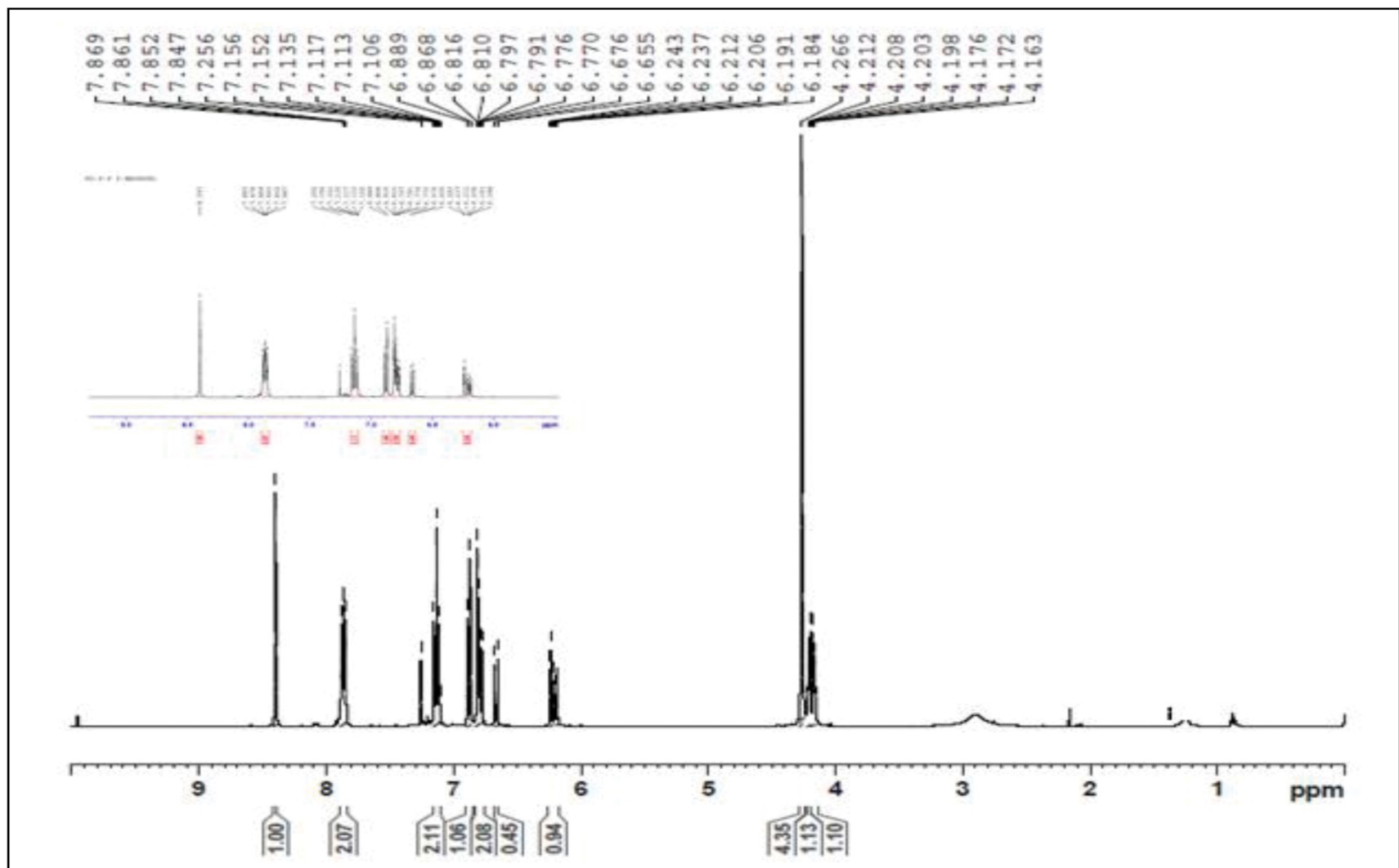


Figure S11. ¹H NMR spectrum of (E)-N-(4-Fluorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (6)

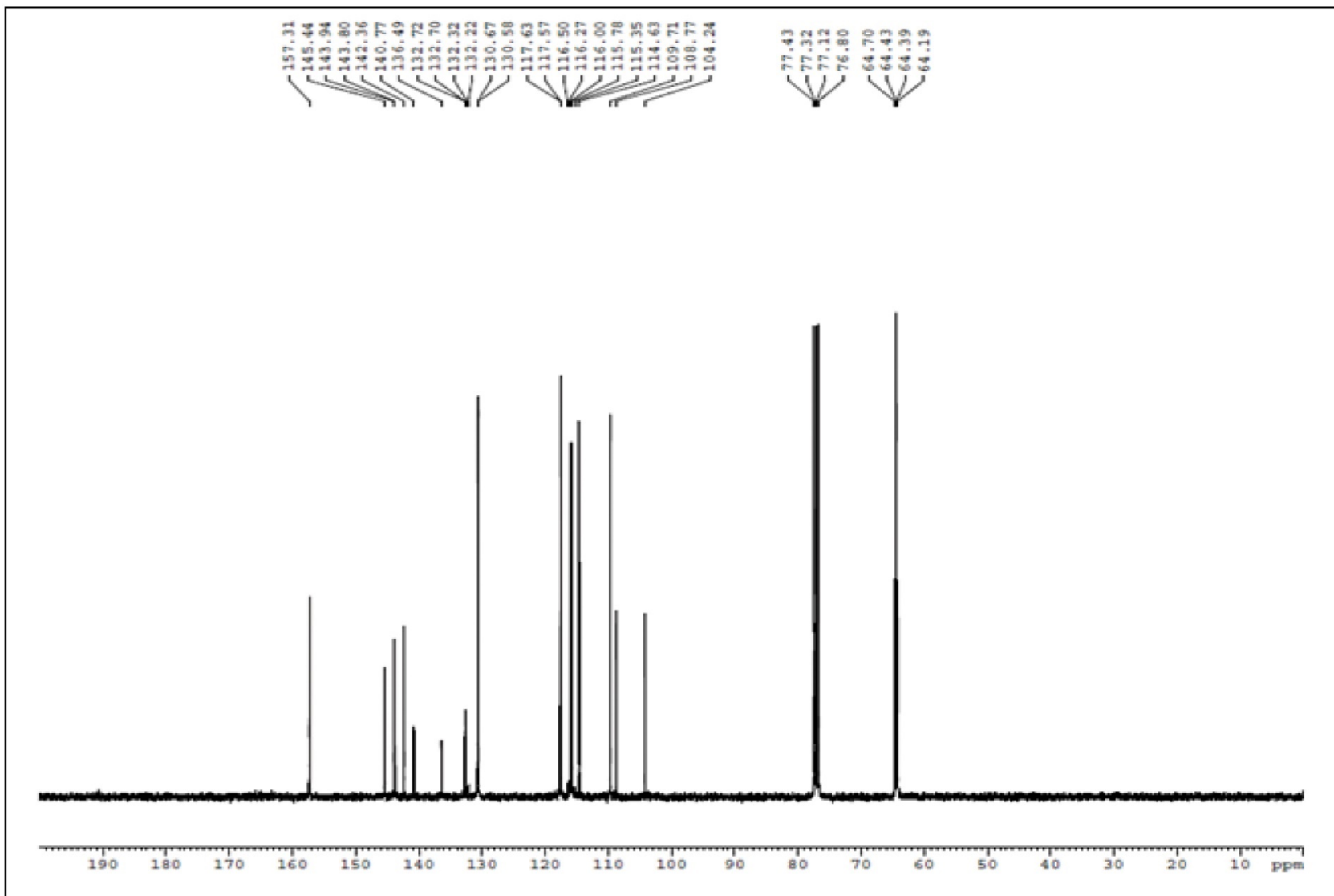


Figure S12. ^{13}C NMR spectrum of (E) - N -(4-Fluorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**6**)

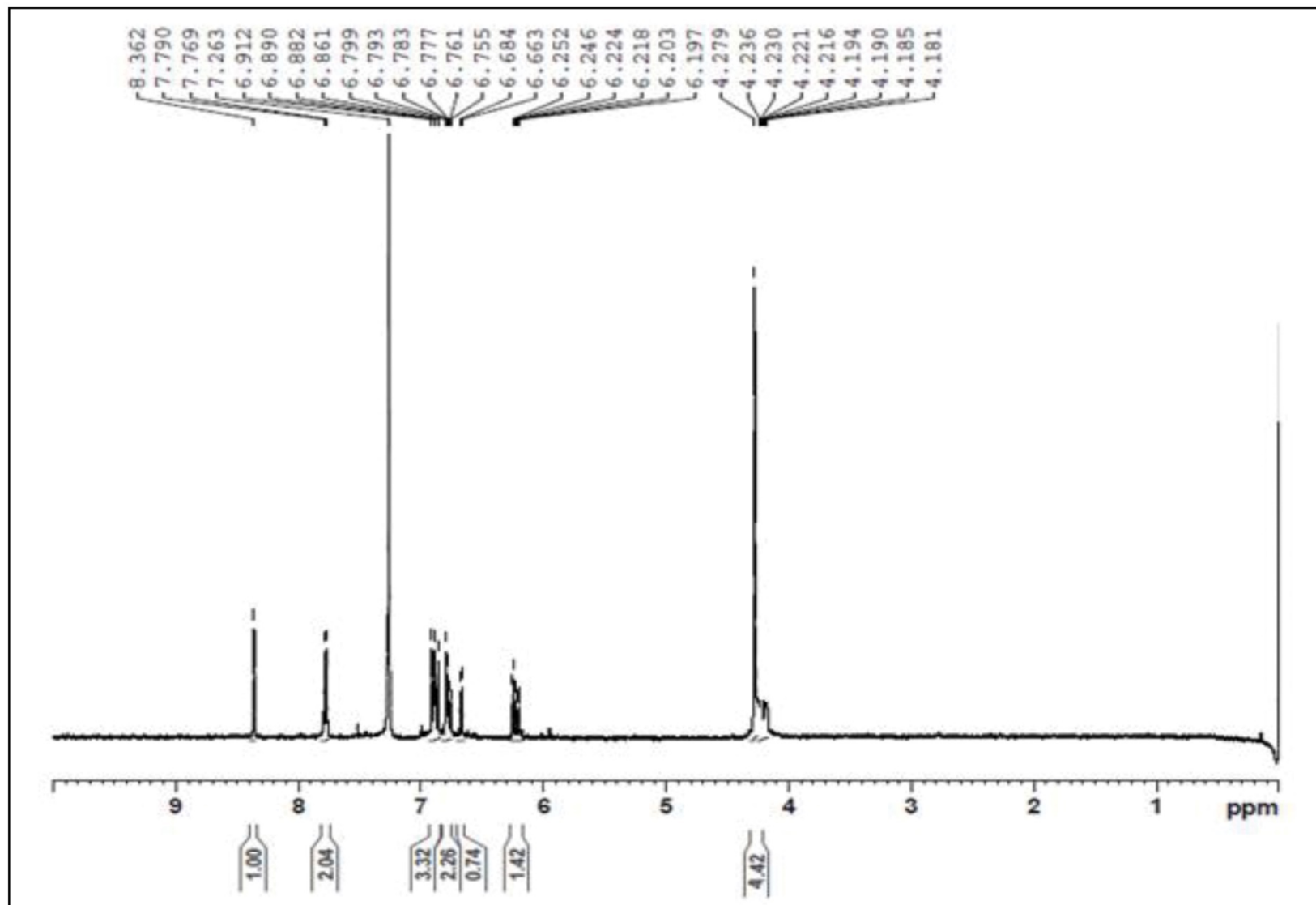


Figure S13. ¹H NMR spectrum of (*E*)-N-(4-Hydroxybenzylidene)-2,3-dihydrobenzo(b)[1,4]- dioxin-6-amine (7)

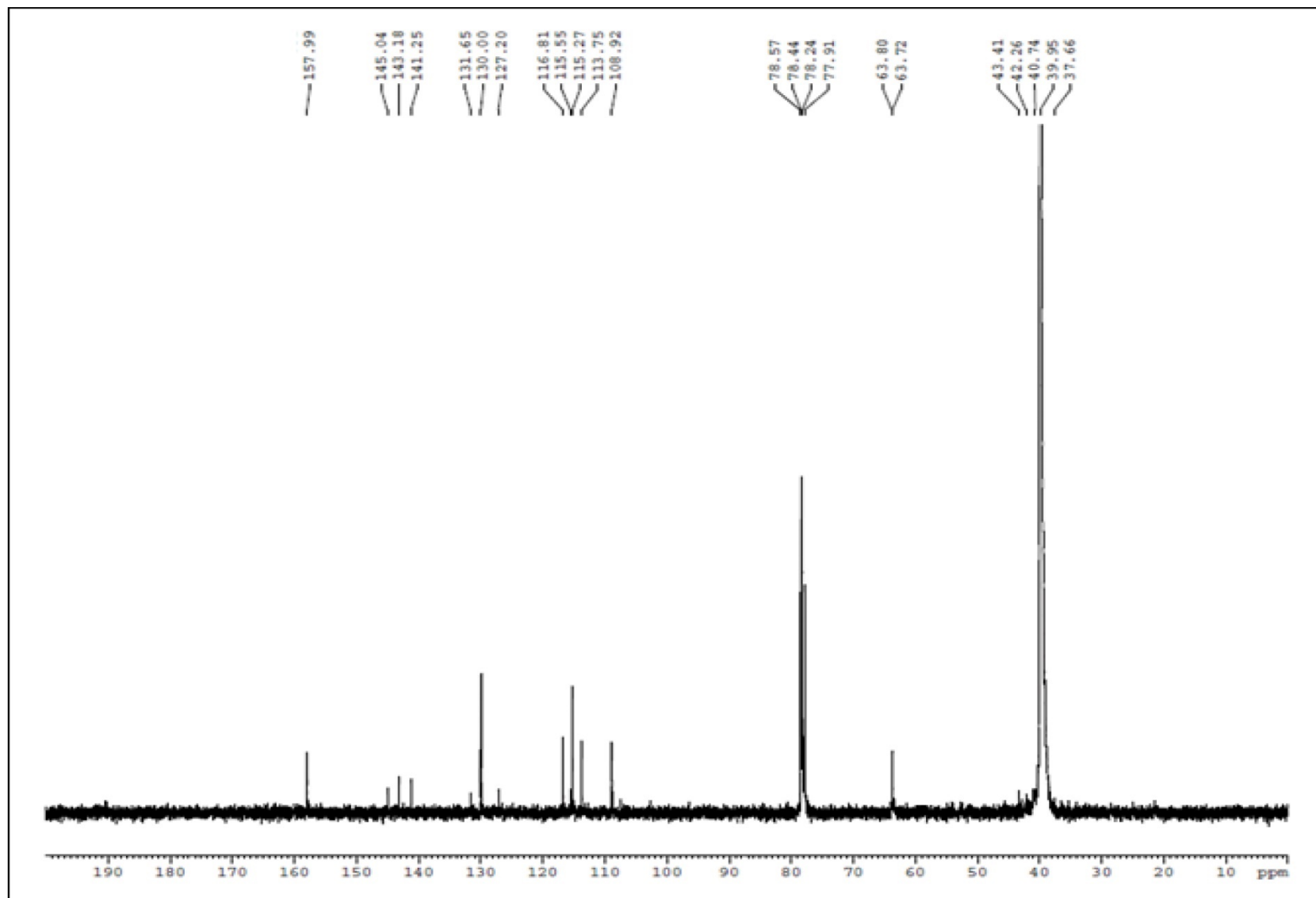


Figure S14. ^{13}C NMR spectrum of (*E*)-*N*-(4-Hydroxybenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**7**)

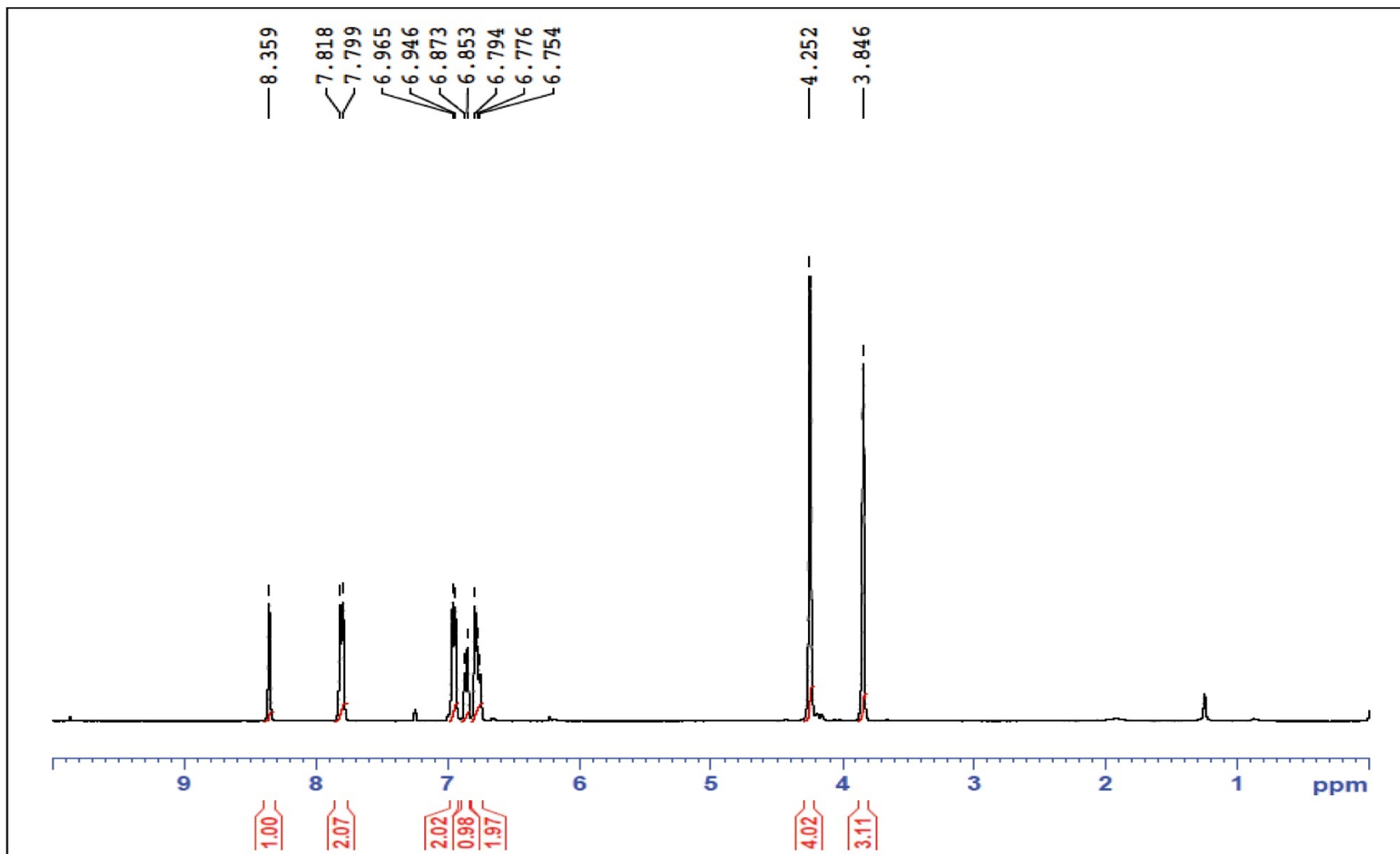


Figure S15. ¹H NMR spectrum of (*E*)-N-(3-Methoxybenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (8)

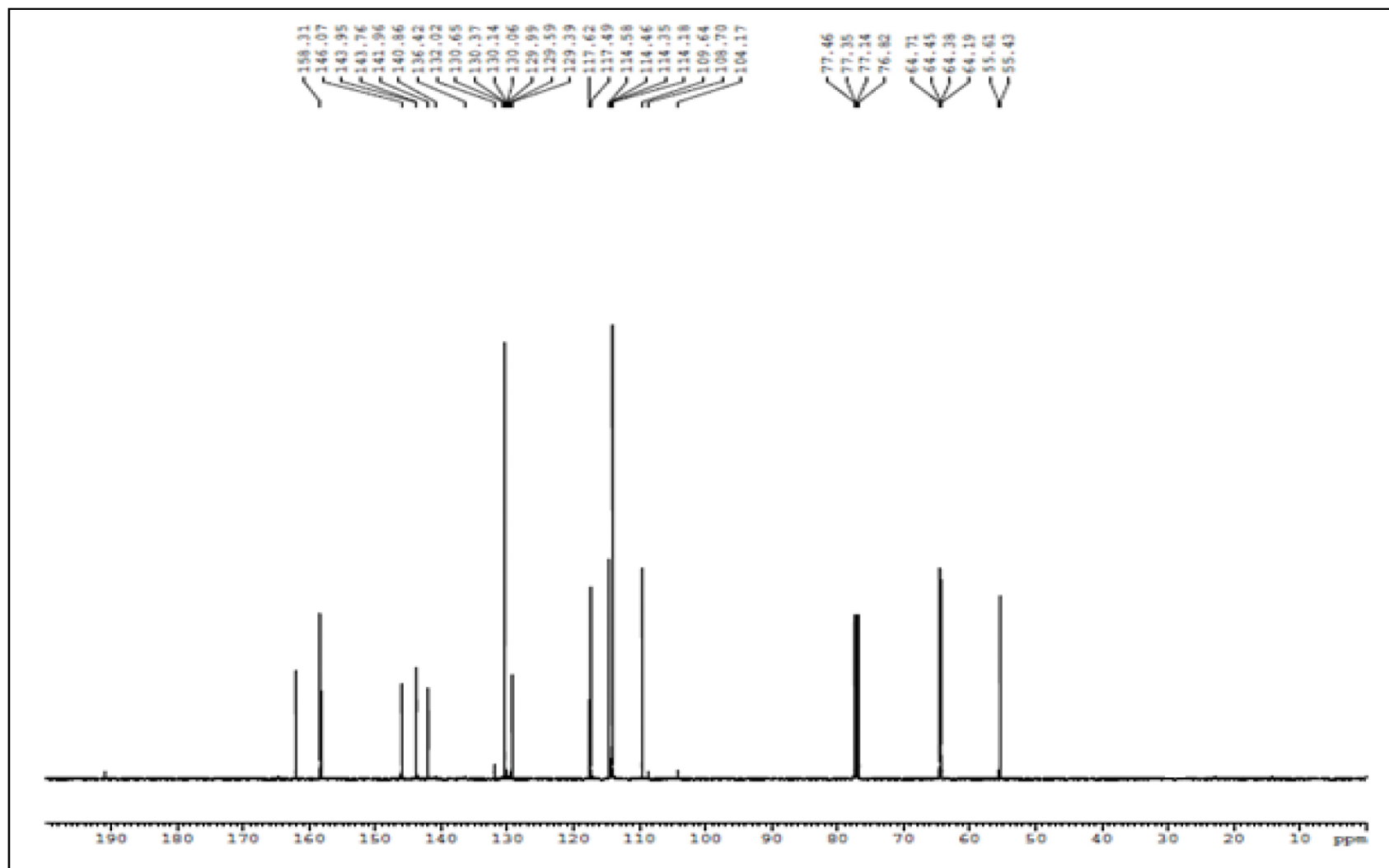


Figure S16. ¹³C NMR spectrum of (*E*)-*N*-(3-Methoxybenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**8**)

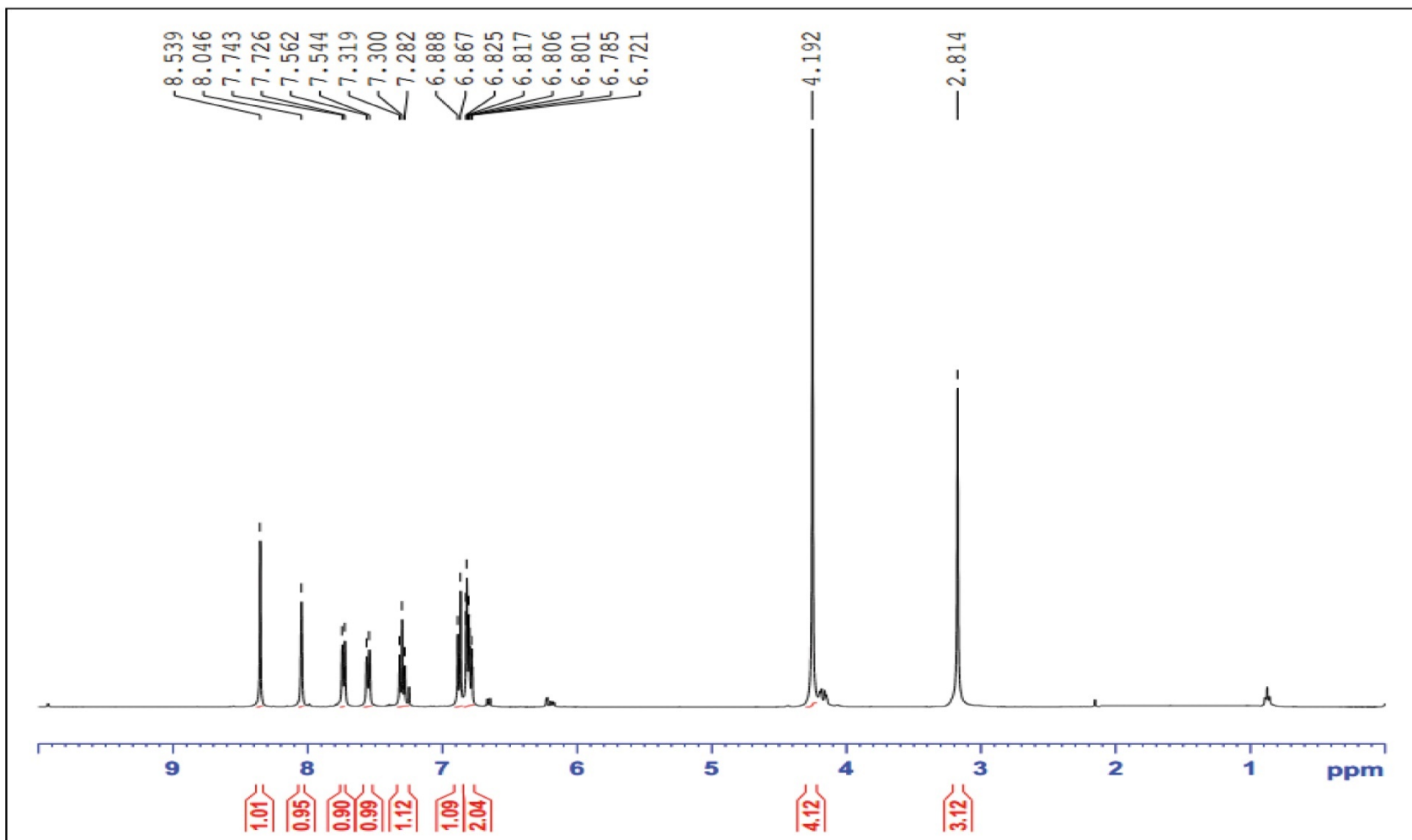


Figure S17. ^1H NMR spectrum of *(E)*-N-(2-Methylbenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (9)

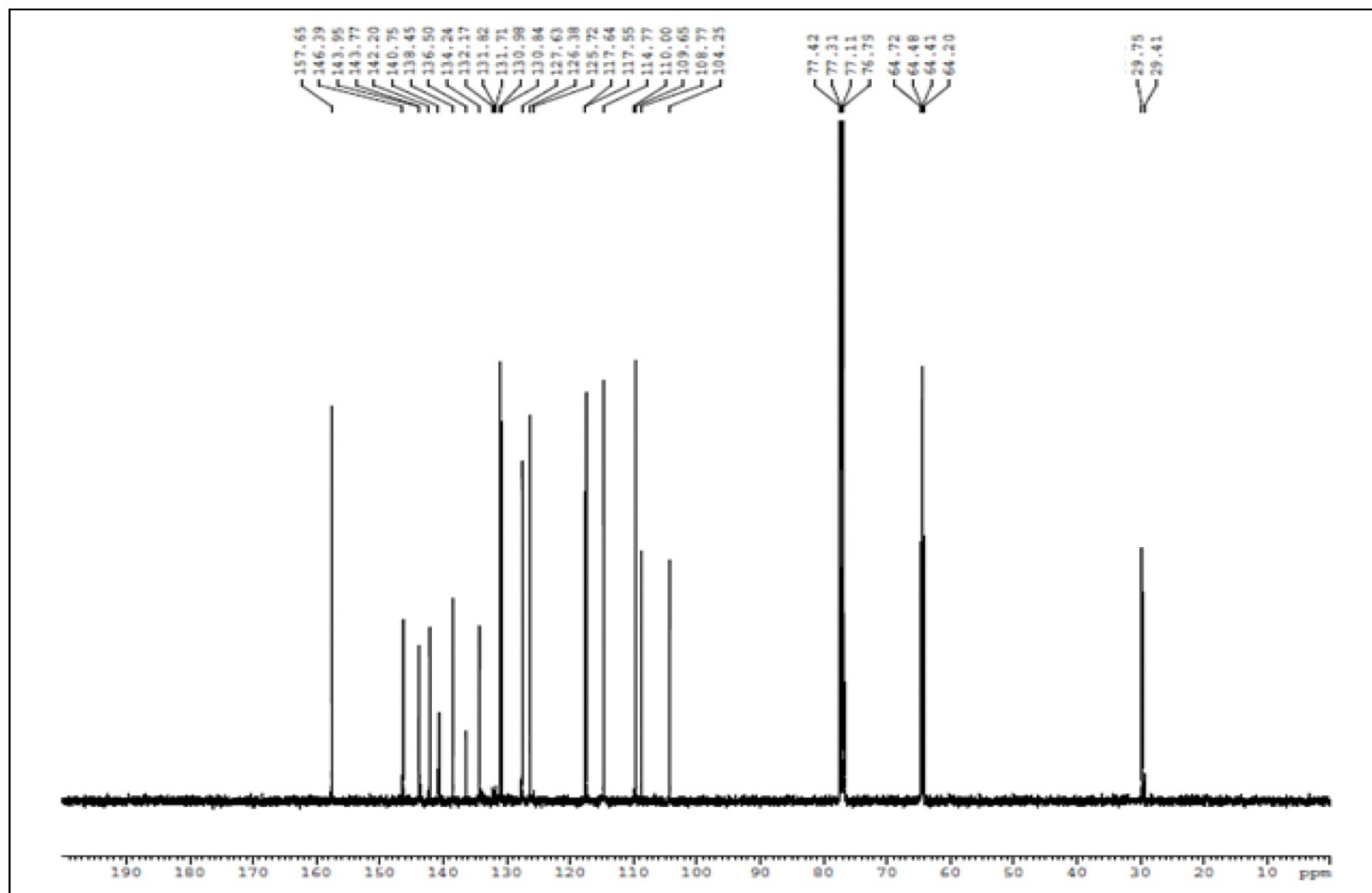


Figure S18. ^{13}C NMR spectrum of (*E*)-*N*-(2-Methylbenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**9**)

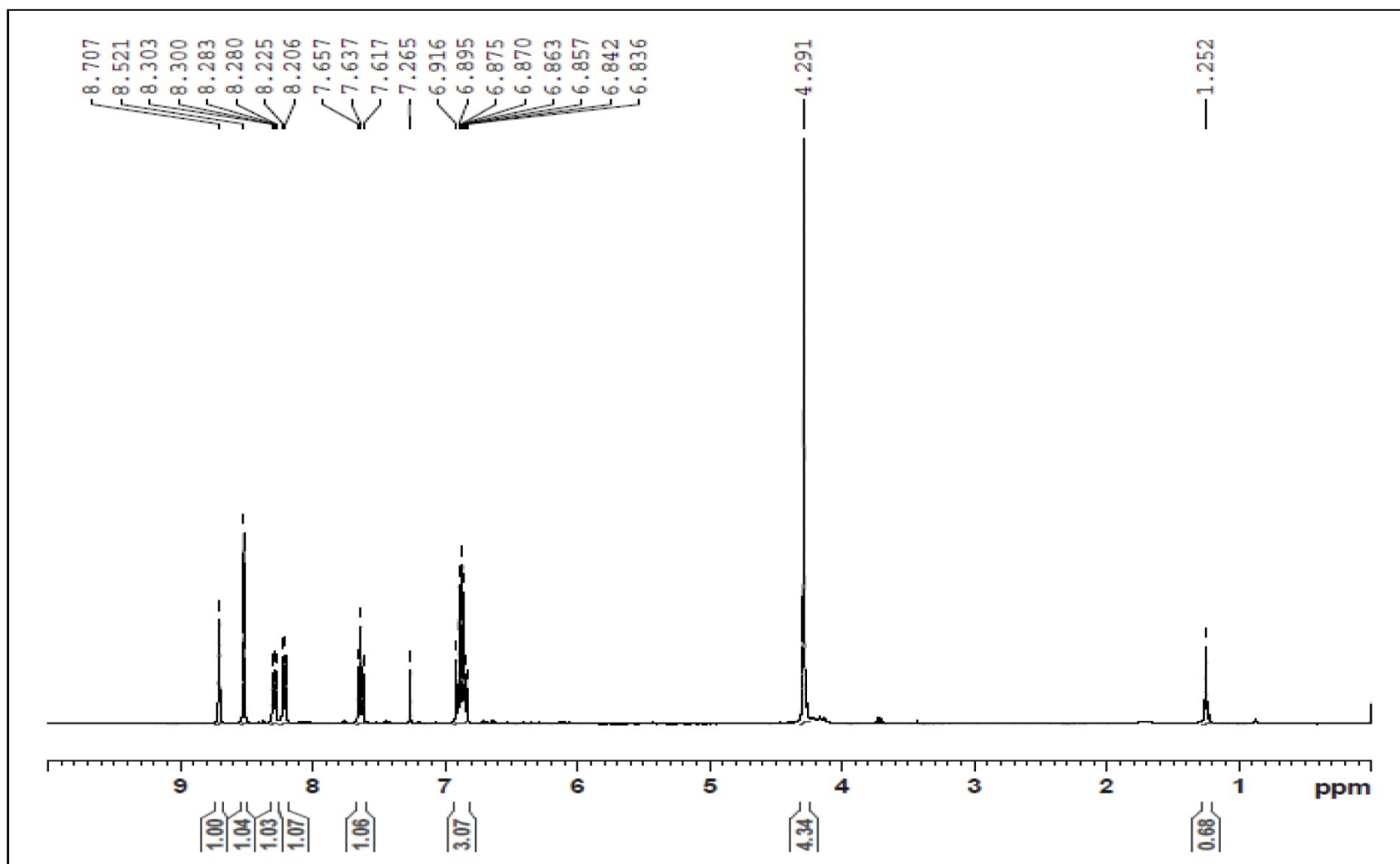


Figure S19. ¹H NMR spectrum of (*E*)-N-(3-Nitrobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**10**)

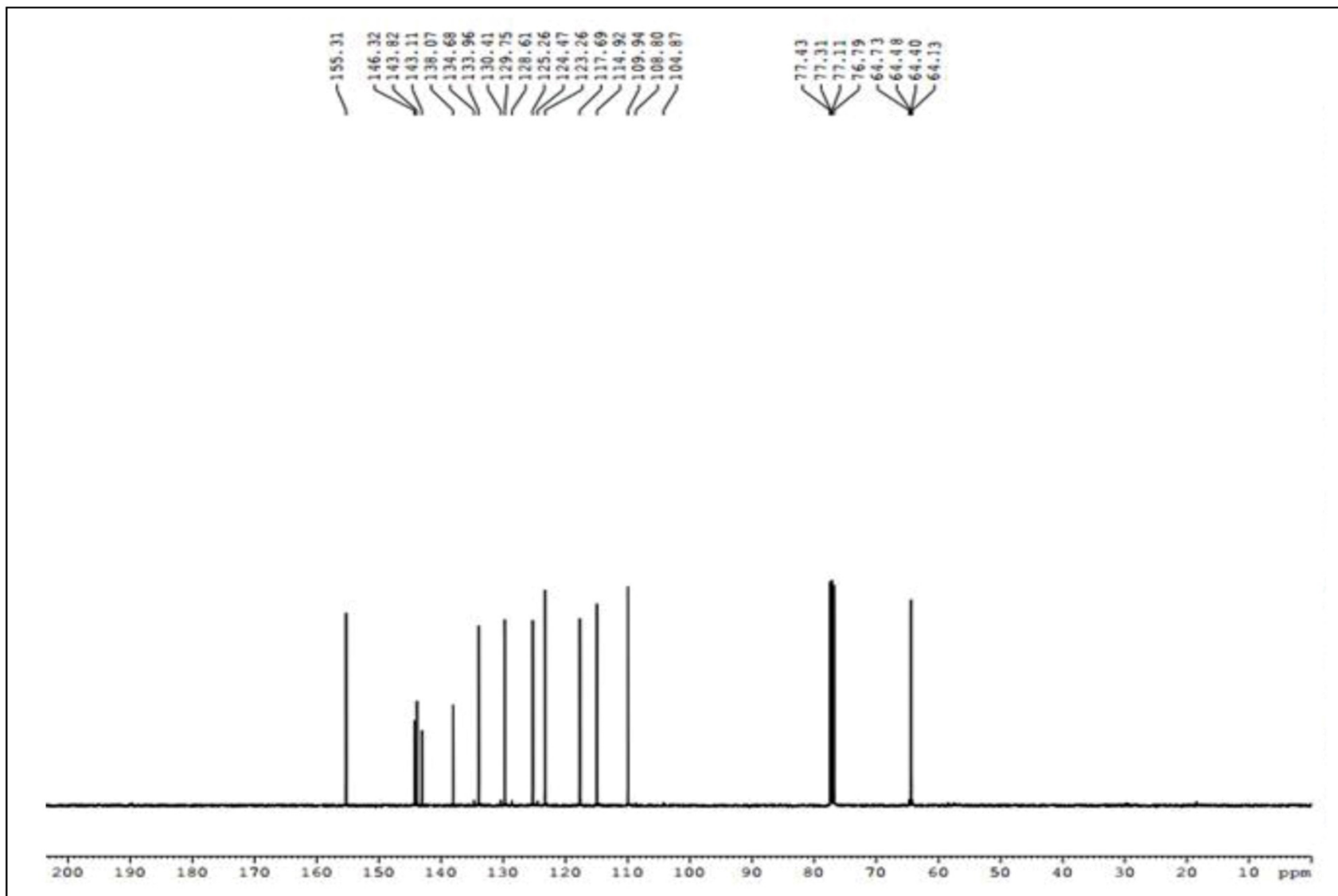


Figure S20. ^{13}C NMR spectrum of (*E*)-*N*-(3-Nitrobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**10**)

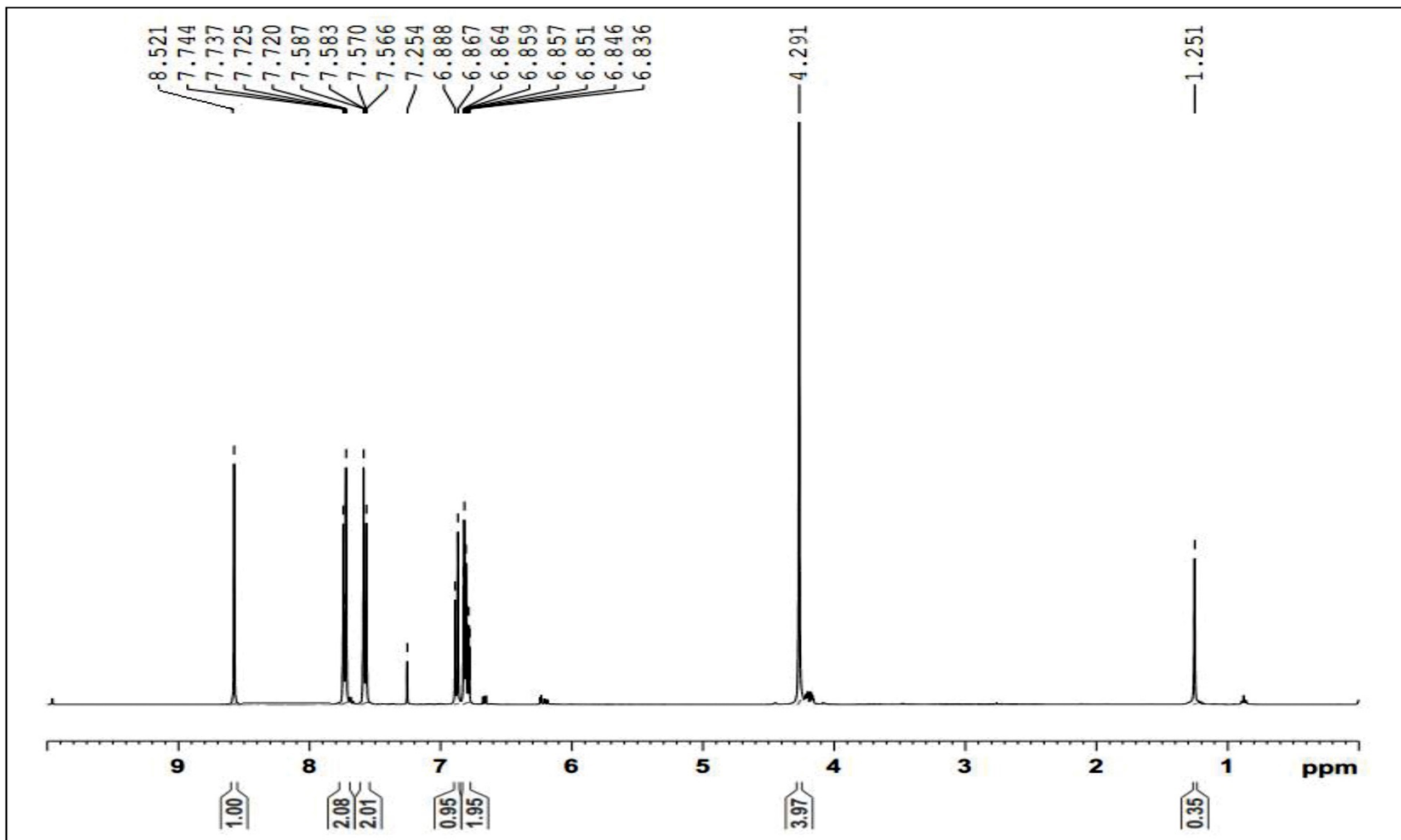


Figure S21. ¹H NMR spectrum of (*E*)-N-(4-Nitrobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**11**)

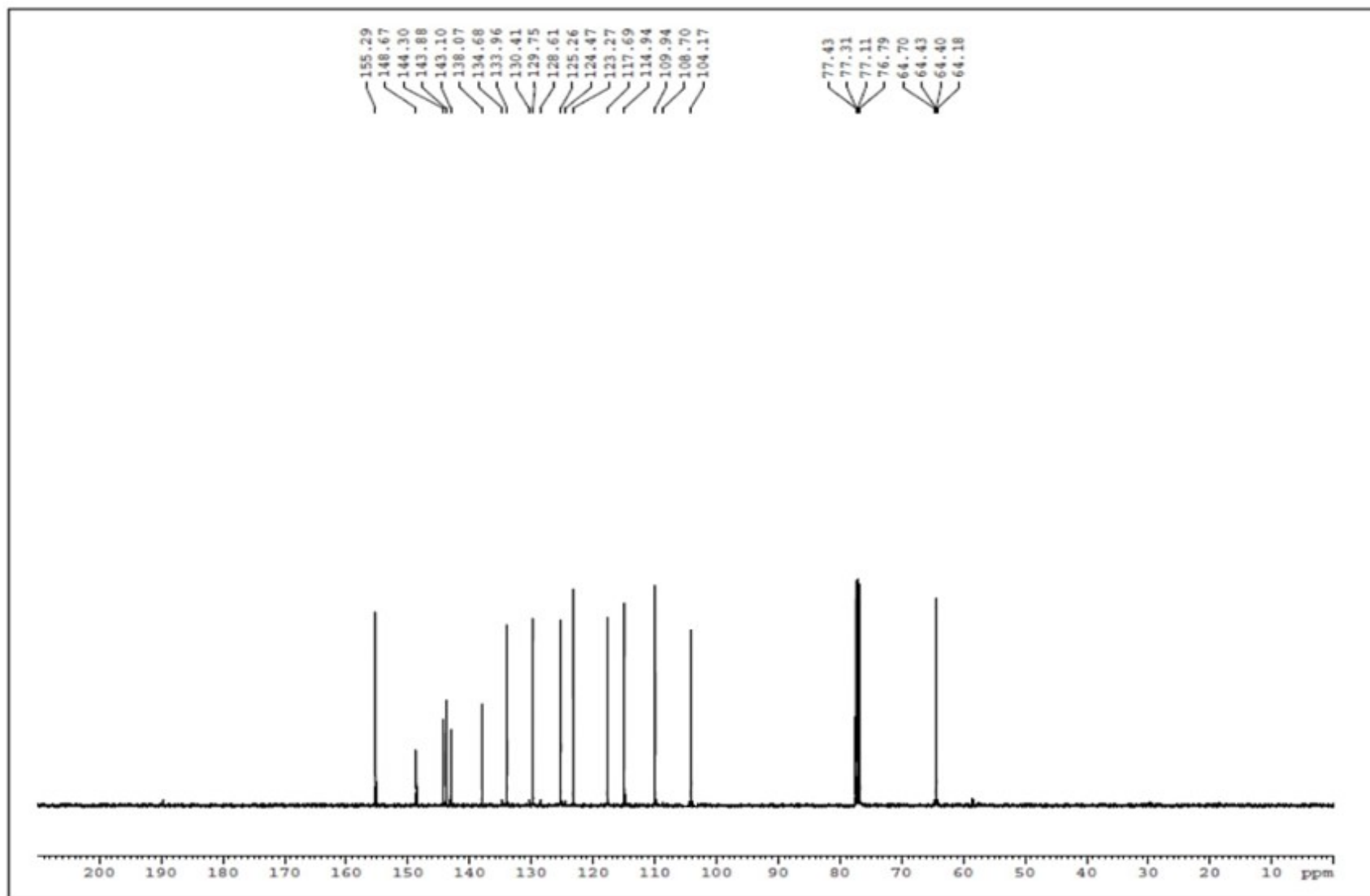


Figure S22. ^{13}C NMR spectrum of (*E*)-*N*-(4-Nitrobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**11**)

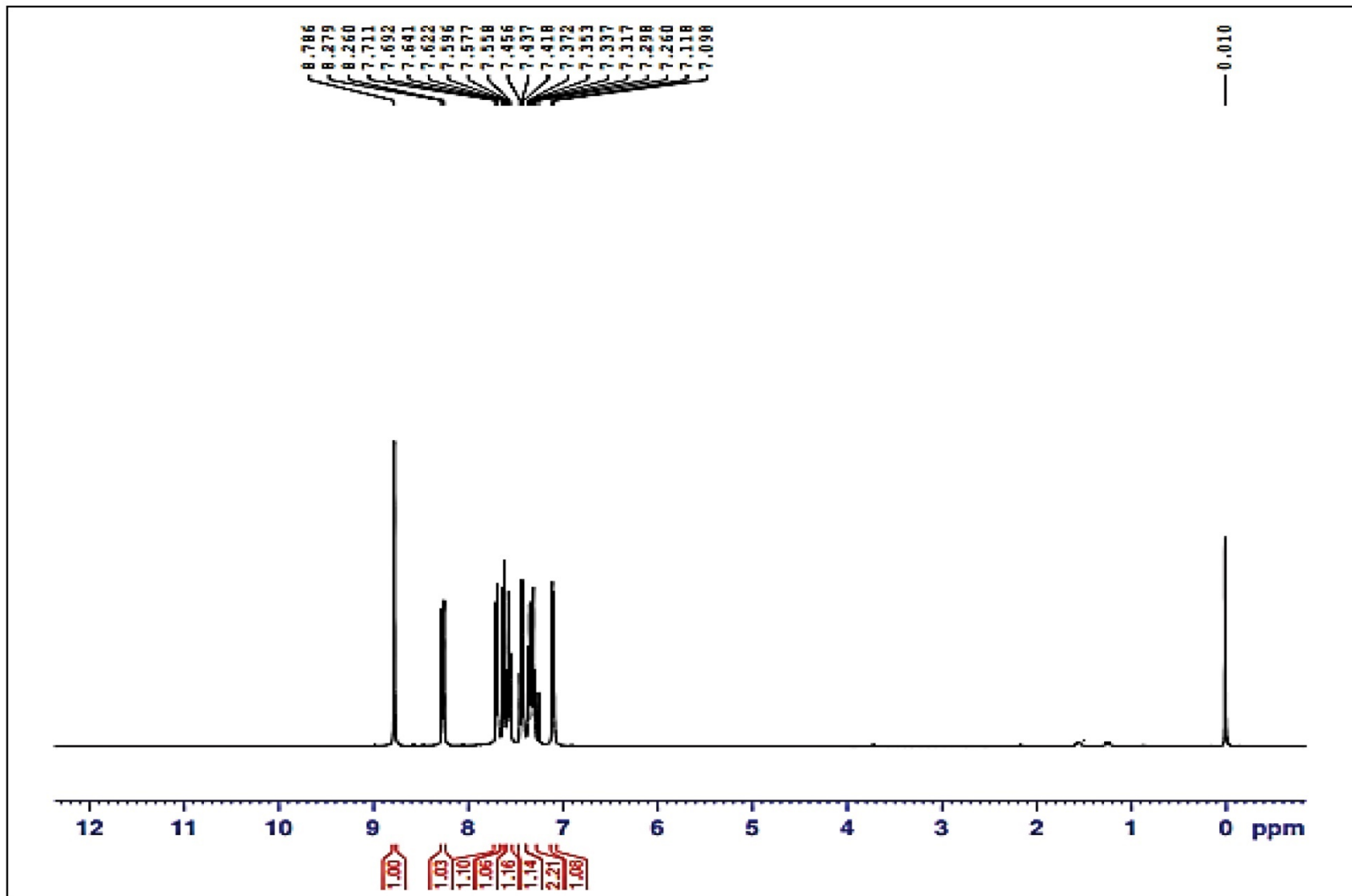


Figure S23. ¹H NMR spectrum of (E)-N-(2-Bromobenzylidene)-2-(trifluoromethyl)aniline (24)

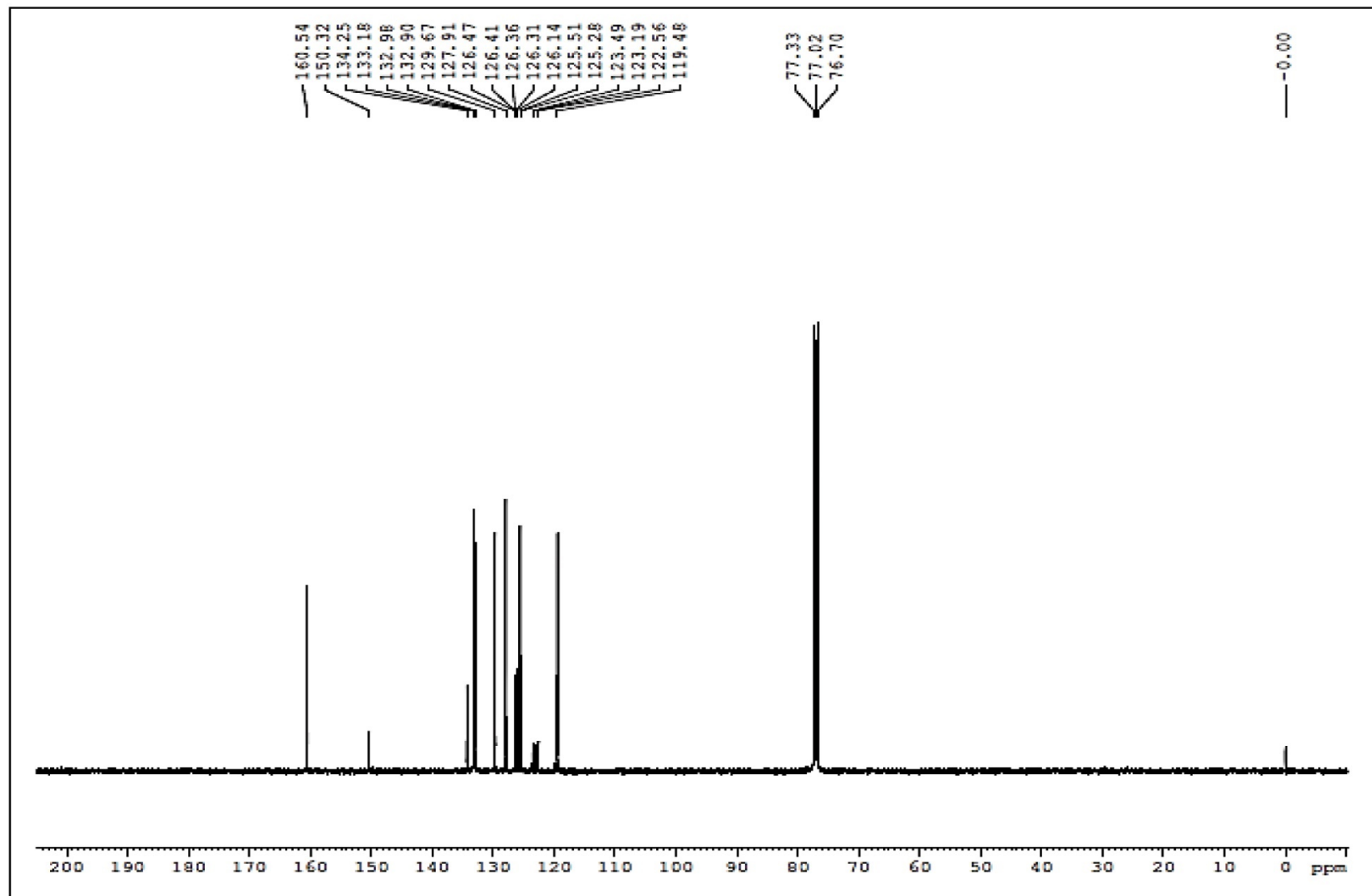


Figure S24. ^{13}C NMR spectrum of *(E)*-N-(2-Bromobenzylidene)-2-(trifluoromethyl)aniline (**24**)

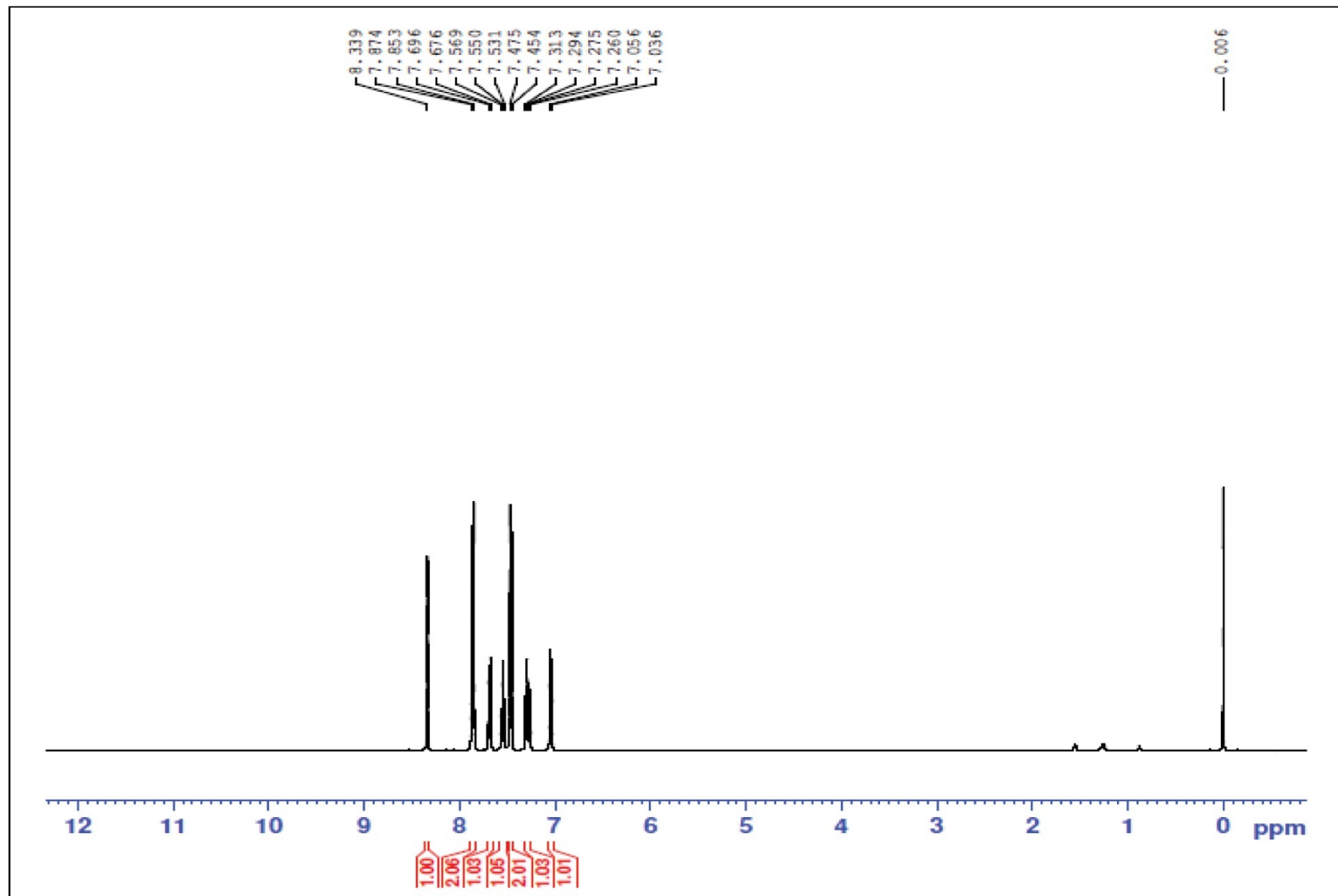


Figure S25. ^1H NMR spectrum of *(E)*-N-(2-Chlorobenzylidene)-2-(trifluoromethyl)aniline (**25**)

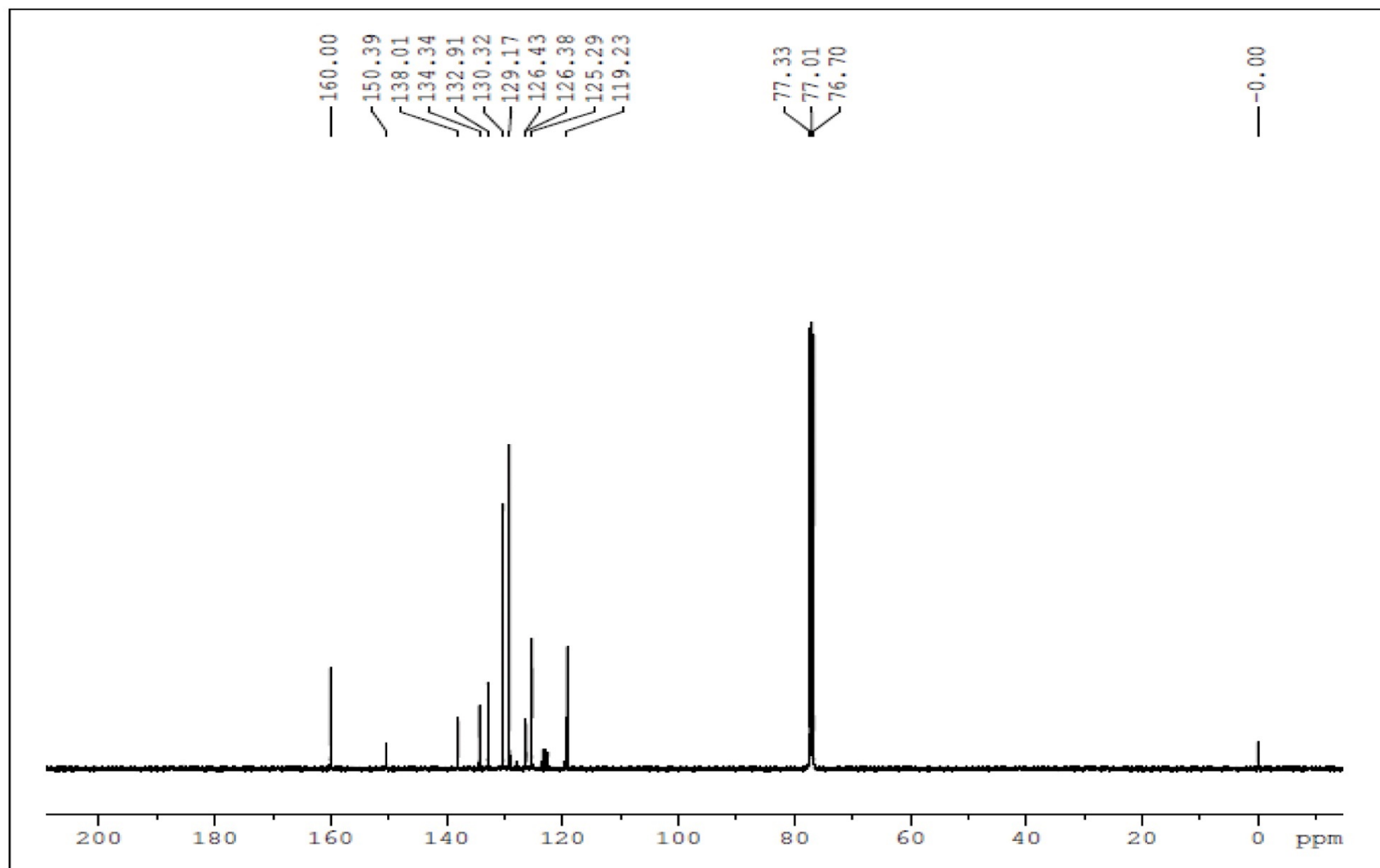


Figure S26. ^{13}C NMR spectrum of (*E*)-*N*-(2-Chlorobenzylidene)-2-(trifluoromethyl)aniline (**25**)

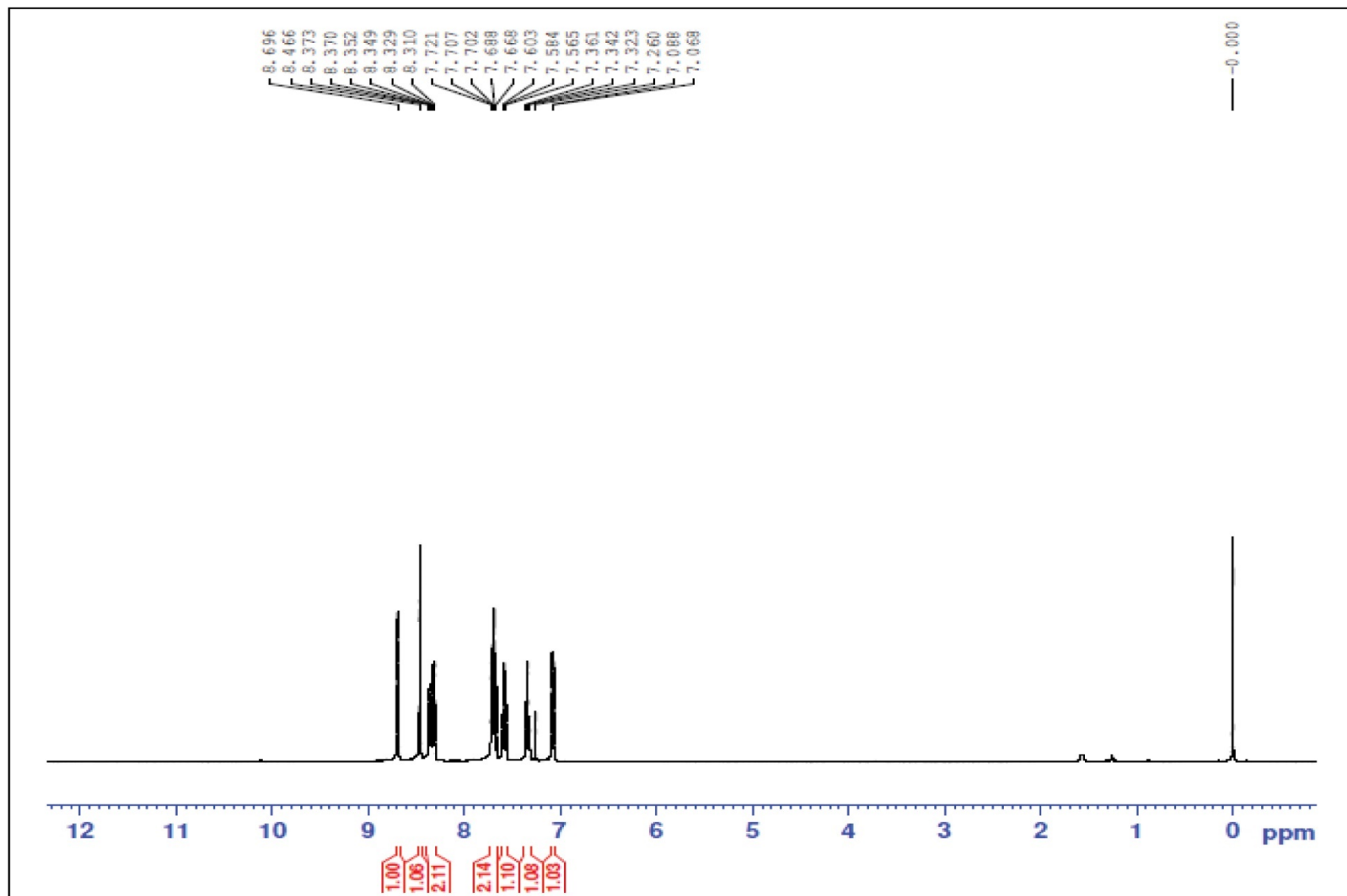


Figure S27. ^1H NMR spectrum of *(E)*-N-(3-nitrobenzylidene)-2-(trifluoromethyl)aniline (26)

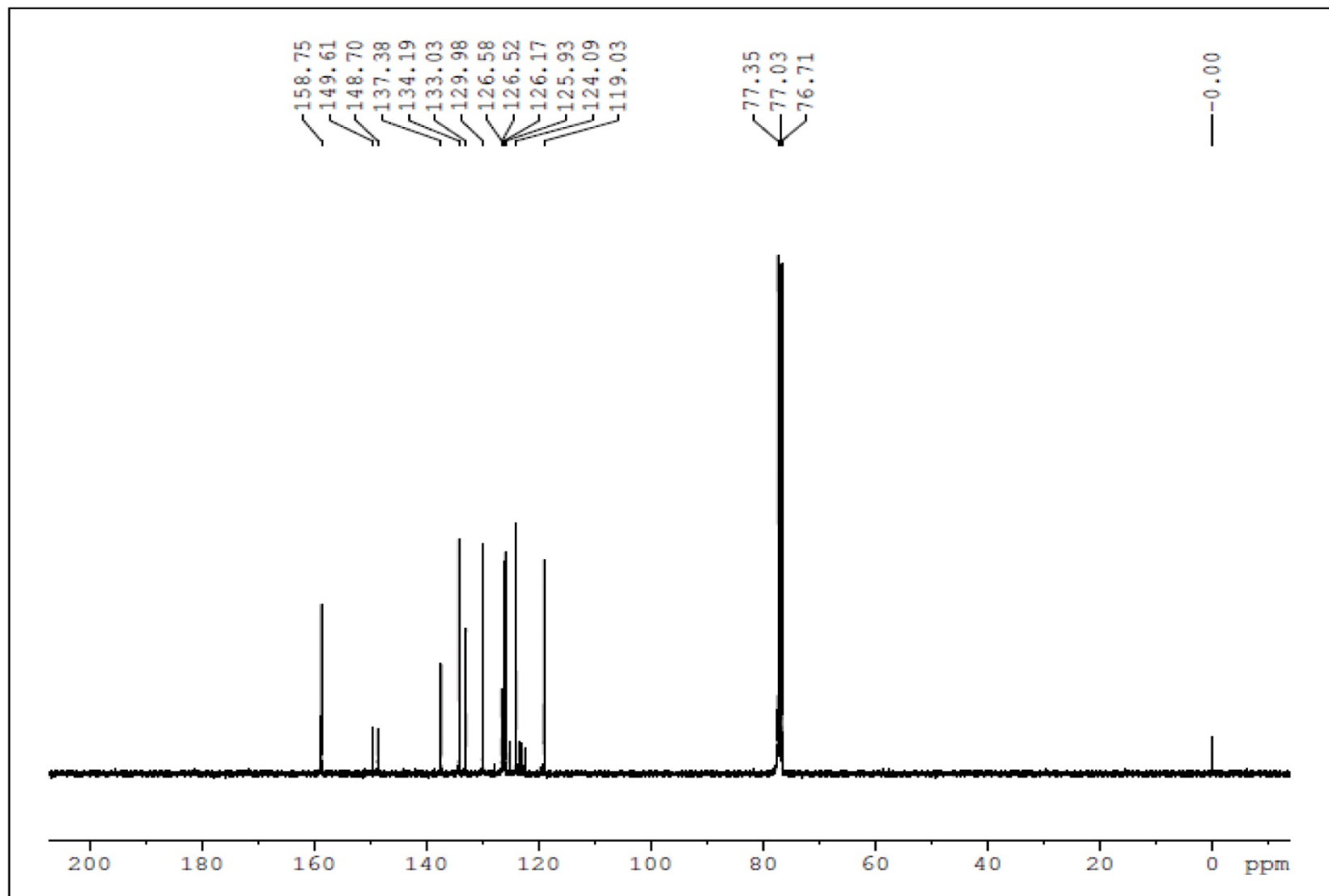


Figure S28. ^{13}C NMR spectrum of (*E*)-*N*-(3-nitrobenzylidene)-2-(trifluoromethyl)aniline (**26**).

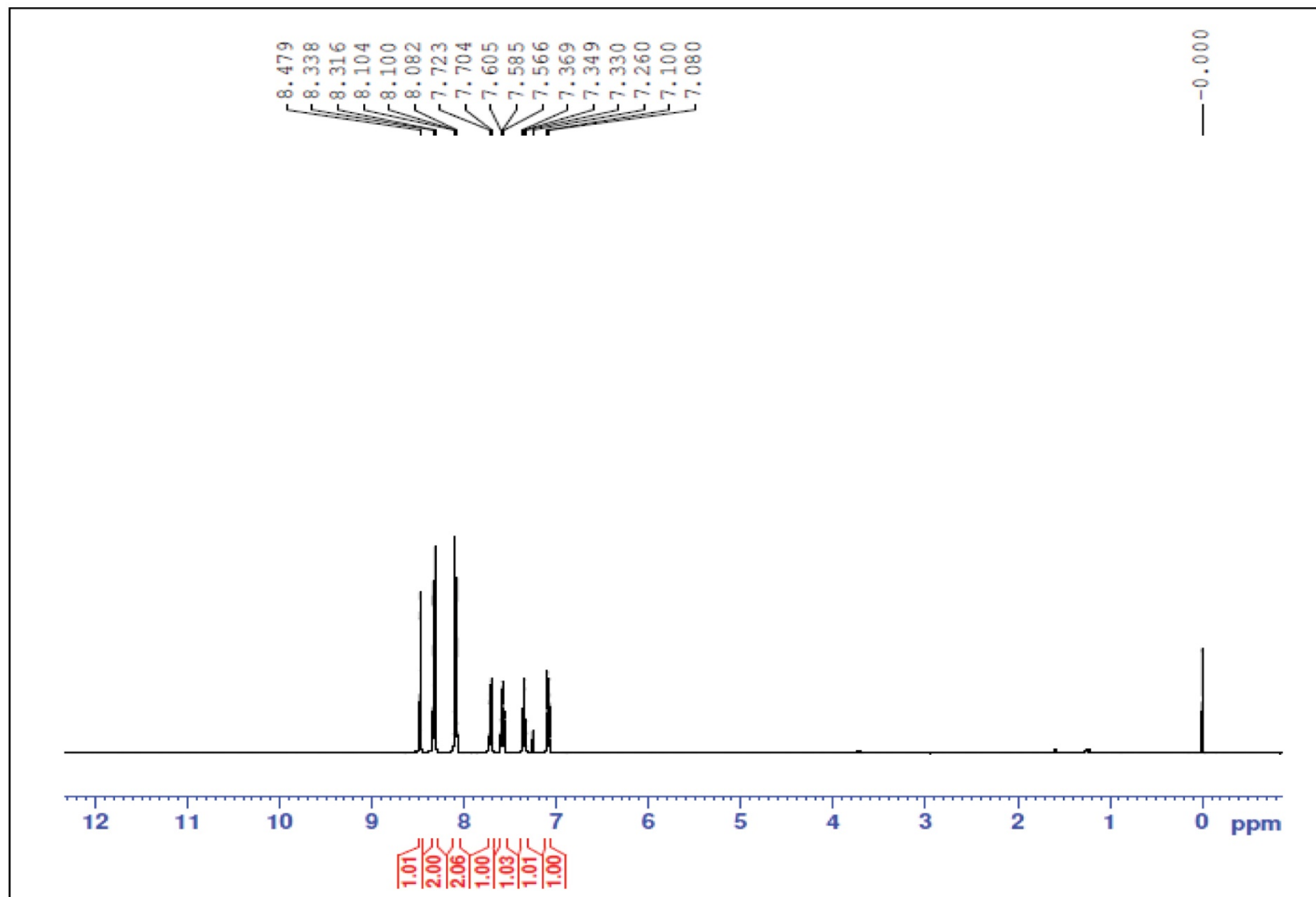


Figure S29. ^1H NMR spectrum of (*E*)-*N*-(4-nitrobenzylidene)-2-(trifluoromethyl)aniline (**27**)

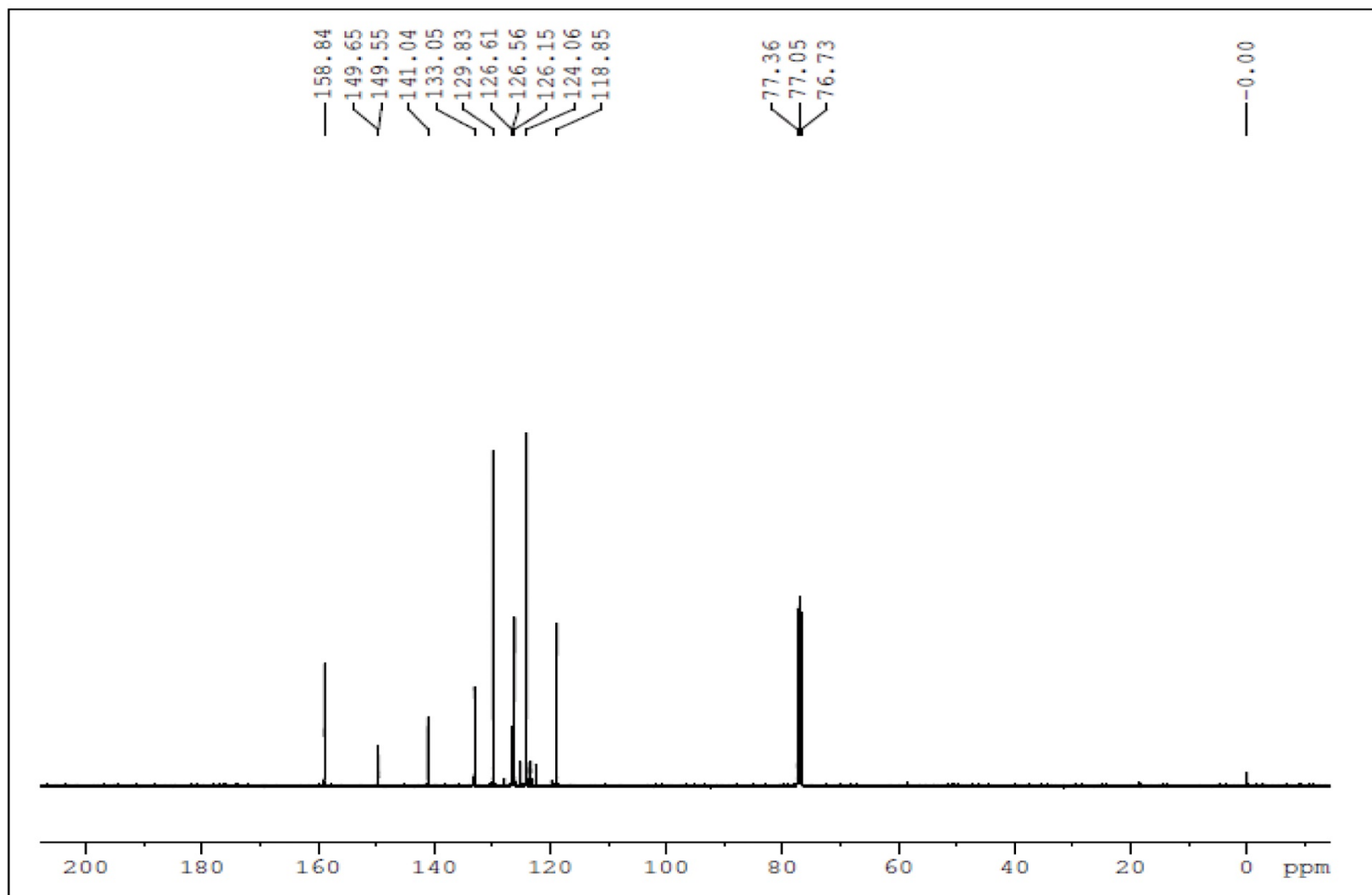


Figure S30. ^{13}C NMR spectrum of (*E*)-*N*-(4-nitrobenzylidene)-2-(trifluoromethyl)aniline (**27**).

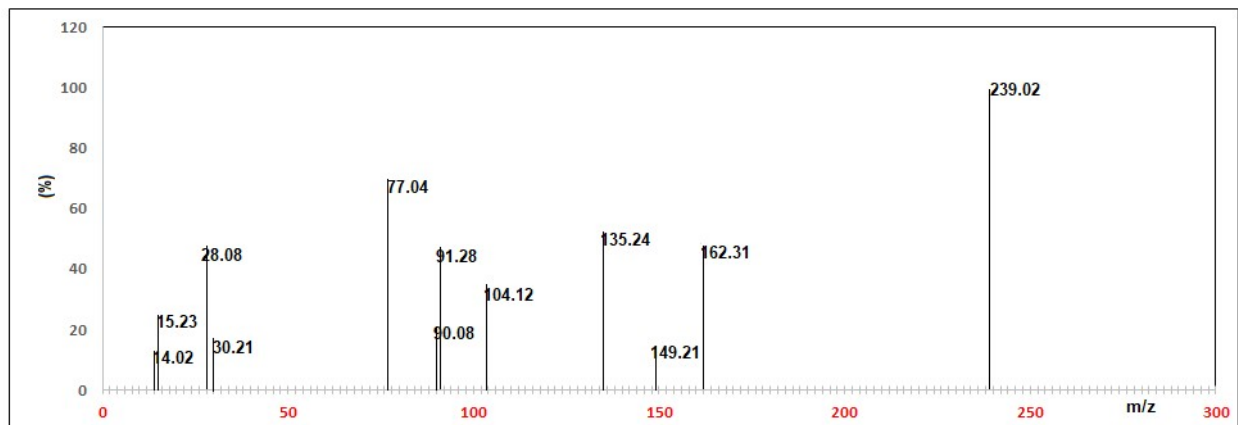


Figure S31. Mass spectrum of (*E*)-N-Benzylidene-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amine (1)

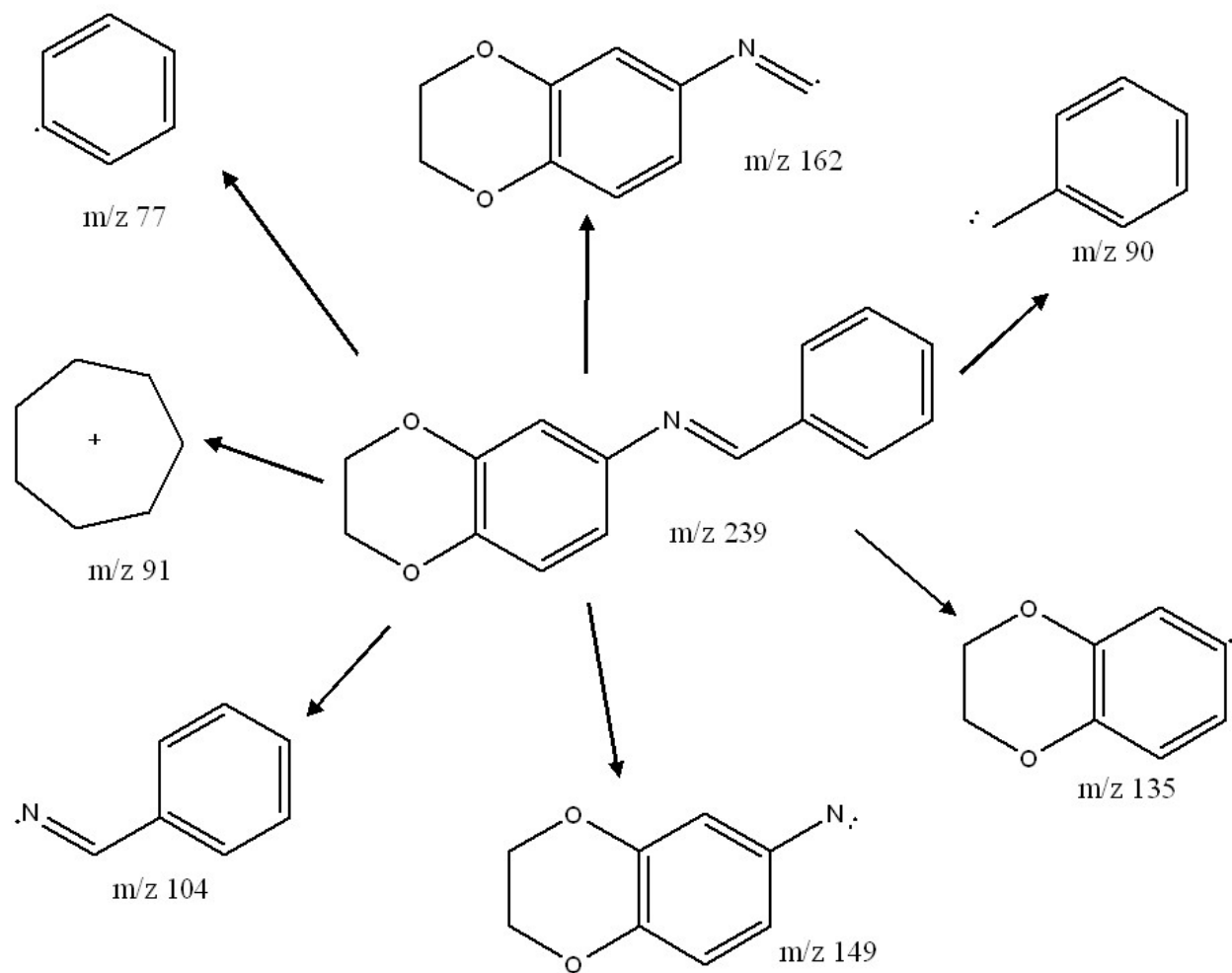


Figure S32. Assigned mass fragments of *(E)*-N-Benzylidene-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amine (**1**)

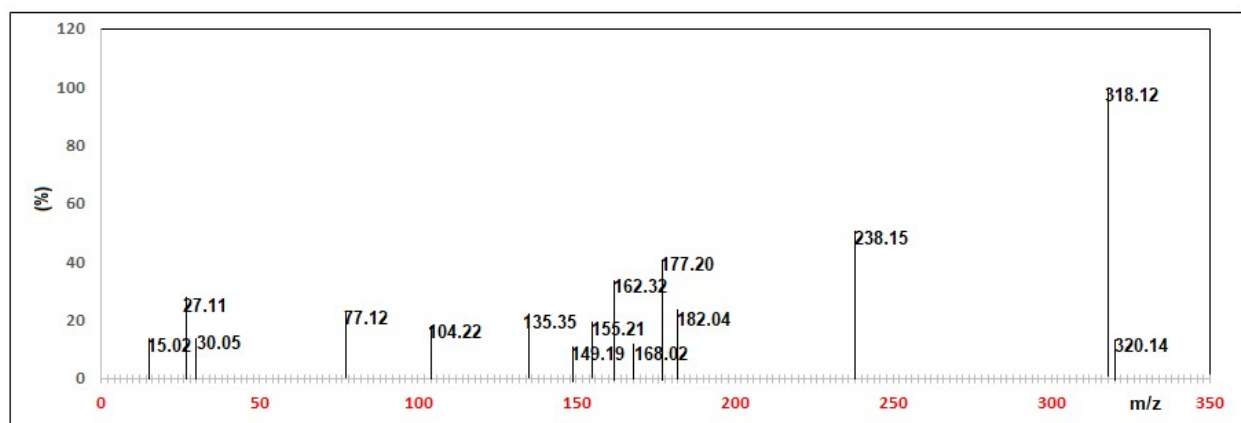


Figure S33. Mass spectrum of (*E*)-N-(3-Bromobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**2**)

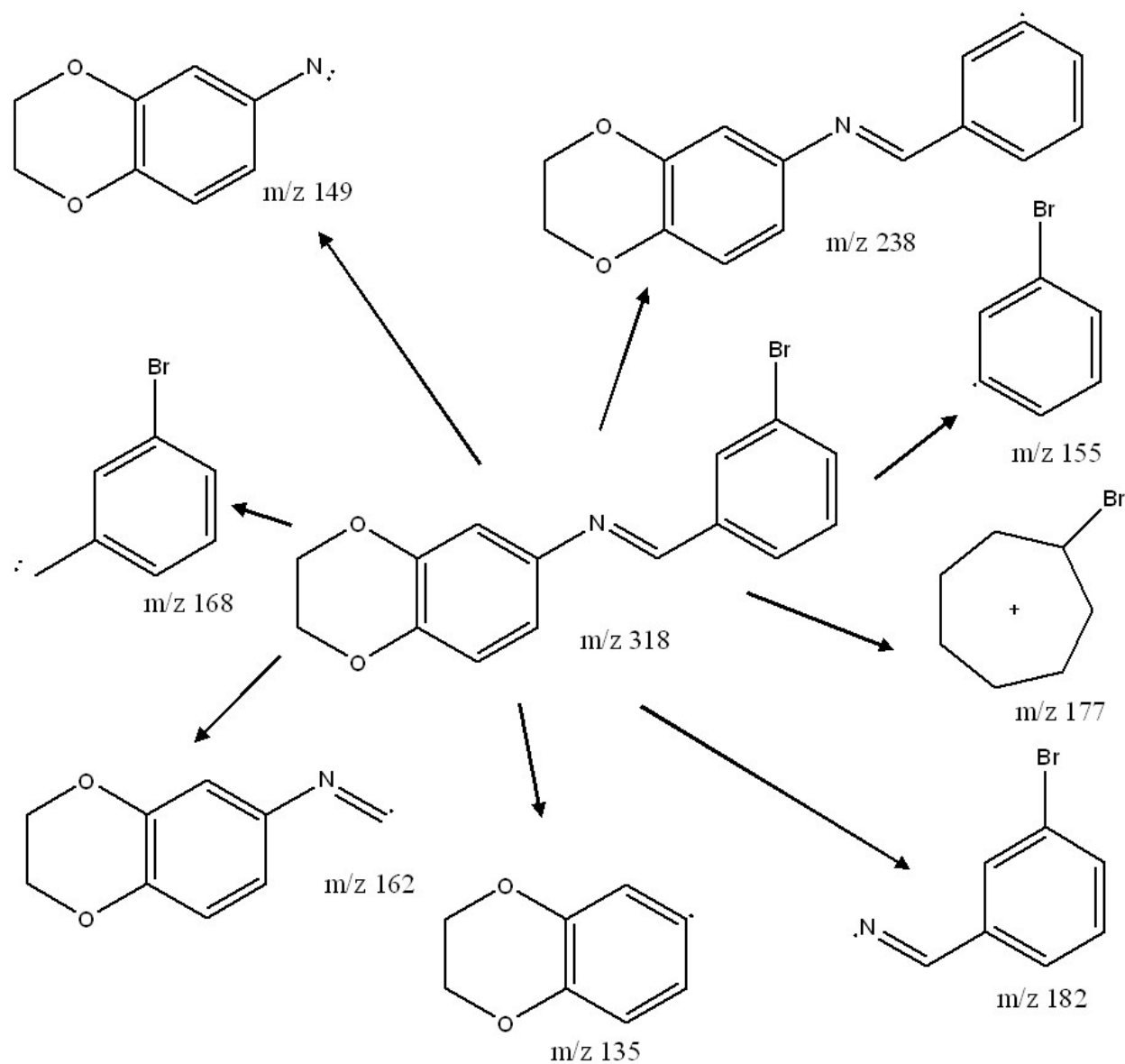


Figure S34. The assigned mass fragments of (E) - N -(3-Bromobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**2**)

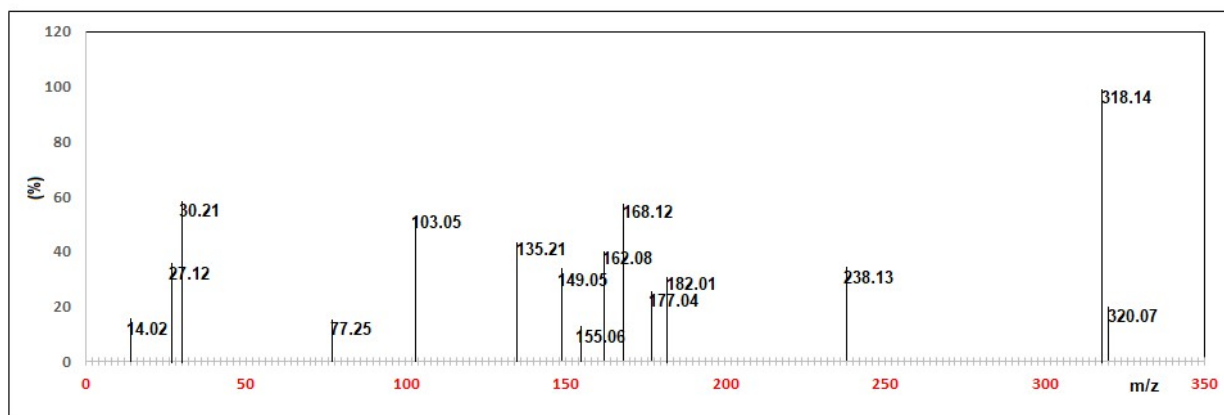


Figure S35. Mass spectrum of (*E*)-*N*-(4-Bromobenzylidene)-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amine (**3**)

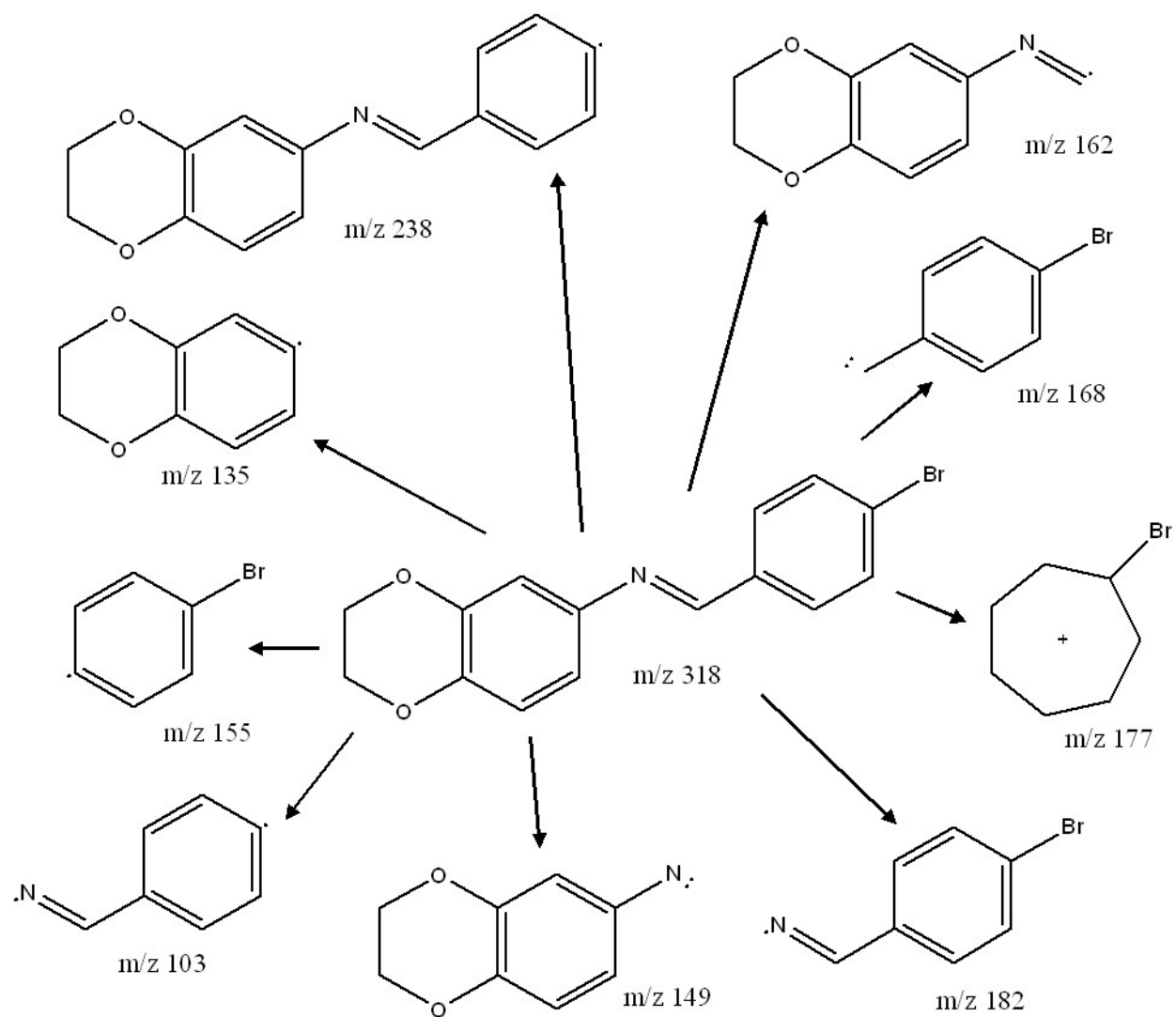


Figure S36. Assigned mass spectral fragments of (E) -N-(4-Bromobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**3**)

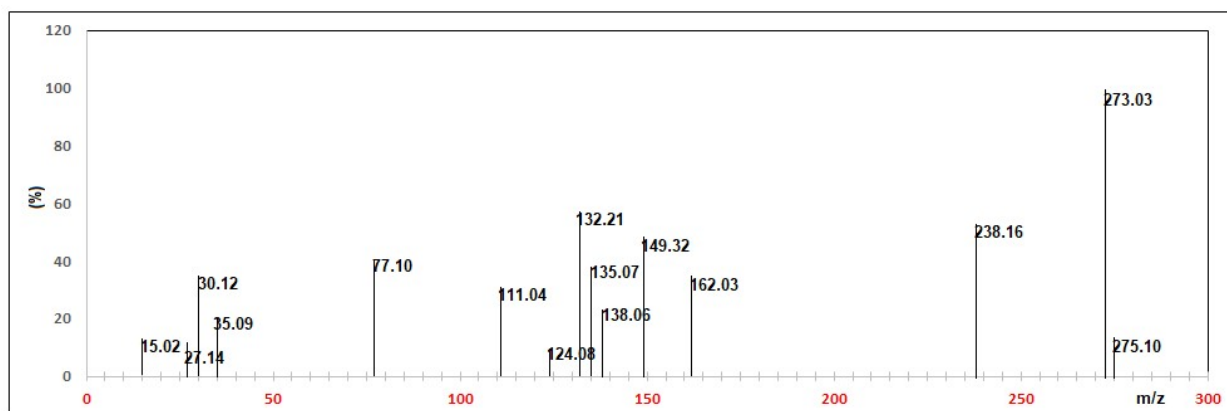


Figure S37. Mass spectrum of (*E*)-*N*-(3-Chlorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**4**)

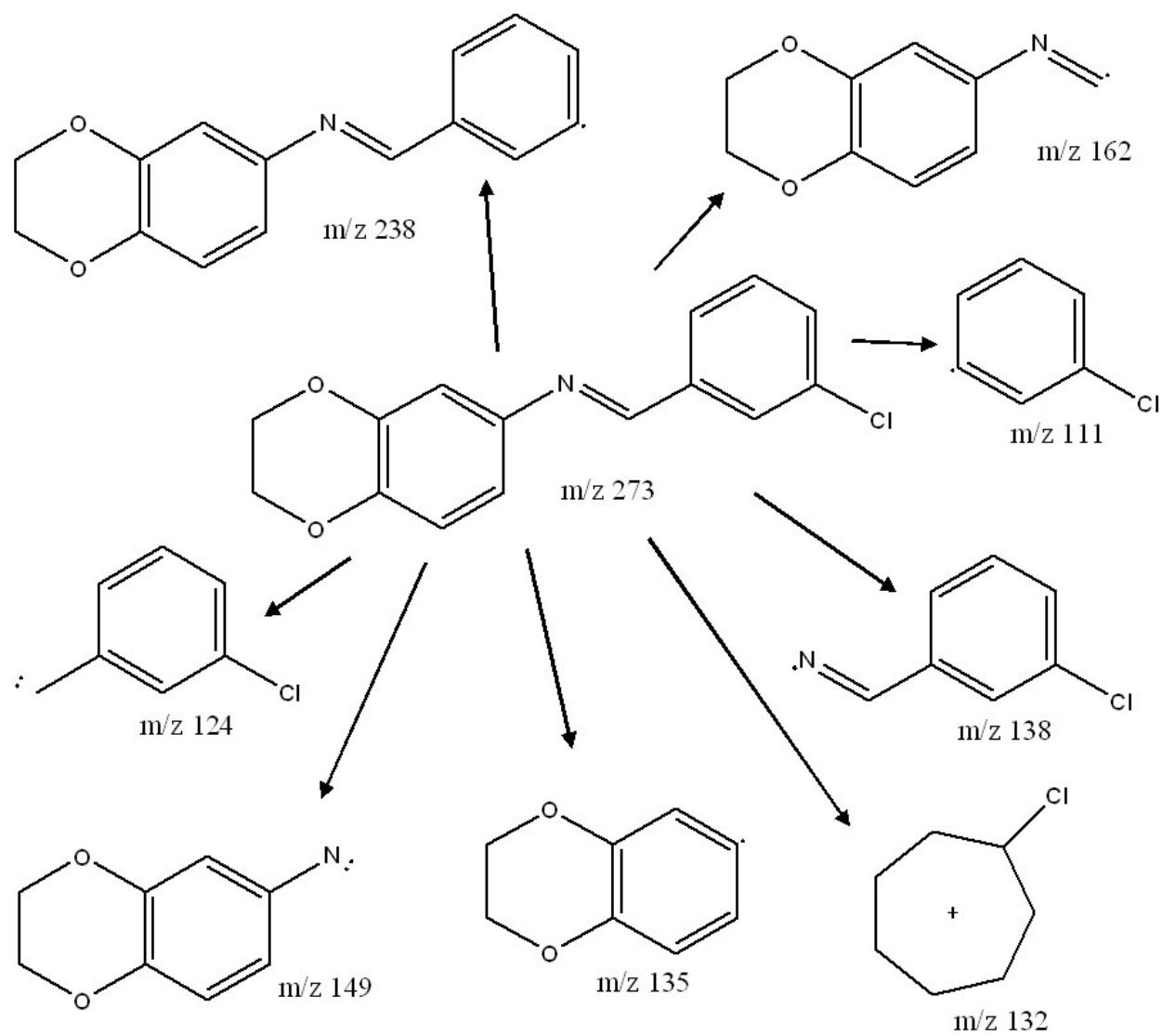


Figure S38. Assigned mass spectral fragments of (E) -N-(3-Chlorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**4**)

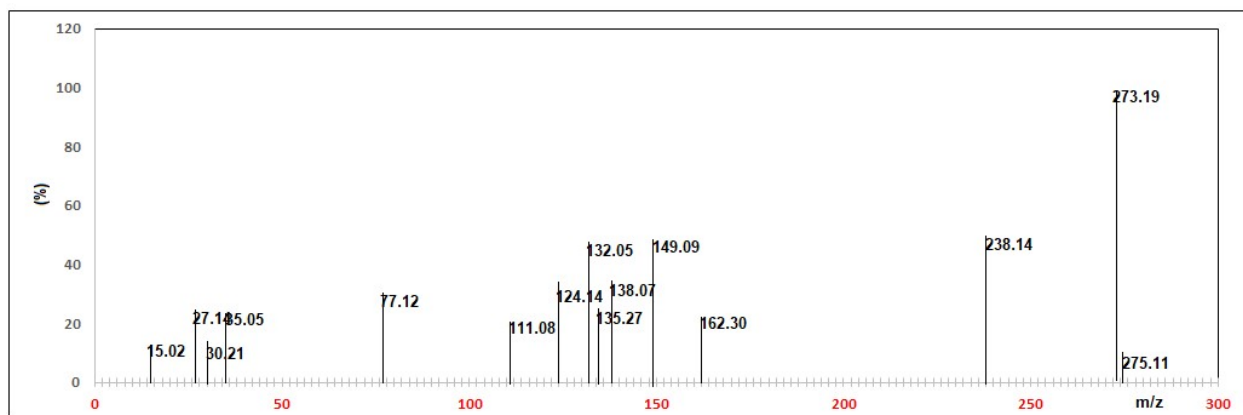


Figure S39. Mass spectrum of (*E*)-*N*-(4-Chlorobenzylidene)-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amine (**5**)

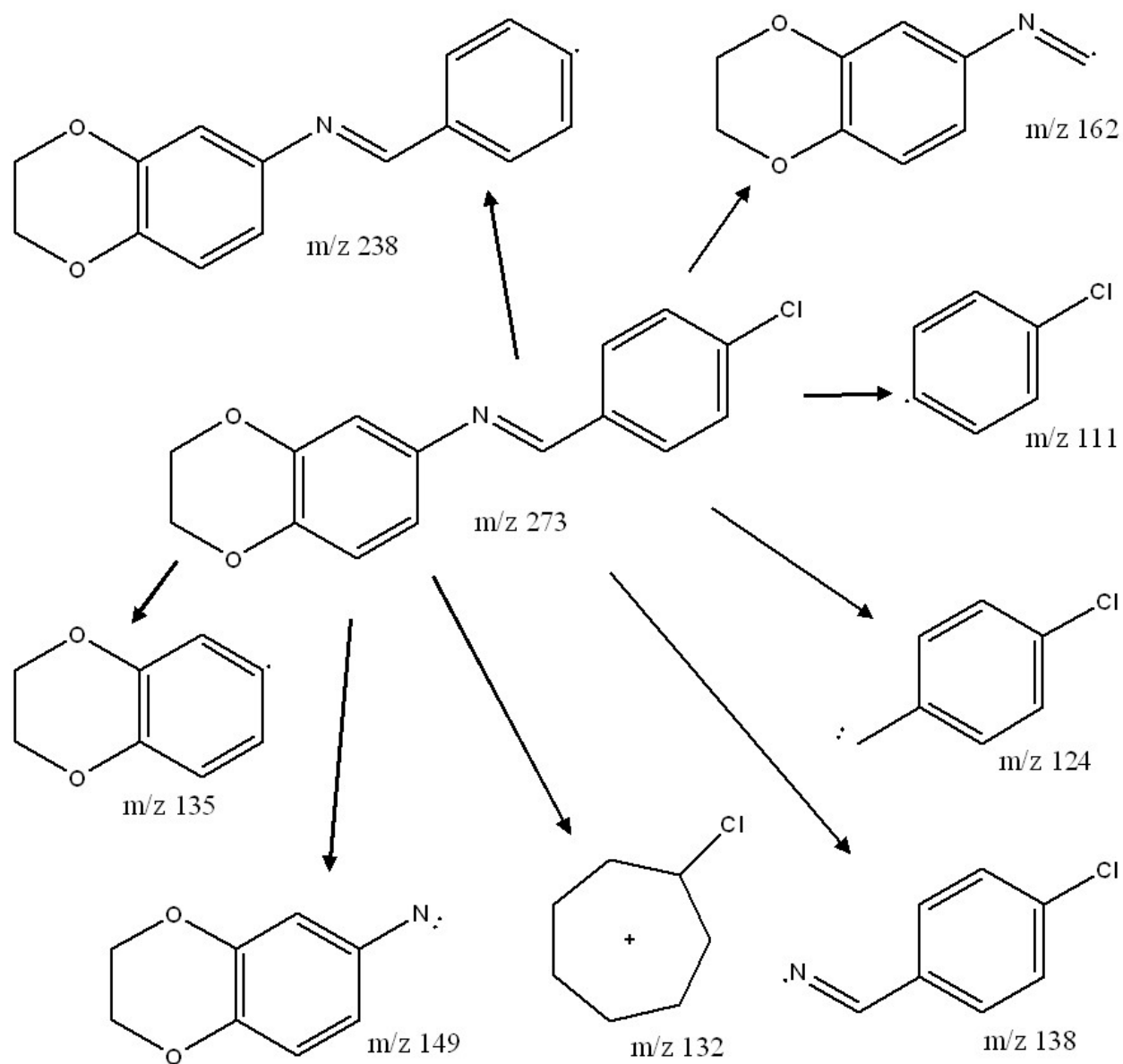


Figure S40. Assigned mass spectral fragments of (E) -N-(4-Chlorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**5**)

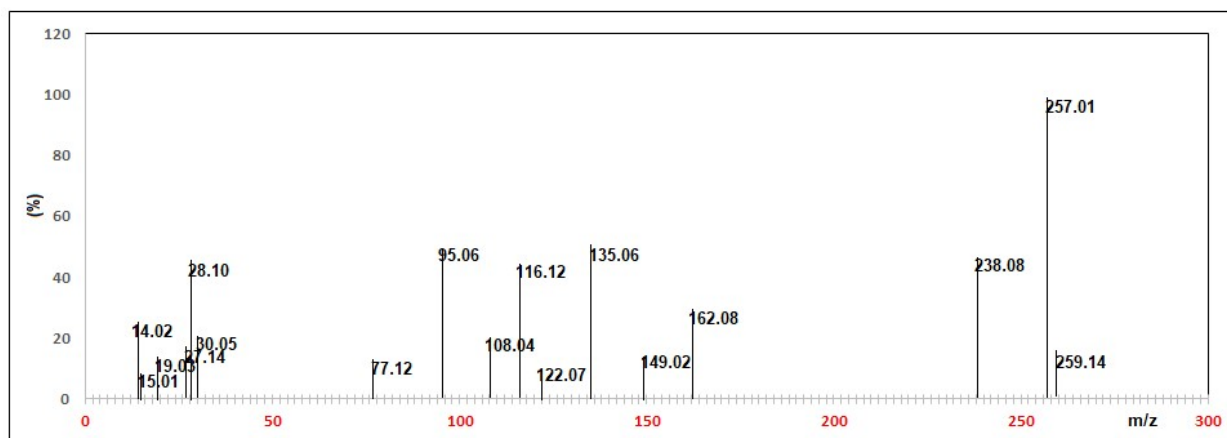


Figure S41. Mass spectrum of (*E*)-N-(4-Fluorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**6**)

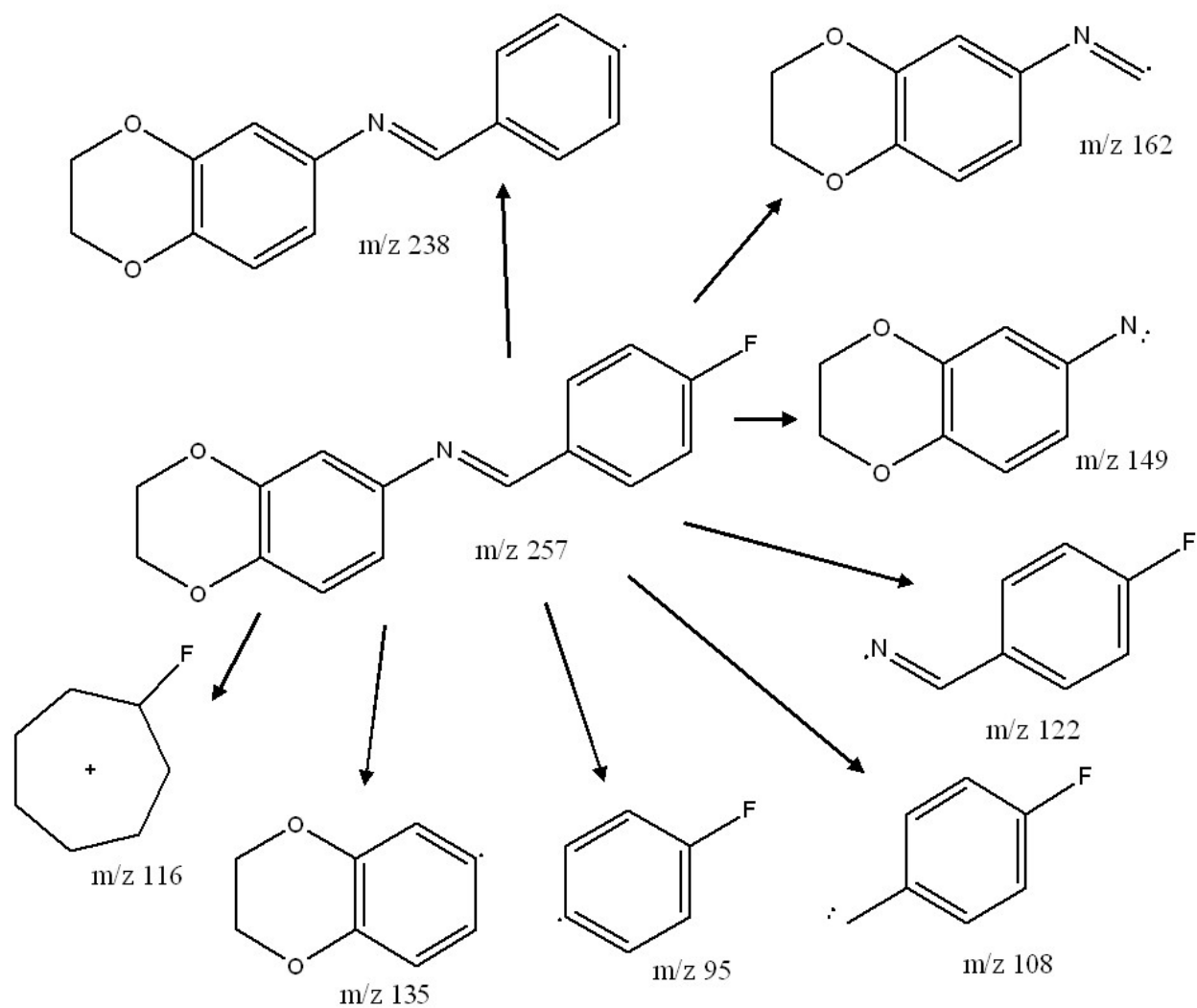


Figure S42. Assigned mass spectral fragments of (*E*)-N-(4-Fluorobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**6**)

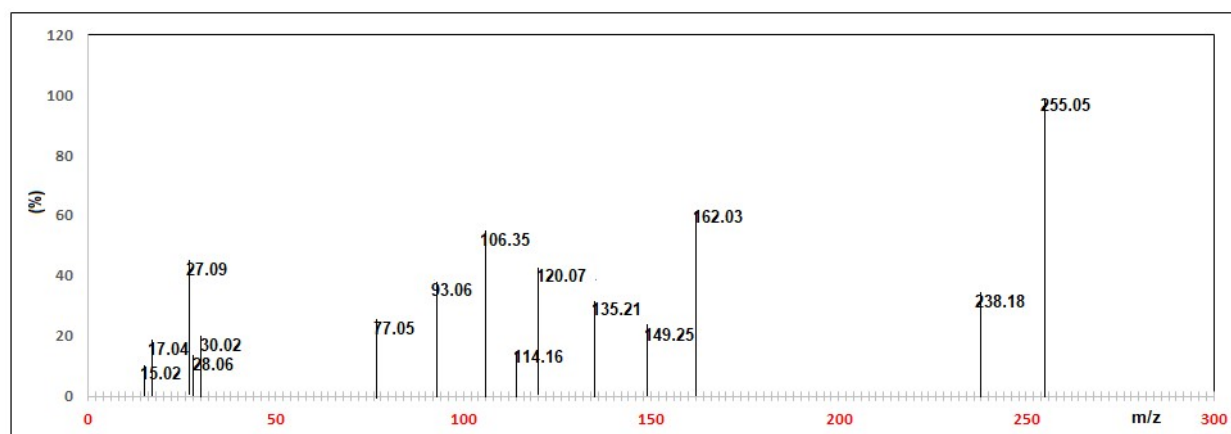


Figure S43. Mass spectrum of (*E*)-*N*-(4-hydroxybenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (7)

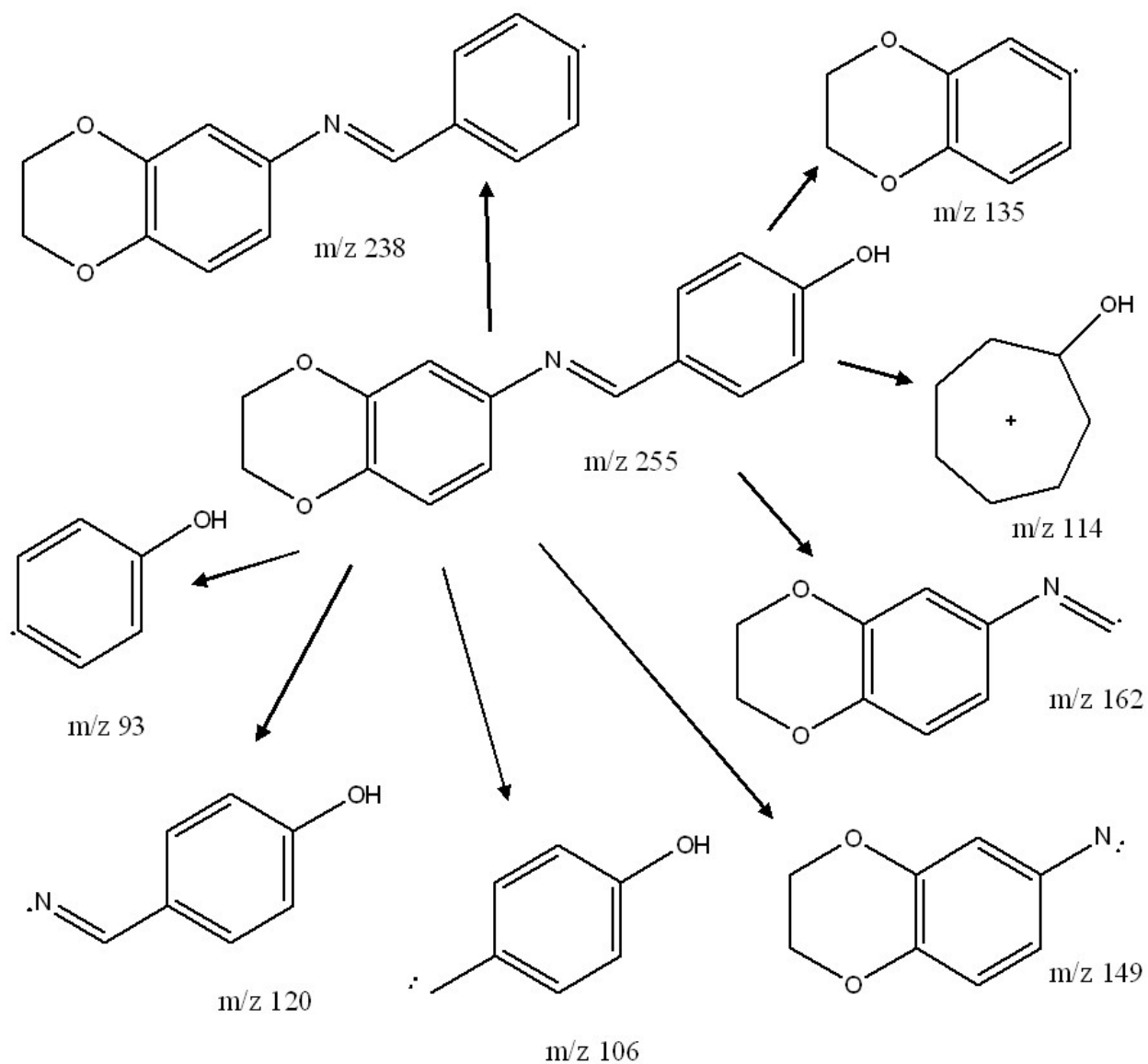


Figure S44. Assigned mass spectral fragments of (E) -N-(4-hydroxybenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (7)

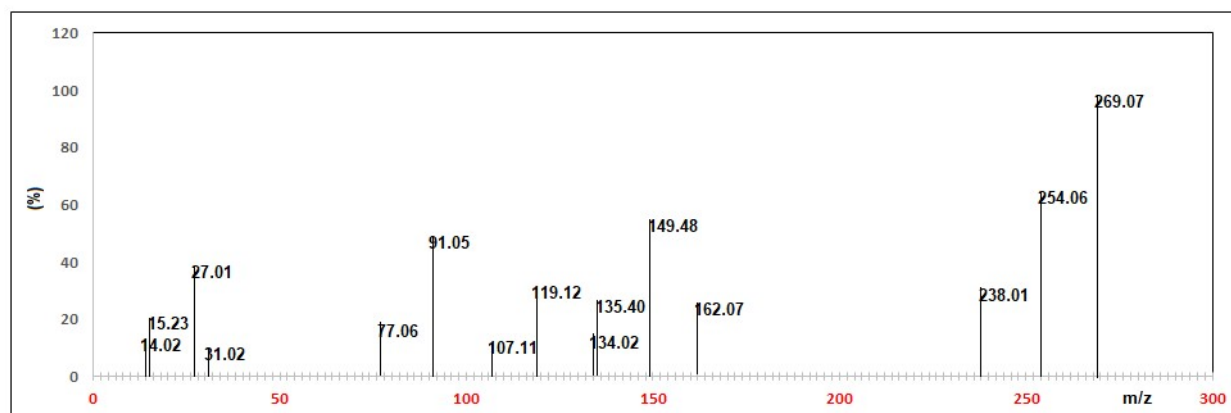


Figure S45. Mass spectrum of (*E*)-*N*-(3-methoxybenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**8**)

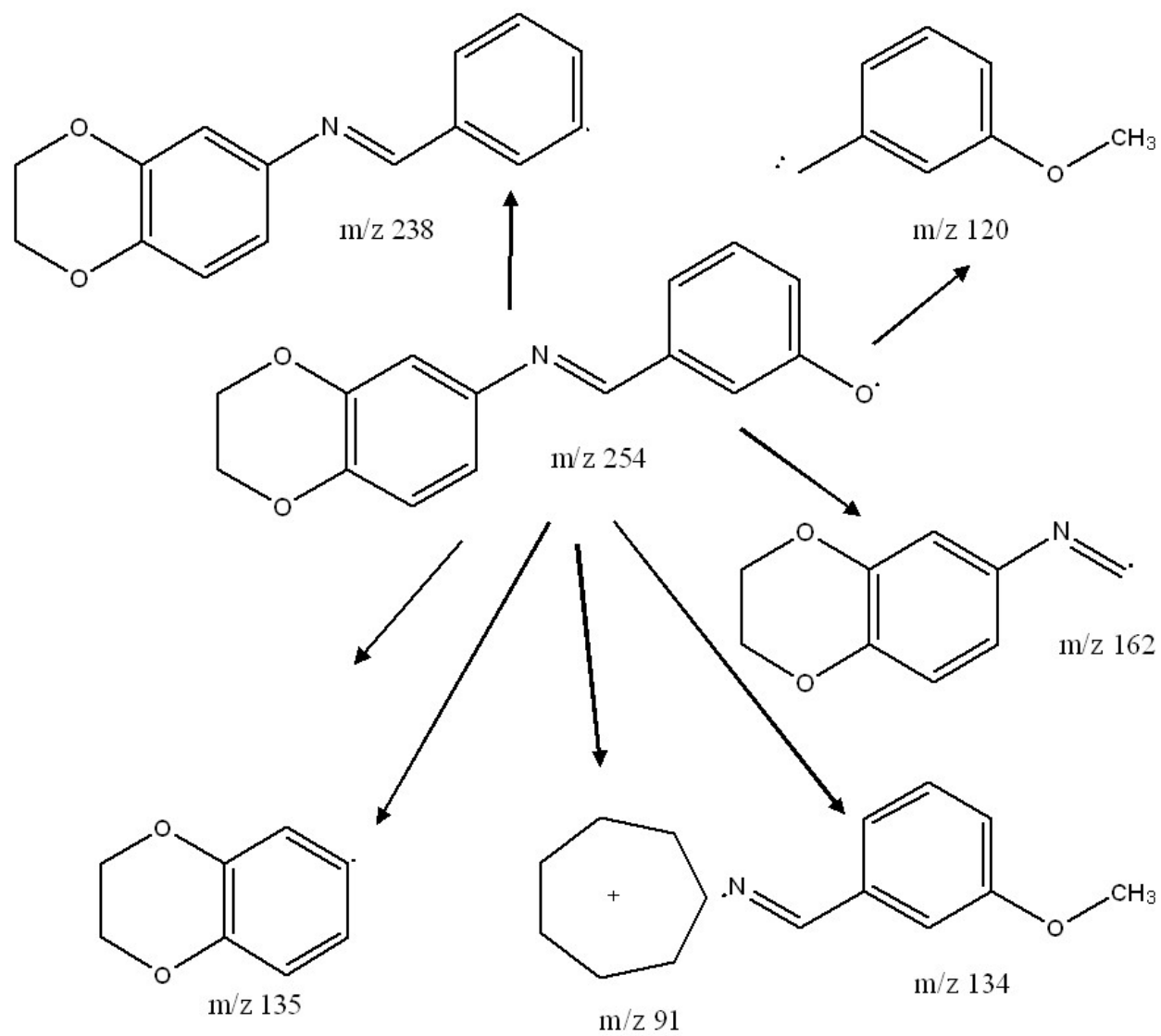


Figure S46. Assigned mass spectral fragments of (E) -N-(3-methoxybenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**8**)

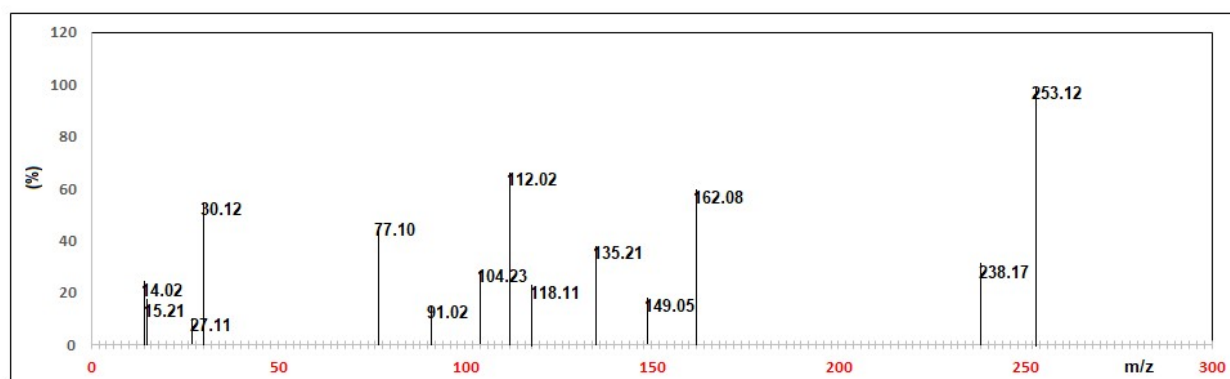


Figure S47. Mass spectrum of (*E*)-*N*-(2-methylbenzylidene)-2,3-dihydrobenzo(*b*)[1,4]-dioxin-6-amine (**9**)

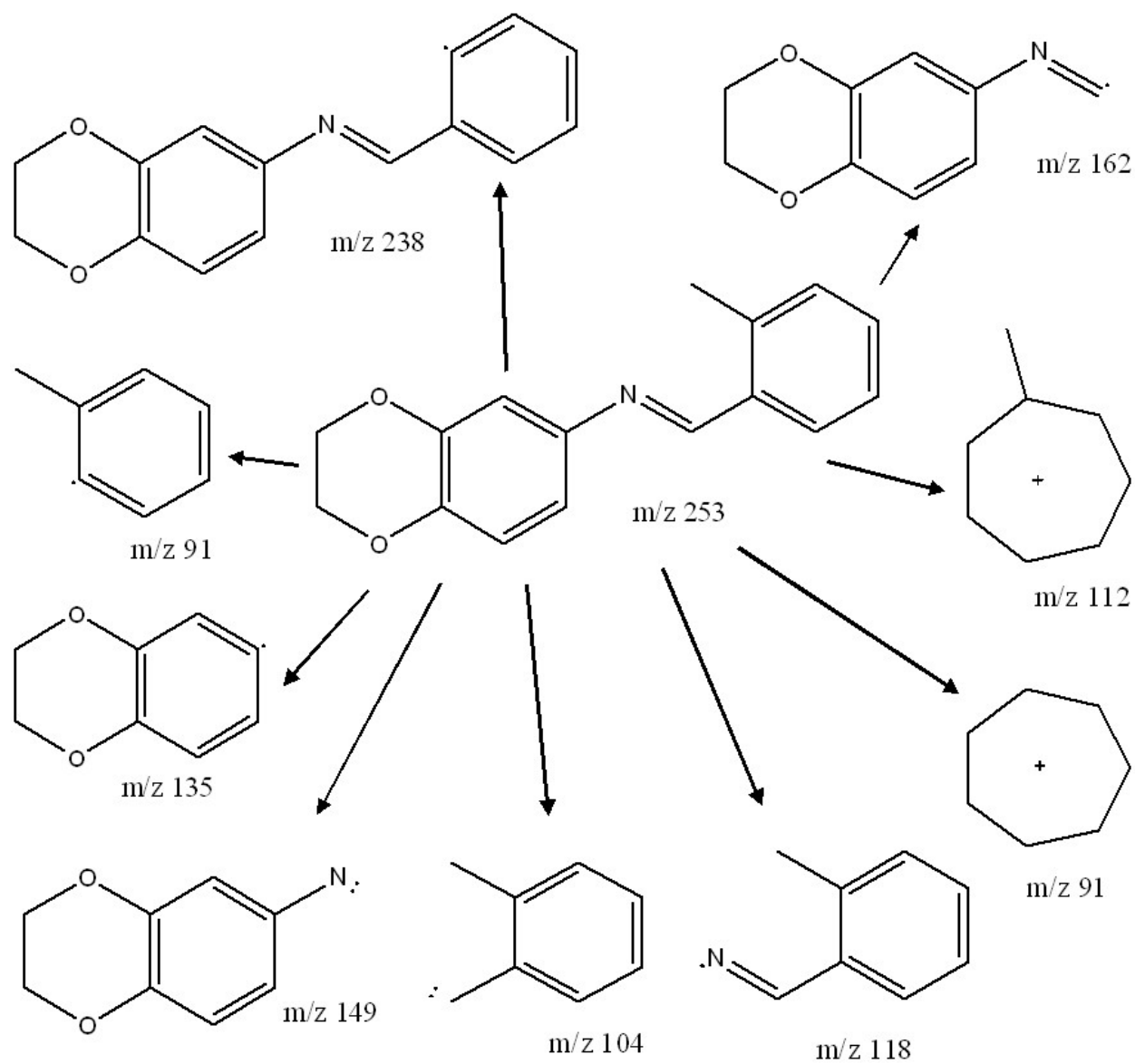


Figure S48. Assigned mass spectral fragments of (*E*)-*N*-(2-methylbenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**9**)

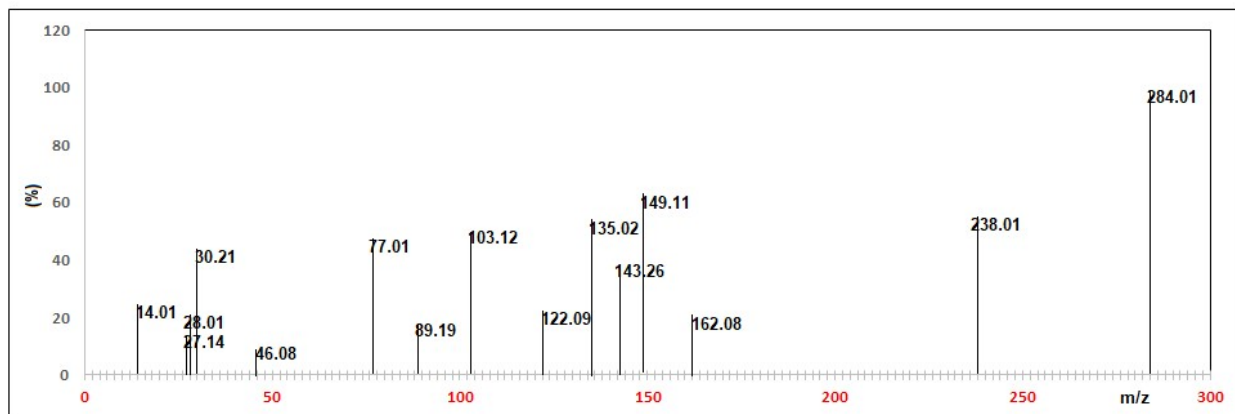


Figure S49. Mass spectrum of (*E*)-N-(3-nitrobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**10**)

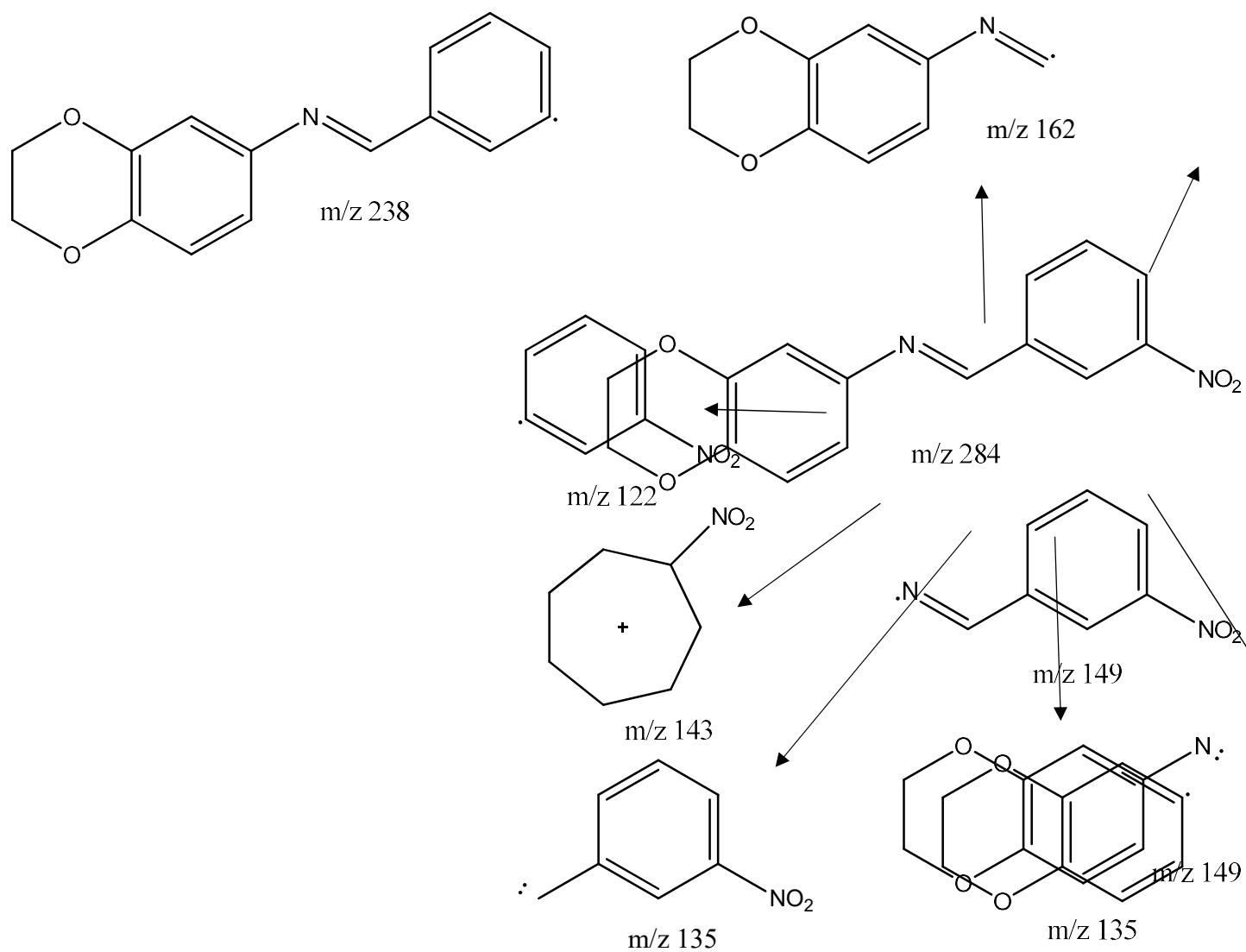


Figure S50. Assigned mass spectral fragments of (E) -N-(3-nitrobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**10**)

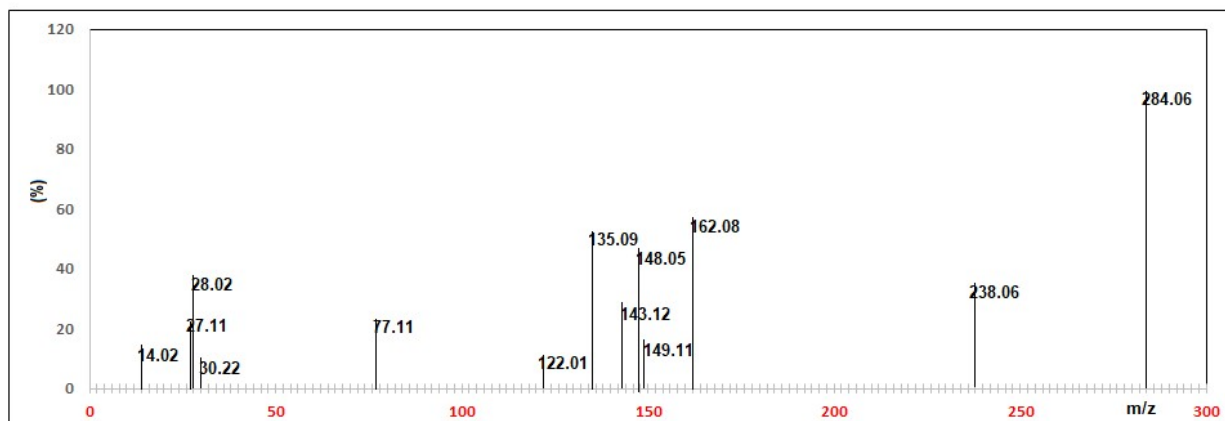


Figure S51. Mass spectrum of (*E*)-N-(4-nitrobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**11**)

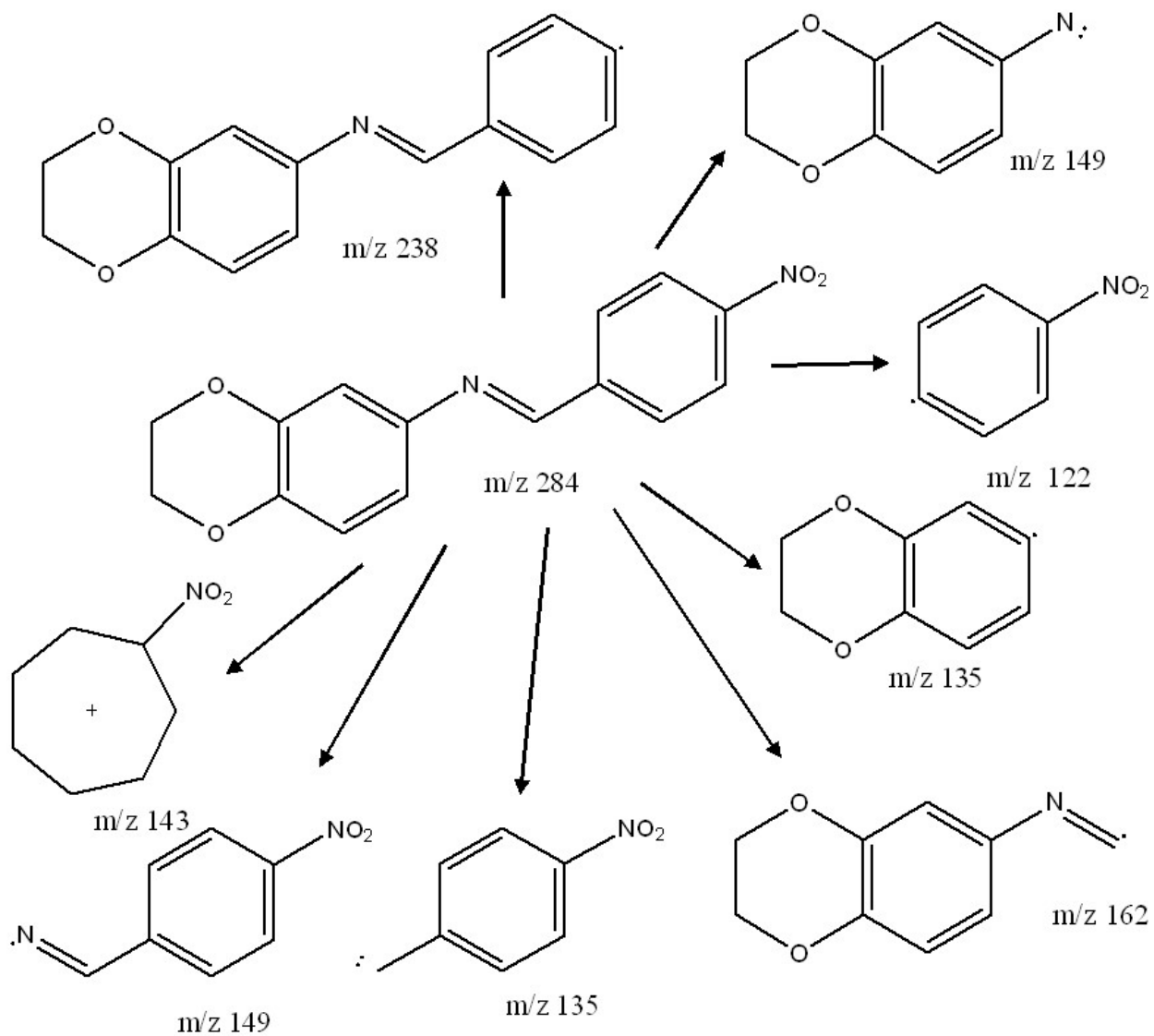


Figure S52. Assigned mass spectral fragments of (E) -N-(4-nitrobenzylidene)-2,3-dihydrobenzo(b)[1,4]-dioxin-6-amine (**11**)

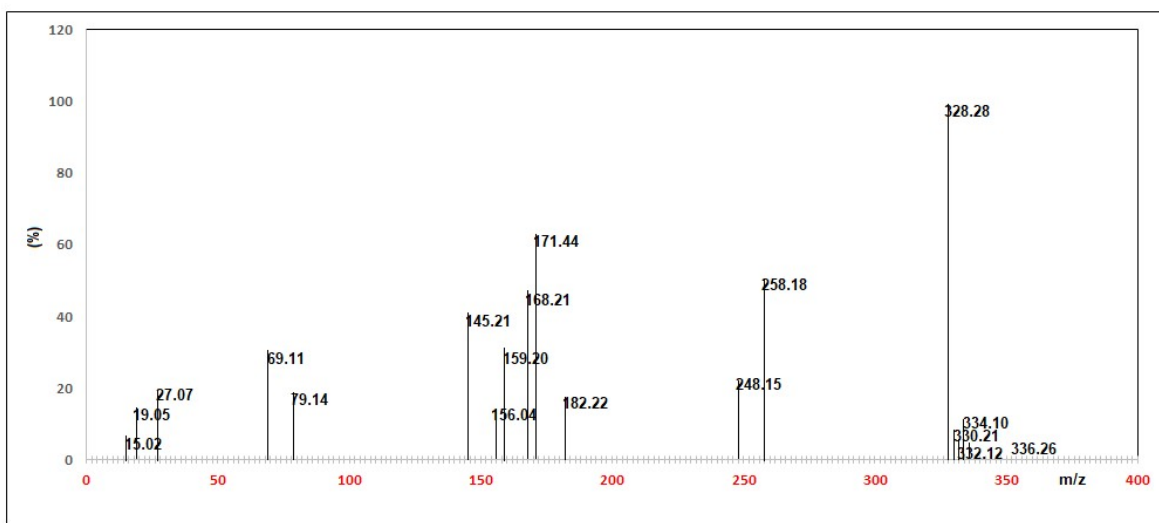


Figure S53. Mass spectrum of (*E*)-N-(2-Bromobenzylidene)-2-(trifluoromethyl)aniline (**24**)

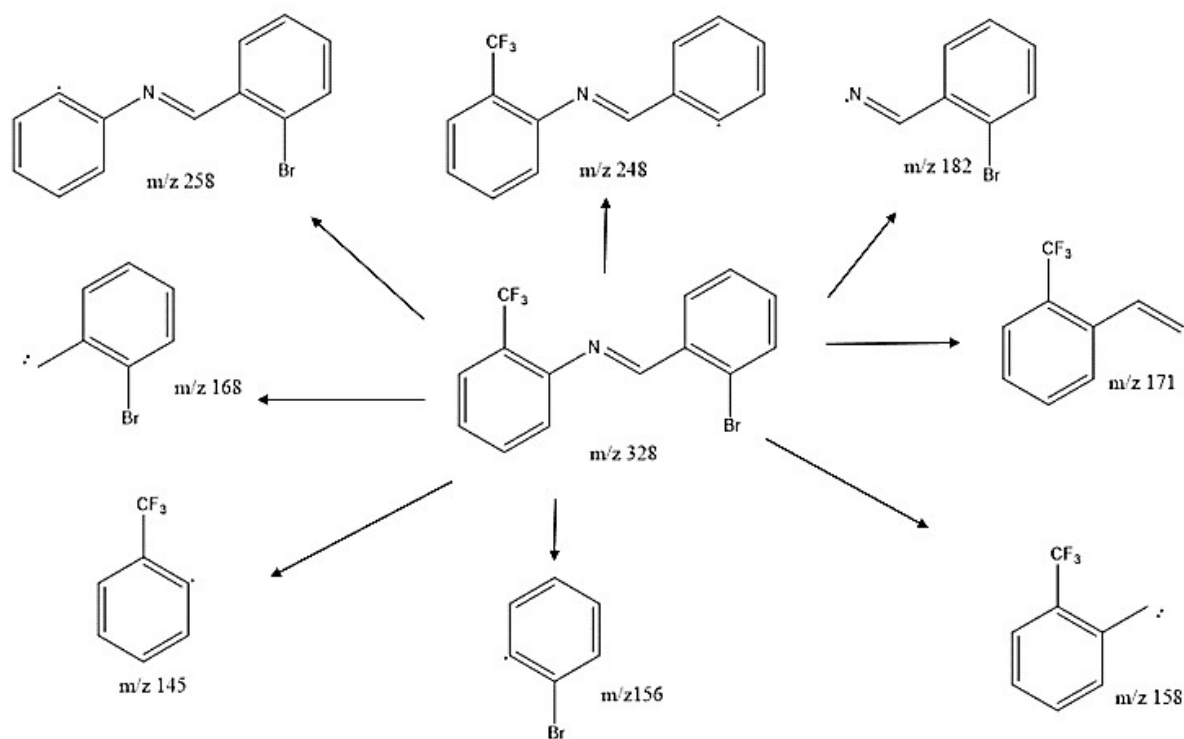


Figure S54. Assigned mass spectral fragments of (E) -N-(2-Bromobenzylidene)-2-(trifluoromethyl)aniline (**24**)

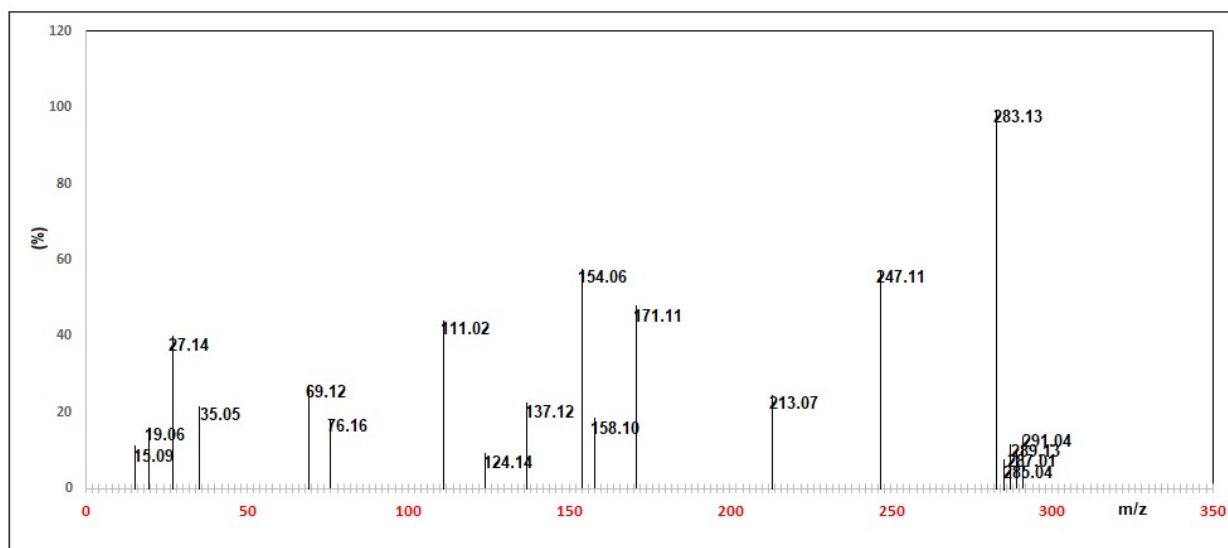


Figure S55. Mass spectrum of (*E*)-N-(4-chlorobenzylidene)-2-(trifluoromethyl)aniline (**25**)

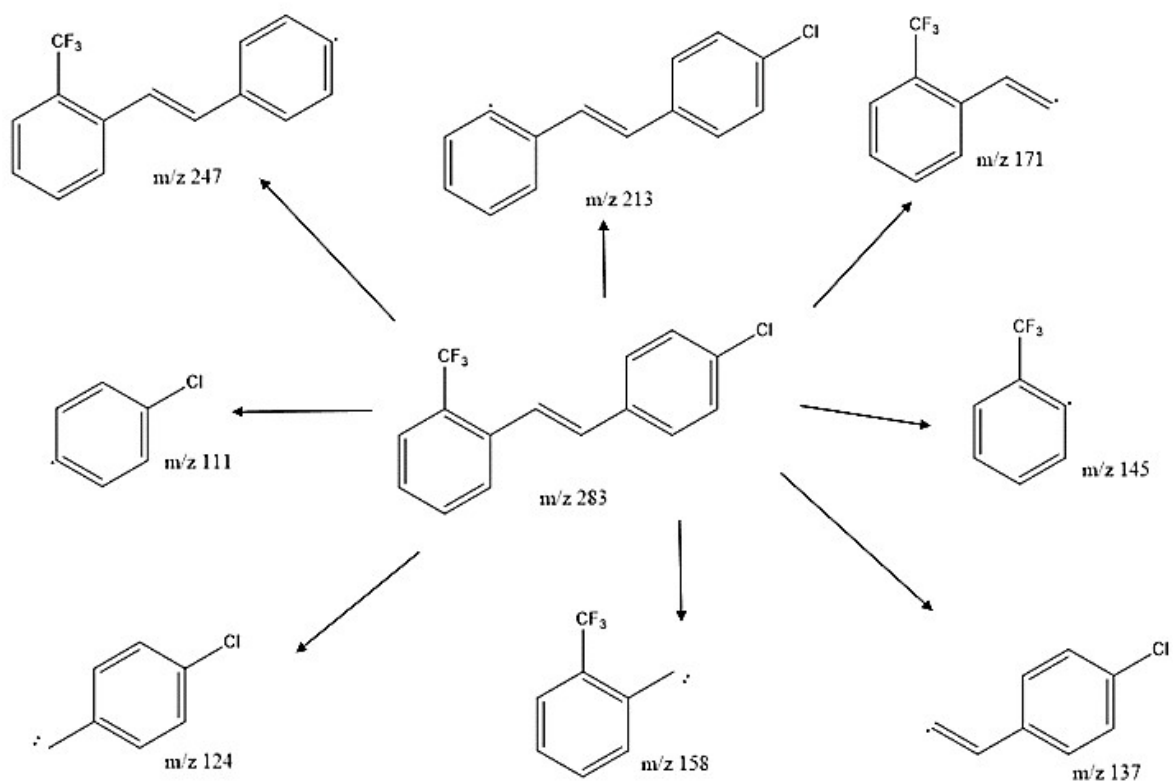


Figure S56. Assigned mass spectral fragments of *(E)*-N-(4-chlorobenzylidene)-2-(trifluoromethyl)aniline (**25**)

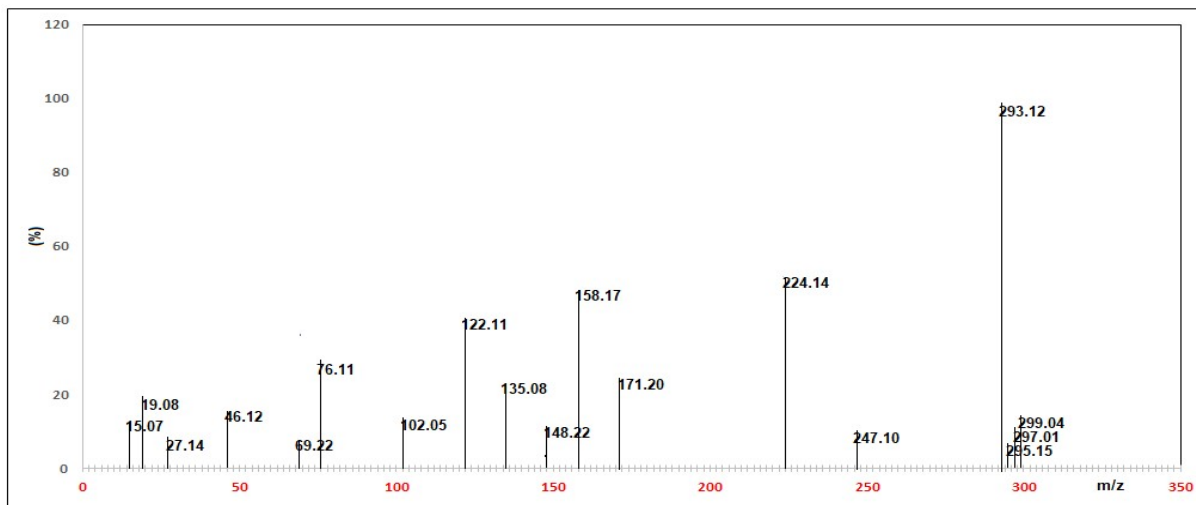


Figure S57. Mass spectrum of (*E*)-N-(3-nitrobenzylidene)-2-(trifluoromethyl)aniline (**26**)

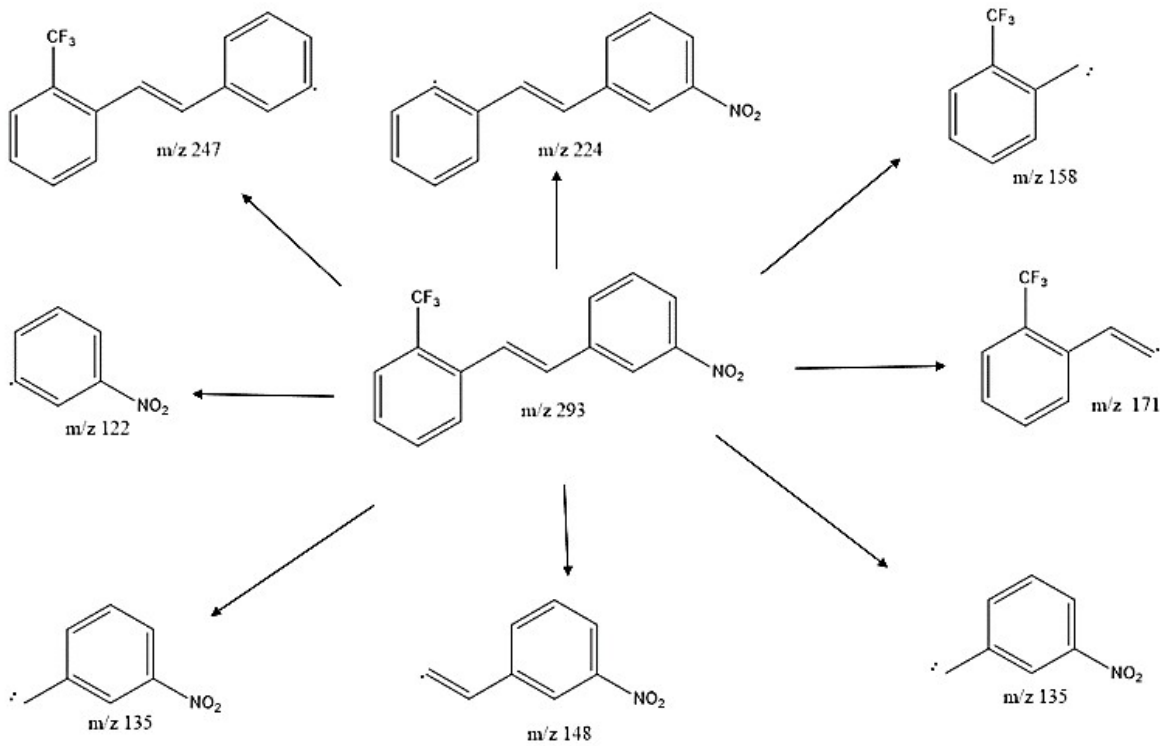


Figure S58. Assigned mass spectral fragments of (E) -N-(3-nitrobenzylidene)-2-(trifluoromethyl)aniline (**26**)

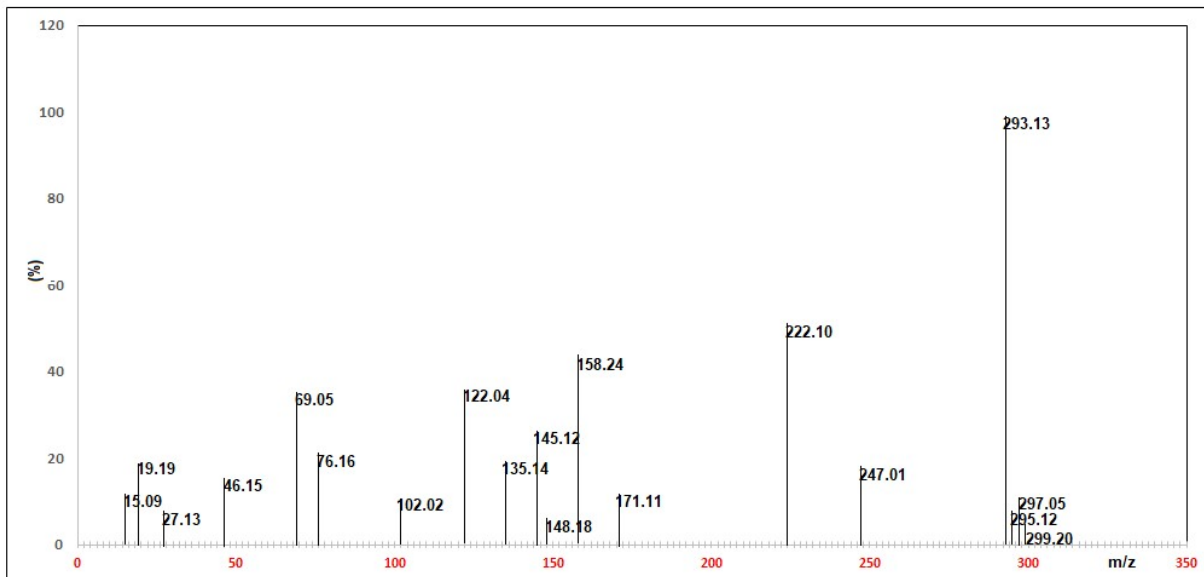


Figure S59. Mass spectrum of (*E*)-N-(4-nitrobenzylidene)-2-(trifluoromethyl)aniline (**27**)

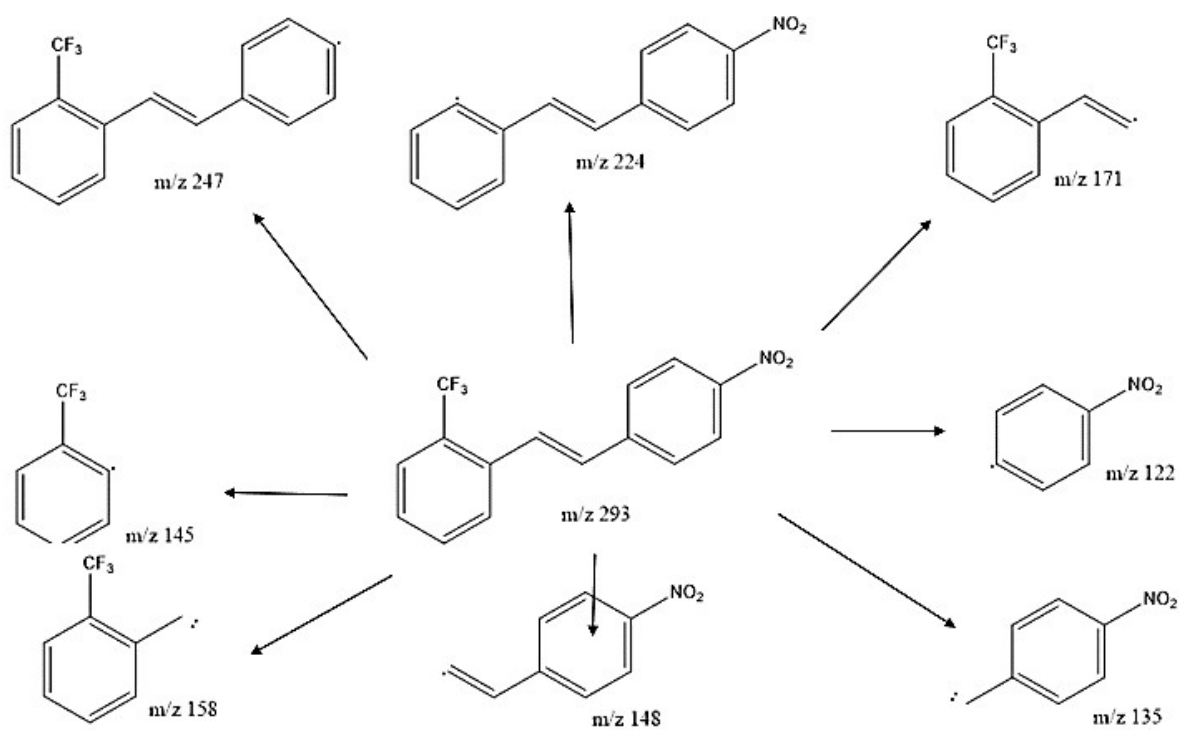


Figure S60. Assigned mass spectral fragments of (*E*)-N-(4-nitrobenzylidene)-2-(trifluoromethyl)aniline (**27**)

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

● **Alert level C**

PLAT242_ALERT_2_C	Low	'MainMol' Ueq as Compared to Neighbors of	N2_2	Check
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...		-11.404	Report
PLAT905_ALERT_3_C	Negative K value in the Analysis of Variance ...		-0.930	Report
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L=	0.600		5 Report
	2 0 0, 0 2 0, -2 -1 1, 2 1 4, 4 3 6,			

● **Alert level G**

PLAT154_ALERT_1_G	The s.u.'s on the Cell Angles are Equal ..(Note)		0.004	Degree
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C14_1	Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of		C14_2	Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .			Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).		1	Note
	0 0 1,			
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L=	0.600	55	Note
PLAT913_ALERT_3_G	Missing # of Very Strong Reflections in FCF		1	Note
	2 0 0,			
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File		2	Note
	2 1 4, -2 -1 1,			
PLAT965_ALERT_2_G	The SHELXL WEIGHT Optimisation has not Converged			Please Check
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value		4.842	Note
	Predicted wR2: Based on SigI**2 3.82 or SHELX Weight 18.13			
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.		2	Info

- 0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
4 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
11 **ALERT level G** = General information/check it is not something unexpected

- 2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
6 ALERT type 2 Indicator that the structure model may be wrong or deficient
5 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check
-
-

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

