

Supporting Information

A novel catalyst-free reaction in water: Synthesis of benzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one derivatives

Junhua Liu ^a, Min Lei ^{b,*}, Lihong Hu ^{a,b,*}

^a *School of Pharmacy, East China University of Science and Technology, 130
Meilong Road, Shanghai 200237, P. R. China*

^b *Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai
201203, P. R. China*

^{*} *To whom correspondence should be addressed. Phone: +86-21-20231965; fax:
+86-21-20231965; E-mail addresses: mlei@mail.shcnc.ac.cn (Lei M.);
simmhulh@mail.shcnc.ac.cn (Hu L.)*

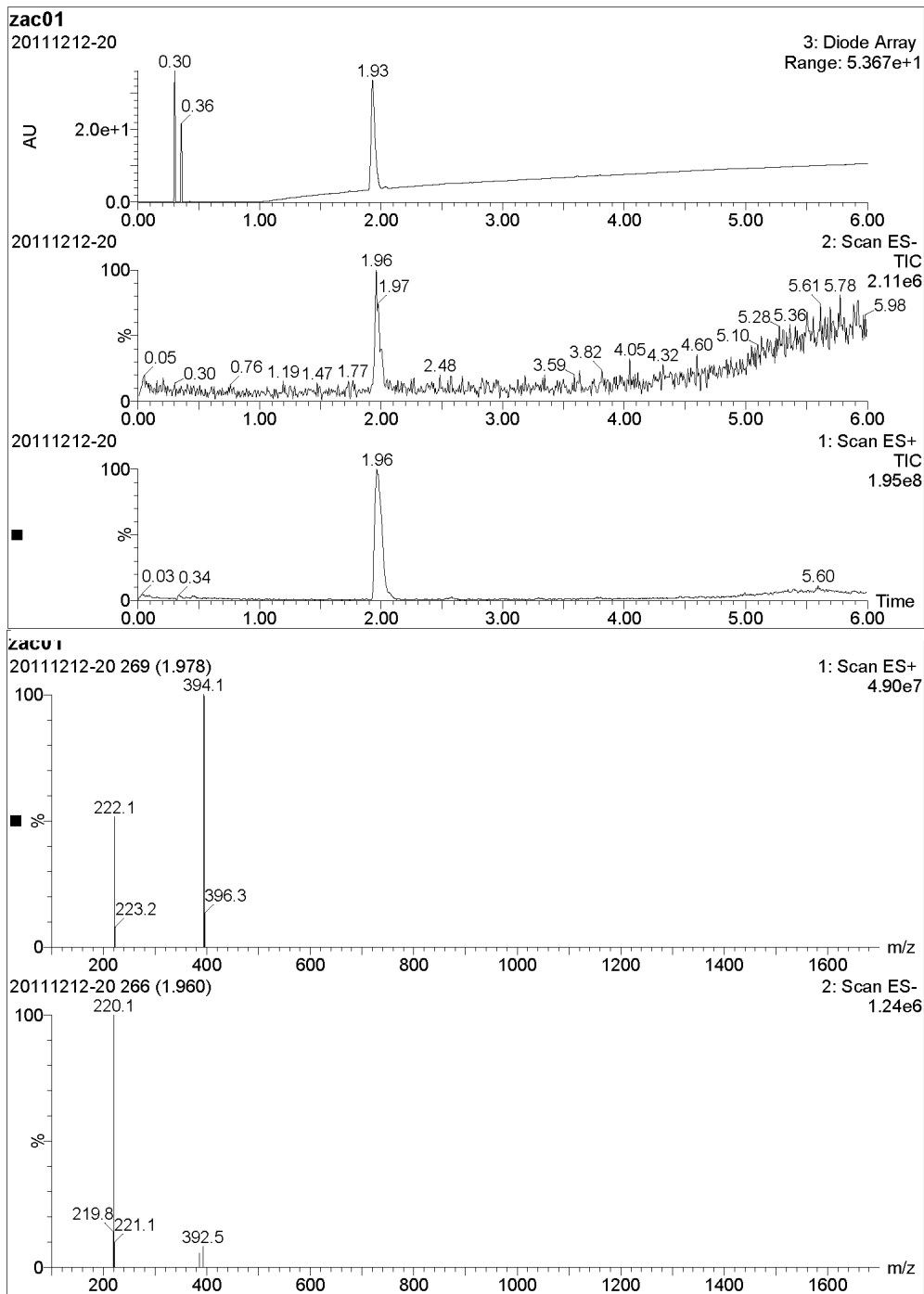
S1.	LCMS	spectrum	of	
2,5-diphenyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4a).6				
S2.	¹ H	NMR	spectrum	of
2,5-diphenyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4a)				
in DMSO- <i>d</i> ₆ 7				
S3.	¹³ C	NMR	spectrum	of
2,5-diphenyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4a)				
in DMSO- <i>d</i> ₆ 8				
S4.	LCMS	spectrum	of	
2,5-bis(4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4b)..... 9				
S5.	¹ H	NMR	spectrum	of
2,5-bis(4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4b) in DMSO- <i>d</i> ₆ 10				
S6.	¹³ C	NMR	spectrum	of
2,5-bis(4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4b) in DMSO- <i>d</i> ₆ 11				
S7.	LCMS	spectrum	of	
2,5-di- <i>p</i> -tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4c). 12				
S8.	¹ H	NMR	spectrum	of
2,5-di- <i>p</i> -tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4c) in DMSO- <i>d</i> ₆ 13				
S9.	¹³ C	NMR	spectrum	of
2,5-di- <i>p</i> -tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4c) in DMSO- <i>d</i> ₆ 14				
S10.	LCMS	spectrum	of	
2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4d). 15				
S11.	¹ H	NMR	spectrum	of
2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4d) in DMSO- <i>d</i> ₆ 16				
S12.	¹³ C	NMR	spectrum	of
2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4d) in DMSO- <i>d</i> ₆ 17				

S13.	HSQC	spectrum	of	2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4d) in DMSO- <i>d</i> ₆	18	
S14.	HMBC	spectrum	of	2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4d) in DMSO- <i>d</i> ₆	19	
S15.	ROESY	spectrum	of	2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4d) in DMSO- <i>d</i> ₆	20	
S16.	LCMS	spectrum	of	4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidine-2,5-diyl)dibenzonitrile (4e).	21	
S17.	¹ H	NMR	spectrum	of	4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidine-2,5-diyl)dibenzonitrile (4e) in DMSO- <i>d</i> ₆	22
S18.	¹³ C	NMR	spectrum	of	4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidine-2,5-diyl)dibenzonitrile (4e) in DMSO- <i>d</i> ₆	23
S19.	LCMS	spectrum	of	dimethyl 4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidine-2,5-diyl)dibenzozoate (4f).....	24	
S20.	¹ H	NMR	spectrum	of	dimethyl 4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidine-2,5-diyl)dibenzozoate (4f) in DMSO- <i>d</i> ₆	25
S21.	¹³ C	NMR	spectrum	of	dimethyl 4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidine-2,5-diyl)dibenzozoate (4f) in DMSO- <i>d</i> ₆	26
S22.	LCMS	spectrum	of	2,5-bis(4-fluorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4g).	27	
S23.	¹ H	NMR	spectrum	of	2,5-bis(4-fluorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4g) in DMSO- <i>d</i> ₆	28
S24.	¹³ C	NMR	spectrum	of	2,5-bis(4-fluorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4g) in DMSO- <i>d</i> ₆	29

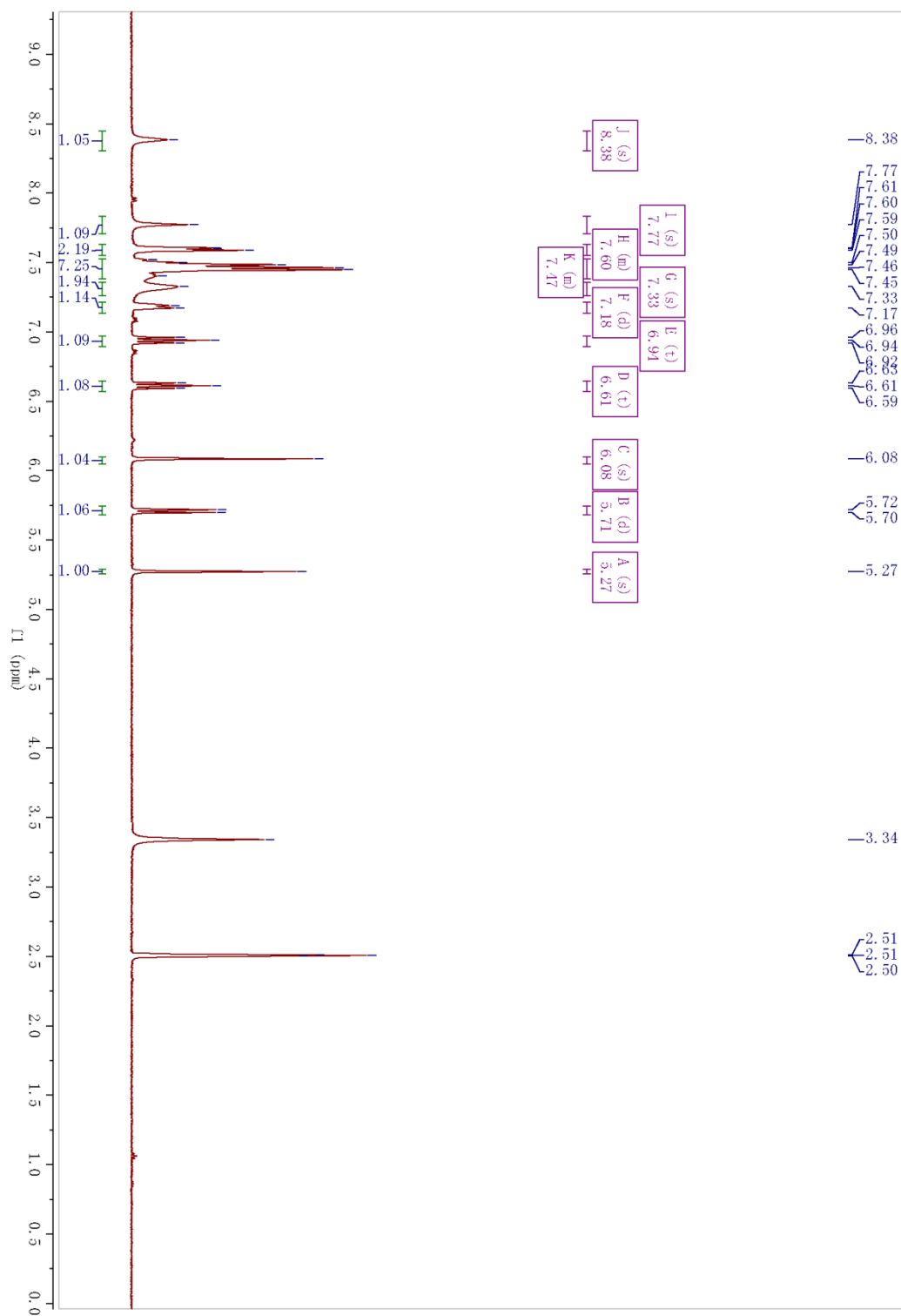
S25.	LCMS	spectrum	of
2,5-bis(4-(trifluoromethyl)phenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4h).			
			30
S26.	¹ H	NMR	spectrum of
2,5-bis(4-(trifluoromethyl)phenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4h) in DMSO- <i>d</i> ₆			
			31
S27.	¹³ C	NMR	spectrum of
2,5-bis(4-(trifluoromethyl)phenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4h) in DMSO- <i>d</i> ₆			
			32
S28.	LCMS	spectrum	of
2,5-bis(3-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4i).			
			33
S29.	¹ H	NMR	spectrum of
2,5-bis(3-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4i) in DMSO- <i>d</i> ₆			
			34
S30.	¹³ C	NMR	spectrum of
2,5-bis(3-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4i) in DMSO- <i>d</i> ₆			
			35
S31.	LCMS	spectrum	of
2,5-di- <i>m</i> -tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4j).			
			36
S32.	¹ H	NMR	spectrum of
2,5-di- <i>m</i> -tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4j) in DMSO- <i>d</i> ₆			
			37
S33.	¹³ C	NMR	spectrum of
2,5-di- <i>m</i> -tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4j) in DMSO- <i>d</i> ₆			
			38
S34.	LCMS	spectrum	of
2,5-di(pyridin-4-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4n).			
			39
S35.	¹ H	NMR	spectrum of
2,5-di(pyridin-4-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4n) in DMSO- <i>d</i> ₆			
			40
S36.	¹³ C	NMR	spectrum of
2,5-di(pyridin-4-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4n) in DMSO- <i>d</i> ₆			
			41

S37.	LCMS	spectrum	of	
2,5-di(pyridin-3-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4o).				
				42
S38.	¹ H	NMR	spectrum	of
2,5-di(pyridin-3-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4o) in DMSO- <i>d</i> ₆				
				43
S39.	¹³ C	NMR	spectrum	of
2,5-di(pyridin-3-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4o) in DMSO- <i>d</i> ₆				
				44
S40.	LCMS	spectrum	of	
2,5-bis(3,4-dimethoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4p).				
				45
S41.	¹ H	NMR	spectrum	of
2,5-bis(3,4-dimethoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4p) in DMSO- <i>d</i> ₆				
				46
S42.	¹³ C	NMR	spectrum	of
2,5-bis(3,4-dimethoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4p) in DMSO- <i>d</i> ₆				
				47
S43.	LCMS	spectrum	of	
2,5-bis(3-hydroxy-4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4q).				
				48
S44.	¹ H	NMR	spectrum	of
2,5-bis(3-hydroxy-4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4q) in DMSO- <i>d</i> ₆				
				49
S45.	¹³ C	NMR	spectrum	of
4-ethyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimidine-3-carboxylate (5q) in DMSO- <i>d</i> ₆				
				50
S46.	LCMS	spectrum	of	
2,5-bis(4-hydroxy-3-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4r).				
				51
S47.	¹ H	NMR	spectrum	of
2,5-bis(4-hydroxy-3-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4r) in DMSO- <i>d</i> ₆				
				52
S48.	¹³ C	NMR	spectrum	of
2,5-bis(4-hydroxy-3-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2- <i>a</i>]pyrimido[4,5- <i>d</i>]pyrimidin-4(1 <i>H</i>)-one (4r) in DMSO- <i>d</i> ₆				
				53

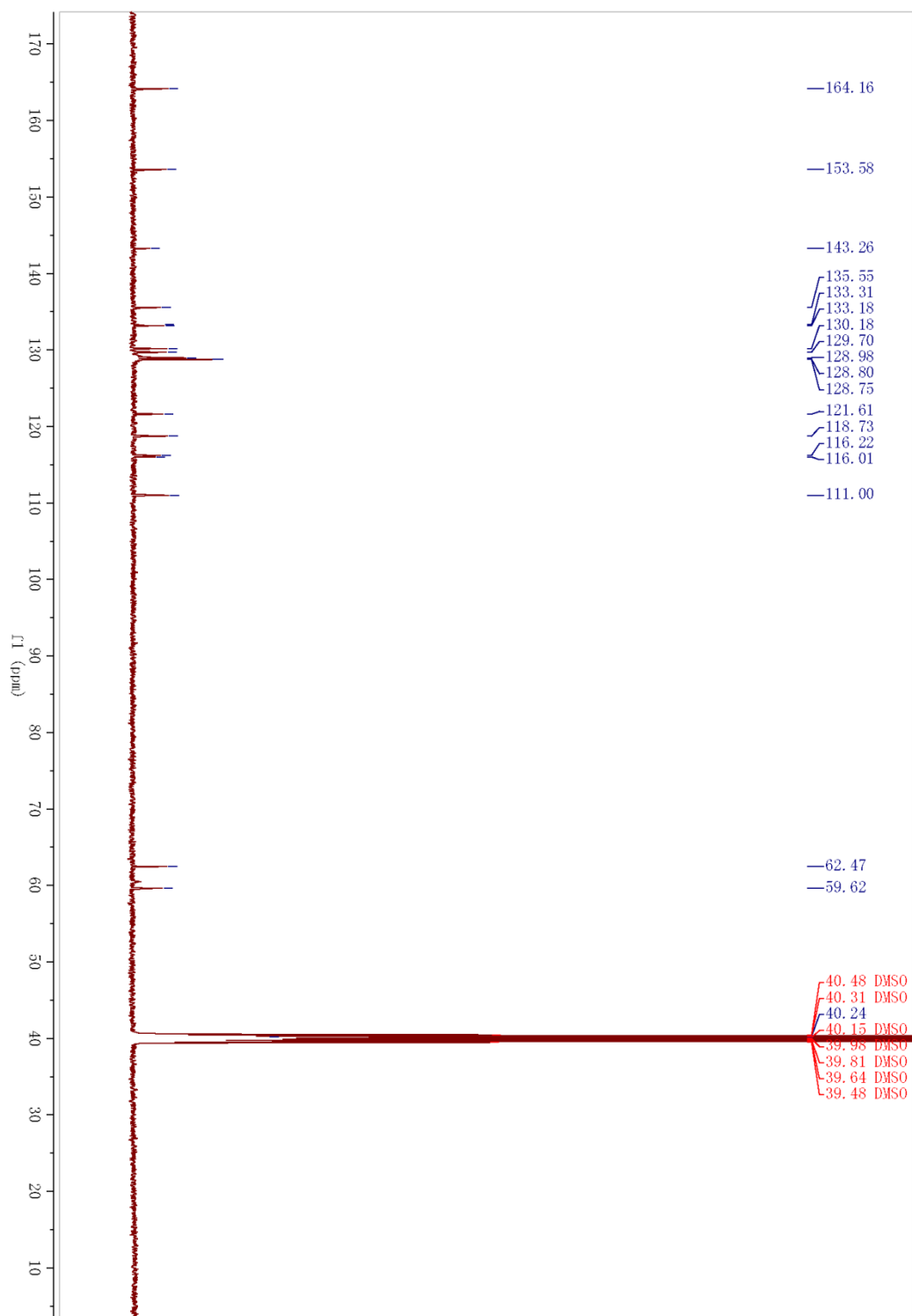
S1. LCMS spectrum of
2,5-diphenyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one
(4a).



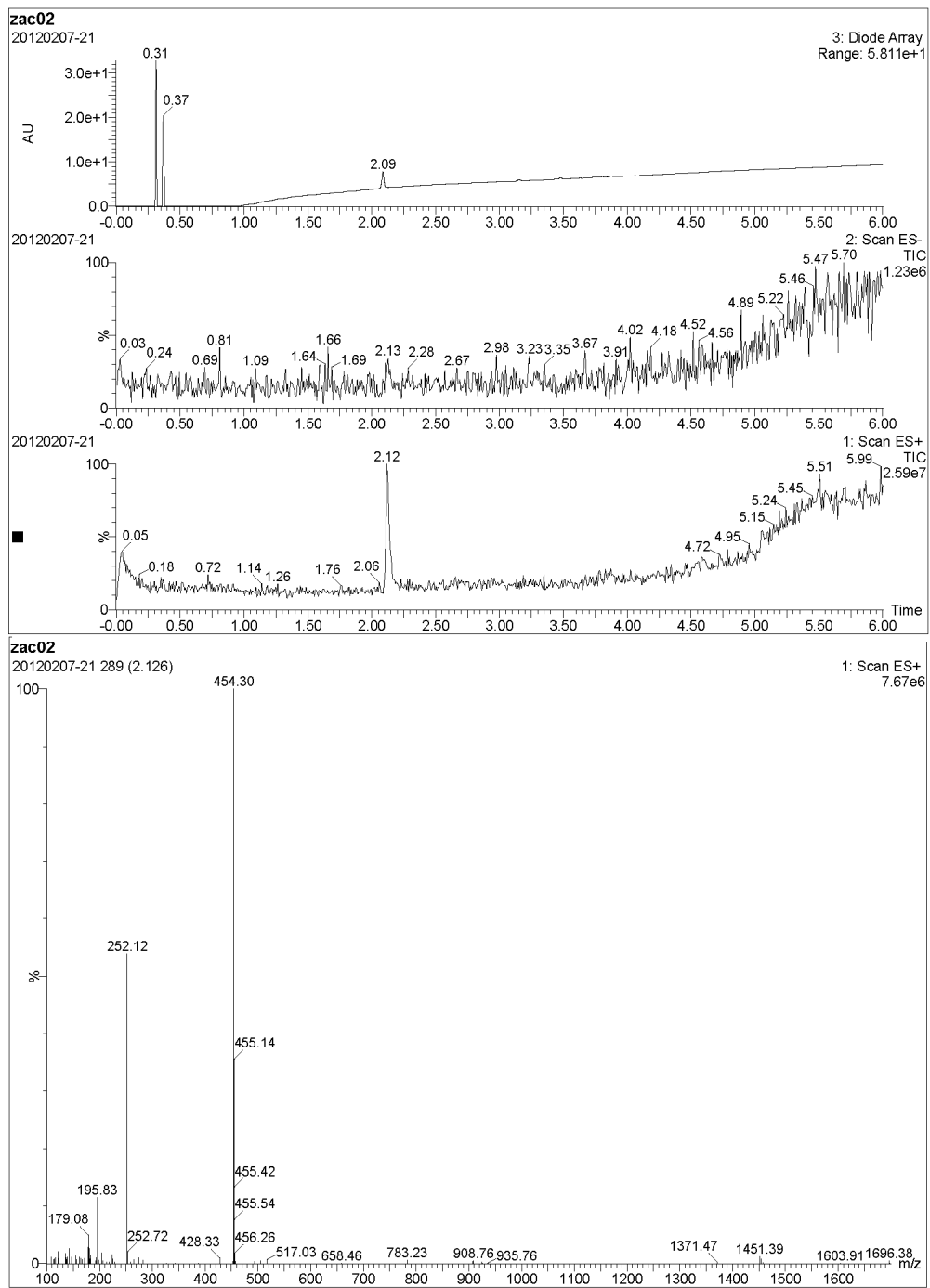
S2. ^1H NMR spectrum of
2,5-diphenyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4
(1*H*)-one (**4a**) in DMSO-*d*₆.



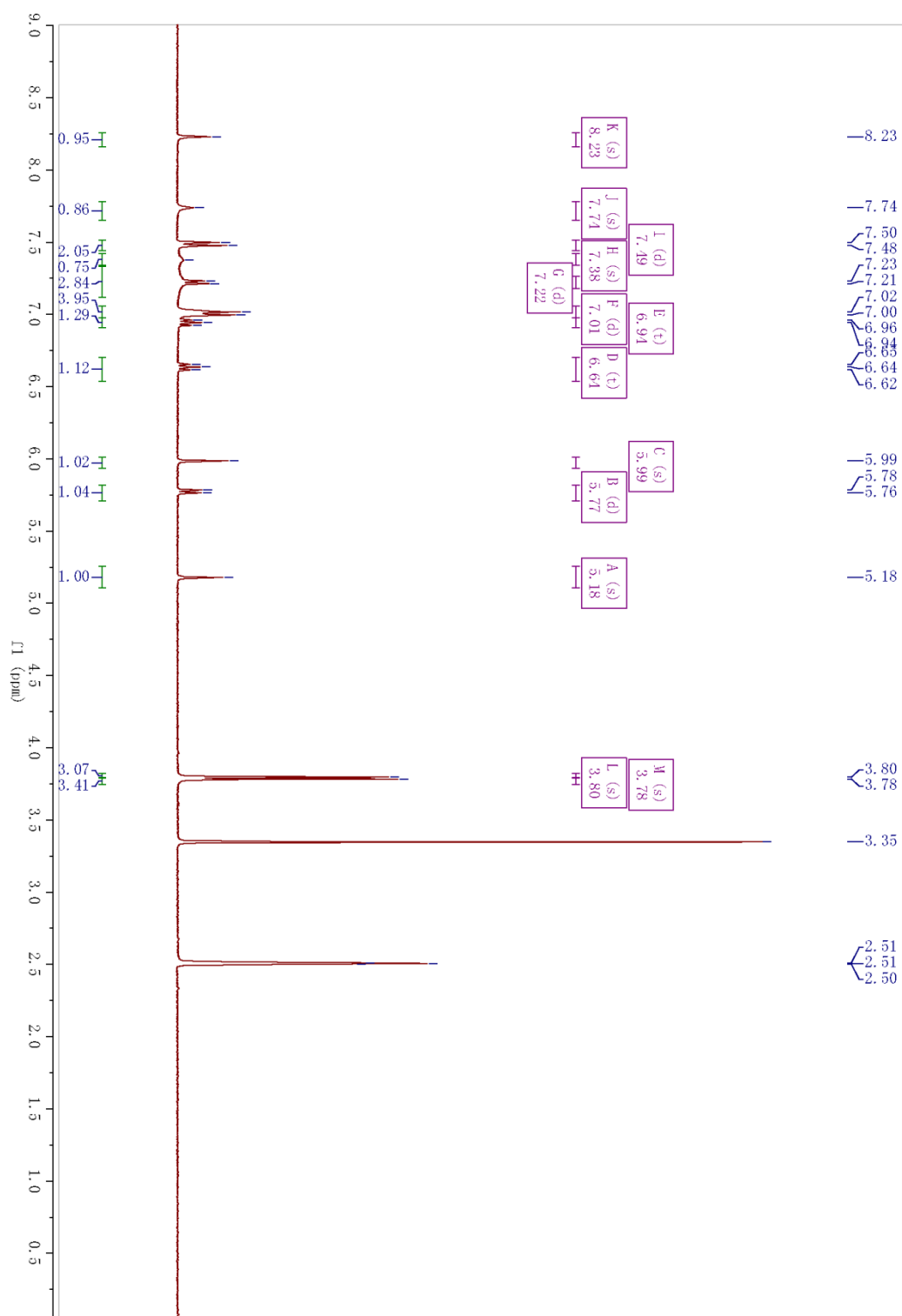
S3. ^{13}C NMR spectrum of
2,5-diphenyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4
(1*H*)-one (**4a**) in DMSO-*d*₆.



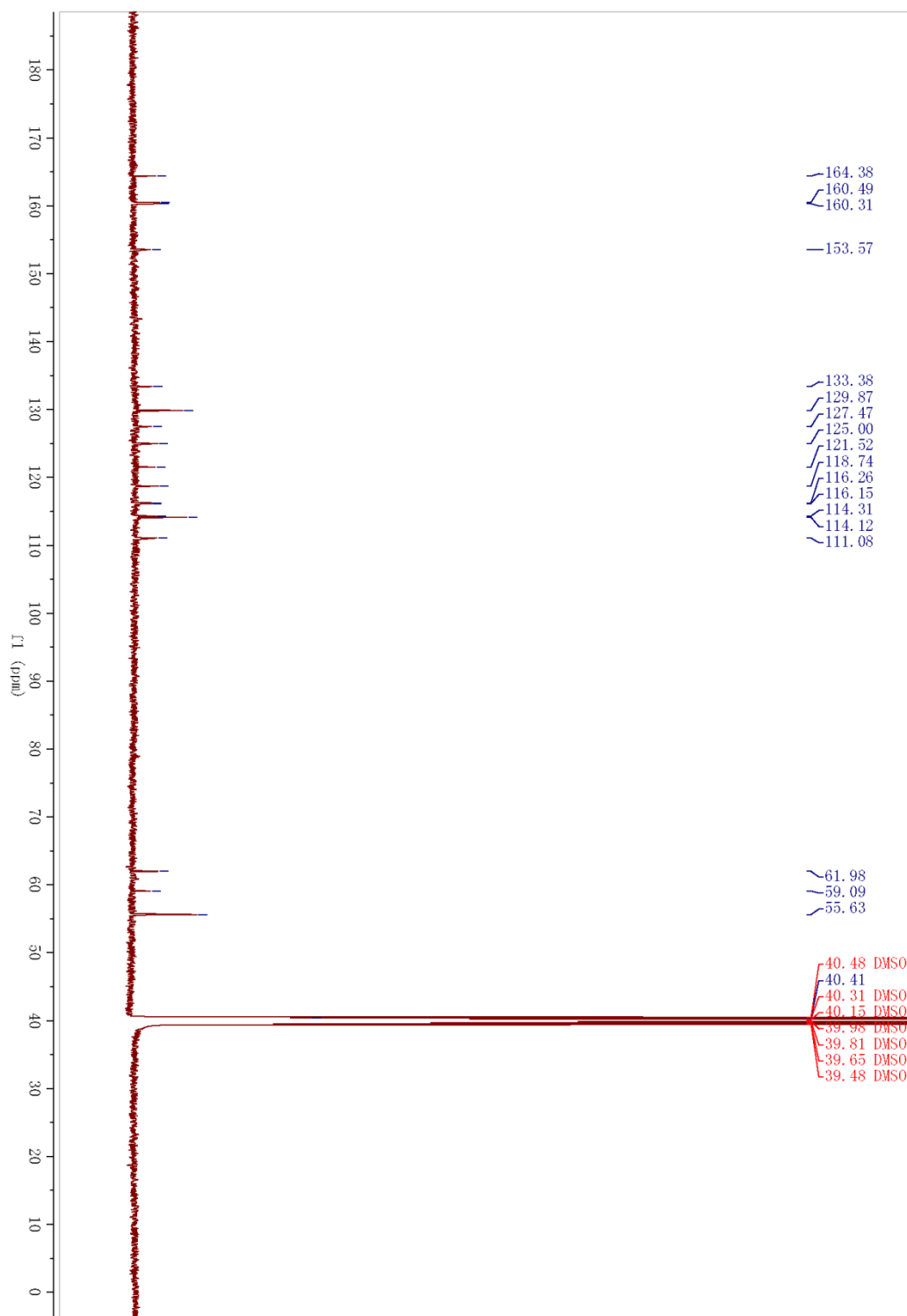
S4. LCMS spectrum of
2,5-bis(4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4b**).



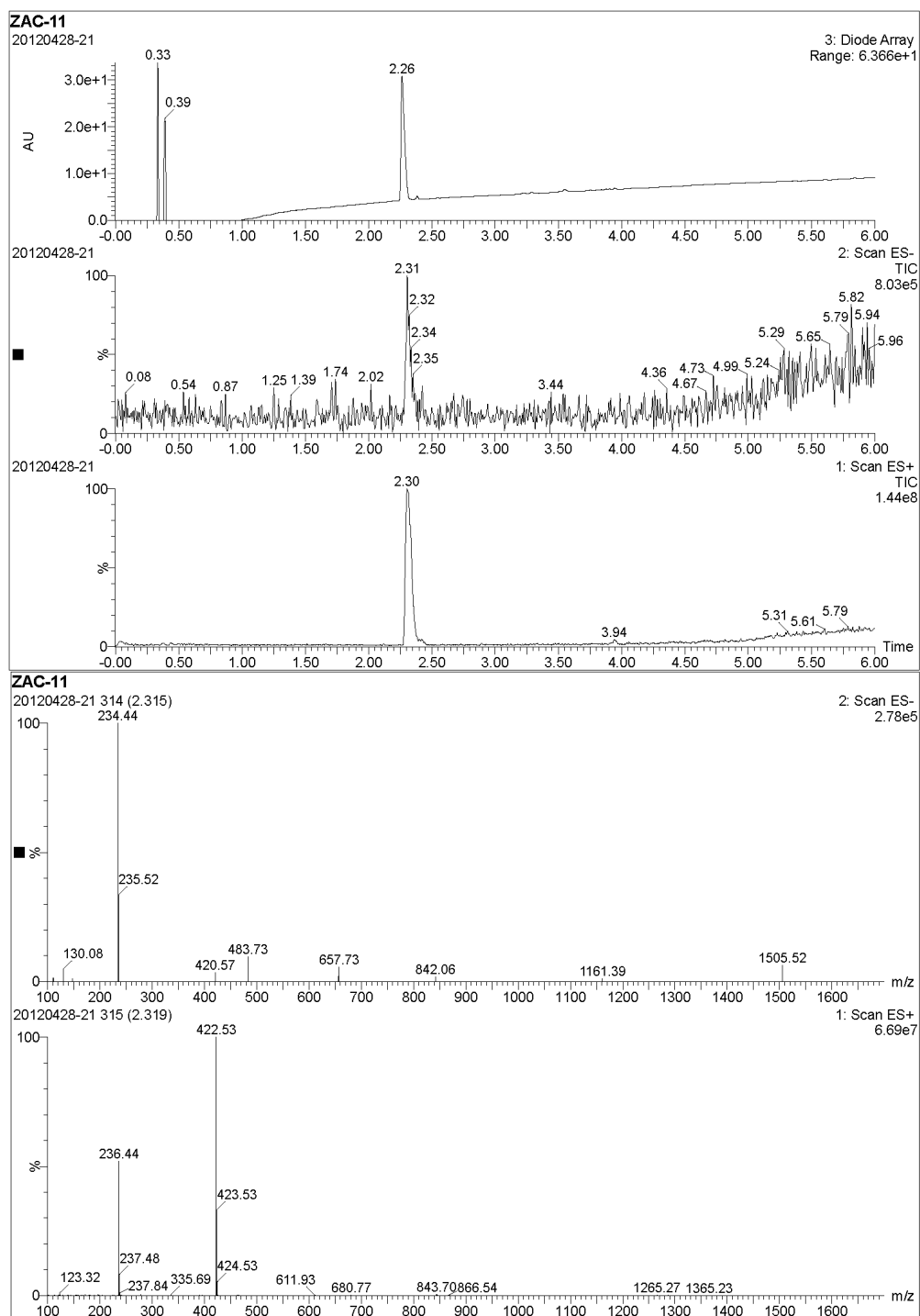
S5. ^1H NMR spectrum of
2,5-bis(4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4b**) in $\text{DMSO-}d_6$.



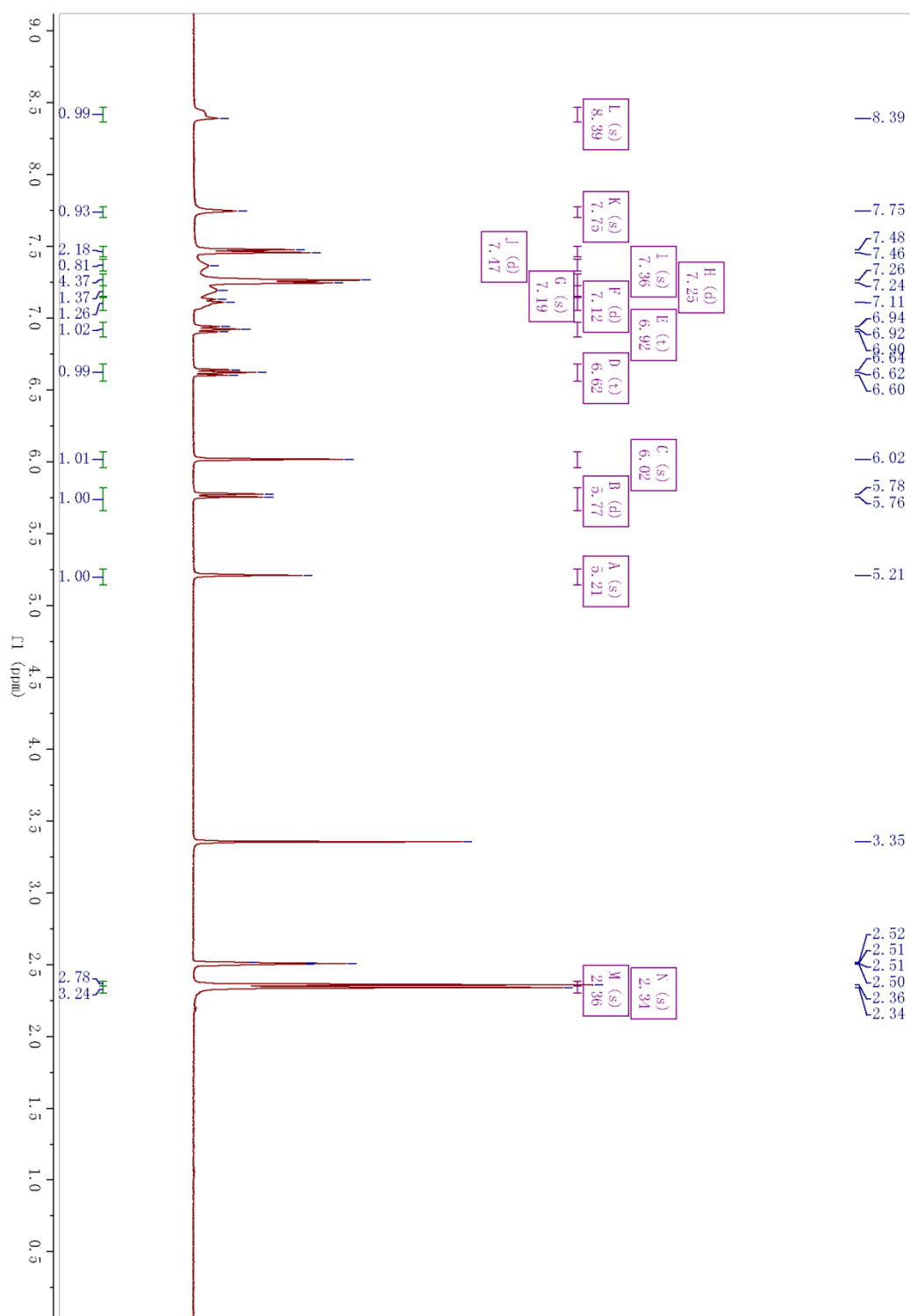
S6. ^{13}C NMR spectrum of
2,5-bis(4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4b**) in DMSO-*d*₆.



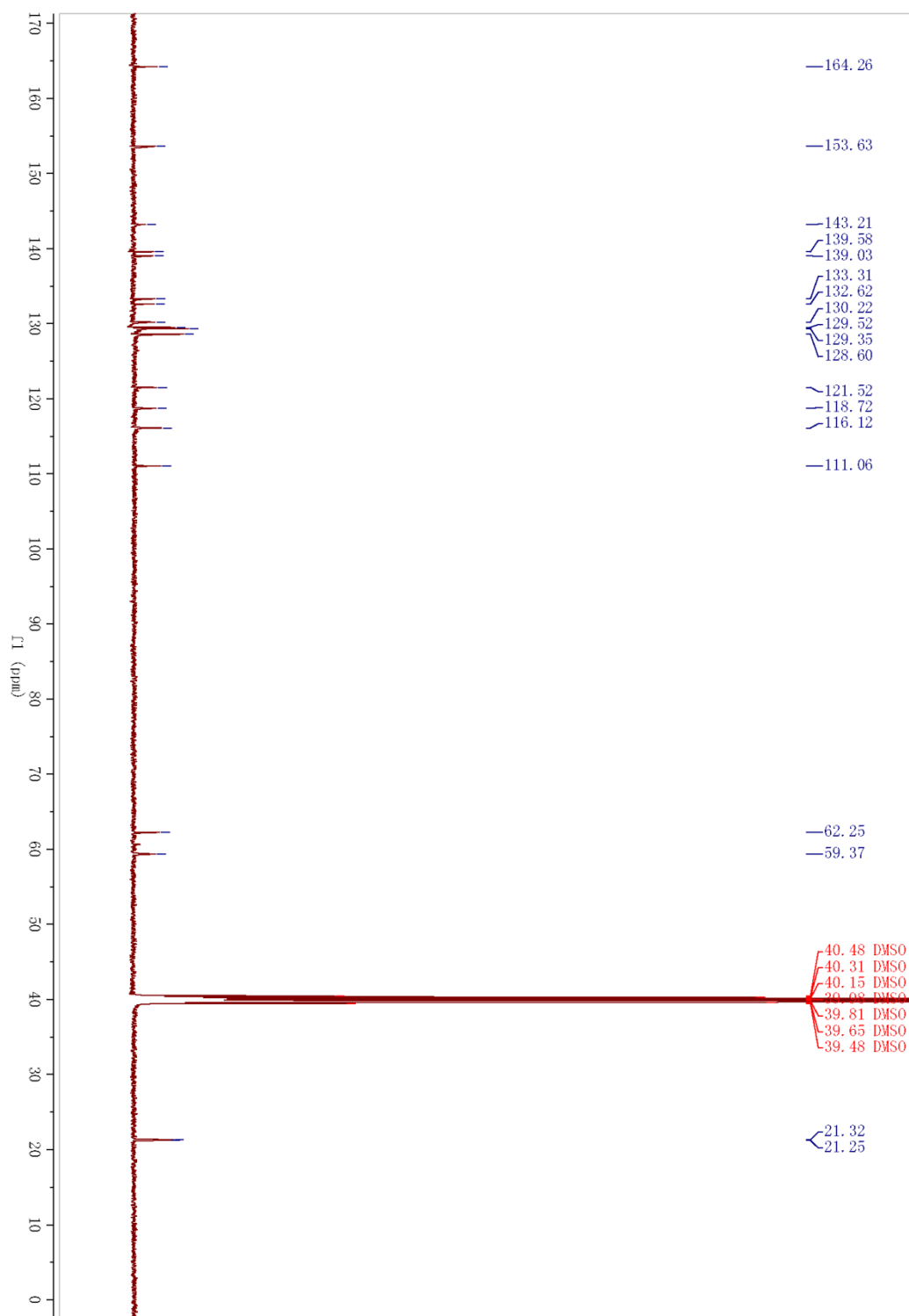
S7. LCMS spectrum of
2,5-di-p-tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-
4(1*H*)-one (**4c**).



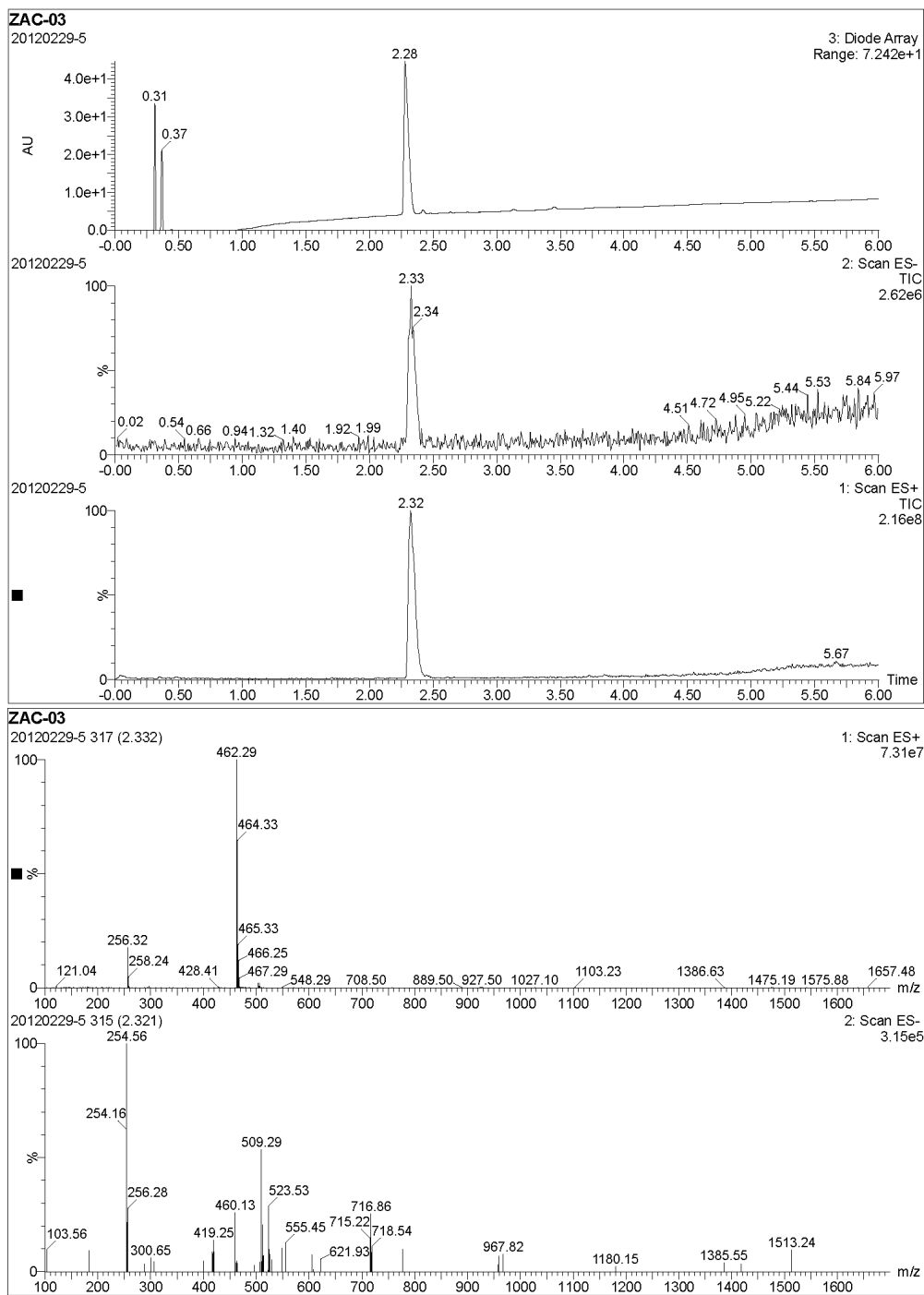
S8. ^1H NMR spectrum of
2,5-di-*p*-tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-
4(1*H*)-one (**4c**) in $\text{DMSO-}d_6$.



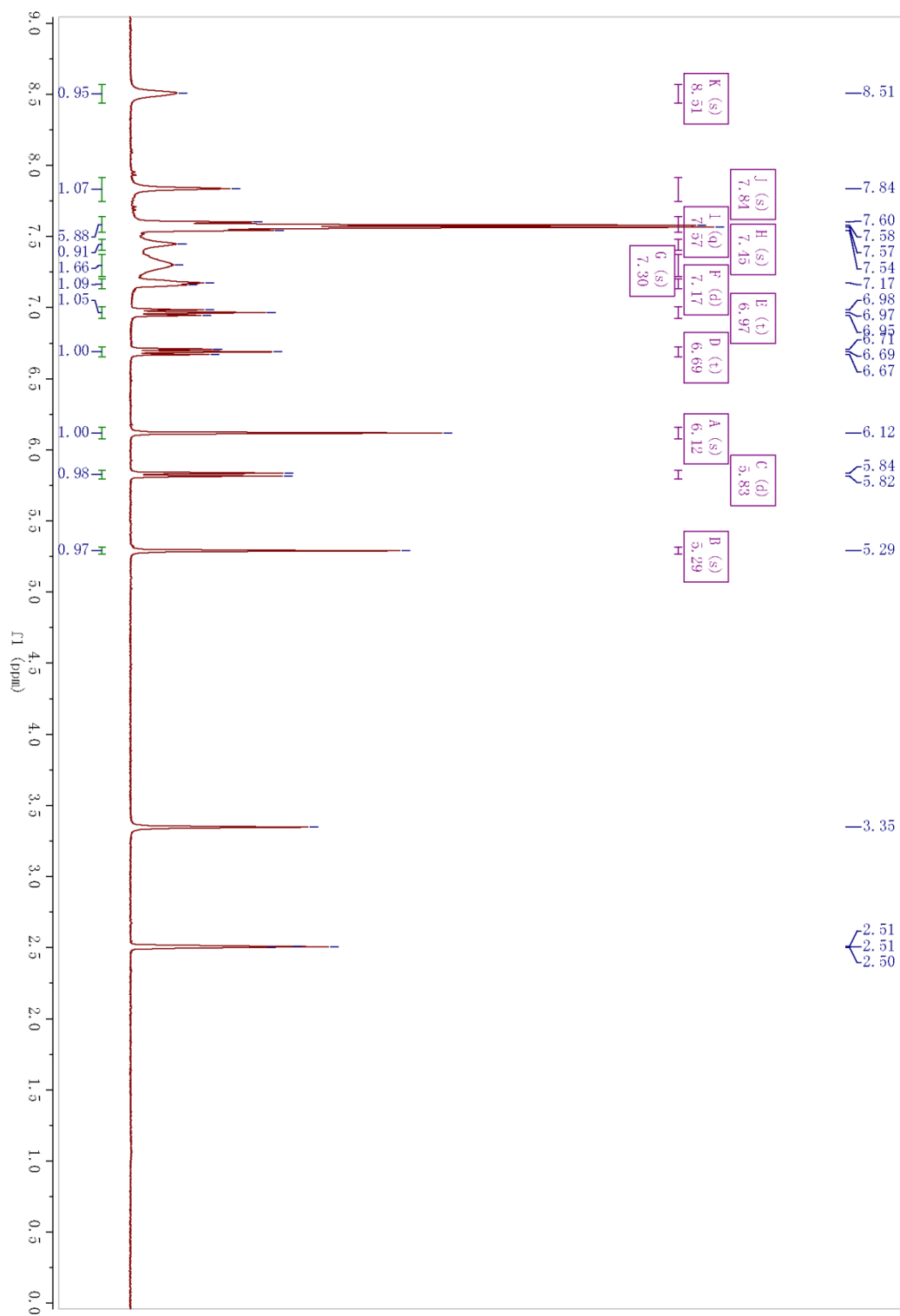
S9. ^{13}C NMR spectrum of
2,5-di-p-tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-
4(1*H*)-one (**4c**) in $\text{DMSO-}d_6$.



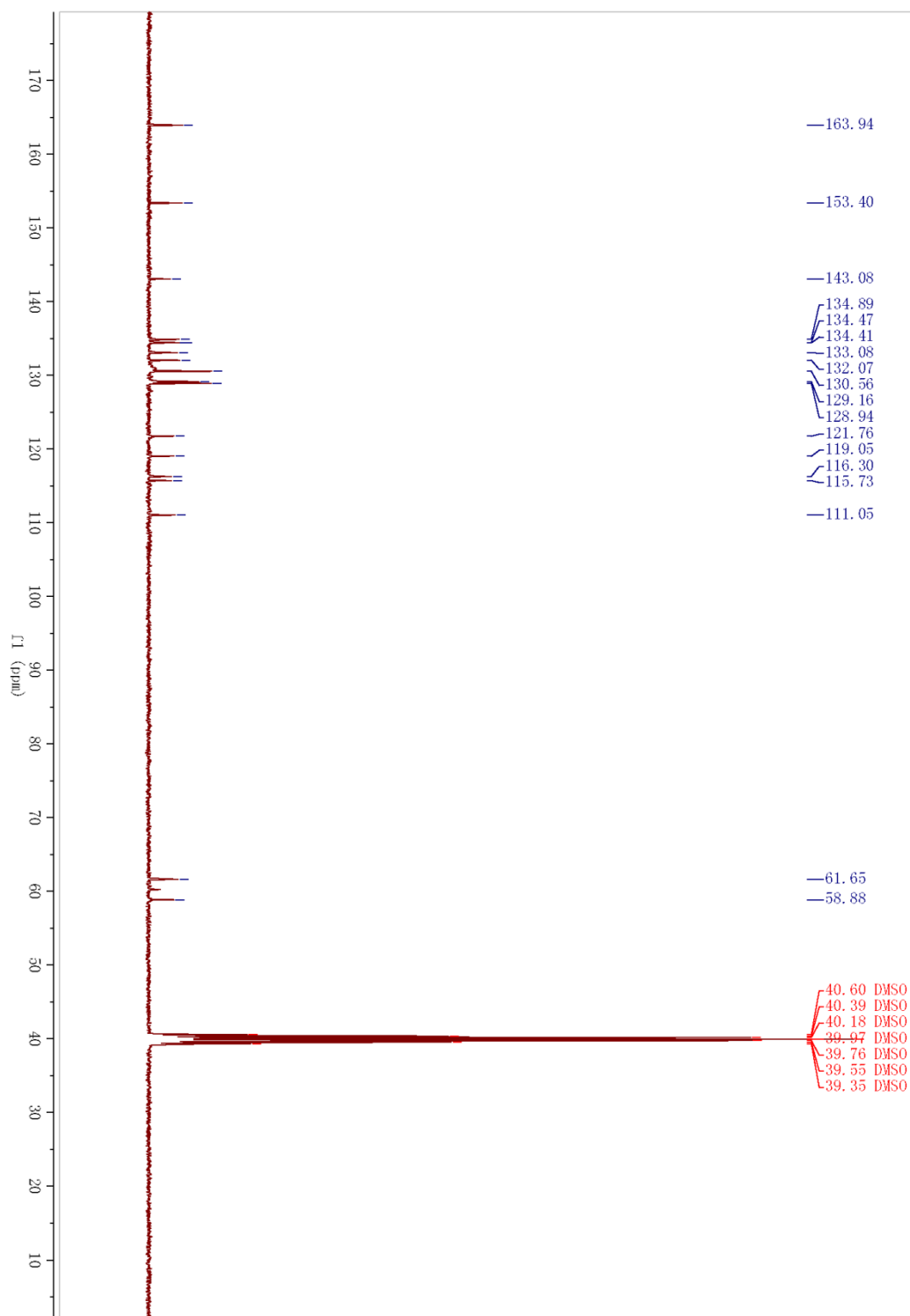
S10. LCMS spectrum of
2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4d**).



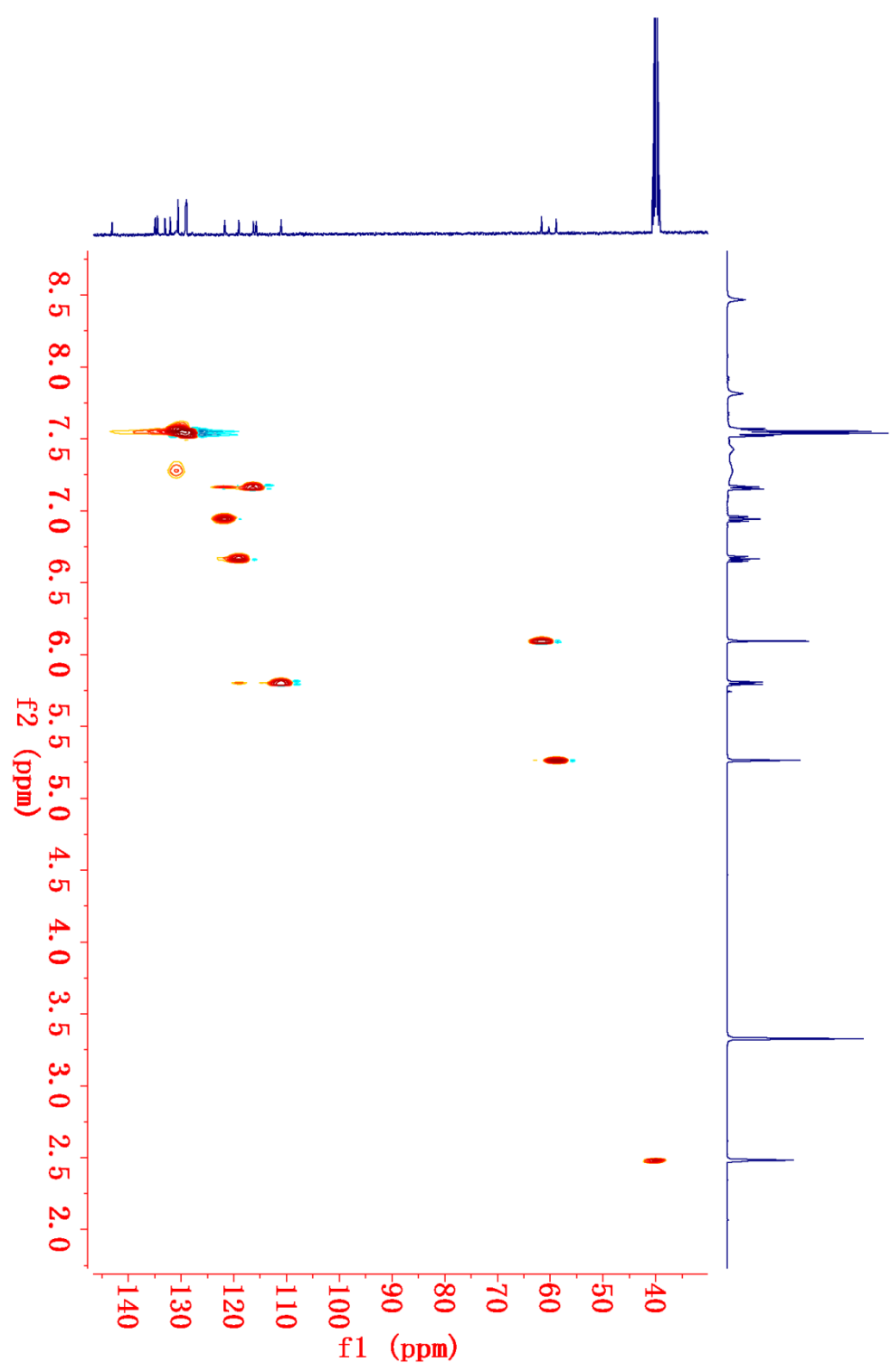
S11. ^1H NMR spectrum of
2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4d**) in $\text{DMSO-}d_6$.



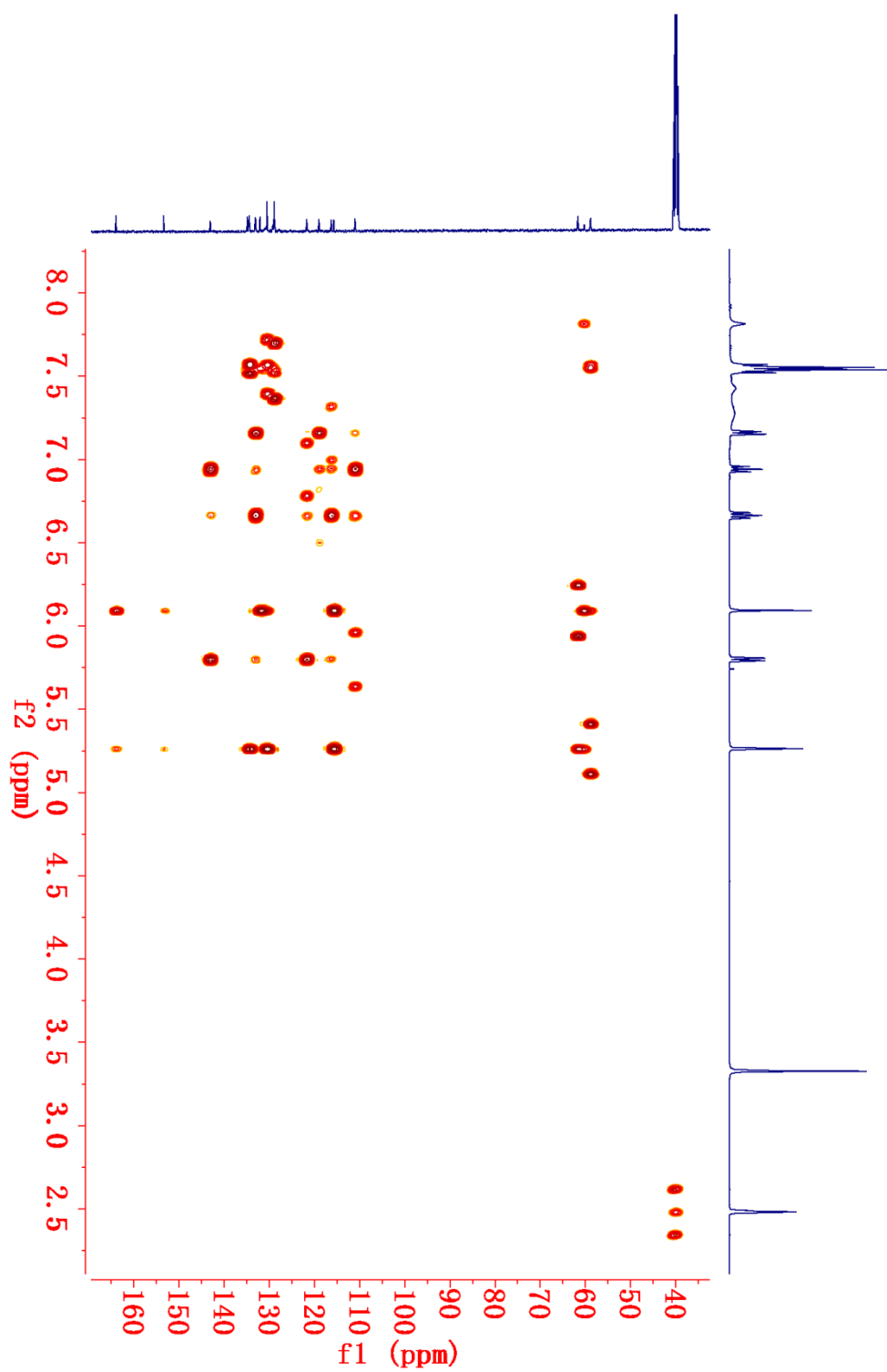
S12. ^{13}C NMR spectrum of
2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4d**) in $\text{DMSO-}d_6$.



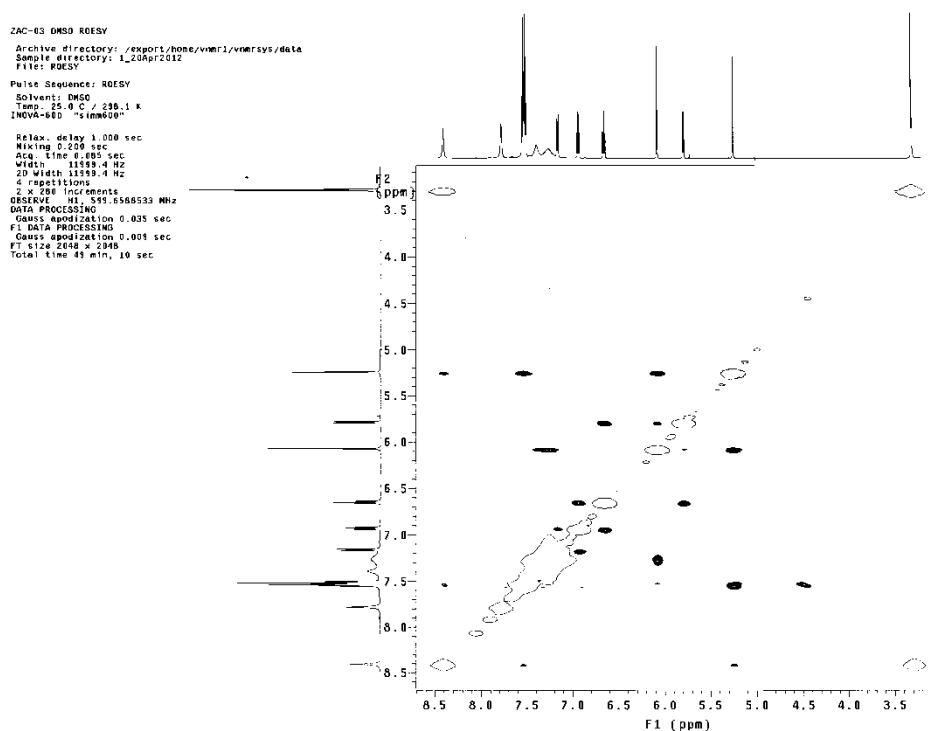
S13. HSQC spectrum of 2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4d**) in DMSO-*d*₆.



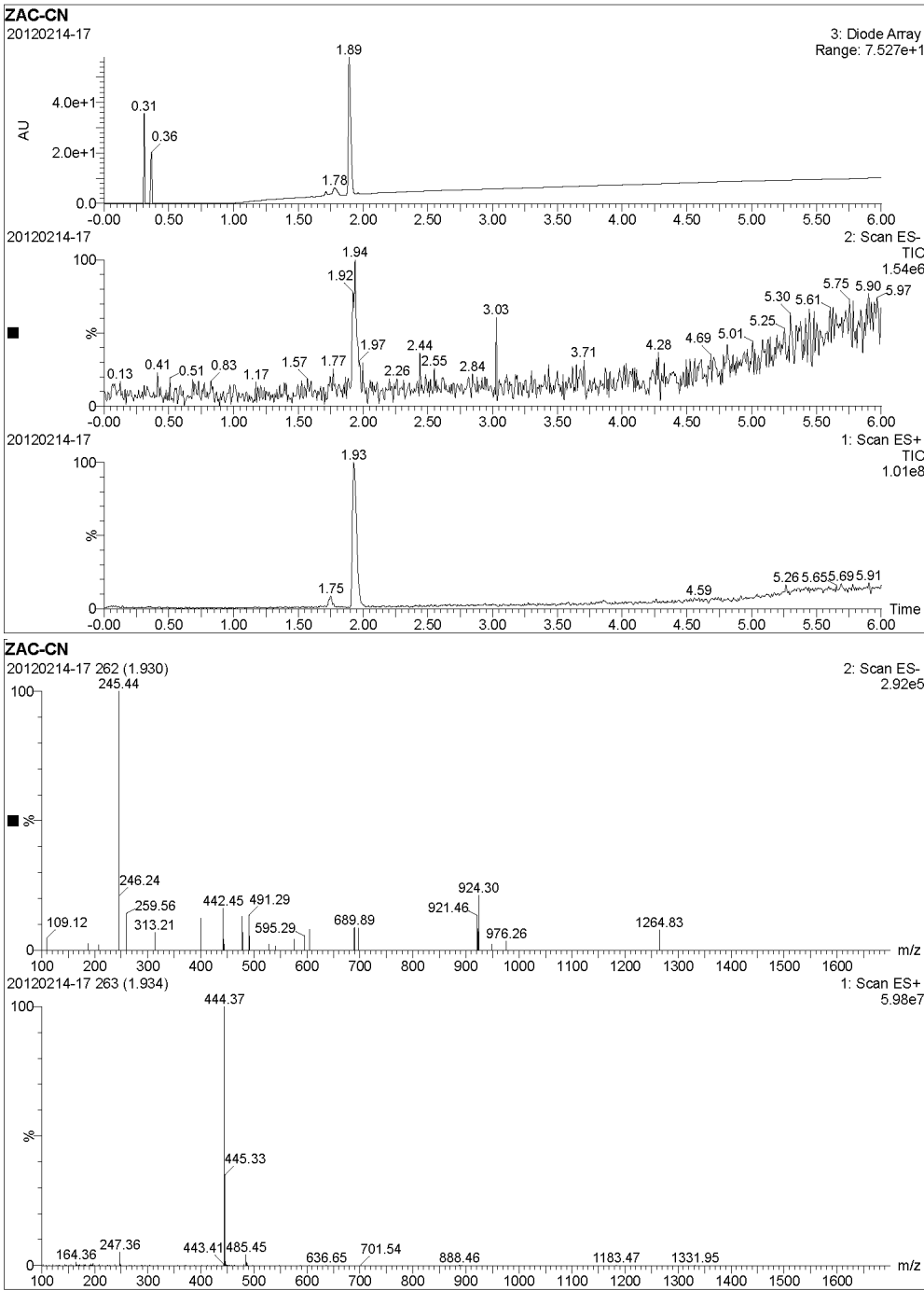
S14. HMBC spectrum of
2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4d**) in DMSO-*d*₆.



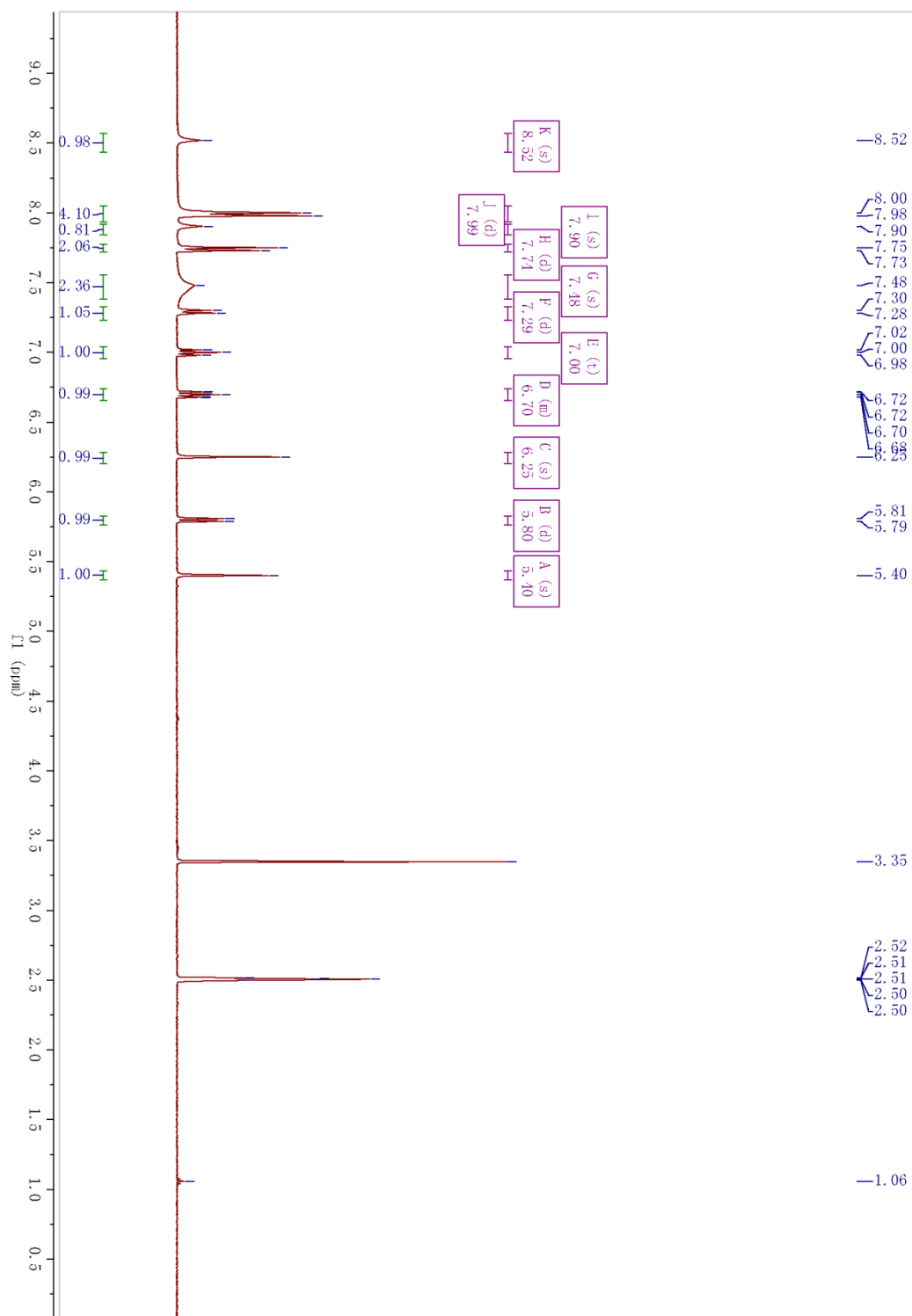
S15. ROESY spectrum of
2,5-bis(4-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4d**) in DMSO-*d*₆.



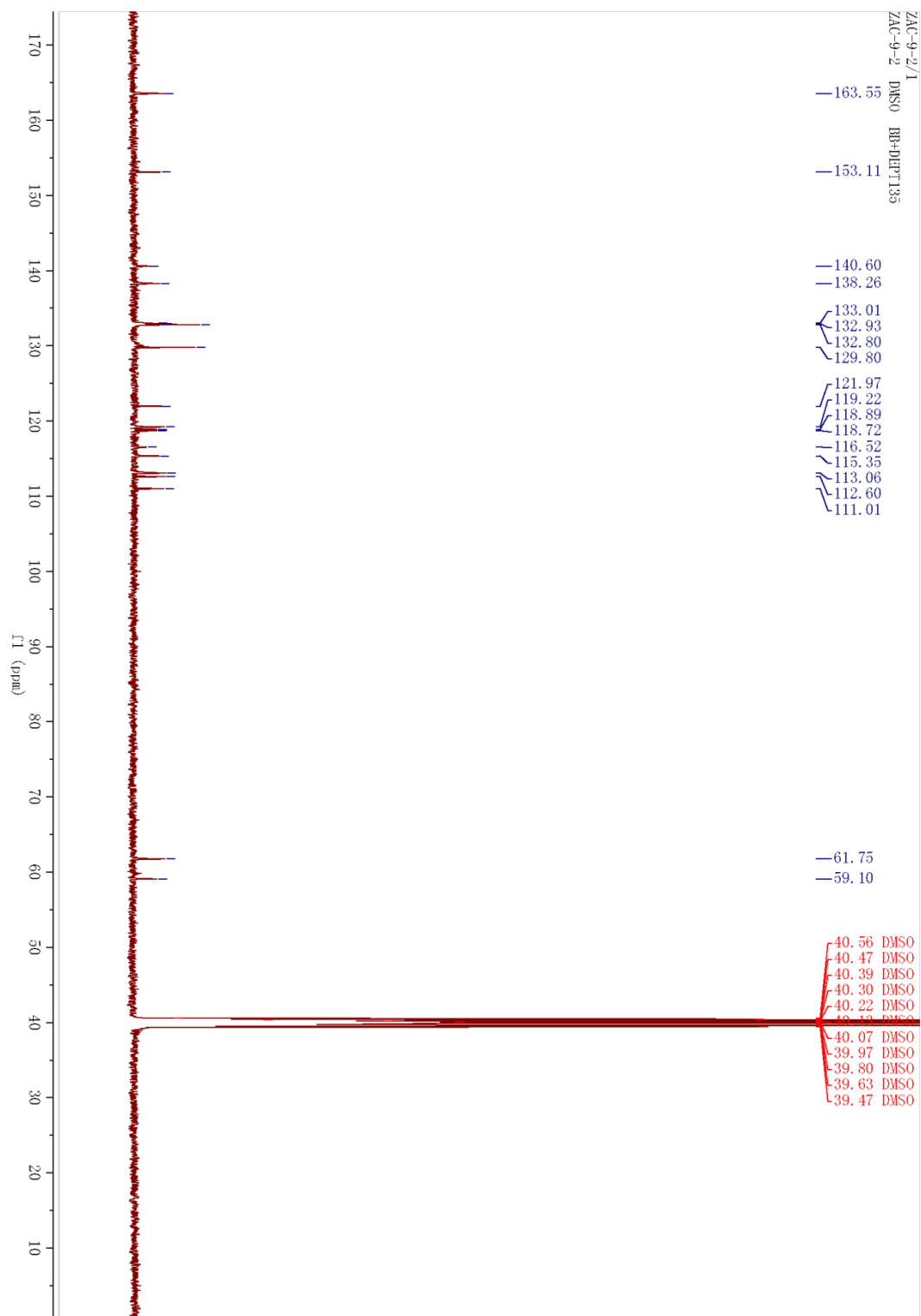
S16. LCMS spectrum of 4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidine-2,5-diyl)dibenzonitrile (**4e**).



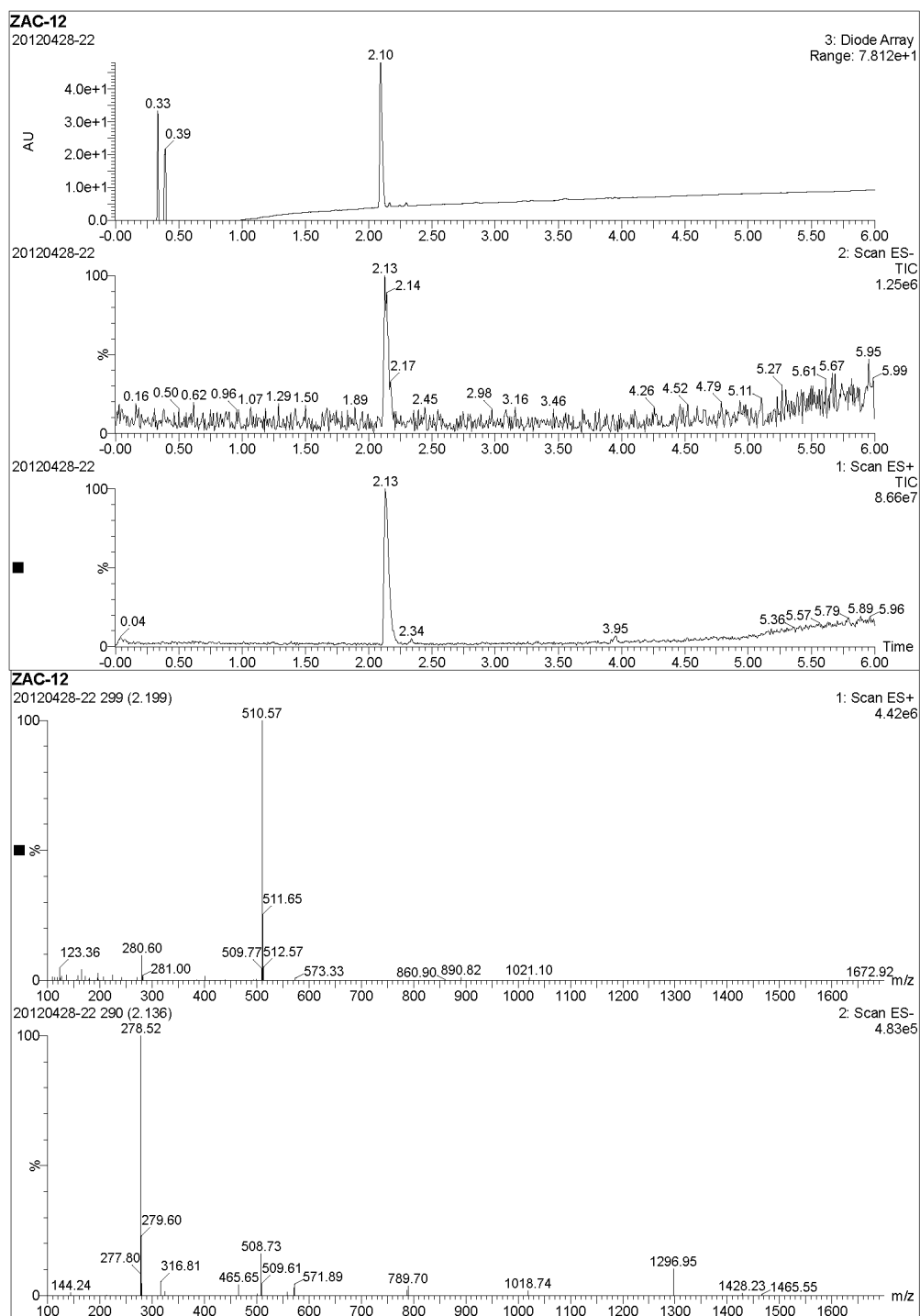
S17. ^1H NMR spectrum of
4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidine-2,5-diyl)dibenzonitrile (**4e**) in $\text{DMSO-}d_6$.



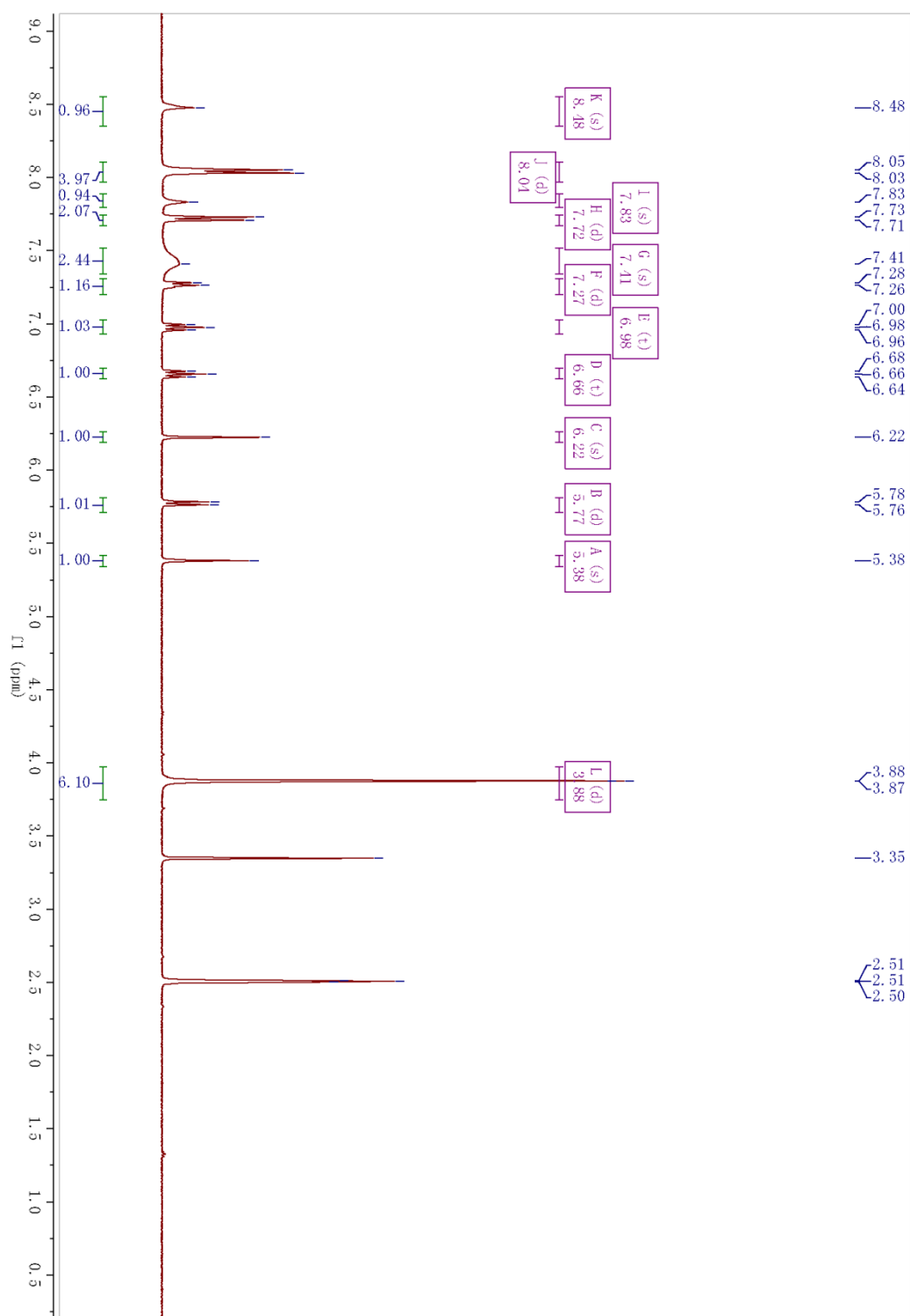
S18. ^{13}C NMR spectrum of
4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-2,5-diyl)dibenzonitrile (**4e**) in $\text{DMSO}-d_6$.



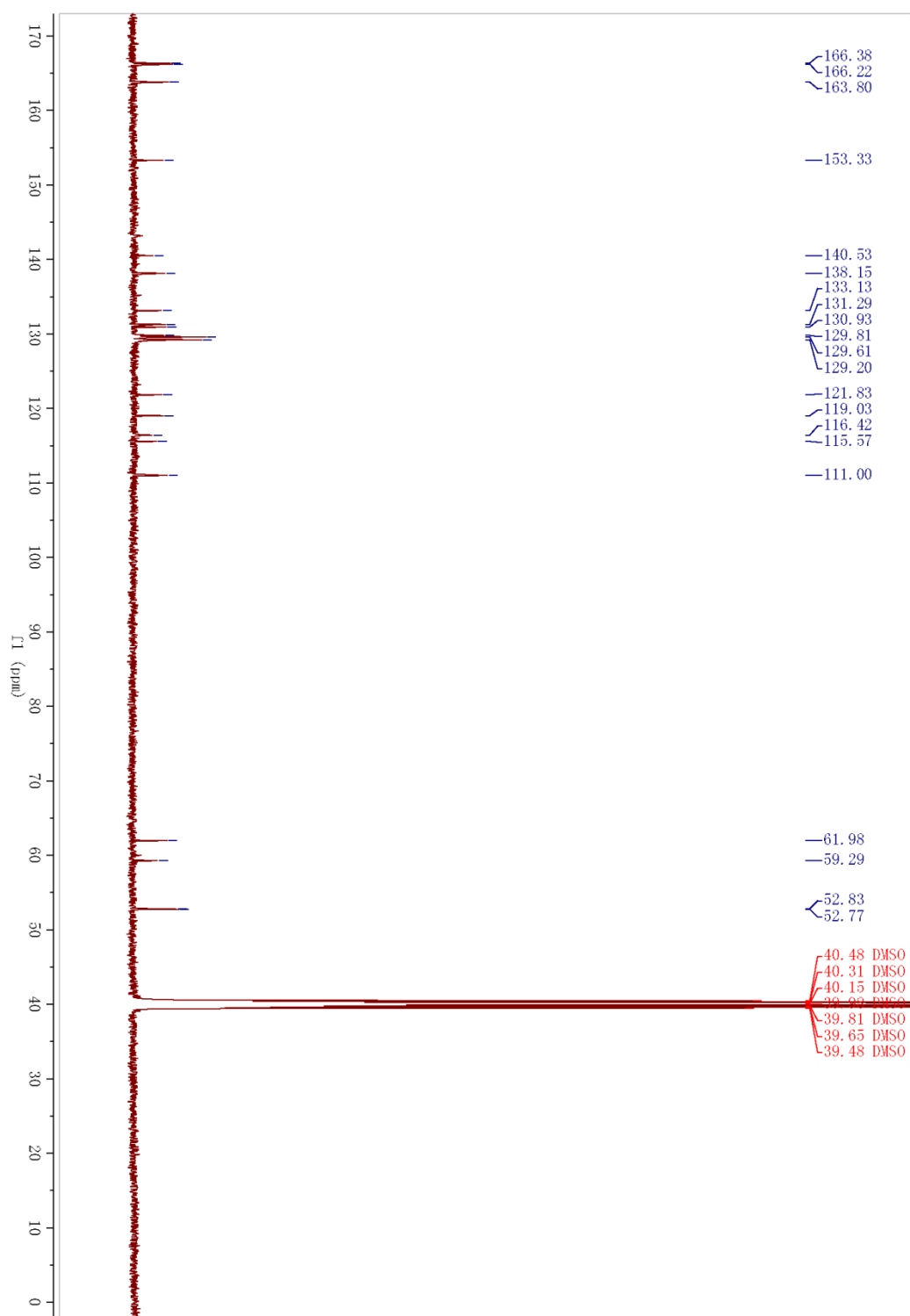
S19. LCMS spectrum of dimethyl 4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidine-2,5-diyl)dibenzoate (**4f**).



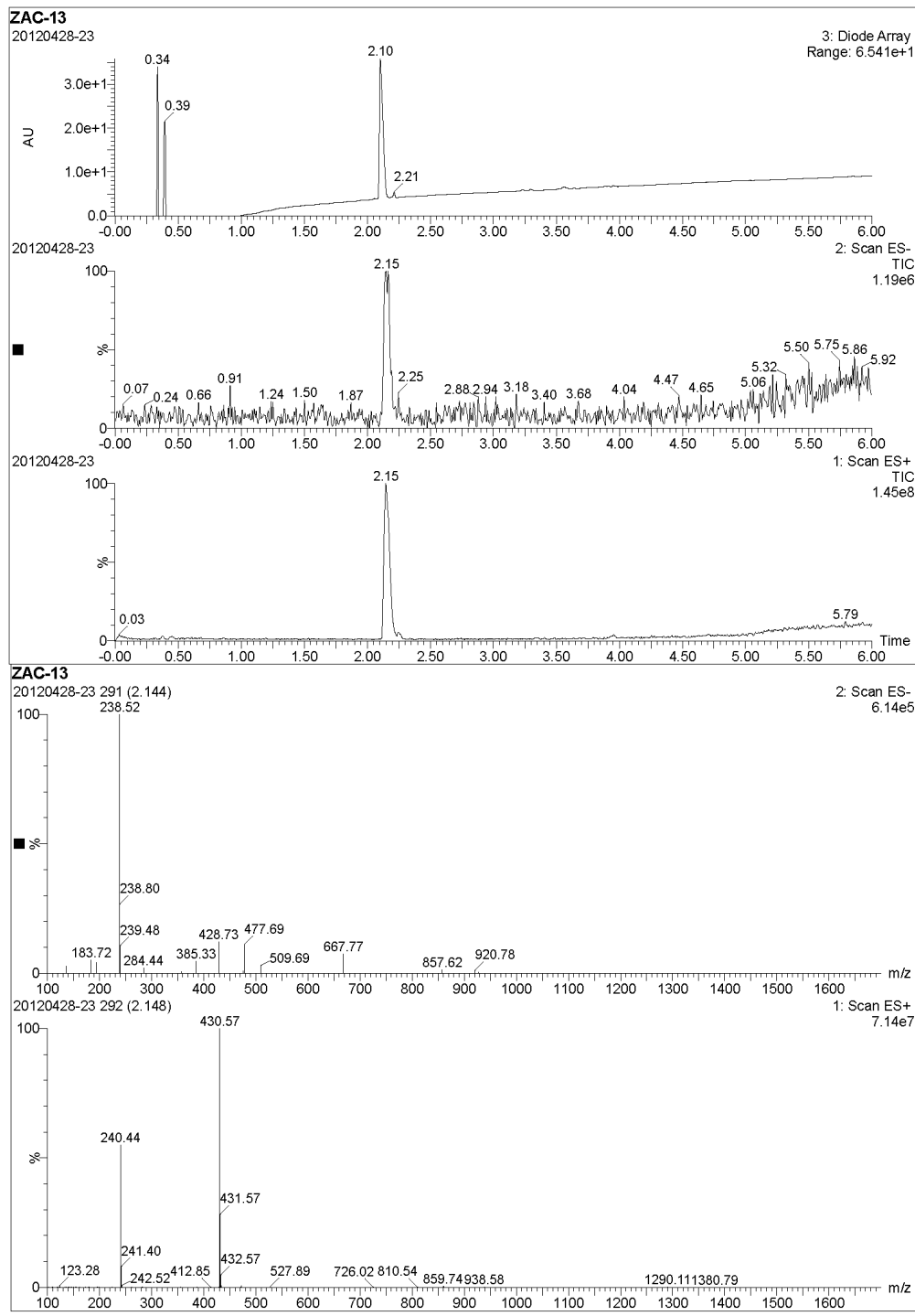
S20. ^1H NMR spectrum of dimethyl 4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidine-2,5-diyl)dibenzoate (**4f**) in $\text{DMSO-}d_6$.



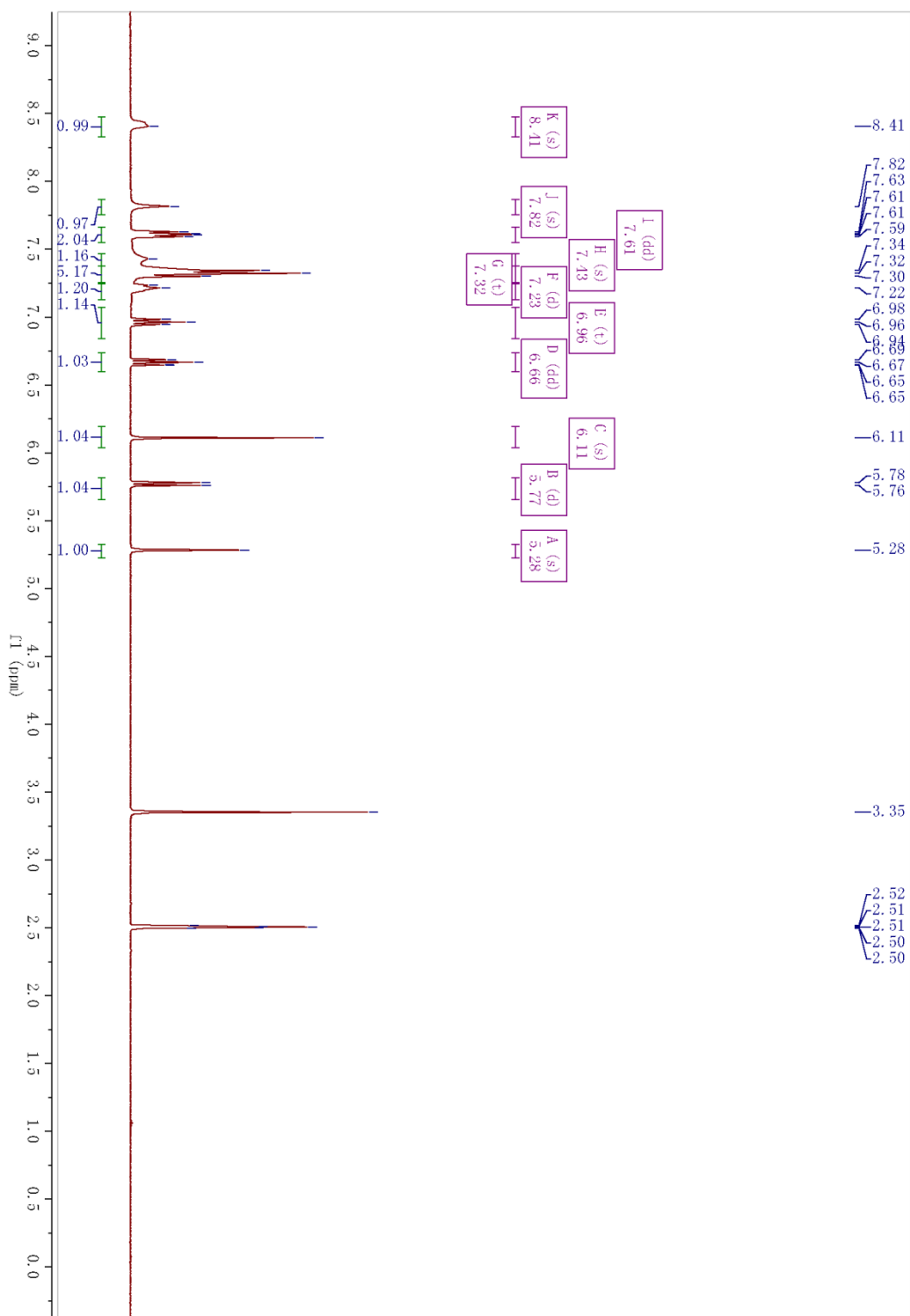
S21. ^{13}C NMR spectrum of dimethyl 4,4'-(4-oxo-1,2,3,4,5,12-hexahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidine-2,5-diyl)dibenzoate (**4f**) in $\text{DMSO-}d_6$.



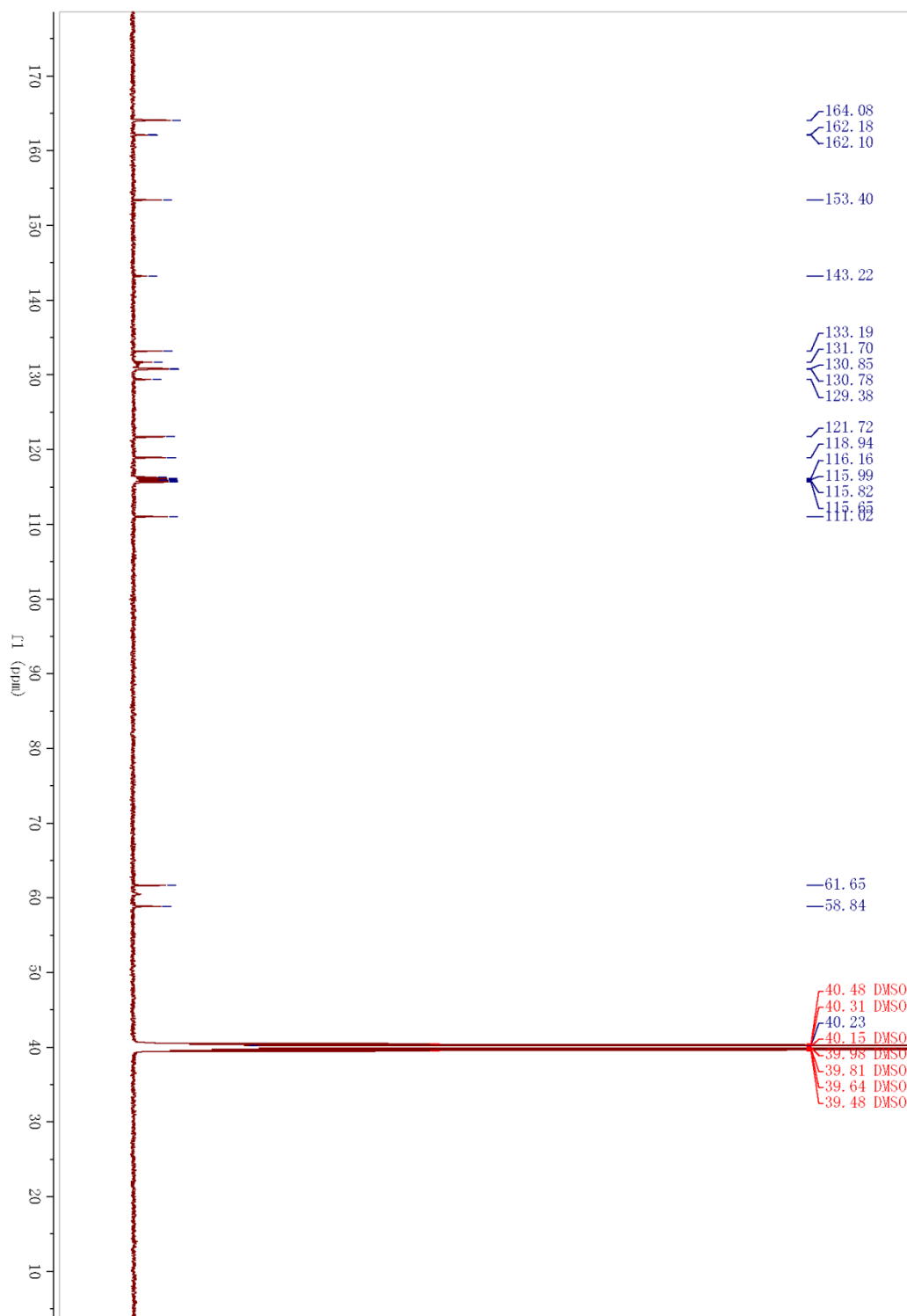
S22. LCMS spectrum of 2,5-bis(4-fluorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4g**).



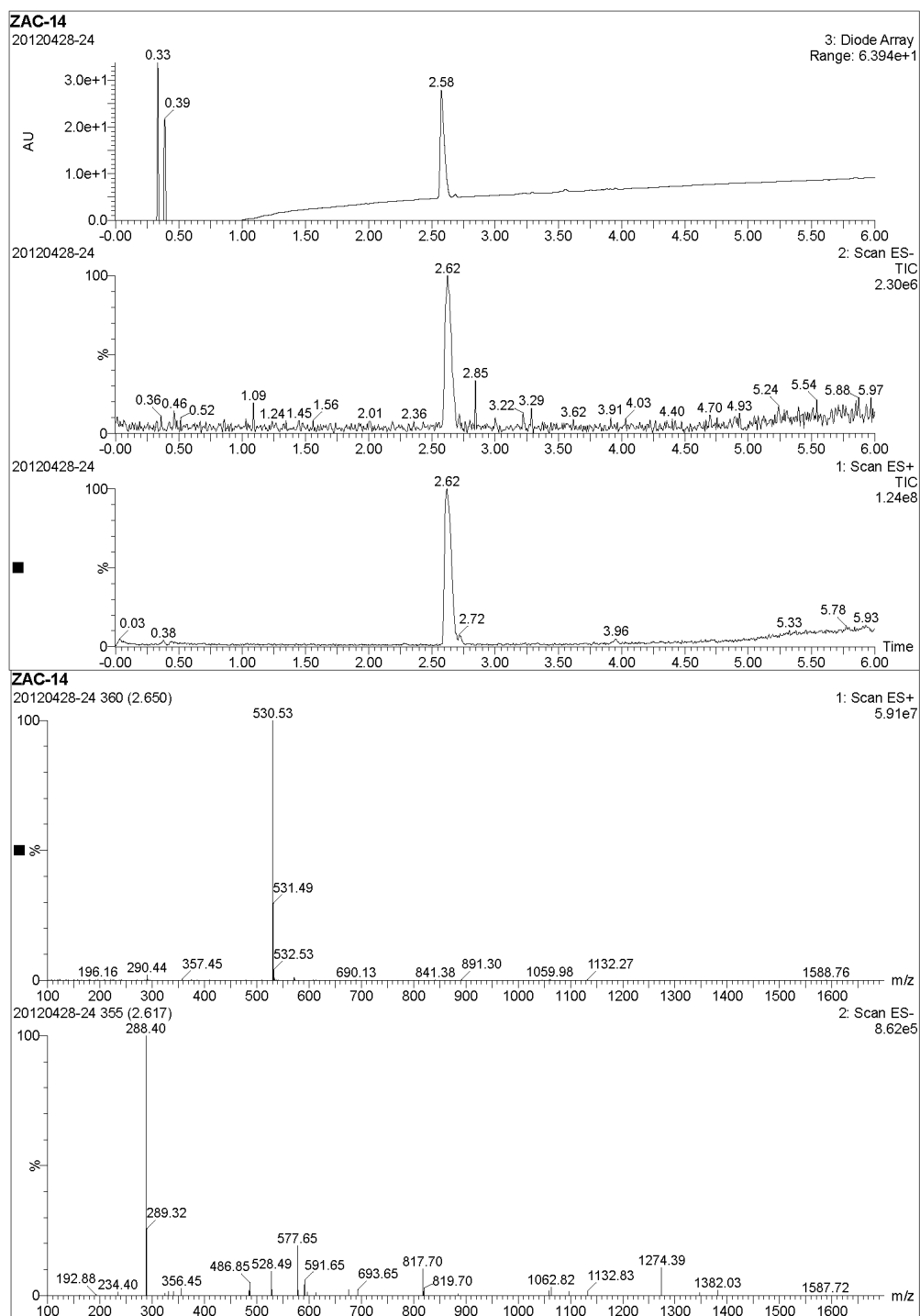
S23. ^1H NMR spectrum of
2,5-bis(4-fluorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4g**) in $\text{DMSO-}d_6$.



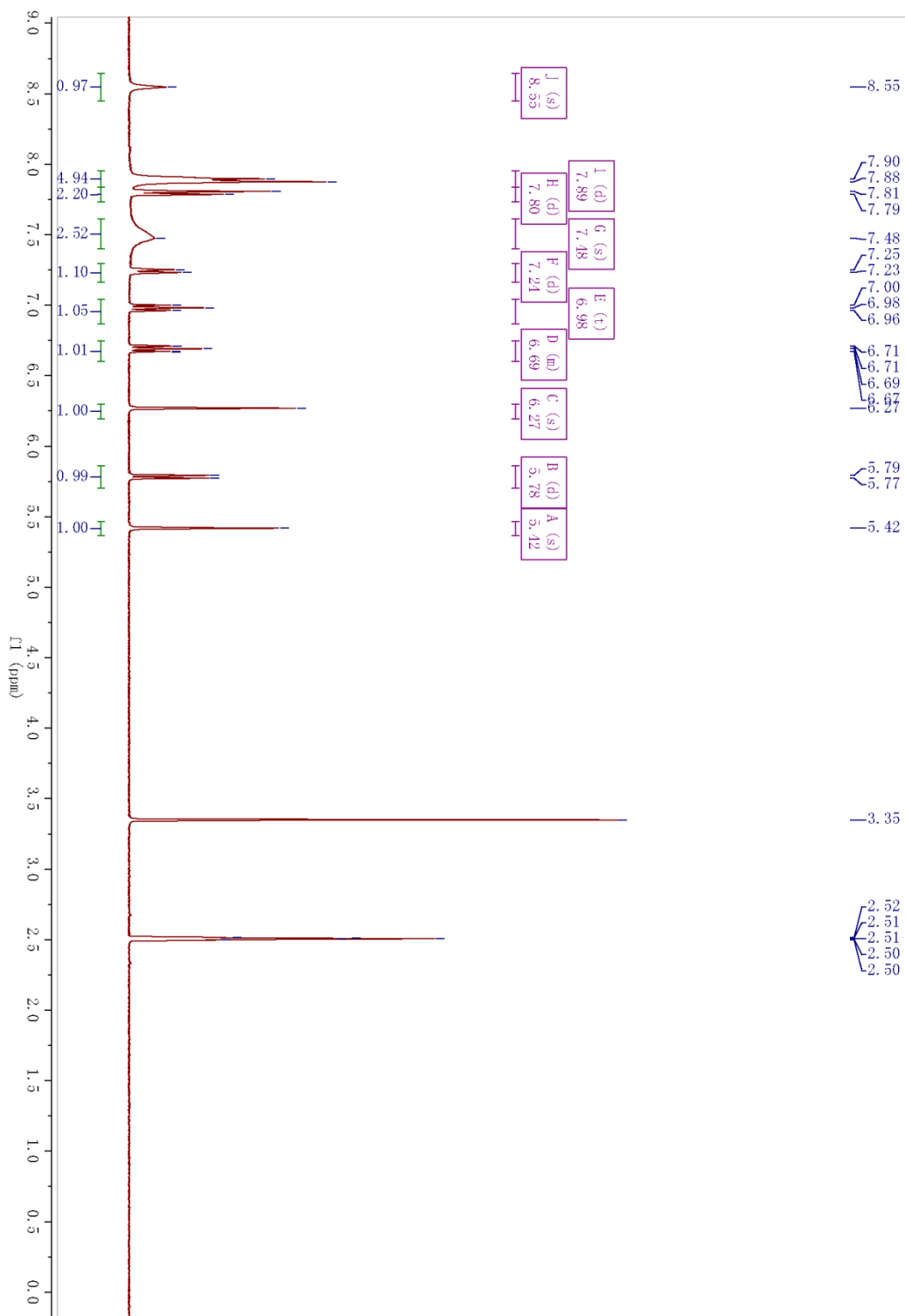
S24. ^{13}C NMR spectrum of
2,5-bis(4-fluorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4g**) in $\text{DMSO-}d_6$.



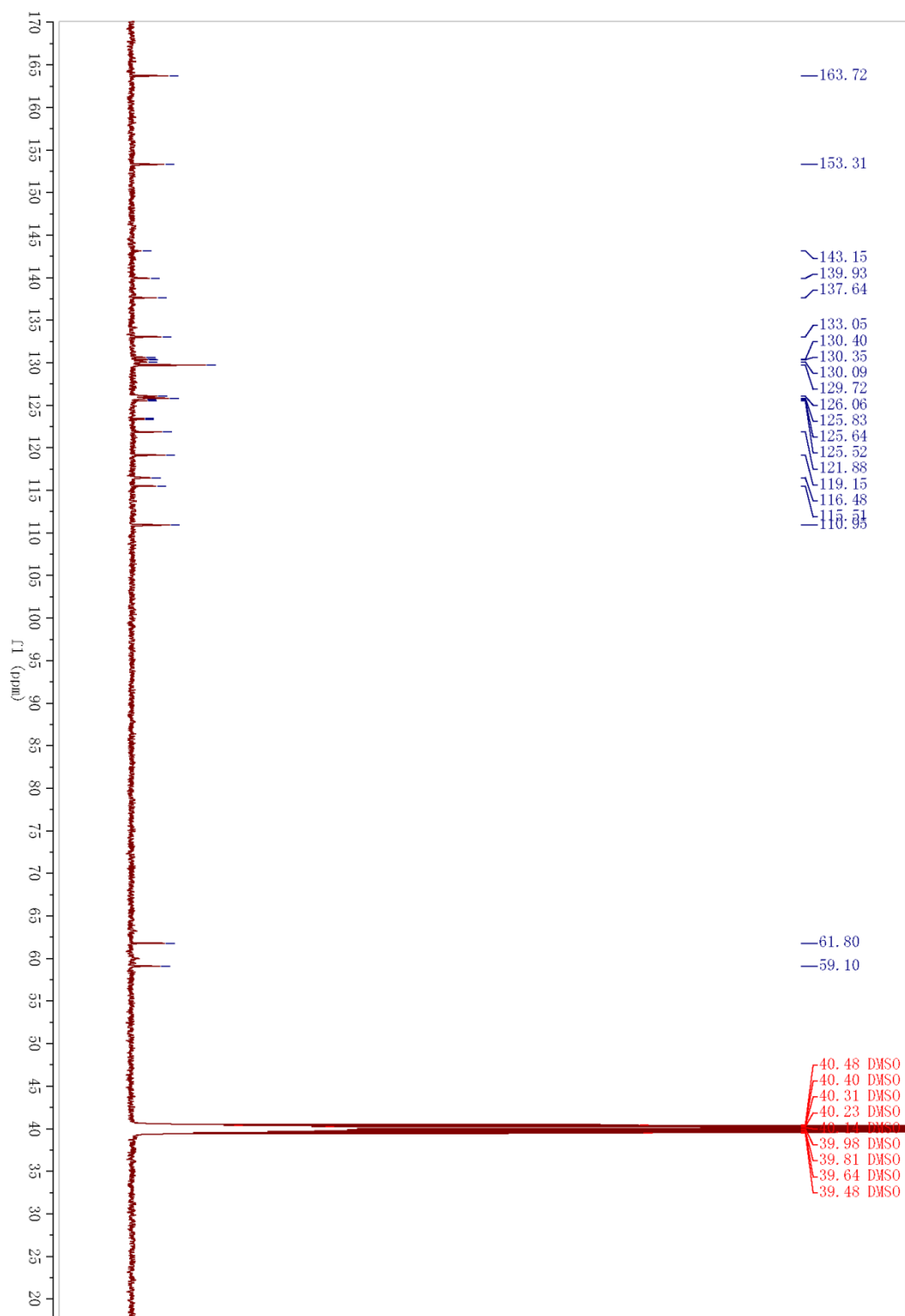
S25. LCMS spectrum of
2,5-bis(4-(trifluoromethyl)phenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4h**).



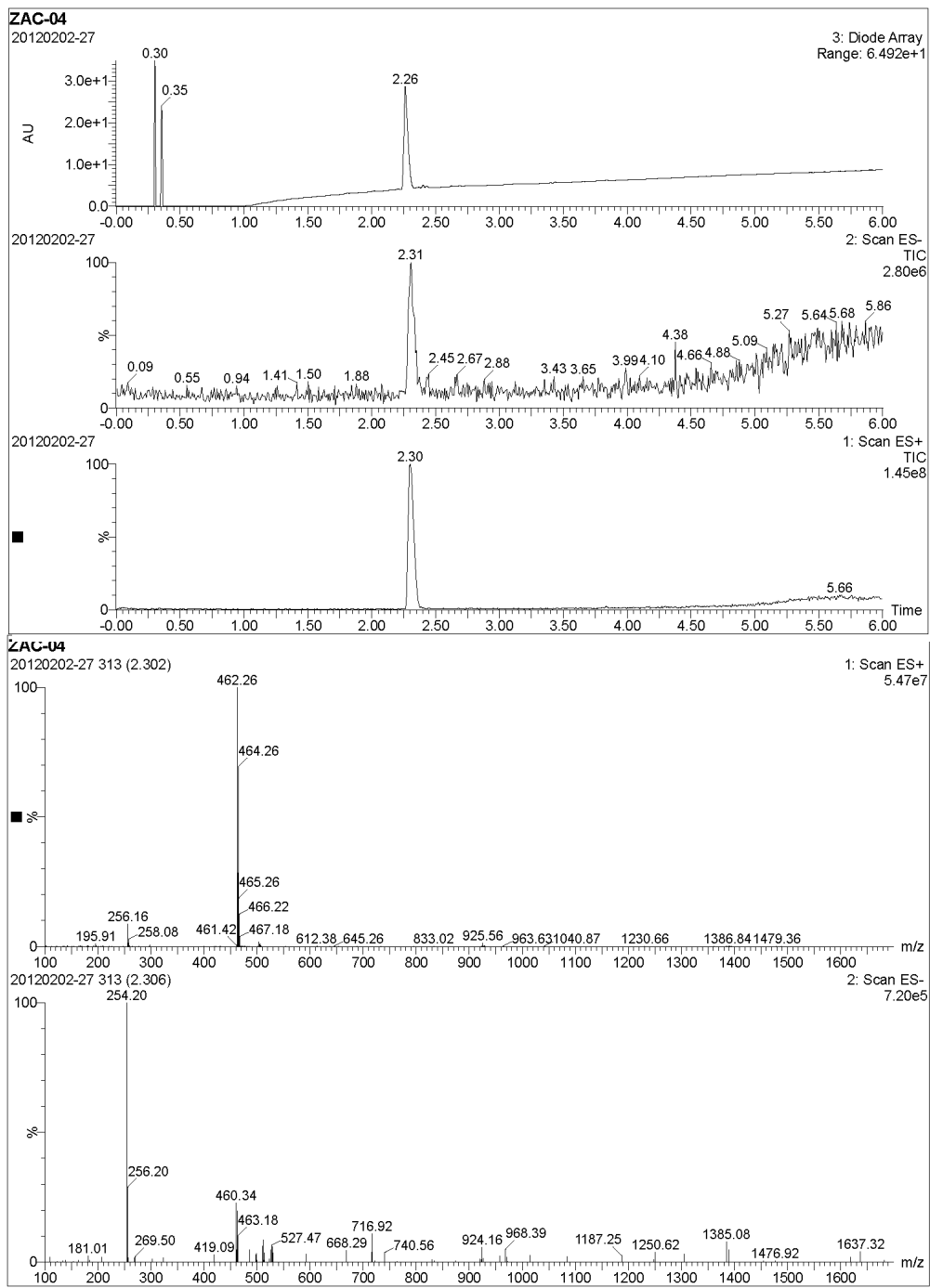
S26. ^1H NMR spectrum of
2,5-bis(4-(trifluoromethyl)phenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrim-
ido[4,5-*d*]pyrimidin-4(1*H*)-one (**4h**) in DMSO-*d*₆.



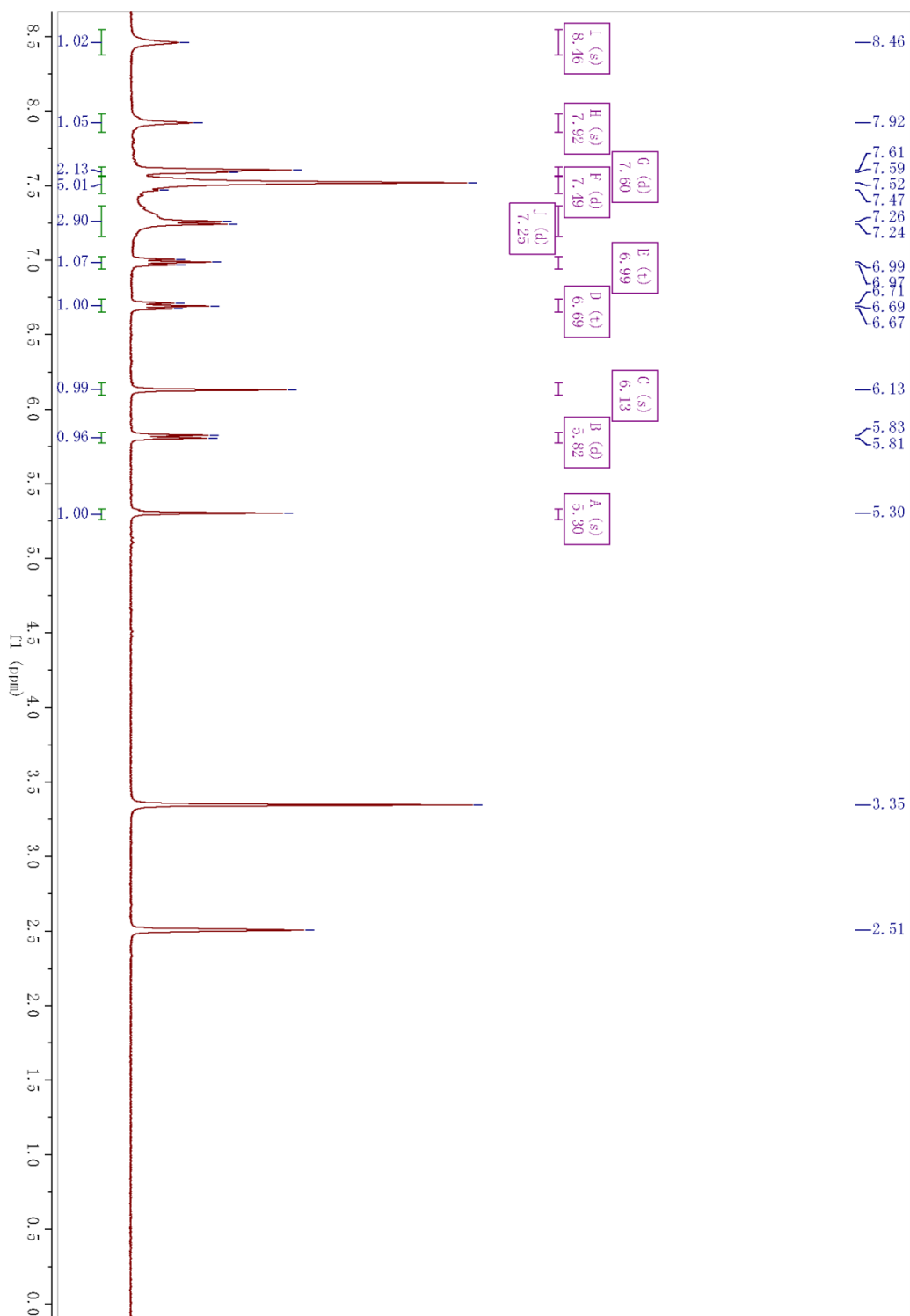
S27. ^{13}C NMR spectrum of
2,5-bis(4-(trifluoromethyl)phenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrim-
ido[4,5-*d*]pyrimidin-4(1*H*)-one (**4h**) in $\text{DMSO-}d_6$.



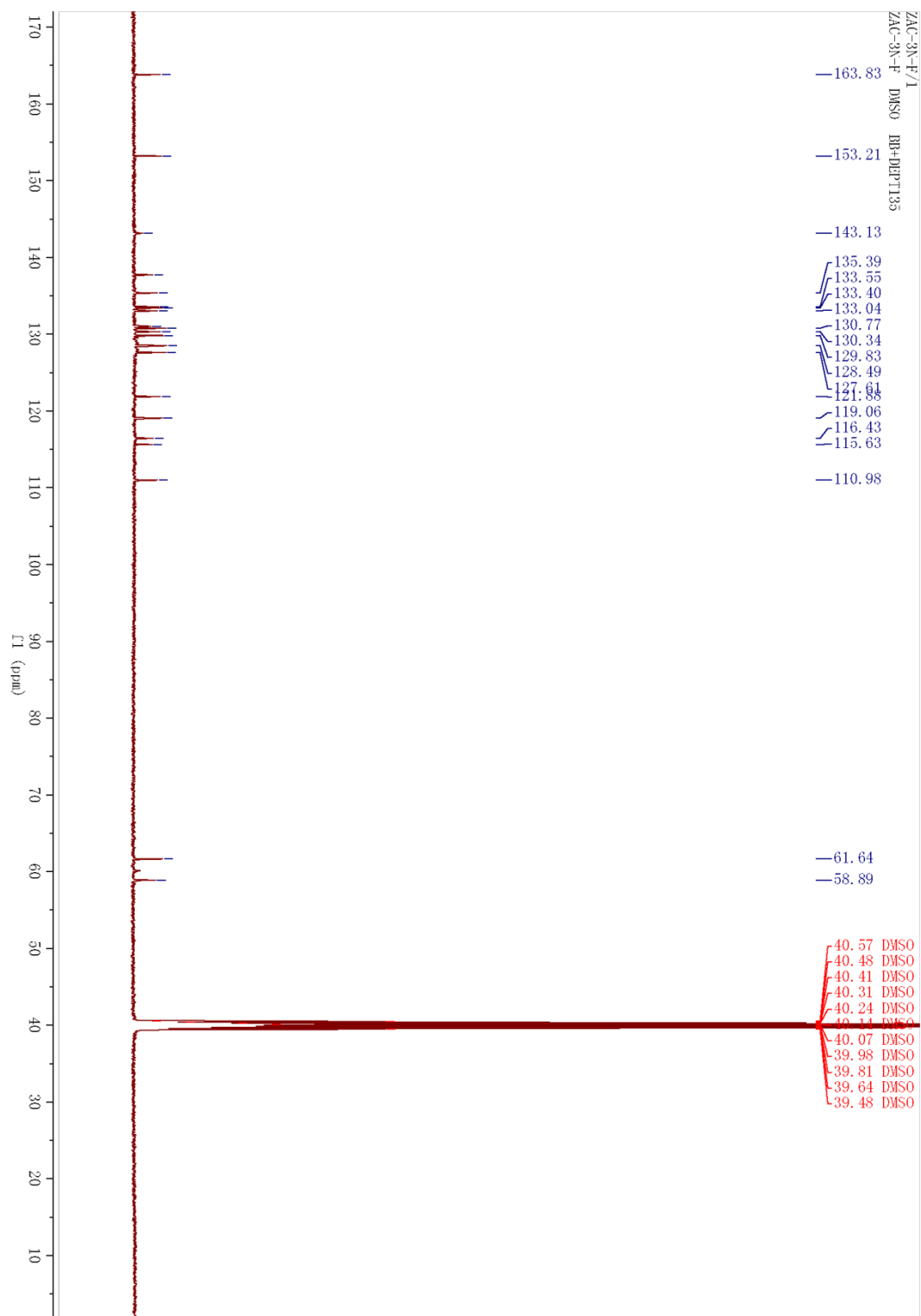
S28. LCMS spectrum of
2,5-bis(3-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4i**).



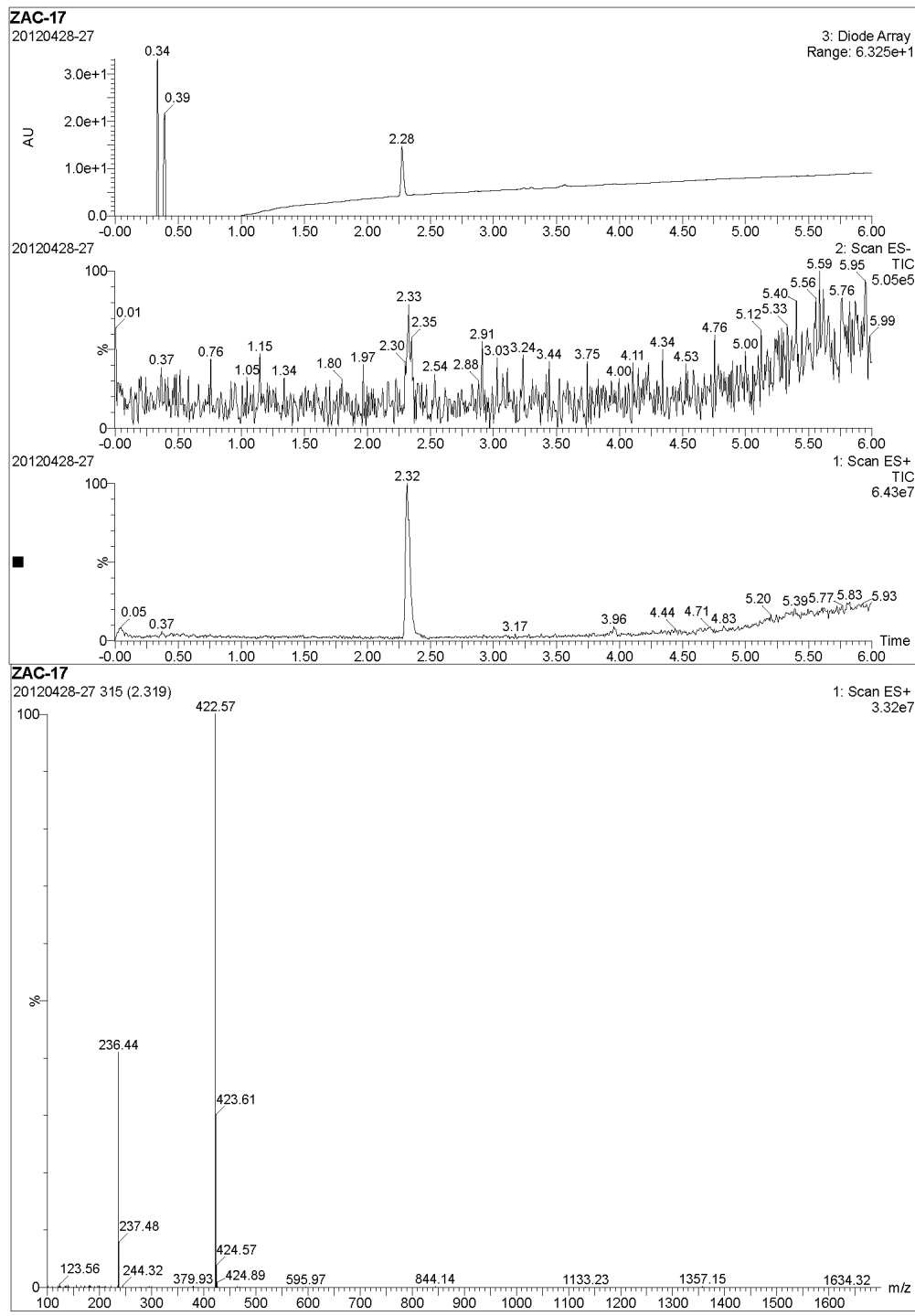
S29. ^1H NMR spectrum of
2,5-bis(3-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4i**) in $\text{DMSO-}d_6$.



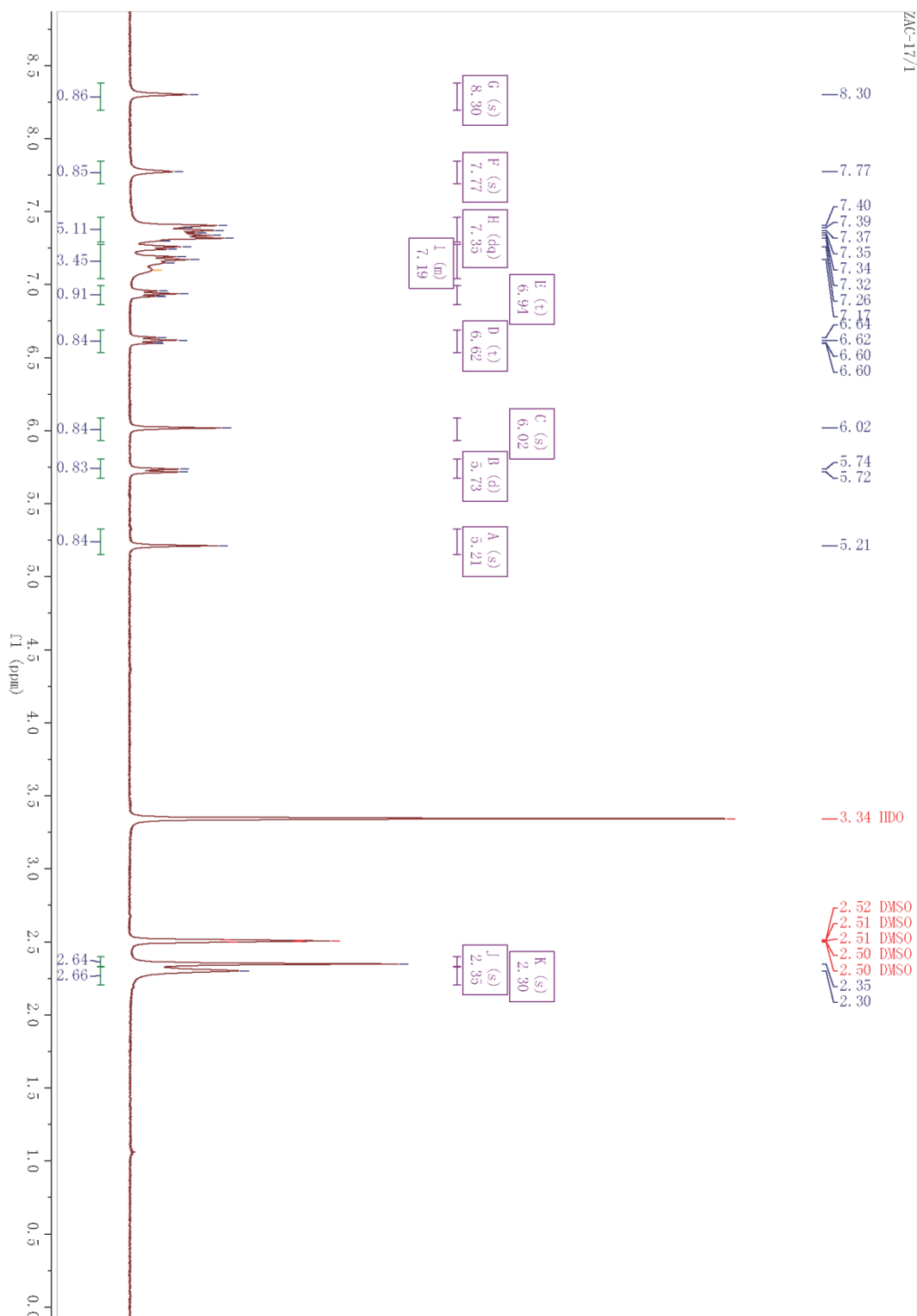
S30. ^{13}C NMR spectrum of
2,5-bis(3-chlorophenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]
pyrimidin-4(1*H*)-one (**4i**) in $\text{DMSO}-d_6$.



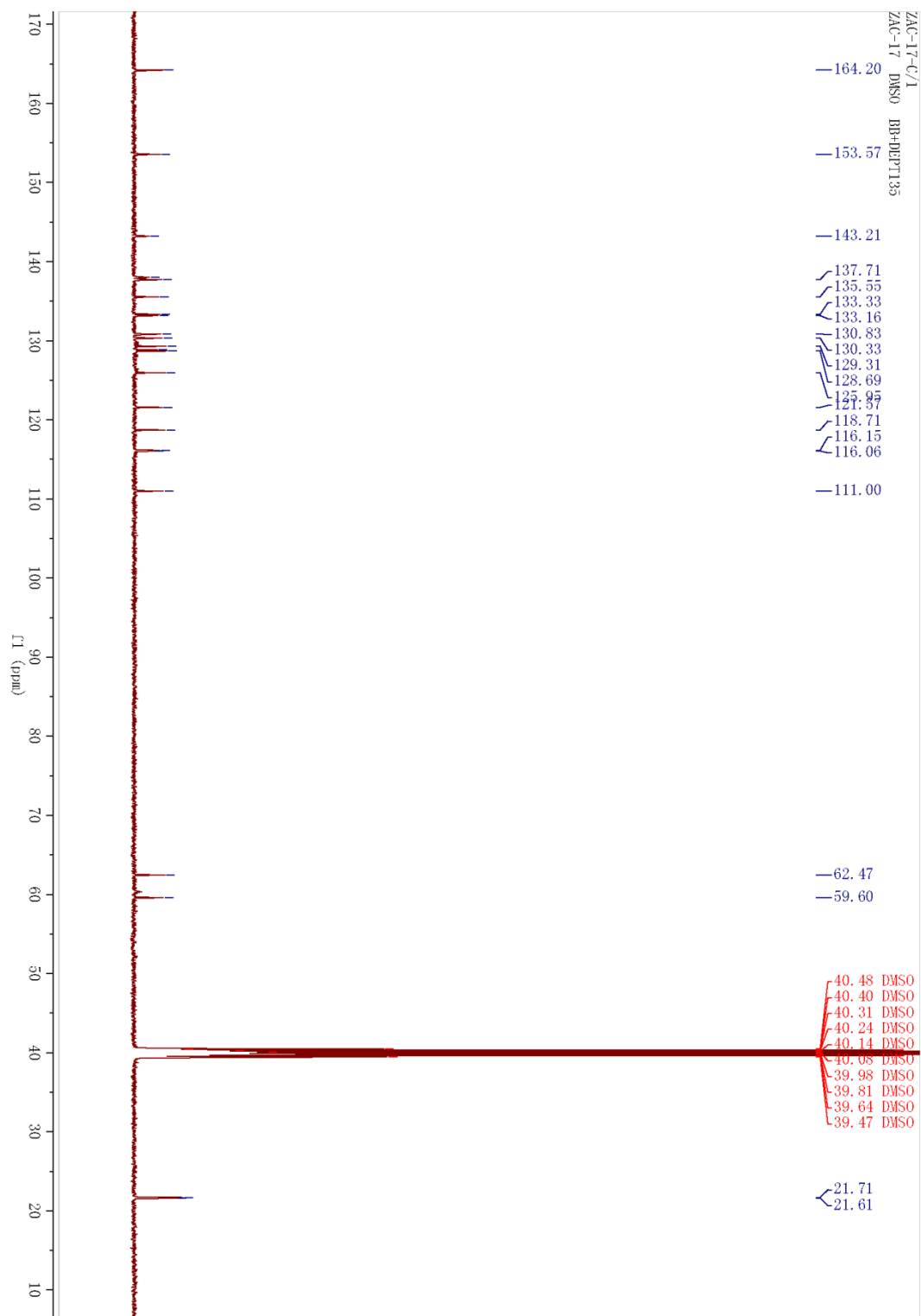
S31. LCMS spectrum of
2,5-di-m-tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin
-4(1*H*)-one (**4j**).



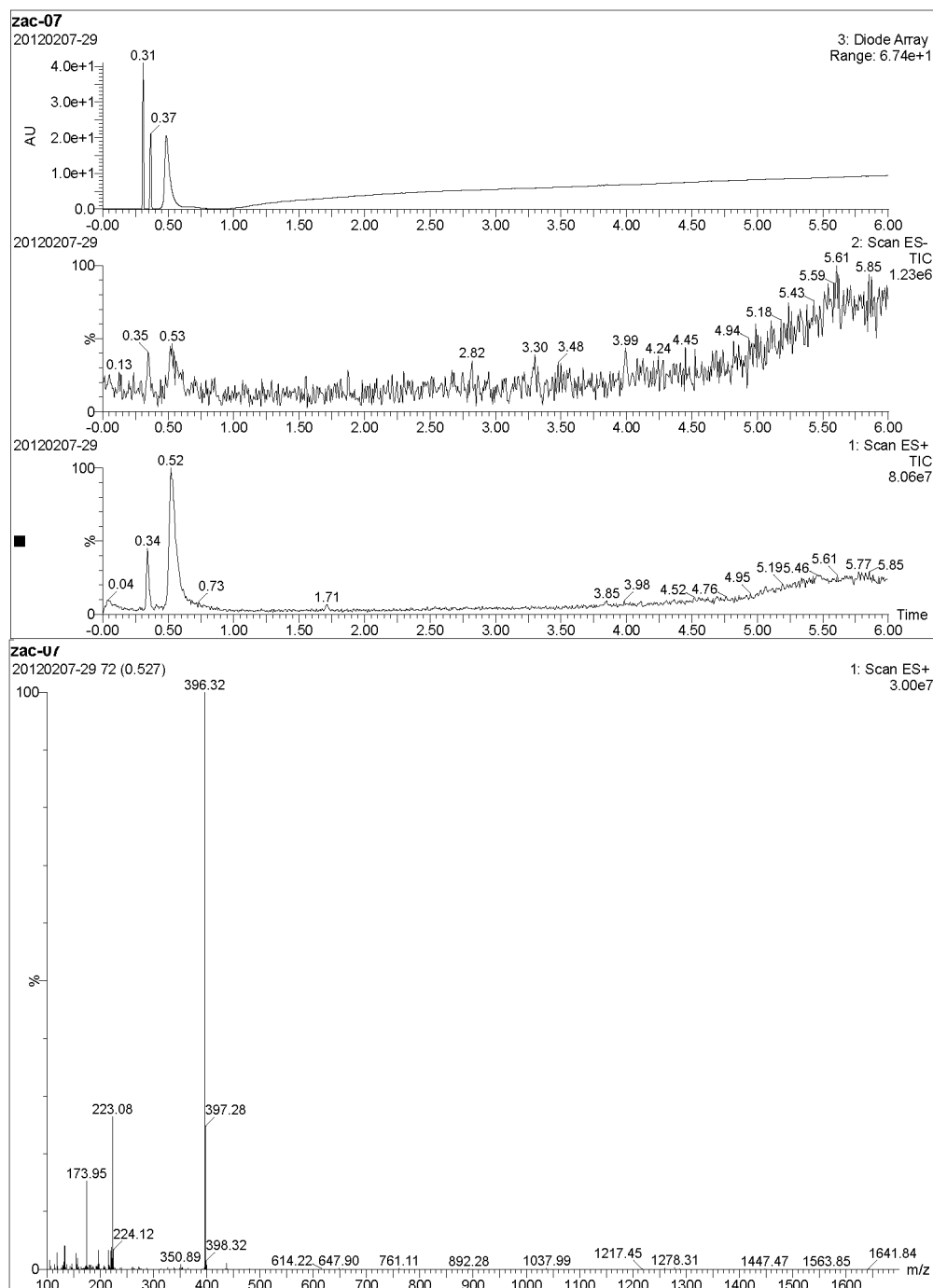
S32. ^1H NMR spectrum of
2,5-di-m-tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin
-4(1*H*)-one (**4j**) in $\text{DMSO-}d_6$.



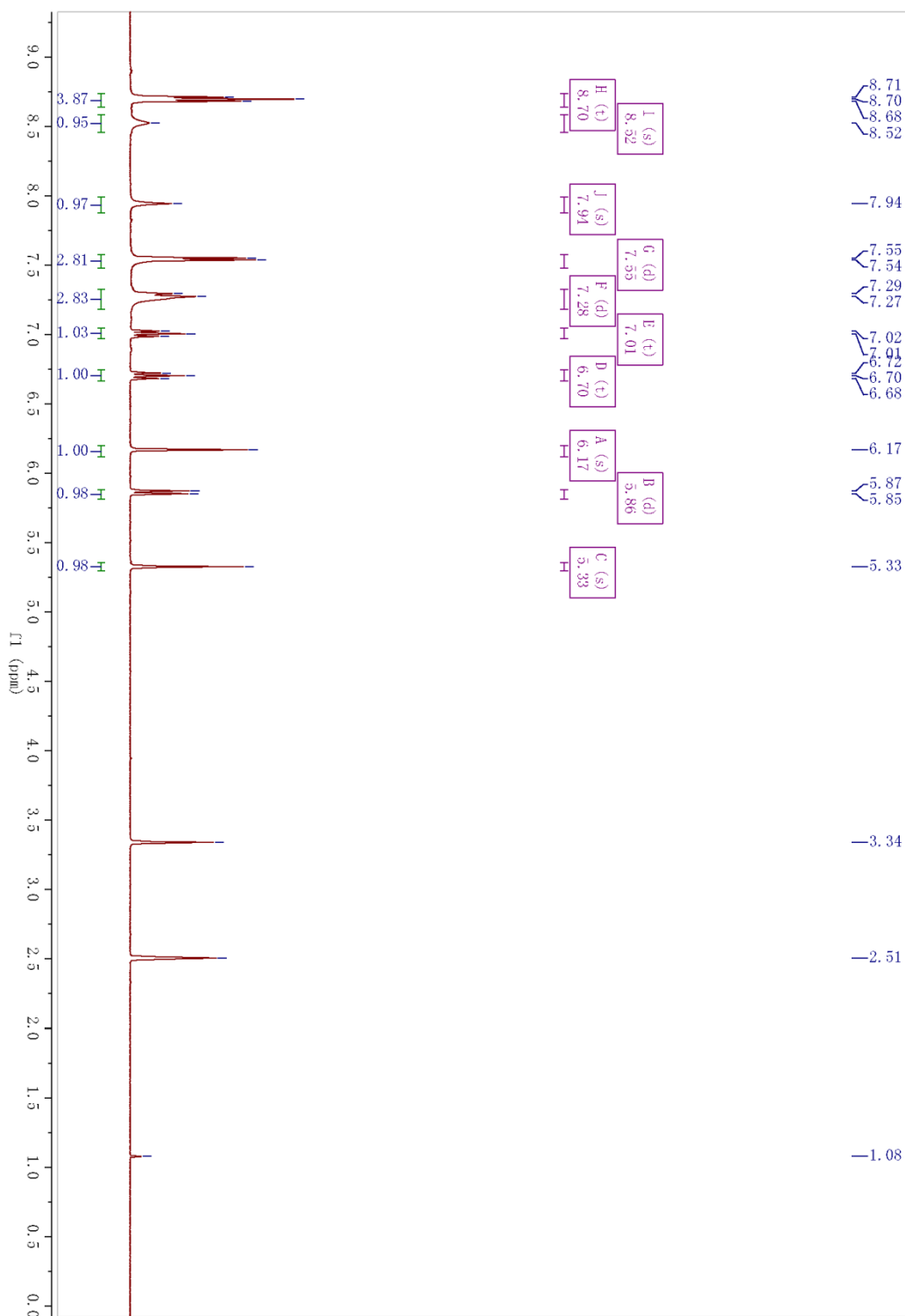
S33. ^{13}C NMR spectrum of
2,5-di-m-tolyl-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin
-4(1*H*)-one (**4j**) in $\text{DMSO-}d_6$.



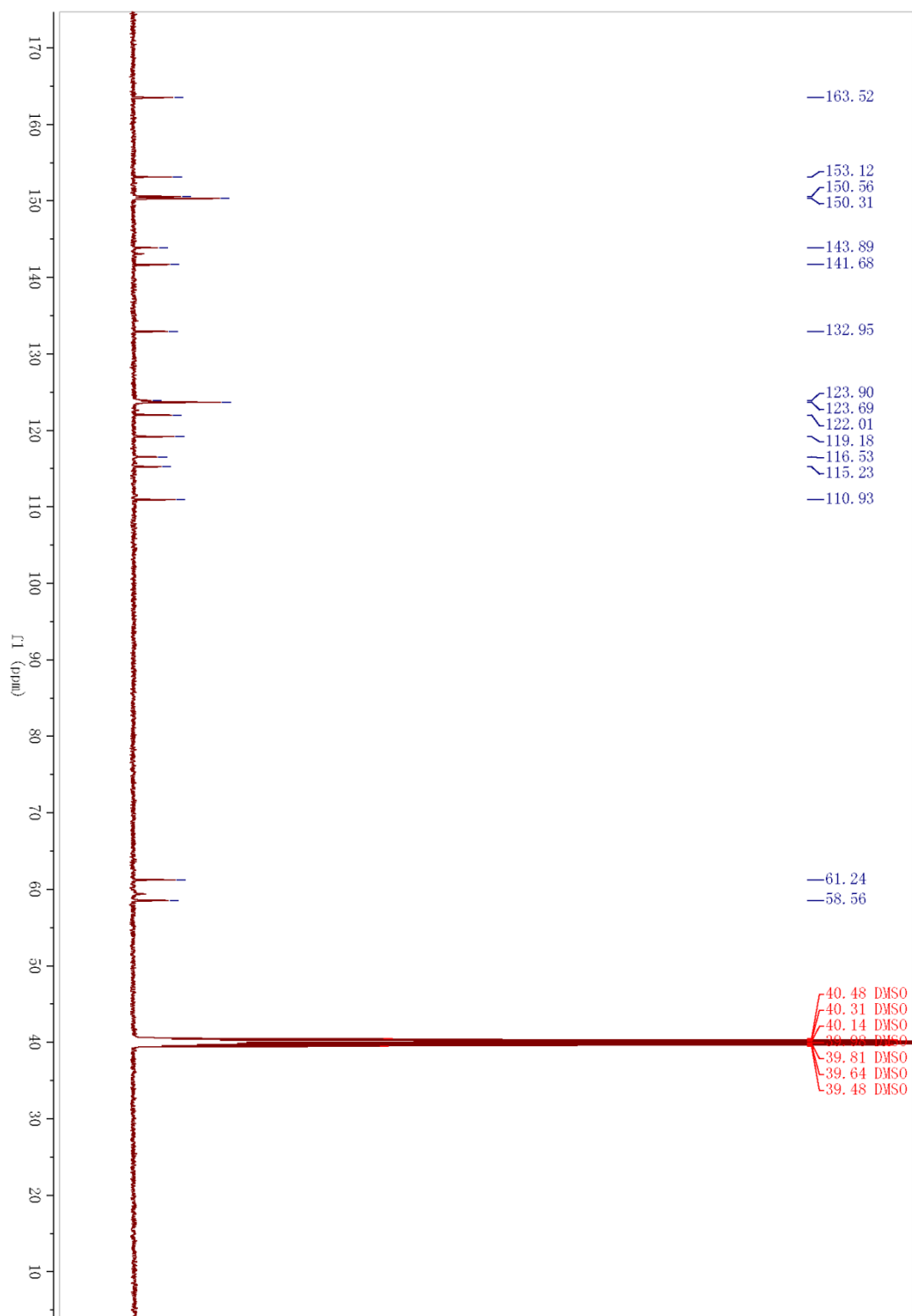
S34. LCMS spectrum of
2,5-di(pyridin-4-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4n**).



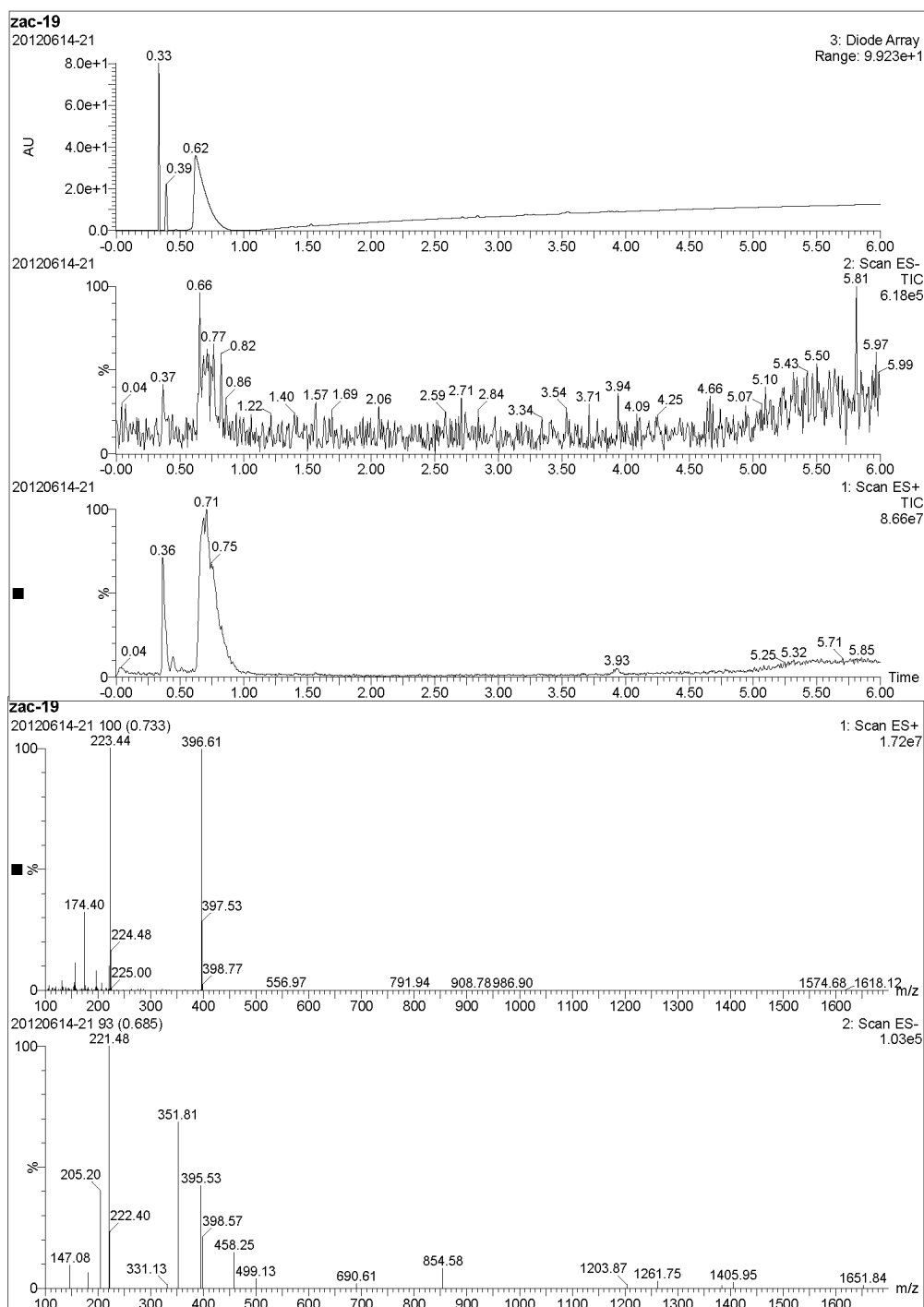
S35. ^1H NMR spectrum of
2,5-di(pyridin-4-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyri-
midin-4(1*H*)-one (**4n**) in $\text{DMSO-}d_6$.



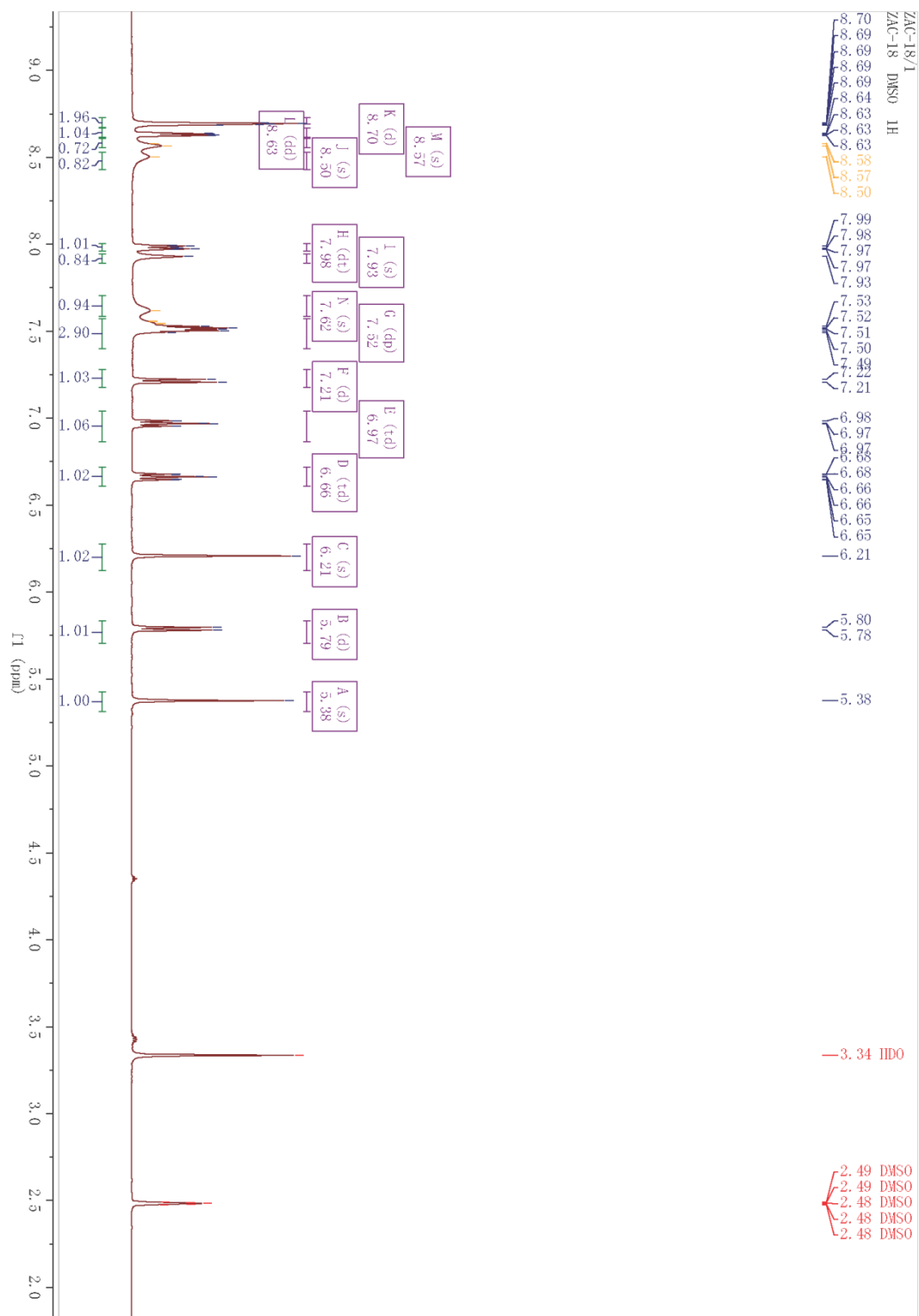
S36. ^{13}C NMR spectrum of
2,5-di(pyridin-4-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyri-
midin-4(1*H*)-one (**4n**) in $\text{DMSO-}d_6$.



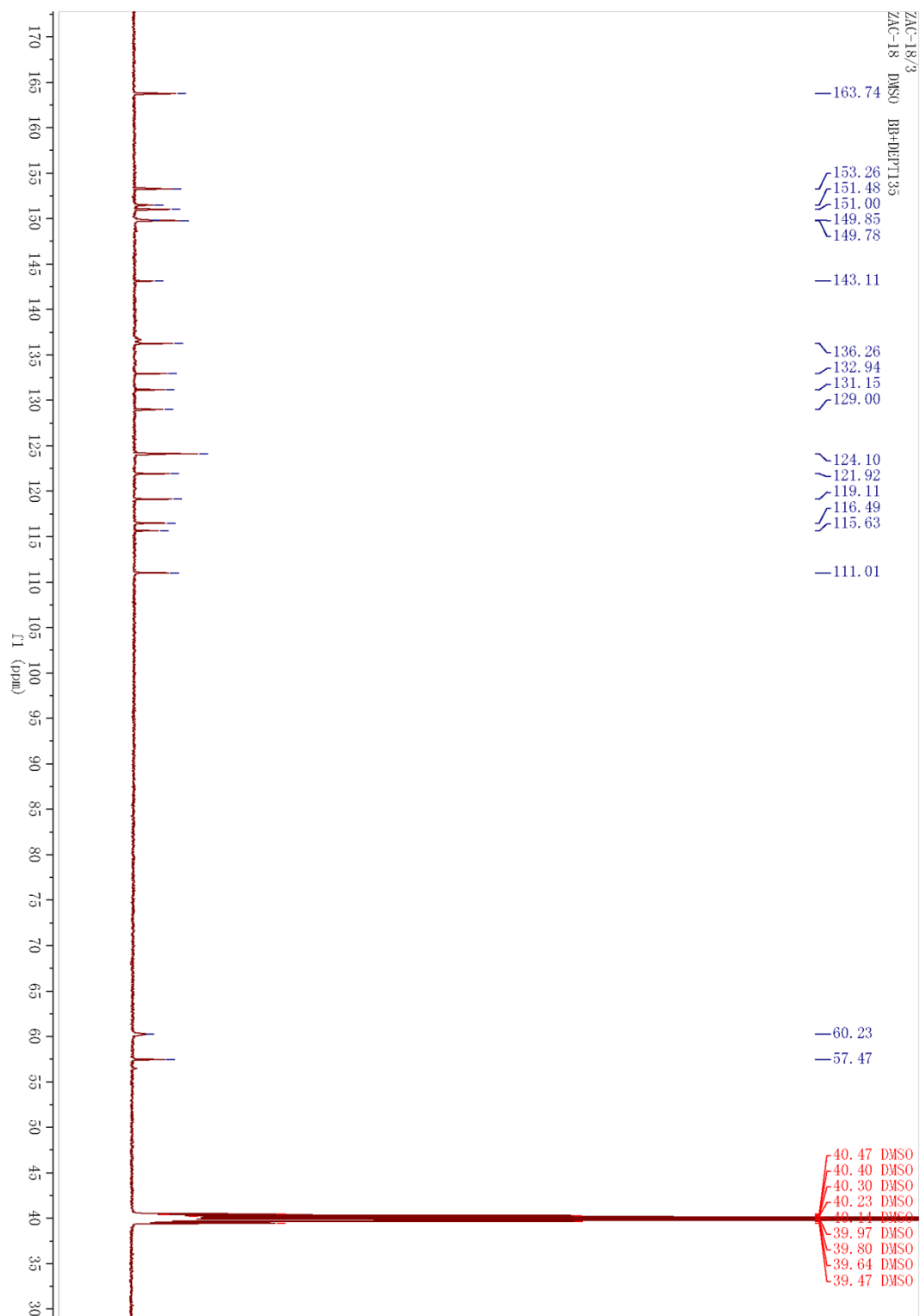
S37. LCMS spectrum of
2,5-di(pyridin-3-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4o**).



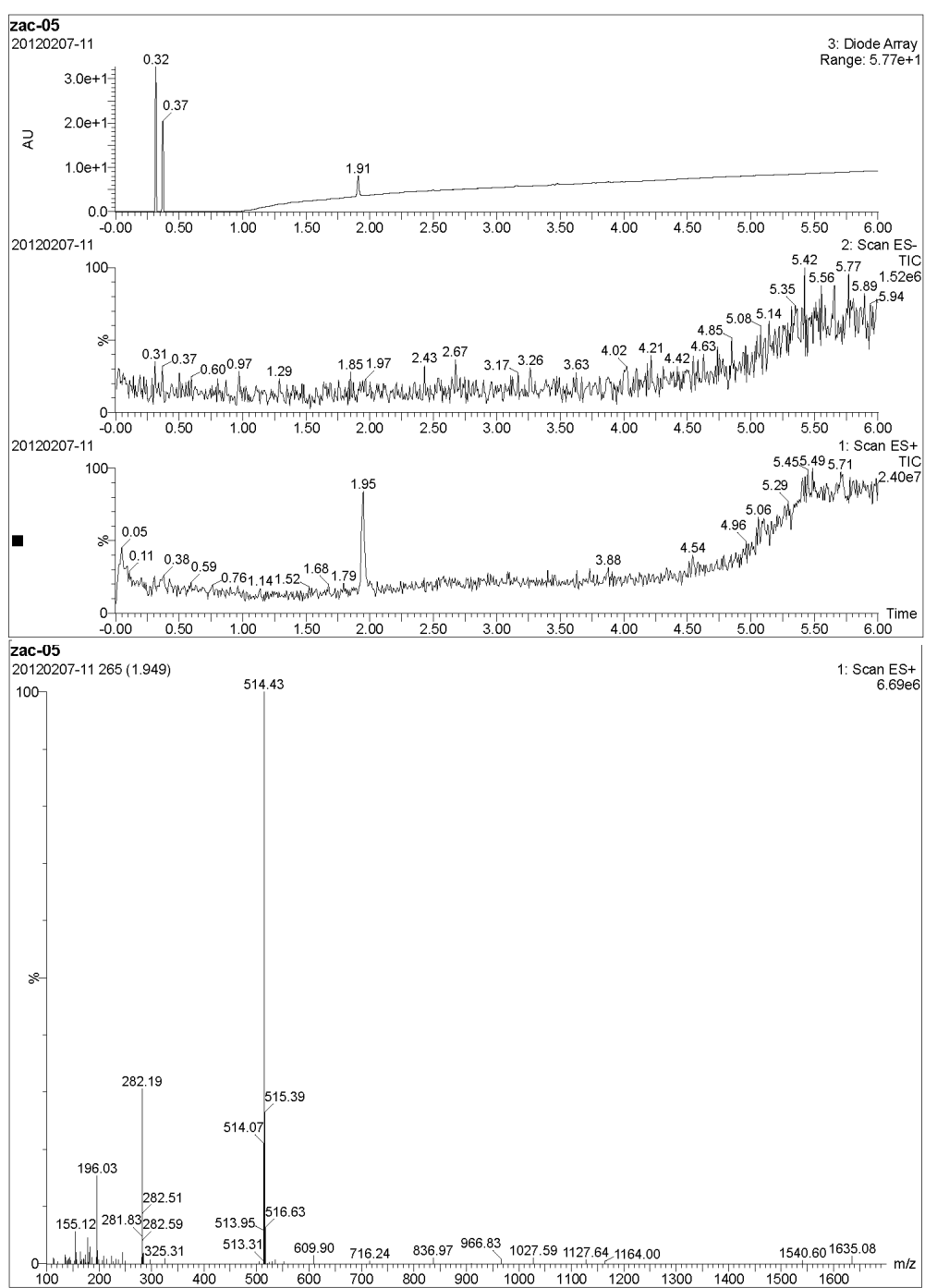
S38. ^1H NMR spectrum of
2,5-di(pyridin-3-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyri-
midin-4(1*H*)-one (**4o**) in DMSO-*d*₆.



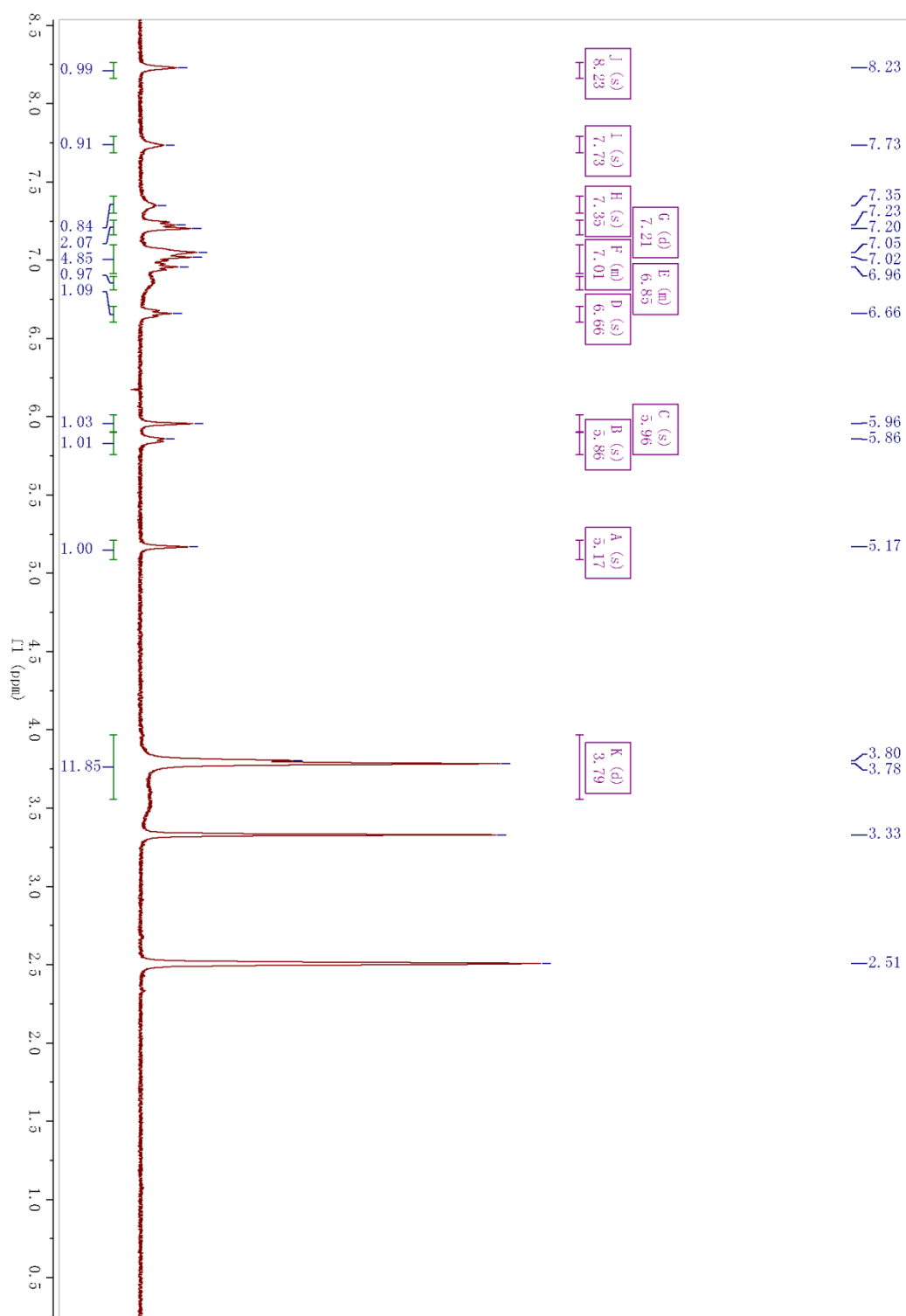
S39. ^{13}C NMR spectrum of
2,5-di(pyridin-3-yl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyri
midin-4(1*H*)-one (**4o**) in DMSO-*d*₆.



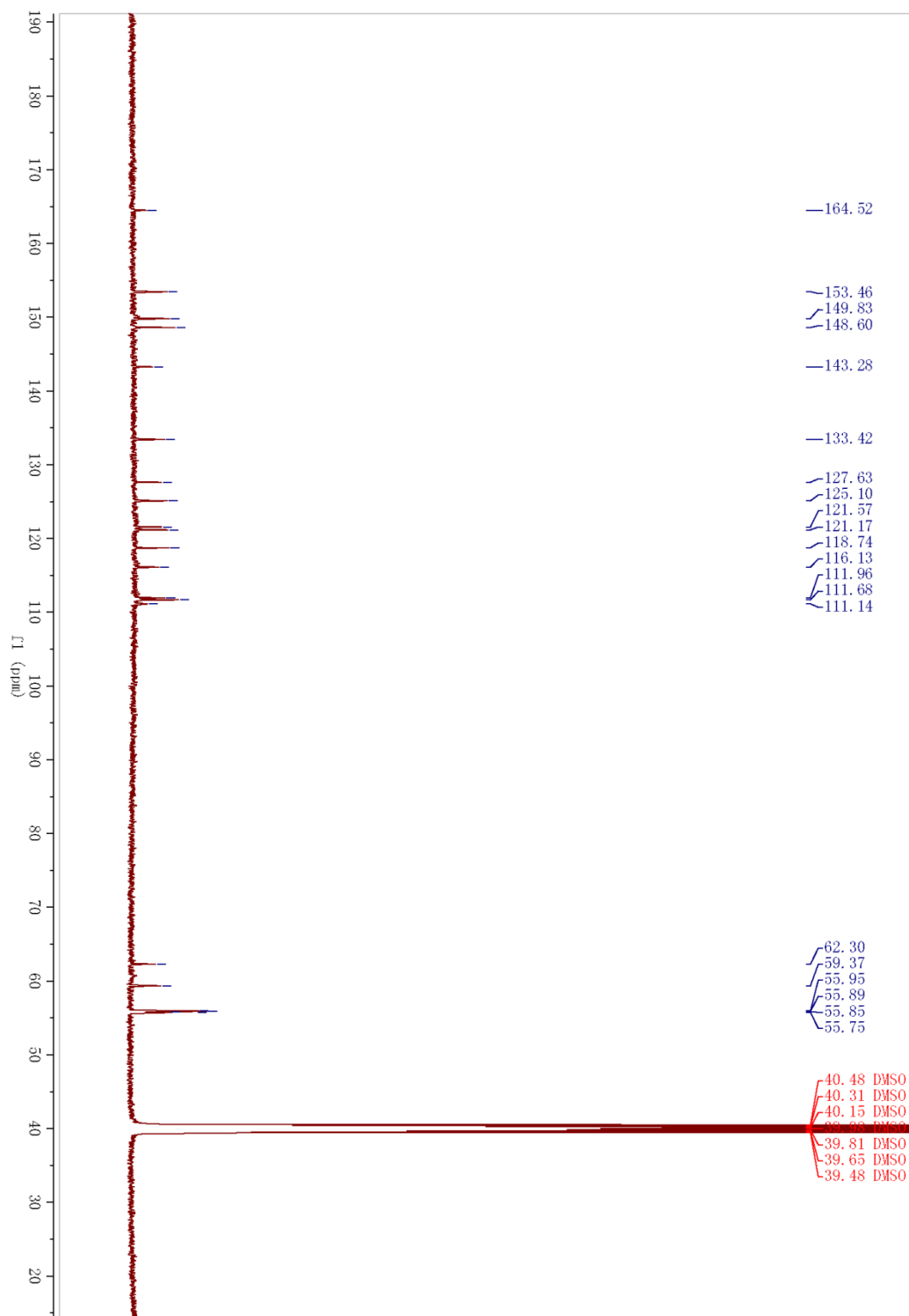
S40. LCMS spectrum of
2,5-bis(3,4-dimethoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4p**).



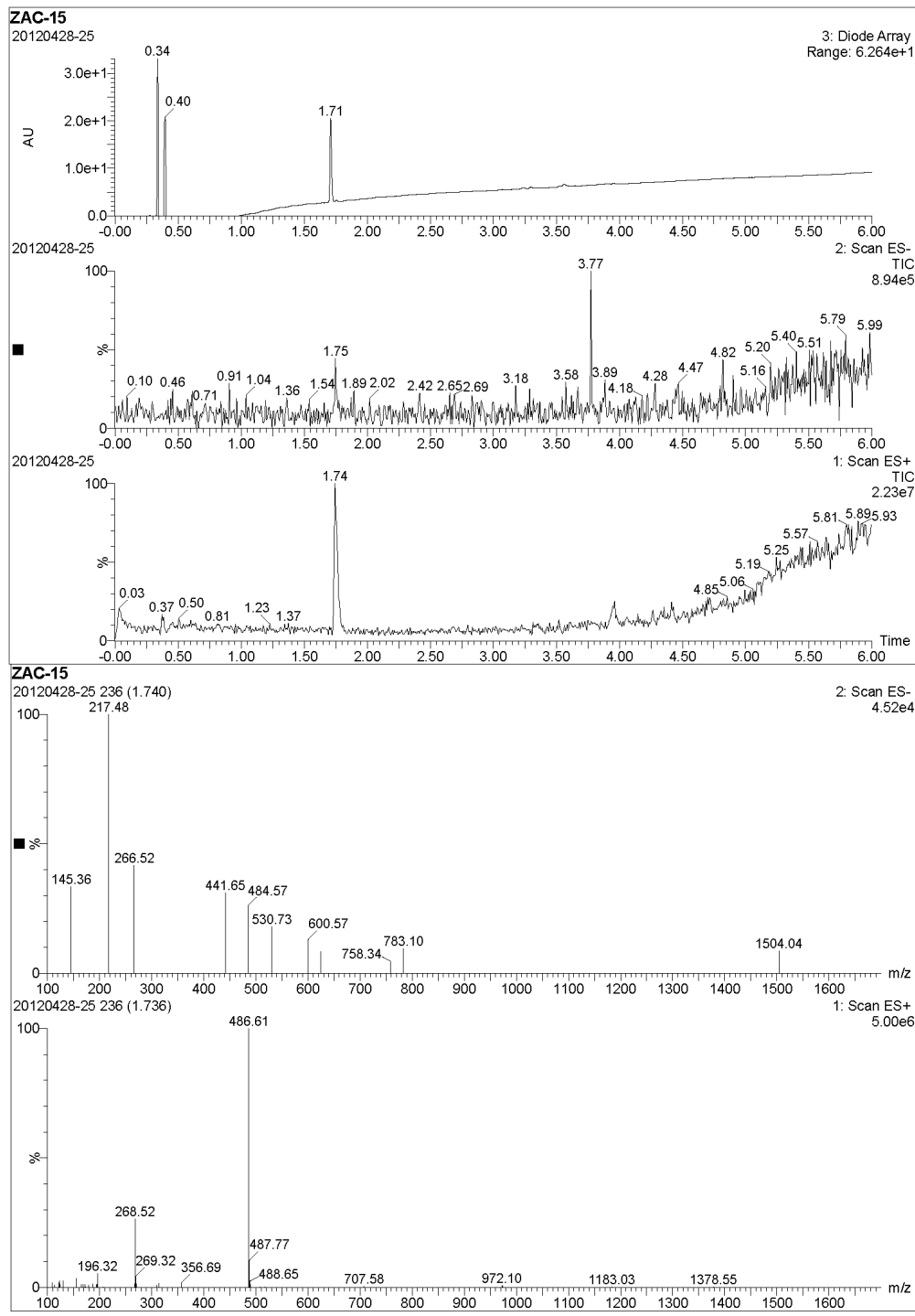
S41. ^1H NMR spectrum of
2,5-bis(3,4-dimethoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4p**) in $\text{DMSO-}d_6$.



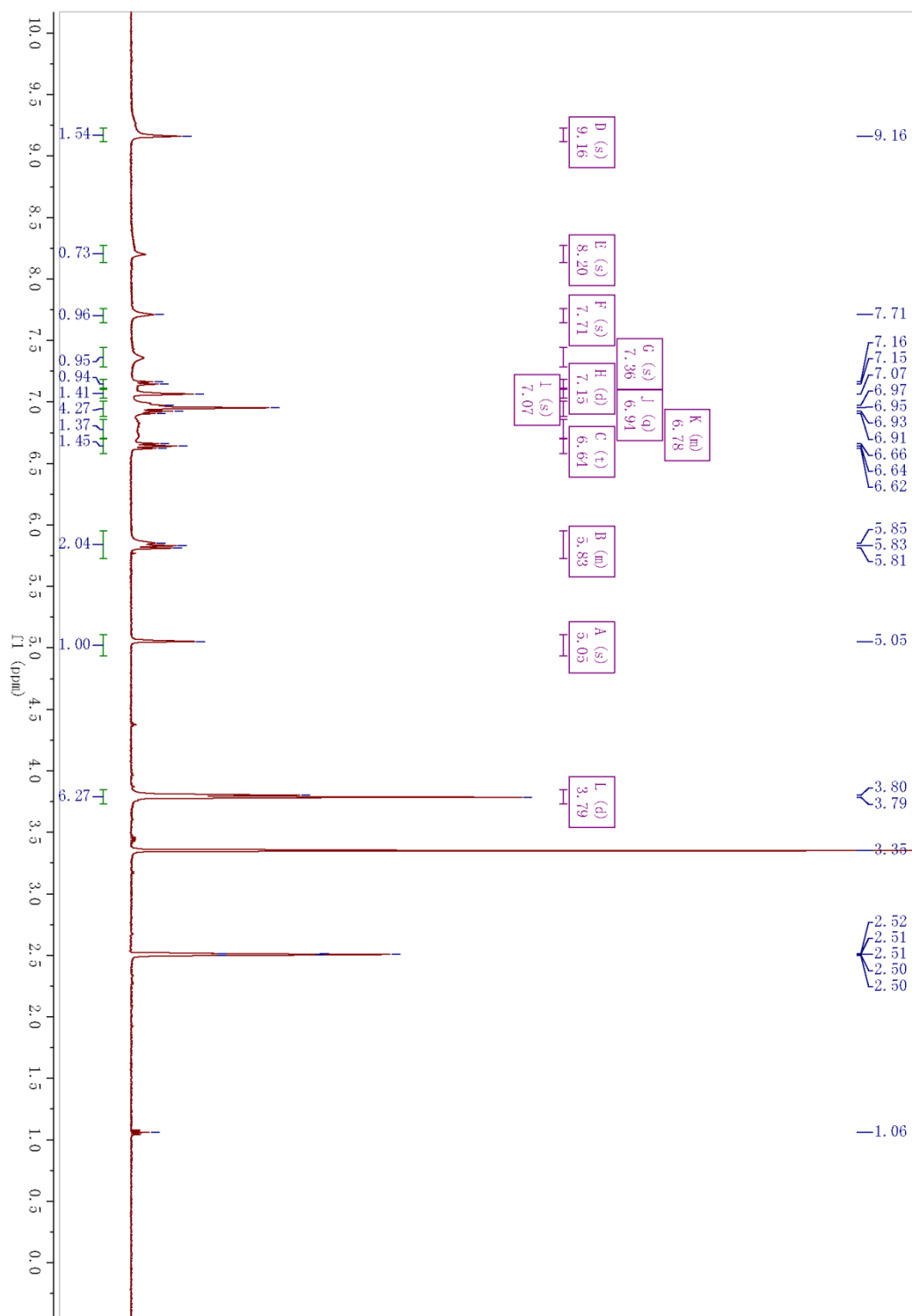
S42. ^{13}C NMR spectrum of
2,5-bis(3,4-dimethoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4p**) in $\text{DMSO-}d_6$.



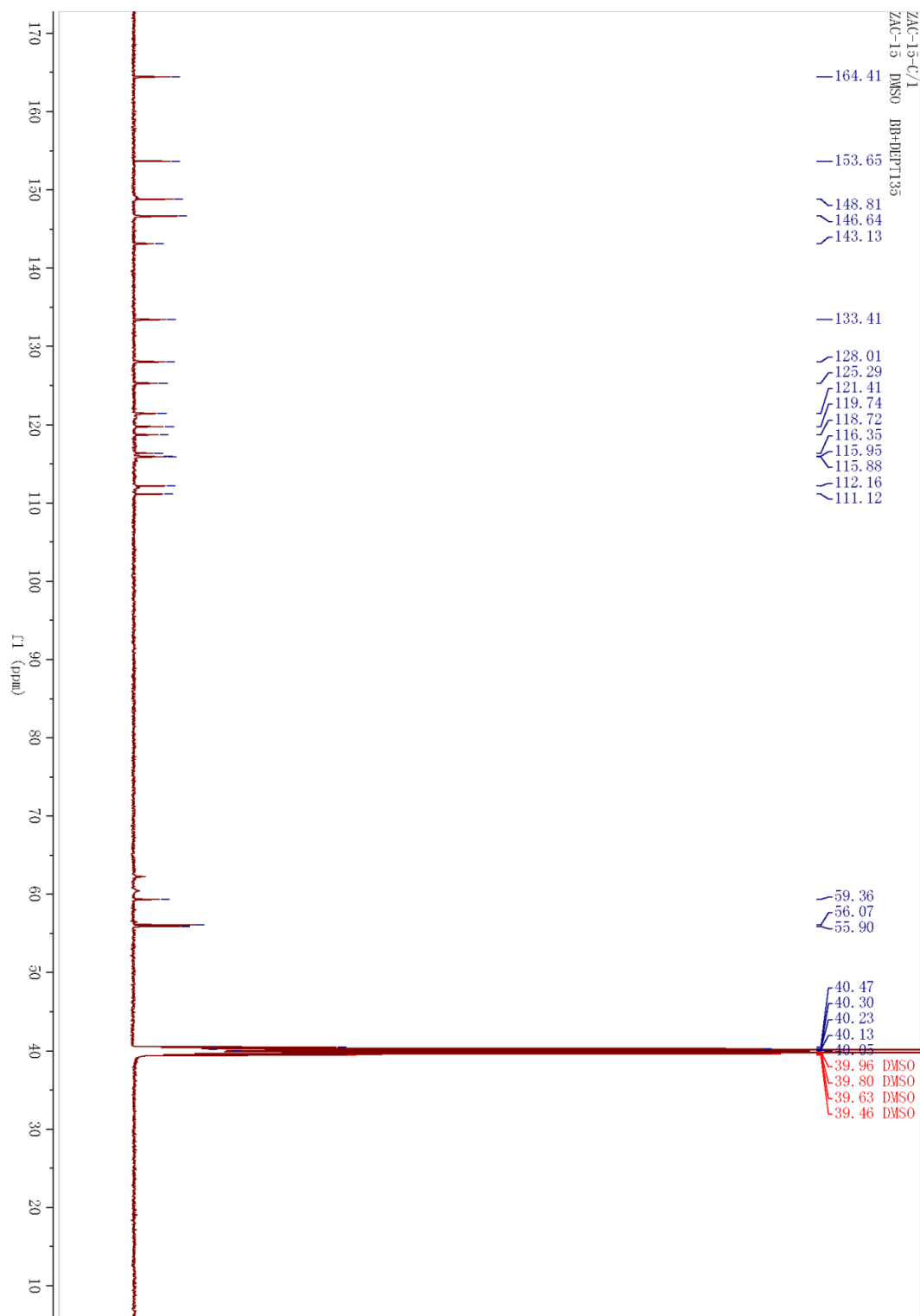
S43. LCMS spectrum of 2,5-bis(3-hydroxy-4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyrimido[4,5-*d*]pyrimidin-4(1*H*)-one (**4q**).



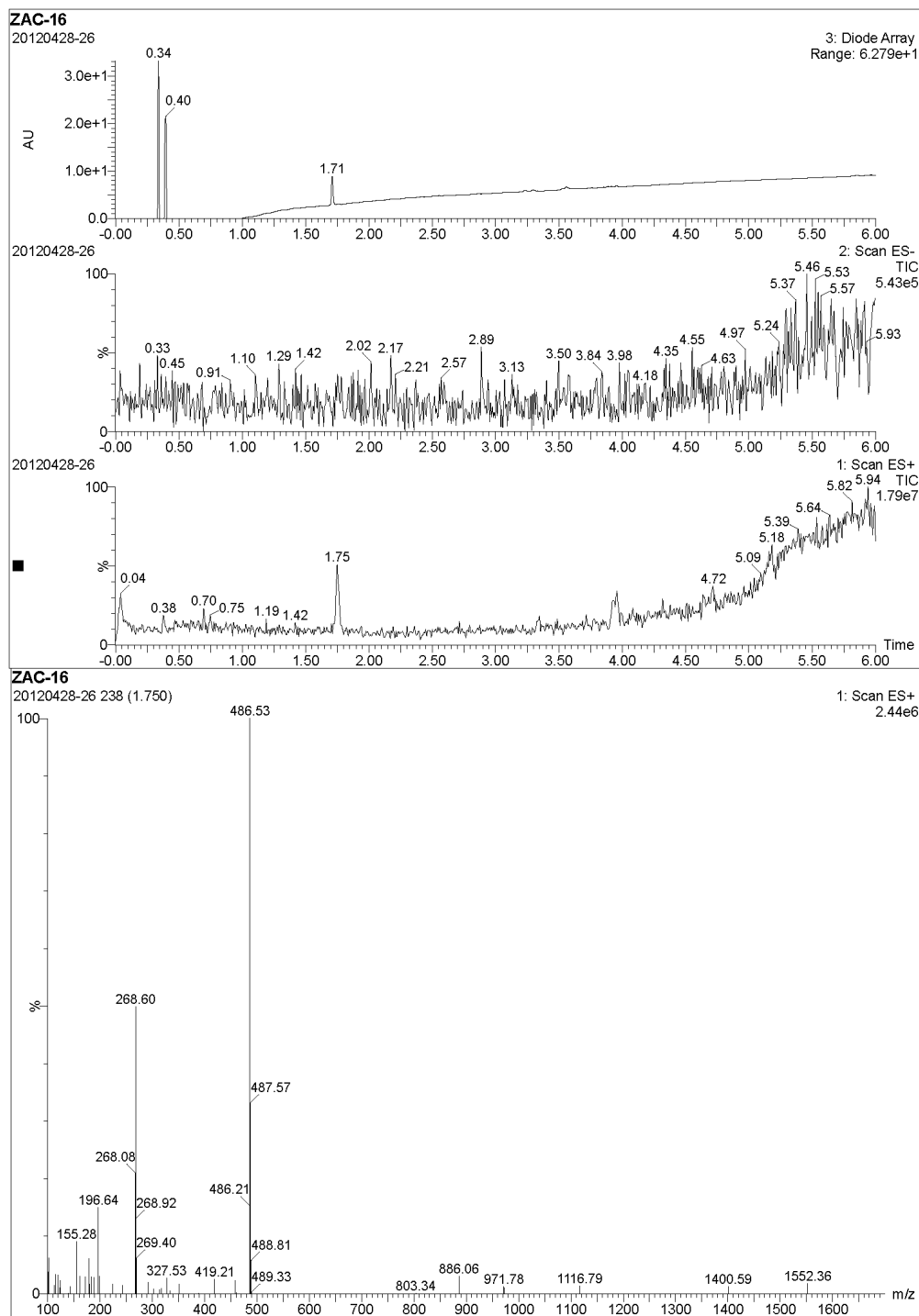
S44. ^1H NMR spectrum of
2,5-bis(3-hydroxy-4-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyr
imido[4,5-*d*]pyrimidin-4(1*H*)-one (**4q**) in $\text{DMSO-}d_6$.



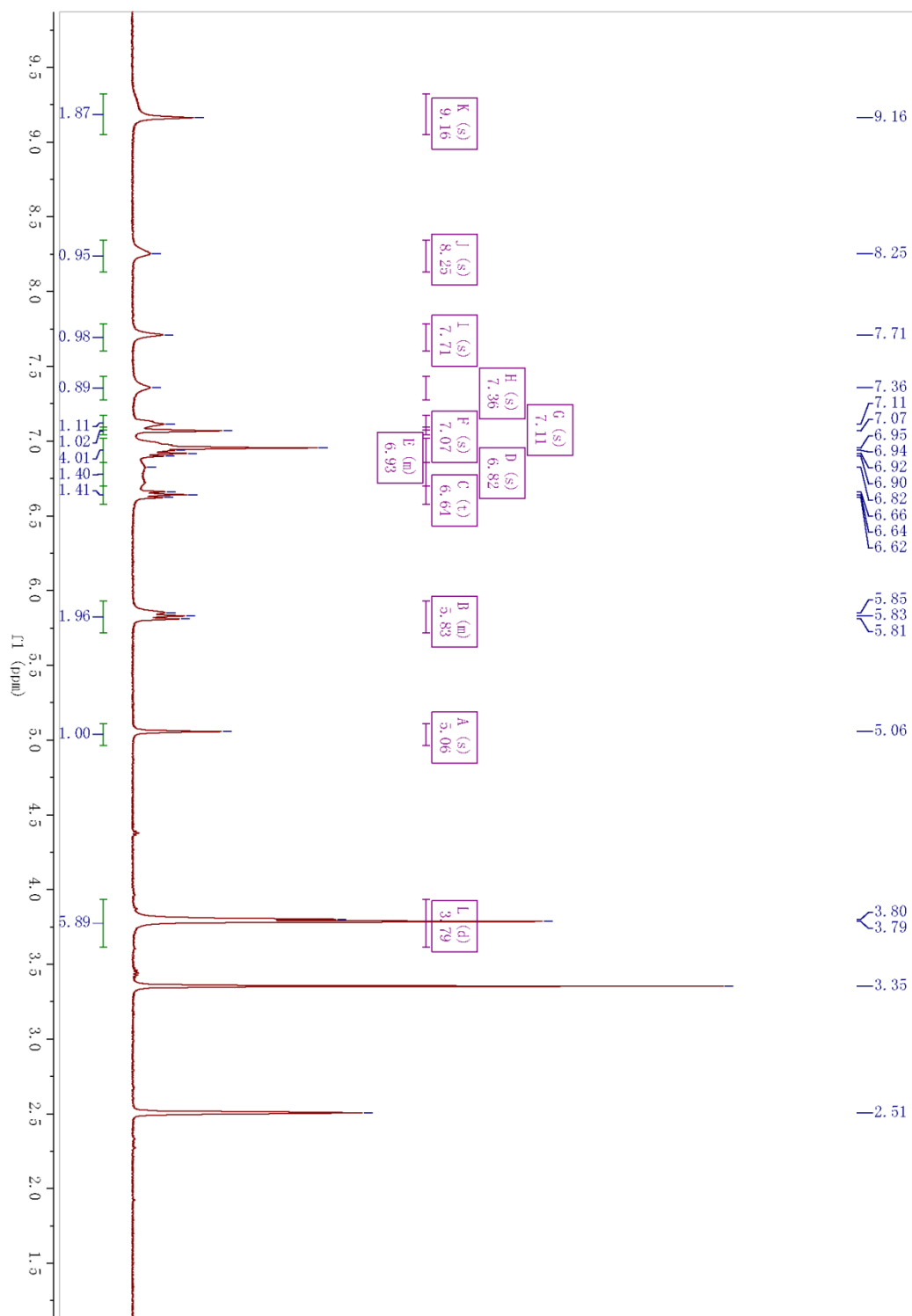
S45. ^{13}C NMR spectrum of ethyl 4-ethyl-2-methyl-1,4-dihydrobenzo[4,5]imidazo[1,2-*a*]pyrimidine-3-carboxylate (**5q**) in $\text{DMSO-}d_6$.



S46. LCMS spectrum of
2,5-bis(4-hydroxy-3-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyr
imido[4,5-*d*]pyrimidin-4(1*H*)-one (**4r**).



S47. ^1H NMR spectrum of
2,5-bis(4-hydroxy-3-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyr
imido[4,5-*d*]pyrimidin-4(1*H*)-one (**4r**) in $\text{DMSO-}d_6$.



S48. ^{13}C NMR spectrum of
2,5-bis(4-hydroxy-3-methoxyphenyl)-2,3,5,12-tetrahydrobenzo[4,5]imidazo[1,2-*a*]pyr
imido[4,5-*d*]pyrimidin-4(1*H*)-one (**4r**) in $\text{DMSO-}d_6$.

