New Journal of Chemistry

Supporting Information for

Synthesis of 1,3,4-Trisubstituted Pyrrolidines as Meropenem Adjuvants Targeting New Delhi Metallo-β-lactamase

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Figure S1. ^{1}H and ^{13}C NMR spectra of **methyl ferulate (4b)**

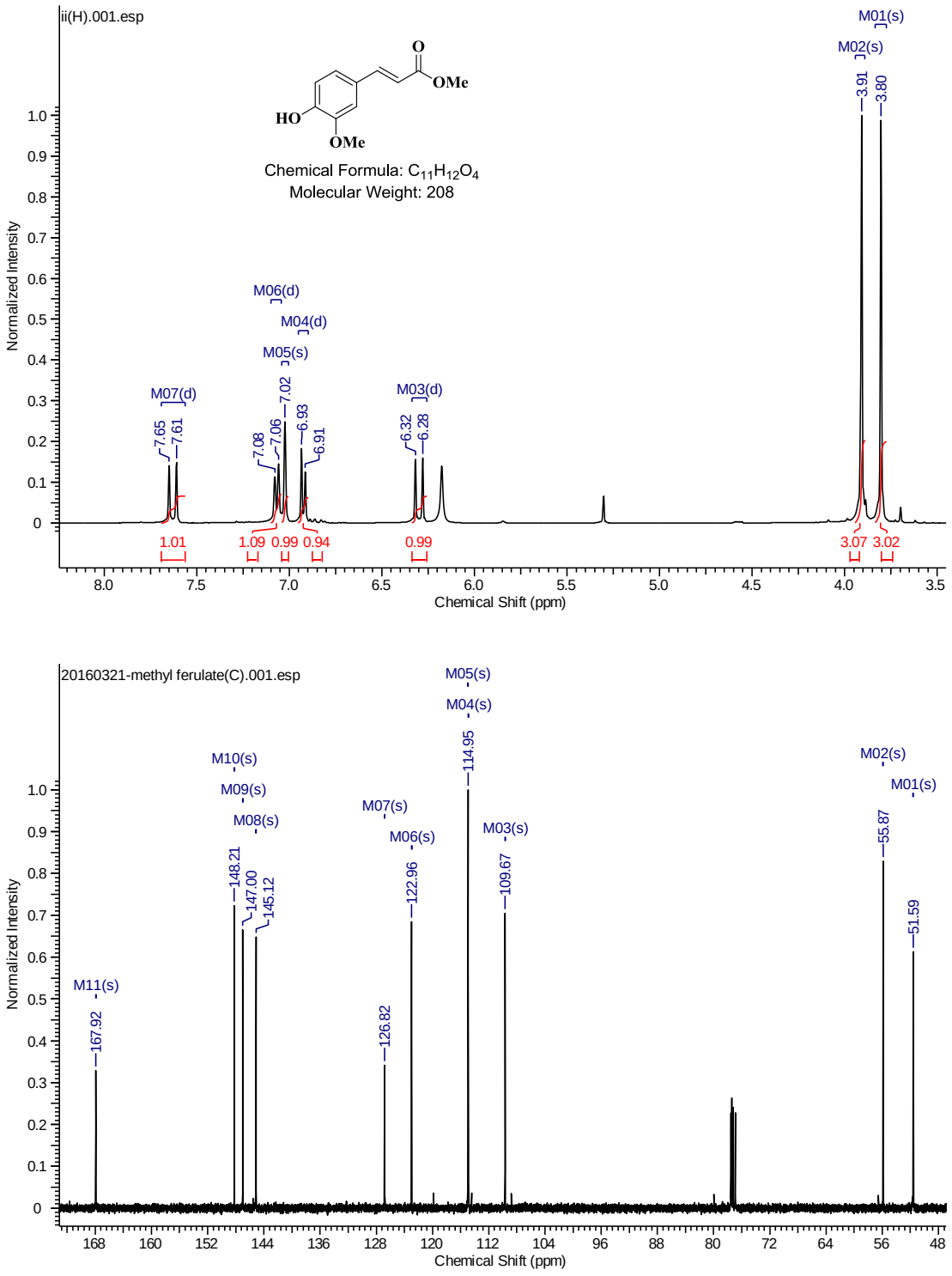


Figure S2. ^{1}H and ^{13}C NMR spectra of **(*E*)-methyl 3-(4-(benzyloxy)-3-methoxyphenyl)acrylate (5a)**

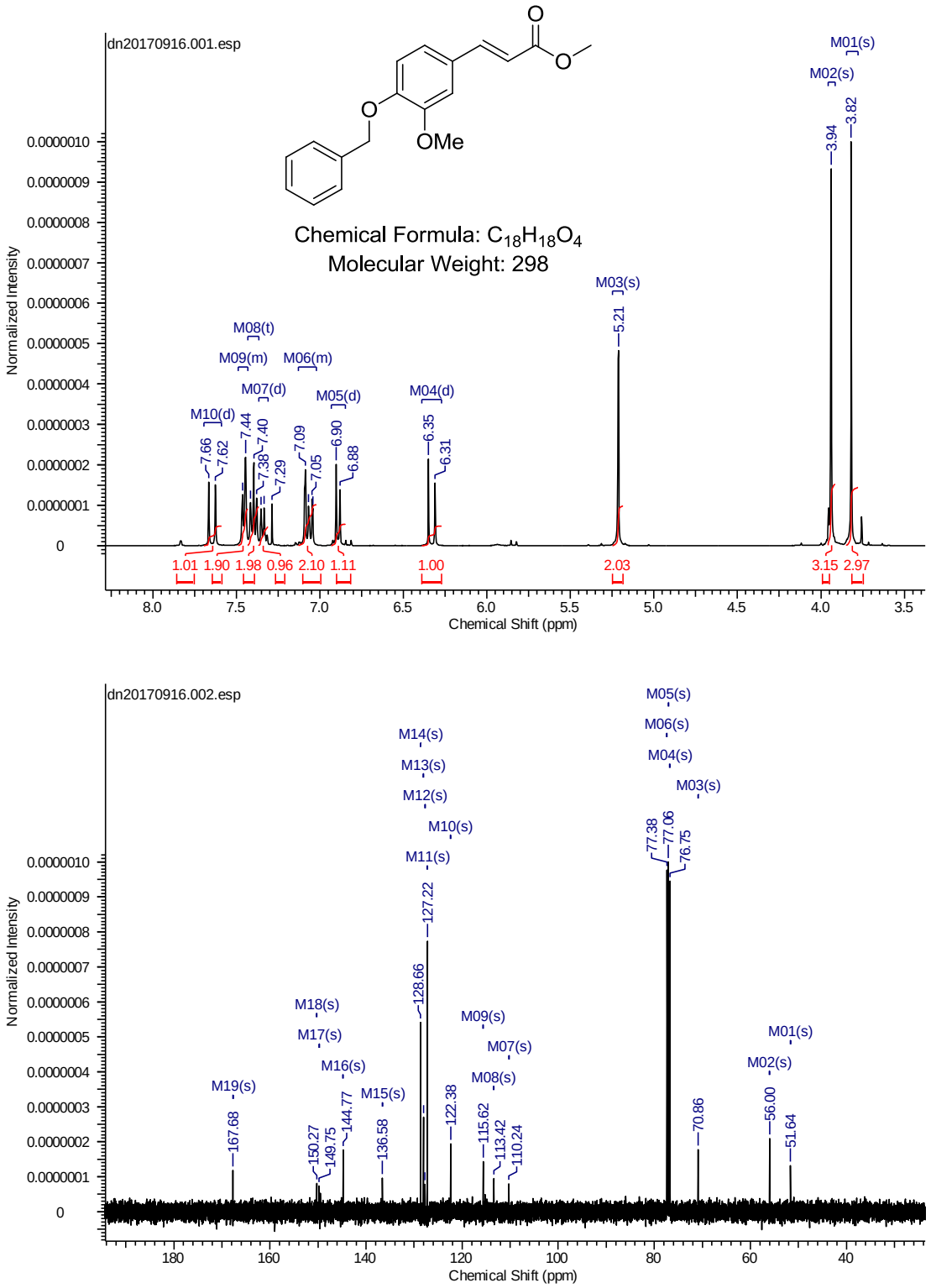


Figure S3. ^{1}H and ^{13}C NMR spectra of **(*E*)-methyl 3-(4-(allyloxy)-3-methoxyphenyl)acrylate (5b)**

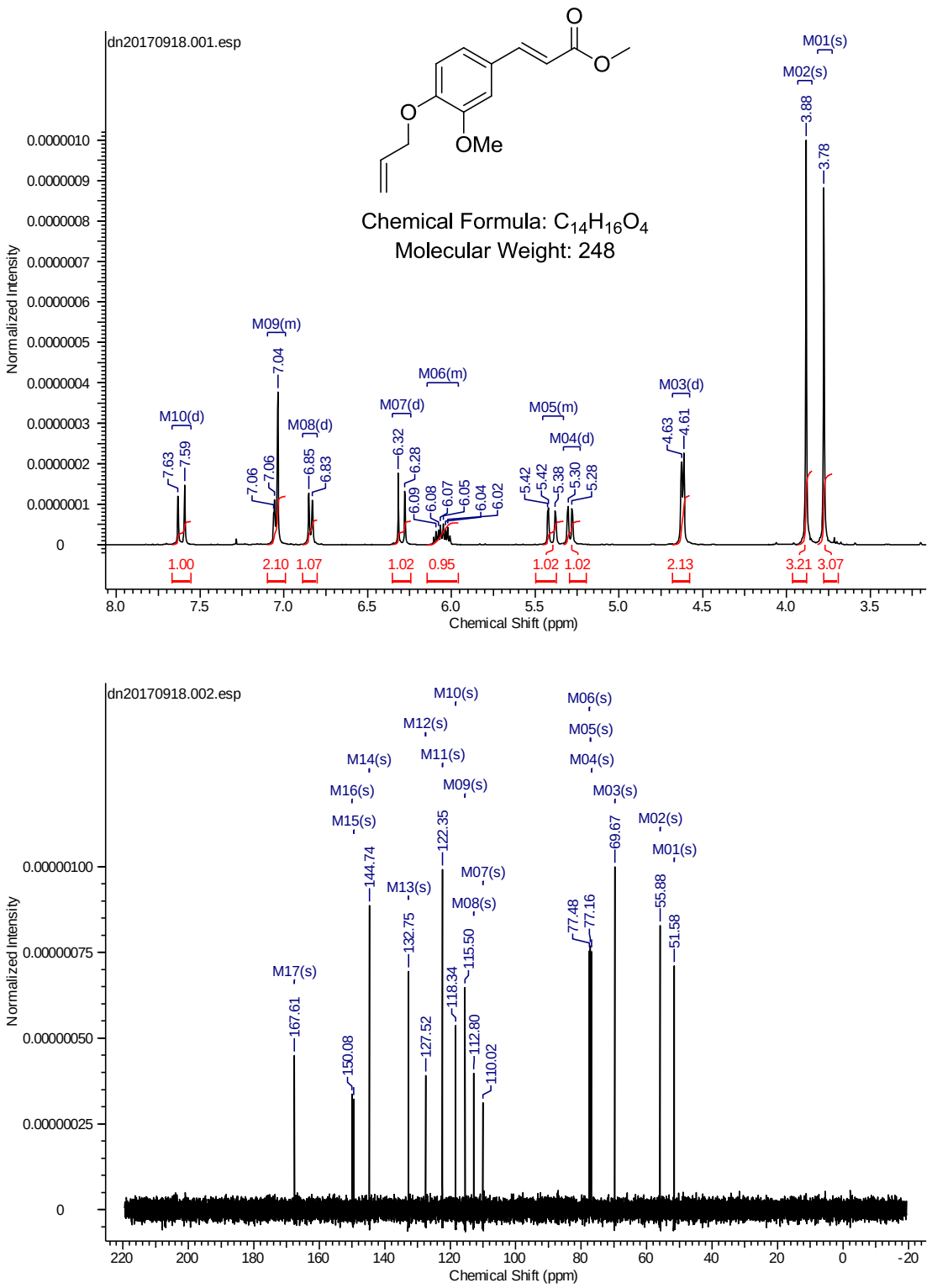


Figure S4. ^{1}H and ^{13}C NMR spectra of **(*E*)-methyl 3-(3-methoxy-4-((methylsulfonyl)oxy)phenyl)acrylate (5c)**

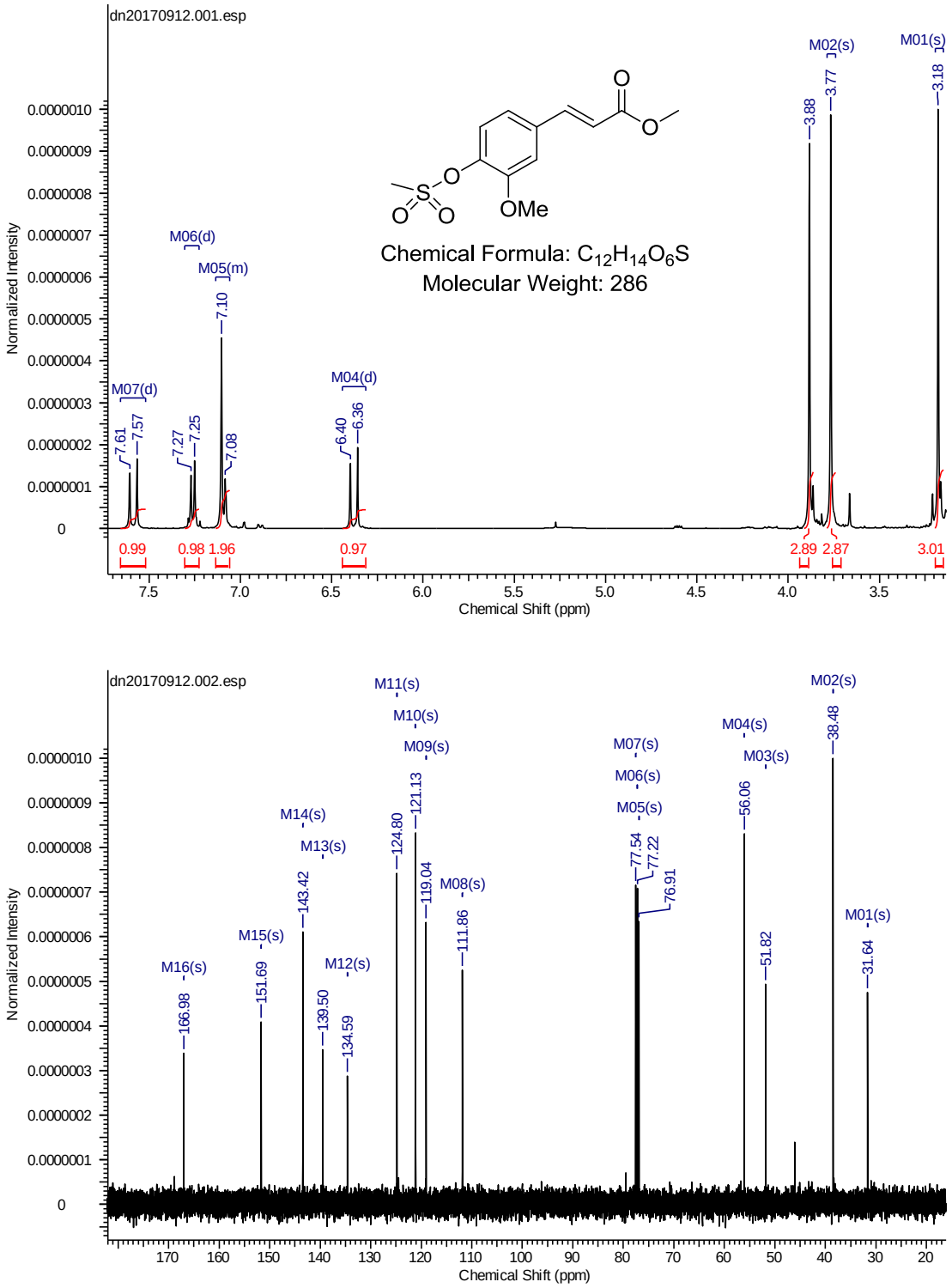


Figure S5. ^{1}H and ^{13}C NMR spectra of **(*E*)-methyl 3-(4-acetoxy-3-methoxyphenyl)acrylate (5d)**

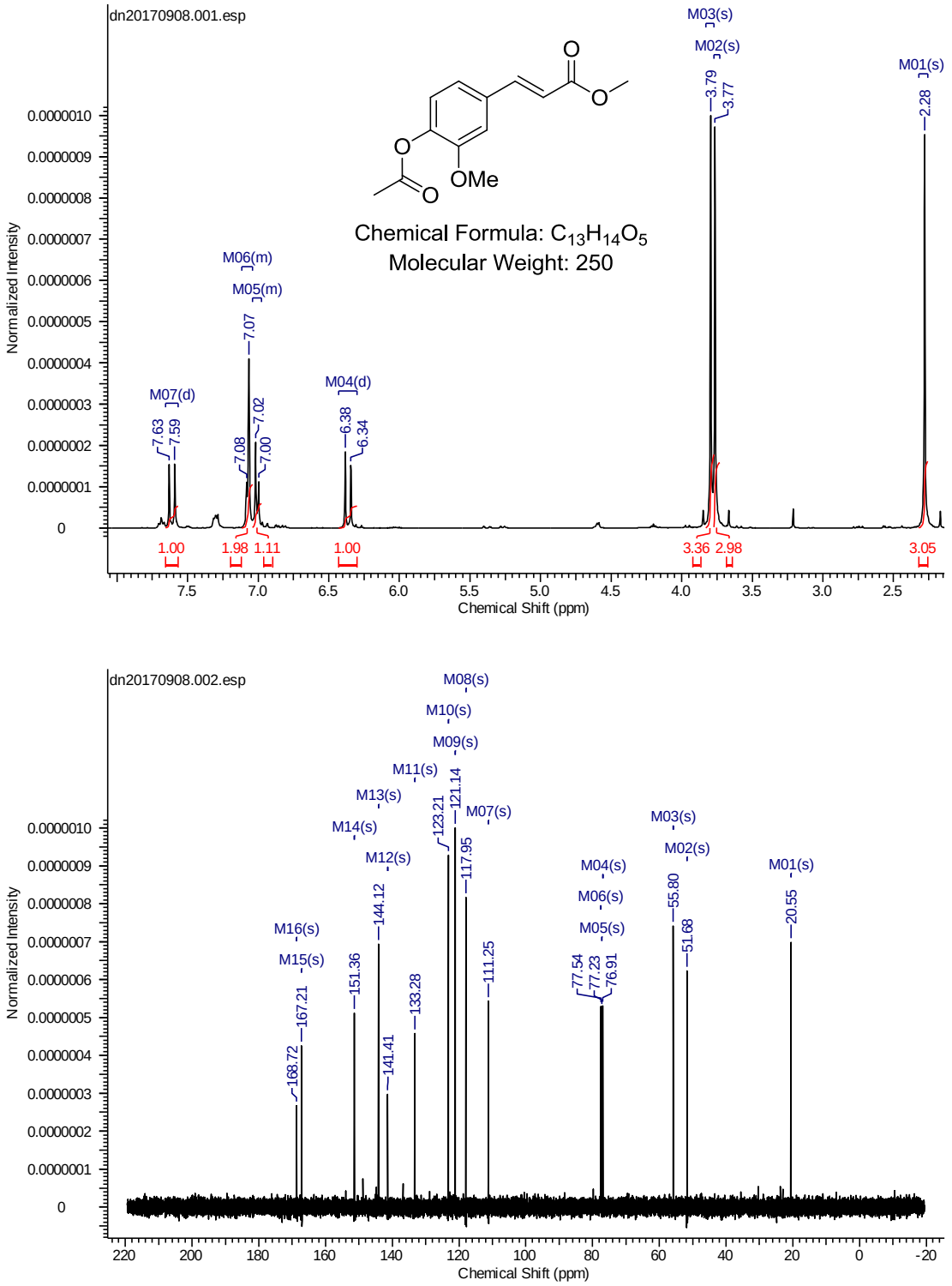


Figure S6. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 1-benzyl-4-(4-(benzyloxy)-3-methoxyphenyl)pyrrolidine-3-carboxylate (6a)**

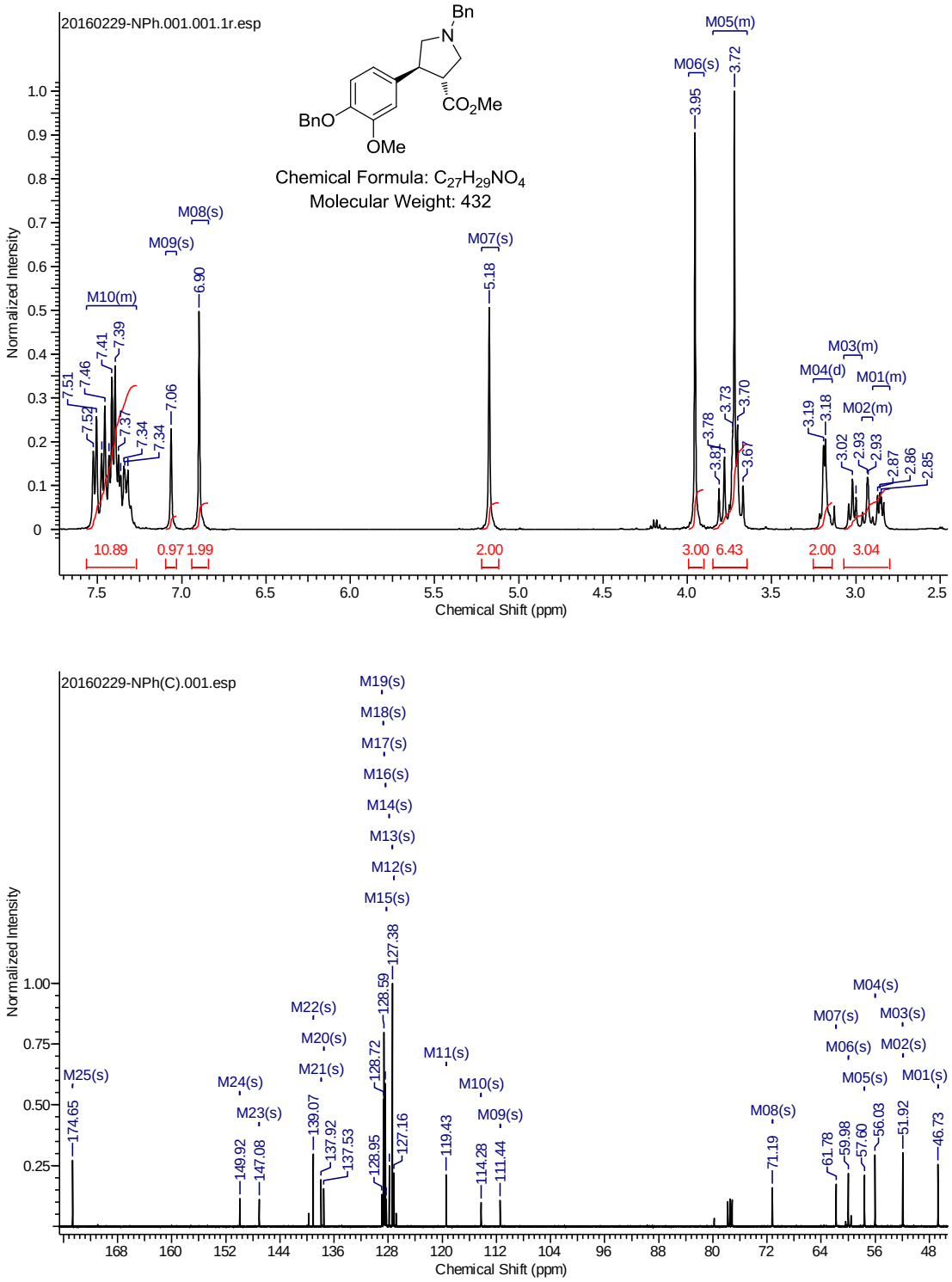


Figure S7. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(allyloxy)-3-methoxyphenyl)-1-benzylpyrrolidine-3-carboxylate (6b)**

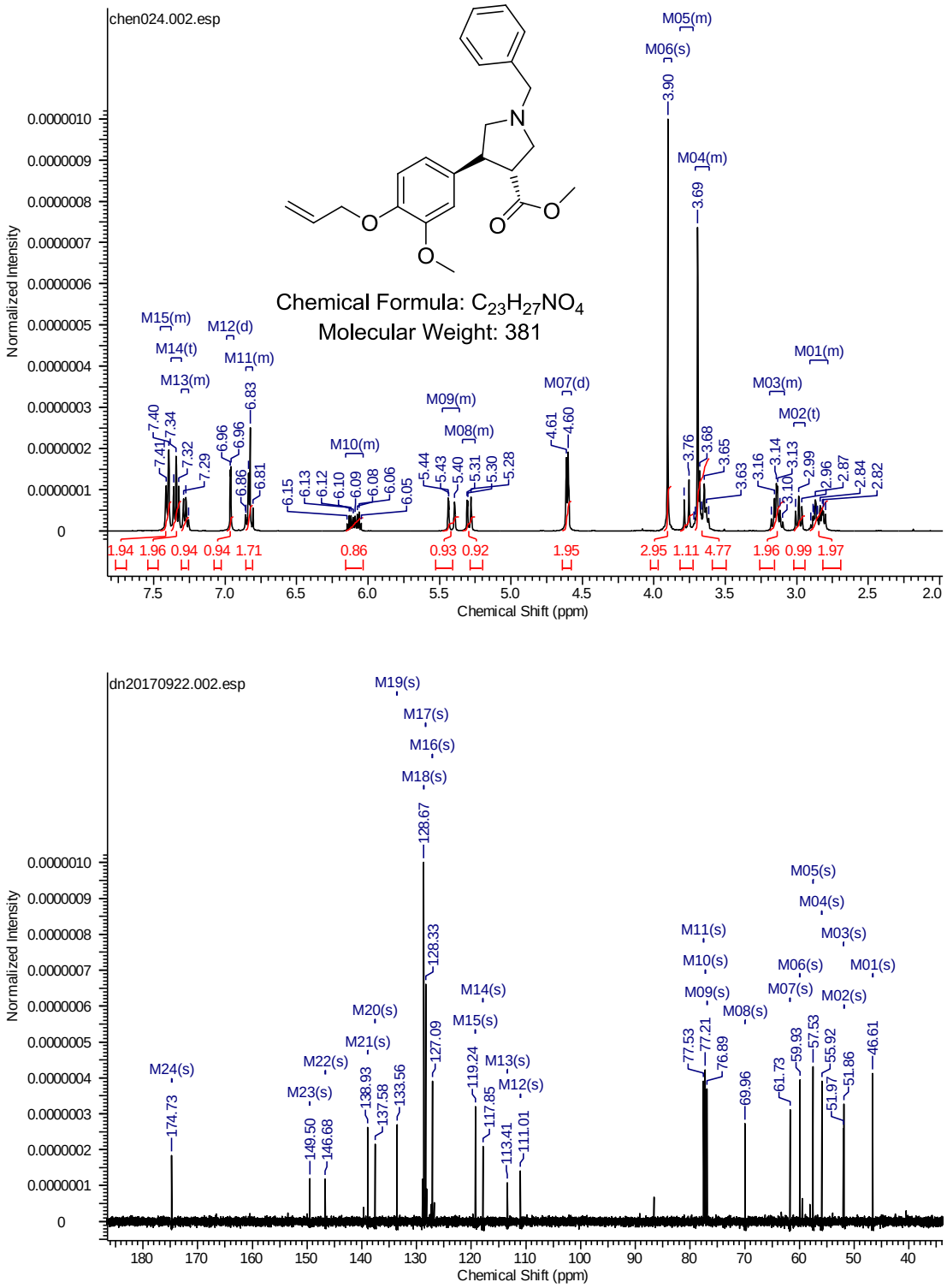


Figure S8. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 1-benzyl-4-(3-methoxy-4-((methylsulfonyl)oxy)phenyl)pyrrolidine-3-carboxylate (6c)**

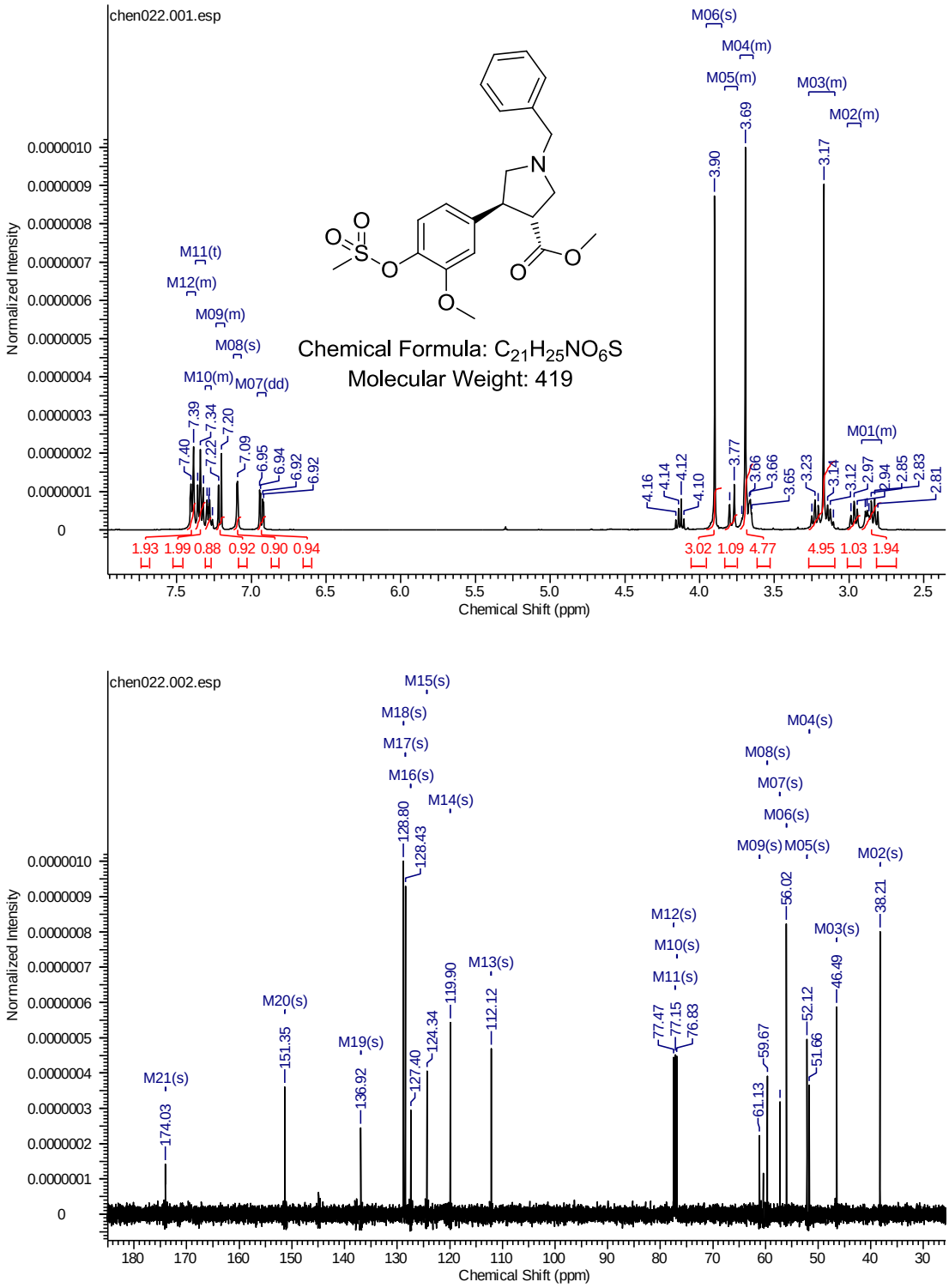


Figure S9. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-acetoxy-3-methoxyphenyl)-1-benzylpyrrolidine-3-carboxylate (6d)**

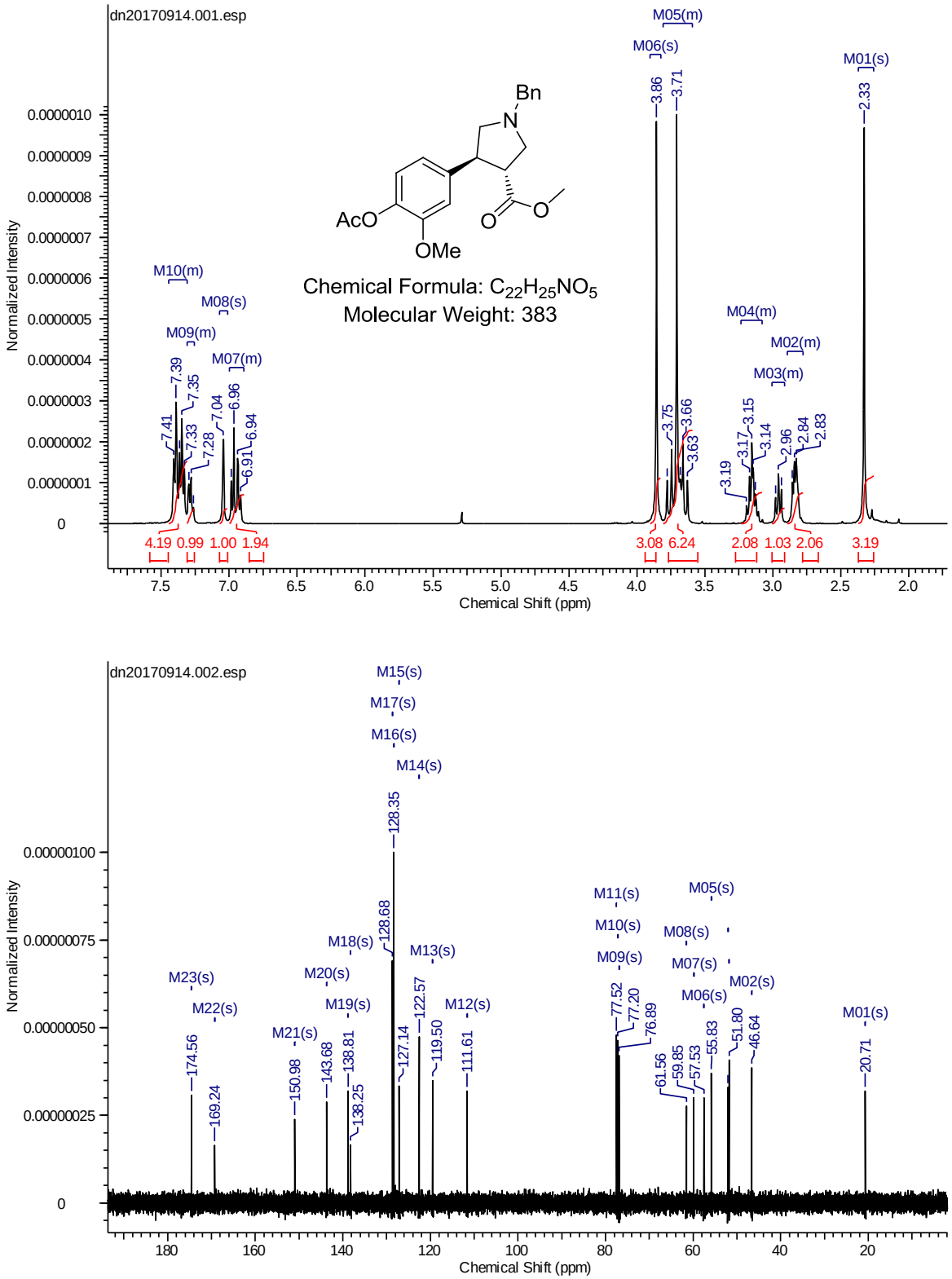


Figure S10. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)pyrrolidine-3-carboxylate (7a)**

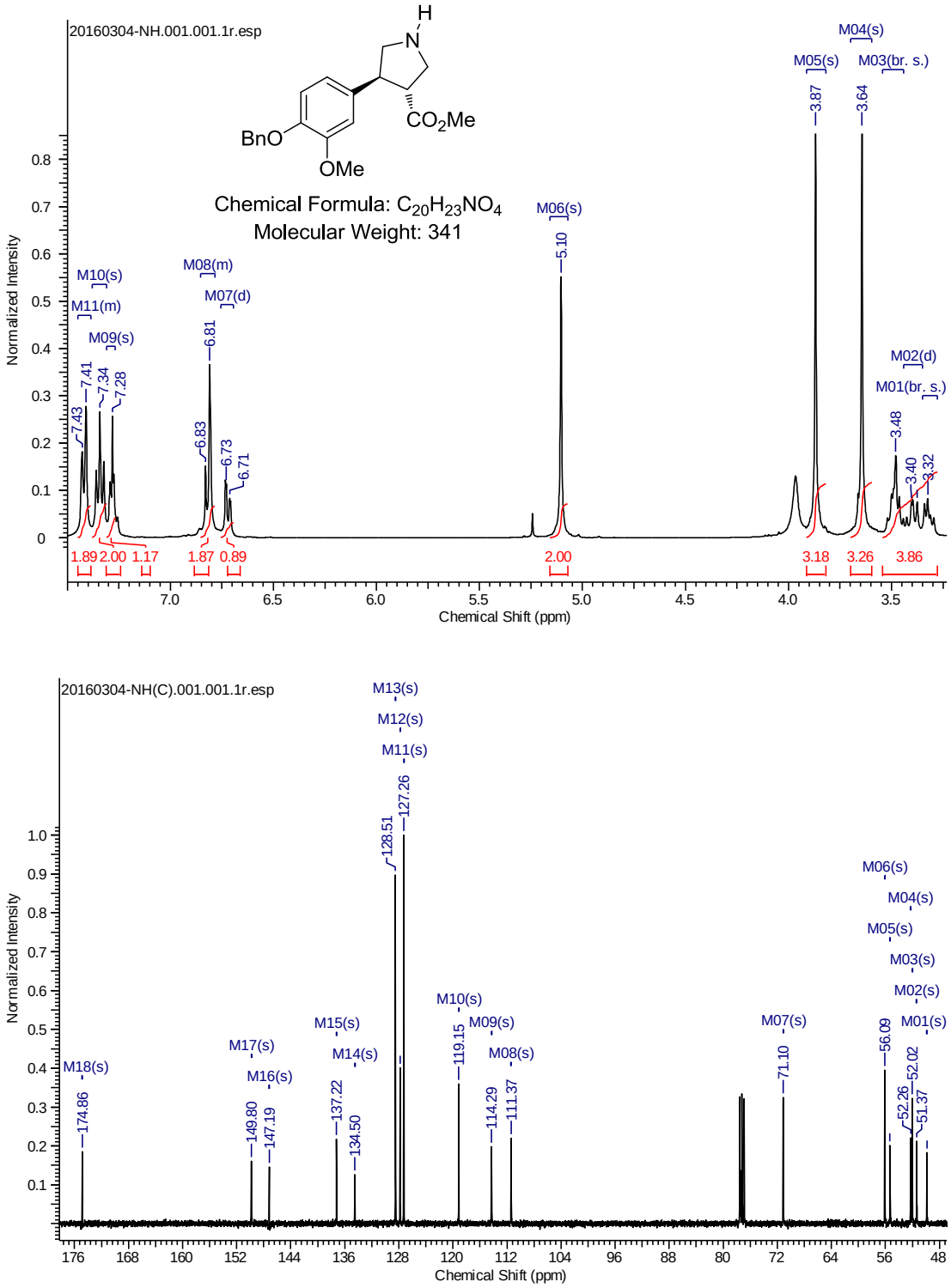


Figure S11. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-(dimethoxyphosphoryl)pyrrolidine-3-carboxylate (8a)**

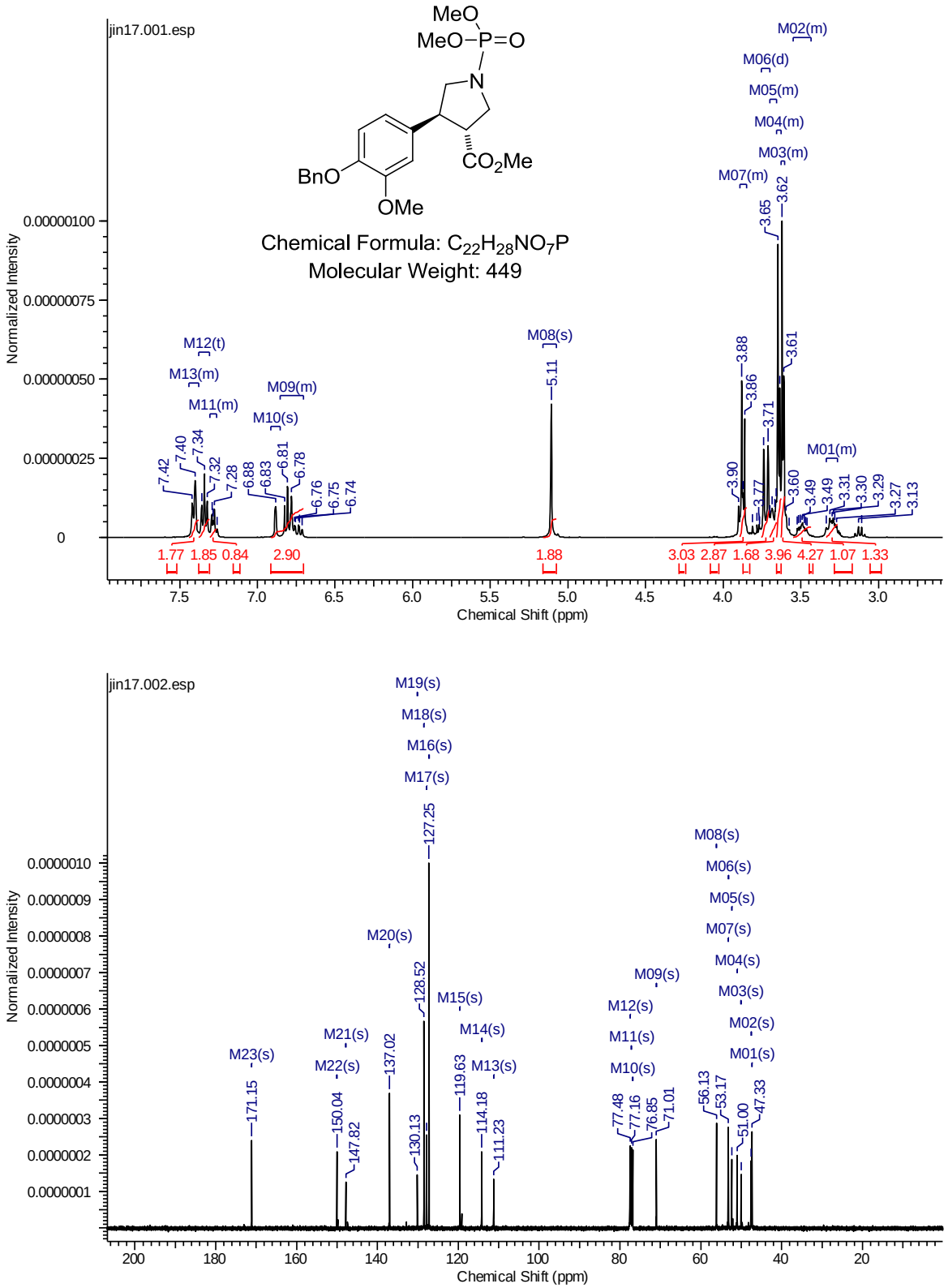


Figure S12. ^{1}H spectrum of **(±)-*trans*-methyl 4-(4-(allyloxy)-3-methoxyphenyl)-1-(dimethoxyphosphoryl)pyrrolidine-3-carboxylate (8b)**

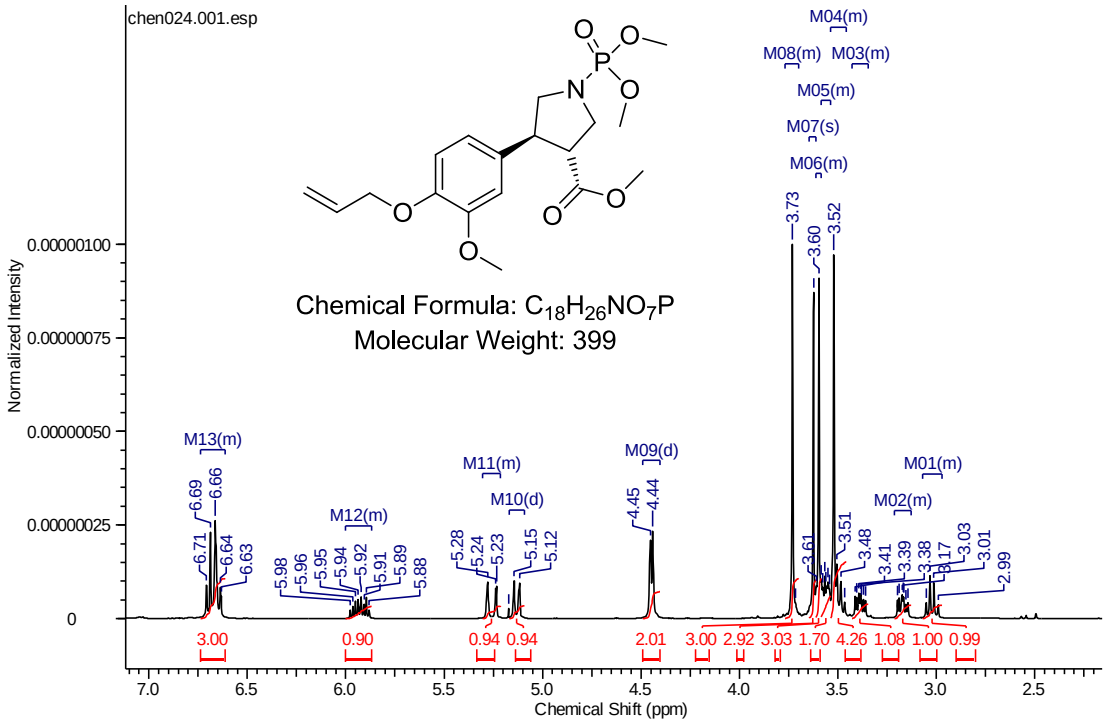


Figure S13. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 1-(dimethoxyphosphoryl)-4-(3-methoxy-4-((methylsulfonyl)oxy)phenyl)pyrrolidine-3-carboxylate (8c)**

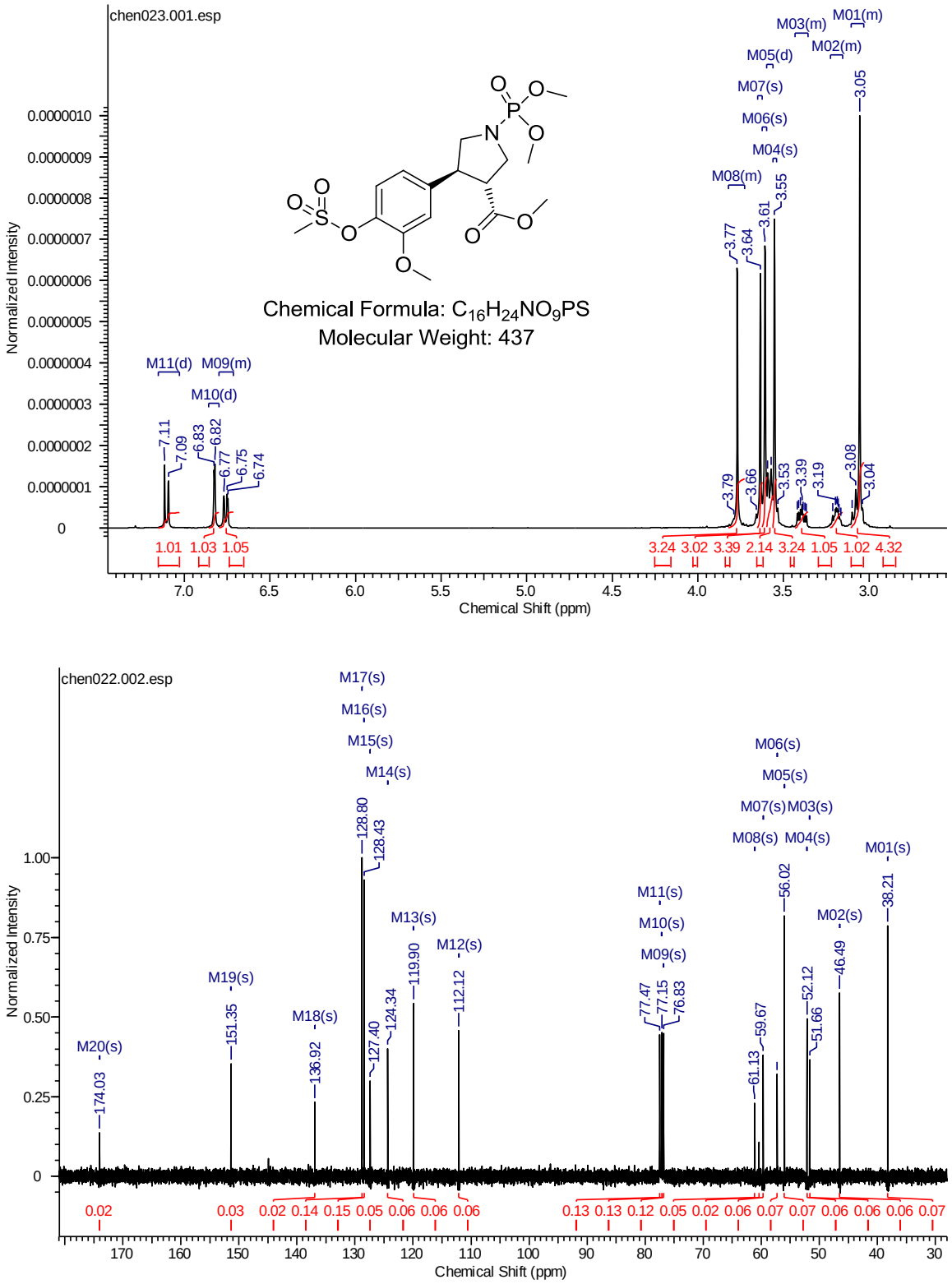


Figure S14. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-acetoxy-3-methoxyphenyl)-1-(dimethoxyphosphoryl)pyrrolidine-3-carboxylate (8d)**

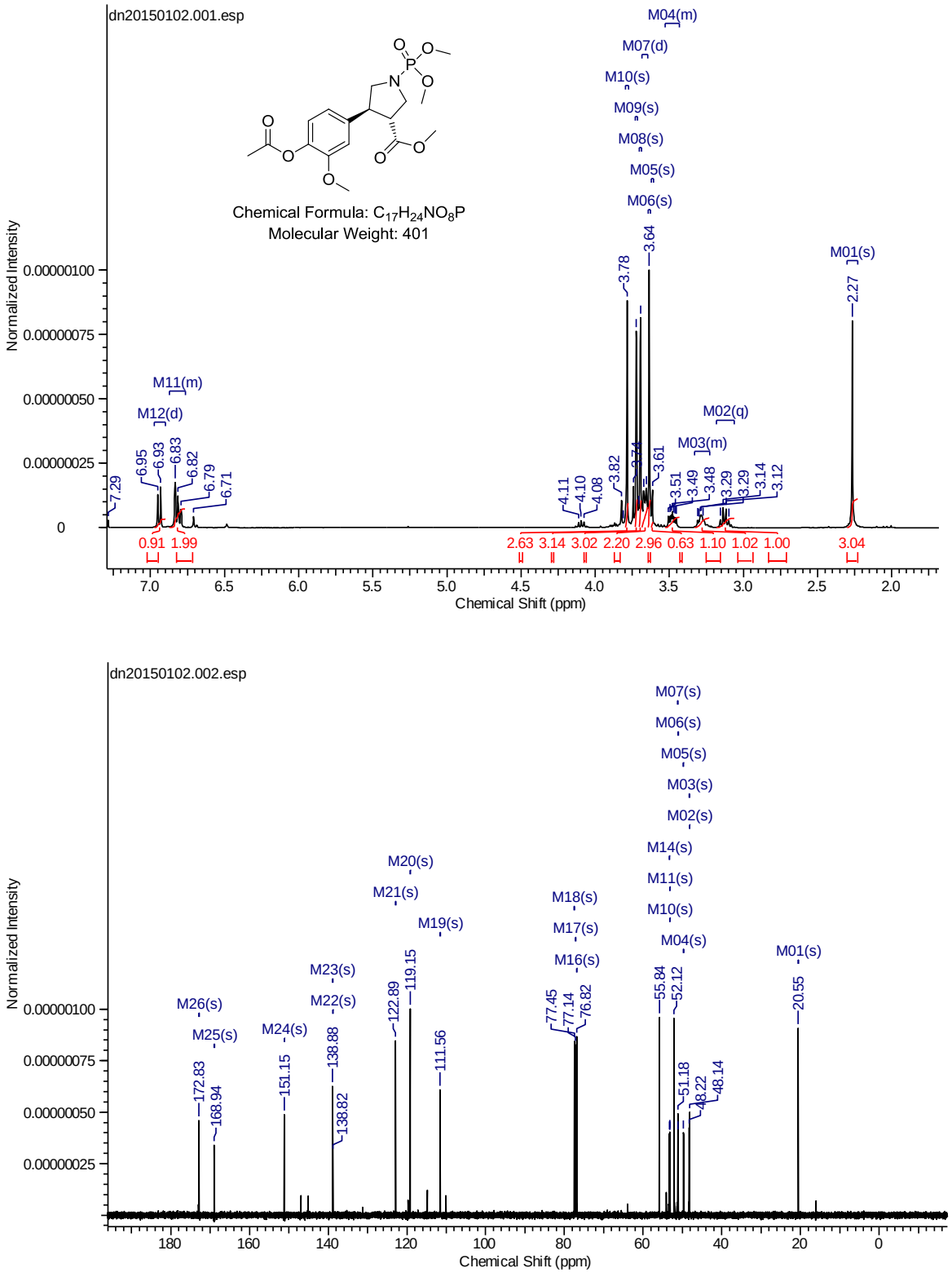


Figure S15. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-1-ethyl 3-methyl 4-(4-benzyloxy)-3-methoxyphenyl)pyrrolidine-1,3-dicarboxylate (7e)**

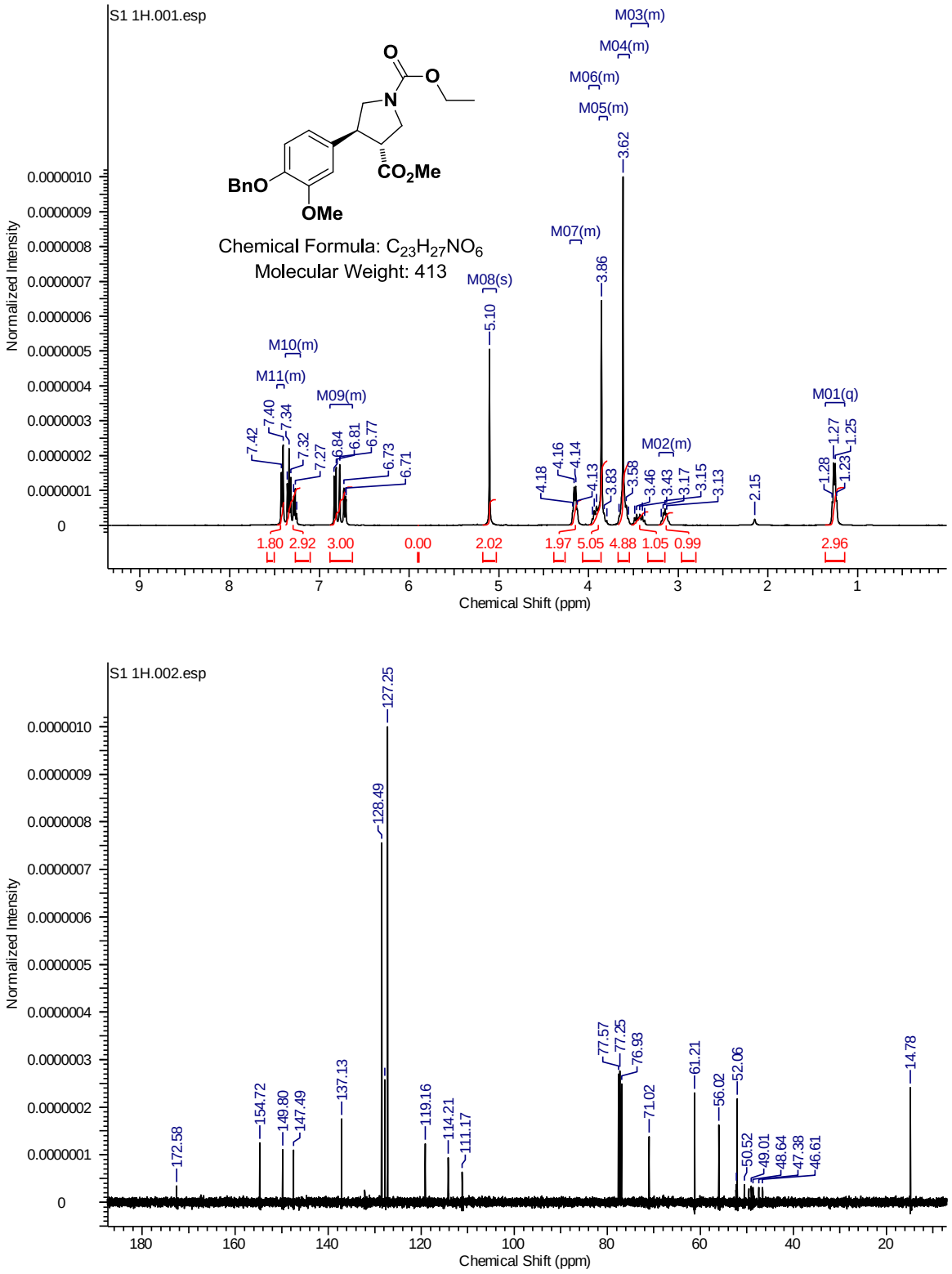


Figure S16. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-4-(4-(benzyloxy)-3-methoxyphenyl)-1-(ethoxycarbonyl)pyrrolidine-3-carboxylic acid (7g)**

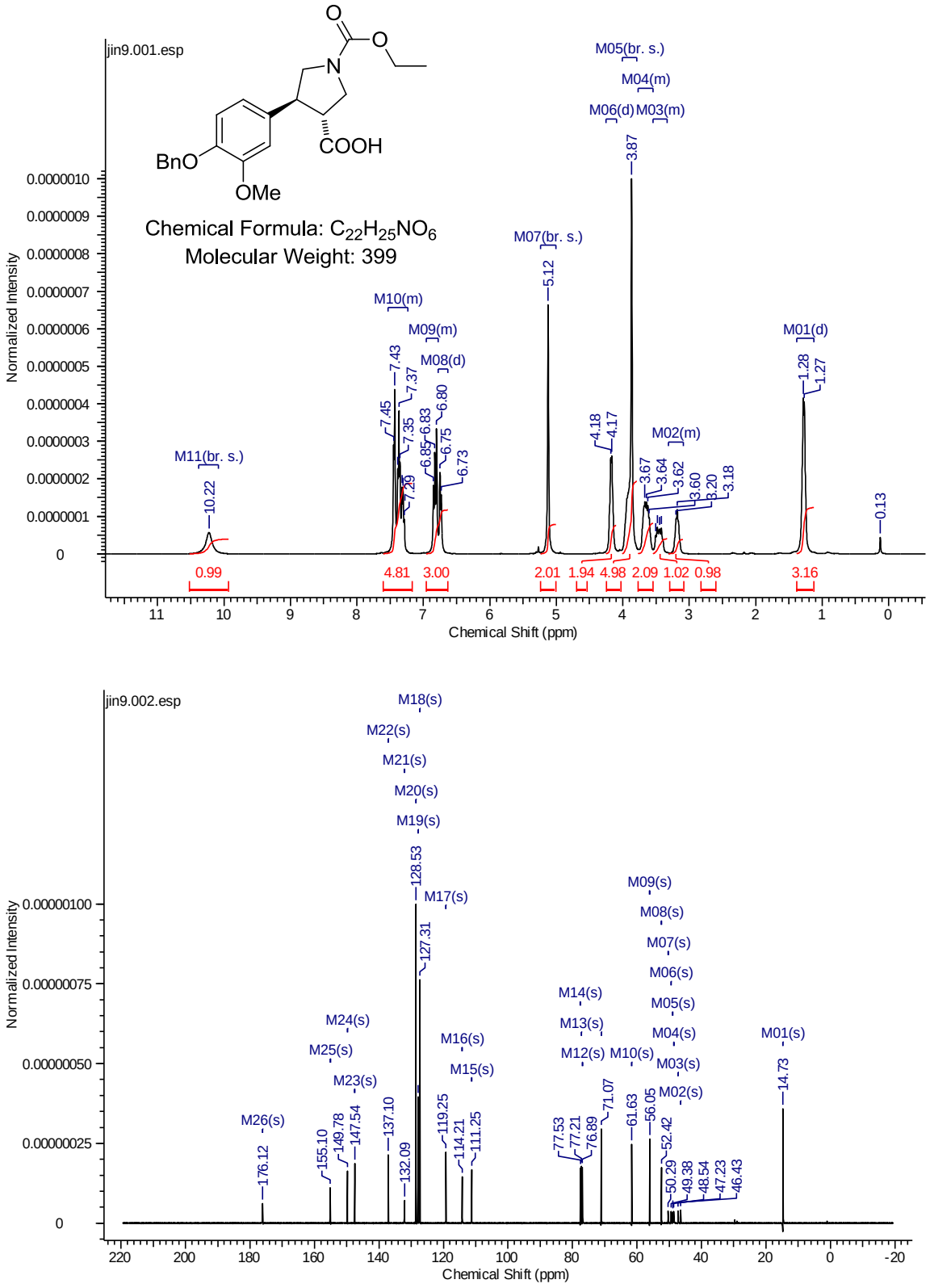


Figure S17. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-ethyl 3-(4-(benzyloxy)-3-methoxyphenyl)-4-carbamoylpyrrolidine-1-carboxylate (7h)**

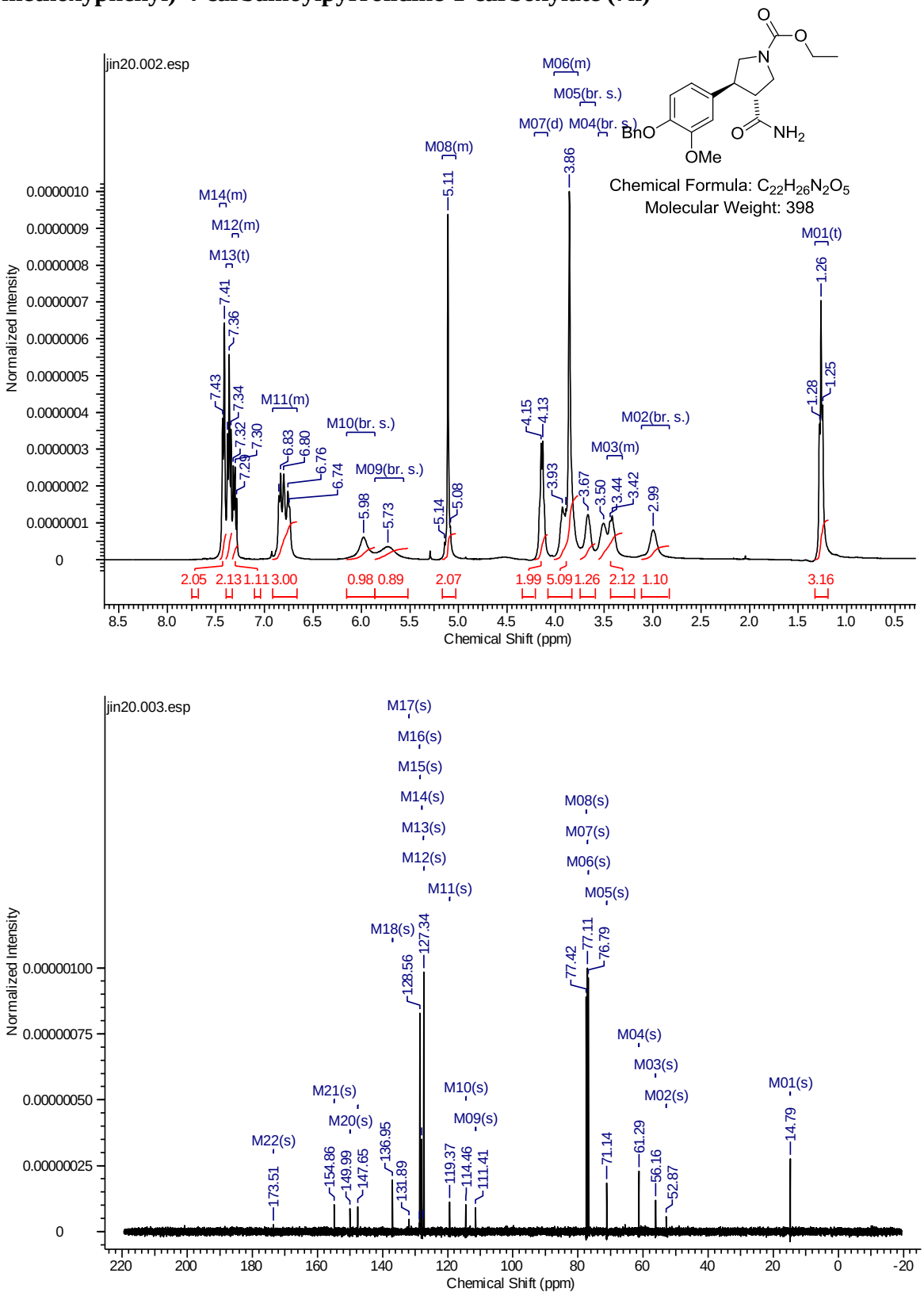


Figure S18. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-ethyl 3-(4-(benzyloxy)-3-methoxyphenyl)-4-(hydroxymethyl)pyrrolidine-1-carboxylate (7f)**

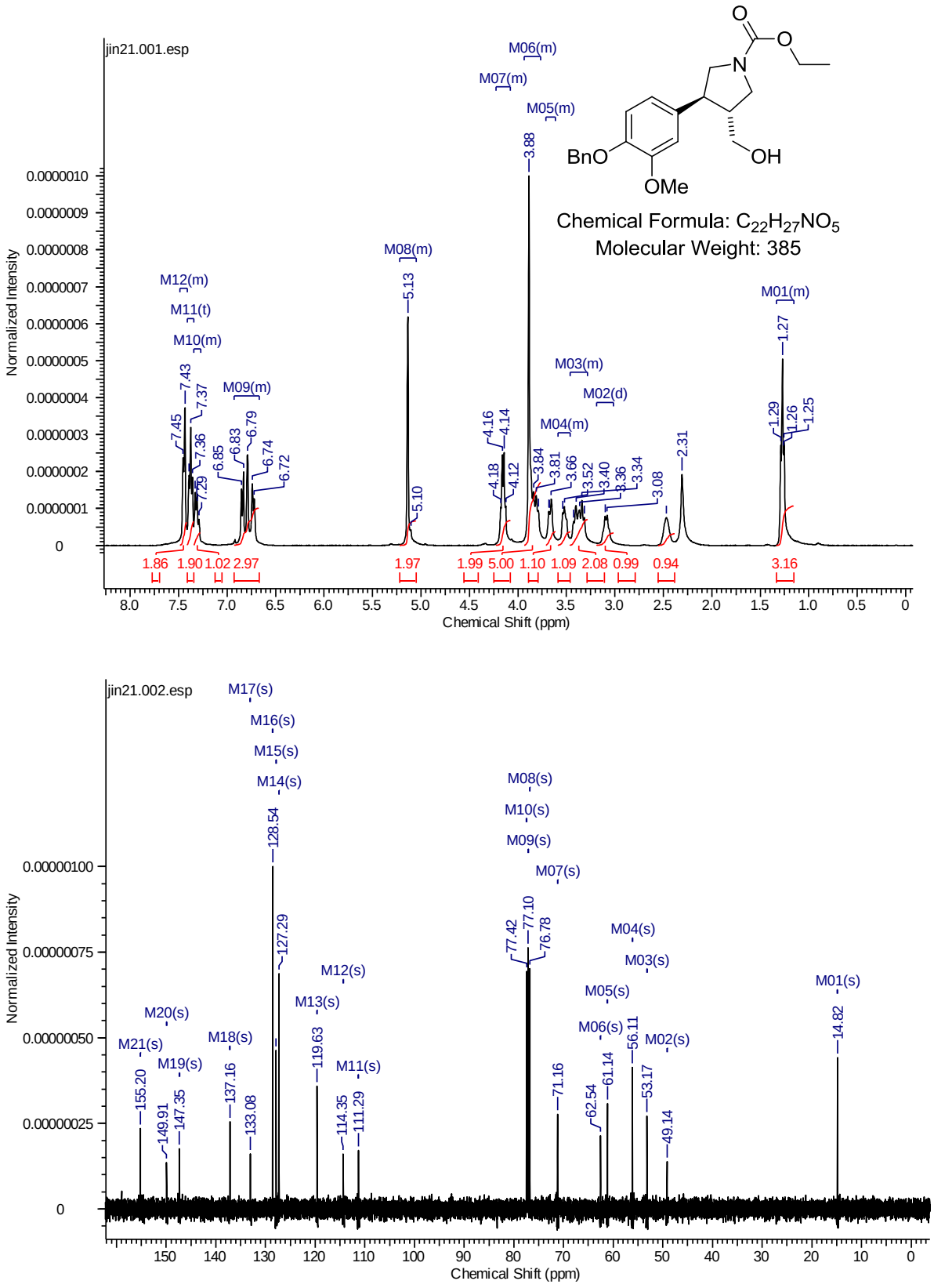


Figure S19. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-1-ethyl 3-methyl 4-(4-hydroxy-3-methoxyphenyl)pyrrolidine-1,3-dicarboxylate (7i)**

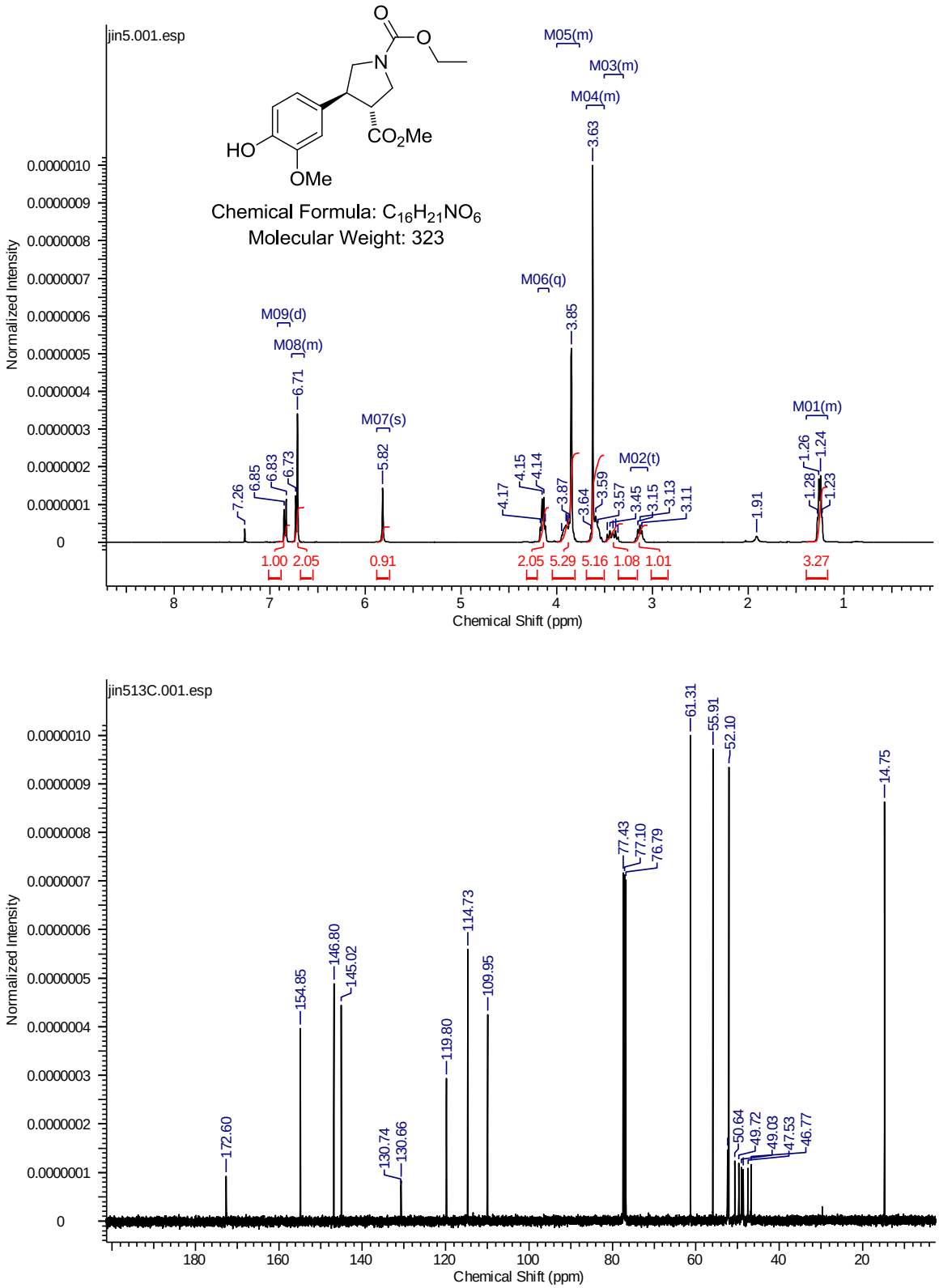


Figure S20. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-1-(ethoxycarbonyl)-4-(4-hydroxy-3-methoxyphenyl)pyrrolidine-3-carboxylic acid (7j)**

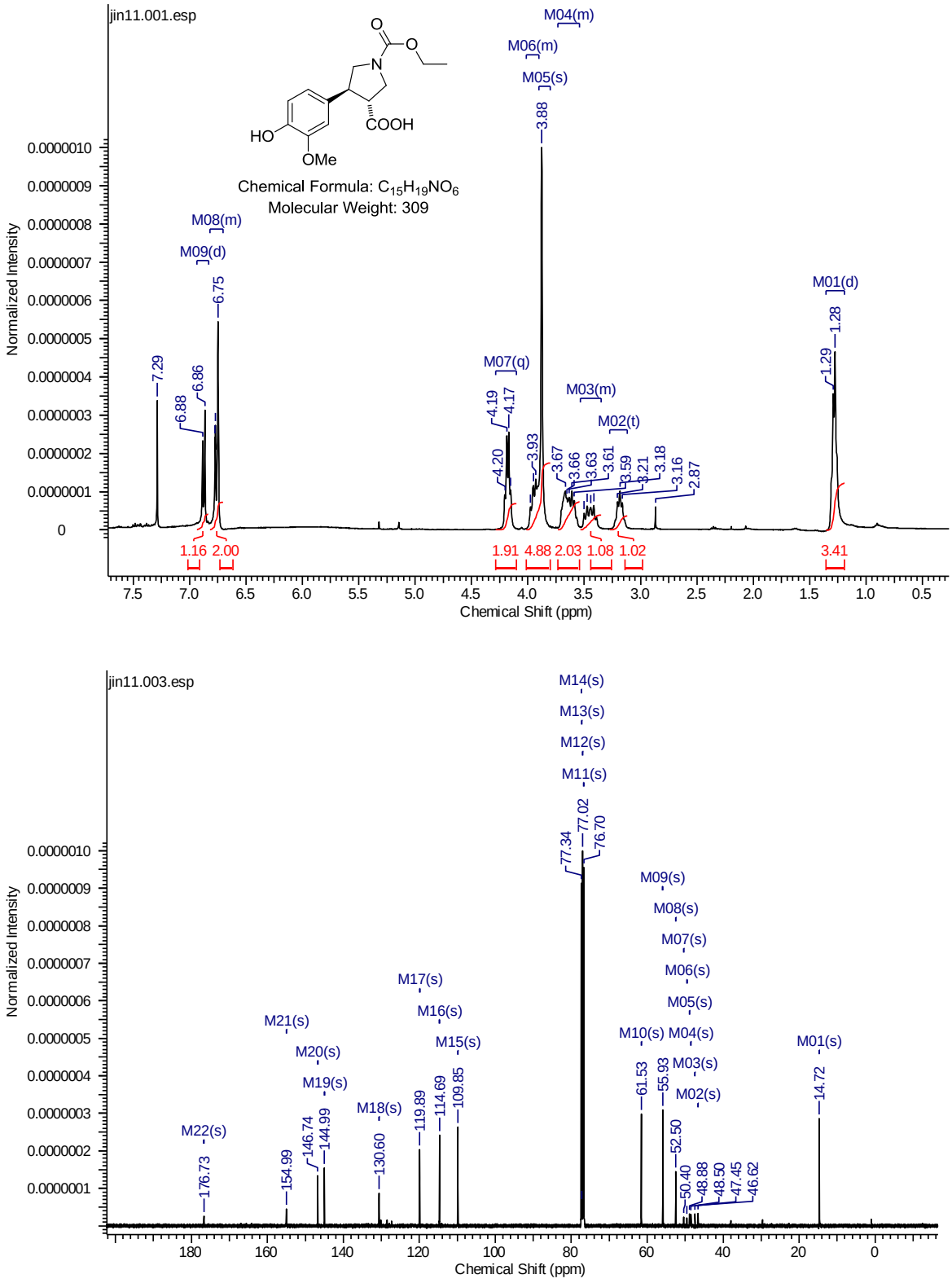
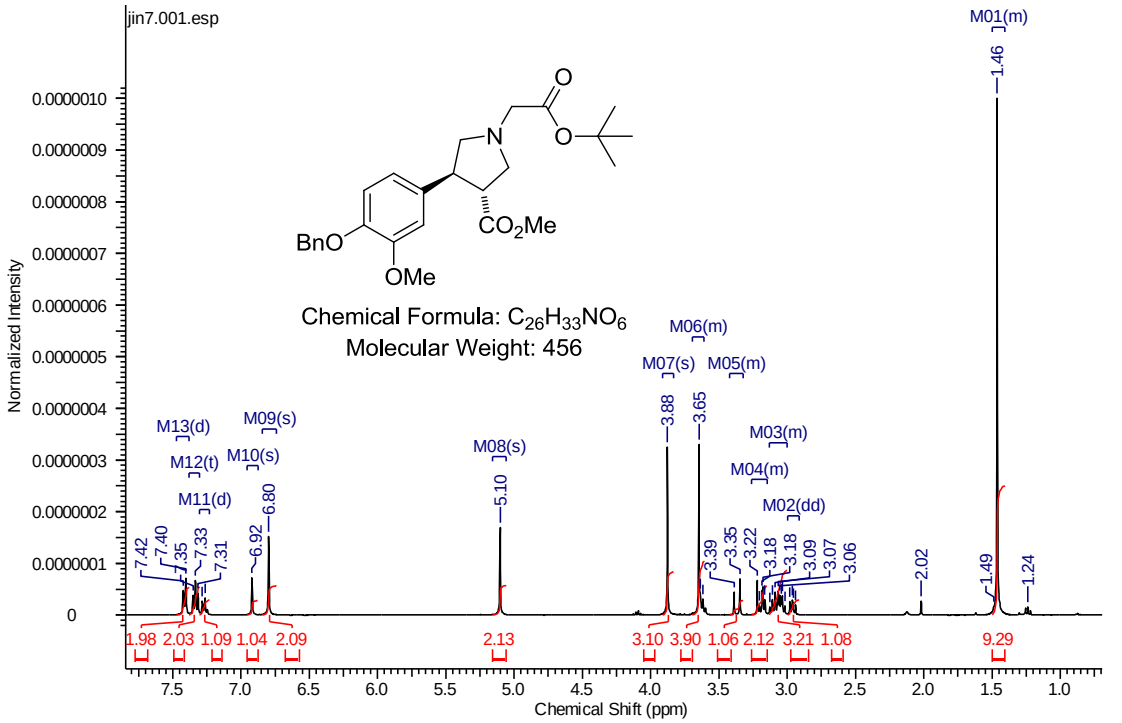


Figure S21. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-(2-(*tert*-butoxy)-2-oxoethyl)pyrrolidine-3-carboxylate (8e)**



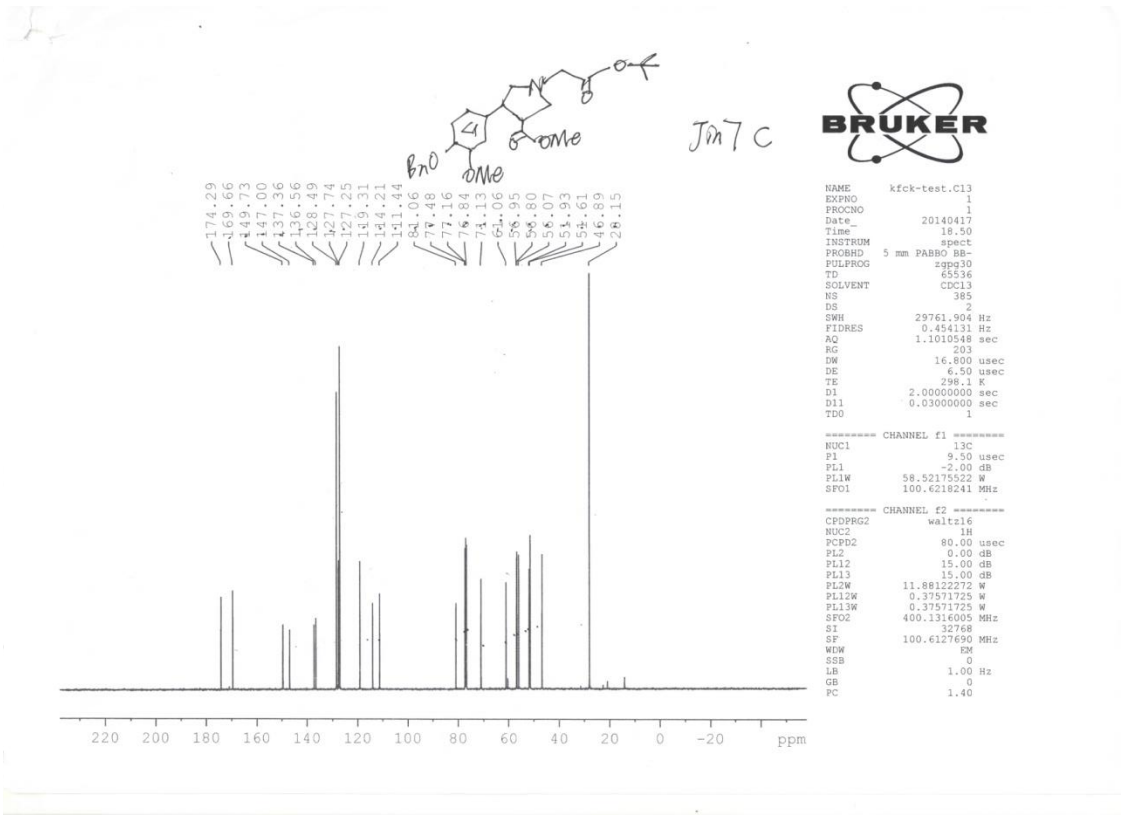


Figure S22. ^{1}H and ^{13}C NMR spectra of **2-((±)-*trans*-3-(4-benzyloxy)-3-methoxyphenyl)-4-(methoxycarbonyl)pyrrolidin-1-yl)acetic acid (8g)**

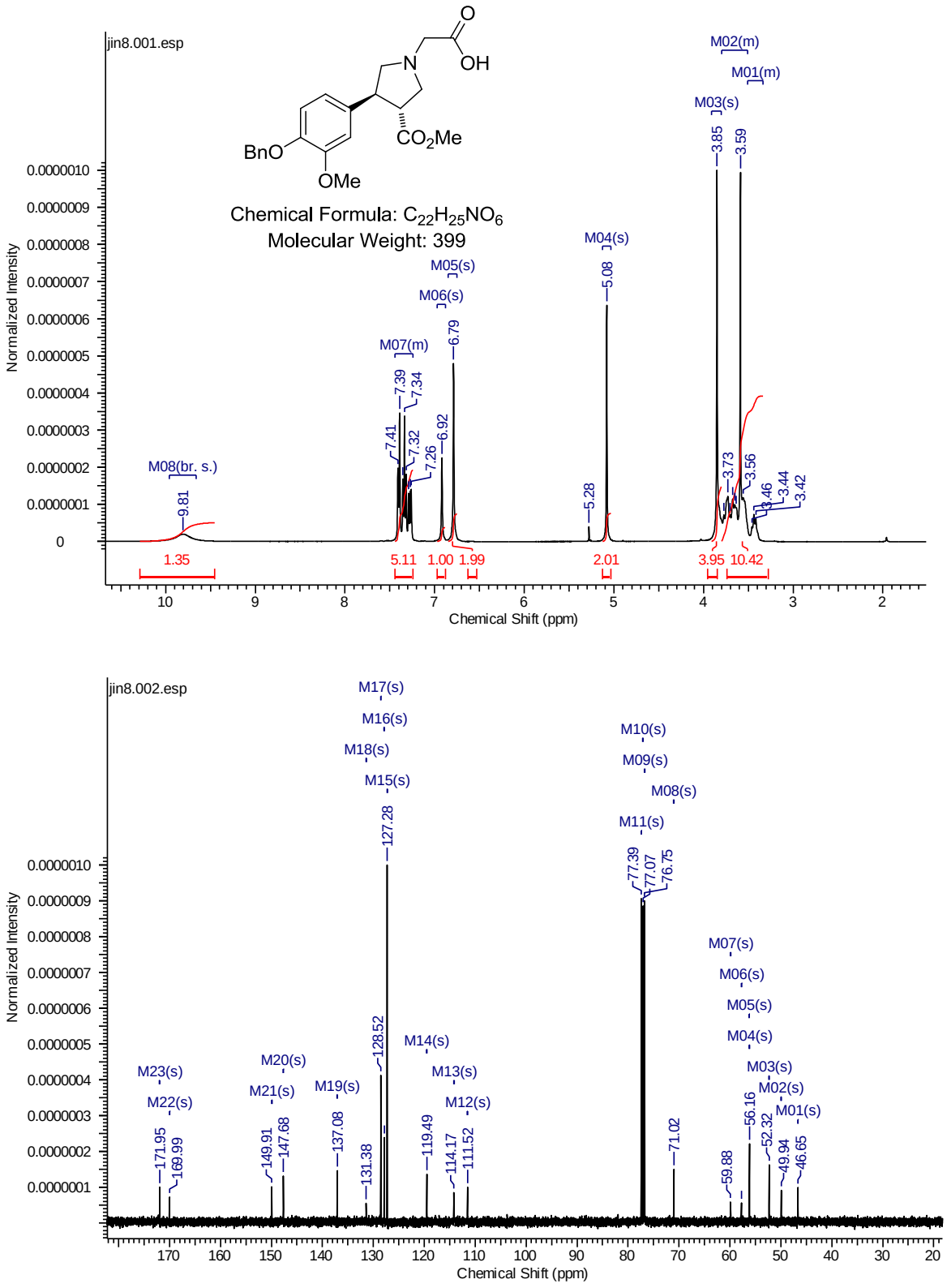


Figure S23. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-(2-isopropoxy-2-oxoethyl)pyrrolidine-3-carboxylate (8f)**

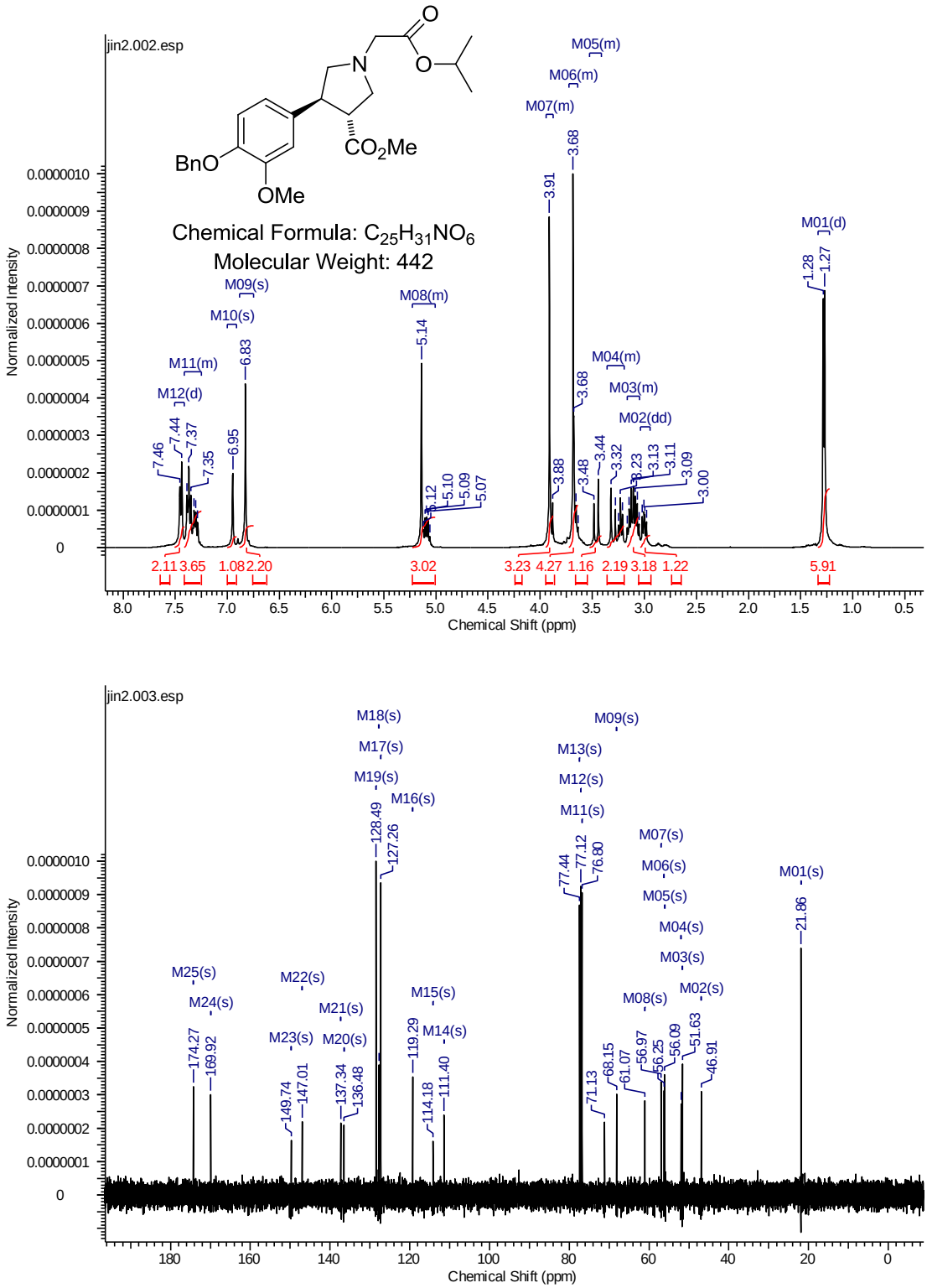


Figure S24. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-(3-ethoxy-3-oxopropyl)pyrrolidine-3-carboxylate (8h)**

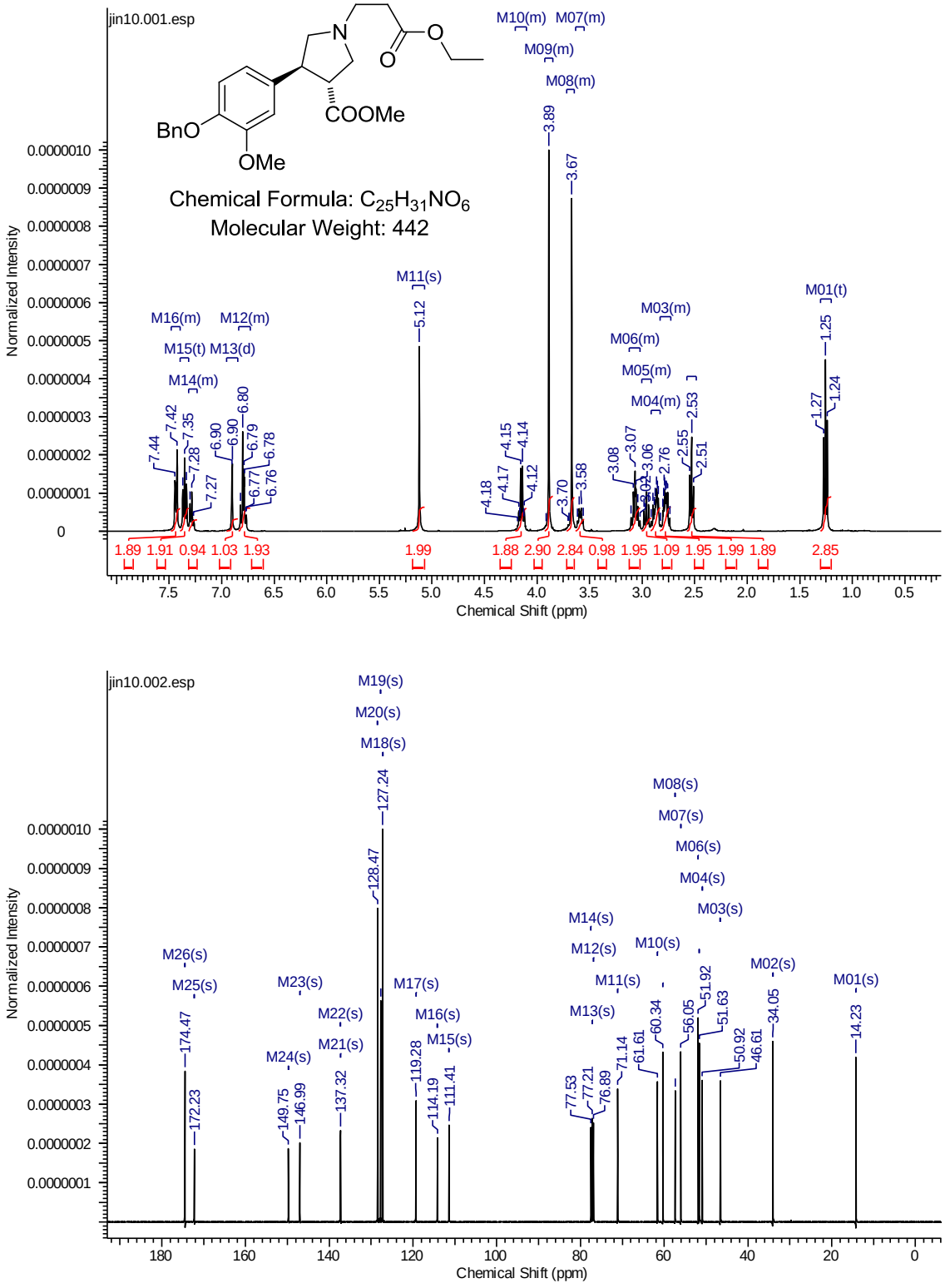


Figure S25. ^{1}H and ^{13}C NMR spectra of**(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-((R)-2,3-dihydroxypropyl)pyrrolidine-3-carboxylate (8i)**

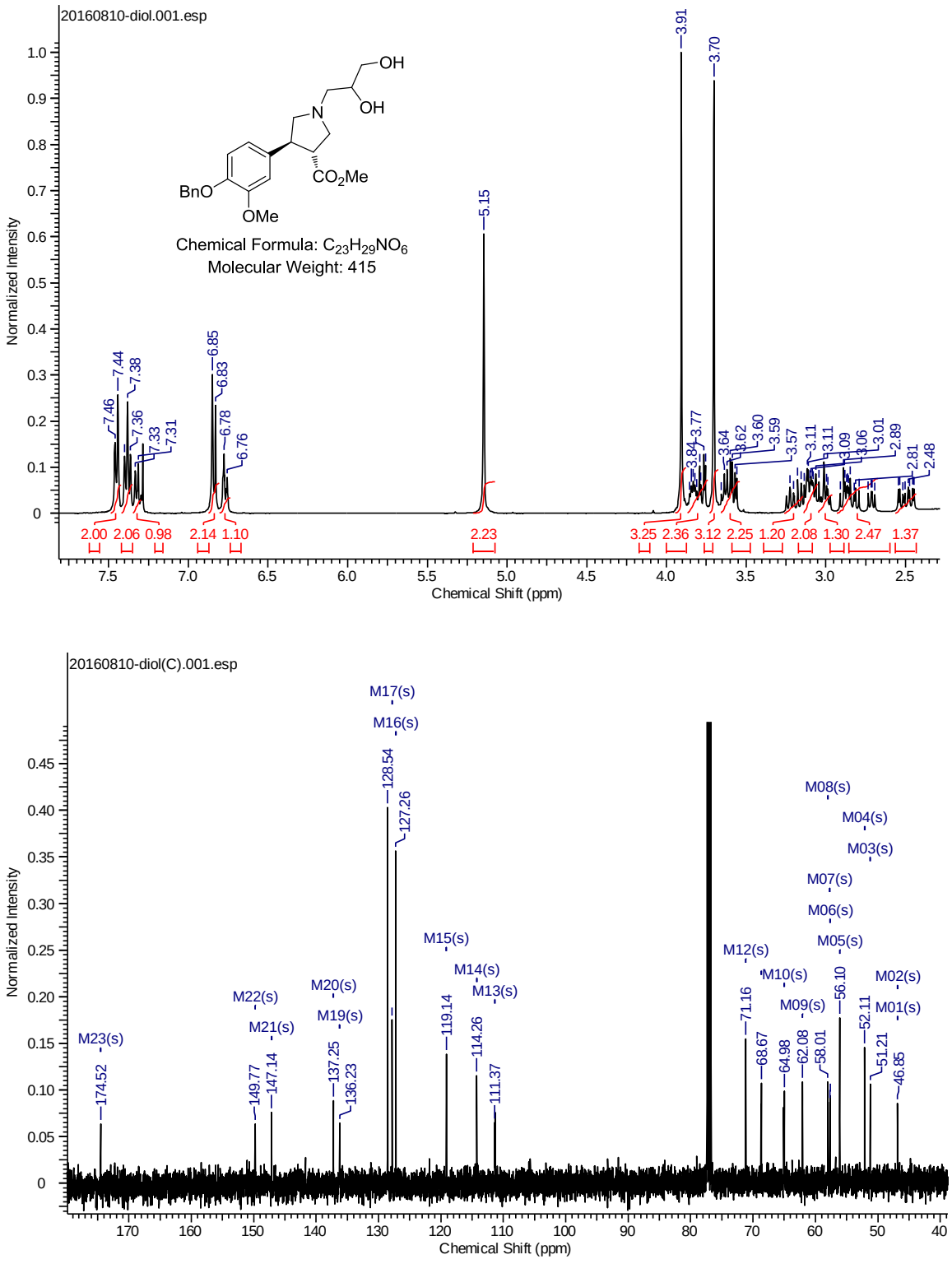


Figure S26. ^{1}H and ^{13}C NMR spectra of **5-((±)-*trans*-3-(4-(benzyloxy)-3-methoxyphenyl)-4-(methoxycarbonyl)pyrrolidin-1-yl)-2,2-dimethyl-5-oxopentanoic acid (8j)**

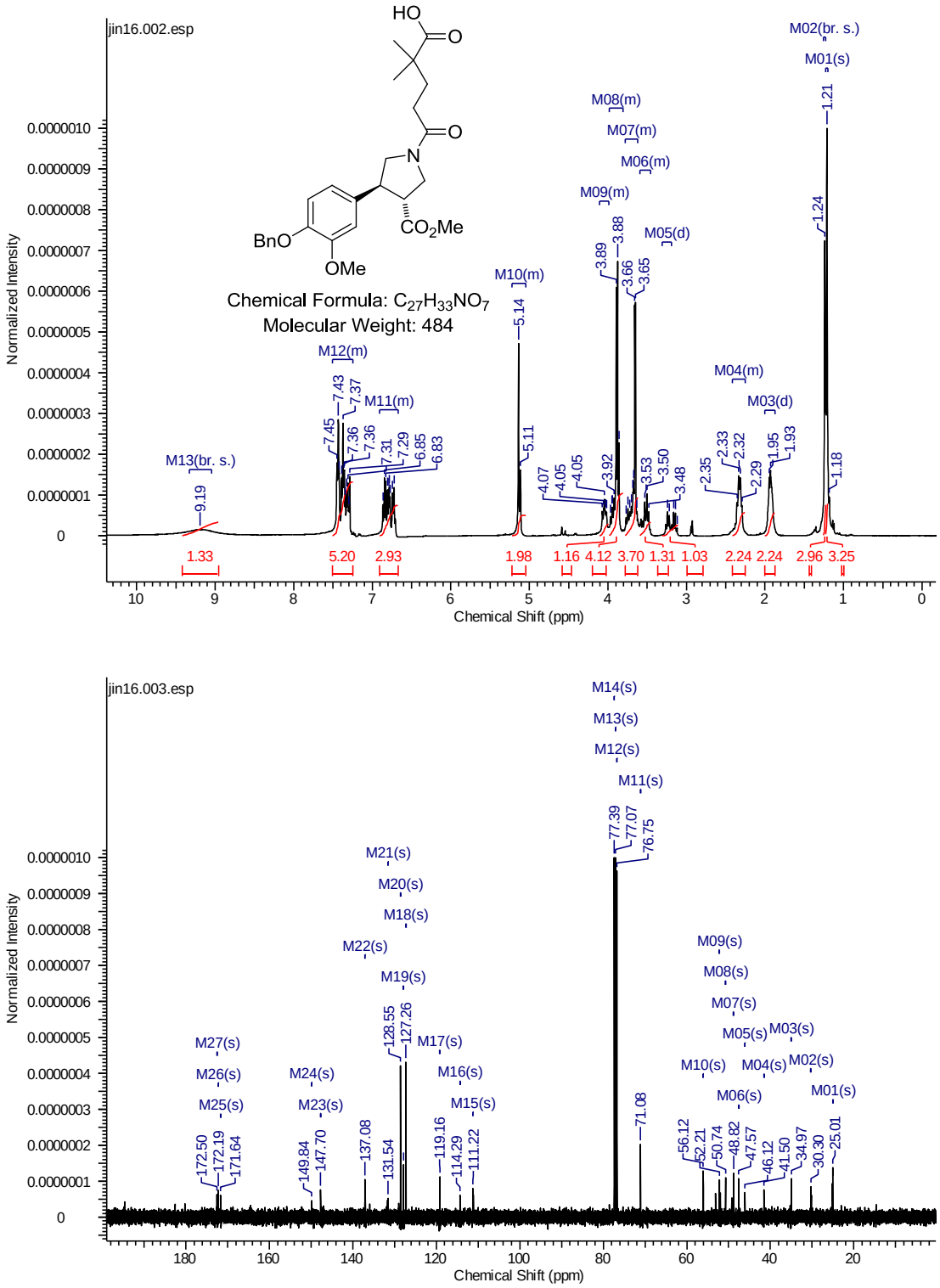


Figure S27. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-4-(4-(benzyloxy)-3-methoxyphenyl)-1-(4-carboxy-3,3-dimethylbutanoyl)pyrrolidine-3-carboxylic acid (8k)**

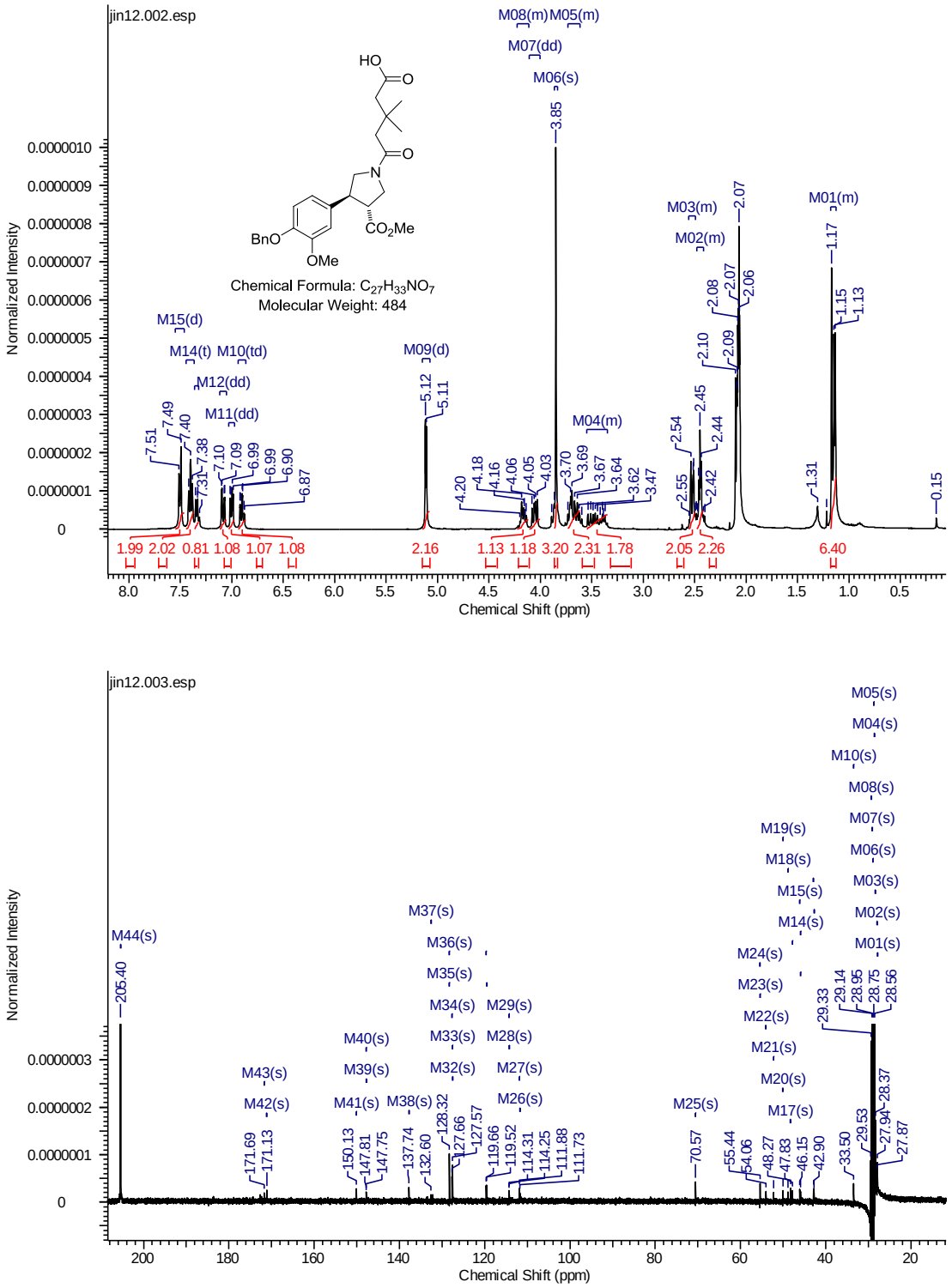


Figure S28. ^{1}H and ^{13}C NMR spectra of **(*E*)-4-((±)-*trans*-3-(4-(benzyloxy)-3-methoxyphenyl)-4-(methoxycarbonyl)pyrrolidin-1-yl)-4-oxobut-2-enoic acid (8l)**

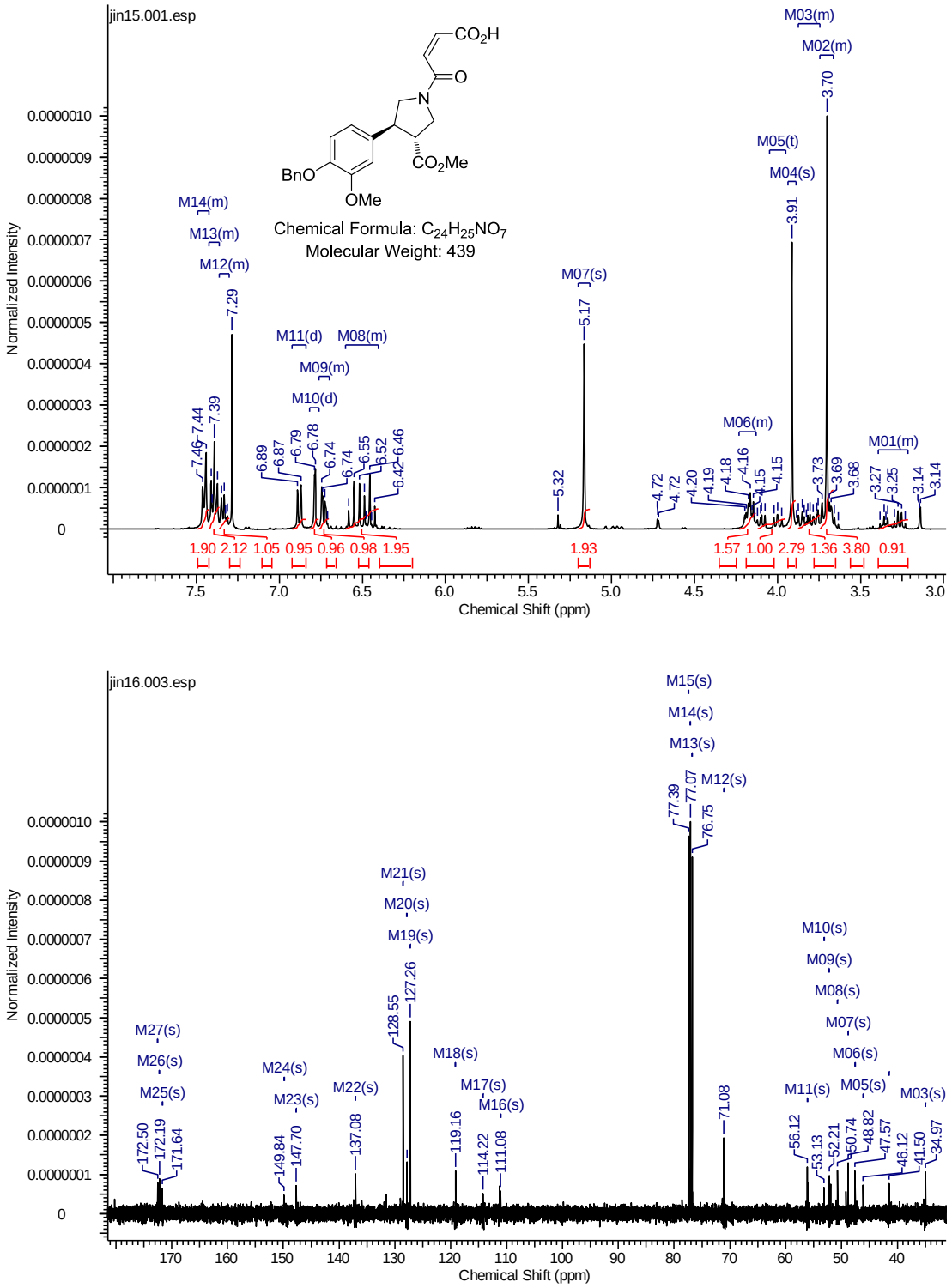


Figure S29. ^{1}H and ^{13}C NMR spectra of **4-((±)-*trans*-3-(4-(benzyloxy)-3-methoxyphenyl)-4-(methoxycarbonyl)pyrrolidine-1-yl)-4-oxobutanoic acid (8m)**

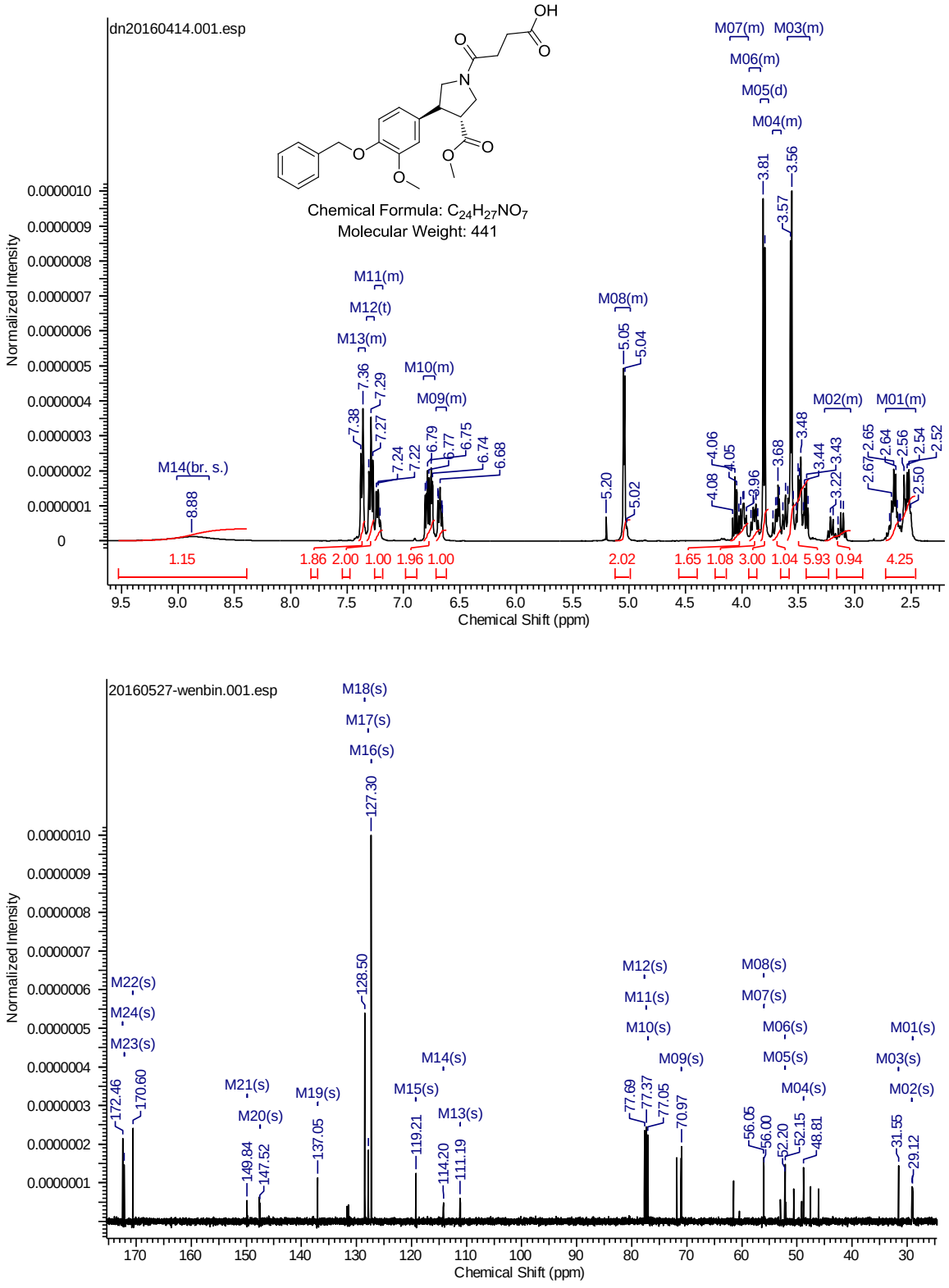


Figure S30. ^{1}H and ^{13}C NMR spectra of **2-(3-(4-(benzyloxy)-3-methoxyphenyl)-4-(methoxycarbonyl)pyrrolidine-1-carbonyl)benzoic acid (8n)**

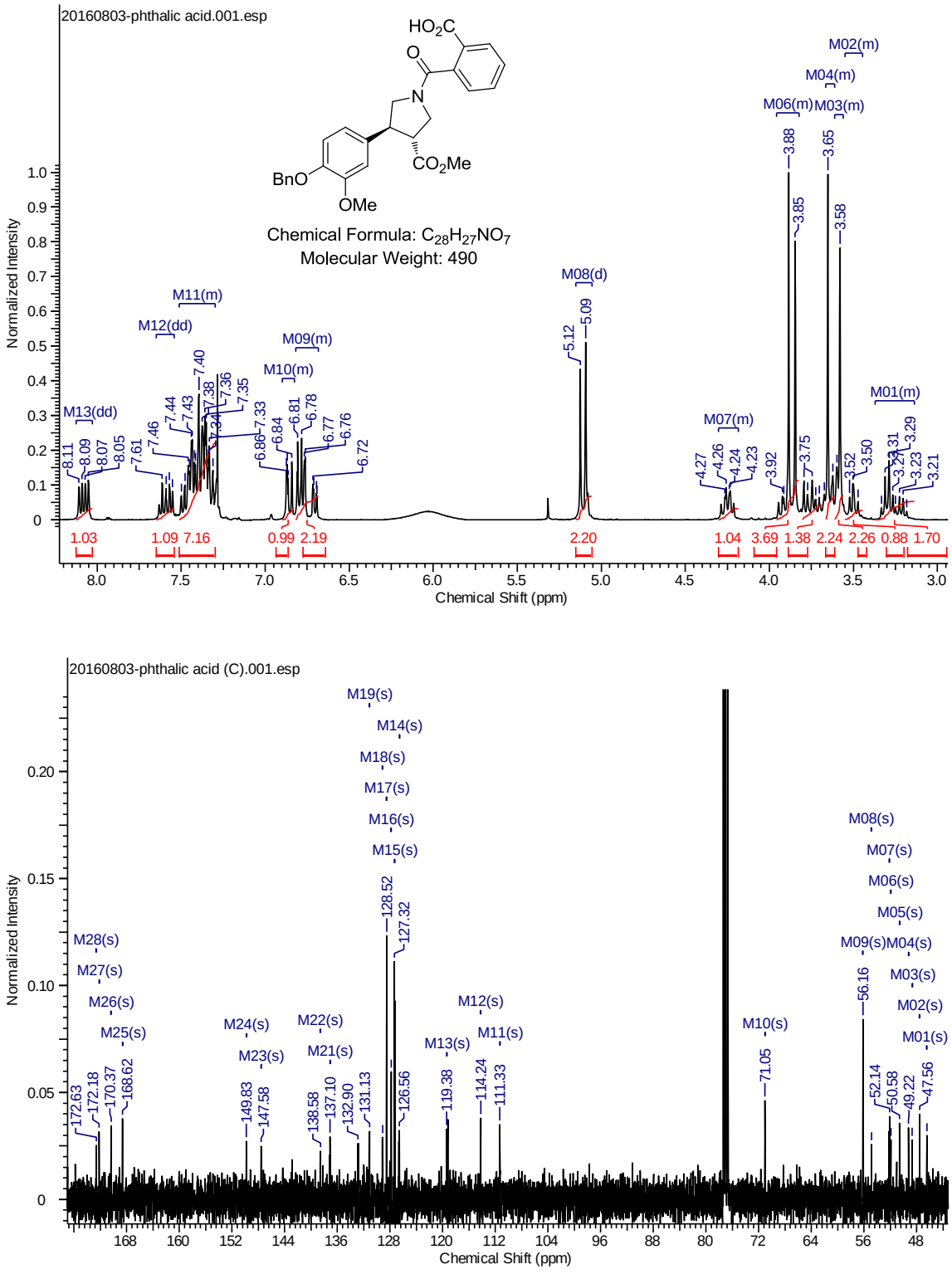


Figure S31. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-(methylsulfonyl)pyrrolidine-3-carboxylate (9a)**

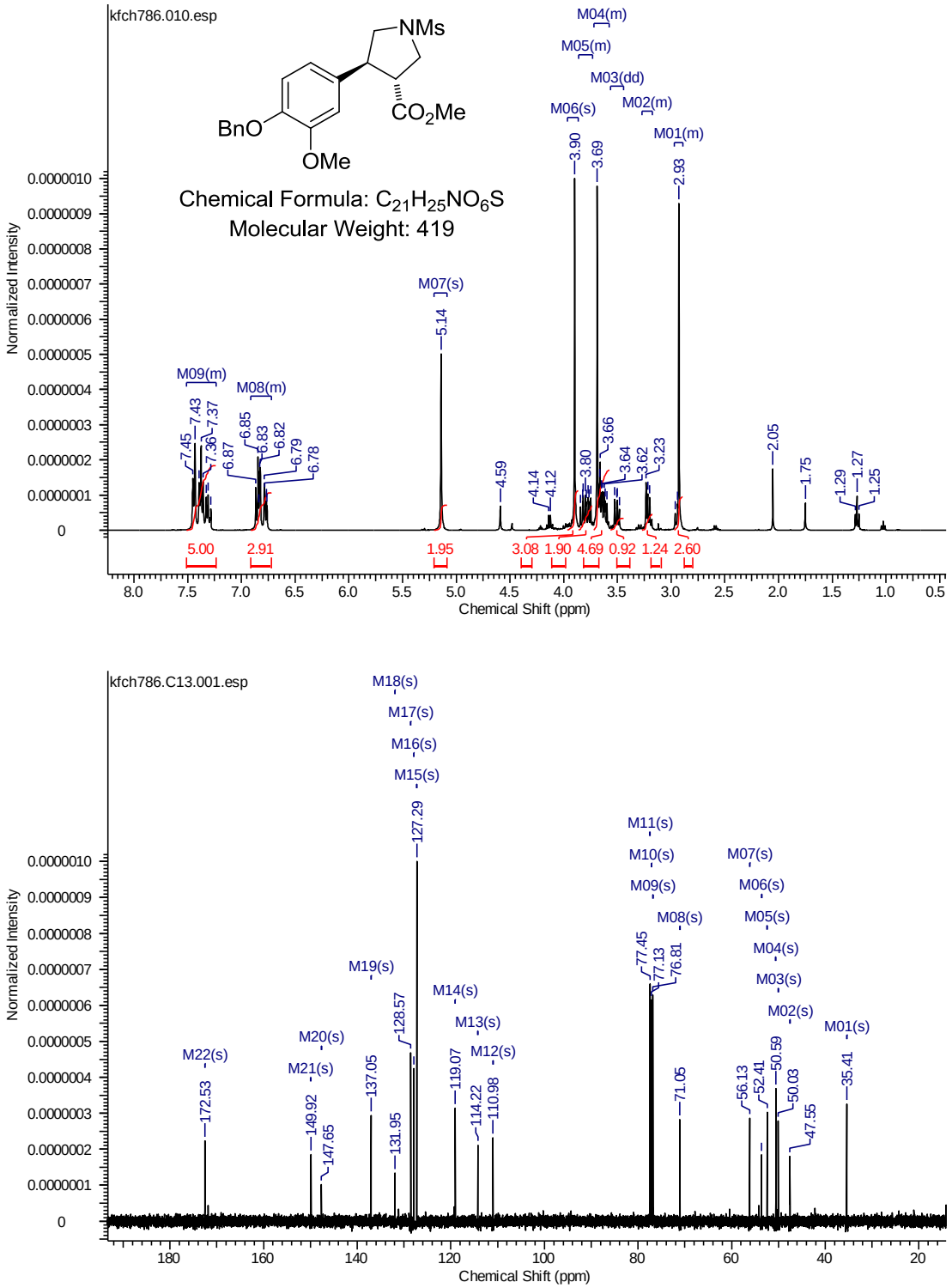


Figure S32. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-hydroxy-3-methoxyphenyl)-1-(methylsulfonyl)pyrrolidine-3-carboxylate (10a)**

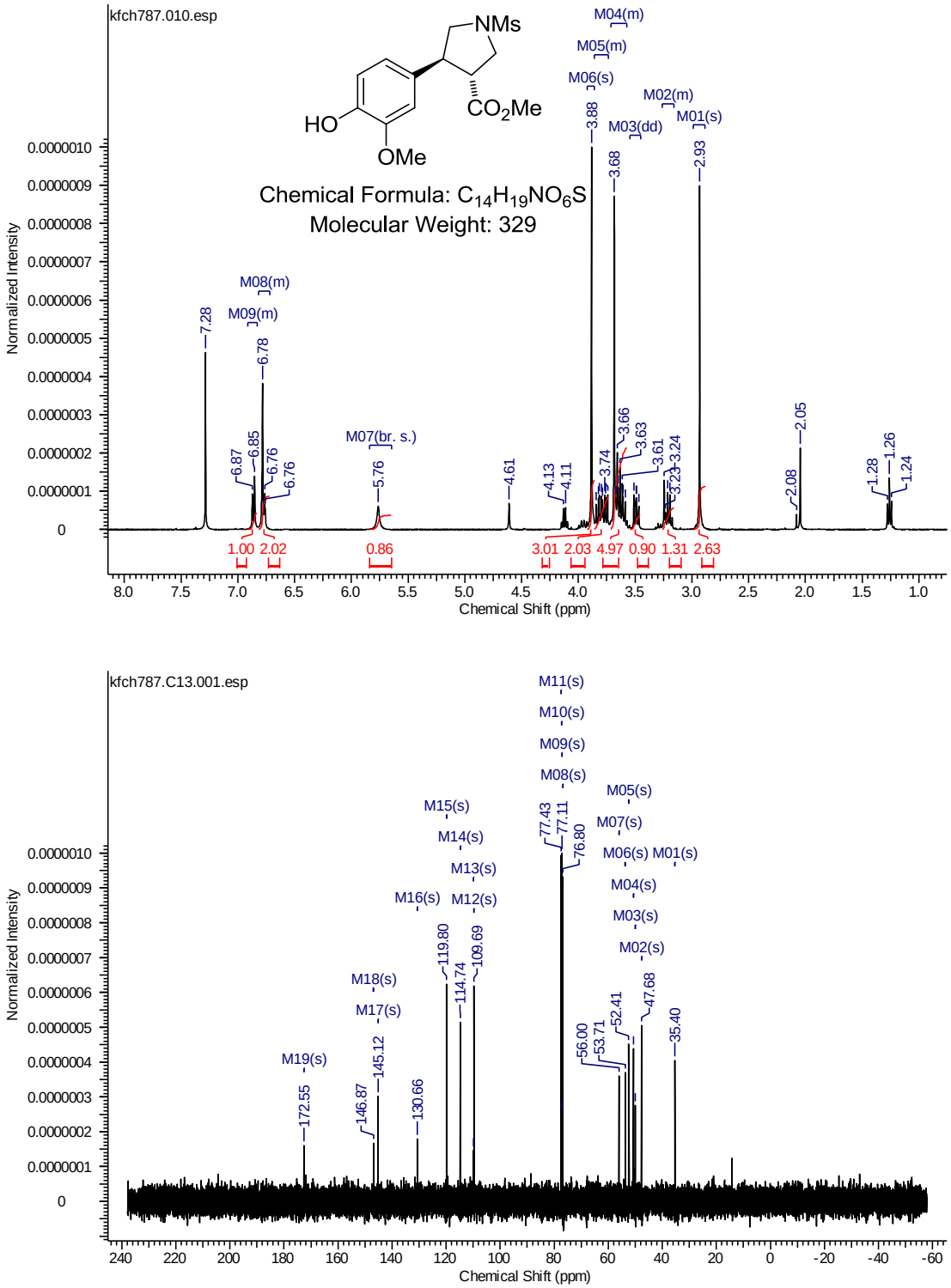


Figure S33. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(3,4-dimethoxyphenyl)-1-(methylsulfonyl)pyrrolidine-3-carboxylate (10b)**

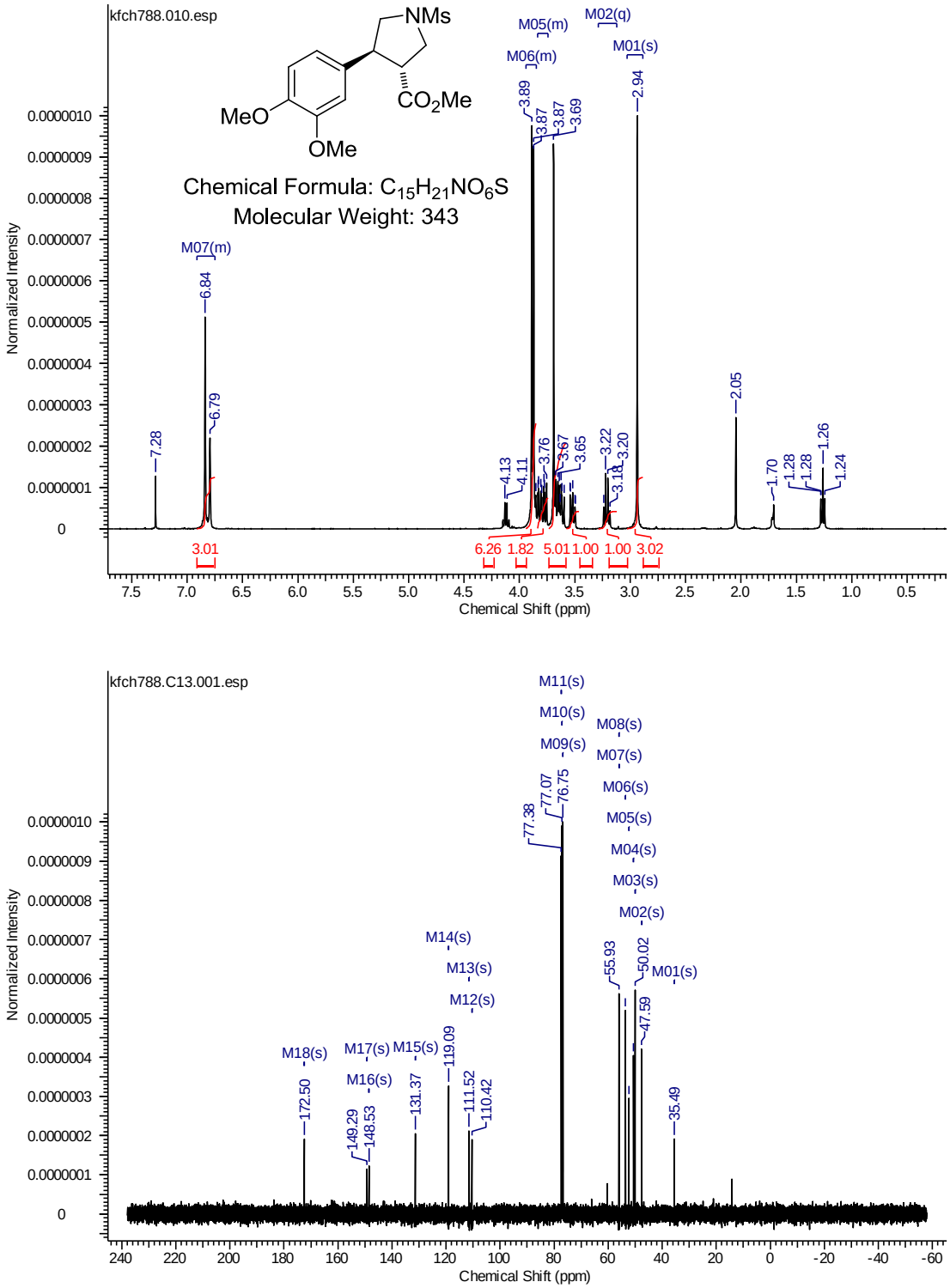


Figure S34. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-(*N*,*N*-dimethylsulfamoyl)pyrrolidine-3-carboxylate (9b)**

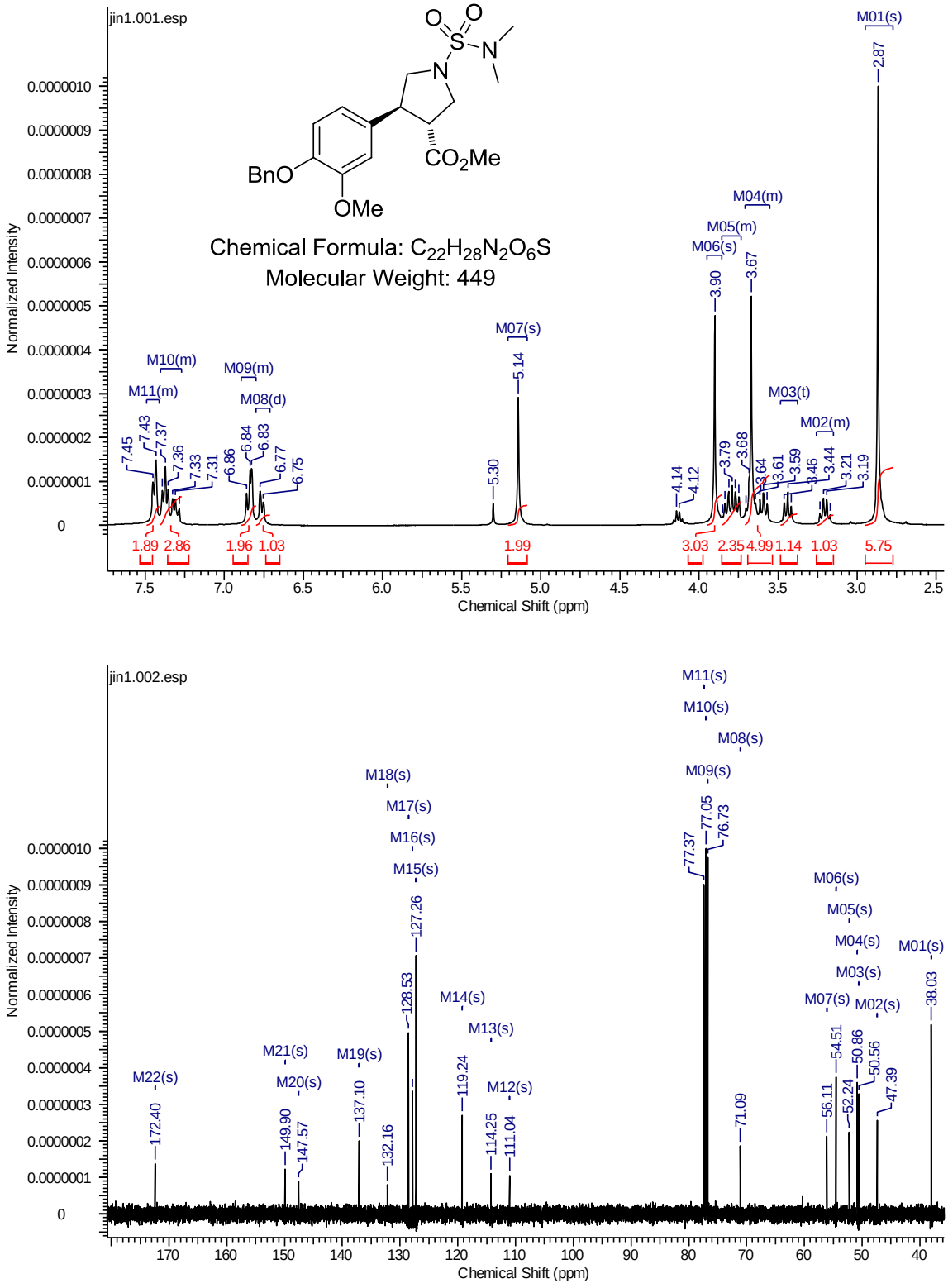


Figure S35. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-4-(4-(benzyloxy)-3-methoxyphenyl)-1-(*N*,*N*-dimethylsulfamonyl)pyrrolidine-3-carboxylic acid (10c)**

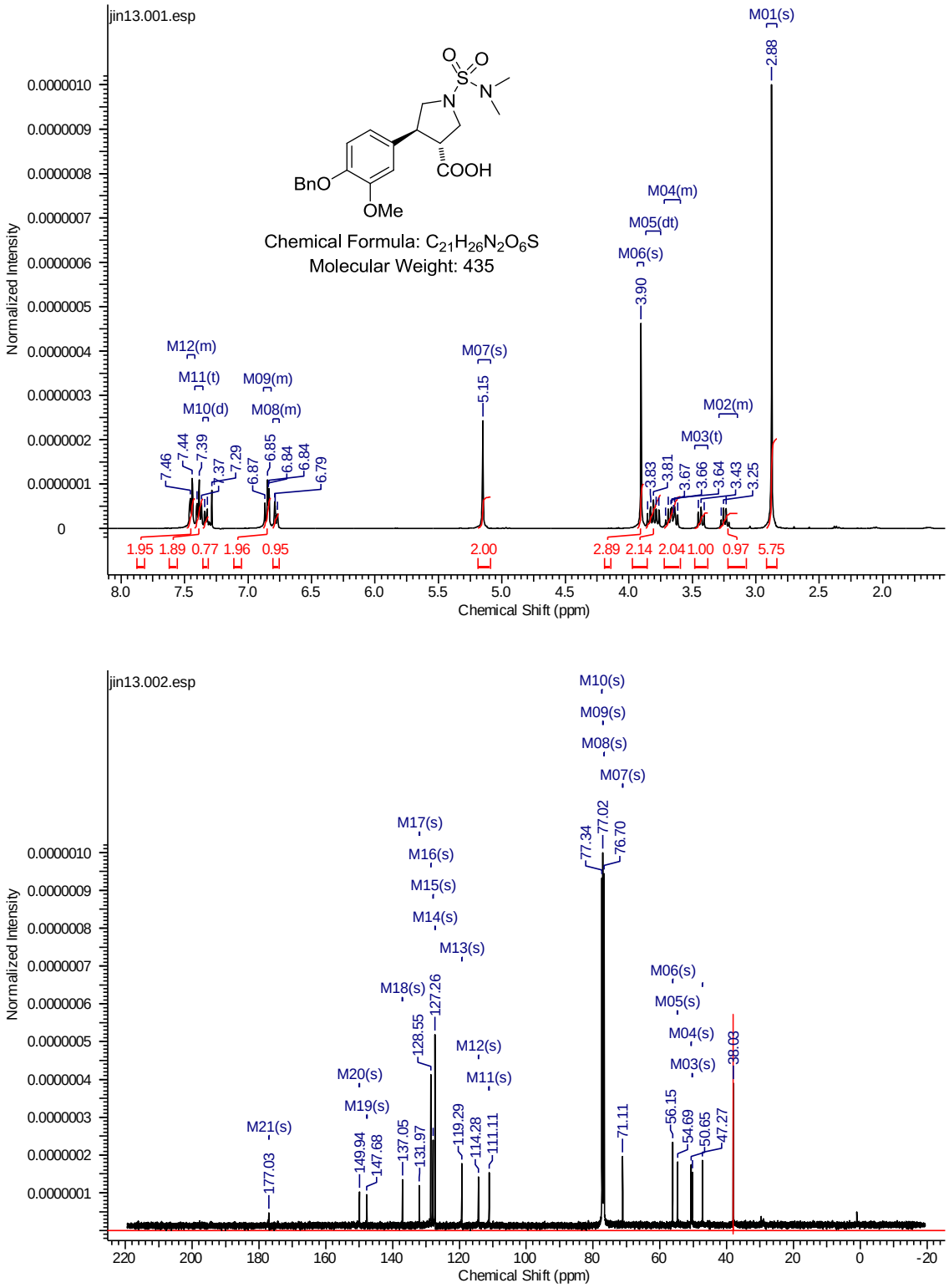


Figure S36. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-(2-(2,6-difluorophenyl)acetyl)pyrrolidine-3-carboxylate (9c)**

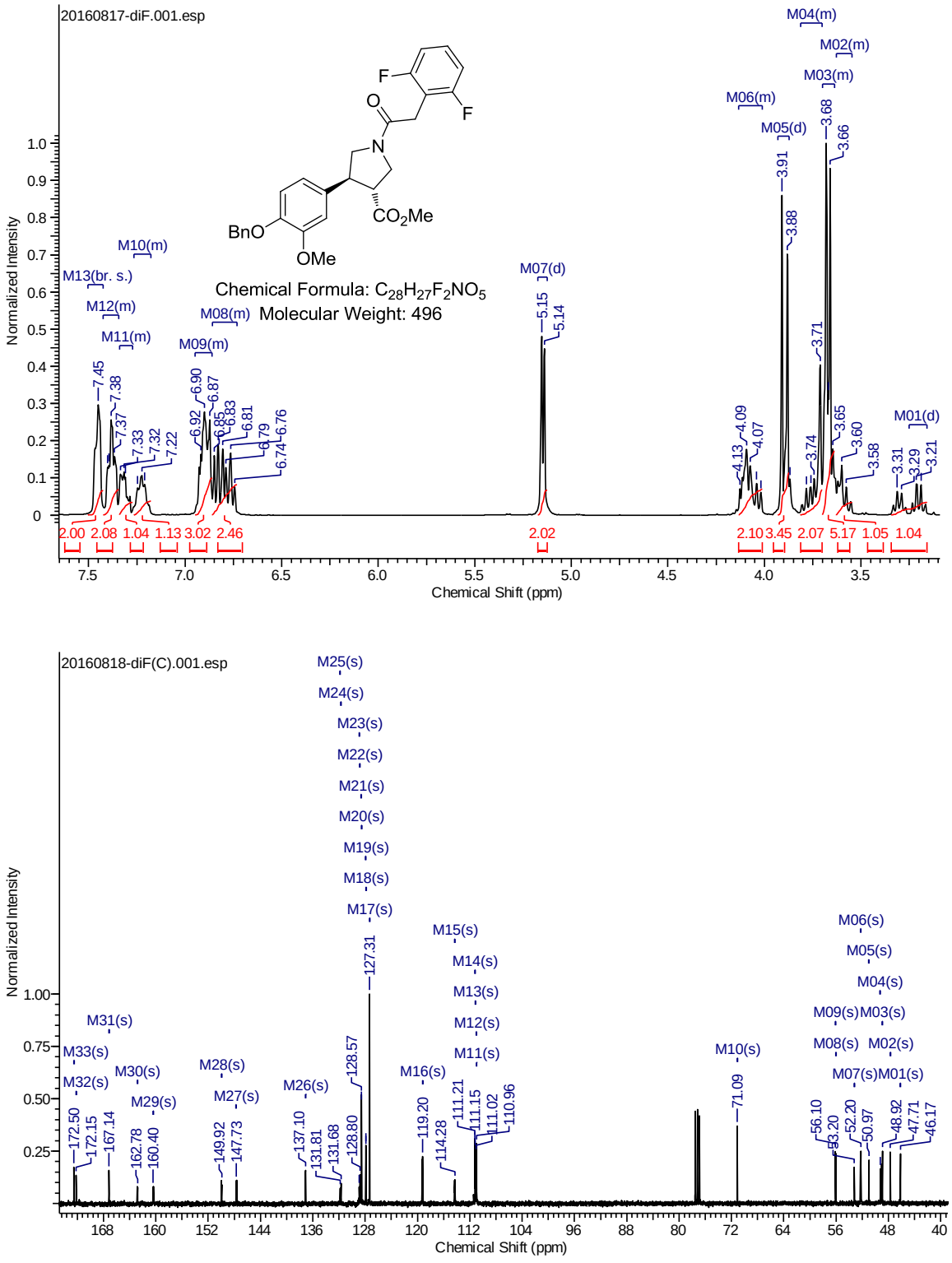


Figure S37. ^{1}H and ^{13}C NMR spectra of **(±)-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-picolinoylpyrrolidine-3-carboxylate (9d)**

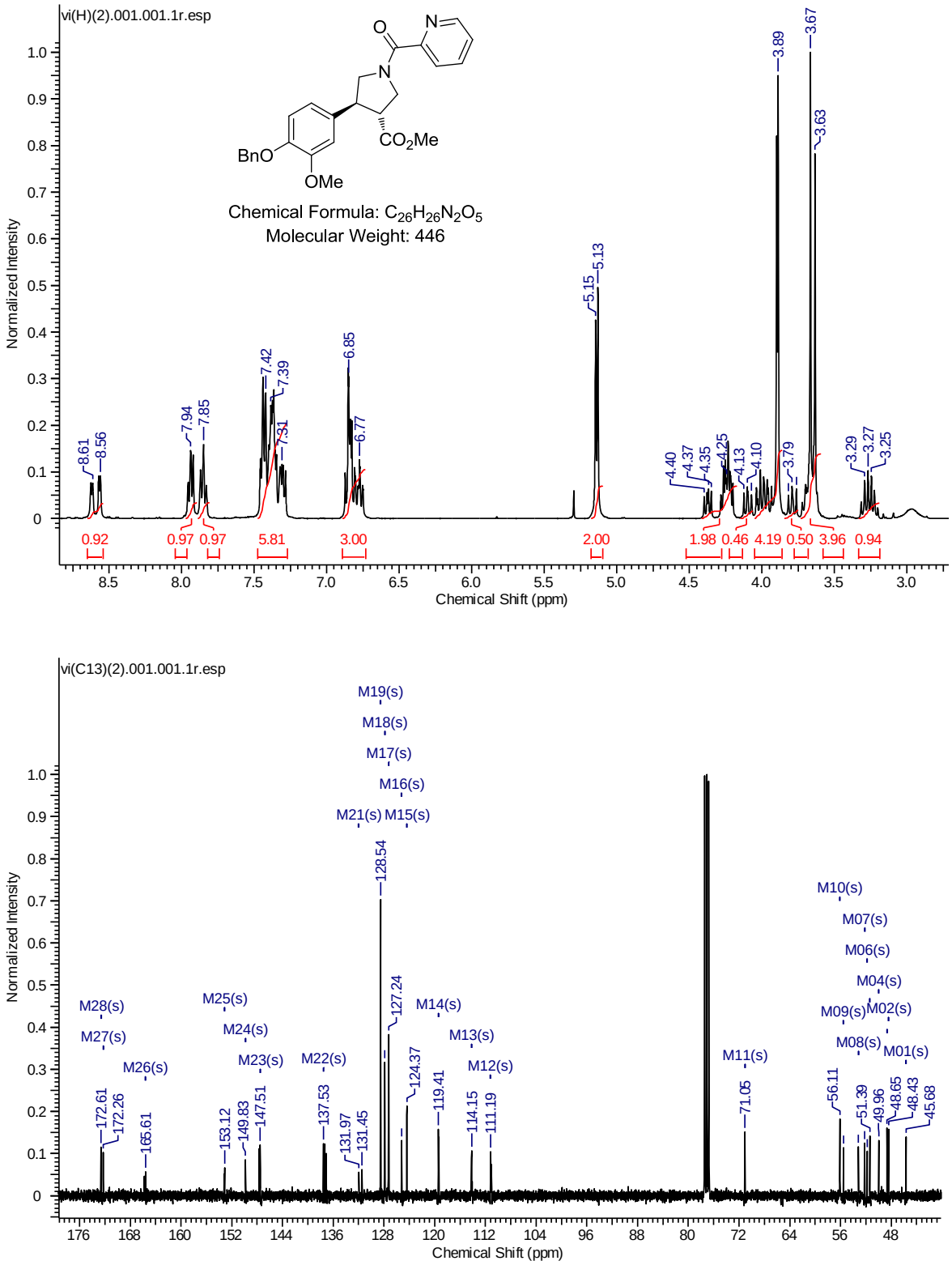


Figure S38. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-(2-chloroacetyl)pyrrolidine-3-carboxylate (9e)**

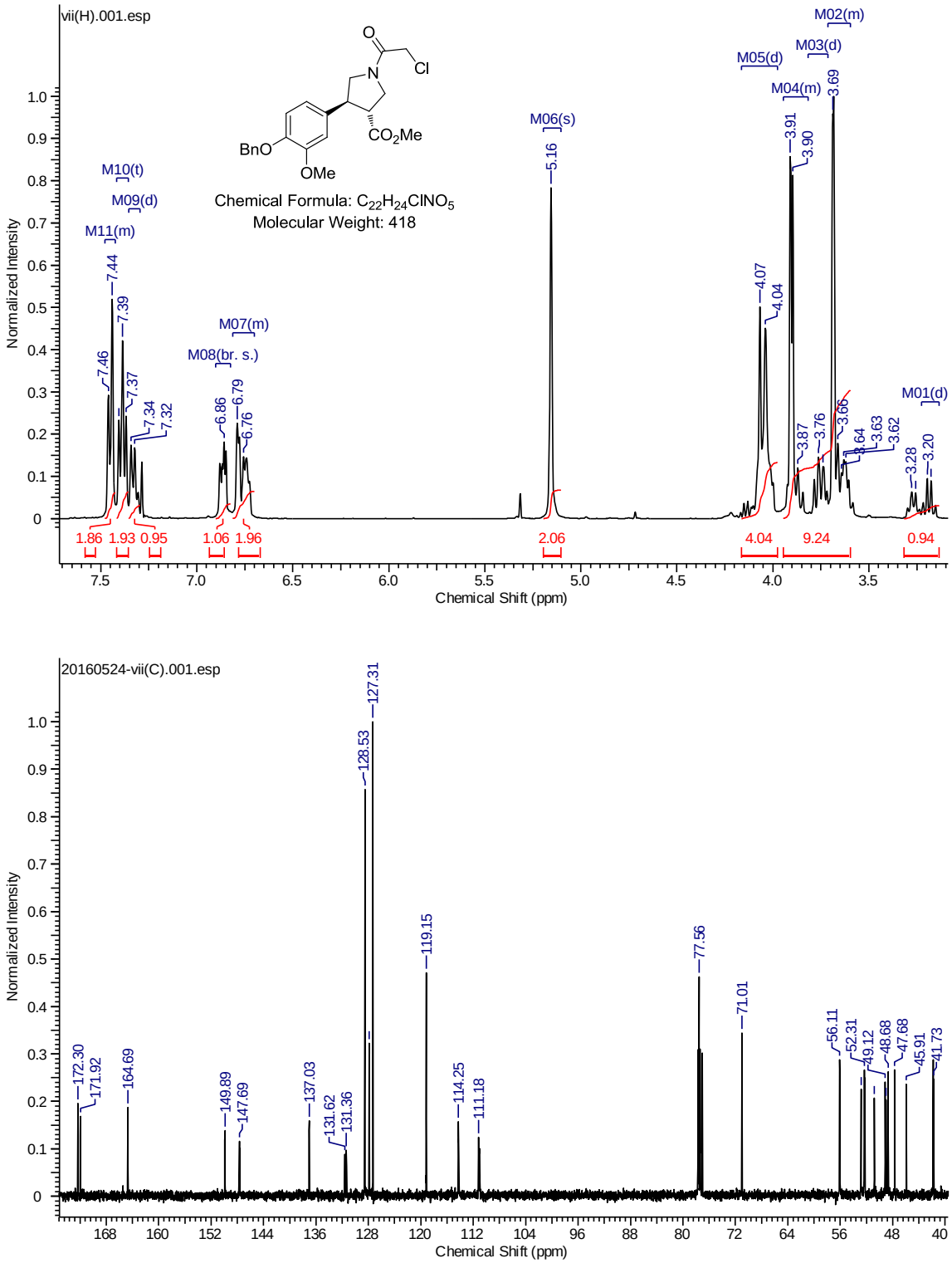


Figure S39. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 1-(2-(acetylthio)acetyl)-4-(4-(benzyloxy)-3-methoxyphenyl)pyrrolidine-3-carboxylate (10d)**

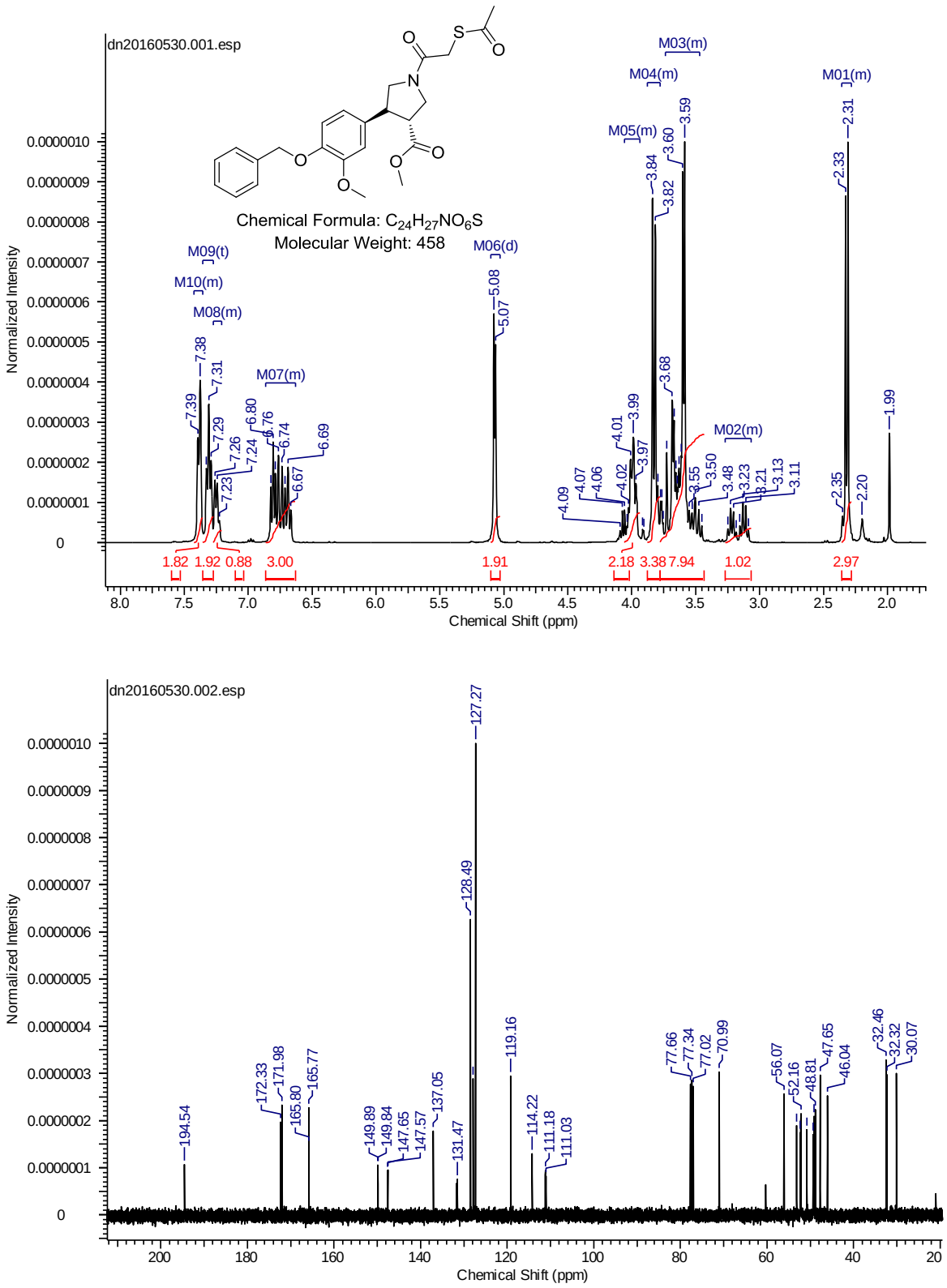
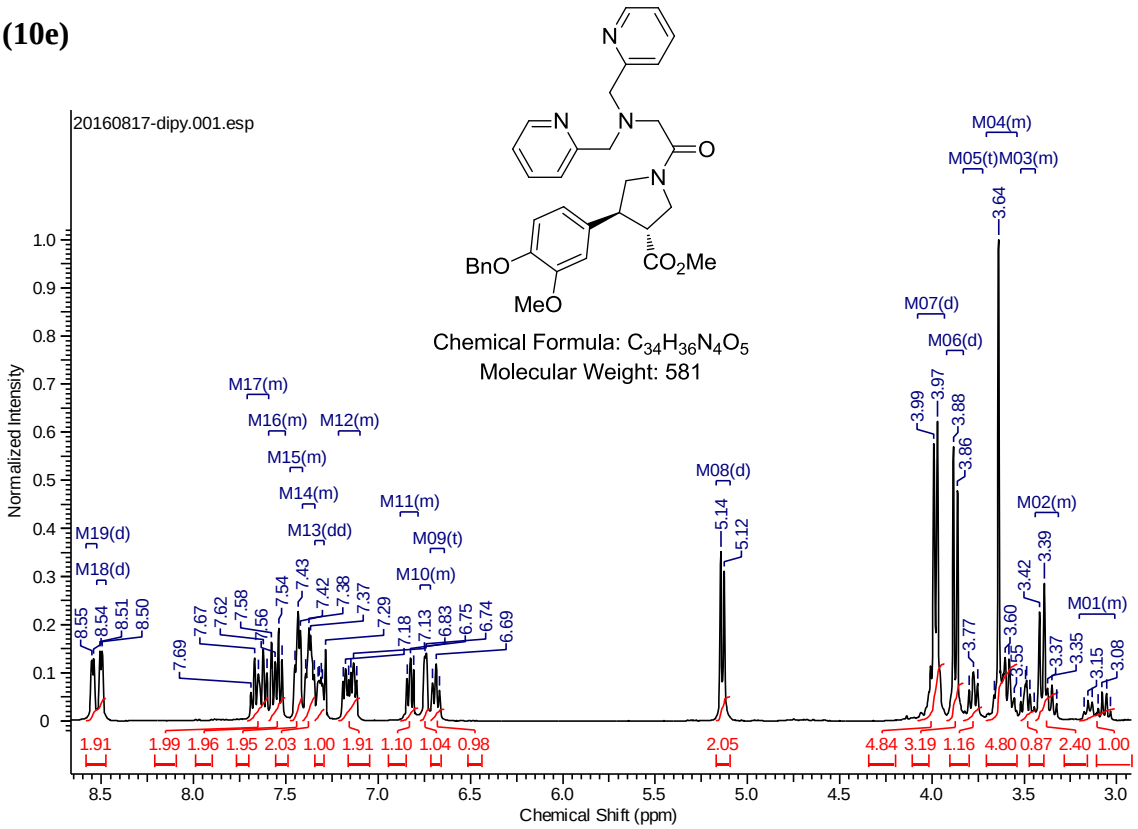


Figure S40. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 4-(4-(benzyloxy)-3-methoxyphenyl)-1-(2-(bis(pyridin-2-ylmethyl)amino)acetyl)pyrrolidine-3-carboxylate (10e)**



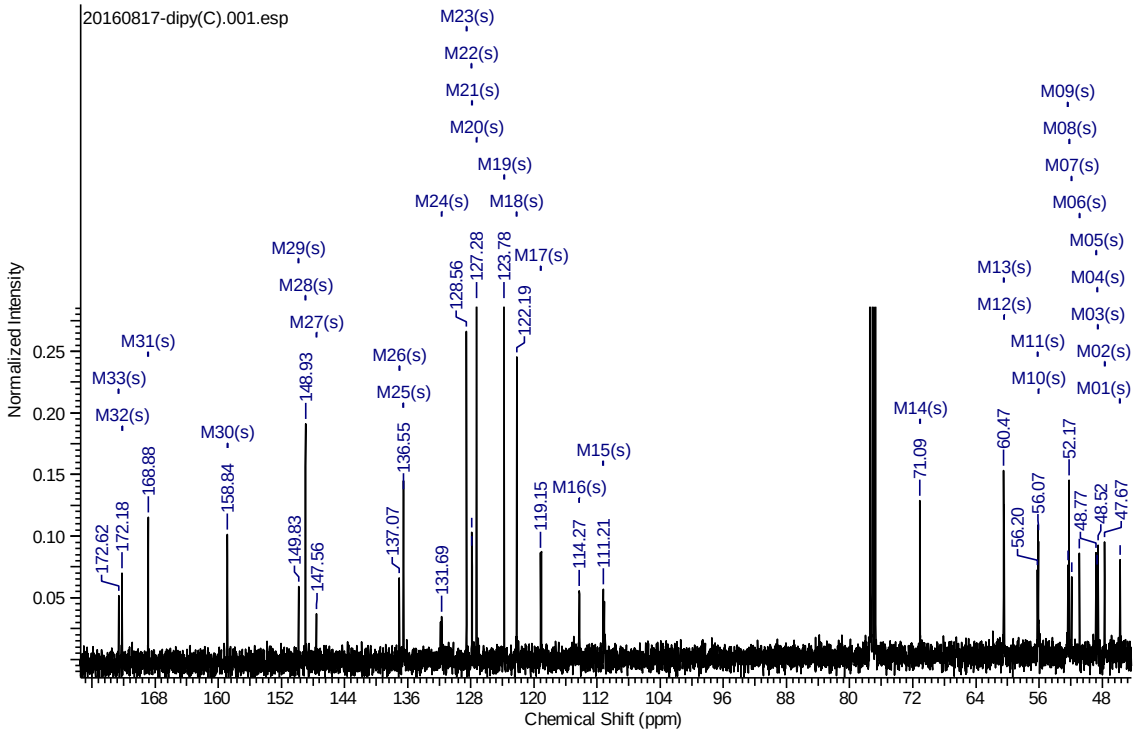


Figure S41. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-methyl 6-((3S,4R)-3-(4-(benzyloxy)-3-methoxyphenyl)-4-(methoxycarbonyl)pyrrolidine-1-carbonyl)picolinate (9f)**

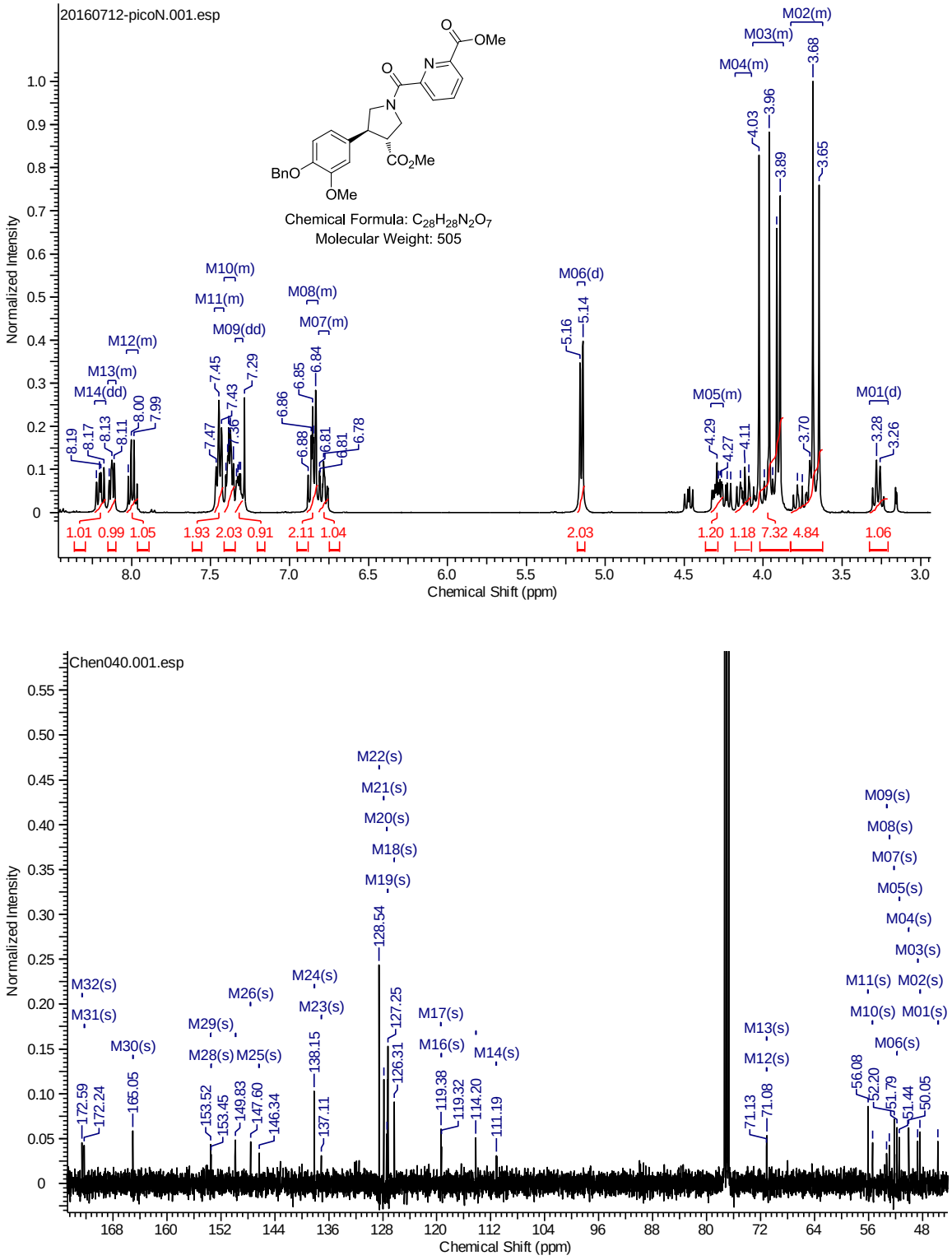


Figure S42. ^{1}H and ^{13}C NMR spectra of **(±)-*trans*-6-(3-(4-(benzyloxy)-3-methoxyphenyl)-4-carboxypyrrolidine-1-carbonyl)picolinic acid (10f)**

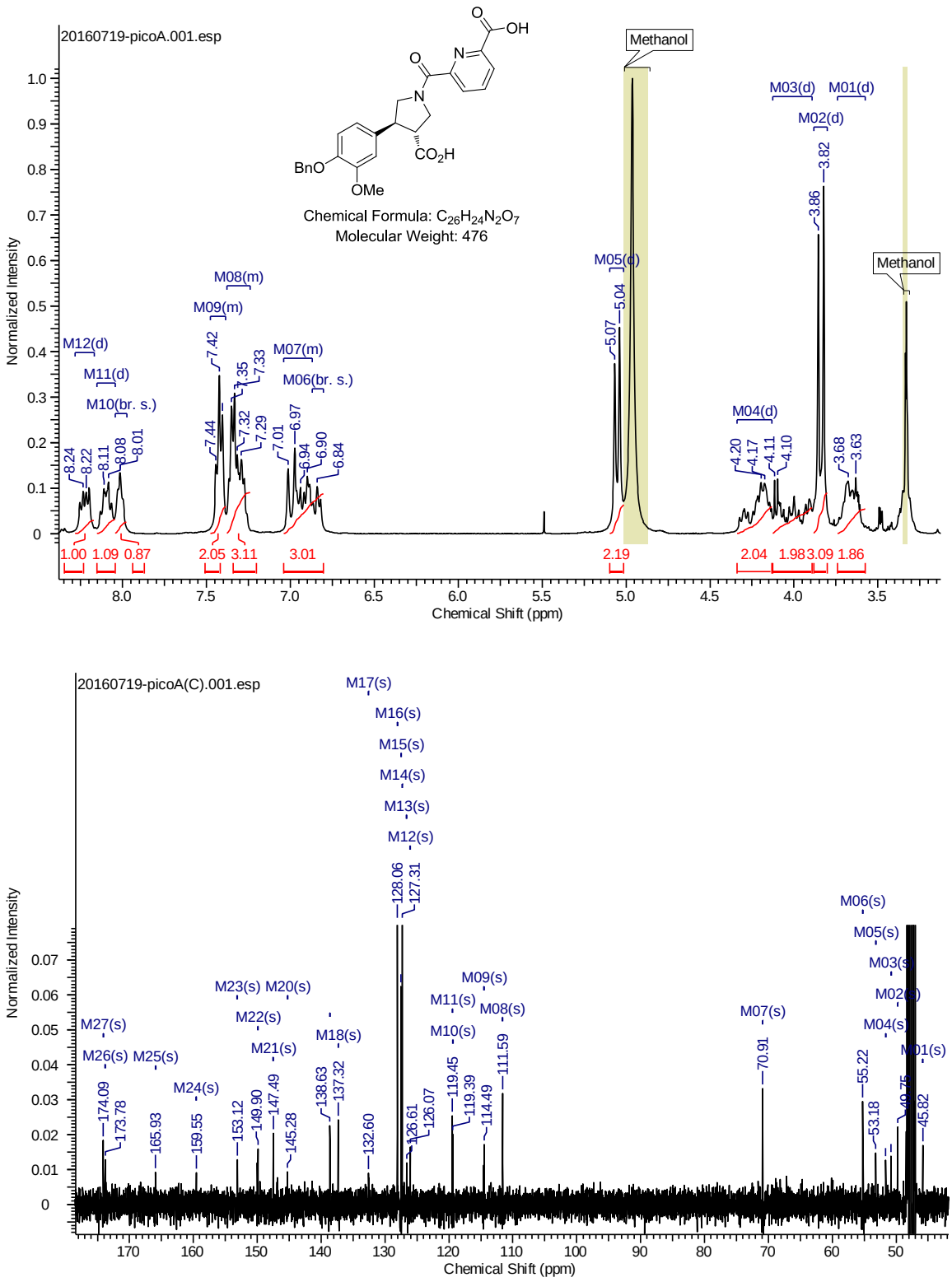
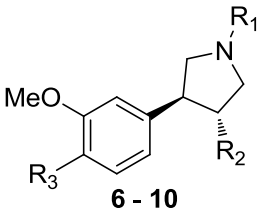
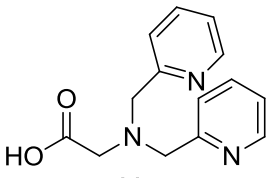


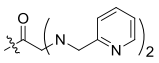
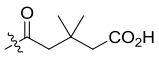
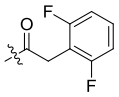
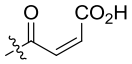
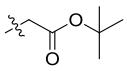
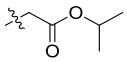
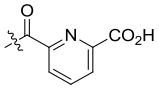
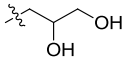
Table S1. MIC screening of compound alone and MRM in the presence of the compound at 100 μM against *E. coli* BL21(NDM-1), calculated cLogP, topological polar surface area (tPSA) and reduction fold (RF).

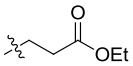
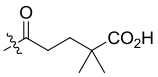
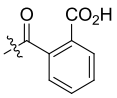
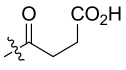


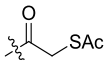
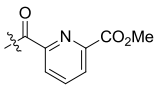
6 - 10



11

Entry	Cpd No.	R_1	R_2	R_3	cLogP[a]	tPSA[a]	MIC (μg/mL)		RF[c]
							Cpd	MRM[b]	
1	MRM	N.A.[d]	N.A.	N.A.	N.A.	N.A.	128	N.A.	N.A.
2	**10e**		CO_2Me	OBn	3.68	93.03	>128	0.5	256
3	**11**	N.A.	N.A.	N.A.	0.53	65.26	>128	4	32
4	**8k**		CO_2Me	OBn	3.80	102.37	>128	8	16
5	**9d**		CO_2Me	OBn	2.97	77.43	>128	8	16
6	**9c**		CO_2Me	OBn	4.82	65.07	>128	8	16
7	**8l**		CO_2Me	OBn	3.15	102.37	>128	16	8
8	**9e**		CO_2Me	OBn	3.04	65.07	>128	16	8
9	**8e**		CO_2Me	OBn	4.79	74.30	>128	32	4
10	**8f**		CO_2Me	OBn	4.39	74.30	>128	32	4
11	**9b**		CO_2H	OBn	2.37	96.38	>128	32	4
12	**7j**		CO_2H	OH	1.52	96.30	>128	32	4
13	**8d**		CO_2Me	OAc	0.68	100.60	>128	32	4
14	**10f**		CO_2H	OBn	2.76	125.73	>128	32	4
15	**8i**		CO_2Me	OBn	2.61	88.46	>128	32	4

16	**7a**		CO_2Me	OBn	3.31	56.79	>128	64	2
17	**9a**		CO_2Me	OBn	2.89	82.14	>128	64	2
18	**10a**		CO_2Me	OH	0.64	93.14	>128	64	2
19	**10b**		CO_2Me	OMe	1.12	82.14	>128	64	2
20	**7e**		CO_2Me	OBn	4.23	74.30	>128	64	2
21	**8g**		CO_2Me	OBn	1.24	85.30	>128	64	2
22	**7g**		CO_2H	OBn	3.76	85.30	>128	64	2
23	**8h**		CO_2Me	OBn	4.36	74.30	>128	64	2
24	**7f**		CH_2OH	OBn	3.66	68.23	>128	64	2
25	**7h**		$CONH_2$	OBn	3.05	91.09	>128	64	2
26	**8j**		CO_2Me	OBn	3.71	102.37	>128	64	2
27	**8a**		CO_2Me	OBn	3.01	83.53	>128	64	2
28	**6c**		CO_2Me	OMs	2.83	82.14	>128	64	2
29	**6b**		CO_2Me	OAllyl	4.25	48.00	>128	64	2
30	**8b**		CO_2Me	OAllyl	2.02	83.53	>128	64	2
31	**8n**		CO_2Me	OBn	4.07	102.37	>128	64	2
32	**6a**		CO_2Me	OBn	5.24	48.00	>128	>128	<1
33	**6d**		CO_2Me	OAc	2.90	65.07	>128	>128	<1
34	**7i**		CO_2Me	OH	1.98	85.30	>128	>128	<1
35	**9b**		CO_2Me	OBn	2.84	85.38	>128	>128	<1
36	**8c**		CO_2Me	OMs	0.60	117.67	>128	>128	<1
37	**8m**		CO_2Me	OBn	2.75	102.37	>128	>128	<1

38	**10d**		CO_2Me	OBn	3.44	82.14	>128	>128	<1
39	**9f**		CO_2Me	OBn	2.60	103.73	>128	>128	<1

[a]Compound's cLogP and tPSA values were calculated using the ChemDraw Ultra (version 12.0). [b]MIC value of MRM in the presence of 100 µM of compound; [c]Reduction fold (RF) was calculated by MIC of MRM alone divided by MIC of MRM in the presence of 100 µM of the test compound; [d]N.A.: Not Applicable; N = 1-3 independent experiments.

Figure S43. X-ray crystal structure of **9b**

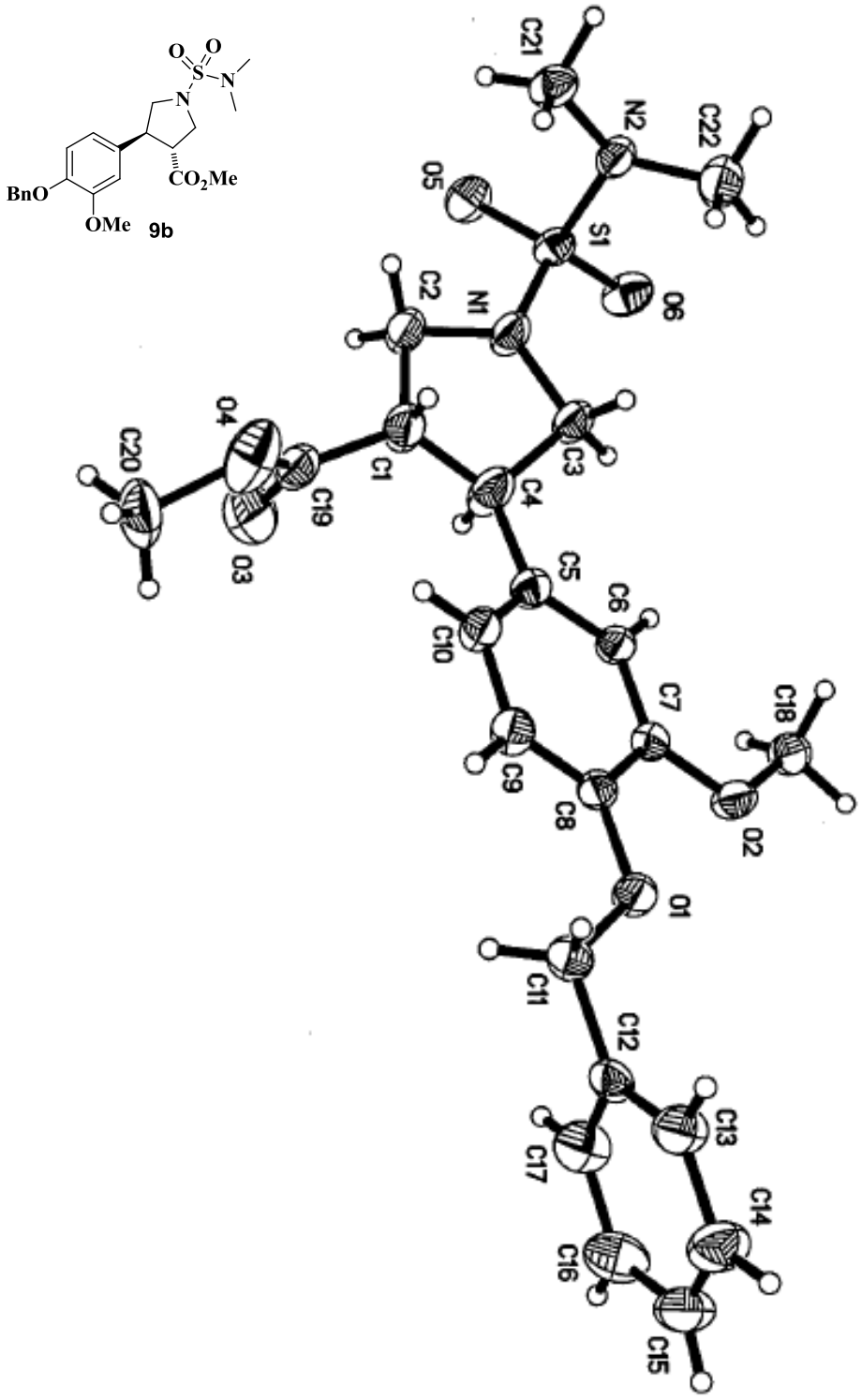
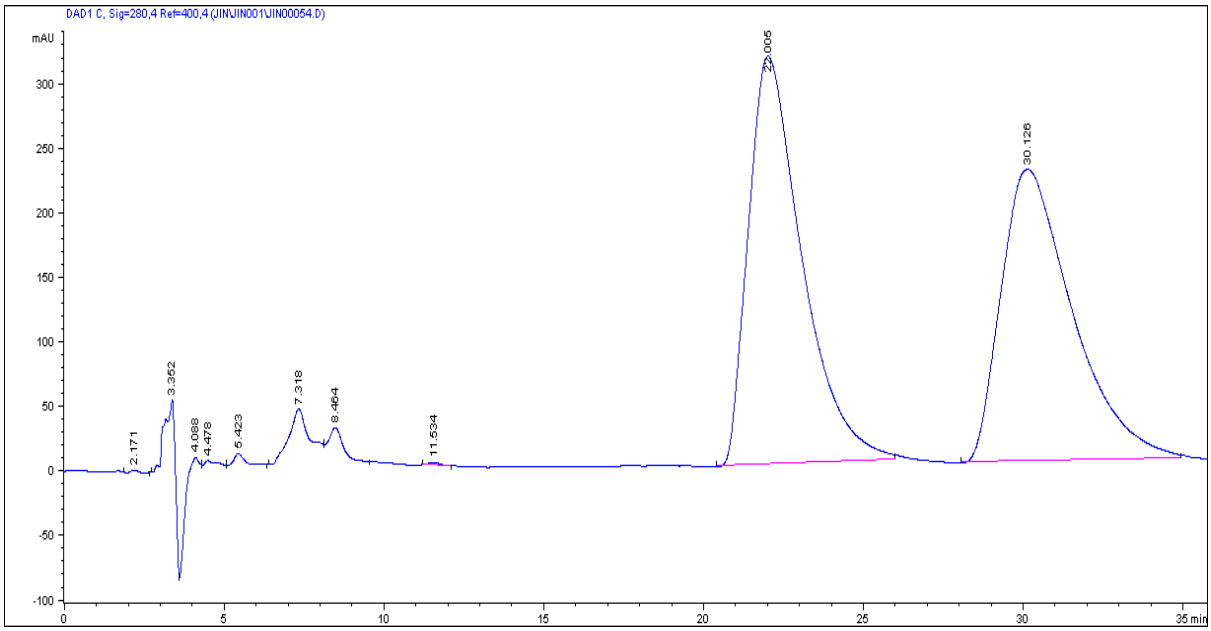


Figure S44. HPLC chromatogram of **6a**



HPLC conditions:
Column: CHIRALCEL® OJ column (4.6 x 250 mm);
Temperature: 23ºC;
Flow rate: 1.0 mL/min;
UV detection: 280 nm (reference 400 nm);
Mobile phase (isocratic elution): 98% Hexane, 2% isopropyl alcohol;
Retention time for less polar enantiomer of **6a**: 22 min;
Retention time for more polar enantiomer of **6a**: 30 min;

Table S2. Crystal data and structure refinement for compound **9b**.

Identification code	jwb1	
Empirical formula	$C_{22}H_{28}N_2O_6S$	
Formula weight	448.52	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 5.64480(10) Å	α= 90°.
	b = 35.3410(9) Å	β= 91.3550(10)°.
	c = 10.9173(3) Å	γ = 90°.
Volume	2177.31(9) $Å^3$	
Z	4	
Density (calculated)	1.368 Mg/m^3	
Absorption coefficient	0.190 mm^{-1}	
F(000)	952	
Crystal size	0.50 x 0.40 x 0.40 mm^3	
Theta range for data collection	1.95 to 27.52°.	
Index ranges	-7<=h<=7, -45<=k<=45, -14<=l<=13	
Reflections collected	47726	
Independent reflections	5001 [R(int) = 0.0358]	
Completeness to theta = 27.52°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6858	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5001 / 0 / 346	

Goodness-of-fit on F^2	1.001
Final R indices [I>2sigma(I)]	R1 = 0.0839, wR2 = 0.1814
R indices (all data)	R1 = 0.1023, wR2 = 0.1926
Largest diff. peak and hole	0.913 and -0.750 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for jwb1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	8761(1)	2450(1)	4022(1)	46(1)
O(1)	16776(3)	747(1)	-708(2)	55(1)
O(2)	13172(3)	1163(1)	-1249(2)	54(1)
O(3)	12248(6)	1026(1)	5194(3)	116(1)
O(4)	15824(5)	1238(1)	5459(2)	102(1)
O(5)	7802(3)	2423(1)	5213(2)	64(1)
O(6)	7251(3)	2469(1)	2959(2)	64(1)
N(1)	10444(5)	2088(1)	3871(2)	66(1)
N(2)	10305(4)	2838(1)	4015(2)	51(1)
C(1)	13156(7)	1599(1)	4271(3)	79(1)
C(2)	11493(6)	1882(1)	4902(2)	68(1)
C(3)	11267(5)	1952(1)	2690(2)	59(1)
C(4)	12357(7)	1581(1)	3032(3)	82(1)
C(5)	13769(5)	1386(1)	2054(2)	48(1)
C(6)	12844(4)	1381(1)	857(2)	45(1)
C(7)	13925(4)	1176(1)	-50(2)	41(1)
C(8)	15928(4)	958(1)	238(2)	43(1)
C(9)	16892(4)	973(1)	1407(2)	50(1)
C(10)	15830(5)	1188(1)	2304(2)	50(1)
C(11)	18613(5)	482(1)	-402(3)	54(1)
C(12)	18955(4)	231(1)	-1493(2)	49(1)

C(13)	20896(5)	272(1)	-2215(3)	62(1)
C(14)	21226(6)	37(1)	-3201(3)	76(1)
C(15)	19652(7)	-246(1)	-3462(3)	75(1)
C(16)	17706(6)	-293(1)	-2741(4)	80(1)
C(17)	17385(5)	-56(1)	-1768(3)	70(1)
C(18)	11221(5)	1395(1)	-1613(3)	55(1)
C(19)	13764(6)	1276(1)	5021(2)	61(1)
C(20)	16260(7)	866(1)	6116(3)	93(1)
C(21)	11943(5)	2900(1)	5055(3)	59(1)
C(22)	11259(6)	2964(1)	2849(3)	70(1)

Table 3. Bond lengths [Å] and angles [°] for jwb1.

S(1)-O(5)	1.423(2)
S(1)-O(6)	1.4247(19)
S(1)-N(1)	1.603(2)
S(1)-N(2)	1.624(2)
O(1)-C(8)	1.369(3)
O(1)-C(11)	1.431(3)
O(2)-C(7)	1.368(3)
O(2)-C(18)	1.422(3)
O(3)-C(19)	1.247(4)
O(4)-C(19)	1.254(4)
O(4)-C(20)	1.516(5)
N(1)-C(2)	1.456(3)
N(1)-C(3)	1.462(3)
N(2)-C(22)	1.463(4)
N(2)-C(21)	1.464(3)
C(1)-C(4)	1.417(4)
C(1)-C(19)	1.443(4)
C(1)-C(2)	1.545(4)
C(1)-H(1A)	0.9800
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-C(4)	1.491(4)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700

C(4)-C(5)	1.515(4)
C(4)-H(4A)	0.9800
C(5)-C(10)	1.379(4)
C(5)-C(6)	1.396(3)
C(6)-C(7)	1.381(3)
C(6)-H(6A)	0.97(2)
C(7)-C(8)	1.398(3)
C(8)-C(9)	1.377(3)
C(9)-C(10)	1.386(4)
C(9)-H(9A)	0.87(3)
C(10)-H(10A)	0.93(3)
C(11)-C(12)	1.501(4)
C(11)-H(11A)	1.00(3)
C(11)-H(11B)	1.00(3)
C(12)-C(13)	1.373(4)
C(12)-C(17)	1.374(4)
C(13)-C(14)	1.377(4)
C(13)-H(13A)	0.90(3)
C(14)-C(15)	1.363(5)
C(14)-H(14A)	0.9300
C(15)-C(16)	1.377(5)
C(15)-H(15A)	0.85(3)
C(16)-C(17)	1.369(5)
C(16)-H(16A)	0.94(4)
C(17)-H(17A)	0.90(4)
C(18)-H(18A)	0.98(3)

C(18)-H(18B)	0.97(3)
C(18)-H(18C)	0.98(3)
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(21)-H(21A)	1.00(3)
C(21)-H(21B)	0.96(3)
C(21)-H(21C)	1.01(4)
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600

O(5)-S(1)-O(6)	120.93(12)
O(5)-S(1)-N(1)	106.24(12)
O(6)-S(1)-N(1)	107.34(12)
O(5)-S(1)-N(2)	106.10(12)
O(6)-S(1)-N(2)	105.47(12)
N(1)-S(1)-N(2)	110.63(13)
C(8)-O(1)-C(11)	116.43(19)
C(7)-O(2)-C(18)	117.97(19)
C(19)-O(4)-C(20)	114.2(3)
C(2)-N(1)-C(3)	112.6(2)
C(2)-N(1)-S(1)	123.41(18)
C(3)-N(1)-S(1)	123.72(18)
C(22)-N(2)-C(21)	113.0(2)
C(22)-N(2)-S(1)	118.03(19)

C(21)-N(2)-S(1)	116.86(18)
C(4)-C(1)-C(19)	124.9(3)
C(4)-C(1)-C(2)	105.8(3)
C(19)-C(1)-C(2)	113.5(3)
C(4)-C(1)-H(1A)	103.4
C(19)-C(1)-H(1A)	103.4
C(2)-C(1)-H(1A)	103.4
N(1)-C(2)-C(1)	102.7(2)
N(1)-C(2)-H(2A)	111.2
C(1)-C(2)-H(2A)	111.2
N(1)-C(2)-H(2B)	111.2
C(1)-C(2)-H(2B)	111.2
H(2A)-C(2)-H(2B)	109.1
N(1)-C(3)-C(4)	101.9(2)
N(1)-C(3)-H(3A)	111.4
C(4)-C(3)-H(3A)	111.4
N(1)-C(3)-H(3B)	111.4
C(4)-C(3)-H(3B)	111.4
H(3A)-C(3)-H(3B)	109.2
C(1)-C(4)-C(3)	108.7(3)
C(1)-C(4)-C(5)	122.1(3)
C(3)-C(4)-C(5)	116.5(2)
C(1)-C(4)-H(4A)	102.0
C(3)-C(4)-H(4A)	102.0
C(5)-C(4)-H(4A)	102.0
C(10)-C(5)-C(6)	118.3(2)

C(10)-C(5)-C(4)	123.2(2)
C(6)-C(5)-C(4)	118.3(2)
C(7)-C(6)-C(5)	121.1(2)
C(7)-C(6)-H(6A)	118.7(15)
C(5)-C(6)-H(6A)	120.2(15)
O(2)-C(7)-C(6)	124.9(2)
O(2)-C(7)-C(8)	115.3(2)
C(6)-C(7)-C(8)	119.8(2)
O(1)-C(8)-C(9)	125.6(2)
O(1)-C(8)-C(7)	115.2(2)
C(9)-C(8)-C(7)	119.1(2)
C(8)-C(9)-C(10)	120.6(2)
C(8)-C(9)-H(9A)	118.8(18)
C(10)-C(9)-H(9A)	120.5(18)
C(5)-C(10)-C(9)	120.9(2)
C(5)-C(10)-H(10A)	121.5(18)
C(9)-C(10)-H(10A)	117.6(18)
O(1)-C(11)-C(12)	107.9(2)
O(1)-C(11)-H(11A)	110.4(19)
C(12)-C(11)-H(11A)	108.1(18)
O(1)-C(11)-H(11B)	105.4(17)
C(12)-C(11)-H(11B)	113.7(17)
H(11A)-C(11)-H(11B)	111(2)
C(13)-C(12)-C(17)	118.2(3)
C(13)-C(12)-C(11)	120.8(2)
C(17)-C(12)-C(11)	121.0(3)

C(12)-C(13)-C(14)	120.6(3)
C(12)-C(13)-H(13A)	121.0(19)
C(14)-C(13)-H(13A)	118.3(19)
C(15)-C(14)-C(13)	120.5(3)
C(15)-C(14)-H(14A)	119.8
C(13)-C(14)-H(14A)	119.8
C(14)-C(15)-C(16)	119.6(3)
C(14)-C(15)-H(15A)	124(2)
C(16)-C(15)-H(15A)	116(2)
C(17)-C(16)-C(15)	119.5(3)
C(17)-C(16)-H(16A)	119(3)
C(15)-C(16)-H(16A)	122(3)
C(16)-C(17)-C(12)	121.7(3)
C(16)-C(17)-H(17A)	119(2)
C(12)-C(17)-H(17A)	119(2)
O(2)-C(18)-H(18A)	109.6(17)
O(2)-C(18)-H(18B)	111.7(17)
H(18A)-C(18)-H(18B)	111(2)
O(2)-C(18)-H(18C)	105.3(18)
H(18A)-C(18)-H(18C)	106(2)
H(18B)-C(18)-H(18C)	112(2)
O(3)-C(19)-O(4)	120.1(3)
O(3)-C(19)-C(1)	119.5(3)
O(4)-C(19)-C(1)	120.4(3)
O(4)-C(20)-H(20A)	109.5
O(4)-C(20)-H(20B)	109.5

H(20A)-C(20)-H(20B)	109.5
O(4)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
N(2)-C(21)-H(21A)	109.9(18)
N(2)-C(21)-H(21B)	108.3(19)
H(21A)-C(21)-H(21B)	110(3)
N(2)-C(21)-H(21C)	108(2)
H(21A)-C(21)-H(21C)	109(3)
H(21B)-C(21)-H(21C)	112(3)
N(2)-C(22)-H(22A)	109.5
N(2)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
N(2)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for jwb1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	41(1)	54(1)	41(1)	-8(1)	2(1)	6(1)
O(1)	62(1)	56(1)	46(1)	1(1)	6(1)	27(1)
O(2)	62(1)	57(1)	42(1)	-9(1)	-5(1)	20(1)
O(3)	170(3)	82(2)	96(2)	16(2)	8(2)	-30(2)
O(4)	80(2)	160(3)	65(1)	13(2)	-8(1)	13(2)
O(5)	62(1)	77(1)	54(1)	-4(1)	22(1)	4(1)
O(6)	51(1)	81(1)	61(1)	-16(1)	-15(1)	8(1)
N(1)	95(2)	67(1)	35(1)	0(1)	6(1)	38(1)
N(2)	57(1)	59(1)	37(1)	-1(1)	-4(1)	-2(1)
C(1)	121(3)	70(2)	45(2)	5(1)	8(2)	43(2)
C(2)	99(2)	66(2)	39(1)	0(1)	1(1)	34(2)
C(3)	78(2)	62(2)	38(1)	-3(1)	6(1)	24(1)
C(4)	111(2)	93(2)	42(1)	-4(1)	3(2)	57(2)
C(5)	56(1)	48(1)	41(1)	-1(1)	6(1)	10(1)
C(6)	48(1)	45(1)	43(1)	-1(1)	2(1)	11(1)
C(7)	44(1)	39(1)	40(1)	1(1)	3(1)	2(1)
C(8)	44(1)	41(1)	44(1)	1(1)	10(1)	5(1)
C(9)	43(1)	58(1)	49(1)	6(1)	5(1)	13(1)
C(10)	52(1)	58(1)	40(1)	1(1)	0(1)	6(1)
C(11)	56(1)	53(1)	55(2)	3(1)	7(1)	20(1)
C(12)	48(1)	41(1)	57(1)	5(1)	5(1)	15(1)

C(13)	61(2)	56(2)	70(2)	-4(1)	15(1)	-4(1)
C(14)	76(2)	77(2)	77(2)	-12(2)	28(2)	3(2)
C(15)	90(2)	61(2)	73(2)	-18(2)	2(2)	14(2)
C(16)	71(2)	62(2)	106(3)	-18(2)	-3(2)	-6(2)
C(17)	56(2)	68(2)	87(2)	-4(2)	15(2)	-4(1)
C(18)	60(2)	55(1)	50(1)	-1(1)	-6(1)	13(1)
C(19)	75(2)	68(2)	39(1)	-3(1)	4(1)	14(2)
C(20)	106(3)	96(2)	77(2)	38(2)	8(2)	43(2)
C(21)	59(2)	66(2)	52(2)	-10(1)	-12(1)	1(1)
C(22)	76(2)	80(2)	53(2)	8(2)	3(2)	-7(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for jwb1.

	x	y	z	U(eq)
H(1A)	14654	1738	4227	95
H(2A)	10293	1751	5362	101(12)
H(2B)	12375	2050	5448	121
H(3A)	12424	2123	2349	82(10)
H(3B)	9959	1920	2107	98
H(4A)	10963	1417	3085	98
H(6A)	11400(40)	1519(7)	650(20)	48(7)
H(9A)	18110(50)	833(8)	1590(20)	54(7)
H(10A)	16570(50)	1195(8)	3070(30)	63(8)
H(11A)	20130(60)	617(9)	-230(30)	77(10)
H(11B)	18060(50)	345(8)	330(30)	68(9)
H(13A)	21950(50)	458(8)	-2070(30)	67(9)
H(14A)	22533	71	-3692	91
H(15A)	19810(60)	-408(9)	-4030(30)	76(10)
H(16A)	16550(70)	-479(12)	-2910(40)	121(14)
H(17A)	16090(70)	-86(11)	-1300(30)	103(13)
H(18A)	11640(50)	1661(9)	-1490(30)	68(9)
H(18B)	9800(50)	1329(8)	-1180(30)	63(8)
H(18C)	11040(50)	1358(9)	-2500(30)	73(9)
H(20A)	17919	840	6311	160(20)

H(20B)	15756	661	5596	147(18)
H(20C)	15379	861	6858	176
H(21A)	13470(50)	2764(9)	4920(30)	73(9)
H(21B)	11220(50)	2802(9)	5780(30)	75(9)
H(21C)	12270(60)	3179(10)	5120(30)	92(11)
H(22A)	12692	2828	2690	80(10)
H(22B)	11593	3230	2890	96(12)
H(22C)	10118	2916	2201	115

Table 6. Torsion angles [°] for jwb1.

O(5)-S(1)-N(1)-C(2)	-23.0(3)
O(6)-S(1)-N(1)-C(2)	-153.7(3)
N(2)-S(1)-N(1)-C(2)	91.7(3)
O(5)-S(1)-N(1)-C(3)	162.9(2)
O(6)-S(1)-N(1)-C(3)	32.3(3)
N(2)-S(1)-N(1)-C(3)	-82.3(3)
O(5)-S(1)-N(2)-C(22)	-172.4(2)
O(6)-S(1)-N(2)-C(22)	-42.9(2)
N(1)-S(1)-N(2)-C(22)	72.8(2)
O(5)-S(1)-N(2)-C(21)	47.7(2)
O(6)-S(1)-N(2)-C(21)	177.10(19)
N(1)-S(1)-N(2)-C(21)	-67.1(2)
C(3)-N(1)-C(2)-C(1)	1.3(4)
S(1)-N(1)-C(2)-C(1)	-173.3(2)
C(4)-C(1)-C(2)-N(1)	-18.5(4)
C(19)-C(1)-C(2)-N(1)	-159.0(3)
C(2)-N(1)-C(3)-C(4)	15.2(3)
S(1)-N(1)-C(3)-C(4)	-170.1(2)
C(19)-C(1)-C(4)-C(3)	163.9(3)
C(2)-C(1)-C(4)-C(3)	29.3(4)
C(19)-C(1)-C(4)-C(5)	-55.9(6)
C(2)-C(1)-C(4)-C(5)	169.5(3)
N(1)-C(3)-C(4)-C(1)	-27.6(4)
N(1)-C(3)-C(4)-C(5)	-170.3(3)

C(1)-C(4)-C(5)-C(10)	4.9(5)
C(3)-C(4)-C(5)-C(10)	142.2(3)
C(1)-C(4)-C(5)-C(6)	179.9(3)
C(3)-C(4)-C(5)-C(6)	-42.8(4)
C(10)-C(5)-C(6)-C(7)	1.6(4)
C(4)-C(5)-C(6)-C(7)	-173.6(3)
C(18)-O(2)-C(7)-C(6)	4.2(4)
C(18)-O(2)-C(7)-C(8)	-176.7(2)
C(5)-C(6)-C(7)-O(2)	-178.5(2)
C(5)-C(6)-C(7)-C(8)	2.4(4)
C(11)-O(1)-C(8)-C(9)	9.1(4)
C(11)-O(1)-C(8)-C(7)	-171.6(2)
O(2)-C(7)-C(8)-O(1)	-3.2(3)
C(6)-C(7)-C(8)-O(1)	176.0(2)
O(2)-C(7)-C(8)-C(9)	176.1(2)
C(6)-C(7)-C(8)-C(9)	-4.7(4)
O(1)-C(8)-C(9)-C(10)	-177.8(2)
C(7)-C(8)-C(9)-C(10)	3.0(4)
C(6)-C(5)-C(10)-C(9)	-3.4(4)
C(4)-C(5)-C(10)-C(9)	171.6(3)
C(8)-C(9)-C(10)-C(5)	1.1(4)
C(8)-O(1)-C(11)-C(12)	169.2(2)
O(1)-C(11)-C(12)-C(13)	105.8(3)
O(1)-C(11)-C(12)-C(17)	-76.7(3)
C(17)-C(12)-C(13)-C(14)	1.2(4)
C(11)-C(12)-C(13)-C(14)	178.8(3)

C(12)-C(13)-C(14)-C(15)	-1.2(5)
C(13)-C(14)-C(15)-C(16)	0.7(5)
C(14)-C(15)-C(16)-C(17)	-0.3(6)
C(15)-C(16)-C(17)-C(12)	0.3(5)
C(13)-C(12)-C(17)-C(16)	-0.8(5)
C(11)-C(12)-C(17)-C(16)	-178.3(3)
C(20)-O(4)-C(19)-O(3)	3.3(4)
C(20)-O(4)-C(19)-C(1)	-174.1(3)
C(4)-C(1)-C(19)-O(3)	-58.5(5)
C(2)-C(1)-C(19)-O(3)	73.1(4)
C(4)-C(1)-C(19)-O(4)	118.8(4)
C(2)-C(1)-C(19)-O(4)	-109.5(4)

Symmetry transformations used to generate equivalent atoms: