Supporting information

Multicomponent/Palladium-Catalyzed Cascade Entry to Benzopyrrolizidine Derivatives: Synthesis and Antioxidant Evaluation

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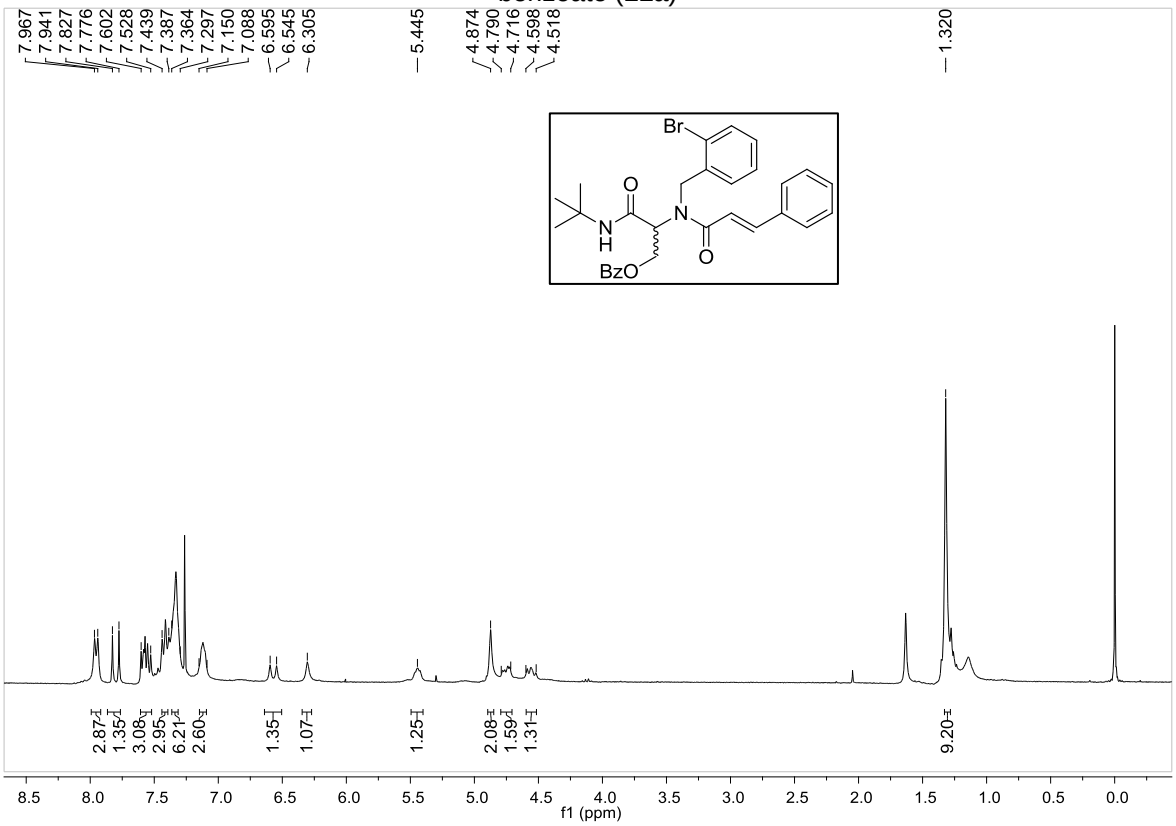
^{1}H-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-phenylprop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11a**)



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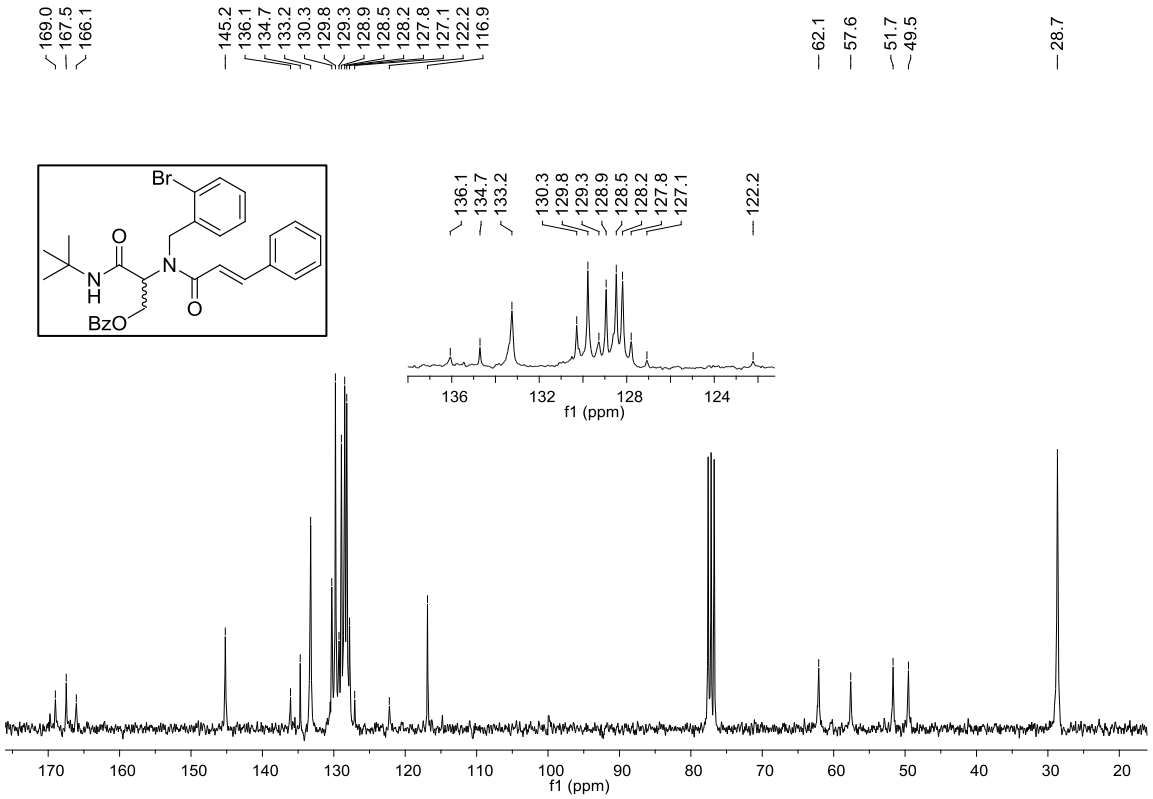
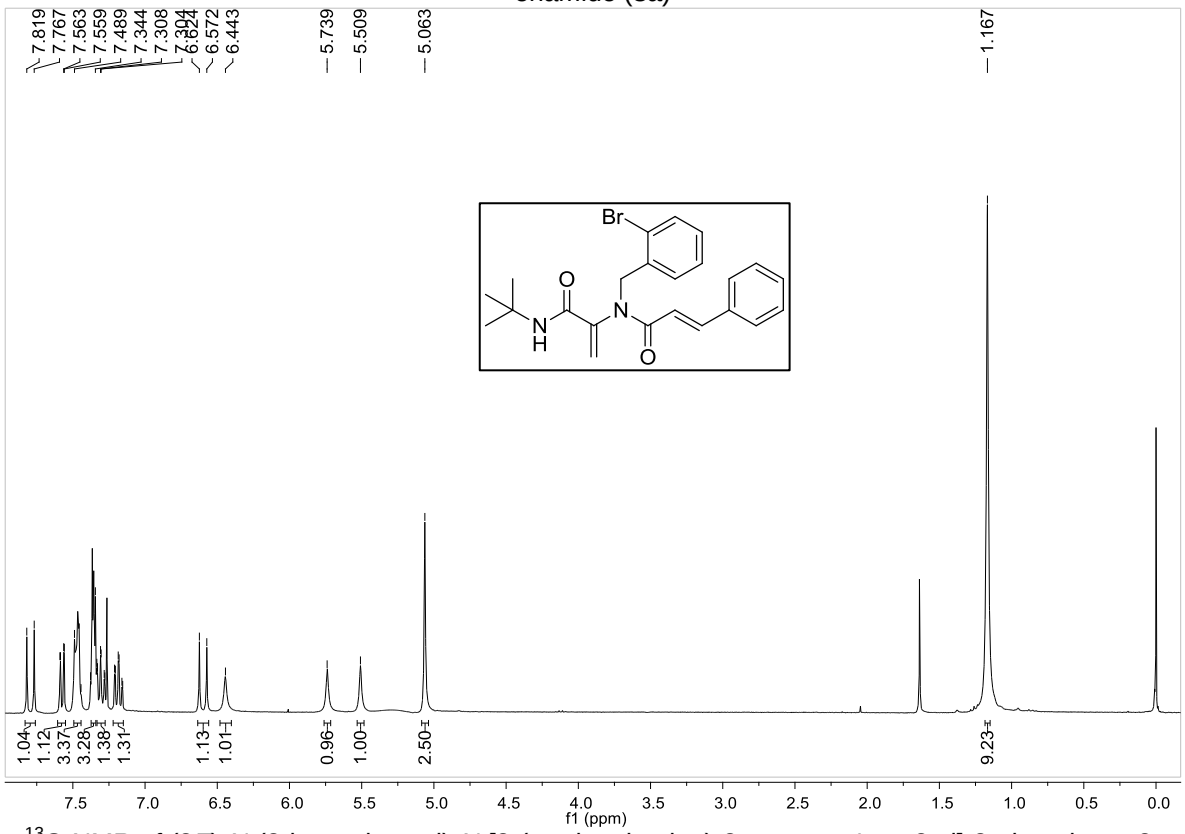


^{1}H-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(tert-butylamino)-3-oxoprop-1-en-2-yl]-3-phenylprop-2-enamide (**8a**)



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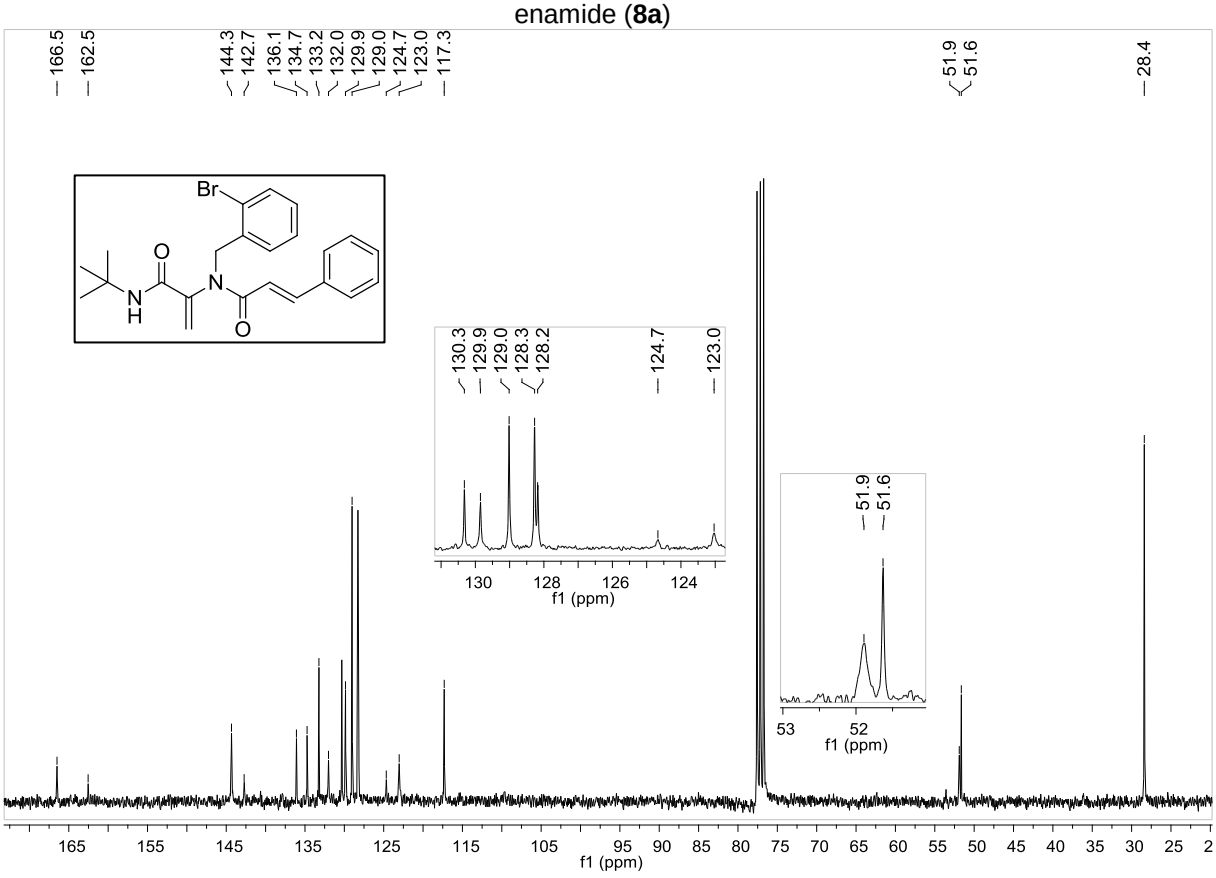

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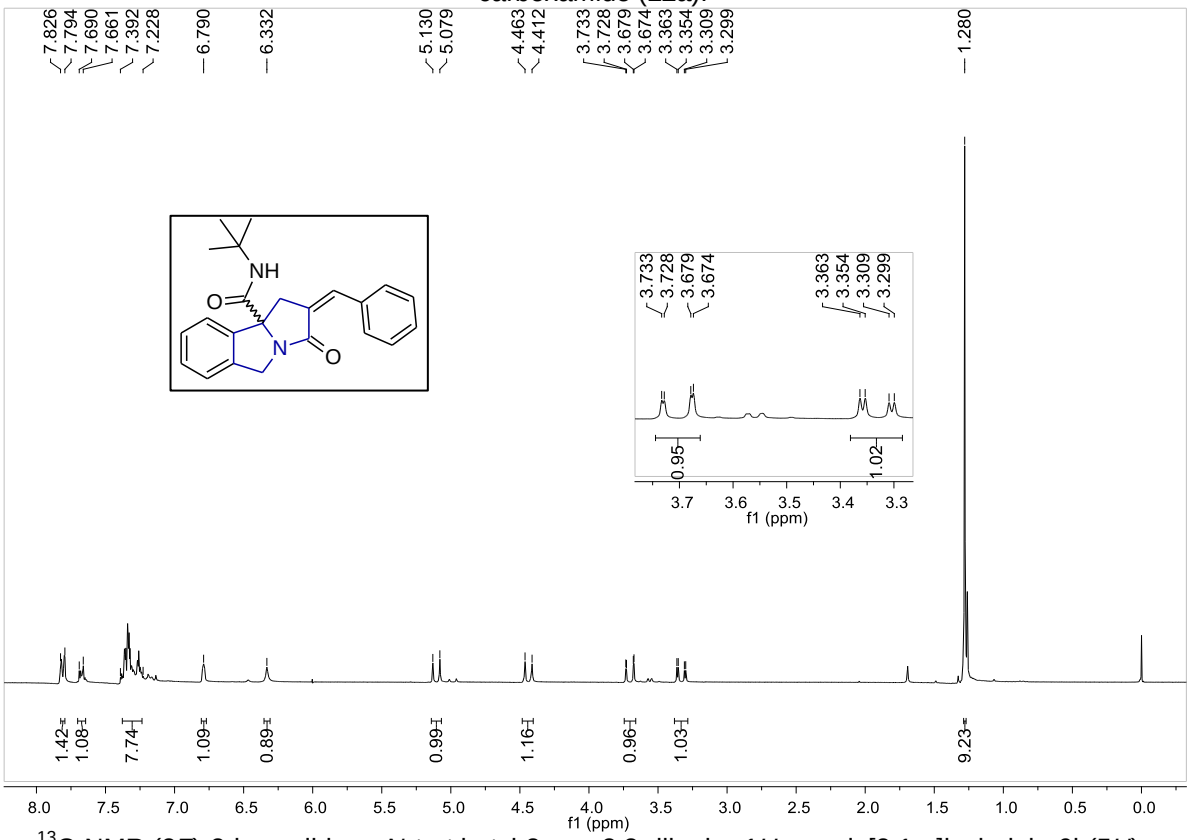

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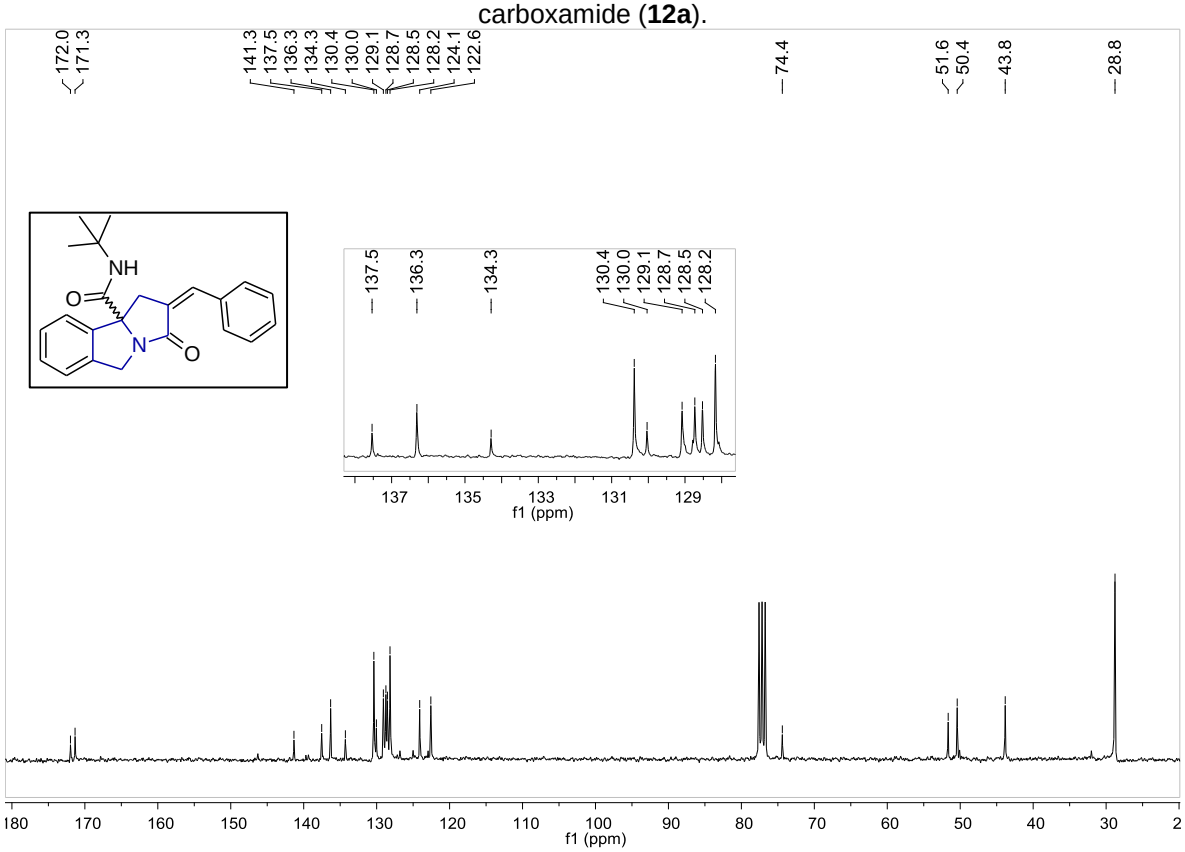
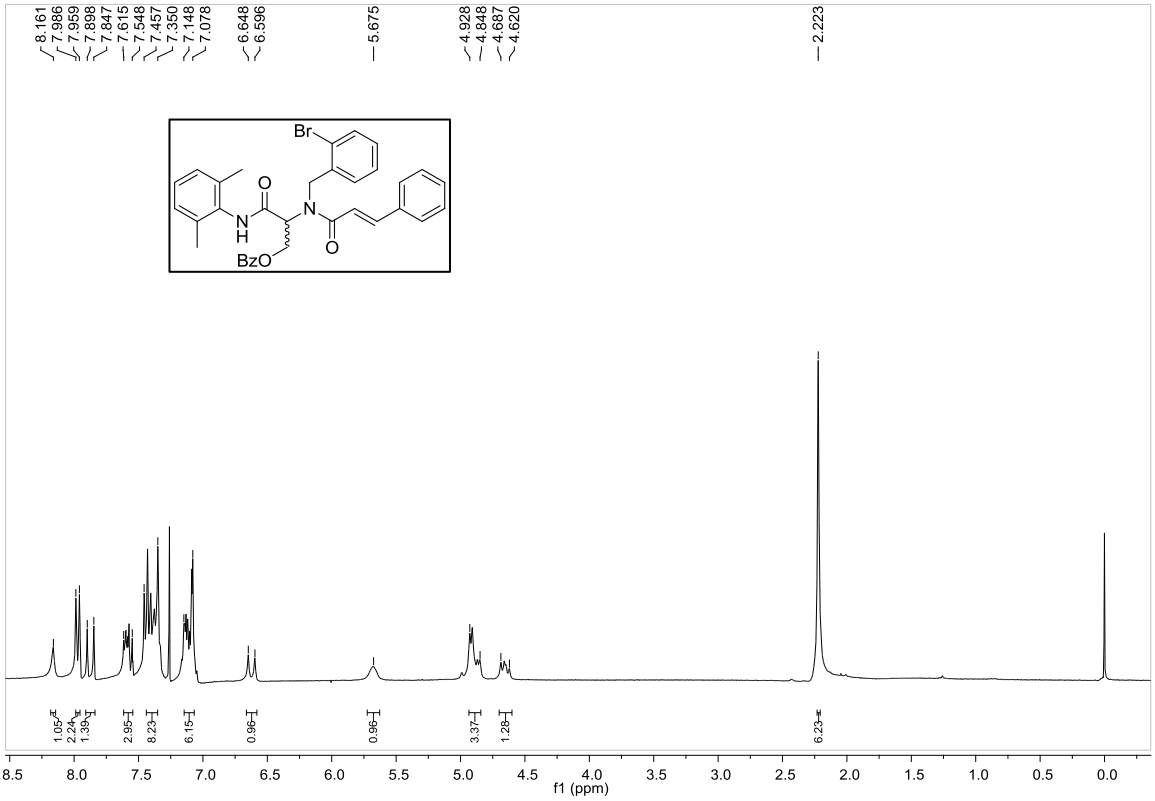
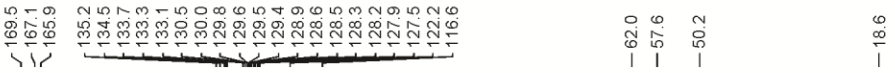
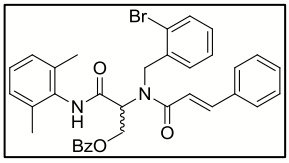


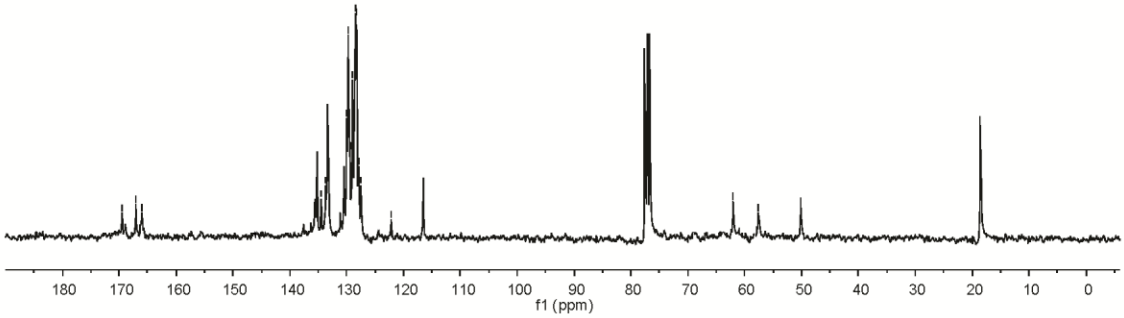
^{1}H-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-phenylprop-2-enoylamino}]-3-[(2,6-dimethylphenyl)amino]-3-oxopropyl benzoate (**11b**)



^{13}C-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-phenylprop-2-enoylamino}]-3-[(2,6-dimethylphenyl)amino]-3-oxopropyl benzoate (**11b**)







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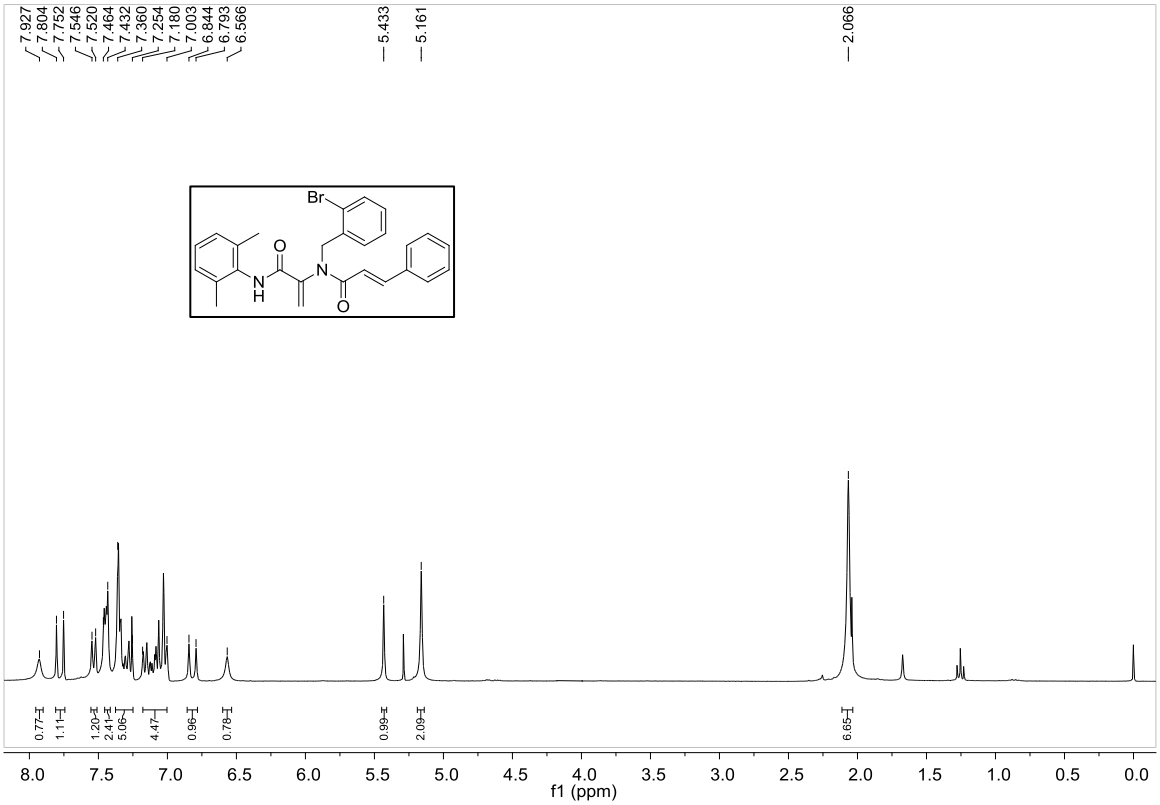

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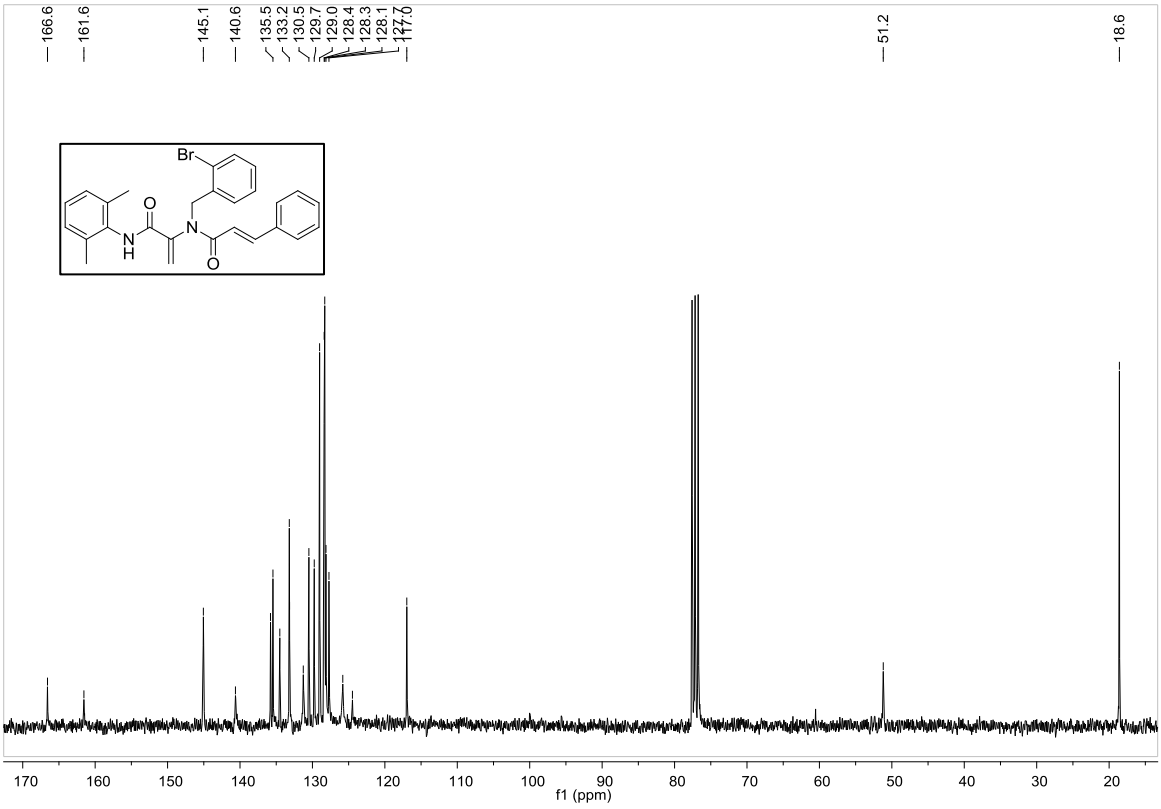

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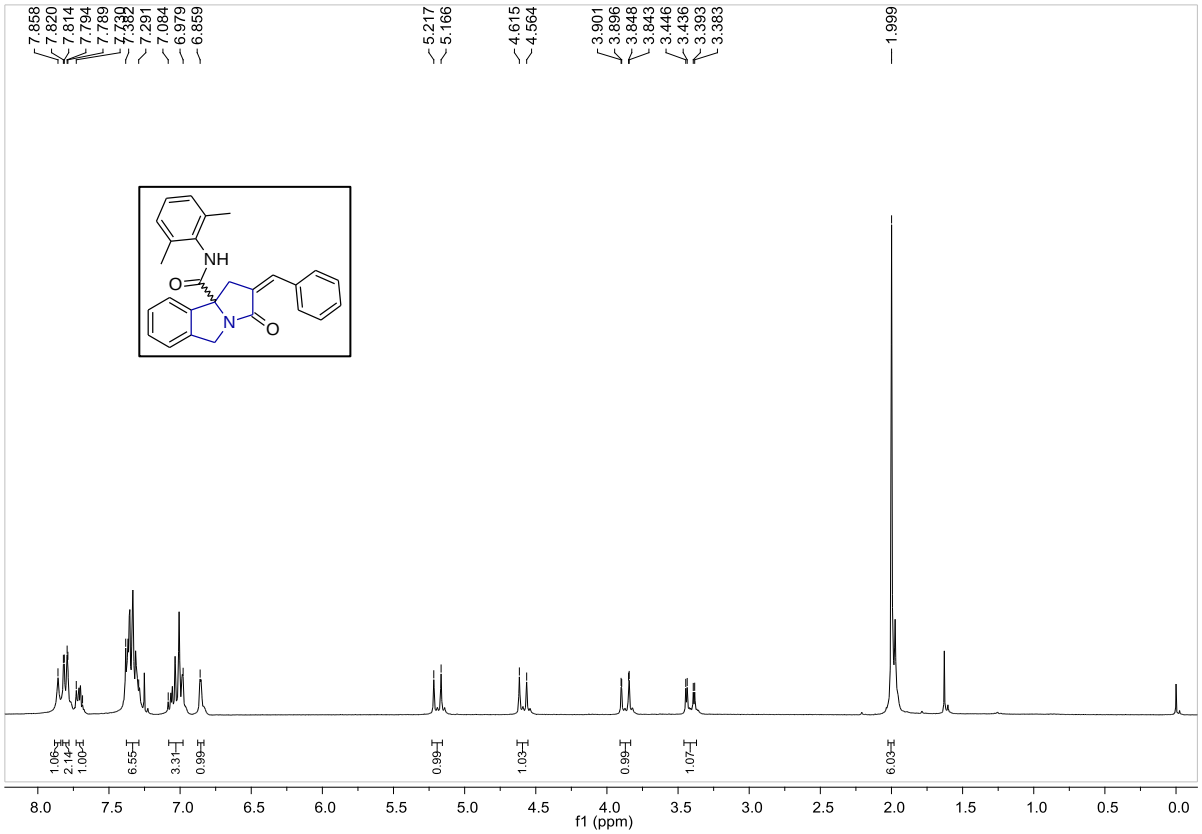

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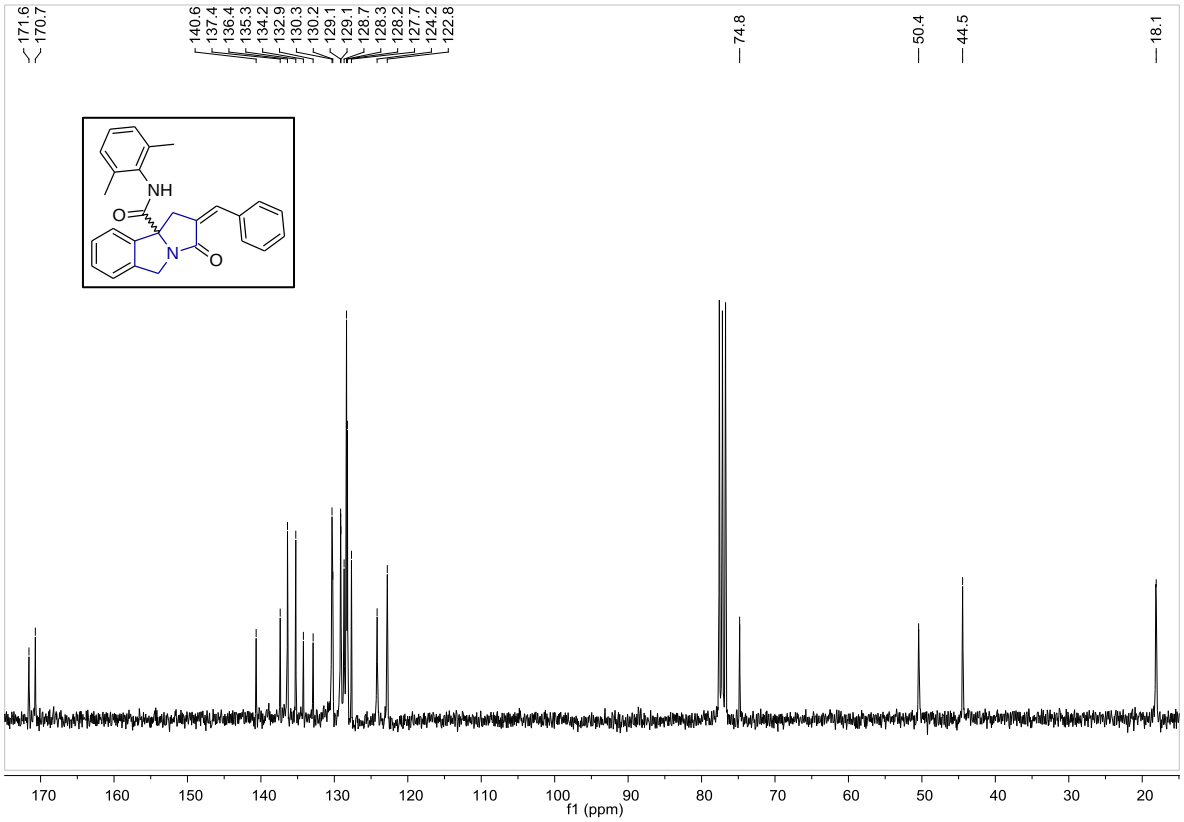
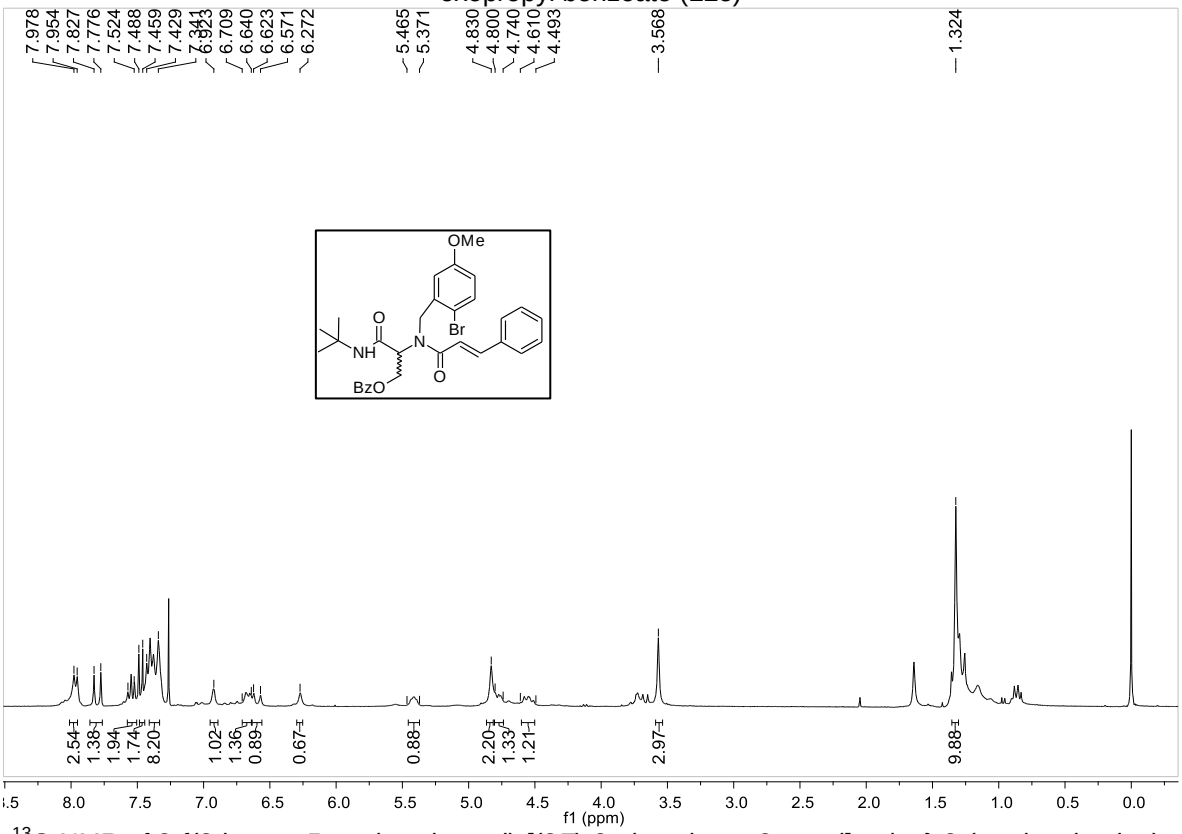


^{1}H-NMR of 2-{(2-bromo-5-methoxybenzyl)-[(2*E*)-3-phenylprop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11c**)



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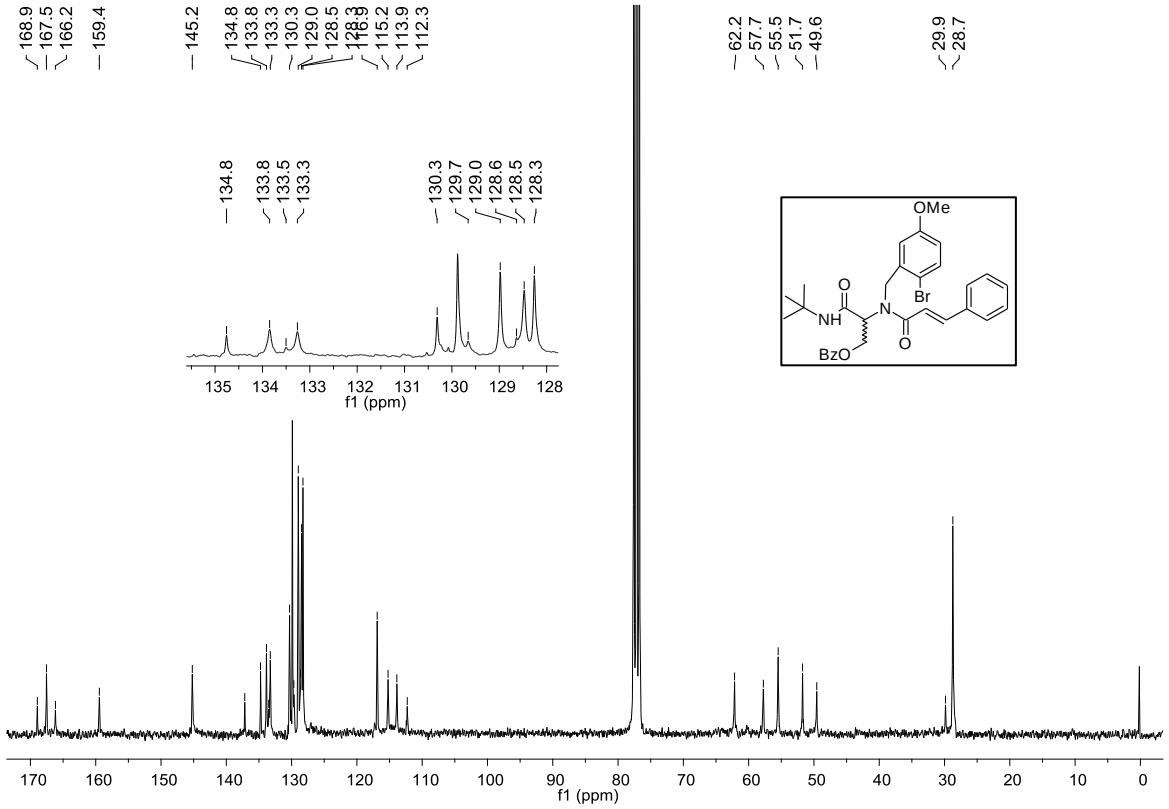

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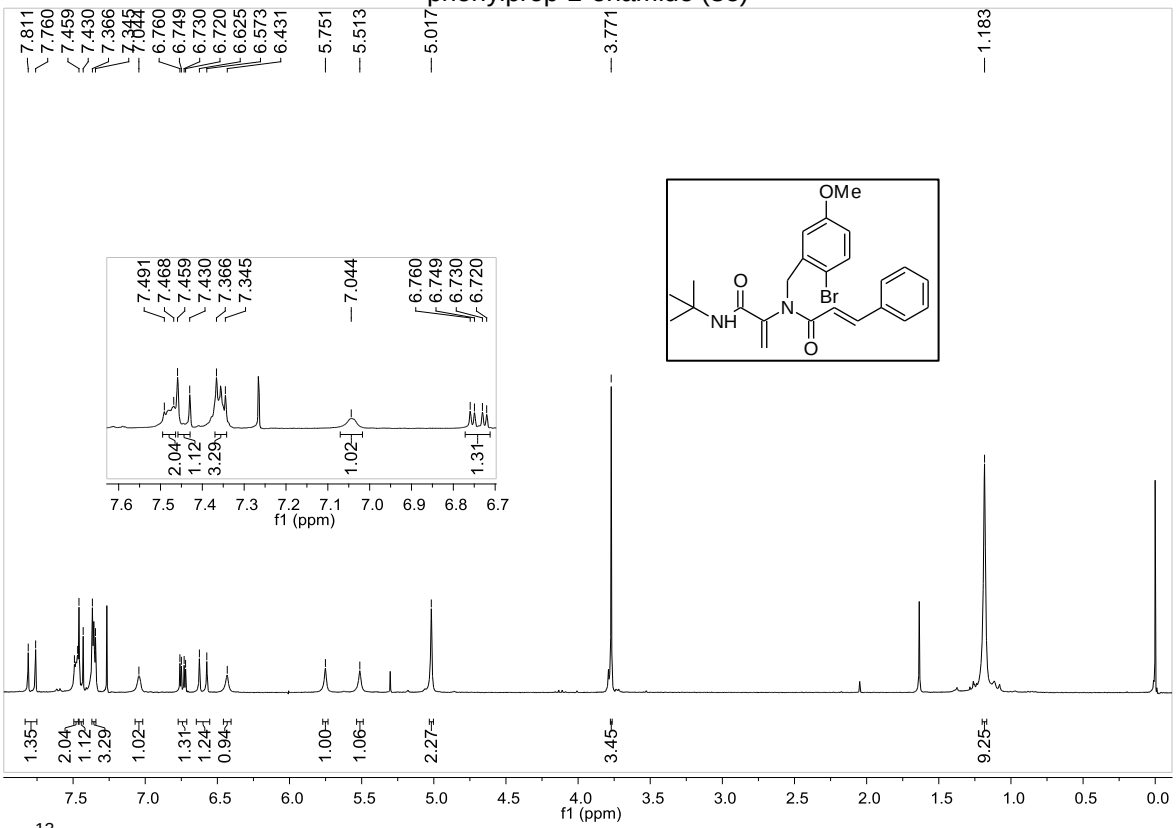

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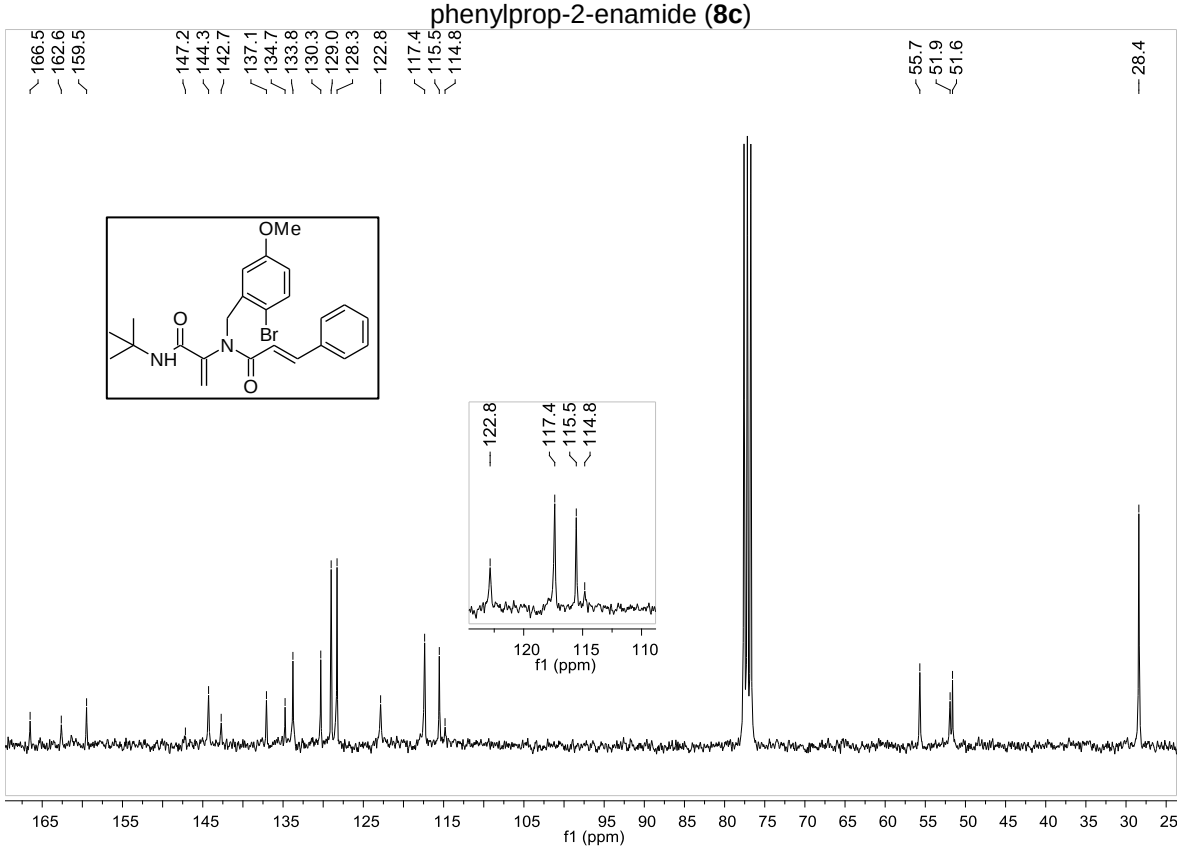

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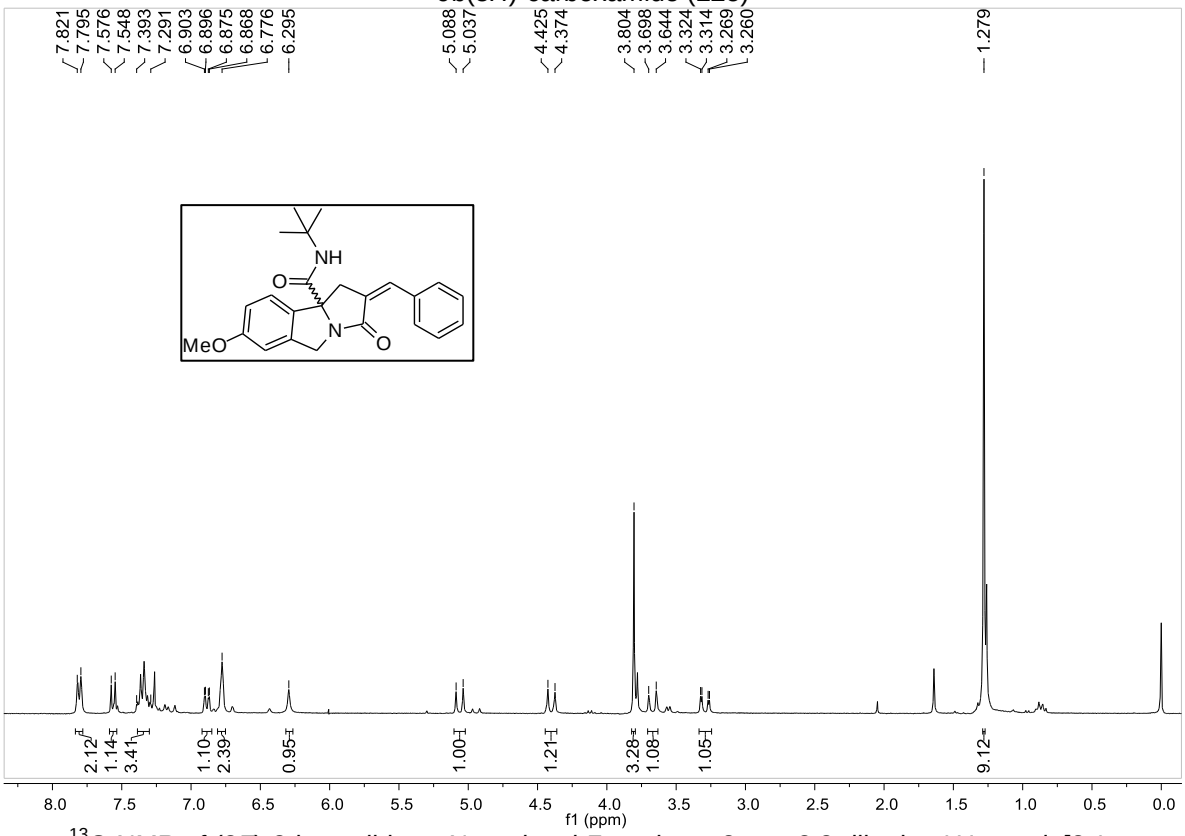

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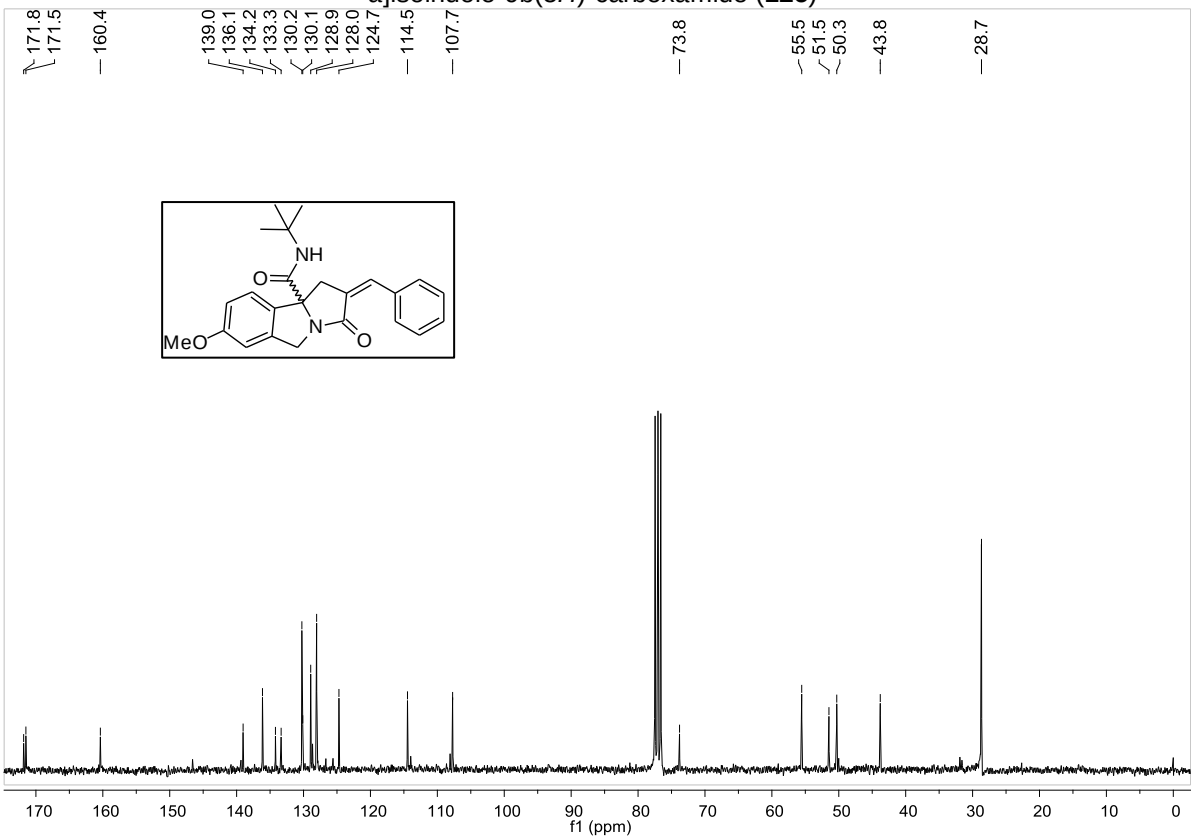

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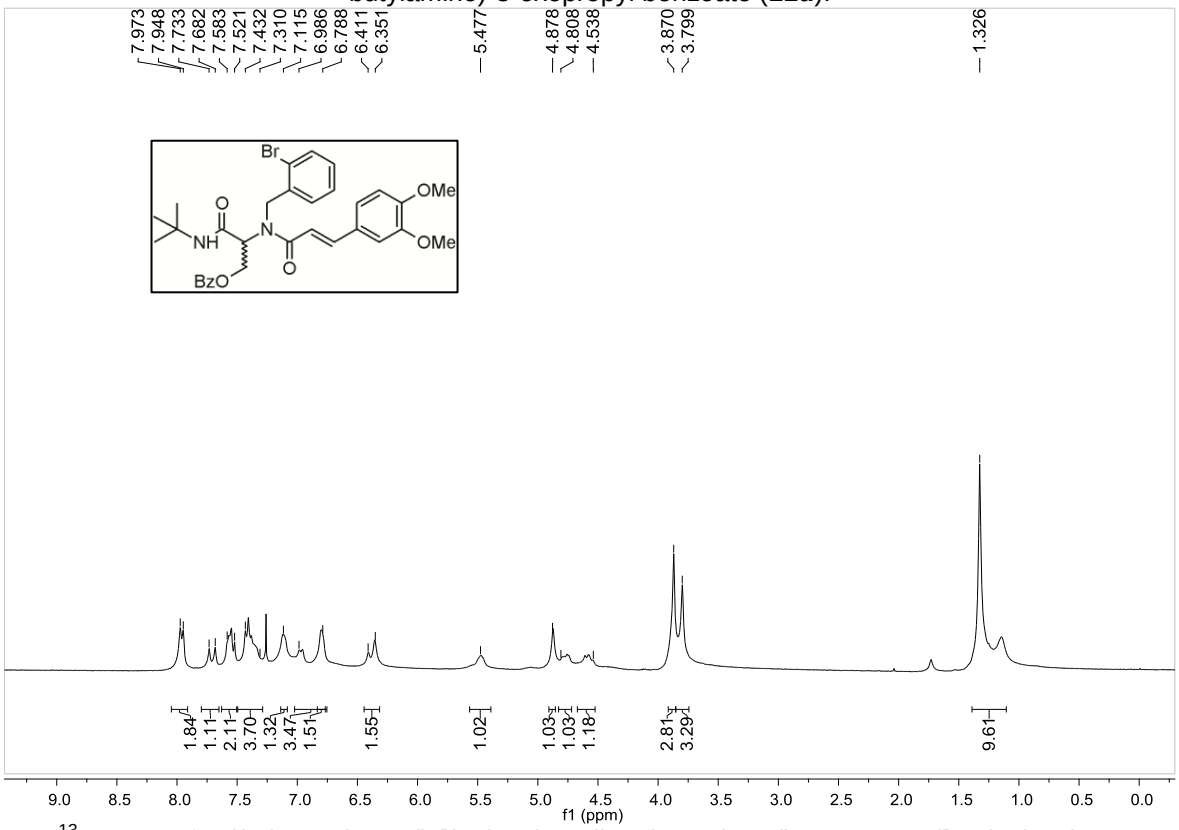

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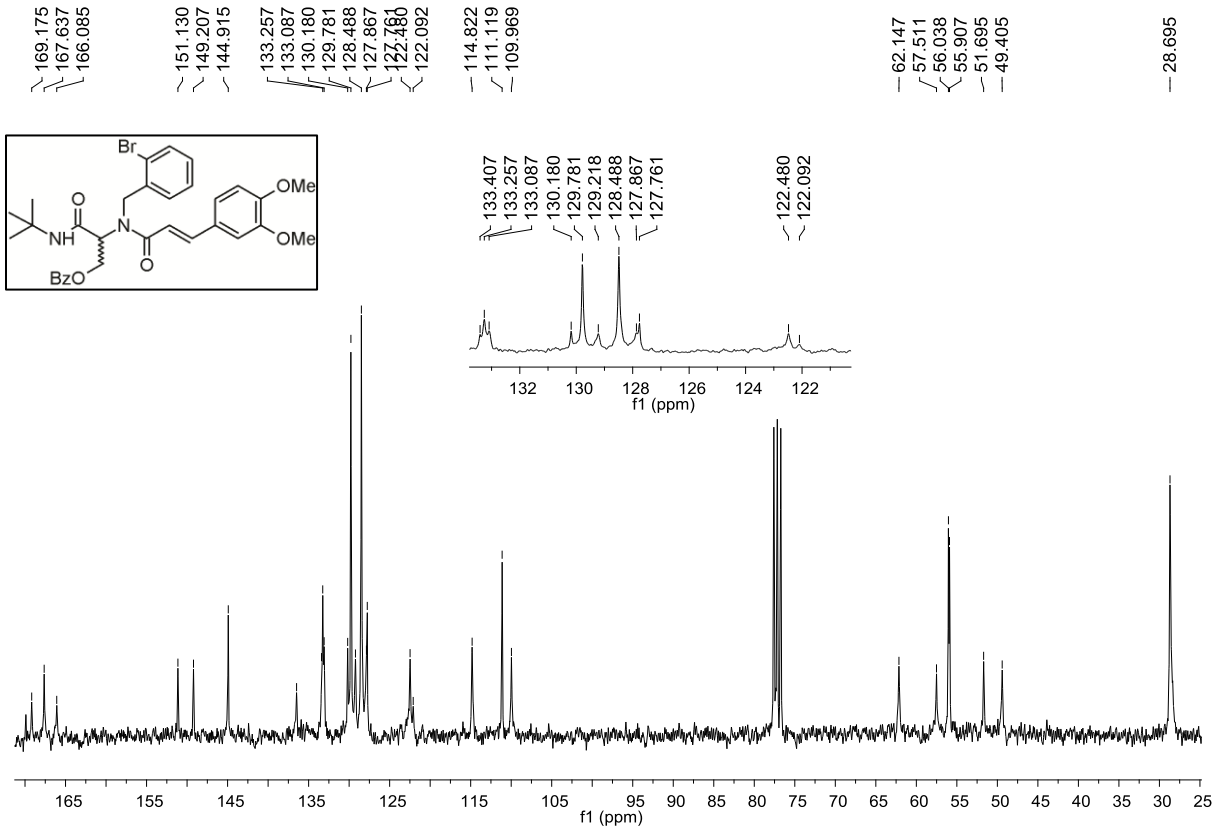

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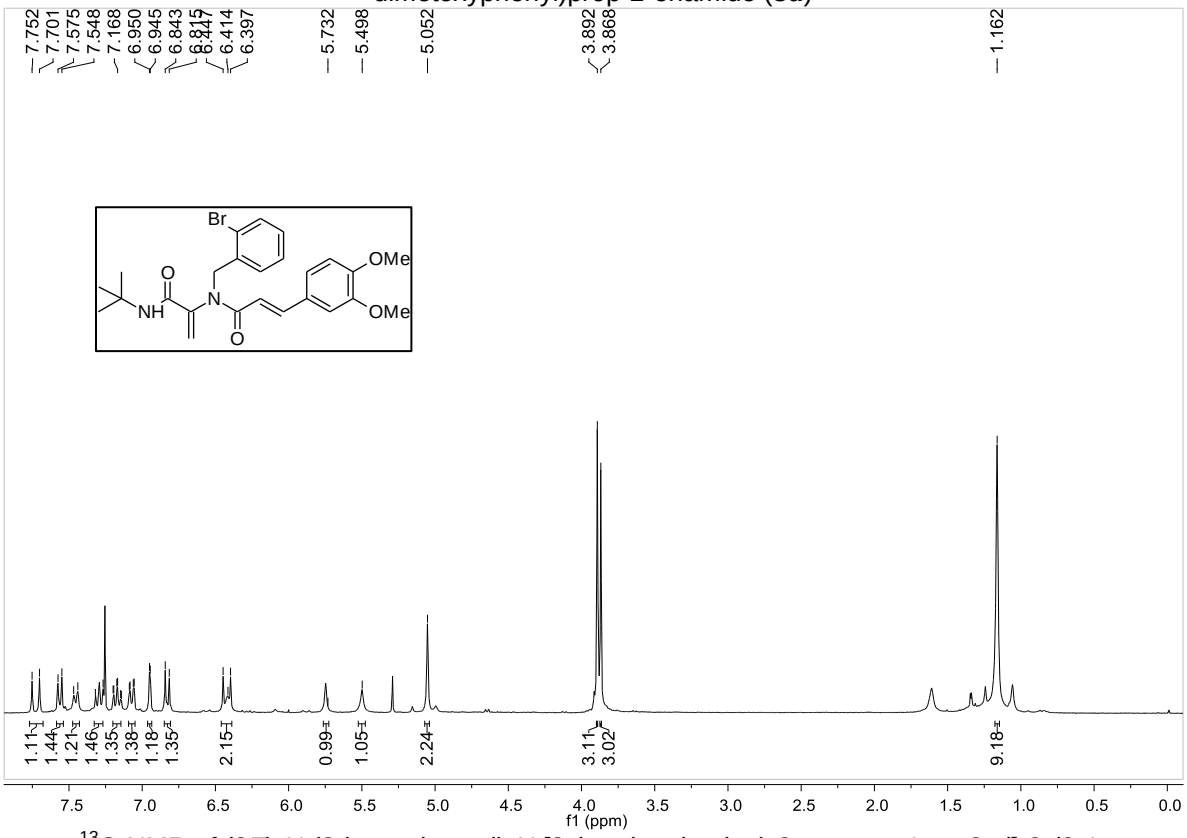

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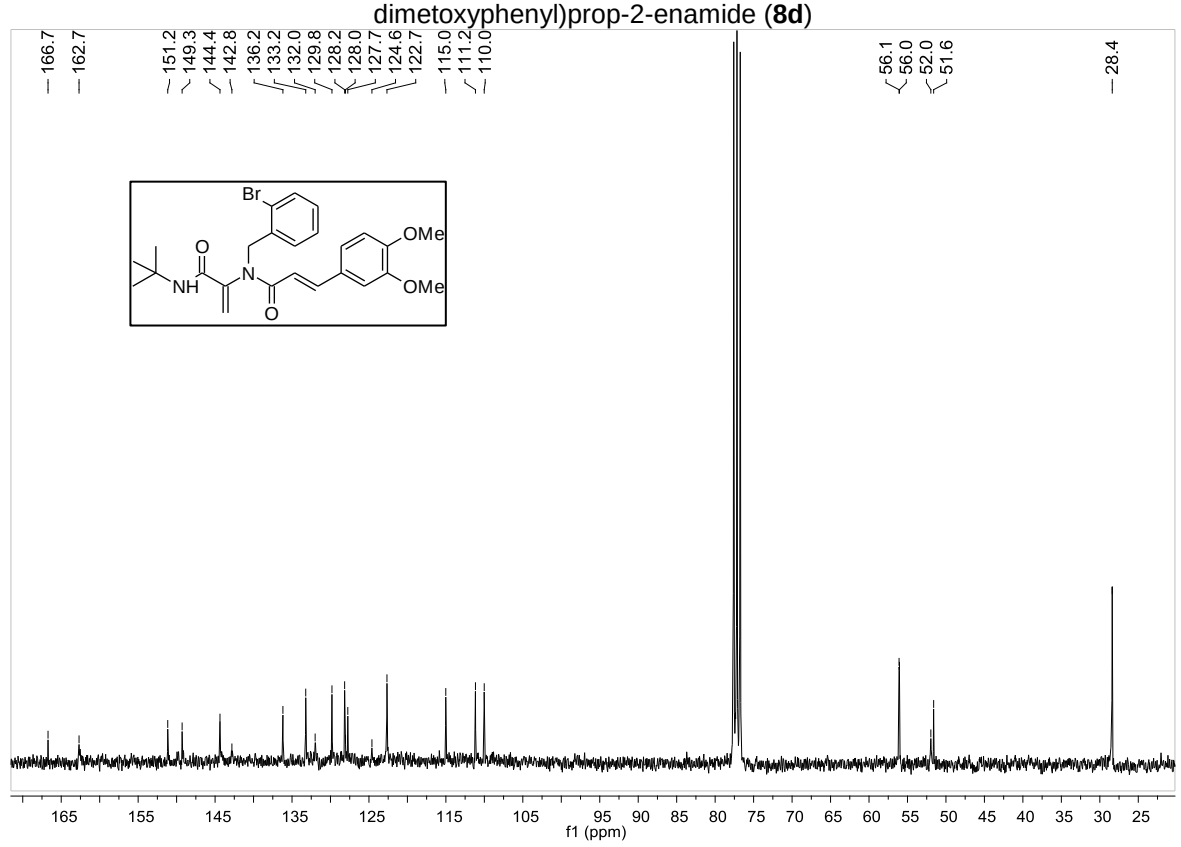

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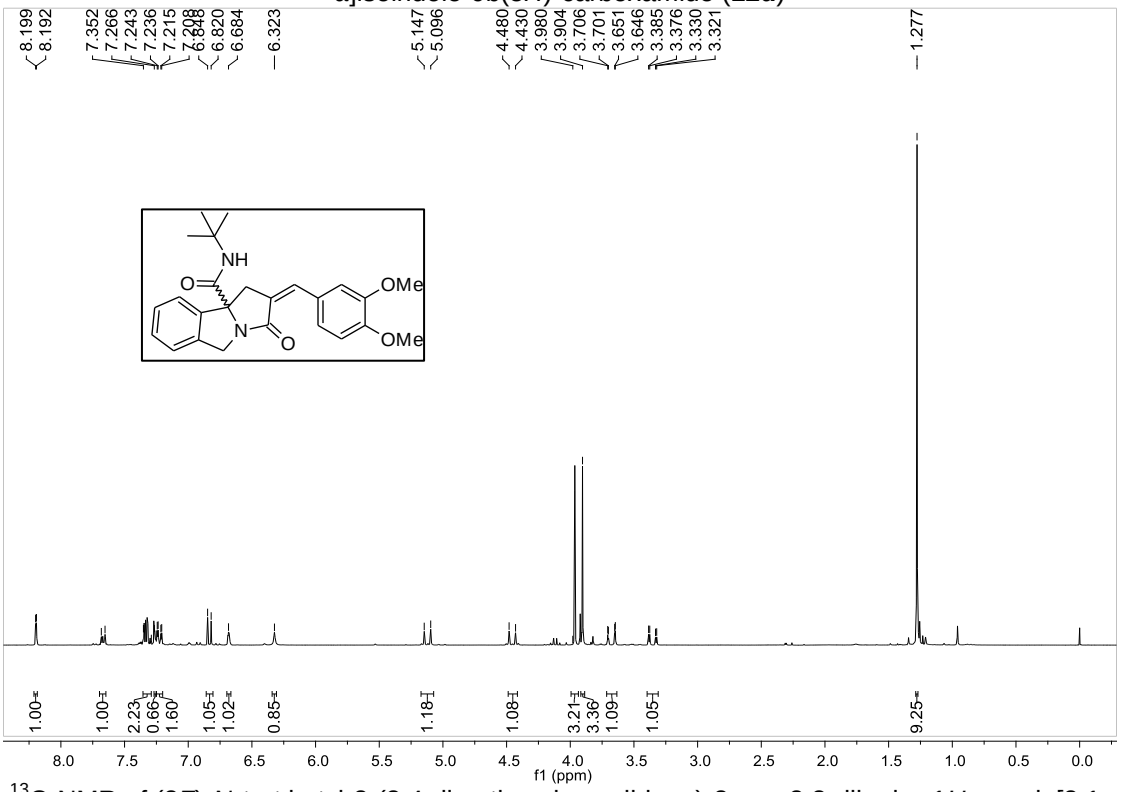

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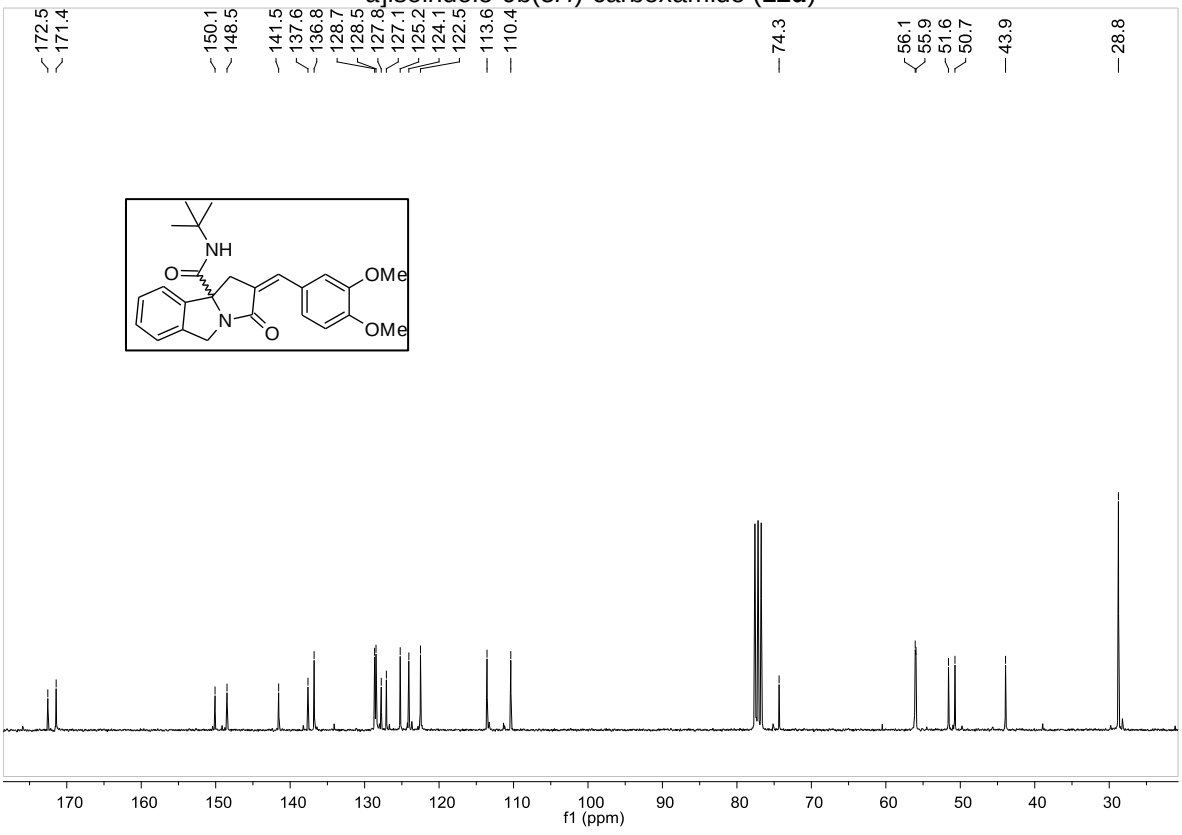

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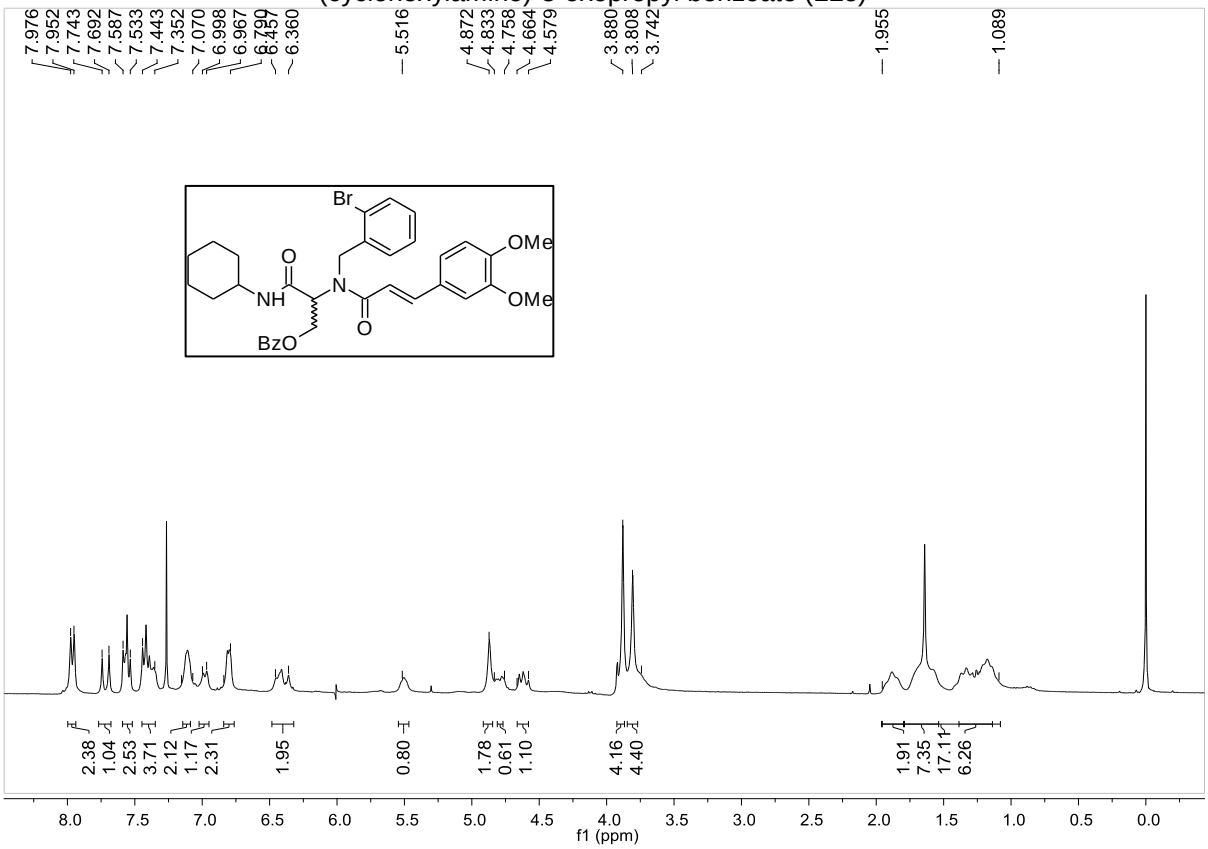

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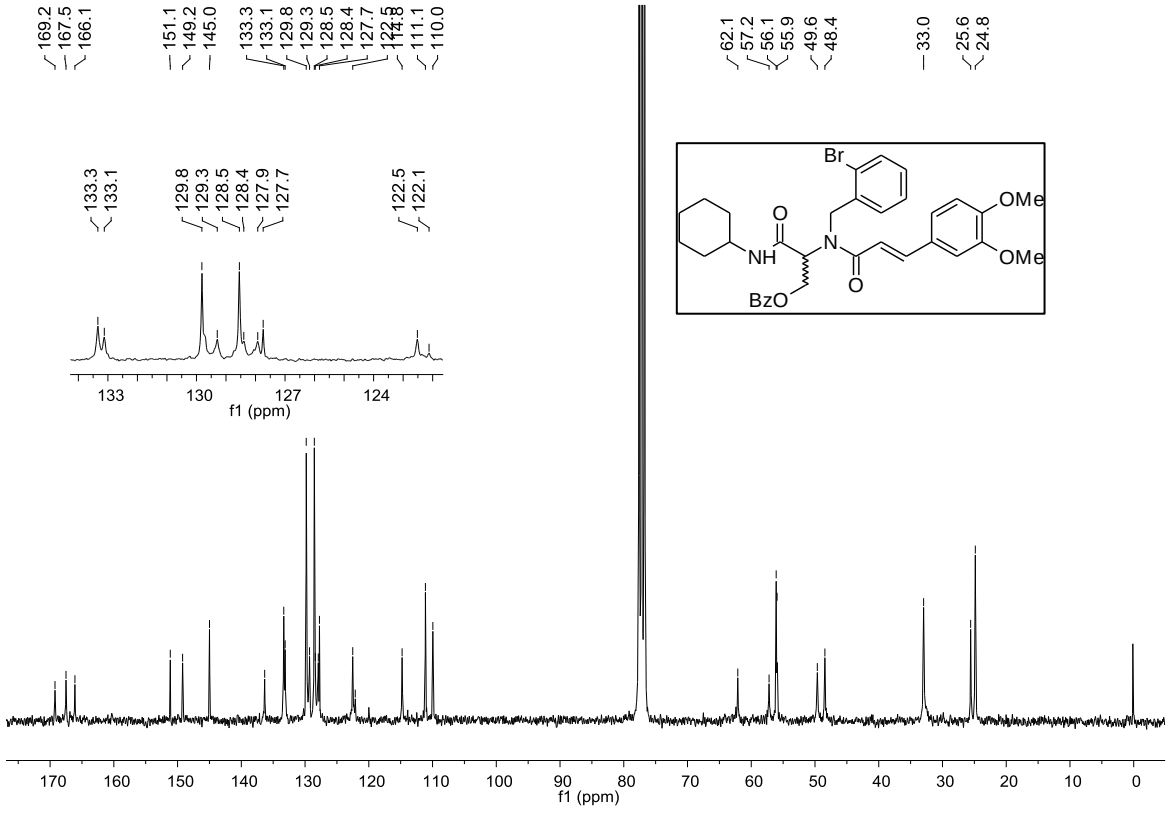

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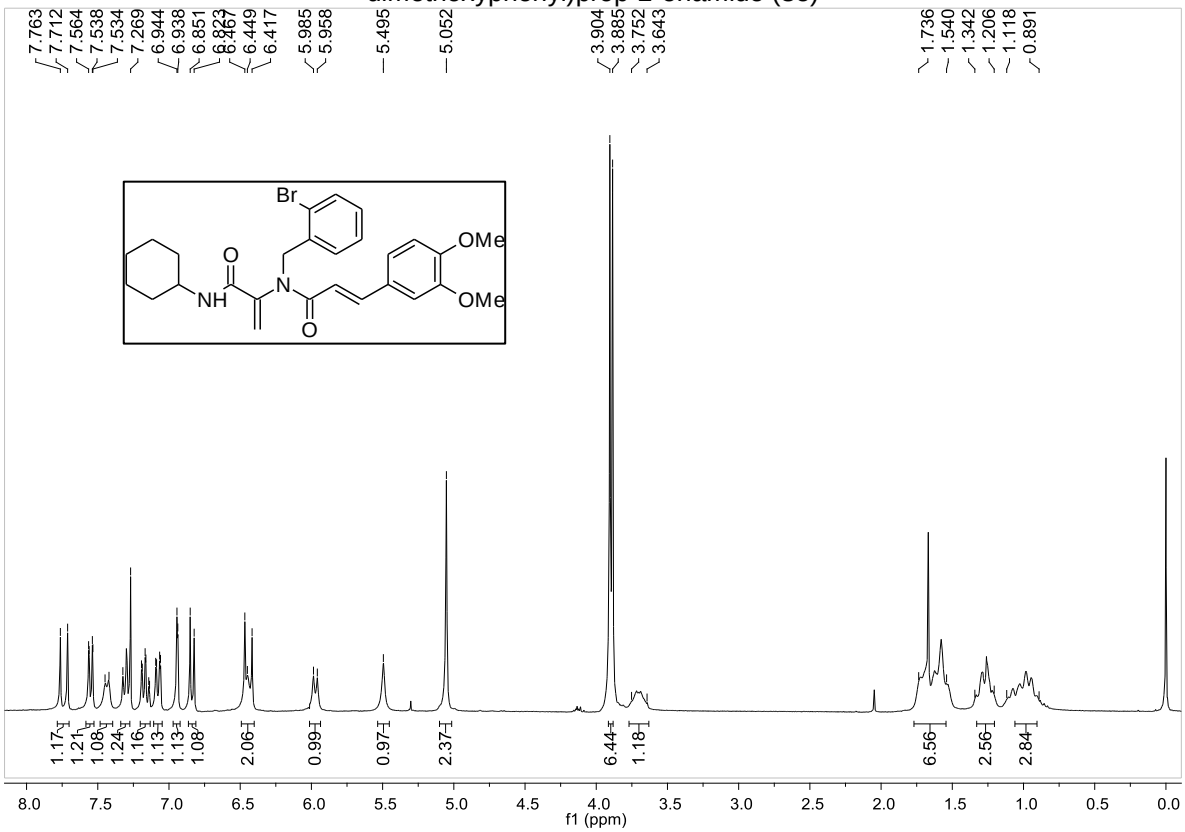

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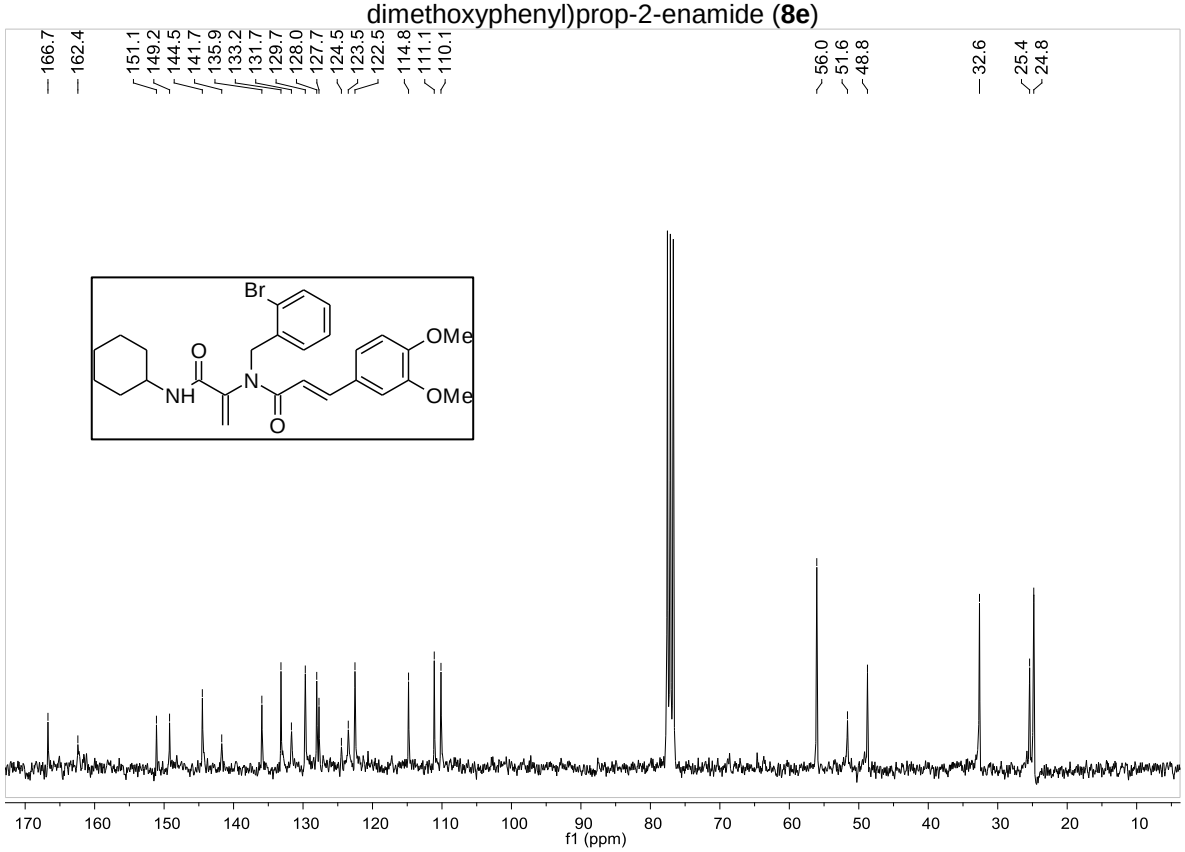

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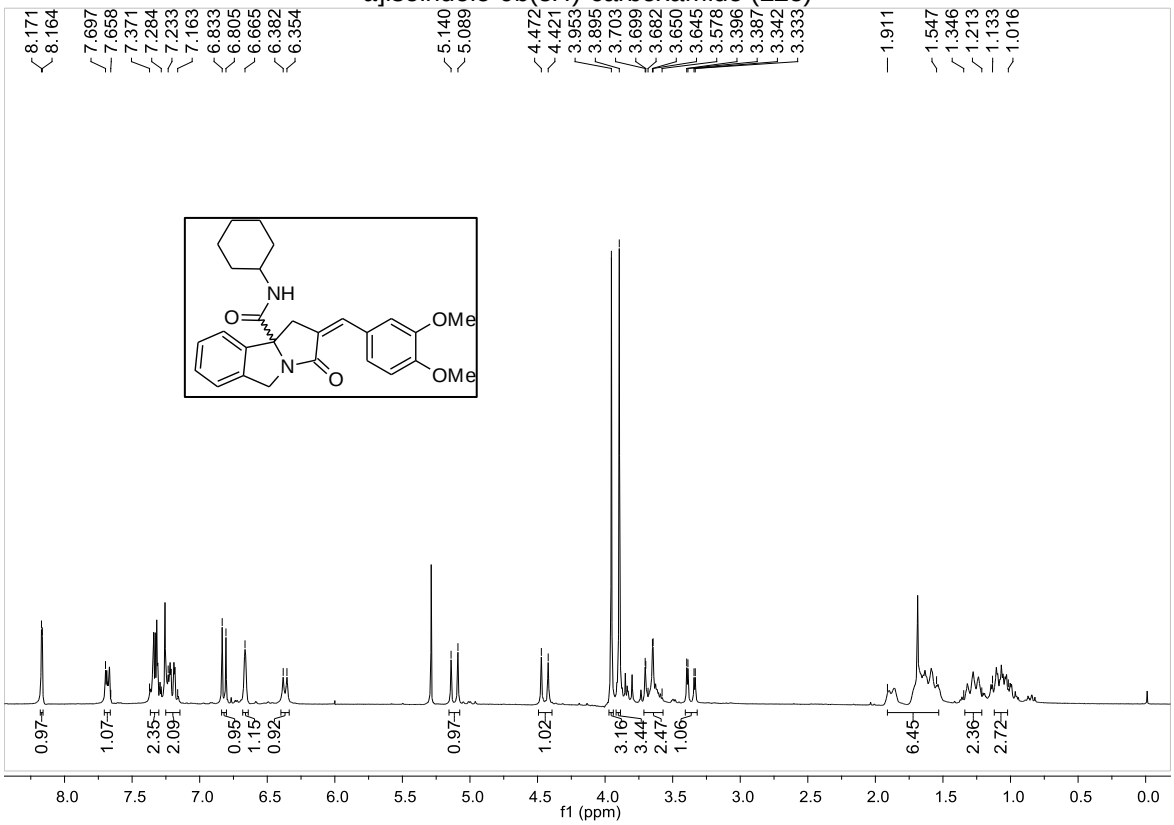

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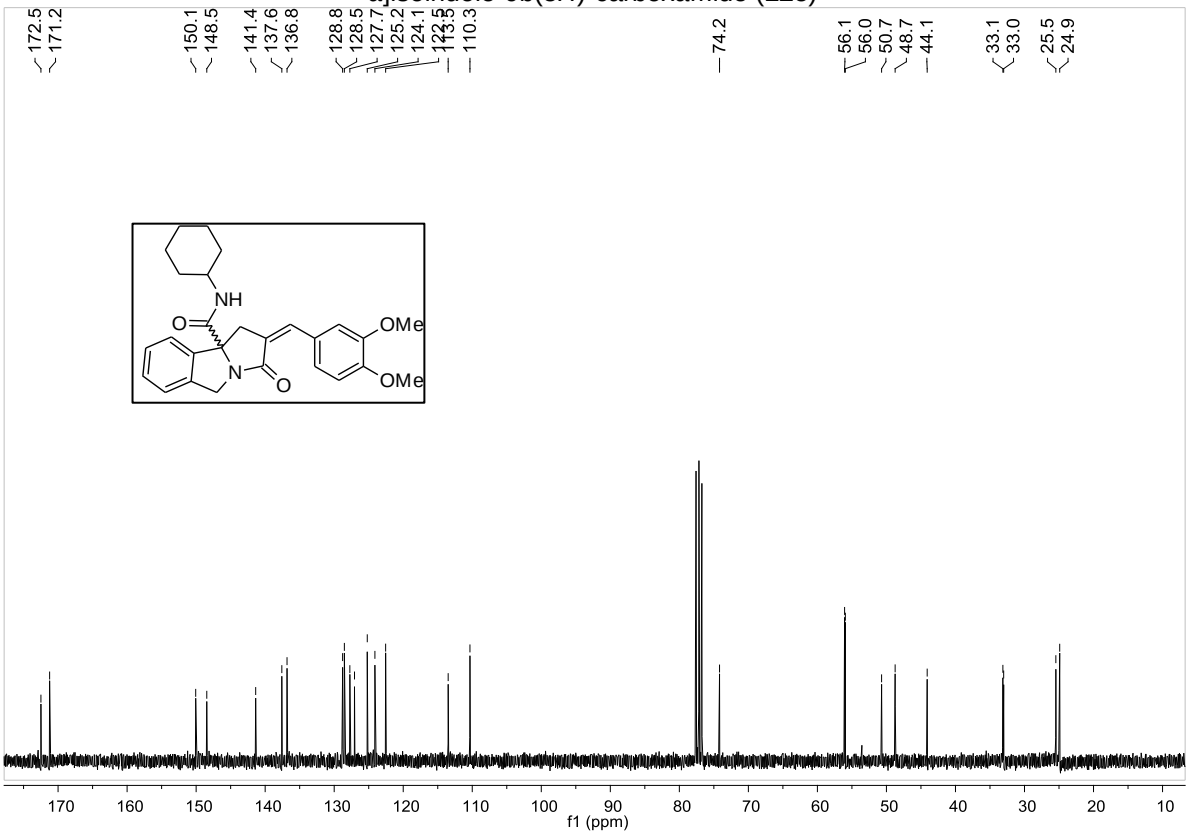

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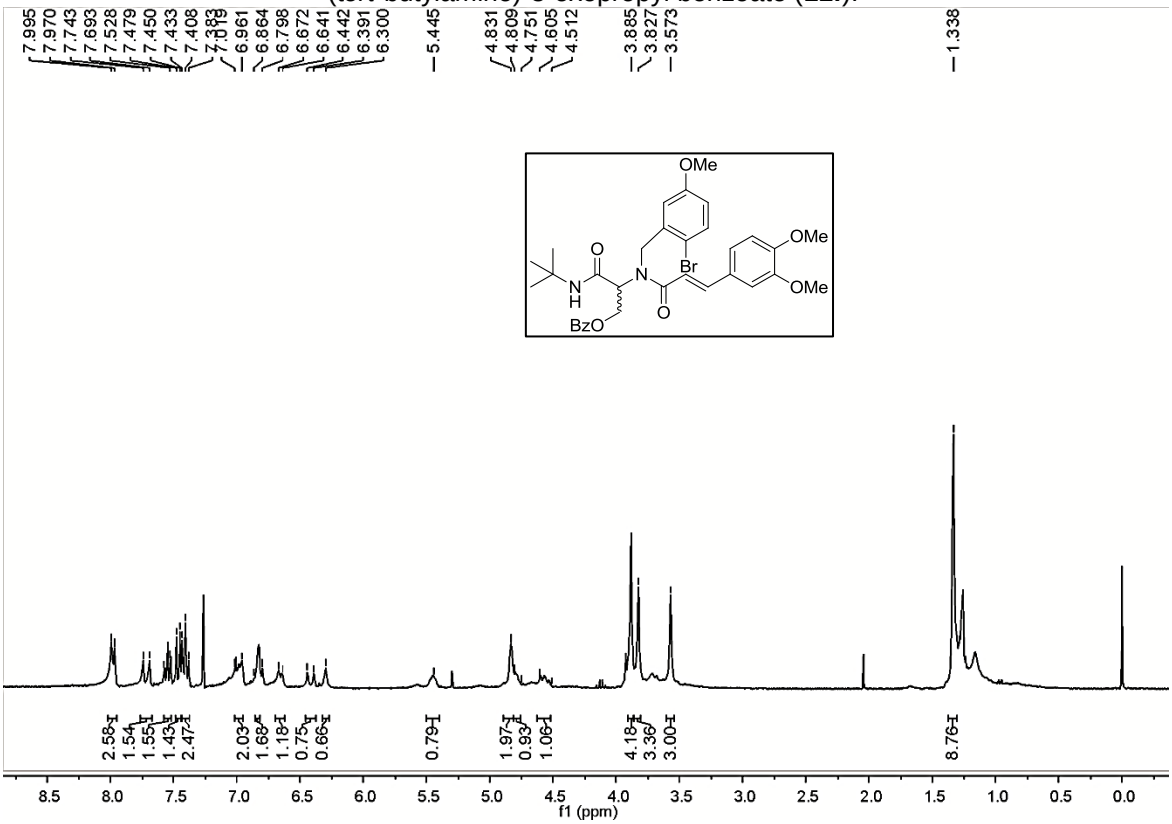

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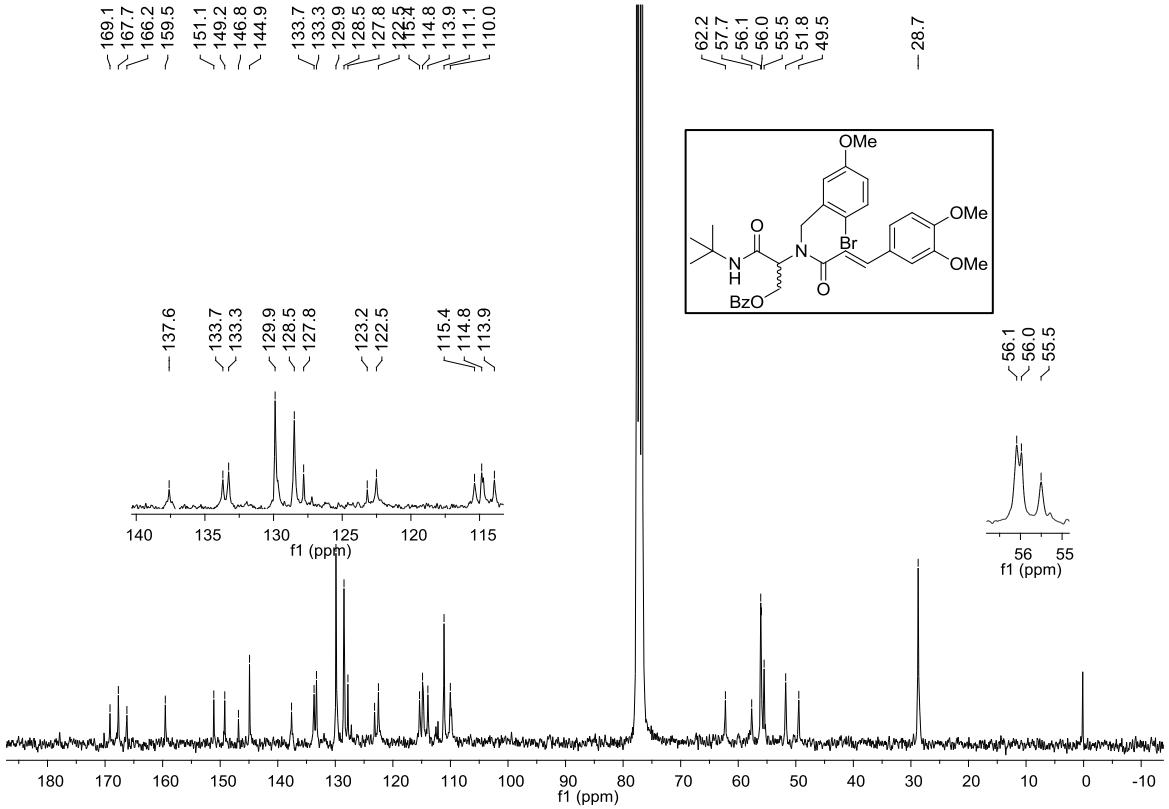

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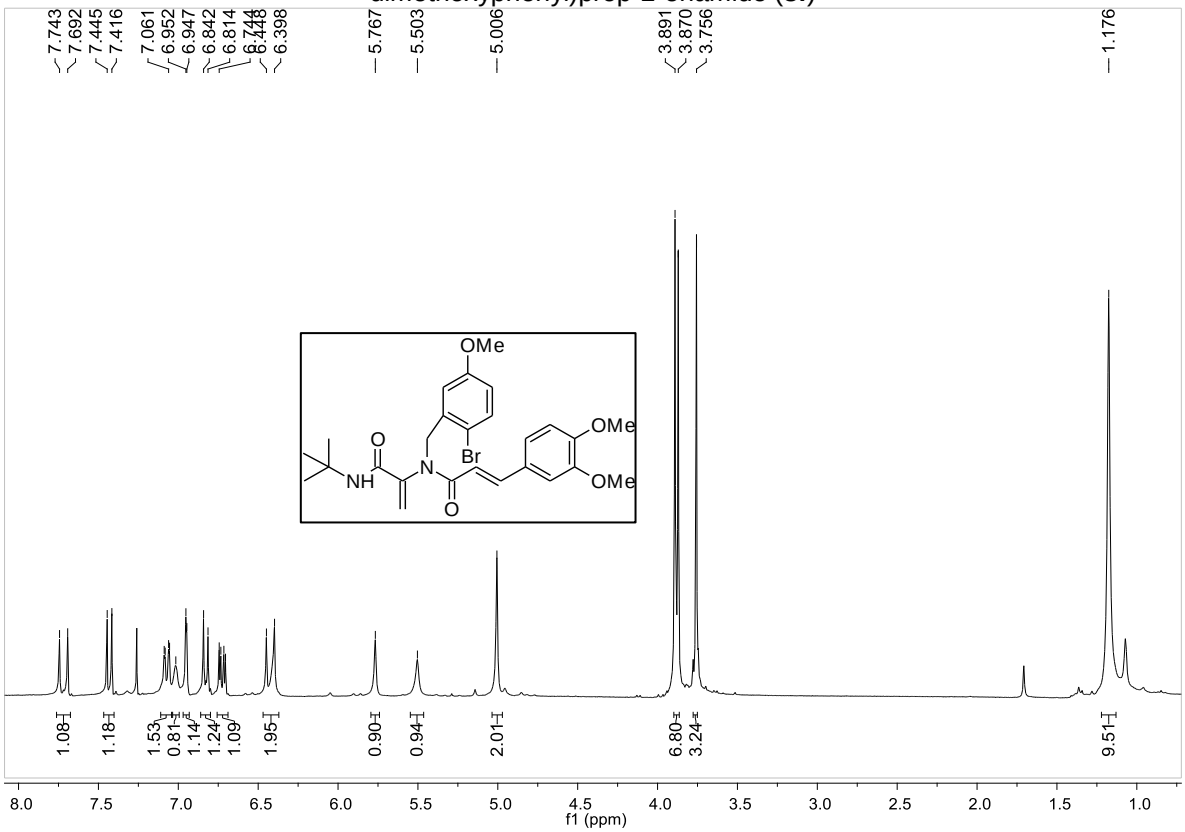

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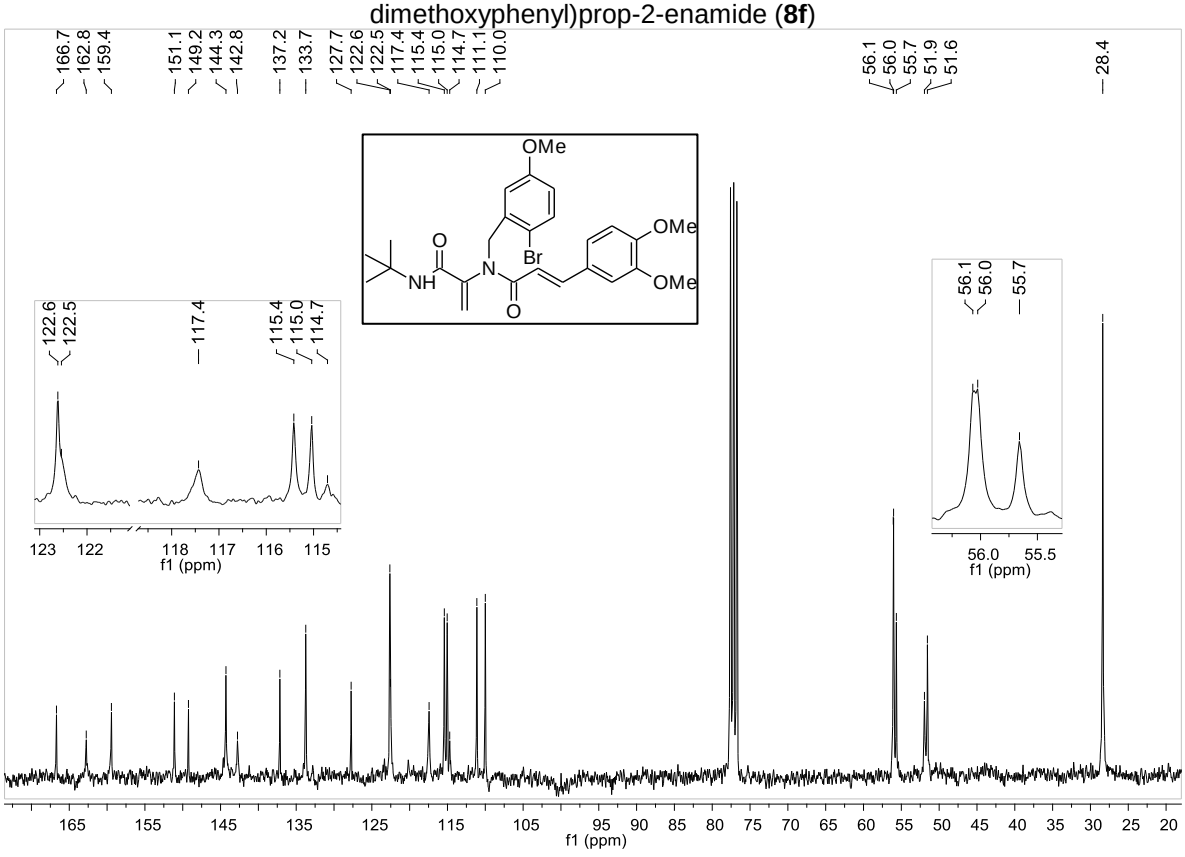

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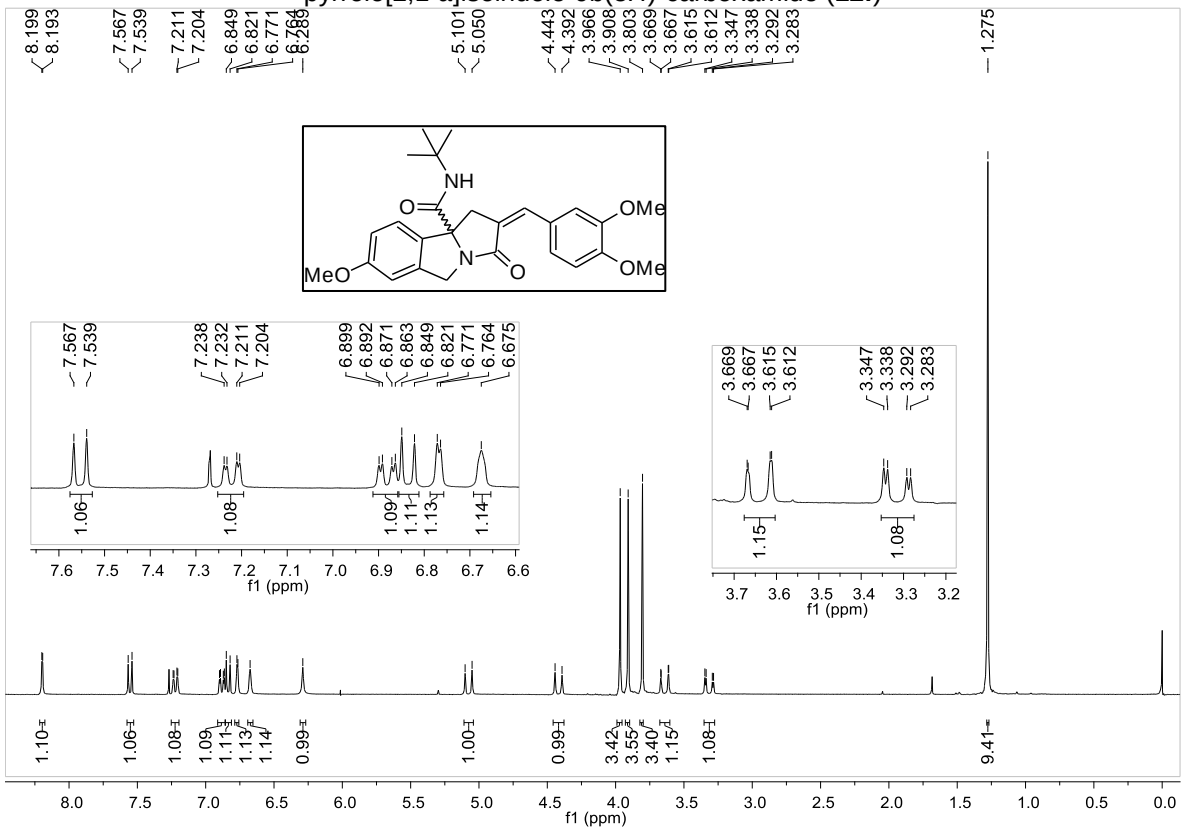

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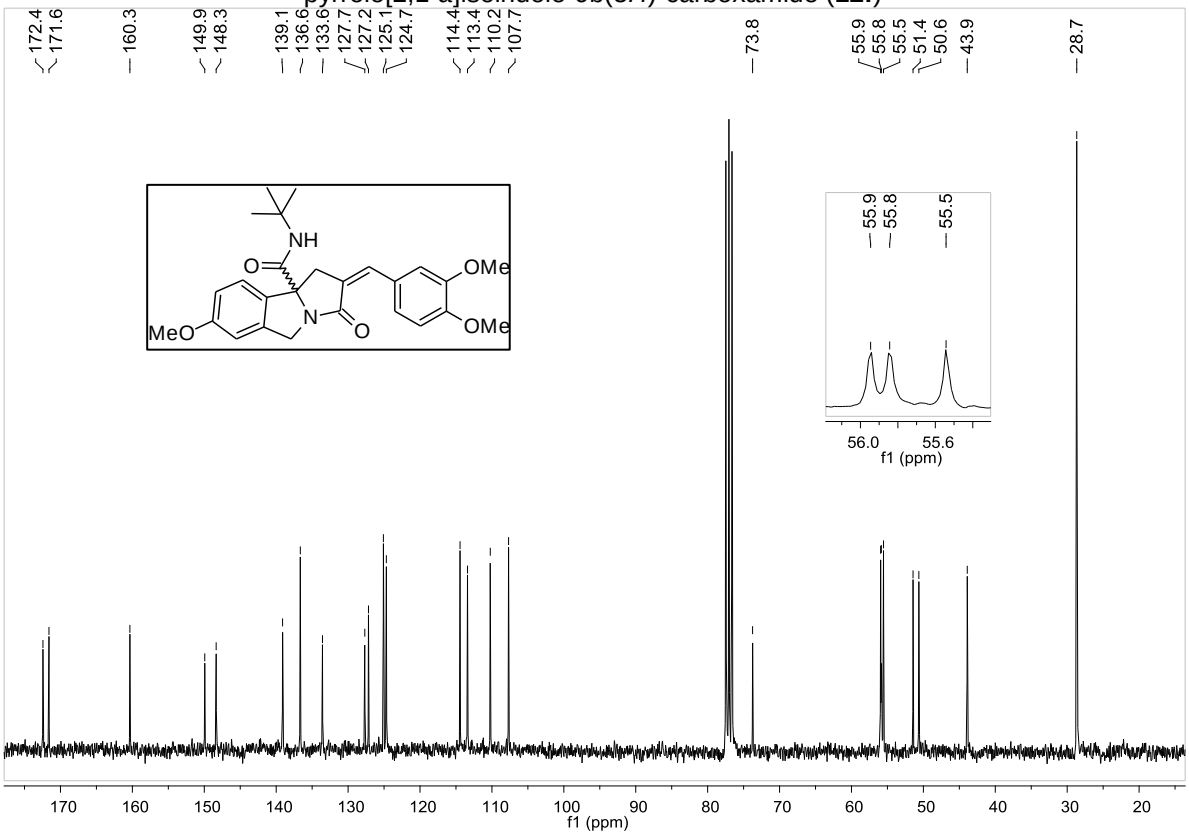

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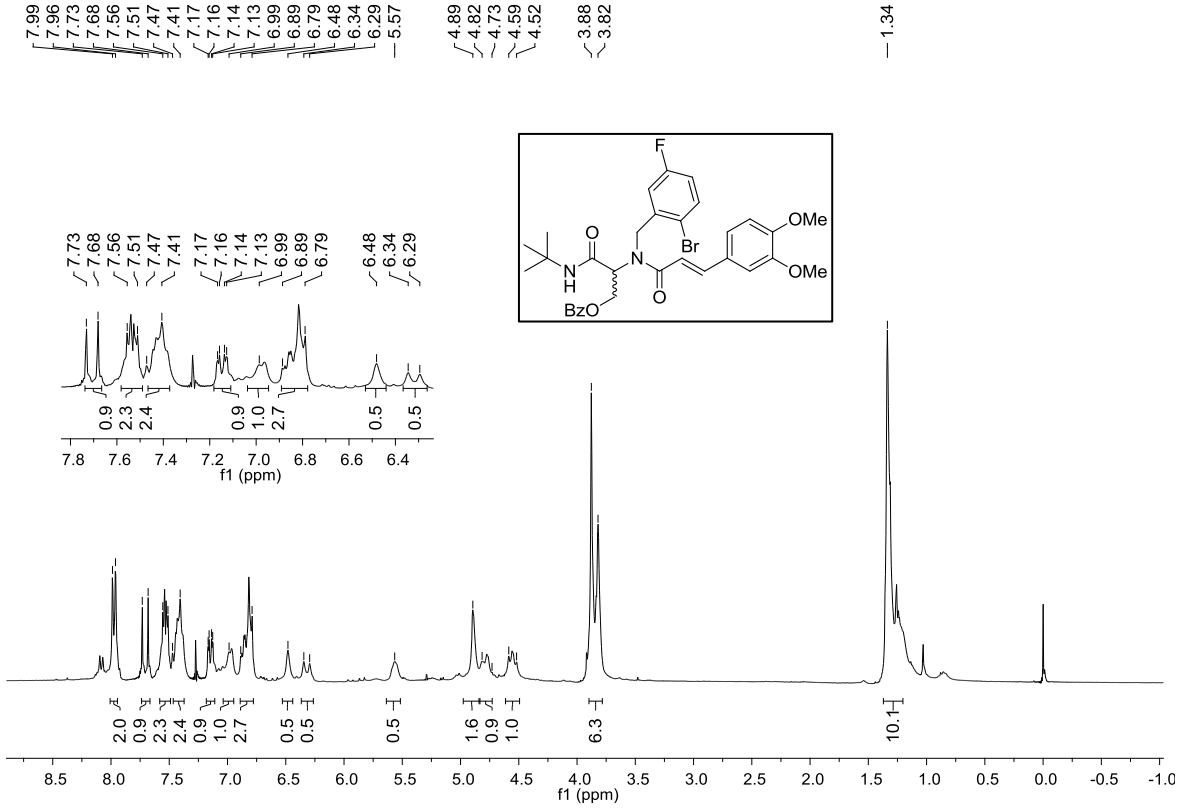
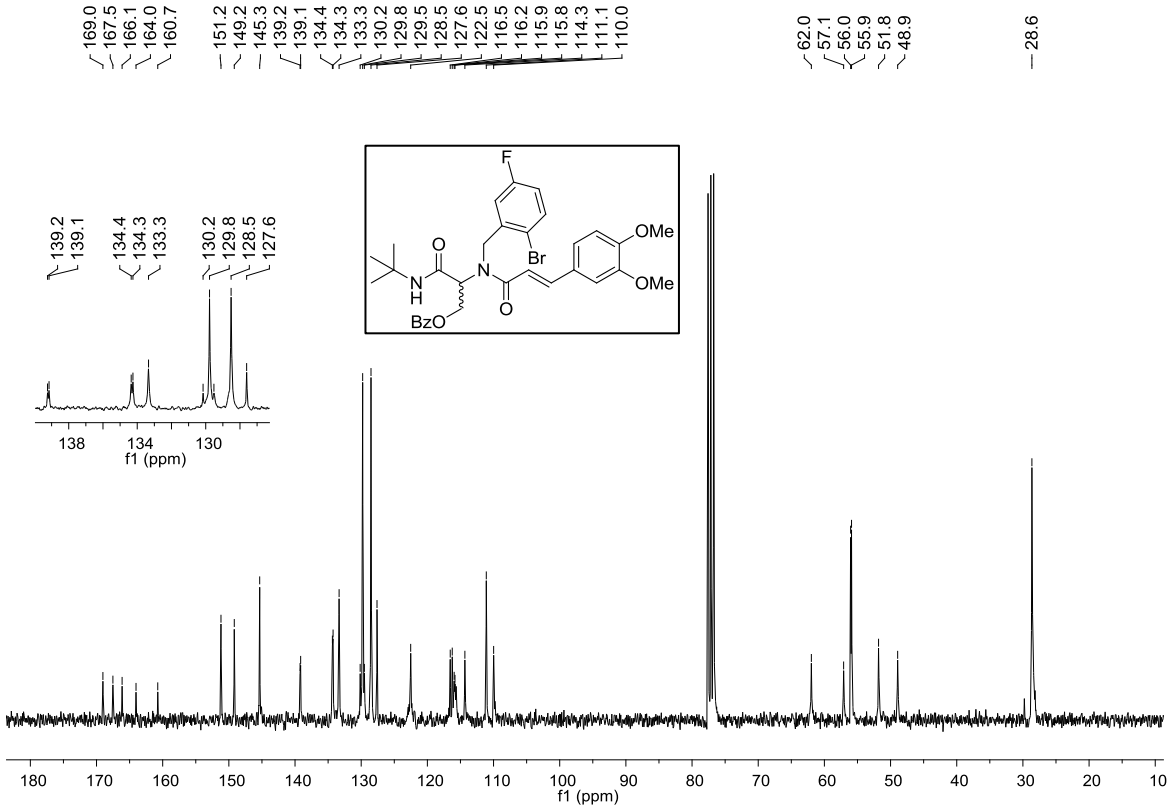
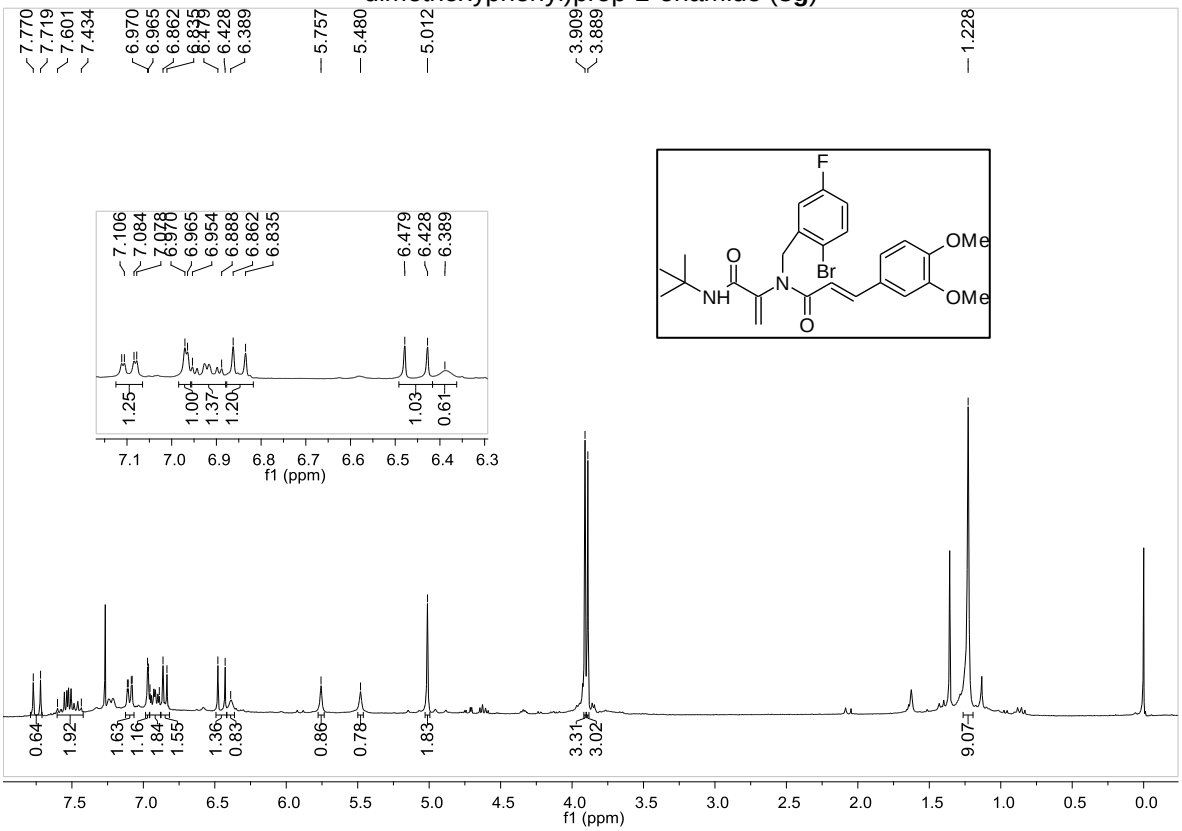


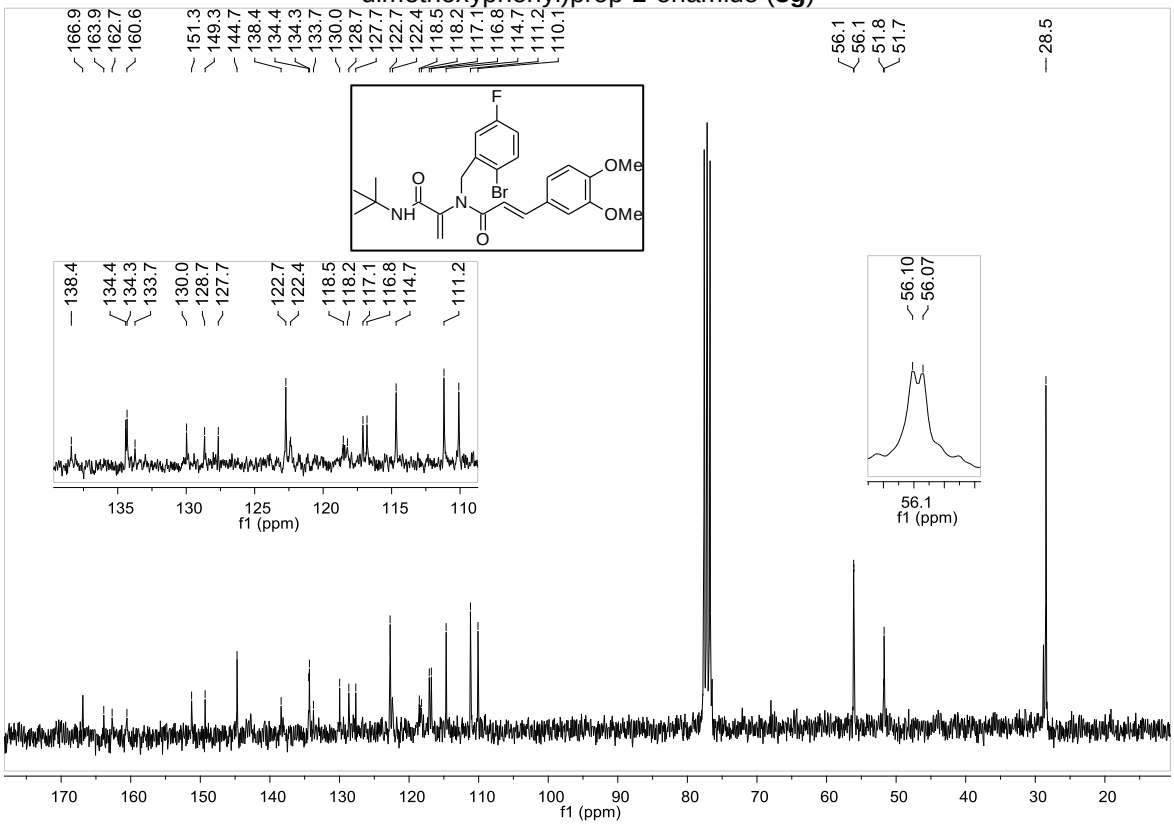
^{13}C-NMR of 2-{(2-bromo-5-fluorobenzyl)-[(2*E*)-3-(3,4-dimethoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11g**)



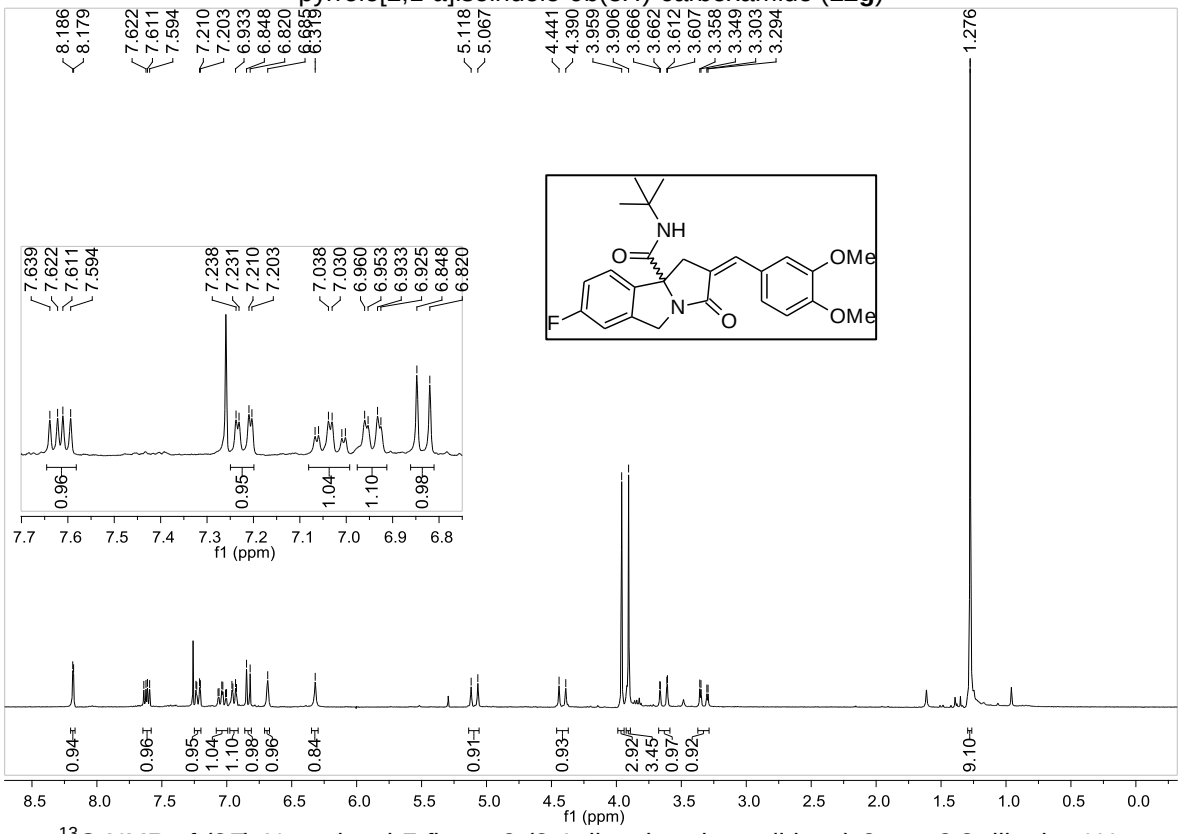
^{1}H-NMR of (2*E*)-*N*-(2-bromo-5-fluorobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(3,4-dimethoxyphenyl)prop-2-enamide (**8g**)



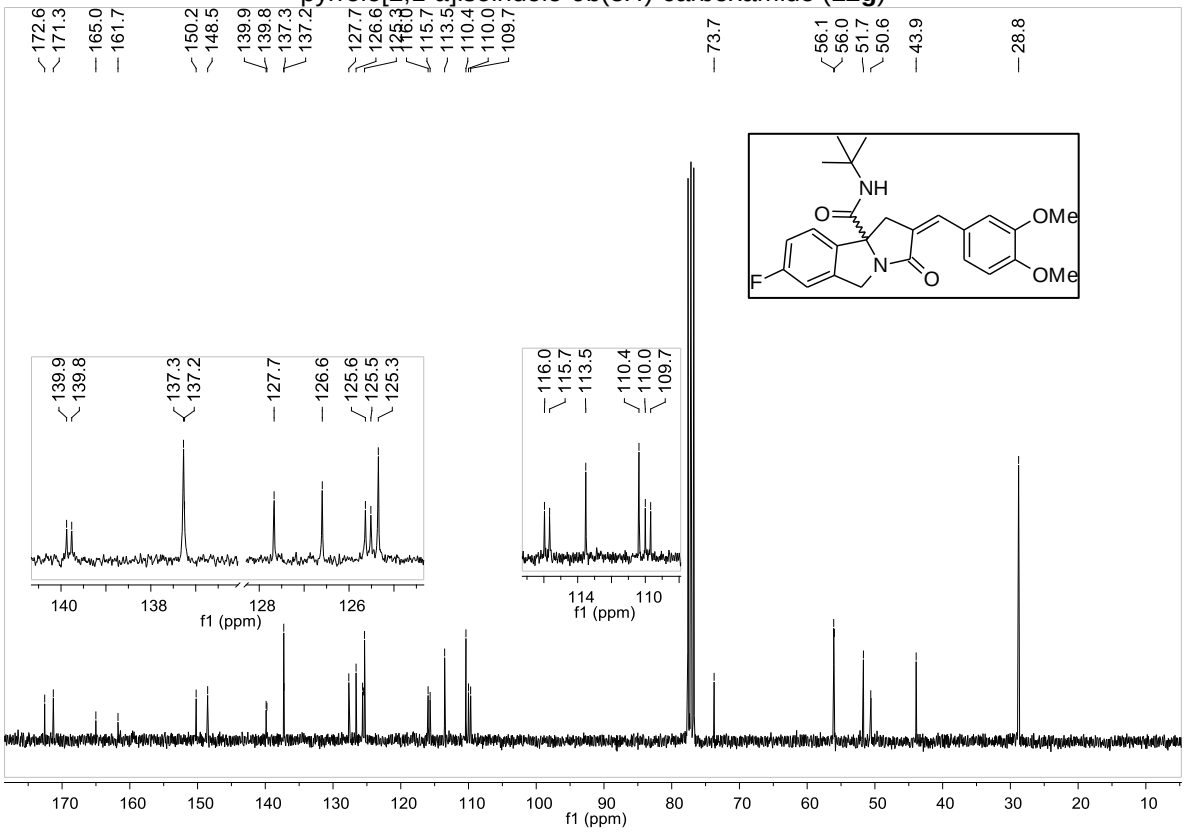
^{13}C-NMR of (2*E*)-*N*-(2-bromo-5-fluorobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(3,4-dimethoxyphenyl)prop-2-enamide (**8g**)



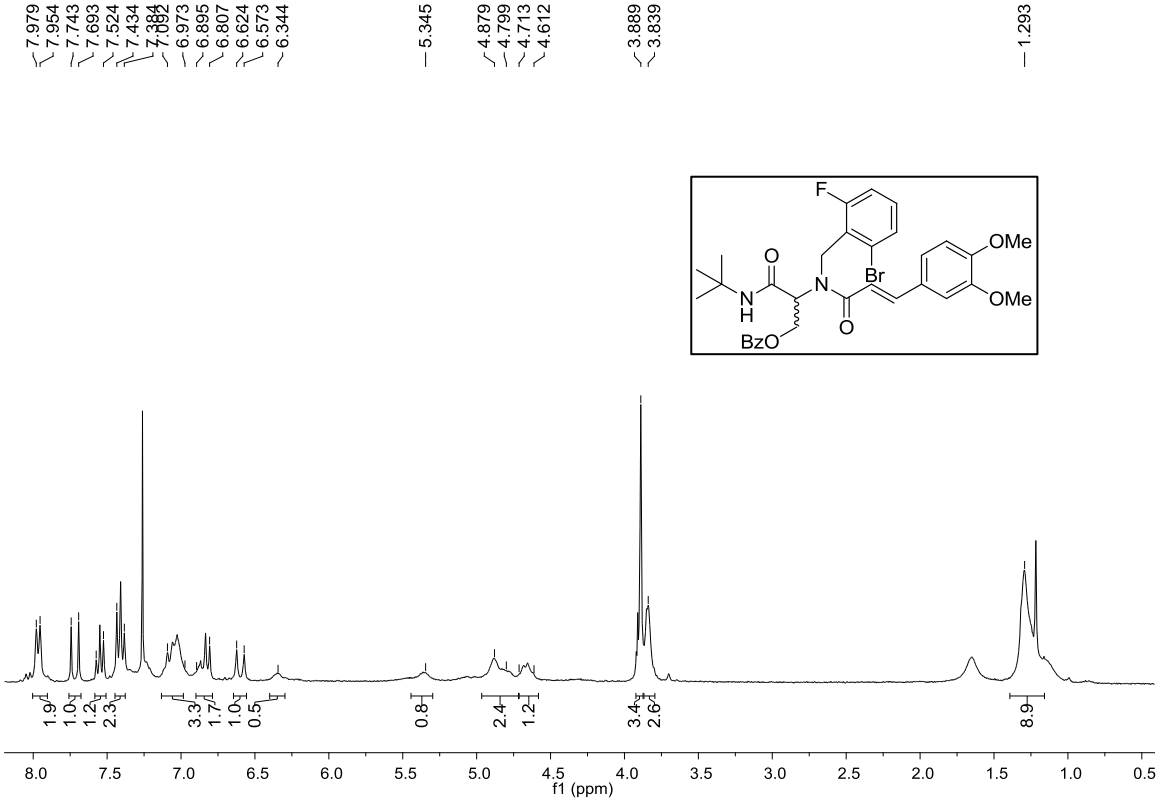
^{1}H-NMR of (2*Z*)-*N*-*tert*-butyl-7-fluoro-2-(3,4-dimethoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12g**)



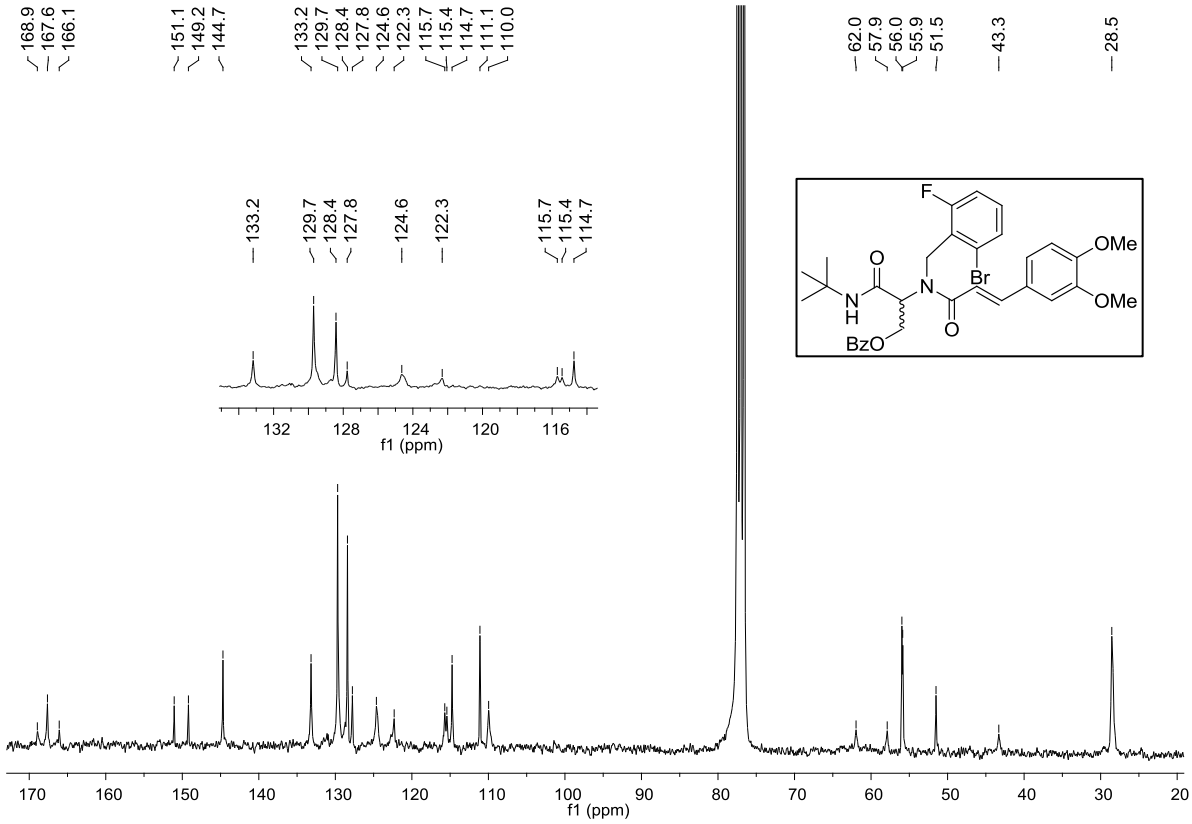
^{13}C-NMR of (2*Z*)-*N*-*tert*-butyl-7-fluoro-2-(3,4-dimethoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12g**)



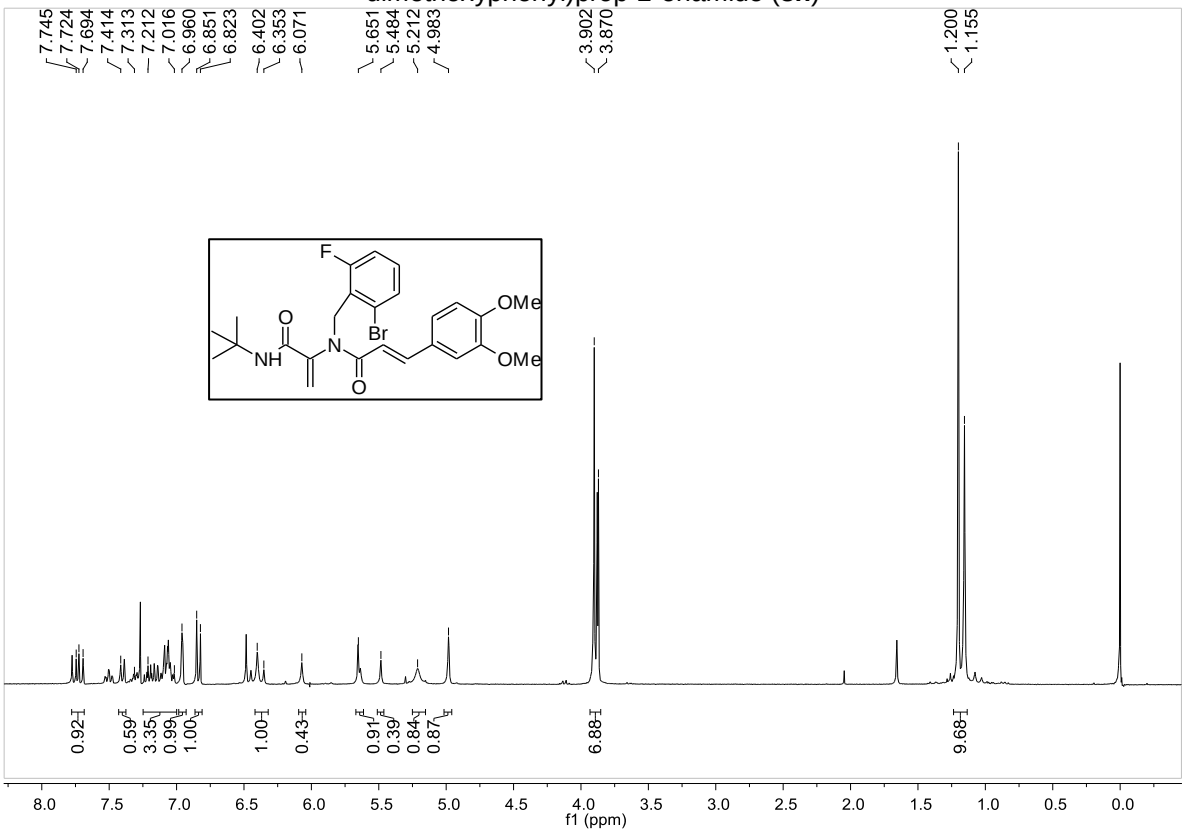
^{1}H-NMR of 2-{(2-bromo-6-fluorobenzyl)-[(2*E*)-3-(3,4-dimethoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11h**).



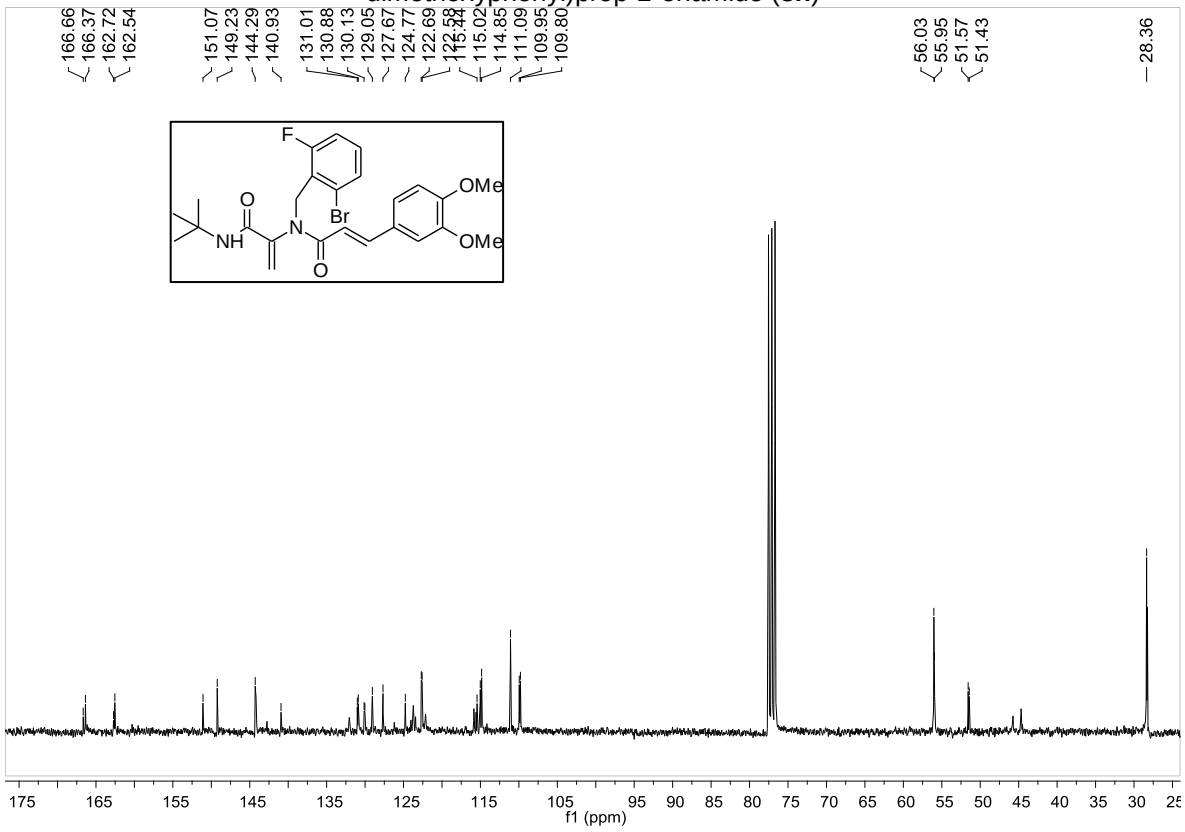
^{13}C-NMR of 2-{(2-bromo-6-fluorobenzyl)-[(2*E*)-3-(3,4-dimethoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11h**).



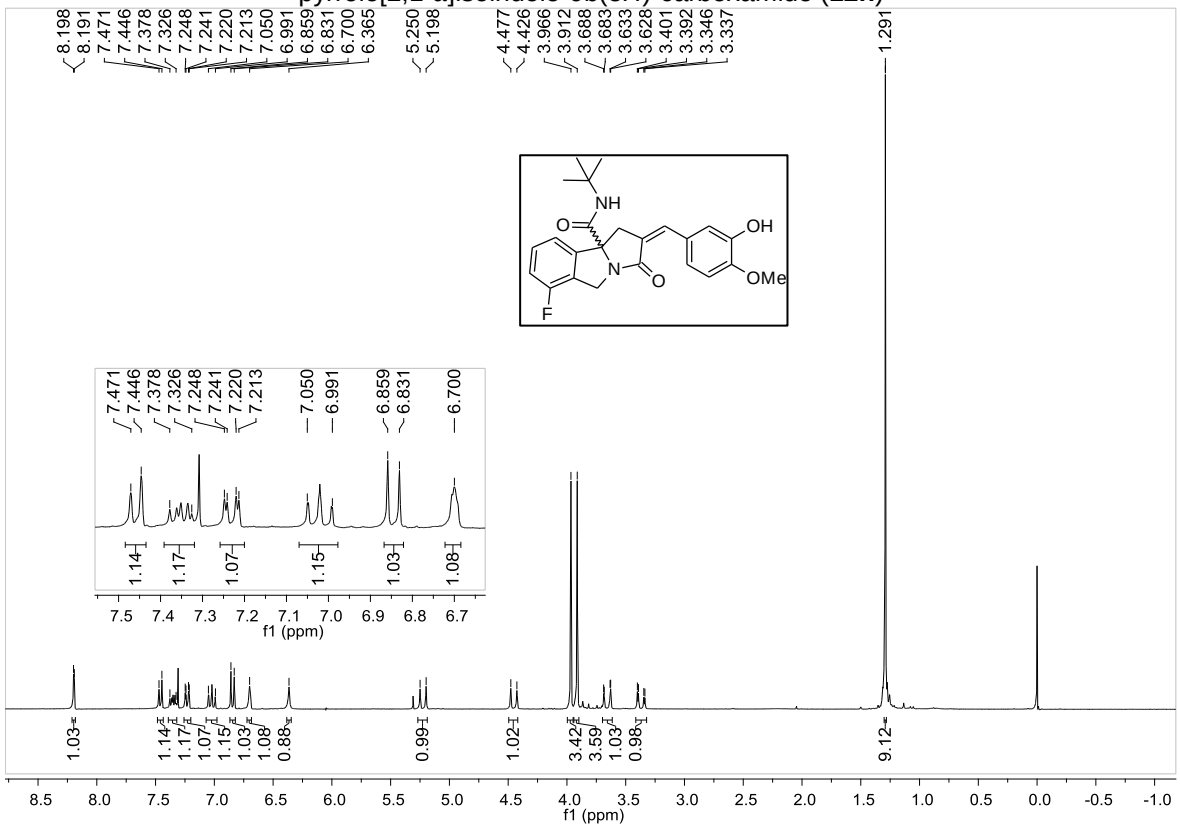
^{1}H-NMR of (2*E*)-*N*-(2-bromo-6-fluorobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(3,4-dimethoxyphenyl)prop-2-enamide (**8h**)



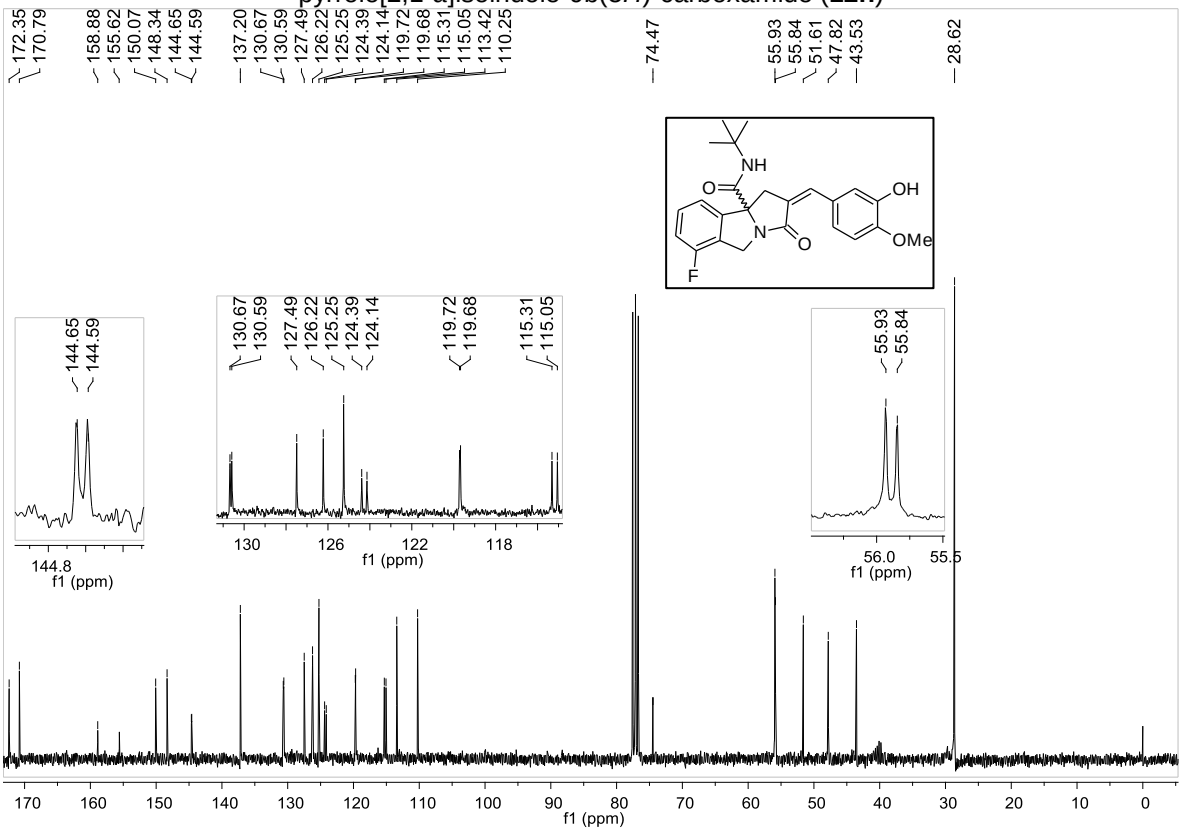
^{13}C-NMR of (2*E*)-*N*-(2-bromo-6-fluorobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(3,4-dimethoxyphenyl)prop-2-enamide (**8h**)



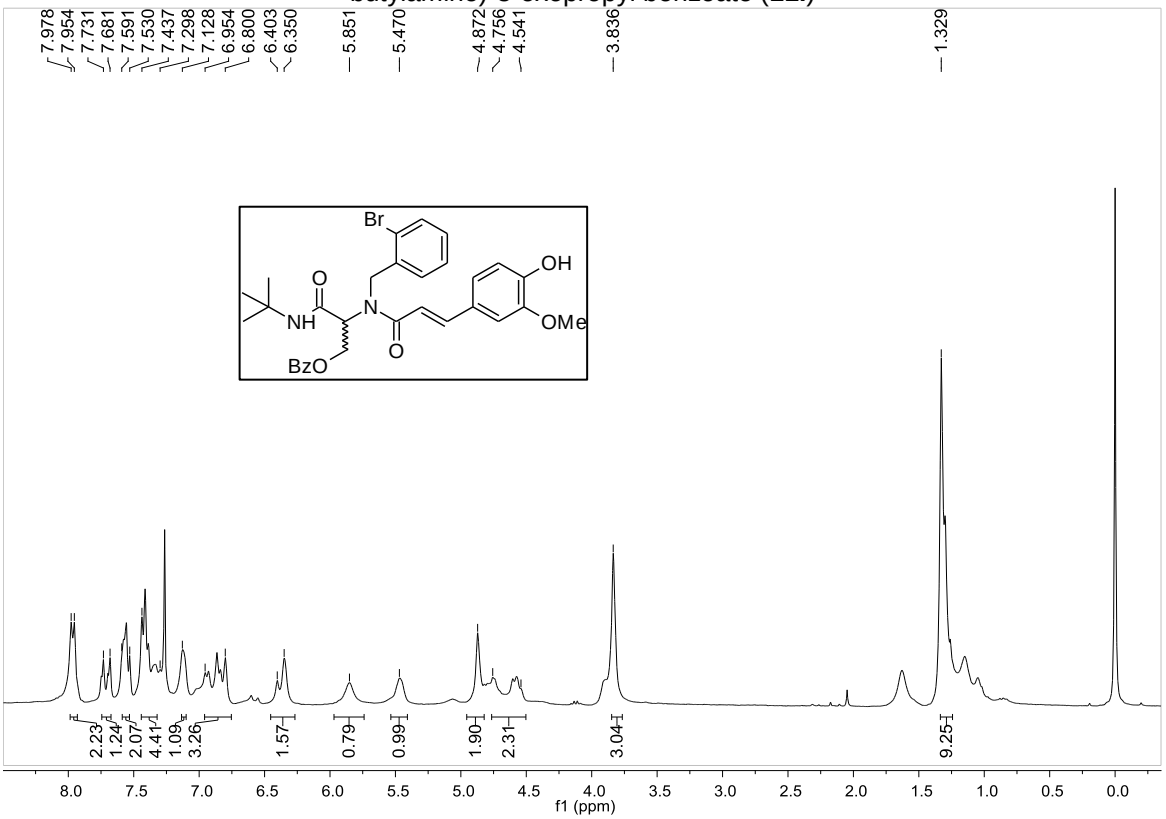
^{1}H-NMR of (2*Z*)-*N*-*tert*-butyl-6-fluoro-2-(3,4-dimethoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12h**)



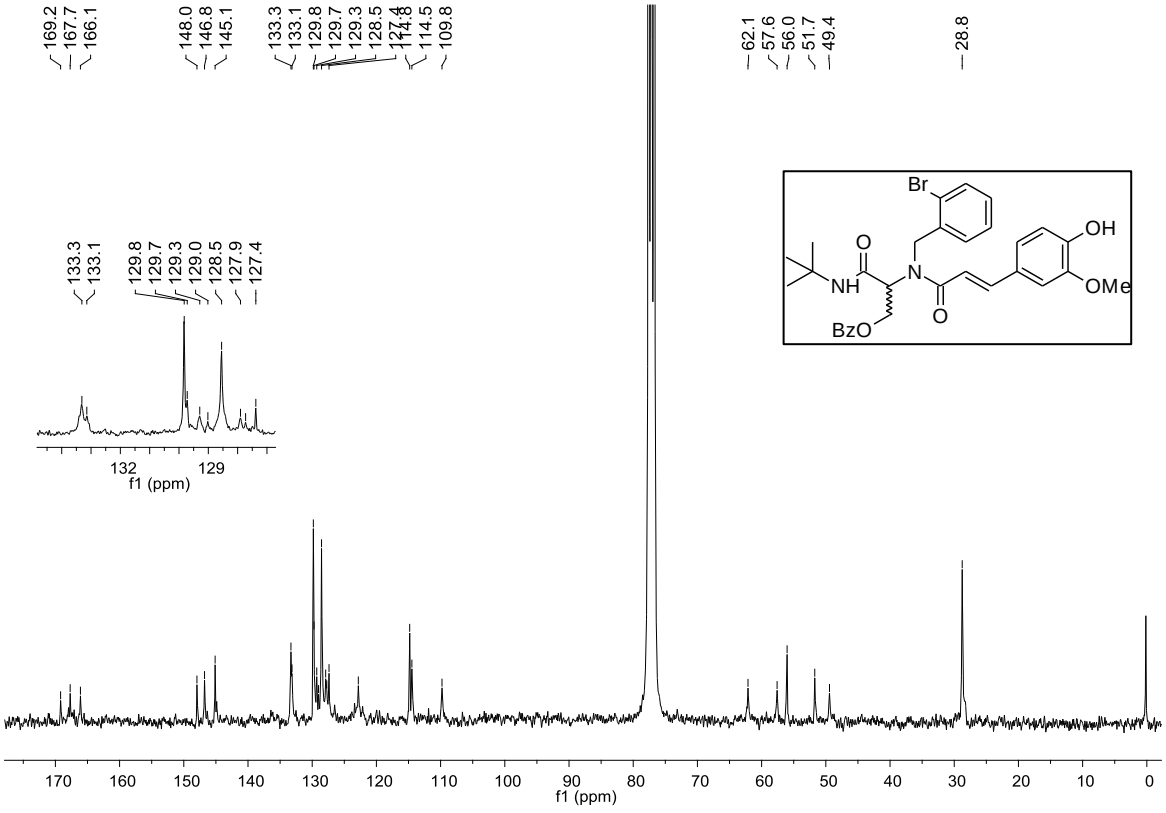
^{13}C-NMR of (2*Z*)-*N*-*tert*-butyl-6-fluoro-2-(3,4-dimethoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12h**)



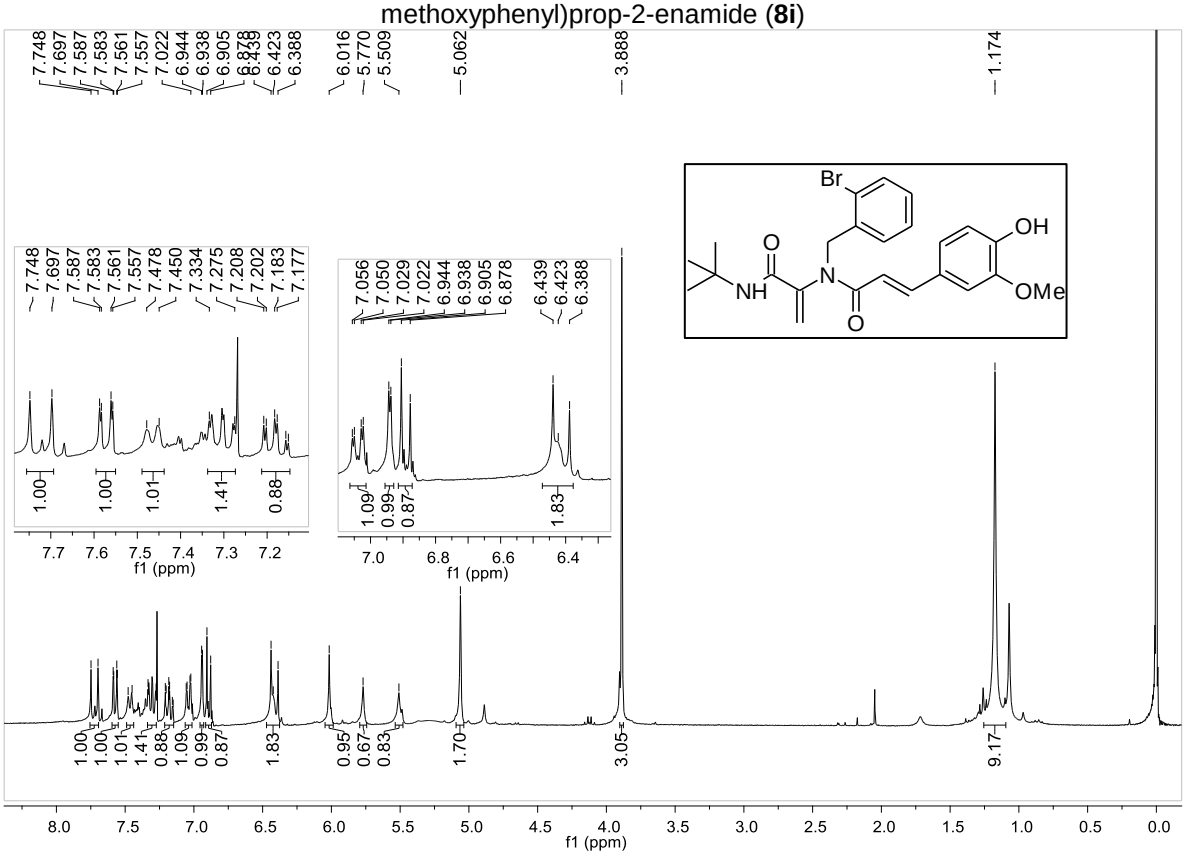
1H-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11i**)



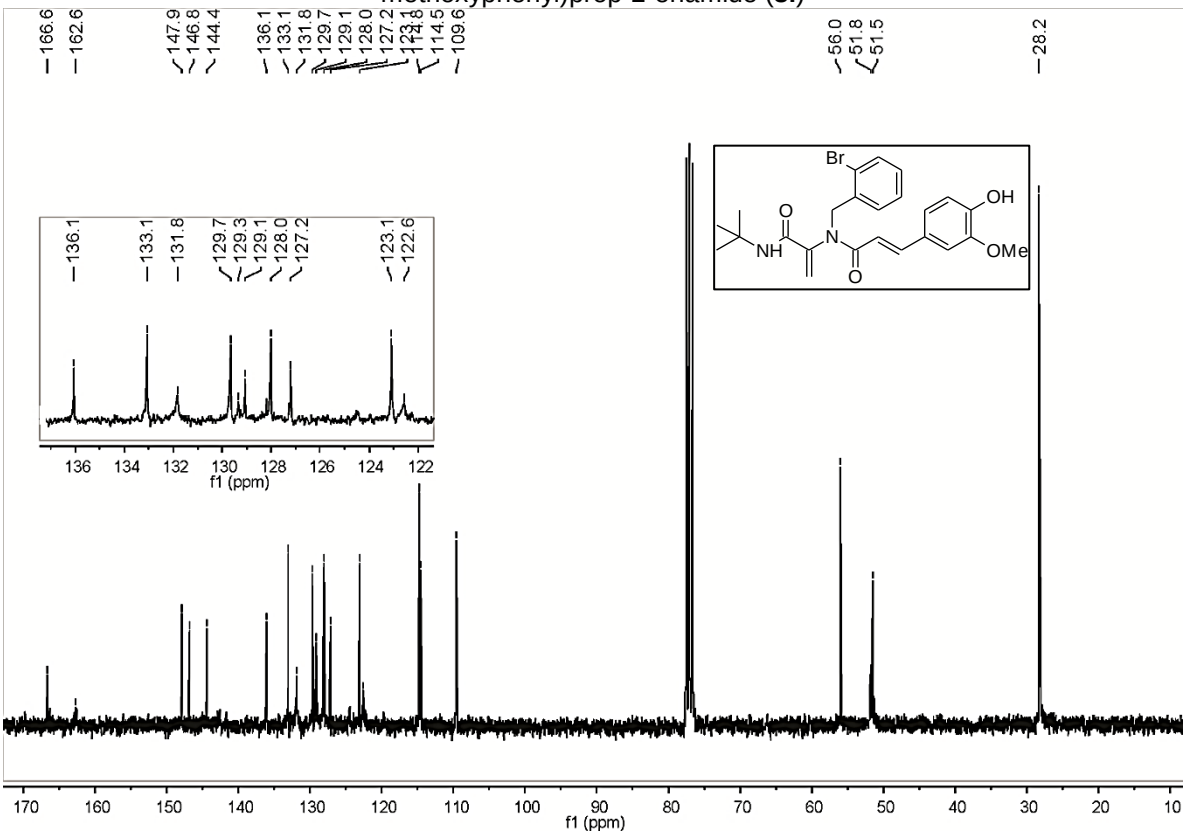
^{13}C-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11i**)



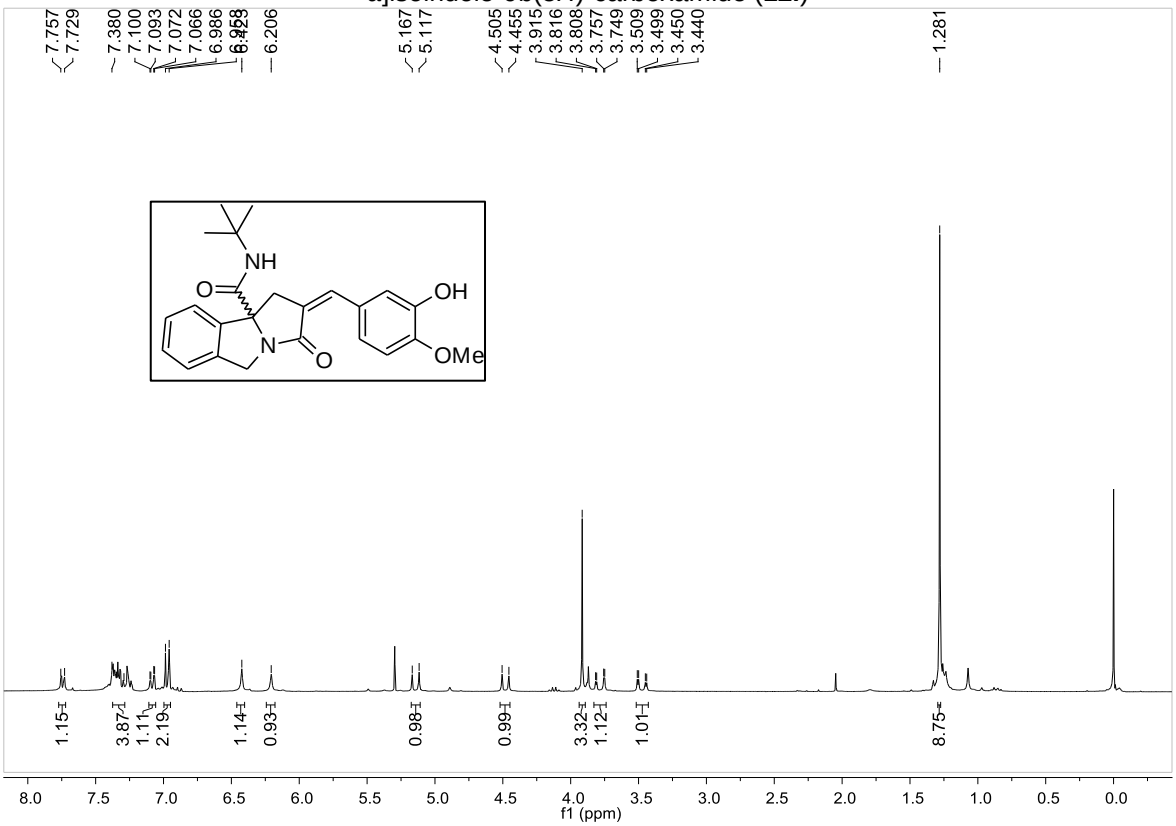
^{1}H-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8i**)



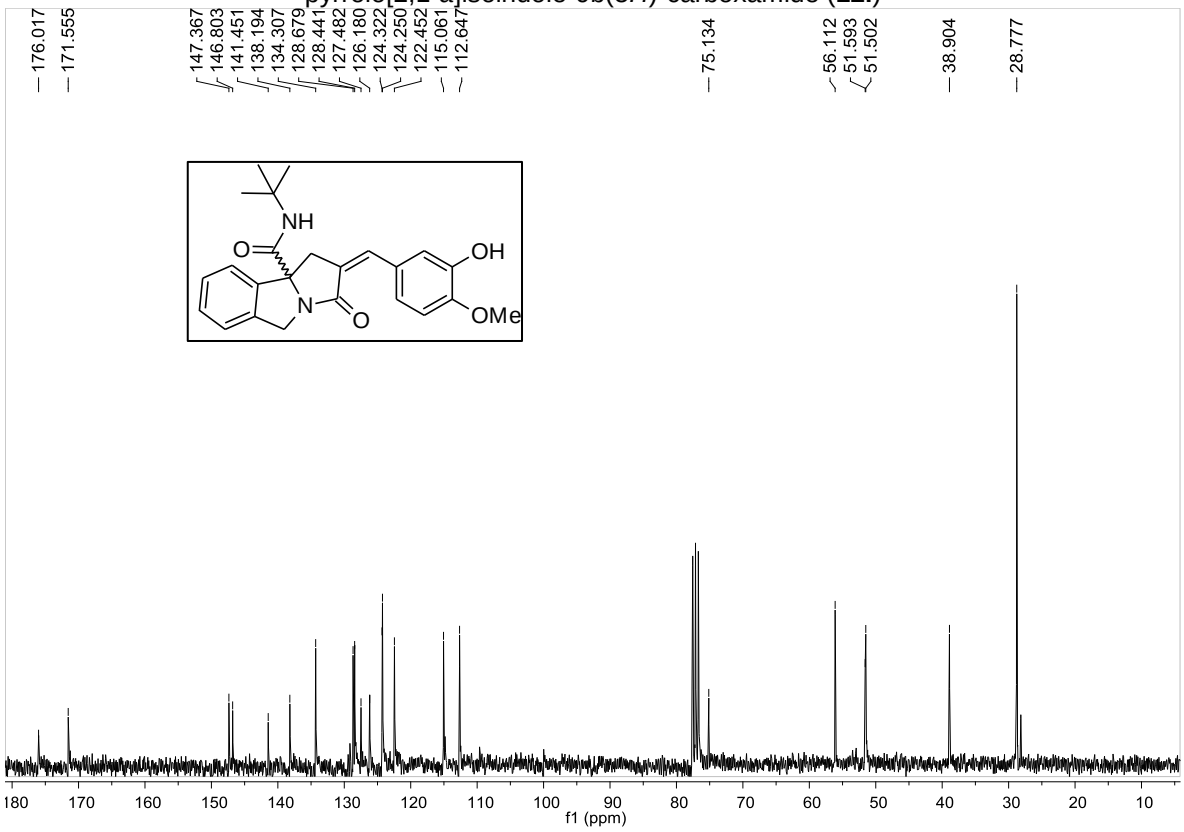
^{13}C-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8i**)



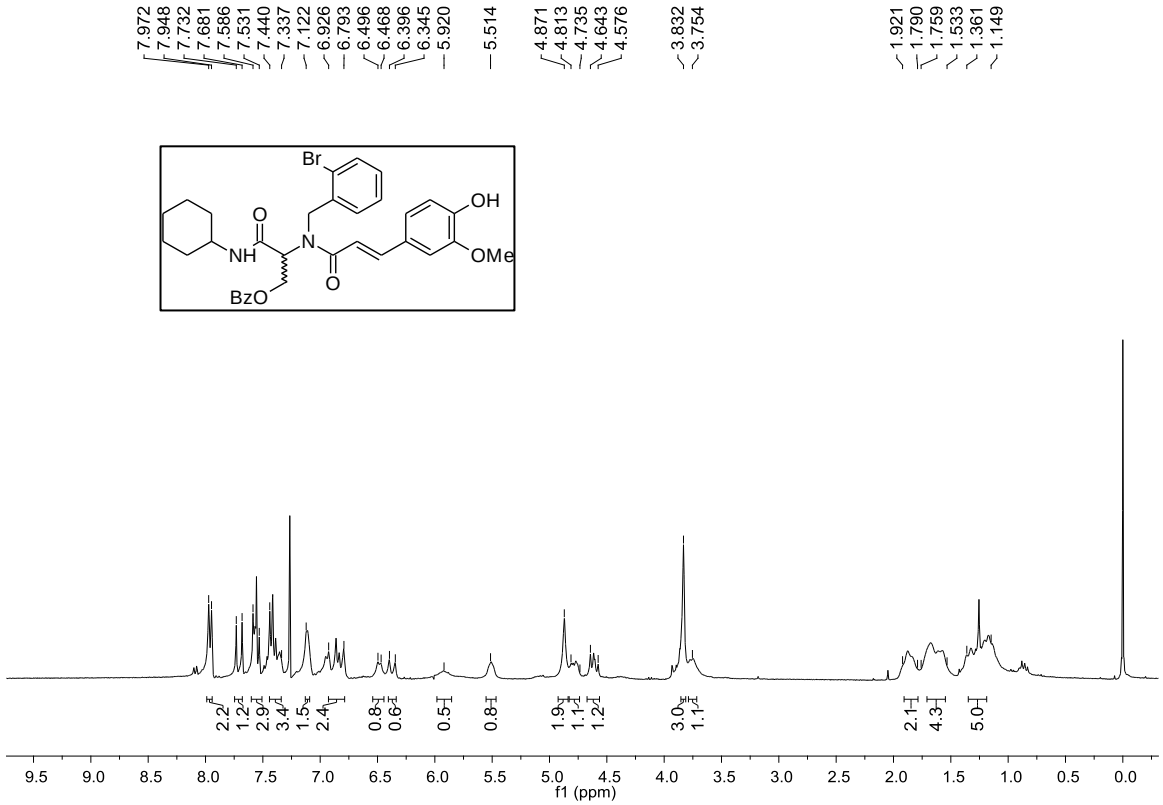
^{1}H-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3-methoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12i**)



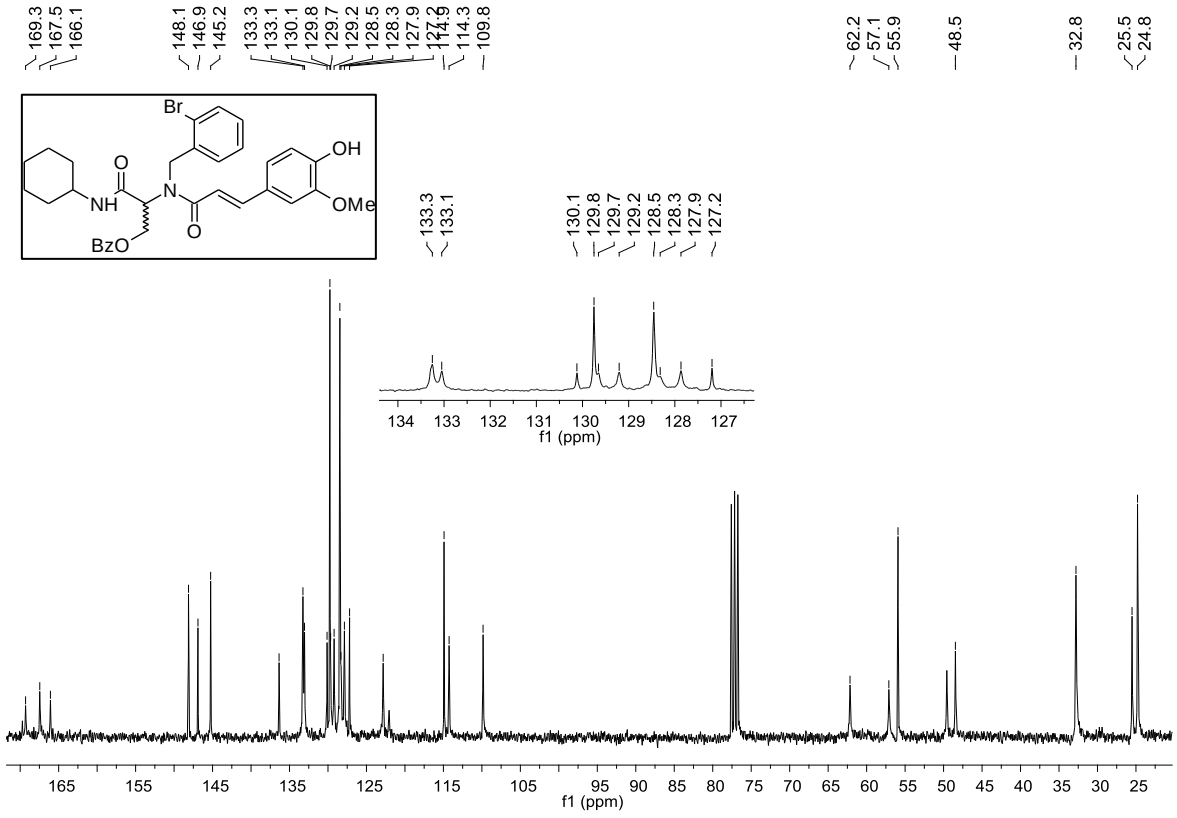
^{13}C-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3-methoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12i**)



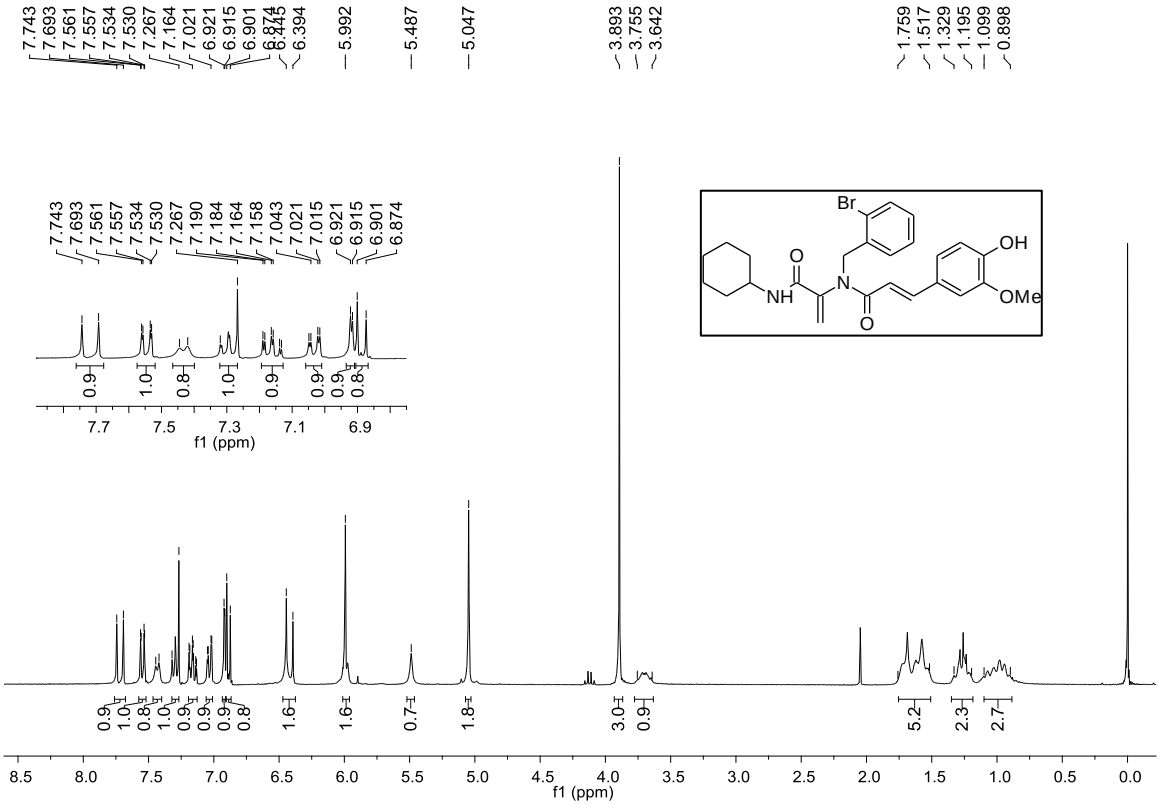
^{1}H-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(cyclohexylamino)-3-oxopropyl benzoate (**11j**)



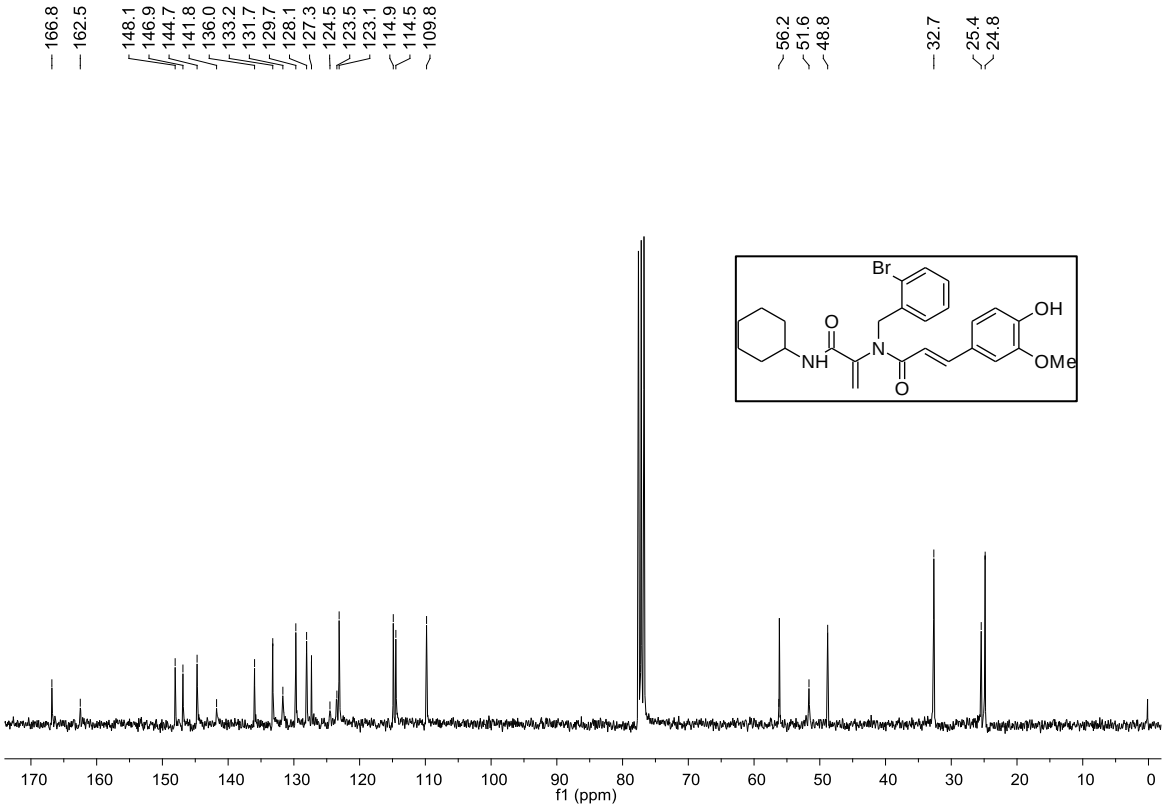
^{13}C-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(cyclohexylamino)-3-oxopropyl benzoate (**11j**)



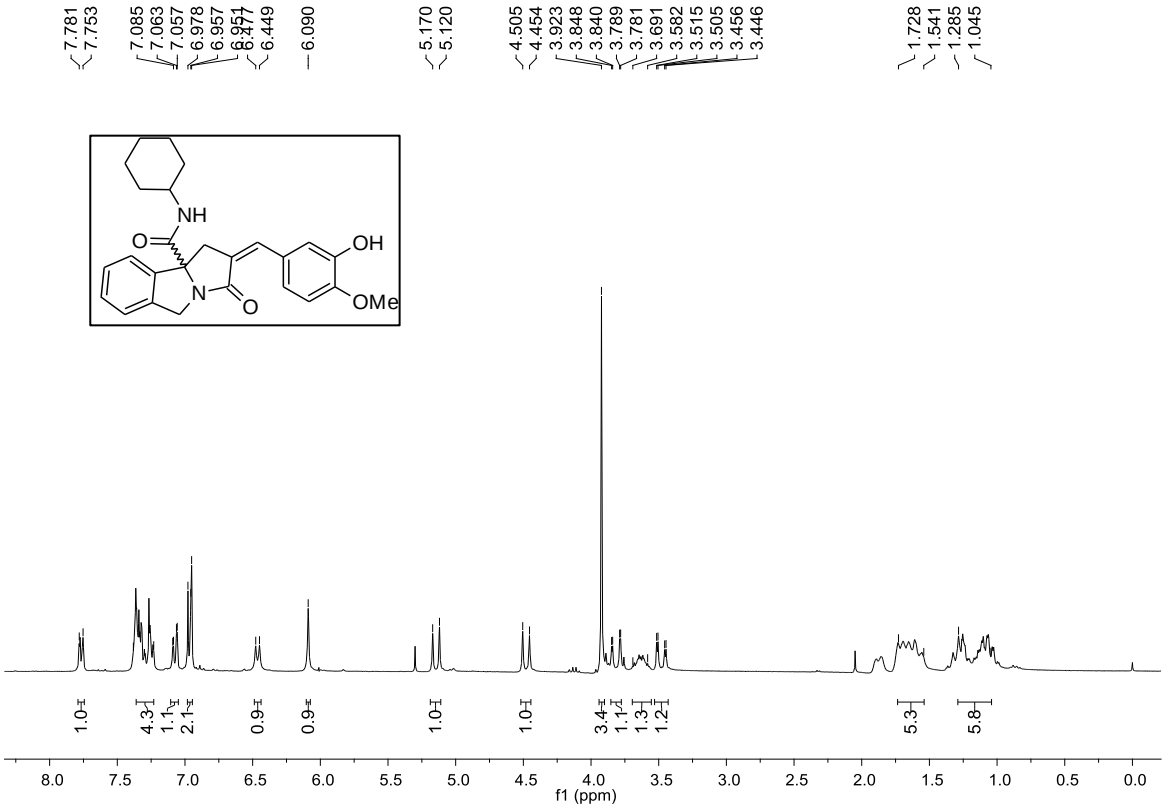
^{1}H-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(cyclohexylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8j**)



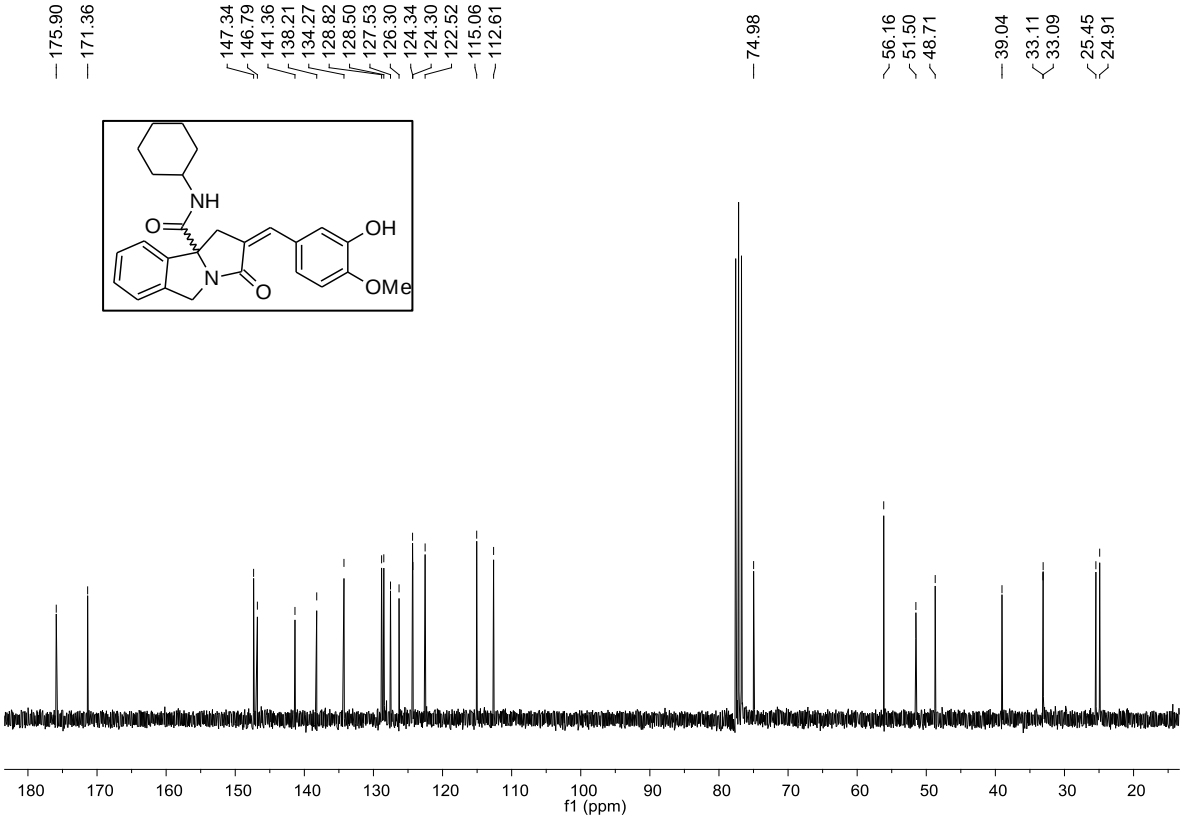
^{13}C-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(cyclohexylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8j**)



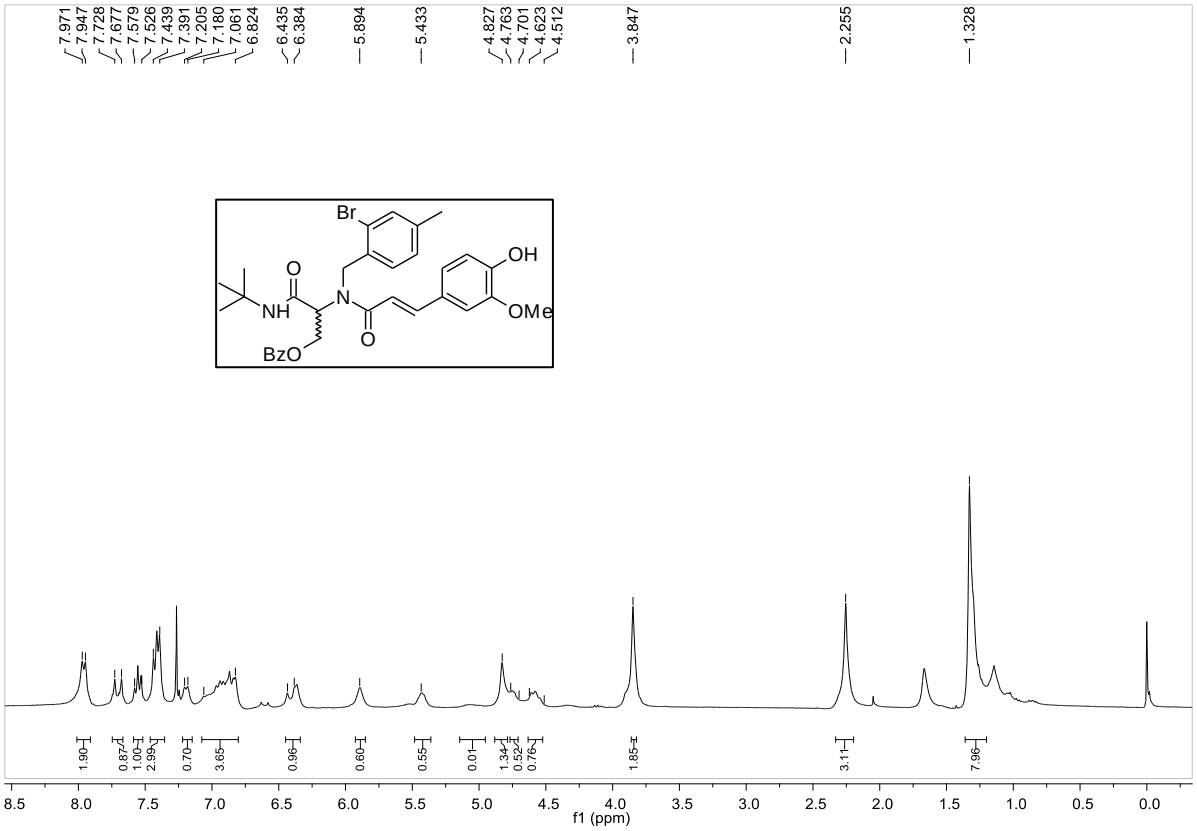
^{1}H-NMR of (2*Z*)-*N*-cyclohexyl-2-(4-hydroxy-3-methoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12j**)



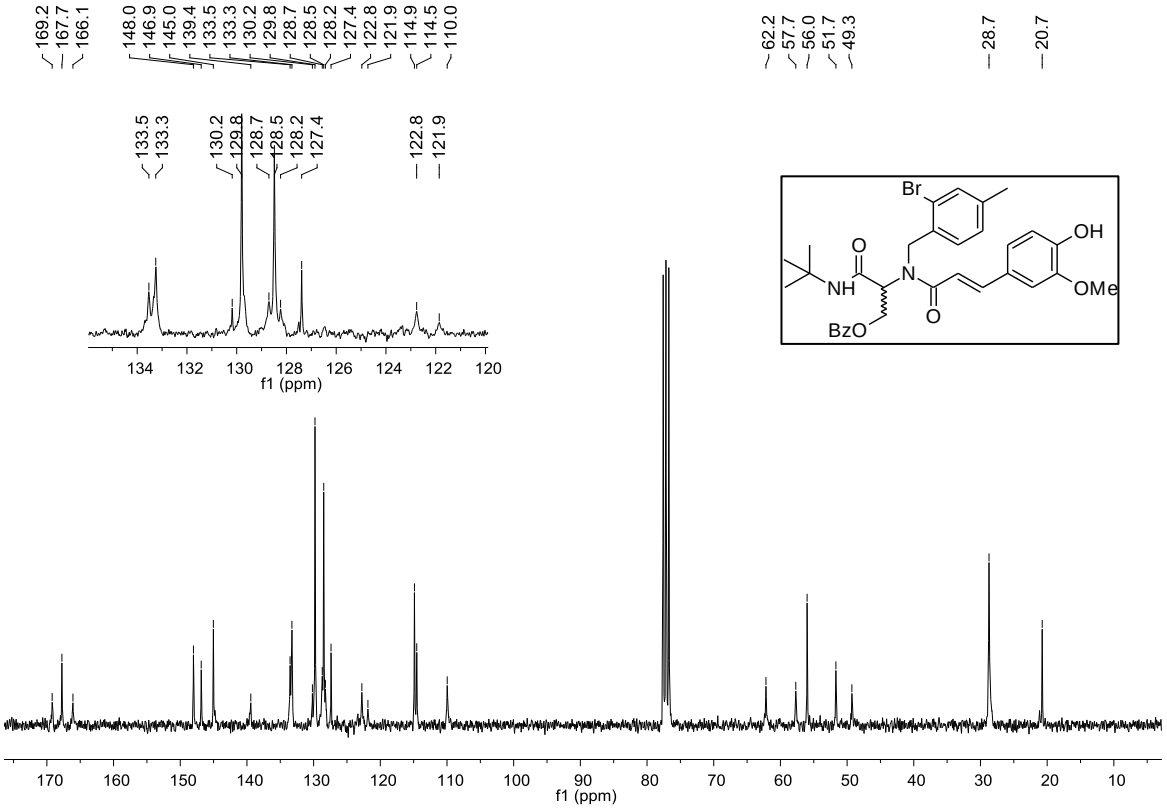
^{13}C-NMR of (2*Z*)-*N*-cyclohexyl-2-(4-hydroxy-3-methoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12j**)



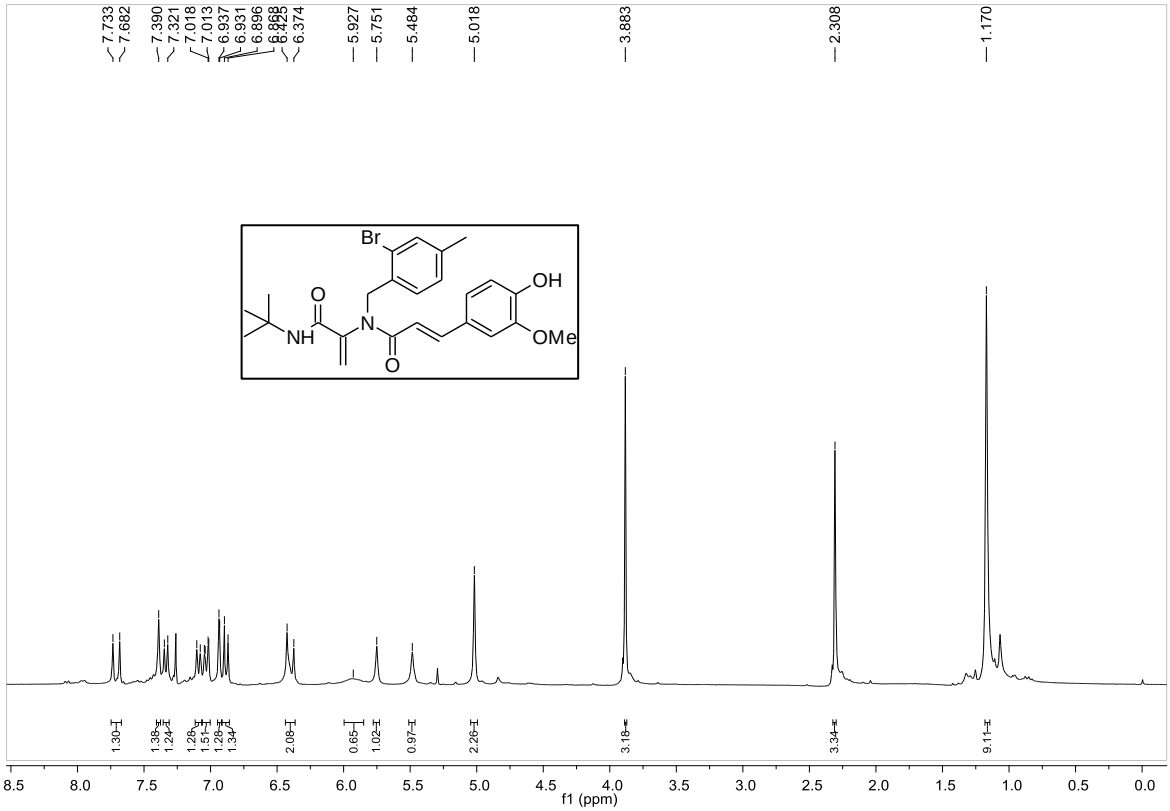
^{1}H-NMR of 2-{(2-bromo-4-methylbenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11k**)



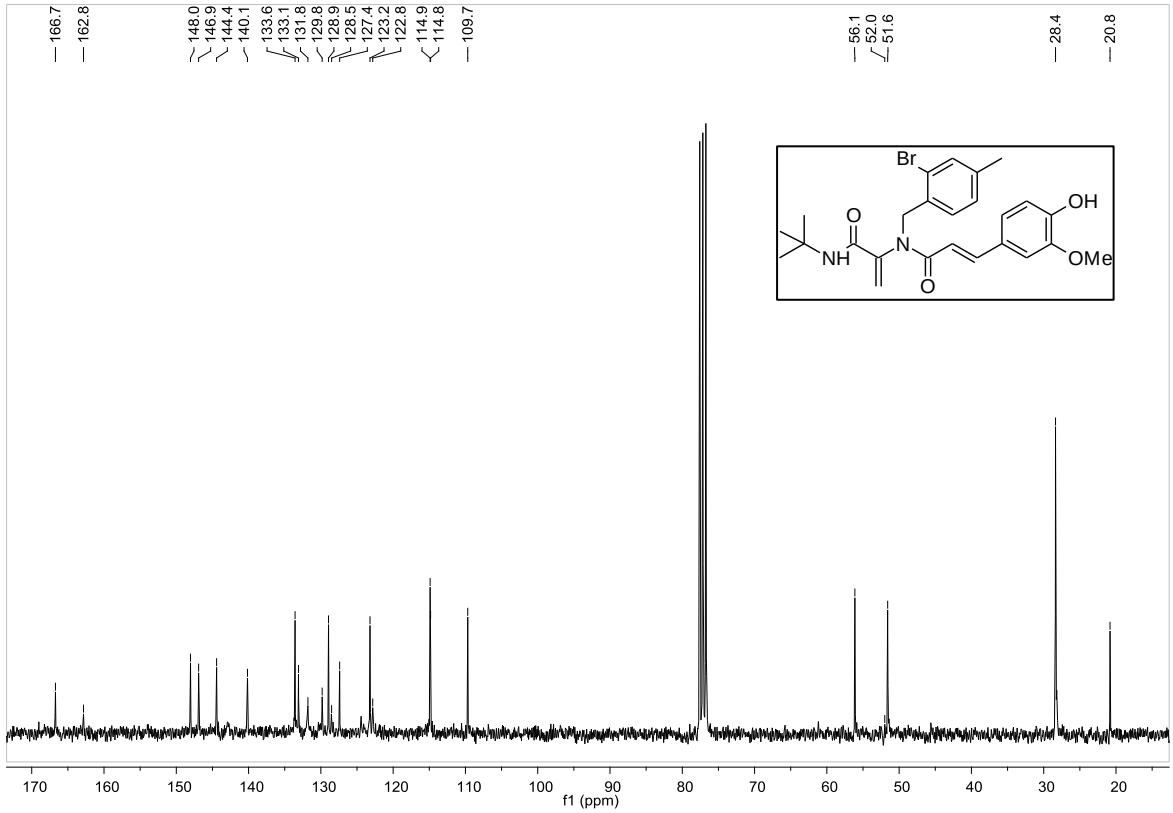
^{13}C-NMR of 2-{(2-bromo-4-methylbenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11k**)



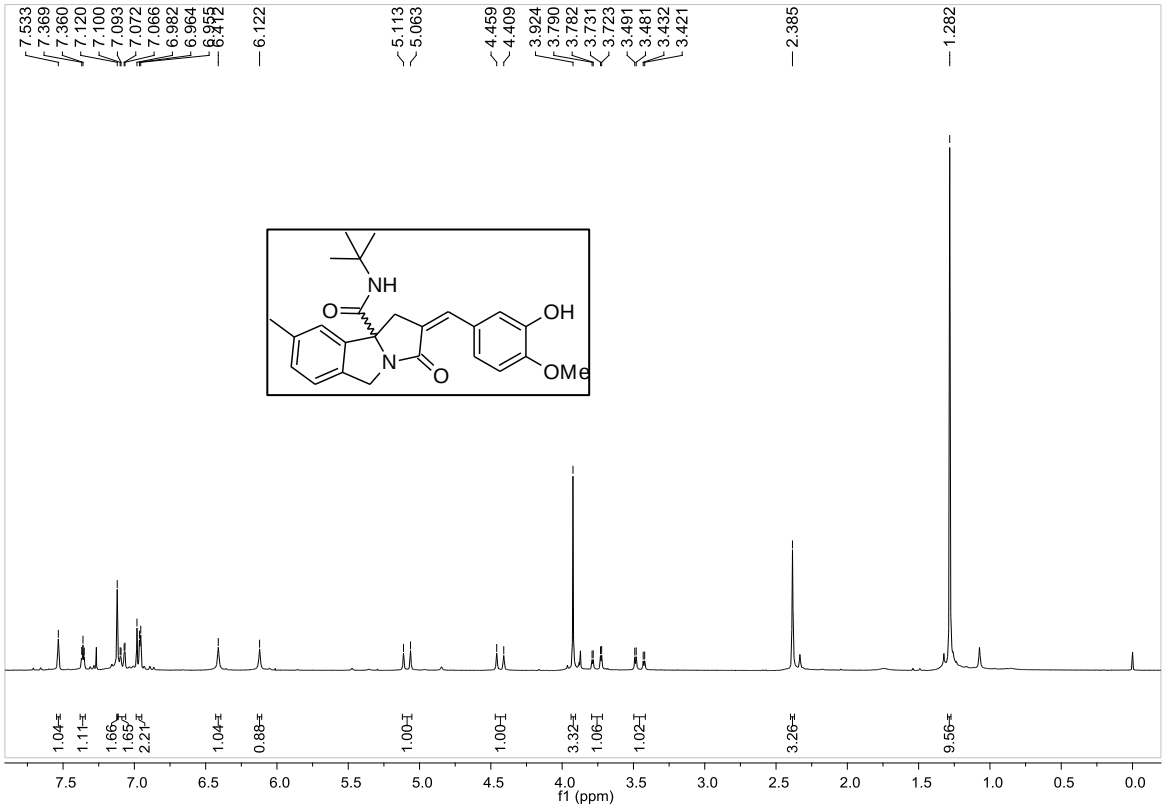
^{1}H-NMR of (2*E*)-*N*-(2-bromo-4-methylbenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8k**)



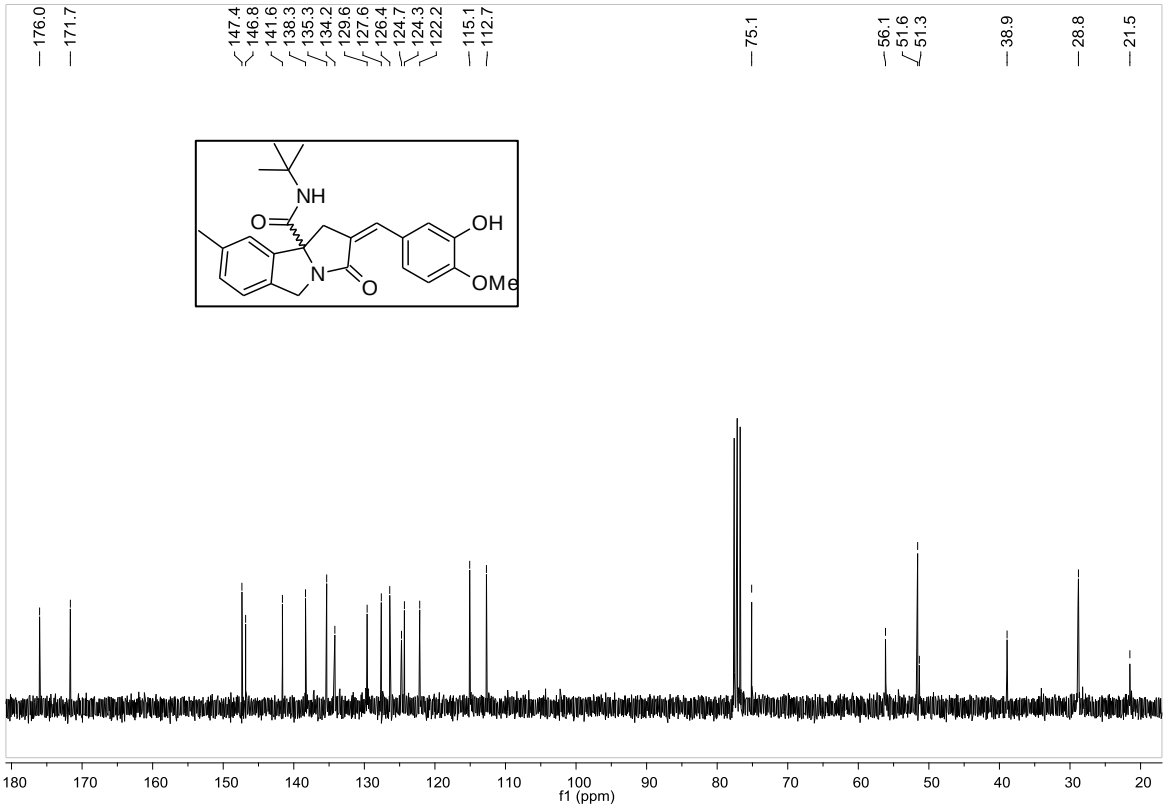
^{13}C-NMR of (2*E*)-*N*-(2-bromo-4-methylbenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8k**)



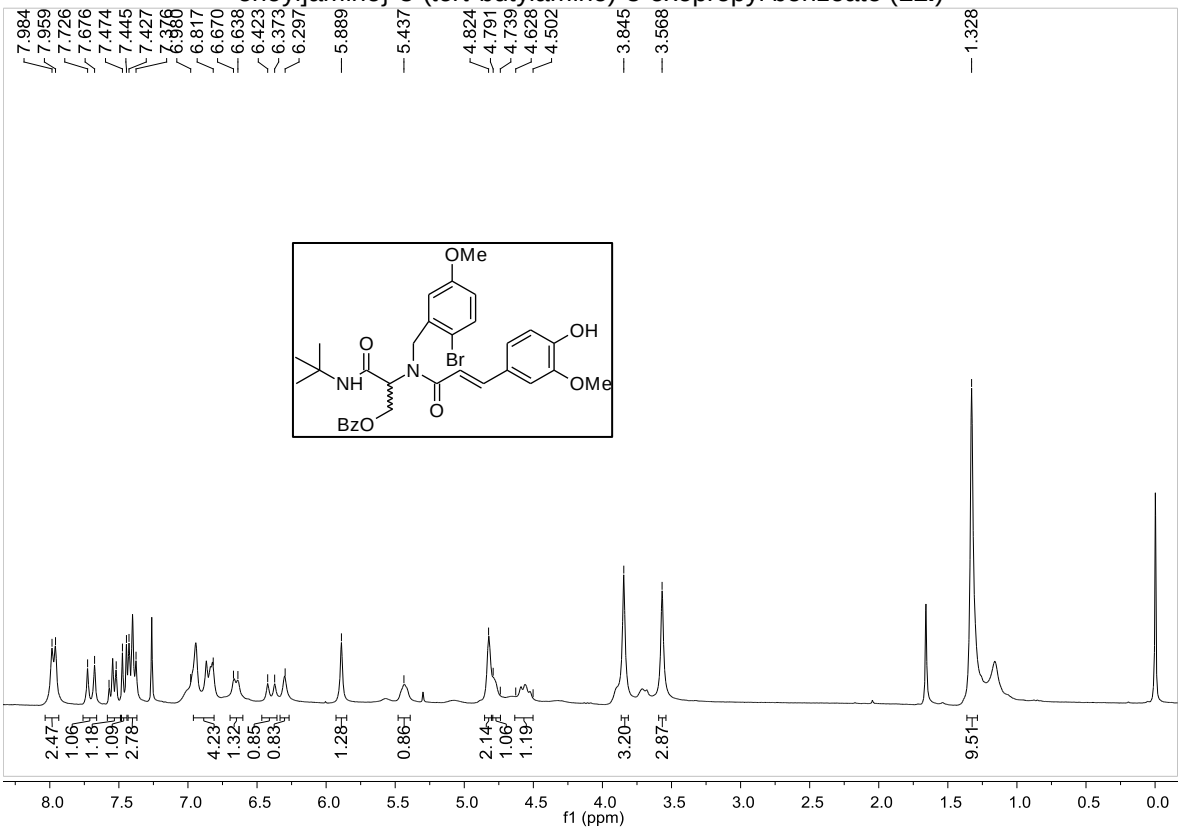
^{1}H-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3-methoxybenzylidene)-8-methyl-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12k**)



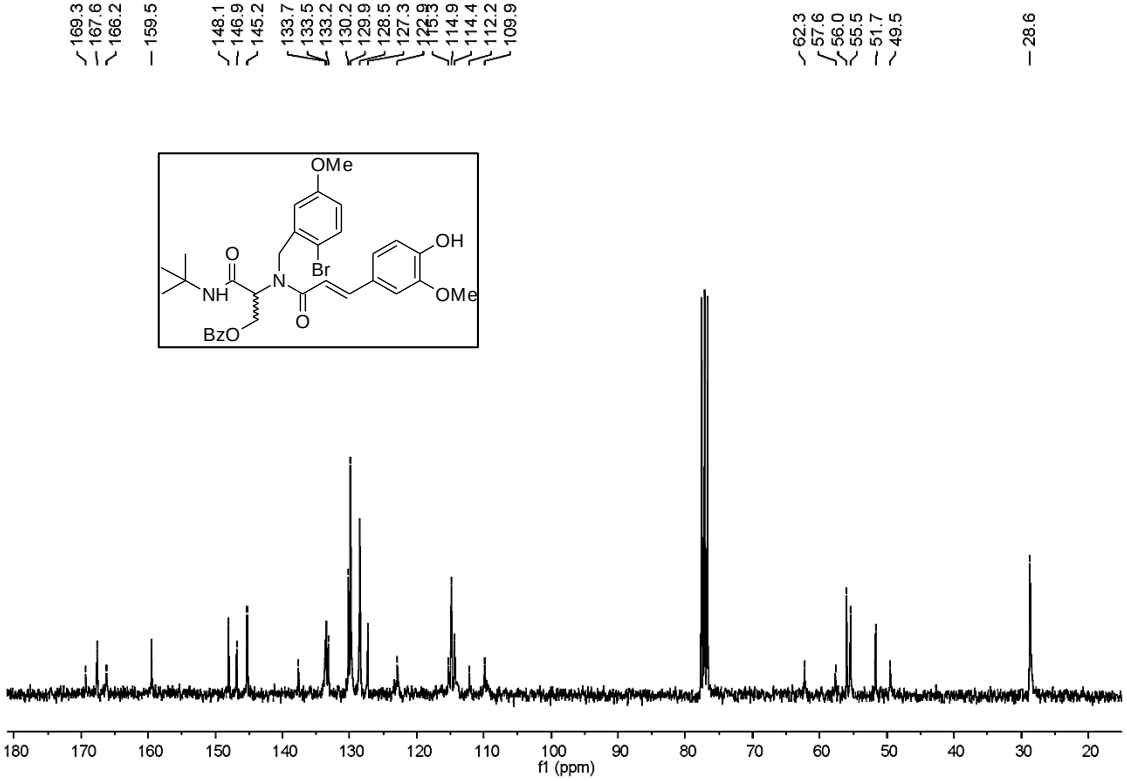
^{13}C-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3-methoxybenzylidene)-8-methyl-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12k**)



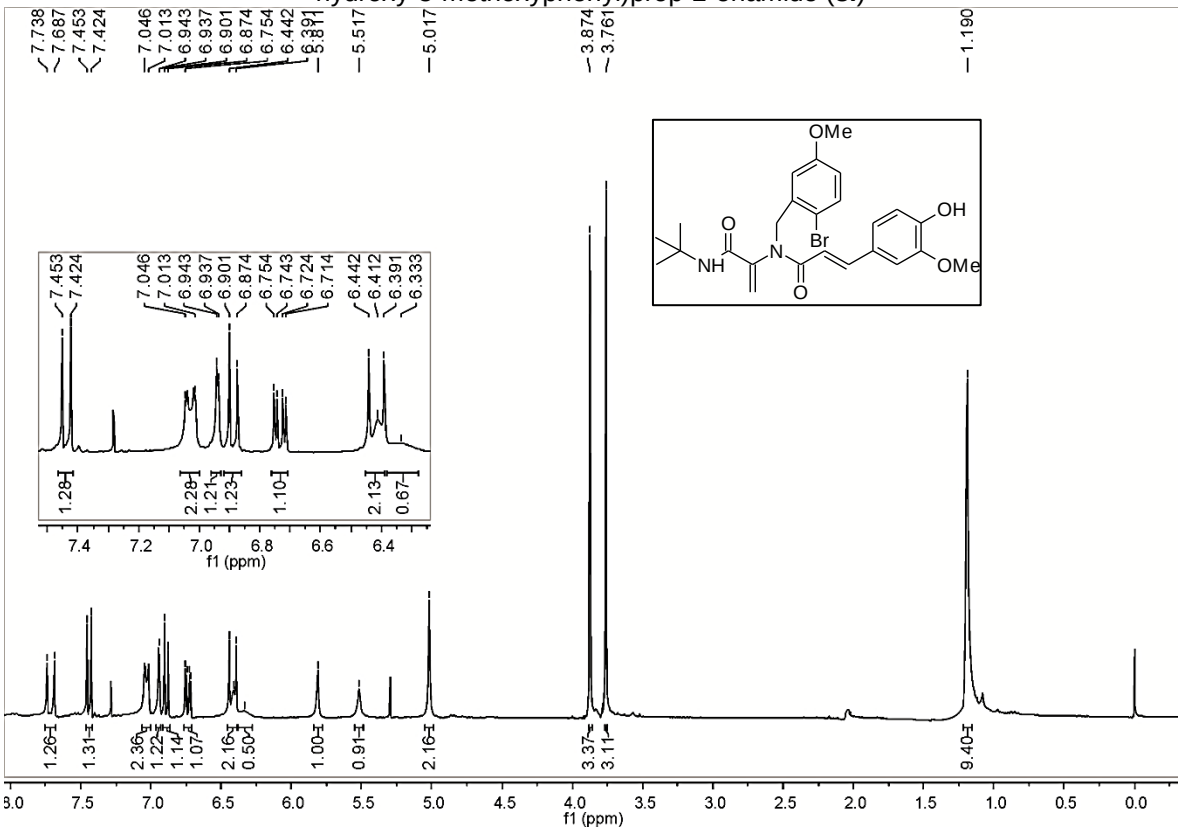
^{1}H-NMR of 2-{(2-bromo-5-methoxybenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11l**)



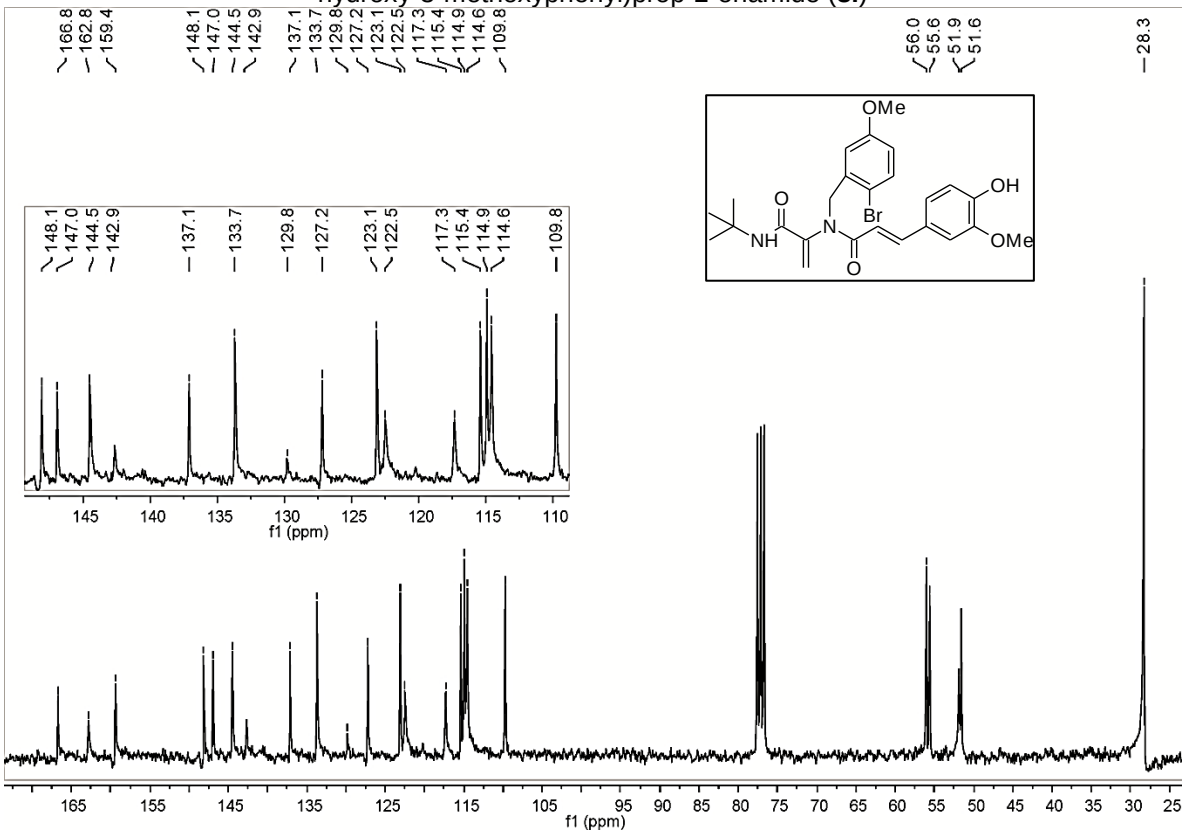
^{13}C-NMR of 2-{(2-bromo-5-methoxybenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11l**)



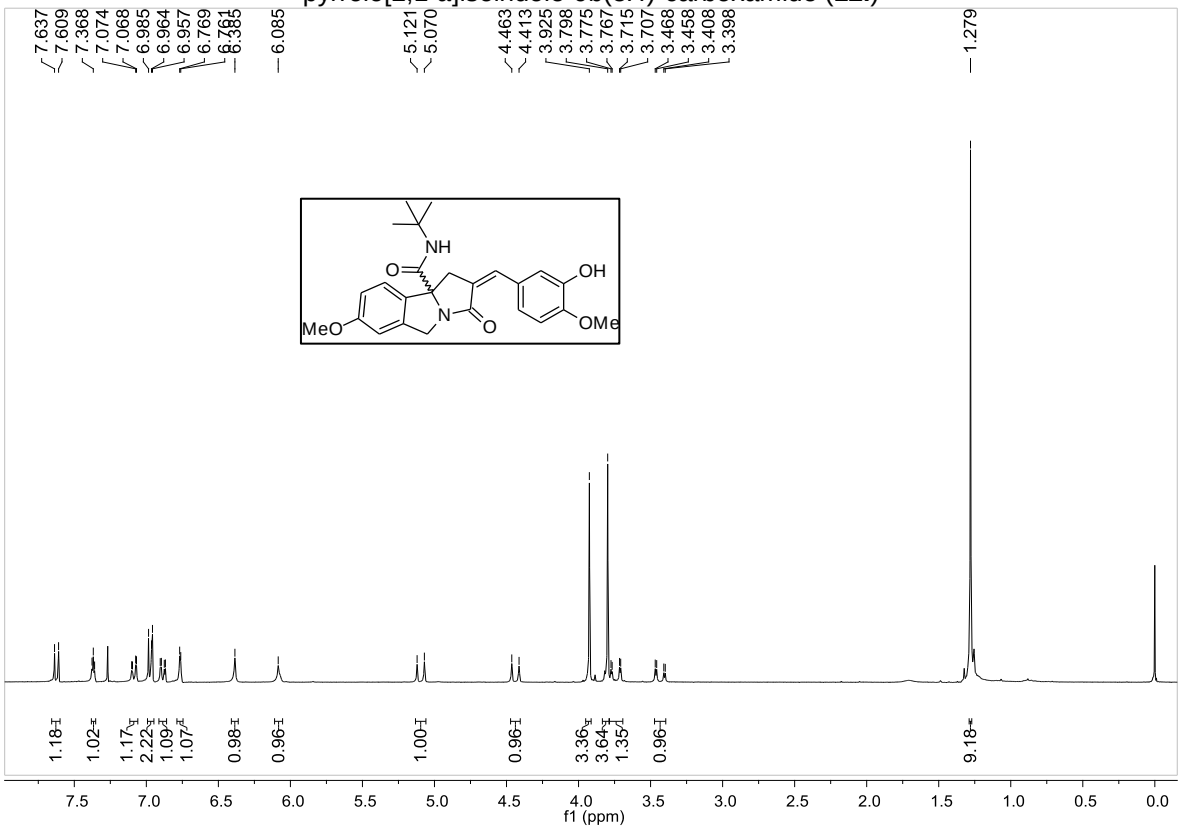
^{1}H-NMR of (2*E*)-*N*-(2-bromo-5-methoxybenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8l**)



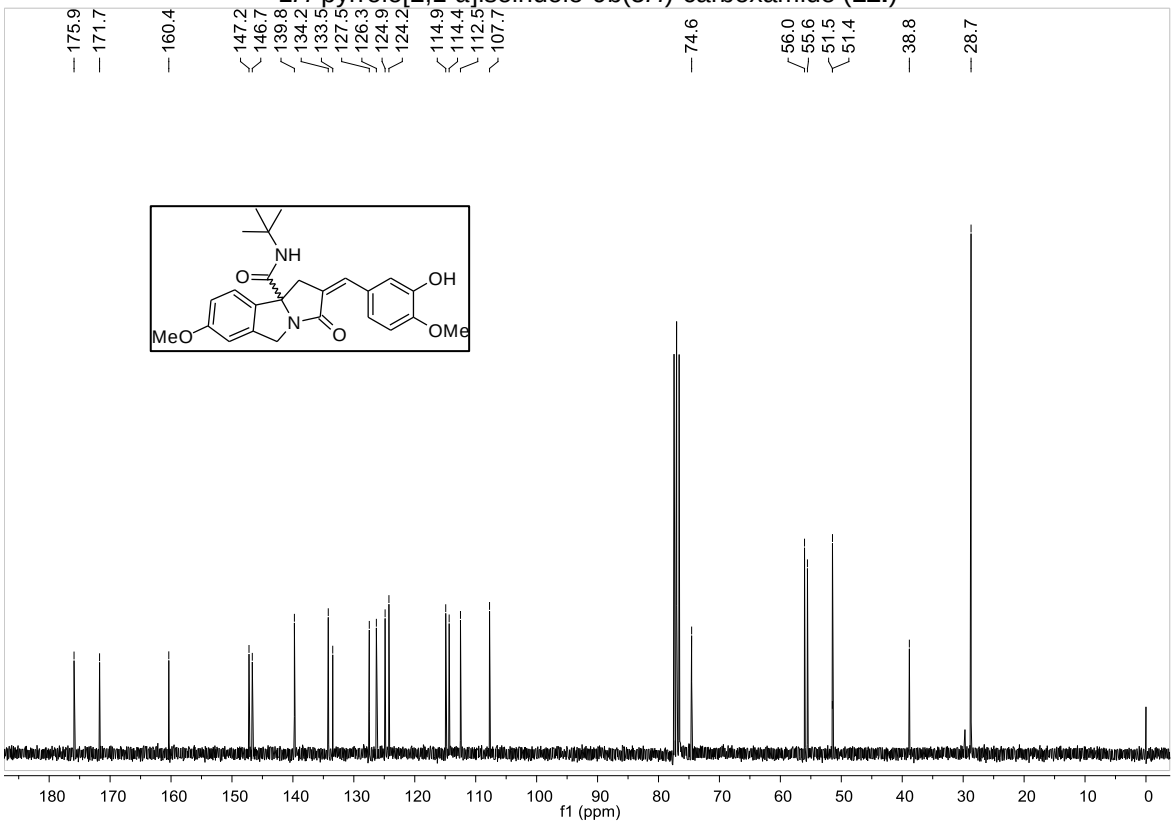
^{13}C-NMR of (2*E*)-*N*-(2-bromo-5-methoxybenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8l**)



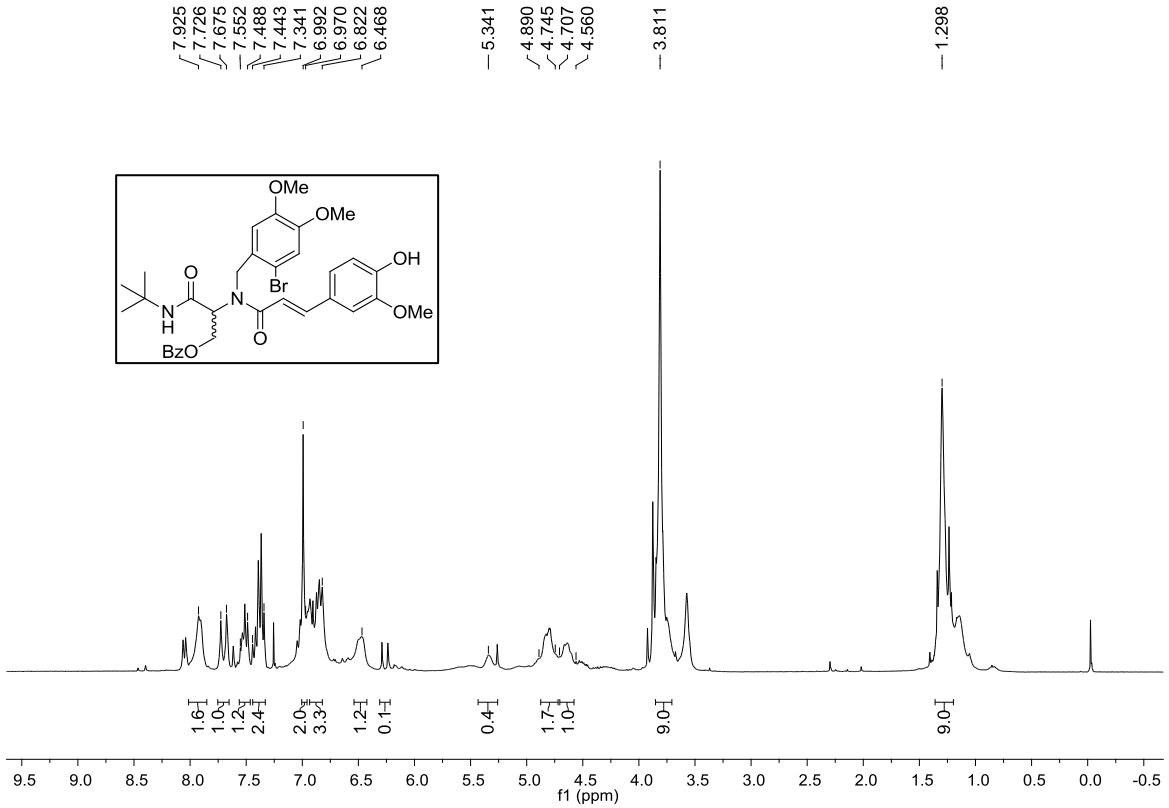
^{1}H-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3-methoxybenzylidene)-7-methoxy-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12l**)



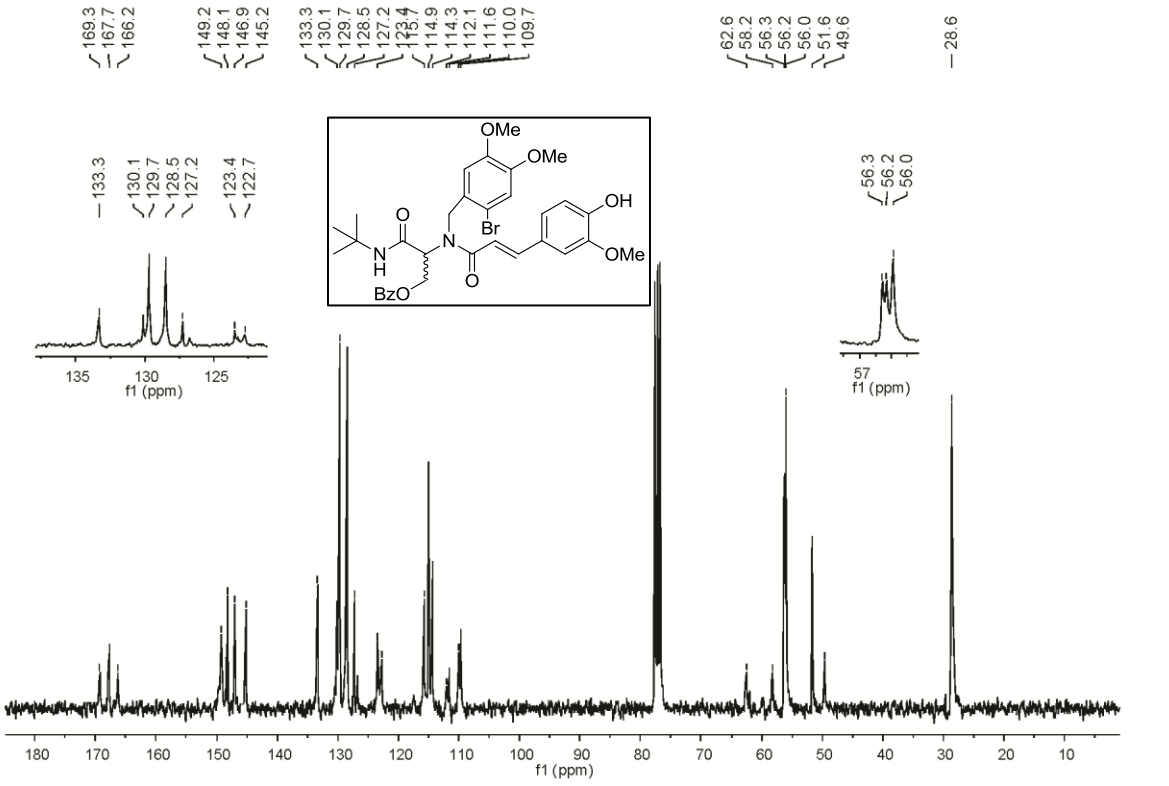
^{13}C-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3-methoxybenzylidene)-7-methoxy-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12l**)



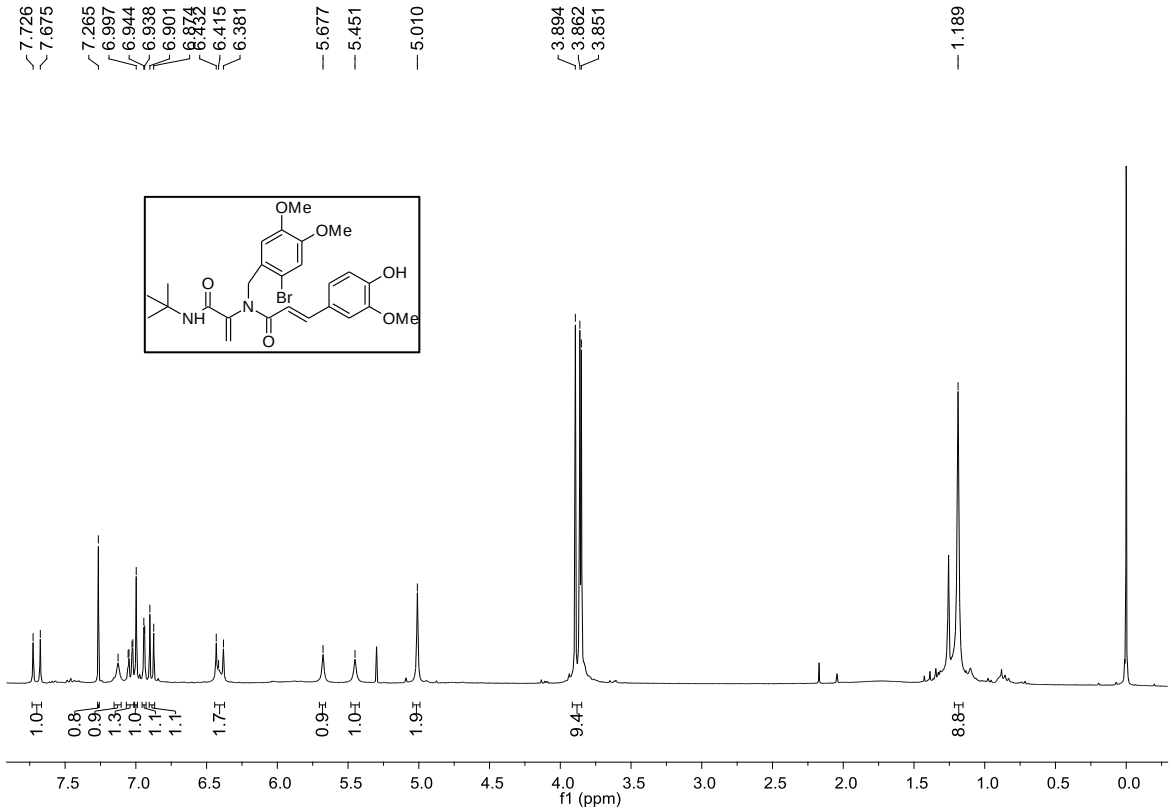
^{1}H-NMR of 2-{(2-bromo-4,5-dimethoxybenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11m**).



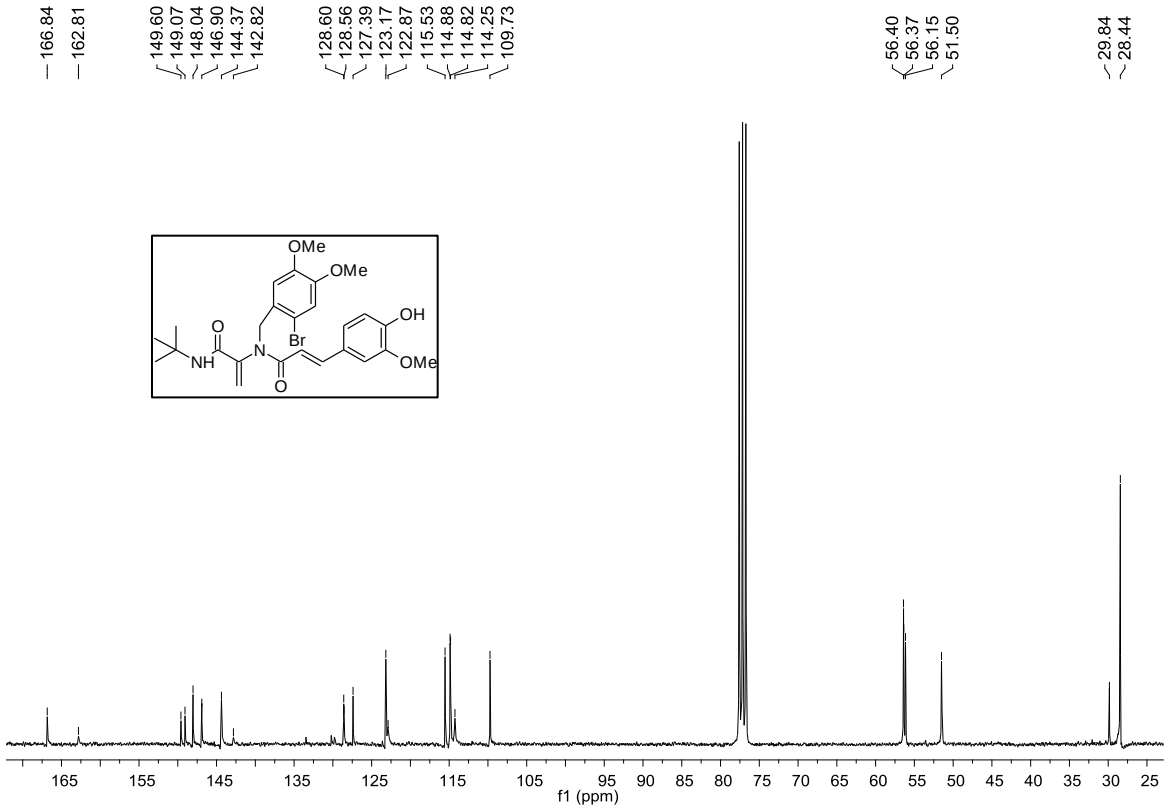
^{13}C-NMR of 2-{(2-bromo-4,5-dimethoxybenzyl)-[(2*E*)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11m**).



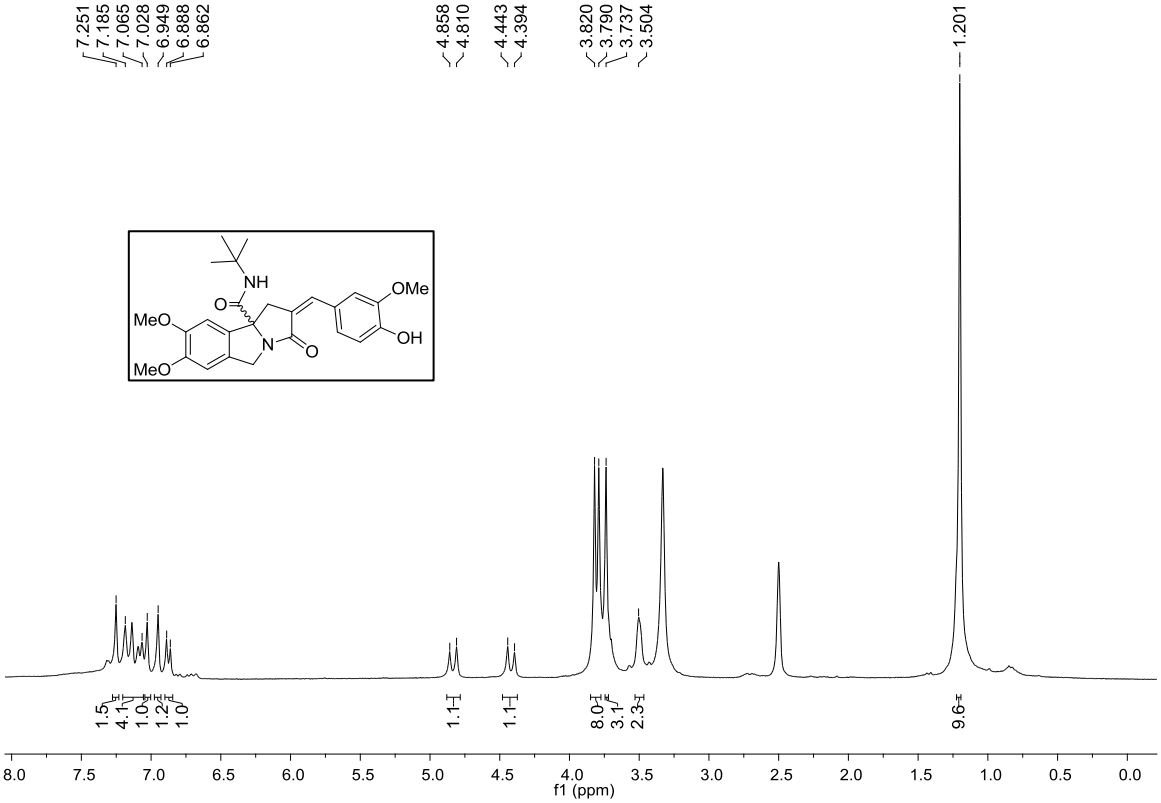
^{1}H-NMR of (2*E*)-*N*-(2-bromo-4,5-dimethoxybenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8m**)



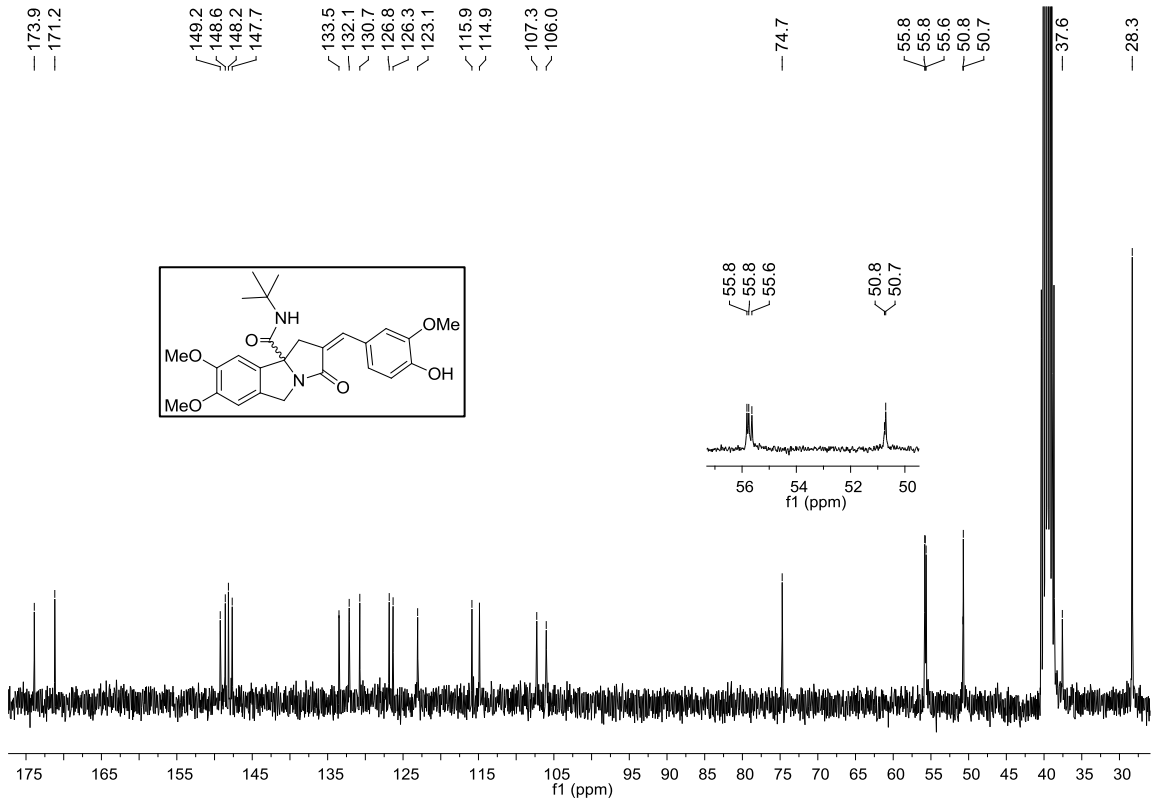
^{13}C-NMR of (2*E*)-*N*-(2-bromo-4,5-dimethoxybenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3-methoxyphenyl)prop-2-enamide (**8m**)



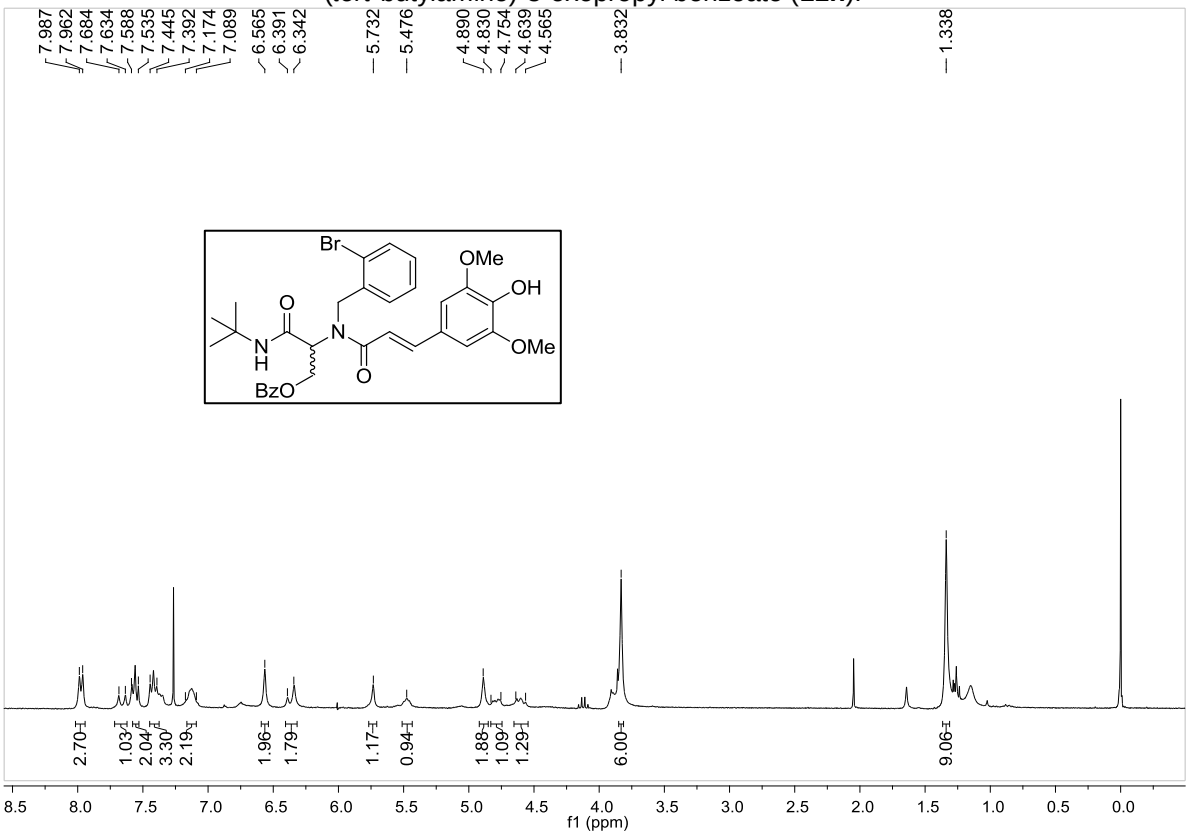
^{1}H-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3-methoxybenzylidene)-7,8-dimethoxy-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12m**)



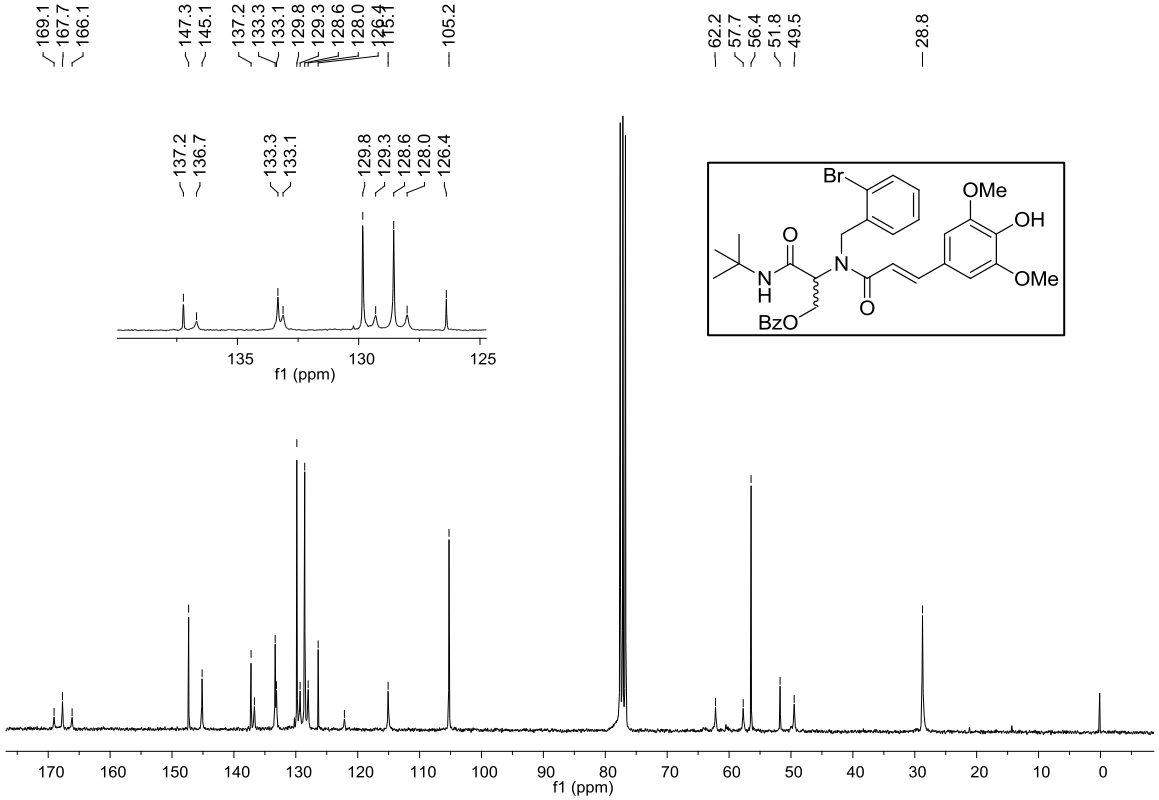
^{13}C-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3-methoxybenzylidene)-7,8-dimethoxy-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12m**)



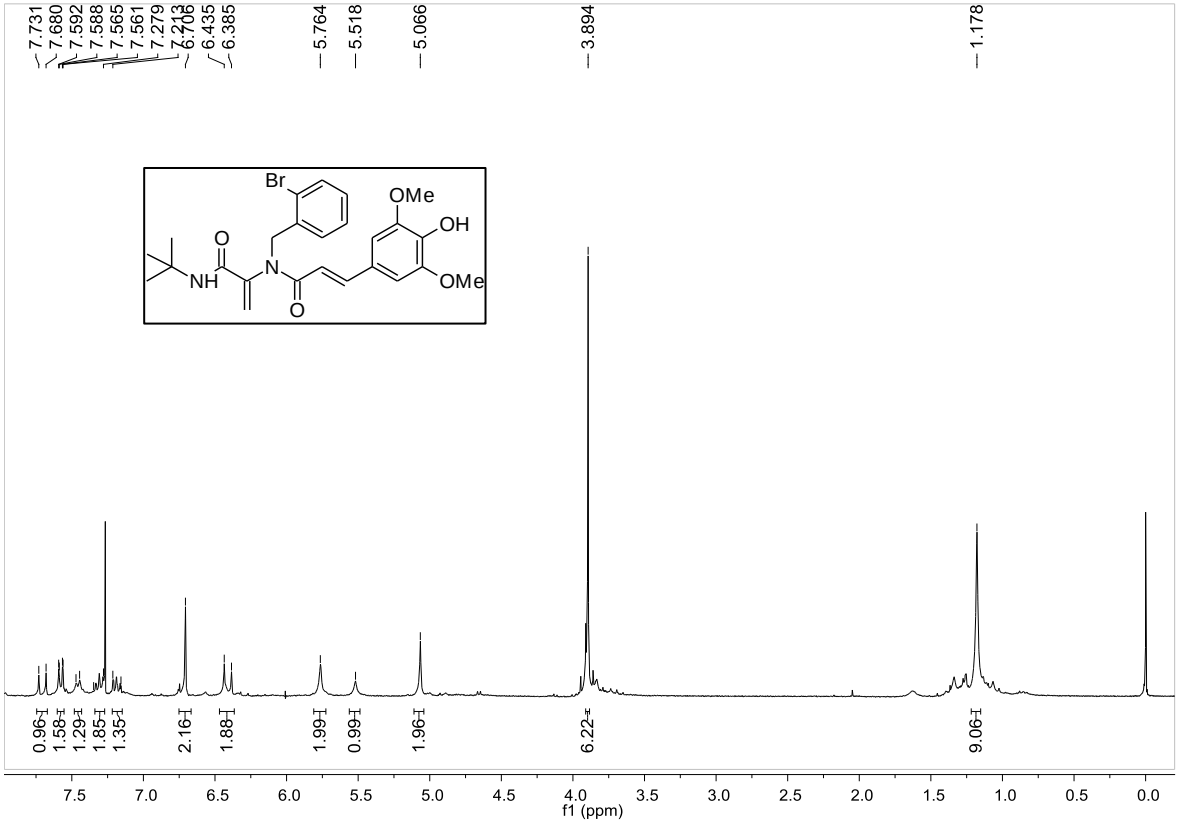
^{1}H-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11n**).



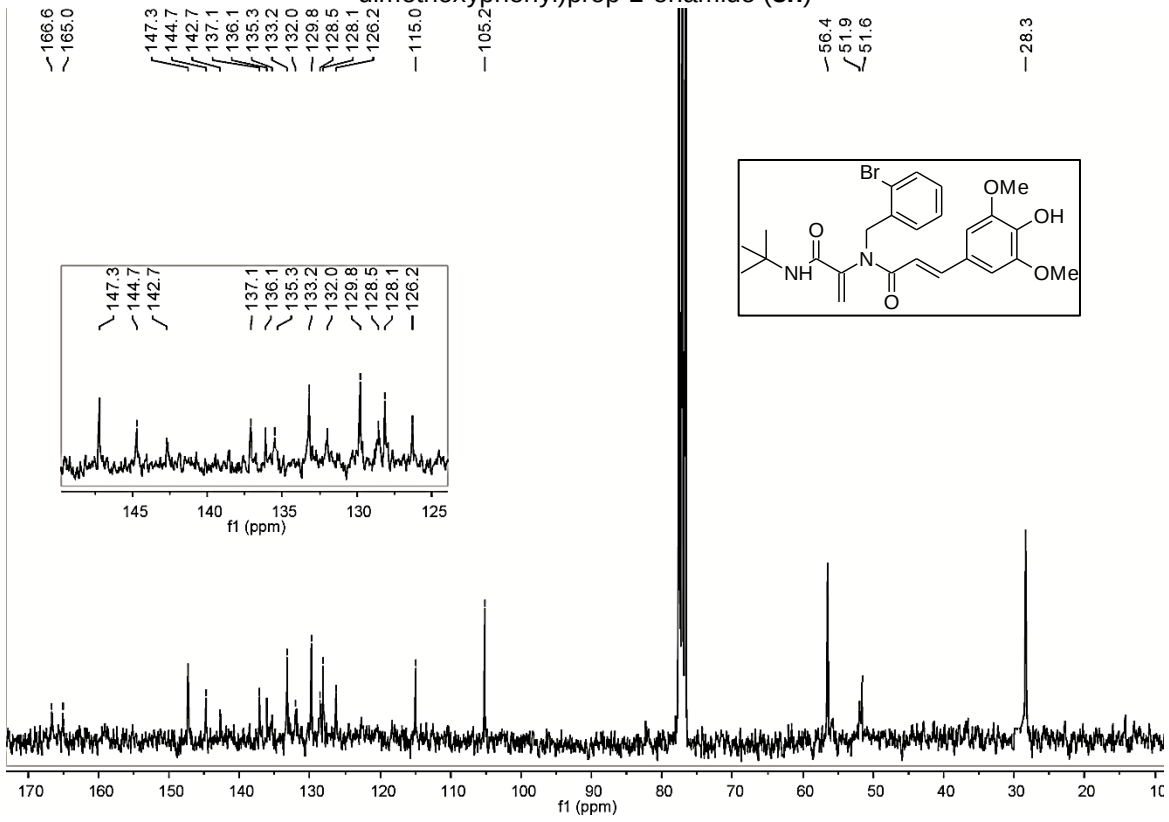
^{13}C-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11n**).



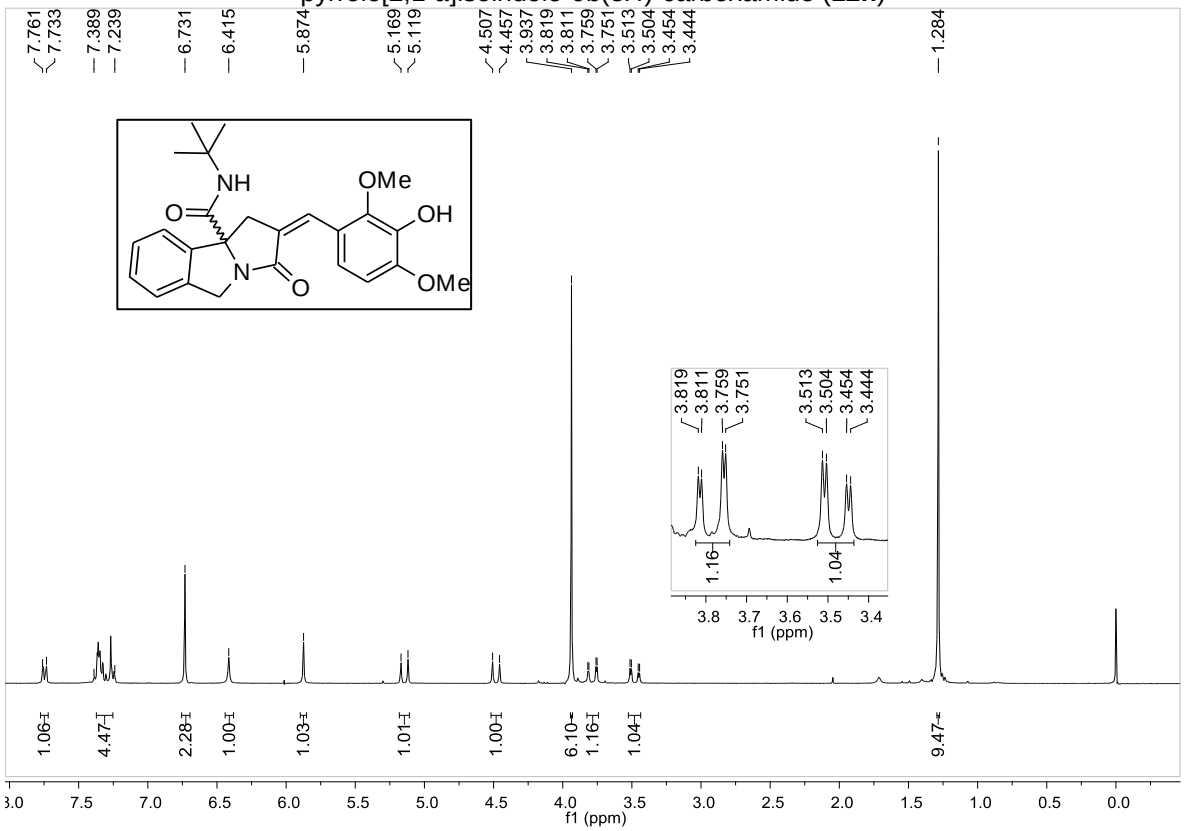
^{1}H-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enamide (**8n**)



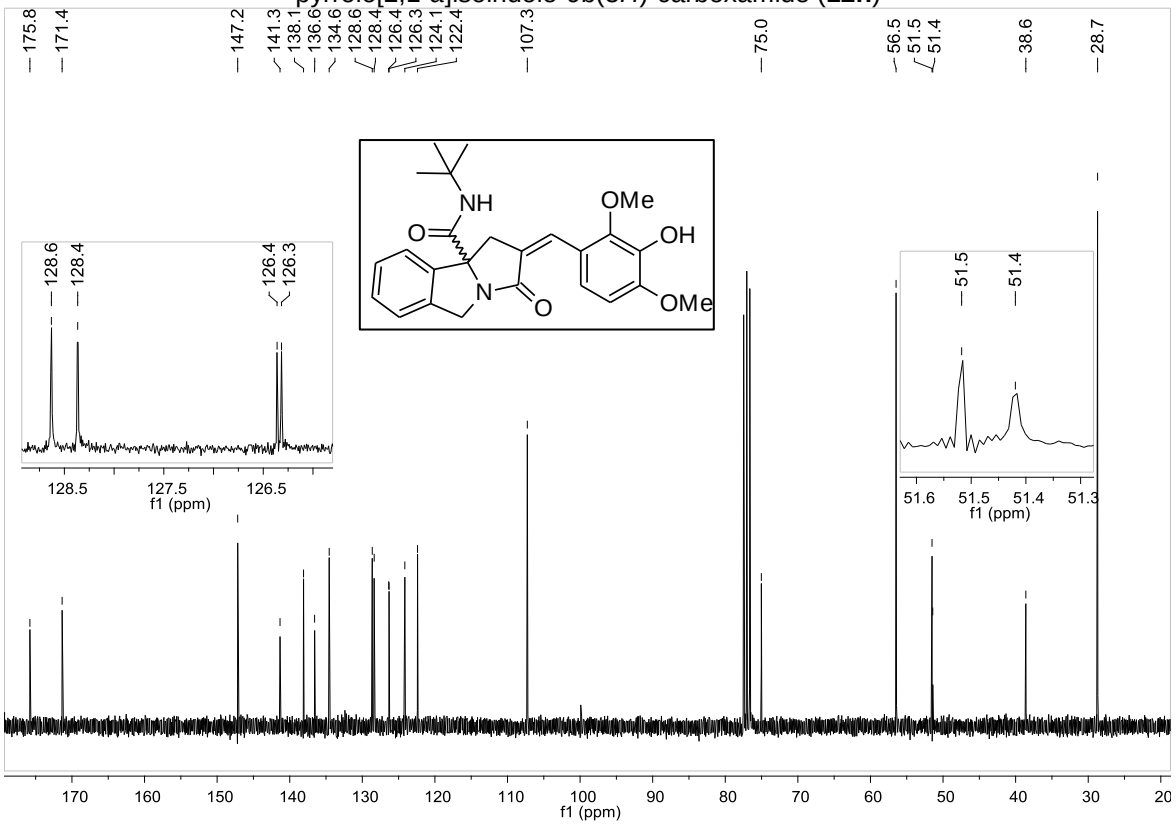
^{13}C-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enamide (**8n**)



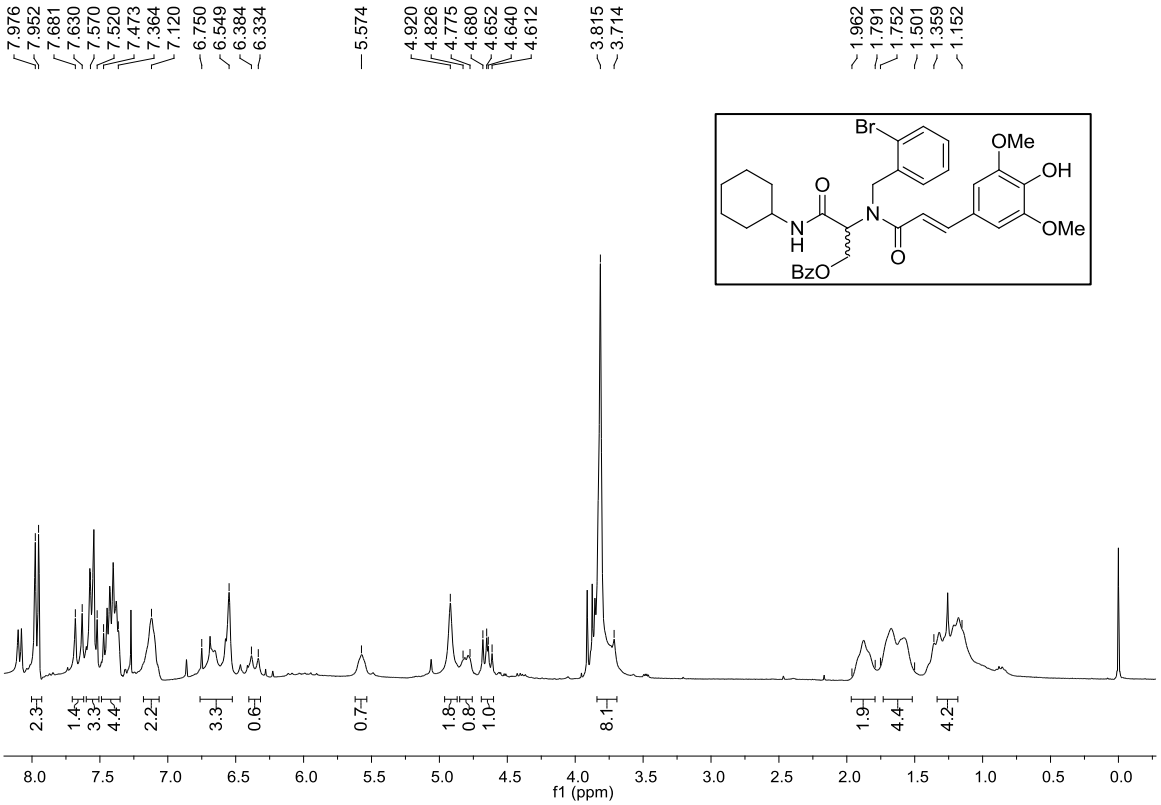
^{1}H-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3,5-dimethoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12n**)



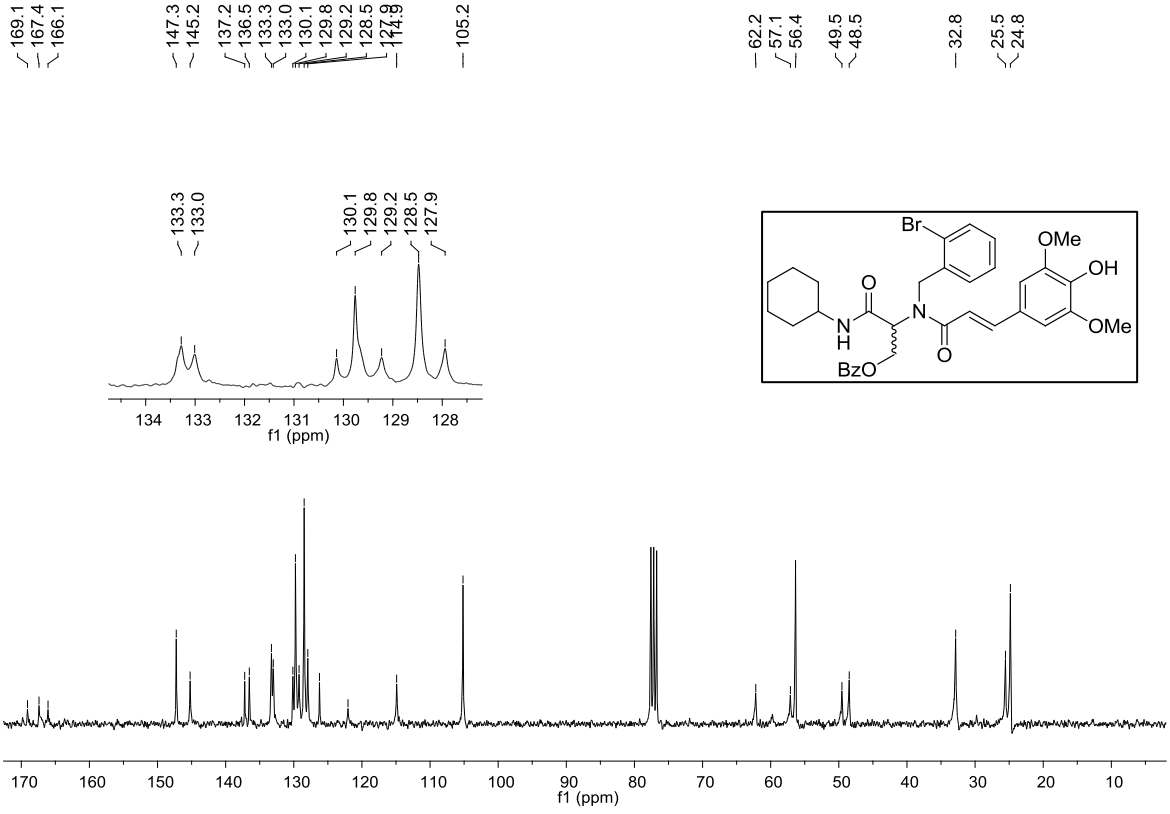
^{13}C-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3,5-dimethoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12n**)



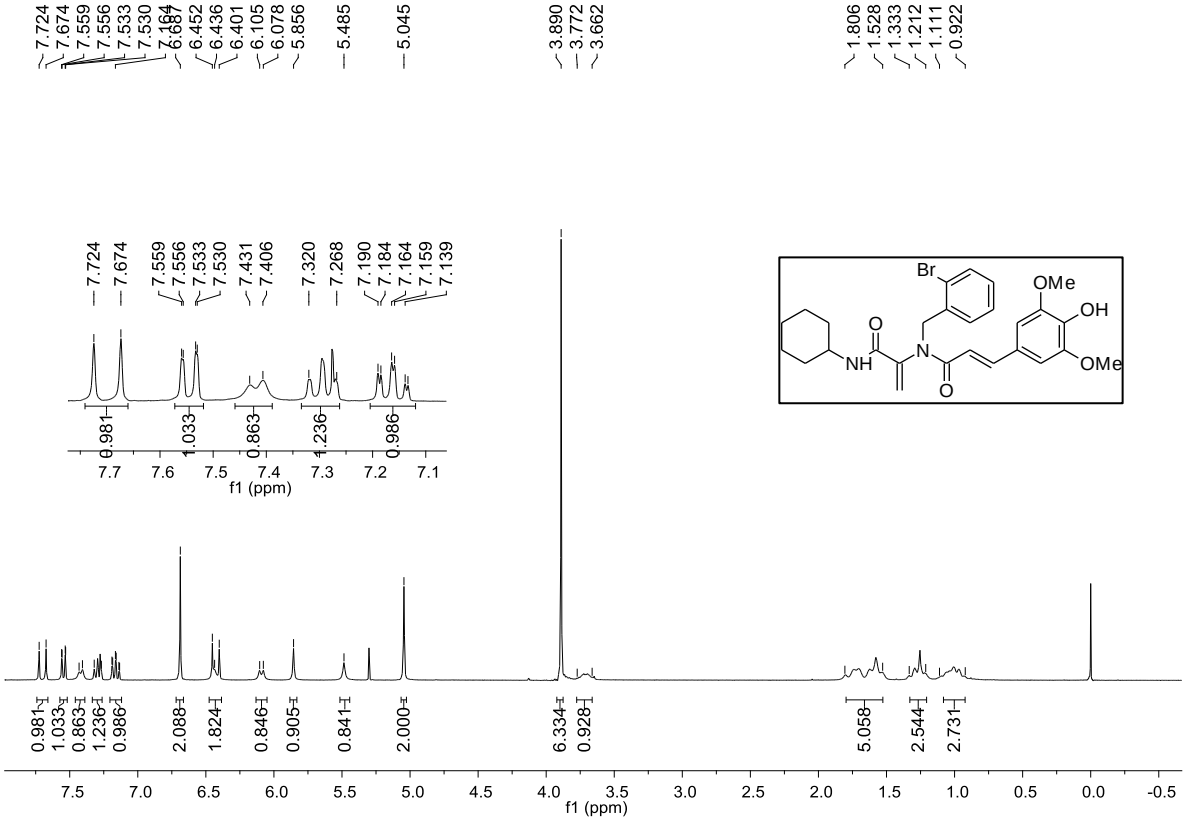
^{1}H-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoyl]amino}-3-(cyclohexylamino)-3-oxopropyl benzoate (**11o**).



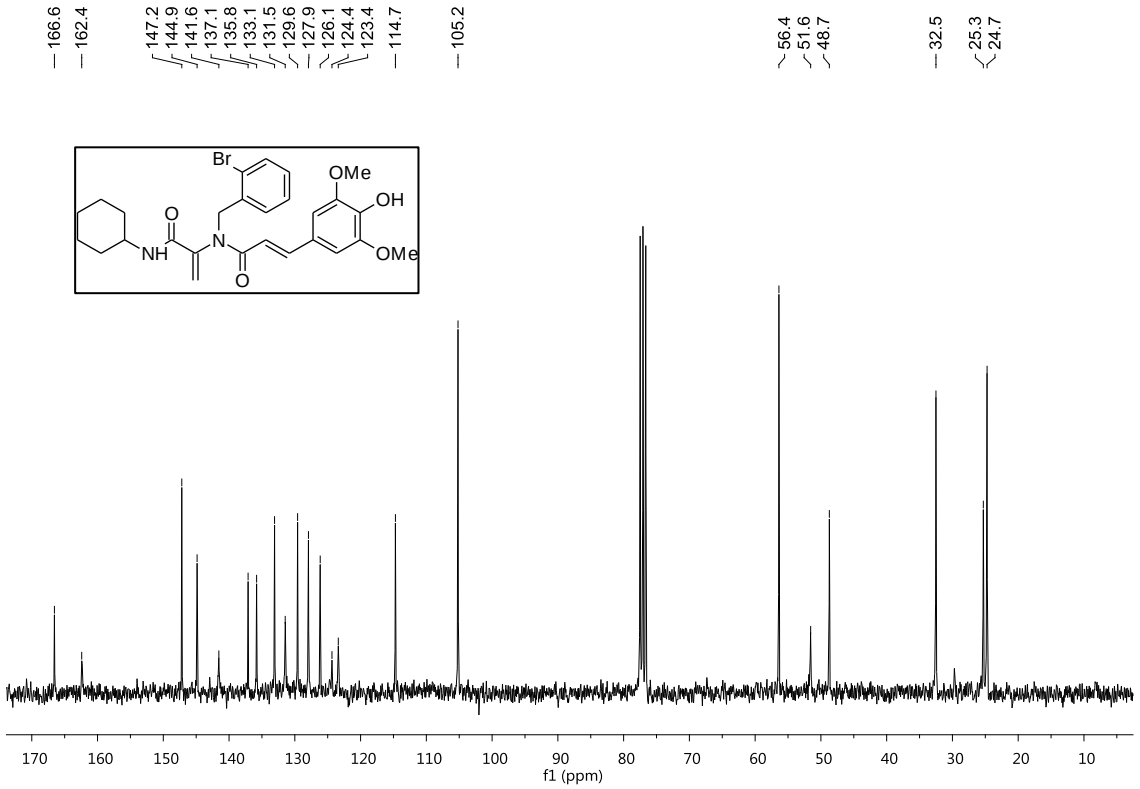
^{13}C-NMR of 2-{(2-bromobenzyl)-[(2*E*)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoyl]amino}-3-(cyclohexylamino)-3-oxopropyl benzoate (**11o**).



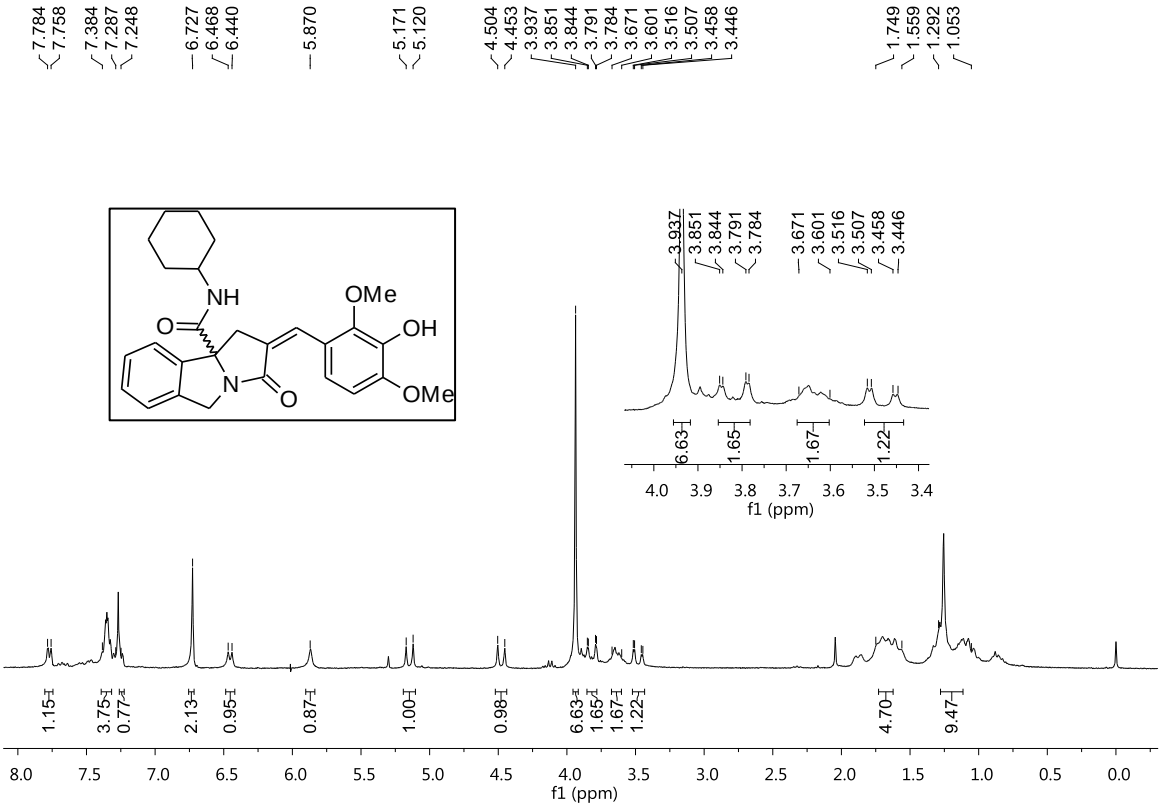
^{1}H-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(cyclohexylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enamide (**8o**)



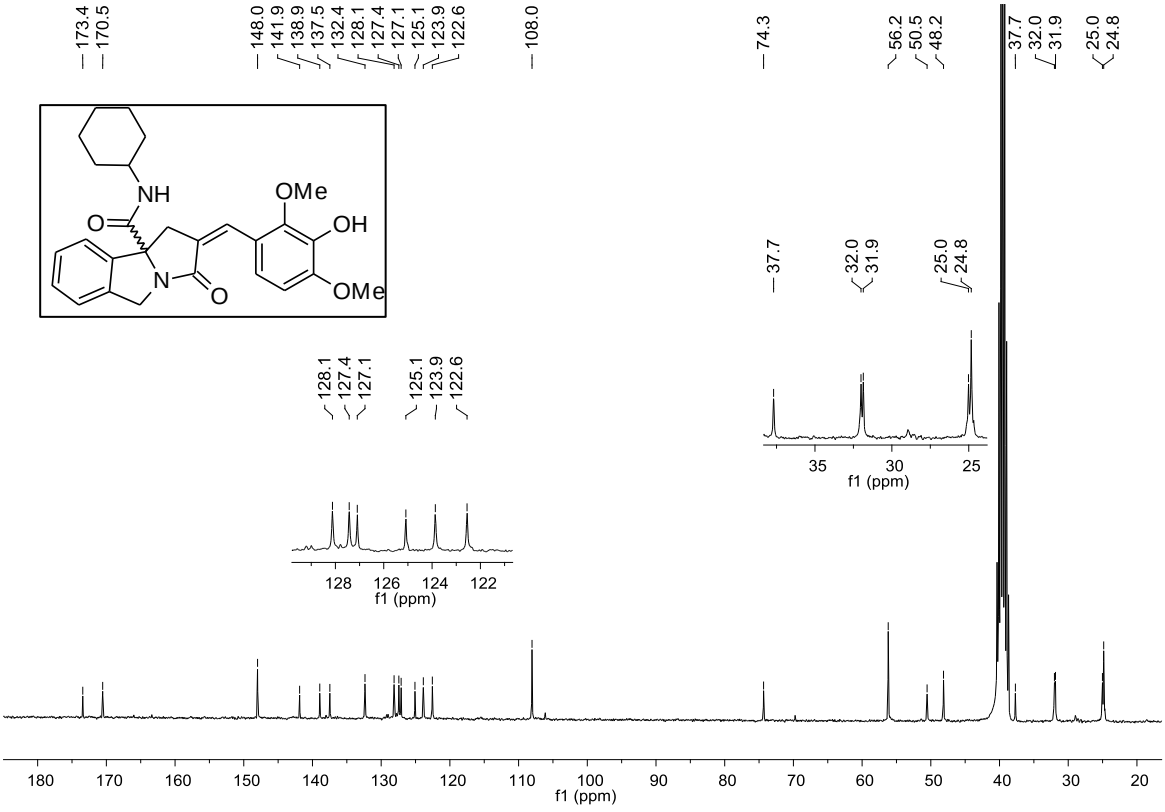
^{13}C-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(cyclohexylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enamide (**8o**)



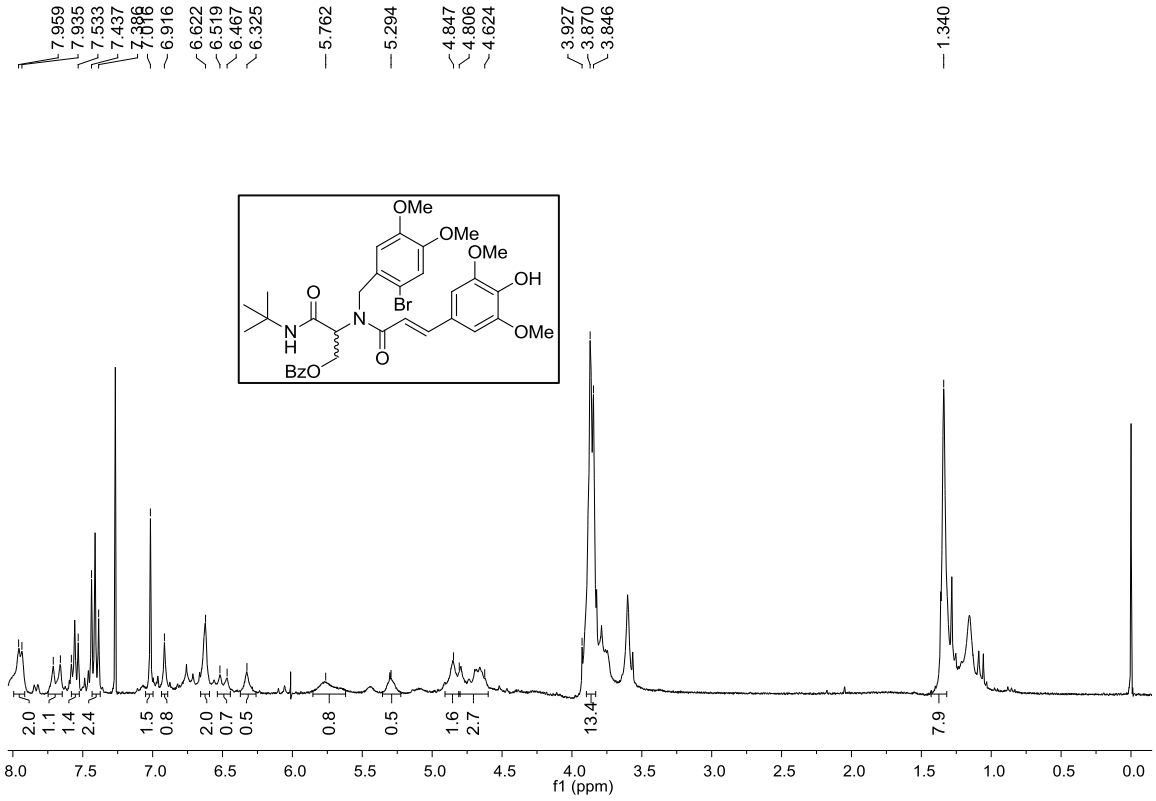
^{1}H-NMR of (2*Z*)-*N*-cyclohexyl-2-(4-hydroxy-3,5-dimethoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12o**)



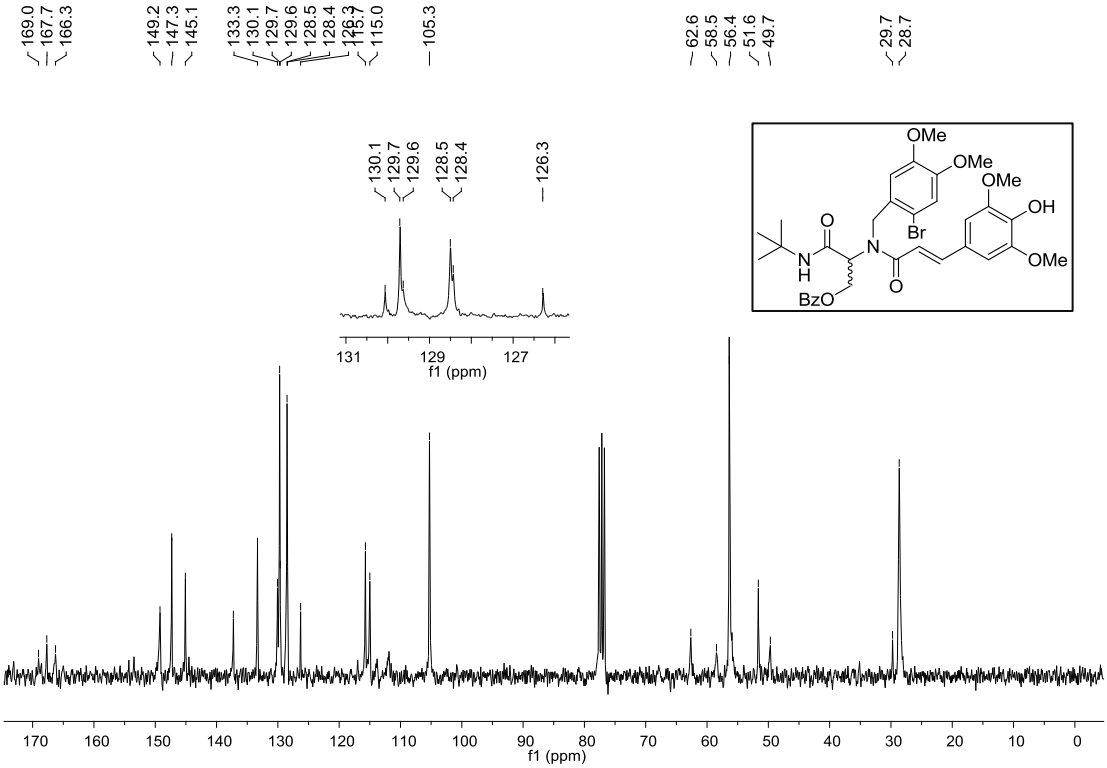
^{13}C-NMR of (2*Z*)-*N*-cyclohexyl-2-(4-hydroxy-3,5-dimethoxybenzylidene)-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12o**)



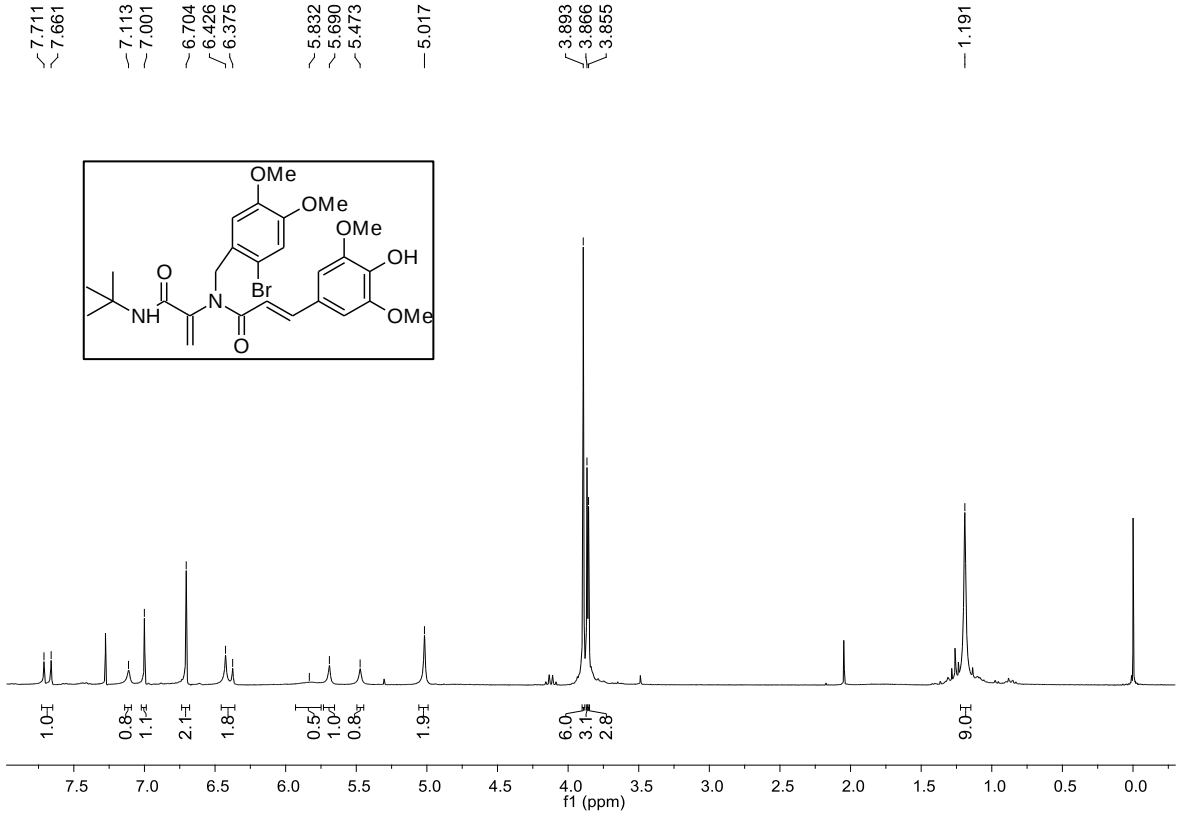
^{1}H-NMR of 2-{(2-bromo-4,5-dimethoxybenzyl)-[(2*E*)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11p**).



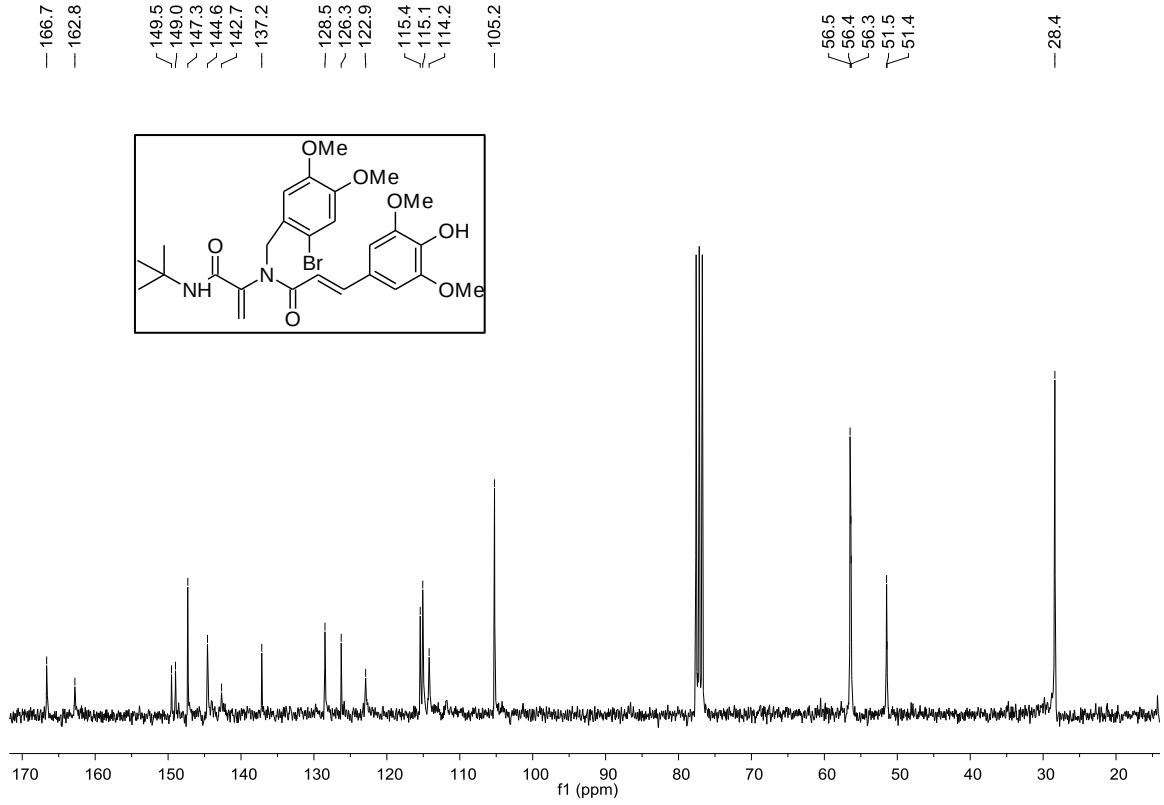
^{13}C-NMR of 2-{(2-bromo-4,5-dimethoxybenzyl)-[(2*E*)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoyl]amino}-3-(*tert*-butylamino)-3-oxopropyl benzoate (**11p**).



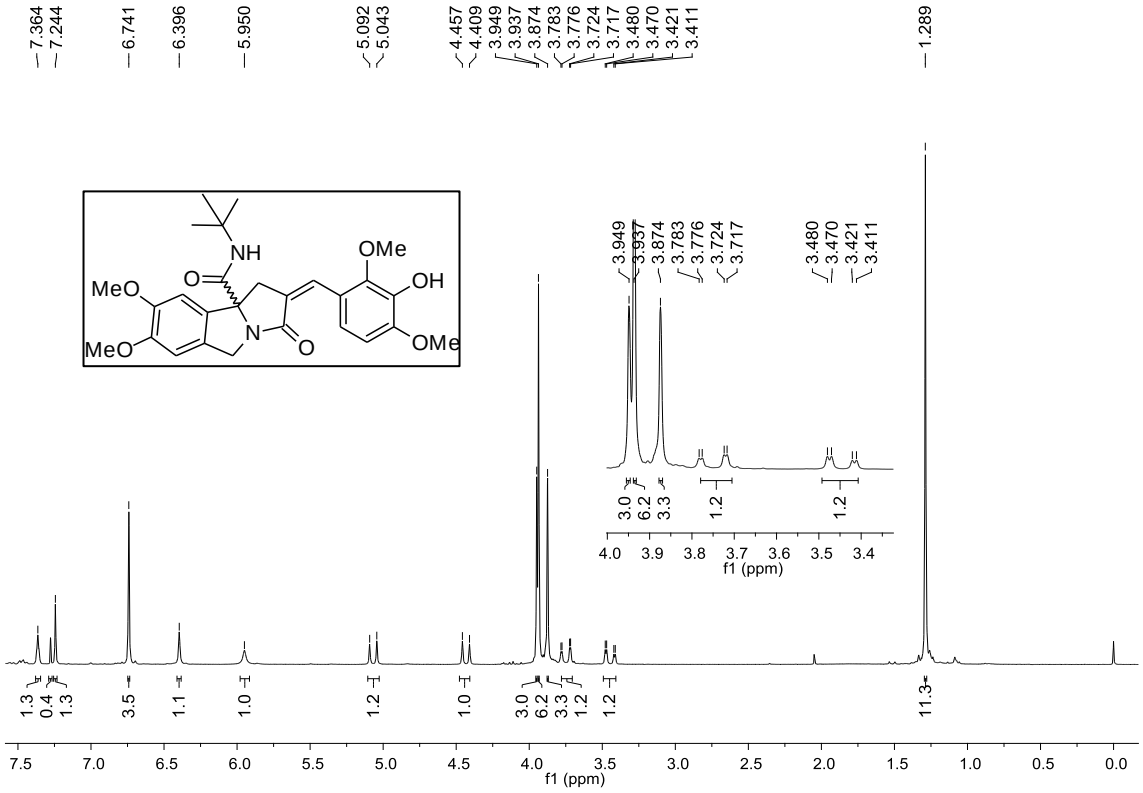
^{1}H-NMR of (2*E*)-*N*-(2-bromo-4,5-dimethoxybenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enamide (**8p**)



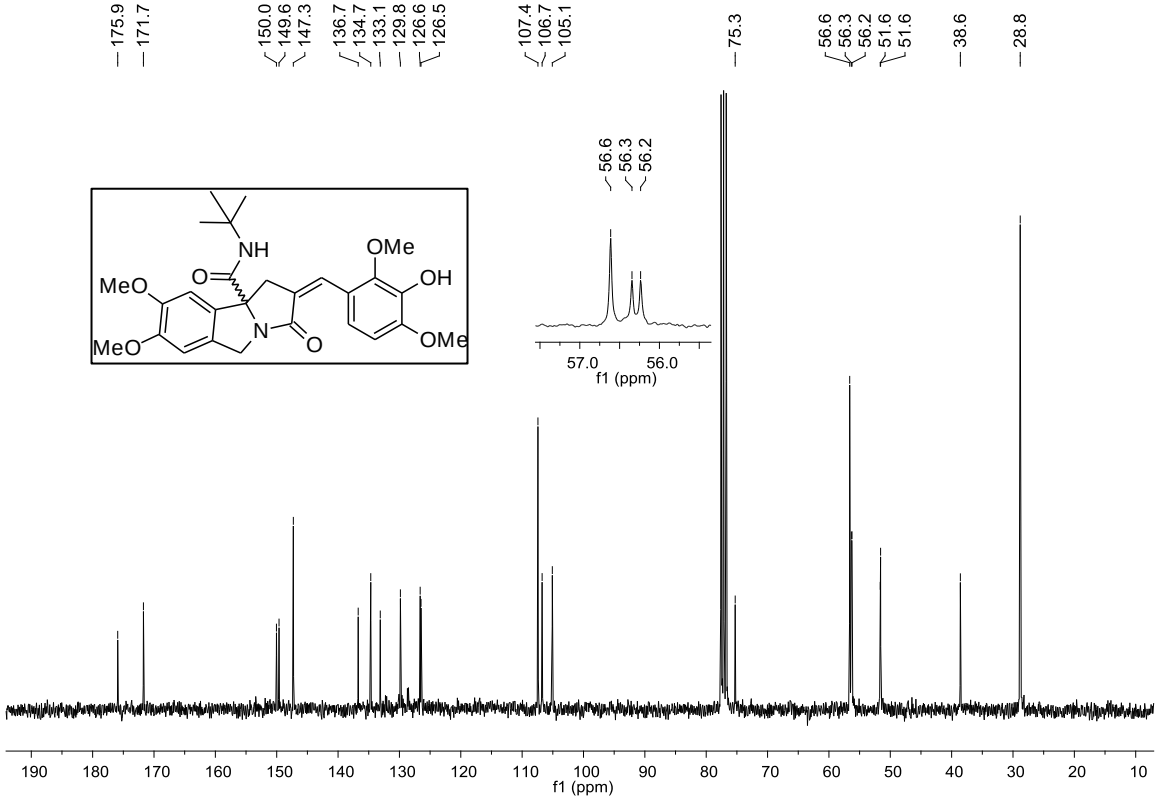
^{13}C-NMR of (2*E*)-*N*-(2-bromo-4,5-dimethoxybenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enamide (**8p**)



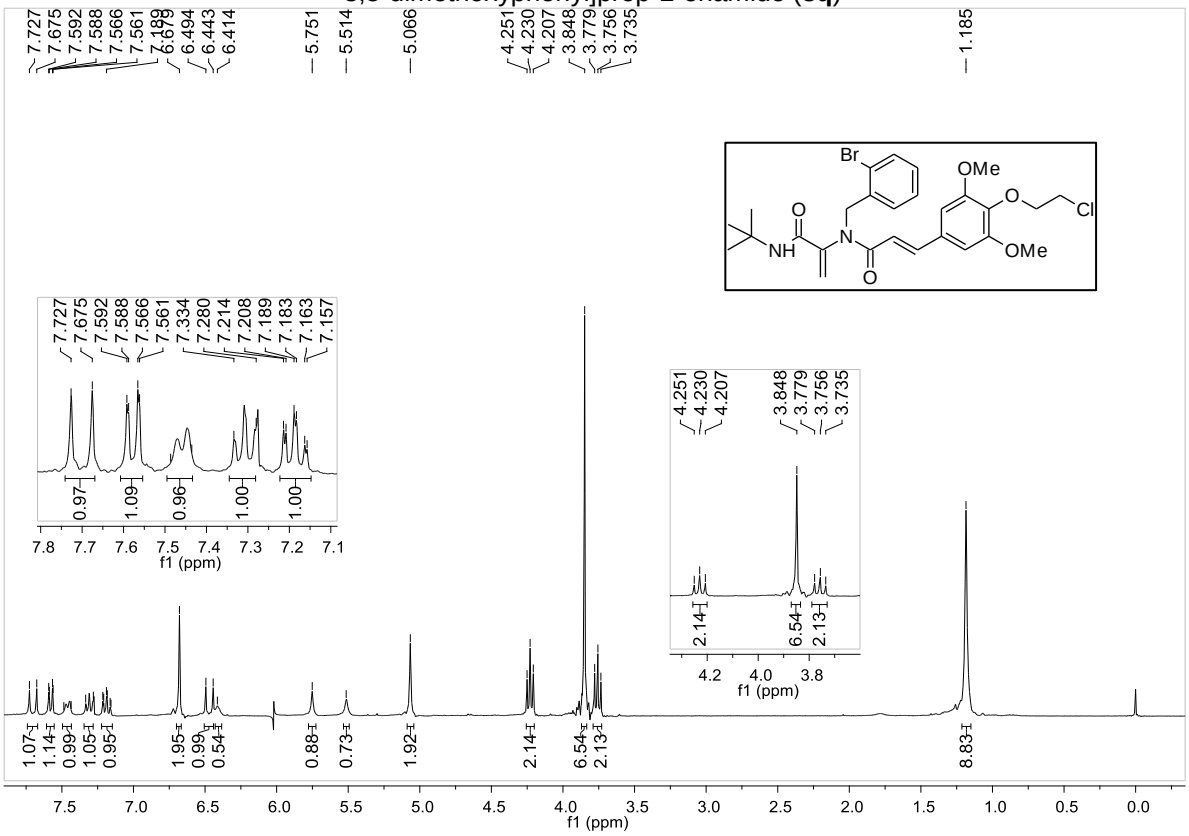
^{1}H-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3,5-dimethoxybenzylidene)-7,8-dimethoxy-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12p**)



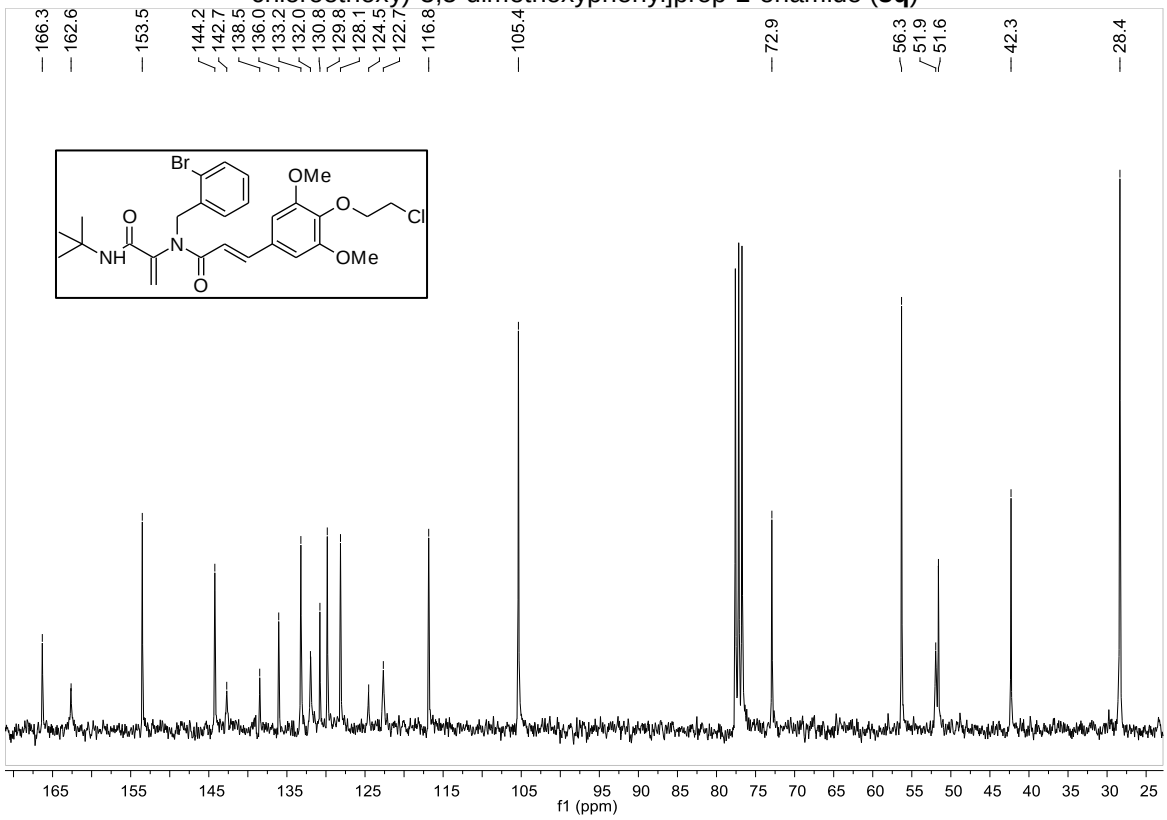
^{13}C-NMR of (2*Z*)-*N*-*tert*-butyl-2-(4-hydroxy-3,5-dimethoxybenzylidene)-7,8-dimethoxy-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12p**)



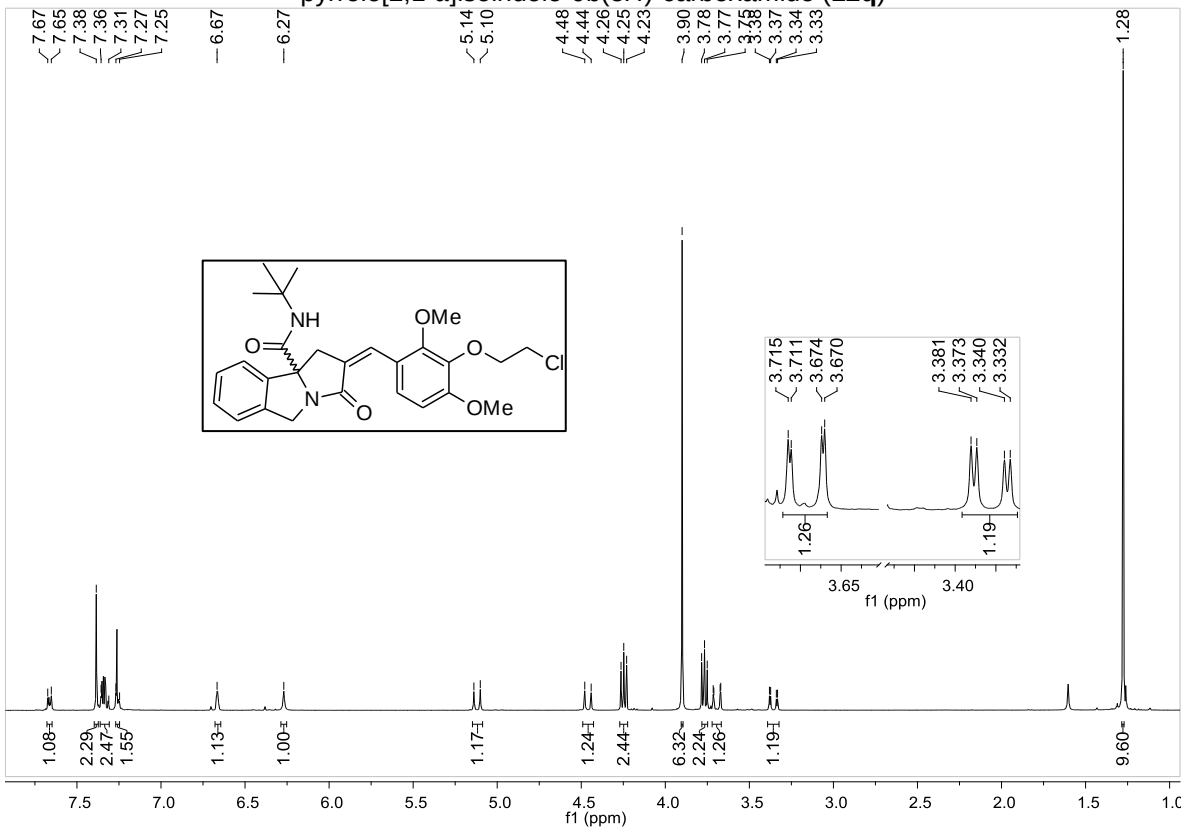
^{1}H-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-[(2-chloroethoxy)-3,5-dimethoxyphenyl]prop-2-enamide (**8q**)



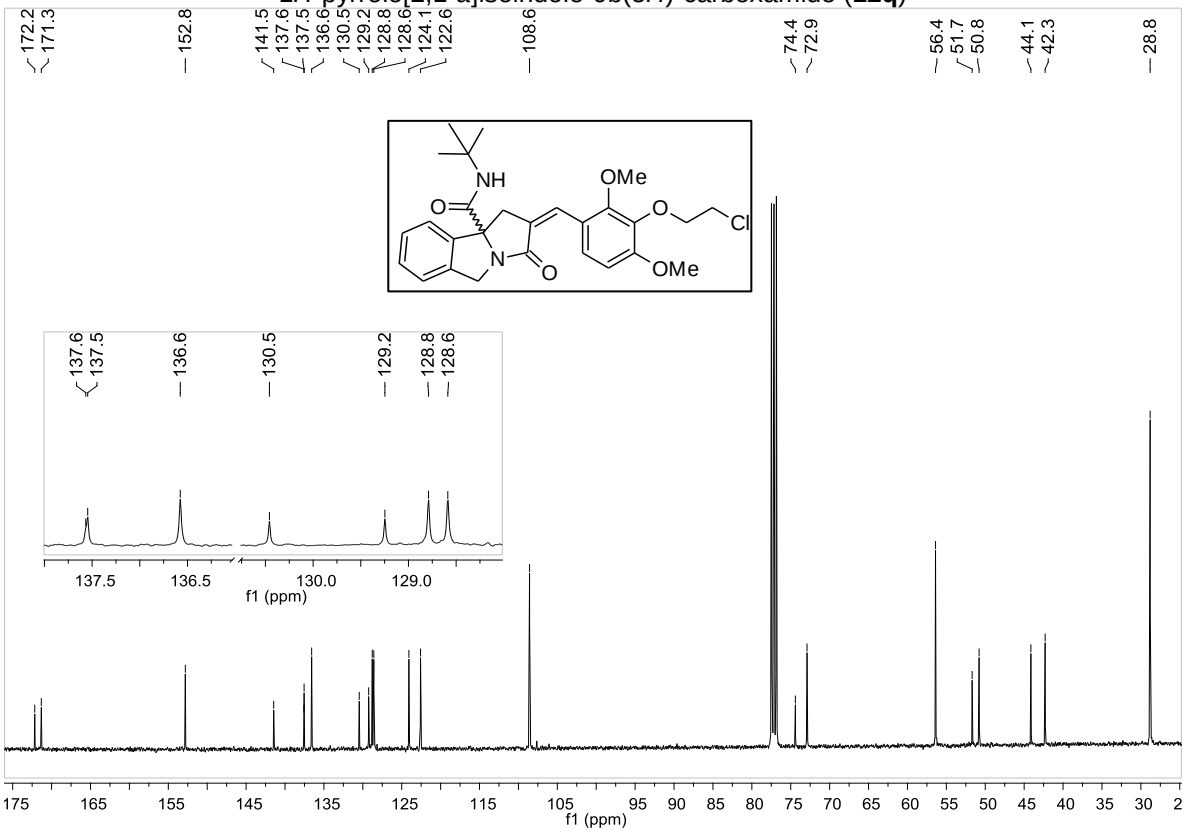
^{13}C-NMR of (2*E*)-*N*-(2-bromobenzyl)-*N*-[3-(*tert*-butylamino)-3-oxoprop-1-en-2-yl]-3-[(2-chloroethoxy)-3,5-dimethoxyphenyl]prop-2-enamide (**8q**)



^{1}H-NMR of (2*Z*)-*N*-*tert*-butyl-2-[4-(2-chloroethoxy)-3,5-dimethoxybenzylidene]-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12q**)



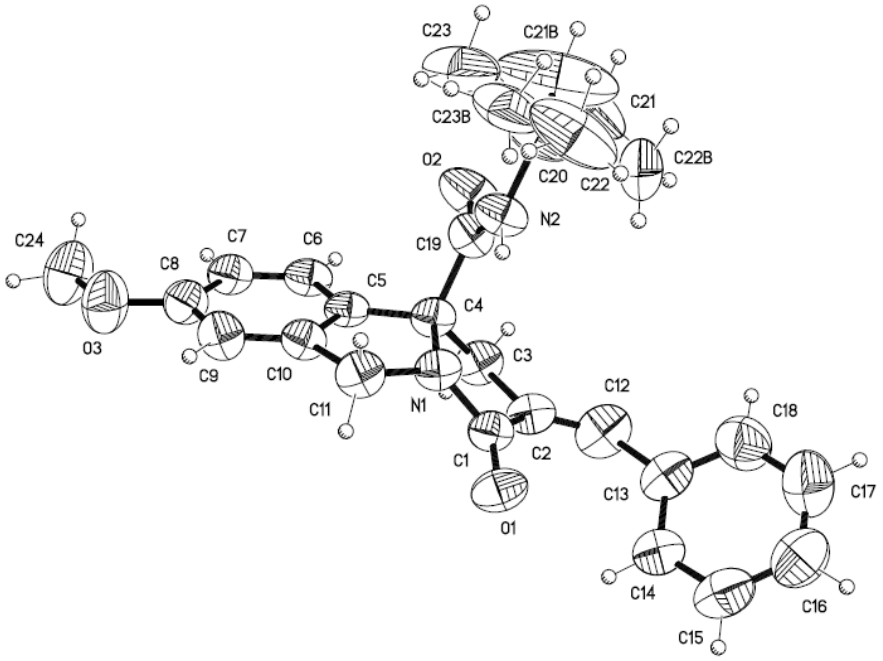
^{13}C-NMR of (2*Z*)-*N*-*tert*-butyl-2-[4-(2-chloroethoxy)-3,5-dimethoxybenzylidene]-3-oxo-2,3-dihydro-1*H*-pyrrolo[2,1-*a*]isoindole-9b(5*H*)-carboxamide (**12q**)

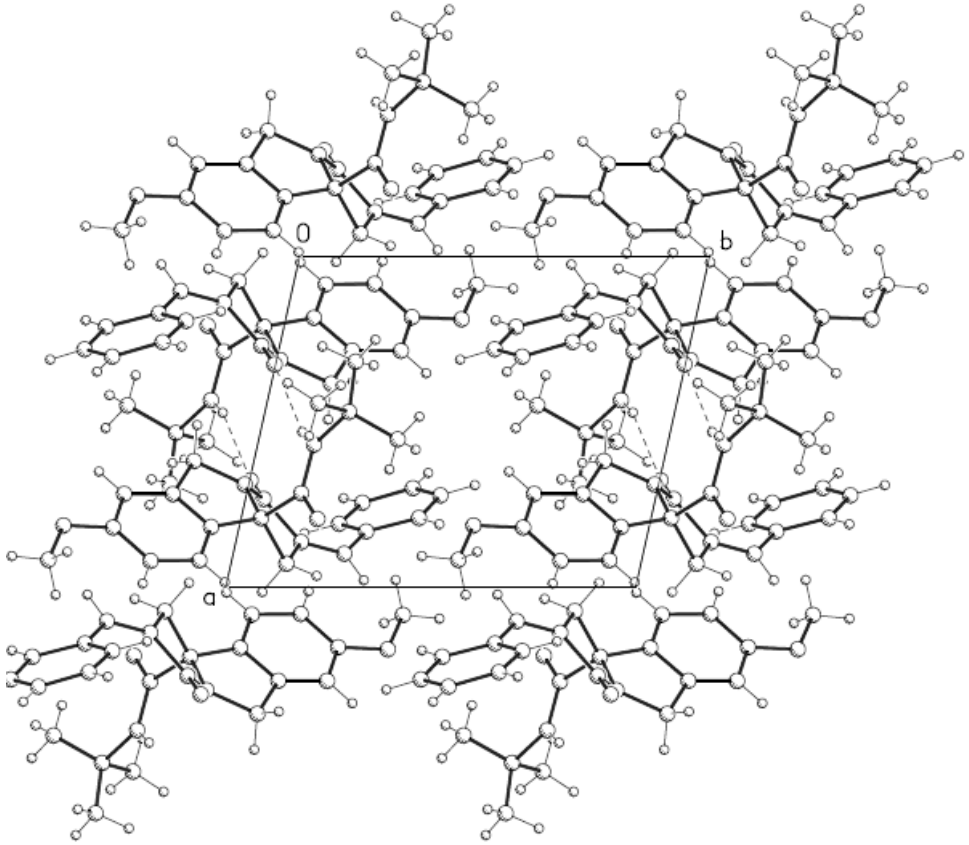


Crystal data and structure refinement for **12c** (CCDC number 1042340)

Empirical formula	$C_{24}H_{26}N_2O_3$	
Formula weight	390.47	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	*P* -1	
Unit cell dimensions	*a* = 8.749(5) Å	α= 104.251(10)°
	b = 10.924(6) Å	β= 92.232(10)°
	c = 11.952(7) Å	γ = 101.630(10)°
Volume	1079.7(11) $Å^3$	
Z	2	
Density (calculated)	1.201 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	416	
Crystal size / colour / shape	0.481 x 0.258 x 0.060 mm / colourless / prism	
Theta range for data collection	2.387 to 26.018°	
Index ranges	$-10 \le h \le 10$, $-13 \le k \le 13$, $-14 \le l \le 14$	
Reflections collected	7776	
Independent reflections	4228 [*R*(int) = 0.0716]	
Completeness to theta = 25.242°	99.4 %	
Measurement device	Bruker Smart Apex CCD diffractometer 01-670-01	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9956 and 0.9657	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4228 / 57 / 301	
Goodness-of-fit on F^2	1.015	
Final *R* indices [*I*>2sigma(*I*)]	*R*1 = 0.0843, *wR*2 = 0.2167	
R indices (all data)	*R*1 = 0.1515, *wR*2 = 0.2647	
Largest diff. peak and hole	0.361 and -0.235 $e.Å^{-3}$	
Remarks	**Main residue disorder 10%**	

Ellipsoid contour plot of compound**12c** (probability level 50 %)





Crystal data and structure refinement for **12q** (CCDC number 1042341)

Empirical formula	$C_{27}\ H_{31}\ Cl\ N_2\ O_5$	
Formula weight	498.99	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\ 2_1/n$	
Unit cell dimensions	a = 8.4979(6) Å	α= 90°
	b = 12.5318(9) Å	β= 99.218(2)°
	c = 24.3558(17) Å	γ = 90°
Volume	2560.2(3) Å^3	
Z	4	
Density (calculated)	1.295 Mg/m^3	
Absorption coefficient	0.189 mm^{-1}	
F(000)	1056	
Crystal size / colour / shape	0.482 x 0.305 x 0.199 mm / colourless / prism	
Theta range for data collection	2.348 to 27.507°	
Index ranges	$-11 \le h \le 11$, $-16 \le k \le 10$, $-24 \le l \le 31$	
Reflections collected	17121	
Independent reflections	5876 [R(int) = 0.0311]	
Completeness to theta = 25.242°	99.9 %	
Measurement device	Bruker Smart Apex CCD diffractometer 01-670-01	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9634 and 0.9085	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5876 / 0 / 324	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2σ(I)]	$R1$ = 0.0534, $wR2$ = 0.1283	
R indices (all data)	$R1$ = 0.0855, $wR2$ = 0.1483	
Largest diff. peak and hole	0.338 and -0.252 e.Å^{-3}	

Ellipsoid contour plot of compound**12q** (probability level 50 %)

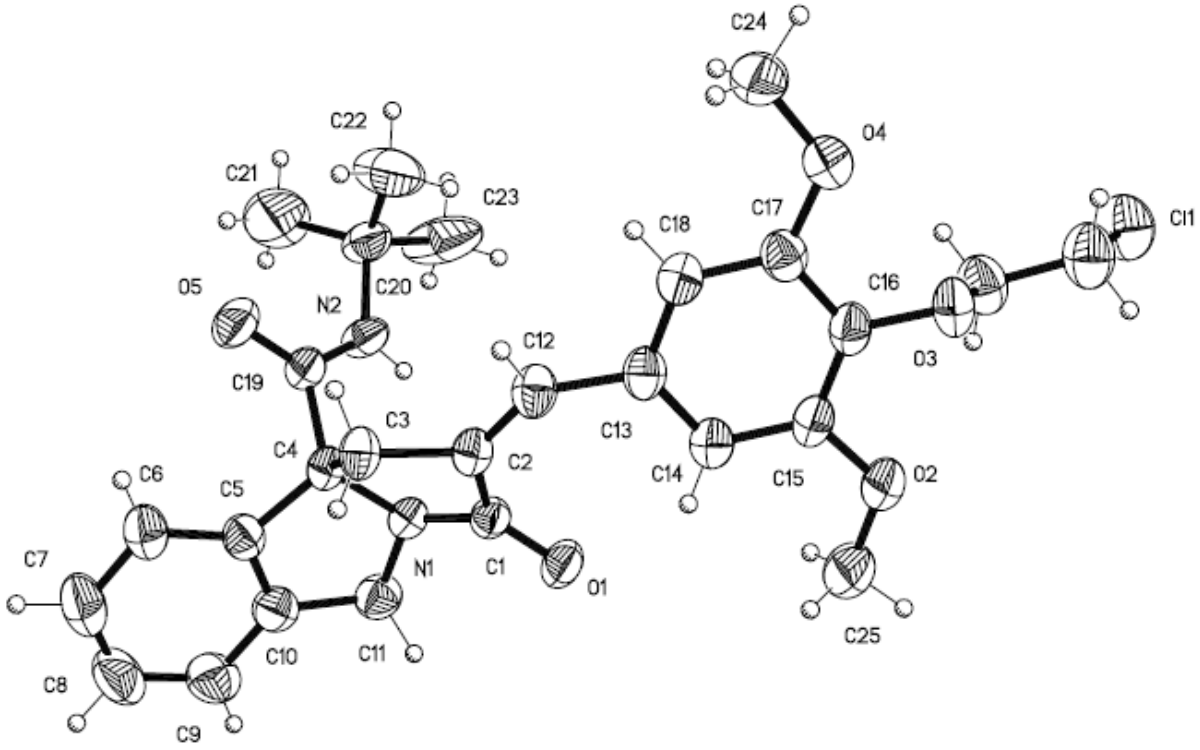


Table S1. DPPH scavenging and lipid peroxidation inhibition of compounds **12a**–**12q**

Compound	% DPPH scavenging				TBARS test	
	100 μM	10 μM	1 μM	IC_{50}	Inhibition at 50 μM (%)	IC_{50} (μM)[a]
12a	-6.44	-5.30	-6.66	ND	17.45	ND
12b	0.87	0.51	-0.77	ND	4.48	ND
12c	1.50	0.57	2.75	ND	21.40	ND
12d	-4.97	-5.19	-7.05	ND	15.96	ND
12e	-1.82	-0.99	-0.99	ND	11.90	ND
12f	-0.11	2.84	-3.17	ND	19.10	ND
12g	-4.75	-3.88	-5.41	ND	18.71	ND
12h	-2.13	-0.42	-1.30	ND	12.25	ND
12i	40.74	3.88	-4.86	ND	74.49	45.48±1.78
12j	48.52	9.67	1.20	ND	95.44	24.60±0.81
12k	34.43	3.69	-0.77	ND	93.44	35.49±2.35
12l	41.34	9.72	-0.31	ND	74.55	ND
12m	40.87	7.85	1.72	ND	78.22	ND
12n	60.40	7.15	-6.06	67.06±7.11	97.15	12.71±0.86
12o	63.55	11.70	2.03	76.45±3.59	96.23	8.26±0.63
12p	66.50	9.80	0.67	65.82±4.88	92.46	31.89±2.46
12q	-5.73	-6.99	-6.50	ND	48.01	ND
Ferulic acid	78.73	14.52	3.06	47.22±2.31	21.79	ND
Sinapinic acid	90.61	23.39	2.65	35.78±1.74	27.52	ND
BHT	-	-	-	74.91±5.76	-	1.22±0.44
α-Tocopherol	-	-	-	31.74±1.06	-	6.78±2.16
Quercetin	--	-	-	10.89±0.47	-	1.496±0.031

As it can be shown in Table S1, the synthesized compounds showed a lower activity than both ferulic and sinapinic acid. The reduction in antioxidant capacity may be attributable to the *E*-configuration in these parent molecules, in contrast with the *Z*-geometry observed in the molecules reported herein. Additionally, there is a deviation in the planarity of the conjugated system due to a distortion of the dihedral angle ϕ O=C-C=C (theoretical = 0°; for 12c and 12 q = -33.55° and 32.89 °, respectively) (see Figure 2). Consequently, a reduction in the number of resonance structures and a decrease in the stability of the phenoxy radical would be expected.

In the TBARS test, compounds lacking a hydroxyl group (**12a**–**h**) had a minimal effect on lipid peroxidation; Surprisingly however, the *O*-chloroethyl compound **12q** had a significant protecting effect (48% of inhibition), which indicated that other mechanisms, such as direct iron reduction, chelation, or a sequential proton loss electron-transfer (SPLET) would be implied in the antioxidant mechanism. This idea was supported since the activity of ferulic and sinapinic acids was lower than 30 % of inhibition at same dose.

Figure S1. Dose-response curves of DPPH scavenging for **12n**–**p**, sinapinic acid, and α-tocopherol. The IC_{50} values are reported as mean± standard error (SEM) with $n = 3$.

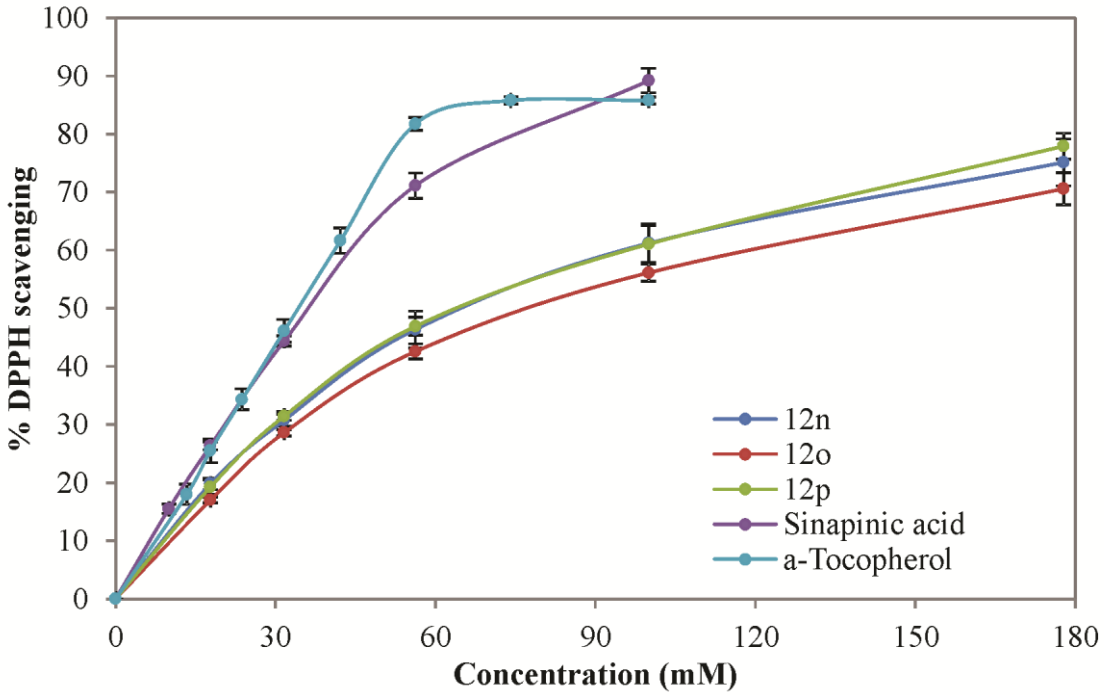


Figure S2. Dose-response curve of TBARS inhibition for the most active compounds. The IC_{50} values are reported as mean± standard error (SEM) with n = 3.