SUPPORTING INFORMATION

Iodine-Promoted Oxidative Cross-Coupling for the Synthesis of (*E*)-2-(3-Oxo-3-Phenylprop-1-en-1-yl)-3-Phenylquinazolin-4(3*H*)-one via C-H Activation: Development of Synthetic TLX Agonists

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1. General Information

All materials were purchased from commercial suppliers and used without further purification. The purities of the final compounds were characterized by high-performance liquid chromatography (LC/MS) using a gradient elution program (Ascentis Express Peptide C18 column, acetonitrile/water 5/95/95/5, 5 min, 0.05% formic acid) and UV detection (254 nM). The purities of final compounds were 95% or greater. NMR spectra was recorded on a Bruker NMR 400 MHz Avance III spectrometer operating at 400 MHz for ^{1}H NMR and 100MHz for ^{13}C NMR. Chemical shifts are given in part per million (ppm) relative to tetramethylsilane (TMS), coupling constants *J* are given in Hertz. HRMS analysis was conducted at Old Dominion University COSMIC using using positive-ion mode electrospray ionization (ESI) in an Apollo II ion source, mounted on a high-field Bruker 10 Tesla with SolariX XR Hybrid FTICR FT-ICR mass spectrometer.

2. Experimental Details:

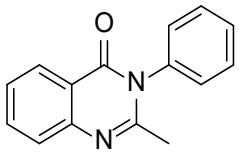
General Procedure for the Synthesis of Starting Meterials (9a-9e):[1]

To a stirred solution of 2-aminobenzoic acid derivative (11.40 mmol) and triphenyl phosphite ($P(OPh)_3$; 3.53 g, 11.40 mmol) in pyridine (15.0 mL), acetic acid (0.41 g, 11.40 mmol) was added dropwise. The resulting mixture was heated to reflux and stirred for 4 hours. Subsequently, the appropriate aniline derivative (11.40 mmol) was added, and the reaction was continued at reflux for an additional 16 hours.

Upon completion, the reaction mixture was cooled to room temperature, diluted with water (5.0 mL), and extracted with ethyl acetate (2 × 100 mL). The combined organic layers were washed with brine, dried over anhydrous sodium sulfate, filtered, and concentrated under reduced pressure.

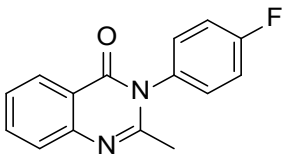
The crude product was purified by flash column chromatography on silica gel (hexane/EtOAc gradient, 100:0 to 4:1) to afford the desired product.

2-Methyl-3-phenylquinazolin-4(3*H*)-one (9a)



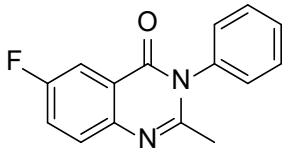
Yield: 1.38 g (80.2%), Colorless solid; m.p. = 148.8-149.5 ºC.; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.28 (dd, J = 7.6, 1.7 Hz, 1H), 7.77 (ddd, J = 8.6, 5.0, 1.5 Hz, 1H), 7.68 (d, J = 8.2 Hz, 1H), 7.61 – 7.42 (m, 4H), 7.27 (dt, J = 8.1, 1.4 Hz, 2H), 2.25 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.25, 154.20, 147.43, 137.72, 134.58, 129.99, 129.28, 127.99, 127.05, 126.74, 126.63, 120.76, 24.39.; LC-MS *m/z* = 237.30 $[M+H]^+$for $C_{15}H_{13}N_2O$. HRMS-ESI: *m/z* calcd for $C_{15}H_{13}N_2O$ $[M + H]^+$: 237.1028, found 237.1021.[2]

3-(4-Fluorophenyl)-2-methylquinazolin-4(3*H*)-one (9b):



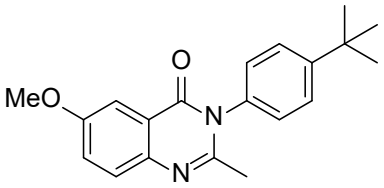
Yield: 1.57 g (84.5%), Colorless solid; m.p. = 140.2-142.8 ºC.; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.27 (dd, J = 7.9, 1.8 Hz, 1H), 7.79 (ddt, J = 8.4, 7.0, 1.3 Hz, 1H), 7.69 (d, J = 8.2 Hz, 1H), 7.49 (td, J = 7.4, 1.3 Hz, 1H), 7.35 – 7.20 (m, 4H), 2.27 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.95, 162.28, 161.47, 154.01, 147.29, 134.73, 133.52 (d, $J_{C,F}$ = 3.0 Hz), 129.84 (d, $J_{C,F}$ = 9.0 Hz), 127.03, 126.78, 120.59, 117.10 (d, $J_{C,F}$ = 23.0 Hz), 24.39.; LC-MS *m/z* = 255.30 $[M+H]^+$for $C_{15}H_{12}FN_2O$. HRMS *m/z* for $C_{15}H_{12}FN_2O$ $[M+H]^+$. Calcd 255.0928, found 255.0928.

6-Fluoro-2-methyl-3-phenylquinazolin-4(3*H*)-one (9c):



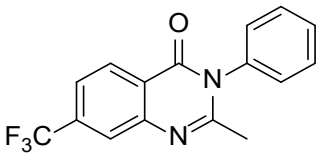
Yield: 1.37g (84.0%), Colorless solid; m.p. = 179.3-180.2 ºC.; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.88 (ddd, J = 8.4, 3.0, 1.6 Hz, 1H), 7.68 (ddd, J = 9.0, 4.8, 1.6 Hz, 1H), 7.61 – 7.43 (m, 4H), 7.29 – 7.21 (m, 2H), 2.23 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.94, 161.54 (d, $J_{C,\,F}$ = 3.0 Hz), 159.47, 153.56, 144.05, 137.45, 130.07, 129.43, 129.12 (d, $J_{C,\,F}$ = 8.0 Hz), 127.88, 123.24, 123.00, 122.01, 121.92, 111.88 (d, $J_{C,\,F}$ = 24.0 Hz), 24.23.; LC-MS *m/z* = 255.30 $[M+H]^+$for $C_{15}H_{12}FN_2O$. HRMS *m/z* for $C_{15}H_{12}FN_2O$ $[M+H]^+$. Calcd 255.0928, found 255.0927.

3-(4-(tert-Butyl)phenyl)-6-methoxy-2-methylquinazolin-4(3*H*)-one (9d):



Yield: 1.0 g (52.0%), Colorless solid; m.p. = 206.8-208.3 ºC.; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 – 7.58 (m, 2H), 7.58 – 7.52 (m, 2H), 7.35 (dd, J = 8.9, 2.9 Hz, 1H), 7.21 – 7.13 (m, 2H), 3.90 (s, 3H), 2.22 (s, 3H), 1.37 (s, 9H).; ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.26, 158.10, 152.22, 152.17, 142.07, 135.09, 128.27, 127.31, 126.90, 124.61, 121.48, 106.43, 55.76, 34.79, 31.30, 24.24.; LC-MS *m/z* = 323.45 $[M+H]^+$for $C_{20}H_{23}N_2O_2$. HRMS *m/z* for $C_{20}H_{23}N_2O_2$ $[M+H]^+$. Calcd 323.1754, found 323.1753.

2-Methyl-3-phenyl-7-(trifluoromethyl)quinazolin-4(3*H*)-one (9e):



Yield: 1.2 g (81.0%), Colorless solid; m.p. = 180.8-181.4 ºC.; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, J = 8.3 Hz, 1H), 7.95 (s, 1H), 7.64 (d, J = 8.4 Hz, 1H), 7.54 (pd, J = 7.2, 3.9 Hz, 3H), 7.25 (d, J = 7.6 Hz, 2H), 2.25 (s, 3H).; ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.47, 155.79, 147.45, 137.24, 136.22, 135.90, 130.17, 129.59, 128.21, 127.80, 124.76, 124.42 (q, $J_{C,F}$ = 3.0 Hz), 123.10, 122.59 (q, $J_{C,F}$ = 3.0 Hz), 122.04, 24.45.; LC-MS *m/z* = 305.27 $[M+H]^+$for $C_{16}H_{12}F_3N_2O$. HRMS *m/z* for $C_{16}H_{12}F_3N_2O$ $[M+H]^+$. Calcd 305.0896, found 305.0895.

3. ^{1}H and ^{13}C NMR spectra of compounds

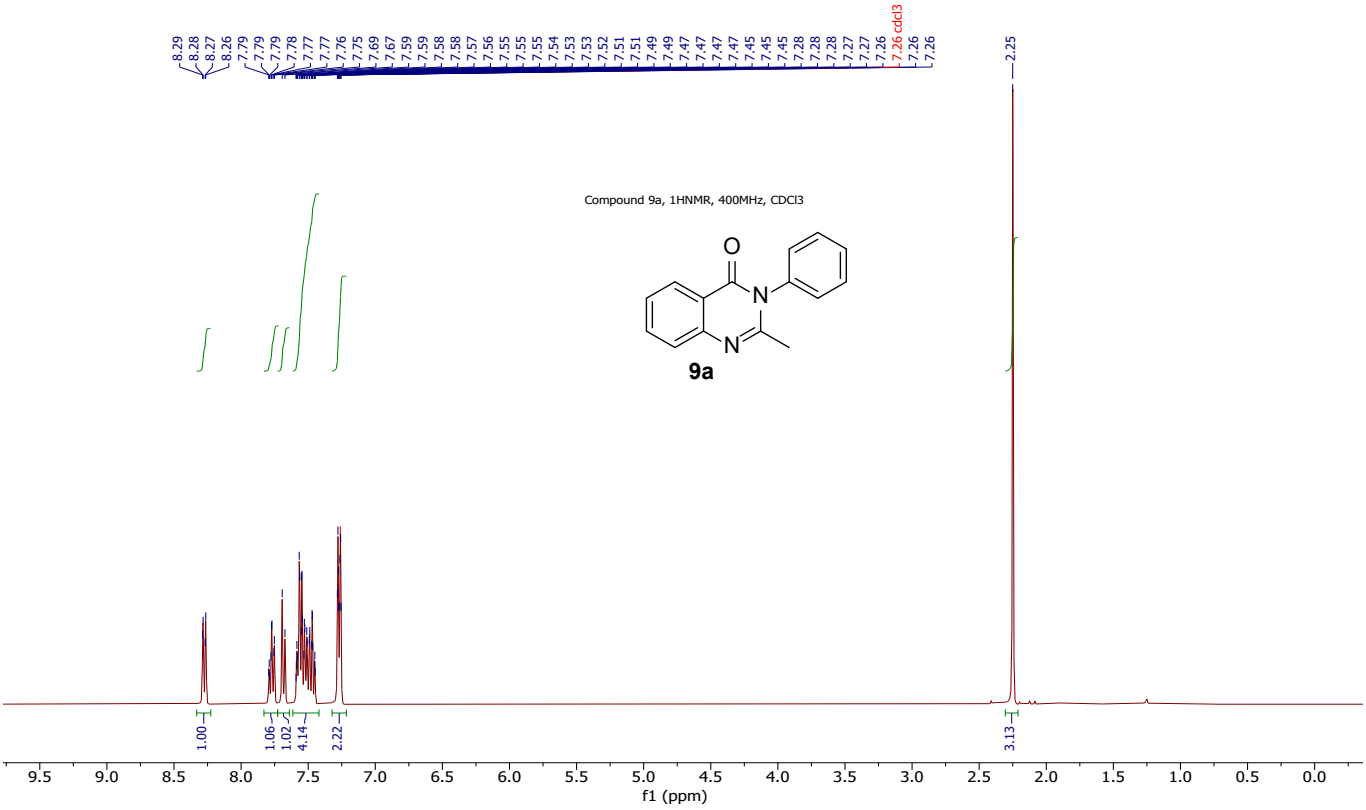


Figure S1. $^{1}HNMR$ spectrum of Compound 9a ($CDCl_3$, 400MHz)

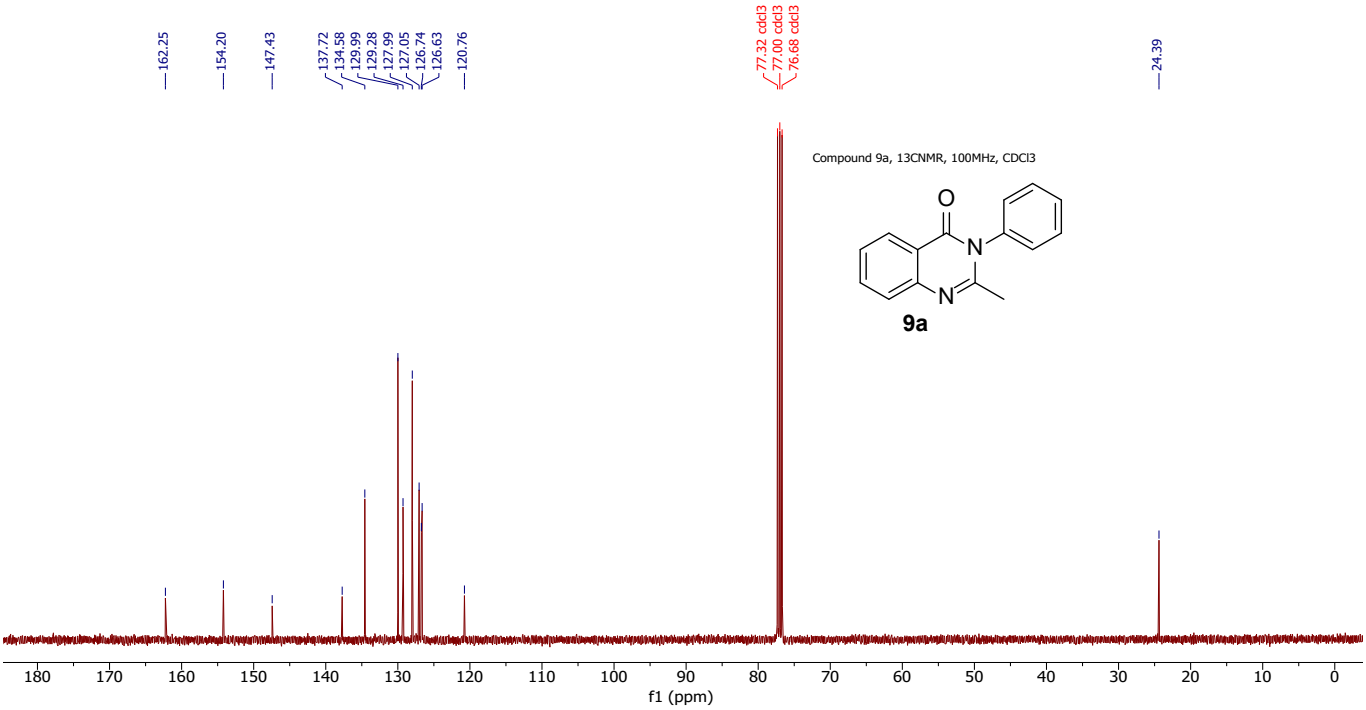


Figure S2. $^{13}CNMR$ spectrum of Compound 9a ($CDCl_3$, 100MHz)

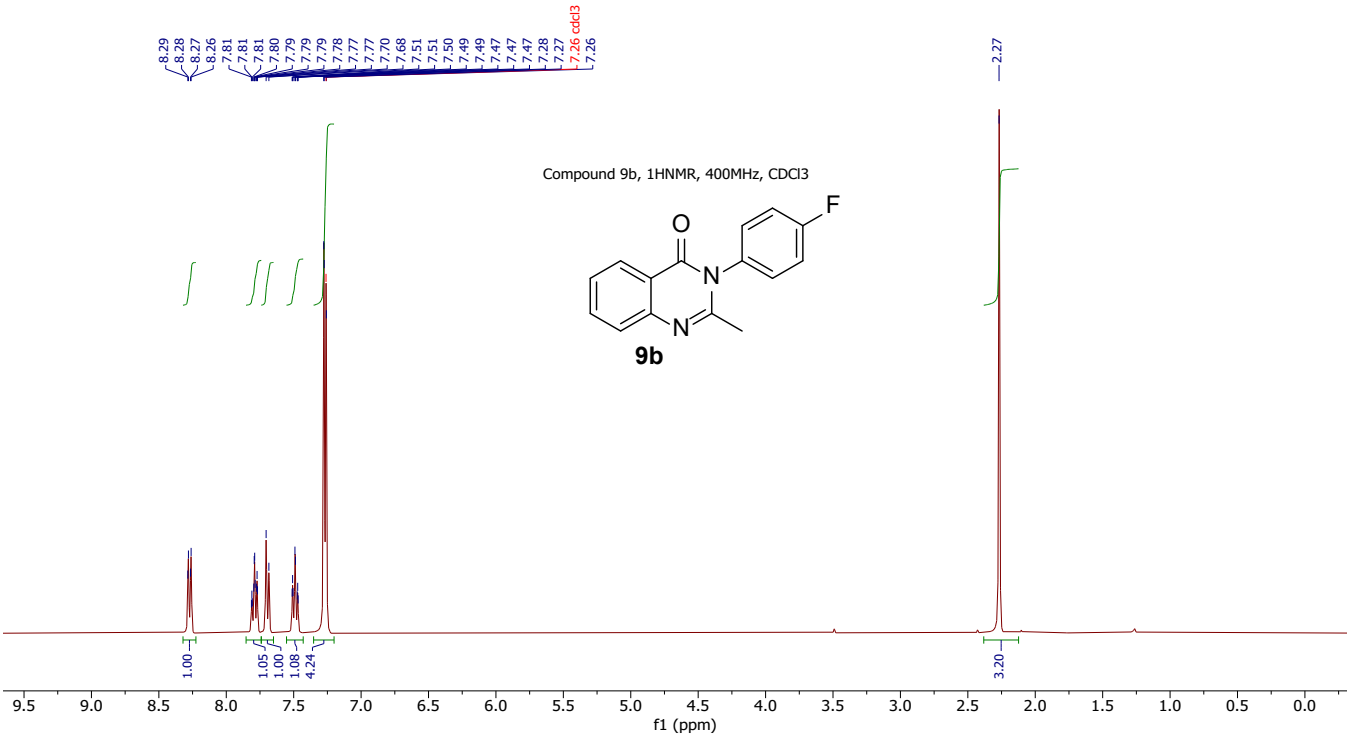


Figure S3. ^{1}HNMR spectrum of Compound 9b ($CDCl_3$, 400MHz) corrected the CDCl3 peak to 7.26

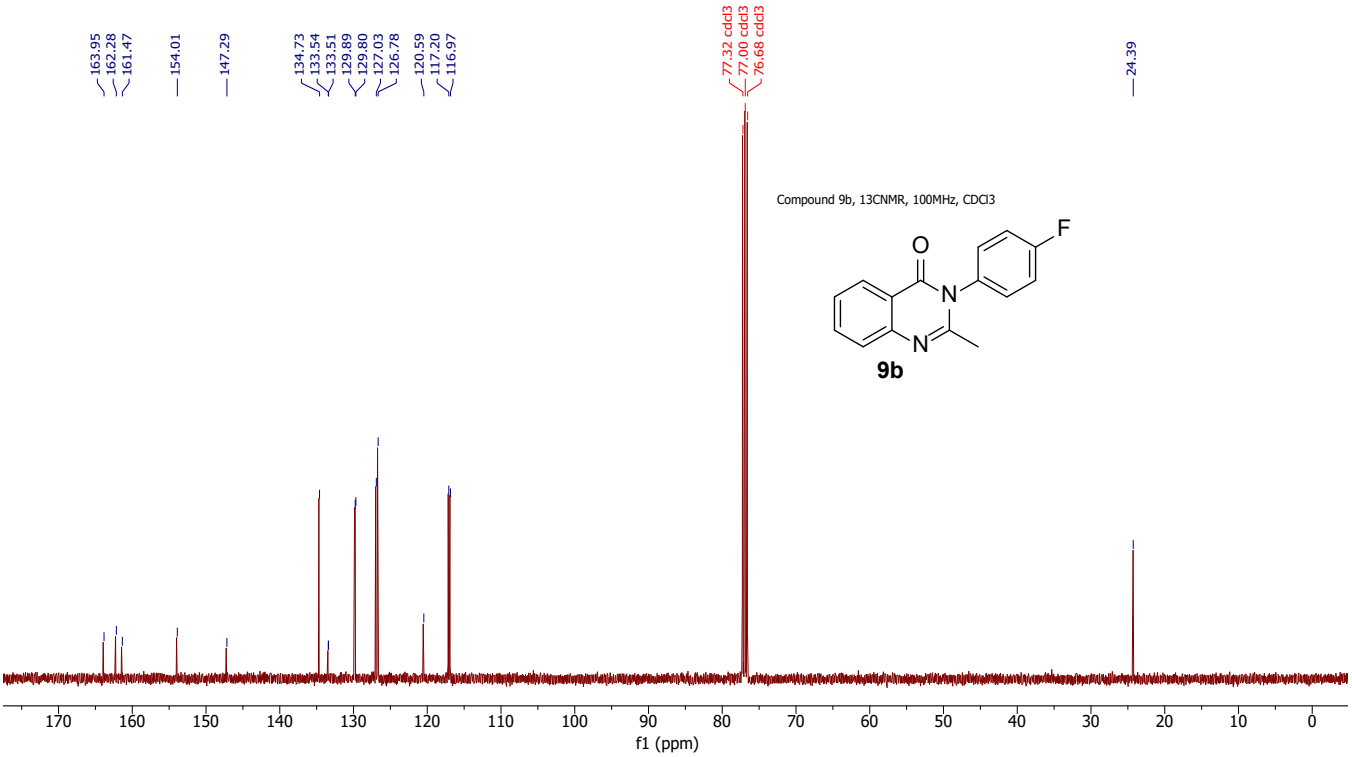


Figure S4. ^{13}CNMR spectrum of Compound 9b ($CDCl_3$, 100MHz)

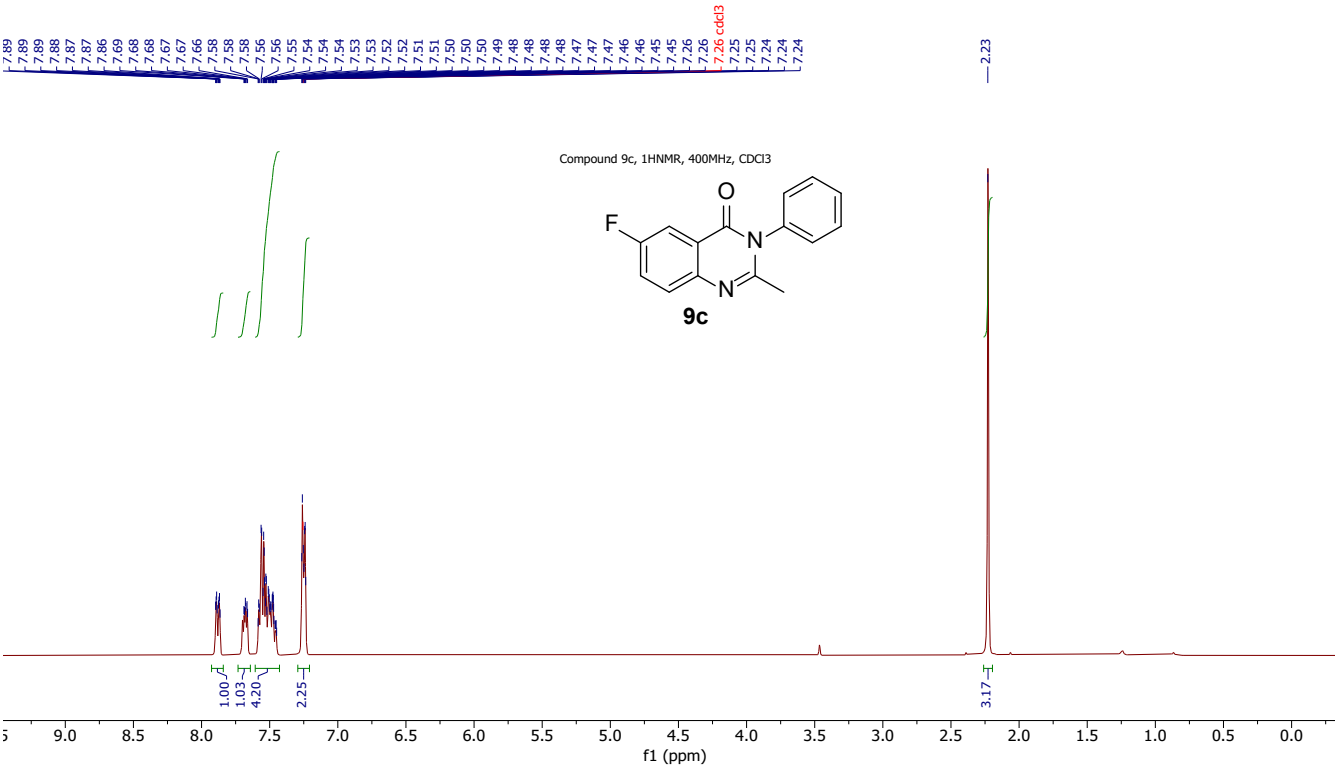


Figure S5. ^{1}HNMR spectrum of Compound 9c ($CDCl_3$, 400MHz)

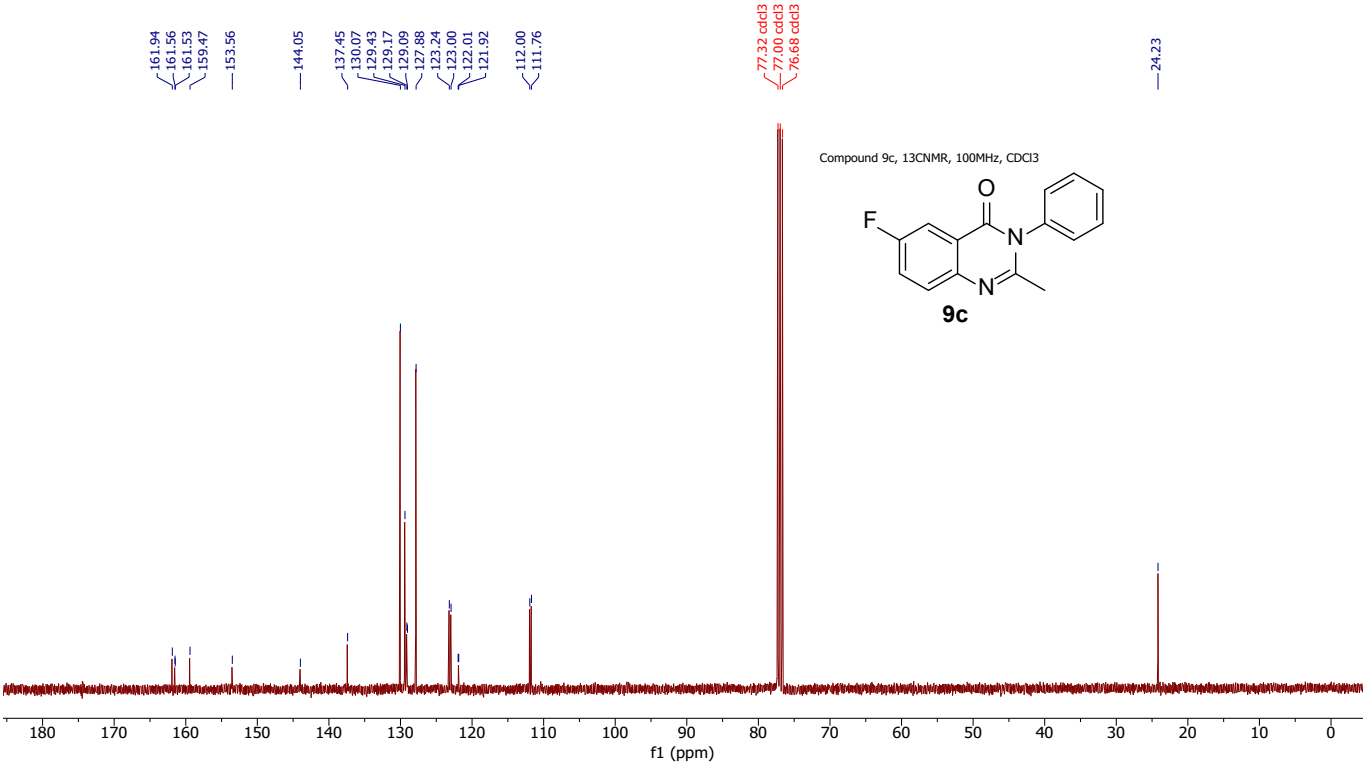


Figure S6. ^{13}CNMR spectrum of Compound 9c ($CDCl_3$, 100MHz)

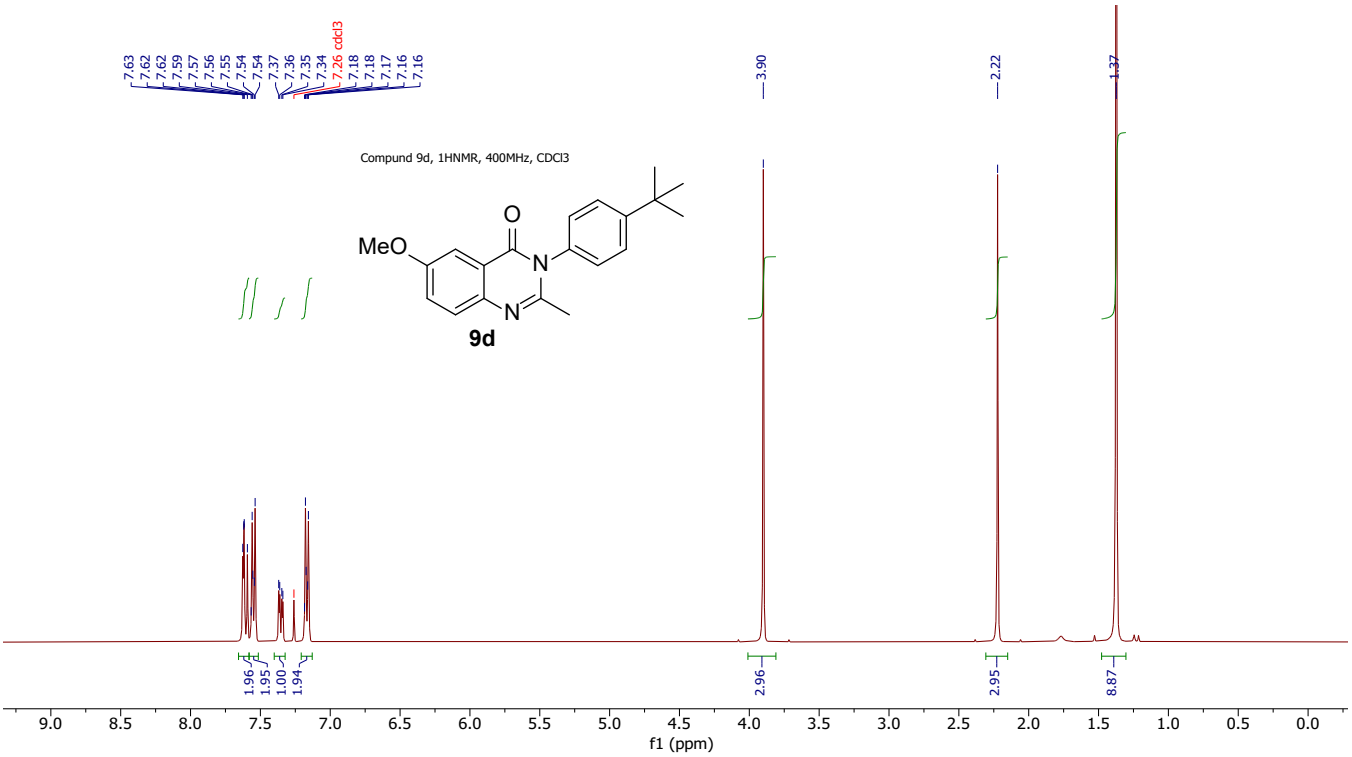


Figure S7. ^{1}HNMR spectrum of Compound 9d ($CDCl_3$, 400MHz)

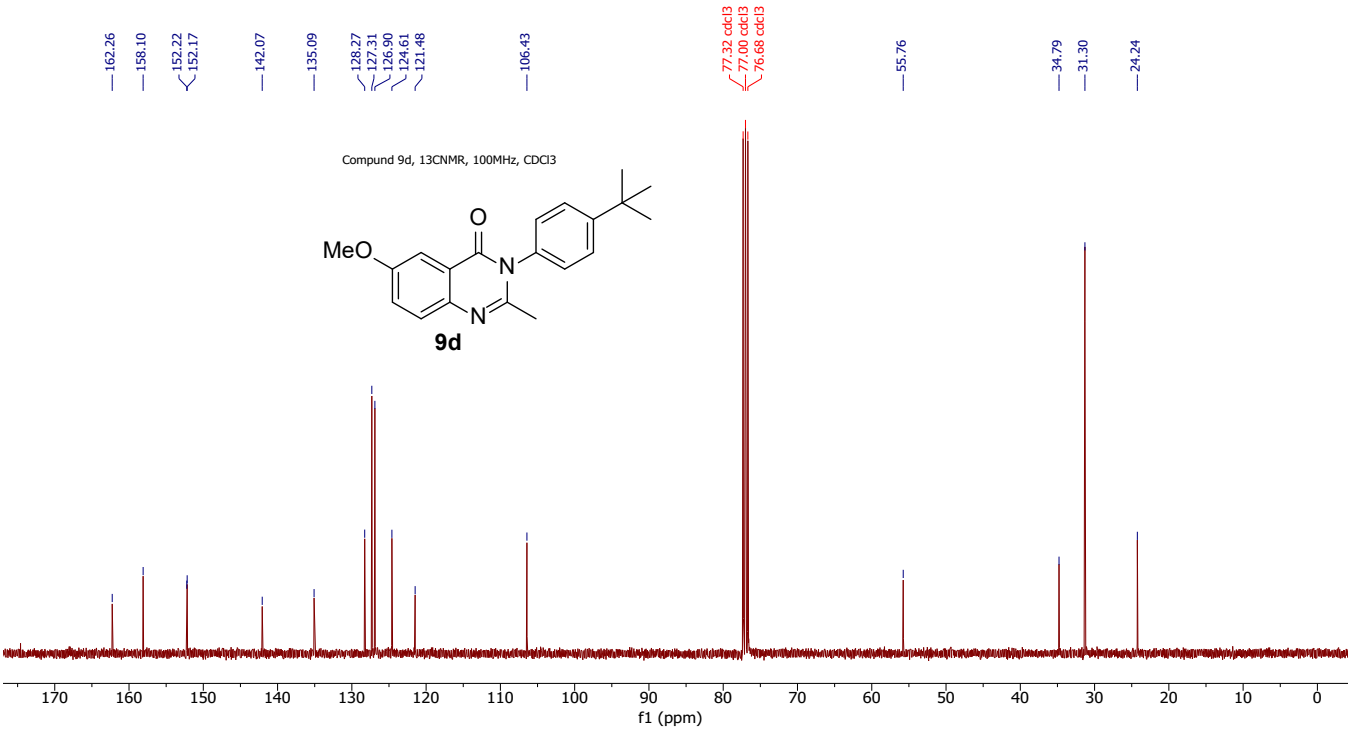


Figure S8. ^{13}CNMR spectrum of Compound 9d ($CDCl_3$, 100MHz)

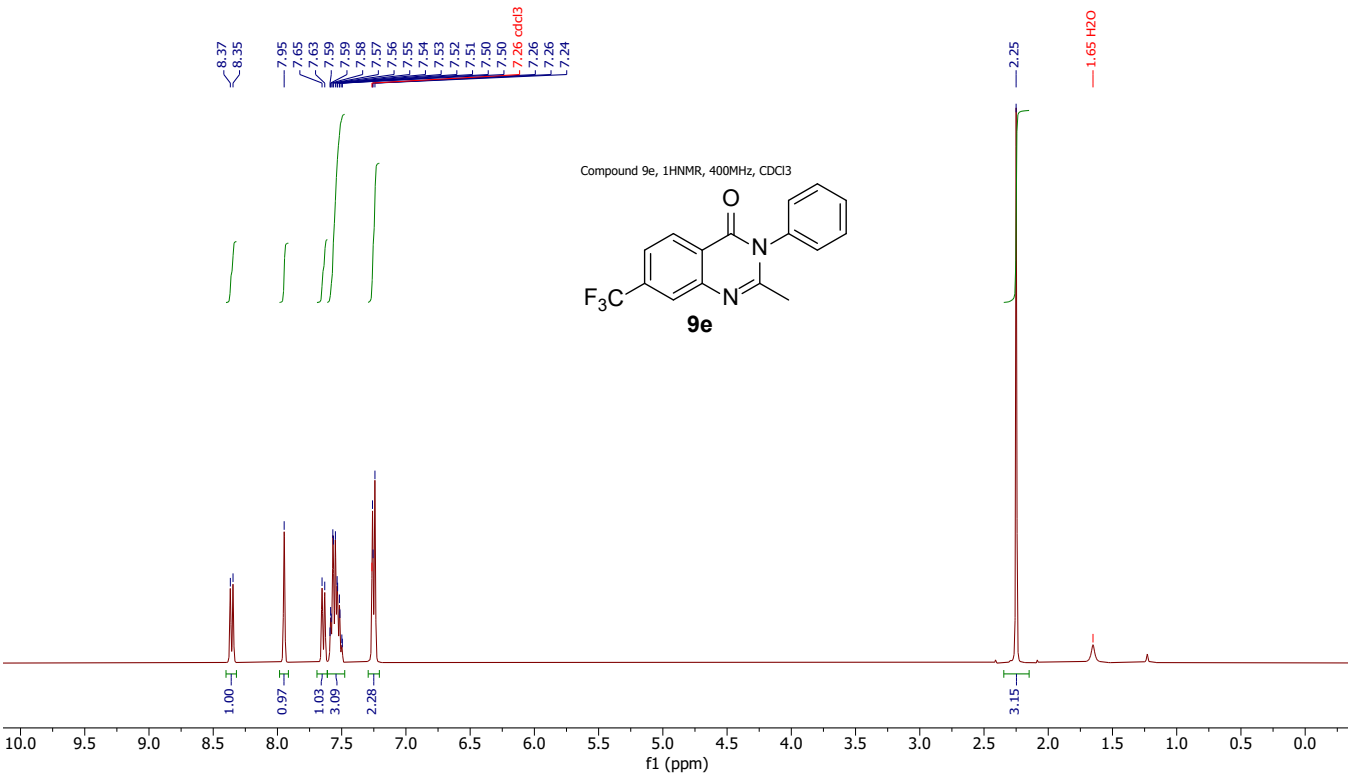


Figure S9. ^{1}HNMR spectrum of Compound 9e ($CDCl_3$, 400MHz)

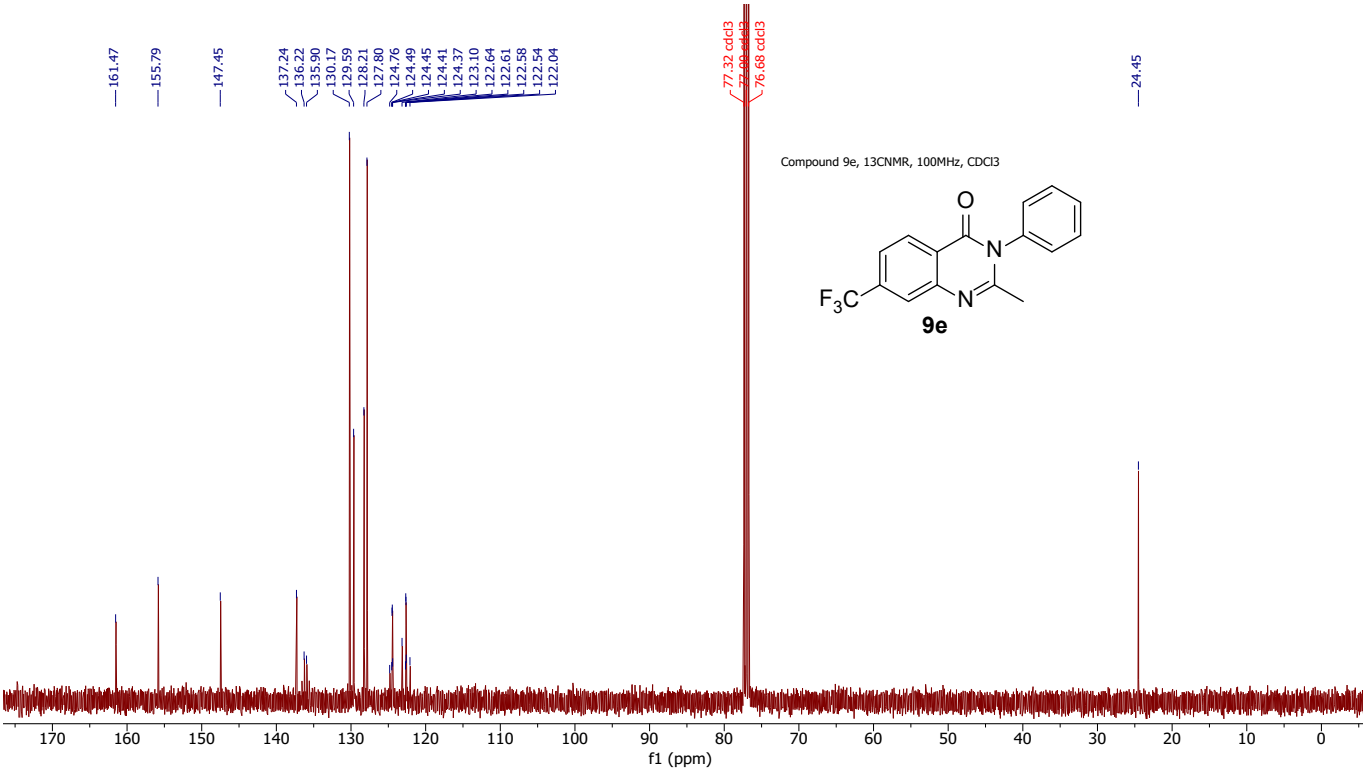


Figure S10. ^{13}CNMR spectrum of Compound 9e ($CDCl_3$, 100MHz)

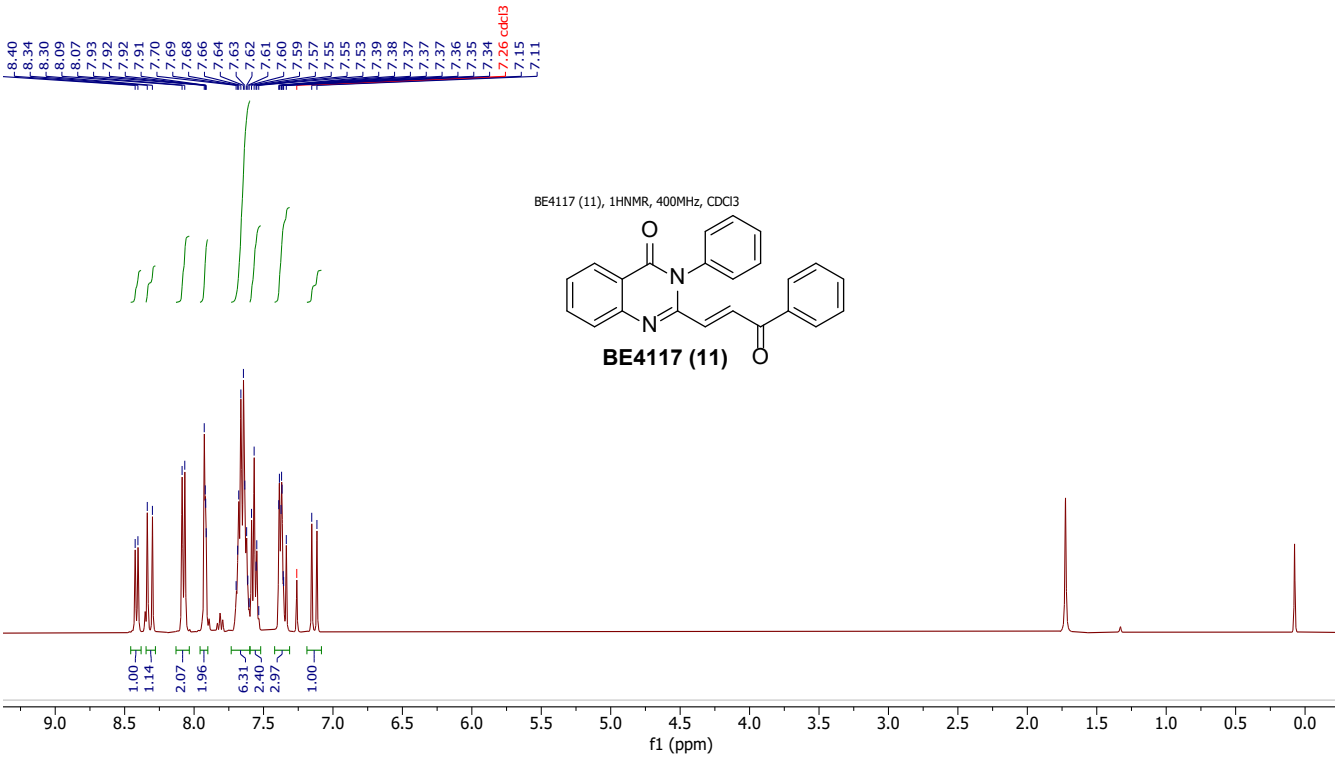


Figure S11. ^{1}HNMR spectrum of BE4117 (11; $CDCl_3$, 400MHz)

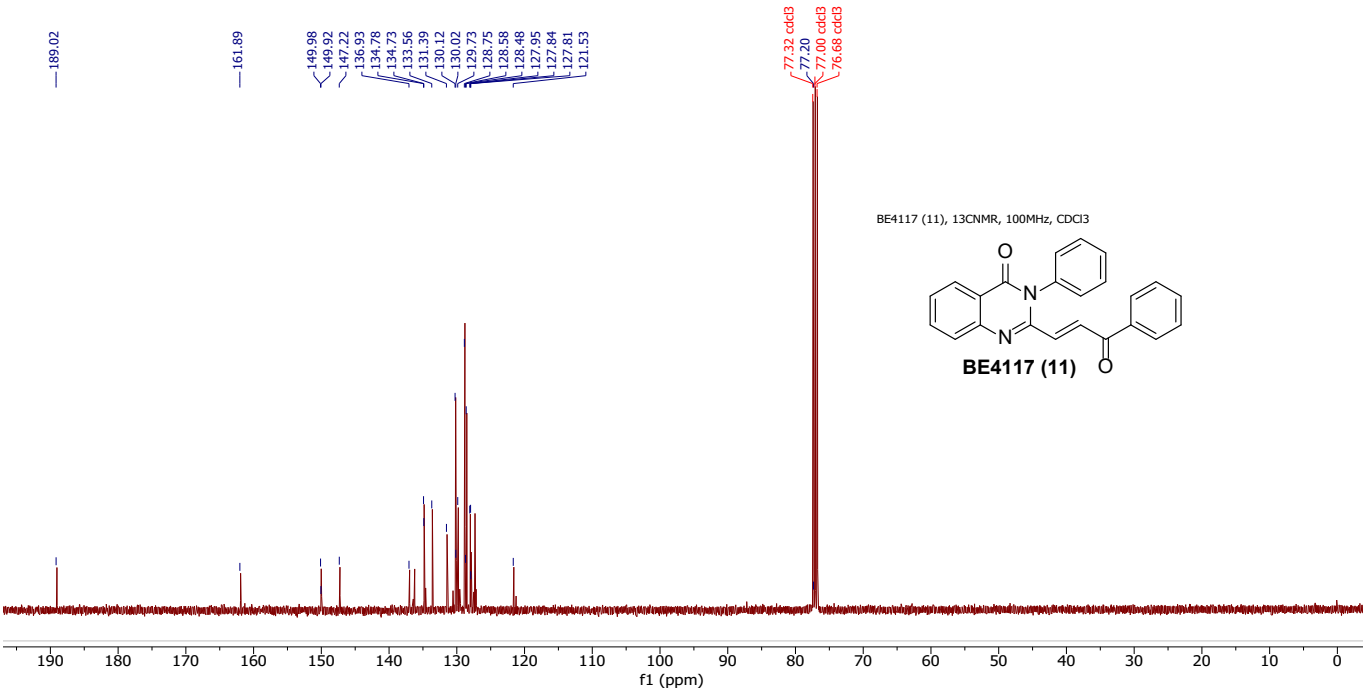


Figure S12. ^{13}CNMR spectrum of 4117 (11, $CDCl_3$, 100MHz)

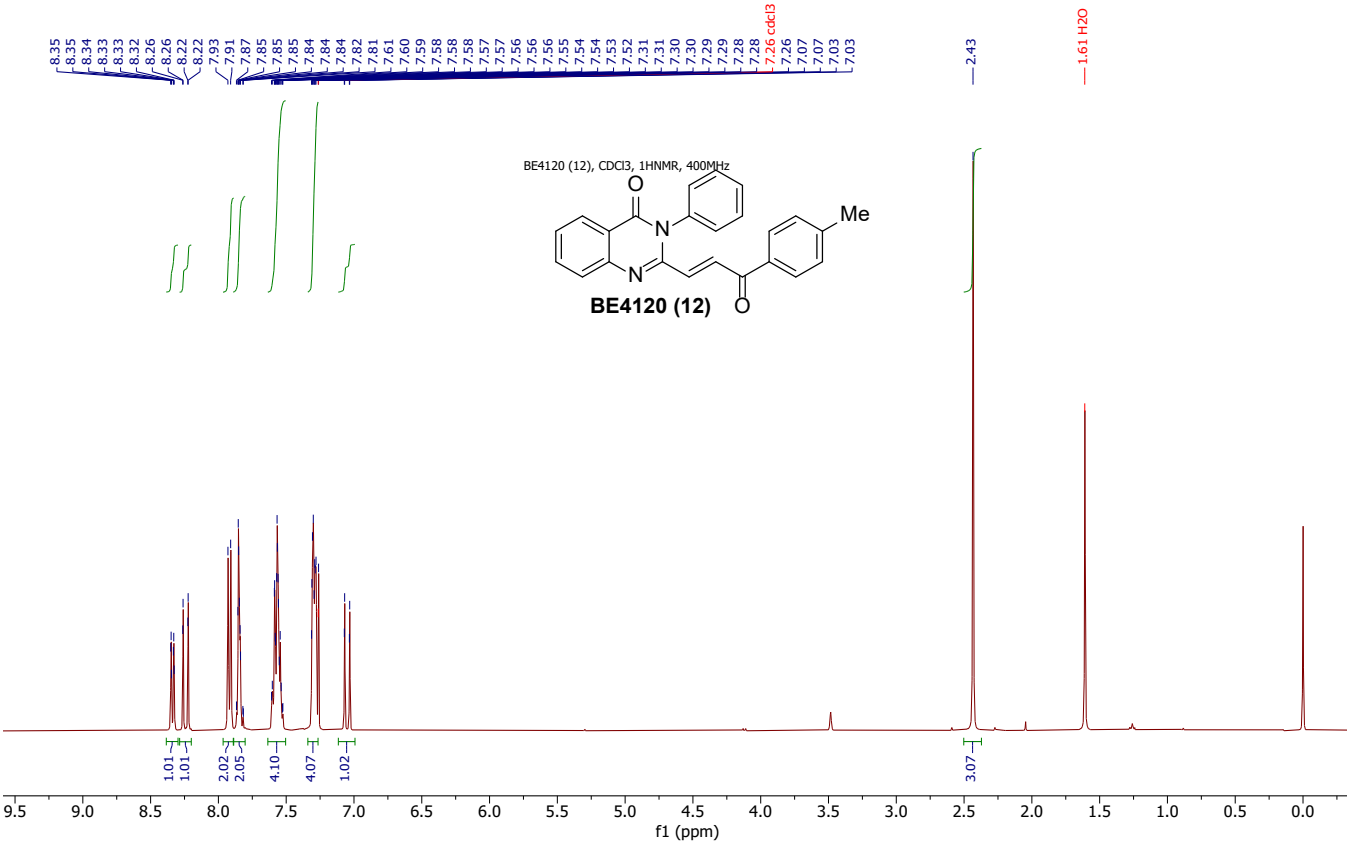


Figure S13. ^{1}HNMR spectra of BE4120 (12; $CDCl_3$, 400MHz)

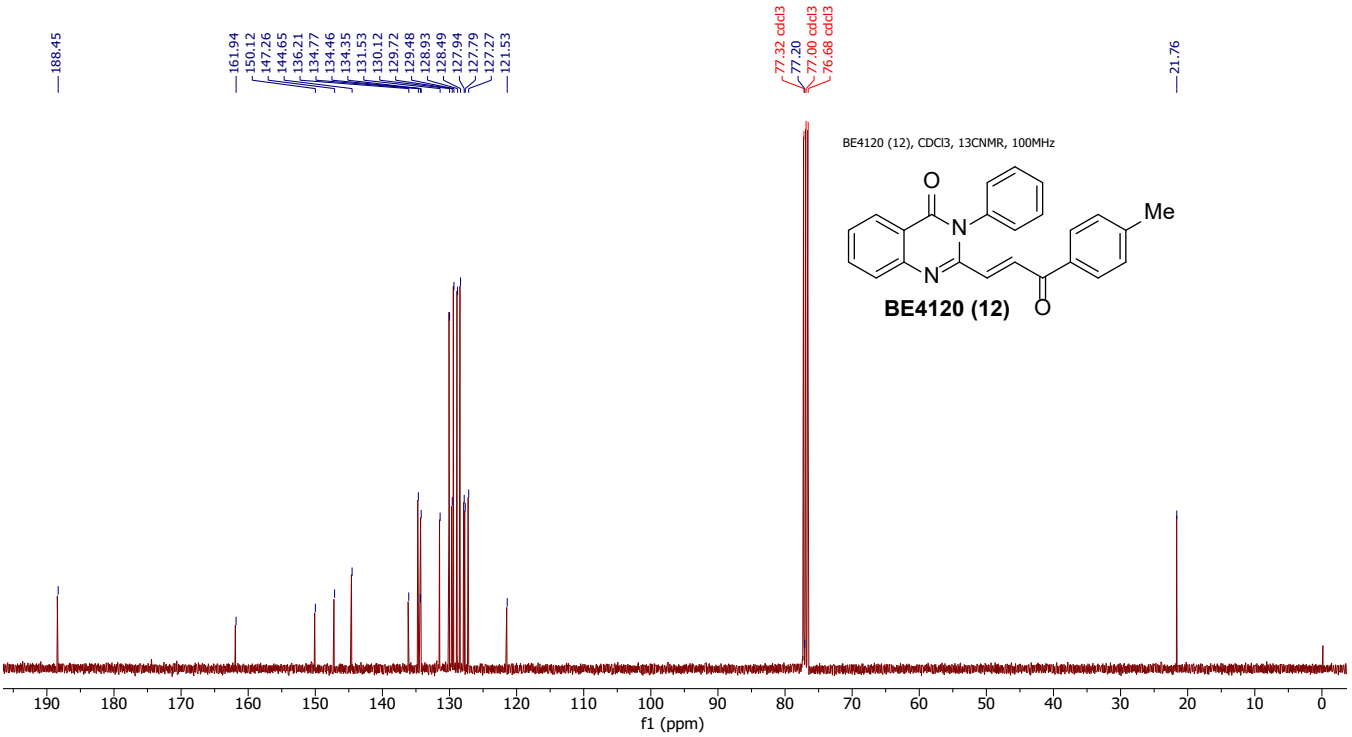


Figure S14. ^{13}CNMR spectra of BE4120 (12; $CDCl_3$, 100MHz)

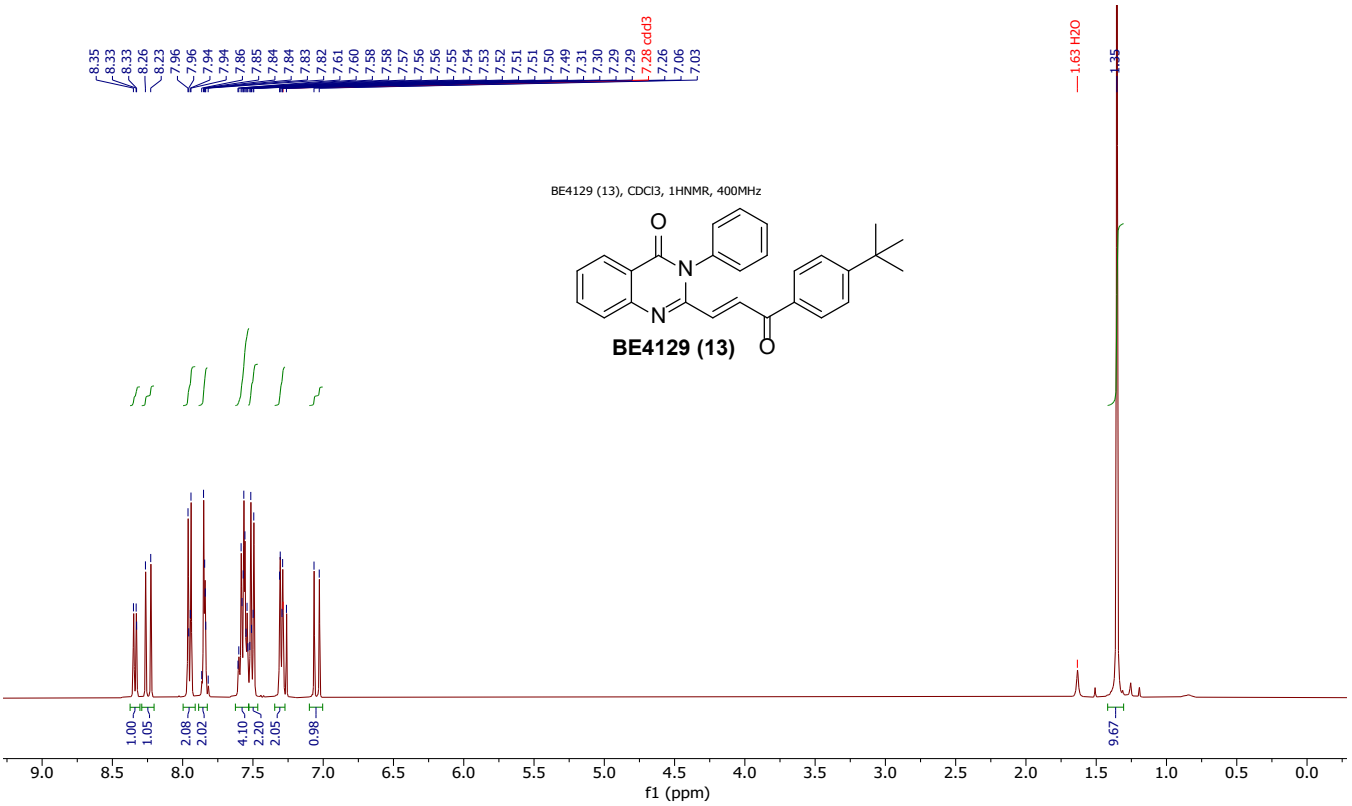


Figure S15. ^{1}HNMR spectra of BE4129 (13; $CDCl_3$, 400MHz)

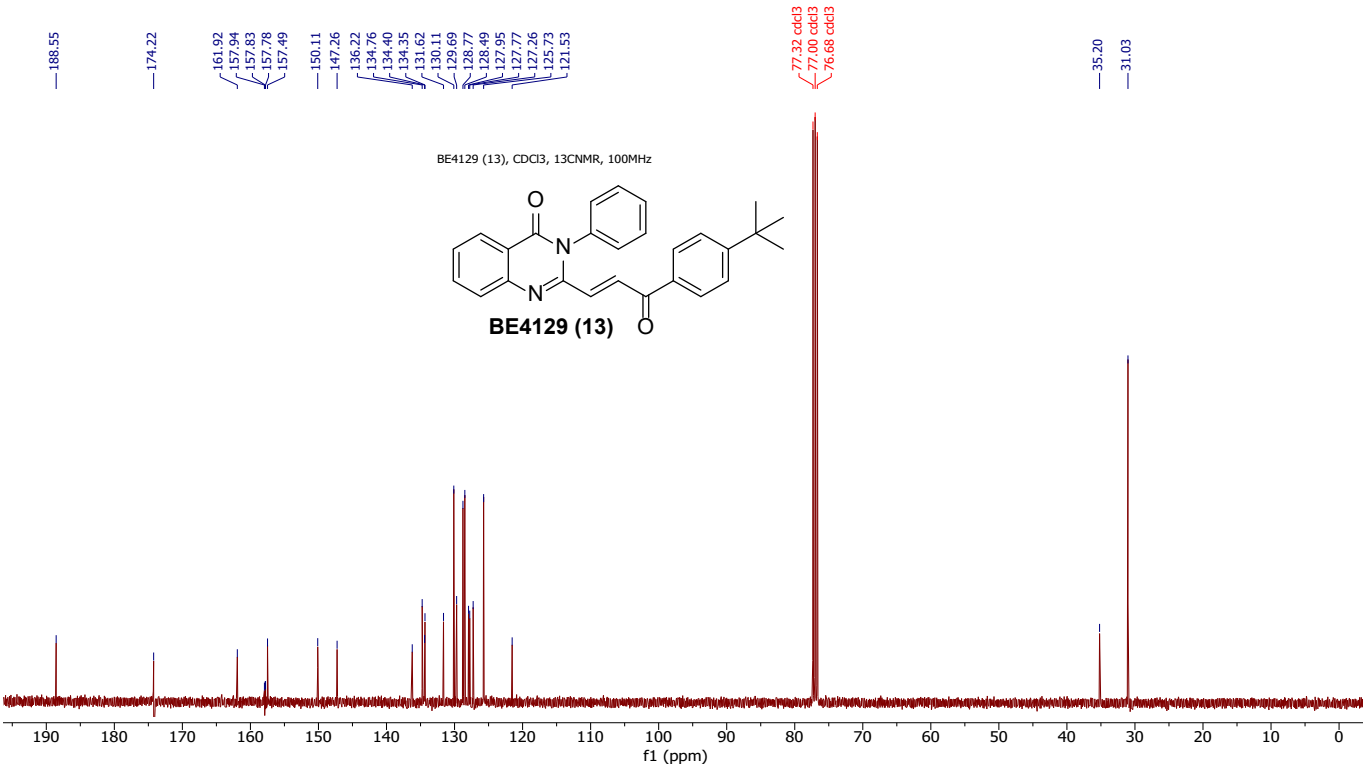


Figure S16. ^{13}CNMR spectra of BE4129 (13; $CDCl_3$, 100MHz)

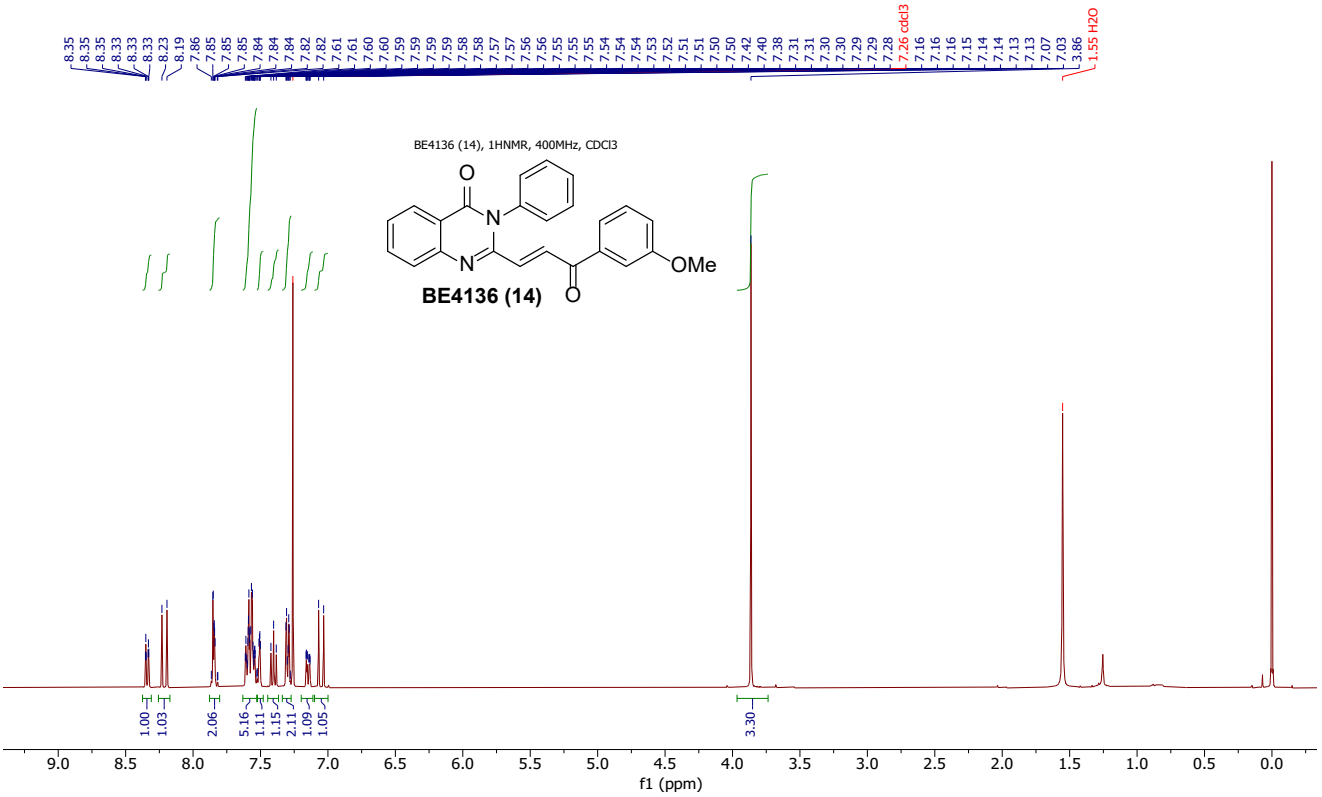


Figure S17. ^{1}HNMR spectra of BE4136 (14, $CDCl_3$, 400MHz)

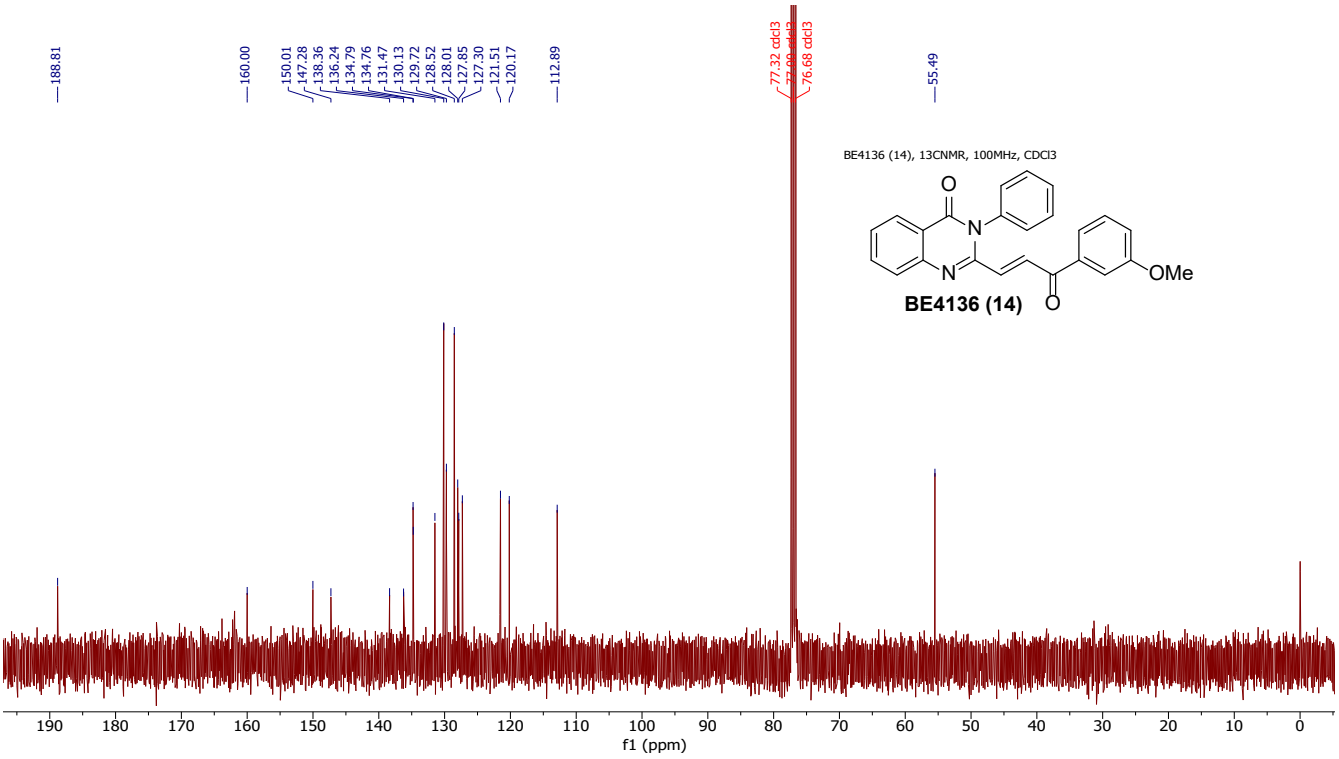


Figure S18. ^{13}CNMR spectra of BE4136 (14, $CDCl_3$, 400MHz)

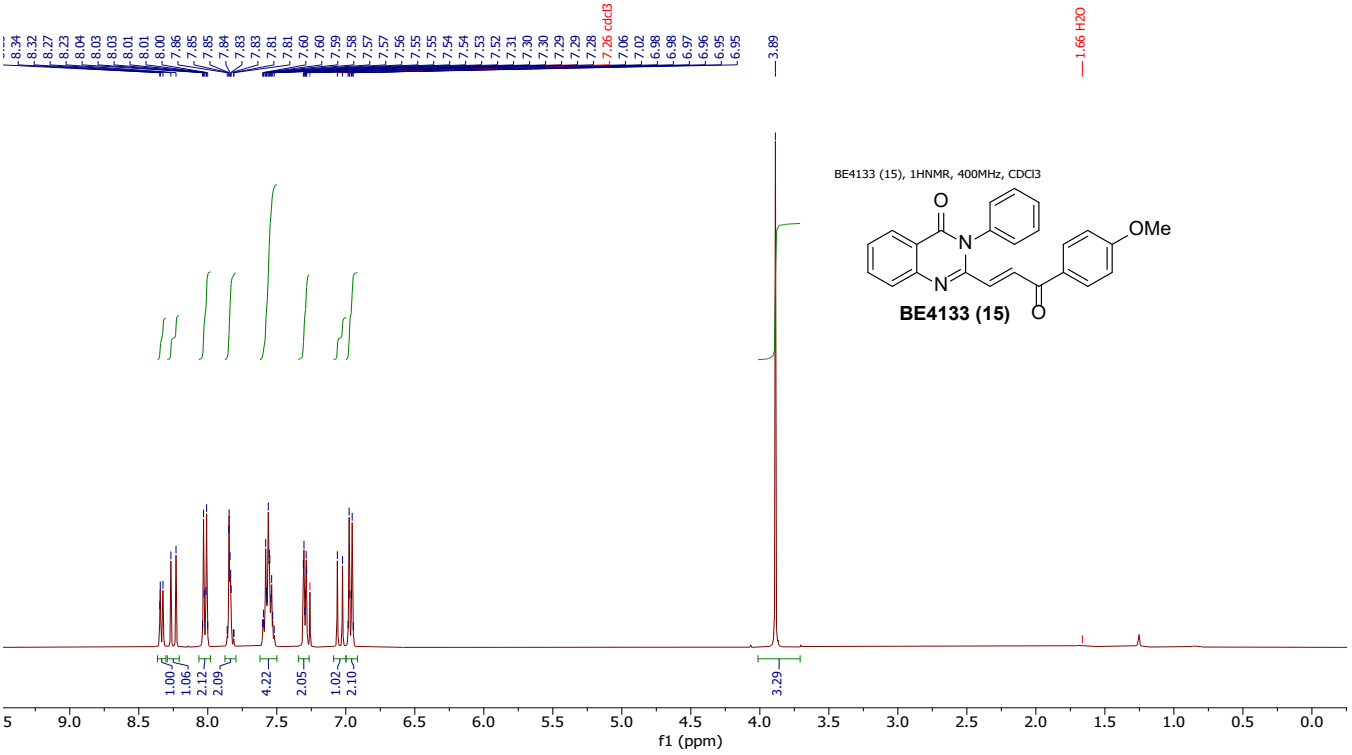


Figure S19. ^{1}HNMR spectra of BE4133 (15; $CDCl_3$, 400MHz)

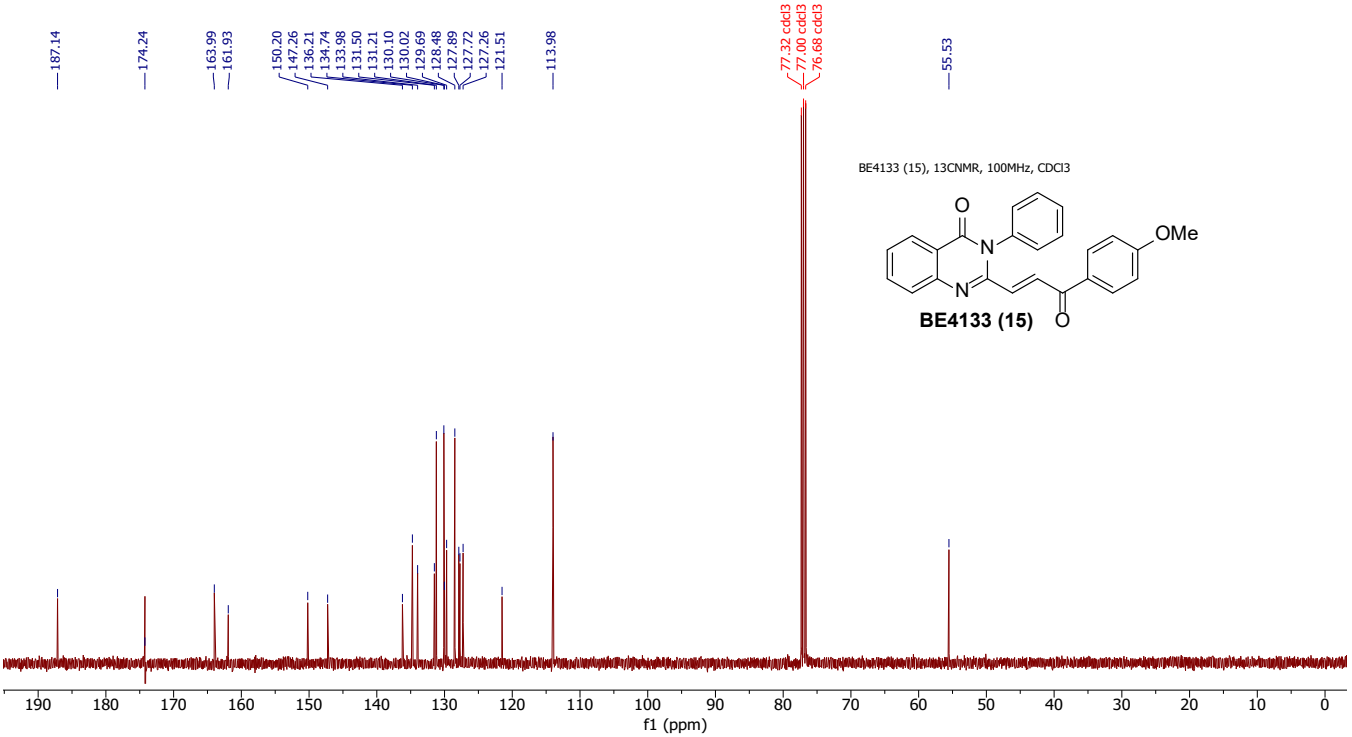


Figure S20. ^{13}CNMR spectra of 4133 (15; $CDCl_3$, 100MHz)

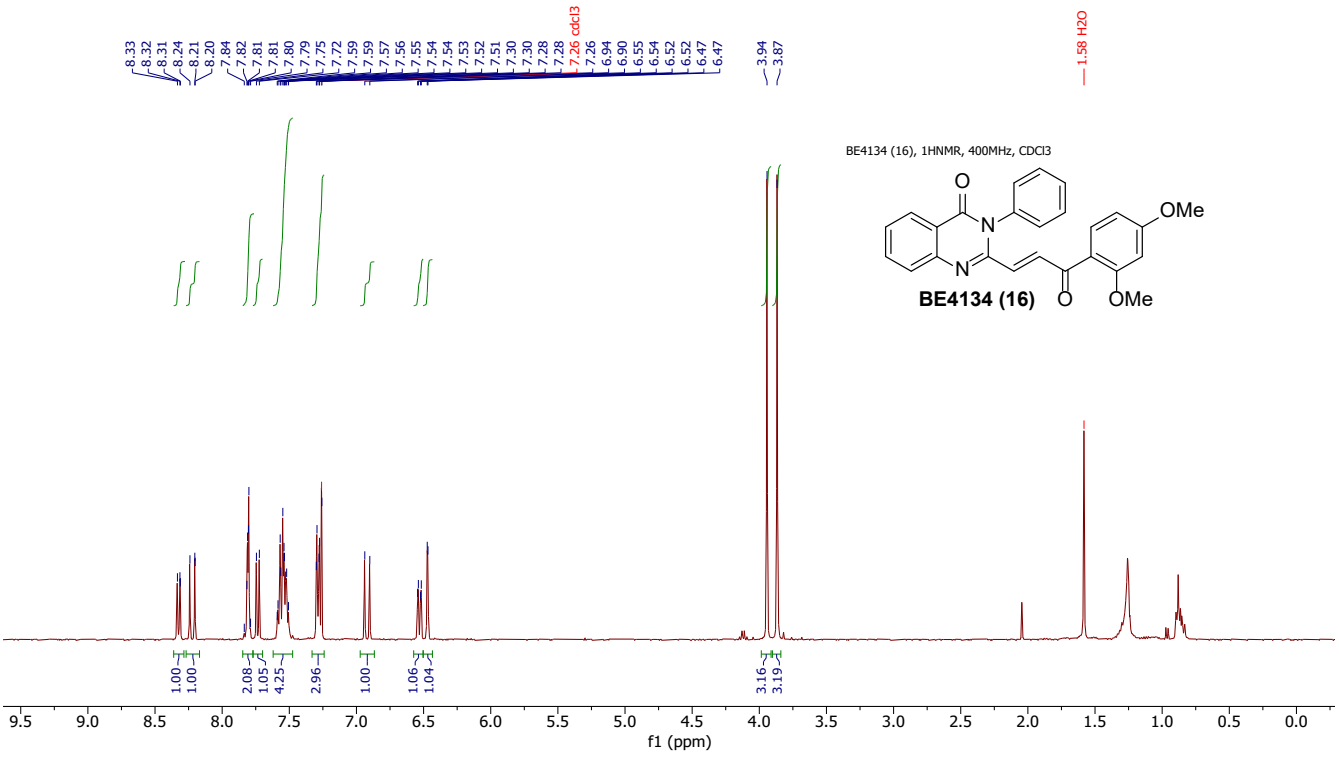


Figure S21. ^{1}HNMR spectra of BE4134 (16; $CDCl_3$, 400MHz)

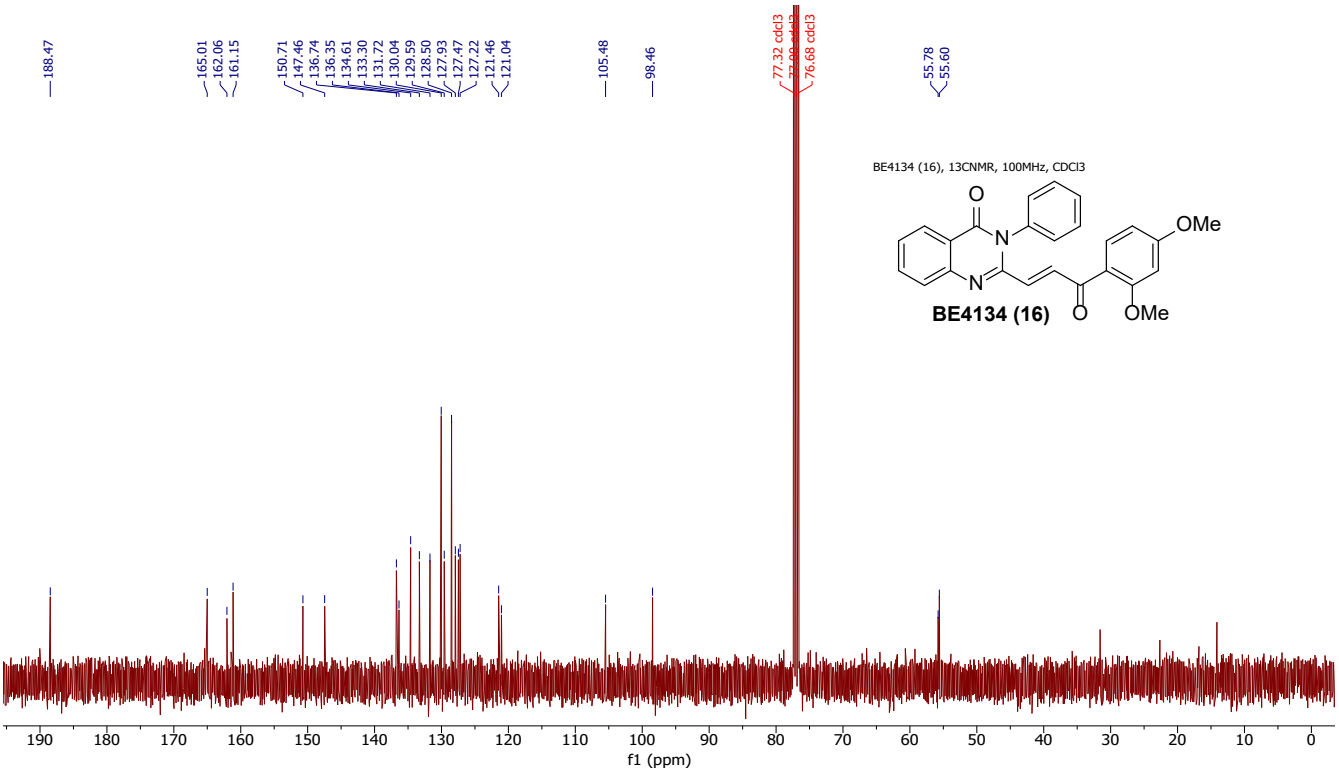


Figure S22. ^{13}CNMR spectra of BE4134 (16; $CDCl_3$, 100MHz)

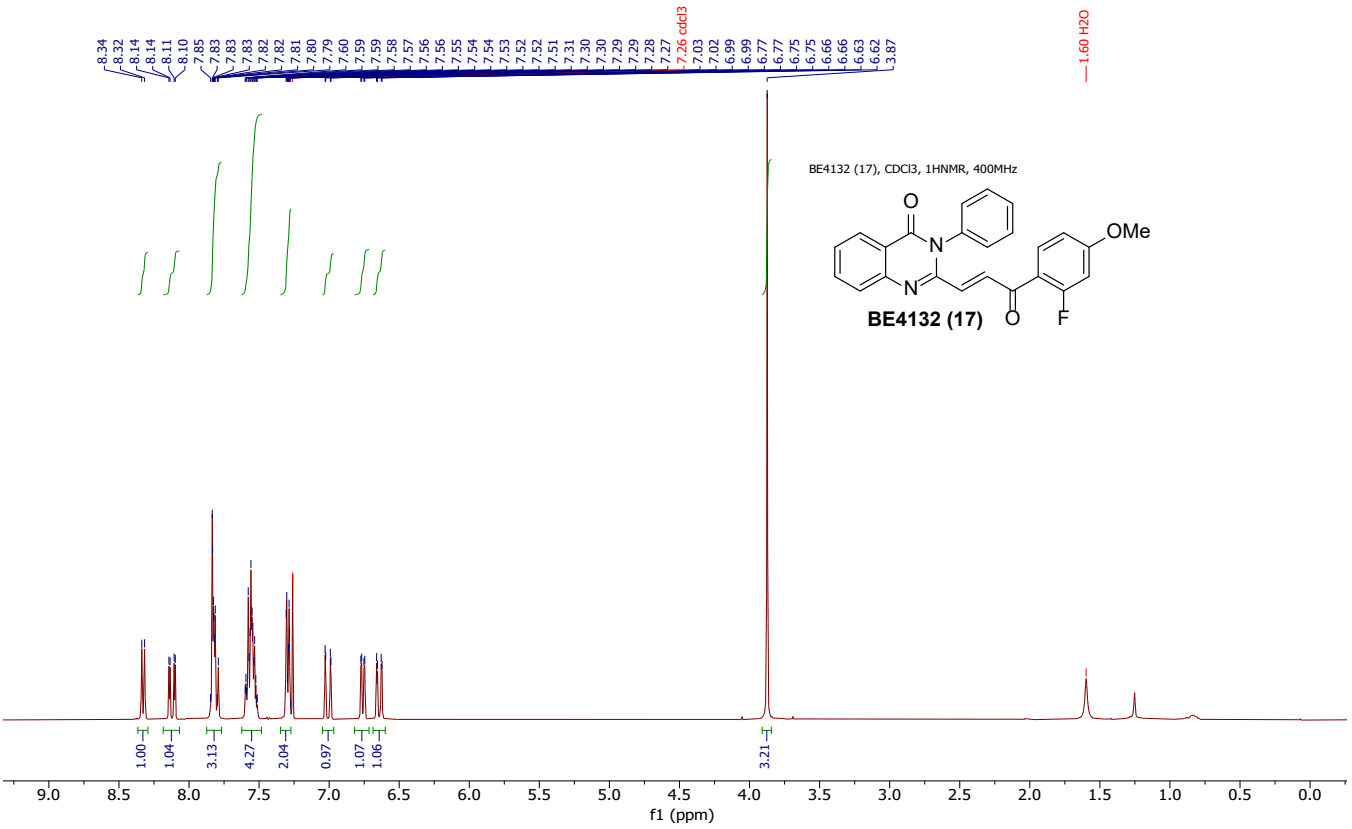


Figure S23. ^{1}HNMR spectra of BE4132 (17; $CDCl_3$, 400MHz)

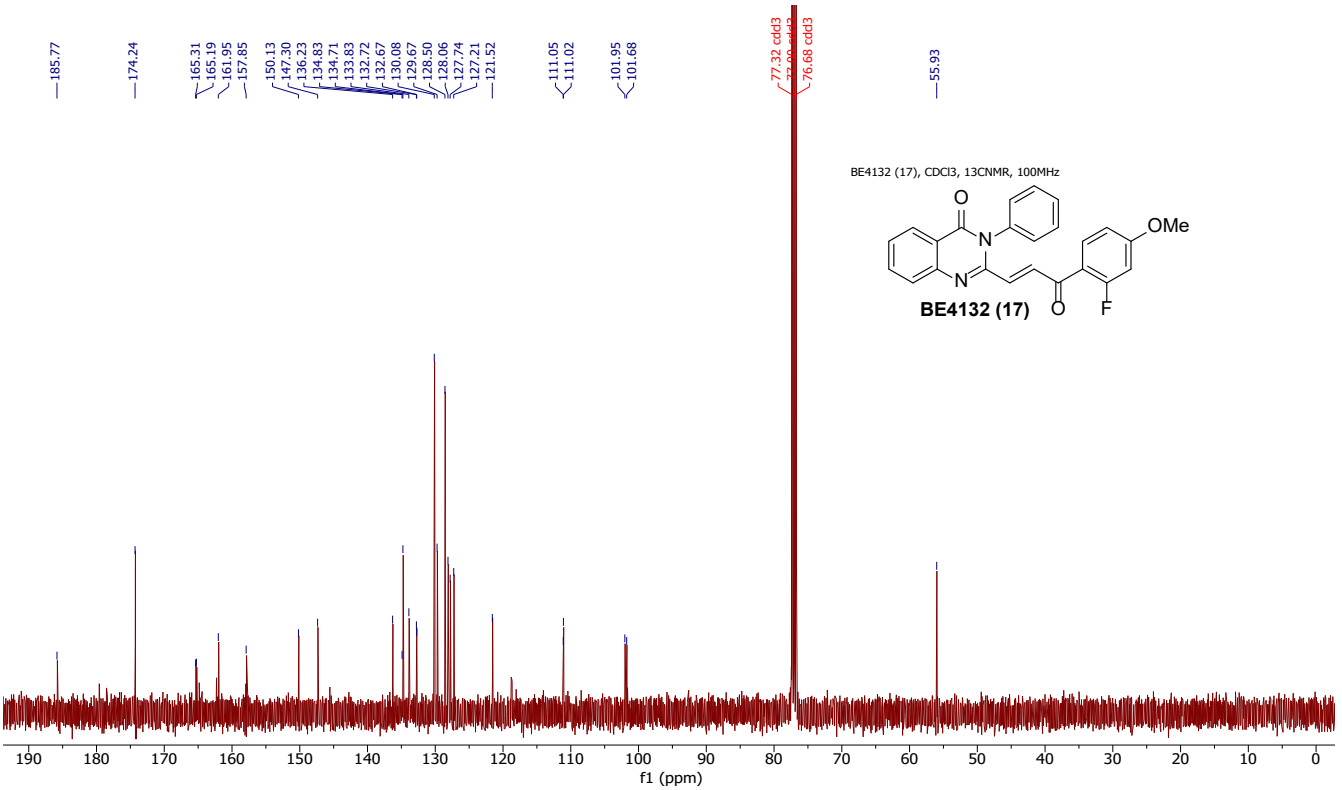


Figure S24. ^{13}CNMR spectra of BE4132 (17; $CDCl_3$, 100MHz)

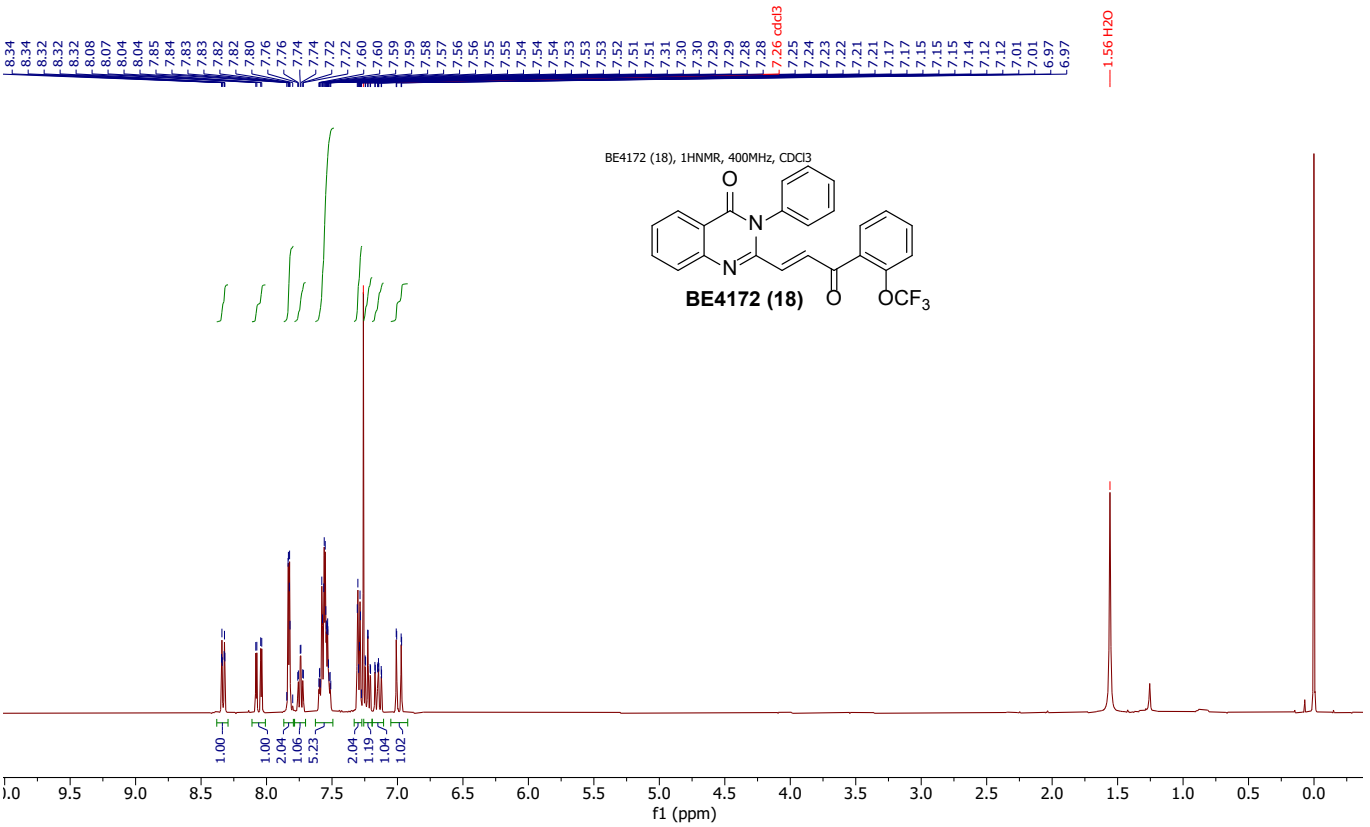


Figure S25. ^{1}HNMR spectra of BE4172 (18; $CDCl_3$, 400MHz)

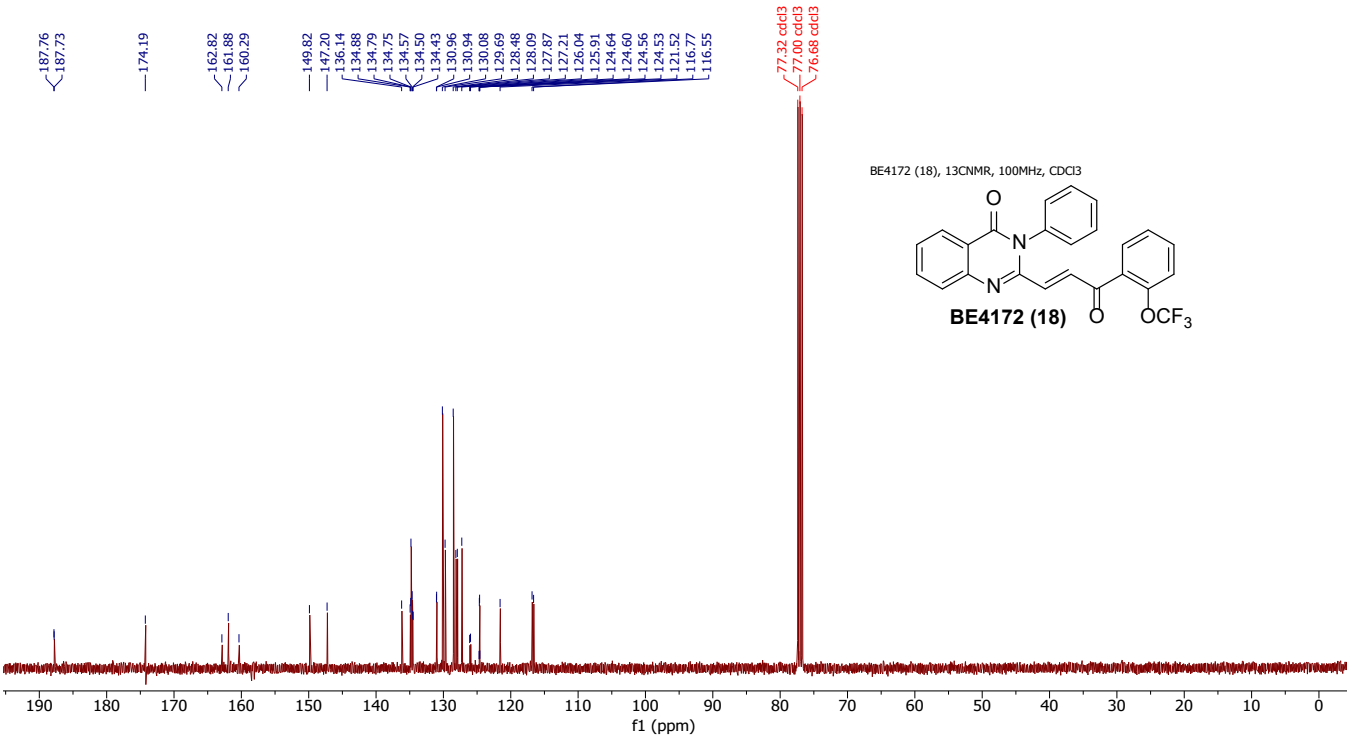


Figure S26. ^{13}CNMR spectra of BE4172 (18; $CDCl_3$, 100MHz)

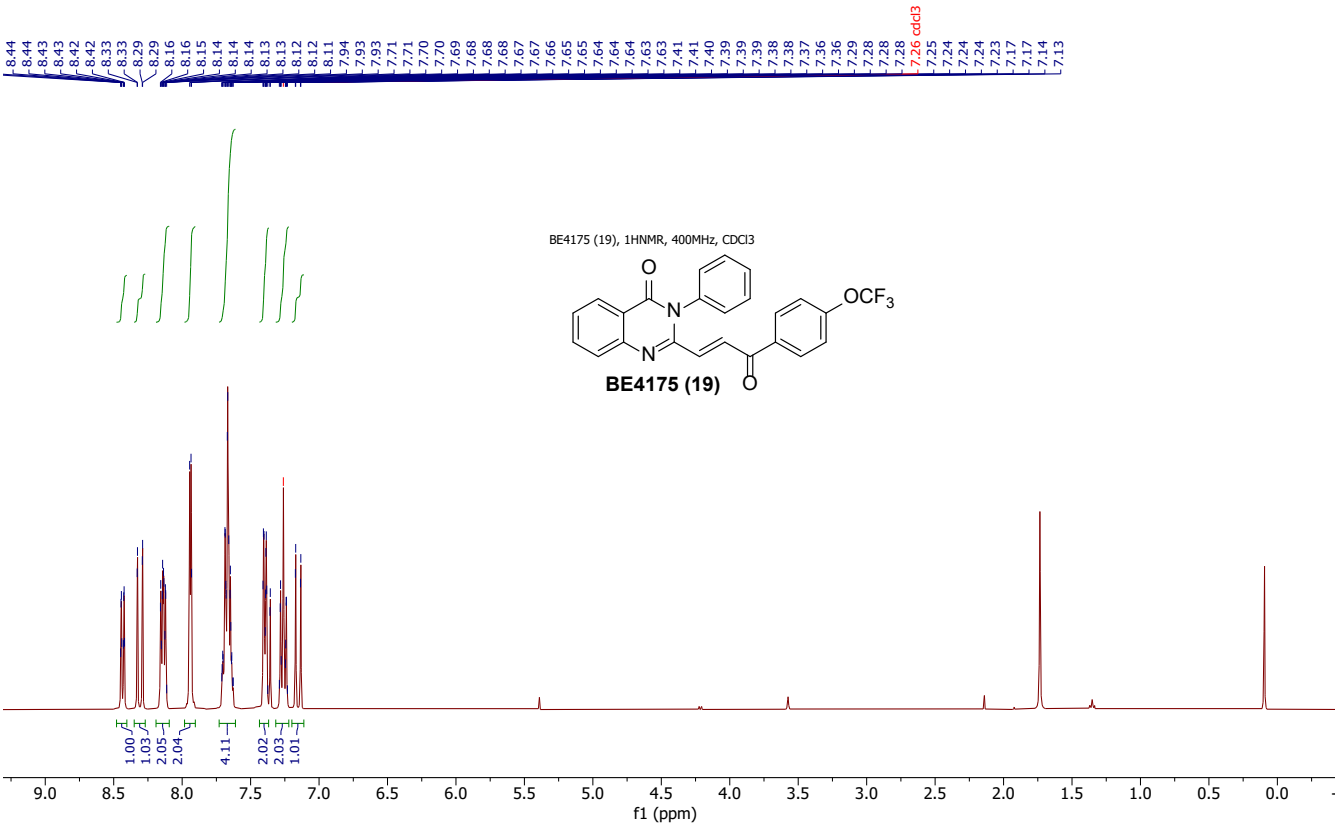


Figure S27. ^{1}HNMR spectra of BE4175 (19; $CDCl_3$, 400MHz)

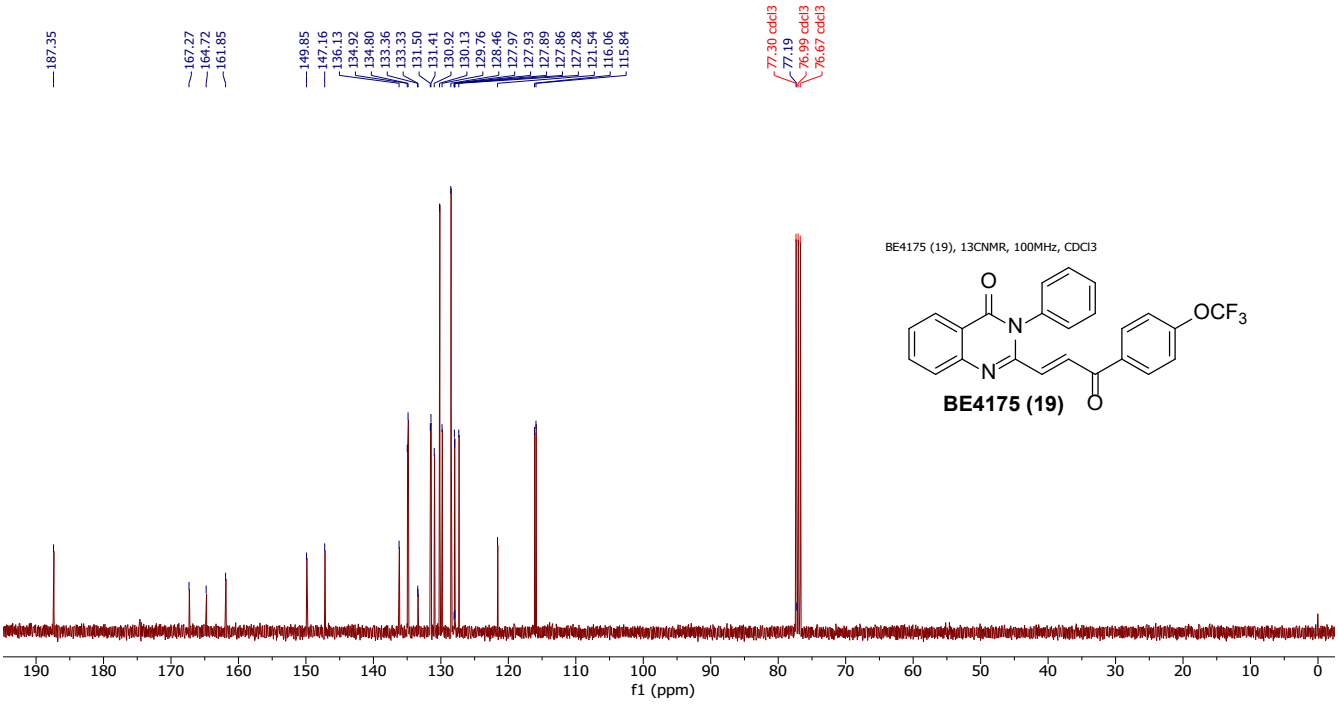


Figure S28. ^{13}CNMR spectra of BE4175 (19; $CDCl_3$, 100MHz)

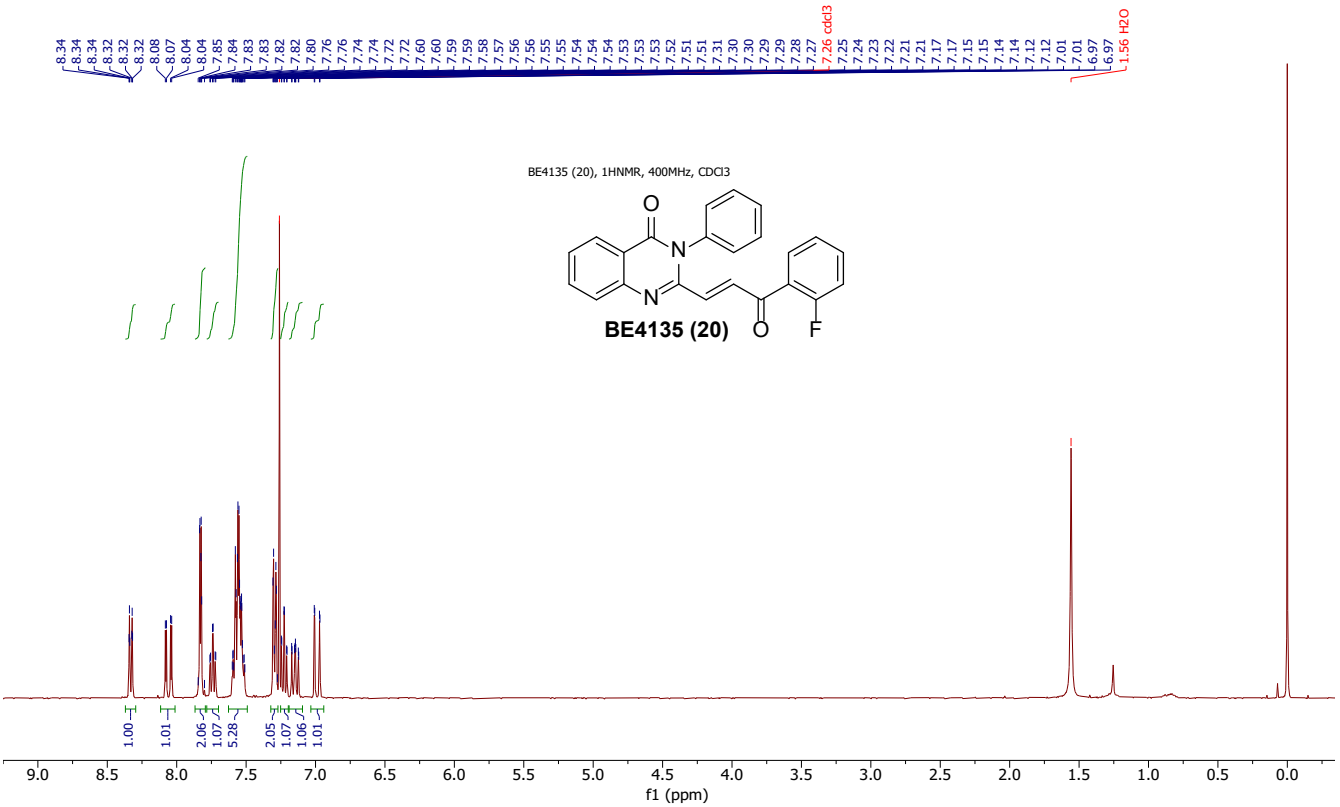


Figure S29. ^{1}HNMR spectrum of BE4135 (20; $CDCl_3$, 400MHz)

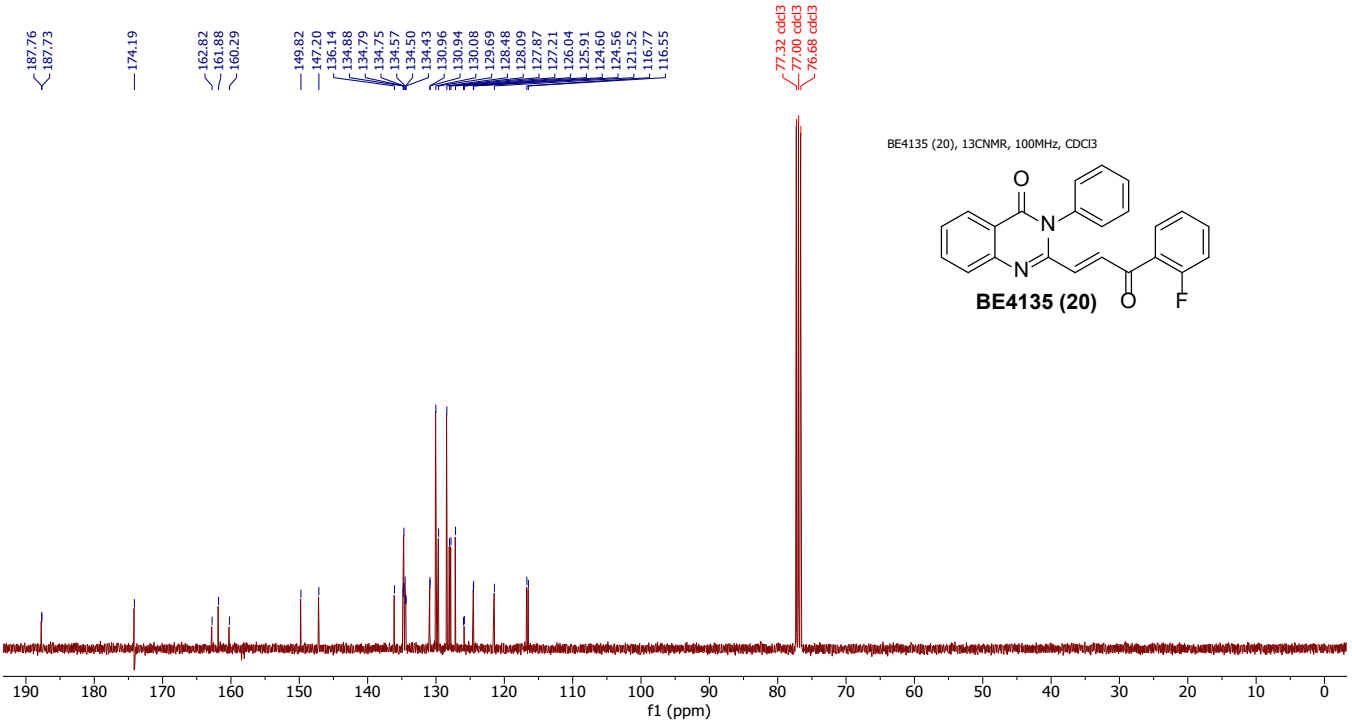


Figure S30. ^{13}CNMR spectra of BE4135 (20; $CDCl_3$, 100MHz)

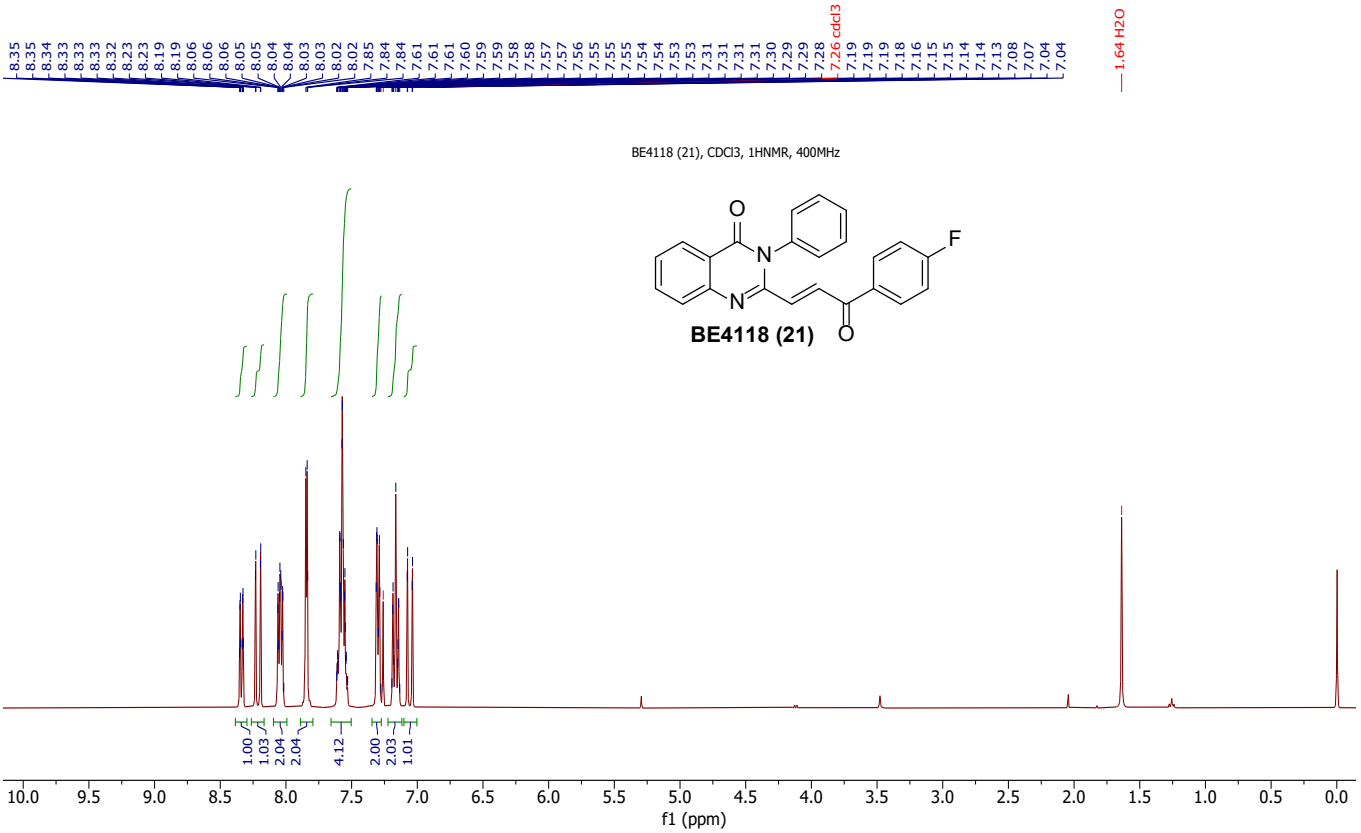


Figure S31. ^{1}HNMR spectra of BE4118 (21; $CDCl_3$, 400MHz)

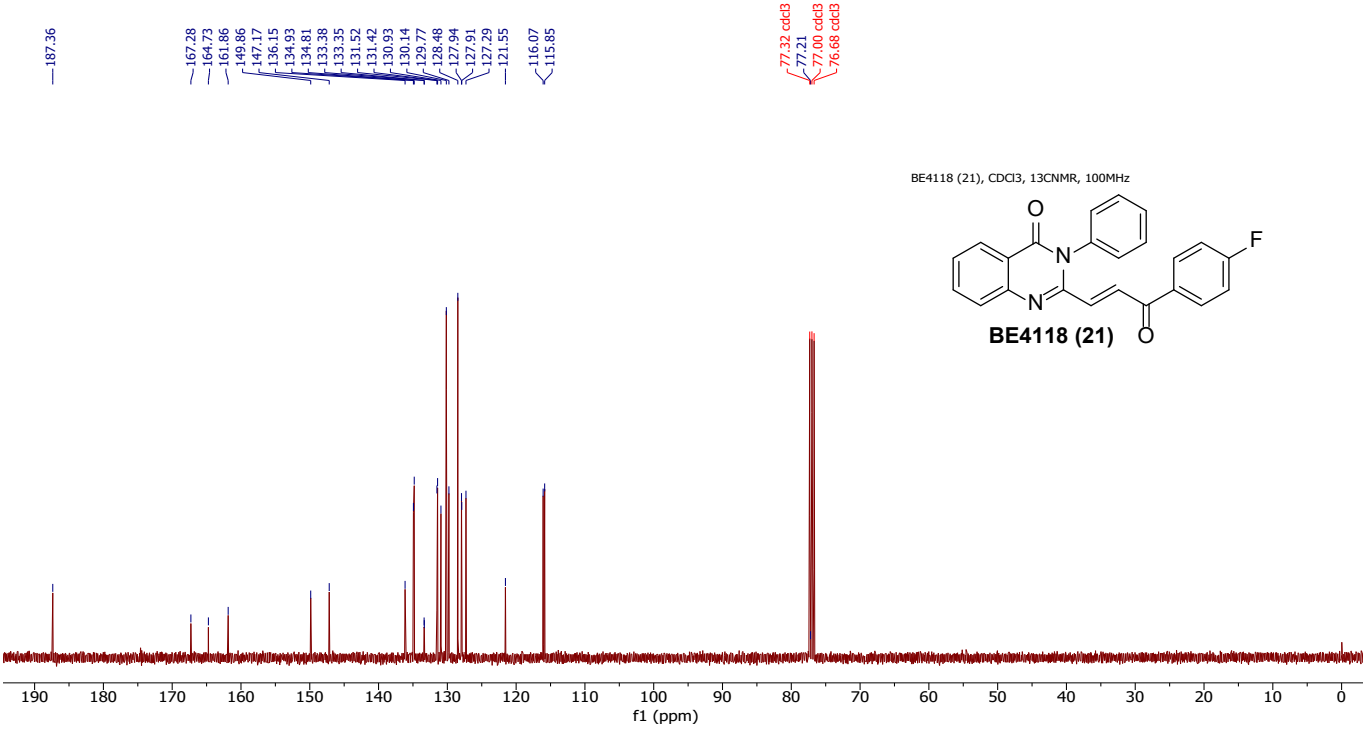


Figure S32. ^{13}CNMR of spectra of BE4118 (21; $CDCl_3$, 100MHz)

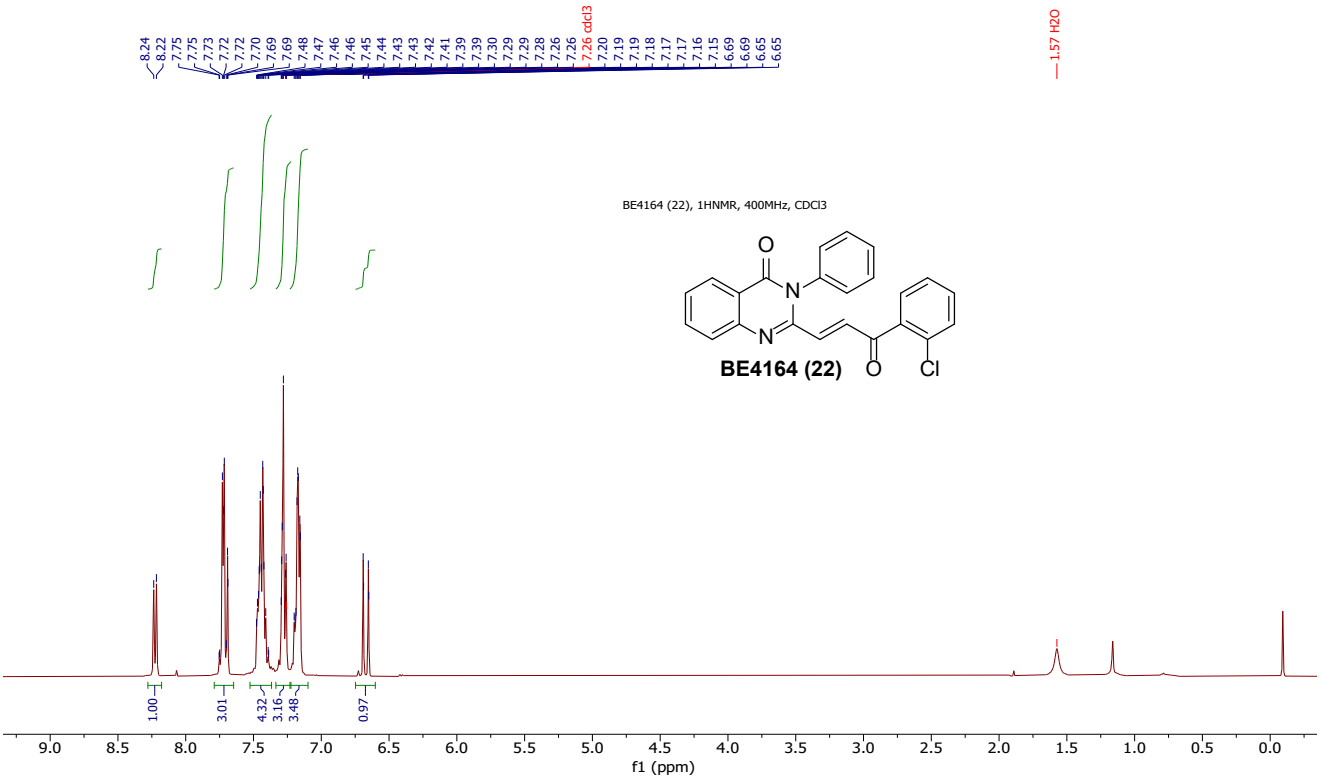


Figure S33. ^{1}HNMR spectra of BE4164 (22; $CDCl_3$, 400MHz)

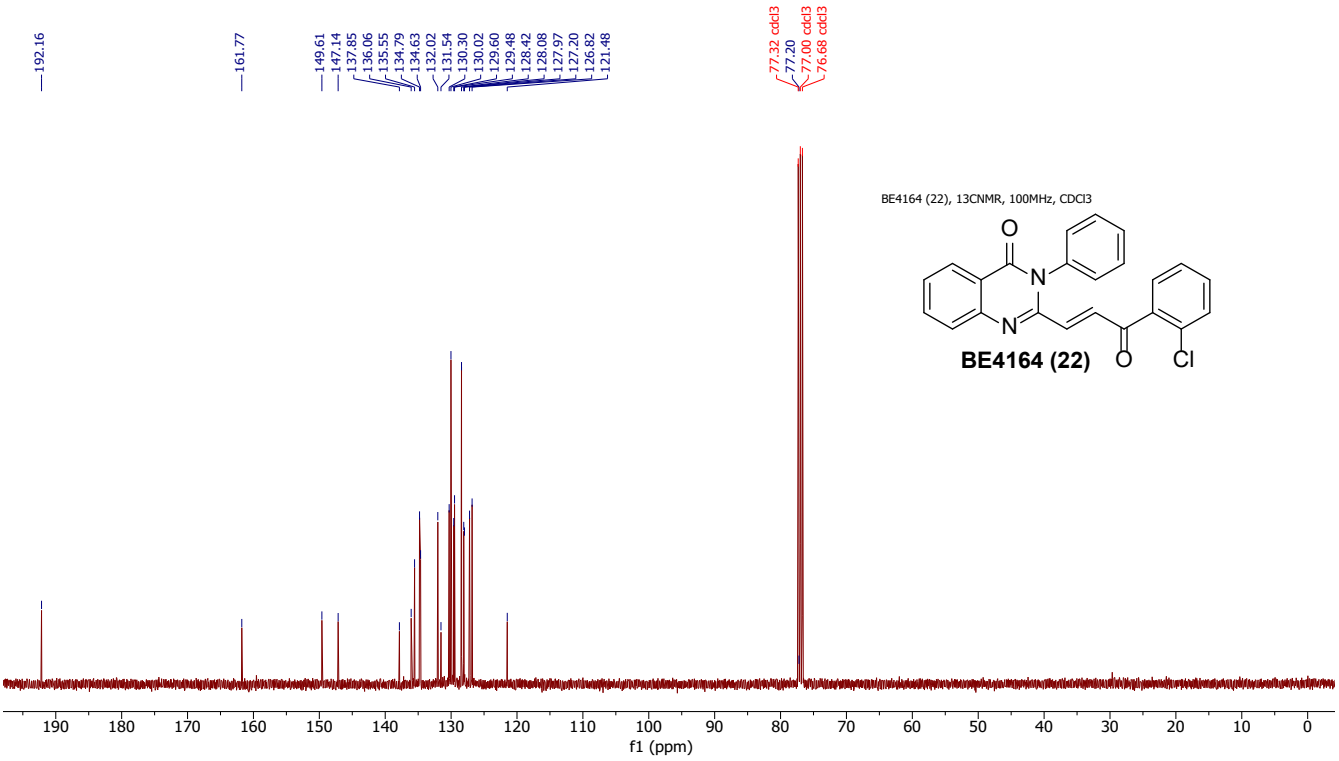


Figure S34. ^{13}CNMR spectra of BE4164 (22; $CDCl_3$, 100MHz)

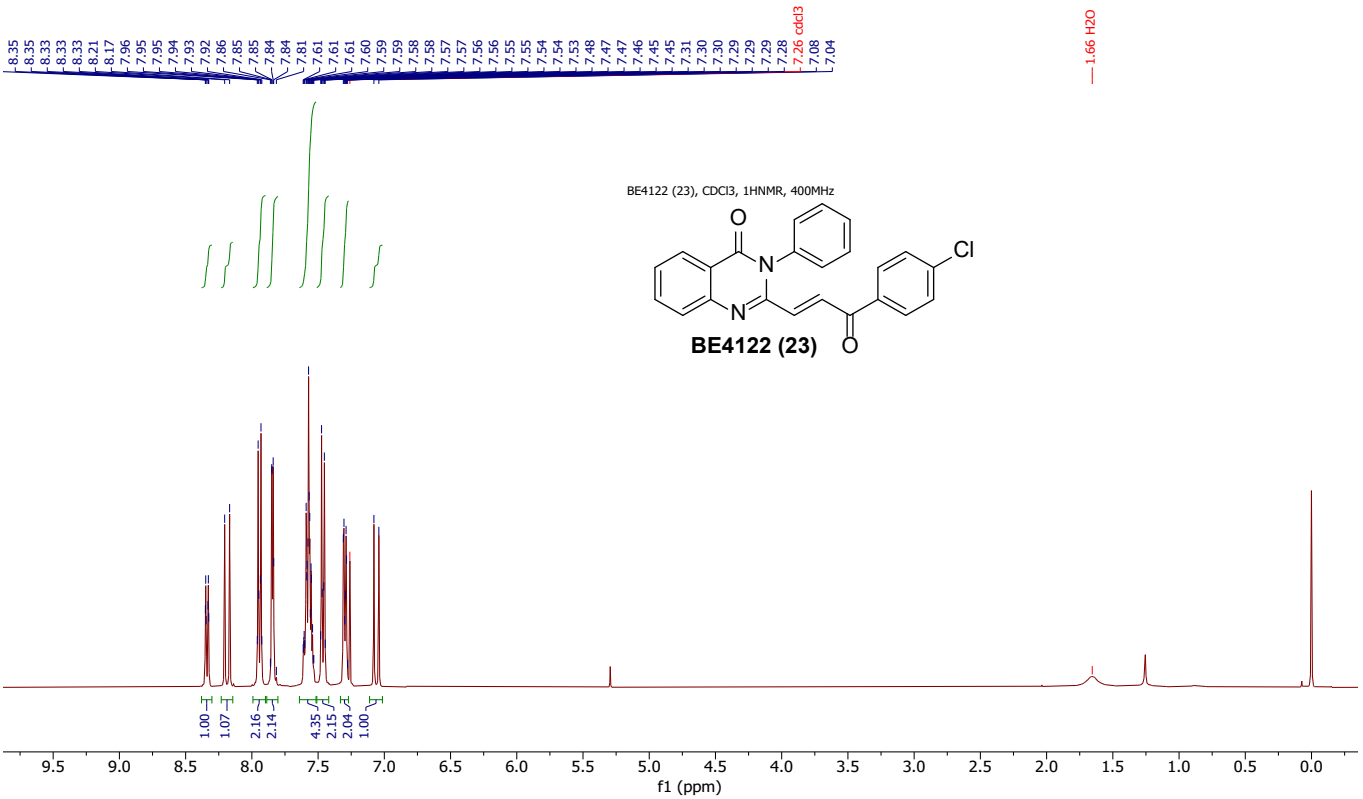


Figure S35. ^{1}HNMR spectra of BE4122 (23; $CDCl_3$, 400MHz)

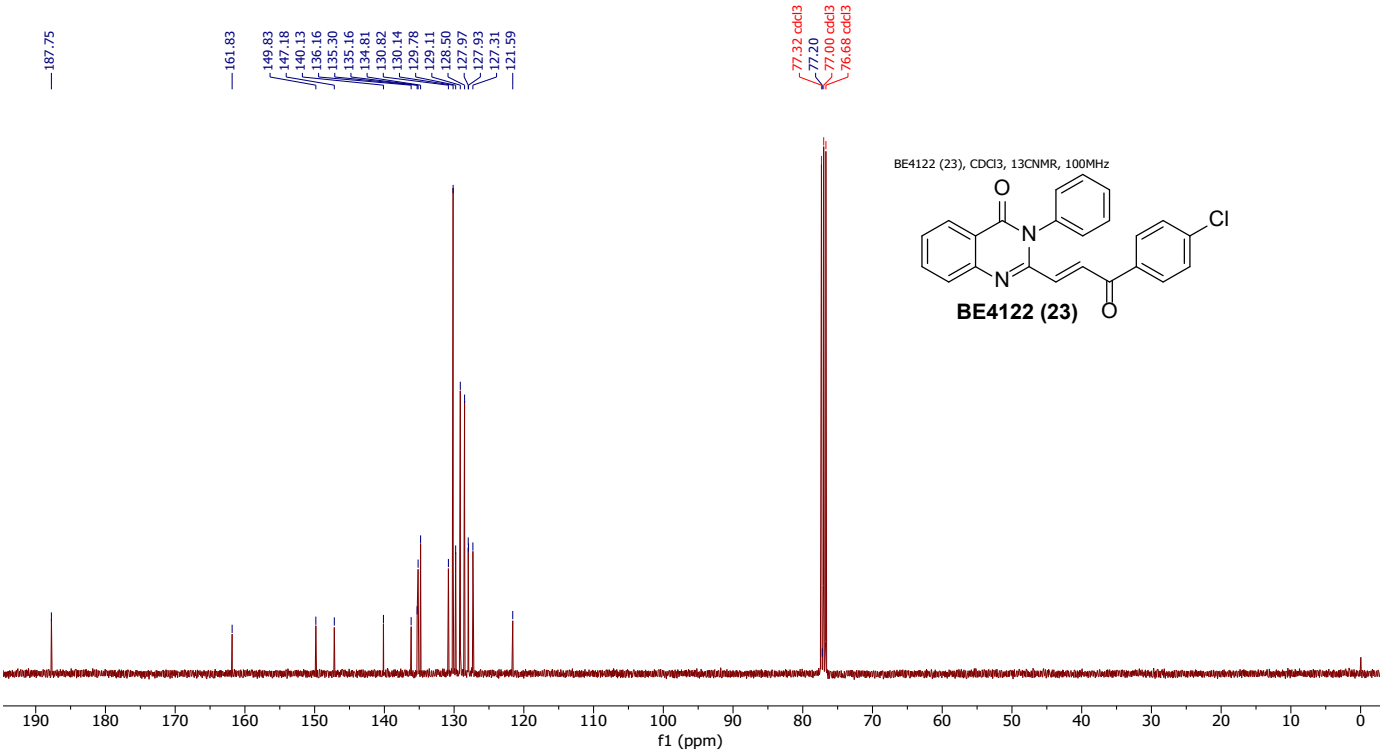


Figure S36. ^{13}CNMR spectra of BE4122 (23; $CDCl_3$, 100MHz)

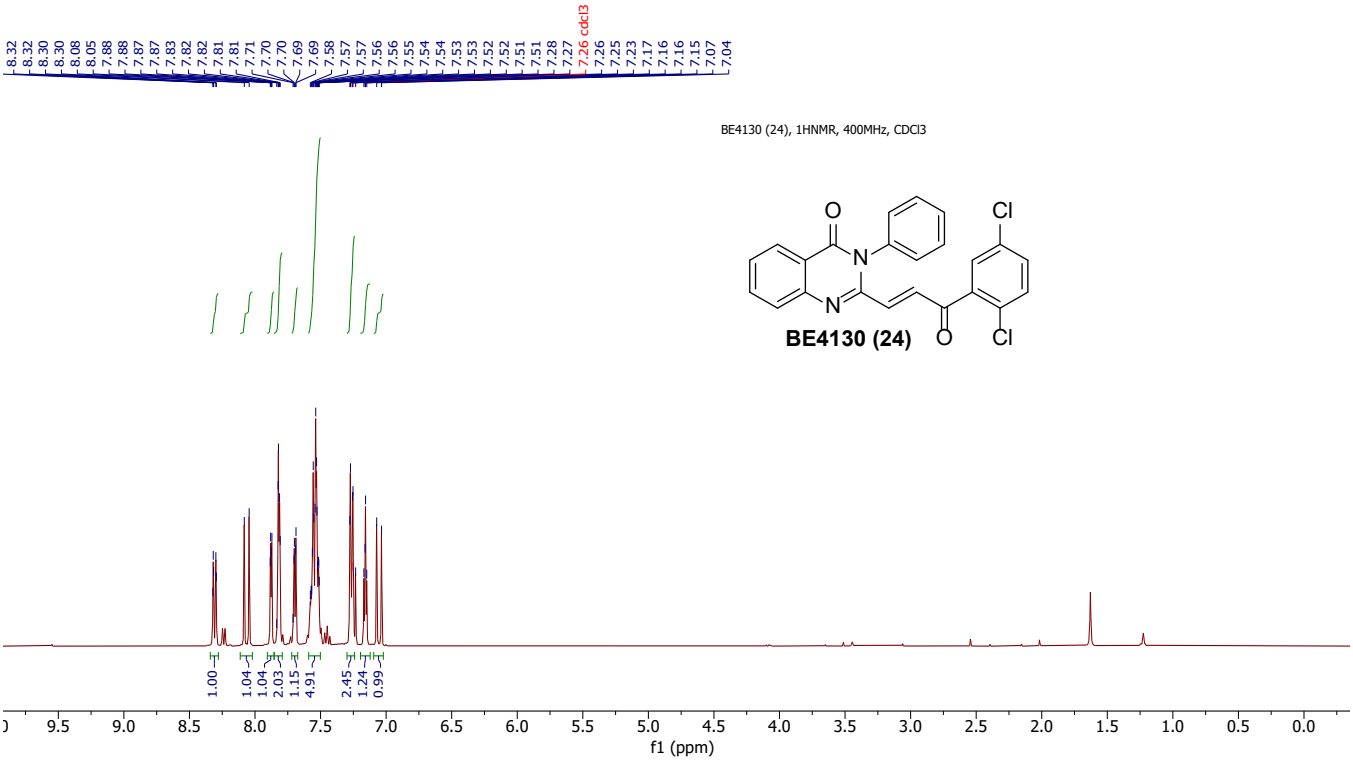


Figure S37. ^{1}HNMR spectra of BE4130 (24; $CDCl_3$, 100MHz)

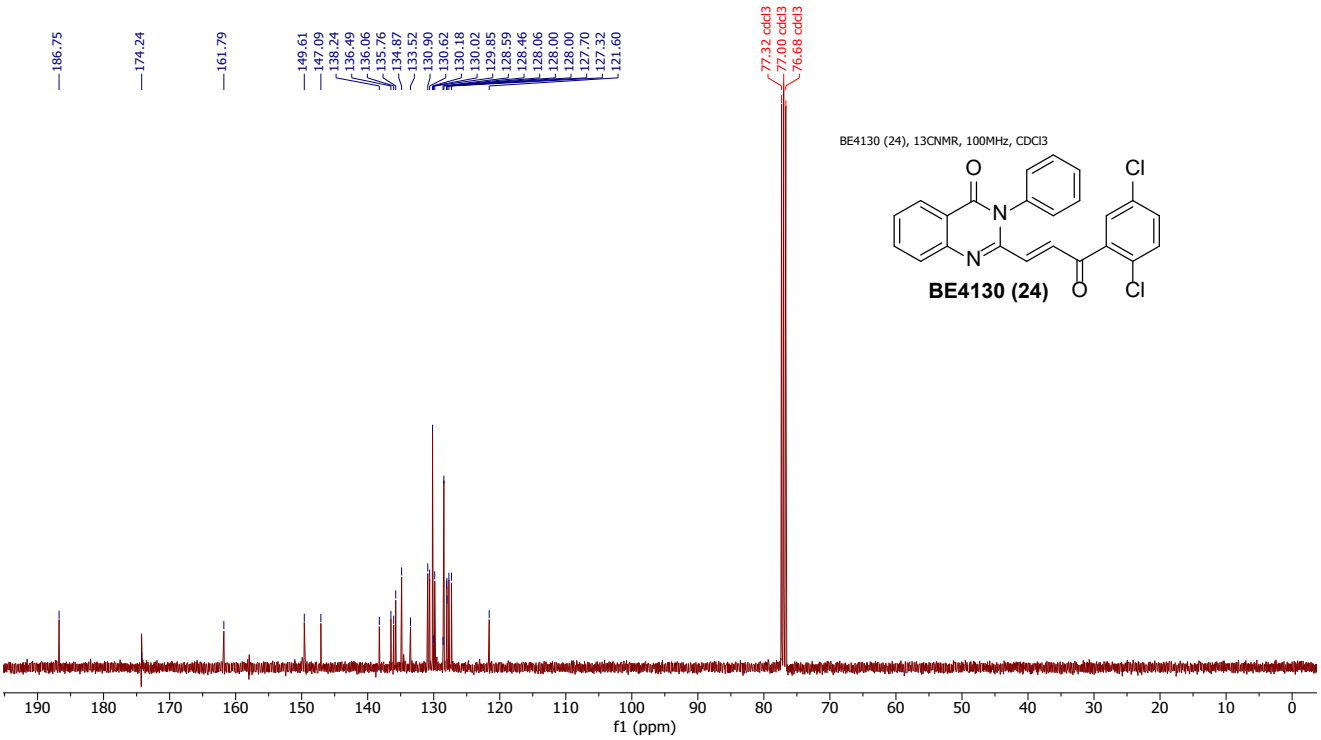


Figure S38. ^{13}CNMR spectra of BE4130 (24; $CDCl_3$, 100MHz)

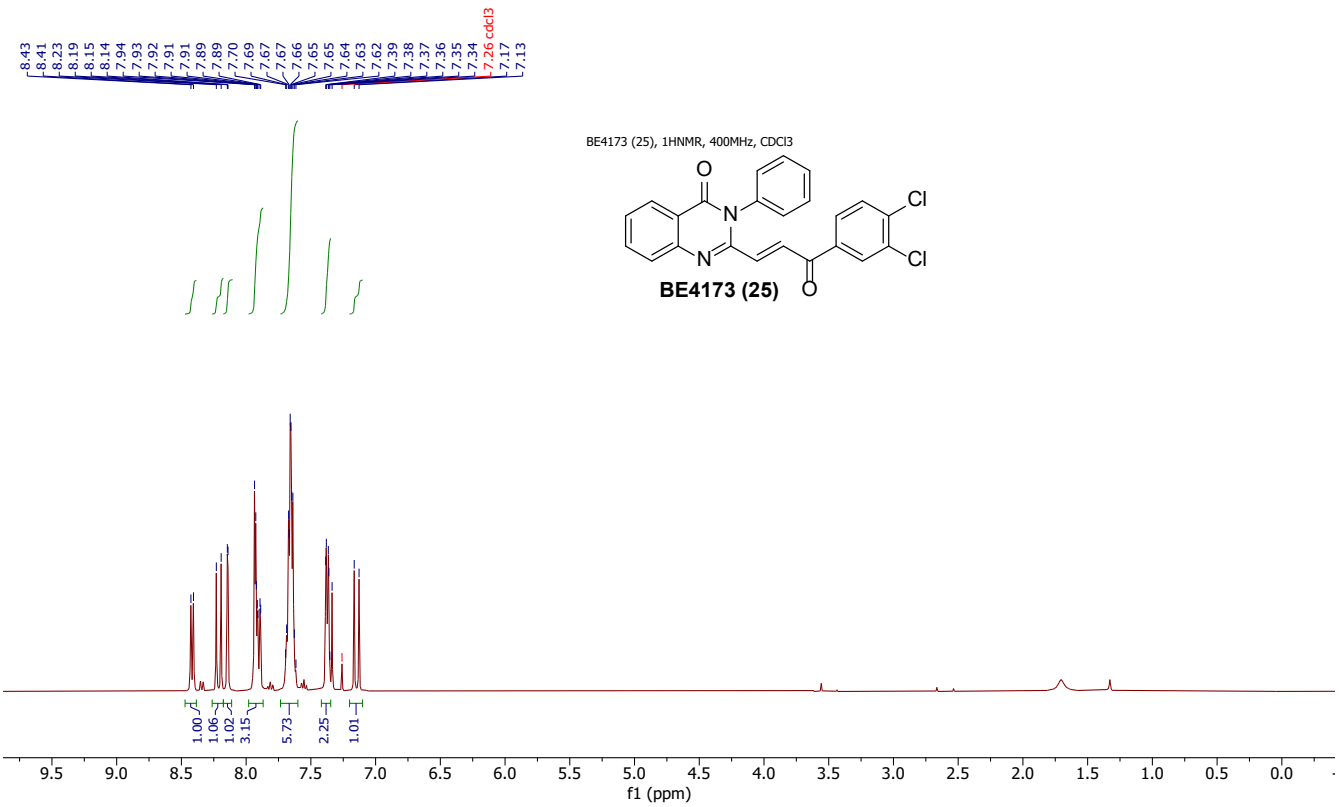


Figure S39. ^{1}HNMR spectra of BE4173 (25; $CDCl_3$, 100MHz)

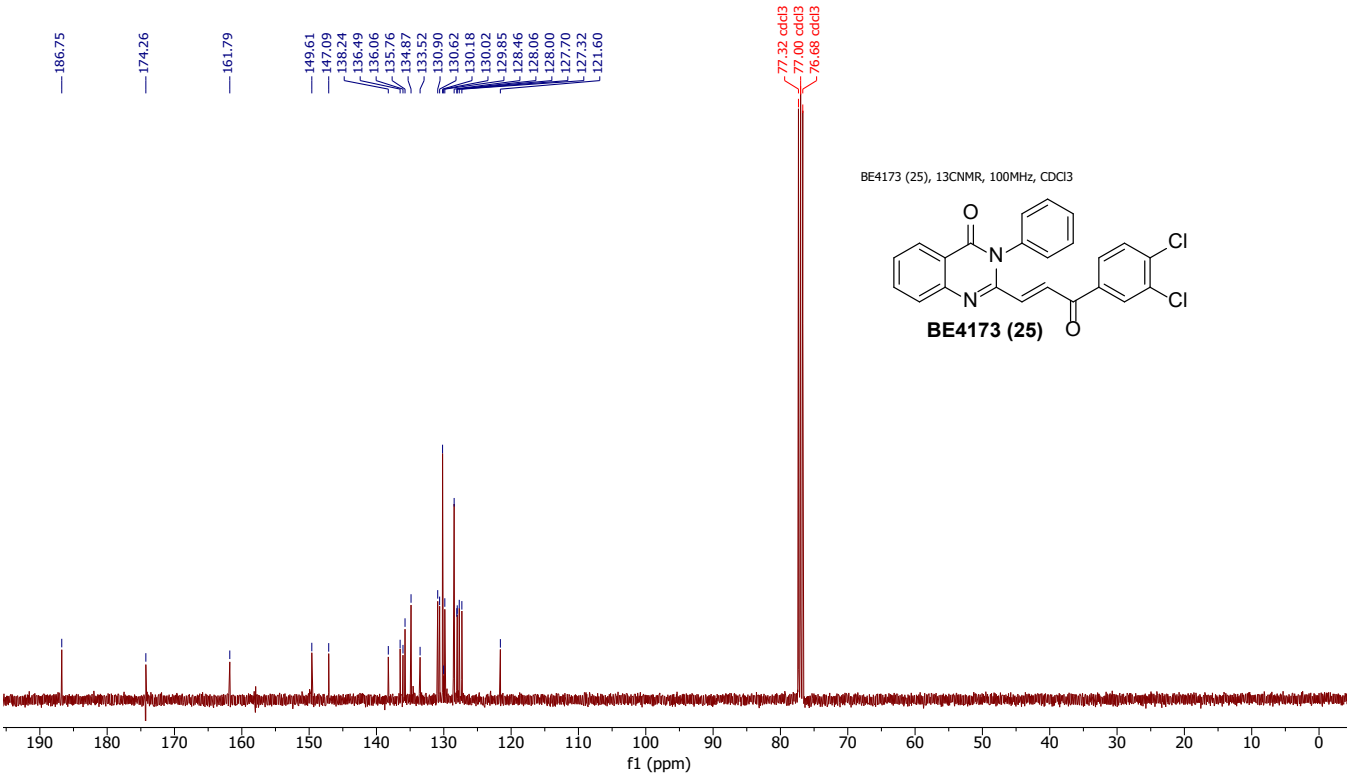


Figure S40. ^{13}CNMR spectra of BE4173 (25; $CDCl_3$, 100MHz)

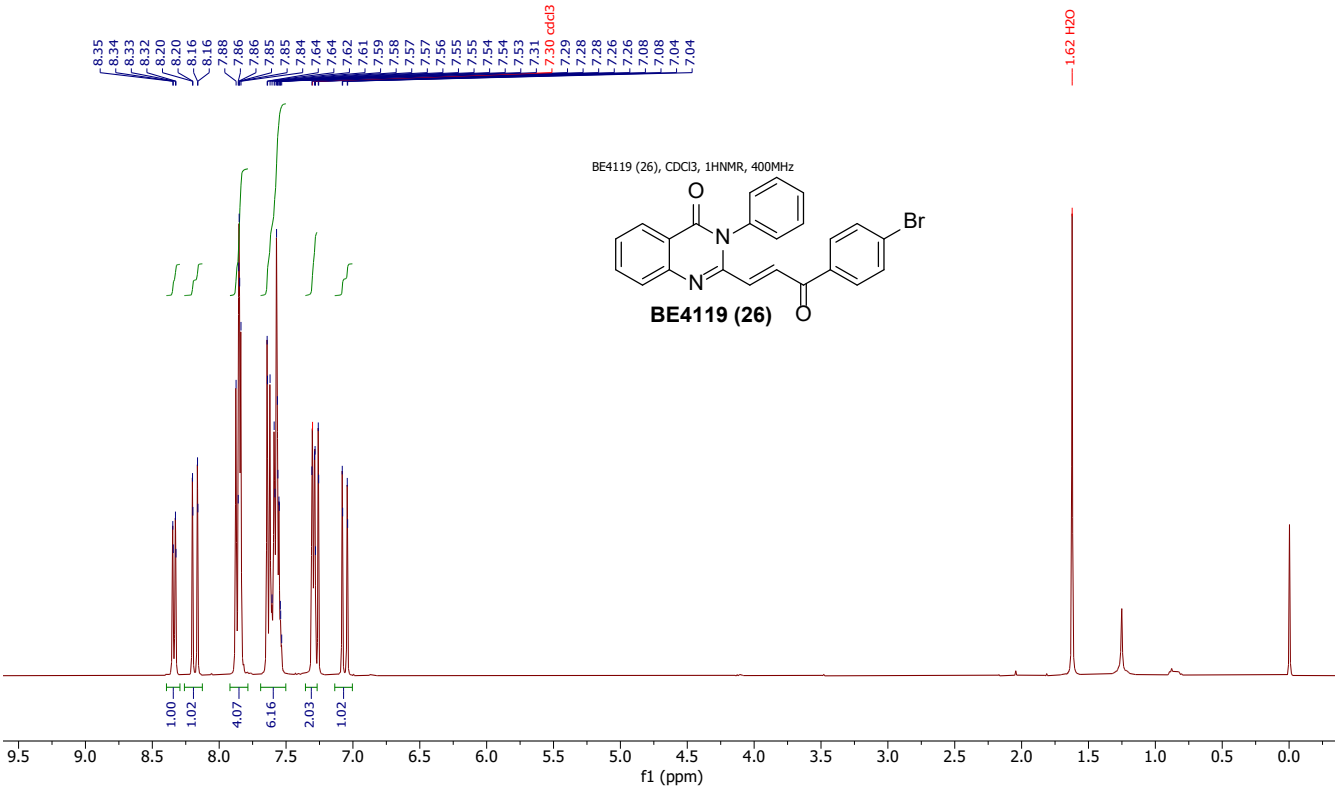


Figure S41. ^{1}HNMR spectra of BE4119 (26; $CDCl_3$, 400MHz)

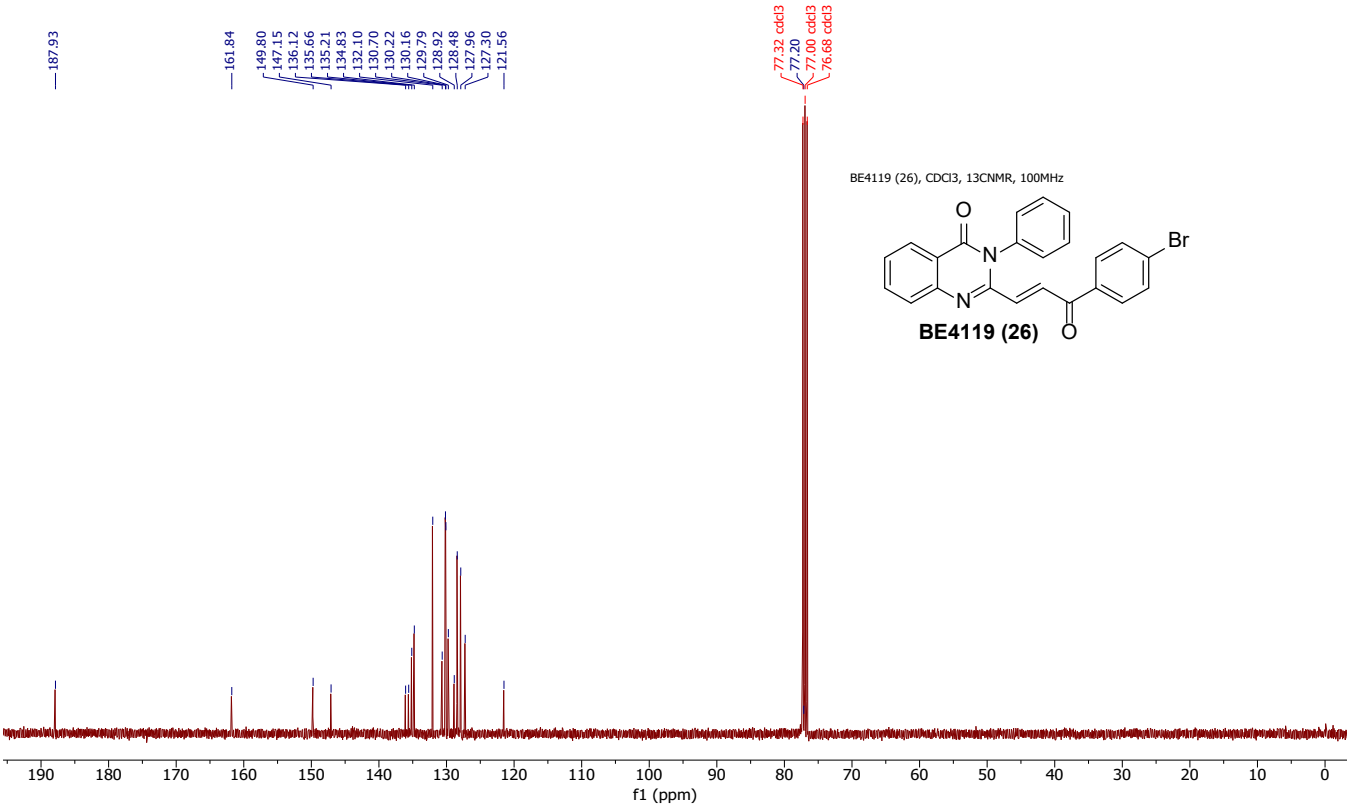


Figure S42. ^{13}CNMR spectra of BE4119 (26; $CDCl_3$, 100MHz)

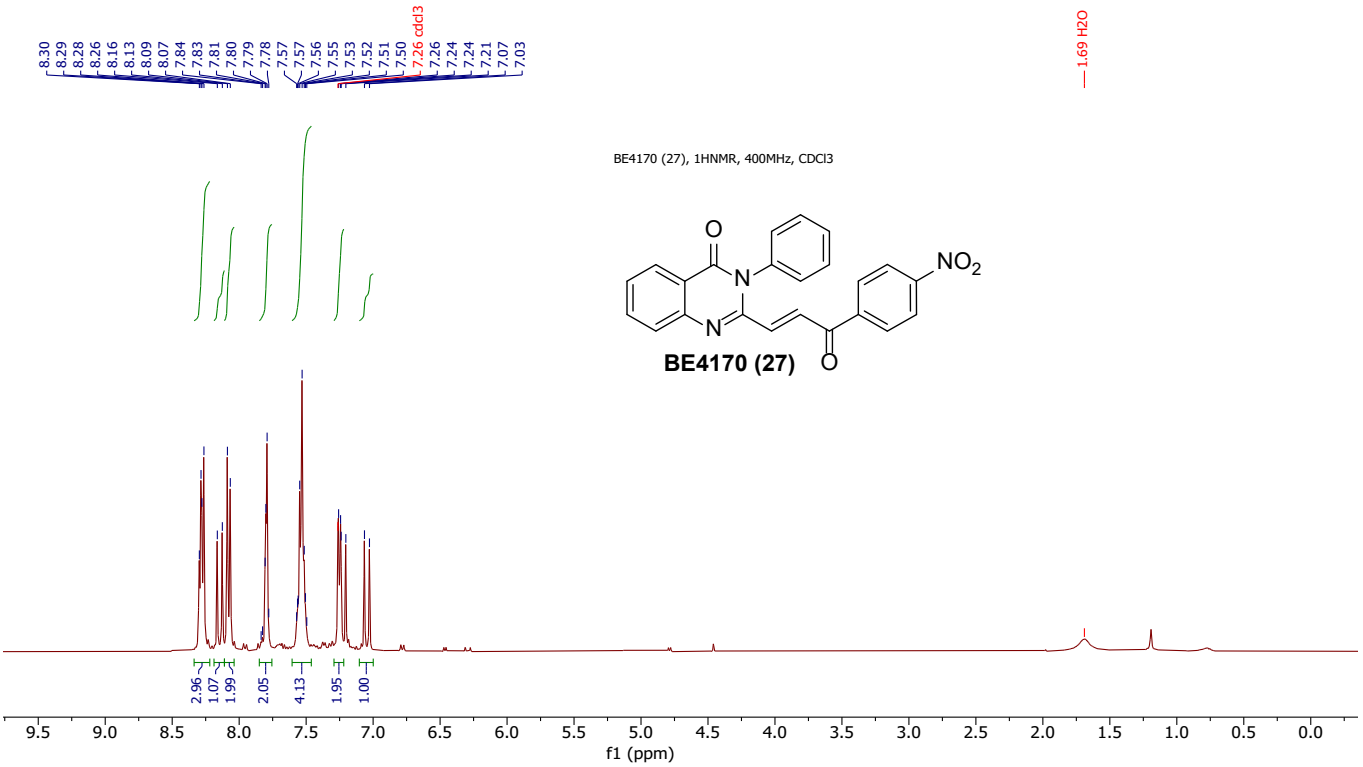


Figure S43. ^{1}HNMR spectra of BE4170 (27; $CDCl_3$, 400MHz)

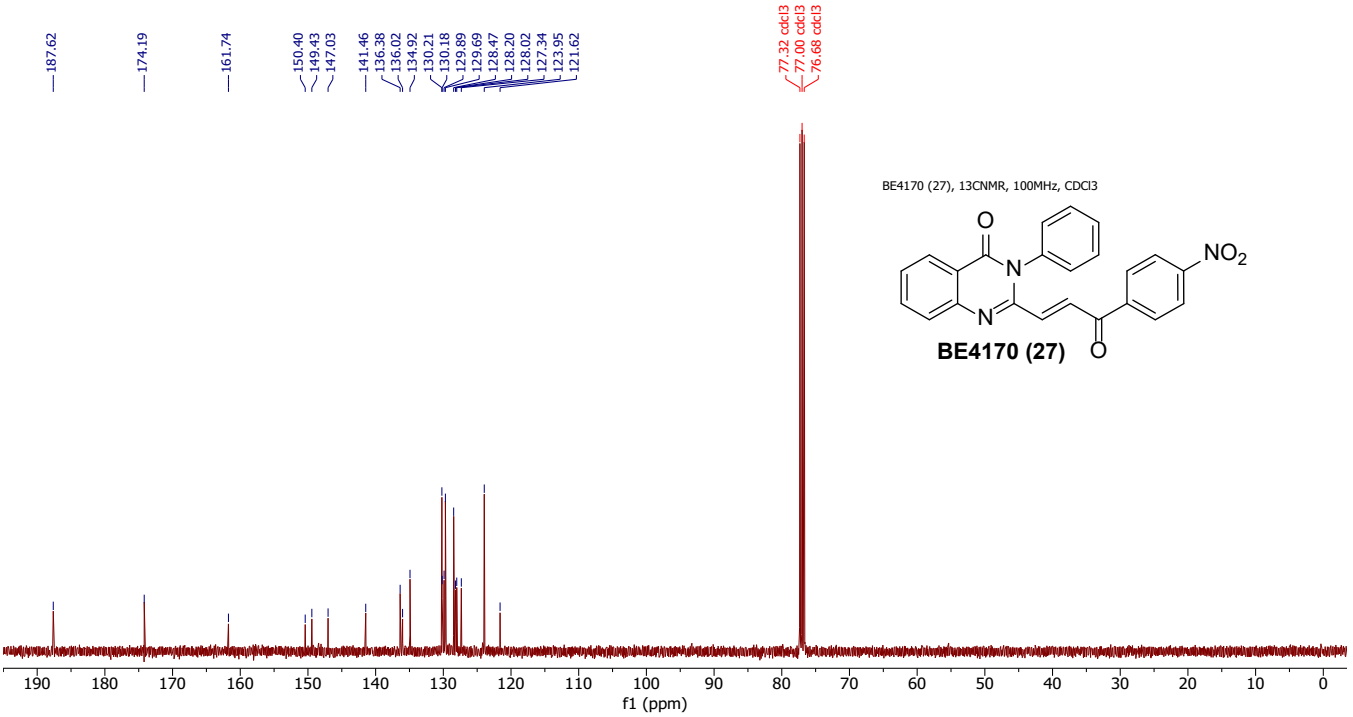


Figure S44. ^{13}CNMR spectra of BE4170 (27; $CDCl_3$, 100MHz)

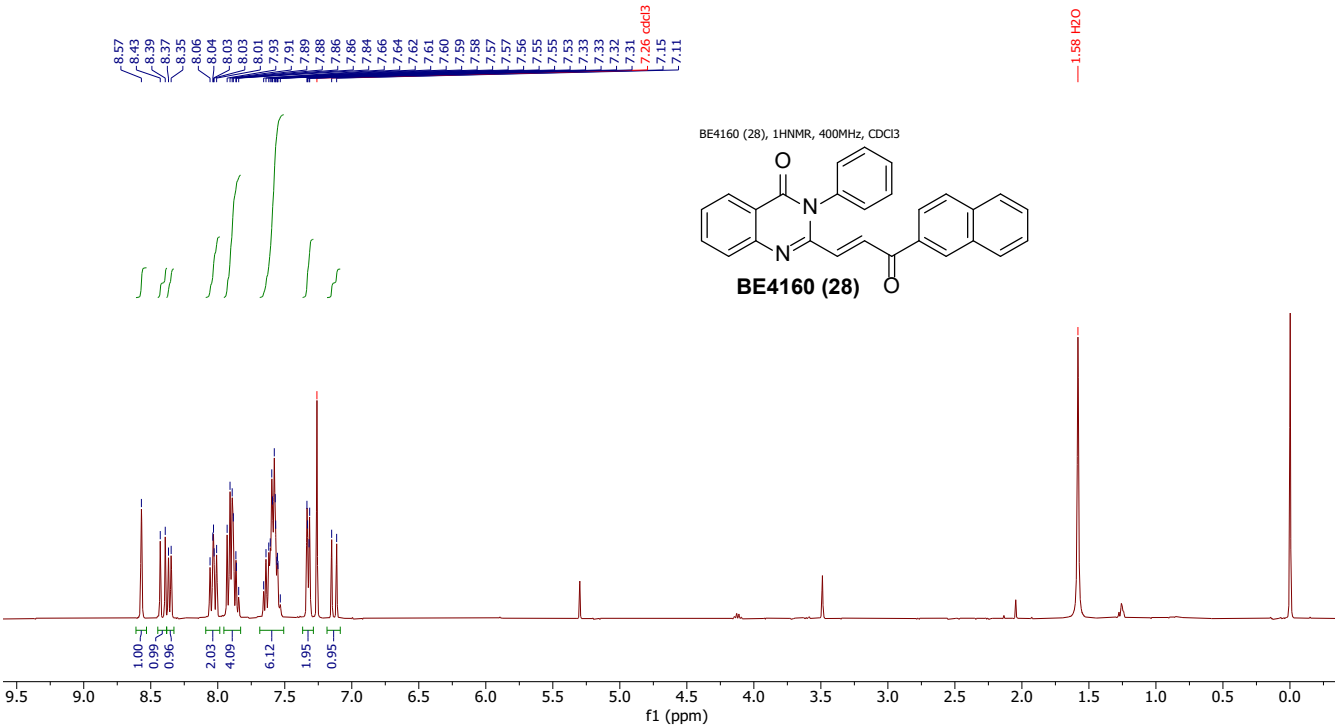


Figure S45. ^{1}HNMR spectra of BE4160 (28; $CDCl_3$, 400MHz)

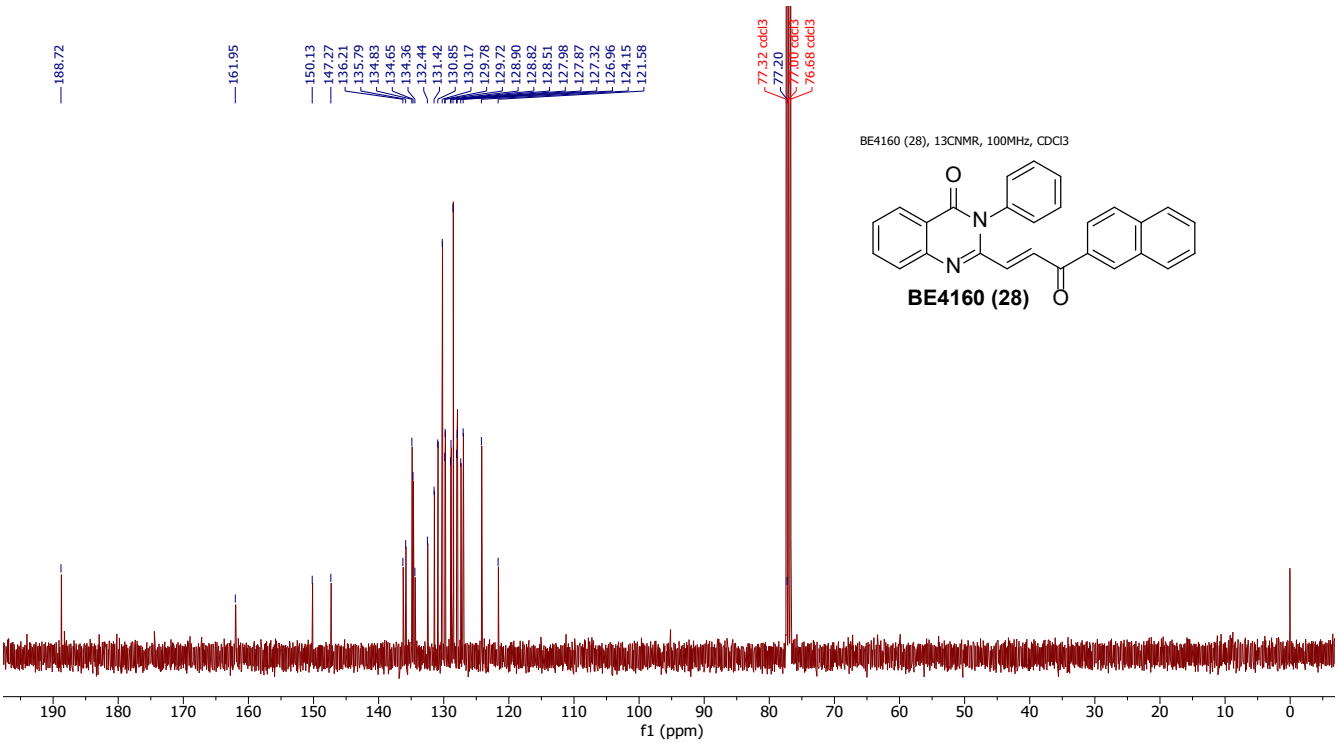


Figure S46. ^{13}CNMR spectra of BE4160 (28; $CDCl_3$, 100MHz)

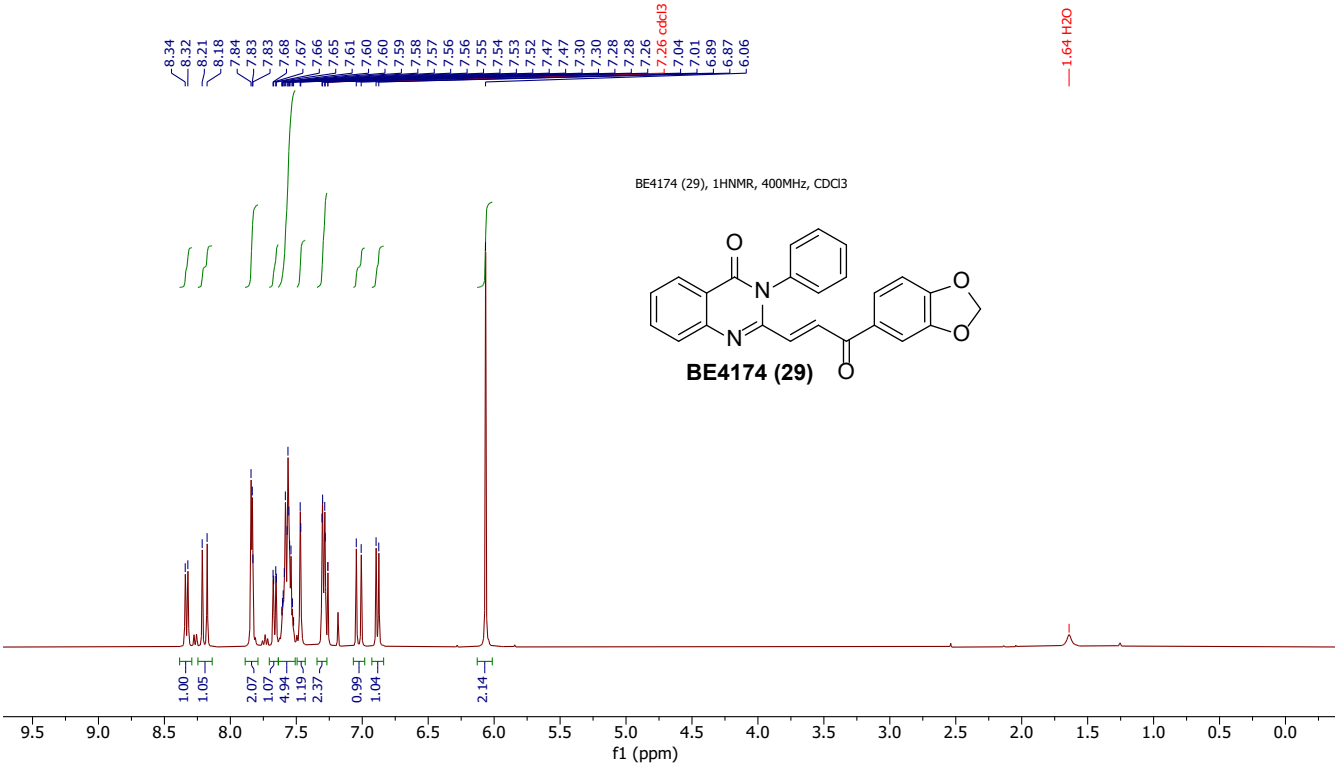


Figure S47. ^{1}HNMR spectra of BE4174 (29; $CDCl_3$, 400MHz)

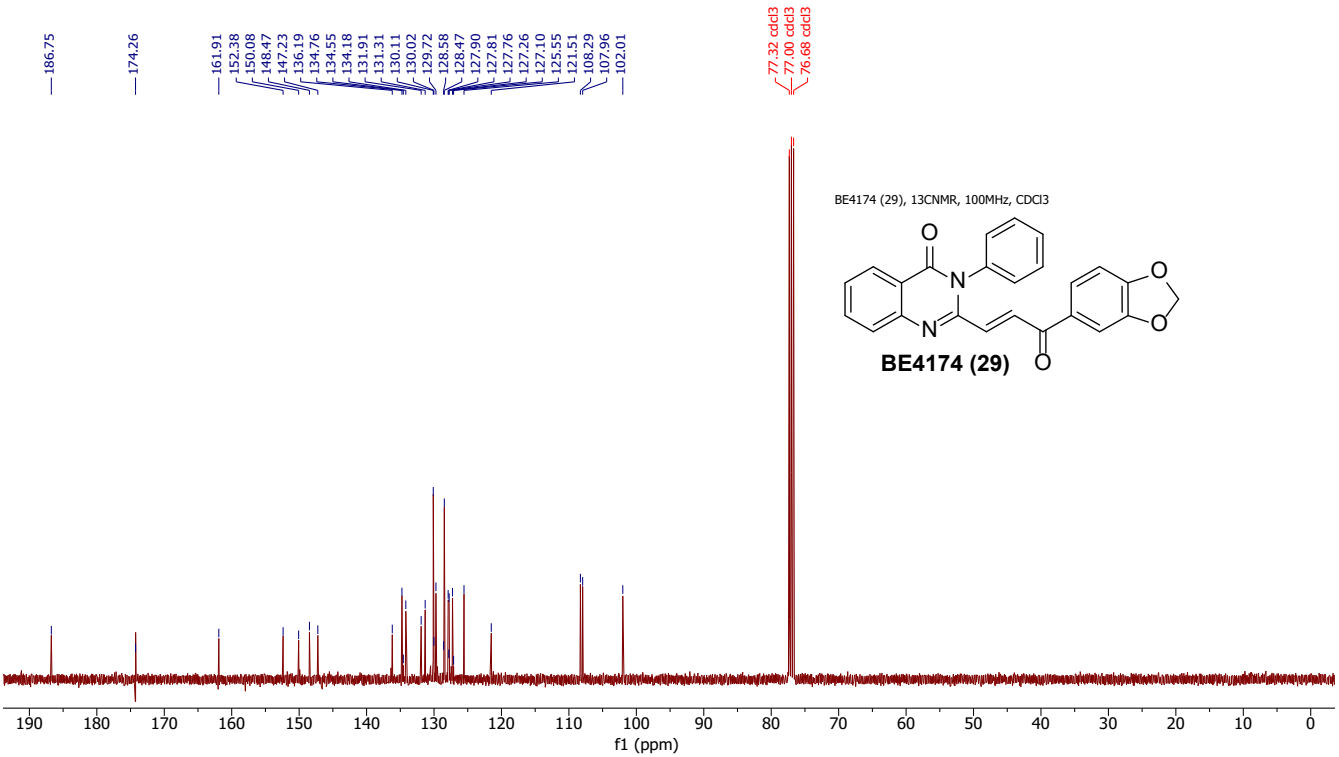


Figure S48. ^{13}CNMR spectra of BE4174 (29; $CDCl_3$, 100MHz)

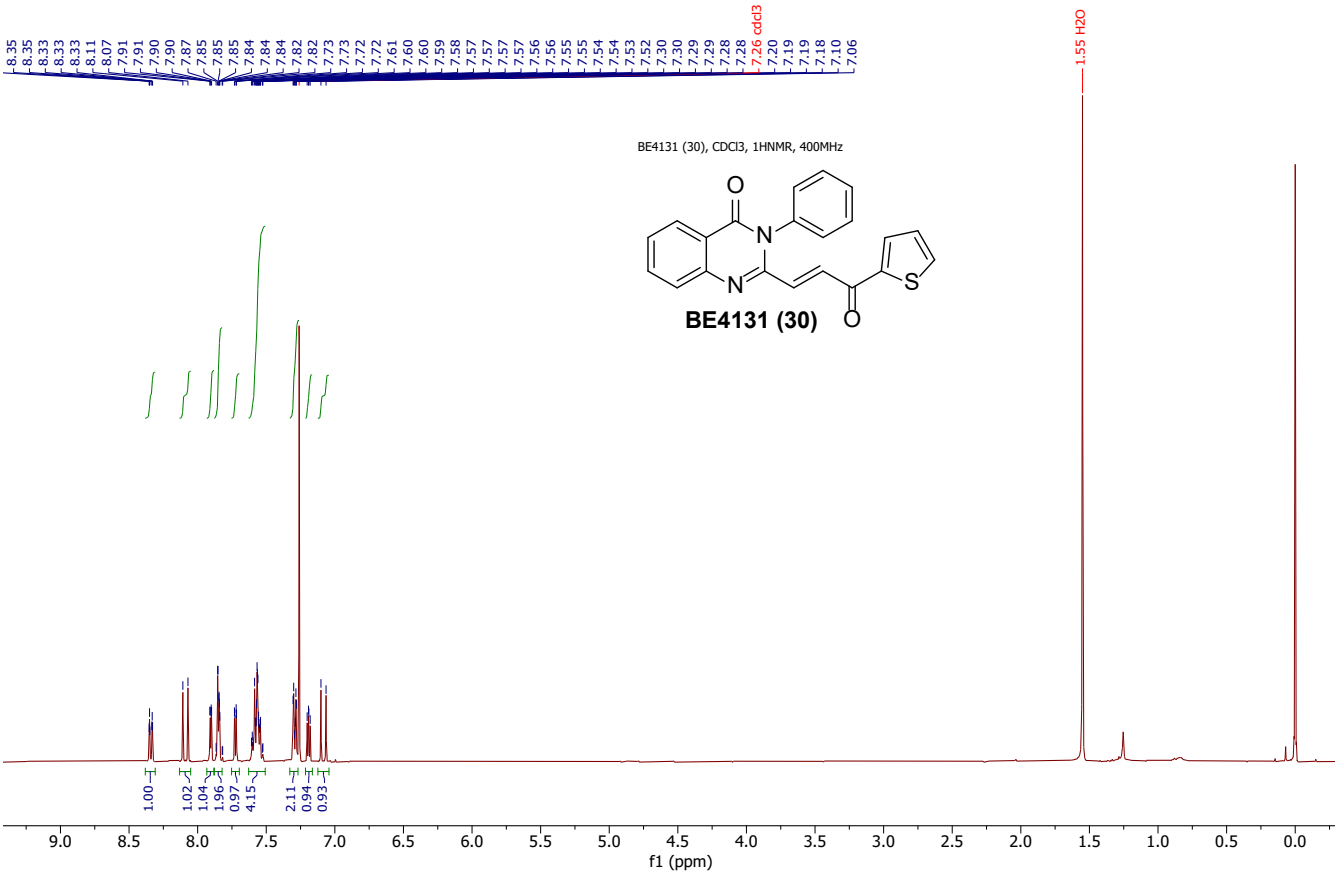


Figure S49. ^{1}HNMR spectra of BE4131 (30; $CDCl_3$, 400MHz)

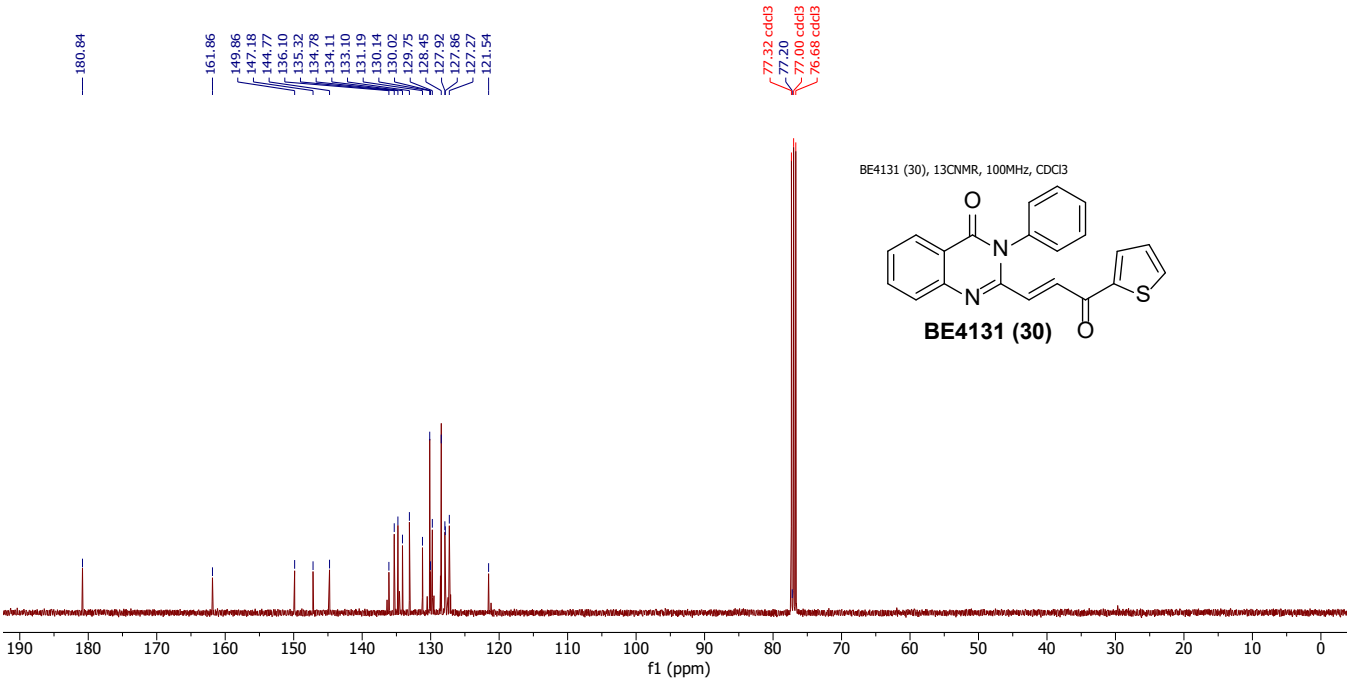


Figure S50. ^{13}CNMR spectra of BE4131 (30; $CDCl_3$, 100MHz)

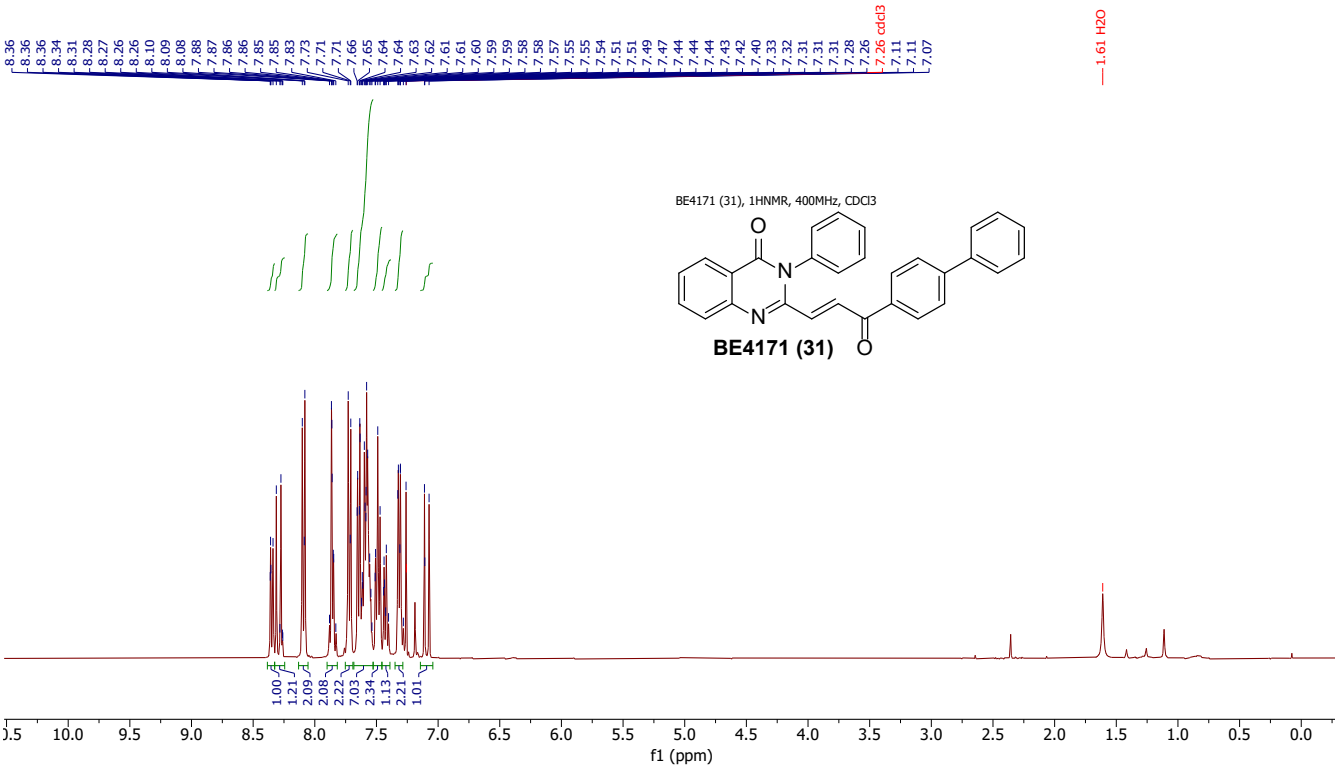


Figure S51. ^{1}HNMR spectra of BE4171 (31; $CDCl_3$, 400MHz)

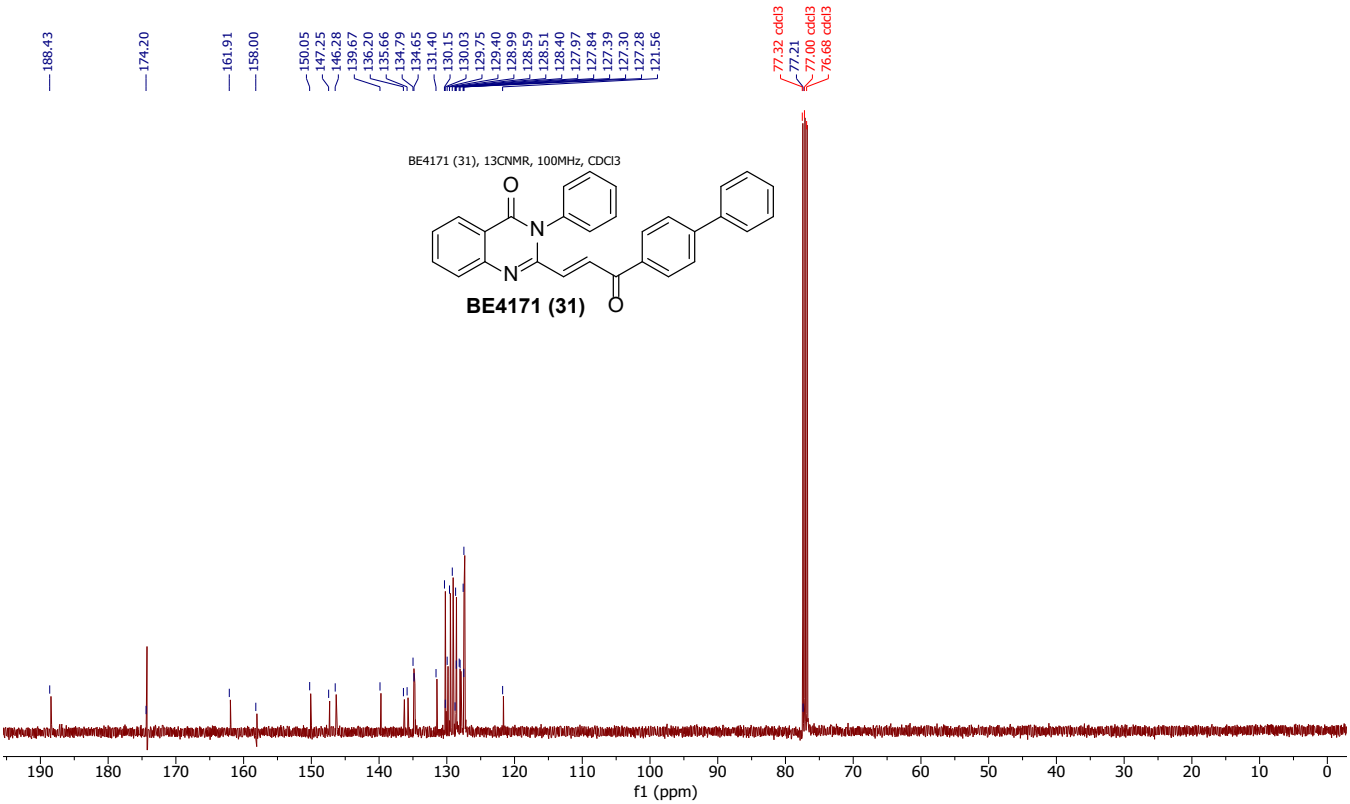


Figure S52. ^{13}CNMR spectra of BE4171 (31; $CDCl_3$, 100MHz)

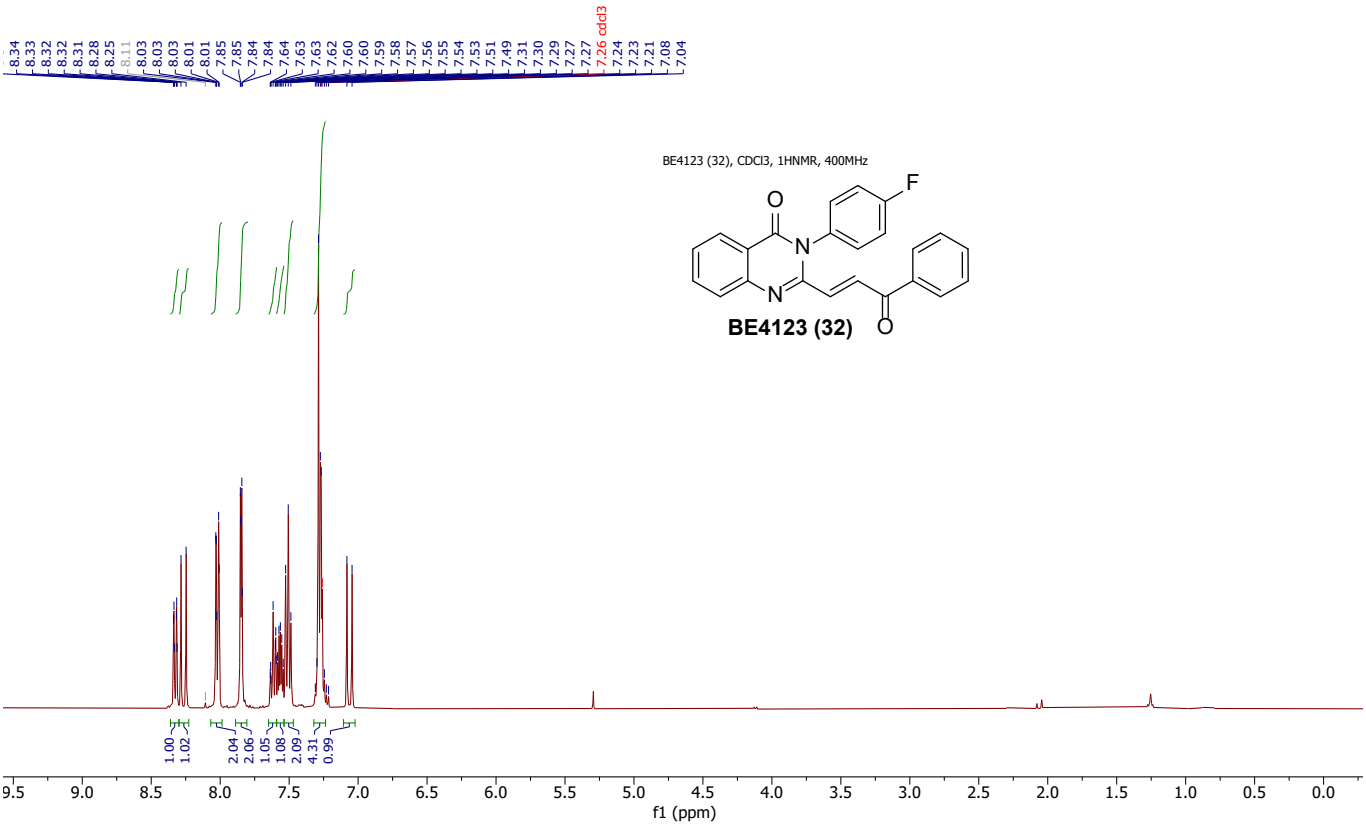


Figure S53. ^{1}HNMR spectra of BE4123 (32; $CDCl_3$, 400MHz)

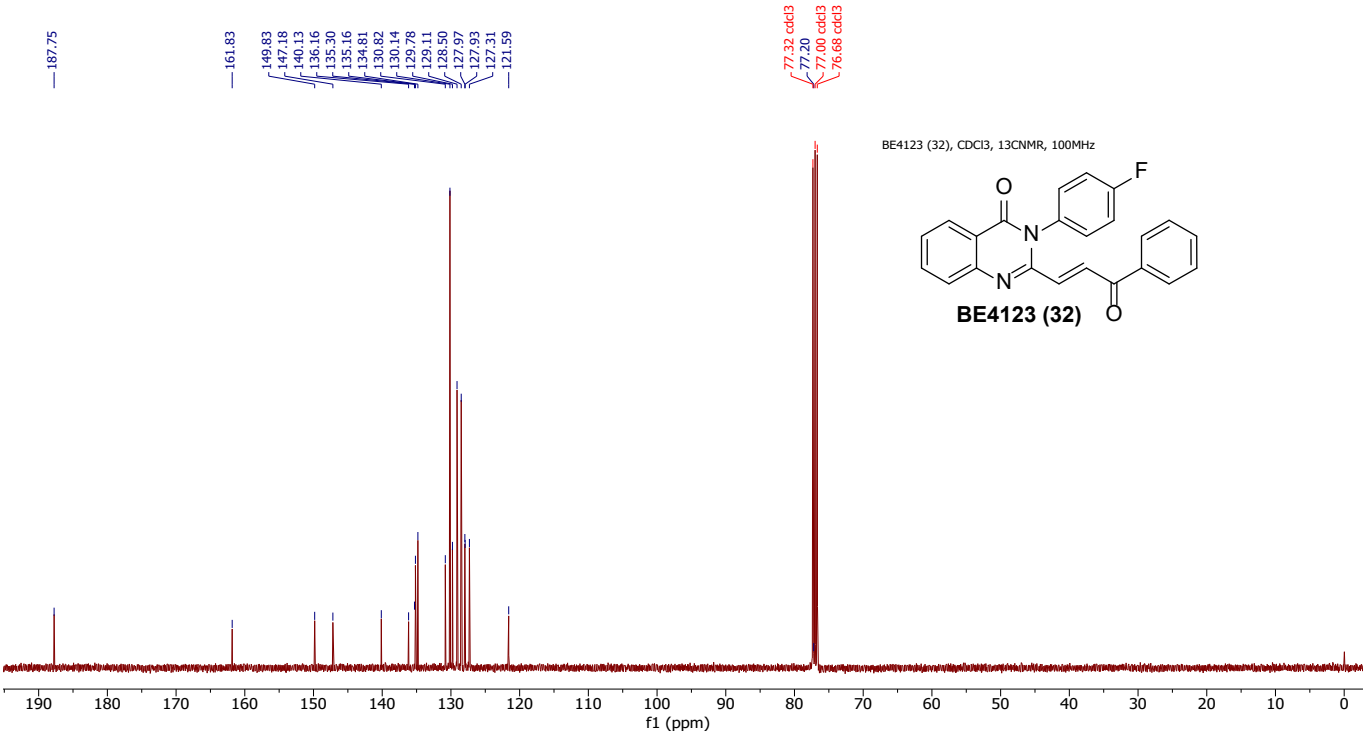


Figure S54. ^{13}CNMR spectra of BE4123 (32; $CDCl_3$, 100MHz)

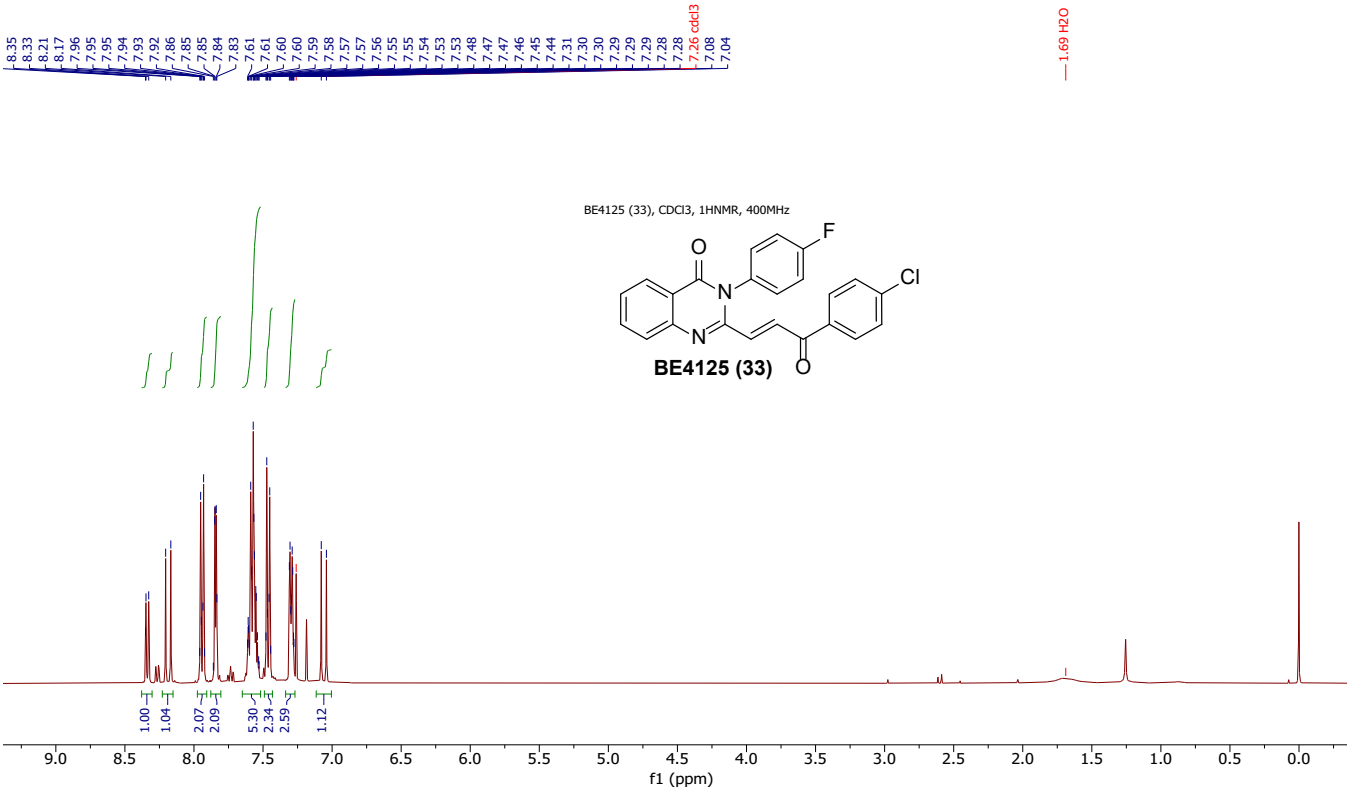


Figure S55. ^{1}HNMR spectra of BE4125 (33; $CDCl_3$, 400MHz)

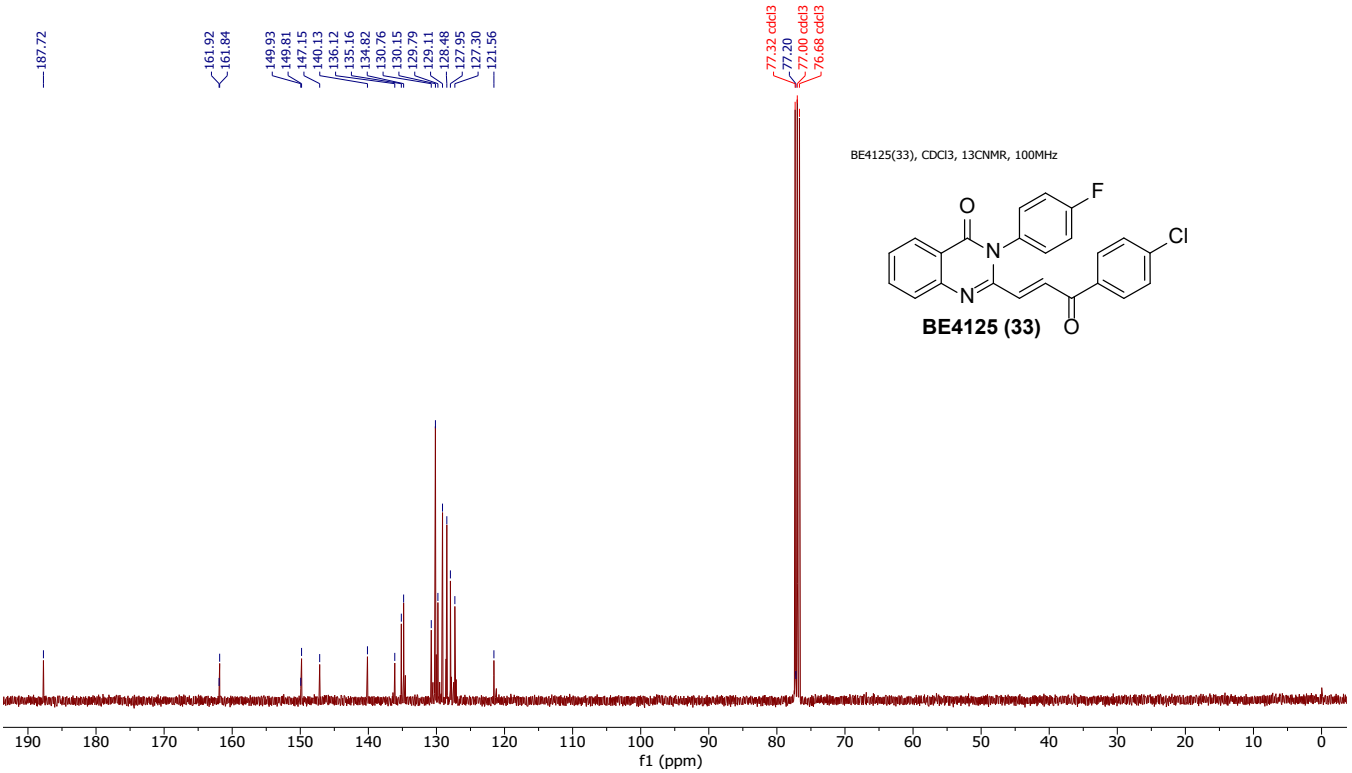


Figure S56. ^{13}CNMR spectra of BE4125 (33; $CDCl_3$, 100MHz)

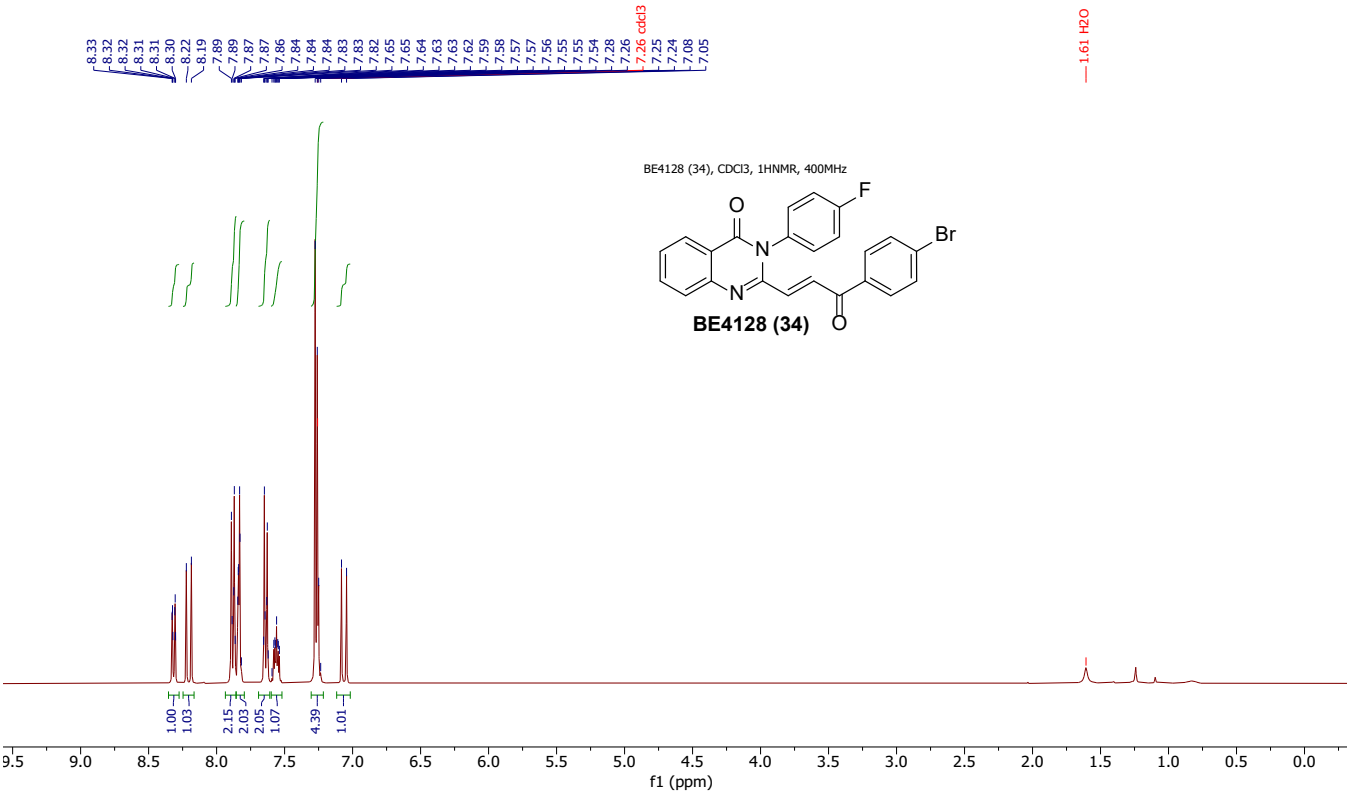


Figure S57. ^{1}HNMR spectra of BE4128 (34; $CDCl_3$, 400MHz)

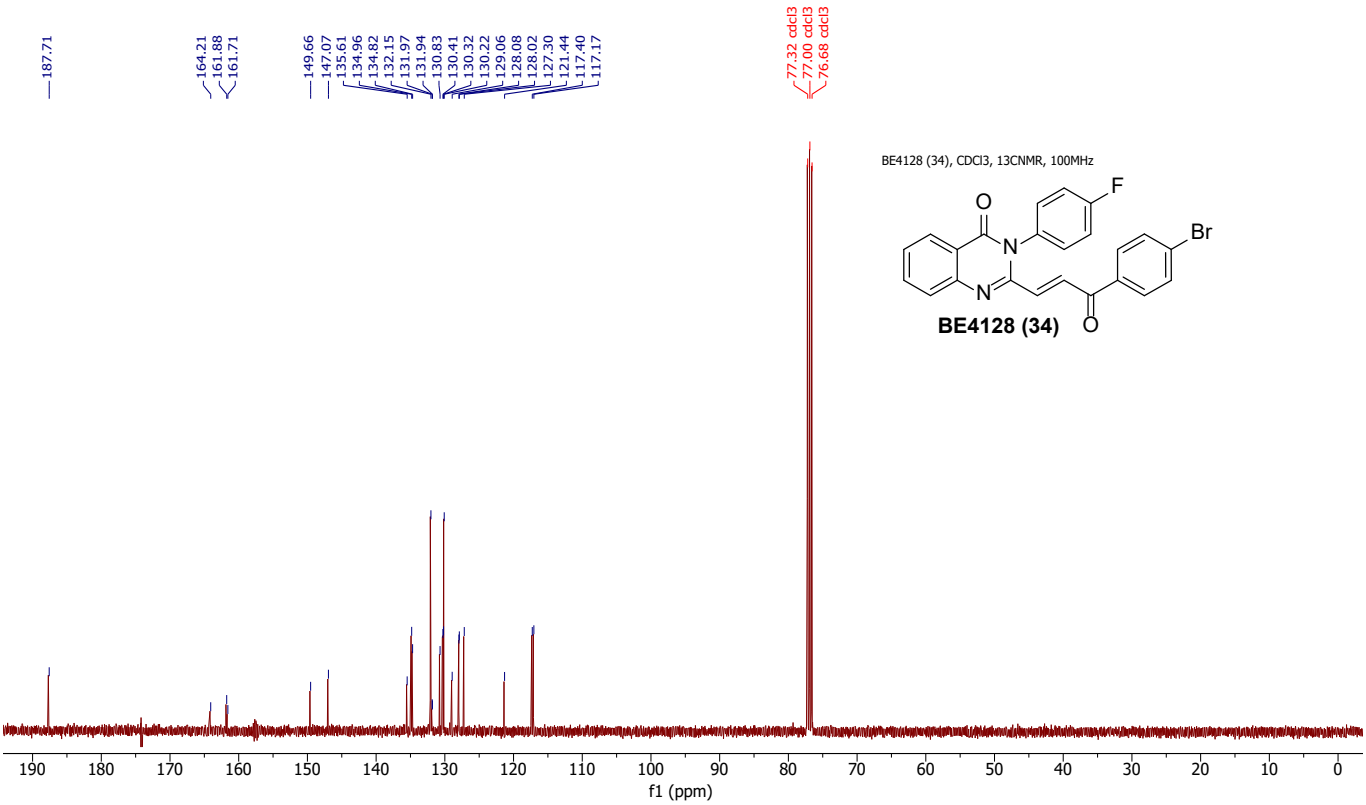


Figure S58. ^{13}CNMR spectra of BE4128 (34; $CDCl_3$, 100MHz)

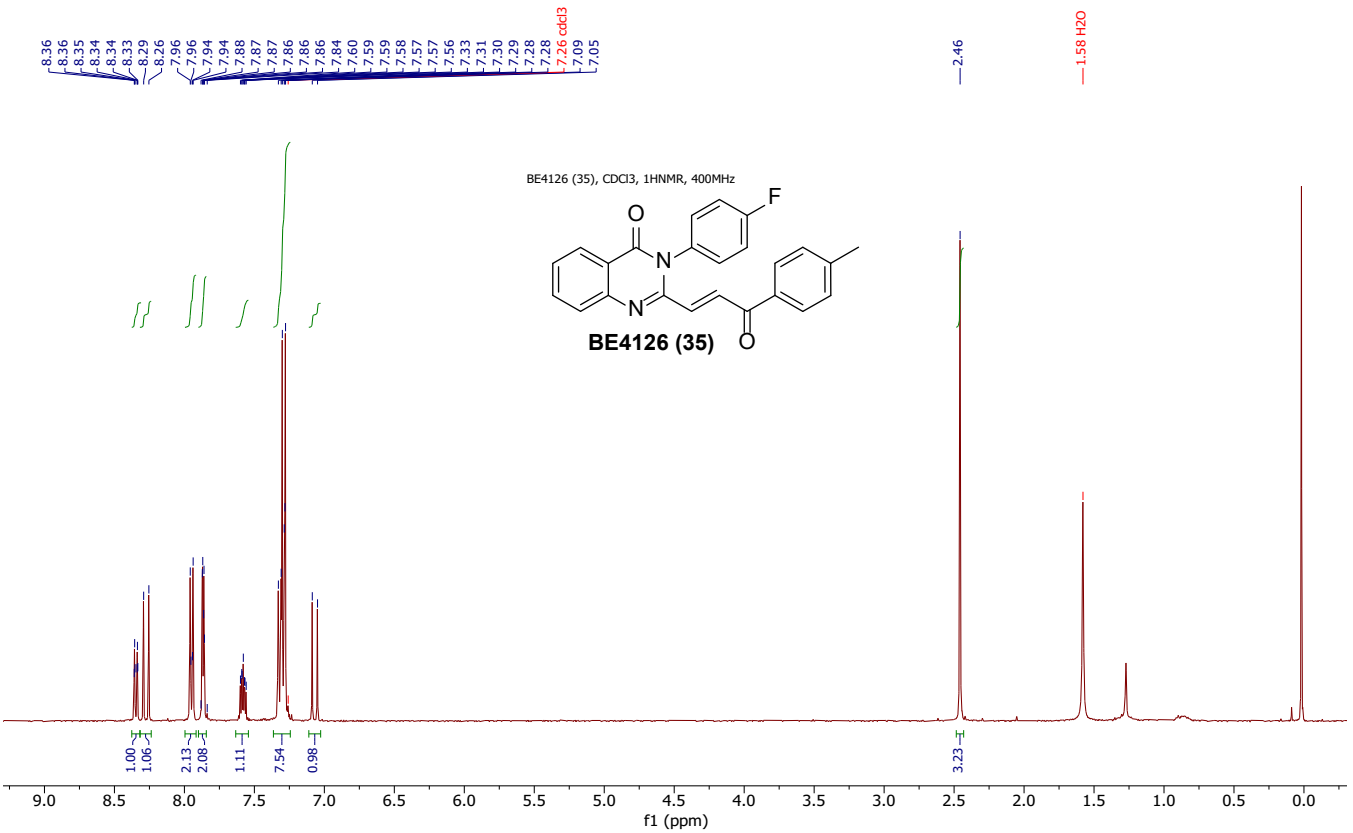


Figure S59. ^{1}HNMR spectra of BE4126 (35; $CDCl_3$, 400MHz)

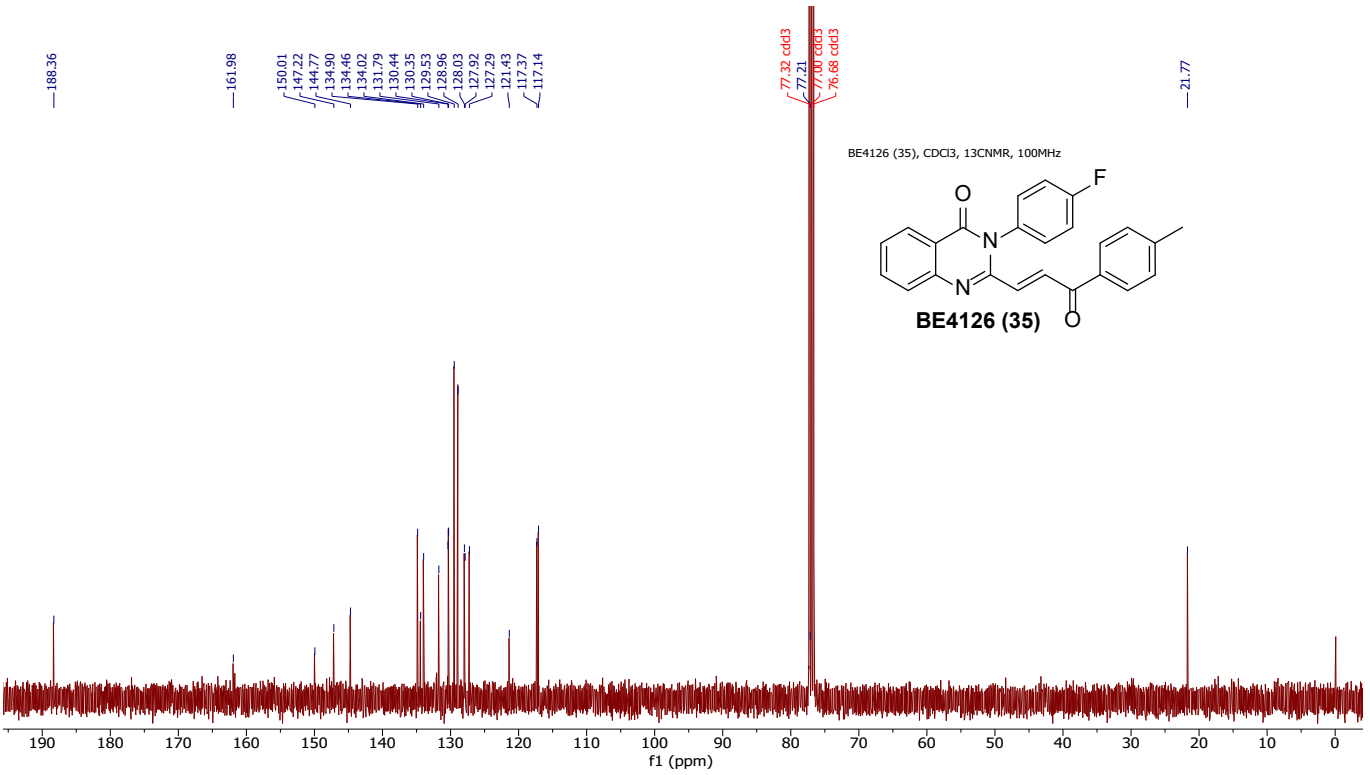


Figure S60. ^{13}CNMR spectra of BE4126 (35; $CDCl_3$, 100MHz)

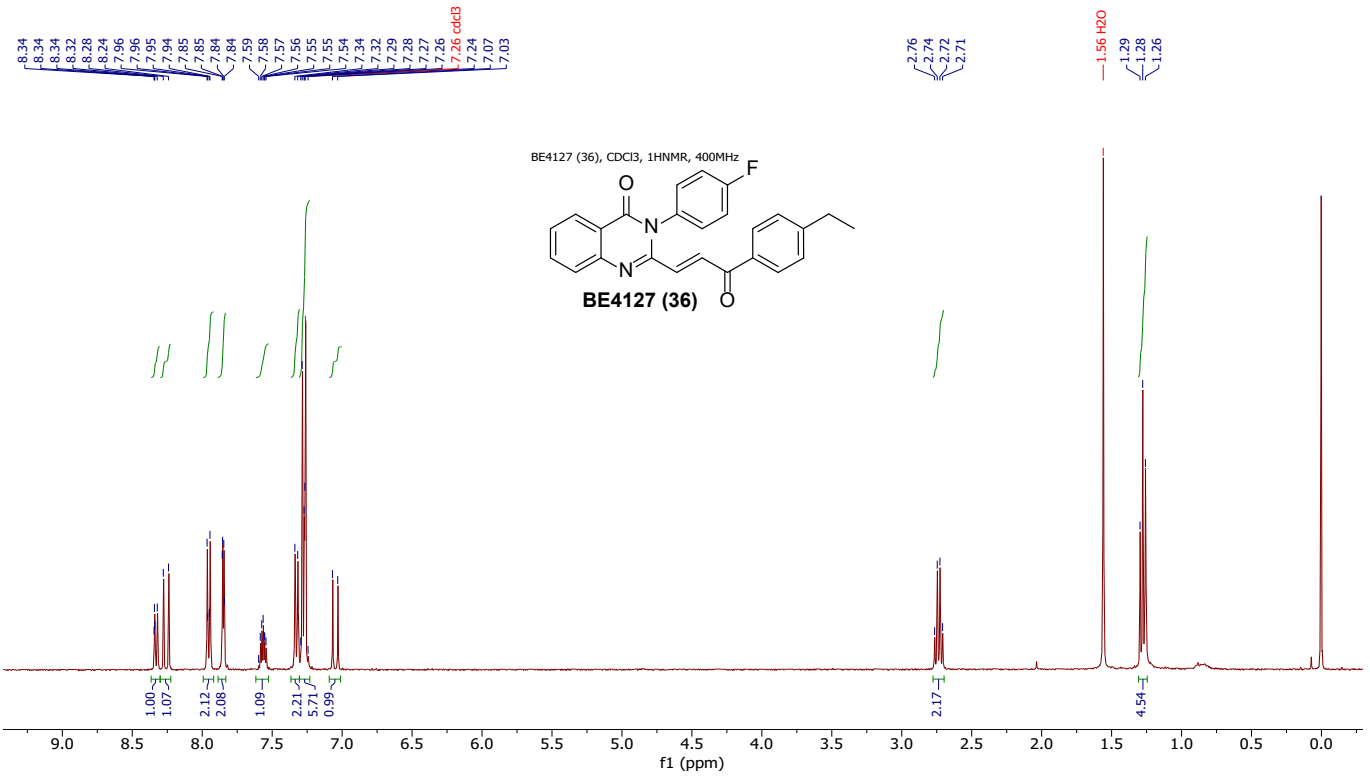


Figure S61. ^{1}HNMR spectra of BE4127 (36; $CDCl_3$, 400MHz)

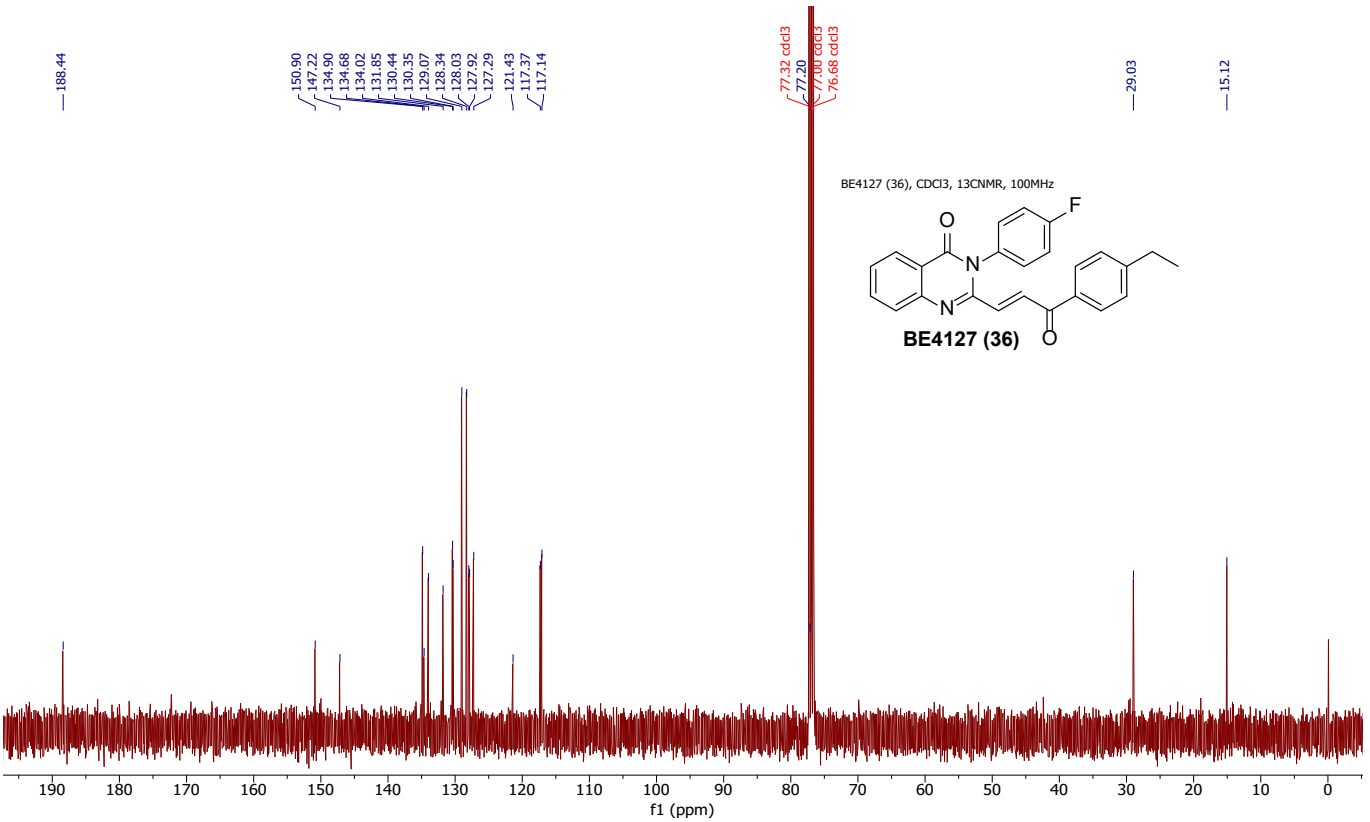


Figure S62. ^{13}CNMR of spctra BE4127 (36; $CDCl_3$, 100MHz)

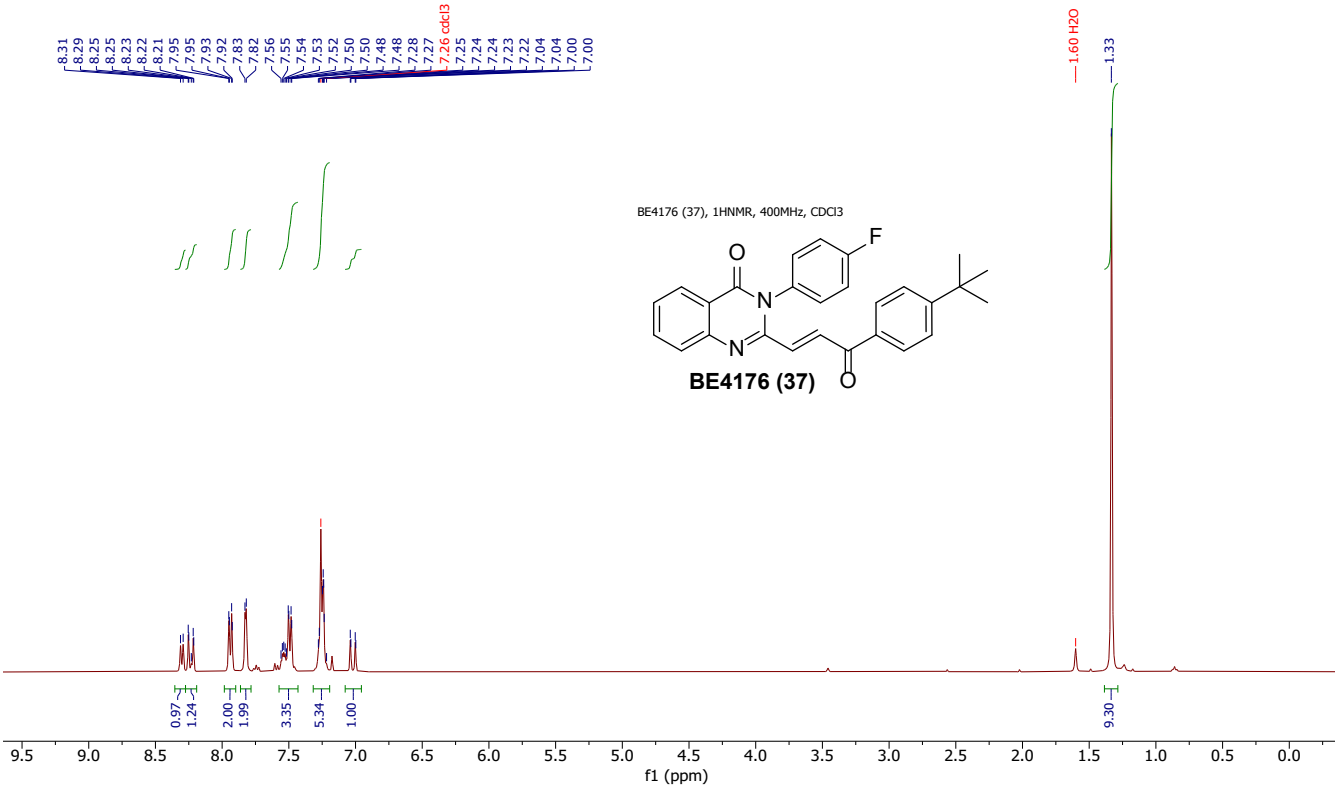


Figure S63. ^{1}HNMR spectra of BE4176 (37; $CDCl_3$, 400MHz)

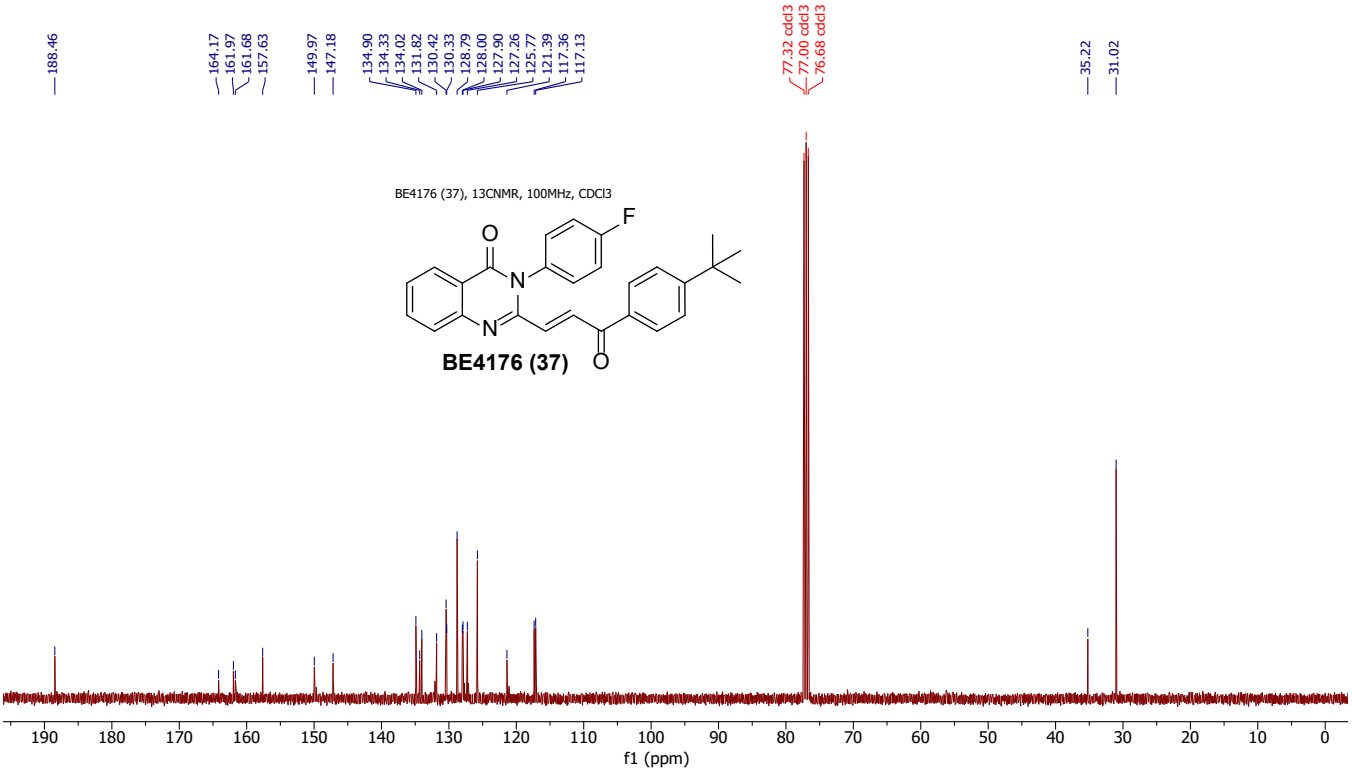


Figure S64. ^{13}CNMR spectra of BE4176 (37; $CDCl_3$, 100MHz)

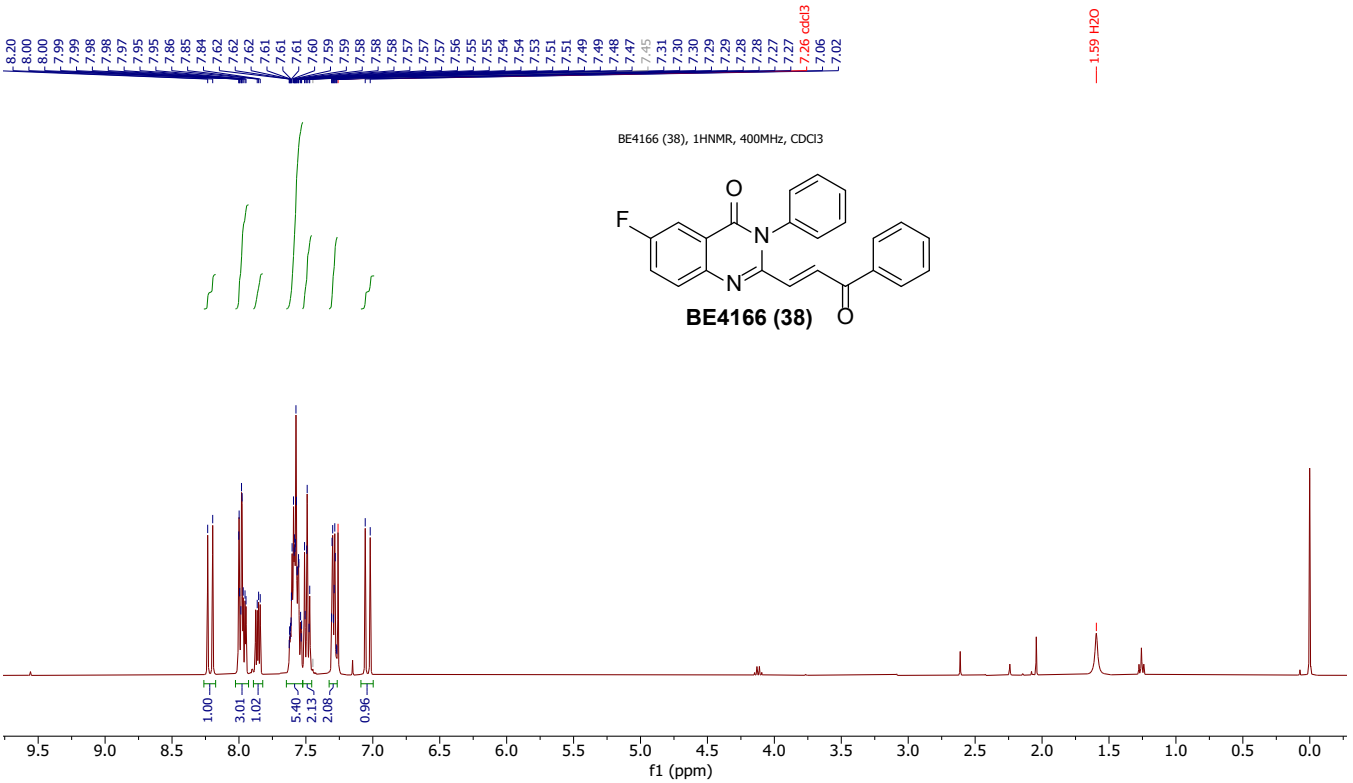


Figure S65. ^{1}HNMR spectra of BE4166 (38; $CDCl_3$, 400MHz)

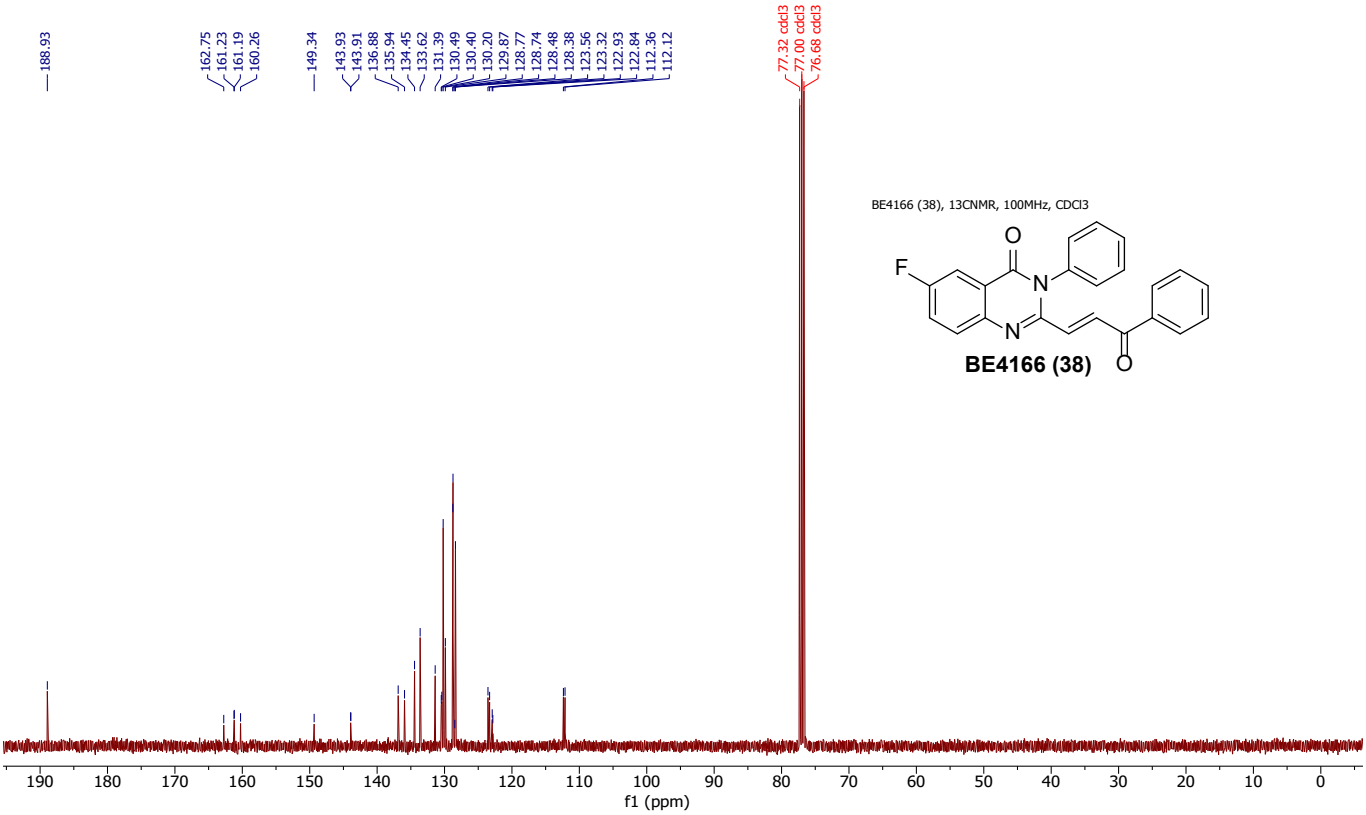


Figure S66. ^{13}CNMR spectra of BE4166 (38; $CDCl_3$, 100MHz)

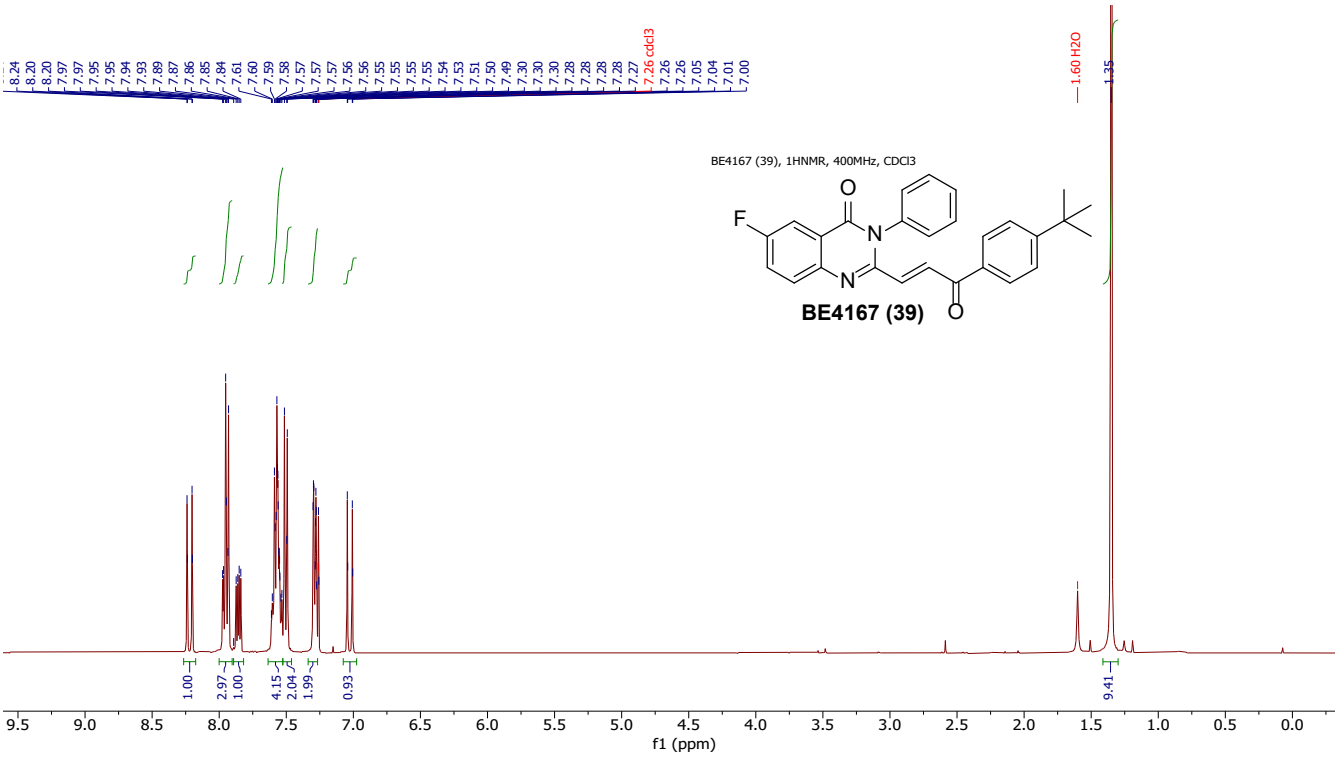


Figure S67. ^{1}HNMR spectra of BE4167 (39; $CDCl_3$, 400MHz)

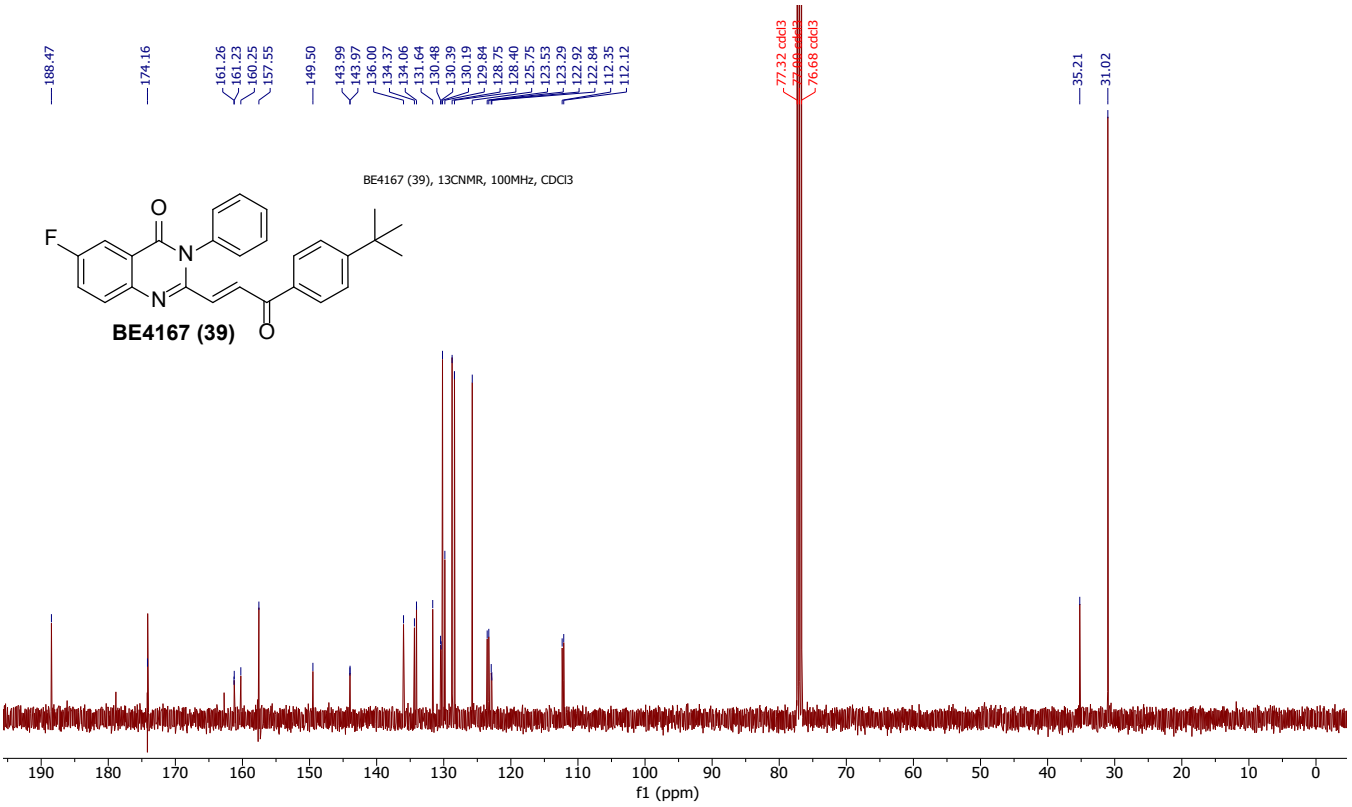


Figure S68. ^{13}CNMR spectra of BE4167 (39; $CDCl_3$, 100MHz)

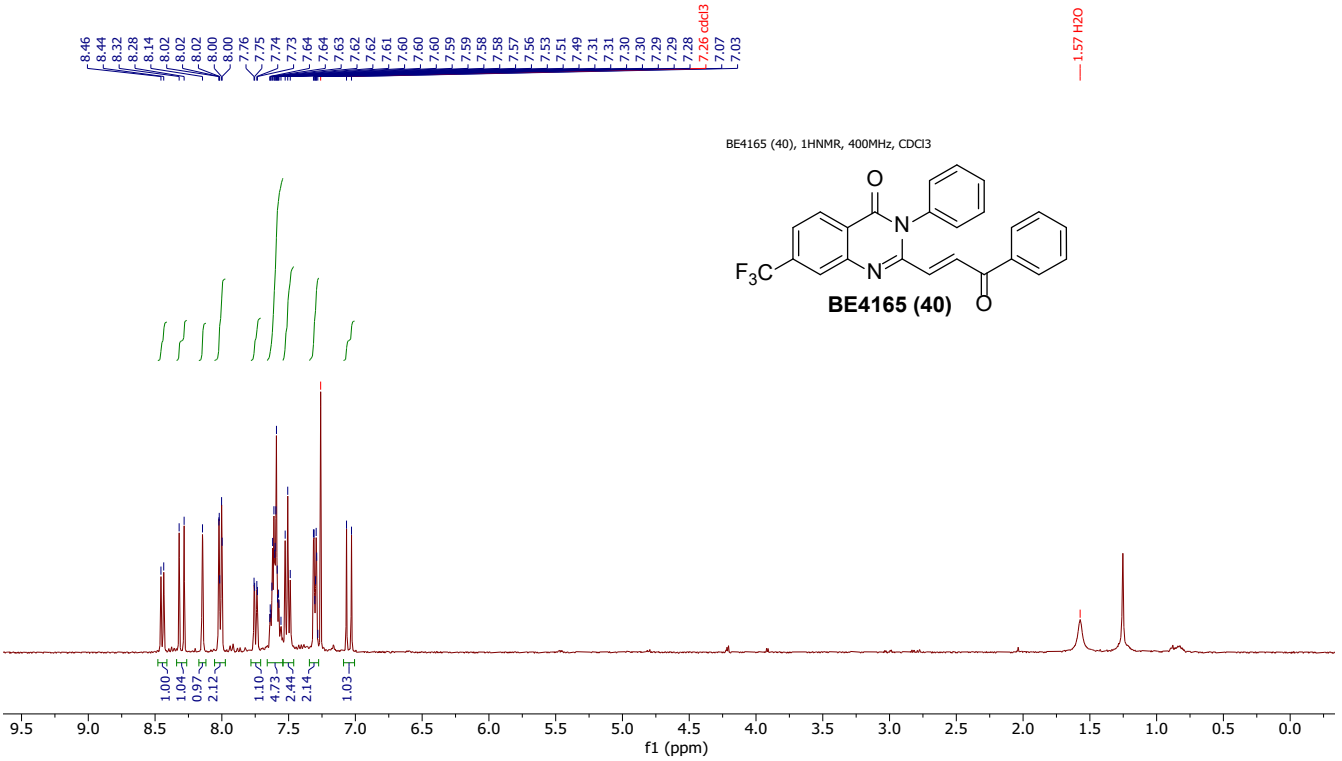


Figure S69. ^{1}HNMR spectra of BE4165 (40; $CDCl_3$, 400MHz)

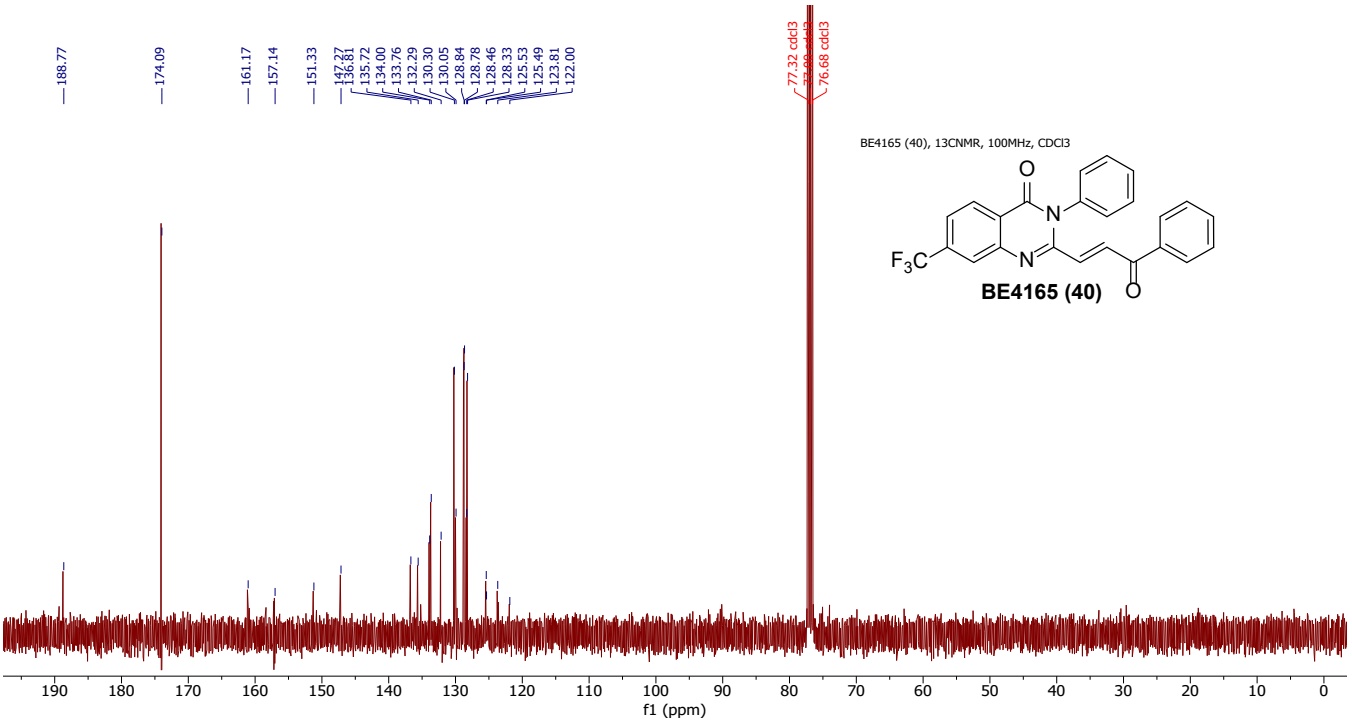


Figure S70. ^{13}CNMR spectra of BE4165 (40; $CDCl_3$, 100MHz)

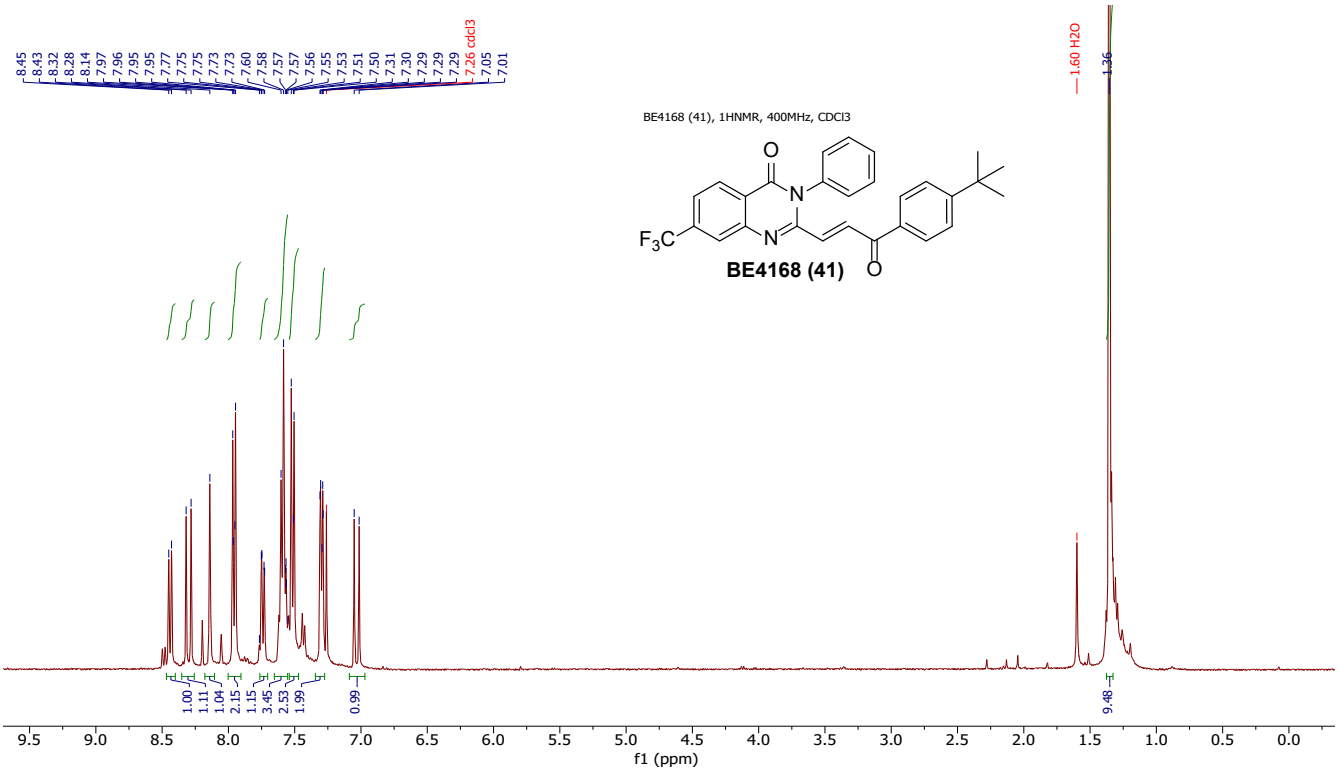


Figure S71. ^{1}HNMR spectra of BE4168 (41; $CDCl_3$, 400MHz)

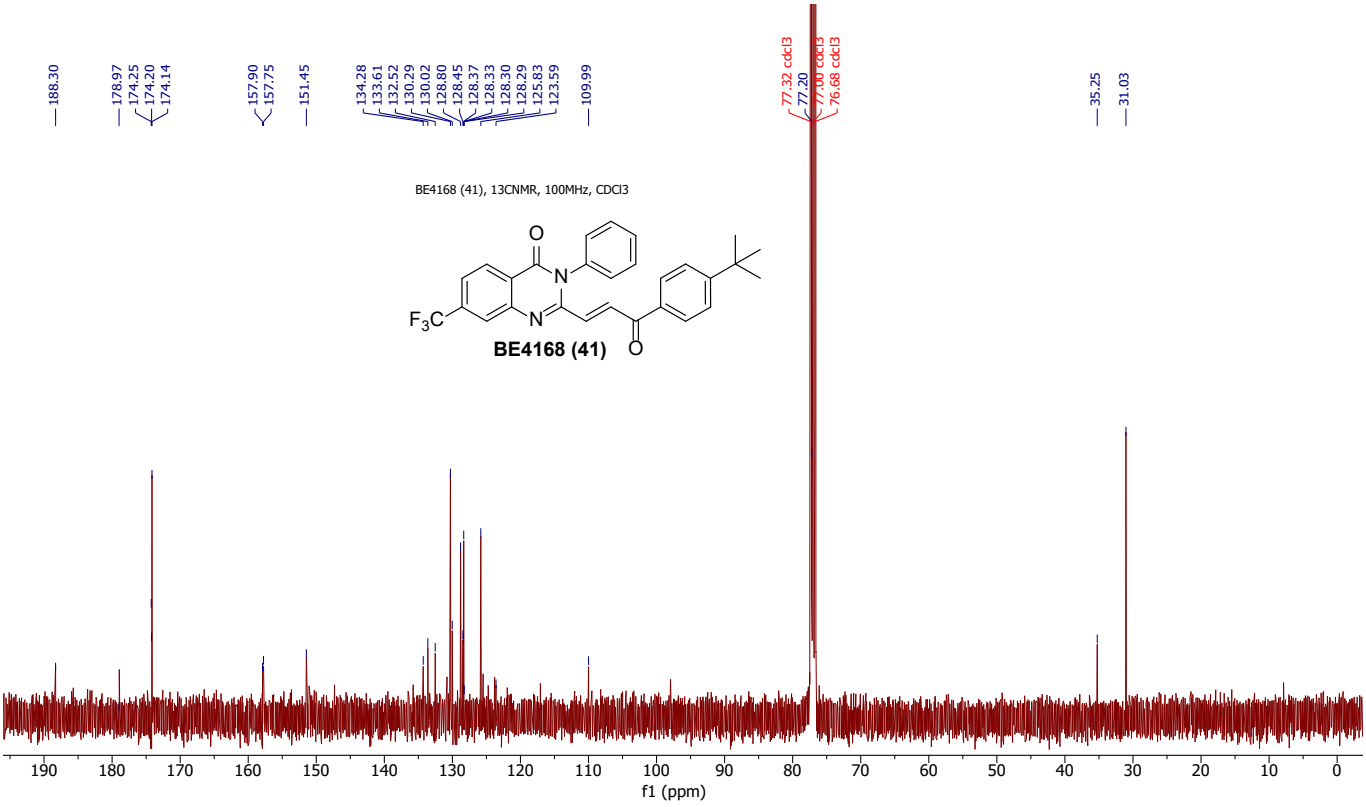


Figure S72. ^{13}CNMR spectra of BE4168 (41; $CDCl_3$, 100MHz)

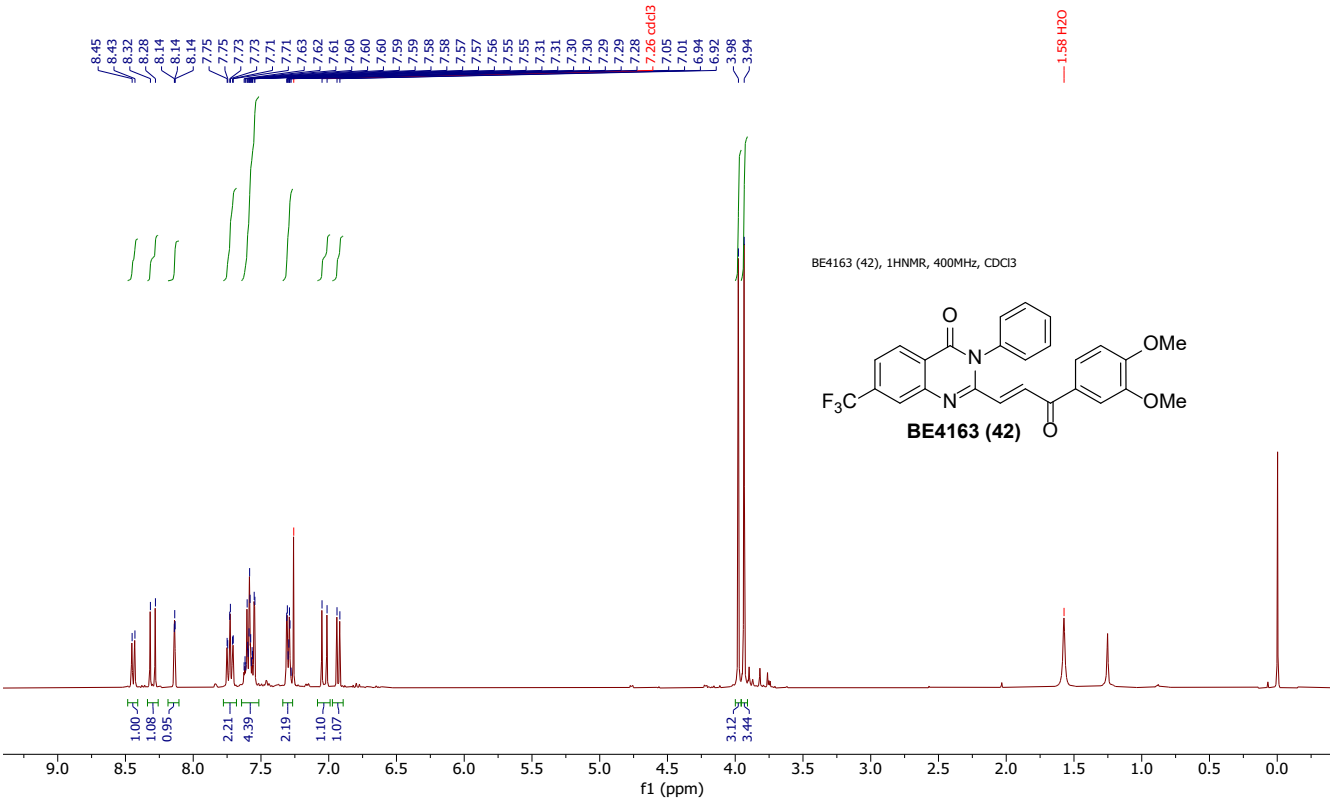


Figure S73. ^{1}HNMR spectra of BE4163 (42; $CDCl_3$, 400MHz)

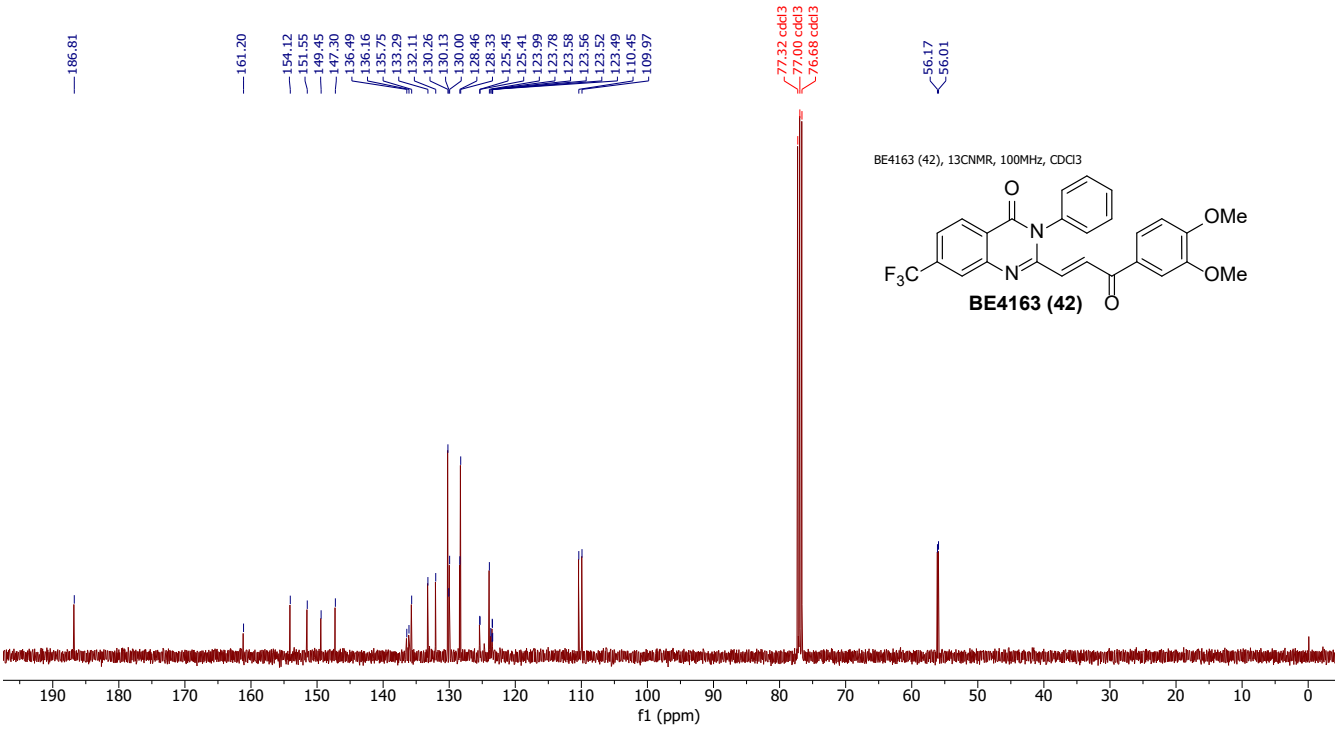


Figure S74. ^{13}CNMR spectra of BE4163 (42; $CDCl_3$, 100MHz)

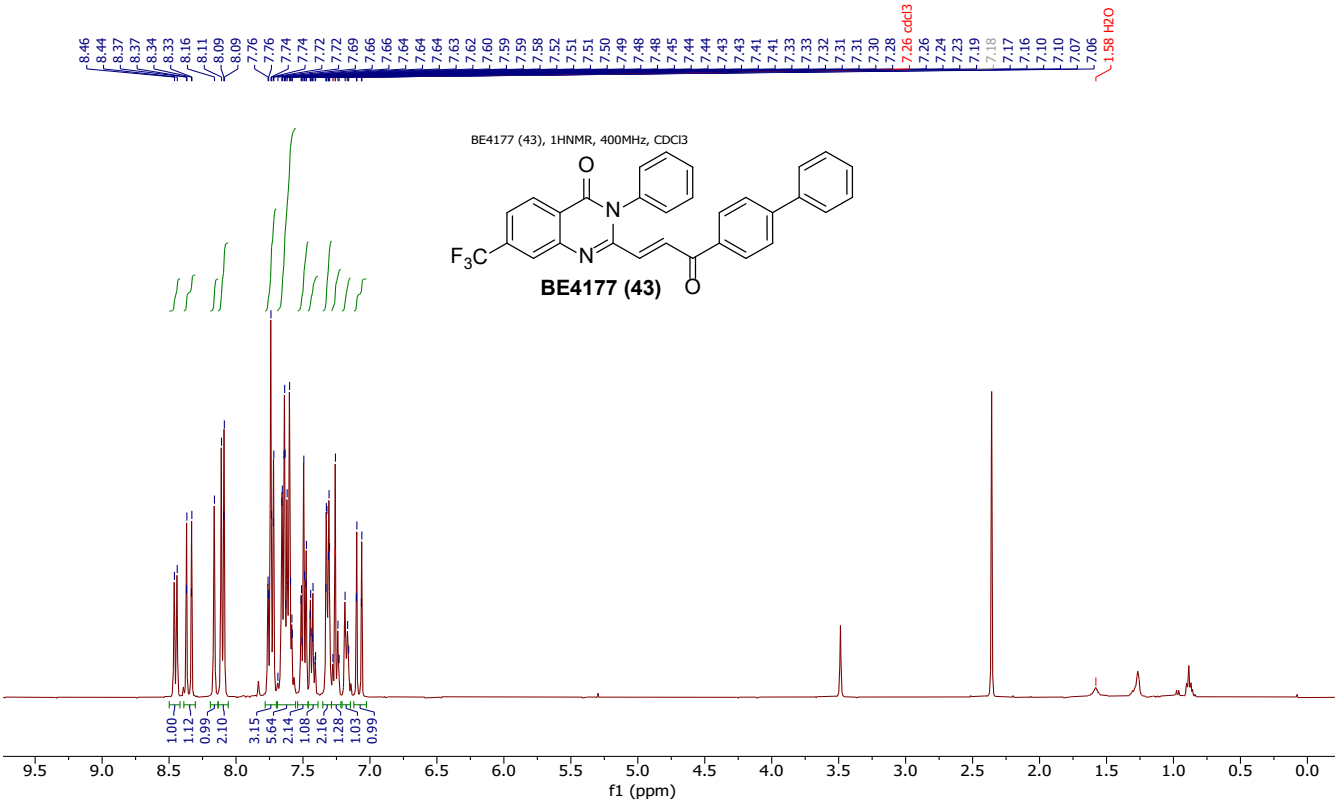


Figure S75. ^{1}HNMR spectra of BE4177 (43; $CDCl_3$, 400MHz)

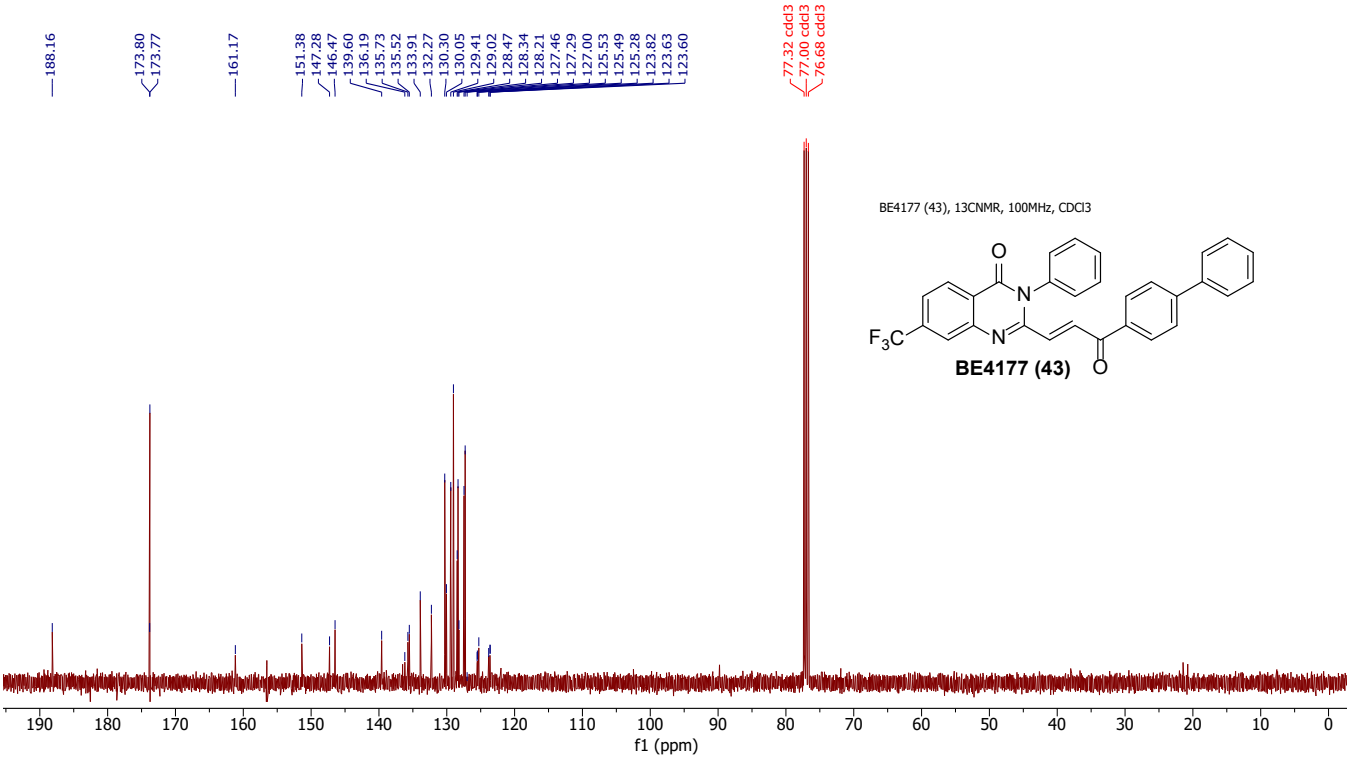


Figure S76. ^{13}CNMR spectra of BE4177 (43; $CDCl_3$, 100MHz)

HRMS Data:

Compound 9b:

Generic Display Report

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Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	compound 9b	Instrument	solariX XR
Comment	compound-9b in MeOH C15H11FN2O H+		

Sample Name	compound-9b in MeOH			
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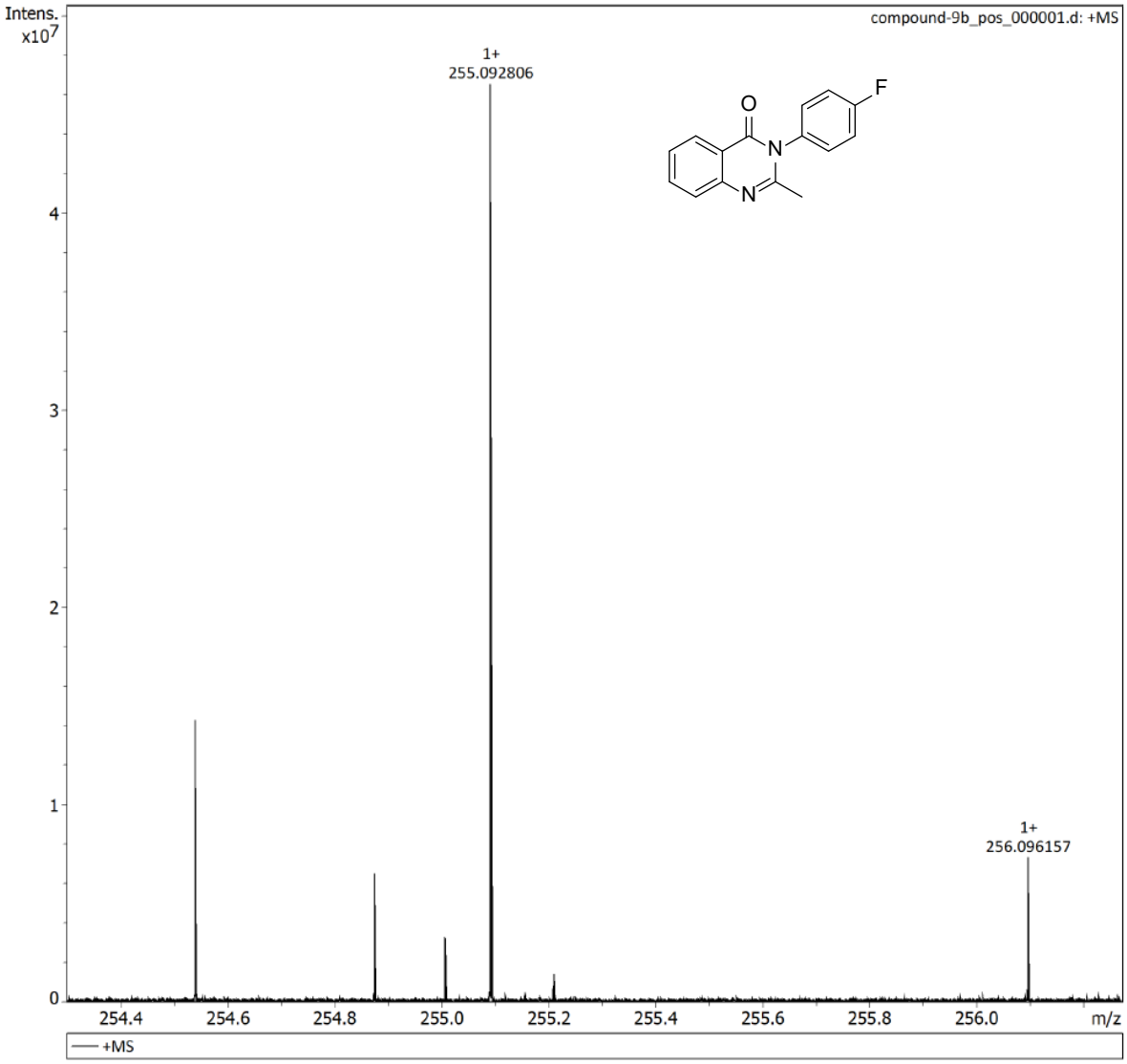
Mass Observed		=	255.092806	m/z

Difference < 1.0 ppm



Compound 9c:

Generic Display Report

Analysis Info

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Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	compound 9c	Instrument	solariX XR
Comment	compound-9c in MeOH C15H11FN2O H+		

Sample Name	compound-9c in MeOH			
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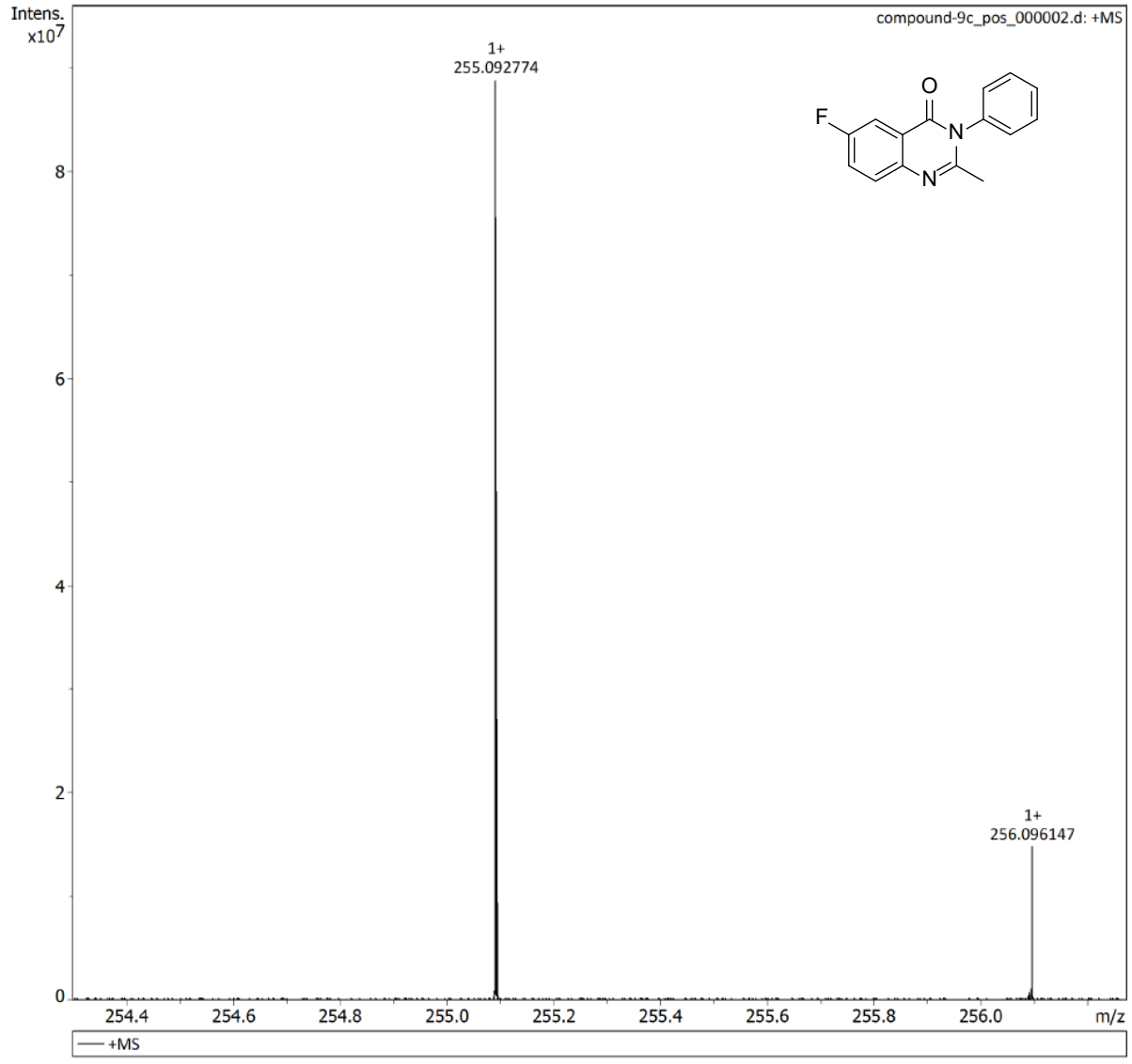
Mass Observed		=	255.092774	m/z

Difference < 1.0 ppm



Compound 9d:

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Analysis Info

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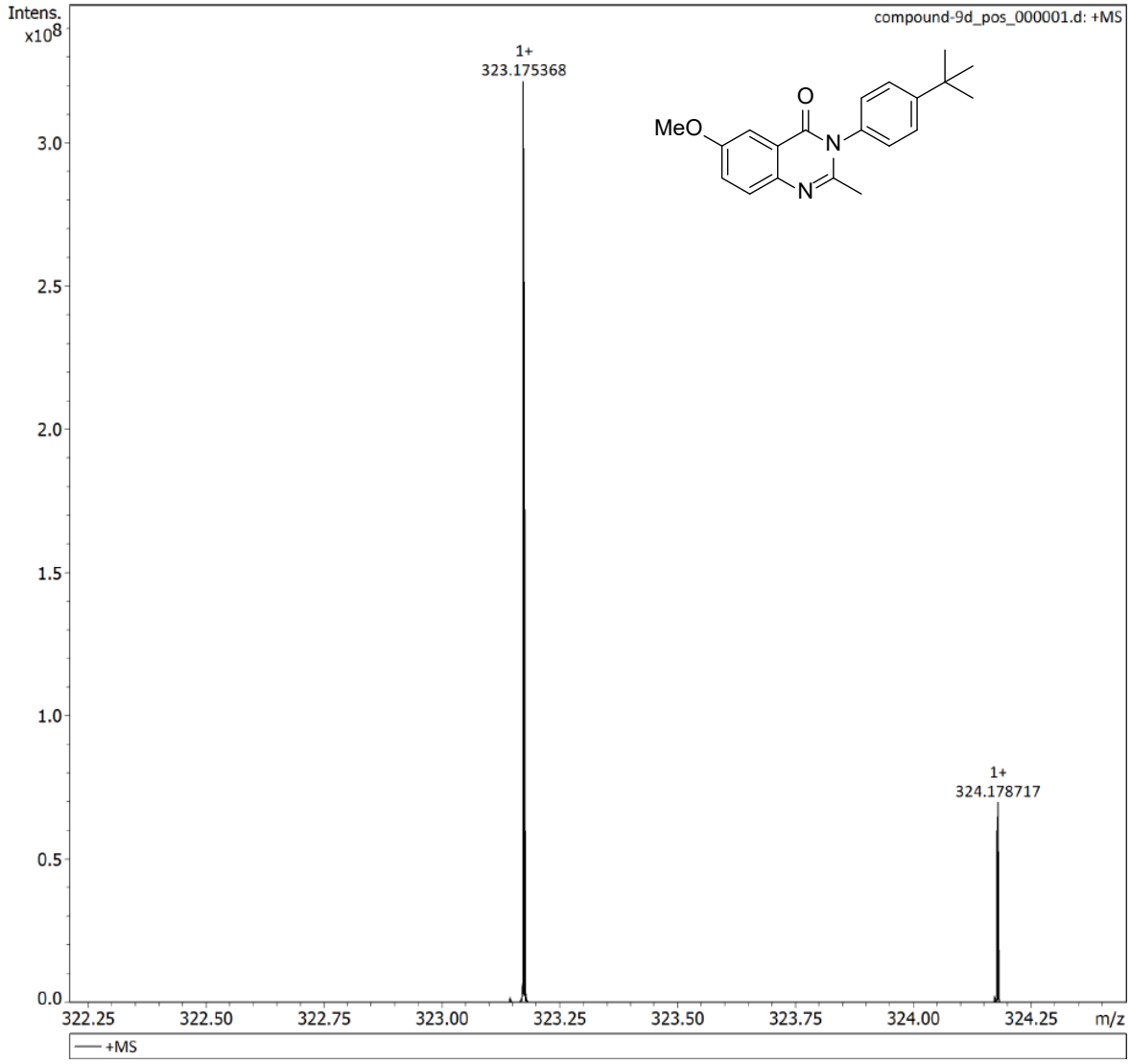
Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	compound 9d	Instrument	solariX XR
Comment	compound-9d in MeOH C20H22N2O2 H+		

Sample Name	compound-9d in MeOH			
Exact Mass of	C20H22N2O2 H+	=	323.175404	m/z
Mass Observed		=	323.175368	m/z

Difference < 1.0 ppm



Compound 9e:

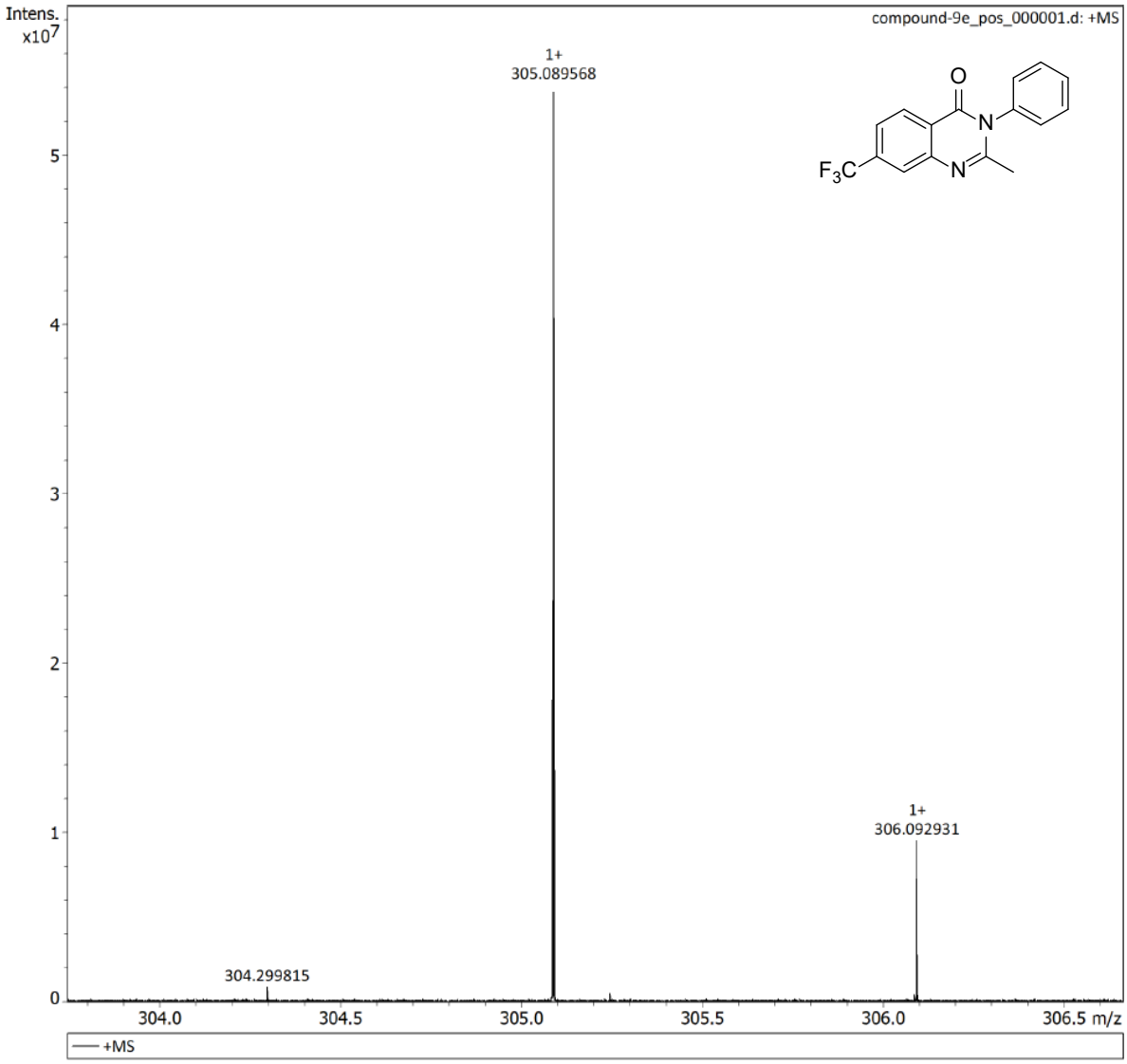
Generic Display Report

Analysis Info

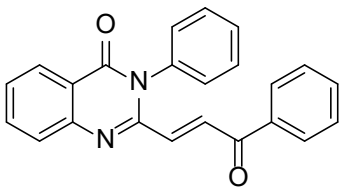
		Acquisition Date	6/3/2025 3:31:20 PM
Analysis Name	F:\MS1 COSMIC\2025\Data_20250603\compound-9e_pos_000001.d		
Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	compound 9e	Instrument	solariX XR
Comment	compound-9e in MeOH C16H11F3N2O H+		

Sample Name	compound-9e in MeOH			
Exact Mass of	C16H11F3N2O H+	=	305.089624	m/z
Mass Observed		=	305.089568	m/z

Difference < 1.0 ppm



(*E*)-2-(3-Oxo-3-phenylprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4117 (11):

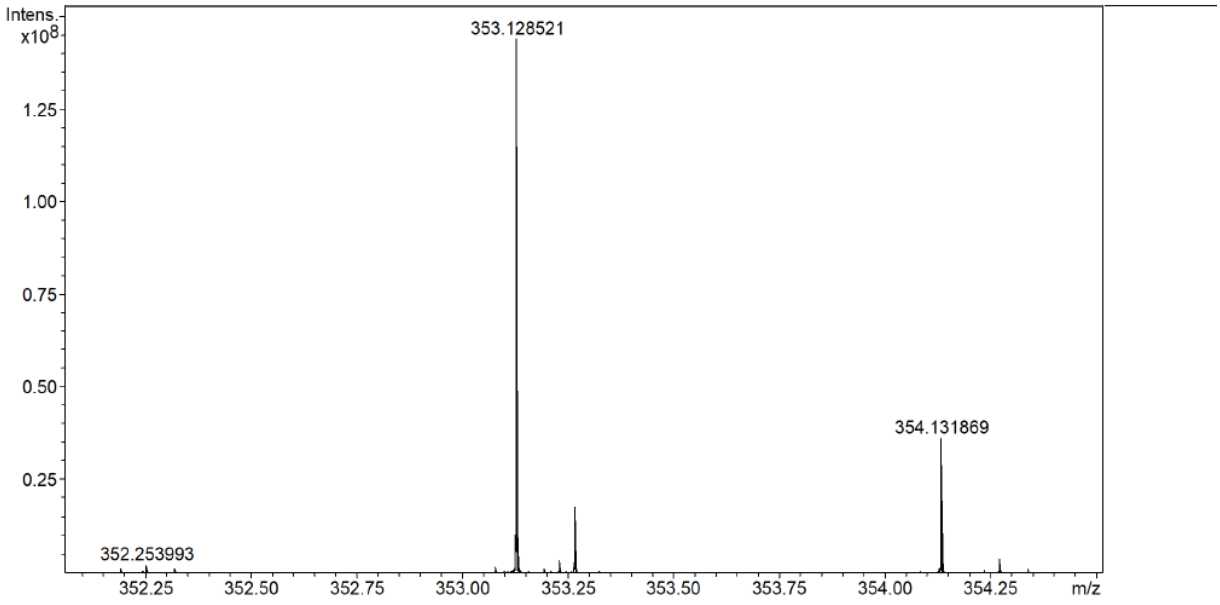


Mass Spectrum List Report

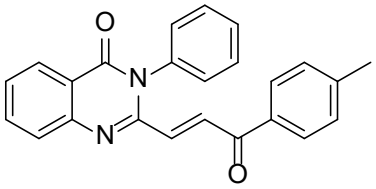
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250530\BE-4117_pos_000001.d	Acquisition Date	5/30/2025 4:57:27 PM
Method		Operator	Admin
Sample Name	BE4117	Instrument	solariX XR
Comment	BE-4117 in MeOH C23H16N2O2 H+		

Sample Name	BE-4117 in MeOH			
Exact Mass of	C23H16N2O2 H+	=	353.128454	m/z
Mass Observed		=	353.128521	m/z

Difference < 1.0 ppm



(*E*)-2-(3-Oxo-3-(p-tolyl)prop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4120 (12):

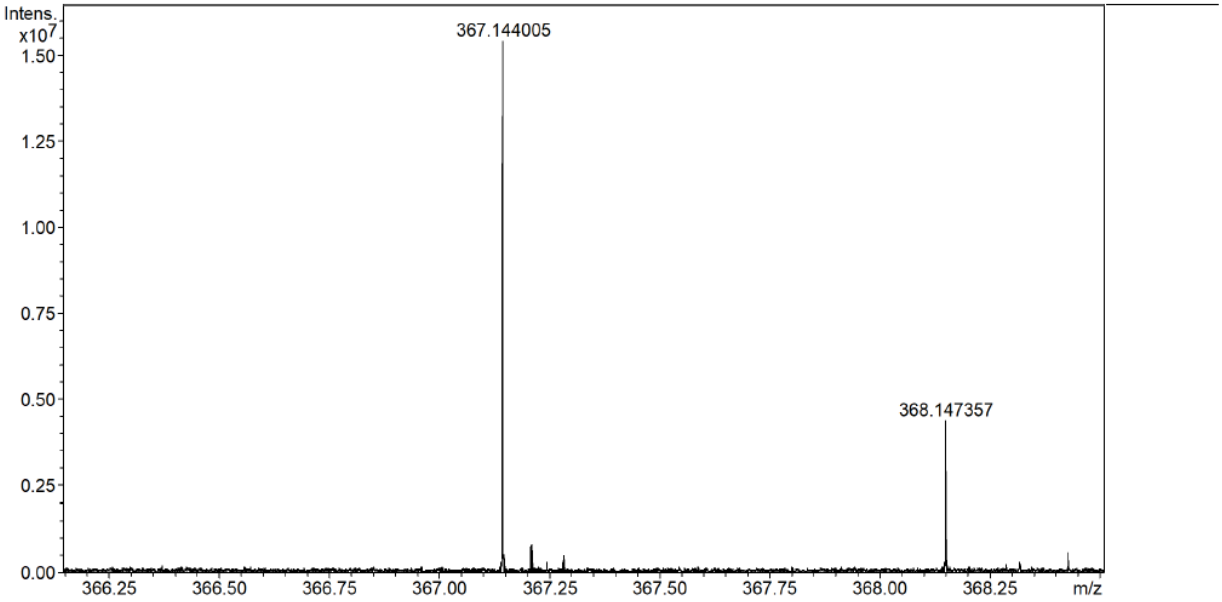


Mass Spectrum List Report

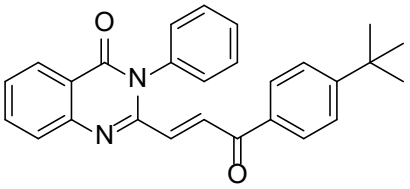
Analysis Info		Acquisition Date	5/30/2025 5:03:49 PM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250530\BE-4120_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4120	Instrument	solariX XR
Comment	BE-4120 in MeOH C24H18N2O2 H+		

Sample Name	BE-4120 in MeOH			
Exact Mass of	C24H18N2O2 H+	=	367.144104	m/z
Mass Observed		=	367.144005	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-(tert-Butyl)phenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4169 (13):

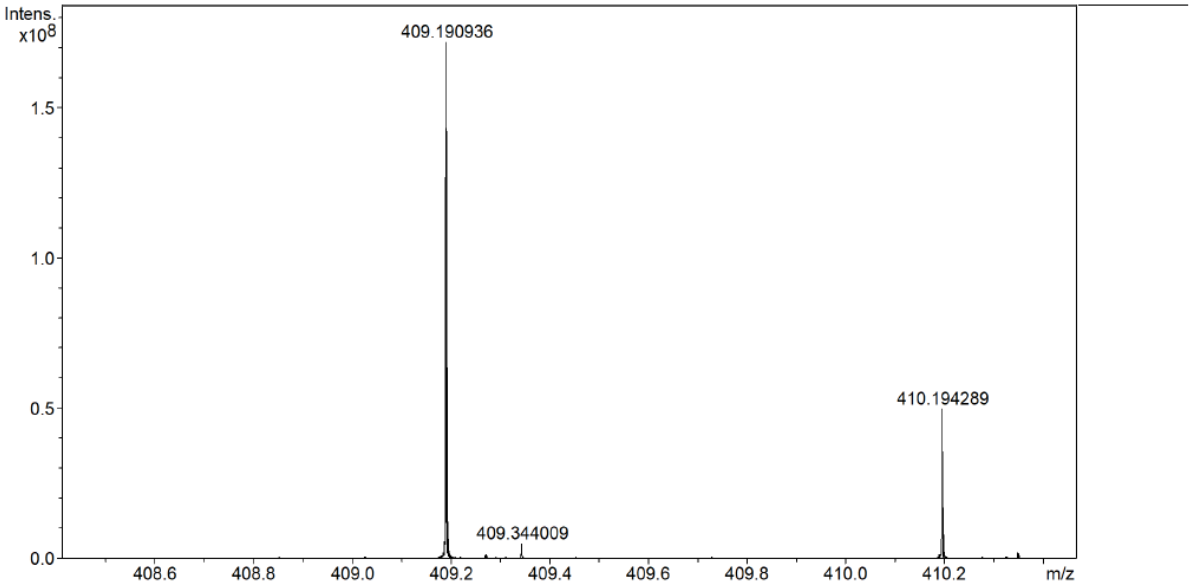


Mass Spectrum List Report

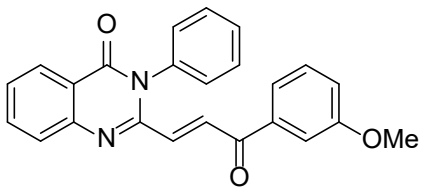
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250530\BE-4169_pos_000002.d	Acquisition Date	5/30/2025 5:12:20 PM
Method		Operator	Admin
Sample Name	BE4169	Instrument	solariX XR
Comment	BE-4169 in MeOH C27H24N2O2 H+		

Sample Name	BE-4169 in MeOH			
Exact Mass of	C27H24N2O2 H+	=	409.191054	m/z
Mass Observed		=	409.190936	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(3-Methoxyphenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4136 (14):

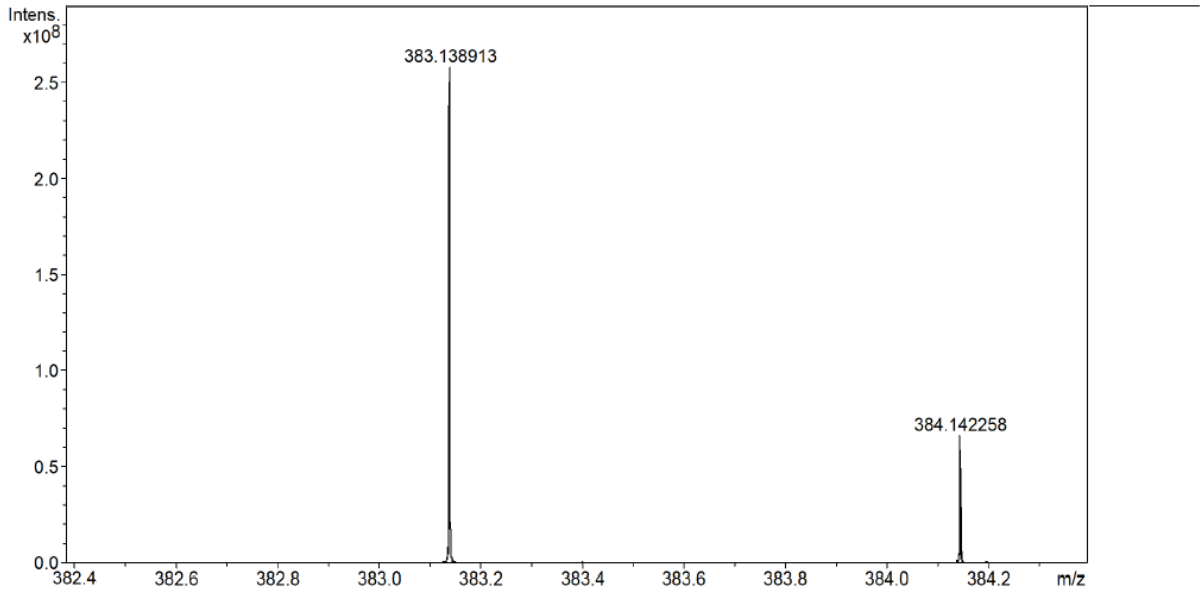


Mass Spectrum List Report

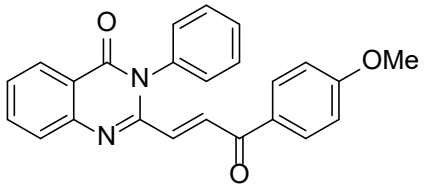
Analysis Info		Acquisition Date	5/30/2025 5:18:26 PM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250530\BE-4136_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4136	Instrument	solariX XR
Comment	BE-4136 in MeOH C24H18N2O3 H+		

Sample Name	BE-4136 in MeOH			
Exact Mass of	C24H18N2O3 H+	=	383.139019	m/z
Mass Observed		=	383.138913	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-Methoxyphenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4133 (15):

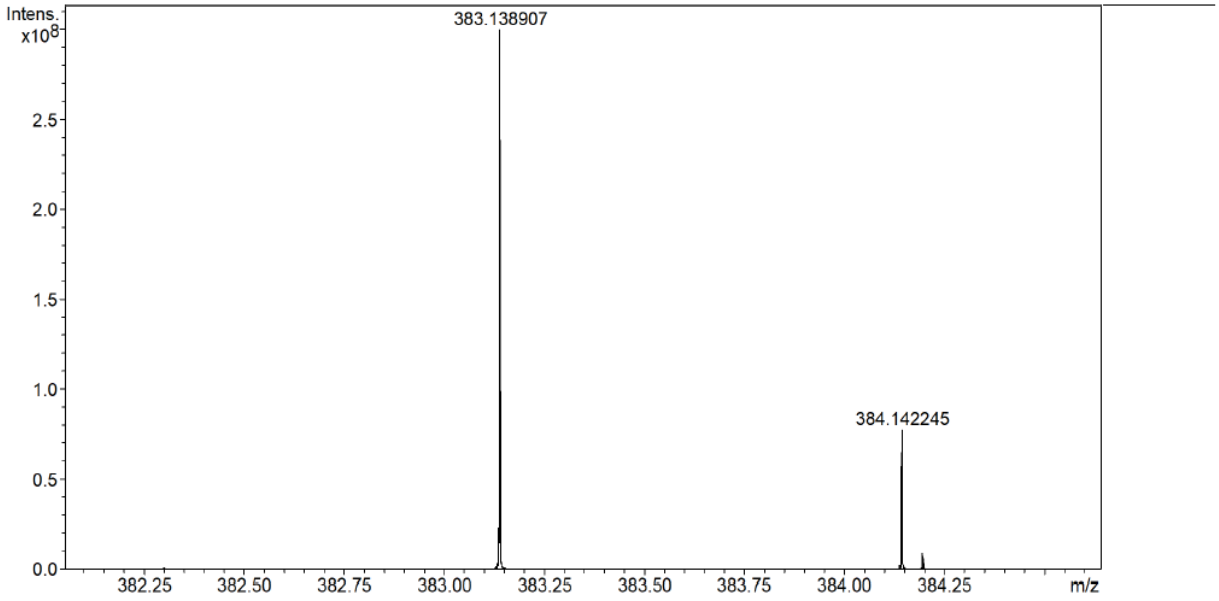


Mass Spectrum List Report

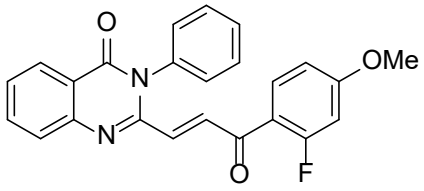
Analysis Info		Acquisition Date	6/2/2025 3:14:16 PM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4133_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4133	Instrument	solariX XR
Comment	BE-4133 in MeOH C24H18N2O3 H+		

Sample Name	BE-4133 in MeOH			
Exact Mass of	C24H18N2O3 H+	=	383.139019	m/z
Mass Observed		=	383.138907	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(2-Fluoro-4-methoxyphenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4132 (17):

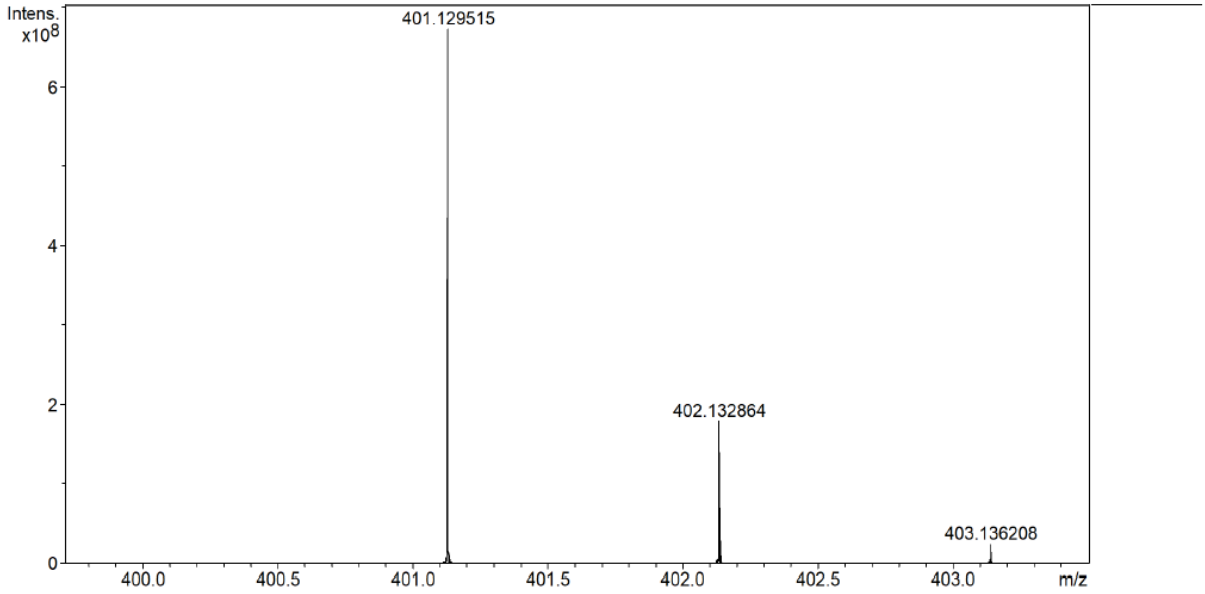


Mass Spectrum List Report

Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4132_pos_000001.d	Acquisition Date	6/2/2025 3:28:20 PM
Method		Operator	Admin
Sample Name	BE4132	Instrument	solariX XR
Comment	BE-4132 in MeOH C24H17FN2O3 H+		

Sample Name	BE-4132 in MeOH			
Exact Mass of	C24H17FN2O3 H+	=	401.129597	m/z
Mass Observed		=	401.129515	m/z

Difference < 1.0 ppm



(*E*)-2-(3-Oxo-3-(2-(trifluoromethoxy)phenyl)prop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4172 (18):

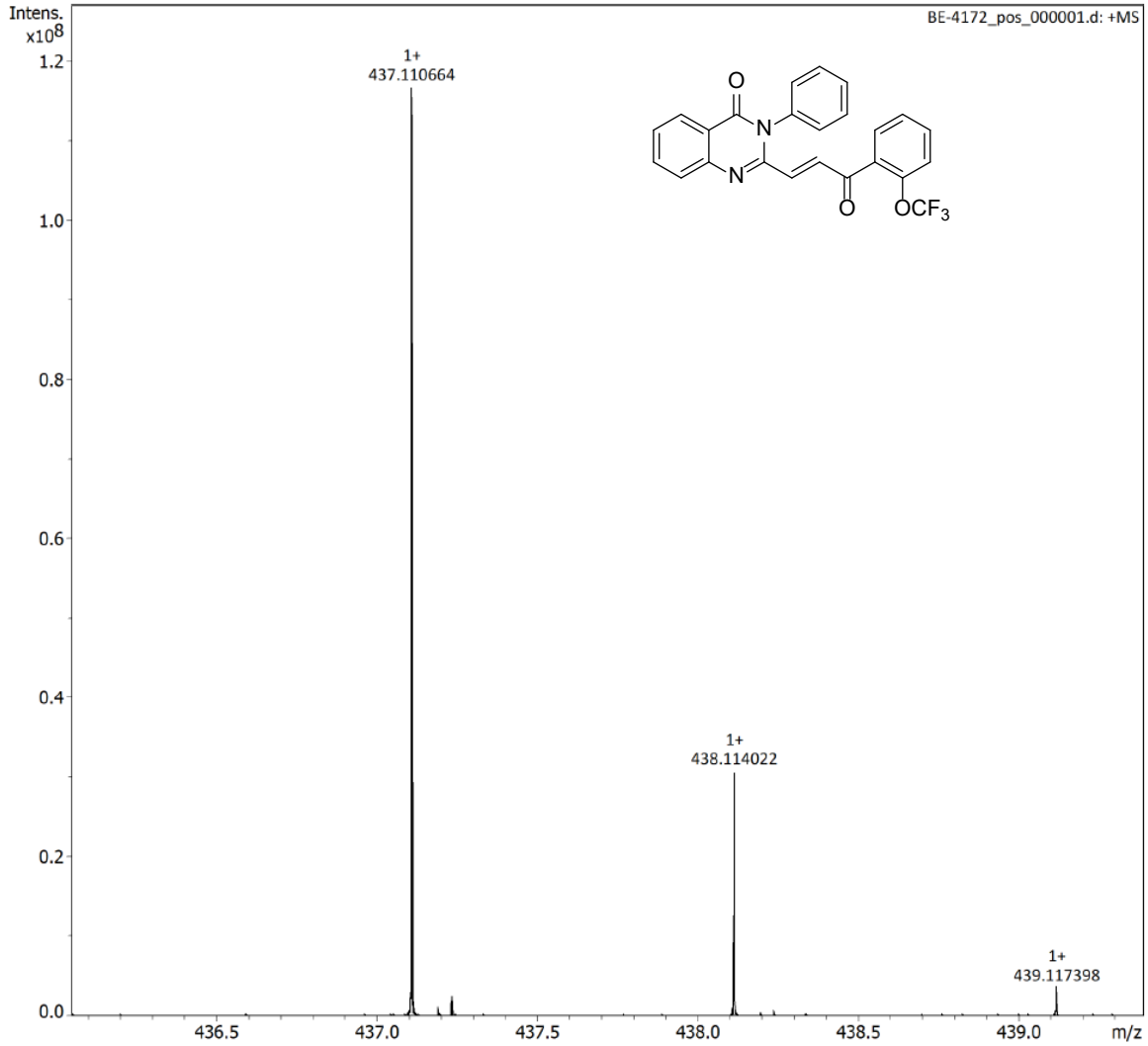
Generic Display Report

Analysis Info

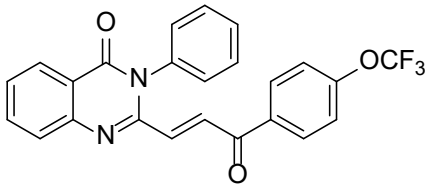
Analysis Name	F:\MS1 COSMIC\2025\Data_20250603\BE-4172_pos_000001.d	Acquisition Date	6/3/2025 12:56:04 PM
Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	BE4172	Instrument	solariX XR
Comment	BE-4172 in MeOH C24H15F3N2O3 H+		

Sample Name	BE-4172 in MeOH			
Exact Mass of	C24H15F3N2O3 H+	=	437.110753	m/z
Mass Observed		=	437.110664	m/z

Difference < 1.0 ppm



(*E*)-2-(3-Oxo-3-(4-(trifluoromethoxy)phenyl)prop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4175 (19):

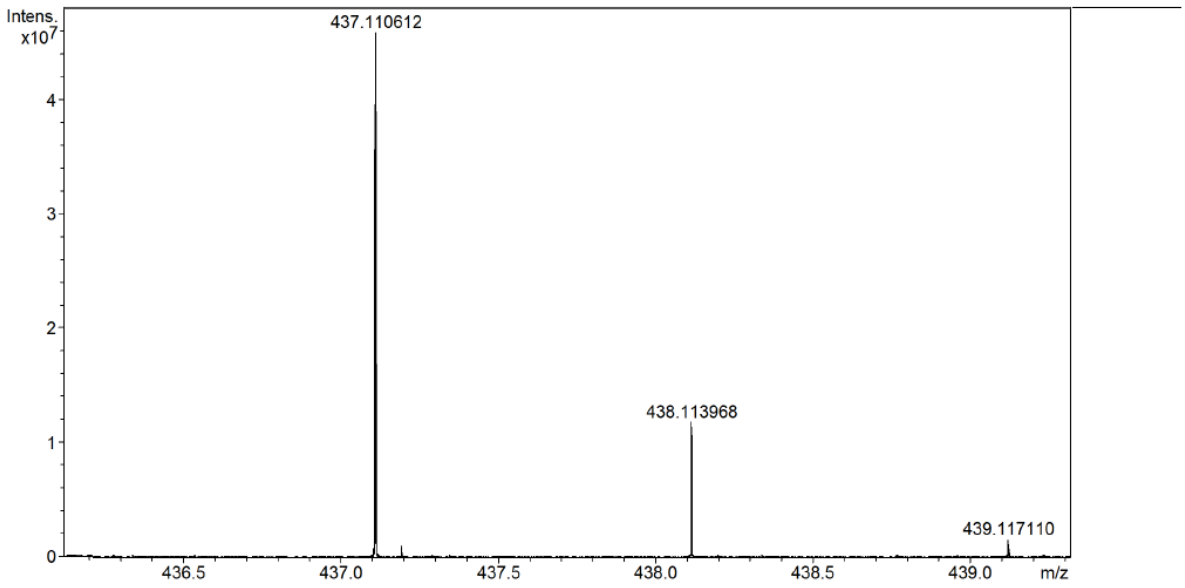


Mass Spectrum List Report

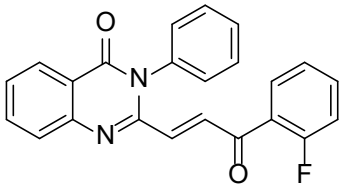
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250603\BE-4175_pos_000001.d	Acquisition Date	6/3/2025 12:18:42 PM
Method		Operator	Admin
Sample Name	BE4175	Instrument	solariX XR
Comment	BE-4175 in MeOH C24H15F3N2O3 H+		

Sample Name	BE-4175 in MeOH			
Exact Mass of	C24H15F3N2O3 H+	=	437.110753	m/z
Mass Observed		=	437.110612	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(2-Fluorophenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4135 (20):

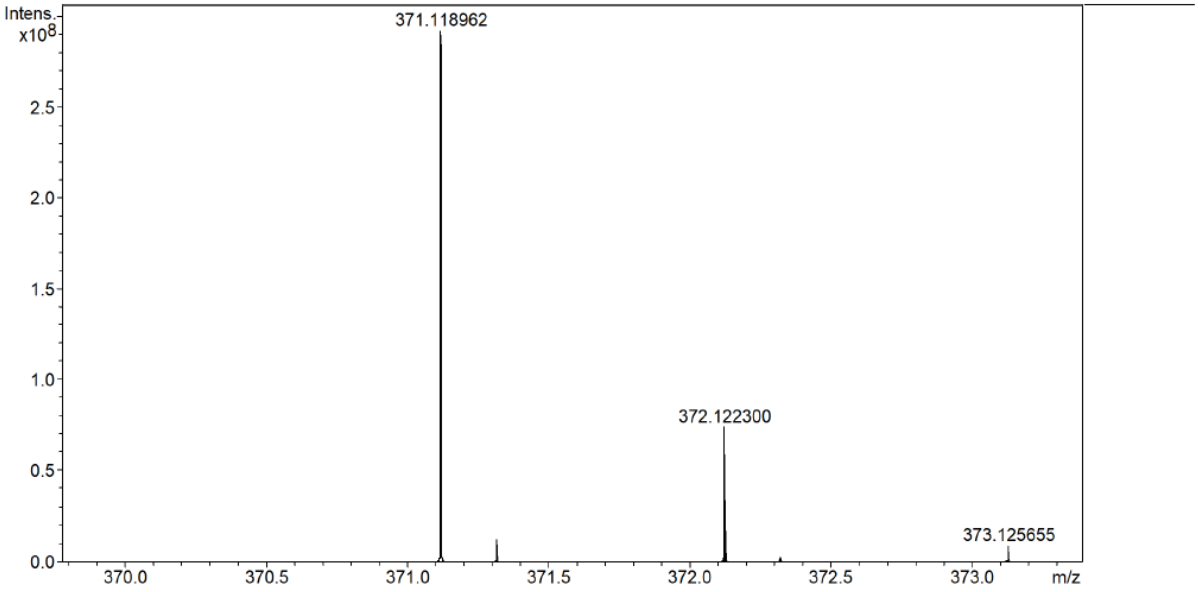


Mass Spectrum List Report

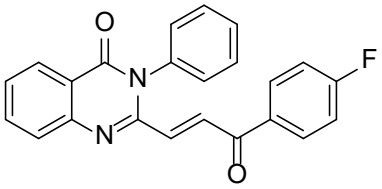
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4135_pos_000001.d	Acquisition Date	6/2/2025 4:45:32 PM
Method		Operator	Admin
Sample Name	BE4135	Instrument	solariX XR
Comment	BE-4135 in MeOH C23H15FN2O2 H+		

Sample Name	BE-4135 in MeOH			
Exact Mass of	C23H15FN2O2 H+	=	371.119032	m/z
Mass Observed		=	371.118962	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-Fluorophenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4118 (21):

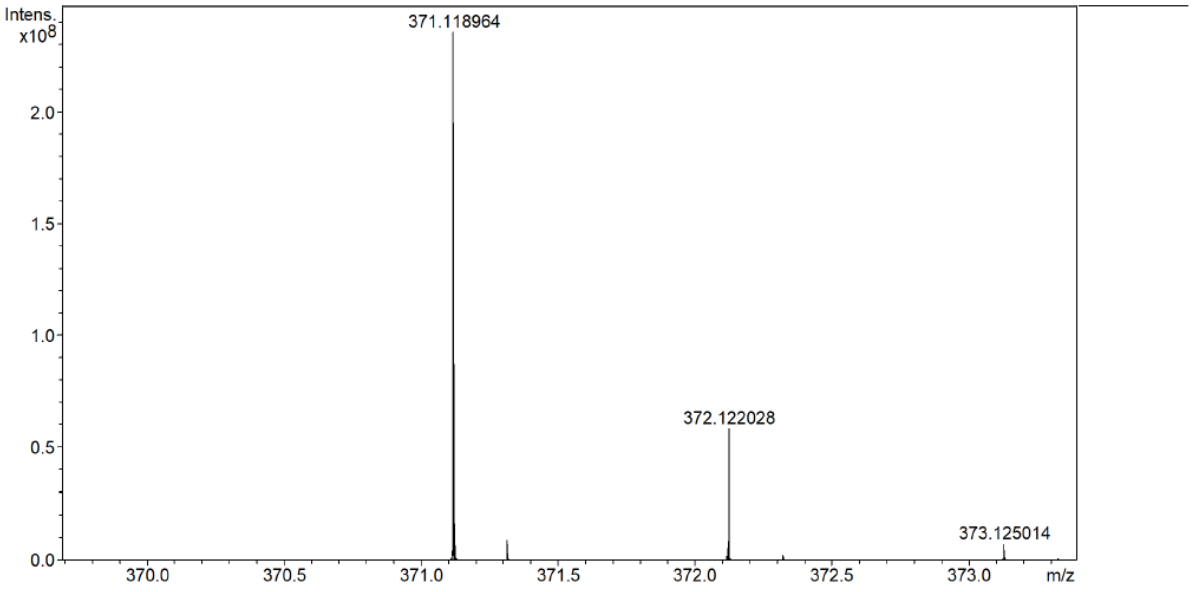


Mass Spectrum List Report

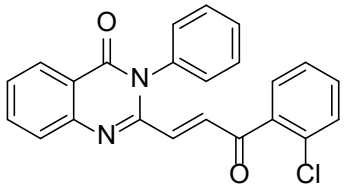
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4118_pos_000001.d	Acquisition Date	6/2/2025 4:31:07 PM
Method		Operator	Admin
Sample Name	BE4118	Instrument	solariX XR
Comment	BE-4118 in MeOH C23H15FN2O2 H+		

Sample Name	BE-4118 in MeOH			
Exact Mass of	C23H15FN2O2 H+	=	371.119032	m/z
Mass Observed		=	371.118964	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(2-Chlorophenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4164 (22):

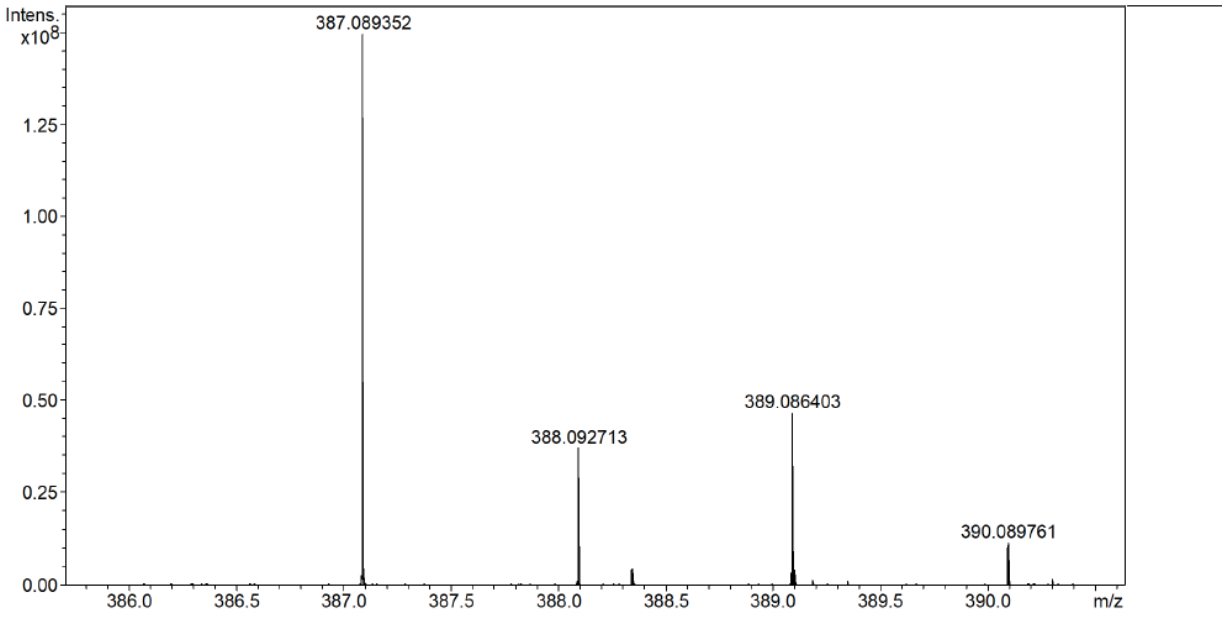


Mass Spectrum List Report

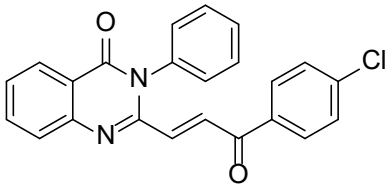
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4164_pos_000001.d	Acquisition Date	6/2/2025 4:26:08 PM
Method		Operator	Admin
Sample Name	BE4164	Instrument	solariX XR
Comment	BE-4164 in MeOH C23H15ClN2O2 H+		

Sample Name	BE-4164 in MeOH			
Exact Mass of	C23H15ClN2O2 H+	=	387.089482	m/z
Mass Observed		=	387.089352	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-Chlorophenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4122 (23):

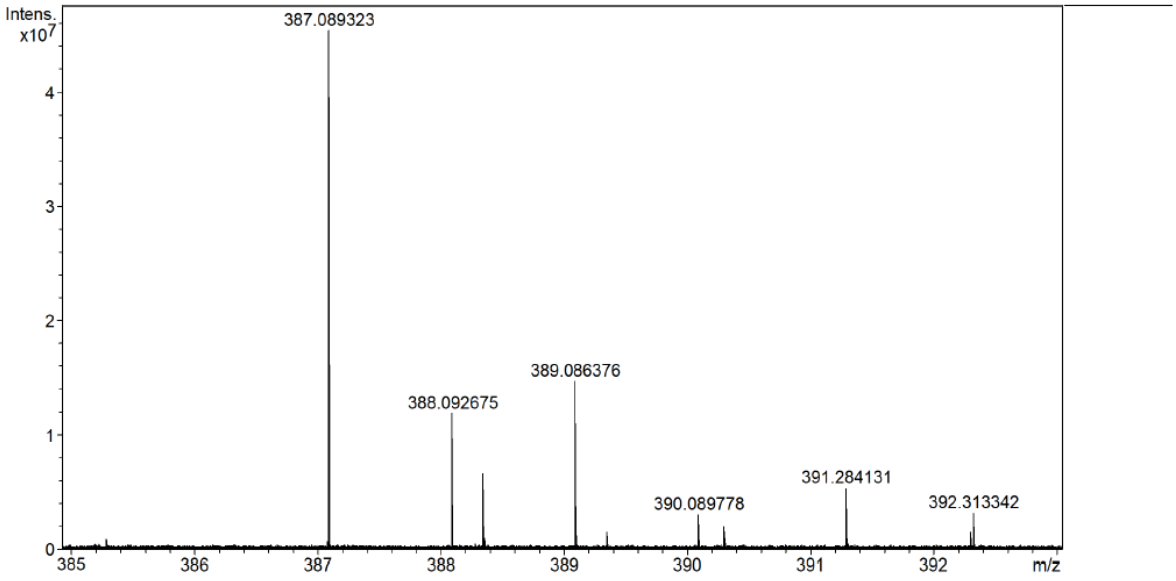


Mass Spectrum List Report

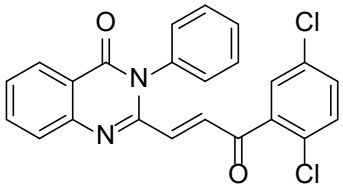
Analysis Info		Acquisition Date	6/2/2025 4:05:34 PM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4122_pos_000002.d		
Method		Operator	Admin
Sample Name	BE4122	Instrument	solariX XR
Comment	BE-4122 in MeOH C23H15ClN2O2 H+		

Sample Name	BE-4122 in MeOH			
Exact Mass of	C23H15ClN2O2 H+	=	387.089482	m/z
Mass Observed		=	387.089323	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(2,5-Dichlorophenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4130 (24):

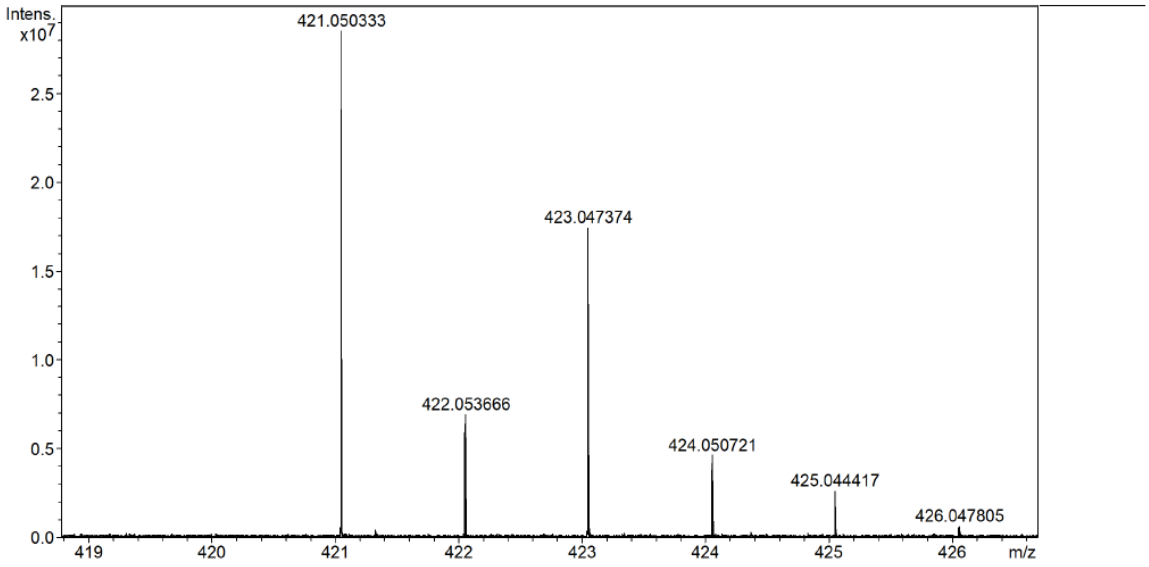


Mass Spectrum List Report

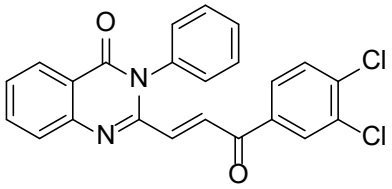
Analysis Info		Acquisition Date	6/2/2025 3:47:17 PM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4130_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4130	Instrument	solariX XR
Comment	BE-4130 in MeOH C23H14Cl2N2O2 H+		

Sample Name	BE-4130 in MeOH			
Exact Mass of	C23H14Cl2N2O2 H+	=	421.050510	m/z
Mass Observed		=	421.050333	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(3,4-Dichlorophenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4173 (25):

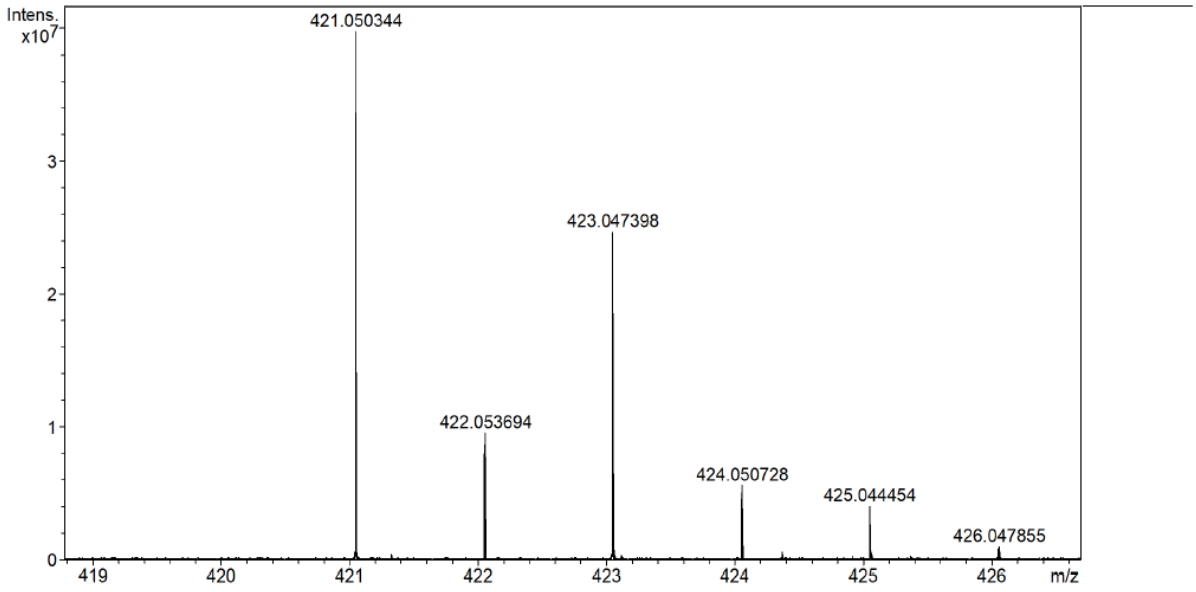


Mass Spectrum List Report

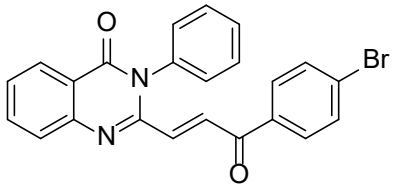
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4173_pos_000001.d	Acquisition Date	6/2/2025 3:35:33 PM
Method		Operator	Admin
Sample Name	BE4173	Instrument	solariX XR
Comment	BE-4173 in MeOH C23H14Cl2N2O2 H+		

Sample Name	BE-4173 in MeOH			
Exact Mass of	C23H14Cl2N2O2 H+	=	421.050510	m/z
Mass Observed		=	421.050344	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-bromophenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4119 (26):

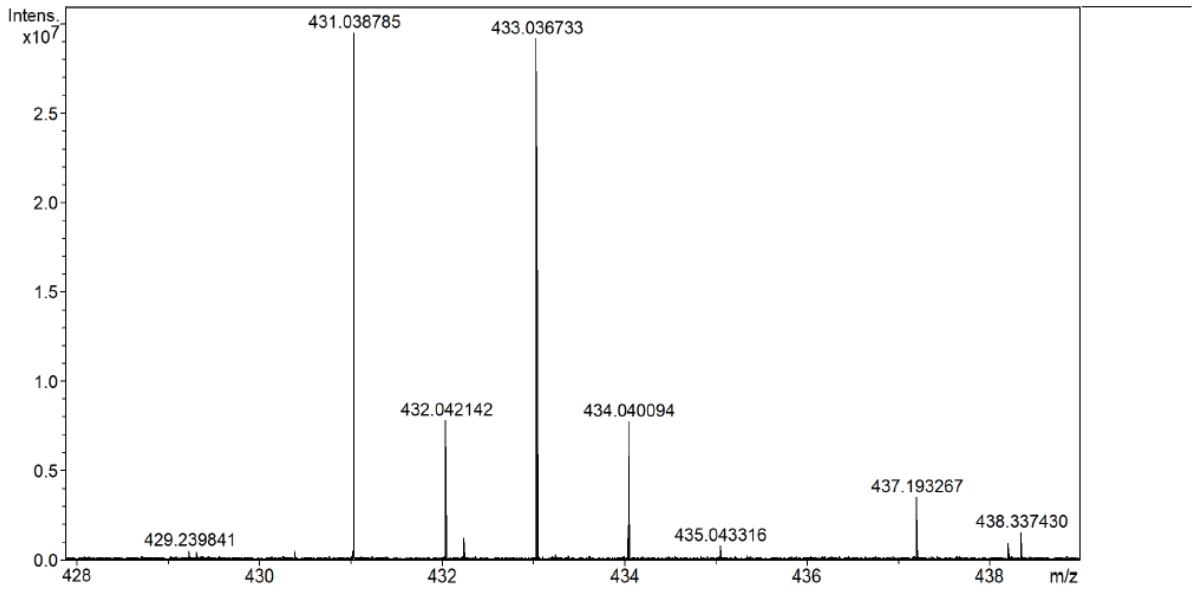


Mass Spectrum List Report

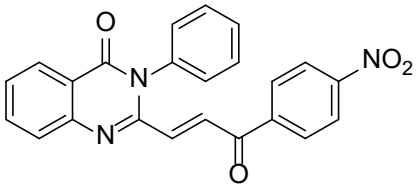
Analysis Info				
			Acquisition Date	6/2/2025 3:41:12 PM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4119_pos_000001.d			
Method			Operator	Admin
Sample Name	BE4119		Instrument	solariX XR
Comment	BE-4119 in MeOH	C23H15BrN2O2 H+		

Sample Name	BE-4119 in MeOH			
Exact Mass of	C23H15BrN2O2 H+	=	431.038967	m/z
Mass Observed		=	431.038785	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-Nitrophenyl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4170 (27):

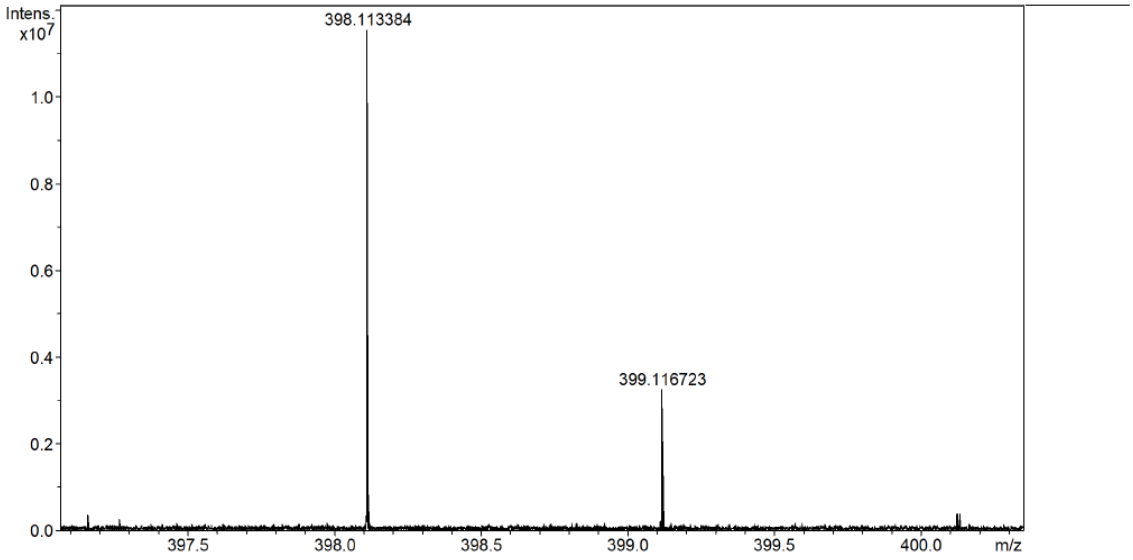


Mass Spectrum List Report

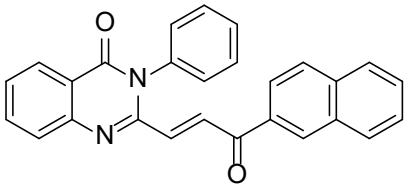
Analysis Info			
		Acquisition Date	6/2/2025 4:40:14 PM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4170_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4170	Instrument	solariX XR
Comment	BE-4170 in MeOH C23H15N3O4 H+		

Sample Name	BE-4170 in MeOH			
Exact Mass of	C23H15N3O4 H+	=	398.113532	m/z
Mass Observed		=	398.113384	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(Naphthalen-2-yl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4160 (28):



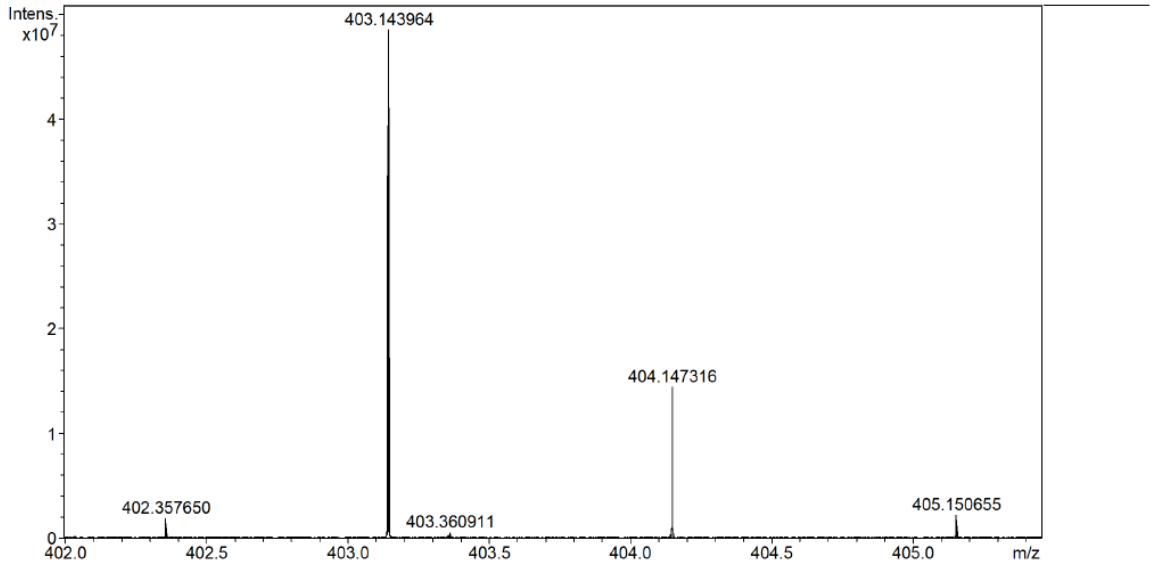
Mass Spectrum List Report

Analysis Info

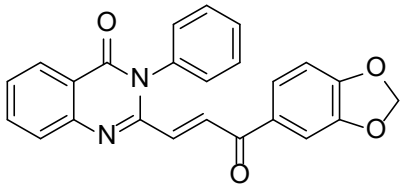
Acquisition Date	6/2/2025 4:49:49 PM		
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4160_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4160	Instrument	solariX XR
Comment	BE-4160 in MeOH C27H18N2O2 H+		

Sample Name	BE-4160 in MeOH			
Exact Mass of	C27H18N2O2 H+	=	403.144104	m/z
Mass Observed		=	403.143964	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(Benzo[d][1,3]dioxol-5-yl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4174 (29):

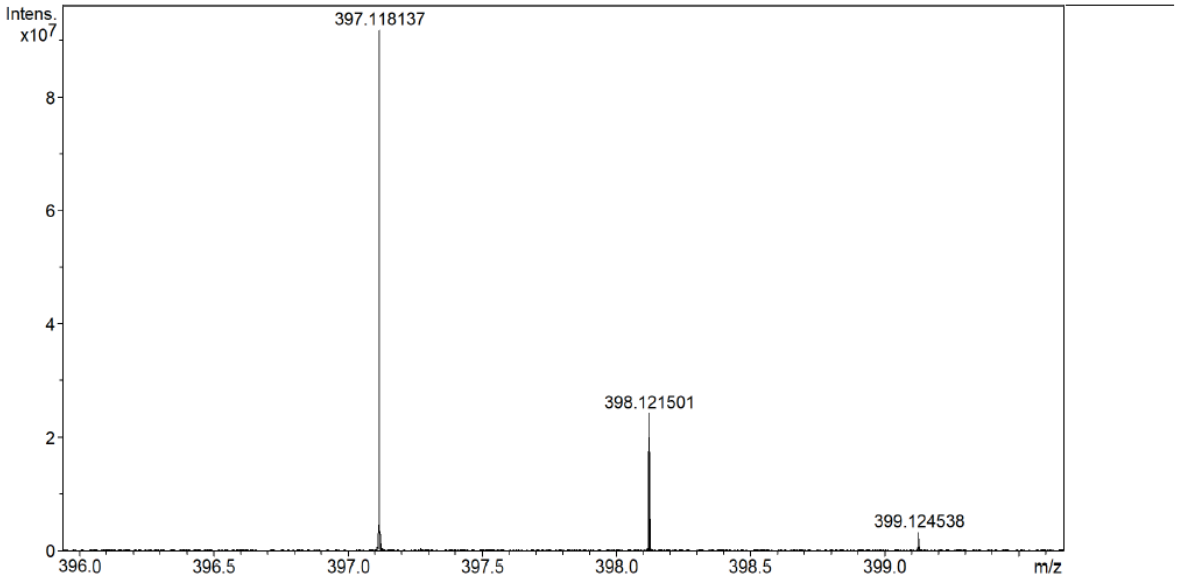


Mass Spectrum List Report

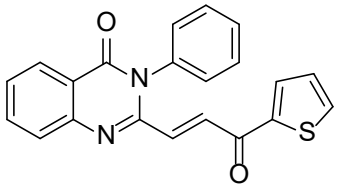
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250602\BE-4174_pos_000002.d	Acquisition Date	6/2/2025 5:25:26 PM
Method		Operator	Admin
Sample Name	BE4174	Instrument	solariX XR
Comment	BE-4174 in MeOH C24H16N2O4 H+		

Sample Name	BE-4174 in MeOH			
Exact Mass of	C24H16N2O4 H+	=	397.118283	m/z
Mass Observed		=	397.118137	m/z

Difference < 1.0 ppm



(*E*)-2-(3-Oxo-3-(thiophen-2-yl)prop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4131 (30):

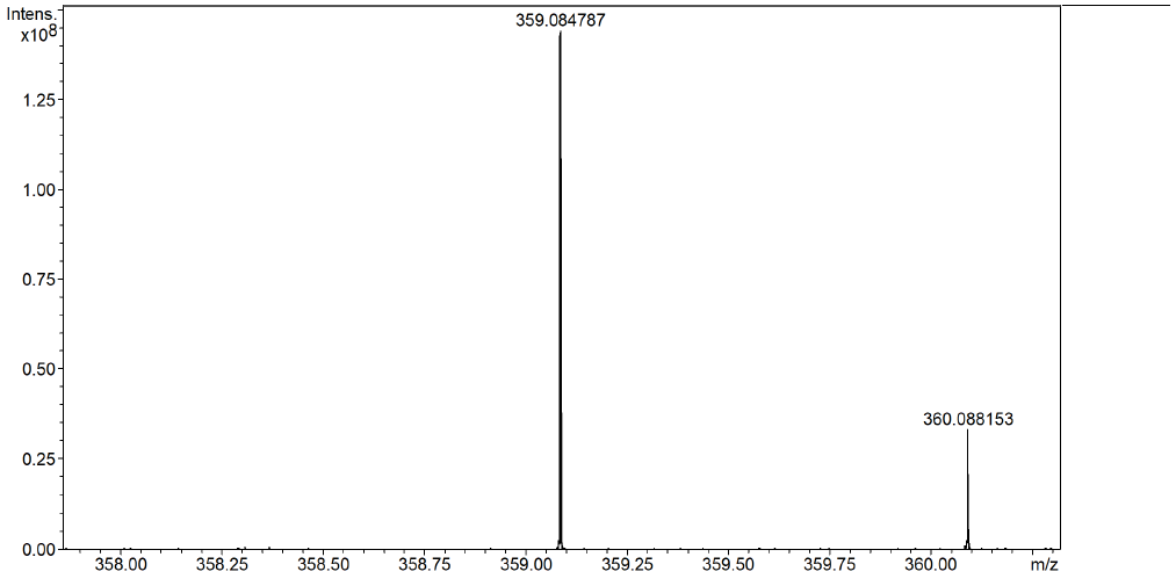


Mass Spectrum List Report

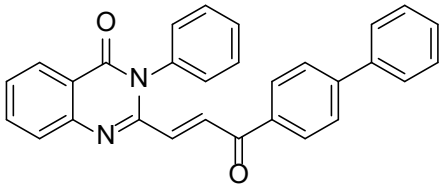
Analysis Info			
Acquisition Date	6/3/2025 10:50:59 AM		
Analysis Name	D:\MS1 COSMIC\2025\Data_20250603\BE-4131_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4131	Instrument	solariX XR
Comment	BE-4131 in MeOH C21H14N2O2S H+		

Sample Name	BE-4131 in MeOH			
Exact Mass of	C21H14N2O2S H+	=	359.084875	m/z
Mass Observed		=	359.084787	m/z

Difference < 1.0 ppm



(*E*)-2-(3-([1,1'-Biphenyl]-4-yl)-3-oxoprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4171 (31):

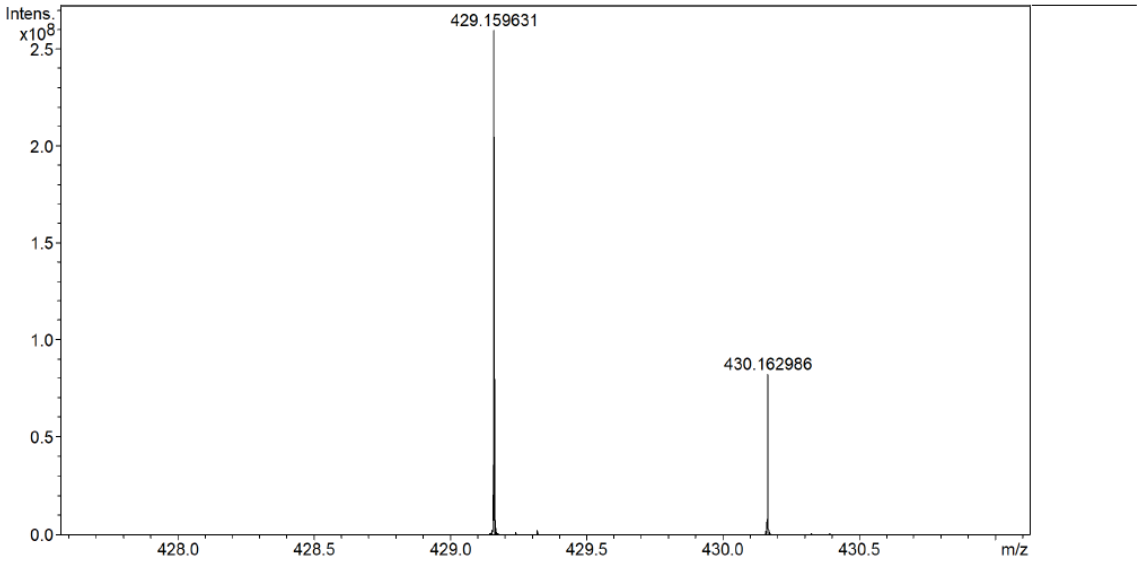


Mass Spectrum List Report

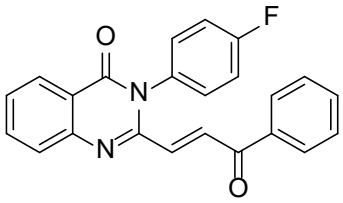
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250603\BE-4171_pos_000001.d	Acquisition Date	6/3/2025 10:56:34 AM
Method		Operator	Admin
Sample Name	BE4171	Instrument	solariX XR
Comment	BE-4171 in MeOH C29H20N2O2 H+		

Sample Name	BE-4171 in MeOH			
Exact Mass of	C29H20N2O2 H+	=	429.15754	m/z
Mass Observed		=	429.159631	m/z

Difference < 1.0 ppm



(*E*)-3-(4-Fluorophenyl)-2-(3-oxo-3-phenylprop-1-en-1-yl)quinazolin-4(3*H*)-one BE4123 (32):

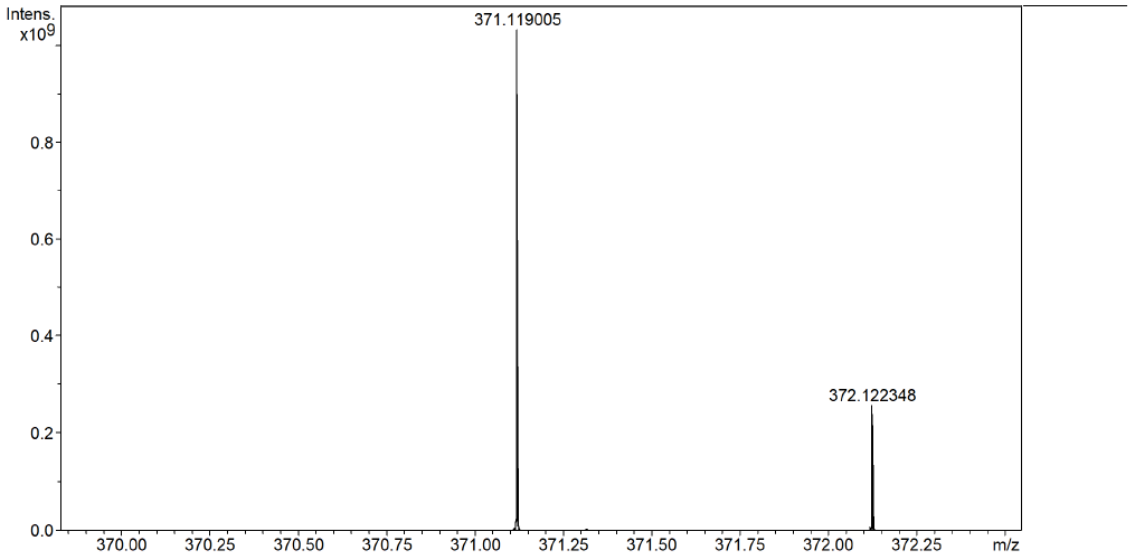


Mass Spectrum List Report

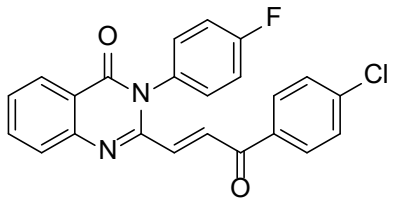
Analysis Info		Acquisition Date	6/3/2025 11:28:40 AM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250603\BE-4123_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4123	Instrument	solariX XR
Comment	BE-4123 in MeOH C23H15FN2O2 H+		

Sample Name	BE-4123 in MeOH			
Exact Mass of	C23H15FN2O2 H+	=	371.119032	m/z
Mass Observed		=	371.119005	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-Chlorophenyl)-3-oxoprop-1-en-1-yl)-3-(4-fluorophenyl)quinazolin-4(3*H*)-one BE4125 (33):



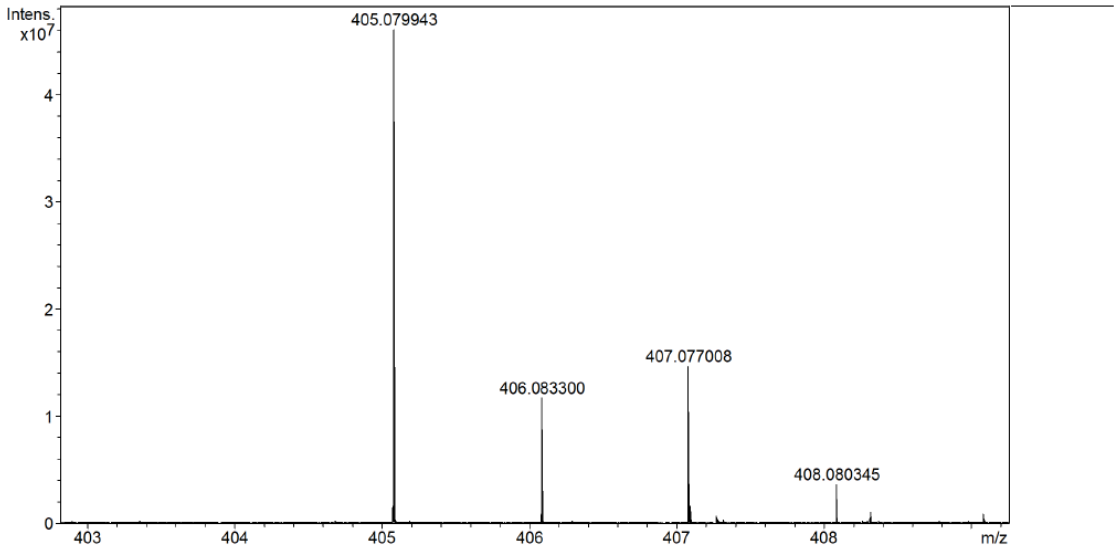
Mass Spectrum List Report

Analysis Info

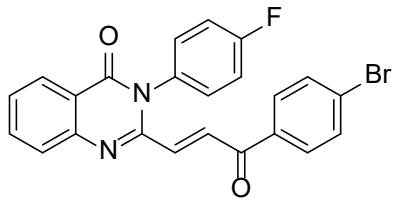
Acquisition Date	6/3/2025 11:33:39 AM		
Analysis Name	D:\MS1 COSMIC\2025\Data_20250603\BE-4125_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4125	Instrument	solariX XR
Comment	BE-4125 in MeOH C23H14ClFN2O2 H+		

Sample Name	BE-4125 in MeOH			
Exact Mass of	C23H14ClFN2O2 H+	=	405.080060	m/z
Mass Observed		=	405.079943	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-Bromophenyl)-3-oxoprop-1-en-1-yl)-3-(4-fluorophenyl)quinazolin-4(3*H*)-one BE4128 (36):

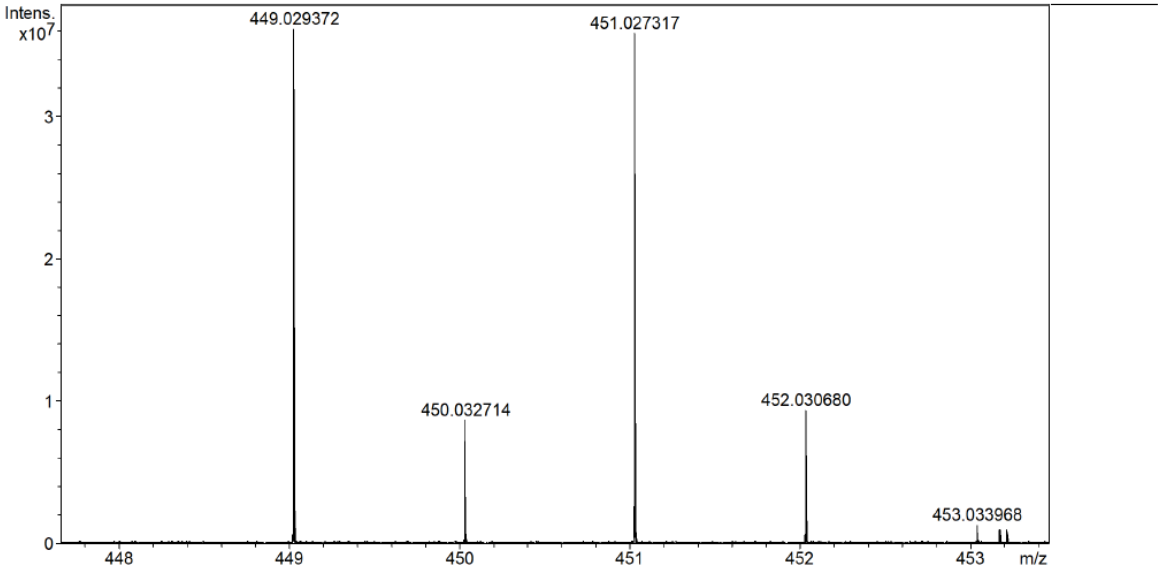


Mass Spectrum List Report

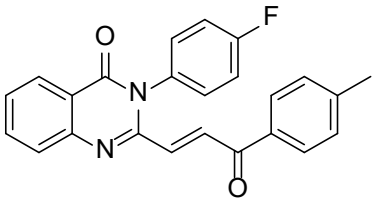
Analysis Info			
Acquisition Date	6/3/2025 12:25:28 PM		
Analysis Name	D:\MS1 COSMIC\2025\Data_20250603\BE-4128_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4128	Instrument	solariX XR
Comment	BE-4128 in MeOH C23H14BrFN2O2 H+		

Sample Name	BE-4128 in MeOH			
Exact Mass of	C23H14BrFN2O2 H+	=	449.029545	m/z
Mass Observed		=	449.029372	m/z

Difference < 1.0 ppm



(*E*)-3-(4-Fluorophenyl)-2-(3-oxo-3-(p-tolyl)prop-1-en-1-yl)quinazolin-4(3*H*)-one BE4126 (35):

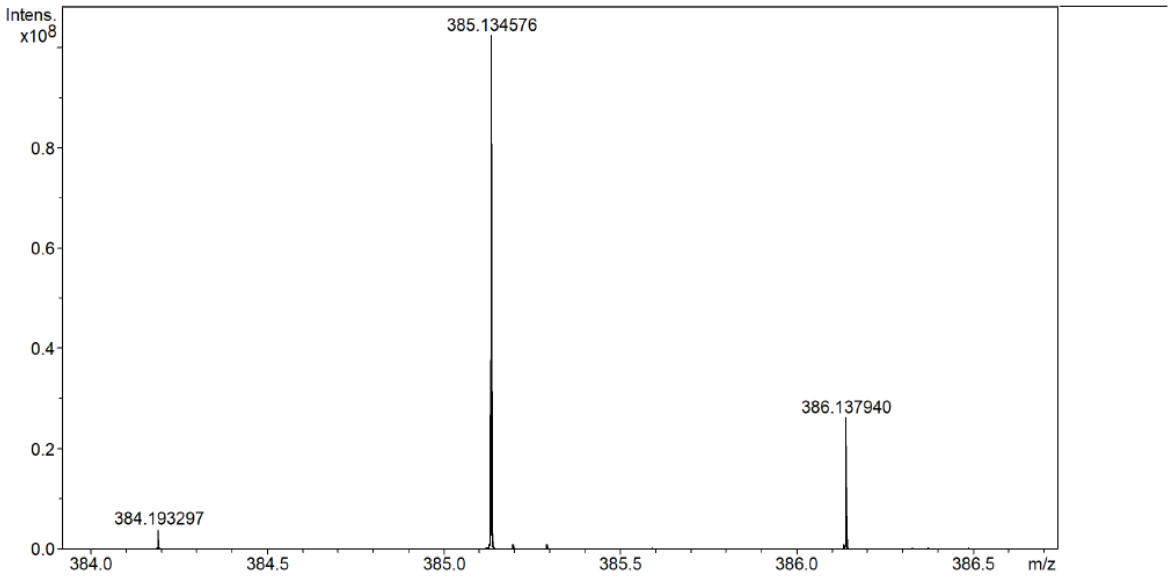


Mass Spectrum List Report

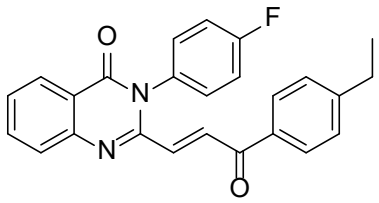
Analysis Info			
Analysis Name	D:\MS1 COSMIC\2025\Data_20250603\BE-4126_pos_000001.d	Acquisition Date	6/3/2025 12:35:12 PM
Method		Operator	Admin
Sample Name	BE4126	Instrument	solariX XR
Comment	BE-4126 in MeOH C24H17FN2O2 H+		

Sample Name	BE-4126 in MeOH			
Exact Mass of	C24H17FN2O2 H+	=	385.134682	m/z
Mass Observed		=	385.134576	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-Ethylphenyl)-3-oxoprop-1-en-1-yl)-3-(4-fluorophenyl)quinazolin-4(3*H*)-one BE4127 (36):

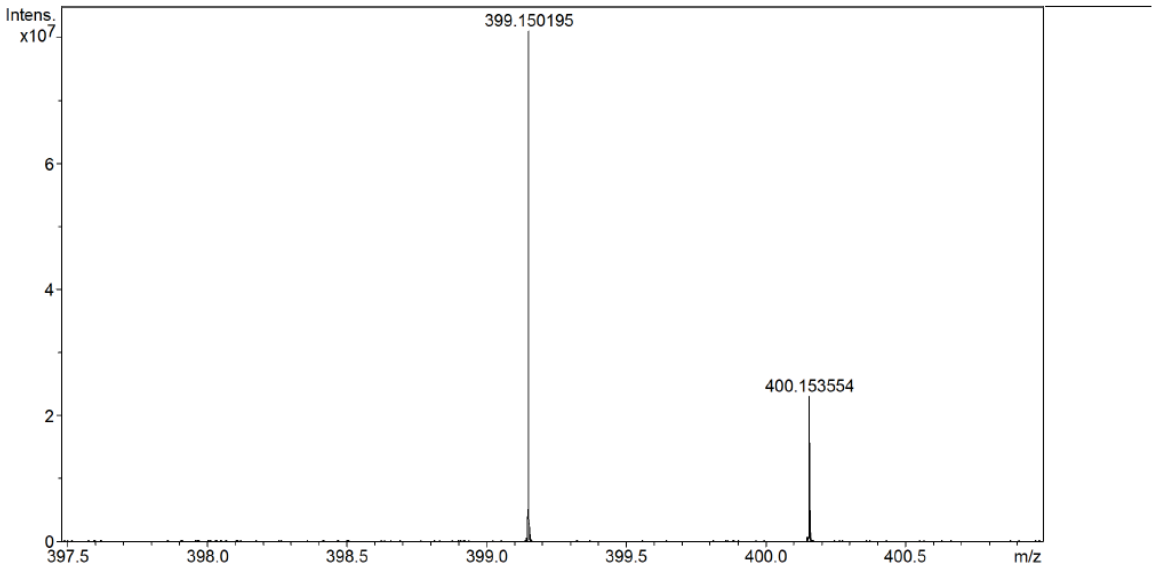


Mass Spectrum List Report

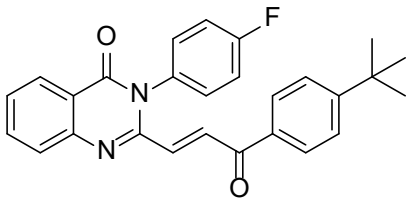
Analysis Info		Acquisition Date	6/3/2025 12:40:16 PM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250603\BE-4127_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4127	Instrument	solariX XR
Comment	BE-4127 in MeOH C25H19FN2O2 H+		

Sample Name	BE-4127 in MeOH			
Exact Mass of	C25H19FN2O2 H+	=	399.150332	m/z
Mass Observed		=	399.150195	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-(tert-Butyl)phenyl)-3-oxoprop-1-en-1-yl)-3-(4-fluorophenyl)quinazolin-4(3*H*)-one BE4176 (37):

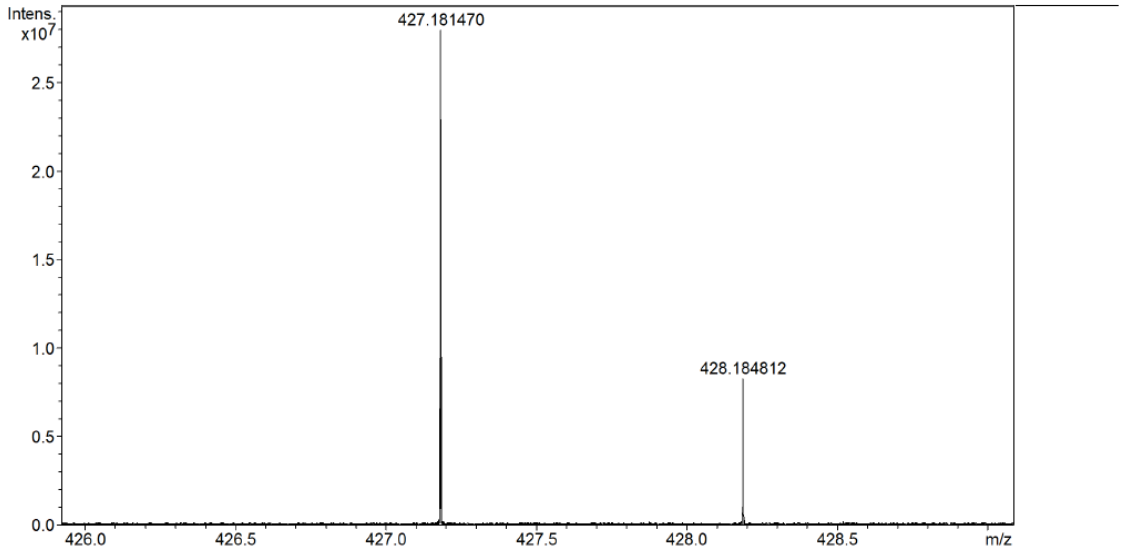


Mass Spectrum List Report

Analysis Info		Acquisition Date	6/3/2025 12:45:20 PM
Analysis Name	D:\MS1 COSMIC\2025\Data_20250603\BE-4176_pos_000001.d		
Method		Operator	Admin
Sample Name	BE4176	Instrument	solariX XR
Comment	BE-4176 in MeOH C27H23FN2O2 H+		

Sample Name	BE-4176 in MeOH			
Exact Mass of	C27H23FN2O2 H+	=	427.181633	m/z
Mass Observed		=	427.181470	m/z

Difference < 1.0 ppm



(*E*)-6-Fluoro-2-(3-oxo-3-phenylprop-1-en-1-yl)-3-phenylquinazolin-4(3*H*)-one BE4166 (38):

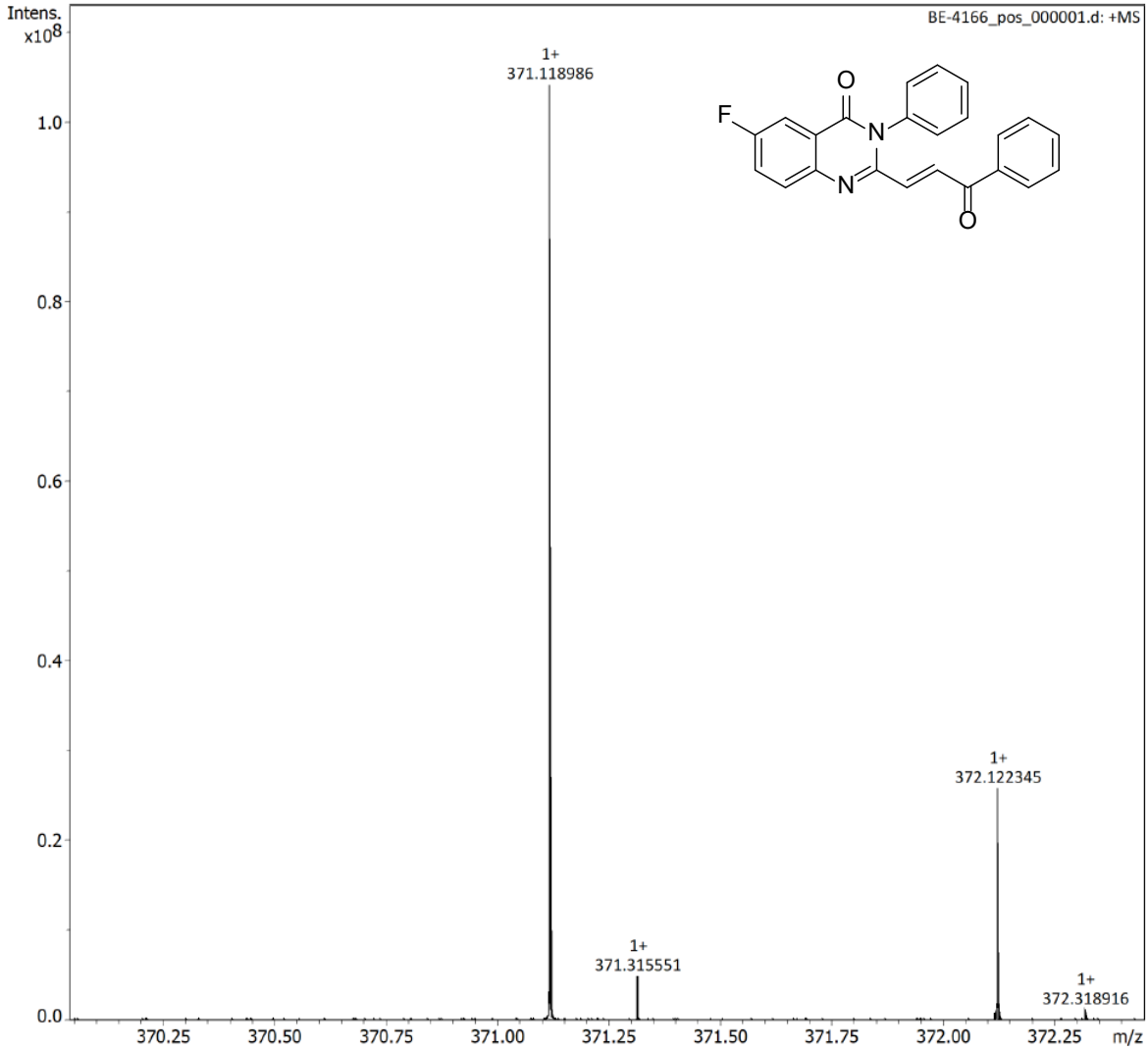
Generic Display Report

Analysis Info

Analysis Name	D:\Data\Data_20250603\BE-4166_pos_000001.d	Acquisition Date	6/3/2025 2:10:38 PM
Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	BE4166	Instrument	solariX XR
Comment	BE-4166 in MeOH C23H15FN2O2 H+		

Sample Name	BE-4166 in MeOH			
Exact Mass of	C23H15FN2O2 H+	=	371.119032	m/z
Mass Observed		=	371.118986	m/z

Difference < 1.0 ppm



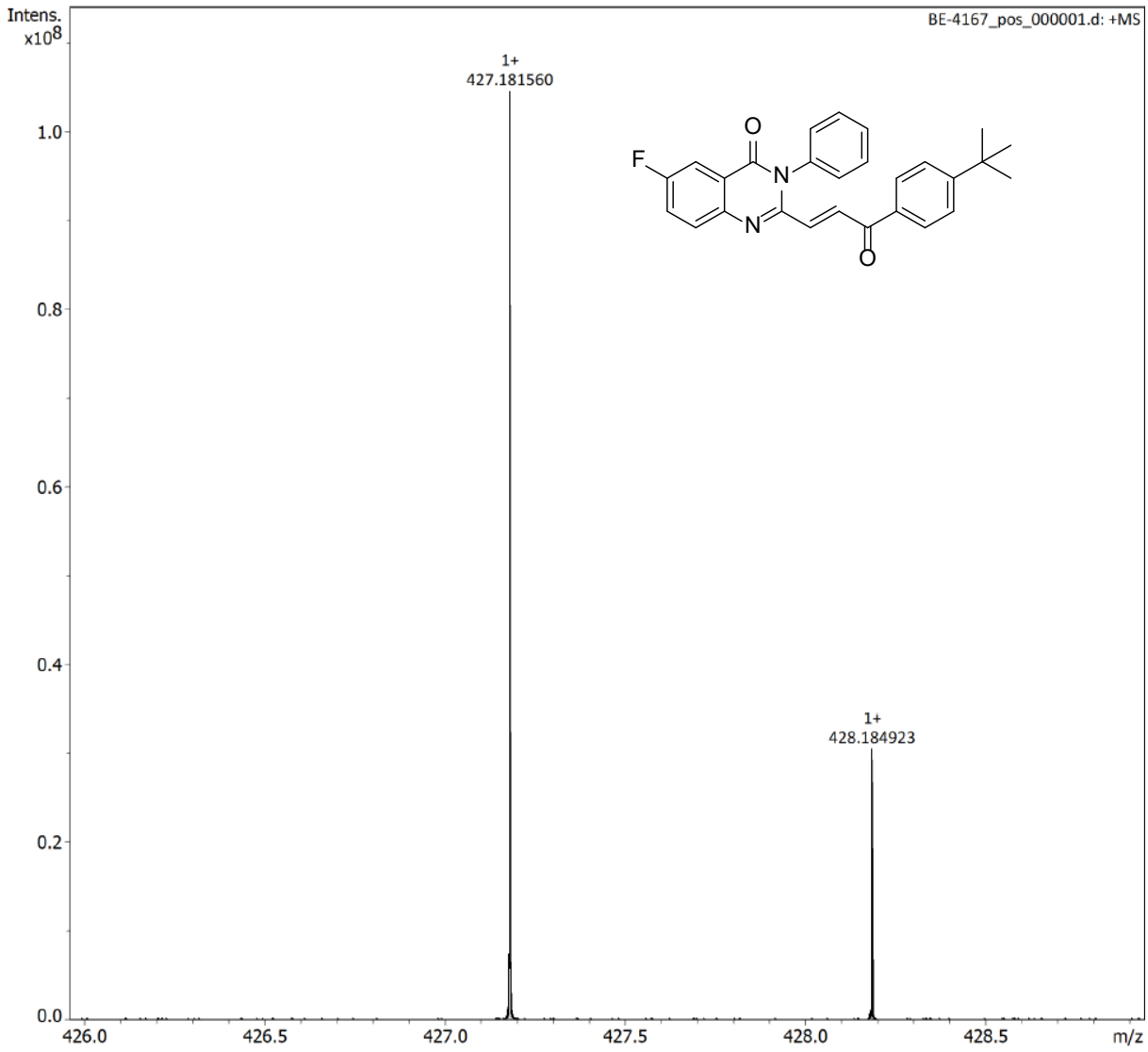
(*E*)-2-(3-(4-(tert-Butyl)phenyl)-3-oxoprop-1-en-1-yl)-6-fluoro-3-phenylquinazolin-4(3*H*)-one BE4167 (39):

Generic Display Report

Analysis Info		Acquisition Date	6/3/2025 2:16:17 PM
Analysis Name	F:\MS1 COSMIC\2025\Data_20250603\BE-4167_pos_000001.d		
Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	BE4167	Instrument	solariX XR
Comment	BE-4167 in MeOH C27H23FN2O2 H+		

Sample Name	BE-4167 in MeOH			
Exact Mass of	C27H23FN2O2 H+	=	427.181633	m/z
Mass Observed		=	427.181560	m/z

Difference < 1.0 ppm



(*E*)-2-(3-Oxo-3-phenylprop-1-en-1-yl)-3-phenyl-7-(trifluoromethyl)quinazolin-4(3*H*)-one BE4165 (40):

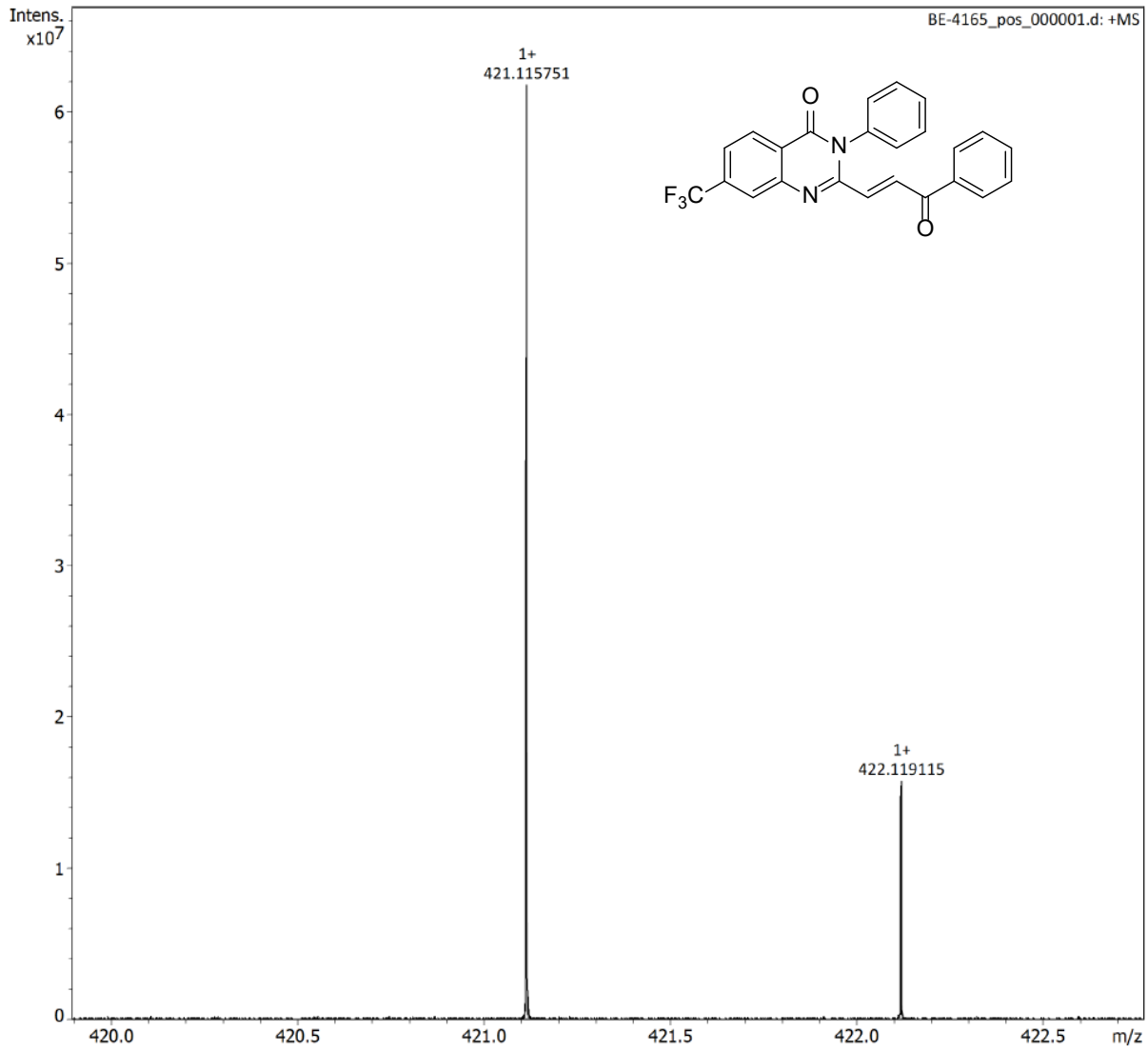
Generic Display Report

Analysis Info

		Acquisition Date	6/3/2025 2:20:55 PM
Analysis Name	F:\MS1 COSMIC\2025\Data_20250603\BE-4165_pos_000001.d		
Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	BE4165	Instrument	solariX XR
Comment	BE-4165 in MeOH C24H15F3N2O2 H+		

Sample Name	BE-4165 in MeOH			
Exact Mass of	C24H15F3N2O2 H+	=	421.115839	m/z
Mass Observed		=	421.115751	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(4-(tert-Butyl)phenyl)-3-oxoprop-1-en-1-yl)-3-phenyl-7-(trifluoromethyl)quinazolin-4(3*H*)-one BE4168 (41):

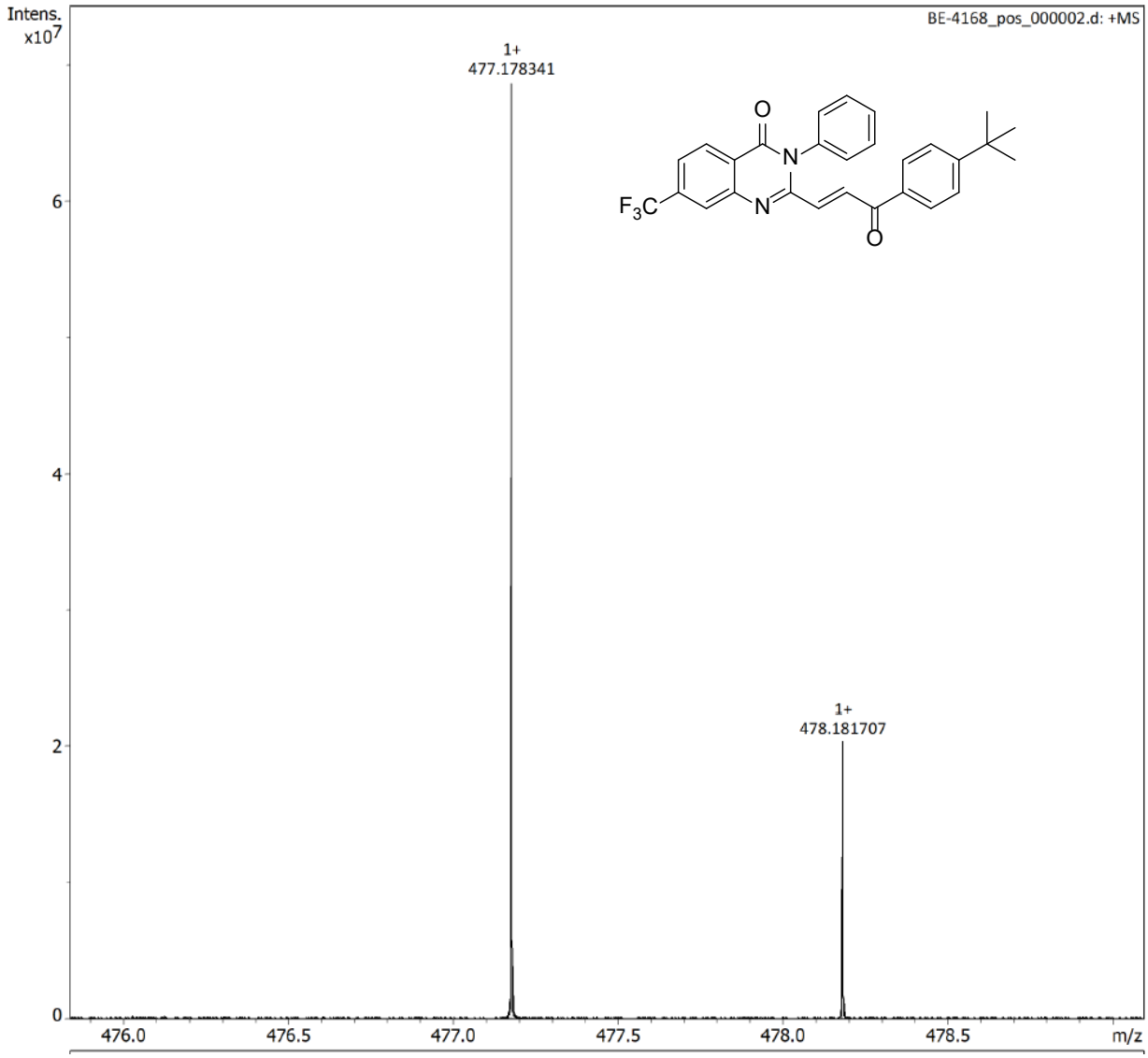
Generic Display Report

Analysis Info

		Acquisition Date	6/3/2025 2:26:43 PM
Analysis Name	F:\MS1 COSMIC\2025\Data_20250603\BE-4168_pos_000002.d		
Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	BE4168	Instrument	solariX XR
Comment	BE-4168 in MeOH C28H23F3N2O2 H+		

Sample Name	BE-4168 in MeOH			
Exact Mass of	C28H23F3N2O2 H+	=	477.178439	m/z
Mass Observed		=	477.178341	m/z

Difference < 1.0 ppm



(*E*)-2-(3-(3,4-Dimethoxyphenyl)-3-oxoprop-1-en-1-yl)-3-phenyl-7-(trifluoromethyl)quinazolin-4(3*H*)-one BE4163 (42):

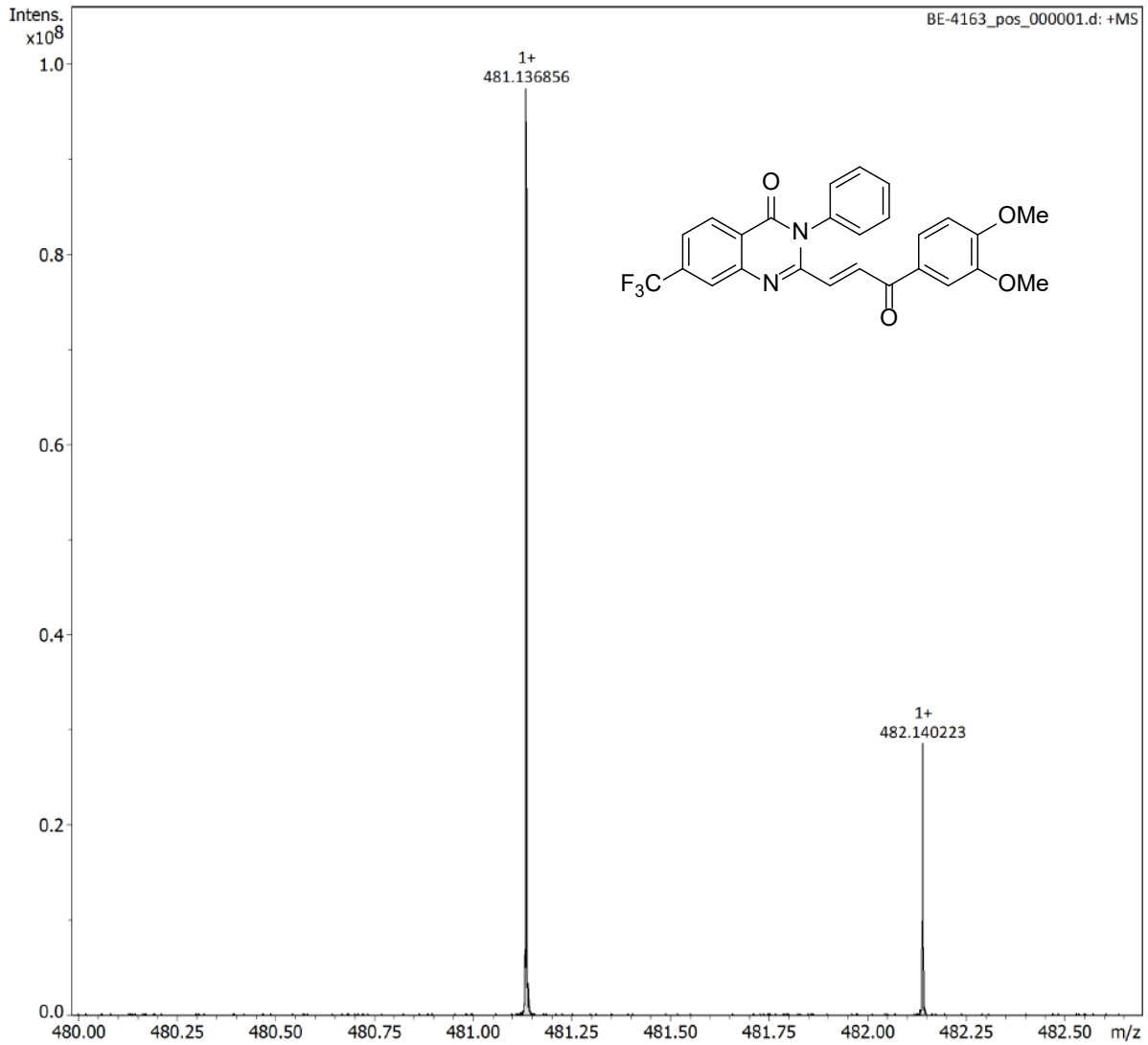
Generic Display Report

Analysis Info

Acquisition Date	6/3/2025 2:32:23 PM		
Analysis Name	F:\MS1 COSMIC\2025\Data_20250603\BE-4163_pos_000001.d		
Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	BE4163	Instrument	solariX XR
Comment	BE-4163 in MeOH C26H19F3N2O4 H+		

Sample Name	BE-4163 in MeOH			
Exact Mass of	C26H19F3N2O4 H+	=	481.136968	m/z
Mass Observed		=	481.136849	m/z

Difference < 1.0 ppm



(*E*)-2-(3-([1,1'-Biphenyl]-4-yl)-3-oxoprop-1-en-1-yl)-3-phenyl-7-(trifluoromethyl)quinazolin-4(3*H*)-one BE4177 (43):

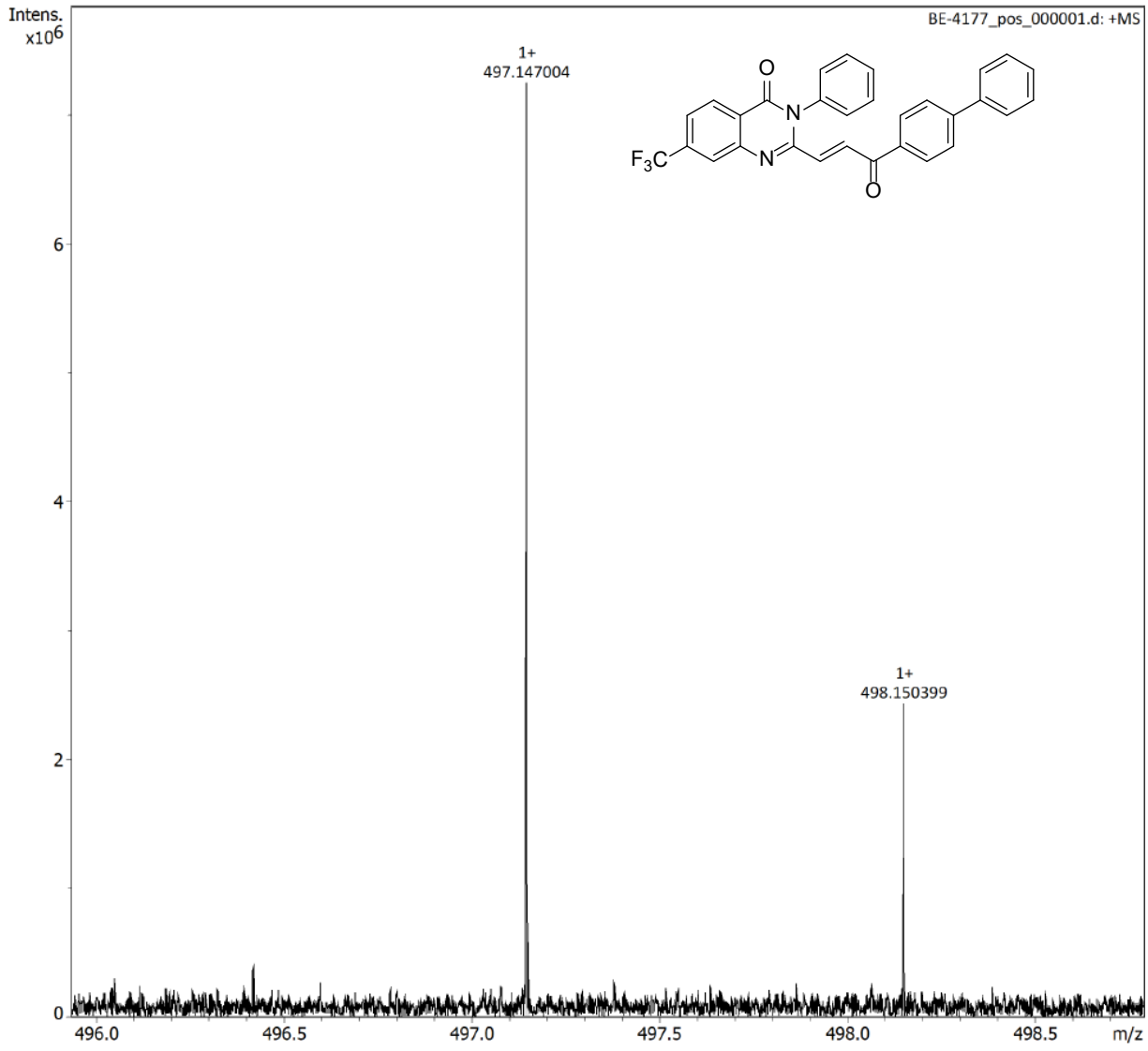
Generic Display Report

Analysis Info

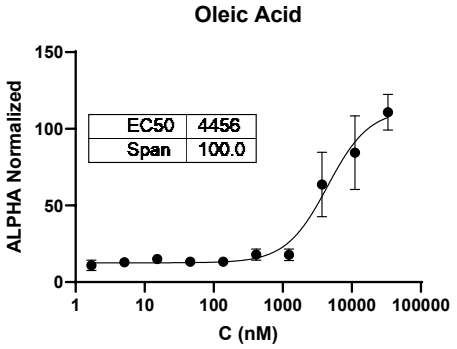
Acquisition Date	6/3/2025 3:19:10 PM		
Analysis Name	F:\MS1 COSMIC\2025\Data_20250603\BE-4177_pos_000001.d		
Method	LowMass_150-1000_050825	Operator	Admin
Sample Name	BE4177	Instrument	solariX XR
Comment	BE-4177 in MeOH C30H19F3N2O2 H+		

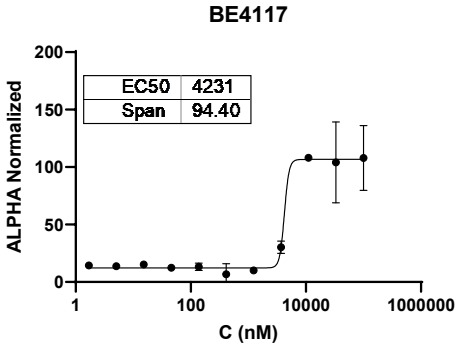
Sample Name	BE-4177 in MeOH			
Exact Mass of	C30H19F3N2O2 H+	=	497.147139	m/z
Mass Observed		=	497.147004	m/z

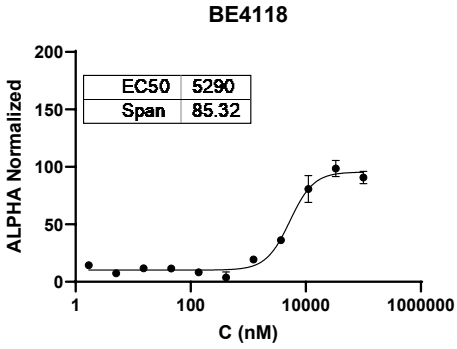
Difference < 1.0 ppm

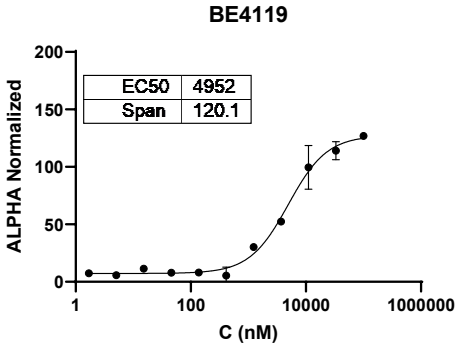


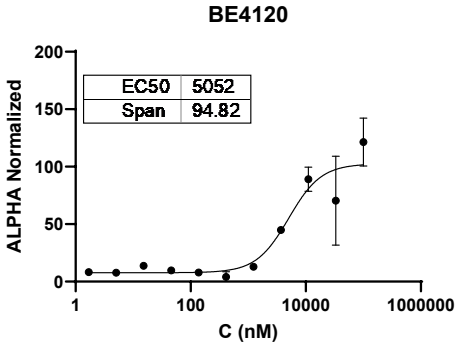
4. Compounds screening in ALPHAscreen

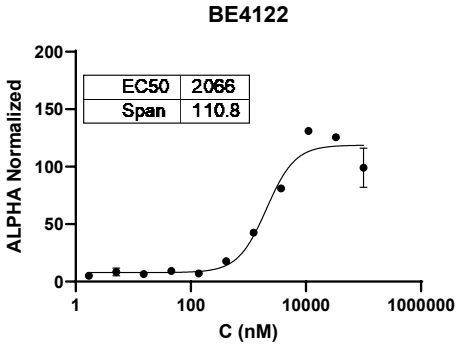


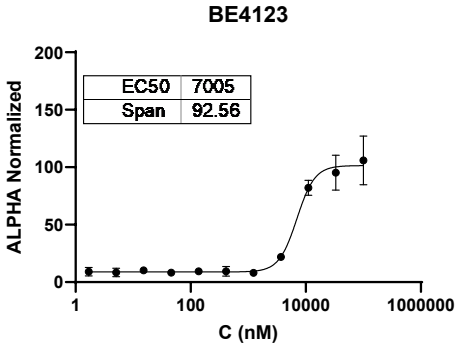


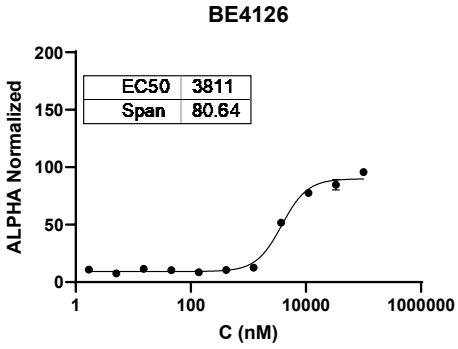












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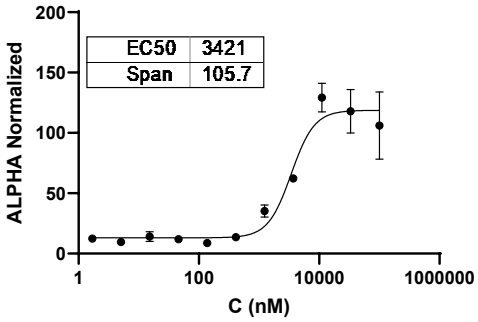

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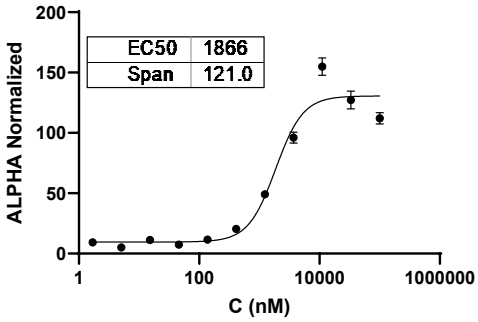

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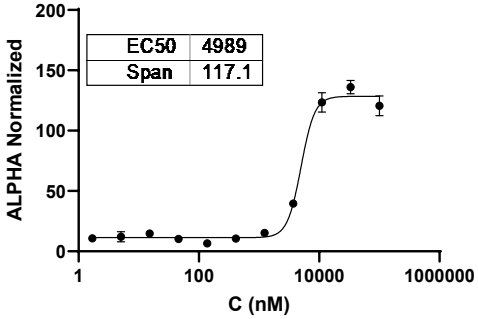

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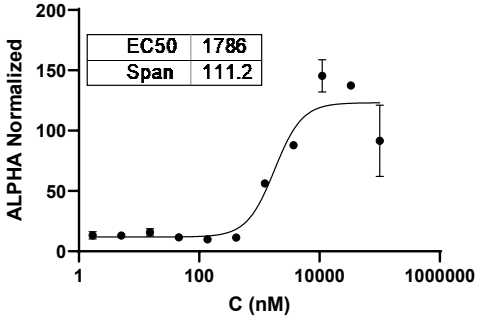

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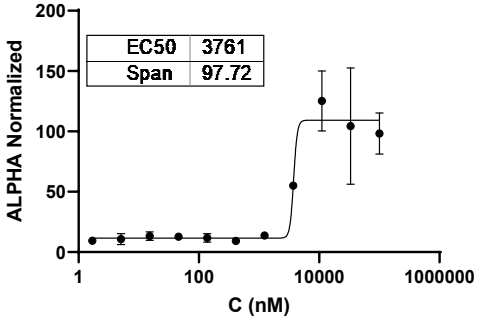

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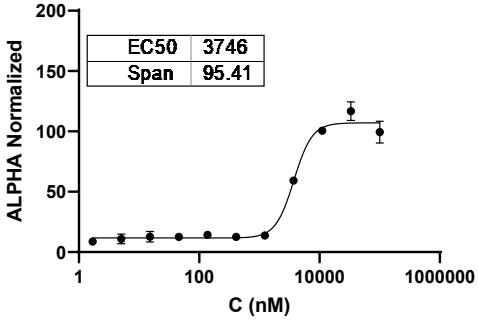

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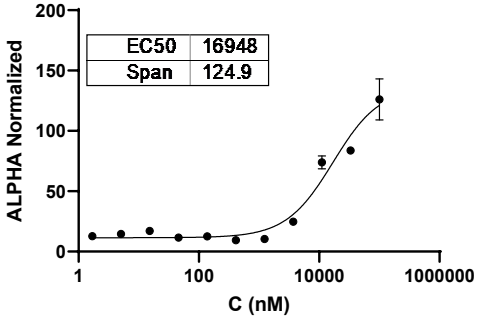

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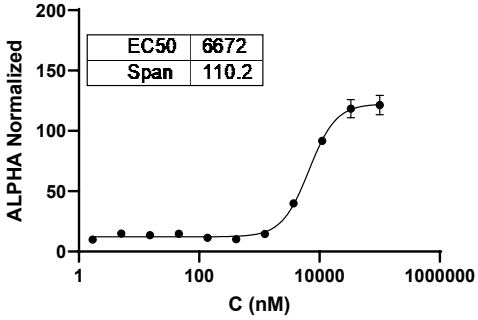

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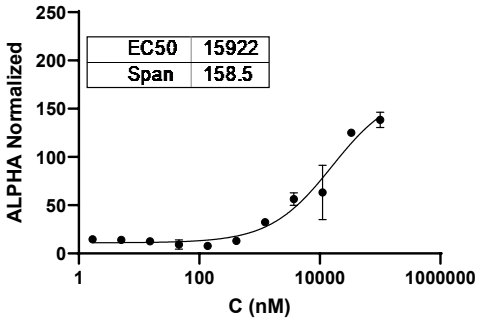

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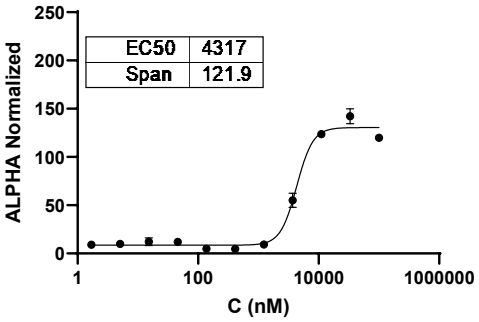

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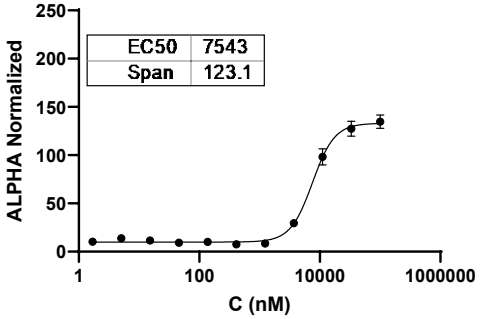

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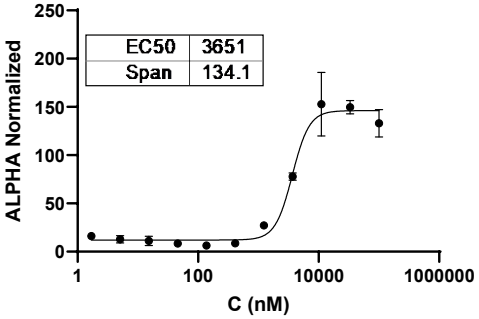

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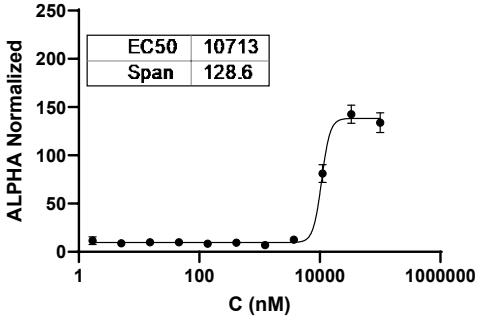

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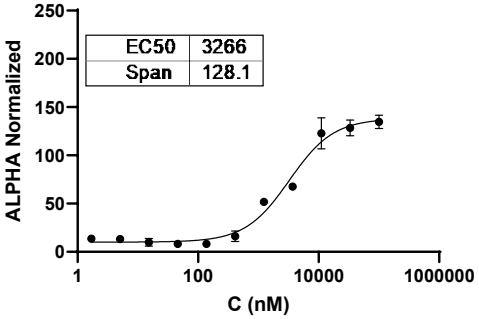

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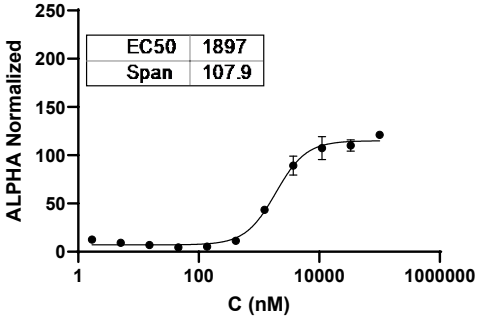

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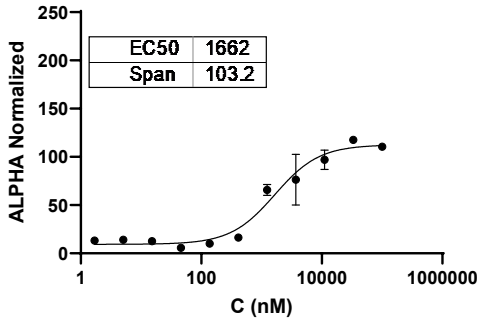

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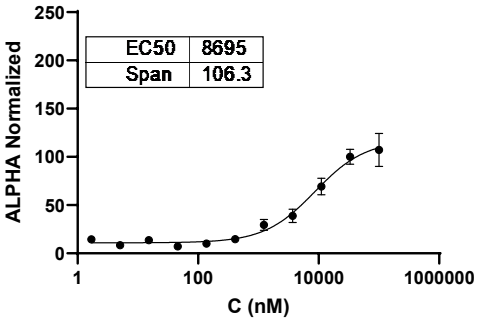

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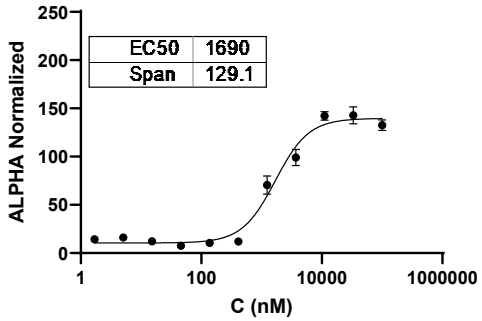

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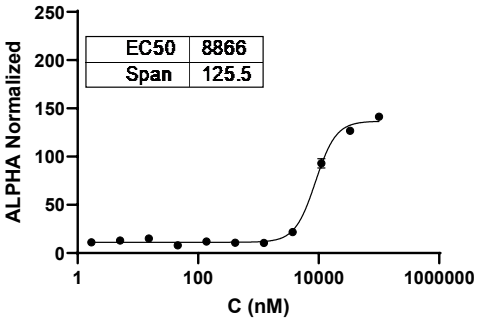

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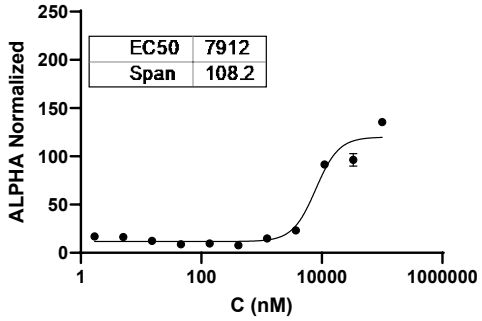

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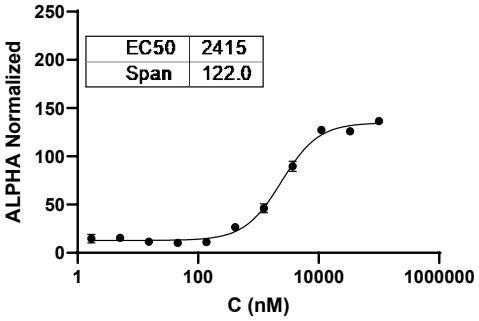

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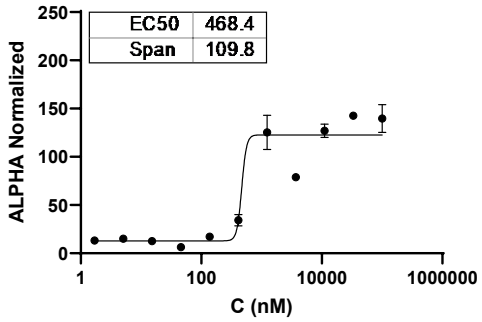
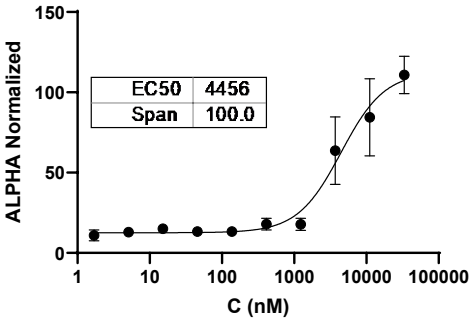
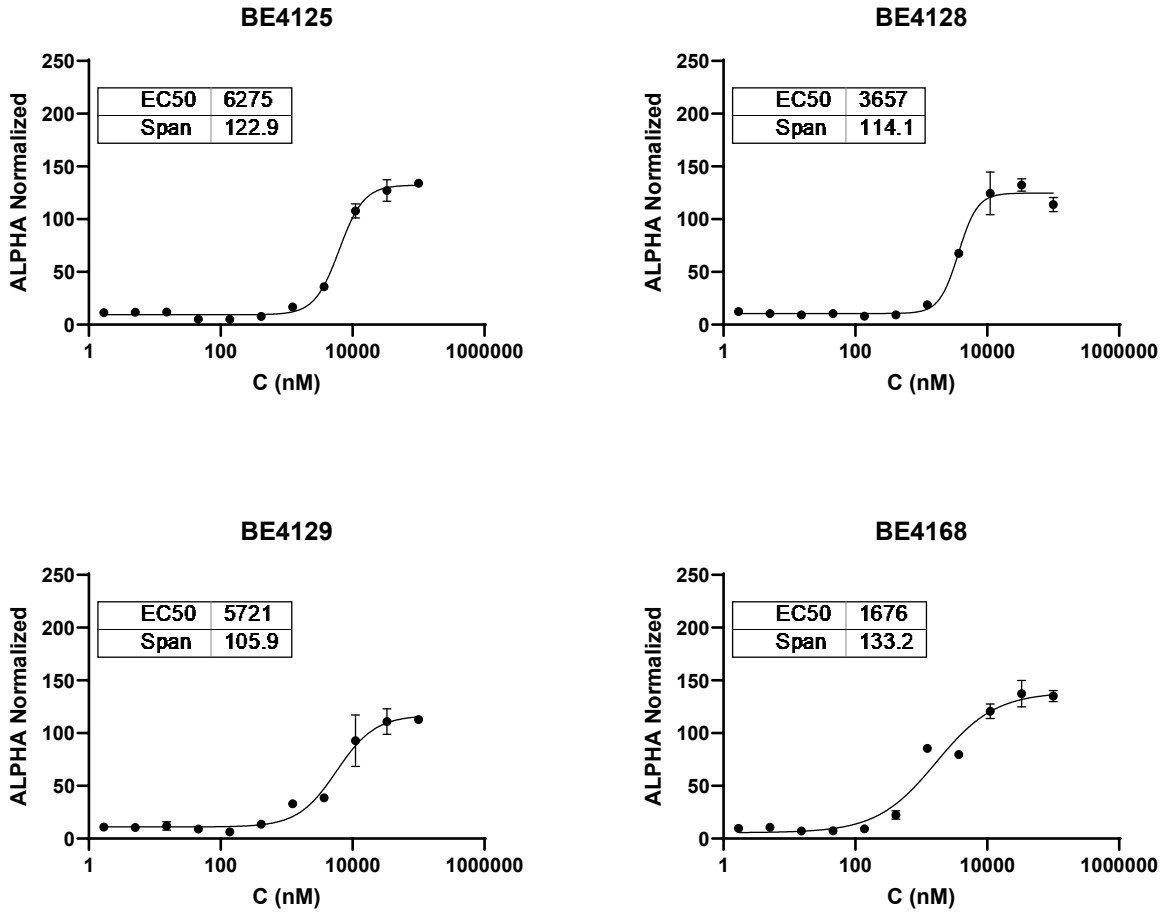


Oleic Acid





5. References

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