Electronic Supplementary Material (ESI) for Chemical Communications.

Synthesis of Quaternary Carbon Centered Indolo[1,2-*a*]quinazolinones and Indazolo[1,2-*a*]indazolones via C-H Functionalization

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Supporting Information

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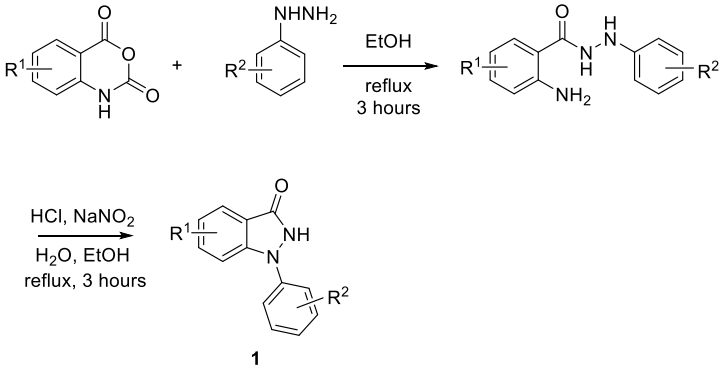
1. General Information

Melting points were measured with a Buchi B-540 melting point apparatus and are uncorrected. NMR spectra were recorded on Bruker Avance III 500 MHz FT NMR spectrometer using tetramethylsilane (TMS) as an internal standard. All the commercially available regents were used directly as received. All experiments were monitored by thin layer chromatography experiment. TLC was performed on Merck TLC Silica gel 60 F254 precoated plates. Column chromatography was performed on silica gel (100-200 mesh, Merck). HRMS data were recorded by electron spray ionization with a Q-TOF mass analyzer.

2. Reaction Procedures

2.1 General procedure for the synthesis of 1-phenyl-1,2-dihydro-3*H*-indazol-3-ones (1)[1]



Scheme SI-1: Synthesis of indazolone derivatives **1**

To a stirred solution of isatoic anhydride (12.0 mmol) in ethanol (20 mL), phenylhydrazine (12.0 mmol) was added. The reaction mixture was refluxed for 2 hours and then it was allowed to cool to room temperature and kept standing at same temperature for 12 hours. The precipitated hydrazide was filtered out and washed with ethanol. Then, 25 mL of 1.0 M HCl was added into this hydrazide. To this slurry, $NaNO_2$ (18.0 mmol, in 10 mL water) was added and the reaction mixture was refluxed for three hours after adding 25 mL of ethanol. The solvent was reduced in vacuo and the reaction mixture was kept overnight. The solid formed was filtered out get the starting compound **1**.

2.2 General procedure for the synthesis of indoloquinazolinones 3 and indazoloindazolones 4

A mixture of 1-phenyl-1,2-dihydro-3*H*-indazol-3-one (**1**, 0.1 mmol), alkyne (**2**, 0.1 mmol), [{$RuCl_2$(*p*-cymene)}$_2$] (5.0 mol %) and CsOAc (0.1 mmol) in ^{t}AmOH (3.0 mL) was stirred at 95 ^{o}C under open air for 24 hours. The solvent ^{t}AmOH was removed under vacuo and water

was added in to the crude reaction mixture which was then extracted with ethylacetate (25 mL x 2). The organic layer was then washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuo and the crude product obtained was purified by silica gel (100-200 mesh) column chromatography using 20% EtOAc in hexane as the eluant to afford indoloquinazolinone derivatives **3** and indazoloindazolones **4**.

2.3 Gram scale synthesis of 3aa

A mixture of **1a** (840 mg, 4.0 mmol), **2a** (712 mg, 4.0 mmol), [{$RuCl_2$(*p*-cymene)}$_2$] (122 mg, 5.0 mol %) and CsOAc (768 mg, 4.0 mmol) in ^{t}AmOH (25 mL) was stirred at 95 ^{o}C under open air for 24 hours. The solvent ^{t}AmOH was removed under vacuo and water was added in to the crude reaction mixture which was then extracted with ethylacetate (30 mL x 3). The organic layer was then washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuo and the crude product obtained was purified by silica gel (100-200 mesh) column chromatography using 20% EtOAc in hexane as the eluant to afford **3aa** (1.16 g, 75%).

2.4 Synthesis of 4aj in the presence of TEMPO

A mixture of **1a** (21 mg, 0.1 mmol), **2j** (11 mg, 0.1 mmol), [{$RuCl_2$(*p*-cymene)}$_2$] (3 mg, 5.0 mol %), TEMPO (16 mg, 0.1 mmol) and CsOAc (19 mg, 0.1 mmol) in ^{t}AmOH (3.0 mL) was stirred at 95 ^{o}C under open air for 24 hours. The solvent ^{t}AmOH was removed under vacuo and water was added in to the crude reaction mixture which was then extracted with ethylacetate (25 mL x 2). The organic layer was then washed with brine and dried over anhydrous Na_2SO_4. The solvent was removed under vacuo and the crude product obtained was purified by silica gel (100-200 mesh) column chromatography using 20% EtOAc in hexane as the eluant to afford **4aj** (8 mg, 23%).

2.4 D/H Exchange reaction for the synthesis of 1a-D

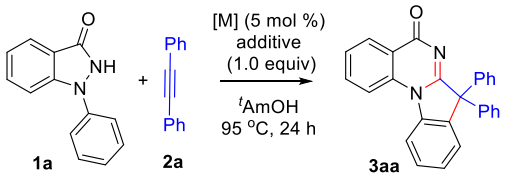
A mixture of **1a** (21 mg, 0.1 mmol), [{$RuCl_2$(*p*-cymene)}$_2$] (3 mg, 5.0 mol %), and CsOAc (19 mg, 0.1 mmol) was stirred in D_2O (3.0 mL, 95 ^{o}C) or CD_3OD (3.0 mL, 60 ^{o}C) under argon for 24 hours. The solvent was removed under and the crude product obtained was purified by silica gel (100-200 mesh) column chromatography using 15-20% EtOAc in hexane as the eluant. The product did not show any H/D exchange.

2.5 General procedure for the synthesis of indolo[1,2-*a*]quinazolinones (4aj′-al′)

A mixture of **1a** (21 mg, 0.1 mmol), **2j-l** (0.1 mmol), [{$RuCl_2$(*p*-cymene)}$_2$] (3 mg, 5.0 mol %), and CsOAc (19 mg, 0.1 mmol) in ^{t}AmOH (3.0 mL) was stirred at 95 ^{o}C under open air for 3 hours. The solvent was removed under vacuo and the crude product obtained was

purified by silica gel (100-200 mesh) column chromatography using 20% EtOAc in hexane as the eluant to afford **4aj′-al′**.

2.6 Optimization of the reaction conditions for 3aa[a] (Table SI-1)



entry	catalyst	additive	solvent	**3aa** (%)[b]
1	$[RuCl_2(PPh_3)_3]$	$Cu(OAc)_2.H_2O$	^{t}AmOH	0
2	$[\{RuCl_2(p\text{-cymene})\}_2]$	$Cu(OAc)_2.H_2O$	^{t}AmOH	38
3	$Pd(OAc)_2$	$Cu(OAc)_2.H_2O$	^{t}AmOH	0
4	$[(Cp^*RhCl_2)_2]$	$Cu(OAc)_2.H_2O$	^{t}AmOH	0
5	$[Cp^*IrCl_2]_2$	$Cu(OAc)_2.H_2O$	^{t}AmOH	0
6	$[\{RuCl_2(p\text{-cymene})\}_2]$	$CuBr_2$	^{t}AmOH	11
7	$[\{RuCl_2(p\text{-cymene})\}_2]$	CsOAc	^{t}AmOH	79
8	$[\{RuCl_2(p\text{-cymene})\}_2]$	AgOAc	^{t}AmOH	37
9	$[\{RuCl_2(p\text{-cymene})\}_2]$	KOAc	^{t}AmOH	31
10	$[\{RuCl_2(p\text{-cymene})\}_2]$	CsOAc	1,4-dioxane	34
11	$[\{RuCl_2(p\text{-cymene})\}_2]$	CsOAc	acetonitrile	62
12	$[\{RuCl_2(p\text{-cymene})\}_2]$	CsOAc	DMF	41
13	$[\{RuCl_2(p\text{-cymene})\}_2]$	CsOAc	toluene	30
14[c]	$[\{RuCl_2(p\text{-cymene})\}_2]$	CsOAc	^{t}AmOH	51
15[d]	$[\{RuCl_2(p\text{-cymene})\}_2]$	CsOAc	^{t}AmOH	77

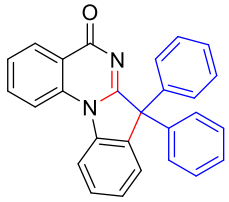
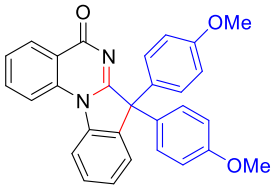
[a]Reaction conditions: **1a** (0.1 mmol), **2a** (0.1 mmol), catalyst (5 mol %), additive (0.1 mmol) and ^{t}AmOH (3.0 mL) at 95 °C under air for 24 h. [b]Isolated yields. [c]Catalyst 2.5 mol %. [d]Catalyst 7.5 mol %.

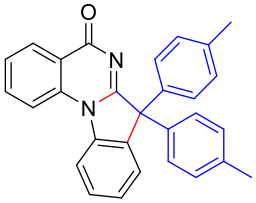
References:

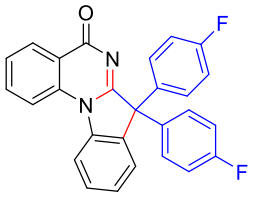
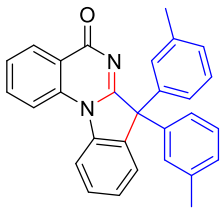
1. (a) P. Singh, N. Kaur, P. Banerjee**,** *J. Org. Chem.* **2020**, *85*, 3393–3406. (b) W. Yang, R. Qiao, J. Chen, X. Huang, M. Liu, W. Gao, J. Ding, H. Wu, *J. Org. Chem.* **2015**, *80*,

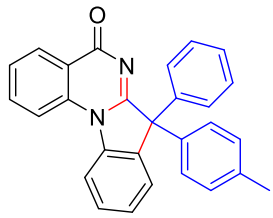
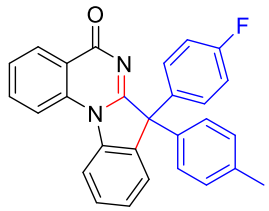
482–489. (c) J. Magano, M. Waldo, D. Greene, E. Nord, *Org. Process Res. Dev*. **2008**, *12*, 877–883.

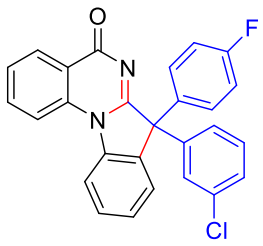
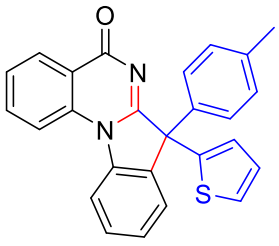
Spectral and analytical data of compounds 3 and 4

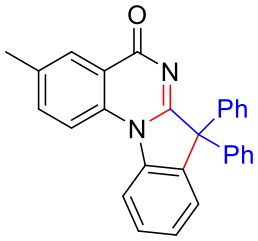
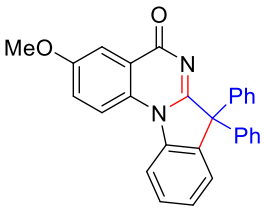
 **3aa**	**7,7-diphenylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3aa):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2a** (18 mg, 0.1 mmol), which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3aa** (30 mg, 79%). M.p.: 266-268 ^{o}C. UV-vis ($CHCl_3$) λ_{max} 325 nm, ε_{max} 3700. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1598, 1554. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 7.9, 1.4 Hz, 1H), 8.26 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.2 Hz, 1H), 7.85 (t, *J* = 8.7 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H), 7.43 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.34-7.25 (m, 10H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.4, 168.7, 141.6, 139.8, 137.7, 136.2, 133.8, 129.6, 128.7, 128.4, 127.7, 127.6, 126.5, 125.9, 119.4, 115.0, 113.7, 63.2. HRMS (+ESI) Calcd for $C_{27}H_{19}N_2O$ $[M+H]^+$: 387.1497; found: 387.1495. Anal. Calcd for $C_{27}H_{18}N_2O$: C, 83.92; H, 4.69; N, 7.25. Found: C, 84.06; H, 4.97; N, 7.38.
 **3ab**	**7,7-bis(4-methoxyphenyl)indolo[1,2-*a*]quinazolin-5(7*H*)-one (3ab):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2b** (24 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3ab** (28 mg, 63%). M.p.: 269-271 ^{o}C. UV-vis ($CHCl_3$) λ_{max} 330 nm, ε_{max} 9500. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1657, 1595, 1556, 1461. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (d, *J* = 8.0 Hz, 1H), 8.24 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.83 (t, *J* = 7.0 Hz, 1H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.41 (d, *J* = 7.5 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 1H), 7.24 (d, *J* = 8.5 Hz, 4H), 6.80 (d, *J* = 8.5 Hz, 4H), 3.76 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.0, 168.8, 159.0, 139.6, 137.8, 136.9, 133.8,

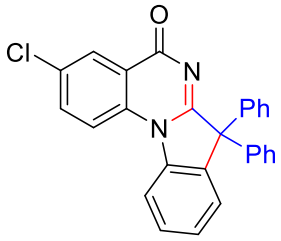
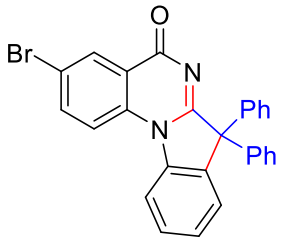
	133.7, 129.8, 129.6, 128.5, 127.4, 126.4, 125.9, 119.4, 114.9, 113.7, 113.6, 62.0, 55.2. HRMS (+ESI) Calcd for $C_{29}H_{23}N_2O_3$ $[M+H]^+$: 447.1709; found: 447.1703. Anal. Calcd for $C_{29}H_{22}N_2O_3$: C, 78.01; H, 4.97; N, 6.27. Found: C, 78.21; H, 4.90; N, 6.36.
 **3ac**	**7,7-di-*p*-tolylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3ac):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2c** (21 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford a white solid of **3ac** (28 mg, 68%). M.p.: 266-268 ^oC. UV-vis ($CHCl_3$) λ_{max} 330 nm, ε_{max} 4600. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1594, 1555, 1460, 743. ^1H NMR (500 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 7.9, 1.4 Hz, 1H), 8.24 (d, *J* = 8.5 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.82 (t, *J* = 8.6 Hz, 1H), 7.55 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 8.0, Hz, 1H), 7.42 (d, *J* = 7.5, Hz, 1H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.20 (d, *J* = 8.5 Hz, 4H), 7.08 (d, *J* = 8.1 Hz, 4H), 2.30 (s, 6H).^{13}C NMR (125 MHz, $CDCl_3$) δ 171.0, 169.0, 140.1, 139.0, 138.1, 137.7, 137.0, 134.0, 129.9, 129.4, 128.9, 128.8, 127.8, 126.7, 126.2, 119.8, 115.2, 113.9, 63.0, 21.2. HRMS (+ESI) Calcd for $C_{29}H_{23}N_2O$ $[M+H]^+$: 415.1810; found: 415.1817. Anal. Calcd for $C_{29}H_{22}N_2O$: C, 84.03; H, 5.35; N, 6.76. Found: C, 83.93; H, 5.18; N, 6.51.

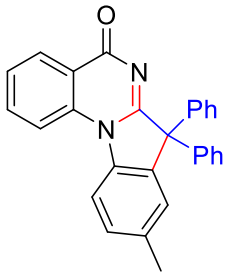
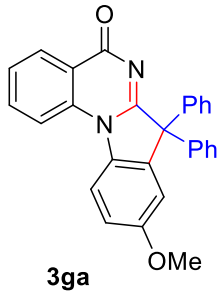
 **3ad**	**7,7-bis(4-fluorophenyl)indolo[1,2-*a*]quinazolin-5(7*H*)-one (3ad):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2d** (21 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3ad** (24 mg, 57% yield). M.p.: 145–147 ^{o}C. UV-vis ($CHCl_3$) λ_{max} 323 nm, ε_{max} 10200. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1596, 1553, 741. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.25 (d, *J* = 8.5 Hz, 1H), 8.05 (d, *J* = 8.3 Hz, 1H), 7.88-7.84 (m, 1H), 7.58 (t, *J* = 7.0 Hz, 1H), 7.56-7.53 (m, 1H), 7.40-7.35 (m, 2H), 7.31-7.27 (m, 4H), 7.00-6.95 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.3 (d, *J* = 203 Hz), 162.2 (d, *J* = 246.3 Hz), 139.7, 137.6, 137.2 (d, *J* = 3.8 Hz), 135.8, 134.0, 130.4 (d, *J* = 8.8 Hz), 129.7, 129.1, 127.3, 126.7, 126.1, 122.3, 119.4, 115.4 (d, *J* = 21.3 Hz), 113.8, 62.0. HRMS (+ESI) Calcd for $C_{27}H_{17}F_2N_2O$ $[M+H]^+$: 423.1309; found: 423.1313. Anal. Calcd for $C_{27}H_{16}F_2N_2O$: C, 76.77; H, 3.82; N, 6.63. Found: C, 76.92; H, 3.97; N, 6.45.
 **3ae**	**7,7-di-*m*-tolylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3ae):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2e** (21 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford white solid of **3ae** (27 mg, 65%). M.p.: 196–198 ^{o}C. UV-vis ($CHCl_3$) λ_{max} 330 nm, ε_{max} 3800. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1598, 1552, 743. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.26 (d, *J* = 8.5 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.84 (t, *J* = 8.7Hz, 1H), 7.56 (t, *J* = 7.0 Hz, 1H), 7.51 (t, *J* = 7.0 Hz, 1H), 7.42 (dd, *J* = 7.6, 1.1 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.20-7.05 (m, 8H), 2.26 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.5, 168.8, 141.5, 139.7, 138.0, 137.8, 136.5, 133.8, 129.6, 129.2, 128.6, 128.5, 128.2, 127.5, 126.4, 125.9, 125.9, 119.5, 115.0, 113.6, 63.2, 21.5. HRMS (+ESI) Calcd for $C_{29}H_{23}N_2O$ $[M+H]^+$: 415.1810; found:

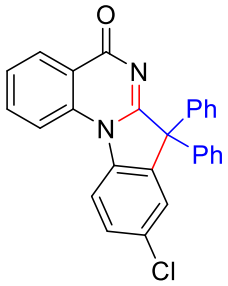
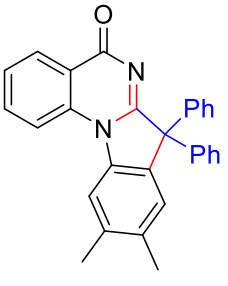
	415.1803. Anal. Calcd for $C_{29}H_{22}N_2O$: C, 84.03; H, 5.35; N, 6.76. Found: C, 84.08; H, 5.60; N, 6.89.
 3af	**7-phenyl-7-(*p*-tolyl)indolo[1,2-*a*]quinazolin-5(7*H*)-one (3af):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2f** (19 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3af** (27 mg, 67%). M.p.: 255–257 °C. UV-vis ($CHCl_3$) λ_{max} 320 nm, ε_{max} 3400. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1659, 1598, 1554, 740. ^1H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 7.9 Hz, 1H), 8.25 (d, *J* = 8.5 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.83 (t, *J* = 7.0 Hz, 1H), 7.55 (t, *J* = 7.0 Hz, 1H), 7.51 (t, *J* = 8.5 Hz, 1H), 7.42 (d, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 7.5 Hz, 1H), 7.33-7.24 (m, 5H), 7.23 (d, *J* = 9.5 Hz. 2H), 7.09 (d, *J* = 9.4 Hz, 2H), 2.30 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.7, 168.9, 141.9, 139.9, 138.6, 137.9, 137.7, 136.5, 133.9, 129.7, 129.2, 128.8, 128.8, 128.5, 127.7, 127.6, 126.6, 126.0, 119.6, 115.1, 113.8, 63.1, 21.1. HRMS (+ESI) Calcd for $C_{28}H_{21}N_2O$ $[M+H]^+$: 401.1654; found: 401.1473. Anal. Calcd for $C_{28}H_{20}N_2O$: C, 83.98; H, 5.03; N, 7.00. Found: C, 83.80; H, 4.92; N, 6.83.
 3ag	**7-(4-fluorophenyl)-7-(*p*-tolyl)indolo[1,2-*a*]quinazolin-5(7*H*)-one (3ag):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2g** (21 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3ag** (27 mg, 64%). M.p.: 263–265°C. UV-vis ($CHCl_3$) λ_{max} 330 nm, ε_{max} 3300. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1652, 1598, 1557. ^1H NMR (500 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.25 (d, *J* = 8.5 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.84 (t, *J* = 8.7 Hz, 1H), 7.56 (t, *J* = 8.0 Hz, 1H), 7.52 (t, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 7.5 Hz, 1H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.32-7.26 (m, 2H), 7.19 (d, *J* = 8.3 Hz, 2H), 7.09 (d, *J* = 8.1 Hz, 2H), 6.97 (t, *J* = 8.7 Hz, 2H), 2.30 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.4,

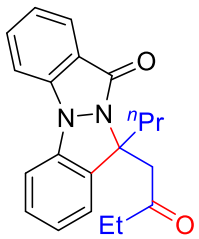
	168.6, 162.1 (d, J = 246.1 Hz), 161.2, 139.7, 138.5, 137.7 (d, J = 3.8 Hz), 137.4 (d, J = 3.3 Hz), 136.2, 133.8, 130.5 (d, J = 8.8 Hz), 129.6, 129.2, 128.8, 128.4, 127.4, 126.5, 126.0, 119.4, 115.3 (d, J = 21.3 Hz), 115.0 (d, J = 23.8 Hz), 115.0, 113.7, 62.3, 20.9. HRMS (+ESI) Calcd for $C_{28}H_{20}FN_2O$ $[M+H]^+$: 419.1560; found: 419.1580. Anal. Calcd for $C_{28}H_{19}FN_2O$: C, 80.37; H, 4.58; N, 6.69. Found: C, 80.43; H, 4.66; N, 6.74.
 **3ah**	**7-(3-chlorophenyl)-7-(4-fluorophenyl)indolo[1,2-*a*]quinazolin-5(7*H*)-one (3ah):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2h** (23 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3ah** (21 mg, 48%). M.p.:156–159 ^oC. UV-vis ($CHCl_3$) λ_{max} 330 nm, ε_{max} 4000. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1596, 1554. ^1H NMR (500 MHz, $CDCl_3$) δ 8.45 (d, J = 8.0 Hz, 1H), 8.34 (s, 1H), 8.18 (d, J = 8.5 Hz, 1H), 8.03 (d, J = 8.2 Hz, 1H), 7.83 (t, J = 7.9 Hz, 1H), 7.60-7.50 (m, 2H), 7.37 (t, J = 7.5 Hz, 1H), 7.29-7.17 (m, 7H), 7.04 (d, J = 7.6 Hz, 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.3, 168.6, 162.7 (d, J = 245.0 Hz), 141.3, 139.4, 137.8, 133.9 (d, J = 12.5 Hz), 133.3 (d, J = 2.5 Hz), 131.7, 131.1, 129.6, 129.1, 126.2, 126.5, 126.4, 125.6, 119.3, 116.3, 115.2, 113.3, 61.9. HRMS (+ESI) Calcd for $C_{27}H_{17}ClFN_2O$ $[M+H]^+$: 439.1013; found: 439.1017. Anal. Calcd for $C_{27}H_{16}ClFN_2O$: C, 73.89; H, 3.67; N, 6.38. Found: C, 74.06; H, 3.54; N, 6.61.
 **3ai**	**7-phenyl-7-(thiophen-2-yl)indolo[1,2-*a*]quinazolin-5(7*H*)-one (3ai):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2i** (20 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford light yellow solid of **3ai** (21 mg, 51%). M.p.: 208–210^oC. UV-vis ($CHCl_3$) λ_{max} 315 nm, ε_{max} 3200. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1598, 1554. ^1H NMR (500 MHz, $CDCl_3$) δ 8.48 (dd, J = 8.0, 1.4

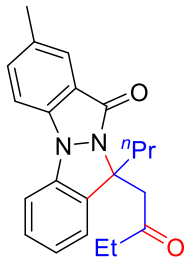
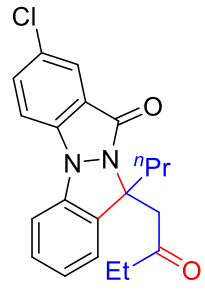
	Hz, 1H), 8.25 (d, *J* = 8.5 Hz, 1H), 8.02 (d, *J* = 8.2 Hz, 1H), 7.85 (t, *J* = 8.7Hz, 1H), 7.60-7.52 (m, 3H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.29-7.26 (m, 1H), 7.21-7.16 (m, 3H), 7.08 (d, *J* = 8.1 Hz, 2H), 6.97-6.95 (m, 1H), 2.30 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.9, 168.7, 143.8, 139.8, 138.4, 138.0, 137.8, 136.6, 134.0, 129.8, 129.2, 128.3, 127.9, 127.3, 126.7, 126.66, 126.2, 126.0, 119.6, 115.1, 113.8, 60.2, 21.1. HRMS (+ESI) Calcd for $C_{26}H_{19}N_2OS$ $[M+H]^+$: 407.1218; found: 407.1081. Anal. Calcd for $C_{26}H_{18}N_2OS$: C, 76.82; H, 4.46; N, 6.89. Found: C, 76.67; H, 4.41; N, 6.94.
 **3ba**	**3-methyl-7,7-diphenylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3ba):** The title compound was prepared by following the general procedure **2.2** from indazolone **1b** (22 mg, 0.1 mmol) and alkyne **2a** (18 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3ba** (27 mg, 68%). M.p.: 301–303 °C. UV-vis ($CHCl_3$) λ_{max} 335 nm, ε_{max} 3850. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1591, 1556. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28 (d, *J* = 1.0 Hz, 1H), 8.15 (d, *J* = 8.6 Hz, 1H), 8.01 (d, *J* = 8.2 Hz, 1H), 7.64 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.55-7.48 (m, 1H), 7.43 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.37-7.27 (m, 11H), 2.51 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.0, 168.9, 141.8, 140.1, 136.8, 136.4, 135.8, 135.0, 129.3, 128.86, 128.8, 128.5, 127.8, 127.6, 125.9, 119.4, 115.0, 113.7, 63.3, 21.1. HRMS (+ESI) Calcd for $C_{28}H_{21}N_2O$ $[M+H]^+$: 401.1654; found: 401.1667. Anal. Calcd for $C_{28}H_{20}N_2O$: C, 83.98; H, 5.03; N, 7.00. Found: C, 83.73; H, 5.18; N, 7.36.
 **3ca**	**3-methoxy-7,7-diphenylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3ca):** The title compound was prepared by following the general procedure **2.2** from indazolone **1c** (24 mg, 0.1 mmol) and alkyne **2a** (18 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3ca** (25 mg, 60%). M.p.: 295–297°C. UV-vis ($CHCl_3$) λ_{max} 340 nm, ε_{max} 4250. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1596,

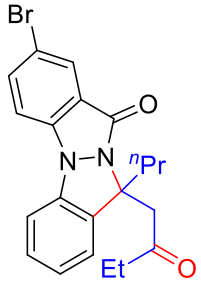
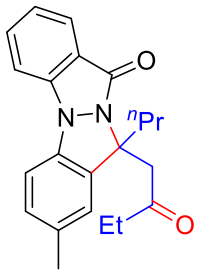
	1561. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.21 (d, *J* = 9.3 Hz, 1H), 8.00 (d, *J* = 8.3 Hz, 1H), 7.89 (d, *J* = 3.1 Hz, 1H), 7.53-7.49 (m, 1H), 7.45-7.41 (m, 2H), 7.37-7.24 (m, 11H), 3.94 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.6, 169.0, 158.2, 141.9, 140.2, 136.7, 132.2, 129.1, 129.0, 128.7, 128.0, 127.8, 126.2, 123.9, 121.3, 117.0, 113.8, 109.6, 63.5, 56.2. HRMS (+ESI) Calcd for $C_{28}H_{21}N_2O_2$ $[M+H]^+$: 417.1603; found: 417.1580. Anal. Calcd for $C_{28}H_{20}N_2O_2$: C, 80.75; H, 4.84; N, 6.73. Found: C, 80.88; H, 4.97; N, 6.92.
 **3da**	**3-chloro-7,7-diphenylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3da):** The title compound was prepared by following the general procedure **2.2** from indazolone **1d** (24 mg, 0.1 mmol) and alkyne **2a** (18 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3da** (24 mg, 57%). M.p.: 315-317 ^{o}C. UV-vis ($CHCl_3$) λ_{max} 328 nm, ε_{max} 2350. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1657, 1589, 1545. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 (d, *J* = 2.5 Hz, 1H), 8.21 (d, *J* = 9.0 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 7.79 (dd, *J* = 9.0 Hz, 2.5 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.32-7.25 (m, 10H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.7, 167.6, 141.5, 139.6, 136.3, 136.2, 134.0, 132.5, 129.2, 128.9, 128.8, 128.6, 127.9, 127.8, 127.5, 127.3, 126.3, 120.9, 116.7, 113.6, 63.3. HRMS (+ESI) Calcd for $C_{27}H_{18}ClN_2O$ $[M+H]^+$: 421.1108; found: 421.1095. Anal. Calcd for $C_{27}H_{17}ClN_2O$: C, 77.05; H, 4.07; N, 6.66. Found: C, 76.83; H, 3.86; N, 6.92.
 **3ea**	**3-bromo-7,7-diphenylindolo[1,2-*a*]quinazolin-5(7*H*)-one(3ea):** The title compound was prepared by following the general procedure **2.2** from indazolone **1e** (29 mg, 0.1 mmol) and alkyne **2a** (18 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3ea** (27 mg, 58%). M.p.: 325–327^{o}C. UV-vis ($CHCl_3$) λ_{max} 330 nm, ε_{max} 3300. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1655, 1590. ^{1}H

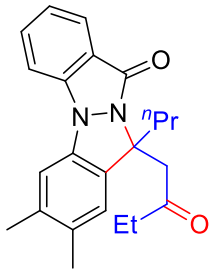
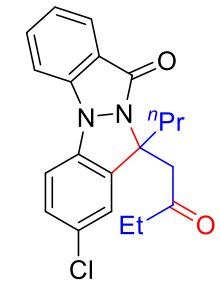
	NMR (500 MHz, $CDCl_3$) δ 8.61 (d, *J* = 2.4 Hz, 1H), 8.15 (d, *J* = 9.0 Hz, 1H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.92 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.53 (t, *J* = 9.0 Hz, 1H), 7.44 (d, *J* = 7.5 Hz, 1H), 7.37 (t, *J* = 7.5 Hz, 1H), 7.33-7.27 (m, 10H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.9, 167.7, 141.7, 139.7, 137.1, 136.8, 136.5, 132.5, 129.2, 129.0, 128.8, 128.1, 128.0, 126.5, 121.2, 120.2, 117.1, 113.9, 63.7. HRMS (+ESI) Calcd for $C_{27}H_{18}BrN_2O$ $[M+H]^+$: 465.0602; found: 465.0428. Anal. Calcd for $C_{27}H_{17}BrN_2O$: C, 69.69; H, 3.68; N, 6.02. Found: C, 69.90; H, 3.49; N, 5.80.
 **3fa**	**1-methyl-7,7-diphenylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3fa):** The title compound was prepared by following the general procedure **2.2** from indazolone **1f** (22 mg, 0.1 mmol) and alkyne **2a** (18 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford light brown solid of **3fa** (26 mg, 65%). M.p.: 246–248 ^oC. UV-vis ($CHCl_3$) λ_{max} 334 nm, ε_{max} 1500. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1598, 1589. ^1H NMR (500 MHz, $CDCl_3$) δ 8.47 (d, *J* = 7.9 Hz, 1H), 8.27 (d, *J* = 8.6 Hz, 1H), 7.87-7.84 (m, 2H), 7.56 (t, *J* = 6.7 Hz, 1H), 7.33-7.27 (m, 11H), 7.16 (d, *J* = 7.6 Hz, 1H), 2.54 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.7, 168.7, 141.7, 139.9, 139, 137.8, 133.8, 133.3, 129.6, 128.7, 128.7, 128.4, 127.6, 127.1, 126.6, 126.4, 115.1, 114.4, 63.0, 22.0. HRMS (+ESI) Calcd for $C_{28}H_{21}N_2O$ $[M+H]^+$:401.1654; found: 401.1659. Anal. Calcd for $C_{28}H_{20}N_2O$: C, 83.98; H, 5.03; N, 7.00. Found: C, 84.26; H, 5.07; N, 7.28.
 **3ga**	**9-methoxy-7,7-diphenylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3ga):** The title compound was prepared by following the general procedure **2.2** from indazolone **1g** (24 mg, 0.1 mmol) and alkyne **2a** (18 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford off white solid of **3ga** (24 mg, 58%). M.p.: 289–291 ^oC. UV-vis ($CHCl_3$) λ_{max} 338 nm, ε_{max} 1250. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1598, 1552. ^1H NMR (500 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 7.9, 1.4 Hz,

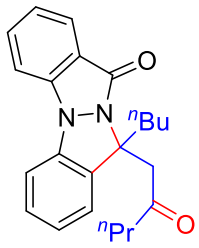
	1H), 8.19 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.9 Hz, 1H), 7.84-7.80 (m, 1H), 7.56-7.52 (m, 1H), 7.35-7.27 (m, 10H), 7.00 (dd, *J* = 8.9, 2.7 Hz, 1H), 6.95 (d, *J* = 2.7 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.1, 168.7, 157.7, 141.6, 138.0, 137.6, 133.7, 133.2, 129.6, 128.7, 128.4, 127.7, 126.3, 119.4, 114.7, 114.4, 113.8, 113.2, 63.5, 55.7. HRMS (+ESI) Calcd for $C_{28}H_{21}N_2O_2$ $[M+H]^+$: 417.1603; found: 417.1590. Anal. Calcd for $C_{28}H_{20}N_2O_2$: C, 80.75; H, 4.84; N, 6.73. Found: C, 80.71; H, 4.83; N, 6.51.
 **3ha**	**9-chloro-7,7-diphenylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3ha):** The title compound was prepared by following the general procedure **2.2** from indazolone **1h** (24 mg, 0.1 mmol) and alkyne **2a** (18 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford off white solid of **3ha** (22 mg, 53%). M.p.: 305–307 °C. UV-vis ($CHCl_3$) λ_{max} 340 nm, ε_{max} 1050. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1656, 1596, 1552. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 7.9, 1.5 Hz, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 7.96 (d, *J* = 8.7 Hz, 1H), 7.87-7.82 (m, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.49 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.38 (d, *J* = 2.2 Hz, 1H), 7.34-7.27 (m, 10H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.0, 168.4, 140.9, 138.3, 138.1, 137.4, 133.9, 131.5, 129.8, 128.8, 128.6, 128.6, 128.0, 127.7, 126.7, 119.4, 114.7, 114.5, 63.2. HRMS (+ESI) Calcd for $C_{27}H_{18}ClN_2O$ $[M+H]^+$: 421.1108; found:. 421.1095. Anal. Calcd for $C_{27}H_{17}ClN_2O$: C, 77.05; H, 4.07; N, 6.66. Found: C, 76.82; H, 4.18; N, 6.40.
 **3ia**	**9,10-dimethyl-7,7-diphenylindolo[1,2-*a*]quinazolin-5(7*H*)-one (3ia):** The title compound was prepared by following the general procedure **2.2** from indazolone **1i** (24 mg, 0.1 mmol) and alkyne **2a** (18 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **3ia** (26 mg, 64%). M.p.: 277–279 °C. UV-vis ($CHCl_3$) λ_{max} 333 nm, ε_{max} 950. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1657, 1601, 1547.

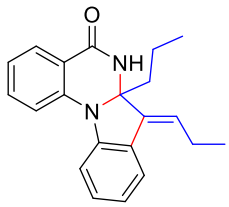
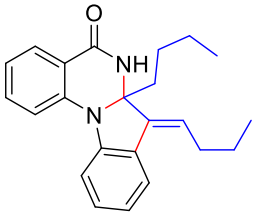
	^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (dd, *J* = 8.0, 1.4 Hz, 1H), 8.26 (d, *J* = 8.5 Hz, 1H), 7.85-7.82 (m, 1H), 7.81 (s, 1H), 7.55 (t, *J* = 7.0 Hz, 1H), 7.34-7.25 (m, 10H), 7.15 (s, 1H), 2.44 (s, 3H), 2.30 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.5, 168.8, 141.9, 137.9, 137.8, 137.3, 134.6, 133.7, 133.6, 129.5, 128.7, 128.3, 128.2, 127.5, 126.3, 119.4, 115.0, 114.8, 63.1, 20.6, 19.8. HRMS (+ESI) Calcd for $C_{29}H_{23}N_2O[M+H]^+$: 415.1810; found: 415.1812. Anal. Calcd for $C_{29}H_{22}N_2O$: C, 84.03; H, 5.35; N, 6.76. Found: C, 84.34; H, 5.24; N, 6.50.
 **4aj**	**12-(2-oxobutyl)-12-propyl-10*H*,12*H*-indazolo[1,2-*a*]indazol-10-one (4aj):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2j** (11 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford a brown thick liquid of **4aj** (21 mg, 62%). UV-vis ($CHCl_3$) λ_{max} 300 nm, ε_{max} 13850. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1719, 1656, 1608, 1501. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.9 Hz, 1H), 7.61-7.58 (m, 1H), 7.49 (d, *J* = 8.3 Hz, 1H), 7.38-7.34 (m, 1H), 7.26-7.28 (m, 1H), 7.20-7.14 (m, 2H), 7.06-7.03 (m, 1H), 4.04 (d, *J* = 17.4 Hz, 1H), 3.26 (d, *J* = 17.3 Hz, 1H), 2.58-2.52 (m , 1H), 2.42-2.26 (m, 2H), 2.01-1.94 (m, 1H), 1.27-1.10 (m, 1H), 1.06-0.98 (m, 1H), 0.83 (t, *J* = 7.3 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.8, 159.0, 138.2, 136.7, 134.7, 131.8, 128.9, 124.3, 122.5, 122.1, 120.9, 119.5, 109.8, 107.9, 67.4, 47.2, 40.9, 36.4, 16.8, 13.6, 7.2. HRMS (+ESI) Calcd for $C_{21}H_{23}N_2O_2$ $[M+H]^+$: 335.1759; found: 335.1758. Anal. Calcd for $C_{21}H_{22}N_2O_2$: C, 75.42; H, 6.63; N, 8.38. Found: C, 75.77; H, 6.41; N, 8.05.

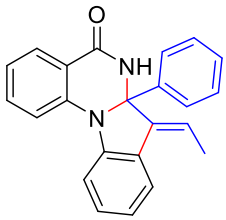
 **4bj**	**8-methyl-12-(2-oxobutyl)-12-propyl-10*H*,12*H*-indazolo[1,2-*a*]indazol-10-one (4bj):** The title compound was prepared by following the general procedure **2.2** from indazolone **1b** (22 mg, 0.1 mmol) and alkyne **2j** (11 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford a yellow gummy liquid of **4bj** (22 mg, 63%). UV-vis ($CHCl_3$) λ_{max} 298 nm, ε_{max} 3250. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1719, 1656, 1500. NMR (400 MHz,) δ 7.64 (s, 1H), 7.40 (d, *J* = 3.9 Hz, 2H), 7.38-7.31 (m, 1H), 7.25-7.21 (m, 1H), 7.18 (d, *J* = 7.5 Hz, 1H), 7.02 (t, *J* = 7.5 Hz, 1H), 4.03 (d, *J* = 17.3 Hz, 1H), 3.24 (d, *J* = 17.3 Hz, 1H), 268-2.46 (m, 1H), 2.43 (s, 3H), 2.42-2.24 (m, 2H), 1.98-1.80 (m, 1H), 1.25-1.17 (m, 1H), 1.05-0.98 (m, 1H), 0.83 (t, *J* = 7.3 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.1, 159.3, 142.0, 136.7, 134.8, 131.0, 127.9, 124.8, 122.5, 122.3, 119.8, 111.2, 107.9, 68.1, 48.5, 42.4, 37.5, 21.2, 18.1, 13.8, 7.4. HRMS (+ESI) Calcd for $C_{22}H_{25}N_2O_2$ $[M+H]^+$: 349.1916; found: 349.1920. Anal. Calcd for $C_{22}H_{24}N_2O_2$: C, 75.83; H, 6.94; N, 8.04. Found: C, 75.49; H, 7.27; N, 8.16.
 **4dj**	**8-chloro-12-(2-oxobutyl)-12-propyl-10*H*,12*H*-indazolo[1,2-*a*]indazol-10-one (4dj):** The title compound was prepared by following the general procedure **2.2** from indazolone **1d** (24 mg, 0.1 mmol) and alkyne **2j** (11 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford yellow gummy liquid of **4dj** (20 mg, 54%). UV-vis ($CHCl_3$) λ_{max} 304 nm, ε_{max} 4800. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1719, 1656, 1493. ^1H NMR (500 MHz, $CDCl_3$) δ 7.83 (d, *J* = 2.0 Hz, 1H), 7.54 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.43 (dd, *J* = 8.7, 0.4 Hz, 1H), 7.38-7.34 (m, 1H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.19-7.17 (m, 1H), 7.08-7.05 (m, 1H), 4.06 (d, *J* = 17.6 Hz, 1H), 3.22 (d, *J* = 17.6 Hz, 1H), 2.53-2.47 (m, 1H), 2.41-2.24 (m, 2H), 1.98-1.92 (m, 1H),1.30-1.20 (m, 1H), 1.05-0.99 (m, 1H), 0.83 (t, *J* = 7.7 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.8, 158.1, 136.6, 136.4, 134.7, 132.2, 129.01, 126.5, 123.9, 122.9, 122.0, 120.5, 110.9,

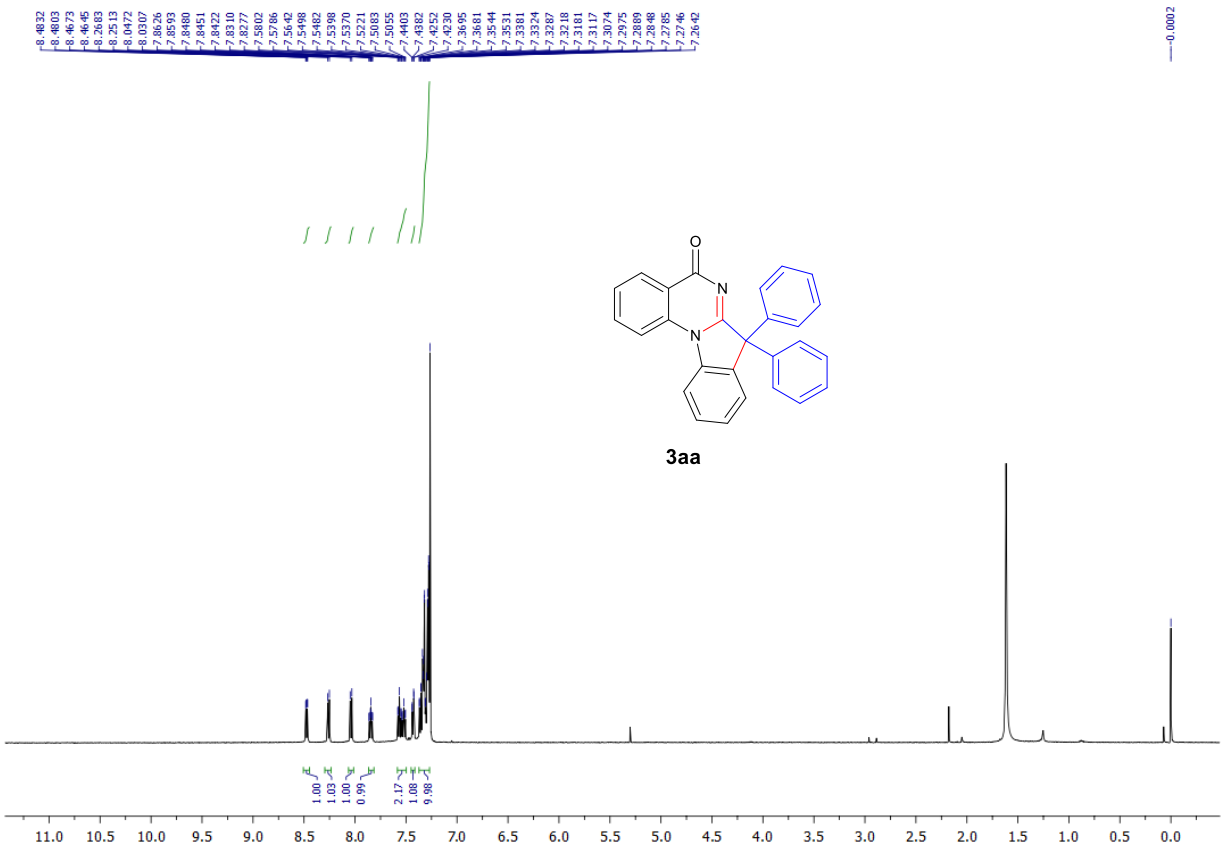
	107.9, 67.6, 46.8, 41.0, 36.4, 16.8, 13.6, 7.2. HRMS (+ESI) Calcd for $C_{21}H_{22}ClN_2O_2$ $[M+H]^+$: 369.1369; found: 369.1361. Anal. Calcd for $C_{21}H_{21}ClN_2O_2$: C, 68.38; H, 5.74; N, 7.59. Found: C, 68.47; H, 5.71; N, 7.90.
 **4ej**	**8-bromo-12-(2-oxobutyl)-12-propyl-10*H*,12*H*-indazolo[1,2-*a*]indazol-10-one (4ej):** The title compounds was prepared by following the general procedure **2.2** from indazolone **1e** (29 mg, 0.1 mmol) and alkyne **2j** (11 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford yellow gummy liquid of **3ej** (24 mg, 59%). UV-vis ($CHCl_3$) λ_{max} 304 nm, ε_{max} 2200. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1719, 1659, 1603, 1500, 1468. ^1H NMR (500 MHz, $CDCl_3$) δ 7.98 (d, *J* = 1.9 Hz, 1H), 7.66 (dd, *J* = 8.7, 1.9 Hz, 1H), 7.40-7.38 (m, 1H), 7.35 (d, *J* = 7.7 Hz, 1H), 7.23 (d, *J* = 7.9 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 4.05 (d, *J* = 17.5 Hz, 1H), 3.22 (d, *J* = 17.5 Hz, 1H), 2.53-2.47 (m, 1H), 2.42–2.23 (m, 2H), 1.98–1.94 (m, 1H), 1.30-1.18 (m, 1H), 1.10-0.86 (m, 1H), 0.83 (t, *J* = 7.3 Hz, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.8, 157.8, 136.8, 136.4, 134.8, 134.7, 129.0, 127.0, 122.9, 122.0, 120.9, 113.5, 111.2, 108.0, 67.6, 46.8, 41.0, 36.4, 16.8, 13.6, 7.2. HRMS (+ESI) Calcd for $C_{21}H_{22}BrN_2O_2$ $[M+H]^+$: 413.0864; found: 413.0863.
 **4fj**	**2-methyl-12-(2-oxobutyl)-12-propyl-10*H*,12*H*-indazolo[1,2-*a*]indazol-10-one (4fj):** The title compound was prepared by following the general procedure **2.2** from indazolone **1f** (22 mg, 0.1 mmol) and alkyne **2j** (11 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford yellow gummy liquid of **4fj** (22 mg, 64%). UV-vis ($CHCl_3$) λ_{max} 300 nm, ε_{max} 9650. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1719, 1656, 1502. ^1H NMR (500 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.9 Hz, 1H), 7.58 (t, *J* = 7.7 Hz, 1H), 7.50 (d, *J* = 8.3 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.10–7.05 (m, 2H), 6.85 (d, *J* = 7.7 Hz, 1H), 4.00 (d, *J* = 17.3 Hz, 1H), 3.23 (d, *J* = 17.2 Hz, 1H), 2.57-2.51 (m, 1H),

	2.37 (s, 3H), 2.37-2.26 (m, 2H), 2.00-1.93 (m, 1H), 1.31-1.14 (m, 1H), 1.06-1.00 (m, 1H), 0.84-0.80 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.9, 158.9, 139.2, 138.0, 136.7, 131.8, 131.7, 124.2, 123.3, 121.9, 120.8, 119.4, 109.7, 108.7, 67.4, 47.2, 40.8, 36.4, 21.6, 16.8, 13.6, 7.2. HRMS (+ESI) Calcd for $C_{22}H_{25}N_2O_2$ $[M+H]^+$: 349.1916; found: 349.1918.
 **4gj**	**2,3-dimethyl-12-(2-oxobutyl)-12-propyl-10H,12H-indazolo[1,2-*a*]indazol-10-one (4gj):** The title compound was prepared by following the general procedure **2.2** from indazolone **1g** (24 mg, 0.1 mmol) and alkyne **2j** (11 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford gummy liquid of **4gj** (18 mg, 51%). UV-vis ($CHCl_3$) λ_{max} 300 nm, ε_{max} 3700. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1719, 1654, 1610, 1500. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 7.8, 0.8 Hz, 1H), 7.59-7.56 (m, 1H), 7.49 (d, *J* = 8.3 Hz, 1H), 7.15-7.10 (m, 1H), 7.06 (s, 1H), 6.94 (s, 1H), 3.99 (d, *J* = 17.2 Hz, 1H), 3.22 (d, *J* = 17.2 Hz, 1H), 2.57-2.50 (m, 1H), 2.40-2.30 (m, 2H), 2.32 (s, 3H), 2.25 (s, 3H), 1.97-1.91 (m, 1H), 1.25-1.15 (m, 1H), 1.15-0.94 (m, 1H), 0.85-0.80 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 207.0, 158.9, 138.0, 137.4, 134.8, 132.0, 131.6, 130.8, 124.2, 123.1, 120.5, 119.1, 109.6, 109.2, 67.4, 47.3, 40.8, 36.4, 20.2, 19.7, 16.8, 13.6, 7.2. HRMS (+ESI) Calcd for $C_{23}H_{27}N_2O_2$ $[M+H]^+$: 363.2072; found: 363.2073. Anal. Calcd for $C_{23}H_{26}N_2O_2$: C, 76.21; H, 7.23; N, 7.73. Found: C, 76.04; H, 7.29; N, 7.62.
 **4ij**	**2-chloro-12-(2-oxobutyl)-12-propyl-10*H*,12*H*-indazolo[1,2-*a*]indazol-10-one (4ij):** The title compound was prepared by following the general procedure **2.2** from indazolone **1i** (24 mg, 0.1 mmol) and alkyne **2j** (11 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford light yellow solid of **4ij** (18 mg, 50%). UV-vis ($CHCl_3$) λ_{max} 300 nm, ε_{max} 3450. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1720, 1653, 1500. M.p.: 172–174 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.85 (d, *J*

	= 7.7 Hz, 1H), 7.60 (t, *J* = 7.3 Hz, 1H), 7.45 (d, *J* = 8.2 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.25-7.13 (m, 3H), 4.09 (d, *J* = 17.7 Hz, 1H), 3.20 (d, *J* = 17.9 Hz, 1H), 2.49-2.33 (m, 3H), 1.92 (t, *J* = 12.7 Hz, 1H), 1.30-1.10 (m, 1H), 1.10-1.00 (m, 1H), 0.89-0.83 (m, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.6, 159.3, 138.5, 136.9, 135.6, 132.0, 128.9, 127.6, 124.4, 122.4, 121.4, 119.5, 109.7, 108.6, 67.3, 46.9, 41.1, 36.2, 16.8, 13.6, 7.2. HRMS (+ESI) Calcd for $C_{21}H_{22}ClN_2O_2$ $[M+H]^+$: 369.1369; found: 369.1367. Anal. Calcd for $C_{21}H_{21}ClN_2O_2$: C, 68.38; H, 5.74; N, 7.59. Found: C, 68.65; H, 5.40; N, 7.78.
 **4ak**	**12-butyl-12-(2-oxopentyl)-10*H*,12*H*-indazolo[1,2-*a*]indazol-10-one (4ak):** The title compound was prepared by following the general procedure **2.2** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2k** (14 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford light brown solid of **4ak** (25 mg, 63%). UV-vis ($CHCl_3$) λ_{max} 300 nm, ε_{max} 3300. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1718, 1656, 1605, 1500. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.9 Hz, 1H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.50 (d, *J* = 9.3 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.26 (d, *J* = 6.3 Hz, 1H), 7.19 (d, *J* = 8.1 Hz, 1H), 7.16 (t, *J* = 7.1 Hz, 1H), 7.05 (t, *J* = 7.5 Hz, 1H), 4.04 (d, *J* = 17.4 Hz, 1H), 3.23 (d, *J* = 17.4 Hz, 1H), 2.60-2.50 (m, 1H), 2.31-2.20 (m, 2H), 2.06-1.95 (m, 1H), 1.42-1.32 (m, 2H), 1.28-1.17 (m, 2H), 1.02-0.90 (m, 2H), 0.77 (t, *J* = 6.9 Hz, 3H), 0.71 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 206.5, 159.0, 138.3, 136.8, 134.7, 131.8, 128.9, 124.3, 122.5, 122.1, 120.1, 119.5, 109.8, 107.9, 67.4, 47.5, 45.2, 38.6, 25.5, 22.3, 16.6, 13.8, 13.3. HRMS (+ESI) Calcd for $C_{23}H_{27}N_2O_2$ $[M+H]^+$: 363.2072; found: 363.2075. Anal. Calcd for $C_{23}H_{26}N_2O_2$: C, 76.21; H, 7.23; N, 7.73. Found: C, 75.89; H, 7.01; N, 7.74.

 **4aj'**	**(*E*)-6a-propyl-7-propylidene-6a,7-dihydroindolo[1,2-*a*]quinazolin-5(6*H*)-one (4aj′):** The title compound was prepared by following the general procedure **2.5** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2j′** (11 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford a yellow thick gum of **4aj′** (10 mg, 33%). UV-vis ($CHCl_3$) λ_{max} 296 nm, ε_{max} 3850. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1663, 1596, 1491. ^1H NMR (500 MHz, $CDCl_3$) δ 8.09 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.64-7.59 (m, 1H), 7.58 (d, *J* = 7.7 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.22 (t, *J* = 7.7 Hz, 1H), 7.20-7.14 (m, 2H), 6.95-6.89 (m, 1H), 6.31 (s, 1H), 5.70 (t, *J* = 7.1 Hz, 1H), 2.61 (pentate, *J* = 7.4 Hz, 2H), 2.17-2.02 (m, 1H), 1.77-1.72 (m, 1H), 1.23 (t, *J* = 7.5 Hz, 3H), 1.19-1.09 (m, 2H), 0.75 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.2, 148.4, 139.9, 138.0, 133.4, 129.4, 128.9, 126.3, 126.0, 125.3, 123,4, 122.3, 122.1, 120.7, 107.6, 80.2, 42.1, 22.0, 17.6, 14.0, 13.8. HRMS (+ESI) Calcd for $C_{21}H_{23}N_2O$ $[M+H]^+$:319.1810; found: 319.1812. Anal. Calcd for $C_{21}H_{22}N_2O$: C, 79.21; H, 6.96; N, 8.80. Found: C, 79.30; H, 7.31; N, 8.69.
 **4ak'**	**(*E*)-6a-butyl-7-butylidene-6a,7-dihydroindolo[1,2-*a*]quinazolin-5(6*H*)-one and (*Z*)-6a-butyl-7-butylidene-6a,7-dihydroindolo[1,2-*a*]quinazolin-5(6*H*)-one (4ak′, *E*:*Z* = 24:1):** The title compounds were prepared by following the general procedure **2.5** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2k′** (14 mg, 0.1 mmol) which was then purified by column chromatography using 15% EtOAc in hexane to afford yellow solid of **4ak′** (12 mg, 36%). M.p.: 164–166 °C. UV-vis ($CHCl_3$) λ_{max} 295 nm, ε_{max} 3750. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1663, 1594, 1491, 1461. ^1H NMR (500 MHz, $CDCl_3$) δ 8.25 (dd, *J* = 7.7, 1.9 Hz, 0.04H), 8.09 (dd, *J* = 7.8, 1.5 Hz, 0.96H), 7.68-7.62 (m, 0.08H), 7.64-7.56 (m, 1.92H), 7.48 (d, *J* = 8.0 Hz, 0.96H), 7.38 (d, *J* = 6.6 Hz, 0.04H), 7.33-7.29 (m, 0.08H) 7.22 (t, *J* = 7.7 Hz, 1H), 7.20-7.10 (m, 1.92H), 6.95-6.85 (m, 1H), 6.35 (bs, 1H), 6.17

	(t, *J* = 8.1 Hz, 0.04H), 5.77-5.66 (m, 0.96H), 2.76 (q, *J* = 6.8 Hz, 0.08H), 2.57 (q, *J* = 7.4 Hz, 1.92H), 2.18-2.05 (m, 1H), 1.82-1.60 (m, 4H), 1.45-1.37 (m, 0.12H), 1.28-1.22 (m, 0.12H), 1.19-1.01 (m, 5.76H), 0.96 (t, *J* = 7.4 Hz, 0.12H), 0.73 (t, *J* = 7.0 Hz, 2.88H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.1, 148.3, 139.8, 138.2, 133.2, 130.4, 129.3, 128.8, 126.0, 125.1, 124.6, 123.3, 122.2, 120.5, 107.5, 80.3, 39.4, 30.4, 26.3, 22.6, 22.2, 14.0, 13.8. HRMS (+ESI) Calcd for $C_{23}H_{27}N_2O$ $[M+H]^+$: 347.2123; found: 347.2126. Anal. Calcd for $C_{23}H_{26}N_2O$: C, 79.73; H, 7.56; N, 8.09. Found: C, 79.79; H, 7.30; N, 7.68.
 **4al'**	**(*E*)-7-ethylidene-6a-phenyl-6a,7-dihydroindolo[1,2-*a*]quinazolin-5(6*H*)-one (4al′):** The title compound was prepared by following the general procedure **2.5** from indazolone **1a** (21 mg, 0.1 mmol) and alkyne **2l′** (13 mg, 0.1 mmol) which was then purified by column chromatography using 20% EtOAc in hexane to afford white solid of **4al′** (22 mg, 65%). M.p.: 209–211 °C. UV-vis ($CHCl_3$) λ_{max} 347 nm, ε_{max} 3850. FTIR ($CHCl_3$, cm^{-1}) ν_{max} 1666, 1591, 1491, 1463. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 1H), 7.51-7.44 (m, 4H), 7.28-7.17 (m, 5H), 7.14-7.10 (m, 1H), 7.02-6.98 (m, 1H), 6.61 (bs, 1H), 5.46 (q, *J* = 7.3 Hz, 1H), 2.03 (d, *J* = 7.4 Hz, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.9, 148.7, 142.8, 142.6, 140.2, 133.2, 129.4, 128.8, 128.1, 128.0, 127.9, 126.4, 126.3, 125.6, 125.2, 123.9, 122.8, 122.2, 121.1, 107.9, 82.1, 14.4. HRMS (+ESI) Calcd for $C_{23}H_{19}N_2O$ $[M+H]^+$: 339.1497; found: 339.1501. Anal. Calcd for $C_{23}H_{18}N_2O$: C, 81.63; H, 5.36; N, 8.28. Found: C, 81.87; H, 5.04; N, 8.02.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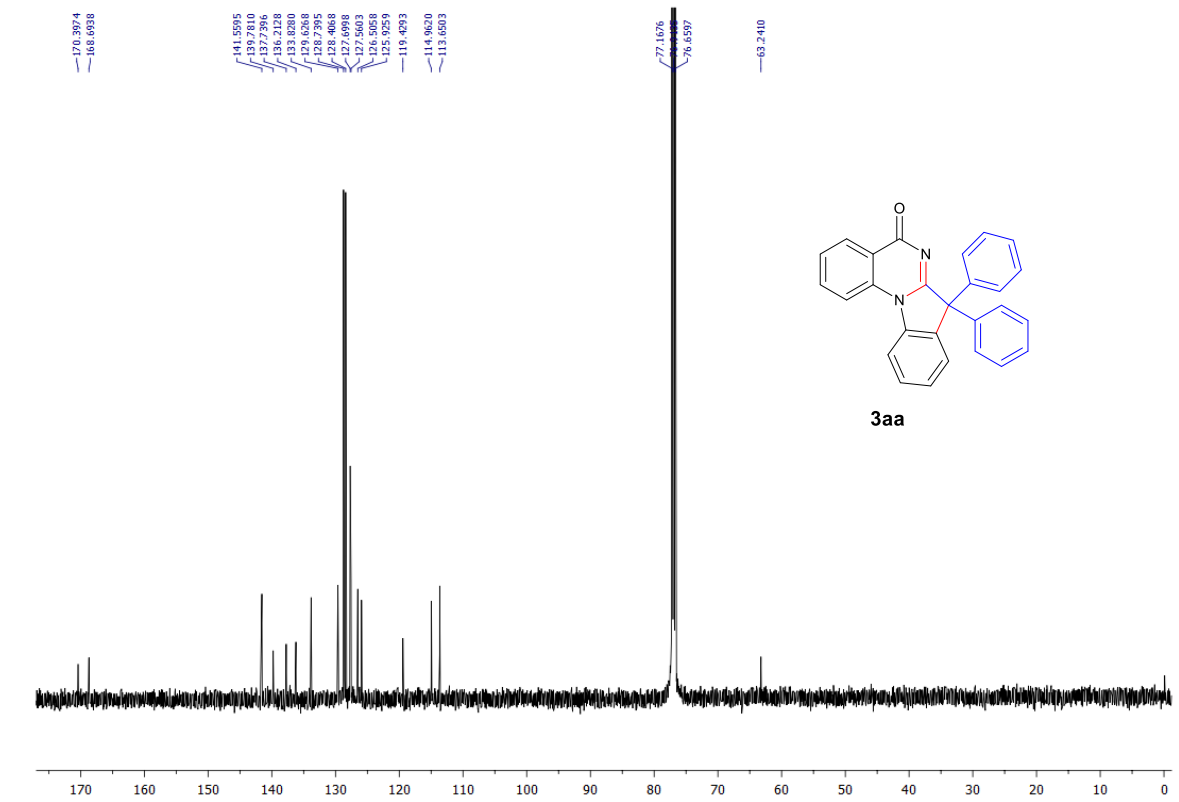
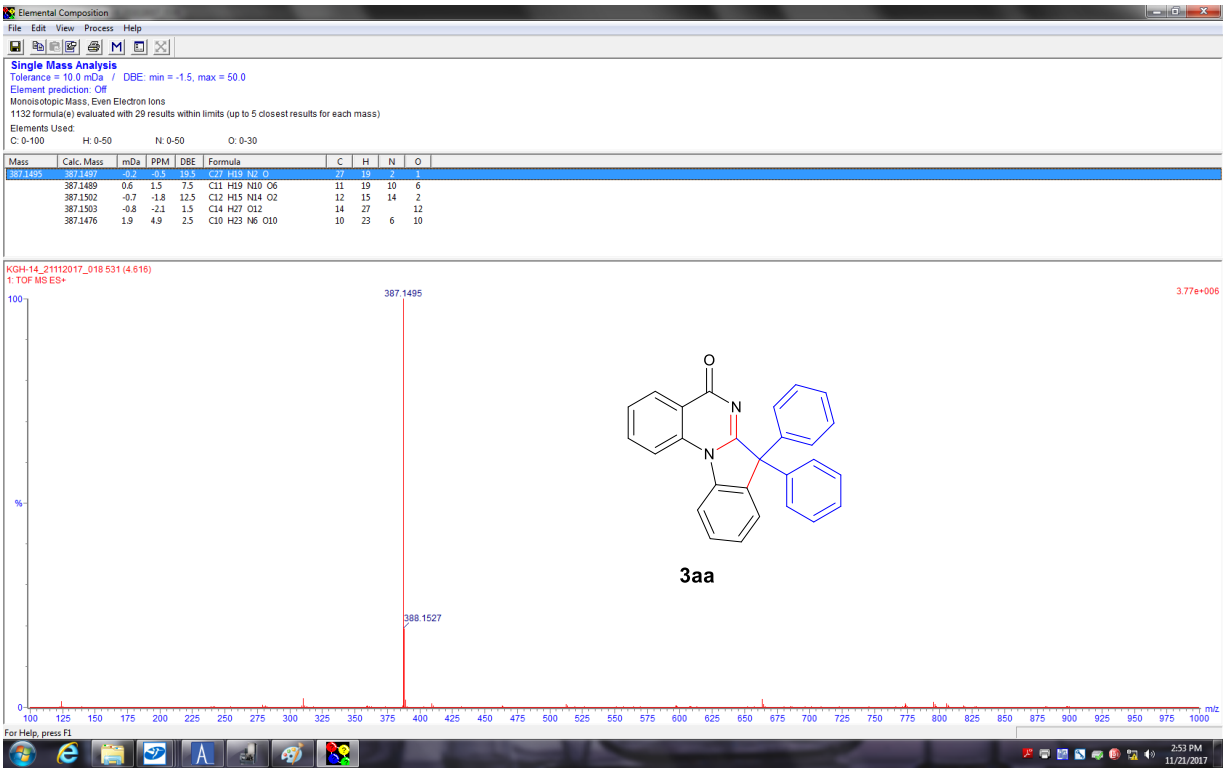

3aa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File Edit View Process Help
Single Mass Analysis
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Element prediction: Off
Monoisotopic Mass, Even Electron Ions
1132 formula(e) evaluated with 29 results within limits (up to 5 closest results for each mass)
Elements Used:
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Mass Calc. Mass mDa PPM DBE Formula C H N O
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387.1489 0.6 1.5 7.5 C11 H19 N10 O6 11 19 10 6
387.1502 -0.7 -1.8 12.5 C12 H15 N14 O2 12 15 14 2
387.1503 -0.8 -2.1 1.5 C14 H27 O12 14 27 12
387.1476 1.9 4.9 2.5 C10 H23 N6 O10 10 23 6 10
KGH-14_21112017_018 531 (4.616)
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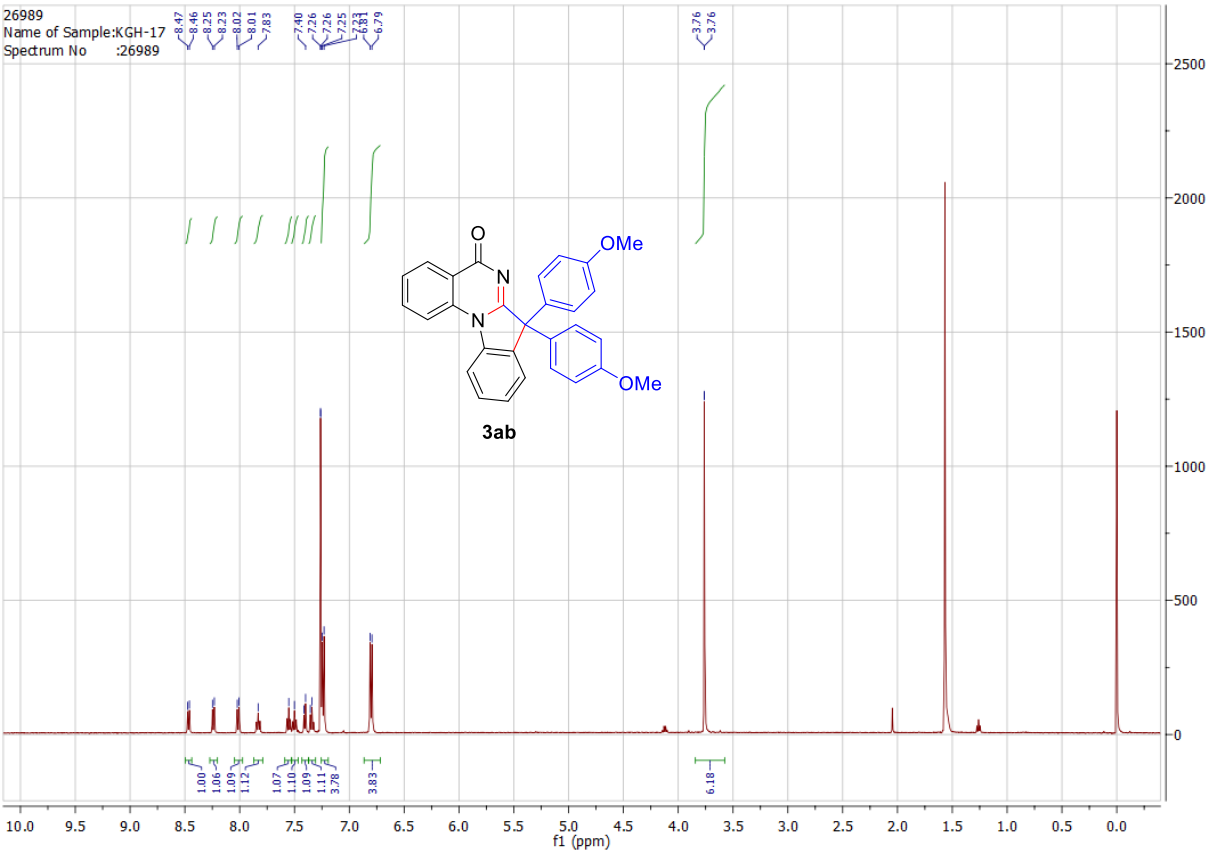
3.77e+006
388.1527
m/z
For Help, press F1
2:53 PM
11/21/2017

3aa


26989
Name of Sample:KGH-17
Spectrum No :26989
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8.01
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7.26
7.26
7.25
7.23
6.81
6.79
3.76
3.76
OMe
OMe
2500
2000
1500
1000
500
0
1.00
1.06
1.09
1.12
1.07
1.10
1.09
1.11
3.78
3.83
6.18
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
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1.0
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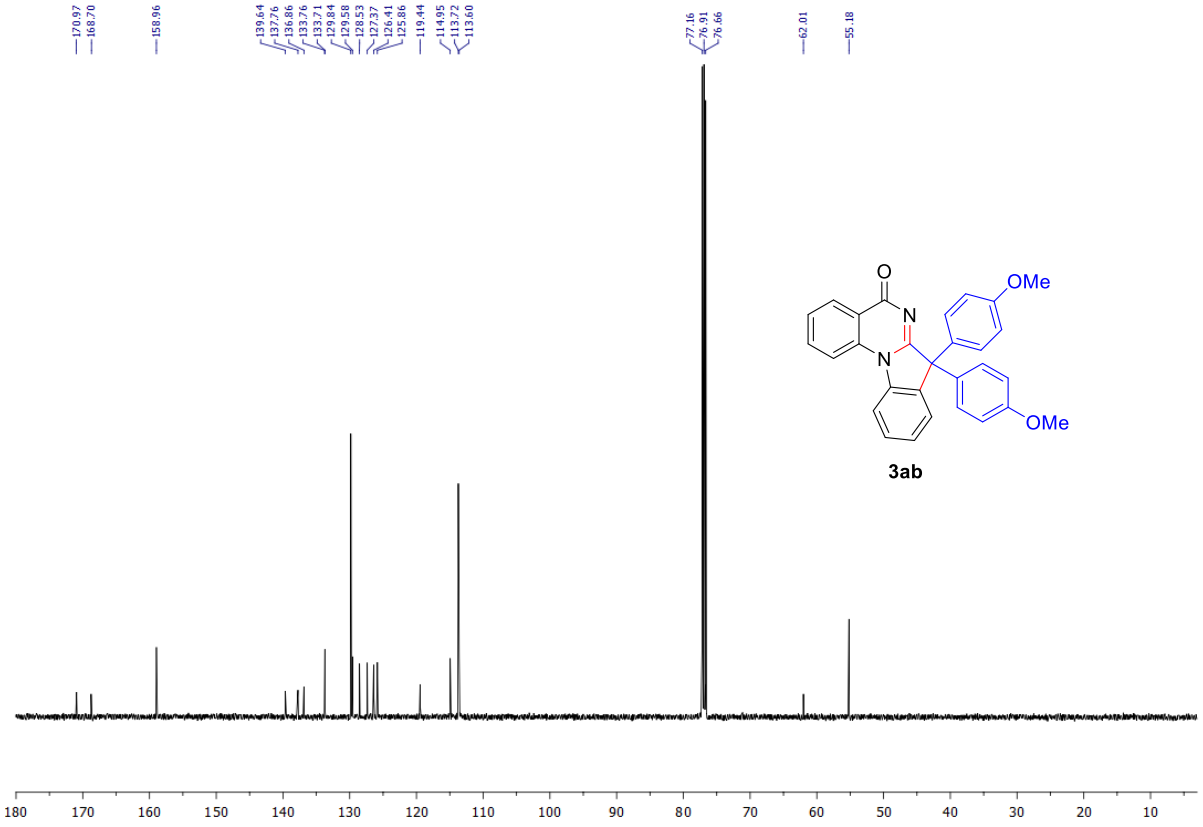
0.0
f1 (ppm)

3ab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168.70
158.96
139.64
137.76
136.96
133.76
133.71
129.84
129.58
128.53
127.37
126.41
125.86
119.44
114.95
113.72
113.60
77.16
76.91
76.66
62.01
55.18
O
N
N
OMe
OMe
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170
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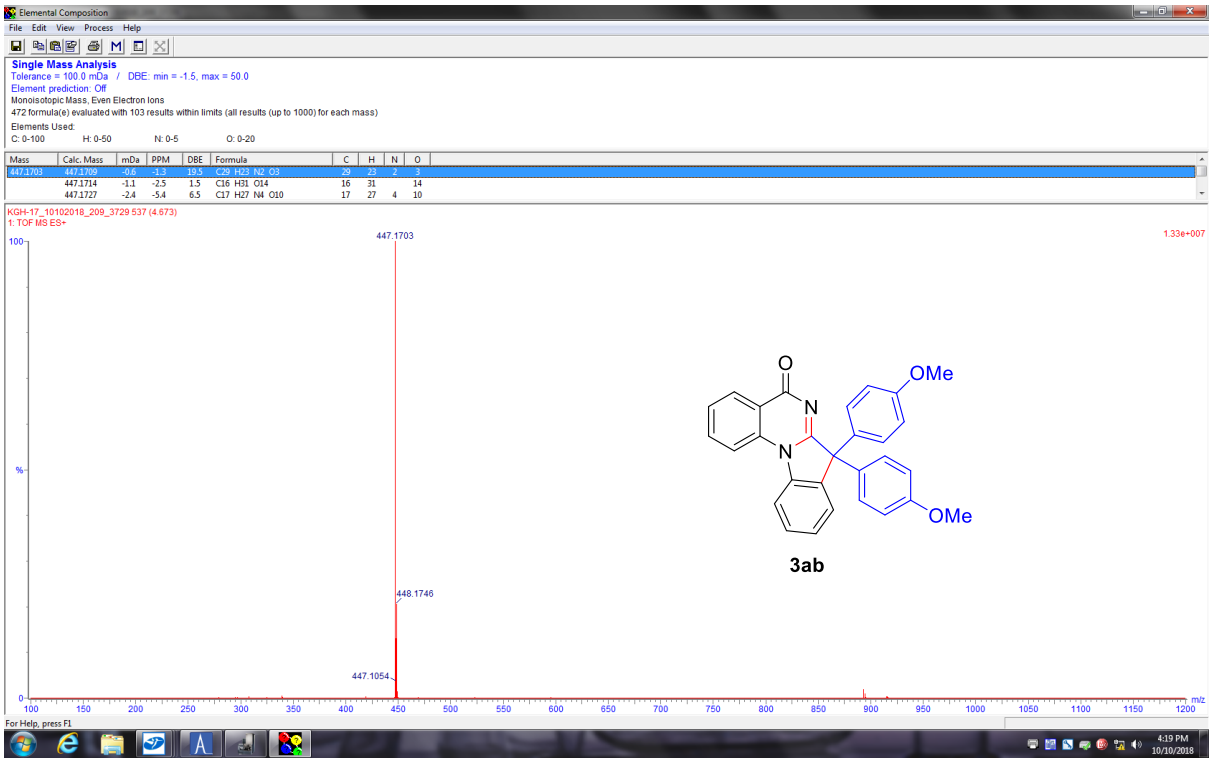
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

3ab


Elemental Composition
File Edit View Process Help
Single Mass Analysis
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Element prediction: Off
Monoisotopic Mass, Even Electron Ions
472 formula(e) evaluated with 103 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-50 N: 0-5 O: 0-20
Mass Calc. Mass mDa PPM DBE Formula C H N O
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447.1714 -1.1 -2.5 1.5 C16 H31 O14 16 31 14
447.1727 -2.4 -5.4 6.5 C17 H27 N4 O10 17 27 4 10
KGH-17_10102018_209_3729 537 (4.673)
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1.33e+007
448.1746
447.1054
100
%
0
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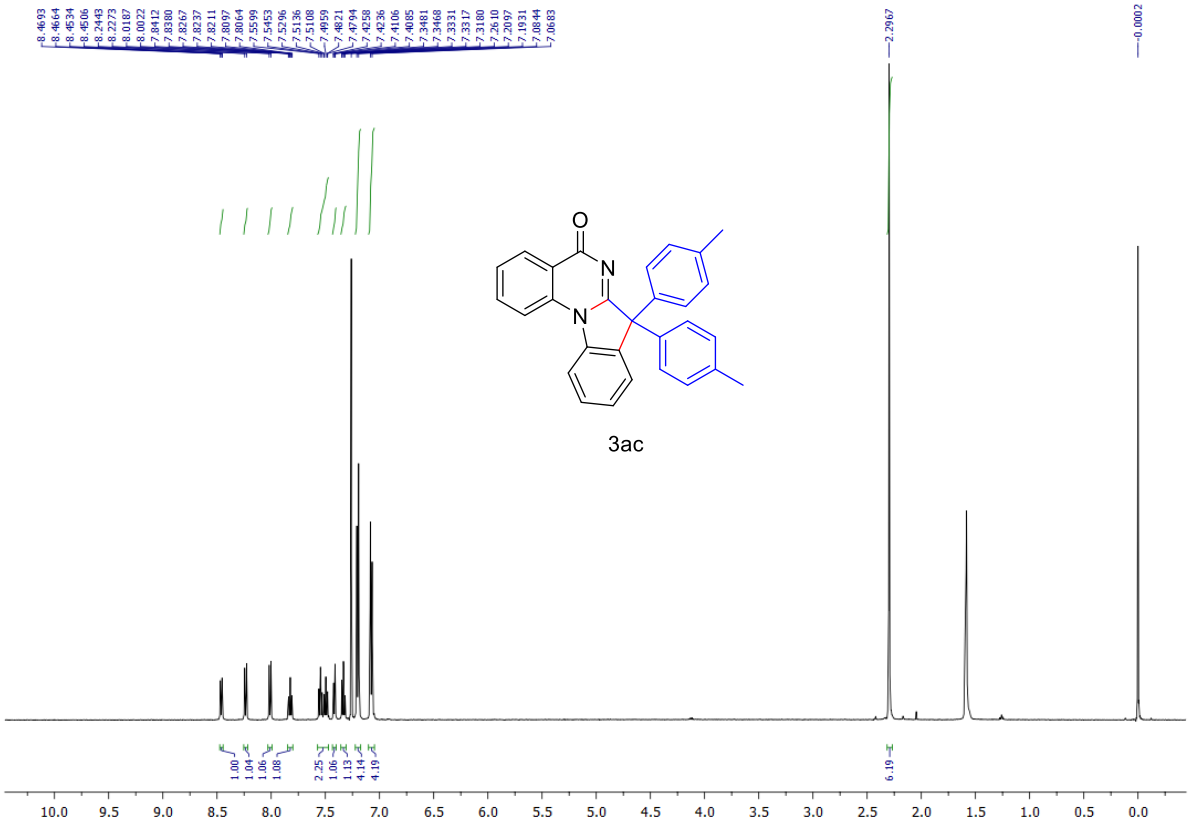
m/z
For Help, press F1
4:19 PM
10/10/2018
O
N
N
OMe
OMe

3ab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8.2443
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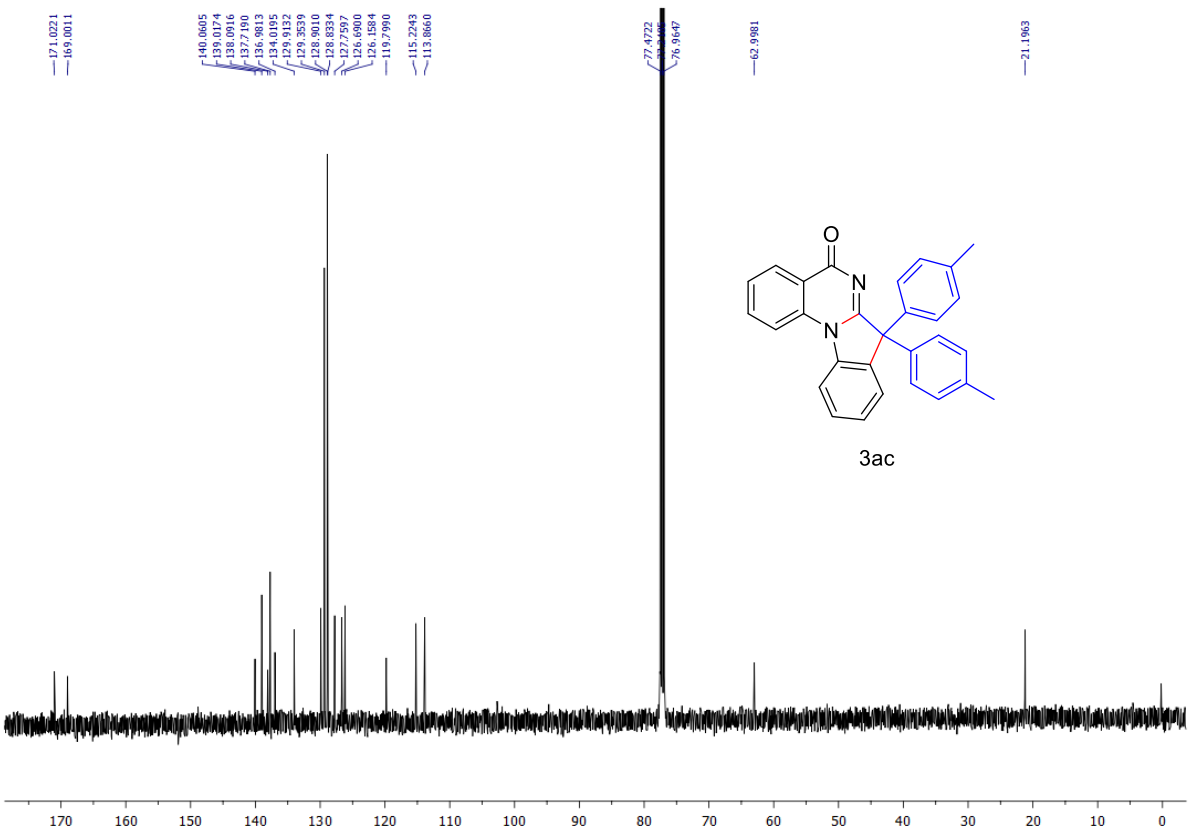
8.0187
8.0022
7.8412
7.8380
7.8267
7.8237
7.8211
7.8097
7.8064
7.5599
7.5453
7.5296
7.5136
7.5108
7.4959
7.4821
7.4794
7.4258
7.4236
7.4106
7.4085
7.3481
7.3468
7.3331
7.3317
7.3180
7.2610
7.2097
7.1931
7.0844
7.0683
2.2967
0.0002
O
N
N
3ac
1.00
1.04
1.06
1.08
2.25
1.06
1.13
4.14
4.19
6.19
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0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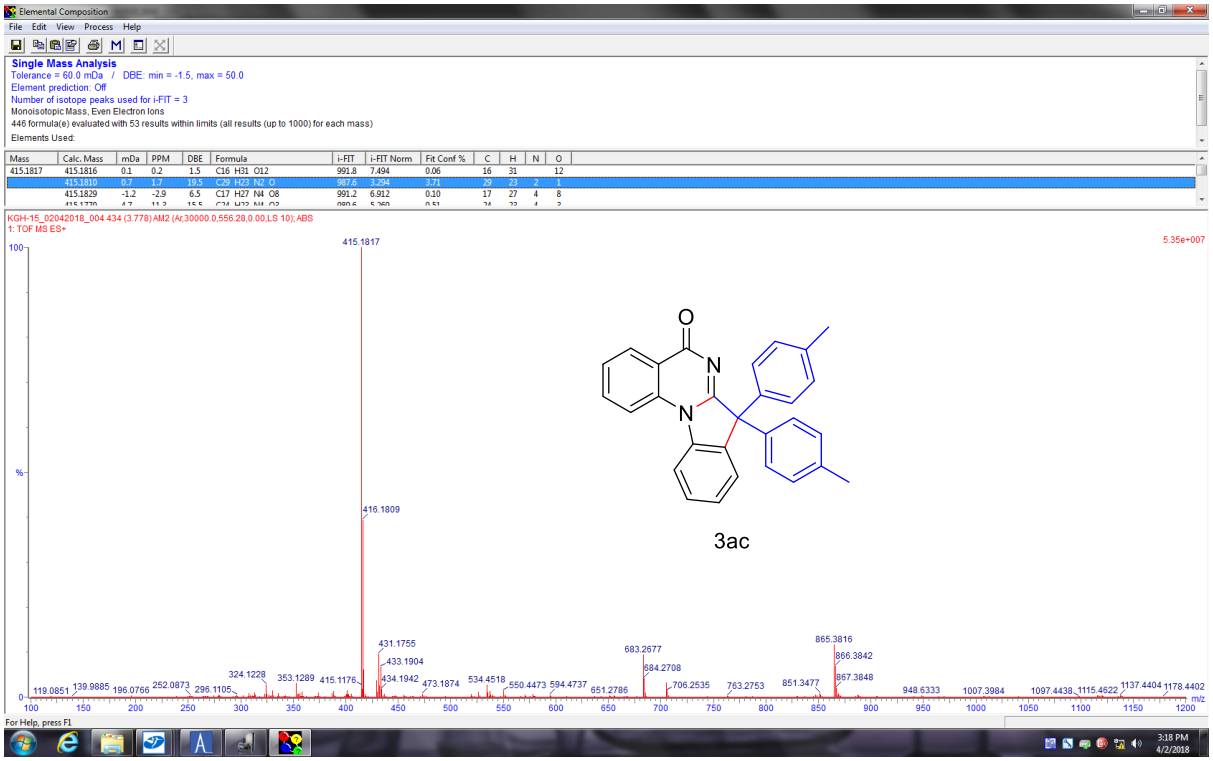
140.0605
139.0174
138.0916
137.7190
136.9813
134.0195
129.9132
129.3539
128.9010
128.8334
127.7597
126.6900
126.1584
119.7990
115.2243
113.8660
77.4722
76.9647
62.9981
21.1963
O
N
N
3ac
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0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Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
446 formula(e) evaluated with 53 results within limits (all results (up to 1000) for each mass)
Elements Used:
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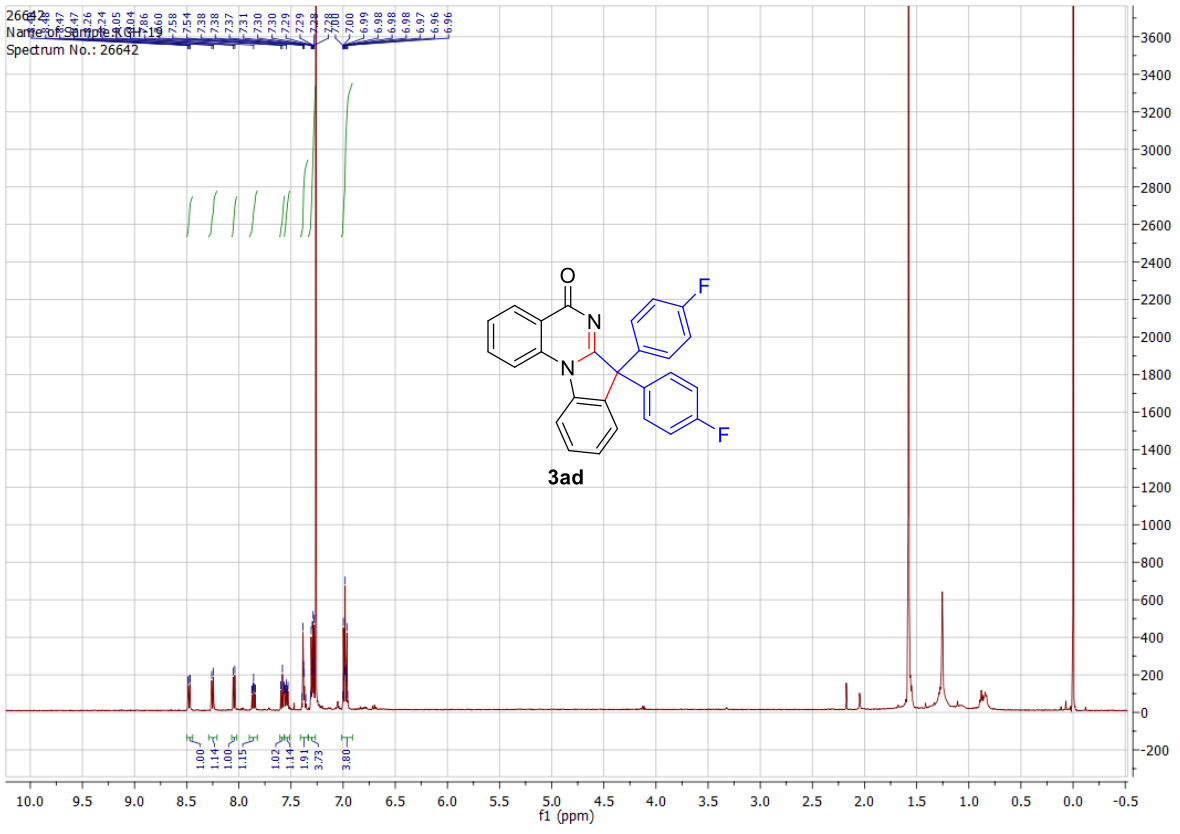
416.1809
3ac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Spectrum No.: 26642
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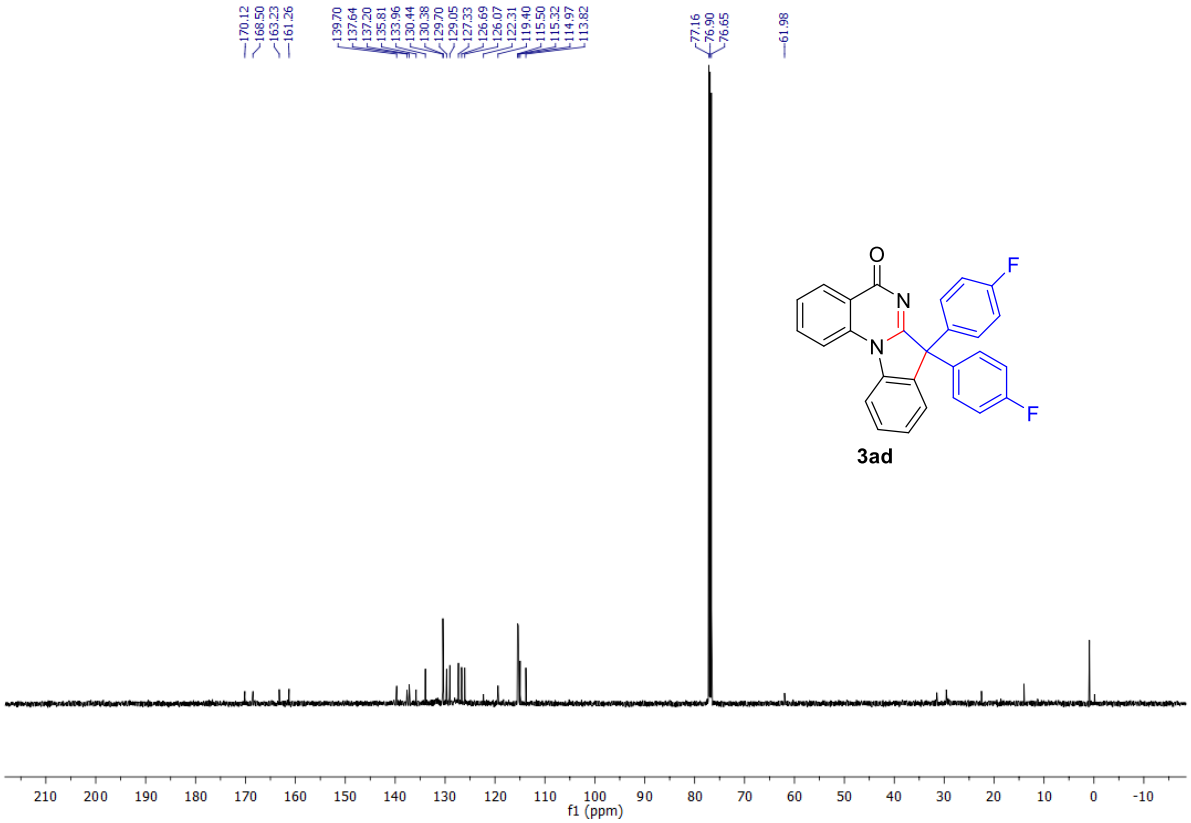
f1 (ppm)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161.26
139.70
137.64
137.20
135.81
133.96
130.44
130.38
129.70
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126.69
126.07
122.31
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115.50
115.32
114.97
113.82
77.16
76.90
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F
3ad
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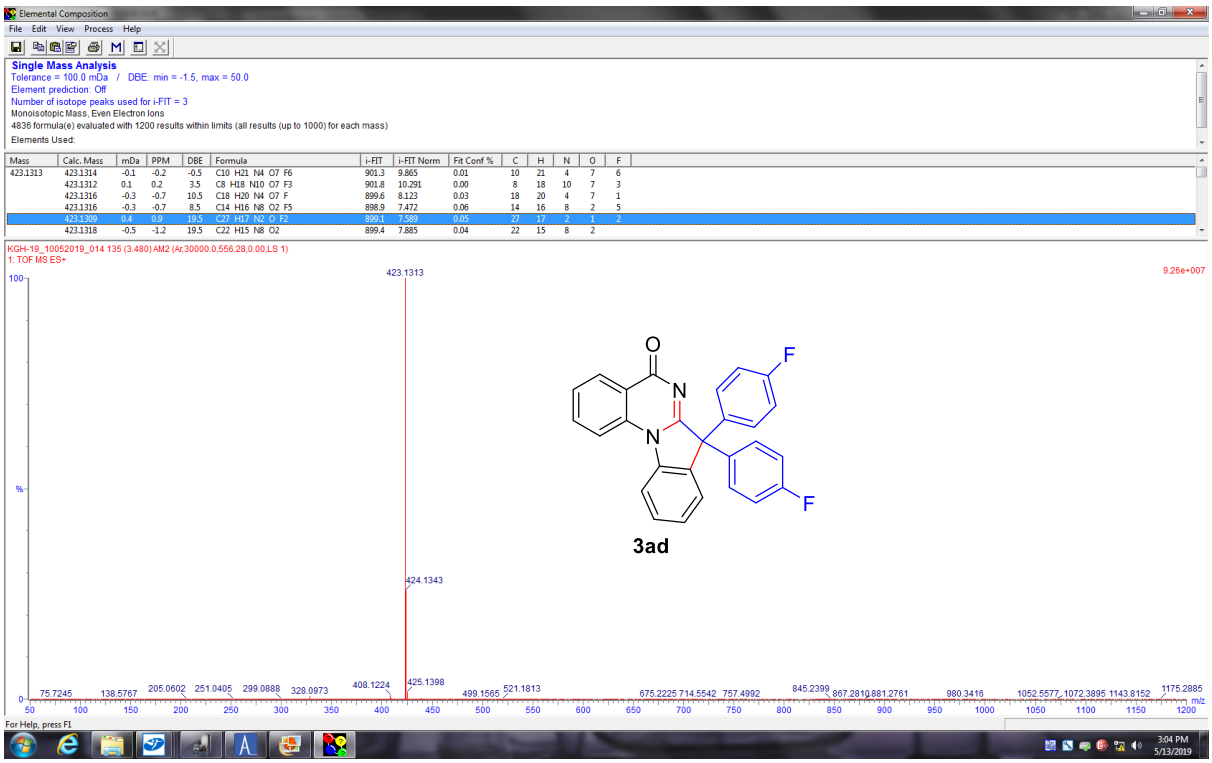
f1 (ppm)


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
4836 formula(e) evaluated with 1200 results within limits (all results (up to 1000) for each mass)
Elements Used:
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423.1312 0.1 0.2 3.5 C8 H18 N10 O7 F3 901.8 10.291 0.00 8 18 10 7 3
423.1316 -0.3 -0.7 10.5 C18 H20 N4 O7 F 899.6 8.123 0.03 18 20 4 7 1
423.1316 -0.3 -0.7 8.5 C14 H16 N8 O2 F5 898.9 7.472 0.06 14 16 8 2 5
423.1309 0.4 0.9 19.5 C27 H17 N2 O F2 899.1 7.589 0.05 27 17 2 1 2
423.1318 -0.5 -1.2 19.5 C22 H15 N8 O2 899.4 7.885 0.04 22 15 8 2
KGH-19_10052019_014 135 (3.480) AM2 (Ar,30000.0,556.28,0.00,LS 1)
1: TOF MS ES+
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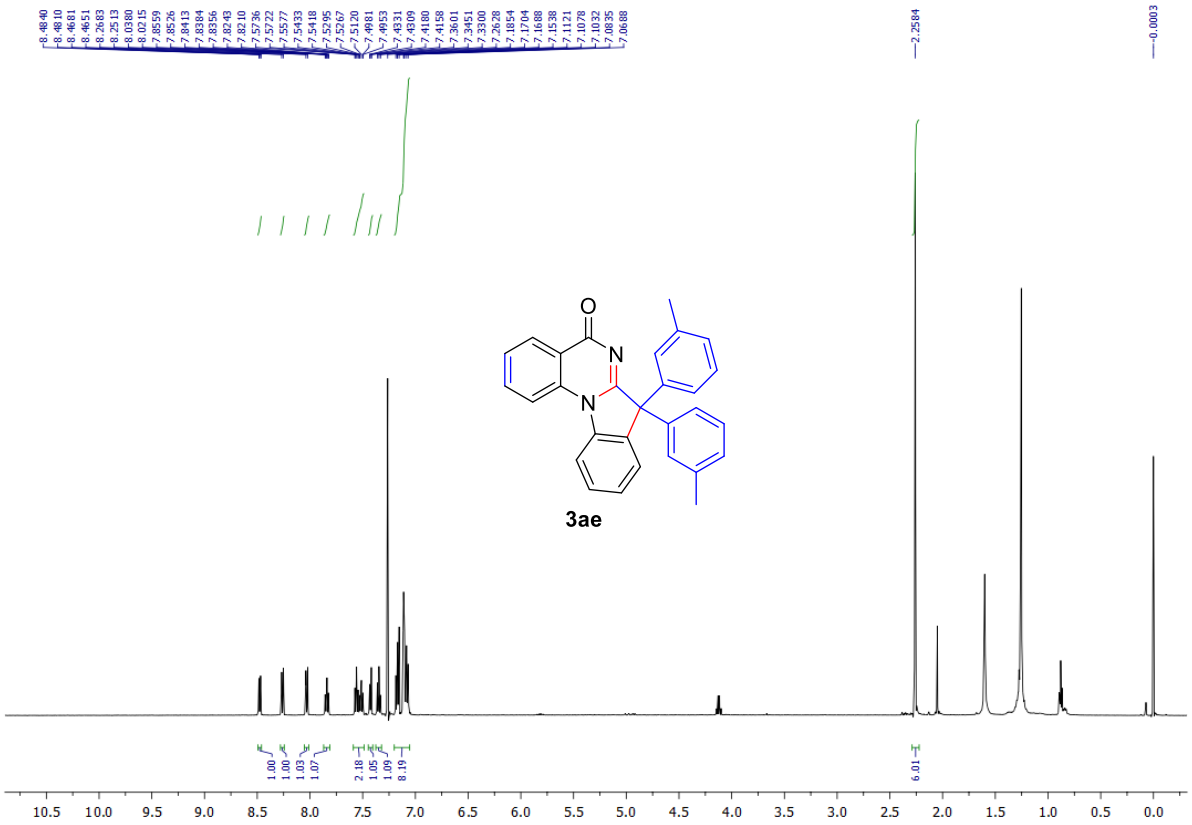
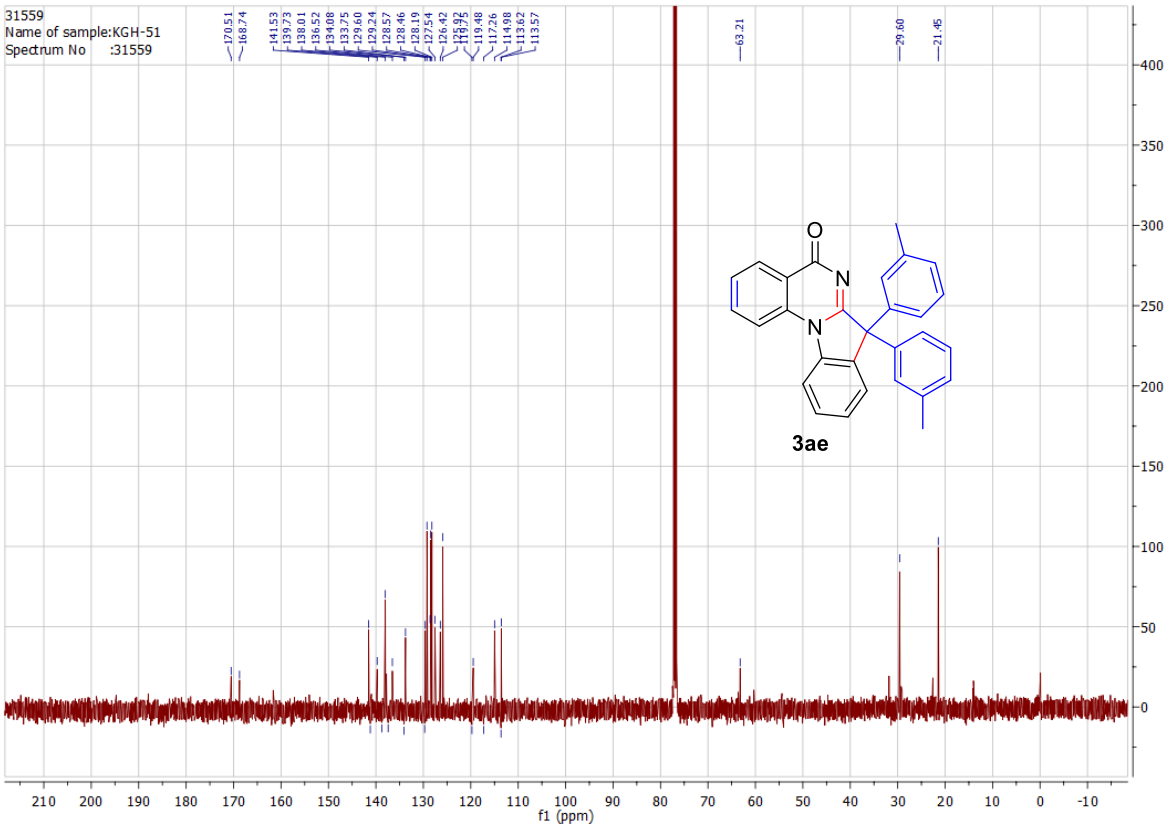
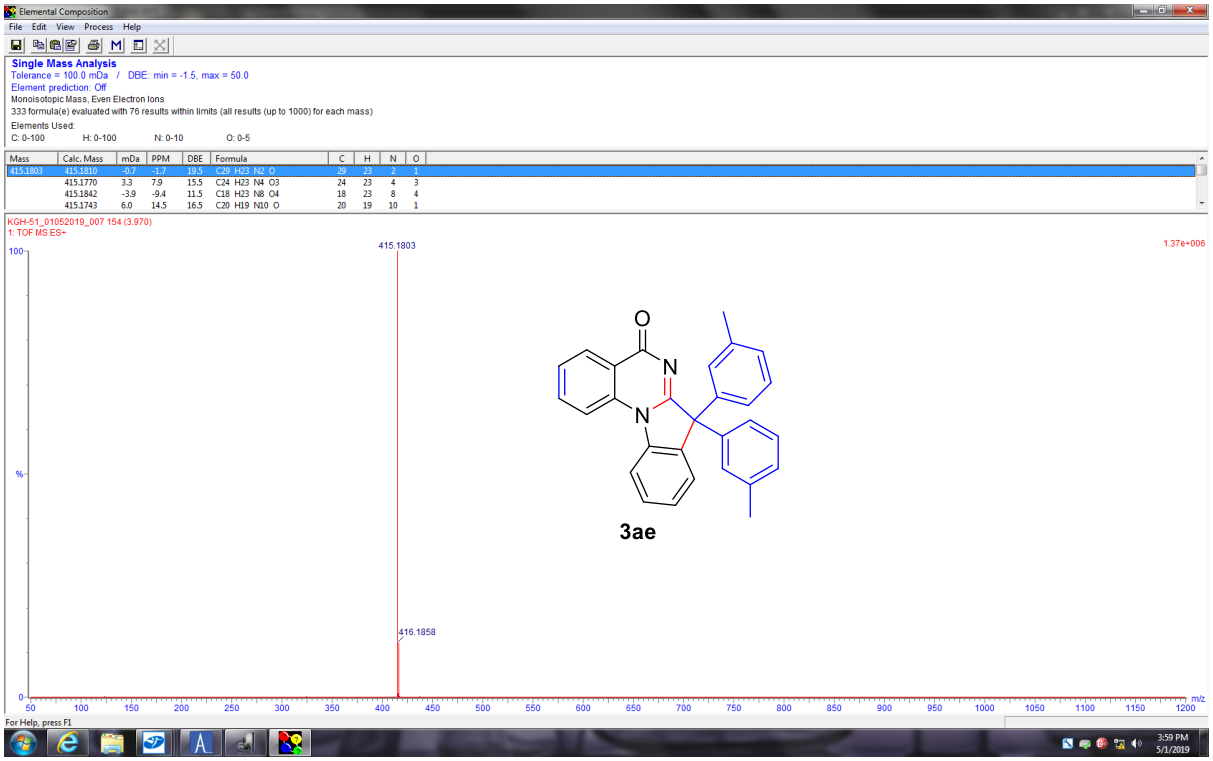
9.26e+007
100
%
424.1343
75.7245 138.5767 205.0602 251.0405 299.0888 328.0973 408.1224 425.1398 499.1565 521.1813 675.2225 714.5542 757.4992 845.2399 867.2810 881.2761 980.3416 1052.5577 1072.3895 1143.8152 1175.2885
m/z
O
N
N
F
F
3ad
For Help, press F1
3:04 PM
5/13/2019


3ae


31559
Name of sample:KGH-51
Spectrum No :31559
3ae
f1 (ppm)


Elemental Composition
File Edit View Process Help
Single Mass Analysis
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Element prediction: Off
Monoisotopic Mass, Even Electron Ions
333 formula(e) evaluated with 76 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-5
Mass Calc. Mass mDa PPM DBE Formula C H N O
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415.1770 3.3 7.9 15.5 C24 H23 N4 O3 24 23 4 3
415.1842 -3.9 -9.4 11.5 C18 H23 N8 O4 18 23 8 4
415.1743 6.0 14.5 16.5 C20 H19 N10 O 20 19 10 1
KGH-51_01052019_007 154 (3.970)
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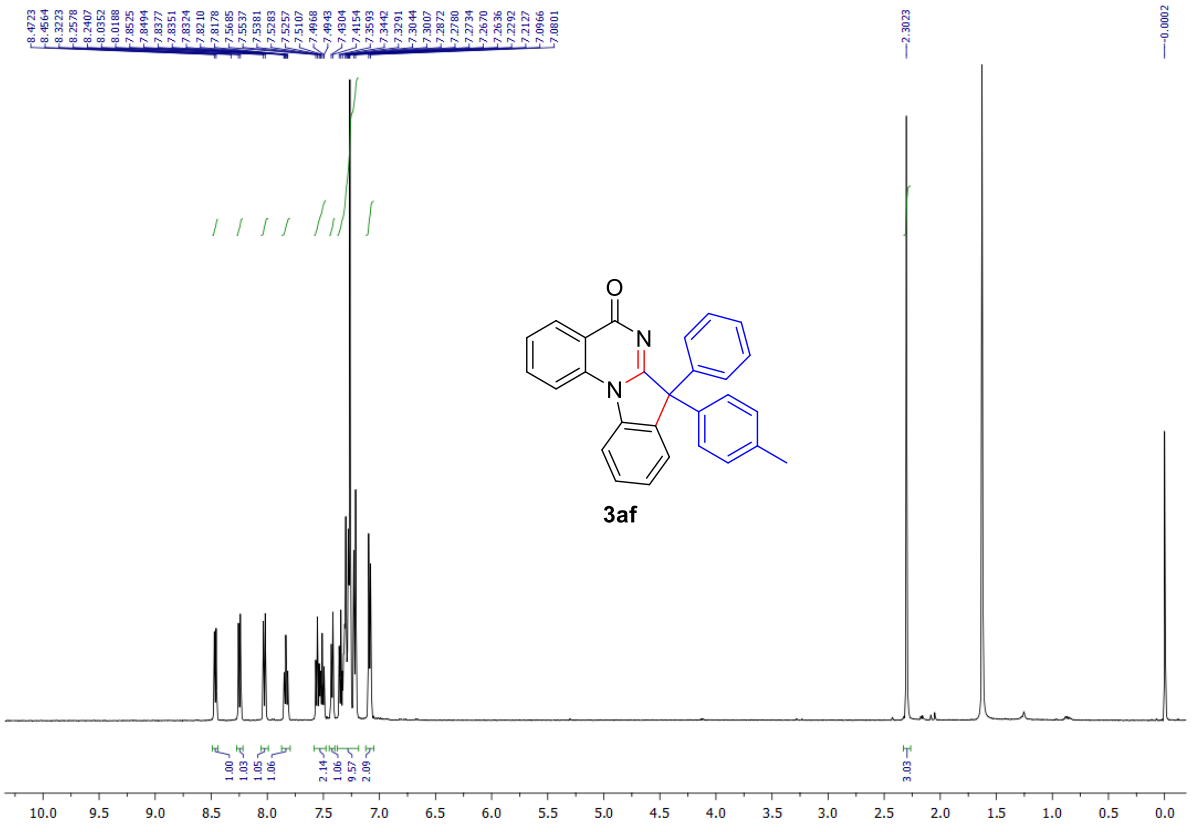
1.37e+006
416.1858
m/z
For Help, press F1
3:59 PM
5/1/2019

3ae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7.8494
7.8377
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7.2872
7.2780
7.2734
7.2670
7.2636
7.2292
7.2127
7.0966
7.0801
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1.03
1.05
1.06
2.14
1.06
9.57
2.09
3.03
10.0
9.5
9.0
8.5
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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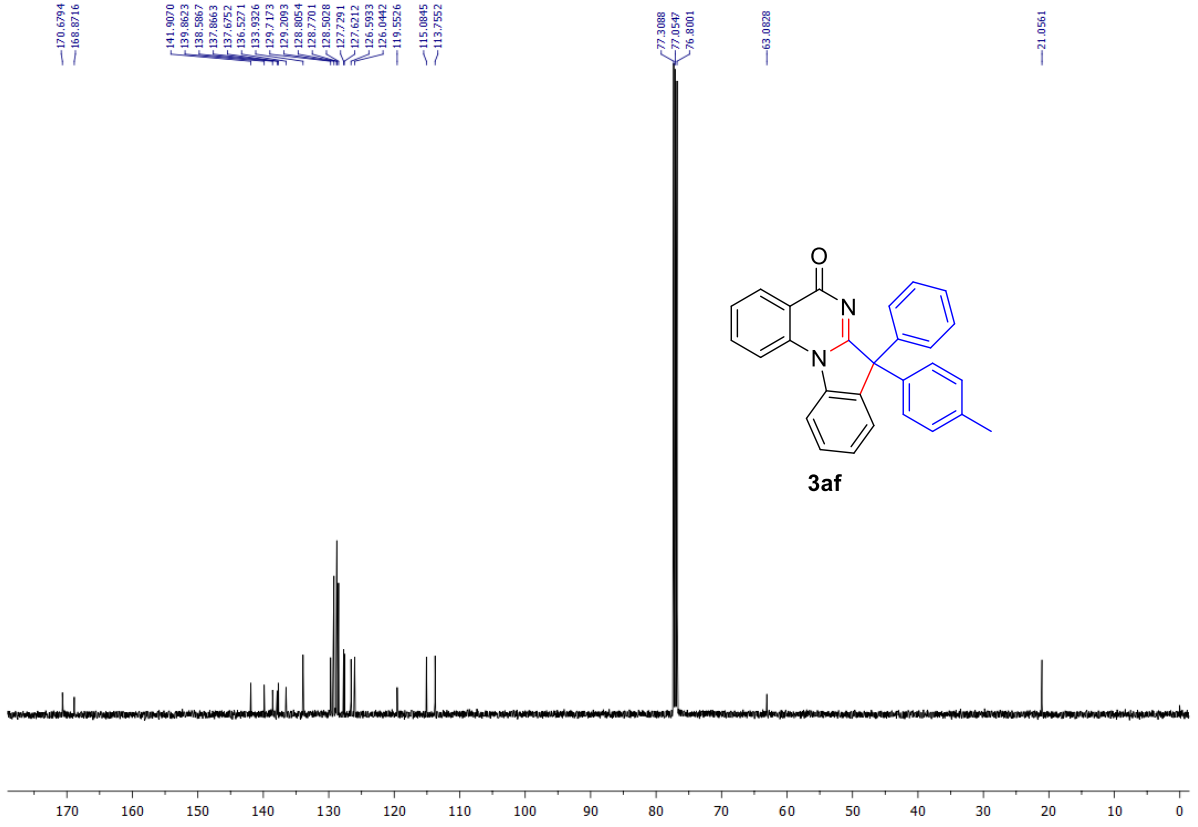
1.5
1.0
0.5
0.0

3af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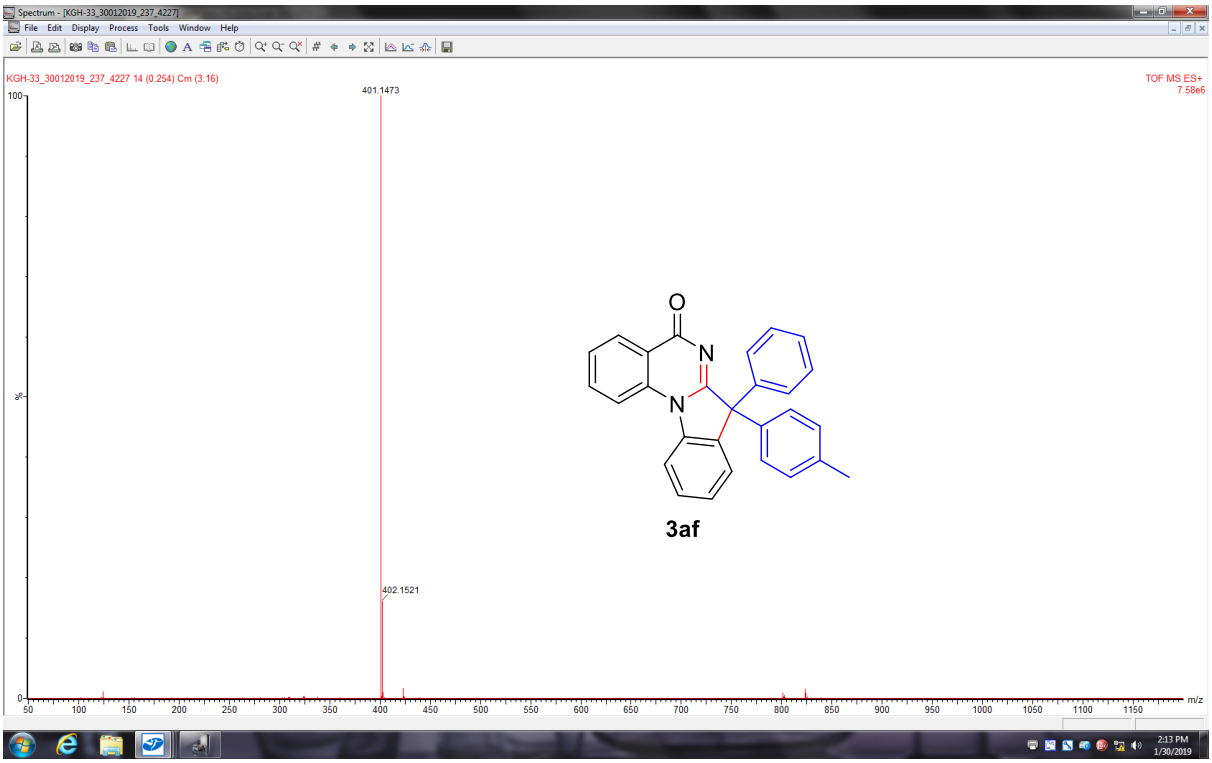
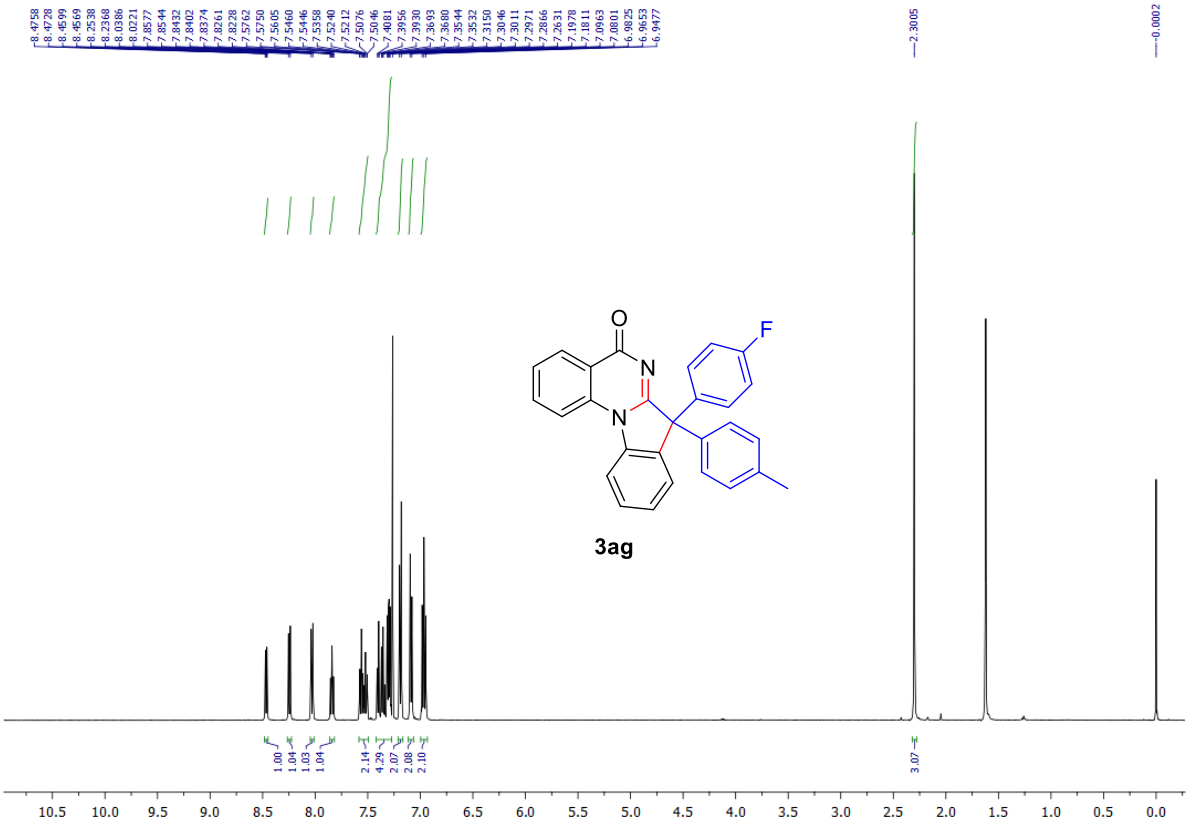
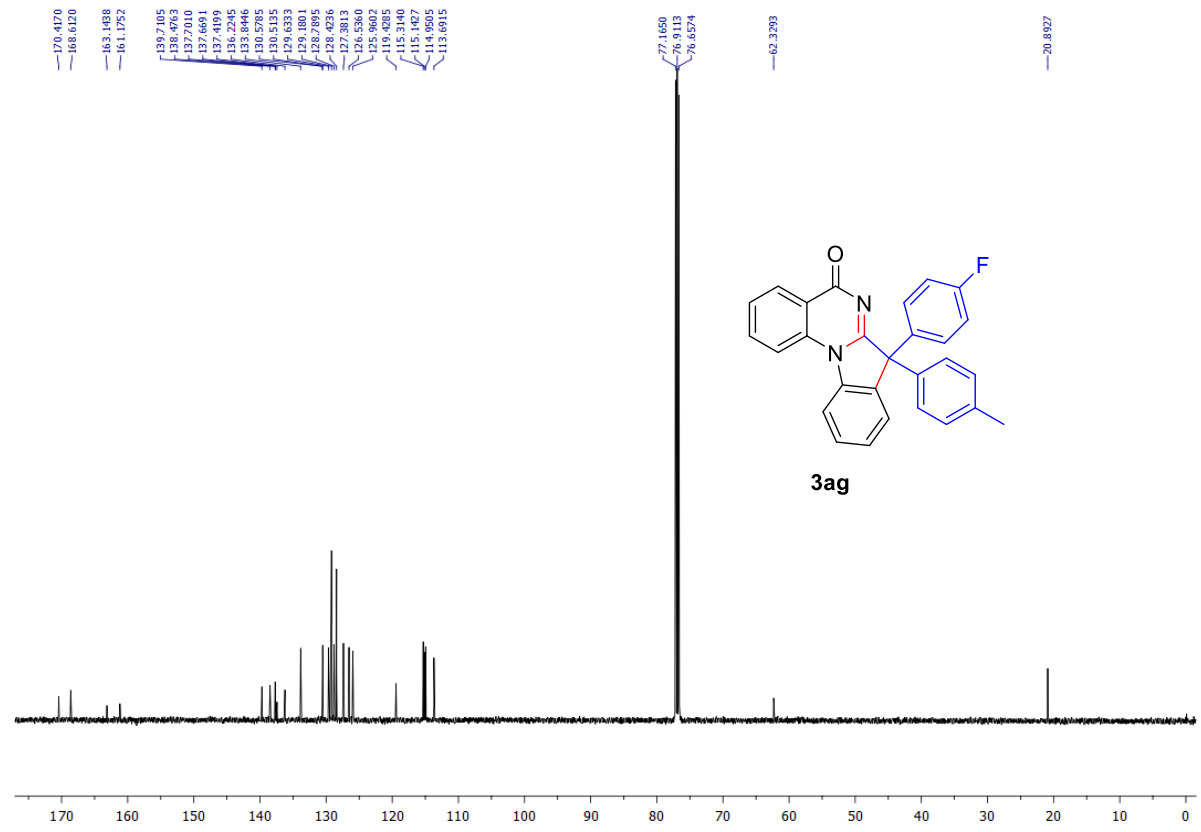
168.8716
141.9070
139.8623
138.5867
137.8863
137.6752
136.5271
133.9326
129.7173
129.2093
128.8054
128.7701
128.5028
127.7291
127.6212
126.5933
126.0442
119.5526
115.0845
113.7552
77.3088
77.0547
76.8001
63.0828
21.0561
O
N
N
3af
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

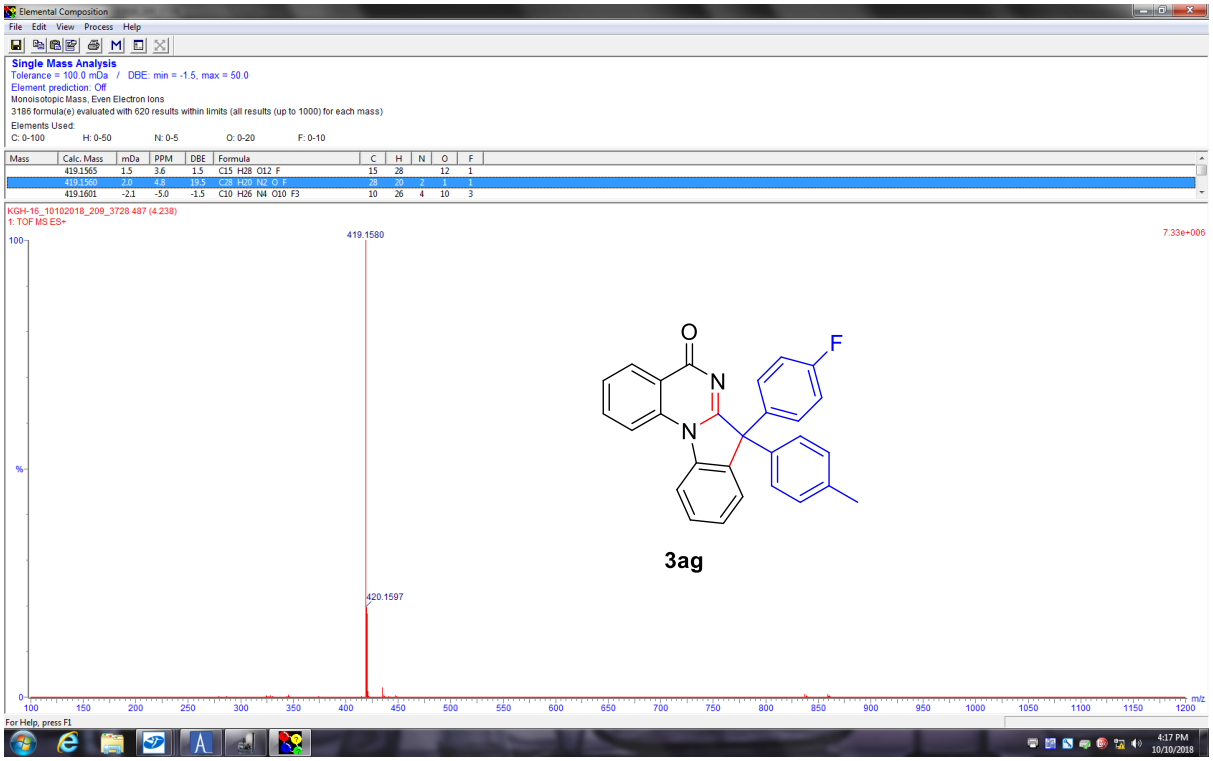

Spectrum - [KGH-33_30012019_237_4227]
File Edit Display Process Tools Window Help
KGH-33_30012019_237_4227 14 (0.254) Cm (3:16)
TOF MS ES+
7.58e6
401.1473
402.1521
100
%
0
O
N
N
3af
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
850
900
950
1000
1050
1100
1150
m/z
2:13 PM
1/30/2019

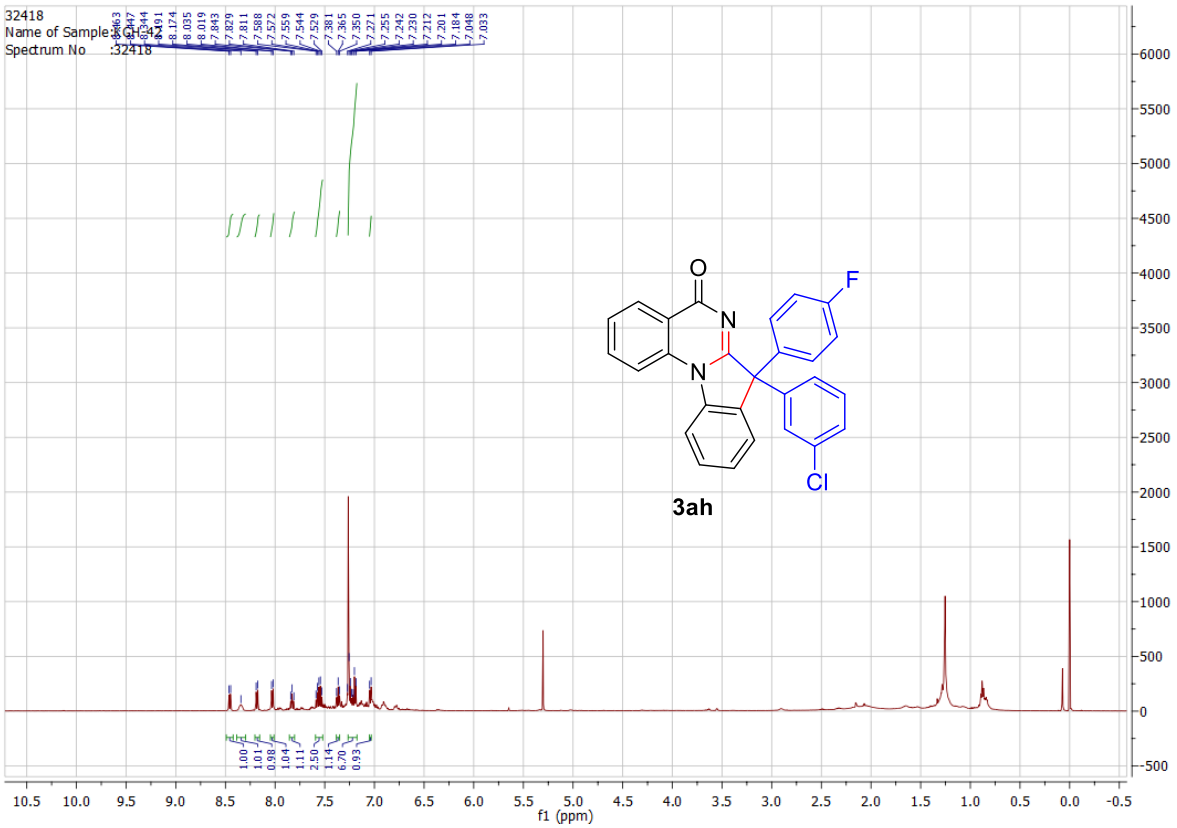

8.4758
8.4728
8.4599
8.4569
8.2538
8.2368
8.0386
8.0221
7.8577
7.8544
7.8432
7.8402
7.8374
7.8261
7.8228
7.5762
7.5750
7.5605
7.5460
7.5446
7.5358
7.5240
7.52.12
7.5076
7.5046
7.4081
7.3956
7.3930
7.3680
7.3644
7.3532
7.3150
7.3046
7.3011
7.2971
7.2866
7.2631
7.1978
7.1811
7.0963
7.0801
6.9825
6.9653
6.9477
2.3005
0.0002
O
N
N
F
1.00
1.04
1.03
1.04
2.14
4.29
2.07
2.08
2.10
3.07
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

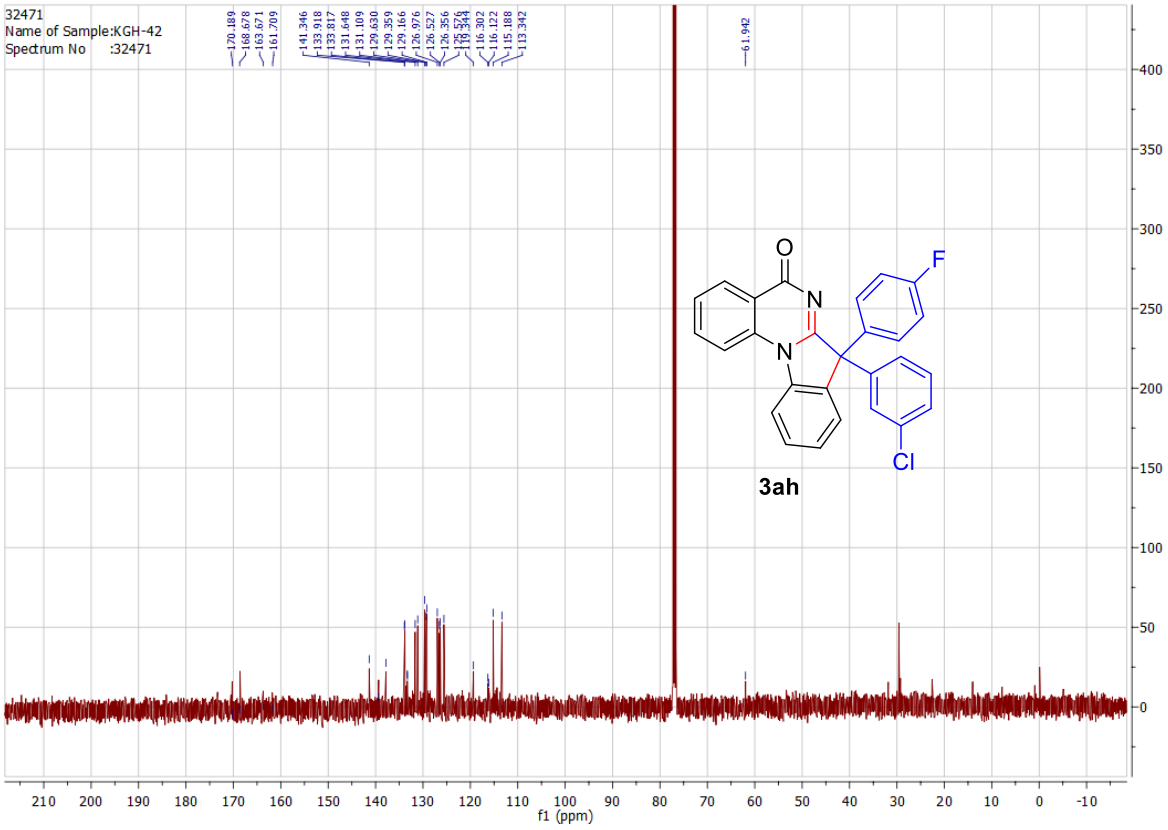
3ag

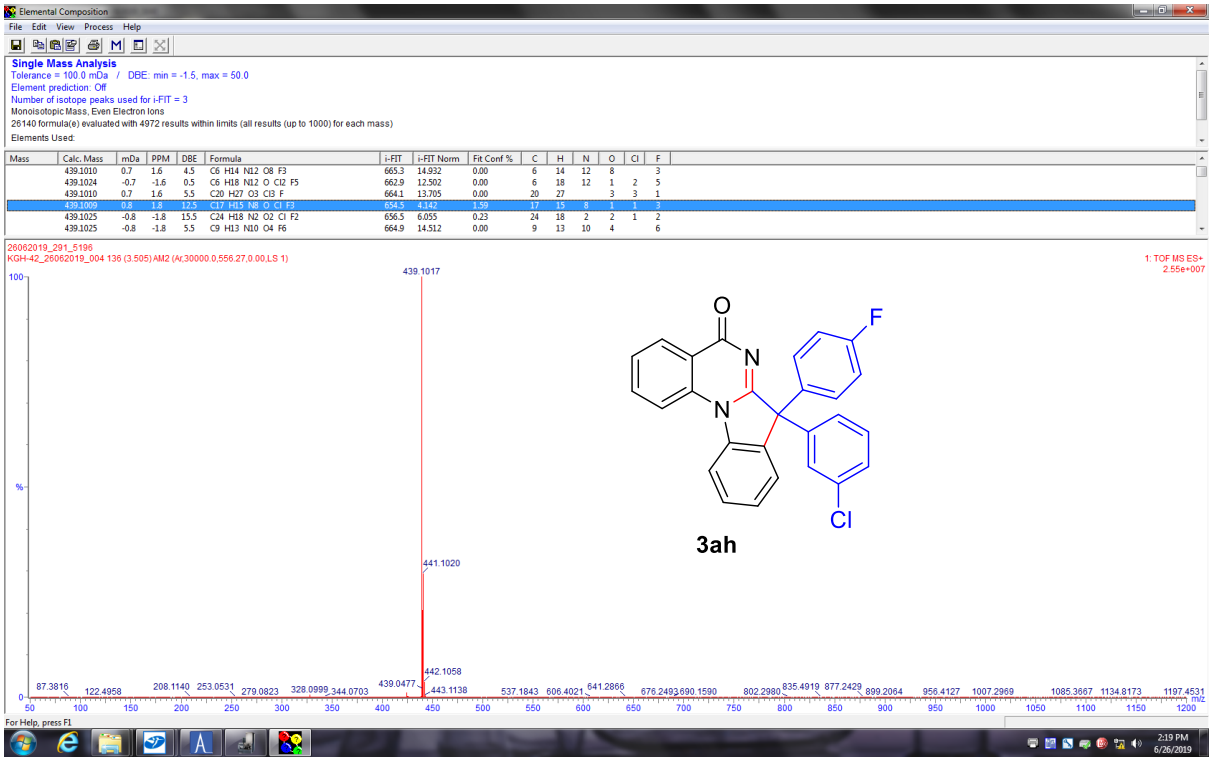

170.4170
168.6120
163.1438
161.1752
139.7105
138.4763
137.7010
137.6691
137.4199
136.2245
133.8446
130.5785
130.5135
129.6333
129.1801
128.7895
128.4236
127.3813
126.5360
125.9602
119.4285
115.3140
115.1427
114.9505
113.6915
77.1650
76.9113
76.6574
62.3293
20.8927
O
N
N
F
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

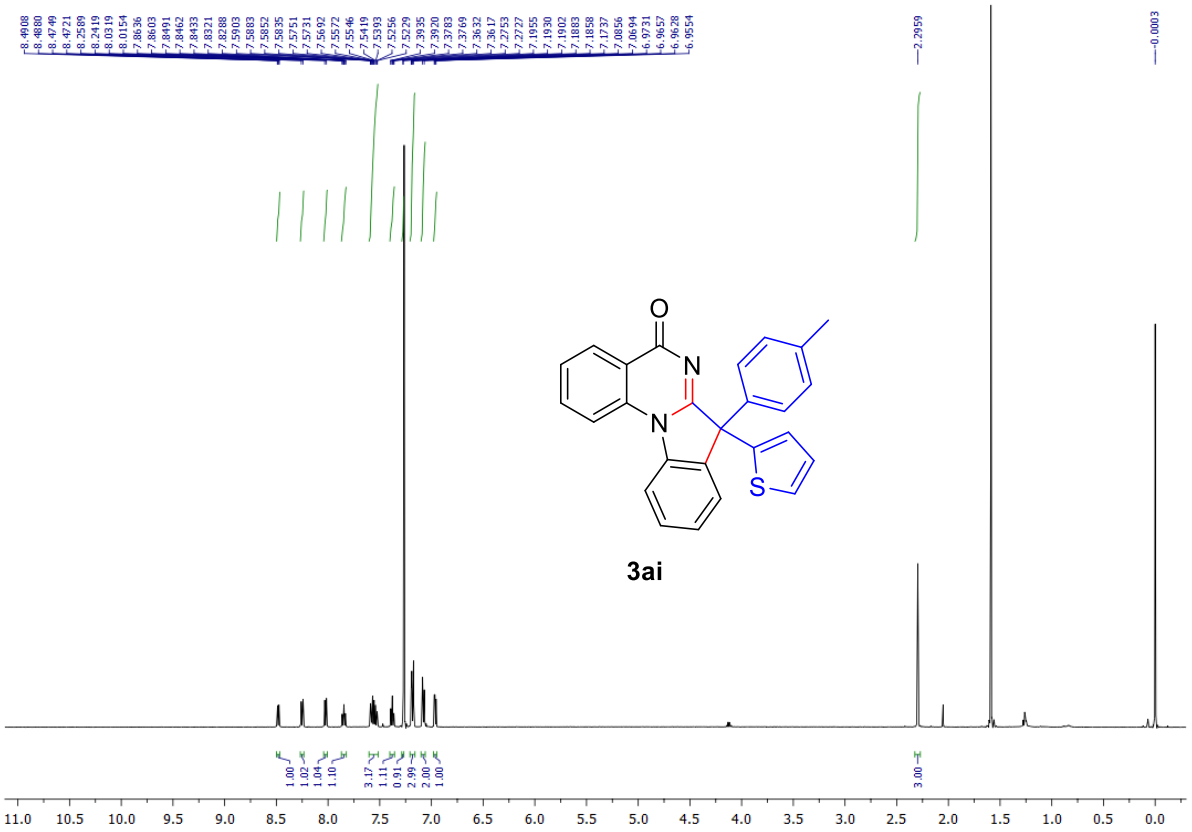
3ag

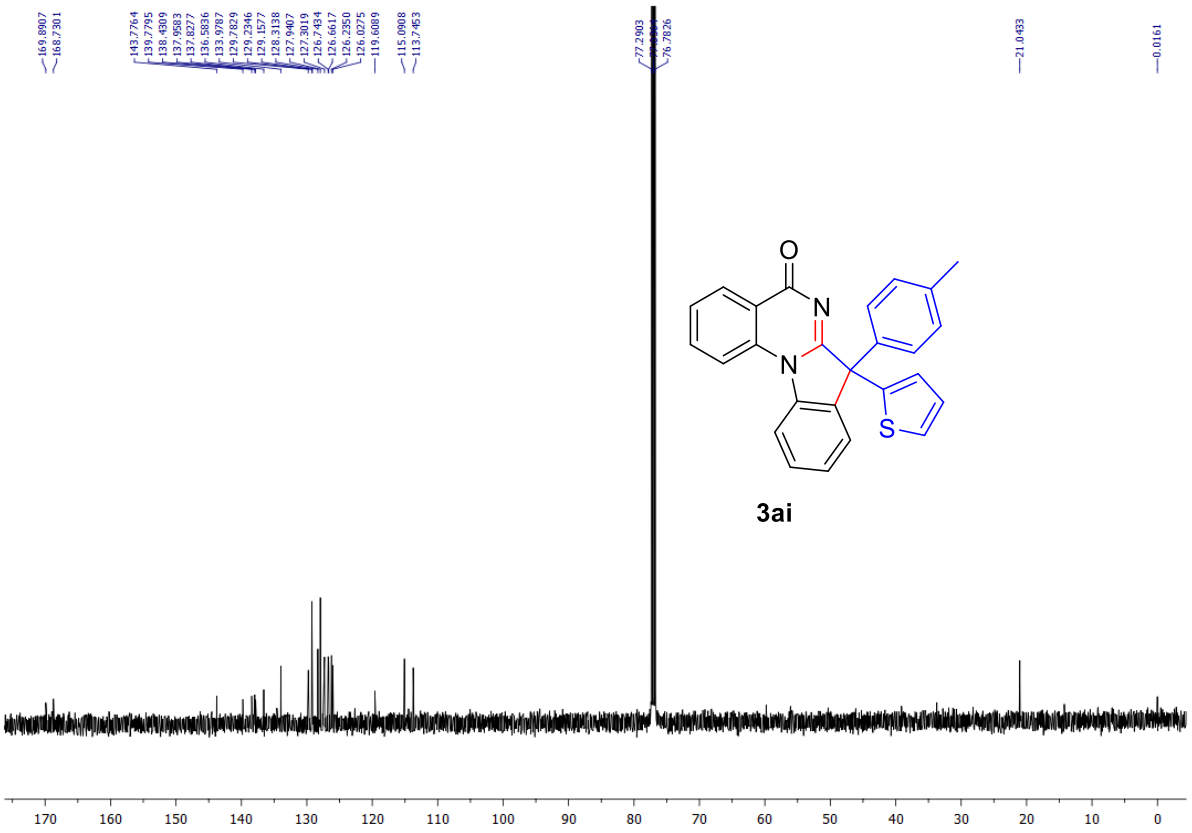

Elemental Composition
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
3186 formula(e) evaluated with 620 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-50 N: 0-5 O: 0-20 F: 0-10
Mass Calc. Mass mDa PPM DBE Formula C H N O F
419.1565 1.5 3.6 1.5 C15 H28 O12 F 15 28 12 1
419.1560 2.0 4.8 19.5 C28 H20 N2 O F 28 20 2 1 1
419.1601 -2.1 -5.0 -1.5 C10 H26 N4 O10 F3 10 26 4 10 3
KGH-16_10102018_209_3728 487 (4.238)
1: TOF MS ES+
419.1580
7.33e+006
420.1597
m/z
For Help, press F1
4:17 PM
10/10/2018
O
N
N
F
3ag

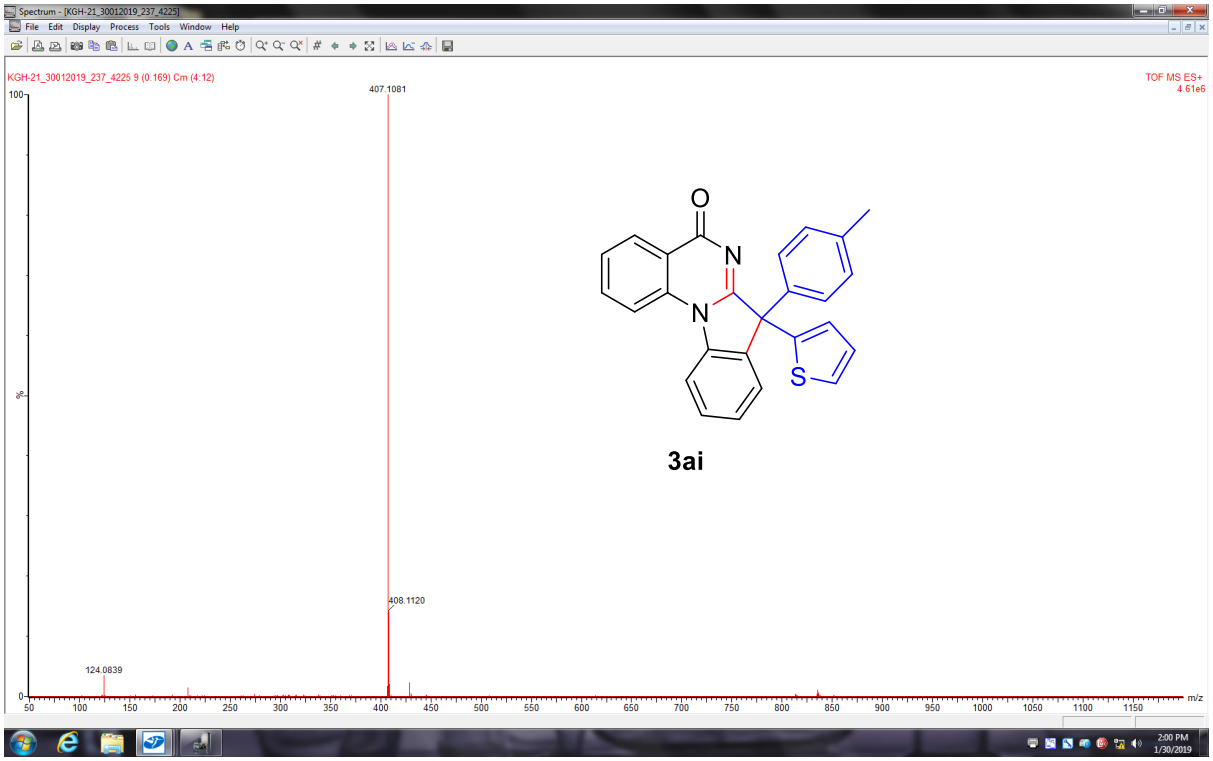

32418
Name of Sample :KGH-42
Spectrum No :32418
8.174
8.035
8.019
7.843
7.829
7.811
7.588
7.572
7.559
7.544
7.529
7.381
7.365
7.350
7.271
7.255
7.242
7.230
7.212
7.201
7.184
7.048
7.033
1.00
1.01
0.98
1.04
1.11
2.50
1.14
6.70
0.93
f1 (ppm)
O
N
N
F
Cl
3ah


32471
Name of Sample:KGH-42
Spectrum No :32471
170.189
168.678
163.671
161.709
141.346
133.918
133.817
131.648
131.109
129.630
129.359
129.166
126.976
126.527
126.356
125.576
119.344
116.302
116.122
115.188
113.342
61.942
O
N
N
F
Cl
3ah
f1 (ppm)

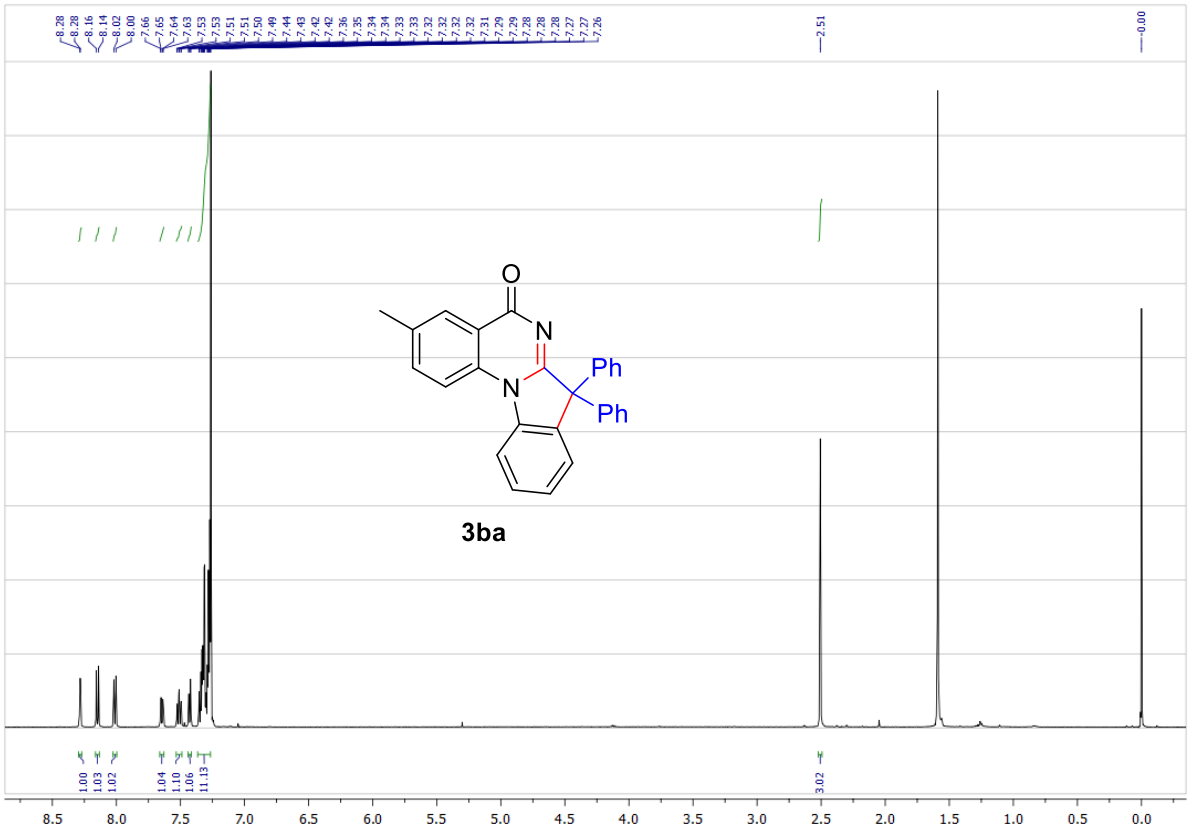

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
26140 formula(e) evaluated with 4972 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O Cl F
439.1010 0.7 1.6 4.5 C6 H14 N12 O8 F3 665.3 14.932 0.00 6 14 12 8 3
439.1024 -0.7 -1.6 0.5 C6 H18 N12 O Cl2 F5 662.9 12.502 0.00 6 18 12 1 2 5
439.1010 0.7 1.6 5.5 C20 H27 O3 Cl3 F 664.1 13.705 0.00 20 27 3 3 1
439.1009 0.8 1.8 12.5 C17 H13 N8 O Cl F3 654.3 4.242 1.53 17 13 8 1 1 3
439.1025 -0.8 -1.8 15.5 C24 H18 N2 O2 Cl F2 656.5 6.055 0.23 24 18 2 2 1 2
439.1025 -0.8 -1.8 5.5 C9 H13 N10 O4 F6 664.9 14.512 0.00 9 13 10 4 6
26062019_291_5196
KGH-42_26062019_004 136 (3.505) AM2 (Ar,30000.0,556.27,0.00,LS 1)
1: TOF MS ES+
2.55e+007
439.1017
441.1020
442.1058
O
N
N
F
Cl
3ah
m/z
For Help, press F1
2:19 PM
6/26/2019


3ai

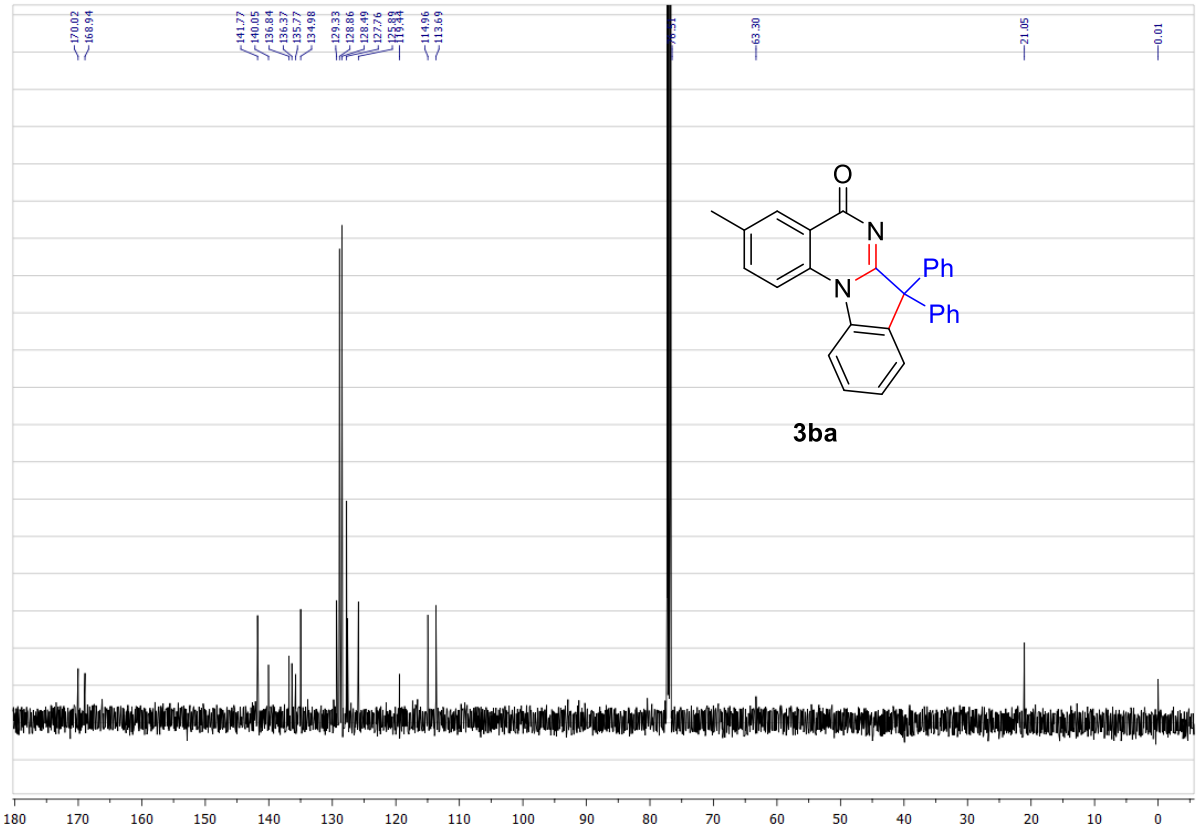

3ai

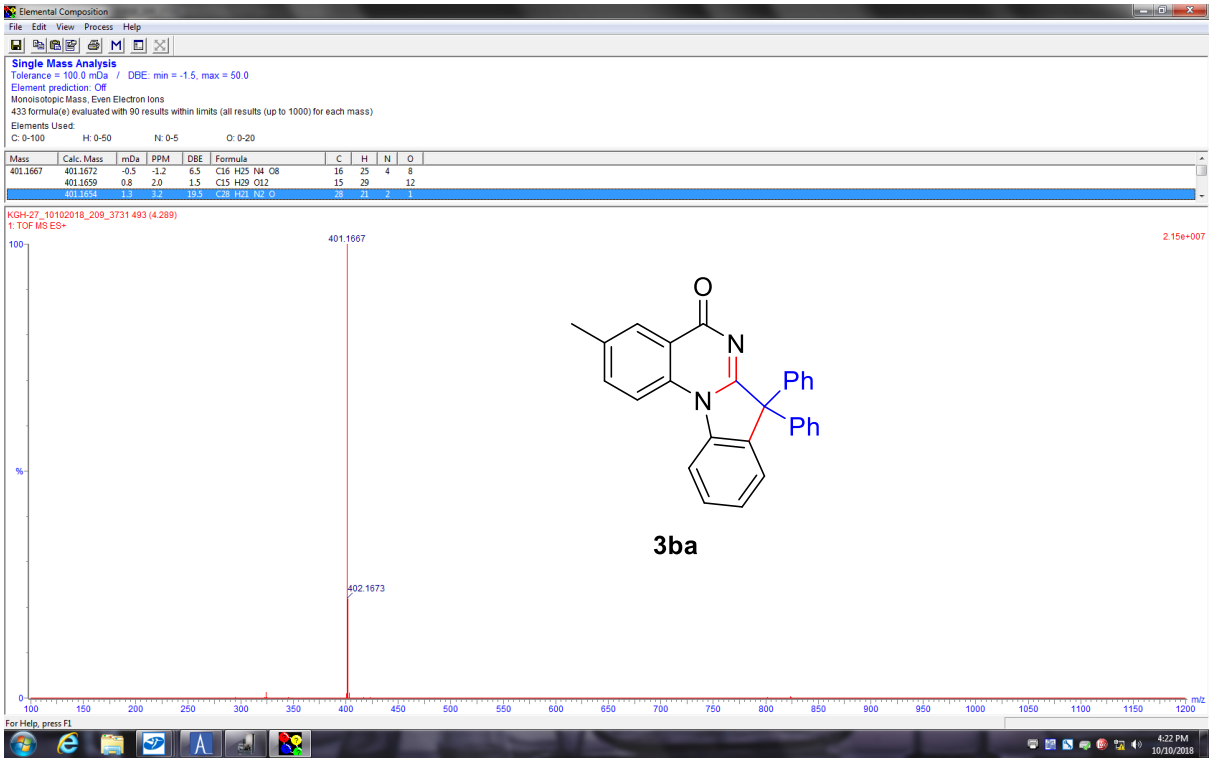

Spectrum - [KGH-21_30012019_237_4225]
File Edit Display Process Tools Window Help
KGH-21_30012019_237_4225 9 (0.169) Cm (4:12)
TOF MS ES+
4.61e6
407.1081
408.1120
124.0839
100
%
0
m/z
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000 1050 1100 1150
O
N
N
S
2:00 PM
1/30/2019

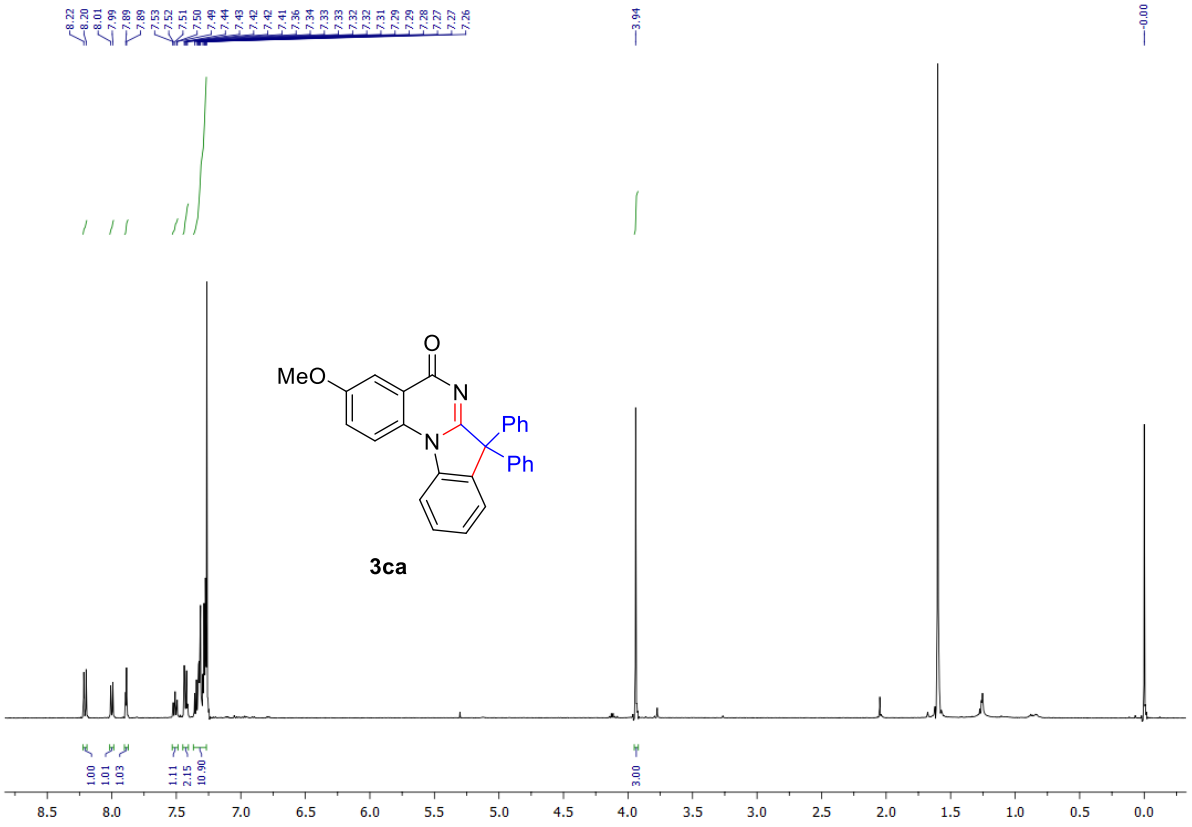
3ai

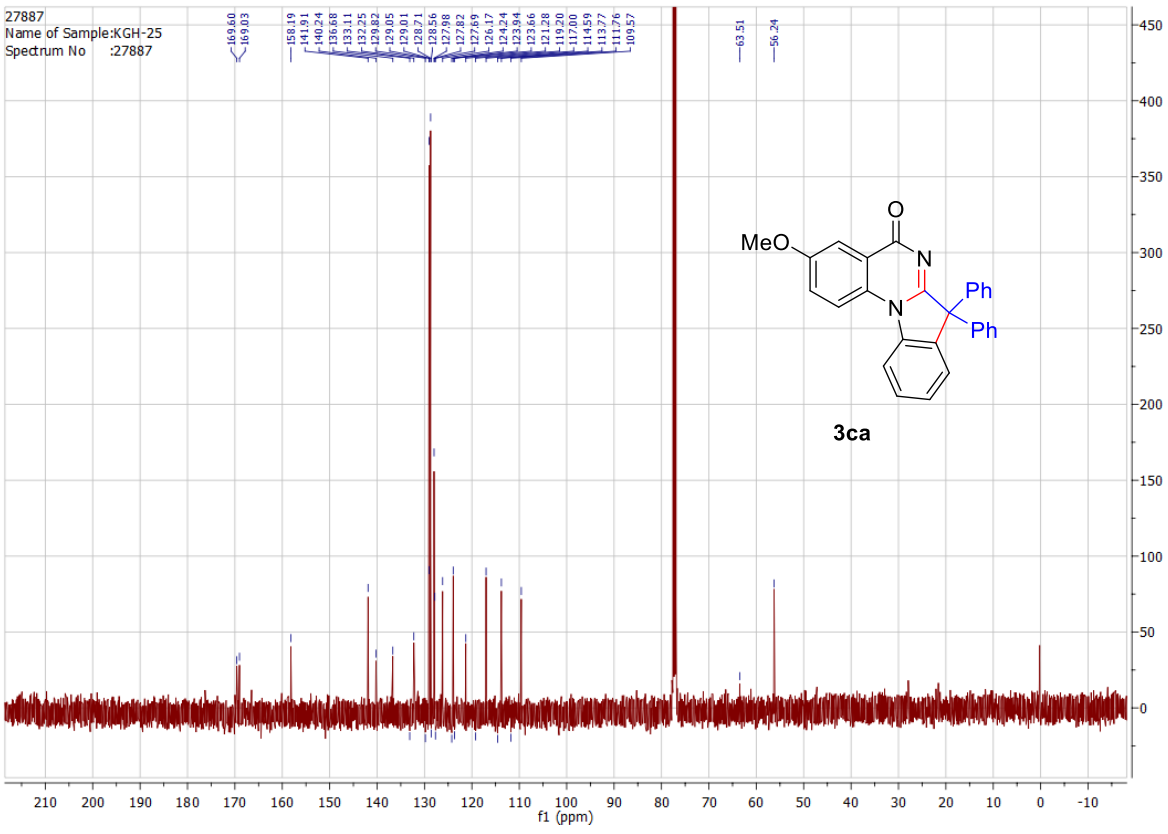

8.28 8.28 8.16 8.14 8.02 8.00 7.66 7.65 7.64 7.63 7.53 7.53 7.51 7.51 7.50 7.49 7.44 7.43 7.42 7.42 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.32 7.32 7.32 7.31 7.29 7.29 7.28 7.28 7.28 7.27 7.27 7.26
2.51
0.00
O
N
N
Ph
Ph
1.00 1.03 1.02 1.04 1.10 1.06 11.13 3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0

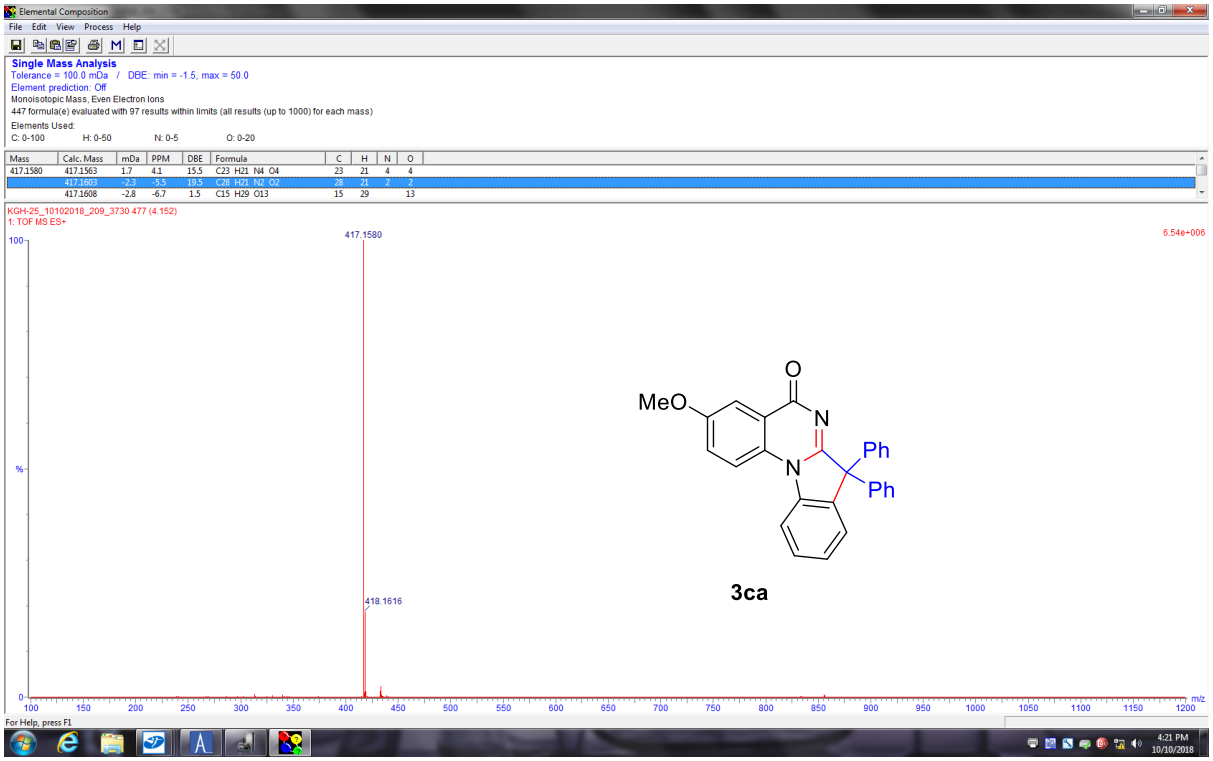
3ba

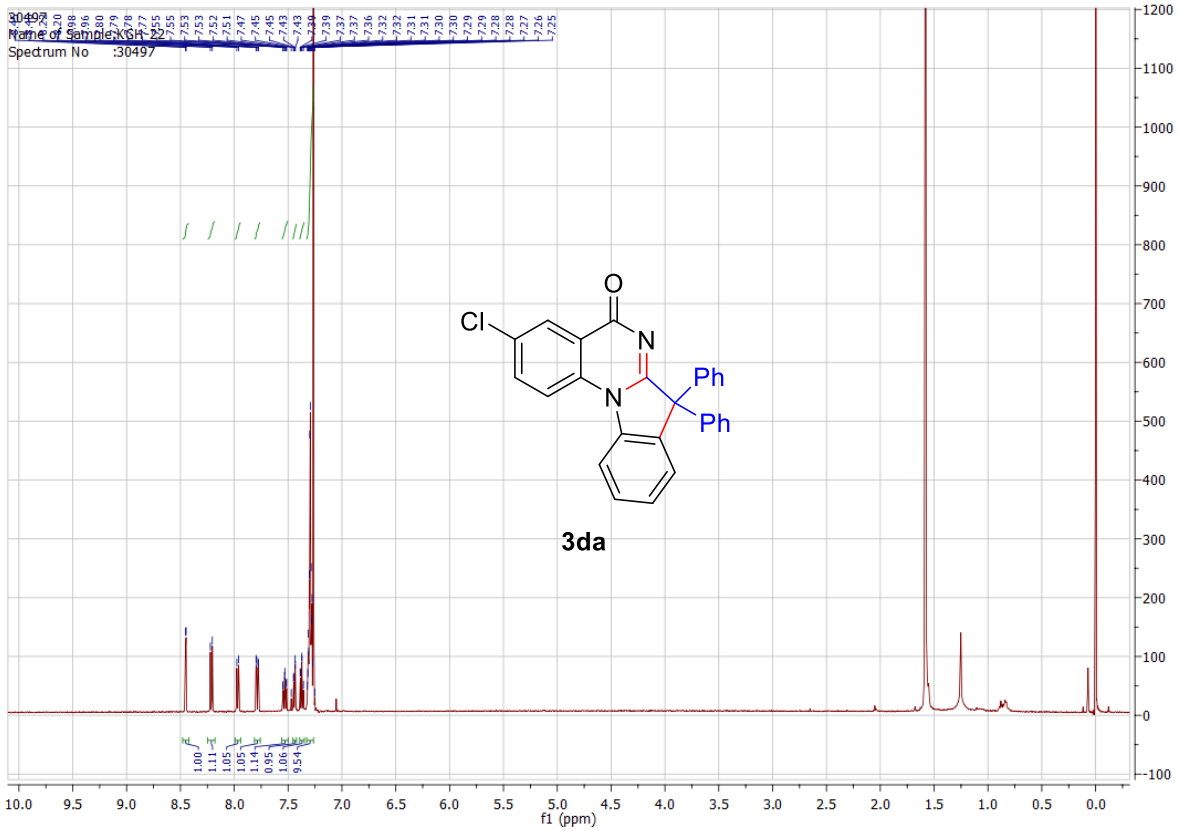

170.02
168.94
141.77
140.05
136.84
136.37
135.77
134.98
129.33
128.86
128.49
127.76
114.96
113.69
63.30
21.05
0.01
O
N
N
Ph
Ph
3ba
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0

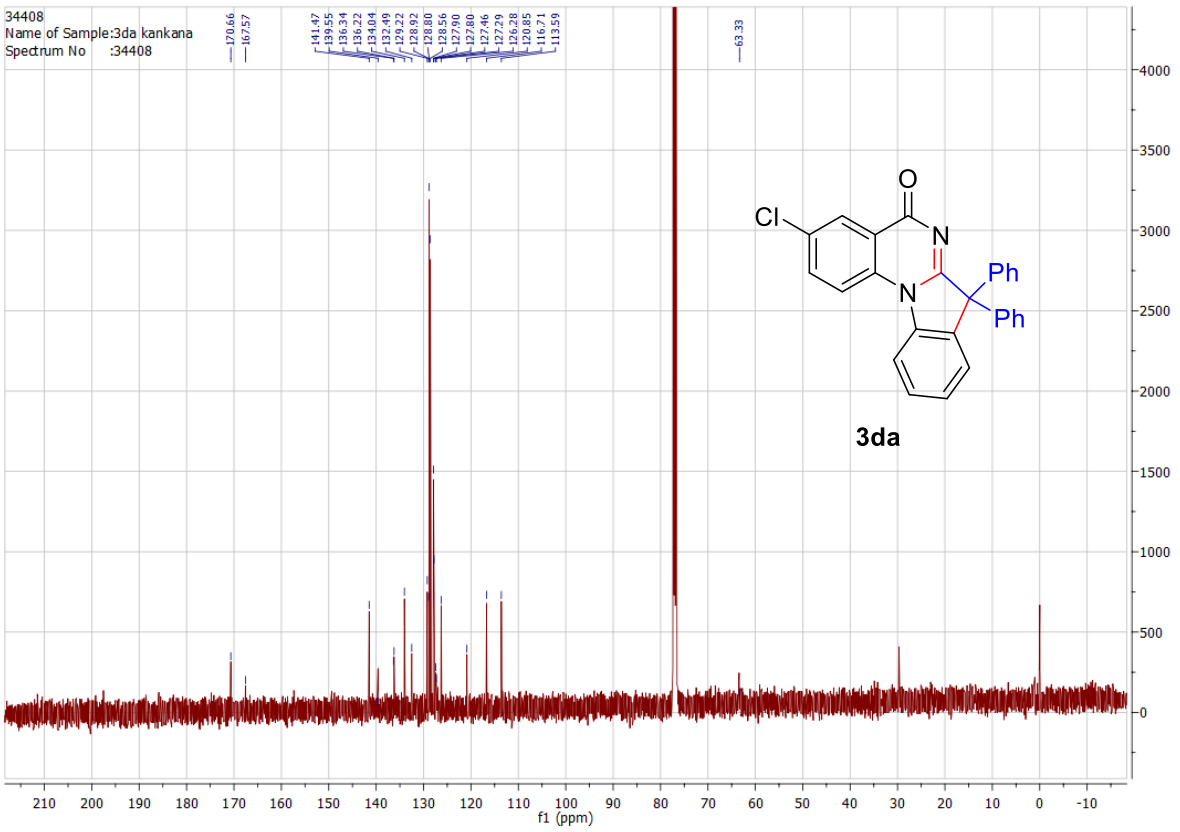

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
433 formula(e) evaluated with 90 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-50 N: 0-5 O: 0-20
Mass Calc. Mass mDa PPM DBE Formula C H N O
401.1667 401.1672 -0.5 -1.2 6.5 C16 H25 N4 O8 16 25 4 8
401.1659 0.8 2.0 1.5 C15 H29 O12 15 29 12
401.1654 1.3 3.2 19.5 C28 H21 N2 O 28 21 2 1
KGH-27_10102018_209_3731 493 (4.289)
1: TOF MS ES+
401.1667
2.15e+007
402.1673
100
%
0
100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000 1050 1100 1150 1200
m/z
O
N
N
Ph
Ph
3ba
For Help, press F1
4:22 PM
10/10/2018

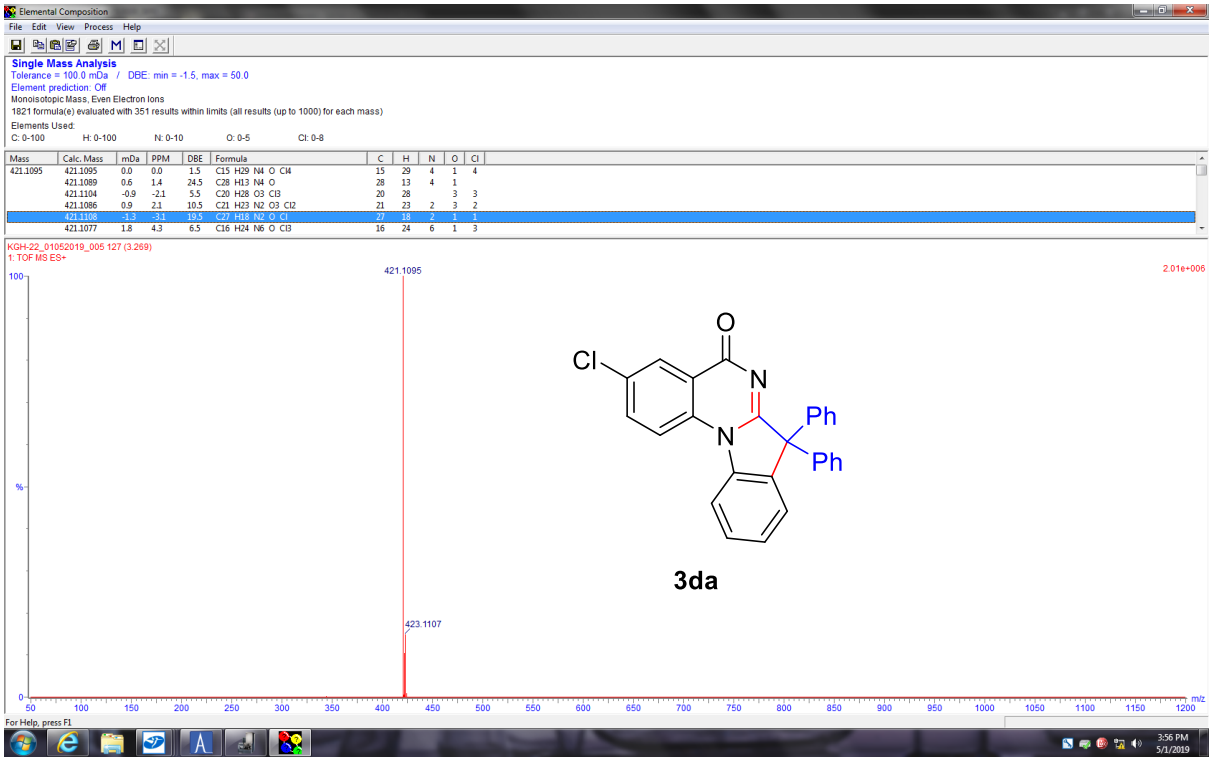

MeO
O
N
N
Ph
Ph
3ca

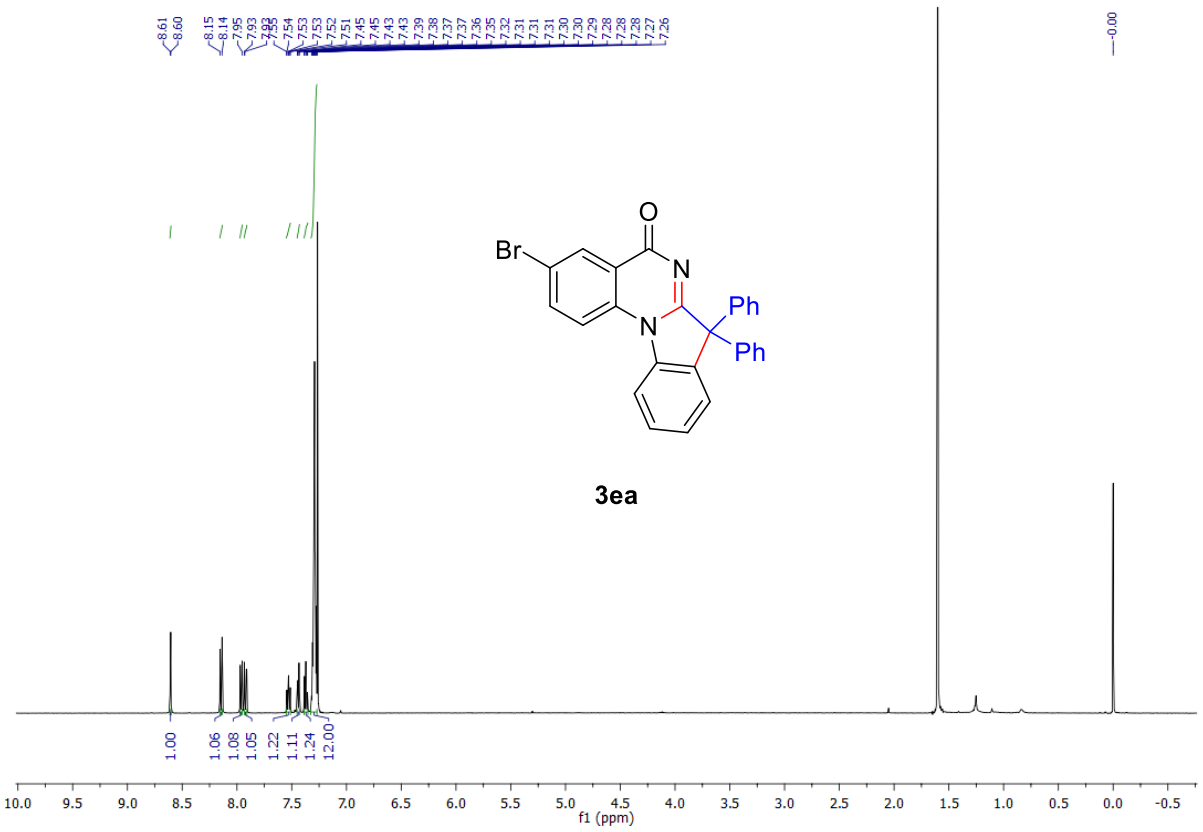

27887
Name of Sample:KGH-25
Spectrum No :27887
MeO
O
N
N
Ph
Ph
3ca
f1 (ppm)


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
447 formula(e) evaluated with 97 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-50 N: 0-5 O: 0-20
Mass Calc. Mass mDa PPM DBE Formula C H N O
417.1580 417.1563 1.7 4.1 15.5 C23 H21 N4 O4 23 21 4 4
417.1603 -2.3 -5.5 19.5 C28 H21 N2 O2 28 21 2 2
417.1608 -2.8 -6.7 1.5 C15 H29 O13 15 29 13
KGH-25_10102018_209_3730 477 (4.152)
1: TOF MS ES+
417.1580
6.54e+006
418.1616
MeO
O
N
N
Ph
Ph
3ca
For Help, press F1
4:21 PM
10/10/2018

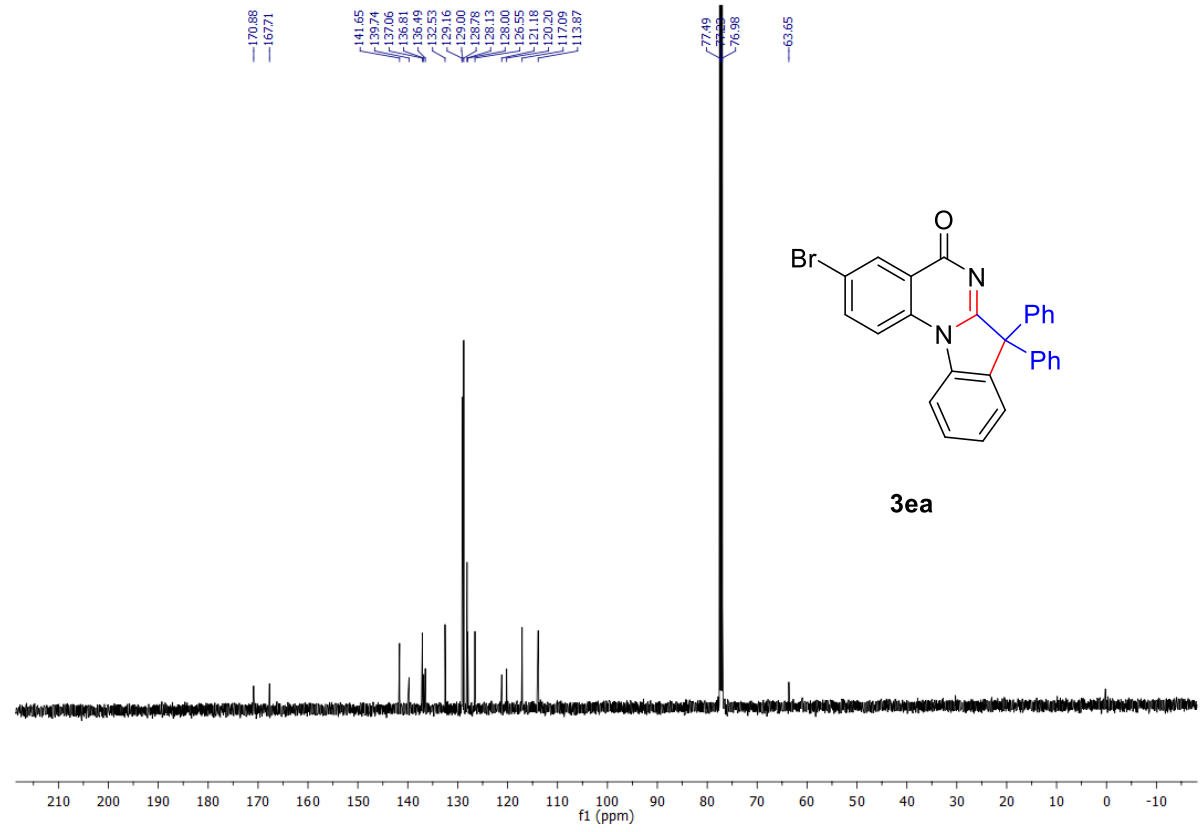

30497
Name of Sample:KGH-22
Spectrum No :30497
Cl
O
N
N
Ph
Ph
3da
1.00
1.11
1.05
1.05
1.14
0.95
1.06
9.54
f1 (ppm)


34408
Name of Sample:3da kankana
Spectrum No :34408
170.66
167.57
141.47
139.55
136.34
136.22
134.04
132.49
129.22
128.92
128.80
128.56
127.90
127.80
127.46
127.29
126.28
120.85
116.71
113.59
63.33
Cl
O
N
N
Ph
Ph
3da
f1 (ppm)

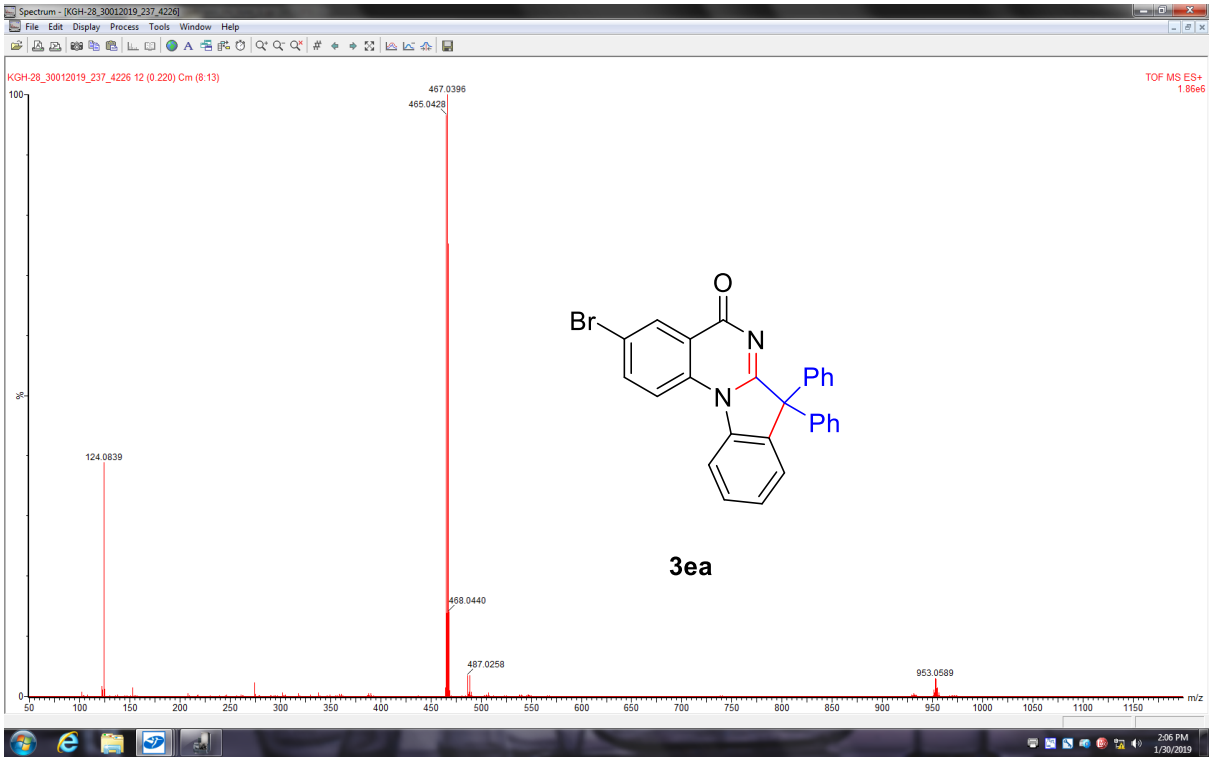

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
1821 formula(e) evaluated with 351 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-5 Cl: 0-8
Mass Calc. Mass mDa PPM DBE Formula C H N O Cl
421.1095 421.1095 0.0 0.0 1.5 C15 H29 N4 O Cl4 15 29 4 1 4
421.1089 0.6 1.4 24.5 C28 H13 N4 O 28 13 4 1
421.1104 -0.9 -2.1 5.5 C20 H28 O3 Cl3 20 28 3 3
421.1086 0.9 2.1 10.5 C21 H23 N2 O3 Cl2 21 23 2 3 2
421.1108 -1.3 -3.1 19.5 C27 H18 N2 O Cl 27 18 2 1 1
421.1077 1.8 4.3 6.5 C16 H24 N6 O Cl3 16 24 6 1 3
KGH-22_01052019_005 127 (3.269)
1: TOF MS ES+
421.1095
2.01e+006
423.1107
Cl
O
N
N
Ph
Ph
3da
m/z
For Help, press F1
3:56 PM
5/1/2019

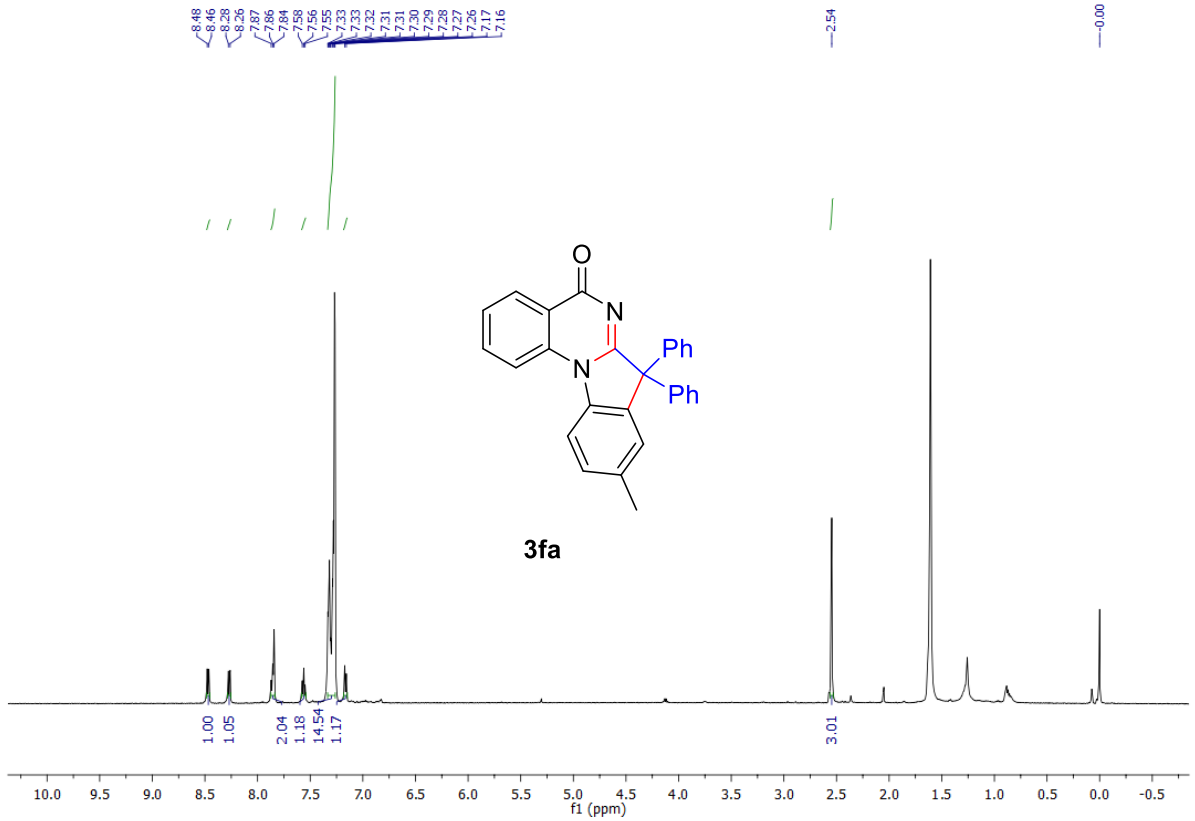

8.61
8.60
8.15
8.14
7.95
7.93
7.54
7.53
7.53
7.52
7.51
7.45
7.43
7.39
7.38
7.37
7.37
7.36
7.35
7.32
7.31
7.31
7.31
7.30
7.30
7.29
7.28
7.28
7.28
7.27
7.26
0.00
1.00
1.06
1.08
1.05
1.22
1.11
1.24
12.00
Br
O
N
N
Ph
Ph
f1 (ppm)

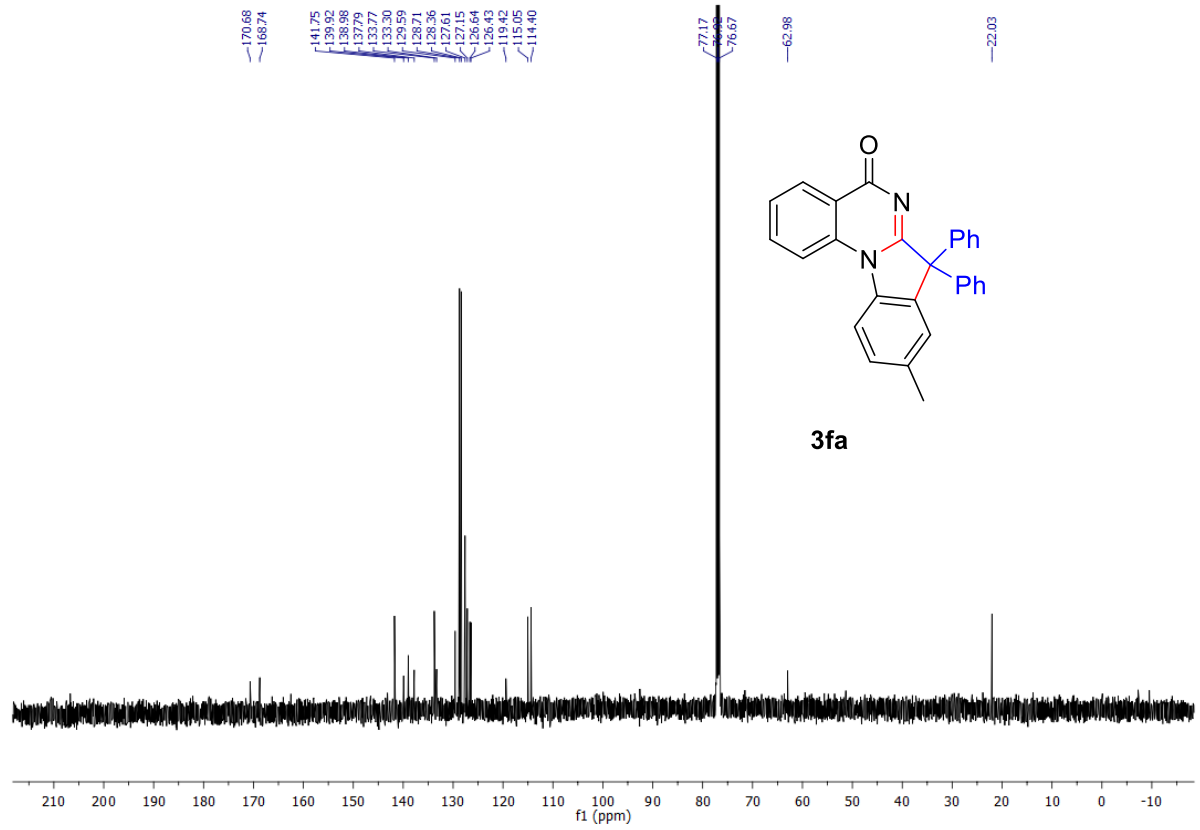
3ea

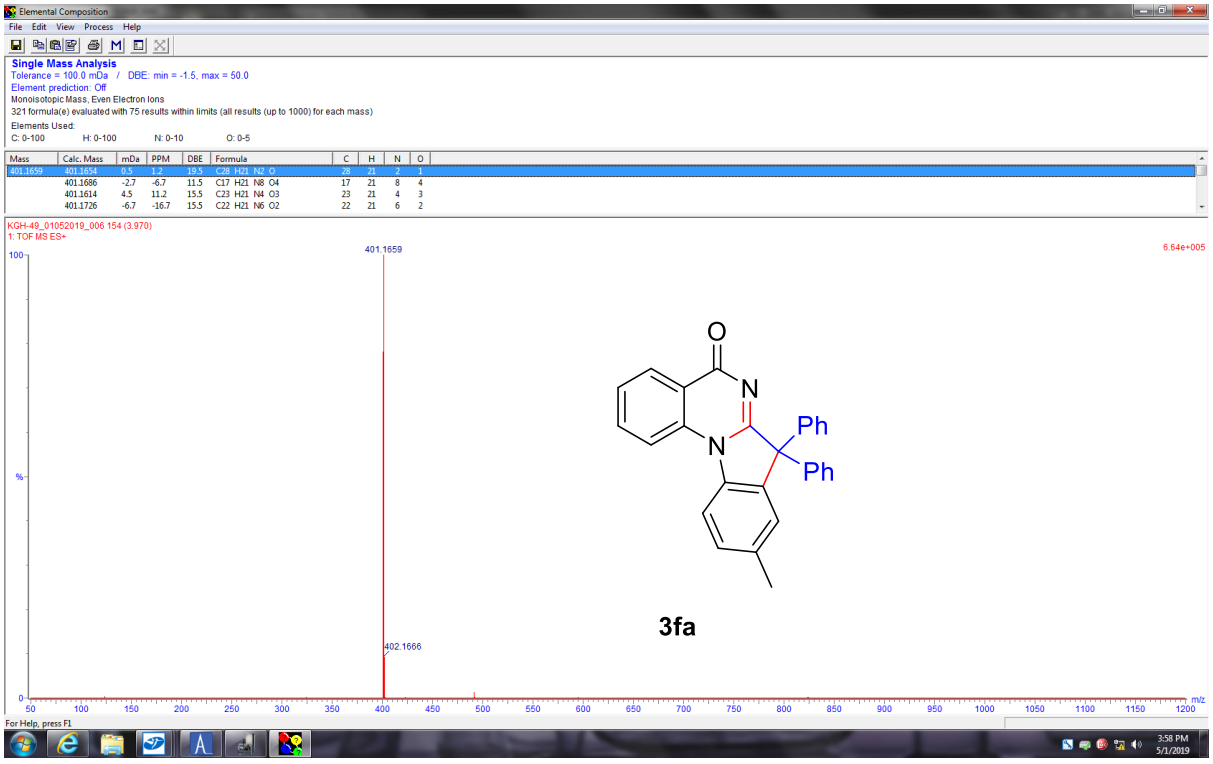

170.88
167.71
141.65
139.74
137.06
136.81
136.49
132.53
129.16
129.00
128.78
128.13
128.00
126.55
121.18
120.20
117.09
113.87
77.49
76.98
63.65
Br
O
N
N
Ph
Ph
f1 (ppm)

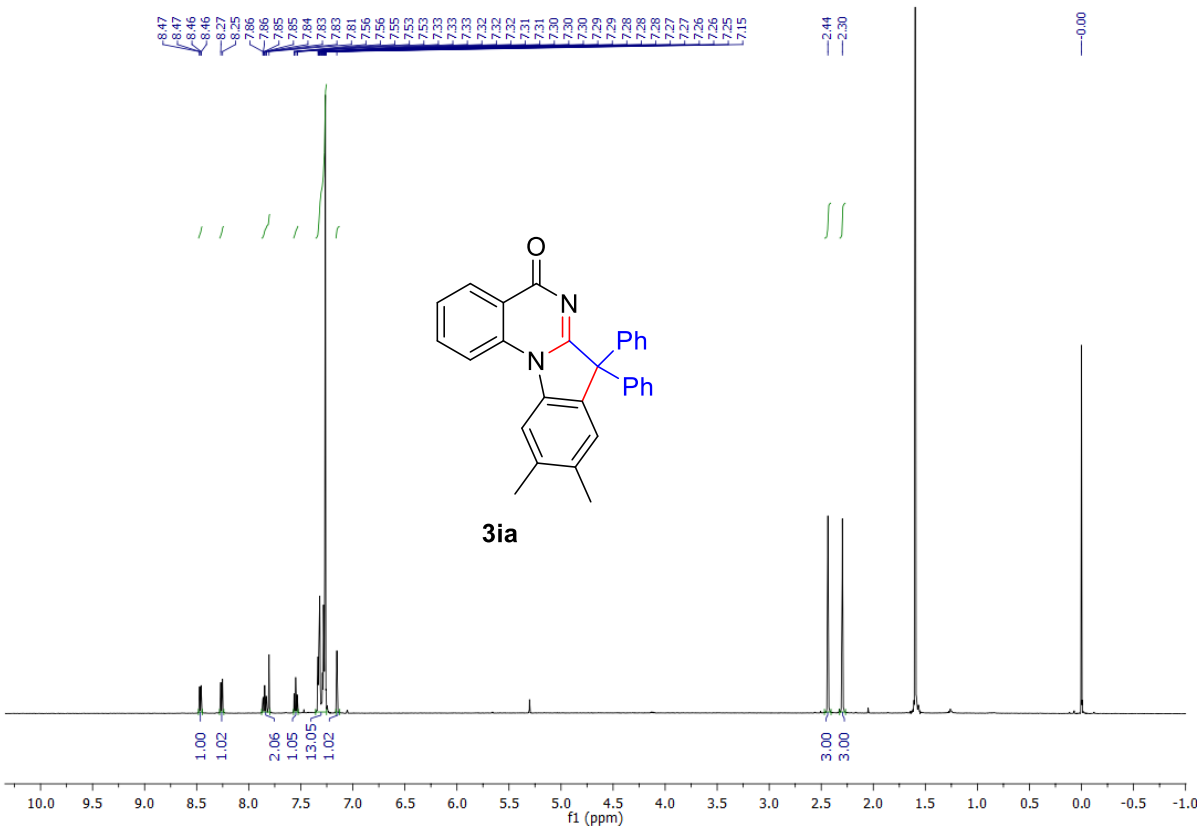
3ea

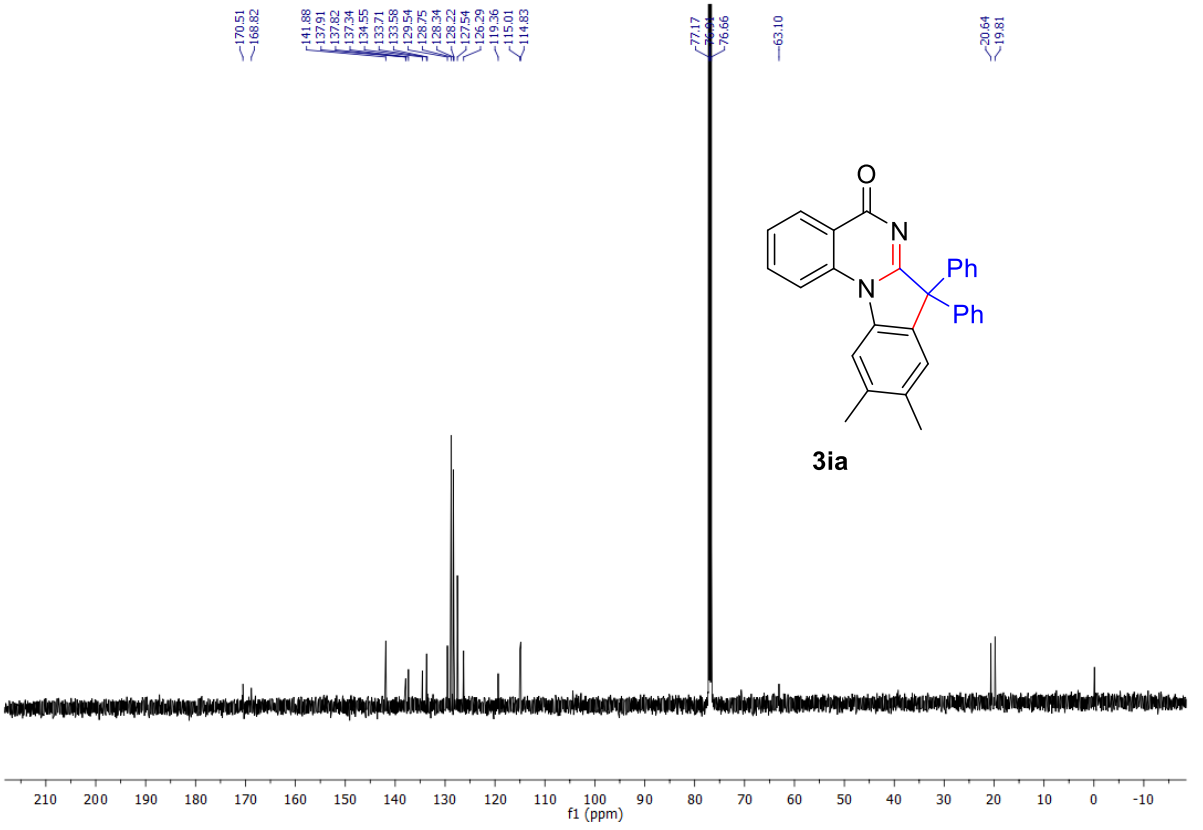

KGH-28_30012019_237_4226 12 (0.220) Cm (8:13)
TOF MS ES+
1.86e6
467.0396
465.0428
124.0839
468.0440
487.0258
953.0589
Br
O
N
N
Ph
Ph
3ea

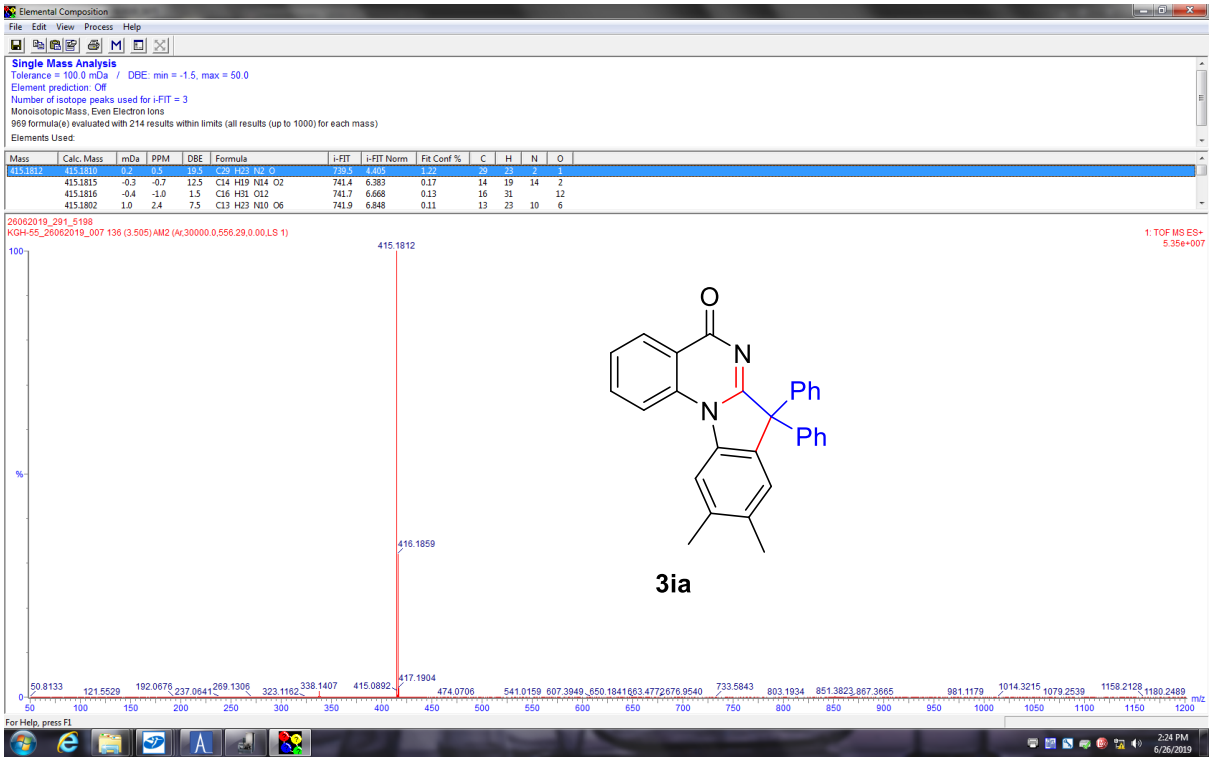

8.48
8.46
8.28
8.26
7.87
7.86
7.84
7.58
7.56
7.55
7.33
7.33
7.32
7.31
7.31
7.30
7.29
7.28
7.27
7.26
7.17
7.16
2.54
0.00
O
N
N
Ph
Ph
3fa
1.00
1.05
2.04
1.18
14.54
1.17
3.01
f1 (ppm)


170.68
168.74
141.75
139.92
138.98
137.79
133.77
133.30
129.59
128.71
128.36
127.61
127.15
126.64
126.43
119.42
115.05
114.40
77.17
76.67
62.98
22.03
O
N
N
Ph
Ph
3fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

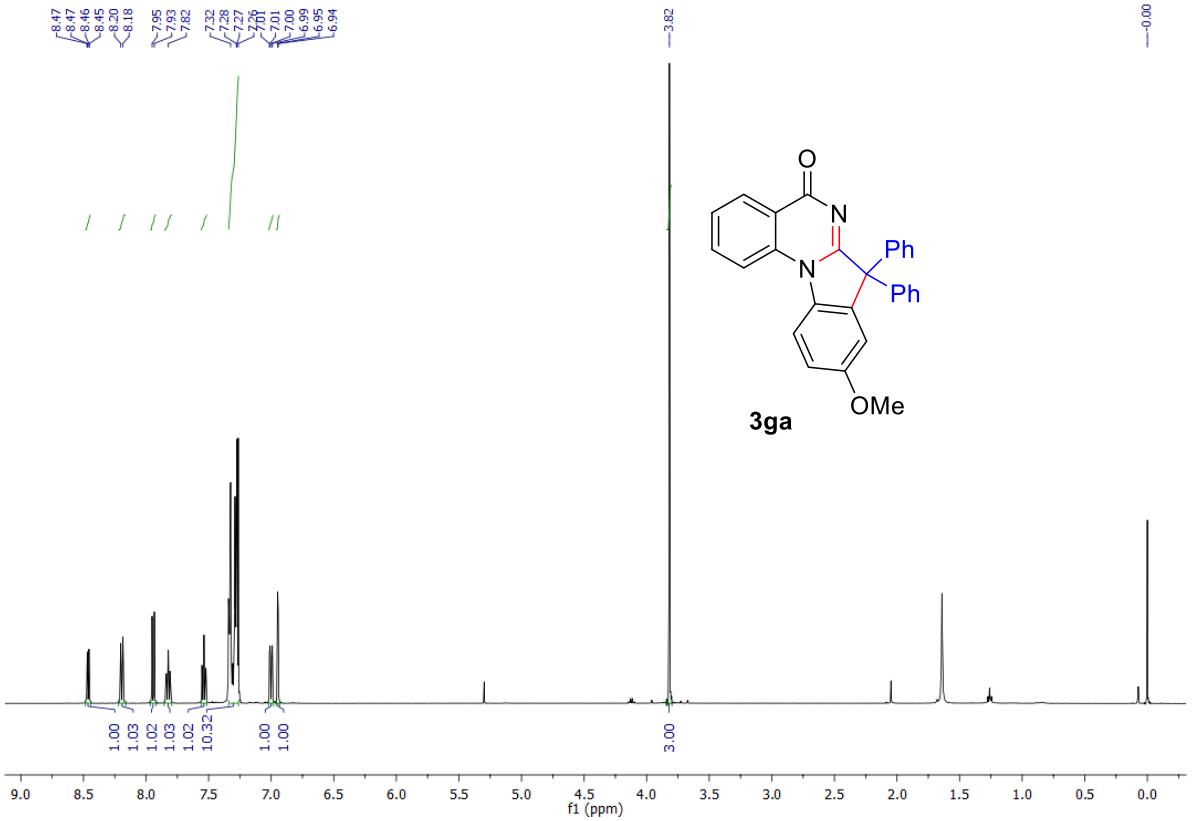

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
321 formula(e) evaluated with 75 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-5
Mass Calc. Mass mDa PPM DBE Formula C H N O
401.1659 401.1654 0.5 1.2 19.5 C28 H21 N2 O 28 21 2 1
401.1686 -2.7 -6.7 11.5 C17 H21 N8 O4 17 21 8 4
401.1614 4.5 11.2 15.5 C23 H21 N4 O3 23 21 4 3
401.1726 -6.7 -16.7 15.5 C22 H21 N6 O2 22 21 6 2
KGH-49_01052019_006 154 (3.970)
1: TOF MS ES+
401.1659
6.64e+005
100
%
0
402.1666
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000 1050 1100 1150 1200
m/z
O
N
N
Ph
Ph
3fa
For Help, press F1
3:58 PM
5/1/2019


8.47
8.46
8.27
7.86
7.85
7.84
7.83
7.81
7.56
7.55
7.53
7.33
7.32
7.31
7.30
7.29
7.28
7.27
7.26
7.25
7.15
2.44
2.30
0.00
O
N
N
Ph
Ph
3ia
1.00
1.02
2.06
1.05
13.05
1.02
3.00
3.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

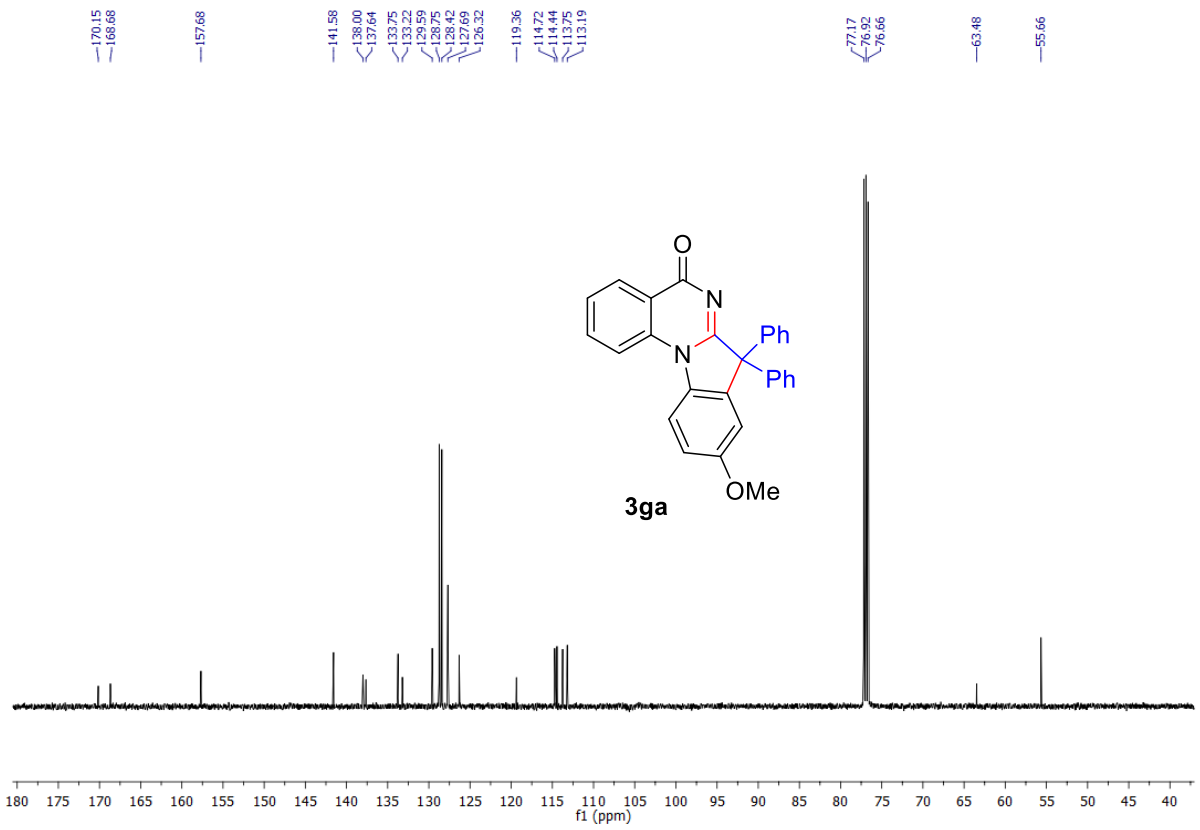

170.51
168.82
141.88
137.91
137.82
137.34
134.55
133.71
133.58
129.54
128.75
128.34
128.22
127.54
126.29
119.36
115.01
114.83
77.17
76.91
76.66
63.10
20.64
19.81
O
N
N
Ph
Ph
3ia
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

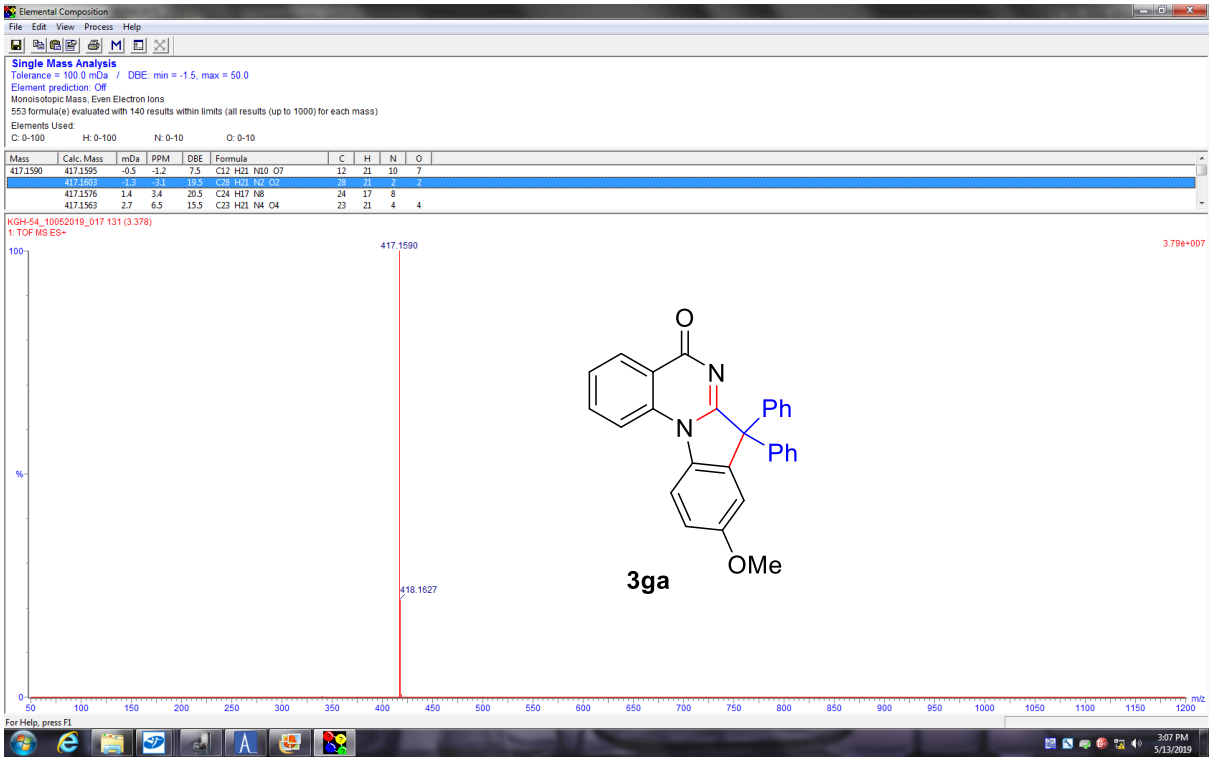

Elemental Composition
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
969 formula(e) evaluated with 214 results within limits (all results (up to 1000) for each mass)
Elements Used:
415.1812
416.1859
417.1904
O
N
N
Ph
Ph

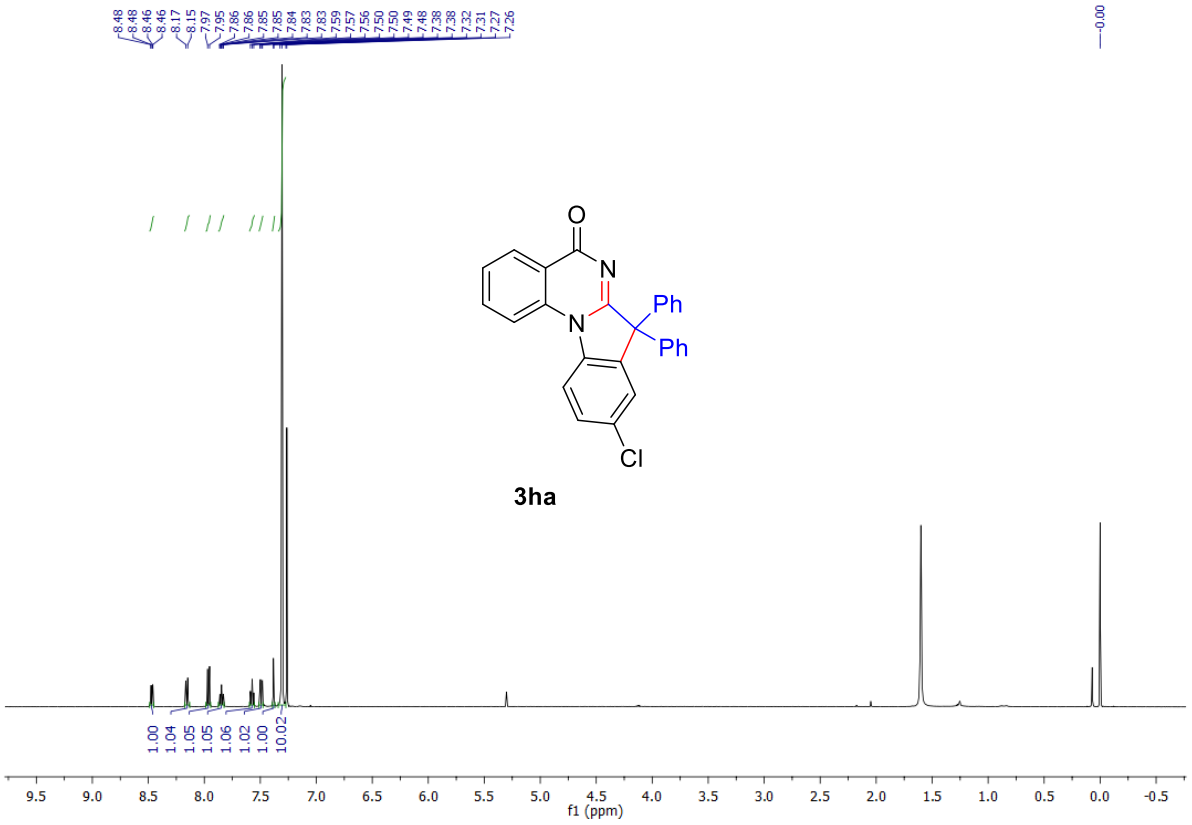
3ia


3.82
0.00
O
N
N
Ph
Ph
OMe
f1 (ppm)

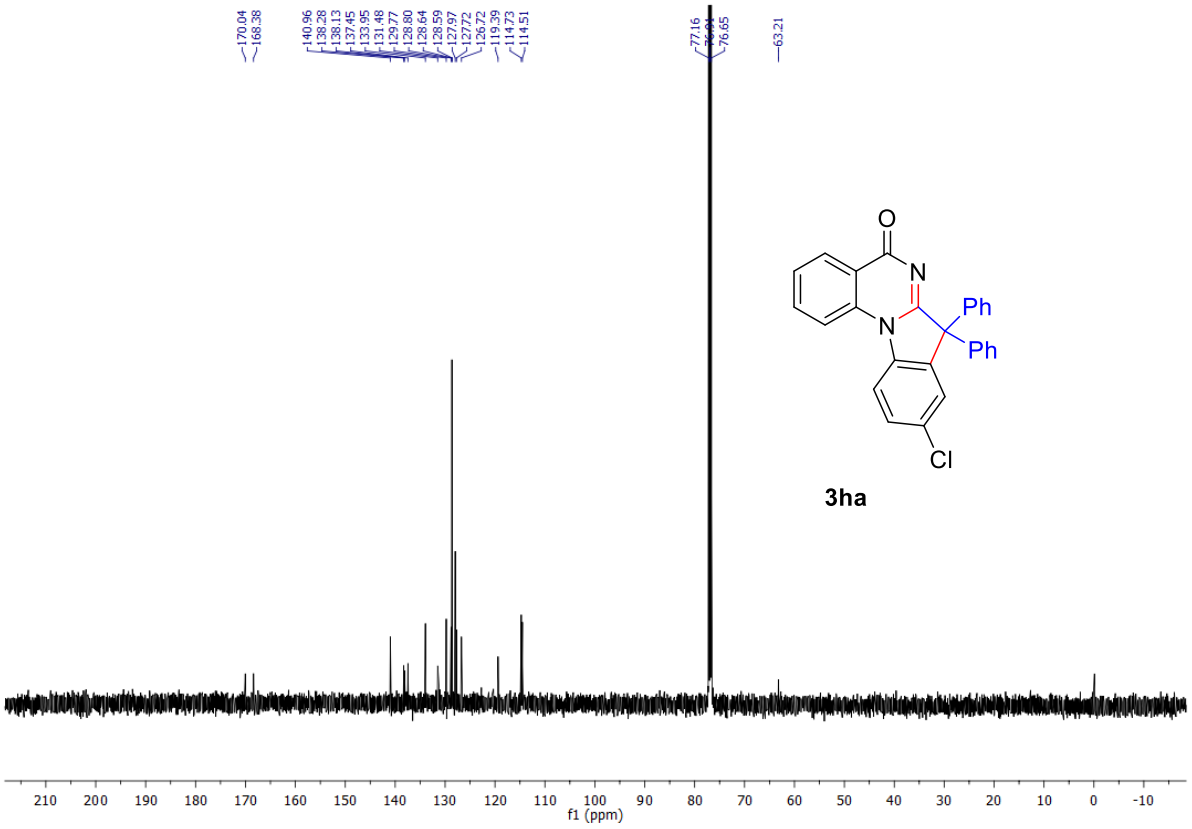
3ga


170.15
168.68
157.68
141.58
138.00
137.64
133.75
133.22
129.59
128.75
128.42
127.69
126.32
119.36
114.72
114.44
113.75
113.19
77.17
76.92
76.66
63.48
55.66
O
N
N
Ph
Ph
OMe
3ga
180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

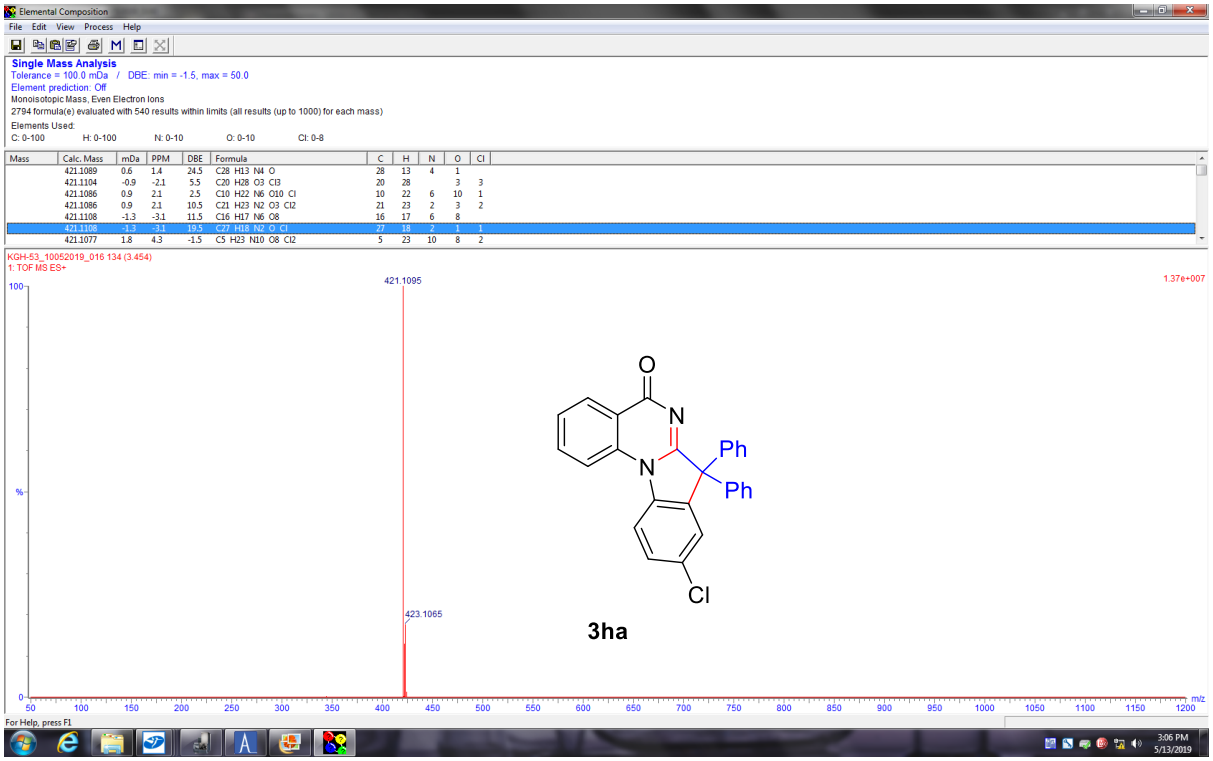

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
553 formula(e) evaluated with 140 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10
Mass Calc. Mass mDa PPM DBE Formula C H N O
417.1590 417.1595 -0.5 -1.2 7.5 C12 H21 N10 O7 12 21 10 7
417.1673 -1.3 -3.1 10.5 C28 H21 N2 O2 28 21 2 2
417.1576 1.4 3.4 20.5 C24 H17 N8 24 17 8
417.1563 2.7 6.5 15.5 C23 H21 N4 O4 23 21 4 4
KGH-54_10052019_017 131 (3.378)
1: TOF MS ES+
417.1590
3.79e+007
418.1627
100
%
0
50 100 150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 1000 1050 1100 1150 1200
m/z
O
N
N
Ph
Ph
OMe
3ga
For Help, press F1
3:07 PM
5/13/2019


8.48
8.48
8.46
8.46
8.17
8.15
7.97
7.95
7.86
7.86
7.85
7.85
7.84
7.83
7.59
7.57
7.56
7.50
7.50
7.49
7.48
7.38
7.38
7.32
7.31
7.27
7.26
0.00
O
N
N
Ph
Ph
Cl
1.00
1.04
1.05
1.05
1.06
1.02
1.00
10.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3ha

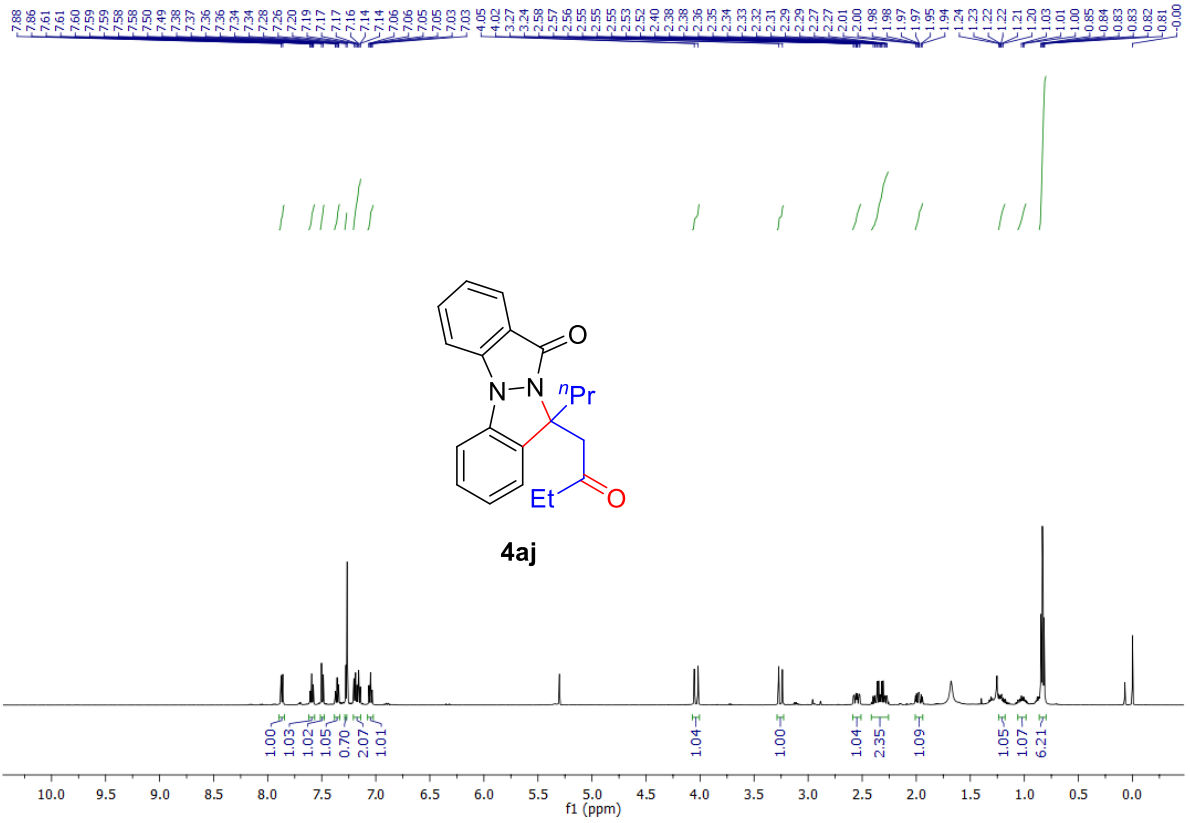

170.04
168.38
140.96
138.28
138.13
137.45
133.95
131.48
129.77
128.80
128.64
128.59
127.97
127.72
126.72
119.39
114.73
114.51
77.16
76.84
76.65
63.21
O
N
N
Ph
Ph
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3ha


Elemental Composition
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
2794 formula(e) evaluated with 540 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-10 Cl: 0-8
Mass Calc. Mass mDa PPM DBE Formula C H N O Cl
421.1089 0.6 1.4 24.5 C28 H13 N4 O 28 13 4 1
421.1104 -0.9 -2.1 5.5 C20 H28 O3 Cl3 20 28 3 3
421.1086 0.9 2.1 2.5 C10 H22 N6 O10 Cl 10 22 6 10 1
421.1086 0.9 2.1 10.5 C21 H23 N2 O3 Cl2 21 23 2 3 2
421.1108 -1.3 -3.1 11.5 C16 H17 N6 O8 16 17 6 8
421.1108 -1.3 -3.1 19.5 C27 H18 N2 O Cl 27 18 2 1 1
421.1077 1.8 4.3 -1.5 C5 H23 N10 O8 Cl2 5 23 10 8 2
KGH-53_10052019_016 134 (3.454)
1: TOF MS ES+
421.1095
423.1065
1.37e+007
m/z
For Help, press F1
3:06 PM
5/13/2019

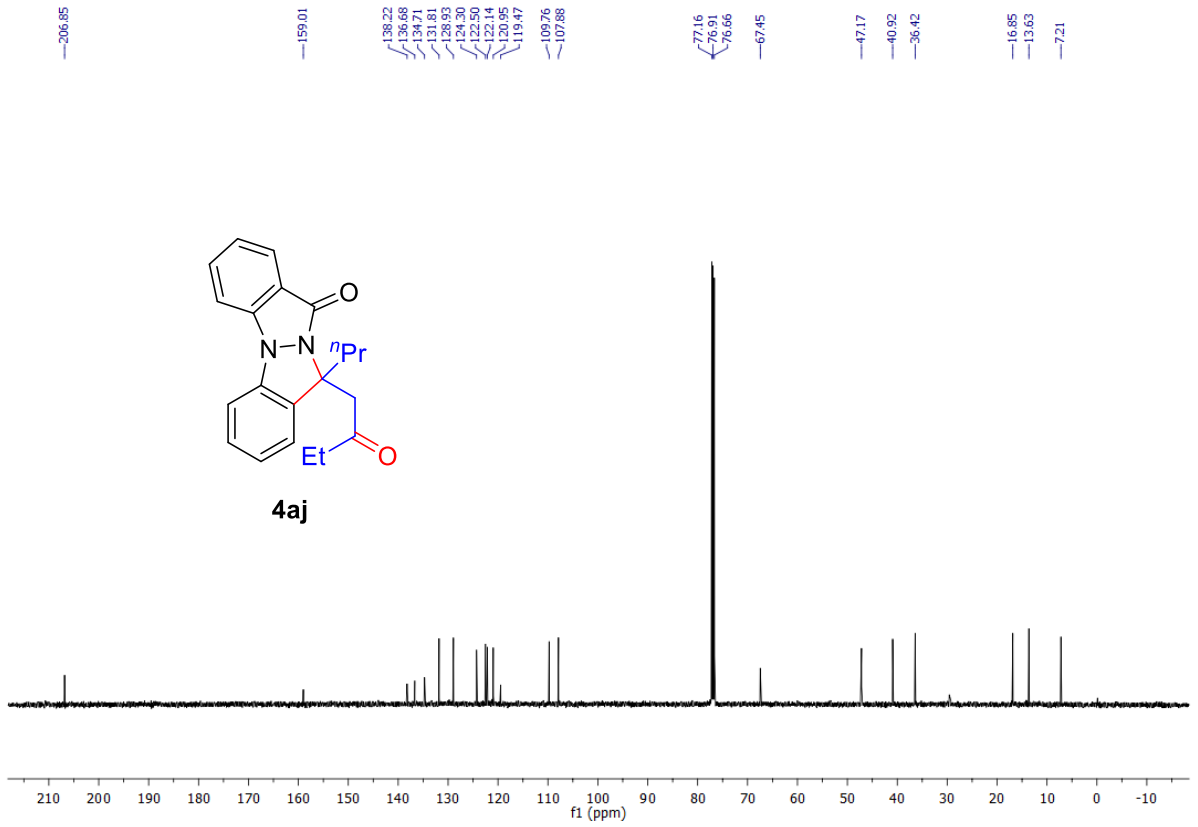
O
N
N
Ph
Ph
Cl

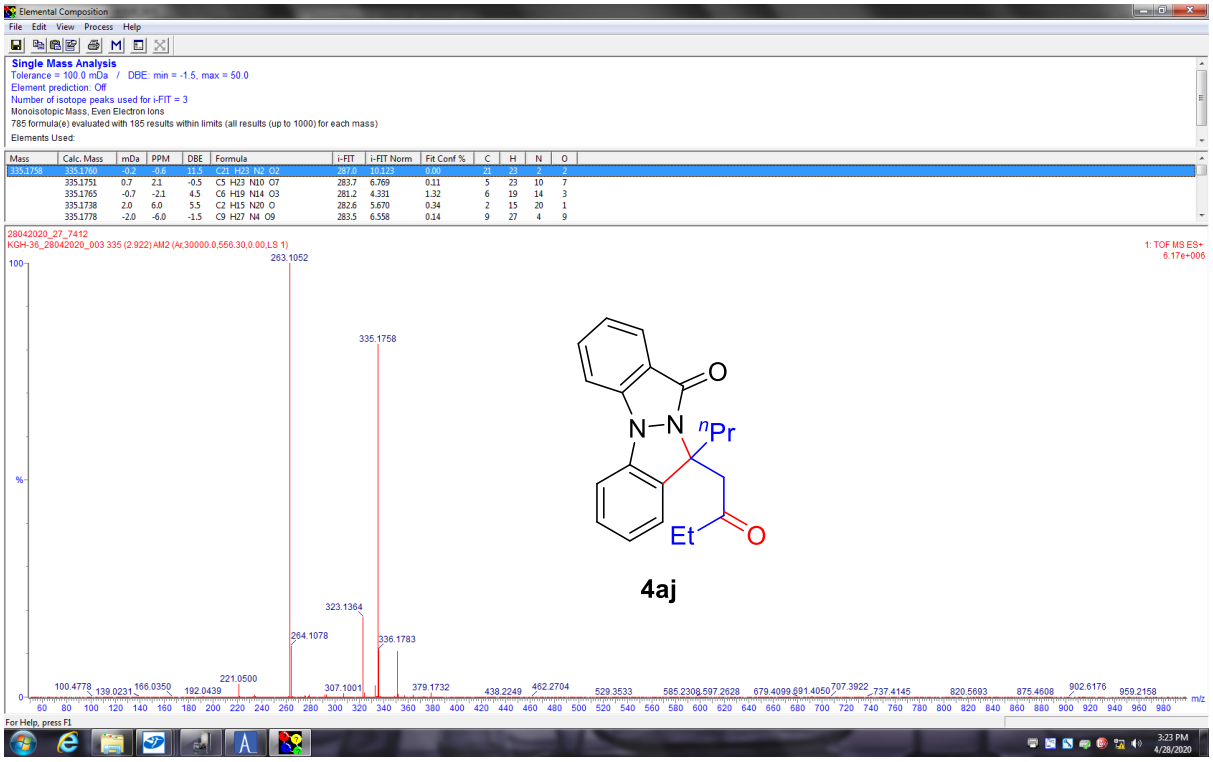
3ha

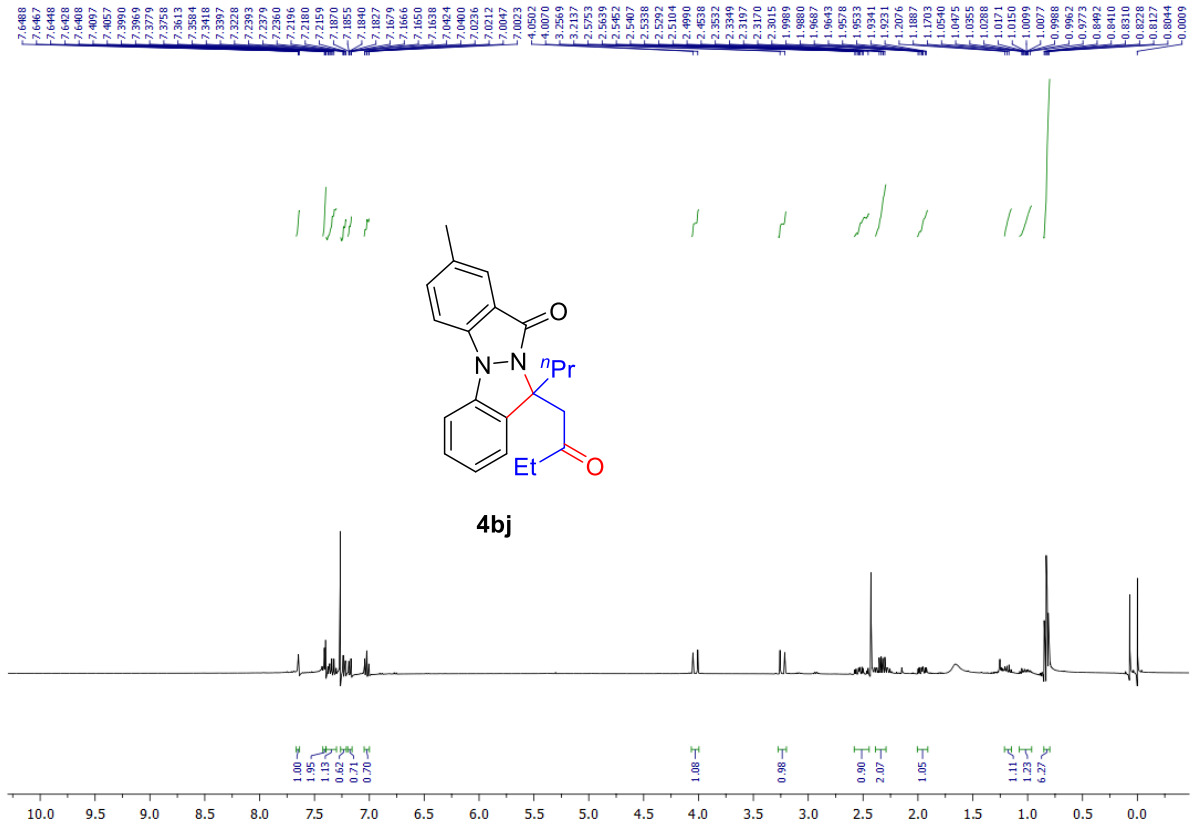

7.88 7.86 7.61 7.61 7.60 7.59 7.59 7.58 7.58 7.50 7.49 7.38 7.37 7.36 7.36 7.34 7.34 7.28 7.26 7.20 7.19 7.17 7.17 7.16 7.14 7.14 7.06 7.06 7.05 7.05 7.03 7.03
4.05 4.02 3.27 3.24 2.58 2.57 2.56 2.55 2.55 2.55 2.53 2.52 2.40 2.38 2.38 2.36 2.35 2.34 2.33 2.32 2.31 2.29 2.29 2.27 2.27 2.01 2.00 1.98 1.98 1.97 1.97 1.95 1.94
1.24 1.23 1.22 1.22 1.21 1.20 1.03 1.01 1.00 0.85 0.84 0.83 0.83 0.82 0.81 0.00
1.00 1.03 1.02 1.05 0.70 2.07 1.01
1.04 1.00 1.04 2.35 1.09 1.05 1.07 6.21
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

O
N–N
nPr
Et
O

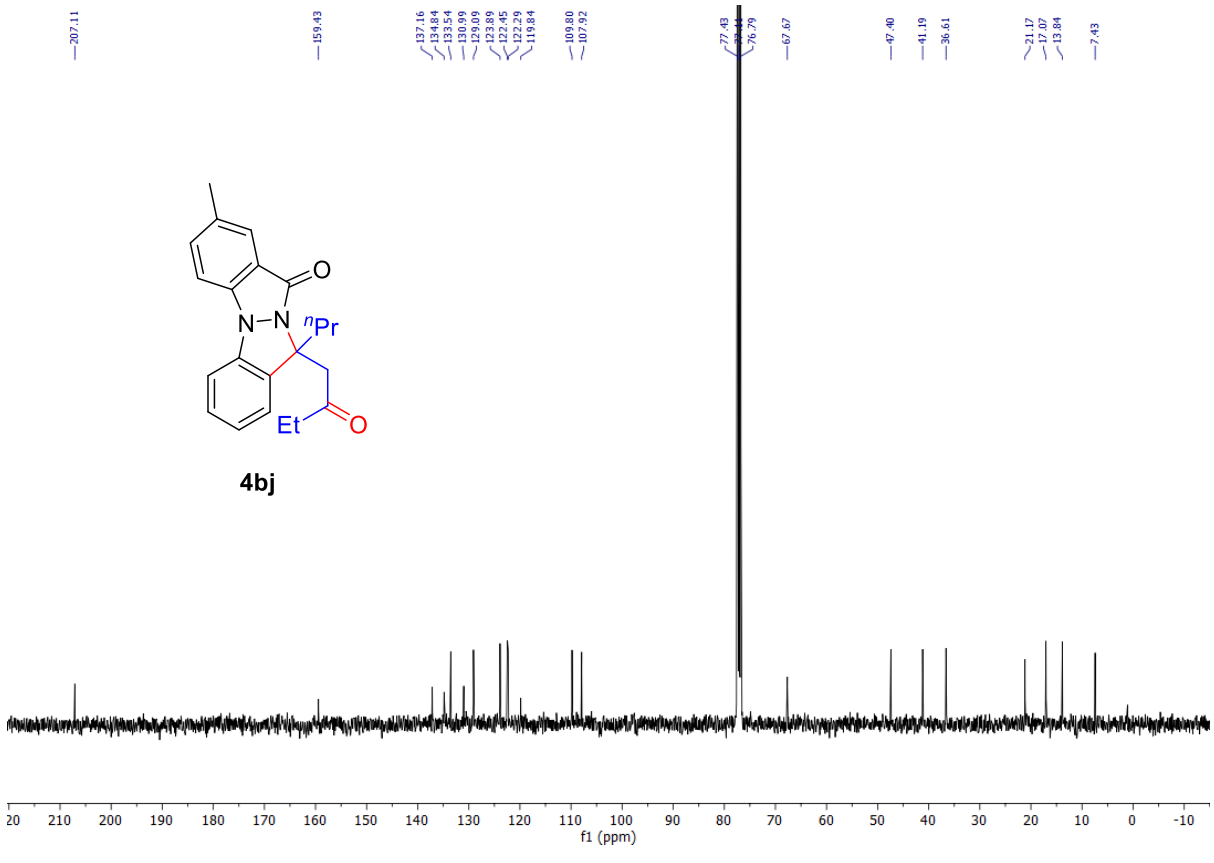
4aj


206.85
159.01
138.22
136.68
134.71
131.81
128.93
124.30
122.50
122.14
120.95
119.47
109.76
107.88
77.16
76.91
76.66
67.45
47.17
40.92
36.42
16.85
13.63
7.21
O
N–N
nPr
Et
O
4aj
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

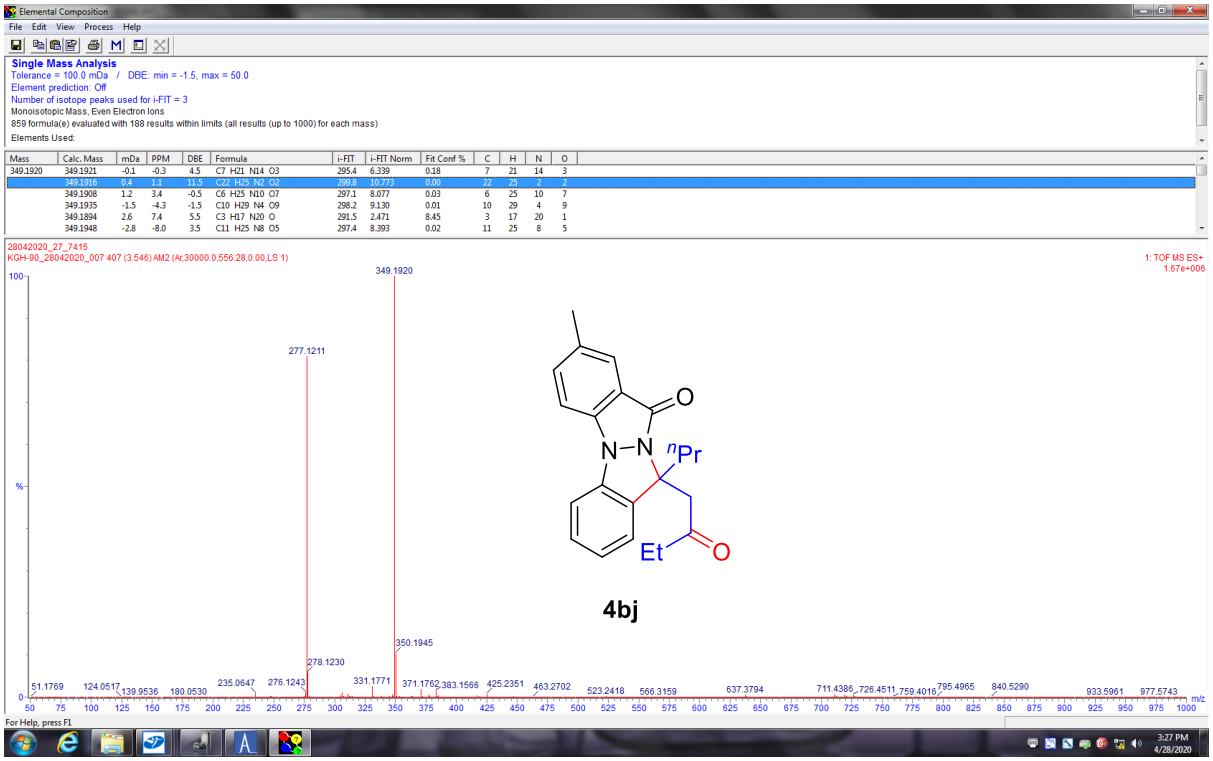

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
785 formula(e) evaluated with 185 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O
335.1758 335.1760 -0.2 -0.6 11.5 C21 H23 N2 O2 287.0 10,123 0.00 21 23 2 2
335.1751 0.7 2.1 -0.5 C5 H23 N10 O7 283.7 6.769 0.11 5 23 10 7
335.1765 -0.7 -2.1 4.5 C6 H19 N14 O3 281.2 4.331 1.32 6 19 14 3
335.1738 2.0 6.0 5.5 C2 H15 N20 O 282.6 5.670 0.34 2 15 20 1
335.1778 -2.0 -6.0 -1.5 C9 H27 N4 O9 283.5 6.558 0.14 9 27 4 9
28042020_27_7412
KGH-36_28042020_003 335 (2.922) AM2 (Ar,30000.0,556.30,0.00 LS 1)
1: TOF MS ES+
6.17e+006
263.1052
335.1758
323.1364
264.1078
336.1783
221.0500
100.4778
139.0231
166.0350
192.0439
307.1001
379.1732
438.2249
462.2704
529.3533
585.2308
597.2628
679.4099
691.4050
707.3922
737.4145
820.5693
875.4608
902.6176
959.2158
m/z
For Help, press F1
O
N–N
nPr
Et
O
4aj


O
N–N
nPr
Et
O
1.00
1.95
1.13
0.62
0.71
0.70
1.08
0.98
0.90
2.07
1.05
1.11
1.23
6.27
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0

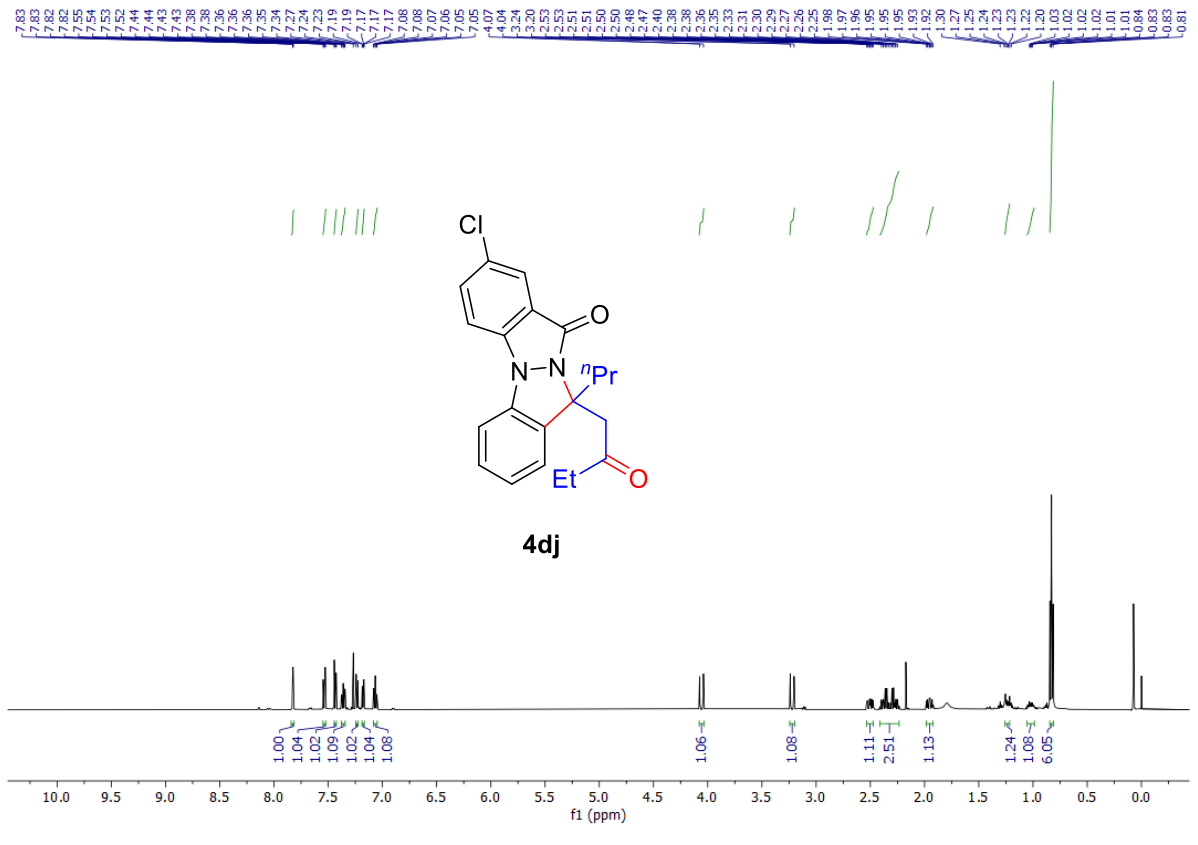
4bj


207.11
159.43
137.16
134.84
133.54
130.99
129.09
123.89
122.45
122.29
119.84
109.80
107.92
77.43
76.79
67.67
47.40
41.19
36.61
21.17
17.07
13.84
7.43
O
N–N
nPr
Et
O
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

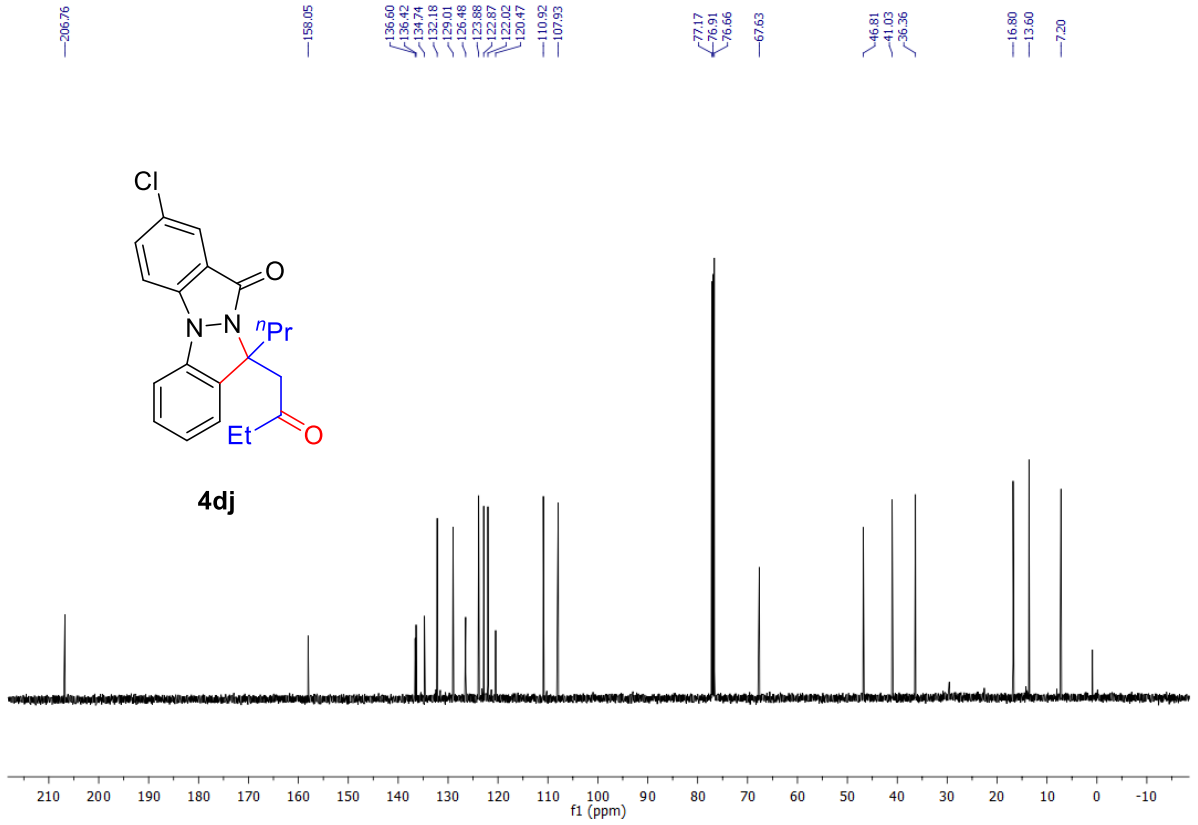
4bj

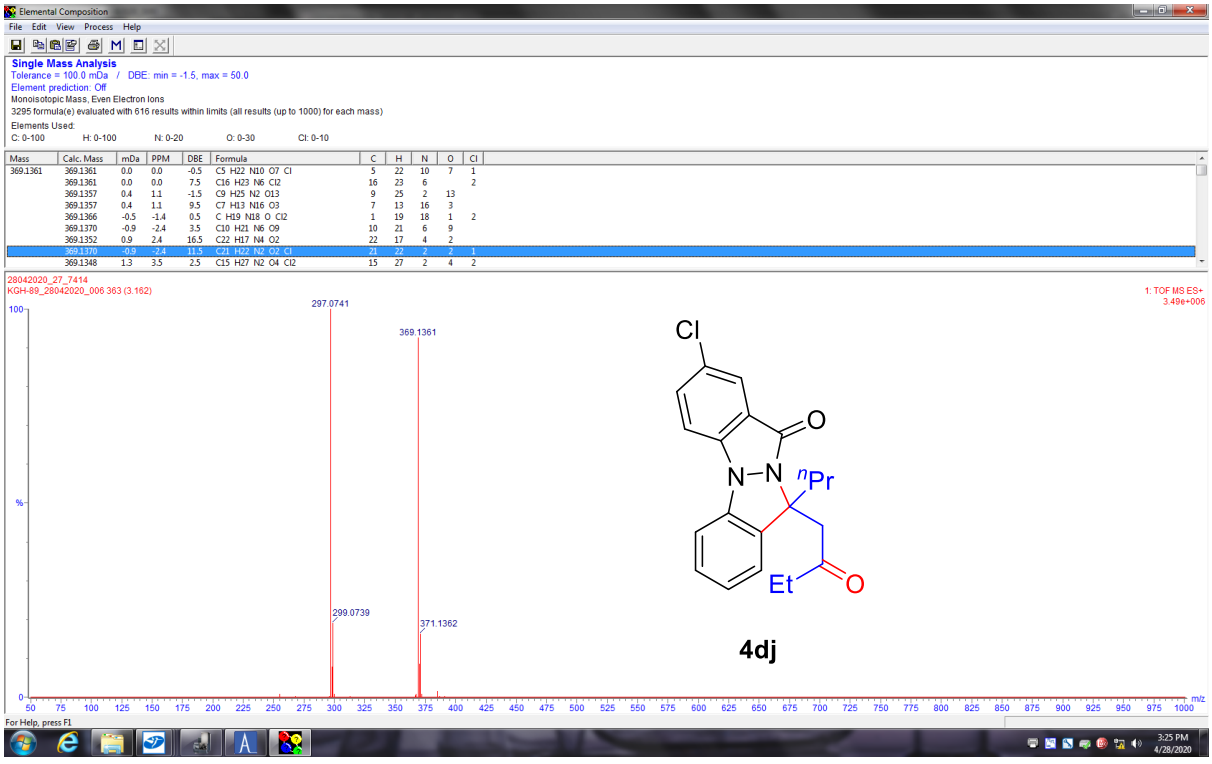

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
859 formula(e) evaluated with 188 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O
349.1920 349.1921 -0.1 -0.3 4.5 C7 H21 N14 O3 295.4 6.339 0.18 7 21 14 3
349.1916 0.4 1.1 11.5 C22 H25 N2 O2 299.8 10.773 0.00 22 25 2 2
349.1908 1.2 3.4 -0.5 C6 H25 N10 O7 297.1 8.077 0.03 6 25 10 7
349.1935 -1.5 -4.3 -1.5 C10 H29 N4 O9 298.2 9.130 0.01 10 29 4 9
349.1894 2.6 7.4 5.5 C3 H17 N20 O 291.5 2.471 8.45 3 17 20 1
349.1948 -2.8 -8.0 3.5 C11 H25 N8 O5 297.4 8.393 0.02 11 25 8 5
28042020_27_7415
KGH-90_28042020_007 407 (3.546) AM2 (Ar,30000.0,556.28,0.00,LS 1)
1: TOF MS ES+
1.67e+006
349.1920
277.1211
278.1230
350.1945
331.1771
For Help, press F1
3:27 PM
4/28/2020

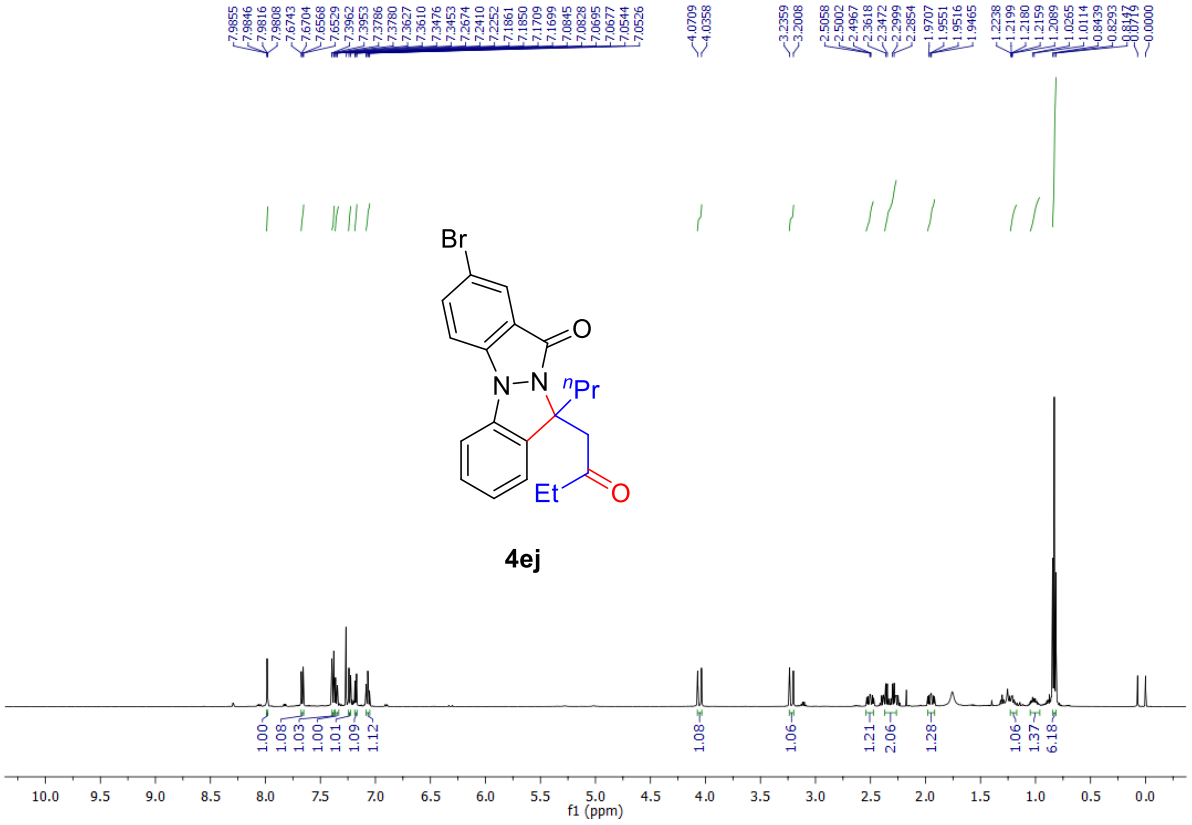
4bj

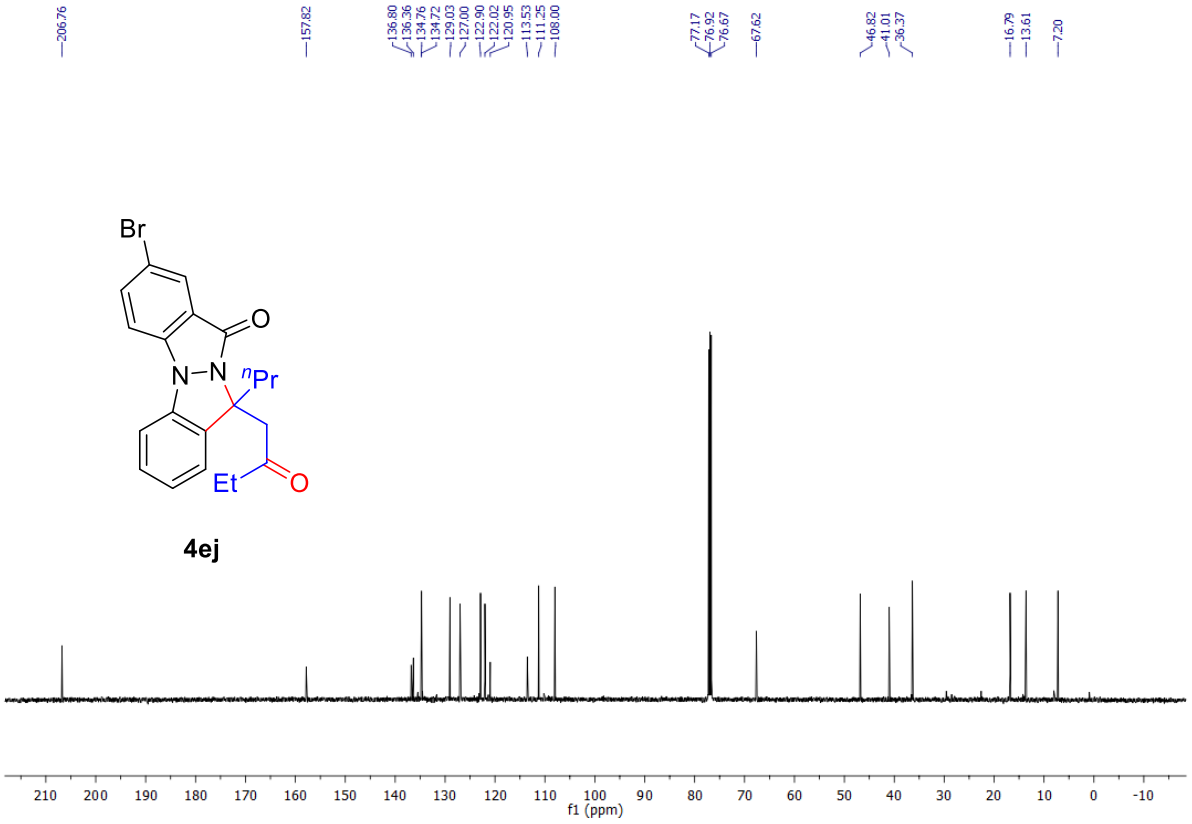


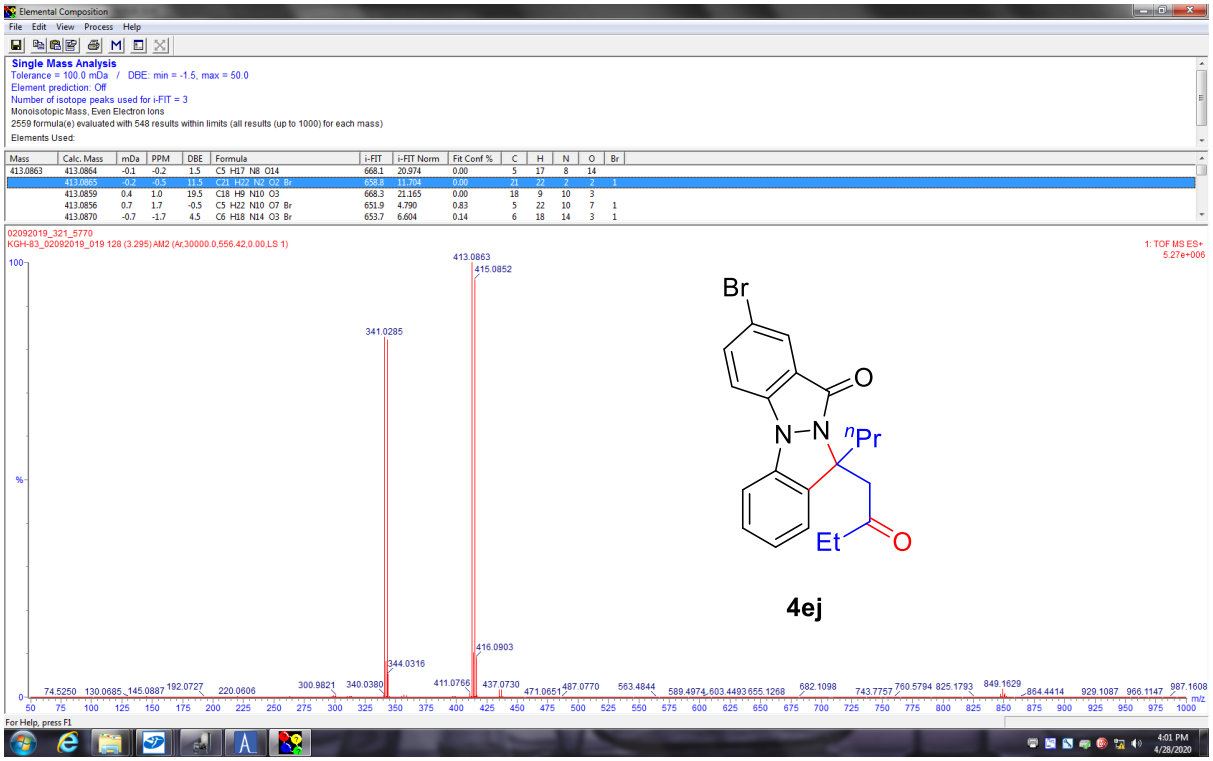
4dj

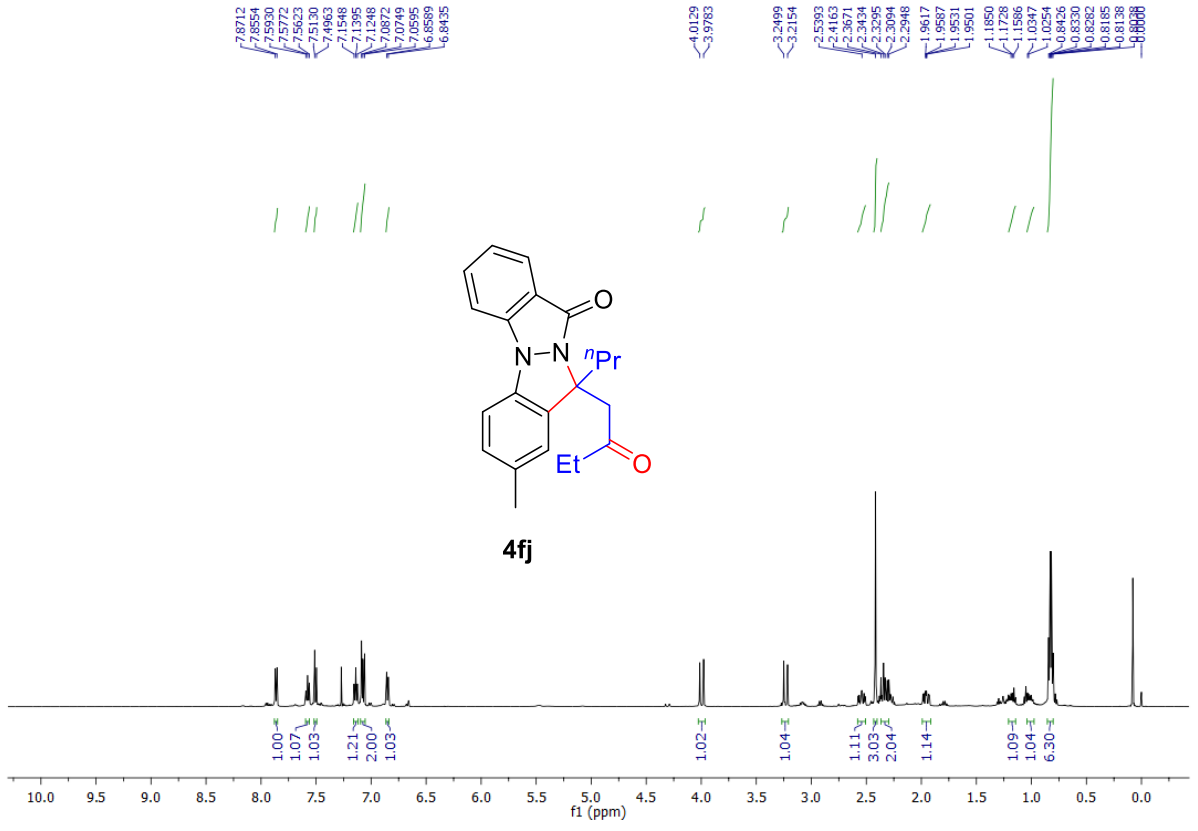

206.76
158.05
136.60
136.42
134.74
132.18
129.01
126.48
123.88
122.87
122.02
120.47
110.92
107.93
77.17
76.91
76.66
67.63
46.81
41.03
36.36
16.80
13.60
7.20
Cl
O
N–N
nPr
Et
O
4dj
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

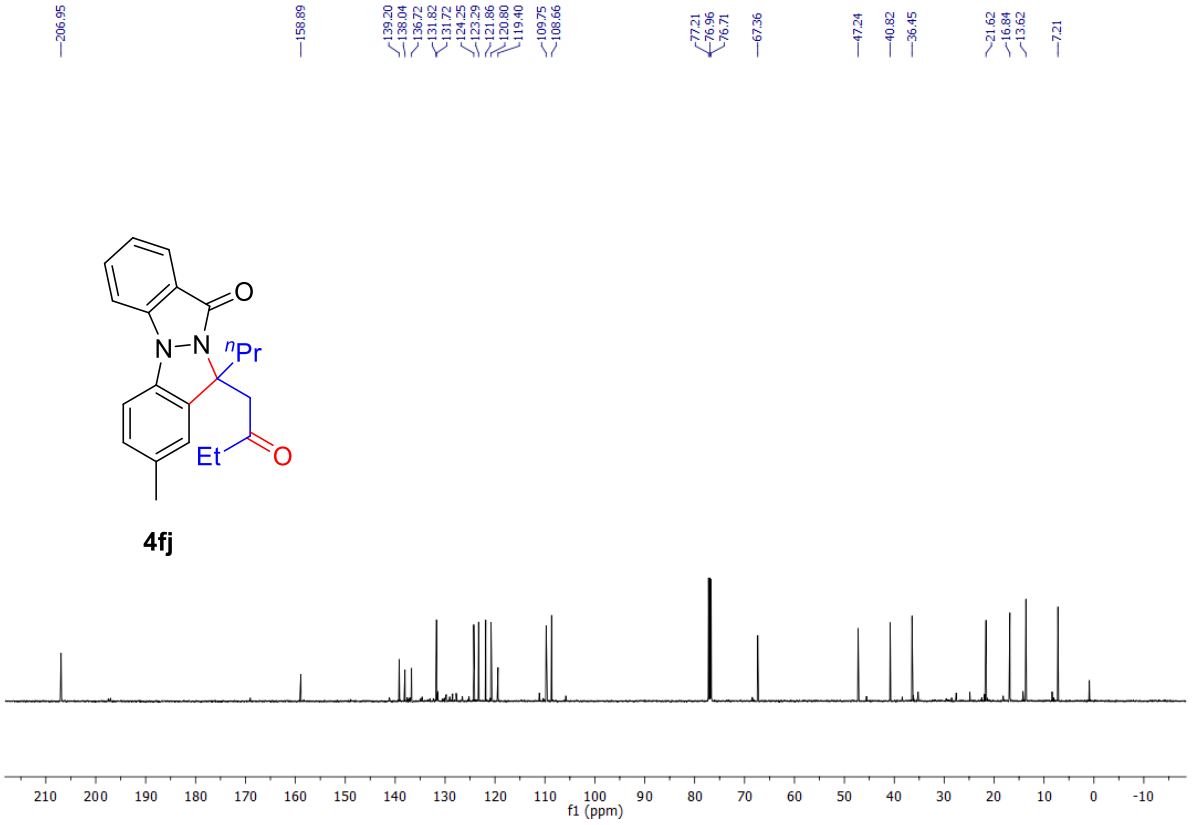

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
3295 formula(e) evaluated with 616 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-20 O: 0-30 Cl: 0-10
Mass Calc. Mass mDa PPM DBE Formula C H N O Cl
369.1361 369.1361 0.0 0.0 -0.5 C5 H22 N10 O7 Cl 5 22 10 7 1
369.1361 0.0 0.0 7.5 C16 H23 N6 Cl2 16 23 6 2
369.1357 0.4 1.1 -1.5 C9 H25 N2 O13 9 25 2 13
369.1357 0.4 1.1 9.5 C7 H13 N16 O3 7 13 16 3
369.1366 -0.5 -1.4 0.5 C H19 N18 O Cl2 1 19 18 1 2
369.1370 -0.9 -2.4 3.5 C10 H21 N6 O9 10 21 6 9
369.1352 0.9 2.4 16.5 C22 H17 N4 O2 22 17 4 2
369.1348 1.3 3.5 2.5 C15 H27 N2 O4 Cl2 15 27 2 4 2
28042020_27_7414
KGH-89_28042020_006 363 (3.162)
1: TOF MS ES+
3.49e+006
297.0741
369.1361
299.0739
371.1362
Cl
O
N–N
nPr
Et
O
4dj
m/z
For Help, press F1
3:25 PM
4/28/2020


Br
O
N–N
nPr
Et
O
4ej
f1 (ppm)

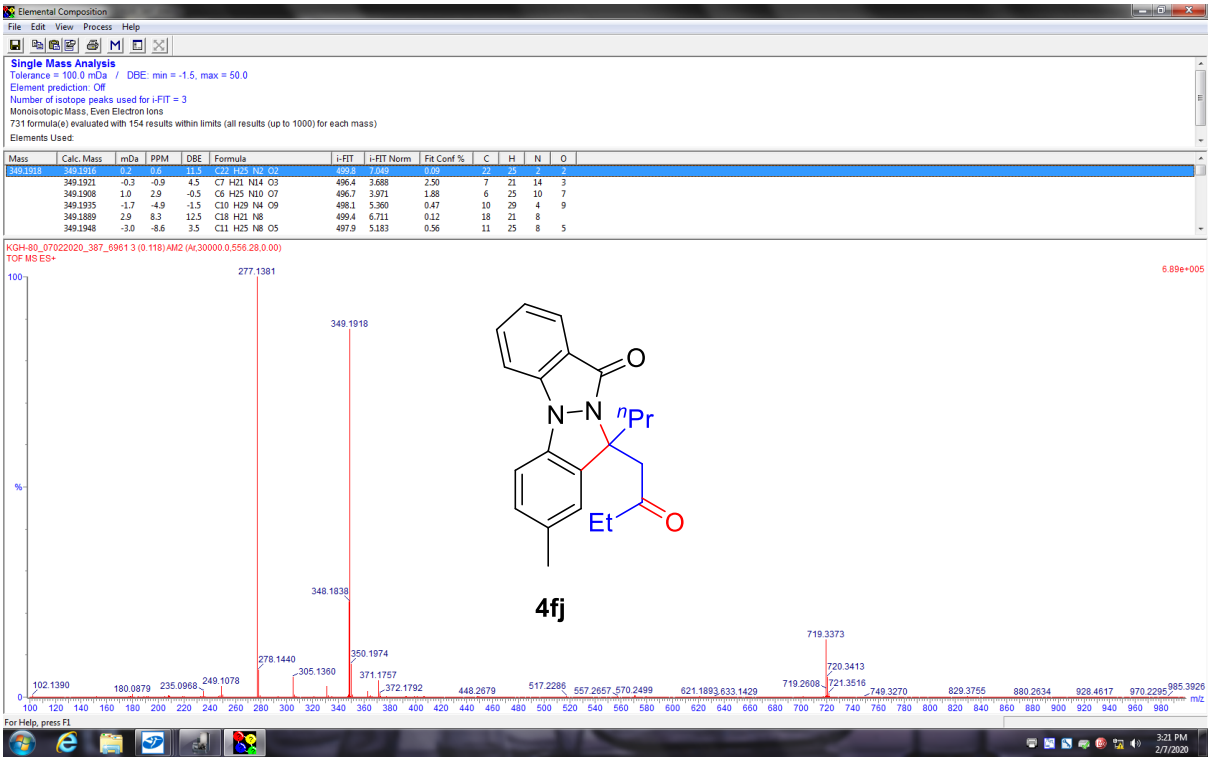

Br
O
N–N
nPr
Et
O
4ej
f1 (ppm)


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
2559 formula(e) evaluated with 548 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O Br
413.0863 413.0864 -0.1 -0.2 1.5 C5 H17 N8 O14 668.1 20.974 0.00 5 17 8 14
413.0865 -0.2 -0.5 11.5 C21 H22 N2 O2 Br 658.8 11.704 0.00 21 22 2 2 1
413.0859 0.4 1.0 19.5 C18 H9 N10 O3 668.3 21.165 0.00 18 9 10 3
413.0856 0.7 1.7 -0.5 C5 H22 N10 O7 Br 651.9 4.790 0.83 5 22 10 7 1
413.0870 -0.7 -1.7 4.5 C6 H18 N14 O3 Br 653.7 6.604 0.14 6 18 14 3 1
02092019_321_5770
KGH-83_02092019_019 128 (3.295) AM2 (Ar,30000.0,556.42,0.00,LS 1)
1: TOF MS ES+
5.27e+006
413.0863
415.0852
341.0285
416.0903
344.0316
Br
O
N–N
nPr
Et
O
4ej
For Help, press F1
4:01 PM
4/28/2020

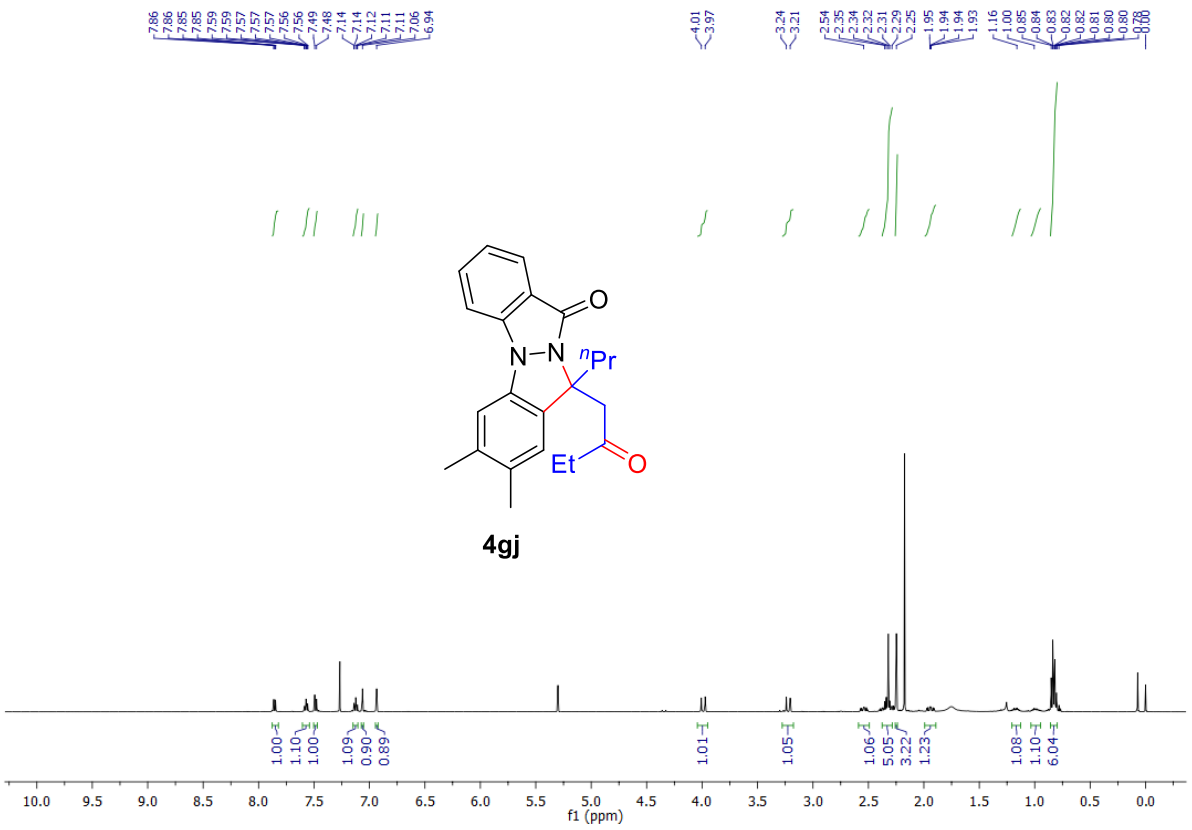

7.8712
7.8554
7.5930
7.5772
7.5623
7.5130
7.4963
7.1548
7.1395
7.1248
7.0872
7.0749
7.0595
6.8589
6.8435
4.0129
3.9783
3.2499
3.2154
2.5393
2.4163
2.3671
2.3434
2.3295
2.3094
2.2948
1.9617
1.9587
1.9531
1.9501
1.1850
1.1728
1.1586
1.0347
1.0254
0.8426
0.8330
0.8282
0.8185
0.8138
O
N–N
nPr
Et
O
4fj
1.00
1.07
1.03
1.21
2.00
1.03
1.02
1.04
1.11
3.03
2.04
1.14
1.09
1.04
6.30
f1 (ppm)

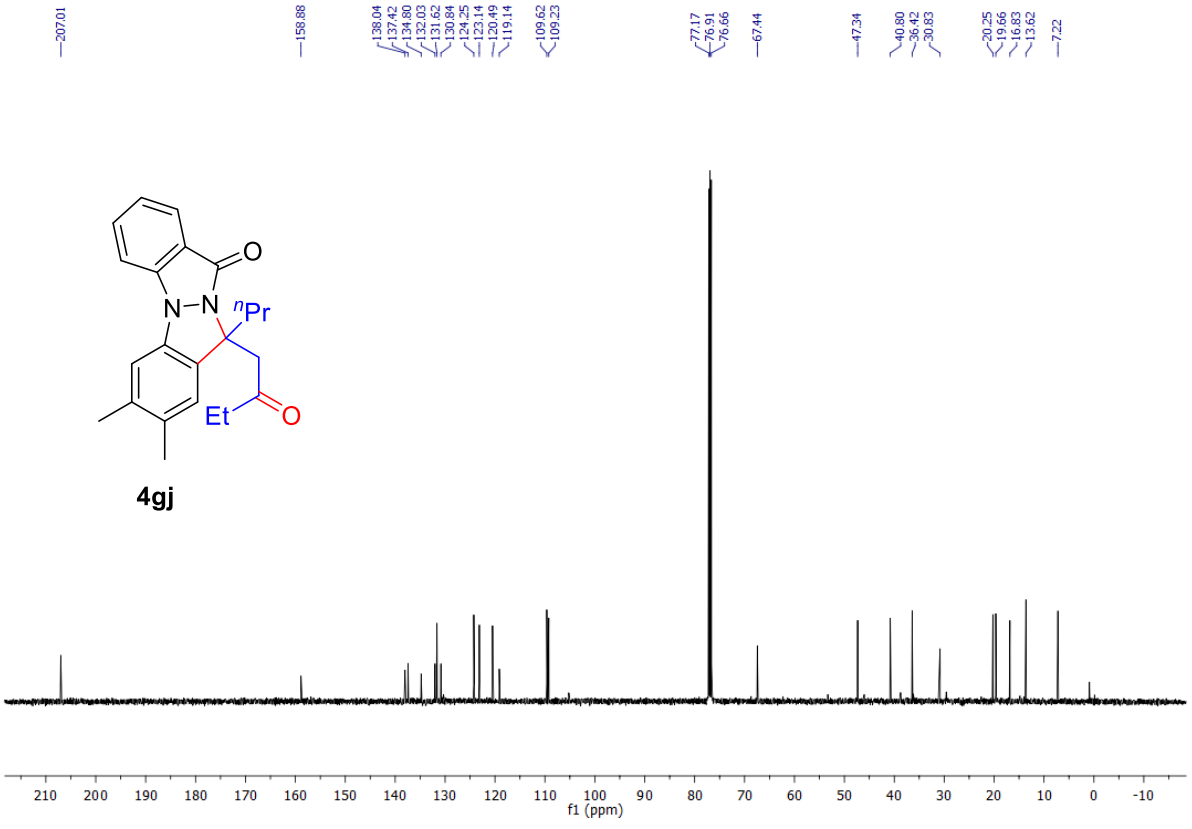

206.95
158.89
139.20
138.04
136.72
131.82
131.72
124.25
123.29
121.86
120.80
119.40
109.75
108.66
77.21
76.96
76.71
67.36
47.24
40.82
36.45
21.62
16.84
13.62
7.21
O
N–N
nPr
Et
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

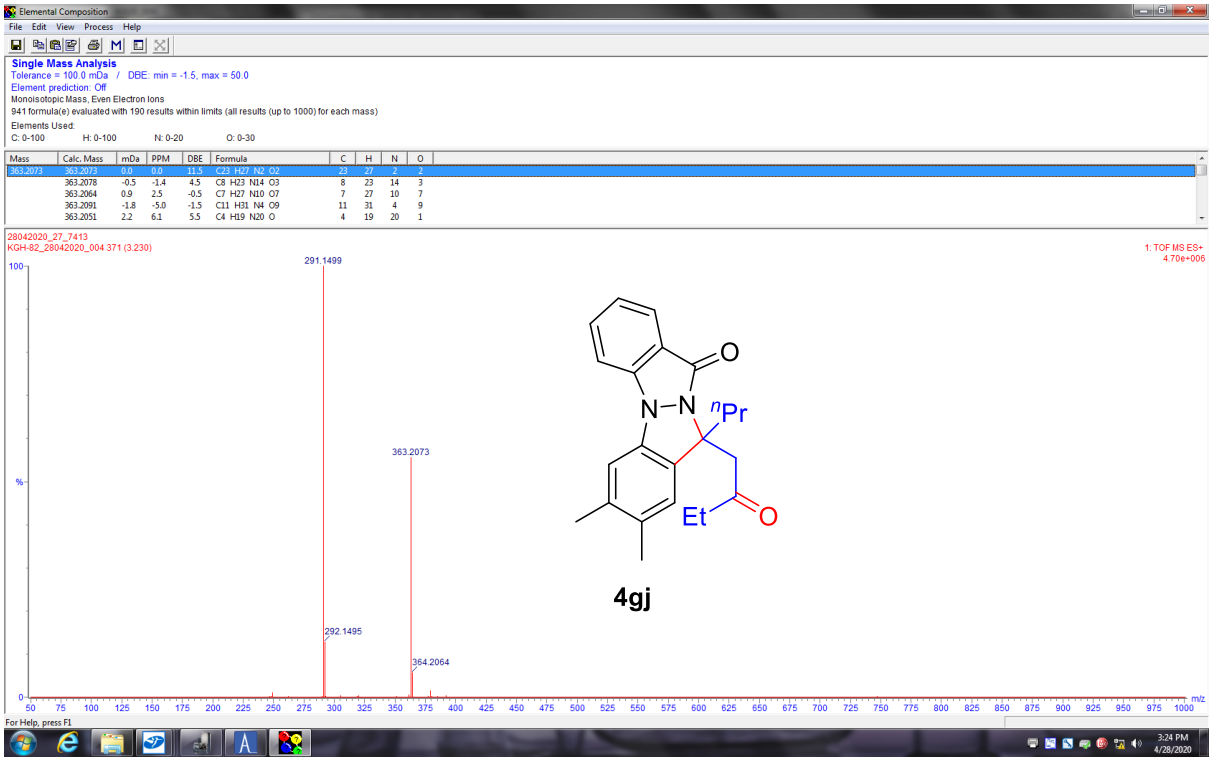
4fj

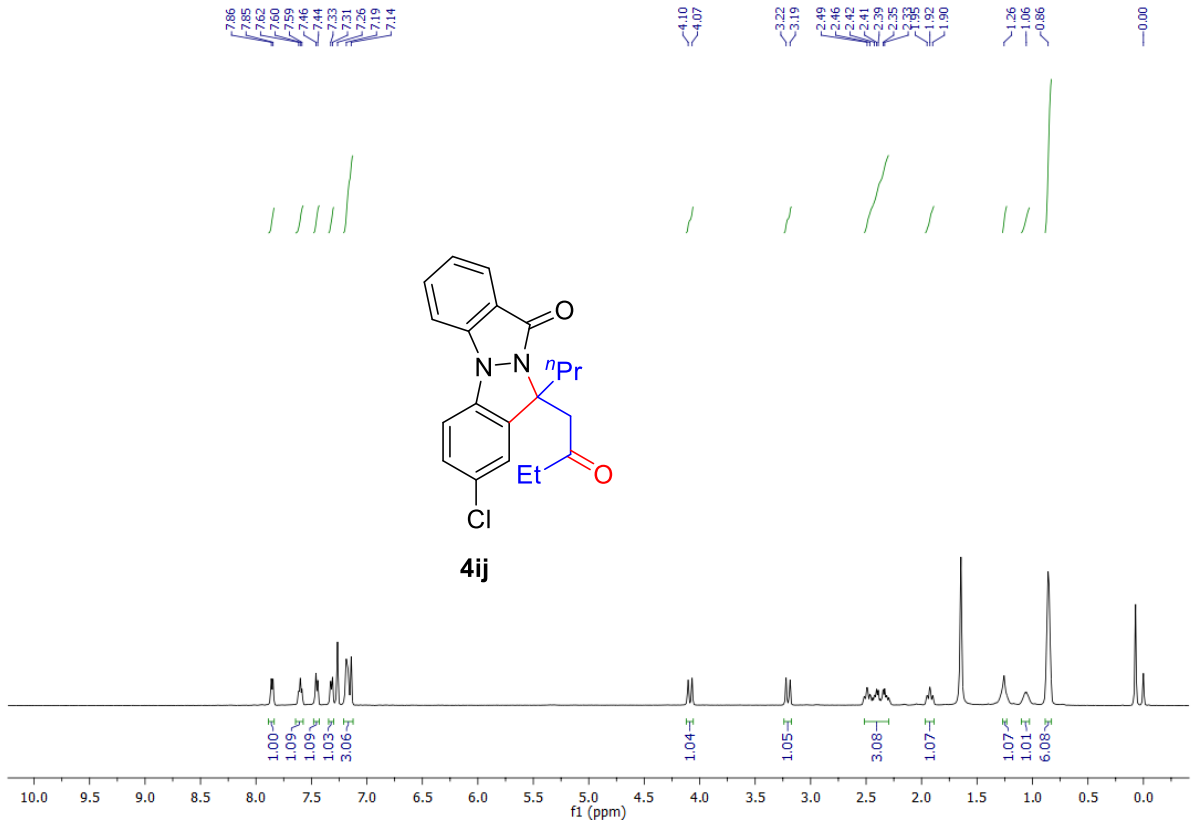

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
731 formula(e) evaluated with 154 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O
349.1918 349.1916 0.2 0.6 11.5 C22 H25 N2 O2 499.8 7.049 0.09 22 25 2 2
349.1921 -0.3 -0.9 4.5 C7 H21 N14 O3 496.4 3.688 2.50 7 21 14 3
349.1908 1.0 2.9 -0.5 C6 H25 N10 O7 496.7 3.971 1.88 6 25 10 7
349.1935 -1.7 -4.9 -1.5 C10 H29 N4 O9 498.1 5.360 0.47 10 29 4 9
349.1889 2.9 8.3 12.5 C18 H21 N8 499.4 6.711 0.12 18 21 8
349.1948 -3.0 -8.6 3.5 C11 H25 N8 O5 497.9 5.183 0.56 11 25 8 5
KGH-80_07022020_387_6961 3 (0.118) AM2 (Ar,30000.0,556.28,0.00)
TOF MS ES+
6.89e+005
277.1381
349.1918
348.1838
278.1440
350.1974
305.1360
371.1757
372.1792
102.1390
180.0879
235.0968
249.1078
448.2679
517.2286
557.2657
570.2499
621.1893
633.1429
719.2608
719.3373
720.3413
721.3516
749.3270
829.3755
880.2634
928.4617
970.2295
985.3926
m/z
For Help, press F1
3:21 PM
2/7/2020

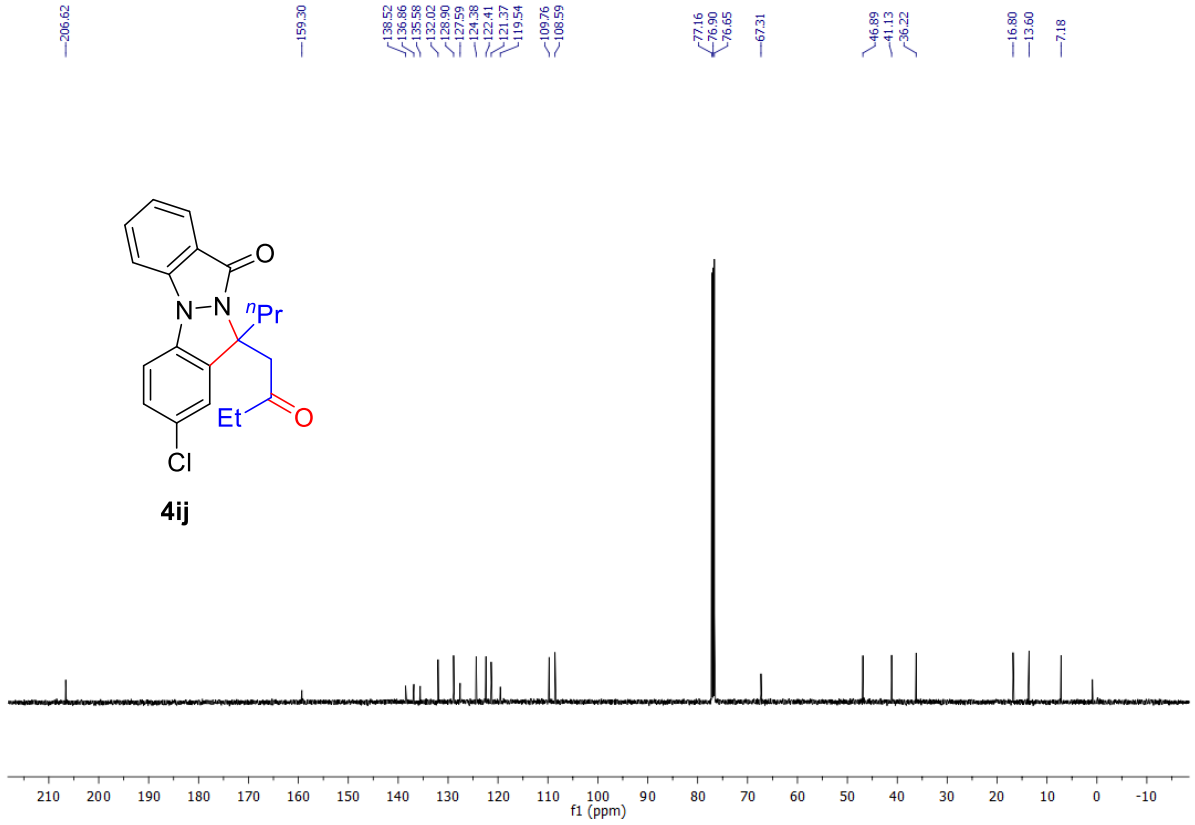
4fj

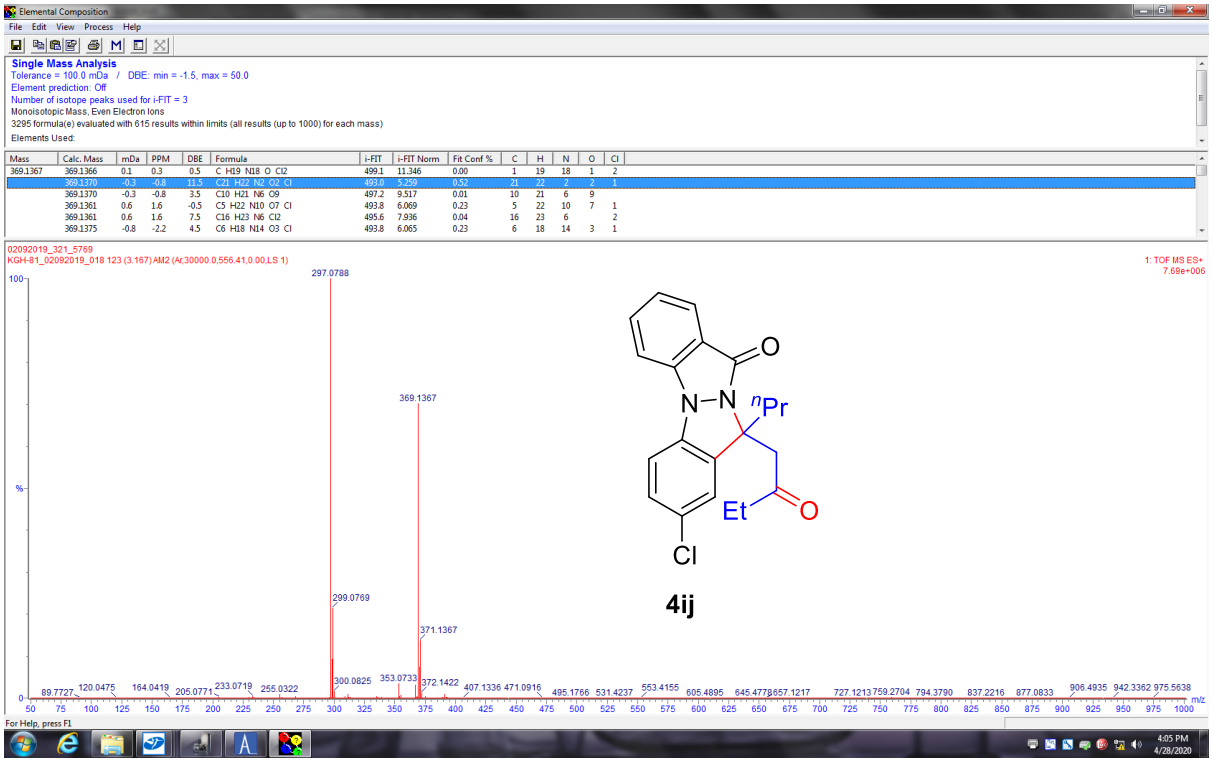

7.86
7.86
7.85
7.85
7.59
7.59
7.57
7.57
7.57
7.56
7.56
7.49
7.48
7.14
7.14
7.12
7.11
7.11
7.06
6.94
4.01
3.97
3.24
3.21
2.54
2.35
2.34
2.32
2.31
2.29
2.25
1.95
1.94
1.94
1.93
1.16
1.00
0.85
0.84
0.83
0.82
0.82
0.81
0.80
0.80
0.78
0.00
O
N–N
nPr
Et
O
4gj
1.00
1.10
1.00
1.09
0.90
0.89
1.01
1.05
1.06
5.05
3.22
1.23
1.08
1.10
6.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

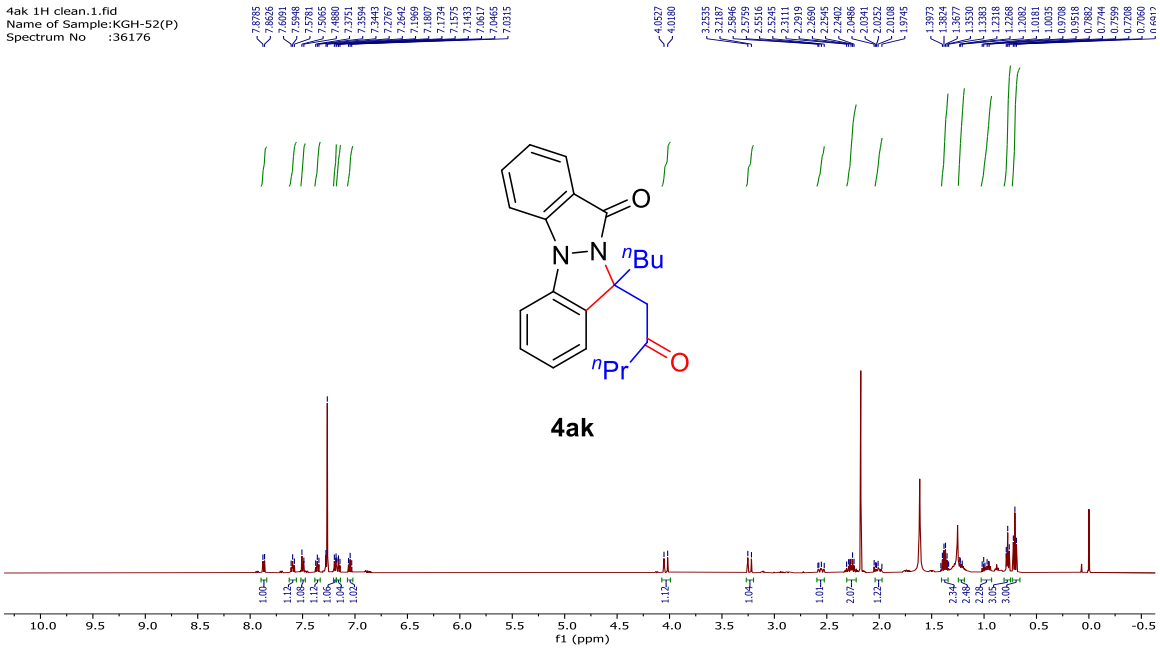

207.01
158.88
138.04
137.42
134.80
132.03
131.62
130.84
124.25
123.14
120.49
119.14
109.62
109.23
77.17
76.91
76.66
67.44
47.34
40.80
36.42
30.83
20.25
19.66
16.83
13.62
7.22
O
N–N
nPr
Et
O
4gj
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

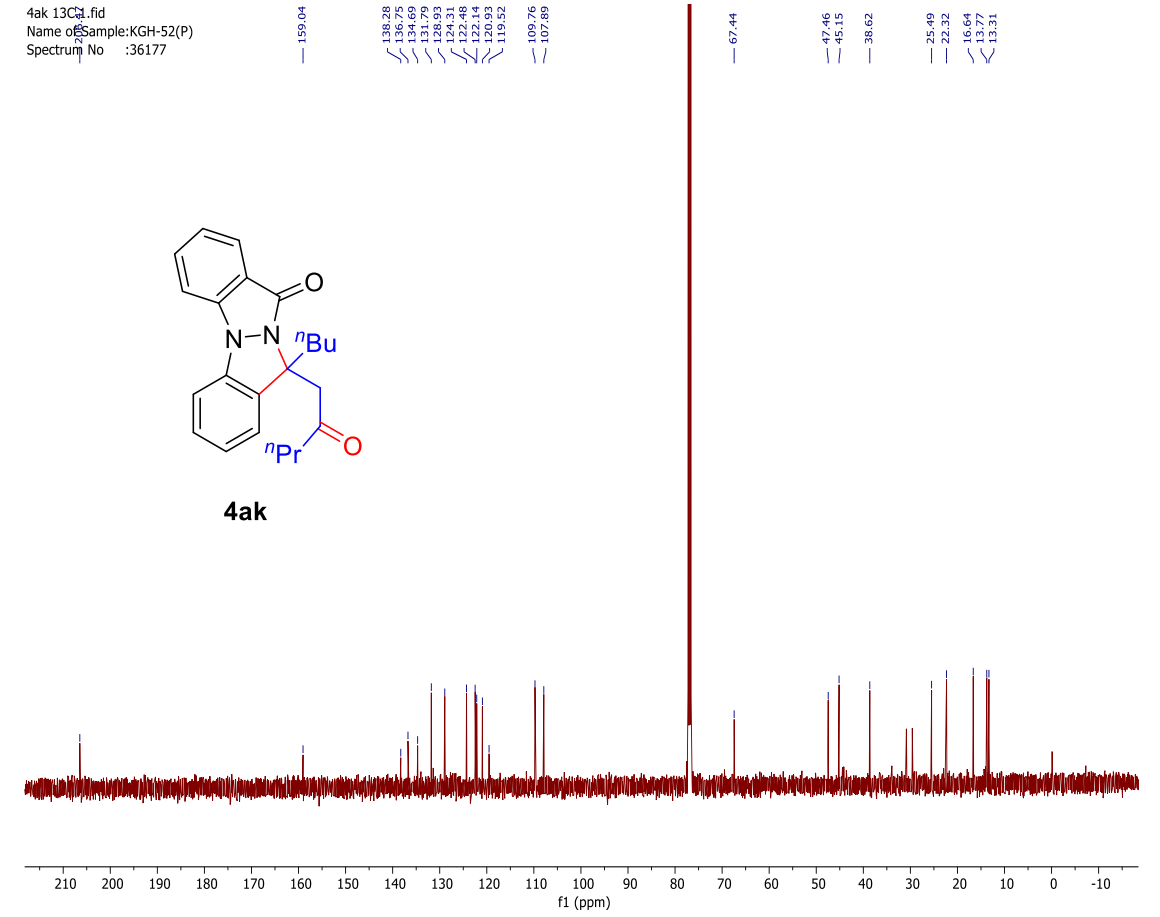

Elemental Composition
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
941 formula(e) evaluated with 190 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-100 H: 0-100 N: 0-20 O: 0-30
Mass Calc. Mass mDa PPM DBE Formula C H N O
363.2073 363.2073 0.0 0.0 11.5 C23 H27 N2 O2 23 27 2 2
363.2078 -0.5 -1.4 4.5 C8 H23 N14 O3 8 23 14 3
363.2064 0.9 2.5 -0.5 C7 H27 N10 O7 7 27 10 7
363.2091 -1.8 -5.0 -1.5 C11 H31 N4 O9 11 31 4 9
363.2051 2.2 6.1 5.5 C4 H19 N20 O 4 19 20 1
28042020_27_7413
KGH-82_28042020_004 371 (3.230)
1: TOF MS ES+
4.70e+006
291.1499
363.2073
292.1495
364.2064
4gj

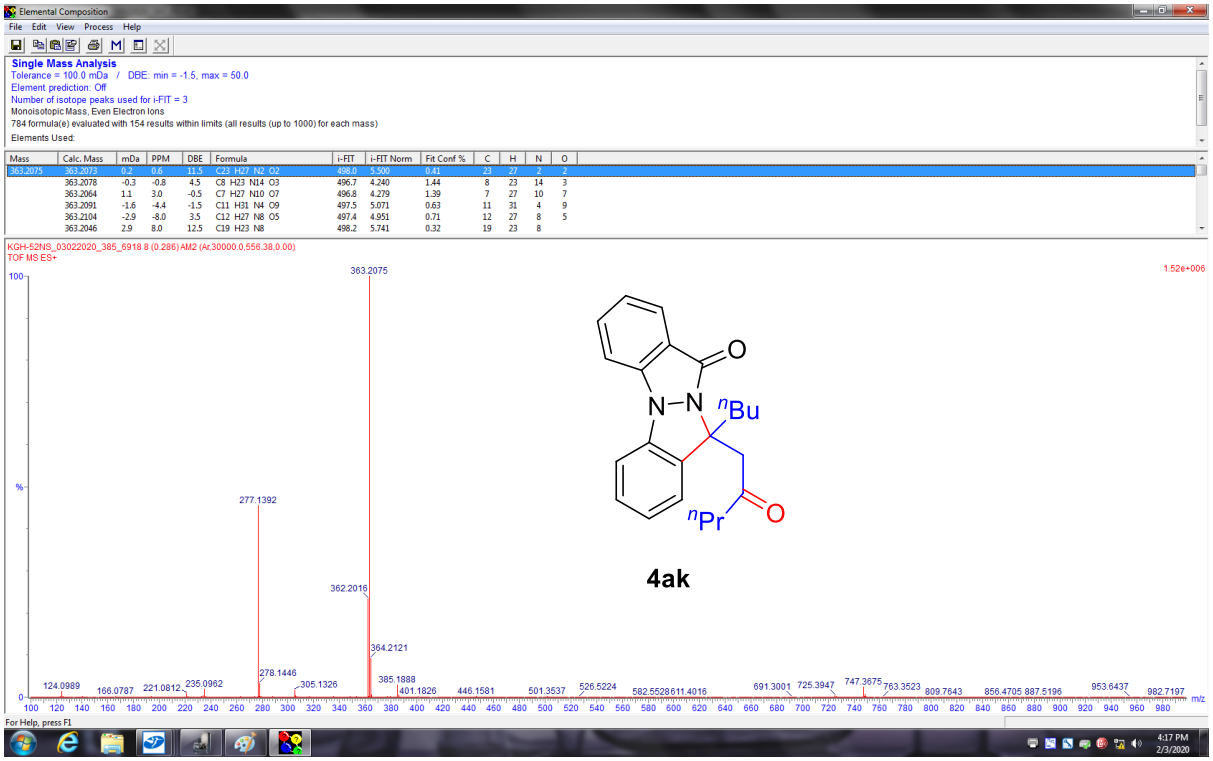

4ij
f1 (ppm)

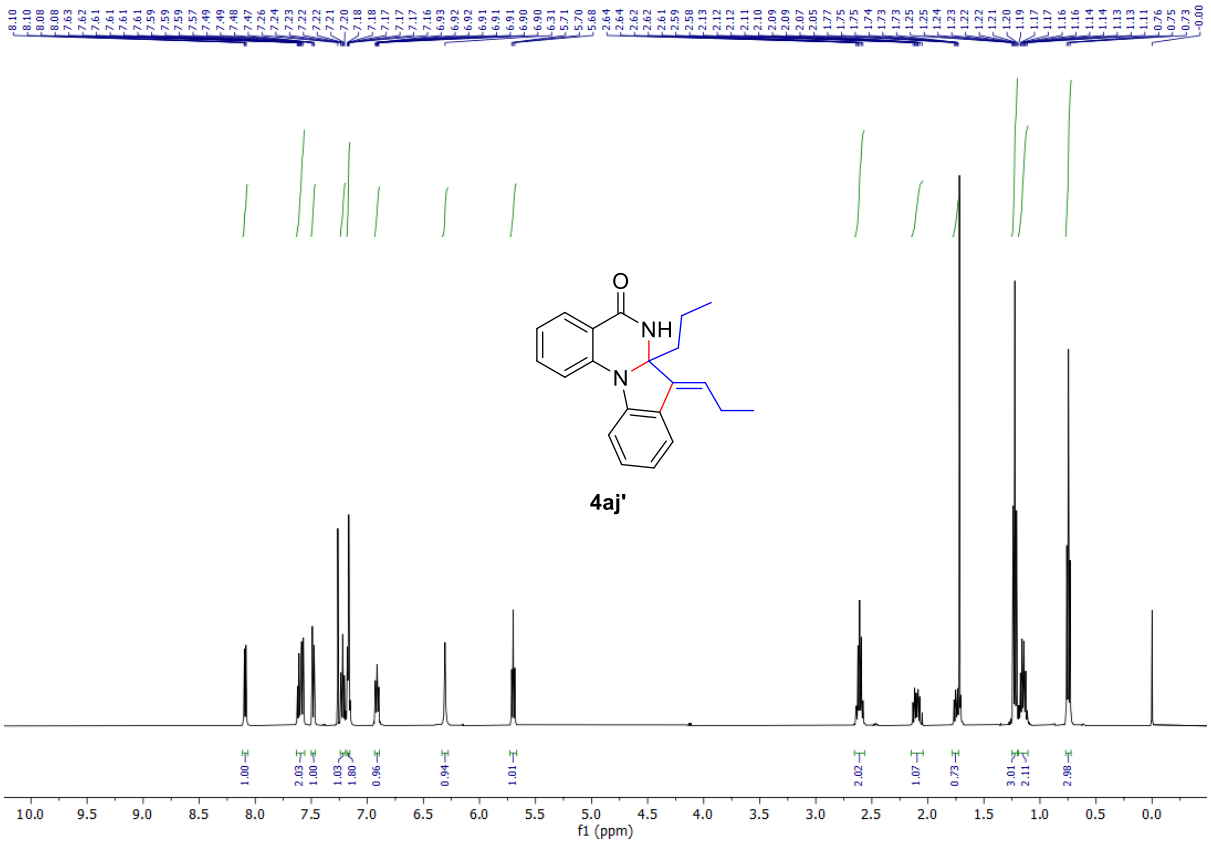

206.62
159.30
138.52
136.86
135.58
132.02
128.90
127.59
124.38
122.41
121.37
119.54
109.76
108.59
77.16
76.90
76.65
67.31
46.89
41.13
36.22
16.80
13.60
7.18
O
N–N
nPr
Et
O
Cl
4ij
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

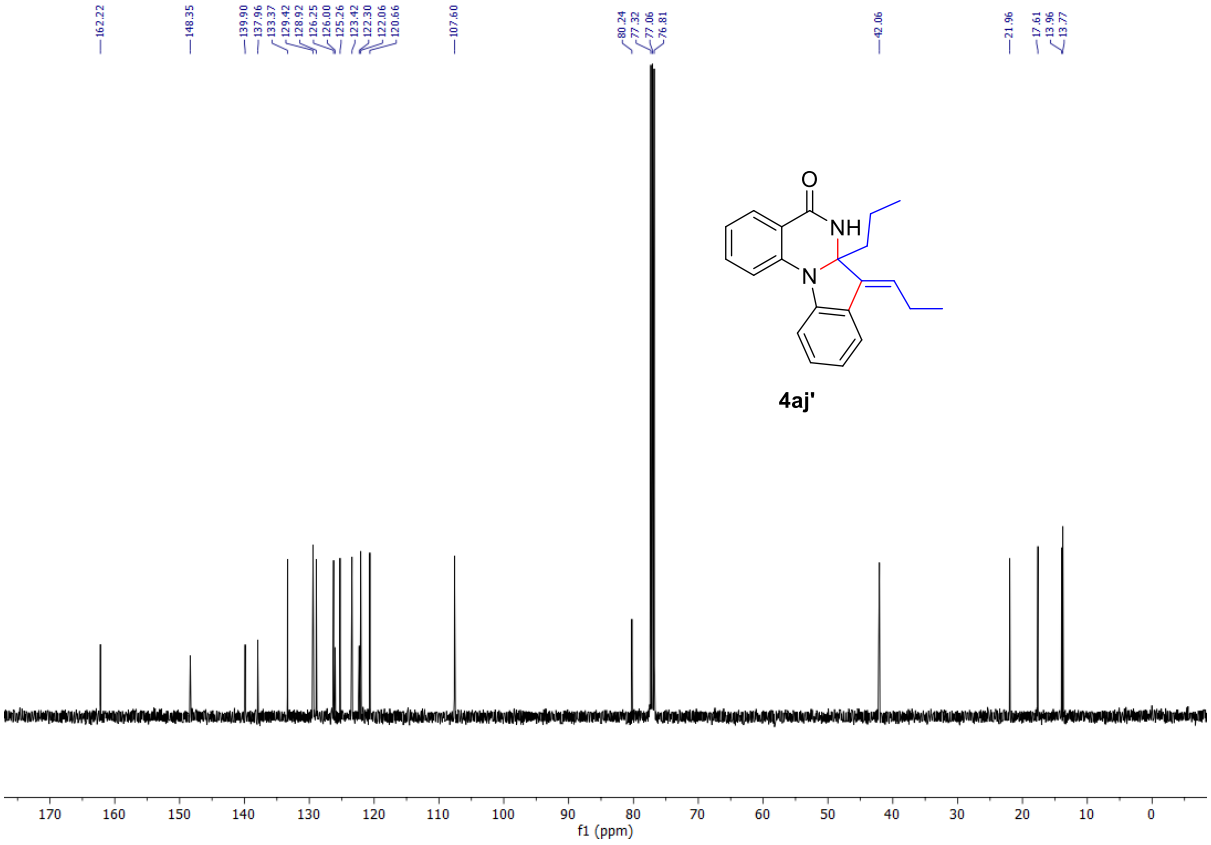

Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
3295 formula(e) evaluated with 615 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O Cl
369.1367 369.1366 0.1 0.3 0.5 C H19 N18 O Cl2 499.1 11.346 0.00 1 19 18 1 2
369.1370 -0.3 -0.8 11.5 C21 H22 N2 O3 Cl 493.8 9.252 0.52 21 22 2 3 1
369.1370 -0.3 -0.8 3.5 C10 H21 N6 O9 497.2 9.517 0.01 10 21 6 9
369.1361 0.6 1.6 -0.5 C5 H22 N10 O7 Cl 493.8 6.069 0.23 5 22 10 7 1
369.1361 0.6 1.6 7.5 C16 H23 N6 Cl2 495.6 7.936 0.04 16 23 6 2
369.1375 -0.8 -2.2 4.5 C6 H18 N14 O3 Cl 493.8 6.065 0.23 6 18 14 3 1
02092019_321_5769
KGH-81_02092019_018 123 (3.167) AM2 (Ar,30000.0,556.41,0.00,LS 1)
1: TOF MS ES+
7.69e+006
100
%
0
297.0788
369.1367
299.0769
371.1367
89.7727 120.0475 164.0419 205.0771 233.0719 255.0322 300.0825 353.0733 372.1422 407.1336 471.0918 495.1766 531.4237 553.4155 605.4895 645.4778 657.1217 727.1213 759.2704 794.3790 837.2216 877.0833 906.4935 942.3362 975.5638
50 75 100 125 150 175 200 225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725 750 775 800 825 850 875 900 925 950 975 1000
m/z
For Help, press F1
O
N–N
nPr
Et
O
Cl
4ij
4:05 PM
4/28/2020


4ak 1H clean.1.fid
Name of Sample:KGH-52(P)
Spectrum No :36176
O
N–N
nBu
nPr
O
4ak
f1 (ppm)

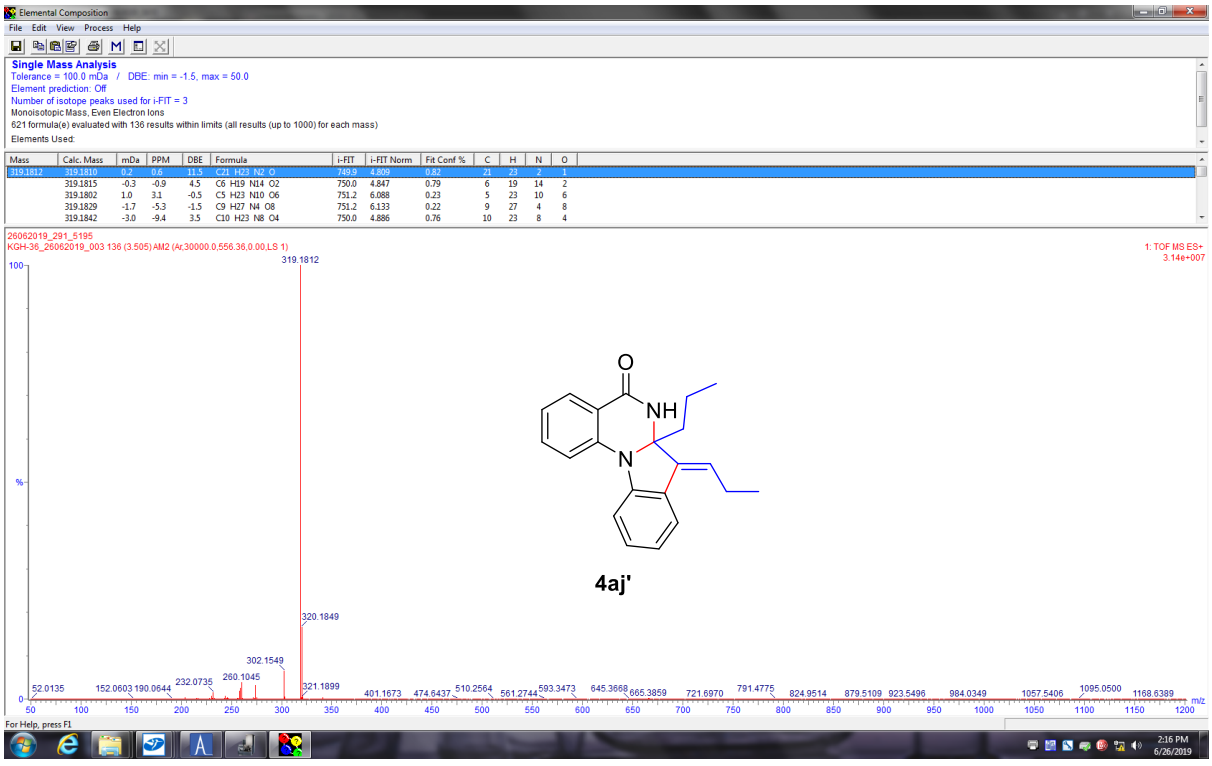

4ak 13C1.fid
Name of Sample:KGH-52(P)
Spectrum No :36177
159.04
138.28
136.75
134.69
131.79
128.93
124.31
122.48
122.14
120.93
119.52
109.76
107.89
67.44
47.46
45.15
38.62
25.49
22.32
16.64
13.77
13.31
O
N–N
nBu
nPr
O
4ak
f1 (ppm)


Elemental Composition
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
784 formula(e) evaluated with 154 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O
363.2075 363.2073 0.2 0.6 11.5 C23 H27 N2 O2 498.0 5.500 0.41 23 27 2 2
363.2078 -0.3 -0.8 4.5 C8 H23 N14 O3 496.7 4.240 1.44 8 23 14 3
363.2064 1.1 3.0 -0.5 C7 H27 N10 O7 496.8 4.279 1.39 7 27 10 7
363.2091 -1.6 -4.4 -1.5 C11 H31 N4 O9 497.5 5.071 0.63 11 31 4 9
363.2104 -2.9 -8.0 3.5 C12 H27 N8 O5 497.4 4.951 0.71 12 27 8 5
363.2046 2.9 8.0 12.5 C19 H23 N8 498.2 5.741 0.32 19 23 8
KGH-52NS_03022020_385_6918 8 (0.286) AM2 (Ar,30000.0,556.38,0.00)
TOF MS ES+
1.52e+006
363.2075
277.1392
362.2016
364.2121
278.1446
385.1888
4ak

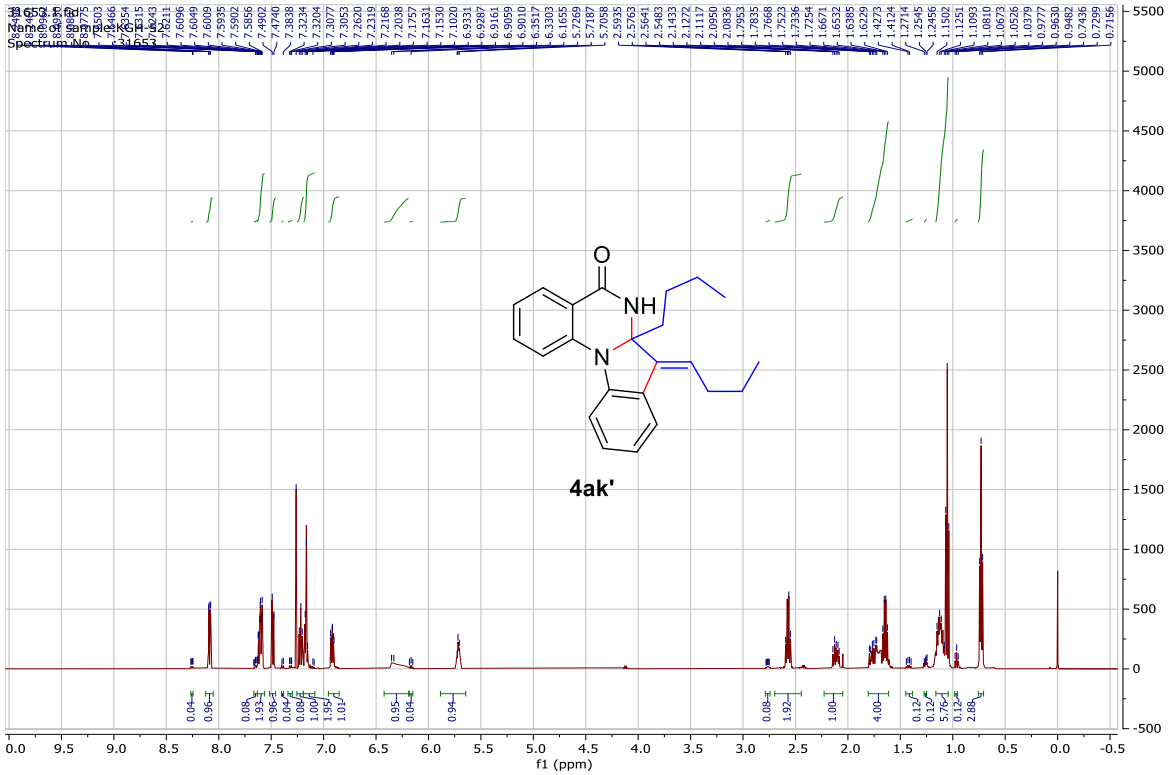

4aj'
f1 (ppm)

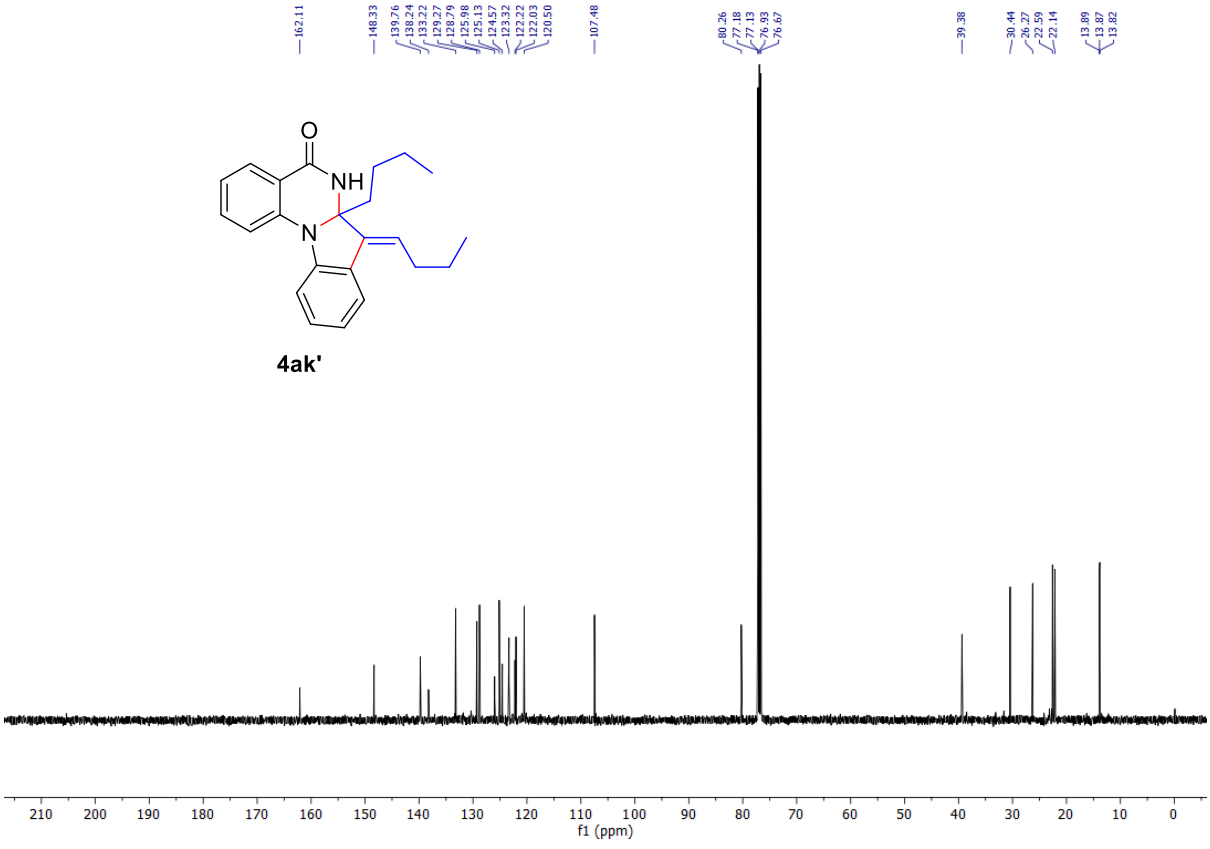

162.22
148.35
139.90
137.96
133.37
129.42
128.92
126.25
126.00
125.26
123.42
122.30
122.06
120.66
107.60
80.24
77.32
77.06
76.81
42.06
21.96
17.61
13.96
13.77
O
NH
N
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

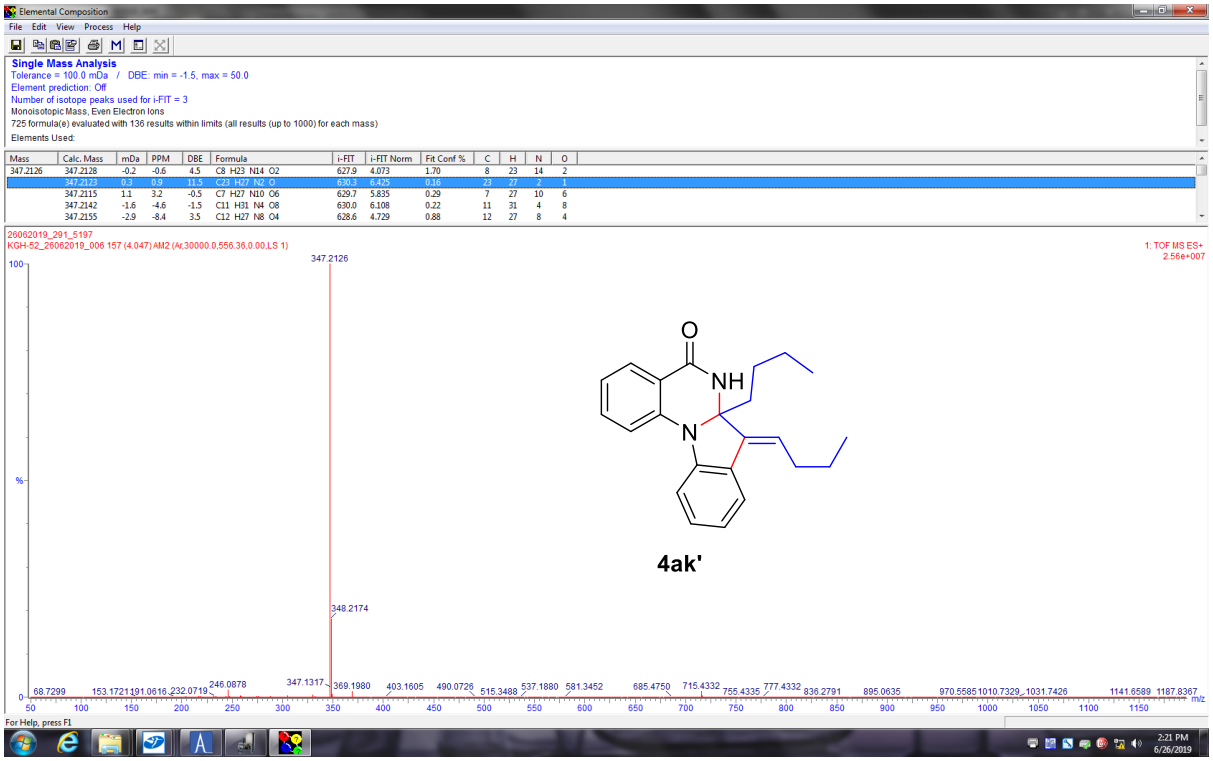
4aj'


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
621 formula(e) evaluated with 136 results within limits (all results (up to 1000) for each mass)
Elements Used:
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O
319.1812 319.1810 0.2 0.6 11.5 C21 H23 N2 O 769.3 4.203 0.82 21 23 2 1
319.1815 -0.3 -0.9 4.5 C6 H19 N14 O2 750.0 4.847 0.79 6 19 14 2
319.1802 1.0 3.1 -0.5 C5 H23 N10 O6 751.2 6.088 0.23 5 23 10 6
319.1829 -1.7 -5.3 -1.5 C9 H27 N4 O8 751.2 6.133 0.22 9 27 4 8
319.1842 -3.0 -9.4 3.5 C10 H23 N8 O4 750.0 4.886 0.76 10 23 8 4
26062019_291_5195
KGH-36_26062019_003 136 (3.505) AM2 (Ar,30000.0,556.36,0.00,LS 1)
1: TOF MS ES+
3.14e+007
319.1812
320.1849
302.1549
260.1045
232.0735
321.1899
52.0135
152.0603
190.0644
401.1673
474.6437
510.2564
561.2744
593.3473
645.3668
665.3859
721.6970
791.4775
824.9514
879.5109
923.5496
984.0349
1057.5406
1095.0500
1168.6389
m/z
For Help, press F1
2:16 PM
6/26/2019

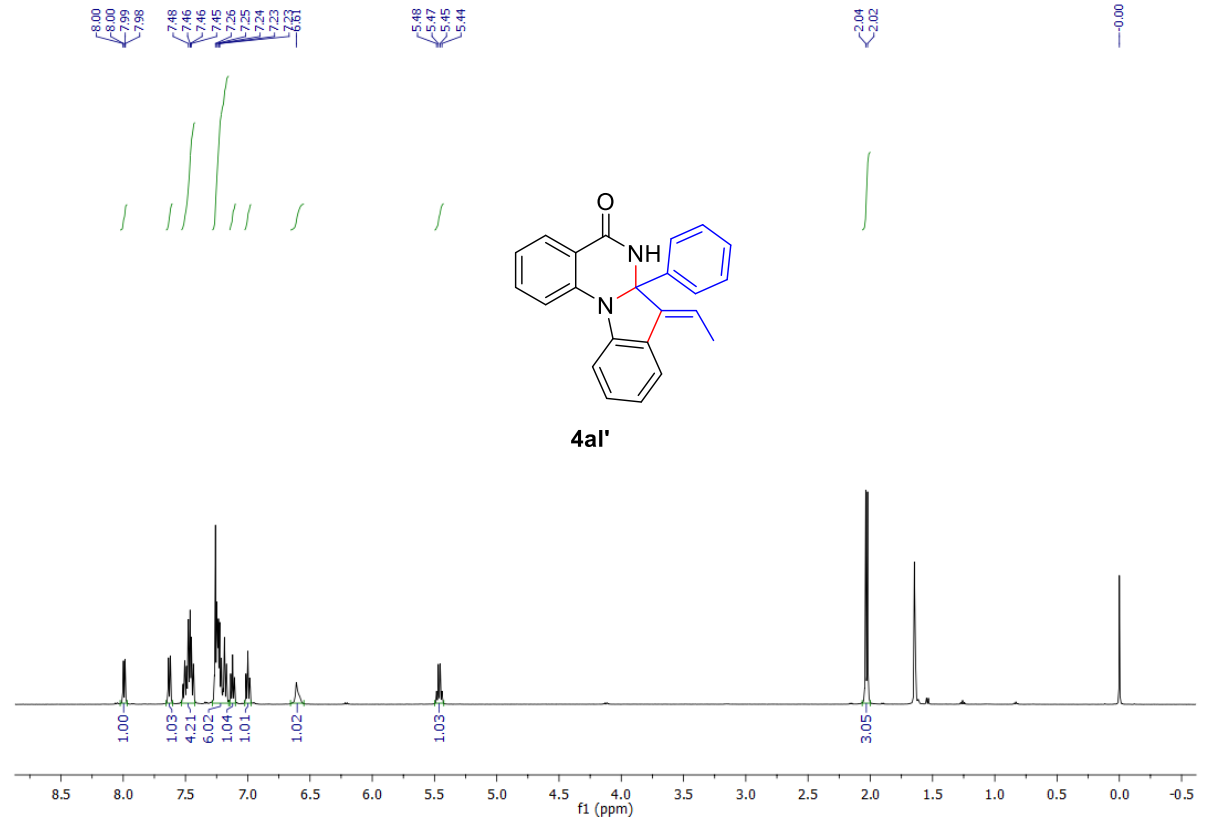
4aj'


Name of sample: KCH-52
Spectrum No. : 31653
O
NH
N
4ak'
f1 (ppm)

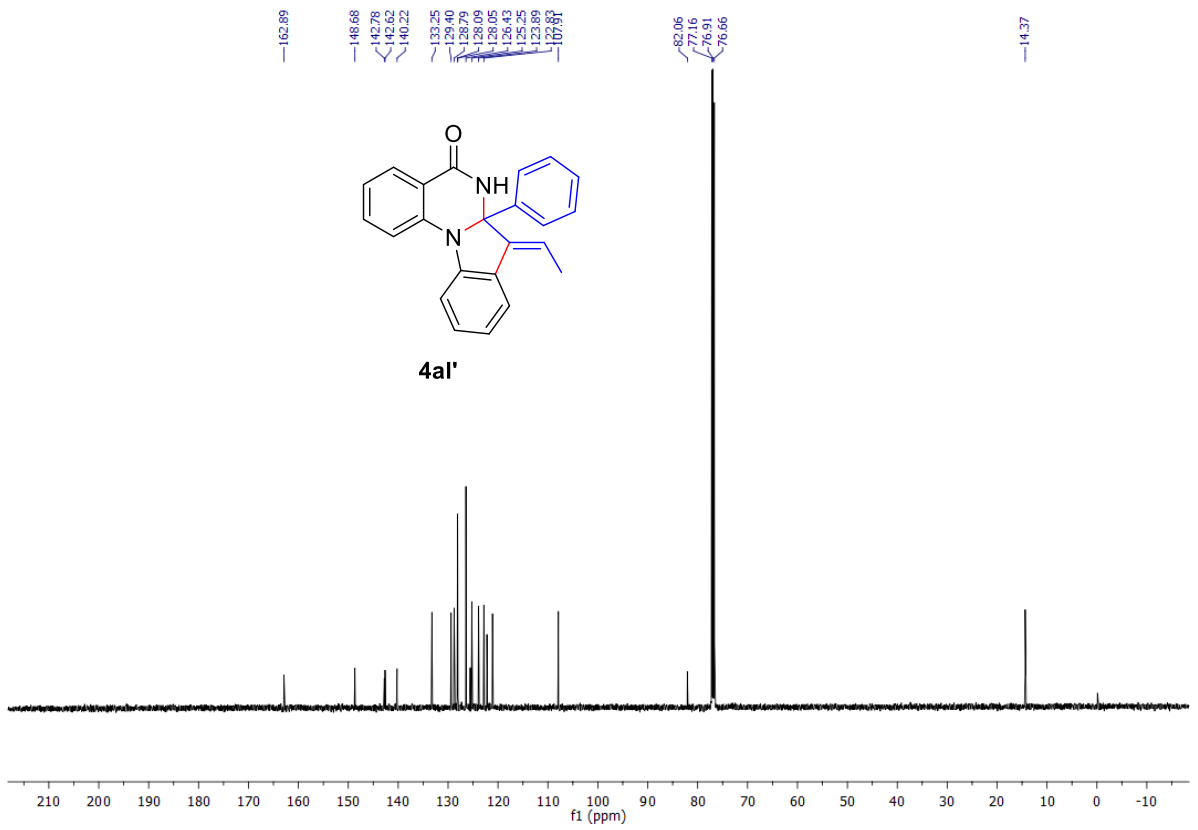

162.11
148.33
139.76
138.24
133.22
129.27
128.79
125.98
125.13
124.57
123.32
122.22
122.03
120.50
107.48
80.26
77.18
77.13
76.93
76.67
39.38
30.44
26.27
22.59
22.14
13.89
13.87
13.82
O
NH
N
4ak'
f1 (ppm)

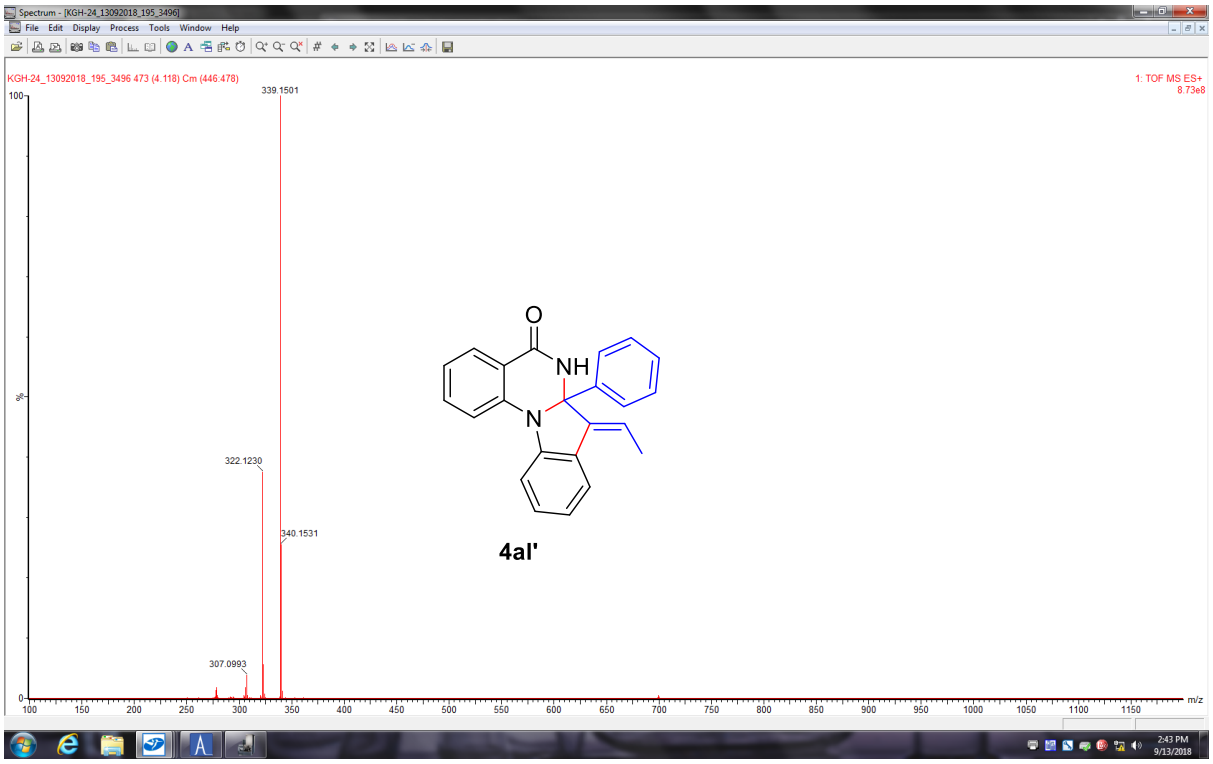

Elemental Composition
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
725 formula(e) evaluated with 136 results within limits (all results (up to 1000) for each mass)
Elements Used:
347.2126
348.2174
1: TOF MS ES+
2.56e+007

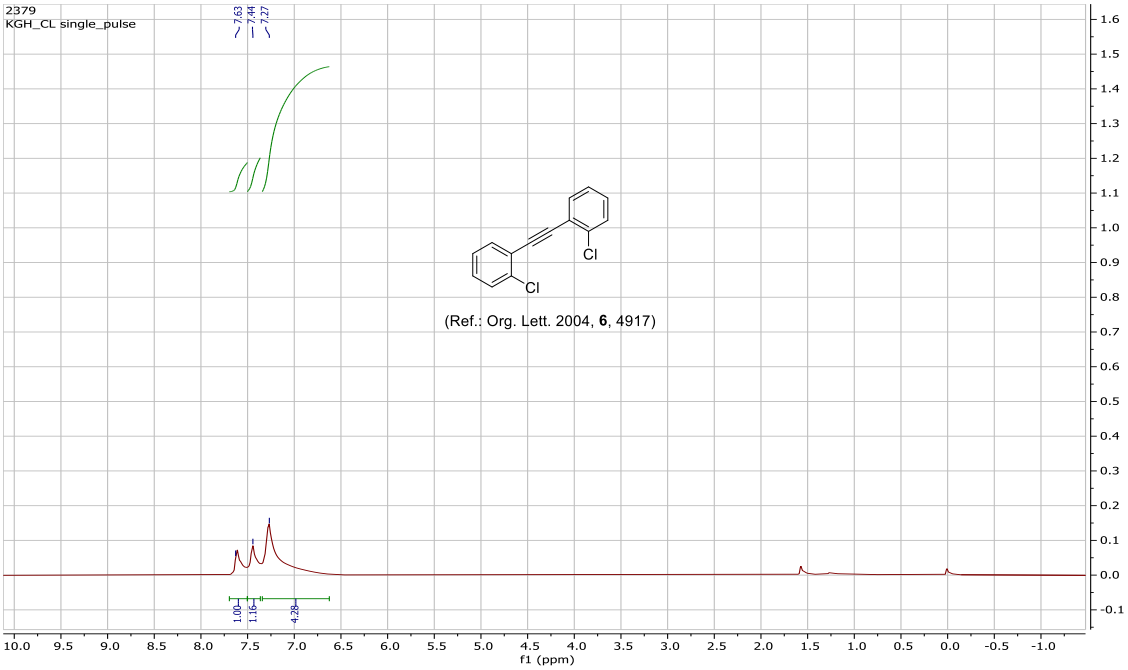
4ak'

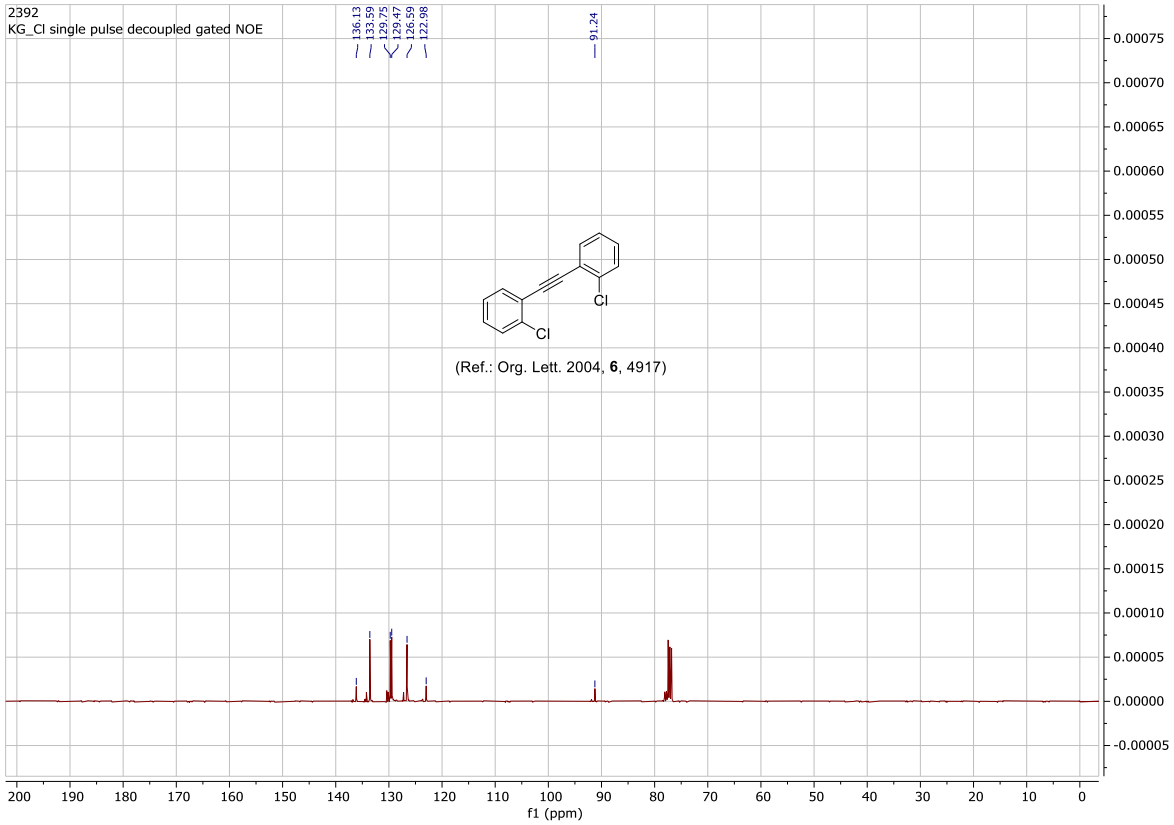


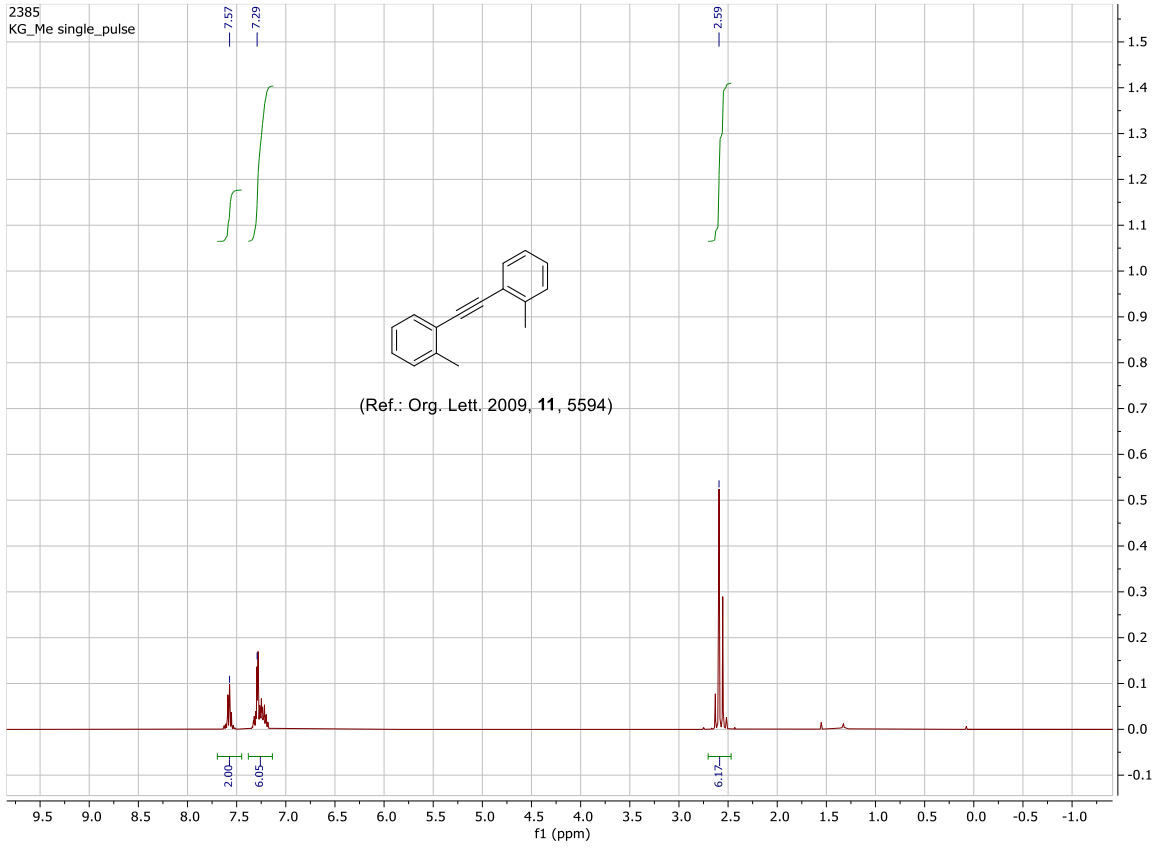
4al'


162.89
148.68
142.78
142.62
140.22
133.25
129.40
128.79
128.09
128.05
126.43
125.25
123.89
82.06
77.16
76.91
76.66
14.37
O
NH
N
4al'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Spectrum - [KGH-24_13092018_195_3496]
File Edit Display Process Tools Window Help
KGH-24_13092018_195_3496 473 (4.118) Cm (446:478)
1: TOF MS ES+
8.73e8
339.1501
322.1230
340.1531
307.0993
O
NH
N
4al'
m/z
2:43 PM
9/13/2018


2379
KGH_CL single_pulse
7.63
7.44
7.27
Cl
Cl
(Ref.: Org. Lett. 2004, 6, 4917)
1.00
1.16
4.28
f1 (ppm)


2392
KG_Cl single pulse decoupled gated NOE
136.13
133.59
129.75
129.27
128.47
126.59
122.98
91.24
Cl
Cl
(Ref.: Org. Lett. 2004, 6, 4917)
f1 (ppm)


2385
KG_Me single_pulse
7.57
7.29
2.59
(Ref.: Org. Lett. 2009, 11, 5594)
2.00
6.05
6.17
f1 (ppm)