

Supplementary Material

Sodium dodecyl sulfate catalyzed one-pot three-component synthesis of structurally diverse 2-amino-3-cyano-4-substitued-4*H*-chromenes in aqueous medium at room temperature

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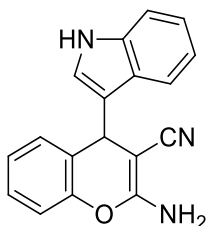
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Table of Contents

Characterization data with scanned spectra of all the synthesized compoundsS2

Characterization data with scanned spectra of all the synthesized compounds:

**4a**

2-Amino-4-(1H-indol-3-yl)-4H-chromene-3-carbonitrile (4a). Yellow solid, yield 94%; mp 166–168 °C; ¹H NMR (500 MHz, DMSO-*d*₆): δ_H/ppm 10.84 (s, 1H, -NH), 7.29 (d, J 8.5 Hz, 1H, aromatic H), 7.23 (d, J 1 Hz, 1H, aromatic H), 7.20 (d, J 7.5 Hz, 1H, aromatic H), 7.15 (t, J 11 Hz, 1H, aromatic H), 7.04 (d, J 7.5 Hz, 1H, aromatic H), 6.99 (t, J 12 Hz, 2H, aromatic H), 6.95 (t, J 11.25 Hz, 1H, aromatic H), 6.82 (t, J 11.25 Hz, 1H, aromatic H), 6.70 (s, 2H, -NH₂), 4.95 (s, 1H, -CH); ¹³C NMR (125 MHz, DMSO-*d*₆): δ_C/ppm 160.6, 148.9, 137.5, 129.8, 128.3, 125.8, 124.9 (2C), 124.3, 123.6, 121.5, 121.3, 119.2, 119.0, 116.3, 112.3, 56.9, 32.9; HRMS (ESI-TOF) *m/z*: For C₁₈H₁₃N₃O Calcd. [M+Na]⁺ 310.0956; Found [M+Na]⁺ 310.0869.

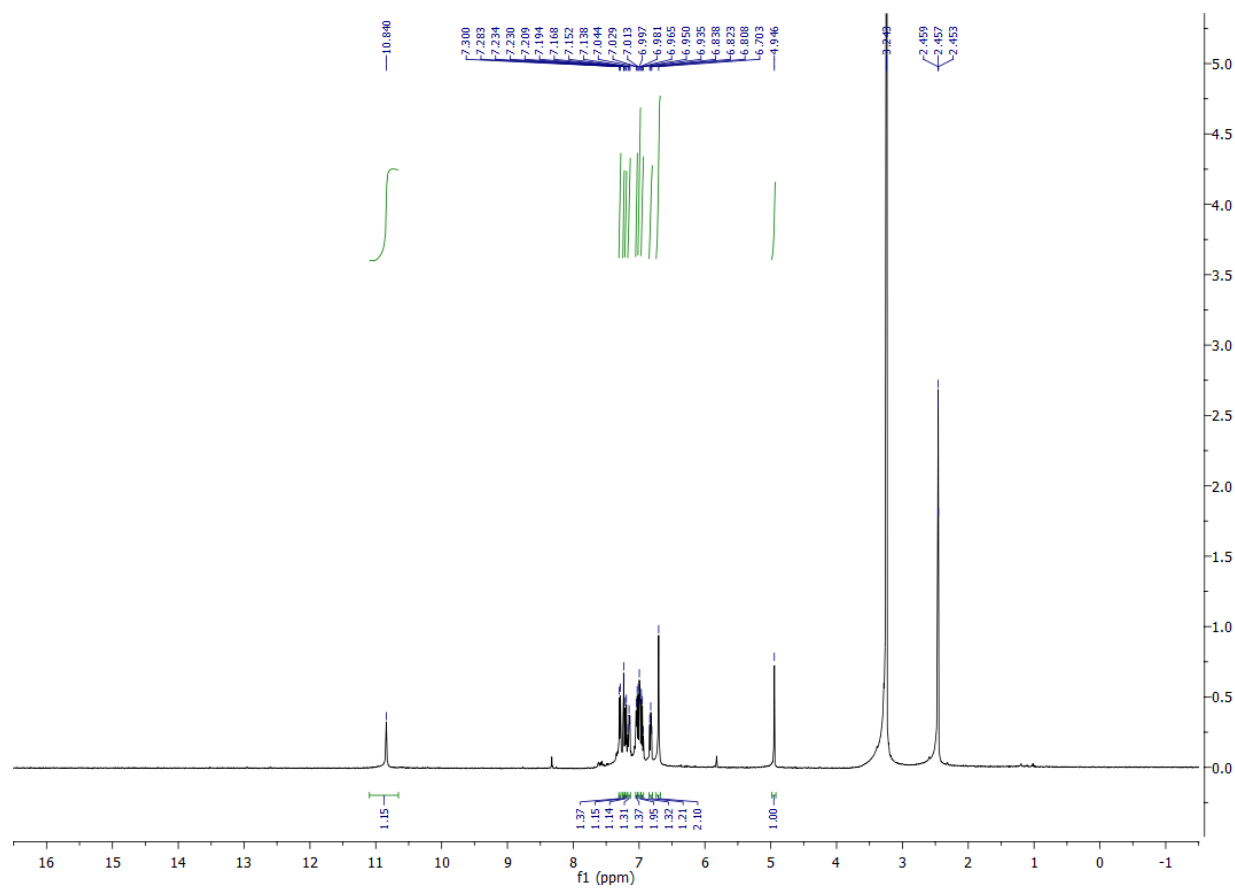


Figure S1. ^1H NMR spectrum of **4a**

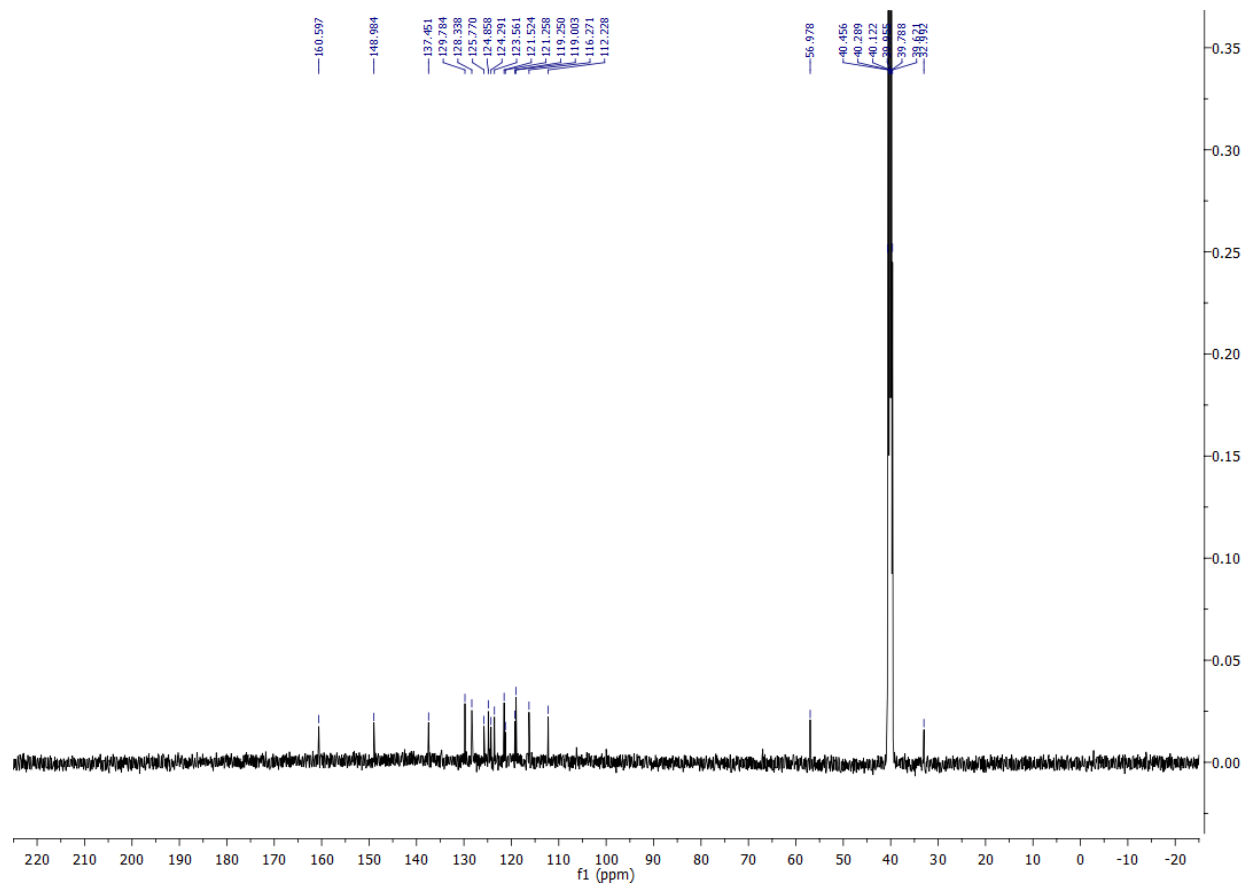


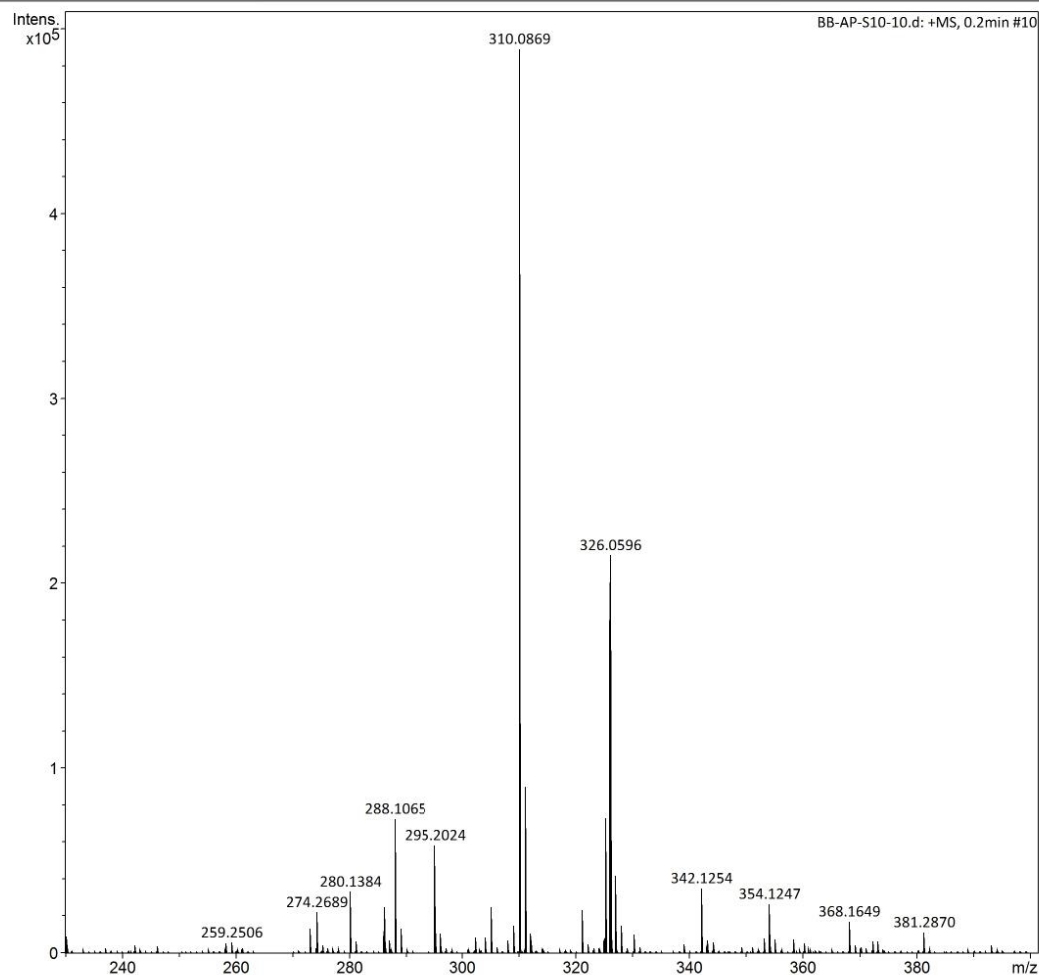
Figure S2. ^{13}C NMR spectrum of 4a

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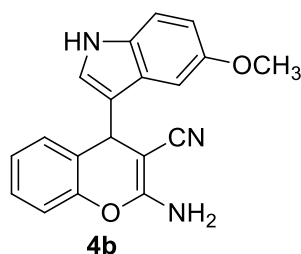
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Page 1 of 1

Figure S3. HRMS spectrum of 4a



2-Amino-4-(5-methoxy-1H-indol-3-yl)-4H-chromene-3-carbonitrile (4b). Off white solid, yield 98%; mp 185–187 °C; ^1H NMR (500 MHz, CDCl_3): δ_{H} /ppm 7.93 (s, 1H, -NH), 7.22 (d, J 9 Hz, 1H, aromatic H), 7.18 (t, J 11.25 Hz, 1H, aromatic H), 7.11 (t, J 4.25 Hz, 2H, aromatic H) 7.03–6.98 (m, 2H, aromatic H), 6.80 (dd, J 8.75 Hz, 2.5 Hz, 1H, aromatic H), 6.77 (d, J 2 Hz, 1H, aromatic H), 5.02 (s, 1H, -CH), 4.56 (s, 2H, -NH₂), 3.73 (s, 3H, -OCH₃); ^{13}C NMR (125 MHz, CDCl_3): δ_{C} /ppm 170.4, 164.1, 158.3, 153.9, 152.1, 148.8, 132.1, 129.6, 128.1, 125.1, 123.2, 122.9, 116.1, 112.1, 112.0, 101.4, 61.5, 55.8, 32.7; HRMS (ESI-TOF) m/z : For $\text{C}_{19}\text{H}_{15}\text{N}_3\text{O}_2$ Calcd. $[\text{M}+\text{Na}]^+$ 340.1062; Found $[\text{M}+\text{Na}]^+$ 340.0804.

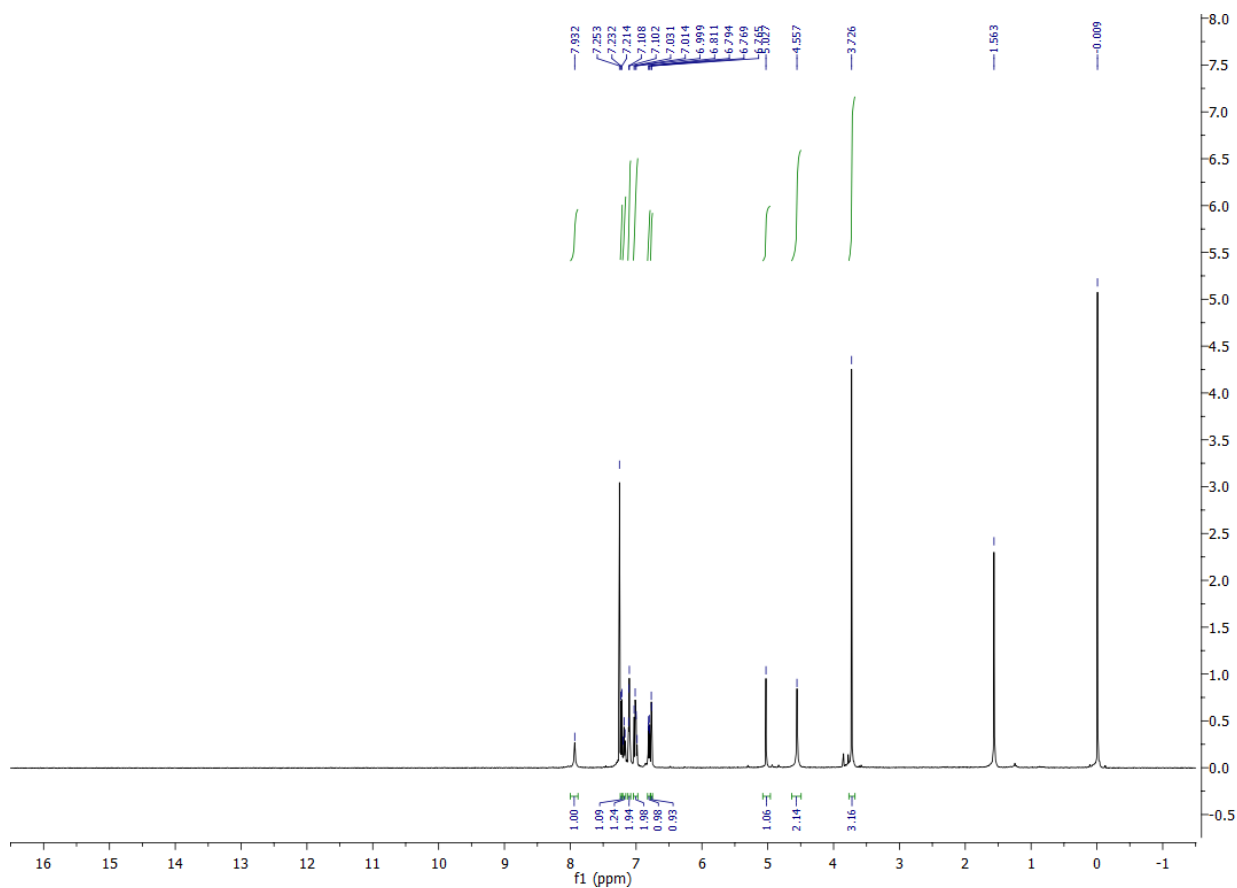


Figure S4. ^1H NMR spectrum of **4b**

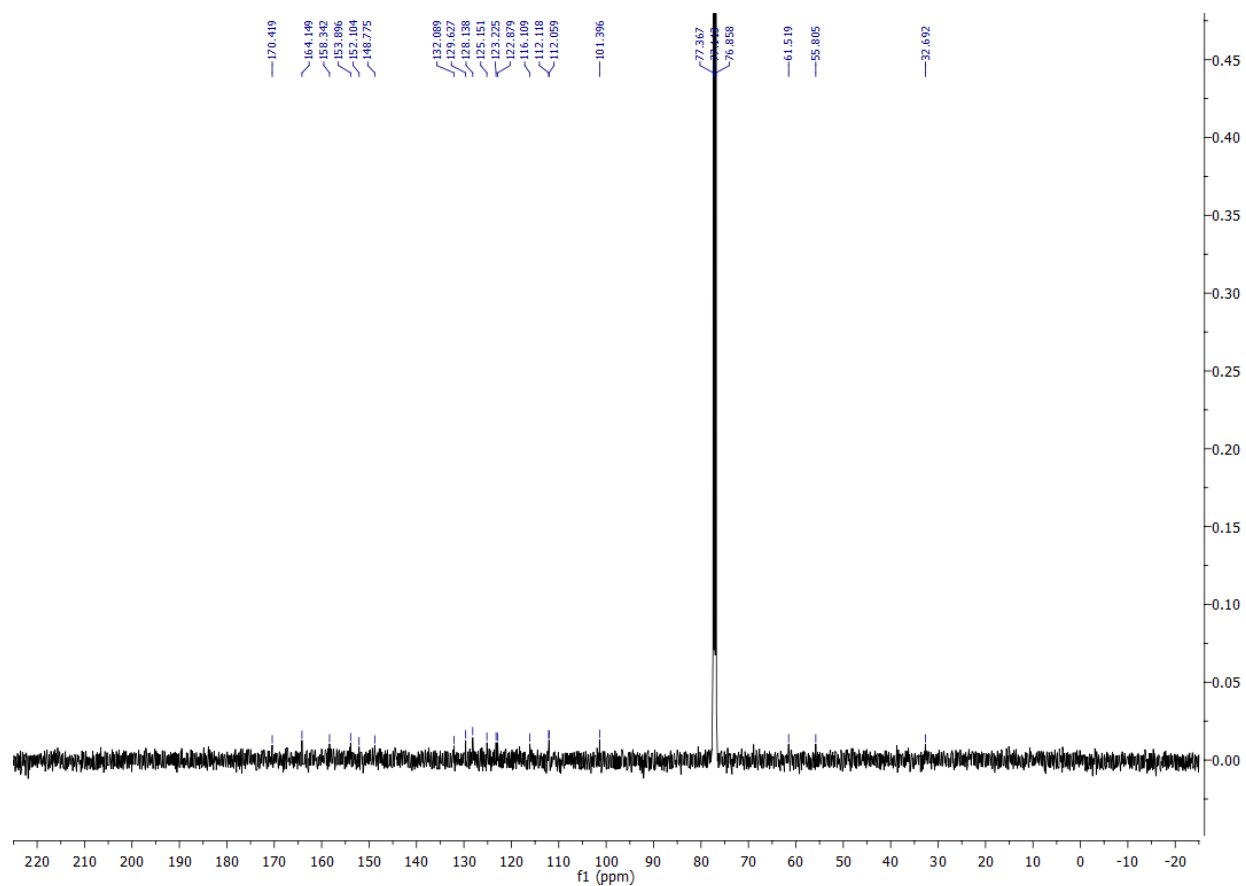


Figure S5. ^{13}C NMR spectrum of **4b**

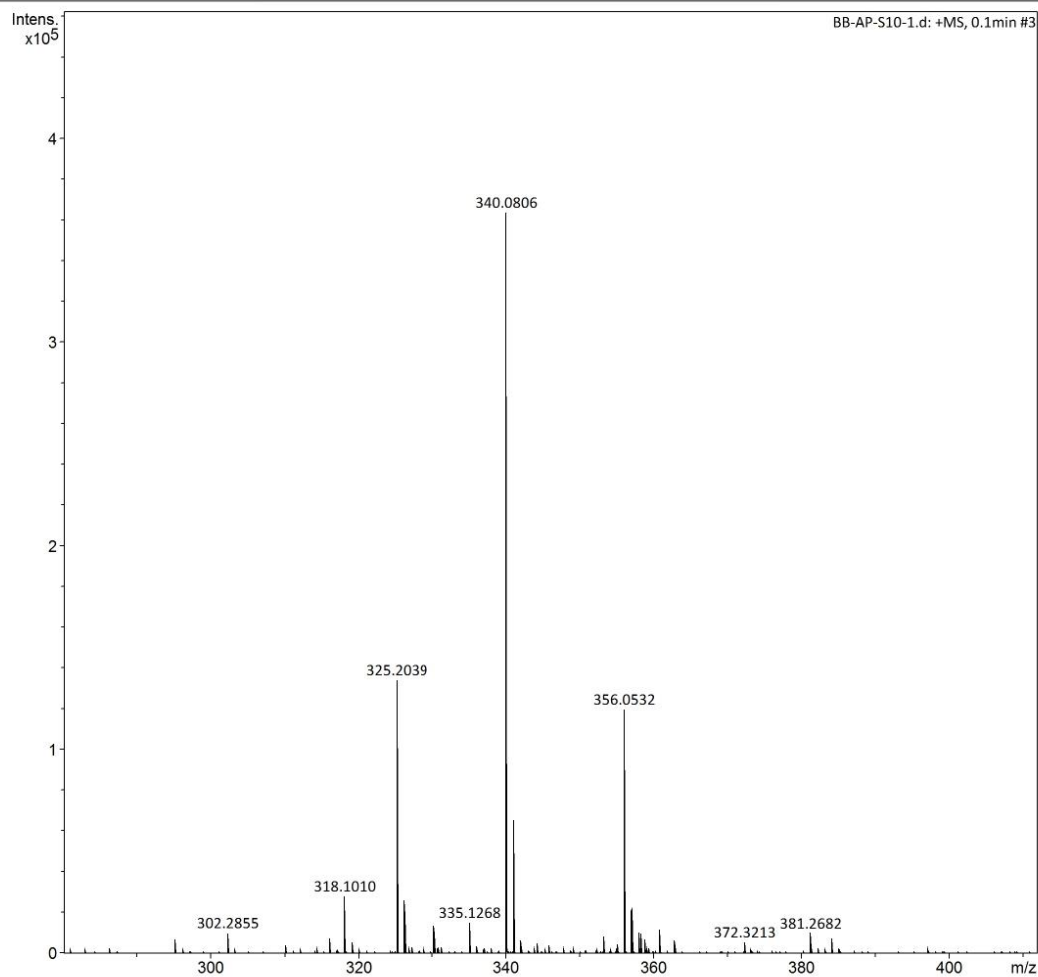
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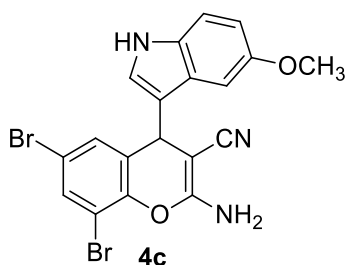
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Figure S6. HRMS spectrum of **4b**



2-Amino-6,8-dibromo-4-(5-methoxy-1H-indol-3-yl)-4H-chromene-3-carbonitrile (4c). Yellow solid, yield 91%; mp 213-215 °C; ^1H NMR (500 MHz, DMSO- d_6): δ_{H} /ppm 10.82 (d, J 2.5 Hz, 1H, -NH) 7.71 (d, J 2.5 Hz, 1H, aromatic H), 7.27 (d, J 3 Hz, 1H, aromatic H), 7.22 (t, J 6 Hz, 2H, aromatic H), 7.03 (s, 2H, -NH $_2$), 6.72 (d, J 2 Hz, 1H, aromatic H), 6.70-6.68 (m, 1H, aromatic H), 5.00 (s, 1H, -CH), 3.64 (s, 3H, -OCH $_3$); ^{13}C NMR (125 MHz, DMSO- d_6): δ_{C} /ppm 160.2, 153.5, 145.4, 133.6, 132.5, 131.6, 128.4, 124.4, 120.6, 118.3, 116.5, 113.1, 111.3, 110.9, 100.9, 100.3, 56.8, 55.7, 33.3; HRMS (ESI-TOF) m/z : For C $_{19}$ H $_{13}$ Br $_2$ N $_3$ O $_2$ Calcd. [M] $^+$ 475.1334; Found [M-H] $^-$ 473.9489.

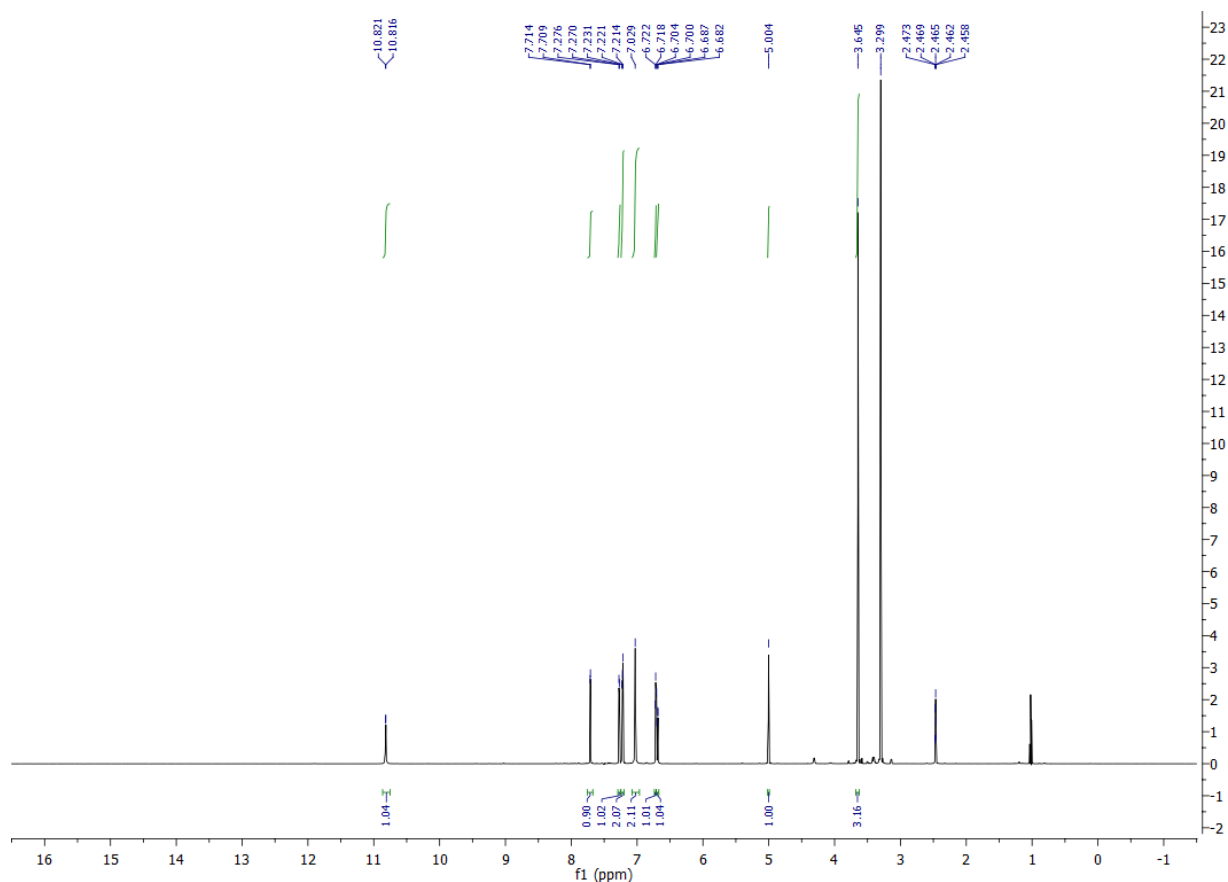


Figure S7. ^1H NMR spectrum of **4c**

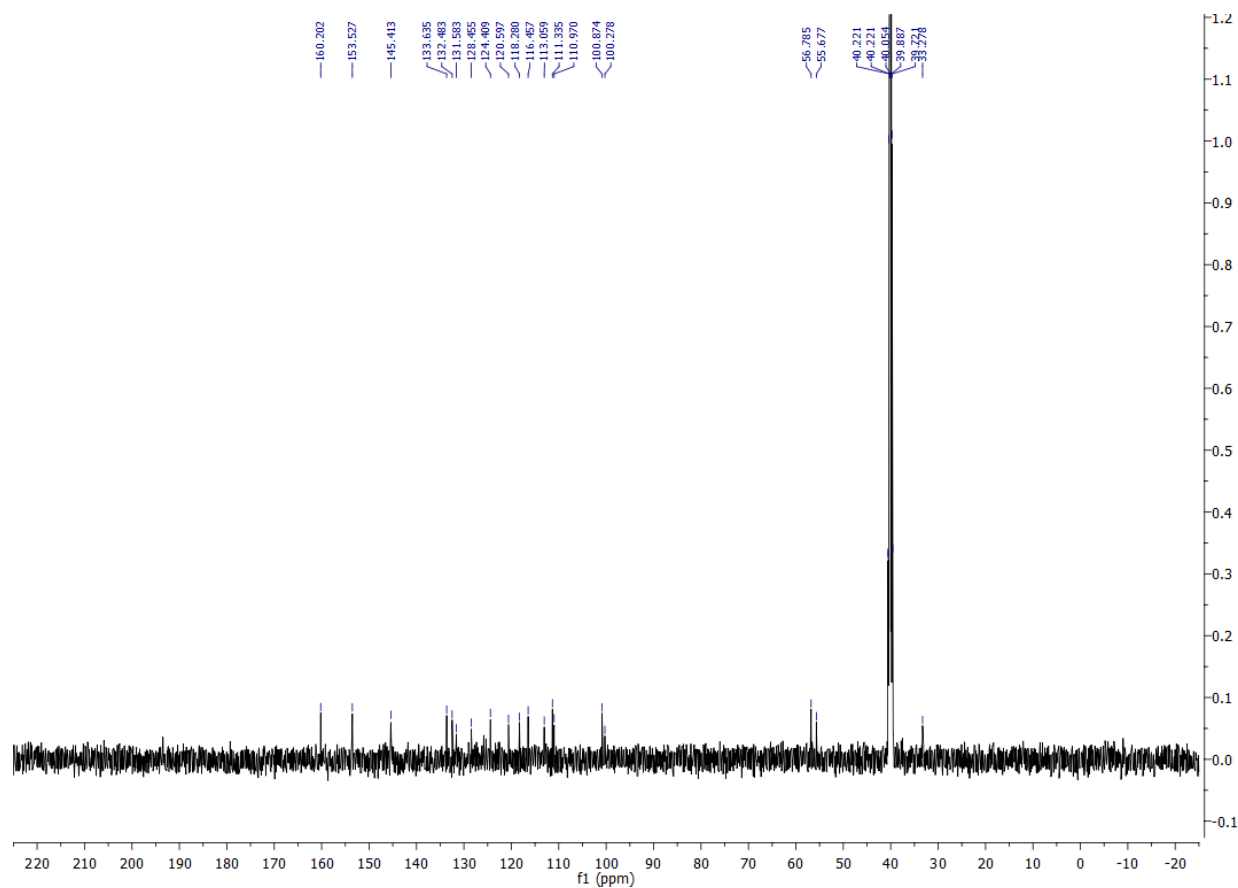


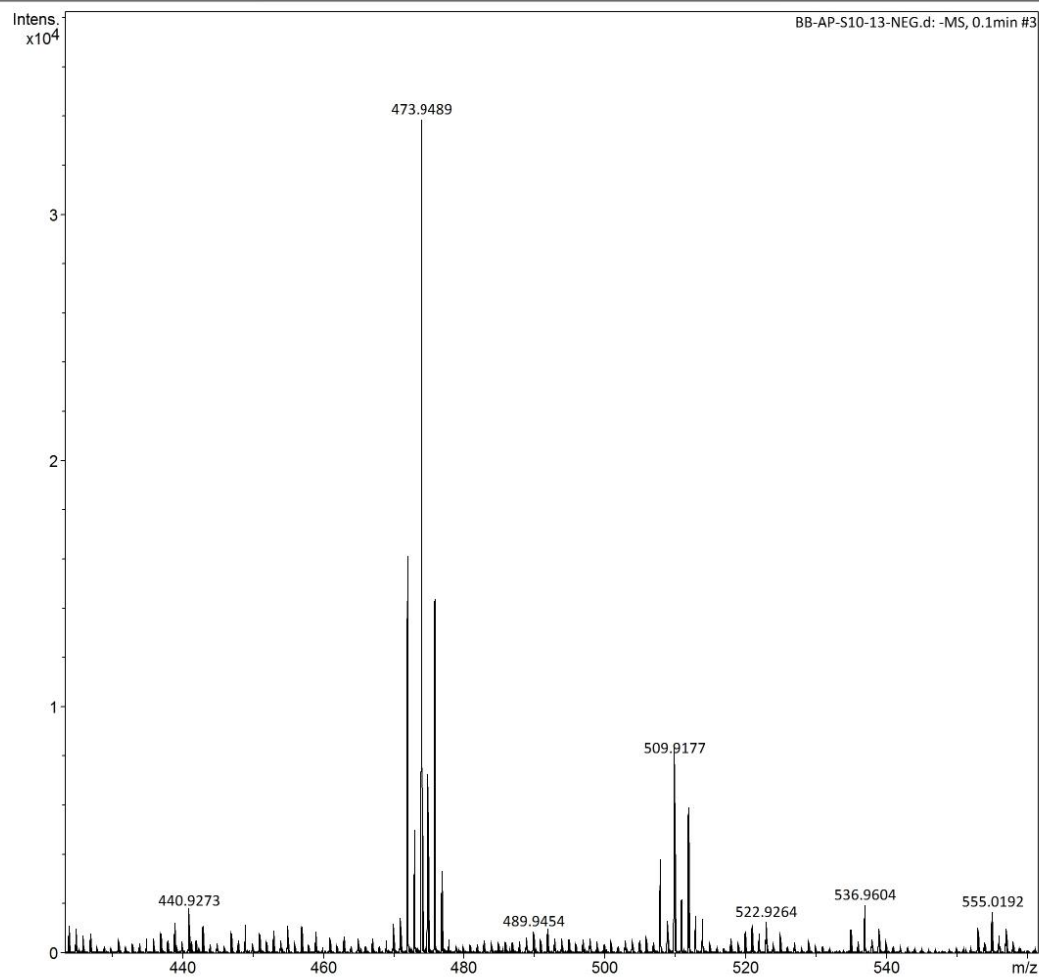
Figure S8. ^{13}C NMR spectrum of **4c**

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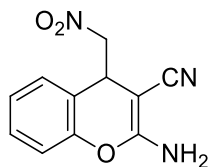
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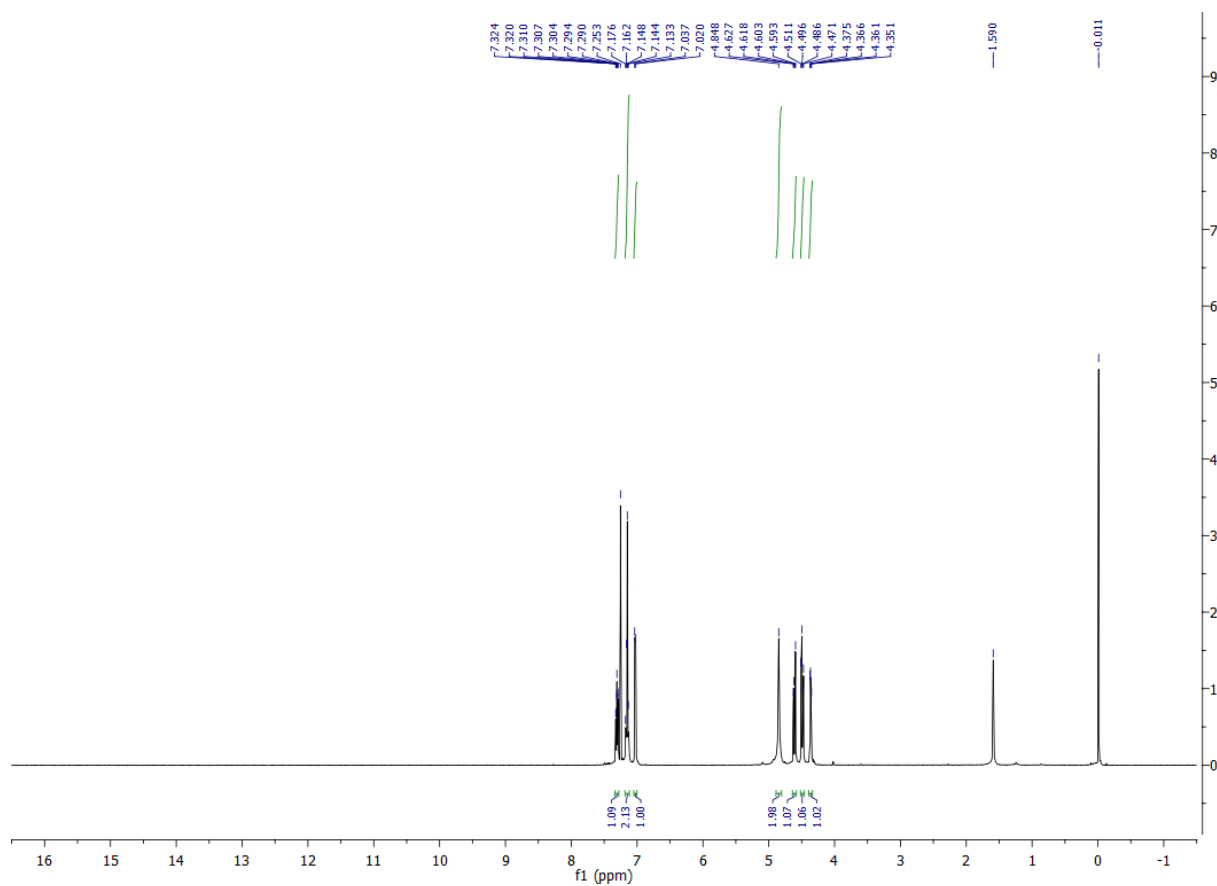
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Page 1 of 1

Figure S9. HRMS spectrum of 4c

**4d**

2-Amino-4-(nitromethyl)-4H-chromene-3-carbonitrile (4d). Off white solid, yield 95%; mp 139–141°C; ^1H NMR (500 MHz, CDCl_3): δ_{H} /ppm 7.32–7.29 (m, 1H, aromatic H), 7.18–7.13 (m, 2H, aromatic H), 7.03 (d, J 8.5 Hz, 1H, aromatic H), 4.85 (s, 2H, $-\text{NH}_2$), 4.61 (dd, J 12.25 Hz, 4.5 Hz, 1H, $-\text{CH}_2$), 4.49 (dd, J 12.5 Hz, 7.5 Hz, 1H, $-\text{CH}_2$), 4.36 (dd, J 7.25 Hz, 4.5 Hz, 1H, $-\text{CH}$); ^{13}C NMR (125 MHz, CDCl_3): δ_{C} /ppm 161.8, 149.3, 129.7, 127.9, 125.8, 118.8, 118.7, 116.9, 80.3, 54.2, 34.8; HRMS (ESI-TOF) m/z : For $\text{C}_{11}\text{H}_9\text{N}_3\text{O}_3$ Calcd. $[\text{M}+\text{Na}]^+$ 254.0542; Found $[\text{M}+\text{Na}]^+$ 254.0508.

**Figure S10.** ^1H NMR spectrum of **4d**

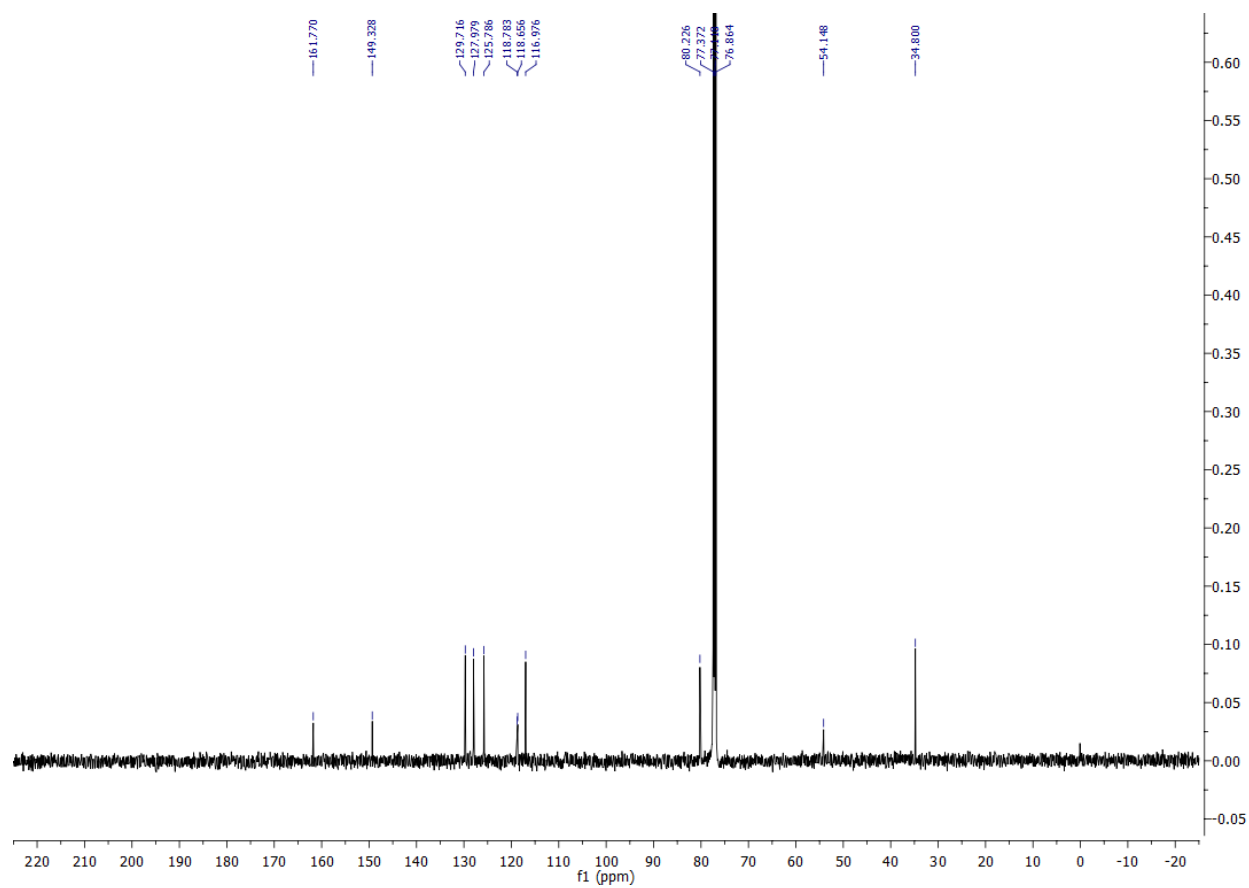


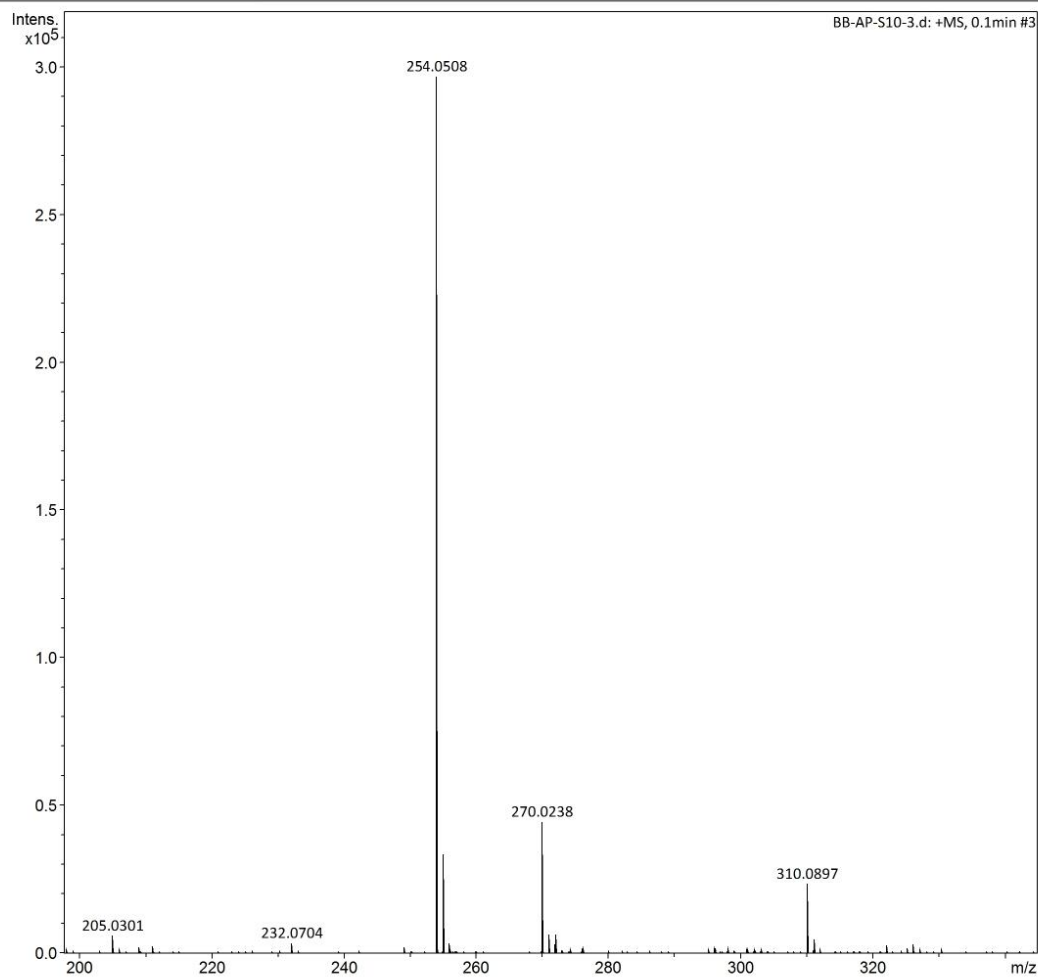
Figure S11. ^{13}C NMR spectrum of 4d

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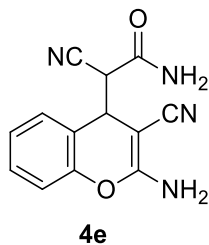
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Bruker Compass DataAnalysis 4.1 printed: 5/12/2023 10:32:10 AM by: HRMS Page 1 of 1

Figure S12. HRMS spectrum of **4d**



2-(2-Amino-3-cyano-4H-chromen-4-yl)-2-cyanoacetamide (**4e**). Off white solid, yield 92%; mp 168-169 °C; ^1H NMR (500 MHz, DMSO- d_6): δ_{H} /ppm 7.78 (s, 1H), 7.52 (s, 1H), 7.32 (t, J 11.25 Hz, 1H, aromatic H), 7.22 (d, J 7.5 Hz, 1H, aromatic H), 7.14 (s, 2H, -NH₂), 7.11 (d, J 7.5 Hz, 1H, aromatic H), 7.04 (d, J 8 Hz, 1H, aromatic H), 4.21 (d, J 5 Hz, 1H, -CH), 3.88 (d, J 5 Hz, 1H, -CH); ^{13}C NMR (125 MHz, DMSO- d_6): δ_{C} /ppm 179.2, 165.4, 163.6, 150.4, 129.8, 129.2, 124.9, 119.9, 117.3, 116.6, 51.9, 48.1, 37.3; HRMS (ESI-TOF) m/z : For C₁₃H₁₀N₄O₂ Calcd. [M+Na]⁺ 277.0701; Found [M+Na]⁺ 277.0937.

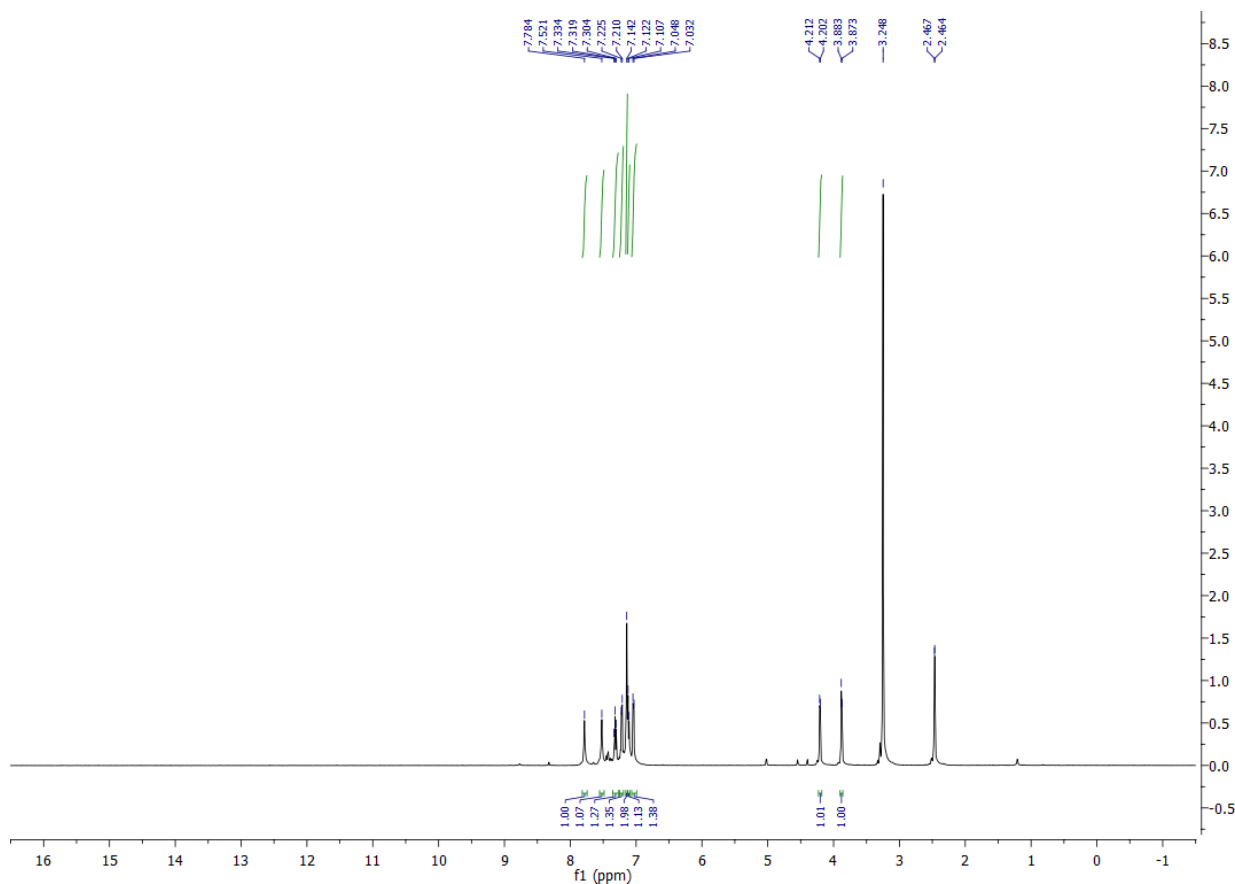


Figure S13. ^1H NMR spectrum of **4e**

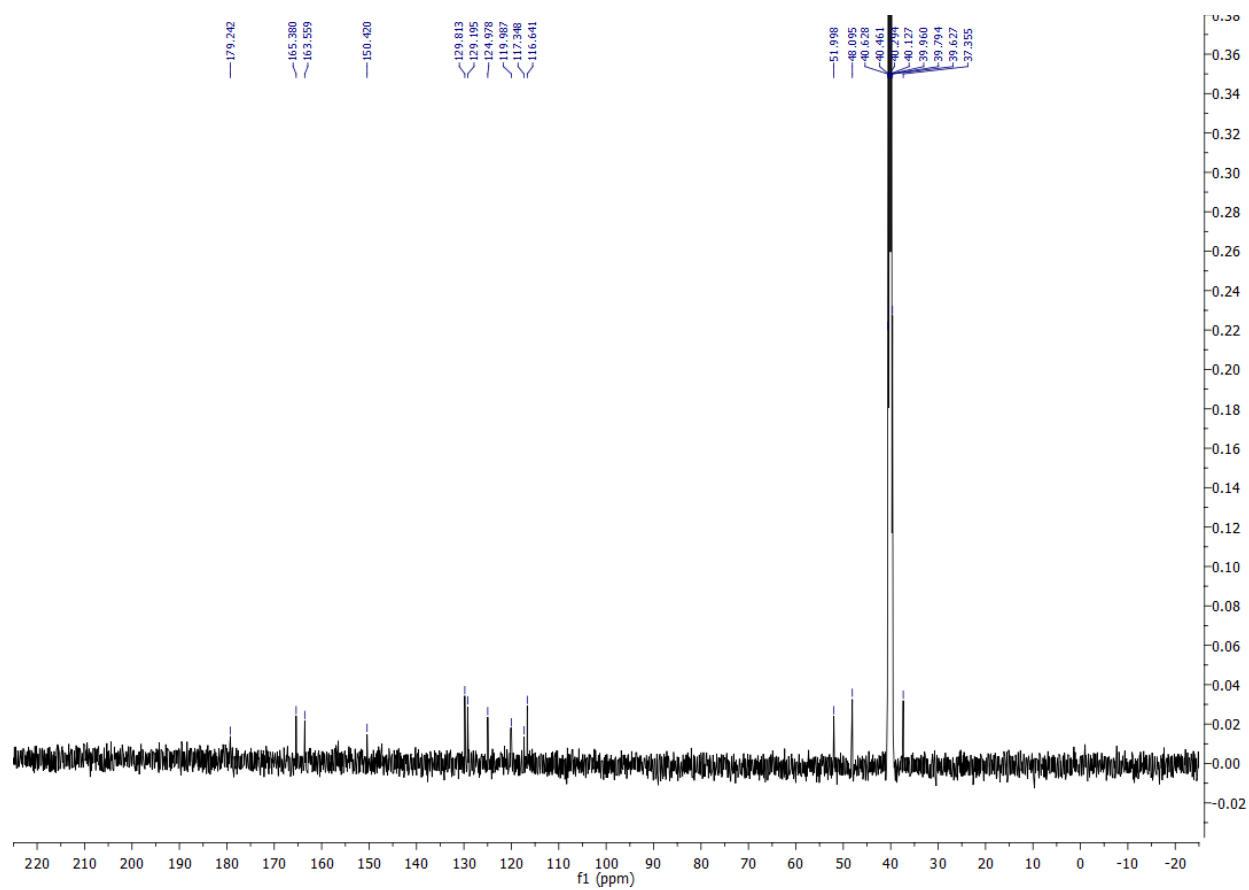


Figure S14. ^{13}C NMR spectrum of **4e**

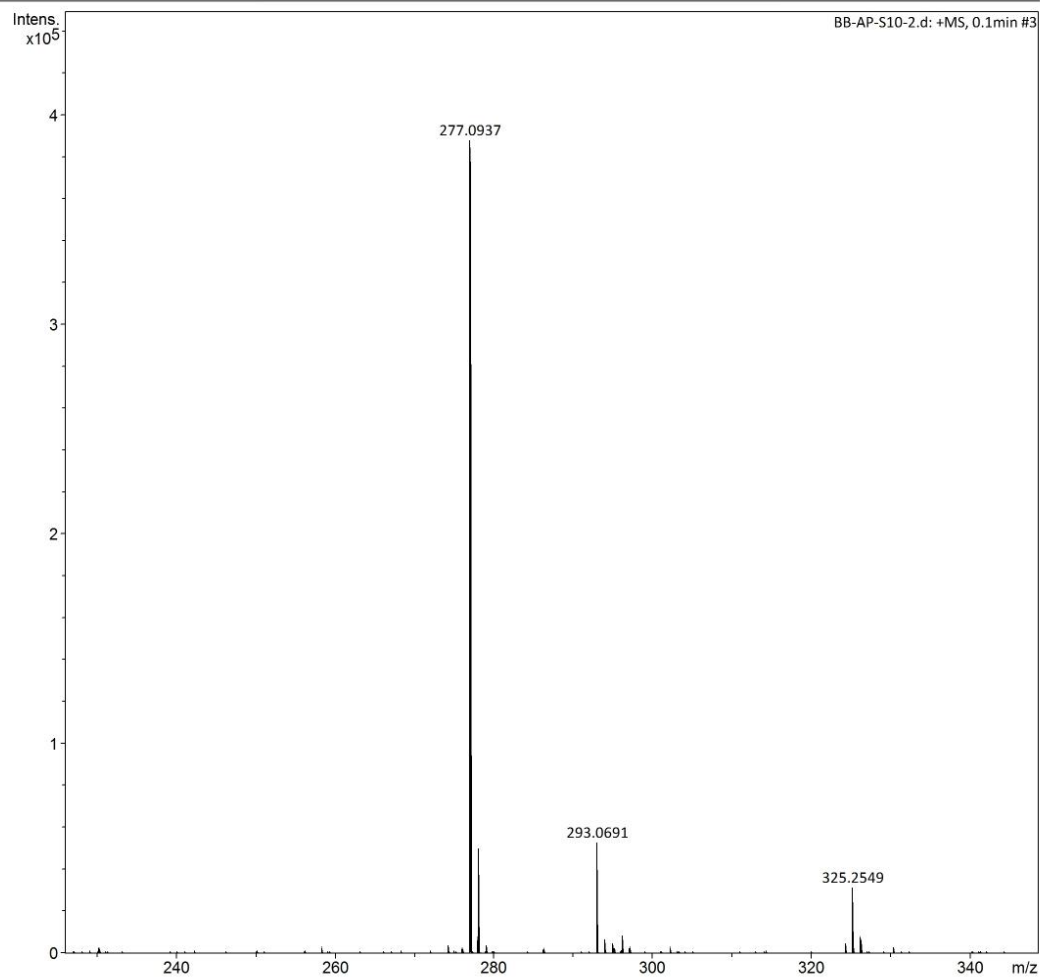
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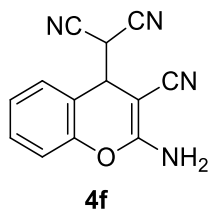
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Page 1 of 1

Figure S15. HRMS spectrum of **4e**



2-(2-Amino-3-cyano-4H-chromen-4-yl)malononitrile (**4f**). White solid, yield 87%; mp 153-155 °C; ^1H NMR (500 MHz, CDCl_3): δ_{H} /ppm 7.53 (s, 2H, $-\text{NH}_2$), 7.48 (d, J 6 Hz, 1H, aromatic H), 7.43 (t, J 9.75 Hz, 1H, aromatic H), 7.28 (t, J 9.5 Hz, 1H, aromatic H), 7.14 (d, J 7 Hz, 1H, aromatic H), 5.08 (d, J 2.5 Hz, 1H, $-\text{CH}$), 4.59 (d, J 2.5 Hz, 1H, $-\text{CH}$); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ_{C} /ppm 163.9, 150.2, 130.6, 129.3, 125.5, 119.8, 118.4, 116.8, 113.5, 113.4, 49.3, 37.6, 32.9; HRMS (ESI-TOF) m/z : For $\text{C}_{13}\text{H}_8\text{N}_4\text{O}$ Calcd. $[\text{M}+\text{K}]^+$ 275.0335; Found $[\text{M}+\text{K}]^+$ 275.0289.

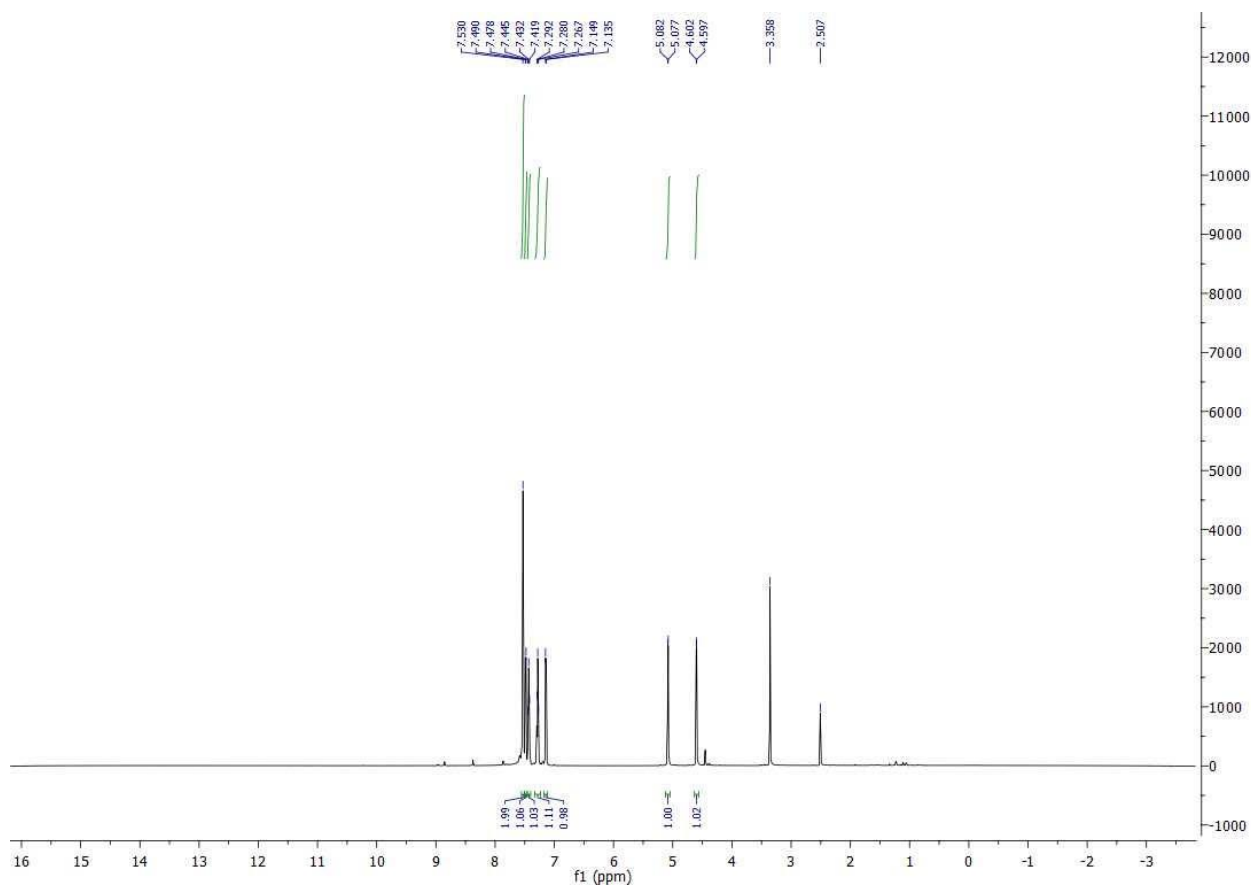


Figure S16. ^1H NMR spectrum of **4f**

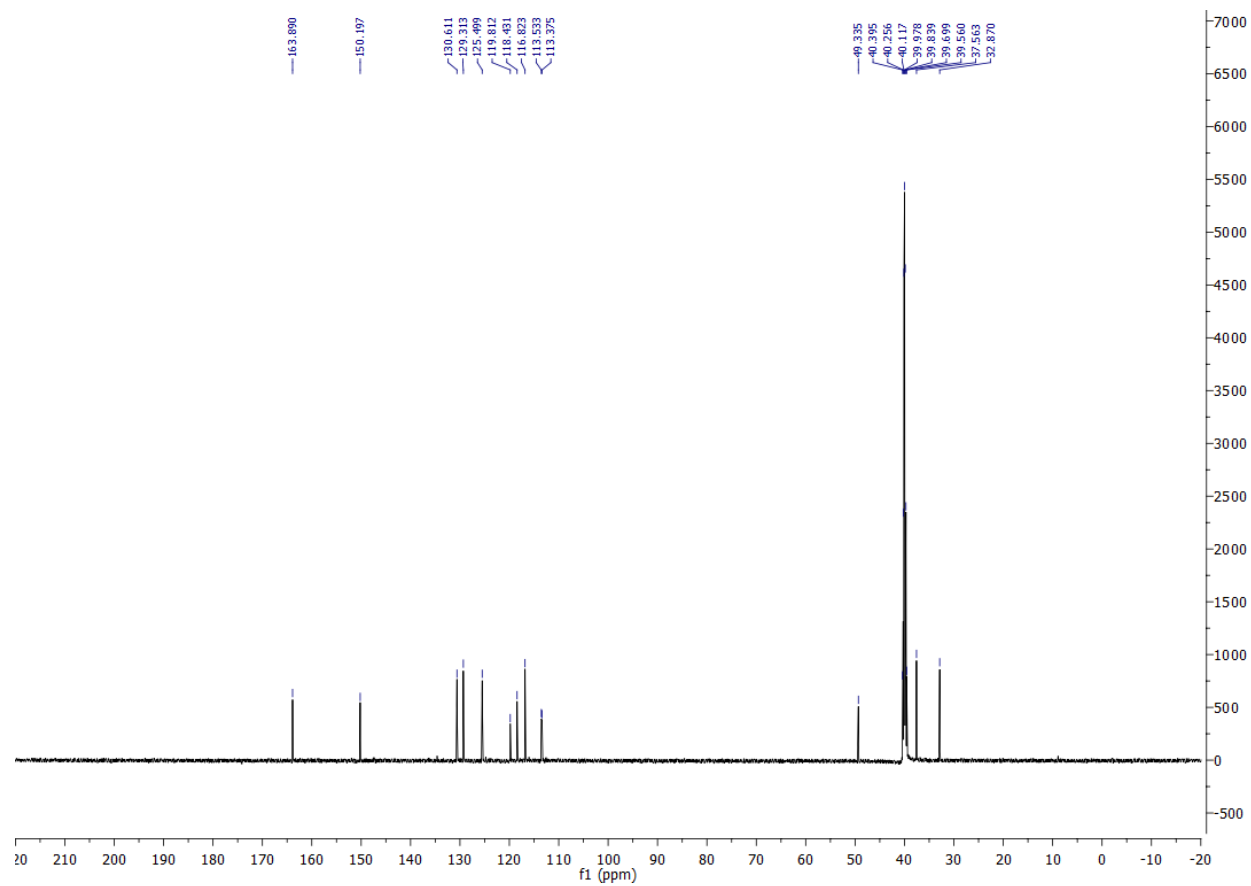


Figure S17. ¹³C NMR spectrum of 4f

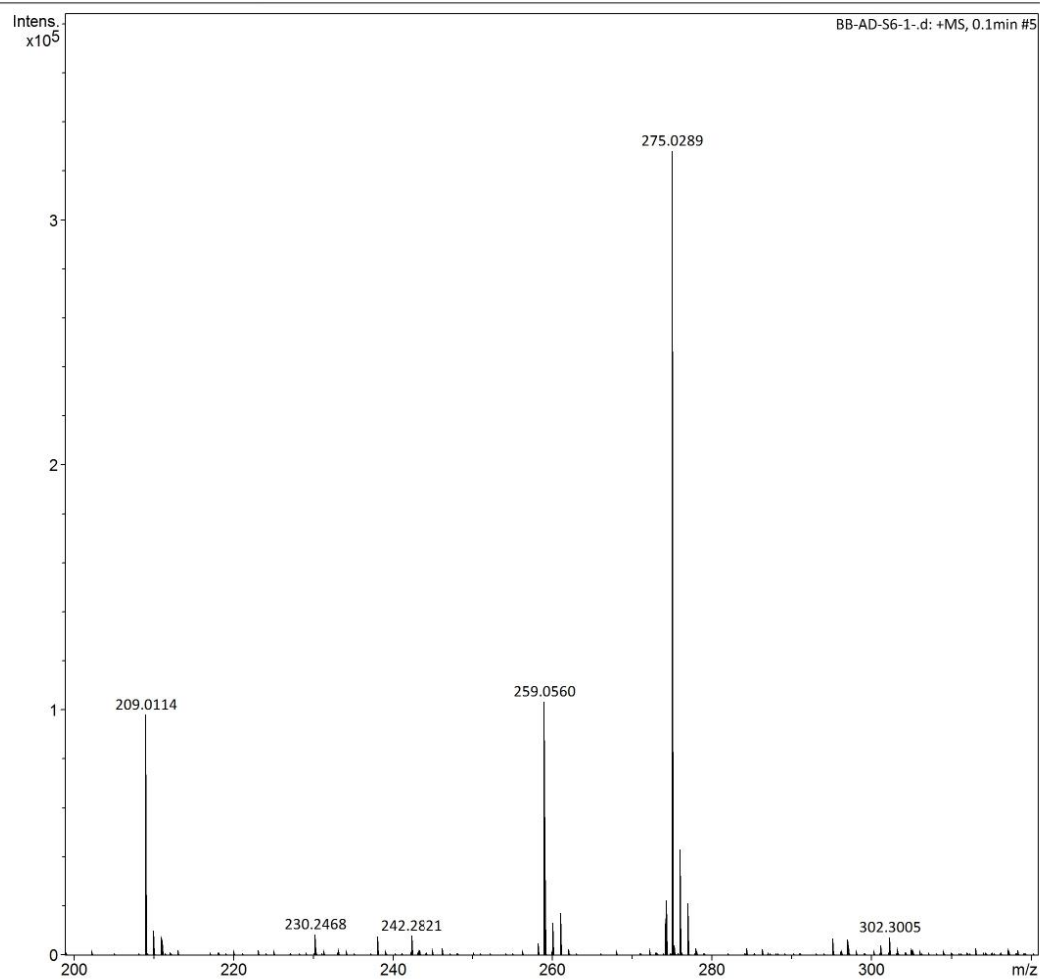
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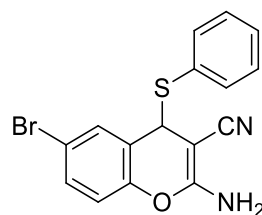
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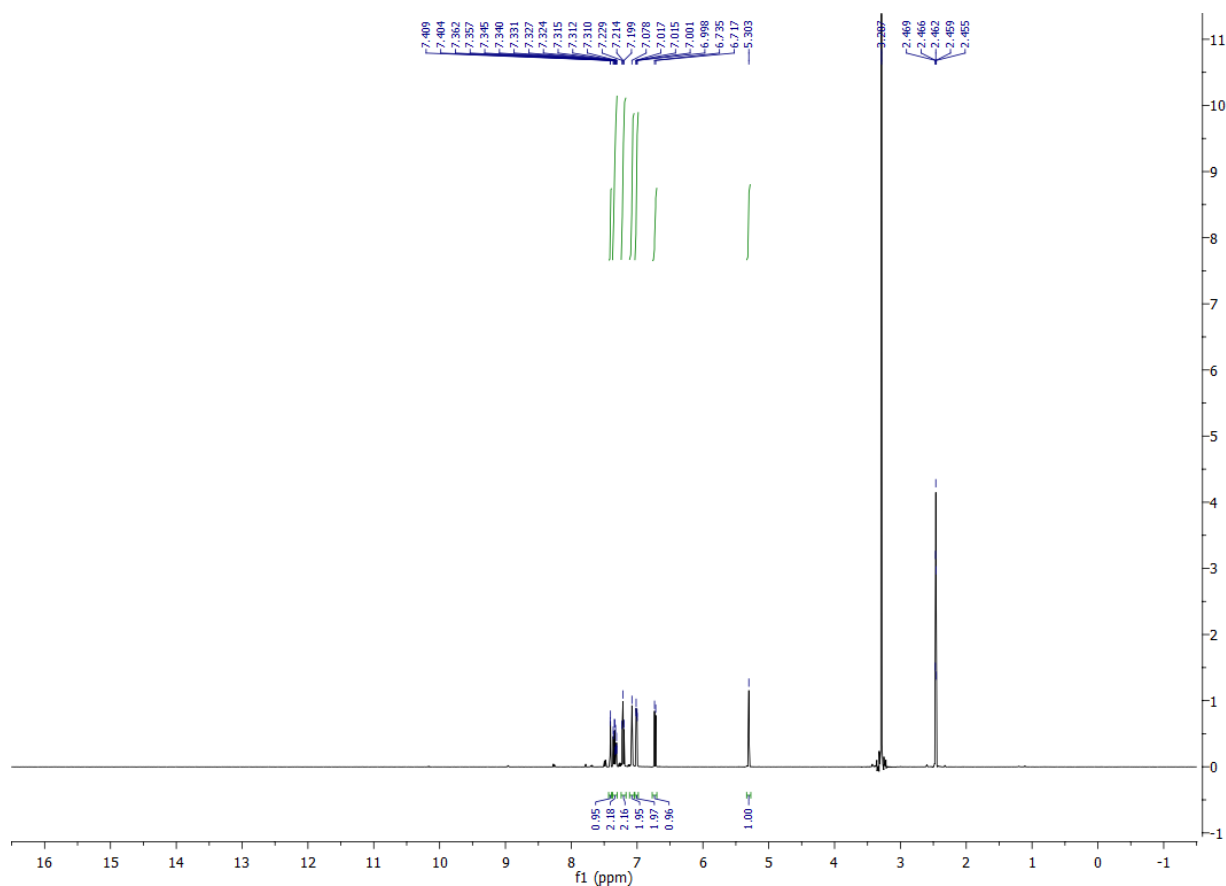
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Page 1 of 1

Figure S18. HRMS spectrum of **4f**

**4g**

2-Amino-6-bromo-4-(phenylthio)-4H-chromene-3-carbonitrile (4g). White solid, yield 88%; mp 181–183 °C; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ_{H} /ppm 7.41 (d, J 2.5 Hz, 1H, aromatic H), 7.36–7.31 (m, 2H, aromatic H), 7.21 (t, J 7.5 Hz, 2H, aromatic H), 7.08 (s, 2H, $-\text{NH}_2$), 7.01 (dd, J 10.5 Hz, 1 Hz, 2H, aromatic H), 6.73 (d, J 9 Hz, 1H, aromatic H), 5.30 (s, 1H, $-\text{CH}$); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ_{C} /ppm 162.43, 136.6, 131.8, 131.7 (2C), 129.6 (2C), 129.7 (2C), 124.4 (2C), 124.0, 118.3, 116.3, 53.6, 46.7; HRMS (ESI-TOF) m/z : For $\text{C}_{16}\text{H}_{11}\text{BrN}_2\text{OS}$ Calcd. $[\text{M}+\text{Na}]^+$ 380.9673; Found $[\text{M}+\text{Na}]^+$ 381.3114.

**Figure S19.** ^1H NMR spectrum of **4g**

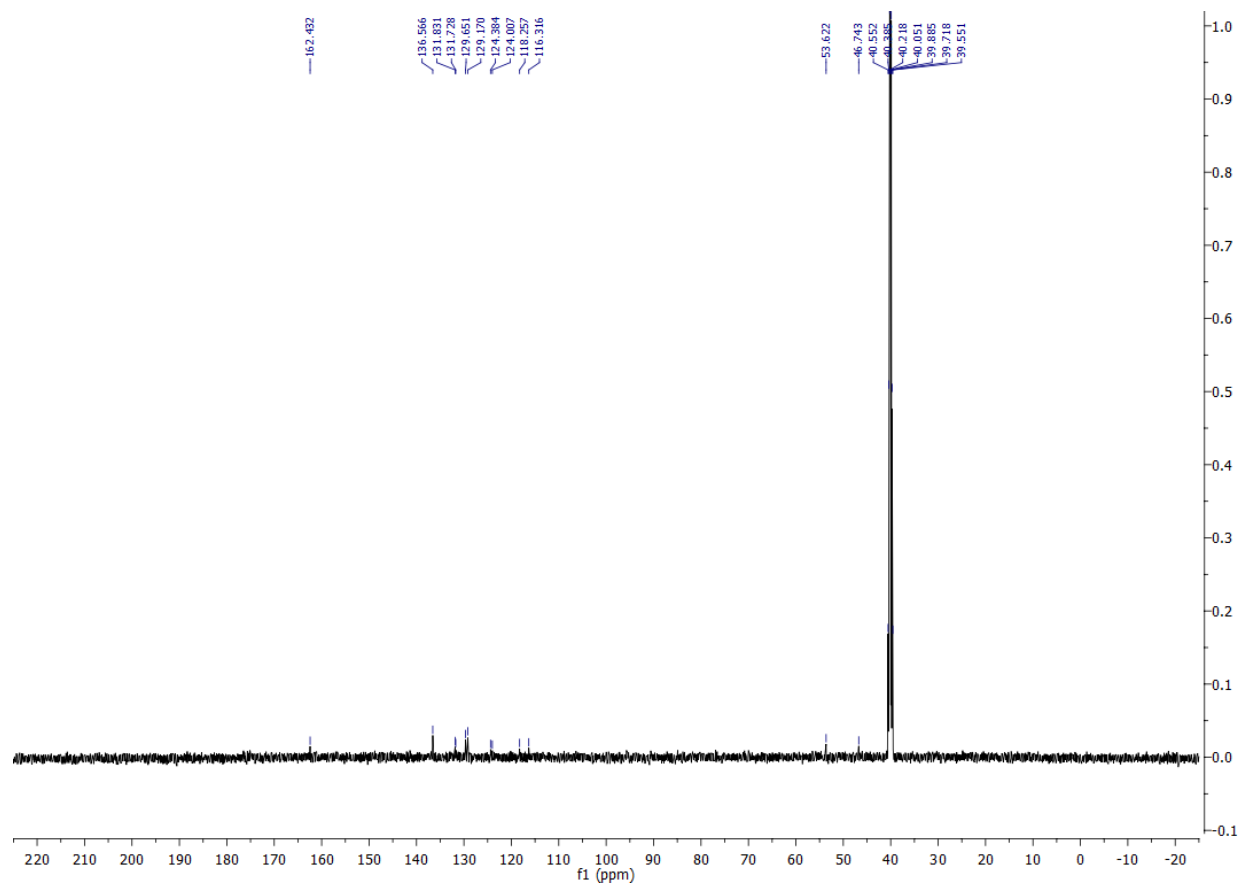


Figure S20. ¹³C NMR spectrum of 4g

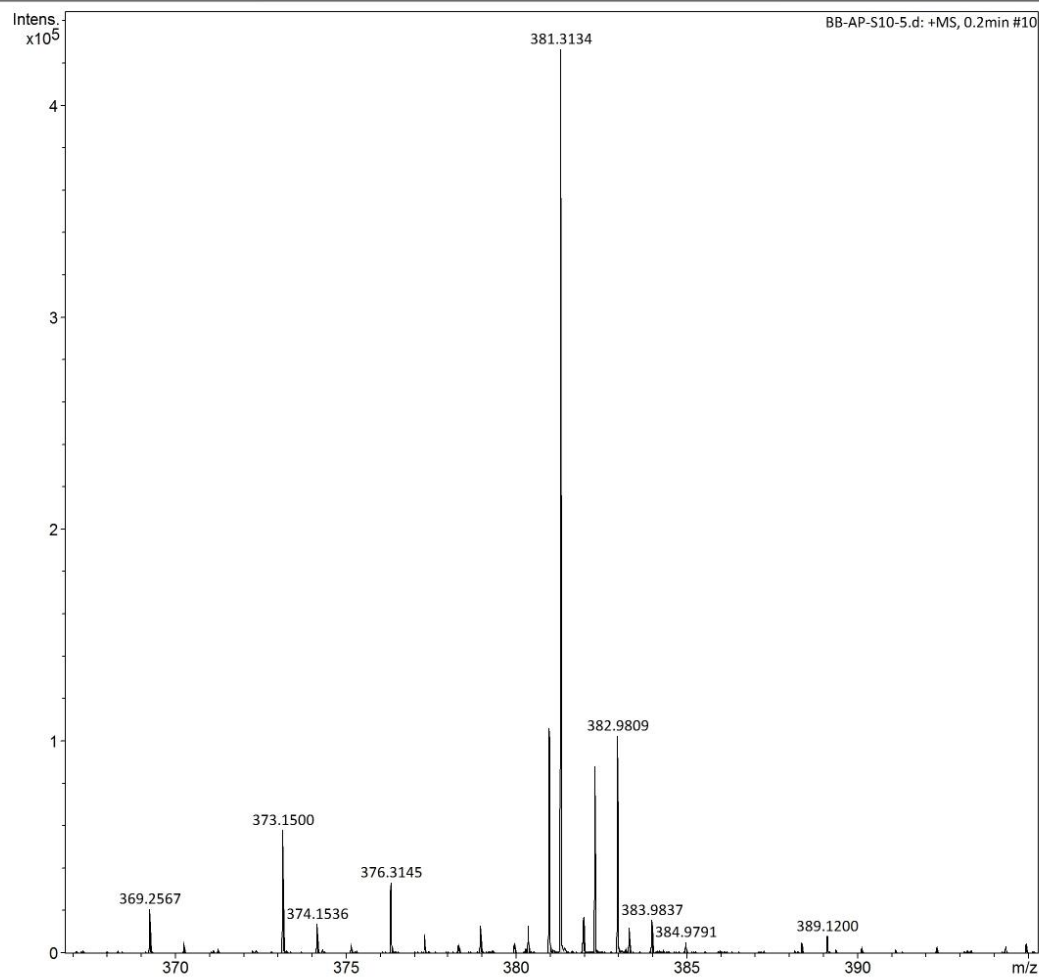
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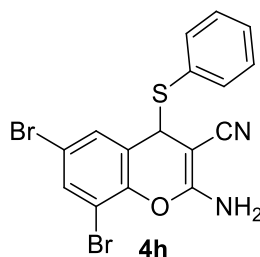
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Page 1 of 1

Figure S21. HRMS spectrum of **4g**



2-Amino-6,8-dibromo-4-(phenylthio)-4H-chromene-3-carbonitrile (4h). Light Yellow solid, yield 82%; mp 171–173 °C; ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ_{H} /ppm 7.74 (d, J 2 Hz, 1H, aromatic H), 7.49 (d, J 7.5 Hz, 1H, aromatic H), 7.41 (d, J 2 Hz, 1H, aromatic H), 7.37-7.34 (m, 3H, aromatic H & $-\text{NH}_2$), 7.26-7.22 (m, 2H, aromatic H), 6.99 (dd, J 8.25 Hz, 1 Hz 1H, aromatic H), 5.34 (s, 1H, $-\text{CH}$), ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$): δ_{C} /ppm 162.1, 145.9, 136.7, 134.2, 130.0 (2C), 129.9, 129.2 (2C), 128.1, 127.7, 119.5, 116.4, 110.5, 53.8, 47.0; HRMS (ESI-TOF) m/z : For $\text{C}_{16}\text{H}_{10}\text{Br}_2\text{N}_2\text{OS}$ Calcd. $[\text{M}+\text{H}]^+$ 436.8959; Found $[\text{M}+\text{H}]^+$ 436.8742.

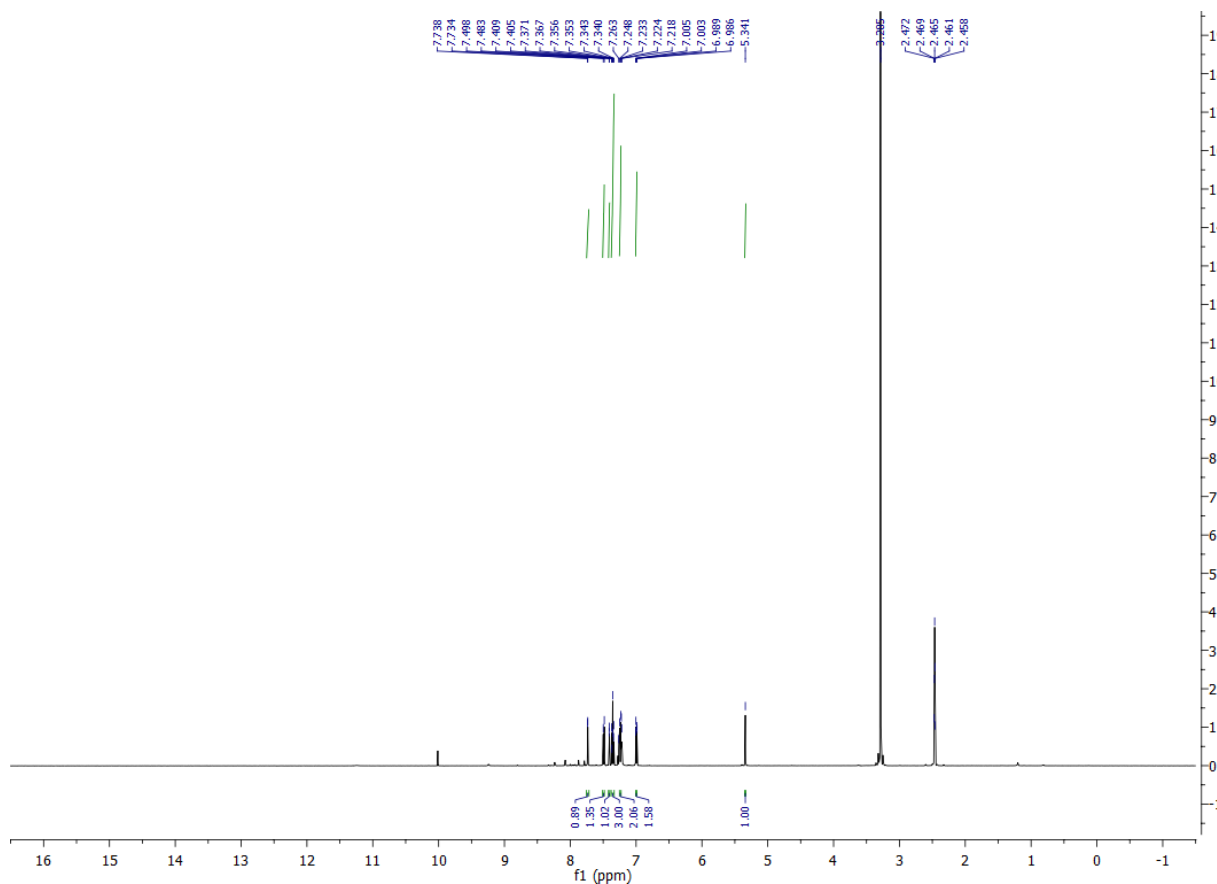


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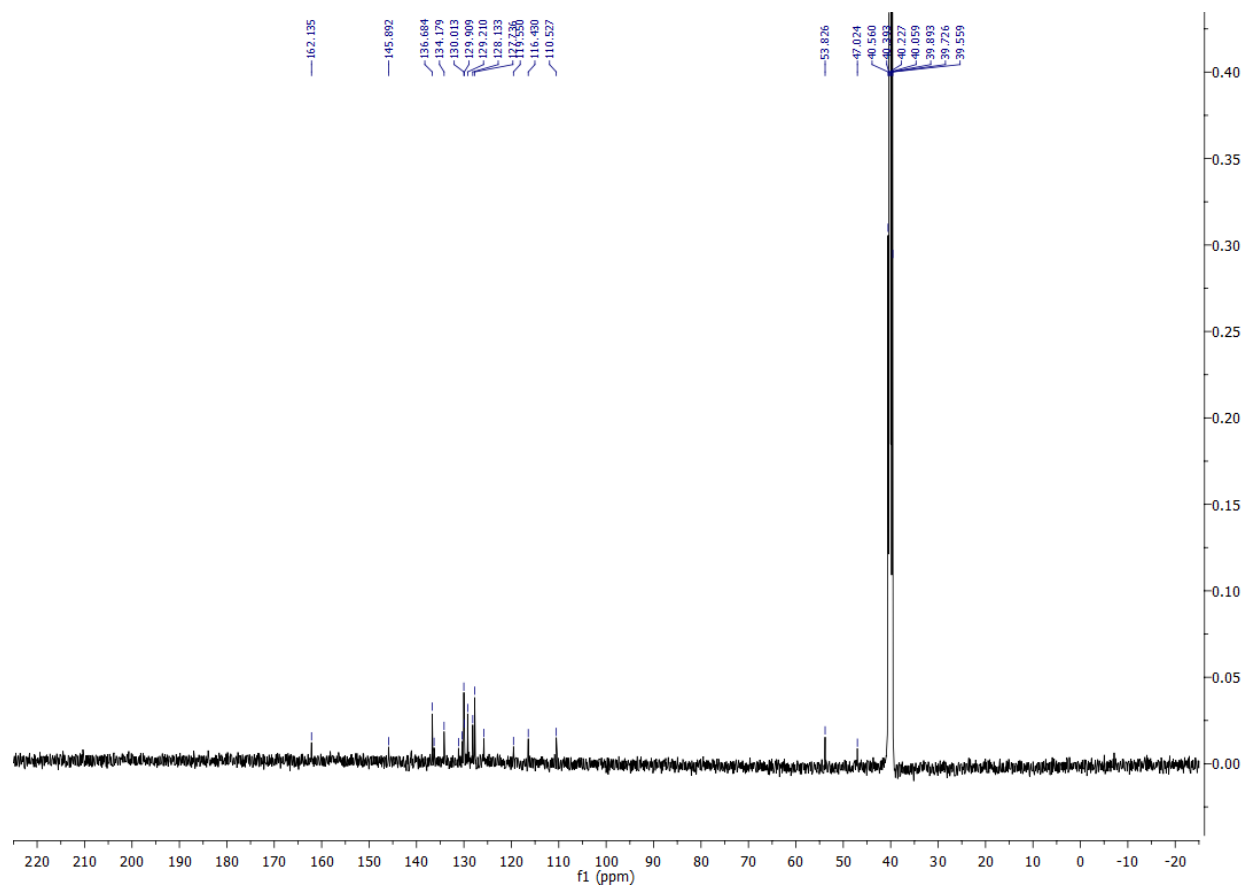


Figure S23. ¹³C NMR spectrum of 4h

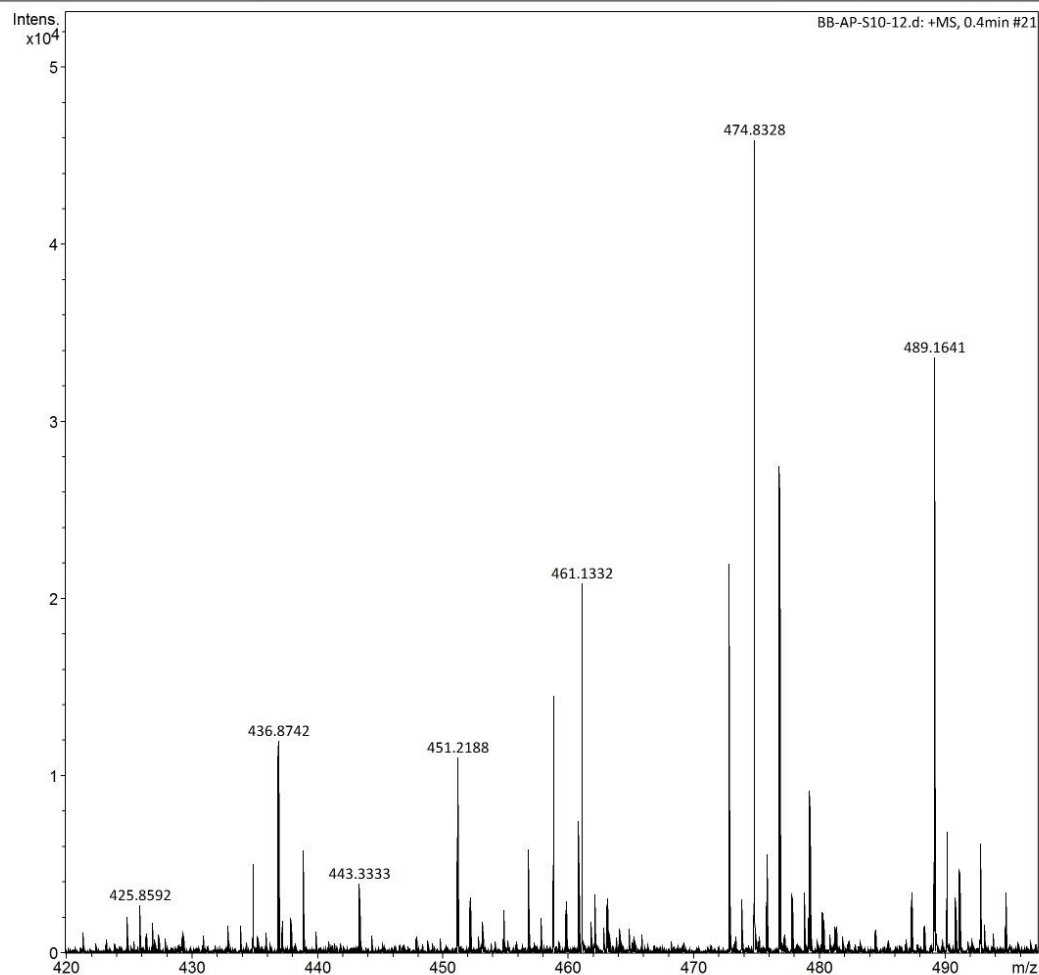
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Focus	Active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
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BB-AP-S10-12.d

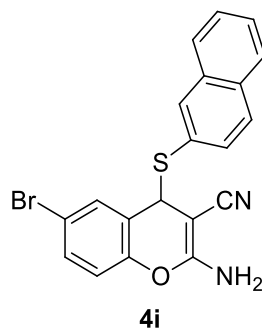
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by: HRMS

Page 1 of 1

Figure S24. HRMS spectrum of 4h



2-Amino-6-bromo-4-(naphthalen-2-ylthio)-4H-chromene-3-carbonitrile (4i). White solid, yield 90%; mp 181-183 °C; ^1H NMR (500 MHz, $\text{DMSO-}d_6$): δ_{H} /ppm 7.87-7.86 (m, 1H, aromatic H), 7.74 (d, J 8.5 Hz, 2H, aromatic H), 7.62 (s, 1H, aromatic H), 7.51-7.48 (m, 2H, aromatic H), 7.46 (d, J 2.5 Hz, 1H, aromatic H), 7.35 (dd, J 8.5 Hz, 2.5 Hz, 1H, aromatic H), 7.09 (dd, J 8.5 Hz, 1.5 Hz, 1H, aromatic H), 7.04 (s, 2H, $-\text{NH}_2$), 6.66 (d, J 8.5 Hz, 1H, aromatic H); 5.40 (s, 1H, $-\text{CH}$); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$): δ_{C} /ppm 162.4, 148.8, 136.5, 133.5, 133.2, 132.9, 131.9, 131.7, 128.6, 128.4, 128.3, 128.0, 127.4, 126.9, 124.5, 119.9, 118.2, 116.4, 53.9, 47.0; HRMS (ESI-TOF) m/z : For $\text{C}_{20}\text{H}_{13}\text{BrN}_2\text{OS}$ Calcd. $[\text{M}+\text{Na}]^+$ 432.2888; Found $[\text{M}+\text{Na}]^+$ 432.9574.

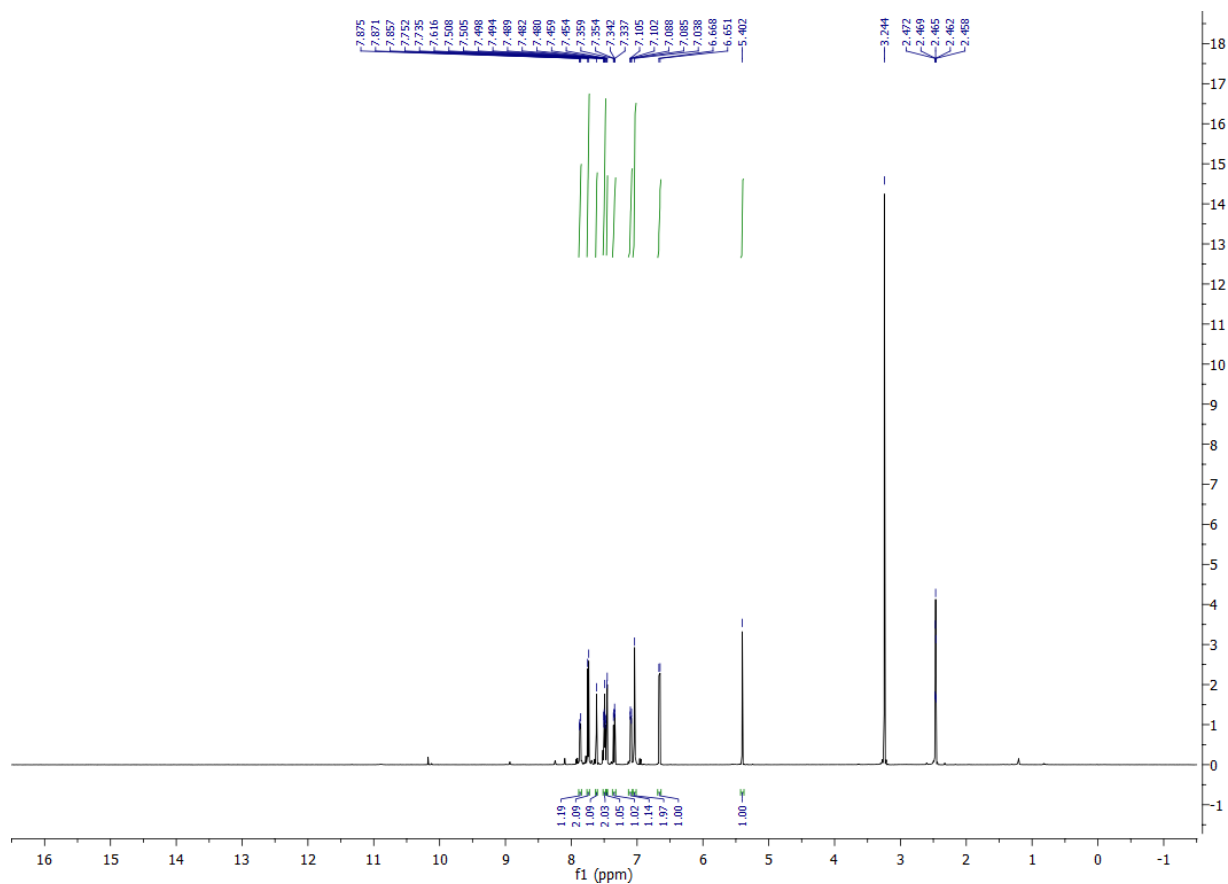


Figure S25. ^1H NMR spectrum of **4i**

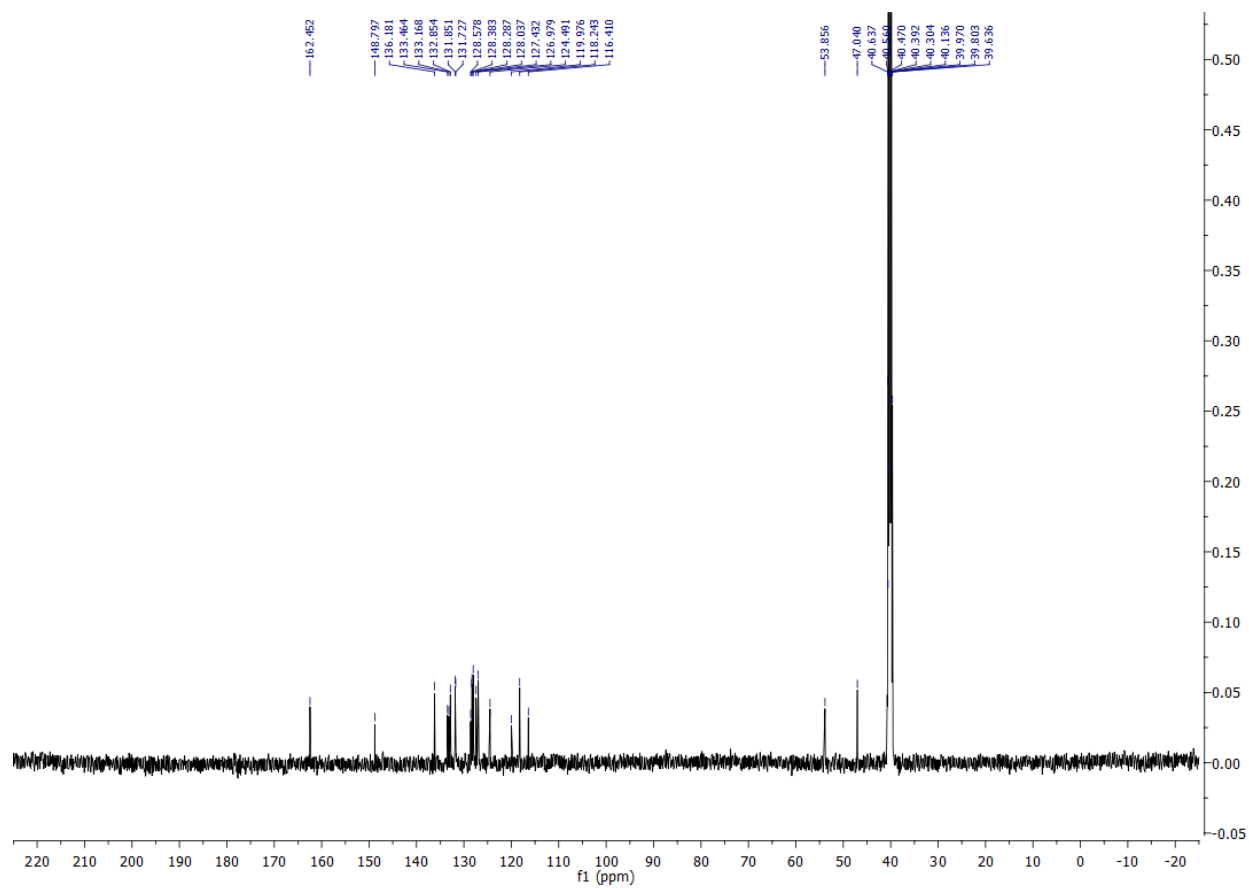


Figure S26. ¹³C NMR spectrum of 4i

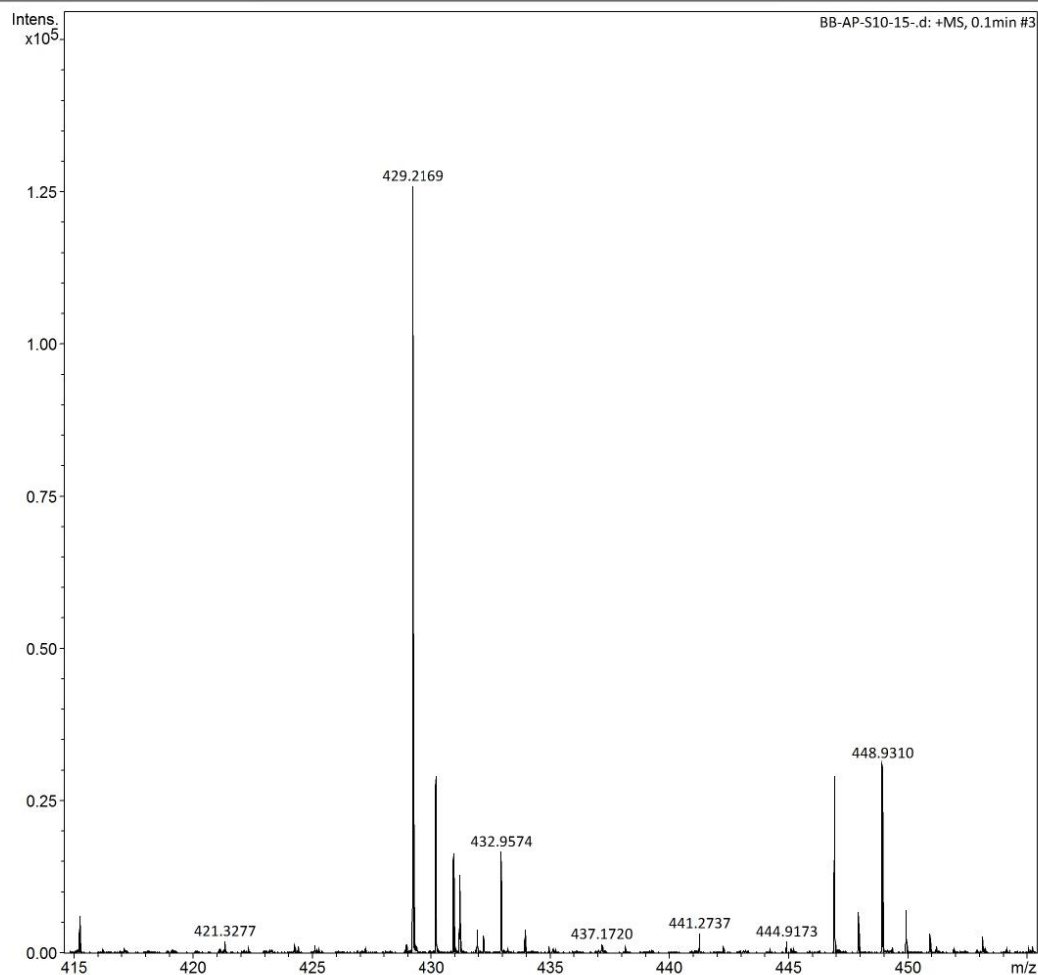
Display Report

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Sample Name
Comment

Acquisition Date 5/11/2023 10:37:28 AM
Operator HRMS
Instrument maXis impact 1819696.00160

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.5 Bar
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		Set Corona	0 nA	Set APCI Heater	0 °C



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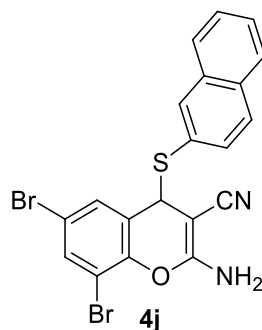
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Page 1 of 1

Figure S27. HRMS spectrum of 4i



2-Amino-6,8-dibromo-4-(naphthalen-2-ylthio)-4H-chromene-3-carbonitrile (4j). Off White solid, yield 94%; mp 173-175 °C; ^1H NMR (500 MHz, $\text{DMSO}-d_6$): δ_{H} /ppm 7.88-7.86 (m, 1H, aromatic H), 7.76 (d, J 8.5 Hz, 1H, aromatic H), 7.72 (d, J 2.5 Hz, aromatic H), 7.51-7.49 (m, 2H, aromatic H), 7.43 (d, J 2.5 Hz, 1H, aromatic H), 7.20 (s, 2H, $-\text{NH}_2$), 7.07 (dd, J 8.5 Hz, 1.5 Hz, 1H, aromatic H) 5.43 (s, 1H, CH); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$): δ_{C} /ppm 162.1, 145.9, 136.4, 134.2, 133.5, 133.3, 132.8, 131.1, 129.8, 128.5, 128.3, 128.1, 127.6, 127.0, 125.9, 119.6, 116.5, 110.6, 53.9, 47.3; HRMS (ESI-TOF) m/z : For $\text{C}_{20}\text{H}_{12}\text{Br}_2\text{N}_2\text{OS}$ Calcd. $[\text{M}+\text{Na}]^+$ 511.1848; Found $[\text{M}+\text{Na}]^+$ 510.8708.

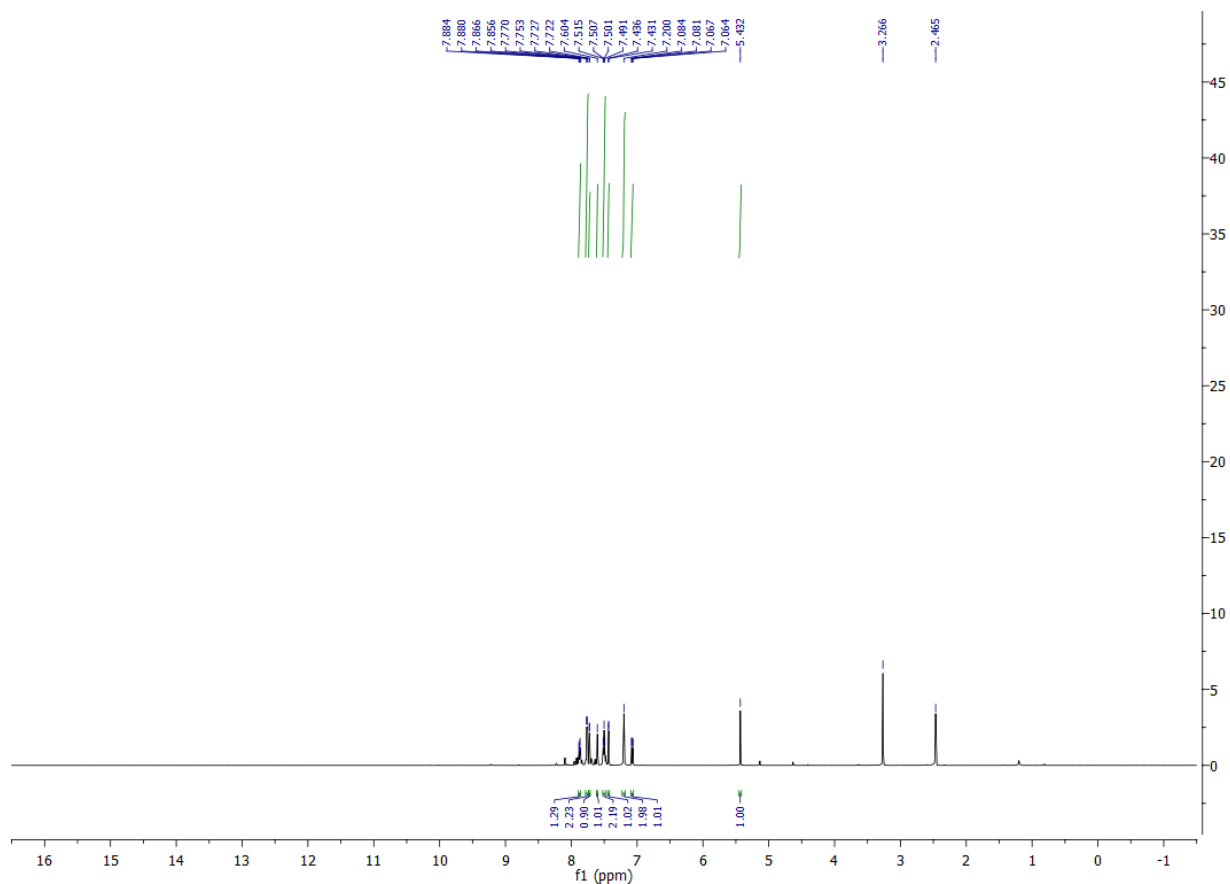


Figure S28. ^1H NMR spectrum of **4j**

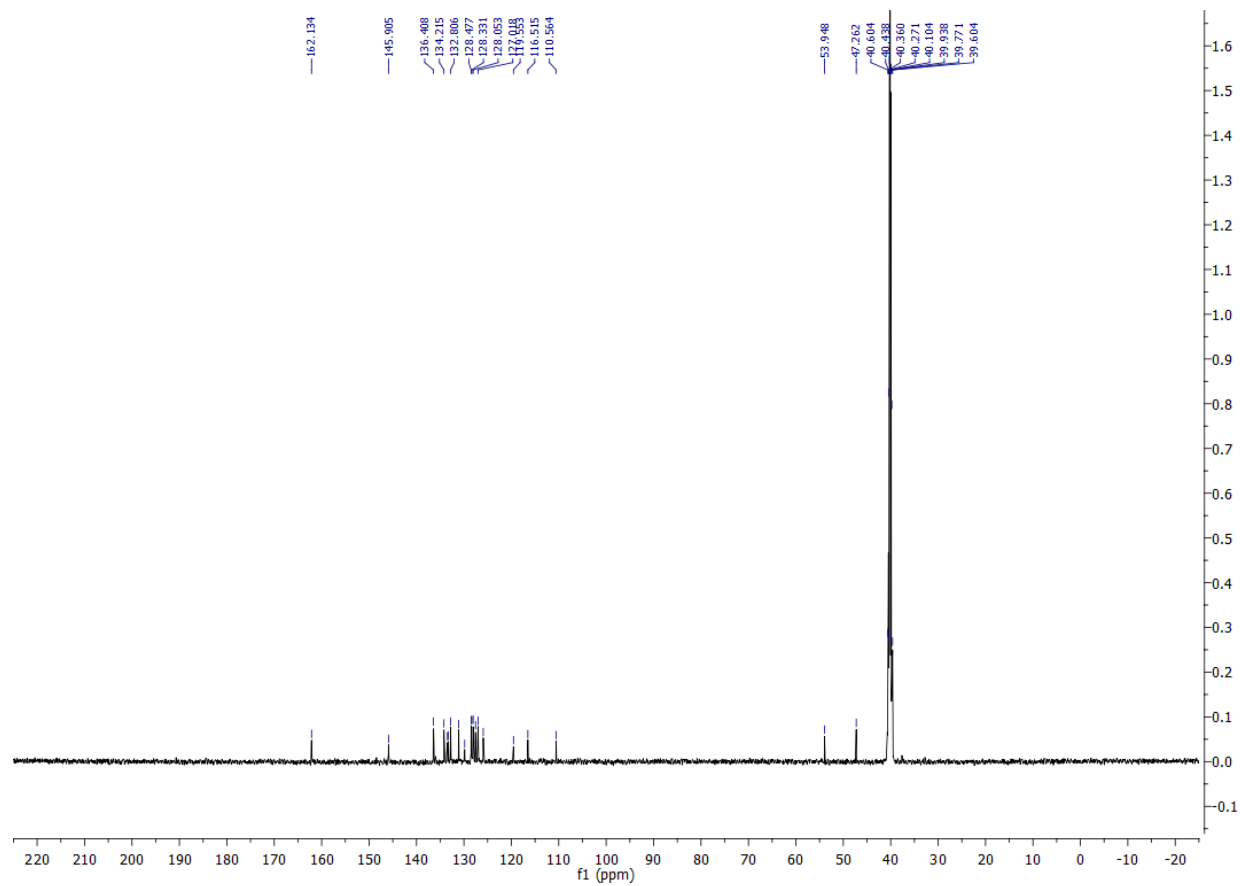


Figure S29. ^{13}C NMR spectrum of 4j

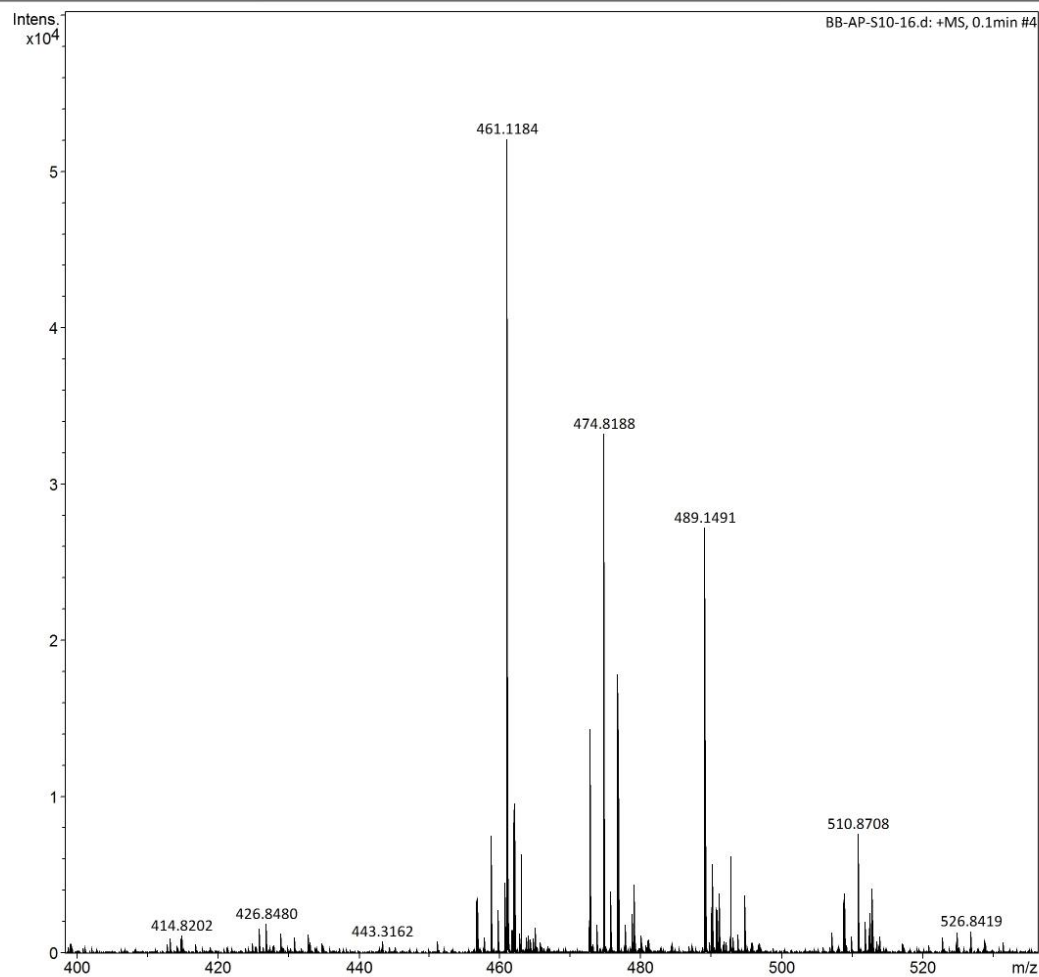
Display Report

Analysis Info
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Operator HRMS
Instrument maXis impact 1819696.00160

Acquisition Parameter

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Scan End	3000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
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Page 1 of 1

Figure S30. HRMS spectrum of 4j