

Supplementary Material

Trisodium citrate dihydrate catalyzed one-pot four component synthesis of spiroprano-indenoquinoxaline derivatives and their molecular docking analysis on the anti-cancer efficacies

Bubun Banerjee,^{1,2*} Aditi Sharma,¹ Pooja A. Chawla,³ Keshav Taruneshwar Jha,³ Kinkar Biswas,⁴ Mayukh Deb,⁵ Manmeet Kaur,¹ Anu Priya,¹ and Arvind Singh¹

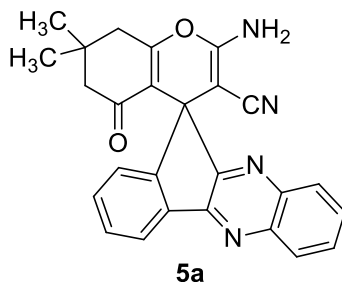
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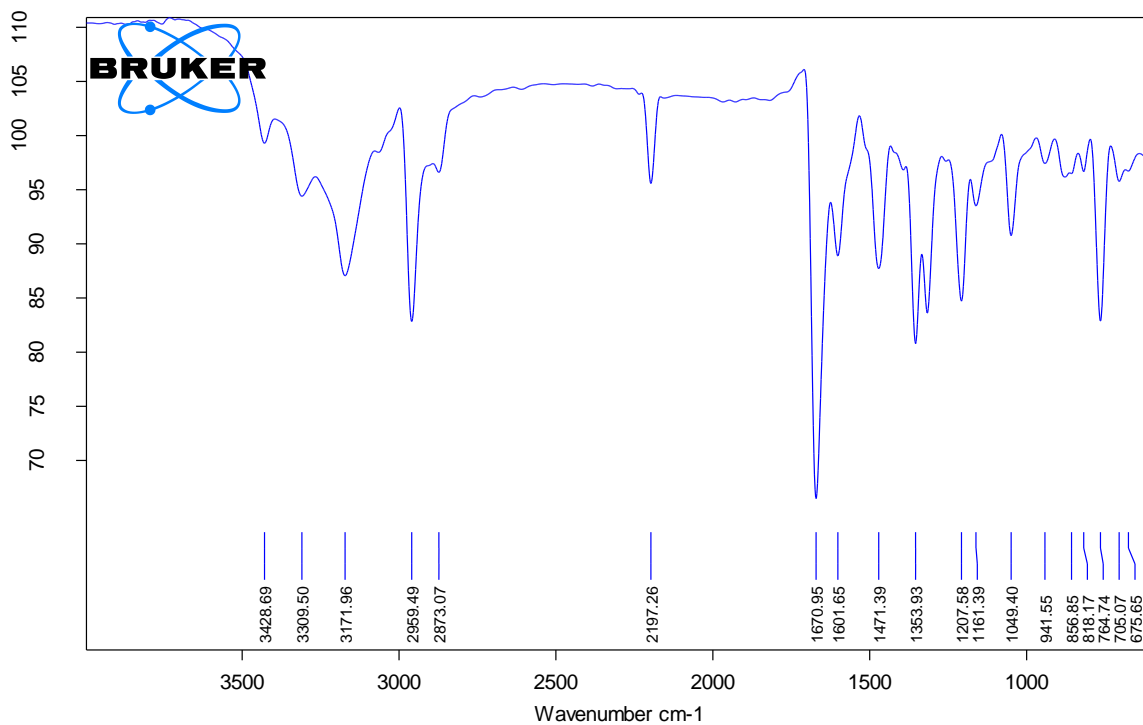
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FTIR, ¹H-NMR, ¹³C-NMR and HRMS spectra.....S2

Characterization data of all the synthesized compounds are given below:

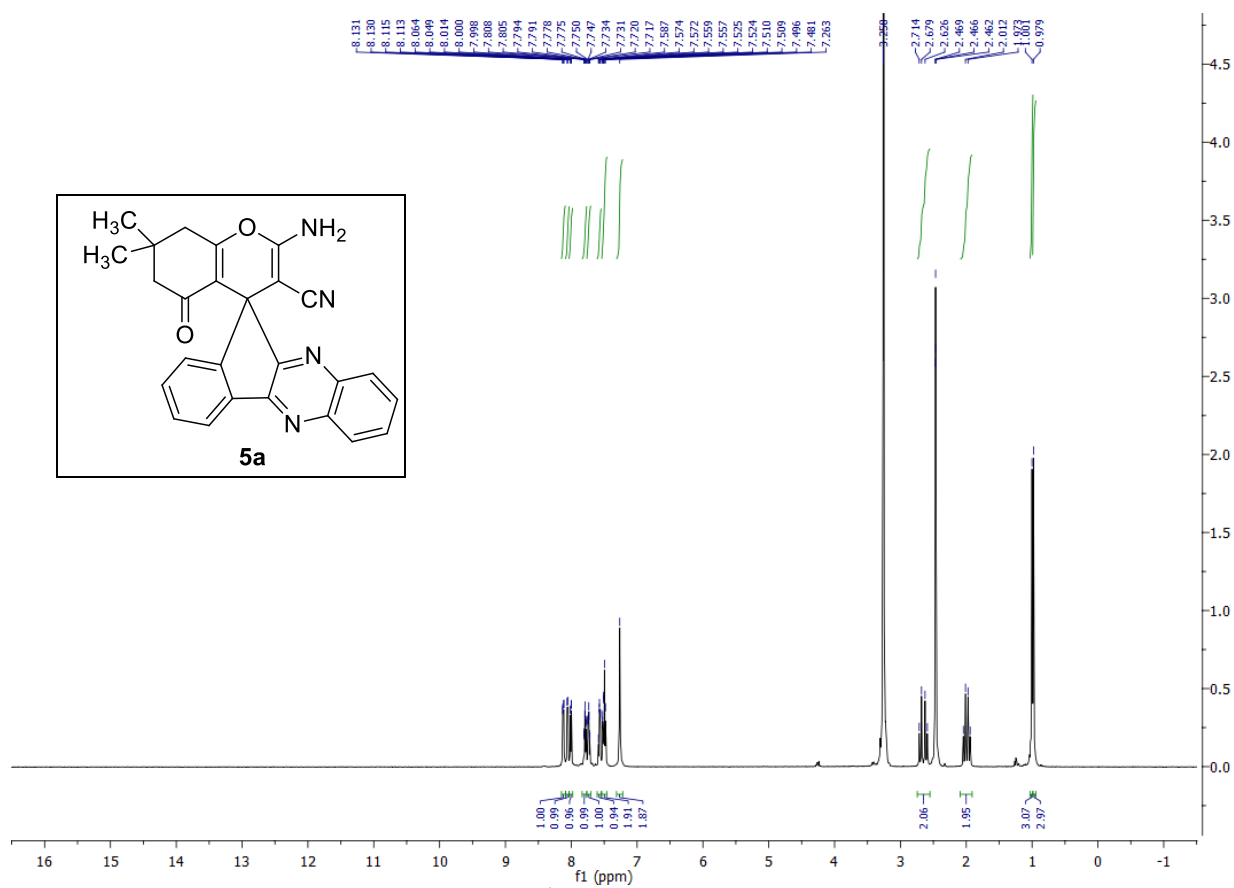


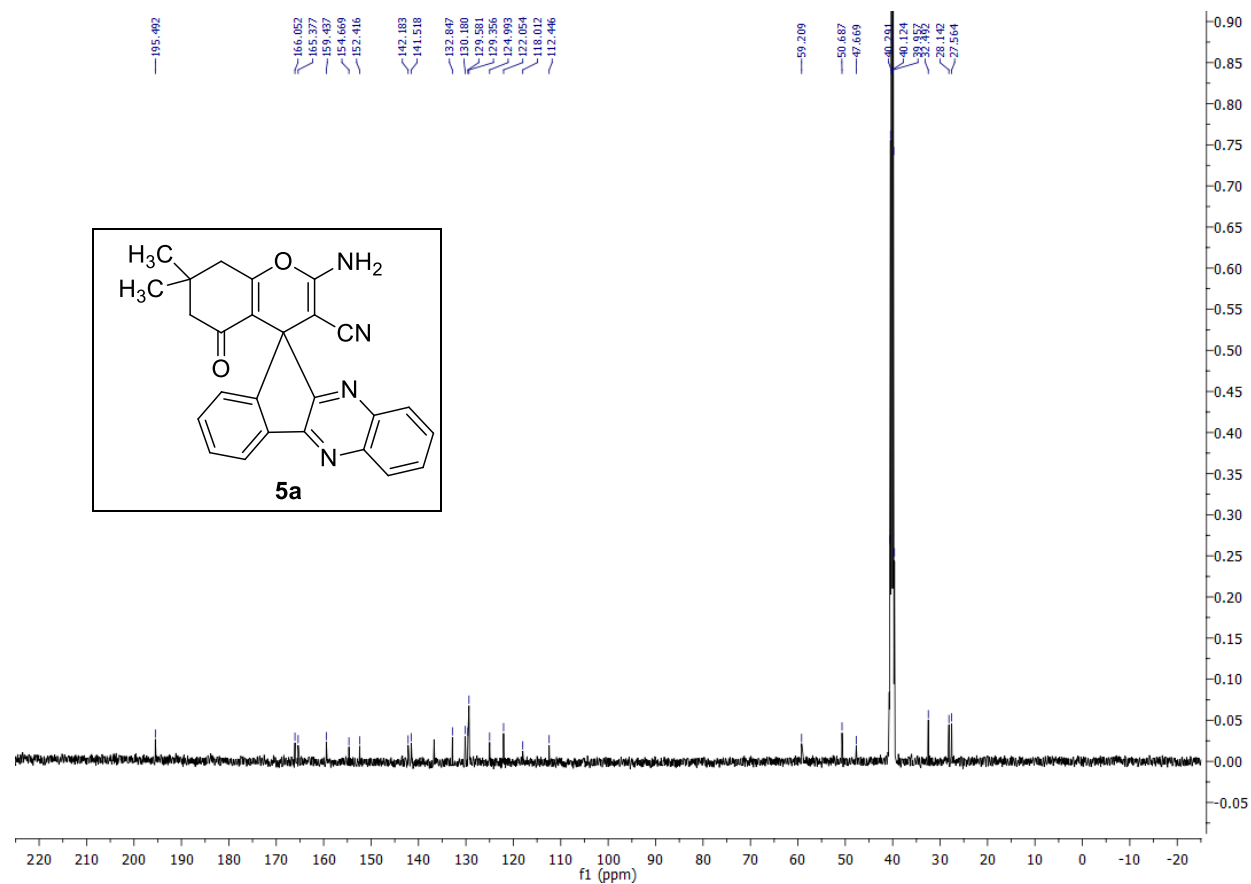
2-Amino-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydrospiro[chromene-4,11'-indeno[1,2-b]quinoxaline]-3-carbonitrile (5a). Orange solid; yield 92%; mp 295-297 °C, (lit. 282 °C)¹; FTIR (cm⁻¹): 3429, 3310, 3172, 2960, 2197, 1671, 1471, 1354, 1208, 765, 705; ¹H NMR (500 MHz, DMSO-d₆): δ_H/ppm: 8.12 (dd, 1H, *J* = 8.25 Hz, aromatic H), 8.06 (d, 1H, *J* = 7.5 Hz, aromatic H), 8.00 (t, 1H, *J* = 7 Hz, aromatic H) 7.81-7.78 (m, 1H, aromatic H), 7.75-7.71 (m, 1H, aromatic H), 7.59-7.56 (m, 1H, aromatic H), 7.53-7.48 (m, 2H, aromatic H), 7.26 (s, 2H, -NH₂), 2.65 (q, 2H, *J* = 17.5 Hz, -CH₂-), 1.99 (q, 2H, *J* = 16 Hz, -CH₂-), 1.00 (s, 3H, -CH₃), 0.98 (s, 3H, -CH₃); ¹³C NMR (125 MHz, DMSO-d₆): δ_C/ppm: 195.49, 166.05, 165.38, 159.44, 154.67, 152.42, 142.18, 141.52, 132.85 (2C), 130.18 (2C), 129.58, 129.36 (2C), 124.99, 122.5 (2C), 118.01, 112.45, 59.21, 50.69, 47.67, 32.49, 28.14, 27.56; MS (ESI-TOF) *m/z*: 419.1146.



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Figure S1. FTIR spectrum of **5a**

Figure S2. ¹H NMR spectrum of **5a**

Figure S3. ^{13}C NMR spectrum of **5a**

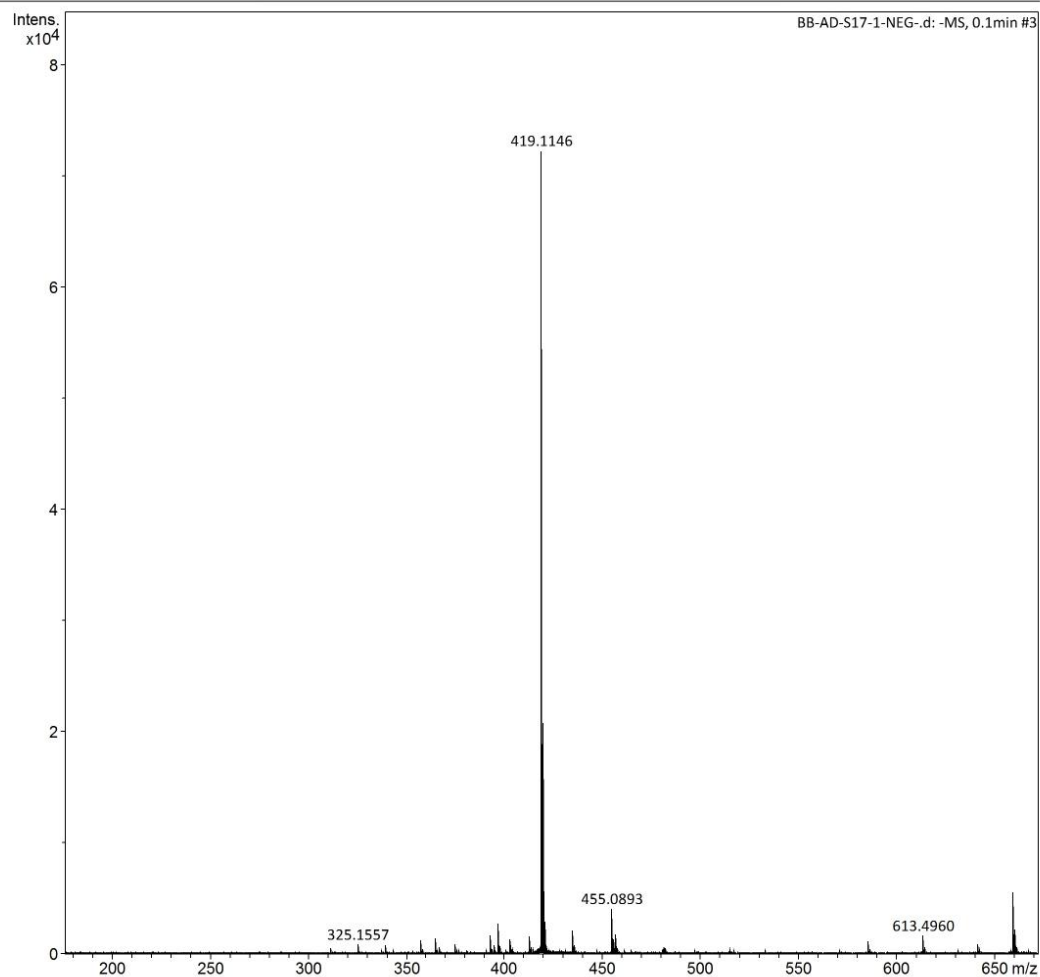
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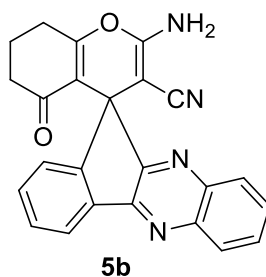
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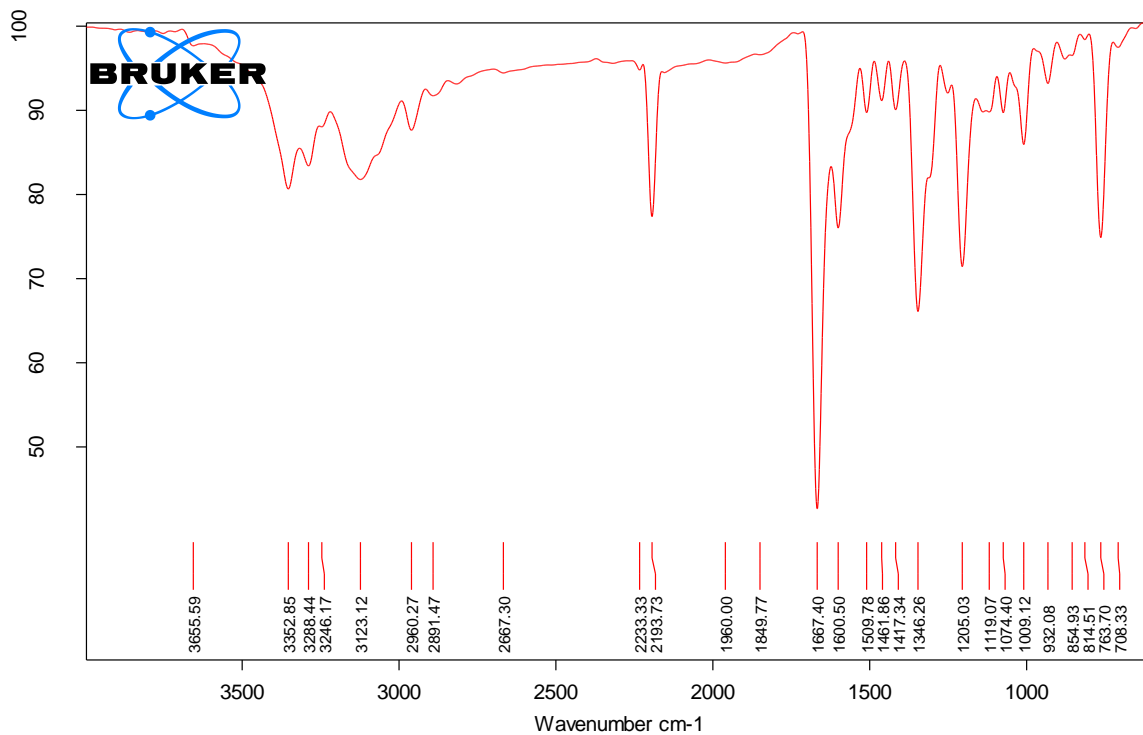
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Figure S4. HRMS spectrum of **5a**



2-Amino-5-oxo-5,6,7,8-tetrahydrospiro[chromene-4,11'-indeno[1,2-b]quinoxaline]-3-carbonitrile (5b). Orange solid; yield 88% mp 287-290 °C, (lit. 282 °C)¹; FTIR (cm⁻¹): 3353, 3288, 3123, 2960, 2233, 1667, 1462, 1346, 1205, 764, 708; ¹H NMR (500 MHz, DMSO-d₆): δ_H/ppm: 8.12 (d, 1H, *J* = 8 Hz, aromatic H), 8.04 (t, 2H, *J* = 8 Hz, aromatic H), 7.79 (t, 1H, *J* = 8 Hz, aromatic H), 7.73 (t, 1H, *J* = 7.5 Hz, aromatic H), 7.56 (t, 1H, *J* = 7.5 Hz, aromatic H), 7.51 (t, 2H, *J* = 7.5 Hz, aromatic H), 7.25 (s, 2H, -NH₂), 2.75 (q, 2H, *J* = 11.75 Hz, -CH₂-), 2.08 (q, 2H, *J* = 10.75 Hz, -CH₂-), 1.90 (t, 2H, *J* = 6.5 Hz, -CH₂-); ¹³C NMR (125 MHz, DMSO-d₆): δ_C/ppm: 195.60, 167.21, 166.15, 159.30, 154.70, 152.59, 142.15, 141.45, 136.63, 132.82, 130.14, 129.53, 129.42, 129.34, 129.31, 125.16, 121.94, 118.04, 113.54, 59.29, 47.74, 37.12, 27.51, 20.29; MS (ESI-TOF) *m/z*: 391.0892.



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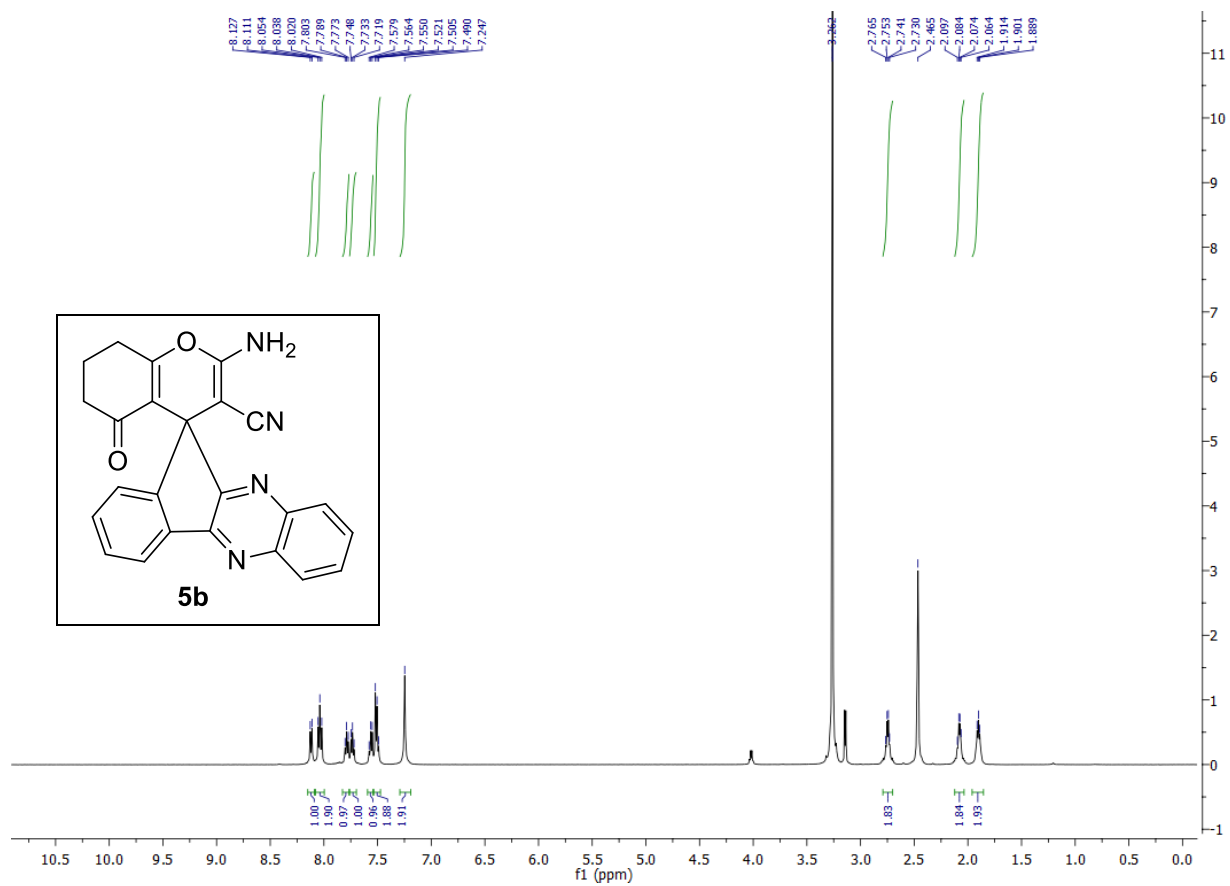
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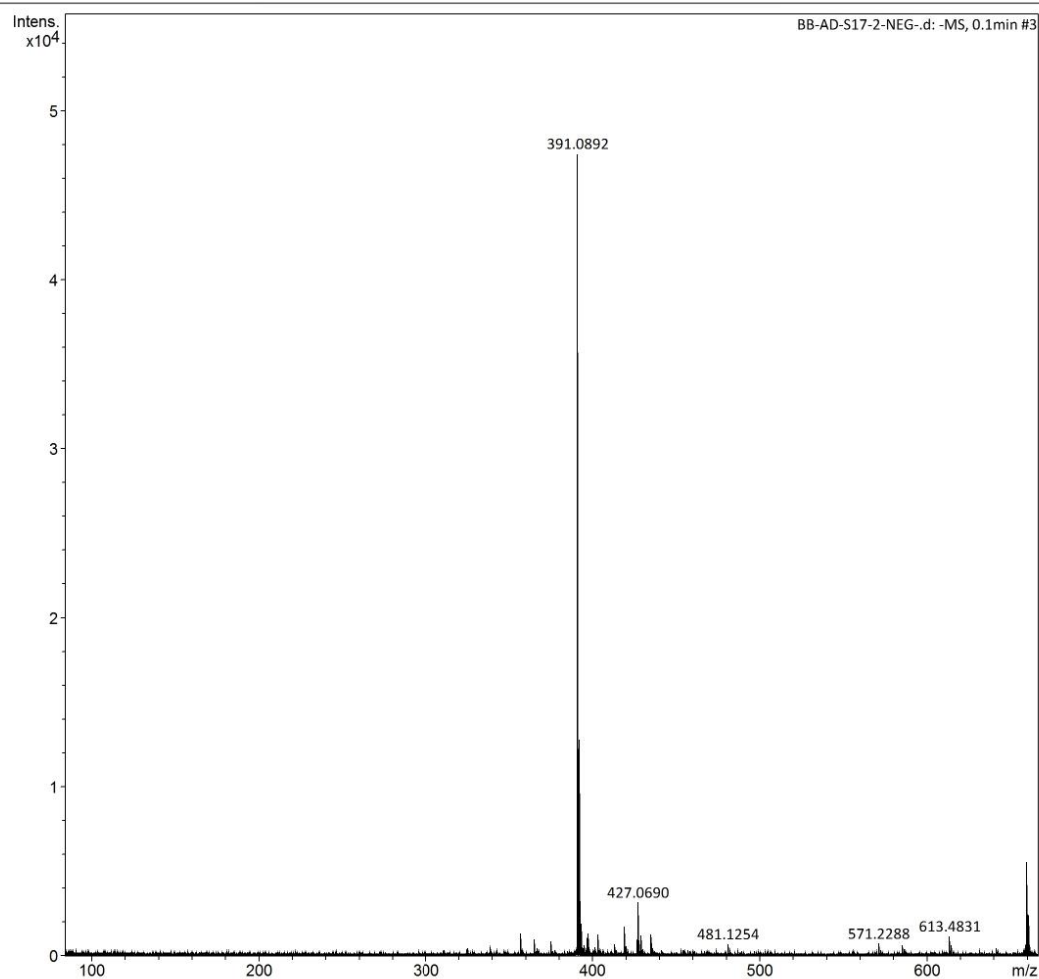
Figure S5. FTIR spectrum of **5b**

Figure S6. ¹H NMR spectrum of **5b**

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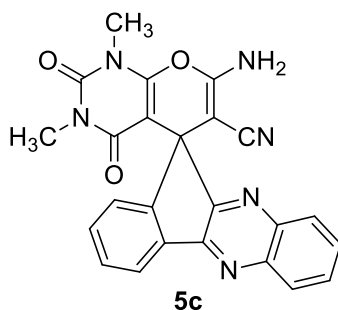
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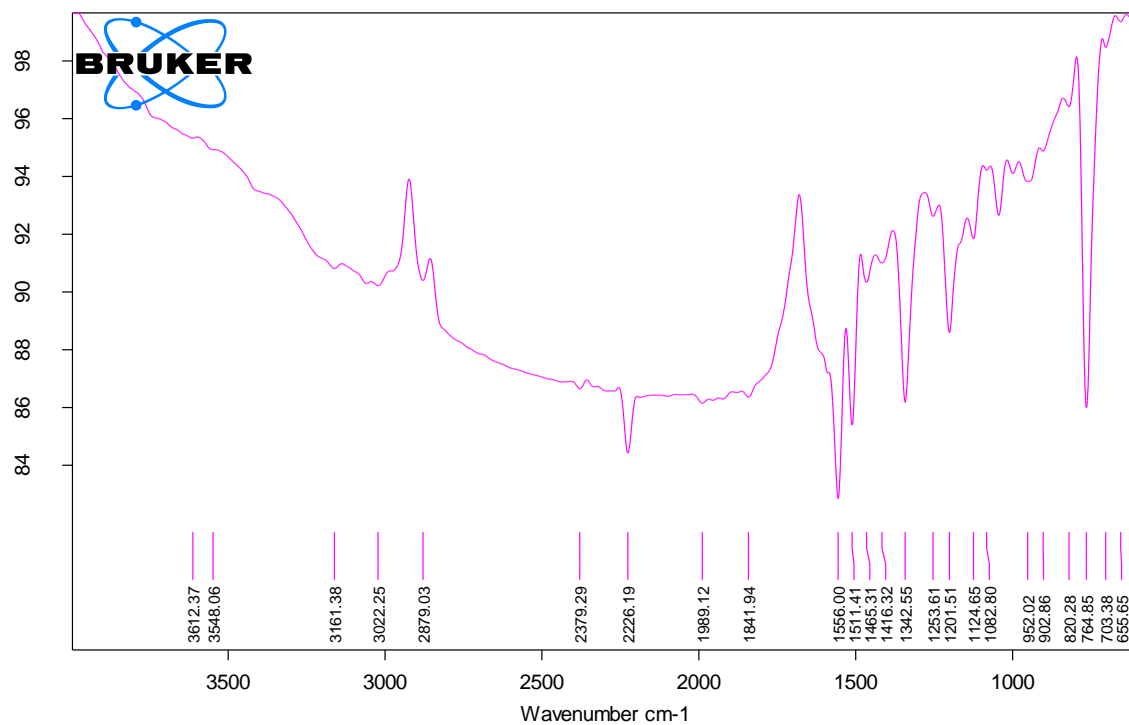
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Figure S8. HRMS spectrum of **5b**



*7'-Amino-1',3'-dimethyl-2',4'-dioxo-1',2',3',4'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,5'-pyrano[2,3-*d*]pyrimidine]-6'-carbonitrile (5c)* Orange solid; yield 85% mp 317-318 °C; FTIR (cm⁻¹): 3548, 3161, 3023, 2879, 2226, 1556, 1465, 1343, 1202, 765, 703; ¹H NMR (500 MHz, DMSO-*d*₆): δ_H/ppm: 8.41 (d, 1H, *J* = 9 Hz, aromatic H), 8.14 (q, 3H, *J* = 8 Hz, aromatic H), 8.07 (d, 1H, *J* = 7 Hz, aromatic H), 7.92-7.81 (m, 4H, aromatic 2H & -NH₂), 7.71-7.67 (m, 1H, aromatic H), 2.60 (s, 3H, -CH₃), 2.33 (s, 3H, -CH₃); ¹³C NMR (125 MHz, CDCl₃): δ_C/ppm: 153.53 (2C), 143.42, 136.04, 135.41, 135.13, 132.82, 132.55, 131.31, 130.45, 130.31, 129.71, 127.09 (2C), 126.79 (2C), 123.20 (2C), 119.28, 113.20, 111.53, 87.87, 57.68 (2C); MS (ESI-TOF) *m/z*: 437.2362.



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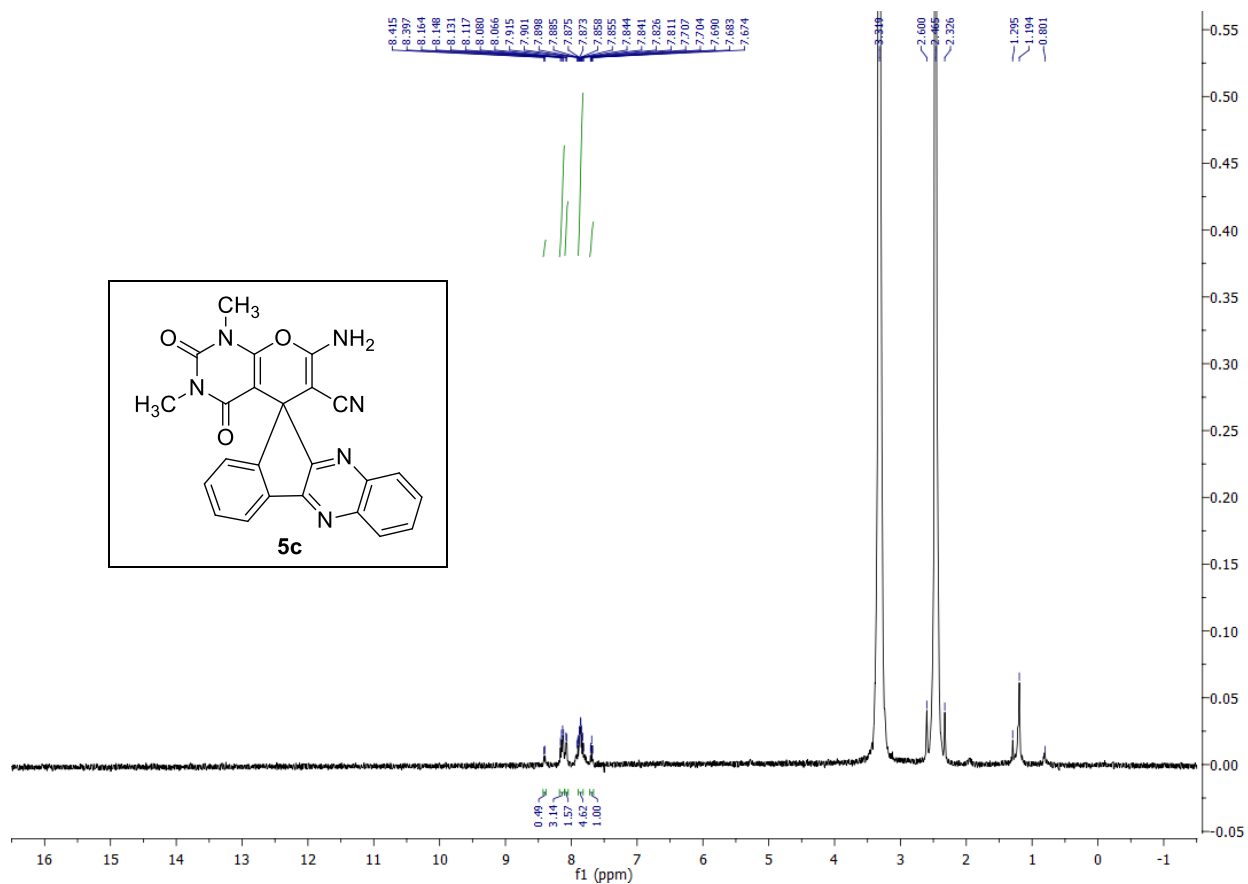
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Instrument type and / or accessory

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Figure S9. FTIR spectrum of **5c**

Figure S10. ^1H NMR spectrum of **5c**

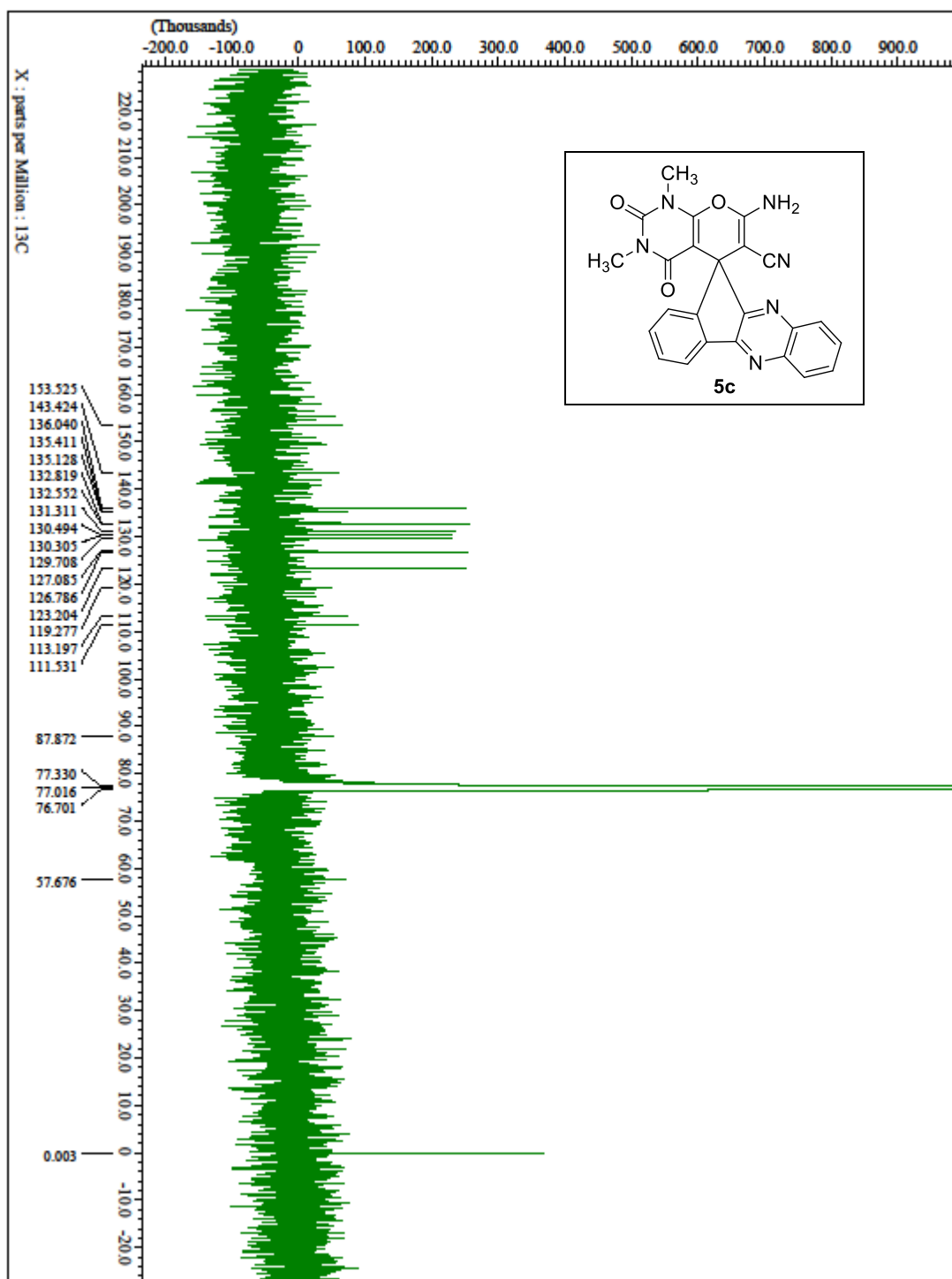


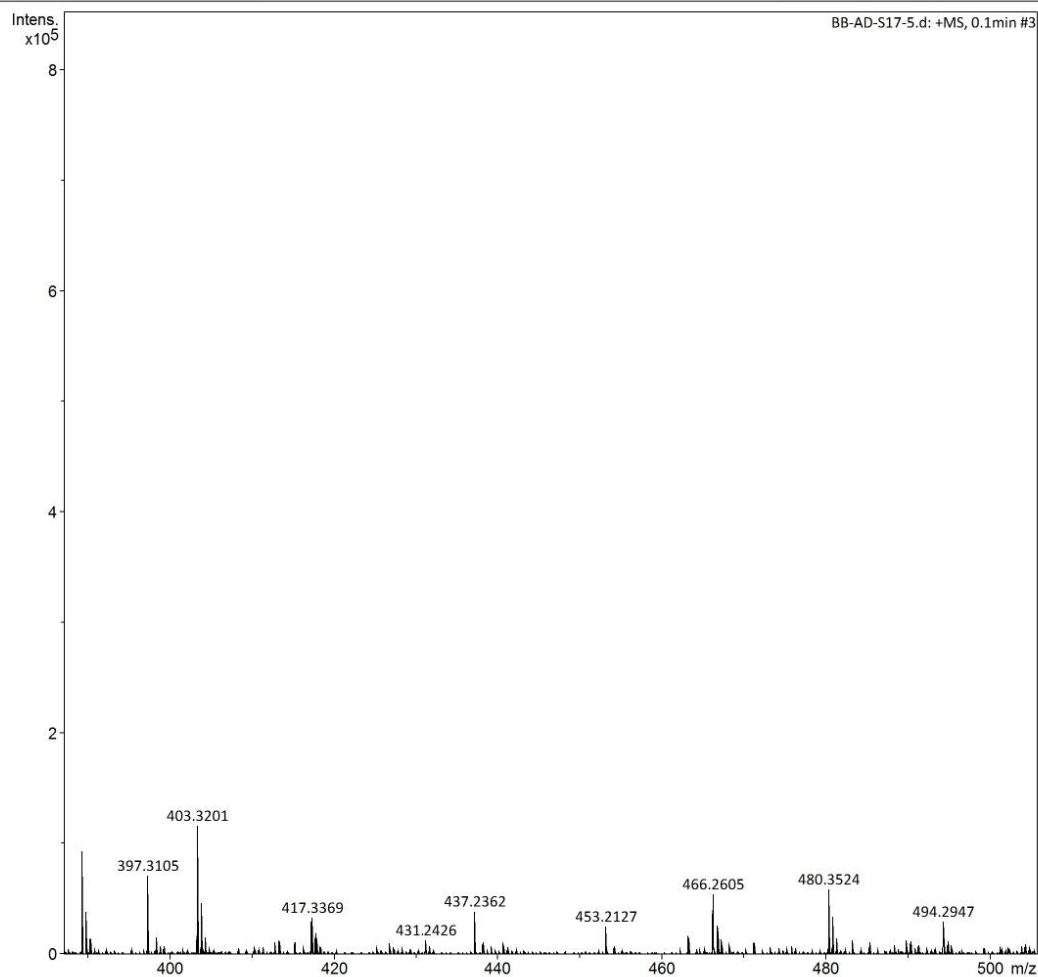
Figure S11. ^{13}C NMR spectrum of **5c** (Due to the low solubility of the molecule, the ^{13}C NMR data was collected with $n_s = 10\text{K}$ in CDCl_3 as solvent. With DMSO-d_6 as solvent we couldn't recognize all the peaks even with $n_s = 10\text{K}$)

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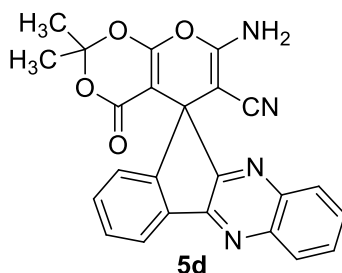
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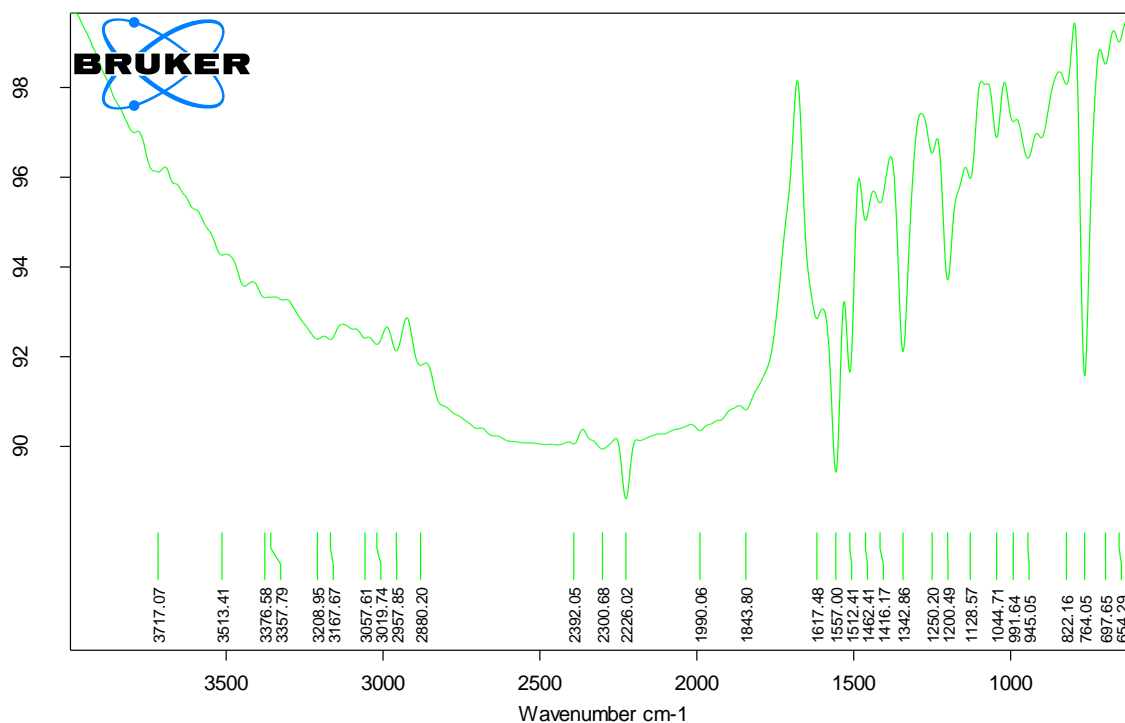
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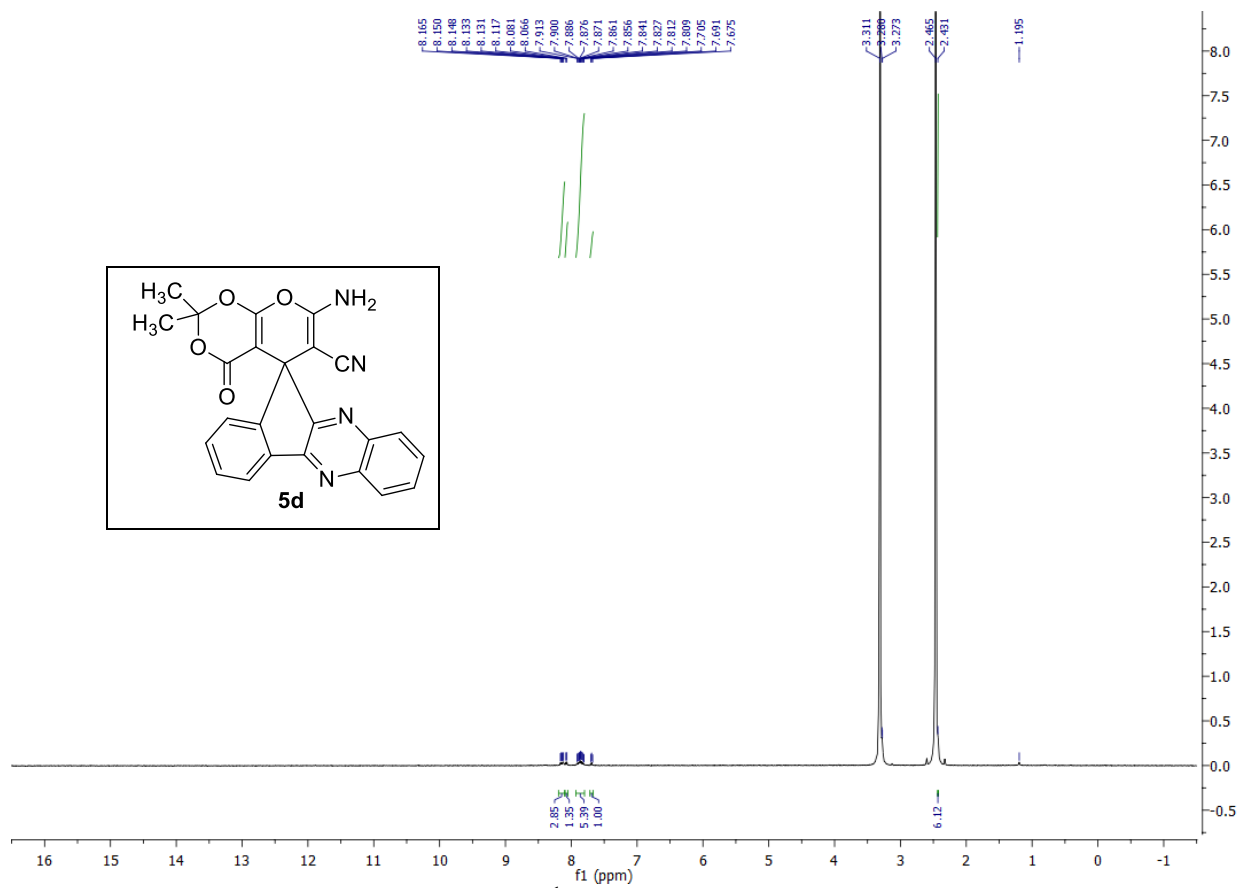
Figure S12. HRMS spectrum of **5c**



7'-Amino-2',2'-dimethyl-4'-oxo-4'H-spiro[indeno[1,2-b]quinoxaline-11,5'-pyrano[2,3-d][1,3]dioxine]-6'-carbonitrile (5d) Orange solid; yield 87% mp 312-315 °C; FTIR (cm⁻¹): 3377, 3208, 2958, 2880, 2226, 1557, 1462, 1343, 1200, 764, 698; ¹H NMR (500 MHz, DMSO-d₆): δ_H/ppm: 8.17-8.12 (m, 3H, aromatic H), 8.07 (d, 1H, *J* = 7.5 Hz, aromatic H), 7.91-7.81 (m, 5H, aromatic 3H & -NH₂), 7.69 (t, 1H, *J* = 7.5 Hz, aromatic H), 2.43 (s, 6H, -CH₃); ¹³C NMR (125 MHz, CDCl₃): δ_C/ppm: 155.52, 143.30, 141.92, 138.63, 136.04, 135.41, 132.82, 132.55, 131.31 (2C), 130.51 (2C), 129.69 (2C), 126.79 (2C), 123.22 (2C), 111.53, 103.91, 90.21, 89.95, 29.71 (2C); MS (ESI-TOF) *m/z*: 424.3493.



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Figure S14. ^1H NMR spectrum of **5d**

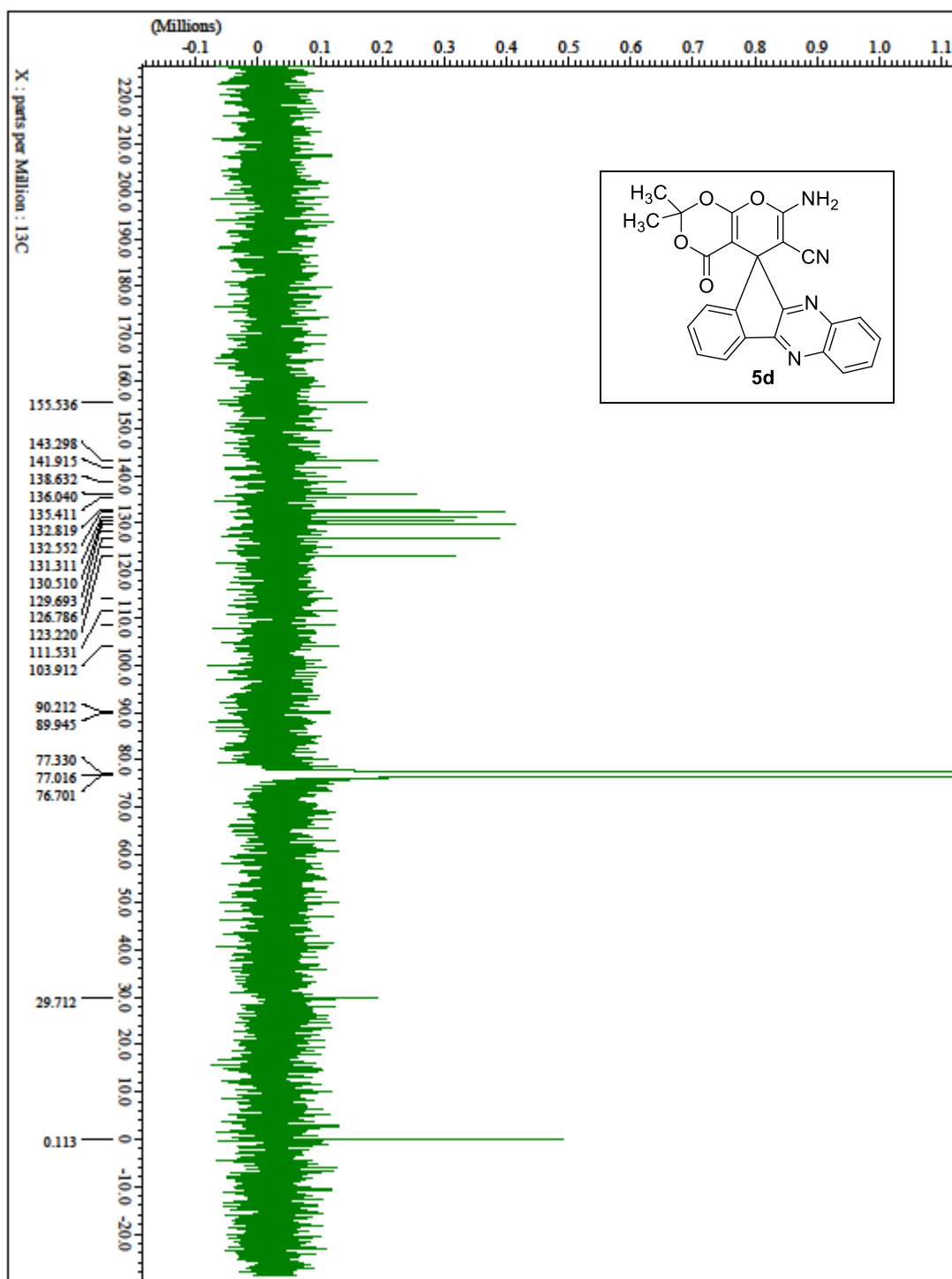


Figure S15. ^{13}C NMR spectrum of **5d** (Due to the low solubility of the molecule, the ^{13}C NMR data was collected with $n_s = 10\text{K}$ in CDCl_3 as solvent. With DMSO-d_6 as solvent we couldn't recognize all the peaks even with $n_s = 10\text{K}$)

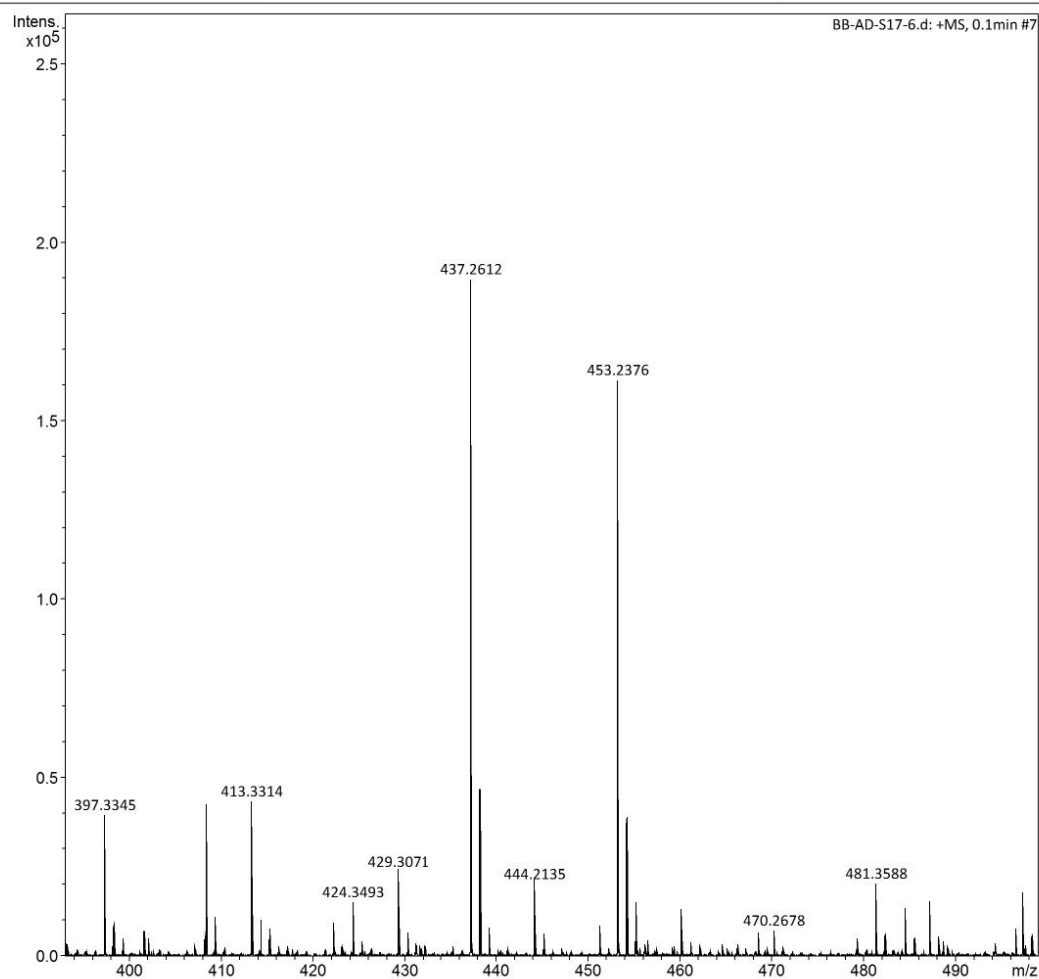
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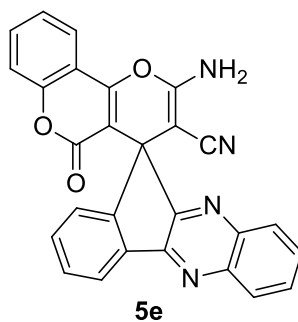
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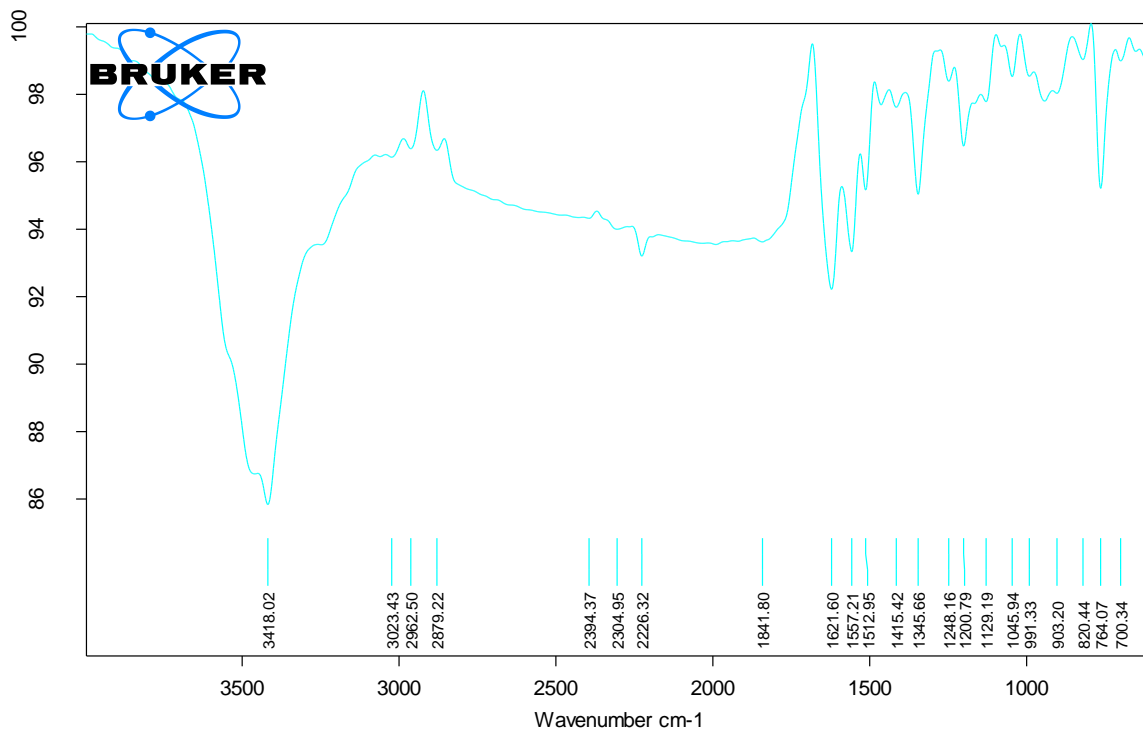
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Figure S16. HRMS spectrum of **5d**



2'-Amino-5'-oxo-5'H-spiro[indeno[1,2-b]quinoxaline-11,4'-pyrano[3,2-c]chromene]-3'-carbonitrile (5e) Orange solid; yield 86% mp 312 °C, (lit. 299 °C)¹; FTIR (cm⁻¹): 3418, 3023, 2963, 2226, 1622, 1415, 1346, 1248, 764, 700; ¹H NMR (500 MHz, DMSO-d₆): δ_H/ppm: 8.41 (d, 1H, *J* = 6 Hz, aromatic H), 8.18-8.07 (m, 4H, aromatic 2H & -NH₂), 8.03 (dd, 1H, *J* = 8, 7 Hz, aromatic H), 7.88-7.82 (m, 3H, aromatic H) 7.77 (t, 3H, *J* = 9, 7 Hz, aromatic H), 7.60-7.57 (m, 1H, aromatic H), 7.43 (d, 1H, *J* = 8 Hz, aromatic H). ¹³C NMR (125 MHz, CDCl₃): δ_C/ppm: 167.21, 153.73, 151.34, 151.03, 136.20 (2C), 136.06 (2C), 132.84 (2C), 132.57 (2C), 132.47 (2C), 131.31 (2C), 130.54 (2C), 129.93 (2C), 129.69 (2C), 123.22, 121.40, 120.88, 54.16, 50.03. MS (ESI-TOF) *m/z*: 441.0979.



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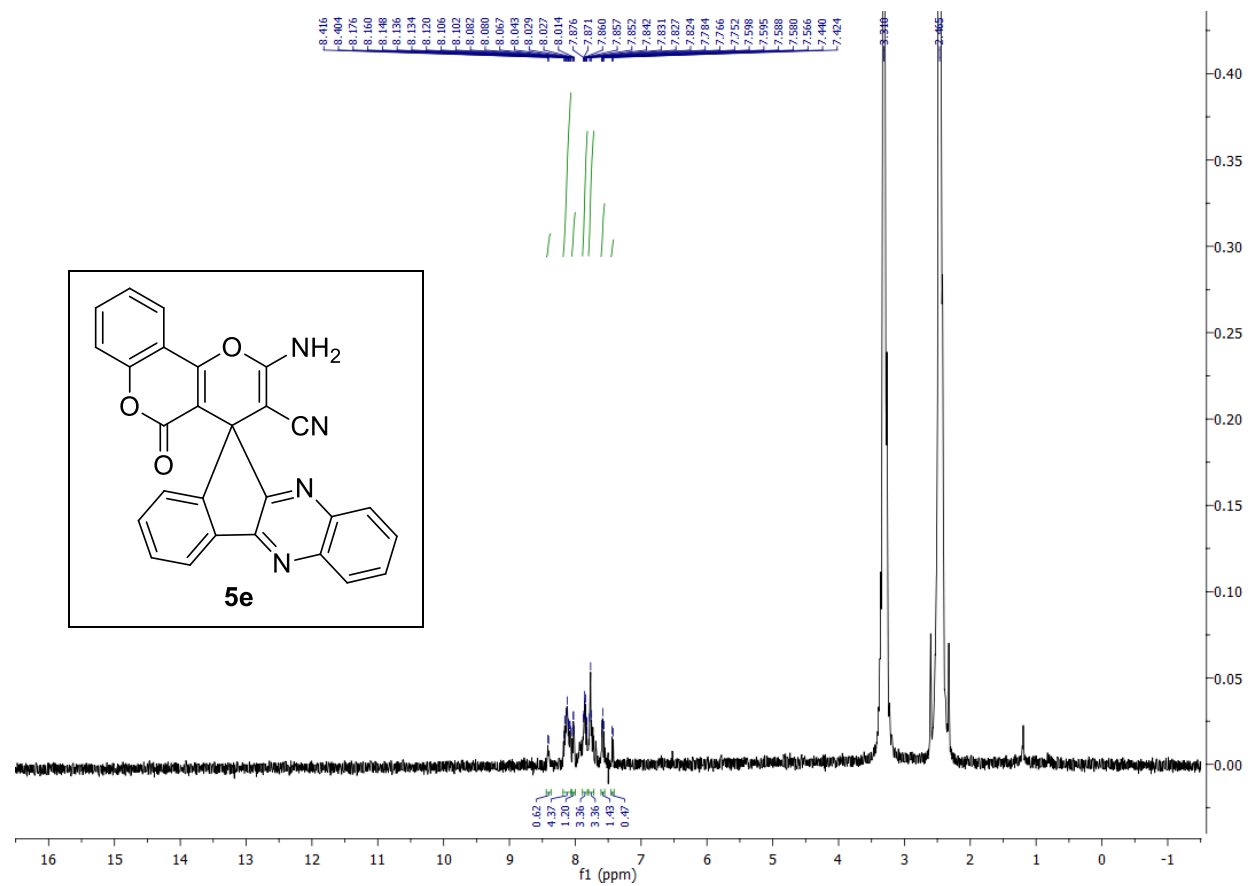
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Figure S17. FTIR spectrum of **5e**

Figure S18. ^1H NMR spectrum of **5e**

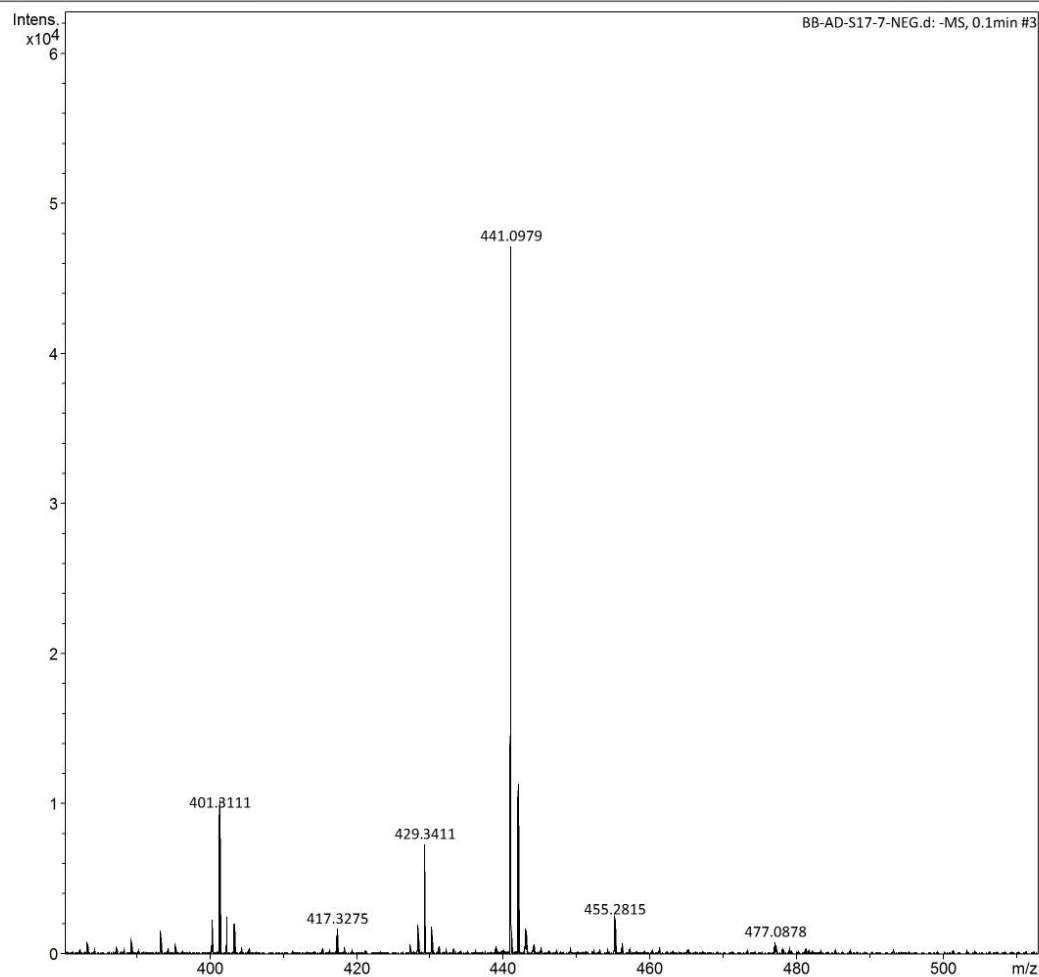
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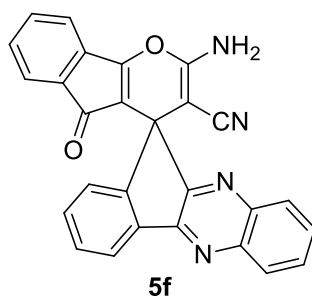
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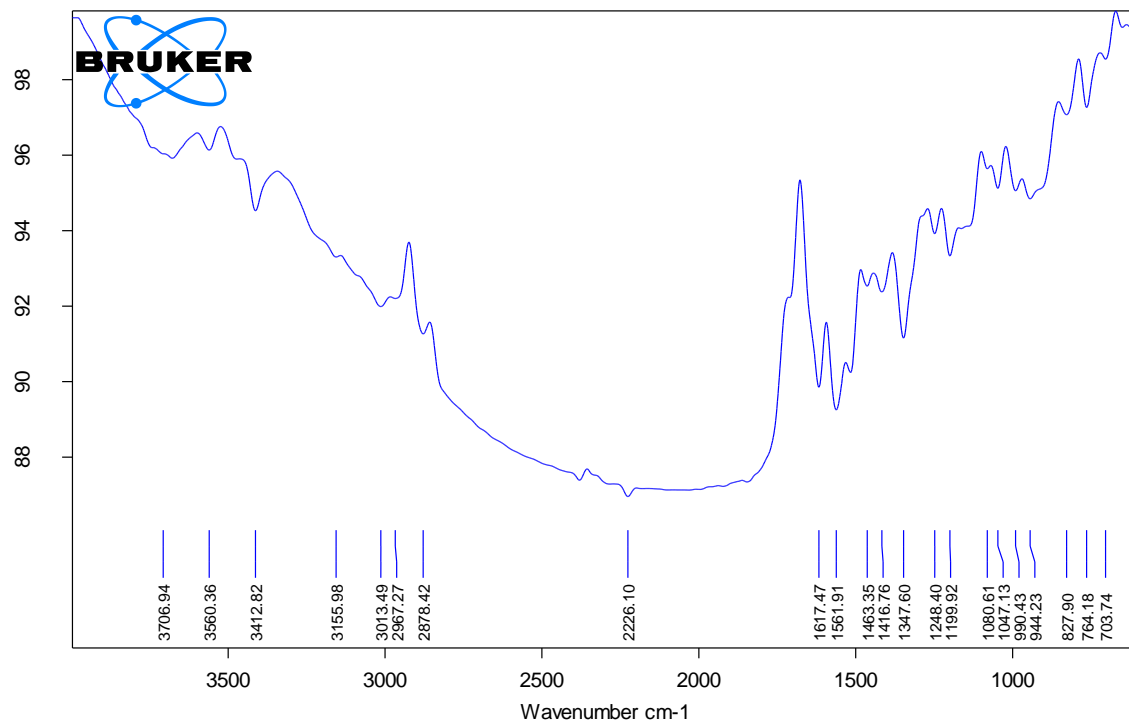
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Figure S20. HRMS spectrum of **5e**



2-Amino-5-oxo-5H-spiro[indeno[1,2-b]pyran-4,11'-indeno[1,2-b]quinoxaline]-3-carbonitrile

(5f) Orange solid; yield 87% mp 315-320 °C; FTIR (cm⁻¹): 3413, 3156, 2967, 2226, 1617, 1463, 1347, 1248, 764, 700; ¹H NMR (500 MHz, DMSO): δ_H/ppm: 8.55 (d, 1H, *J* = 7.5 Hz, aromatic H), 8.22 (d, 1H, aromatic 1H), 8.14-8.09 (m, 3H, aromatic 1H & -NH₂), 7.83 (t, 1H, *J* = 8 Hz, aromatic H), 7.76 (q, 3H, *J* = 8, 7.5 Hz, aromatic H), 7.63 (t, 1H, *J* = 8 Hz, aromatic H), 7.25 (d, 4H, *J* = 3.5 Hz, aromatic H). ¹³C NMR (125 MHz, CDCl₃): δ_C/ppm: 187.62, 153.57, 149.69, 143.25, 141.90, 140.95, 138.90, 136.06, 135.40, 132.84 (2C), 132.57 (2C), 131.31 (2C), 130.51 (2C), 129.69 (2C), 126.79 (2C), 123.22 (2C), 113.21, 111.55, 88.80, 78.57. MS (ESI-TOF) *m/z*: 427.2750.



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Instrument type and / or accessory

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Figure S21. FTIR spectrum of **5f**

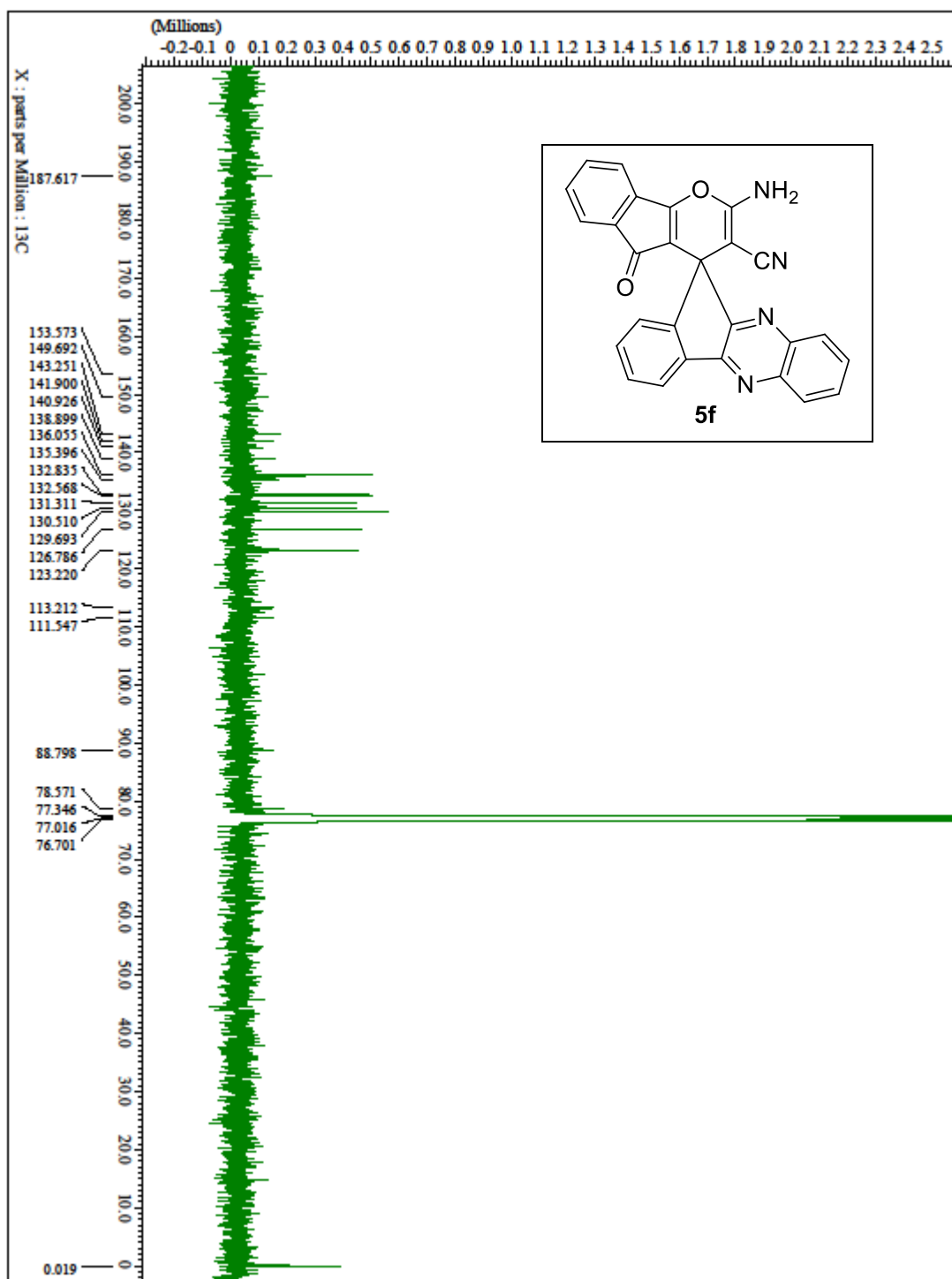


Figure S23. ^{13}C NMR spectrum of **5f** (Due to the low solubility of the molecule, the ^{13}C NMR data was collected with $ns = 10\text{K}$ in CDCl_3 as solvent. With DMSO-d_6 as solvent we couldn't recognize all the peaks even with $ns = 10\text{K}$)

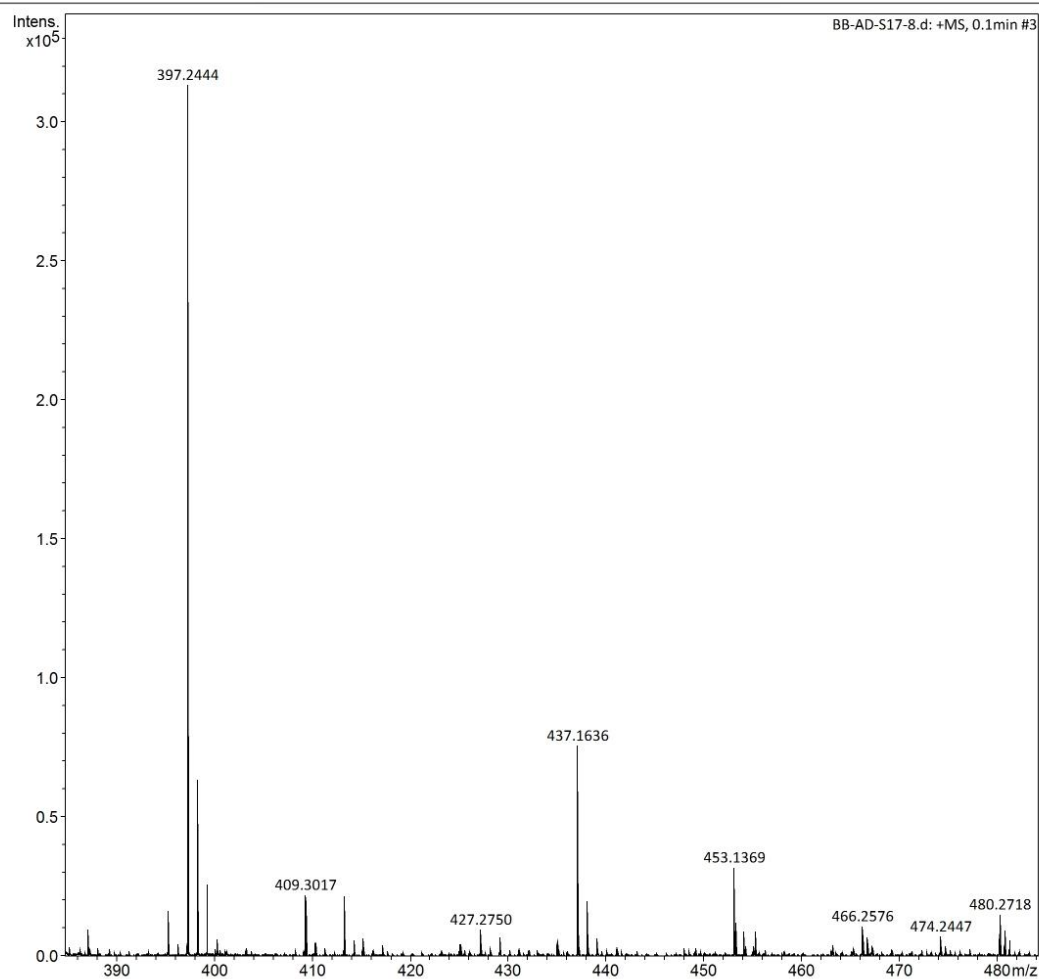
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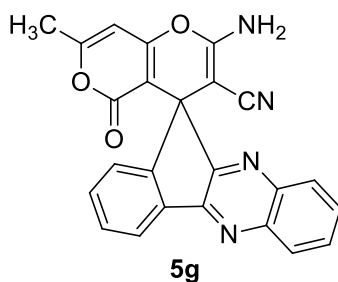
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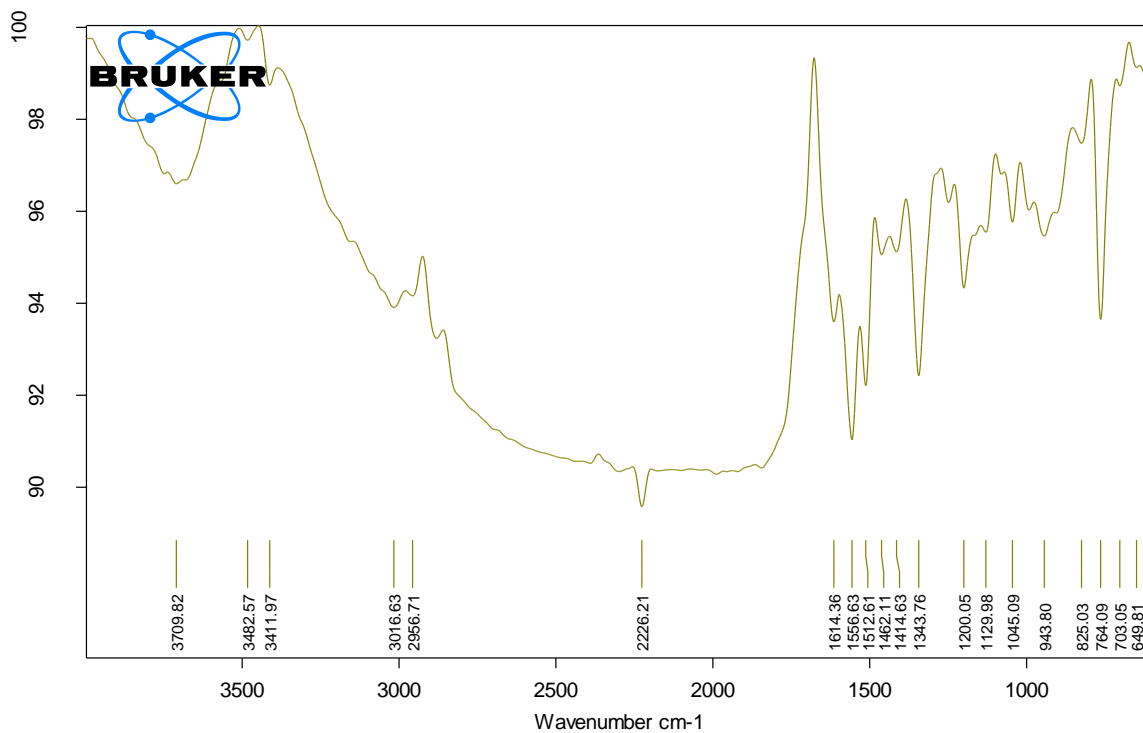
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Figure S24. HRMS spectrum of **5f**

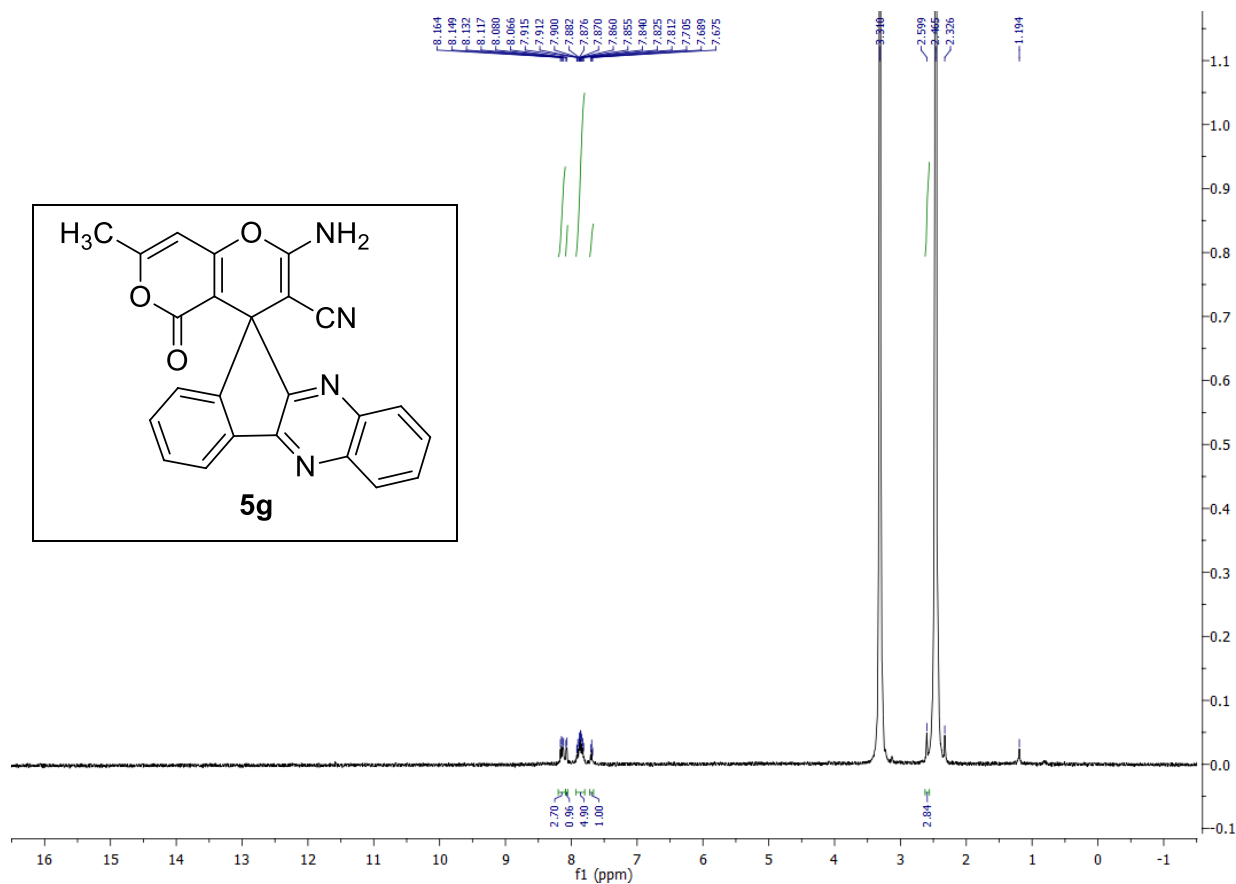


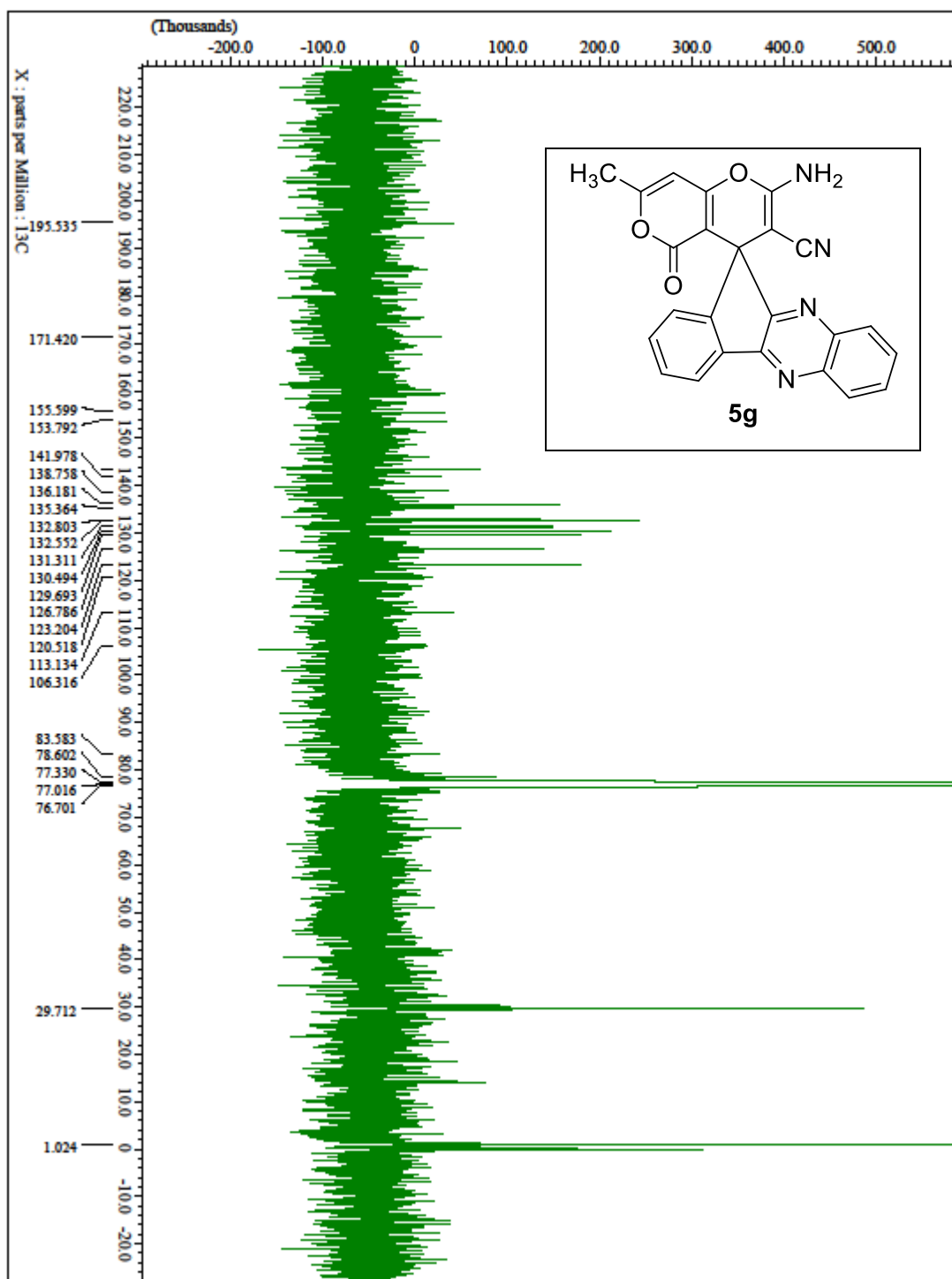
2'-Amino-7'-methyl-5'-oxo-5'H-spiro[indeno[1,2-b]quinoxaline-11,4'-pyrano[4,3-b]pyran]-3'-carbonitrile (5g) Orange solid; yield 86% mp 316-317 °C; FTIR (cm⁻¹): 3483, 3017, 2957, 2226, 1614, 1557, 1344, 1200, 764, 703; ¹H NMR (500 MHz, DMSO-d₆): δ_H/ppm: 8.14 (q, 3H, *J* = 8.5, 7.5 Hz, aromatic H), 8.07 (d, 1H, *J* = 7 Hz, aromatic H), 7.92-7.81 (m, 6H, aromatic 4H & -NH₂), 7.69 (t, 1H, *J* = 7.5 Hz, aromatic H), 2.60 (s, 3H, -CH₃). ¹³C NMR (125 MHz, CDCl₃): δ_C/ppm: 195.54, 171.42, 155.60, 153.79, 141.98, 138.76, 136.18, 135.36, 132.80 (2C), 132.55 (2C), 131.31, 130.49, 129.69, 126.79, 123.20 (2C), 120.52, 113.13, 106.32, 83.58, 78.60, 29.71. MS (ESI-TOF) *m/z*: 430.2016.



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Figure S25. FTIR spectrum of **5g**

Figure S26. ^1H NMR spectrum of **5g**



Display Report

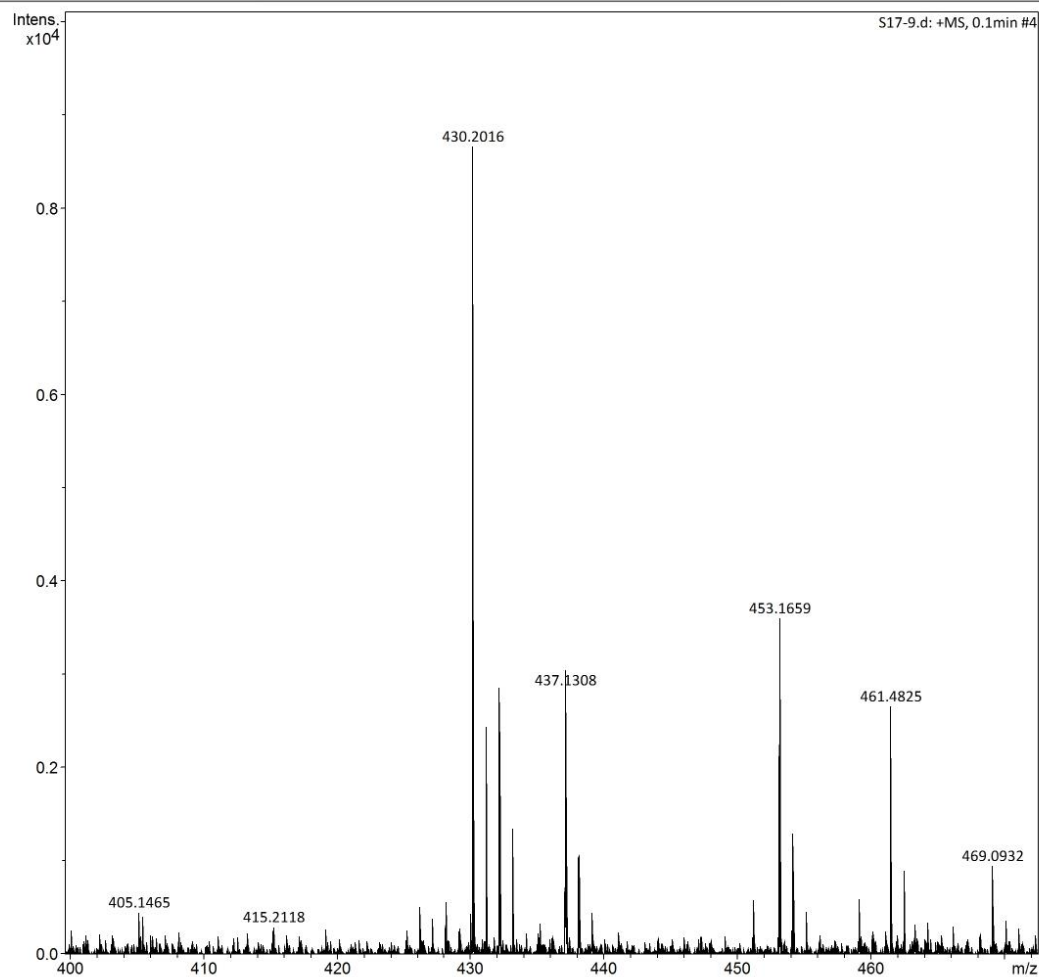
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Method Tune_pos_Mid.m
Sample Name
Comment

Acquisition Date 1/9/2024 12:47:18 PM
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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S17-9.d

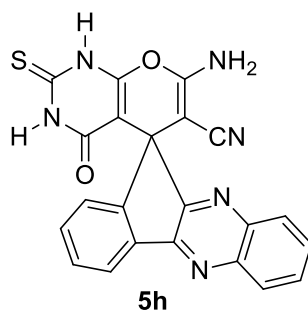
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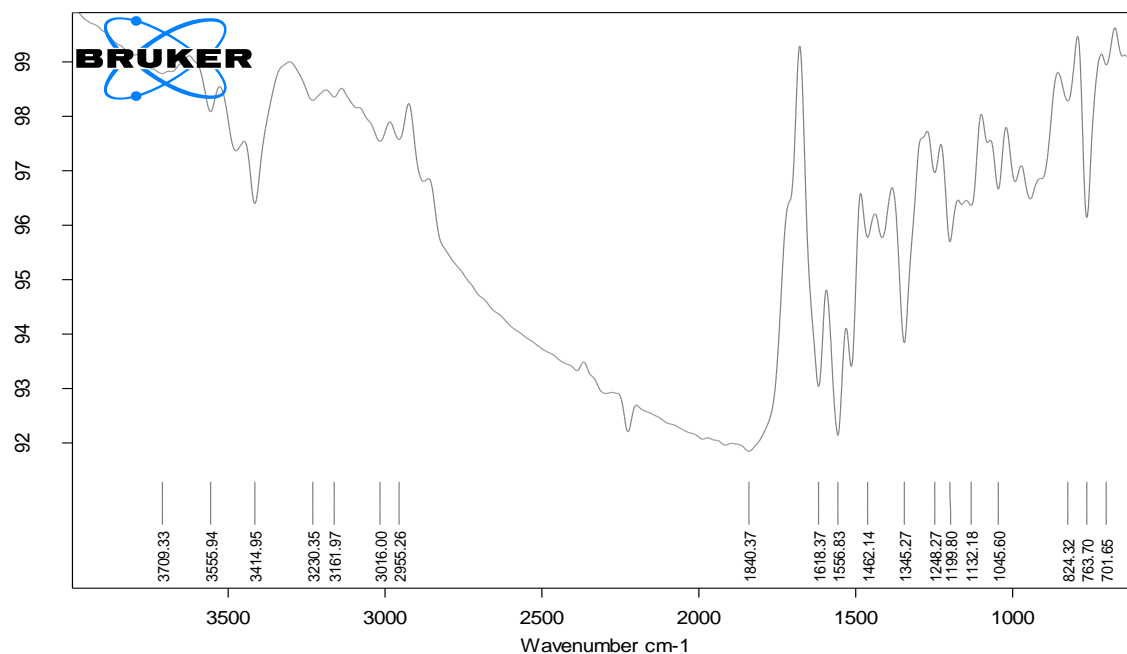
by: HRMS

Page 1 of 1

Figure S28. HRMS spectrum of **5g**



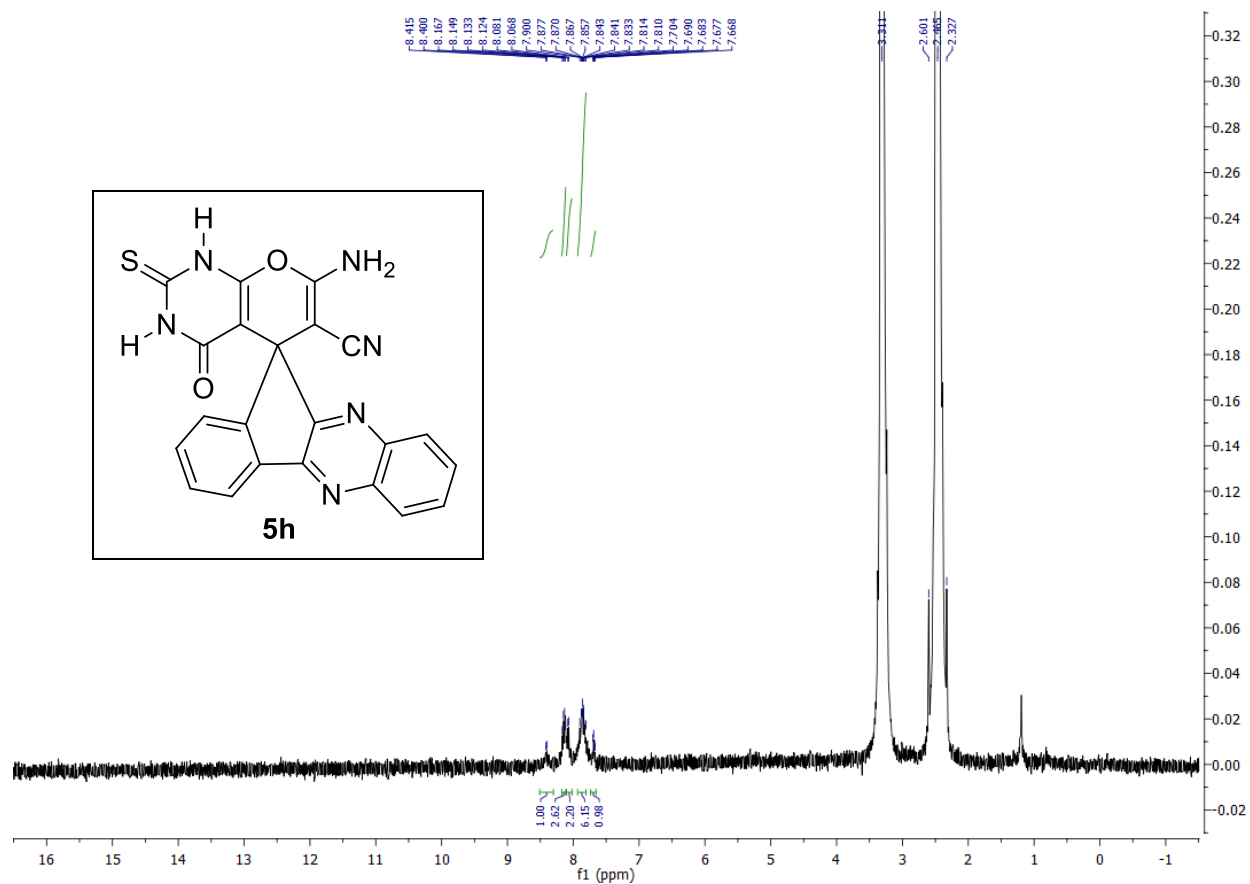
*7'-Amino-4'-oxo-2'-thioxo-1',2',3',4'-tetrahydrospiro[indeno[1,2-*b*]quinoxaline-11,5'-pyrano[2,3-*d*]pyrimidine]-6'-carbonitrile (5h)* Orange solid; yield 85% mp >300 °C; FTIR (cm⁻¹): 3415, 3230, 3016, 2955, 2226, 1618, 1557, 1345, 1248, 764, 702; ¹H NMR (500 MHz, DMSO-*d*₆): δ_H/ppm: 8.41 (d, 1H, *J* = 7.5 Hz, aromatic H), 8.14, (br s, 2H, NH), 8.75 (d, 2H, *J* = 6.5 Hz, aromatic 4H), 7.90-7.81 (m, 6H, 4 x aromatic H & -NH₂), 7.70-7.67 (m, 1H, aromatic H); ¹³C NMR (125 MHz, CDCl₃): δ_C/ppm: 212.31, 203.16, 158.63, 154.59, 142.14, 138.176, 135.03, 131.77, 131.48, 130.26 (2C), 129.44, 129.13, 128.64 (2C), 125.73 (2C), 122.26, 122.14, 115.33, 112.06, 93.21; MS (ESI-TOF) *m/z*: 425.2723.



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Figure S29. FTIR spectrum of **5h**

Figure S30. ¹H NMR spectrum of **5h**

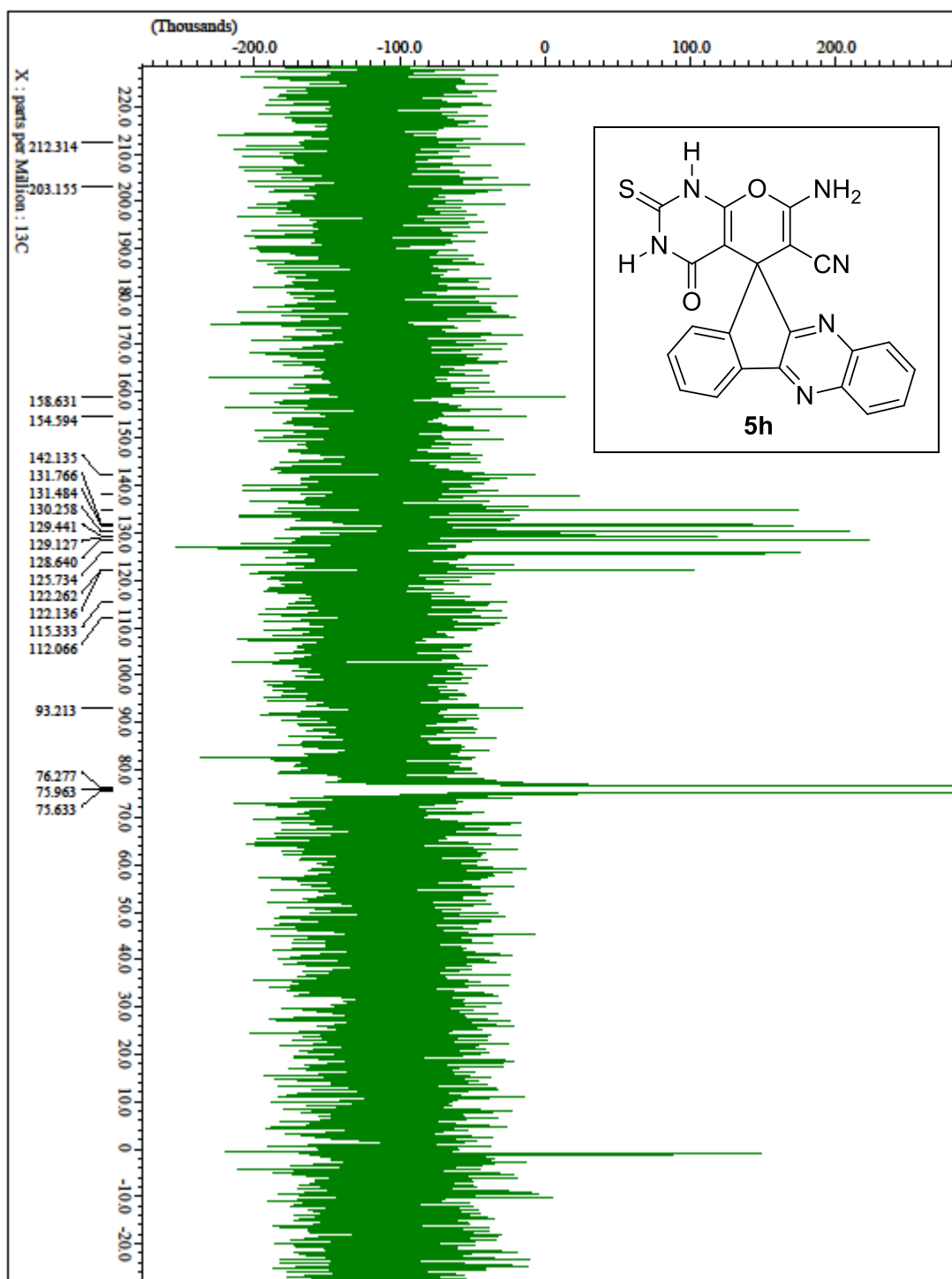


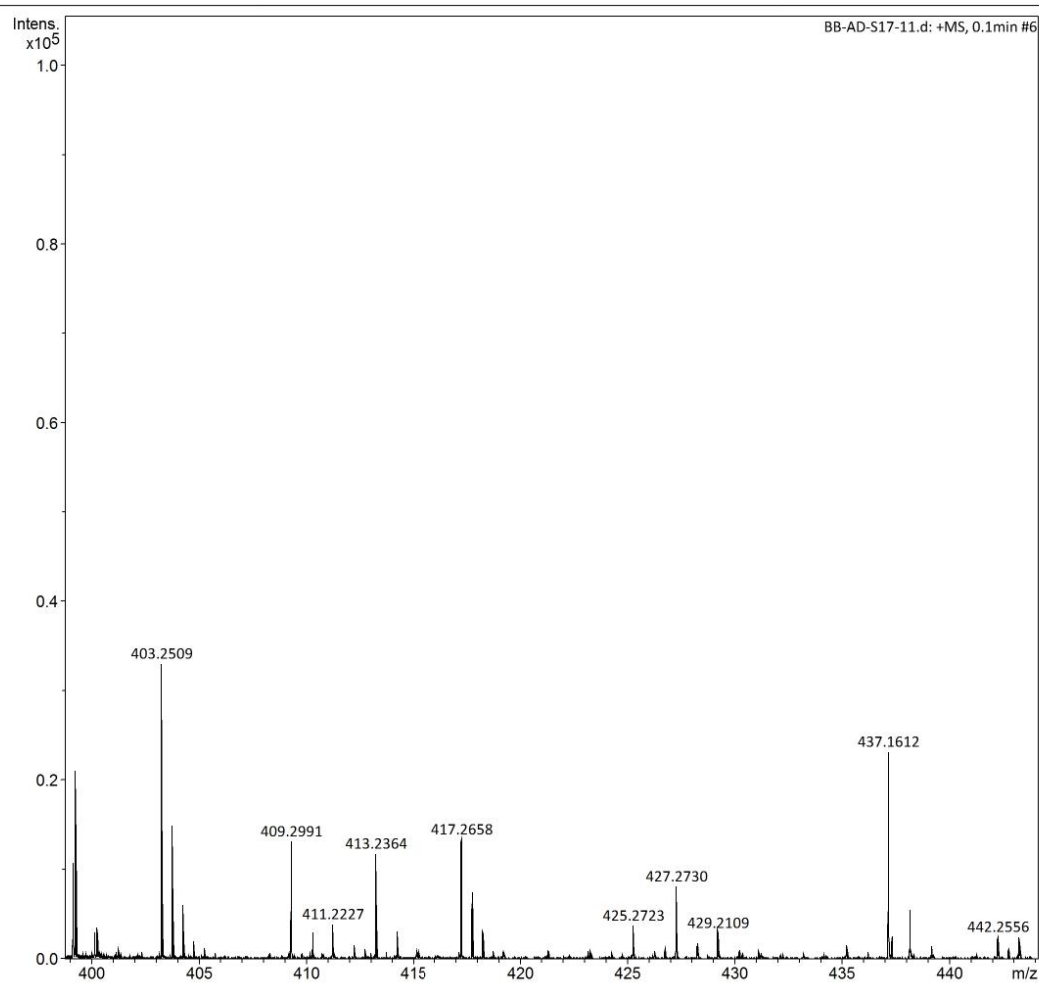
Figure S31. ^{13}C NMR spectrum of **5h** (Due to the low solubility of the molecule, the ^{13}C NMR data was collected with $n_s = 10\text{K}$ in CDCl_3 as solvent. With DMSO-d_6 as solvent we couldn't recognize all the peaks even with $n_s = 10\text{K}$)

Display Report

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Sample Name MEOH
Comment
Acquisition Date 5/17/2023 12:18:08 PM
Operator HRMS
Instrument maXis impact 1819696.00160

Acquisition Parameter

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Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
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BB-AD-S17-11.d

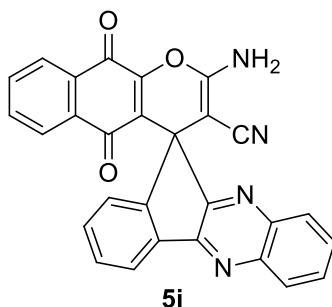
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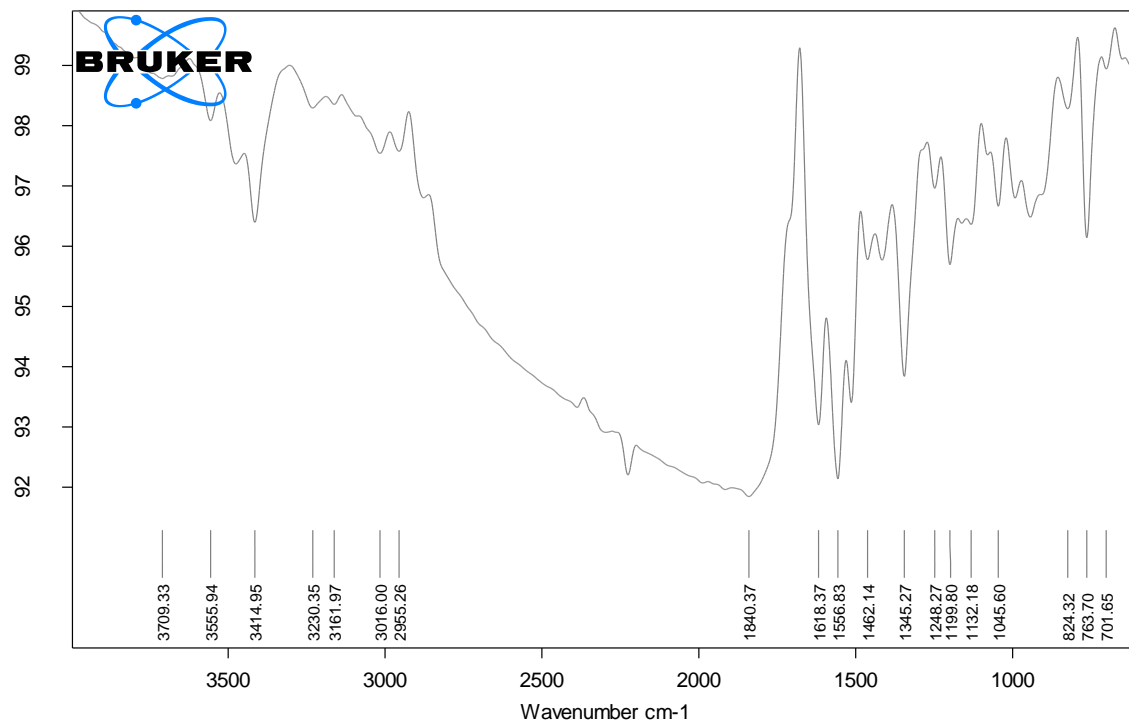
by: HRMS

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Figure S32. HRMS spectrum of **5h**



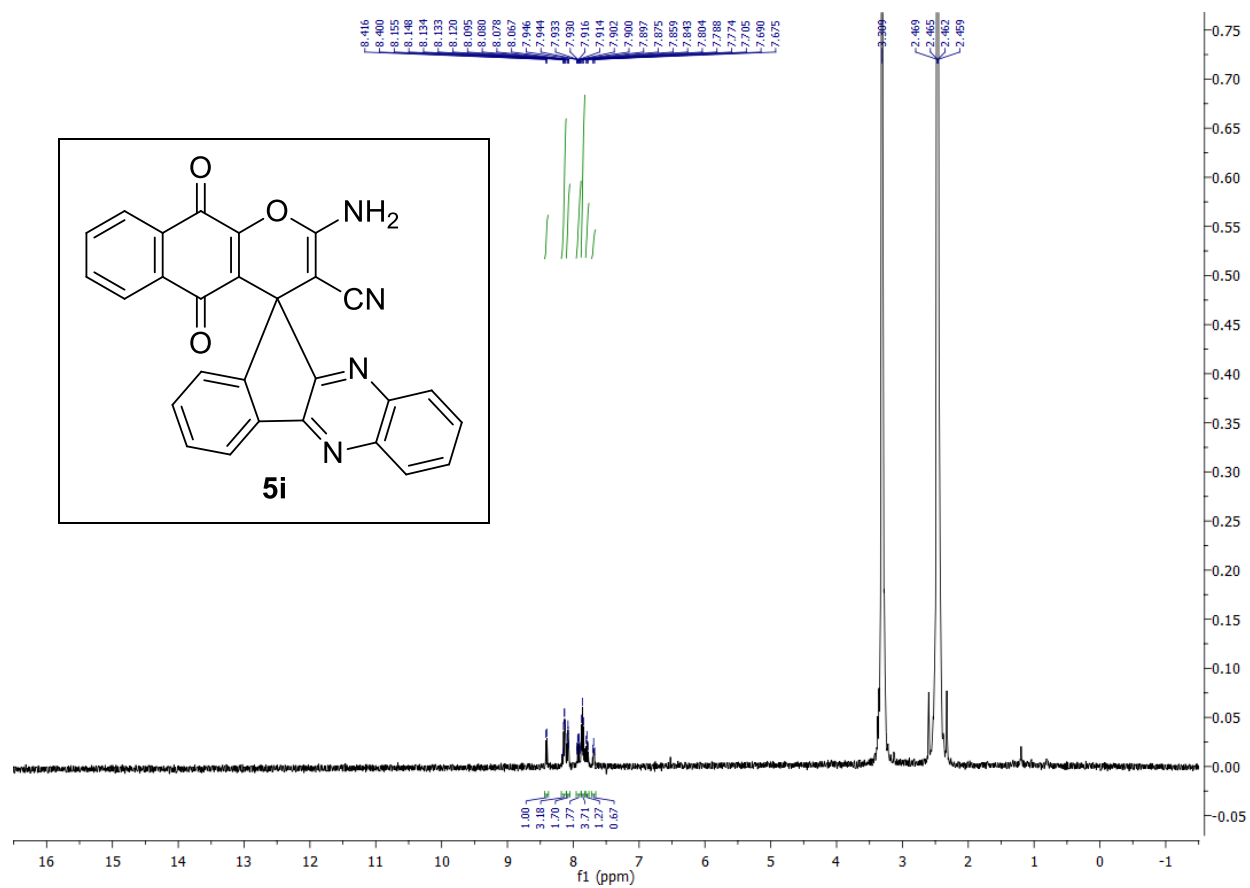
*2-Amino-5,10-dioxo-5,10-dihydrospiro[benzo[*g*]chromene-4,11'-indeno[1,2-*b*]quinoxaline]-3-carbonitrile (5i)* Orange solid; yield 90% mp 318-319 °C; FTIR (cm⁻¹): 3413, 3014, 2949, 2226, 1617, 1558, 1345, 1199, 764, 705; ¹H NMR (500 MHz, DMSO-*d*₆): δ_H/ppm: 8.41 (d, 1H, *J* = 8 Hz, aromatic H), 8.16-8.12 (m, 3H, aromatic 1H & -NH₂), 8.08 (dd, 2H, *J* = 7.5 Hz, aromatic H), 7.95-7.90 (m, 2H, aromatic H), 7.86 (t, 4H, *J* = 8 Hz, aromatic H), 7.79 (t, 1H, *J* = 7.5 Hz, aromatic H), 7.69 (t, 1H, *J* = 7.5 Hz, aromatic H). ¹³C NMR (125 MHz, DMSO-*d*₆): δ_C/ppm: 195.79 (2C), 158.10, 147.24, 146.77, 141.92, 141.49, 141.16, 138.13, 137.53, 137.30, 134.99, 133.72, 133.54, 133.07, 131.63, 131.26, 130.35, 129.63, 129.55, 129.24, 127.89, 126.44, 125.73, 123.55, 103.98, 103.76, 89.07; MS (ESI-TOF) *m/z*: 455.5160.



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Figure S33. FTIR spectrum of **5i**

Figure S34. ¹H NMR spectrum of **5i**

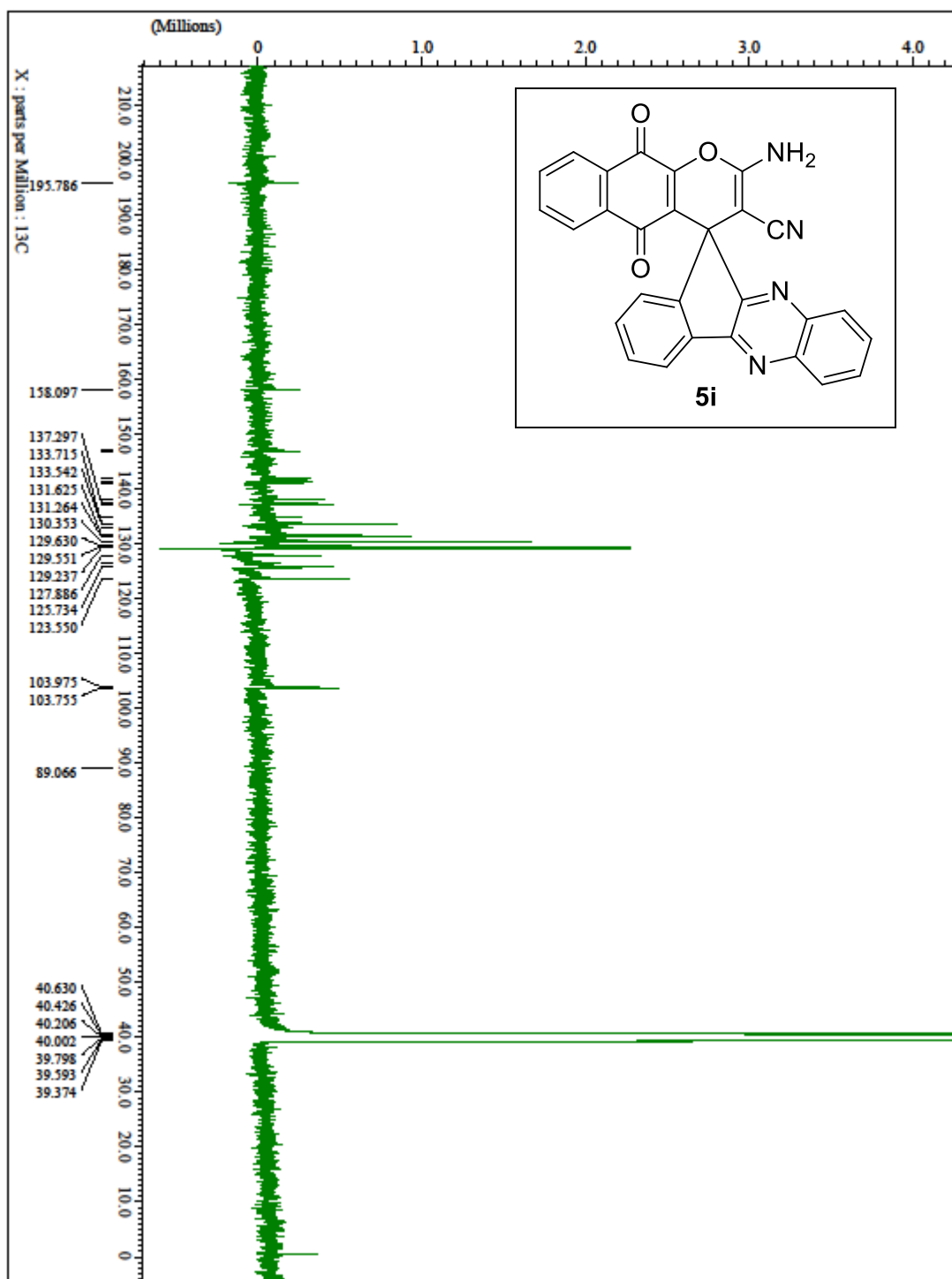
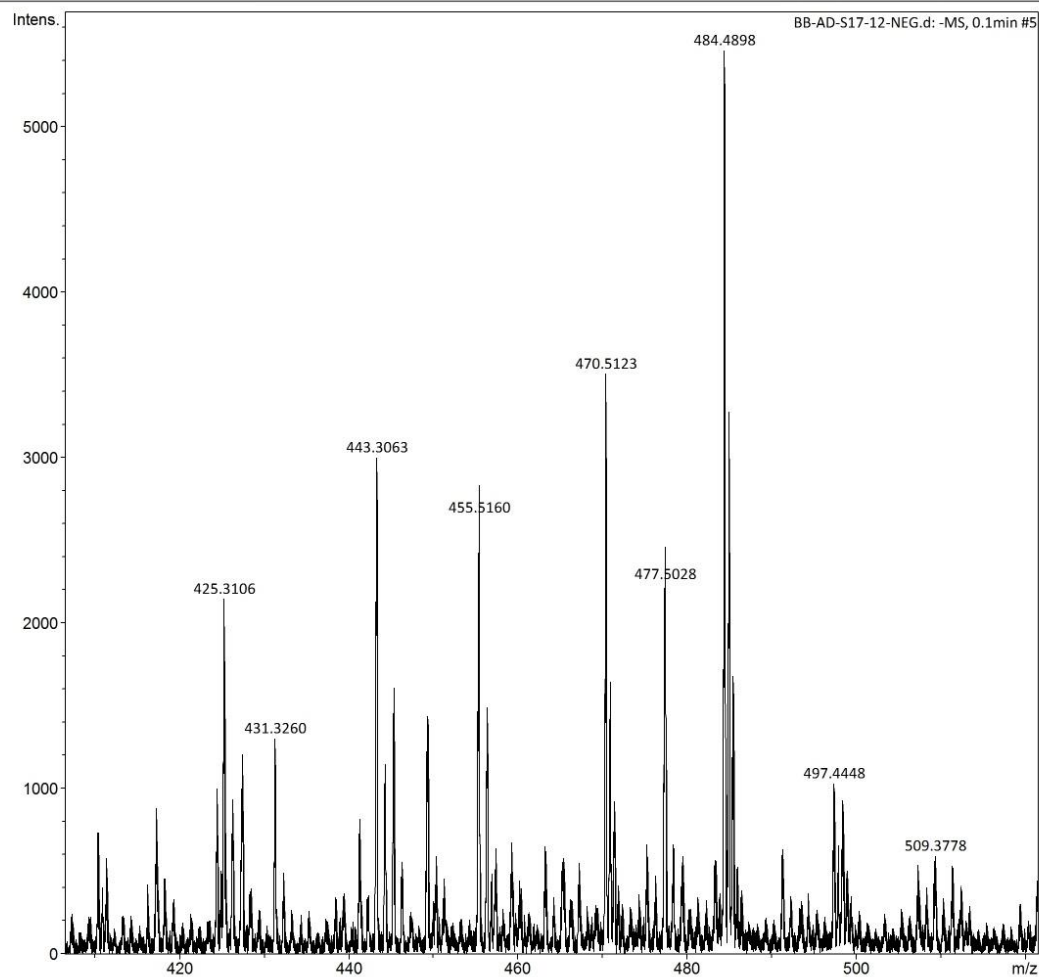


Figure S35. ^{13}C NMR spectrum of **5i** (Due to the low solubility of the molecule, the ^{13}C NMR data was collected with $ns = 10\text{K}$ in DMSO-d_6 as solvent)

Display Report

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Comment
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Operator HRMS
Instrument maXis impact 1819696.00160

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Set Corona 0 nA Set APCI Heater 0 °C



BB-AD-S17-12-NEG.d

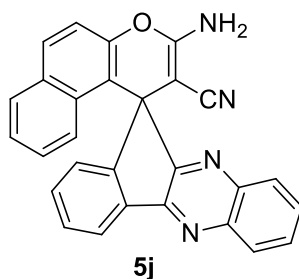
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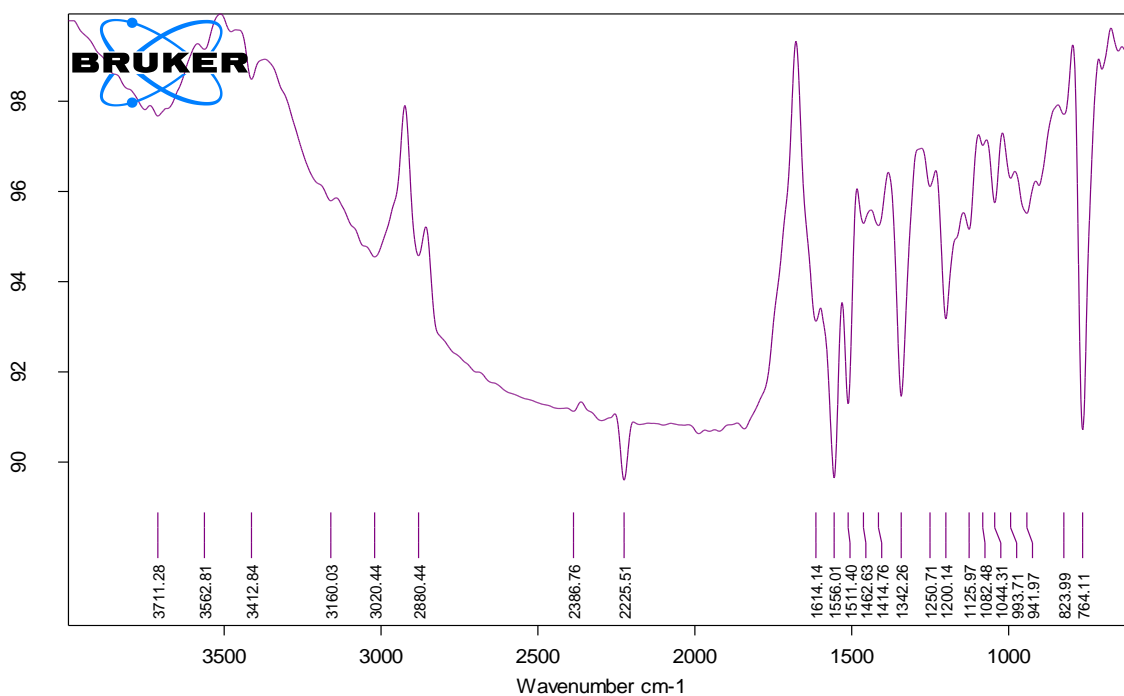
by: HRMS

Page 1 of 1

Figure S36. HRMS spectrum of **5i**



3-Aminospiro[benzo[f]chromene-1,11'-indeno[1,2-b]quinoxaline]-2-carbonitrile (5j) Orange solid; yield 89% mp 303-305 °C; FTIR (cm⁻¹): 3413, 3020, 2880, 2226, 1614, 1556, 1342, 1200, 825, 764; ¹H NMR (500 MHz, DMSO-d₆): δ_H/ppm: 8.17-8.12 (m, 4H, aromatic 2H & -NH₂), 8.07 (d, 2H, *J* = 7.5 Hz, aromatic H), 7.90-7.83 (m, 8H, aromatic H), 7.69 (t, 2H, *J* = 7.5 Hz, aromatic H); ¹³C NMR (125 MHz, CDCl₃): δ_C/ppm: 143.31, 141.92, 141.57 (2C), 138.73 (2C), 136.79 (2C), 136.13 (2C), 132.82 (2C), 132.54 (2C), 131.63 (2C), 131.31 (2C), 130.49 (2C), 129.69 (2C), 126.79, 123.20, 117.486, 114.31, 113.20, 89.66; MS (ESI-TOF) *m/z*: 425.2837.



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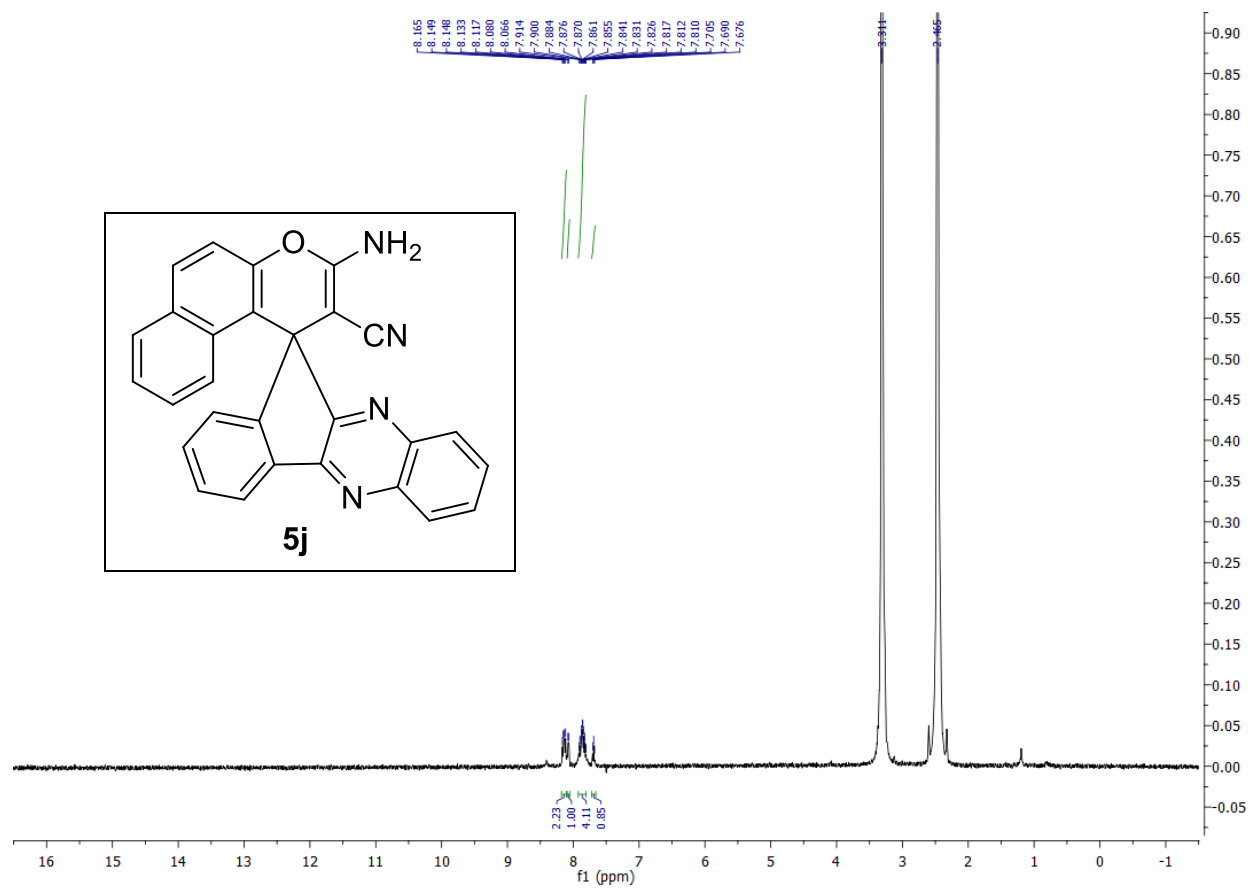
BB-AD-517-14

Instrument type and / or accessory

19/08/2022

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Figure S37. FTIR spectrum of **5j**

Figure S38. ¹H NMR spectrum of **5j**

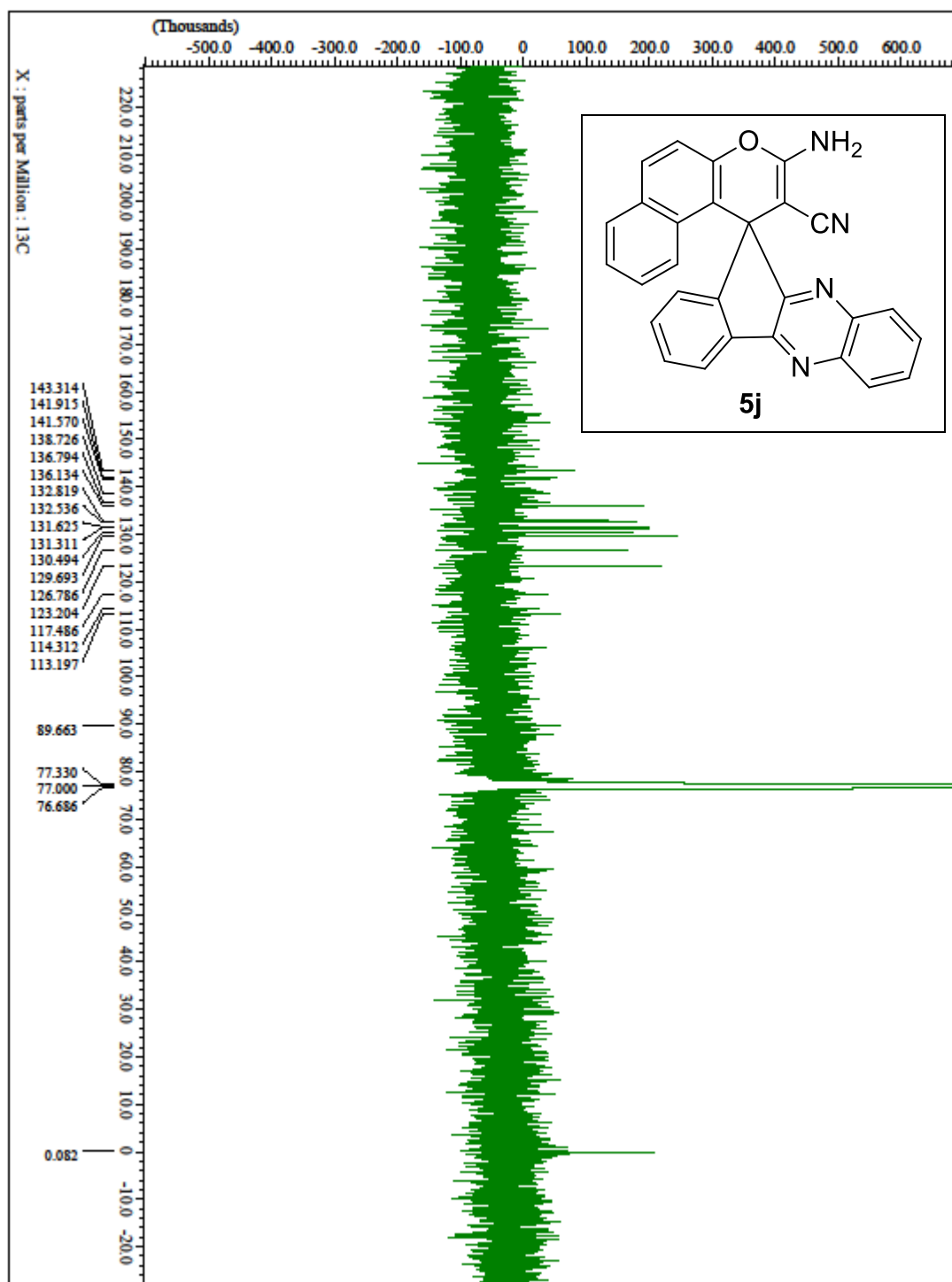


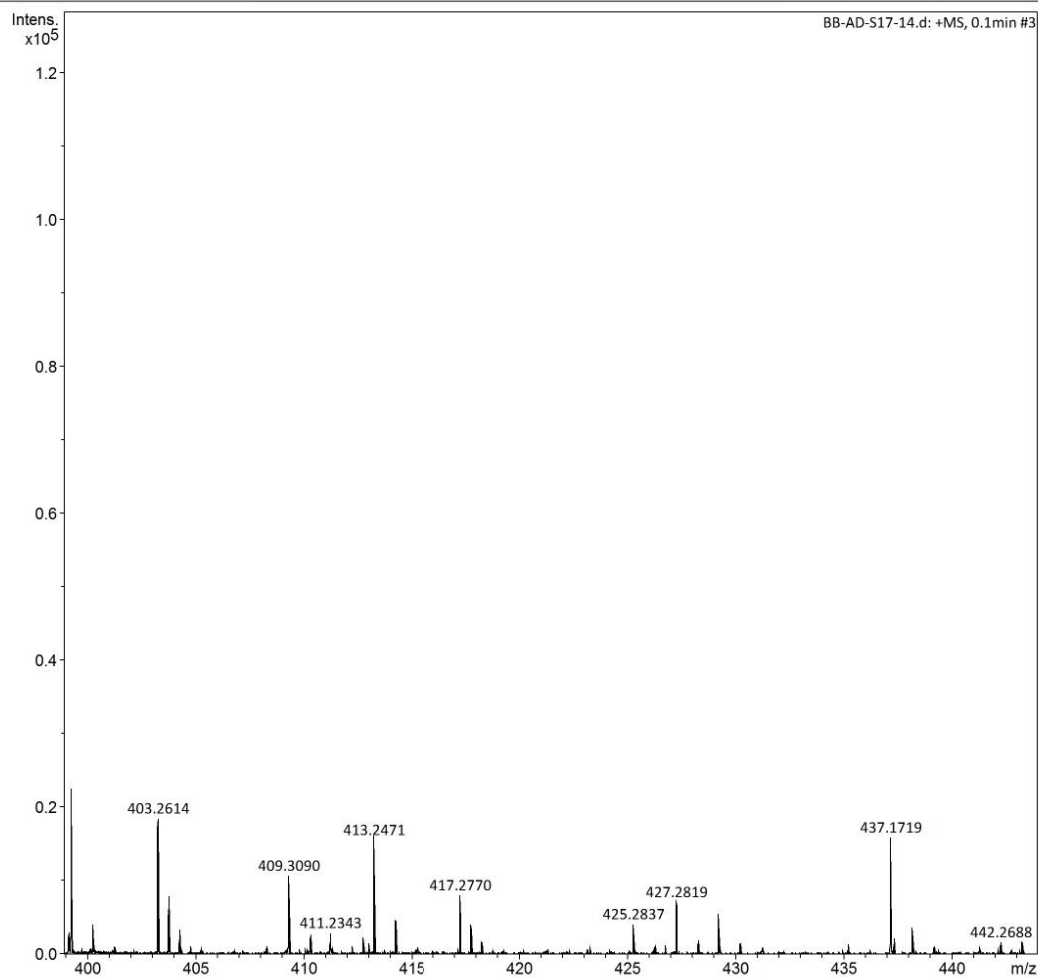
Figure S39. ¹³C NMR spectrum of **5j** (Due to the low solubility of the molecule, the ¹³C NMR data was collected with ns = 10K in CDCl₃ as solvent. With DMSO-d₆ as solvent we couldn't recognize all the peaks even with ns = 10K)

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Instrument maXis impact 1819696.00160

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BB-AD-S17-14.d

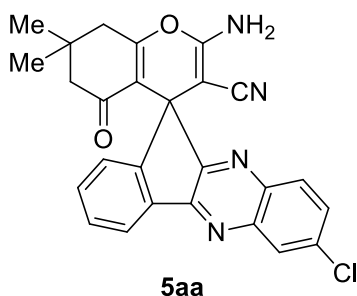
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by: HRMS

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Figure S40. HRMS spectrum of **5j**



2-Amino-7'-chloro-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydrospiro[chromene-4,11'-indeno[1,2-b]quinoxaline]-3-carbonitrile (5aa) Brown solid; yield 80% mp 289 °C; FTIR (cm⁻¹): 3321, 3081, 2952, 2178, 1659, 1593, 1466, 1310, 1211, 750, 711; ¹H NMR (500 MHz, DMSO-d₆): δ_H/ppm: 8.19-8.02 (m, 3H, aromatic H), 7.83-7.75 (m, 1H, aromatic H), 7.59 (s, 1H, aromatic H), 7.51 (s, 2H, aromatic H), 7.30 (s, 2H, -NH₂), 2.65 (q, 2H, -CH₂), 2.00 (q, 2H, -CH₂), 0.99 (t, 6H, *J* = 5.5, 4.5 Hz, -CH₃); ¹³C NMR (125 MHz, DMSO-d₆): δ_C/ppm: 195.54, 166.60, 165.50, 159.46, 155.62, 152.65, 142.67, 134.51, 133.36, 131.11, 130.03 (2C), 129.51 (2C), 128.13 (2C), 125.08 (2C), 122.32 (2C), 117.94, 112.29, 58.89, 50.61, 47.73, 32.50, 28.13, 27.55; MS (ESI-TOF) *m/z*: 454.0525.

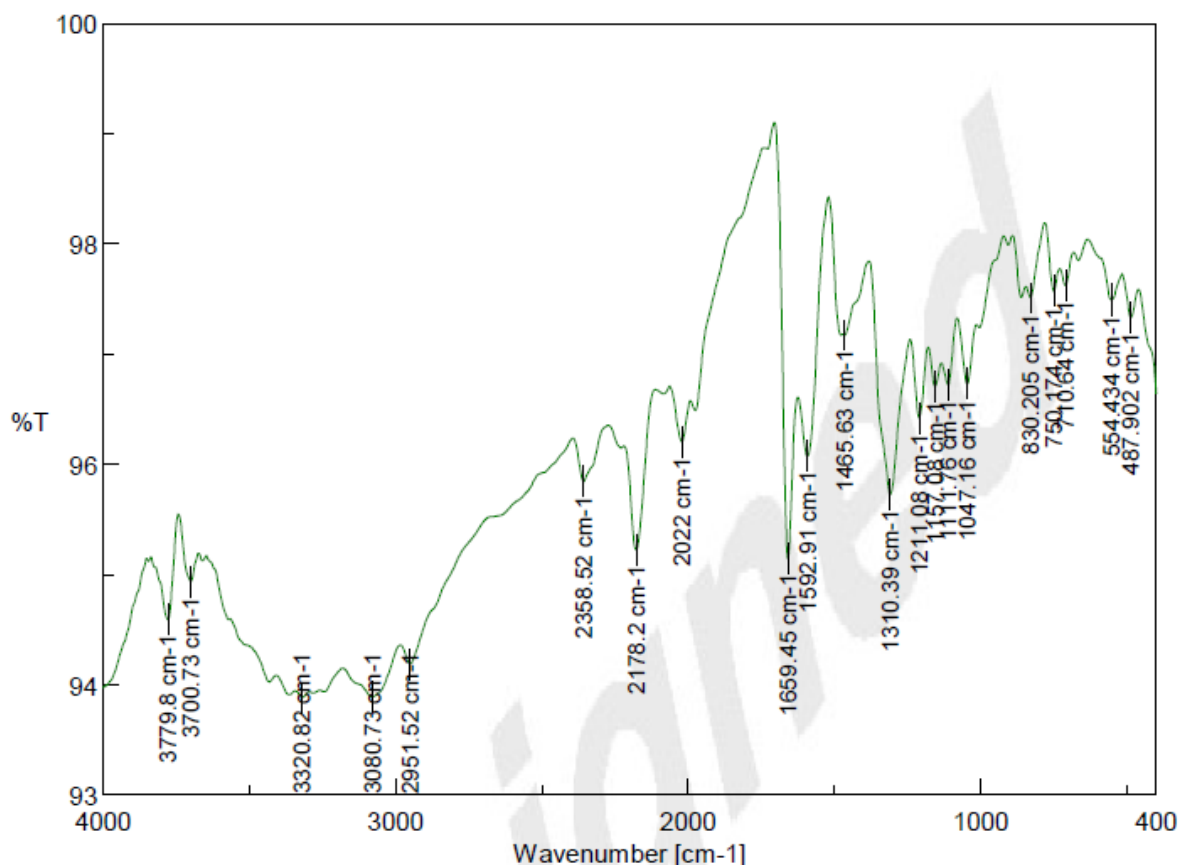
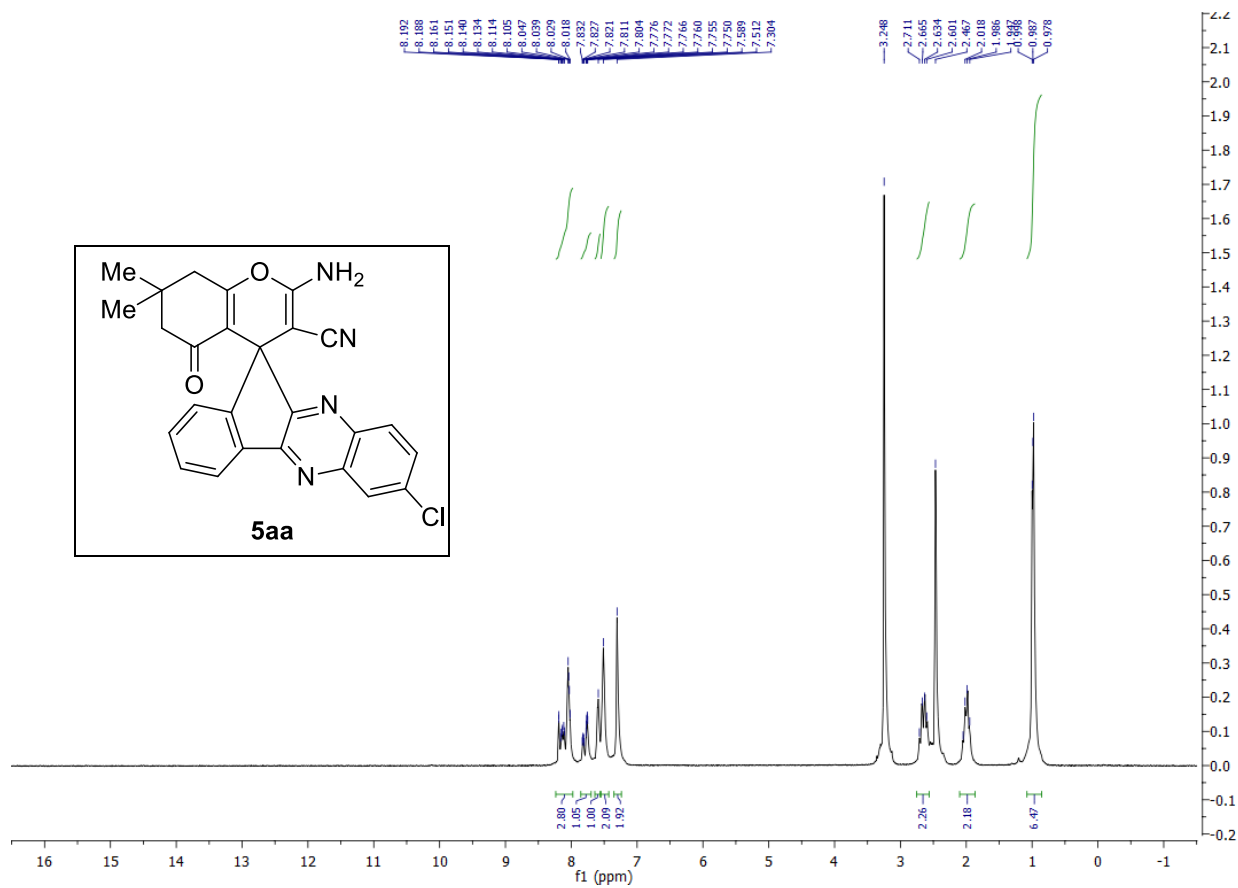
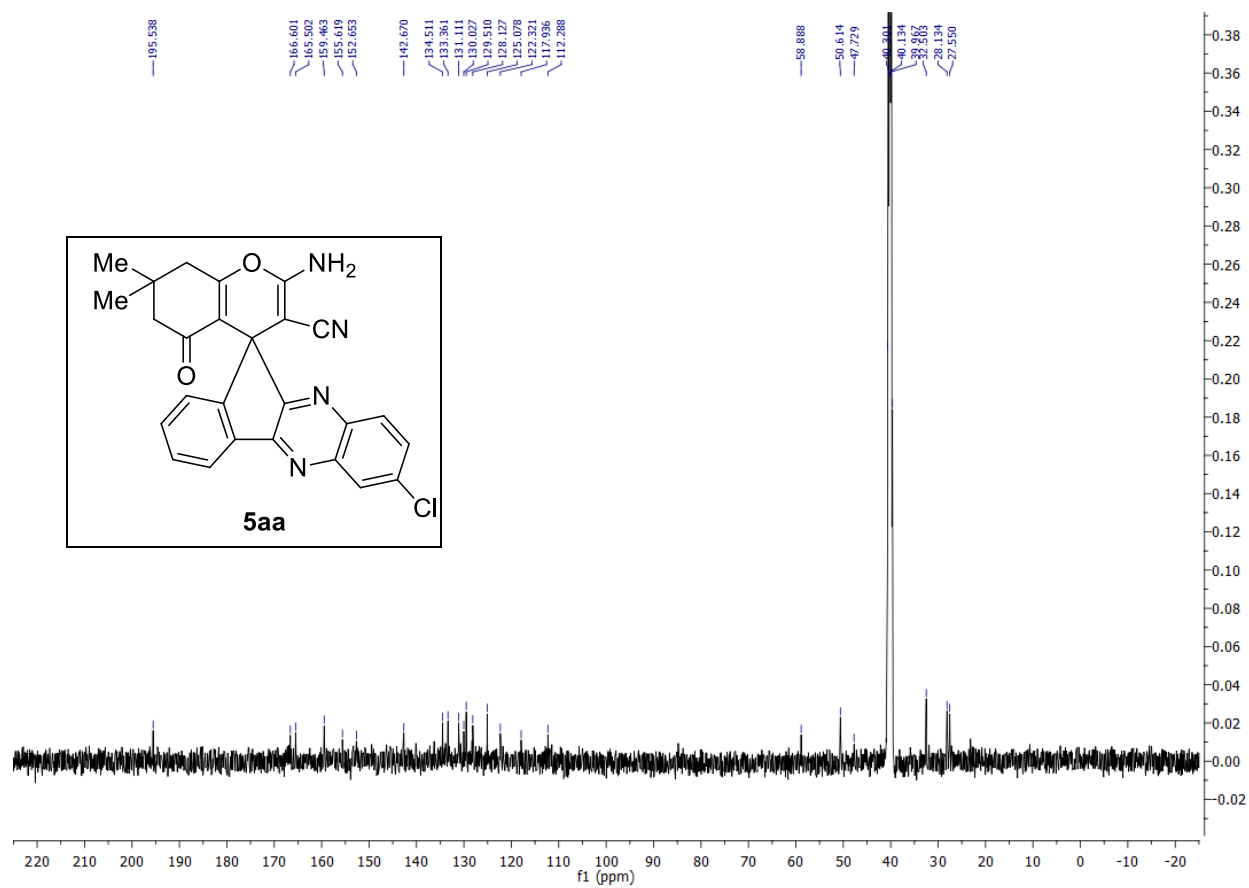


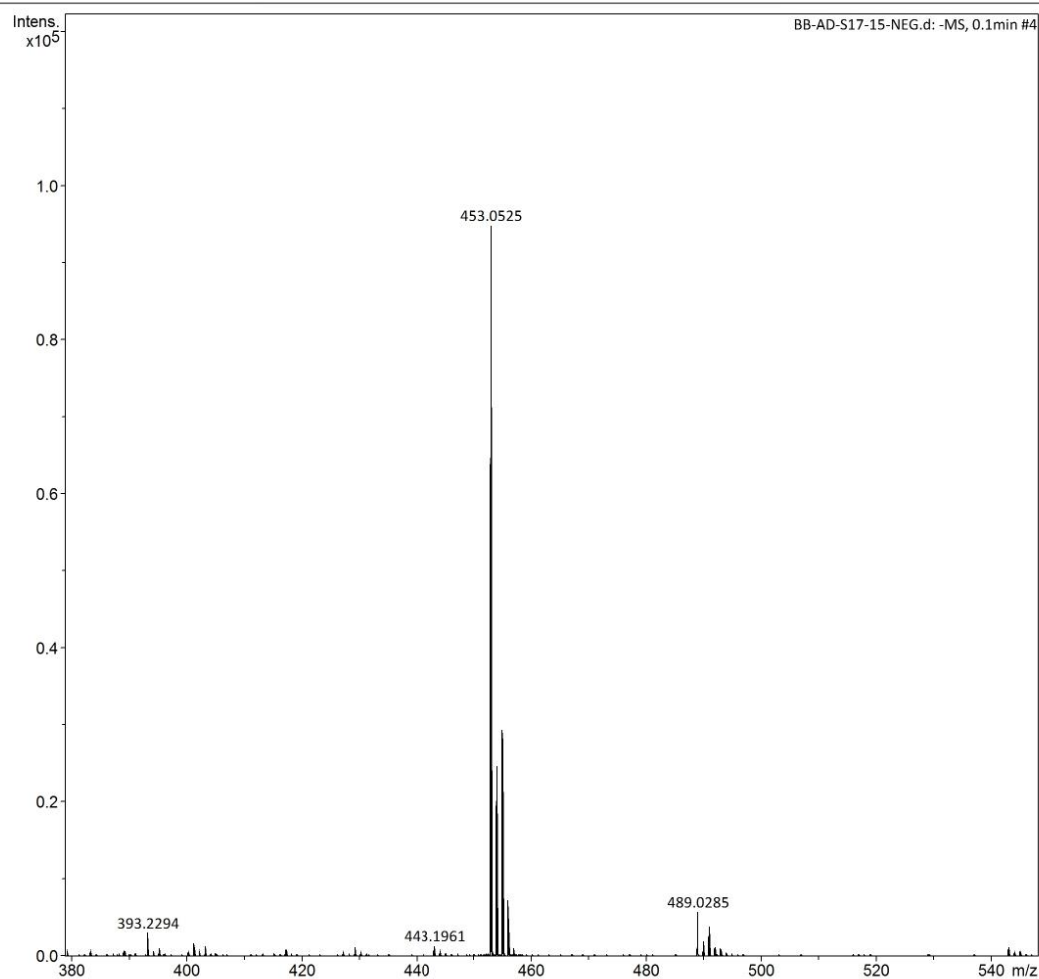
Figure S41. FTIR spectrum of **5aa**

Figure S43. ¹³C NMR spectrum of **5aa**

Display Report

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Sample Name
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Instrument maXis impact 1819696.00160

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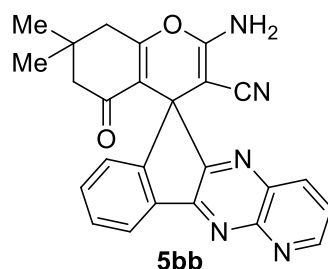
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by: HRMS

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Figure S44. HRMS spectrum of **5aa**



*2-Amino-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydrospiro[chromene-4,6'-indeno[1,2-b]pyrido[3,2-*e*]pyrazine]-3-carbonitrile (5bb)* Brown solid; yield 78% mp 277-280 °C; FTIR (cm⁻¹): 3389, 3290, 3175, 2959, 2193, 1651, 1591, 1317, 1214, 861, 783; ¹H NMR (500 MHz, DMSO-d₆): δ_H/ppm: 9.04 (br s, 1H, aromatic H), 8.47 (d, 1H, *J* = 7 Hz, aromatic H), 8.12 (d, 1H, *J* = 7.5 Hz, aromatic H), 7.77 (t, 1H, *J* = 4, 3.5 Hz, aromatic H), 7.62 (d, 1H, *J* = 7 Hz, aromatic H), 7.55 (q, 2H, *J* = 7, 7.5 Hz, aromatic H), 7.33 (s, 2H, -NH₂), 2.66 (q, 2H, -CH₂), 2.00 (q, 2H, -CH₂), 0.99 (s, 6H, -CH₃); ¹³C NMR (125 MHz, DMSO-d₆): δ_C/ppm: 195.58, 167.03, 165.58, 159.51, 157.64, 153.50, 153.03, 151.49, 138.42, 136.25, 133.68, 129.63, 125.12, 122.71, 122.29, 119.85, 117.92, 112.24, 111.63, 58.76, 50.58, 47.59, 32.50, 28.15, 27.54; MS (ESI-TOF) *m/z*: 444.1320.

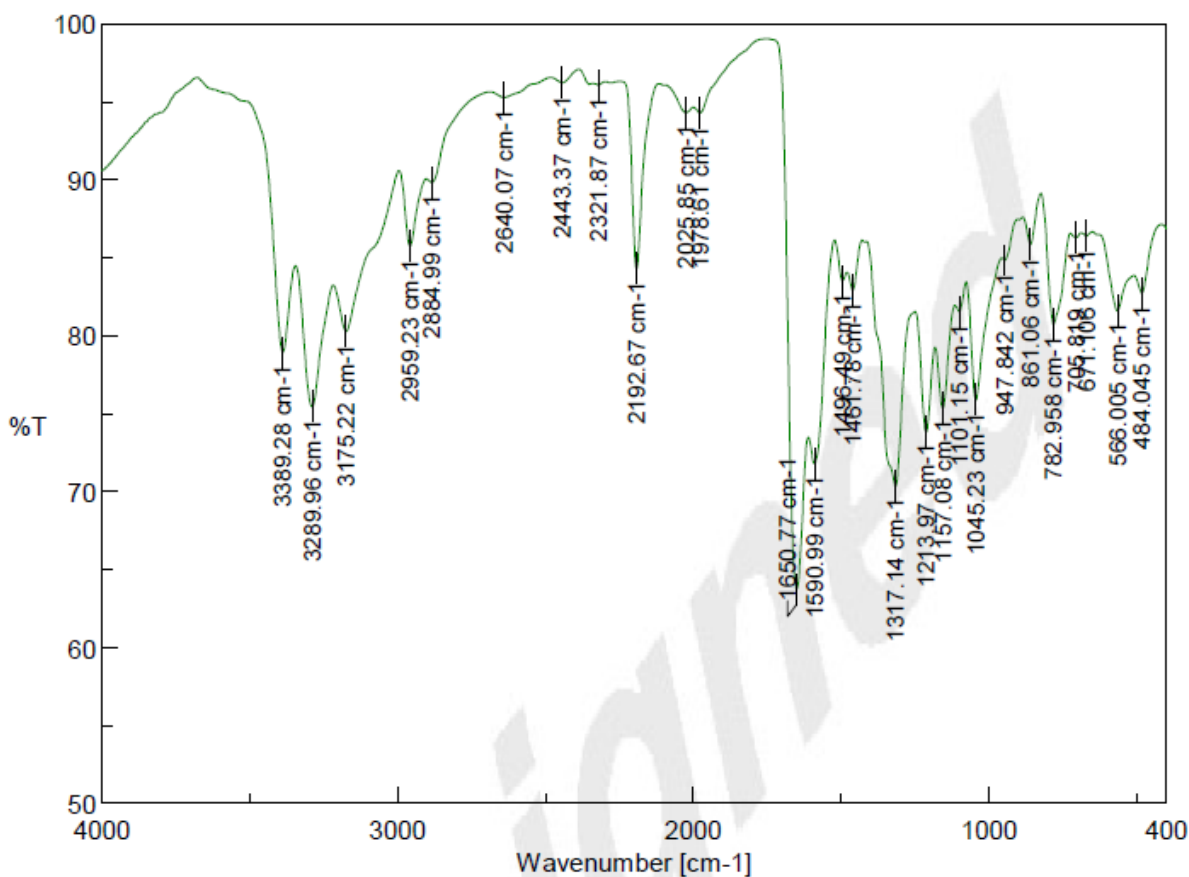
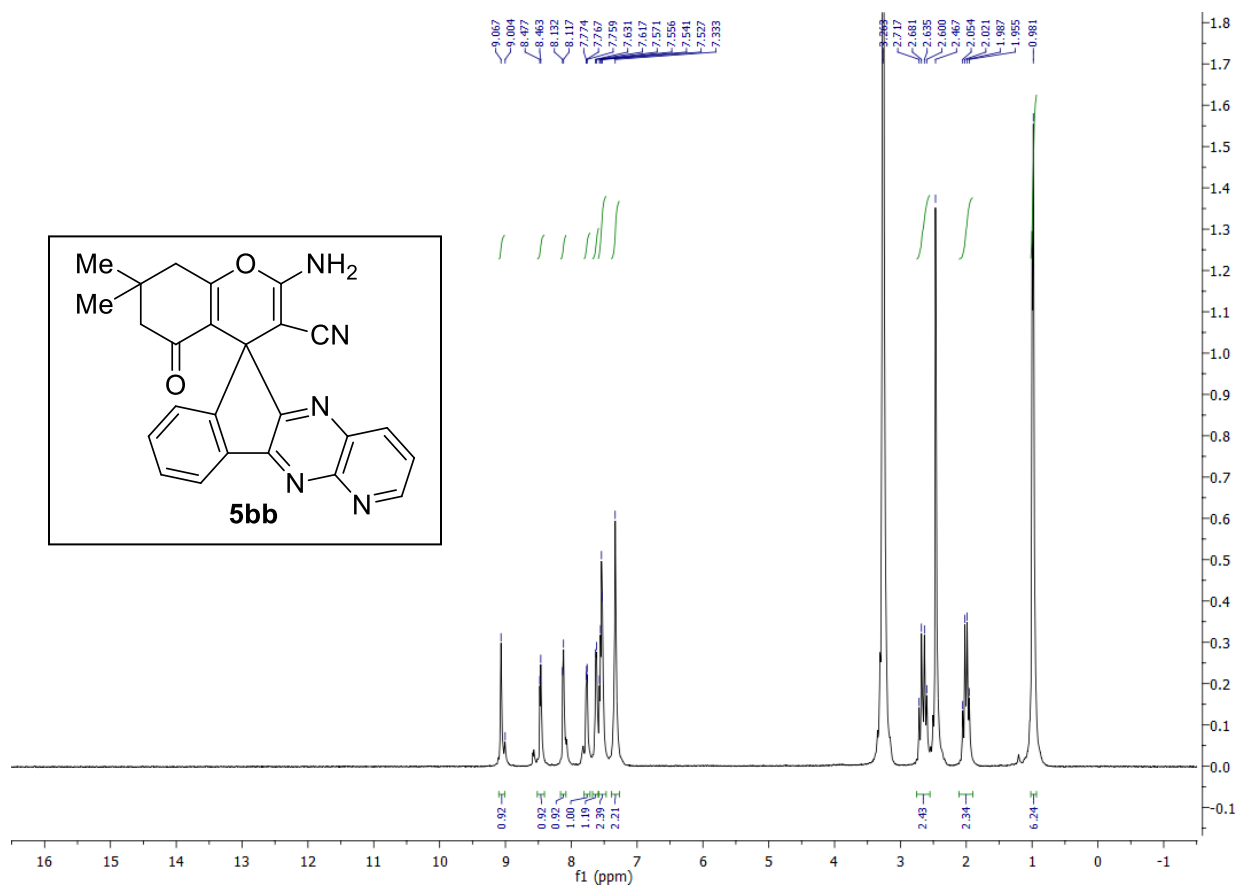
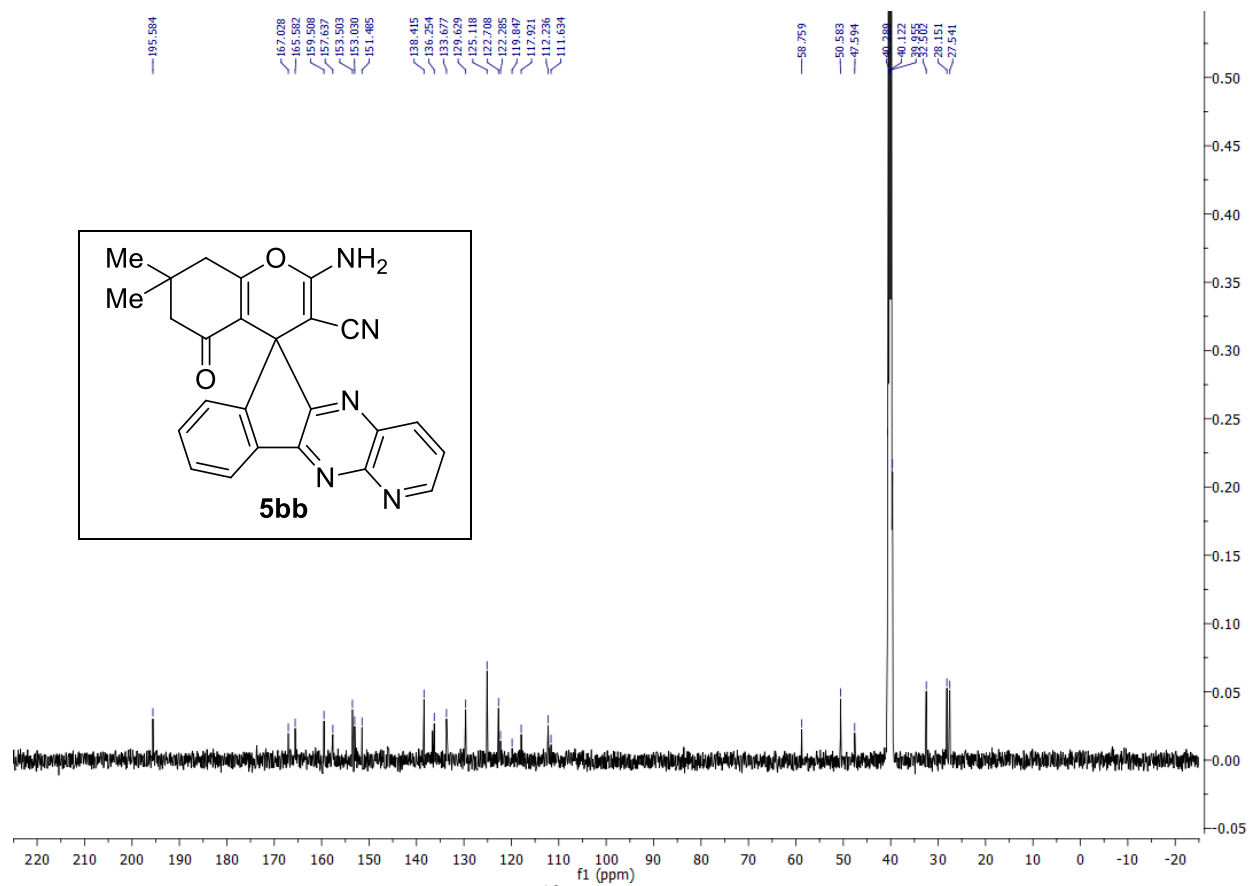


Figure S45. FTIR spectrum of **5bb**Figure S46. ¹H NMR spectrum of **5bb**

Figure S47. ¹³C NMR spectrum of **5bb**

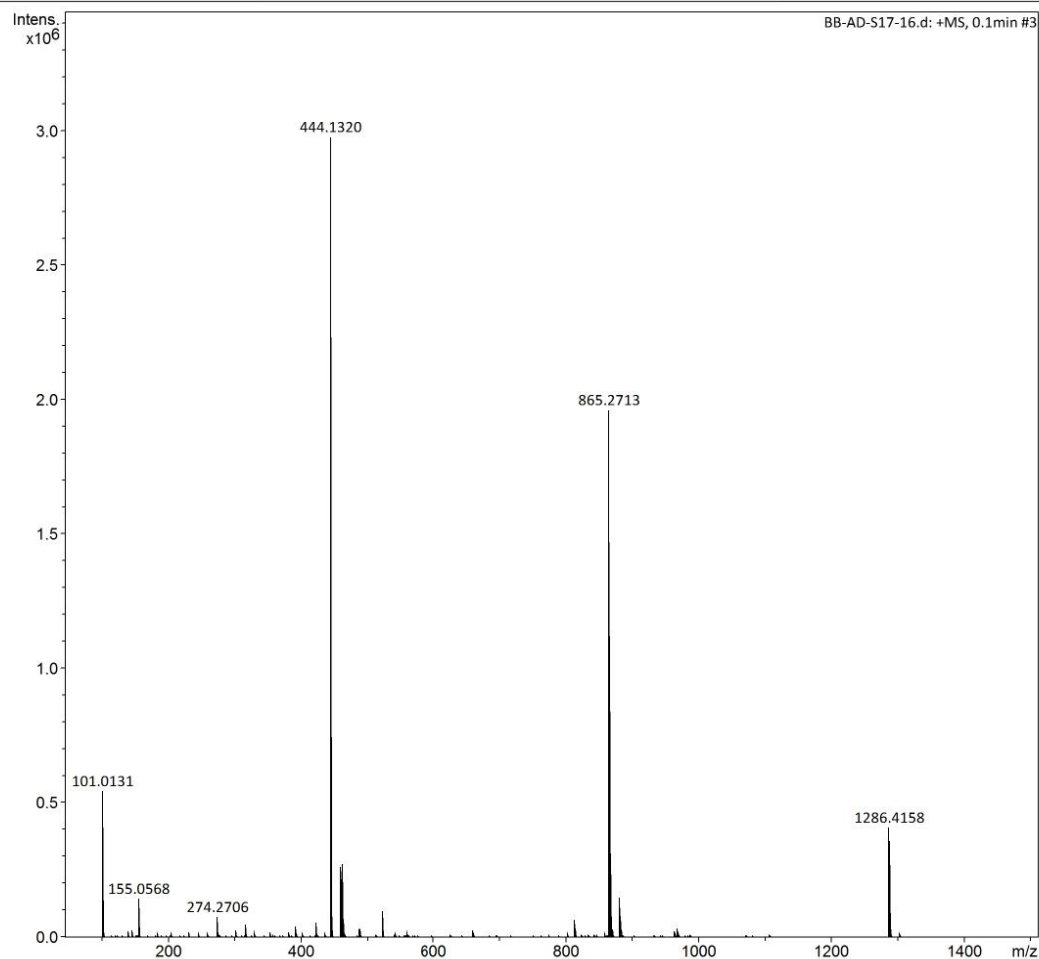
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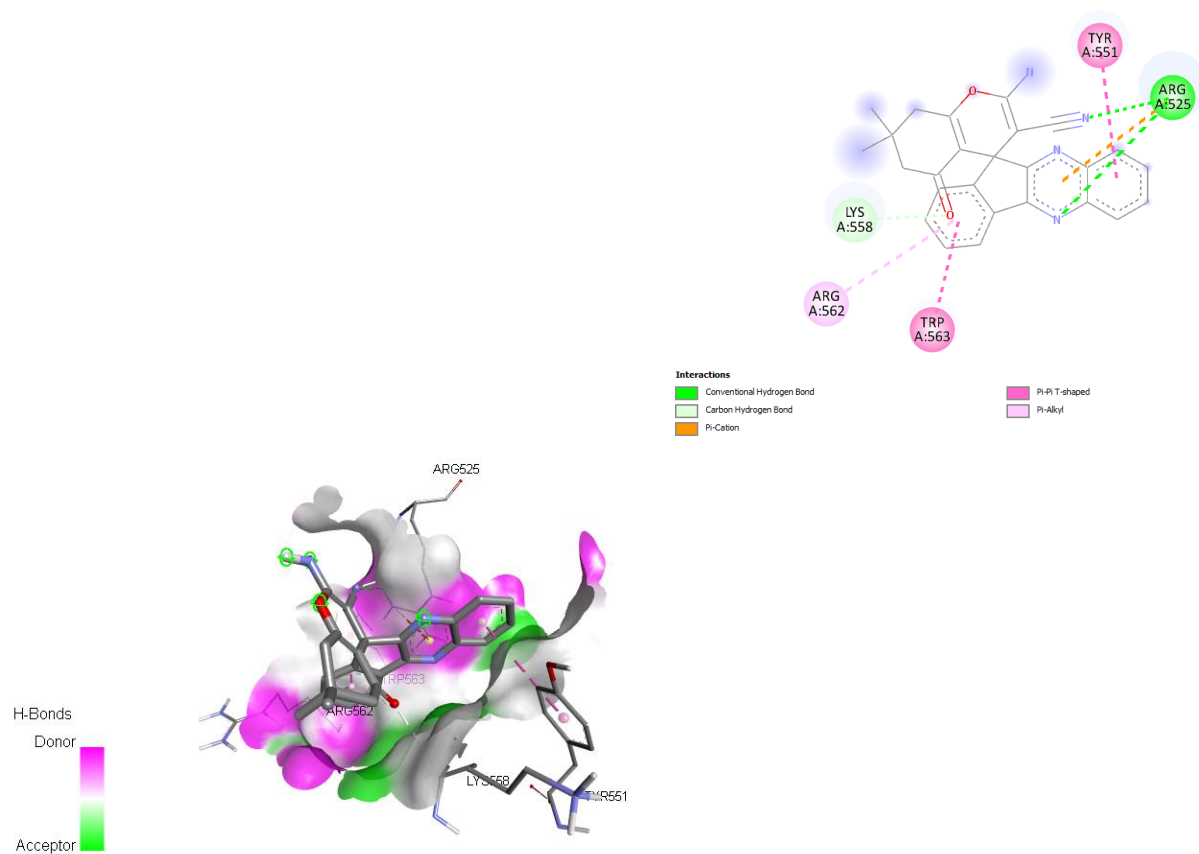
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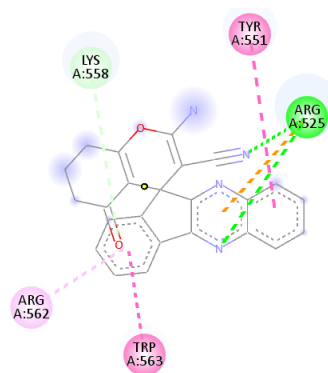
Figure S48. HRMS spectrum of **5bb**

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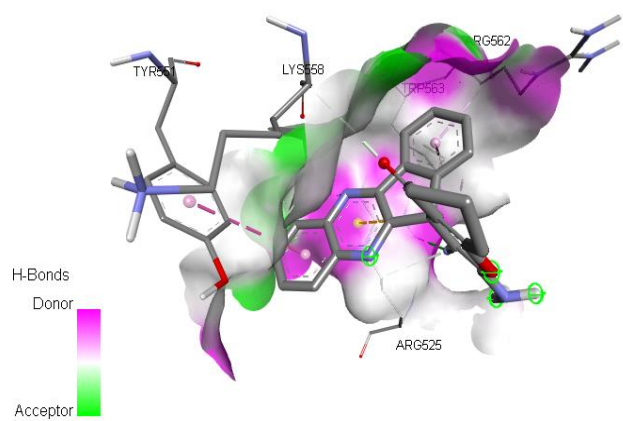


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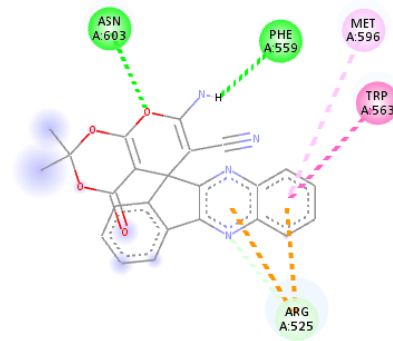
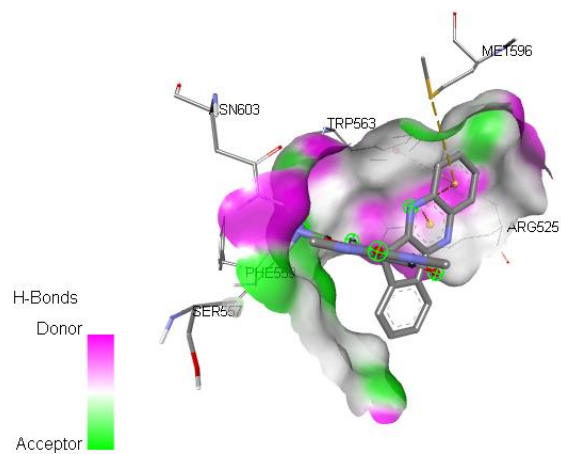


Interactions

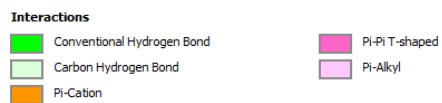
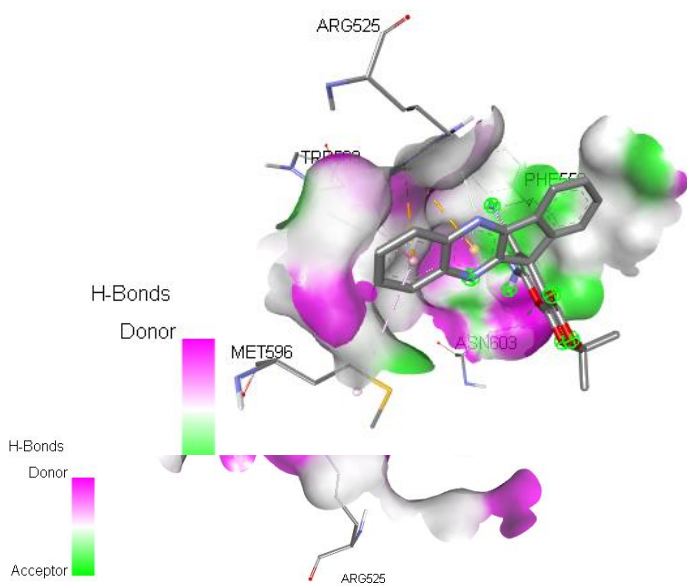
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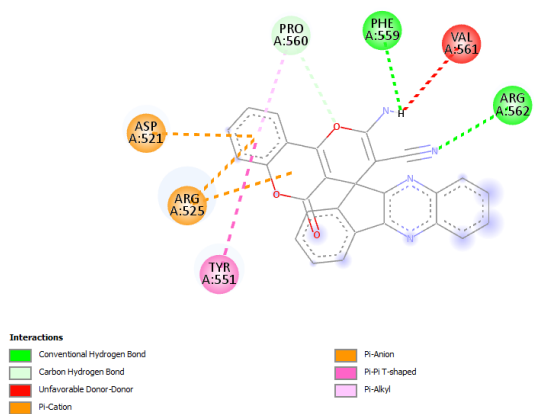
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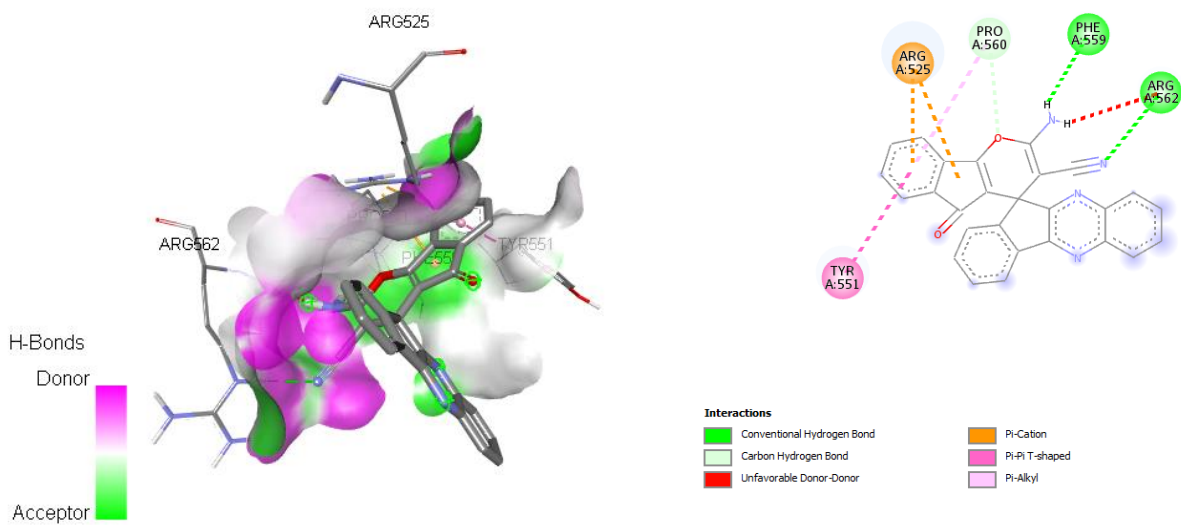
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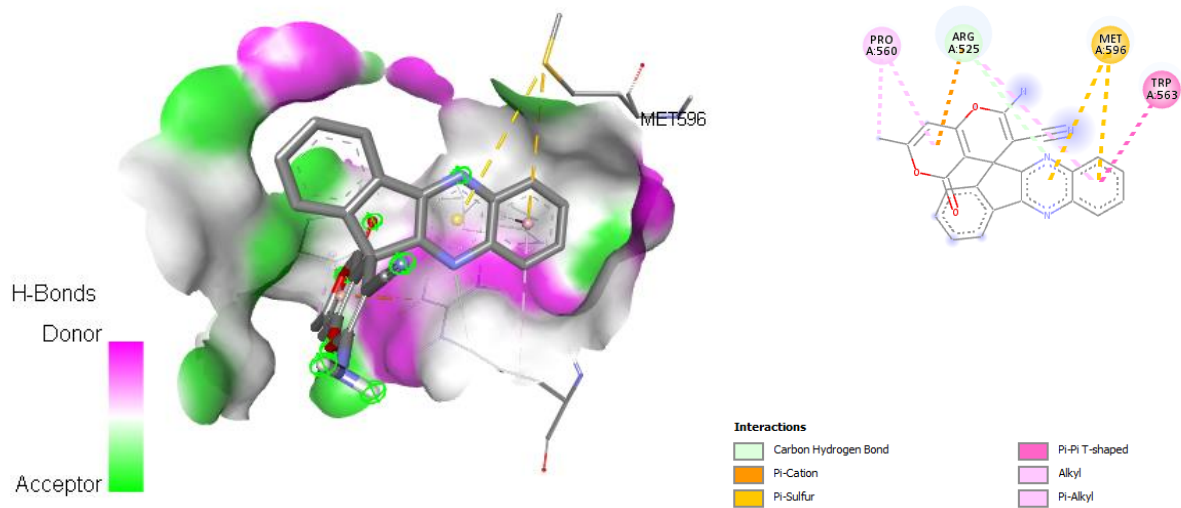
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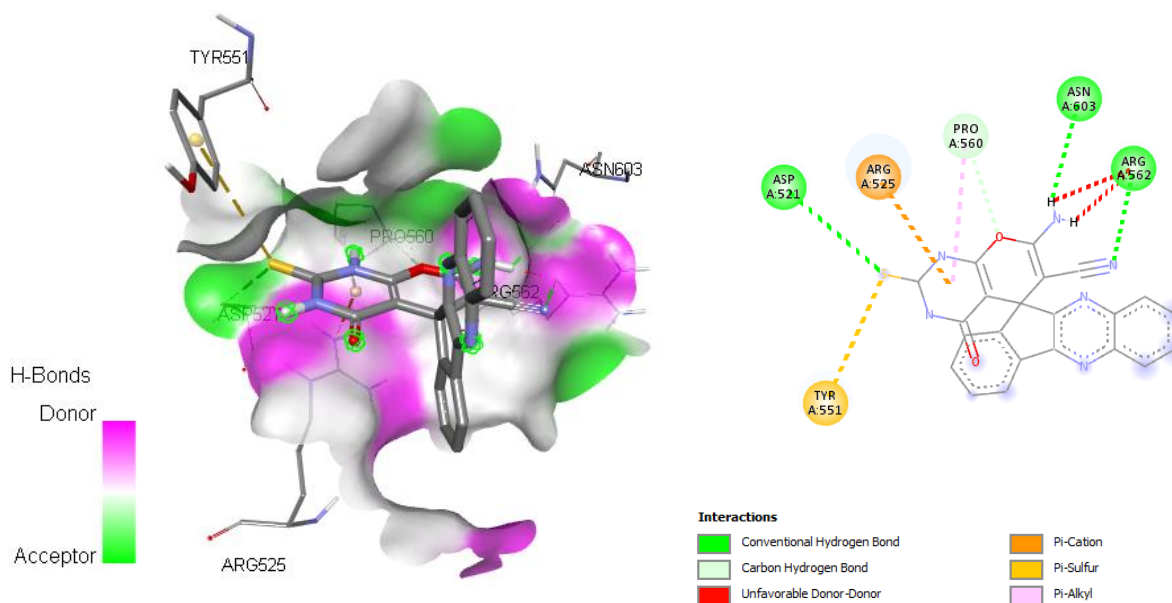
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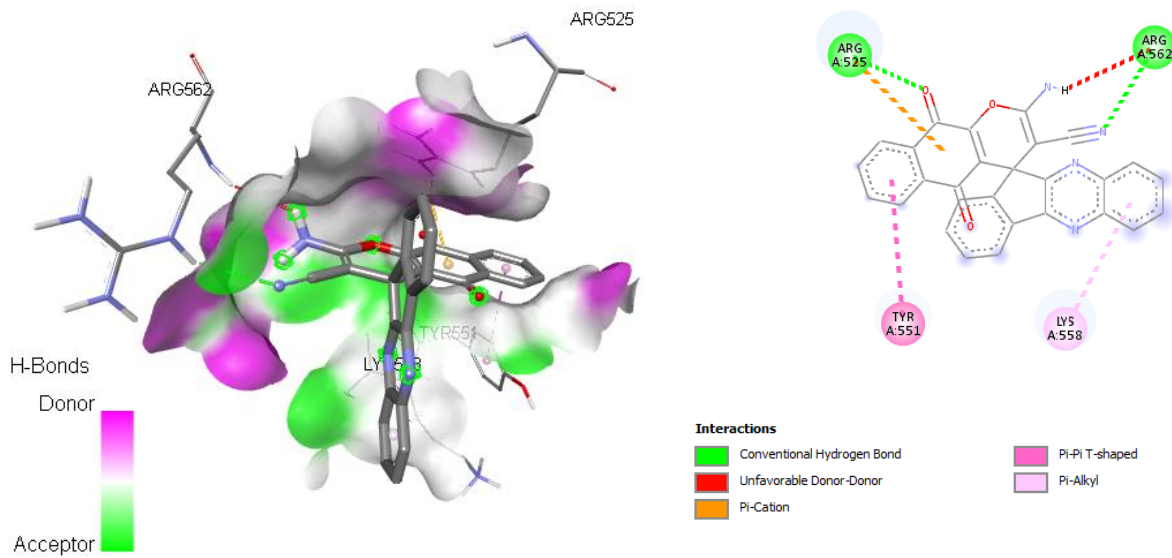
Compound 5g

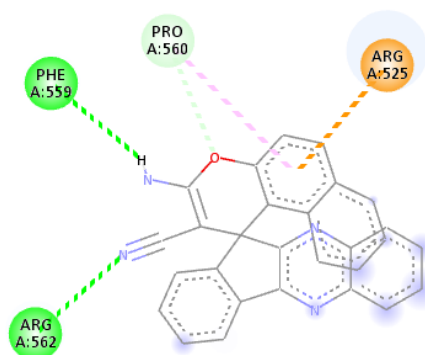
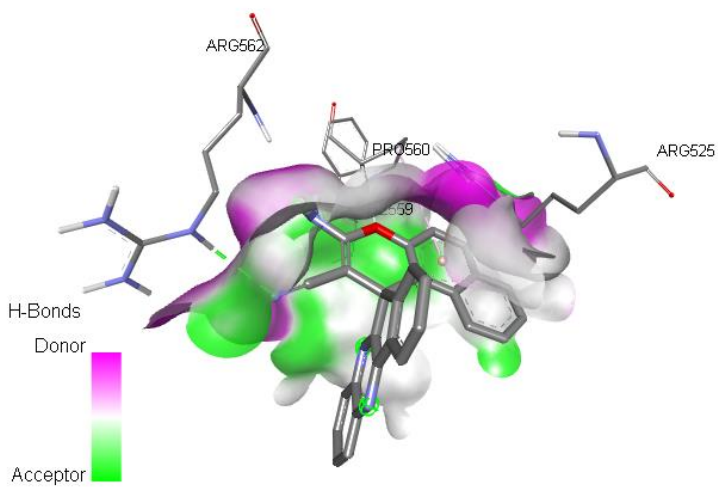


Compound 5h



Compound 5i

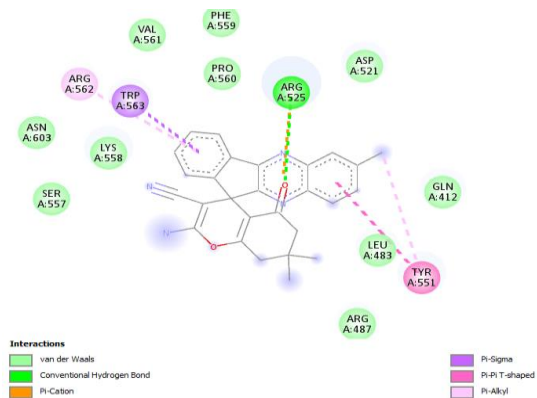
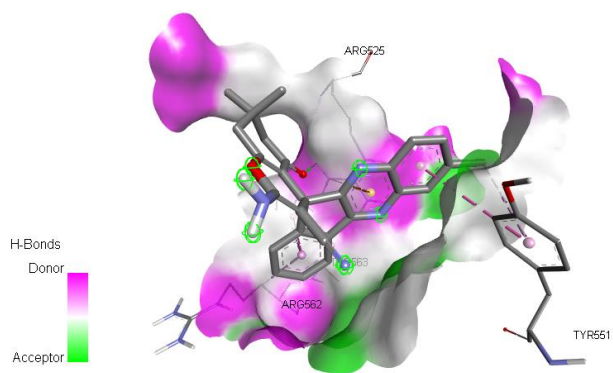


Compound 5j**Interactions**

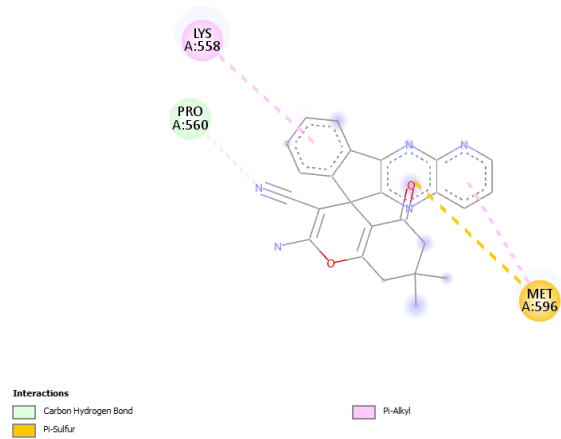
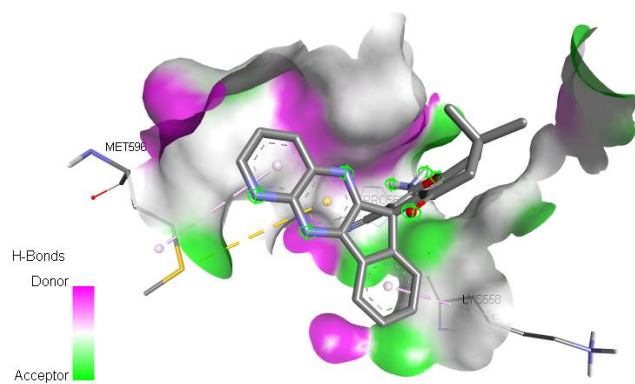
Conventional Hydrogen Bond
Carbon Hydrogen Bond

Pi-Cation
Pi-Alkyl

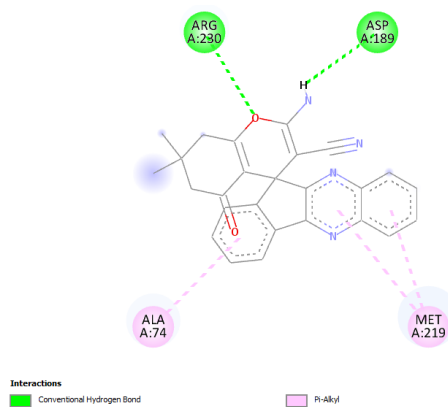
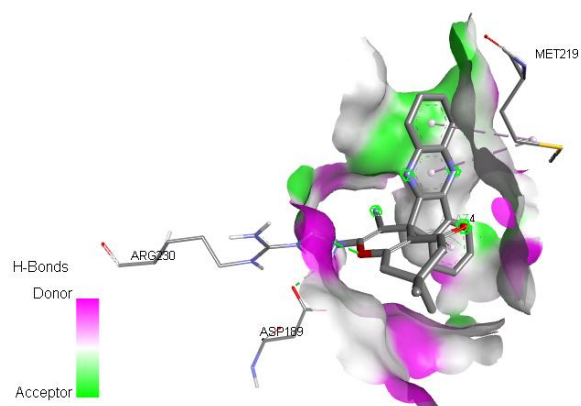
Compound 5aa

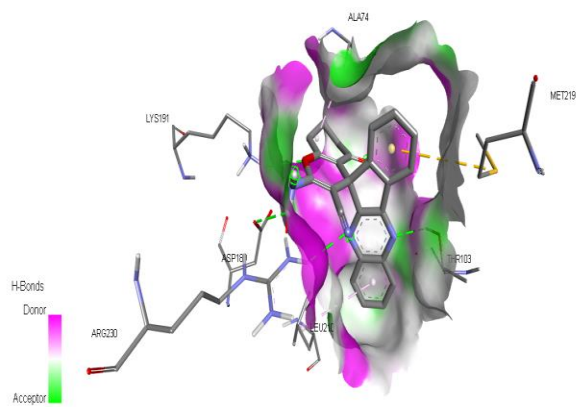
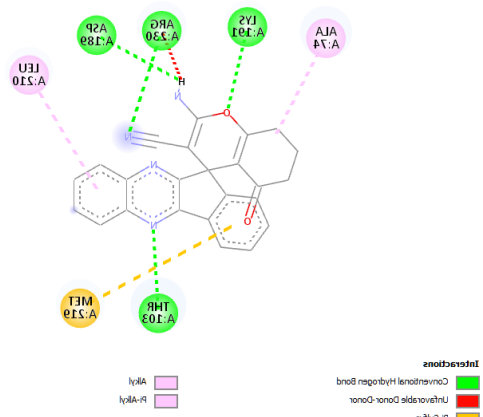


Compound 5bb

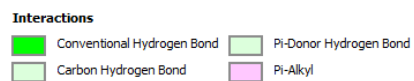
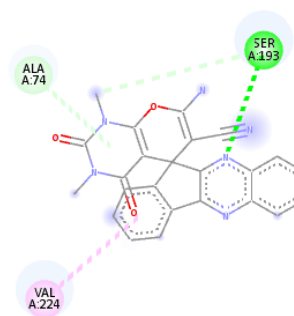
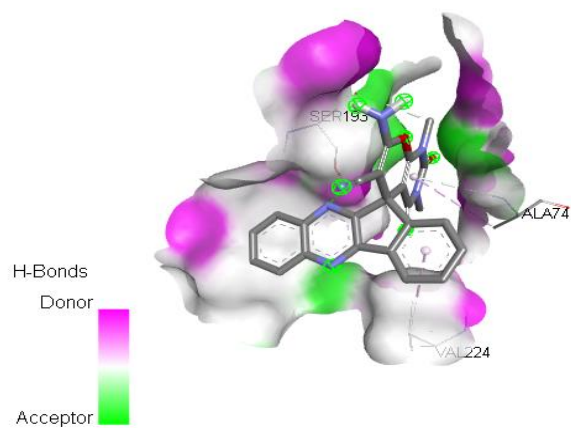


DOCKING POSES WITH (PDB: 1PMV): HEPATIC CANCER

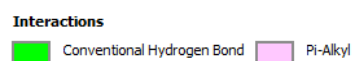
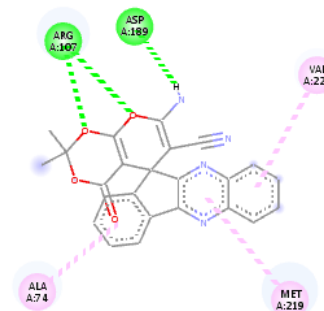
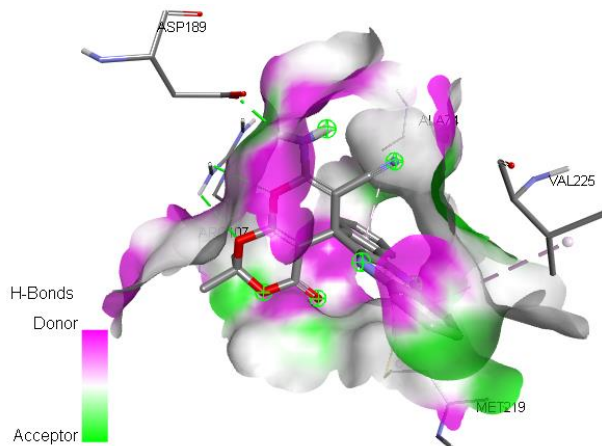
Compound 5a**Compound 5b**



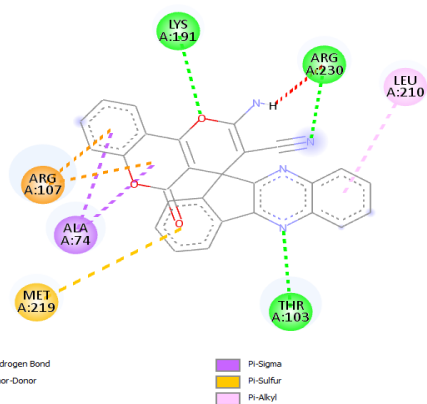
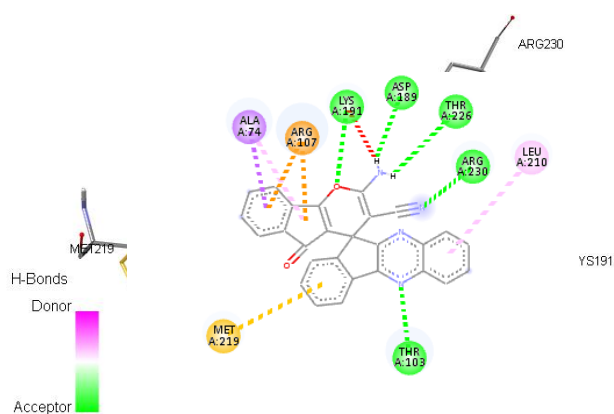
Compound 5c



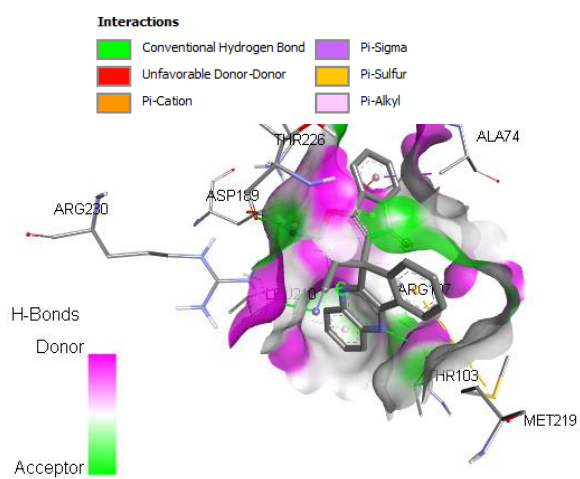
Compound 5d



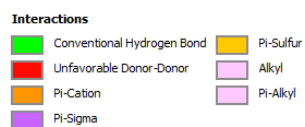
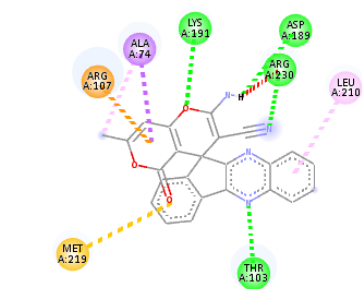
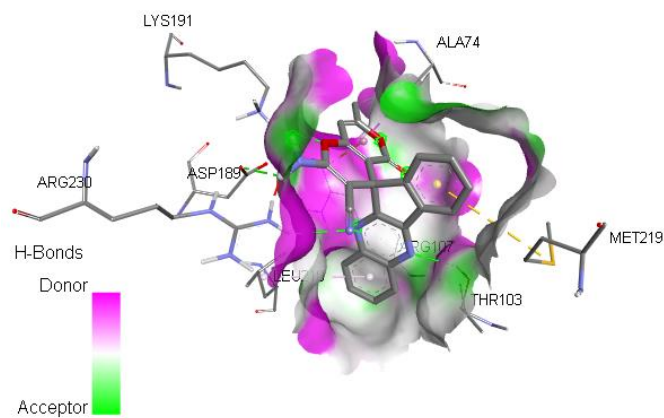
Compound 5e



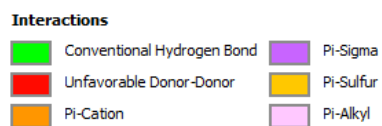
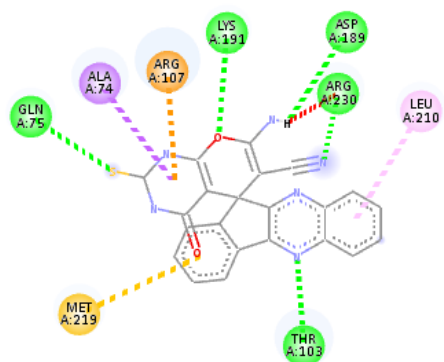
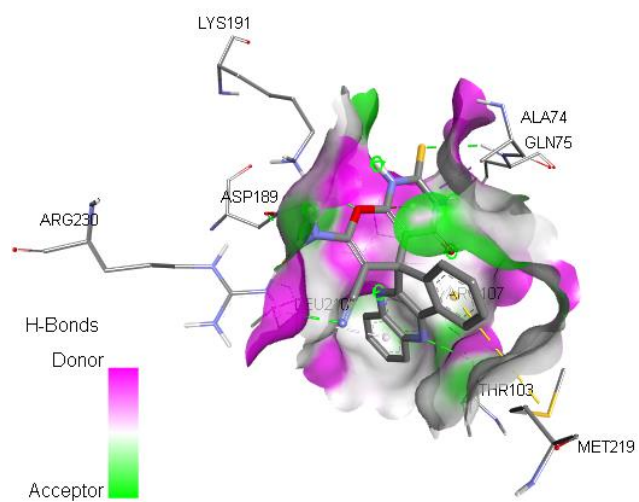
Compound 5f



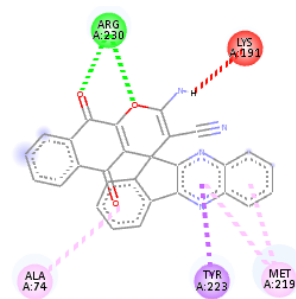
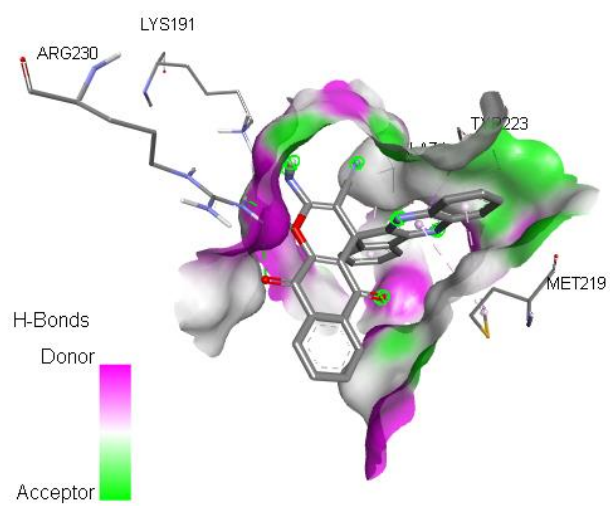
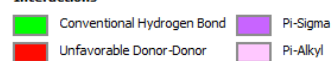
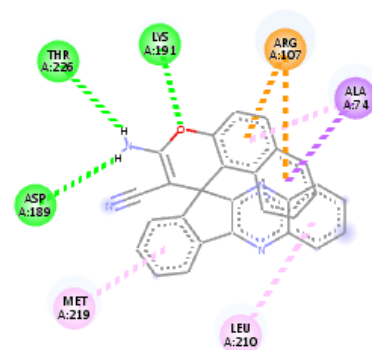
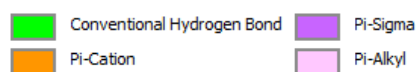
Compound 5g

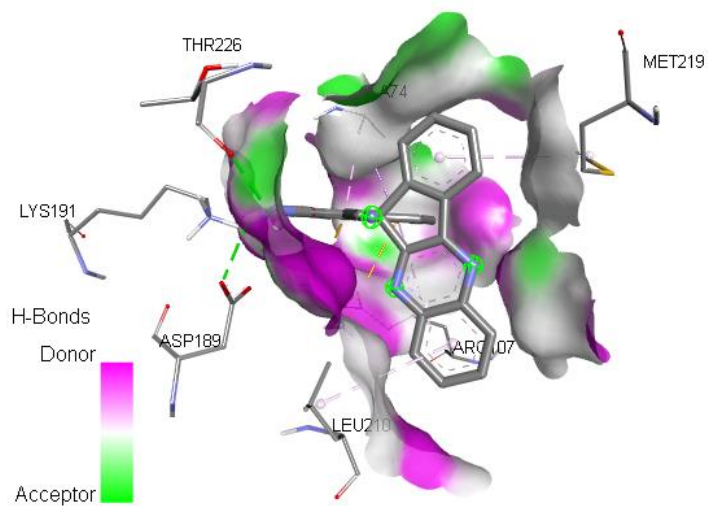


Compound 5h

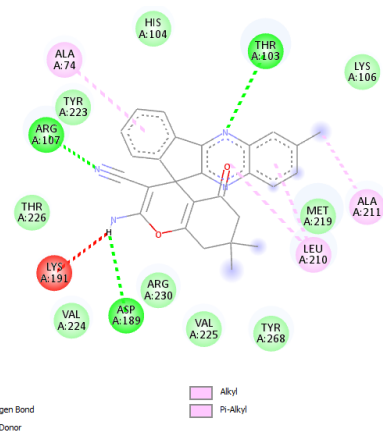
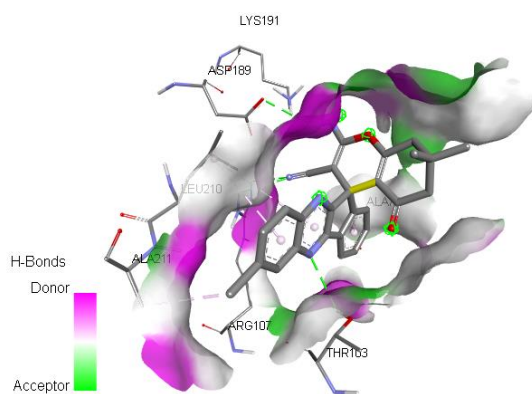


Compound 5i

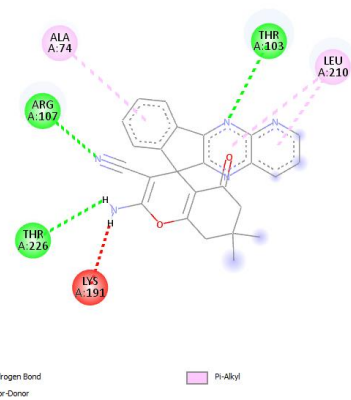
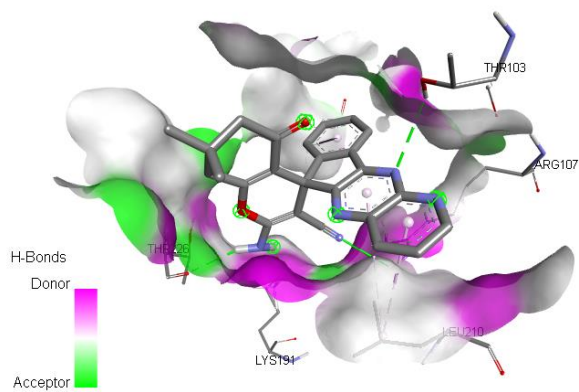
**Interactions****Compound 5j****Interactions**



Compound 5aa

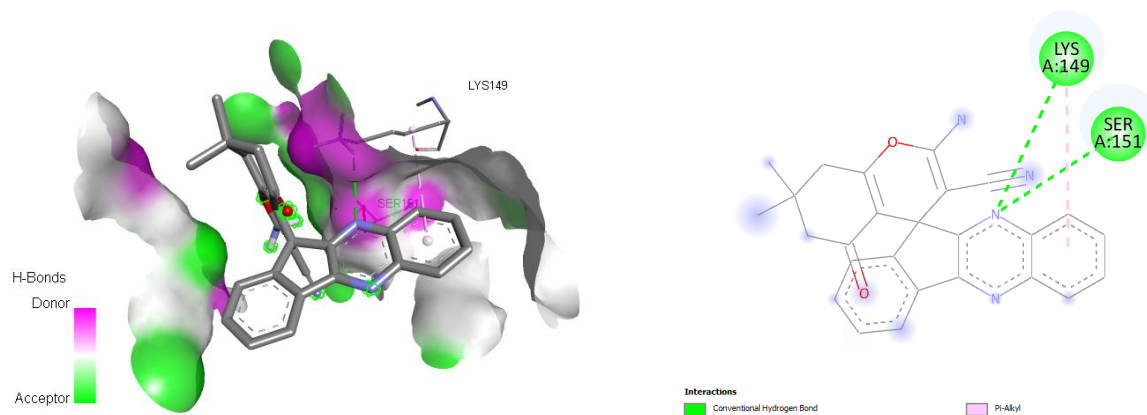


Compound 5bb

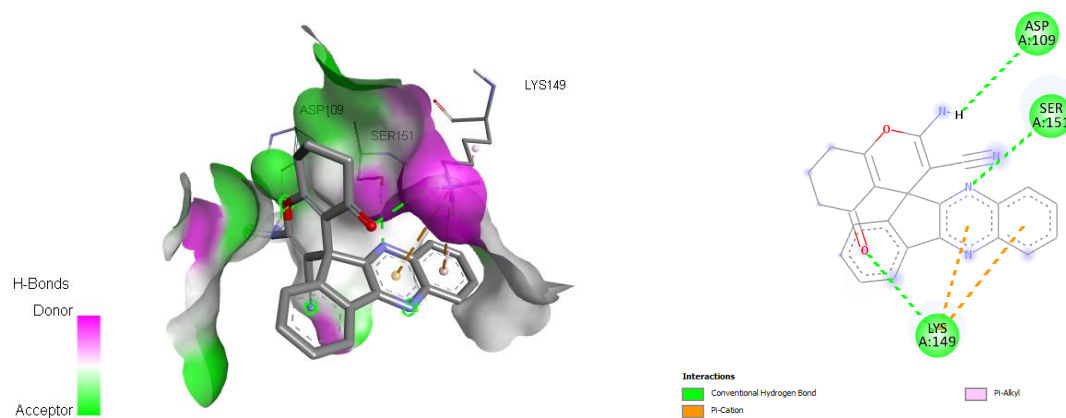


DOCKING POSES WITH (PDB: 3I5Z): LUNG CANCER

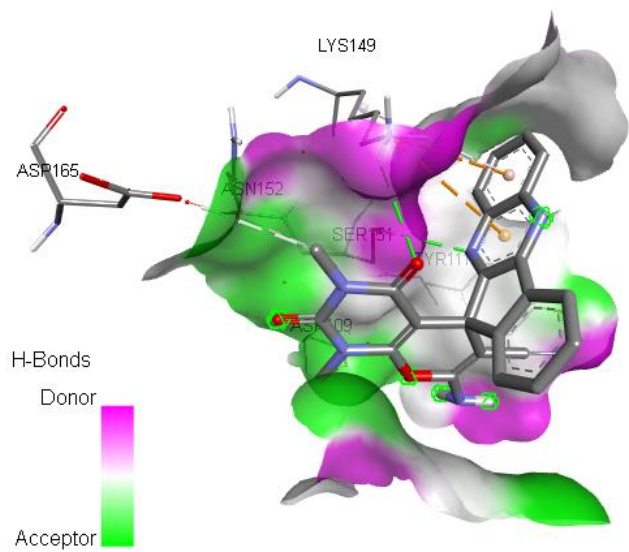
Compound 5a



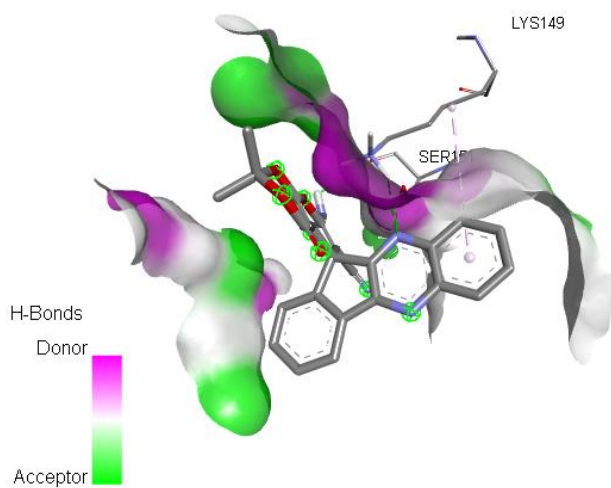
Compound 5b



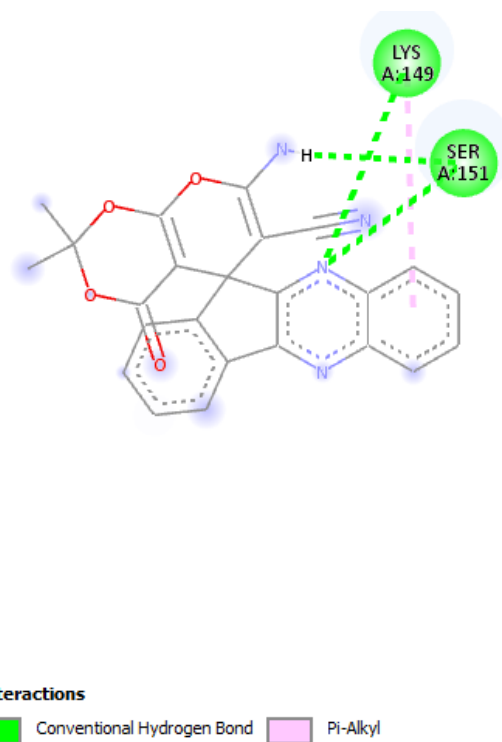
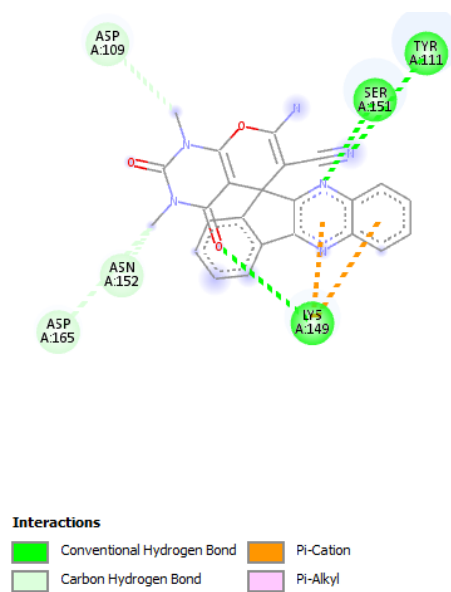
Compound 5c

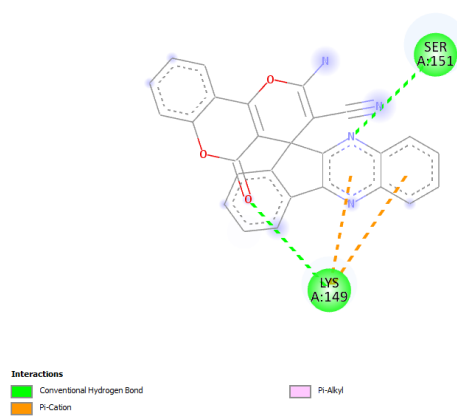
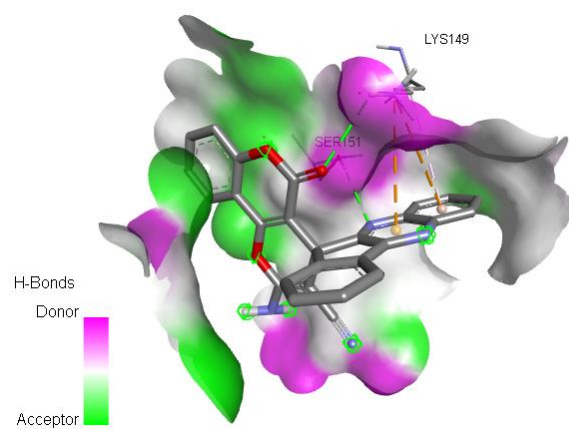


Compound 5d

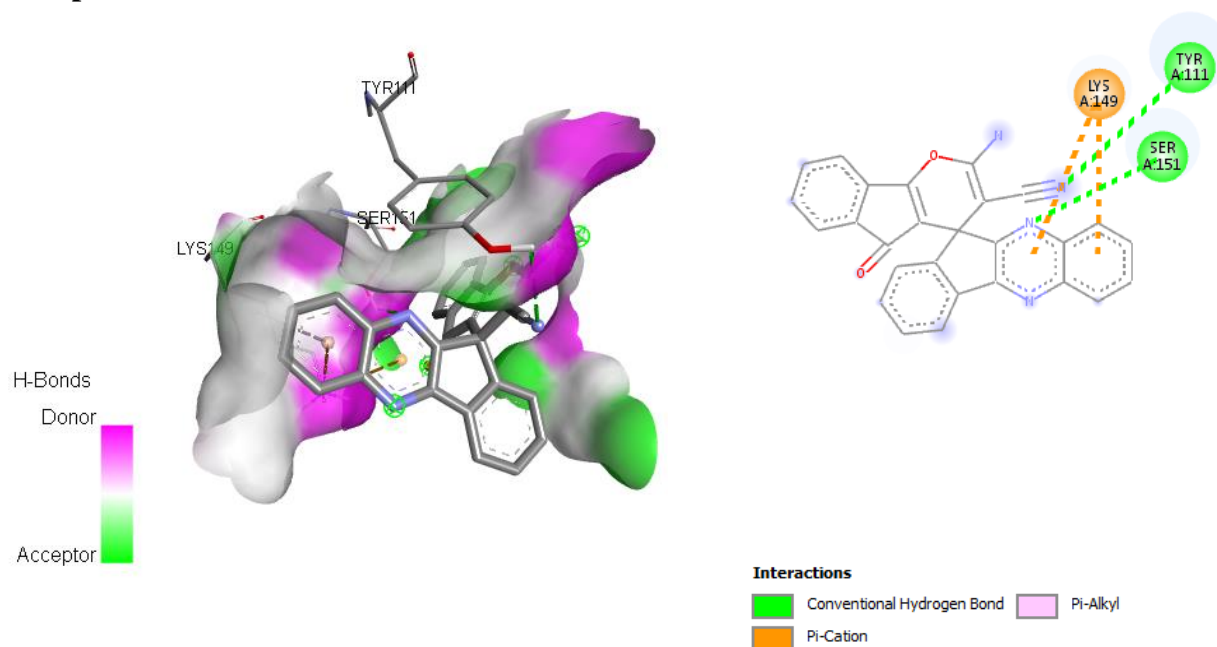


Compound 5e

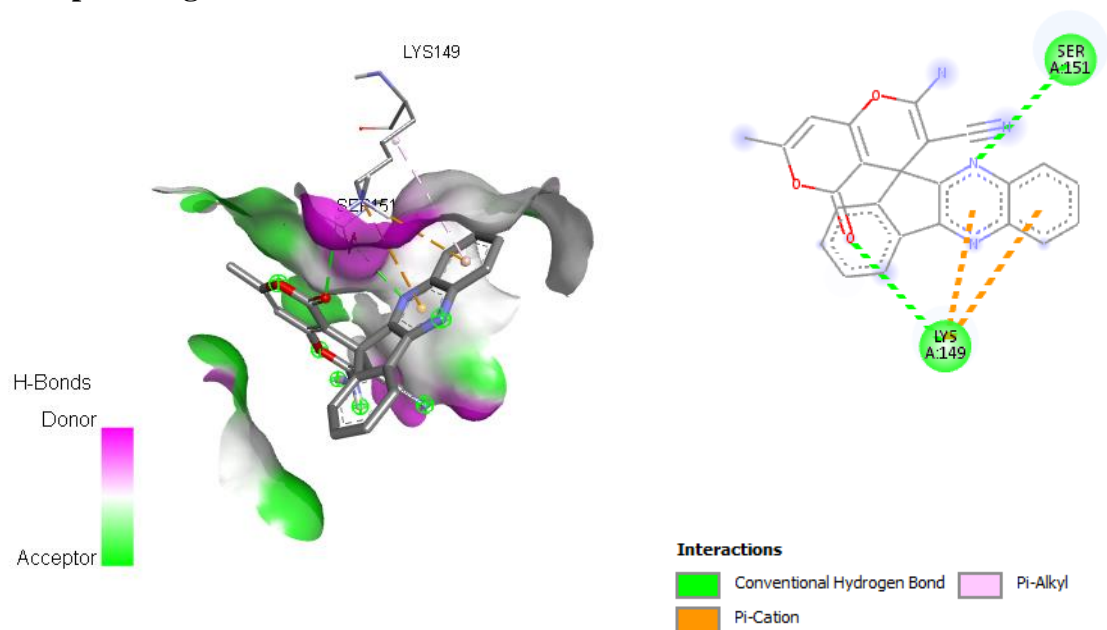




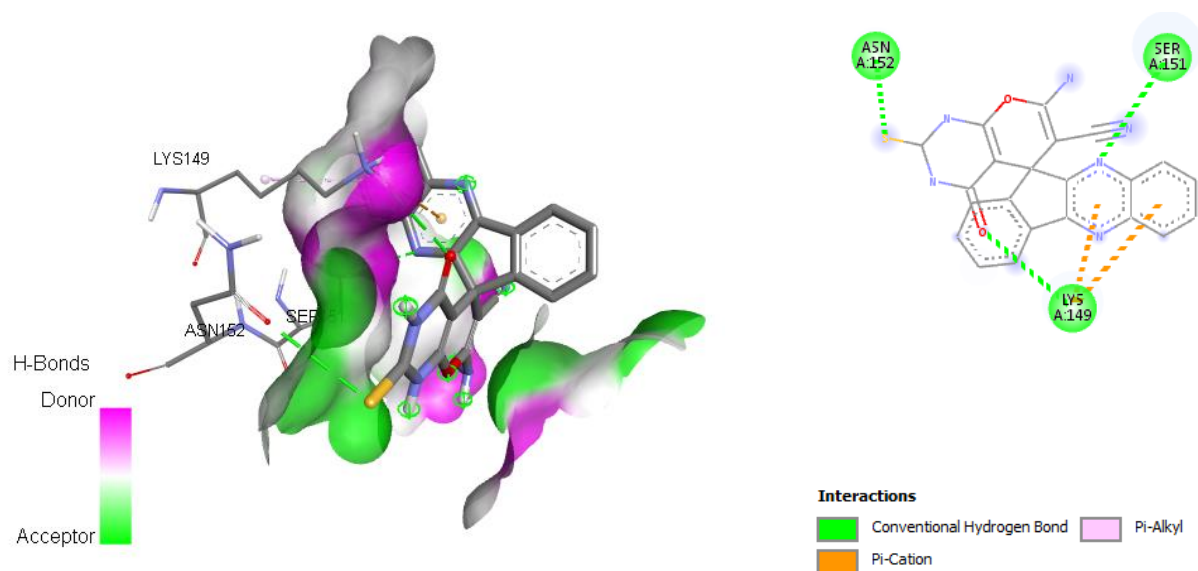
Compound 5f



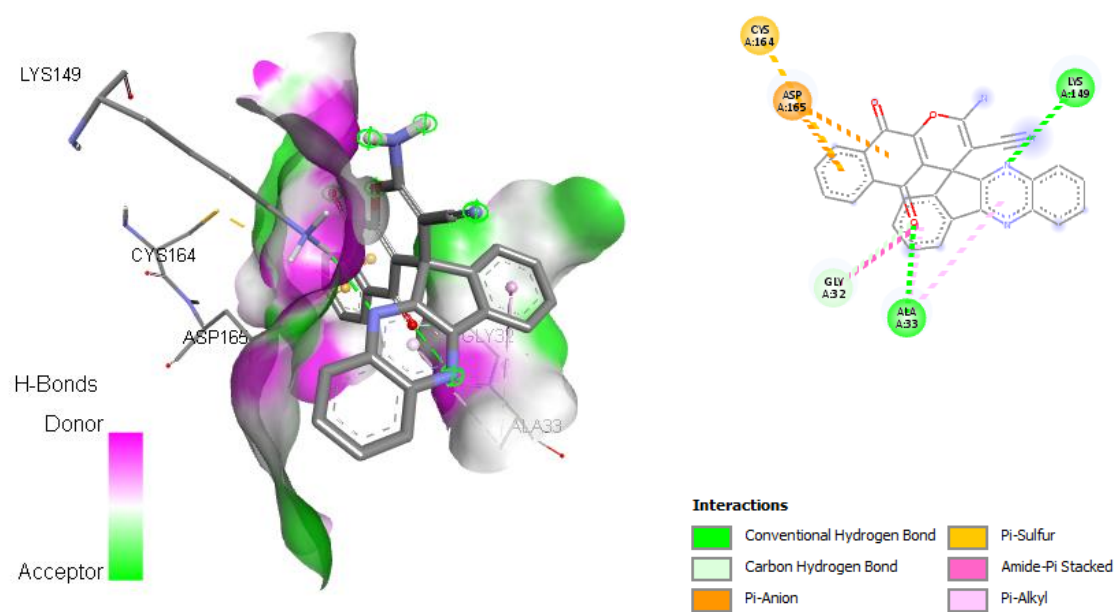
Compound 5g



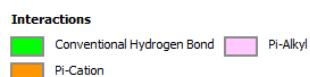
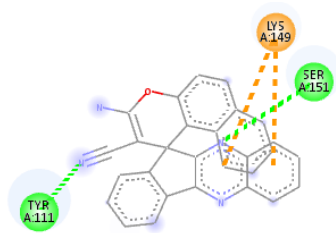
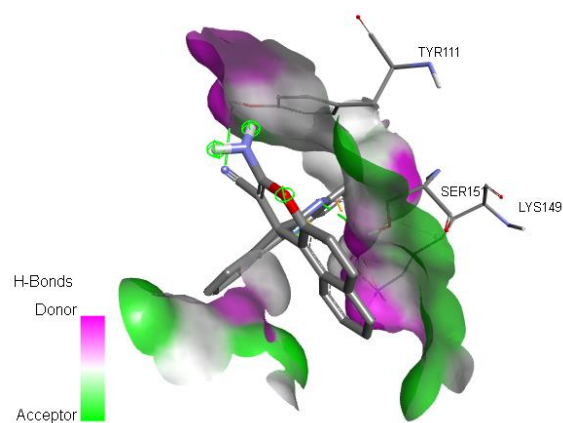
Compound 5h



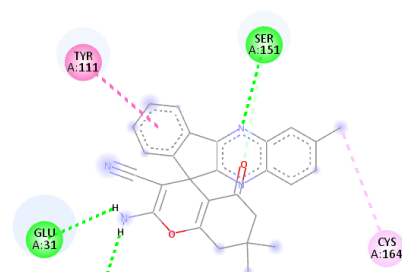
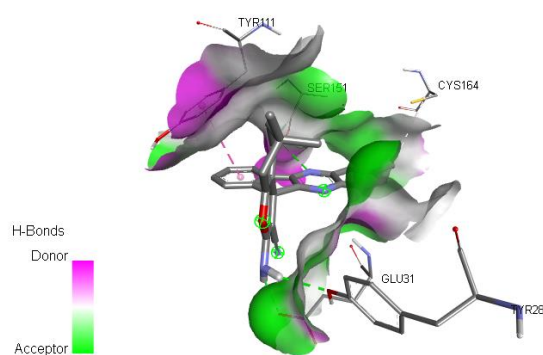
Compound 5i



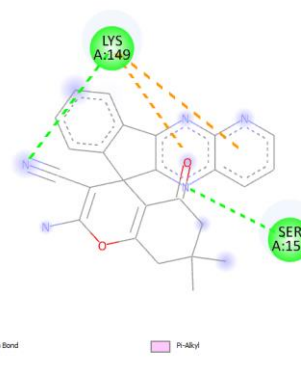
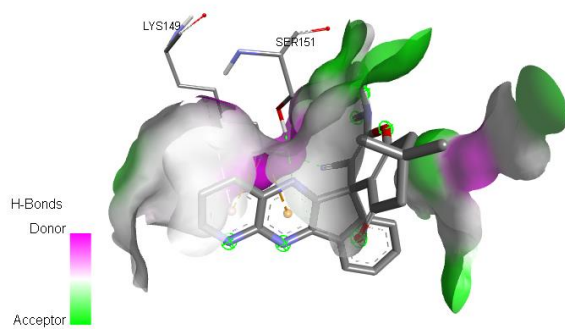
Compound 5j



Compound 5aa



Compound 5bb



References

- [1] Moosavi-Zare, A. R.; Zolfigol, M. A.; Noroozizadeh, E.; Zarei, M.; Karamian, R.; Asadbegy, M. *Mol. Catal. A Chem.* **2016**, *425*, 217-228.