Supporting Information for

Discovery of novel biphenyl-substituted diarylpyrimidines with a cyanomethyl linker as HIV-1 NNRTIs by a molecular hybridization strategy Design of Biphenyl-Substituted Diarylpyrimidines with a Cyanomethyl Linker as HIV-1 NNRTIs via a Molecular Hybridization Strategy

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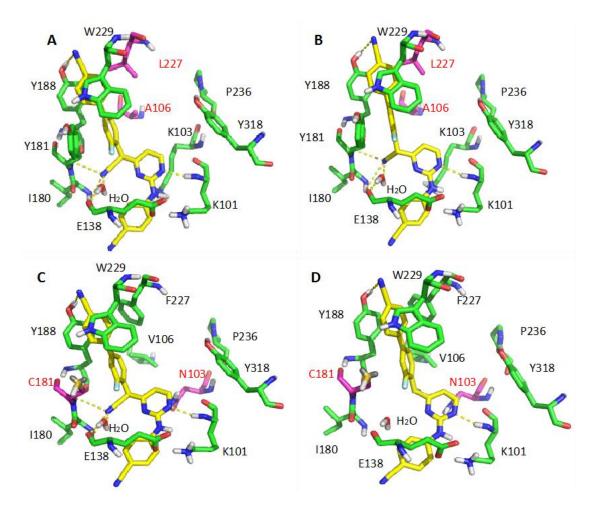
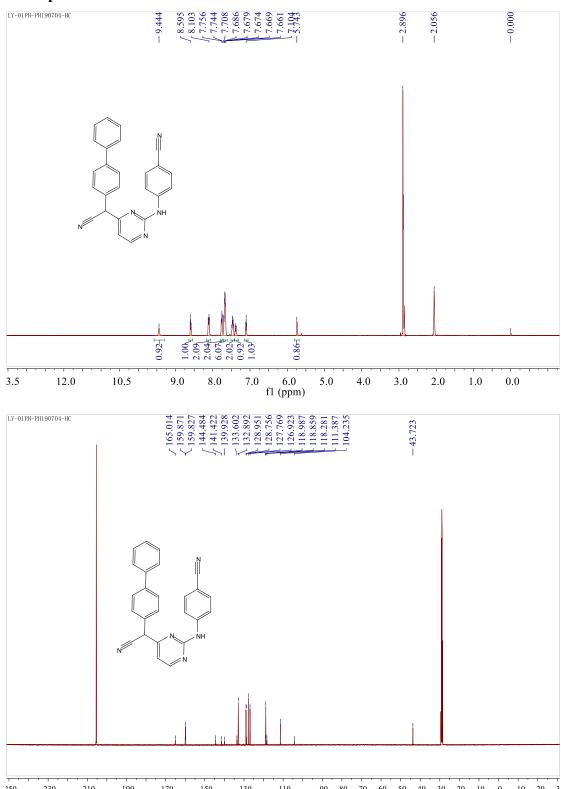


Figure S1 Predicted binding modes of **10p** with double mutant (F227L + V106A, K103N + Y181C) RT (PDB: 2ZD1). (A) F227L + V106A mutant RT with **10p**-S; (B) F227L + V106A mutant RT with **10p**-R; (C) K103N + Y181C mutant RT with **10p**-S; (D) K103N + Y181C mutant RT with **10p**-R.

¹H-NMR, ¹³C-NMR and MS spectra of compounds

1. Spectra of compound 10a



Display Report Analysis Info 1/7/2020 15:15:57 PM Acquisition Date Analysis Name D:\Data\data\2019\H-H_BB1_01_3080.d Method MS-Pos-10min.m Operator BDAL@DE Н-Н compact 8255754.20127 Sample Name Instrument Comment **Acquisition Parameter** 2.0 Bar 200 °C 8.0 l/min Source Type ESI Ion Polarity Positive Set Nebulizer Set Capillary Set End Plate Offset Set Charging Voltage Set Corona Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater Focus Scan Begin 5000 V -500 V 2000 V Active 50 m/z 1500 m/z Waste 0 °C Scan End 0 nA Intens. x10⁵ +MS, 7.8-8.0min #456-472, Background Subtracted 1+ 388.1572 0.8 0.6 0.4 1+ 389.1601 0.2 1+ 390.1630 x105 C₂₅H₁₈N₅, 388.1557 1.2 1+ 388.1557 1.0 0.8 0.6 0.4 1+ 389.1587 0.2 1+ 390.1616 0.0 390 387 388 389 391 m/z H-H_BB1_01_3080.d

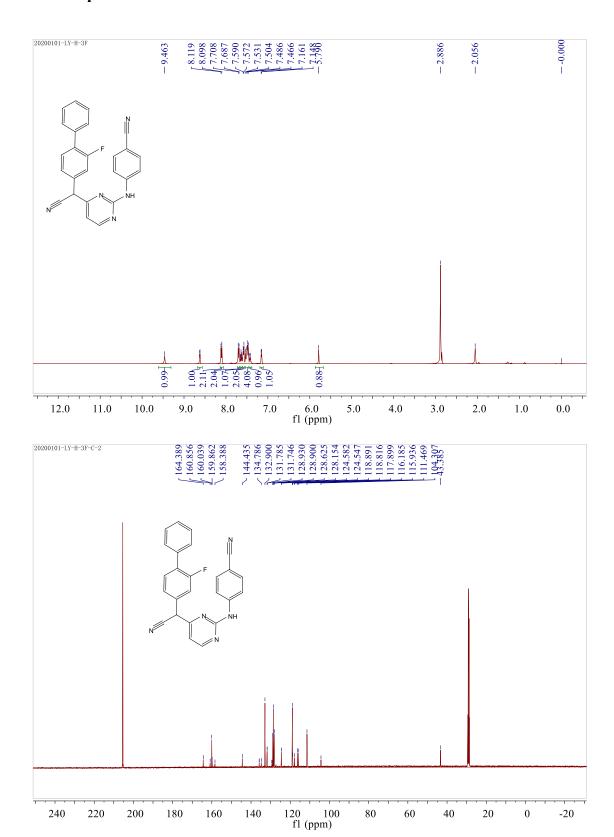
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2. Spectra of compound 10b



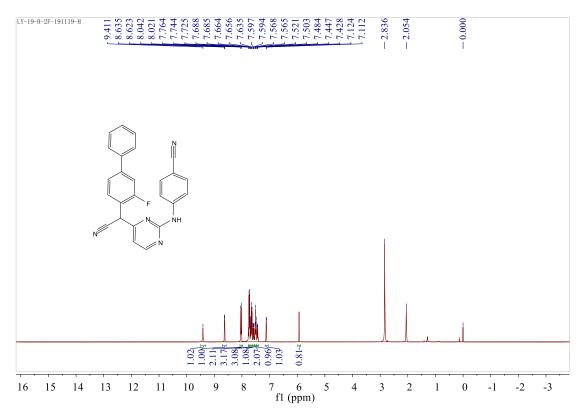
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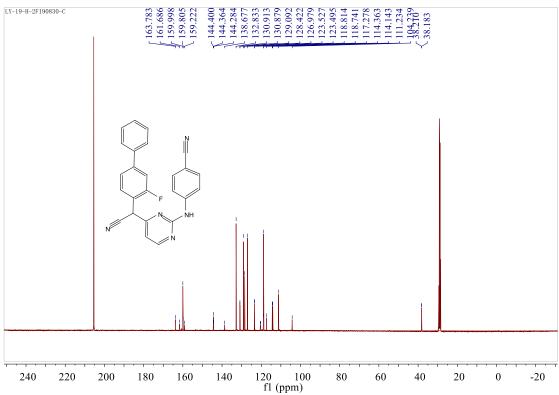
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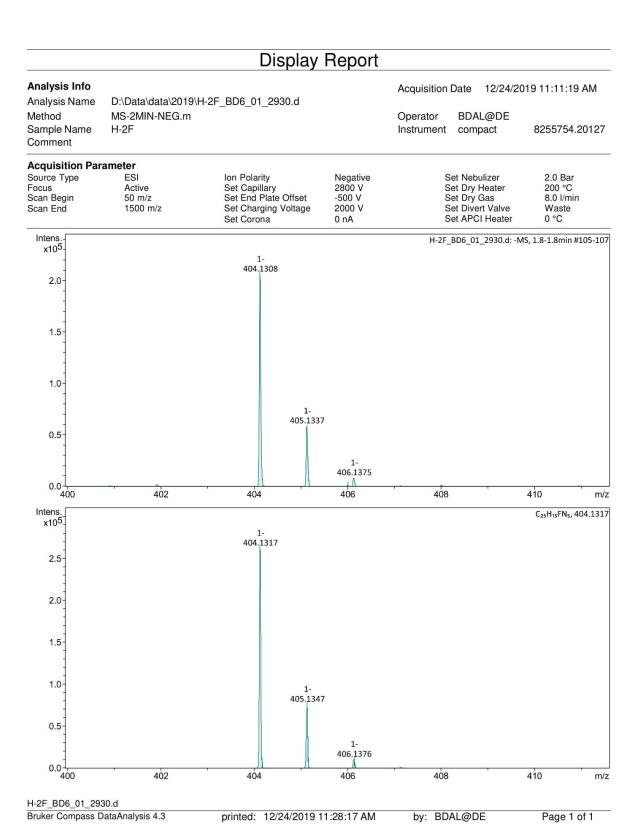
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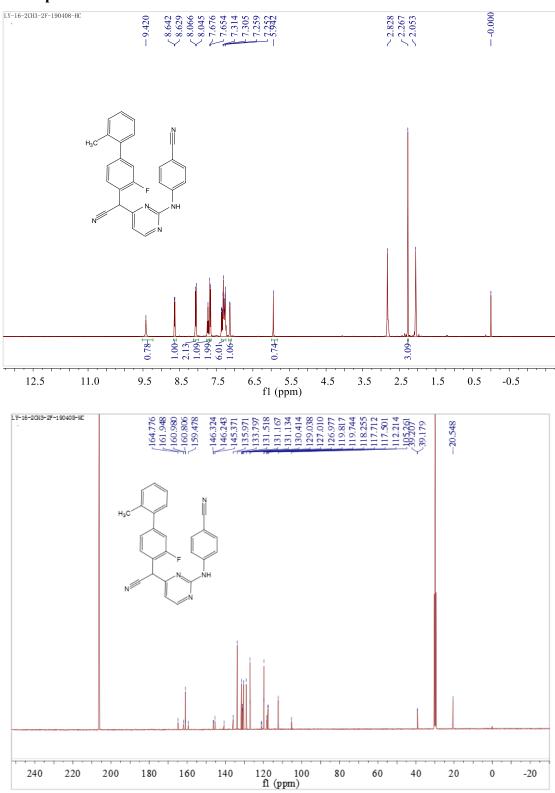
3. Spectra of compound 10c







4. Spectra of compound 10d



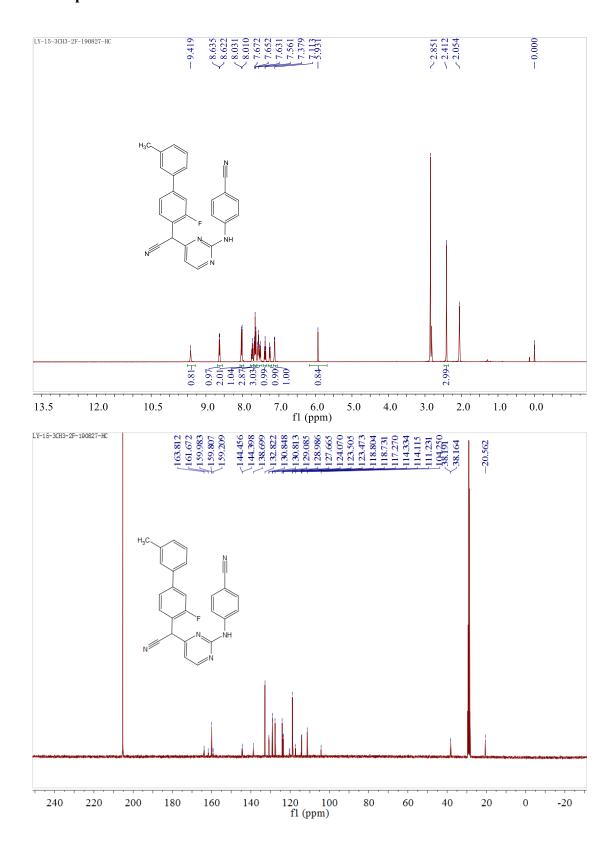
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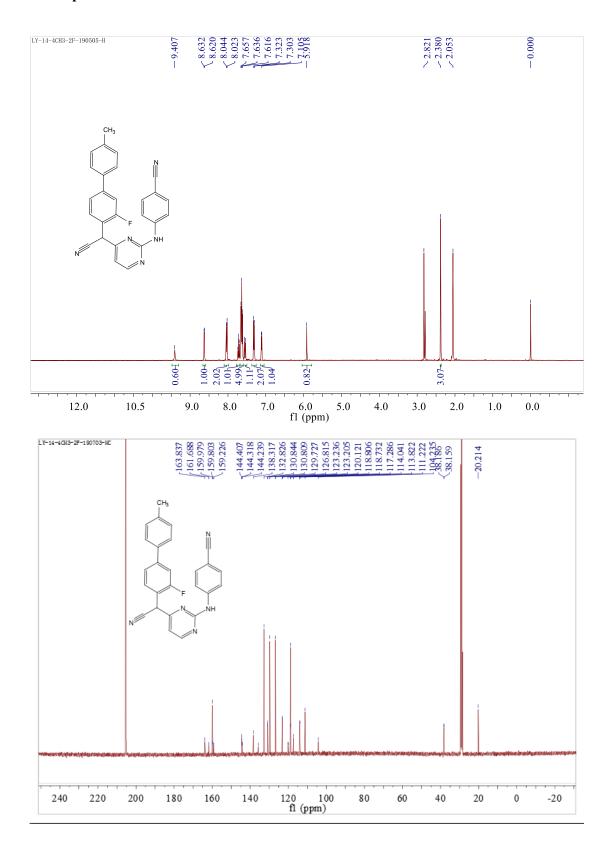
5. Spectra of compound 10e



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6. Spectra of compound 10 f



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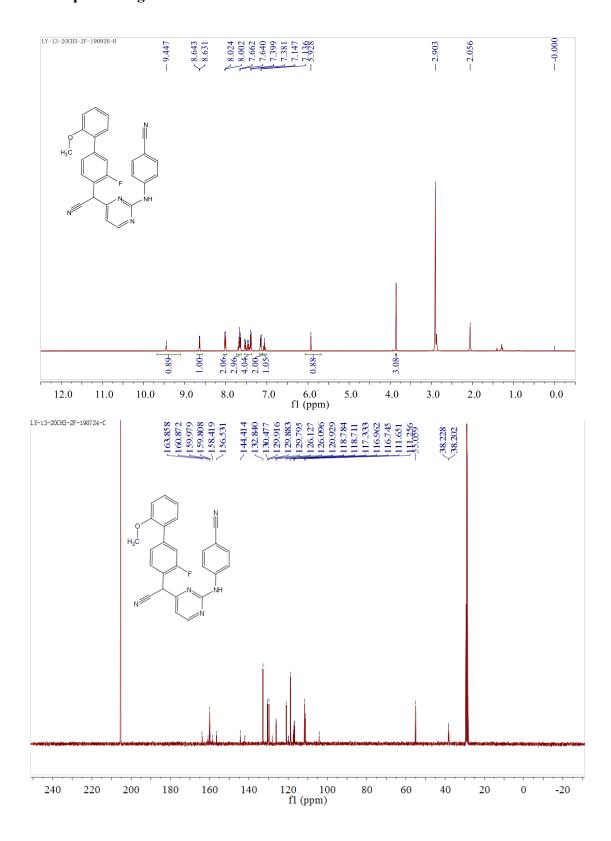
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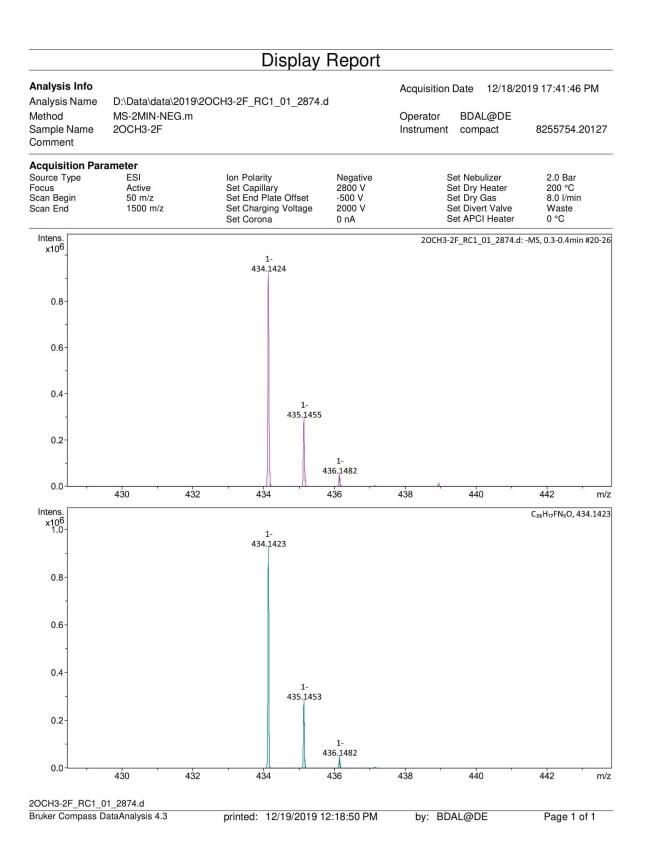
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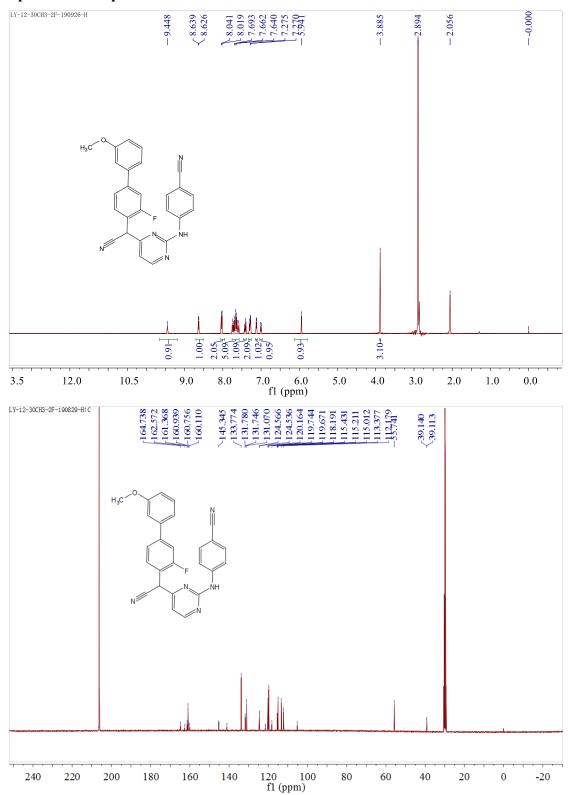
7. Spectra of compound 10g





S15

8. Spectra of compound 10h



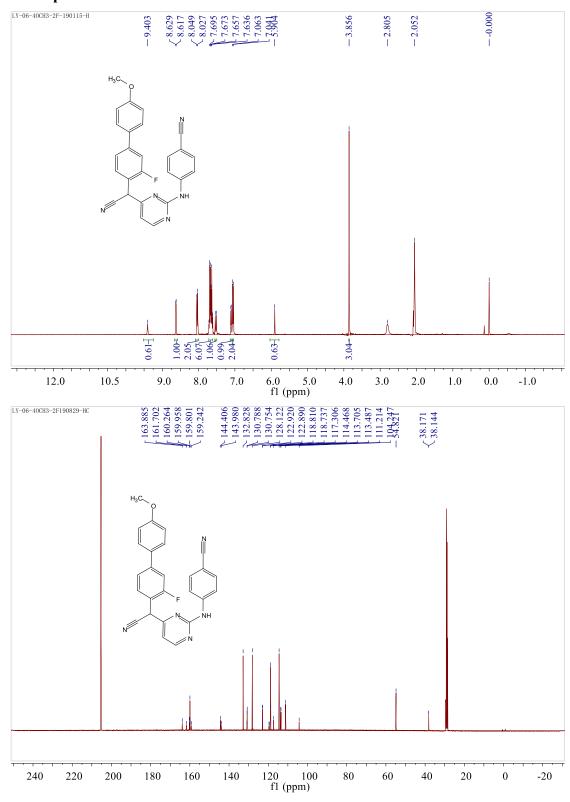
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9. Spectra of compound 10i



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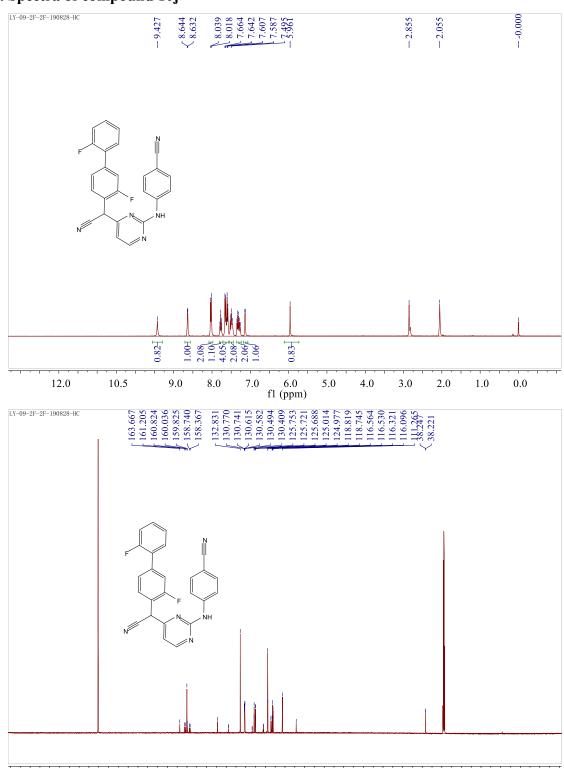
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10. Spectra of compound 10j



-20

120 100 fl (ppm)

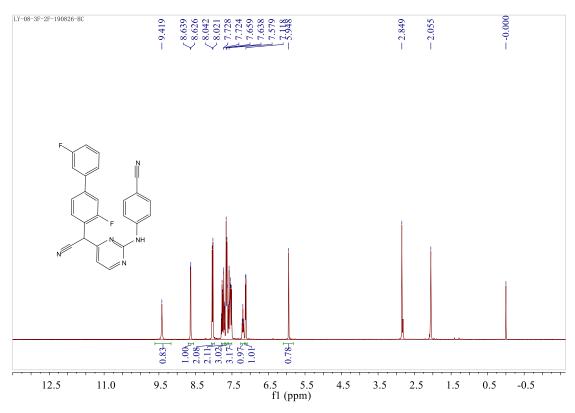
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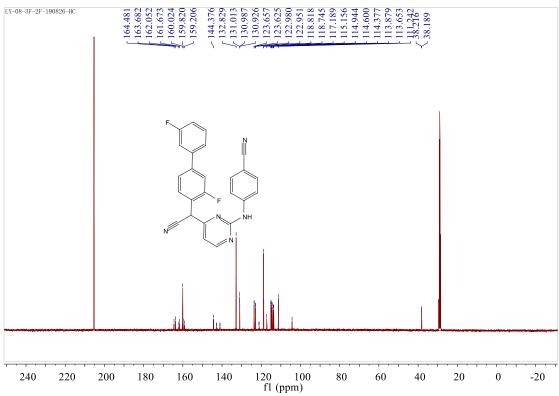
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11. Spectra of compound 10k





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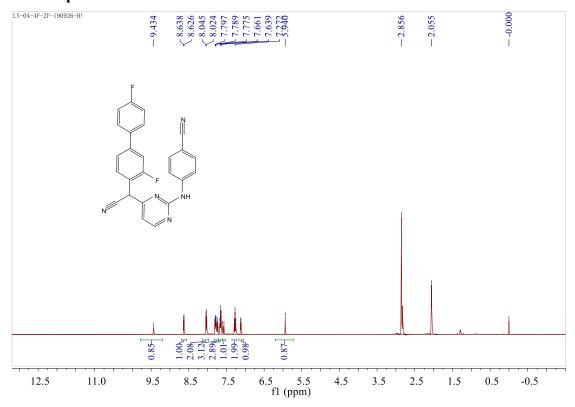
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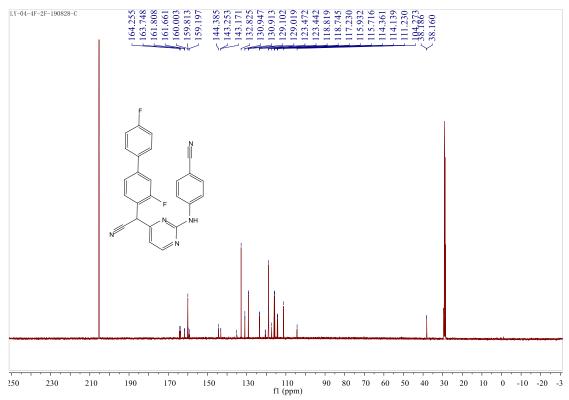
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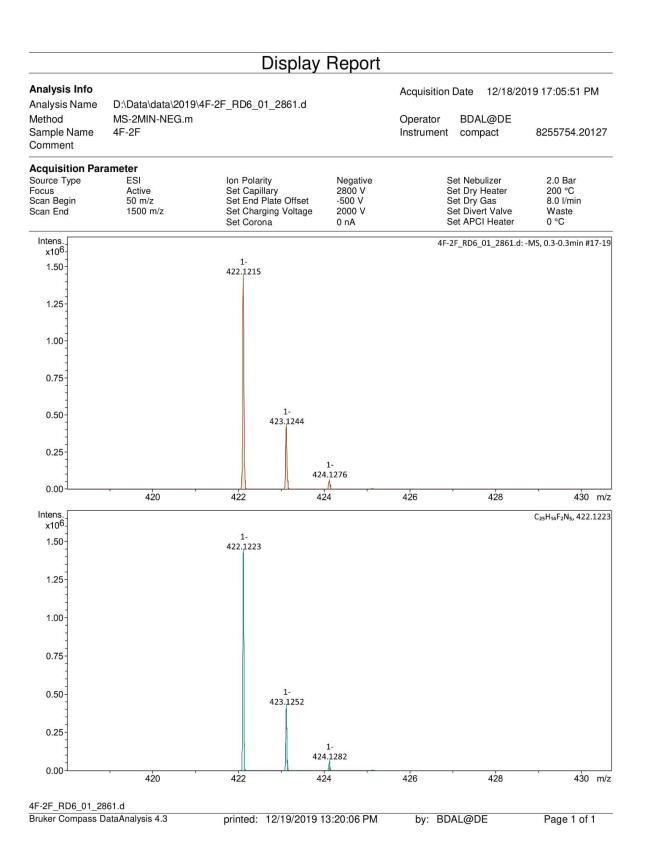
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12. Spectra of compound 10k

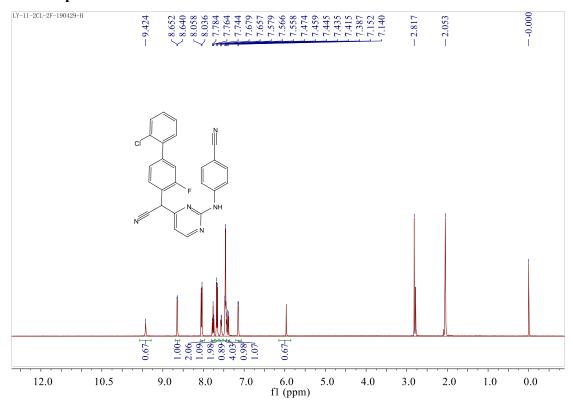


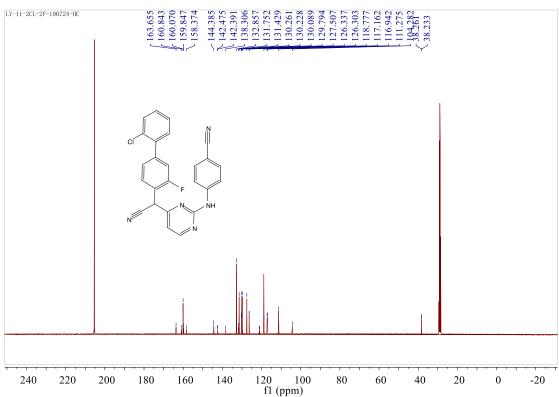




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13. Spectra of compound 10m



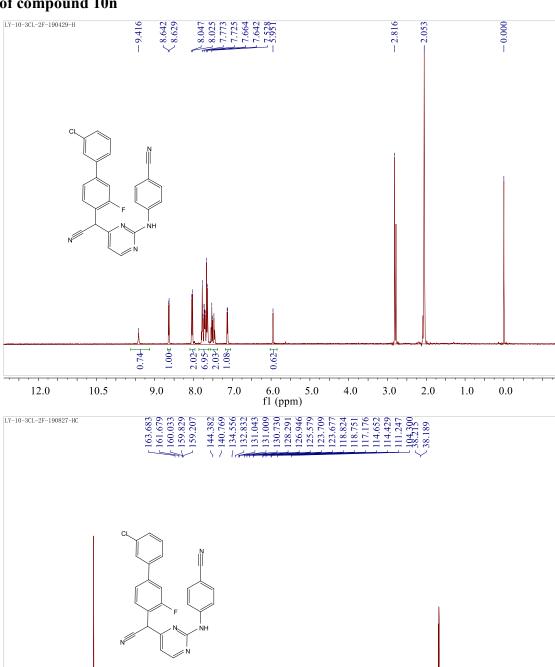


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2CL-2F_RD8_01_2859.d

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14. Spectra of compound 10n



120 100 fl (ppm)

-20

Display Report Analysis Info 12/18/2019 17:27:57 PM Acquisition Date Analysis Name D:\Data\data\2019\3CL-2F_RC6_01_2869.d MS-2MIN-NEG.m Method Operator BDAL@DE Sample Name 3CL-2F Instrument compact 8255754.20127 Comment **Acquisition Parameter** Negative 2800 V -500 V 2000 V Source Type ESI Ion Polarity Set Nebulizer 2.0 Bar Set Capillary Set End Plate Offset Set Charging Voltage Set Corona Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater Focus Scan Begin 200 °C 8.0 l/min Waste Active 50 m/z 1500 m/z Scan End 0 nA 0°C Intens. 3CL-2F_RC6_01_2869.d: -MS, 0.3-0.3min #17-19 x106 1-438.0925 1.25 1.00 0.75 1-440.0905 0.50 439.0956 0.25 1-441.0929 1-442.0959 0.00 434 436 438 442 444 440 m/z Intens. C₂₅H₁₄CIFN₅, 438.0927 x10⁶ 1-438.0927 1.25 1.00 0.75 1-440.0908 0.50 439.0957 0.25 1-441.0931 442.0959 0.00 434 436 438 440 442 444 m/z 3CL-2F_RC6_01_2869.d

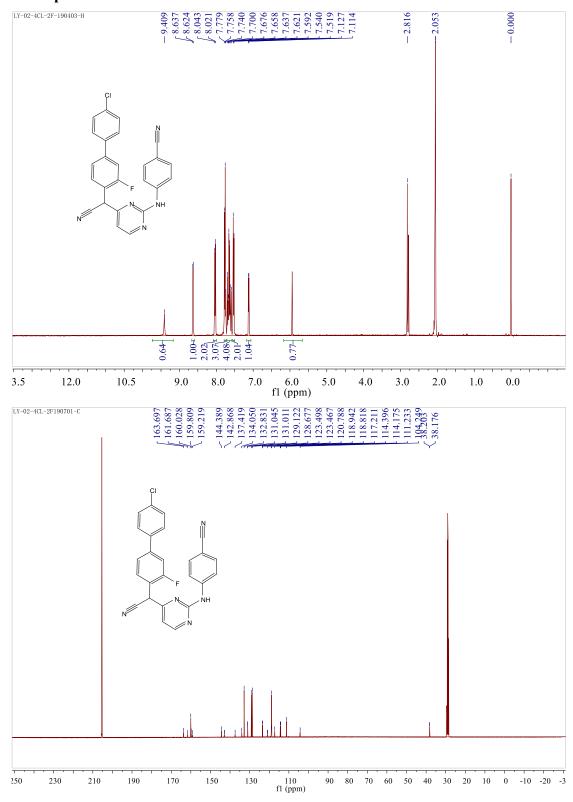
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15. Spectra of compound 10o



Display Report Analysis Info 12/18/2019 17:03:06 PM Acquisition Date Analysis Name D:\Data\data\2019\4CL-2F_RD7_01_2860.d MS-2MIN-NEG.m Method Operator BDAL@DE Sample Name 8255754.20127 4CL-2F Instrument compact Comment **Acquisition Parameter** Negative 2800 V -500 V 2000 V Source Type ESI Ion Polarity Set Nebulizer 2.0 Bar Set Capillary Set End Plate Offset Set Charging Voltage Set Corona Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater Focus Scan Begin 200 °C 8.0 l/min Waste Active 50 m/z 1500 m/z Scan End 0 nA 0°C Intens. x10⁶ 4CL-2F_RD7_01_2860.d: -MS, 0.2-0.3min #13-18 1-438.<mark>0</mark>917 2.0 1.5 1.0 1-440.0896 1-439.0945 0.5 1-441.0920 1-442.0943 0.0 436 434 438 440 442 444 m/z Intens. C₂₅H₁₄CIFN₅, 438.0927 x10⁶ 1-438.0927 2.0 1.5 1.0 1-440.0908 439.0957 0.5 1-441.0931 442.0959 0.0 434 436 438 440 442 444 m/z 4CL-2F_RD7_01_2860.d

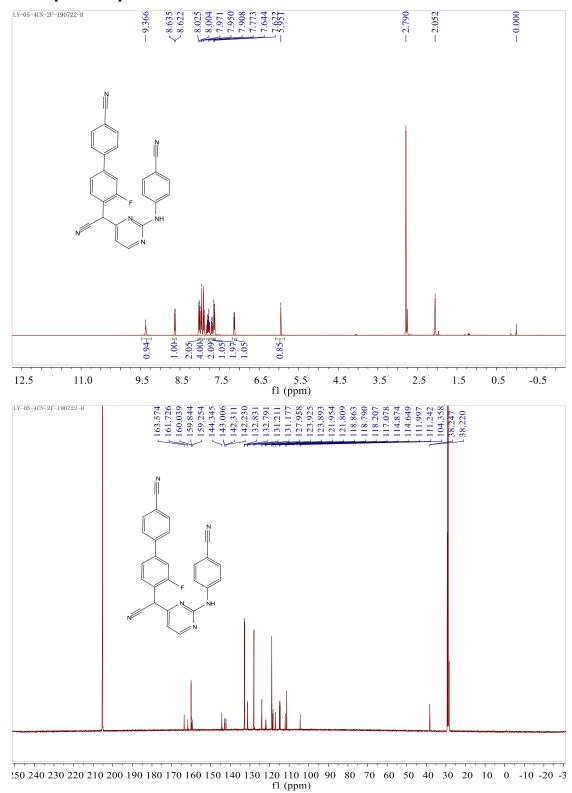
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16. Spectra of compound 10p



Display Report Analysis Info 12/18/2019 12:26:12 PM Acquisition Date Analysis Name D:\Data\data\2019\LY191212-4CN-2F_GD8_01_2850.d Method MS-2MIN-NEG.m Operator BDAL@DE LY191212-4CN-2F compact 8255754.20127 Sample Name Instrument Comment **Acquisition Parameter** Negative 2800 V -500 V 2000 V Source Type ESI Ion Polarity Set Nebulizer 2.0 Bar Set Capillary Set End Plate Offset Set Charging Voltage Set Corona Set Nebulizer Set Dry Heater Set Dry Gas Set Divert Valve Set APCI Heater Focus Scan Begin 200 °C 8.0 l/min Active 50 m/z 1500 m/z Scan End Waste 0 nA 0°C Intens. LY191212-4CN-2F_GD8_01_2850.d: -MS, 0.3-0.3min #15-18 1-429.1264 3 1-430.1291 1-431.1322 0 426 428 432 434 436 430 m/z Intens. C₂₆H₁₄FN₆, 429.1269 1-429.1269 3 1-430.1299 1-431.1328 426 428 432 434 436 430 m/z

LY191212-4CN-2F_GD8_01_2850.d

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