Supporting Information

The conjugates of 5'-deoxy-5-fluorocytidine and hydroxycinnamic acids synthesis, anti-pancreatic cancer activity and molecular docking studies

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compound	MW ^a	dipole ^b	volc	SASAd	dHB ^e	aHB ^f	logP ^g	logS ^h	metab ⁱ	P ^j	Ro3 ^k	Ro5 ¹
1	517.5	2.54	1540.4	857.6	1	14.2	1.6	-5.3	1	68.8	0	2
2	517.5	7.06	1539.8	853.2	1	14.2	1.8	-5.3	1	97.3	0	2
3	517.5	4.88	1541.0	863.3	1	14.2	1.6	-5.4	1	69.3	0	2
4	575.5	4.88	1683.2	928.9	1	16.7	1.1	-5.3	1	29.8	0	2
5	575.5	4.61	1687.0	928.8	1	16.7	1.1	-5.3	1	31.1	0	2
6	491.4	5.21	1423.3	792.5	3	13.2	1.0	-4.9	3	25.5	0	1
30	491.4	9.36	1441.2	811.6	3	16.1	-0.1	-4.3	3	23.8	0	1
31	407.4	9.58	1178.2	678.8	5	12.6	-0.5	-3.5	5	16.9	1	0
32	633.5	4.79	1832.0	997.0	1	19.2	0.7	-5.3	1	16.9	1	2
33	507.4	6.92	1470.2	832.5	4	14.0	0.3	-5.1	4	5.6	1	2
34	423.4	6.09	1199.7	694.7	6	13.4	-1.2	-3.4	6	5.1	1	2
5-dFCR	245.2	5.85	691.2	416.1	4	9.1	-1.4	-1.8	3	80.6	0	0
benazepril	424.5	3.78	1360.8	744.9	2	8.5	1.7	-4.7	7	30.8	1	0
capecitabine	373.4	7.50	1107.9	635.8	3	11.1	0.3	-3.2	3	93.3	0	0
cis-ermethrin	391.3	2.61	1150.2	611.5	0	2.5	6.0	-5.9	2	5009	1	1
irinotecan	586.7	13.88	1780.8	952.1	1	12.8	3.4	-6.7	4	50.6	1	1

^aMW – molecular weight (Da); ^bdipole – dipole moment (D); ^cvol – total molecular volume (Å³); ^dSASA – solvent accessible surface (Å²); ^edHB – estimated number of hydrogen bonds that would be donated by the solute to water molecules in an aqueous solution; ^faHB – estimated number of hydrogen bonds that would be accepted by the solute from water molecules in an aqueous solution; ^glogP – octanol/water partition coefficient; ^glogS – predicted aqueous solubility (mol/dm³); ⁱmetab – number of likely metabolic reactions; ^jP – apparent Caco-2 permeability (nm/sec); ^kRo3 – number of violations of Jorgensen's rule of three; ^lRo5 – number of violations of Lipinski's rule of five.

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compound	FOSA ^a	FISA ^b	PISAc	glob ^d	HERG ^e	BB ^f	MDCK ^g	Kp ^h	HSA ⁱ	Jm ^j	LD ₅₀ k
1	406.9	227.6	191.2	0.75	-6.5	-2.5	41.0	-4.4	-0.5	0.000	5000
2	388.6	211.7	210.9	0.76	-6.5	-2.2	67.7	-4.0	-0.5	0.000	5000
3	415.2	227.3	187.5	0.75	-6.5	-2.5	42.1	-4.4	-0.5	0.000	5000
4	488.2	265.9	142.9	0.74	-6.5	-3.1	16.6	-5.1	-0.7	0.000	5000
5	486.5	264.0	146.5	0.74	-6.5	-3.1	17.3	-5.1	-0.7	0.000	5000
6	296.6	273.0	181.0	0.77	-6.1	-2.9	15.9	-5.1	-0.4	0.000	5000
30	339.4	276.3	153.9	0.76	-6.1	-3.0	14.7	-5.3	-0.9	0.000	1000
31	162.5	291.8	182.5	0.79	-5.7	-2.9	10.2	-5.5	-0.8	0.000	1000
32	558.8	292.0	113.3	0.73	-6.5	-3.6	9.1	-5.6	-0.9	0.000	5000
33	308.1	342.4	149.0	0.75	-6.3	-3.9	2.8	-6.4	-0.5	0.000	5000
34	161.8	346.3	153.5	0.79	-5.7	-3.6	2.5	-6.5	-0.9	0.000	1000
5-dFCR	122.9	220.3	28.6	0.91	-3.1	-1.3	56.8	-5.2	-0.8	0.025	3390
benazepril	282.7	137.9	324.4	0.80	-5.3	-1.0	16.2	-4.1	0.1	0.001	4019
capecitabine	350.6	213.6	27.3	0.81	-4.7	-2.0	66.5	-4.6	-0.7	0.007	1000
cis-permethrin	201.9	31.2	293.7	0.87	-5.1	0.1	8214.0	-0.5	1.0	0.166	85
irinotecan	638.0	178.0	136.1	0.75	-7.0	-1.4	21.8	-6.0	0.6	0.000	765

Table S2. Predicted selected ADMET properties of the tested compounds, cont.

^aFOSA – hydrophobic component of the SASA; ^bFISA – hydrophilic component of the SASA; ^cPISA – π (carbon and attached hydrogen) component of the SASA; ^dglob – globularity descriptor; ^eHERG – predicted IC₅₀ value for blockage of HERG K⁺ channels; ^fBB – predicted brain/blood partition coefficient; ^gMDCK – predicted apparent MDCK cell permeability (nm/sec); ^gK_p – predicted skin permeability; ⁱHSA – prediction of binding to human serum albumin; ⁱJ_m – Predicted maximum transdermal transport rate ($\mu g \text{ cm}^{-2} \text{ hr}^{-1}$); ^kLD₅₀ – predicted value of median lethal dose (mg/kg).

(3,4-diallyloxy)cinnamic acid (18)

Methyl ester **12** [1] (1.00 g, 5.15 mM) was dissolved in acetone (30 mL), then K_2CO_3 (2.84, 20.60 mM) and allyl bromide (2.49 g, 20.60 mM) were added. The mixture was stirred overnight at ambient temperature. The inorganic salts were filtered off, and solvents were evaporated to oily residue. Then, methanol (10 mL) was added, followed by the addition of a NaOH (0.41 g, 10.30 mM) solution in water (5 mL). After stirring in r.t. for 1 h, the mixture was diluted with water (100 mL) and washed twice with methylene chloride. The aqueous layer was acidified to pH 1 with conc. HCl aq. The product was extracted with methylene chloride (3x30 mL). The combined organic layers were dried under anhydrous MgSO₄, evaporated, and dried *in vacuo* to give **18** as white solid. Yield 1.19 g (89%); m.p. 161.7°C (159-160°C [2]); ¹H NMR (500 MHz, CDCl₃) δ 7.71 (d, 1H, J = 15.8 Hz, H-10), 7.13-7.08 (m, 2H, H-12, H-16), 6.88 (d, 1H, *J* = 8.1 Hz, H-15), 6.28 (d, 1H, *J* = 15.8 Hz, H-9), 6.14-6.02 (m, 2H, H-18, H-21), 5.47-5.40 (m, 2H, H-19, H-22), 5.34-5.28 (m, 2H, H-19, H-22), 4.67-4.62 (m, 4H, H-17, H-20). ¹³C NMR (125 MHz, CDCl₃) δ 172.6 (C-8), 151.0 (C-14), 148.6 (C-13), 146.9 (C-10), 133.0 (C-18), 132.8 (C-21), 127.1 C-11), 123.1 (C-16), 118.0 (C-22), 117.9 (C-19), 114.9 (C-9), 113.3 (C-12), 112.8 (C-15), 69.9 (C-17), 69.7 (C-20); HRMS (ESI, m/z): calculated for C₁₅H₁₇O₄ [M + H]⁺ 261.1127; found 261.1139, calculated for C₁₅H₁₆O₄Na [M + Na]⁺ 283.0946; found 283.0951.

5'-deoxy-5-fluoro-2',3'-O-isopropylidene-N⁴, N⁴-(bis(3,4-diallyloxy)cinnamoyl)cytidine (26)



5'-deoxy-5-fluoro-2',3'-O-isopropylidenocytidine (27) (0.110 g, 0.386 mM) and 3,4-di-O-allycaffeic acid (17) (0,100 g, 0.39 mM) were dissolved in dry pyridine (2 mL) and cooled to -25°C. To the stirred on an ice-salt bath solution the POCl₃ (0.04 mL) was added dropwise over a period of 5 min. with the temperature kept below -20°C. The reaction was stirred 4 hours at -20°C, then it was allowed to reach ambient temperature and stirred overnight. After extraction by water/methylene chloride system, the separated organic layer was dried over anhydrous MgSO4, and the solvent was distilled off under reduced pressure. The crude oil was purified using flash column chromatography on a silica gel with hexanes: ethyl acetate 3:1 to 1:1 (v/v), to give two main products: monosubstituted 28 with the yield of 0.067 g (33%) as a yellow solid and disubstituted 26 as a yellow solid. Yield of 26 0.016 g (5.4%); m.p. 83°C (dec.); ¹H NMR (500 MHz, CDCl₃) δ 7.87 (d, 1H, J = 4.9 Hz, H-6, double bound in flucytosine ring), 7.78 (d, 2H, J = 15.4 Hz, H-10, double bond), 7.12 (dd, 2H, J₁ = 8.4 Hz, J₂ = 1.9 Hz, H-16, aromatic CA), 7.05 (d, 2H, J = 1.9 Hz, H-12, aromatic CA), 6.86 (d, 2H, J = 8.4 Hz, H-15, aromatic CA), 6.61 (d, 2H, J = 15.4 Hz, H-9, double bond), 6.11-6.00 (m, 4H, H-18, H-21, allyl CH), 5.78 (d, 1H, J = 1.6 Hz, H-1', deoxyribose), 5.46-5.39 (m, 4H, H-19, H-22, allyl CH₂), 5.33-5.25 (m, 4H, H-19, H-22, allyl CH₂), 4.96 (dd, 1H, J₁ = 6.3 Hz, J₂ = 1.8 Hz, H-2', deoxyribose), 4.64 (m, 4H, H-20, CH₂), 4.59 (m, 4H, H-17, CH₂), 4.51 (dd, 1H, J₁ = 6.3 Hz, J₂ = 4.1 Hz, H-3', deoxyribose), 4,42 (dq, 1H, J₁ = 6.6 Hz, J₂ = 4.1 Hz, H-4', deoxyribose), 1.58 (s, 3H, H-7' or H-8', isopropylidene CH₃), 1.43 (d, J = 6.6 Hz, 3H, H-5', deoxyribose CH₃), 1.36 (s, 3H, H-7' or H-8', isopropylidene CH₃); ¹³C NMR (125 MHz, CDCl₃) δ 167.3 (C-8, C=O CA), 157.3 (d, J_{CF} = 13.4 Hz, C-4, flucytosine ring), 152.4 (C-2, C=O flucytosine ring), 151.4 (C-14, aromatic CA), 148.5 (C-13, aromatic CA), 146.7 (C-10, double bond), 140.4 (d, J_{CF} = 247.7 Hz, C-5, flucytosine ring), 133.0 (C-18, allyl CH), 132.7 (C-21, allyl CH), 130.6 (d, J_{CF} = 34.1 Hz, C-6, flucytosine ring), 127.3 (C-11, aromatic CA), 123.5 (C-16, aromatic CA), 118.1 (C-22, allyl CH₂), 118.1 (C-19, allyl CH₂), 117.3 (C-9, double bond), 114.6 (C-6', isopropylidene), 113.5 (C-12, aromatic CA), 113.3 (C-15, aromatic CA), 94.7 (C-1', deoxyribose), 85.6 (C-2', deoxyribose), 84.6 (C-3', deoxyribose), 84.3 (C-4', deoxyribose), 70.1 (C-17, CH₂), 69.7 (C-20, CH₂), 27.1 (C-7' or C-8', isopropylidene CH₃), 25.3 (C-7' or C-8', isopropylidene CH₃), 19.3 (C-5', deoxyribose CH₃); HRMS (ESI, m/z): calculated for $C_{42}H_{45}N_3O_{10}F$ [M + H]⁺ 770.3089; found 770.3081, calculated for $C_{42}H_{44}N_3O_{10}FNa$ [M + Na]⁺ 792.2908; found 792.2902.

5'-deoxy-5-fluoro-2',3'-O-isopropylidene-N⁴-(3,4-diallyloxy)cinnamoyl)cytidine (28)



To 5'-deoxy-5-fluoro-2',3'-O-isopropylidenocytidine (**27**) (1.10 g, 3.86 mmol) in methylene chloride (4 mL), 50% NaOH (0.925 g; 11.57 mM) was added. Then, after 1 min. stirring in ambient temperature, the solution (3,4-diallyloxy)cinnamoyl chloride (**24**) (1.08, 3.86 mM) in methylene chloride (6 mL) was added dropwise. The reaction mixture was heated with stirring for 1 h at 50°C. After cooling, it was extracted with water/methylene chloride. The separated organic layer was dried over anhydrous MgSO₄, and the solvent was distilled off under reduced pressure. The crude product **28** was purified by flash column chromatography on a silica gel with hexanes: ethyl acetate 4:1to 1:1 (v/v). Yield 1,85 g (91%); m.p. 85°C (dec.); ¹H NMR (500 MHz, CDCl₃) δ 7.82 (d, 1H, *J* = 15.6 Hz, H-10, double bond), 7.56 (bs, 1H, H-7, NH), 7.22-7.12 (m, 2H, H-12, H-16, aromatic CA), 6.87 (d, 1H, *J* = 8.3 Hz, H-15, aromatic CA), 6.15-6.00 (m, 2H, H-18, H-21, allyl CH), 5.67 (s, 1H, H-1', CHN deoxyribose), 5.55-5.38 (d, 2H, *J* = 15.3 Hz, H-19, H-22, allyl CH₂), 5.30 (d, 2H, *J* = 10.5 Hz, H-19, H-22, allyl CH₂), 4.92 (d, 1H, *J*

= 5.5 Hz, H-2', deoxyribose), 4.65 (d, 4H, J = 4.5 Hz, H-17, H-20, CH₂), 4.51 (dd, 1H, $J_1 = J_2 = 4.6$ Hz, H-3', deoxyribose), 4.31 (m, 1H, H-4', deoxyribose), 1.57 (s, 3H, H-7' or H-8', isopropylidene CH₃), 1.41 (d, 3H, J = 6.5 Hz, H-5', deoxyribose CH₃), 1.34 (s, 3H, H-7' or H-8', isopropylidene CH₃); ¹³C NMR (125 MHz, CDCl₃) δ 150.9 (C-14, aromatic CA), 148.5 (C-13, aromatic CA), 146.0 (C-10, double bound), 133.0 (C-18, allyl CH), 132.9 (C-21, allyl CH), 127.8 (C-11, aromatic CA), 123.3 (C-16, aromatic CA), 118.0 (C-19, C-22, allyl CH₂), 114.7 (C-6', isopropylidene), 113.3 (C-15, aromatic CA), 113.1 (C-12, aromatic CA), 93.9 (C-1', deoxyribose), 85.3 (C-2', deoxyribose), 84.7 (C-3', deoxyribose), 83.5 (C-4', deoxyribose), 69.9 (C-17, CH₂), 69.7 (C-20, CH₂), 27.1 (C-7' or C-8', isopropylidene CH₃), 25.3 (C-7' or C-8', isopropylidene CH₃), 19.1 (C-5', deoxyribose CH₃); HRMS (ESI, m/z): calculated for C₂₇H₃₁N₃O₇F [M + H]⁺ 528.2146; found 528.2145, calculated for C₂₇H₃₀N₃O₇FNa [M + Na]⁺ 550.1965; found 550.1964.

5'-deoxy-5-fluoro-N⁴-(3,4-diallyloxy)cinnamoyl)cytidine (29)



To 5'-deoxy-5-fluoro-2',3'-O-isopropylidenocytidine (27) (0.48 g, 1.68 mmol) in methylene chloride (2 mL), 50% NaOH (0.27 g, 3.37 mM) was added. Then, after 1 min. stirring in ambient temperature, the solution of (3,4-diallyloxy)cinnamoyl chloride (24) (0.47 g, 1.69 mM) in methylene chloride (3 mL) was added dropwise. The reaction mixture was heated with stirring for 1 h at 50°C. After cooling, 5 M HCl aq. (2.5 mL) and methanol (2 mL) were added to reaction mixture and stirred 20 min. in ambient temperature. Due to the lack of progress, methylene chloride was distilled off and another portion of methanol (10 mL) and conc. HCl aq. (1.5 mL) were added to reaction mixture. After additional 1 h stirring, it was diluted with an aqueous saturated sodium bicarbonate solution, then extracted with methylene chloride. The organic layer was dried over anhydrous MgSO₄, and the solvent was distilled off under reduced pressure. The crude product 29 was purified by flash column chromatography on a silica gel with methylene chloride: methanol 50:1 to 25:1. Yield 0.19 g (23%); m.p. 59°C (dec.); ¹H NMR (500 MHz, CDCl₃) δ 7.75 (d, 1H, J = 15.6 Hz, H-10, double bond), 7.16 (d, 1H, J = 8.2 Hz, H-16, aromatic CA), 7.13 (d, 1H, J = 1.5 Hz, H-12, aromatic CA), 6.84 (d, 1H, J = 8.4 Hz, H-15, aromatic CA), 6.11-6.01 (m, 2H, H-18, H-21, allyl CH), 5.72 (d, 1H, J = 3.7 Hz, H-1', CHN deoxyribose), 5.47-4.38 (m, 2H, H-19, H-22, allyl CH₂), 5.32-5.27 (m, 2H, H-19, H-22, allyl CH₂), 4.63 (m, 2H, H-17, CH₂), 4.61 (m, 2H, H-20, CH₂), 4.30 (bs, 1H, H-4', deoxyribose), 4.27 (m, 1H, H-2', deoxyribose), 3.86 (bs, 1H, H-3', deoxyribose), 3.56 (bs, 1H, deoxyribose OH), 1.38 (d, 3H, J = 6,5 Hz, H-5', CH₃ deoxyribose), ¹³C NMR (125 MHz, CDCl₃) δ 151.1 (C-14, aromatic CA), 148.4 (C-13, aromatic CA), 146.6 (C-10, double bond), 133.0 (C-18, allyl CH), 132.8 (C-21, allyl CH), 127.5 (C-11, aromatic CA), 123.2 (C-16, aromatic CA), 118.0 (C-19, C-22, allyl CH₂), 113.7 (C-12, aromatic CA), 113.3 (C-15, aromatic CA), 92.9 (C-1', deoxyribose), 81.9 (C-4', deoxyribose), 76.2 (C-2', deoxyribose), 75.3 (C-3', deoxyribose), 70.0 (C-17, CH₂), 69.6 (C-20, CH₂), 18.8 (C-5', deoxyribose CH₃); HRMS (ESI, m/z): calculated for C₂₄H₂₇N₃O₇F [M + H]⁺ 488.1833; found 488.1830.

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Figure S1. ¹H NMR spectrum of compound 18 (CDCl₃)



Figure S2. ¹³C NMR spectrum of compound 18 (CDCl₃)



Figure S3. ¹H NMR spectrum of compound **26** (CDCl₃)



Figure S4. ¹³C NMR spectrum of compound 26 (CDCl₃)



Figure S5. ¹H NMR spectrum of compound **28** (CDCl₃)



Figure S6. ¹³C NMR spectrum of compound 28 (CDCl₃)



Figure S7. ¹H NMR spectrum of compound 29 (CDCl₃)



Figure S8. ¹³C NMR spectrum of compound 29 (CDCl₃)



Figure S9. ¹H NMR spectrum of compound **1** (DMSO- d_6)



Figure S10. ¹³C NMR spectrum of compound **1** (DMSO- d_6)



Figure S11. ¹H NMR spectrum of compound **2** (DMSO- d_6)

Figure S12. ¹³C NMR spectrum of compound 2 (DMSO- d_6)

Figure S13. ¹H NMR spectrum of compound 3 (DMSO-*d*₆)

Figure S14. ¹³C NMR spectrum of compound 3 (DMSO- d_6)

Figure S15. ¹H NMR spectrum of compound **4** (DMSO- d_6)

Figure S16. ¹³C NMR spectrum of compound **4** (DMSO- d_6)

Figure S17. ¹H NMR spectrum of compound **5** (DMSO- d_6)

Figure S18. ¹H NMR spectrum of compound 5 (CDCl₃)

Figure S19. ¹³C NMR spectrum of compound (DMSO- d_6)

Figure S20. ¹³C NMR spectrum of compound 5 (CDCl₃)

Figure S21. ¹H NMR spectrum of compound **6** (DMSO- d_6)

Figure S22. ¹³C NMR spectrum of compound 6 (DMSO- d_6)

210914_7_79	1: 0-70 N: 0 _1A 16 (0.177)	D-6 О: (Ст (13:23-)	D-15 F: 1 (87:100+2:8))	-1						то	F MS ES
100-				518.1577							2.17e+00
				5	19 1608						
- 512	1928 514	1096	516 0982 51	8.0929	520.163	31 521.10	659	524.1657	525.1688	528.4417 ₅₂₉	1417
0	2.0 514		516.0	518.0	520.0	52 St	2.0	524.0	526.0	528.0	i i i i m
Virimum: Vaximum			5 Q	-1.5 85 0							
lass	Cale. Ma	ss mDa	PPM	DBE	1 - F 1 1	Norm	Conff) Formul			
518.1577	518,1575		с.4	13.5			99.89		5 N3 09 F		
	519,1556	2.1	4.2	26.5	868.6	6.814	0.11	C36 H2	1 N 02 F		
Aonoisotopi 159 formula Elements Us 2 0-60 H:	c Mass. Even (e) evaluated sed: 0-70 N: 0-6	Electron with 2 res	lons ults within I	imits (all re Na: 1-1	858.6 sults (up to	6, 814 1000) for	e.ii each mas	C36 H2	5 X 02 F		
Monoisotopi 559 formula Elements Us 2: 0-60 H: 210914_7_79	c Mass. Even (e) evaluated sed: 0-70 N: 0-6 _1A 16 (0.177)	Electron with 2 res O: 0-11 Cm (13:23-	tons ults within I 5 F: 1-1 87:100+2:8))	26.5 imits (all re Na: 1-1	asults (up to	6. 811 1000) for	each mas	C36 H2	1 N 02 F	то	F-MS-ES
Monoisotopi 559 formula Elements Use C: 0-60 H: 210914_7_79 100	c Mass. Even (e) evaluated sed: 0-70 N: 0-6 _1A 16 (0.177))	Electron with 2 res O: 0-11 Cm (13:23-	lons ults within I 5 F: 1-1 87:100+2:8))	imits (all re Na: 1-1	868.6 sults (up to 0.1400	6, 814 1000) for	each mas	C36 H2	1 N 02 F	то	F MS ES 2.88e+0
Monoisotopi 559 formula; Elements Us C: 0-60 H: 210914_7_79 100	c Mass. Even (e) evaluated sed: 0-70 N: 0-6 _1A 16 (0.177))	Electron with 2 res O: 0-1 Cm (13:23-	lons ults within I 5 F: 1-1 87:100+2:8))	imits (all re Na: 1-1	868.6 sults (up to 0.1400	8, 814 1000) for	e.i1	C36 H2	2 X 02 F	то	F MS ES 2.88e+0
Monoisotopi 559 formula: Elements Us C: 0-60 H: 210914_7_79 100	c Mass. Even (e) evaluated sed: _1A 16 (0.177) 1	Electron with 2 res O: 0-18 Cm (13:23-1	lons ults within I 5 F: 1-1 87:100+2:8))	26.5 imits (all re Na: 1-1 540	sults (up to 0.1400 541.1429 4 542 1	6, 414 1000) for	each mas	C36 H2 (5)	5 X 02 F	то	F MS ES 2.880+0

Figure S23. HRMS data of compound 1

Monoisotopio	o Mass, Even Ele	ectron lons										
577 formula(e) evaluated with	1 2 results v	within lim	its (all re	esults (up t	o 1000) fo	r each ma	iss)				
C: 0-60 H	: 0-70 N: 0-6	O: 0-15	F: 1-1									TOF MS F
100-				518.158	0							8.15e+(
- 509	2580 511 2710	514 1029	518	519 1.0945	9.1609 520.1628	521.1653	524.1656 (525.1686	50	99 1435 530).1430	533 3480
0	510.0 512.0	514.0	516 .0	518.0	520.0	522.0	524.0	526.0	528.0	530.0	532	.0 534.0
Minimum: Maximum:		5.0	5.0	-1.5 80.0								
	Calc. Mass			DBE	1-F12	Nozm	Coní () Eber	u_a			
518.1580	518.1575	0.5	1.0	13.5	549.3		98.88		1125 N			
Monoisotopio 559 formula(Elements Us C: 0-60 H:	: Mass, Even Ele e) evaluated with ed: 0-70 N: 0-6 C	ectron lons 1 2 results v D: 0-15 F	within lim : 1-1 Na	its (all re a: 1-1	esults (up te	o 1000) fo	r each ma	155)				
Monoisotopio 559 formula(Elements Us C: 0-60 H: 210914_7_81_	c Mass. Even Ele e) evaluated with ed: 0-70 N: 0-6 C _1A 16 (0.177) Cm (ectron lons 12 results v D: 0-15 F 15:20-(3:8+1	within lim : 1-1 Ni 131:145))	its (all re a: 1-1	isults (up ti	o 1000) fo	r each ma	155)				TOF MS E
Monoisotopio 559 formula(Elements Us C: 0-60 H: 210914_7_81_ 100	c Mass. Even Ele e) evaluated with ed: 0-70 N: 0-6 C _1A 16 (0.177) Cm (ectron lons 1 2 results v D: 0-15 F 15:20-(3:8+1	within lim : 1-1 Na (31:145))	its (all re a: 1-1	sults (up t 540 1398	o 1000) fo	r each ma	iss)				TOF MS E 2.27e+0
Monoisotopia 559 formula(Elements Us C: 0-60 H: 210914_7_81_ 100	c Mass, Even Ele ed: 0-70 N: 0-6 C 1A 16 (0.177) Cm (ectron Ions 12 results v D: 0-15 F 15:20-(3:8+1	within lim : 1-1 N: 31:145))	its (all re a. 1-1	sults (up t 540 1398 541 1/	o 1000) fo 427	r each ma	155)				TOF MS E 2.27e+(
Monoisotopio 559 formula(Elements Us C: 0-60 H: 210914_7_81_ 100 	c Mass. Even Ele e) evaluated with ed: 0-70 N: 0-6 C _1A 16 (0.177) Cm (1430 533 3480	ectron lons 12 results v D: 0-15 F 15:20-(3:8+1	vithin lim : 1-1 N: (31:145)) 537 (1320	its (all re a: 1-1	540 1398 541.1-	o 1000) fo 427 542.1454	r each ma	155) 1181 ⁵⁴⁶	.1216	548 1226		TOF MS E 2.27c+0 552.0714
Monoisotopio 559 formula(Elements Us C: 0-60 H: 210914_7_81_ 100 	c Mass. Even Ele e) evaluated with ed: 0-70 N: 0-6 C 1A 16 (0.177) Cm (1430 <u>533.3480</u> 532.0 534	ectron Ions 1 2 results v D; 0-15 F 15:20-(3.8+1) 535,0994 4.0 536	vithin lim : 1-1 Ni :31:145)) :537:1320	its (all re a: 1-1) 538.134 38.0	540 1398 540 1398 541.1- 13 540.0	o 1000) fo 427 542.1454 542.0	r each ma 545.	1181 546 546.0	.1216	548.1226 .0 55	0.0	TOF MS E 2.27c+(552.0714 r 552.0
Monoisotopio 559 formula(Elements Us 210914_7_81_ 100 	c Mass, Even Ele ed: 0-70 N: 0-6 C 1A 16 (0.177) Cm (1430 533 3480 532 0 534	ctron lons 1 2 results v D: 0-15 F 15:20-(3:8+1 5:55,0994 4.0 536 5:0	vithin lim : 1-1 N: (31:145)) 537:1320 :0 5:	its (all re a: 1-1) 538.134 38.0	sults (up 6 540.1398 541.14 13 540.0	o 1000) fo 427 542.1454 542.0	r each ma 545. 544.0	1181 546 546.0	.1216 548	548 1226 .0 55	0.0	TOF MS E 2.27o+(552.0714 552.0
Monoisotopio 559 formula(Elements Us C: 0-60 H: 210914_7_81_ 100 	c Mass. Even Ele e) evaluated with ed: 0-70 N: 0-6 C 1A 16 (0.177) Cm (1430 <u>533,3480</u> 532,0 534	ctron lons 12 results v 0; 0-15 F 15:20-(3:8+1 15:20-(3:8+1 15:20-(3:8+1 15:20-(3:8+1 15:20-(3:8+1 15:20-(3:8+1 15:20-(3:8+1 15:20-(3:8+1)15:20-(3:8+1) 15:20-(3:8+1)15:20-(3:8+1) 15:	vithin lim : 1-1 Ni :31:145)) :537:1320 :0 5: :0 5: :0	its (all re a: 1-1) 538.134 38.0 –1 .5 80.0 DBR	540 1398 540 1398 541.1- 13 540.0	o 1000) fo 427 542,1454 542,0	r each ma 545. 544.0	1181 546 546.0	.1216 1.548	548.1226 .0 55	0.0	TOF MS E 2.27c+(552.0714 552.0

Figure S24. HRMS data of compound 2

Monoisotopi	c Mass, Even Ele	ectron Ion	S							
577 formula Elements Us	(e) evaluated with sed:	n 2 results	within lim	iits (all re	sults (up to	o 1000) for	each mass	3)		
C: 0-60 ⊢ 210914_7_64	<mark>l: 0-70 N: 0-6</mark> _1A 16 (0.177) Cm (O: 0-1: (15:23-(1:7-	5 F: 1-1 +142:150))							TOF MS E
100-						518	3.1579			1.14e+
							519.1608			
0-1 501	1.9659503.9613 506	6,1074	510.3	752 514.	1066 516.15	86 518.093	0 520.16	33523.16515	24.1657 525. ⁻	1688 529,1428
500.0	502.5 505.0	507.5	510.0	512	.5 515.	0 517.	5 520.0) 522.5	525.0	527.5 530.0
linimum: aximum:		5.0	5.0	-1.5 80.0						
	Cale. Mass		ээм	DBE	1-F12	Noim	Coní ()	Formula		
18.1579	518.1575	0.4	0.8	13.5	960.7		98.66	C24 H25		
	518.1556	2.3	4.4	26.5		4.312	1.34	C36 H21	N O2 F	
	a Maari Euro El									
Aonoisotopi 59 formula	c Mass. Even Ele (e) evaluated with	ectron Ion 1 2 results	s s within lim	its (all re	sults (up to) 1000) for	each mass	5)		
Monoisotopi 159 formula Elements Us C: 0-60 H:	c Mass. Even Ele (e) evaluated with sed: 0-70 N: 0-6 (ectron Ion 1 2 results D: 0-15	s : within lim F: 1-1 N	iits (all re: a: 1-1	sults (up to	o 1000) for	each mass	5)		
Monoisotopi 559 formula Elements Us 2: 0-60 H: 210914_7_64	c Mass. Even Ele (e) evaluated with sed: 0-70 N: 0-6 (_1A 16 (0.177) Cm (ectron Ion 1 2 results O: 0-15 (15:23-(1:7)	s ⊊within lim F: 1-1 N +142:150))	iits (all re: a: 1-1	sults (up to	9 1000) for	each mass	5)		TOF MS E
Monoisotopi 59 formulat Elements Us 2: 0-60 H: 2:10914_7_64,	c Mass. Even Ele (e) evaluated with sed: 0-70 N: 0-6 (_1A 16 (0.177) Cm (ectron Ion 1 2 results D: 0-15 (15:23-(1:7)	s Within lim F: 1-1 N: +142:150))	iits (all re: a: 1-1 54	sults (up to	9 1000) for	each mass	5)		TOF MS E 2.890+
Monoisotopi 159 formula(20 ments Us 20 0-60 H: 210914_7_64 100	c Mass. Even Ele (e) evaluated with sed: 0-70 N: 0-6 (_1A 16 (0.177) Cm (ectron Ion n 2 results D: 0-15 (15:23-(1.7)	s : within lim F: 1-1 N +142:150))	iits (all re: a: 1-1 54	sults (up to 10.1398	o 1000) for	each mass	s)		TOF MS E 2.890+
Monoisotopi 159 formula 21ements Us 210914_7_64 100	c Mass. Even Ele (e) evaluated with sed: 0-70 N: 0-6 (_1A 16 (0.177) Cm (ectron Ion 1 2 results D: 0-15 (15:23-(1.7	s ⊧within lim F: 1-1 – N ⊧142:150))	iits (all re: a: 1-1 54	sults (up to 10.1398	o 1000) for	each mass	5)		TOF MS E 2.890+
Monoisotopi 59 formula Clements Us 2: 0-60 H: 2:10914_7_64 100 	c Mass. Even Ele (e) evaluated with sed: 0-70 N: 0-6 (_1A 16 (0.177) Cm (ectron Ion n 2 results D: 0-15 (15:23-(1 7-	s ⊧within lim F: 1-1 N ⊧142:150))	iits (all re: a: 1-1 54	sults (up to 10.1398 541.14	5 1000) for	each mass	5)		TOF MS E 2.89c+
1000isotopi 59 formula 21ements Us 210914_7_64 100 	c Mass. Even Ele (e) evaluated with sed: 0-70 N: 0-6 C _1A 16 (0.177) Cm (533.3264 535 10	ectron Ion 1 2 results 0: 0-15 (15:23-(1:7 (15:23-(1:7 (15:23-(1:7))	s : within lim F: 1-1 N +142:150)) 7.1318:537.	iits (all re: a: 1-1 54 6331	sults (up to 10.1398 541,14	26 542.1452	each mass 543.1475 52	5) 15.1183545.61	91 ⁵⁴⁷ 1196	TOF MS E 2.890+ 550.1320 ^{550.7}
Aonoisotopi 59 formular 1000 H: 10014_7_64 100 	c Mass. Even Ele (e) evaluated with sed: 0-70 N: 0-6 (_1A 16 (0.177) Cm (ectron Ion 1 2 results 0: 0-15 (15:23-(1 7) (15:23-(1 7) (15:23-(1 7) (15:23-(1 7) (15:23-(1 7)) (15:23-(1 7)) (15	s within lim F: 1-1 N ⊧142:150)) 7.1318 <i>5</i> 37. 538.0	iits (all re: a: 1-1 54 6331 5	sults (up to 10.1398 541.14 40.0	26 542.1452 542.0	each mass 543.1475 54 544.0	5) 15.1183545.61 546.0	91 547 1196 548.0	TOF MS E 2.890+ 550.1320 ^{550.7} 550.0
Monoisotopi 159 formula 21ements Us 210914_7_64 100 	c Mass. Even Ele (e) evaluated with sed: _1A 16 (0.177) Cm (ectron Ion 1 2 results 0: 0-15 (15:23-(1.7 061 53 536.0 5. 0	s within lim F: 1-1 N +142:150)) 7.1318 537 538.0	iits (all re: a: 1-1 6331 54 53 - 1 . 5 80 . 0	sults (up to 10.1398 541.14 40.0	26 542.1452 542.0	each mass 543.1475 ₅₄ 544.0	3) 15 1183 545 61 546.0	91 547.1196 548.0	TOF MS E 2.89c+ 550.1320 ^{550.7} 550.0
Aonoisotopi i59 formula Elements Us 2: 0-60 H: 2:10914_7_64 100 	c Mass, Even Ele (e) evaluated with sed: 0-70 N: 0-6 (1A 16 (0.177) Cm (533.3264 535 10 533.0	ectron Ion 1 2 results D: 0-15 (15:23-(1.7- 061 53 536.0 5., 0 5., 0	s within lim F. 1-1 N +142:150)) 7.1318 537. 538.0 5 . 0	its (all re: a: 1-1 54 6331 5 	sults (up to 10.1398 541.14 40.0	26 542.1452 542.0	each mass 543.1475 ₅₄ 544.0	5) 15.1183 545 61 546.0	91 547 1196 548.0	TOF MS E 2.896+ 550.1320 ^{550.7} 550.0
Aonoisotopi i59 formulat Elements Us 2: 0-60 H: 210914_7_64, 100 	c Mass, Even Ele (e) evaluated with sed: 0-70 N: 0-6 (1A 16 (0.177) Cm (1A 16 (0.177) Cm (533.3264 535.10 533.0 533.0 Call a. Maaa	ectron Ion 1 2 results 0: 0-15 (15:23-(1 7) (15:23-(1 7) (15:23-(1 7) (15:23-(1 7) (15:23-(1 7)) (15:23-(1 7)) (15	s within lim F: 1-1 N +142:150)) 7.1318 <i>5</i> 37. 538.0 5.0	iits (all re: a: 1-1 54 6331 5 	suits (up to 10.1398 541.14 40.0	26 542.1452 542.0	each mass 543.1475 ₅₄ 544.0	5) 15.1183.545.61 546.0	91 547 1196 548.0	TOF MS E 2.896+ 550.1320 550.7

Figure S25. HRMS data of compound 3

Monc 624 fe Elem C: 0- 21091	oisotopic Mass. Even Electron Ions formula(e) evaluated with 3 results within limits (all results rents Used: -60 H; 0-70 N; 0-6 O; 0-15 F; 1-1 14_7_82_2A 16 (0.177) Cm (14.22-(3.6+169:194))	(up to 1000) for each r	nass)
100-	576.1631		
	577.1664		
	572.2082 573.1130 574.1273 ^{574.6337}	578.1687 579.1705 58	0.1387 581.1692 ^{582.1710} 583.
	572.0 573.0 574.0 575.0 576.0 577.0	578.0 579.0 58	0.0 581.0 582.0 583.
Mini Maxi	imum: -1.5 mom: 5.0 5.0 80.0		

- 576,1631 - 576,1630 - 0.1 - 6.2 - 14.5 - 711.9 - 0.699 - 96,61 - 626 刊27 N3 - 611 - 576,1621 - 0.7 - 1.2 - 32,5 - 715,2 - 3,636 - 3,52 - 639 H29 N5 - 576,1611 - 2.6 - 3,5 - 27,5 - 714,6 - 2,785 - 6,17 - 638 刊23 文 04 内		Calc. Mass			DBE	1 - F - C	Norm	Coni()	s o smulla
	576.1631	576.1630 576.1624 576.1610	0.1 0.7 2.0	$\begin{array}{c} 0 & 0 \\ 1 & 2 \\ 3 & 5 \end{array}$	14.5 32.5 27.5	711.9 715.2 714.6	0 099 3 436 2 785	90.61 3.22 6.17	026 H27 X3 011 5 039 H19 X5 2 038 H23 X 04 F

210914 7 8	2_2A 16 (0.177) Cm	(14:22-(3:6	+169:194))								TOF MS
100				598.1	451						2.830
					599.1487						
		_	05 4000 50	6 1396	600	1510		- 604 12	48		
589.15	584 ^{592.0408} 5	93.2136 5	95.1369 59				603.123.	2 004.12	606.627	8 609.1	1586 610.7085
0	592.0408 5 590.0 592.0	93.2136 594.0	596.0	598.0	0 600	.0 602	2.0 6	04.0	606.627 606.0	8 609.1 608.0	610.0
0- ¹⁵⁸⁹¹⁵ Minimum: Maximum:	592.0408 5 590.0 592.0	93.2136 594.0	596.0 5.0	-1.5 80.0	0 600	.0 602	2.0 6	04.0	606.0	8 609.1 608.0	1586 610.7085 610.0
0- ^{1589.15} Minimum: Maximum: Vass	592.0408 5 590.0 592.0 Calc. Mage	9 <u>3.2136</u> 594.0 594.0	596.0 5.0 5.0	598.0 598.0 80.0 DBT	600. 600	.0 60: Nomi	2.0 6) Form	⁴⁰ 606.627 606.0	<u>8 609.1</u> 608.0	610.0

Figure S26. HRMS data of compound 4

TOF MS ES+ 1.35e+007

Monoisotopic Mass. Even Electron Ions
624 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-60 H: 0-70 N: 0-6 O: 0-15 F: 1-1

210914 7	20 3	A 16 (0.177) Cm (11:25-	(2:8+108:176))

					E	577.1664				
	567.5176 569.10	45	572.4350	574.1373	576.0916	578.1687	7 579.1714	582.1714	583.1744	586.5336
566.0	568.0	570.0	572.0	574.0	576.0	578.0	580.0	582.0	584.0	586.0
Minimum: Maximum:		5.0	5.0	-0.5 80.0						
	Cald Mass				i-rop					
576.1633	576.1630 576.1604 576.1600	0.3 0.9 7.2	0.5 1.6 3.8	14.5 32.5 27.8	845.9 850.0 849.2	0.651 9 4.229 1 3.358 3	5.06 C2 .46 C1 .48 C1	26 H27 N3 39 H19 N5 38 H23 N C	011 - 7 4 F	

Monoisotopic Mass. Even Electron Ions 616 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass) Elements Used: C: 0-60 H: 0-70 N: 0-6 O: 0-15 F: 1-1 Na: 1-1

TOF	MS	ES
4	.59e	+00

100					598.1448							
					599	1487						
590.	7978 59	94.1952	595.137	j <u>596</u> .136	7	600.1512	6	03.1234603.62	248 606.62	78607.1301 609	5566	610.7121
	592.0	594.0		596.0	598.0	600.0	602.0	604.0	606.0	608.0	610.0	
Minimum: Maximum:			5.0	5.0	-1.5 80.0							
	Cal.c.					i HRDD						
598.1448	598.1/ 598.1/ 598.1/		-0-1 0-4 1-7	-0.2 0.7 2.8	14.5 32.5 27.5	1046.5 1050.9 1050.6	0.028 4.433 4.183	97.29 1.19 1.53	C26 H26 N3 C39 N18 N5 C38 N22 N	011 - Na 7 Na 04 F Na		

Figure S27. HRMS data of compound 5

Elements Us C: 0-60 H 210914 7 31	ed: : 0-70 N: 0- 2A 16 (0 177) Cr	-6 O: 0- m (13:24-(4)	15 F: 1 8+43:50))	-1							TOF MS FS
100-					492.1418						4.50e+00
		400	1400 400	1240 401	493.	1449	405 1402	100 1100	400 1421		502.2540
0	3.2339 485.114 484.0	400. 486.0	488.0	490.0	492.0	494.1400	495.1492	498.1488	499.1421 1111111111111111111111111111111111	502.1694	503.3549 11111 m 504.0
Mirimum:				-1.5							
Maximum:		5.0	5.0	80.0							
	Cald. Mas			DBE	1400.0	NO2m	CONL()	eormula			
	492.1400	0.0 1.8	0.0 3.7	25.5	1403.3 1406.6		26.34 3.66	- C/2 11/3 - C34 1129	N3 09 F N 02 F		
Monoisotopio i31 formula(Elements Us 2: 0-60 H:	c Mass. Even F e) evaluated w ed: 0-70 N: 0-6	Electron Io /ith 2 resul O: 0-15	ns ts within li F: 1-1	mits (all re Na: 1-1	sults (up to	1000) for	each mass	5)			
Monoisotopio 531 formula(Elements Us C: 0-60 H: 210914_7_31_	c Mass, Even E e) evaluated w ed: 0-70 N: 0-6 _2 16 (0.177) Cm	Electron Io /ith 2 resul O: 0-15 1 (13:24-(4:8	ns ts within li F: 1-1 +43:50))	mits (all re Na: 1-1	sults (up to	1000) for	each mass	5)		t:	TOF MS ES 7.840+0
Monoisotopia 531 formula(Elements Us C: 0-60 H: 210914_7_31_ 100	c Mass. Even E e) evaluated w ed: 0-70 N: 0-6 _2 16 (0.177) Cm	Electron Io vith 2 resul O: 0-15 • (13:24-(4:8	ns ts within li F: 1-1 +43:50))	mits (all re Na. 1-1	sults (up to	1000) for 514.1234	each mass	5)		t	TOF MS ES 7.84e+0
Monoisotopio 531 formula(Elements Us C: 0-60 H: 210914_7_31_ 100	c Mass, Even F e) evaluated w ied: 0-70 N: 0-6 _2 16 (0.177) Cm	Electron lo vith 2 resul O: 0-15 (13:24-(4:8	ns ts within li F: 1-1 +43:50))	mits (all re Na: 1-1	sults (up to	1000) for 514.1234	each mass	s)		1.	TOF MS ES 7.84e+0
Monoisotopio 531 formula(Elements Us C: 0-60 H: 210914_7_31_ 100	c Mass, Even E e) evaluated w ed: 0-70 N: 0-6 _2 16 (0.177) Cm	Electron Io ith 2 resul O: 0-15 (13:24-(4:8	ns ts within li F: 1-1 +43:50))	mits (all re Na: 1-1	sults (up to	1000) for 514.1234 515. 46	each mass 1266 516.1287	5)	16 520.1046	1:	TOF MS ES 7.84c+0 524.1268
Monoisotopio 531 formula(Elements Us 210914_7_31_ 100 	c Mass. Even F e) evaluated w ed: 0-70 N: 0-6 _2 16 (0.177) Cm 03.1273 505.3	Electron lo vith 2 resul 0: 0-15 (13:24-(4:8 3212 505.95 506.0	ns ts within li +43:50)) 03 508.02 508.0	mits (all re Na: 1-1	sults (up to	1000) for 514.1234 515. 46 514.0	each mass 1266 516,1287 516,0	519.10 518.0	16 520.1046 520.0	521.9871 522.0	TOF MS ES 7.84c+0 524.1268 524.1268
Monoisotopio 531 formula(Elements Us 210914_7_31_ 100 5 5 502.0	c Mass. Even B e) evaluated w ed: 0-70 N: 0-6 _2 16 (0.177) Cm 03.1273 505.3 504.0	Electron lo rith 2 resul 0; 0-15 r(13:24-(4:8 3212 505.95 506.0	ns ts within li +43:50)) 03 508.02 508.0	mits (all re Na: 1-1 79 511. 510.0 5	sults (up to 1155 512.112 512.0	1000) for 514.1234 515. 16 514.0	each mass 1266 516.1287 516.0	5) 519.10 518.0	16 520.1046 520.0) 521.9871 522.0 5	TOF MS ES 7.840+0 524.1268
Monoisotopic 531 formula(Elements US 210914_7_31_ 100 	c Mass. Even E e) evaluated w ied: 0-70 N: 0-6 _2 16 (0.177) Cm 03.1273 505.3 504.0	Electron lo ith 2 resul 0: 0-15 (13:24-(4:8 3212 505.95 506.0 5. 0 5. 0	ns ts within li +43:50)) 03 508.02 508.0 5.0	mits (all re Na: 1-1 510.0 5 80.0	sults (up to 1155 512.114 512.0	1000) for 514.1234 515. 16 514.0	each mass 1266 516,1287 516.0	5) 519.10 518.0	16 520.1046 520.0	1: 5521.9871 552.0 5	TOF MS ES 7.846+00 524.1268 24.0
Monoisotopio 531 formula(Elements Us 210914_7_31_ 100 % 05 502.0	c Mass. Even F e) evaluated w ed: 0-70 N: 0-6 _2 16 (0.177) Cm 03.1273 505.3 504.0	Electron lo vith 2 resul 0: 0-15 (13:24-(4:8 3212:505.95 506.0	ns ts within li +43:50)) 03 508.02 508.0	mits (all re Na: 1-1 79 511. 510.0	sults (up to 1155 512.114 512.0	1000) for 514.1234 515. 66 514.0	each mass 1266 516.1287 516.0	5) 519.10 518.0	16 520.1046 520.0	1: 3 521.9871 522.0 5	TOF MS ES 7.840+00 524 1268

Figure S28. HRMS data of compound 6