Supporting Information

Transition-metal-, oxidant- and additive-free multi-component synthesis of alkyl heteroaryl BCPs enabled by visible-lightinduced phosphine-catalyzed halogen-atom transfer

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General Information

All reagents and deuterated solvents were commercially available and used without further purification. All products were separated by silica gel (200-300 mesh) column chromatography with petroleum ether (PE) (60-90°C) and ethyl acetate (EA). ¹H, ¹³C, ¹⁹F and ³¹P NMR spectra were recorded on a Bruker Advance 500 spectrometer at ambient temperature with CDCl₃ as solvent and tetramethylsilane (TMS) as the internal standard. Melting points were determined on an X-5 Data microscopic melting point apparatus. Analytical thin layer chromatography (TLC) was performed on Merk precoated TLC (silica gel 60 F254) plates. Compounds for HRMS were analyzed by positive mode electrospray ionization (ESI) using Agilent 6530 QTOF mass spectrometer.

1. Experimental Section

1.1 Preparation of the solution of [1.1.1]propellane in hexane

Ph-Br
$$\xrightarrow{n-Bu_2O}$$
 Ph-Li + \xrightarrow{Cl} $\xrightarrow{n-Bu_2O}$ decompress
Br Br distillation

A 150 mL three-neck round bottom flask equipped with a magnetic stirring bar was charged with bromobenzene (100 mmol, 1.0 equiv.) and n-Bu₂O (20 mL). Then the reaction mixture was cooled down to -30 °C and n-BuLi (100 mmol, 1.0 equiv., 2.5 M in hexane) was added dropwise. After the addition was completed, the reaction mixture was allowed to warm to room temperature, and stirred at room temperature for 1 h. The reaction mixture was used directly in the next step.

A solution of the above prepared PhLi in *n*-Bu₂O/hexane (65 mL) was added dropwise to a suspension of 1,1-dibromo-2,2-bis(chloromethyl)cyclopropane (45.0 mmol) in anhydrous *n*-Bu₂O (20 mL) at -20 °C. After the addition was completed, the reaction mixture was allowed to warm to 0 °C and stirred for 2 h. Then the addition funnel was swapped out for a distillation head with attached 100 mL round bottom flask in a bath (liquid nitrogen). A vacuum was slowly applied to the system and the distillate was collected, while maintaining the reaction/distillation flask below 0 °C. Approximately 30 mL of distillate was collected. The concentration of [1.1.1]propellane (0.4-0.6 M) was measured by ¹H NMR using dichloromethane as the standard.

1.2 Preparation of the starting material azauracils



All the azauracils are known compounds.¹ The general synthesis procedures were described as follows: To a round bottom flask charged with 6-azuracil (4.0 mmol), K₂CO₃ (2.0 mmol) and DMF (40 mL) was added alkyl halides (3.6 mmol) dropwise. The reaction mixture was allowed to stir at room temperature for 16 h, and then quenched by water and extracted with EtOAc. The combined organic layer was washed with brine, dried over MgSO₄. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel). To a round bottom flask charged with *N*-1-alkyl-6-azauracils (2.0 mmol), K₂CO₃ (1.0 mmol) and DMF (20 mL) was added alkyl halides (2.0 mmol) dropwise. The reaction mixture was allowed

to stir at room temperature for 16 h, and then quenched by water and extracted with EtOAc. The combined organic layer was washed with brine, dried over MgSO₄. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.3 Preparation of the starting material pyrazinones



All the pyrazinones are known compounds.¹ The general synthesis procedures were described as follows: To a round bottom flask charged with glycinamide hydrochloride (20.0 mmol) and MeOH (18 mL) was added water (4.4 mL). To the above suspension was added 12.5 M aqueous NaOH solution (28.6 mmol) at -30 °C, followed by a solution of NaOH (20.0 mmol) in MeOH (9 mL). Glyoxal monohydrate (20.0 mmol) was then added at -30 °C and the resulting mixture was allowed to stir at -30 °C for 2 h. The resulting mixture was further stirred at room temperature for 1 h. The reaction mixture was cooled in an ice bath and acidified with AcOH. The precipitate separated was collected by filtration and dried to afford pyrazinones as a pale red solid. To a round bottom flask charged with sodium hydride (5.2 mmol, 60% dispersion in mineral oil) was added DMF (2 mL) under N₂ atmosphere. To the above suspension was added a solution of pyrazinones (3.5 mmol) in DMF (2 mL) and THF (2 mL) dropwise at 0 °C. A solution of the corresponding alkyl halide (4.6 mmol) in THF (1 mL) was added dropwise after 15 minutes at 0 °C. Then tetra-butyl ammonium iodide (0.35 mmol) was added to the reaction mixture. The reaction mixture was allowed to stir at room temperature for 3 h, and then quenched by ice water and extracted with EtOAc. The combined organic layer was washed with brine, dried over MgSO₄. The solvent was removed in vacuo, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.4 Preparation of the starting material quinoxaline-2(1H)-ones



All the quinoxaline-2(1*H*)-ones are known compounds.² The general synthesis procedures were described as follows: To a round bottom flask charged with *o*-arylenediamine (10 mmol) and ethanol (50 mL) was added ethyl glyoxylate (12 mmol). The mixture was stirred at reflux for 3 h. The precipitated solid was filtered and washed with ethanol, then dried to give the first step product. To a suspension of the first step product (10 mmol) in DMF was added potassium carbonate (12 mmol) and halogenoalkanes (16 mmol). The mixture was stirred at room temperature for 12 h. The reaction was quenched by water and extracted with EtOAc. The combined organic layer was washed with brine, dried over MgSO₄. The solvent was removed *in vacuo*, and the obtained residue was purified by silica gel column chromatography (200-300 mesh silica gel).

1.5 Preparation of the starting material 4-azacoumarin



The 4-azacoumarin is a known compound.³ The general synthesis procedure was described as follows: To a round bottom flask charged with 2-aminophenol (10.0 mmol), ethyl glyoxylate solution (~50% in toluene) in anhydrous toluene (0.25 M), and dried 4Å molecular sieves (0.6 g/mmol). Then reflux the reaction overnight, cool the mixture to room temperature and filter the resulting mixture through a plug of celite. Then the solvent was removed in vacuo. The residue was purified by flash column chromatography on silica (pentane/acetone 20:1), affording the compound **3al** as a yellow crystalline solid.

1.6 Preparation of the starting material cinnolinones



The cinnolinones are known compounds.⁴ The general synthesis procedure was described as follows: To a round bottom flask charged with cinnolin-4(1*H*)-one (2.0 mmol), K₂CO₃ (3.0 mmol) and DMF (20 mL) was added alkyl halides (2.6 mmol) dropwise. The reaction mixture was allowed to stir at room temperature for 24 h, and then quenched by water and extracted with EtOAc. The combined organic layer was washed with brine, dried over MgSO₄. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.7 Preparation of the starting material drug derivatives



All the drug derivatives are known compounds.⁵ The general synthesis procedures were described as follows: To a round bottom flask charged with quinoxalin-2(1*H*)-one (10 mmol), K₂CO₃ (30 mmol) and DMF (50 mL) was added 2-bromoethanol (12 mmol). The mixture was stirred at room temperature for 24 h, and then quenched by water and extracted with EtOAc. The combined organic layer was washed with brine, dried over MgSO₄. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel). To a round bottom flask charged with 1-(2-hydroxyethyl)quinoxalin-2(1*H*)-one (4.0 mmol), DMAP (0.4 mmol), EDCl (10 mmol), and DMF (50 mL) was added carboxylic acid drug molecules (4.4 mmol). The mixture was stirred at room temperature for 24 h, and then quenched by water and extracted with EtOAc. The combined organic layer was washed with brine, dried over MgSO₄. The solvent was removed *in vacuo*, and the obtained residue was removed *in vacuo*, and the purified by silica gel column chromatography (200-300 mesh silica gel).

1.8 General procedure for the multicomponent reaction



A mixture of heteroarene (1) (0.2 mmol), [1.1.1]propellane (2) (0.5 mmol), alkyl halides (3) (0.4 mmol), PPh₃ (20 mol%) and NMP (2.0 mL) in a 25-mL Schlenk tube was stirred with the irradiation of blue LEDs (10 W) at room temperature under a nitrogen atmosphere for 6 h. After completion of the reaction, a saturated NH₄Cl solution was added to the mixture. The mixture was then extracted with EtOAc, and the collected organic layer was washed with brine, and dried with MgSO₄. The solvent was removed *in vacuo*, and the obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.9 General procedure for the synthesis of compound 88



A mixture of compound (26) (0.2 mmol), zidovudine (0.3 mmol), Et₃N (0.4 mmol), CuI (20 mol%) and MeCN (10 mL) in a round bottom flask was stirred at room temperature for 12 h. After completion of the reaction, the reaction mixture was filtered and the solution was concentrated *in vacuo*. The obtained residue was further purified by silica gel column chromatography (200-300 mesh silica gel).

1.10 Ineffective substrates for the multicomponent reaction



1.11 Determine the amount of phosphine residues in the product by HPLC



数据文件:	2024-08-10 11-44-48+08-00-01. d	x	
序列名称:	HPLC1260-2024-08-10 11-44- 39+08-00	项目名称:	TEST
样品名称:	Ph3P	操作者:	SYSTEM
仪器:	HPLC1260	进样日期:	2024-08-10 11:46:14+08:00
进样体积:	10.000 µL	位置:	62
采集方法:	HY-CH30H. amx	类型:	样品
处理方法:	GC_LC 面积百分比_DefaultMethod.pmx	样品含量:	0.00
手动修改:	手动积分		



信号:	VWD1A, Wave	length=264 nm				
保留时间 [min]	类型	峰宽 [min]	峰面积	峰高	峰面积%	名称
22. 557	BB	14.81	93439.63	1879. 21	100.00	
		总和	93439.63			

数据文件:	2024-08-10 12-31-19+08-00-02. dx	с.	
序列名称:	HPLC1260-2024-08-10 11-44- 39+08-00	项目名称:	TEST
样品名称:	4	操作者:	SYSTEM
仪器:	HPLC1260	进样日期:	2024-08-10 12:32:44+08:00
进样体积:	10.000 µL	位置:	63
采集方法:	HY-CH30H. amx	类型:	样品
处理方法:	GC_LC 面积百分比_DefaultMethod.pmx	样品含量:	0.00
手动修改:	手动积分		



信号:	号: VWD1A, Wavelength=264 nm		01A,Wavelength=264 nm			
保留时间 [min]	类型	峰宽 [min]	峰面积	峰高	峰面积%	名称
34, 828	BB	8.92	53346.02	776.86	100.00	
		总和	53346.02			

1.12 Visible light irradiation on/off experiments



Figure S1 Visible light irradiation on/off experiments.

1.13 Proposed mechanism



2 References

- 1. P. Ghosh, N. Y. Kwon, S. Kim, S. Han, S. H. Lee, W. An, N. K. Mishra, S. B. Han and I. S. Kim, *Angew. Chem. Int. Ed.*, 2021, **60**, 191.
- 2. J. Zhou, Q. Ren, N. Xu, C. Wang, S. Song, Z. Chen and J. Li, Green Chem., 2021, 23, 5753.
- 3. J. H. Ye, P. Bellotti, T. O. Paulisch, C. G. Daniliuc and F. Glorius, *Angew. Chem. Int. Ed.*, 2021, **60**, 13671.
- 4. P.; Marshall, B.; Mooney and R. Prager, Aust. J. Chem., 1981, 34, 2619.
- 5. J. Zhu, Y. Guo, Y. Zhang, W. Li, P. Zhang and J. Xu, Green Chem., 2023, 25, 986.

3 Characterization of Products

2,4-Dibenzyl-6-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (4)



Obtained as a light yellow solid (X = I, 78 mg, 68% yield); M. P. = 115-116 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.48 (d, *J* = 6.5 Hz, 2H), 7.42 – 7.27 (m, 8H), 5.06 (d, *J* = 17.5 Hz, 4H), 2.39 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.3, 149.0, 140.6, 135.5, 135.5, 129.6, 128.8, 128.8, 128.6, 128.4, 128.2, 55.5, 51.0, 44.1, 38.9, 38.2 (t, *J* = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.05 – -81.10 (m), -116.60 – -116.66 (m), -122.26 – -122.32 (m), -126.01 – -126.08 (m); HRMS (ESI+): Calculated for C₂₆H₂₀F₉N₃O₂: [M+Na]⁺ 600.1304, Found 600.1303.

2,4-Dimethyl-6-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (5)



Obtained as a light yellow solid (X = I, 55 mg, 65% yield); M. P. = 98-99 °C; IR (KBr) v/cm⁻¹ 2965, 2924, 1763, 1604, 1467, 1296, 1186, 1096, 1018, 753, 717; ¹H NMR (500 MHz, CDCl₃) δ 3.62 (s, 3H), 3.33 (s, 3H), 2.40 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.8, 149.2, 139.9, 51.0, 39.6, 38.8, 38.2 (t, *J* = 30.2 Hz), 26.9, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.05 – -81.10 (m), -116.60 – -116.68 (m), -122.28 – -122.35 (m), -126.02 – -126.09 (m); HRMS (ESI+): Calculated for C₁₄H₁₂F₉N₃O₂: [M+Na]⁺ 448.0678, Found 448.0679.

2,4-Diethyl-6-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2H,4H)-dione (6)



Obtained as a white solid (X = I, 56 mg, 62% yield); M. P. = 92-93 °C; ¹H NMR (500 MHz, CDCl₃) δ 3.98 (dq, J = 21.1, 7.1 Hz, 4H), 2.40 (s, 6H), 1.32 (t, J = 7.2 Hz, 3H), 1.24 (t, J = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 155.3, 148.5, 140.2, 51.0, 46.9, 38.9, 38.2 (t, J = 30.2 Hz), 35.9, 13.3, 12.4, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.02 – -81.14 (m), -116.63 – -116.69 (m), -122.35 – -122.38 (m), -126.05 – -126.11 (m); HRMS (ESI+): Calculated for C₁₆H₁₆F₉N₃O₂: [M+H]⁺ 454.1172, Found 454.1171.

2,4-bis(4-Methylbenzyl)-6-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (7)



Obtained as a white solid (X = I, 77 mg, 67% yield); M. P. = 188-189 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.40 (d, *J* = 7.9 Hz, 2H), 7.31 (d, *J* = 7.9 Hz, 2H), 7.15 (dd, *J* = 15.5, 7.8 Hz, 4H), 5.04 (s, 2H), 5.01 (s, 2H), 2.40 (s, 6H), 2.35 (s, 3H), 2.33 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 155.3, 149.0, 140.5, 138.2, 138.0, 132.5, 132.5, 129.6, 129.4, 129.3, 128.8, 55.2, 51.0, 43.8, 38.9, 38.2 (t, *J* = 30.2 Hz), 21.2, 21.2, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ - 81.05 - 81.09 (m), -116.62 - 116.67 (m), -122.30 - -122.34 (m), -126.01 - -126.08 (m); HRMS (ESI+): Calculated for C₂₆H₂₀F₉N₃O₂: [M+Na]⁺ 628.1617, Found 628.1612.

6-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2,4-bis(2-oxo-2-phenylethyl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (8)



Obtained as a light yellow solid (X = I, 87 mg, 69% yield); M. P. = 112-113 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.98 (dd, J = 7.1, 5.8 Hz, 4H), 7.63 (dd, J = 15.5, 7.6 Hz, 2H), 7.51 (dd, J = 15.7, 7.9 Hz, 4H), 5.42 (s, 2H), 5.36 (s, 2H), 2.41 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 191.4, 190.3, 155.1, 149.0, 141.1, 134.5, 134.3, 134.2, 129.0, 128.9, 128.2, 128.1, 57.6, 51.1, 46.3, 38.8, 38.2 (t, J = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ - 81.07 - -81.11 (m), -116.60 - -116.68 (m), -122.30 - -122.37 (m), -126.03 - -126.09 (m); HRMS (ESI+): Calculated for C₂₈H₂₀F₉N₃O₄: [M+H]⁺ 634.1383, Found 634.1375.

2,4-Diallyl-6-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2H,4H)-dione (9)



Obtained as a yellow solid (X = I, 57 mg, 60% yield); M. P. = 63-64 °C; ¹H NMR (500 MHz, CDCl₃) δ 5.98 – 5.81 (m, 2H), 5.36 – 5.23 (m, 4H), 4.53 (dd, *J* = 18.4, 6.1 Hz, 4H), 2.40 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.1, 148.5, 140.5, 131.2, 130.2, 119.6, 119.3, 54.3, 51.0, 42.8, 38.8, 38.2 (t, *J* = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.04 – -81.09 (m), -116.61 – -116.69 (m), -122.32 – -122.38 (m), -126.01 – -126.08 (m); HRMS (ESI+): Calculated for C₁₈H₁₆F₉N₃O₂: [M+H]⁺ 478.1172, Found 478.1170.

6-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2,4-di(prop-2-yn-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (10)



Obtained as a white solid (X = I, 60 mg, 63% yield); M. P. = 124-125 °C; ¹H NMR (500 MHz, CDCl₃) δ 4.74 (d, J = 2.4 Hz, 2H), 4.68 (d, J = 2.4 Hz, 2H), 2.44 (s, 6H), 2.37 (t, J = 2.4 Hz, 1H), 2.24 (t, J = 2.4 Hz, 1H); ¹³C NMR (126 MHz, CDCl₃) δ 154.3, 147.5, 141.2, 76.5, 76.3, 73.7, 71.9, 51.1, 41.6, 38.7, 38.3 (t, J = 30.2 Hz), 29.9, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.04 – -81.08 (m), -116.62 – -116.69 (m), -122.30 – -122.34 (m), -126.00 – -126.07 (m); HRMS (ESI+): Calculated for C₁₈H₁₂F₉N₃O₂: [M+Na]⁺ 496.0678, Found 496.0680.

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1H)-one (11)



Obtained as a light yellow solid (X = I, 47 mg, 43% yield); M. P. = 146-147 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.40 (d, *J* = 6.7 Hz, 3H), 7.21 – 7.18 (m, 2H), 7.13 (s, 5H), 3.30 (s, 3H), 2.55 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 154.3, 150.6, 136.9, 136.6, 131.6, 131.5, 128.9, 128.6, 128.3, 128.1, 126.7, 126.0, 50.0, 40.8, 36.9 (t, *J* = 30.2 Hz), 32.6, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.04 – -81.08 (m), -116.49 – -116.57 (m), -122.27 – -122.32 (m), -125.98 – -126.05 (m); HRMS (ESI+): Calculated for C₂₆H₁₉F₉N₂O: [M+H]⁺ 547.1426, Found 547.1427.

5,6-bis(4-Fluorophenyl)-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)pyrazin-2(1*H*)-one (12)



Obtained as a light yellow solid (X = I, 47 mg, 40% yield); M. P. = 116-117°C; ¹H NMR (500 MHz, CDCl₃) δ 7.20 – 7.15 (m, 2H), 7.13 – 7.06 (m, 4H), 6.84 (dd, *J* = 12.0, 5.4 Hz, 2H), 3.29 (s, 3H), 2.54 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 163.5 (d, *J* = 165.1 Hz), 161.5 (d, *J* = 160.0 Hz), 155.2, 152.1, 136.9, 133.5 (d, *J* = 165.1 Hz), 132.0, 131.9, 131.0 (d, *J* = 7.6 Hz), 128.4 (d, *J* = 3.8 Hz), 116.6 (d, *J* = 8.8 Hz), 114.9 (d, *J* = 8.8 Hz), 51.0, 41.8, 37.9 (t, *J* = 30.2 Hz), 33.6, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.08 – -81.12 (m), -109.6, -114.6, -116.55 – -116.62 (m), -122.28 – -122.33 (m), -126.01 – -126.08 (m); HRMS (ESI+): Calculated for C₂₆H₁₇F₁₁N₂O: [M+H]⁺ 583.1238, Found 583.1238.

5,6-bis(4-Bromophenyl)-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)pyrazin-2(1*H*)-one (13)



Obtained as a light yellow solid (X = I, 59 mg, 42% yield); M. P. = 134-135 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.57 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.5 Hz, 2H), 7.07 (d, *J* = 8.3 Hz, 2H), 6.99 (d, *J* = 8.5 Hz, 2H), 3.28 (s, 3H), 2.53 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.1, 152.3, 136.9, 136.3, 132.7, 131.5, 131.1, 131.0, 130.9, 124.4, 121.6, 51.0, 41.7, 37.9 (t, *J* = 30.2 Hz), 33.7, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – -81.07 (m), -116.58 – -116.66 (m), -122.27 – -122.31 (m), -125.98 – -126.04 (m); HRMS (ESI+): Calculated for C₂₆H₁₇Br₂F₉N₂O: [M+H]⁺ 702.9637, Found 702.9641.

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-di-p-tolylpyrazin-2(1H)-one (14)



Obtained as a light yellow solid (X = I, 56 mg, 49% yield); M. P. = 168-169 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.20 (d, *J* = 7.9 Hz, 2H), 7.05 (dd, *J* = 17.1, 8.1 Hz, 4H), 6.94 (d, *J* = 8.1 Hz, 2H), 3.28 (s, 3H), 2.53 (s, 6H), 2.38 (s, 3H), 2.25 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 155.4, 151.2, 139.6, 137.8, 136.7, 134.9, 132.7, 129.8, 129.8, 129.7, 129.1, 128.5, 51.0, 41.8, 37.9 (t, *J* = 30.2 Hz), 33.6, 21.4, 21.1, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ - 81.03 – -81.08 (m), -116.48 – -116.55 (m), -122.27 – -122.34 (m), -125.98 – -126.04 (m); HRMS (ESI+): Calculated for C₂₈H₂₃F₉N₂O: [M+Na]⁺ 597.1559, Found 597.1557.

1-Ethyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (15)



Obtained as a yellow liquid (X = I, 50 mg, 45% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.42 – 7.37 (m, 3H), 7.23 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.11 (s, 5H), 3.86 (q, *J* = 7.1 Hz, 2H), 2.55 (s, 6H), 1.17 (d, *J* = 7.0 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 154.6, 152.0, 137.8, 137.7, 132.8, 132.2, 130.1, 129.5, 129.3, 128.9, 127.7, 127.0, 51.1, 41.3, 37.9 (t, *J* = 30.2 Hz), 29.7, 13.6, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.04 – -81.08 (m), -116.50 – -116.59 (m), -122.26 – -122.35 (m), -125.97 – -126.05 (m); HRMS (ESI+): Calculated for C₂₇H₂₁F₉N₂O: [M+H]⁺ 561.1583, Found 561.1587.

1-Benzyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1H)-one (16)



Obtained as a light yellow solid (X = I, 62 mg, 50% yield); M. P. = 89-90 °C;¹H NMR (500 MHz, CDCl₃) δ 7.35 (t, J = 7.5 Hz, 1H), 7.26 – 7.19 (m, 5H), 7.14 – 7.08 (m, 5H), 6.99 (d, J = 7.3 Hz, 2H), 6.86 (dd, J = 6.5, 2.8 Hz, 2H),5.11 (s, 2H), 2.58 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.0, 152.5, 137.9,137.5, 136.0, 132.9, 131.9, 130.5, 129.5, 129.3, 128.6, 128.5, 127.7, 127.5, 127.2, 127.0, 51.1, 48.7, 41.9, 37.9 (t, J = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – -81.07 (m), -116.50 – -116.57 (m), -122.27 – -122.33 (m), -125.96 – -126.02 (m); HRMS (ESI+): Calculated for C₃₂H₂₃F₉N₂O: [M+H]⁺ 623.1739, Found 623.1736.

1-(4-Chlorobenzyl)-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (17)



Obtained as a light yellow solid (X = I, 66 mg, 50% yield); M. P. = 145-146 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.37 (t, *J* = 7.5 Hz, 1H), 7.29 – 7.26 (m, 2H), 7.18 (d, *J* = 8.4 Hz, 2H), 7.11 (s, 5H), 7.00 (d, *J* = 7.2 Hz, 2H), 6.80 (d, *J* = 8.4 Hz, 2H), 5.07 (s, 2H), 2.58 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.0, 152.6, 137.6, 137.4, 134.5, 133.5, 133.1, 131.8, 130.5, 129.7, 129.3, 128.8, 128.7, 127.7, 127.1, 51.1, 48.1, 41.9, 37.9 (t, *J* = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – -81.07 (m), -116.51 – -116.58 (m), -122.27 – -122.30 (m), -125.96 – -126.03 (m); HRMS (ESI+): Calculated for C₃₂H₂₂ClF₉N₂O: [M+H]⁺ 657.1350, Found 657.1351.

1-Allyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1H)-one (18)



Obtained as a light yellow solid (X = I, 53 mg, 46% yield); M. P. = 136-137 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.37 (dt, J = 14.6, 7.2 Hz, 3H), 7.24 – 7.19 (m, 2H), 7.12 (d, J = 1.9 Hz, 5H), 5.80 (ddd, J = 22.6, 10.6, 5.4 Hz, 1H), 5.16 (dd, J = 10.3, 0.8 Hz, 1H), 4.91 (dd, J = 17.2, 0.8 Hz, 1H), 4.42 (d, J = 5.4 Hz, 2H), 2.56 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 154.6, 152.2, 137.9, 137.6, 132.8, 132.0, 131.4, 130.4, 129.7, 129.3, 128.7, 127.7, 127.0, 118.3, 51.1, 48.2, 41.8, 37.9 (t, J = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.04 – -81.08 (m), -116.52 – -116.59 (m), -122.30 – -122.35 (m), -125.98 – -126.05 (m); HRMS (ESI+): Calculated for C₂₈H₂₁F₉N₂O: [M+H]⁺ 573.1583, Found 573.1584.

1-Benzyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-5-phenylpyrazin-2(1*H*)-one (19)



Obtained as a yellow liquid (X = I, 42 mg, 38% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.70 – 7.67 (m, 2H), 7.45 (s, 1H), 7.39 (d, *J* = 6.3 Hz, 4H), 7.36 (dd, *J* = 6.5, 3.3 Hz, 3H), 7.32 (d, *J* = 7.4 Hz, 1H), 5.13 (s, 2H), 2.54 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 154.7, 153.8, 135.5, 134.8, 132.7, 129.2, 128.8, 128.7, 128.5, 128.1, 124.9, 123.7, 52.1, 51.1, 41.9, 37.9 (t, *J* = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – -81.07 (m), -116.53 – -116.61 (m), -122.28 – -122.33 (m), -125.98 – -126.05 (m); HRMS (ESI+): Calculated for C₂₆H₁₉F₉N₂O: [M+H]⁺ 547.1426, Found 547.1429.

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (20)



Obtained as a light yellow solid (X = I, 62 mg, 70% yield); M. P. = 70-71 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.88 – 7.83 (m, 1H), 7.59 – 7.53 (m, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 3.68 (s, 3H), 2.56 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 154.8, 154.5, 133.5, 132.8, 130.5, 130.2, 123.7, 113.6, 51.2, 42.1, 37.9 (t, *J* = 30.2 Hz), 28.6, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.04 – -81.08 (m), -116.57 – -116.65 (m), -122.26 – -122.34 (m), -125.98 – -126.06 (m); HRMS (ESI+): Calculated for C₁₈H₁₃F₉N₂O: [M+H]⁺ 445.0957, Found 445.0957.

1-Benzyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (21)



Obtained as a light yellow solid (X = I, 68 mg, 65% yield); M. P. = 93-94 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.86 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.44 – 7.41 (m, 1H), 7.33 – 7.29 (m, 3H), 7.27 (d, *J* = 7.2 Hz, 1H), 7.23 (t, *J* = 8.1 Hz, 3H), 5.46 (s, 2H), 2.59 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.0, 154.5, 135.1, 133.0, 132.9, 130.5, 130.3, 129.0, 127.8, 126.9, 123.8, 114.5, 51.3, 45.6, 42.1, 37.9 (t, *J* = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – 81.07 (m), -116.56 – -116.63 (m), -122.27 – -122.31 (m), -125.96 – -126.03 (m); HRMS (ESI+): Calculated for C₂₄H₁₇F₉N₂O: [M+H]⁺ 521.1270, Found 521.1266.

1-(2-Oxo-2-phenylethyl)-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl) quinoxalin-2(1*H*)-one (22)



Obtained as a yellow liquid (X = I, 70 mg, 64% yield); ¹H NMR (500 MHz, CDCl₃) δ 8.07 (d, J = 7.3 Hz, 2H), 7.89 (dd, J = 8.0, 1.2 Hz, 1H), 7.68 (t, J = 7.5 Hz, 1H), 7.55 (t, J = 7.8 Hz, 2H), 7.48 – 7.40 (m, 1H), 7.33 (t, J = 7.6 Hz, 1H), 6.94 (d, J = 8.3 Hz, 1H), 5.70 (s, 2H), 2.56 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 191.0, 154.5, 154.2, 134.5, 134.4, 132.9, 130.5, 130.5, 129.1, 128.2, 123.9, 113.5, 51.3, 48.0, 42.0, 37.9 (t, J = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.05 – -81.09 (m), -116.56 – -116.64 (m), -122.28 – -122.34 (m), -125.99 – 126.06 (m); HRMS (ESI+): Calculated for C₂₅H₁₇F₉N₂O₂: [M+H]⁺ 549.1219, Found 549.1219.

1-Ethyl-2-(2-oxo-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-1(2*H*)-yl)acetate (23)



Obtained as a light yellow solid (X = I, 72 mg, 70% yield); M. P. = 88-89 °C;¹H NMR (500 MHz, CDCl₃) δ 7.87 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.35 (t, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 8.3 Hz, 1H), 4.99 (s, 2H), 4.26 (q, *J* = 7.1 Hz, 2H), 2.56 (s, 6H), 1.29 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 167.0, 154.7, 154.0, 132.8, 132.6, 130.6, 130.5, 124.0, 113.1, 62.2, 51.3, 43.1, 41.9, 37.9 (t, *J* = 30.2 Hz), 14.1, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.04 – -81.08 (m), -116.58 – -116.66 (m), -122.30 – -122.35 (m), -125.99 – -126.05 (m); HRMS (ESI+): Calculated for C₂₁H₁₇F₉N₂O₃: [M+H]⁺ 517.1168, Found 517.1170.

3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1-phenylquinoxalin-2(1H)-one (24)



Obtained as a yellow liquid (X = I, 53 mg, 52% yield);¹H NMR (500 MHz, CDCl₃) δ 7.92 – 7.88 (m, 1H), 7.65 – 7.61 (m, 2H), 7.59 – 7.54 (m, 1H), 7.34 (ddd, J = 14.3, 7.2, 1.7 Hz, 2H), 7.31 – 7.29 (m, 2H), 6.72 – 6.67 (m, 1H), 2.58 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.6, 154.2, 135.4, 134.3, 132.6, 130.4, 130.1, 129.8, 129.6, 128.2, 123.9, 115.5, 51.4, 42.0, 37.9 (t, J = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.06 – -81.11 (m), -116.59 – -116.65 (m), -122.33 – -122.37 (m), -125.99 – -126.06 (m); HRMS (ESI+): Calculated for C₂₃H₁₅F₉N₂O: [M+H]⁺ 507.1113, Found 507.1110.

1-Allyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (25)



Obtained as a yellow liquid (X = I, 53 mg, 56% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.86 (dd, J = 8.0, 1.3 Hz, 1H), 7.54 – 7.50 (m, 1H), 7.35 – 7.31 (m, 1H), 7.28 (d, J = 8.4 Hz, 1H), 5.93 (ddd, J = 22.3, 10.4, 5.2 Hz, 1H), 5.23 (dd, J = 50.4, 13.9 Hz, 2H), 4.87 (d, J = 5.1 Hz, 2H), 2.56 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 154.9, 154.0, 132.9, 132.7, 130.5, 130.4, 130.3, 123.7, 118.3, 114.2, 51.3, 44.2, 42.0, 37.9 (t, J = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.05 – -81.10 (m), -116.60 – -116.66 (m), -122.31 – -122.35 (m), -125.99 – 126.06 (m); HRMS (ESI+): Calculated for C₂₀H₁₅F₉N₂O: [M+H]⁺ 471.1113, Found 471.1101.

3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-1-(prop-2-yn-1-yl)quinoxalin-2(1H)-one (26)



Obtained as a yellow liquid (X = I, 54 mg, 58% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.86 (dd, J = 8.0, 1.2 Hz, 1H), 7.61 – 7.56 (m, 1H), 7.46 (d, J = 8.4 Hz, 1H), 7.40 – 7.35 (m, 1H), 5.02 (d, J = 2.5 Hz, 2H), 2.56 (s, 6H), 2.30 (t, J = 2.5 Hz, 1H); ¹³C NMR (126 MHz, CDCl₃) δ 154.7, 153.4, 132.9, 132.0, 130.6, 130.3, 124.1, 114.1, 76.6, 73.3, 51.3, 42.0, 37.9 (t, J = 30.2 Hz), 31.1, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.08 – -81.13 (m), -116.61 – -116.68 (m), -122.30 – -122.34 (m), -126.01 – -126.09 (m); HRMS (ESI+): Calculated for C₂₀H₁₃F₉N₂O: [M+H]⁺ 469.0957, Found 469.0957.

1,5-Dimethyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (27)



Obtained as a light yellow solid (X = I, 66 mg, 72% yield); M. P. = 133-134 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.46 – 7.40 (m, 1H), 7.20 (d, J = 7.4 Hz, 1H), 7.13 (d, J = 8.4 Hz, 1H), 3.66 (s, 3H), 2.66 (s, 3H), 2.54 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 154.4, 152.8, 139.1, 133.6, 131.3, 130.2, 125.0, 111.5, 51.1, 42.3, 37.8 (t, J = 30.2 Hz), 28.7, 17.3, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.04 – -81.08 (m), -116.53 – -116.62 (m), -122.26 – -122.31 (m), -125.98 – -126.06 (m); HRMS (ESI+): Calculated for C₁₉H₁₅F₉N₂O: [M+H]⁺ 459.1113, Found 459.1114.

5-Chloro-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (28)



Obtained as a light yellow solid (X = I, 62 mg, 65% yield); M. P. = 81-82 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.45 (t, *J* = 4.9 Hz, 2H), 7.22 (dd, *J* = 7.6, 2.0 Hz, 1H), 3.68 (s, 3H), 2.58 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.2, 154.1, 135.2, 135.0, 130.4, 129.4, 124.7, 112.5, 51.3, 42.2, 38.0 (t, *J* = 30.2 Hz), 29.1, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ - 81.03 – -81.08 (m), -116.56 – -116.66 (m), -122.26 – -122.33 (m), -125.97 – -126.06 (m); HRMS (ESI+): Calculated for C₁₈H₁₂ClF₉N₂O: [M+H]⁺ 479.0567, Found 479.0563.

6-Fluoro-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (29)



Obtained as a yellow solid (X = I, 62 mg, 67% yield); M. P. = 95-96 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.55 (dd, J = 8.7, 2.7 Hz, 1H), 7.33 – 7.28 (m, 1H), 7.26 (dd, J = 9.3, 4.6 Hz, 1H), 3.67 (s, 3H), 2.55 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 158.7 (d, J = 244.4 Hz), 156.3, 154.1, 133.3 (d, J = 11.3 Hz), 130.2 (d, J = 2.5 Hz), 118.2 (d, J = 23.9 Hz), 115.6 (d, J = 22.7 Hz), 114.7 (d, J = 7.6 Hz), 51.2, 42.1, 37.9 (t, J = 31.5 Hz), 28.9, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.05 – -81.09 (m), -116.63 – -116.70 (m), 118.80 (s), -122.30 – -122.34 (m), - 126.01 – -126.07 (m); HRMS (ESI+): Calculated for C₁₈H₁₂F₁₀N₂O: [M+H]⁺ 463.0863, Found 463.0866.

1,6,7-Trimethyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (30)



Obtained as a yellow liquid (X = I, 65 mg, 69% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.62 (s, 1H), 7.06 (s, 1H), 3.65 (s, 3H), 2.54 (s, 6H), 2.42 (s, 3H), 2.35 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 154.6, 153.5, 140.4, 132.7, 131.5, 131.1, 130.2, 114.2, 51.2, 42.1, 37.9 (t, *J* = 30.0 Hz), 28.5, 20.6, 19.1, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – -81.07 (m), -116.52 – -116.60 (m), -122.27 – -122.34 (m), -125.96 – -126.04 (m); HRMS (ESI+): Calculated for C₂₀H₁₇F₉N₂O: [M+H]⁺ 473.1270, Found 473.1264.

6,7-Dichloro-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (31)



Obtained as a light yellow solid (X = I, 53 mg, 52% yield); M. P. = 94-95 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.94 (s, 1H), 7.39 (s, 1H), 3.63 (s, 3H), 2.54 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 156.3, 153.9, 134.6, 132.9, 131.8, 131.0, 127.6, 115.2, 51.3, 42.0, 37.9 (t, *J* = 30.2 Hz), 28.9, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – -81.08 (m), -116.63 – -116.70 (m), -122.23 – -122.35 (m), -125.95 – -126.09 (m); HRMS (ESI+): Calculated for C₁₈H₁₁Cl₂F₉N₂O: [M+H]⁺ 513.0177, Found 513.0185.

6,7-Difluoro-1-methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1*H*)-one (32)



Obtained as a light yellow solid (X = I, 50 mg, 50% yield); M. P. = 89-90 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.66 (dd, J = 10.1, 8.2 Hz, 1H), 7.09 (dd, J = 11.2, 7.0 Hz, 1H), 3.62 (s, 3H), 2.53 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.4 (d, J = 3.8 Hz), 154.0, 151.6 (dd, J = 277.2, 13.9 Hz), 146.7 (dd, J = 262.1, 13.9 Hz), 130.7 (dd, J = 11.3, 1.3 Hz), 129.0 (dd, J = 11.3, 2.5 Hz), 117.8 (dd, J = 20.2, 2.5 Hz), 102.3 (d, J = 22.7 Hz), 51.2, 41.9, 37.9 (t, J = 30.2 Hz), 29.1, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.06 – 81.10 (m), -116.64 – -116.71 (m), - 122.30 – -122.34 (m), -126.01 – -126.08 (m), -130.06 (d, J = 18.8 Hz), -141.79 (d, J = 18.8 Hz); HRMS (ESI+): Calculated for C₁₈H₁₁F₁₁N₂O: [M+H]⁺ 481.0768, Found 481.0769.

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)benzo[g]quinoxalin-2(1H)-one (33)



Obtained as a light yellow solid (X = I, 59 mg, 60% yield); M. P. = 126-127 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.37 (s, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 7.90 (d, *J* = 8.3 Hz, 1H), 7.60 – 7.56 (m, 2H), 7.51 – 7.47 (m, 1H), 3.73 (s, 3H), 2.59 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.4, 154.4, 133.8, 132.0, 131.8, 129.8, 129.5, 128.5, 128.1, 127.2, 125.4, 110.0, 51.4, 42.2, 37.9 (t, *J* = 30.2 Hz), 28.6, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.02 – -81.06 (m), -116.55 – -116.64 (m), -122.24 – -122.28 (m), -125.97 – -126.04 (m); HRMS (ESI+): Calculated for C₂₂H₁₅F₉N₂O: [M+H]⁺ 495.1113, Found 495.1103.

2-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxaline (34)



Obtained as a colourless liquid (X = I, 24 mg, 28% yield); ¹H NMR (500 MHz, CDCl₃) δ 8.02 (t, J = 9.4 Hz, 2H), 7.75 – 7.66 (m, 2H), 2.83 (s, 3H), 2.61 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 152.4, 151.1, 141.1, 141.0, 129.8, 129.2, 128.9, 128.2, 51.4, 43.1, 38.0 (t, J = 30.2 Hz), 23.9, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.00 – -81.04 (m), -116.60 – -116.66 (m), -122.17 – -122.23 (m), -125.96 – -126.04 (m); HRMS (ESI+): Calculated for C₁₈H₁₃F₉N₂: [M+H]⁺ 429.1008, Found 429.1004.

2-Chloro-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxaline (35)



Obtained as a colourless liquid (X = I, 30 mg, 33% yield); ¹H NMR (500 MHz, CDCl₃) δ 8.11 – 8.04 (m, 1H), 8.04 – 7.97 (m, 1H), 7.77 (dd, J = 6.3, 3.5 Hz, 2H), 2.67 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 149.9, 146.2, 141.3, 140.8, 130.9, 130.4, 129.0, 128.1, 51.5, 42.5, 38.0 (t, J = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.01 – -81.06 (m), -116.58 – -116.67 (m), -122.21 – -122.26 (m), -125.97 – -126.05 (m); HRMS (ESI+): Calculated for C₁₇H₁₀ClF₉N₂: [M+H]⁺ 449.0462, Found 449.0456.

2,6-Dichloro-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxaline (36)



Obtained as a light yellow solid (X = I, 44 mg, 46% yield); M. P. = 49-50 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.07 (d, *J* = 2.2 Hz, 1H), 7.92 (d, *J* = 8.9 Hz, 1H), 7.70 (dd, *J* = 8.9, 2.3 Hz, 1H), 2.66 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 150.0, 145.4, 140.0, 138.7, 135.3, 130.9, 128.2, 127.0, 50.5, 41.4, 37.1 (t, *J* = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – -81.07 (m), -116.63 – -116.70 (m), -122.21 – -122.26 (m), -125.99 – -126.06 (m); HRMS (ESI+): Calculated for C₁₇H₉Cl₂F₉N₂: [M+H]⁺ 483.0072, Found 483.0079.

3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2H-benzo[b][1,4]oxazin-2-one (37)



Obtained as a light yellow solid (X = I, 63 mg, 73% yield); M. P. = 117-118 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.67 (dd, J = 7.9, 1.2 Hz, 1H), 7.47 – 7.37 (m, 1H), 7.29 (dd, J = 11.1, 4.2 Hz, 1H),

7.20 (d, J = 8.2 Hz, 1H), 2.46 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 152.2, 151.8, 146.7, 131.4, 131.1, 129.2, 125.6, 116.4, 51.3, 41.3, 37.9 (t, J = 30.2 Hz), ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.12 – -81.16 (m), -116.75 – -116.78 (m), -122.33 – -122.35 (m), -126.06 – -126.13 (m); HRMS (ESI+): Calculated for C₁₇H₁₀F₉NO₂: [M+H]⁺ 432.0641, Found 432.0648.

1-Methyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)cinnolin-4(1H)-one (38)



Obtained as a light yellow solid (X = I, 38 mg, 43% yield); M. P. = 88-89 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.32 (d, *J* = 7.9 Hz, 1H), 7.74 (dd, *J* = 11.5, 4.2 Hz, 1H), 7.42 (dd, *J* = 12.4, 6.0 Hz, 2H), 4.08 (s, 3H), 2.49 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 170.8, 145.3, 141.4, 133.7, 125.9, 124.8, 124.1, 114.8, 51.0, 43.6, 37.8 (t, *J* = 30.2 Hz), 29.7, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – -81.07 (m), -116.51 – -116.59 (m), -122.27 – -122.31 (m), -125.96 – -126.03 (m); HRMS (ESI+): Calculated for C₁₈H₁₃F₉N₂O: [M+H]⁺ 445.0957, Found 445.0958.

1-Benzyl-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)cinnolin-4(1H)-one (39)



Obtained as a light yellow solid (X = I, 58 mg, 56% yield); M. P. = 111-112 °C; ¹H NMR (500 MHz, CDCl₃) δ 8.31 (d, *J* = 8.3 Hz, 1H), 7.76 (d, *J* = 8.5 Hz, 1H), 7.69 (ddd, *J* = 8.4, 6.8, 1.3 Hz, 1H), 7.52 (ddd, *J* = 8.0, 6.9, 1.0 Hz, 1H), 7.35 (t, *J* = 8.0 Hz, 3H), 6.99 – 6.91 (m, 2H), 5.89 (s, 2H), 2.66 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 171.4, 148.1, 139.5, 134.7, 132.6, 129.3, 128.4, 128.3, 126.4, 125.4, 125.2, 123.8, 65.0, 53.5, 39.2 (t, *J* = 30.2 Hz), 38.5, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.06 – -81.10 (m), -116.63 – -116.70 (m), -122.24 – 122.30 (m), -126.03 – -126.10 (m); HRMS (ESI+): Calculated for C₂₄H₁₇F₉N₂O: [M+H]⁺ 521.1270, Found 521.1270.

1-Methyl-3-(3-(perfluoropropyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (40)



Obtained as a light yellow solid (X = I, 54 mg, 68% yield); M. P. = 72-73 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.85 (dd, J = 8.0, 1.3 Hz, 1H), 7.56 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.38 – 7.33 (m, 1H), 7.30 (d, J = 8.4 Hz, 1H), 3.68 (s, 3H), 2.58 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 154.7, 154.5, 133.5, 132.7, 130.5, 130.2, 123.8, 113.6, 52.2, 42.0, 36.5 (d, J = 25.2 Hz), 28.6, ¹³C NMR for ^{*i*}C₃F₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -74.63(d, J = 9.4 Hz), -183.23 – -183.40 (m); HRMS (ESI+): Calculated for C₁₇H₁₃F₇N₂O: [M+H]⁺ 395.0989, Found 395.0988.

1-methyl-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (41)



Obtained as a light yellow solid (X = I, 78 mg, 72% yield); M. P. = 85-86 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.86 (dd, J = 8.0, 1.1 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.38 – 7.33 (m, 1H), 7.30 (d, J = 8.4 Hz, 1H), 3.68 (s, 3H), 2.56 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 154.8, 154.5, 133.5, 132.8, 130.5, 130.2, 123.7, 113.6, 51.2, 42.1, 38.0 (t, J = 31.5 Hz), 28.6, ¹³C NMR for C₆F₁₃ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.77 – -80.82 (m), 116.34 – -116.41 (m), 121.28 – 121.38 (m), 121.84 – -121.93 (m), 122.86 – -122.93 (m), 126.07 – -126.16 (m); HRMS (ESI+): Calculated for C₂₀H₁₃F₁₃N₂O: [M+Na]⁺ 567.0713, Found 567.0710.

3-(3-(Perfluorooctyl)-1-methylquinoxalin-2(1H)-one (42)



Obtained as a light yellow solid (X = I, 85 mg, 66% yield); M. P. = 99-100 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.78 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.53 – 7.45 (m, 1H), 7.28 (dd, *J* = 11.3, 4.0 Hz, 1H), 7.23 (d, *J* = 8.4 Hz, 1H), 3.61 (s, 3H), 2.49 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 154.8, 154.5, 133.5, 132.8, 130.5, 130.2, 123.7, 113.6, 51.2, 42.1, 38.0 (t, *J* = 30.2 Hz), 28.6, ¹³C NMR for C₈F₁₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.73 – -80.78 (m), -116.32 – -116.40 (m), -121.20 – -121.31 (m), -121.61 – -121.68 (m), -121.87 – -121.96 (m), -122.64 – -122.75 (m), -126.05 – -126.12 (m); HRMS (ESI+): Calculated for C₂₂H₁₃F₁₇N₂O: [M+H]⁺ 645.0829, Found 645.0828.

1-Ethyl-2,2-difluoro-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo [1.1.1]pentan-1-yl)acetate (43)



Obtained as a light yellow liquid (X = I, 42 mg, 60% yield; X = Br, 31 mg, 45% yield; X = Cl, 16 mg, 23% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.85 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.55 (ddd, *J* = 8.6, 7.4, 1.5 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 4.37 (q, *J* = 7.1 Hz, 2H), 3.67 (s, 3H), 2.44 (s, 6H), 1.38 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 163.3 (t, *J* = 32.8 Hz), 155.3, 154.5, 133.5, 132.8, 130.4, 130.2, 123.7, 113.6, 112.2 (t, *J* = 249.5 Hz), 62.8, 50.5 (t, *J* = 3.8 Hz), 41.5, 39.2 (t, *J* = 31.5 Hz), 28.6, 14.2; ¹⁹F NMR (471 MHz, CDCl₃) δ -111.56 (s); HRMS (ESI+): Calculated for C₁₈H₁₈F₂N₂O₃: [M+H]⁺ 349.1358, Found 349.1357.

Diethyl-(difluoro(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1] pentan-1yl)methyl)phosphonate (44)



Obtained as a yellow liquid (X = Br, 31 mg, 38% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.84 (dd, J = 8.0, 1.4 Hz, 1H), 7.53 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.34 – 7.31 (m, 1H), 7.28 (d, J = 8.4 Hz, 1H), 4.32 – 4.25 (m, 4H), 3.66 (s, 3H), 2.48 (s, 6H), 1.38 (t, J = 7.1 Hz, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.6, 154.6, 133.4, 132.8, 130.3, 130.1, 123.6, 113.6, 64.3 (d, J = 7.6 Hz), 51.0 (d, J = 2.5 Hz), 42.0, 39.0 (td, J = 27.6, 15.9 Hz), 28.6, 16.4, 16.4; ¹⁹F NMR (471 MHz, CDCl₃) δ -114.77 (s), -115.01 (s); ³¹P NMR (202 MHz, CDCl₃) δ 6.25 (t, J = 111.4 Hz); HRMS (ESI+): Calculated for C₁₉H₂₃F₂N₂O₄P: [M+H]⁺ 413.1440, found 413.1440.

3-(3-(Dichloromethyl)bicyclo[1.1.1]pentan-1-yl)-1-methylquinoxalin-2(1*H*)-one (45)



Obtained as a light yellow solid (X = Br, 22 mg, 36% yield); M. P. = 193-194 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.86 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.54 (ddd, *J* = 8.6, 7.3, 1.5 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 5.89 (s, 1H), 3.67 (s, 3H), 2.38 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.8, 154.6, 133.4, 132.8, 130.3, 130.1, 123.7, 113.6, 71.9, 50.6, 45.2, 40.8, 28.6; HRMS (ESI+): Calculated for C₁₅H₁₄Cl₂N₂O: [M+H]⁺ 309.0556, found 309.0553.

1-Methyl-3-(3-(trichloromethyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (46)



Obtained as a yellow solid (X = Br, 25 mg, 37% yield; X = Cl, 20 mg, 29% yield); M. P. = 189-190 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.87 (dd, J = 8.0, 1.3 Hz, 1H), 7.58 – 7.54 (m, 1H), 7.38 – 7.34 (m, 1H), 7.32 – 7.30 (m, 1H), 3.69 (s, 3H), 2.51 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.5, 154.5, 133.5, 132.8, 130.4, 130.2, 123.7, 113.6, 97.9, 52.5, 50.9, 38.9, 28.7; HRMS (ESI+): Calculated for C₁₅H₁₃Cl₃N₂O: [M+H]⁺ 343.0166, found 343.0162.

3-(3-(Dibromofluoromethyl)bicyclo[1.1.1]pentan-1-yl)-1-methylquinoxalin-2(1H)-one (47)



Obtained as a yellow liquid (X = Br, 33 mg, 40% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.86 (dd, J = 8.0, 1.3 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.30 (d, J = 8.3 Hz, 1H), 3.68 (s,

3H), 2.52 – 2.43 (m, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.0, 154.5, 133.5, 132.8, 130.4, 130.2, 123.7, 113.6, 57.9, 51.4 (d, J = 1.3 Hz), 50.9, 39.0, 28.7; ¹⁹F NMR (471 MHz, CDCl₃) δ -52.97 (s); HRMS (ESI+): Calculated for C₁₅H₁₃Br₂FN₂O: [M+H]⁺ 414.9451, found 414.9454.

3-(3-(Dibromomethyl)bicyclo[1.1.1]pentan-1-yl)-1-methylquinoxalin-2(1H)-one (48)



Obtained as a yellow solid (X = Br, 34 mg, 43% yield); M. P. = 186-187 °C;^zH NMR (500 MHz, CDCl₃) δ 7.86 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.58 – 7.52 (m, 1H), 7.37 – 7.32 (m, 1H), 7.30 (d, *J* = 8.3 Hz, 1H), 5.90 (s, 1H), 3.68 (s, 3H), 2.37 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.6, 154.6, 133.4, 132.8, 130.3, 130.2, 123.7, 113.6, 51.2, 46.7, 45.8, 39.8, 28.6; HRMS (ESI+): Calculated for C₁₅H₁₄Br₂N₂O: [M+H]⁺ 396.9546, found 396.9547.

1-Ethyl-2-(2-oxo-3-(3-(perfluoropropyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-1(2*H*)-yl)acetate (49)



Obtained as a yellow liquid (X = I, 61 mg, 65% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.86 (dd, J = 8.0, 1.3 Hz, 1H), 7.56 – 7.48 (m, 1H), 7.39 – 7.32 (m, 1H), 7.06 (d, J = 8.3 Hz, 1H), 4.98 (s, 2H), 4.26 (q, J = 7.1 Hz, 2H), 2.58 (s, 6H), 1.29 (t, J = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 170.0, 154.5, 154.0, 132.8, 132.6, 130.6, 130.5, 124.0, 113.1, 62.2, 52.3 (d, J = 2.5 Hz), 43.1, 41.8, 36.5 (d, J = 25.2 Hz), 14.1, ¹³C NMR for ^{*i*}C₃F₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -74.6 (d, J = 9.4 Hz), -183.37 – -183.44 (m); HRMS (ESI+): Calculated for C₂₀H₁₇F₇N₂O₃: [M+Na]⁺ 489.1020, Found 489.1018.

1-Ethyl-2-(2-oxo-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-1(2*H*)-yl)acetate (50)



Obtained as a yellow solid (X = I, 86 mg, 70% yield); M. P. = 89-90 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.87 (dd, J = 8.0, 1.1 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.06 (d, J = 8.3 Hz, 1H), 4.99 (s, 2H), 4.26 (q, J = 7.1 Hz, 2H), 2.56 (s, 6H), 1.29 (t, J = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 167.0, 154.7, 154.0, 132.8, 132.6, 130.6, 130.5, 124.0, 113.1, 62.2, 51.3, 43.1, 41.9, 38.0 (t, J = 25.2 Hz), 14.1, ¹³C NMR for C₆F₁₃ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.81 – -80.86 (m), 116.40 – -116.47 (m), 121.32 – -121.40 (m), 121.88 – -121.96 (m),

122.88 - -122.98 (m), 126.10 - -126.18 (m); HRMS (ESI+): Calculated for $C_{23}H_{17}F_{13}N_2O_3$: [M+H]⁺ 617.1104, Found 617.1094.

1-Ethyl-2-(2-oxo-3-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-1(2*H*)-yl)acetate (51)



Obtained as a light yellow solid (X = I, 103 mg, 72% yield); M. P. = 123-124 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.87 (dd, J = 8.0, 1.3 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.39 – 7.32 (m, 1H), 7.06 (d, J = 8.2 Hz, 1H), 4.99 (s, 2H), 4.26 (q, J = 7.1 Hz, 2H), 2.56 (s, 6H), 1.29 (t, J = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 167.0, 154.7, 154.0, 132.8, 132.6, 130.6, 130.5, 124.0, 113.1, 62.2, 51.3, 43.1, 41.9, 38.0 (t, J = 31.5 Hz), 14.1, ¹³C NMR for C₈F₁₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.79 – -80.84 (m), -116.39 – -116.47 (m), -121.25 – -121.34 (m), -121.65 – 121.73 (m), -121.91 – -121.99 (m), -122.71 – -122.79 (m), -126.10 – -126.16 (m); HRMS (ESI+): Calculated for C₂₅H₁₇F₁₇N₂O₃: [M+H]⁺ 717.1040, Found 717.1045.

1,6,7-Trimethyl-3-(3-(perfluoropropyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (52)



Obtained as a light yellow solid (X = I, 53 mg, 63% yield); M. P. = 146-147 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.60 (s, 1H), 7.06 (s, 1H), 3.64 (s, 3H), 2.56 (s, 6H), 2.42 (s, 3H), 2.34 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 154.6, 153.4, 140.4, 132.7, 131.5, 131.2, 130.2, 114.2, 52.2 (d, *J* = 3.8 Hz), 42.0, 36.4 (d, *J* = 25.2 Hz), 28.5, 20.6, 19.1, ¹³C NMR for ^{*i*}C₃F₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -74.6 (d, *J* = 9.4 Hz), -183.31 – -183.39 (m); HRMS (ESI+): Calculated for C₁₉H₁₇F₇N₂O: [M+H]⁺ 423.1302, Found 423.1306.

1,6,7-Trimethyl-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (53)



Obtained as a light yellow solid (X = I, 74 mg, 65% yield); M. P. = 114-115 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.61 (s, 1H), 7.06 (s, 1H), 3.65 (s, 3H), 2.54 (s, 6H), 2.42 (s, 3H), 2.34 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 154.6, 153.5, 140.4, 132.7, 131.5, 131.2, 130.2, 114.2, 51.2, 42.1, 37.9 (t, *J* = 30.2 Hz), 28.5, 20.6, 19.1, ¹³C NMR for C₆F₁₃ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.77 – -80.82 (m), 116.34 – -116.41 (m), 121.28 – -121.38 (m), 121.84 – -121.93 (m),

122.86 – -122.93 (m), 126.07 – -126.16 (m); HRMS (ESI+): Calculated for $C_{22}H_{17}F_{13}N_2O$: [M+H]⁺ 573.1206, Found 573.1207.

1,6,7-Trimethyl-3-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (54)



Obtained as a light yellow solid (X = I, 91 mg, 68% yield); M. P. = 83-84 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.61 (s, 1H), 7.06 (s, 1H), 3.65 (s, 3H), 2.54 (s, 6H), 2.42 (s, 3H), 2.35 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 154.6, 153.5, 140.4, 132.7, 131.5, 131.2, 130.2, 114.2, 51.2, 42.1, 37.9 (t, *J* = 30.2 Hz), 28.5, 20.6, 19.1, ¹³C NMR for C₈F₁₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.73 - -80.77 (m), -116.32 - -116.40 (m), -121.20 - -121.31 (m), -121.61 - -121.68 (m), -121.87 - -121.96 (m), -122.64 - -122.75 (m), -126.05 - -126.12 (m); HRMS (ESI+): Calculated for C₂₄H₁₇F₁₇N₂O: [M+H]⁺ 673.1142, Found 673.1139.

2,4-Dimethyl-6-(3-(perfluoropropyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (55)



Obtained as a light yellow solid (X = I, 26 mg, 63% yield); M. P. = 77-78 °C; ¹H NMR (500 MHz, CDCl₃) δ 3.62 (s, 3H), 3.33 (s, 3H), 2.42 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.8, 149.2, 139.8, 52.0 (d, *J* = 3.8 Hz), 39.6, 38.7, 36.8 (d, *J* = 25.2 Hz), 26.9, ¹³C NMR for ^{*i*}C₃F₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -74.69 (d, *J* = 9.4 Hz), -183.31 – -183.35 (m); HRMS (ESI+): Calculated for C₁₃H₁₂F₇N₃O₂: [M+Na]⁺ 398.0710, Found 398.0707.

2,4-Dimethyl-6-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (56)



Obtained as a light yellow solid (X = I, 69 mg, 66% yield); M. P. = 59-60 °C; ¹H NMR (500 MHz, CDCl₃) δ 3.62 (s, 3H), 3.33 (s, 3H), 2.40 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.8, 149.2, 139.9, 51.0, 39.6, 38.8, 38.3 (t, *J* = 25.2 Hz), 26.9, ¹³C NMR for C₆F₁₃ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.78 – -80.83 (m), 116.40 – -116.48 (m), 121.30 – -121.39 (m), 121.89 – -121.98 (m), 122.89 – -123.00 (m), 126.08 – -126.16 (m); HRMS (ESI+): Calculated for C₁₆H₁₂F₁₃N₃O₂: [M+Na]⁺ 548.0614, Found 548.0619.

2,4-Dimethyl-6-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (57)



Obtained as a light yellow solid (X = I, 85 mg, 68% yield); M. P. = 99-100 °C; ¹H NMR (500 MHz, CDCl₃) δ 3.62 (s, 3H), 3.33 (s, 3H), 2.41 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.8, 149.2, 139.9, 51.0, 39.6, 38.8, 38.3 (t, *J* = 30.2 Hz), 26.9, ¹³C NMR for C₈F₁₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.75 – -80.80 (m), -116.40 – -116.48 (m), -121.24 – -121.32 (m), -121.64 – -121.74 (m), -121.89 – -121.99 (m), -122.67 – -122.77 (m), -126.06 – -126.16 (m); HRMS (ESI+): Calculated for C₁₈H₁₂F₁₇N₃O₂: [M+Na]⁺ 648.0550, Found 648.0545.

2,4-Dibenzyl-6-(3-(perfluoropropyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (58)



Obtained as a light yellow solid (X = I, 47 mg, 65% yield); M. P. = 92-93 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.52 – 7.46 (m, 2H), 7.41 (dd, *J* = 7.8, 1.4 Hz, 2H), 7.39 – 7.28 (m, 6H), 5.07 (d, *J* = 16.7 Hz, 4H), 2.42 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.3, 149.0, 140.5, 135.5, 135.4, 129.6, 128.8, 128.6, 128.4, 128.2, 55.5, 52.0 (d, *J* = 3.8 Hz), 44.1, 38.7, 36.8 (d, *J* = 25.2 Hz), ¹³C NMR for ^{*i*}C₃F₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -74.66 (d, *J* = 9.4 Hz), -183.28 – -183.35 (m); HRMS (ESI+): Calculated for C₂₅H₂₀F₇N₃O₂: [M+Na]⁺ 550.1336, Found 550.1346.

2,4-Dibenzyl-6-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (59)



Obtained as a white solid (X = I, 99 mg, 73% yield); M. P. = 101-102 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.52 – 7.47 (m, 2H), 7.41 (dd, *J* = 7.8, 1.4 Hz, 2H), 7.38 – 7.29 (m, 6H), 5.07 (d, *J* = 17.9 Hz, 4H), 2.41 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.3, 149.0, 140.6, 135.5, 135.4, 129.6, 128.8, 128.8, 128.6, 128.4, 128.2, 55.5, 51.0, 44.1, 38.8, 38.3 (t, *J* = 25.2 Hz), ¹³C NMR for C₆F₁₃ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.80 – -80.84 (m), 116.42 – -116.48 (m), 121.29 – -121.37 (m), 121.90 – -121.98 (m), 122.89 – -122.96 (m), 126.09 – -126.17 (m); HRMS (ESI+): Calculated for C₂₈H₂₀F₁₃N₃O₂: [M+Na]⁺ 700.1240, Found 700.1244.

2,4-Dibenzyl-6-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)-1,2,4-triazine-3,5(2*H*,4*H*)-dione (60)



Obtained as a white solid (X = I, 113 mg, 73% yield); M. P. = 123-124 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.49 (d, *J* = 6.6 Hz, 2H), 7.40 (d, *J* = 6.5 Hz, 2H), 7.38 – 7.28 (m, 6H), 5.07 (d, *J* = 17.6 Hz, 4H), 2.40 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.3, 149.0, 140.6, 135.5, 135.5, 129.6, 128.8, 128.8, 128.6, 128.4, 128.2, 55.5, 51.0, 44.1, 38.8, 38.3 (t, *J* = 30.2 Hz), ¹³C NMR for C₈F₁₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.77 – -80.81 (m), -116.42 – -116.47 (m), -121.26 – -121.30 (m), -121.68 – -121.76 (m), -121.90 – -121.96 (m), -122.69 – -122.73 (m), -126.09 – -126.15 (m); HRMS (ESI+): Calculated for C₃₀H₂₀F₁₇N₃O₂: [M+Na]⁺ 800.1176, Found 800.1172.

1-Methyl-3-(3-(perfluoropropyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (61)



Obtained as a light yellow solid (X = I, 43 mg, 43% yield); M. P. = 175-176 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.42 – 7.37 (m, 3H), 7.19 (dd, *J* = 7.5, 1.8 Hz, 2H), 7.12 (s, 5H), 3.30 (s, 3H), 2.57 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.3, 151.4, 138.0, 137.6, 132.7, 132.5, 130.0, 129.6, 129.3, 129.2, 127.7, 127.1, 52.0 (d, *J* = 2.5 Hz), 41.7, 36.5 (d, *J* = 25.2 Hz), 33.7, ¹³C NMR for ^{*i*}C₃F₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -74.62 (d, *J* = 9.4 Hz), -183.23 – 183.30 (m); HRMS (ESI+): Calculated for C₂₅H₁₉F₇N₂O: [M+H]⁺ 497.1458, Found 497.1457.

1-Methyl-3-(3-(perfluorohexyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (62)



Obtained as a light yellow solid (X = I, 58 mg, 45% yield); M. P. = 125-126 °C; ¹H NMR (500 MHz, CDCl₃) δ 77.44 – 7.36 (m, 3H), 7.22 – 7.17 (m, 2H), 7.16 – 7.08 (m, 5H), 3.30 (s, 3H), 2.55 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.3, 151.6, 138.0, 137.6, 132.7, 132.5, 130.0, 129.6, 129.3, 129.1, 127.7, 127.0, 51.0, 41.8, 38.0 (t, *J* = 25.2 Hz), 33.7, ¹³C NMR for C₆F₁₃ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.79 – -80.83 (m), 116.29 – -116.36 (m), 121.27 – 121.36 (m), 121.82 – -121.95 (m), 122.85 – -122.96 (m), 126.08 – -126.16 (m); HRMS (ESI+): Calculated for C₂₈H₁₉F₁₃N₂O: [M+Na]⁺ 669.1182, Found 669.1178.

1-Methyl-3-(3-(perfluorooctyl)bicyclo[1.1.1]pentan-1-yl)-5,6-diphenylpyrazin-2(1*H*)-one (63)



Obtained as a light yellow solid (X = I, 69 mg, 65% yield); M. P. = 159-160 °C;¹H NMR (500 MHz, CDCl₃) δ 7.40 (qd, J = 5.8, 1.7 Hz, 3H), 7.21 – 7.17 (m, 2H), 7.13 (s, 5H), 3.30 (s, 3H), 2.55 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.3, 151.6, 138.0, 137.6, 132.7, 132.5, 130.0, 129.6, 129.3, 129.1, 127.7, 127.0, 51.0, 41.8, 38.0 (t, J = 30.2 Hz), 33.7, ¹³C NMR for C₈F₁₇ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.75 – -80.80 (m), -116.29 – -116.36 (m), -121.23 – -121.29 (m), -121.61 – -121.68 (m), -121.89 – -121.96 (m), -122.67 – -122.75 (m), -126.06 – -126.14 (m); HRMS (ESI+): Calculated for C₃₀H₁₉F₁₇N₂O: [M+Na]⁺ 769.1118, Found 769.1111.

1-Ethyl-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1]pentan-1-yl)acetate (64)



Obtained as a light yellow liquid (X = I, 36 mg, 58% yield; X = Br, 19 mg, 30% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.85 (dd, J = 8.0, 1.3 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.34 – 7.30 (m, 1H), 7.28 (d, J = 9.4 Hz, 1H), 4.17 (q, J = 7.1 Hz, 2H), 3.66 (s, 3H), 2.62 (s, 2H), 2.30 (s, 6H), 1.30 (d, J = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 171.3, 156.5, 154.7, 133.4, 132.9, 130.1, 129.9, 123.5, 113.5, 60.3, 53.0, 42.5, 37.8, 36.9, 28.6, 14.4; HRMS (ESI+): Calculated for C₁₈H₂₀N₂O₃: [M+Na]⁺ 335.1366, Found 335.1367.

tert-Butyl-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1]pentan-1-yl)acetate (65)



Obtained as a yellow solid (X = Br, 23 mg, 34% yield); M. P. = 104-105 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.85 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.34 – 7.30 (m, 1H), 7.28 (d, *J* = 7.9 Hz, 1H), 3.66 (s, 3H), 2.53 (s, 2H), 2.29 (s, 6H), 1.48 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 170.7, 156.6, 154.7, 133.4, 132.9, 130.0, 129.9, 123.5, 113.5, 80.4, 53.0, 42.4, 39.2, 37.1, 28.6, 28.2; HRMS (ESI+): Calculated for C₂₀H₂₄N₂O₃: [M+H]⁺ 341.1868, found 341.1864.

3-(3-(3,3-Dimethyl-2-oxobutyl)bicyclo[1.1.1]pentan-1-yl)-1-methylquinoxalin-2(1H)-one (66)



Obtained as a yellow liquid (X = Br, 21 mg, 32% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.84 (dd, J = 8.0, 1.2 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.33 – 7.28 (m, 1H), 7.26 (d, J = 4.0 Hz, 1H), 3.65 (s, 3H), 2.77 (s, 2H), 2.28 (s, 6H), 1.13 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 213.9, 156.6, 154.7, 133.4,

132.9, 130.0, 129.8, 123.5, 113.5, 53.3, 44.4, 43.0, 38.3, 37.4, 28.6, 26.0; HRMS (ESI+): Calculated for $C_{20}H_{24}N_2O_2$: [M+H]⁺ 325.1911, found 325.1913.

2-(3-(4-Methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1]pentan-1-yl)acetonitrile (67)



Obtained as a brown liquid (X = I, 30 mg, 57% yield; X = Br, 19 mg, 36% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.85 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.36 – 7.31 (m, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 3.67 (s, 3H), 2.69 (s, 2H), 2.35 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.6, 154.6, 133.4, 132.8, 130.2, 130.1, 123.6, 117.3, 113.6, 52.5, 42.1, 35.6, 28.6, 21.2; HRMS (ESI+): Calculated for C₁₆H₁₅N₃O: [M+H]⁺ 266.1288, Found 266.1280.

1-Methyl-3-(3-(4-nitrobenzyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (68)



Obtained as a light yellow solid (X = Br, 33 mg, 46% yield); M. P. = 174-175 °C; ¹H NMR (400 MHz, CDCl₃) δ 8.17 (d, *J* = 8.6 Hz, 2H), 7.82 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.55 – 7.48 (m, 1H), 7.32 (t, *J* = 7.3 Hz, 3H), 7.27 (d, *J* = 5.2 Hz, 1H), 3.64 (s, 3H), 2.14 (s, 6H); ¹³C NMR (101 MHz, CDCl₃) δ 156.5, 154.6, 147.2, 146.5, 146.5, 133.4, 132.8, 130.0, 129.8, 123.7, 123.6, 113.6, 52.0, 42.8, 40.4, 39.0, 28.6; HRMS (ESI+): Calculated for C₂₁H₁₉N₃O₃: [M+H]⁺ 362.1499, Found 362.1503.

tert-Butyl-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1]pentan-1-yl)propanoate (69)



Obtained as a yellow liquid (X = Br, 28 mg, 40% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.85 (dd, J = 8.0, 1.3 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.35 – 7.30 (m, 1H), 7.28 (d, J = 9.4 Hz, 1H), 3.67 (s, 3H), 2.22 (s, 6H), 1.48 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 173.5, 156.9, 154.7, 133.4, 132.9, 130.0, 129.9, 123.5, 113.5, 80.2, 51.1, 41.7, 41.3, 28.6, 28.3, 13.3; HRMS (ESI+): Calculated for C₂₁H₂₆N₂O₃: [M+Na]⁺ 377.1836, Found 377.1832.

1-Benzyl-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1]pentan-1-yl)propanoate (70)



Obtained as a brown liquid (X = Br, 31 mg, 40% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.84 (dd, J = 8.0, 1.4 Hz, 1H), 7.51 (ddd, J = 8.6, 7.3, 1.5 Hz, 1H), 7.37 (s, 2H), 7.36 (d, J = 4.5 Hz, 2H), 7.35 – 7.32 (m, 1H), 7.31 (dd, J = 6.2, 2.2 Hz, 1H), 7.27 – 7.25 (m, 1H), 5.14 (s, 2H), 3.65 (s, 3H), 2.77 (q, J = 7.0 Hz, 1H), 2.21 (s, 6H), 1.20 (d, J = 7.0 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 174.0, 156.6, 154.6, 136.1, 133.4, 132.8, 130.0, 129.9, 128.6, 128.3, 128.2, 123.5, 113.5, 66.2, 51.1, 41.5, 41.3, 40.9, 28.6, 13.4; HRMS (ESI+): Calculated for C₂₄H₂₄N₂O₃: [M+H]⁺ 389.1867, found 389.1865.

1-Ethyl-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1]pentan-1-yl)-2-phenylacetate (71)



Obtained as a yellow liquid (X = Br, 30 mg, 39% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.82 (dd, J = 8.0, 1.4 Hz, 1H), 7.50 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.36 – 7.30 (m, 5H), 7.29 – 7.27 (m, 1H), 7.25 (s, 1H), 4.19 (dd, J = 17.2, 7.1 Hz, 2H), 3.84 (s, 1H), 3.64 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 171.8, 156.7, 154,6, 136.5, 133.4, 132.9, 130.0, 129.9, 128.6, 128.4, 127.1, 123.5, 113.5, 60.7, 53.4, 51.7, 42.5, 41.5, 28.6, 14.3; HRMS (ESI+): Calculated for C₂₄H₂₄N₂O₃: [M+H]⁺ 389.1860, found 389.1856.

Diethyl-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1]pentan-1-yl)malonate (72)



Obtained as a brown liquid (X = Br, 29 mg, 38% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.85 (dd, J = 8.0, 1.3 Hz, 1H), 7.52 (ddd, J = 8.5, 7.3, 1.5 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.28 (d, J = 8.4 Hz, 1H), 4.23 (q, J = 7.1 Hz, 4H), 3.67 (s, 3H), 2.40 (s, 6H), 1.30 (t, J = 7.1 Hz, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 167.6, 156.2, 154.6, 133.4, 132.9, 130.1, 130.0, 123.5, 113.5, 61.3, 53.6, 52.5, 42.5, 37.7, 28.6, 14.2; HRMS (ESI+): Calculated for C₂₁H₂₄N₂O₅: [M+Na]⁺ 407.1577, Found 407.1572.

Ethyl-2-methyl-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1] pentan-1-yl)pr opanoate (74)



Obtained as a brown liquid (X = Br, 22 mg, 32% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.85 (dd, J = 8.0, 1.4 Hz, 1H), 7.55 - 7.49 (m, 1H), 7.33 (dd, J = 11.7, 4.6 Hz, 1H), 7.28 (d, J = 8.4 Hz, 1H),

4.15 (q, J = 7.1 Hz, 2H), 3.67 (s, 3H), 2.19 (s, 6H), 1.28 (t, J = 7.1 Hz, 3H), 1.20 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 176.0, 157.0, 154.7, 133.4, 132.9, 130.0, 129.9, 123.5, 113.5, 60.3, 49.7, 45.6, 42.1, 40.0, 28.6, 21.7, 14.4; HRMS (ESI+): Calculated for C₂₀H₂₄N₂O₃: [M+H]⁺ 341.1860, Found 341.1860.

1-Benzyl-2-methyl-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo[1.1.1] pentan-1-yl)propanoate (75)



Obtained as a yellow liquid (X = Br, 35 mg, 44% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.83 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.53 – 7.49 (m, 1H), 7.37 (d, *J* = 5.1 Hz, 2H), 7.35 (d, *J* = 2.3 Hz, 2H), 7.35 – 7.32 (m, 1H), 7.30 (dd, *J* = 4.2, 2.6 Hz, 1H), 7.27 – 7.25 (m, 1H), 5.13 (s, 2H), 3.64 (s, 3H), 2.17 (s, 6H), 1.23 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 175.9, 156.9, 154.7, 136.3, 133.4, 132.9, 130.0, 129.9, 128.5, 128.0, 128.0, 123.5, 113.5, 66.2, 49.7, 45.6, 42.4, 40.0, 28.6, 21.8; HRMS (ESI+): Calculated for C₂₅H₂₆N₂O₃: [M+H]⁺ 403.2016, found 403.2014.

Diethyl-2-methyl-2-(3-(4-methyl-3-oxo-3,4-dihydroquinoxalin-2-yl)bicyclo [1.1.1]pentan-1-yl) malonate (76)



Obtained as a brown liquid (X = Br, 32 mg, 40% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.85 (dd, J = 8.0, 1.4 Hz, 1H), 7.52 (ddd, J = 8.6, 7.4, 1.5 Hz, 1H), 7.35 – 7.31 (m, 1H), 7.28 (d, J = 8.4 Hz, 1H), 4.22 (qd, J = 7.1, 1.2 Hz, 4H), 3.67 (s, 3H), 2.35 (s, 6H), 1.46 (s, 3H), 1.29 (t, J = 7.1 Hz, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 170.8, 156.6, 154.6, 133.4, 132.9, 130.1, 130.0, 123.5, 113.5, 61.1, 54.1, 51.0, 42.3, 41.3, 28.6, 18.4, 14.2; HRMS (ESI+): Calculated for C₂₂H₂₆N₂O₅: [M+H]⁺ 399.1914, Found 399.1908.

Methyl-3-(3-(2-nitropropan-2-yl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-2(1H)-one (77)



Obtained as a yellow solid (X = Br, 28 mg, 45% yield); M. P. = 167-168 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.84 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.57 – 7.51 (m, 1H), 7.36 – 7.32 (m, 1H), 7.29 (d, *J* = 8.4 Hz, 1H), 3.67 (s, 3H), 2.27 (s, 6H), 1.62 (s, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 155.8, 154.6, 133.4 132.8, 130.2, 130.1, 123.6, 113.6, 86.8, 49.9, 45.2, 39.0, 28.6, 22.8; HRMS (ESI+): Calculated for C₁₇H₁₉N₃O₃: [M+H]⁺ 314.1499, Found 314.1499.

3-(3-(Tert-butyl)bicyclo[1.1.1]pentan-1-yl)-1-methylquinoxalin-2(1H)-one (78)



Obtained as a yellow liquid (X = I, 13 mg, 23% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.88 (dd, J = 8.0, 1.1 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.34 – 7.30 (m, 1H), 7.28 (d, J = 8.6 Hz, 1H), 3.67 (s, 3H), 2.10 (s, 6H), 0.92 (s, 9H); ¹³C NMR (126 MHz, CDCl₃) δ 157.8, 154.7, 133.4, 132.9, 129.9, 129.8, 123.4, 113.5, 48.8, 48.5, 39.6, 29.6, 28.6, 25.9; HRMS (ESI+): Calculated for C₁₈H₂₂N₂O: [M+H]⁺ 283.1805, Found 283.1805.

2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)ethyl 2-(4isobutylphenyl)propanoate (79)



Obtained as a light yellow solid (X = I, 81 mg, 61% yield); M. P. = 80-81 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.84 (dd, J = 8.0, 1.3 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.37 – 7.31 (m, 2H), 7.08 (d, J = 8.1 Hz, 2H), 7.04 (d, J = 8.1 Hz, 2H), 4.49 (ddd, J = 9.9, 6.9, 2.2 Hz, 1H), 4.45 – 4.35 (m, 3H), 3.58 (q, J = 7.1 Hz, 1H), 2.54 (s, 6H), 2.43 (d, J = 7.2 Hz, 2H), 1.83 (dt, J = 13.5, 6.8 Hz, 1H), 1.42 (d, J = 7.2 Hz, 3H), 0.89 (d, J = 6.6 Hz, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 174.7, 154.6, 154.3, 140.8, 137.2, 133.0, 132.9, 130.5, 130.4, 129.4, 127.1, 123.8, 113.8, 61.0, 51.2, 45.0, 45.0, 41.9, 40.6, 37.9 (t, J = 30.2 Hz), 30.2, 22.4, 18.3, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03– -81.08 (m), -115.59 – -116.67 (m), -121.29 – -122.33(m), -125.97 – -126.04 (m); HRMS (ESI+): Calculated for C₃₂H₃₁F₉N₂O₃: [M+H]⁺ 663.2264, Found 663.2262.

2-(2-Oxo-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-1(2*H*)-yl)ethyl 2-(1-(4chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl)acetate (80)



Obtained as a yellow liquid (X = I, 80 mg, 49% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.86 - 7.79 (m, 1H), 7.67 - 7.58 (m, 2H), 7.50 - 7.45 (m, 2H), 7.45 - 7.40 (m, 1H), 7.31 (t, J = 7.6 Hz, 2H),

6.88 (d, J = 2.4 Hz, 1H), 6.84 (d, J = 9.0 Hz, 1H), 6.66 (dd, J = 9.0, 2.5 Hz, 1H), 4.48 (s, 4H), 3.80 (s, 3H), 3.60 (s, 2H), 2.55 (s, 6H), 2.28 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 170.8, 168.2, 156.1, 154.6, 154.3, 139.4, 136.0, 133.8, 132.9, 131.2, 130.8, 130.5, 130.5, 130.5, 129.2, 123.8, 115.0, 113.4, 111.9, 111.6, 101.3, 61.2, 55.7, 51.3, 41.9, 40.7, 30.1, 14.2, 13.3, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.02 - -81.06 (m), -116.58 - -116.64 (m), -122.27 - -122.32 (m), -125.97 - -126.04 (m); HRMS (ESI+): Calculated for C₃₈H₂₉CF₉N₃O₅: [M+Na]⁺ 836.1544, Found 836.1547.

2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)ethyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (81)



Obtained as a yellow liquid (X = I, 77 mg, 55% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.86 – 7.81 (m, 1H), 7.53 (d, *J* = 7.9 Hz, 2H), 7.45 (dd, *J* = 16.2, 8.4 Hz, 3H), 7.35 (dt, *J* = 17.2, 7.6 Hz, 4H), 6.99 (t, *J* = 9.4 Hz, 2H), 4.53 – 4.42 (m, 4H), 3.64 (q, *J* = 7.1 Hz, 1H), 2.54 (s, 6H), 1.46 (d, *J* = 7.2 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 173.9, 159.6 (d, *J* = 249.5 Hz), 154.6, 154.3, 141.2 (d, *J* = 7.6 Hz), 135.3, 132.9 (d, *J* = 10.1 Hz), 130.9 (d, *J* = 3.8 Hz), 130.5, 130.4, 128.9 (d, *J* = 2.5 Hz), 128.5, 128.0, 127.9, 127.8, 123.8, 123.4 (d, *J* = 3.8 Hz), 115.2 (d, *J* = 23.9 Hz), 113.7, 61.3, 51.2, 44.9, 41.9, 40.6, 37.9 (t, *J* = 30.2 Hz), 18.2, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -80.02 – -81.06 (m), -116.60 – -116.66 (m), -117.25 (s), -122.29 – -122.33 (m), -125.98 – -126.05 (m); HRMS (ESI+): Calculated for C₃₄H₂₆F₁₀N₂O₃: [M+H]⁺ 701.1857, Found 701.1857.

2-(3-(3-(Perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)ethyl 2-(4-((2-oxocyclopentyl)methyl)phenyl)propanoate (82)



Obtained as a yellow liquid (X = I, 63 mg, 45% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.84 (dd, J = 8.0, 1.3 Hz, 1H), 7.50 – 7.45 (m, 1H), 7.37 – 7.31 (m, 2H), 7.08 (d, J = 8.1 Hz, 2H), 7.04 (d, J = 8.1 Hz, 2H), 4.49 (ddd, J = 9.9, 6.9, 2.2 Hz, 1H), 4.45 – 4.35 (m, 3H), 3.58 (q, J = 7.1 Hz, 1H), 2.54 (s, 6H), 2.43 (d, J = 7.2 Hz, 2H), 1.83 (dt, J = 13.5, 6.8 Hz, 1H), 1.42 (d, J = 7.2 Hz, 3H), 0.89 (d, J =

6.6 Hz, 6H); ¹³C NMR (126 MHz, CDCl₃) δ 220.1, 174.5, 154.6, 154.3, 139.1, 137.8, 132.9, 132.9, 130.5, 130.4, 129.2, 127.4, 123.8, 113.7, 61.0, 51.2, 51.0, 45.0, 41.9, 40.5, 38.2, 38.2 (t, *J* = 30.2 Hz), 35.2, 29.3, 20.5, 18.3, ¹³C NMR for C₄F₉ could not be assigned; ¹⁹F NMR (471 MHz, CDCl₃) δ -81.03 – -81.08 (m), -116.59 – -116.67 (m), -122.29 – -122.33 (m), -125.97 – -126.04 (m); HRMS (ESI+): Calculated for C₃₄H₃₁F₉N₂O₄: [M+H]⁺ 703.2213, Found 703.2218.

(3*R*,5*S*,8*R*,9*S*,10*S*,13*S*,14*S*)-10,13-Dimethyl-17-oxohexadecahydro-1*H*-cyclopenta[*a*]phenanthr en-3-yl-2-(3-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)bicyclo[1.1.1]pentan-1-yl)propanoate (83)



Obtained as a light yellow solid (X = Br, 55 mg, 39% yield); M. P. = 70-71 °C; ¹H NMR (500 MHz, CDCl₃) δ 7.39 (d, J = 6.9 Hz, 2H), 7.32 (d, J = 7.0 Hz, 2H), 7.29 – 7.17 (m, 6H), 4.99 (s, 2H), 4.95 (s, 2H), 4.78 – 4.55 (m, 1H), 2.53 (q, J = 6.8 Hz, 1H), 2.36 (dd, J = 19.3, 8.8 Hz, 1H), 2.03 – 1.98 (m, 1H), 1.96 (s, 6H), 1.88 – 1.83 (m, 1H), 1.72 (d, J = 12.3 Hz, 3H), 1.67 (d, J = 13.3 Hz, 1H), 1.59 – 1.52 (m, 2H), 1.48 – 1.39 (m, 3H), 1.32 (s, 1H), 1.27 (s, 1H), 1.23 (d, J = 3.0 Hz, 1H), 1.16 (ddd, J = 14.5, 9.5, 4.5 Hz, 4H), 1.03 (d, J = 7.0 Hz, 3H), 0.98 (dd, J = 13.7, 3.8 Hz, 1H), 0.91 (dd, J = 12.2, 4.8 Hz, 1H), 0.78 (s, 6H), 0.68 – 0.62 (m, 1H); ¹³C NMR (126 MHz, CDCl₃) δ 173.5, 155.4, 149.1, 142.3, 135.7, 135.7, 129.5, 128.8, 128.7, 128.6, 128.2, 128.0, 73.4, 55.3, 54.3 (d, J = 1.3 Hz), 51.4, 50.9, 47.8, 44.7 (d, J = 2.5 Hz), 43.9, 42.0, 40.8, 37.9, 36.7 (d, J = 1.3 Hz), 35.9, 35.7, 35.1, 34.2 (d, J = 12.6 Hz), 31.5, 30.8, 28.3, 27.7 (d, J = 15.1 Hz), 21.8, 20.5, 13.8, 13.3, 12.3; HRMS (ESI+): Calculated for C₄₄H₅₃N₃O₅: [M+Na]⁺ 726.3877, Found 726.3875.

(2*S*,5*R*)-2-Isopropyl-5-methylcyclohexyl-2-(3-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)bicyclo[1.1.1]pentan-1-yl)-2-methylpropanoate (84)



Obtained as a light yellow liquid (X = Br, 40 mg, 34% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.50 – 7.46 (m, 2H), 7.41 (dd, J = 7.8, 1.4 Hz, 2H), 7.36 – 7.27 (m, 6H), 5.07 (s, 2H), 5.04 (s, 2H), 4.66 (td, J = 10.9, 4.3 Hz, 1H), 2.00 (s, 6H), 2.00 – 1.95 (m, 1H), 1.95 – 1.88 (m, 1H), 1.82 – 1.57 (m, 3H), 1.49 (ddd, J = 8.6, 7.3, 4.5 Hz, 1H), 1.43 – 1.38 (m, 1H), 1.15 (d, J = 8.8 Hz, 6H), 1.06 (dd, J = 12.8, 2.9 Hz, 1H), 0.96 (d, J = 11.2 Hz, 1H), 0.91 (dd, J = 6.8, 2.1 Hz, 6H), 0.80 – 0.71 (m, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 175.4, 155.5, 149.1, 142.6, 135.8, 135.7, 129.6, 128.8, 128.7, 128.6, 128.2, 128.0, 74.3, 55.3, 49.5, 47.1, 46.0, 43.9, 42.1, 41.1, 36.9, 34.3, 31.4, 26.0, 23.1, 22.1, 22.1, 21.8, 20.9, 16.0; HRMS (ESI+): Calculated for C₃₆H₄₅N₃O₄: [M+Na]⁺ 606.3302, Found 606.3300.

(*R*)-3,7-Dimethyloct-6-en-1-yl-2-(3-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)bicyclo[1.1.1]pentan-1-yl)-2-methylpropanoate (85)



Obtained as a light yellow liquid (X = Br, 44 mg, 57% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.50 – 7.45 (m, 2H), 7.39 (dd, J = 7.9, 1.3 Hz, 2H), 7.36 – 7.26 (m, 6H), 5.05 (d, J = 13.8 Hz, 4H), 4.15 – 4.06 (m, 2H), 2.00 (s, 6H), 2.00 – 1.86 (m, 2H), 1.68 (d, J = 5.6 Hz, 1H), 1.66 (s, 3H), 1.59 (s, 3H), 1.57 – 1.52 (m, 1H), 1.44 (dd, J = 13.4, 6.3 Hz, 1H), 1.35 (ddd, J = 8.6, 6.4, 3.1 Hz, 1H), 1.15 (s, 6H), 0.92 (d, J = 6.6 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 175.9, 155.5, 149.1, 142.5, 135.7, 135.7, 131.3, 129.6, 128.8, 128.7, 128.6, 128.2, 128.0, 124.6, 62.9, 55.3, 49.5, 46.0, 44.0, 42.1, 37.0, 36.7, 35.6, 29.5, 25.7, 25.4, 21.8, 19.4, 17.7; HRMS (ESI+): Calculated for C₃₆H₄₅N₃O₄: [M+H]⁺ 584.3483, Found 584.3482.

1-Methyl-2-((2-(3-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)bicyclo[1.1.1]pe ntan-1-yl)propanoyl)oxy)benzoate (86)



Obtained as a light yellow liquid (X = Br, 51 mg, 45% yield); ¹H NMR (500 MHz, CDCl₃) δ 8.01 (dd, J = 7.8, 1.5 Hz, 1H), 7.56 (td, J = 7.9, 1.6 Hz, 1H), 7.52 – 7.47 (m, 2H), 7.44 – 7.39 (m, 2H), 7.37 – 7.28 (m, 7H), 7.09 (d, J = 8.0 Hz, 1H), 5.08 (s, 2H), 5.06 (s, 2H), 3.87 (s, 3H), 3.01 (q, J = 7.0 Hz, 1H), 2.19 (s, 6H), 1.33 (d, J = 7.1 Hz, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 172.5, 165.0, 155.5, 150.5, 149.1, 142.3, 135.7, 135.7, 133.7, 131.7, 129.5, 128.8, 128.7, 128.6, 128.2, 128.0, 126.0, 123.8, 123.6, 55.4, 52.2, 51.0, 44.0, 41.7, 40.7, 38.3, 13.5; HRMS (ESI+): Calculated for C₃₃H₃₁N₃O₆: [M+Na]⁺ 588.2105, Found 588.2104.

2-(4-(3-(3-Chloro-10*H*-phenothiazin-10-yl)propyl)piperazin-1-yl)ethyl-2-(3-(2,4-dibenzyl-3,5-dioxo-2,3,4,5-tetrahydro-1,2,4-triazin-6-yl)bicyclo[1.1.1]pentan-1-yl)-2-methylpropanoate (87)



Obtained as a brown liquid (X = Br, 66 mg, 40% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.46 (d, J = 6.8 Hz, 2H), 7.38 (dd, J = 7.9, 1.4 Hz, 2H), 7.35 – 7.27 (m, 6H), 7.16 – 7.12 (m, 1H), 7.10 (dd, J = 7.6, 1.4 Hz, 1H), 7.00 (d, J = 8.1 Hz, 1H), 6.92 (td, J = 7.5, 0.8 Hz, 1H), 6.89 – 6.85 (m, 2H), 6.83 (d, J = 2.0 Hz, 1H), 5.05 (s, 2H), 5.01 (s, 2H), 4.19 (t, J = 5.8 Hz, 2H), 3.88 (t, J = 6.7 Hz, 2H), 2.61 (t, J = 5.8 Hz, 2H), 2.50 (d, J = 29.5 Hz, 10H), 2.01 (s, 6H), 1.97 – 1.90 (m, 2H), 1.14 (s, 6H); ¹³C

NMR (126 MHz, CDCl₃) δ 175.6, 155.4, 149.1, 146.5, 144.5, 142.5, 135.7, 135.7, 133.3, 129.5, 128.8, 128.7, 128.6, 128.2, 128.0, 127.9, 127.5, 127.5, 124.8, 123.6, 123.0, 122.3, 115.9, 115.9, 61.7, 60.4, 56.7, 55.4, 55.4, 53.2, 49.5, 46.0, 45.3, 44.0, 42.1, 36.7, 25.5, 21.8; HRMS (ESI+): Calculated for C₄₇H₅₁ClN₆O₄S: [M+H]⁺ 831.3454, Found 831.3451.

1-(5-(Hydroxymethyl)-4-(5-((2-oxo-3-(3-(perfluorobutyl)bicyclo[1.1.1]pentan-1-yl)quinoxalin-1(2H)-yl)methyl)-1H-1,2,3-triazol-1-yl)tetrahydrofuran-2-yl)-5-methylpyrimidine-2,4(1H,3H)dione (88)



Obtained as a yellow liquid (100 mg, 68% yield); ¹H NMR (500 MHz, CDCl₃) δ 7.97 – 7.74 (m, 3H), 7.56 (t, J = 7.8 Hz, 1H), 7.48 (s, 1H), 7.33 (t, J = 7.5 Hz, 1H), 6.24 (t, J = 6.5 Hz, 1H), 5.48 (dd, J = 24.1, 15.3 Hz, 2H), 5.40 (dd, J = 13.3, 5.5 Hz, 1H), 4.44 – 4.32 (m, 1H), 3.96 (d, J = 12.2 Hz, 1H), 3.83 – 3.67 (m, 1H), 2.89 (dd, J = 15.1, 7.0 Hz, 4H), 2.54 (s, 6H), 1.89 (s, 3H); ¹³C NMR (126 MHz, CDCl₃) δ 163.8, 154.2, 150.5, 142.5, 137.5, 132.9, 132.5, 130.8, 130.2, 123.9, 114.7, 111.2, 88.2, 85.2, 61.5, 59.5, 51.3, 46.0, 41.9, 37.7, 37.6, 12.4, 9.6; ¹⁹F NMR (471 MHz, CDCl₃) δ - 81.07 (m), -116.58 – -116.65 (m), -122.26 – -122.32 (m), -125.98 – -126.05 (m); HRMS (ESI+): Calculated for C₃₀H₂₆F₉N₇O₅: [M+H]⁺ 736.1924, Found 736.1916.
4 Copies of ¹H, ¹³C, and ¹⁹F NMR Spectra



4 ¹³C NMR (126 MHz, CDCl₃)





5 ¹H NMR (500 MHz, CDCl₃)





5¹⁹F NMR (471 MHz, CDCl₃)









7¹H NMR (500 MHz, CDCl₃)





7¹⁹F NMR (471 MHz, CDCl₃)





8¹³C NMR (126 MHz, CDCl₃)









9¹⁹F NMR (471 MHz, CDCl₃)





10¹³C NMR (126 MHz, CDCl₃)





11 ¹H NMR (500 MHz, CDCl₃)





11 ¹⁹F NMR (471 MHz, CDCl₃)





12 ¹³C NMR (126 MHz, CDCl₃)





13 ¹H NMR (500 MHz, CDCl₃)





13¹⁹F NMR (471 MHz, CDCl₃)





14 ¹³C NMR (126 MHz, CDCl₃)





15 ¹H NMR (500 MHz, CDCl₃)





15¹⁹F NMR (471 MHz, CDCl₃)





16¹³C NMR (126 MHz, CDCl₃)





17 ¹H NMR (500 MHz, CDCl₃)





17¹⁹F NMR (471 MHz, CDCl₃)





18 ¹³C NMR (126 MHz, CDCl₃)





19 ¹H NMR (500 MHz, CDCl₃)





19¹⁹F NMR (471 MHz, CDCl₃)





20 ¹³C NMR (126 MHz, CDCl₃)









21 ¹⁹F NMR (471 MHz, CDCl₃)





22 ¹³C NMR (126 MHz, CDCl₃)









23 ¹⁹F NMR (471 MHz, CDCl₃)





24 ¹³C NMR (126 MHz, CDCl₃)





25 ¹H NMR (500 MHz, CDCl₃)





25¹⁹F NMR (471 MHz, CDCl₃)





26¹³C NMR (126 MHz, CDCl₃)





27 ¹H NMR (500 MHz, CDCl₃)





27¹⁹F NMR (471 MHz, CDCl₃)




28 ¹³C NMR (126 MHz, CDCl₃)





29 ¹H NMR (500 MHz, CDCl₃)









30 ¹³C NMR (126 MHz, CDCl₃)





31 ¹H NMR (500 MHz, CDCl₃)





31 ¹⁹F NMR (471 MHz, CDCl₃)









33 ¹H NMR (500 MHz, CDCl₃)





33 ¹⁹F NMR (471 MHz, CDCl₃)





34 ¹³C NMR (126 MHz, CDCl₃)























-2.66

8.07 68.07 7.73 7.71 7.71 7.71 7.71 7.71 7.69 7.69

36 ¹³C NMR (126 MHz, CDCl₃)













































40 ¹³C NMR (126 MHz, CDCl₃)







26 26 26 26 26 26 26 26 26 26 26 26 26 2	68	56
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43 ¹H NMR (500 MHz, CDCl₃)









44 ¹³C NMR (126 MHz, CDCl₃)





45 ¹H NMR (500 MHz, CDCl₃)





46 ¹H NMR (500 MHz, CDCl₃)





47 ¹H NMR (500 MHz, CDCl₃)





47¹⁹F NMR (471 MHz, CDCl₃)





48 ¹³C NMR (126 MHz, CDCl₃)





49¹³C NMR (126 MHz, CDCl₃)





50 ¹H NMR (500 MHz, CDCl₃)





50¹⁹F NMR (471 MHz, CDCl₃)





51 ¹³C NMR (126 MHz, CDCl₃)





52 ¹H NMR (500 MHz, CDCl₃)





52 ¹⁹F NMR (471 MHz, CDCl₃)




53 ¹³C NMR (126 MHz, CDCl₃)





54 ¹H NMR (500 MHz, CDCl₃)





54 ¹⁹F NMR (471 MHz, CDCl₃)





55 ¹³C NMR (126 MHz, CDCl₃)





56 ¹H NMR (500 MHz, CDCl₃)





56 ¹⁹F NMR (471 MHz, CDCl₃)





57 ¹³C NMR (126 MHz, CDCl₃)









58 ¹⁹F NMR (471 MHz, CDCl₃)





59 ¹³C NMR (126 MHz, CDCl₃)









60¹⁹F NMR (471 MHz, CDCl₃)





61 ¹³C NMR (126 MHz, CDCl₃)





62 ¹H NMR (500 MHz, CDCl₃)





62 ¹⁹F NMR (471 MHz, CDCl₃)





63 ¹³C NMR (126 MHz, CDCl₃)









65 ¹H NMR (500 MHz, CDCl₃)





66 ¹H NMR (500 MHz, CDCl₃)





67 ¹H NMR (500 MHz, CDCl₃)















70 ¹H NMR (500 MHz, CDCl₃)





71 ¹H NMR (500 MHz, CDCl₃)





72 ¹H NMR (500 MHz, CDCl₃)





74 ¹H NMR (500 MHz, CDCl₃)









76 ¹H NMR (500 MHz, CDCl₃)









78 ¹H NMR (500 MHz, CDCl₃)





79 ¹H NMR (500 MHz, CDCl₃)





79¹⁹F NMR (471 MHz, CDCl₃)





80 ¹³C NMR (126 MHz, CDCl₃)









81 ¹⁹F NMR (471 MHz, CDCl₃)





82 ¹³C NMR (126 MHz, CDCl₃)








84 ¹H NMR (500 MHz, CDCl₃)





85 ¹H NMR (500 MHz, CDCl₃)













88 ¹H NMR (500 MHz, CDCl₃)





88 ¹⁹F NMR (471 MHz, CDCl₃)

