

Supplementary Information

5-Phenoxy primaquine analogs and the tetraoxane hybrid as anti-malarial agents

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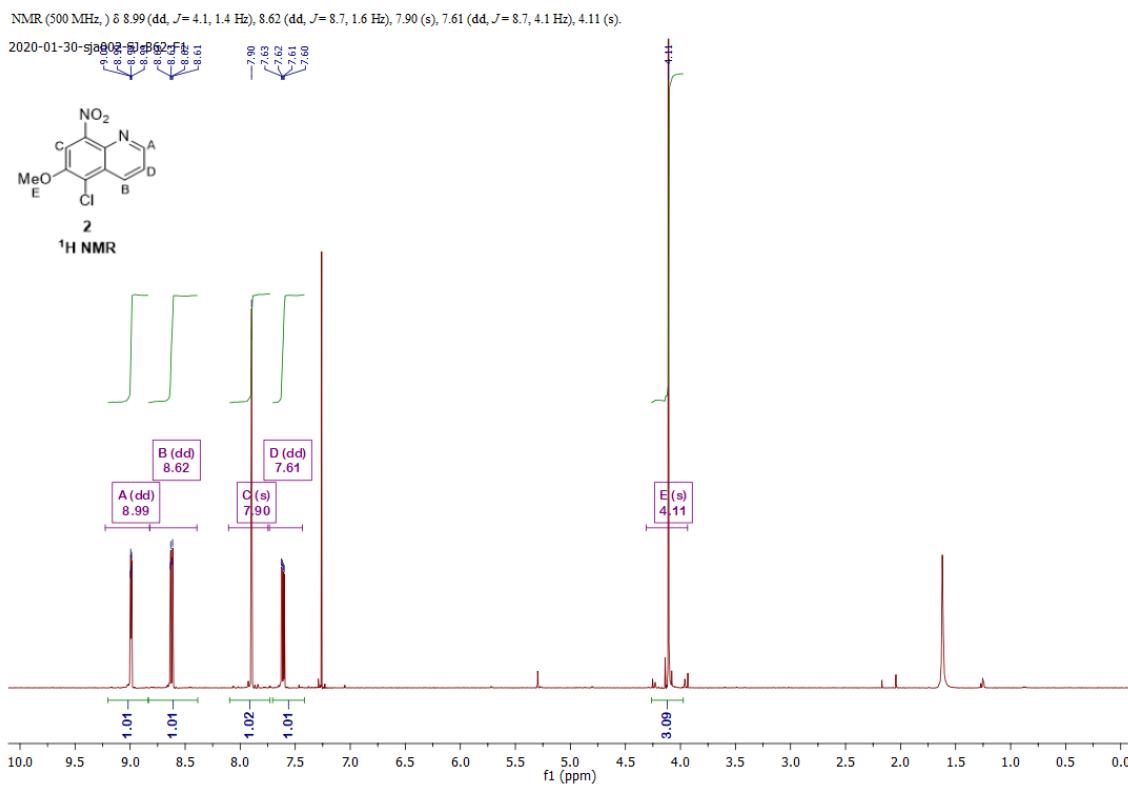
² *National Center for Genetic Engineering and Biotechnology (BIOTEC), Pathum Thani 12120, Thailand*

**Corresponding author*

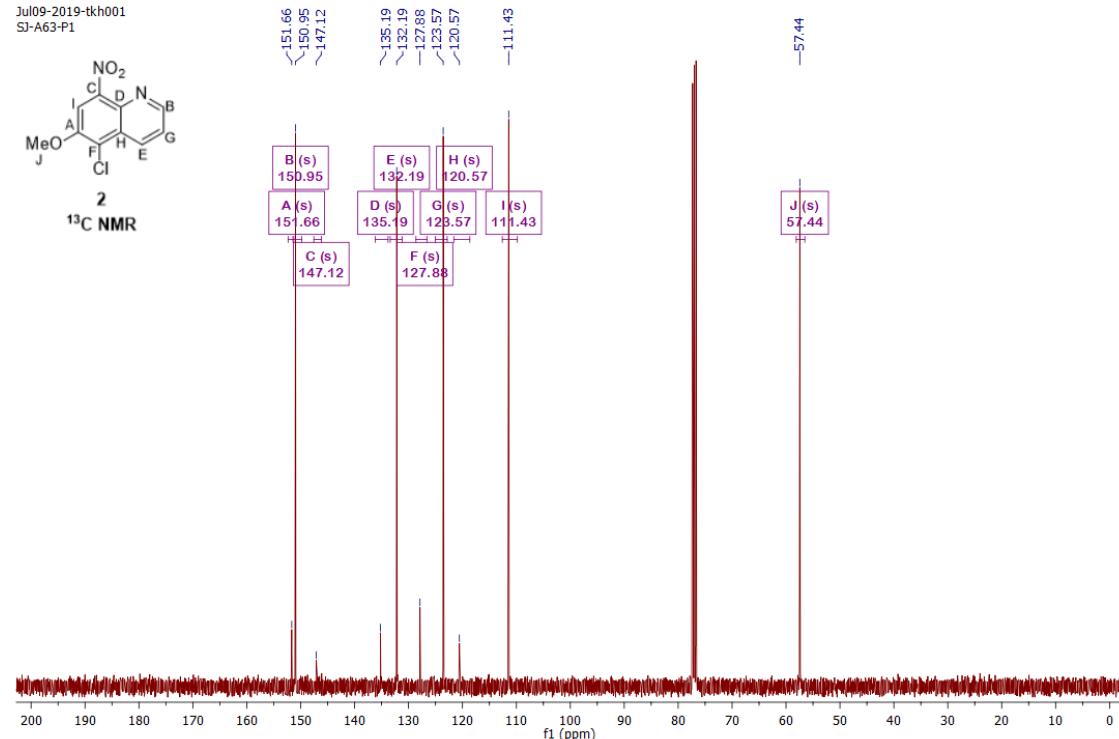
†These authors contributed equally to this work.

NMR and HRMS spectra

5-Chloro-6-methoxy-8-nitroquinoline (2)



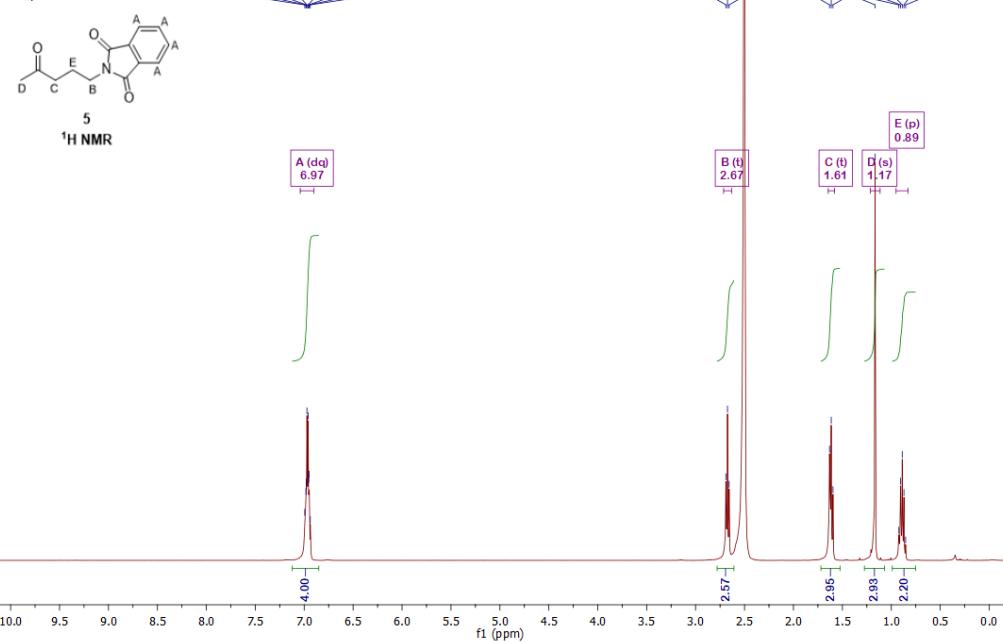
^{13}C NMR (101 MHz, CDCl₃) δ 151.66 (s), 150.95 (s), 147.12 (s), 135.19 (s), 132.19 (s), 127.88 (s), 123.57 (s), 120.57 (s), 111.43 (s), 57.44 (s).



2-(4-Oxopentyl)isoindoline-1,3-dione (5)

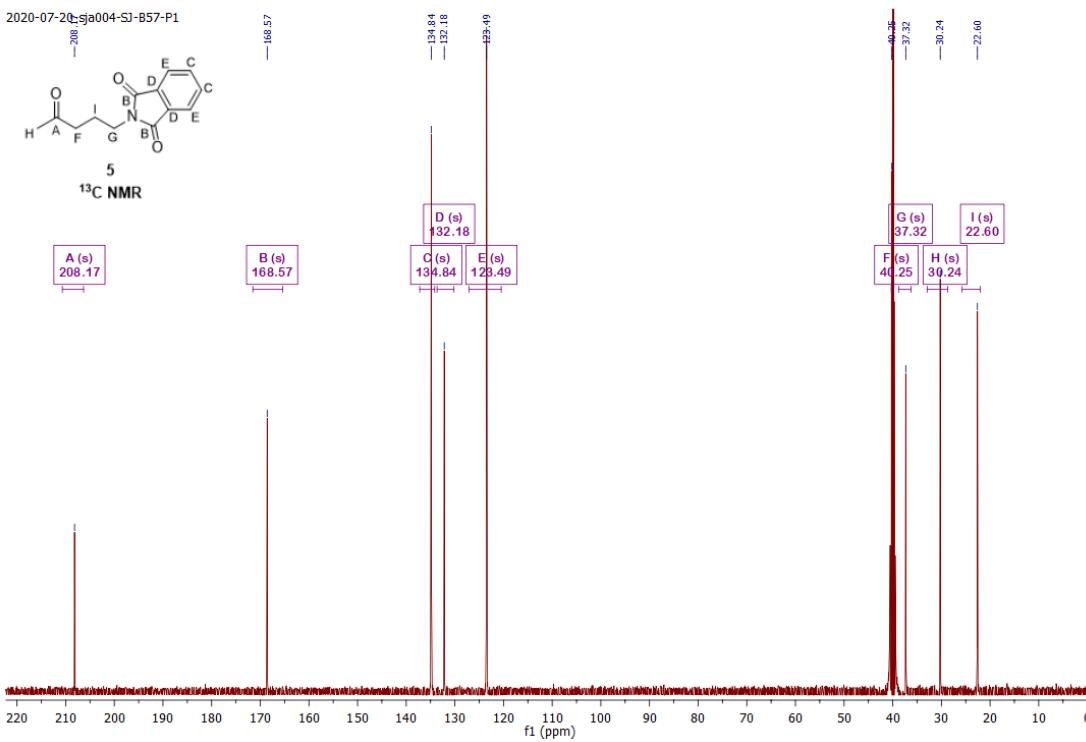
¹H NMR (400 MHz, DMSO) δ 6.97 (dq, *J* = 6.2, 4.8 Hz, 1H), 2.67 (t, *J* = 6.8 Hz, 1H), 1.61 (t, *J* = 7.1 Hz, 1H), 1.17 (s, 1H), 0.89 (p, *J* = 6.9 Hz, 1H).

Jun06-2019-thk001
chula_proton 1H



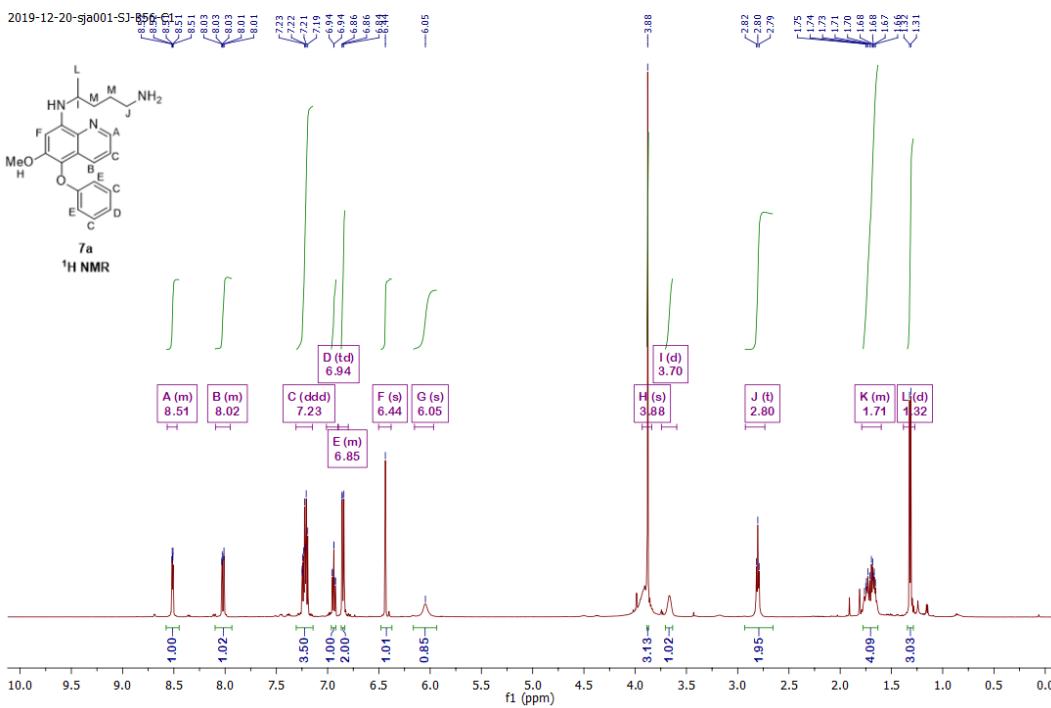
NMR (126 MHz,) δ 208.17 (s), 168.57 (s), 134.84 (s), 132.18 (s), 123.49 (s), 40.25 (s), 37.32 (s), 30.24 (s), 22.60 (s).

2020-7-20:sja004-SJ-B57-P1

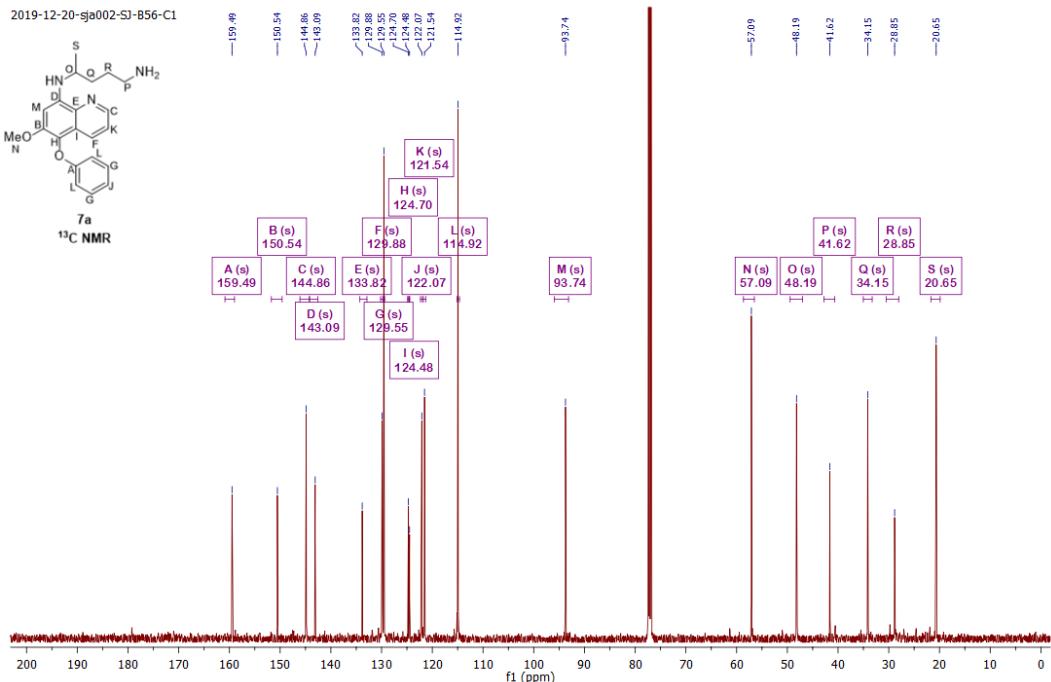


***N*⁴-(6-Methoxy-5-phenoxyquinolin-8-yl)pentane-1,4-diamine (7a)**

NMR (500 MHz, CDCl_3) δ 8.56 – 8.47 (m), 8.09 – 7.95 (m), 7.23 (ddd, $J = 15.7, 7.2, 3.9$ Hz), 6.94 (td, $J = 7.4, 0.7$ Hz), 6.89 – 6.80 (m), 6.44 (s), 6.05 (s), 3.88 (s), 2.80 (t, $J = 6.7$ Hz), 1.79 – 1.60 (m), 1.32 (d, $J = 6.3$ Hz).



NMR (126 MHz, CDCl_3) δ 159.49 (s), 150.54 (s), 144.86 (s), 143.09 (s), 133.82 (s), 129.88 (s), 129.55 (s), 124.70 (s), 124.48 (s), 122.07 (s), 121.54 (s), 114.92 (s), 93.74 (s), 57.09 (s), 48.19 (s), 41.62 (s), 34.15 (s), 28.85 (s), 20.65 (s).



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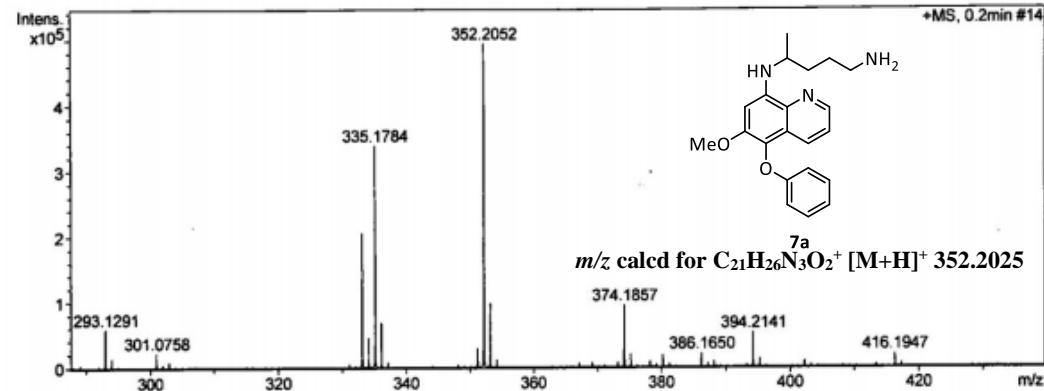
High resolution report

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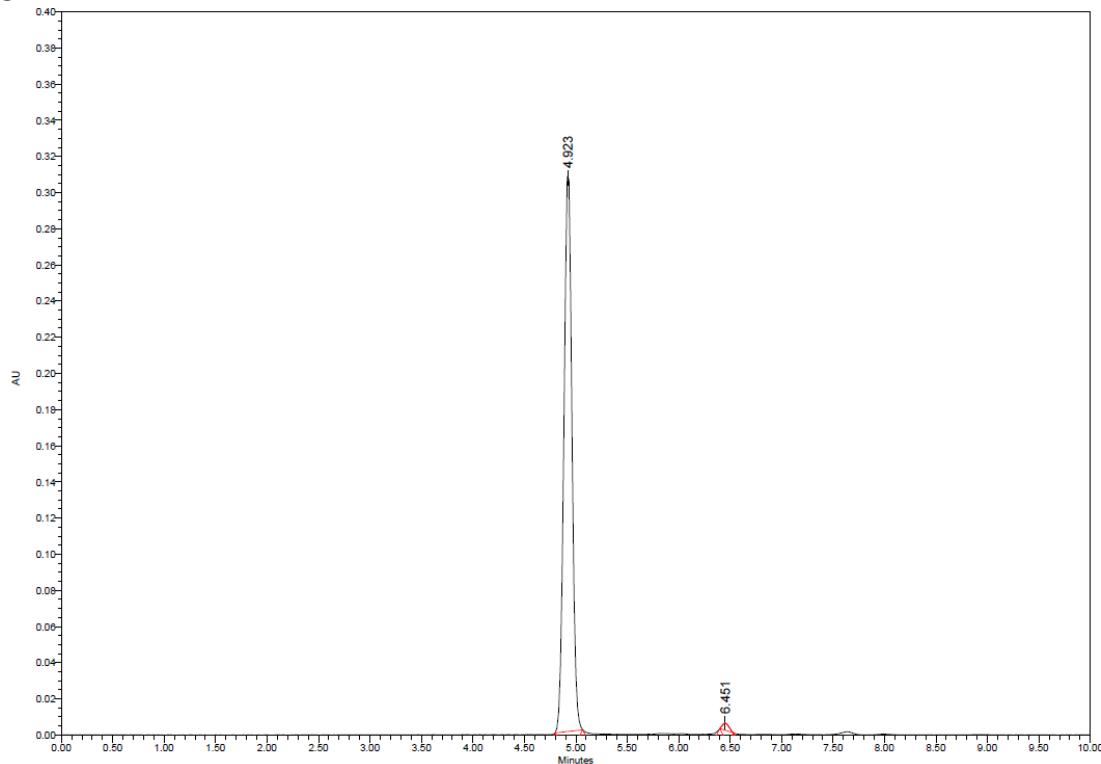
Calibrate by Sodium Formate

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
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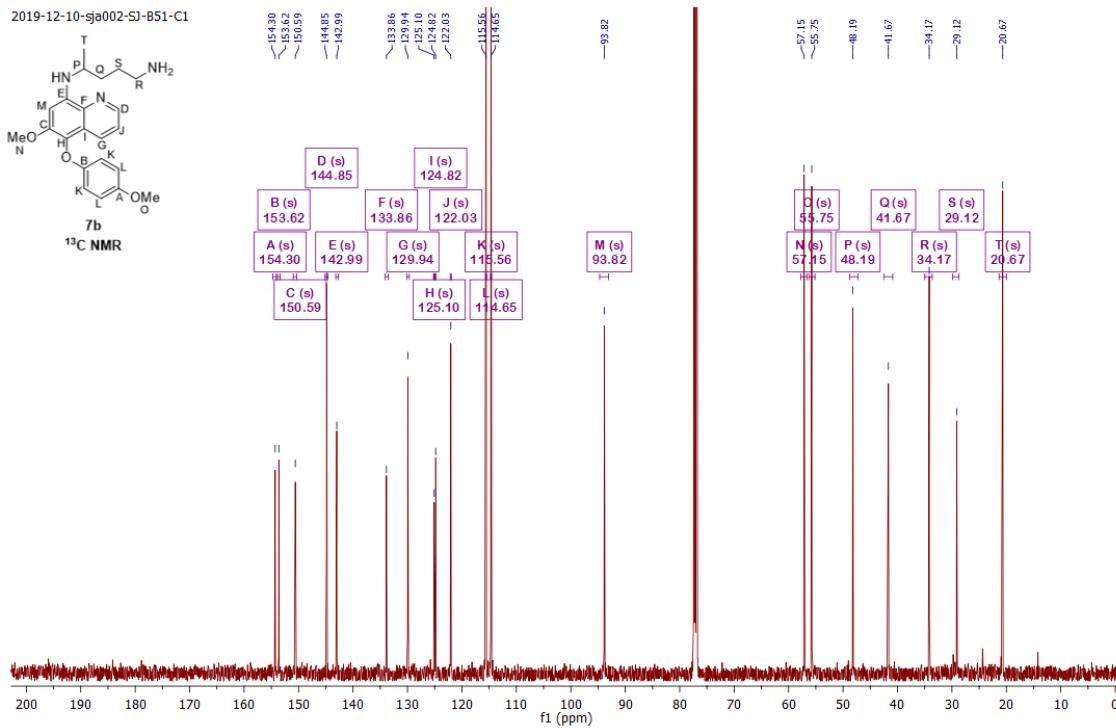
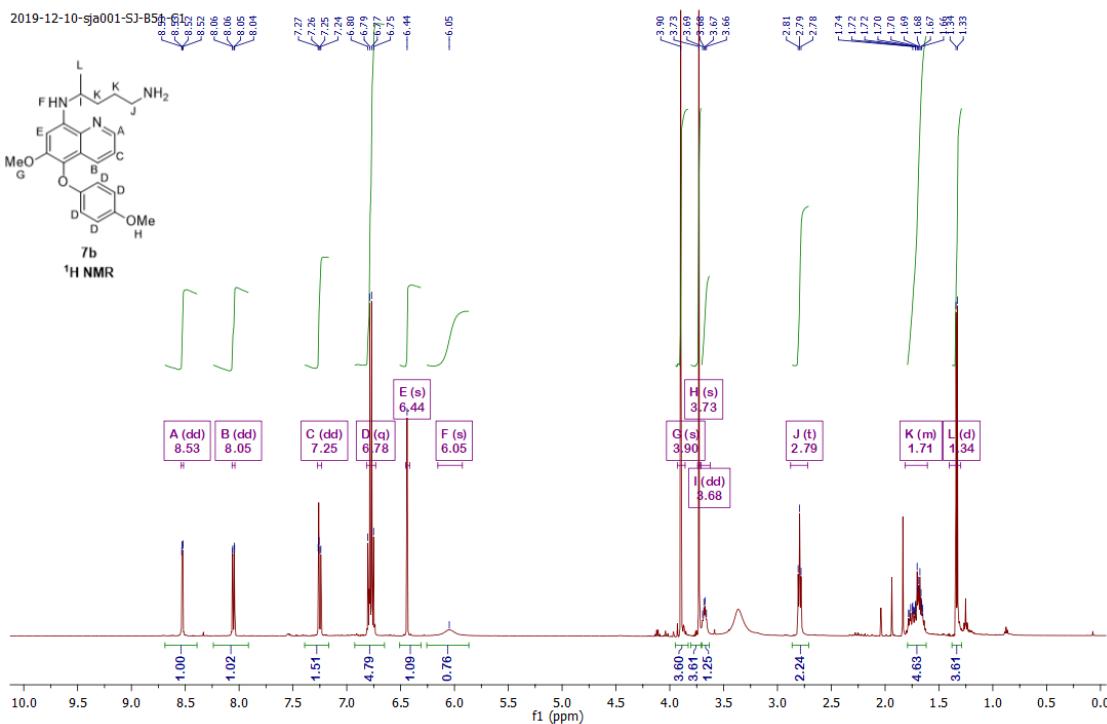


HPLC



N⁴-(6-Methoxy-5-(4-methoxyphenoxy)quinolin-8-yl)pentane-1,4-diamine (7b)

NMR (500 MHz, δ) 8.53 (dd, $J = 4.1, 1.6$ Hz), 8.05 (dd, $J = 8.4, 1.5$ Hz), 7.25 (dd, $J = 8.5, 4.1$ Hz), 6.78 (q, $J = 9.3$ Hz), 6.44 (s), 6.05 (s), 3.90 (s), 3.73 (s), 3.68 (dd, $J = 11.9, 5.9$ Hz), 2.79 (t, $J = 6.8$ Hz), 1.82 – 1.61 (m), 1.34 (d, $J = 6.3$ Hz).



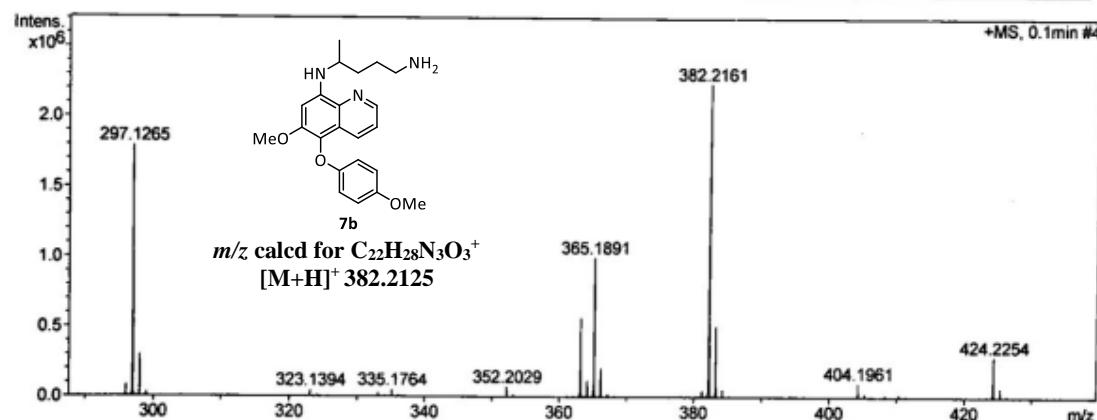
BIORESOURCES RESEARCH UNIT

High resolution report

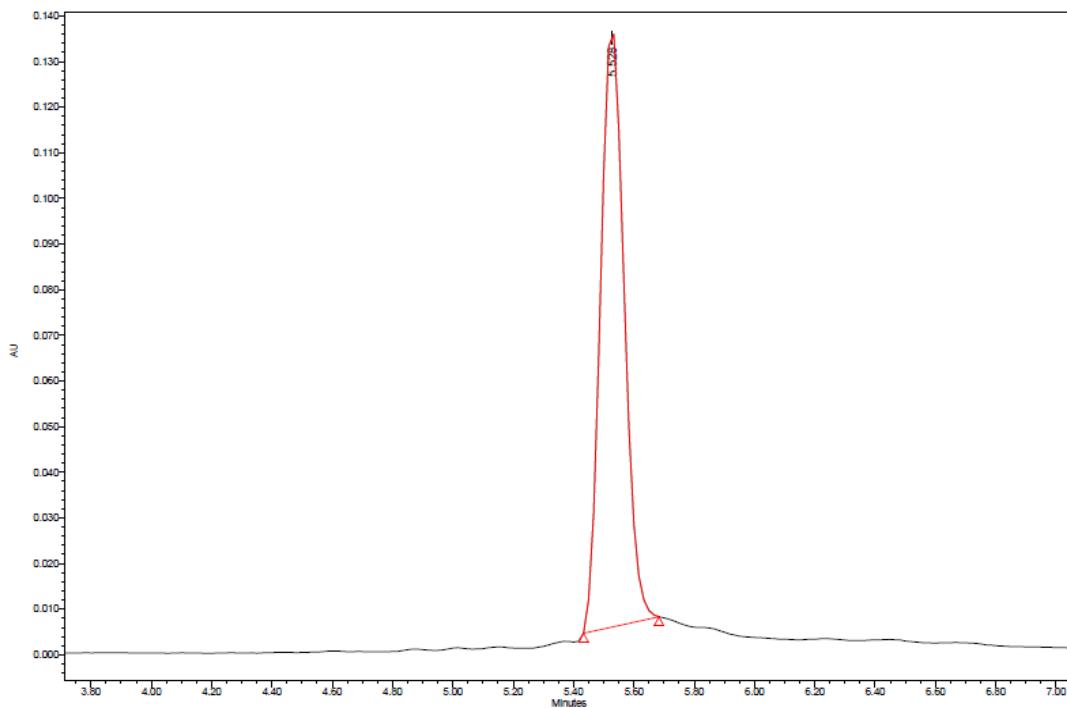
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		Calibrate by	Sodium Formate

Acquisition Parameter

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Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



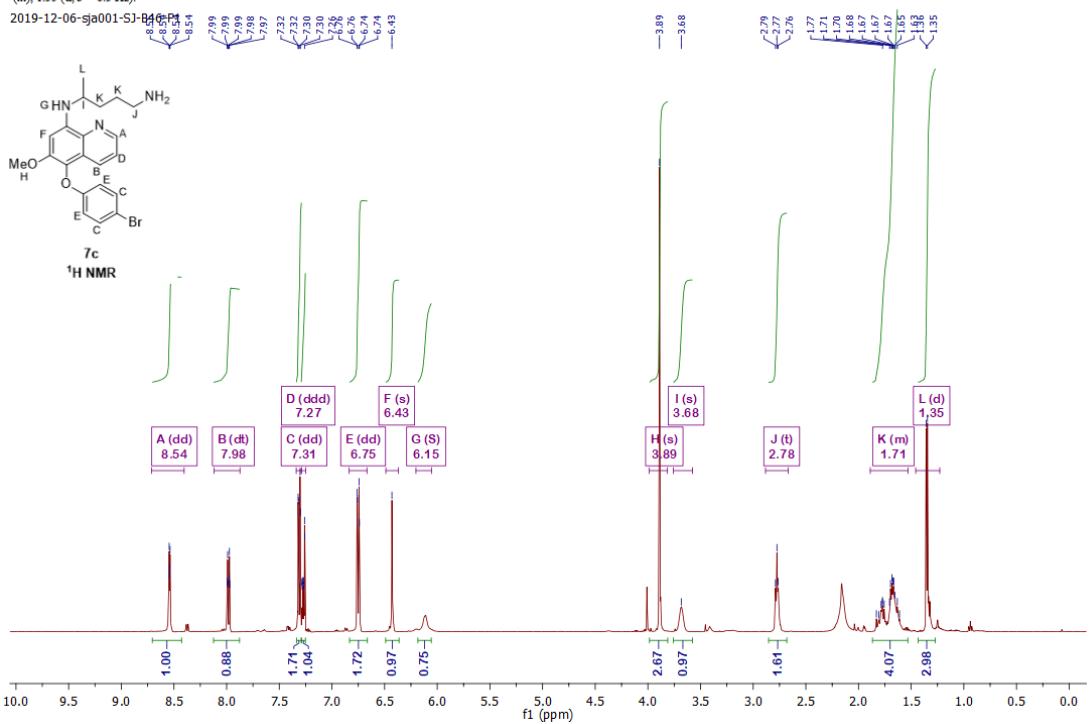
HPLC



N⁴-(5-(4-Bromophenoxy)-6-methoxyquinolin-8-yl)pentane-1,4-diamine (7c)

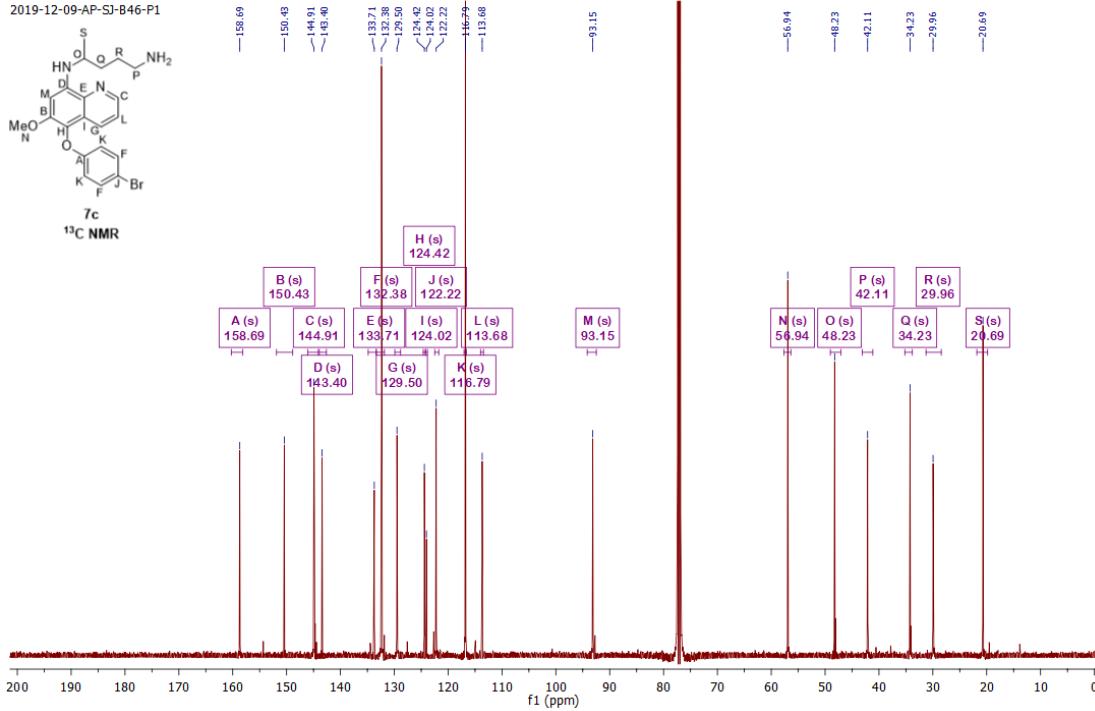
NMR (500 MHz, δ) 8.54 (dd, $J=2.7, 1.5$ Hz), 7.98 (dt, $J=8.5, 1.5$ Hz), 7.31 (dd, $J=9.1, 1.4$ Hz), 7.27 (ddd, $J=8.5, 4.2, 1.4$ Hz), 6.75 (dd, $J=9.1, 1.4$ Hz), 6.43 (s), 3.89 (s), 3.68 (s), 2.78 (t, $J=6.4$ Hz), 1.89 – 1.53 (m), 1.35 (d, $J=6.3$ Hz).

2019-12-06-sja001-SJ-B46-P1



NMR (126 MHz, δ) 8 158.69 (s), 150.43 (s), 144.91 (s), 143.40 (s), 133.71 (s), 132.38 (s), 129.50 (s), 124.42 (s), 124.02 (s), 122.22 (s), 116.79 (s), 113.68 (s), 93.15 (s), 56.94 (s), 48.23 (s), 42.11 (s), 34.23 (s), 29.96 (s), 20.69 (s).

2019-12-09-AP-SJ-B46-P1



BIORESOURCES RESEARCH UNIT

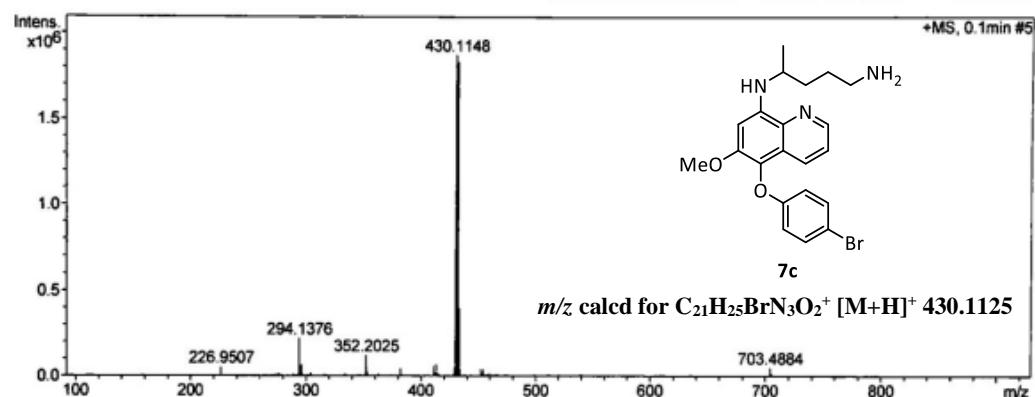
High resolution report

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 Sample Name SJ B56 P1 Br

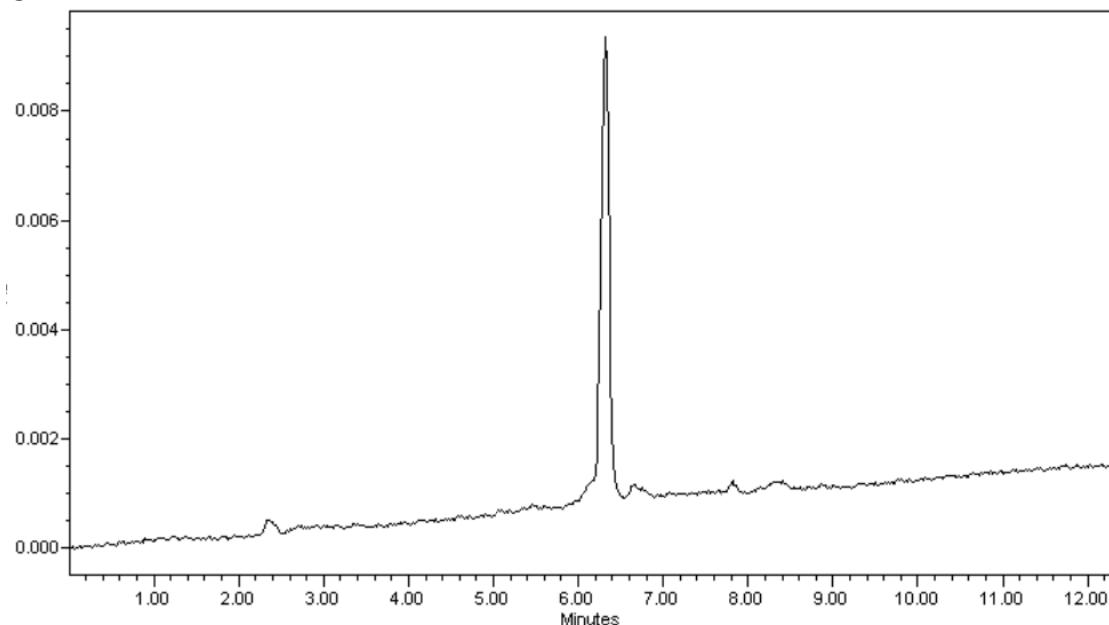
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 Operator Sutchai
 Instrument micrOTOF Ext: 3560
 Calibrate by Sodium Formate

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

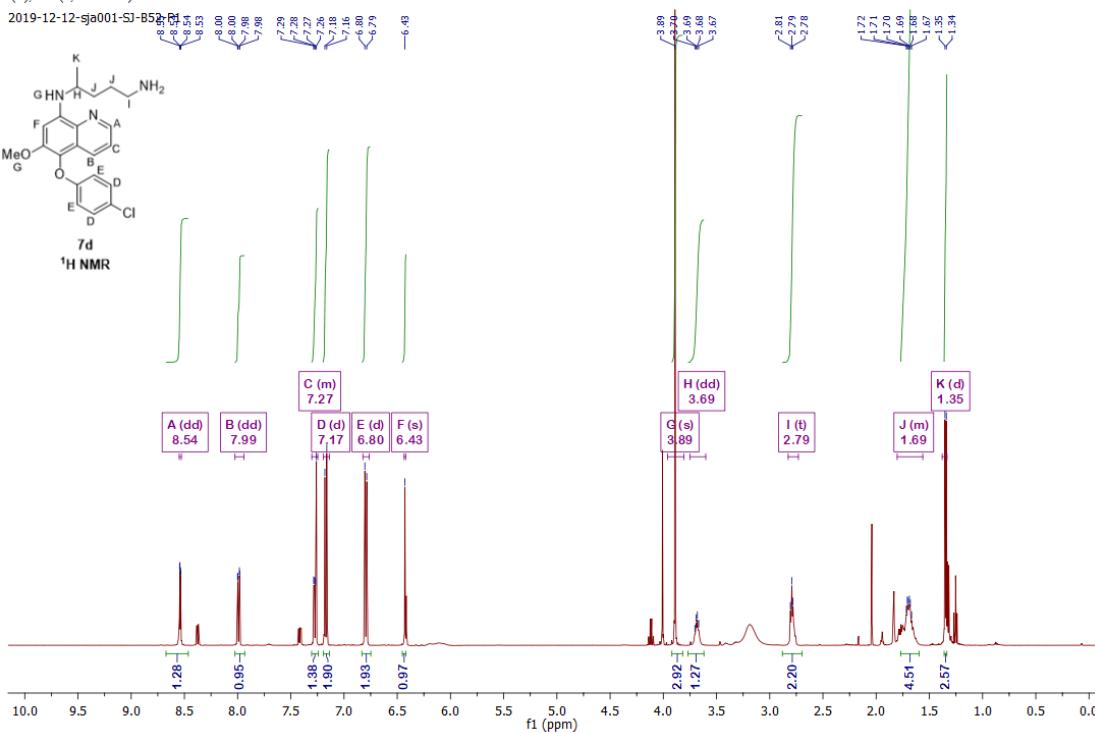


HPLC

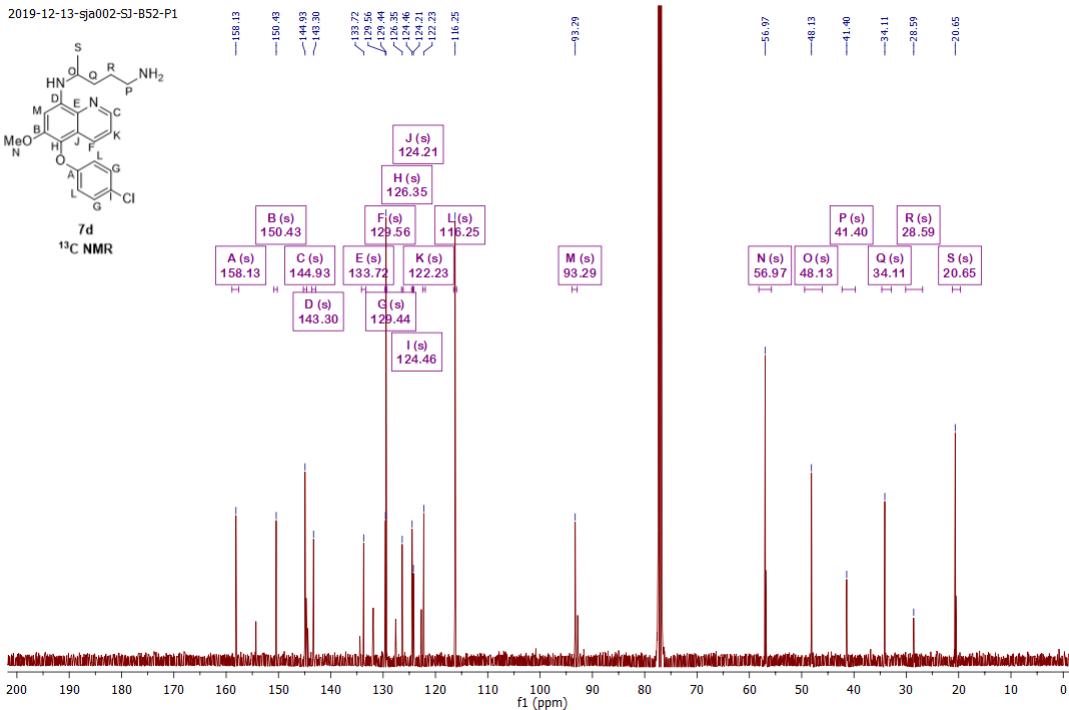


N⁴-(6-Methoxy-5-(4-chlorophenoxy)quinolin-8-yl)pentane-1,4-diamine (7d)

NMR (500 MHz, δ) 8.54 (dd, $J = 4.2, 1.6$ Hz), 7.99 (dd, $J = 8.5, 1.6$ Hz), 7.30 – 7.25 (m), 7.17 (d, $J = 9.0$ Hz), 6.80 (d, $J = 9.0$ Hz), 6.43 (s), 3.89 (s), 3.69 (dd, $J = 11.8, 5.8$ Hz), 2.79 (t, $J = 6.1$ Hz), 1.80 – 1.56 (m), 1.35 (d, $J = 6.3$ Hz).



NMR (126 MHz, δ) 158.13 (s), 150.43 (s), 144.93 (s), 143.30 (s), 133.72 (s), 129.56 (s), 129.44 (s), 126.35 (s), 124.46 (s), 124.21 (s), 122.23 (s), 116.25 (s), 93.29 (s), 56.97 (s), 48.13 (s), 48.13 (s), 41.40 (s), 34.11 (s), 34.11 (s), 20.65 (s).



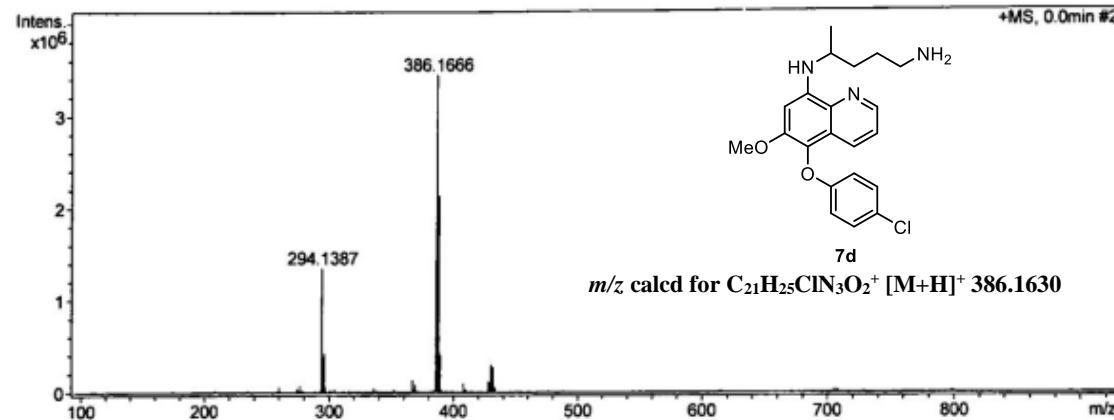
BIORESOURCES RESEARCH UNIT

High resolution report

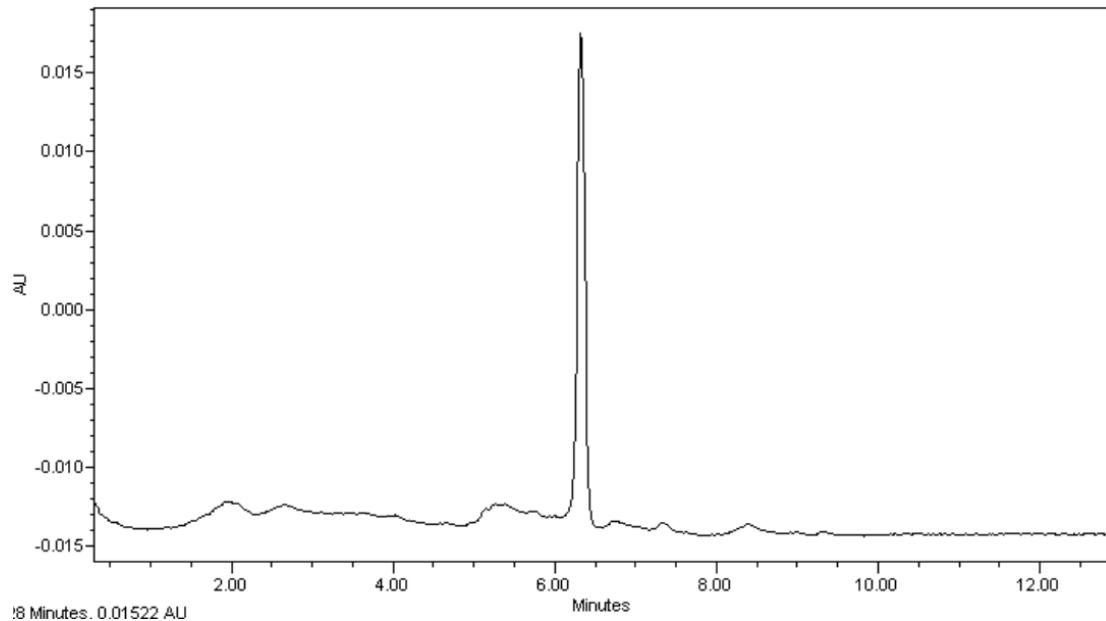
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			Sodium Formate

Acquisition Parameter

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Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

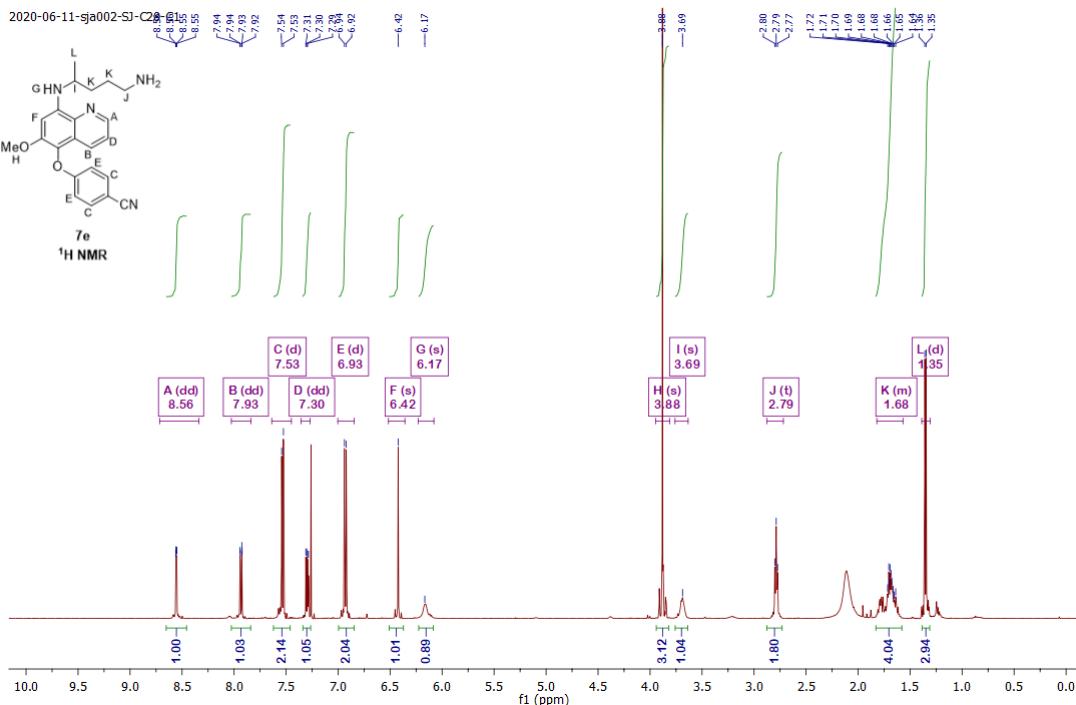


HPLC

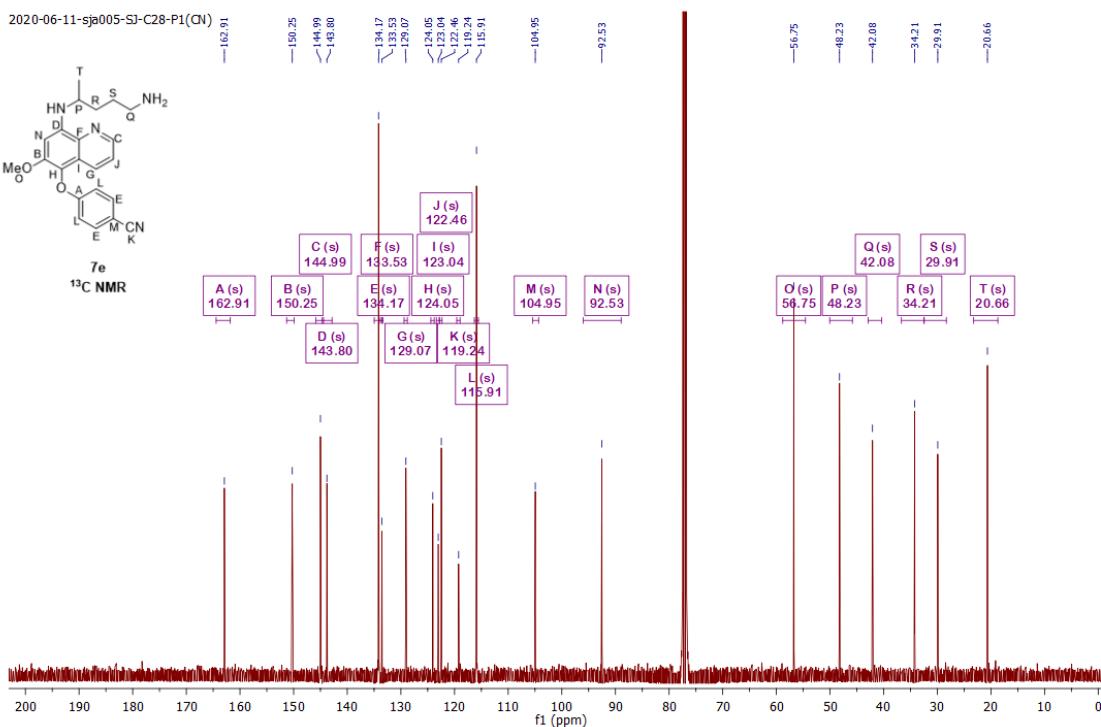


4-((8-((5-Aminopentan-2-yl)amino)-6-methoxyquinolin-5-yl)oxy)benzonitrile (7e)

NMR (500 MHz , CDCl_3) δ 8.56 (dd, $J = 4.2, 1.4 \text{ Hz}$), 7.93 (dd, $J = 8.5, 1.5 \text{ Hz}$), 7.53 (d, $J = 8.7 \text{ Hz}$), 7.30 (dd, $J = 8.5, 4.1 \text{ Hz}$), 6.93 (d, $J = 8.7 \text{ Hz}$), 6.42 (s), 6.17 (s), 3.88 (s), 3.69 (s), 2.79 (t, $J = 6.8 \text{ Hz}$), 1.82 – 1.57 (m), 1.35 (d, $J = 6.3 \text{ Hz}$).



NMR (126 MHz , CDCl_3) δ 162.91 (s), 150.25 (s), 144.99 (s), 143.80 (s), 134.17 (s), 133.53 (s), 129.07 (s), 124.05 (s), 123.04 (s), 122.46 (s), 119.24 (s), 115.91 (s), 104.95 (s), 92.53 (s), 56.75 (s), 48.23 (s), 42.08 (s), 34.21 (s), 29.91 (s), 20.66 (s).



High resolution report

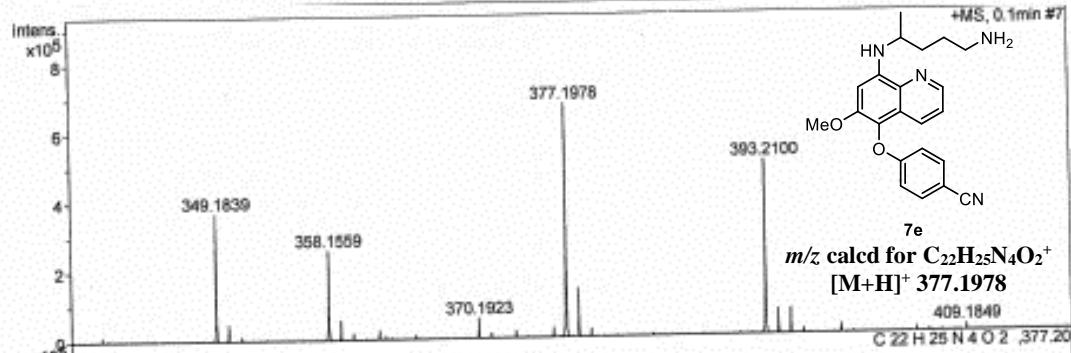
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 Method NaFormate_pos.m
 Sample Name SJ C 28 P1 N

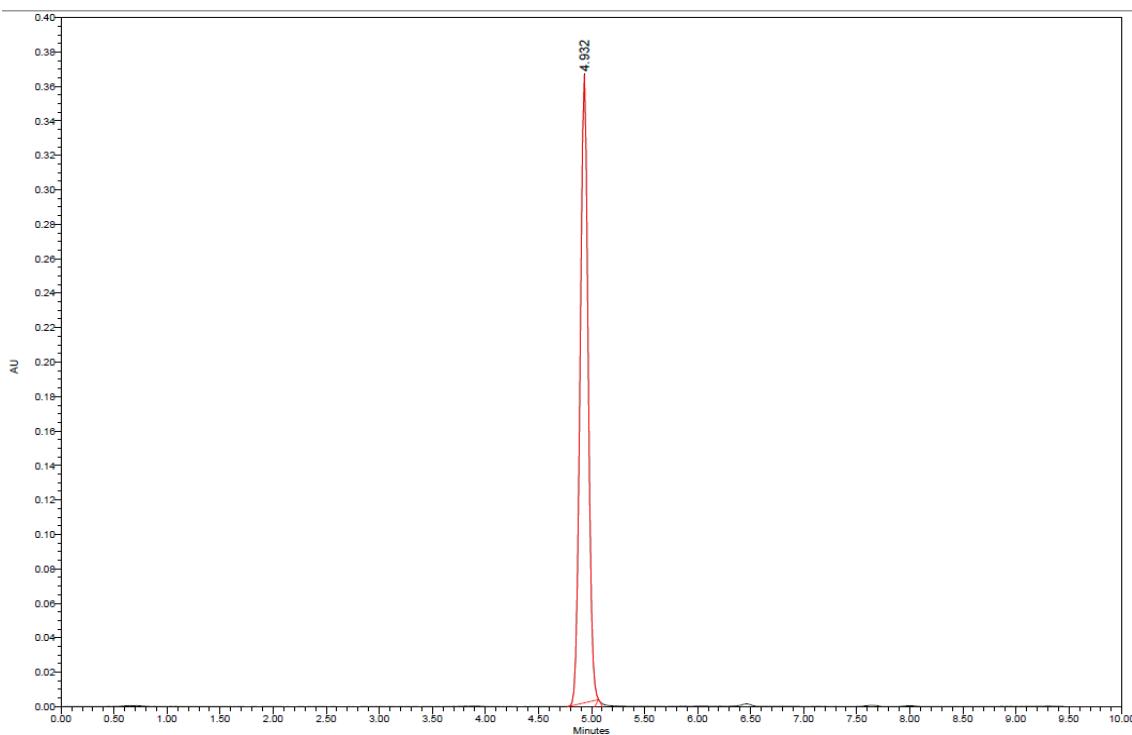
Operator Sutichai Ext: 3560
 Instrument micrOTOF Bruker
 Calibrate by Sodium Formate

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
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Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

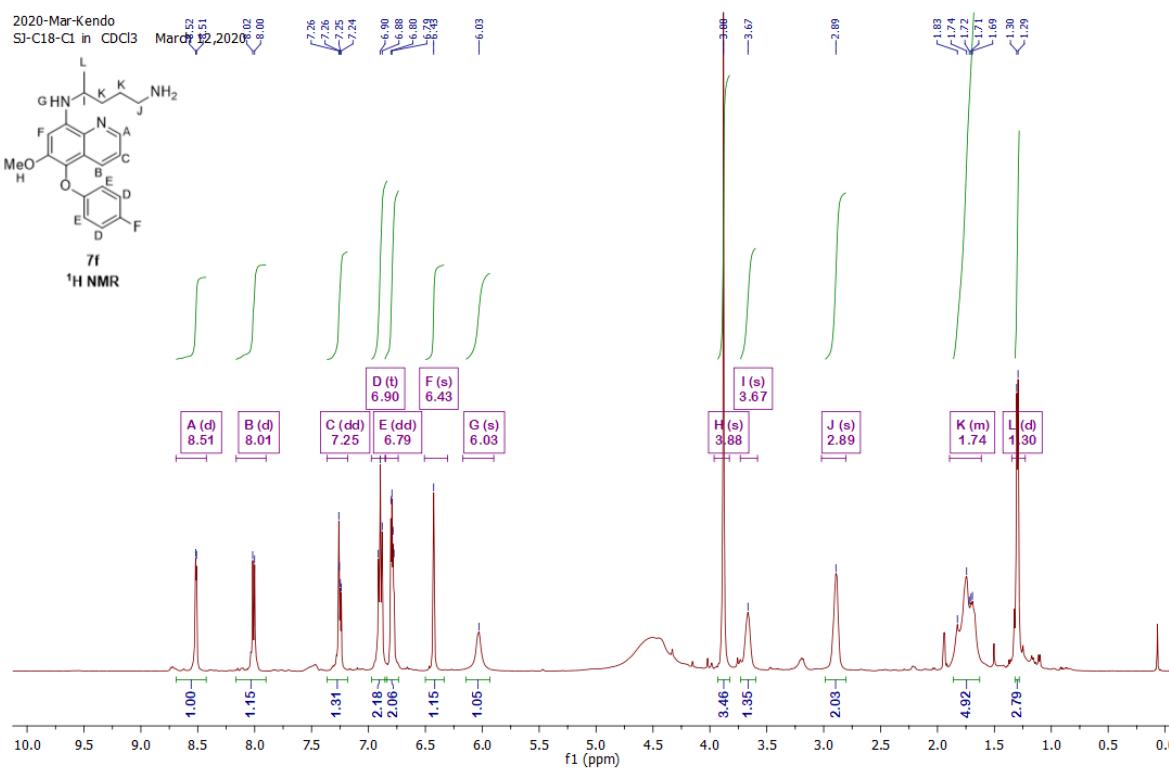


HPLC

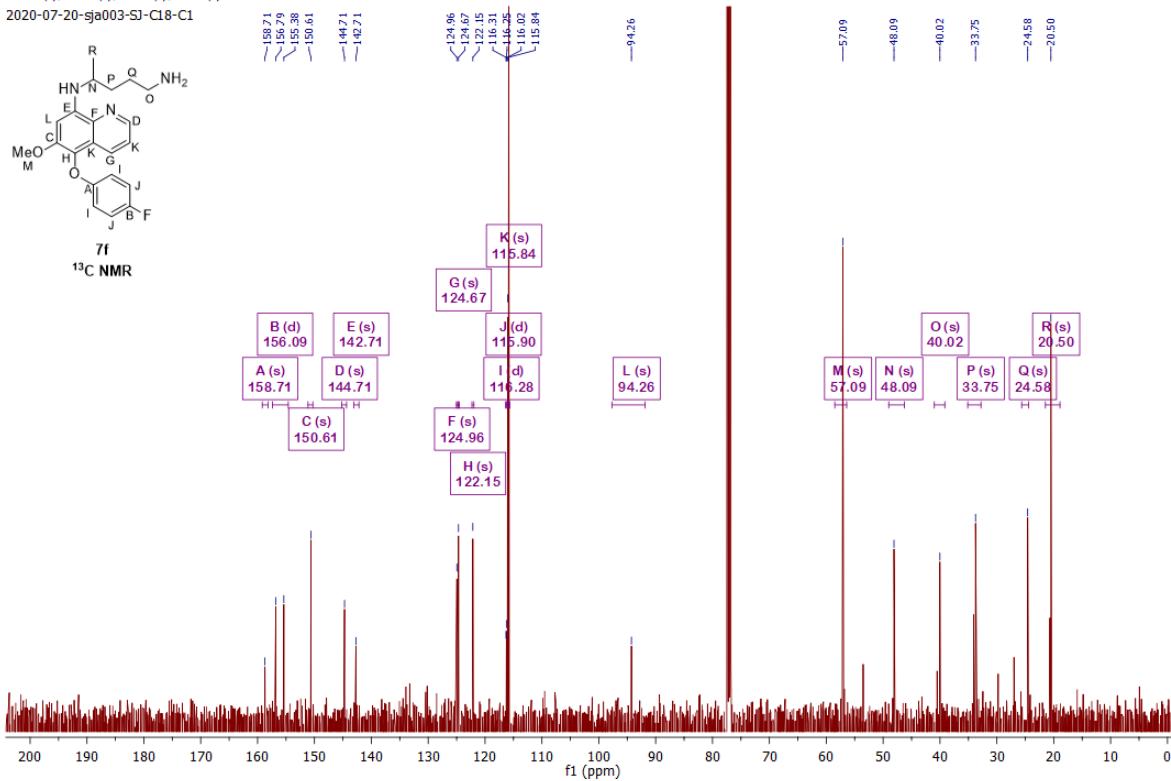


N⁴-(5-(4-Fluorophenoxy)-6-methoxyquinolin-8-yl)pentane-1,4-diamine (7f)

¹H NMR (500 MHz, CDCl₃) δ 8.51 (d, *J* = 4.0 Hz, 1H), 8.01 (d, *J* = 8.4 Hz, 1H), 7.25 (dd, *J* = 7.7, 3.2 Hz, 1H), 6.90 (t, *J* = 8.6 Hz, 2H), 6.79 (dd, *J* = 9.0, 4.2 Hz, 2H), 6.43 (s, 1H), 6.03 (s, 1H), 3.88 (s, 3H), 3.67 (s, 1H), 2.89 (s, 2H), 1.89 – 1.62 (m, 4H), 1.30 (d, *J* = 6.0 Hz, 3H).

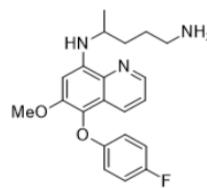


NMR (126 MHz) δ 158.71 (s), 156.09 (d, *J* = 177.0 Hz), 150.61 (s), 144.71 (s), 142.71 (s), 124.96 (s), 124.67 (s), 122.15 (s), 116.28 (d, *J* = 7.9 Hz), 115.90 (d, *J* = 31.5 Hz), 115.84 (s), 94.26 (s), 57.09 (s), 48.09 (s), 40.02 (s), 33.75 (s), 24.58 (s), 20.50 (s).

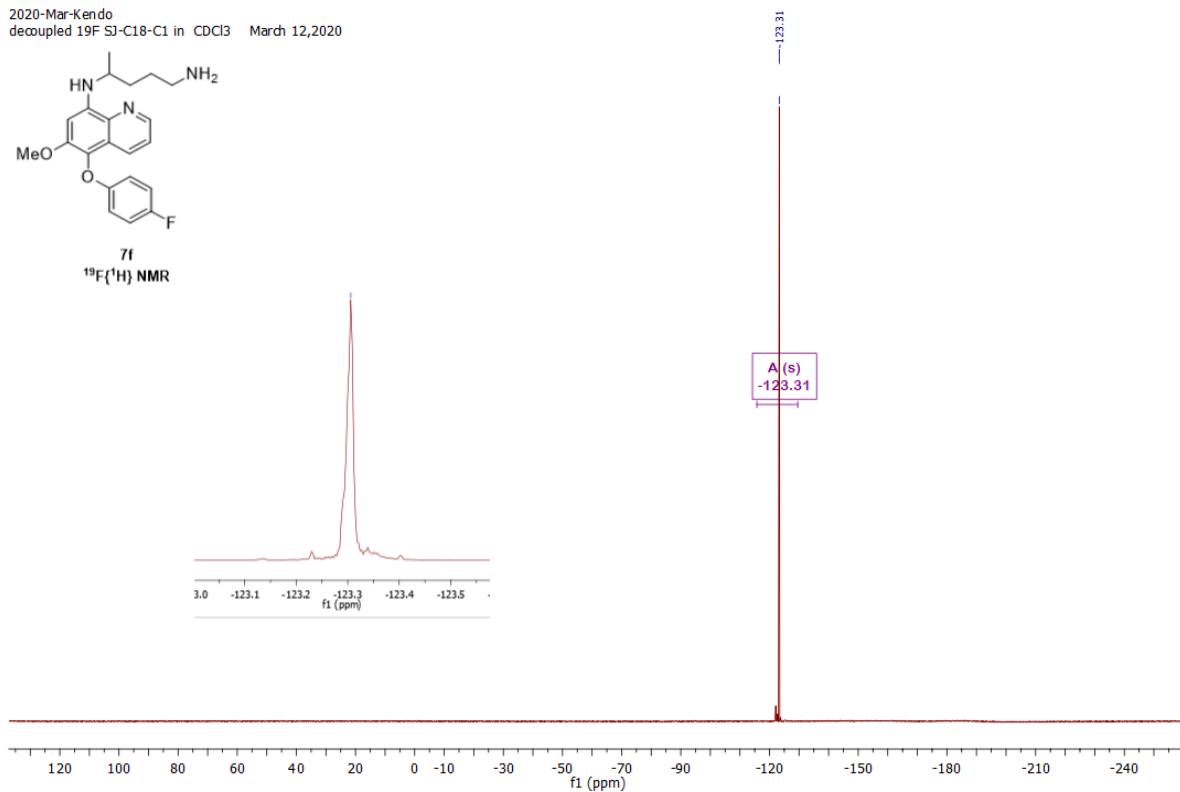


¹⁹F NMR (471 MHz, CDCl₃) δ -123.31 (s).

2020-Mar-Kendo
decoupled 19F SJ-C18-C1 in CDCl₃ March 12,2020



7f
¹⁹F(¹H) NMR



High resolution report

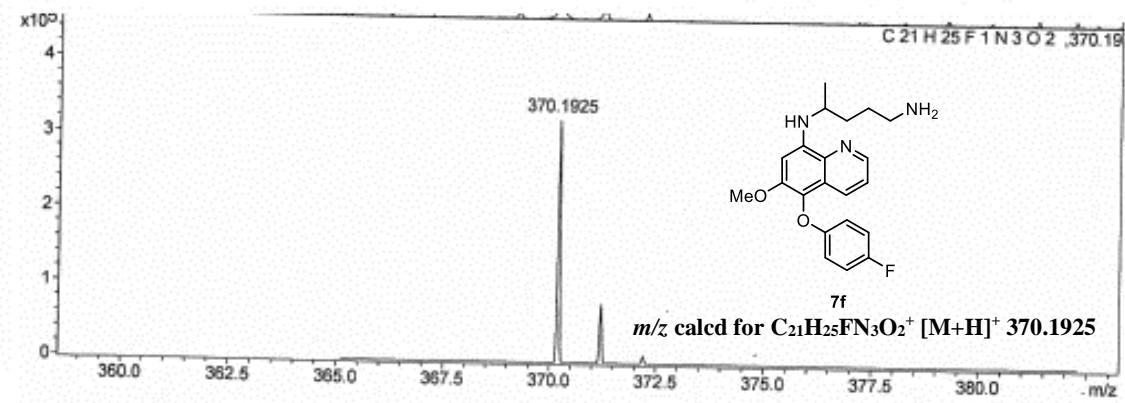
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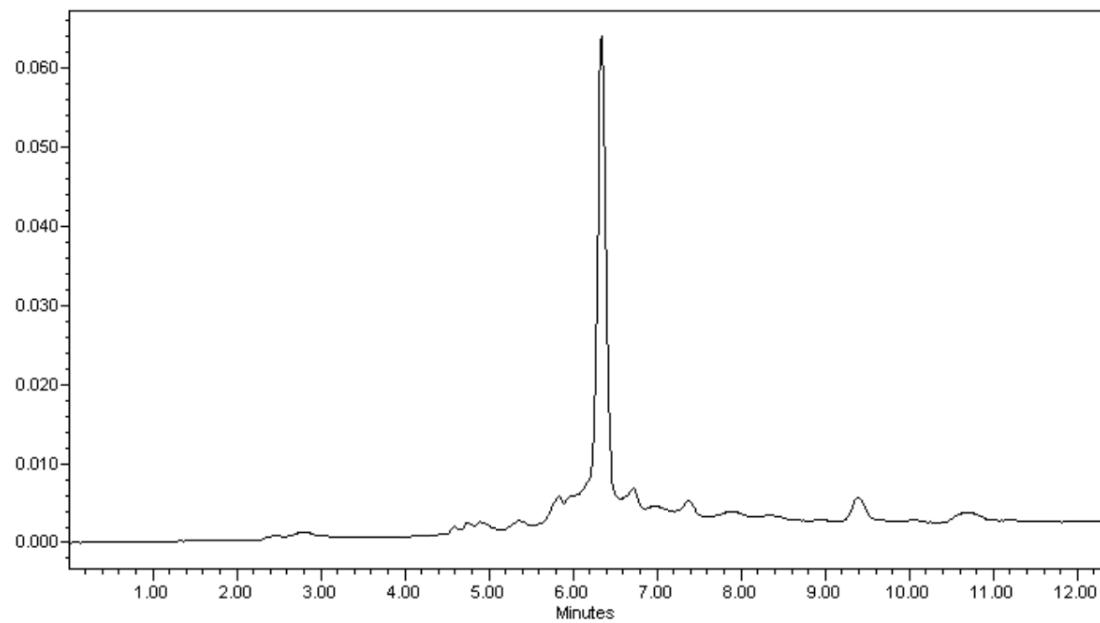
Operator Sutichai Ext: 3560
Instrument micrOTOF Bruker
Calibrate by Sodium Formate

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
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Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source

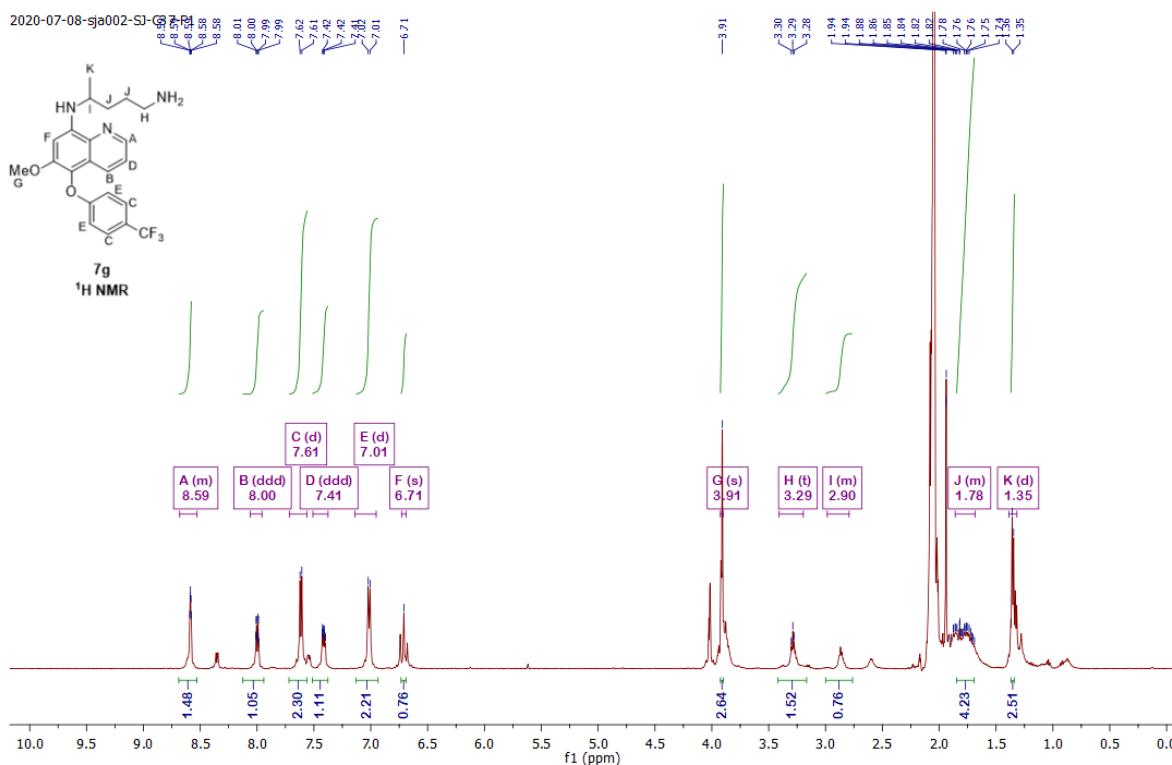


HPLC

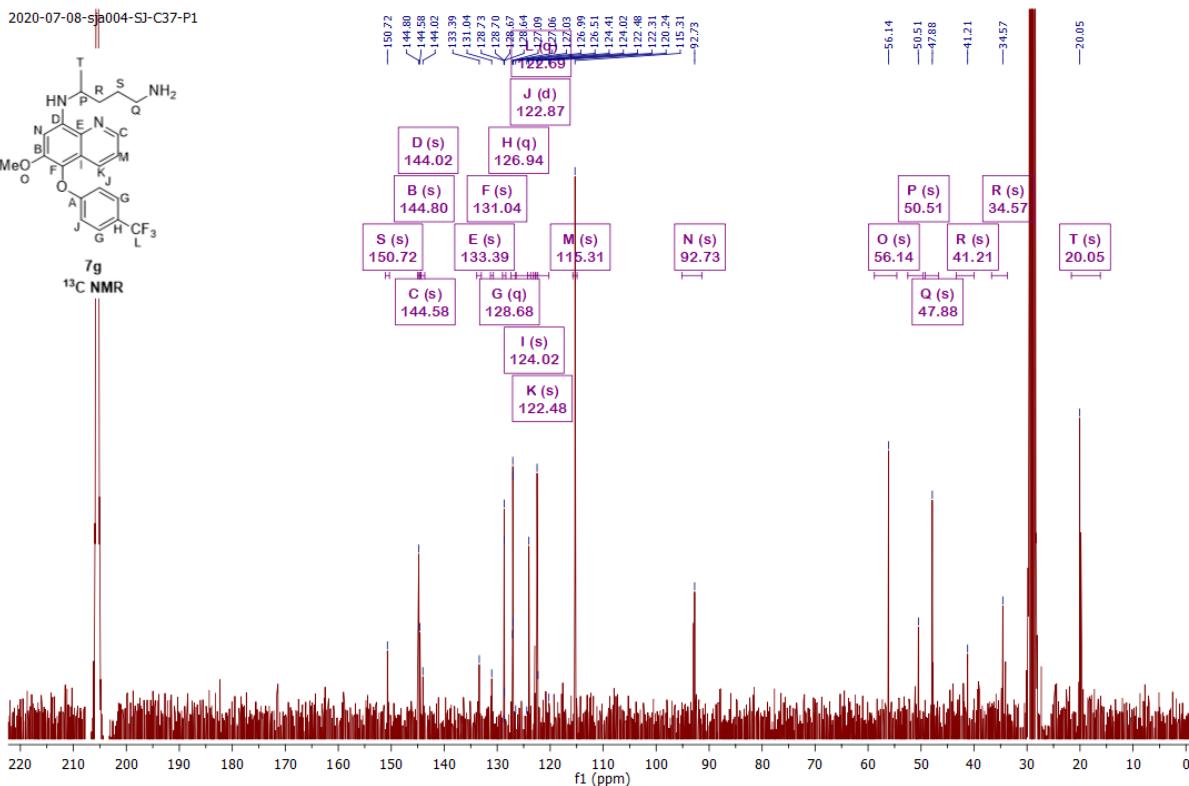


***N*⁴-(5-(4-Fluorophenoxy)-6-methoxyquinolin-8-yl)pentane-1,4-diamine (7g)**

NMR (500 MHz) δ 8.68 – 8.53 (m), 8.00 (ddd, $J = 8.5, 3.5, 1.7$ Hz), 7.61 (d, $J = 8.0$ Hz), 7.41 (ddd, $J = 8.3, 4.1, 1.5$ Hz), 7.01 (d, $J = 8.3$ Hz), 6.71 (dd, $J = 16.1, 14.9$ Hz), 3.91 (dd, $J = 4.4, 1.7$ Hz), 3.29(m), 1.94 (t, $J = 6.2$ Hz), 2.98 – 2.79 (m) 1.86 – 1.68 (m), 1.35 (d, $J = 6.3$ Hz).

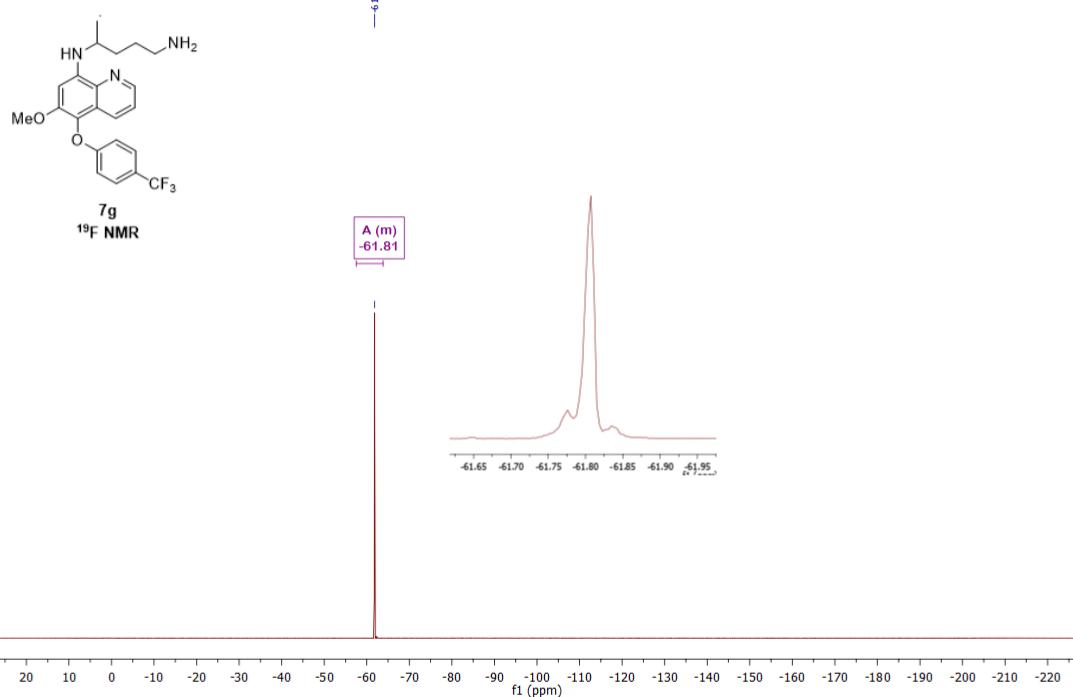


NMR (126 MHz) δ 150.72 (s), 144.80 (s), 144.58 (s), 144.02 (s), 133.39 (s), 131.04 (s), 128.68 (q, $J = 4.1$ Hz), 126.94 (q, $J = 65.1$ Hz), 124.02 (s), 122.87 (d, $J = 7.7$ Hz), 122.69 (q, $J = 265.0$ Hz), 122.48 (s), 115.31 (s), 92.73 (s), 56.14 (s), 50.51 (s), 47.88 (s), 41.21 (s), 34.57 (s), 20.05 (s).



NMR (471 MHz) δ -57.53 – -63.84 (m).

2020-07-08-sja002-SJ-C37-P1



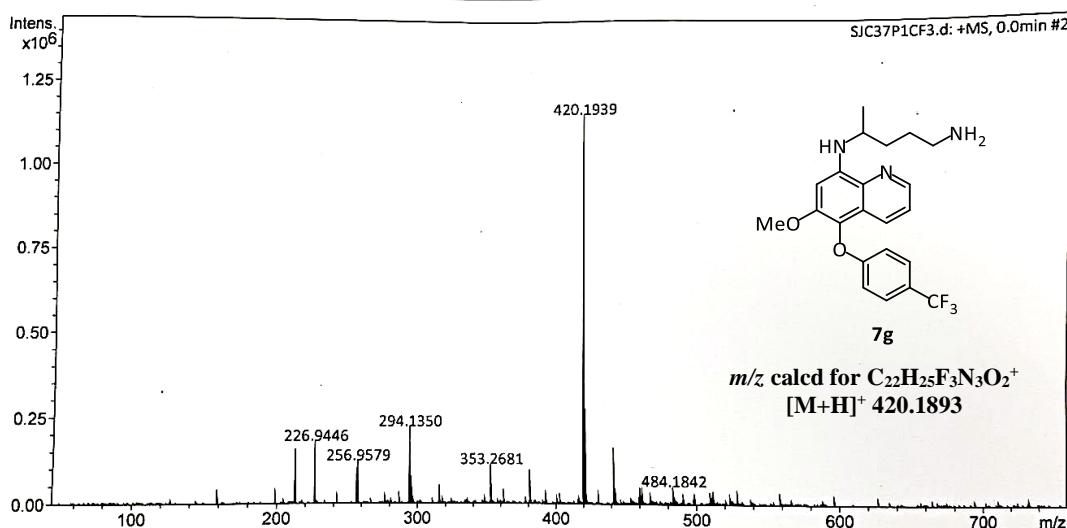
High resolution report

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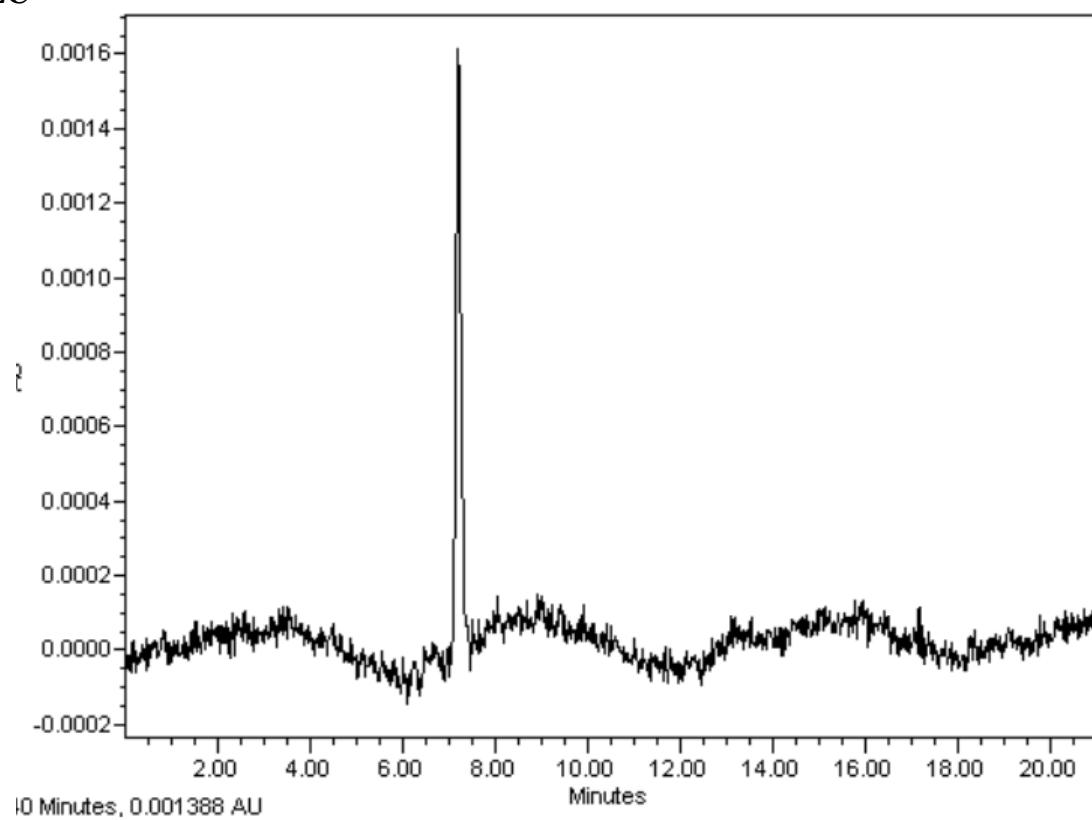
Acquisition Date 17/11/2563 13:24:20
Operator Sutichai
Instrument micrOTOF
Calibrate by Sodium Formate Ext: 3560
Bruker

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Not active			Set Dry Heater	200 °C
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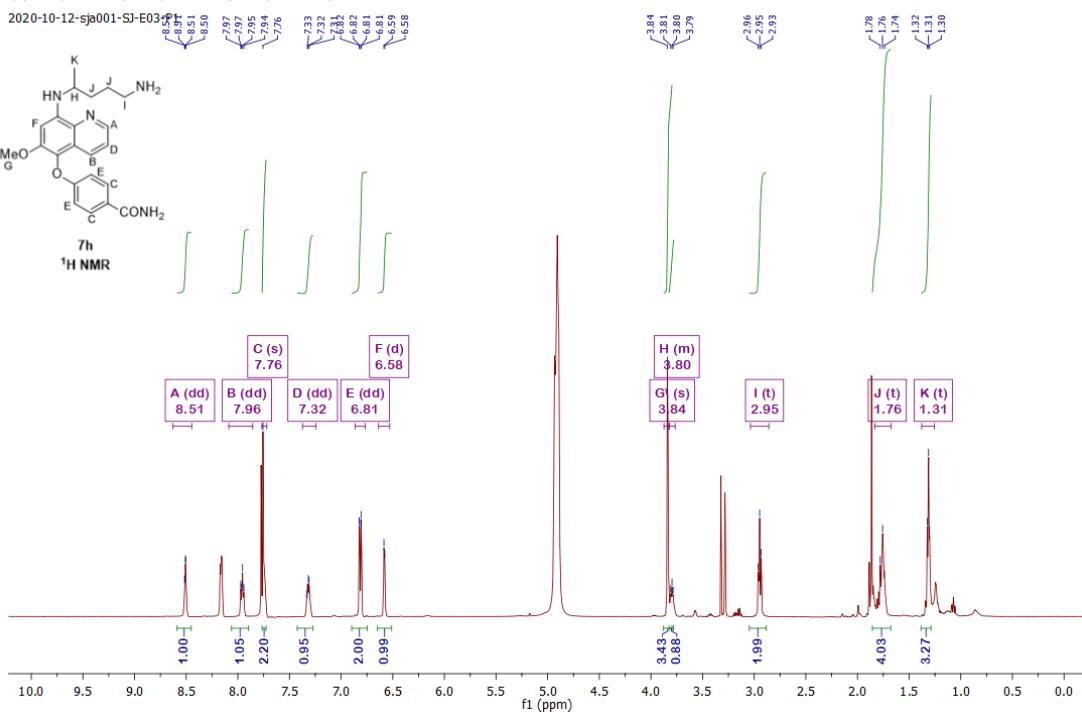


HPLC

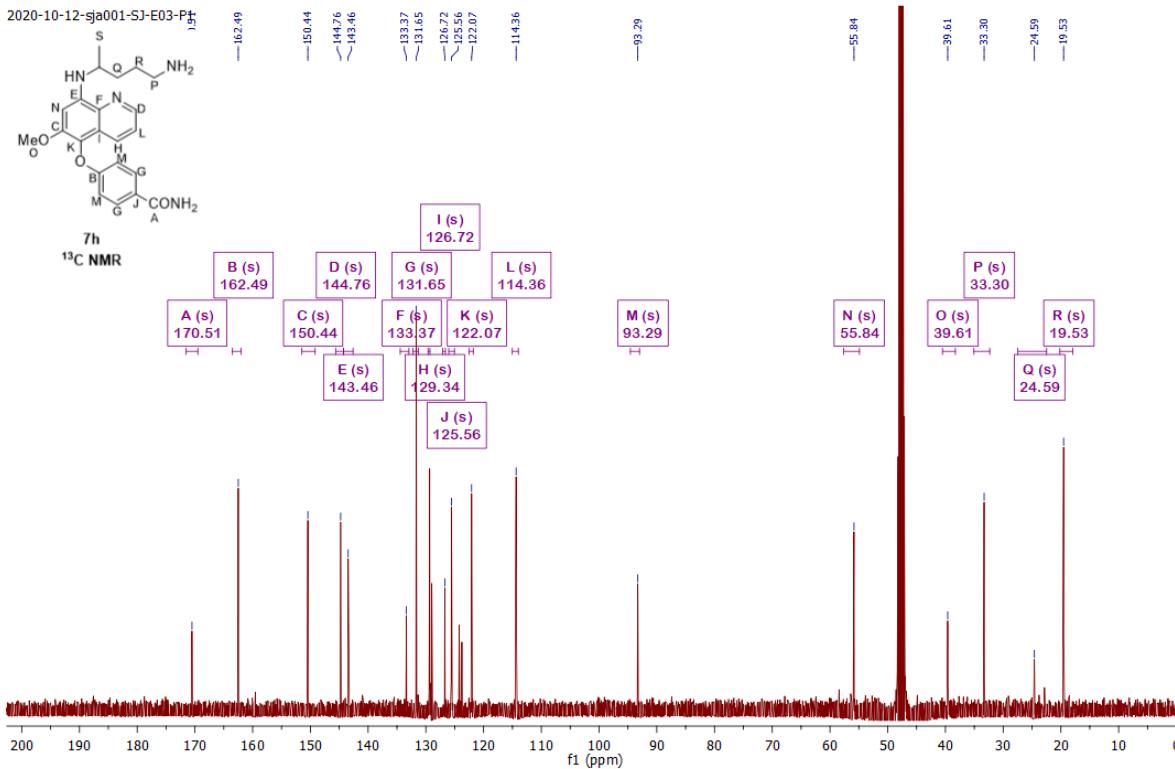


4-((8-((5-Aminopentan-2-yl)amino)-6-methoxyquinolin-5-yl)oxy)benzamide (7h)

NMR (500 MHz) δ 8.51 (dd, $J = 4.1, 1.4$ Hz), 8.16 (dd, $J = 5.7, 3.4$ Hz), 7.96 (dd, $J = 11.1, 4.1$ Hz), 7.77 (s), 7.76 (s), 7.32 (dd, $J = 8.4, 4.1$ Hz), 6.81 (dd, $J = 8.3, 1.4$ Hz), 6.58 (d, $J = 4.1$ Hz), 3.84 (s), 3.82 – 3.77 (m), 2.95 (t, $J = 7.2$ Hz), 1.76 (t, $J = 10.6$ Hz), 1.31 (t, $J = 5.5$ Hz).



NMR (126 MHz) δ 170.51 (s), 162.49 (s), 150.44 (s), 144.76 (s), 143.46 (s), 133.37 (s), 131.65 (s), 129.34 (s), 128.97 (s), 126.72 (s), 125.56 (s), 124.22 (s), 123.76 (s), 122.07 (s), 114.36 (s), 93.29 (s), 55.84 (s), 39.61 (s), 33.30 (s), 19.53 (s).



Mass Spectrum List Report

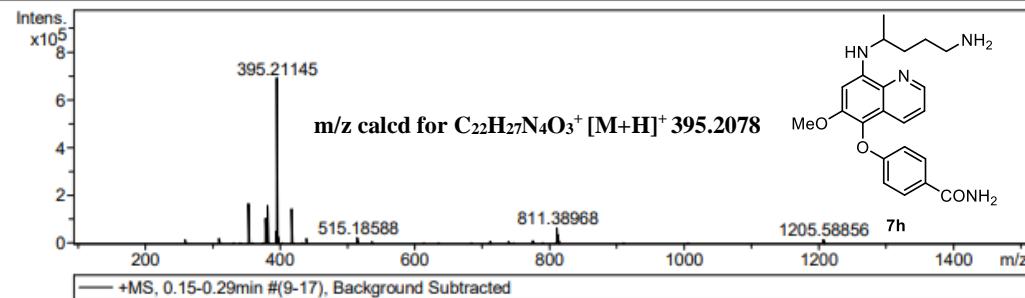
Analysis Info

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Method nv_pos_5min_profile_190214.m
Sample Name SJ-E03-P1
Comment

Acquisition Date 12/14/2020 6:45:27 PM
Operator CU.
Instrument / Ser# micrOTOF-Q II 10335

Acquisition Parameter

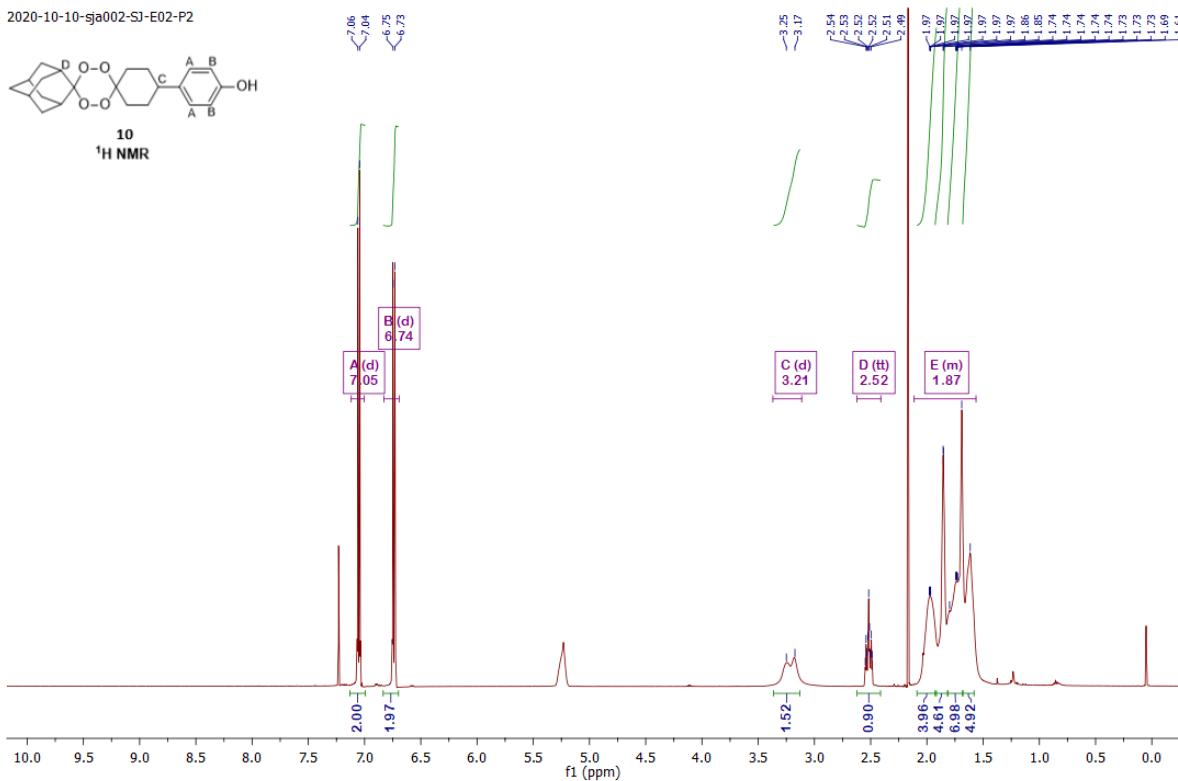
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	200 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	8.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	250.0 Vpp	Set Divert Valve	Waste



4-(Dispiro[cyclohexane-1,3'-[1,2,4,5]tetroxane-6',2'']-tricyclo[3.3.1.13,7]decan]-4-yl)phenol (10)

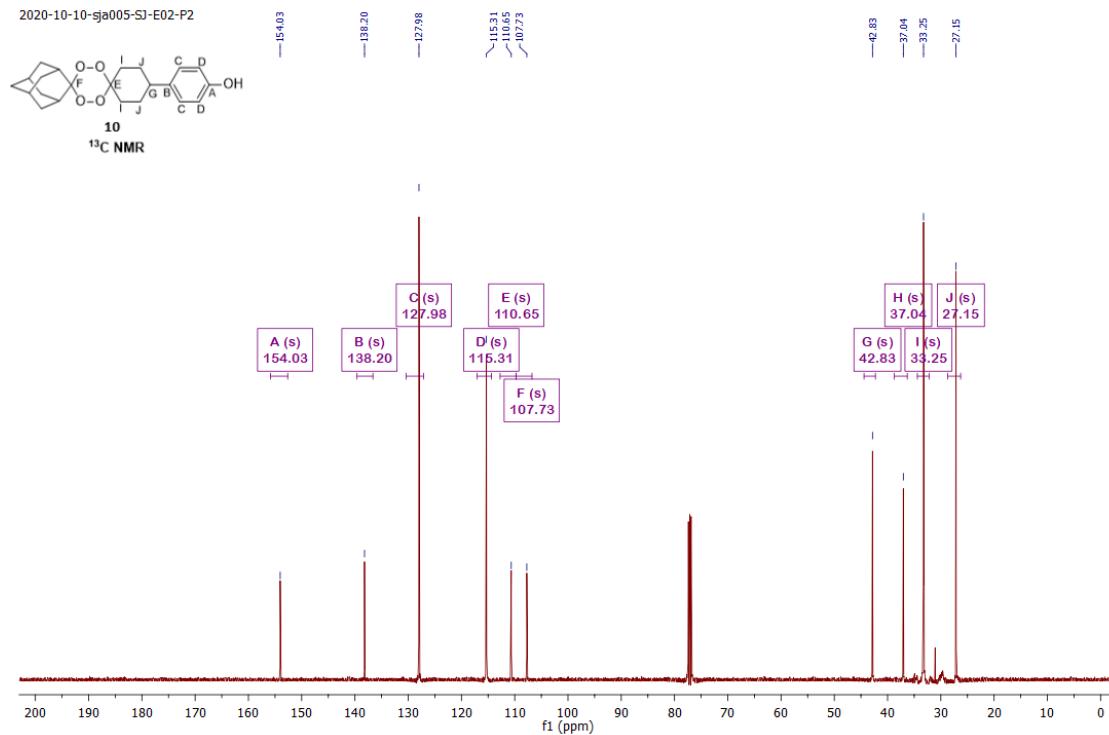
NMR (500 MHz,) δ 7.05 (d, J = 8.5 Hz), 6.74 (d, J = 8.1 Hz), 3.21 (d, J = 38.1 Hz), 2.52 (tt, J = 11.8, 3.6 Hz), 2.11 – 1.56 (m).

2020-10-10-sja002-SJ-E02-P2



NMR (126 MHz,) δ 154.03 (s), 138.20 (s), 127.98 (s), 115.31 (s), 110.65 (s), 107.73 (s), 42.83 (s), 37.04 (s), 33.25 (s), 27.15 (s).

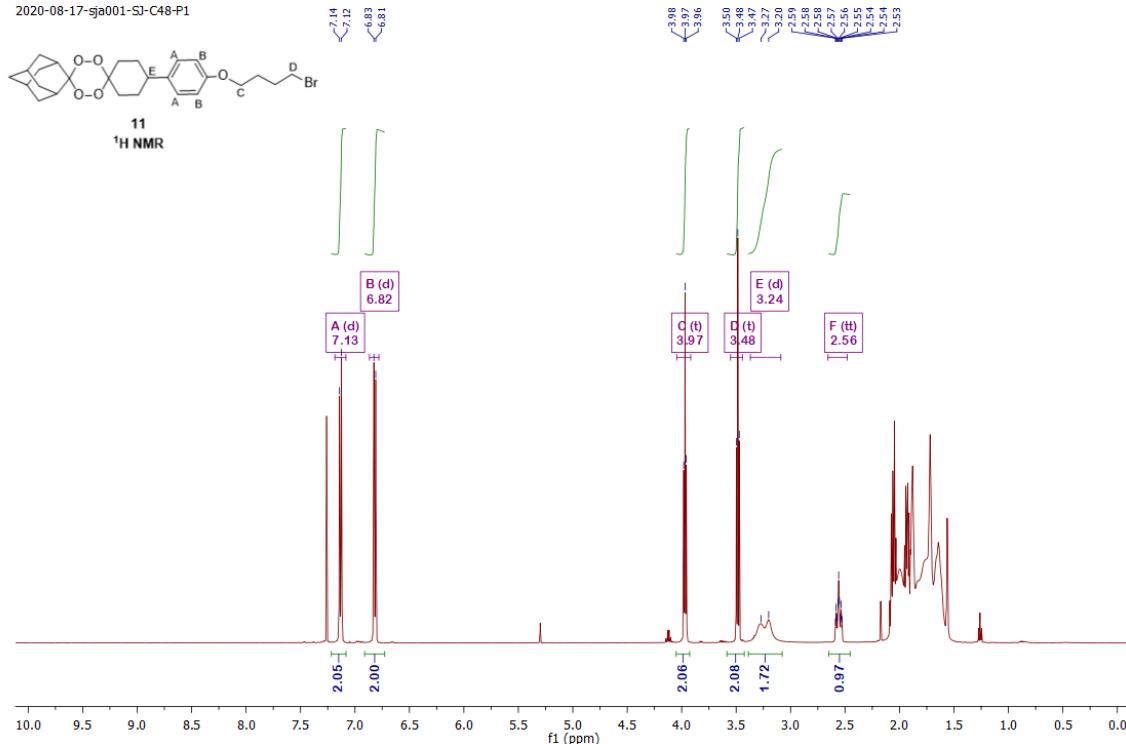
2020-10-10-sja005-SJ-E02-P2



(1*r*,3*r*,5*r*,7*r*)-4''-(4-(4-bromobutoxy)phenyl)dispiro[adamantane-2,3'-[1,2,4,5]tetraoxane-6',1''-cyclohexane] (11)

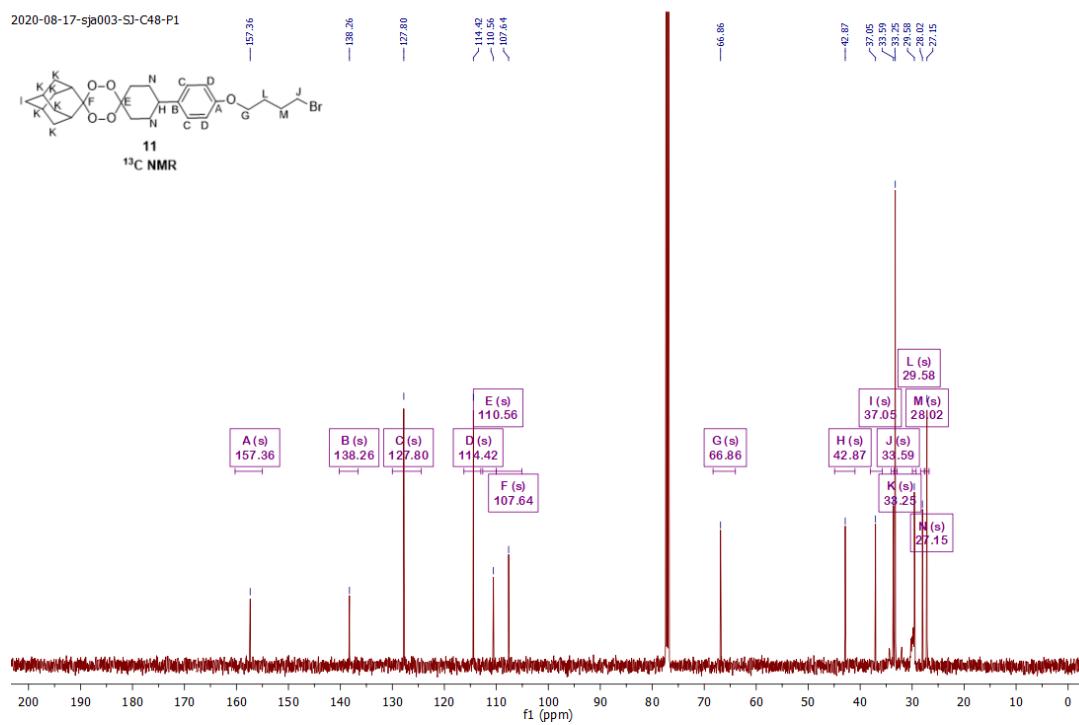
NMR (500 MHz,) δ 7.13 (d, J = 8.6 Hz), 6.82 (d, J = 8.6 Hz), 3.97 (t, J = 6.0 Hz), 3.48 (t, J = 6.7 Hz), 3.24 (d, J = 34.4 Hz), 2.56 (tt, J = 11.8, 3.5 Hz).

2020-08-17-sja001-SJ-C48-P1



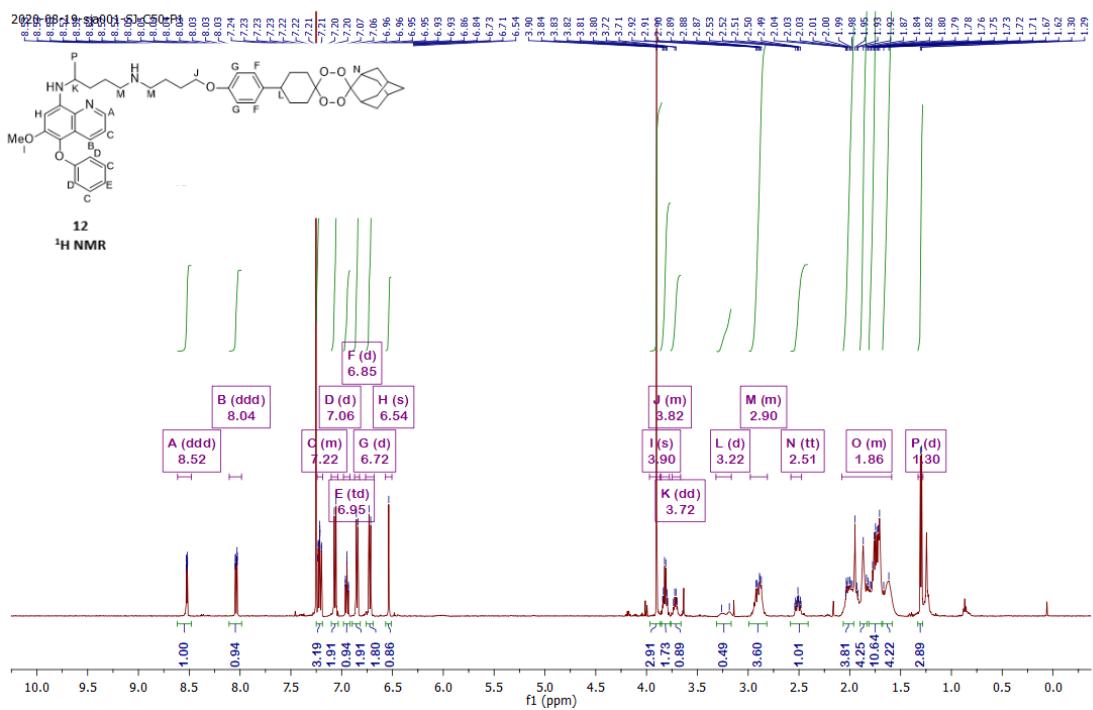
NMR (126 MHz,) δ 157.36 (s), 138.26 (s), 127.80 (s), 114.42 (s), 110.56 (s), 107.64 (s), 66.86 (s), 42.87 (s), 37.05 (s), 33.59 (s), 33.25 (s), 29.58 (s), 28.02 (s), 27.15 (s).

2020-08-17-sja003-SJ-C48-P1

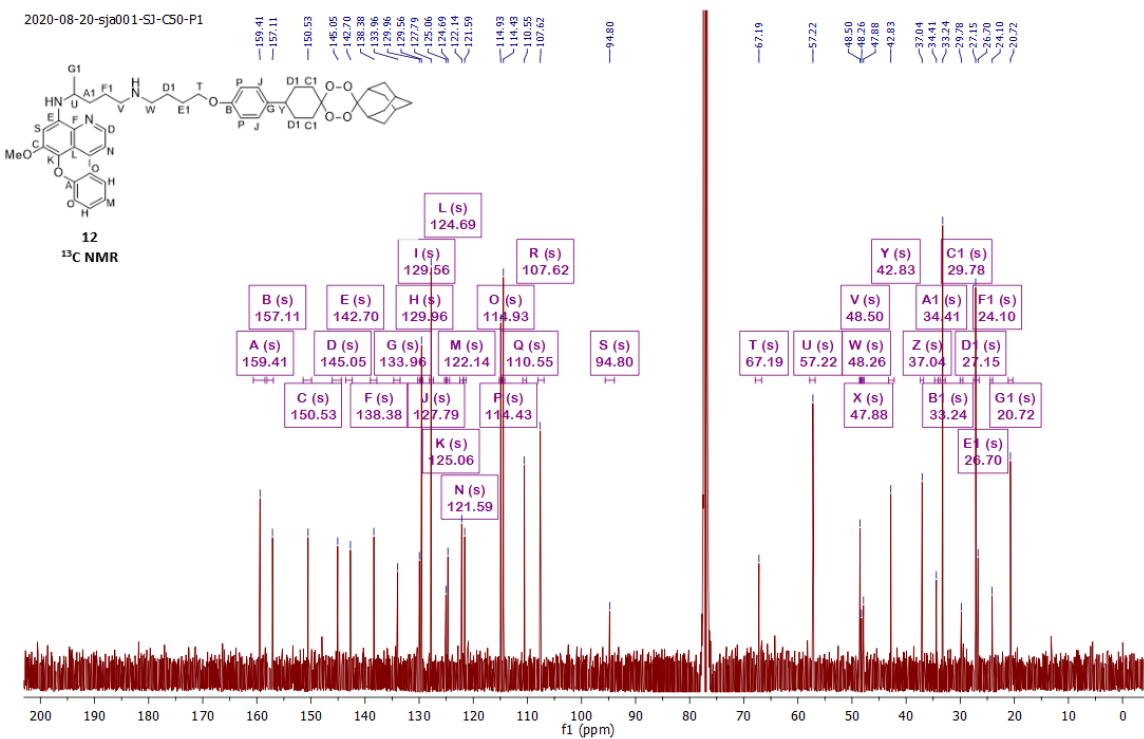


*N*¹-(4-((1*r*,3*r*,5*r*,7*r*)-dispiro[adamantane-2,3'-[1,2,4,5]tetraoxane-6',1''-cyclohexan]-4''-yl)phenoxybutyl)-*N*⁴-(6-methoxy-5-phenoxyquinolin-8-yl)pentane-1,4-diamine (12)

NMR (500 MHz, δ) 8.52 (ddd, $J = 4.1, 1.6, 0.5$ Hz), 8.04 (ddd), 7.24 – 7.19 (m), 7.06 (d, $J = 8.7$ Hz), 6.95 (td, $J = 7.3, 0.5$ Hz), 6.85 (d, $J = 7.8$ Hz), 6.72 (d, $J = 8.4$ Hz), 6.54 (s), 3.90 (s), 3.86 – 3.77 (m), 3.72 (dd, $J = 12.5, 6.3$ Hz), 3.22 (d, $J = 38.2$ Hz), 2.98 – 2.81 (m), 2.51 (tt, $J = 11.6, 3.5$ Hz), 2.08 – 1.59 (m), 1.30 (d, $J = 6.3$ Hz).



NMR (126 MHz), δ 159.41 (s), 157.11 (s), 150.53 (s), 145.05 (s), 142.70 (s), 138.38 (s), 133.96 (s), 129.96 (s), 129.56 (s), 127.79 (s), 125.06 (s), 124.69 (s), 122.14 (s), 121.59 (s), 114.93 (s), 114.43 (s), 110.55 (s), 107.62 (s), 94.80 (s), 67.19 (s), 57.22 (s), 48.50 (s), 48.26 (s), 47.88 (s), 42.83 (s), 37.04 (s), 34.41 (s), 33.24 (s), 29.78 (s), 27.15 (s), 26.70 (s), 24.10 (s), 20.72 (s).



High resolution report

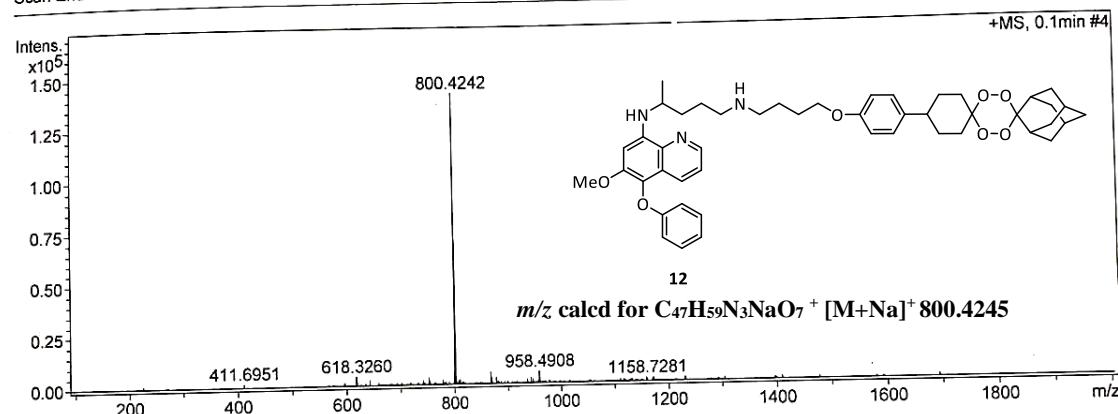
Acquisition Date 9/9/2020 3:01:38 PM

Analysis Name D:\Data\customer\SJ C50 P1.d
 Method NaFormate_pos.m
 Sample Name SJ C50 P1

Operator Sutichai Ext: 3560
 Instrument micrOTOF Bruker
 Calibrate by Sodium Formate

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	100 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



Primary data for heme polymerization inhibition assay

	Control	T	T-							
	1	0.5446	1.3240							
	2	0.5361	1.3336							
	3	0.5828	1.3263							
	Average	0.5545	1.3280							
PQ	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3
	400	1.1201	1.1807	1.1501	0.269	0.190	0.230	73.12	80.96	77.01
	200	0.9117	0.8333	0.8610	0.538	0.640	0.604	46.18	36.04	39.63
	100	0.7047	0.7321	0.7060	0.806	0.770	0.804	19.42	22.96	19.59
	50	0.6525	0.5004	0.5950	0.873	1.070	0.948	12.67	-7.00	5.24
	10	0.4823	0.6216	0.5831	1.093	0.913	0.963	-9.33	8.67	3.70
	2	0.5384	0.6796	0.5908	1.021	0.838	0.953	-2.08	16.17	4.69
							IC50	312.8	309.9	336.8
7a R = H	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3
	400	1.3420	1.3328	1.2949	-0.018	-0.006	0.043	101.81	100.63	95.73
	200	1.2442	1.2371	1.2369	0.108	0.118	0.118	89.17	88.25	88.23
	100	0.9465	1.0180	0.9378	0.493	0.401	0.505	50.68	59.92	49.55
	50	0.7077	0.7989	0.7428	0.802	0.684	0.757	19.81	31.60	24.35
	10	0.5876	0.6523	0.6299	0.957	0.874	0.903	4.28	12.65	9.75
	2	0.5604	0.6189	0.5991	0.992	0.917	0.942	0.76	8.32	5.77
							IC50	104.9	96.0	103.9
7b R = OMe	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3
	400	1.2860	1.2564	1.3151	0.054	0.093	0.017	94.57	90.75	98.34
	200	1.0747	1.0745	1.1075	0.328	0.328	0.285	67.25	67.23	71.49
	100	0.8648	0.8585	0.8842	0.599	0.607	0.574	40.12	39.30	42.63
	50	0.6724	0.7042	0.6810	0.848	0.806	0.837	15.24	19.36	16.35
	10	0.5933	0.6127	0.6461	0.950	0.925	0.882	5.02	7.53	11.84
	2	0.5750	0.5950	0.5688	0.974	0.948	0.982	2.65	5.23	1.85
							IC50	162.1	159.6	156.7
7c R = Br	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3
	400	1.2540	1.2423	1.2580	0.096	0.111	0.091	90.44	88.93	90.95
	200	1.0445	1.0467	1.0307	0.367	0.364	0.384	63.35	63.64	61.57
	100	0.7978	0.8029	0.8502	0.685	0.679	0.618	31.46	32.12	38.23
	50	0.6525	0.6955	0.6376	0.873	0.818	0.893	12.67	18.23	10.74
	10	0.6204	0.5995	0.6111	0.915	0.942	0.927	8.52	5.82	7.32
	2	0.6135	0.6058	0.5650	0.924	0.934	0.986	7.63	6.63	1.36
							IC50	170.0	180.6	174.8
7d R = Cl	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3
	400	1.3014	1.3228	1.2608	0.034	0.007	0.087	96.57	99.33	91.32
	200	1.1881	1.1676	1.1406	0.181	0.207	0.242	81.92	79.27	75.78
	100	0.8563	0.9389	0.8664	0.610	0.503	0.597	39.02	49.70	40.32
	50	0.7722	0.7133	0.7552	0.719	0.795	0.741	28.15	20.53	25.95
	10	0.6479	0.6889	0.6284	0.879	0.826	0.905	12.08	17.37	9.55
	2	0.6147	0.6029	0.5760	0.922	0.937	0.972	7.78	6.26	2.78
							IC50	135.4	124.7	136.6

7e	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3		
R = CN	400	1.1611	1.2140	1.0931	0.216	0.147	0.304	78.42	85.27	69.64		
	200	0.9587	0.9868	0.9039	0.477	0.441	0.548	52.26	55.89	45.17		
	100	0.7875	0.7915	0.6884	0.699	0.694	0.827	30.12	30.64	17.31		
	50	0.7039	0.6810	0.7223	0.807	0.837	0.783	19.32	16.35	21.70		
	10	0.5837	0.6538	0.6274	0.962	0.872	0.906	3.78	12.84	9.43		
	2	0.6189	0.5844	0.6159	0.917	0.961	0.921	8.32	3.87	7.94		
							IC50	291.1	269.3	297.1	285.8	Average
											11.9	SD
7f	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3		
R = F	400	1.2465	1.2646	1.3609	0.105	0.082	-0.043	89.47	91.81	104.26		
	200	1.0774	1.1136	1.1214	0.324	0.277	0.267	67.61	72.28	73.29		
	100	0.8393	0.8052	0.8321	0.632	0.676	0.641	36.82	32.41	35.89		
	50	0.7010	0.7465	0.6951	0.811	0.752	0.818	18.94	24.82	18.18		
	10	0.6656	0.6128	0.6293	0.856	0.925	0.903	14.36	7.54	9.67		
	2	0.6011	0.5685	0.6436	0.940	0.982	0.885	6.02	1.81	11.52		
							IC50	155.3	170.6	175.4	167.1	Average
											8.6	SD
7g	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3		
R = CF3	400	1.2701	1.3094	1.3367	0.075	0.024	-0.011	92.52	97.60	101.13		
	200	1.2291	1.2514	1.2888	0.128	0.099	0.051	87.22	90.10	94.94		
	100	0.9072	0.9439	0.9565	0.544	0.497	0.480	45.60	50.34	51.98		
	50	0.7905	0.8434	0.7615	0.695	0.627	0.732	30.51	37.35	26.76		
	10	0.6662	0.7085	0.6369	0.856	0.801	0.894	14.44	19.91	10.65		
	2	0.5617	0.6305	0.6619	0.991	0.902	0.861	0.93	9.83	13.89		
							IC50	107.6	114.2	107.2	109.7	Average
											3.2	SD
7h	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3		
R = CONH2	400	1.2292	1.2707	1.3532	0.128	0.074	-0.033	87.23	92.60	103.26		
	200	1.0705	1.1566	1.2061	0.333	0.222	0.158	66.71	77.84	84.25		
	100	0.8632	0.9015	0.8701	0.601	0.551	0.592	39.91	44.86	40.80		
	50	0.7271	0.7882	0.7887	0.777	0.698	0.697	22.32	30.21	30.28		
	10	0.6189	0.6897	0.6984	0.917	0.825	0.814	8.33	17.48	18.60		
	2	0.6080	0.5767	0.6640	0.931	0.971	0.858	6.92	2.87	14.16		
							IC50	153.6	161.7	146.0	153.8	Average
											6.4	SD
12	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3		
conjugate	400	1.3771	1.2946	1.3063	-0.063	0.043	0.028	106.35	95.69	97.20		
	200	1.2526	1.2954	1.2334	0.098	0.042	0.122	90.25	95.79	87.78		
	100	1.1903	1.1218	1.0502	0.178	0.267	0.359	82.20	73.34	64.09		
	50	0.9274	0.9397	0.9501	0.518	0.502	0.489	48.21	49.80	51.14		
	10	0.7022	0.7176	0.6639	0.809	0.789	0.859	19.10	21.09	14.14		
	2	0.6519	0.6822	0.6232	0.874	0.835	0.911	12.59	16.51	8.88		
							IC50	64.5	64.3	71.8	66.9	Average
											3.5	SD
CQ	conc	1	2	3	HCF1	HCF2	HCF3	%Inh1	%Inh2	%Inh3		
	400	1.3721	1.2840	1.3079	-0.057	0.057	0.026	105.70	94.31	97.41		
	200	1.2998	1.1170	1.2177	0.036	0.273	0.143	96.36	72.73	85.74		
	100	1.2104	1.1826	1.0987	0.152	0.188	0.296	84.80	81.20	70.36		
	50	0.9397	0.8390	1.0169	0.502	0.632	0.402	49.80	36.78	59.78		
	10	0.7031	0.7685	0.7640	0.808	0.723	0.729	19.21	27.67	27.09		
	2	0.6704	0.6490	0.6412	0.850	0.878	0.888	14.98	12.22	11.21		
							IC50	61.3	59.6	62.8	61.2	Average
											1.3	SD