

Supplementary information

Pyridinyl 4-(2-oxoalkylimidazolidin-1-yl)benzenesulfonates and their hydrochloride salts as novel water soluble antimitotic prodrugs bioactivated by cytochrome P450 1A1 in breast cancer cells

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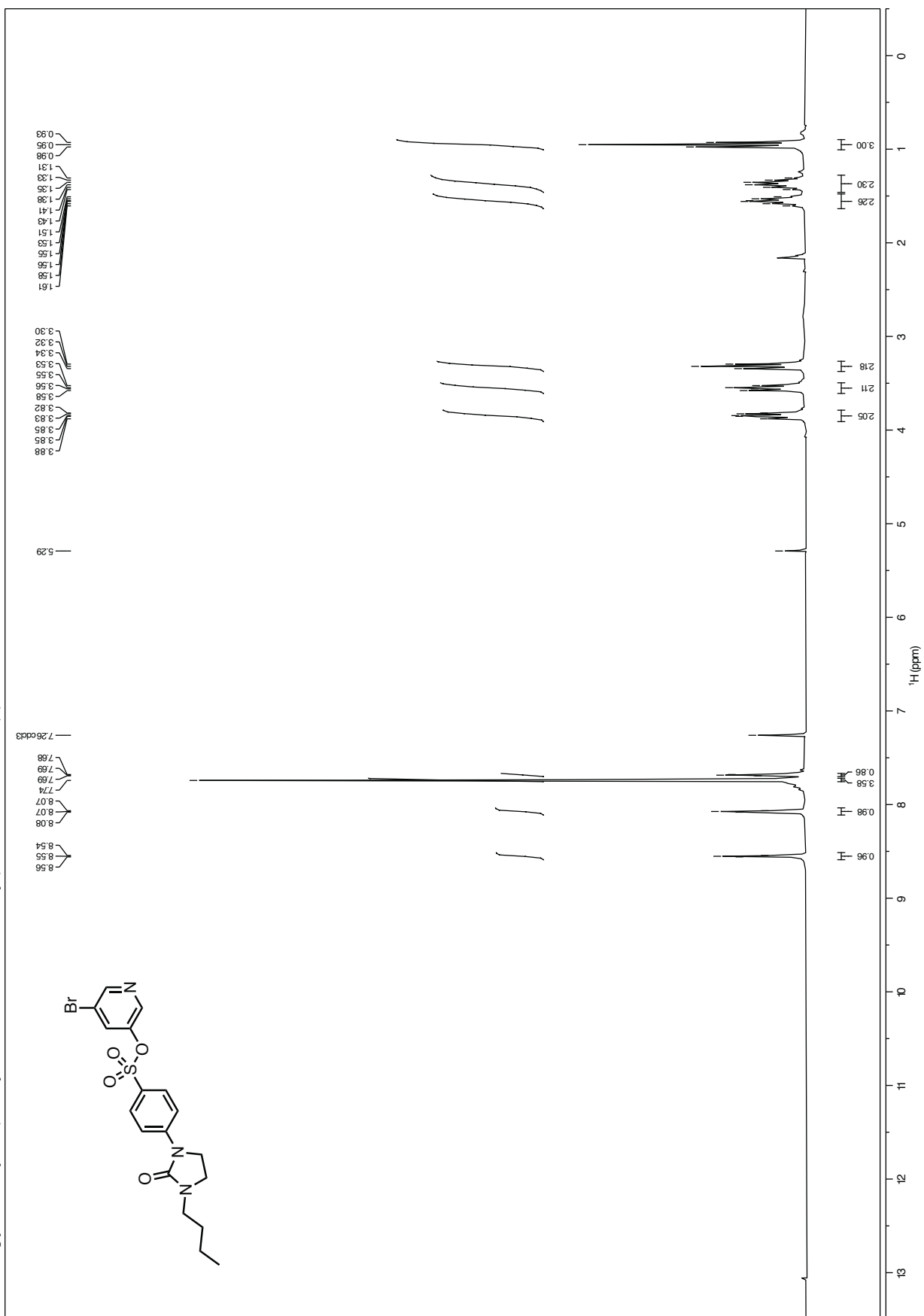
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^c *Centre de recherche de l'Institut universitaire de cardiologie et de pneumologie de Québec-Université Laval (IUCPQ), 2725 Ch Ste-Foy, Québec, QC, G1V 4G5, Canada.*

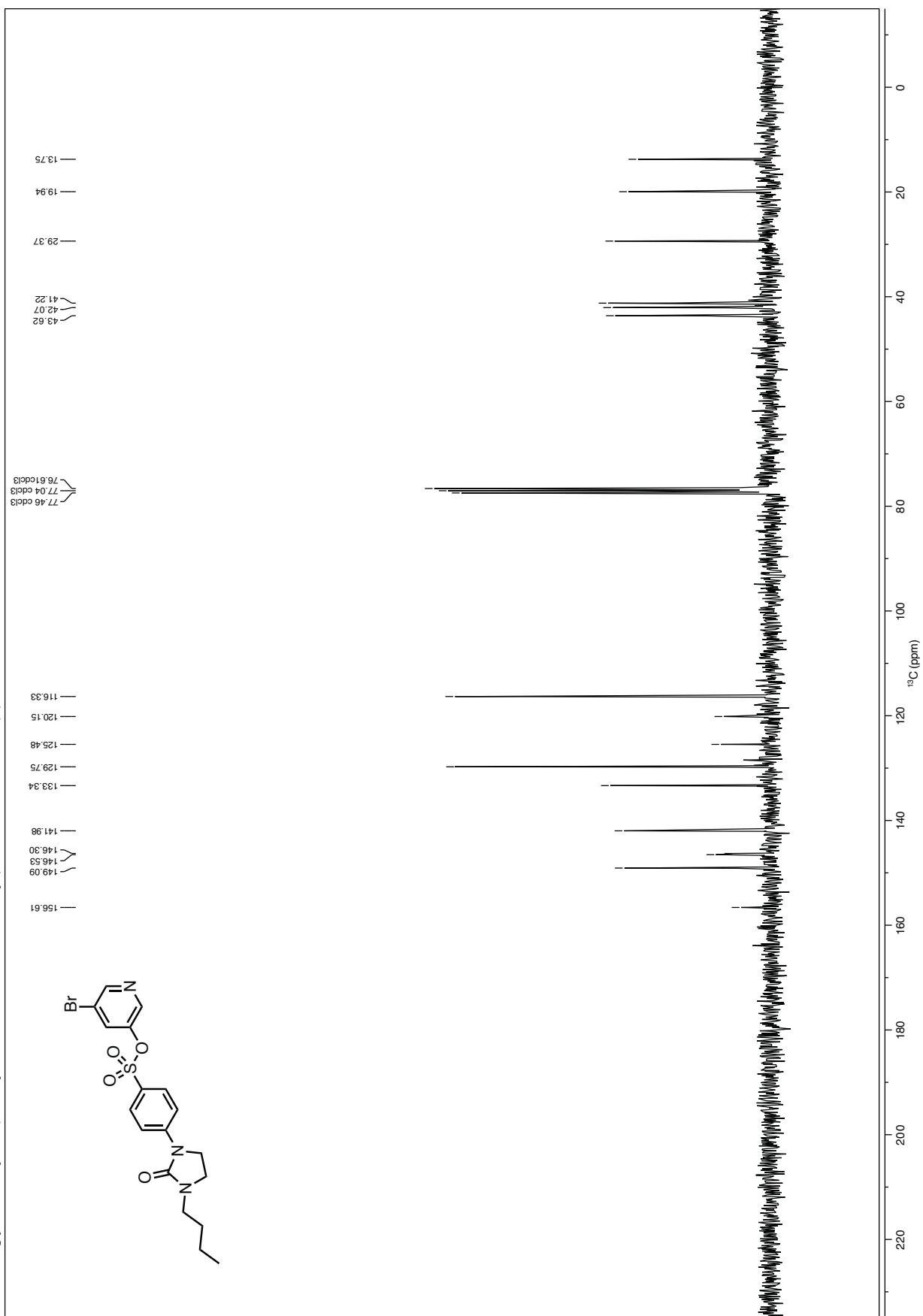
***Corresponding author:** Sébastien Fortin, Faculté de pharmacie, Université Laval and Centre de recherche du CHU de Québec-Université Laval, 10, rue de l'Espinay, Québec, Québec, G1L 3L5, Canada, Tel.: (418) 525-4444 ext. 52364, e-mail: sebastien.fortin@pha.ulaval.ca

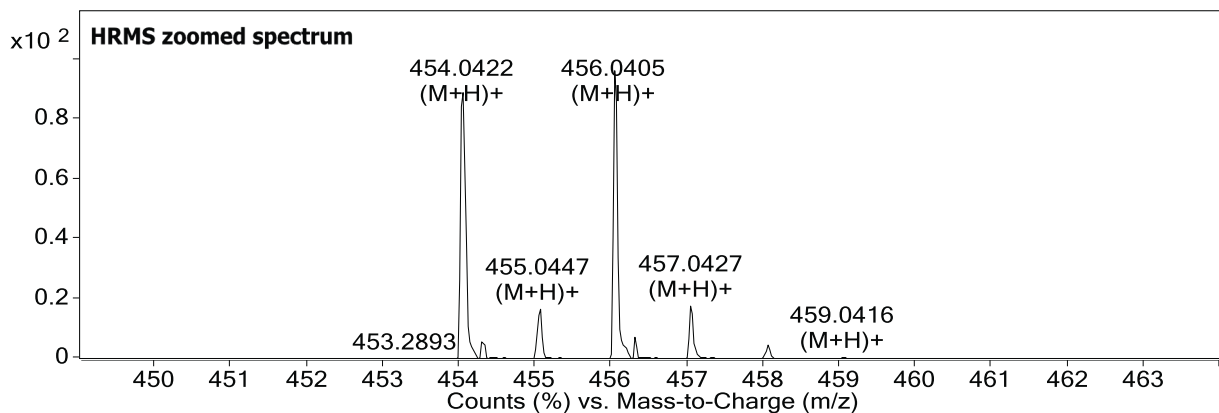
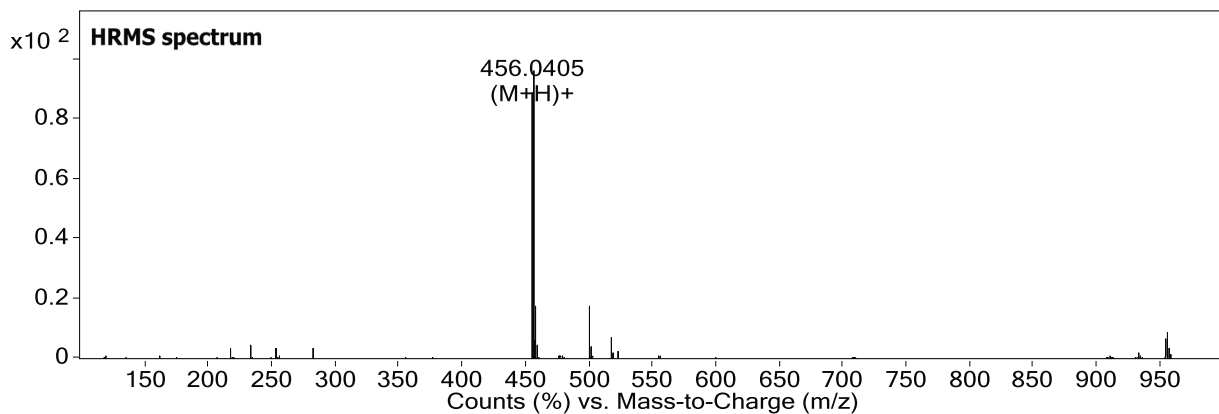
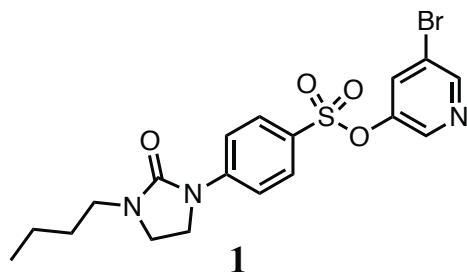
Contents: ¹H NMR, ¹³C NMR and HRMS spectra for all compounds and calculated physicochemical, pharmacokinetics and drug-likeness properties by SwissADME tool for the most potent PYRIB-SOs **4** and **5** assessed in our biofunctional assays.

5-Bromopyridin-3-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (**1**)



5-Bromopyridin-3-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (**1**)

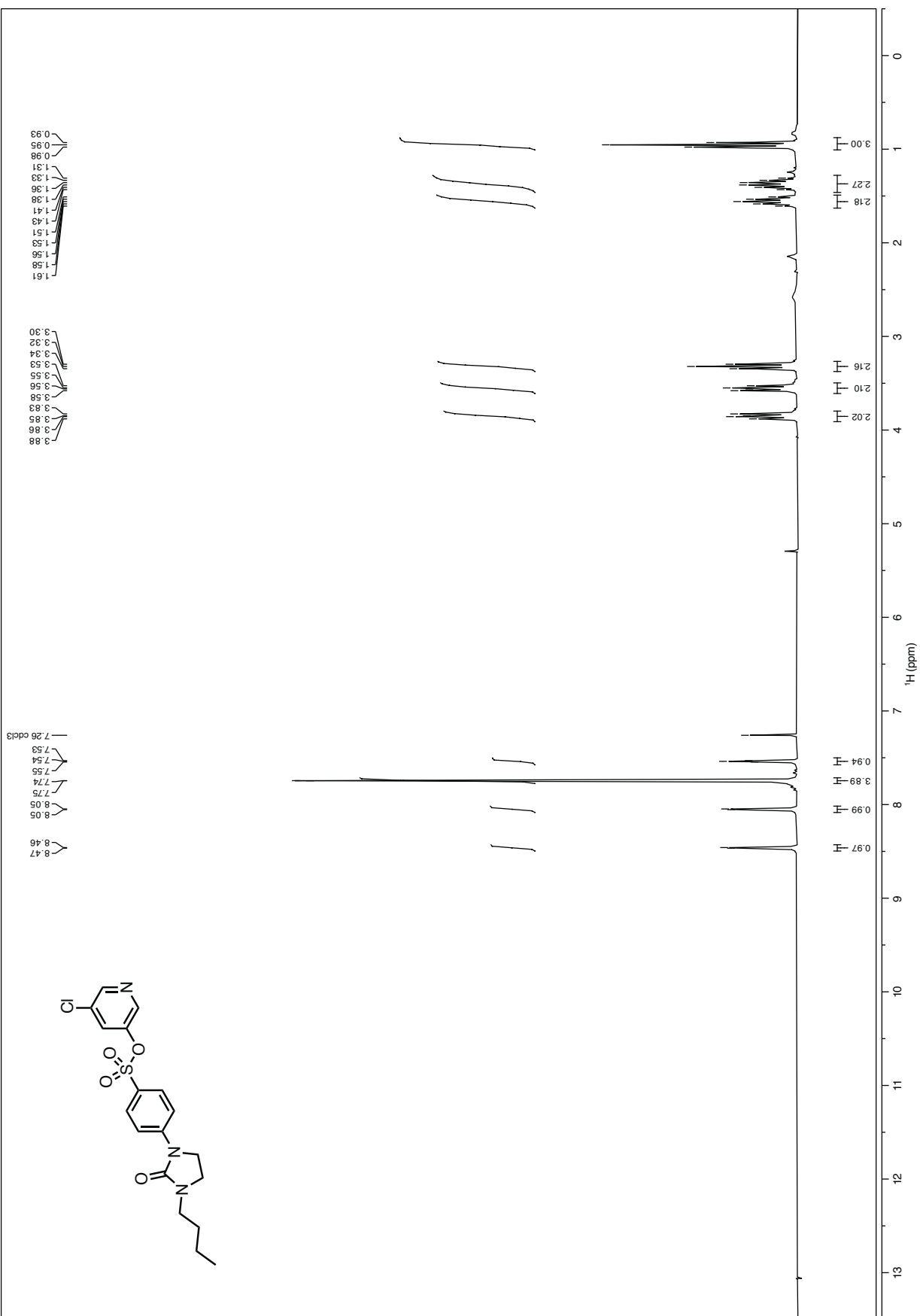




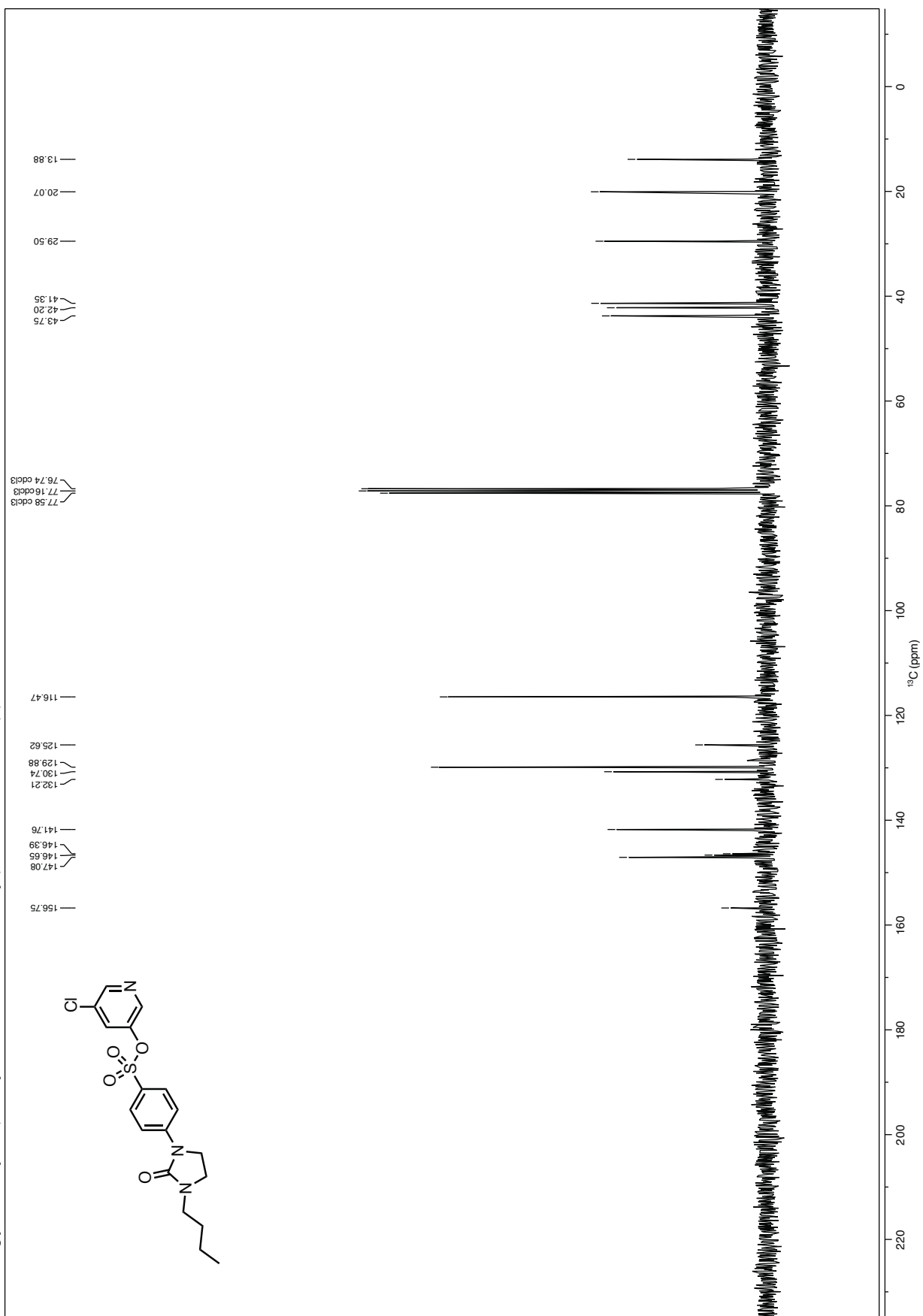
MS spectrum peak list

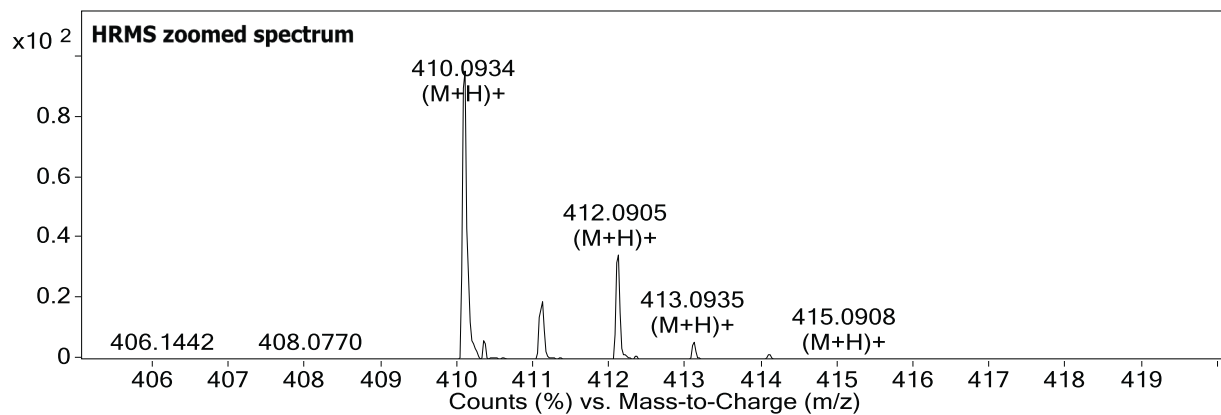
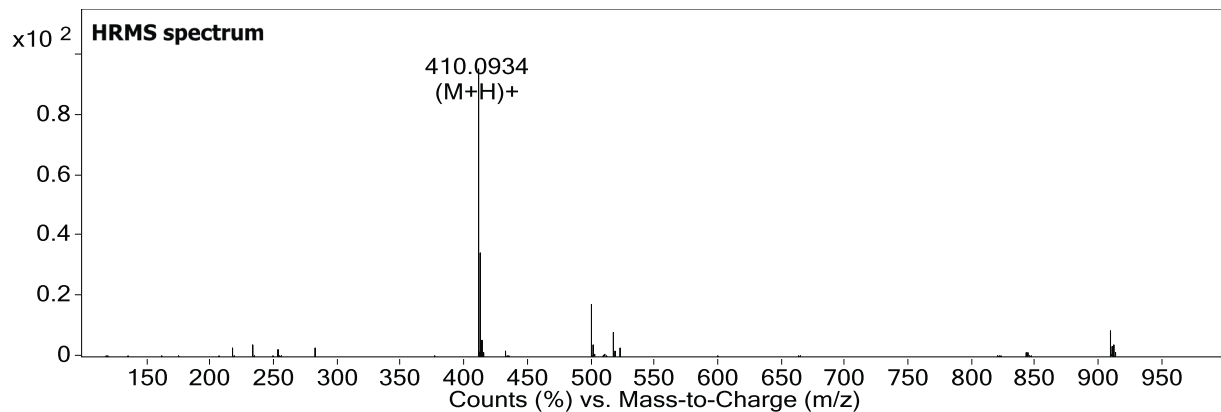
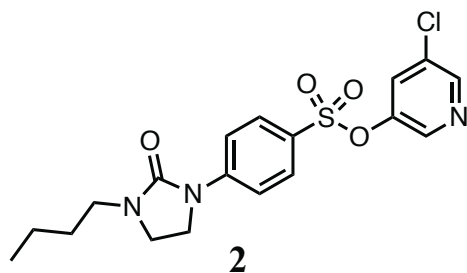
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	Abund	Formula	Ion
454.0422	454.0431	-1.83	267375	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺
455.0447	455.046	-2.8	48956	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺
456.0405	456.0411	-1.47	286349	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺
457.0427	457.044	-2.8	52786	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺
458.0398	458.0408	-2.23	14114	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺
459.0416	459.0423	-1.43	1919	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺
460.0433	460.0435	-0.45	308	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺

5-Chloropyridin-3-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (2)



5-Chloropyridin-3-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (2)

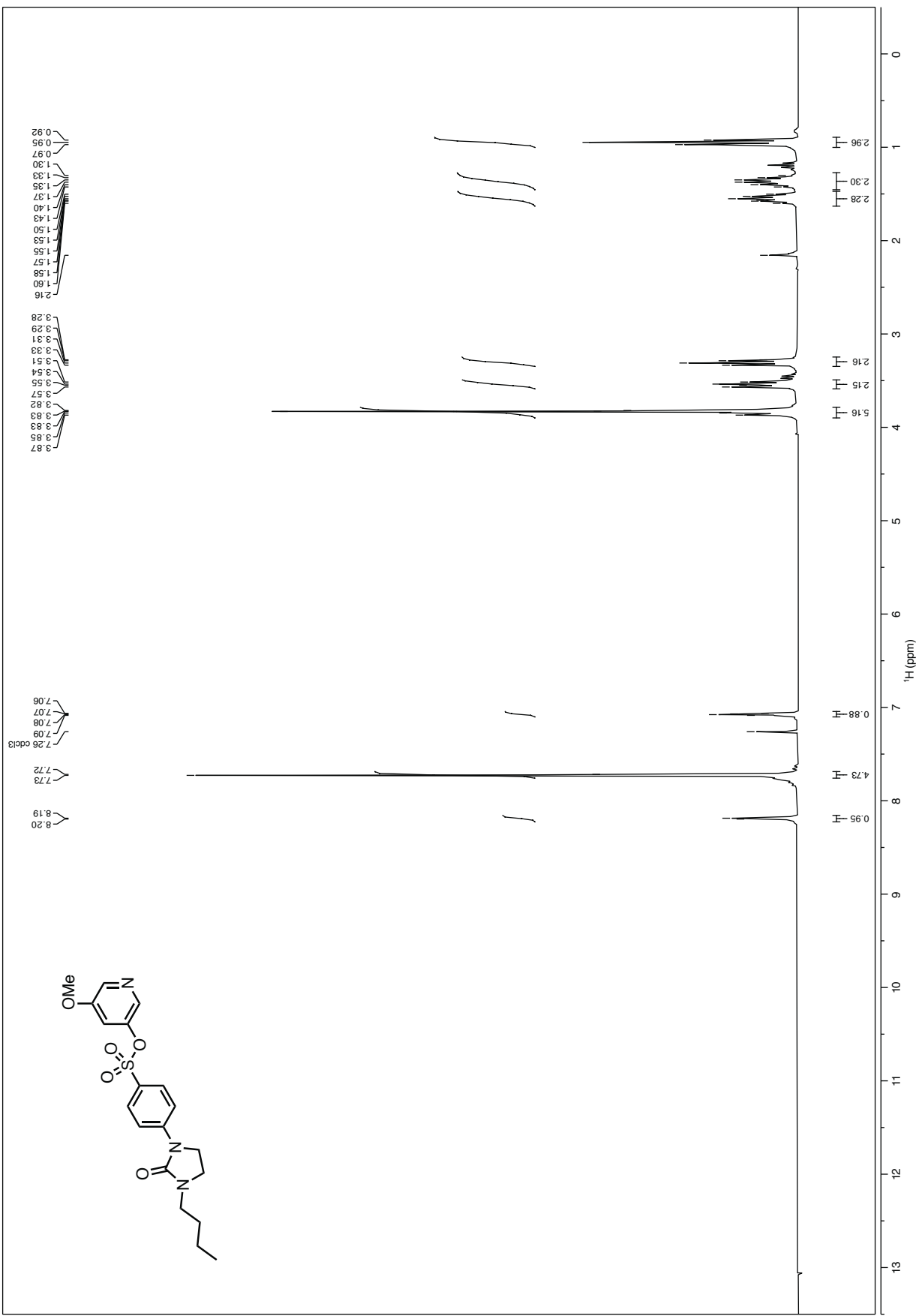




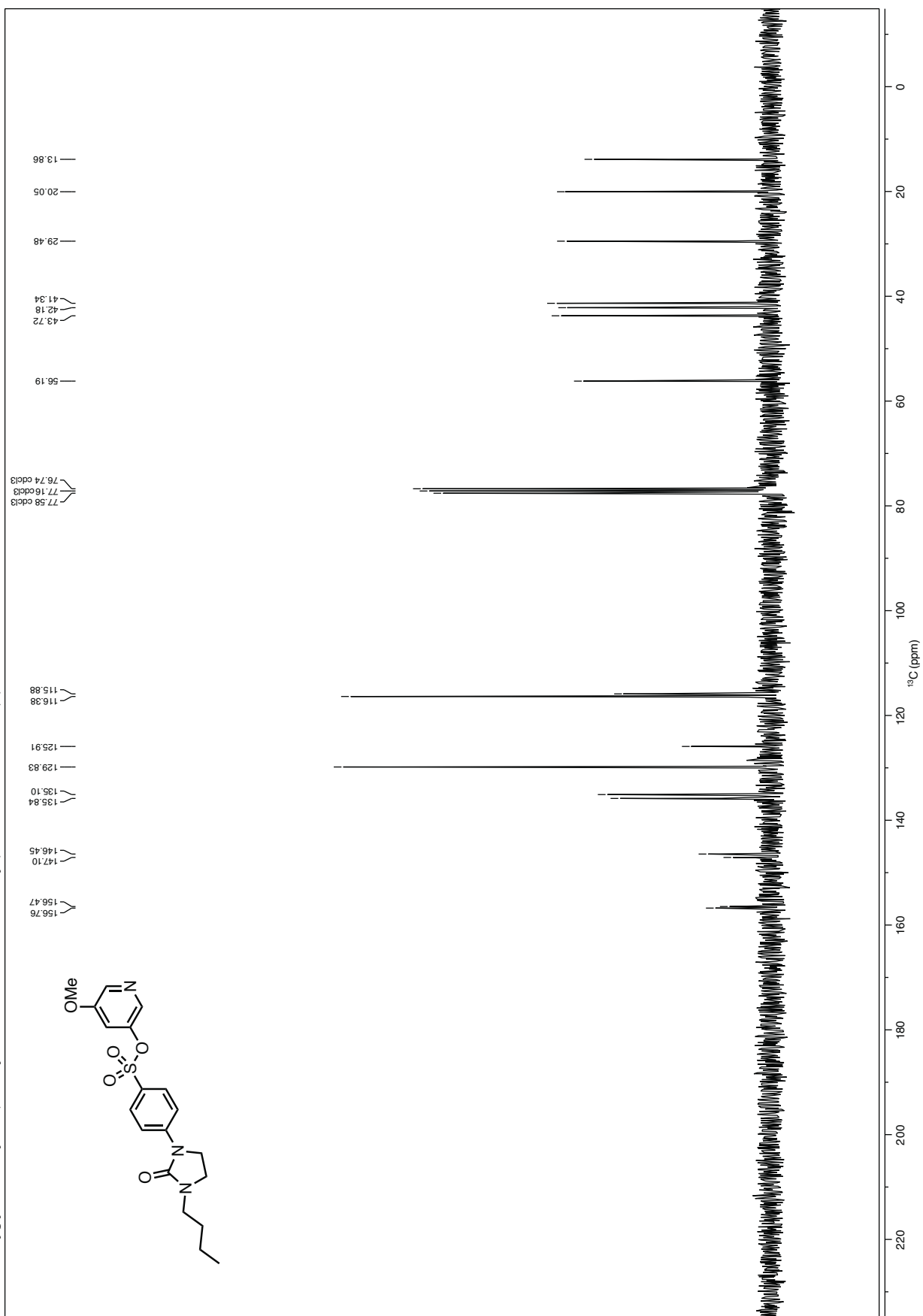
MS spectrum peak list

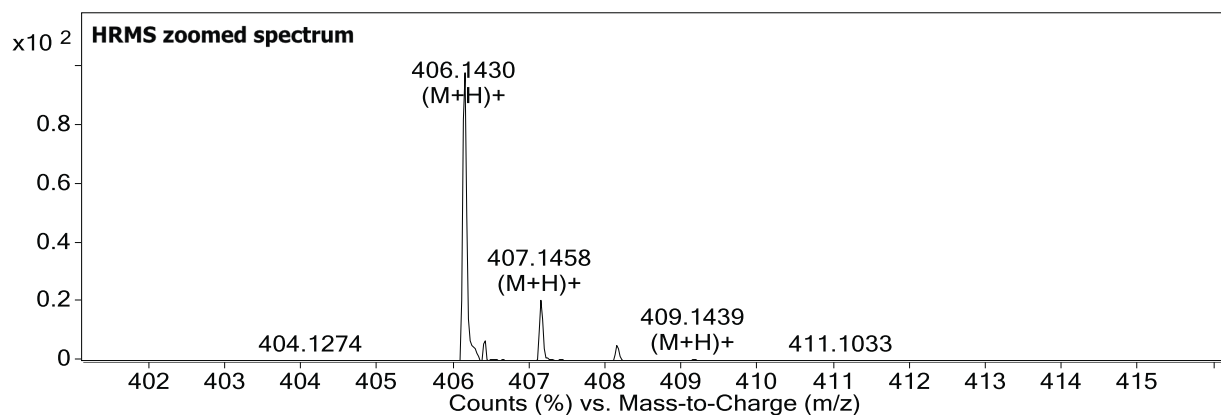
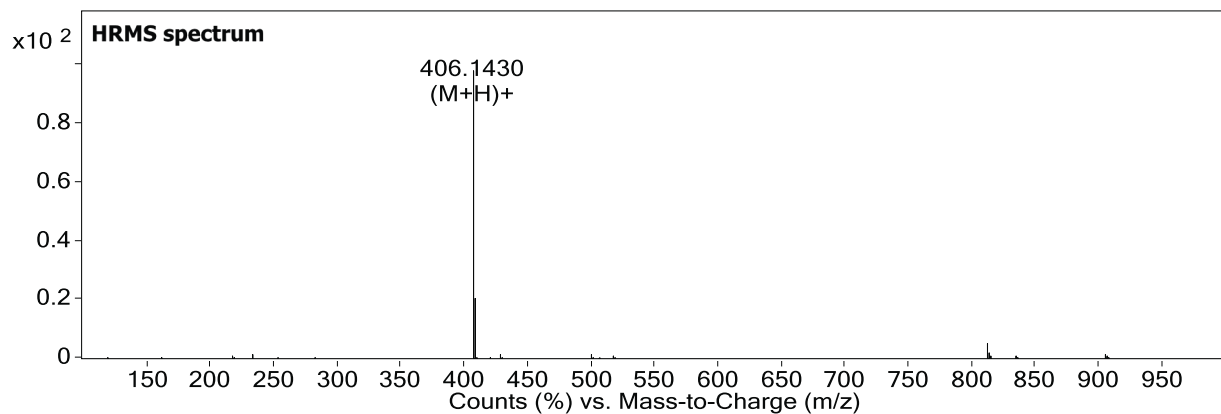
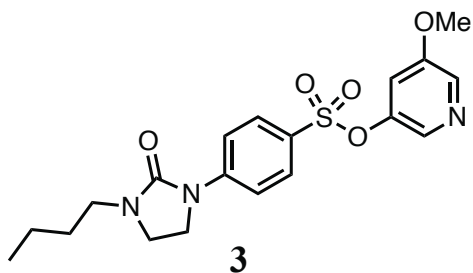
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	Abund	Formula	Ion
410.0934	410.0936	-0.51	297896	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
411.0962	411.0965	-0.84	56760	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
412.0905	412.0911	-1.44	108195	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
413.0935	413.0937	-0.55	17660	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
414.0909	414.0907	0.32	4382	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
415.0908	415.0921	-2.95	719	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺

5-Methoxypyridin-3-yl 4-(3-buty-2-oxoimidazolidin-1-yl)benzenesulfonate (**3**)



5-Methoxypyridin-3-yl 4-(3-buty[2-oxoimidazolidin-1-yl]benzenesulfonate (**3**)

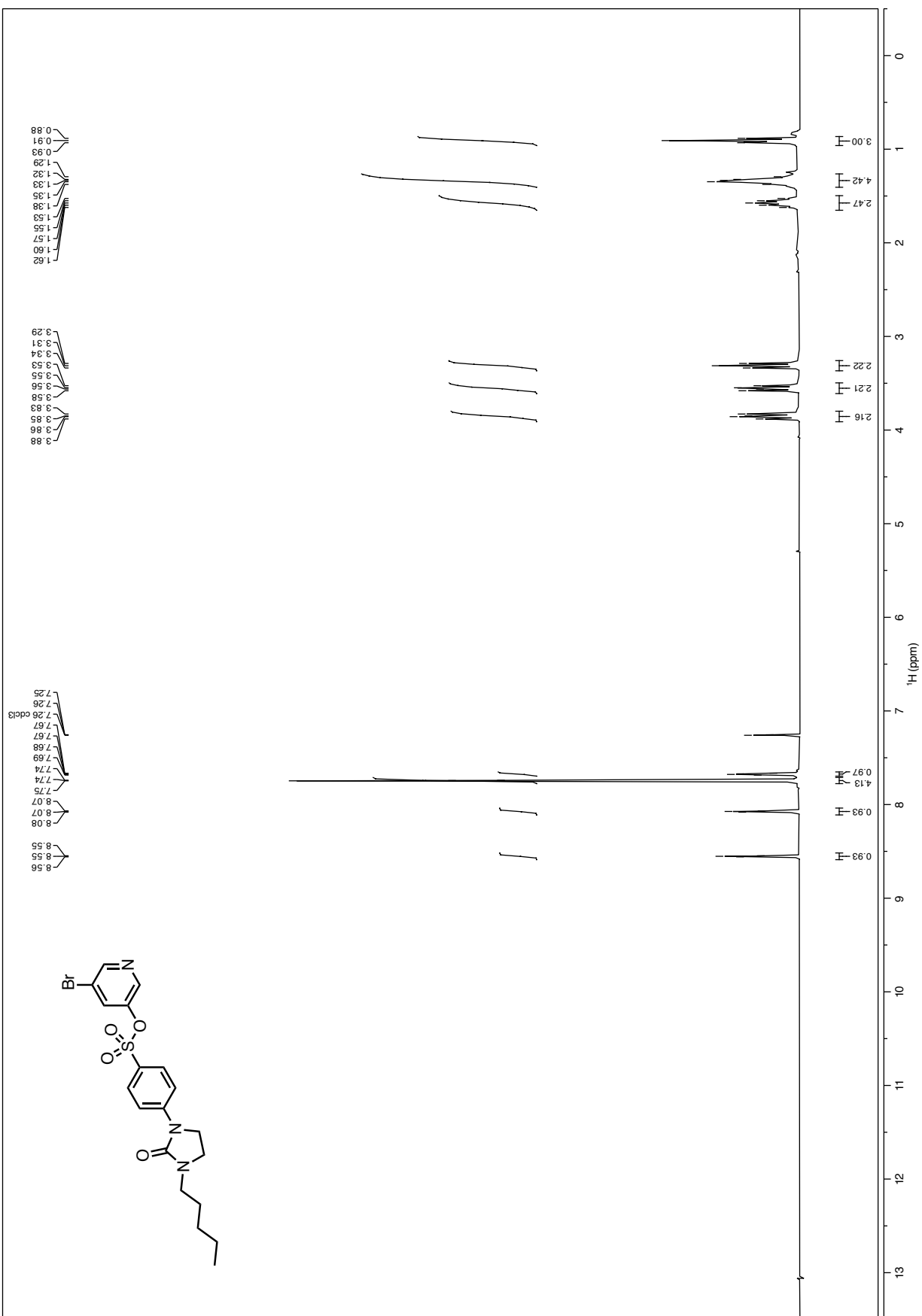




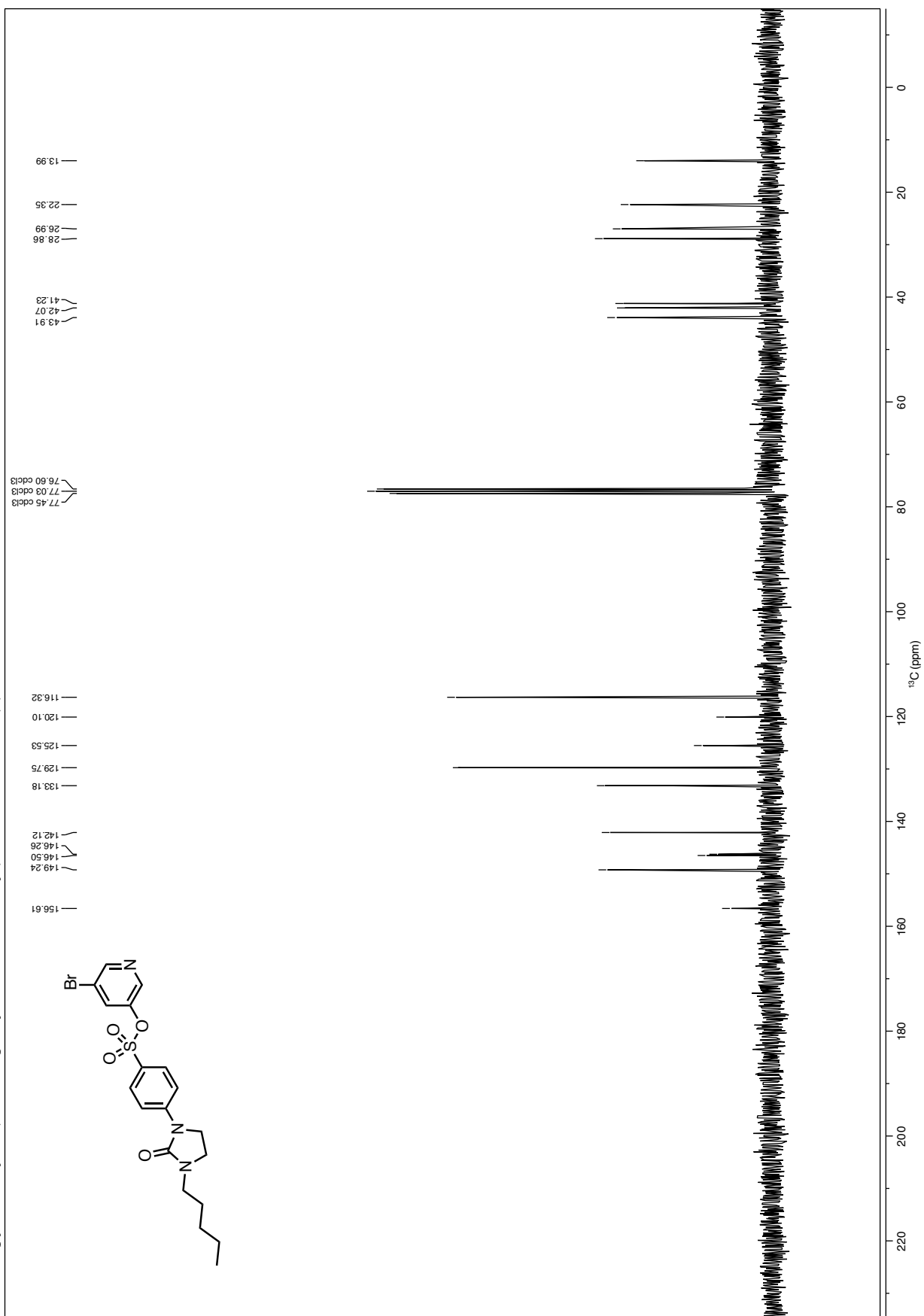
MS spectrum peak list

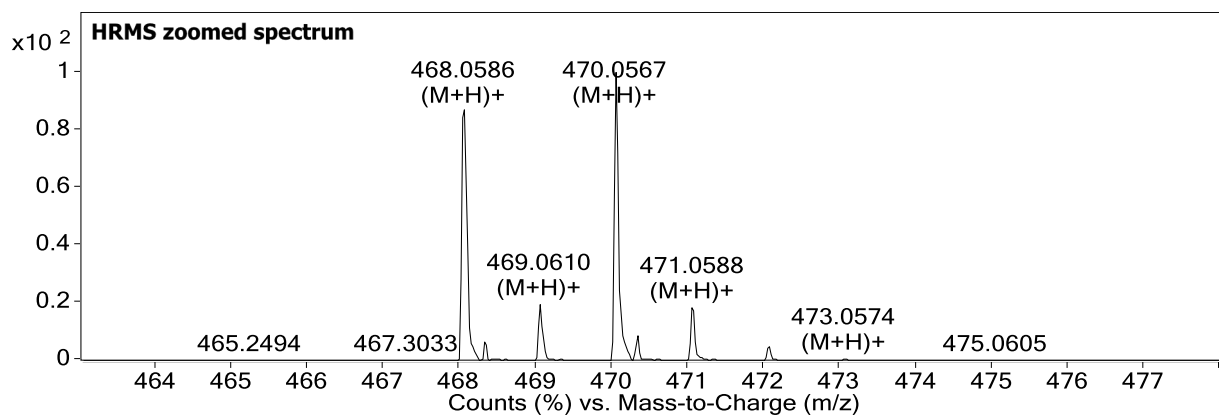
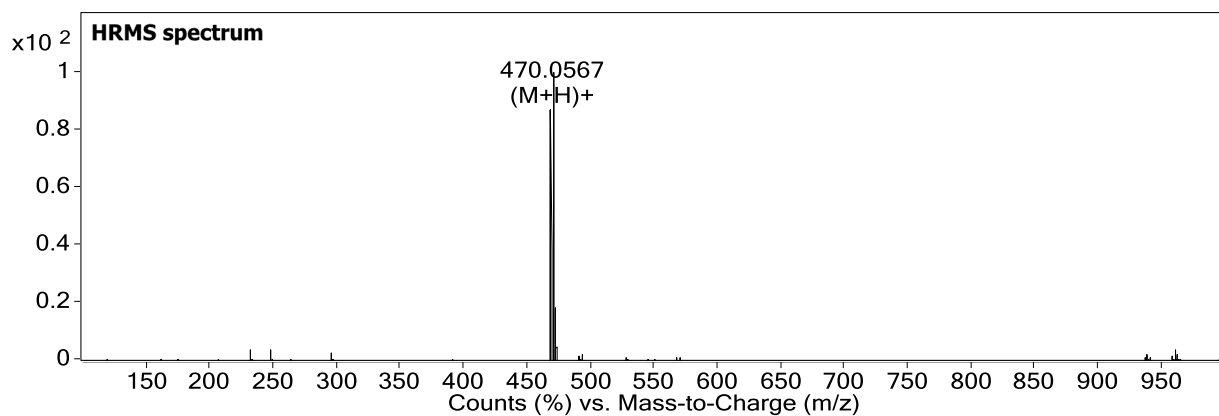
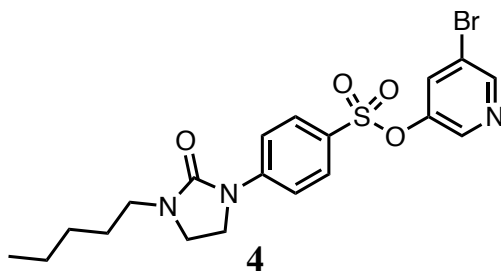
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	Abund	Formula	Ion
406.143	406.1431	-0.3	361649	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺
407.1458	407.1461	-0.71	74417	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺
408.1432	408.1432	0.02	20415	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺
409.1439	409.1446	-1.71	2802	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺
410.1433	410.1459	-6.41	425	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺

5-Bromopyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**4**)



5-Bromopyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**4**)

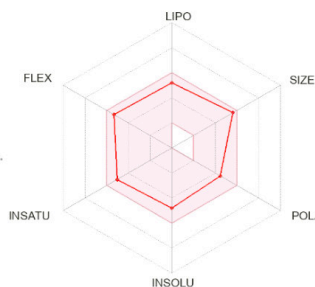
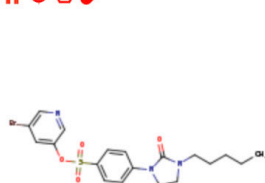




MS spectrum peak list

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	Abund	Formula	Ion
468.0586	468.0587	-0.34	328082	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
469.061	469.0617	-1.4	68626	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
470.0567	470.0568	-0.22	358121	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
471.0588	471.0596	-1.87	70399	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
472.0561	472.0567	-1.34	17982	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
473.0574	473.0581	-1.39	2657	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
474.0582	474.0594	-2.35	396	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺

Molecule 4



SMILES CCCCCN1CCN(C1=O)c1ccc(cc1)S(=O)(=O)Oc1cncc(c1)Br

Physicochemical Properties

Formula	C19H22BrN3O4S
Molecular weight	468.36 g/mol
Num. heavy atoms	28
Num. arom. heavy atoms	12
Fraction Csp3	0.37
Num. rotatable bonds	8
Num. H-bond acceptors	5
Num. H-bond donors	0
Molar Refractivity	117.51
TPSA ²	88.19 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP) ²	3.46
Log $P_{o/w}$ (XLOGP3) ²	3.58
Log $P_{o/w}$ (WLOGP) ²	4.36
Log $P_{o/w}$ (MLOGP) ²	3.09
Log $P_{o/w}$ (SILICOS-IT) ²	2.50
Consensus Log $P_{o/w}$ ²	3.40

Water Solubility

Log S (ESOL) ²	-4.79
Solubility	7.62e-03 mg/ml ; 1.63e-05 mol/l
Class ²	Moderately soluble
Log S (Ali) ²	-5.12
Solubility	3.57e-03 mg/ml ; 7.62e-06 mol/l
Class ²	Moderately soluble
Log S (SILICOS-IT) ²	-6.31
Solubility	2.27e-04 mg/ml ; 4.85e-07 mol/l
Class ²	Poorly soluble

Pharmacokinetics

GI absorption ²	High
BBB permeant ²	No
P-gp substrate ²	No
CYP1A2 inhibitor ²	No
CYP2C19 inhibitor ²	Yes
CYP2C9 inhibitor ²	Yes
CYP2D6 inhibitor ²	No
CYP3A4 inhibitor ²	Yes
Log K_p (skin permeation) ²	-6.62 cm/s

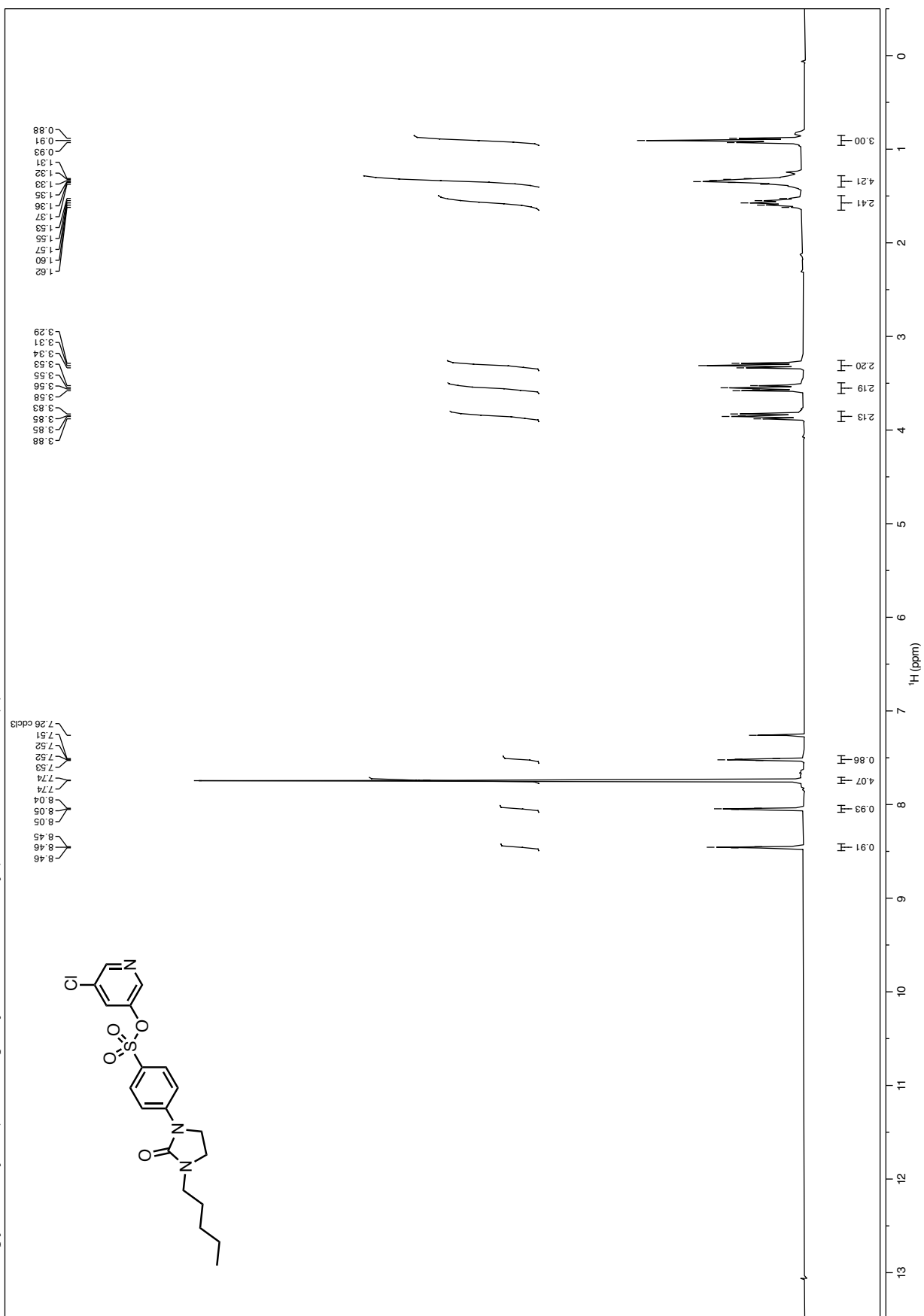
Druglikeness

Lipinski ²	Yes; 0 violation
Ghose ²	Yes
Veber ²	Yes
Egan ²	Yes
Muegge ²	Yes
Bioavailability Score ²	0.55

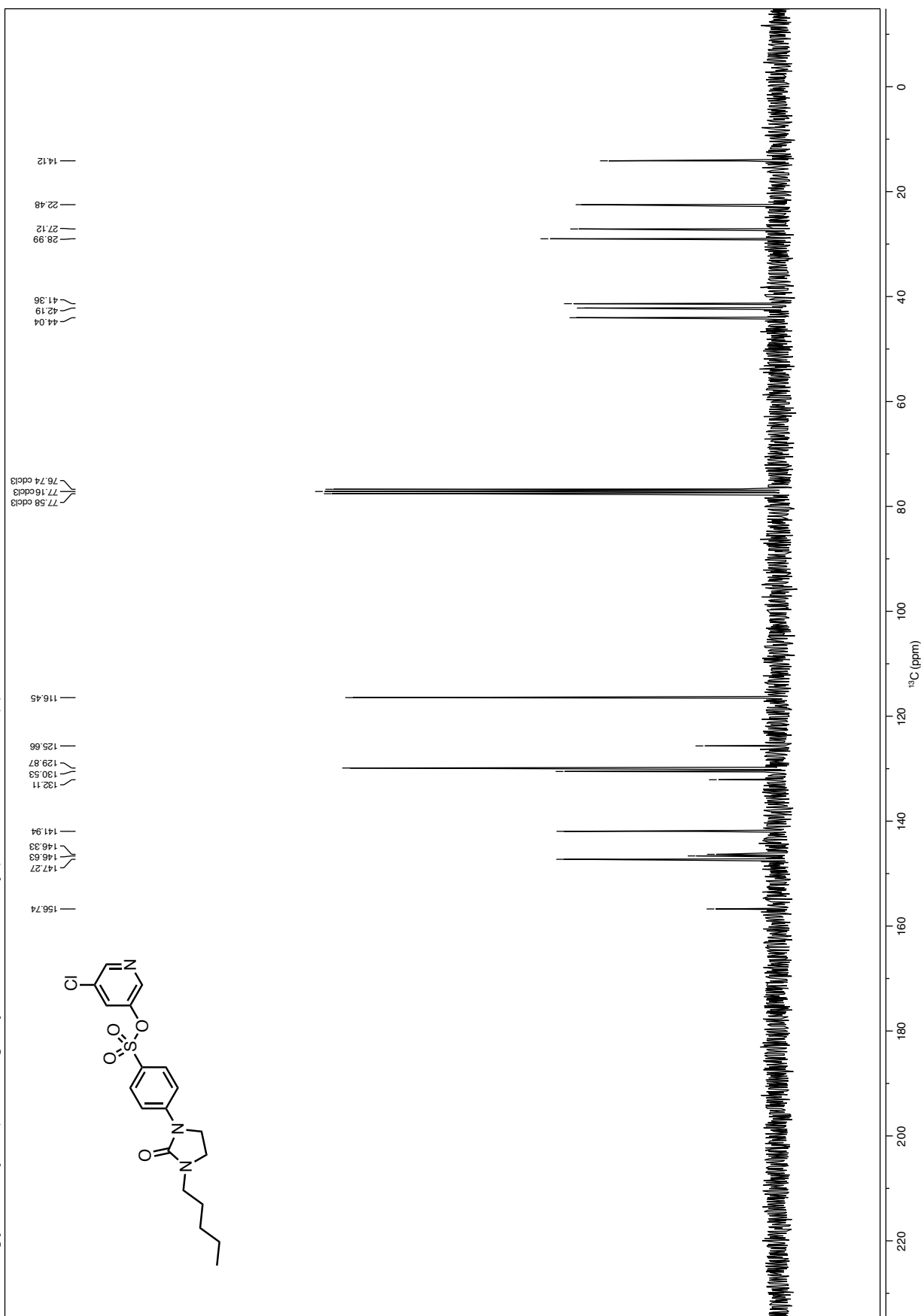
Medicinal Chemistry

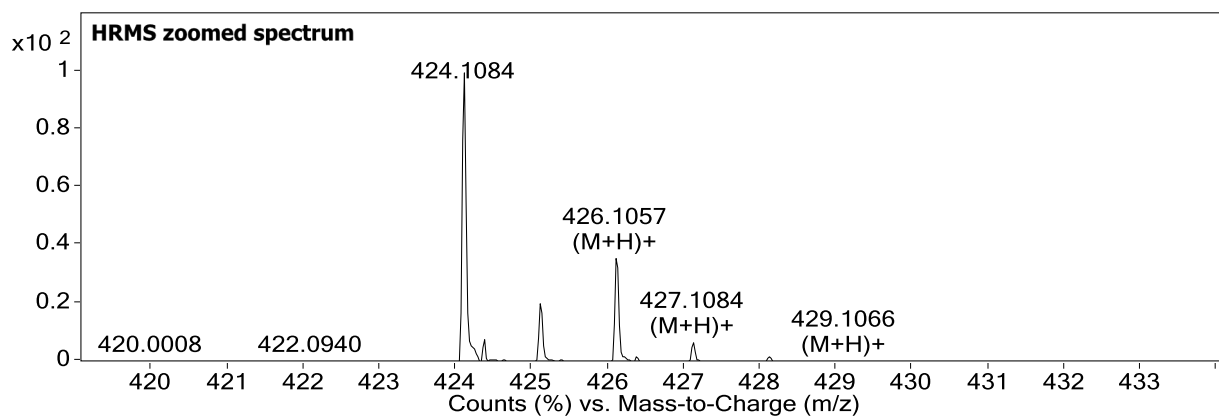
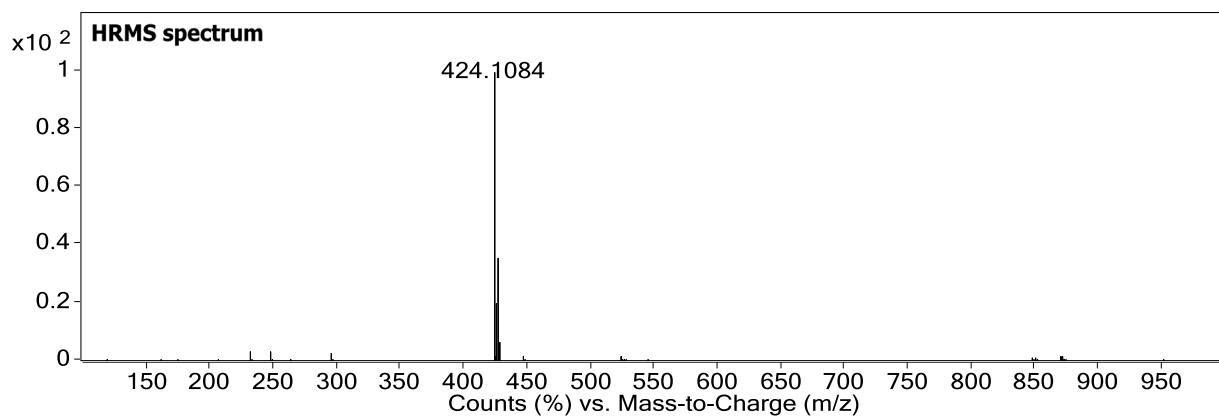
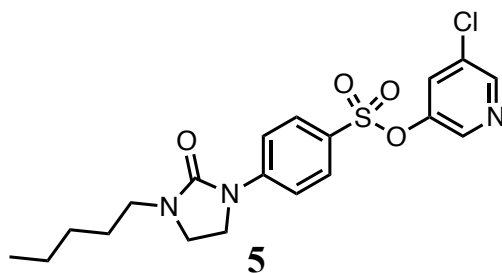
PAINS ²	0 alert
Brenk ²	1 alert: sulfonic_acid_1 ²
Leadlikeness ²	No; 3 violations: MW>350, Rotors>7, XLOGP3>3.5
Synthetic accessibility ²	3.32

5-Chloropyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**5**)



5-Chloropyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**5**)

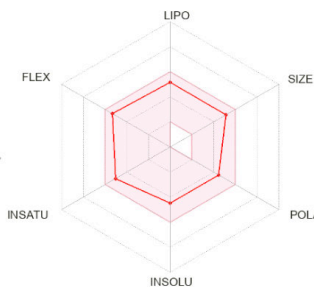
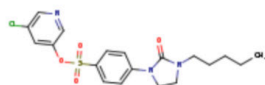




MS spectrum peak list

<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
424.1084	424.1092	-2.03	1	373280	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺
425.1112	425.1122	-2.36		76186	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺
426.1057	426.1068	-2.63		138012	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺
427.1084	427.1094	-2.38		23994	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺
428.106	428.1066	-1.4		6093	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺
429.1066	429.1079	-3.01		953	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺

Molecule 5



SMILES CCCCCN1CCN(C1=O)c1ccc(cc1)S(=O)(=O)Oc1cncc(c1)Cl

Physicochemical Properties

Formula	C ₁₉ H ₂₂ ClN ₃ O ₄ S
Molecular weight	423.91 g/mol
Num. heavy atoms	28
Num. arom. heavy atoms	12
Fraction Csp ³	0.37
Num. rotatable bonds	8
Num. H-bond acceptors	5
Num. H-bond donors	0
Molar Refractivity	114.82
TPSA ²	88.19 Å ²

Lipophilicity

Log <i>P</i> _{o/w} (iLOGP) ²	3.41
Log <i>P</i> _{o/w} (XLOGP3) ²	3.52
Log <i>P</i> _{o/w} (WLOGP) ²	4.25
Log <i>P</i> _{o/w} (MLOGP) ²	2.98
Log <i>P</i> _{o/w} (SILICOS-IT) ²	2.46
Consensus Log <i>P</i> _{o/w} ²	3.32

Water Solubility

Log <i>S</i> (ESOL) ²	-4.48
Solubility	1.42e-02 mg/ml ; 3.35e-05 mol/l
Class ²	Moderately soluble
Log <i>S</i> (Ali) ²	-5.06
Solubility	3.73e-03 mg/ml ; 8.79e-06 mol/l
Class ²	Moderately soluble
Log <i>S</i> (SILICOS-IT) ²	-6.12
Solubility	3.20e-04 mg/ml ; 7.55e-07 mol/l
Class ²	Poorly soluble

Pharmacokinetics

GI absorption ²	High
BBB permeant ²	No
P-gp substrate ²	No
CYP1A2 inhibitor ²	No
CYP2C19 inhibitor ²	Yes
CYP2C9 inhibitor ²	Yes
CYP2D6 inhibitor ²	No
CYP3A4 inhibitor ²	Yes
Log <i>K</i> _p (skin permeation) ²	-6.39 cm/s

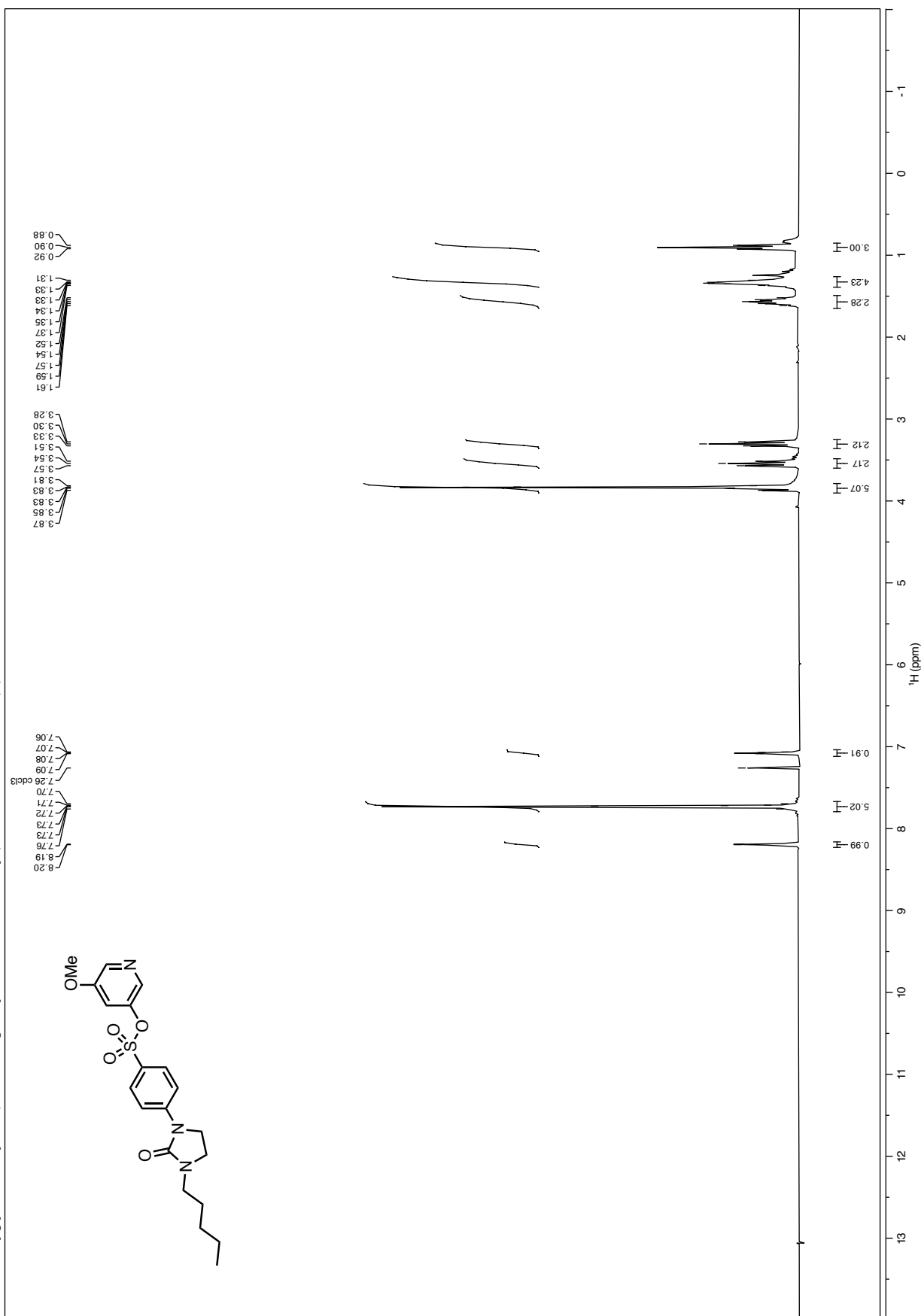
Druglikeness

Lipinski ²	Yes; 0 violation
Ghose ²	Yes
Veber ²	Yes
Egan ²	Yes
Muegge ²	Yes
Bioavailability Score ²	0.55

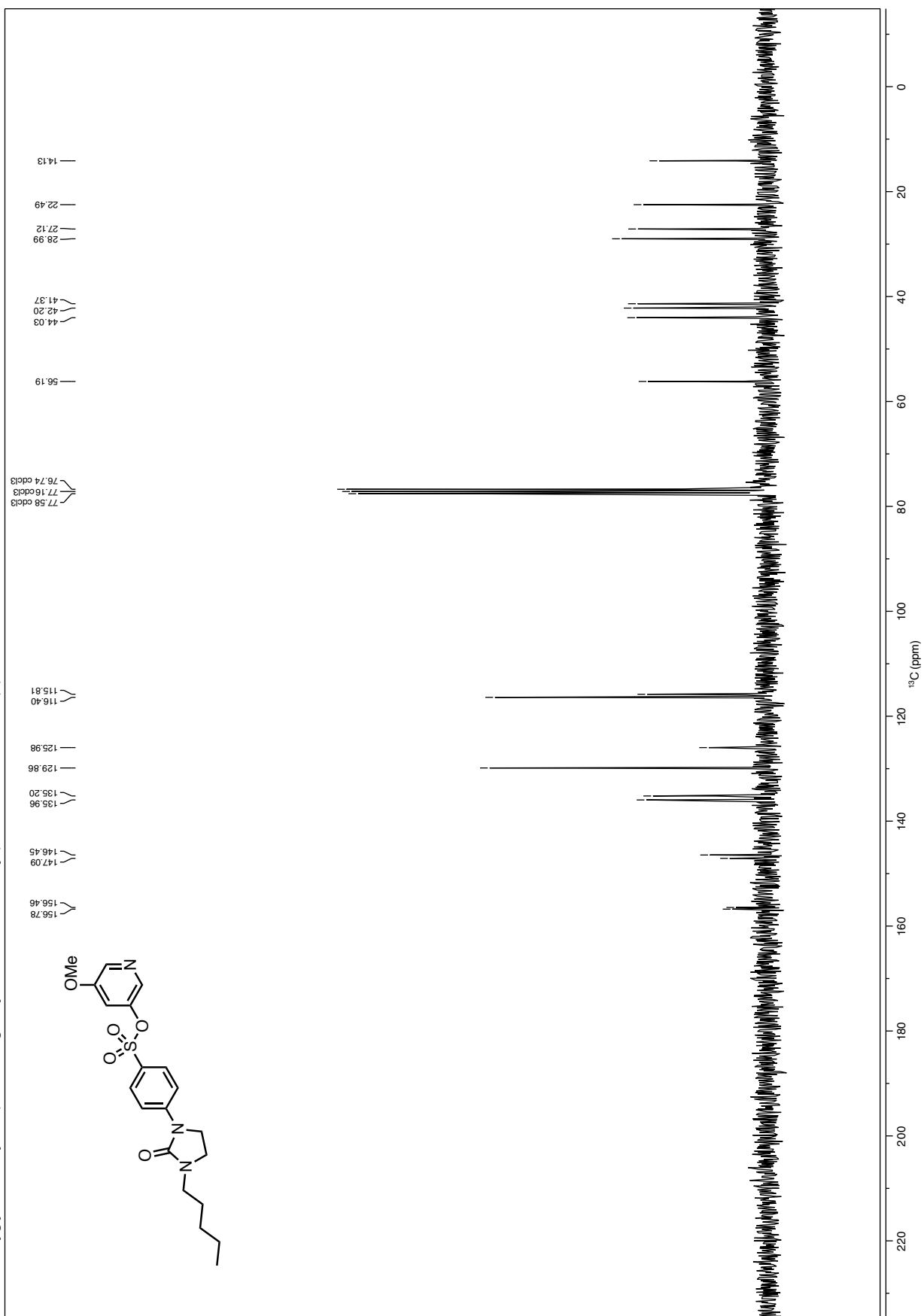
Medicinal Chemistry

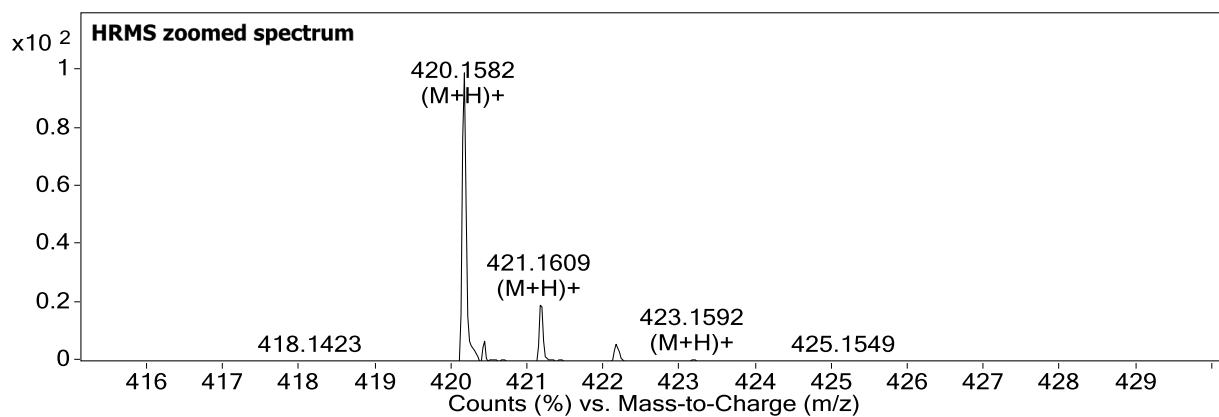
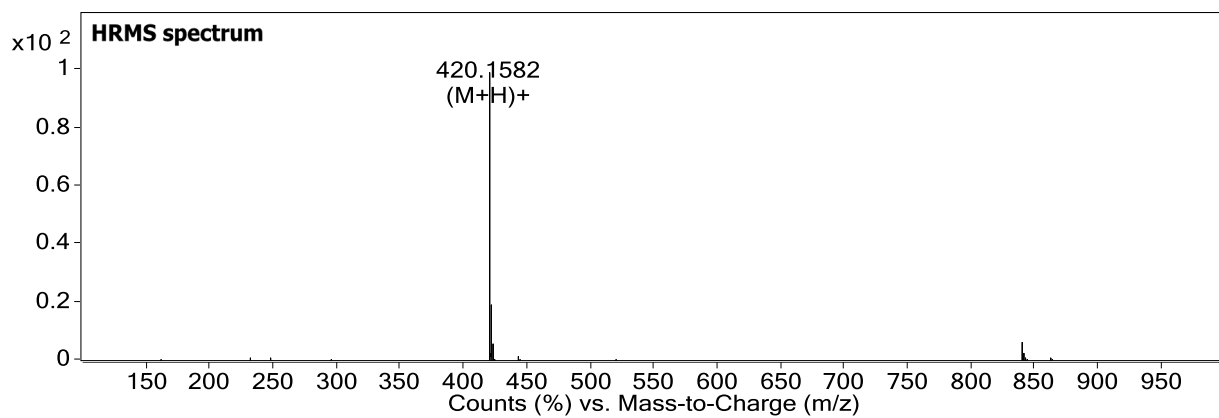
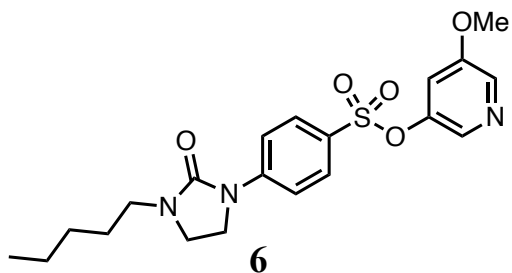
PAINS ²	0 alert
Brenk ²	1 alert: sulfonic_acid_1 ²
Leadlikeness ²	No; 3 violations: MW>350, Rotors>7, XLOGP3>3.5
Synthetic accessibility ²	3.29

5-Methoxypyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**6**)



5-Methoxypyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**6**)

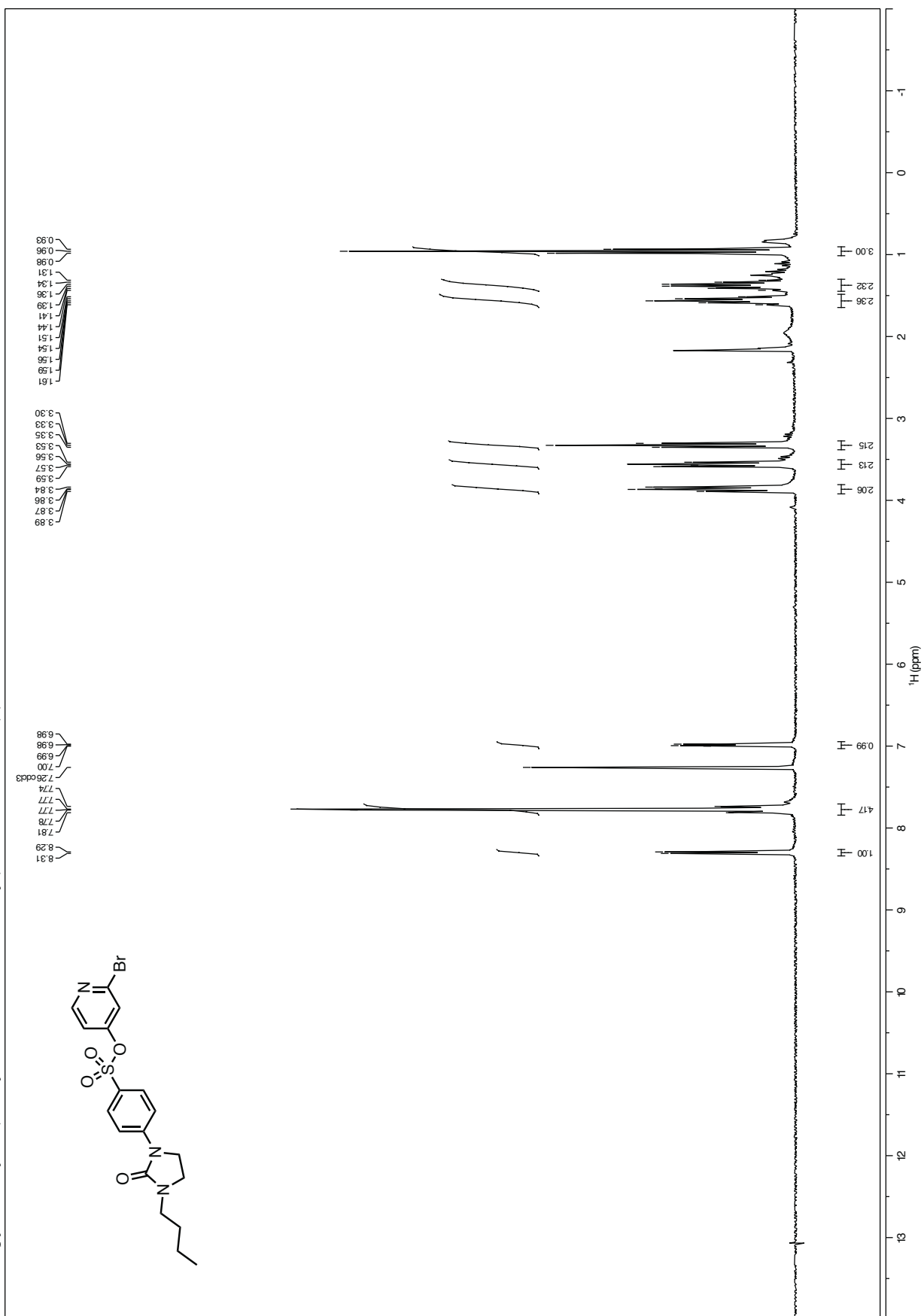




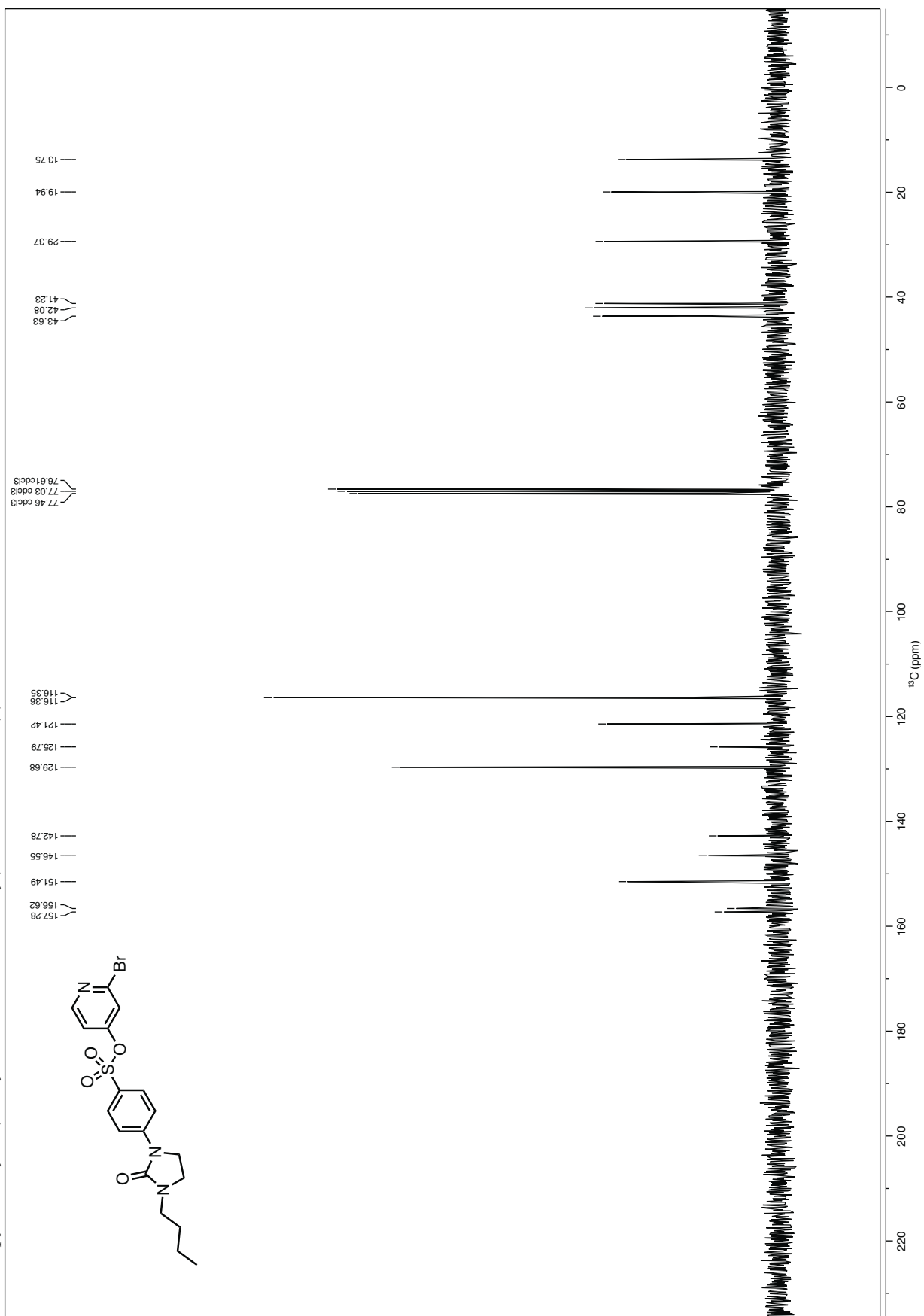
MS spectrum peak list

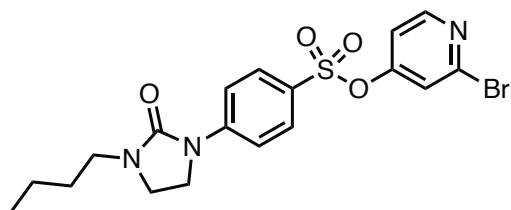
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	Abund	Formula	Ion
420.1582	420.1588	-1.34	350684	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺
421.1609	421.1617	-1.93	72490	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺
422.1588	422.159	-0.4	20368	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺
423.1592	423.1604	-2.78	2992	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺
424.1603	424.1617	-3.23	459	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺

2-Bromopyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (7)

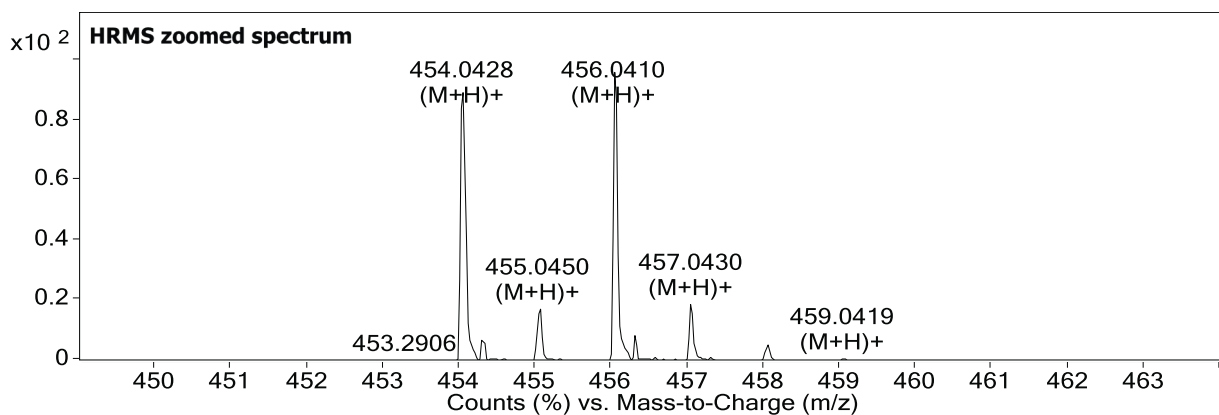
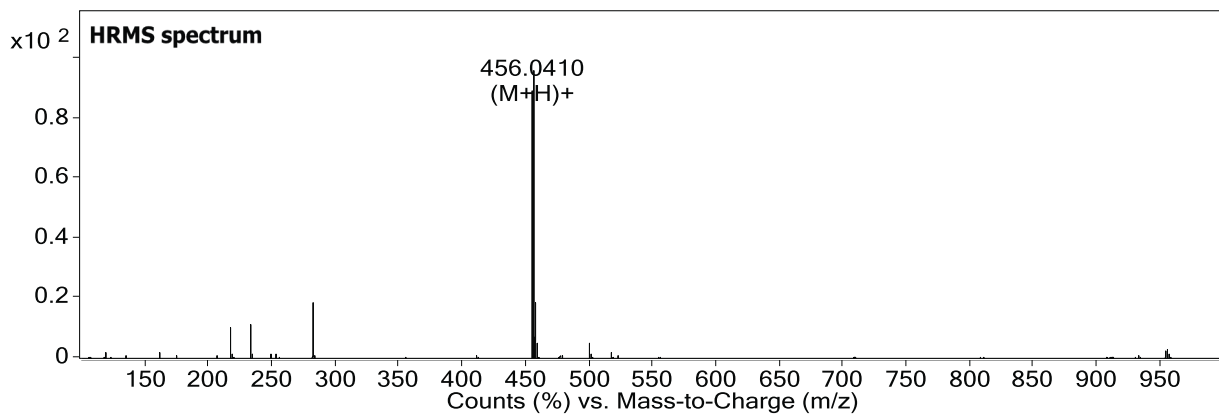


2-Bromopyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (7)





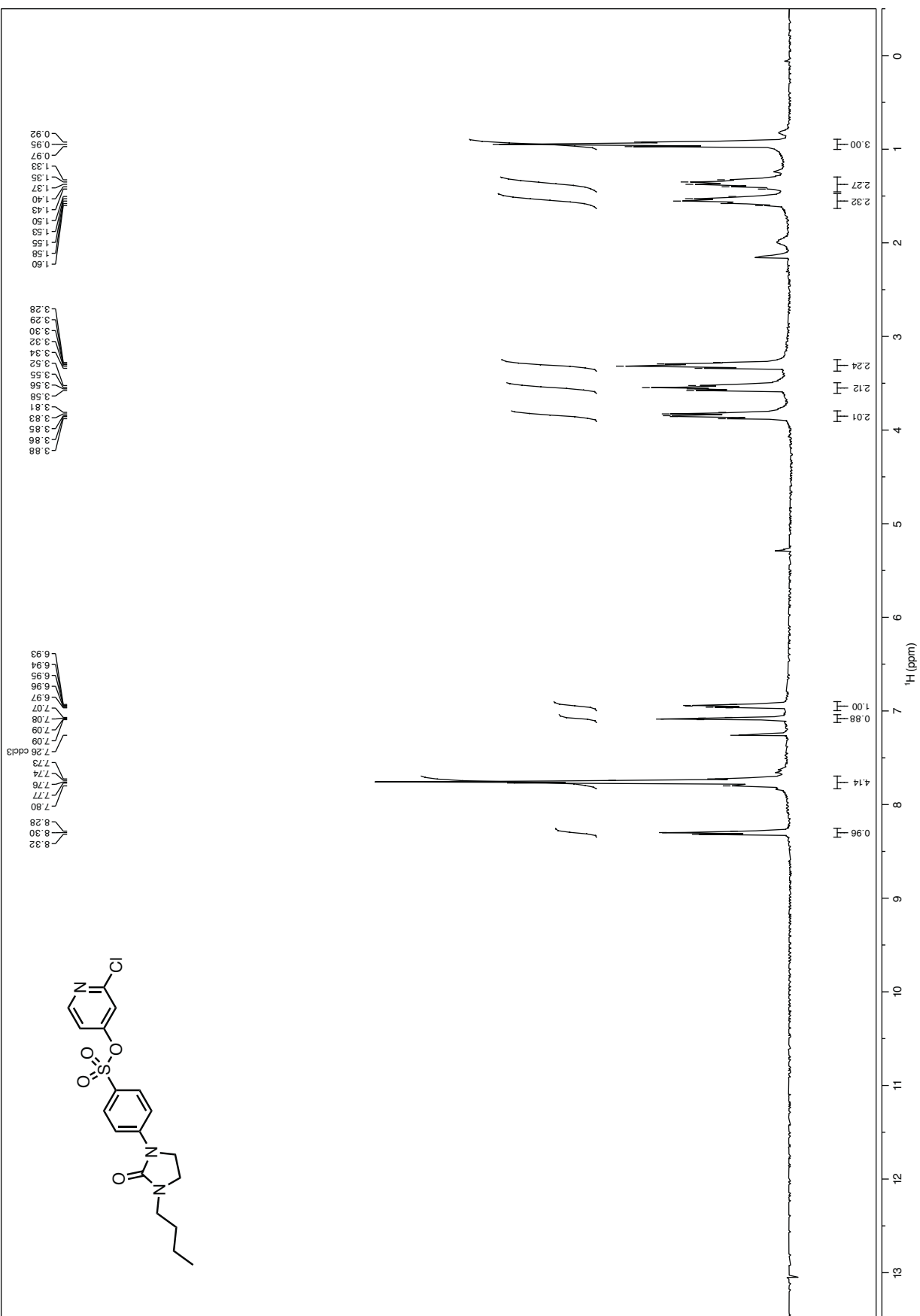
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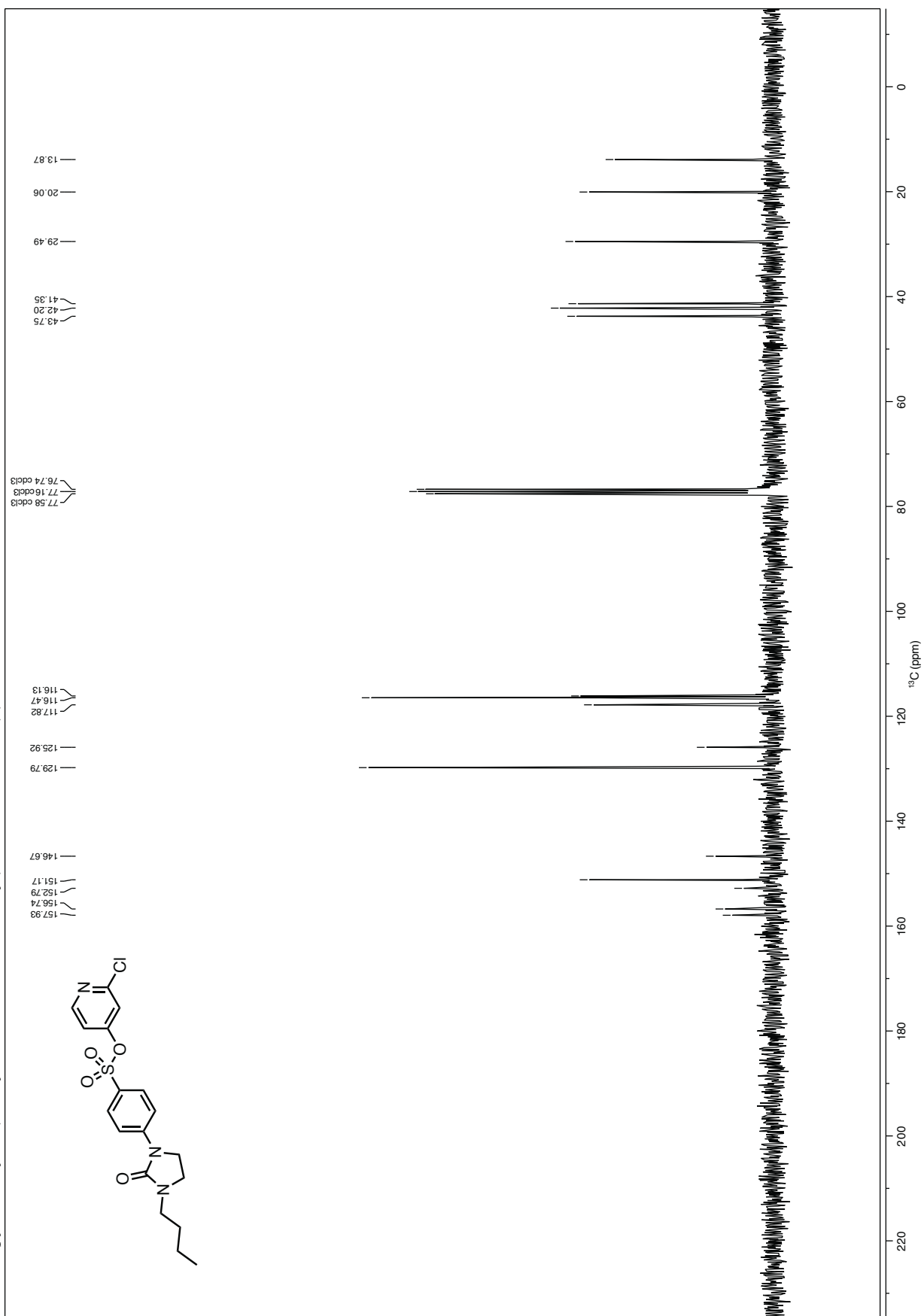
MS spectrum peak list

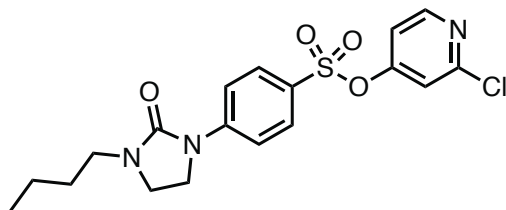
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
454.0428	454.0431	-0.58	359007	C18 H21 Br N3 O4 S	(M+H)+
455.045	455.046	-2.27	68252	C18 H21 Br N3 O4 S	(M+H)+
456.041	456.0411	-0.33	382873	C18 H21 Br N3 O4 S	(M+H)+
457.043	457.044	-2.11	73266	C18 H21 Br N3 O4 S	(M+H)+
458.04	458.0408	-1.79	19734	C18 H21 Br N3 O4 S	(M+H)+
459.0419	459.0423	-0.93	2703	C18 H21 Br N3 O4 S	(M+H)+
460.0435	460.0435	-0.03	399	C18 H21 Br N3 O4 S	(M+H)+

2-Chloropyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (**8**)

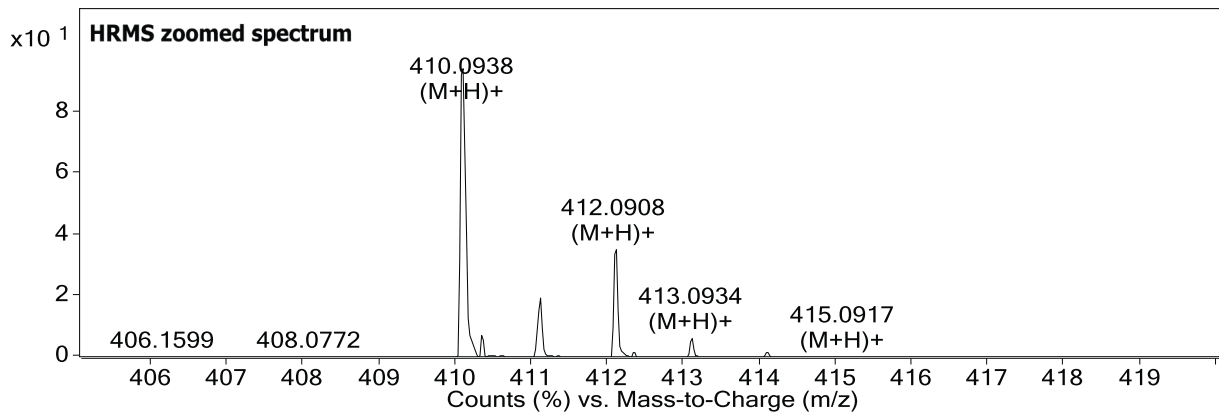
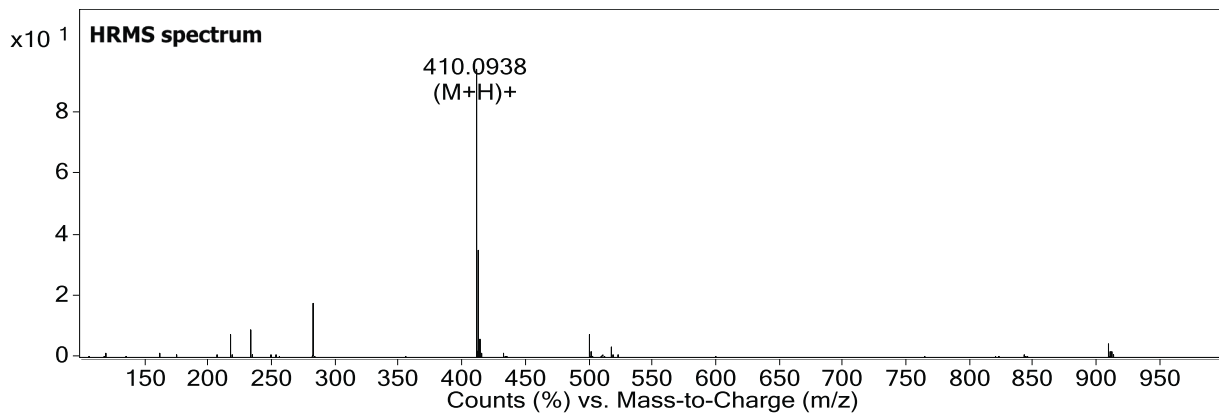


2-Chloropyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (**8**)





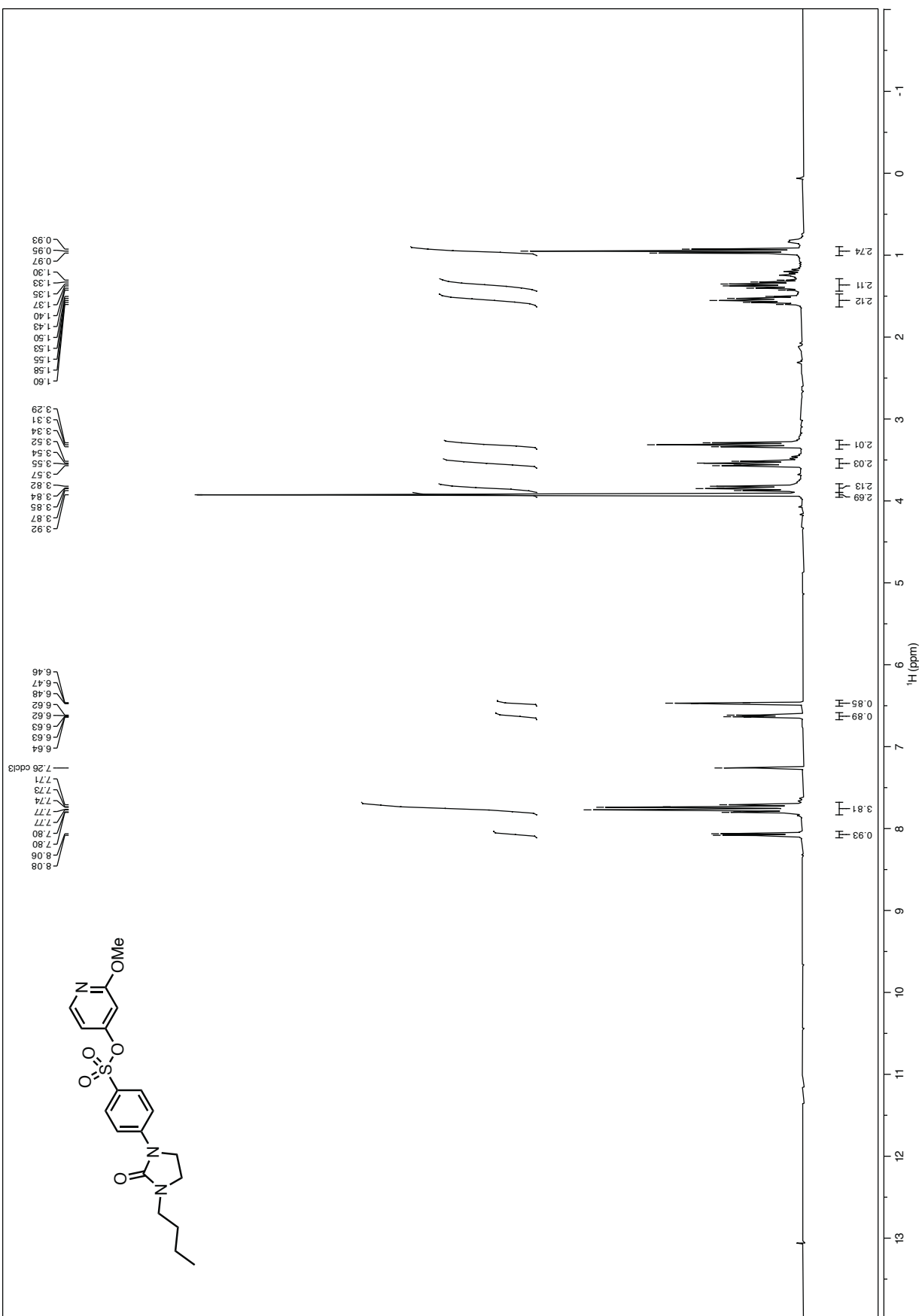
8



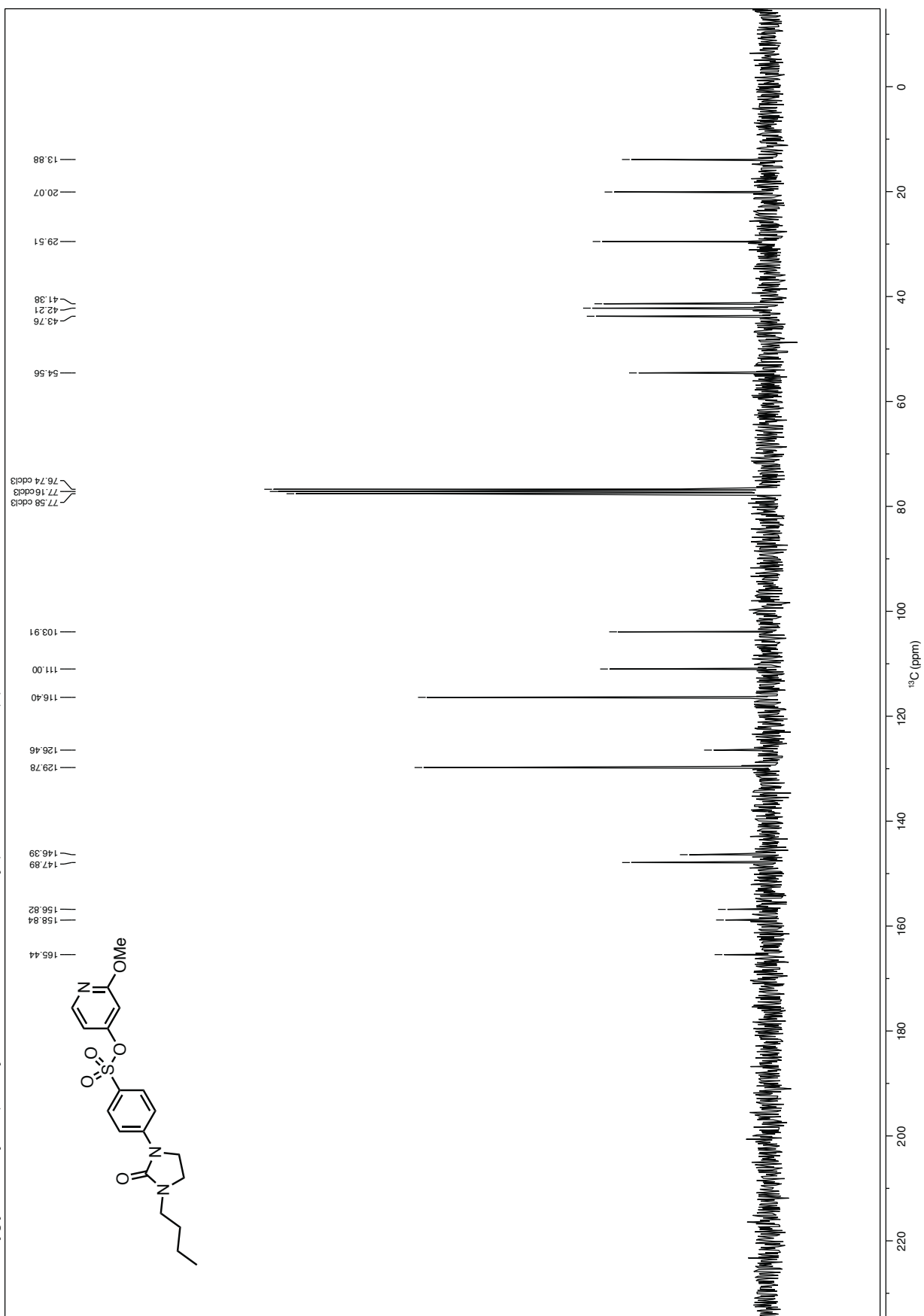
MS spectrum peak list

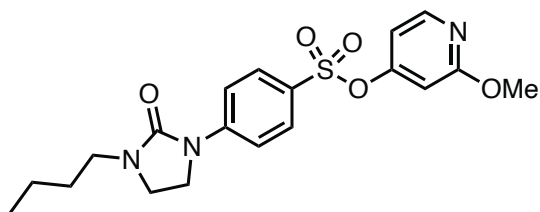
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
410.0938	410.0936	0.42	377201	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
411.0963	411.0965	-0.45	73821	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
412.0908	412.0911	-0.73	139781	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
413.0934	413.0937	-0.79	23215	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
414.0909	414.0907	0.47	5984	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺
415.0917	415.0921	-0.94	938	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺

2-Methoxypyridin-4-yl 4-(3-buty-2-oxoimidazolidin-1-yl)benzenesulfonate (**9**)

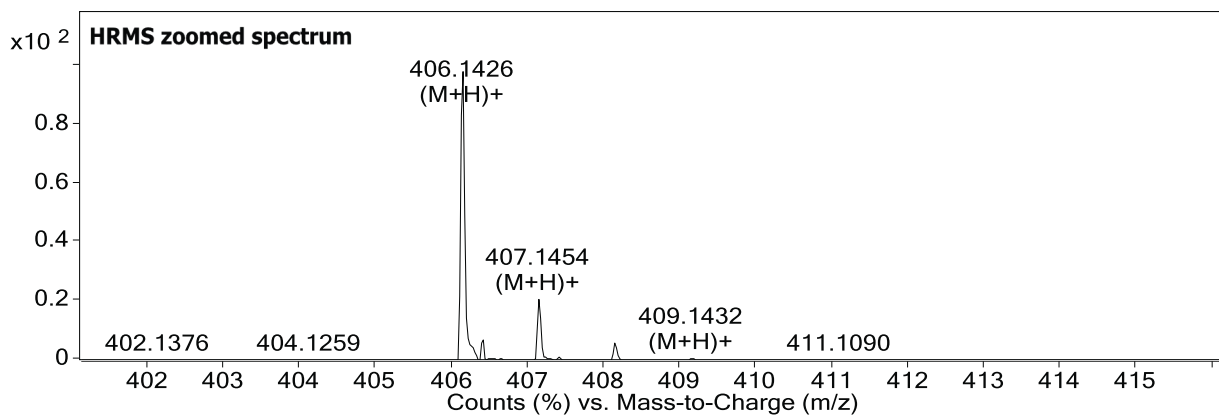
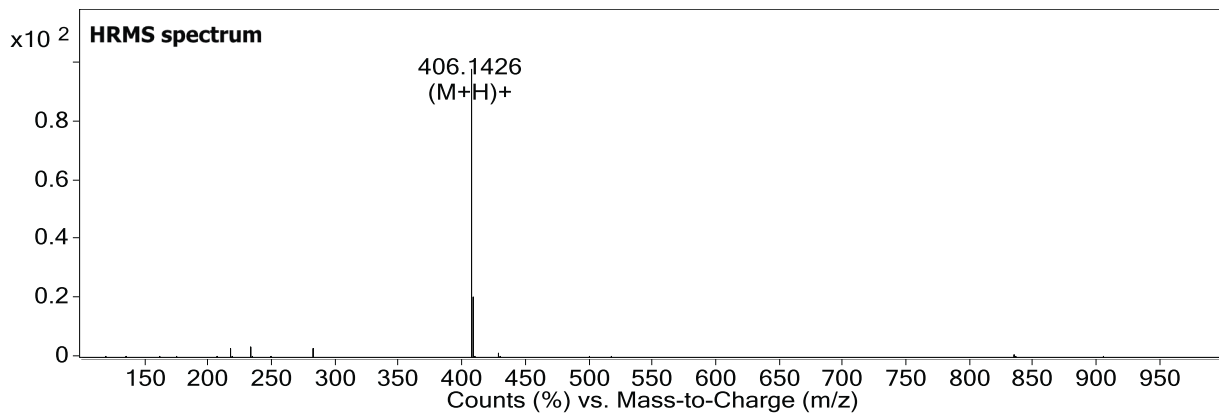


2-Methoxypyridin-4-yl 4-(3-buty-2-oxoimidazolidin-1-yl)benzenesulfonate (**9**)





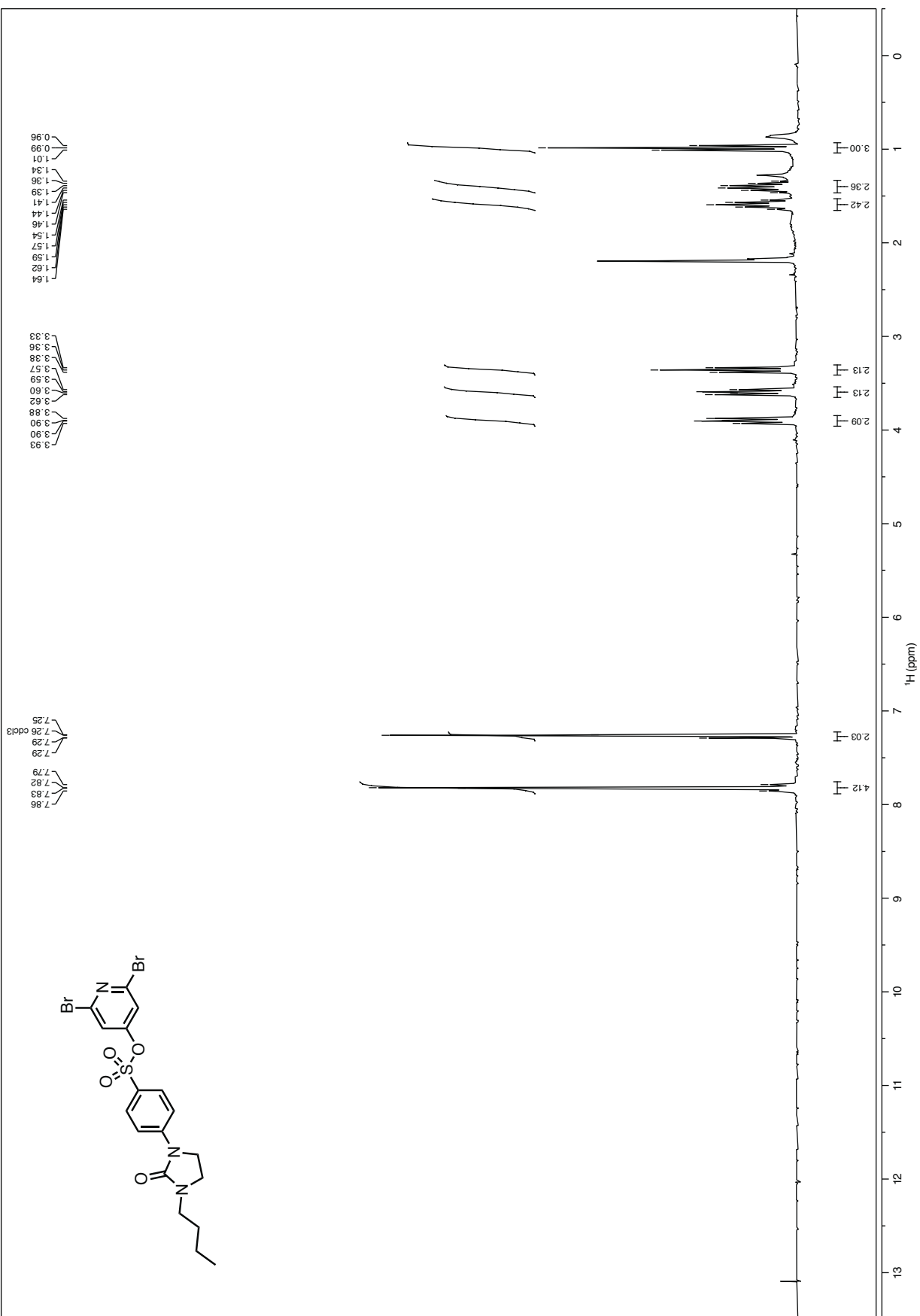
9



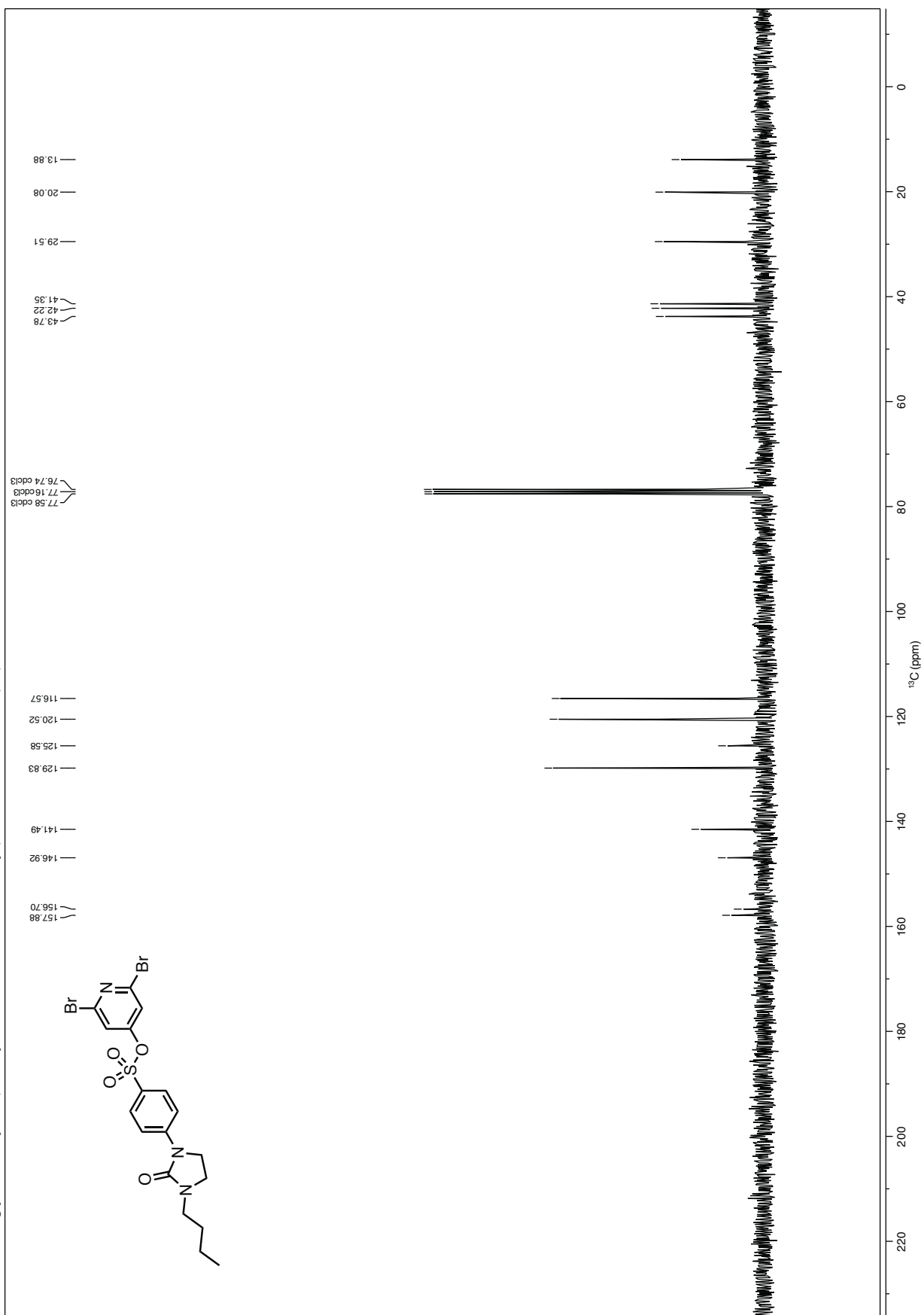
MS spectrum peak list

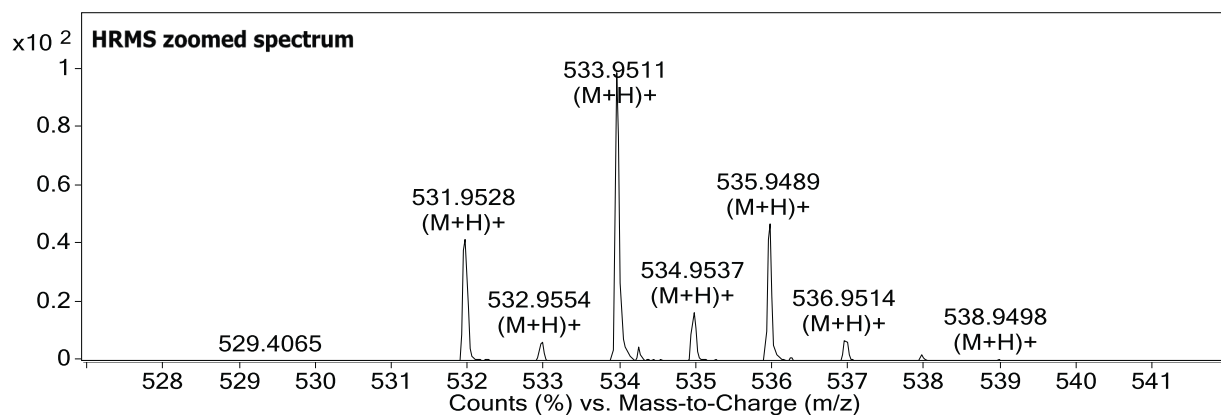
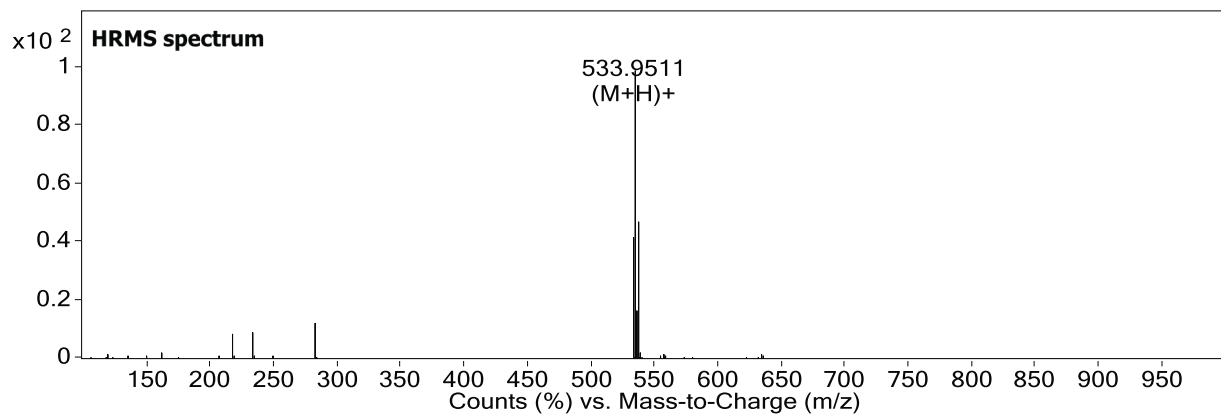
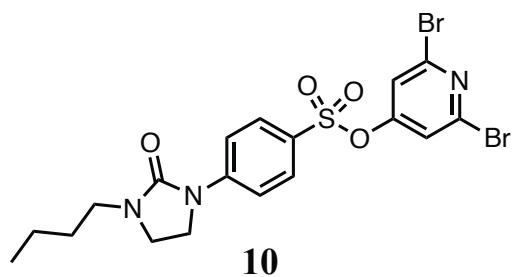
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
406.1426	406.1431	-1.36	380289	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺
407.1454	407.1461	-1.64	79371	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺
408.1427	408.1432	-1.02	21751	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺
409.1432	409.1446	-3.56	3011	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺

2,6-Dibromopyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (**10**)



2,6-Dibromopyridin-4-yl 4-(3-buty1-2-oxoimidazolidin-1-yl)benzenesulfonate (**10**)

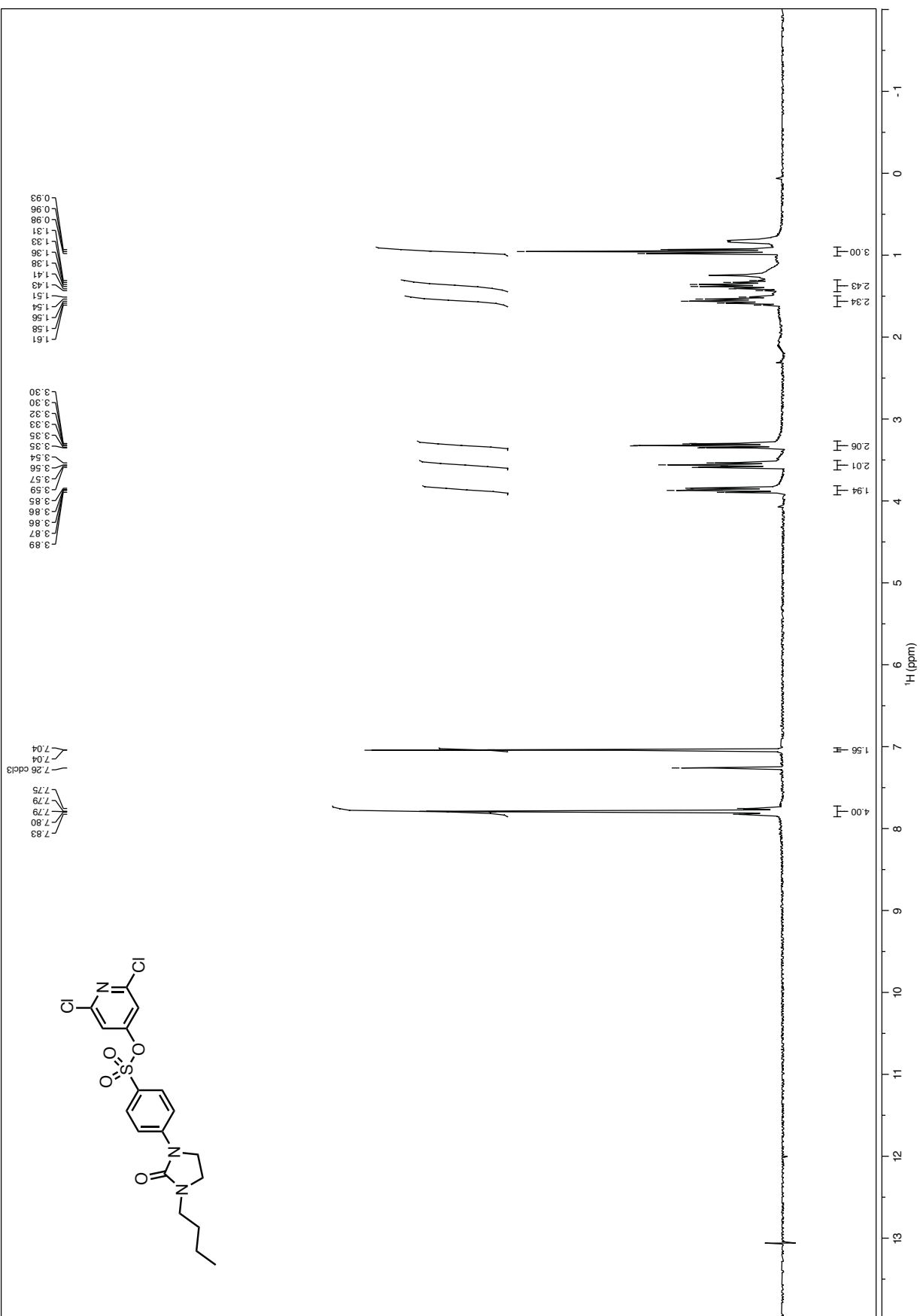




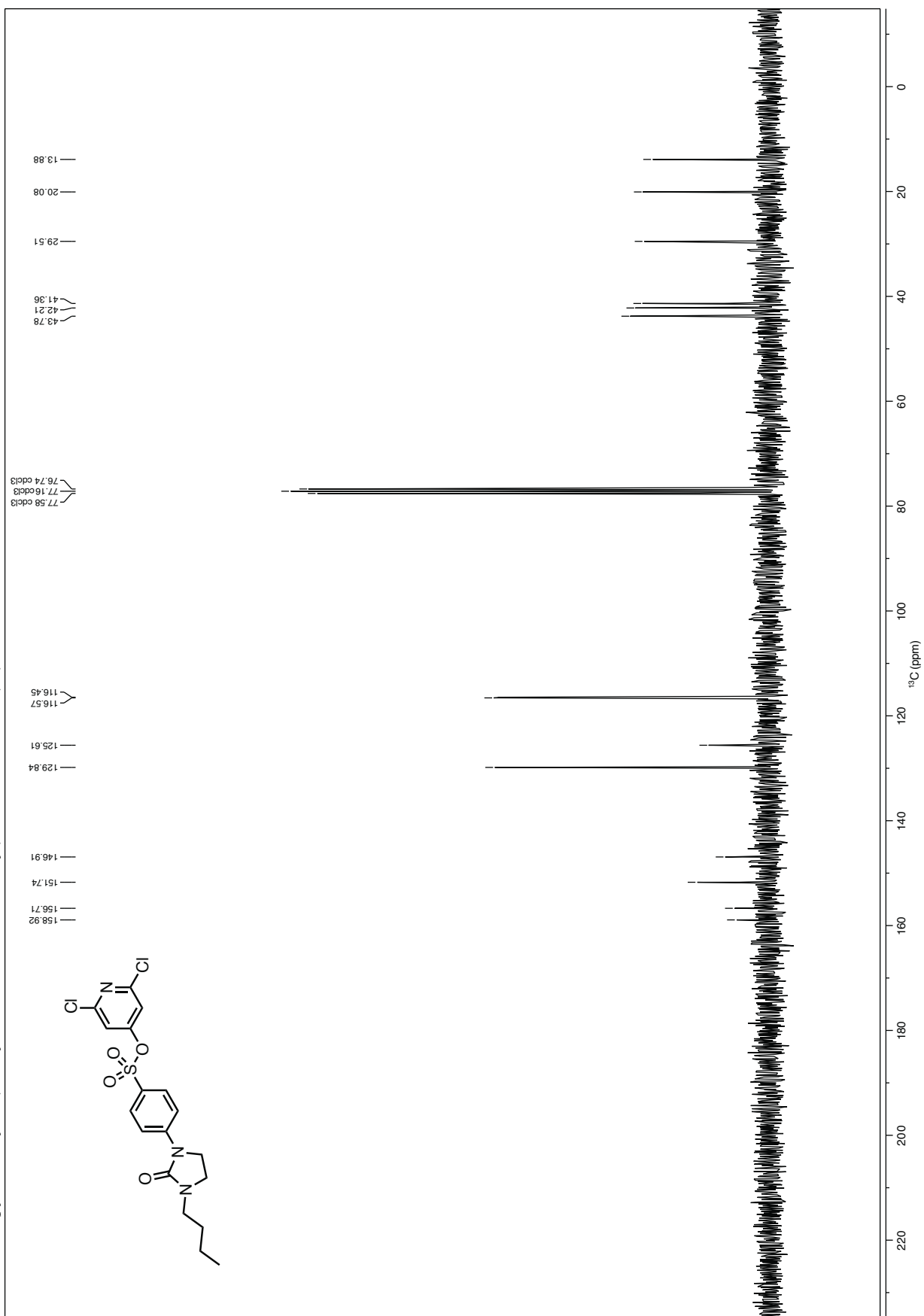
MS spectrum peak list

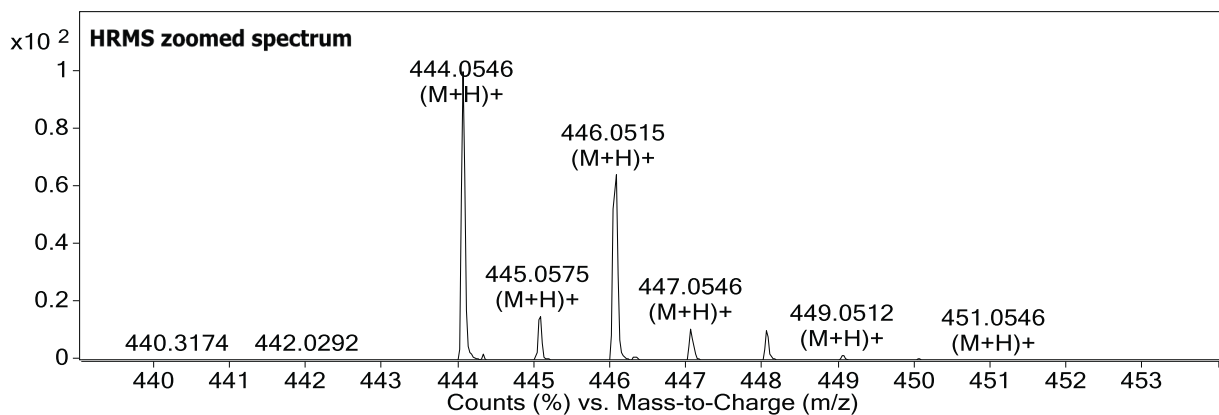
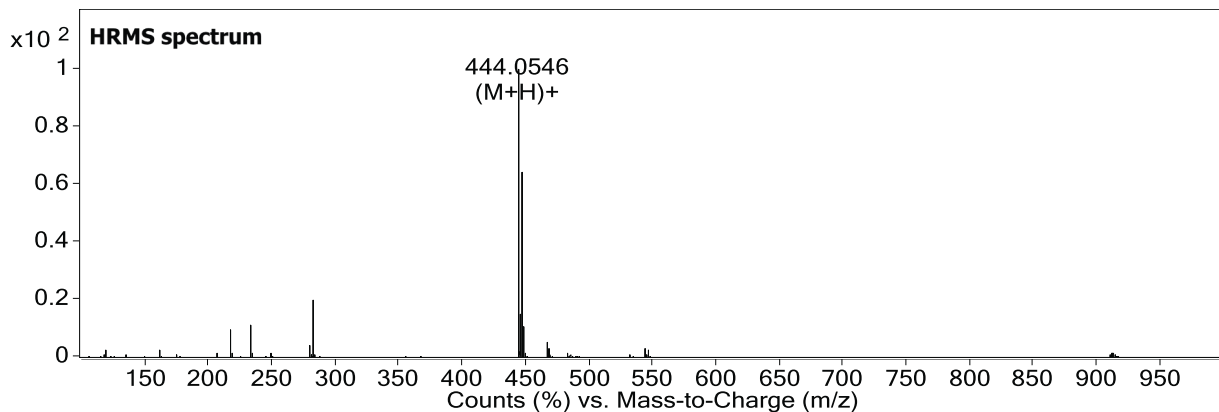
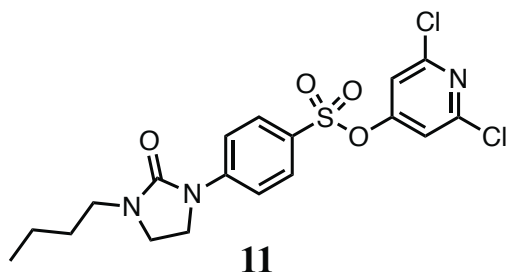
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
531.9528	531.9536	-1.49		67239	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H) ⁺
532.9554	532.9565	-2.12		10211	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H) ⁺
533.9511	533.9516	-0.97		154416	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H) ⁺
534.9537	534.9545	-1.43		25847	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H) ⁺
535.9489	535.9497	-1.51		75355	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H) ⁺
536.9514	536.9525	-1.95		11476	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H) ⁺
537.9492	537.9494	-0.3		3019	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H) ⁺
538.9498	538.9508	-1.88	1	450	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H) ⁺

2,6-Dichloropyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (**11**)



2,6-Dichloropyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate (**11**)

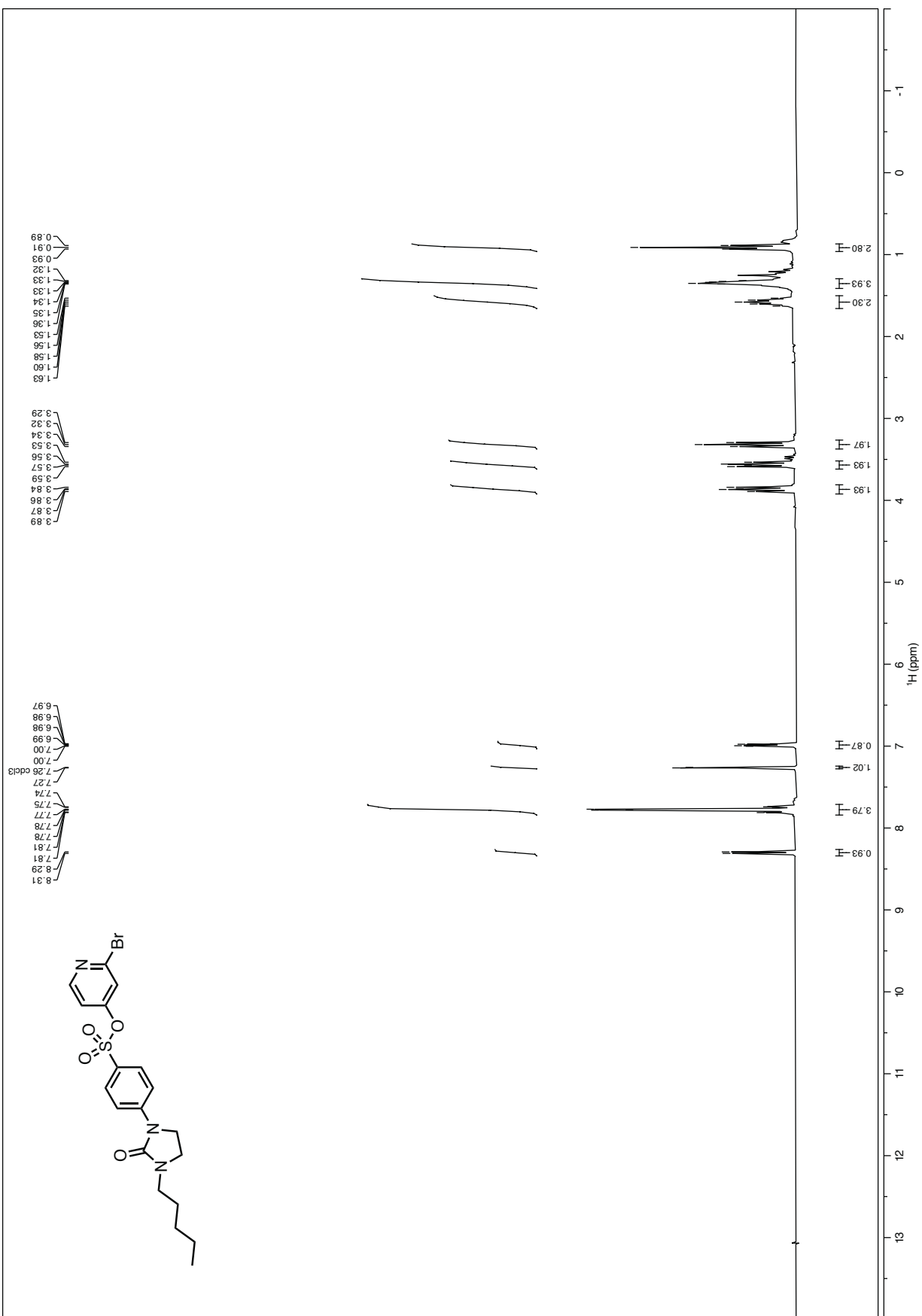




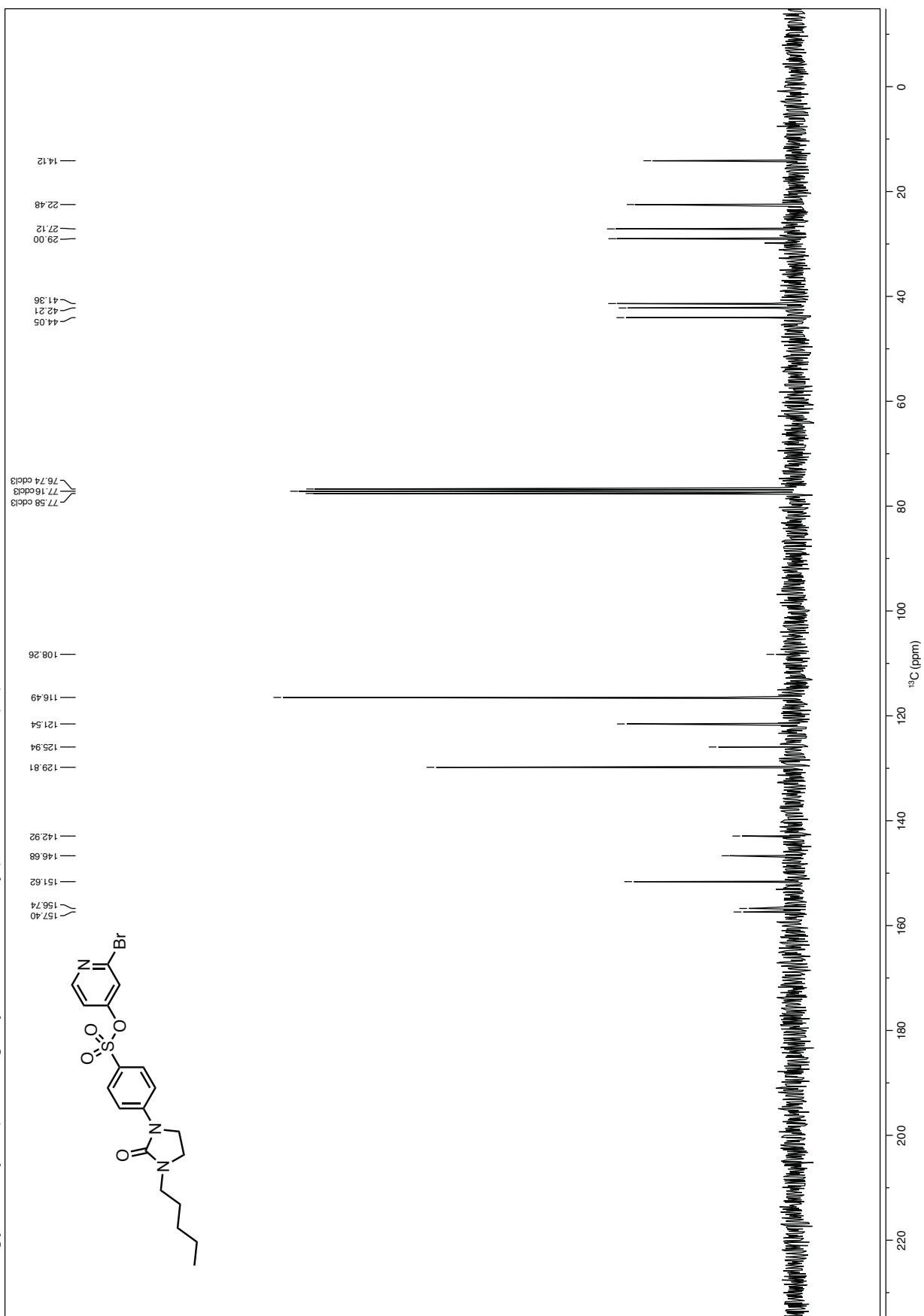
MS spectrum peak list

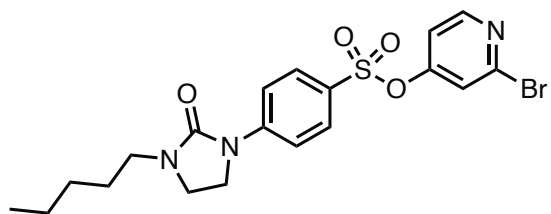
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
444.0546	444.0546	0.08		76874	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺
445.0575	445.0575	0		12097	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺
446.0515	446.0519	-0.88		50732	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺
447.0546	447.0547	-0.16		8244	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺
448.0499	448.0496	0.46		8233	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺
449.0512	449.052	-1.8		1327	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺
450.0488	450.0491	-0.79	1	410	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺
451.0546	451.0504	9.33	1	74	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺

2-Bromopyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**12**)

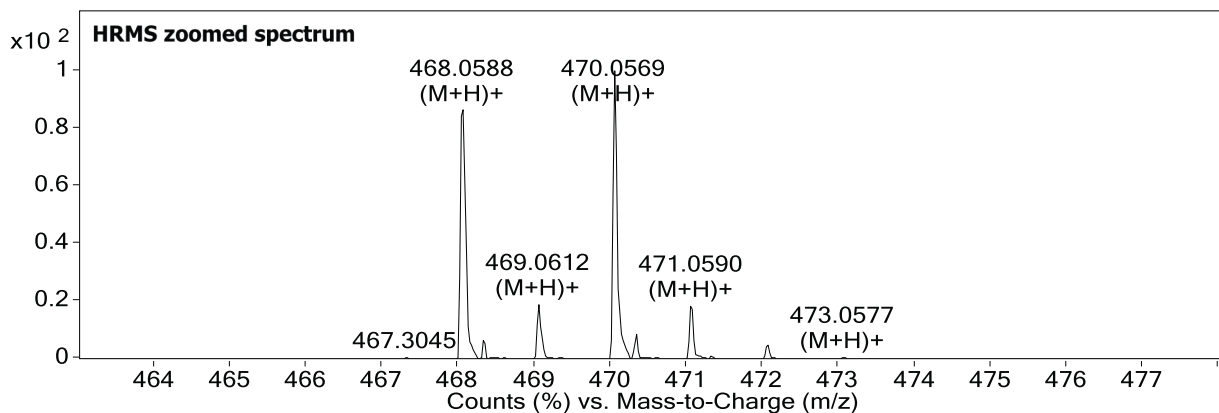
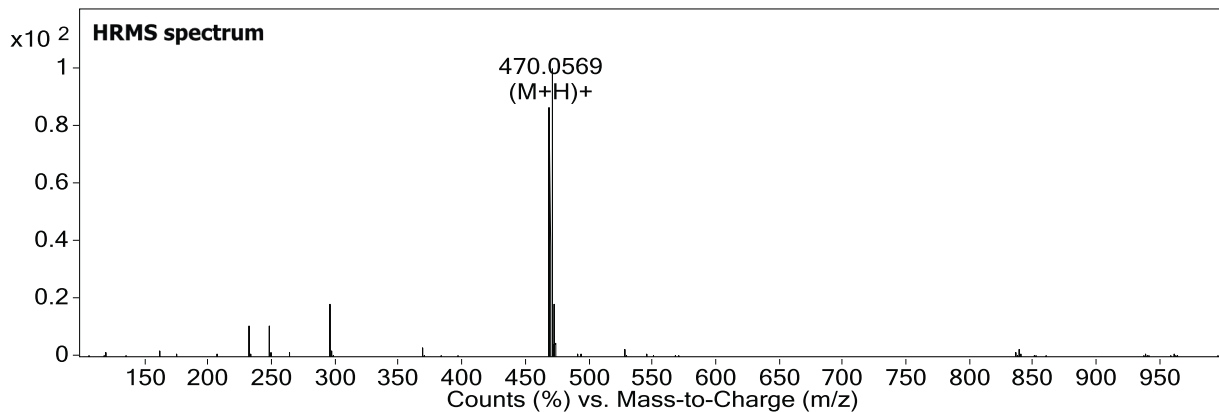


2-Bromopyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**12**)





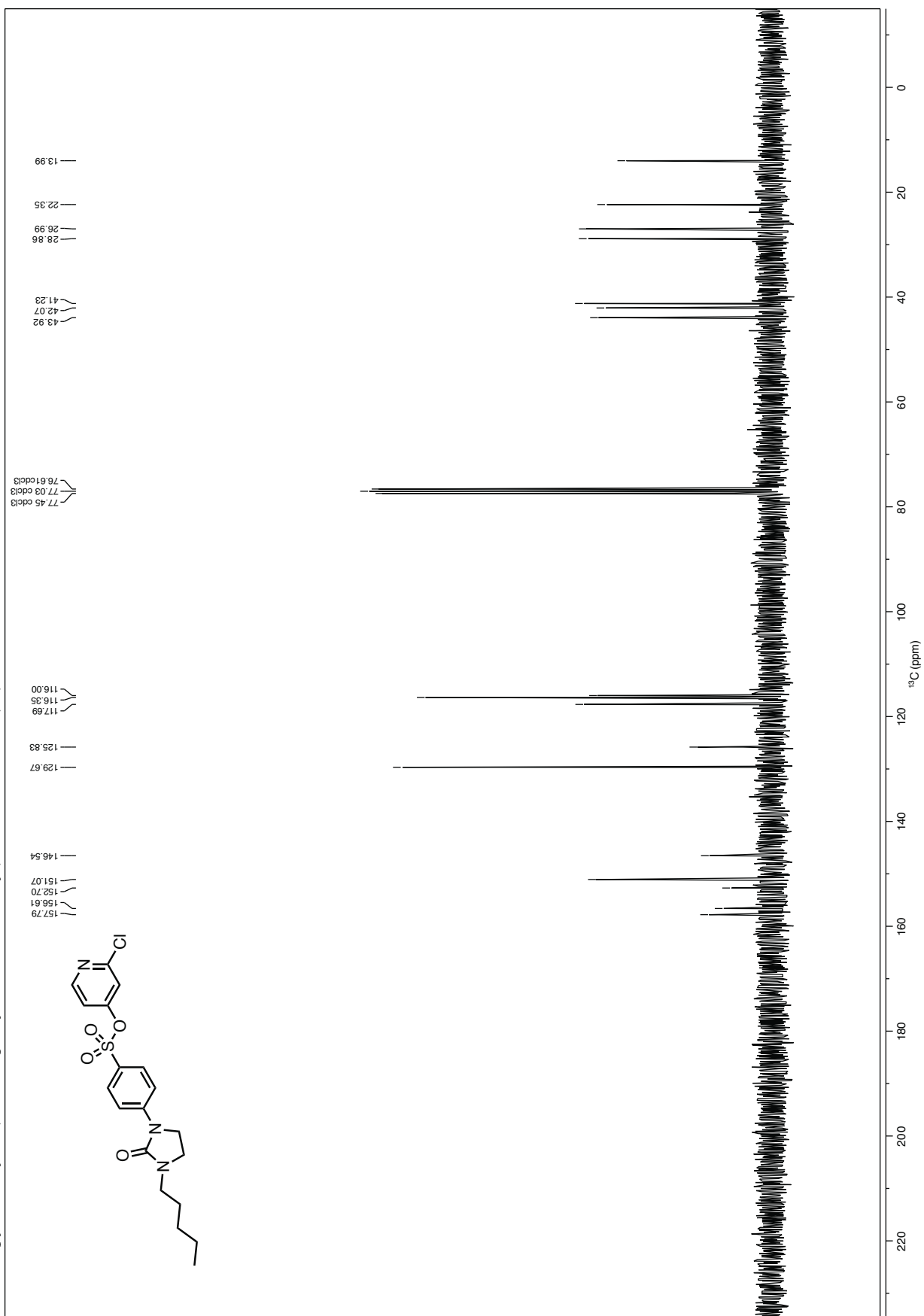
12

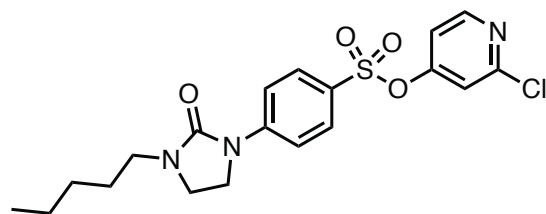


MS spectrum peak list

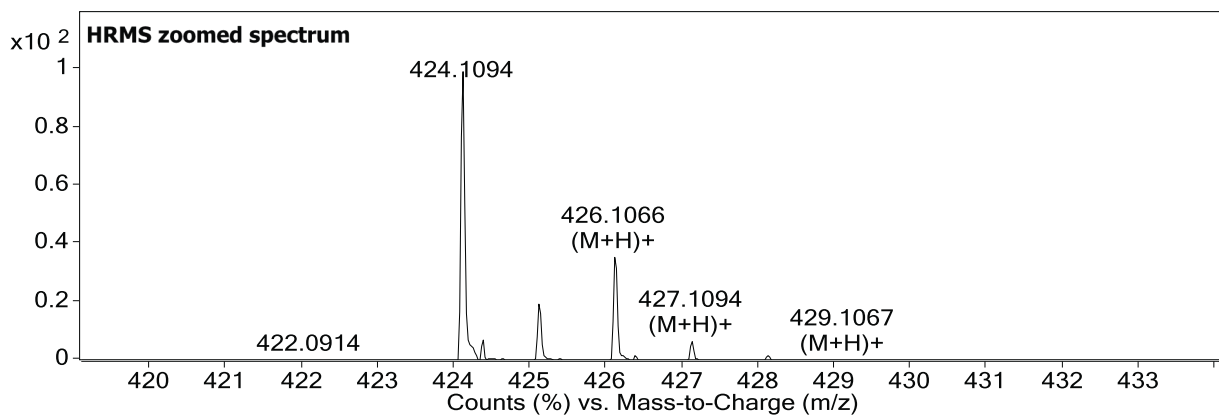
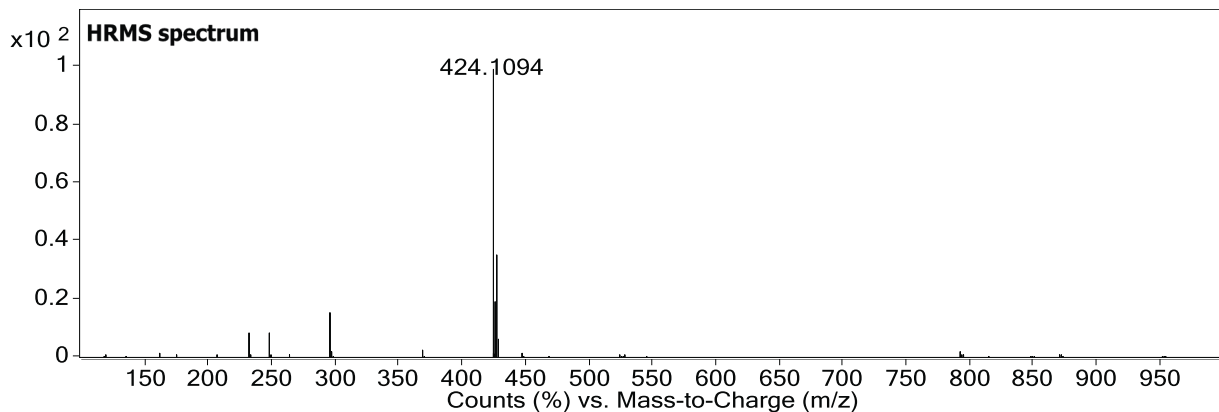
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
468.0588	468.0587	0.08	326440	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
469.0612	469.0617	-0.99	67916	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
470.0569	470.0568	0.27	356399	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
471.059	471.0596	-1.27	69994	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
472.0562	472.0567	-1.09	17974	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
473.0577	473.0581	-0.83	2646	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺
474.0587	474.0594	-1.29	407	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺

2-Chloropyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**13**)





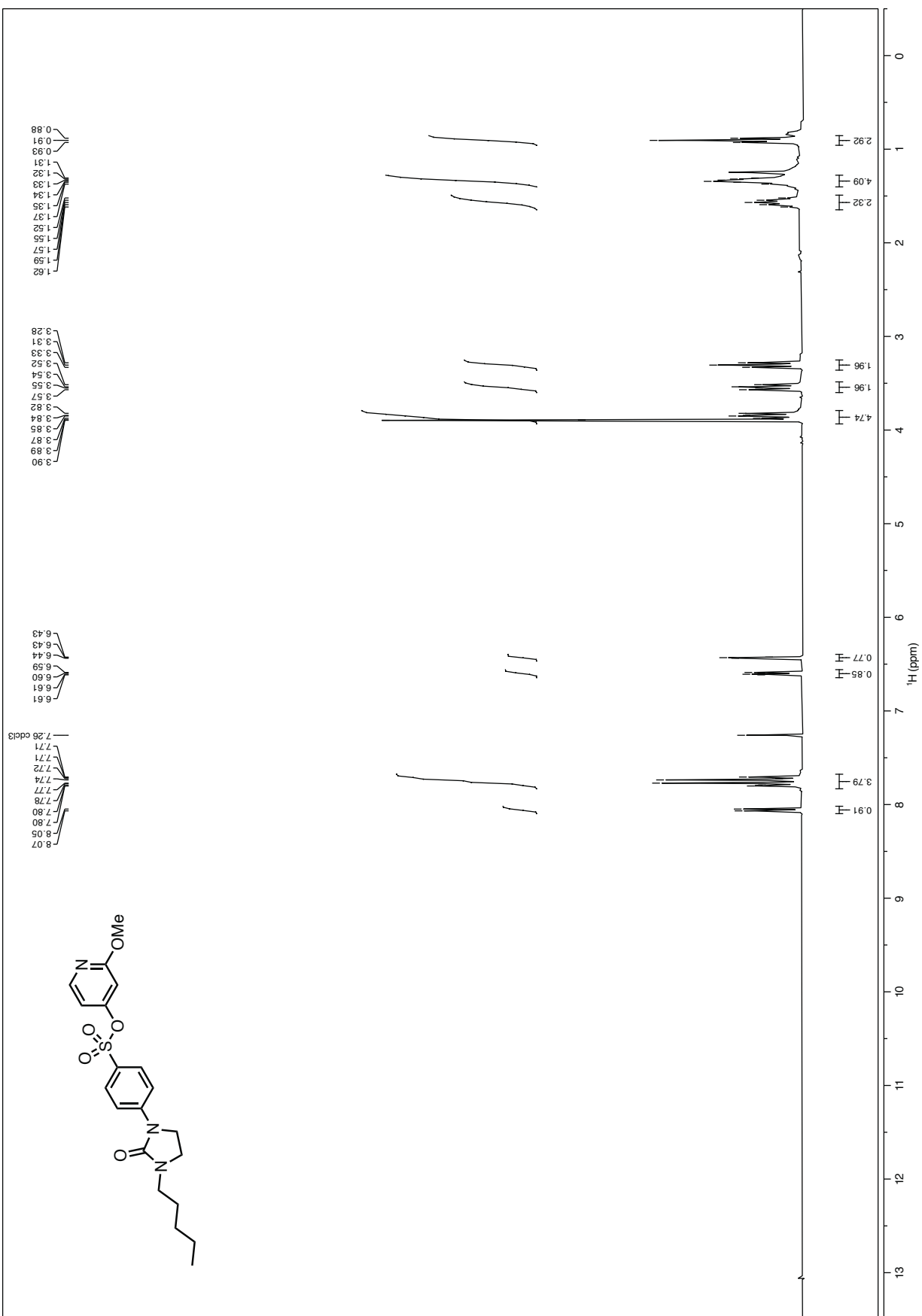
13



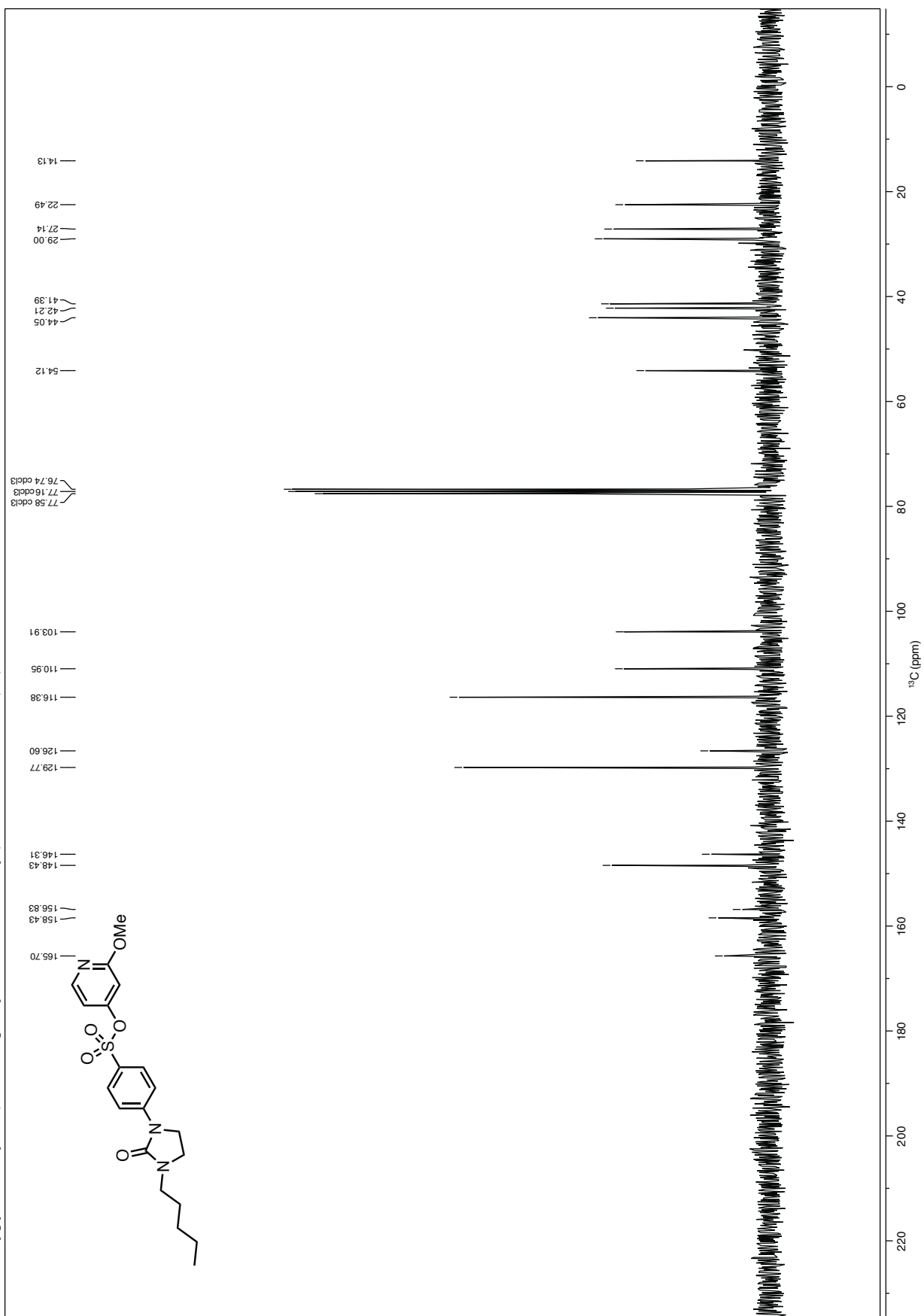
MS spectrum peak list

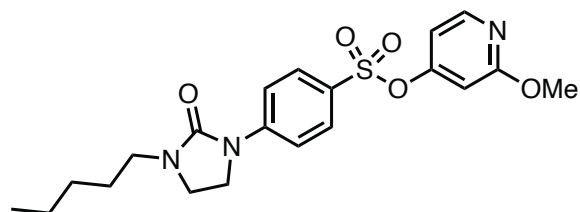
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
424.1094	424.1092	0.29	1	357439	C19 H23 Cl N3 O4 S	(M+H)+
425.1123	425.1122	0.34		71589	C19 H23 Cl N3 O4 S	(M+H)+
426.1066	426.1068	-0.46		131456	C19 H23 Cl N3 O4 S	(M+H)+
427.1094	427.1094	-0.06		22528	C19 H23 Cl N3 O4 S	(M+H)+
428.107	428.1066	1.01		5789	C19 H23 Cl N3 O4 S	(M+H)+
429.1067	429.1079	-2.8	1	954	C19 H23 Cl N3 O4 S	(M+H)+

2-Methoxypyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**14**)

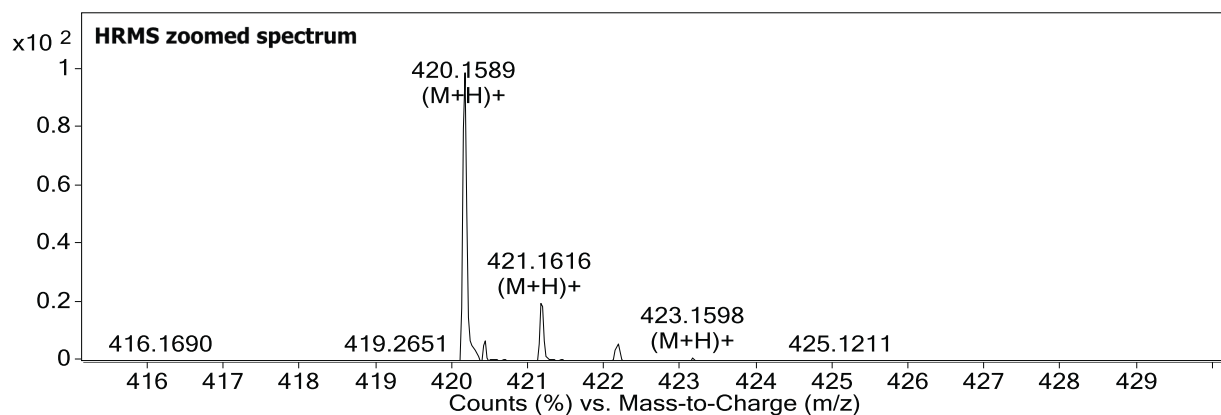
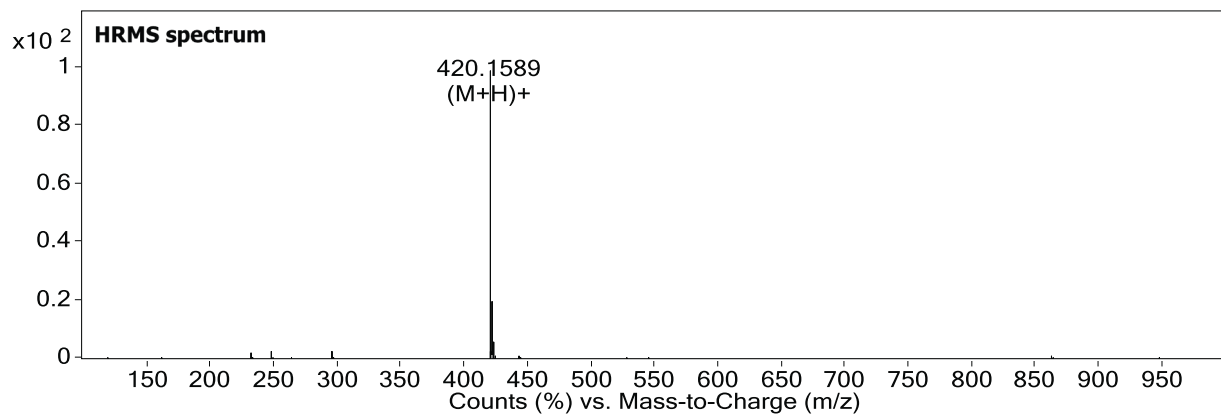


2-Methoxypyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**14**)





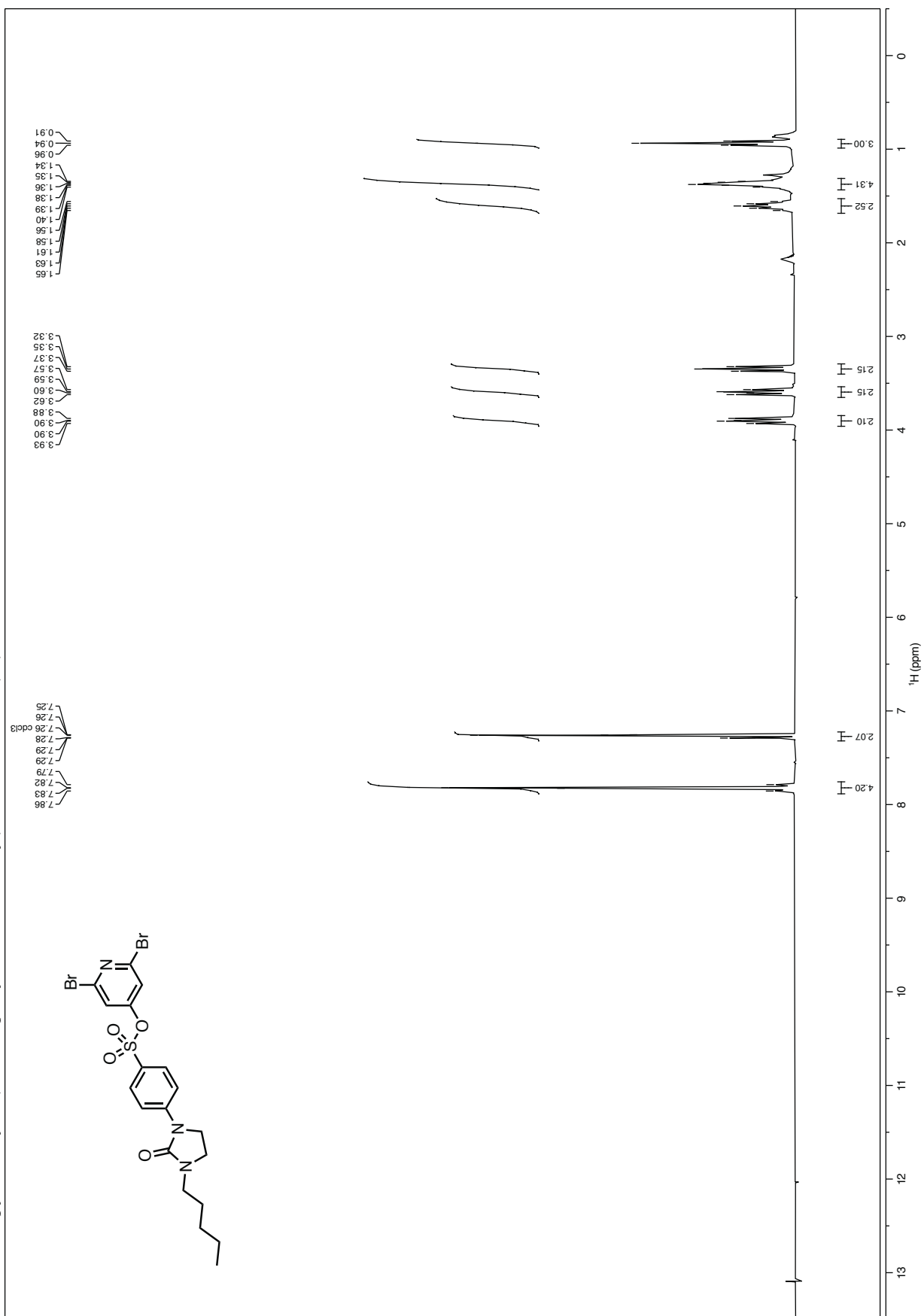
14



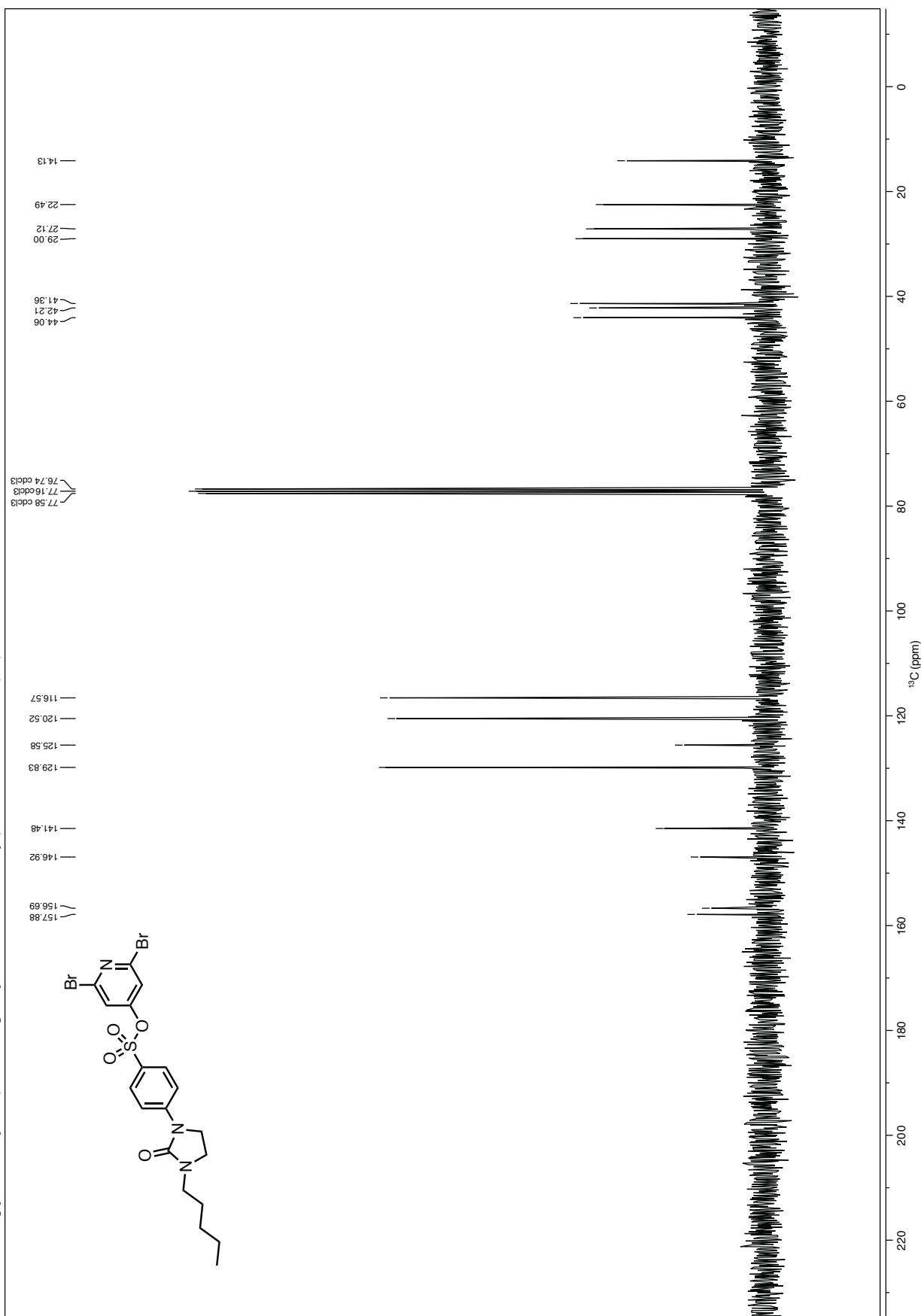
MS spectrum peak list

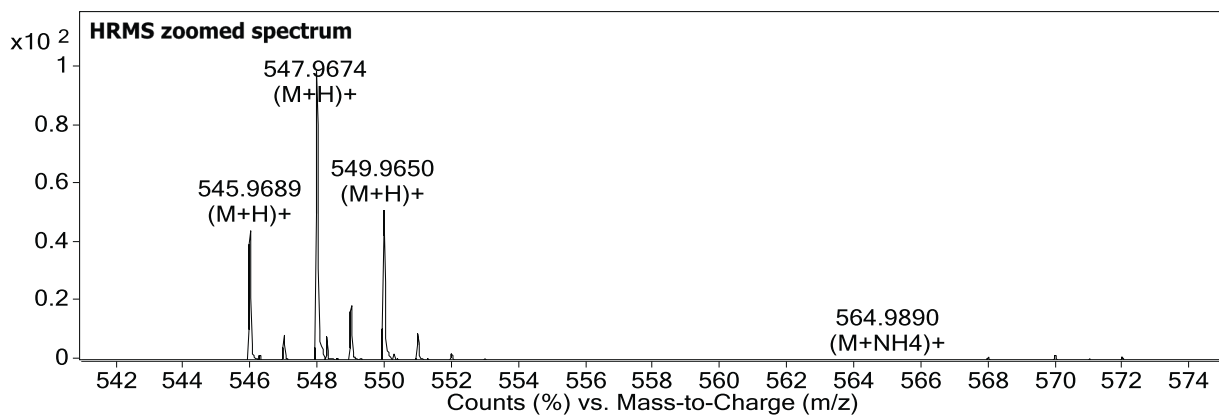
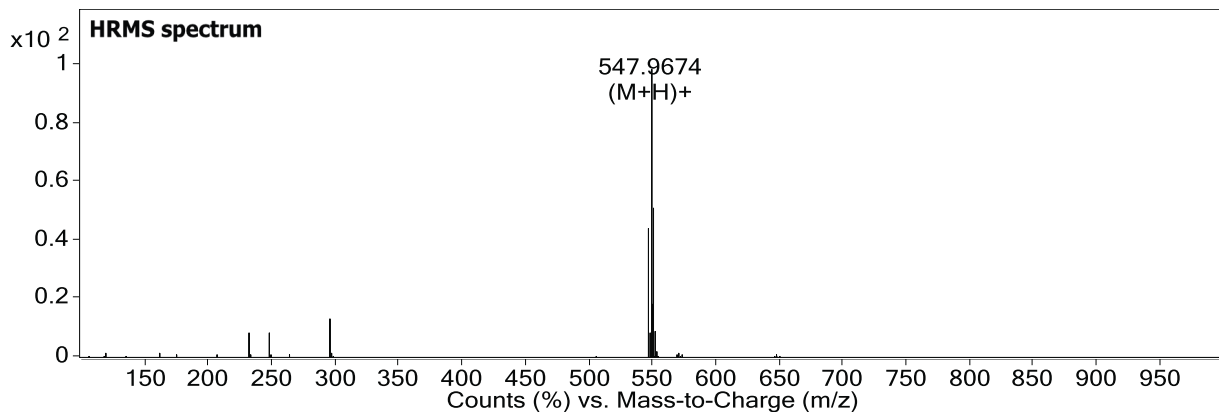
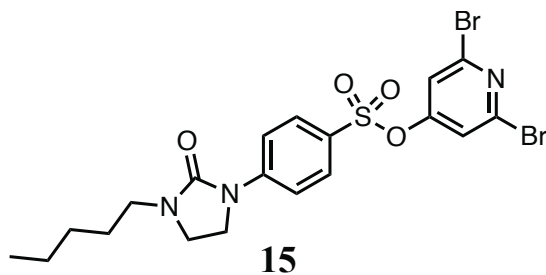
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
420.1589	420.1588	0.2	359321	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺
421.1616	421.1617	-0.4	74995	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺
422.1593	422.159	0.61	20899	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺
423.1598	423.1604	-1.5	3083	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺

2,6-Dibromopyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**15**)



2,6-Dibromopyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**15**)

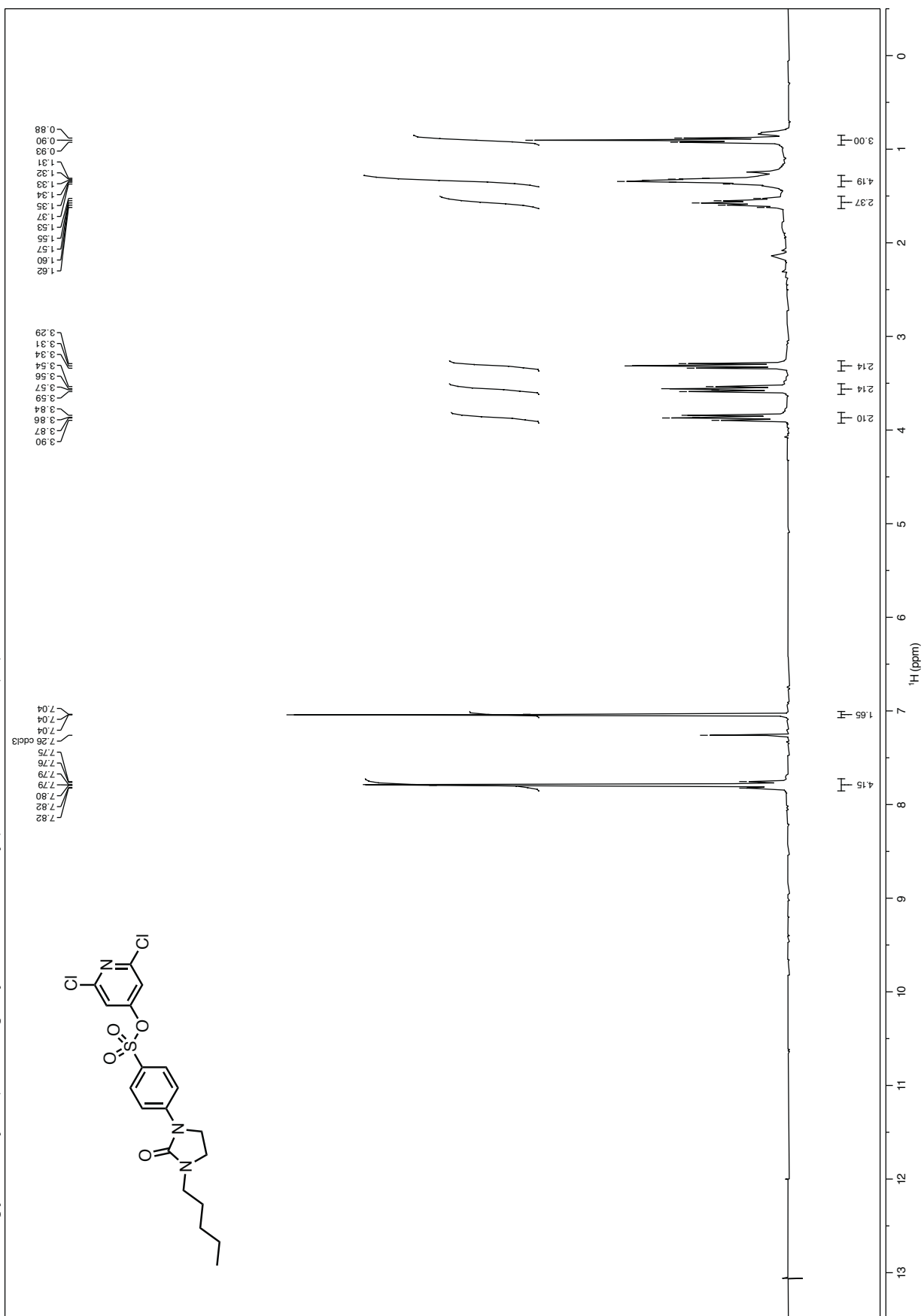




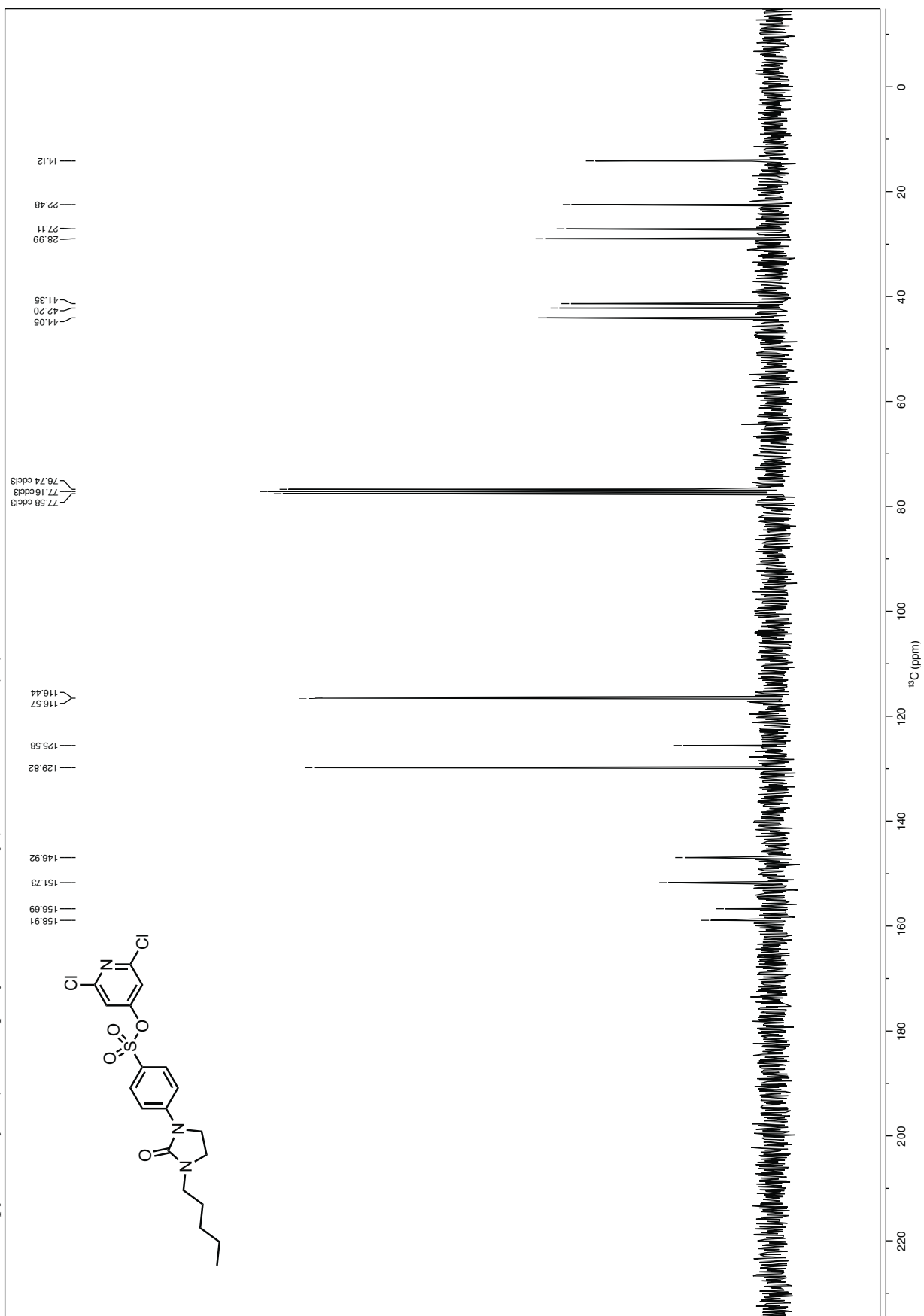
MS spectrum peak list

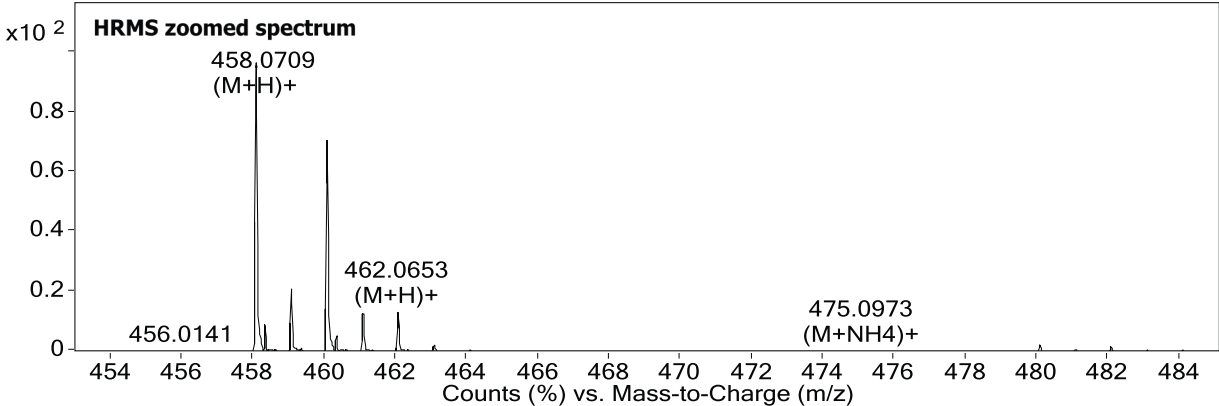
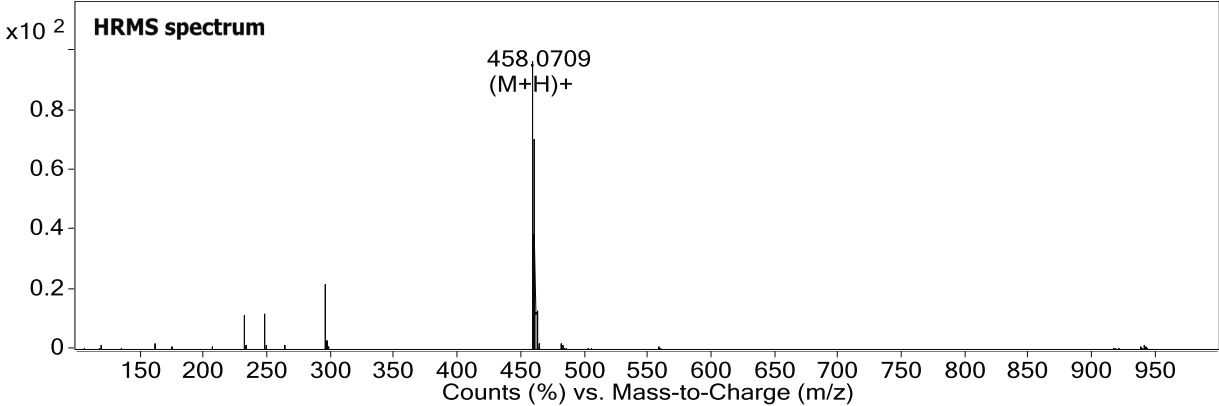
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>z</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
545.9689	545.9692	-0.57		171224	C ₁₉ H ₂₂ Br ₂ N ₃ O ₄ S	(M+H) ⁺
546.9717	546.9722	-0.8		31115	C ₁₉ H ₂₂ Br ₂ N ₃ O ₄ S	(M+H) ⁺
547.9674	547.9673	0.24		374516	C ₁₉ H ₂₂ Br ₂ N ₃ O ₄ S	(M+H) ⁺
548.9697	548.9701	-0.76		71434	C ₁₉ H ₂₂ Br ₂ N ₃ O ₄ S	(M+H) ⁺
549.965	549.9654	-0.78		194028	C ₁₉ H ₂₂ Br ₂ N ₃ O ₄ S	(M+H) ⁺
550.9681	550.9681	-0.08		34461	C ₁₉ H ₂₂ Br ₂ N ₃ O ₄ S	(M+H) ⁺
551.9654	551.9653	0.29		8689	C ₁₉ H ₂₂ Br ₂ N ₃ O ₄ S	(M+H) ⁺
552.9667	552.9666	0.14		1325	C ₁₉ H ₂₂ Br ₂ N ₃ O ₄ S	(M+H) ⁺

2,6-Dichloropyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**16**)



2,6-Dichloropyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate (**16**)

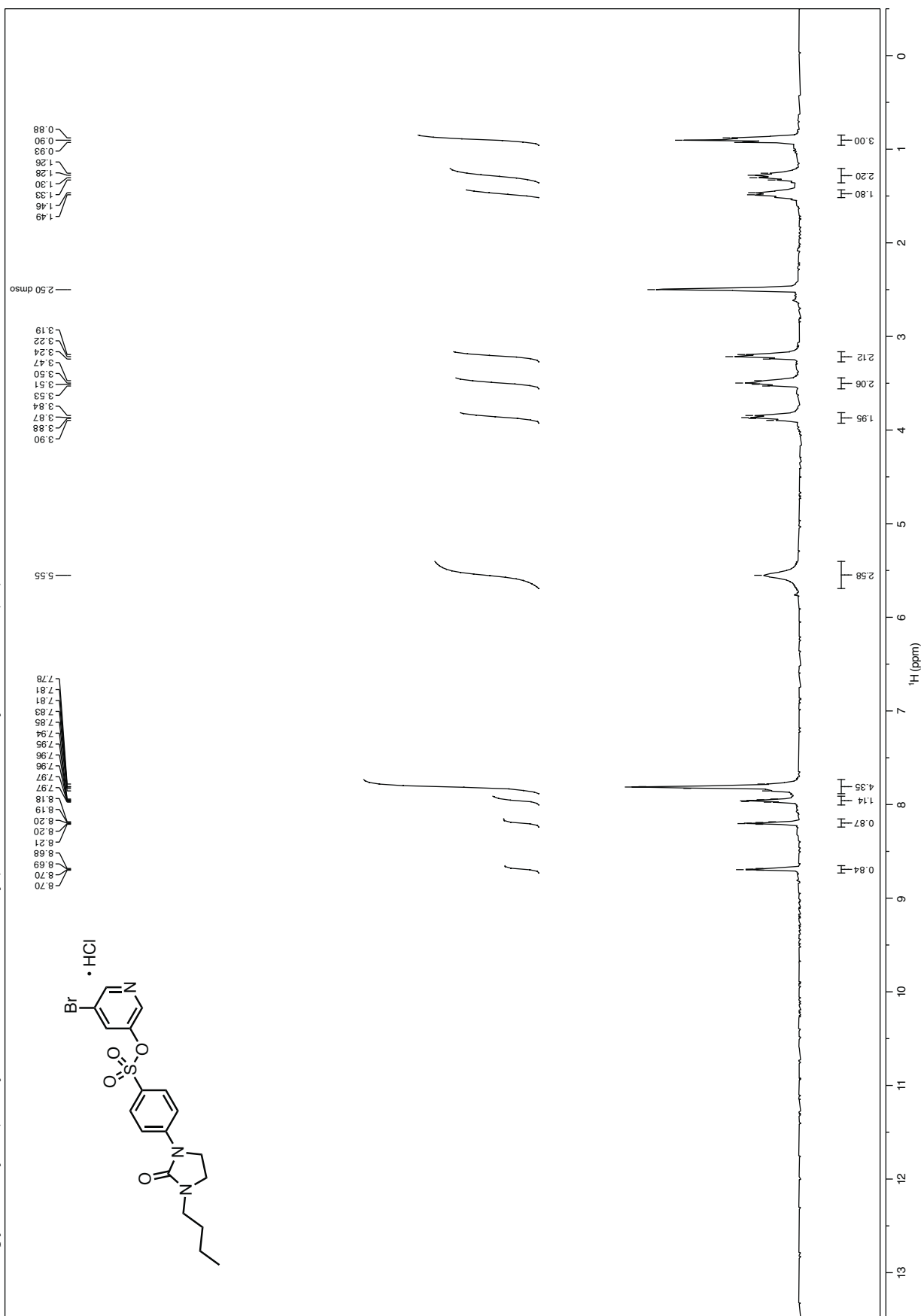




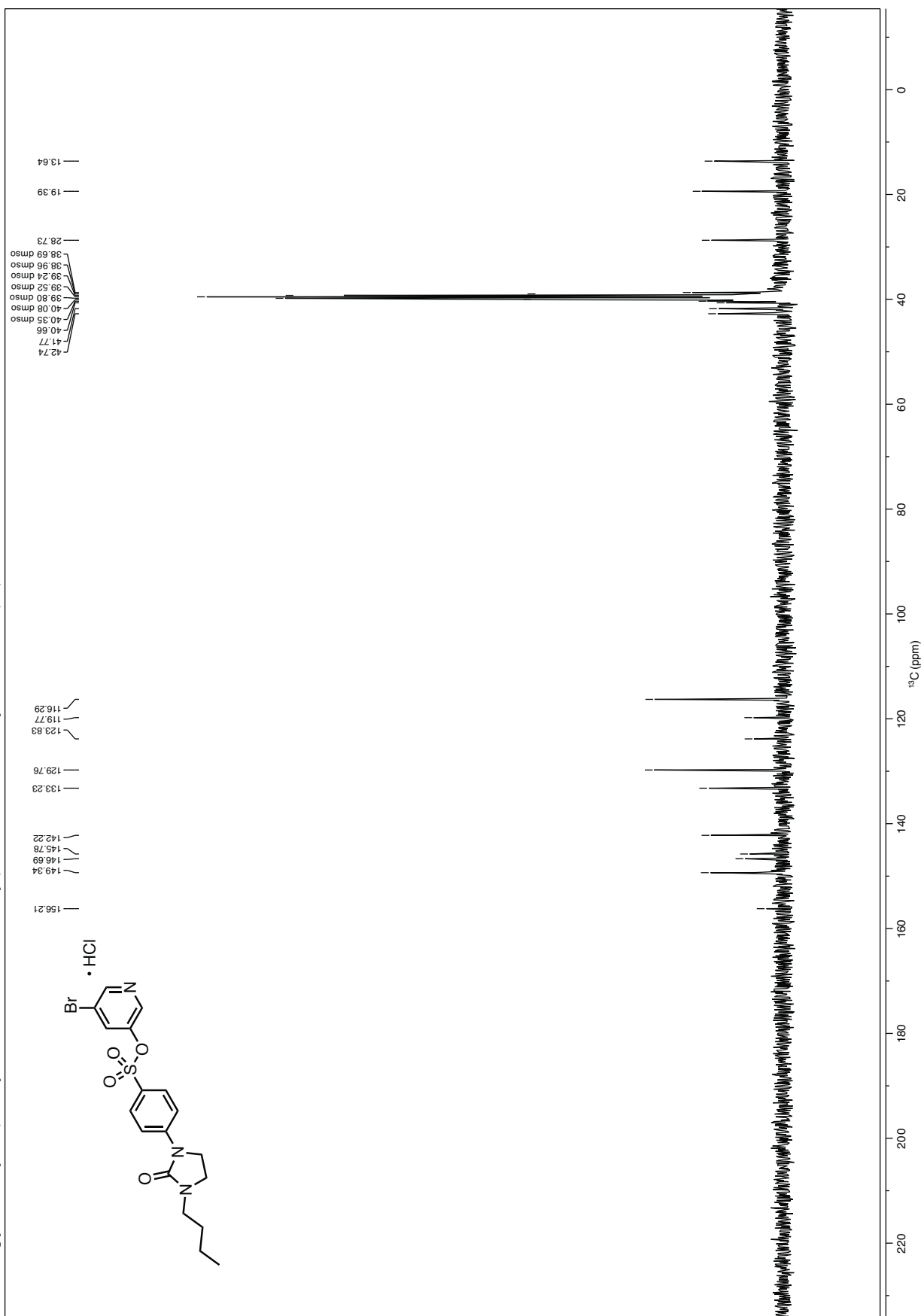
MS spectrum peak list

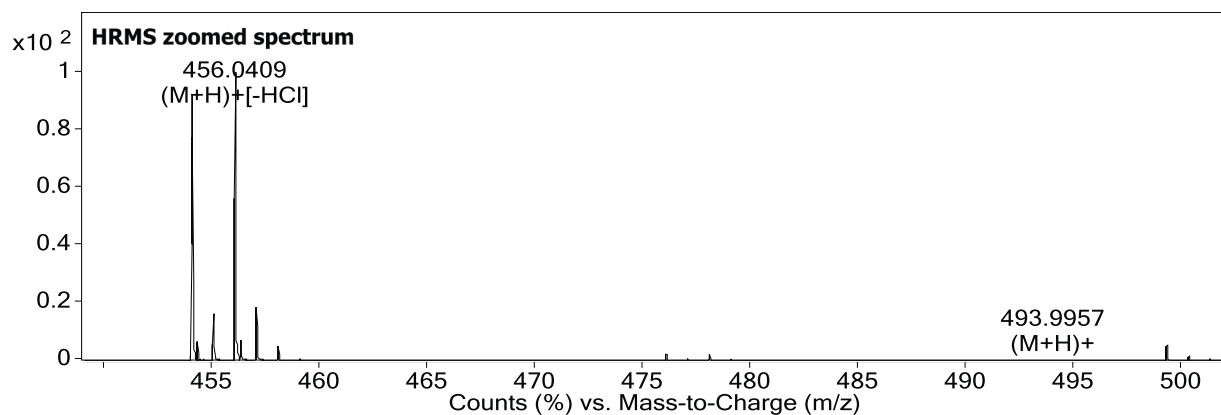
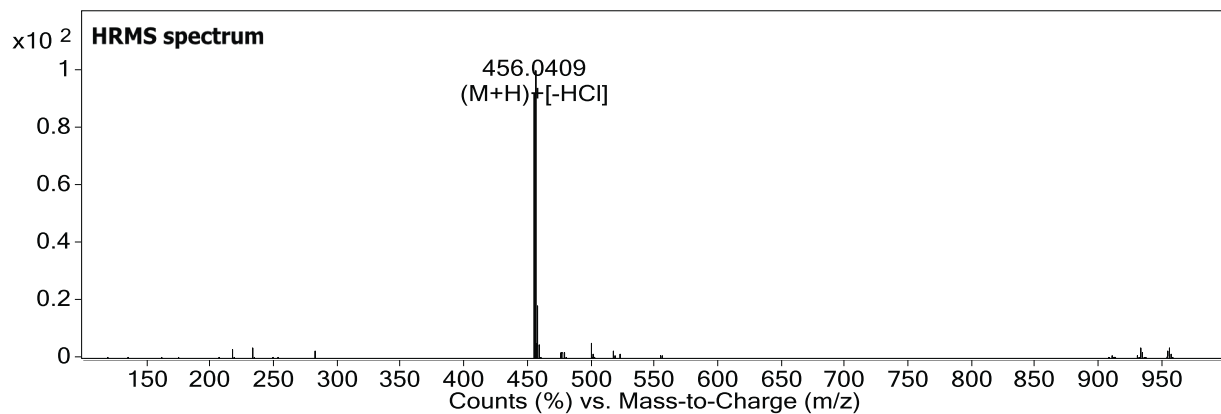
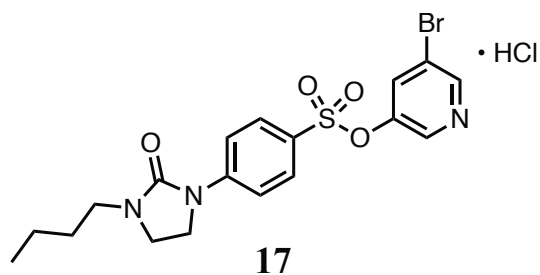
m/z	Calc m/z	Diff(ppm)	z	Abund	Formula	Ion
458.0709	458.0703	1.44		519006	C19 H22 Cl2 N3 O4 S	(M+H)+
459.0732	459.0732	-0.09		109195	C19 H22 Cl2 N3 O4 S	(M+H)+
460.0679	460.0676	0.58		370030	C19 H22 Cl2 N3 O4 S	(M+H)+
461.07	461.0704	-0.86		69740	C19 H22 Cl2 N3 O4 S	(M+H)+
462.0653	462.0654	-0.15		68262	C19 H22 Cl2 N3 O4 S	(M+H)+
463.0676	463.0677	-0.24	1	10440	C19 H22 Cl2 N3 O4 S	(M+H)+
464.0654	464.065	0.83	1	2668	C19 H22 Cl2 N3 O4 S	(M+H)+
465.0669	465.0662	1.59	1	479	C19 H22 Cl2 N3 O4 S	(M+H)+

5-Bromopyridin-3-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**17**)



5-Bromopyridin-3-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**17**)

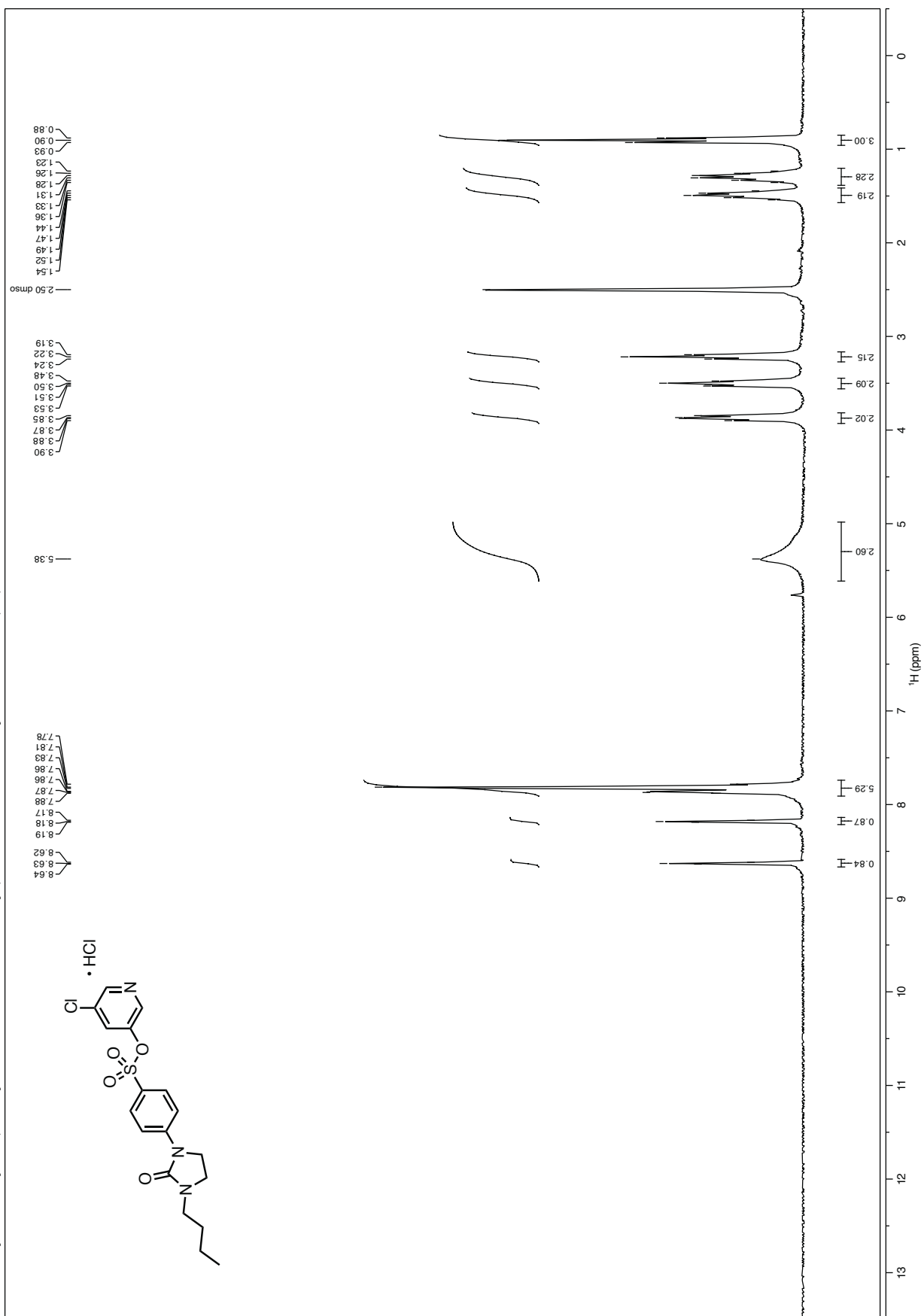




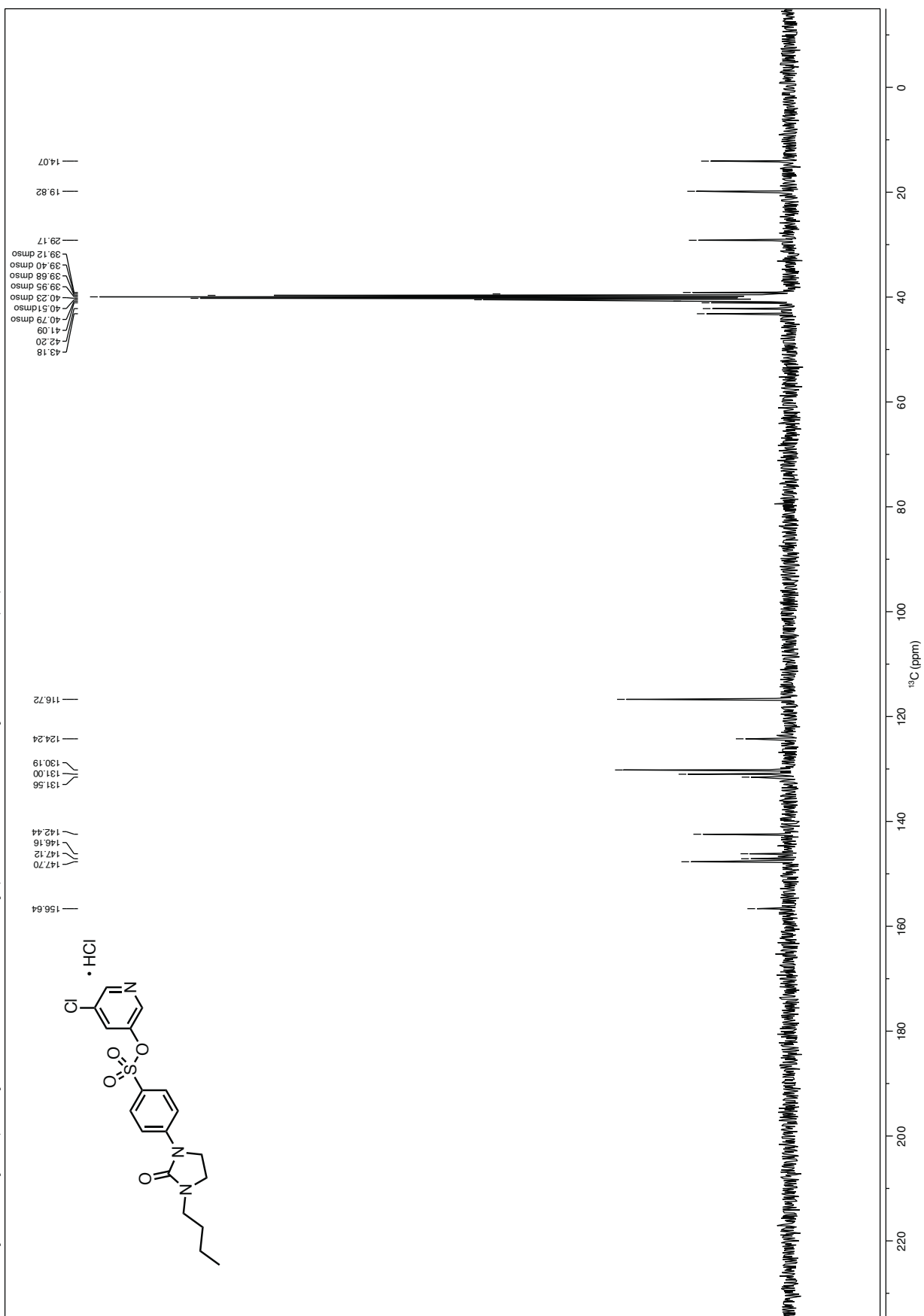
MS spectrum peak list

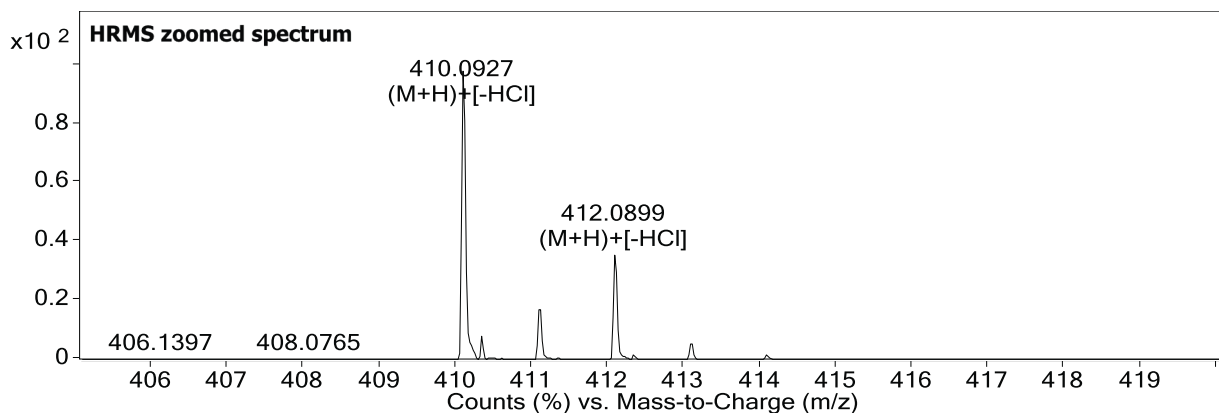
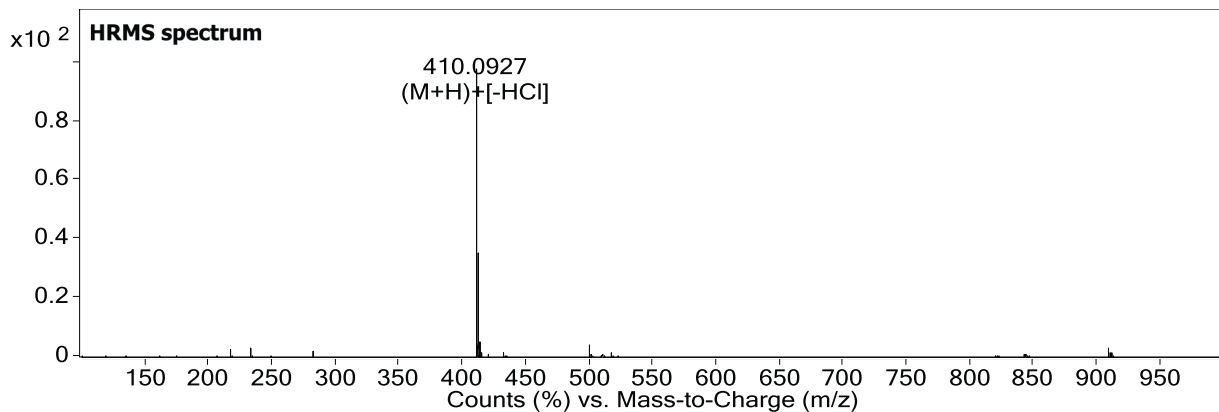
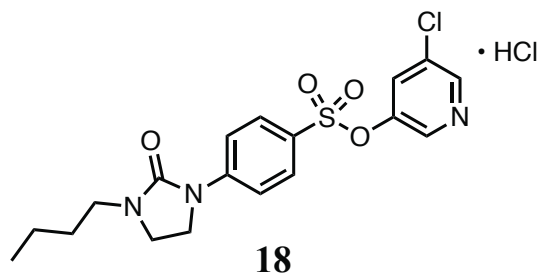
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
454.0428	454.0431	-0.51		249909	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
455.0453	455.046	-1.44		45006	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
456.0409	456.0411	-0.45		265041	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
457.0434	457.044	-1.14		48148	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
458.0402	458.0408	-1.41		12546	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
459.0418	459.0423	-1.13		1797	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
460.0424	460.0435	-2.42		280	C ₁₈ H ₂₁ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
491.9984	492.0176	-38.98	1	429	C ₁₈ H ₂₂ Br Cl N ₃ O ₄ S	(M+H) ⁺

5-Chloropyridin-3-yl 4-(3-buty[2-oxoimidazolidin-1-yl])benzenesulfonate hydrochloride (**18**)



5-Chlorouracil-3-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**18**)

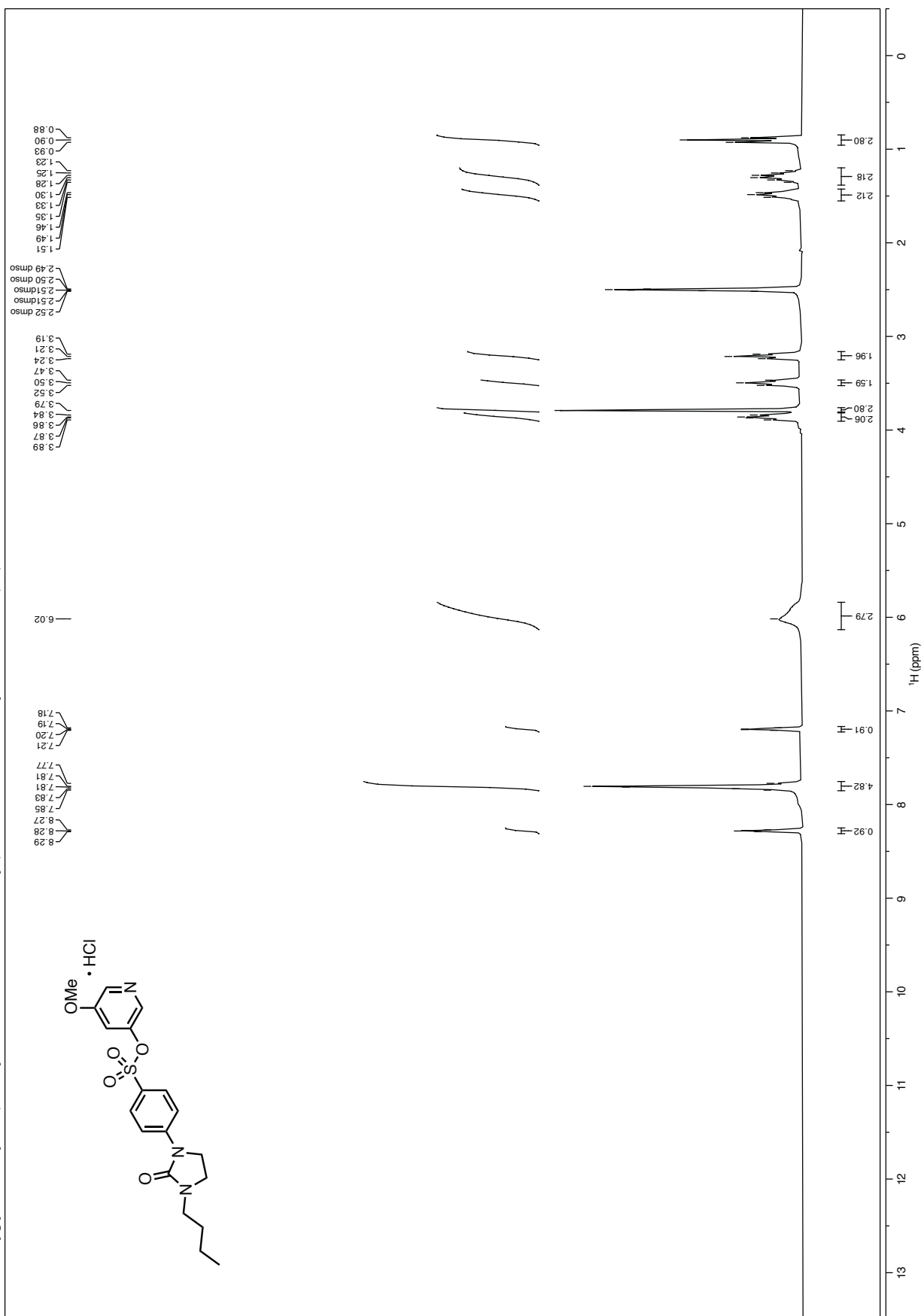




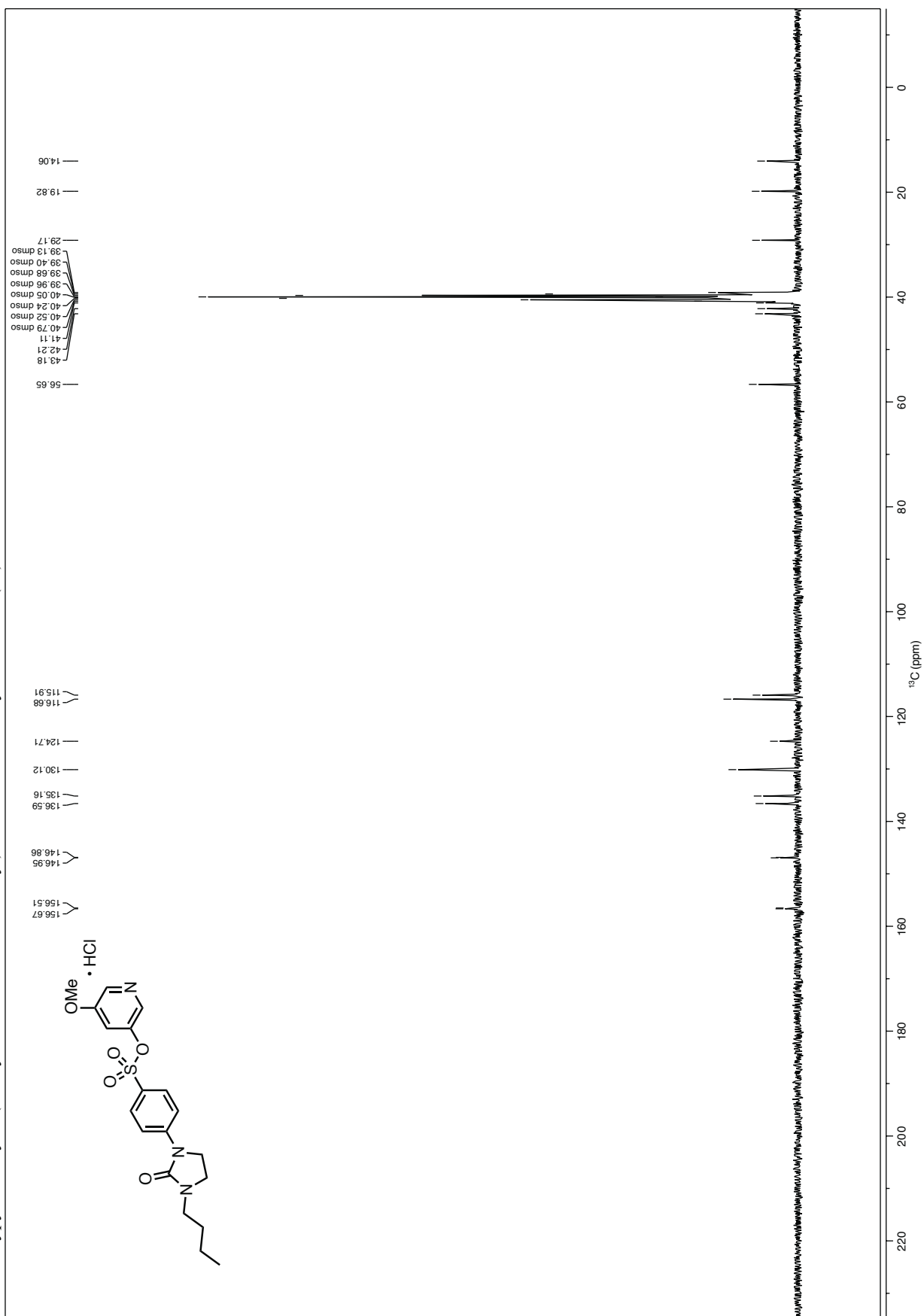
MS spectrum peak list

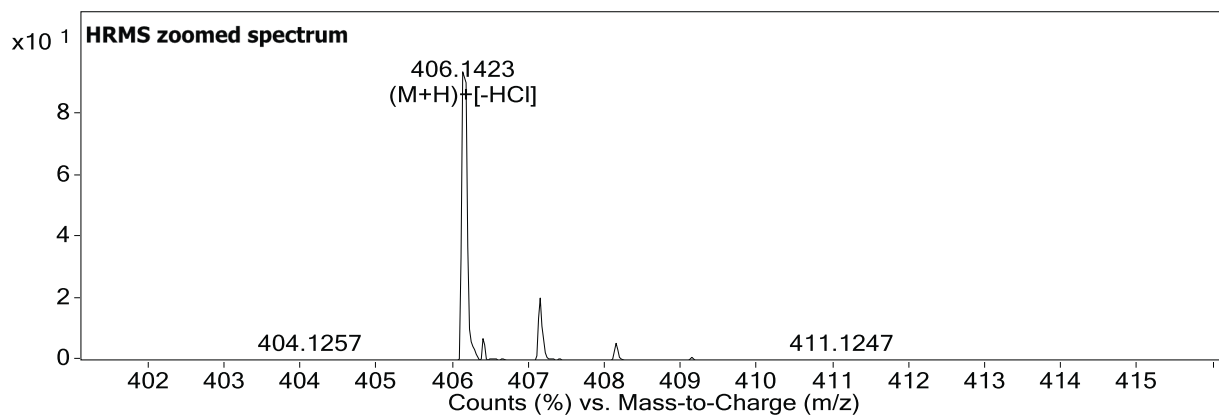
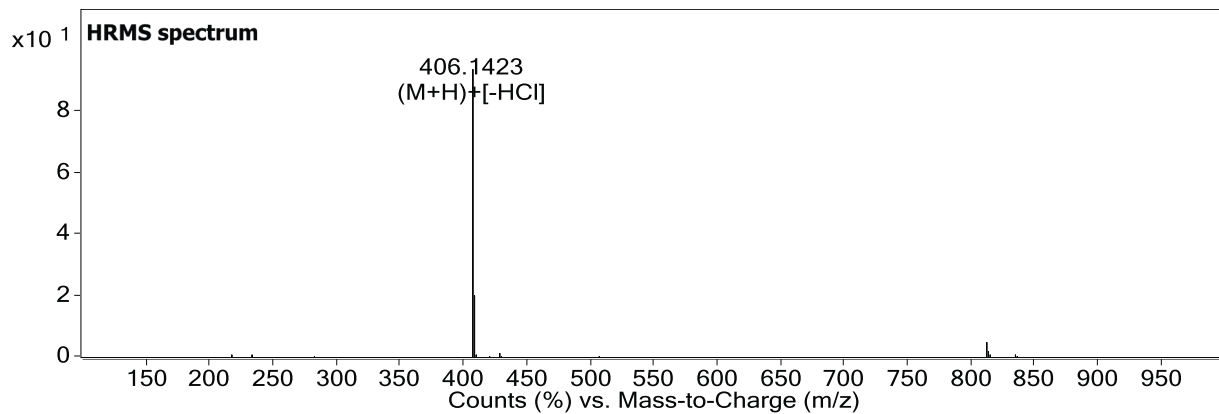
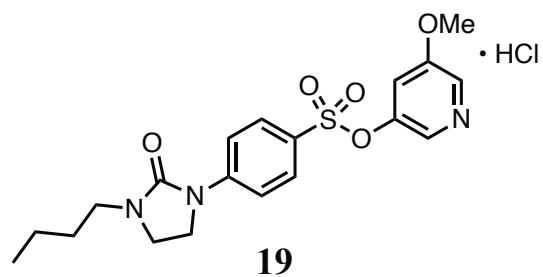
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
410.0927	410.0936	-2.15	364926	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
411.0952	411.0965	-3.25	67706	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
412.0899	412.0911	-2.92	132950	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
413.0926	413.0937	-2.71	21448	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
414.09	414.0907	-1.66	5605	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
415.0905	415.0921	-3.8	885	C ₁₈ H ₂₁ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]

5-Methoxypyridin-3-yl 4-(3-buty-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**19**)



5-Methoxypyridin-3-yl 4-(3-buty-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**19**)

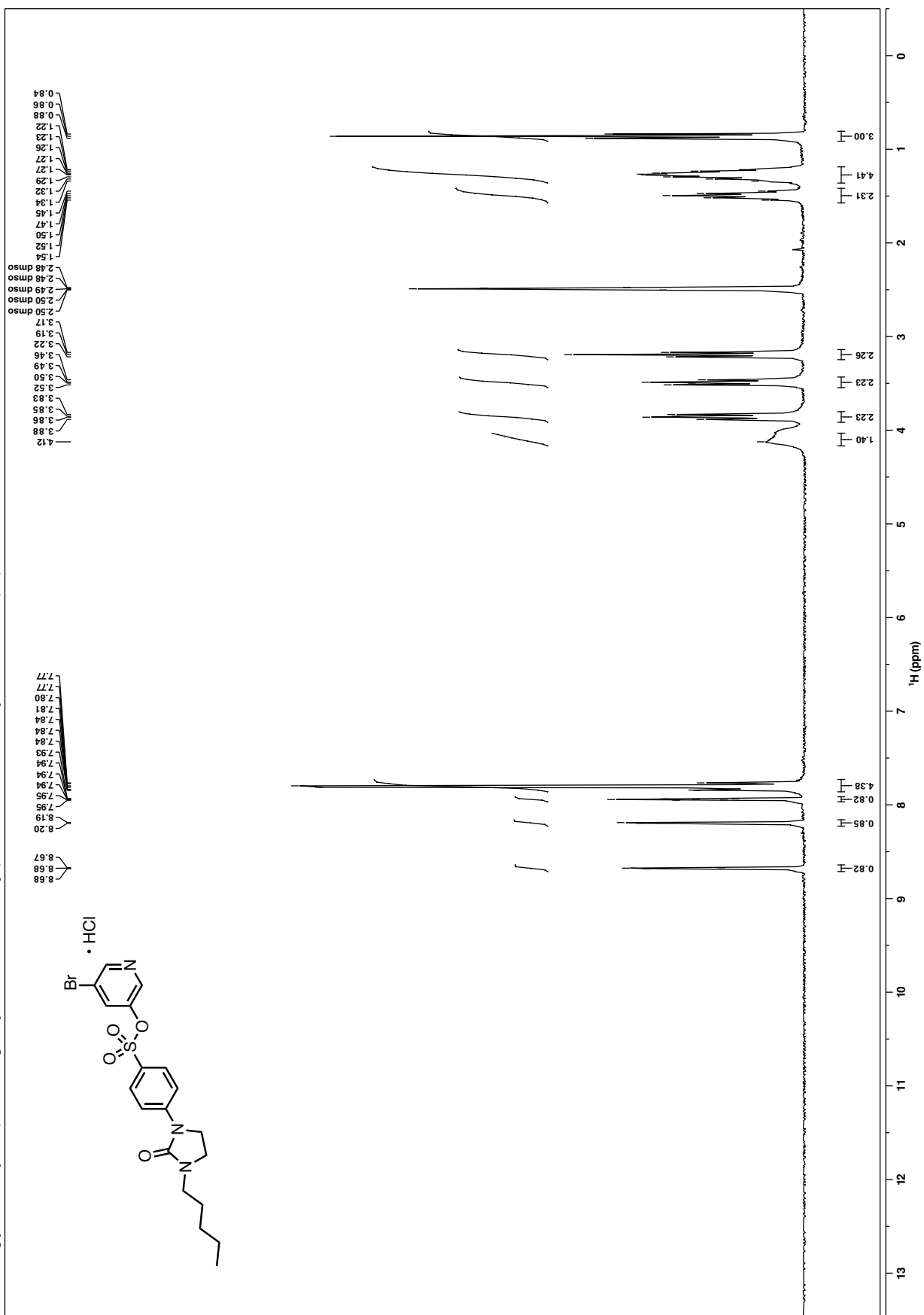




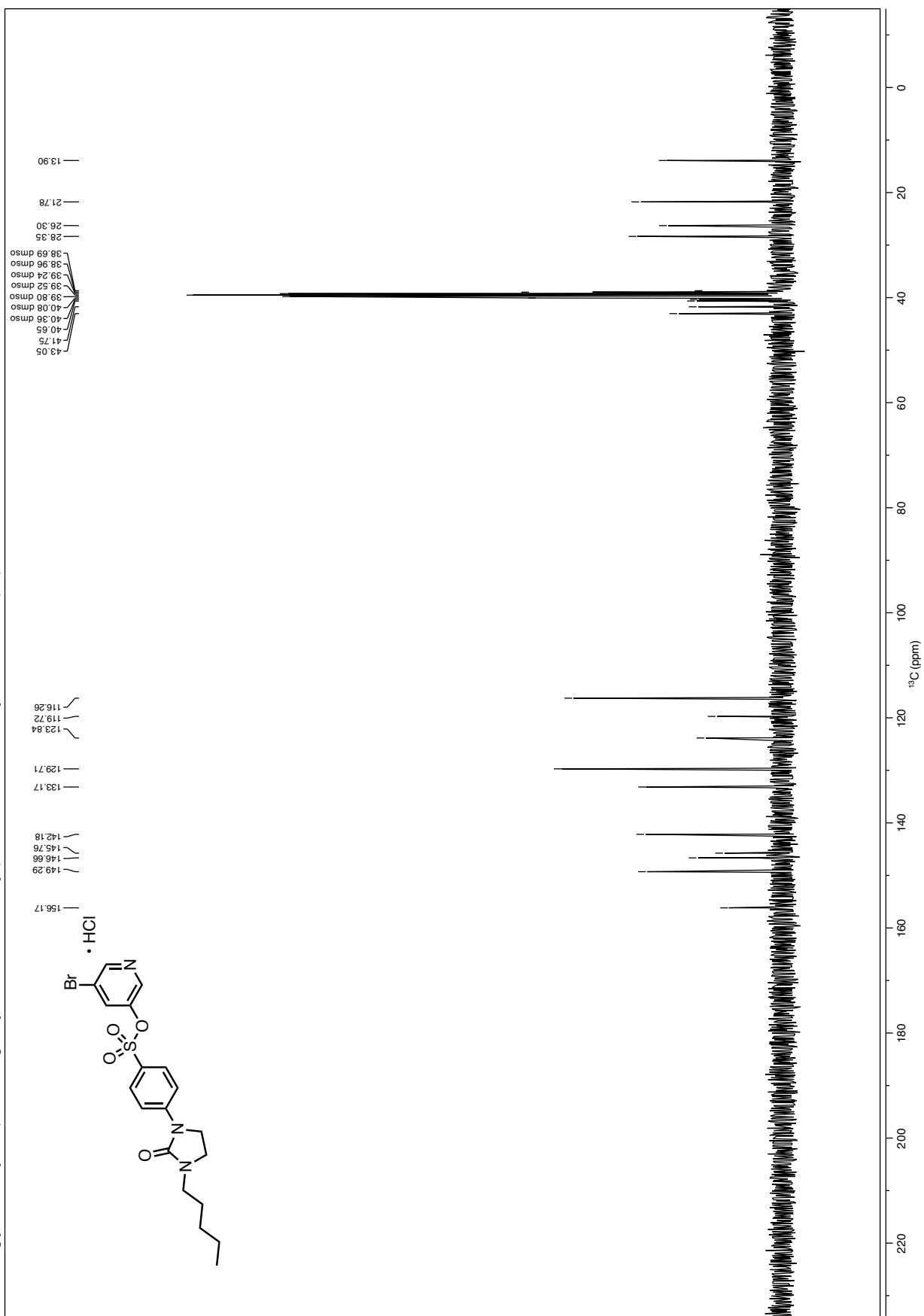
MS spectrum peak list

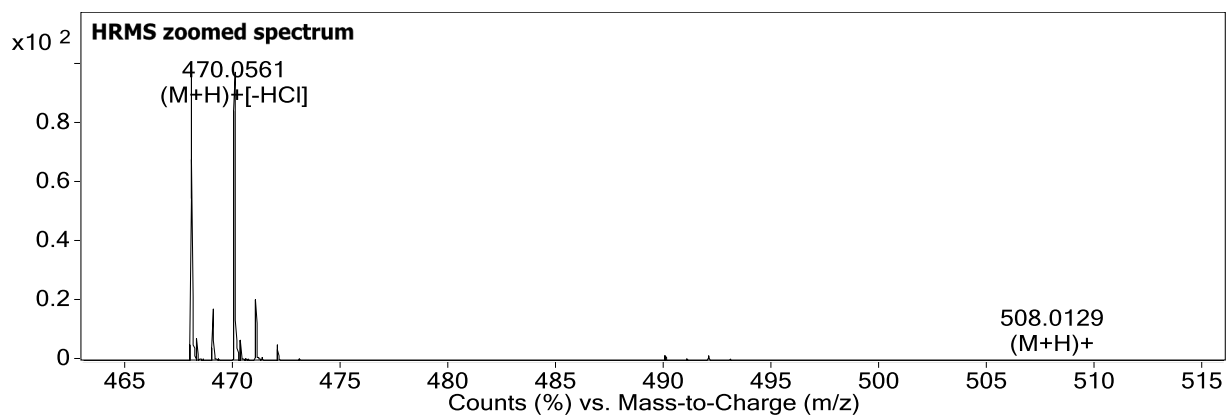
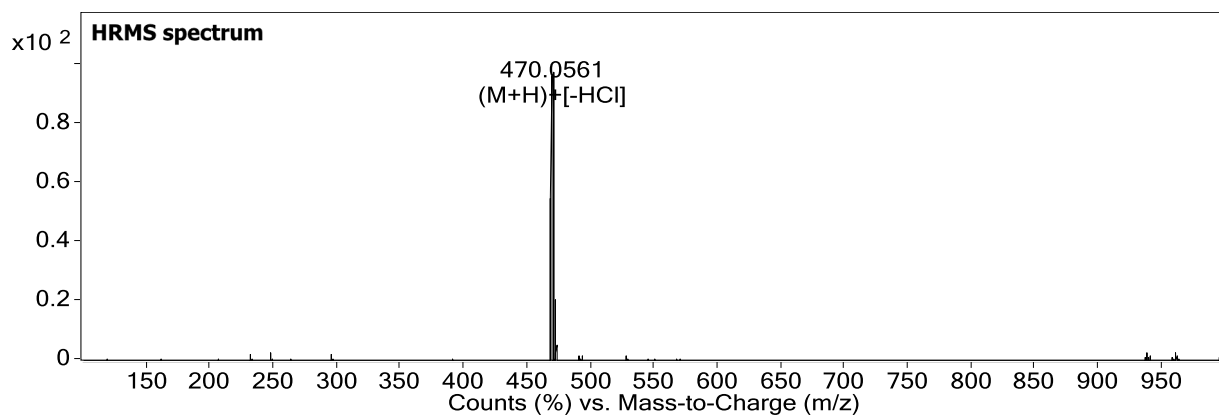
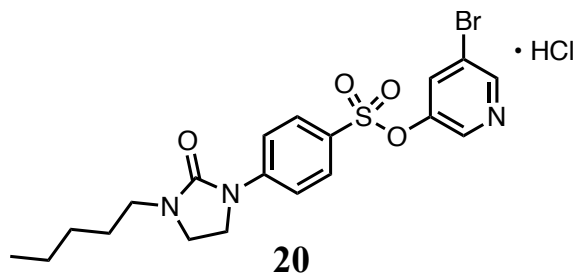
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	Abund	Formula	Ion
406.1423	406.1431	-1.94	339666	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
407.1451	407.1461	-2.4	68725	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
408.1425	408.1432	-1.53	19178	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
409.1429	409.1446	-4.34	2813	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
410.1421	410.1459	-9.11	413	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺ [-HCl]

5-Bromopyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**20**)



5-Bromopyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**20**)

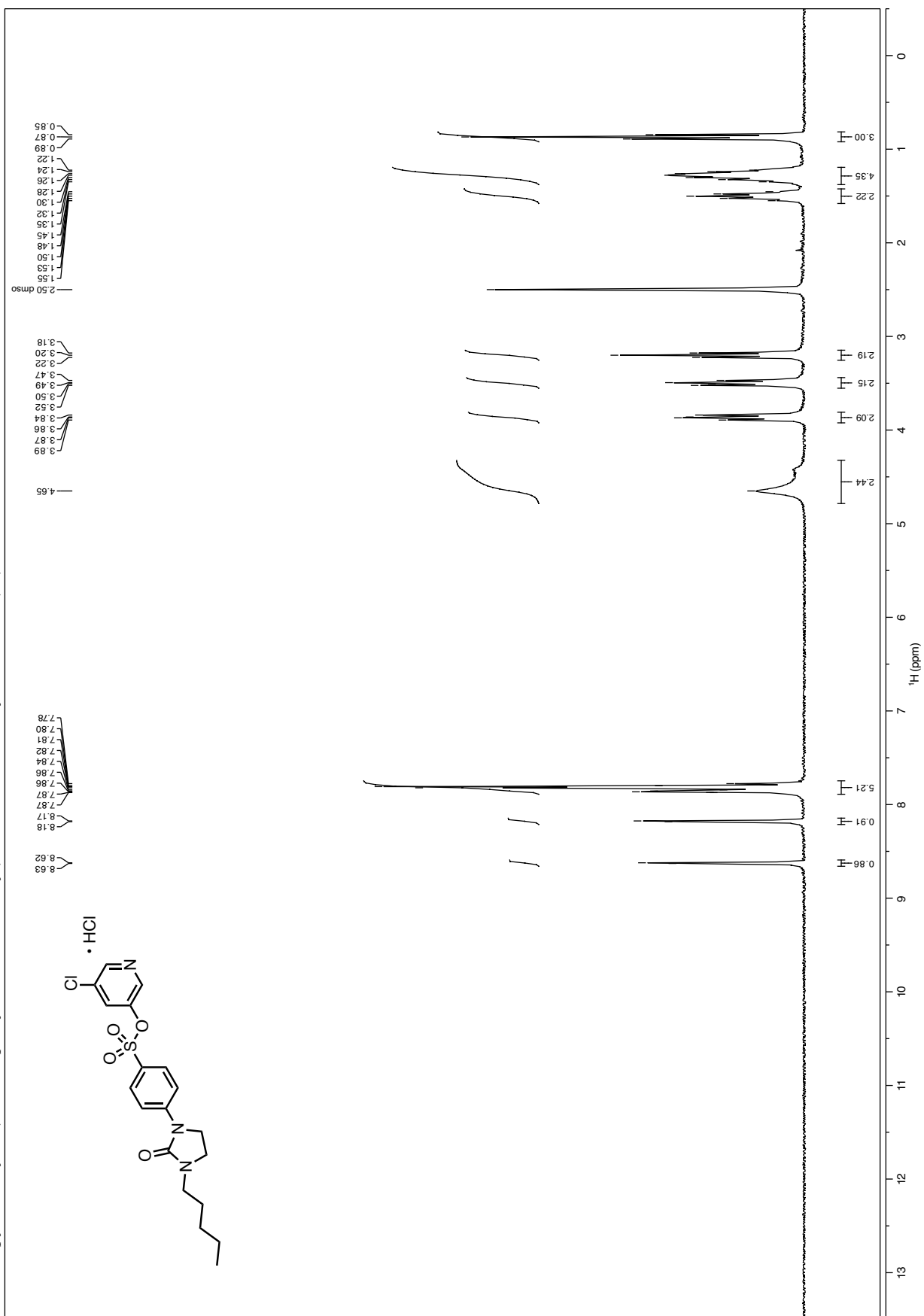




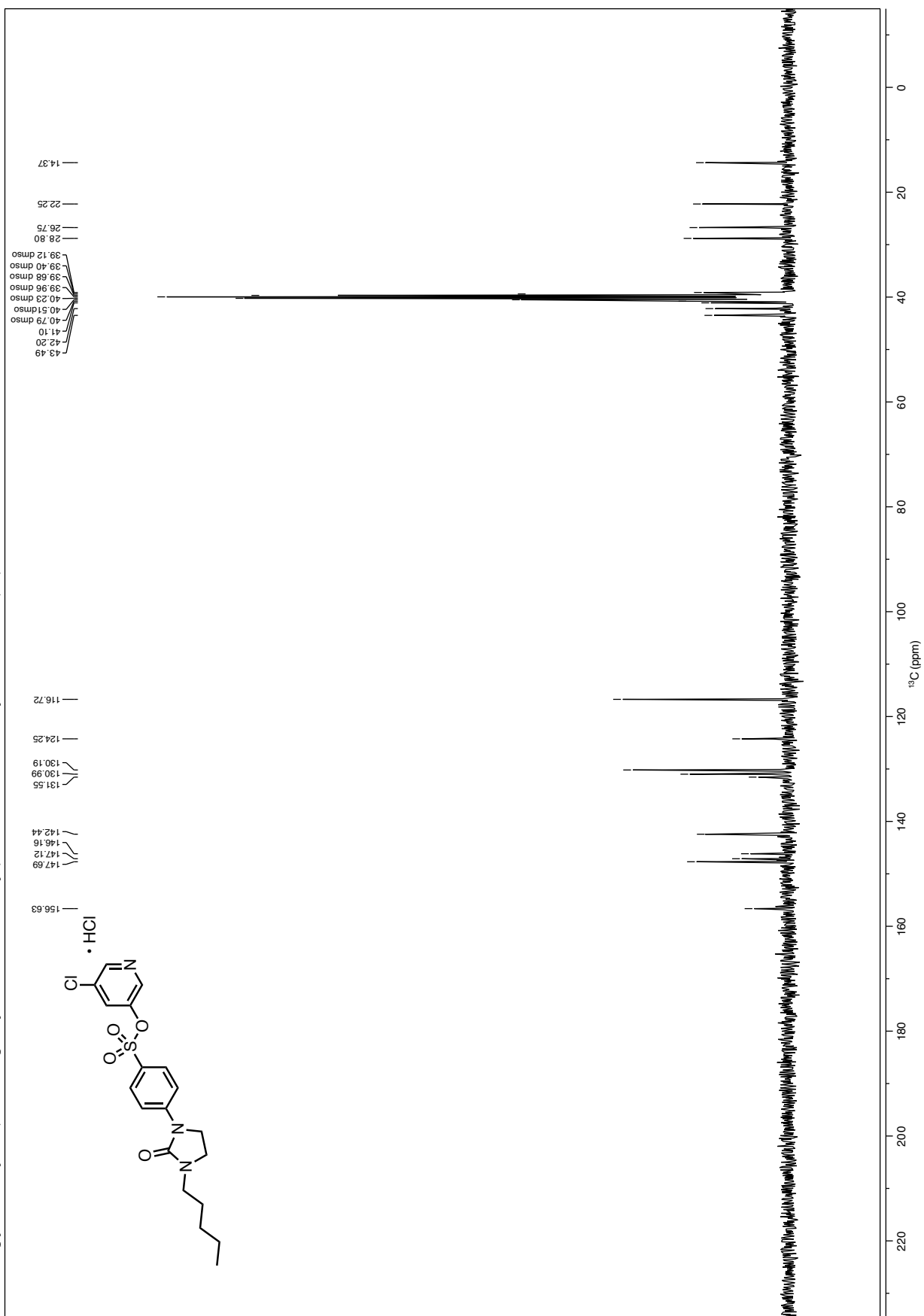
MS spectrum peak list

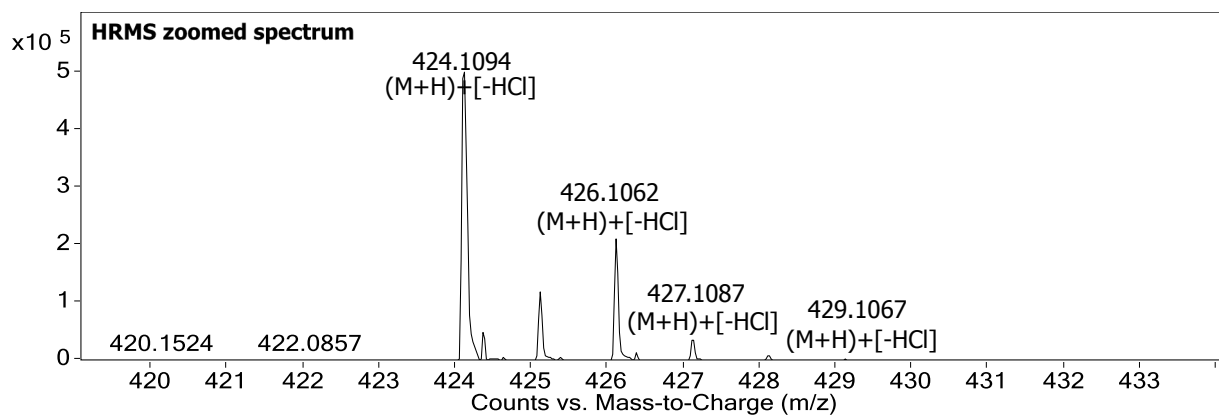
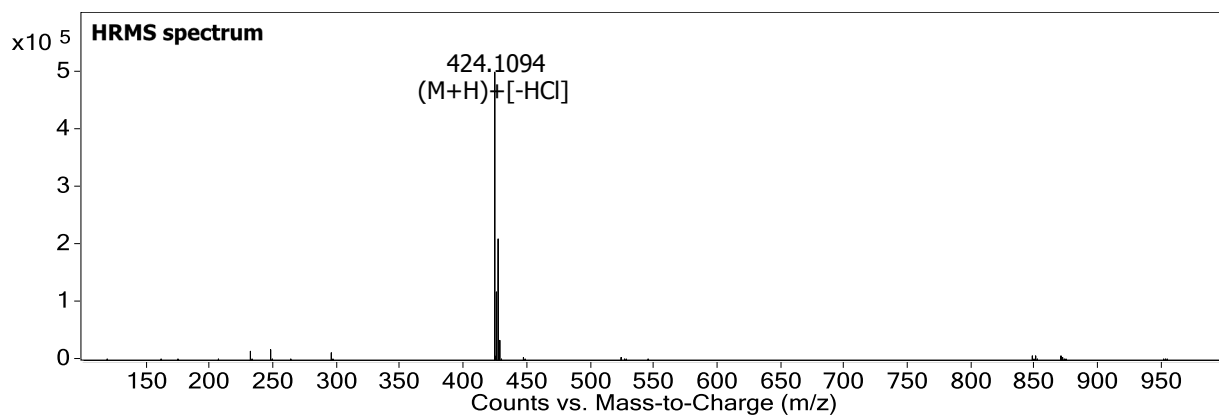
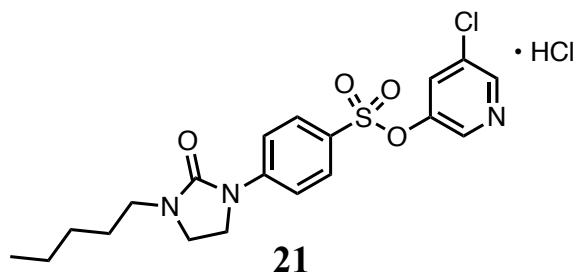
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
468.058	468.0587	-1.48	1	276802	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
469.0602	469.0617	-3.05		53064	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
470.0561	470.0568	-1.59		286117	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
471.0585	471.0596	-2.42		58083	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
472.0568	472.0567	0.27		15344	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
473.0577	473.0581	-0.79		2162	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
474.065	474.0594	11.82		307	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H) ⁺ [-HCl]
506.0125	506.0332	-40.91	1	276	C ₁₉ H ₂₄ Br Cl N ₃ O ₄ S	(M+H) ⁺

5-Chloropyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**21**)



5-Chloropyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**21**)

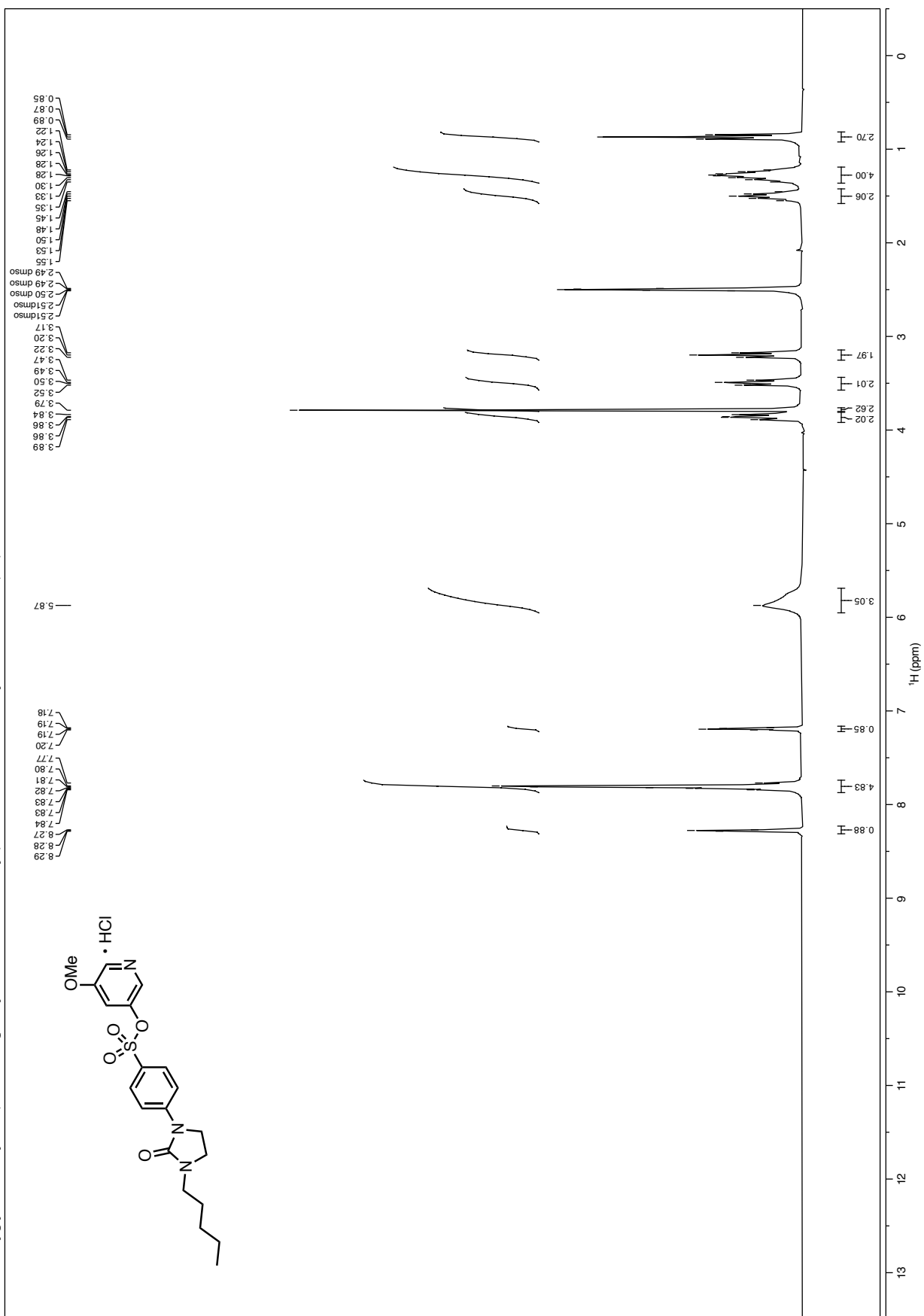




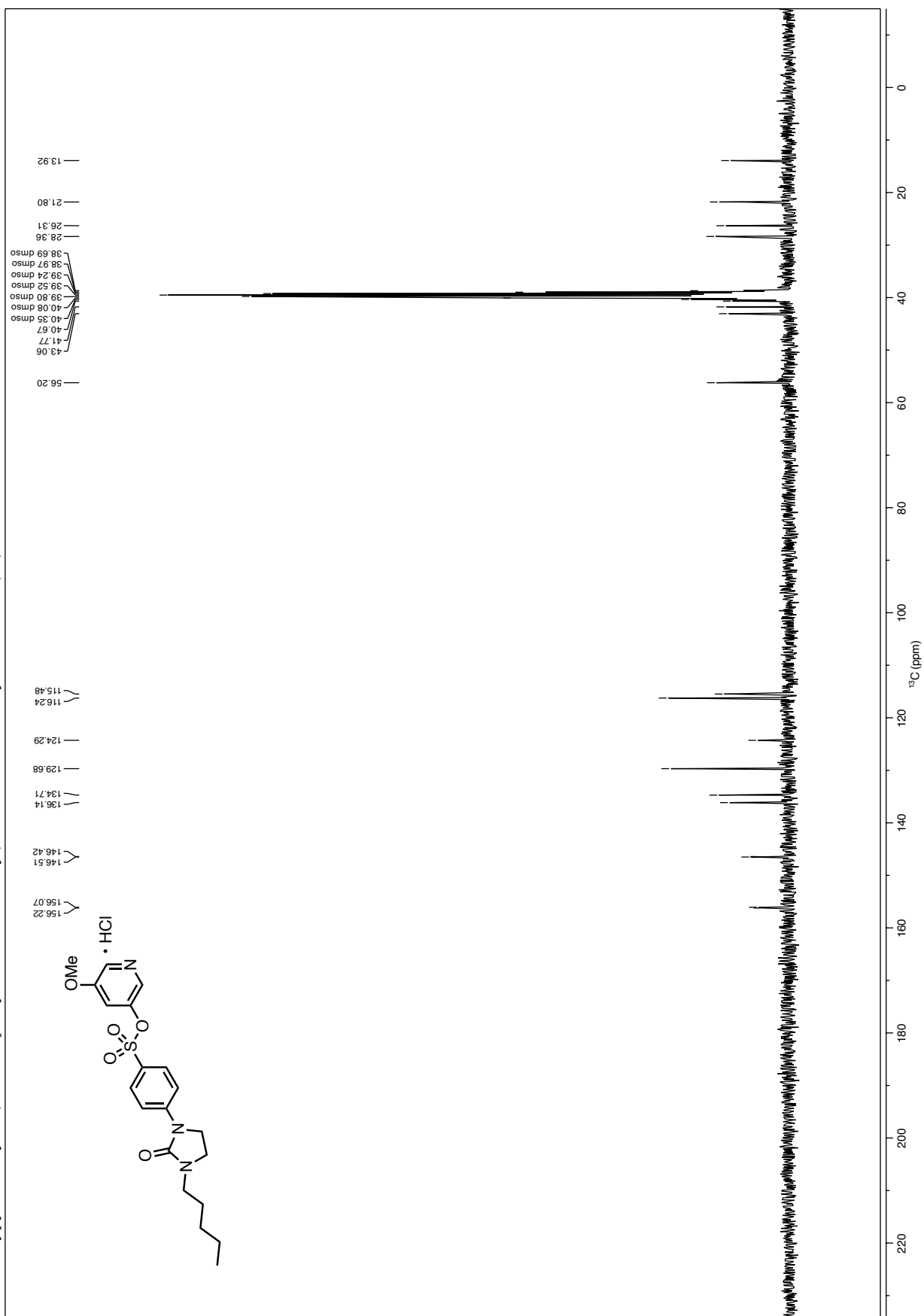
MS spectrum peak list

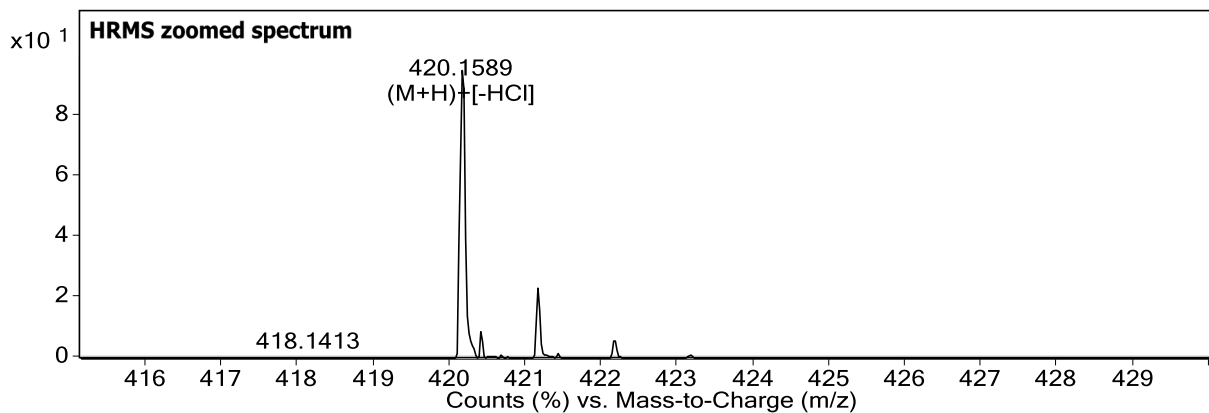
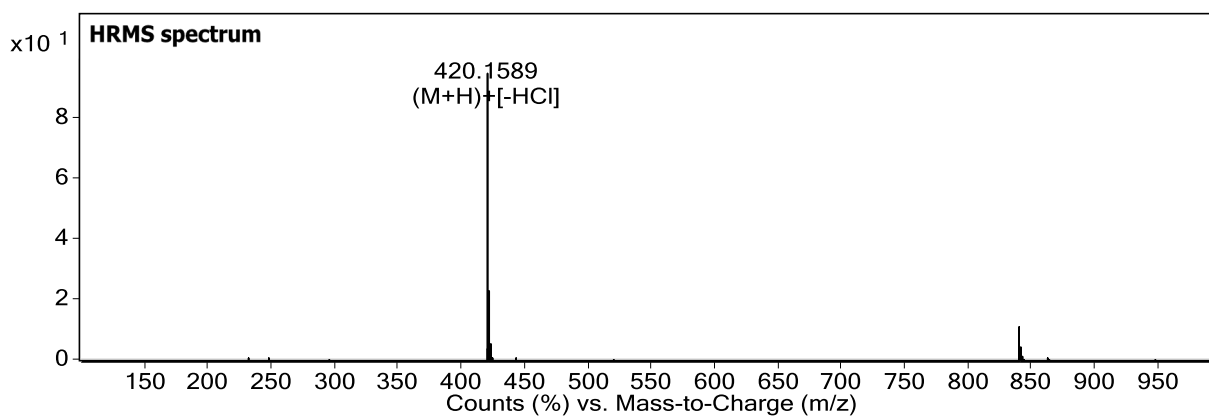
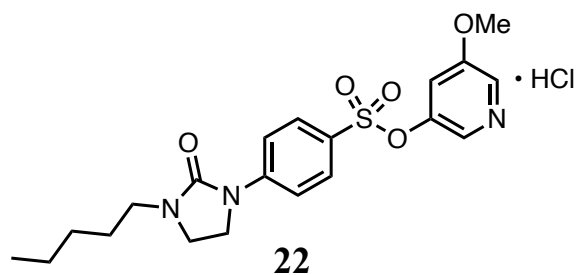
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
424.1094	424.1092	0.38	1	527690	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
425.1117	425.1122	-1.1		118507	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
426.1062	426.1068	-1.41		211477	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
427.1087	427.1094	-1.79		37128	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
428.1062	428.1066	-1		9130	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]
429.1067	429.1079	-2.76		1422	C ₁₉ H ₂₃ Cl N ₃ O ₄ S	(M+H) ⁺ [-HCl]

5-Methoxypyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (22)



5-Methoxypyridin-3-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**22**)

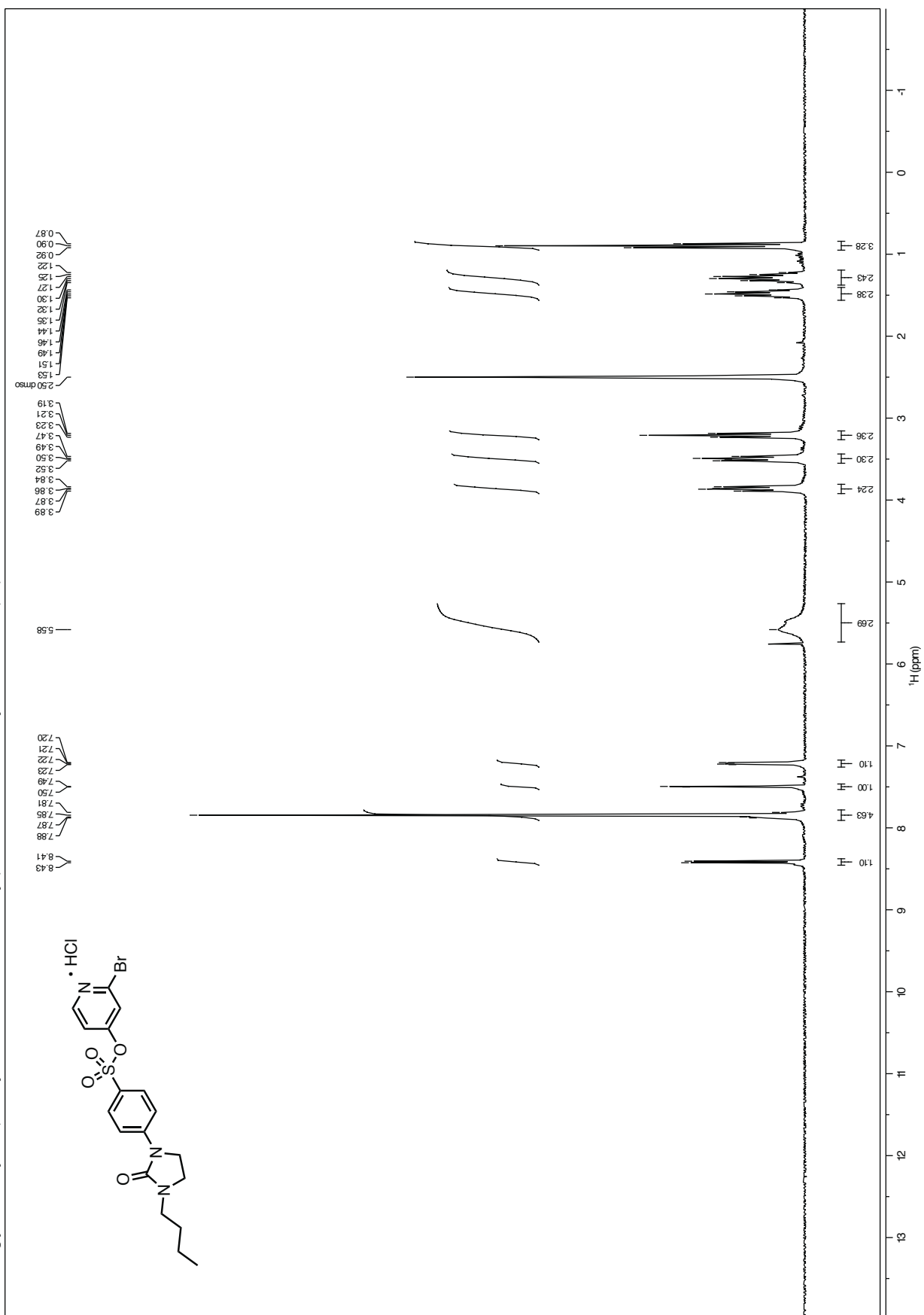




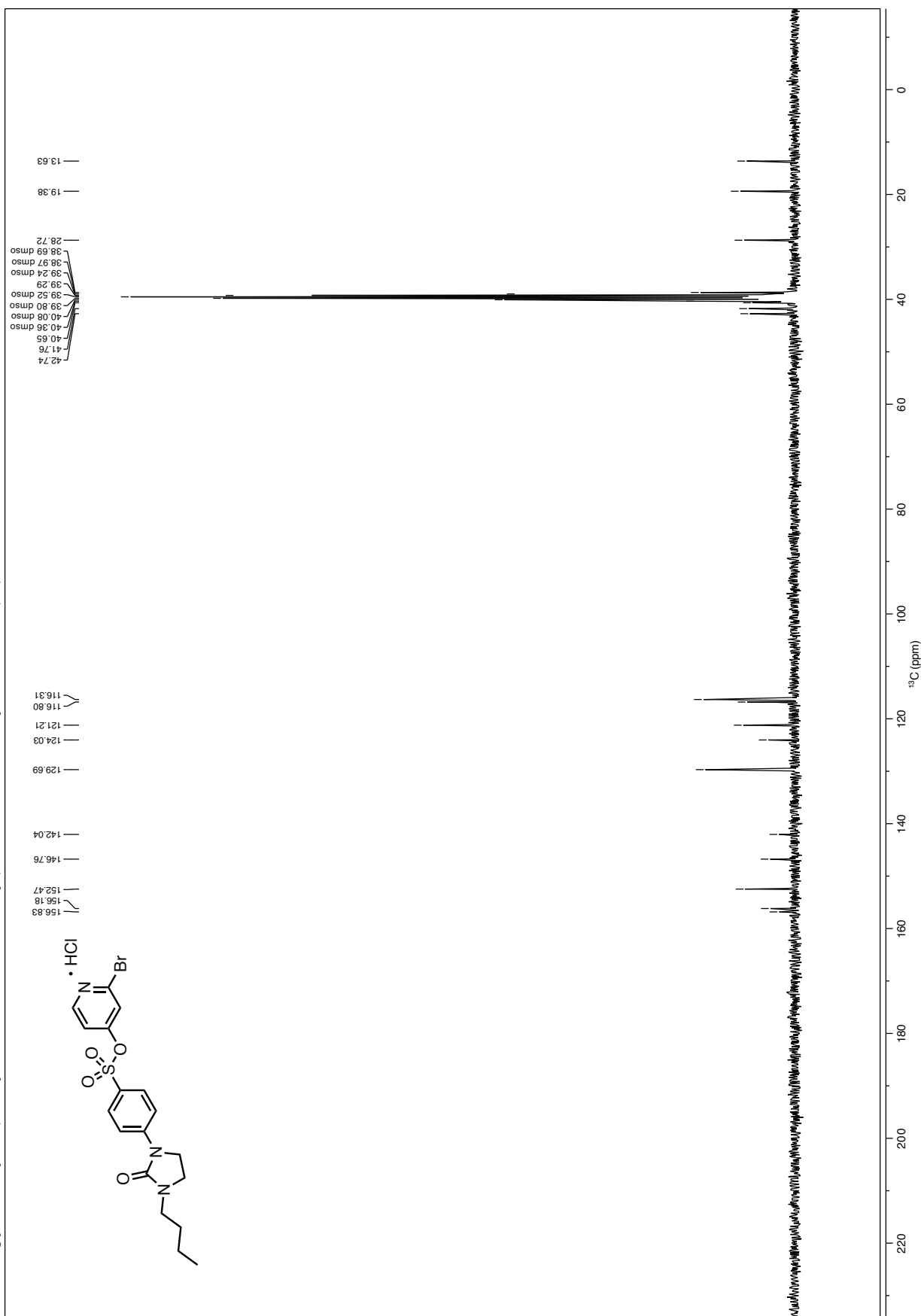
MS spectrum peak list

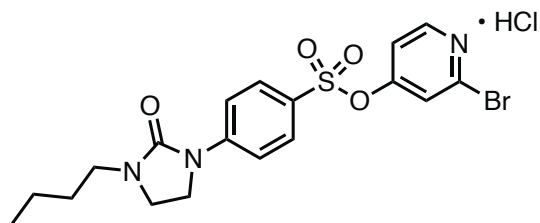
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	Abund	Formula	Ion
420.1589	420.1588	0.4	412114	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
421.1611	421.1617	-1.63	95925	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
422.1582	422.159	-1.8	25990	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
423.1593	423.1604	-2.56	3900	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
424.1565	424.1617	-12.26	571	C ₂₀ H ₂₆ N ₃ O ₅ S	(M+H) ⁺ [-HCl]

2-Bromopyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**23**)

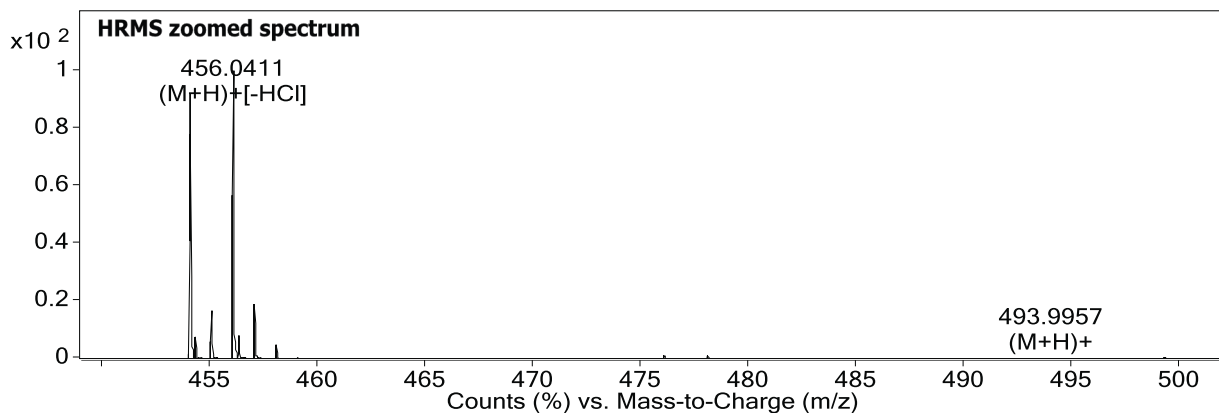
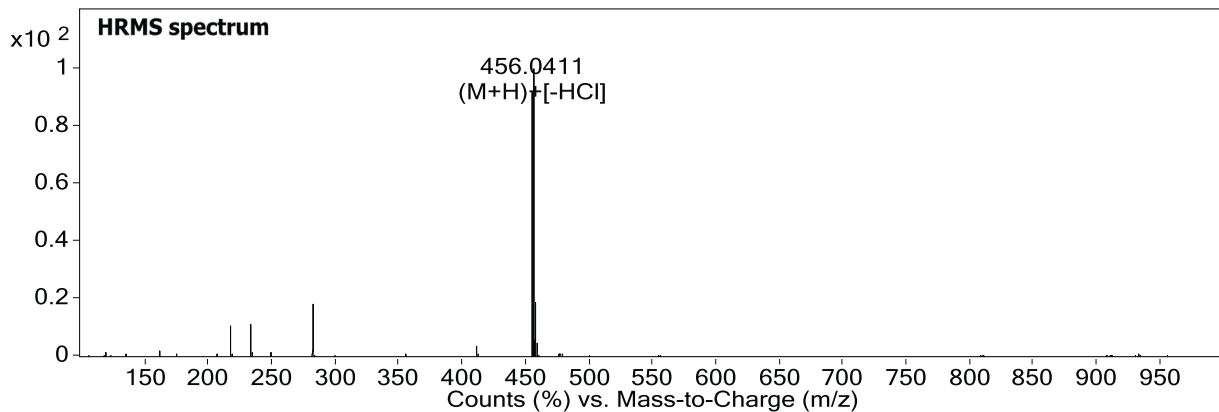


2-Bromopyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**23**)





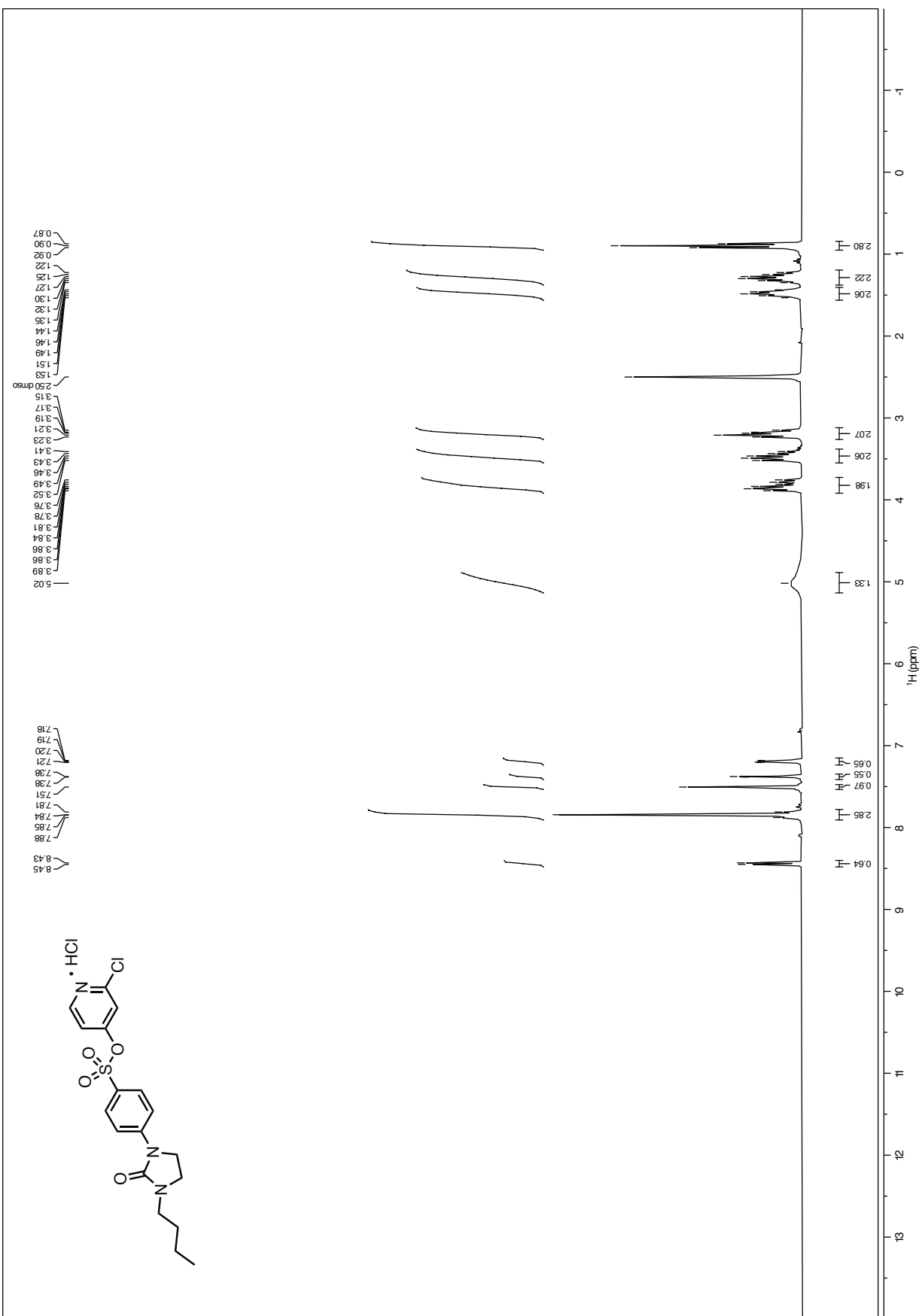
23



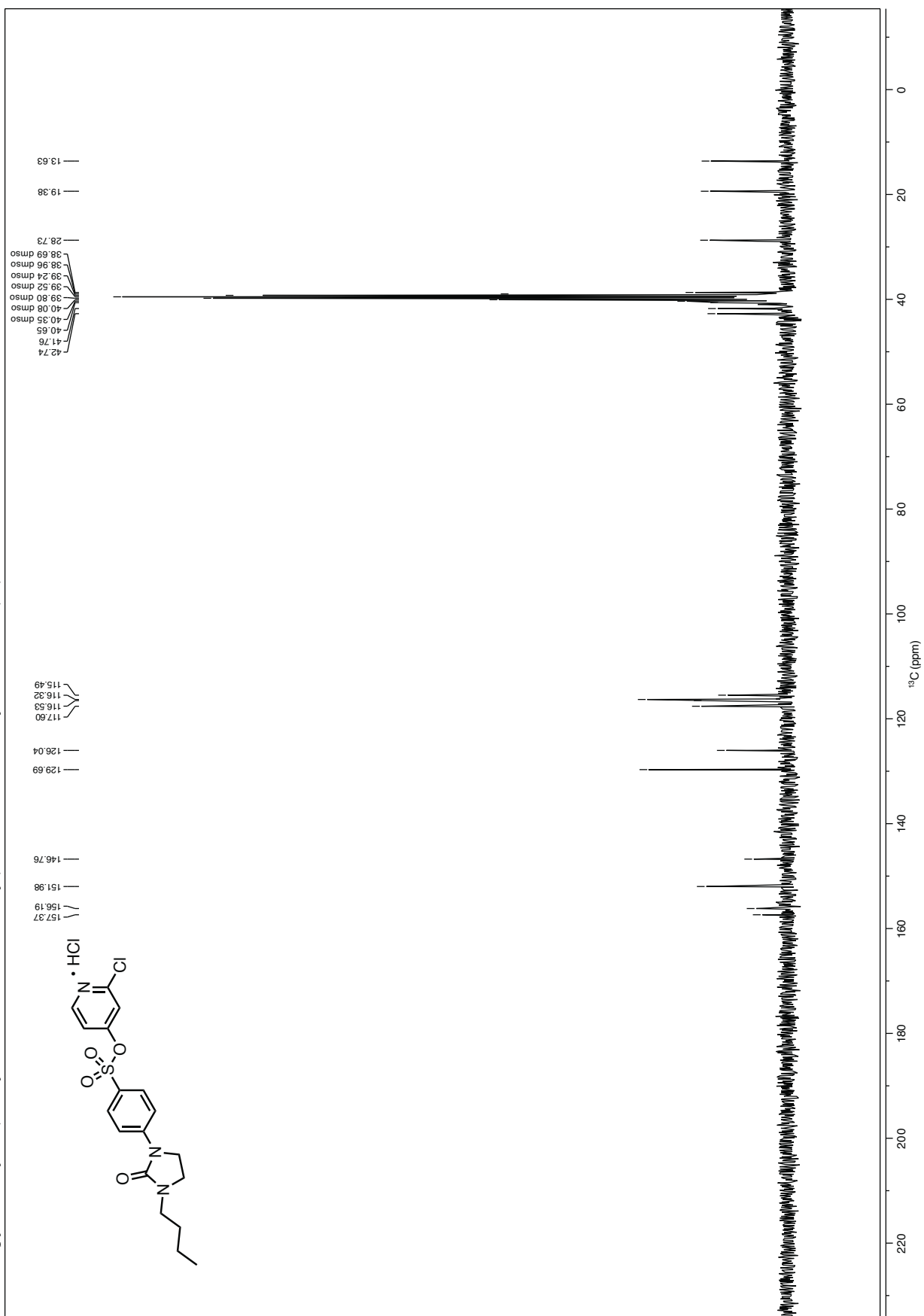
MS spectrum peak list

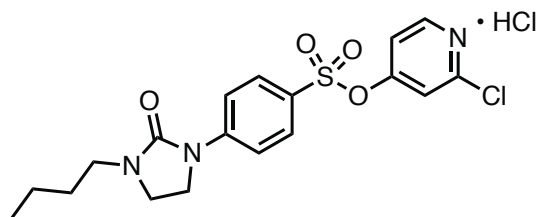
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
454.0431	454.0431	-0.01		335413	C18 H21 Br N3 O4 S	(M+H) ⁺ [-HCl]
455.0453	455.046	-1.46		62552	C18 H21 Br N3 O4 S	(M+H) ⁺ [-HCl]
456.0411	456.0411	-0.03		356655	C18 H21 Br N3 O4 S	(M+H) ⁺ [-HCl]
457.0434	457.044	-1.22		66875	C18 H21 Br N3 O4 S	(M+H) ⁺ [-HCl]
458.0402	458.0408	-1.37		17409	C18 H21 Br N3 O4 S	(M+H) ⁺ [-HCl]
459.0413	459.0423	-2.16		2258	C18 H21 Br N3 O4 S	(M+H) ⁺ [-HCl]
460.0422	460.0435	-3		378	C18 H21 Br N3 O4 S	(M+H) ⁺ [-HCl]
491.9989	492.0176	-37.98	1	326	C18 H22 Br Cl N3 O4 S	(M+H) ⁺

2-Chloropyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**24**)

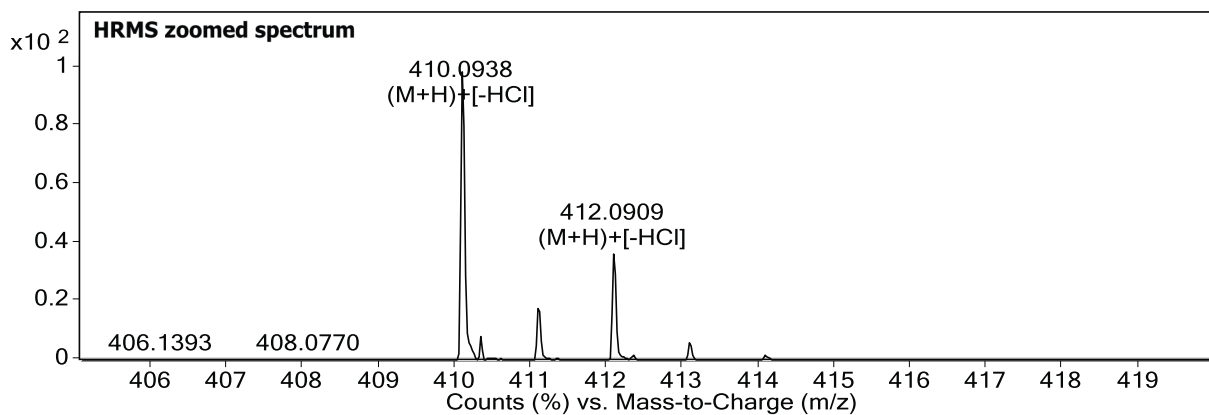
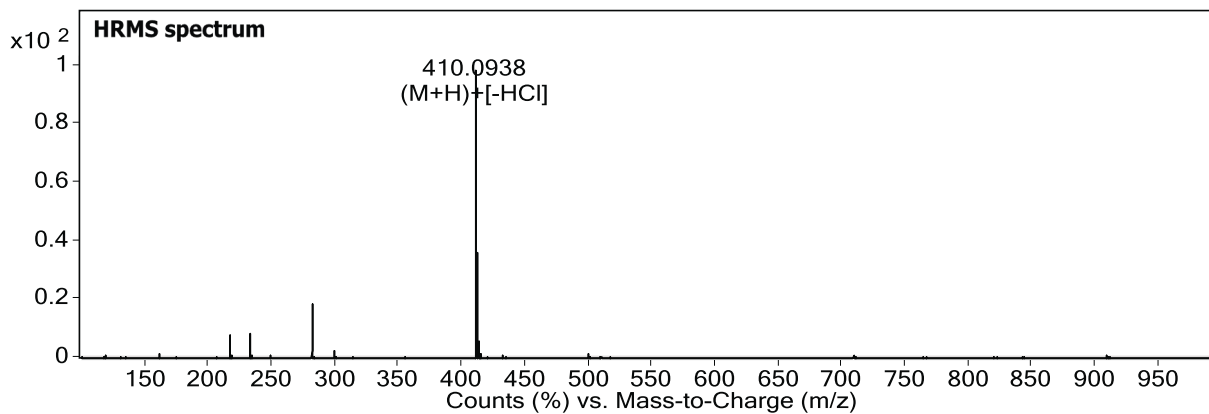


2-Chloropyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**24**)





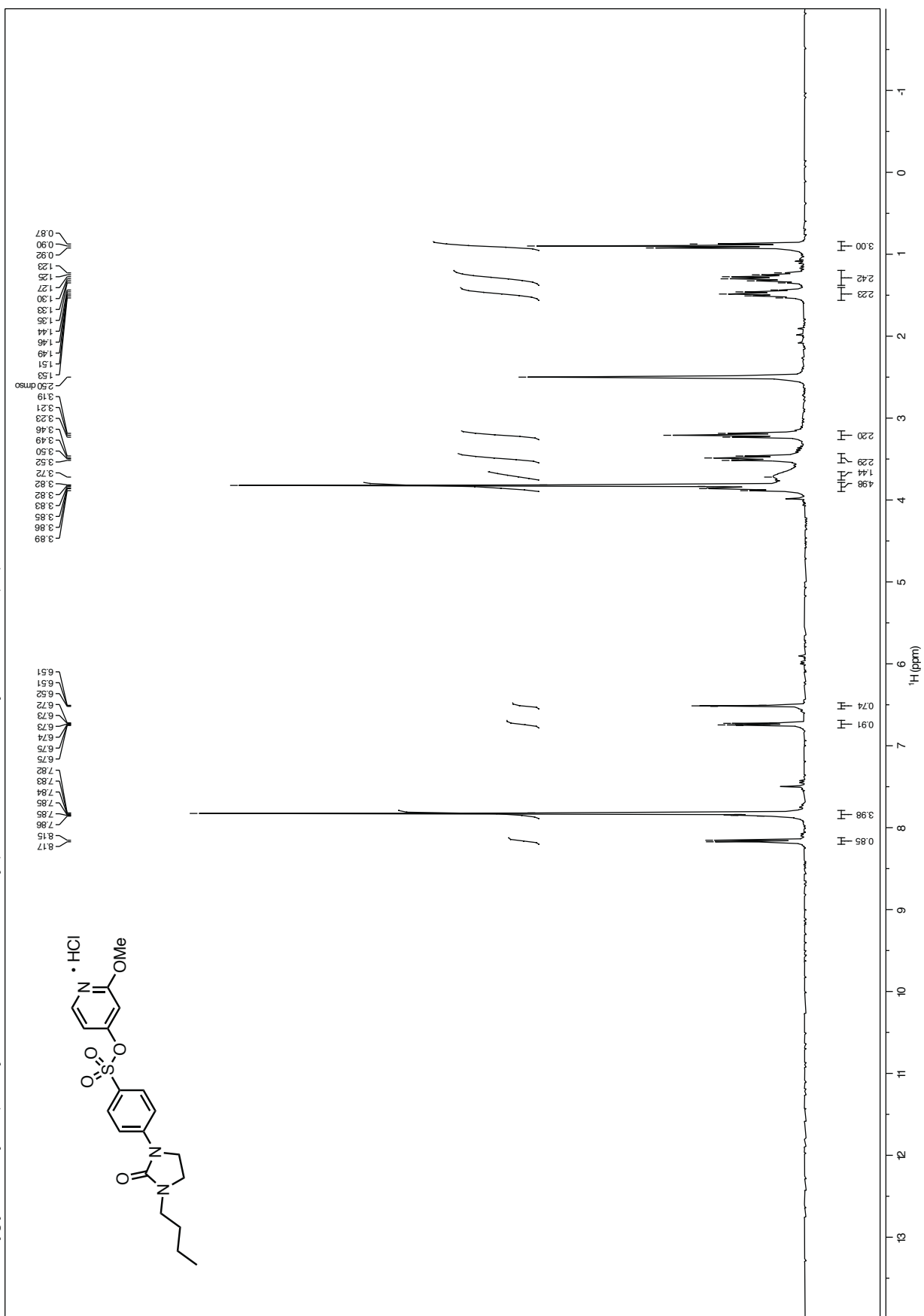
24



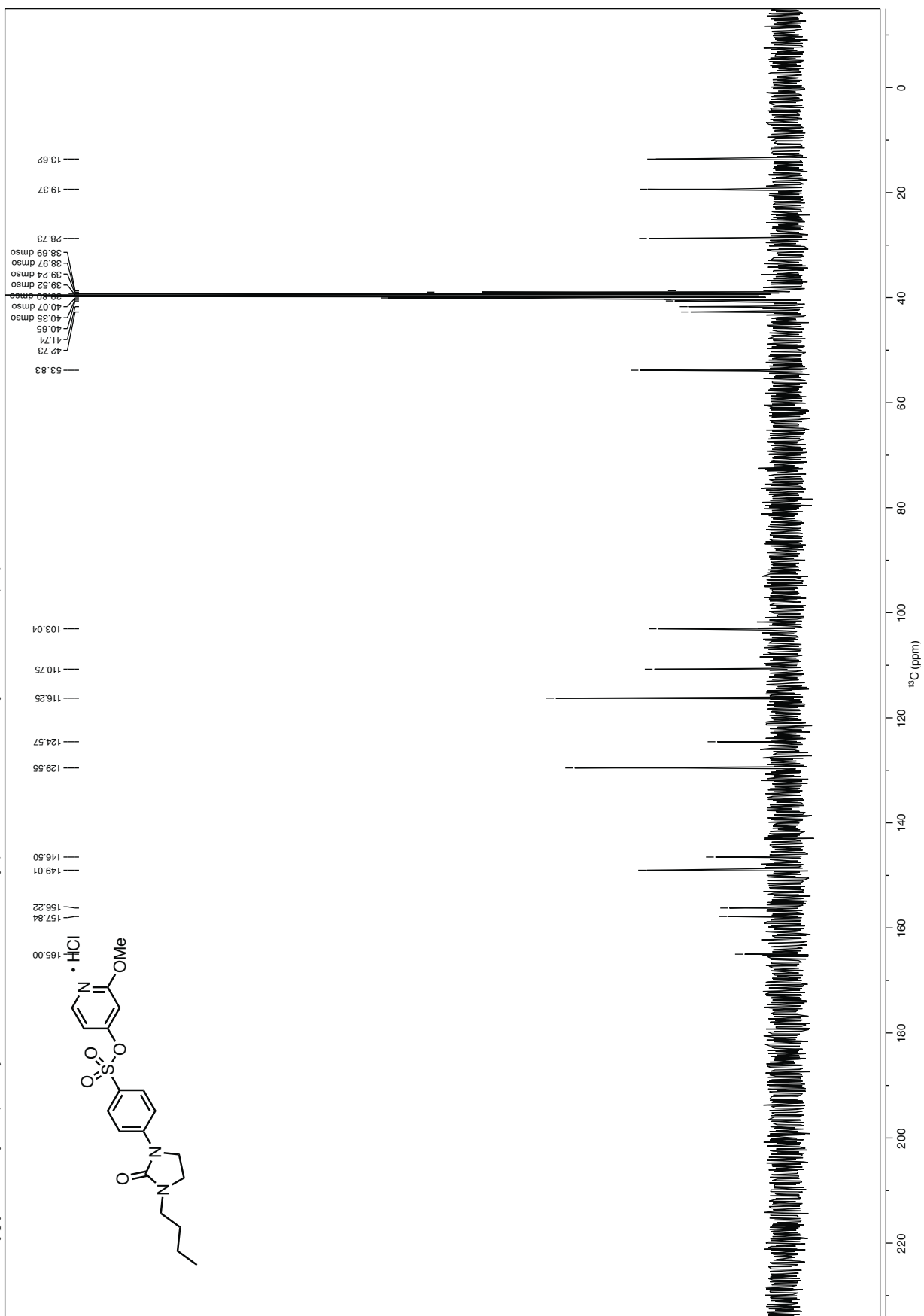
MS spectrum peak list

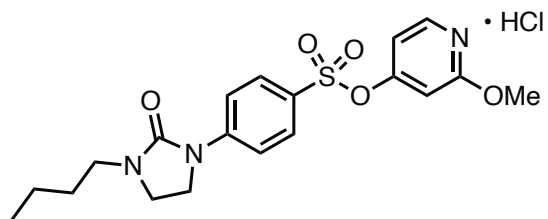
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
410.0938	410.0936	0.45	361684	C18 H21 Cl N3 O4 S	(M+H)+[-HCl]
411.0962	411.0965	-0.65	67251	C18 H21 Cl N3 O4 S	(M+H)+[-HCl]
412.0909	412.0911	-0.52	133221	C18 H21 Cl N3 O4 S	(M+H)+[-HCl]
413.0936	413.0937	-0.43	21478	C18 H21 Cl N3 O4 S	(M+H)+[-HCl]
414.0907	414.0907	-0.03	5677	C18 H21 Cl N3 O4 S	(M+H)+[-HCl]
415.0913	415.0921	-1.91	893	C18 H21 Cl N3 O4 S	(M+H)+[-HCl]

2-Methoxypyridin-4-yl 4-(3-buty-1-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (25)

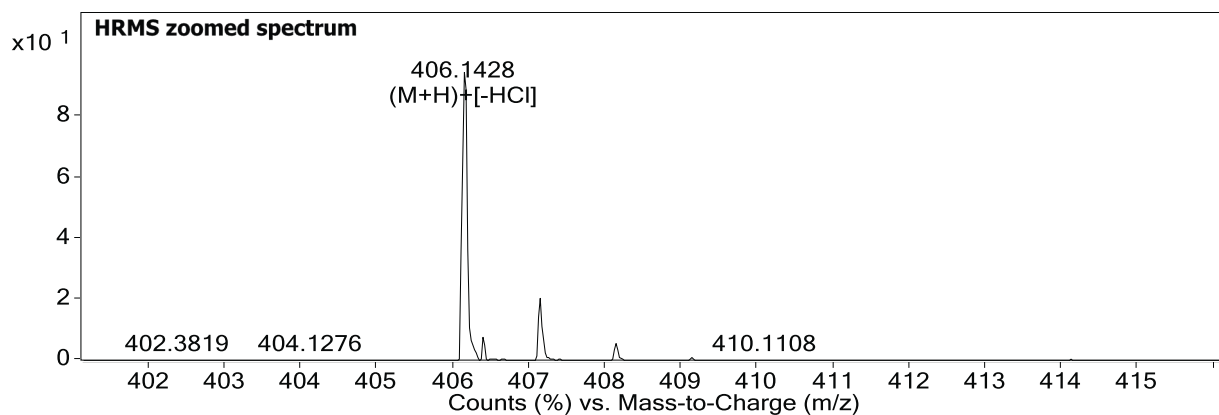
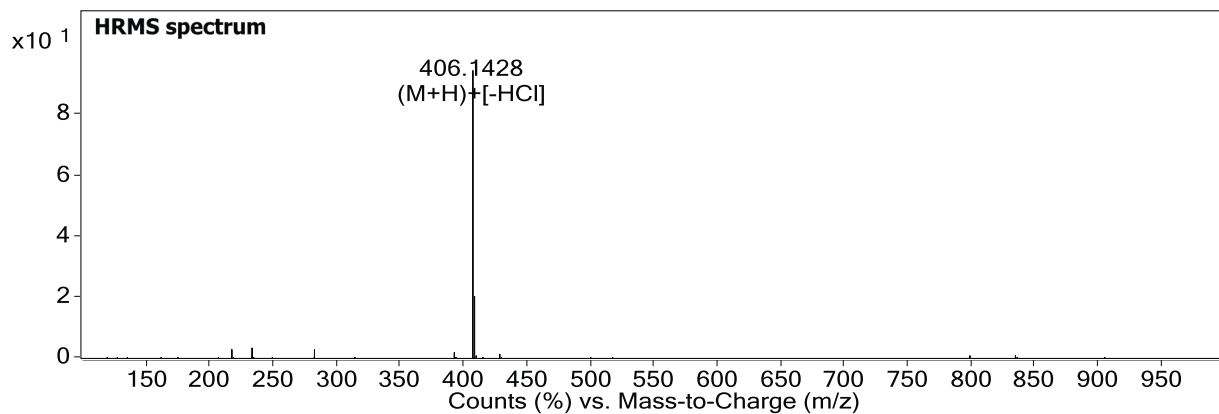


2-Methoxypyridin-4-yl 4-(3-buty-1-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (25)





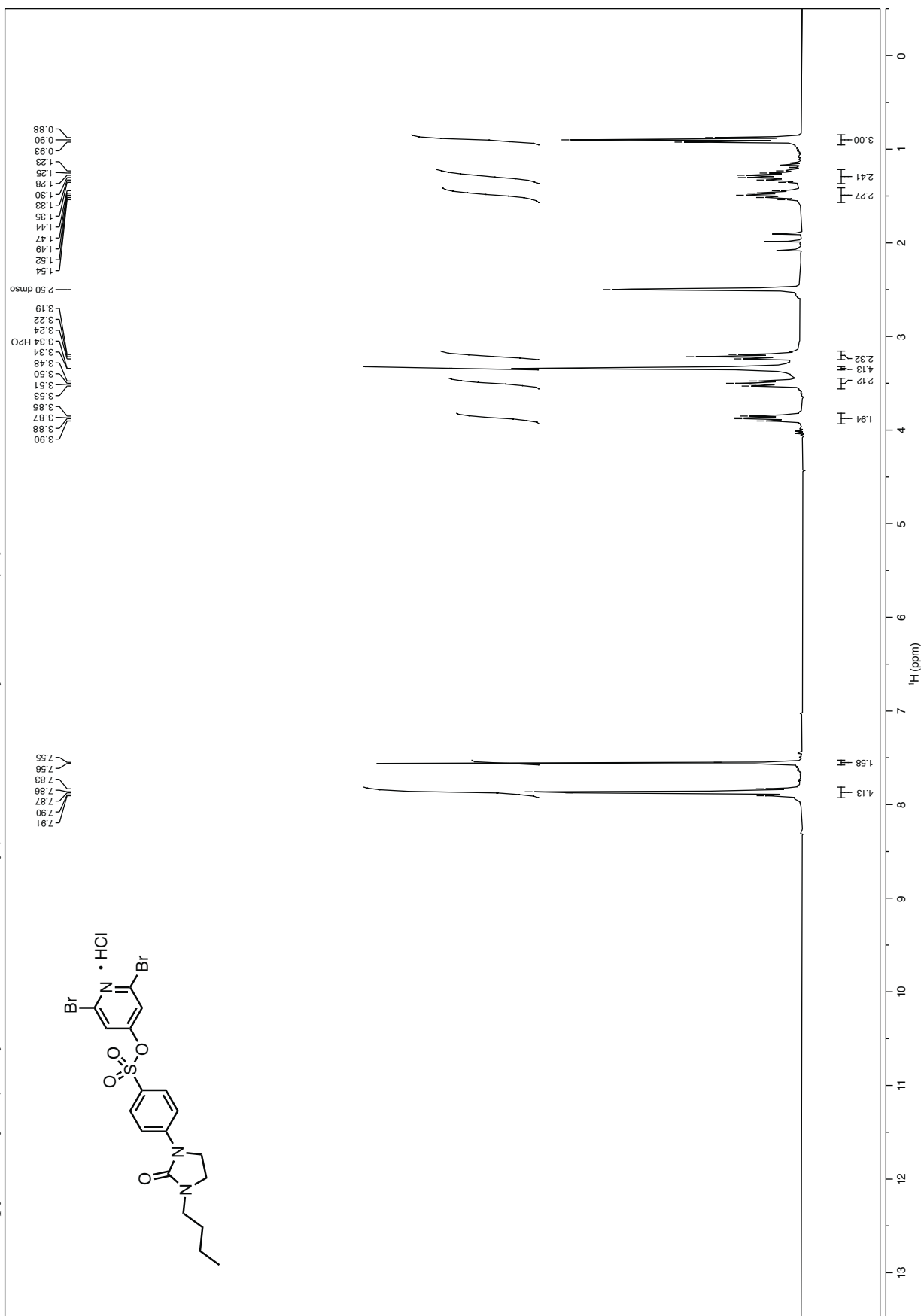
25



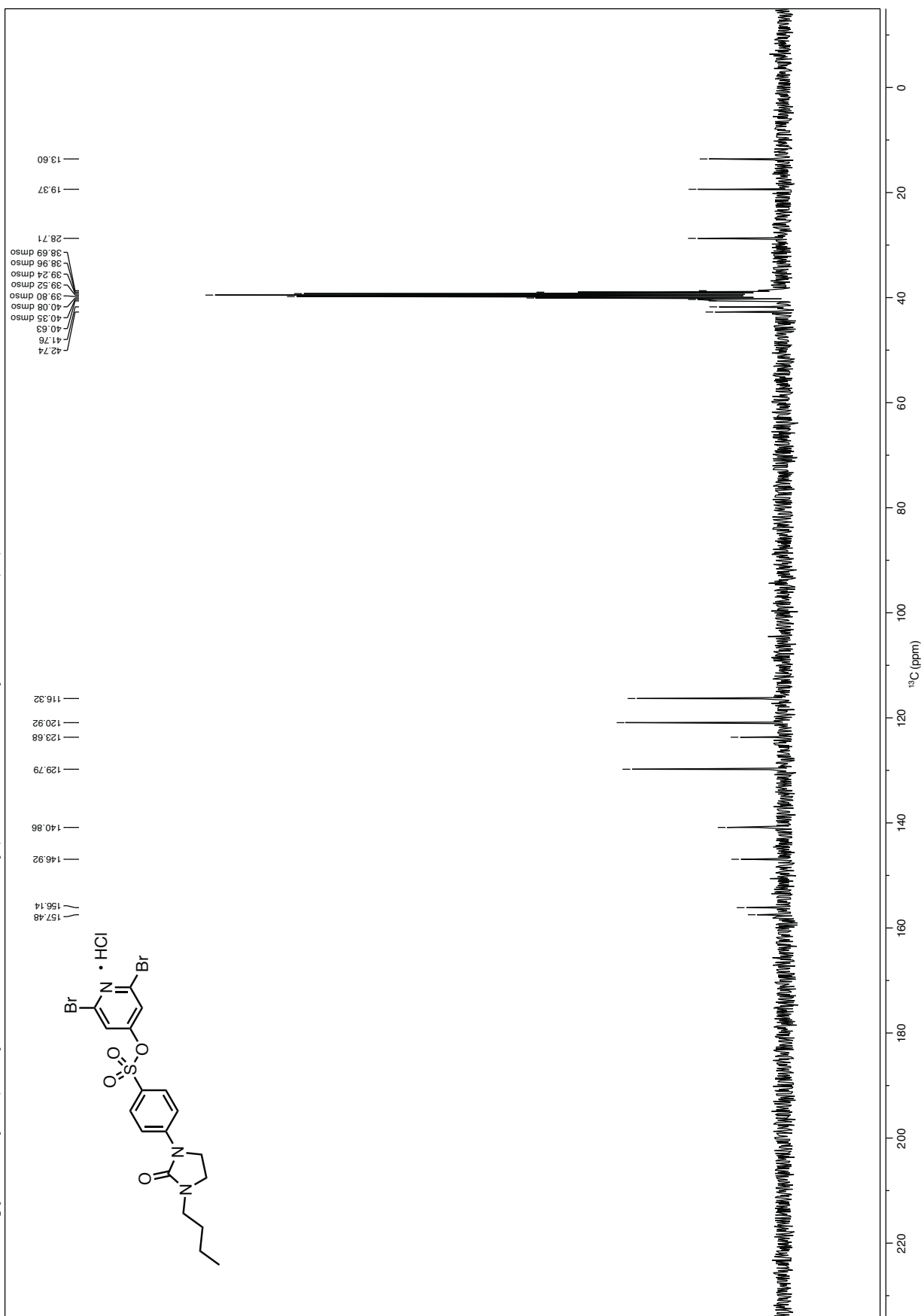
MS spectrum peak list

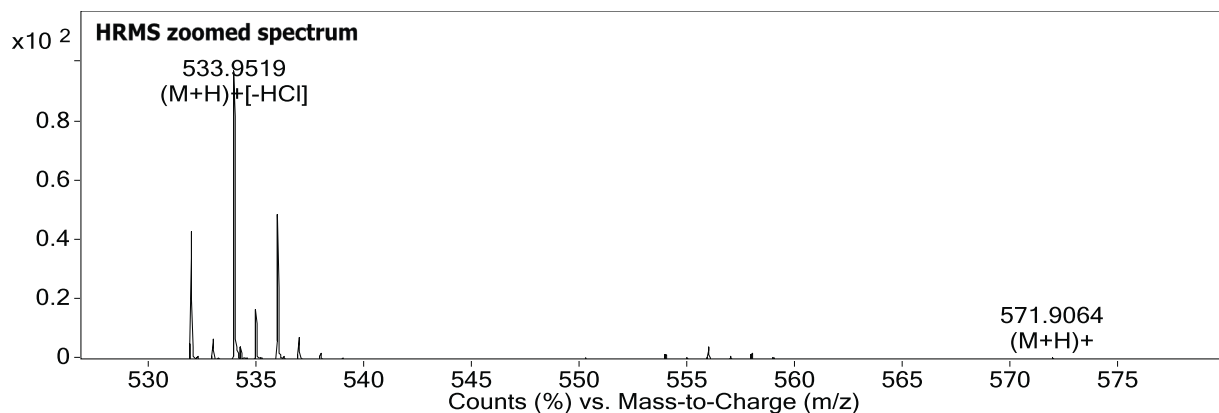
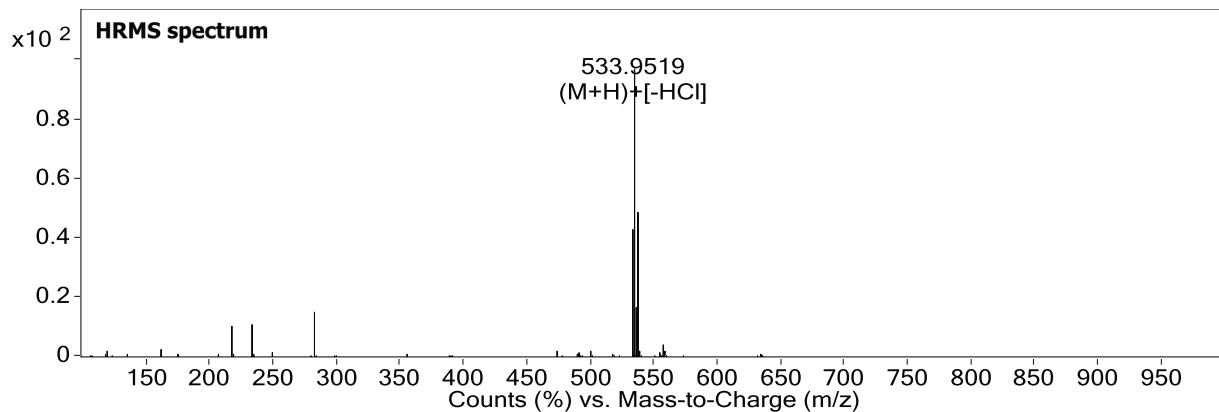
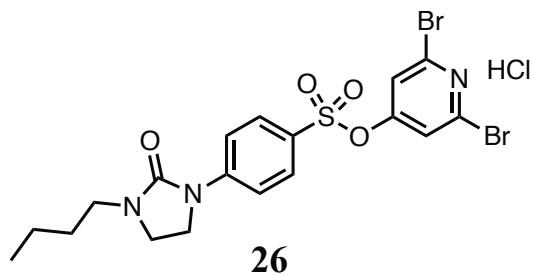
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
406.1428	406.1431	-0.86	383389	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
407.1453	407.1461	-1.93	78765	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
408.1426	408.1432	-1.35	22338	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺ [-HCl]
409.1434	409.1446	-2.91	3169	C ₁₉ H ₂₄ N ₃ O ₅ S	(M+H) ⁺ [-HCl]

2,6-Dibromopyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (26)



2,6-Dibromopyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (**26**)

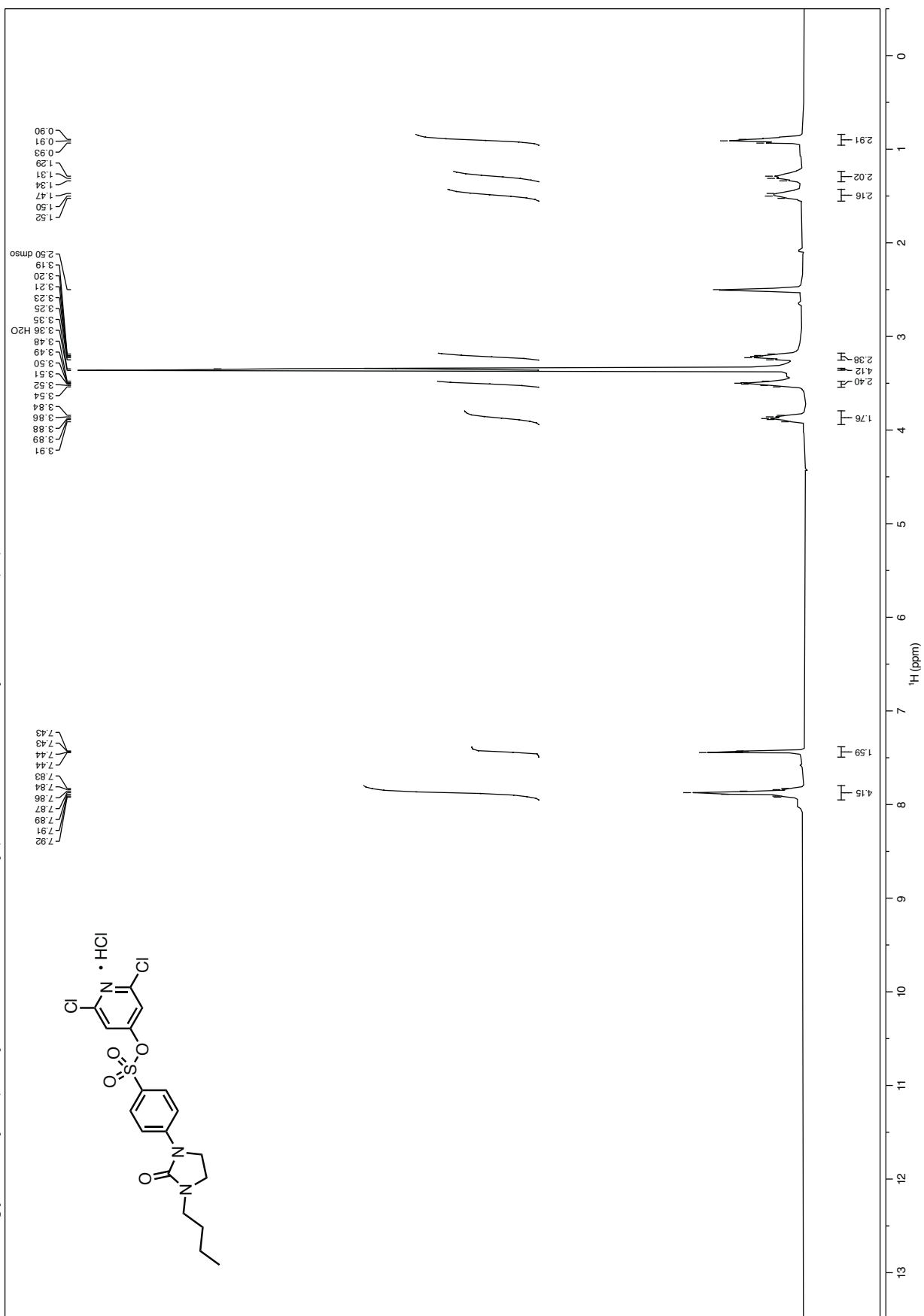




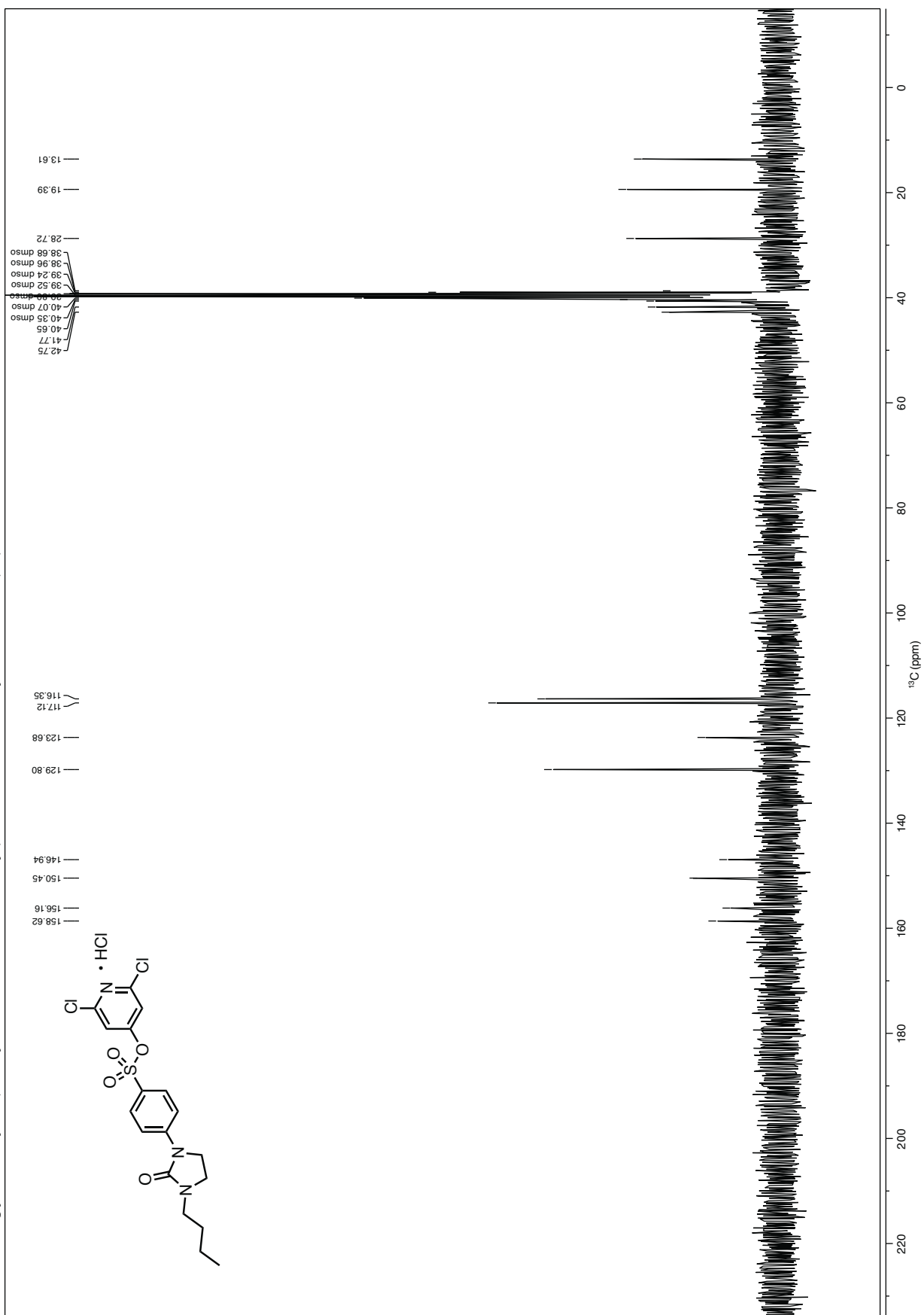
MS spectrum peak list

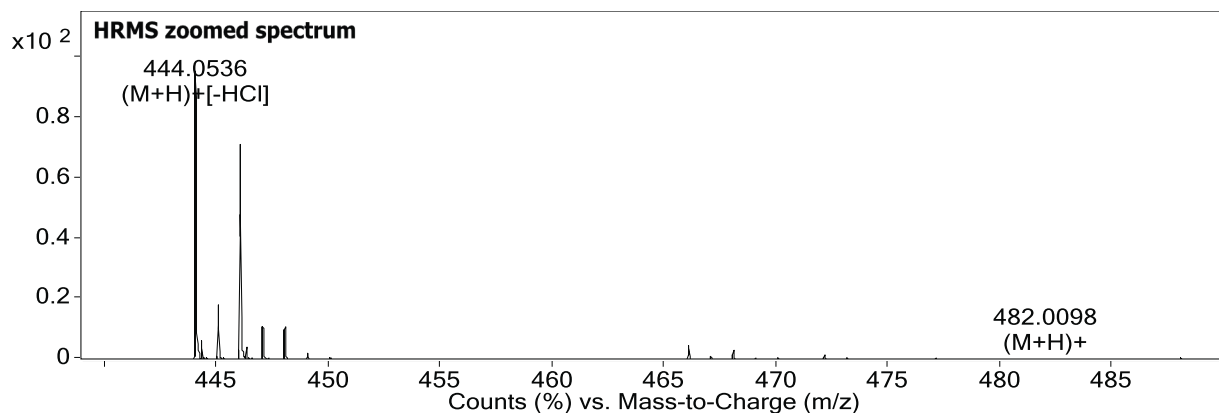
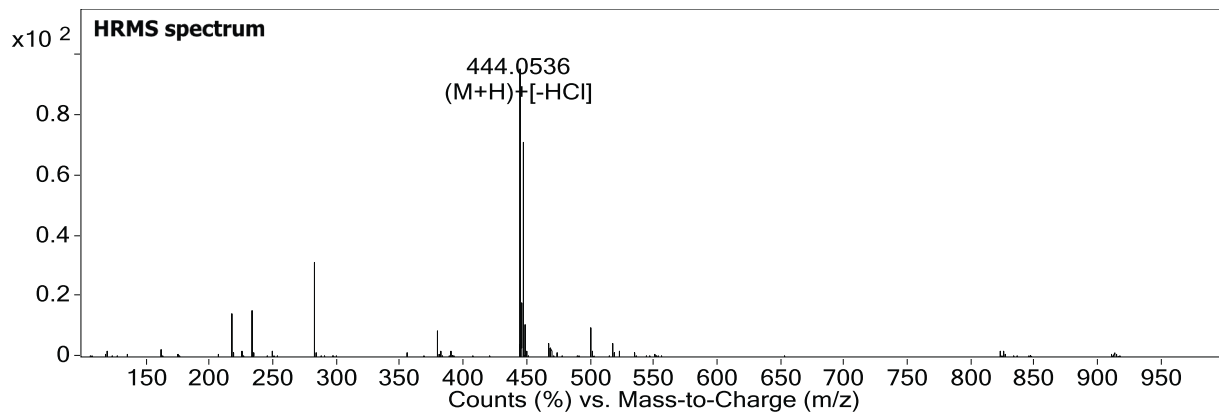
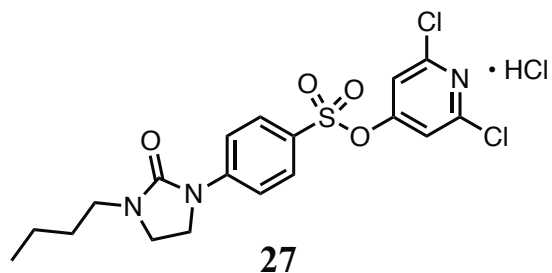
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
531.9536	531.9536	0.02		59602	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H)+[-HCl]
532.9564	532.9565	-0.18		9393	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H)+[-HCl]
533.9519	533.9516	0.48		136360	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H)+[-HCl]
534.9544	534.9545	-0.15		22910	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H)+[-HCl]
535.9498	535.9497	0.07		67264	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H)+[-HCl]
536.9523	536.9525	-0.22		10228	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H)+[-HCl]
537.9497	537.9494	0.59		2829	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H)+[-HCl]
538.9509	538.9508	0.18	1	461	C ₁₈ H ₂₀ Br ₂ N ₃ O ₄ S	(M+H)+[-HCl]

2,6-Dichloropyridin-4-yl 4-(3-butyl-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (27)



2,6-Dichloropyridin-4-yl 4-(3-buty]-2-oxoimidazolidin-1-yl)benzenesulfonate hydrochloride (27)

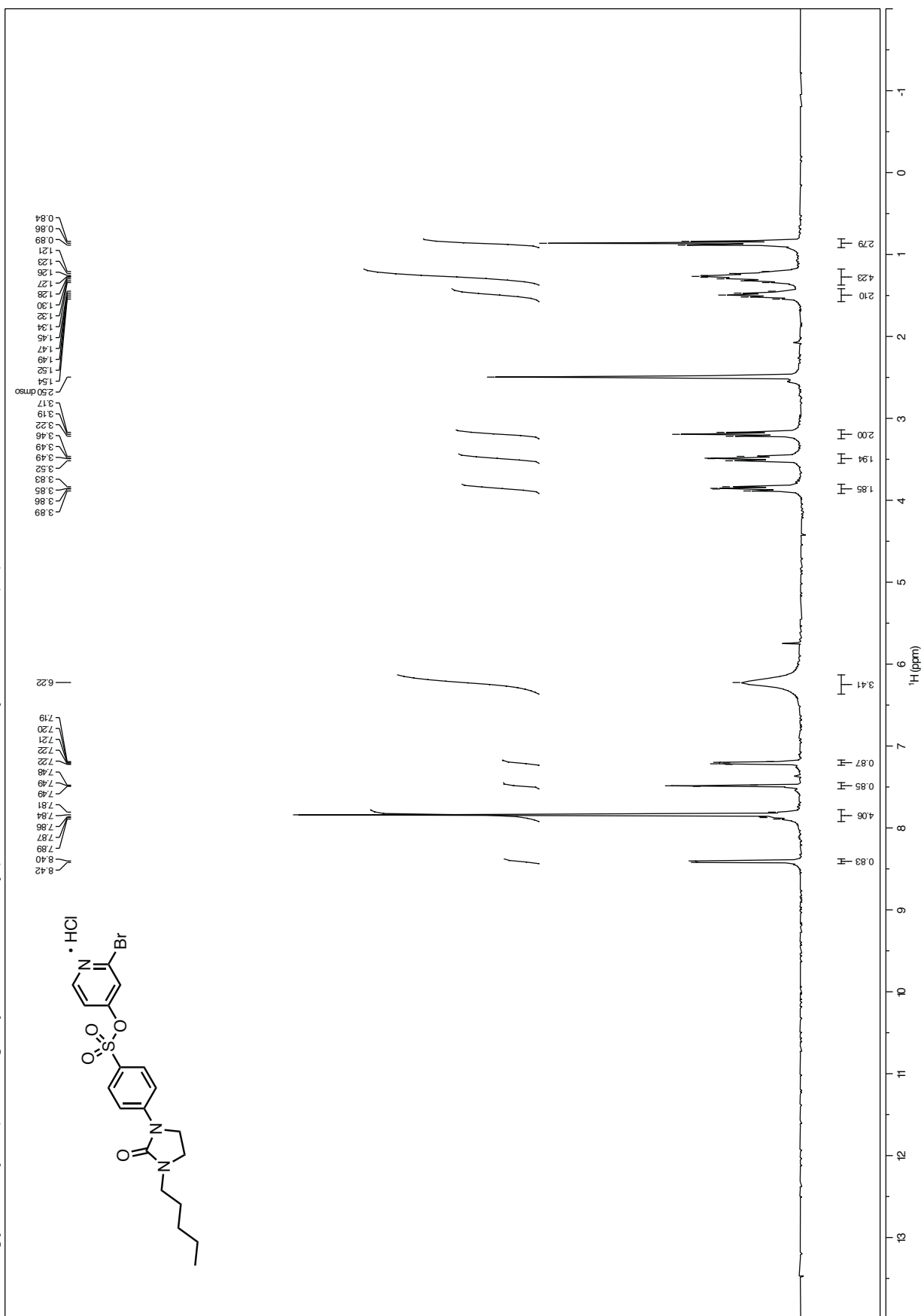




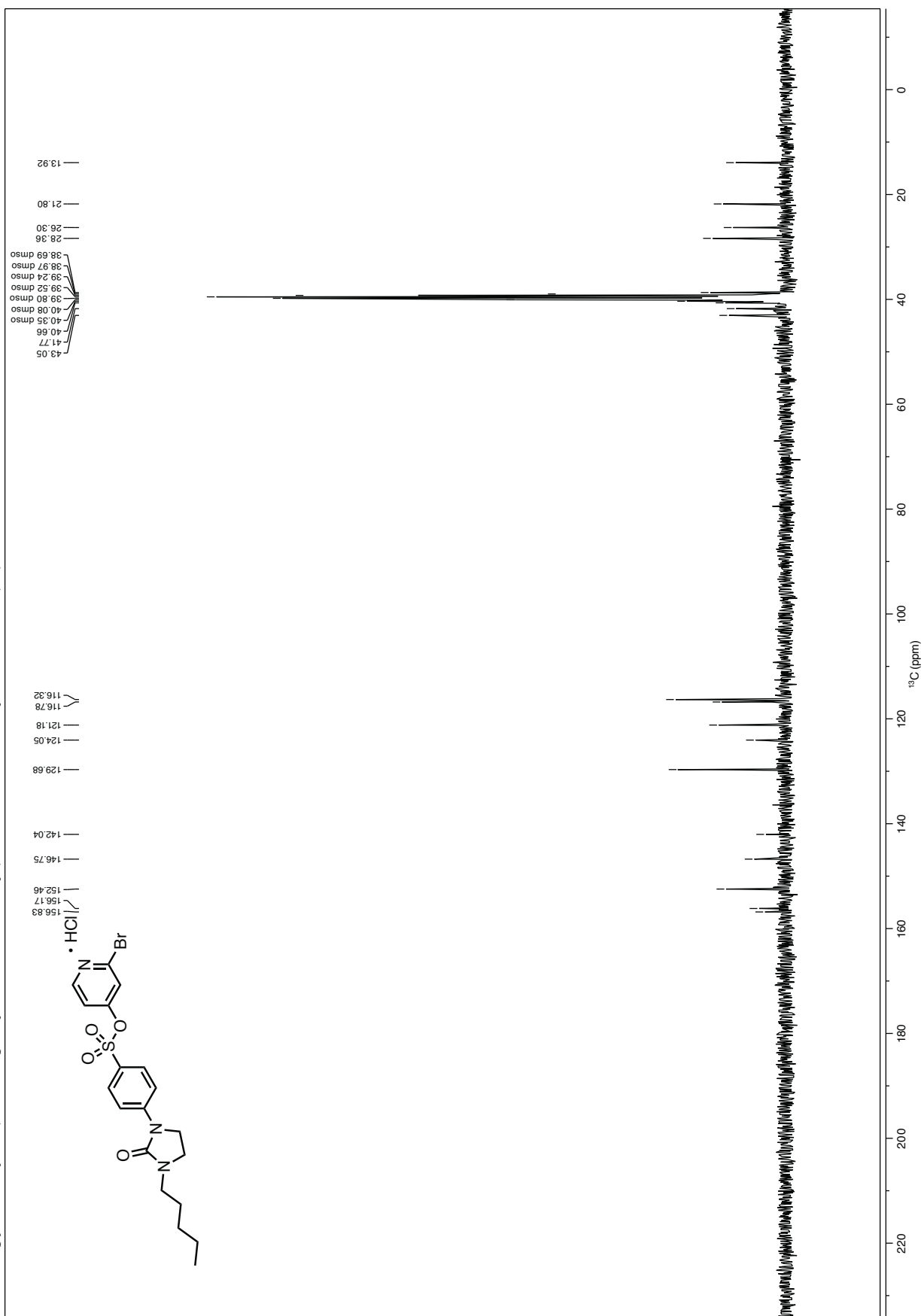
MS spectrum peak list

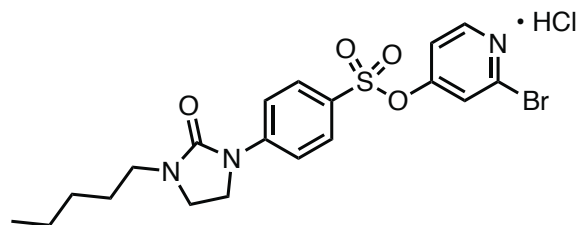
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
444.0536	444.0546	-2.32		211565	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
445.0565	445.0575	-2.35		38160	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
446.0508	446.0519	-2.6		150668	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
447.0531	447.0547	-3.55		24404	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
448.0484	448.0496	-2.74		23909	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
449.051	449.052	-2.16	1	3986	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
450.0478	450.0491	-2.94	1	1060	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
451.0489	451.0504	-3.32	1	195	C ₁₈ H ₂₀ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]

2-Bromopyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**28**)

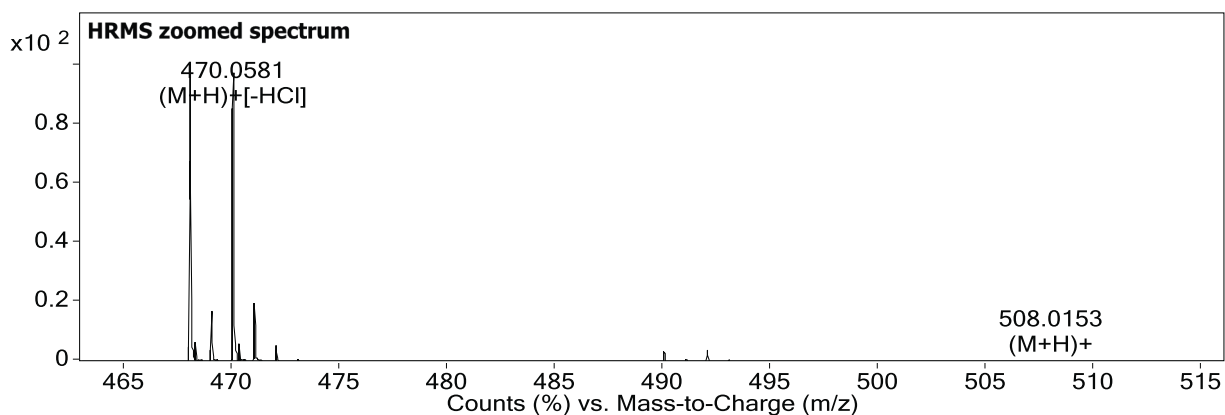
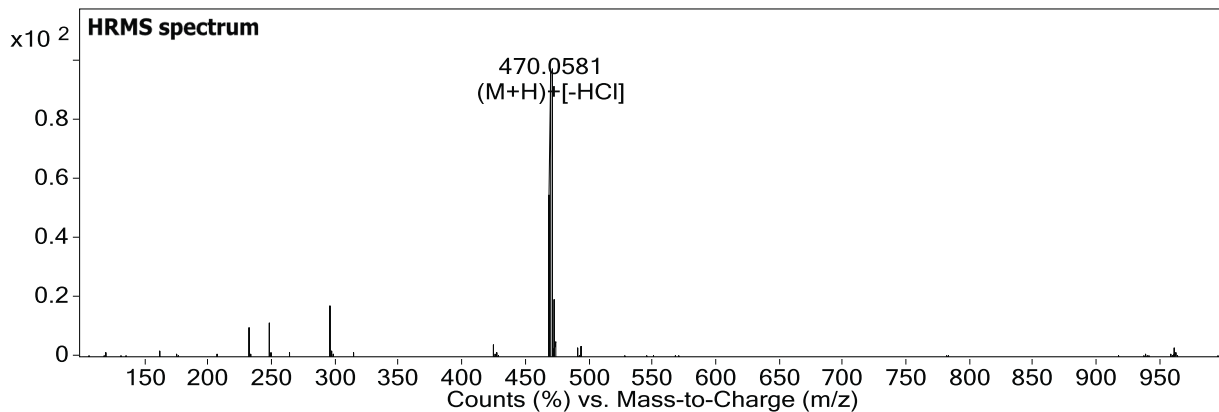


2-Bromopyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**28**)





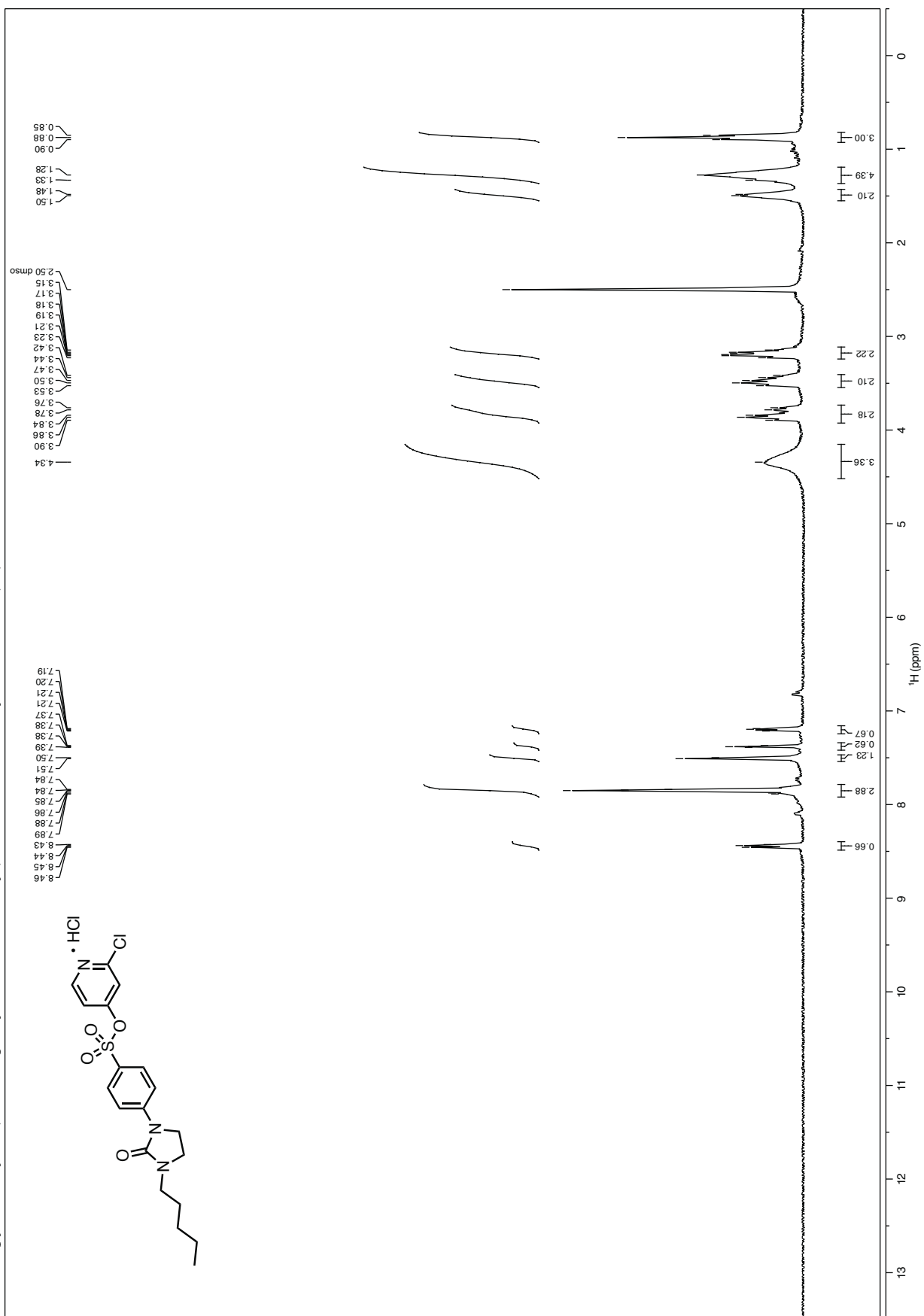
28



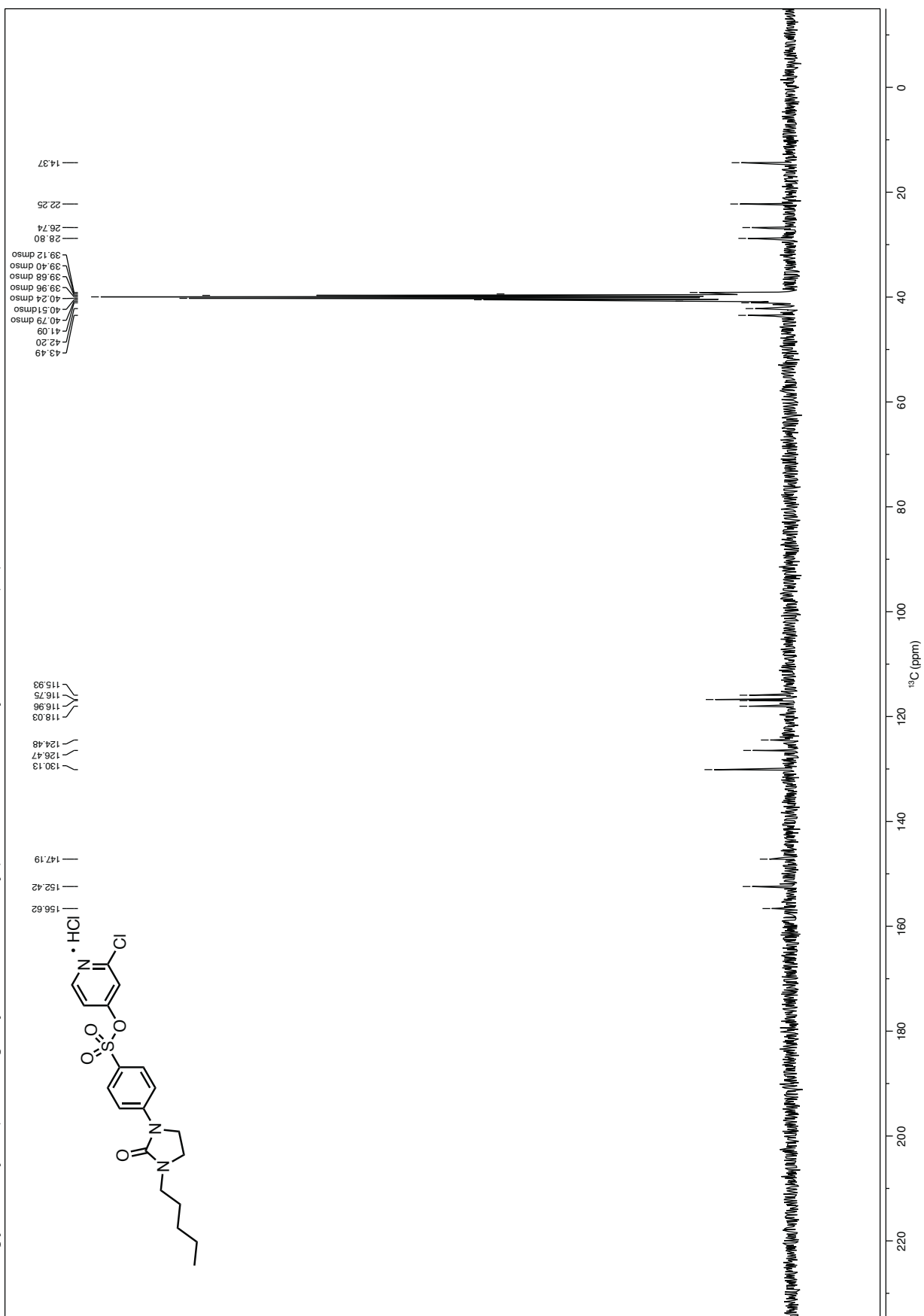
MS spectrum peak list

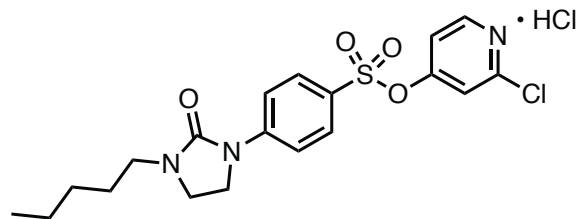
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
468.0601	468.0587	3.01		223751	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H)+[-HCl]
469.0625	469.0617	1.86		41250	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H)+[-HCl]
470.0581	470.0568	2.78		231398	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H)+[-HCl]
471.0609	471.0596	2.56		45406	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H)+[-HCl]
472.0589	472.0567	4.58		11857	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H)+[-HCl]
473.0597	473.0581	3.57		1686	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H)+[-HCl]
474.0668	474.0594	15.82		262	C ₁₉ H ₂₃ Br N ₃ O ₄ S	(M+H)+[-HCl]
506.0152	506.0332	-35.65	1	342	C ₁₉ H ₂₄ Br Cl N ₃ O ₄ S	(M+H)+

2-Chloropyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (29)

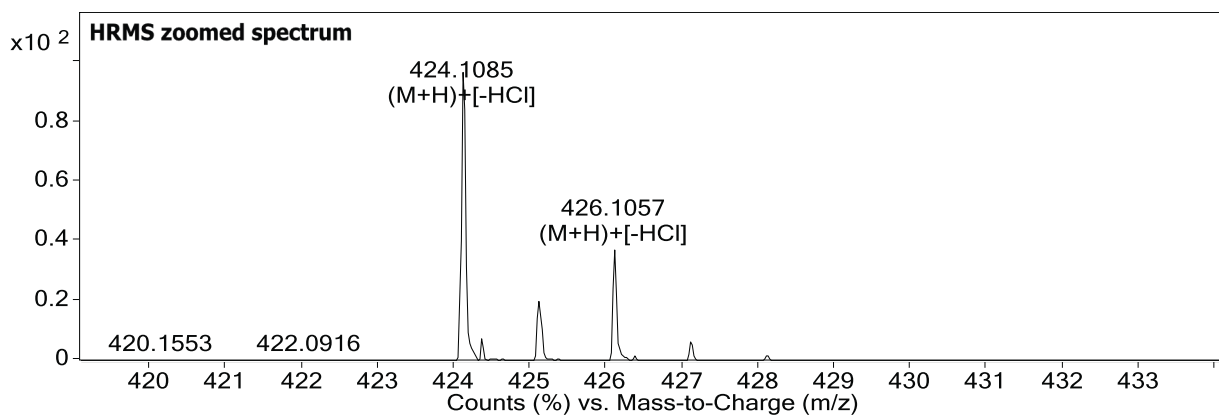
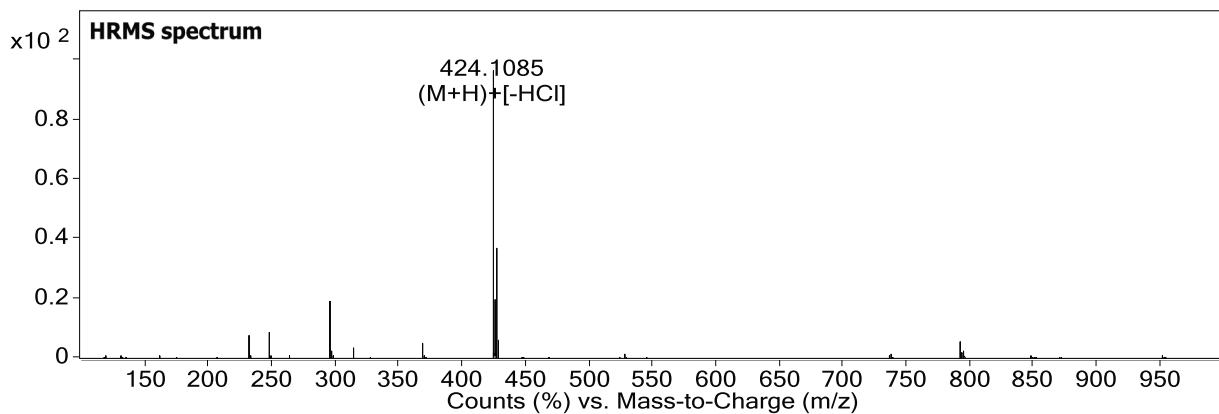


2-Chloropyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (29)





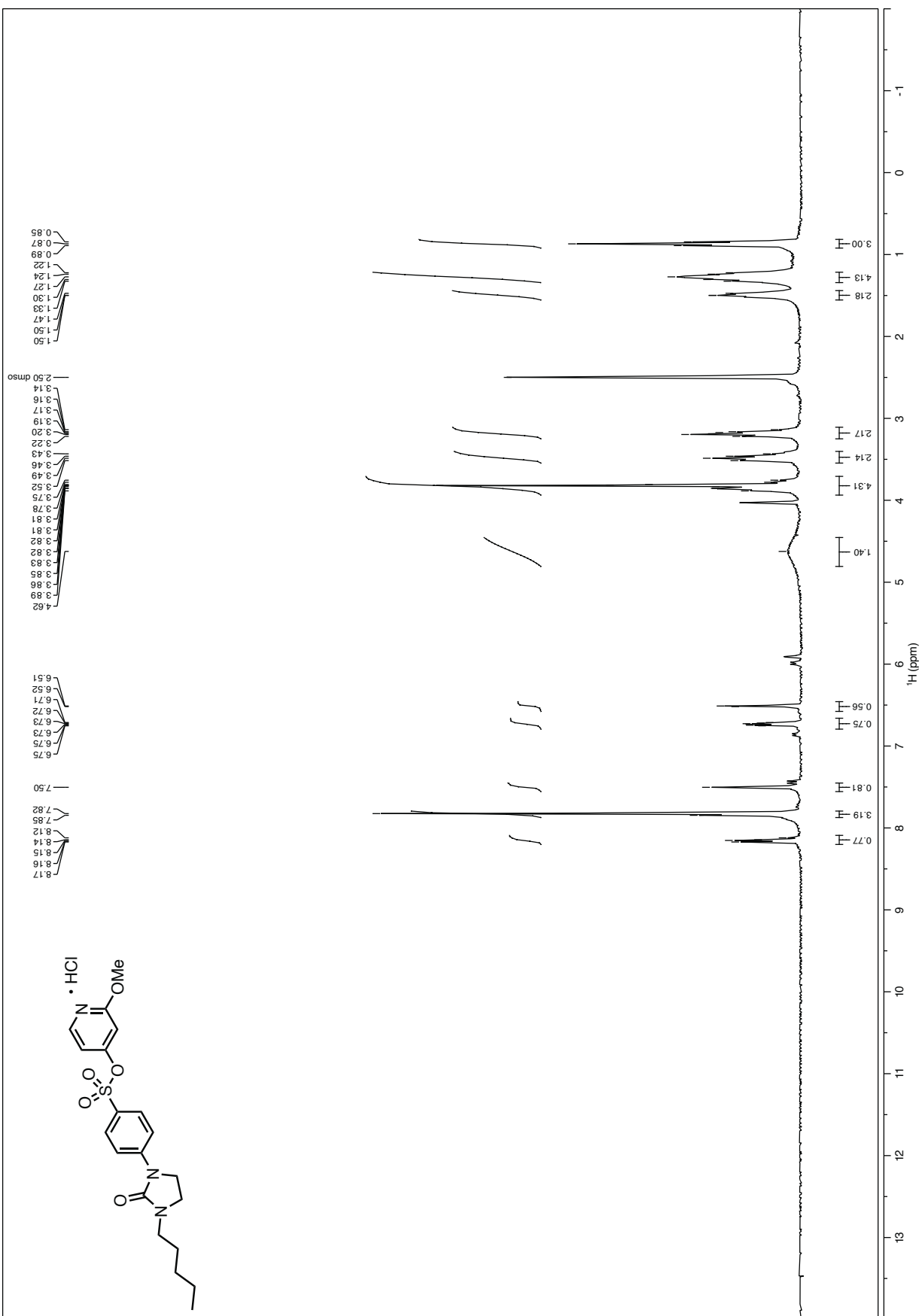
29



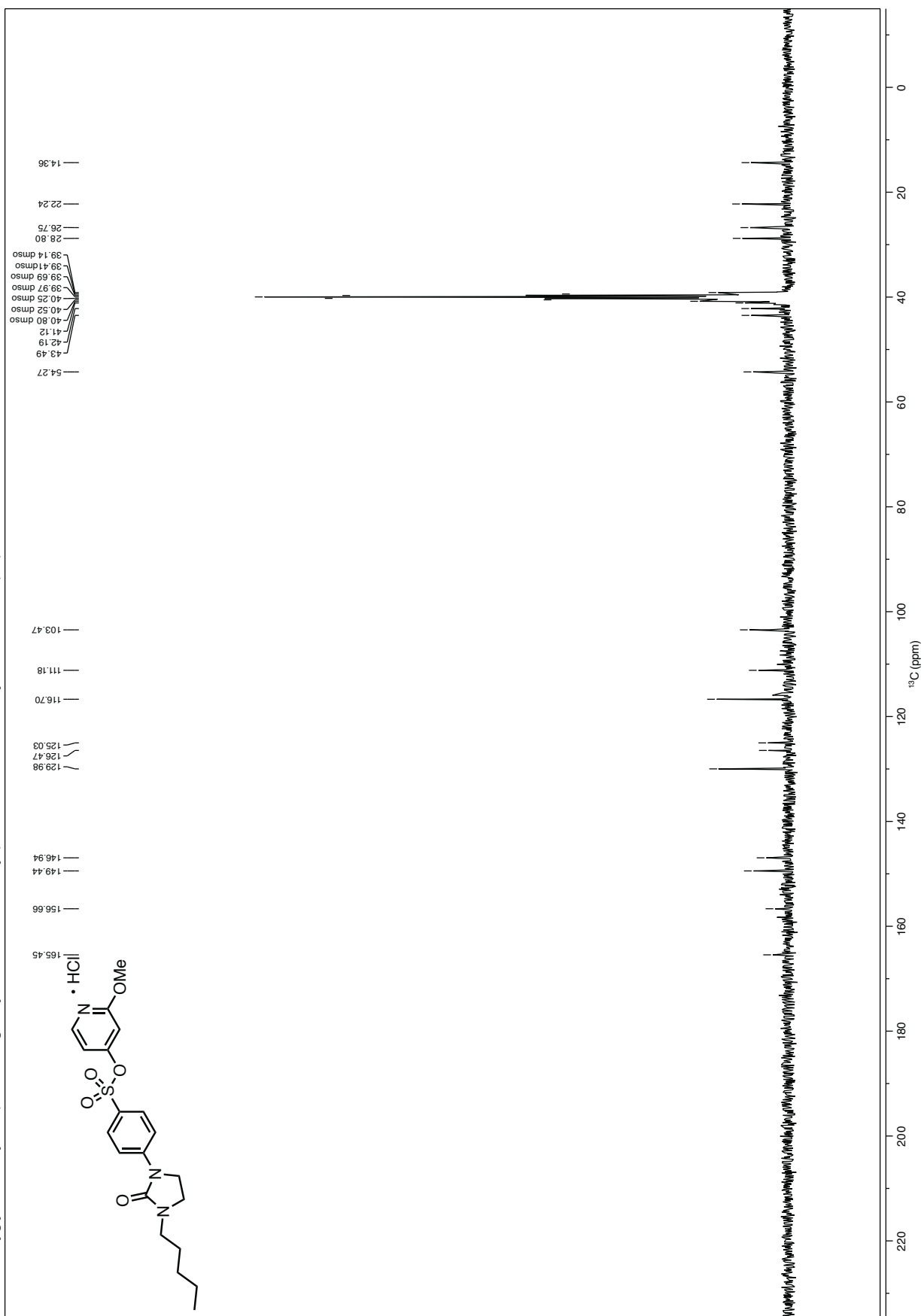
MS spectrum peak list

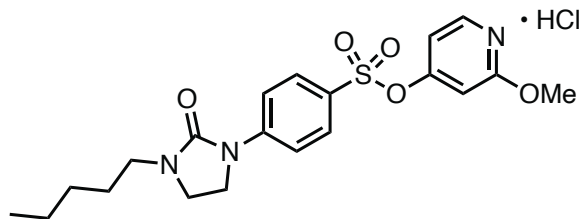
<i>m/z</i>	<i>Calc m/z</i>	Diff(ppm)	<i>z</i>	Abund	Formula	Ion
424.1085	424.1092	-1.67		254092	C19 H23 Cl N3 O4 S	(M+H)+[-HCl]
425.1113	425.1122	-2.09		50737	C19 H23 Cl N3 O4 S	(M+H)+[-HCl]
426.1057	426.1068	-2.72		94214	C19 H23 Cl N3 O4 S	(M+H)+[-HCl]
427.1084	427.1094	-2.37		16165	C19 H23 Cl N3 O4 S	(M+H)+[-HCl]
428.1058	428.1066	-1.94		3974	C19 H23 Cl N3 O4 S	(M+H)+[-HCl]
429.1065	429.1079	-3.08	1	655	C19 H23 Cl N3 O4 S	(M+H)+[-HCl]

2-Methoxypyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (30)

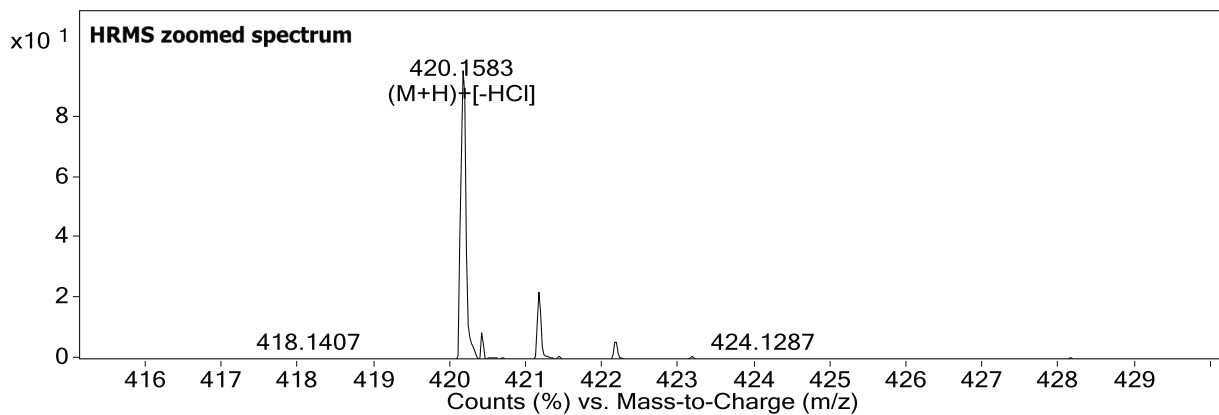
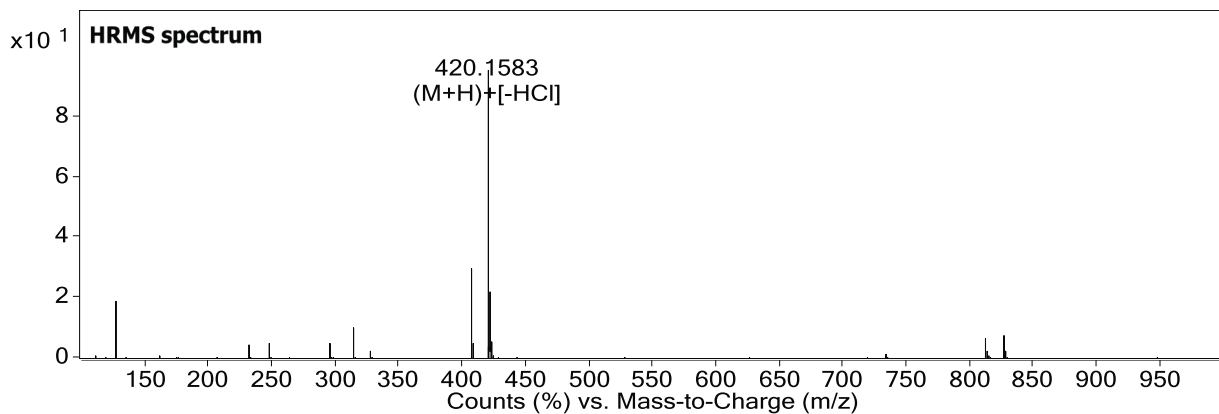


2-Methoxypyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**30**)





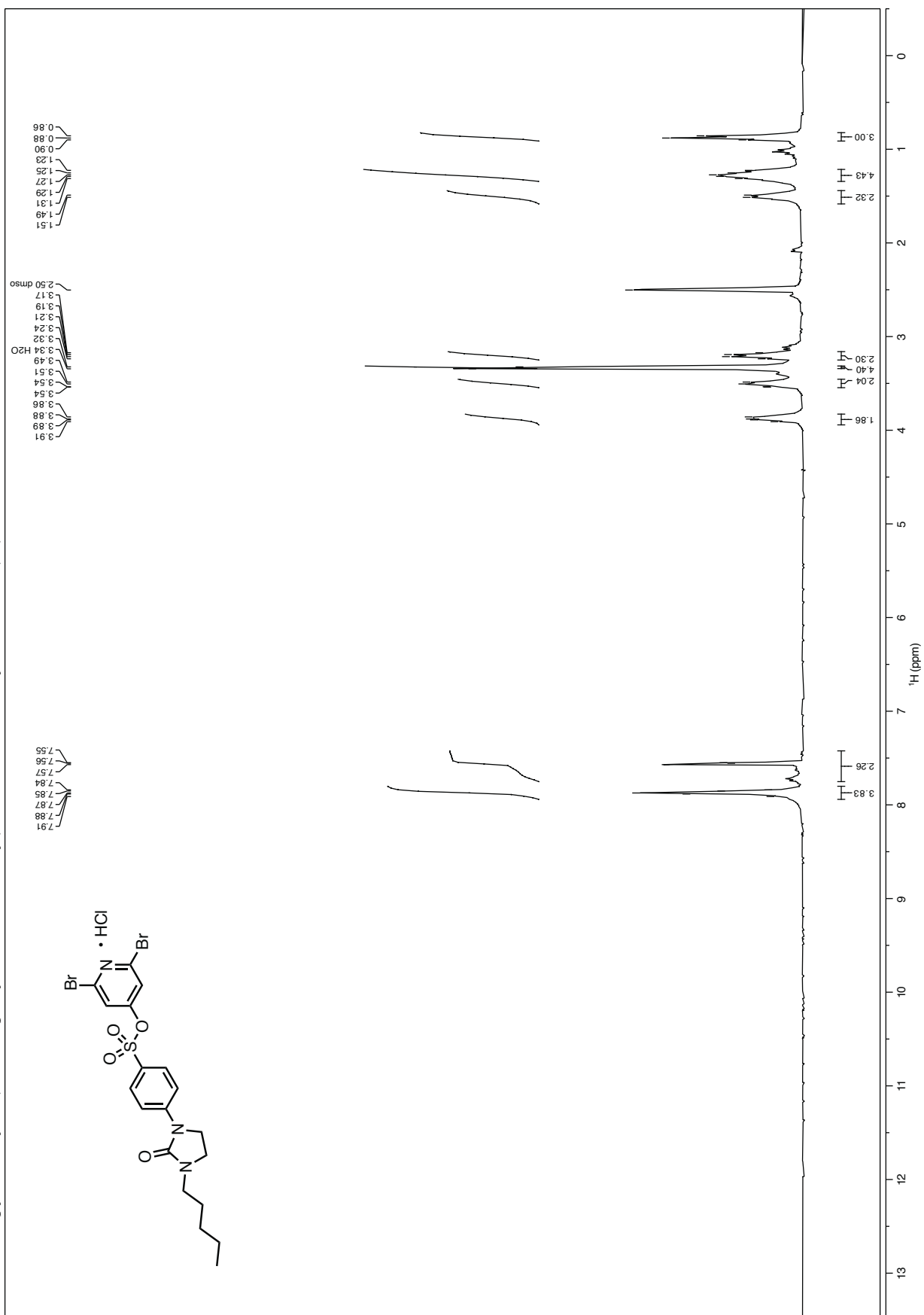
30



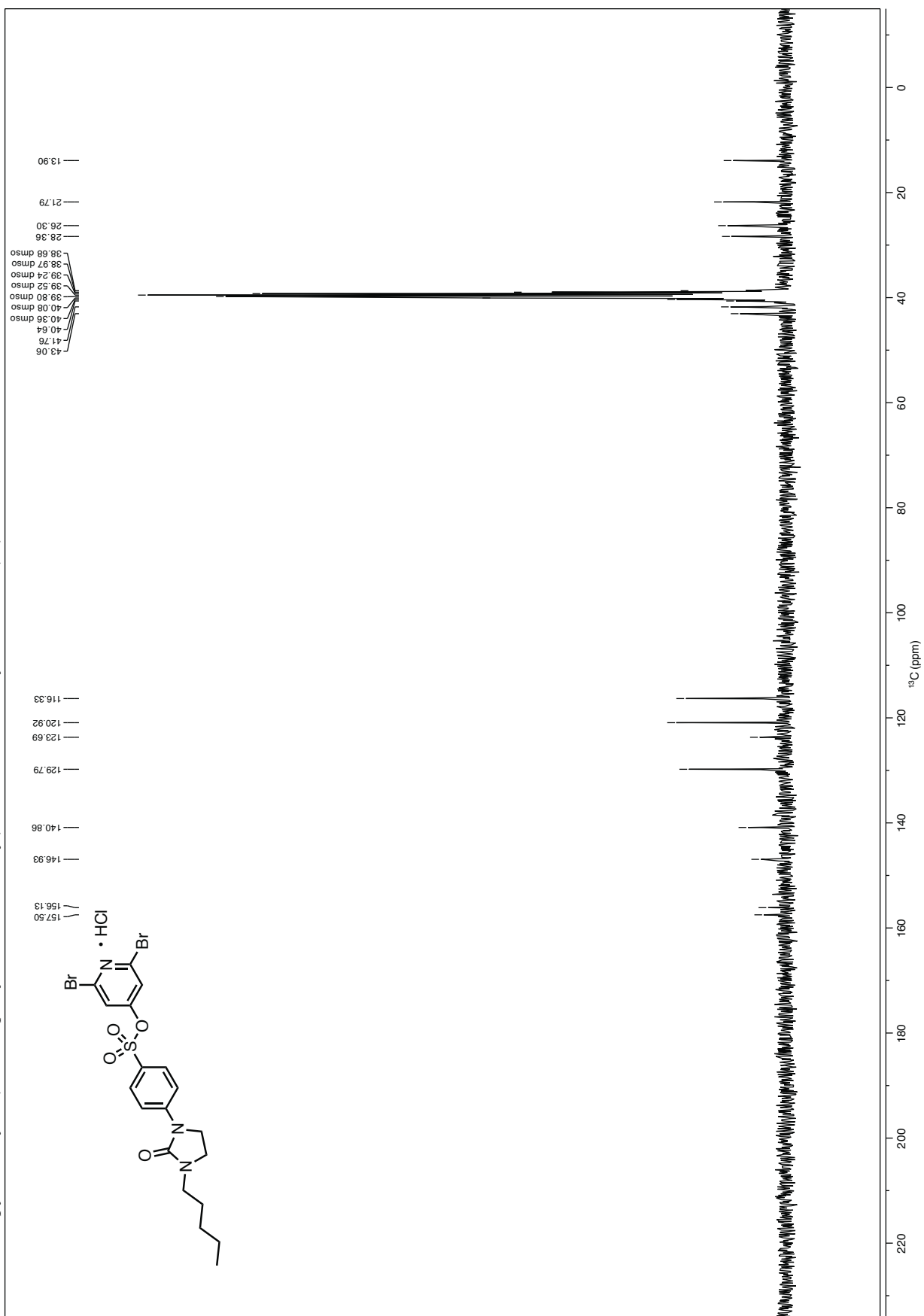
MS spectrum peak list

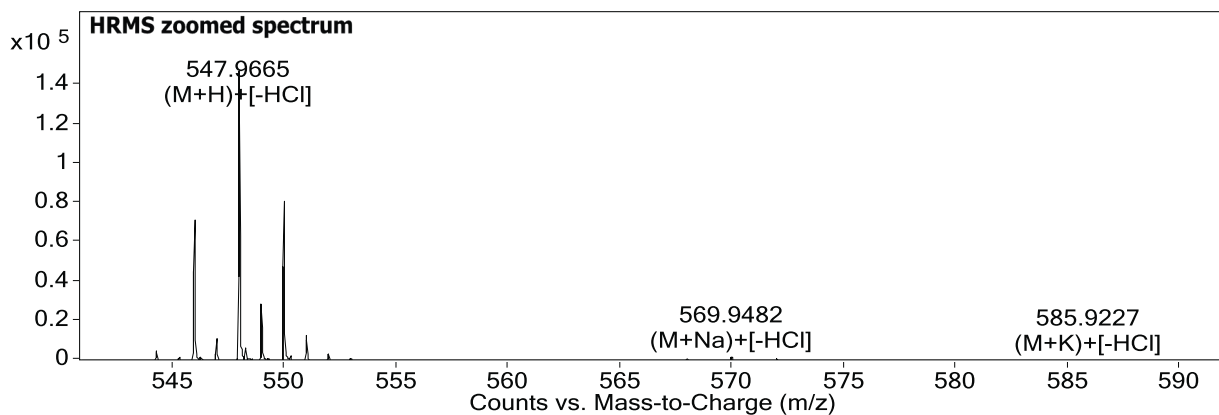
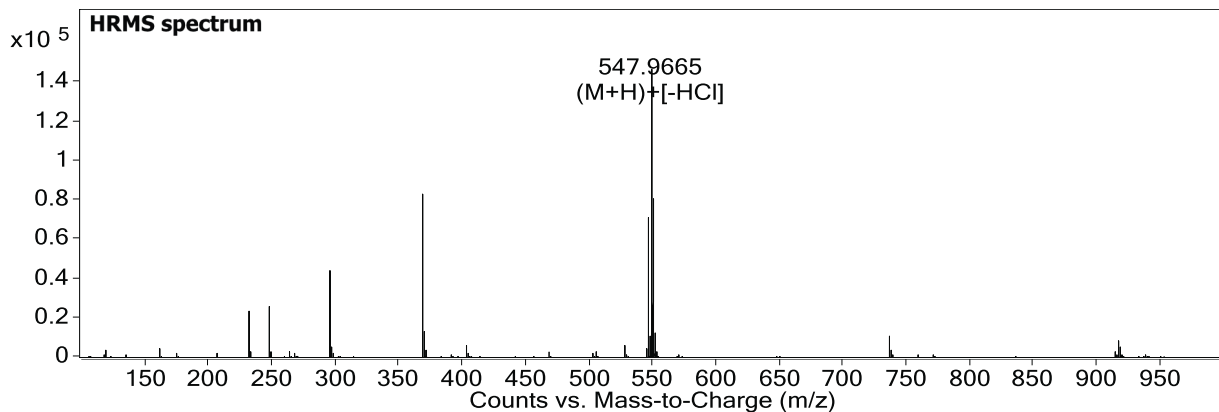
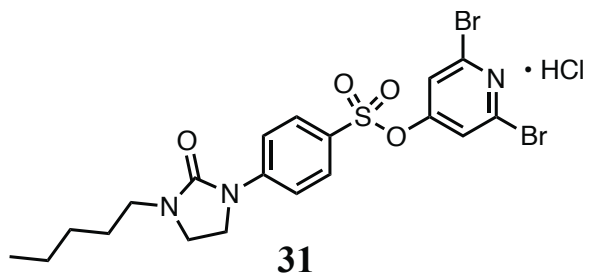
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
420.1583	420.1588	-1	411133	C20 H26 N3 O5 S	(M+H)+[-HCl]
421.161	421.1617	-1.83	92226	C20 H26 N3 O5 S	(M+H)+[-HCl]
422.1582	422.159	-1.8	24521	C20 H26 N3 O5 S	(M+H)+[-HCl]
423.1593	423.1604	-2.56	3727	C20 H26 N3 O5 S	(M+H)+[-HCl]

2,6-Dibromopyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**31**)



2,6-Dibromopyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**31**)

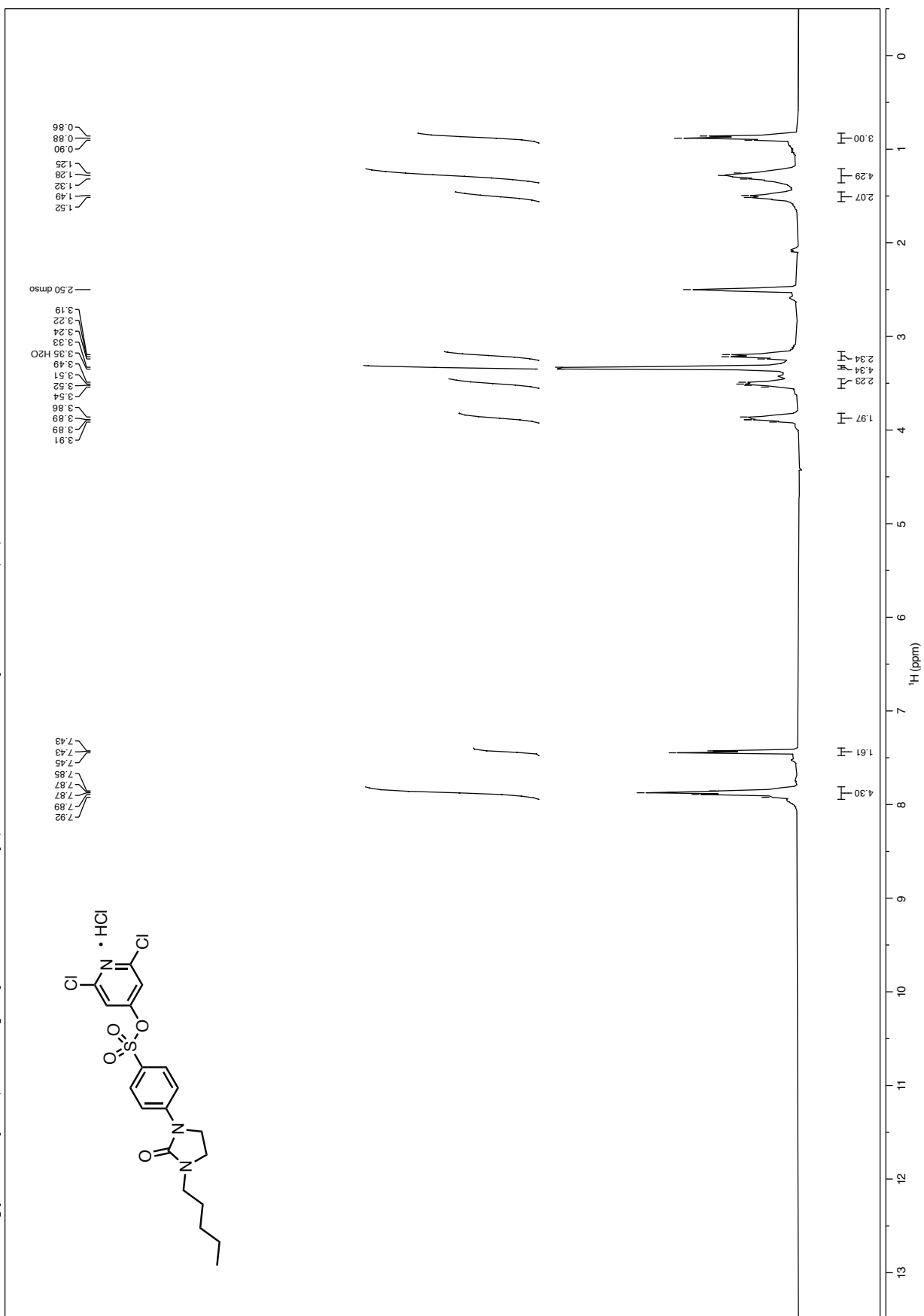




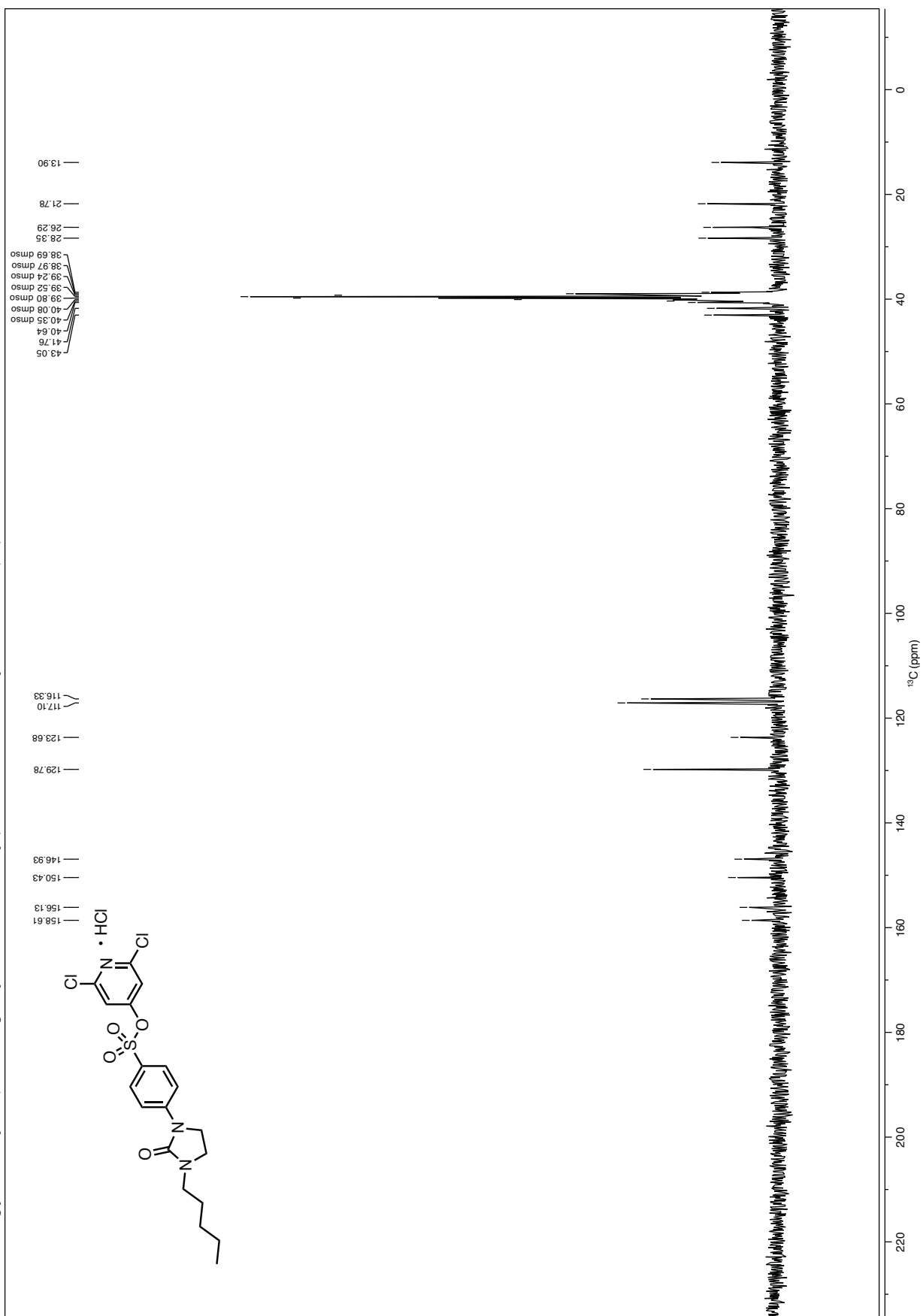
MS spectrum peak list

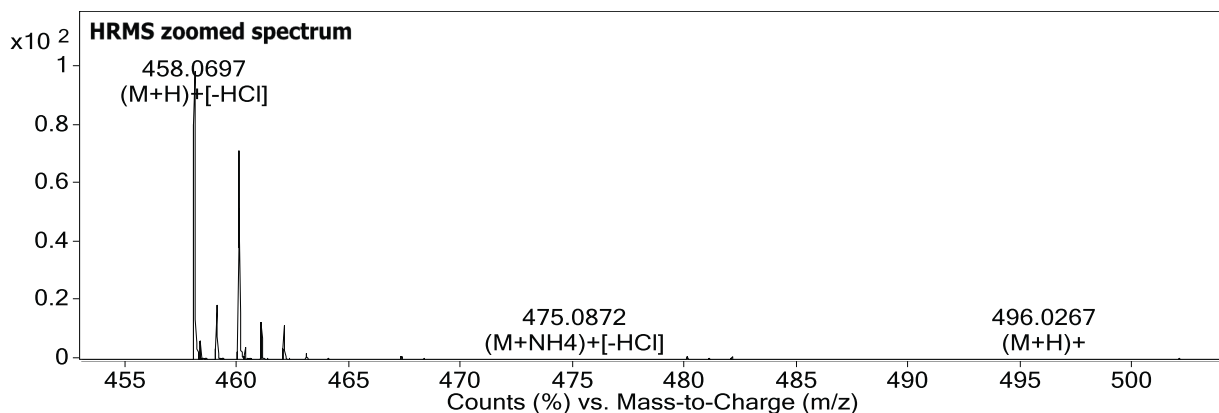
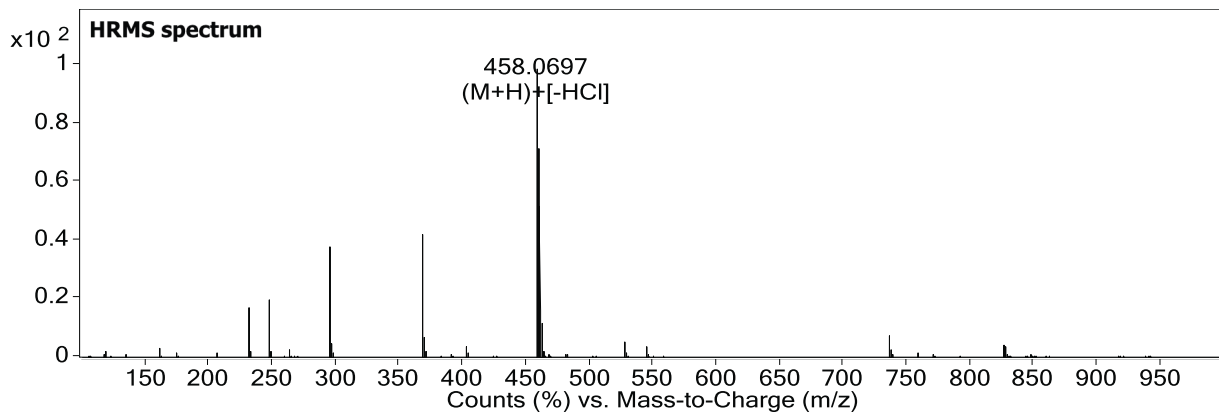
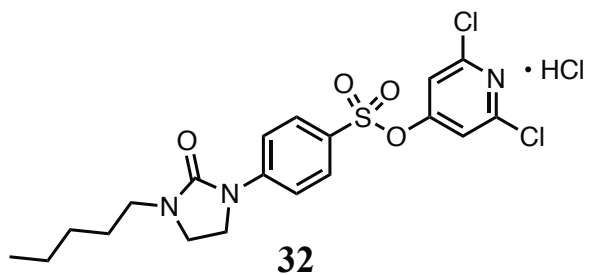
<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>z</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
545.9687	545.9692	-0.93		71347	C19 H22 Br2 N3 O4 S	(M+H)+[-HCl]
546.9712	546.9722	-1.78		12002	C19 H22 Br2 N3 O4 S	(M+H)+[-HCl]
547.9665	547.9673	-1.37		155322	C19 H22 Br2 N3 O4 S	(M+H)+[-HCl]
548.9698	548.9701	-0.6		28392	C19 H22 Br2 N3 O4 S	(M+H)+[-HCl]
549.9649	549.9654	-1.01		80895	C19 H22 Br2 N3 O4 S	(M+H)+[-HCl]
550.9671	550.9681	-1.88		12950	C19 H22 Br2 N3 O4 S	(M+H)+[-HCl]
551.965	551.9653	-0.5		3308	C19 H22 Br2 N3 O4 S	(M+H)+[-HCl]
552.9663	552.9666	-0.52		580	C19 H22 Br2 N3 O4 S	(M+H)+[-HCl]

2,6-Dichloropyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (32)



2,6-Dichloropyridin-4-yl 4-(2-oxo-3-pentylimidazolidin-1-yl)benzenesulfonate hydrochloride (**32**)





MS spectrum peak list

<i>m/z</i>	<i>Calc m/z</i>	<i>Diff(ppm)</i>	<i>z</i>	<i>Abund</i>	<i>Formula</i>	<i>Ion</i>
458.0697	458.0703	-1.18		255473	C ₁₉ H ₂₂ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
459.0722	459.0732	-2.17		48891	C ₁₉ H ₂₂ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
460.0671	460.0676	-1.2		183014	C ₁₉ H ₂₂ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
461.0696	461.0704	-1.66		33231	C ₁₉ H ₂₂ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
462.0644	462.0654	-2.1		30895	C ₁₉ H ₂₂ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
463.0667	463.0677	-2.2	1	5133	C ₁₉ H ₂₂ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
464.0638	464.065	-2.73	1	1243	C ₁₉ H ₂₂ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]
465.0652	465.0662	-2.16	1	236	C ₁₉ H ₂₂ Cl ₂ N ₃ O ₄ S	(M+H) ⁺ [-HCl]