

Supplementary materials

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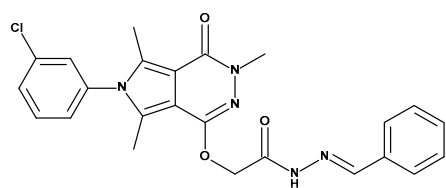
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Table S1 - Structures of new compounds

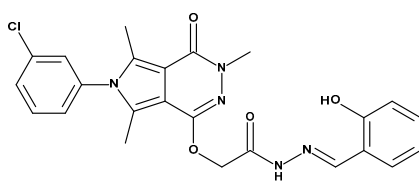
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5a	6a	7a
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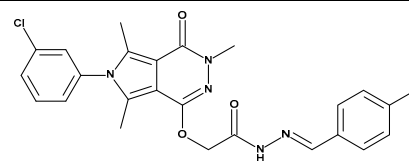
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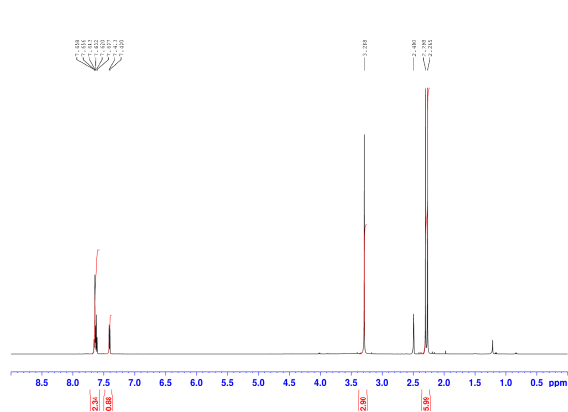


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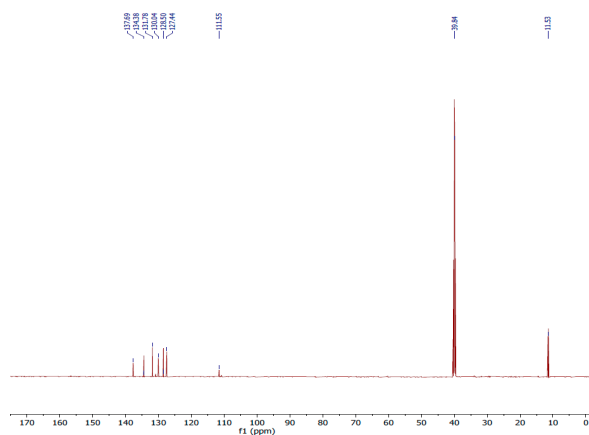


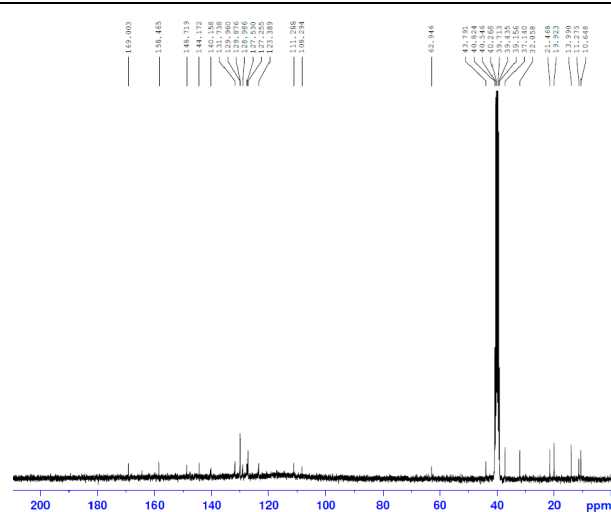
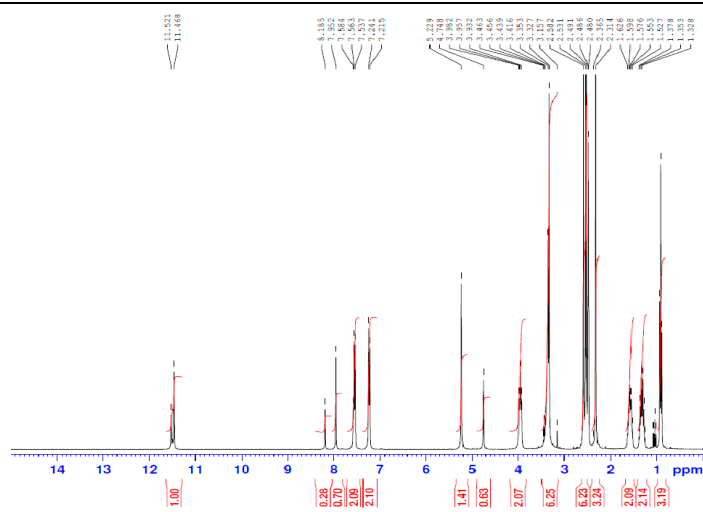
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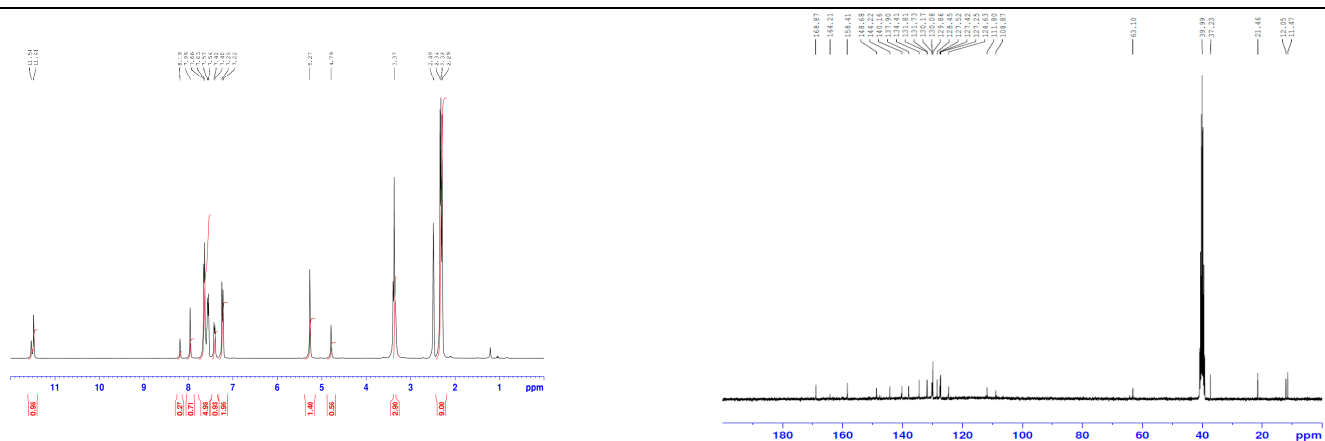
Table S2 - NMR spectra of new compounds



2c

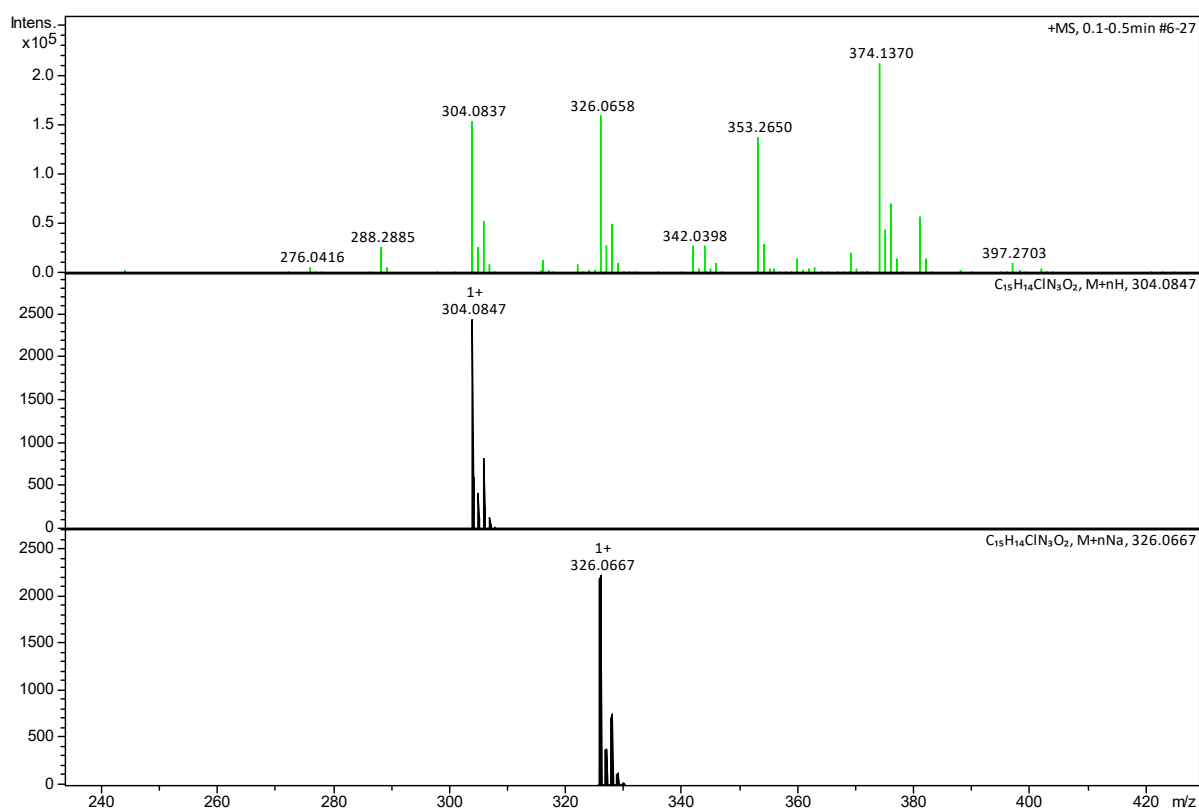




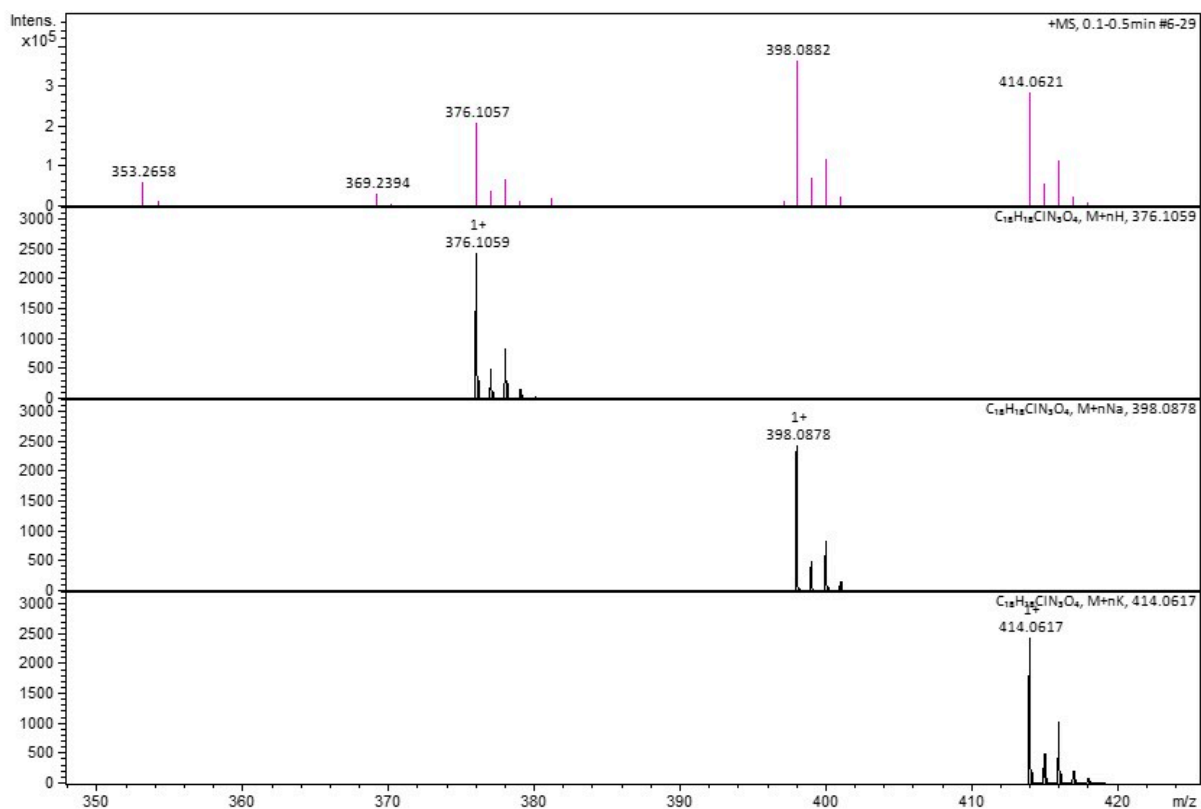


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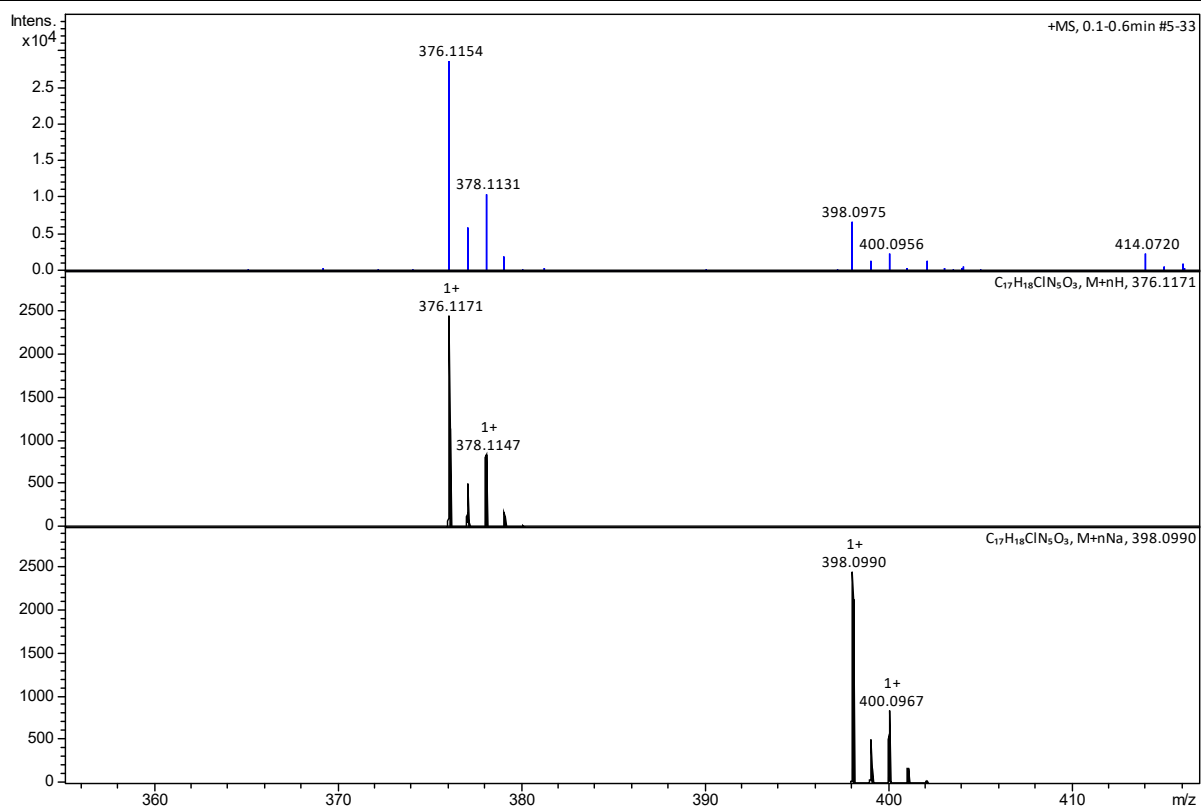
Table S3 - Mass spectra of new compounds



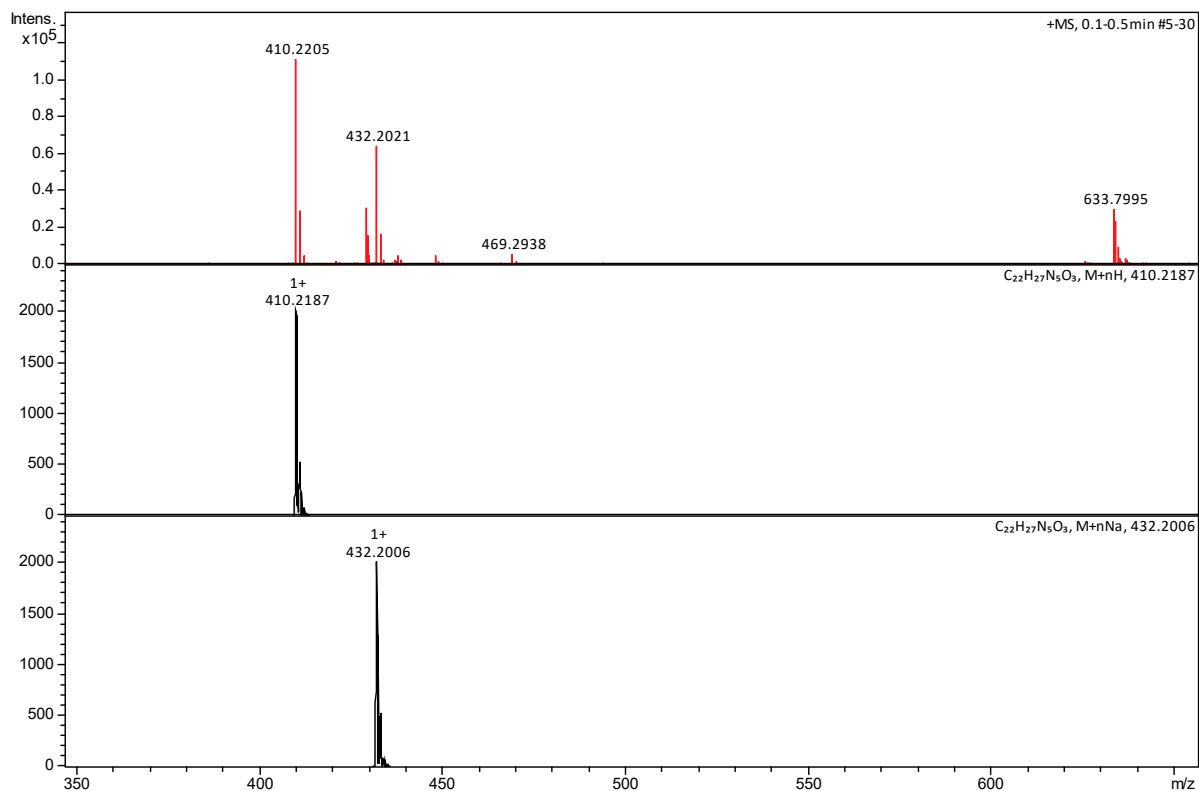
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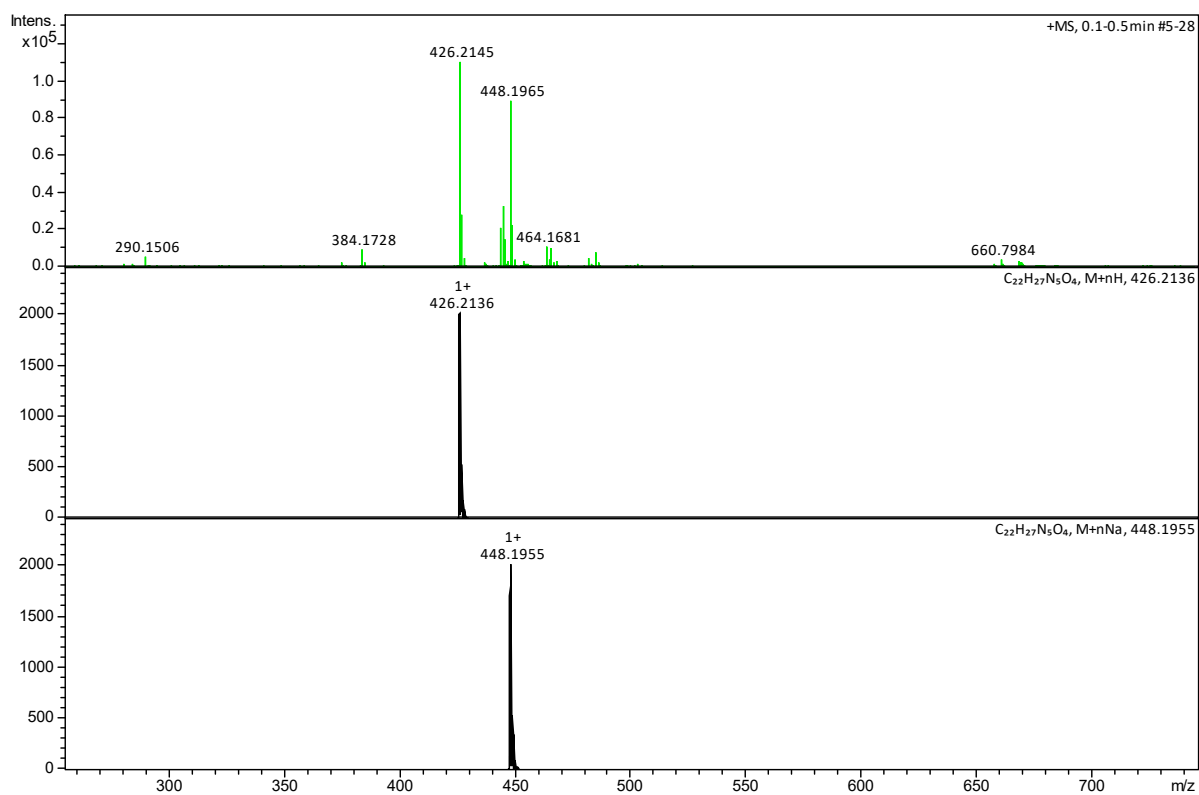
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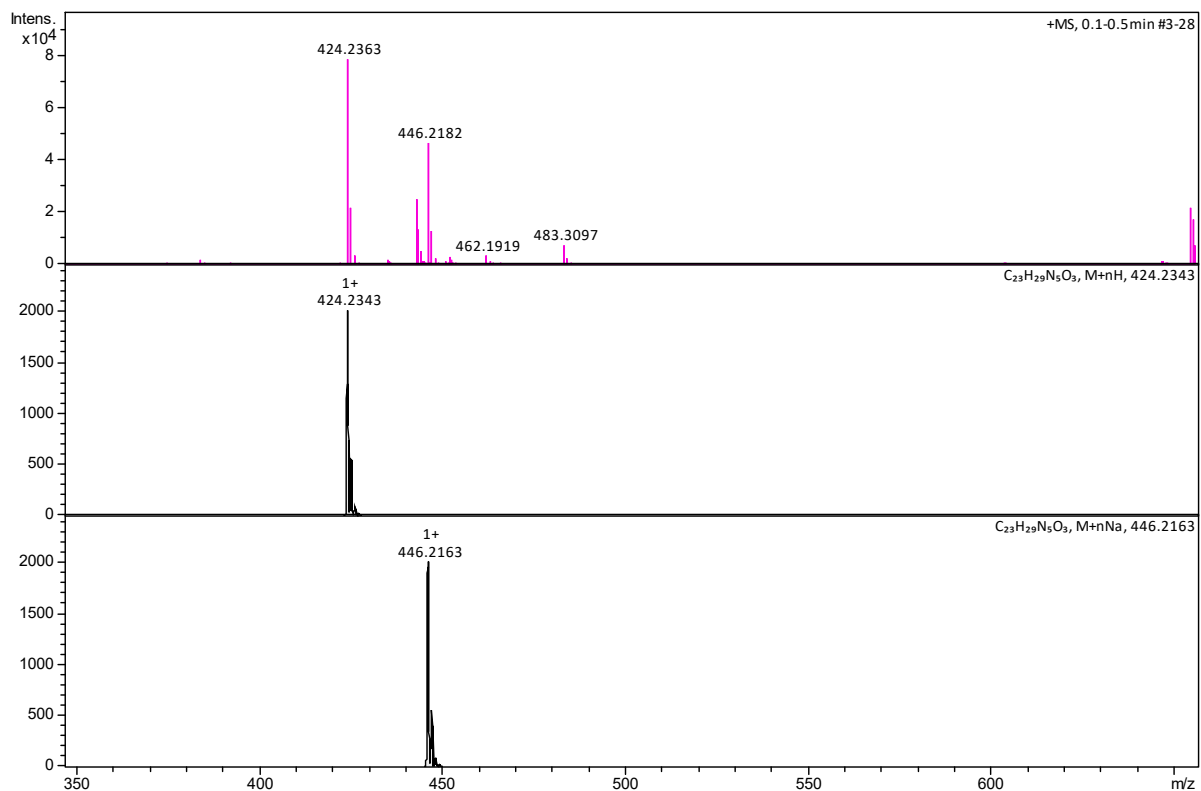
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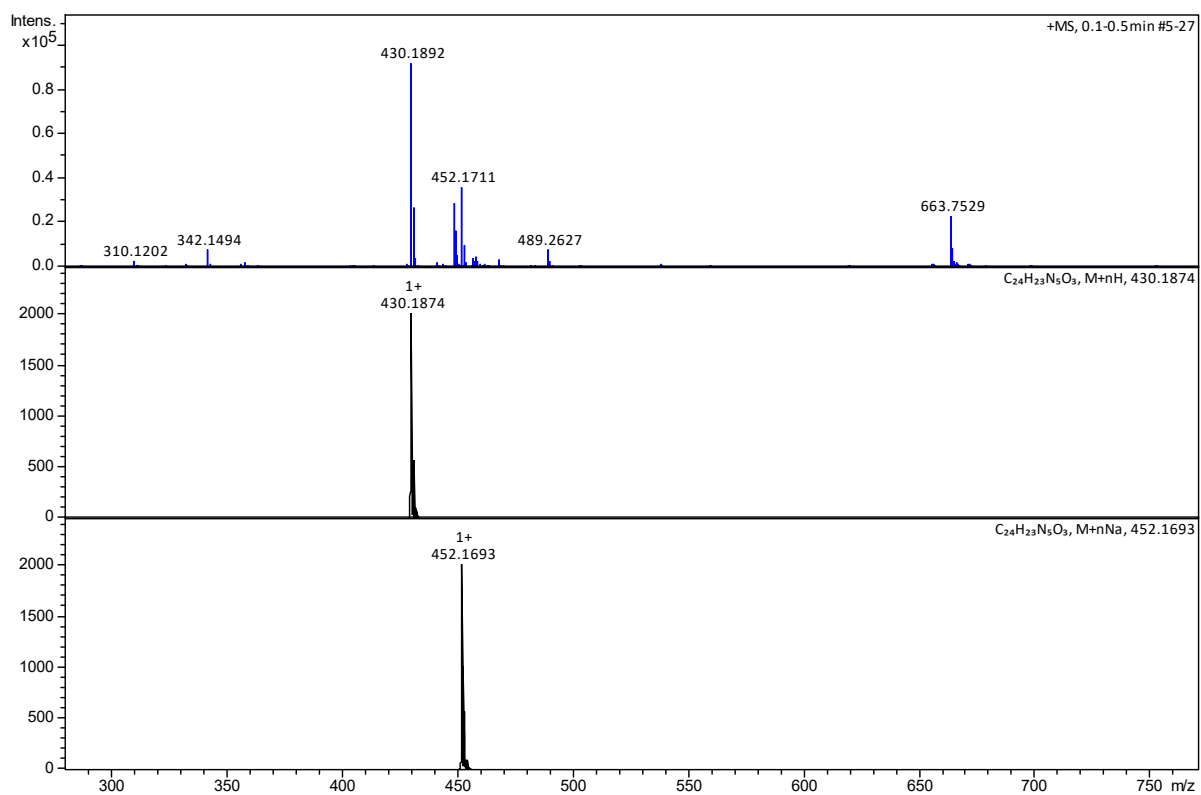
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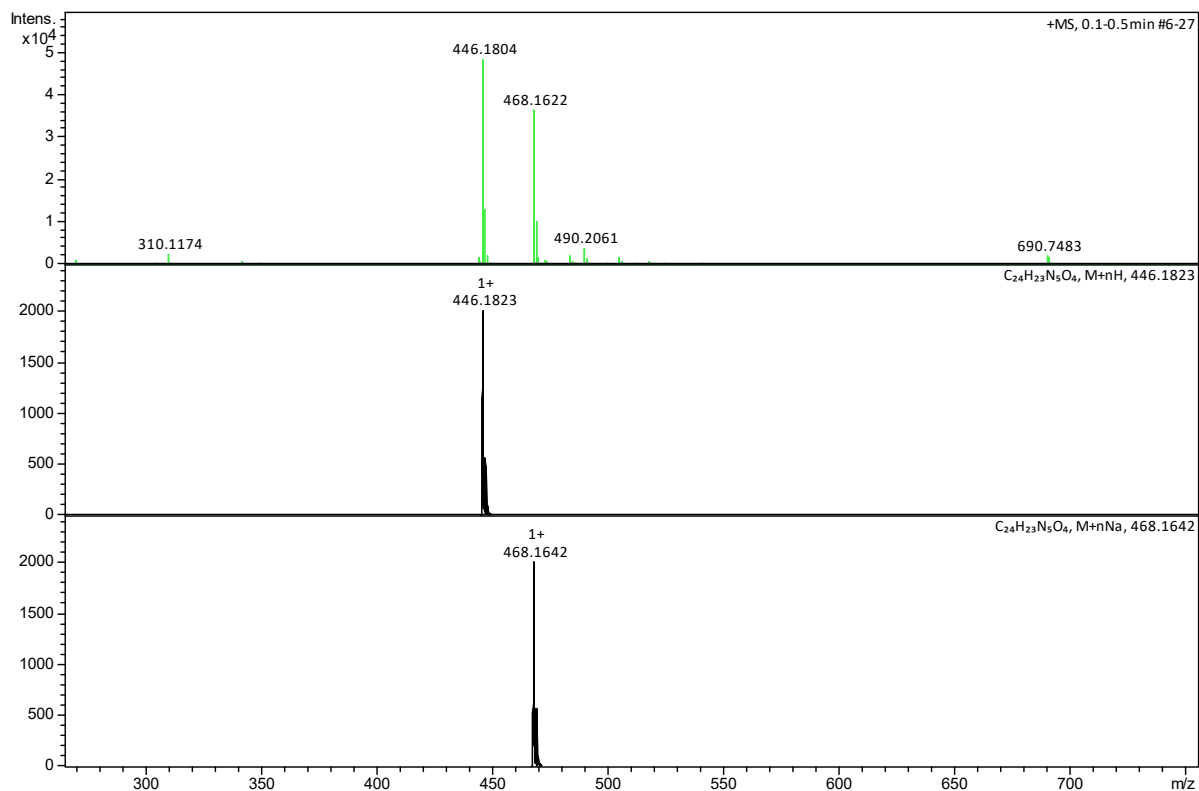
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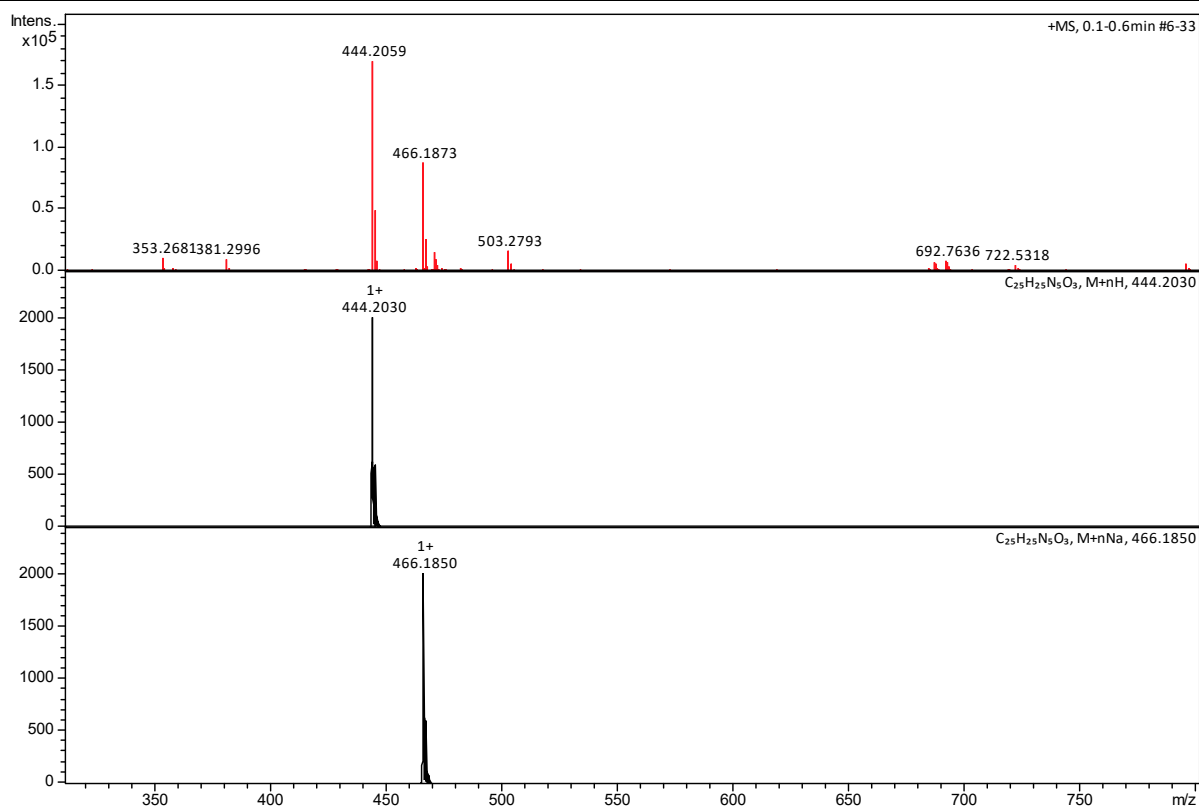
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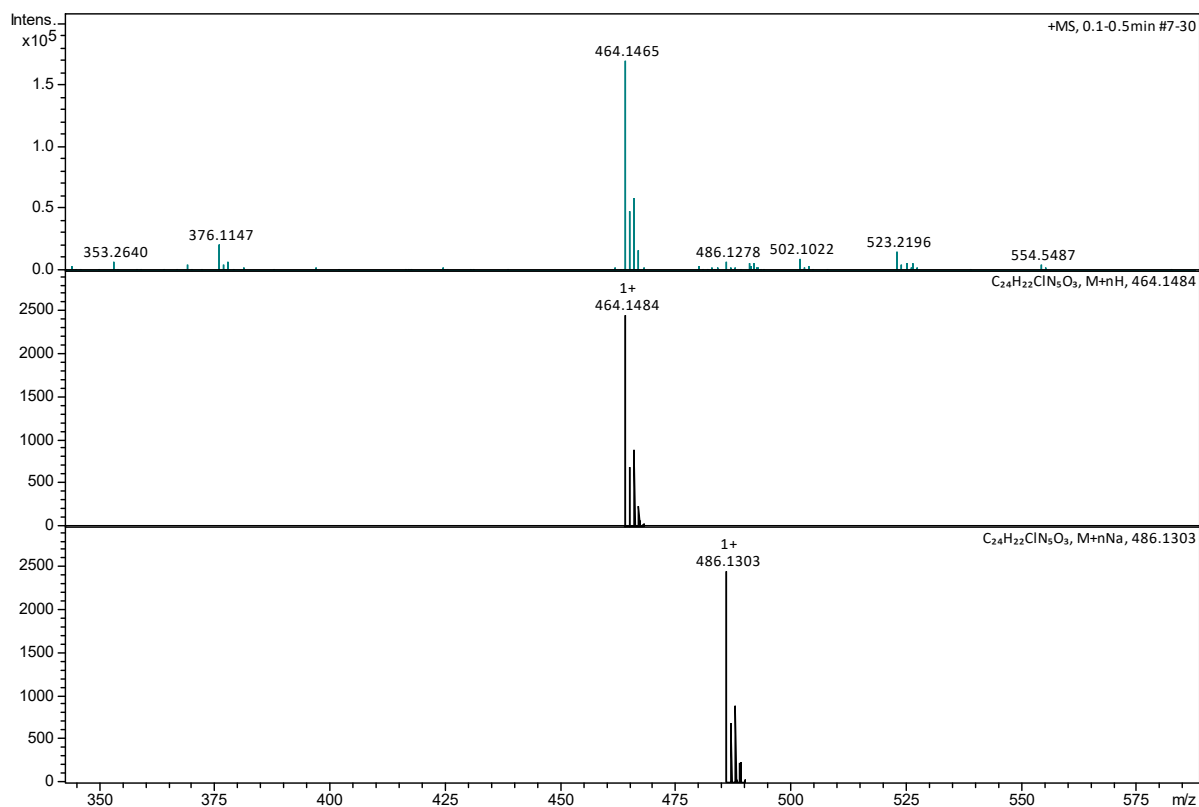
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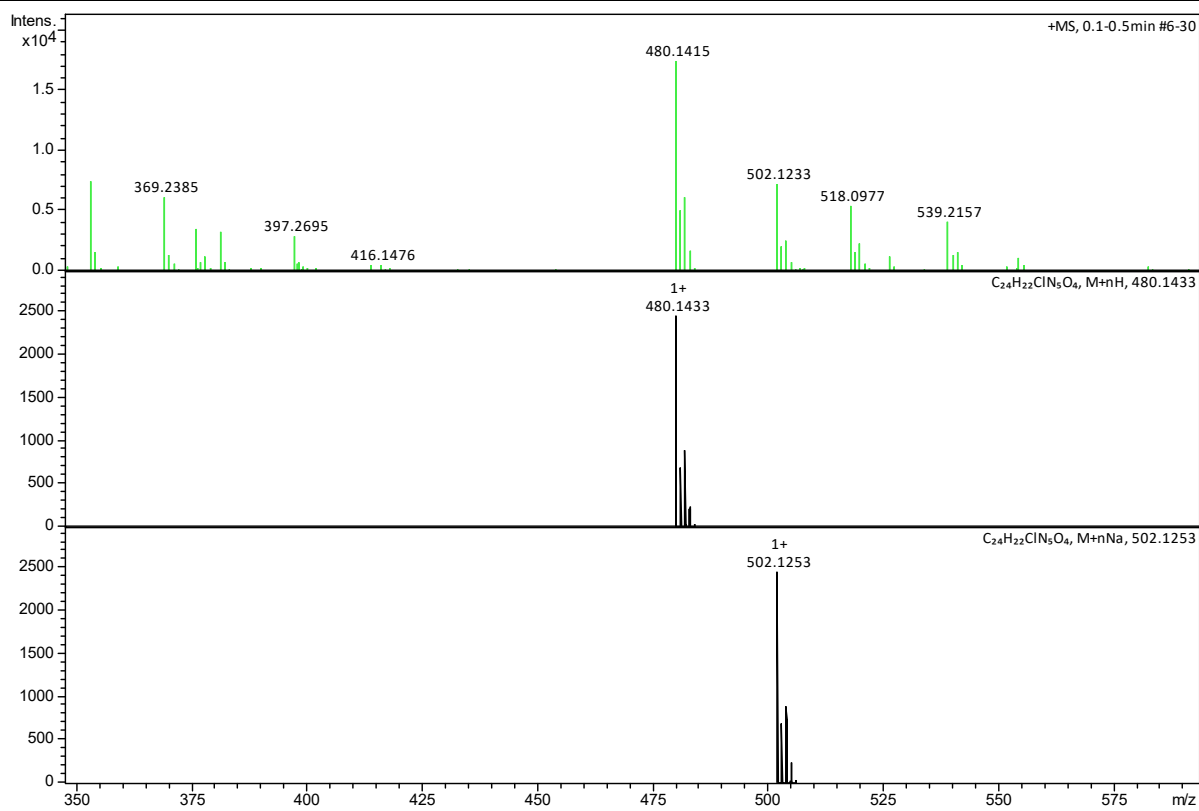
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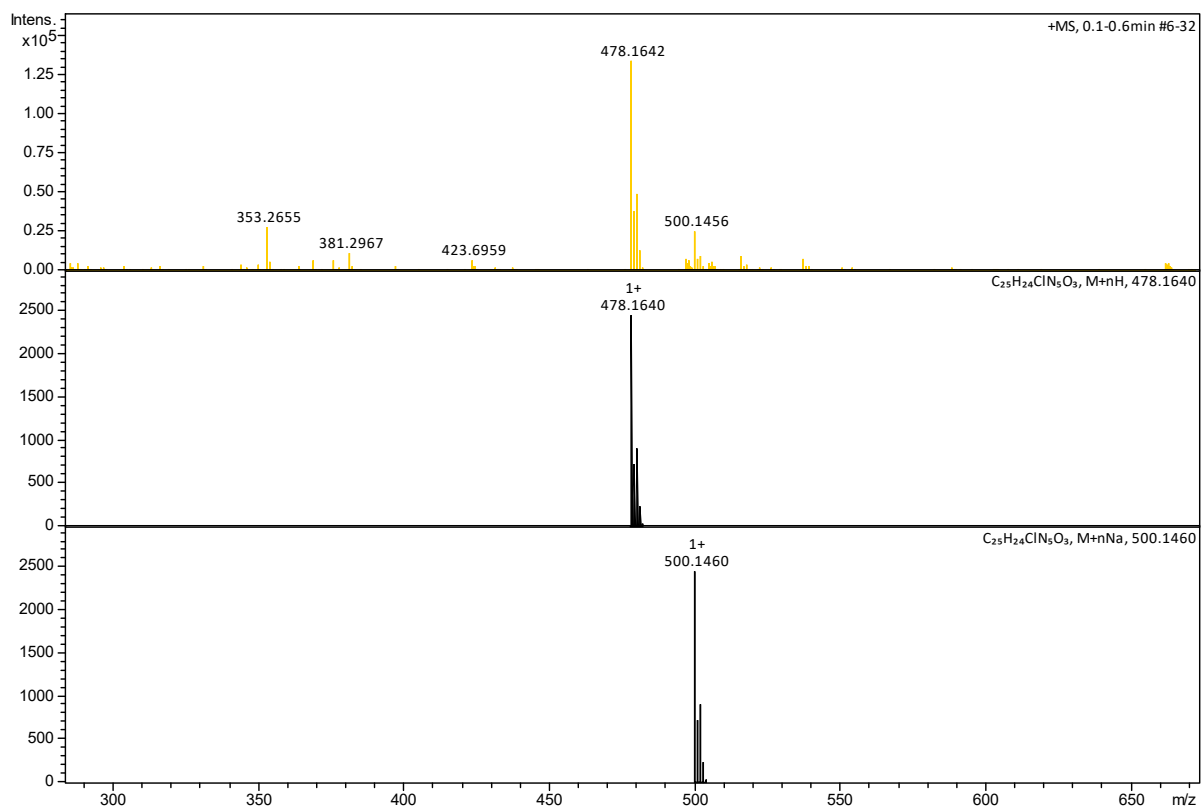
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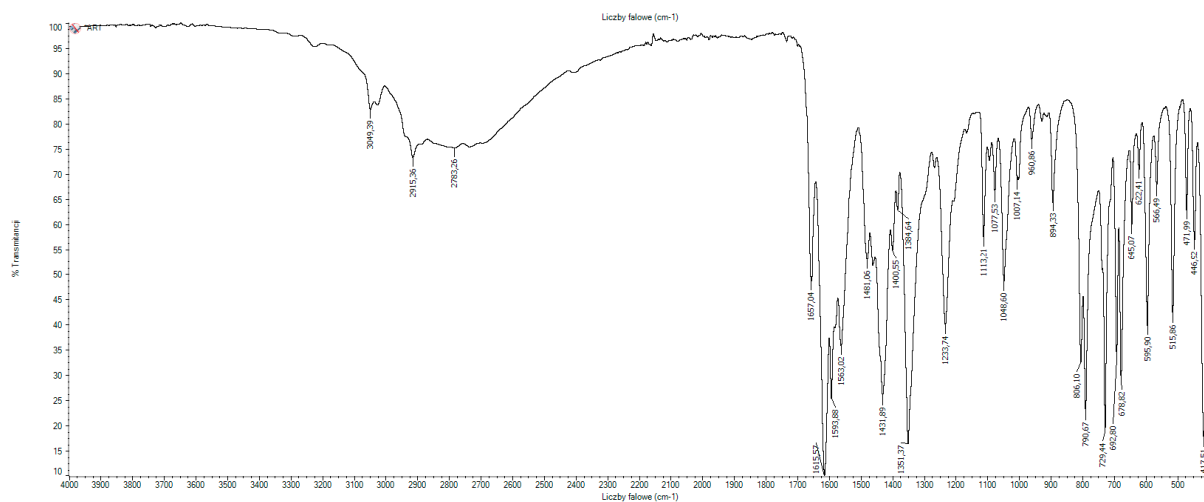


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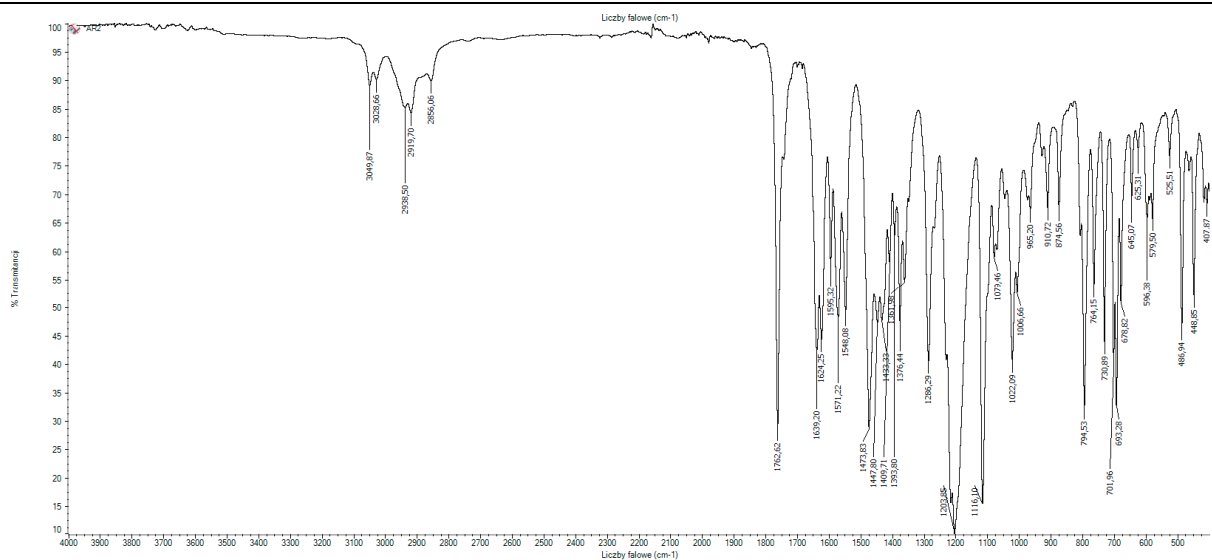


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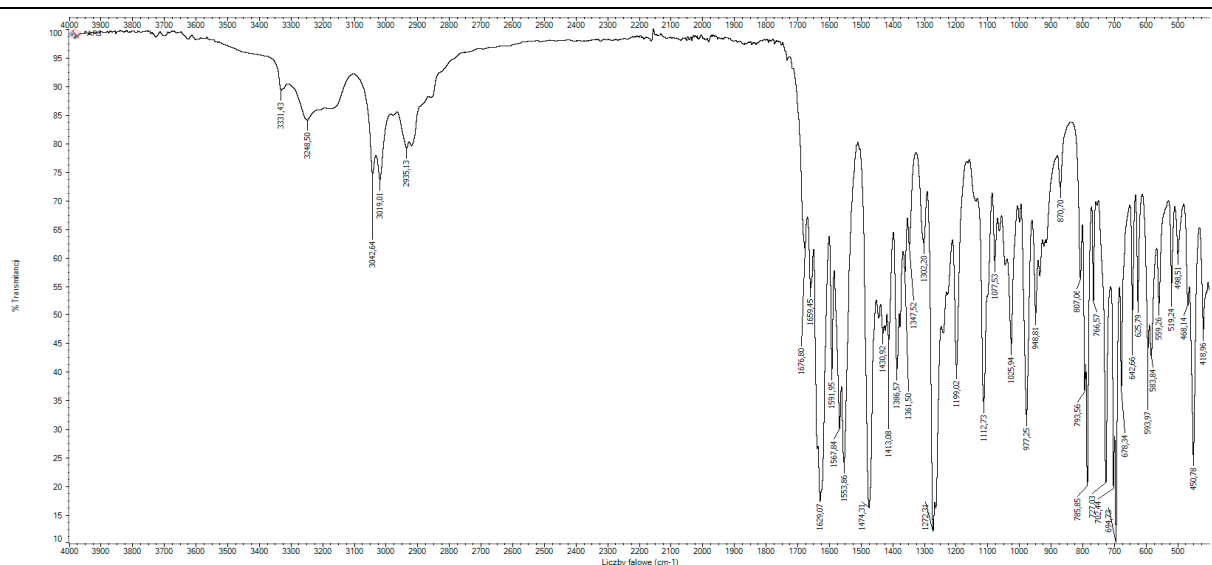
Table S4 – FT-IR spectra of new compounds



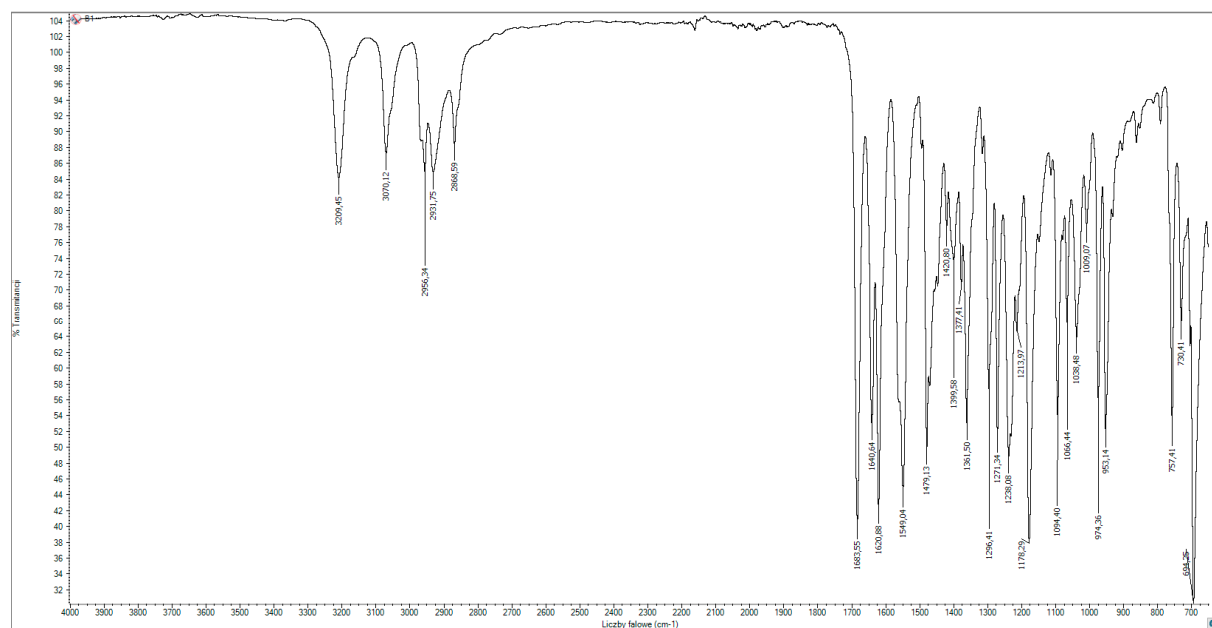
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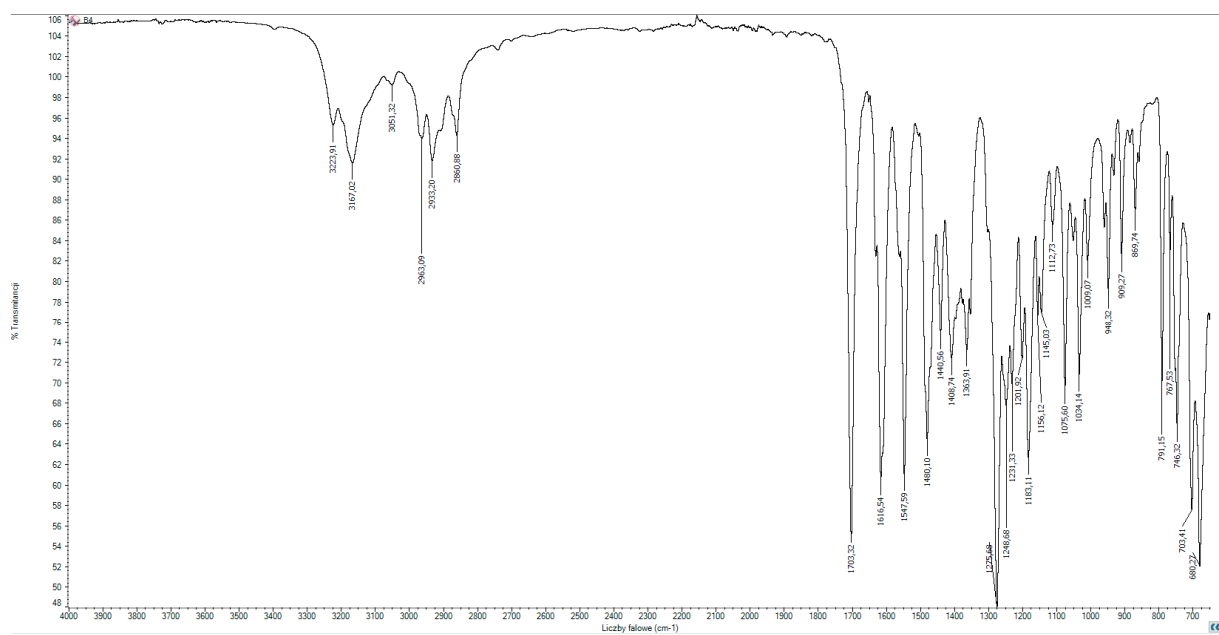
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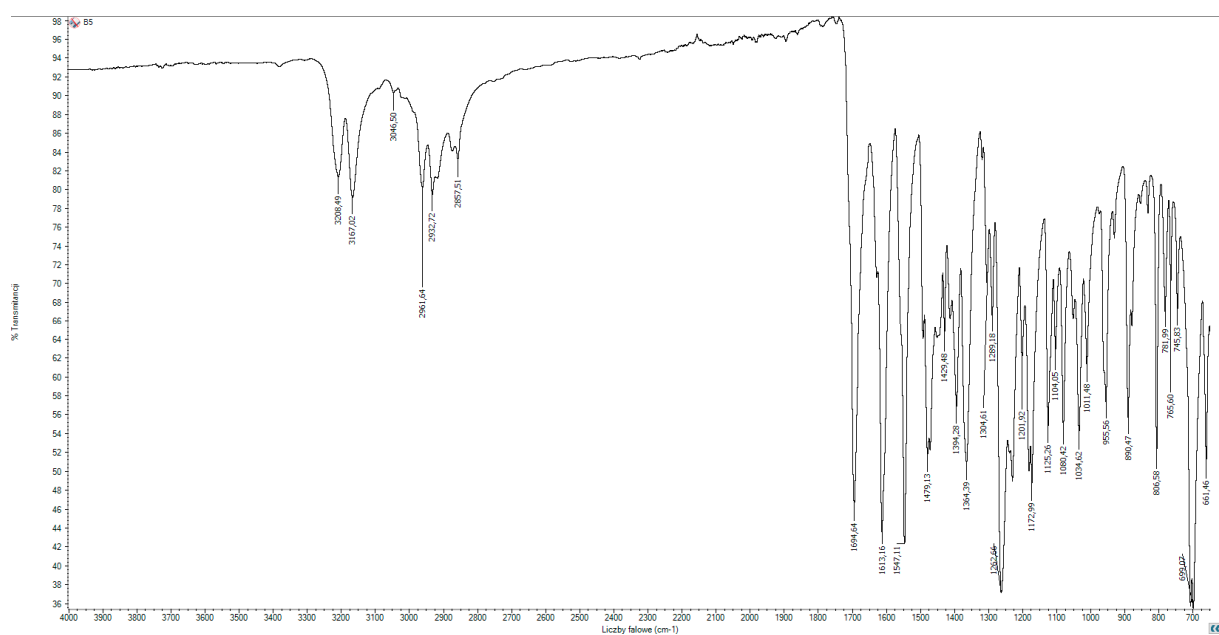
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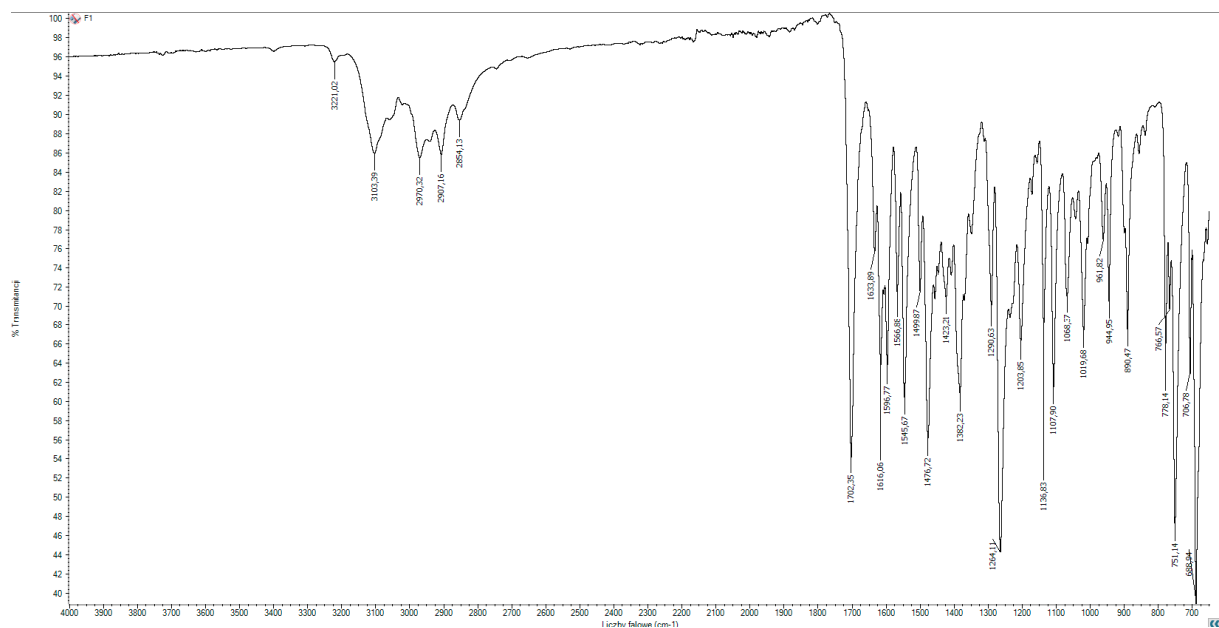
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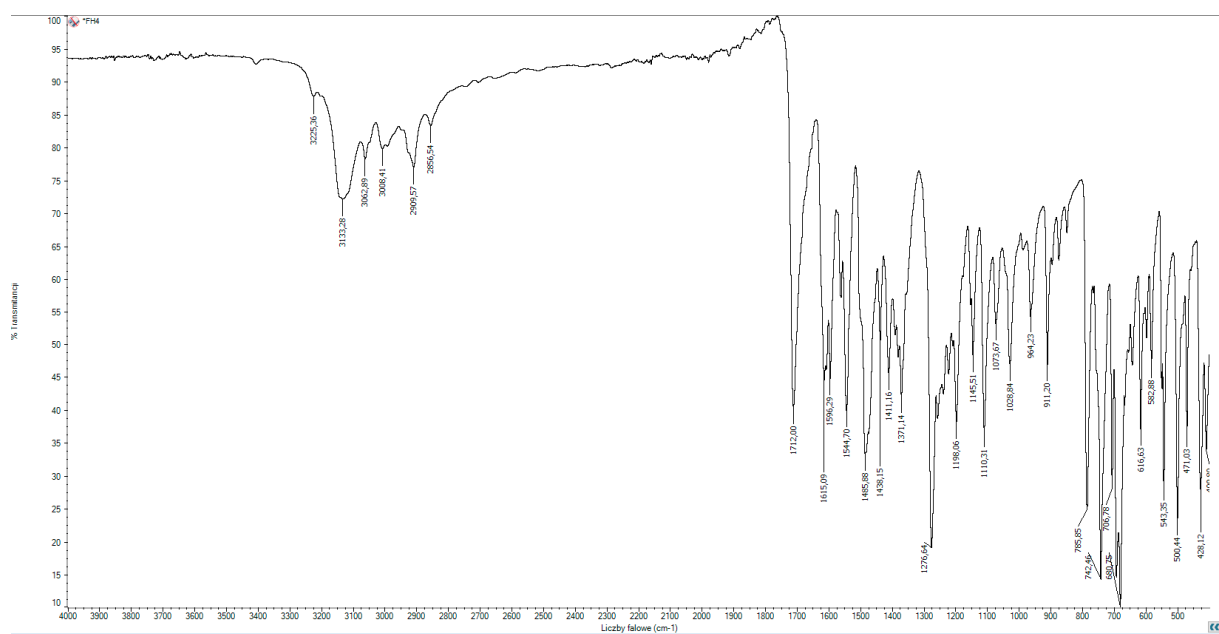
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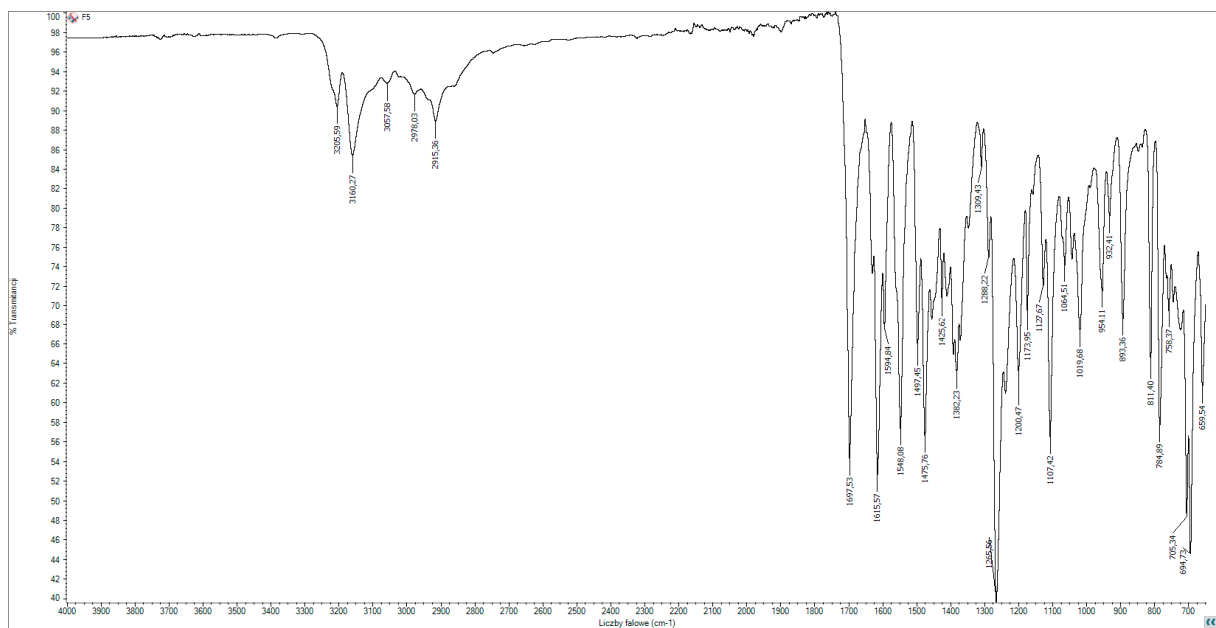
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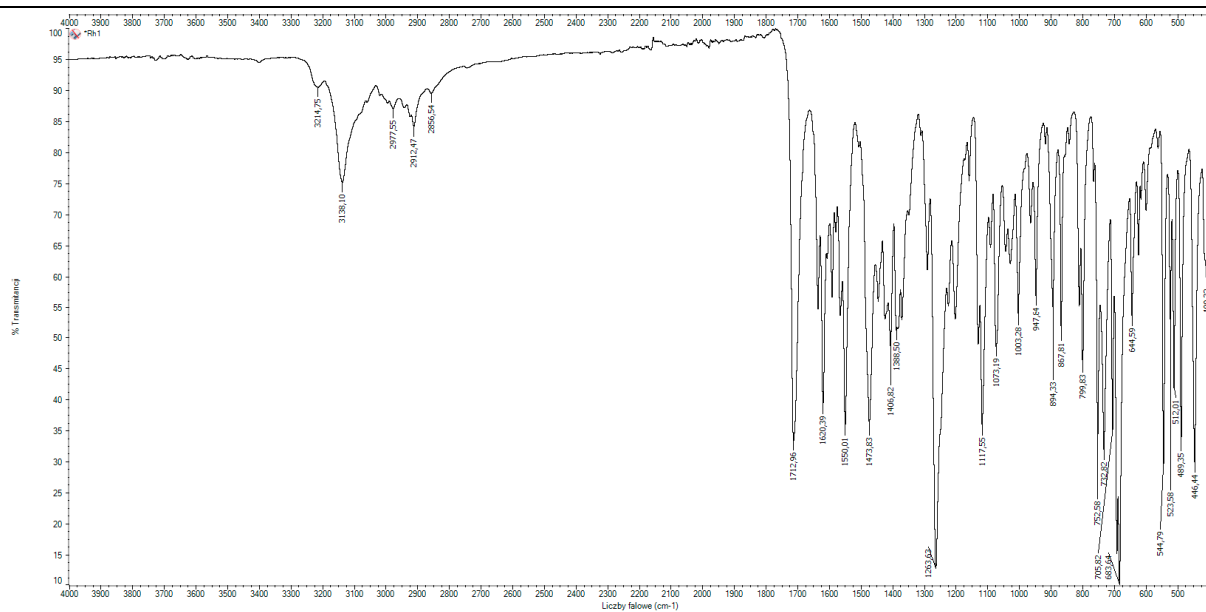
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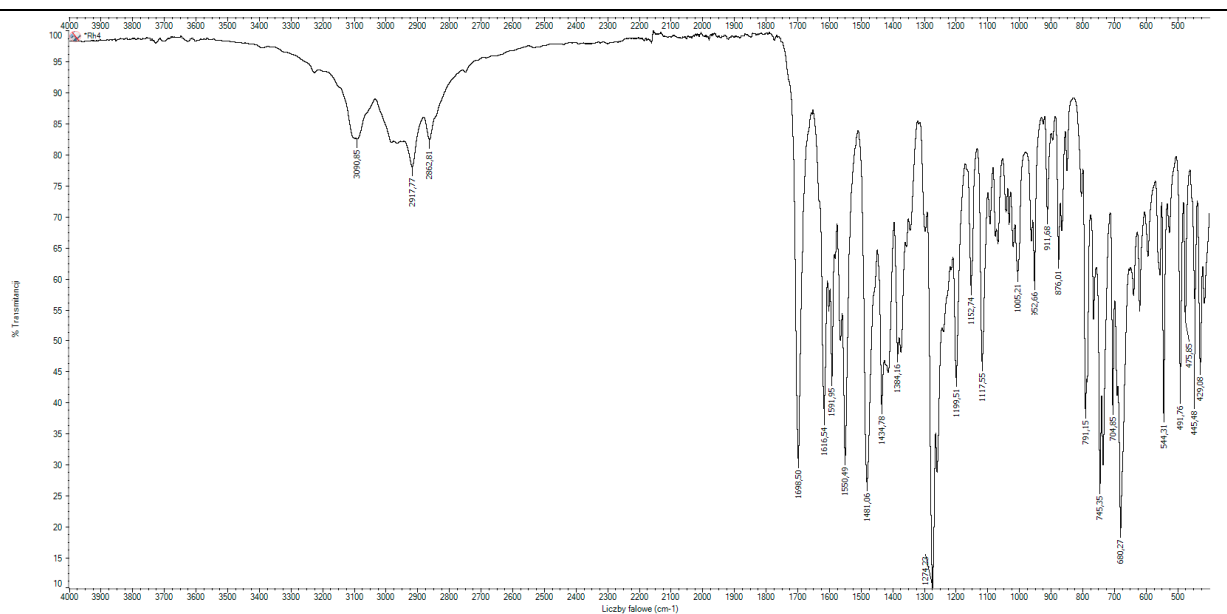
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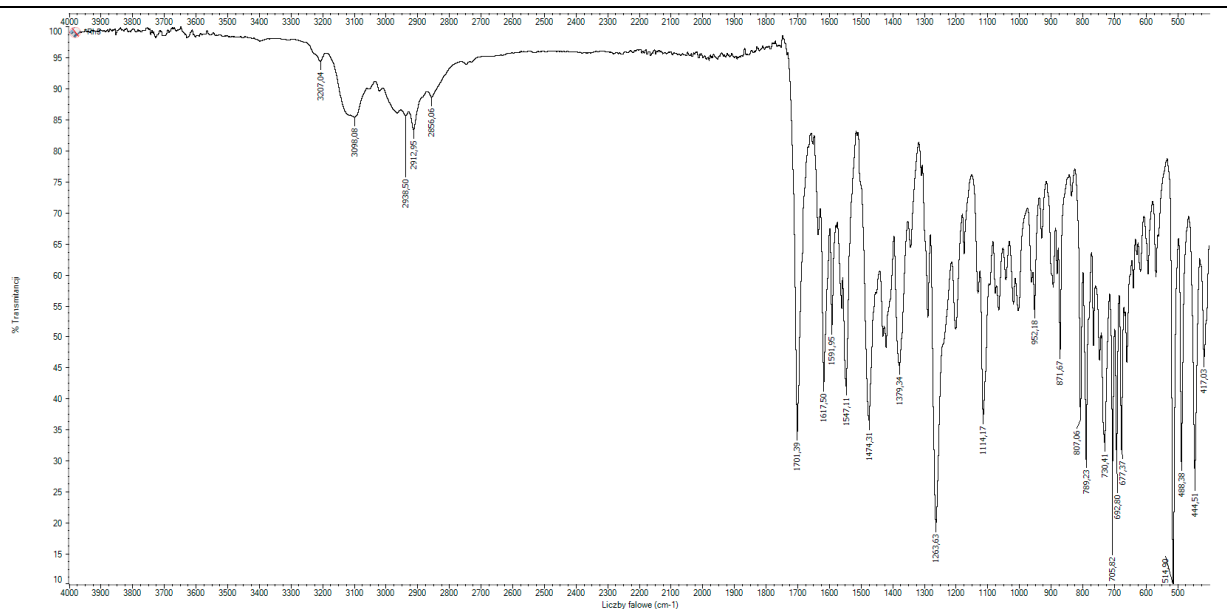
7b



5c



6c



7c

Table S5 – Molecular formula strings (CSV) of reported compounds

	SMILE
2c	<chem>CN1NC(=O)c2c(C)n(c(C)c2C1=O)c3cccc(Cl)c3</chem>
3c	<chem>COC(=O)COC1=NN(C)C(=O)c2c(C)n(c(C)c12)c3cccc(Cl)c3</chem>
4c	<chem>CN1N=C(OCC(=O)NN)c2c(C)n(c(C)c2C1=O)c3cccc(Cl)c3</chem>
5a	<chem>CCCCn1c(C)c2C(=O)N(C)N=C(OCC(=O)N\N=C\c3ccccc3)c2c1C</chem>
6a	<chem>CCCCn1c(C)c2C(=O)N(C)N=C(OCC(=O)N\N=C\c3ccccc3O)c2c1C</chem>
7a	<chem>CCCCn1c(C)c2C(=O)N(C)N=C(OCC(=O)N\N=C\c3ccc(C)cc3)c2c1C</chem>

5b CN1N=C(OCC(=O)N\N=C\c2cccc2)c3c(C)n(c(C)c3C1=O)c4cccc4
6b CN1N=C(OCC(=O)N\N=C\c2cccc2O)c3c(C)n(c(C)c3C1=O)c4cccc4
7b CN1N=C(OCC(=O)N\N=C\c2ccc(C)cc2)c3c(C)n(c(C)c3C1=O)c4cccc4
5c CN1N=C(OCC(=O)N\N=C\c2cccc2)c3c(C)n(c(C)c3C1=O)c4cccc(Cl)c4
6c CN1N=C(OCC(=O)N\N=C\c2cccc2O)c3c(C)n(c(C)c3C1=O)c4cccc(Cl)c4
7c CN1N=C(OCC(=O)N\N=C\c2ccc(C)cc2)c3c(C)n(c(C)c3C1=O)c4cccc(Cl)c4

Figure S1 - Flowchart summarizing the Materials and Methods section

