

# Supporting Information

**Design and synthesis of pyridyl and 2-hydroxyphenyl chalcones with remarkable antituberculosis activity.**

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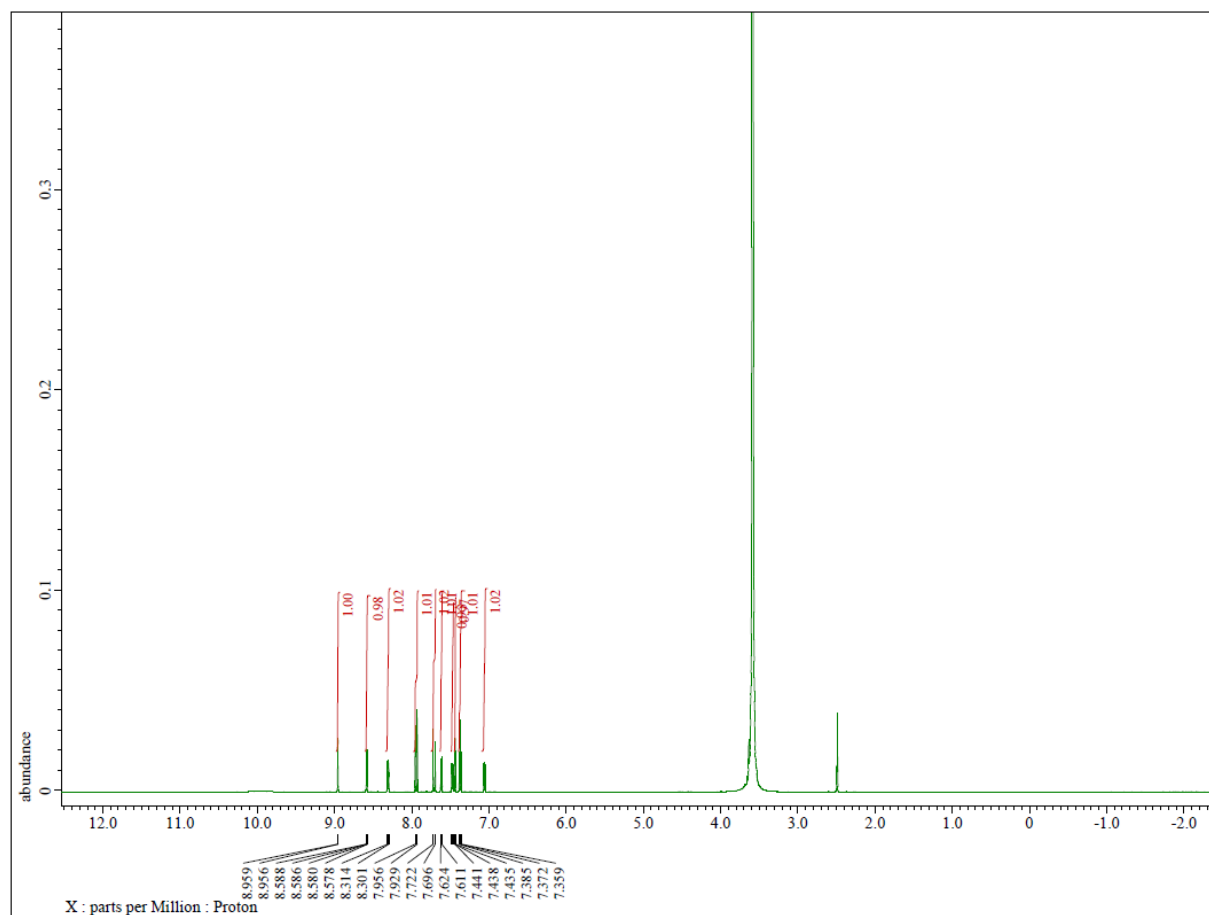
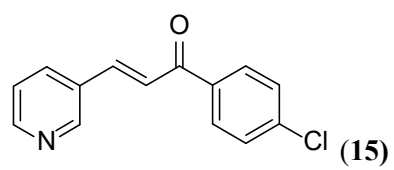
<sup>3</sup>UCL School of Pharmacy, UCL, London WC1N 1AX, UK

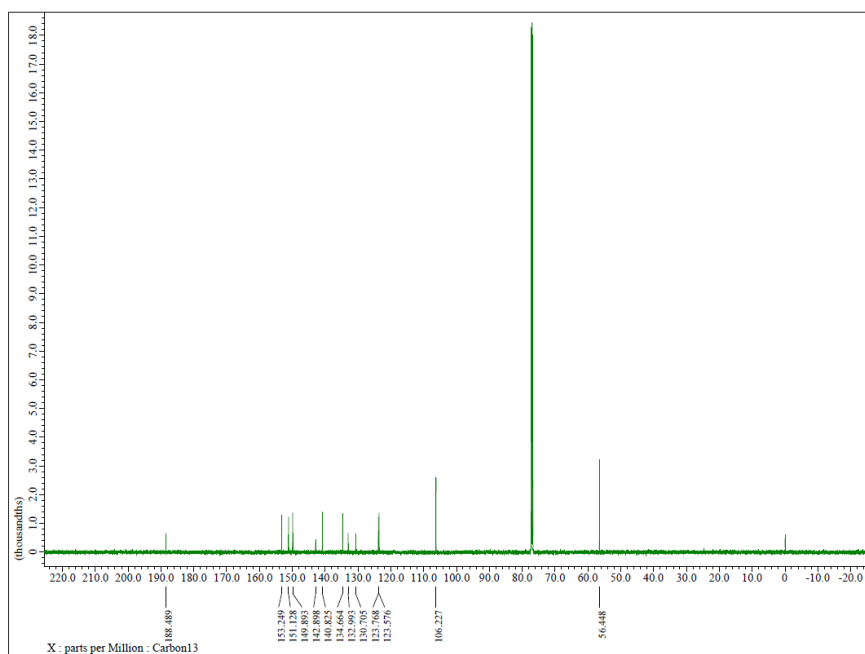
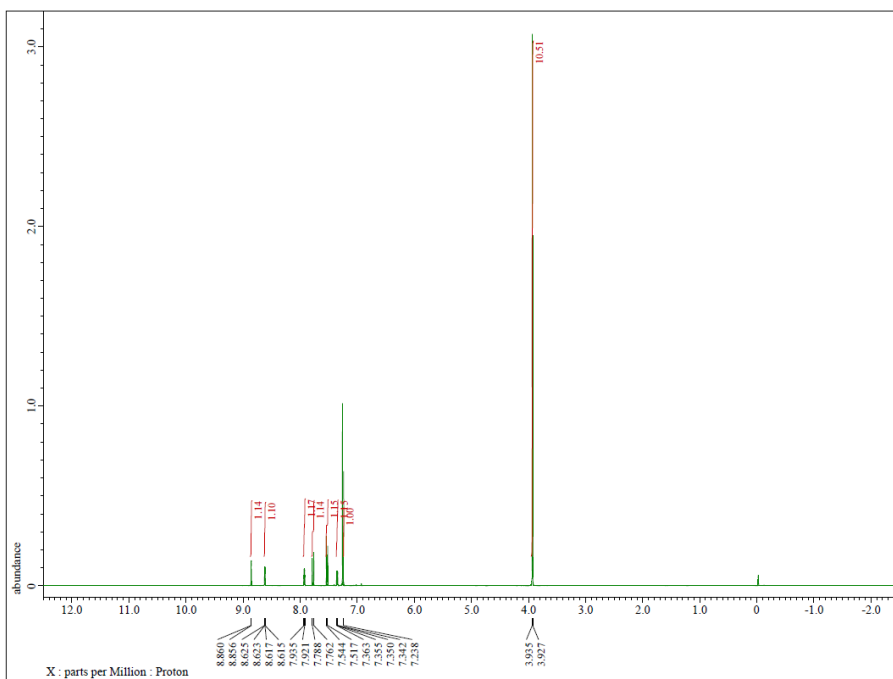
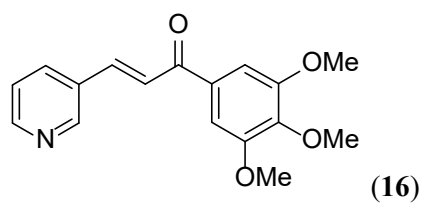
<sup>4</sup>Center for Global Infectious Disease Research, Seattle Children's Research Institute, 307 Westlake Avenue North, Suite 500, Seattle, USA.

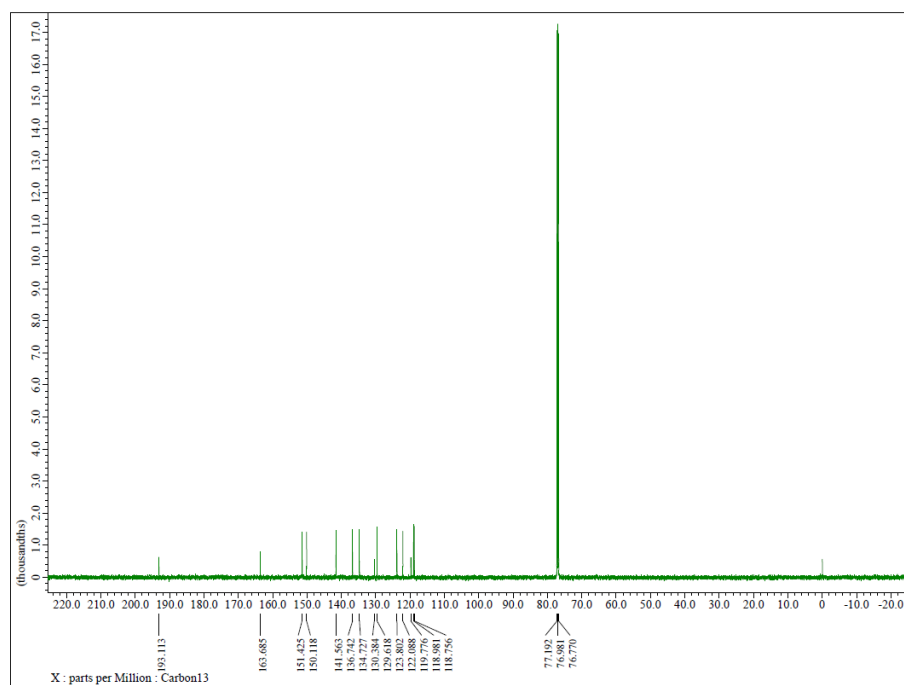
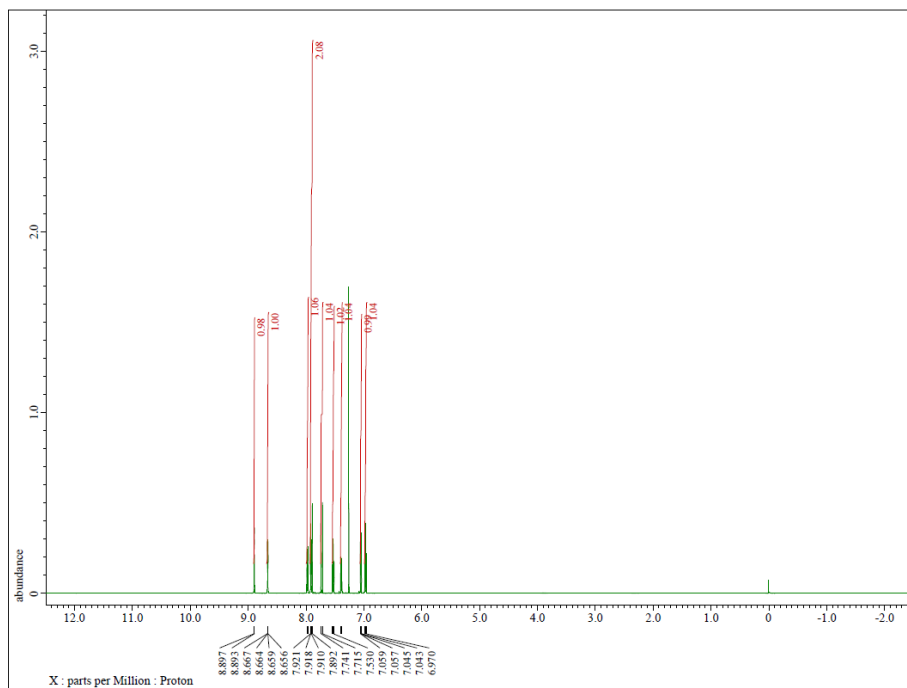
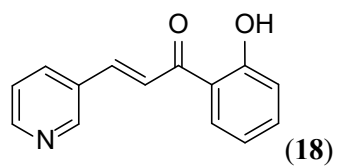
\*Corresponding author: Dr F. Brucoli.

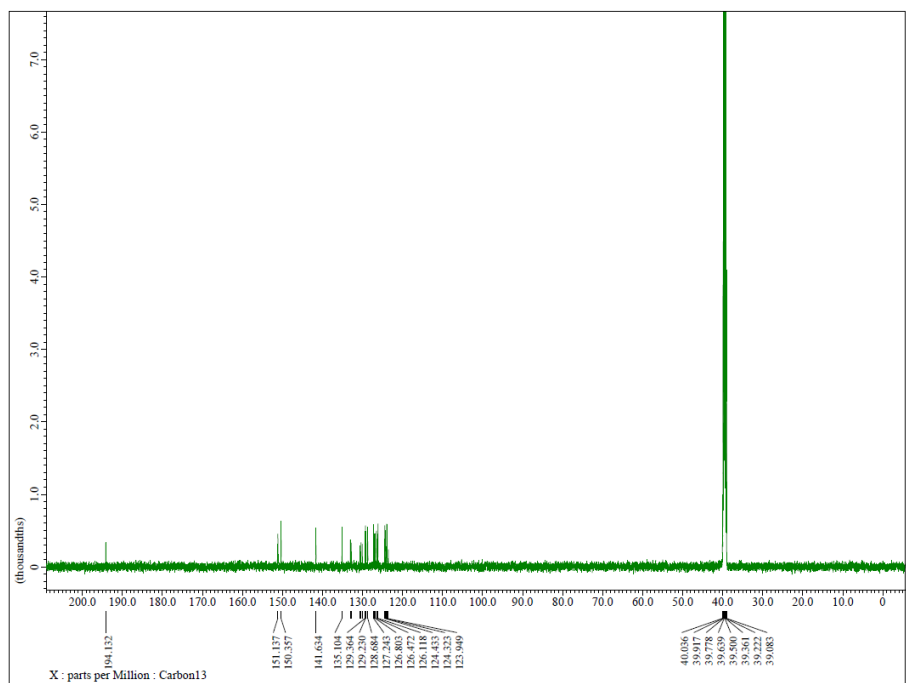
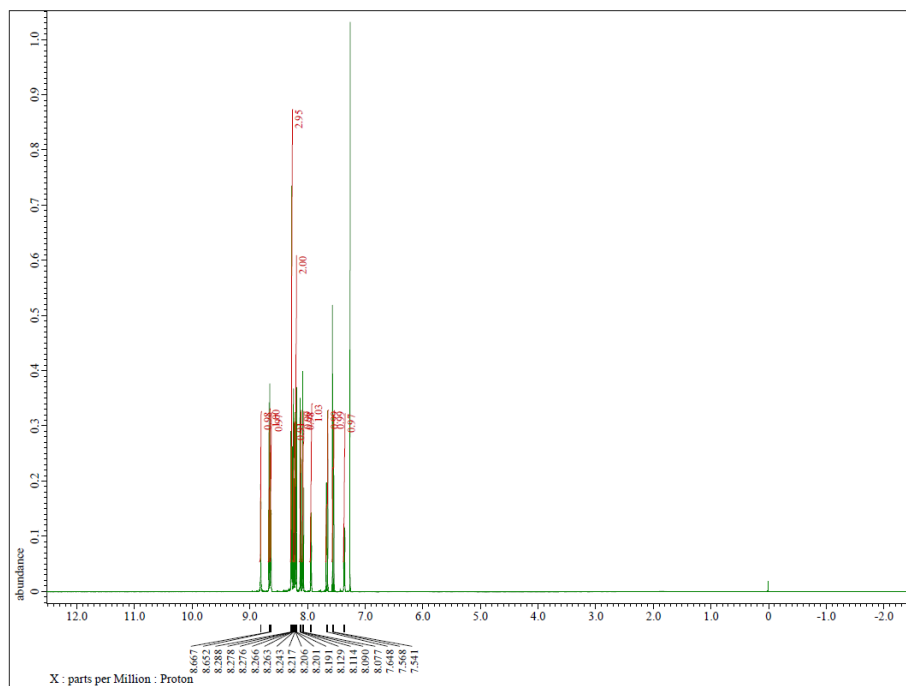
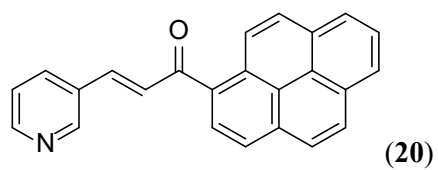
E-mail: federico.brucoli@dmu.ac.uk; orcid.org/ 0000-0001-8661-2910

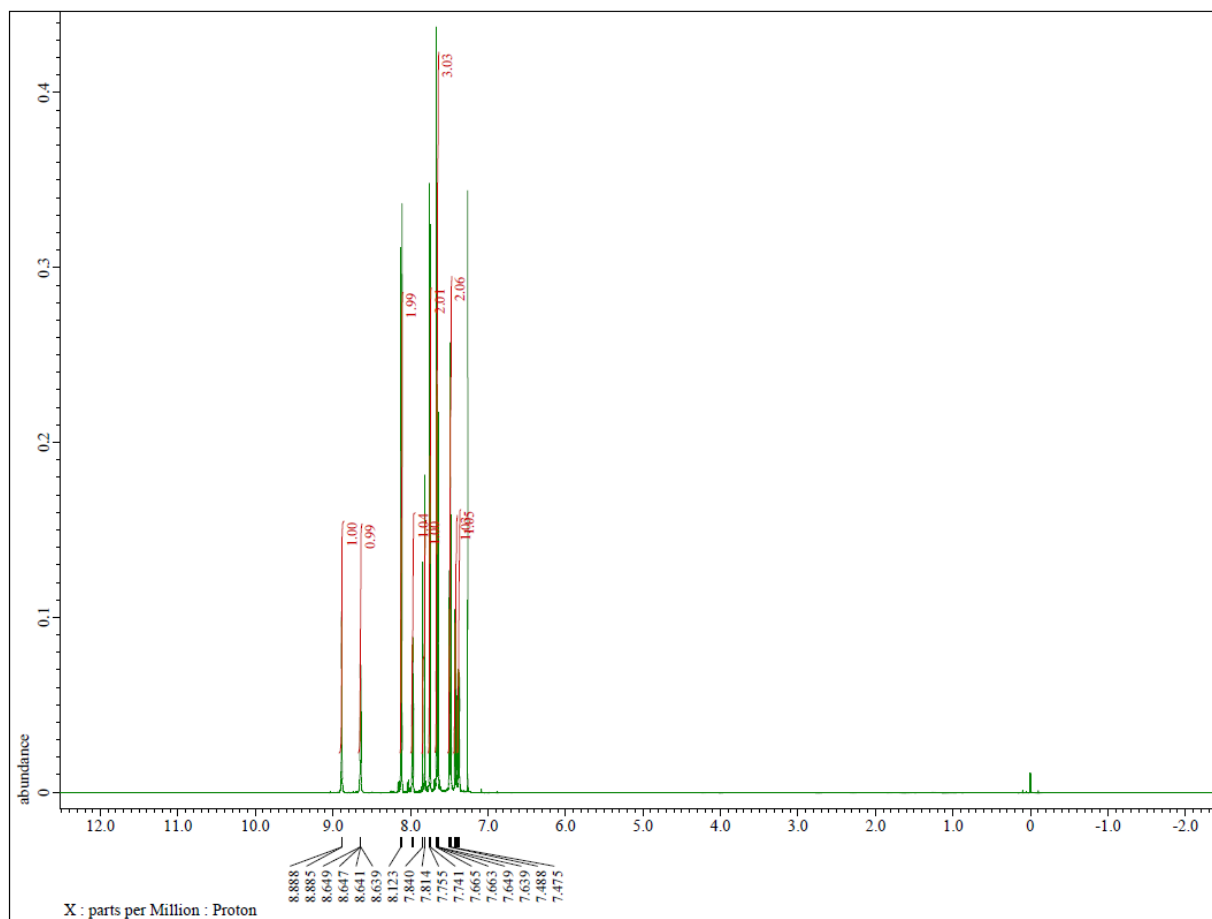
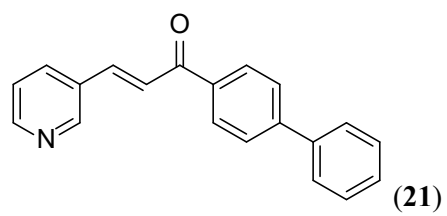
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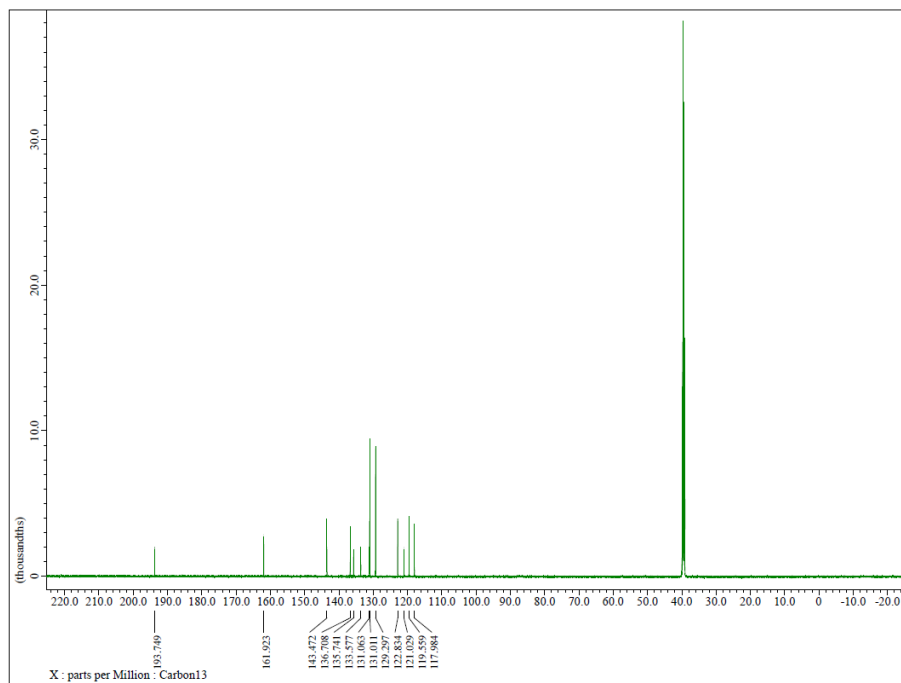
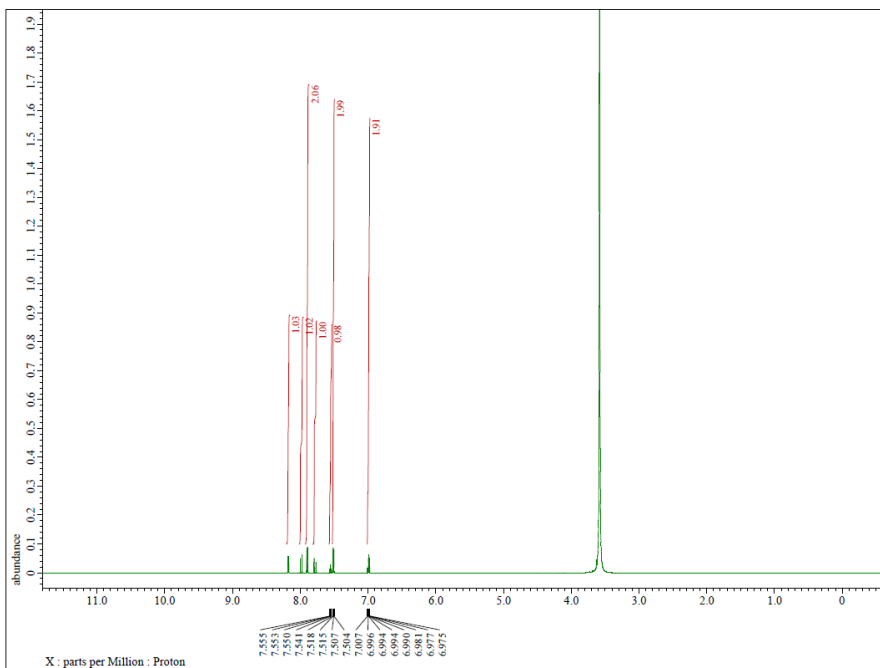
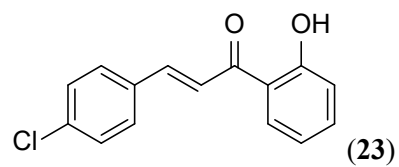


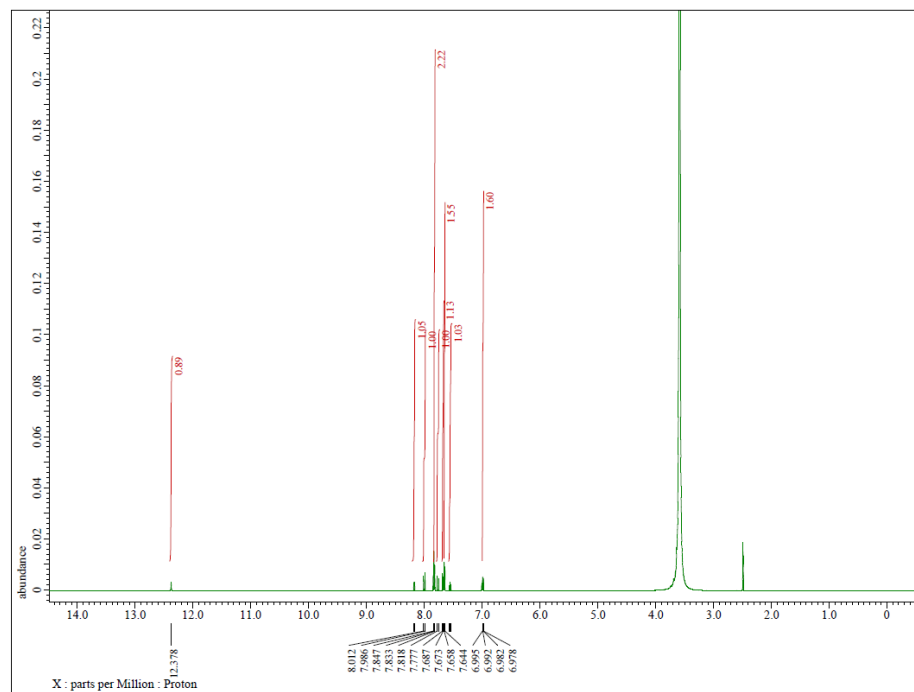
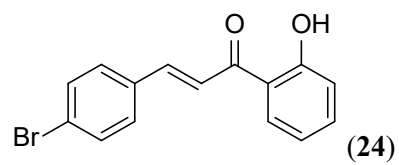




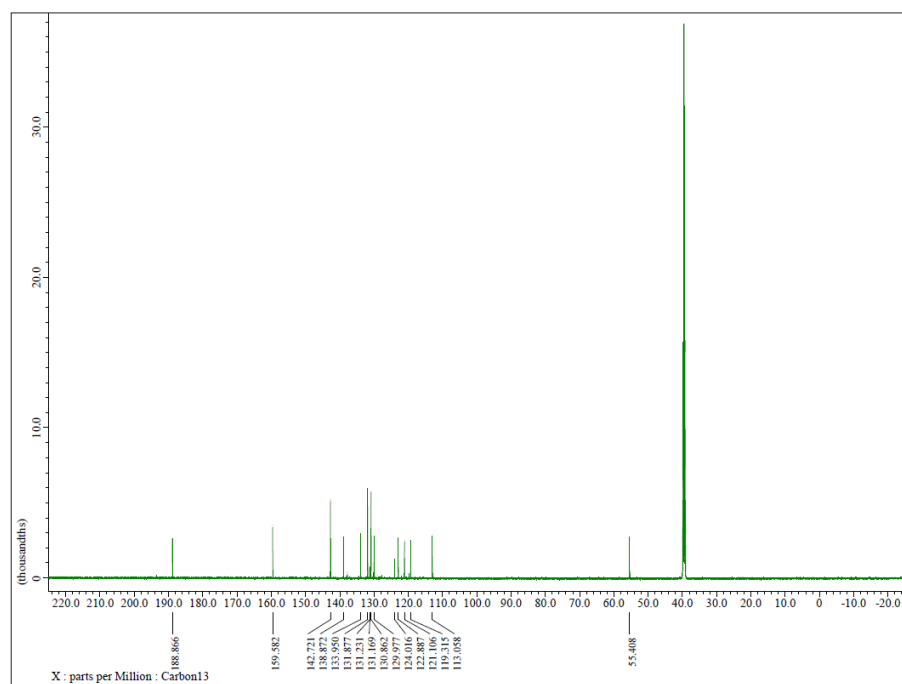
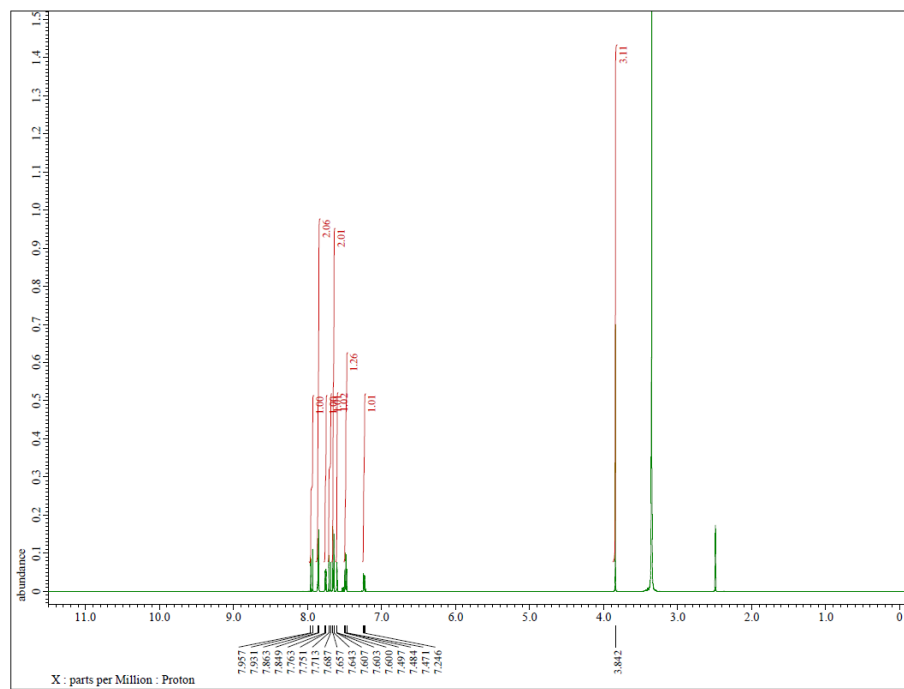
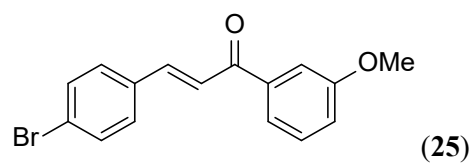


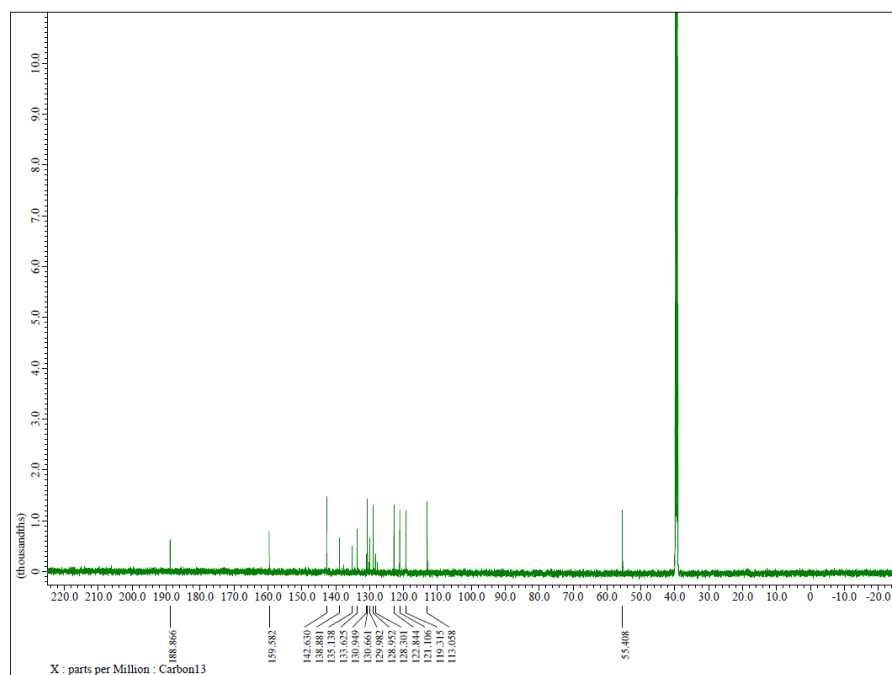
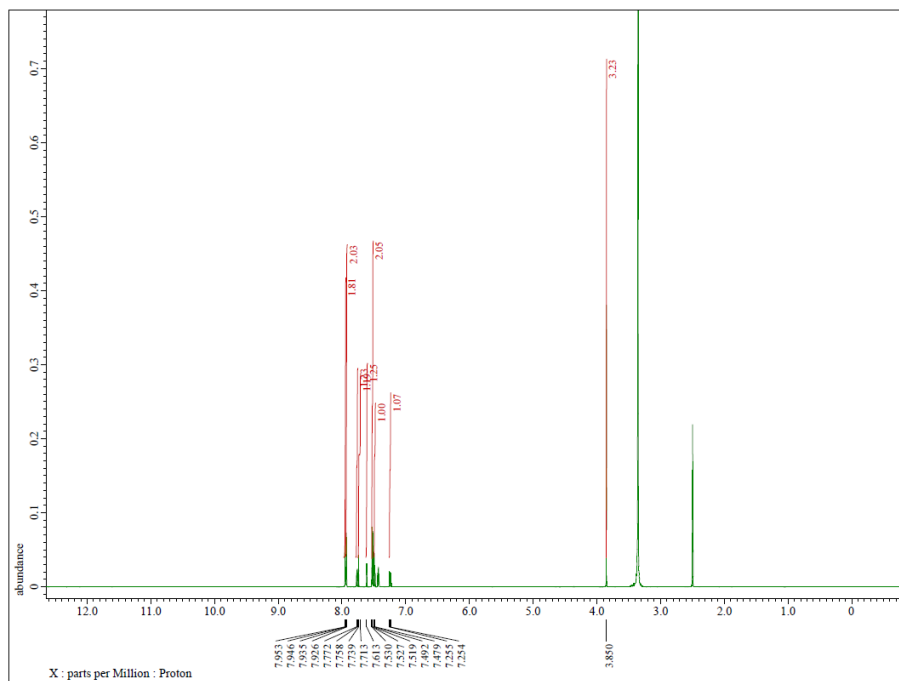
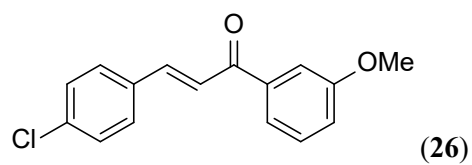


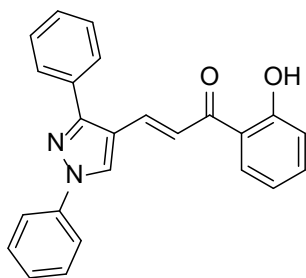


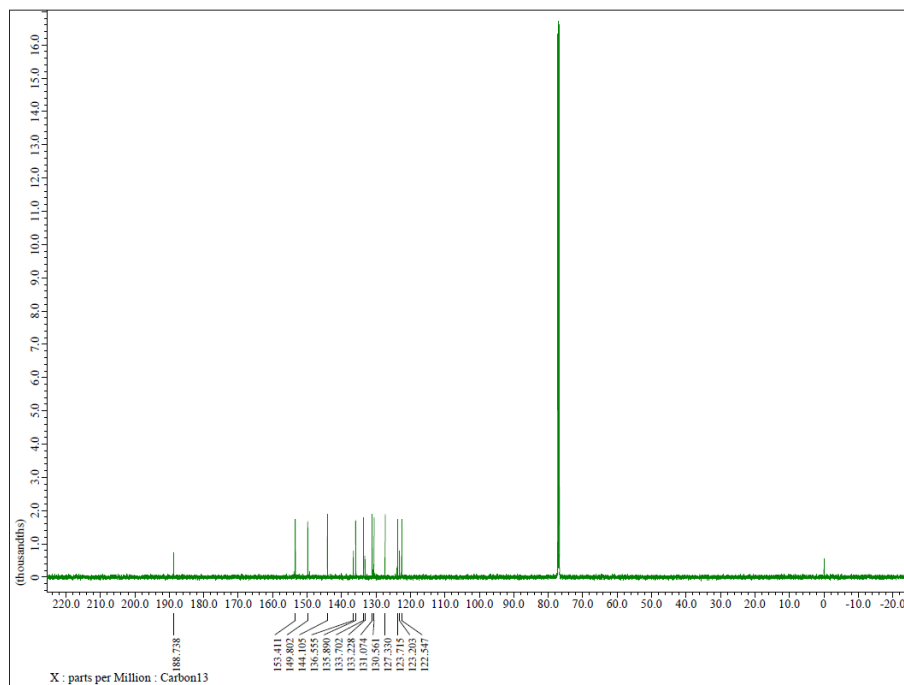
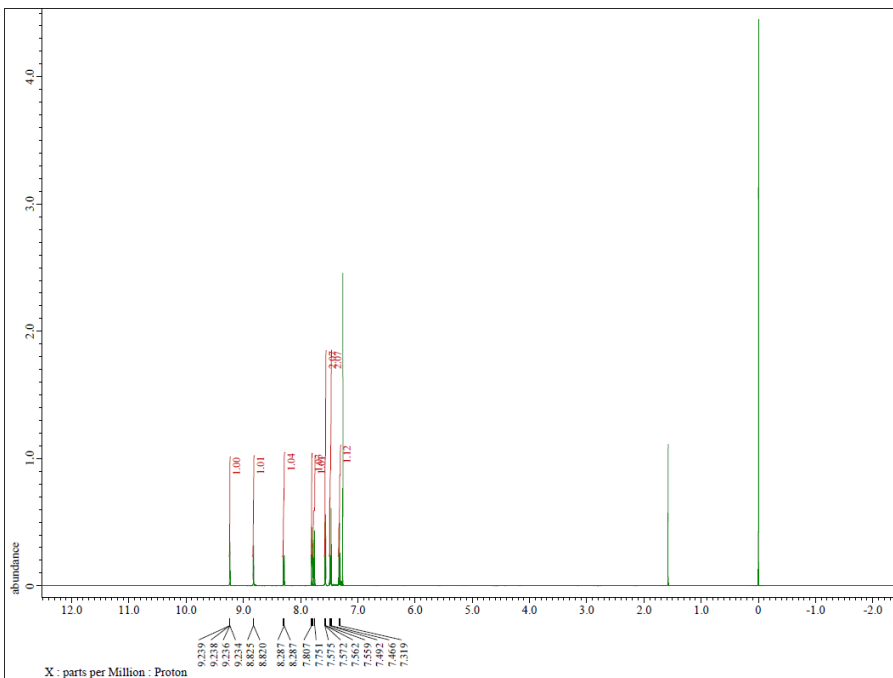
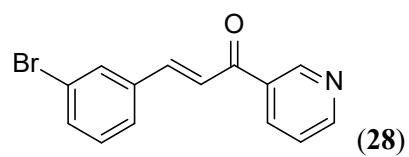


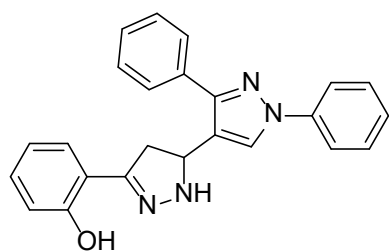




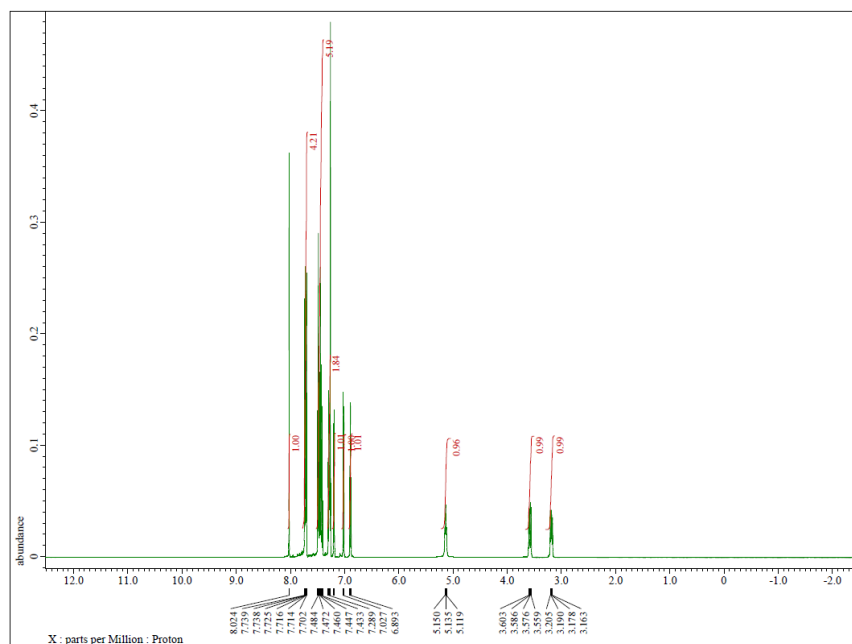


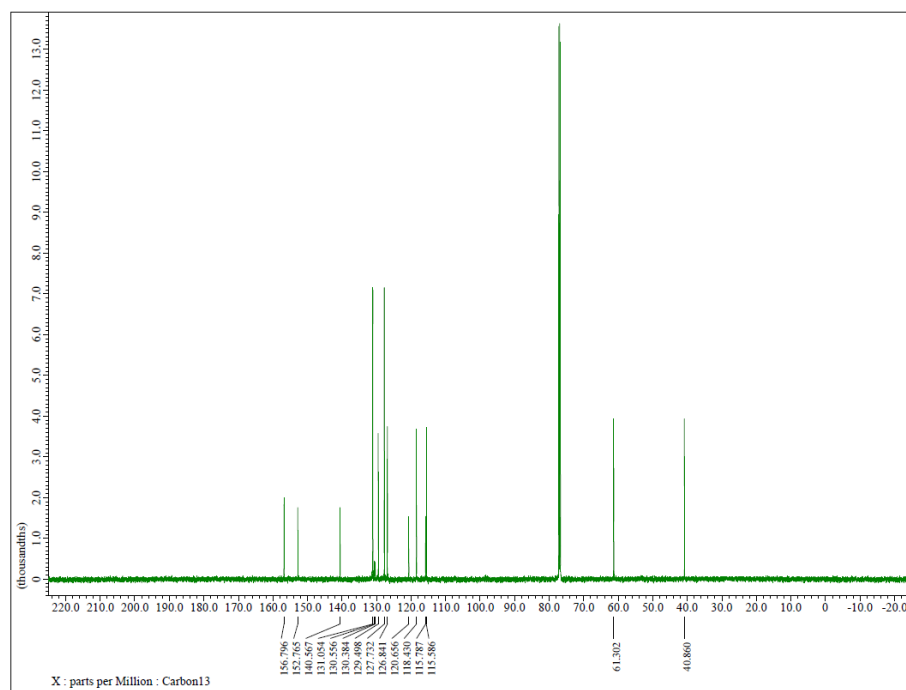
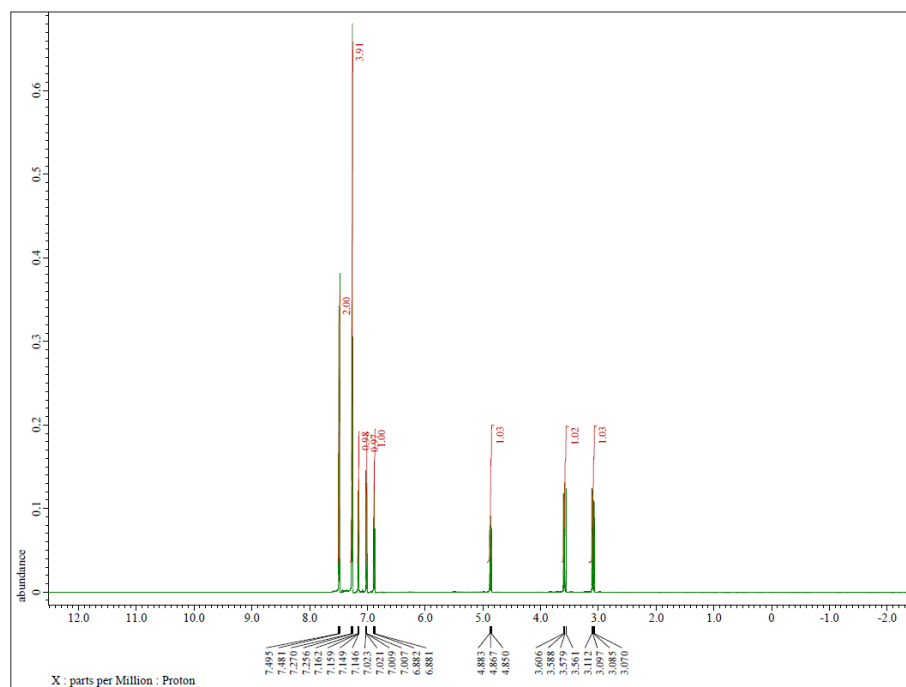
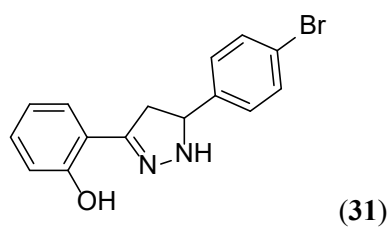






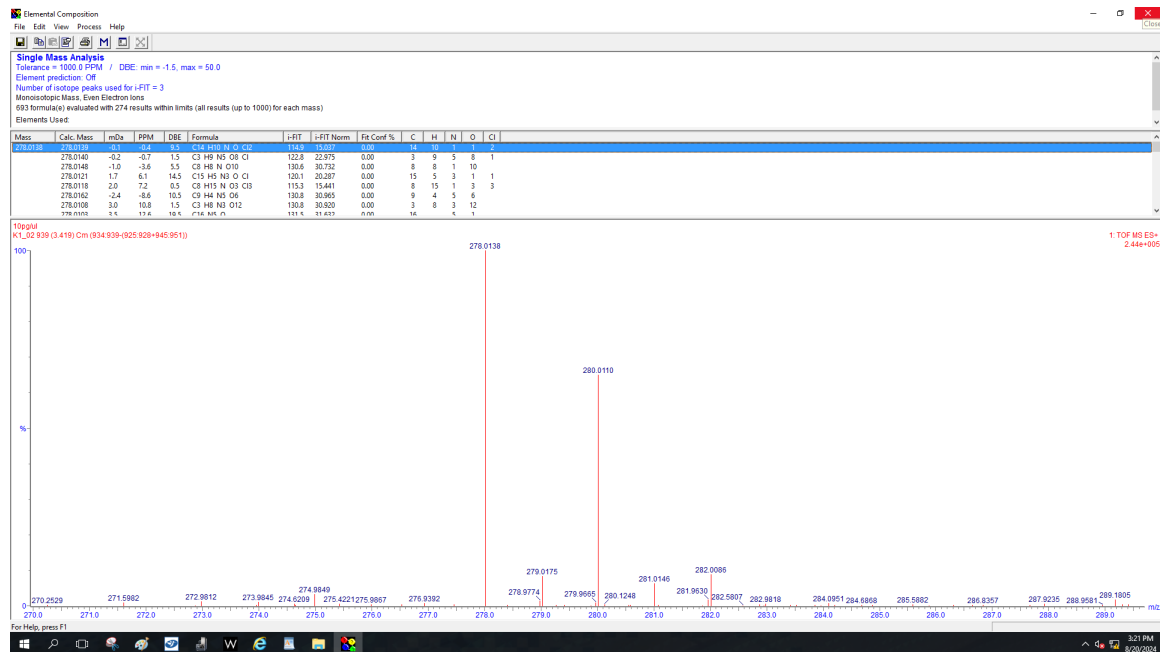
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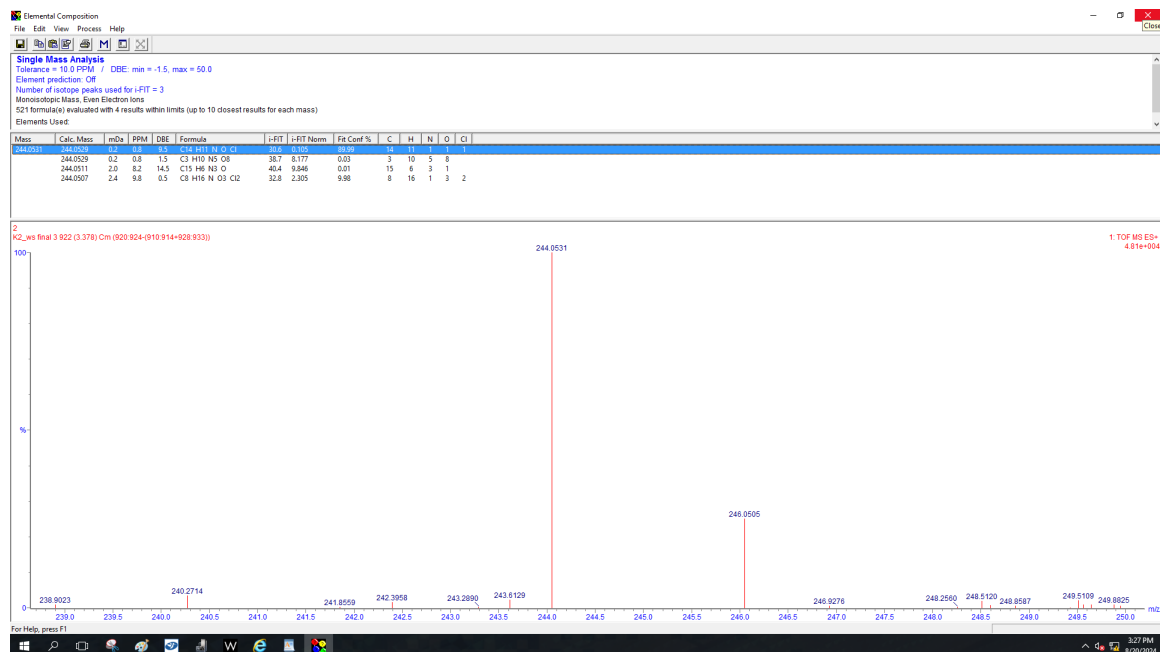


## Accurate mass determination of selected compounds

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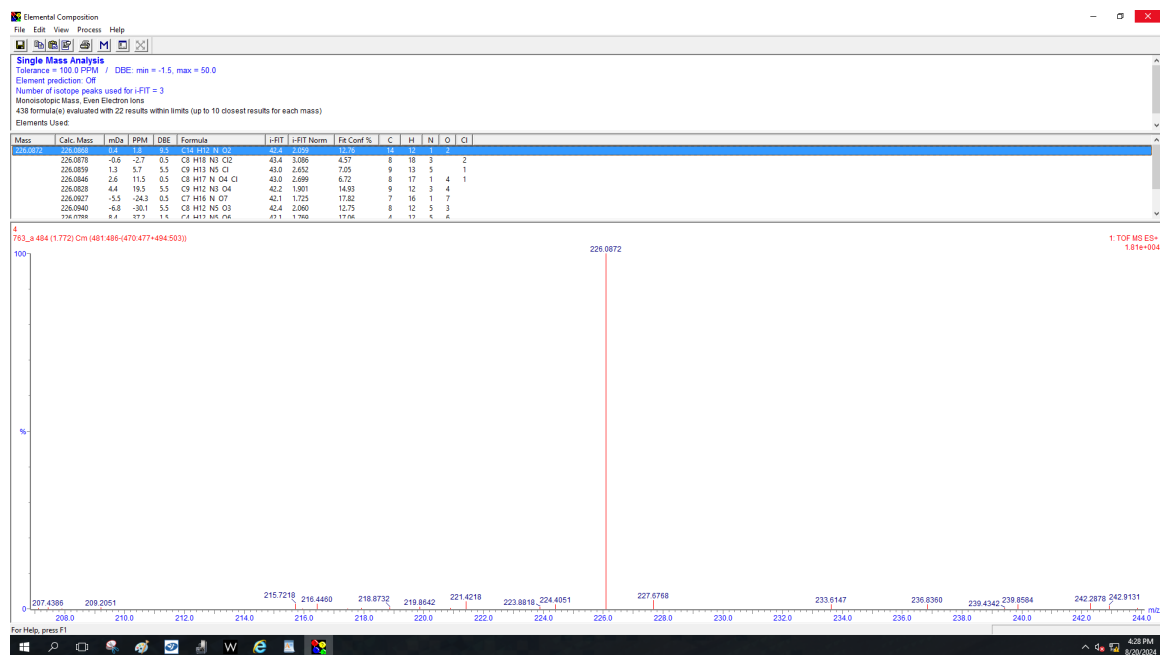
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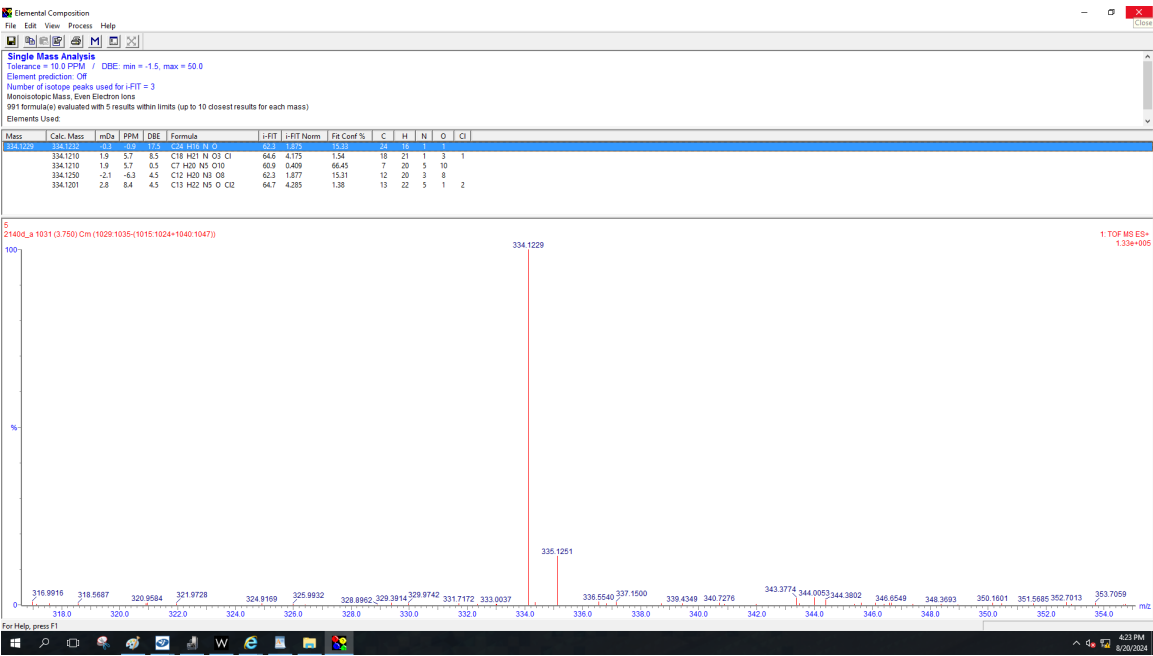


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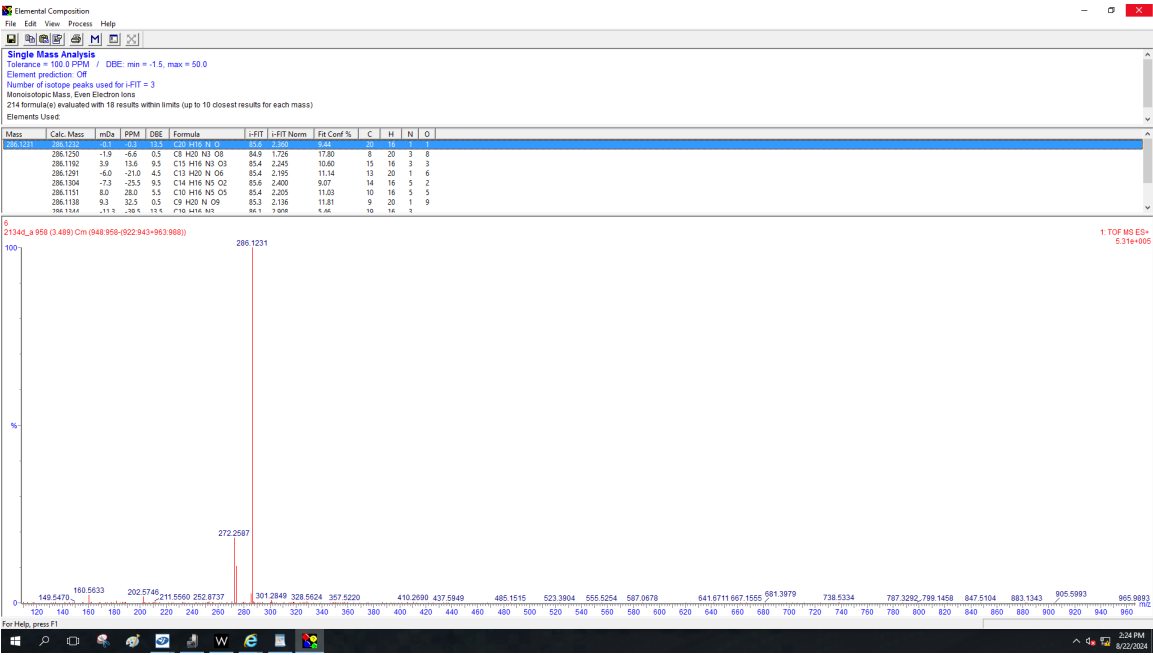




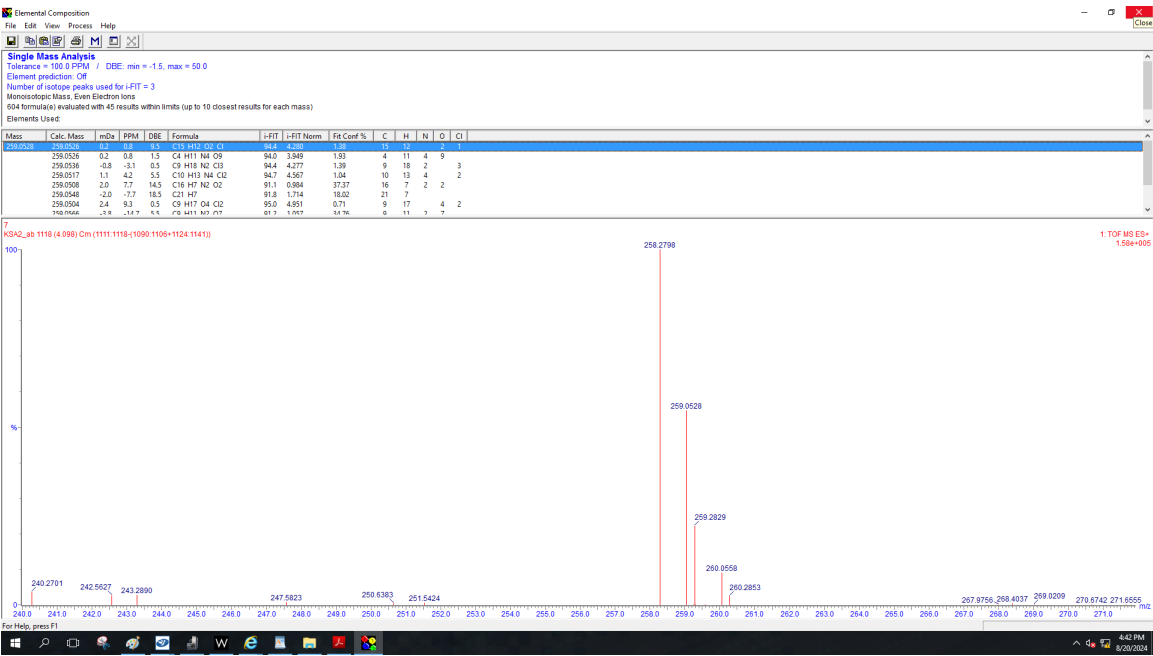
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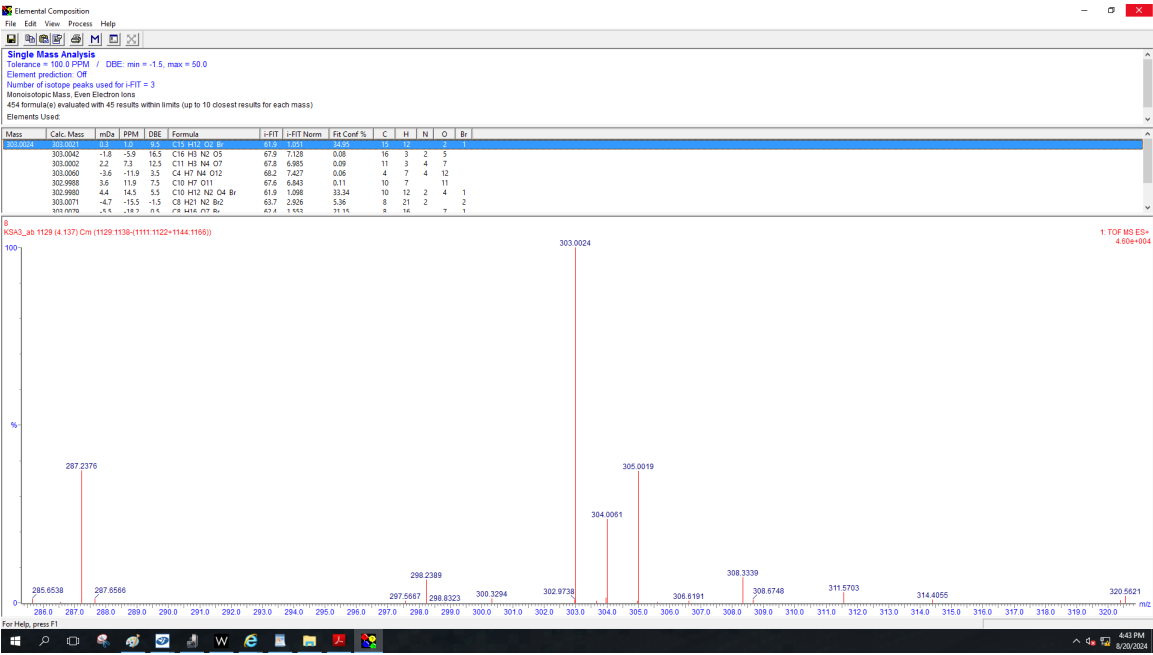
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**Elemental Composition**

File Edit View Process Help

Single Mass Analysis  
Tolerance = 100.0 PPM / DDE: min = -1.5, max = 50.0  
Element prediction: C#H  
Number of isotope peaks used for fFIT = 3  
Monoisotopic Mass, Even Electron ions  
490 formula(s) evaluated with 52 results within limits (up to 10 closest results for each mass)  
Elements Used:

Mass	Calc. Mass	mDa	PPM	DDE	Formula	fFIT	fFIT Norm	Ft Coef %	C	H	N	O	Br
317.0158	1.7	5.4	12.3	C12 H5 N4 O7	65.3	3.546	2.88	12	5	4	7		
317.0198	-2.3	-7.3	16.5	C17 H5 N2 O5	65.9	3.839	1.95	17	5	2	5		
317.0345	3.0	8.5	7.5	C11 H9 O11	65.4	3.450	3.17	11	9		11		
317.0140	3.5	11.0	25.5	C24 H4 N2	66.3	4.333	1.31	24	1	2			
317.0137	3.8	12.0	5.5	C11 H14 N2 O4 Br	64.3	2.370	8.25	11	14	2	4	1	
317.0217	-4.2	-13.2	3.3	C3 H9 N4 O12	64.6	2.646	7.10	5	9	4	12		
317.0198	-5.1	-14.9	-1.5	C20 H4 N2 K2 Br2	61.9	1.705	50.71	6	15	5		5	

9  
K3AS\_ab\_1095 (4.007) Cm (1093.1095-1080.1089-1100.1100)

1. TOF MS ES+  
3.41e+004

For Help, press F1

Elemental Composition

File Edit View Help

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: C#

Number of isotope peaks used for rFIT = 3

Monoisotopic Mass, Even Electron Ions

676 formula(s) evaluated with 47 results within limits (up to 10 closest results for each mass)

Elements Used:

Mass	Calc. Mass	mDa	PPM	DBE	Formula	rFIT	rFIT Norm	Fit Conf %	C	H	N	O	Cl
273.0685	273.0683	0.2	0.7	1.5	C <sub>5</sub> H <sub>13</sub> N <sub>4</sub> O <sub>9</sub>	98.2	20.384	0.00	5	13	4	9	
273.0685	273.0685	0.0	0.0	1.5	C <sub>5</sub> H <sub>13</sub> N <sub>4</sub> O <sub>9</sub>	98.2	20.384	0.00	5	13	4	9	
273.0682	-0.7	-2.6	0.5	C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> Cl <sub>3</sub>	87.7	9.890	0.01	10	20	2		3	
273.0674	1.1	4.0	5.5	C <sub>11</sub> H <sub>15</sub> N <sub>4</sub> Cl <sub>2</sub>	85.4	7.659	0.05	11	15	4		2	
273.0704	-1.9	-7.0	18.5	C <sub>22</sub> H <sub>8</sub>	99.0	21.177	0.00	22	8				
273.0664	2.1	7.7	14.5	C <sub>17</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub>	86.5	20.705	0.00	17	8	2		2	
273.0660	2.5	8.2	0.5	C <sub>10</sub> H <sub>15</sub> O <sub>4</sub> Cl <sub>2</sub>	87.5	8.661	0.01	10	15		4	2	
273.0773	-1.8	-11.0	4.5	C <sub>19</sub> H <sub>41</sub> N <sub>2</sub> F <sub>7</sub>	88.8	35.187	0.99	19	41	2			

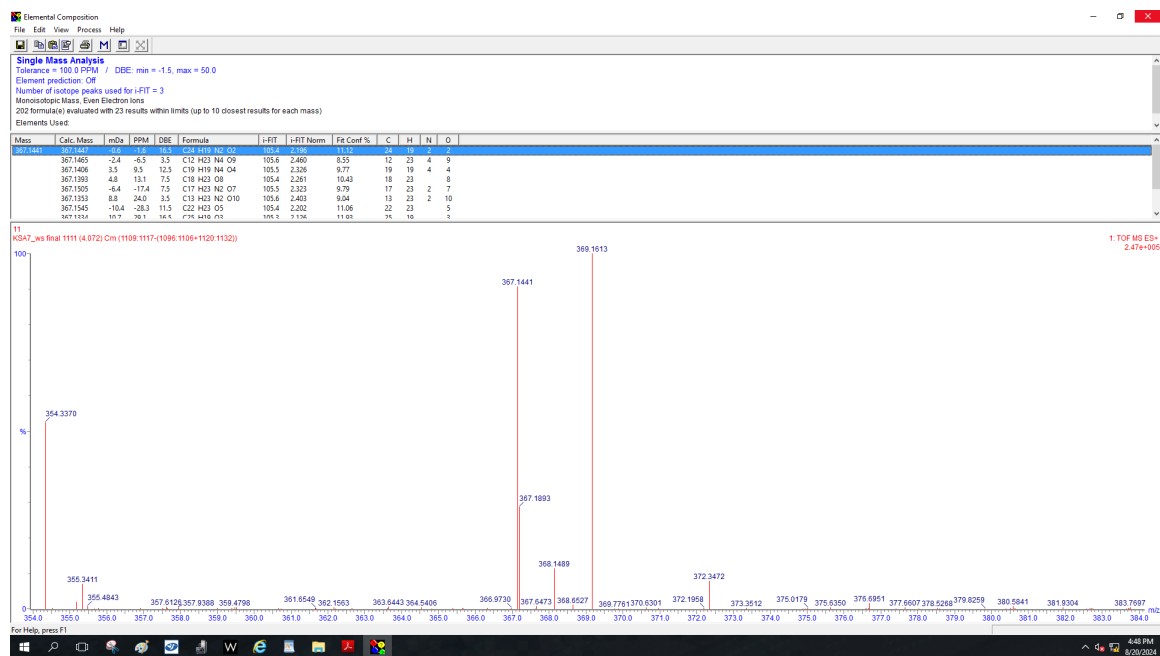
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MS/MS: 273.0685 (3.965) Cm (1074.1083-1083.1071+1086.1095)

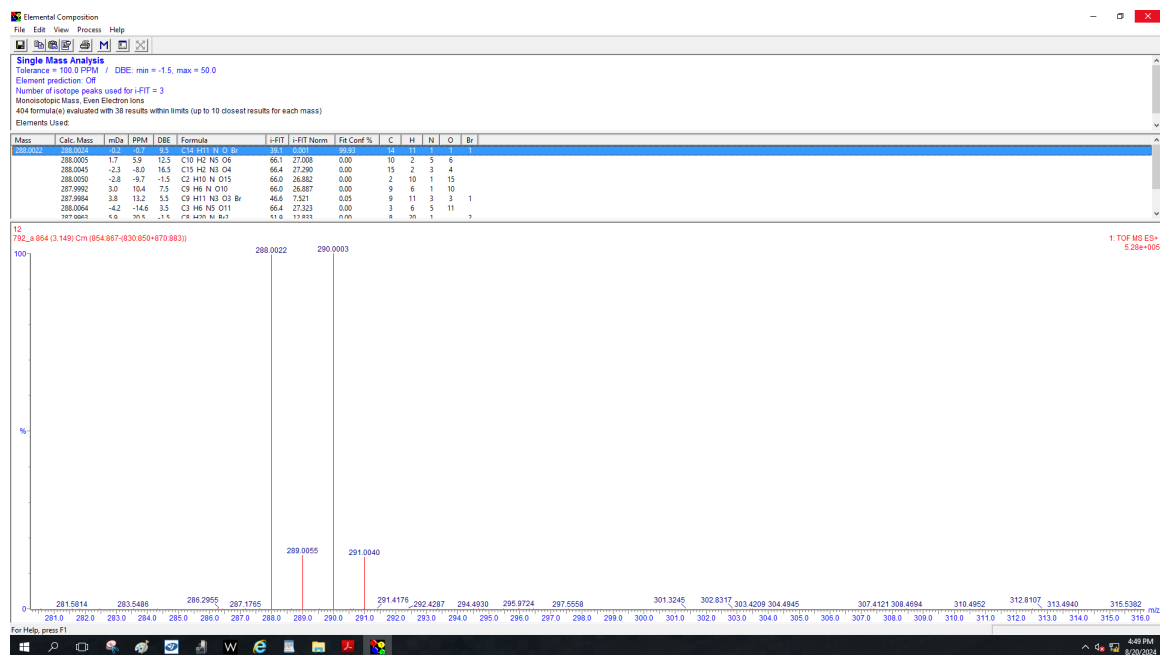
1. TOF MS ES+  
2.87e+005

For Help, press F1

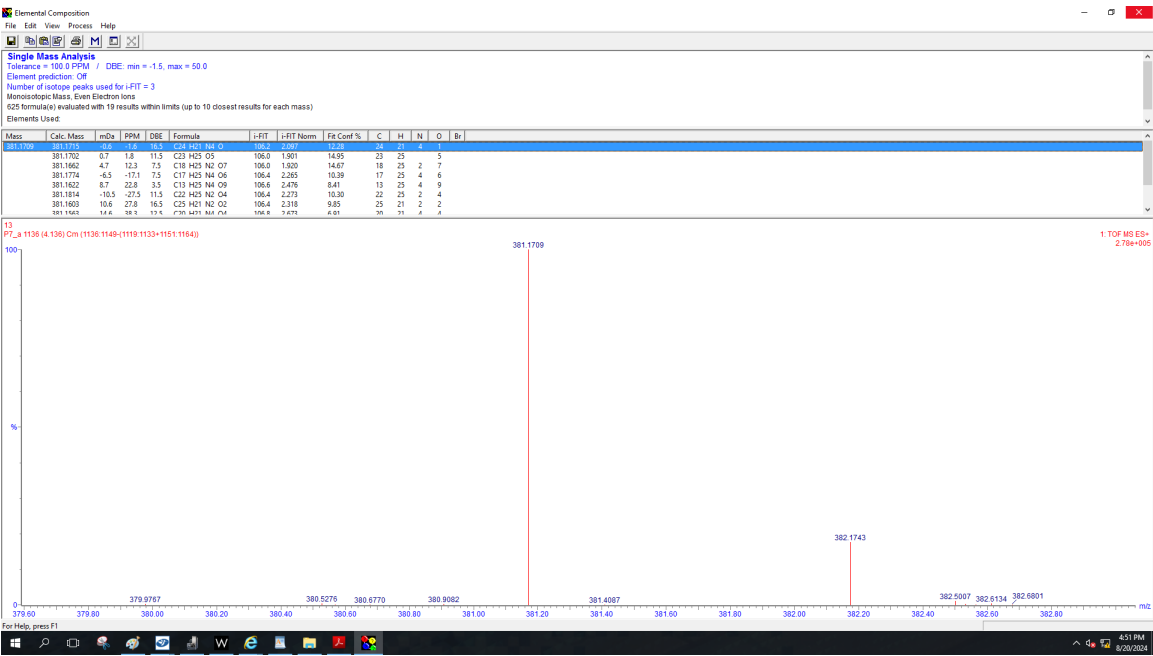
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