

Supplementary material for the article:

Živković, M. B.; Matić, I. Z.; Rodić, M. V.; Novaković, I. T.; Krivokuća, A. M.; Sladić, D. M.; Krstić, N. M. Anticancer Potential of New Steroidal Thiazolidin-4-One Derivatives. Mechanisms of Cytotoxic Action and Effects on Angiogenesis in Vitro. *Journal of Steroid Biochemistry and Molecular Biology* **2017**, *174*, 72–85.
<https://doi.org/10.1016/j.jsbmb.2017.07.031>

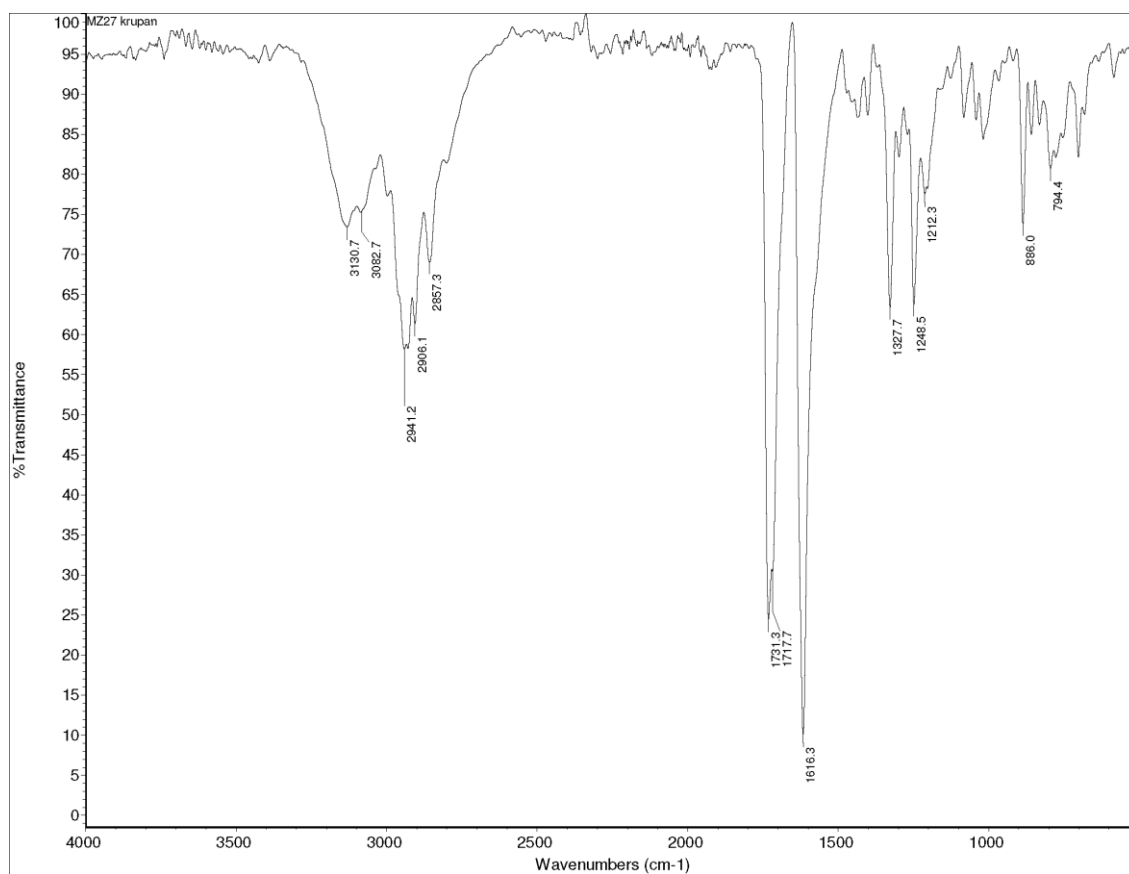
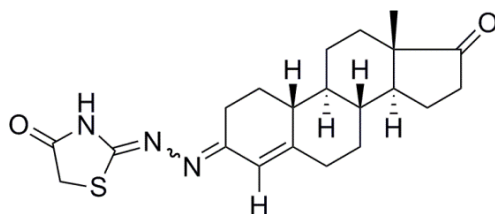
Supplementary data

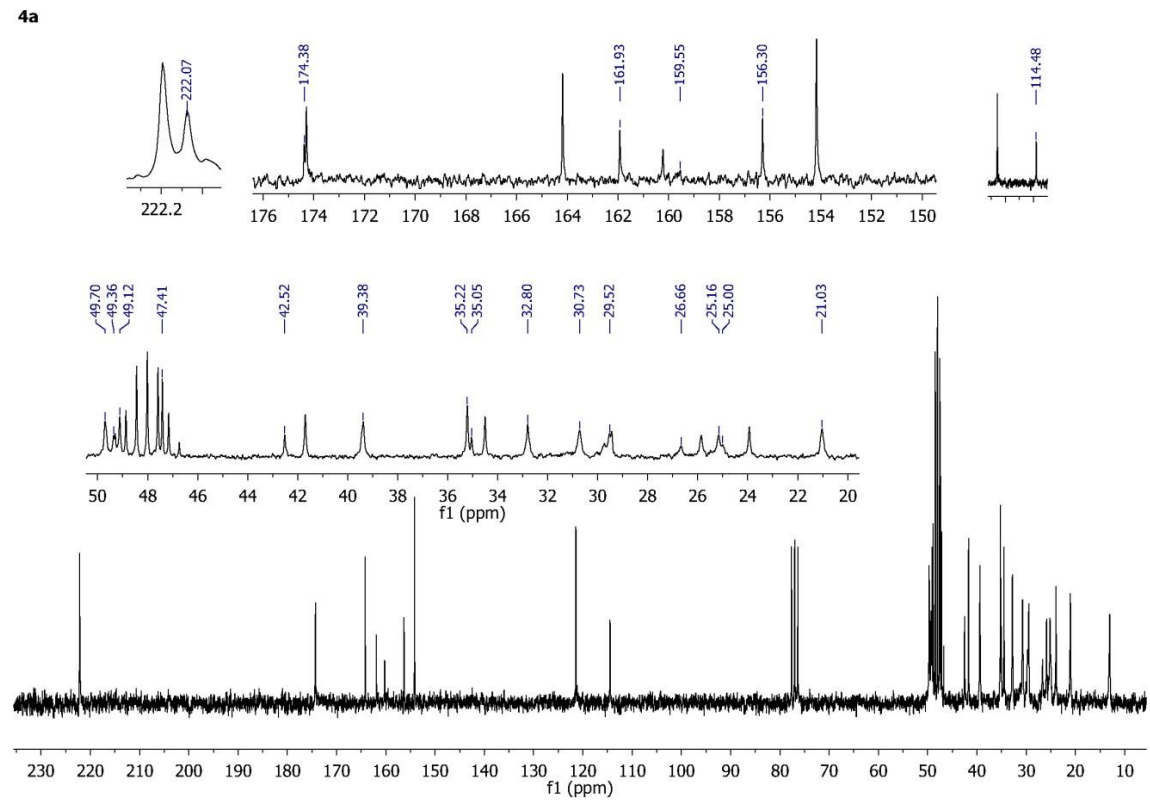
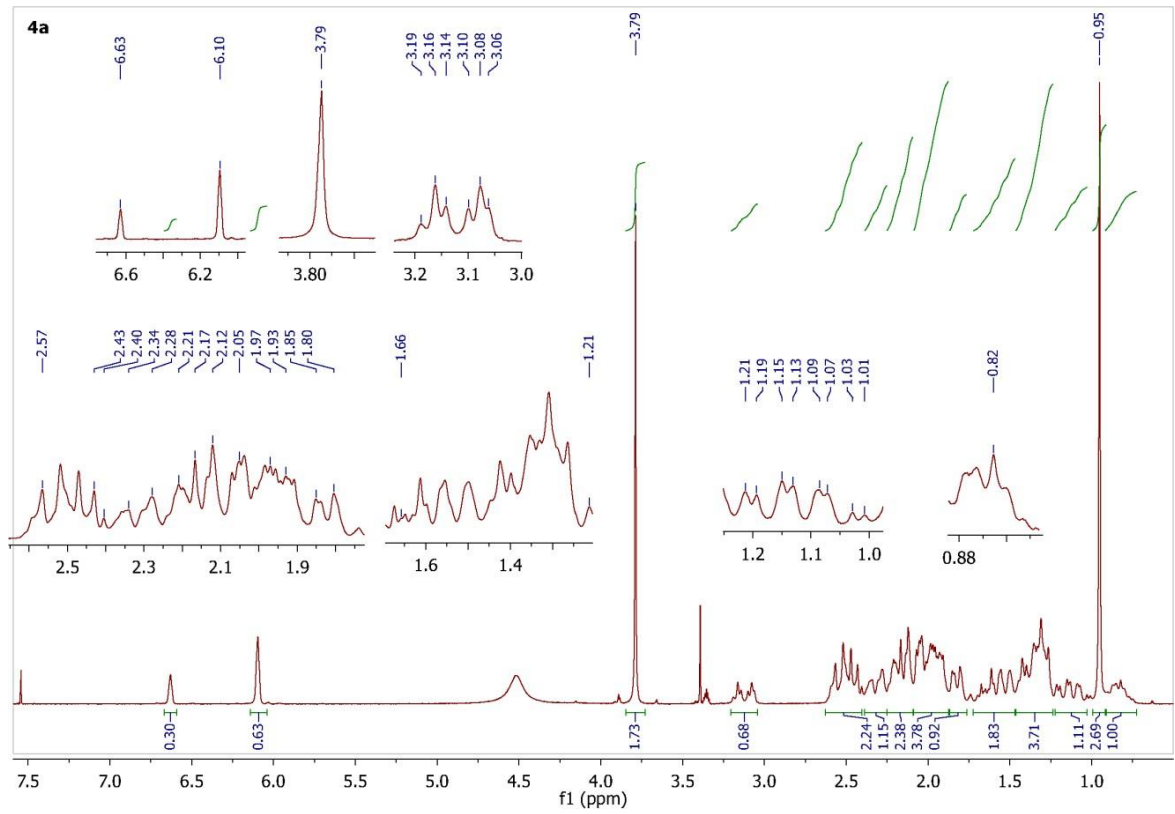
Anticancer potential of new steroidal 4-oxo-thiazolidine derivatives. Mechanisms of cytotoxic action and effects on angiogenesis *in vitro*

Marijana B. Živković^a, Ivana Z. Matić^b, Marko V. Rodić^c, Irena T. Novaković^a, Ana M. Krivokuća^b, Dušan M. Sladić^d, Natalija M. Krstić^{a,1}

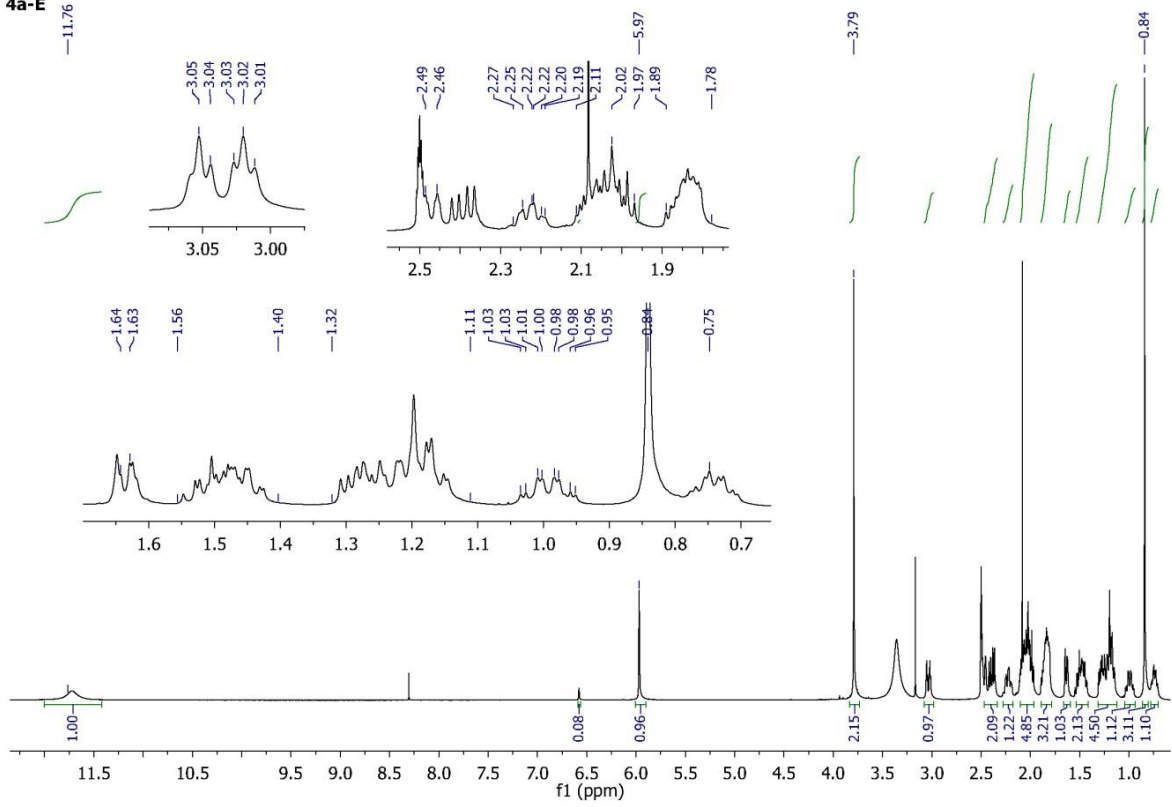
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Compound 4a

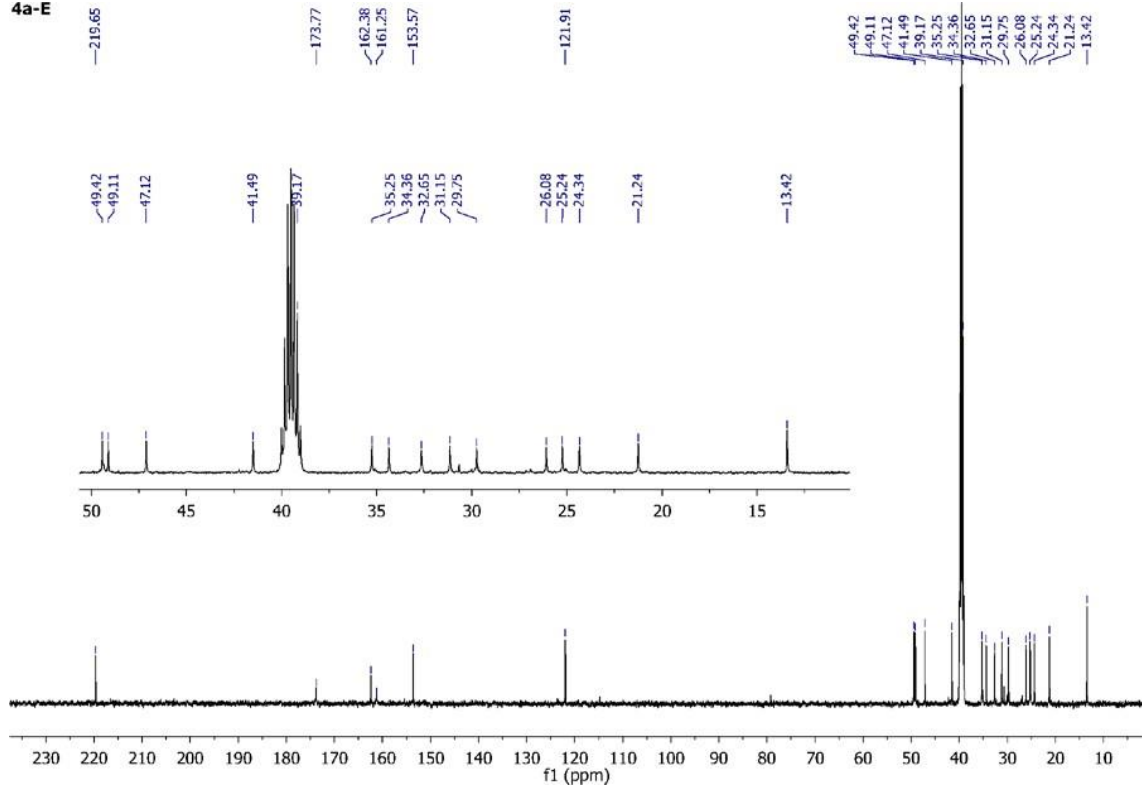




4a-E

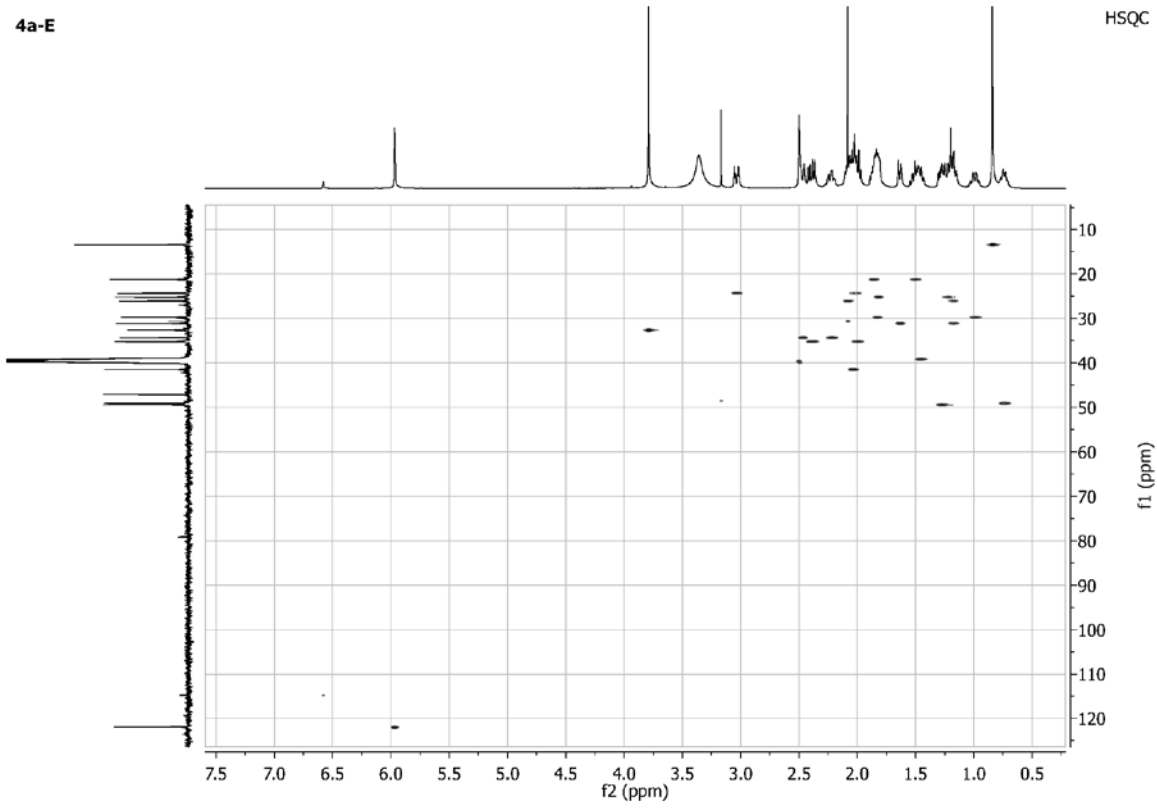


4a-E



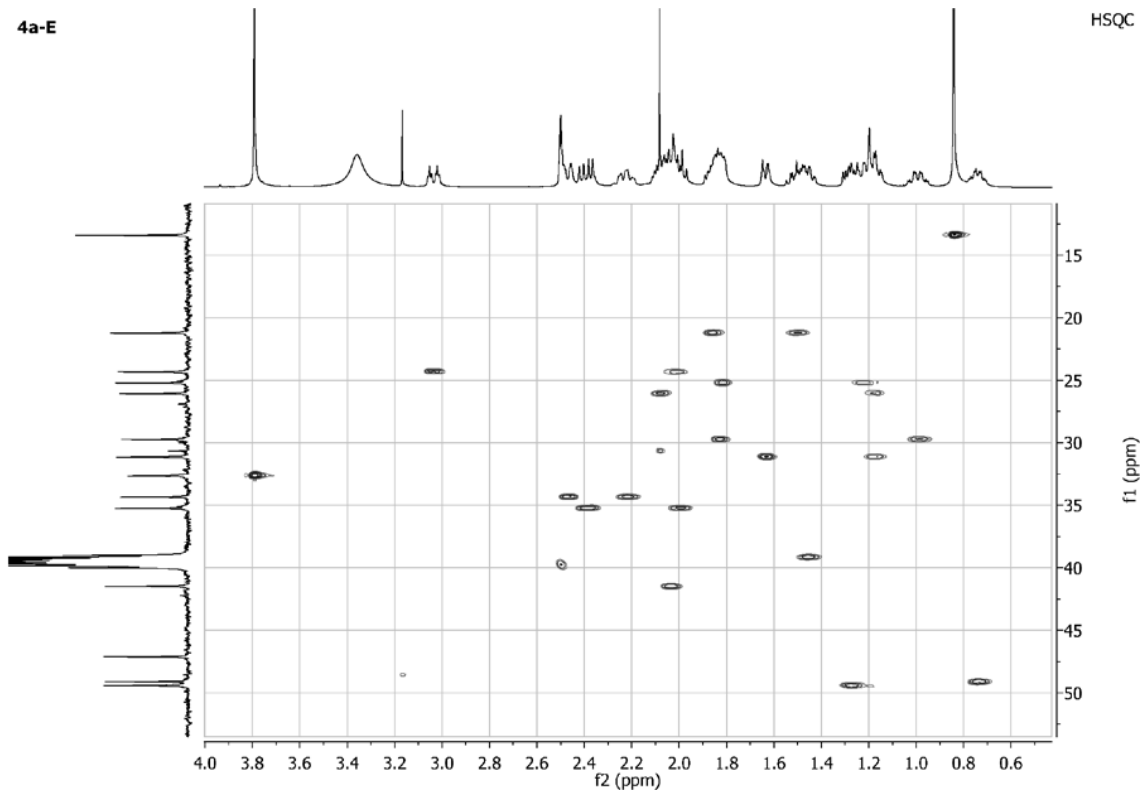
4a-E

HSQC

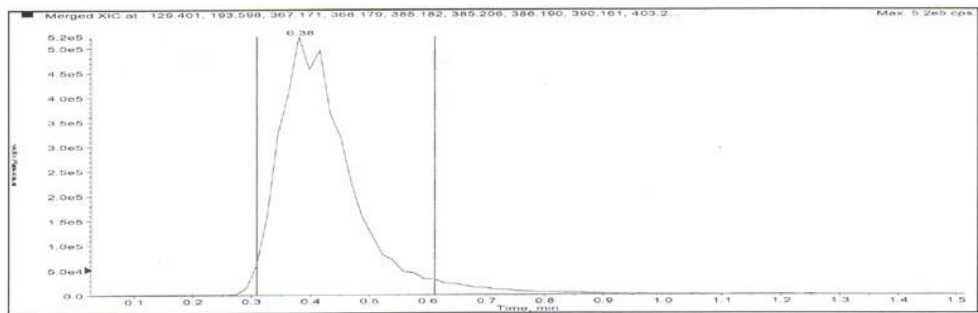


4a-E

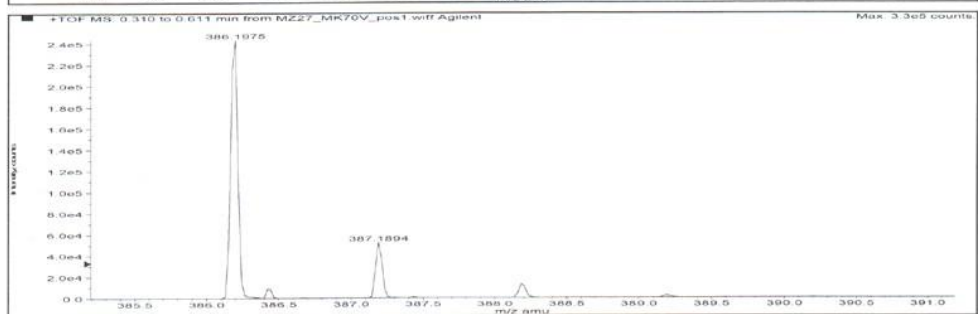
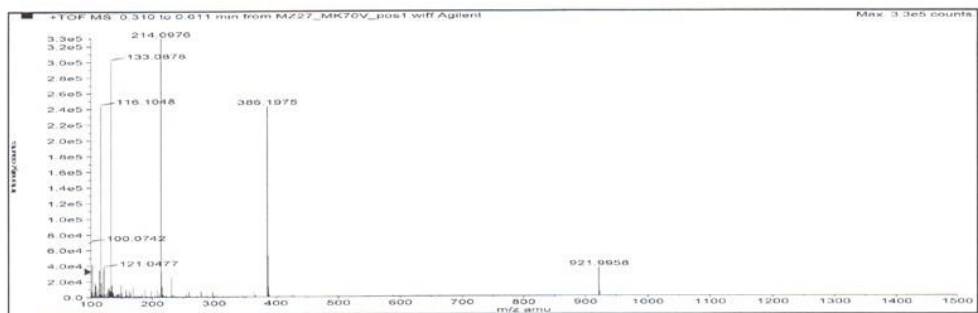
HSQC



Sample Name: M227 Sample Location: P1-C6 Sample Id: Operator: Milka
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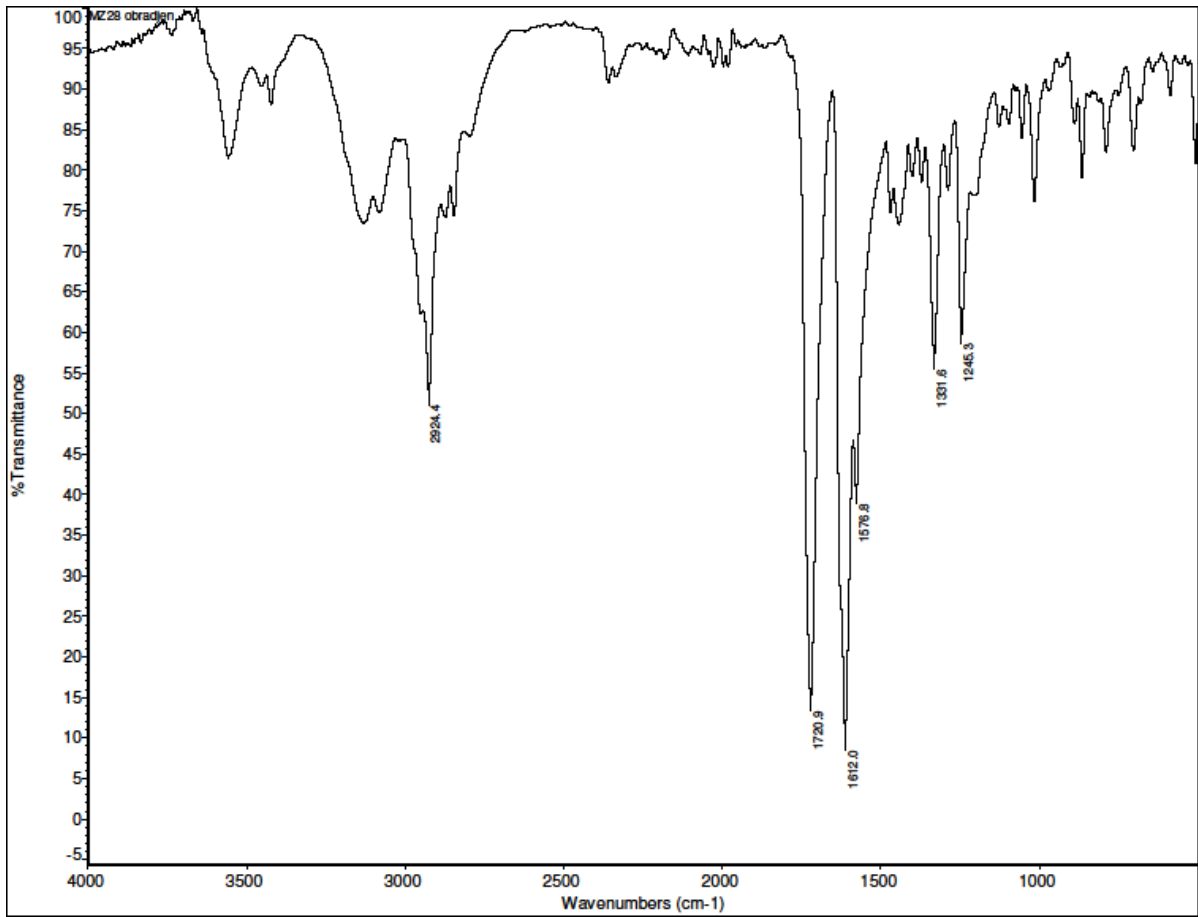
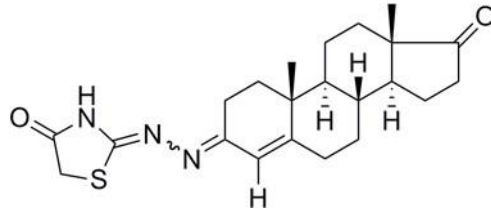
Merged XIC, Period# : 1 Experiment# : 1

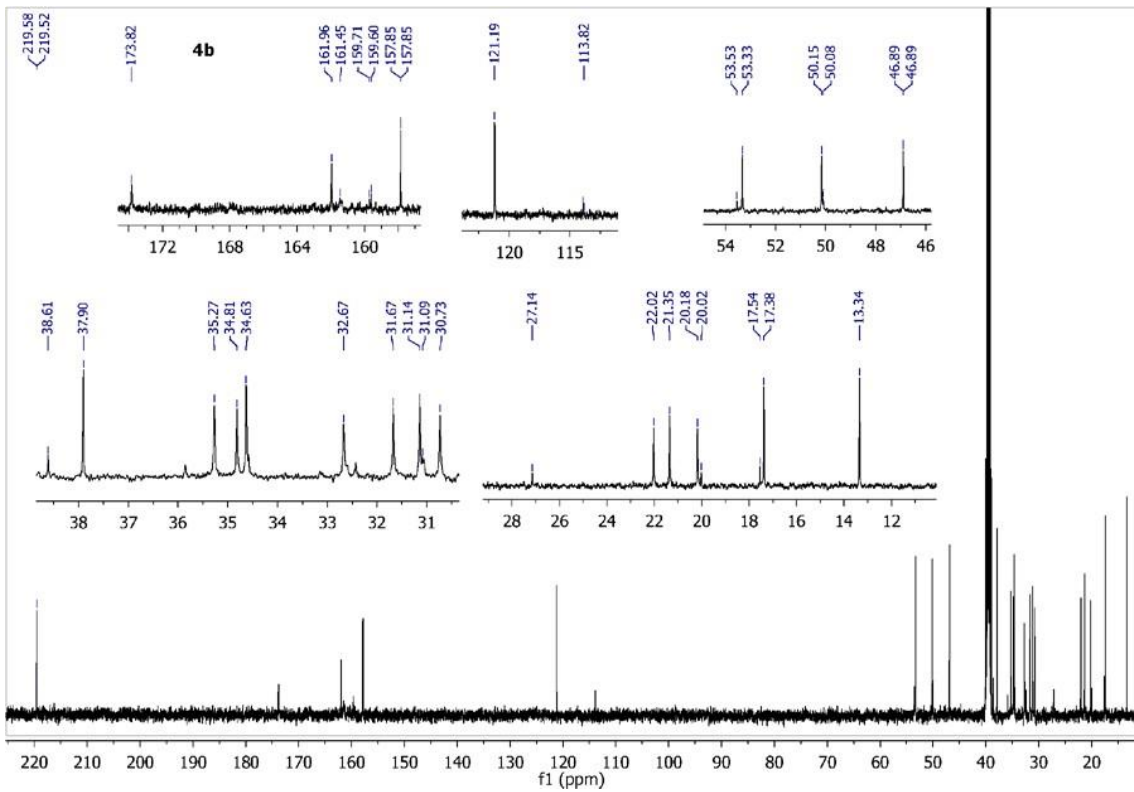
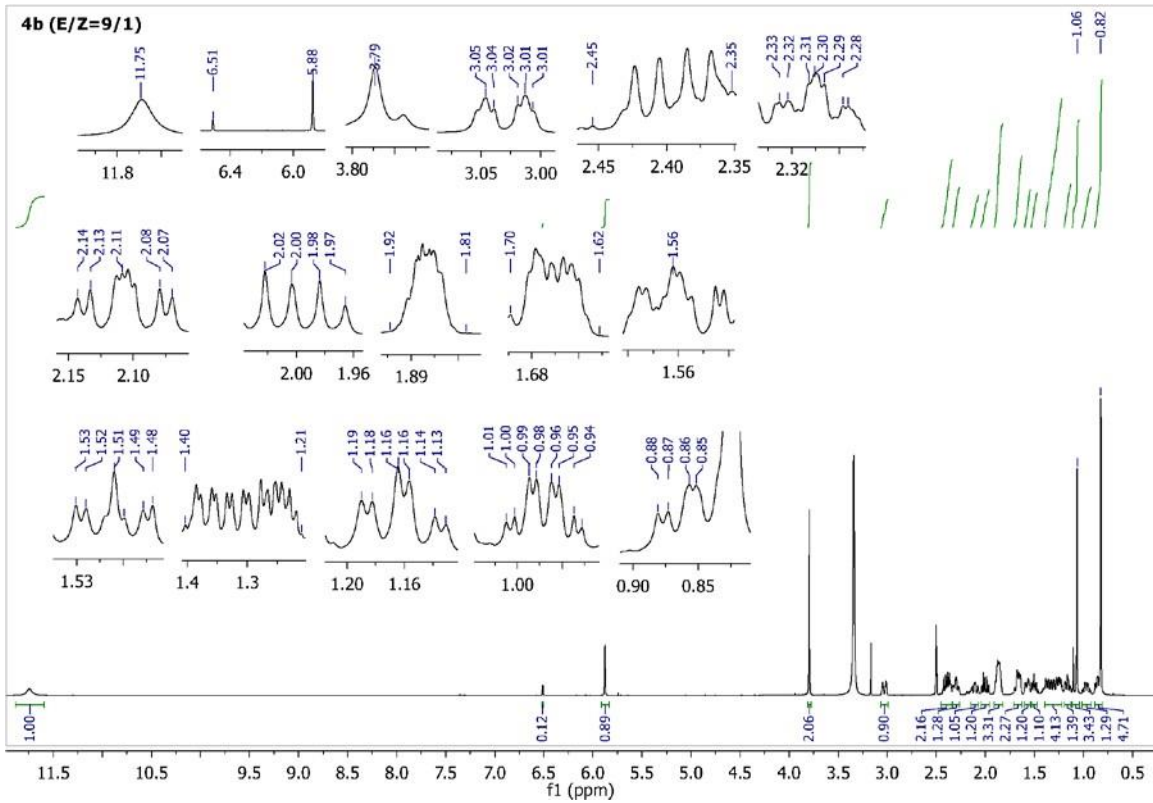


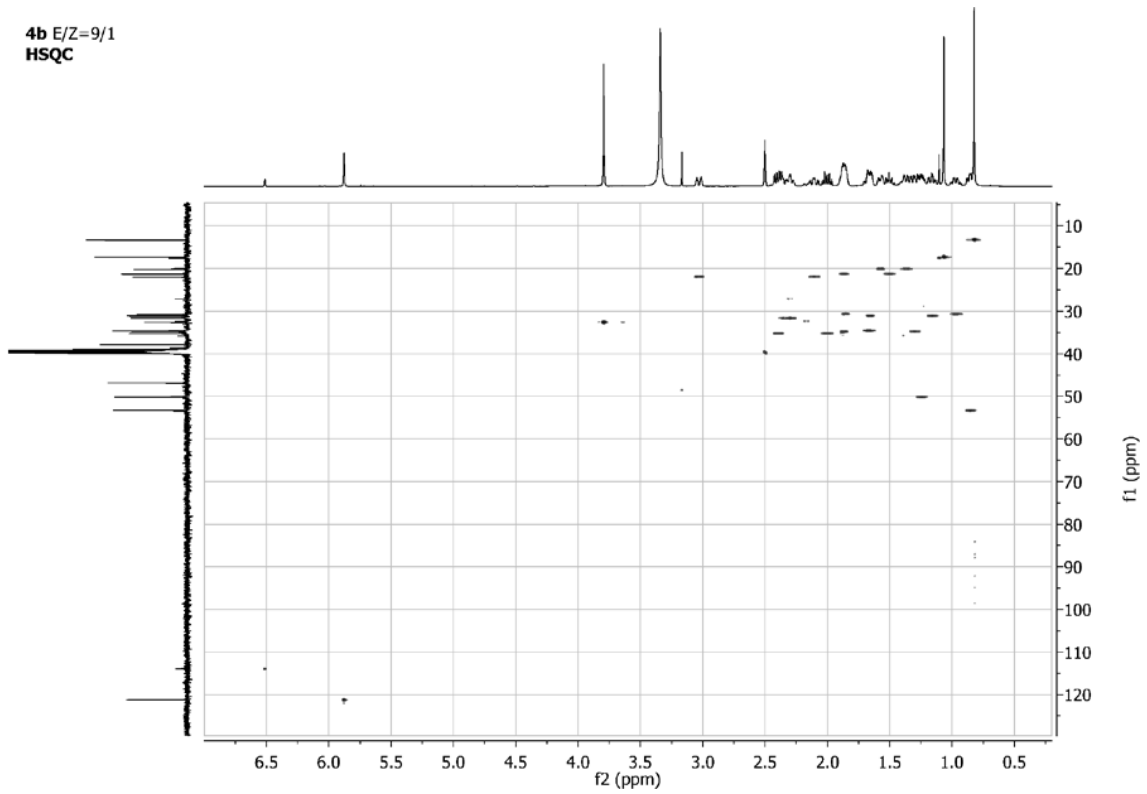
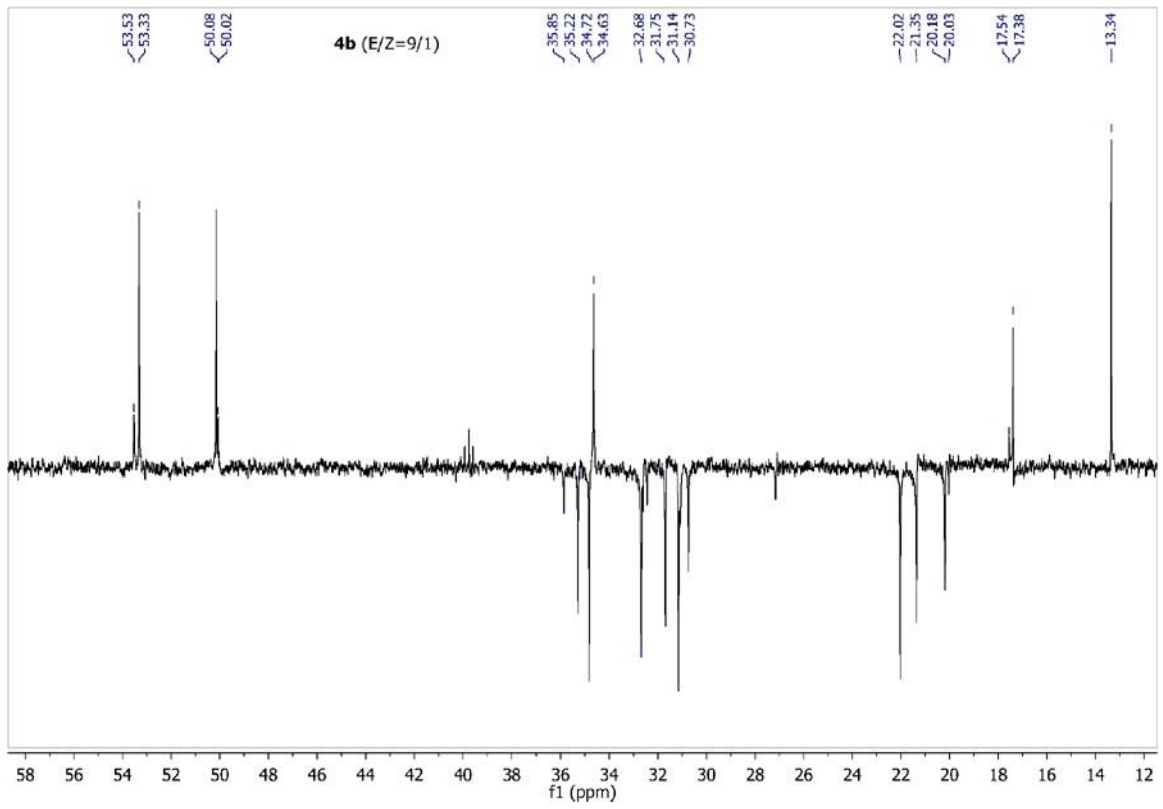
| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|-------------|---------------|-----------|---------------|------------|-------------|
| C21H27N3O2S | -- | 385.18240 | 0.38 | 4.31106 E6 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|--------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+H] ⁺ | 252584.55 | 386.18967 | 386.18961 | -0.06638 | -0.17 | -- |

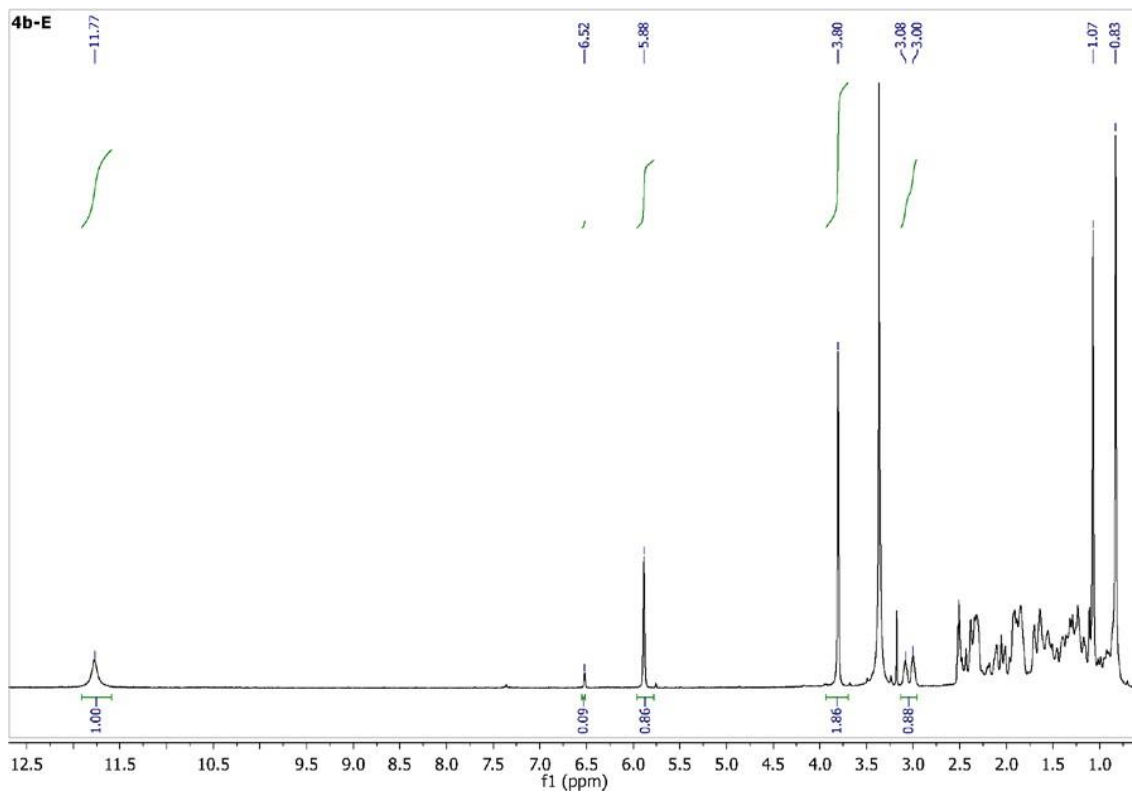
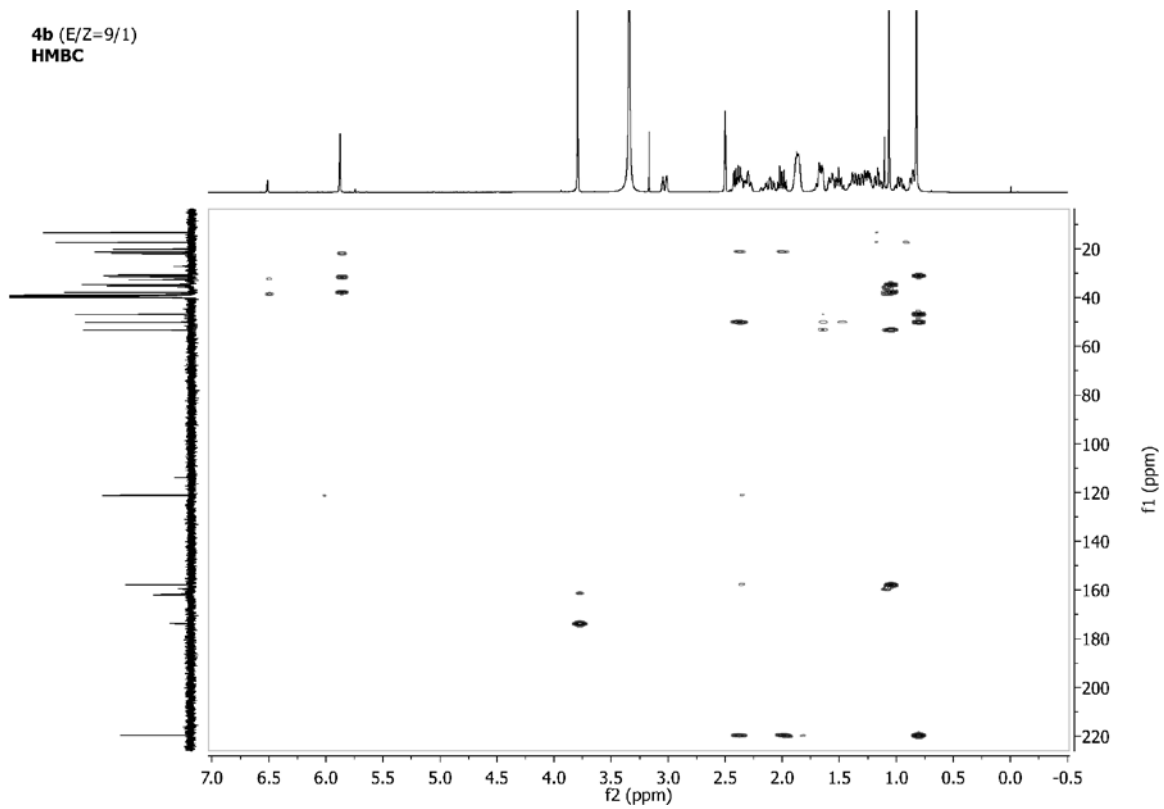
Compound 4b

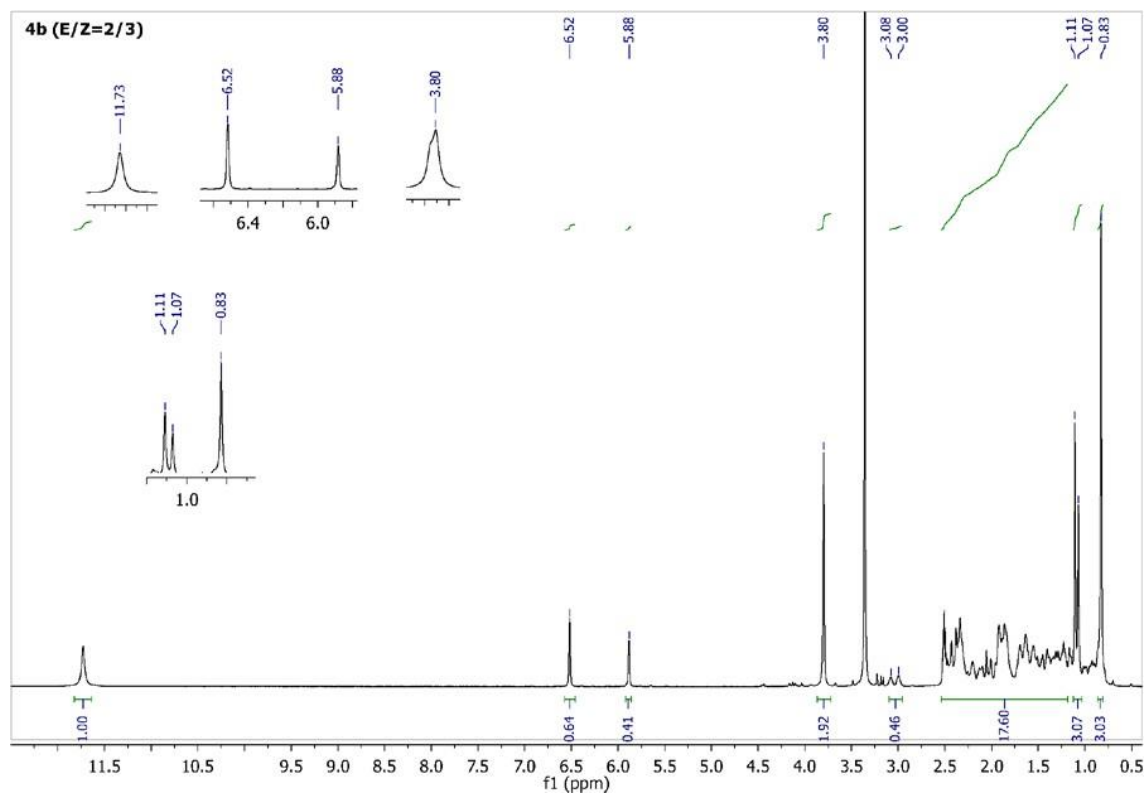
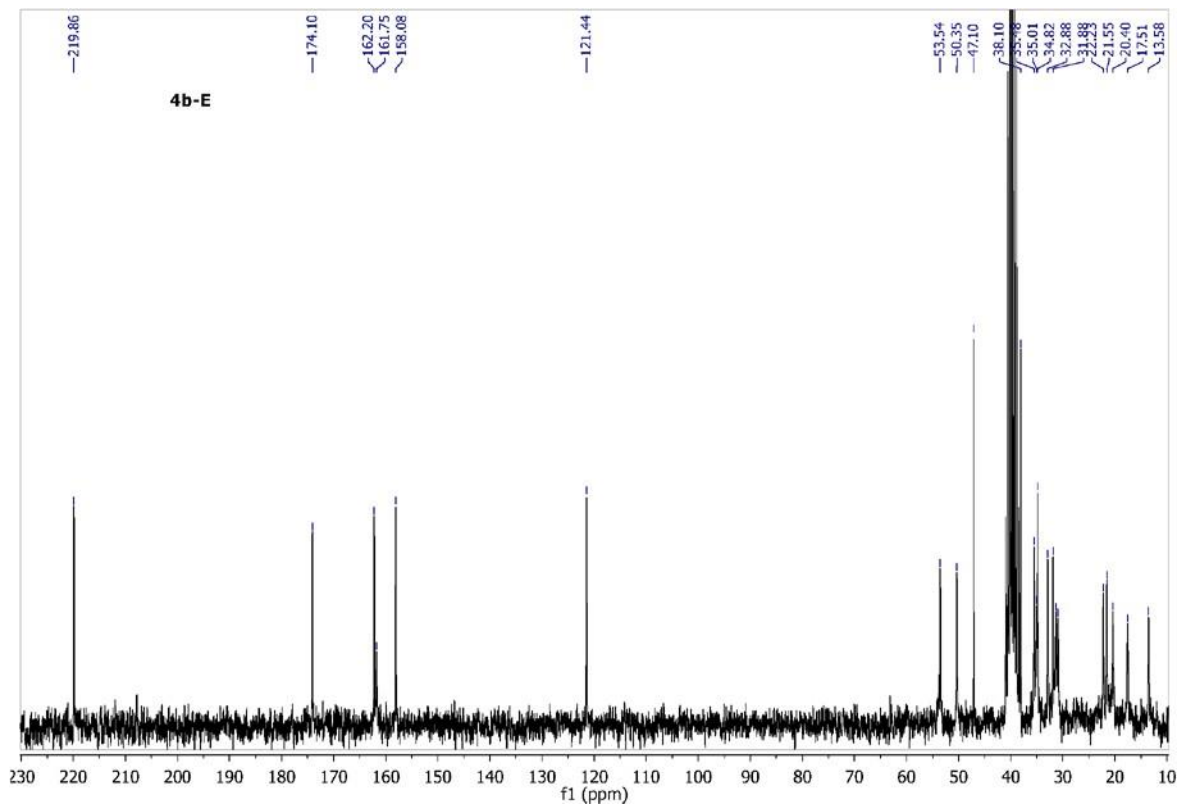




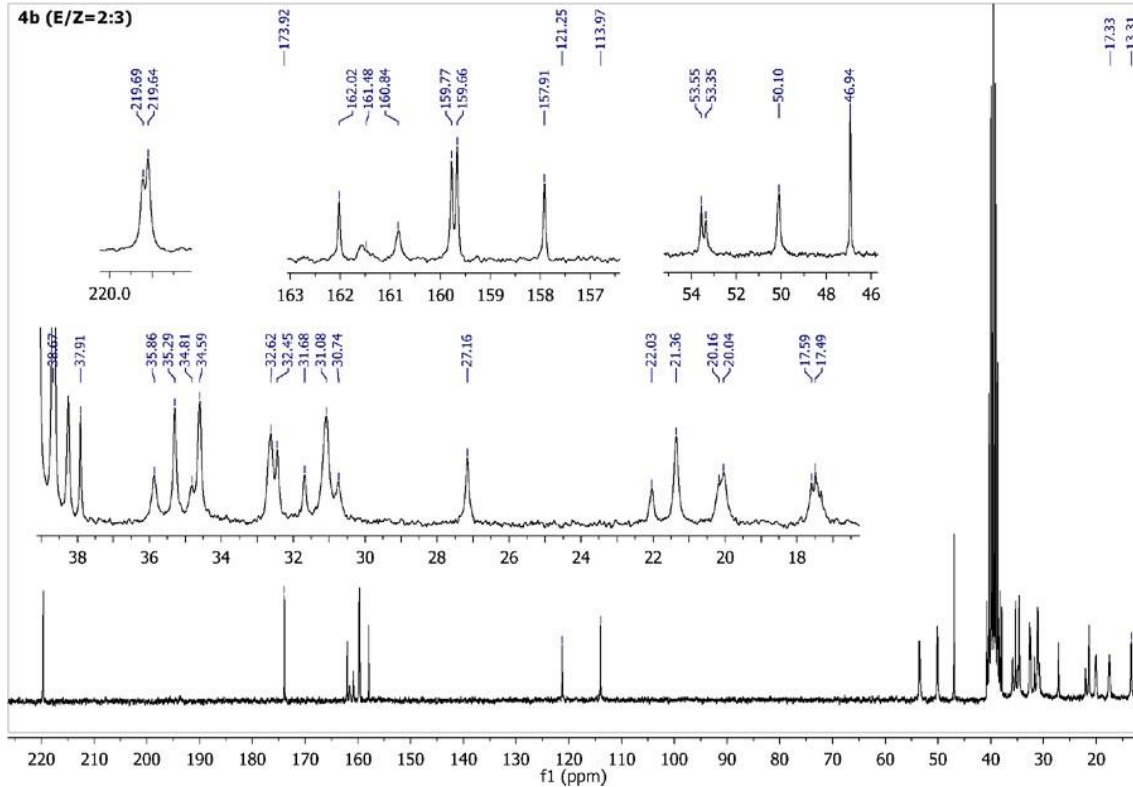


4b (E/Z=9/1)
HMBC

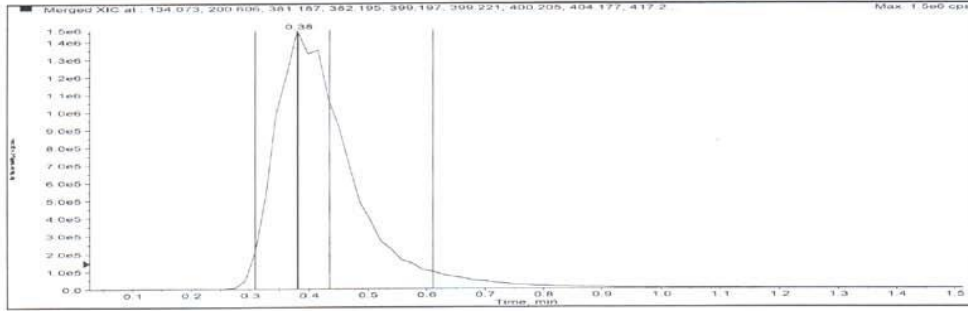




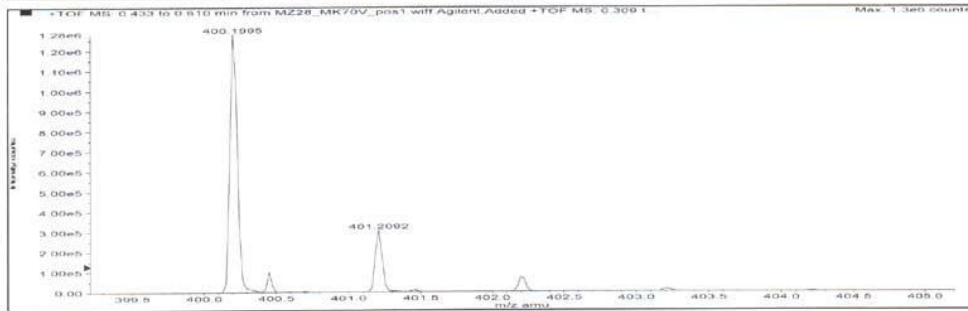
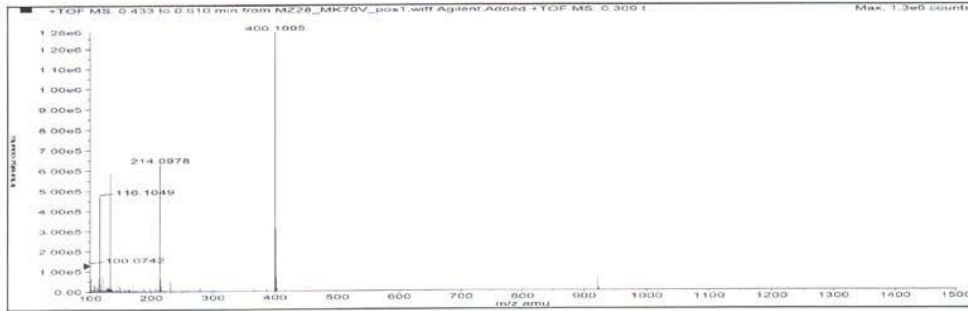
4b (E/Z=2:3)



Sample Name: MZ28 Sample Location: P1-C7 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ28_MK70V_pos1.wiff Acq Time: February 02 2016, 12:12:05 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anm\efc.xml



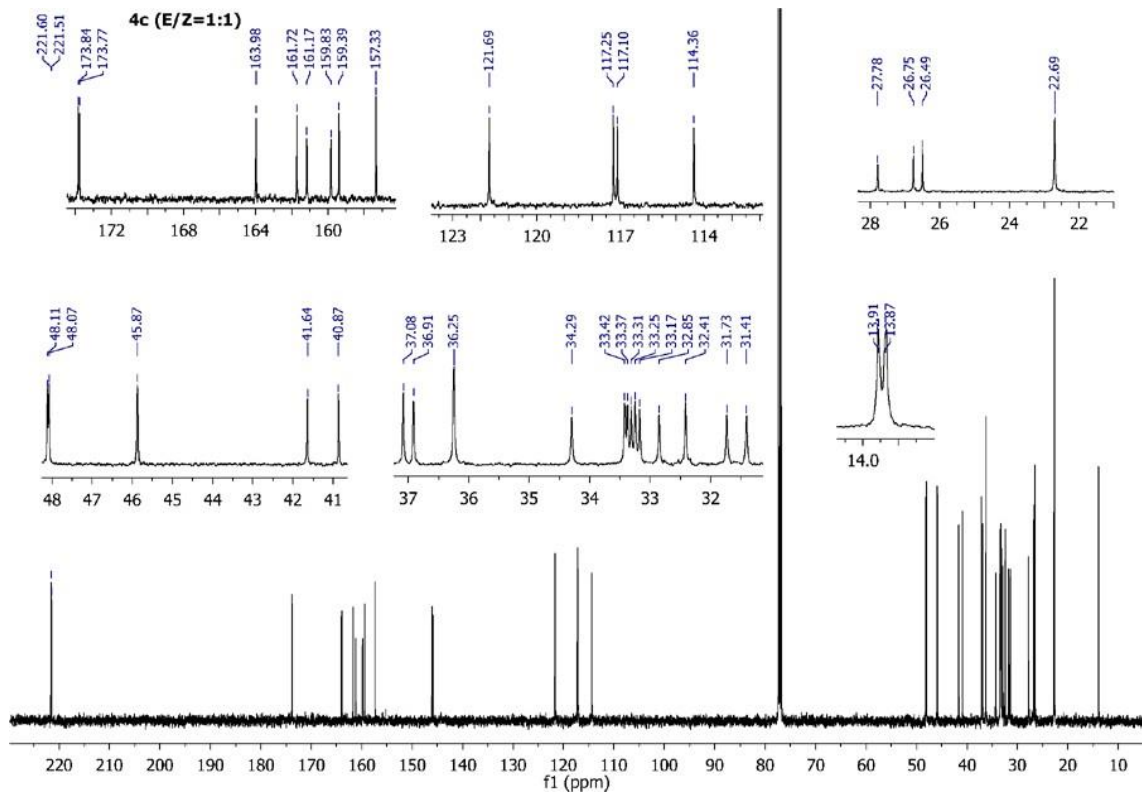
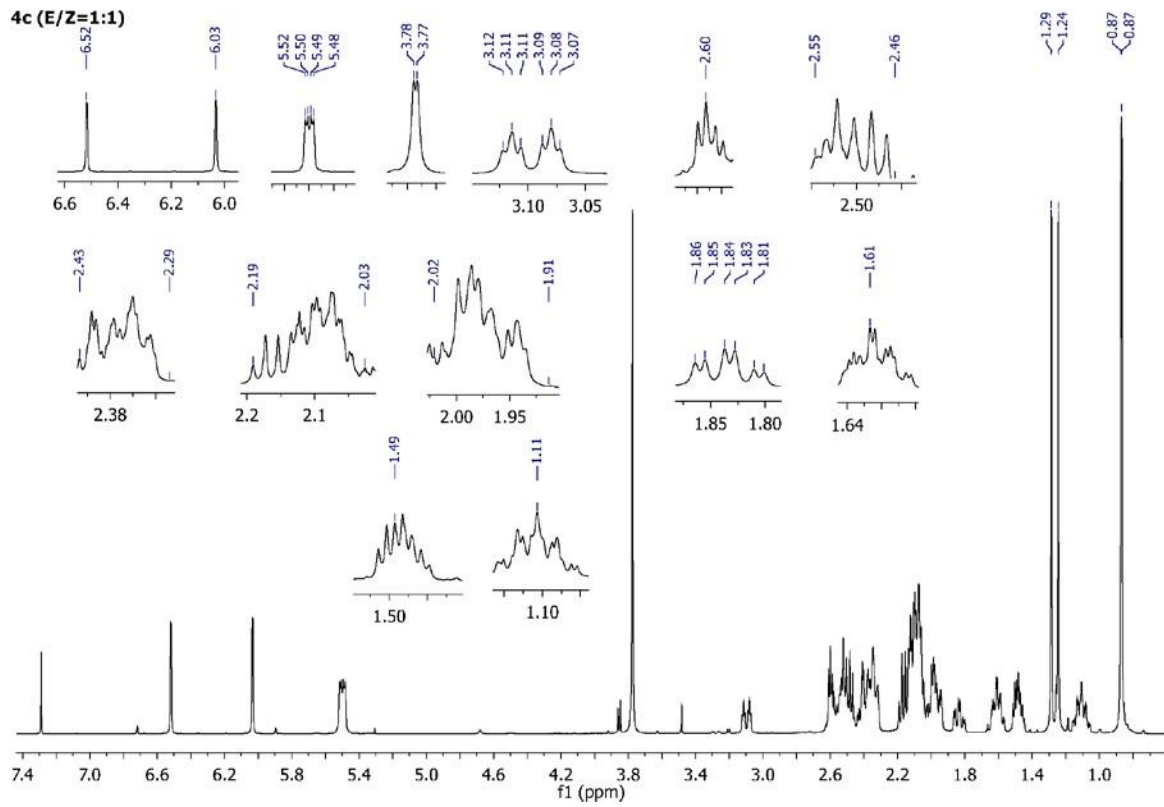
Merged XIC, Period# : 1 Experiment# : 1



| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|-------------|---------------|-----------|---------------|------------|-------------|
| C22H29N3O2S | -- | 399.19805 | 0.38 | 1.27682 E7 | -- |

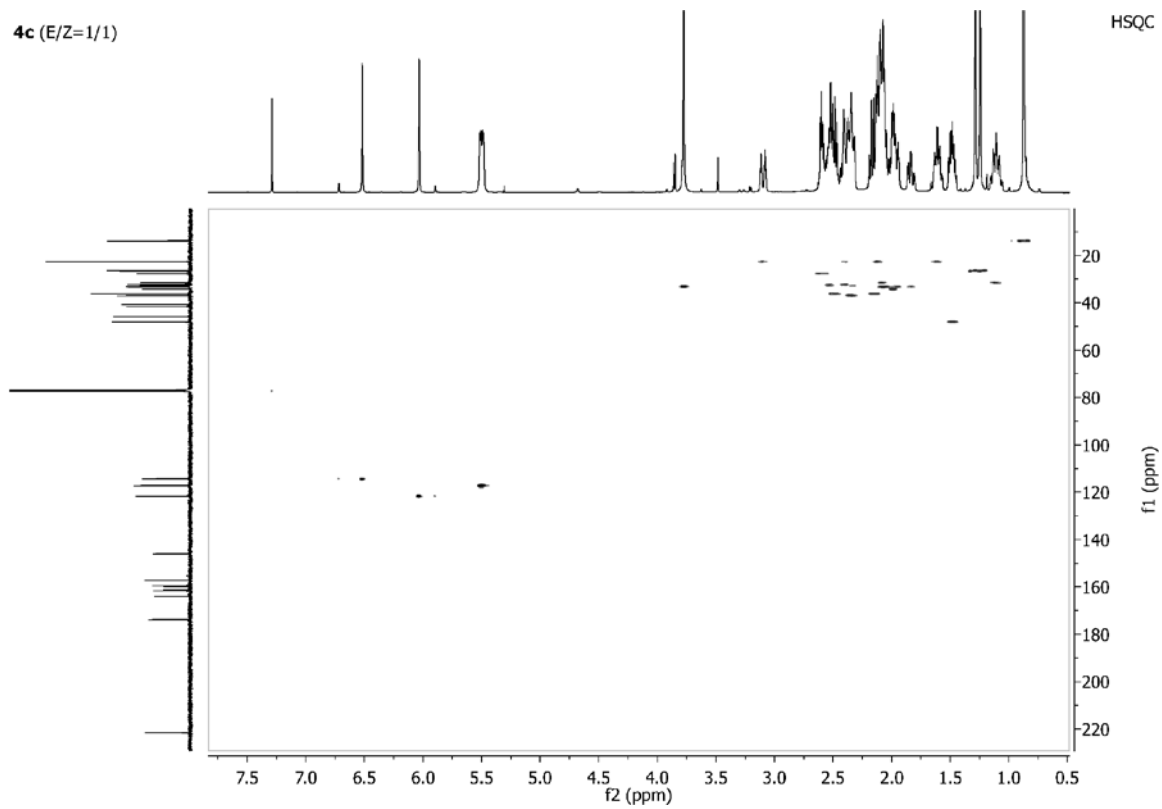
| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|--------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+H] ⁺ | 1305288 12 | 400.20532 | 400.20549 | 0.16967 | 0.42 | -- |

4c (E/Z=1:1)



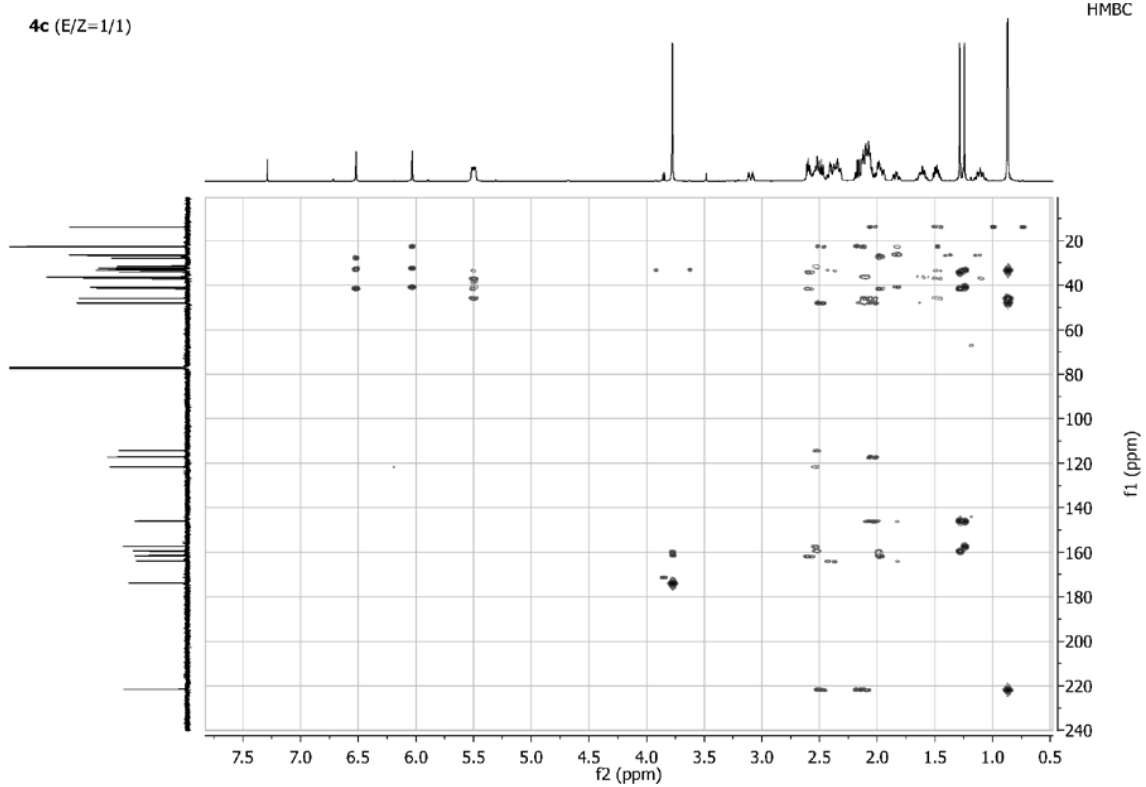
4c (E/Z=1/1)

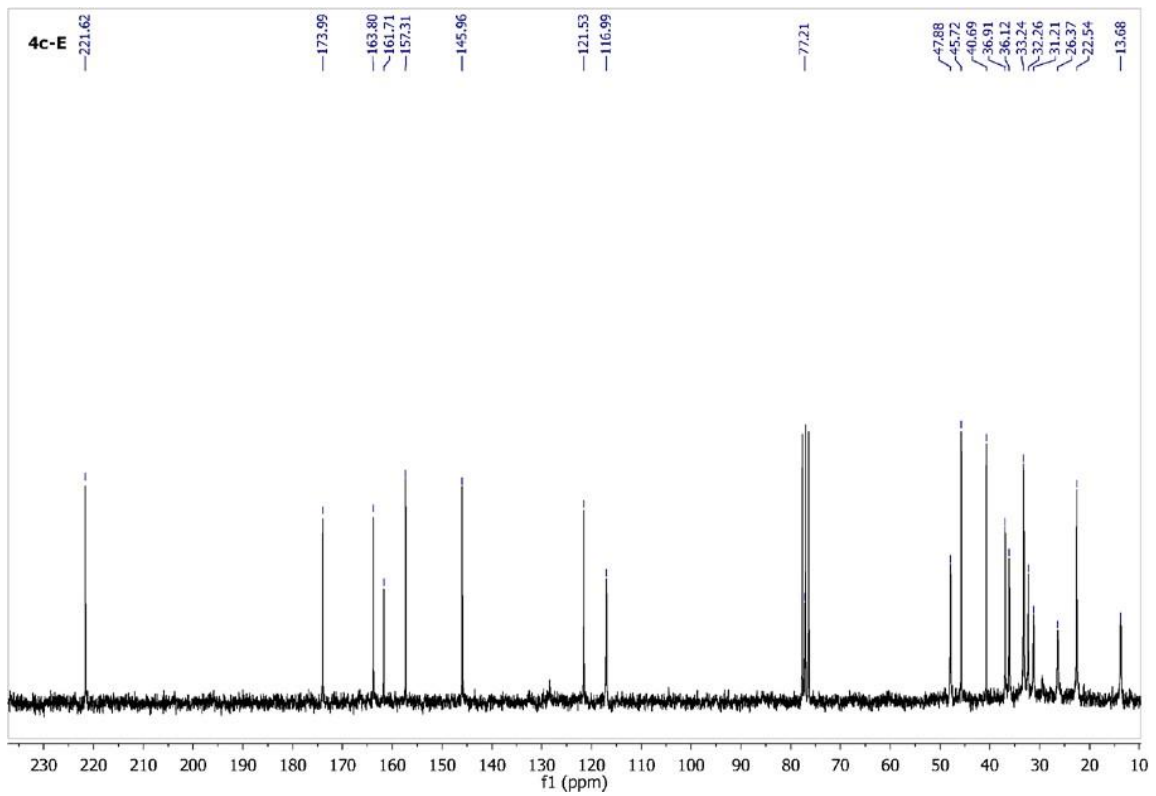
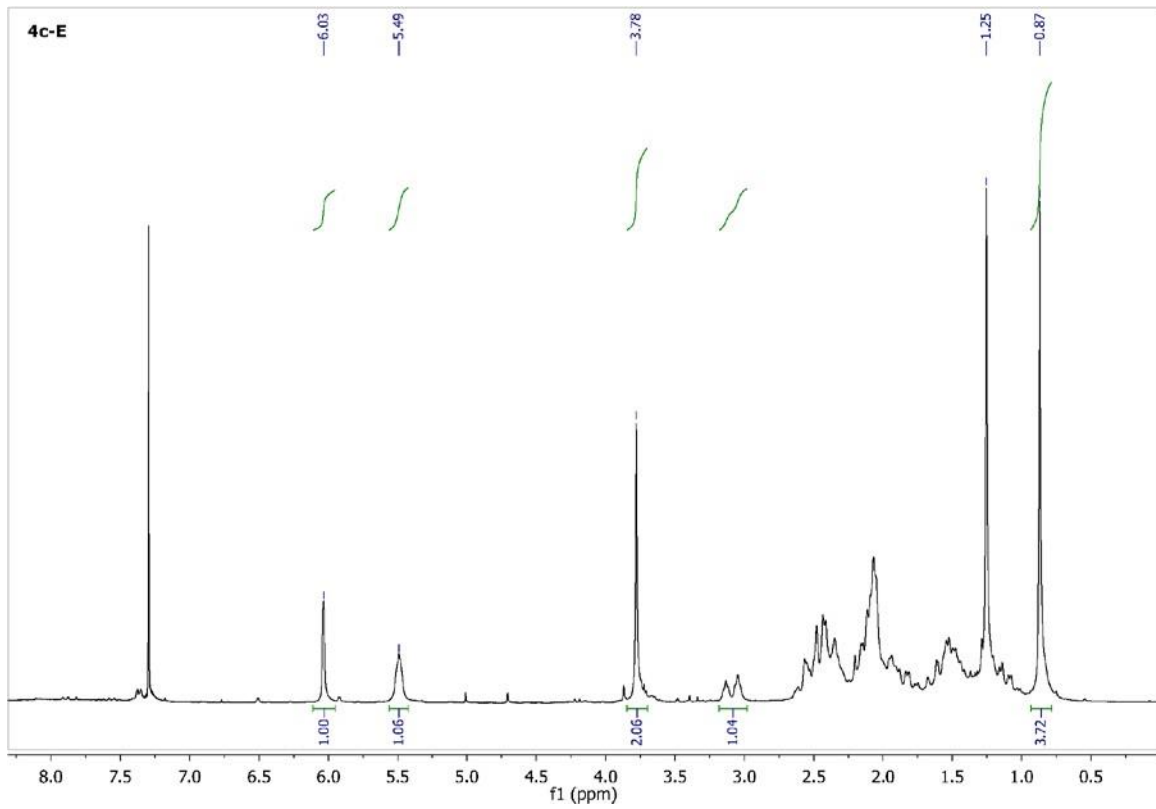
HSQC

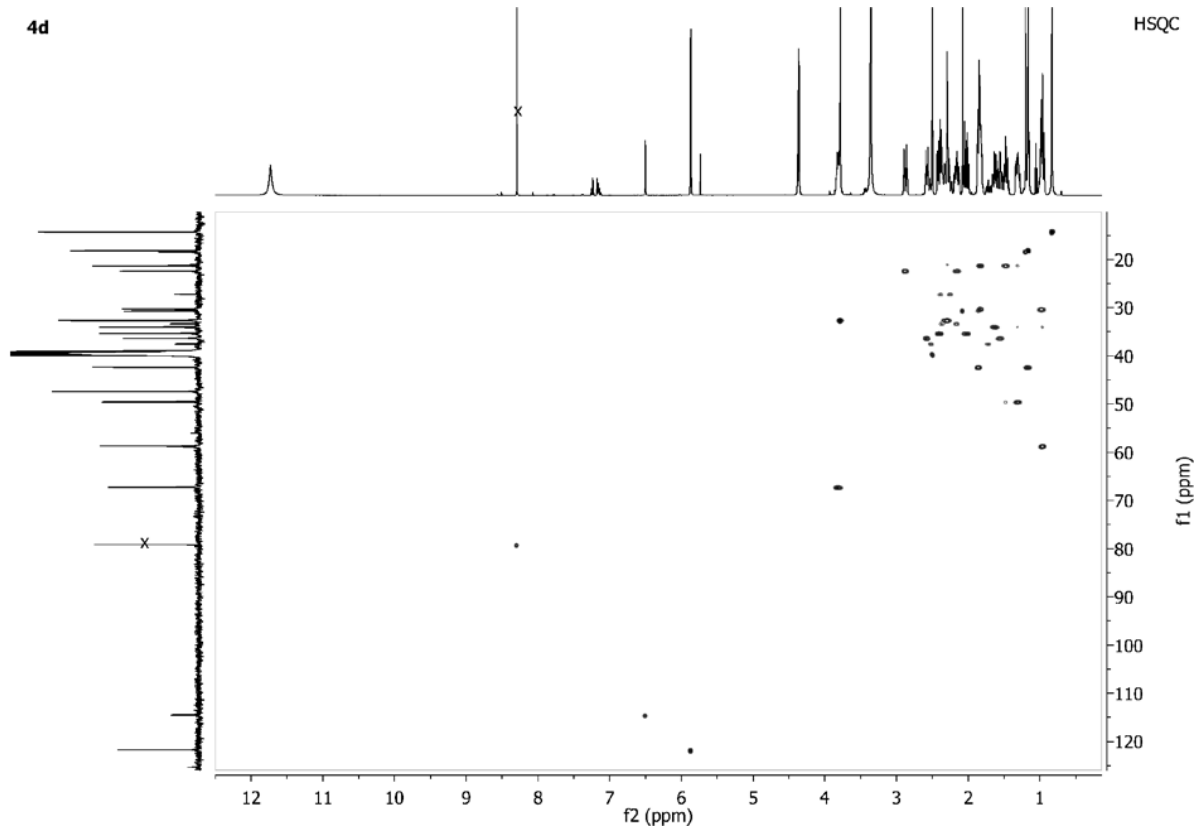
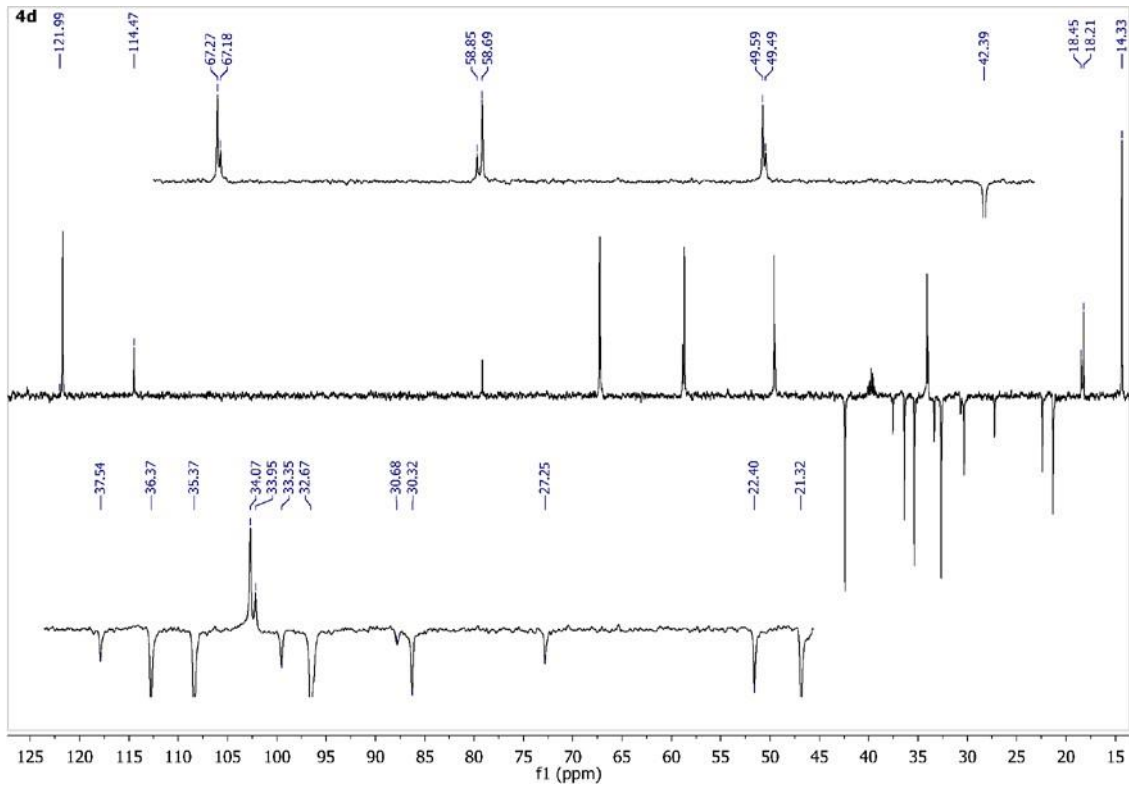


4c (E/Z=1/1)

HMBC

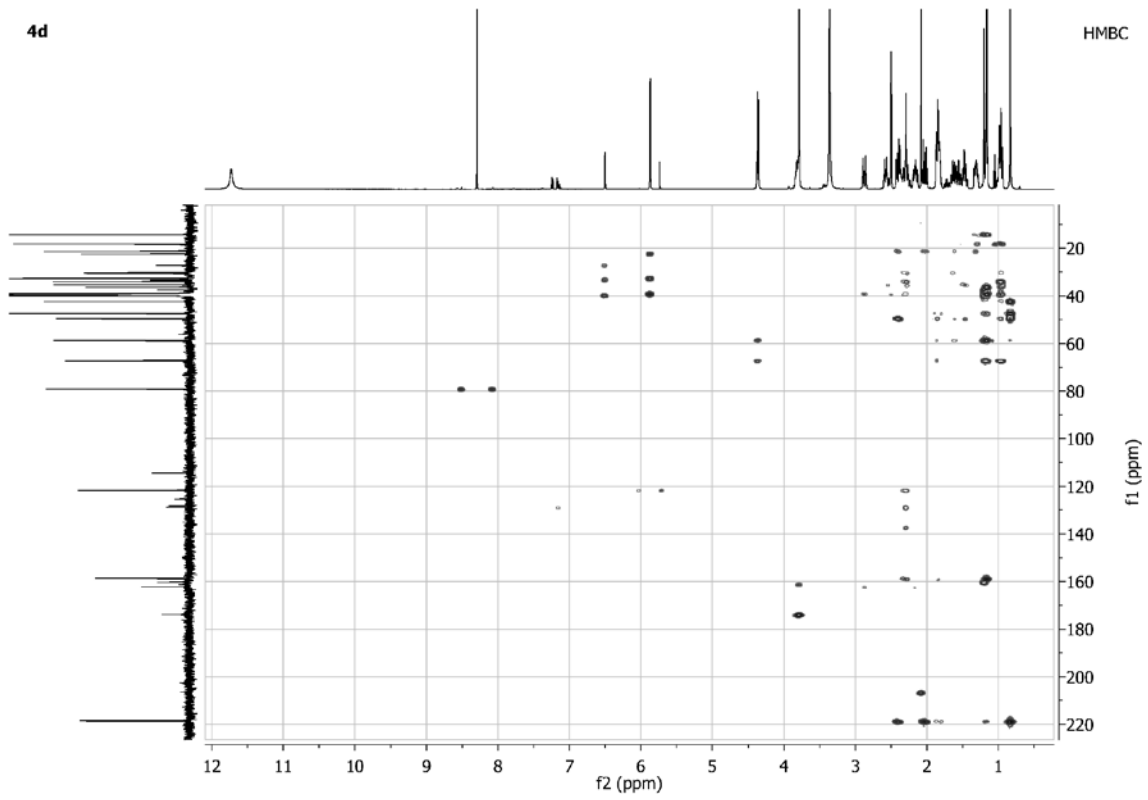






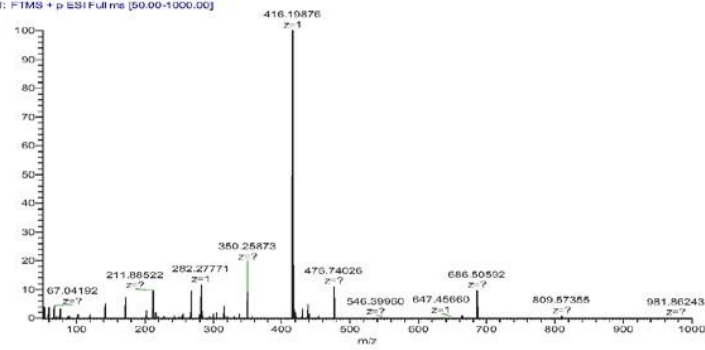
4d

HMBC

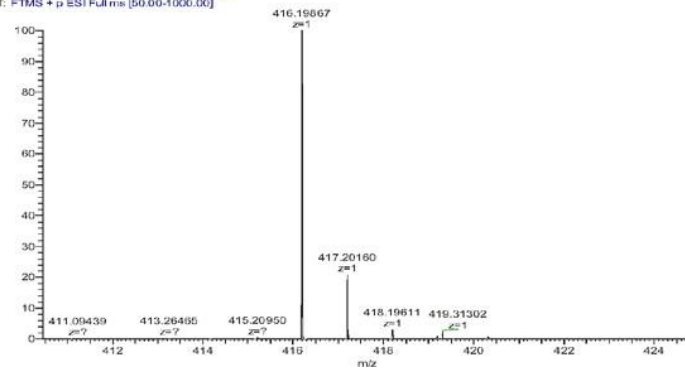


OB5028 1 ug/mL MZ44 in MeOH

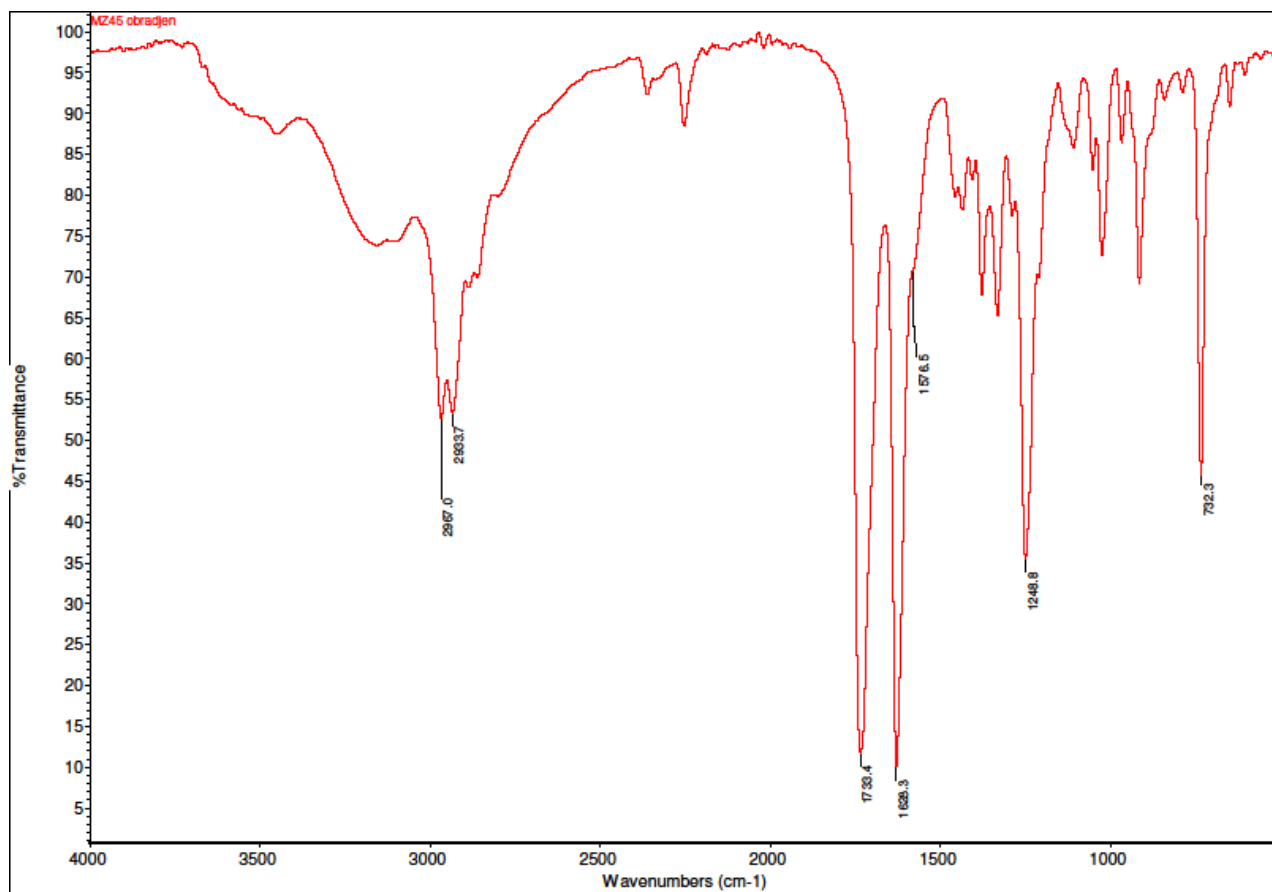
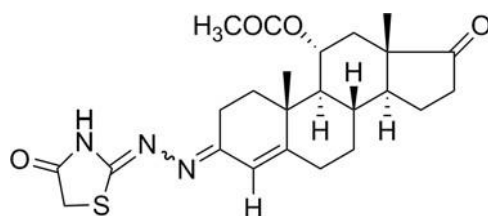
OB5028 #11 RT: 0.08 AV: 1 NL: 2.73E7
T: FTMS + p ESI Full ms [50.00-1000.00]

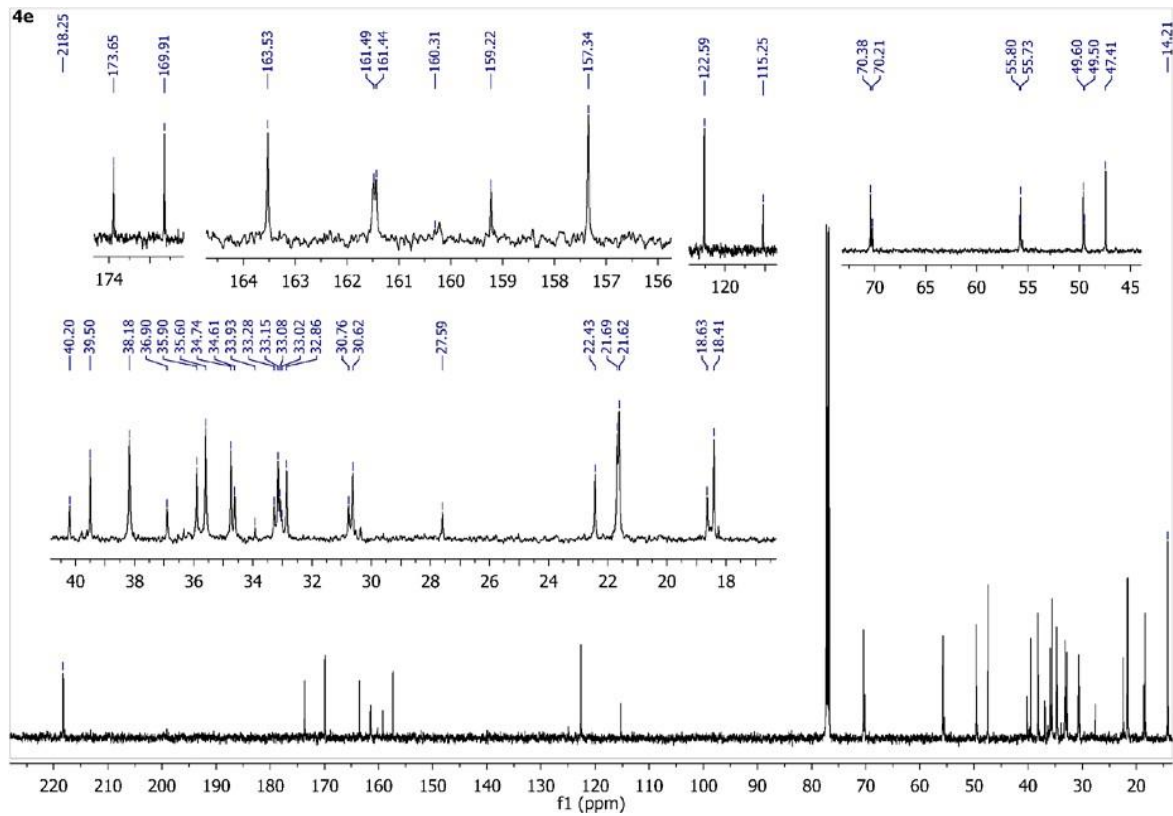
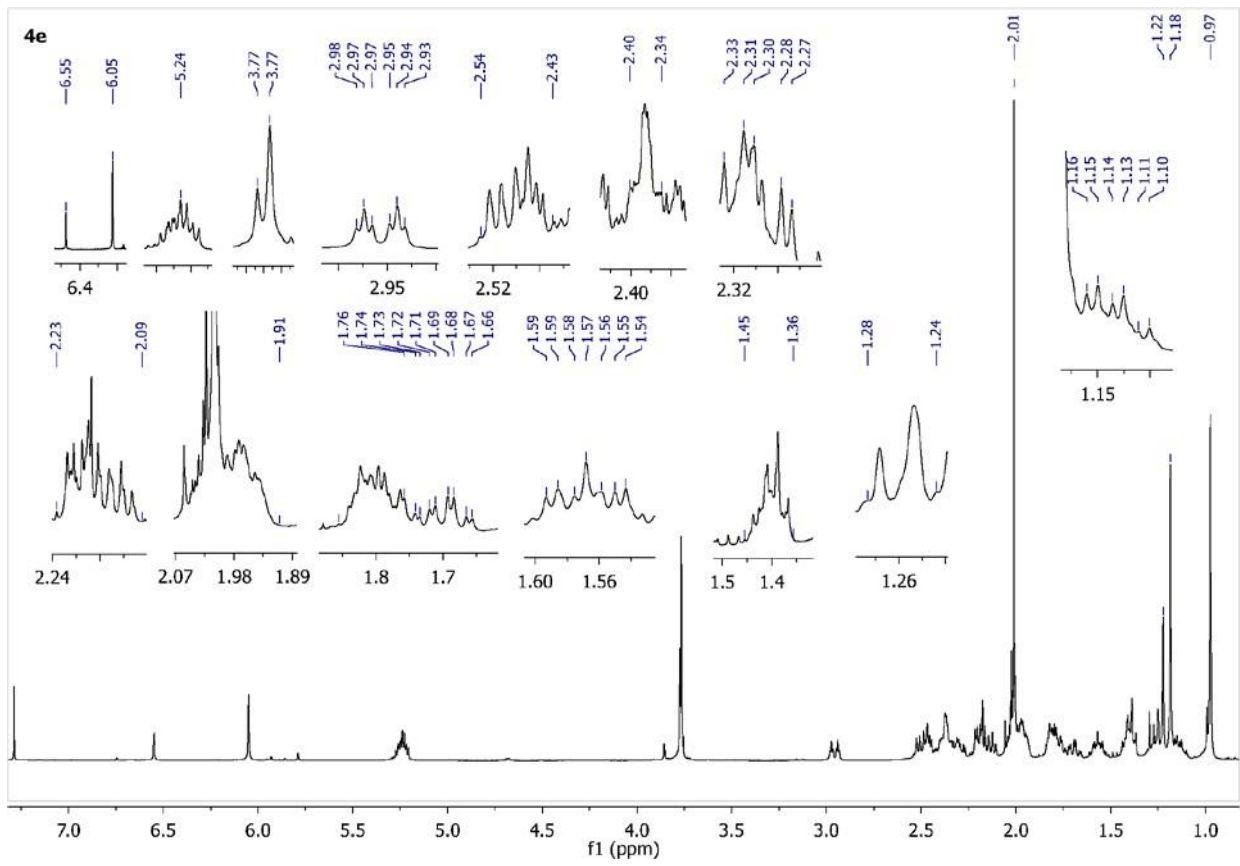


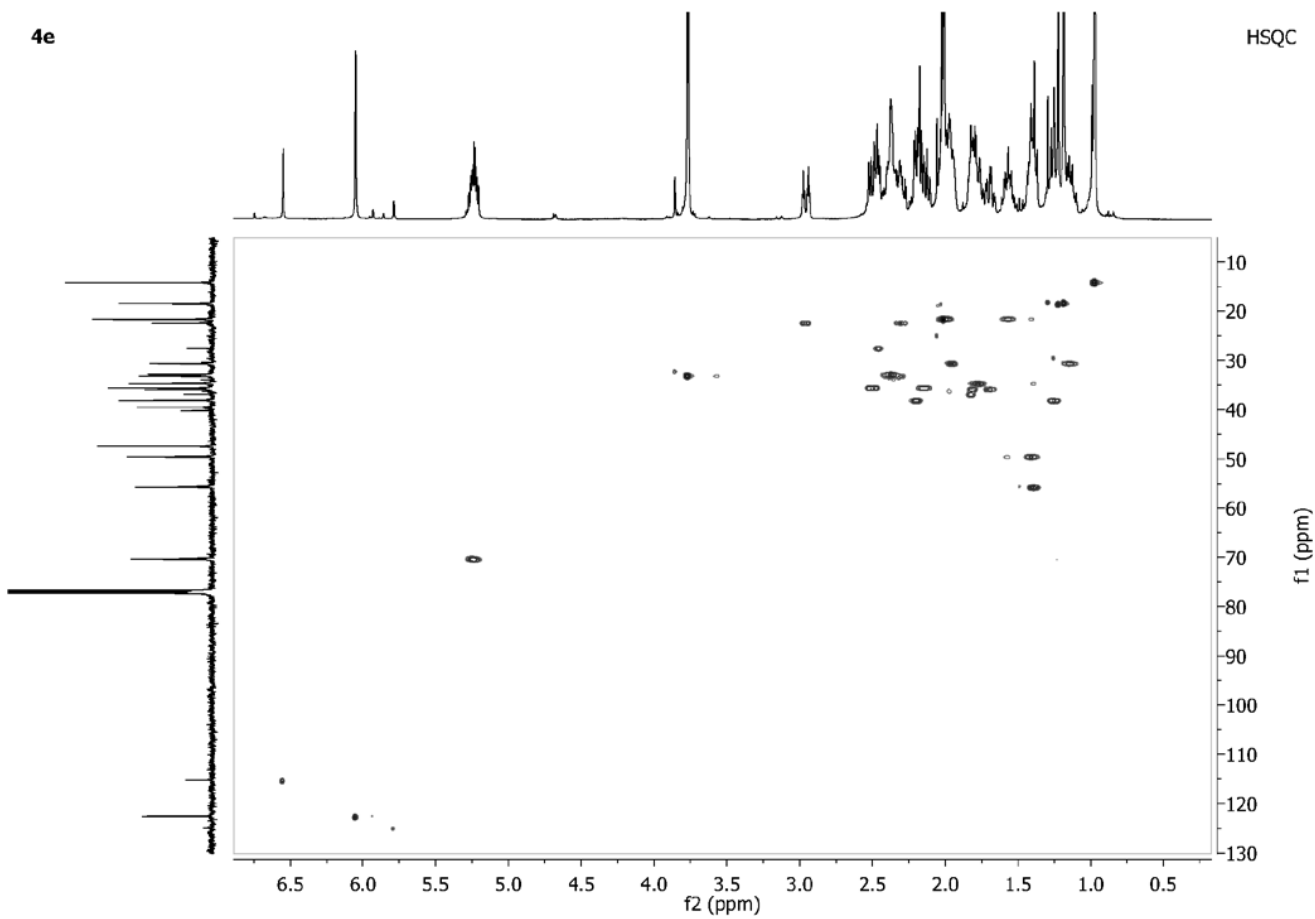
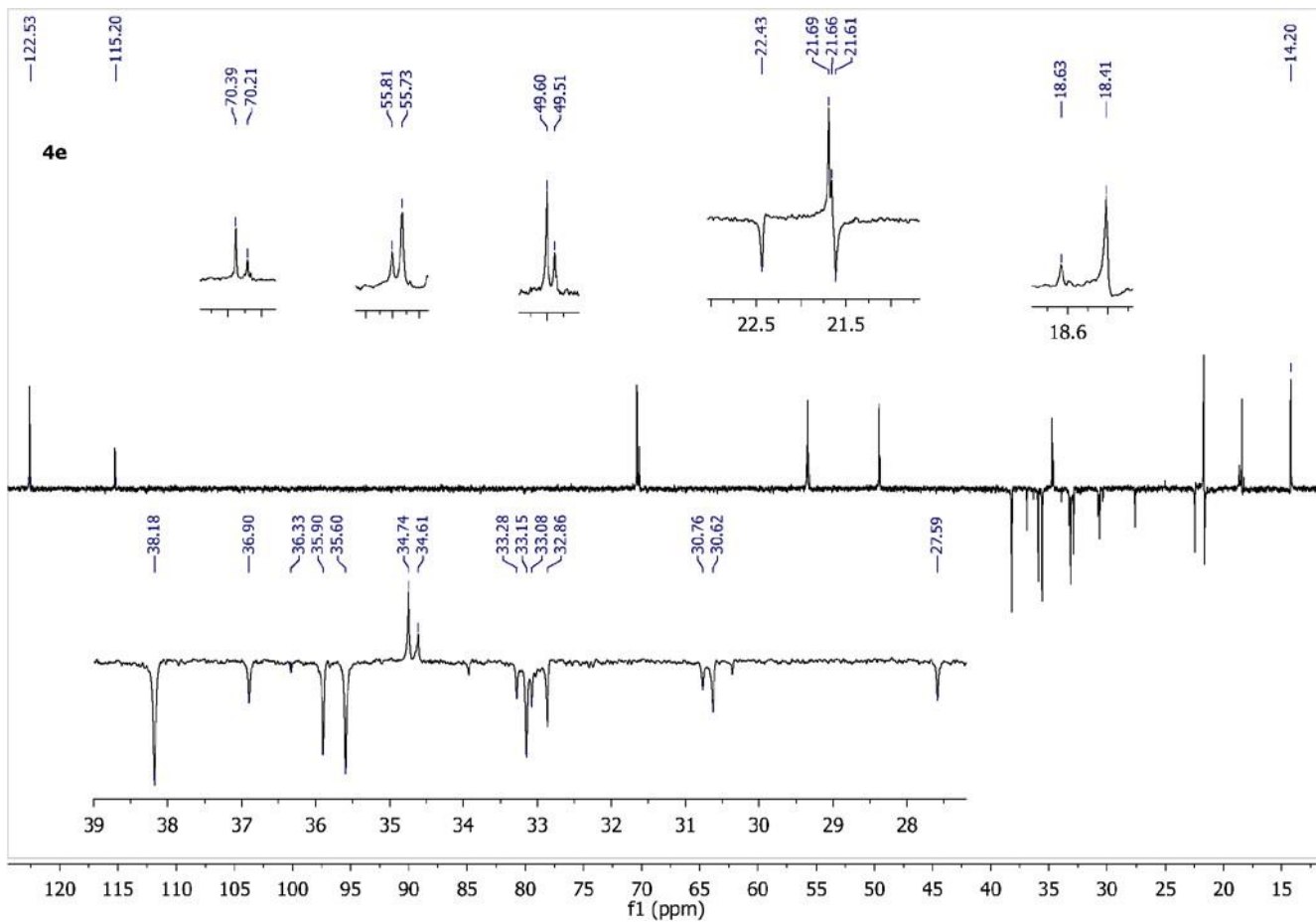
OB5028 #44 RT: 0.36 AV: 1 NL: 3.04E7
T: FTMS + p ESI Full ms [50.00-1000.00]



Compound 4e

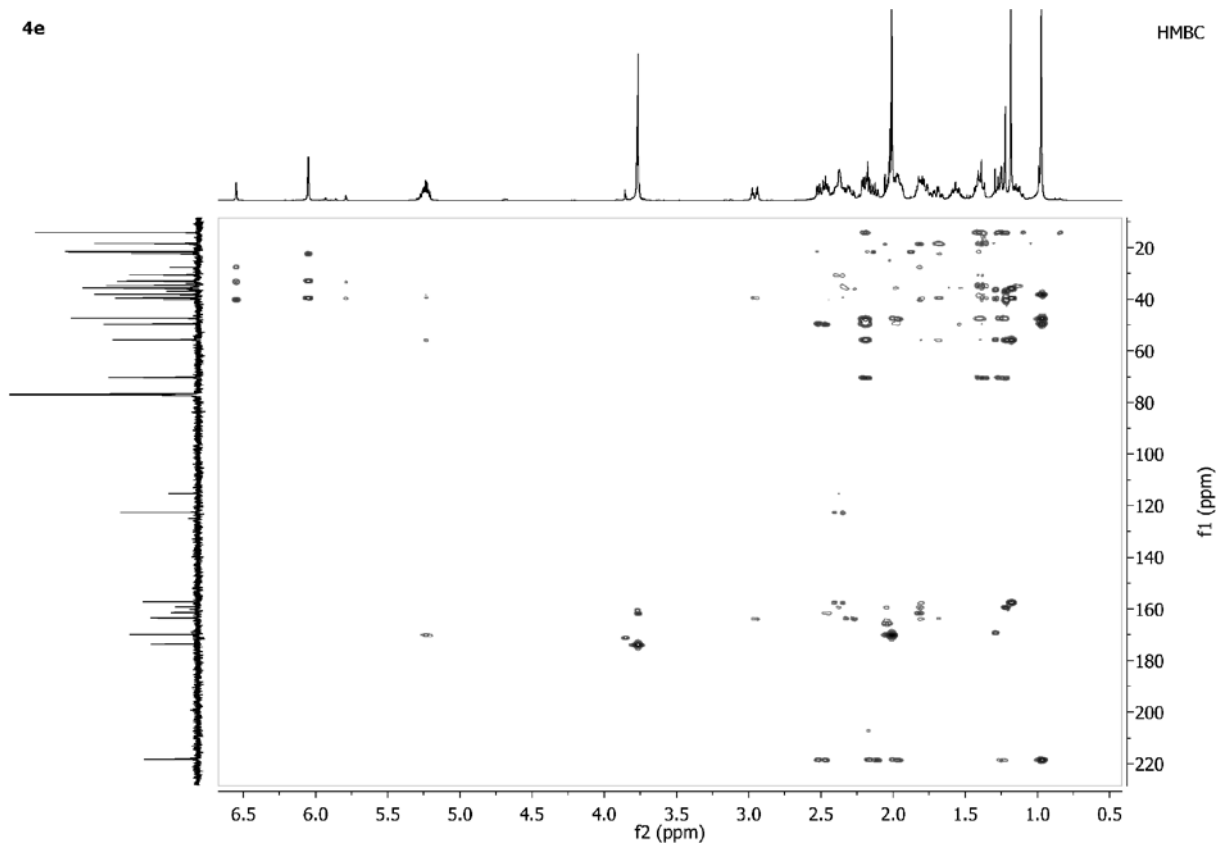




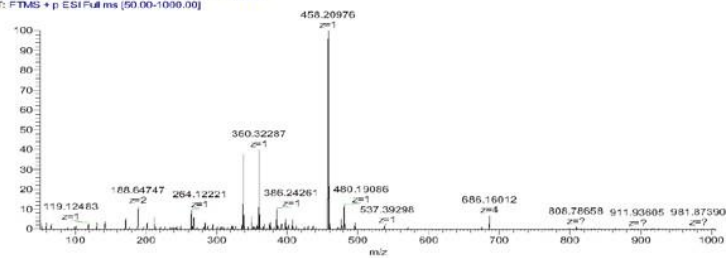


4e

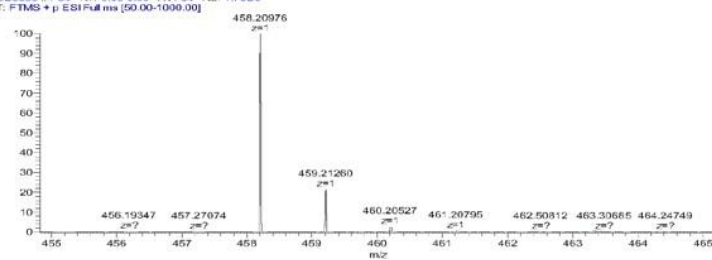
HMBC



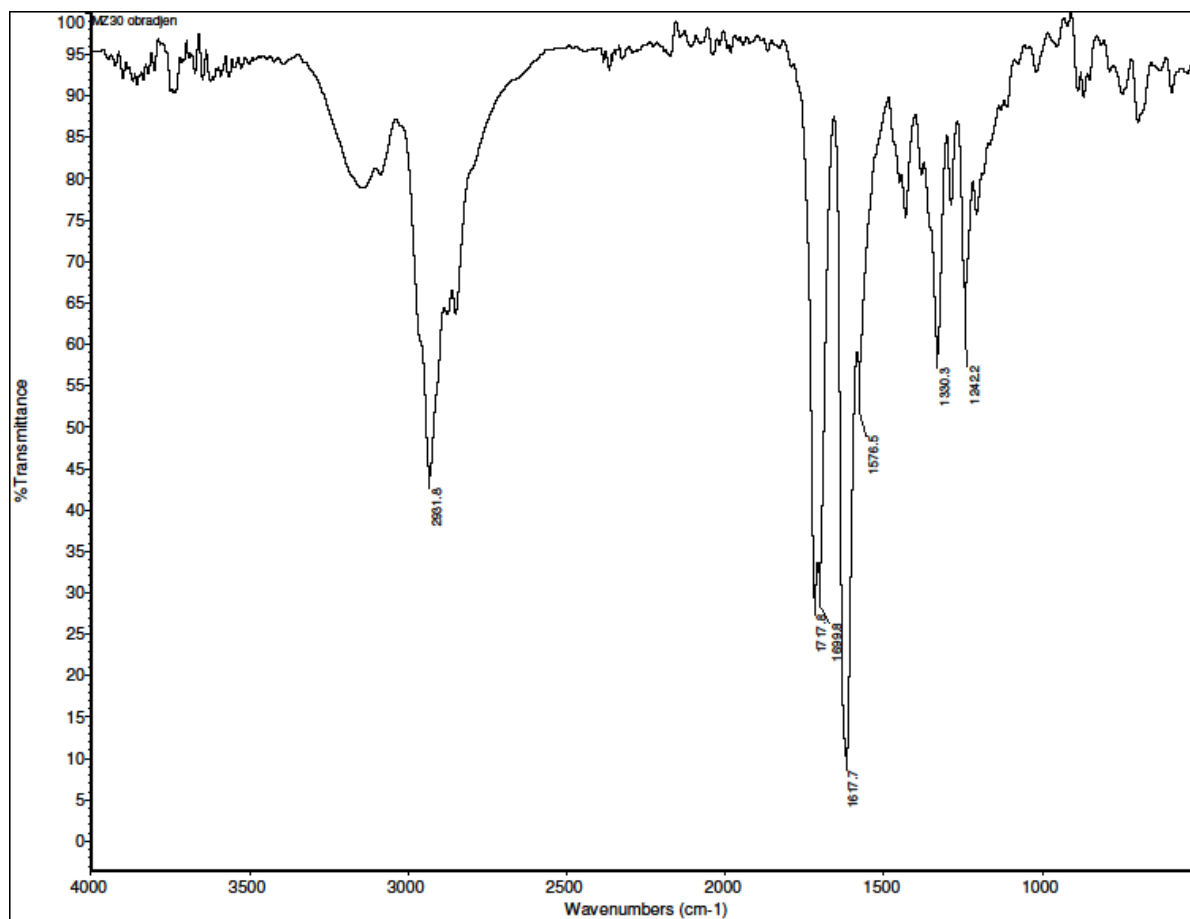
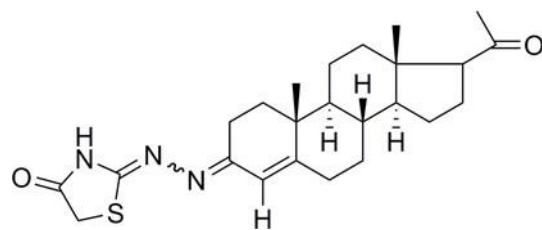
OB5055 MZ45 in MeOH
 OB5055 #1-54 RT: 0.00-0.50 AV: 54 NL: 1.76E6
 T: FTMS + p ESIFull.ms [50.00-1000.00]



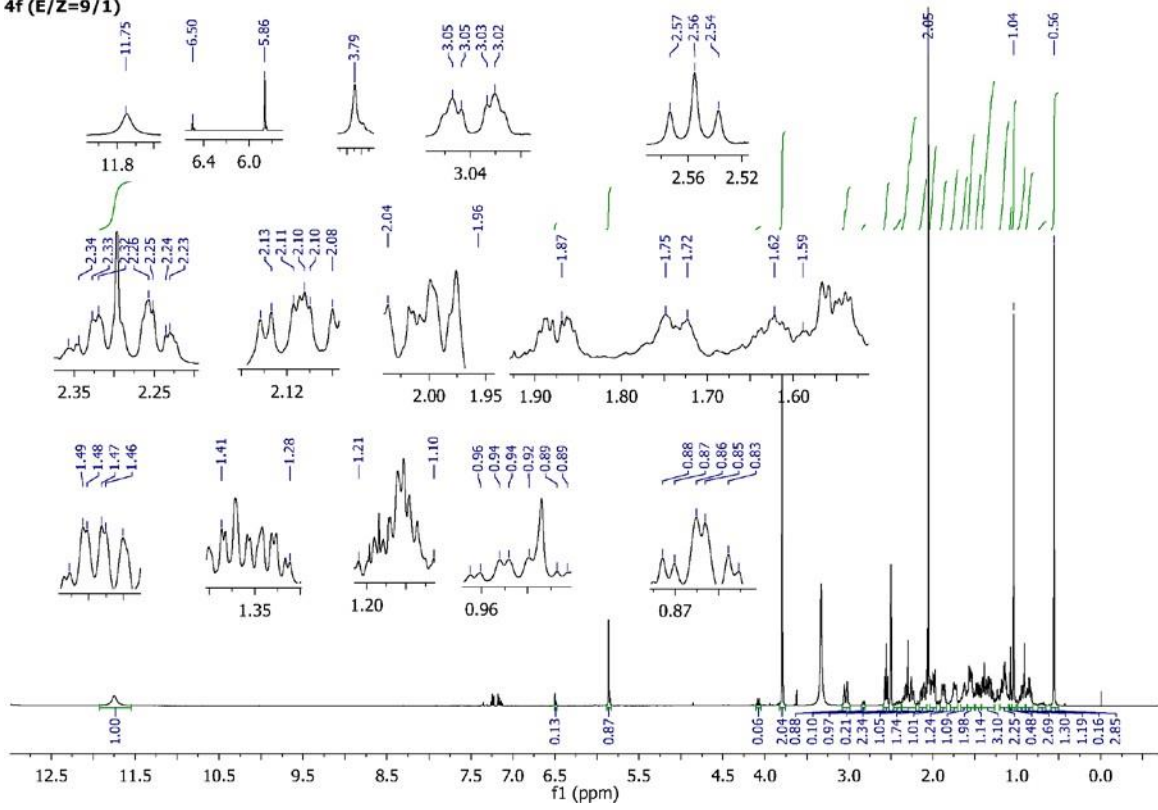
OB5055 #1-54 RT: 0.00-0.50 AV: 54 NL: 1.76E6
 T: FTMS + p ESIFull.ms [50.00-1000.00]



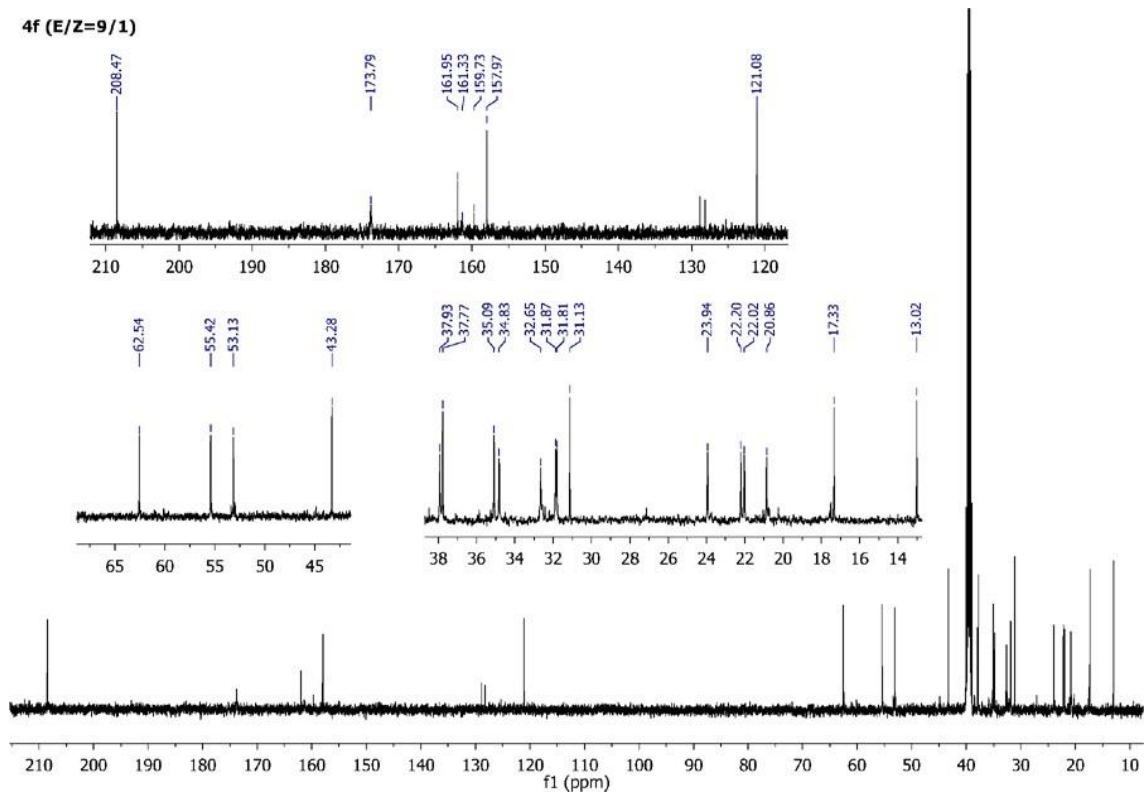
Compound 4f



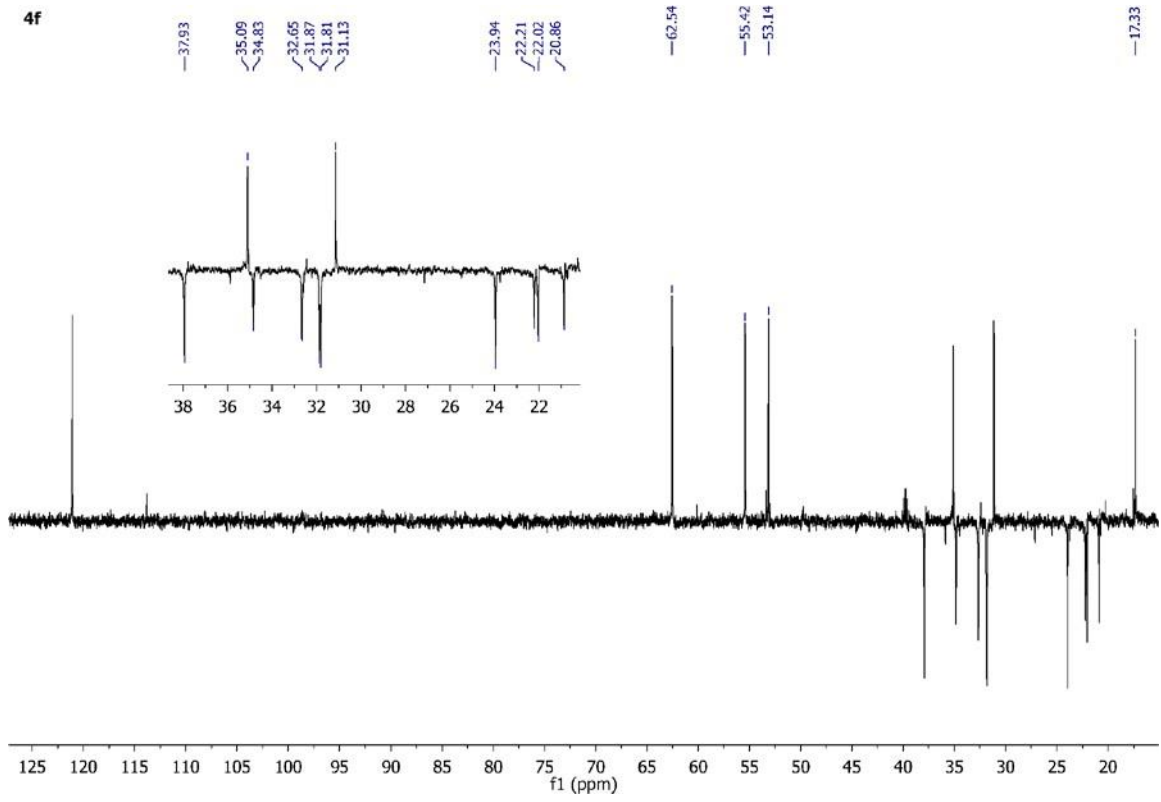
4f (E/Z=9/1)



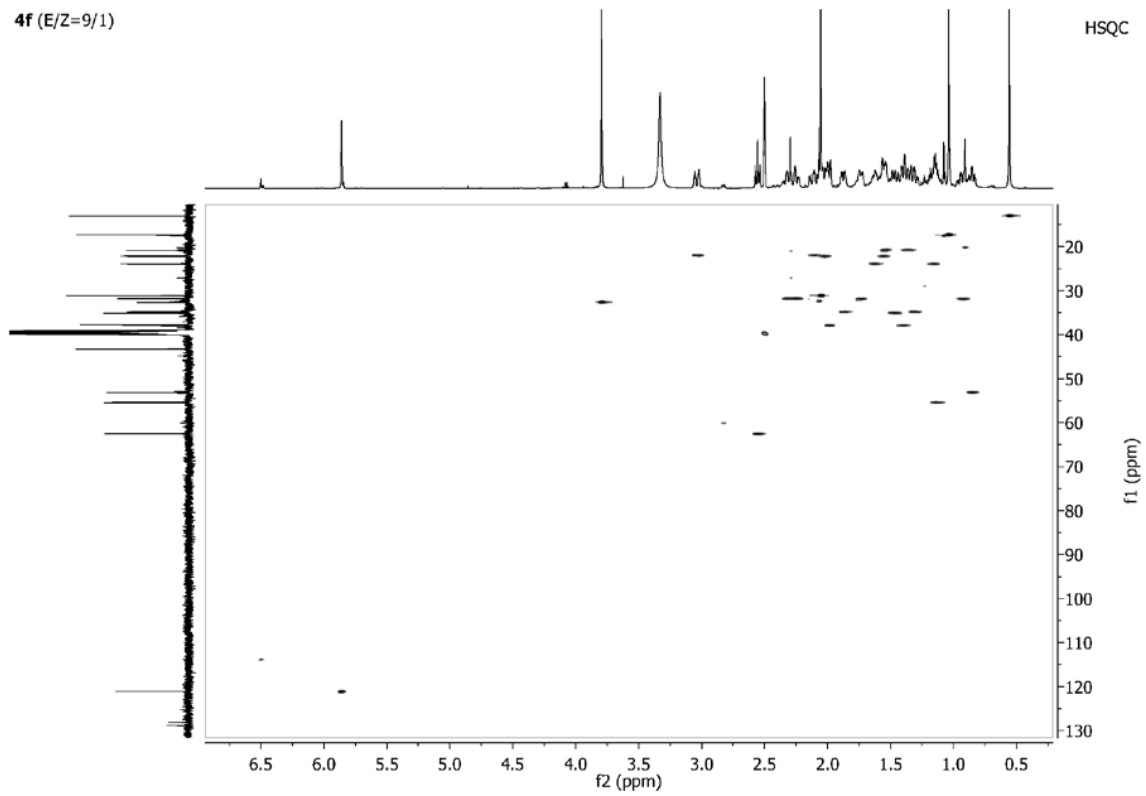
4f (E/Z=9/1)



4f

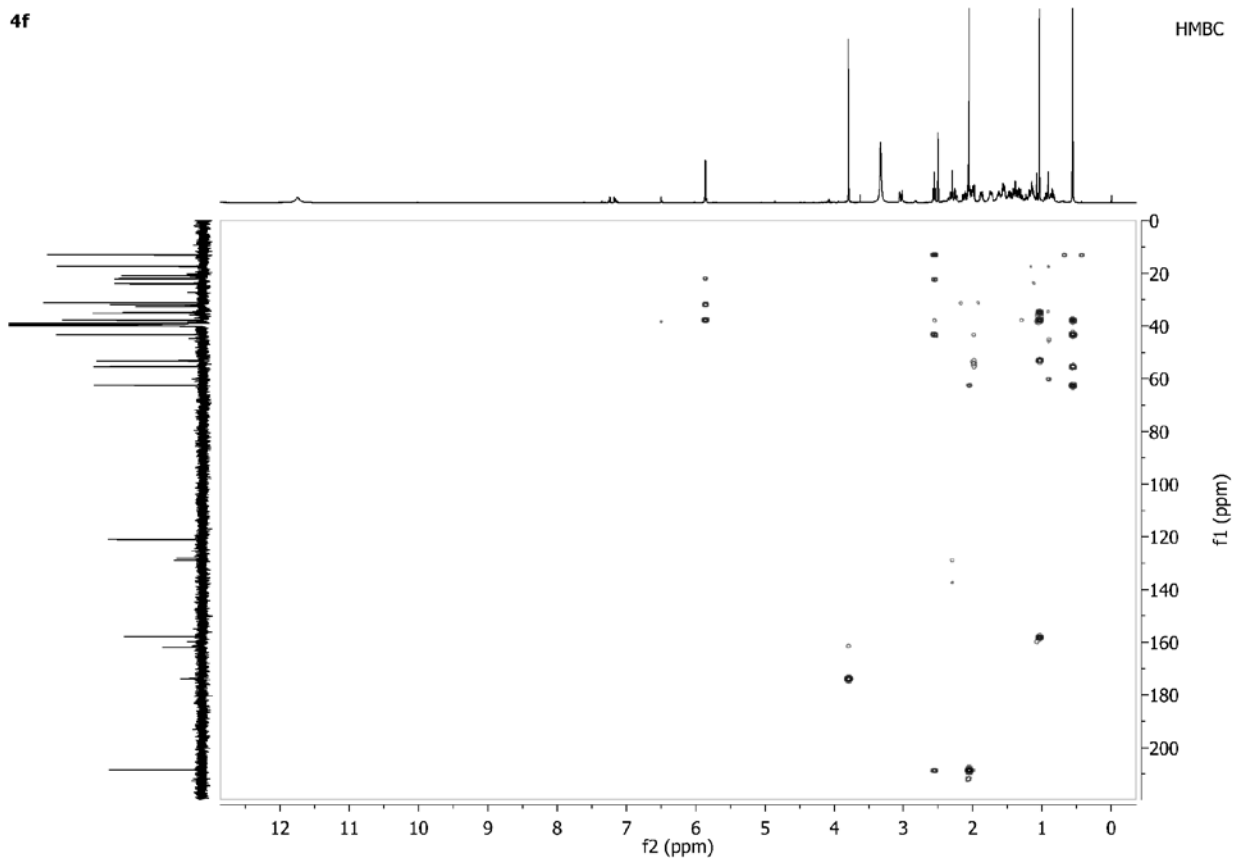


4f (E/Z=9/1)

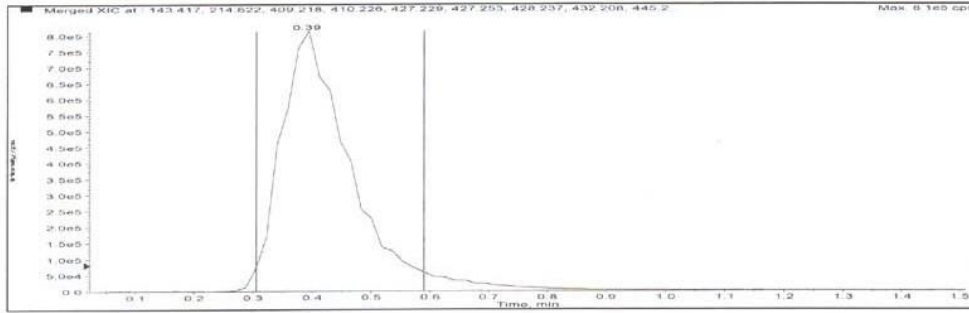


4f

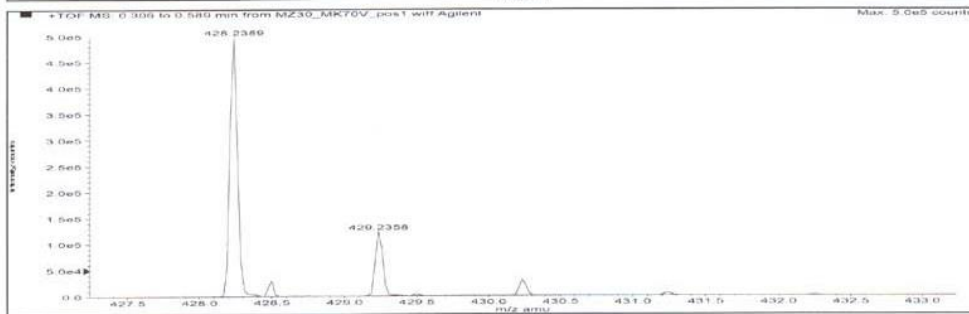
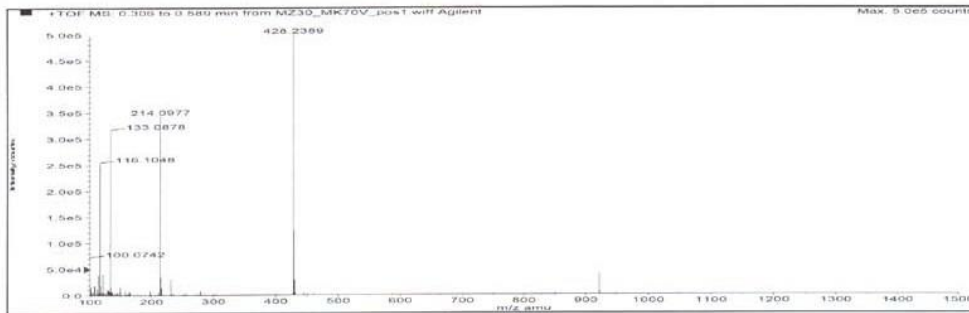
HMBC



Sample Name: MZ30 Sample Location: P1-C9 Sample Id: Operator: Milka
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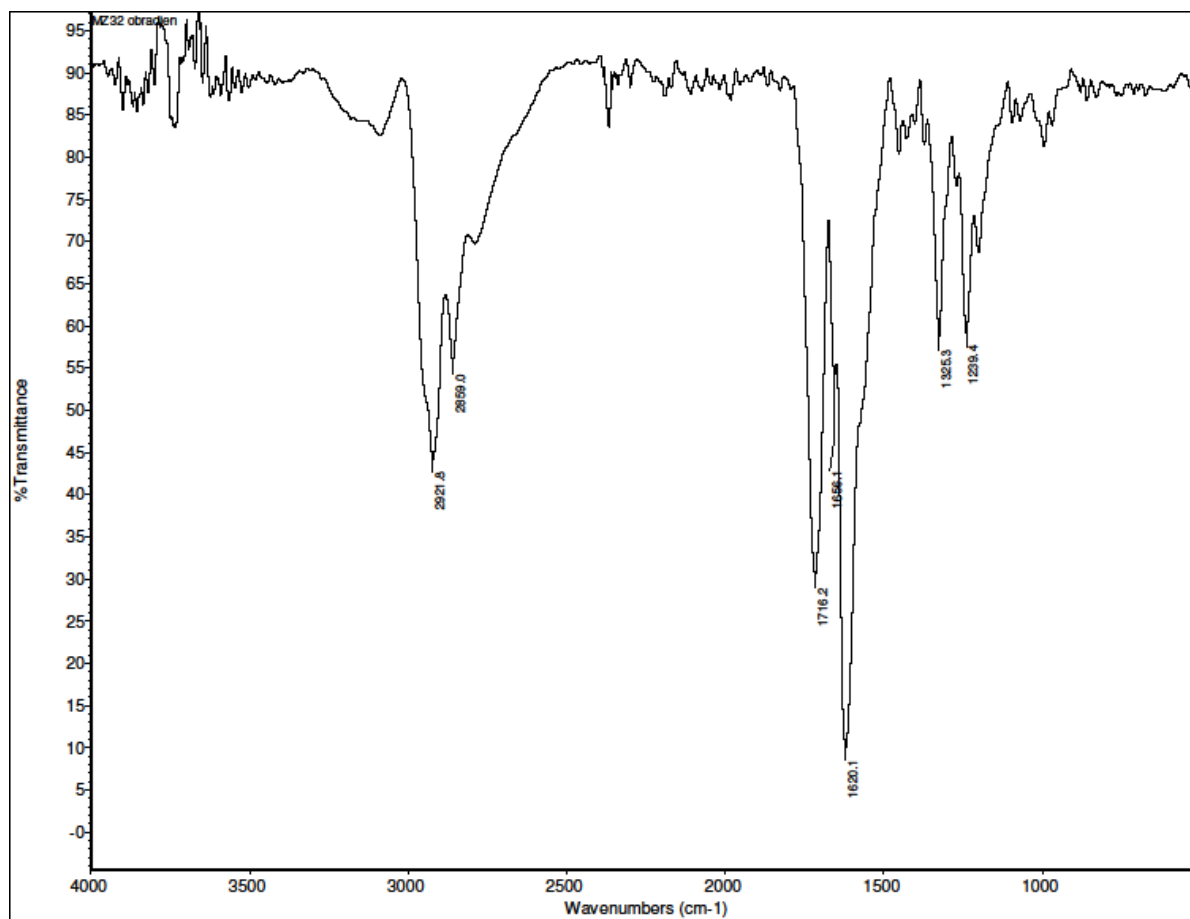
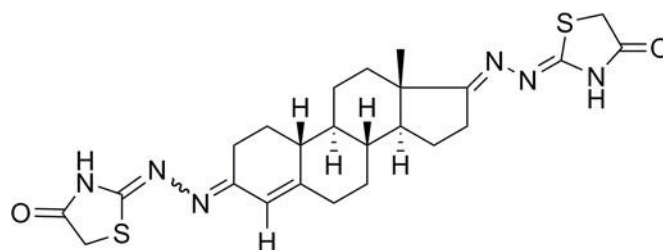
Merged XIC, Period# : 1 Experiment# : 1

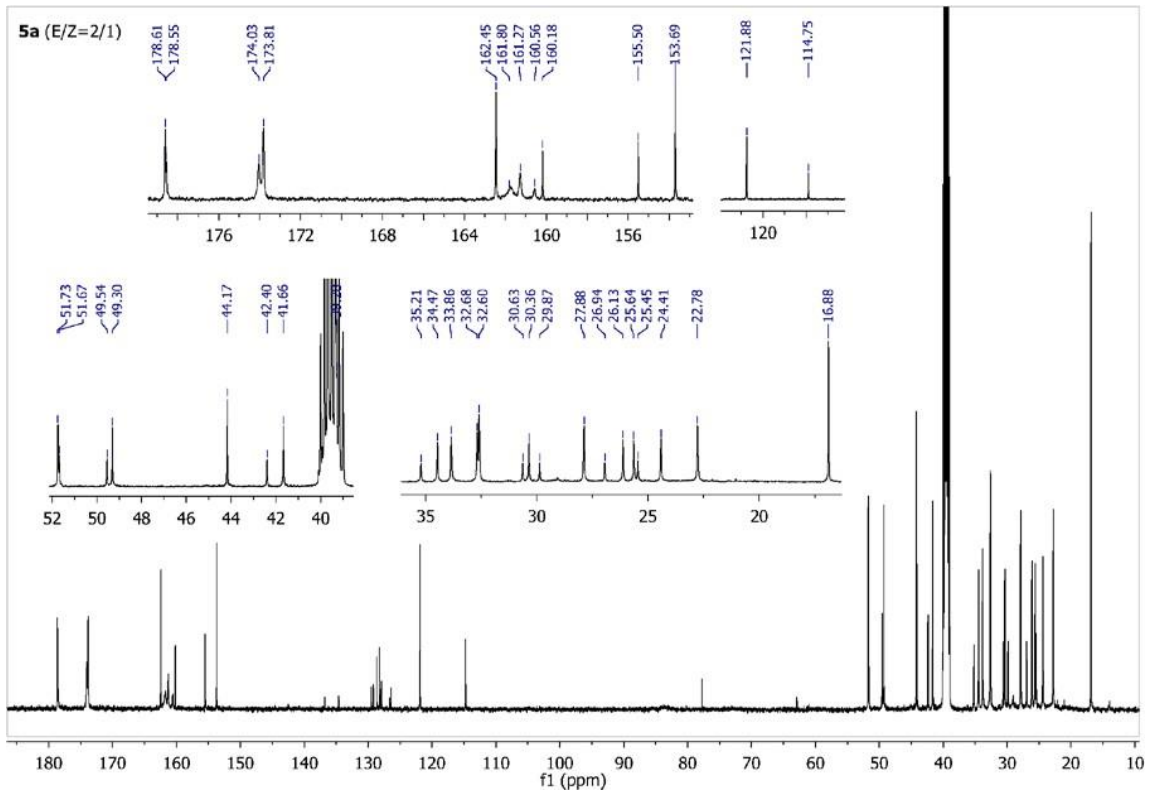
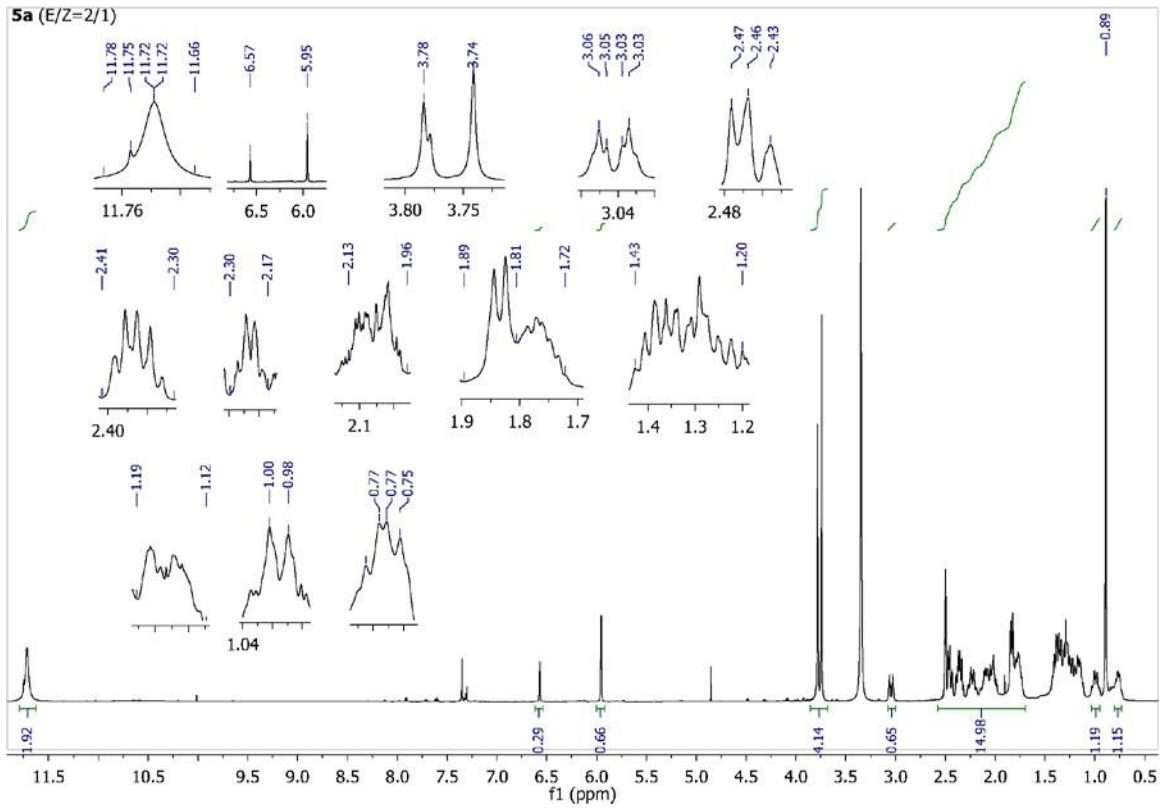


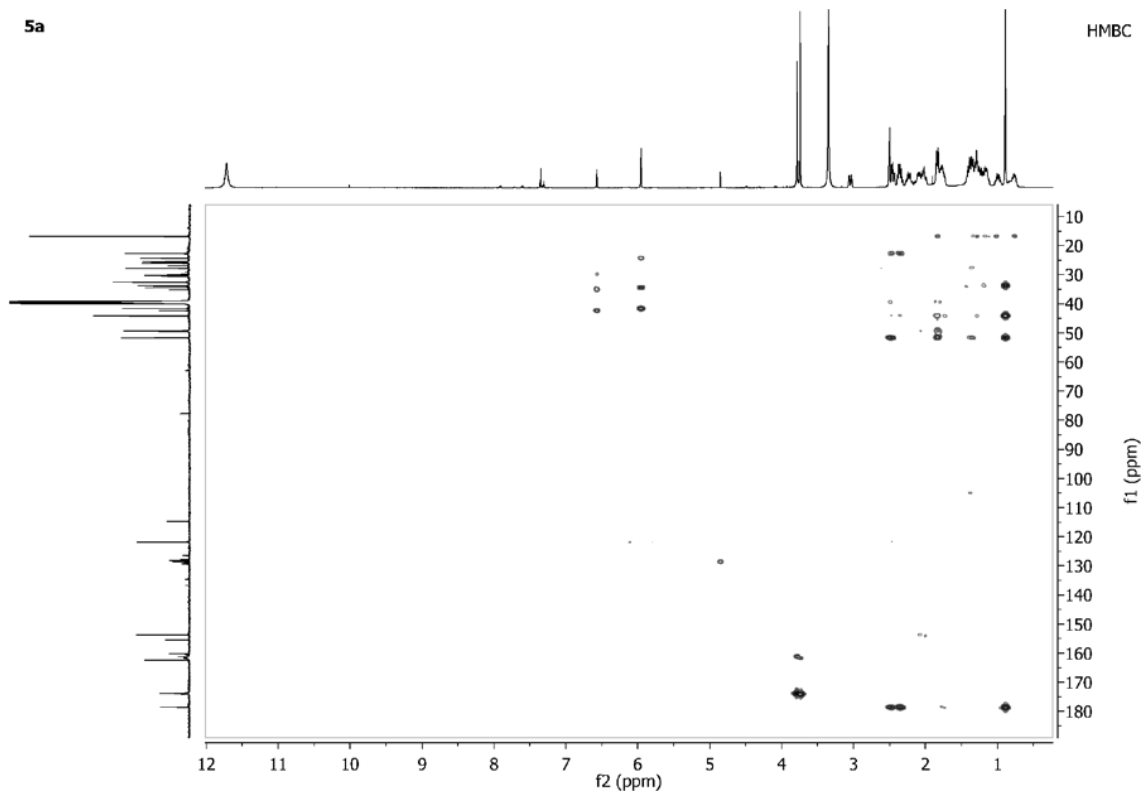
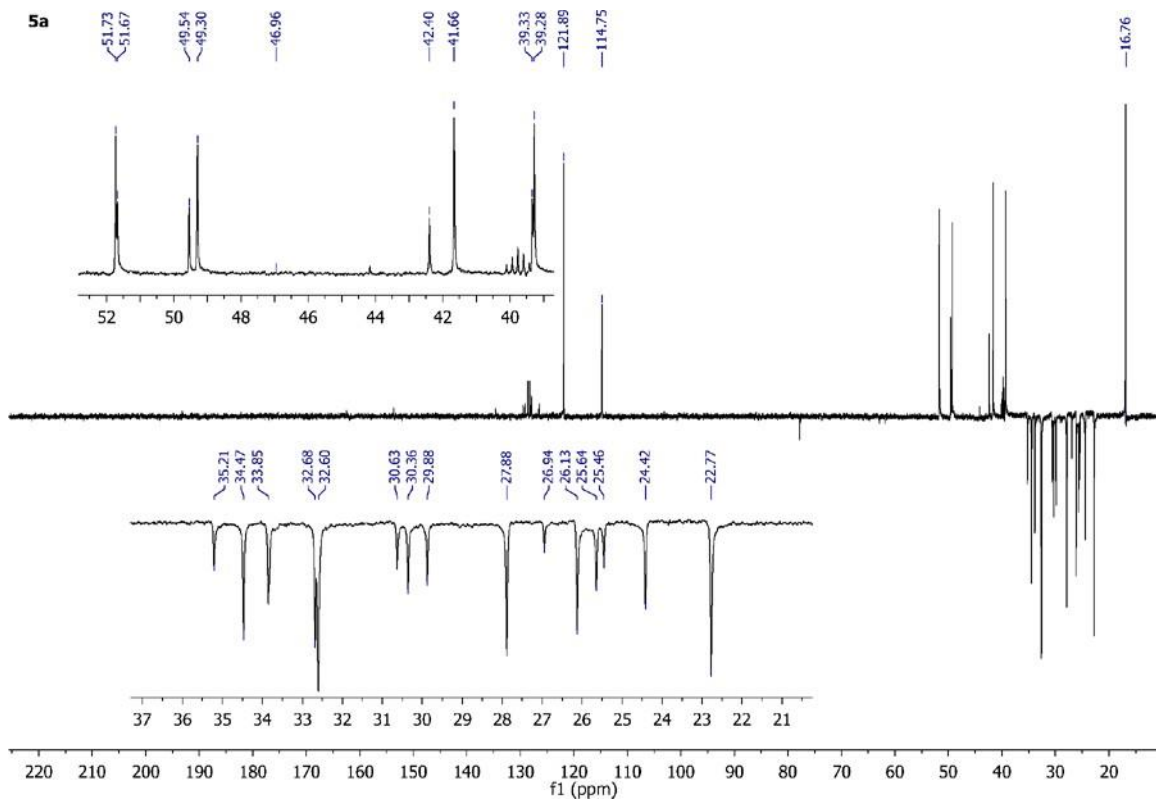
| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|-------------|---------------|-----------|---------------|------------|-------------|
| C24H33N3O2S | - | 427.22935 | 0.39 | 6.57191 E6 | - |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|--------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+H] ⁺ | 500607.97 | 428.23662 | 428.23653 | -0.09033 | -0.21 | - |

Compound 5a

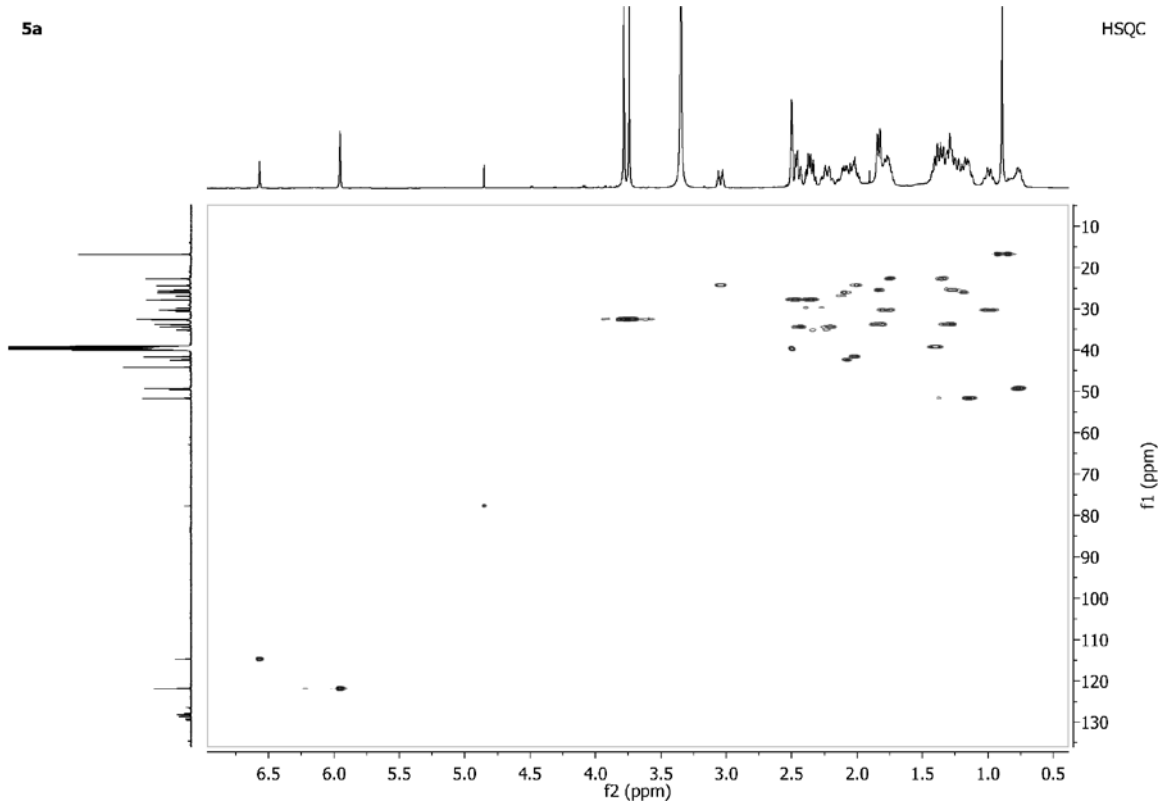






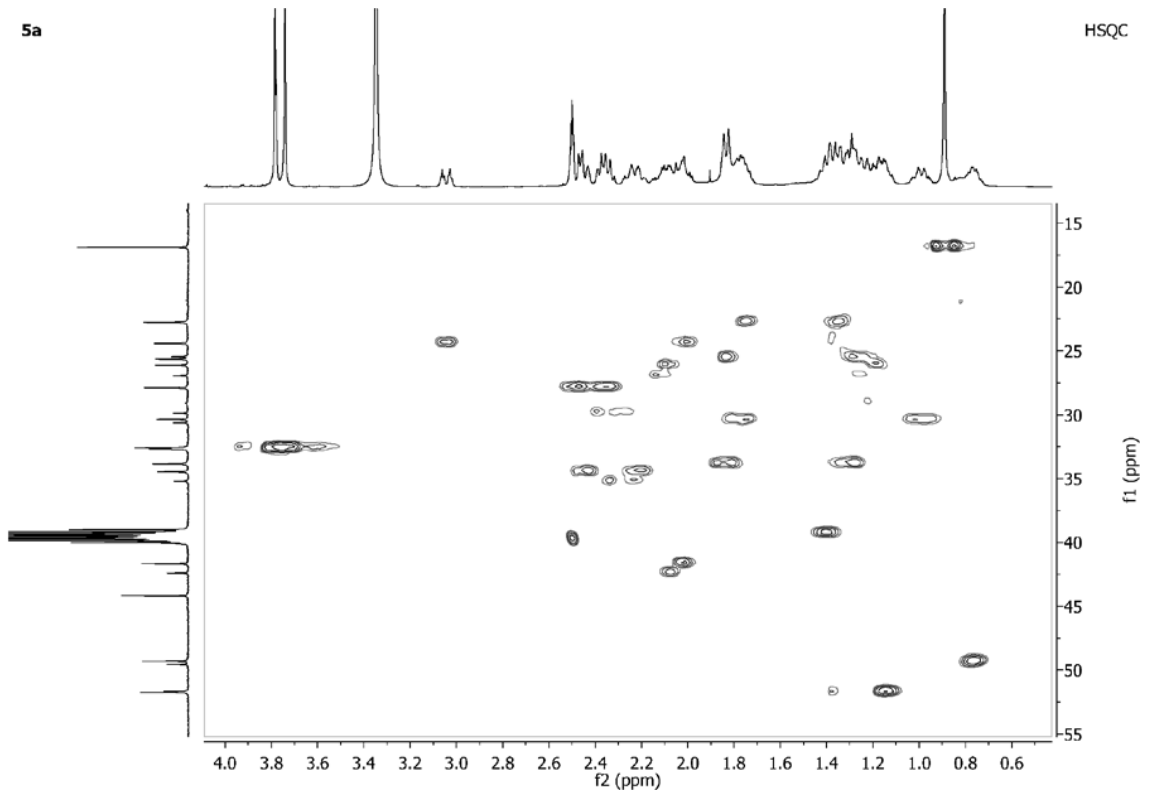
5a

HSQC

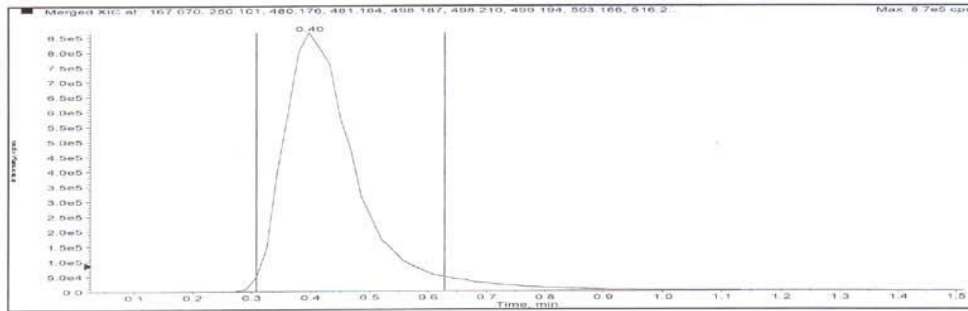


5a

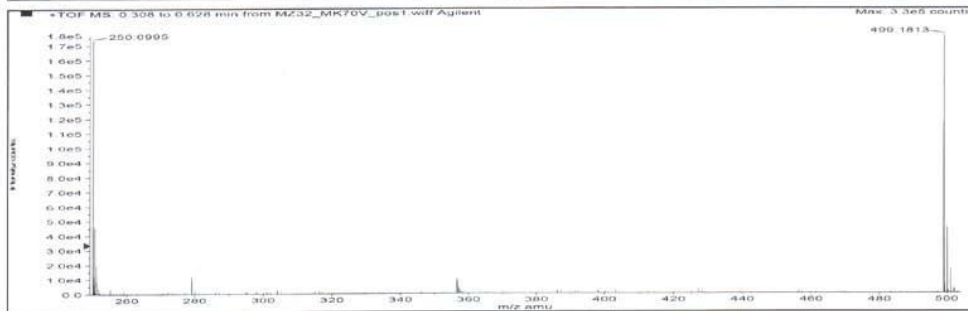
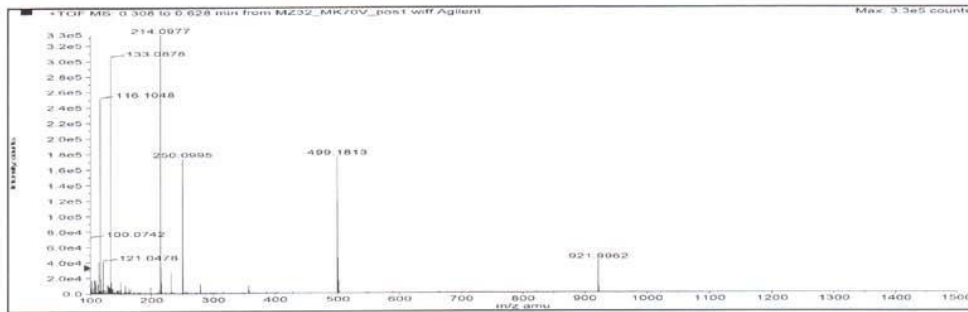
HSQC



Sample Name: MZ32 Sample Location: P1-D2 Sample Id: Operator: Milka
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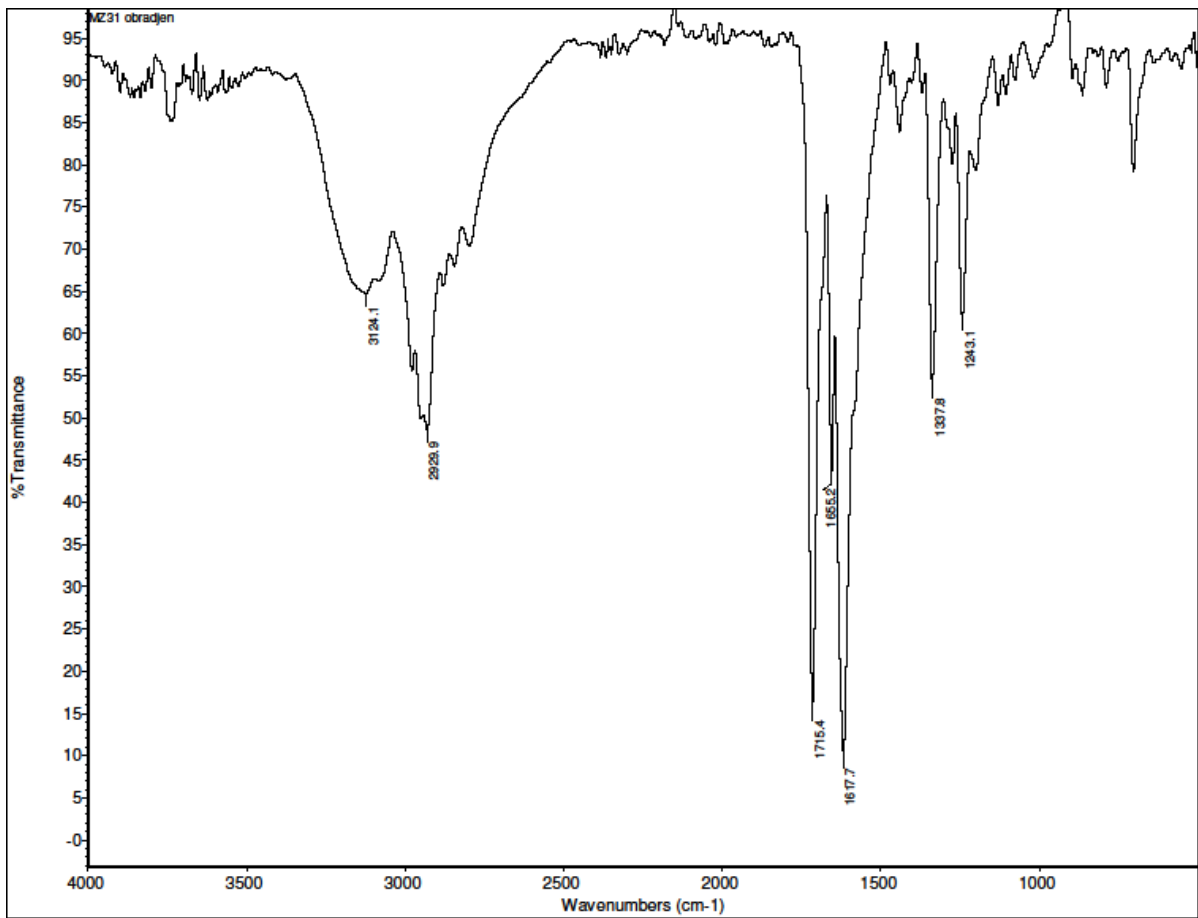
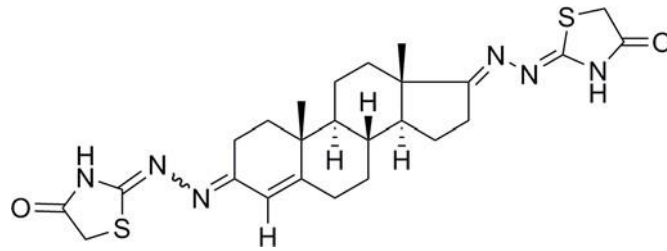
Merged XIC, Period# : 1 Experiment# : 1

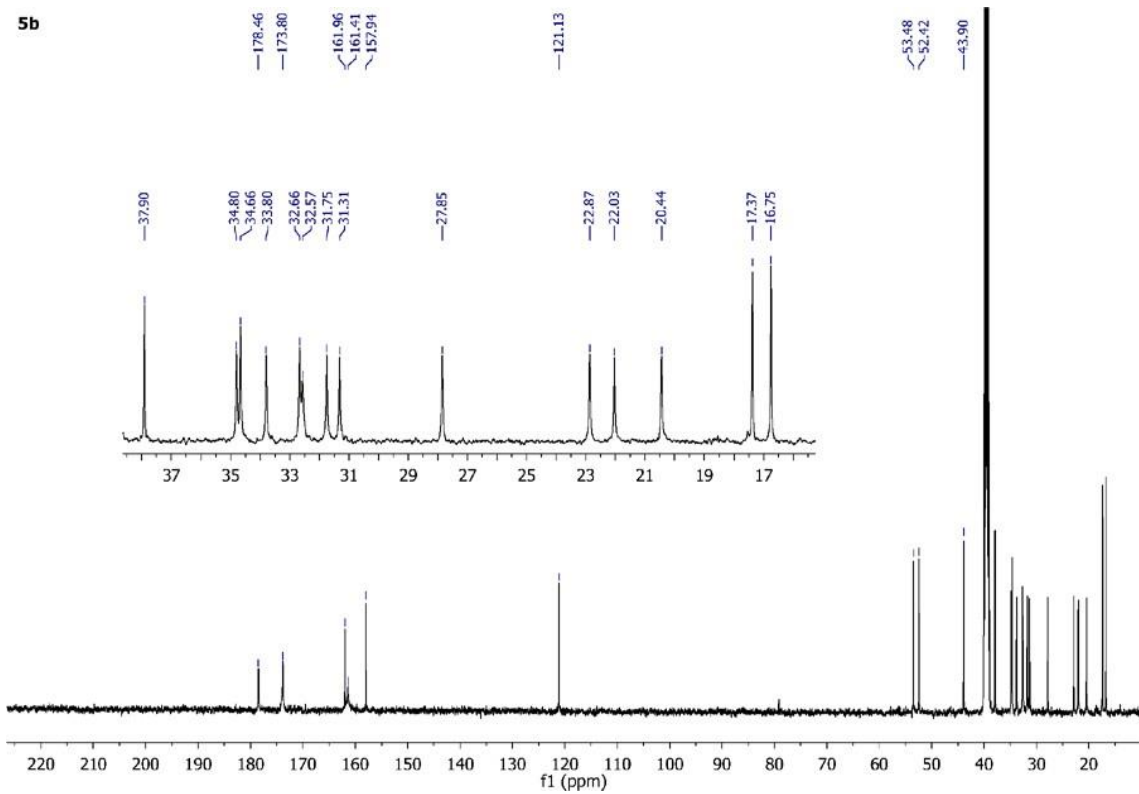
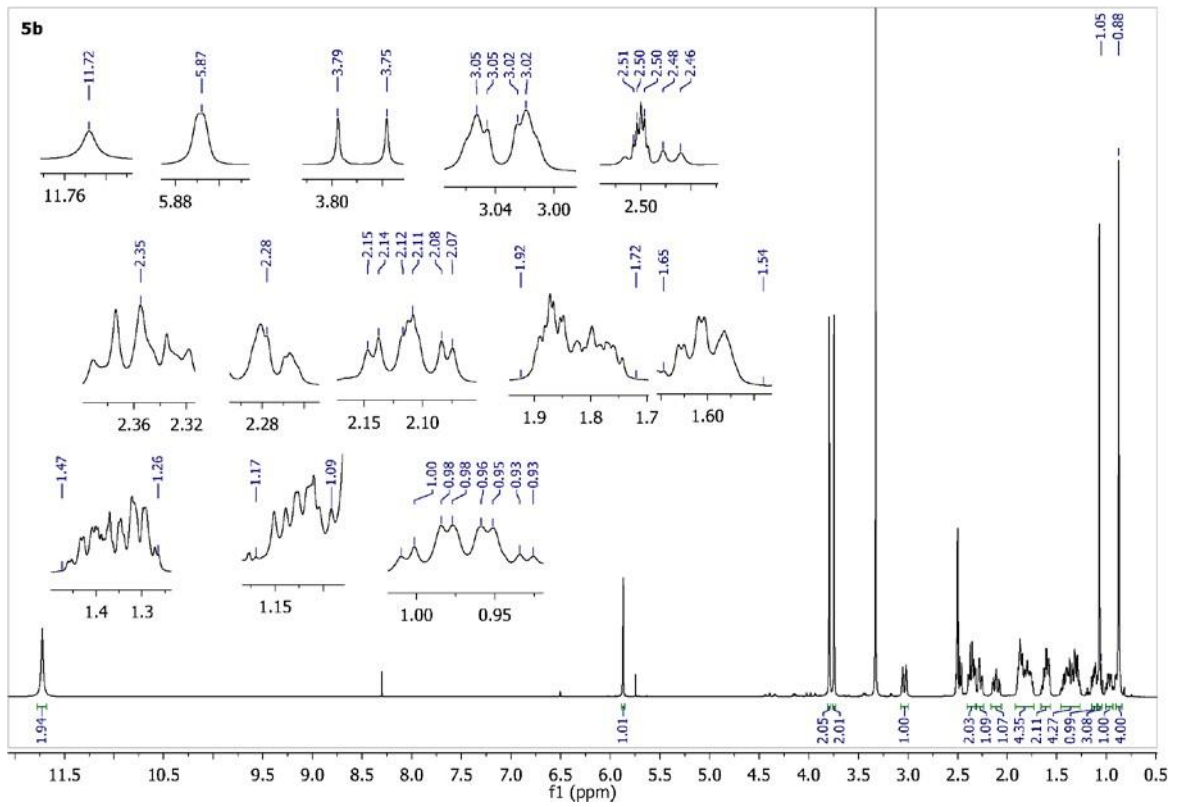


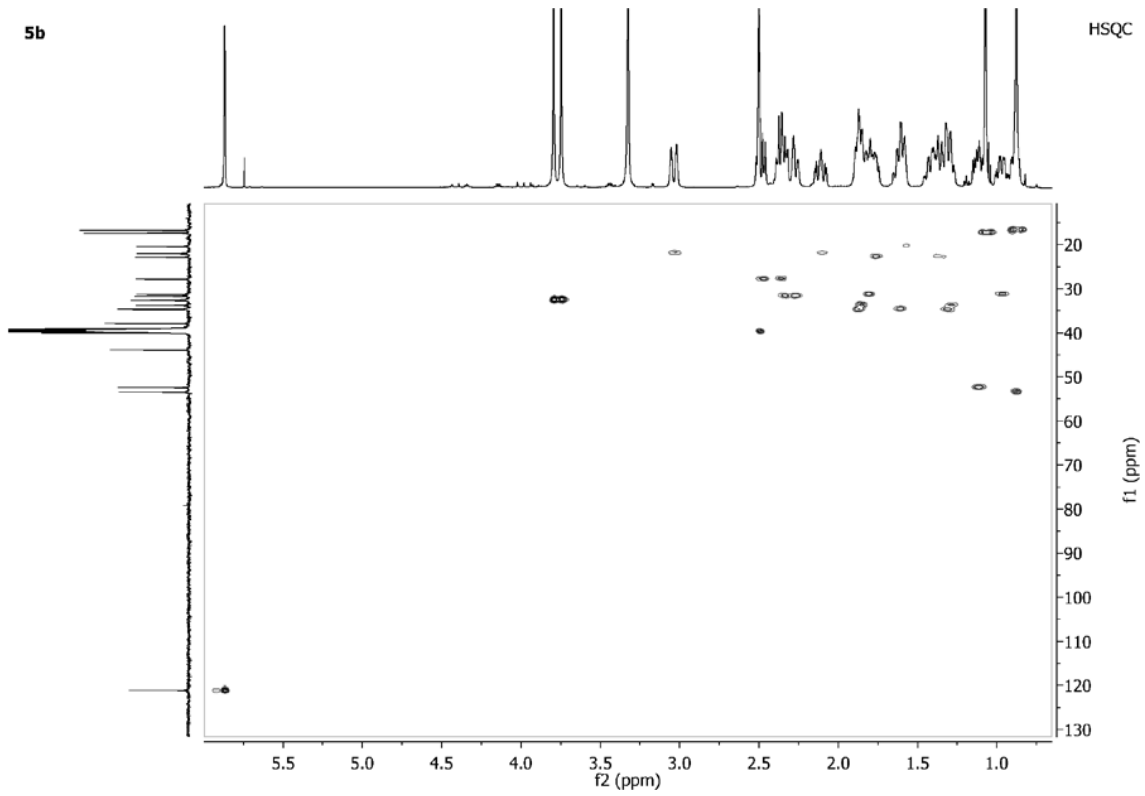
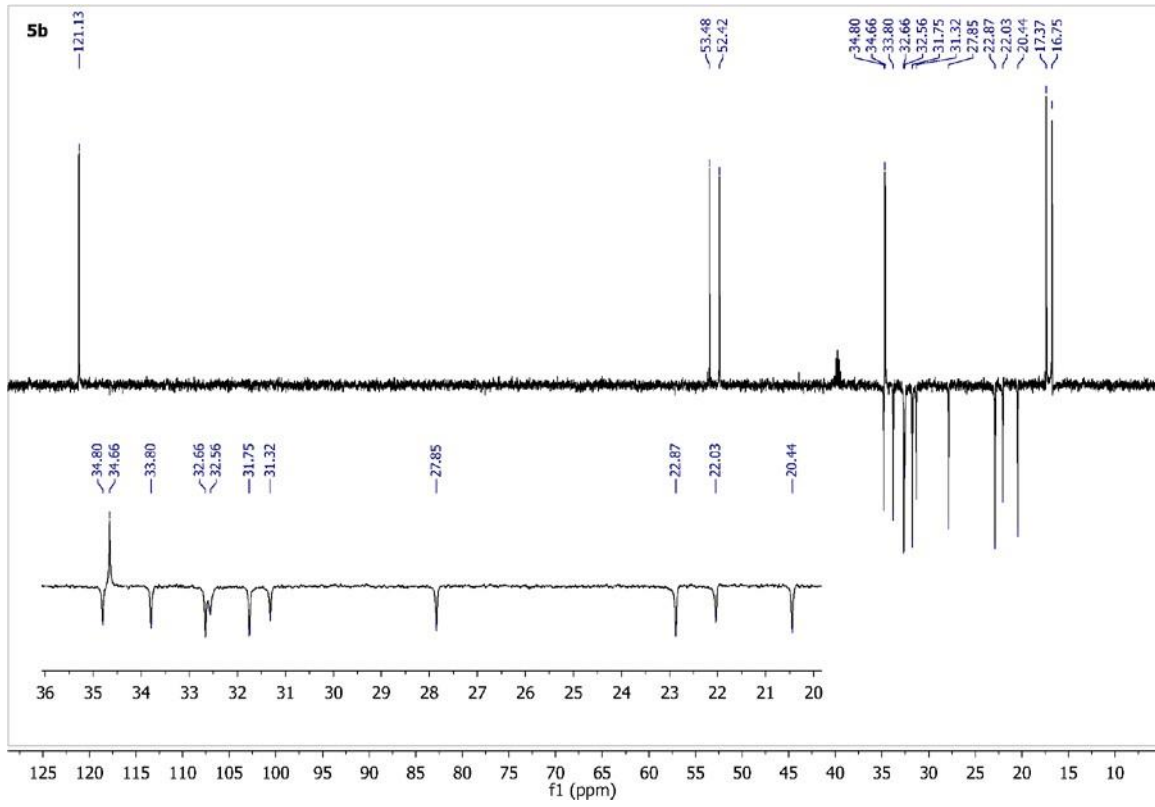
| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|--------------|---------------|-----------|---------------|------------|-------------|
| C24H30N6O2S2 | -- | 498.18717 | 0.40 | 7.34072 E6 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|----------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+2H] ²⁺ | 174314.82 | 250.10086 | 250.10125 | 0.38728 | 1.55 | -- |
| [M+H] ⁺ | 190340.14 | 499.19444 | 499.19400 | -0.44628 | -0.89 | -- |

Compound **5b**

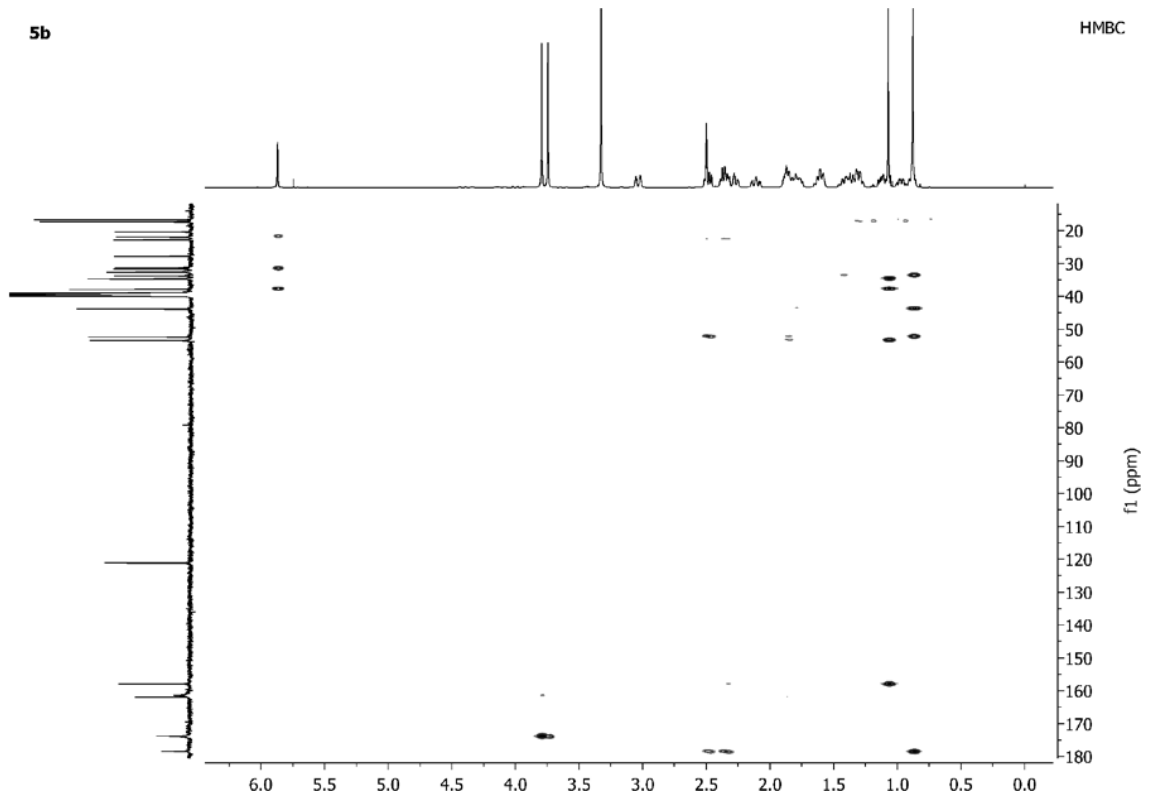




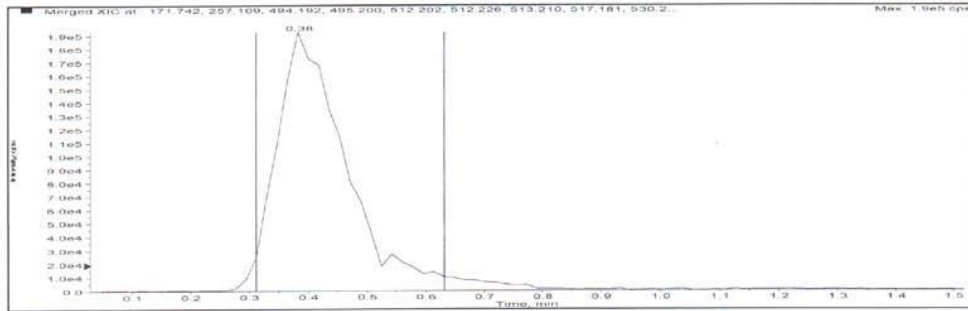


5b

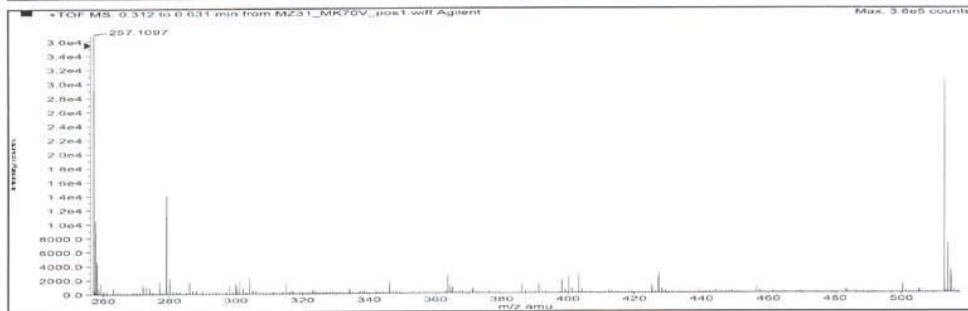
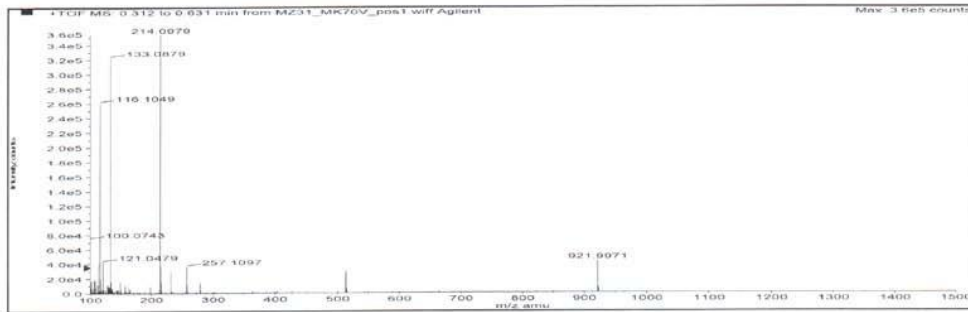
HMBC



Sample Name: MZ31 Sample Location: P1-D1 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ31_MK70V_pos1.wiff Acq Time: February 02 2016, 12:19:17 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anml\efc.xml



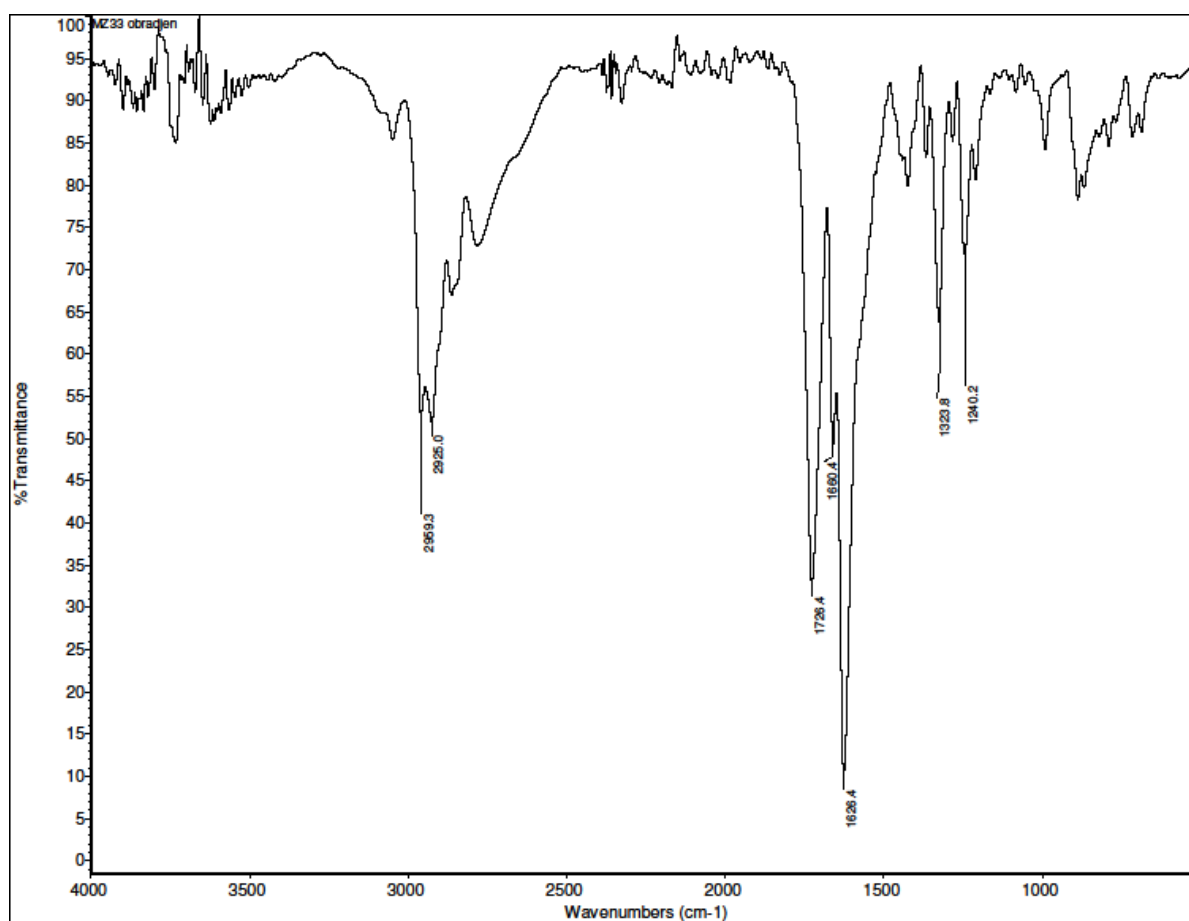
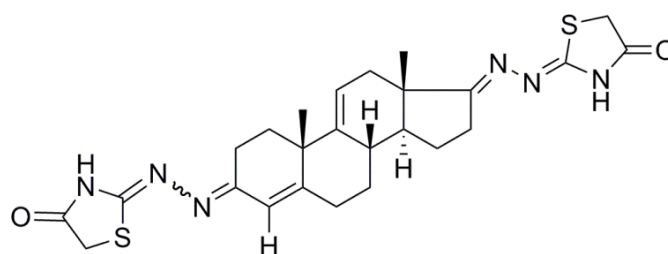
Merged XIC, Period# : 1 Experiment# : 1



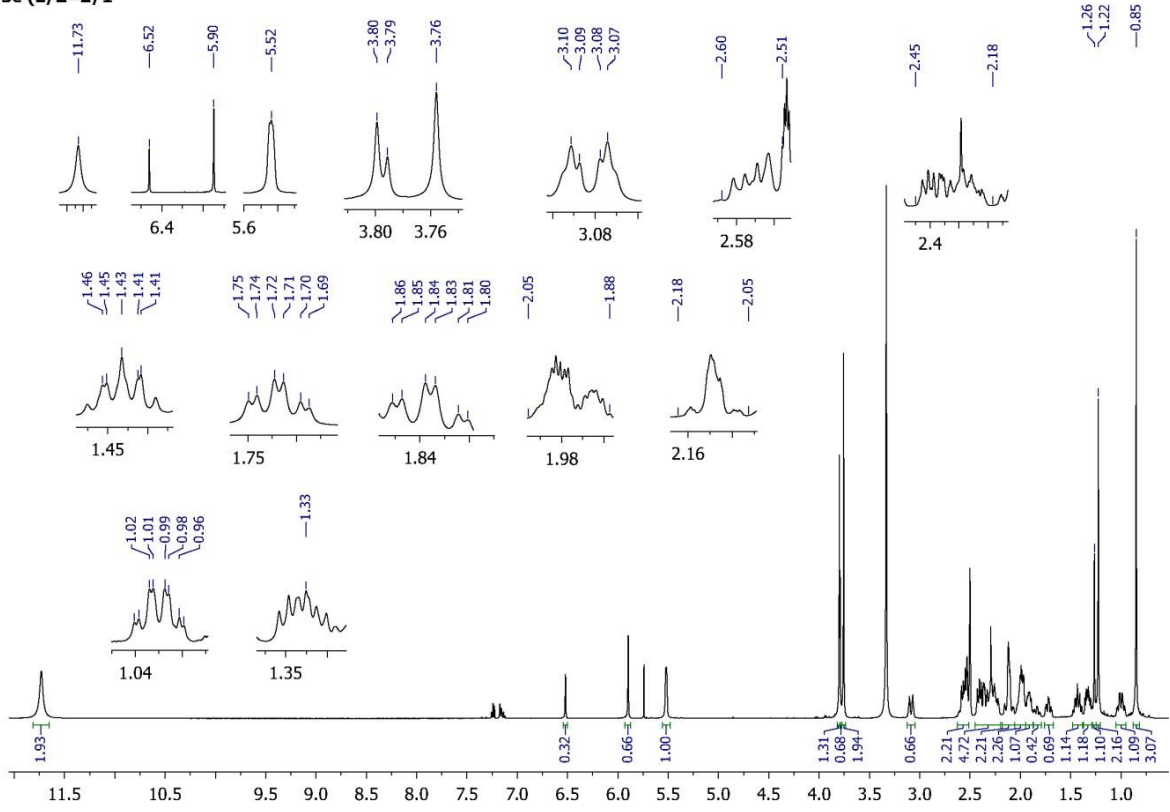
| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|--------------|---------------|-----------|---------------|------------|-------------|
| C25H32N6O2S2 | -- | 512.20282 | 0.38 | 1.61132 E6 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|----------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+2H] ²⁺ | 36873.28 | 257.10868 | 257.10937 | 0.68760 | 2.67 | -- |
| [M+H] ⁺ | 30190.77 | 513.21009 | 513.21057 | 0.48028 | 0.94 | -- |

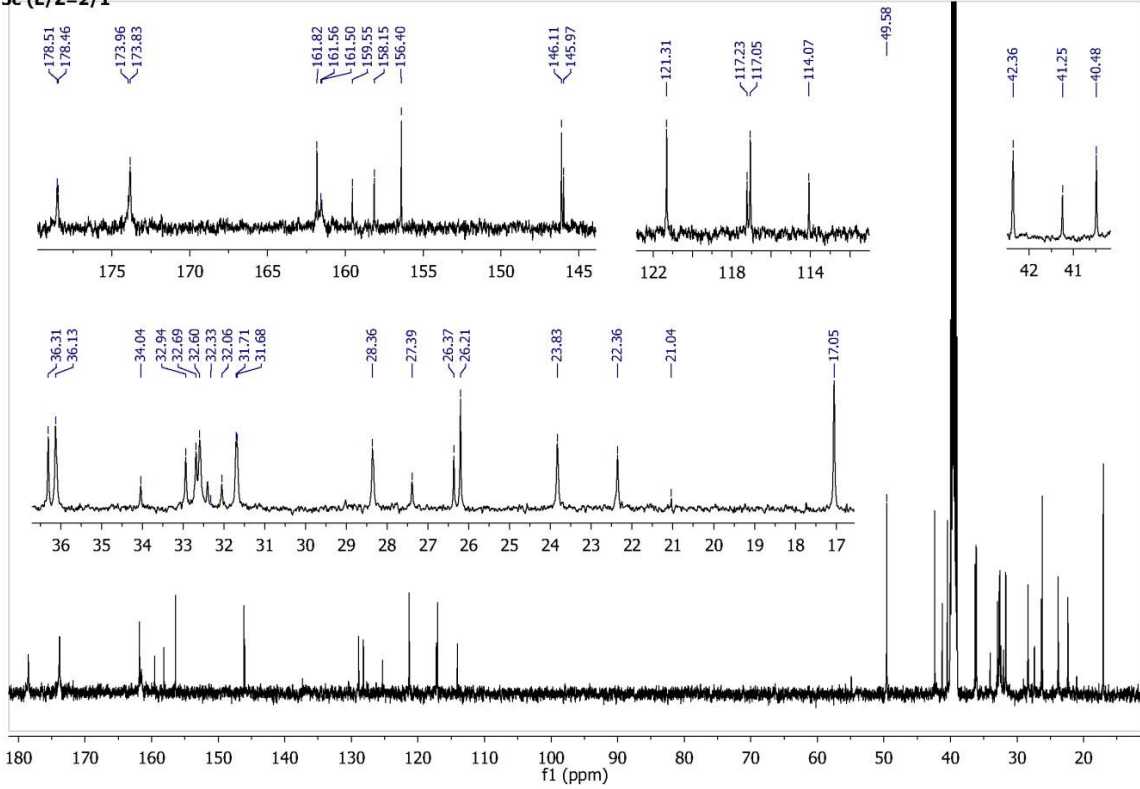
Compound 5c

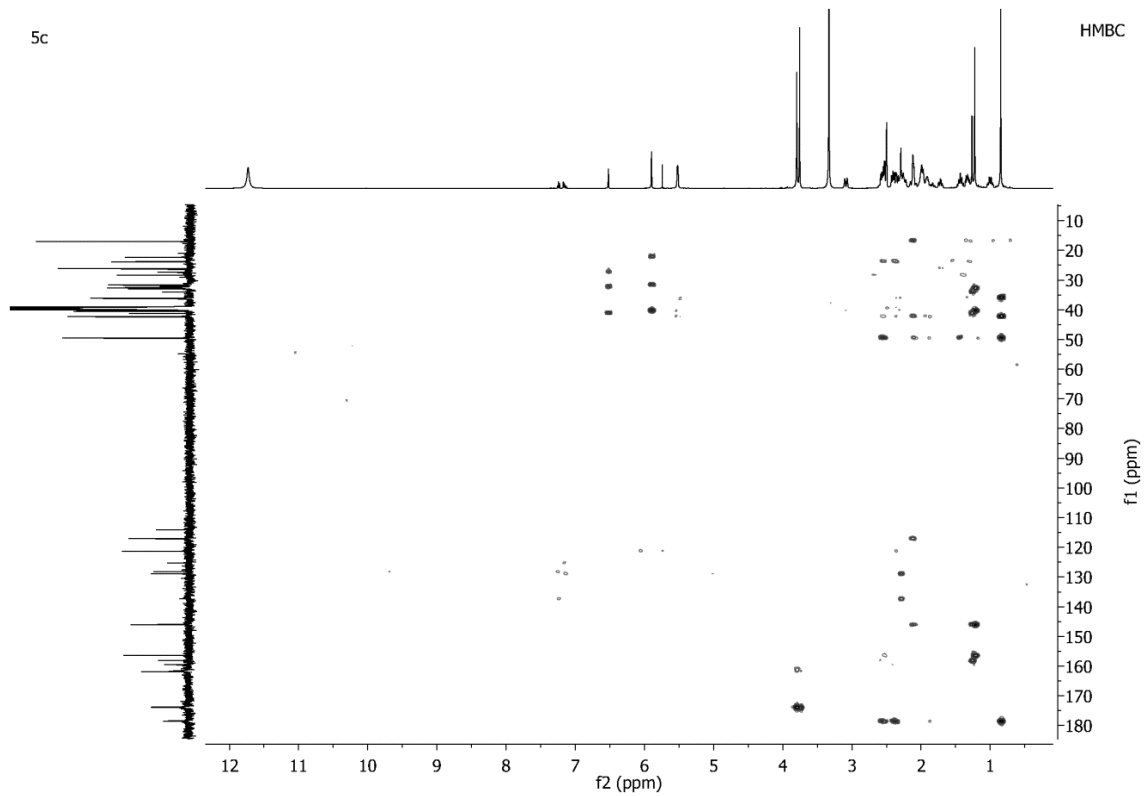
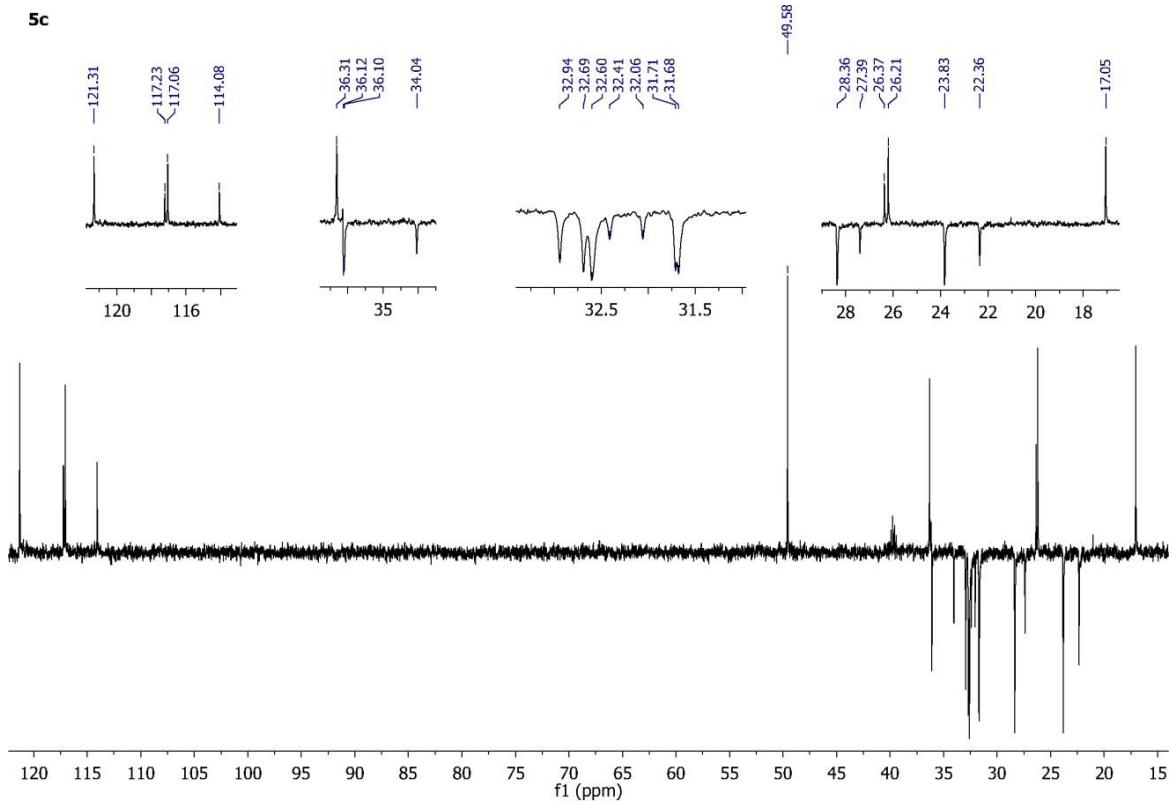


5c (E/Z=2/1)



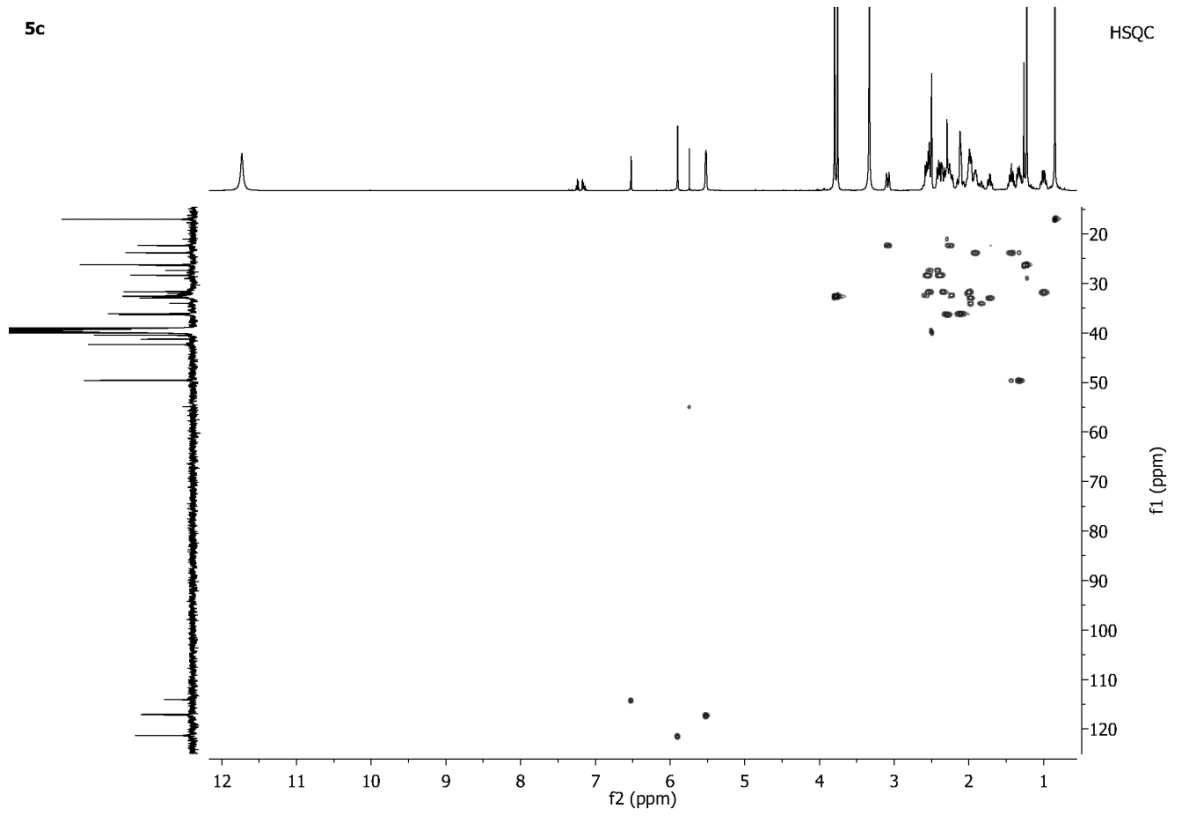
5c (E/Z=2/1)





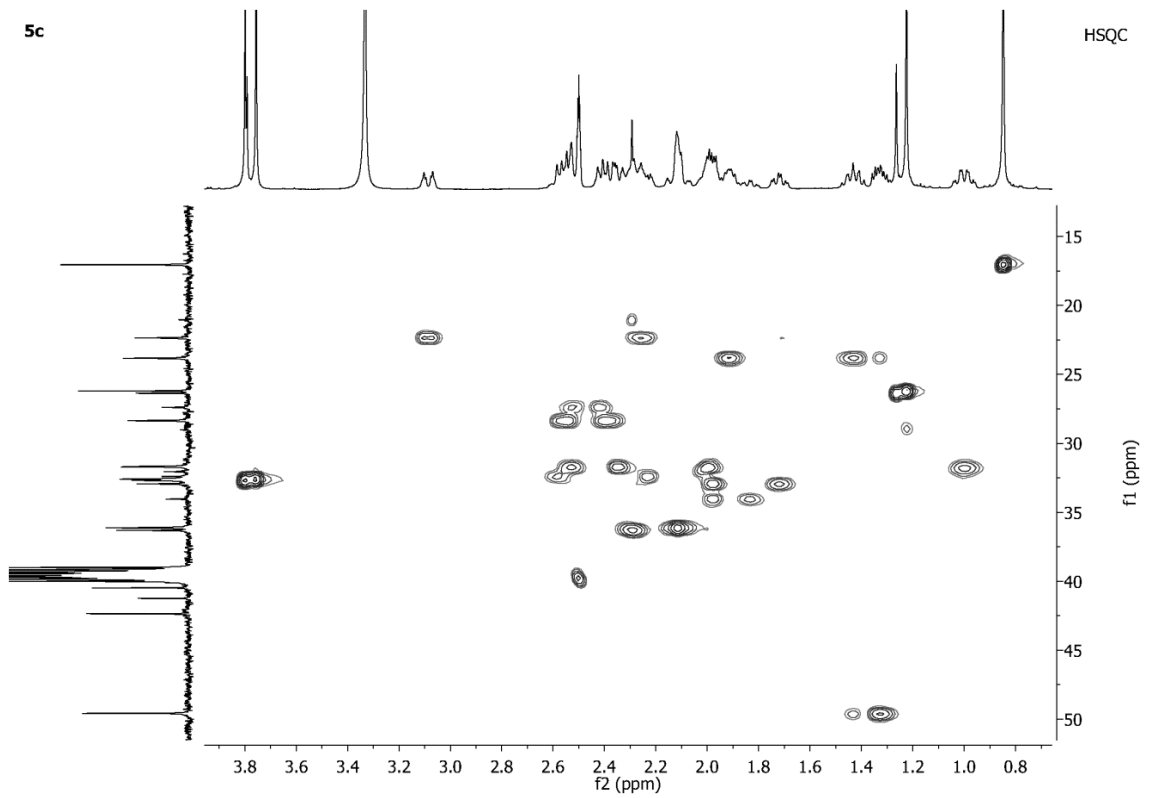
5c

HSQC

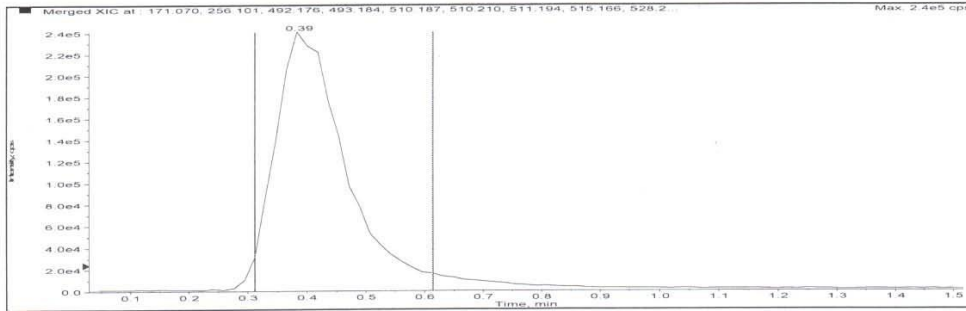


5c

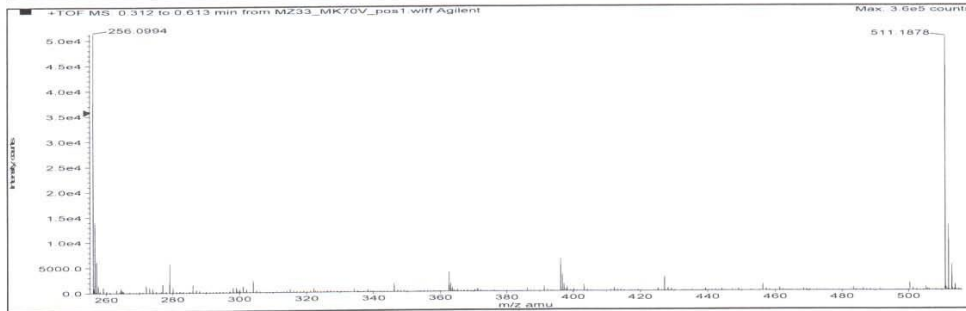
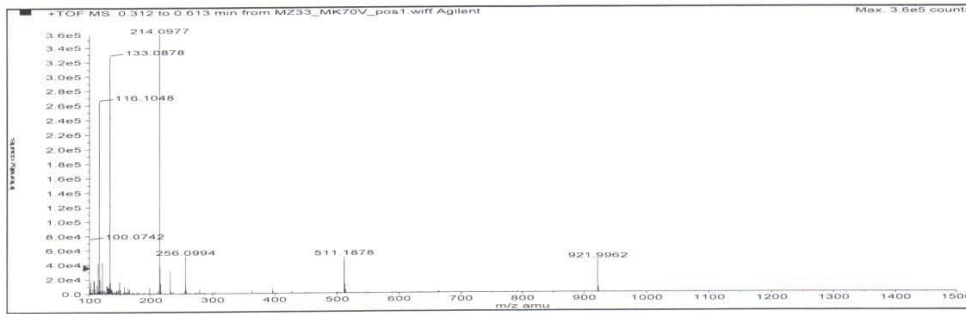
HSQC



Sample Name: MZ33 Sample Location: P1-D3 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ33_MK70V_pos1.wiff Acq Time: February 02 2016, 12:24:11 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_ident1.anml\efc.xml



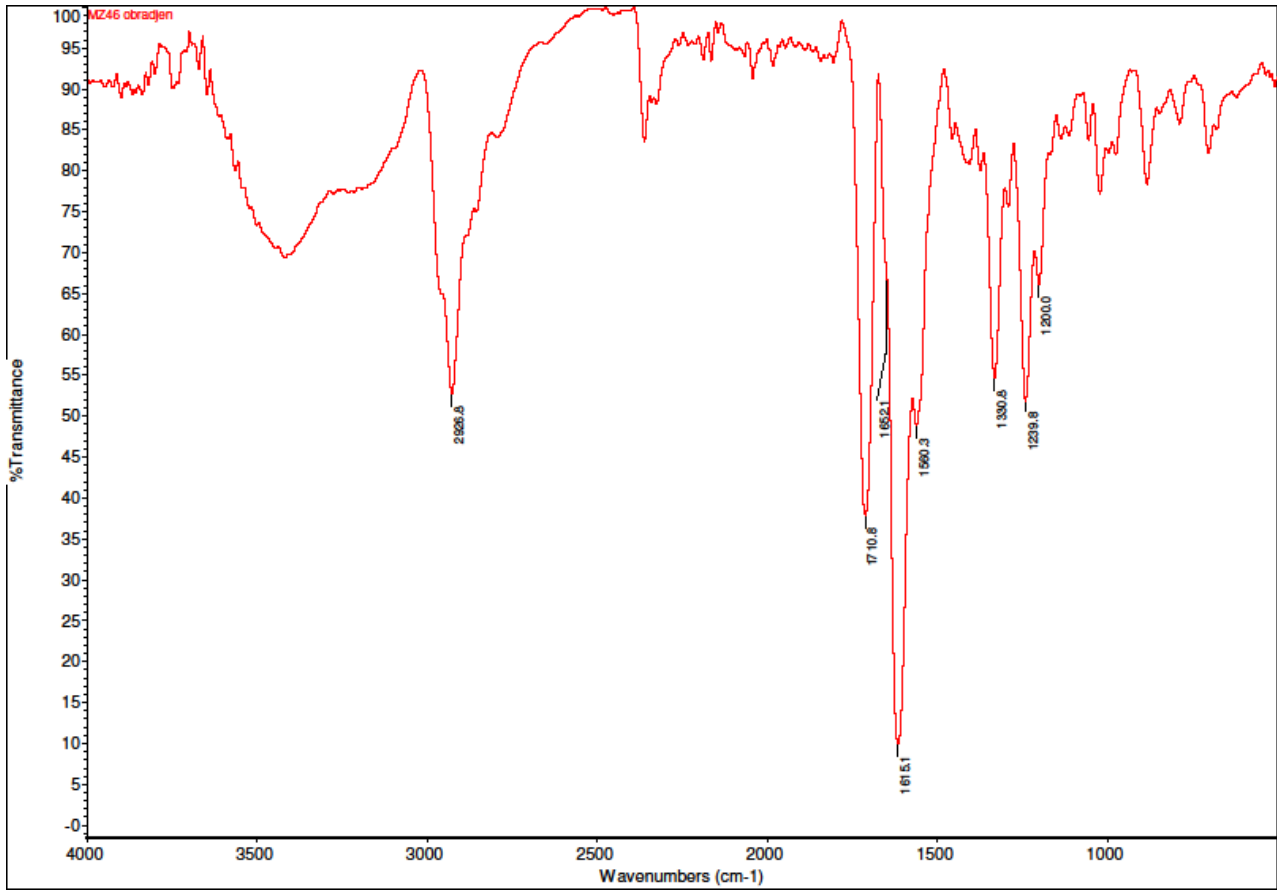
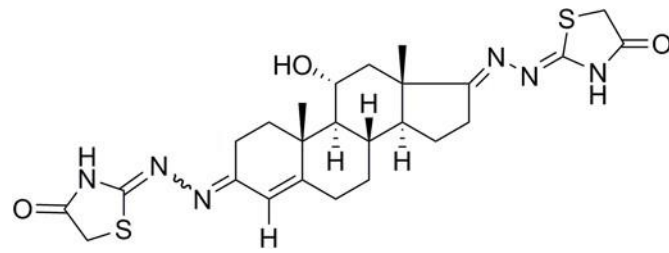
Merged XIC, Period# : 1 Experiment# : 1



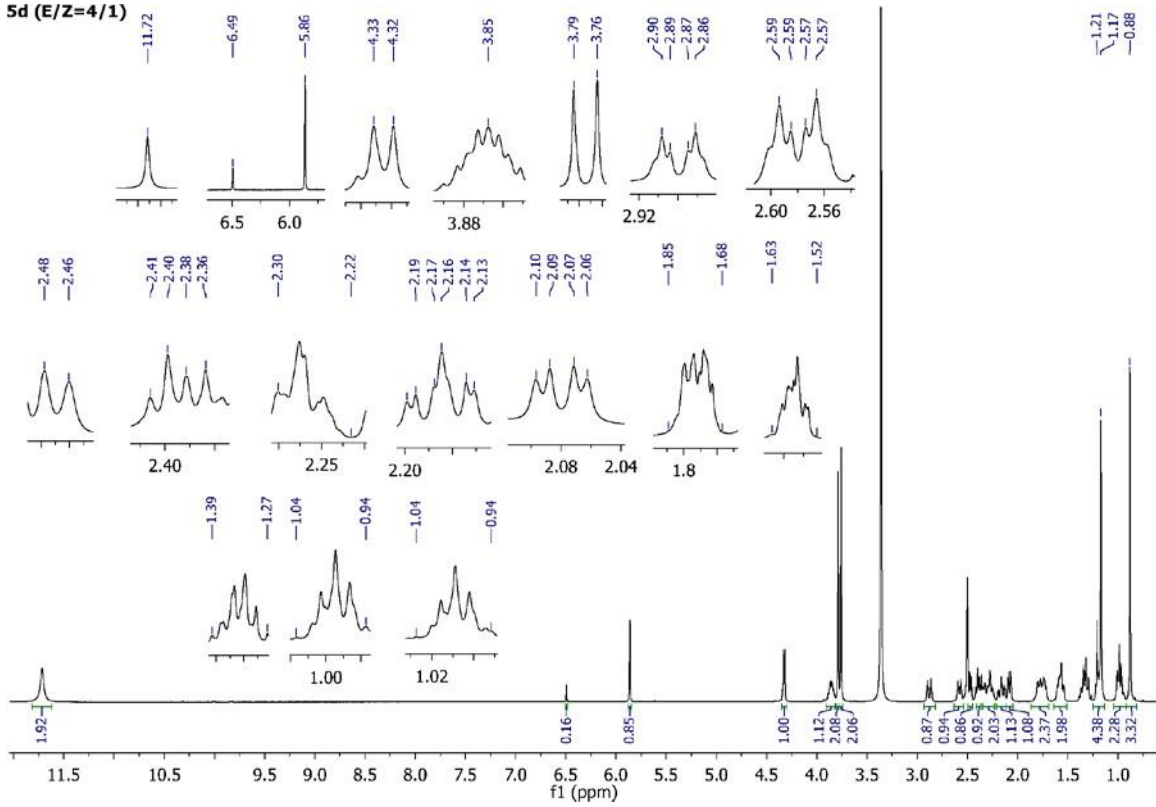
| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|--|---------------|-----------|---------------|------------|-------------|
| C ₂₅ H ₃₀ N ₆ O ₂ S ₂ | -- | 510.18717 | 0.39 | 2.04044 E6 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|----------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+2H] ²⁺ | 51504.23 | 256.10086 | 256.10172 | 0.85889 | 3.35 | -- |
| [M+H] ⁺ | 51096.74 | 511.19444 | 511.19440 | -0.04512 | -0.09 | -- |

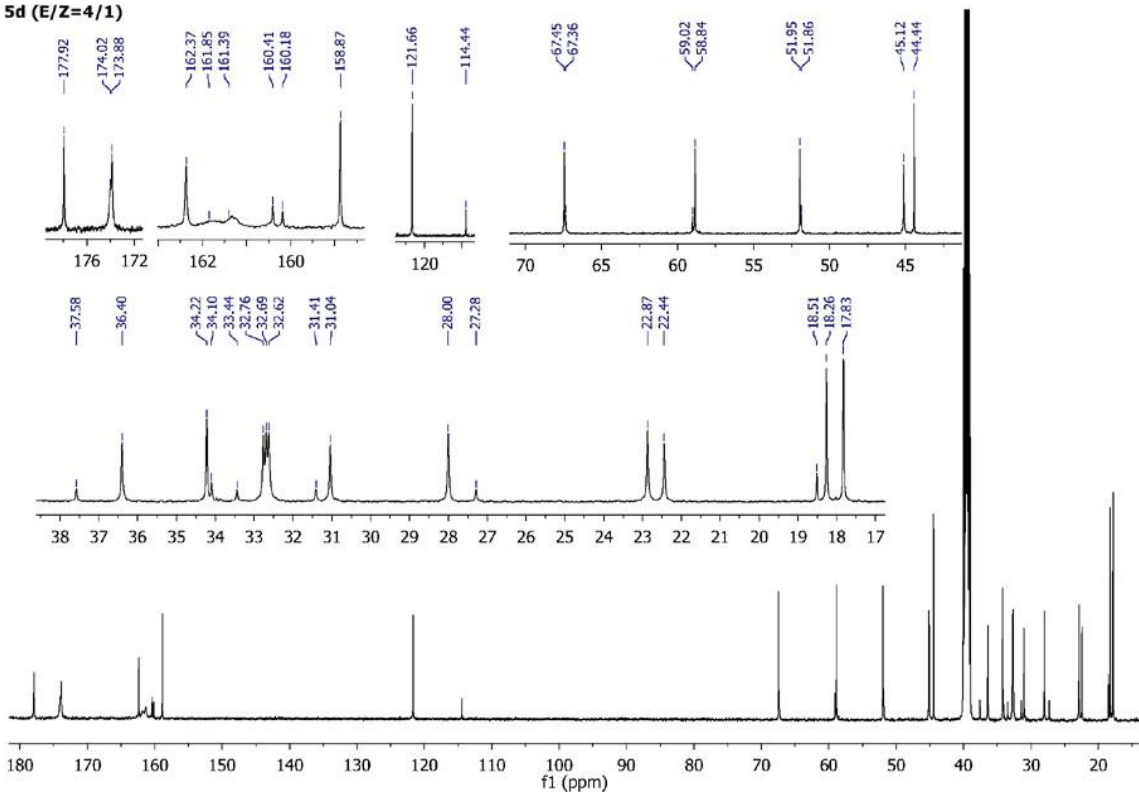
Compound 5d

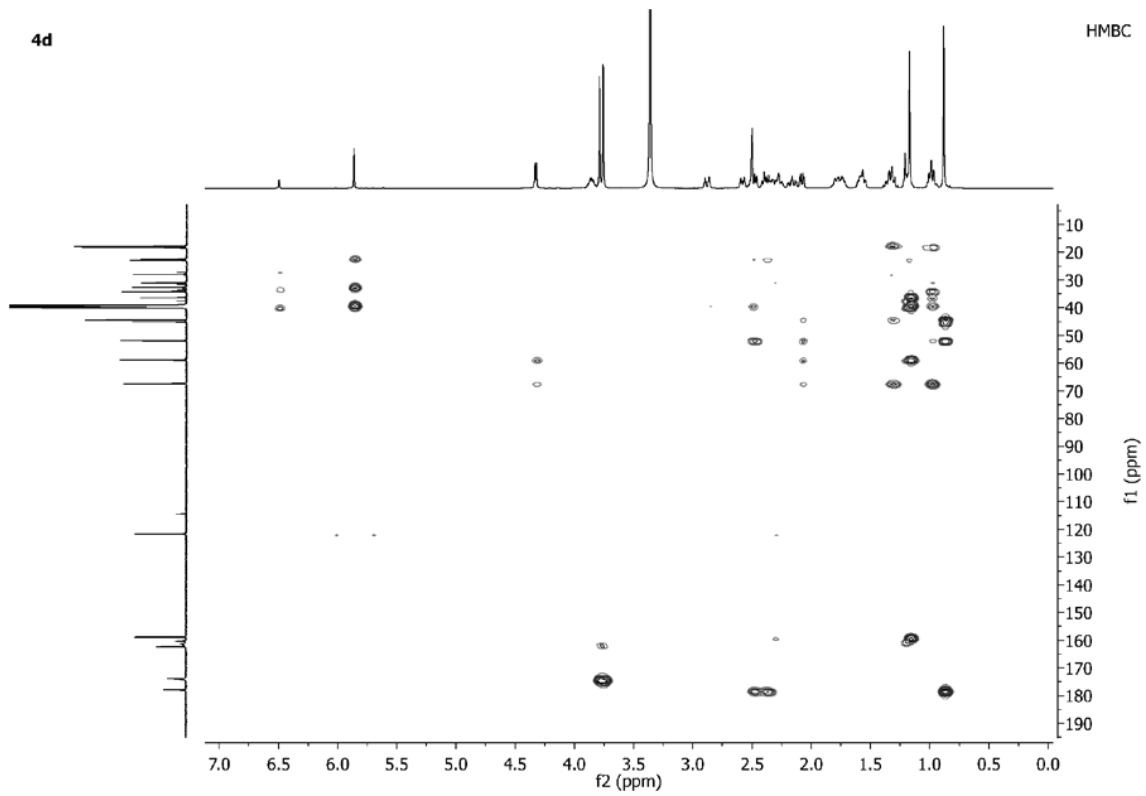
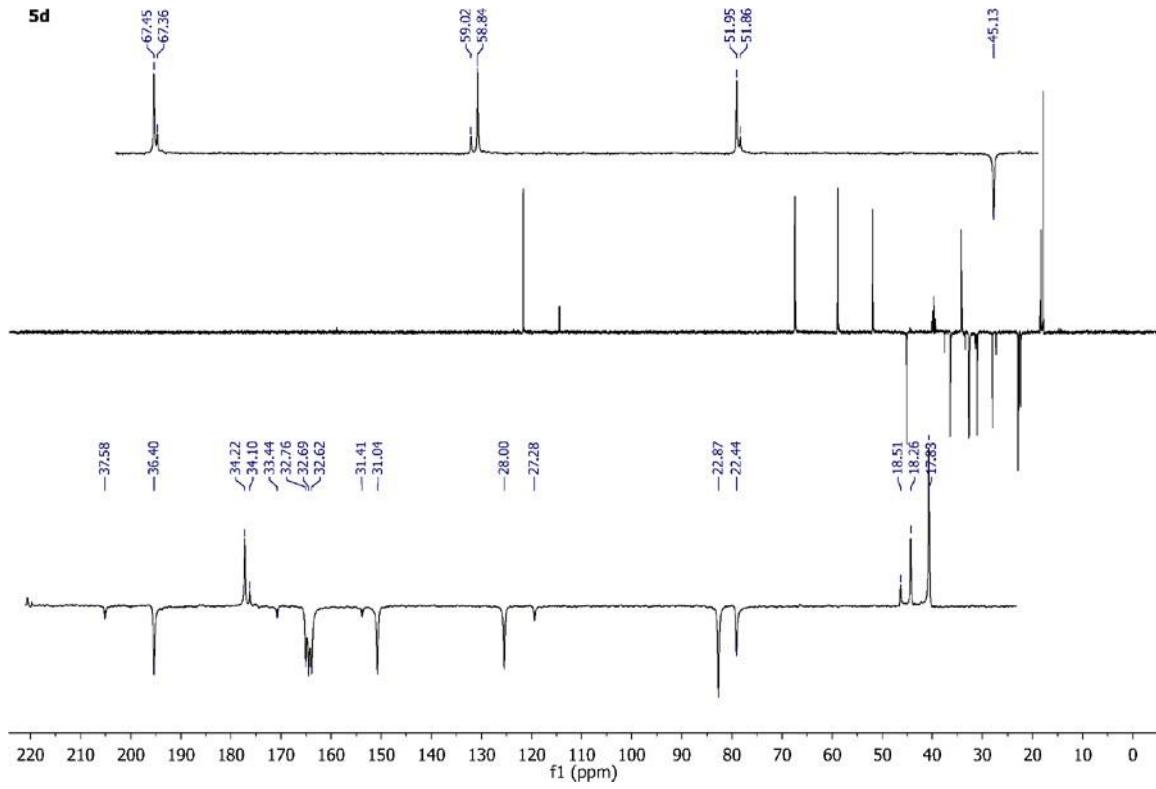


5d (E/Z=4/1)



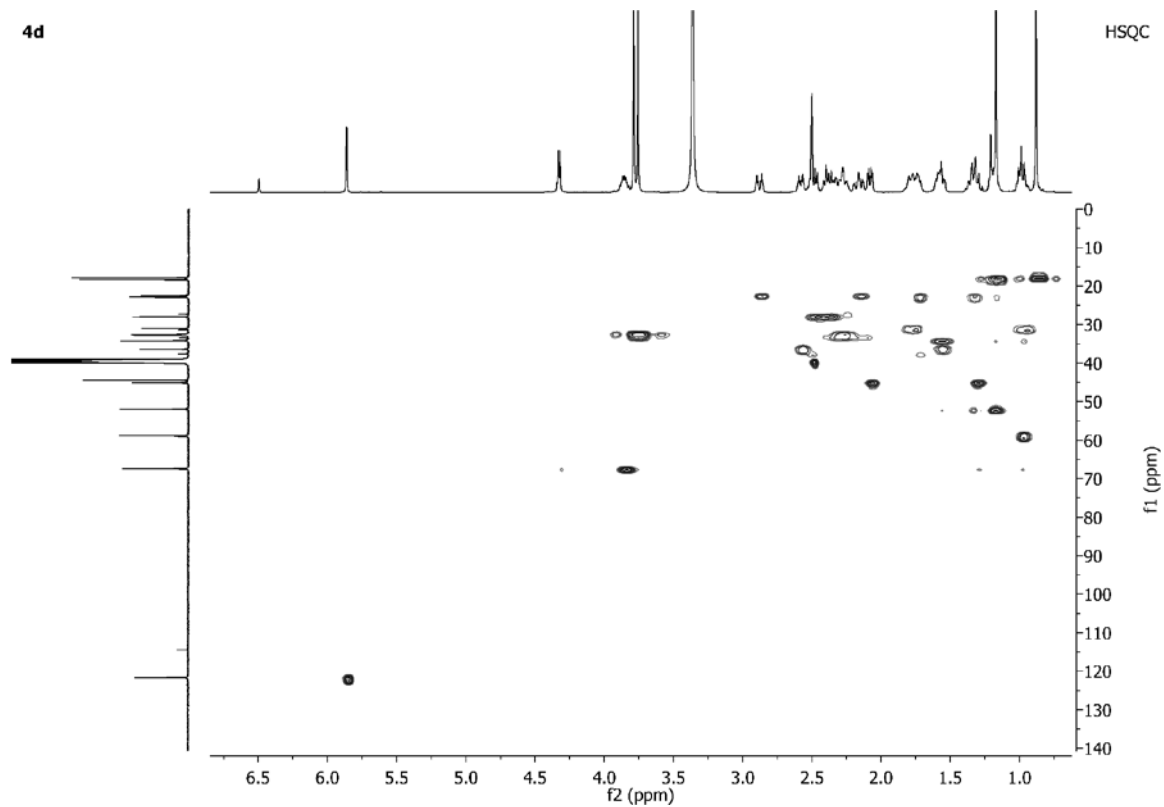
5d (E/Z=4/1)





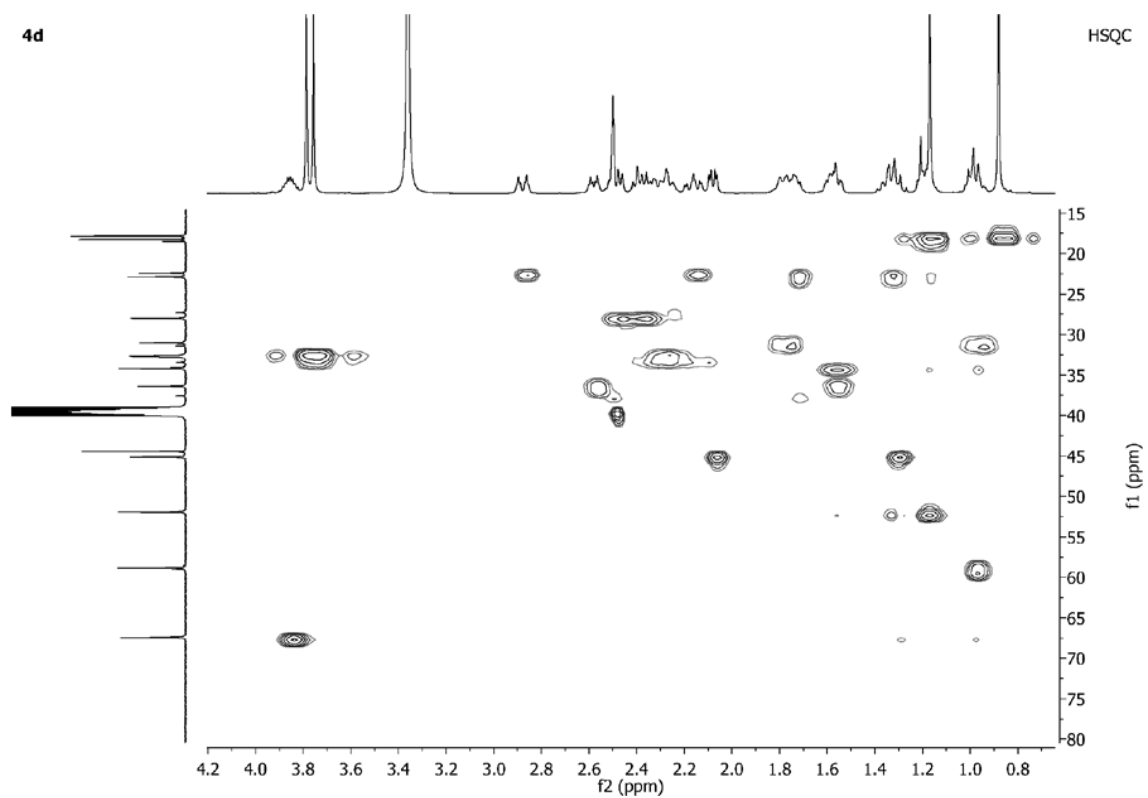
4d

HSQC



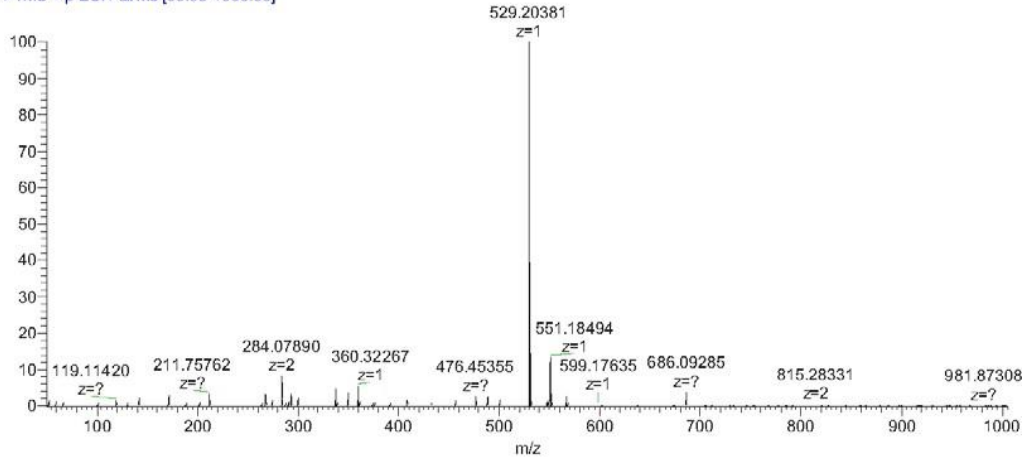
4d

HSQC

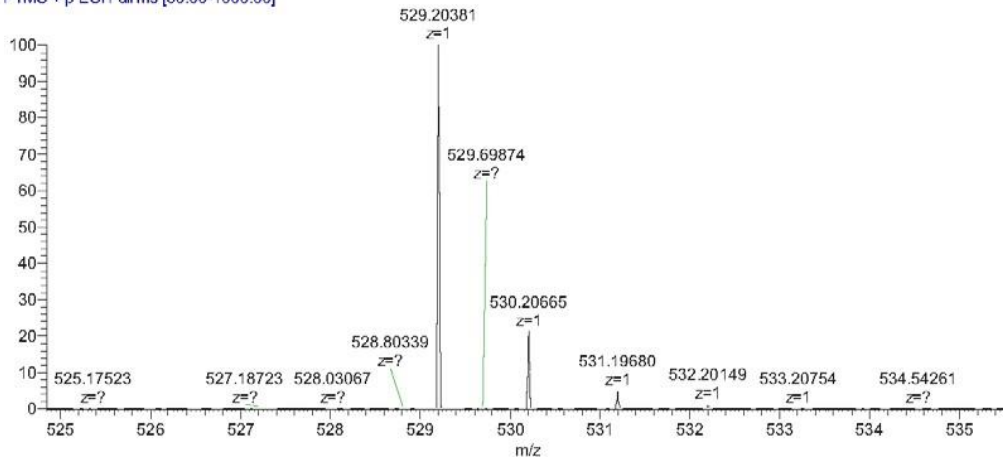


OB5056 MZ46 in MeOH

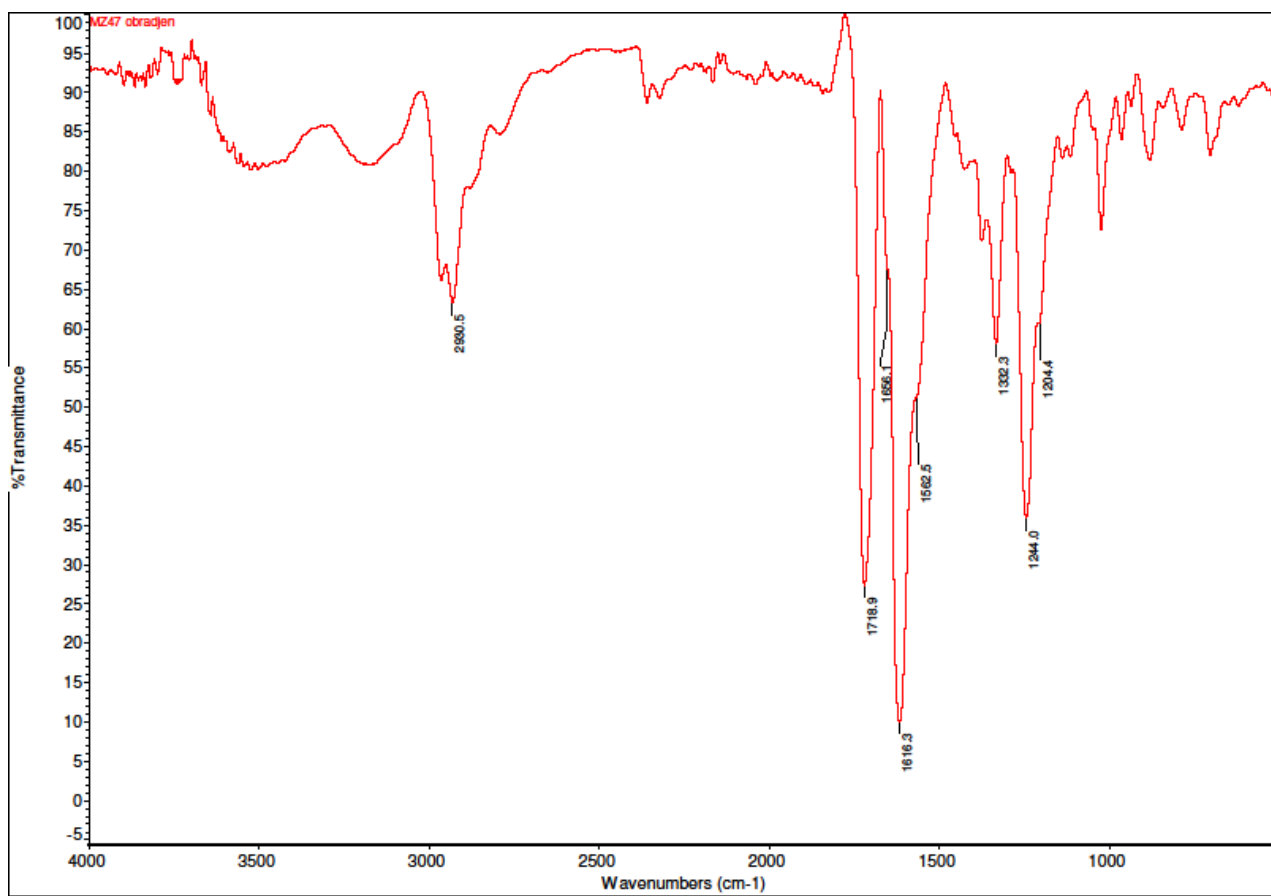
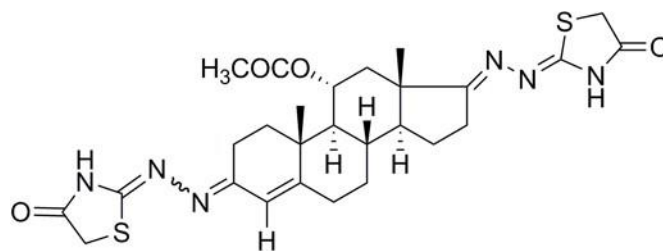
OB5056 #1-54 RT: 0.00-0.50 AV: 54 NL: 4.47E6
T: FTMS + p ESI Full ms [50.00-1000.00]

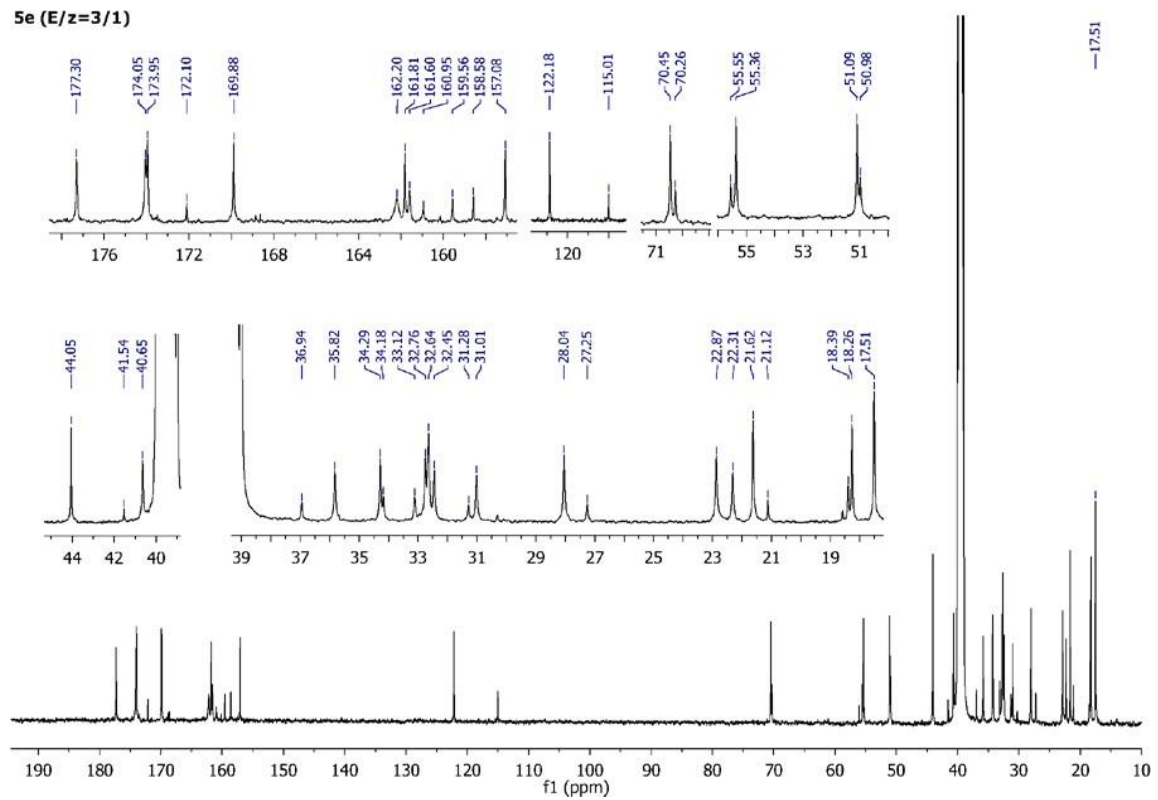
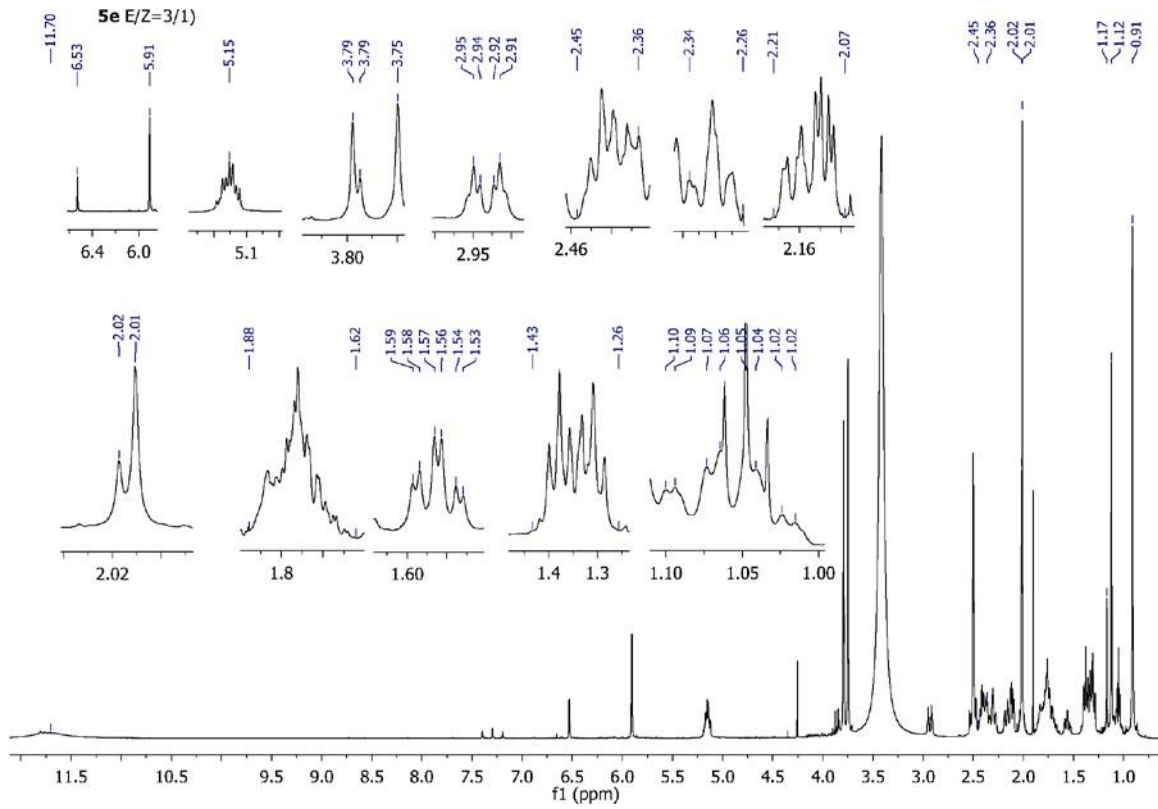


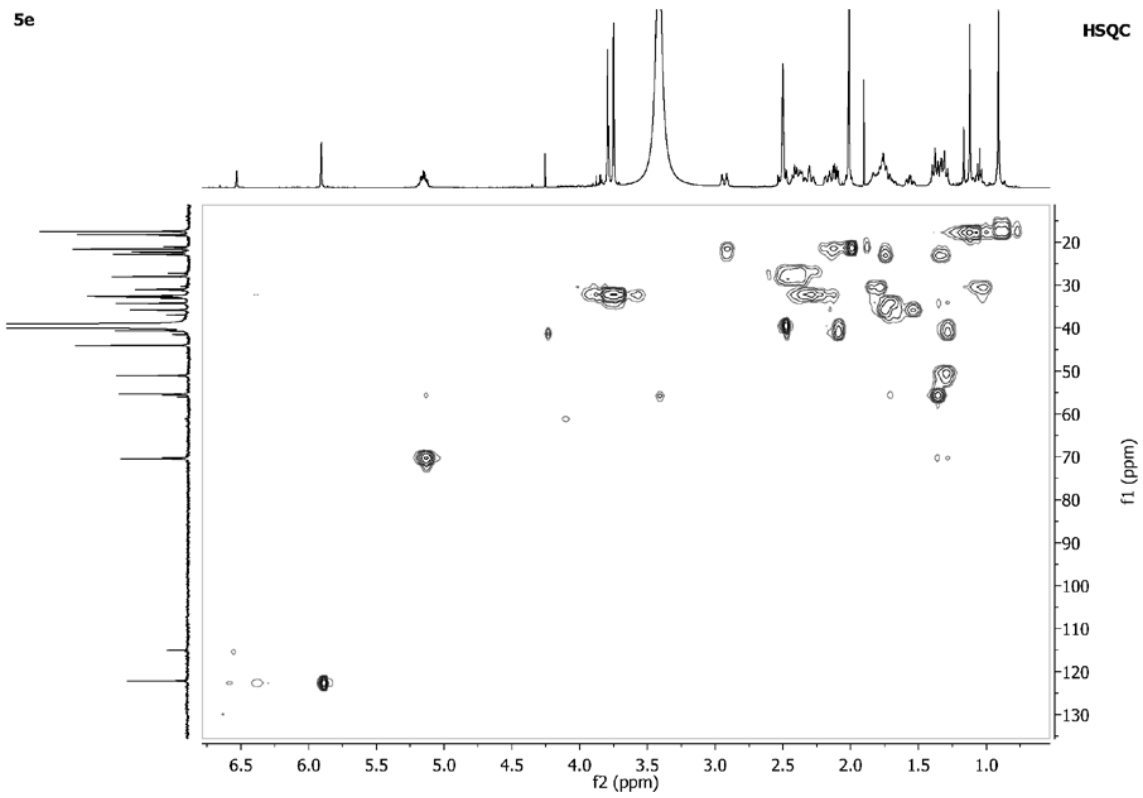
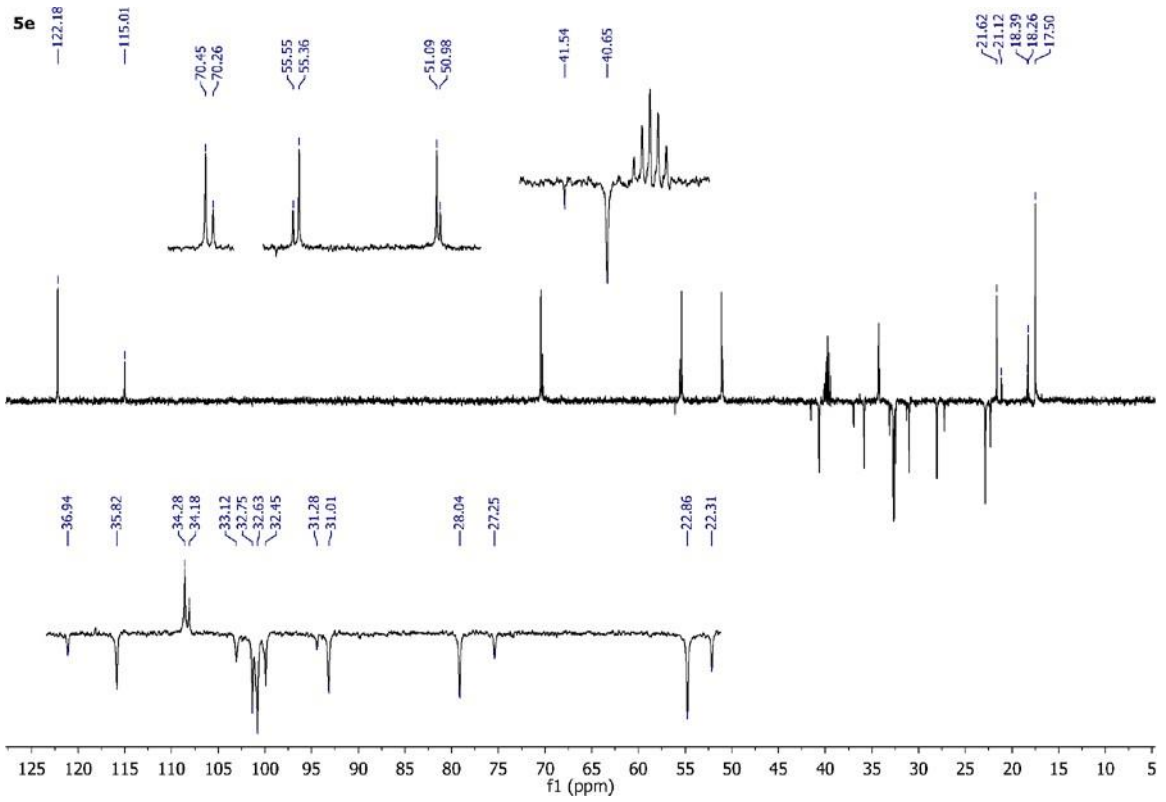
OB5056 #1-54 RT: 0.00-0.50 AV: 54 NL: 4.47E6
T: FTMS + p ESI Full ms [50.00-1000.00]



Compound 5e

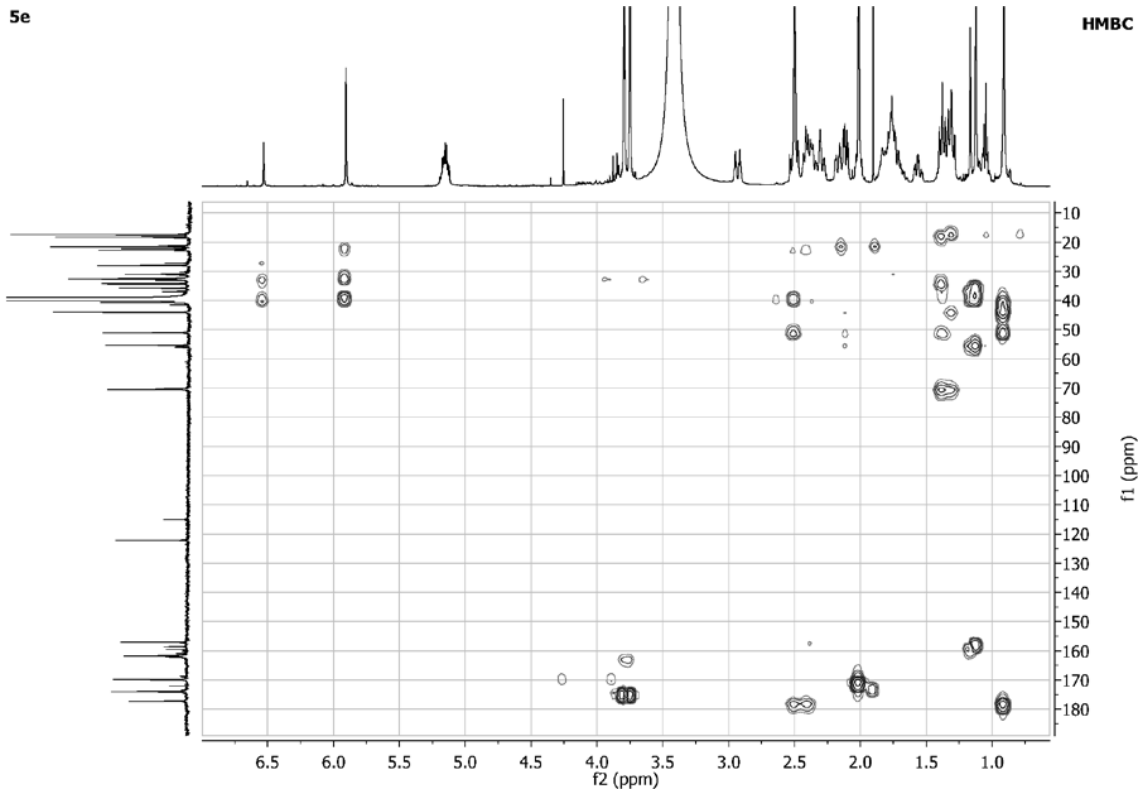






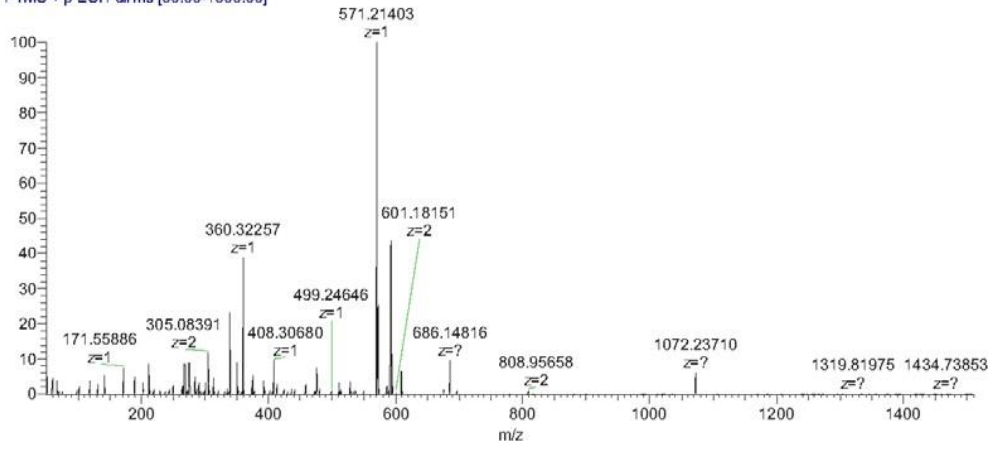
5e

HMBC

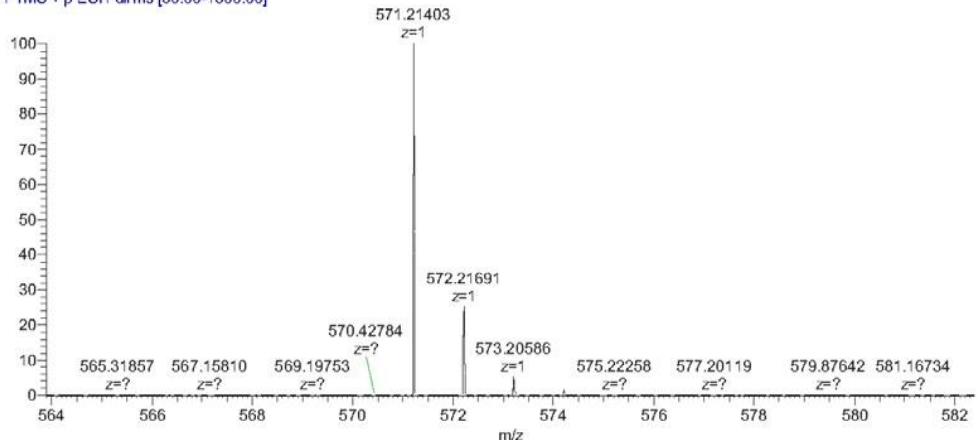


OB5057 MZ47R2 in MeOH

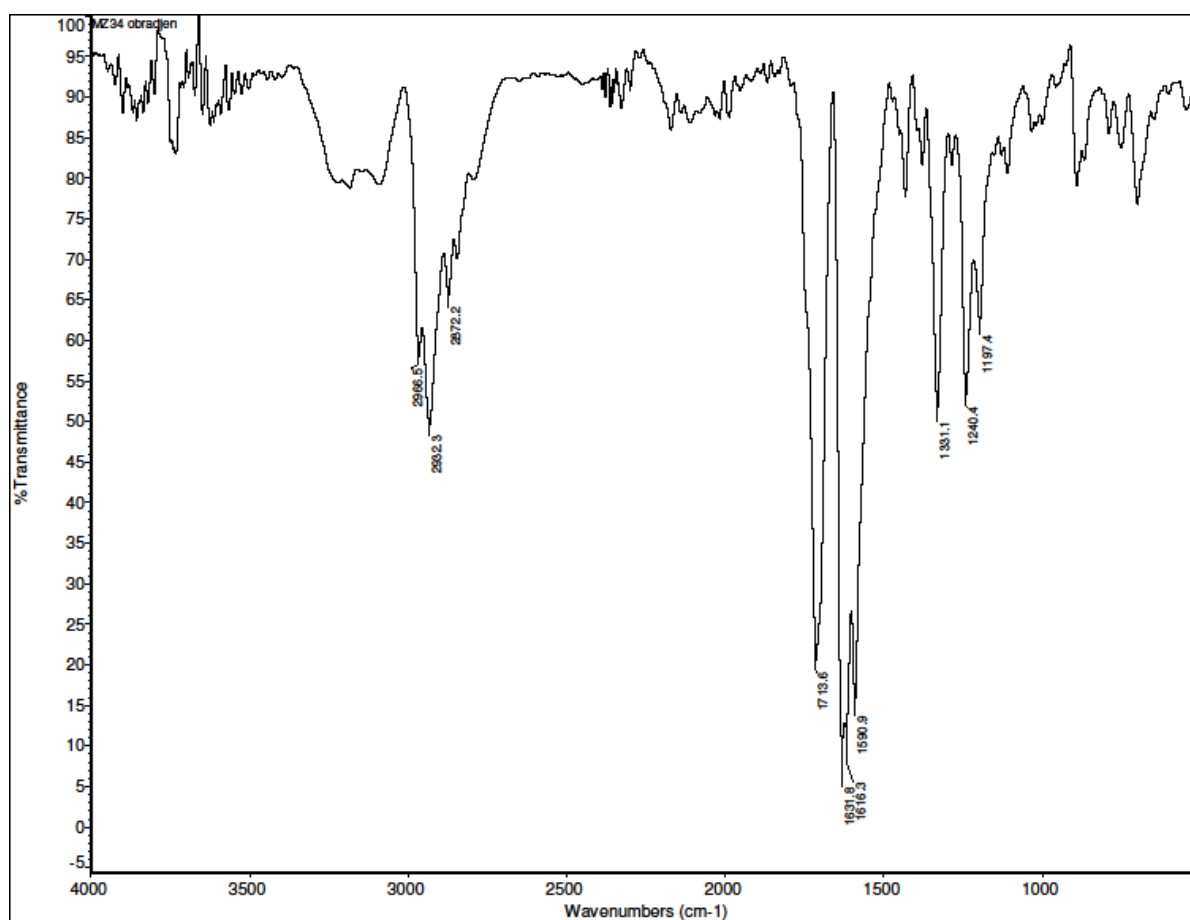
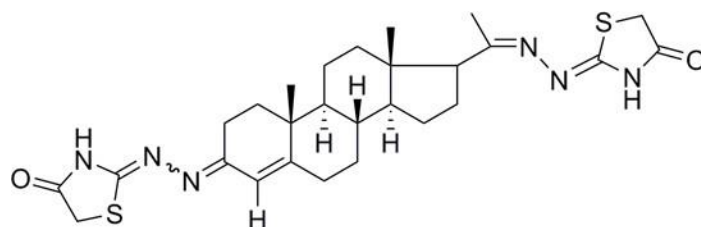
OB5057 #1-53 RT: 0.01-0.50 AV: 53 NL: 1.21E6
T: FTMS + p ESI Full ms [50.00-1500.00]



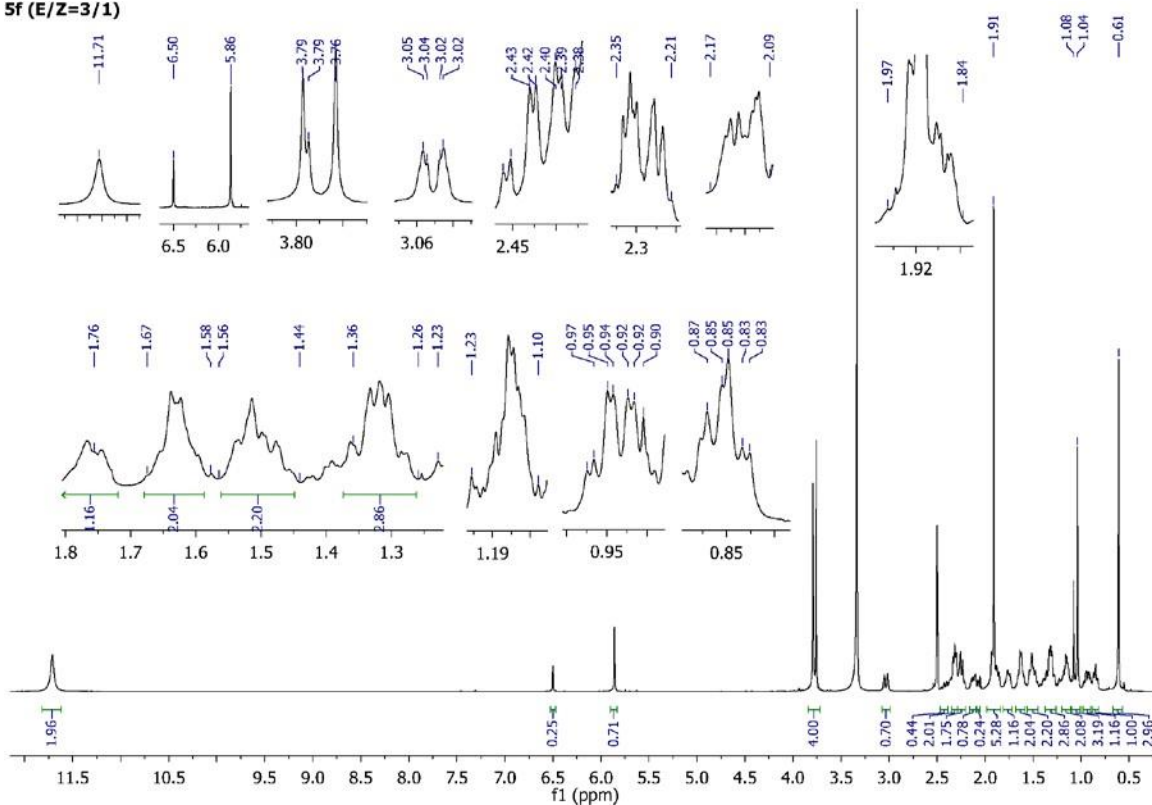
OB5057 #1-53 RT: 0.01-0.50 AV: 53 NL: 1.21E6
T: FTMS + p ESI Full ms [50.00-1500.00]



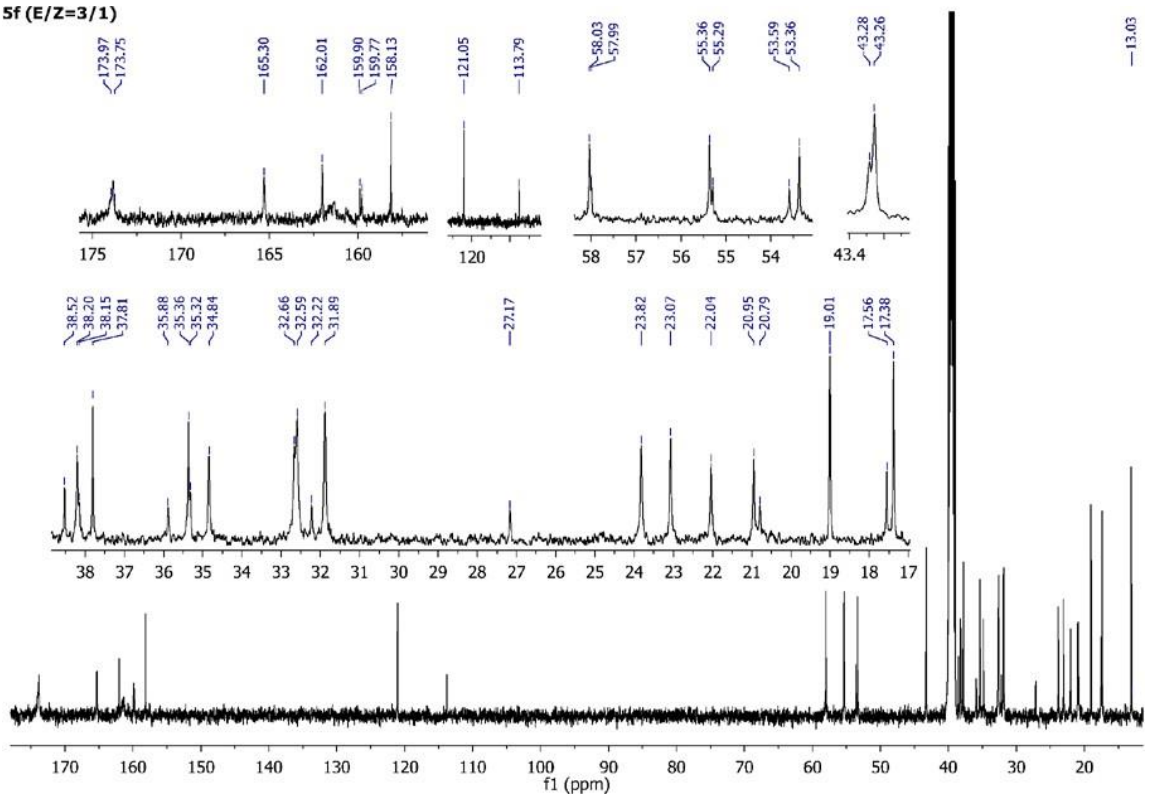
Compound 5f



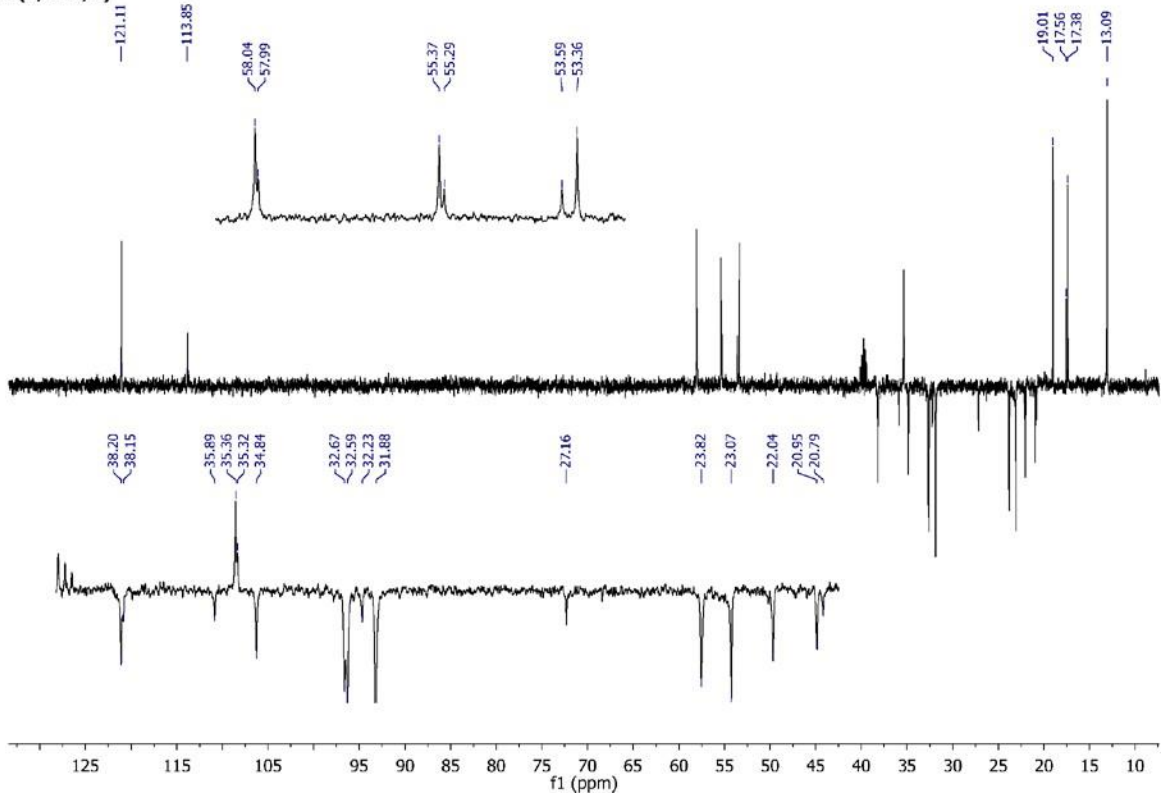
5f (E/Z=3/1)



5f (E/Z=3/1)

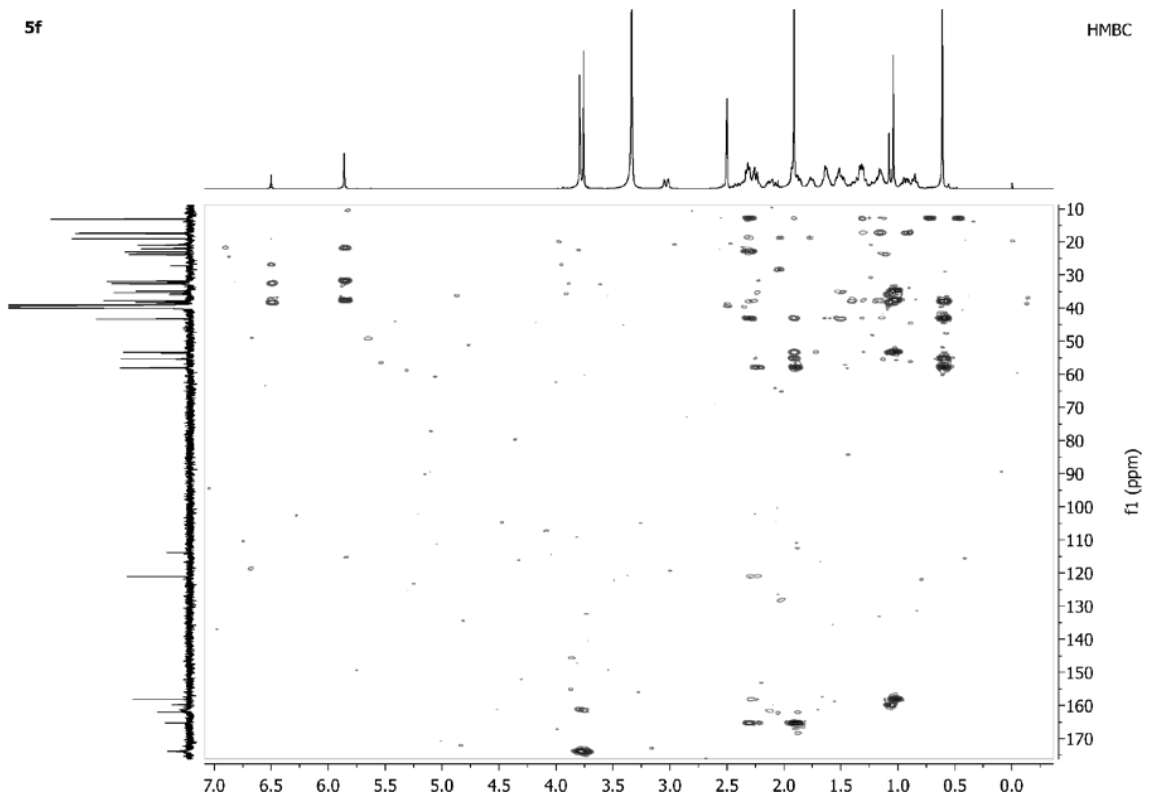


5f (E/Z=3/1)



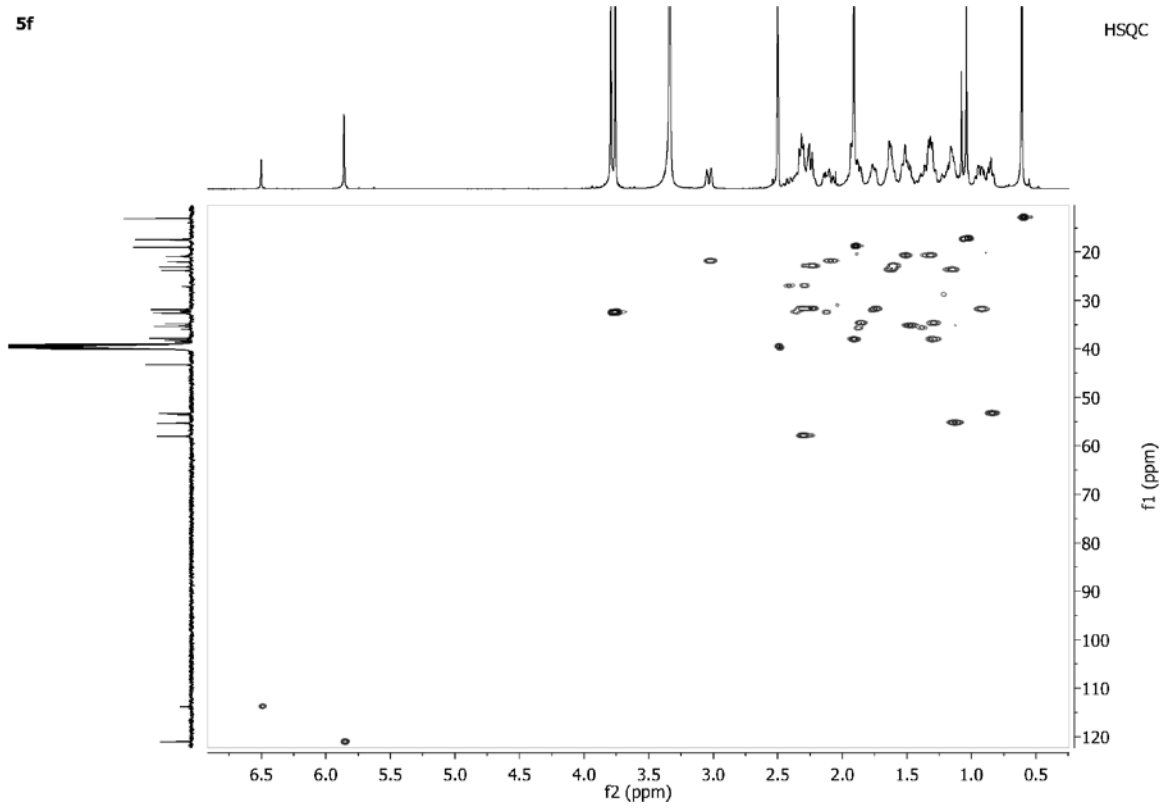
5f

HMBC



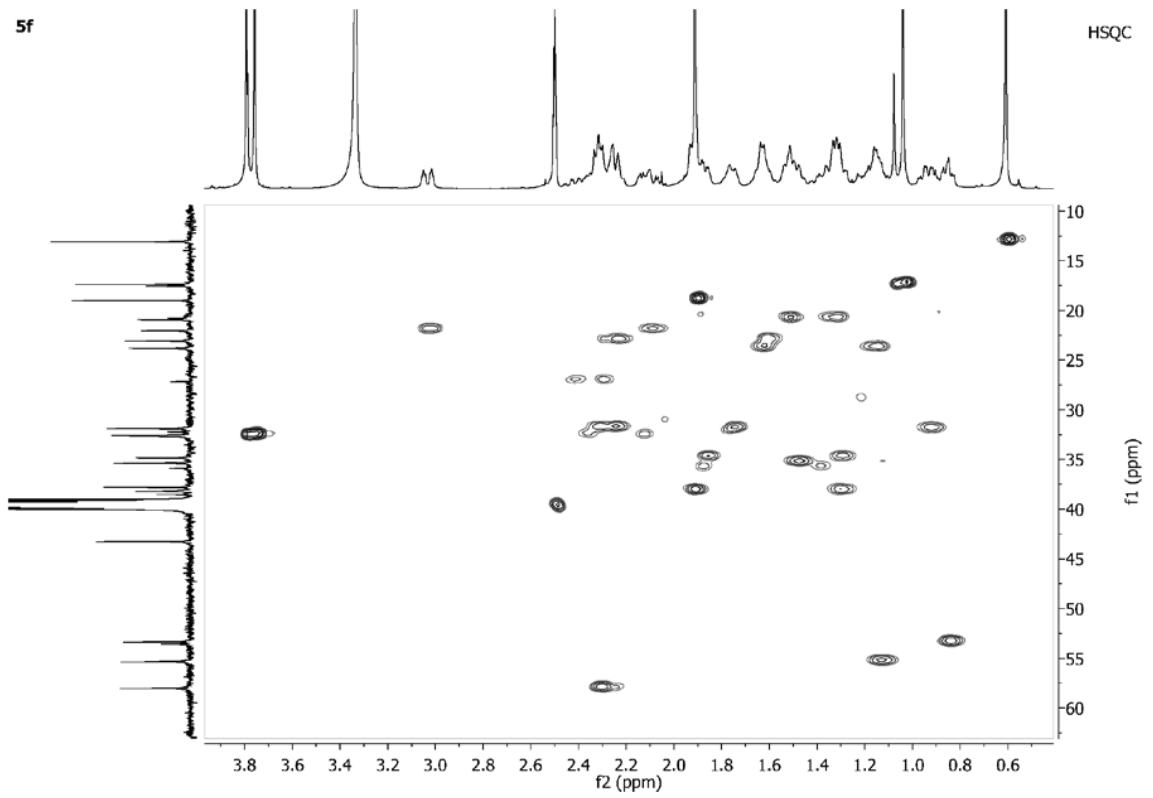
5f

HSQC

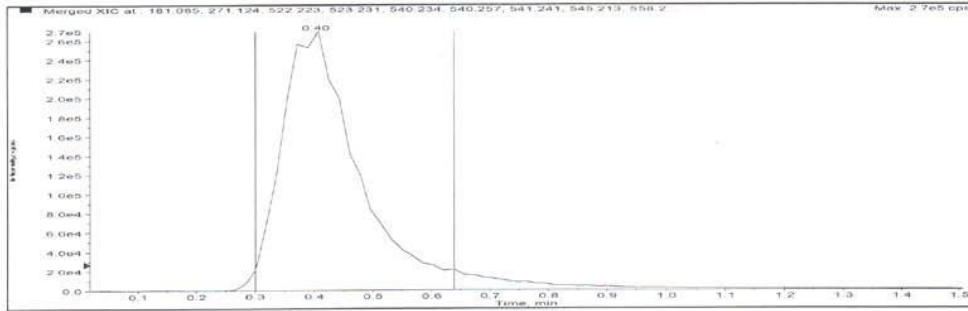


5f

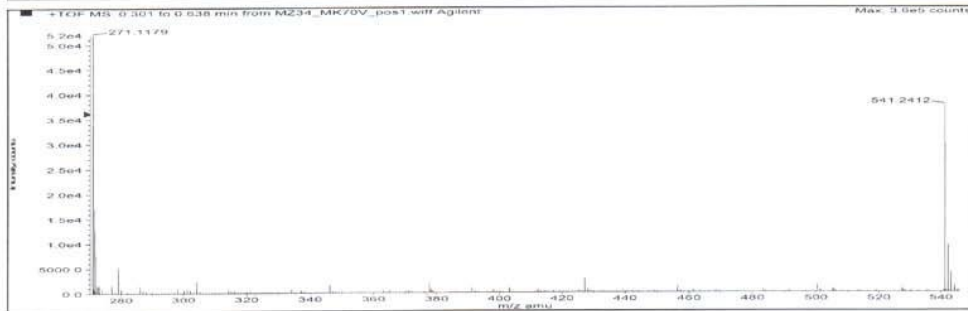
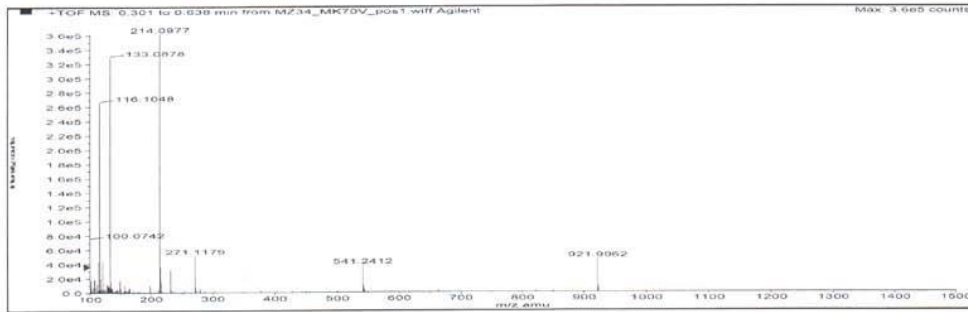
HSQC



Sample Name: MZ34 Sample Location: P1-D4 Sample Id: Operator: Milka
 Data File Name: D:\PE Sciex Data\Projects\Sladic\Data\MZ34_MK70V_pos1.wiff Acq Time: February 02 2016, 12:26:33 PM
 Method: d:\TOF_Data\damethods\Night_Seq_Comp_Ident1.anml\efc.xml



Merged XIC, Period#: 1 Experiment#: 1



| Formula | Compound name | Mass | Peak RT (min) | Peak area | Description |
|--------------|---------------|-----------|---------------|------------|-------------|
| C27H36N6O2S2 | -- | 540.23412 | 0.40 | 2.45726 E6 | -- |

| Species | Abundance (counts) | Ion Mass | Measured Mass | Error (mDa) | Error (ppm) | Ret. Time Error (min) |
|----------------------|--------------------|-----------|---------------|-------------|-------------|-----------------------|
| [M+2H] ²⁺ | 54175.16 | 271.12433 | 271.12463 | 0.29171 | 1.08 | -- |
| [M+H] ⁺ | 37573.94 | 541.24139 | 541.24142 | 0.02349 | 0.04 | -- |

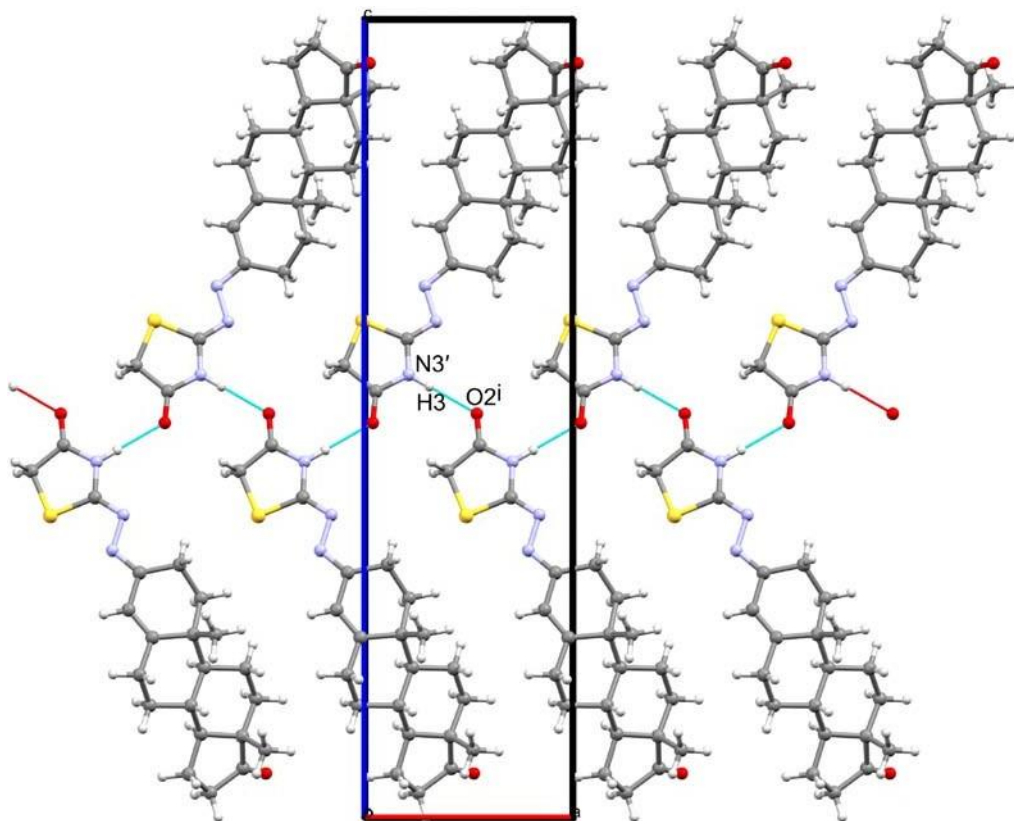


Figure S1. Chain of hydrogen bonded molecules propagating along crystallographic axis a , as supramolecular motif in crystal structure of 1. Hydrogen bond data: $N3'-H3 = 0.86 \text{ \AA}$, $H3 \cdots O2^i = 2.05(4) \text{ \AA}$, $N3' \cdots O2^i = 2.903(5) \text{ \AA}$, $\angle(N-H \cdots O3^i) = 170.1^\circ$; symmetry code (i): $1/2+x, 1/2-y, 1-z$.