

# Supporting Information

## Ring closure mechanisms mediated by laccase to synthesize phenothiazines, phenoxazines, and phenazines

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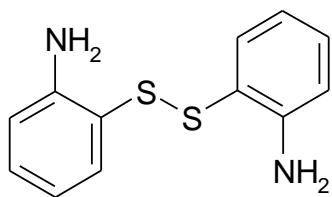
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## Structural Data of Compounds

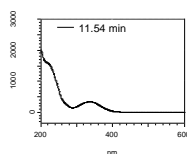
**Table S1:** Data of structural characterization of product **6** - product resulted from **3a**

**6** **2-Aminophenyl disulfide**

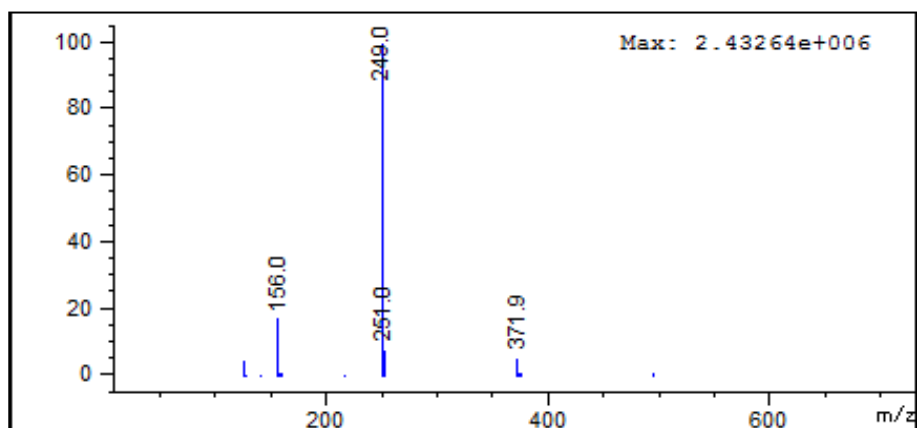


248.37 g/mol

**Fig. S1** UV-vis spectrum for product **6**



**Figure. S2** MS spectrum for product **6** - AP-ESI: pos. ion mode

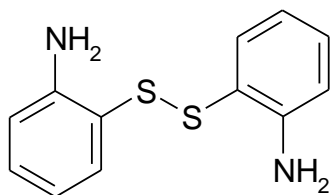


$R_f$  (HPLC) 11.54 min, UV-vis (MeOH)  $\lambda_{max}$  215, 334 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  249.0 (100).

**Table S2:** Data of structural characterization of **6(ref)** - 2-Aminophenyl disulfide (received from commercial supplier)

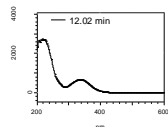
**6(ref)**

**2-Aminophenyl disulfide**

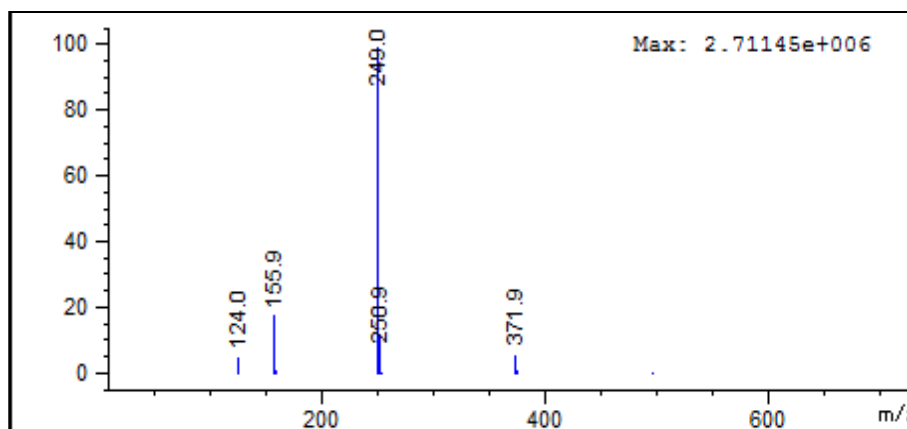


248.37 g/mol

**Figure. S3** UV-vis spectrum for **6(ref)**



**Figure. S4** MS spectrum for **6(ref)** - AP-ESI: pos. ion mode

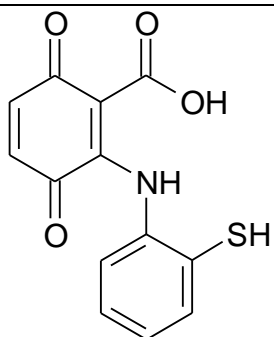


$R_f$  (HPLC) 12.02 min, UV-vis (MeOH)  $\lambda_{\max}$  218, 335 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  249.0 (100).

**Table S3:** Data of structural characterization of product **4a** - product resulted from **1a** and **3a**

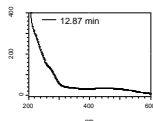
**4a**

**2-(2-Mercaptophenylamino)-3,6-dioxocyclohexa-1,4-diene-1-carboxylic acid**

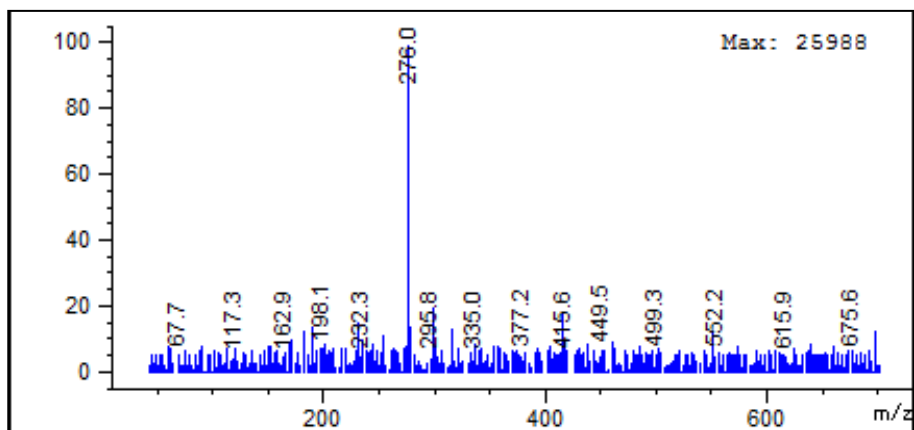


275.28 g/mol

**Figure. S5** UV-vis spectrum for product **4a**



**Figure. S6** MS spectrum for product **4a** - AP-ESI: pos. ion mode

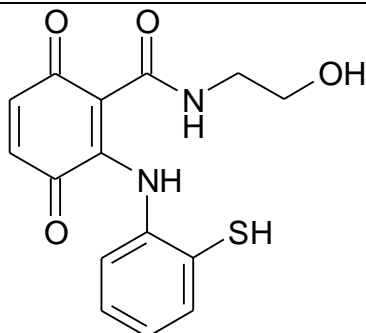


$R_f$  (HPLC) 12.87 min, UV-vis (MeOH)  $\lambda_{\max}$  448 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  276.0 (100).

**Table S4:** Data of structural characterization of product **4b** - product resulted from **1b** and **3a**

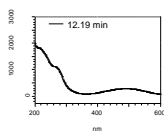
**4b**

**2-(2-Mercaptophenylamino)-N-(2-hydroxyethyl)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide**

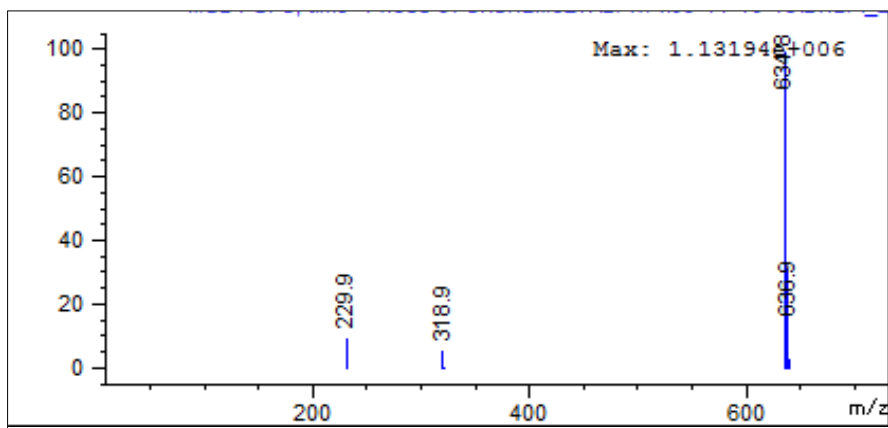


318.35 g/mol

**Figure. S7** UV-vis spectrum for product **4b**



**Figure. S8** MS spectrum for product **4b** - AP-ESI: pos. ion mode

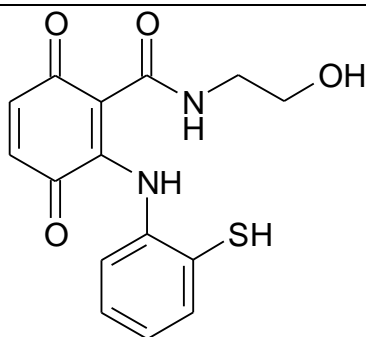


$R_f$  (HPLC) 12.19 min, UV-vis (MeOH)  $\lambda_{max}$  215, 263, 488 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  318.9 (5).

**Table S5:** Data of structural characterization of product **4b** - product resulted from **1a** and 2-aminophenyl disulfide (received from commercial supplier)

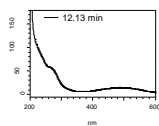
**4b**

**2-(2-Mercaptophenylamino)-N-(2-hydroxyethyl)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide**

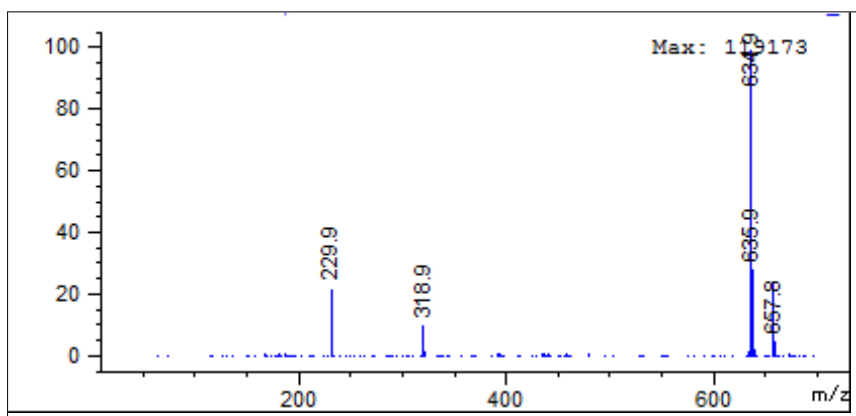


318.35 g/mol

**Figure. S9** UV-vis spectrum for product **4b**



**Figure. S10** MS spectrum for product **4b** - AP-ESI: pos. ion mode



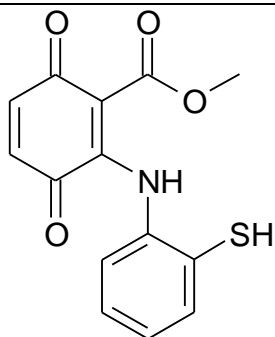
$R_f$  (HPLC) 12.13 min, UV-vis (MeOH)  $\lambda_{\max}$  214, 261, 486 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  318.9 (10).



**Table S6:** Data of structural characterization of product **4c** - product resulted from **1c** and **3a**

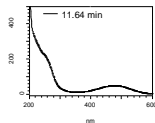
**4c**

**2-(2-Mercaptophenylamino)-3,6-dioxocyclohexa-1,4-diene-1-carboxylic acid methylester**

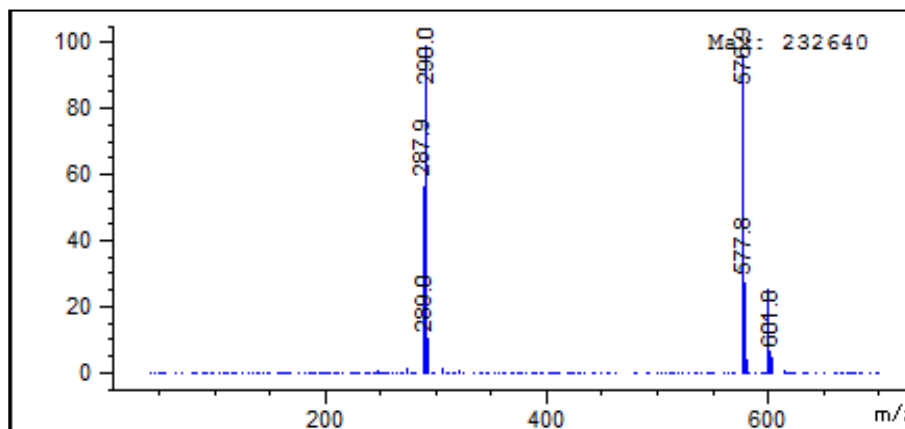


289.31 g/mol

**Figure. S11** UV-vis spectrum for product **4c**



**Figure. S12** MS spectrum for product **4c** - AP-ESI: pos. ion mode

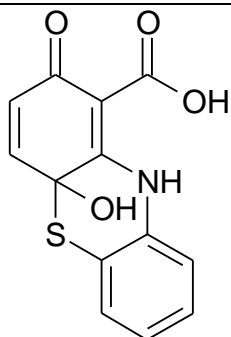


$R_f$  (HPLC) 11.64 min, UV-vis (MeOH)  $\lambda_{\max}$  210, 413 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  290.0 (100).

**Table S7:** Data of structural characterization of product **5a** - product resulted from **1a** and **3a**

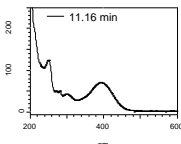
**5a**

**4a-Hydroxy-N-(2-hydroxyethyl)-2-oxo-10H-phenothiazine-1-carboxylic acid**

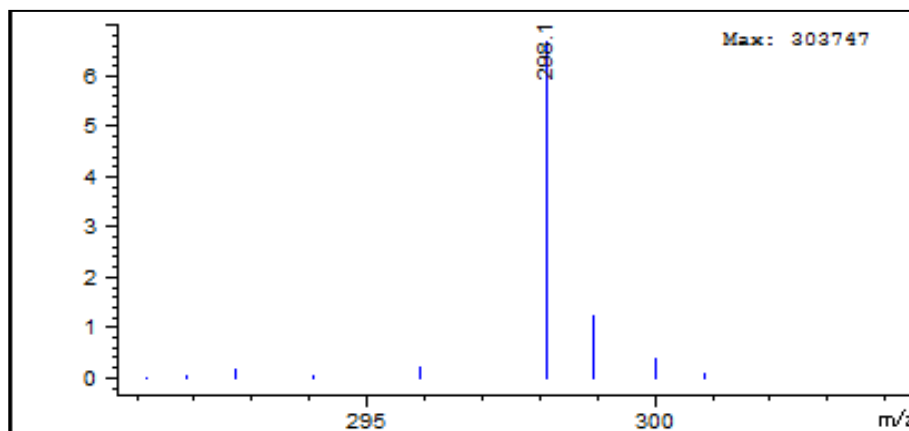
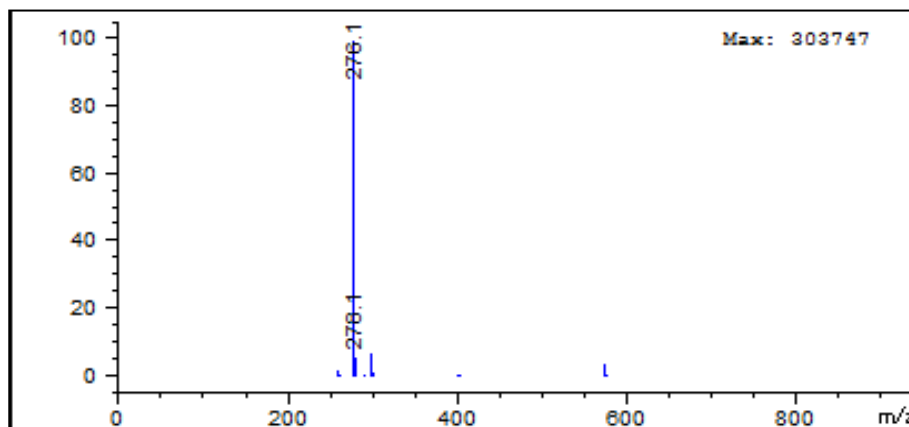


275.28 g/mol

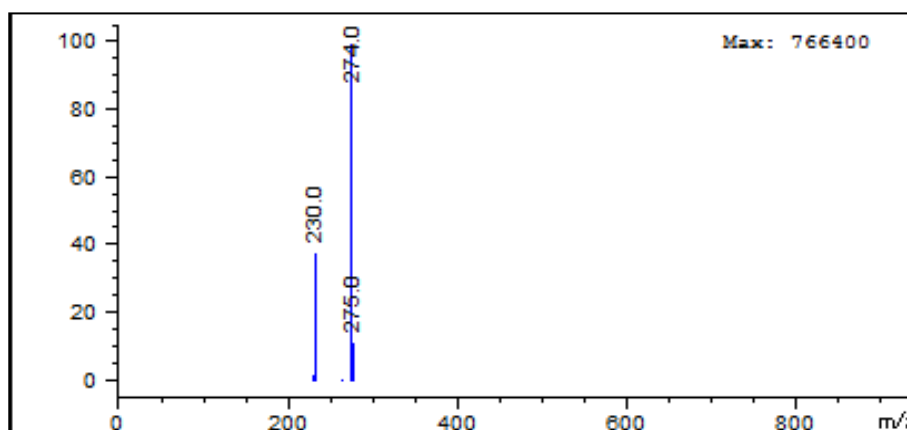
**Figure. S13** UV-vis spectrum for product **5a**



**Figure. S14** MS spectra for product **5a** - AP-ESI: pos. ion mode



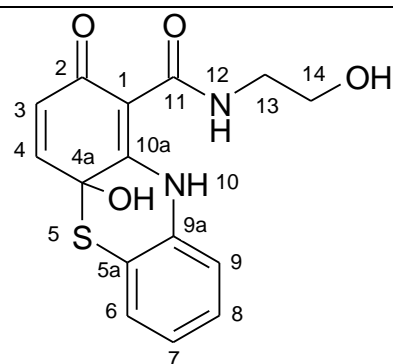
**Figure. S15** MS spectrum for product **5a** - AP-ESI: neg. ion mode



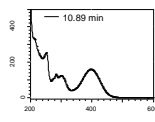
Synthesis and isolation as described above.  $R_f$  (HPLC) 11.16 min, UV-vis (MeOH)  $\lambda_{\max}$  250, 280, 299, 393 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  276.1 (100),  $[M+Na]^+$  298.1 (7); AP-ESI: neg. ion mode  $[M-H]^-$  274.0 (100).

**Table S8:** Data of structural characterization of product **5b** - product resulted from **1b** and **3a**

**5b** **4a-Hydroxy-N-(2-hydroxyethyl)-2-oxo-10H-phenothiazine-1-carboxamide**

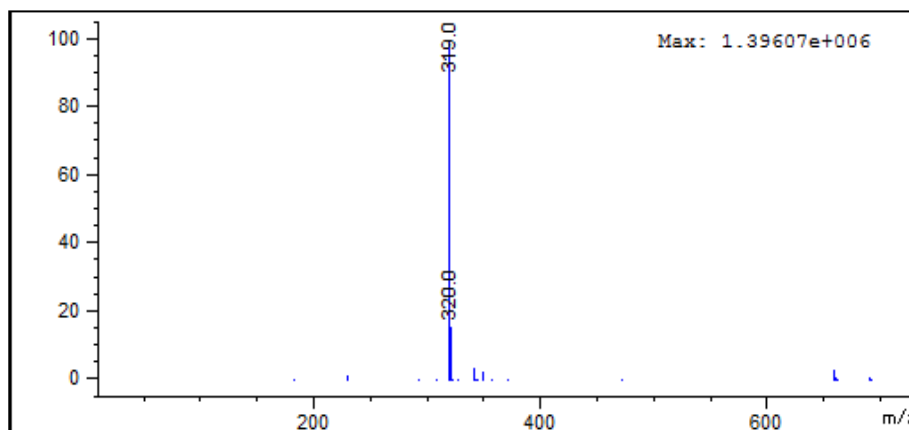


**Figure. S16** UV-vis spectrum for product **5b**

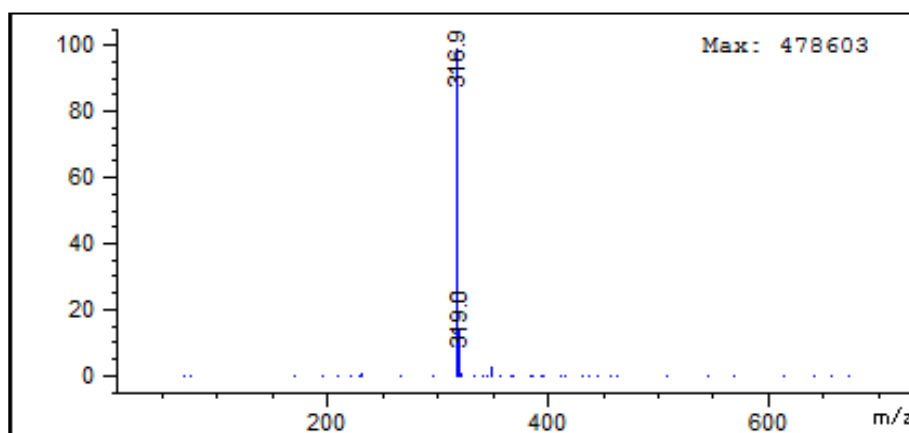


318.35 g/mol

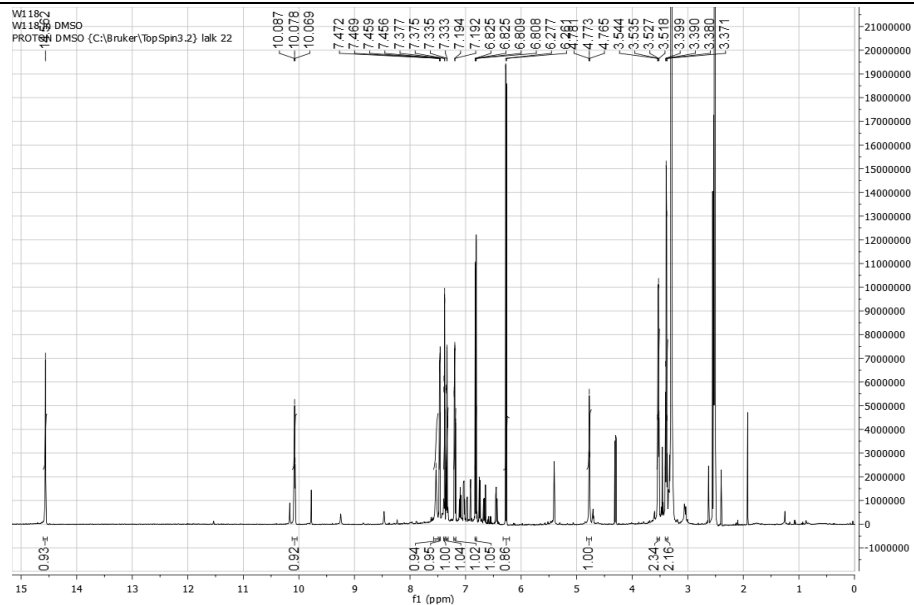
**Figure. S17** MS spectrum for product **5b** - AP-ESI: pos. ion mode



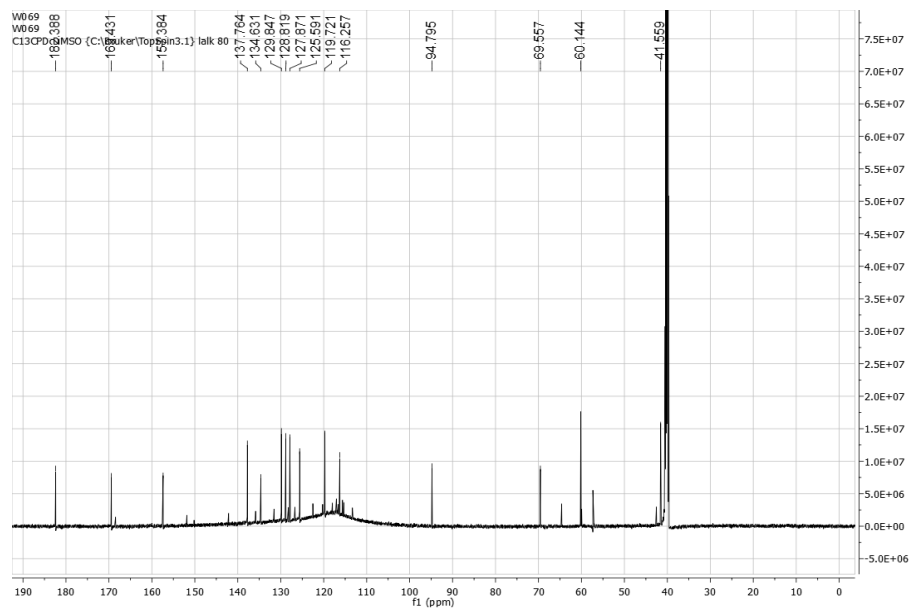
**Figure. S18** MS spectrum for product **5b** - AP-ESI: neg. ion mode



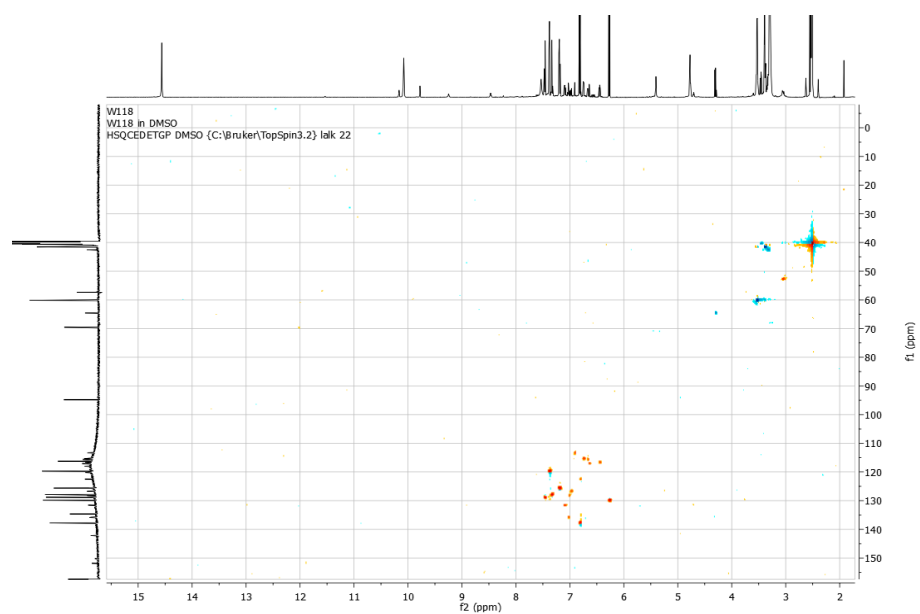
**Figure. S19**  $^1\text{H}$  NMR for product **5b**



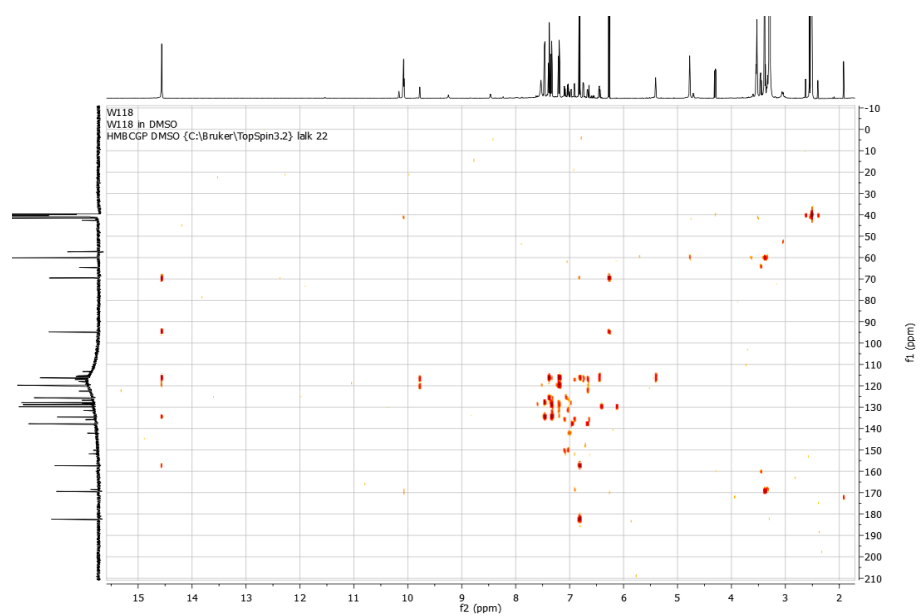
**Figure. S20**  $^{13}\text{C}$  NMR for product **5b**



**Figure. S21 HSQC for product 5b**



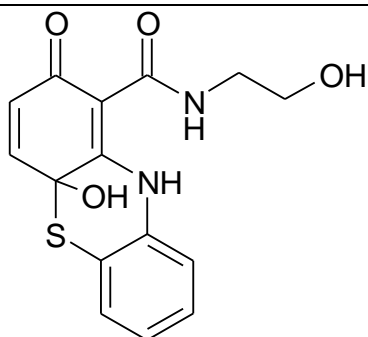
**Figure. S22 HMBC for product 5b**



**Table S9:** Data of structural characterization of product **5b** - product resulted from **1b** and 2-aminophenyl disulfide

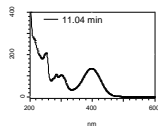
**5b**

**4a-Hydroxy-N-(2-hydroxyethyl)-2-oxo-10H-phenothiazine-1-carboxamide**

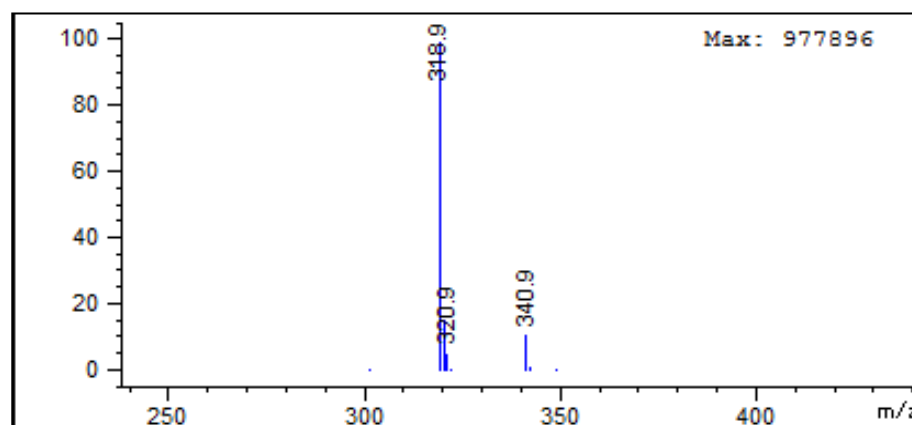
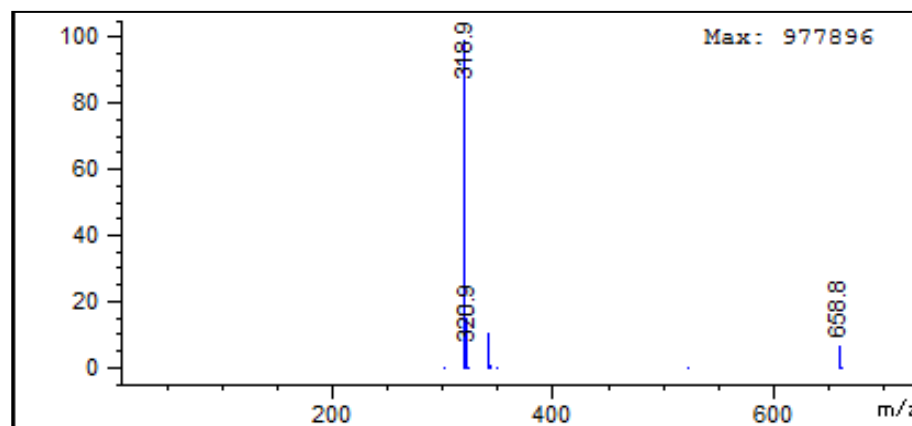


318.35 g/mol

**Figure. S23** UV-vis spectrum for product **5b**



**Figure. S24** MS spectra for product **5b** - AP-ESI: pos. ion mode



$R_f$  (HPLC) 11.05 min, UV-vis (MeOH)  $\lambda_{\max}$  252, 284, 300, 397 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  318.9 (100),  $[M+Na]^+$  340.9 (11),  $[2M+Na]^+$  658.8 (5).

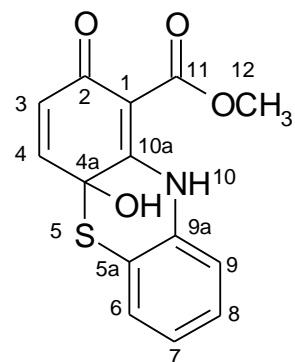
**Table S10:** Data of structural characterization of product **5c** - product resulted from **1c** and **3a**

**5c**

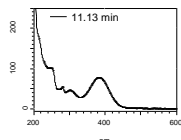
**4a-Hydroxy-N-(2-hydroxyethyl)-2-oxo-10H-phenothiazine-1-carboxylic acid methylester**

**5c**

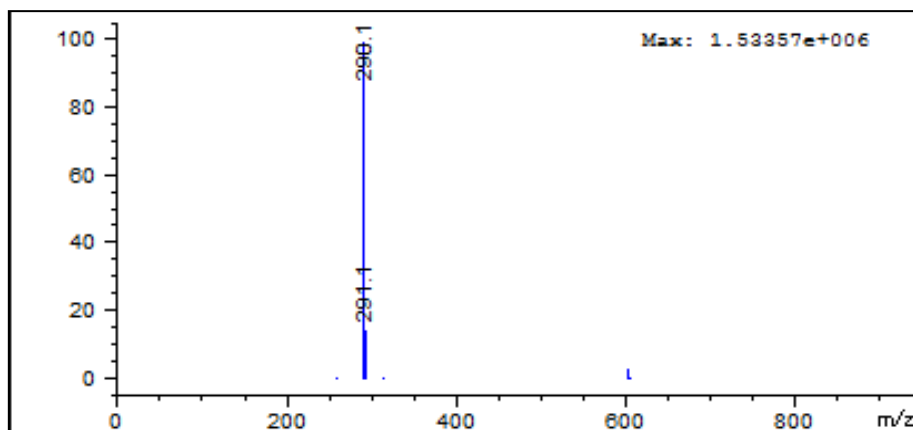
**Figure. S25** UV-vis spectrum for product **5c**



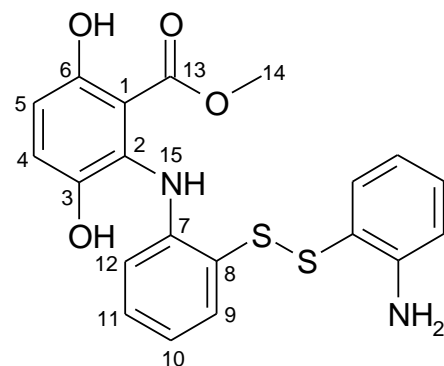
289.31 g/mol



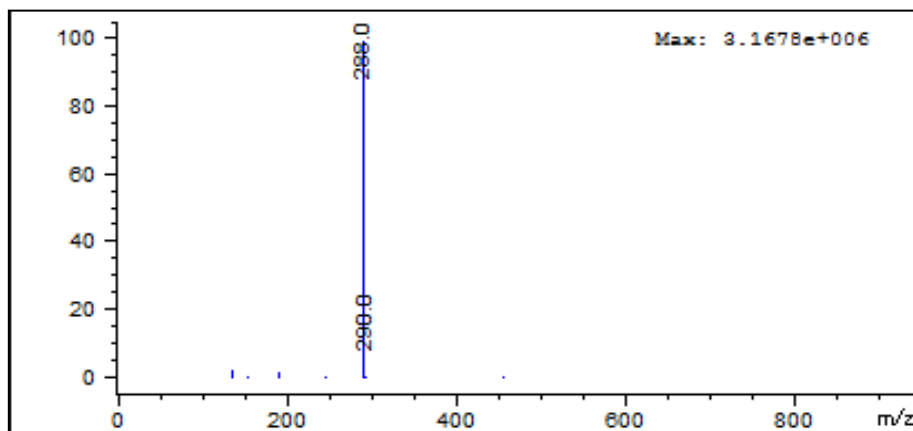
**Figure. S26** MS spectrum for product **5c** - AP-ESI: pos. ion mode



**8c**

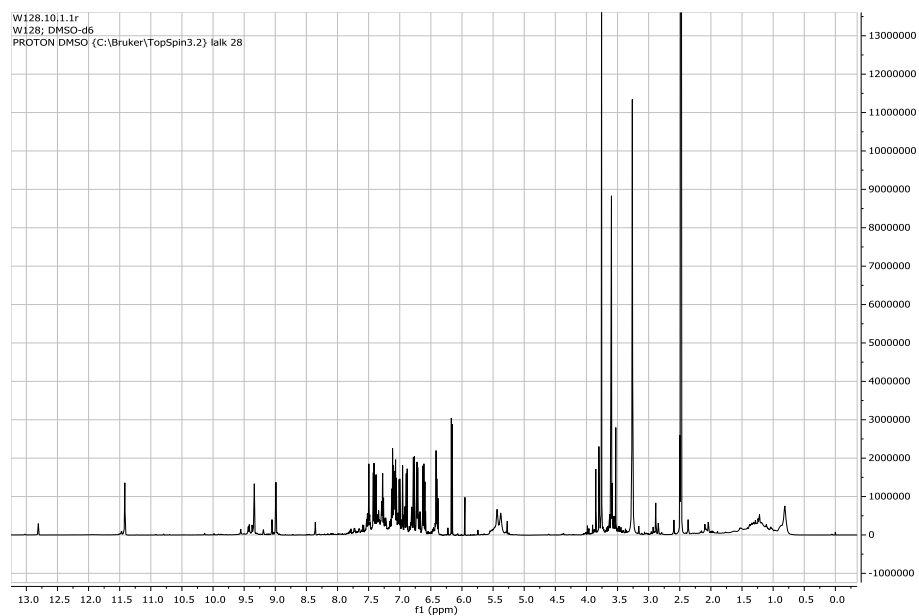


**Figure. S27** MS spectrum for product **5c** - AP-ESI: neg. ion mode





**Figure. S28**  $^1\text{H}$  NMR for product **5c** and **8c**



**Figure. S29**  $^{13}\text{C}$  NMR for product **5c** (**8c**)

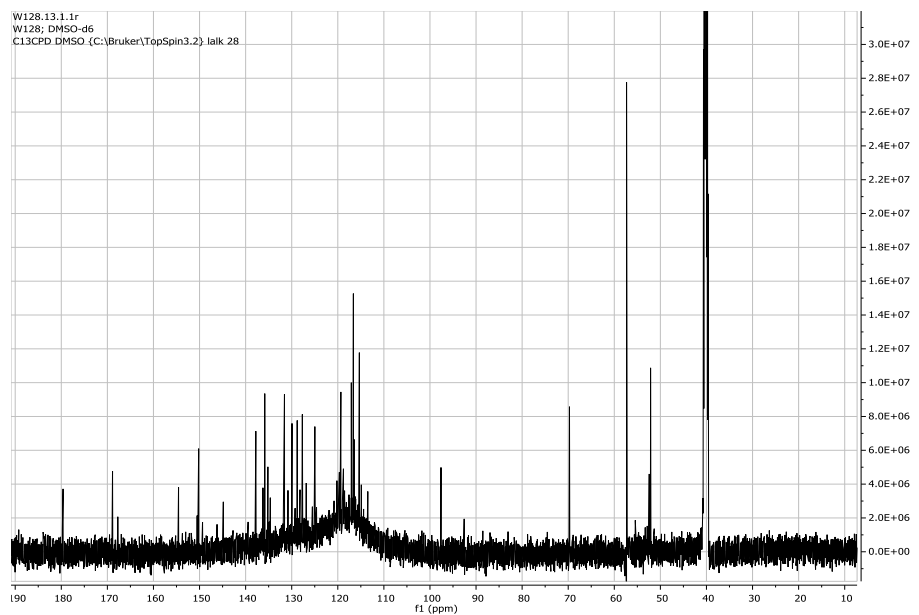


Figure. S30 HSQC for product 5c (8c)

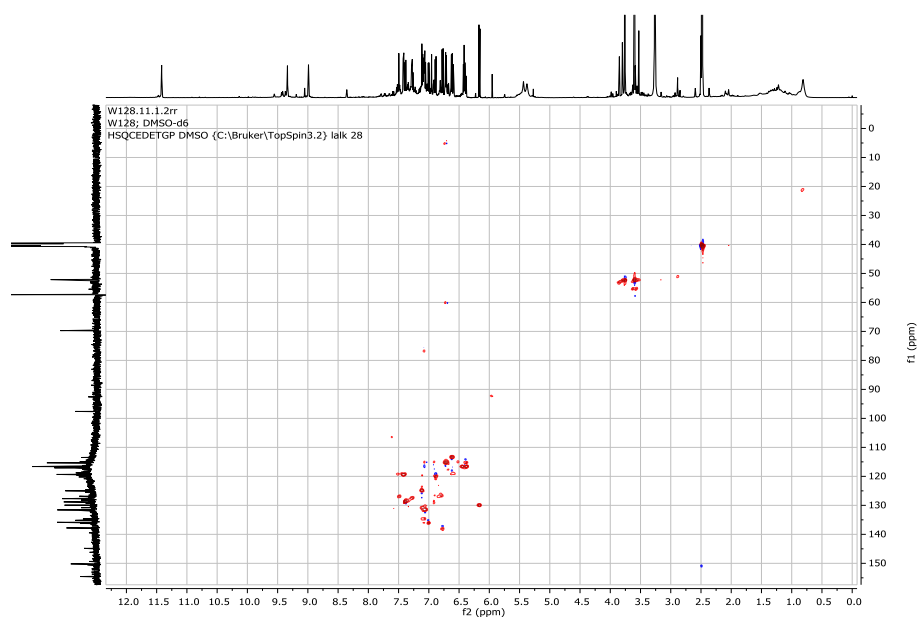
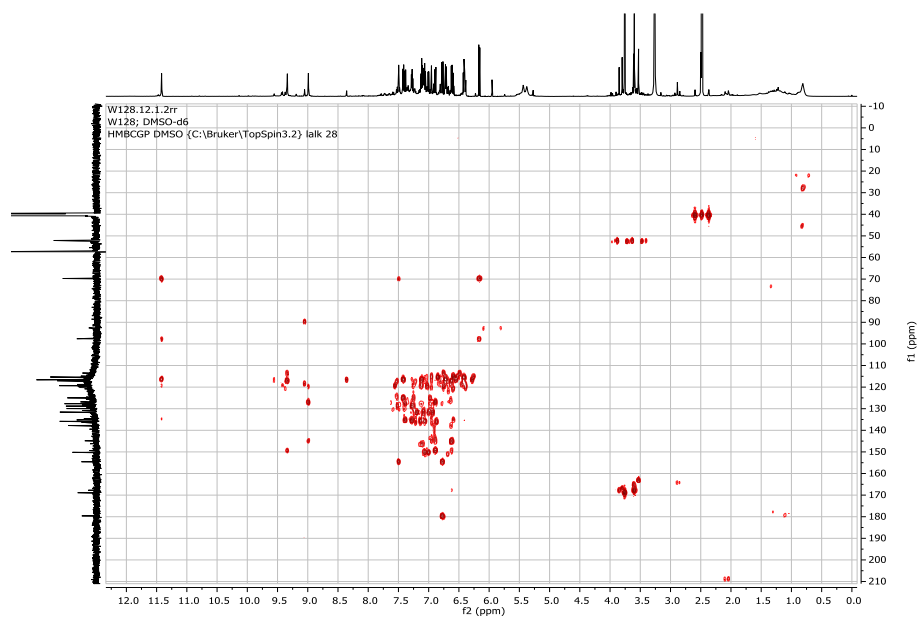


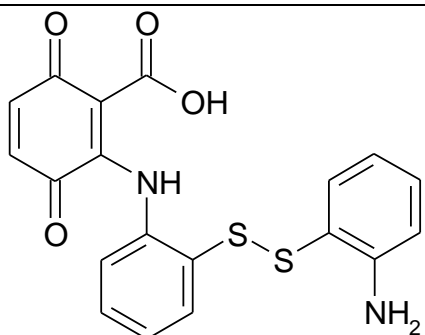
Figure. S31 HMBC for product 5c (8c)



**Table S11:** Data of structural characterization of product **7a** - product resulted from **1a** and **3a**

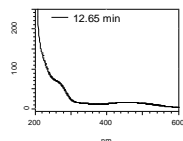
**7a**

**[2-[(2-Aminophenyl)disulfanyl]anilino]-3,6-dioxocyclohexa-1,4-diene-1-carboxylic acid**

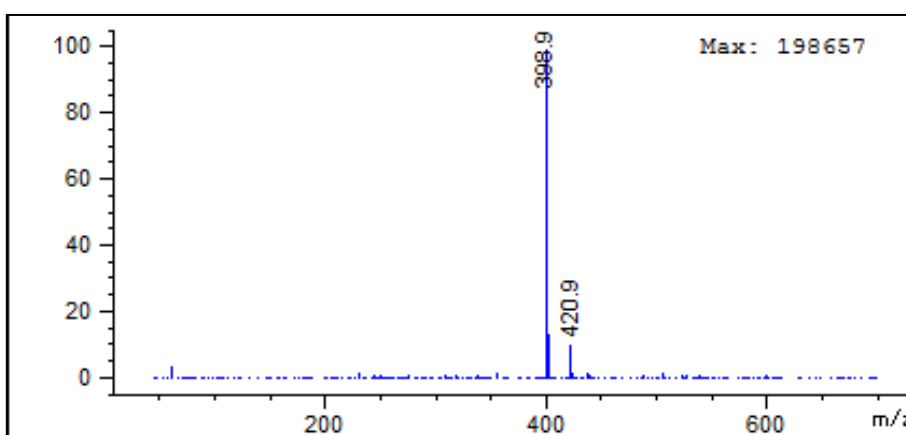


398.46 g/mol

**Figure. S32** UV-vis spectrum for product **7a**



**Figure. S33** MS spectrum for product **7a** - AP-ESI: pos. ion mode

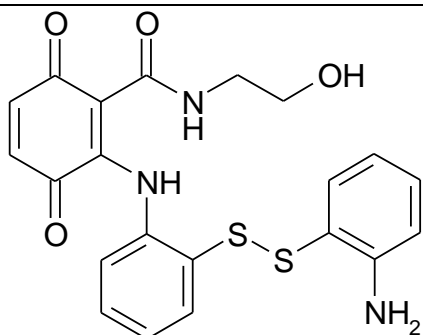


$R_f$  (HPLC) 12.60 min, UV-vis (MeOH)  $\lambda_{\max}$  210, 455 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  398.9 (100),  $[M+Na]^+$  420.9 (10).

**Table S12:** Data of structural characterization of product **7b** - product resulted from **1b** and **3a**

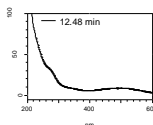
**7b**

**2-[2-[(2-Aminophenyl)disulfanyl]anilino]-N-(2-hydroxyethyl)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide**

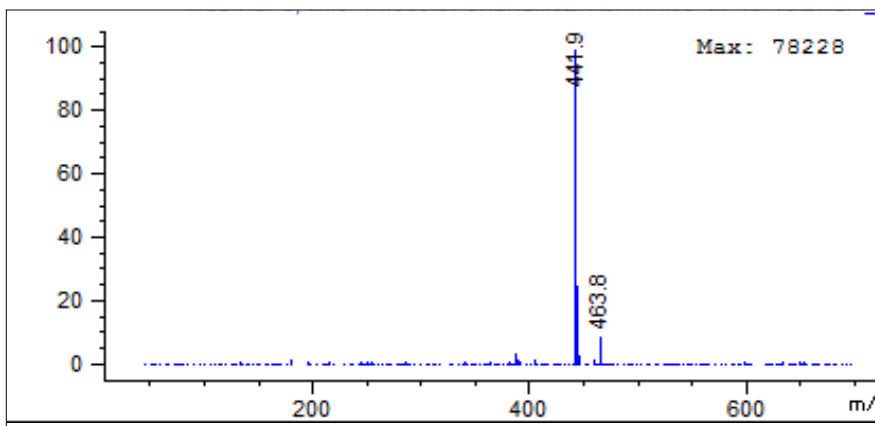


441.53 g/mol

**Figure. S34** UV-vis spectrum for product **7b**



**Figure. S35** MS spectrum for product **7b** - AP-ESI: pos. ion mode

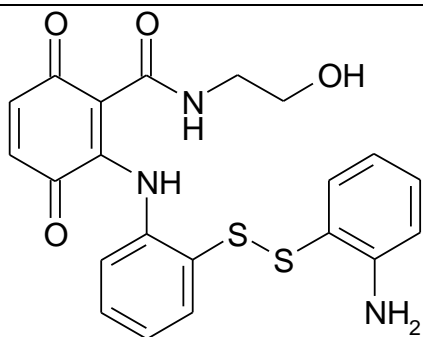


$R_f$  (HPLC) 12.48 min, UV-vis (MeOH)  $\lambda_{\max}$  209, 492 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  441.9 (100),  $[M+Na]^+$  463.9 (8).

**Table S13:** Data of structural characterization of product **7b** - product resulted from **1b** and 2-aminophenyl disulfide (received from commercial supplier)

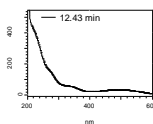
**7b**

**2-[2-[(2-Aminophenyl)disulfanyl]anilino]-N-(2-hydroxyethyl)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide**

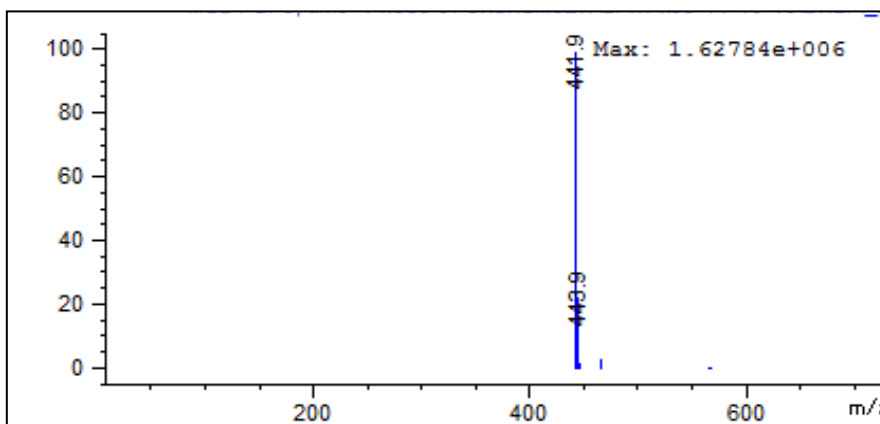


441.53 g/mol

**Figure. S36** UV-vis spectrum for product **7b**



**Figure. S37** MS spectrum for product **7b** - AP-ESI: pos. ion mode



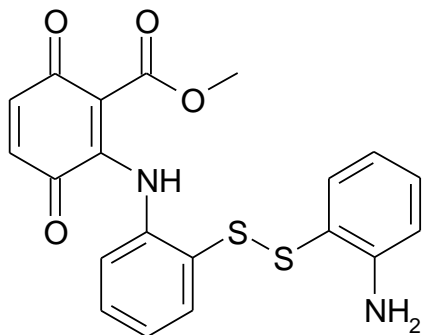
$R_f$  (HPLC) 12.43 min, UV-vis (MeOH)  $\lambda_{\max}$  209, 492 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  441.9 (100).

**Table S14:** Data of structural characterization of products **7c**, **8c** - products resulted from **1c** and **3a**

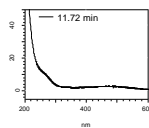
**7c** [2-[(2-Aminophenyl)disulfanyl]anilino]-3,6-dioxocyclohexa-1,4-diene-1-carboxylic acid methylester

**8c** [2-[(2-aminophenyl)disulfanyl]anilino]-3,6-dihydroxy-benzoic acid

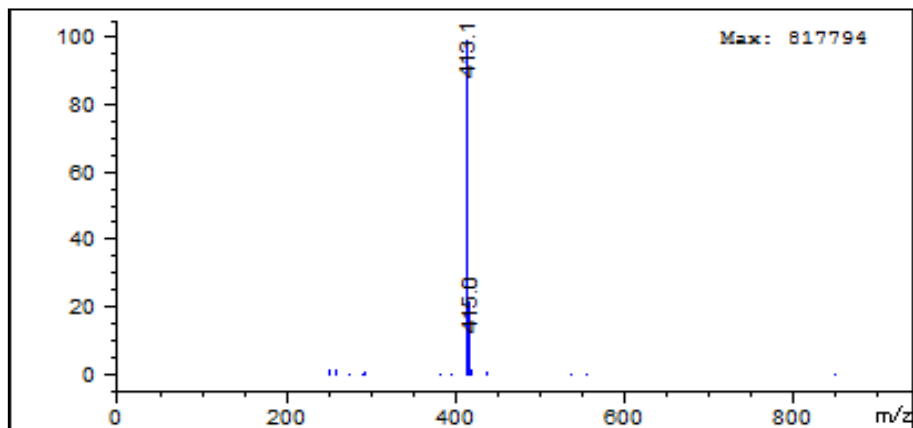
**7c** **Figure. S38** UV-vis spectrum for product **7c**



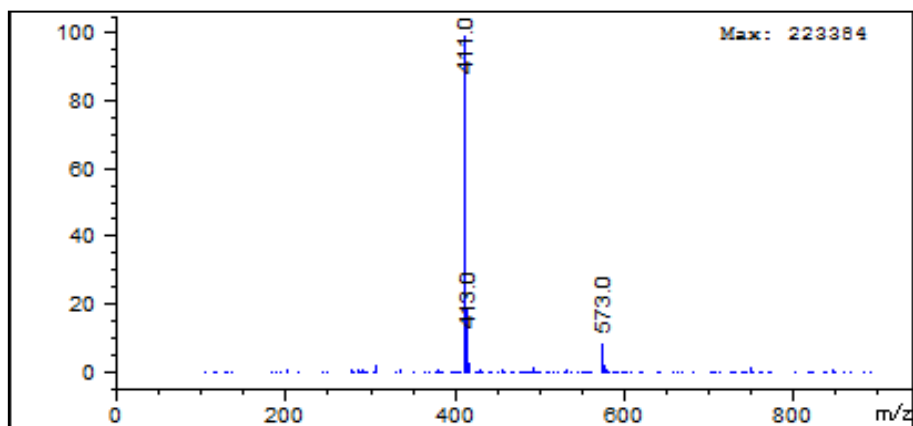
412.49 g/mol



**Figure. S39** MS spectrum for product **7c** - AP-ESI: pos. ion mode

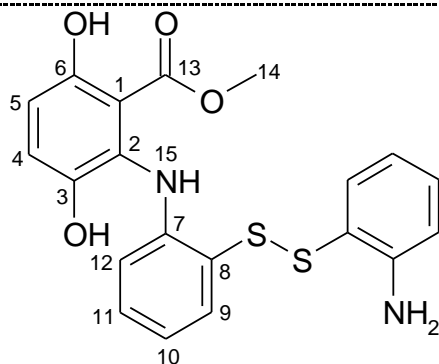


**Figure. S40** MS spectrum for product **7c** - AP-ESI: neg. ion mode



**8c** for <sup>1</sup>H NMR, <sup>13</sup>C NMR, HMBC, and HSQC spectra see structural data of product **5c** 4a-Hydroxy-N-(2-hydroxyethyl)-2-oxo-10H-

phenothiazine-1-carboxylic acid methylester



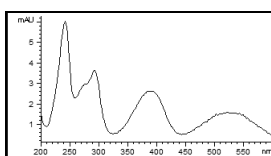
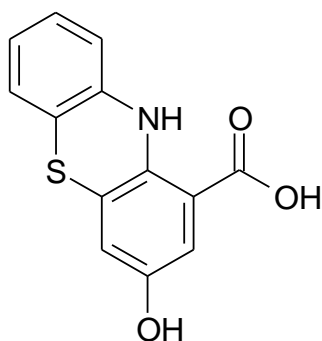
Data for **7c**:  $R_f$  (HPLC) 11.72 min, UV-vis (MeOH)  $\lambda_{\max}$  210, 473 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  413.1 (100); AP-ESI: neg. ion mode  $[M-H]^-$  411.0 (100).

**Table S15:** Data of structural characterization of products **9a**, **10a** - product resulted from **1a** and **3a**

**9a** **3-Hydroxy-10H-phenothiazine-1-carboxylic acid**

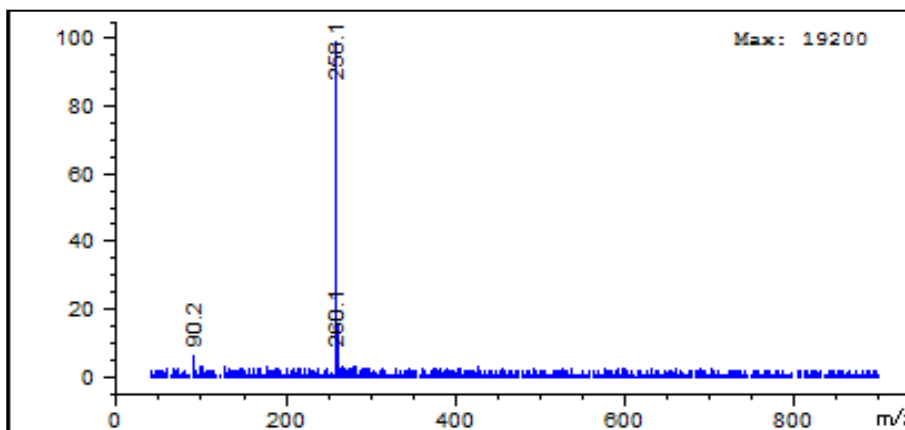
**10a** **3-Oxo-phenothiazine-1-carboxylic acid**

**9a** **Figure. S41 UV-vis spectrum for product 9a, 10a**

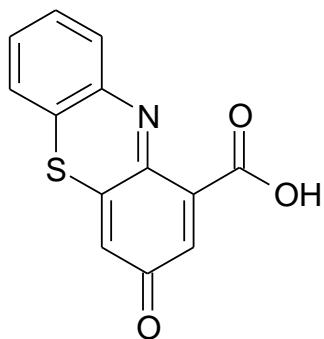


**Figure. S42** MS spectrum for product **9a**, **10a** - AP-ESI: pos. ion mode

259.29 g/mol



**10a**



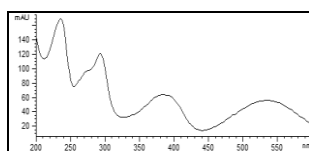
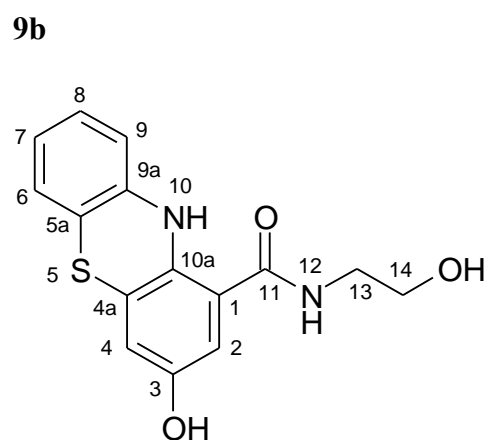
257.27 g/mol

**10a:**  $R_f$  (LC/MS) 5.81 min, UV-vis (MeOH)  $\lambda_{\text{max}}$  240, 292, 390, 528 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  258.1 (100). **9a:** MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  260.1 (6)

**Table S16:** Data of structural characterization of products **9b**, **10b** - products resulted from **1b** and **3a**

<b>9b</b>	<b>3-Hydroxy-N-(2-hydroxyethyl)-10H-phenothiazine-1-carboxamide</b>
<b>10b</b>	<b>N-(2-Hydroxyethyl)-3-oxo-phenothiazine-1-carboxamide</b>

**Figure. S43** UV-vis spectrum for product **9b**, **10b**

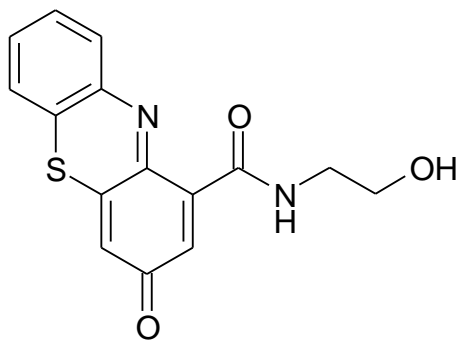


302.35 g/mol

**10b**

**Figure. S44** MS spectra for product **9b**, **10b** - AP-ESI: pos. ion mode





300.34 g/mol

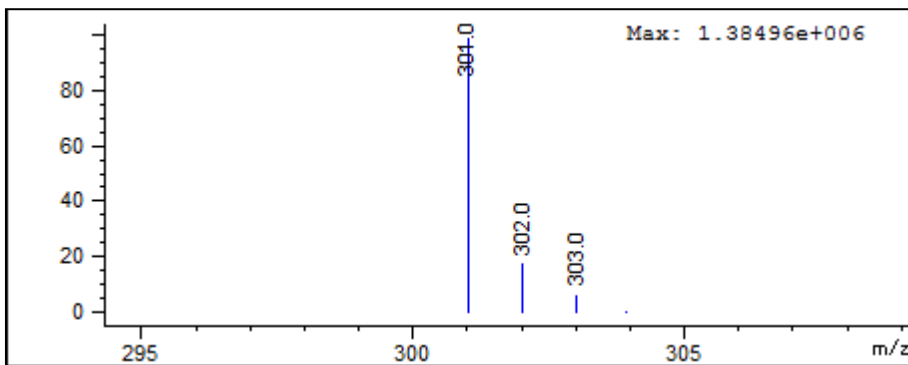
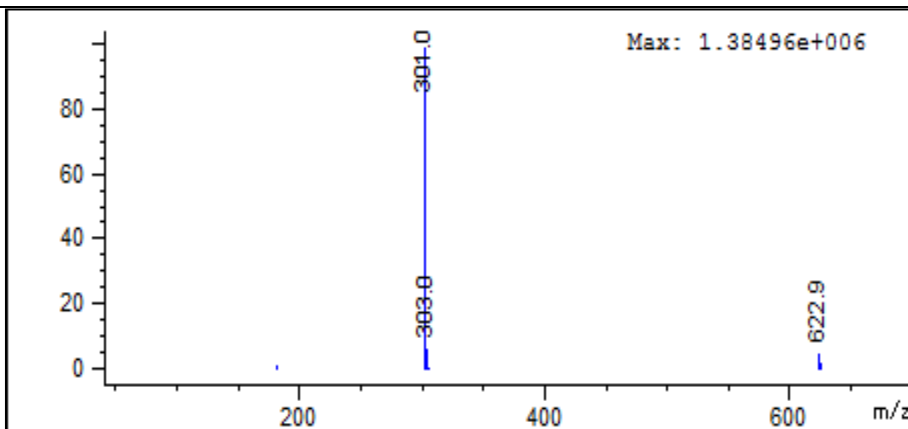


Figure. S45 <sup>1</sup>H NMR for product 9b

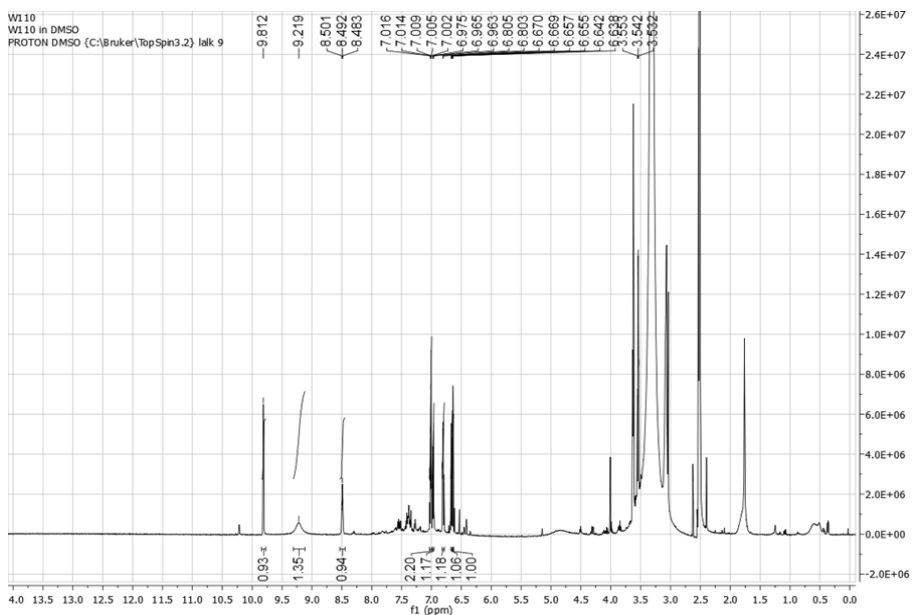


Figure. S46  $^{13}\text{C}$  NMR for product **9b**

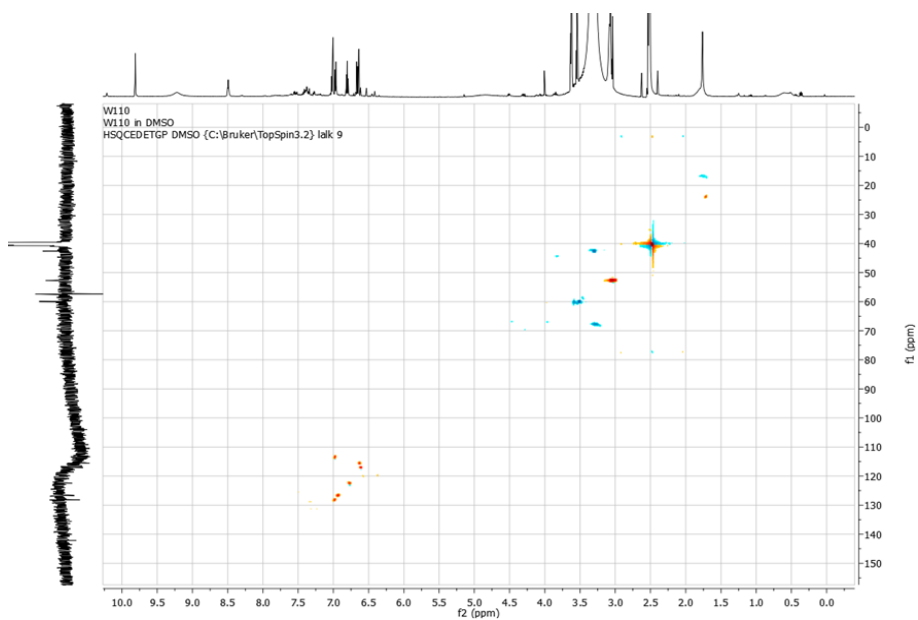
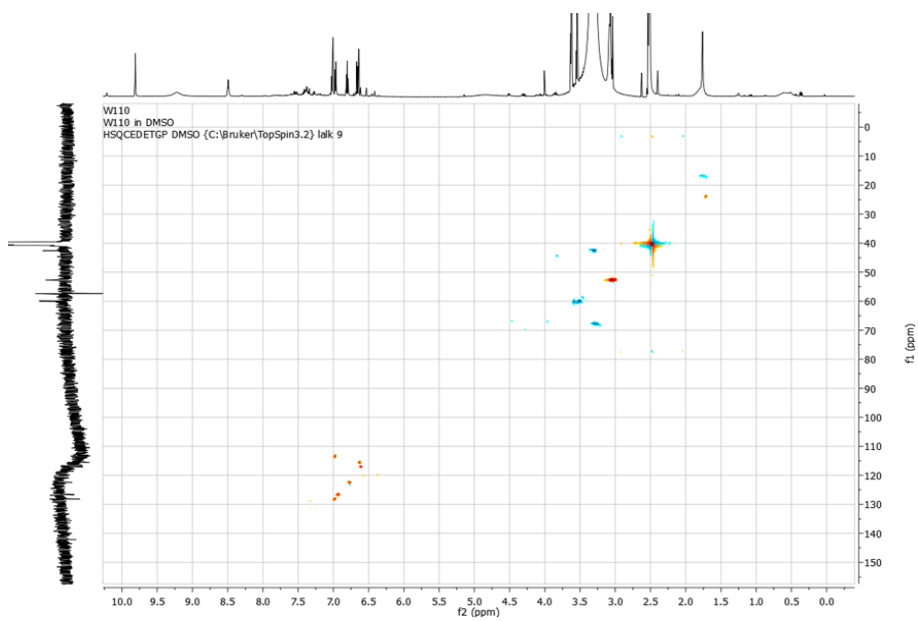
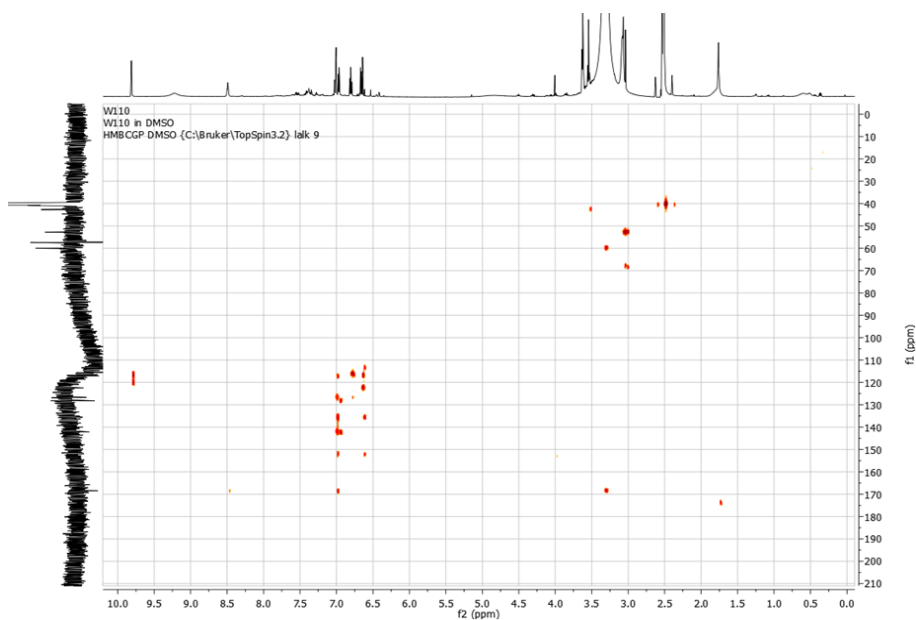


Figure. S47 HSQC for product **9b**



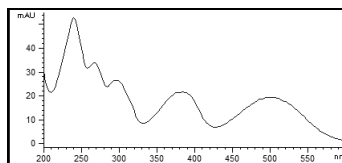
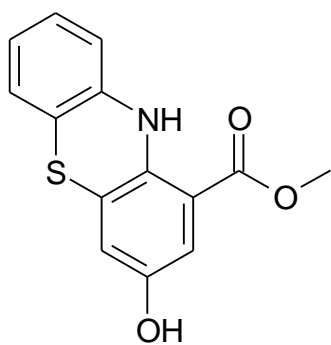
**Figure. S48** HMBC for product **9b**



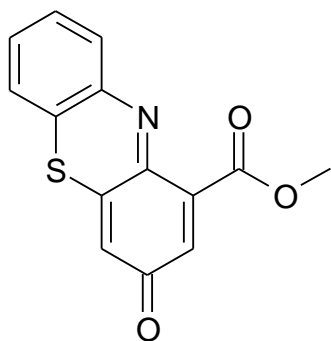
**Table S17:** Data of structural characterization of products **9c**, **10c** - product resulted from **1c** and **3a**

<b>9c</b>	<b>3-Hydroxy-10H-phenothiazine-1-carboxylic acid methylester</b>
<b>10c</b>	<b>3-Oxo-phenothiazine-1-carboxylic acid methylester</b>

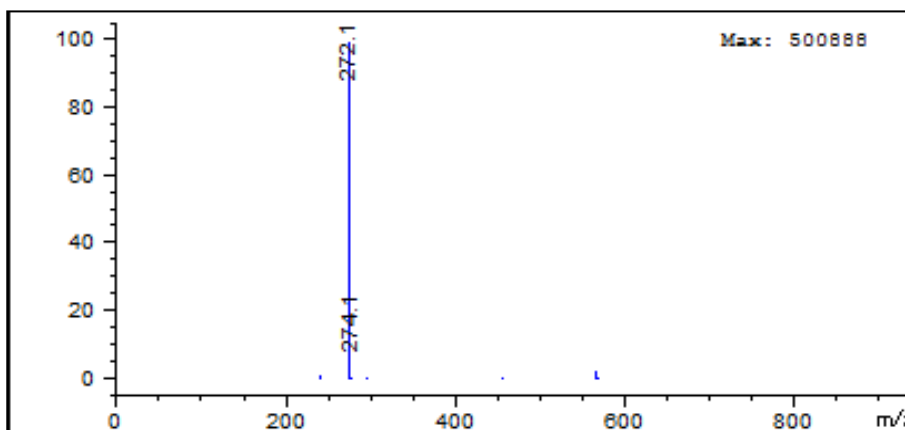
**9c** **Figure. S49** UV-vis spectrum for product **9c**, **10c**



273.31 g/mol

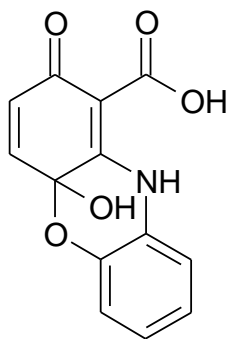
**10c****Figure. S50** MS spectrum for product **9c**, **10c** - AP-ESI: pos. ion mode

271.30 g/mol

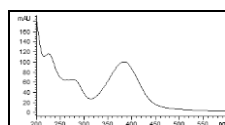


**10c**:  $R_f$  (LC/MS) 14.67 min, UV-vis (MeOH)  $\lambda_{\max}$  241, 269, 297, 382, 503 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  272.1 (100). **9c**: MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  274.1 (4).

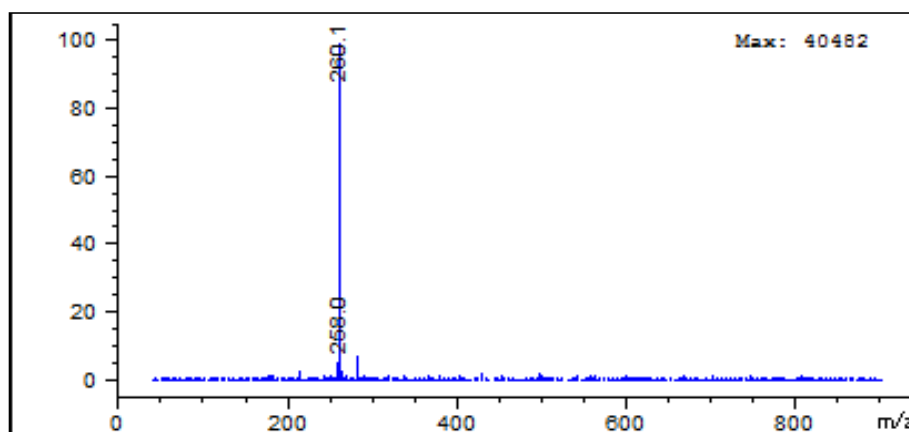
**Table S18**: Data of structural characterization of product **11a** - product resulted from **1a** and **3b**

**11a****4a-Hydroxy-2-oxo-10H-phenoxazine-1-carboxylic acid****Figure. S51** UV-vis spectrum for product **11a**

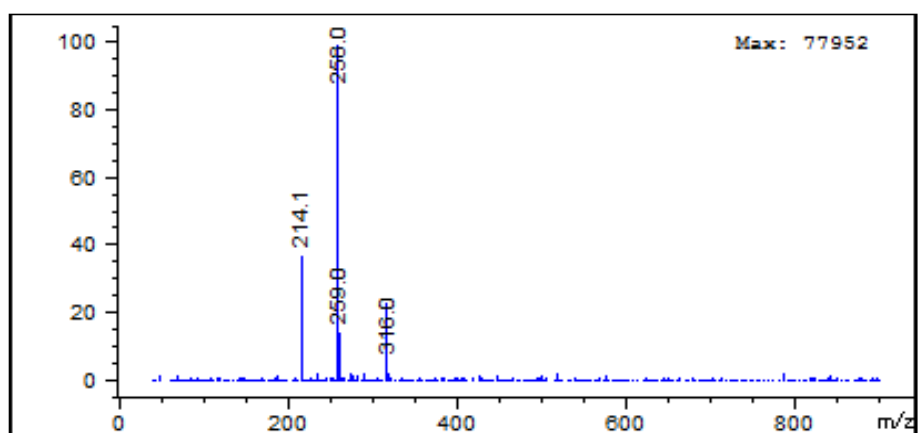
259.22 g/mol



**Figure. S52** MS spectra for product **11a** - AP-ESI: pos. ion mode



**Figure. S53** MS spectra for product **11a** - AP-ESI: neg. ion mode

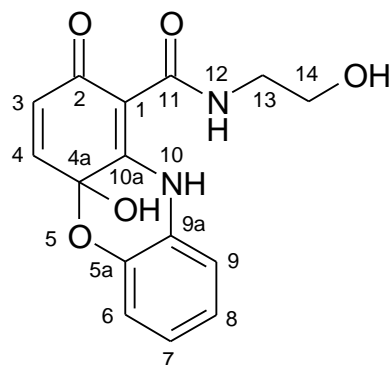


$R_f$  (HPLC) 10.72 min, UV-vis (MeOH)  $\lambda_{\max}$  225, 280, 381 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  260.1 (100); AP-ESI: neg. ion mode  $[M-H]^-$  258.0 (100).

**Table S19:** Data of structural characterization of product **11b** - product resulted from **1b** and **3b**

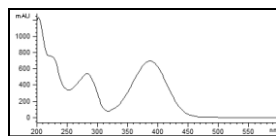
**11b**

**4a-Hydroxy-N-(2-hydroxyethyl)-2-oxo-10H-phenoxazine-1-carboxamide**

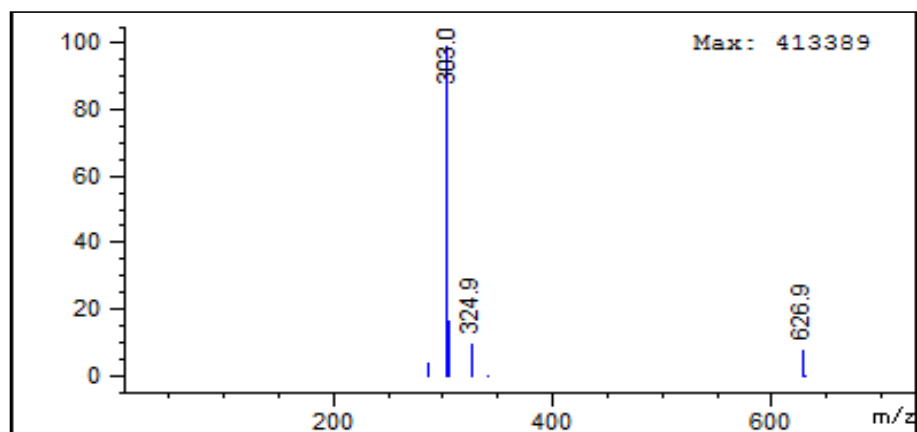


302.29 g/mol

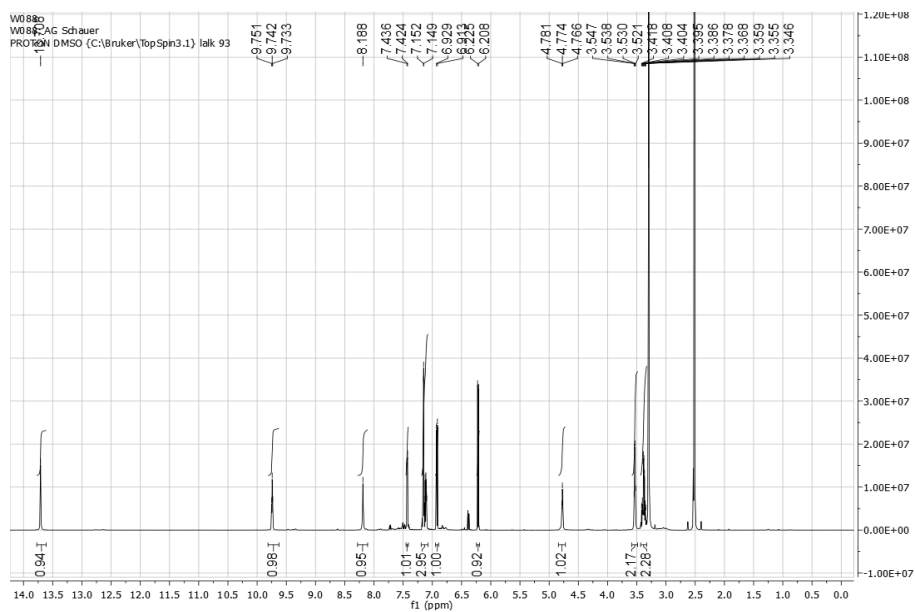
**Fig. S54** UV-vis spectrum for product **11b**



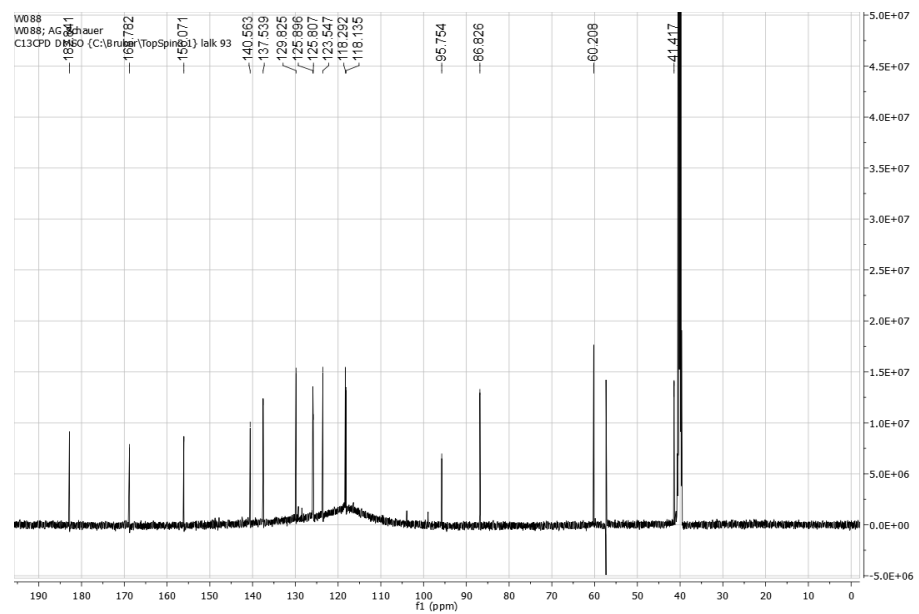
**Figure. S55** MS spectrum for product **11b** - AP-ESI: pos. ion mode



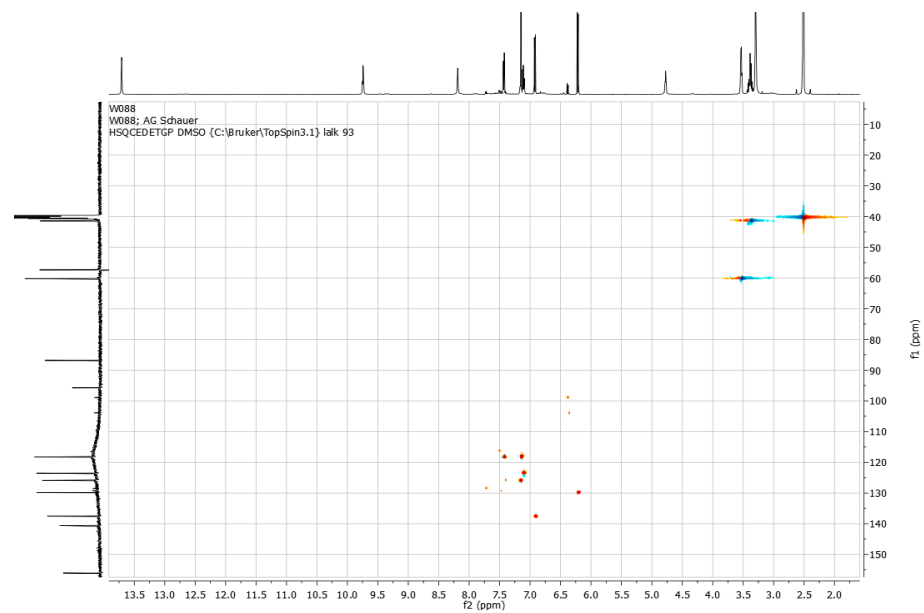
**Figure. S56**  $^1\text{H}$  NMR for product **11b**



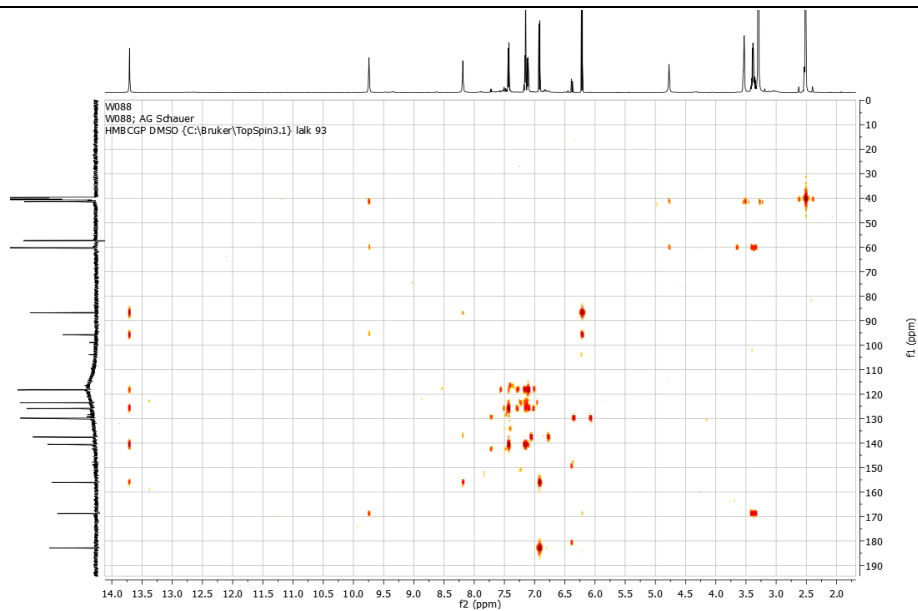
**Figure. S57**  $^{13}\text{C}$  NMR for product **11b**



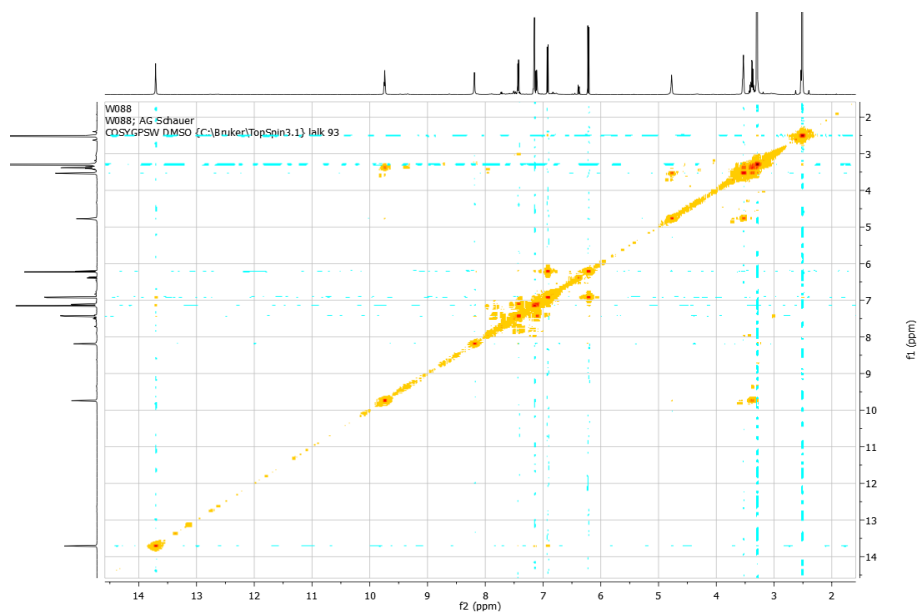
**Figure. S58** HSQC for product **11b**



**Figure. S59** HMBC for product **11b**



**Figure. S60** <sup>1</sup>H <sup>1</sup>H COSY for product **11b**

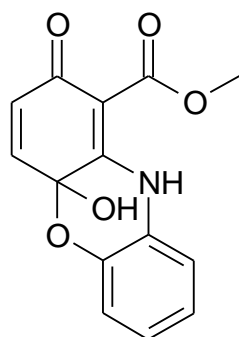


**Table S20:** Data of structural characterization of product **11c** - product resulted from **1c** and **3b**



11c

4a-Hydroxy-2-oxo-10H-phenoxazine-1-carboxylic acid  
methylester



273.25 g/mol

Figure. S61 UV-vis spectrum for product 11c

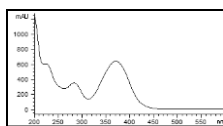


Figure. S62 MS spectrum for product 11c - AP-ESI: pos. ion mode

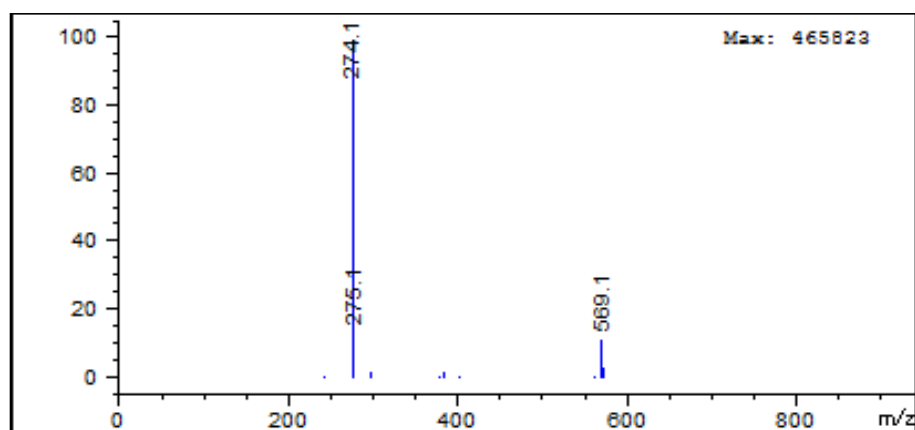
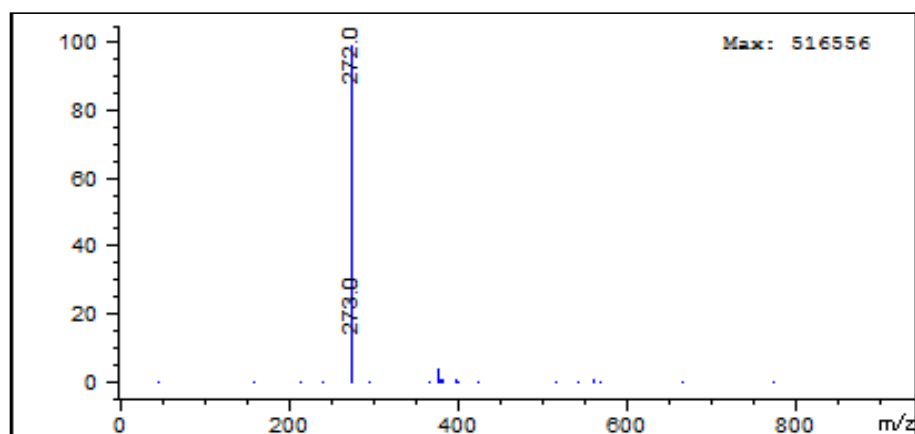


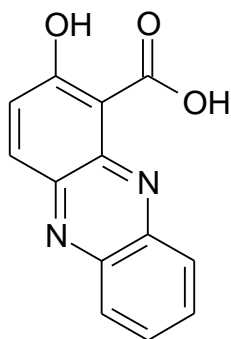
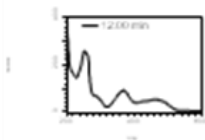
Figure. S63 MS spectrum for product 11c - AP-ESI: neg. ion mode



$R_f$  (HPLC) 10.72 min, UV-vis (MeOH)  $\lambda_{\max}$  225, 286, 371 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  274.1 (100),  $[2M+Na]^+$  569.1 (11); AP-ESI: neg. ion mode  $[M-H]^-$  272.0 (100).

Table S21: Data of structural characterization of product 12a - product resulted from 1a and 3c

Figure. S64 UV-vis spectrum for product 12a



240.22 g/mol

Figure. S65 MS spectrum for product 12a - AP-ESI: pos. ion mode

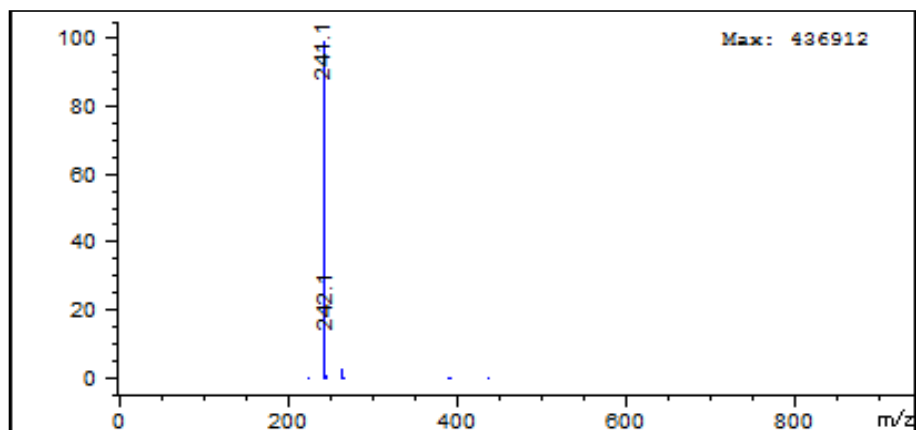
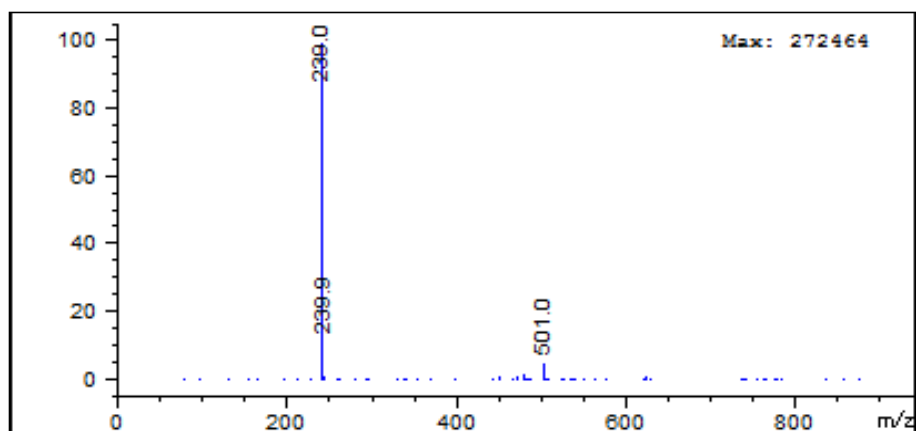


Figure. S66 MS spectrum for product 12a - AP-ESI: neg. ion mode



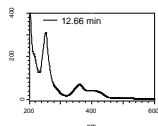
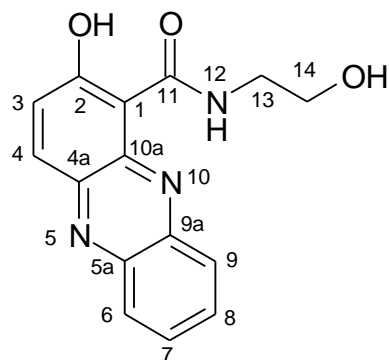
$R_f$  (HPLC) 12.00 min, UV-vis (MeOH)  $\lambda_{\max}$  220, 254, 369, 463 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  241.1 (100); AP-ESI: neg. ion mode  $[M-H]^-$  239.0 (100).

**Table S22:** Data of structural characterization of product **12b** - product resulted from **1b** and **3c**

**12b**

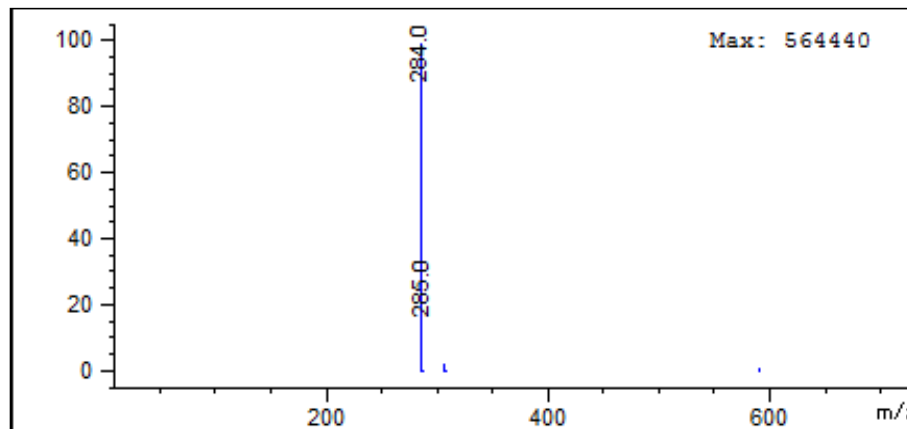
**2-Hydroxy-N-(2-hydroxyethyl)-phenazine-1-carboxamide**

**Figure. S67** UV-vis spectrum for product **12b**

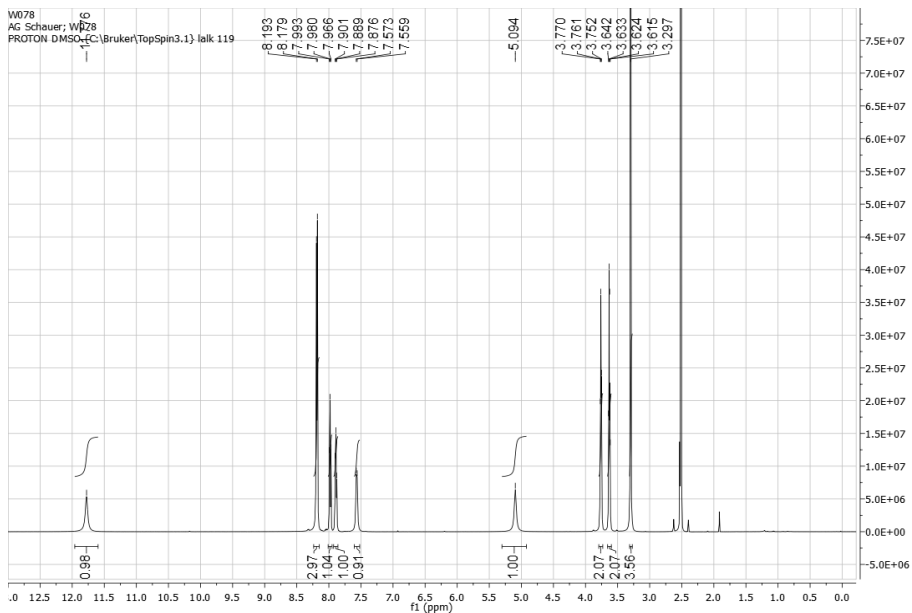


283.29 g/mol

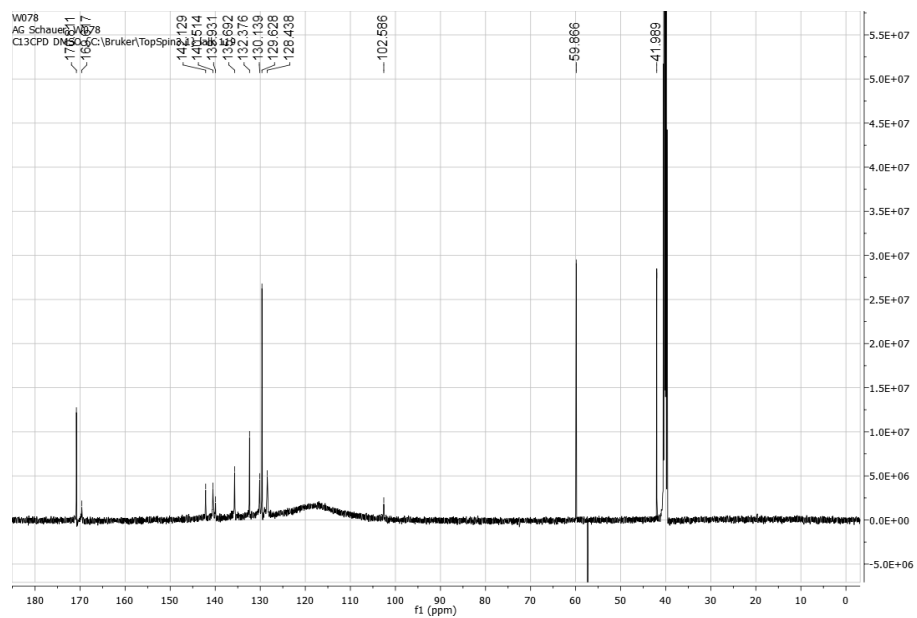
**Figure. S68** MS spectrum for product **12b** - AP-ESI: pos. ion mode



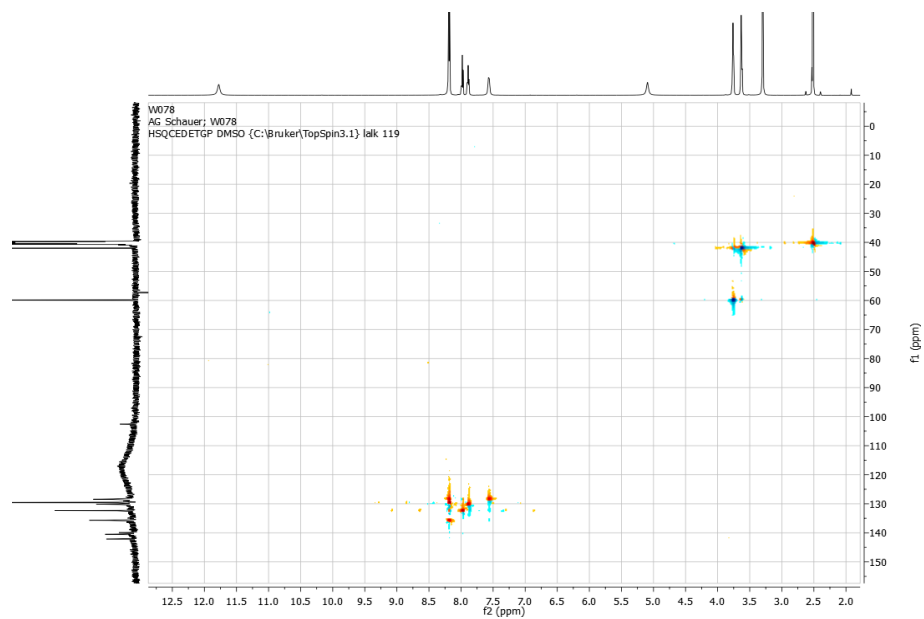
**Figure. S69**  $^1\text{H}$  NMR for product **12b**



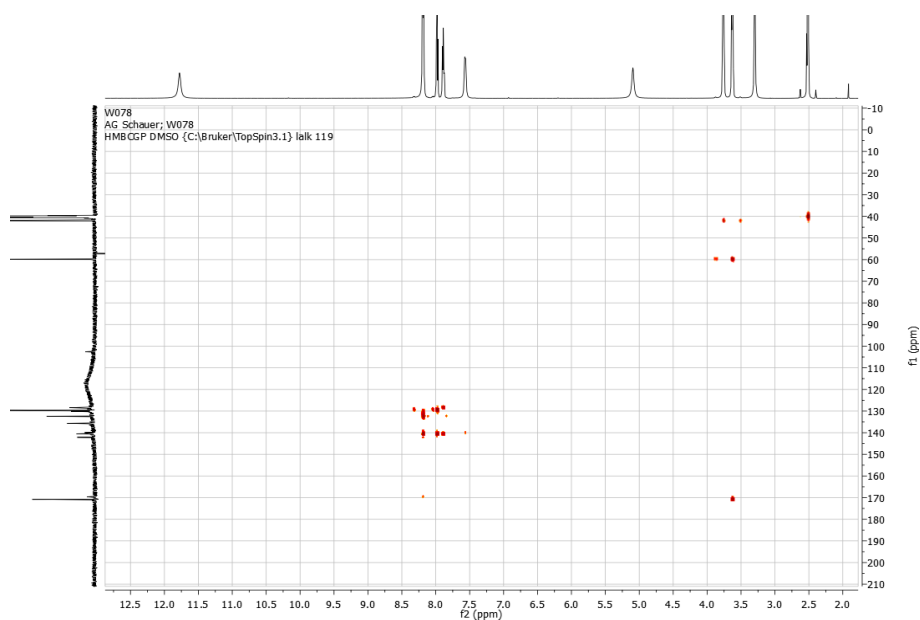
**Figure. S70**  $^{13}\text{C}$  NMR for product **12b**



**Figure. S71** HSQC for product **12b**



**Figure. S72** HMBC for product **12b**

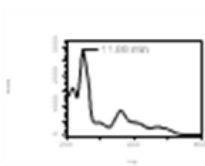
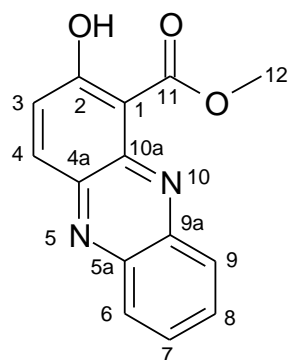


**Table S23:** Data of structural characterization of product **12c** - product resulted from **1c** and **3c**

**12c**

**2-Hydroxyphenazine-1-carboxylic acid methylester**

**Figure. S73** UV-vis spectrum for product **12c**



254.25 g/mol

Figure. S74 MS spectrum for product **12c** - AP-ESI: pos. ion mode

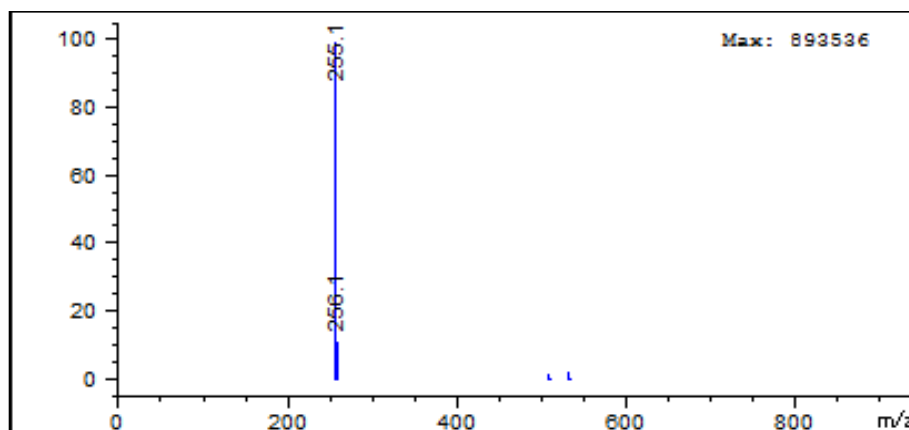


Figure. S75 MS spectrum for product **12c** - AP-ESI: neg. ion mode

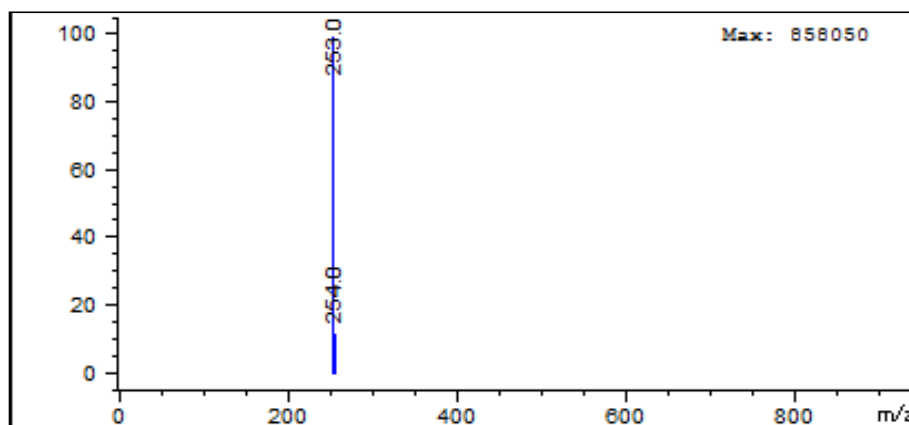


Figure. S76  $^1\text{H}$  NMR for product **12c**

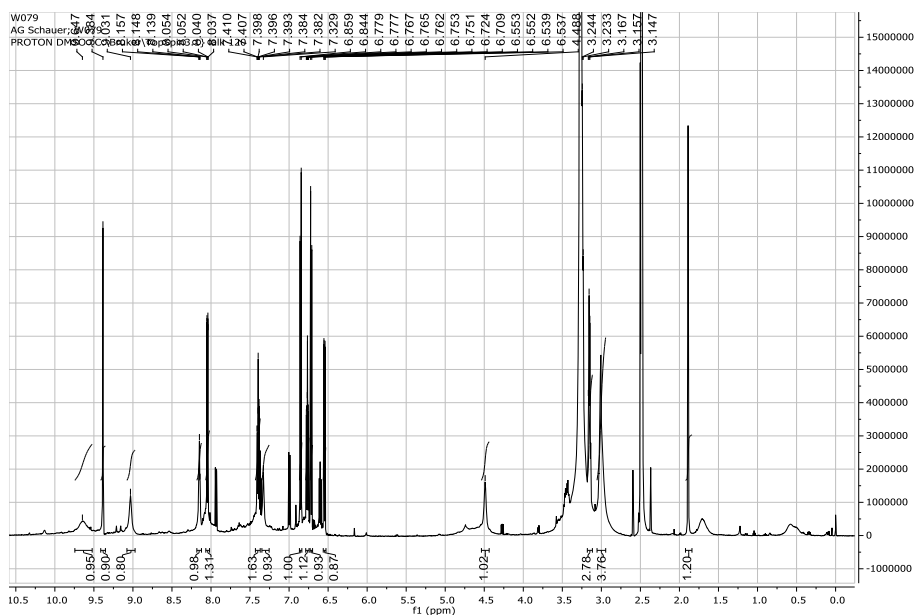


Figure. S77  $^{13}\text{C}$  NMR for product 12c

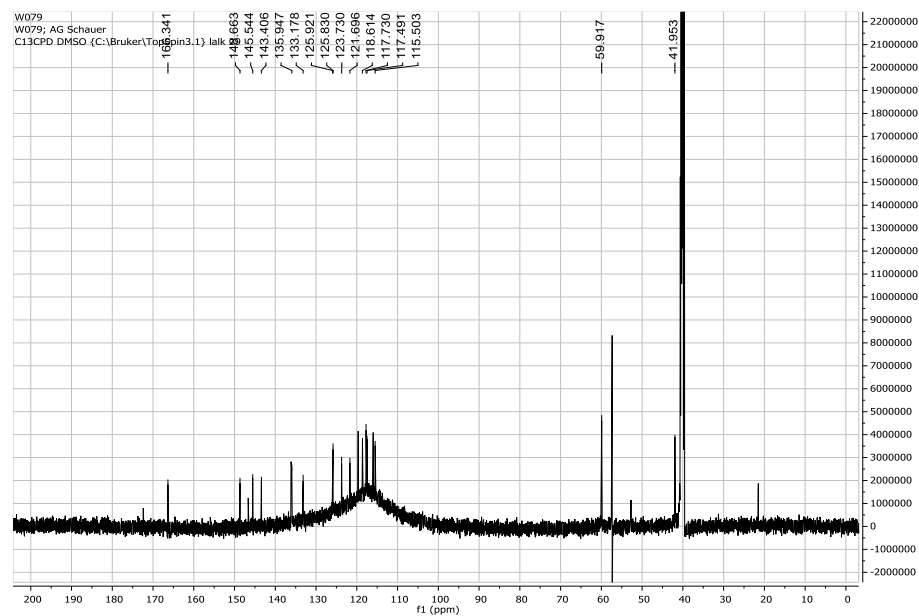
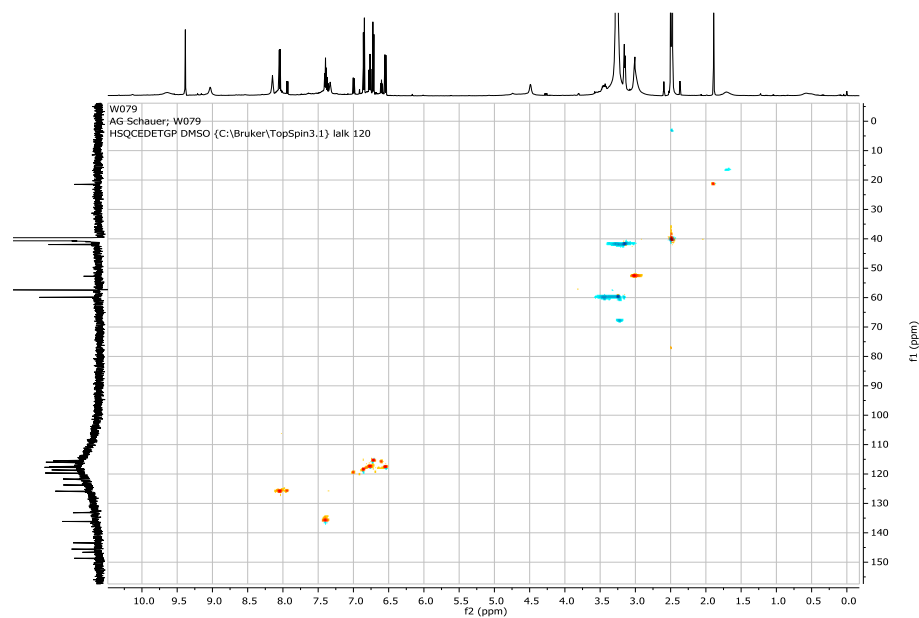
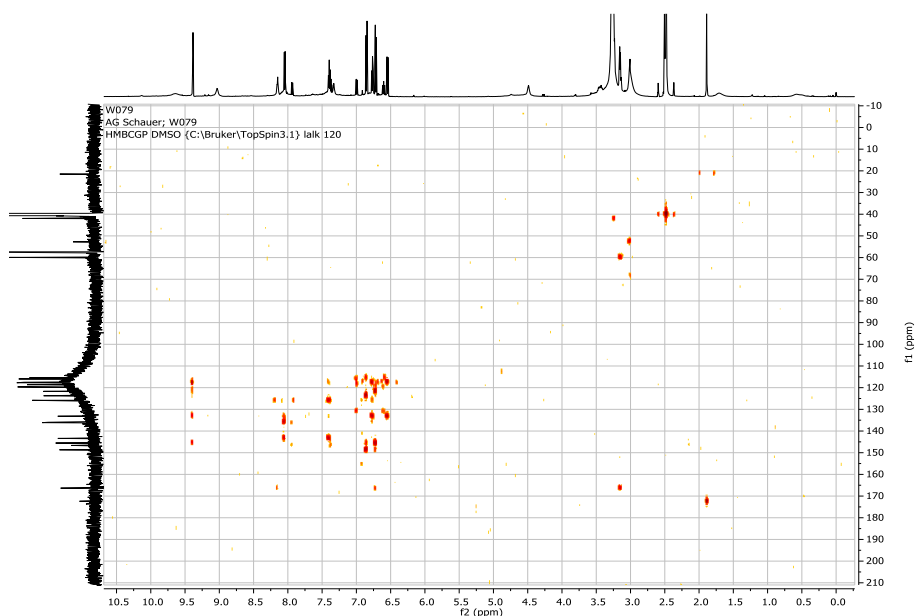


Figure. S78 HSQC for product 12c



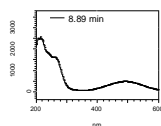
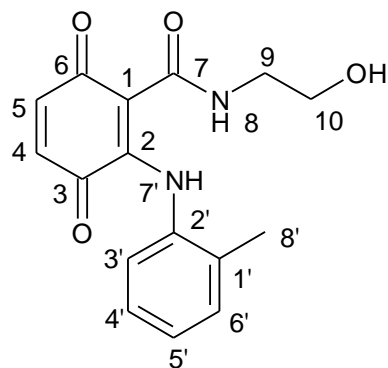
**Figure. S79** HMBC for product **12c**



**Table S24:** Data of structural characterization of products **13a**, **14a** - products resulted from **1b** and **3d**

<b>13a</b>	<b>N-(2-Hydroxyethyl)-2-(2-methylanilino)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide</b>
<b>14a</b>	<b>3,6-Dihydroxy-N-(2-hydroxyethyl)-2-(2-methylanilino)benzamide</b>

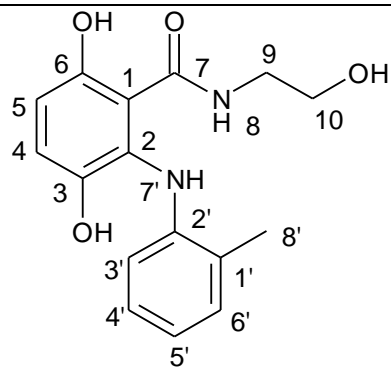
**13a** **Figure. S80** UV-vis spectrum for product **13a**



300.32 g/mol

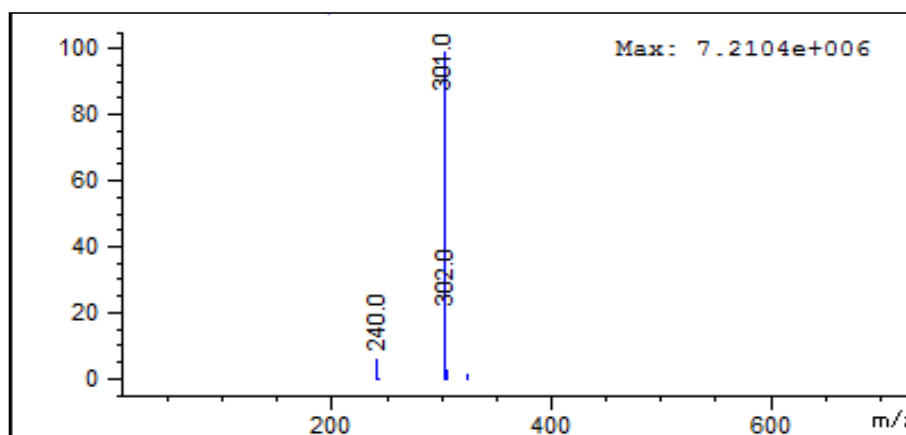
**14a**



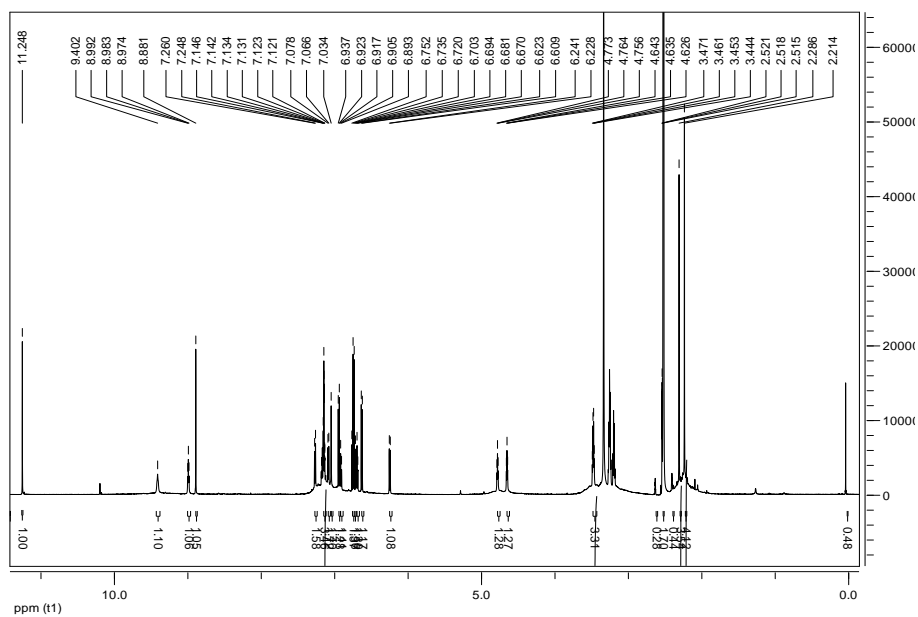


302.33 g/mol

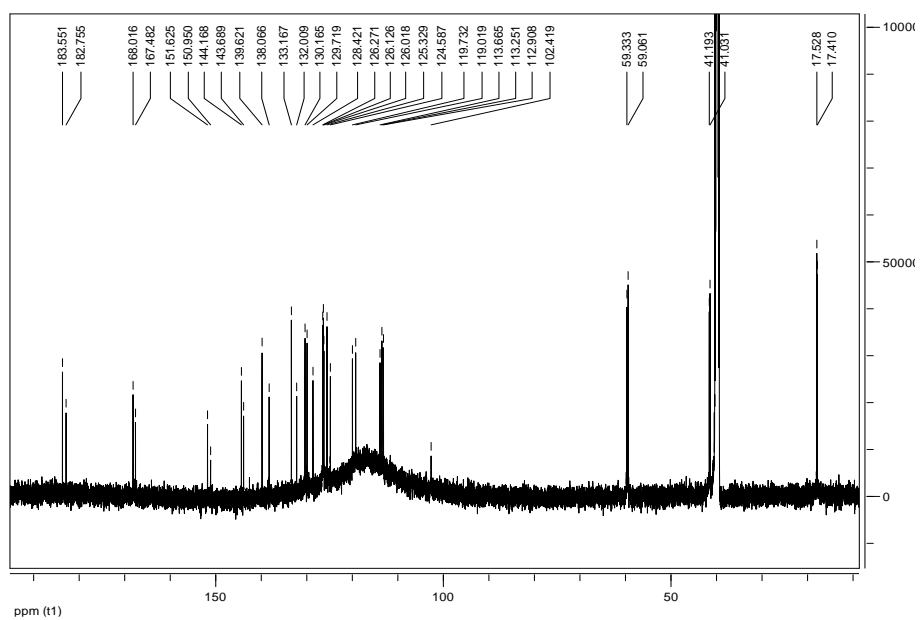
**Figure. S81** MS spectrum for product **13a** - AP-ESI: pos. ion mode



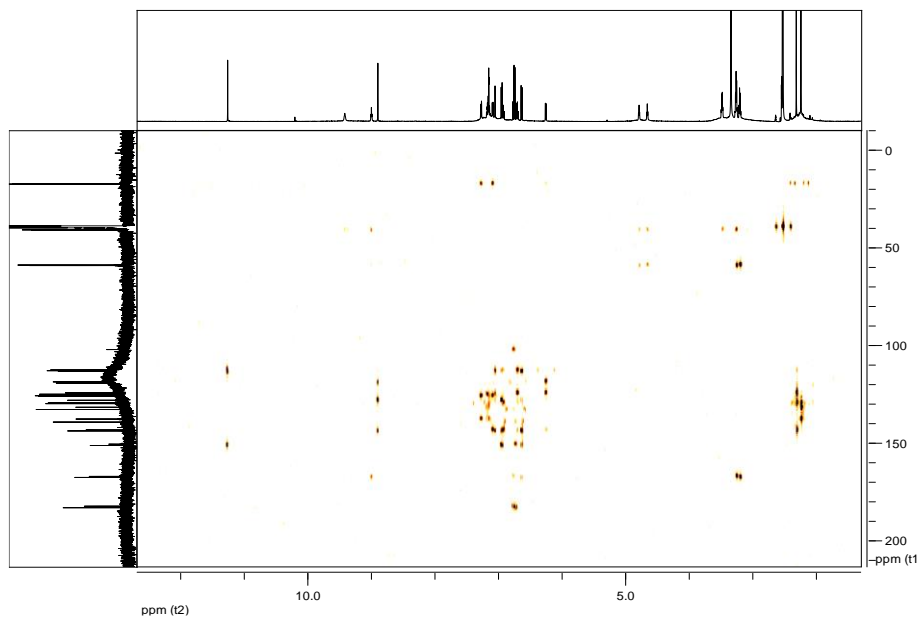
**Figure. S82**  $^1\text{H}$  NMR for product **13a**, **14a**



**Figure. S83**  $^{13}\text{C}$  NMR for product **13a**, **14a**



**Figure. S84** HMBC for product **13a**, **14a**



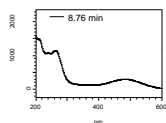
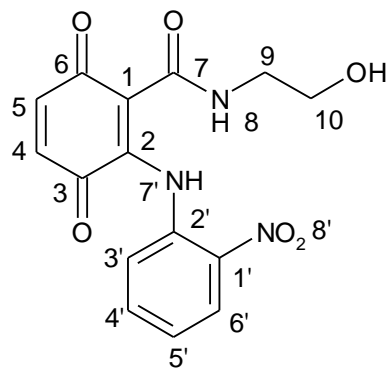
**Table S25:** Data of structural characterization of products **13b**, **14b** - products resulted from **1b** and

**3e**

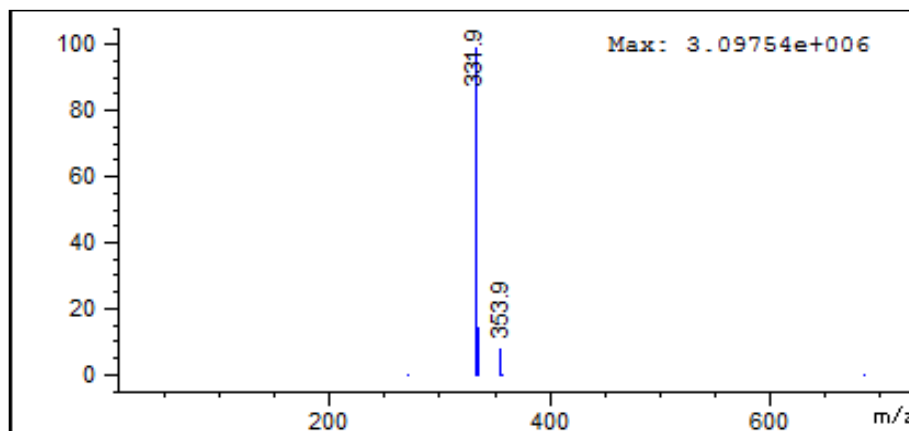
**13b** **N-(2-Hydroxyethyl)-2-(2-nitroanilino)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide**

**14b** **3,6-Dihydroxy-N-(2-hydroxyethyl)-2-(2-nitroanilino)benzamide**

**13b** **Figure. S85** UV-vis spectrum for product **13b**

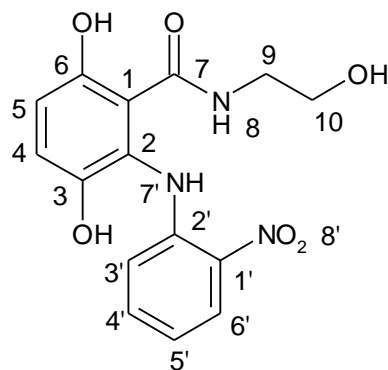


**Figure. S86** MS spectrum for product **13b** - AP-ESI: pos. ion mode



331.29 g/mol

**14b**



333.30 g/mol

Figure. S87 <sup>1</sup>H NMR for product 14b

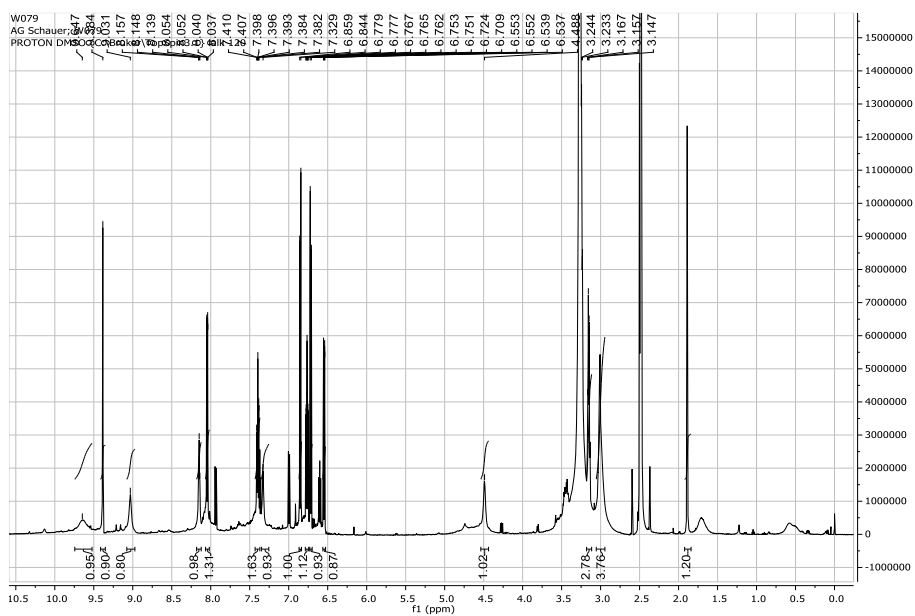


Figure. S88 <sup>13</sup>C NMR for product 14b

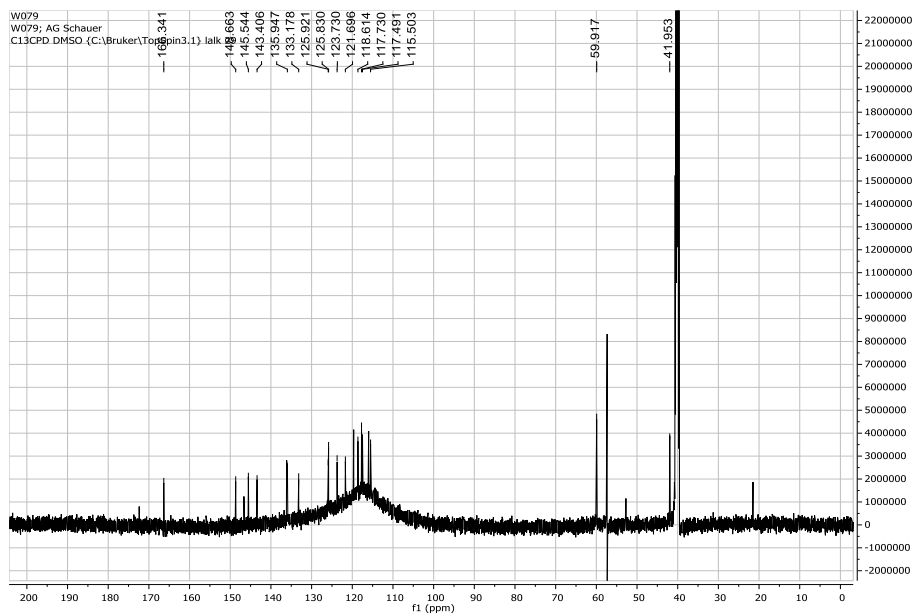


Figure. S89 HSQC for product 14b

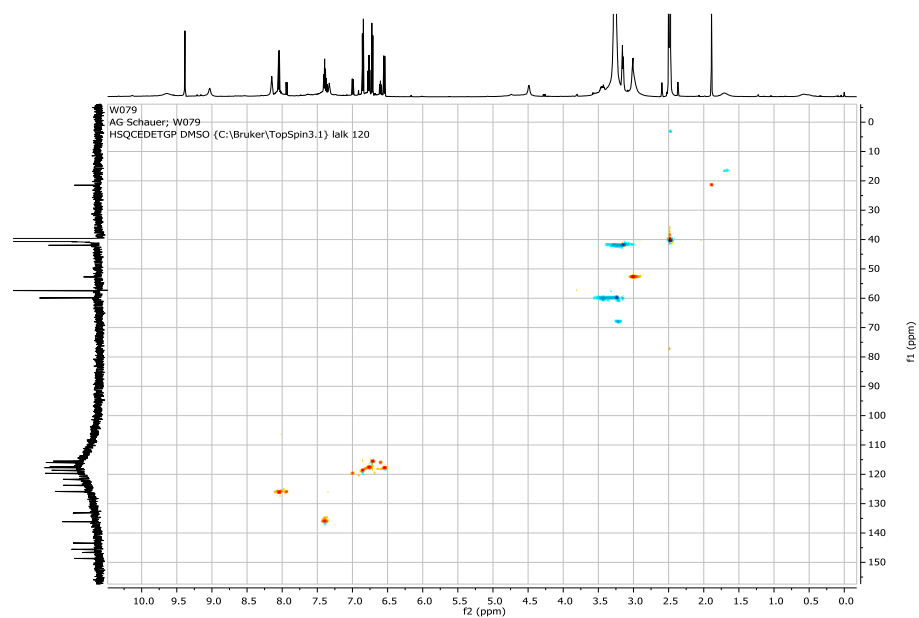
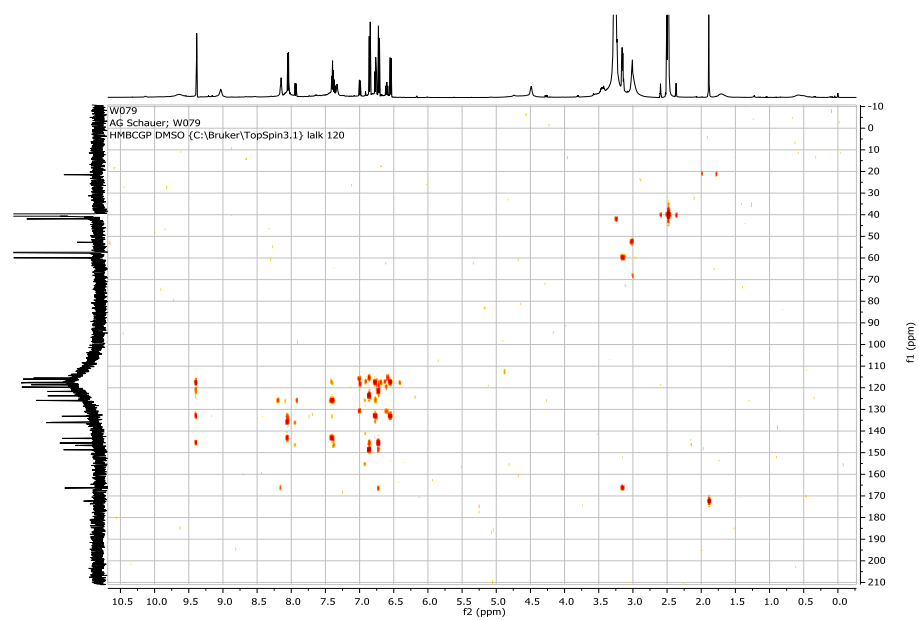


Figure. S90 HMBC for product 14b

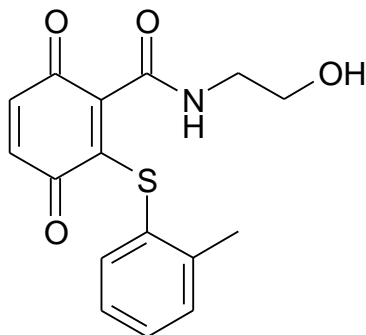


**Table S26:** Data of structural characterization of product **13c** - product resulted from **1b** and **3f**

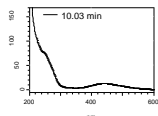
**13c**

**N-(2-Hydroxyethyl)-2-(o-tolylsulfonyl)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide**

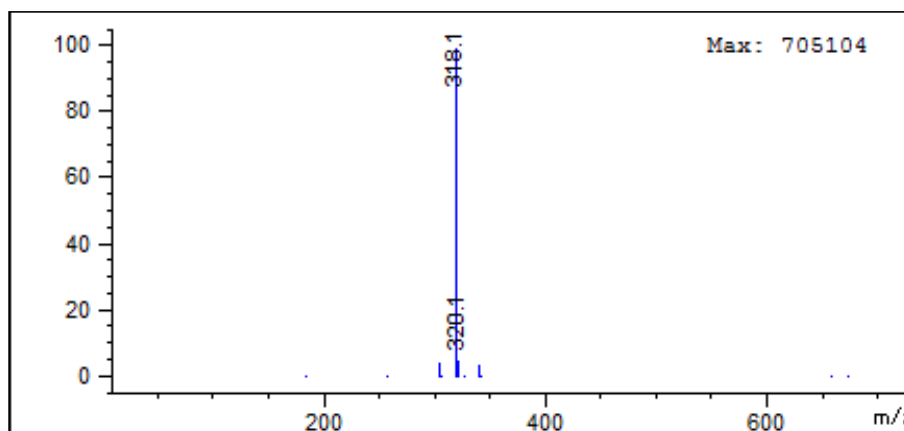
**Figure. S91** UV-vis spectrum for product **13c**



317.37 g/mol



**Figure. S92** MS spectrum for product **13c** - AP-ESI: pos. ion mode



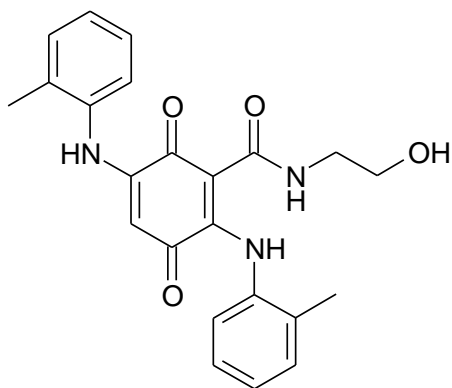
$R_f$  (HPLC) 10.04 min, UV-vis (MeOH)  $\lambda_{max}$  205, 245, 440 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  318.1 (100).

**Table S27:** Data of structural characterization of product **15a** - product resulted from **1b** and **3d**

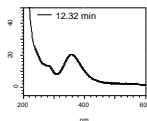
**15a**

**N-(2-Hydroxyethyl)-2,5-bis(2-methylanilino)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide**

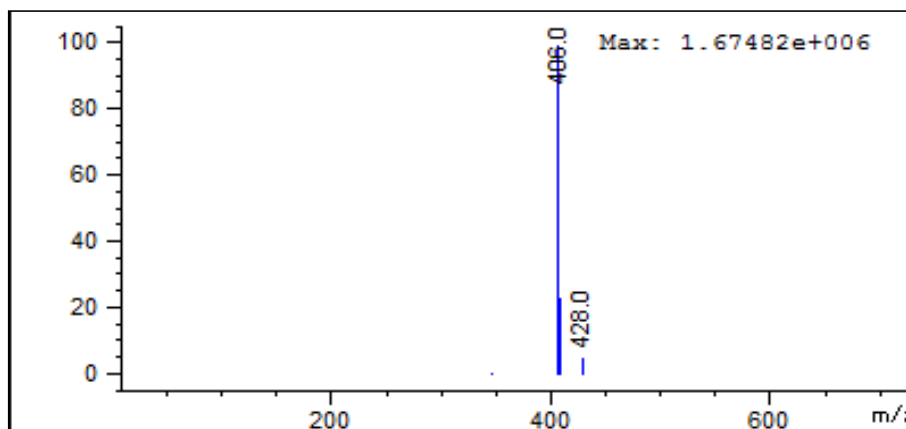
**Figure. S93** UV-vis spectrum for product **15a**



405.46 g/mol



**Figure. S94** MS spectrum for product **15a** - AP-ESI: pos. ion mode



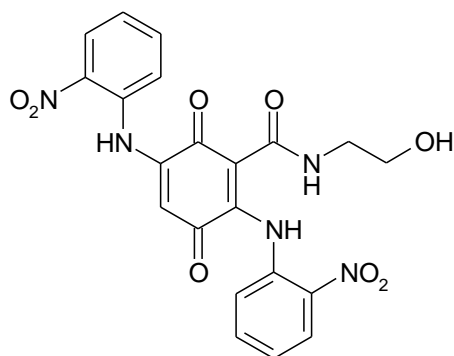
$R_f$  (HPLC) 12.32 min, UV-vis (MeOH)  $\lambda_{\max}$  210, 281, 359 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  406.0 (100),  $[M+Na]^+$  428.0 (5).

**Table S28:** Data of structural characterization of product **15b** - product resulted from **1b** and **3e**

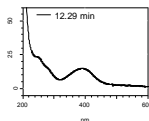
**15b**

**N-(2-Hydroxyethyl)-2,5-bis(2-nitroanilino)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide**

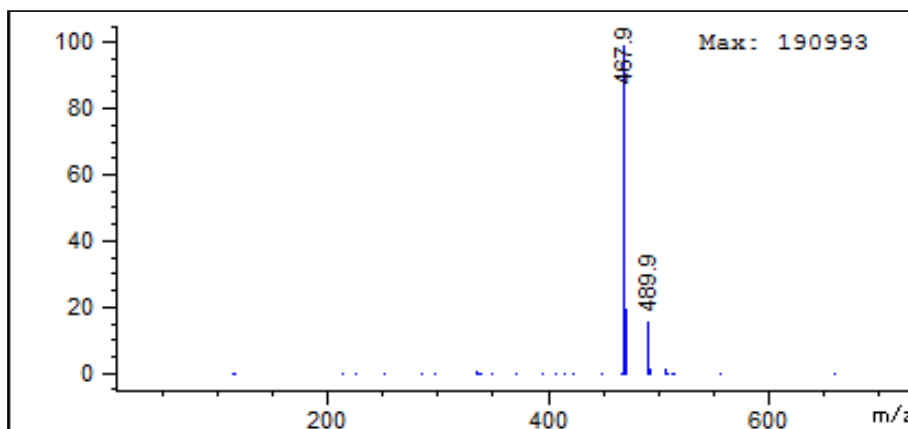
**Figure. S95** UV-vis spectrum for product **15b**



467.40 g/mol



**Figure. S96** MS spectrum for product **15b** - AP-ESI: pos. ion mode



$R_f$  (HPLC) 9.00 min, UV-vis (MeOH)  $\lambda_{\max}$  209, 262, 383 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  467.9 (100),  $[M+Na]^+$  489.9 (16).

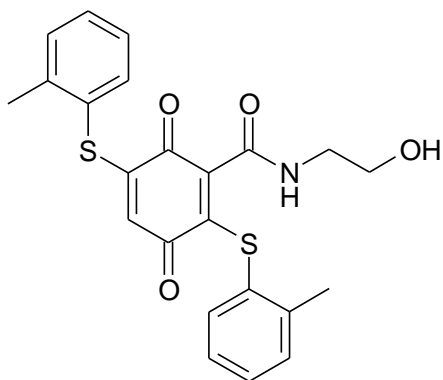


**Table S29:** Data of structural characterization of product **15c** - product resulted from **1b** and **3f**

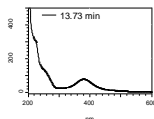
**15c**

**N-(2-Hydroxyethyl)-2,5-bis(o-tolylsulfanyl)-3,6-dioxocyclohexa-1,4-diene-1-carboxamide**

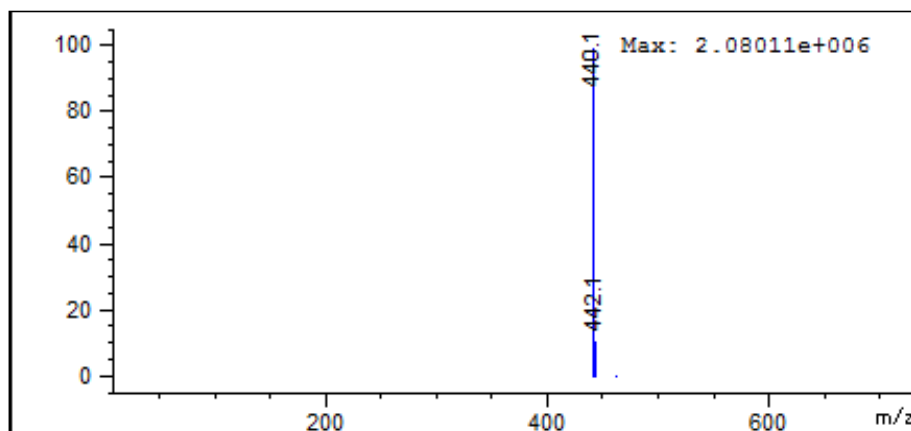
**Figure. S97** UV-vis spectrum for product **15c**



439.56 g/mol



**Figure. S98** MS spectrum for product **15c** - AP-ESI: pos. ion mode



$R_f$  (HPLC) 10.04 min, UV-vis (MeOH)  $\lambda_{\max}$  205, 225, 379 nm. MS  $m/z$  (rel. intensity) AP-ESI: pos. ion mode  $[M+H]^+$  440.1 (100).