

## Supplementary Information

### *Hetero-Diels-Alder Reactions of in situ-Generated Azoalkenes with Thioketones; Experimental and Theoretical Studies*

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## 1. Experimental

**Generals:** For general information and preparation procedures, see the main manuscript, pp. 12-13.

### 1.1. The $^1\text{H}$ NMR and $^{13}\text{C}$ NMR spectra of all new compounds 9a-p, 9s and 11a-b:

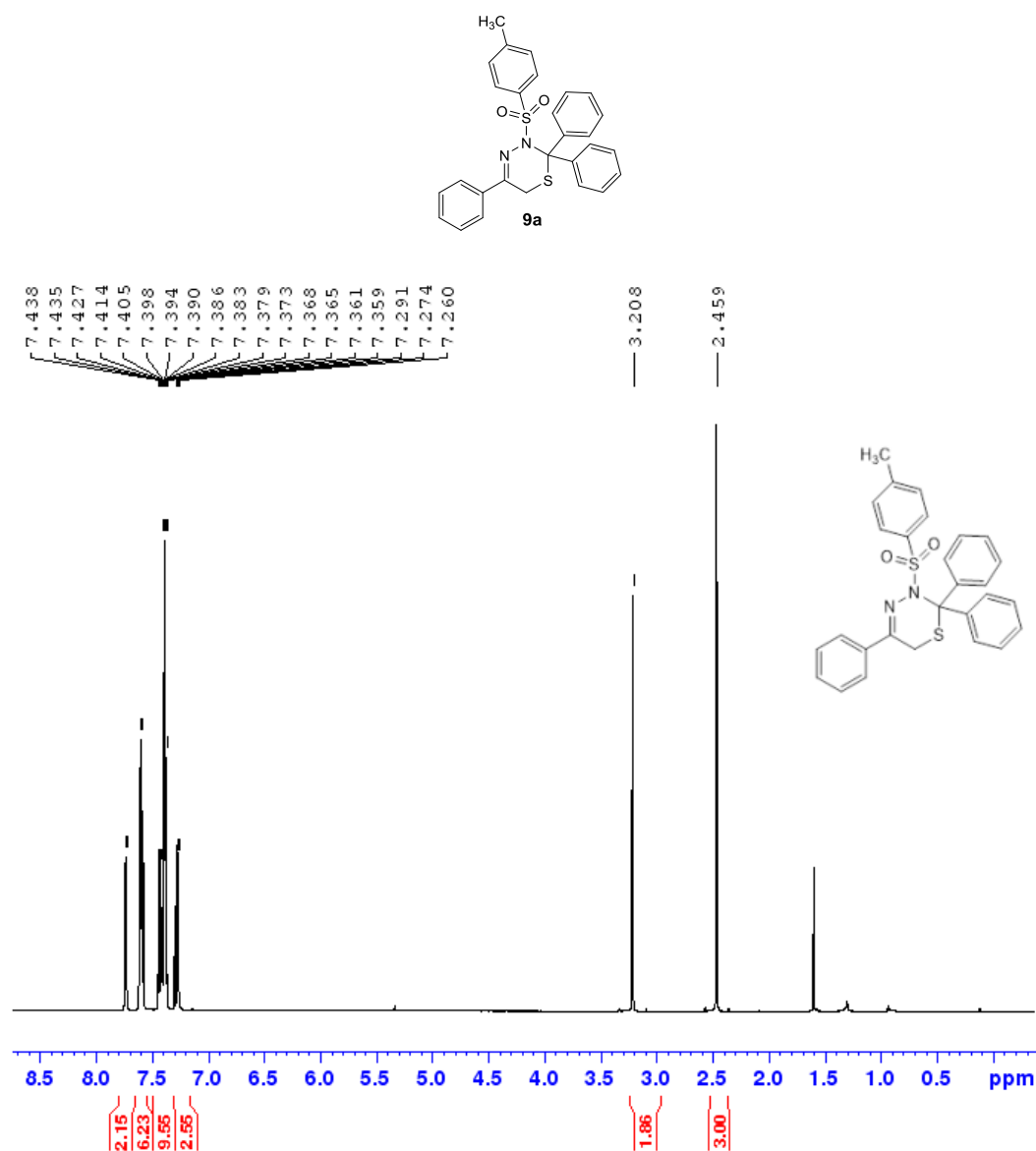


Fig. 1a.  $^1\text{H}$ -NMR for compound 9a.

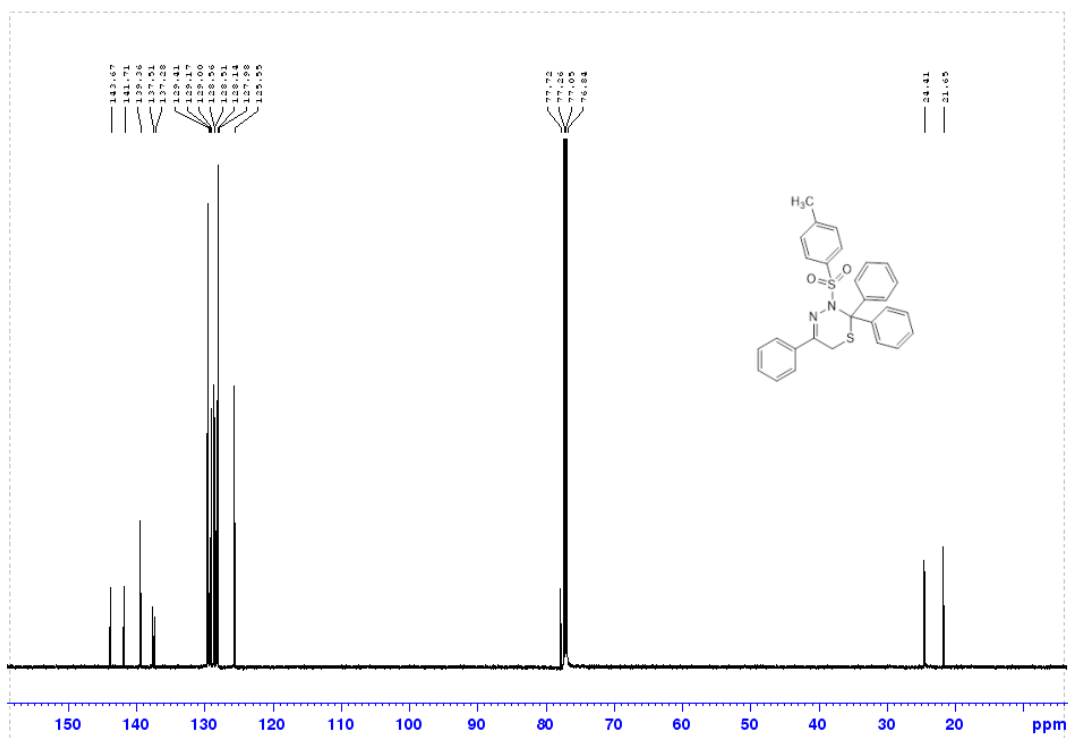


Fig. 1b. <sup>13</sup>C-NMR for compound **9a**

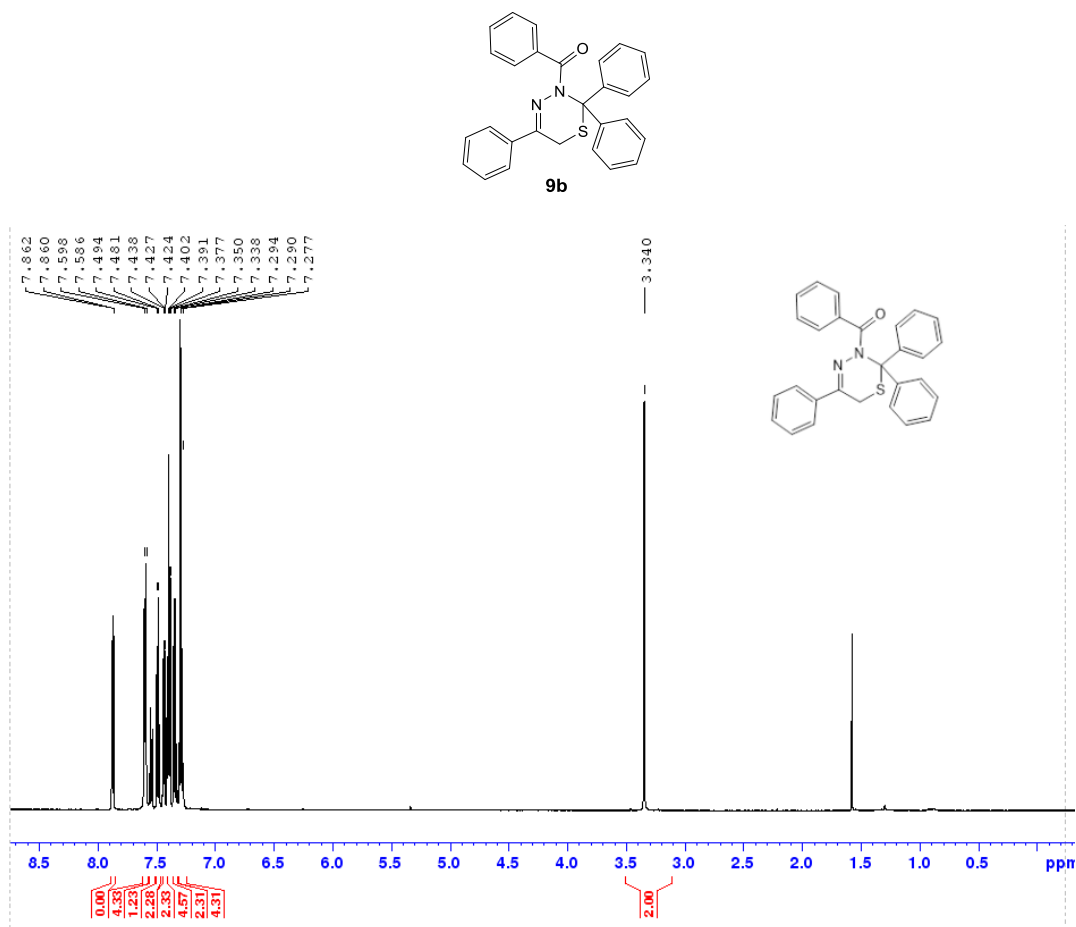


Fig. 2a. <sup>1</sup>H-NMR for compound **9b**.

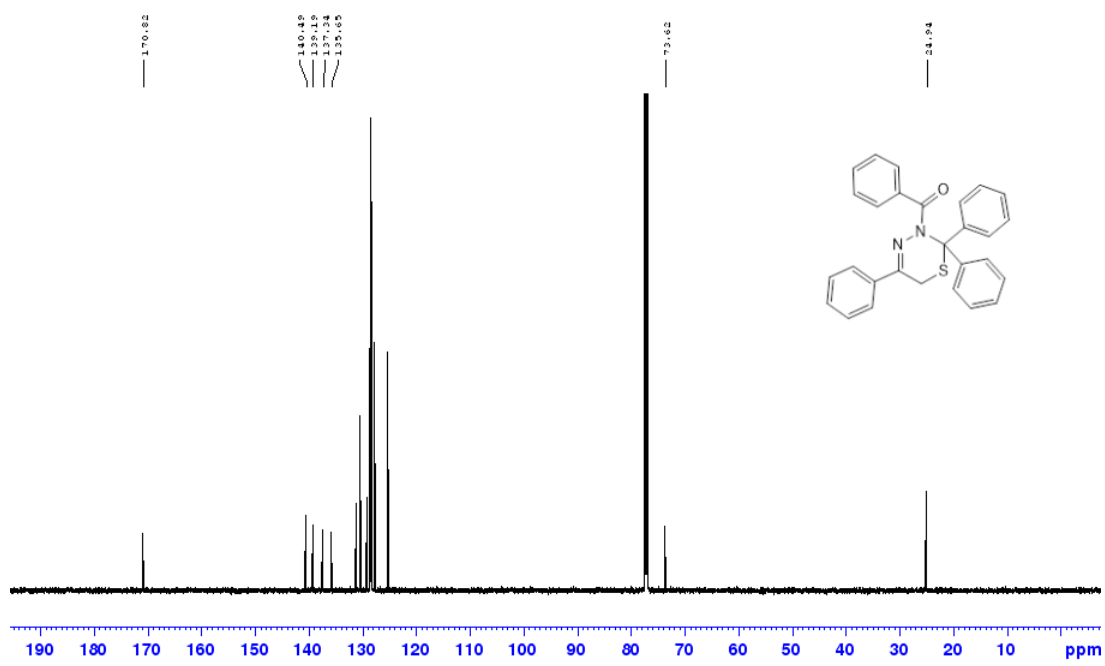


Fig. 2b. <sup>13</sup>C NMR for compound 9b.

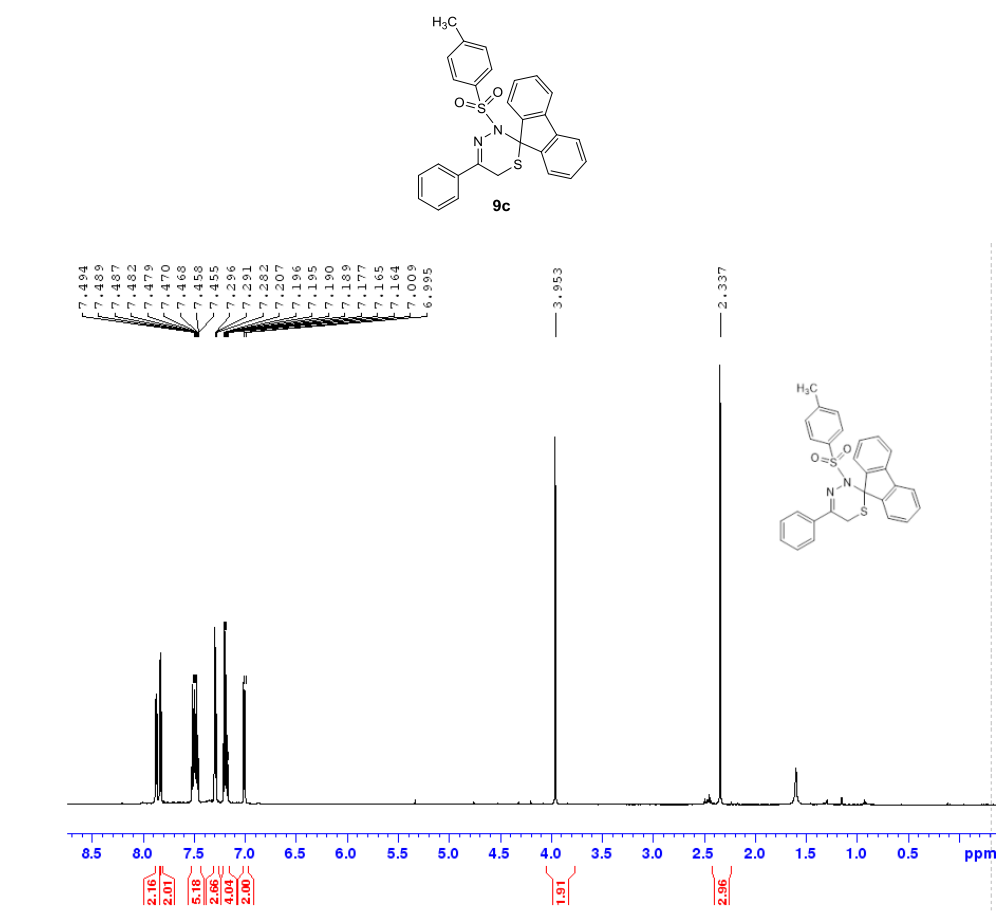


Fig. 3a. <sup>1</sup>H NMR for compound 9c.

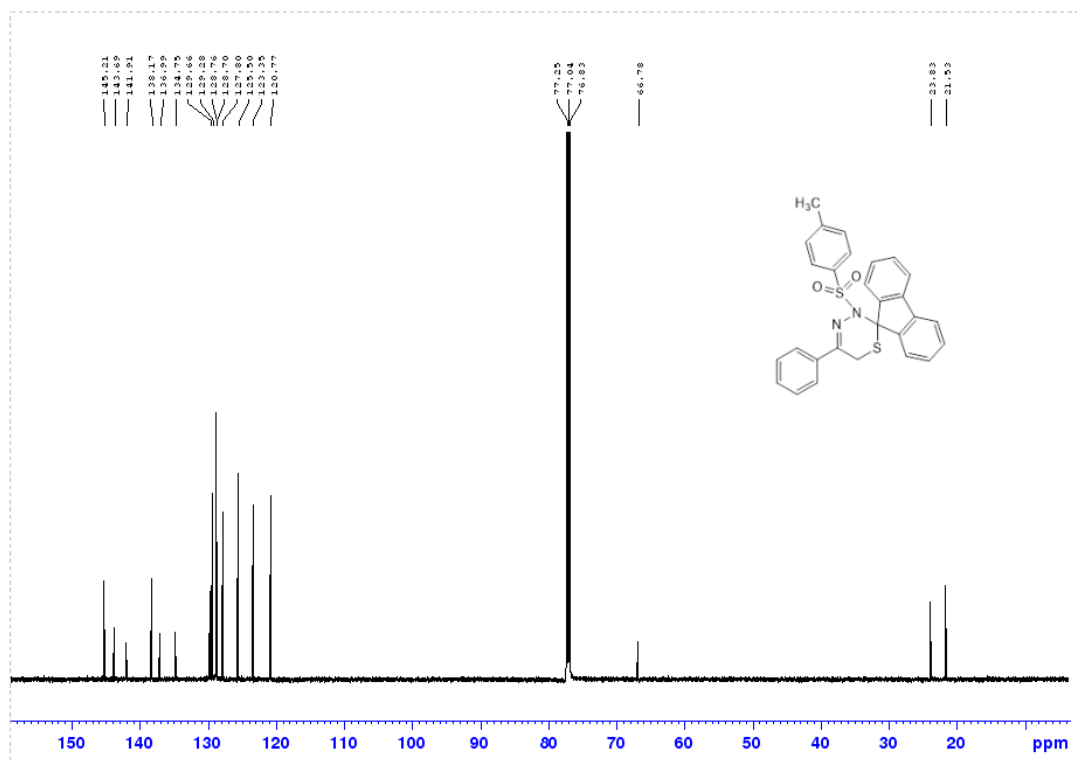


Fig. 3b. <sup>13</sup>C NMR for compound 9c.

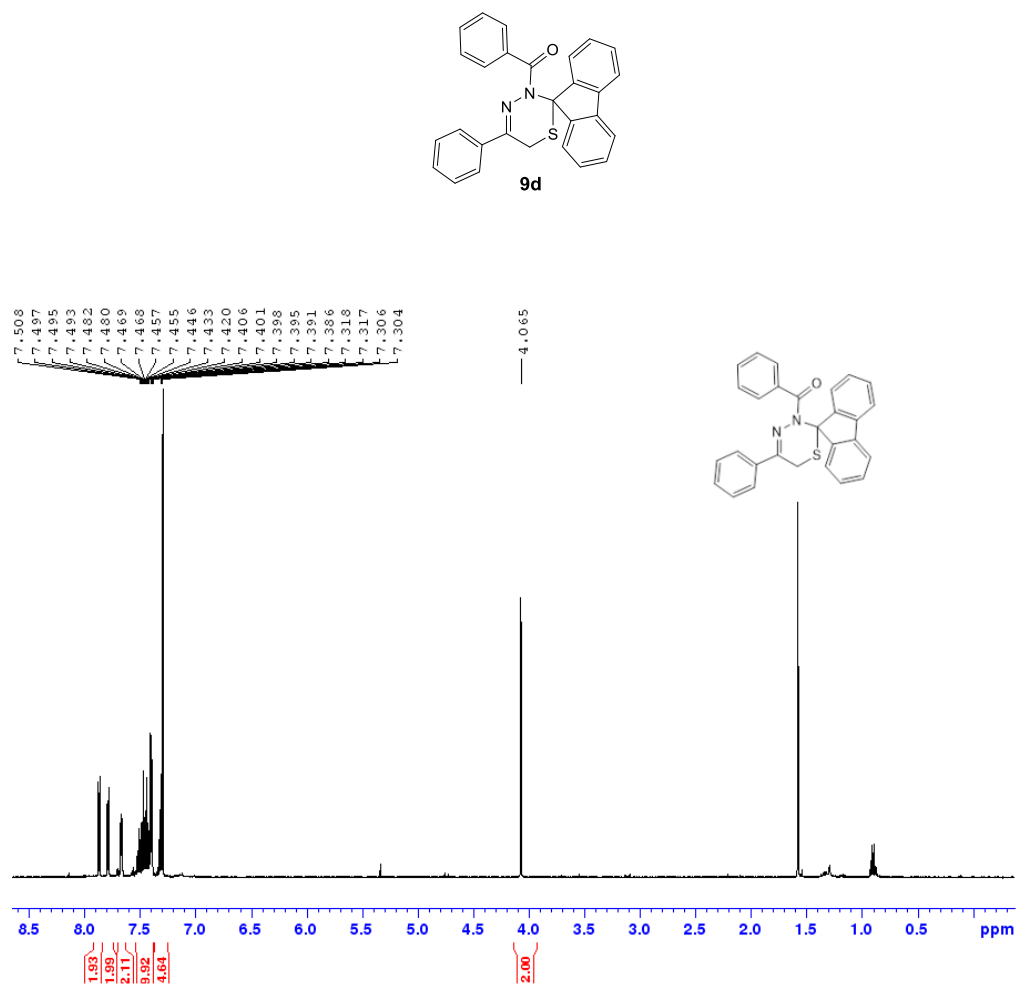


Fig. 4a.  $^1\text{H}$  NMR for compound 9d.

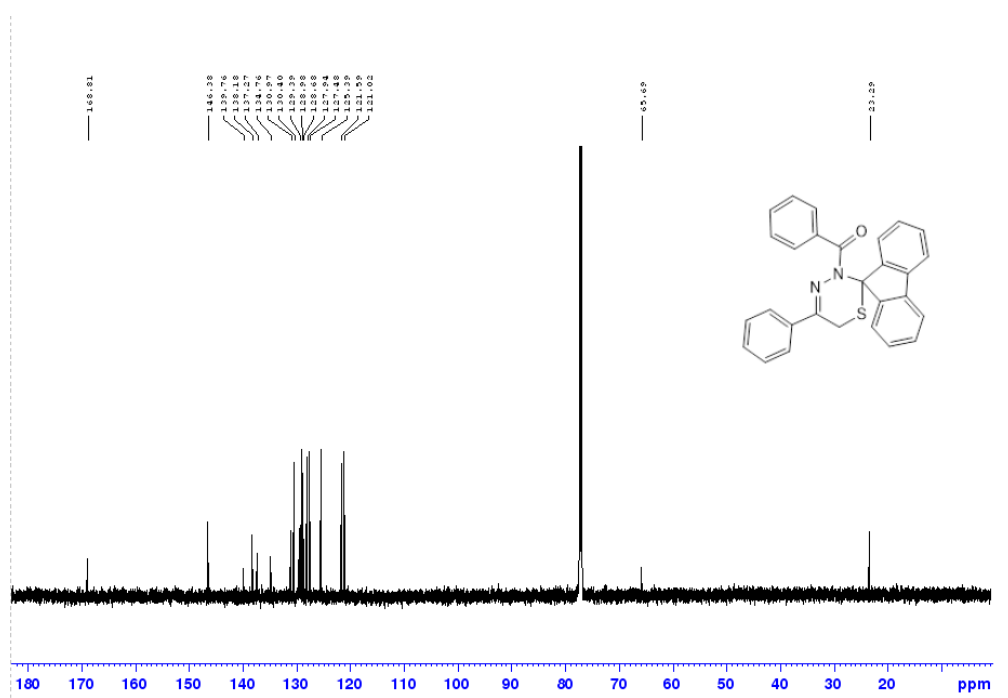


Fig. 4b.  $^{13}\text{C}$  NMR for compound 9d.

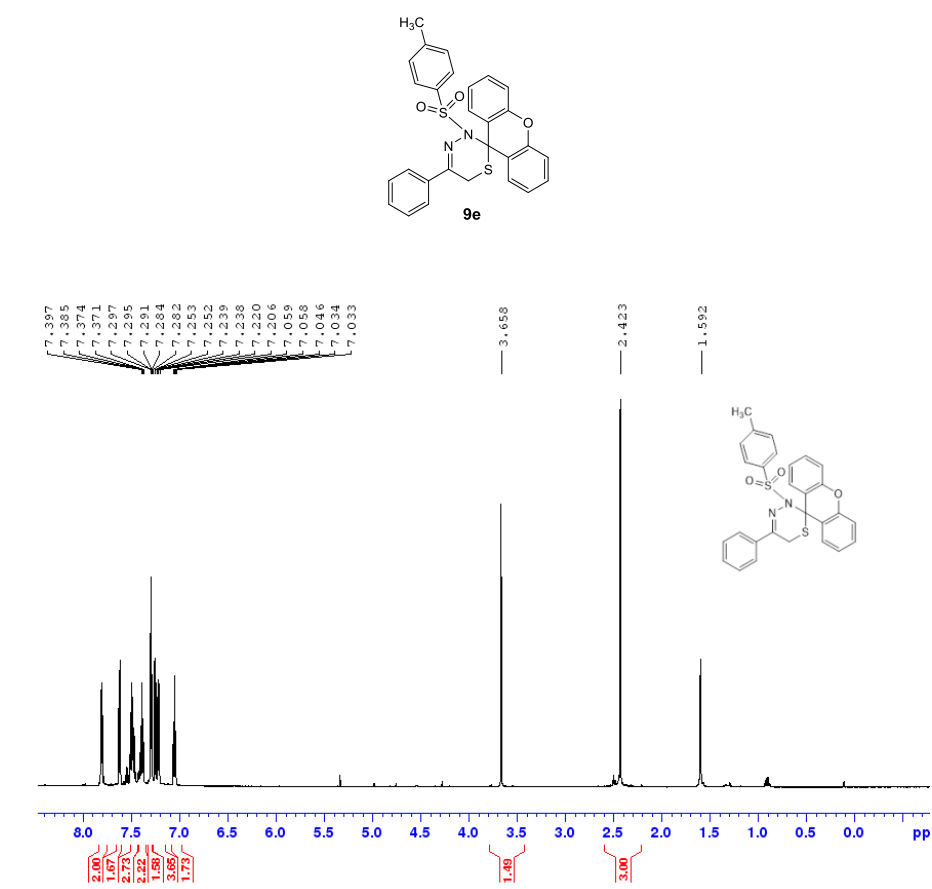


Fig. 5a.  $^1\text{H}$  NMR for compound 9e.

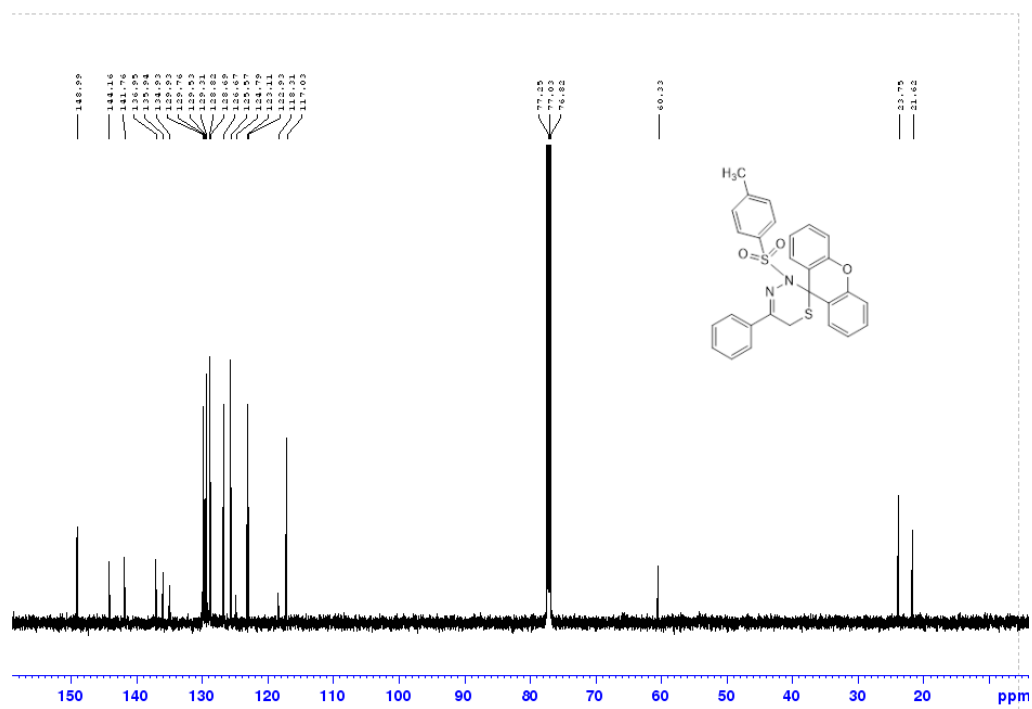


Fig. 5b.  $^{13}\text{C}$  NMR for compound 9e.

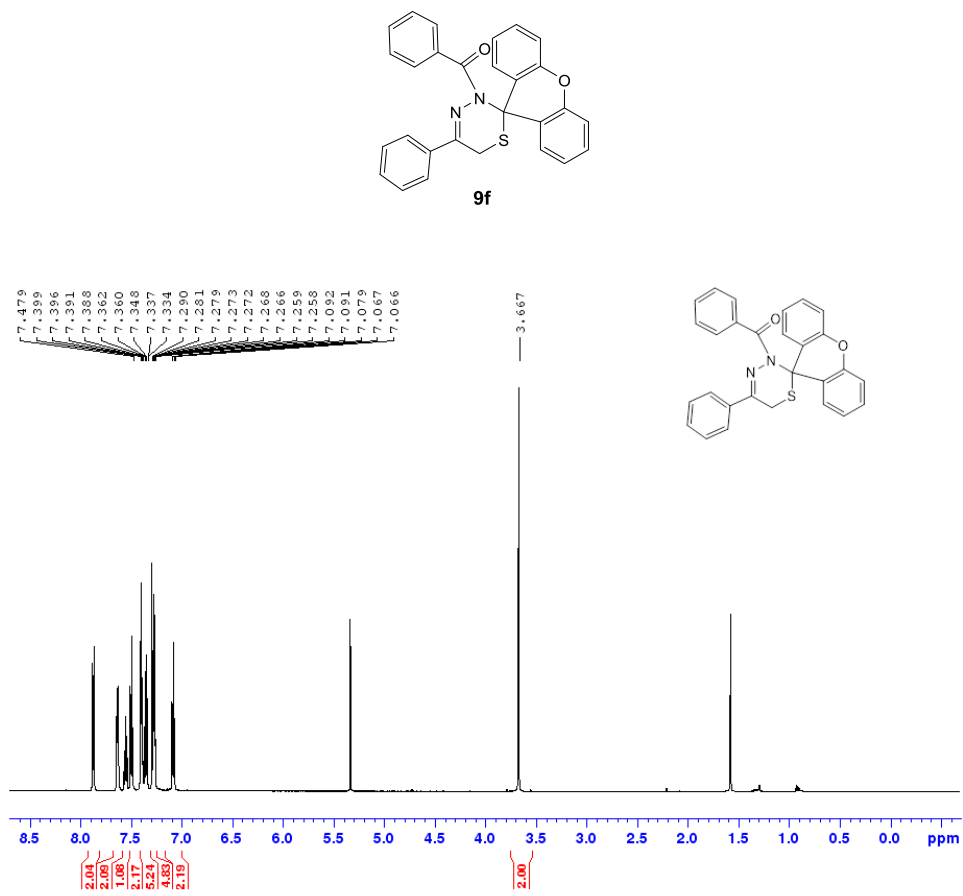


Fig. 6a.  $^1\text{H}$  NMR for compound 9f.

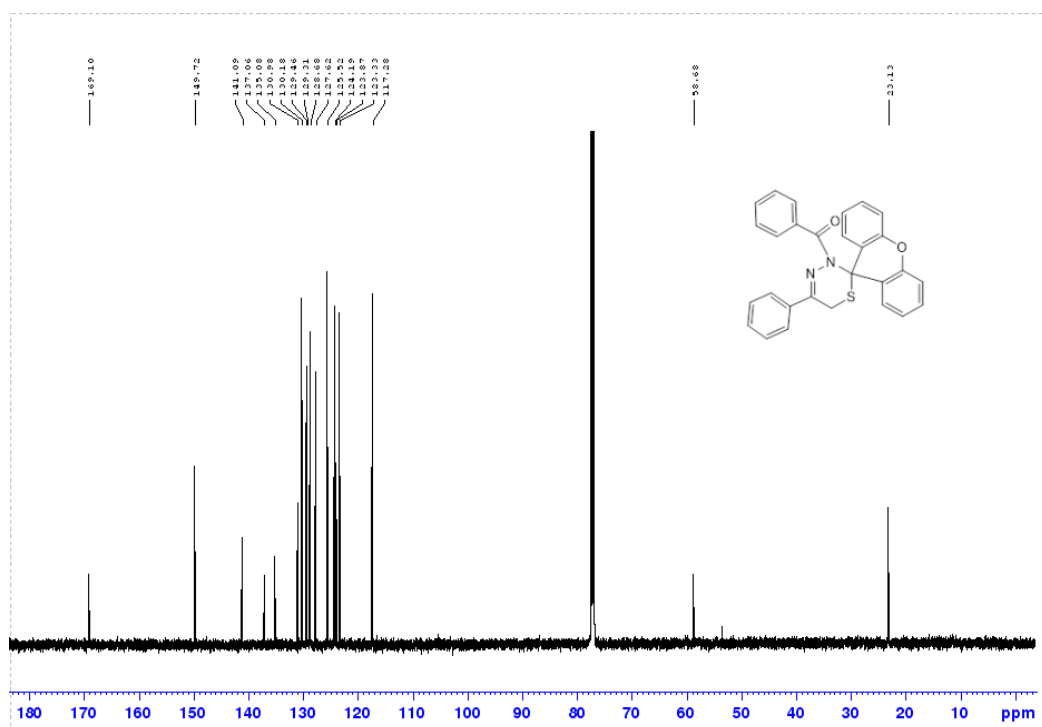


Fig. 6b. <sup>13</sup>C NMR for compound 9f.

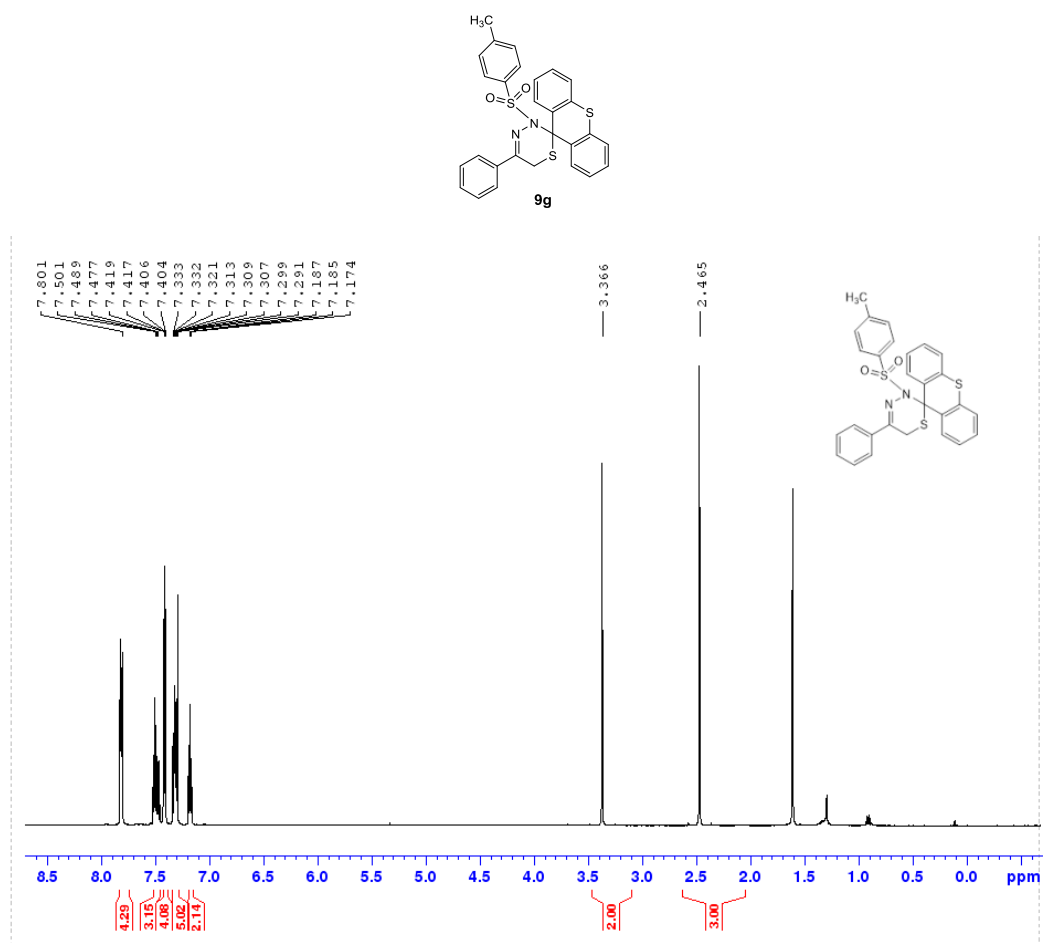




Fig. 7a.  $^1\text{H}$  NMR for compound 9g.

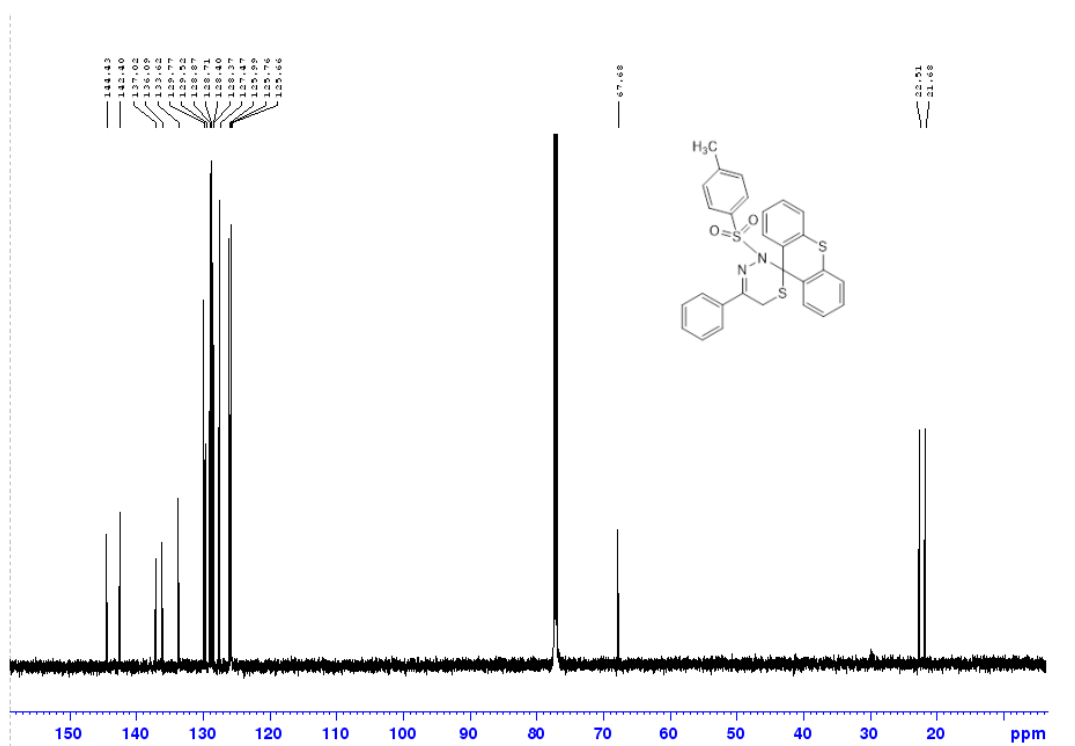


Fig. 7b.  $^{13}\text{C}$  NMR for compound 9g.

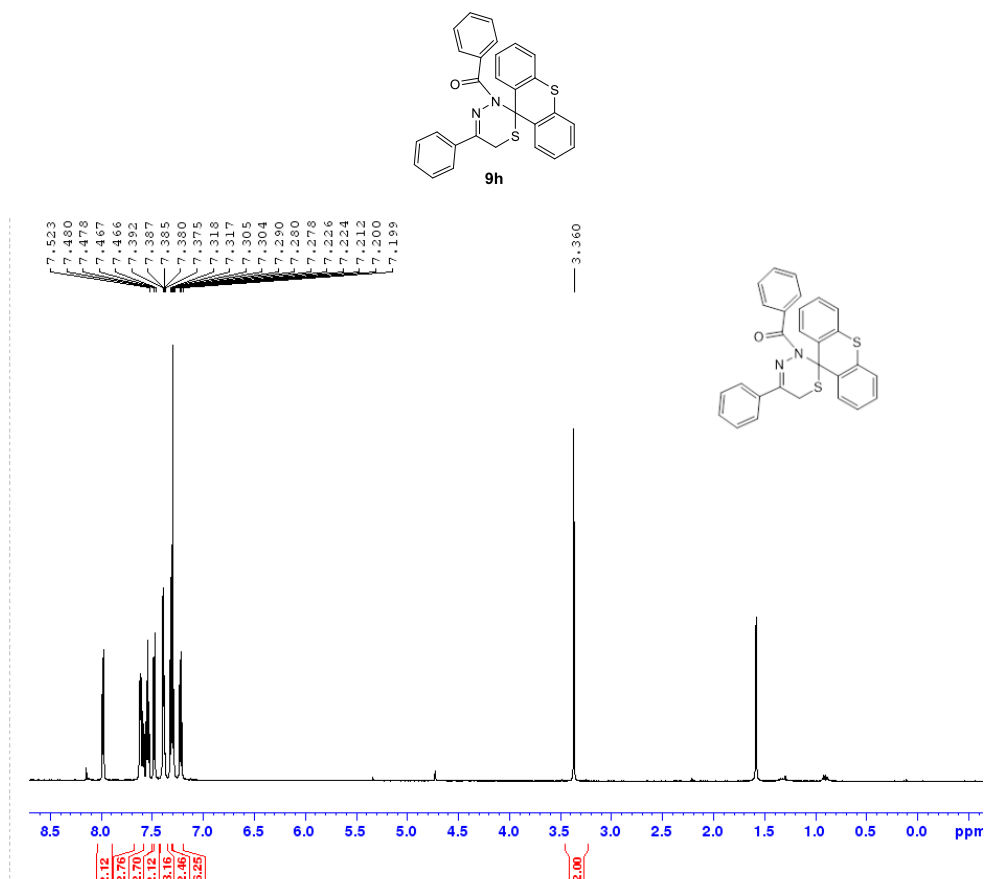


Fig. 8a.  $^1\text{H}$  NMR for compound 9h.

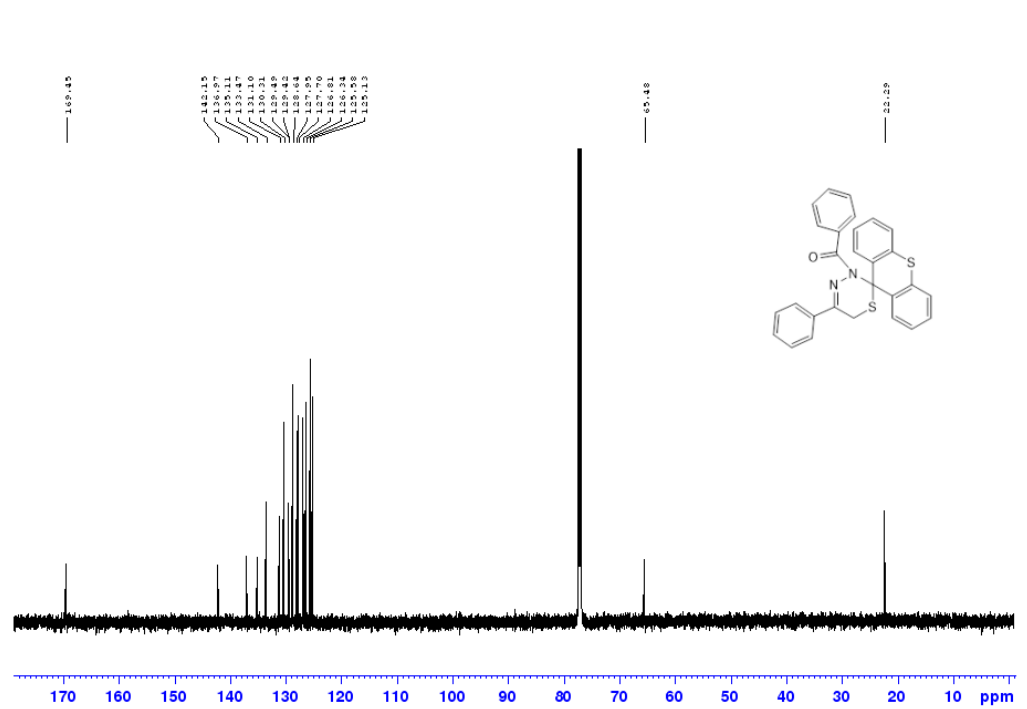
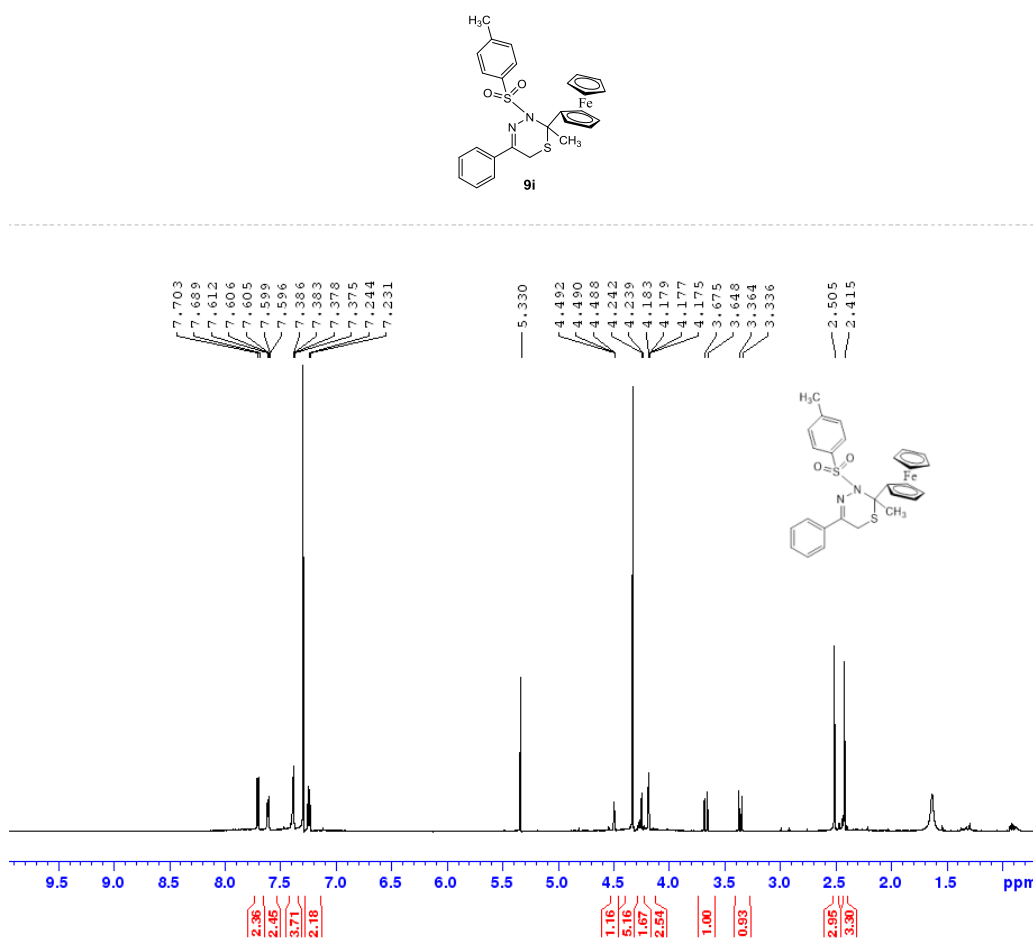


Fig. 8b.  $^{13}\text{C}$  NMR for compound 9h.



Chemical structure of compound 10 is shown as an inset. The structure is a ferrocene derivative with a sulfonamide group and a methyl group. The chemical structure is: Cc1ccc(S(=O)(=O)Nc2ccccc2)cc1 (Note: The structure in the image is more complex, involving a ferrocene core and a sulfonamide group, but the SMILES provided is a simplified representation of the sulfonamide part).

Chemical structure of **9j** is shown above the spectrum. The structure is a 1,3-diphenyl-4-methyl-5-(ferrocenyl)thiazolidine-2-one derivative. The spectrum displays peaks corresponding to the protons in the molecule, with chemical shifts ranging from approximately 1.5 to 7.5 ppm. Integration values are provided below the baseline.

**Chemical Shifts (ppm):** 7.416, 7.406, 7.397, 7.394, 7.381, 7.381, 7.289, 7.280, 7.285, 7.277, 7.273, 7.262, 7.258, 4.396, 4.394, 4.392, 4.390, 4.387, 4.384, 4.381, 4.379, 4.377, 4.375, 4.345, 4.243, 4.240, 4.239, 4.236, 4.235, 4.232, 4.203, 4.200, 4.199, 4.196, 4.195, 4.192, 4.153, 3.823, 3.794, 3.468, 3.439, 2.455, 1.578.

**Integration Values:** 1.80, 4.52, 4.38, 7.31, 0.85, 0.80, 2.36.

Fig. 10a.  $^1\text{H}$  NMR for compound 9j.

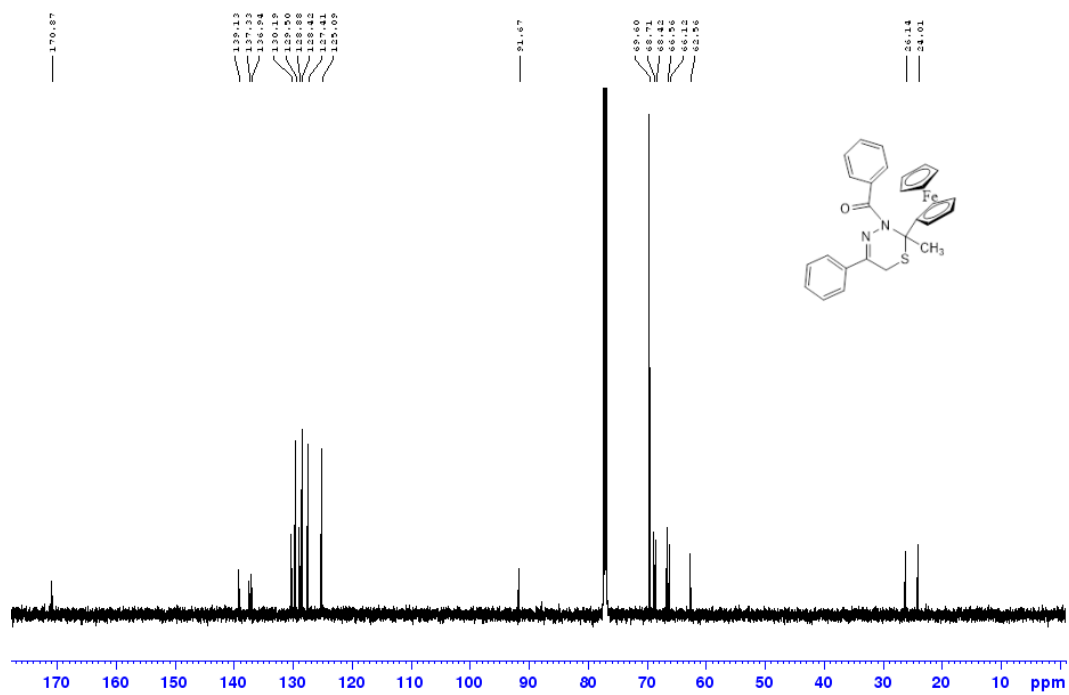
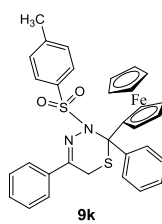


Fig. 10b.  $^{13}\text{C}$  NMR for compound 9j.



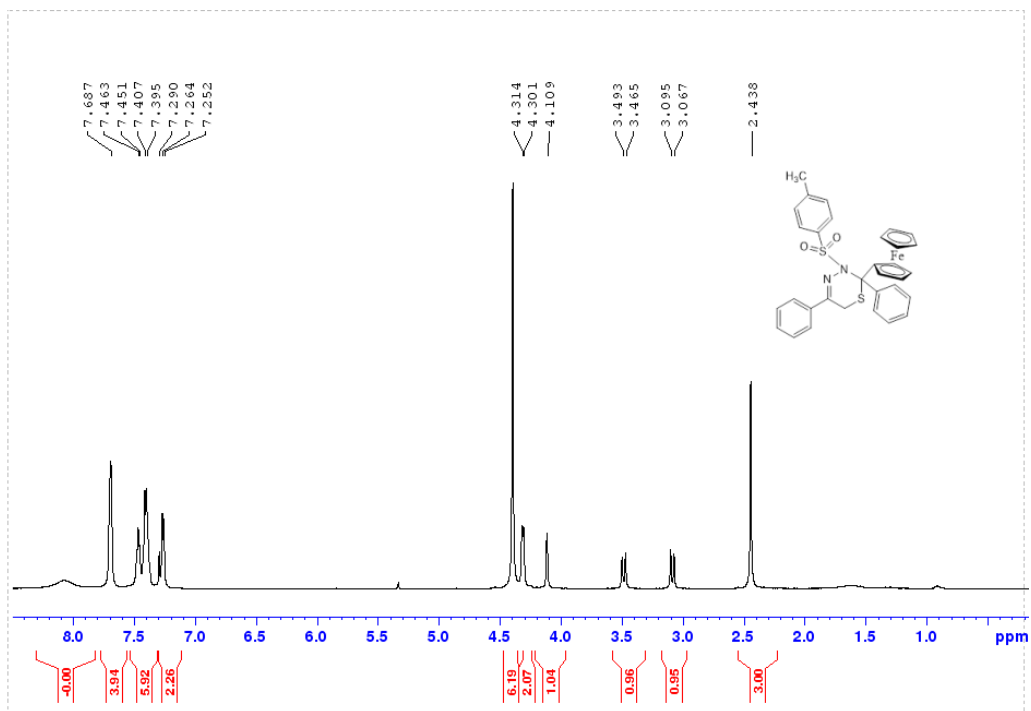


Fig. 11a. <sup>1</sup>H NMR for compound 9k.

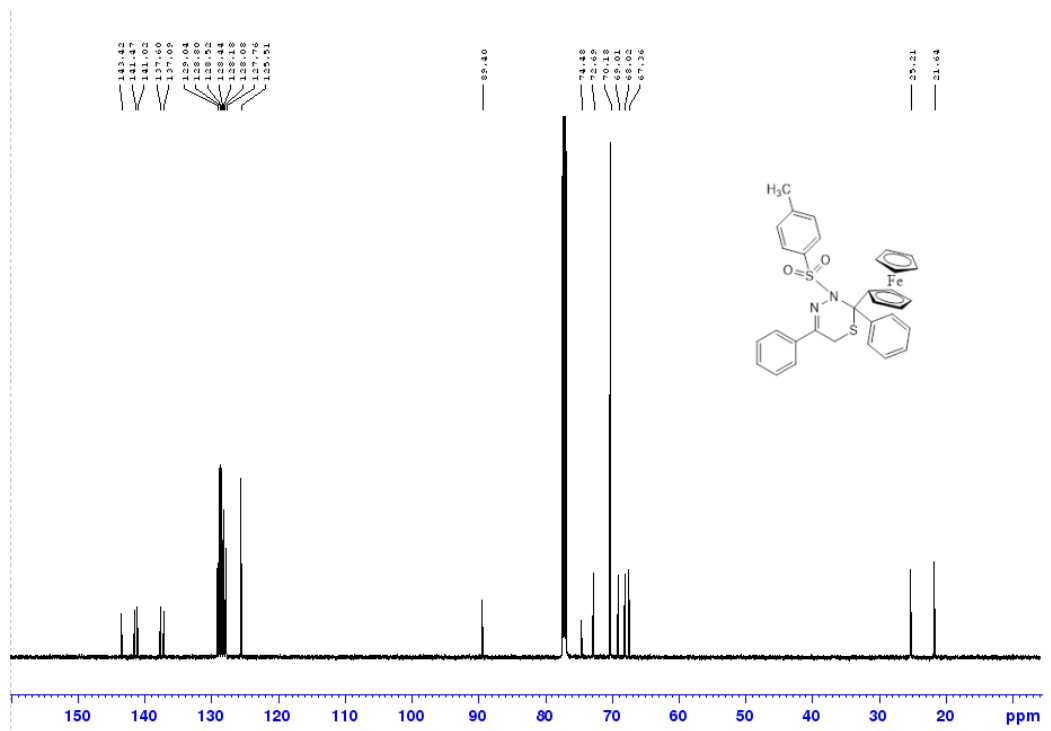
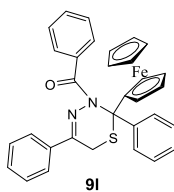


Fig. 11b. <sup>13</sup>C NMR for compound 9k.



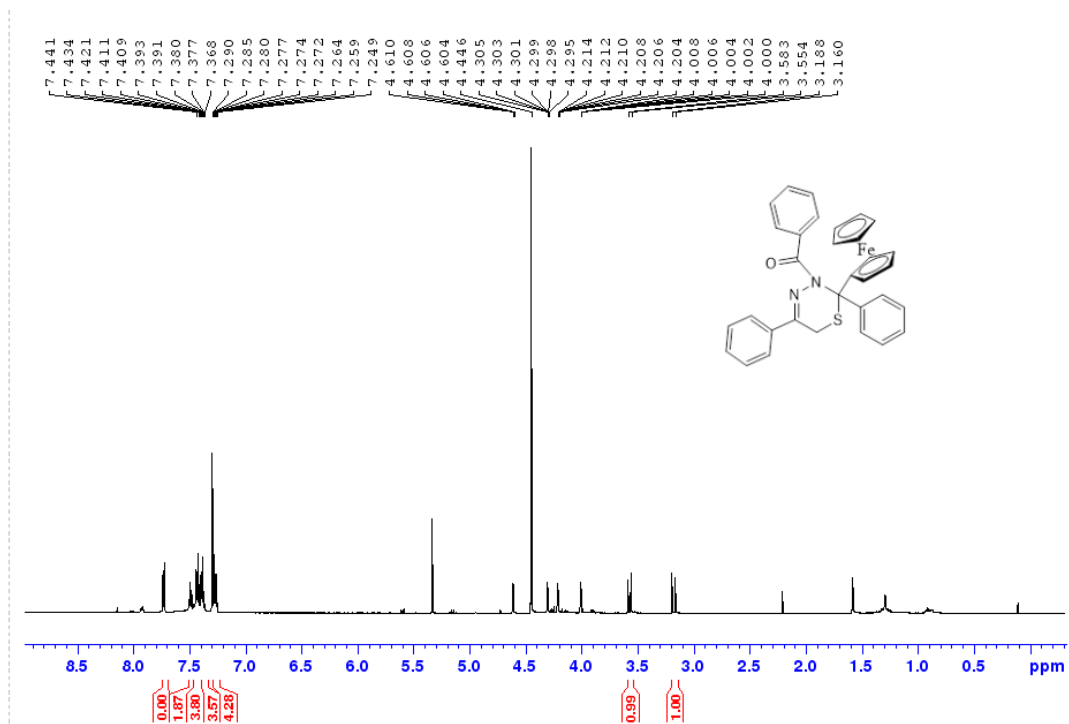


Fig. 12a. <sup>1</sup>H NMR for compound 9l.

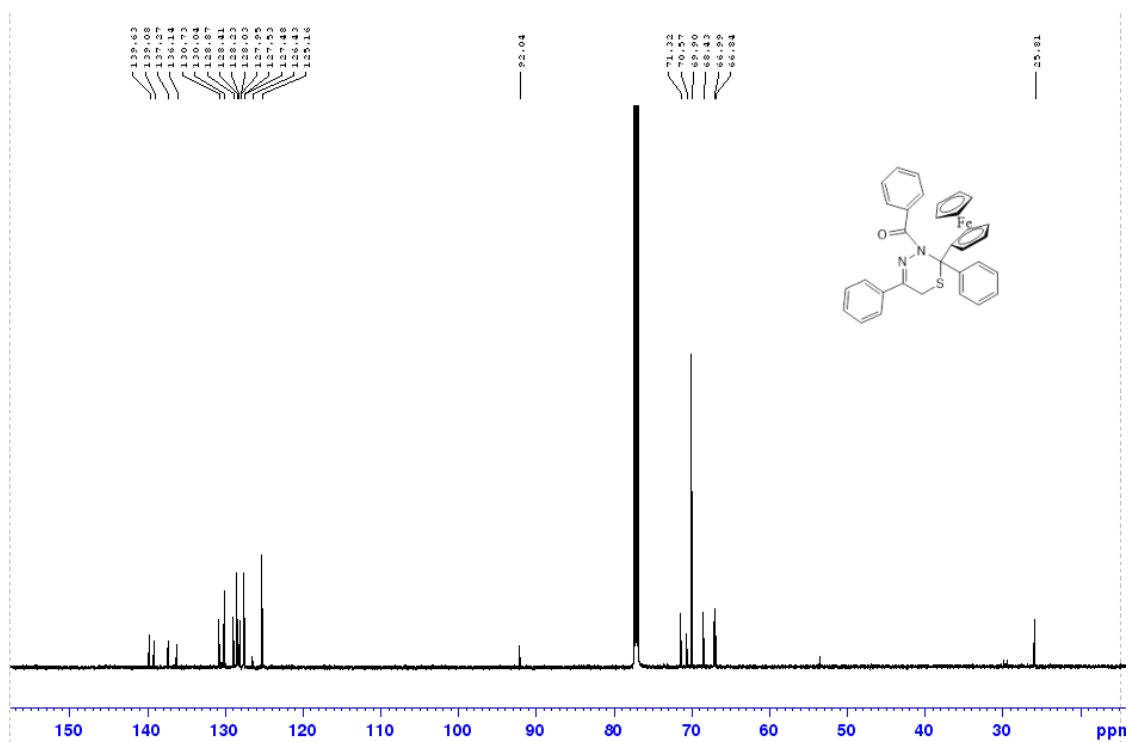
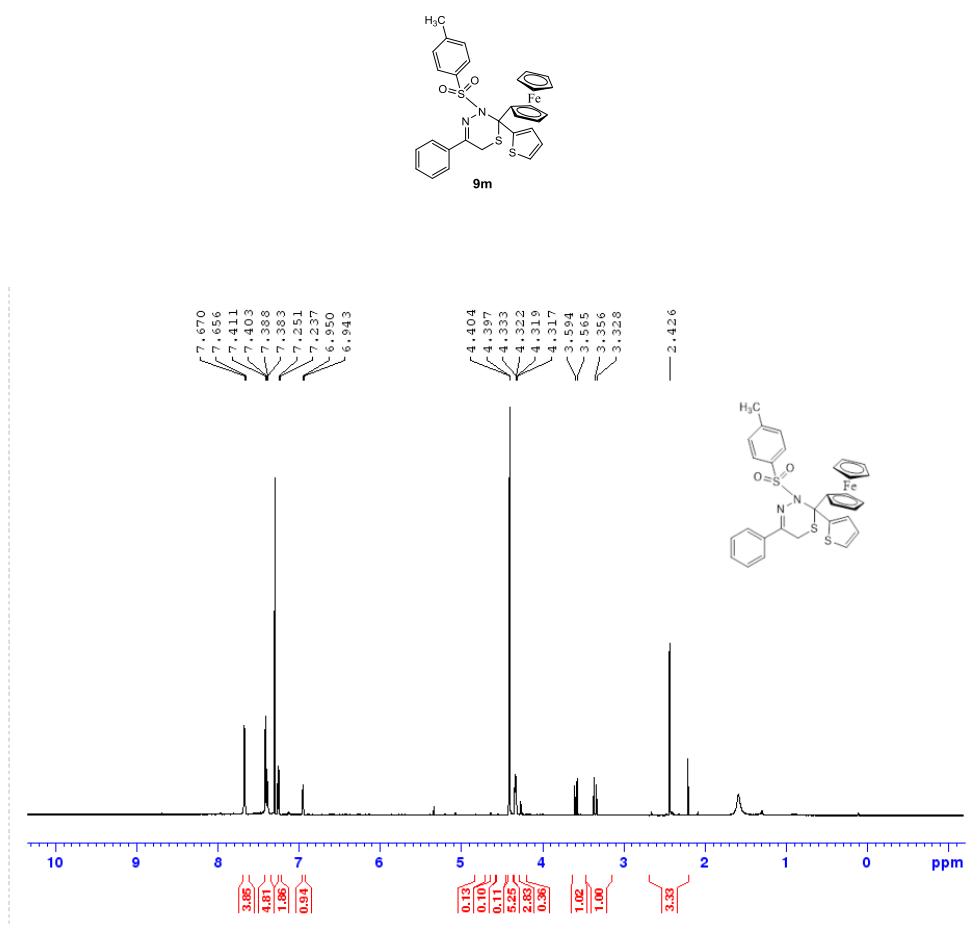
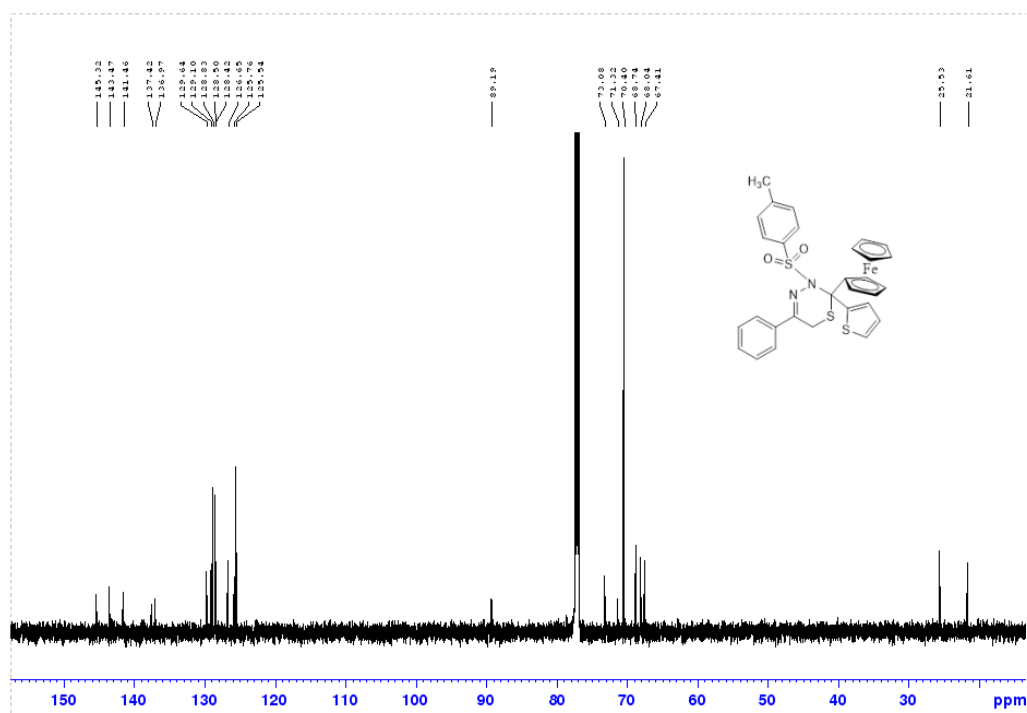


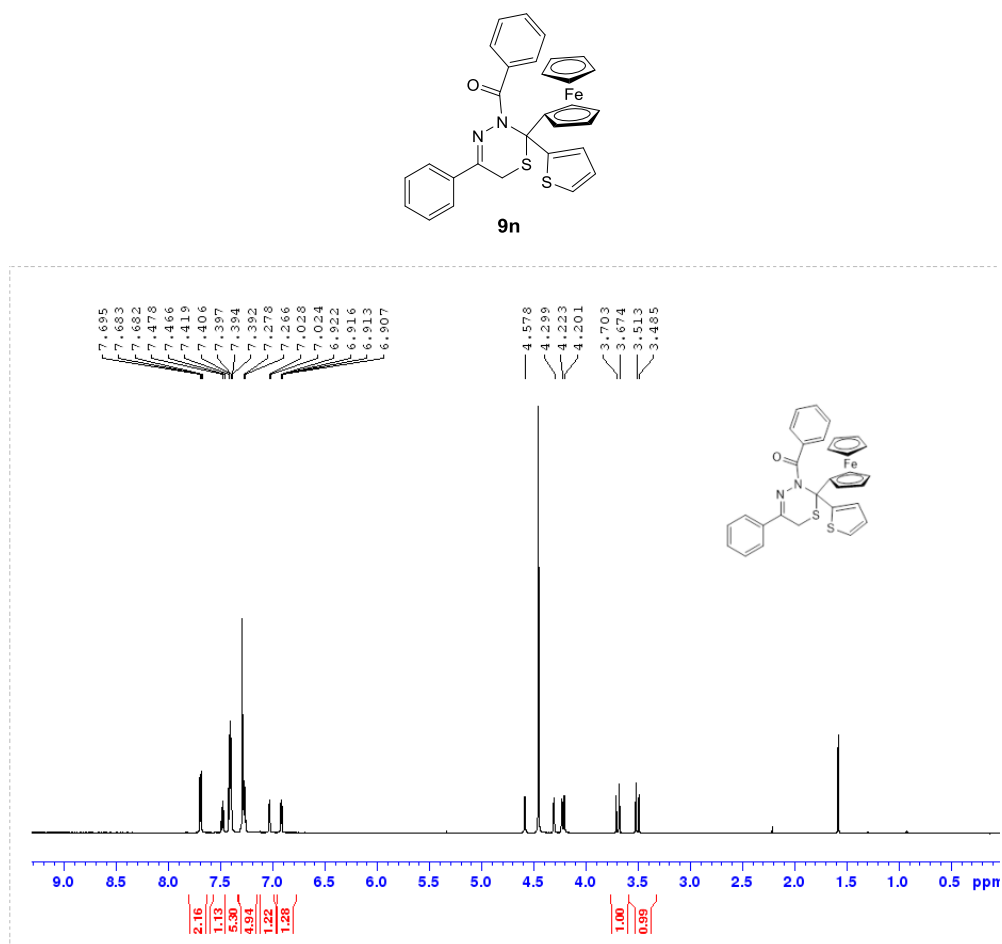
Fig. 12b. <sup>13</sup>C NMR for compound 9l.



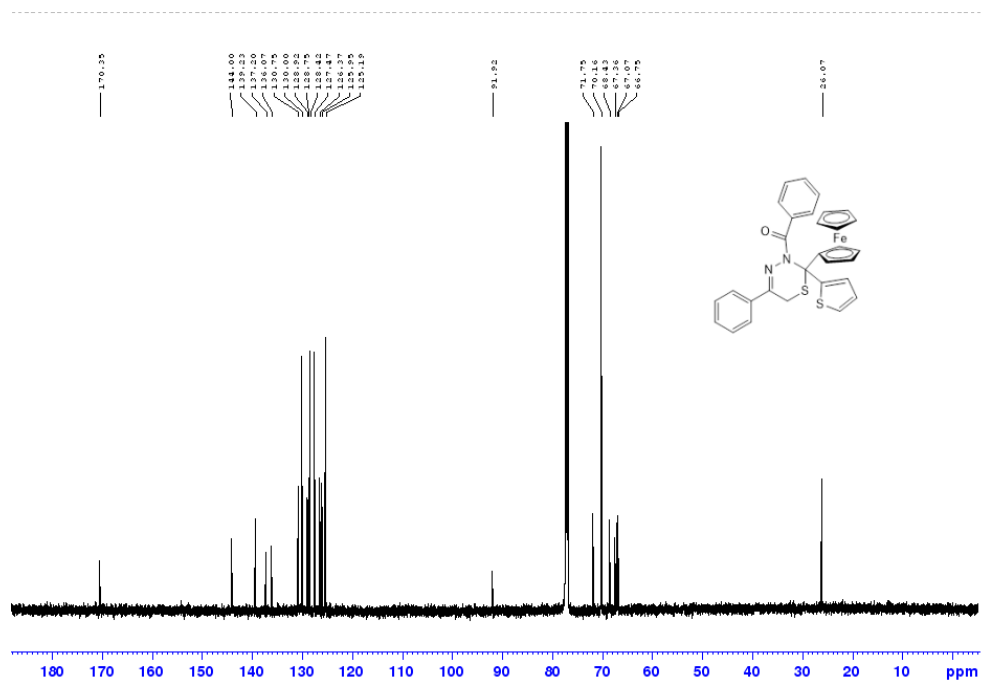
**Fig. 13a.** <sup>1</sup>H NMR for compound **9m**.



**Fig. 13b.** <sup>13</sup>C NMR for compound **9m**.

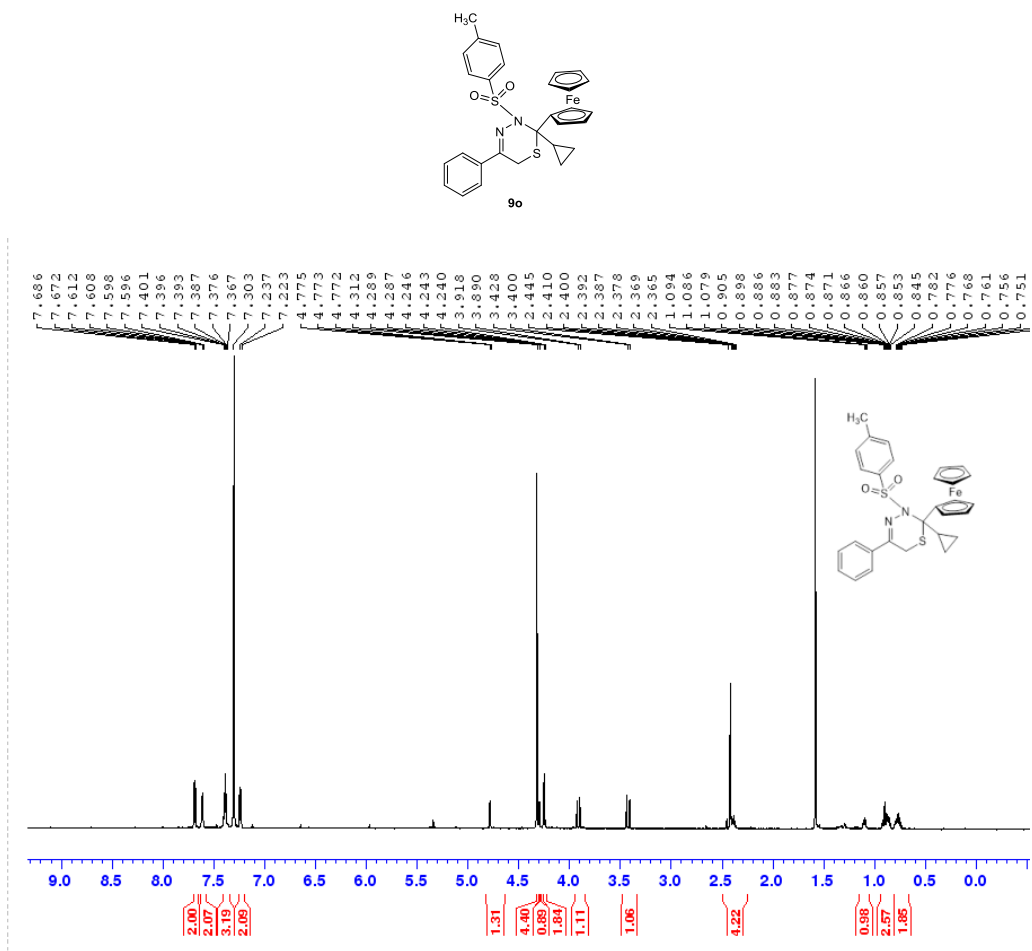


**Fig. 14a.**  $^1\text{H}$  NMR for compound **9n**.

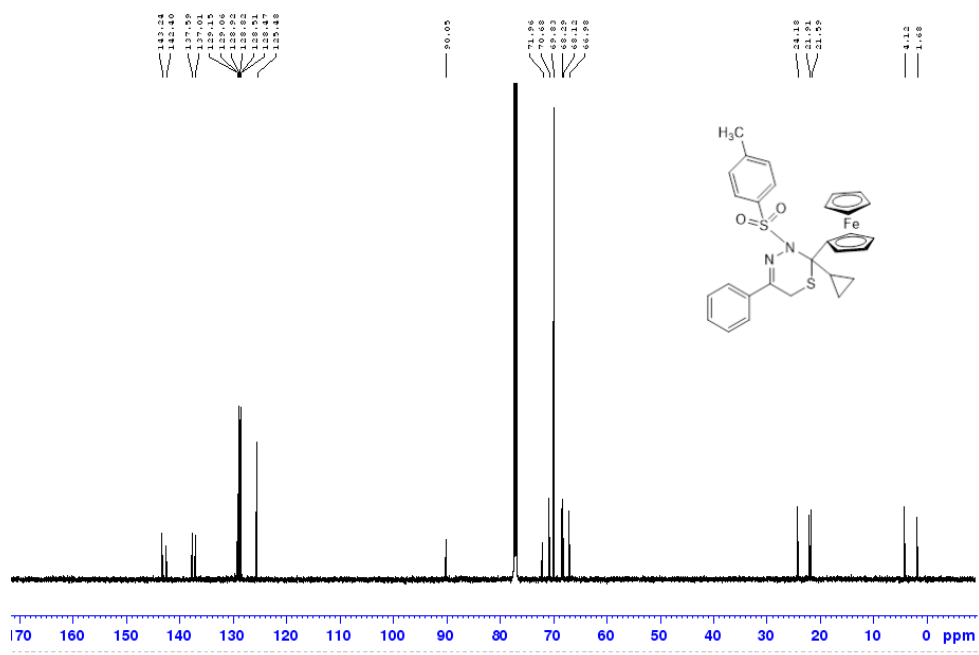


**Fig. 14b.**  $^{13}\text{C}$  NMR for compound **9n**.

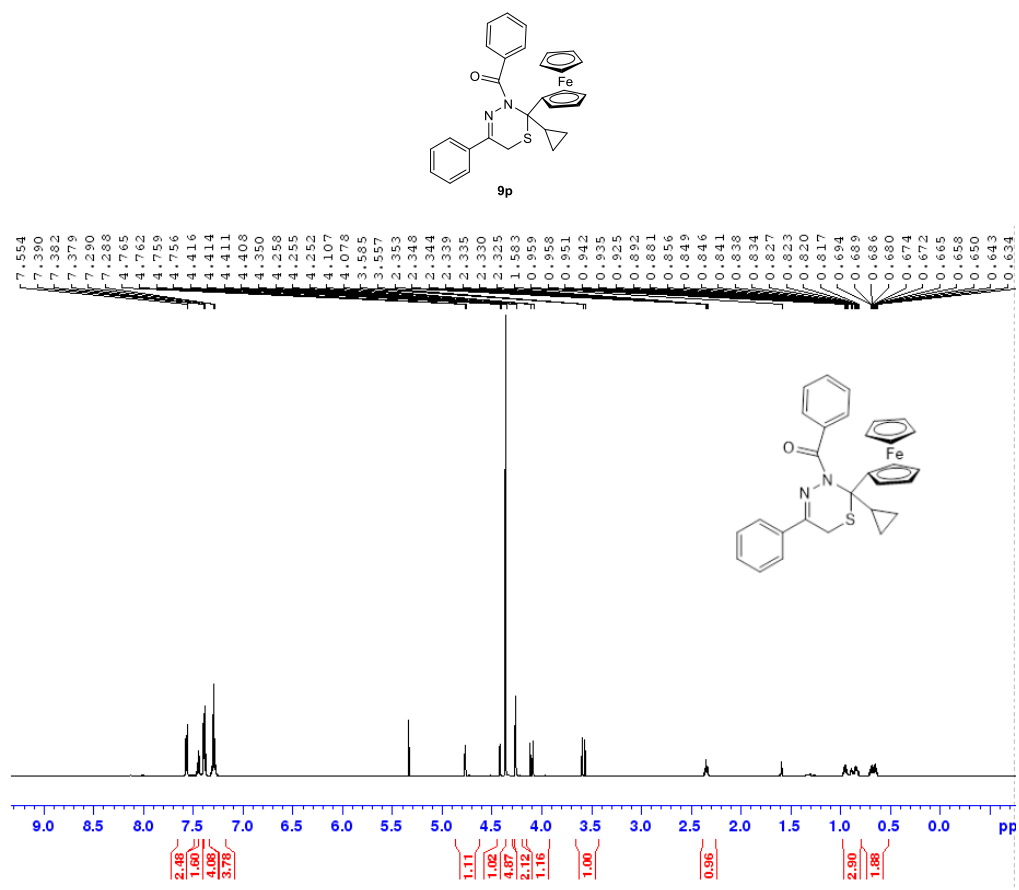




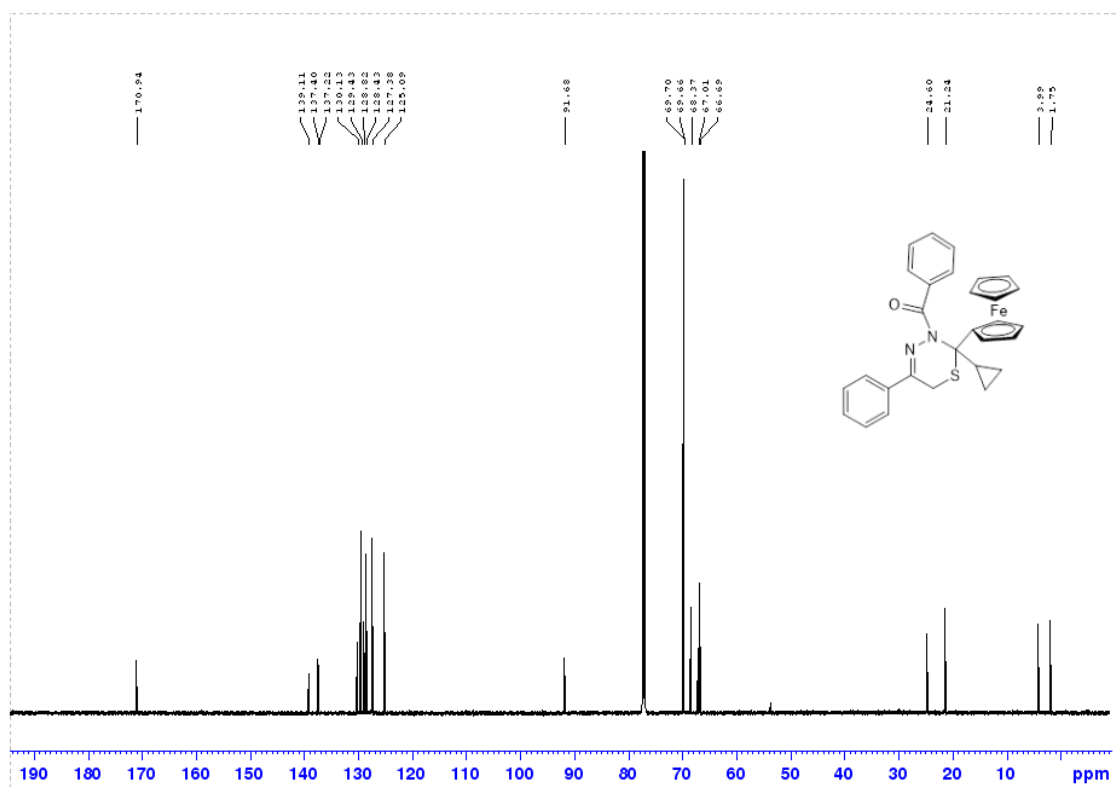
**Fig. 15a.** <sup>1</sup>H NMR for compound **9o**.



**Fig. 15b.** <sup>13</sup>C NMR for compound **9o**.



**Fig. 16a.** <sup>1</sup>H-NMR for compound **9p**.



**Fig. 16b.** <sup>13</sup>C-NMR for compound **9p**.

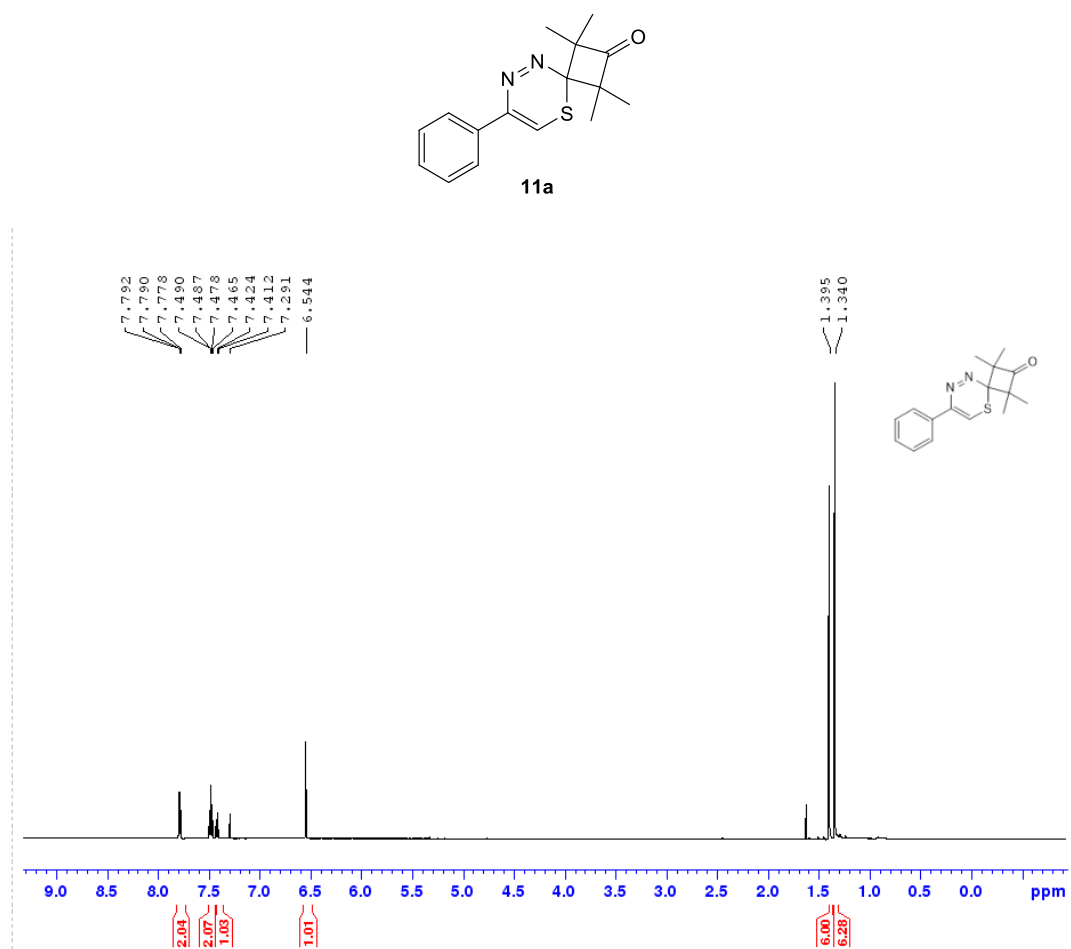


Fig. 17a. <sup>1</sup>H-NMR for compound 11a.

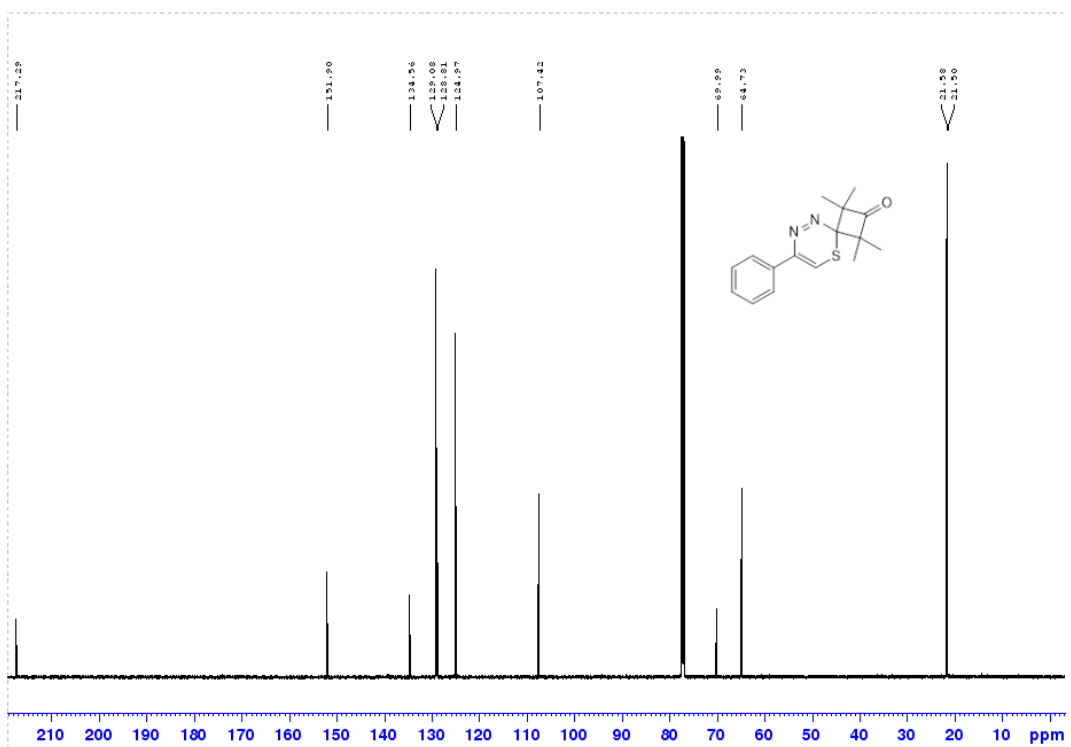
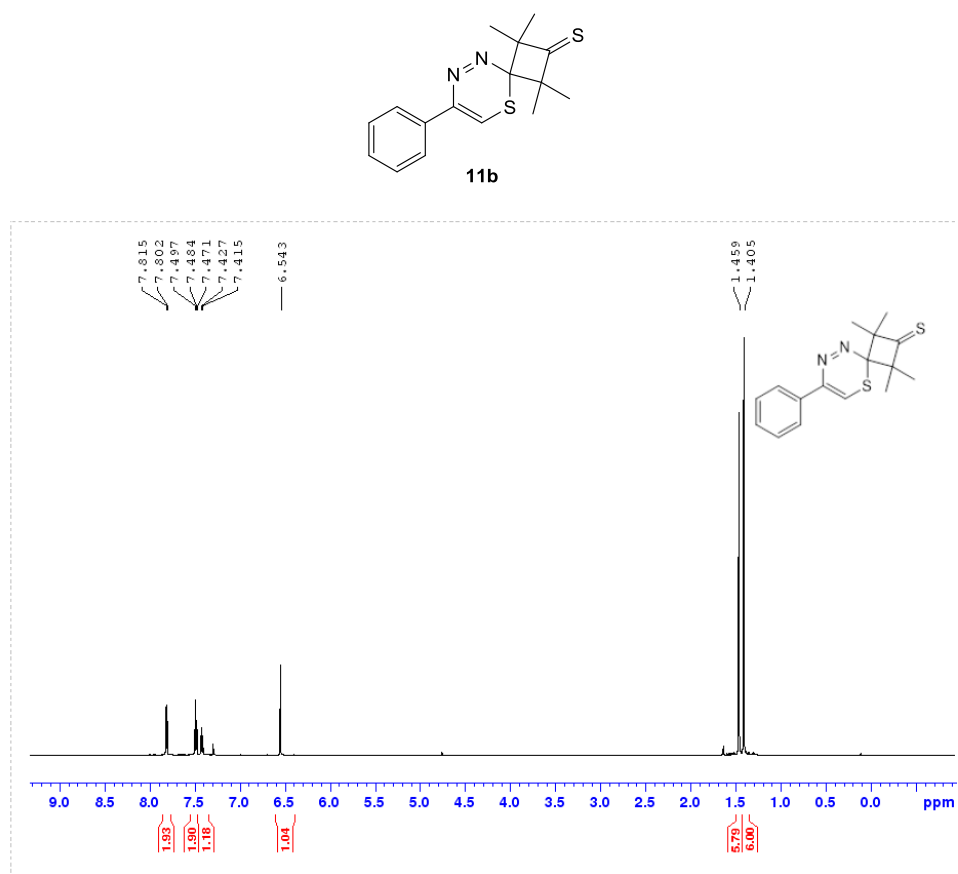
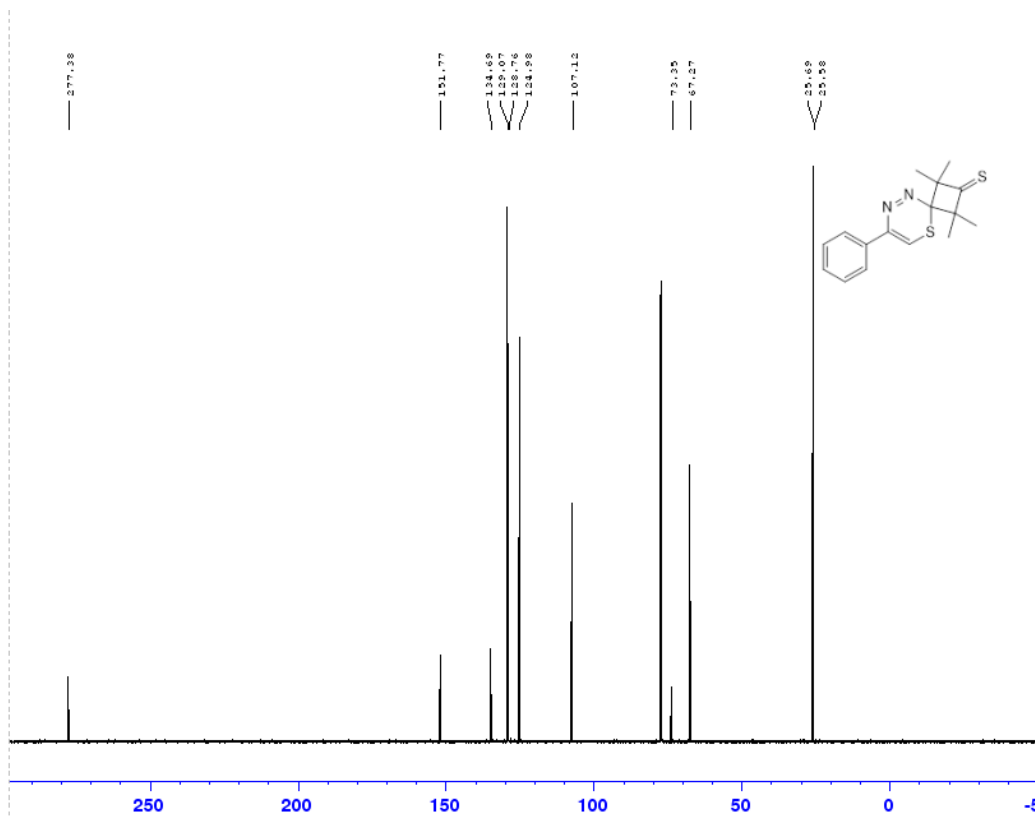


Fig. 17b. <sup>13</sup>C-NMR for compound 11a.



**Fig. 18a.**  $^1\text{H}$ -NMR for compound **11b**.



**Fig. 18b.**  $^{13}\text{C}$ -NMR for compound **11b**.

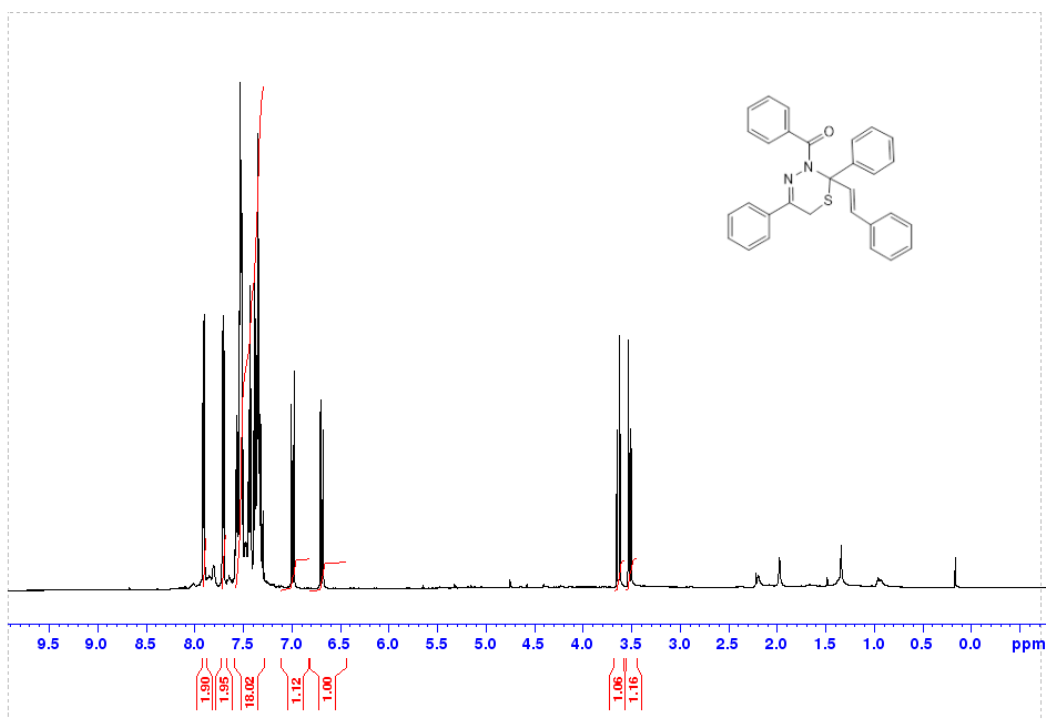
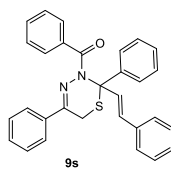


Fig. 19a. <sup>1</sup>H-NMR for compound 9s.

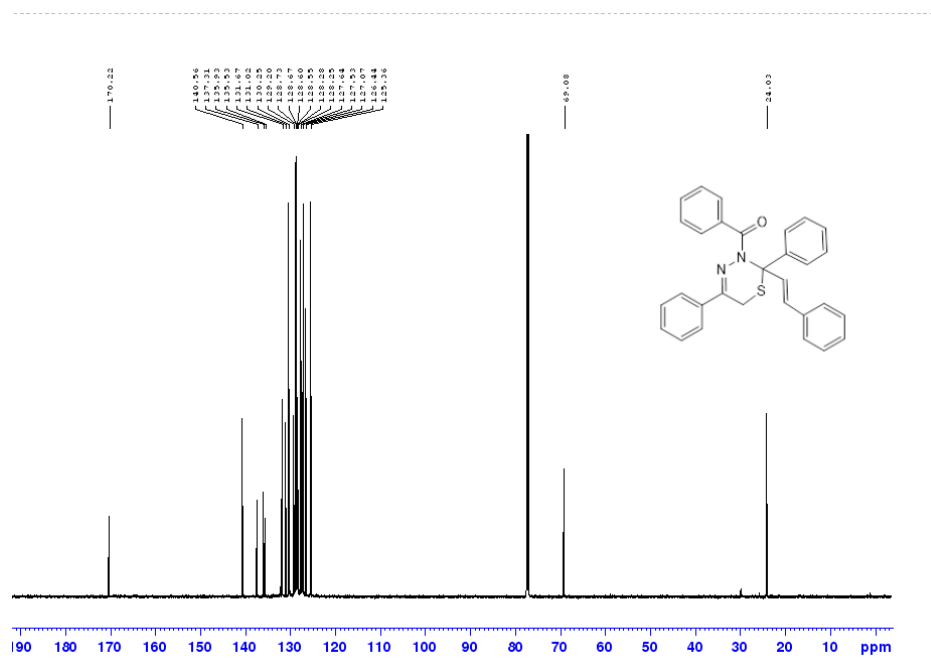
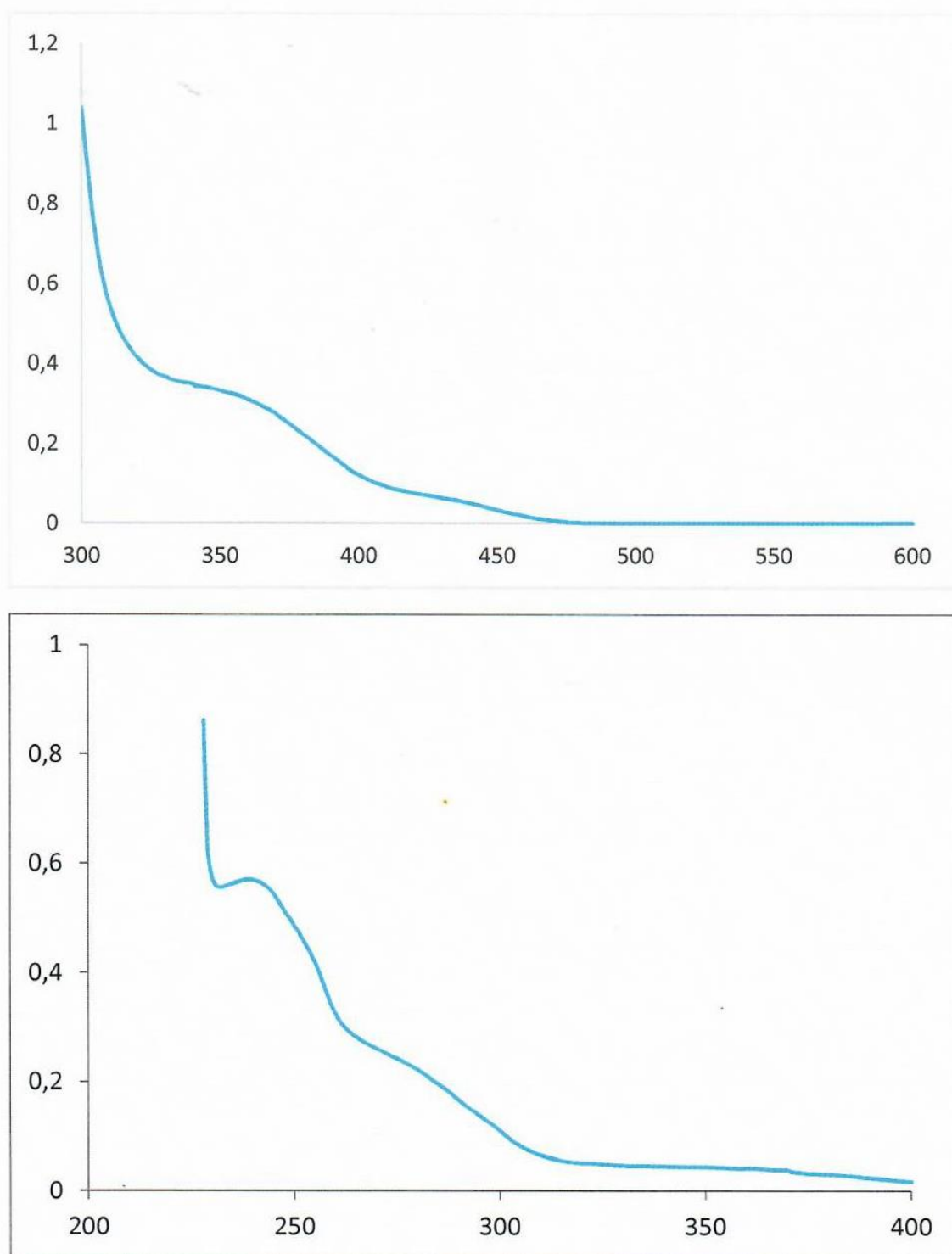
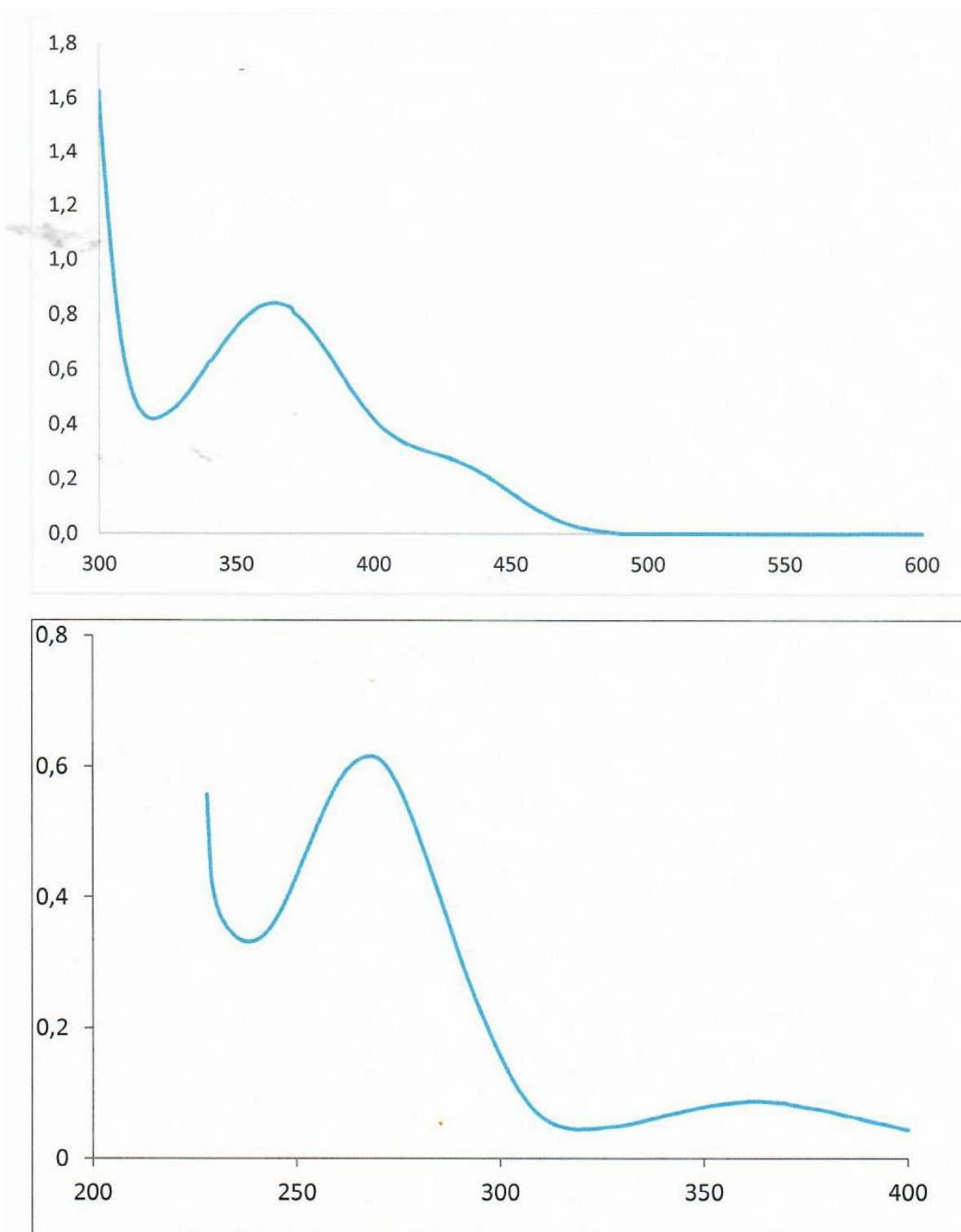


Fig. 19b. <sup>13</sup>C-NMR for compound 9s.

## 1.2. The UV-Vis spectra for products 11a-11b.



**Fig. 20a.** UV-Vis registered for **11a** (Concentration:  $c = 4,400 \times 10^{-5} \text{ mol/dm}^3$ ;  $\lambda_1$ : 239 nm,  $\epsilon_1 = 1.3 \times 10^4$ ;  $\lambda_2$ : 283 nm,  $\epsilon_2 = 3.7 \times 10^3$ ;  $\lambda_3$ : 358 nm,  $\epsilon_3 = 7.4 \times 10^2$ ;  $\lambda_4$ : 430 nm,  $\epsilon_4 = 1.6 \times 10^2$ ).



**Fig. 20b.** UV-Vis registered for **11b** (Concentration:  $4,398 \times 10^{-4} \text{ mol/dm}^3$ ; Absorptions:  $\lambda_1$  268 nm,  $\epsilon_1 = 1.36 \times 10^4$ ;  $\lambda_2$  364 nm,  $\epsilon_2 = 1.91 \times 10^3$ ;  $\lambda_3$ : 426 nm,  $\epsilon_3 = 5.8 \times 10^2$ ).

## 2. The X-Ray structure determinations

**Table S1.** Crystallographic data and structure refinement details for compounds **9c** and **9g**.

Compound	<b>9c</b>	<b>9g</b>
CCDC number	2072033	2072034
Formula	C <sub>28</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> S <sub>2</sub>	C <sub>28</sub> H <sub>22</sub> N <sub>2</sub> O <sub>2</sub> S <sub>3</sub>
<i>M<sub>r</sub></i>	482.60	514.65
Crystal size (mm)	0.39 x 0.16 x 0.04	0.15 x 0.1 x 0.05
Crystal system	monoclinic	triclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>c</i>	<i>P</i> -1
Temperature (K)	100	100
<i>a</i> (Å)	10.5875(4)	10.2742(3)
<i>b</i> (Å)	15.0374(6)	10.3516(3)
<i>c</i> (Å)	14.4764(5)	11.6550(3)
$\alpha$ (°)	90	81.401(1)
$\beta$ (°)	91.419(2)	77.990(1)
$\gamma$ (°)	90	82.594(1)
<i>V</i> (Å <sup>3</sup> )	2304.06(15)	1192.66(6)
<i>Z</i>	4	2
<i>D<sub>x</sub></i> (g cm <sup>-3</sup> )	1.391	1.433
$\lambda$ (Å)	0.71073	0.71073
$\mu$ (mm <sup>-1</sup> )	0.26	0.341
Transmissions	0.905–0.990	0.892–0.954
<i>F</i> (000)	1008	536
2 $\theta$ <sub>max</sub>	61.0	70.3
Refl. measured	64825	34181
Refl. indep.	7053	11499
<i>R</i> <sub>int</sub>	0.059	0.0295
Parameters	308	317
<i>wR</i> ( <i>F</i> <sup>2</sup> , all refl.)	0.1203	0.1071
<i>R</i> ( <i>F</i> , >4 $\sigma$ ( <i>F</i> ))	0.0395	0.0354
<i>S</i>	1.054	1.505
Max. $\Delta\rho$ (e Å <sup>-3</sup> )	0.380, –0.425	0.57, –0.43



### 3. DFT calculations

All calculations were performed using the GAUSSIAN 16, B.01 package of programs [1]. The structures were fully optimized first using the B3LYP/6-31G(d)[2,3]+GD3BJ [4,5] method, then the PBE1PBE/def2tzvp[6–10]+GD3BJ [4,5] functional including the PCM-solvent sphere for dichloromethane [11]. Zero point vibrational energies and free enthalpy contributions were determined analytically.

**Table S2:** Total energies ( $E_{\text{tot}}$ ) and Gibbs free energies ( $G_{298}$ ) [a.u.], of thiones (1)-azoalkene 7a-cycloadducts 9 and 10, respectively, van der Waals complexes and transition states and the relative energies with respect to the corresponding educts (last column) [kcal/mol].

Species	$E_{\text{tot}}$ [a.u.]	$E_{\text{rel}}$ [kcal/mol]	$G_{298}$ [a.u.]	$E_{\text{rel}}$ [kcal/mol]
1a	-899,06563		-898,91347	
7a	-1.237,34909		-1.237,13653	
Sum of 1a+7a	-2.136,41472	0.00	-2.136,05000	0.00
1a+7a->9a	-2.136,47789	-39,64	-2.136,08308	-20,76
vdW from 1a + 7a	-2.136,42596	-7,05	-2.136,04310	4,33
TS for 9a	-2.136,42240	-4,82	-2.136,03690	8,22
1a+7a->10a	-2.136,47314	-36,66	-2.136,08074	-19,29
TS for 10a	-2.136,40840	3,97	-2.136,01930	19,26
1b	-897,88171		-897,74937	
Sum of 1b + 7a	-2.135,23079	0.00	-2.134,88589	0.00
1b+7a->9c	-2.135,30019	-43,55	-2.134,92418	-24,02
vdW from 1b + 7a	-2.135,24502	-8,93	-2.134,88108	3,02
TS for 9c	-2.135,23749	-4,20	-2.134,86995	10,00
1b+7a->10c	-2.135,29415	-39,76	-2.134,92199	-22,65
TS for 10c	-2.135,22766	1,97	-2.134,85793	17,55
1m	-975,21672		-975,05214	
Sum of 1m+7a	-2.212,56580	0.00	-2.212,18866	0.00
1m+7a->9m	-2.212,62248	-35,56	-2.212,21346	-15,56
vdW from 1m+7a	-2.212,57931	-15.09	-2.212,18337	3,32
TS for 9m	-2.212,56876	-1,85	-2.212,16780	13,09
1m+7a->10m	-2.212,62629	-37,96	-2.212,21852	-18,74
TS for 10m	-2.212,53590	18,77	-2.212,13515	33,58

Table S2 continued.

Species	E <sub>tot</sub> [a.u.]	E <sub>rel</sub> [kcal/mol]	G <sub>298</sub> [a.u.]	E <sub>rel</sub> [kcal/mol]
<b>1n</b>	-976,43164		-976,24474	
<b>Sum of 1n+7a</b>	-2.213,78073	0.00	-2.213,38127	0.00
<b>1n+7a-&gt;9n</b>	-2.213,84387	-39,62	-2.213,41218	-19,40
<b>vdW from 1n + 7a</b>	-2.213,79526	-9,12	-2.213,37501	3,93
<b>TS for 9n</b>	-2.213,78692	-3,88	-2.213,36224	11,94
<b>1n+7a-&gt;10n</b>	-2.213,83438	-33,66	-2.213,40562	-15,28
<b>TS for 10n</b>	-2.213,75097	18,68	-2.213,32794	33,46
<b>1i</b>	-785,04269		-784,89811	
<b>Sum of 1i+7a</b>	-2.022,39178	0.00	-2.022,03464	0.00
<b>1i+7a-&gt;9q</b>	-2.022,45640	-40,55	-2.022,06501	-19,06
<b>vdW from 1i + 7a</b>	-2.022,40293	-7,00	-2.022,02787	4,25
<b>TS1-stepwise</b>	-2.022,39264	-0,54	-2.022,01364	13,17
<b>Z (Intermediate)</b>	-2.022,40302	-7,05	-2.022,01945	9,53
<b>TS2-stepwise</b>	-2.022,40177	-6,27	-2.022,01547	12,03
<b>1i+7a-&gt;10q</b>	-2.022,46135	-43,65	-2.022,07099	-22,81
<b>TS for 10q</b>	-2.022,37772	8,82	-2.021,99340	25,88
<b>11a</b>	-1.202,66061		-1.202,39925	
<b><i>p</i>-tolylsulfinic acid 12</b>	-819,76099		-819,66041	
<b>TS for 1i+7a (NNC)<sup>a)</sup></b>	-2.022,36888	14,37	-2.021,98357	32,05
<b>1i+7a (NNC)<sup>a)</sup></b>	-2.022,43486	-27,03	-2.022,04115	-4,09
<b>TS for 1i+7a (NNO)<sup>a)</sup></b>	-2.022,35652	22,13	-2.021,97281	38,80
<b>1i+7a (NNO)<sup>a)</sup></b>	-2.022,40164	-6,19	-2.022,01265	13,80

<sup>a)</sup> Addition to C=O bond of **1i**.

### 3.1. Gaussian Archive Entries

(Total energies (a.u.), number of imaginary frequencies (for transition states: imaginary frequencies), coordinates)

#### 1a

HF=-899.0656303 a.u. (0)

1\1\GINC-R08N09\FOpt\RPBE1PBE\def2TZVP\C13H10S1\WURTHWE\  
13-Feb-2021\0\ \# pbe1pbe/def2tzvp emp=gd3bj Opt nosym Pop=NBO Freq  
scrf=(solvent=dichloromethane)\ \ 1a Thiobenzophenone\ \ 0,1\C,0,-  
0.0000000004,0.042711794\S,0.0000000001,0,1.6837354658\C,1.2557467119,  
0.0884042861,-0.7175425213\C,-1.2557467119,-0.0884042865,-0.7175425212\  
C,1.4057634606,-0.6117728542,-1.9191088769\C,2.6078212372,-0.5791812938,-  
2.6060403986\C,3.6661419372,0.1755513656,-2.1205121721\C,3.52345991,  
0.887239145,-0.9349427787\C,2.3337451933,0.8341792594,-0.2331937183\  
H,0.584192158,-1.2067951338,-2.2982731448\H,2.7176554922,-1.1442445435,-  
3.5240433945\H,4.6022675673,0.2113620108,-2.6655457571\H,4.3448251108,  
1.4852857373,-0.5582433018\H,2.2144083461,1.380041514,0.6947214337\C,-  
1.4057634604,0.6117728538,-1.9191088769\C,-2.607821237,0.5791812939,-  
2.6060403985\C,-3.6661419373,-0.1755513652,-2.120512172\C,-3.5234599102,-  
0.8872391447,-0.9349427786\C,-2.3337451935,-0.8341792595,-0.2331937182\H,-  
0.5841921576,1.2067951332,-2.2982731448\H,-2.7176554919,1.1442445436,-  
3.5240433944\H,-4.6022675674,-0.2113620102,-2.665545757\H,-4.3448251112,-  
1.4852857368,-0.5582433017\H,-2.2144083464,-1.3800415141,0.6947214338\ \  
Version=ES64L-G16RevB.01\HF=-899.0656303\RMSD=3.877e-09\RMSF=  
9.391e-06\Dipole=0,0,-1.805389\Quadrupole=6.8796793,-5.3016639,-  
1.5780154,3.8736704,0,0.\PG =C02 [C2(C1S1), X(C12H10)]\ \@

#### 7a

HF=-1237.349088 a.u. (0)

1\1\GINC-R08N05\FOpt\RPBE1PBE\def2TZVP\C15H14N2O2S1\  
WURTHWE\ 05-Mar-202 0\0\ \# pbe1pbe/ def2tzvp Opt=readfc geom=check  
guess=read scrf=(solvent=dichloromethane) freq pop=nbo emp=gd3bj  
nosym\ \ 7a Tosylazoalkene\ \ 0,1\C,-0.1476006043,-0.0571155243,-  
0.140160722\C,0.0058651256,0.0348141764,1.2433905715\C,1.2903450417,  
0.1704767518,1.7736813537\C,2.3946036608,0.1899228894,0.9360954454\  
C,2.2344194585,0.0831316289,-0.4376440746\C,0.9581989886,-0.0379698151,-  
0.9726044737\C,-1.1713079966,-0.0027030352,2.1259390395\C,-2.3290009924,-  
0.6173703708,1.8738755755\N,-0.9326588434,0.5781080728,3.39817785\N,-  
1.8763591229,1.1534628411,3.9238461006\S,-1.5175406729,1.7665045356,

5.5144761968\O,-1.7455286349,3.1769147077,5.397137409\C,0.1727601006,  
 1.4461813991,5.8026006615\C,0.550605182,0.2450962506,6.3872807765\  
 C,1.8968915908,-0.0281548254,6.5462142653\C,2.8699991064,0.8766356417,  
 6.123137358\C,2.4608462098,2.0730848471,5.5340873599\C,1.11987051,  
 2.3646386166,5.3682783225\C,4.3225941321,0.5824656765,6.319103989\O,-  
 2.3364850737,0.9725299396,6.3840635662\H,1.4199093838,0.2523311994,2.84533  
 08306\H,3.3864790545,0.2891634535,1.3617671833\H,3.0988217918,  
 0.102532506,-1.0909830763\H,0.8227729827,-0.1071200872,-2.0456231076\H,-  
 1.1407886424,-0.124755364,-0.5684664586\H,-2.4796720777,-1.1763623556,  
 0.9603094979\H,-3.1246891805,-0.6086416184,2.6074294262\H,2.2002322584,-  
 0.9633375719,7.0032409125\H,-0.2030087941,-0.4609971385,6.7119945392\  
 H,0.805168379,3.2923235363,4.907458842\H,3.2063160545,2.7848796295,5.19770  
 7859\H,4.9287363952,1.0389702333,5.5354477513\H,4.5124988041,-  
 0.4914138612,6.3305353555\H,4.6655132597,0.9875965776,7.2760925324\ \  
 Version=ES64L-G16RevB.01\HF=-1237.349088\RMSD=3.701e-09\RMSF=  
 2.169e-06\Dipole=2.7504301,-1.3458846,-1.2804855\Quadrupole=11.2036248,-  
 3.5918655,-7.6117594,11.4512086,32.9203444,-14.0202401\PG=C01  
 [X(C15H14N2O2S1)]\ \@

### 9a (from 1a and 7a)

HF=-2136.4778897 a.u (0)

1\1\GINC-R09N15\FOpt\RPBE1PBE\def2TZVP\C28H24N2O2S2\  
 WURTHWE\13-Feb-202 0\0\ \# pbe1pbe/def2tzvp Opt=readfc geom=check  
 guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=dichloromethane)  
 \ \ 9a NNC-Product\ \ 0,1\C,-1.9393748698,-0.66373739,-0.3385230461\C,-  
 3.265097497,-0.5850208377,0.0467489798\C,-3.8491899784,-1.6221973124,  
 0.7651069396\C,-3.0955282801,-2.7400645105,1.0878672316\C,-1.7671840576,-  
 2.8233669853,0.6963925644\C,-1.1699284446,-1.7829625394,-0.0145458799\  
 C,0.2523818672,-1.8587626745,-0.3999628631\C,0.9044077691,-3.2020134134,-  
 0.501315892\N,0.8323833255,-0.746806339,-0.6489826444\N,2.1306794622,-  
 0.6215334171,-0.9800928\S,2.5068029001,1.017009308,-1.1491073841\  
 O,3.9342355659,1.1137694641,-1.1173613247\O,1.7758310119,1.5166891823,-  
 2.2750328959\C,0.8752415972,3.0008958568,2.5875873701\C,0.057535288,  
 2.8096109176,1.472005933\C,0.5396678358,2.2032589817,0.3291925427\  
 C,1.860399422,1.7737559433,0.2956405607\C,2.7001660145,1.968222836,  
 1.3826255942\C,2.2005908055,2.5803342037,2.5205990199\C,0.3297146293,  
 3.6410043217,3.8240806891\C,3.0953779483,-1.730303626,-1.0594371439\  
 S,2.1727901067,-3.16083592,-1.7660946121\C,4.4835591164,-2.9368336404,  
 2.8434389339\C,3.6488738716,-1.8408717244,2.7133044089\C,3.2070742468,-  
 1.4429736998,1.4569713584\C,3.5958458637,-2.13122503,0.3170001125\  
 C,4.416482884,-3.2509689683,0.459619566\C,4.8640276186,-3.6436363244,  
 1.7080187046\C,5.5279854526,-1.4398862423,-1.7779639617\C,6.4769820942,-

1.1907547755,-2.7584834433\ C,6.0868716164,-0.9441396386,-4.0656477469\  
 C,4.7366267676,-0.9442373658,-4.3874288611\ C,3.7894076308,-1.1978975954,-  
 3.4101828723\ C,4.1769846632,-1.4497726107,-2.0954628271\ H,-1.4831682629,  
 0.136000706,-0.9071610259\ H,-3.8509199515,0.2870334392,-0.2205195177\ H,-  
 4.8886644175,-1.5599647693,1.0652989278\ H,-3.5408778629,-3.5540195267,  
 1.6480098118\ H,-1.1918749806,-3.7011700137,0.966221099\ H,1.3284727314,-  
 3.5274638288,0.4535640719\ H,0.1783648933,-3.9505699097,-0.8196601291\ H,-  
 0.9735220723,3.1445363857,1.5021026965\ H,-0.0922290347,2.0656481204,-  
 0.537167752\ H,3.7339645452,1.651564753,1.3320821231\ H,2.8556693323,  
 2.7384228965,3.3699557982\ H,1.1221217528,3.8748842323,4.535044366\ H,-  
 0.2058663297,4.5623130106,3.5850195501\ H,-0.3824068502,2.9741124932,  
 4.3184622288\ H,4.8300665034,-3.2486204394,3.8217650479\ H,3.3297767815,-  
 1.287907387,3.589189775\ H,2.5413596456,-0.5948510073,1.3798489714\  
 H,4.6995217913,-3.8212712592,-0.4167974332\ H,5.508594375,-4.5103536015  
 ,1.7970046074\ H,5.8477159892,-1.6024976718,-0.7577503866\ H,7.5277349446,-  
 1.1814359691,-2.492905619\ H,6.8300132289,-0.7472179419,-4.8295514797\  
 H,4.417386853,-0.7445276647,-5.403620195\ H,2.7361141473,-1.1852854812,-  
 3.6644208476\ \ Version=ES64L-G16RevB.01\ HF=-2136.4778897\ RMSD=  
 3.516e-09\ RMSF=1.275e-06\ Dipole=-0.9525195,-0.808447,2.7391283\  
 Quadrupole=0.1676077,0.8836617,-1.0512694,-8.5167297,7.4089125,  
 4.6575909\ PG=C01 [X(C28H24N2O2S2)]\ \@

### 1a + 7a vdW-complex

HF=-2136.425961 a.u.(0)

1\1\GINC-R10N37\FOpt\RPBE1PBE\def2TZVP\C28H24N2O2S2\  
 WURTHWE\13-Feb-202 0\0\ \# pbe1pbe/def2tzvp opt=readfc geom=check  
 guess=read scrf=(solvent =dichloromethane) freq pop=nbo emp=gd3bj  
 nosym\ \ 1a + 7a vdW-complex\ \ 0,1\ C,0.231977665,2.8374631356,-  
 3.6161122983\ C,0.3713738998,2.7905928972,-2.2260658986\ C,1.5139236086,  
 2.1955615487,-1.6797198677\ C,2.476884226,1.6406438273,-2.5070635672\  
 C,2.3310879494,1.7004275543,-3.8853931996\ C,1.2092731201,2.3086340653,-  
 4.4380254797\ C,-0.6998138999,3.2760372551,-1.3431792511\ S,-2.2768187417,  
 3.1227705423,-1.7727623291\ C,-0.311054726,3.8730585795,-0.0597117433\  
 C,0.8521206258,4.6437465527,0.0386720317\ C,1.1983903927,5.2414967632,1.238  
 1543542\ C,0.4056181348,5.0545390746,2.3619627072\ C,-0.744760389,  
 4.2797441474,2.2784031373\ C,-1.1067881531,3.7038658532,1.0756114689\ C,-  
 1.0803815665,-0.5390347932,-2.2323240295\ C,-1.1524104295,-1.401737153,-  
 1.2164265796\ C,-1.786577985,-2.730045572,-1.2502418325\ C,-1.3299701704,-  
 3.7608807224,-0.426743208\ C,-1.9227587005,-5.0127477758,-0.4787023613\ C,-  
 2.9812527693,-5.2519717732,-1.3429404867\ C,-3.4497977036,-4.2266047408,-  
 2.1543976253\ C,-2.8612424813,-2.9744877158,-2.105333252\ N,-0.4692485738,-  
 1.1458492899,-0.0012071201\ N,-0.4522451699,0.0125342243,0.3951013091\

S,0.4396410385,0.212510696,1.880992534\O,-0.555564005,0.628304143,  
 2.8251283633\C,1.0532546889,-1.365104168,2.3058678819\C,0.2606986647,-  
 2.2213826695,3.0589085504\C,0.7230742755,-3.4949325017,3.3330664825\  
 C,1.9628518652,-3.9274967407,2.8623460743\C,2.7350906564,-3.0474859648,  
 2.1047959564\C,2.2887187982,-1.7700448087,1.8194549913\C,2.4634974104,-  
 5.2986925934,3.1851416816\O,1.5215057571,1.0897741162,1.5364664978\H,-  
 0.5037722693,-3.5784864543,0.2485901797\H,-1.5537177809,-5.8058300186,  
 0.1614627398\H,-3.4461402115,-6.2302622775,-1.3789518182\H,-4.2861591434,-  
 4.4000892787,-2.8214701344\H,-3.250896548,-2.172813227,-2.7217905753\H,-  
 0.5642458713,0.4042986173,-2.1207516043\H,-1.4906766859,-0.784125672,-  
 3.2026991776\H,0.1097649322,-4.1694837196,3.9199182298\H,-0.7038924282,-  
 1.8895293112,3.4213279086\H,2.888179733,-1.0901406368,1.2274379065\  
 H,3.6994683874,-3.3712117032,1.7296978773\H,2.9942775772,-5.2928918355,  
 4.1420974184\H,1.6414548859,-6.0104588078,3.2725997348\H,3.159634389,-  
 5.656471047,2.4257216756\H,3.0905415729,1.2750163777,-4.5311651303\  
 H,3.343899246,1.1582427871,-2.0711847523\H,1.6211161627,2.1269892429,-  
 0.6047586536\H,-0.6525084805,3.3006909583,-4.0359738188\H,1.0978037596,  
 2.3668028837,-5.5143237634\H,1.4713190523,4.792810281,-0.8372784447\  
 H,2.0919315396,5.8516208314,1.2971048211\H,0.6866118997,5.50837211,  
 3.3052953201\H,-1.3554479362,4.1165490413,3.1582675908\H,-1.995699095,  
 3.0900958658,1.0019425784\ \ Version=ES64L-G16RevB.01\ HF=-2136.425961\  
 RMSD=8.518e-09\RMSF=1.117e-06\Dipole=1.84845,-3.038735,-0.2895545\  
 Quadrupole=-6.2283789,6.2379413,-0.0095625,6.759272,0.34714,-  
 7.5968848\PG=C01[X(C28H24N2O2S2)]\ \ @

### TS for 9a

HF=-2136.4224007 a.u. (1, -86,8511cm<sup>-1</sup>)

1\1\GINC-R08N29\FTS\RPBE1PBE\def2TZVP\C28H24N2O2S2\  
 WURTHWE\14-Feb-2020\0\ \ # pbe1pbe/def2tzvp Opt=(ts,noeigentest,  
 readfc) geom=check guess=read freq pop=nbo emp=gd3bj nosym  
 scrf=(solvent=dichloromethane)\ \ TS for 9a \ \ 0,1\C,0.4014402519,-  
 0.3765159971,0.153198678\C,0.0820383761,-0.1323584563,1.4928766126\  
 C,1.1074231569,-0.1502842009,2.4450745452\C,2.412226576,-0.4111369304,  
 2.0631990684\C,2.7178083952,-0.6418990895,0.7289880033\C,1.7082802645,-  
 0.6206620807,-0.225991715\C,-1.308429988,0.0812730062,1.9054350678\S,-  
 2.5432151983,-0.6554759652,1.1043000927\C,-1.588125835,0.9628682728,  
 3.0444652765\C,-0.8046432207,2.0987699036,3.2684795507\C,-1.0927938168,  
 2.9547219852,4.3186393551\C,-2.1500038705,2.677016075,5.1726660518\C,-  
 2.9304201049,1.5452106535,4.9635822376\C,-2.6604570029,0.7036436897,  
 3.9027964747\C,-1.8690591672,-3.1381365419,1.2978242742\C,-2.6000780819,-  
 3.4522197224,2.4003877347\C,-3.9560627879,-4.0197211218,2.3675242982\C,-  
 4.8076894435,-3.8689205257,3.464229865\C,-6.0966969517,-4.3758823226,

3.4340630426\ C,-6.5615332082,-5.0421043853,2.3090026374\ C,-5.7220464309,-  
5.2013573146,1.2144050377\ C,-4.4323033879,-4.6983500268,1.2438712894\ N,-  
2.1074907514,-3.210003876,3.6795645723\ N,-1.0821602085,-2.5120270336,  
3.7648517491\ S,-0.5590776705,-2.3541343092,5.4035917784\ O,-1.593153229,-  
2.7212856408,6.3293923991\ C,0.7126896343,-3.5544033067,5.4328162435\  
C,0.4326035781,-4.8380777498,5.8854465334\ C,1.4337617564,-5.7907467086,  
5.8611425071\ C,2.7096079863,-5.4846025728,5.3855588326\ C,2.9601350403,-  
4.1913697455,4.9300231839\ C,1.9716180365,-3.2236607703,4.9493211245\  
C,3.7891288666,-6.5192416394,5.3880147719\ O,0.0220608013,-1.0420225644,  
5.4636284338\ H,-4.4497739742,-3.345938642,4.3421900385\ H,-6.7435963117,-  
4.2445197135,4.2939032467\ H,-7.5699974071,-5.4382654156,2.2855968607\ H,-  
6.070560147,-5.7295322477,0.3343584342\ H,-3.784986101,-4.8544519291,  
0.389069382\ H,-0.835471892,-2.8350984577,1.4009917362\ H,-2.2240385006,-  
3.3696096318,0.304136752\ H,1.2237891408,-6.7934071433,6.2168388197\ H,-  
0.5567068376,-5.077298259,6.2544618364\ H,2.1693068529,-2.2194285376,  
4.5976062883\ H,3.9453991064,-3.9396052852,4.5537875674\ H,4.587952727,-  
6.2626955669,4.691660785\ H,4.2319199443,-6.6047231589,6.3849980118\  
H,3.3952066392,-7.5020188239,5.1234668952\ H,3.7416480984,-0.8375521304,  
0.4319252961\ H,3.195983165,-0.4364129964,2.8115033904\ H,0.8644952541,-  
0.0054736002,3.4895478011\ H,-0.3909374987,-0.3555044728,-0.5852018474\  
H,1.9434411166,-0.7910949892,-1.2699326451\ H,0.0179139446,2.3223626832,  
2.6005228976\ H,-0.4874474127,3.8404209424,4.4711545989\ H,-2.3653018857,  
3.3389142532,6.0034161347\ H,-3.7482940248,1.3170523657,5.6367248883\ H,-  
3.2597060306,-0.1833590661,3.7373191449\ \ Version=ES64L-G16RevB.01\ HF=-  
2136.4224007\ RMSD=8.341e-09\ RMSF=1.903e-06\ Dipole=2.2151311,-  
1.1203046,-1.4114871\ Quadrupole=7.0313603,16.9801704,-24.0115307,-  
10.4322825,15.4841978,-0.2366612\ PG=C01[X(C28H24N2O2S2)]\ \@

### 10a (from 1a and 7a)

HF=-2136.4731387 a.u. (0)

1\1\GINC-R09N28\FOpt\RPBE1PBE\def2TZVP\C28H24N2O2S2\  
WURTHWE\12-Feb-2020\0\# pbe1pbe/def2tzvp Opt=readfc geom=check  
guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=dichloromethane)  
\10a NNS-Product\0,1\ C,-1.6028265051,-0.8445503227,0.1150750005\ C,-  
2.9599604395,-1.0366581732,0.2934129849\ C,-3.4224043498,-1.9347962833,  
1.2491234715\ C,-2.5126400937,-2.6398785973,2.0206525093\ C,-1.1496288293,-  
2.4541257312,1.8380945865\ C,-0.6760925573,-1.5514456476,0.8863904584\  
C,0.772216558,-1.3337366084,0.7003181595\ C,1.7250558682,-2.3455920297,  
1.2761410517\ N,1.0991906228,-0.2803996757,0.0527882428\ N,2.3875819026,  
0.0166067494,-0.2047809521\ S,2.5868475613,1.5394147923,-0.880750471\  
O,3.9950222092,1.6474864588,-1.1160697678\ O,1.6526859716,1.6405192781,-  
1.9567705939\ C,1.3510149866,4.2936681222,2.4897328008\ C,0.405685761,3.800

719061,1.5902463367\ C,0.7761084551,2.979492919,0.5414973554\  
 C,2.1159063065,2.6440066458,0.3892106727\ C,3.0777154625,3.1144282084,  
 1.2734194715\ C,2.687092034,3.938147981,2.3145067934\ C,0.940670949,  
 5.2052012265,3.6021058202\ S,3.6904840596,-0.6312325005,0.734299278\  
 C,3.1007692911,-2.3507393451,0.616619958\ C,2.9225262734,-3.9482751365,-  
 3.3986117503\ C,3.5585404565,-2.738607499,-3.1711802014\ C,3.6142331765,-  
 2.2040287685,-1.8913213937\ C,3.0317734809,-2.8679910213,-  
 0.8187917316\ C,2.4036763677,-4.0902760832,-1.0556586487\ C,2.3482425965,-  
 4.625655402,-2.3319428433\ C,4.1402571848,-3.1389918131,1.4021122251\  
 C,3.8283353374,-3.8569405289,2.551028156\ C,4.8103497063,-4.5752907135,  
 3.2208623039\ C,6.1161579704,-4.5768483582,2.7578374158\ C,6.4364825806,-  
 3.8618401662,1.6111523113\ C,5.4555259128,-3.1554415426,0.9368812062\ H,-  
 1.2394016491,-0.1489262957,-0.6307393063\ H,-3.6645497572,-0.4866477298,-  
 0.319797156\ H,-4.4868470081,-2.084712965,1.387 0769956\ H,-2.8614804669,-  
 3.3405670276,2.7702773811\ H,-0.4581428893,-3.0111430358,2.4581984222\  
 H,1.8362110699,-2.1493234394,2.3450253734\ H,1.2662829775,-3.3316036144,  
 1.1861509345\ H,-0.6385587311,4.0651344388,1.7150975153\ H,0.0407662309,  
 2.5990310763,-0.1551129841\ H,4.1175551782,2.8441573847,1.1395439558\ H,  
 3.4341231406,4.3126344165,3.0053636721\ H,1.6611760807,5.1831357485,  
 4.4203915424\ H,0.8772301,6.2375355114,3.2447386528\ H,-0.041895283,  
 4.9356290157,3.992619841\ H,2.8765137788,-4.3636148326,-4.3985346411\  
 H,4.0156453099,-2.1997081777,-3.9930240209\ H,4.117883621,-1.25921397,-  
 1.7303742636\ H,1.9671177227,-4.6486925756,-0.2359991225\ H,1.8559838685,-  
 5.5780570517,-2.4913222963\ H,2.8168260296,-3.875802194,2.934918128\  
 H,4.5475816546,-5.1344648749,4.1112959989\ H,6.8812939869,-5.1350078291,  
 3.2845165339\ H,7.4532339064,-3.8594514619,1.2361312796\ H,5.7075088604,-  
 2.6154100113,0.0311713481\ \ Version=ES64L-G16RevB.01\ HF=-2136.4731387\  
 RMSD=1.876e-09\RMSF=7.665e-07\ Dipole=-0.8453885,-0.9723161,2.7634561\  
 Quadrupole=-6.9501085,10.4827683,-3.5326597,-8.3860117,9.6868797,  
 5.2668306\ PG=C01[X(C28H24N2O2S2)]\ \@

### TS for 10a

HF=-2136.408398 a.u. (1, -268,3840 cm<sup>-1</sup>)

1\1\ GINC-R09N23\ FTS\ RPBE1PBE\ def2TZVP\ C28H24N2O2S2\  
 WURTHWE\ 13-Feb-2020 \0\ \# pbe1pbe/def2tzvp Opt=(ts,noeigentest,  
 readfc) geom=check guess=read freq pop=nbo emp=gd3bj nosym  
 scrf=(solvent=dichloromethane)\ \ TS for 10a \ \ 0,1\ C,-0.104165093,  
 0.0161225207,-0.0750968794\ C,0.0350983503,0.0177177445,1.3200748696\  
 C,1.3232425917,0.0022317148,1.8564376642\ C,2.4349704784,-0.0565648849,  
 1.0285501362\ C,2.2803791191,-0.0860966311,-0.3467754411\ C,1.0028922503,-  
 0.0392410249,-0.8962743302\ C,-1.1447789652,0.0984138394,2.1950567041\ S,-  
 0.9795510396,0.4665289573,3.819345598\ C,-2.4224393048,-0.5403963337,



1.7901325836\ C,-2.4037039406,-1.6709238989,0.9698450126\ C,-3.5794745777,-  
2.3292433932,0.6411513493\ C,-4.7959662721,-1.8708762705,1.1201140314\ C,-  
4.8257519818,-0.7549089082,1.9489700237\ C,-3.6541935805,-0.1049750703,  
2.2869528312\ N,-0.2752970051,2.4982203724,3.7551651295\ S,0.8834989752,  
2.4834308543,5.0512151265\ O,2.1137028478,1.8701532732,4.6413788863\ N,  
0.2717109908,2.9130820403,2.6775820531\ C,-0.5129725931,2.9207025496,  
1.5656832128\ C,0.1712175075,3.3233076324,0.3259833977\ C,1.564284926,3.332  
2679538,0.2578392084\ C,2.208976796,3.6890671187,-0.9143327949\ C,  
1.4747048554,4.0369531662,-2.0396871311\ C,0.0874697973,4.0391647986,-  
1.979660402\ C,-0.5583837557,3.69135914,-0.8050648794\ C,-1.7889010919,  
2.4313778618,1.5989060705\ C,1.1374615975,4.2000394601,5.26571042\ C,  
2.2055790953,4.8185970726,4.6301446511\ C,2.3813867945,6.180550078,  
4.7900095194\ C,1.5051843394,6.9336900524,5.5716775197\ C,0.4385913122,  
6.2860231124,6.1934596594\ C,0.246407452,4.9240898631,6.0460946195\ C,  
1.7219481359,8.4012128817,5.7593627603\ O,0.1515213238,1.9626999758,  
6.1695431992\ H,2.1324177845,3.0301258455,1.1271944811\ H,3.2922122604,  
3.6812954108,-0.9541910231\ H,1.9803578099,4.3088528657,-2.9590627728\ H,-  
0.4944402876,4.3220816656,-2.8491810366\ H,-1.640738727,3.7215160501,-  
0.7646602584\ H,-2.3145738737,2.3720903677,2.5383971641\ H,-2.3588483078,  
2.2897177639,0.6913773673\ H,3.2131829025,6.6716015807,4.2973222167\ H,  
2.884209341,4.2347749808,4.0223043621\ H,-0.5803821675,4.422634675,  
6.5329630184\ H,-0.2518411879,6.8585987185,6.8025697965\ H,0.7860976061,  
8.9162674473,5.9792168244\ H,2.4016594148,8.5803289487,6.5981234745\ H,  
2.1714838361,8.8519304215,4.873434619\ H,3.1489358187,-0.1268862202,-  
0.9936297121\ H,3.4257605447,-0.0741389355,1.4671786668\ H,1.449007066,  
0.0230204531,2.9315472452\ H,-1.0920603076,0.0878956206,-0.5133051837\ H,  
0.8739433979,-0.0278632162,-1.9721245958\ H,-3.6882486736,0.7518827091,  
2.9478761137\ H,-5.7700473745,-0.3895566439,2.335542257\ H,-5.7151851336,-  
2.3813640191,0.8580651671\ H,-3.5378930995,-3.2098967673,0.0107793024\ H,-  
1.4593987928,-2.0544130242,0.6062236992\ \ Version=ES64L-G16RevB.01\ HF=-  
2136.408398\ RMSD=3.742e-09\ RMSF=9.475e-07\ Dipole=-0.5932683,1.7392088,  
-2.3245434\ Quadrupole=4.8773489,22.8564334,-27.7337823,6.9889022,-  
4.3496174,17.4276774\ PG=C01 [X(C28H24N2O2S2)]\ \@

## 1b

HF=-897.8817061 a.u. (0)

1\1\GINC-R08N08\FOpt\RPBE1PBE\def2TZVP\C13H8S1\WURTHWE\12-  
Feb-2020\0\ \ # pbe1pbe/def2tzvp Opt=readfc geom=check guess=read  
Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=dichloromethane)\ \  
Compound 1b: Thiofluorenone \ \ 0,1\ S,0.1246976562,0.0000000006,  
0.0178002009\ C,-0.0131962887,-0.0000000004,1.6402010187\ C,1.0777841126,-  
0.0000000001,2.6256638253\ C,-1.2550507172,0.0000000002,2.427050491\

C,0.5300290741,0.0000000002,3.9208007862\ C,1.3559727108,0.0000000021,  
 5.0266308363\ C,2.7362253914,0.0000000015,4.8234718862\ C,3.2767734922,  
 0.0000000001,3.5427505382\ C,2.4457487001,-0.0000000008,2.427111056\  
 H,0.9509072867,-0.0000000011,6.0318979533\ H,3.3992170317,0.0000000007,  
 5.6809962783\ H,4.352480398,-0.0000000019,3.4145953824\ H,2.8515486487,-  
 0.0000000004,1.4217696546\ C,-0.9341845743,-0.0000000003,3.7961524253\ C,-  
 1.9352584101,0.0000000009,4.746396586\ C,-3.2612510691,-0.0000000004,  
 4.3126216722\ C,-3.5774341649,-0.0000000004,2.9589332058\ C,-2.5696852599,  
 0.0000000014,1.9999452337\ H,-1.7062958095,-0.000000001,5.8057871028\ H,-  
 4.0598270922,-0.000000001,5.0455663518\ H,-4.6159469341,0.0000000005,  
 2.6506113429\ H,-2.7994112263,-0.0000000004,0.9404108439\ \ Version=ES64L-  
 G16RevB.01\ HF=-897.8817061\ RMSD=7.138e-09\ RMSF=3.640e-05\ Dipole=-  
 0.1532857,0.,1.8070194\ Quadrupole=3.0668293,-14.1035865,11.0367572,0.,-  
 0.244343,0.\ PG=CS [SG(C13H8S1)]\ \@

### 9c (from 1b and 7a)

HF=-2135.3001907 a.u (0)

1\1\GINC-R07N14\FOpt\RPBE1PBE\def2TZVP\C28H22N2O2S2\  
 WURTHWE\12-Feb-2020\0\ \ # pbe1pbe/def2tzvp Opt=readfc geom=check  
 guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=dichloromethane)  
 \ \ Compound 9c\ \ 0,1\ C,-0.2377940873,-0.1215409627,-0.0220186334\ C,-  
 0.3243952515,0.0156433215,1.3641924468\ C,0.798517508,-0.1870400308,  
 2.1527629338\ C,1.9941562239,-0.5269348576,1.5332595738\ C,2.067602739,-  
 0.6702795481,0.15086197\ C,0.9427185375,-0.4748936418,-0.641699038\ C,-  
 1.6039048318,0.0742124001,-0.6412973976\ N,-1.6693118969,1.009198295,-  
 1.7708803494\ N,-2.7278173541,1.0276635896,-2.6160641151\ C,-3.5875692291,  
 0.0916463027,-2.742468621\ C,-3.6014019073,-1.1976146707,-1.9827033308\ S,-  
 1.9965382261,-1.5826382324,-1.2952878039\ C,-4.6708552887,0.3379152845,-  
 3.7169881191\ C,-4.5709334846,1.3811365366,-4.6416153752\ C,-5.5952875451,  
 1.6284914986,-5.5363409728\ C,-6.7419949824,0.8418840234,-5.5262348808\ C,-  
 6.8501012222,-0.1969163152,-4.6155224321\ C,-5.8209664307,-0.4508312057,-  
 3.7200927831\ S,-1.0855104718,2.5993812231,-1.6173005004\ C,-2.3551858053,  
 3.4848899842,-0.8008146602\ C,-3.5122400407,3.8284213376,-1.4883248215\ C,-  
 4.5332756462,4.4641751123,-0.8044004127\ C,-4.4135943968,4.7693157532,  
 0.5505935451\ C,-3.2311710911,4.4343059425,1.2080656744\ C,-2.2048460994,  
 3.7878196242,0.5458751683\ C,-5.5378496136,5.4180255438,1.2933075001\ C,-  
 2.4649221328,0.4421974522,0.5495572688\ C,-3.7935973745,0.8248413672,  
 0.5989387603\ C,-4.354896507,1.1275373882,1.8345610863\ C,-3.5980344618,  
 1.0488367462,2.9971045924\ C,-2.2598513749,0.679481731,2.9481623935\ C,-  
 1.693970037,0.382720074,1.7179713256\ O,0.0524687052,2.5234934614,-  
 0.7547918712\ O,-0.9486008122,3.091653578,-2.9519980025\ H,-3.6732233304,  
 1.9863529516,-4.6516156963\ H,-5.4985267128,2.4370052183,-6.2518119756\ H,-

7.5434633526,1.0369257806,-6.2291411831\H,-7.7390595437,-0.816571701,-  
 4.5985038407\H,-5.9310631882,-1.2647397894,-3.0139032154\H,-4.3656906311,-  
 1.1846244957,-1.1990086723\H,-3.8438049844,-2.0209734678,-2.6571977634\H,-  
 5.4408637868,4.7322794249,-1.333840434\H,-3.6092269995,3.5950507023,-  
 2.5403148865\H,-1.2956840975,3.510313788,1.0626516153\H,-3.117696906,  
 4.6736102852,2.2595057529\H,-5.1661332174,6.1325614192,2.0296398452\H,-  
 6.2182507738,5.9351544637,0.6160744752\H,-6.1179542605,4.6648992058,  
 1.8357824254\H,-4.0532917417,1.2911582789,3.9503129541\H,-5.390736454,  
 1.441141318,1.8863744046\H,-4.388496175,0.9330808386,-0.2983931911\H,-  
 1.6689434551,0.6359977662,3.8558933176\H,0.7487983297,-0.0840152828,  
 3.2306496163\H,2.8822520279,-0.6849747931,2.1340877996\H,3.0108491429,-  
 0.9353418518,-0.311797676\H,0.9953085393,-0.5797463562,-1.7190358778\ \\  
 Version =ES64L-G16RevB.01\HF=-2135.3001907\RMSD=5.733e-09\RMSF=  
 1.055e-06\Dipole=-2.9401751,-0.2722377,1.6474728\ Quadrupole=24.8314556,-  
 15.7934435,-9.0380121,-14.5513673,6.1943607,13.2720414\PG=C01  
 [X(C28H22N2O2S2)]\ \@

### 1b + 7a-vdW-complex

HF=-2135.2450211 a.u (0)

1\1\GINC-R08N07\FOpt\RPBE1PBE\def2TZVP\C28H22N2O2S2\  
 WURTHWE\12-Feb-2020\0\ \# pbe1pbe/def2tzvp Opt=readfc geom=check  
 guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=dichloromethane)  
 \ 1b + 7a-vdW-complex \ 0,1\C,-1.6881929114,-1.4618646275,0.9727525651\  
 C,-0.5982740521,-1.3144950797,1.9461219319\C,0.2296811578,-2.4470365056,  
 1.8488893908\C,-0.2866247531,-3.3312342376,0.7977445769\C,-1.4942524783,-  
 2.6699397838,0.2811181575\C,-0.2940611094,-0.3028214316,2.8339293413\  
 C,0.8426132147,-0.4429433601,3.6308206313\C,1.6532367207,-1.5684496808,  
 3.5432282747\C,1.3519813527,-2.5848841734,2.6439976871\S,0.3601692262,-  
 4.737875772,0.2878972198\C,0.8970505524,-1.0455515666,-1.6329071448\  
 C,1.5610162657,-0.3832392451,-0.6813266724\N,1.1489466457,0.9360725941,-  
 0.3421753289\N,-0.0621172536,1.1131053235,-0.3144408895\C,-2.7578179241,-  
 0.6461635937,0.6660971595\C,-3.6299296109,-1.0507395772,-0.3435455369\C,-  
 3.4356213479,-2.2438935728,-1.0311392709\C,-2.3592023473,-3.0682120683,-  
 0.7210447717\S,-0.4897301501,2.7689127939,0.0531955519\O,0.6695358976,  
 3.600624105,0.1945215954\C,2.7816819711,-0.8233553651,0.0111474248\  
 C,3.4780702332,0.0500869875,0.8466967721\C,4.6111241519,-0.3743748397,  
 1.5236055701\C,5.064852664,-1.6761464599,1.3812822602\C,4.3736960296,-  
 2.5547466517,0.555835264\C,3.2433499991,-2.13426739,-0.1202377262\C,-  
 1.3383156905,3.1552059206,-1.4204650928\C,-0.6699842798,3.8219714472,-  
 2.4401551147\C,-1.3438829595,4.0908090313,-3.6166127761\C,-2.6700485502,  
 3.6951408066,-3.7942896158\C,-3.3152147354,3.0272906994,-2.7536380755\C,-  
 2.6597550633,2.7519849238,-1.5680756187\C,-3.3771204814,3.9637982737,-

5.0835821252\O,-1.4226763031,2.6335701091,1.1369911193\H,3.1277103611,  
 1.0669298712,0.9657081551\H,5.1379229577,0.3182859504,2.1696939081\H,  
 5.9481267968,-2.0089669372,1.9138376921\H,4.7115197984,-3.5787180145,  
 0.4463739685\H,2.7030652289,-2.8438309618,-0.7341180143\H,0.0160865828,-  
 0.6096370861,-2.0848829868\H,1.2351457767,-2.0035993187,-2.001621325\H,-  
 0.8341576144,4.6213013458,-4.412999727\H,0.3581360476,4.1317413291,-  
 2.3021302816\H,-3.1644933452,2.2415269806,-0.7581161425\H,-4.3489821157,  
 2.7235779759,-2.8739801605\H,-4.4577522583,4.0048337151,-4.9437944674\H,-  
 3.0439840581,4.9016115537,-5.5302859492\H,-3.1670071053,3.1666041306,-  
 5.8032638726\H,-4.4747612401,-0.4216878968,-0.6004818599\H,-4.1285944301,-  
 2.5316120216,-1.8126179685\H,-2.1925336133,-4.0008001074,-1.2481955748\H,-  
 2.9086215679,0.294441538,1.1820875948\H,-0.9069050846,0.5881338247,  
 2.9006045115\H,1.1011670702,0.3455097931,4.328284552\H,2.5334429727,-  
 1.6460011246,4.1694944098\H,1.9834367589,-3.4602605733,2.5505758044  
 \ \ Version=ES64L-G16RevB.01\ HF=-2135.2450211\ RMSD=9.794e-  
 09\RMSF=1.503e-06\ Dipole=-0.9998872,0.7428053,-2.0989043\  
 Quadrupole=9.9314628,-21.2366687,11.305206,-10.4764446,19.3715698,-  
 11.8520089\ PG=C01[X(C28H22N2O2S2)]\ \@

### TS for 9c

HF = -2135.237493 a.u. (1, -186,7306cm<sup>-1</sup>)

1\1\GINC-R09N40\FTS\RPBE1PBE\def2TZVP\C28H22N2O2S2\  
 WURTHWE\13-Feb-2020\0\ \ # pbe1pbe/def2tzvp Opt=(ts,noeigentest,readfc)  
 geom=check guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=  
 dichloromethane)\ \ TS for 9c \ \ 0,1\C,0.0807414012,-0.3208192441,  
 0.1532155652\C,0.7593555003,-0.1716399365,1.4442743735\C,2.0401427836,-  
 0.742834591,1.332100182\C,2.1970578459,-1.2903544179,-0.0159539435\  
 C,0.9533560703,-0.9936079201,-0.7246813148\C,0.3584974686,0.4134561772,  
 2.6279826125\C,1.2540996069,0.4329266208,3.6957038473\C,2.5237725845,-  
 0.1231712115,3.5805861129\C,2.9280642567,-0.7207304885,2.3926067234\  
 S,3.4949929036,-2.1133490966,-0.5807968673\C,4.258597415,-0.8958108083,-  
 2.4934785443\C,5.1231947104,-0.0425405775,-1.8565473047\N,4.6587279632,  
 1.1634833274,-1.3529846523\N,3.4220323522,1.2718712866,-1.2536520832\C,-  
 1.1713833415,0.0722521515,-0.2773605081\C,-1.5407124977,-0.2040432709,-  
 1.5938291311\C,-0.6782586158,-0.867055145,-2.4592279066\C,0.5792548678,-  
 1.2749087358,-2.0265595088\S,2.9418169572,2.8263332822,-0.6917590846\  
 O,4.0516129294,3.7295981111,-0.5739617574\C,6.554012799,-0.2950496487,-  
 1.6580981561\C,7.405915756,0.7323445149,-1.2419295684\C,8.7592225789,  
 0.4980705972,-1.0637602583\C,9.2895088481,-0.7650363159,-1.2859780387\  
 C,8.4499171269,-1.7958316454,-1.6875835056\C,7.0977900705,-1.5647329004,-  
 1.8714283238\C,1.9424123719,3.2891040184,-2.0500682011\C,2.4285676642,  
 4.183882283,-2.9929974227\C,1.6350250434,4.5111013678,-4.0786857145\

C,0.3689716958,3.9503289144,-4.2404695937\ C,-0.0891499092,3.0453927983,-  
 3.2820279395\ C,0.6854529953,2.7122196973,-2.1875681447\ C,-0.4916482296,  
 4.3271135011,-5.4038638177\ O,2.1097067078,2.5646300163,0.4486553412\  
 H,6.9950080141,1.7170941128,-1.0628449571\ H,9.4039289755,1.3095593029,-  
 0.7462036594\ H,10.347938104,-0.9476362021,-1.1420198045\ H,8.8497640356,-  
 2.7894657894,-1.853641068\ H,6.4607488718,-2.3893760144,-2.1678718964\  
 H,3.2716771793,-0.5350535976,-2.7501240707\ H,4.6236486314,-1.7580390461,-  
 3.0328252608\ H,2.0058248036,5.2132500499,-4.8170971278\ H,3.4134796092,  
 4.6161885878,-2.8699568277\ H,0.3253663319,2.0095717572,-1.4468923059\ H,-  
 1.0680068917,2.5930346158,-3.3977017976\ H,-1.1556485156,5.1539326446,-  
 5.1334431509\ H,0.1087187257,4.6525927293,-6.2541887885\ H,-1.1213416736,  
 3.4930472783,-5.7172432399\ H,-2.5181430691,0.1030986678,-1.9475835362\ H,-  
 0.9907016496,-1.0708681437,-3.4762314332\ H,1.248153773,-1.8121283647,-  
 2.6892701133\ H,-1.8560614591,0.5890504871,0.3850451941\ H,-0.623617893,  
 0.8604310352,2.7298093519\ H,0.9577554833,0.8940155214,4.6307436578\  
 H,3.2025111447,-0.0882016977,4.4242410612\ H,3.9164207877,-1.1543036459,  
 2.2906503066\ \ Version=ES64L-G16RevB.01\ HF=-2135.237493\ RMSD=7.391e-  
 09\ RMSF=8.760e-07\ Dipole=-1.7361092,-0.7548112,-2.1586515\ Quadrupole=-  
 4.3087511,-12.3779693,16.6867204,-18.198321,-1.9559807,-8.0178744\ PG=C01  
 [X(C28H22N2O2S2)]\ \@

### 10c (from 1b and 7a)

HF=-2135.2941496 a.u. (0)

1\1\GINC-R08N08\FOpt\RPBE1PBE\def2TZVP\C28H22N2O2S2\  
 WURTHWE\12-Feb-2020\0\ \ # pbe1pbe/def2tzvp Opt=readfc geom=check  
 guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=dichloromethane)  
 \ \ Product 10c (NNS)\ \ 0,1\ C,0.2849395569,-0.4221579311,-0.1184568522\  
 C,0.1958140135,-0.4958616191,1.2762535958\ C,1.0933006334,0.1699627578,  
 2.0886058104\ C,2.1008260706,0.9189229363,1.4883581023\ C,2.1948215021,  
 0.9943246757,0.1028591742\ C,1.290061439,0.3259973668,-0.712754956\ C,-  
 0.9876251096,-1.342560209,1.6771185213\ C,-0.659717219,-2.454335196,  
 2.6625061772\ C,-1.8462903317,-3.0488209047,3.3691841685\ N,-3.0195469565,-  
 2.5398764127,3.4332165233\ N,-3.3226973685,-1.3726316181,2.8290386422\ S,-  
 2.1169235758,-0.1752328331,2.5068533037\ C,-1.6727749283,-4.3516087451,  
 4.0436034184\ C,-2.7856754556,-5.0849689102,4.4644629715\ C,-2.6278083958,-  
 6.2986647388,5.1064738461\ C,-1.355169578,-6.8052123189,5.3467922103\ C,-  
 0.2446808026,-6.0866521021,4.934088355\ C,-0.4010519083,-4.8709844497,  
 4.2834359566\ S,-4.8686718232,-0.8331734966,3.2198423765\ C,-4.7915719783,-  
 0.5103350286,4.9355645403\ C,-5.0375520878,-1.5377081437,5.8377974146\ C,-  
 4.9084103369,-1.2864804535,7.1913099033\ C,-4.5374983815,-0.0260123375,  
 7.6592338944\ C,-4.2938627036,0.9850136913,6.7311690645\ C,-4.4150447232,  
 0.7530494069,5.3725202616\ C,-4.4304420947,0.240153605,9.1269722876\ C,-

1.5348282266,-1.7954843373,0.3451460762\ C,-2.5914580774,-2.6452473356,  
0.0719282912\ C,-2.9055517129,-2.9106270123,-1.2575706417\ C,-2.1726686683,-  
2.3388036436,-2.2912148918\ C,-1.1025348552,-1.4962989494,-2.0193228366\ C,-  
0.784896937,-1.2306873439,-0.6962813243\ O,-5.0156214058,0.3959168444,  
2.5022773174\ O,-5.7536426332,-1.930937109,2.9900844651\ H,-3.7748402789,-  
4.6889656742,4.2730042734\ H,-3.5021674386,-6.8576678675,5.4194619422\ H,-  
1.2330241226,-7.7570574827,5.8503848718\ H,0.7519621815,-6.4710793907  
,5.1168920627\ H,0.4822250141,-4.325912468,3.974868194\ H,0.0439856417,-  
2.0732363464,3.4074320181\ H,-0.1422917589,-3.2534124114,2.1234926471\ H,-  
5.0981742108,-2.0844223921,7.9006315319\ H,-5.3263828709,-2.5161202097,  
5.4774098775\ H,-4.2293210844,1.5433103144,4.6560696511\ H,-4.004569477,  
1.9705666279,7.0785058669\ H,-3.7536192755,1.0702405445,9.3322861527\ H,-  
5.4097567868,0.5032018855,9.5383763963\ H,-4.0777385444,-0.6413115286,  
9.6645665231\ H,-2.4354738066,-2.5584926673,-3.319472505\ H,-3.7319883116,-  
3.5725968209,-1.4879235141\ H,-3.1703334516,-3.1004324764,0.8650929313\ H,-  
0.525545142,-1.0620831253,-2.8279356532\ H,1.0183733732,0.1171384736,  
3.1692955157\ H,2.8175529329,1.4474713607,2.1054381364\ H,2.9866070883,  
1.5823679429,-0.346559694\ H,1.3731804149,0.390112156,-1.791536346\ \\  
Version=ES64L-G16RevB.01\ HF=-2135.2941496\ RMSD=4.562e-09\ RMSF=  
8.341e-07\ Dipole=2.5312294,-0.407672,1.7674484\ Quadrupole=-34.4240773,-  
1.476824,35.9009013,0.4923791,-5.7444886,-5.1816626\ PG=C01  
[X(C28H22N2O2S2)]\ \@

### TS for 10c

HF=-2135.2276585 a.u (1, -278,3394cm<sup>-1</sup>)

1\1\GINC-R10N14\FTS\RPBE1PBE\def2TZVP\C28H22N2O2S2\  
WURTHWE\06-Mar-2020\0\ \# pbe1pbe/def2tzvp Opt=(ts,noeigentest,  
readfc) geom=check guess=read freq pop=nbo emp=gd3bj nosym  
scrf=(solvent=dichloromethane)\ \ TS for 10c\ \ 0,1\ C,-0.0600830678,-  
0.0962309809,0.0617919924\ C,0.0298259423,-0.1136481145,1.5221892221\  
C,1.3863517473,-0.0266817468,1.8873210041\ C,2.1967749667,0.0723687254,  
0.6508213266\ C,1.2461557743,-0.0258531803,-0.4580297608\ C,1.772939051,-  
0.0502781338,3.2141596148\ C,0.7866793538,-0.1455658527,4.1889545098\ C,-  
0.5576874469,-0.218073944,3.835370247\ C,-0.9467107599,-0.2061127949,  
2.5000760553\ C,-1.1425211371,-0.1508506942,-0.7969969194\ C,-0.9045370882,-  
0.143498297,-2.1699883134\ C,0.3891534107,-0.0966038643,-2.6764682199\  
C,1.4845864005,-0.0407414232,-1.8207371869\ S,3.839985109,-0.151413937,  
0.5202209505\ N,4.3797305697,1.7646447362,-0.4759726472\ S,5.5705000917,  
1.2087377448,-1.622069065\ O,4.9338578452,0.5839763752,-2.7456442843\  
N,3.4455963591,2.375247924,-1.0864682837\ C,2.3773923408,2.767541949,-  
0.3468062794\ C,1.2881368502,3.413118327,-1.0961106854\ C,1.2479612352,  
3.3446117885,-2.4897600052\ C,0.2203699729,3.9474291213,-3.1947245618\ C,-

0.7892637017,4.6213728191,-2.5215948915\ C,-0.7562308186,4.6996399817,-  
 1.1359395355\ C,0.2762481735,4.1060422868,-0.4297538751\ C,2.2820596652,  
 2.4179237984,0.9774552719\ C,6.2685620962,2.7304321882,-2.1232445574\  
 C,5.7838460279,3.3625242678,-3.2606099679\ C,6.3297971564,4.5761831243,-  
 3.6349174497\ C,7.3461023883,5.1708895139,-2.8868352002\ C,7.8143856362,  
 4.5113048464,-1.751150257\ C,7.2812789004,3.2962923479,-1.3603424238\  
 C,7.9060377817,6.4992155913,-3.2838430454\ O,6.5135148002,0.4834390386,-  
 0.8224879027\ H,2.0235000722,2.7997304362,-3.0109204977\ H,0.200855012,  
 3.8800607647,-4.2763373767\ H,-1.597234945,5.0866903269,-3.0741346383\ H,-  
 1.5338651735,5.2331950691,-0.6020731631\ H,0.3011971038,4.2003754688,  
 0.649136724\ H,3.1731832583,2.1951467648,1.5447204593\ H,1.3701772339,2.593  
 030428,1.5293038753\ H,5.9640433923,5.0722523049,-4.5269956494\  
 H,4.9975072959,2.8997165381,-3.842303067\ H,7.6508687448,2.7825869709,-  
 0.4819669208\ H,8.6127920592,4.9551001401,-1.1670881952\ H,7.8755875286,  
 6.6354227341,-4.3656748039\ H,7.3190939634,7.3068018877,-2.8355529323\  
 H,8.9358440185,6.6143919276,-2.9438406852\ H,-1.7434185661,-0.1848620763,-  
 2.8550874835\ H,0.5448164995,-0.1013279735,-3.7486892405\ H,2.4979873842,-  
 0.0116963168,-2.2051399654\ H,-2.1569759266,-0.2047404679,-0.4186403896\  
 H,2.8214321458,0.0069094574,3.4841524054\ H,1.0671843342,-0.1659397021,  
 5.2354277474\ H,-1.3106348695,-0.2919336853,4.6113346235\ H,-1.9957125978,-  
 0.27288308,2.2347796034\ \ Version=ES64L-G16RevB.01\ HF=-2135.2276585\  
 RMSD=5.342e-09\ RMSF=1.057e-06\ Dipole=-1.6640437,2.9624584,0.2110799\  
 Quadrupole=-12.058361,8.6756078,3.3827532,29.0283882,-1.0187103,-  
 12.0859347\ PG=C01[X(C28H22N2O2S2)]\ \@

# 1m

HF=-975.2167163 a.u. (0)

1\1\GINC-R10N32\FOpt\RPBE1PBE\def2TZVP\C15H10S1\WURTHWE\  
 09-Feb-2021\0\ \# pbe1pbe/def2tzvp Opt=readfc geom=check guess=read  
 Pop=NBO Freq emp= gd3bj nosym scrf=(solvent=dichloromethane)\ \ Educt  
 1m\ \0,1\ C,0.0456181386,-0.2770719488,0.019785706\ C,0.0118539522,-  
 0.0788157192,1.4158841719\ C,1.2144407141,0.1619276201,2.0942119651\  
 C,2.4224305389,0.2050909904,1.4328164972\ C,2.4543307901,0.0565002988,0.048  
 9500679\ C,1.2809493787,-0.1643294134,-0.637401866\ C,-1.2232492783,-  
 0.0454347941,2.2102858899\ S,-1.431437415,1.1231933263,3.3442372248\ C,-  
 1.1047761568,-0.540895469,-0.8124051315\ C,-2.2852710658,-1.0819941299,-  
 0.4719691179\ C,-2.7297243683,-1.5490491581,0.820274292\ C,-2.229156951,-  
 1.1056292693,2.0622037072\ C,-2.7544176602,-1.6567153283,3.2389121635\ C,-  
 3.7397021172,-2.6194868139,3.2103536661\ C,-4.2689751933,-3.0255740794,  
 1.9884299602\ C,-3.7776819428,-2.4830594502,0.8218166452\ H,-4.1918624884,-  
 2.7891975903,-0.1323527469\ H,-5.0621981509,-3.762827338,1.9521979767\ H,-  
 4.1079016172,-3.0432088329,4.1369076668\ H,-2.3597176398,-1.3084063502,

4.1848668824\H,1.2986964084,-0.2727352985,-1.716137769\H,3.3941338164  
,0.1140262683,-0.4872351492\H,3.3372545126,0.3697239463,1.9892331331\  
H,1.1740231052,0.3104014554,3.1657788402\H,-2.9789165198,-1.2797297001,-  
1.283619383\H,-0.947676498,-0.3482736448,-1.8693591459\ \ Version=ES64L-  
G16RevB.01\HF=-975.2167163\RMSD=7.360e-09\RMSF=1.860e-06\Dipole=  
0.2348835,-1.2229344,-1.1259307\Quadrupole=6.6605945,-4.2182755,-  
2.442319,9.762549,2.6896425,-5.7201003\PG=C01[X(C15H10S1)]\ \@

### 9m (from 1m and 7a)

HF=-2212.6224788 a.u. (0)

1\1\GINC-R10N11\FOpt\RPBE1PBE\def2TZVP\C30H24N2O2S2\  
WURTHWE\10-Feb-2021\0\ \ # pbe1pbe/def2tzvp Opt=readfc geom=check  
guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=dichloromethane)  
\ \ Product 9m (NNC) \ \ 0,1\C,0.0392424484,0.267478909,0.0656142486\  
C,0.0048574585,0.1491152349,1.4692274175\C,1.2286456994,0.0804175504,  
2.1356380479\C,2.4483187586,0.1524304491,1.4825067206\C,2.4803421455,0.28  
71544827,0.1070262807\C,1.2829106827,0.3336651089,-0.5773497514\C,-  
1.2526222285,-0.0733588183,2.3096571286\N,-0.9323938159,0.181133242,  
3.7317495184\N,-0.4993853048,-0.7071477406,4.6456994657\C,-0.214866704,-  
1.9284591369,4.3936513545\C,-0.3486374459,-2.5607376548,3.0453579375\S,-  
1.7426863918,-1.8438618838,2.1789088866\C,-2.592199888,0.6080505345,  
1.9809587399\C,-3.0672070251,0.8596712404,0.6835906293\C,-4.361015373,  
1.3879342509,0.5323324004\C,-5.1881504876,1.6461685632,1.6020969157\C,-  
4.738453697,1.3361188733,2.8760733479\C,-3.4699771402,0.8164104012,  
3.046460294\C,-2.3862213547,0.5808218095,-0.5637961182\C,-1.1008502876,  
0.3228610175,-0.8218706604\S,-0.7655680507,1.7455349488,4.3553544972\O,-  
1.5695919511,1.8181592377,5.5385653018\C,0.2825052216,-2.7292279391,  
5.5263830792\C,0.0323062236,-2.3326289047,6.8422101976\C,0.5284858476,-  
3.0665029018,7.9040610753\C,1.2826722741,-4.2114683469,7.6735389287\  
C,1.5310960706,-4.6170750711,6.3713143394\C,1.0306382468,-3.885081659,  
5.3045896816\C,0.910755261,1.8964486063,4.8461366118\C,1.3439778377,  
1.3286066905,6.0387253408\C,2.6703357425,1.4604421115,6.4019177955\  
C,3.572307836,2.1626021398,5.6005765882\C,3.108074025,2.7325604777,  
4.4179415104\C,1.7849515069,2.6018805939,4.0321654284\C,4.9990726124,2.31  
80904267,6.0208546937\O,-1.0083547353,2.6275866029,3.2540365267\H,-  
0.5681007606,-1.4485709427,7.0166874157\H,0.3190718495,-2.7501443469,  
8.9194686859\H,1.6682244511,-4.7872049921,8.5068123381\H,2.1182447392,-  
5.5079105726,6.1809941045\H,1.2452622787,-4.21187918,4.2939678983\  
H,0.5683953966,-2.4536336183,2.4574635761\H,-0.5683160745,-3.6246591753,  
3.136247697\H,3.0149768146,1.0109219051,7.3267064138\H,0.6481894705,  
0.7863186173,6.6636729379\H,1.4290118239,3.0367901852,3.1076400102\H,3.79  
41668165,3.283201007,3.7842012892\H,5.6327393119,2.6035494372,



5.1807655027\H,5.0890297456,3.0955309005,6.7854586719\H,5.3861099882,  
 1.393584666,6.4532651691\H,3.4206862527,0.3454201021,-0.4278144949\  
 H,3.363169998,0.0971906335,2.0601823938\H,1.2548758273,-0.0444593415,  
 3.2065103709\H,1.2877356091,0.4290684464,-1.6575278766\H,-4.7095183998,  
 1.5867479282,-0.4750196696\H,-6.177284953,2.0590128051,1.4440980355\H,-  
 5.373593703,1.4846456553,3.7410807953\H,-3.1608436712,0.5571181708,  
 4.0481531966\H,-3.0396221702,0.6273418889,-1.4297465944\H,-0.8460223442,  
 0.1885717001,-1.868676767\ \ Version=ES64L-G16RevB.01\ HF=-2212.6224788\  
 RMSD=3.298e-09\RMSF=6.082e-07\ Dipole=2.7533317,-1.3979449,-0.247879\  
 Quadrupole=7.588917,-9.9339671,2.3450501,2.6115682,26.8141571,-  
 14.7629818\ PG=C01[X(C30H24N2O2S2)]\ \@

### vdW (from 1m and 7a)

HF=-2212.5793122 a.u. (0)

1\1\GINC-R08N27\FOpt\RPBE1PBE\def2TZVP\C30H24N2O2S2\  
 WURTHWE\21-Mar-2021\0\ \ # pbe1pbe/def2tzvp Opt Pop=NBO Freq  
 emp=gd3bj nosym scrf=(solvent=dichloromethane)\ \ vdw-complex from 1m  
 and 7a\ \ 0,1\C,-0.0235162154,-0.0359298647,-0.0008371596\C,-0.0006017884,-  
 0.0471329109,1.3883049216\C,1.197579799,-0.0148630903,2.0912766579\  
 C,2.3845397283,0.0463989453,1.3856549583\C,2.392565035,0.0664336601,-  
 0.0096266556\C,1.1748644257,0.0198137142,-0.6874009906\S,-1.5078487343,-  
 0.1678814527,2.2568774554\O,-2.5606424248,0.4556213425,1.5092938148\  
 C,3.6813191309,0.1592443809,-0.7613534661\N,-1.7982845063,-1.8825838747,  
 2.0269302906\N,-1.7758005263,-2.4995359367,3.0836643676\C,-1.9362713787,-  
 3.9069120864,2.9694408308\C,-2.7328221664,-4.5031762686,4.0518714647\C,-  
 2.9152284468,-3.8302128813,5.2603288846\C,-3.6909614558,-4.3900298854,  
 6.2634748489\C,-4.3010835915,-5.6210343108,6.0730205619\C,-4.1304854639,-  
 6.2928381947,4.8690176501\C,-3.3554671313,-5.7379233634,3.8657040579\C,-  
 1.2998418537,-4.5670174905,1.9991913921\O,-1.3105340912,0.1513994485,  
 3.6410103157\C,-5.3535452522,-0.4304196085,-0.7129311411\C,-5.3833563586,-  
 1.2902792786,0.4446367322\C,-4.8164439133,-2.5802470711,0.5209270051\C,-  
 4.962390221,-3.3066437037,1.7105500976\C,-5.6072888933,-2.7864739664,  
 2.8097667628\C,-6.1876308393,-1.5235816426,2.7289121145\C,-6.0915085442,-  
 0.8079866162,1.5565164553\C,-4.1102259767,-3.2486772875,-0.5776542608\S,-  
 4.3445502706,-4.8565411001,-0.8413702521\C,-3.1222947059,-2.5291033438,-  
 1.3941596663\C,-3.3344788854,-1.2546357639,-1.9608162303\C,-2.3693397095,-  
 0.752928401,-2.8509823966\C,-1.2000243577,-1.4284137456,-3.1172261786\C,-  
 0.9637610408,-2.6560589312,-2.504035713\C,-1.9241527206,-3.1994200707,-  
 1.6802847798\C,-4.4906591713,-0.4207968956,-1.7406967922\H,-2.445996572,-  
 2.8666218036,5.409757516\H,-3.821774989,-3.8573171121,7.198182799\H,-  
 4.9139726359,-6.0532702418,6.8552416458\H,-4.6142715988,-7.2487121547,  
 4.7058993394\H,-3.254758106,-6.255800282,2.9188190204\H,-0.7277789429,-

4.0265110057,1.2565928805\H,-1.2970283504,-5.6478512567,1.9626292221\  
H,3.3243992007,0.0773802899,1.9254010761\H,1.1904721694,-0.0323219838,  
3.1736564474\H,-0.9660782491,-0.0721926024,-0.5322866688\H,1.1665066509,  
0.0249445233,-1.7714281853\H,3.5841208471,-0.2475367707,-1.7684482106\  
H,3.9901759706,1.2048416913,-0.8557717621\H,4.4817850741,-0.3707126844,-  
0.243101086\H,-0.4690792699,-1.0022839921,-3.7943008225\H,-0.0394642946,-  
3.1918448552,-2.6833372903\H,-1.7687541149,-4.1719935701,-1.232026314\H,-  
2.5582302587,0.2054414374,-3.3215390267\H,-6.5543108384,0.1696322707,  
1.4821136403\H,-6.7145042196,-1.1055770944,3.5784745286\H,-5.6620494435,-  
3.3644831488,3.7246627002\H,-4.5325376107,-4.2973088336,1.7534641696\H,-  
6.0950341994,0.3626402341,-0.6995107307\H,-4.6132449563,0.3764640015,-  
2.4673573882\ \ Version=ES64L-G16RevB.01\HF=-2212.5793122\RMSD=  
6.750e-09\RMSF=3.204e-06\Dipole=2.2740592,0.1364263,-0.6285507\  
Quadrupole=0.7196855,-4.465192,3.7455065,-9.2594486,-11.1557799,-  
17.3996976\PG=C01[X(C30H24N2O2S2)]\ \@

### TS for 9m

HF=-2212.5687574 a.u (1, -262.4891cm<sup>-1</sup>)

1\1\GINC-R09N27\FTS\RPBE1PBE\def2TZVP\C30H24N2O2S2\  
WURTHWE\13-Feb-2021 \0\ \# pbe1pbe/def2tzvp opt=(ts,noeigentest,readfc)  
geom=check guess=read scrf=(solvent= dichloromethane) freq pop=nbo  
emp=gd3bj nosym\ \ TS for 9m \ \0,1\C,0.0922161821,1.1673964191,  
0.3306975444\C,0.4340938887,0.0244420502,1.097713702\C,1.8066990755,-  
0.2226259746,1.2934794969\C,2.7957041255,0.5856586812,0.7883384358\  
C,2.4539591892,1.6883243011,0.0099379559\C,1.1251801585,1.954493687,-  
0.2132963806\C,-0.5012594882,-0.9484357765,1.6717541928\N,0.4096254564,-  
0.0544817047,4.4183989466\N,-0.1107375071,-0.8719367004,5.2150066239\  
C,0.1078222477,-2.2006576198,4.9431902312\C,1.0475697415,-2.5702571508,  
3.9996598674\S,0.0687939273,-2.5266430032,1.898023826\C,-1.8795693729,-  
0.6803442553,2.0758269186\C,-2.7263091286,0.3455953543,1.5761173097\C,-  
4.0253734594,0.4637214131,2.0944725781\C,-4.4968923616,-0.3439061075,  
3.103782395\C,-3.6760030887,-1.3514534528,3.5979973396\C,-2.4188815498,-  
1.5231686551,3.0685134579\C,-2.4148290287,1.2756150036,0.5288977986\C,-  
1.2303503399,1.6149835248,-0.0021473683\S,0.0239910811,1.5613873209,  
4.813358386\O,-0.4832560829,1.6893300341,6.151688273\C,-0.7530628366,-  
3.1422525591,5.6640446464\C,-1.4716475667,-2.7329445418,6.7922003412\C,-  
2.2971132631,-3.6191852988,7.462047286\C,-2.4344127873,-4.9278893098,  
7.0172429306\C,-1.7355170214,-5.3412320855,5.8915897026\C,-0.9036480008,-  
4.4594642191,5.221511402\C,1.6185537722,2.2769439203,4.7204457142\  
C,2.3950116167,2.3799349247,5.8675081571\C,3.6586809197,2.9340572542,  
5.7757694008\C,4.1611711286,3.383371604,4.5542916772\C,3.3584762836,3.270  
799226,3.4203672527\C,2.0918024048,2.7195156497,3.4933432952\

C,5.54082474,3.9535676979,4.4615566531\O,-0.7649916666,2.0394122726,  
 3.7100780344\H,-1.3745343999,-1.7111785719,7.1351634524\H,-2.8404085542,-  
 3.2843378088,8.3383447871\H,-3.085112078,-5.6185341881,7.5406569508\H,-  
 1.8428116942,-6.3562943269,5.5268573444\H,-0.3865700475,-4.7968840943,  
 4.3313279104\H,1.790575147,-1.8322283949,3.731279581\H,1.3426157084,-  
 3.6069476952,3.9080166894\H,4.2665889021,3.0264525563,6.6689832214\  
 H,2.0041107047,2.0391943327,6.8180949128\H,1.4689354911,2.6368497659,  
 2.6119738145\H,3.7311776438,3.6231429295,2.4647944739\H,5.6297311727,  
 4.6440808243,3.6220434311\H,5.8157814076,4.4783681079,5.377668564\  
 H,6.2736116938,3.1548665661,4.3104255159\H,3.2192028332,2.3278595908,-  
 0.4134769153\H,3.8339973983,0.356345721,0.9949070664\H,2.0882725053,-  
 1.0940374481,1.8629902332\H,0.8431887372,2.8064079171,-0.8211241474\H,-  
 4.6652811267,1.2361981884,1.6838176226\H,-5.4977624883,-0.2022765832,  
 3.4937087127\H,-4.0190077809,-2.0121469769,4.385090106\H,-1.8118540545,-  
 2.3393536618,3.4257219857\H,-3.2750962474,1.8199714991,0.1521234388\H,-  
 1.2557742627,2.3951588267,-0.7562997759\ \ Version=ES64L-G16RevB.01\HF=-  
 2212.5687574\RMSD=5.700e-09\RMSF=1.845e-06\ Dipole=1.7986227,  
 0.3263485,-1.3403736\ Quadrupole=22.2068619,1.2028199,-23.4096818,  
 13.723574,13.004707,-13.3242687\ PG=C01 [X(C30H24N2O2S2)]\ \@

### 10m (from 1m and 7a)

HF=-2212.6262902 a.u (0)

1\1\GINC-R08N03\FOpt\RPBE1PBE\def2TZVP\C30H24N2O2S2\  
 WURTHWE\10-Feb-2021\0\ \# pbe1pbe/def2tzvp opt=readfc geom=check  
 guess=read pop=nbo freq emp=gd3bj nosym scrf= (solvent=dichloromethane)  
 \ \ Product 10m (NNS)\ \0,1\C,-0.0450558047,0.4566567639,0.2314111631\C,-  
 0.1207669517,0.067987743,1.5677072743\C,1.0582159931,0.0924342329,  
 2.3371949431\C,2.2373505283,0.5739371321,1.7553645868\C,2.2899497967,0.96  
 37776597,0.433290356\C,1.1398638869,0.8892668178,-0.3378943512\C,-  
 1.4539516117,-0.3192045212,2.1806314394\C,-2.642696495,-0.0344803135,  
 1.2626574008\C,-2.8662478759,1.4211481229,0.9434735235\N,-2.4704210217,  
 2.4161364734,1.6433939332\N,-1.8488767344,2.2108886018,2.8286939778\S,-  
 1.8395195383,0.7298923946,3.6510053359\C,-1.4494389584,-1.7576918042,  
 2.6652044406\C,-0.599822354,-2.1652157432,3.7127687396\C,-0.7273429011,-  
 3.4668223139,4.2170270426\C,-1.6056044685,-4.3772045417,3.6678296126\C,-  
 2.3938750878,-3.9928511432,2.5922741506\C,-2.3203952735,-2.6967367808,2  
 .1131312277\C,0.447700203,-1.3480143335,4.2966163391\C,1.1624060477,-  
 0.3815619206,3.7027506181\C,-3.5596926617,1.7569288145,-0.3171232321\C,-  
 3.4358603768,3.0335471825,-0.8718326155\C,-4.0804189319,3.353369569,-  
 2.0520823985\C,-4.8693565335,2.4085466186,-2.6991350605\C,-5.0026509791,  
 1.1408789521,-2.1555192117\C,-4.3482610926,0.8145533832,-0.9761837251\S,-  
 0.7704549149,3.4474301028,3.2108097078\O,0.140892772,3.6718352,

2.1289021139\ C,-1.8477307632,4.8221221466,3.3221439954\ C,-1.8959126055,  
5.7443600888,2.2899155139\ C,-2.7595872138,6.8228141176,2.3911761217\ C,-  
3.5741792318,6.9892078842,3.5076645562\ C,-3.5061735047,6.0421606473,  
4.5318633863\ C,-2.6511019854,4.960918283,4.4475720096\ C,-4.492405351,  
8.1641037224,3.6230758818\ O,-0.2665056606,3.108521436,4.508281815\ H,-  
2.8209983155,3.7659133343,-0.3642688895\ H,-3.9657817764,4.3450530028,-  
2.4744290572\ H,-5.3749776992,2.6613647152,-3.62378381\ H,-5.6184378059,  
0.3981812551,-2.649182349\ H,-4.4723606131,-0.1801579101,-0.565780947\ H,-  
3.5417826511,-0.4397735827,1.7304386229\ H,-2.5224648257,-0.5664521666,  
0.3165623363\ H,-2.8034182909,7.547257417,1.5856617937\ H,-1.2636978011,  
5.613252193,1.4215576985\ H,-2.6015639175,4.2301463721,5.2455084401\ H,-  
4.135370863,6.1570287448,5.4076388699\ H,-5.4776786188,7.8595587965,  
3.9817559062\ H,-4.0977985711,8.889666339,4.3404104928\ H,-4.6119613639,  
8.6711587742,2.6654499468\ H,3.2183890717,1.3242201111,0.0066442052\ H,  
3.1311138167,0.6170097181,2.3681940146\ H,-0.9271260664,0.4444002949,-  
0.3937208576\ H,1.1536915505,1.1907889833,-1.3785492659\ H,-2.9695915173,-  
2.4215442987,1.2939482746\ H,-3.0842780755,-4.6934011438,2.1378007269\ H,-  
1.6729620179,-5.3810941472,4.0699476208\ H,-0.0917047026,-3.7602401768,  
5.0453356674\ H,1.9882037832,0.0381181728,4.2693680488\ H,0.7492948461,-  
1.6405088314,5.29799 50339\ \ Version=ES64L-G16RevB.01\ HF=-2212.6262902\  
RMSD=3.739e-09\ RMSF=1.187e-06\ Dipole=-1.9556518,-0.2840783,-0.9928155\  
Quadrupole=1.6054277,12.5352795,-14.1407072,-13.1597633,-2.8730922,-  
6.3250355\ PG=C01[X(C30H24N2O2S2)]\ \@

## TS for 10m

HF=-2212.5358951 a.u (1, -251.2265cm<sup>-1</sup>)

1\1\GINC-R10N02\FTS\RPBE1PBE\def2TZVP\C30H24N2O2S2\  
WURTHWE\12-Feb-2021 \0\ \# pbe1pbe/def2tzvp opt=(ts,noeigentest,readfc)  
geom=check guess=read freq pop=nbo emp=gd3bj nosym scrf=(solvent=  
dichloromethane)\ \ TS for 10m\ \0,1\ C,-0.3625619924,-0.1073322324,-  
0.0545180222\ C,0.0276093285,-0.3774399464,1.2506331404\ C,1.3603439653,-  
0.769473139,1.49634231\ C,2.2744232893,-0.7451897006,0.4382821044\  
C,1.8822921237,-0.4218415246,-0.8462680502\ C,0.5501308695,-0.1255888938,-  
1.0961060841\ C,-0.856568696,-0.2852717446,2.4502395305\ C,-  
2.9602967533,0.6931557089,1.5990469356\ C,-2.6758449835,1.9101485632,  
1.0348958545\ N,-2.1840861062,2.929179832,1.793520625\ N,-2.0671666778,  
2.7021735221,3.0267410008\ S,-0.6380622465,0.9269581834,3.5650957235\ C,-  
1.2902325147,-1.6176171254,2.9761303679\ C,-0.2816043122,-2.3697943789,  
3.6177563355\ C,-0.6331148743,-3.5769400432,4.2309479859\ C,-1.9227384606,-  
4.0676483234,4.1777874068\ C,-2.8991430356,-3.3413656376,3.5121265912\ C,-  
2.5826998295,-2.1281120824,2.9228099511\ C,1.1138738446,-1.963077085,  
3.6855240619\ C,1.8215113857,-1.2635233758,2.7817937376\ C,-2.7469110727,

2.1840955049,-0.4071846091\ C,-1.8860916297,3.1135595196,-0.992846799\ C,-  
1.9358799546,3.3514308946,-2.3558803903\ C,-2.8417327913,2.6644360595,-  
3.1531541728\ C,-3.7053878537,1.7423176682,-2.5779143375\ C,-3.6616176921,  
1.5062810982,-1.2136560212\ S,-1.2814663226,4.0456078287,3.8179216237\ O,-  
0.2180960065,4.5547594403,3.0026364703\ C,-2.5927979711,5.1997216081,  
3.8599545684\ C,-2.7211520391,6.12659388,2.8330026352\ C,-3.778676808,  
7.0158618822,2.8641208199\ C,-4.7110992096,6.9917122313,3.9022577692\ C,-  
4.5600866198,6.0462546892,4.9153586374\ C,-3.5087192517,5.1471885857,  
4.9021099088\ C,-5.8338914282,7.9783608222,3.9376018286\ O,-1.0190856734,  
3.5635741251,5.1418155906\ H,-1.1674151892,3.6308150646,-0.3701480185\ H,-  
1.256540168,4.0692717949,-2.8004978124\ H,-2.8770044426,2.8495533733,-  
4.2203802961\ H,-4.4241836809,1.2128784128,-3.1921313784\ H,-4.3584241942,  
0.8055405803,-0.7682536685\ H,-3.1832720717,0.6367892174,2.6539486478\ H,-  
3.2509179839,-0.1341849555,0.9656730072\ H,-3.8854230794,7.7443021065,  
2.0680206753\ H,-1.9974994564,6.1461333682,2.0285141905\ H,-3.3905482476,  
4.4159526374,5.6916378419\ H,-5.2778926674,6.014451311,5.7272490912\ H,-  
6.2018098016,8.1953275042,2.9335392517\ H,-6.6635757728,7.6155365055,  
4.5450035909\ H,-5.4943842503,8.9239707557,4.3712476976\ H,2.6076616441,-  
0.4153073237,-1.6511337094\ H,3.3053957545,-1.0155406289,0.6397886983\ H,-  
1.3889031002,0.1419215579,-0.2694955218\ H,0.2169536698,0.1117670094,-  
2.0996238807\ H,-3.3700895378,-1.5745887615,2.4353510546\ H,-3.9175690601,-  
3.7081640026,3.4625481032\ H,-2.16674915,-5.0099065148,4.6536505776\ H,  
0.1393605261,-4.1382086863,4.7454445533\ H,2.8857853132,-1.1534004582,  
2.9672105349\ H,1.6624869466,-2.3644732819,4.5324777413\ \ Version=ES64L-  
G16RevB.01\ HF=-2212.5358951\ RMSD=8.226e-09\ RMSF=5.900e-07\ Dipole=-  
2.5653294,-0.4188974,-1.8646733\ Quadrupole=16.483117,5.4248372,-21.9079542,  
-24.021884,-11.4863347,-12.3770406\ PG=C01[X(C30H24N2O2S2)]\ \@

# 1n

HF=-976.4316442 a.u. (0)

1\1\GINC-R10N32\FOpt\RPBE1PBE\def2TZVP\C15H12S1\  
WURTHWE\10-Feb-2021\0\ \# pbe1pbe/def2tzvp Opt=readfc geom=check  
guess=read Pop=NBO Freq emp= gd3bj nosym scrf=(solvent=  
dichloromethane)\ \ Educt 1n\ \ 0,1\ C,-0.0509744032,0.6190787537,  
0.3832179939\ C,0.1944886834,0.185313682,1.6973866971\ C,1.3489554061,-  
0.5800467844,1.9514656737\ C,2.1906646844,-0.8754182027,0.8784344421\  
C,1.9229318935,-0.4602986227,-0.4112193653\ C,0.7862123112,0.2976939564,-  
0.6618445845\ C,-0.837181708,0.5343327217,2.6947761949\ S,-1.6534688926,  
1.9527113114,2.6299725589\ C,-1.2168342453,-0.452271419,3.7269054197\ C,-  
2.5456871547,-0.8654340752,3.817201646\ C,-2.9336881592,-1.7773637714,  
4.7832250598\ C,-2.0001916232,-2.2579957049,5.6909443489\ C,-0.6830862116,-  
1.8307244924,5.6169925512\ C,-0.2721895849,-0.9392842464,4.6336450308\

H,3.0929097332,-1.4445342682,1.0779360235\H,2.6002889406,-0.7205293722,-  
 1.2163051803\H,0.5535272305,0.6316877009,-1.6658082138\H,-0.9452540876,  
 1.2015967488,0.2025426131\H,0.044573353,-2.1903101223,6.3369618212\H,-  
 2.2987177678,-2.9608183011,6.4600883708\H,-3.9654520784,-2.1046138335,  
 4.8327331791\H,-3.2677307054,-0.4673623168,3.1143319119\C,1.8163124223,-  
 1.07522984,3.2951764678\C,1.1480869566,-0.4901953329,4.5263421069\  
 H,1.7038862576,-2.1660717998,3.3166743428\H,2.892377929,-0.887783256,  
 3.353670255\H,1.7012824554,-0.8073522662,5.4121898469\H,1.2000709752,  
 0.6035040983,4.4921397743\ \ Version=ES64L-G16RevB.01\ HF=-976.4316442\  
 RMSD=7.008e-09\RMSF=8.890e-06\Dipole=1.1466488,-1.4051155,0.0378185\  
 Quadrupole=1.9084913,-6.874804,4.9663128,1.3825374,5.5626083,-11.3290622\  
 PG=C01[X(C15H12S1)]\ \@

### 9n (from 1n and 7a)

HF=-2213.8438687 a.u. (0)

1\1\GINC-R09N43\FOpt\RPBE1PBE\def2TZVP\C30H26N2O2S2\  
 WURTHWE\10-Feb-2021\0\ \ # pbe1pbe/def2tzvp Opt=readfc geom=check  
 guess=read Pop=NBO Freq emp=gd3bj nosym scrf= (solvent=  
 dichloromethane)\ \ Product 9n NNC\ \ 0,1\C,-0.0704597294,-0.0708985487,-  
 0.1370535199\C,0.205855136,-0.3167091785,1.2106255679\C,1.5418550078,-  
 0.4148192127,1.6082863946\C,2.5931624322,-0.2968864662,0.7214306838\  
 C,2.3156048282,-0.0964346462,-0.6219600914\C,1.0024565561,0.0059211514,-  
 1.0325553085\C,-1.456741157,0.07923746,-0.7936734877\N,-1.3652342635,  
 1.1675986592,-1.7908940676\N,-1.8827651823,1.1836422117,-3.0313006679\C,-  
 2.5977183665,0.2484670952,-3.5318595579\C,-2.9372588674,-1.0230964052,-  
 2.8215844376\S,-1.5811219545,-1.494751616,-1.7516962885\C,-3.103628484,  
 0.4738792401,-4.8977858374\C,-2.4888932942,1.4026319873,-5.7407849818\C,-  
 2.9834642222,1.6349463945,-7.0110959566\C,-4.1012696277,0.9443295176,-  
 7.4656677251\C,-4.7153940467,0.0164277548,-6.6387872467\C,-4.2178817095,-  
 0.2218623264,-5.3659419224\S,-0.784647435,2.7041268421,-1.4006446958\C,-  
 2.1307210493,3.7899237321,-1.6917216352\C,-2.4034856135,4.2371713697,-  
 2.9787854586\C,-3.4767567149,5.0829322226,-3.1828508903\C,-4.2797679786,  
 5.4999693565,-2.1200446736\C,-3.9770849254,5.0456908078,-0.8388798323\C,-  
 2.910206488,4.1918309715,-0.6166713725\C,-5.4235572006,6.4345571246,-  
 2.3544476077\C,-2.7476016799,0.2206794073,0.0081036037\C,-3.7539872576,  
 1.038816304,-0.5037947464\C,-5.0045446468,1.1277207602,0.088740568\C,-  
 5.2821644474,0.378963421,1.2161952756\C,-4.2931889022,-0.4432044753,  
 1.7333049494\C,-3.0350308987,-0.5407288765,1.1504013674\O,-0.5126664937,  
 2.6734562393,0.0048840245\O,0.2510931328,3.0277108494,-2.3347875873\H,-  
 1.610778448,1.9280834079,-5.3870595508\H,-2.4900946384,2.3530428224,-  
 7.6560587017\H,-4.4860977628,1.1254904603,-8.4624476918\H,-5.5876644644,-  
 0.526825841,-6.9832046894\H,-4.7183979826,-0.9429464791,-4.7305375727\H,-

3.8672682516,-0.9322446947,-2.2517503932\H,-3.0548855746,-1.8416847169,-  
3.5320800852\H,-3.6988086104,5.4273731824,-4.1869293951\H,-1.7833458823,  
3.917047895,-3.804587664\H,-2.682178309,3.8339086189,0.3786677925\H,-  
4.5885260754,5.3613123359,-0.0009367137\H,-6.1298430203,6.4157981413,-  
1.5239918132\H,-5.0617094151,7.4616443295,-2.4608838513\H,-5.9565122456,  
6.1828928253,-3.2731533658\H,-6.2533366515,0.4328877536,1.6940731941\H,-  
5.751649351,1.784114223,-0.3415715203\H,-3.5777911924,1.6270293236,-  
1.3915650528\C,-2.0026026827,-1.3844504752,1.8194387306\H,-4.4931275531,-  
1.0280556554,2.6248217749\C,-0.8275198353,-0.5270430464,2.2751521896\  
H,1.7468129725,-0.6015126345,2.6571640178\H,3.6156015015,-0.3767353514,  
1.0718912631\H,3.1143441595,-0.0197843182,-1.3499634192\H,0.7963251602,  
0.1661449205,-2.0826259731\H,-0.335511538,-1.0017253098,3.12624502\H,-  
1.2056547669,0.436140216,2.6353480159\H,-2.4562587735,-1.8779745999,  
2.6804115766\H,-1.6436026242,-2.1728710093,1.1497572803\ \ Version=ES64L-  
G16RevB.01\HF=-2213.8438687\RMSD=4.448e-09\RMSF=1.295e-06\Dipole=-  
3.0114955,-0.1729583,-0.2421688\Quadrupole=11.4464035,-11.4719434,  
0.0255399,-16.7228691,14.1098468,-6.9212651\PG=C01  
[X(C30H26N2O2S2)]\ \@

### 1n + 7a -vdW-Complex

HF=-2213.795258 a.u (0)

1\1\GINC-R07N15\FOpt\RPBE1PBE\def2TZVP\C30H26N2O2S2\  
WURTHWE\02-Mar-2021\0\ \# pbe1pbe/def2tzvp opt=(maxstep=10,readfc)  
geom=check guess=read scrf=(solvent=dichloromethane) freq pop=nbo  
emp=gd3bj nosym\ \ 1n + 7a -vdW-Complex \ \ 0,1\C,0.3102227815,  
0.1114224377,0.3442135861\C,-0.0085495082,-0.2419774772,1.658082551\  
C,1.0095410412,-0.3601279363,2.6057976043\C,2.326277661,-0.1095022794,  
2.267094535\C,2.6466243917,0.2316825506,0.9602459013\C,1.6420325129,  
0.3340180316,0.0111497272\C,-1.3955381167,-0.5658133675,2.0548445925\S,-  
1.6537228096,-1.9981462654,2.8162410058\C,-0.7727341223,0.2307062453,-  
0.6762838454\C,-1.6573835033,1.430247229,-0.3938640566\C,-2.5697989347,  
1.3414913324,0.7976372662\C,-2.48534958,0.4080775841,1.8499701445\C,-  
3.4809659292,0.4290011297,2.8424299609\C,-4.5032091796,1.3498181058,  
2.8415564878\C,-4.5716070917,2.2822719256,1.8144619911\C,-3.623164468,  
2.2557211347,0.8116324294\C,-0.9190918292,1.038772081,5.6663954984\C,-  
1.8894537252,1.9166052094,5.4009531442\C,-3.2507471579,1.9027163415,  
5.9551075607\C,-4.00717408,3.072661463,6.022695694\C,-5.3018363768,  
3.042746928,6.517204104\C,-5.8615836808,1.8474563858,6.9432874292\C,-  
5.1154074099,0.677400241,6.8741368332\C,-3.8222539036,0.7039160566,  
6.3824965666\N,-1.5944670251,3.063911727,4.6168063218\N,-0.8815125121,  
2.8652877089,3.6416705014\S,-0.4606730153,4.358178873,2.8211303253\O,-  
1.0752590443,5.4928619683,3.4464864089\C,1.2530136082,4.340173068,

3.1437234583\ C,1.7695460513,5.1324972195,4.1613195116\ C,3.1254994525,5.08  
0369556,4.4254933849\ C,3.9692867821,4.2421525463,3.6961359775\  
C,3.4192236105,3.4479810995,2.6902315141\ C,2.0674080123,3.489352945,  
2.4057580515\ C,5.4380892503,4.2125900838,3.9726209434\ O,-0.7000689243,  
4.0751725144,1.4357039275\ H,-3.5766387306,4.0058077893,5.6837210525\ H,-  
5.8772689121,3.9599318867,6.5648310627\ H,-6.8769051352,1.8240631728,  
7.3213566741\ H,-5.5482658267,-0.263460991,7.193321637\ H,-3.2615687763,-  
0.2201094819,6.3033148127\ H,0.0590852486,1.1581709202,5.2200251463\ H,-  
1.0682053634,0.2290801,6.3674479095\ H,3.5390612986,5.6990553087,  
5.2139610881\ H,1.1135752029,5.7808190319,4.7281977313\ H,1.645854307,  
2.8673058834,1.626042682\ H,4.0608877959,2.7831063331,2.1232841191\  
H,5.8703248904,3.2436396725,3.7198716829\ H,5.9518015438,4.9685453202,  
3.3707004704\ H,5.6496625075,4.4301116767,5.0203167666\ H,3.6774383188,0.41  
47304845,0.6791923838\ H,3.1014531054,-0.1862889637,3.0202079779\  
H,0.74896426,-0.6523442456,3.615214057\ H,1.8898433349,0.5846366051,-  
1.0148589023\ H,-3.6904055951,2.9674613075,-0.0043674696\ H,-5.3640201205,  
3.0215046434,1.7925836161\ H,-5.2286110334,1.3531749024,3.6461672819\ H,-  
3.4036181283,-0.2888547311,3.6474713226\ H,-2.2844348433,1.6228332267,-  
1.269014819\ H,-1.0305087868,2.3201225569,-0.2689419887\ H,-0.328346297,  
0.3419037225,-1.6670297368\ H,-1.3775802832,-0.6825636535,-0.6983191191\  
Version=ES64L-G16RevB.01\ HF=-2213.795258\ RMSD=6.813e-  
09\ RMSF=7.810e-07\ Dipole=1.9706076,0.4338433,0.6749444\  
Quadrupole=18.2804011,-27.6283066,9.3479055,11.9645084,7.0333533,  
4.9192994\ PG=C01[X(C30H26N2O2S2)]\ \@

### TS for 9n

HF=-2213.786918 a.u. (1, -221.4444cm<sup>-1</sup>)

1\1\GINC-

R10N19\ FTS\ RPBE1PBE\ def2TZVP\ C30H26N2O2S2\ WURTHWE\ 12-Feb-  
2021 \0\ \# pbe1pbe/def2tzvp opt=(ts,noeigentest,readfc) geom=check  
guess=read freq pop=nbo emp=gd3bj nosym scrf=(solvent=dichloromethane)  
\\ TS for 9n \\ 0,1\ C,-1.4721969372,-0.9363240016,-1.0618680254\ C,-  
0.3580709554,-0.6517403295,-0.2287512825\ C,0.914227126,-0.708034966,-  
0.7811542858\ C,1.1422686255,-1.0636198054,-2.1016937683\ C,0.0710769107,-  
1.4289777771,-2.8981078875\ C,-1.202214275,-1.3726948548,-2.3740397362\ C,-  
2.8787585058,-0.725886991,-0.7170689315\ N,-2.5043890468,1.9480911508,-  
2.1215149483\ N,-1.994049307,1.617848853,-3.2145017577\ C,-2.6837785556,  
0.6748877835,-3.9471830916\ C,-3.9723700009,0.337029018,-3.5989371046\ S,-  
4.081218307,-1.1950477605,-1.7906358795\ C,-1.9665968452,0.1228161865,-  
5.1022365328\ C,-0.8107267544,0.7427785619,-5.5838373486\ C,-0.1208000785,  
0.2108342992,-6.6601547115\ C,-0.5614137945,-0.9546495811,-7.2726297795\ C,-  
1.7055685715,-1.5816965887,-6.7978319266\ C,-2.4025696712,-1.0481654802,-



5.7265244539\ S,-1.5731387413,3.1291444097,-1.3024463993\ C,-2.7677111158,  
4.4031604142,-1.1821916766\ C,-2.8050565582,5.4057706648,-2.1426812637\ C,-  
3.7679447,6.3936047111,-2.045048888\ C,-4.6997308117,6.3917169817,-  
1.0067495357\ C,-4.6370558777,5.3744180693,-0.0554260866\ C,-3.6792906449,  
4.3793926059,-0.1353268612\ C,-5.7550370416,7.4486227679,-0.9296525403\ C,-  
3.3742559303,-0.0990544746,0.5237383707\ C,-4.4925944441,0.742296791,  
0.4357790998\ C,-5.0631306713,1.3117779939,1.5551515583\ C,-4.5413321254,  
1.0275196883,2.810008441\ C,-3.4325382339,0.2056030178,2.9141033709\ C,-  
2.8248575112,-0.3459260464,1.7911042914\ O,-1.3441983074,2.5824189624,  
0.0068094178\ O,-0.4588308117,3.5837721162,-2.0864869679\ H,-0.4556274226,  
1.6418724367,-5.0976186024\ H,0.7723274117,0.7087701287,-7.020238547\ H,-  
0.0165005485,-1.3731987036,-8.1106261712\ H,-2.0561939814,-2.4969207768,-  
7.2609040681\ H,-3.2805320549,-1.5670870273,-5.3597334967\ H,-4.5065888313,  
1.012504193,-2.9443464668\ H,-4.5707605699,-0.2787443576,-4.2560833412\ H,-  
3.7958637889,7.1856906342,-2.7851968067\ H,-2.0793104042,5.4125868049,-  
2.9462375053\ H,-3.62937621,3.5917702815,0.6058554482\ H,-5.3473222171,  
5.3657141535,0.7640936446\ H,-6.1266237738,7.5660862751,0.0888364709\ H,-  
5.3779100832,8.411241893,-1.2785097087\ H,-6.6064732506,7.183292256,-  
1.563898739\ H,-4.9881746415,1.4528764686,3.701194961\ H,-5.9134222085,  
1.9750974234,1.4486664765\ H,-4.8969536798,0.9613577994,-0.5423219779\ C,-  
1.5573951798,-1.1147594562,1.9466369911\ H,-3.0100071657,-0.0087447293,  
3.88974409\ C,-0.4353587508,-0.3679534286,1.2389890167\ H,1.759517288,-  
0.484545928,-0.1393927938\ H,2.154372119,-1.0877906735,-2.4888191767\ H,  
0.2182550351,-1.74897677,-3.9223005356\ H,-2.040125638,-1.6799606177,-  
2.9821130622\ H,0.526649815,-0.6391771752,1.6790403673\ H,-0.5607369352,  
0.7087346238,1.3962678745\ H,-1.3264472621,-1.2140551638,3.0081788922\ H,-  
1.6468666005,-2.1270759546,1.5391538873\ \ Version=ES64L-G16RevB.01\ HF=-  
2213.786918\ RMSD=5.607e-09\ RMSF=9.481e-07\ Dipole=-1.4155313,0.3185062,  
0.2812759\ Quadrupole=4.7126272,-1.9742129,-2.7384143,-26.2679964,  
0.2949862,3.5131805\ PG=C01 [X(C30H26N2O2S2)]\ \@

### 10n (from 1n and 7a)

HF=-2213.8343802 a.u (0)

1\1\GINC-R10N10\FOpt\RPBE1PBE\def2TZVP\C30H26N2O2S2\  
WURTHWE\10-Feb-2021\0\ \ # pbe1pbe/def2tzvp Opt=readfc geom=check  
guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=dichloromethane)  
\ \ Product 10n (NNS)\ \ 0,1\ C,-0.0259896739,-0.1010202247,-0.076071345\ C,-  
0.0297775488,-0.1583750366,1.3301943226\ C,1.2005825559,-0.2869938145,  
1.9859231479\ C,2.4052760505,-0.3419326703,1.3111176393\ C,2.4113130099,-  
0.2569821676,-0.0705217406\ C,1.2068856721,-0.142672249,-0.7339045196\ C,-  
1.3039147935,-0.0740149445,2.1726705949\ C,-1.0291798118,-0.2153821844,  
3.6727213602\ C,-2.2054799645,0.1225274167,4.555392466\ N,-3.1961444755,

0.867725194,4.2378217918\ N,-3.2560974814,1.41379372,3.0022513416\ S,-  
1.8337955551,1.6928378434,2.0834700268\ C,-2.2450814348,-0.4596798812,  
5.9114741526\ C,-3.4514558061,-0.5317960385,6.6127570681\ C,-3.4944318194,-  
1.0710457038,7.8849831589\ C,-2.3333916611,-1.5451449503,8.4855430988\ C,-  
1.1314347801,-1.4782646912,7.7988861275\ C,-1.0873315969,-0.9451022811,  
6.5186507552\ S,-4.6045786931,2.3750350327,2.7482361012\ C,-4.3286022918,  
3.7813061531,3.750025944\ C,-4.719582157,3.7588569905,5.0828209998\ C,-  
4.4379265188,4.8511913388,5.8828422656\ C,-3.7725816585,5.9662395054,  
5.3740992944\ C,-3.3888628977,5.9597084556,4.0340655402\ C,-3.6589820328,  
4.8754326243,3.2180413247\ C,-3.5017414222,7.1533785421,6.2425679876\ C,-  
2.403453215,-1.0289379165,1.714976777\ C,-3.028967736,-0.909965807,  
0.4640991124\ C,-4.0393878275,-1.8034344501,0.1221936094\ C,-4.4437055872,-  
2.8156023712,0.9759479012\ C,-3.8187688544,-2.946075341,2.2026689388\ C,-  
2.816473989,-2.0583396066,2.5606307011\ O,-4.5367091516,2.7494089948,  
1.3686865841\ O,-5.72662296,1.654033041,3.260697889\ H,-4.3534242591,-  
0.16588038,6.1386387185\ H,-4.4399799512,-1.128371305,8.4118396422\ H,-  
2.3689134446,-1.9681632674,9.4827093594\ H,-0.2202132327,-1.8426802305,  
8.2586666533\ H,-0.1359671832,-0.896258737,6.0031753695\ H,-0.2137690056,  
0.4534202198,3.9469229922\ H,-0.6915015372,-1.2268378082,3.9081653773\ H,-  
4.7399784278,4.8394214161,6.9242813161\ H,-5.2371355169,2.8954830836,  
5.4798030631\ H,-3.3627511623,4.8768870321,2.1765698468\ H,-2.8699609668,  
6.8184585216,3.6228962909\ H,-2.6502881157,7.7280768555,5.8764015609\ H,-  
4.3689230764,7.8206926676,6.2567499705\ H,-3.3050543232,6.8534076781,  
7.2729868135\ H,-5.236361467,-3.4941731812,0.6829644054\ H,-4.517315394,-  
1.6936892854,-0.8455200688\ C,-2.6235089511,0.1242720382,-0.5347036414\ H,-  
2.3599071503,-2.1935528203,3.5306380205\ H,-4.107898812,-3.7310589416,  
2.8914088667\ H,1.23646155,-0.3599525306,3.0622625104\ H,3.3289720588,-  
0.4464239505,1.867671583\ H,3.340992902,-0.2860340859,-0.6267216341\ H,  
1.202728047,-0.0911700241,-1.81815871\ C,-1.2011647374,-0.0606381585,-  
1.030301069\ H,-3.2823967593,0.0454676713,-1.4023549315\ H,-2.7619481952,  
1.1249414752,-0.126717896\ H,-0.9910509876,0.7208367812,-1.7667971433\ H,-  
1.1642534031,-1.0032113966,-1.5896203279\ \ Version=ES64L-G16RevB.01\ HF=-  
2213.8343802\ RMSD=4.984e-09\ RMSF=7.855e-07\ Dipole=2.2372081,  
0.3405148,1.2401726\ Quadrupole=-32.7400991,8.5172046,24.2228946,1.602744,  
1.4266541,10.4193469\ PG=C01 [X(C30H26N2O2S2)]\ \@

## TS for 10n

HF = -2213.7509673 a.u (1, -264.9009cm<sup>-1</sup>)

1\1\GINC-R07N17\FTS\RPBE1PBE\def2TZVP\C30H26N2O2S2\

WURTHWE\15-Feb-2021\0\ \ # pbe1pbe/def2tzvp opt=(ts,noeigentest,readfc,  
maxstep=5) geom=check guess=read scrf=(solvent= dichloromethane) freq  
pop=nbo emp=gd3bj nosym\ \ TS for 10n\ \ 0,1\ C,0.0825161352,-0.0294487112,

0.1915746208\ C,0.2807951289,-0.3255295908,1.5333551028\ C,1.5315853072,-  
 0.8169564969,1.940785889\ C,2.5637801846,-0.8978999006,1.0148195746\  
 C,2.3744041425,-0.5303822576,-0.3088411851\ C,1.1199905477,-0.1183913109,-  
 0.7244114228\ C,-0.7737430025,-0.2346827877,2.5903362775\ S,-0.701211423,  
 0.921978075,3.7848845968\ C,1.6848160745,-1.4000599496,3.3076700967\  
 C,0.8709628021,-2.6851700469,3.4206634006\ C,-0.6405678229,-2.6320375226,  
 3.3238631539\ C,-1.4343813228,-1.5254549075,2.9677611152\ C,-2.8250942473,-  
 1.6436947337,3.0329316021\ C,-3.4416010523,-2.8276544533,3.3876193649\ C,-  
 2.6658834959,-3.9325890369,3.7042242121\ C,-1.2900350861,-3.8160493088  
 ,3.6789942382\ C,-2.6197457526,1.0864227971,1.4365943059\ C,-2.0074695776,  
 2.2064746534,0.9342616829\ C,-1.8790714462,2.4998760537,-0.5017283765\ C,-  
 0.7889002526,3.2265435862,-0.9821492161\ C,-0.6625510928,3.4871749264,-  
 2.3360389662\ C,-1.6180722356,3.022140468,-3.2300753877\ C,-2.7067373714,  
 2.3003279995,-2.7605451411\ C,-2.8389623757,2.0444396504,-1.4052312431\ N,-  
 1.3659945806,3.0715495698,1.7575729483\ N,-1.4265557418,2.834751298,  
 3.0027364566\ S,-0.4197831223,3.9618680618,3.8748298568\ O,0.8680747742,  
 4.0697798046,3.2554399043\ C,-1.3107713533,5.4450842906,3.6277928986\ C,-  
 0.9640439494,6.2851680816,2.5777925366\ C,-1.6918519772,7.4437207751,  
 2.3806093486\ C,-2.761267443,7.7740166179,3.2135729713\ C,-3.0893579749,  
 6.9085555822,4.2561296512\ C,-2.3733246049,5.74445405,4.4697364506\ C,-  
 3.5222460672,9.0442901969,3.0065587157\ O,-0.5394782368,3.5501764262,  
 5.2429940749\ H,-0.034349639,3.5653484162,-0.2838050065\ H,0.1926122555,  
 4.0463734967,-2.697519448\ H,-1.5156163551,3.223499503,-4.2900545552\ H,-  
 3.4624235535,1.9443787951,-3.4509374116\ H,-3.7063183252,1.5043297007,-  
 1.0435528491\ H,-2.9516378214,1.0977365758,2.4621000092\ H,-3.0173634172,  
 0.3252752261,0.778322126\ H,-1.4276214436,8.1059729656,1.5636761615\ H,-  
 0.1347269914,6.0288148986,1.9316891734\ H,-2.6273140309,5.0756134535,  
 5.2822779322\ H,-3.9190995221,7.1512166829,4.9104651199\ H,-3.5797168442,  
 9.3035094428,1.9483863084\ H,-4.5343209004,8.9712127906,3.4060478114\ H,-  
 3.0239564494,9.872864297,3.5191494053\ H,3.1958190078,-0.5900778008,-  
 1.0133874323\ H,3.5283361879,-1.2732109498,1.3405481445\ H,-0.8912312555,  
 0.2753426253,-0.1550844628\ H,0.9382276556,0.1401401743,-1.7610344869\ H,-  
 3.4444574776,-0.7926887637,2.7952637723\ H,-4.5234057803,-2.883325561,  
 3.4153812217\ H,-3.1282596482,-4.8718706066,3.9840599939\ H,-0.6783339064,-  
 4.6675895376,3.9607378685\ H,2.7333907956,-1.6466691293,3.4849114626\  
 H,1.3914409606,-0.6896051263,4.0837334122\ H,1.1075908242,-3.159937545,  
 4.3775147077\ H,1.2284514805,-3.3788895385,2.6505047934\ \ Version=ES64L-  
 G16RevB.01\ HF=-2213.7509673\ RMSD=4.186e-09\ RMSF=6.778e-07\ Dipole=-  
 1.7344252,0.051883,-1.9357272\ Quadrupole=4.2829266,21.3148587,-25.5977853,  
 -20.0541323,-8.1976797,-12.6094287\ PG=C01[X(C30H26N2O2S2)]\ \@

**1i**

HF=-785.0426912 a.u. (0)

1\1\GINC-R08N11\FOpt\RPBE1PBE\def2TZVP\C8H12O1S1\  
WURTHWE\14-Feb-2020\0\ \# pbe1pbe/def2tzvp Opt=readfc geom=check  
guess=read scrf=(solvent=dichloromethane) Pop=NBO Freq emp=gd3bj  
nosym\ \ 1i Educt\ \ 0,1\C,0.0872732654,-0.0000973704,-0.1136745034\C,  
0.1785190402,-0.0000043865,1.4195276857\C,1.7145342261,-0.0001077294,  
1.4138201545\C,1.6122855168,-0.000187838,-0.1076296596\O,-0.6399140115,  
0.000108923,2.2914832111\C,2.3433417753,-1.2603116979,1.9942005467\  
C,2.3435153024,1.2600740773,1.9940589892\S,2.7094145502,-0.0003176702, -  
1.2767033248\C,-0.5313203581,1.2601714975,-0.7047742657\C,-0.5314626531,-  
1.2603774482,-0.7046037702\H,3.4101071314,-1.2727339757,1.7617629793\  
H,2.2179385805,-1.2663758874,3.078521009\H,1.8921179803,-2.1666717516,  
1.587217124\H,3.4102812088,1.2723262052,1.7616146334\H,1.8924123664,  
2.1664505184,1.5869785123\H,2.218117729,1.2662745157,3.078379237\H,-  
0.3611287383,1.2755567912,-1.7831899567\H,-1.6065556865,1.2635304182,-  
0.5167696985\H,-0.1010785595,2.1664229399,-0.2754156862\H,-0.3612795644,-  
1.2759244716,-1.7830184078\H,-0.1013165921,-2.1666186868,-0.2751274796\H,-  
1.6066973268,-1.2635937109,-0.5165924632\ \ Version=ES64L-G16RevB.01\HF=-  
785.0426912\RMSD=5.583e-09\RMSF=5.540e-06\Dipole=0.0365281,-  
0.0000268,-0.0378073\Quadrupole=-1.5444807,4.3564253,-  
2.8119447,0.0008388,8.2509848,-0.0009799\PG=C01[X(C8H12O1S1)]\ \@

**9q (from 1i and 7a)**

HF=-2022.4563956 a.u. (0)

1\1\GINC-R08N11\FOpt\RPBE1PBE\def2TZVP\C23H26N2O3S2\  
WURTHWE\15-Feb-2020\0\ \# pbe1pbe/def2tzvp Opt=(maxstep=8,readfc)  
geom=check guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=  
dichloromethane)\ \ 9q NNC-Product\ \ 0,1\C,-0.0955905159,0.6179846118, -  
0.0600441658\C,-0.0706783505,-0.8330422579,0.3905052888\O,0.7902420676,-  
1.6669060695,0.3845991412\C,-1.6726787345,0.5024495183,0.0016182803\N,-  
2.431202272,1.4838432542,0.7398886606\N,-3.7333580338,1.1060797579,  
1.1182291147\C,-4.4257523543,0.4274843859,0.2801556353\C,-4.0694983295,  
0.0473151343,-1.1273039017\S,-2.3642090229,0.2978723323,-1.6607008065\C,-  
5.7685523649,0.0220771917,0.7449282033\C,-6.0439763639,-0.0240754124,  
2.1132162336\C,-7.3032588144,-0.3758693282,2.5642437671\C,-8.3083770456,-  
0.6878666188,1.6573168919\C,-8.0437202343,-0.6483672754,0.2965690887\C,-  
6.7813090367,-0.3014111015,-0.1584009671\S,-2.4350495852,3.1284492017,  
0.3804262611\C,-3.7718347743,3.4004693487,-0.7252189274\C,-3.5250487063,  
3.4715696925,-2.0890659492\C,-4.5886112277,3.6385013489,-2.9589279752\C,-  
5.8974155306,3.729403086,-2.4883067006\C,-6.1173152756,3.6650249944,-  
1.1121082096\C,-5.066027435,3.5069077095,-0.2288479108\C,-7.0409236416,

3.9202616671,-3.4328341136\C,-1.531739374,-0.873516777,0.8018144296\O,-  
 2.7413093146,3.7901509313,1.6119924944\O,-1.2094404567,3.4061611294,-  
 0.3058891884\H,-5.2549632181,0.2166708948,2.8136686859\H,-7.5013296089,-  
 0.4129381969,3.6290102955\H,-9.2942803715,-0.9652033884,2.0116721565\H,-  
 8.8228795822,-0.888050111,-0.4172134631\H,-6.6009356345,-0.2680215237,-  
 1.2253329901\H,-4.3606117116,-0.9897208198,-1.3003092665\H,-4.6886407747,  
 0.6685812122,-1.7831720616\H,-4.3997581248,3.6937781634,-4.0252378723\H,-  
 2.5118824246,3.3891796235,-2.4578006624\H,-5.2417596135,3.4514642014,  
 0.8375484601\H,-7.1288470834,3.734457432,-0.7277737305\H,-7.2968653252,  
 4.9812753365,-3.5110696947\H,-6.7937907238,3.5659922063,-4.434127971\H,-  
 7.9327902283,3.3964641485,-3.0849212437\C,0.5471399798,0.8812914163,-  
 1.4074763596\C,0.5739949211,1.4871979186,1.0092002716\C,-2.2827219243,-  
 2.1074323948,0.3439116349\C,-1.6587338837,-0.7412750414,2.3200742128\H,-  
 1.2528963599,-1.6437372407,2.7812325414\H,-1.1311723761,0.1181785783  
 ,2.7260282411\H,-2.7097647172,-0.6534759404,2.5978529614\H,-1.7889684208,-  
 2.9853842868,0.7656395578\H,-3.3125922478,-2.102803909,0.7070692563\H,-  
 2.2807282151,-2.2084527927,-0.7412973217\H,1.6267981492,0.7481208722,-  
 1.3143234514\H,0.1955837072,0.194431444,-2.1796060897\H,0.3499463249,  
 1.9064774576,-1.7221453309\H,1.5565237503,1.0634146269,1.2281197019\H,  
 0.7042406368,2.5001184339,0.6363854329\H,0.0074564883,1.5402921505,  
 1.9363491135\ \ Version=ES64L-G16RevB.01\ HF=-2022.4563956\ RMSD=  
 2.388e-09\ RMSF=7.126e-07\ Dipole=-3.5913399,-0.7791846,-1.6159389\  
 Quadrupole=37.0747269,-30.6832701,-6.3914568,2.3261389,14.0222959,-  
 13.4765874\ PG=C01 [X(C23H26N2O3S2)]\ \@

### 1i + 7a vdW-complex

HF=-2022.4029297 a.u (0)

1\1\GINC-R09N10\FOpt\RPBE1PBE\def2TZVP\C23H26N2O3S2\  
 WURTHWE\25-Feb-2021\0\ \# pbe1pbe/def2tzvp opt=(maxstep=9) freq  
 pop=nbo emp=gd3bj nosym scrf=(solvent= dichloromethane)\ \ 1i + 7a vdW-  
 complex \ \ 0,1\C,-0.3659475506,0.0574479337,0.0306313998\C,-0.1911805496,  
 0.2216414584,1.4041283961\C,1.0849092379,0.0686926544,1.9497880102\  
 C,2.163796109,-0.2258551261,1.1313612133\C,1.9838008316,-0.3793214808,-  
 0.2359222554\C,0.7152363929,-0.2360631129,-0.7830976758\C,-1.3478616828,  
 0.5094236298,2.2658380539\C,-2.4246491904,1.2239751564,1.9362814418\N,-  
 1.1776050711,0.0286044192,3.5882930168\N,-2.174364796,-0.421672791,  
 4.1380496298\S,-1.8840019266,-0.9540549712,5.7711646072\O,-2.727781395,-  
 0.1109319645,6.5663304836\C,-0.2023849045,-0.6380020015,6.1098809961\  
 C,0.1715757783,0.6116097589,6.5869353008\C,1.5134892755,0.8799590285,6.781  
 8241441\C,2.48788604,-0.0783365008,6.5020637499\C,2.0832536851,-  
 1.3231780415,6.0214686804\C,0.7456560659,-1.610190664,5.8208241592\  
 C,3.9344706964,0.215629259,6.7380809396\O,-2.1215555564,-2.3683610874,

5.7168038398\ S,-3.2992917264,-2.2688491163,0.9335810909\ C,-2.6560349462,-  
 3.6276104719,1.4883759173\ C,-3.2612330104,-4.8876571854,2.0993611214\ C,-  
 1.8345781551,-5.4550422714,2.0961469537\ O,-1.3716455273,-6.5205678476,  
 2.3820245639\ C,-1.2249349751,-4.1504054234,1.5625042898\ C,-0.3857908571,-  
 3.4392378804,2.6212280557\ C,-0.4917301033,-4.2392292718,0.2351754444\ C,-  
 3.85561757,-4.6758533212,3.4872761568\ C,-4.2256615438,-5.6236465134,  
 1.1800451171\ H,1.226537436,0.1809608327,3.0173953685\ H,3.1502882862,-  
 0.3382899551,1.5660018453\ H,2.8272944073,-0.6175932774,-0.8732671315\ H,  
 0.5643012364,-0.3692970681,-1.8479924868\ H,-1.3602201494,0.1261718928,-  
 0.3931660206\ H,-3.2180511227,1.3842828218,2.6547750291\ H,-2.5056791156,  
 1.6938836335,0.9653691932\ H,2.8289251802,-2.0779524919,5.7984638385\ H,  
 0.436396839,-2.5777547578,5.4475705594\ H,-0.5818939663,1.3589632131,  
 6.8011233281\ H,1.8133872703,1.8528029859,7.1547894055\ H,4.2054653362,-  
 0.021454428,7.7714684743\ H,4.5727875118,-0.3816516642,6.086023189\ H,  
 4.1558472995,1.271539881,6.5768401615\ H,-4.0920540332,-5.6431198505,  
 3.9349585329\ H,-3.1773298363,-4.137657595,4.1504993814\ H,-4.7760678444,-  
 4.0948928793,3.3981121824\ H,-4.4834813576,-6.5906711799,1.6159692735\ H,-  
 5.1372475769,-5.0336611728,1.0649932203\ H,-3.7969792257,-5.7913671828,  
 0.1903595789\ H,0.4484468598,-4.7781612583,0.3675562592\ H,-1.0848782869,-  
 4.7541867748,-0.5223070989\ H,-0.2697701205,-3.2315258554,-0.1235779352\ H,  
 0.5332132164,-4.0033113335,2.7934554898\ H,-0.1239749269,-2.4410477522,  
 2.2670496469\ H,-0.920892,-3.3444211313,3.5670076164\ \ Version=ES64L-  
 G16RevB.01\ HF=-2022.4029297\ RMSD=7.295e-09\ RMSF=2.959e-06\ Dipole=  
 2.7840968,1.4811968,-1.0515384\ Quadrupole=10.6478831,-8.856214,-1.791669,-  
 4.0958863,33.2380452,16.3447583\ PG=C01[X(C23H26N2O3S2)]\ \@

### TS1 for zwitterionic intermediate Z for 9q

HF=-2022.3926436 a.u.(1, -214.2616cm<sup>-1</sup>)

1\1\GINC-R08N33\FTS\RPBE1PBE\def2TZVP\C23H26N2O3S2\

WURTHWE\08-Mar-2021\0\ \# pbe1pbe/def2tzvp

opt=(ts,noeigentest,calcfc,maxstep=6) freq pop= nbo emp=gd3bj nosym

scrf=(solvent=dichloromethane)\ \ TS1 for zwitterionic intermediate Z for 9q

\ \ 0,1\ C,-0.0289386837,0.1557780445,-0.0220291722\ C,-0.0156276805,  
 0.0562964413,1.3744100637\ C,1.2238597291,0.0001162567,2.018217604\ C,  
 2.4045186255,0.0387124653,1.2944225302\ C,2.3778300349,0.1320202085,-  
 0.0898252278\ C,1.1529217024,0.1896455467,-0.7414670514\ C,-1.2746411067,  
 0.0304800749,2.1299794558\ C,-1.3574732985,-0.0221207301,3.5129439394\ N,-  
 2.410132941,0.129786665,1.3710237013\ N,-3.5053459039,0.2723664896,  
 1.9626309728\ S,-4.836920099,0.262011919,0.9053612107\ O,-5.3434185038,-  
 1.0841325397,0.9106903023\ C,-4.2215626646,0.6529432296,-0.6862800574\ C,-  
 4.0646641939,1.9844663034,-1.0452132337\ C,-3.5021688174,2.2895573082,-  
 2.2715948568\ C,-3.0889475854,1.2834438328,-3.1441527535\ C,-3.2575115086,-

0.0456290943,-2.7578574086\ C,-3.8179244953,-0.36821229,-1.5350142791\ C,-  
2.5005052941,1.6219196827,-4.4767197733\ O,-5.6872228397,1.3226649548,  
1.3752614038\ S,-1.258897507,2.2197801082,3.890443179\ C,-2.6833405282,  
2.847771045,4.2991004609\ C,-3.7697237952,2.5156100726,5.3165784893\ C,-  
4.6609730725,1.3186196632,5.0125334368\ C,-3.3375309759,4.1504761646,  
3.8491522599\ C,-3.8761988155,4.0933779287,2.4222436844\ C,-2.5152224822,  
5.4077350053,4.0885377978\ C,-4.4025671971,3.858353966,4.9149691218\ O,-  
5.3603150118,4.4576754526,5.3038147282\ C,-3.2573000094,2.4797505945,  
6.7523553514\ H,-0.9794425779,0.2077502282,-0.5369850745\ H,1.1160076282,  
0.2654175271,-1.8224824536\ H,3.3022412294,0.1612680934,-0.6545442804\ H,  
3.3524492793,-0.0052239161,1.81834876\ H,1.2807202165,-0.0727472107,  
3.097405701\ H,-2.3248645878,-0.2129387341,3.9567972372\ H,-0.499261765,-  
0.2897081381,4.1115241671\ H,-3.3776088138,3.3281405642,-2.5573953416\ H,-  
4.3818932834,2.7695177463,-0.3705322186\ H,-3.9404915552,-1.4005974042,-  
1.2336635638\ H,-2.937819294,-0.8395972834,-3.4236787796\ H,-3.285929046,  
1.6784915764,-5.2366236664\ H,-1.9963391049,2.5888884874,-4.4540176941\ H,-  
1.7877035638,0.8619149607,-4.799822548\ H,-5.5395417869,1.3662418422,  
5.6590924694\ H,-4.9848830022,1.3008618567,3.9729972596\ H,-4.1303733278,  
0.3890312764,5.2256166757\ H,-4.105427871,2.453663906,7.4390918655\ H,-  
2.6558948327,1.5808908709,6.9026374639\ H,-2.6431954131,3.3498231351,  
6.9896086462\ H,-3.1359886106,6.2885064229,3.914669096\ H,-2.1257715657,  
5.4515429361,5.1069134783\ H,-1.6723520409,5.4325049979,3.3946172598\ H,-  
4.4697840484,4.9881188652,2.224243932\ H,-3.0358733013,4.0660890431,  
1.7247500529\ H,-4.4977575478,3.2138769575,2.2532510245\ \ Version=ES64L-  
G16RevB.01\ HF=-2022.3926436\ RMSD=3.792e-09\ RMSF=1.220e-06\ Dipole  
=3.1835734,0.8323929,-0.4054359\ Quadrupole=-40.8176163, 7.3823372,  
33.4352792,2.5626379,17.5241849,-5.0687835\ PG=C01[X(C23H26N2O3S2)]\ \@

### Zwitterionic intermediate Z for 9q

HF=-2022.403018 a.u (0)

1\1\GINC-

R08N08\FOpt\RPBE1PBE\def2TZVP\C23H26N2O3S2\WURTHWE\08-  
Mar-2021\0\ \# pbe1pbe/def2tzvp opt=(maxstep=8) freq pop=nbo emp=gd3bj  
nosym scrf=(solvent=dichloro methane)\ \ zwitterionic Z intermediate for 9q  
\ \ 0,1\ C,0.2241311216,-0.2845436396,0.1860900077\ C,0.1718881995,-  
0.1396020681,1.580138702\ C,1.367847311,-0.2544976798,2.2949663881\ C,  
2.5662608183,-0.5133366915,1.645320864\ C,2.600434209,-0.6634327006,  
0.2683023699\ C,1.4183381812,-0.5476095398,-0.4562158878\ C,-1.1075751202,  
0.1269773546,2.2409650834\ C,-1.1814847584,0.5875190003,3.6464511286\ N,-  
2.2018621999,0.0497267685,1.5210757987\ N,-3.3314016811,0.3992257353,  
2.0779556533\ S,-4.592625888,0.0990457833,1.0595097932\ O,-4.7966901939,-  
1.323955924,0.9195168759\ C,-4.1461245587,0.7237423182,-0.5271250426\ C,-

4.4673141706,2.0291408698,-0.8674223497\ C,-4.0680078316,2.5325360996,-  
2.0946662446\ C,-3.3433247589,1.7507182409,-2.9912296459\ C,-3.0344617827,  
0.4399720636,-2.6286534226\ C,-3.4324251649,-0.0779353367,-1.4090030042\ C,-  
2.9321752468,2.2909250329,-4.3249003693\ O,-5.6918154107,0.885856802,  
1.568755769\ S,-1.2940686796,2.4010741207,3.3803173459\ C,-2.7693431608,  
2.8483809857,3.878814983\ C,-3.7297904395,2.4482440303,4.9977150115\ C,-  
4.7106234205,1.3026598089,4.7953931682\ C,-3.4638434841,4.1596517503,  
3.5701352955\ C,-4.2638818243,4.061984921,2.2648165301\ C,-2.639430569,  
5.4320336056,3.6332065994\ C,-4.3560677493,3.837787133,4.7771726356\ O,-  
5.2021988499,4.4477746985,5.355108792\ C,-3.0200554146,2.3411686538,  
6.348247011\ H,-0.6929484524,-0.1811021067,-0.3797221903\ H,1.4316862957,-  
0.6552472886,-1.535115897\ H,3.5370406656,-0.8645651789,-0.2382666956\ H,  
3.4779800215,-0.6007251609,2.2251934683\ H,1.379552025,-0.1549374053,  
3.3732068201\ H,-2.095475065,0.2676461182,4.1392757141\ H,-0.3089991954,  
0.389767216,4.2595900347\ H,-4.3242824844,3.5521580988,-2.3617919813\ H,-  
5.0367420833,2.6397326429,-0.1789089803\ H,-3.1953757229,-1.097366486,-  
1.1347643658\ H,-2.4725644276,-0.1845352112,-3.3151091707\ H,-3.655161625,  
2.0044488068,-5.0947939636\ H,-2.8782244803,3.3802823531,-4.3132097208\ H,-  
1.9609847579,1.8968703292,-4.6292673996\ H,-5.4729219521,1.3848033025,  
5.5730657396\ H,-5.1841800428,1.3315248764,3.8169669448\ H,-4.2119031839,  
0.3392801756,4.9009163355\ H,-3.7740125949,2.3469856479,7.1372037662\ H,-  
2.4643652562,1.4035957162,6.4063325272\ H,-2.3295384698,3.1679390827,  
6.5210371499\ H,-3.3060608052,6.2944031736,3.5845011006\ H,-2.0577859839,  
5.4931567152,4.5539272093\ H,-1.9556814139,5.4807785389,2.7830239474\ H,-  
4.9341458512,4.9209101299,2.2003996113\ H,-3.5707300095,4.0824013758,  
1.4221027483\ H,-4.8492061384,3.1435557178,2.2097827567\ \ Version=ES64L-  
G16RevB.01\ HF=-2022.403018\ RMSD=6.608e-09\ RMSF=3.921e-06\ Dipole  
=3.5402853,2.6993474,0.9847448\ Quadrupole=-45.1662667,10.4823557,  
34.683911,-10.6033122,13.9608596,4.6191774\ PG=C01[X(C23H26N2O3S2)]\ \@

## TS2 for zwitterionic intermediate Z for 9q

HF=-2022.4017695 a.u. (1, -67.9594cm<sup>-1</sup>)

1\1\GINC-R08N07\FTS\RPBE1PBE\def2TZVP\C23H26N2O3S2\  
WURTHWE\09-Mar-2021\0\ \# pbe1pbe/def2tzvp opt=(ts,noeigentest,  
calcf, maxstep=8) freq pop= nbo emp=gd3bj nosym scrf=(solvent=  
dichloromethane)\ \ TS2 for zwitterionic intermediate Z for 9q  
\ \ 0,1\ C,0.0015615338,-0.0254382252,0.0065343091\ C,0.0021954345,  
0.0094908559,1.4029771946\ C,1.2353222778,0.0499160322,2.0652715066\  
C,2.41986879,0.0700437448,1.3532071272\ C,2.4059955639,0.0394504897,-  
0.0368295444\ C,1.1918737129,-0.0091442707,-0.7046709262\ C,-1.2449580772,  
0.0236994719,2.1740990224\ C,-2.5139681211,-0.4866652631,1.6169219423\ S,-  
2.5622267017,-2.1058802845,2.4735792325\ C,-3.5341055788,-1.7926977236,



3.7637621598\ C,-4.9725908326,-1.2418344573,3.8551767177\ C,-5.2783856982,  
0.2032335966,4.2015134121\ N,-1.1790277467,0.4044620655,3.4246166971\ N,-  
2.274462605,0.3656385563,4.1501322484\ S,-1.9812734936,1.1523086363,  
5.5899367877\ O,-1.9232962275,2.5656853672,5.3079658866\ C,-0.3934212343,  
0.6732476658,6.1836285909\ C,0.745798686,1.2866001487,5.6723533444\ C,1.990  
5520945,0.8888022164,6.121574853\ C,2.1248817449,-0.1119558161,7.08548185\ C,  
0.9704718784,-0.6961535156,7.5973568457\ C,-0.2849851301,-  
0.3127953373,7.1511295883\ C,3.4809350972,-0.5366507063,7.5540140924\ O,-  
2.9839579685,0.6977332652,6.5218548525\ C,-3.7205474939,-2.7886583596,  
4.909159509\ C,-3.6735670648,-4.2570302164,4.4954224669\ C,-5.1400556274,-  
2.2209012752,5.0264762627\ O,-6.0524522792,-2.4573006697,5.7597813055\ C,-  
2.8646472727,-2.5487012032,6.1442441999\ C,-5.8053476632,-1.6888982487,  
2.6482229505\ H,1.2433515062,0.0605325749,3.1477463098\ H,3.3639646958,  
0.0992825484,1.8854660872\ H,3.3357160635,0.0490055498,-0.59354821\ H,  
1.1671694692,-0.0302080328,-1.7880491314\ H,-0.9317661321,-0.0434975126,-  
0.5430096862\ H,-3.3840516654,0.0892585003,1.923244648\ H,-2.5197292833,-  
0.6711184107,0.5484038641\ H,1.0527530615,-1.4607526476,8.3620528801\ H,-  
1.1758088022,-0.763492145,7.5667814988\ H,0.6480517292,2.070706208,  
4.934109018\ H,2.8784237125,1.3666060401,5.7209753439\ H,4.0629829521,  
0.3215510077,7.8983030599\ H,3.4127492503,-1.2555029808,8.3707749916\ H,  
4.0441223361,-1.0005366226,6.7395211072\ H,-6.3534815034,0.2788063065,  
4.3787253962\ H,-4.7479592284,0.5272464526,5.0920814997\ H,-5.0166525417,  
0.86697615,3.3774295857\ H,-6.8622305099,-1.5472648137,2.8797829446\ H,-  
5.5569746118,-1.0791313464,1.7774163809\ H,-5.6422195651,-2.7369215848,  
2.394194798\ H,-4.045208694,-4.8695831981,5.3185153378\ H,-4.2813633261,-  
4.456475001,3.611728314\ H,-2.6437603153,-4.5547283602,4.2856713756\ H,-  
3.1756834228,-3.2392483655,6.9301985494\ H,-1.8165941155,-2.7380061047,  
5.904081708\ H,-2.9691788555,-1.5273778648,6.502381812\ \ Version=ES64L-  
G16RevB.01\ HF=-2022.4017695\ RMSD=5.567e-09\ RMSF=7.490e-07\ Dipole=  
1.3792324,-2.9328151,-2.6242571\ Quadrupole=12.3477107,7.2039798,-  
19.5516905,10.6075505,38.2498962,-26.2548119\ PG=C01  
[X(C23H26N2O3S2)]\ \@

### 10q (from 1i and 7a)

HF=-2022.4613472 a.u. (0)

1\1\GINC-

R08N28\FOpt\RPBE1PBE\def2TZVP\C23H26N2O3S2\WURTHWE\ 16-  
Feb-202 0\0\ \# pbe1pbe/def2tzvp Opt=(maxstep=8,readfc) geom=check  
guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=dichloromethane)  
\ \ 10q NNS-Product\ \0,1\ C,0.1963029522,-0.048644251,0.4424462251\ C,-  
0.9660857791,0.310979988,1.1183812972\ C,-0.9707098434,1.3596244964,  
2.025222932\ C,0.205210784,2.0559588477,2.2544092895\ C,1.3862372443,1.7073

520676,1.6061275161\ C,1.3614105156,0.6472926005,0.6962804683\ S,-  
2.426328395,-0.6124962312,0.857418433\ O,-3.4918206082,-0.0200702284,1  
.6083425633\ C,2.6626662928,2.4349613349,1.883144789\ N,-2.1742917606,-  
2.1022493348,1.6012461088\ S,-2.4283374812,-2.1549777955,3.3195948637\ C,-  
1.0530860379,-3.2123077548,3.7859320152\ C,-1.0550650725,-4.4072079676,  
2.8428357168\ C,-0.9023962976,-4.004835045,1.4066899938\ N,-1.4075626932,-  
2.9436123174,0.8978523782\ C,-0.1074639018,-4.8467965063,0.4924763414\  
C,0.3410491976,-4.3397520426,-0.730600574\ C,1.0883173047,-5.1235334738,-  
1.589287446\ C,1.4007636039,-6.4353979432,-1.2498802227\ C,0.9538297779,-  
6.9526404401,-0.0447512089\ C,0.2082622048,-6.1650631546,0.8209707481\ O,-  
2.5736607452,-0.8853741292,-0.5369226145\ H,0.0932997843,-3.3204388487,-  
0.9974436076\ H,1.4339317742,-4.7093119571,-2.529465216\ H,1.9883028877,-  
7.0484663888,-1.9231971343\ H,1.1829583425,-7.976377047,0.2272901395\ H,-  
0.1406151724,-6.5983249005,1.7502639151\ H,-1.9794496961,-4.9734107593,  
2.9809946707\ H,-0.2379388901,-5.0775925163,3.1047248804\ H,0.2056066276,  
2.8808191411,2.9578930174\ H,-1.8849795567,1.6218211509,2.5410328282\  
H,0.1815850392,-0.8643030677,-0.2690477789\ H,2.2714655783,0.3683919605,  
0.1767185478\ H,3.1657473935,2.7132181008,0.9546760196\ H,2.4876254222,3.33  
80096221,2.4678260992\ H,3.35181511,1.7973219212,2.4443683888\ C,-  
1.1641514985,-3.6208759334,5.3120575362\ C,0.3808100031,-2.5918706144,  
4.0505780697\ C,0.3122033842,-3.2590674416,5.41624437\ O,1.1383890919,-  
3.4799661513,6.2561948036\ C,-2.0253129734,-2.7032323365, 6.1792242154\ C,-  
1.4958109058,-5.0669347168,5.6284827696\ C,0.4268714444,-1.076356197,  
4.1968901649\ C,1.5348378194,-3.0375511232,3.169167864\ H,-1.3763509313,-  
5.2315345975,6.7009138465\ H,-2.5339111332,-5.2867530438,5.3682711922\ H,-  
0.8484182051,-5.7747882967,5.1111317575\ H,-1.8235958091,-2.9175389488,  
7.2301952609\ H,-1.8303054619,-1.6440583312,6.0114027655\ H,-3.0851889368,-  
2.8949271997,5.9954118384\ H,2.468805821,-2.6667678097,3.5957500542\  
H,1.6207710229,-4.1207093922,3.0841834339\ H,1.4348848772,-2.617150687,  
2.1663254387\ H,1.3614642487,-0.7940071534,4.6858006771\ H,0.4027465641,-  
0.6110994304,3.2119441753\ H,-0.4011835329,-0.67420921,4.7779984827\ \\  
Version=ES64L-G16RevB.01\ HF=-2022.4613472\ RMSD=6.796e-09\ RMSF  
=1.921e-06\ Dipole=2.2441014,-0.359812,0.9538492\ Quadrupole=-15.5772539,  
19.4280143,-3.8507603,4.6139469,-12.5617994,0.186872\ PG=C01  
[X(C23H26N2O3S2)]\ \@

### TS for 9q

HF=-2022.3777236 a.u. (1, -270.4678 cm<sup>-1</sup>)

1\1\GINC-R08N39\FTS\RPBE1PBE\def2TZVP\C23H26N2O3S2\  
WURTHWE\08-Mar-2020\0\ \# pbe1pbe/def2tzvp Opt=(ts,noeigentest,  
readfc) geom=check guess=read freq pop=nbo emp=gd3bj nosym  
scrf=(solvent=dichloromethane)\ \ TS for 9q \ \ 0,1\C,0.1543957247,

0.0127801442,0.011184154\ C,0.0445979859,-0.1132782885,1.3897719241\  
C,1.1696384583,-0.2743197713,2.1885008843\ C,2.4169805701,-0.3055905764,  
1.5918686607\ C,2.5572884562,-0.1797542243,0.2101249264\ C,1.409810047,-  
0.0251919627,-0.5673169178\ S,-1.5270461534,0.0198556168,2.1396041853\ O,-  
2.5612197648,-0.3119595554,1.206141903\ C,3.9081455094,-0.2368699628,-  
0.4282046777\ N,-1.749743036,1.7160368535,2.4698979724\ N,-0.7043467638,  
2.2024029029,2.9723263662\ C,-0.6920354403,3.5452903394,3.2070136715\ C,-  
1.7380316906,4.3365926226,2.8094129571\ C,0.5583014146,4.0600643348,  
3.7848043368\ C,0.5709435048,5.2594142515,4.4964666879\ C,1.7534811312,  
5.7537554408,5.0215728123\ C,2.9394437128,5.0527233784,4.8509684199\  
C,2.9340628397,3.8514614469,4.1547675478\ C,1.754163599,3.357476677,3.62468  
14771\ O,-1.5008896616,-0.6040801879,3.4313507366\ C,-1.7932863584,  
4.2060262973,0.3864509591\ C,-0.4905384036,4.7777751977,-0.2228054907\  
C,0.2093067707,3.8616327993,-1.2103923201\ S,-2.3005498765,2.6424002979,  
0.3641665458\ C,-2.6431509042,5.434938234,-0.0598173788\ C,-3.8423221864,  
5.083849995,-0.9246879178\ C,-3.0318715917,6.492926928,0.9668911056\ C,-  
1.3936287119,5.845610156,-0.8444980712\ O,-1.2031331033,6.6840394946,-  
1.6782516373\ C,0.5258838827,5.4155969827,0.7172293115\ H,1.7506763829,  
2.4294898596,3.0668915077\ H,3.8565616657,3.2994478743,4.0167488001\  
H,3.8639277821,5.439335725,5.2636224535\ H,1.7469282558,6.6847698613,  
5.576087152\ H,-0.3538837273,5.7998616601,4.6615996846\ H,-2.7184541153,  
3.9057216153,2.674935054\ H,-1.6690632664,5.4074125584,2.921436408\  
H,1.5031091406,0.0720199972,-1.6432156434\ H,-0.7333063998,0.1443666062,-  
0.5929766592\ H,1.0615173858,-0.3711820886,3.2606749628\ H,3.2998707674,-  
0.4269392054,2.209600579\ H,4.6827100502,0.1261600705,0.2485369497\  
H,4.1600439397,-1.2685006974,-0.6924718953\ H,3.9384270763,0.3522248297,-  
1.3457569347\ H,-3.489879432,7.3341662999,0.4434564452\ H,-3.7626525499,  
6.0901084248,1.670706802\ H,-2.1779240857,6.8780794766,1.5237150673\ H,-  
4.2354410856,5.9889680624,-1.3913633457\ H,-3.5787369827,4.3709898334,-  
1.7076154638\ H,-4.6277047089,4.6397602554,-0.3099379319\ H,1.2191456814,  
6.0198057358,0.1287223444\ H,0.0646187032,6.0597713494,1.4653700848\  
H,1.0951028299,4.6431475549,1.2340378209\ H,0.9872541097,4.4150072912,-  
1.7399077457\ H,0.673968485,3.0297499884,-0.6765221959\ H,-0.4879342251,  
3.4474967109,-1.9401537301\ \ Version=ES64L-G16RevB.01\ HF=-2022.3777236\  
RMSD=9.033e-09\ RMSF=6.714e-07\ Dipole=2.5977032,1.9916079,0.0491534\  
Quadrupole=3.4290743,5.1399416,-8.5690159,-7.2158341,7.8784068,27.5120413\  
PG=C01[X(C23H26N2O3S2)]\ \@

# 11a

HF=-1202.6606138 a.u (0)

1\1\GINC-R09N16\FOpt\RPBE1PBE\def2TZVP\C16H18N2O1S1\  
WURTHWE\15-Feb-2020\0\# pbe1pbe/def2tzvp Opt=(maxstep=8,readfc)

```

geom=check guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=
dichloromethane)\ \ 11a product after elimination\ \ 0,1\ N,-2.2308542831,-
1.7656836403,2.2145857764\ C,-1.7594510288,-2.7011593463,3.2436393109\
S,0.0253164193,-2.5856728294,3.2386761334\ C,0.216719055,-2.9562793518,
1.5859664335\ C,-0.8086553503,-2.806735599,0.7074596305\ N,-1.8437772549,-
1.9442875894,1.0494184301\ C,-2.4022721241,-2.4492085777,4.6500778581\ C,-
3.5542644719,-1.4527716016,4.6426305398\ C,-2.394664322,-4.1571316192,
3.1842469872\ C,-3.5565680764,-4.2989887985,2.2064046944\ C,-0.7567319602,-
3.2586357711,-0.6852442877\ C,-1.4779676892,-2.6052328026,-1.6868416966\ C,-
1.4212514865,-3.0531274457,-2.9960387798\ C,-0.6476068534,-4.1574223644,-
3.3290993437\ C,0.0640034742,-4.8187958414,-2.3378285328\ C,0.0033684498,-
4.3789024319,-1.0255183397\ C,-2.8923110184,-3.8884713446,4.6005371354\ O,-
3.4465490007,-4.5853300782,5.4025251505\ C,-1.4611490274,-2.1663590307,
5.8092392251\ C,-1.4729492452,-5.3595756594,3.0993728146\ H,-2.0728003405,-
1.7385379624,-1.4289784304\ H,-1.982228757,-2.5329401789,-3.7640344297\ H,-
0.6064188067,-4.5055967469,-4.3545321338\ H,0.658305368,-5.6910425553,-
2.5843551045\ H,0.5338189989,-4.9223844667,-0.2515059254\ H,1.2139622147,-
3.2309175252,1.2637377493\ H,-4.1085923588,-5.2098631446,2.4455478852\ H,-
4.2487549901,-3.4578099189,2.2510491515\ H,-3.1855884959,-4.38001445,
1.1827004859\ H,-2.0309153893,-6.2476259023,3.4037986944\ H,-1.1203876884,-
5.5078109936,2.0776408671\ H,-0.6072582698,-5.263554096,3.755400814\ H,-
2.0235829156,-2.1982513865,6.7438765215\ H,-0.6552596307,-2.8994190487,
5.8812866622\ H,-1.0210763611,-1.1713267165,5.7105374472\ H,-4.0842585445,-
1.5235079648,5.5943071556\ H,-3.1714204515,-0.4375283786,4.5268027843\ H,-
4.2616988424,-1.6364867768,3.834626449\ \ Version=ES64L-G16RevB.01\ HF=-
1202.6606138\ RMSD=5.862e-09\ RMSF=1.475e-06\ Dipole=1.1444287,-0.382703
,-0.6216292\ Quadrupole=-3.5533183,4.4433261,-0.8900078,-10.9119578,
10.0066762,11.4132912\ PG=C01[X(C16H18N2O1S1)]\ \@

```

### ***p*-Tolyl sulfinic acid 12**

HF=-819.7609899 a.u (0)

1\1\GINC-

R09N16\FOpt\RPBE1PBE\def2TZVP\C7H8O2S1\WURTHWE\15-Feb-

2020\0\ \# pbe1pbe/def2tzvp Opt=(maxstep=8,readfc) geom=check

guess=read Pop=N BO Freq emp=gd3bj nosym scrf=(solvent=

dichloromethane)\ \ 12: pTol-Sulfinic acid\ \ 0,1\ C,-0.0075143323,-

0.1453753017,-0.1268213732\ C,-0.0509764712,-0.3349947177,1.2493367372\

C,1.1199325555,-0.2550758852,1.978650675\ C,2.3424315096,0.0015083206,

1.3531617243\ C,2.3587632993,0.1717748581,-0.0275218028\ C,1.191617028,

0.0918170657,-0.7734373072\ H,-0.9939528978,-0.5323169522,1.7467572375\

H,1.0901866089,-0.394595506,3.0540337023\ C,3.599983543,0.0943238805,

2.1589252197\ H,3.300464604,0.3660119977,-0.5293147894\ H,1.199713315,

0.220669182,-1.849069481\ S,-1.4896194071,-0.3239173212,-1.092899062\ O,-  
 2.245012295,0.9460037278,-0.3787344754\ O,-1.1315137152,0.0499358583,-  
 2.4655638099\ H,-3.1977793453,0.8122262222,-0.4790439926\ H,4.4780185693,  
 0.1718059602,1.517415583\ H,3.5780587206,0.9726834001,2.8100338059\  
 H,3.7193477623,-0.7799847894,2.8030214173\ \ Version=ES64L-G16RevB.01\  
 HF=-819.7609899\ RMSD=3.994e-09\ RMSF=1.565e-06\ Dipole=0.2165909,-  
 0.2928595,1.7205771\ Quadrupole=11.0546291,-5.2740712,-5.7805579,  
 0.6259801,-0.3715821,-0.3506783\ PG=C01[X(C7H8O2S1)]\ \@

### TS for 1i+7a (NNC), Addition to C=O bond

HF=-2022.3688762 a.u. (1, -297.9983cm<sup>-1</sup>)

1\1\GINC-

R08N27\ FTS\ RPBE1PBE\ def2TZVP\ C23H26N2O3S2\ WURTHWE\ 12-Mar-  
 2020\0\ \ # pbe1pbe/def2tzvp Opt=(ts,noeigentest,readfc) geom=check  
 guess=read scrf=(solvent=dichloromethane) freq pop=nbo emp=gd3bj  
 nosym\ \ TS for 1i+7a (NNC) (C=O-addition)\ \ 0,1\ C,-0.3156714279,-  
 0.2369831923,0.2381909757\ C,-0.248970395,-0.0280513028,1.6226719981\  
 C,1.0178639869,0.1322247095,2.1932391264\ C,2.1655995574,0.0911175181,1.416  
 0596492\ C,2.0837492659,-0.115333575,0.0473263408\ C,0.8320093282,-  
 0.2811387859,-0.5330544704\ C,-1.4805217656,0.0268468702,2.418878488\ N,-  
 2.6334566437,-0.1020926142,1.7684894327\ N,-3.7201234314,0.060114408,  
 2.4315328821\ S,-5.0896097496,-0.0320616643,1.4993075081\ O,-6.0193269882,-  
 0.8651431785,2.218944171\ C,-4.6446739952,-0.8163968849,-0.01004644\ C,-  
 4.2367010037,-0.0489674698,-1.091278438\ C,-3.8213916252,-0.678675174,-  
 2.2514538185\ C,-3.8047765758,-2.0692132944,-2.3487139349\ C,-4.2190016627,-  
 2.8176954194,-1.2481817648\ C,-4.6353990818,-2.2016850746,-0.0806786662\ C,-  
 3.376590186,-2.7421347556,-3.614581926\ O,-5.5094308065,1.3192971305,  
 1.2005805008\ C,-1.5023355624,0.188180751,3.8335263319\ O,-2.1193714978,  
 1.6712539861,4.3751688246\ C,-2.3594637074,2.6731805647,3.714845698\ C,-  
 3.1876691202,3.8532639038,4.1568334797\ C,-2.9367772817,4.421677597,  
 5.5390786841\ C,-1.8672185071,3.3511036507,2.4331113767\ C,-2.3732719148,  
 2.9170272141,1.0632039928\ C,-2.5954798199,4.58977259,2.9659877146\ S,-  
 2.6672107465,6.1042405853,2.4630828235\ C,-0.3475016636,3.5247366527,  
 2.440728\ C,-4.675288466,3.5360746048,3.922766559\ H,-1.2869941197,-  
 0.366672565,-0.2230368552\ H,0.7474362181,-0.444243378,-1.6019249016\  
 H,2.9811773886,-0.1471732734,-0.5590099801\ H,3.1321033337,0.2219204662,  
 1.8897070702\ H,1.1254014904,0.3006571318,3.2580804782\ H,-2.2896578122,-  
 0.3667958563,4.3353790744\ H,-0.5640949632,0.1891104087,4.3728399477\ H,-  
 3.499022593,-0.0808752606,-3.0971896671\ H,-4.2450450379,1.031103801,-

1.0182613274\H,-4.9515774927,-2.7880662469,0.7731617354\H,-4.211007946,-  
3.90067556,-1.3065377187\H,-4.2318339719,-2.8800180223,-4.2832676307\H,-  
2.6364138806,-2.1455619188,-4.1499239487\H,-2.9537928556,-3.7280589716, -  
3.4164612367\H,-5.2312528103,4.473158939,3.9767600642\H,-4.8600071492,  
3.0680432813,2.9550557485\H,-5.0214903751,2.8593862294,4.7051693342\H,-  
3.4914196072,5.3552593949,5.6442094519\H,-3.2846155782,3.7213713319,  
6.2996603367\H,-1.8785039615,4.6274172419,5.7043704626\H,-  
0.0986880932,4.3026501027,1.7168081618\H,0.031618421,3.8308025984,  
3.41717501\H,0.1358434978,2.5937768693,2.1451726214\H,-2.225026711,  
3.7631348248,0.3889618552\H,-1.8046985851,2.0659733604,0.6934798237\H,-  
3.4312493576,2.659109 4997,1.0772297377\ \ Version=ES64L-G16RevB.01 \ HF=-  
2022.3688762 \ RMSD=3.754e-09 \ RMSF=1.560e-06 \ Dipole=3.1721972,  
0.7674747,0.5960845 \ Quadrupole=-41.008038,7.162435,33.8456029,0.1041996,  
12.2149359,18.6685396 \ PG=C01[X(C23H26N2O3S2)] \ \ @

### 1i+7a (NNC) Addition to C=O bond

HF=-2022.4348601 a.u. (0)

1\1\GINC-R09N18\FOpt\RPBE1PBE\def2TZVP\C23H26N2O3S2\  
WURTHWE\15-Feb-2020\0\ \ # pbe1pbe/def2tzvp Opt=(maxstep=8,readfc)  
geom=check guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=  
dichloromethane) 1i+7a (NNC) C=O addition \ \ 0,1\C,0.0240293644,-  
0.0546454234,0.1430489388\C,0.118977292,0.0681915276,1.5294045243\  
C,1.3662580742,0.3097544606,2.1078509769\C,2.4939891244,0.4198656507,1.315  
0179601\C,2.3930674881,0.2894078099,-0.0648155765\C,1.157251095,  
0.0507003886,-0.6476694939\C,-1.0709541227,-0.0743758153,2.3803671912\C,-  
2.4185104161,0.0636644431,1.735389312\O,-3.4967883499,0.1886867833,  
2.6385118197\C,-3.0927979851,0.4850999548,3.9484930475\N,-2.0775220134,-  
0.448070796,4.3832602867\N,-0.8870274771,-0.3529022011,3.6175111789\S,-  
2.3869021786,-2.0812767819,4.6592242854\O,-1.2436448475,-2.5693034209,  
5.3671982892\C,-4.3584355793,0.7726702734,4.8361544484\C,-5.6944883224,  
0.3250862806,4.277914628\C,-2.6560198629,2.0040611601,4.1224386619\C,-  
2.3710843288,2.8335200768,2.8825088225\O,-3.6906881579,-2.1767076228,  
5.2409856544\C,-4.270993088,0.4313075337,6.3289631521\C,-4.038757952,  
2.240997975,4.681607301\S,-4.8835434216,3.5776068171,4.966176258\C,-  
1.567669299,2.2496028494,5.1637848907\C,-2.4331785476,-2.8511488218  
,3.0825650199\C,-1.2488403998,-3.2270331027,2.4612409129\C,-1.2958444959,-  
3.7607771756,1.1861865073\C,-2.5100936561,-3.9353089075,0.5232097509\C,-  
3.685862666,-3.5658283341,1.1764177085\C,-3.6564808301,-3.0226548818,  
2.4481585951\C,-2.5515068141,-4.5314259708,-0.8473923853\H,1.4333076319,  
0.4142840677,3.1831824509\H,3.4567368237,0.6133105664,1.7731607775\  
H,3.2775219061,0.3775130205,-0.6848393052\H,1.0731750875,-0.0547116896,-

1.7226959517\H,-0.9304570301,-0.2526434113,-0.3290104639\H,-2.4091054177,  
0.9078957805,1.0411968888\H,-2.5920739925,-0.8429001962,1.1442386772\H,-  
4.638787999,-3.69946924,0.6766424982\H,-4.5695498289,-2.7229571331,  
2.9453082431\H,-0.3039508799,-3.0875215499,2.9701513961\H,-0.3720180293,-  
4.0418684943,0.6930593335\H,-2.612327823,-5.6222657459,-0.7854782379\H,-  
3.4227676744,-4.1857874258,-1.4050824829\H,-1.6516025527,-4.2864000738,-  
1.4132229741\H,-1.5481987695,3.3136700384,5.4064658264\H,-1.7237690217,  
1.6882272307,6.0820536903\H,-0.59739725,1.9647217477,4.7530891896\H,-  
2.4096969856,3.8868033873,3.1671562947\H,-1.3756096276,2.6303218418,  
2.4833572093\H,-3.1186402297,2.6748558949,2.1057495395\H,-6.492036255,  
0.7791903563,4.869002363\H,-5.8193967582,0.6220880784,3.2379576454\H,-  
5.7804807333,-0.7596735173,4.3529940972\H,-4.9217168228,1.1243717817,  
6.8656925469\H,-4.6098211739,-0.5857020301,6.5020181391\H,-3.2628709178,  
0.527192421,6.7278380275\ \ Version=ES64L-G16RevB.01\HF=-2022.4348601\  
RMSD=6.425e-09\RMSF=5.811e-07\Dipole=1.1140665,-0.476779,-3.9719059\  
Quadrupole=12.1853576,9.9589874,-22.1443451,11.8348811,20.2091236,  
11.8607859\PG=C01[X(C23H26N2O3S2)]\ \@

### TS for 1i+7a (NNO) Addition to C=O bond

HF=-2022.3565188 a.u. (1, -429.2590 cm<sup>-1</sup>)

1\1\GINC-R09N13\FTS\RPBE1PBE\def2TZVP\C23H26N2O3S2\  
WURTHWE\10-Mar-2020\0\ \ # pbe1pbe/def2tzvp Opt=(ts,noeigentest,  
readfc) geom=check guess=read scrf=(solvent=dichloro methane) freq pop=nbo  
emp=gd3bj nosym\ \ TS for 1i+7a (NNO)-C=O-addition\ \ 0,1\C,-0.2450818418,  
0.488521147,0.2944945644\C,-0.2956089825,0.2544557146,1.6721042834\  
C,0.8951802821,0.2263939662,2.4014557929\C,2.107587385,0.4402676683,  
1.7704378115\C,2.148114487,0.6814662446,0.4032821511\C,0.9696544364  
,0.7015572492,-0.3317890287\C,-1.5733094329,0.0281962112,2.3386915411\C,-  
1.858539831,0.3232380369,3.6665554228\C,-3.2102707354,1.7133870738,  
3.6780667982\O,-4.1624999849,1.2617713536,2.9987419059\N,-3.6671980283,-  
0.655789119,2.0948976323\N,-2.6045077081,-0.3371766108,1.5257216452\S,-  
4.9780197107,-0.8204484637,0.9543564867\O,-4.726622602,-2.08536266,  
0.3229846042\C,-3.3881822398,2.0952763788,5.2081685357\C,-2.7010535383,  
3.3977757598,4.8625296812\S,-2.2461837151,4.6465330277,5.7699301151\C,-  
2.5477584994,3.1171421974,3.3818115186\C,-1.1213521406,3.2387067569,  
2.8846324987\C,-4.7706402672,0.4728325269,-0.1972029737\C,-5.3389285406,  
1.7120291104,0.0656221912\C,-5.1313155816,2.7455239409,-0.8291530082\C,-  
4.3540696499,2.5642848424,-1.9727817332\C,-3.7987591655,1.3075325233,-  
2.2125600043\C,-3.9994981406,0.2597281317,-1.3328799279\C,-4.1018917087,  
3.7011527814,-2.9106444642\O,-6.1658470736,-0.6287543517,1.7256522773\C,-  
4.8698924431,2.28926716,5.5210426076\C,-2.7312882346,1.3097952546,  
6.3268878065\C,-3.466372388,3.9765440112,2.5192773459\H,-1.1687032579,

0.5251103947,-0.26884541\H,0.9981764753,0.8931193499,-1.3979132319\  
H,3.0984255348,0.8504029356,-0.089352876\H,3.0256063437,0.409968862,  
2.3449250679\H,0.8742635352,0.0116292495,3.4632424755\H,-2.584626994,-  
0.3247586279,4.1471700188\H,-1.0528252889,0.6940297959,4.2826974167\H,-  
5.5787619147,3.7142512556,-0.636527041\H,-5.9279264646,1.8566810078,  
0.9610429269\H,-3.5724803598,-0.7166271766,-1.5212146697\H,-3.2030717087,  
1.1480399459,-3.104416704\H,-3.2021381606,4.247107467,-2.6102159802\H,-  
3.9450570563,3.3480903743,-3.9306300213\H,-4.9306480784,4.4102308906,-  
2.9072566783\H,-2.9314668293,1.810623151,7.2764183402\H,-3.1527611109,  
0.3032767494,6.3814529739\H,-1.6497702271,1.2361247074,6.2187510017\H,-  
4.9750891745,2.7934527969,6.4834856914\H,-5.3768649865,2.8782143754,  
4.7570838456\H,-5.3580755029,1.3145131452,5.5740065111\H,-0.8196110345,  
4.2874447127,2.9351340631\H,-0.4146321689,2.662225074,3.480653441\H,-  
1.0522245231,2.9116181957,1.8462768149\H,-3.118108866,5.0111520744,  
2.5362499495\H,-3.4433088989,3.6097855966,1.4915107518\H,-4.500060528,  
3.9474152343,2.863634811\ \ Version=ES64L-G16RevB.01\HF=-2022.3565188  
\RMSD=5.076e-09\RMSF=1.936e-06\ Dipole=2.8835817,1.5579383,-1.3127246\  
Quadrupole=-16.5669721,1.2203163,15.3466558,-18.0215084,15.573721,-  
16.1694893\PG=C01[X(C23H26N2O3S2)]\ \@

### 1i+7a (NNO) Addition to C=O bond

HF=-2022.4016417 a.u. (0)

1\1\GINC-R10N25\FOpt\RPBE1PBE\def2TZVP\C23H26N2O3S2\  
WURTHWE\15-Feb-2020\0\ \# pbe1pbe/def2tzvp Opt=(maxstep=8,readfc)  
geom=check guess=read Pop=NBO Freq emp=gd3bj nosym scrf=(solvent=  
dichloromethane)\ \ 1i+7a (NNO) C=O-addition\ \0,1\C,0.0313834557,  
0.2962213103,-0.0383348507\C,-0.0423329156,-0.2452671108,1.2444477936\  
C,1.0540727346,-0.9502587473,1.7470967699\C,2.1989505418,-1.0994289557,  
0.9862379683\C,2.2667728448,-0.5501472123,-0.2887347664\C,1.1816263003,  
0.1480989125,-0.7973314564\C,-1.2447940042,-0.0839696527,2.0669801727\C,-  
2.5826436282,0.2655933689,1.5115590931\C,-3.6462535201,-0.6714882297,  
2.0653813998\O,-3.327603418,-0.9835451359,3.4063557984\N,-2.3620648435,-  
0.0919729976,3.9663366264\N,-1.1440238886,-0.2170654728,3.3400328183\S,-  
2.2410652317,-0.5329975449,5.6199551594\O,-1.1971362581,0.3020142092,  
6.1249000766\C,-5.1351299465,-0.2280887091,1.8245778051\C,-5.3759897003,  
1.1174892009,1.1633367191\C,-3.9151703002,-1.9877108788,1.2495723585\C,-  
3.0136792441,-2.2889255145,0.0648309286\C,-1.7297634061,-2.1994772388,  
5.6057314177\C,-0.3751034869,-2.494862912,5.5093648082\C,0.0166604452,-  
3.8180345383,5.4210611203\C,-0.9219900969,-4.8496347632,5.4261258654\C,-  
2.2742126206,-4.5232196712,5.5226132365\C,-2.6862280978,-3.2062863116,  
5.609414885\C,-0.4855272335,-6.2781377669,5.3569479672\O,-3.572436403,-  
0.4309393072,6.1288653473\C,-5.2695595922,-1.4142672799,0.8942960159\S,-



6.4075498817,-1.867897503,-0.1469729721\ C,-6.0153324008,-0.3673117243,  
 3.0621474648\ C,-4.0434858001,-3.2368502346,2.1195628019\ H,0.9860779407,-  
 1.38889245,2.7348316044\ H,3.0408103133,-1.6541966927,1.3836937146\  
 H,3.16271523,-0.6719394373,-0.8861533053\ H,1.2291043733,0.5804934239,-  
 1.7896992553\ H,-0.8026715068,0.854360593,-0.445742624\ H,-2.8139319676,  
 1.2742144974,1.8740200572\ H,-2.6054516051,0.2870652468,0.4275583868\ H,-  
 3.0157600741,-5.3143073383,5.5246651988\ H,-3.7360321169,-2.9533264128,  
 5.6779025297\ H,0.35330562,-1.6949302804,5.5061529307\ H,1.0716765214,-  
 4.0568667138,5.3457610198\ H,-0.3205719782,-6.6739731194,6.3637632051\ H,-  
 1.2428858107,-6.9018616565,4.8803589697\ H,0.4511396843,-6.3809786583,  
 4.8075382528\ H,-6.4255658238,1.1902809945,0.8720889526\ H,-5.1577836697,  
 1.929869473,1.8602761962\ H,-4.7720545189,1.2539797401,0.2652095596\ H,-  
 7.0609541579,-0.2543649842,2.7702655681\ H,-5.8945374308,-1.3302459972,  
 3.5557479574\ H,-5.7604791635,0.4131485532,3.7814436877\ H,-3.393437385,-  
 3.1666987041,-0.4609160593\ H,-2.9741894305,-1.4691959773,-0.653035192\ H,-  
 1.9988015436,-2.5066795888,0.4059733657\ H,-4.4617278308,-4.0430329387,  
 1.5143742361\ H,-3.0586684487,-3.5363113495,2.4817384512\ H,-4.6868766309,-  
 3.0842966682,2.9845304238\ \ Version=ES64L-G16RevB.01\ HF=-2022.4016417\  
 RMSD=4.146e-09\RMSF=7.846e-07\ Dipole=1.6579838,-1.7724789,-1.8736575\  
 Quadrupole=-5.7278046,28.4256563,-22.6978518,-5.5570527,7.2912398,-  
 26.0708373\ PG=C01[X(C23H26N2O3S2)]\ \@

#### 4. References

- [1] Gaussian 16, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B.G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, V.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, V.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2016.
- [2] Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **1993**, *98*, 5648–5652.

- [3] Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **1988**, *37*, 785–789.
- [4] Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* **2011**, *32*, 1456–1465.
- [5] Grimme, S.; Hansen, A.; Brandenburg, J. G.; Bannwarth, C. Dispersion-corrected mean-field electronic structure methods. *Chem. Rev.* **2016**, *116*, 5105–5154.
- [6] Perdew, J. P.; Burke, K.; Ernzerhof, M. Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1996**, *77*, 3865–3868.
- [7] Perdew, J. P.; Burke, K.; Ernzerhof, M. Errata: Generalized gradient approximation made simple. *Phys. Rev. Lett.* **1997**, *78*, 1396.
- [8] Adamo, C.; Barone, V. Toward reliable density functional methods without adjustable parameters: The PBE0 model. *J. Chem. Phys.* **1999**, *110*, 6158–6169.
- [9] Ernzerhof, M.; Scuseria, G. E. Assessment of the Perdew-Burke-Ernzerhof exchange-correlation functional. *J. Chem. Phys.* **1999**, *110*, 5029–5036.
- [10] Weigend, R.; Ahlrichs, R. Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: Design and assessment of accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297–3305.
- [11] Tomasi, J.; Mennucci, B.; Cammi, R. Quantum Mechanical Continuum Solvation Models. *Chem. Rev.* **2005**, *105*, 2999–3093.