

## **SUPPORTING INFORMATION**

# Regioselective Synthesis of Enantiopure 1,2- and 1,3-Dispirooxindoles along with DFT Study

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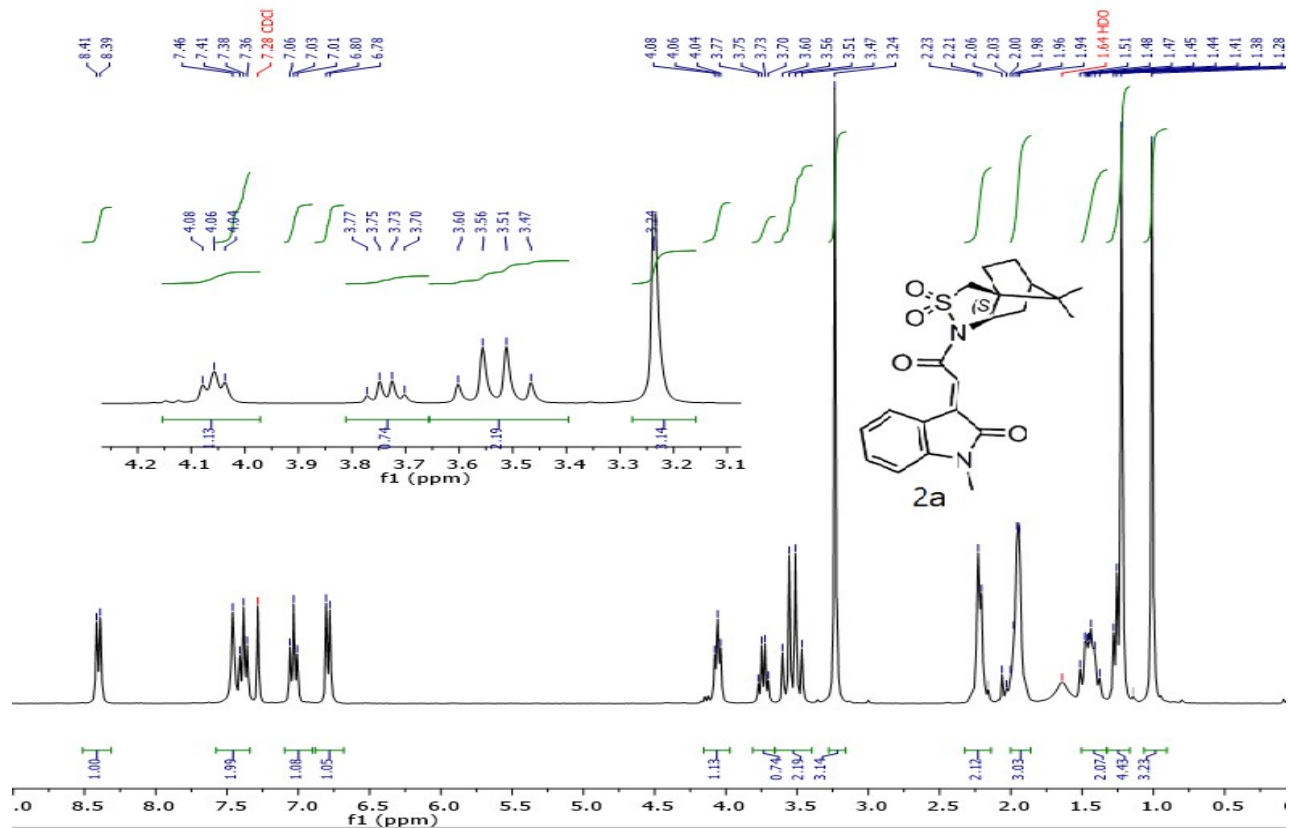
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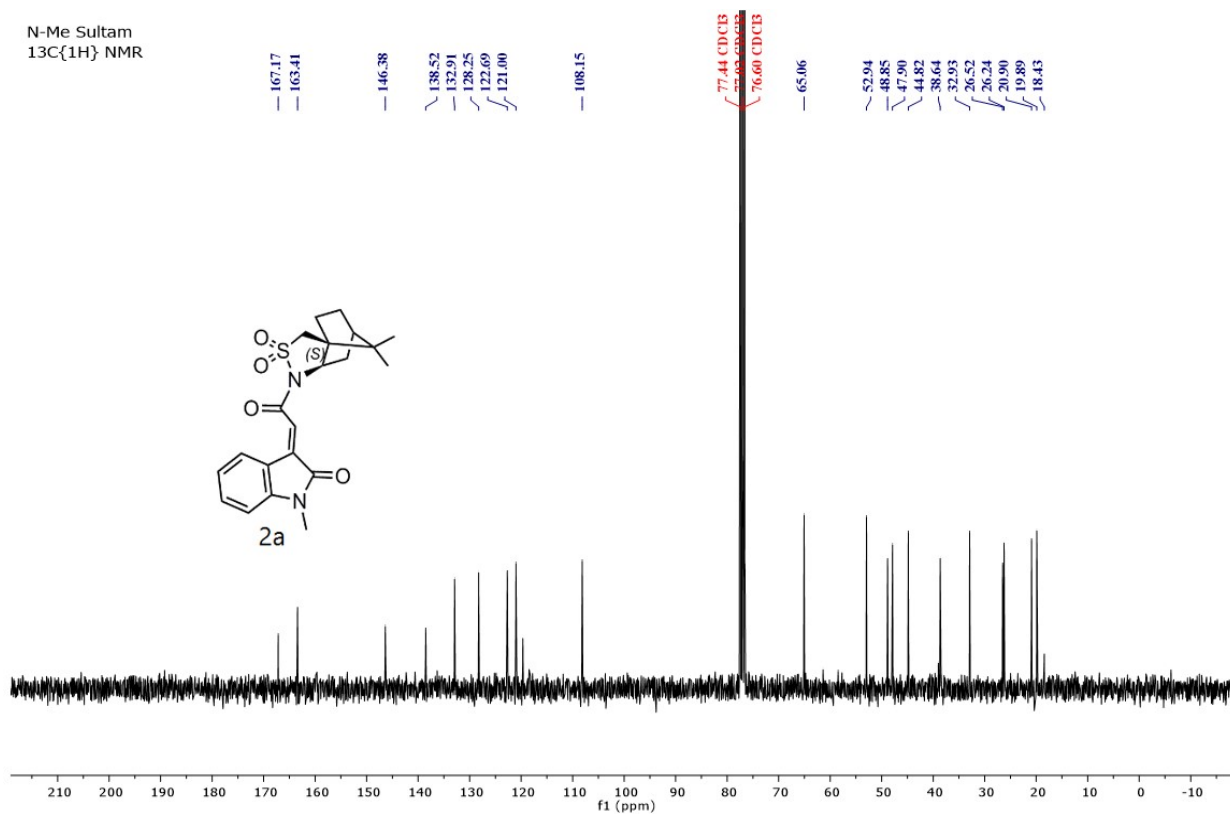
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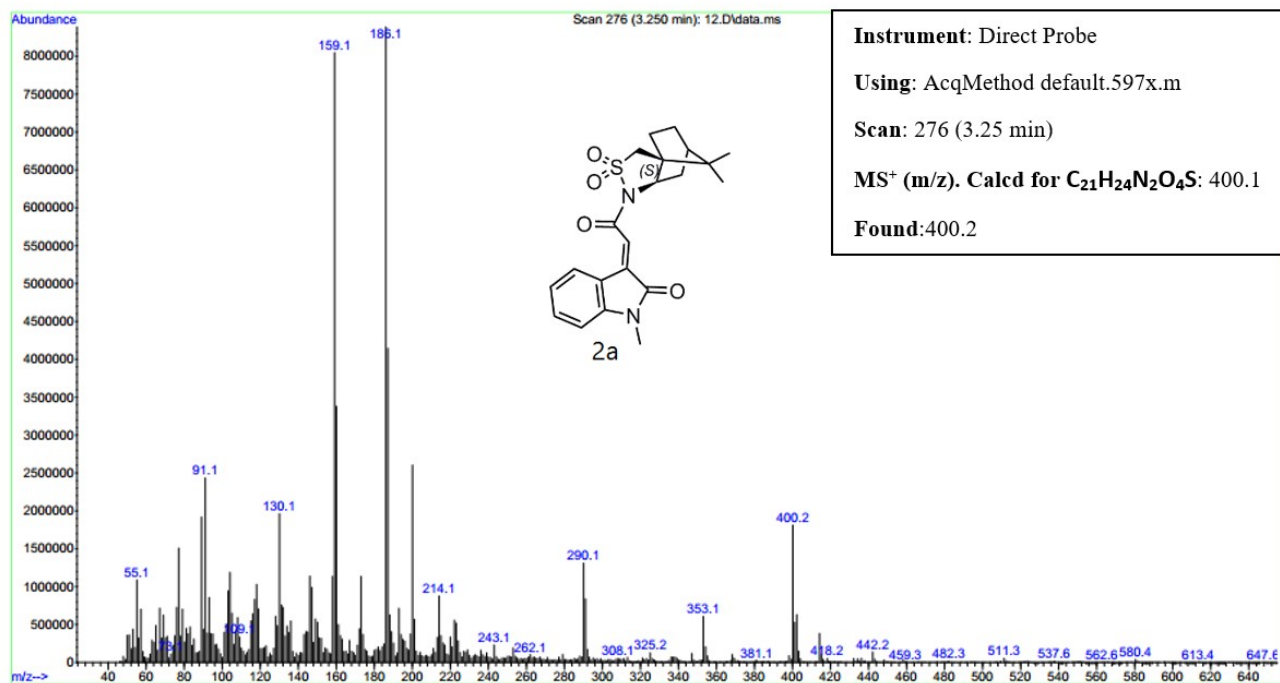
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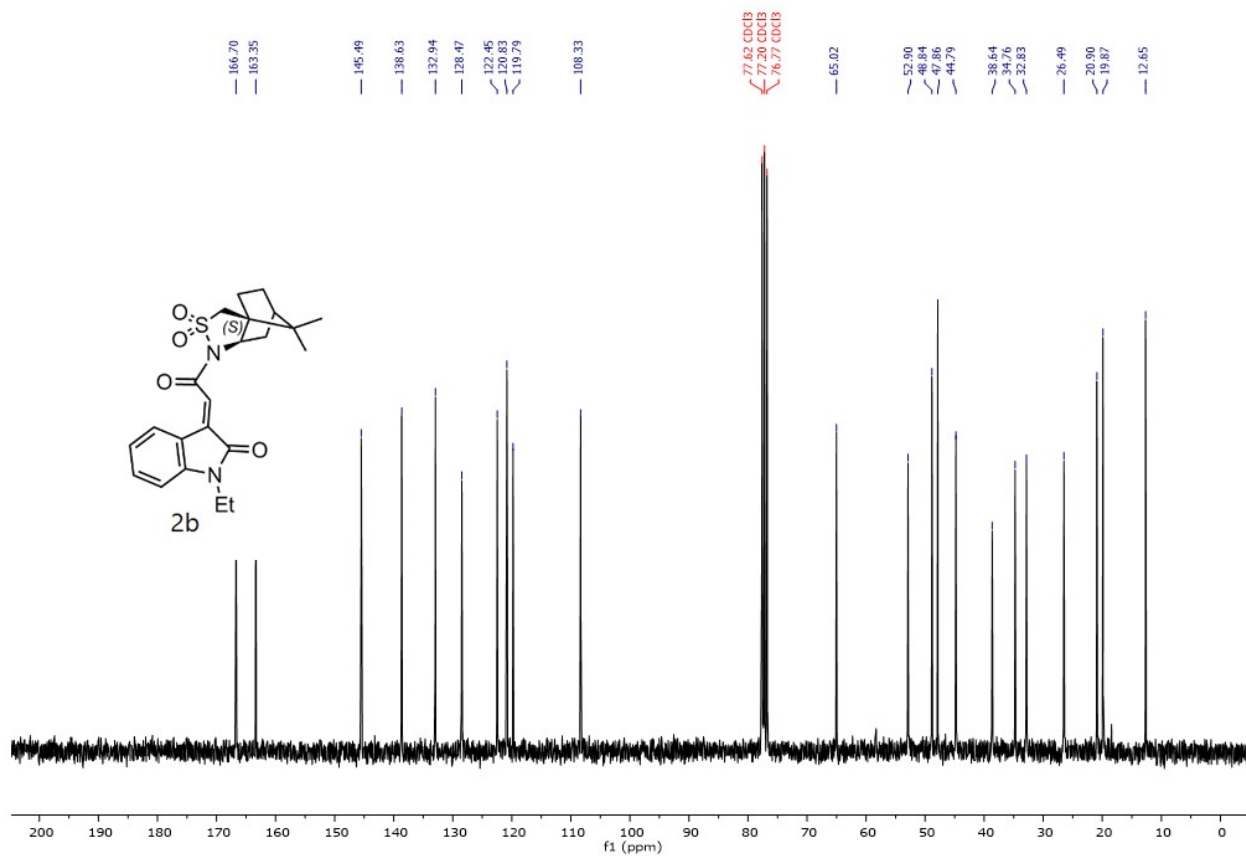
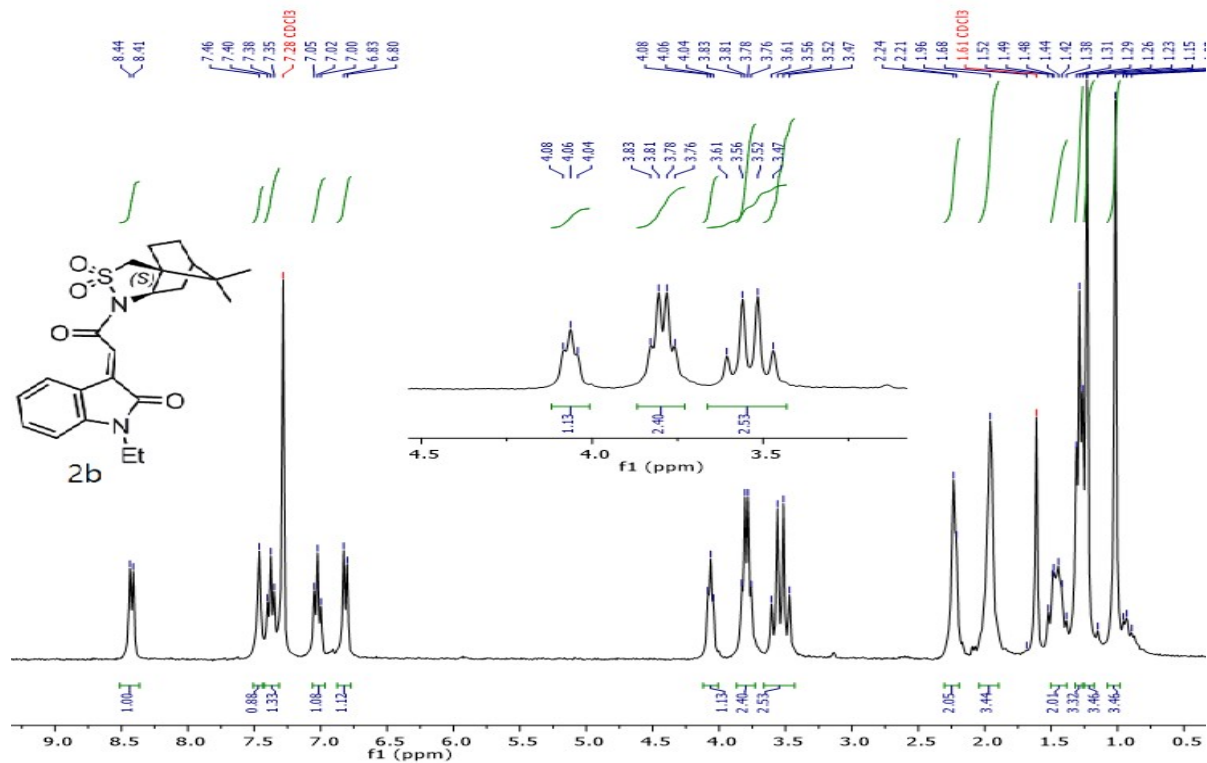
N-Me Sultam  
<sup>13</sup>C{<sup>1</sup>H} NMR



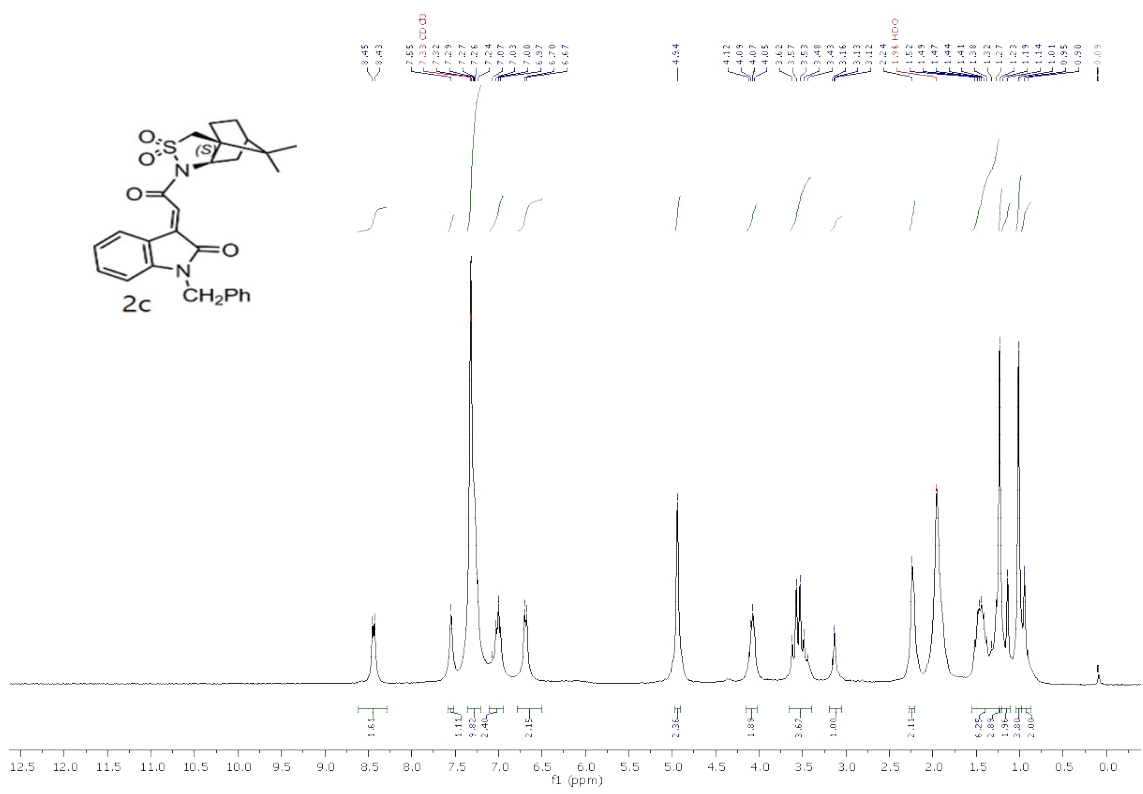
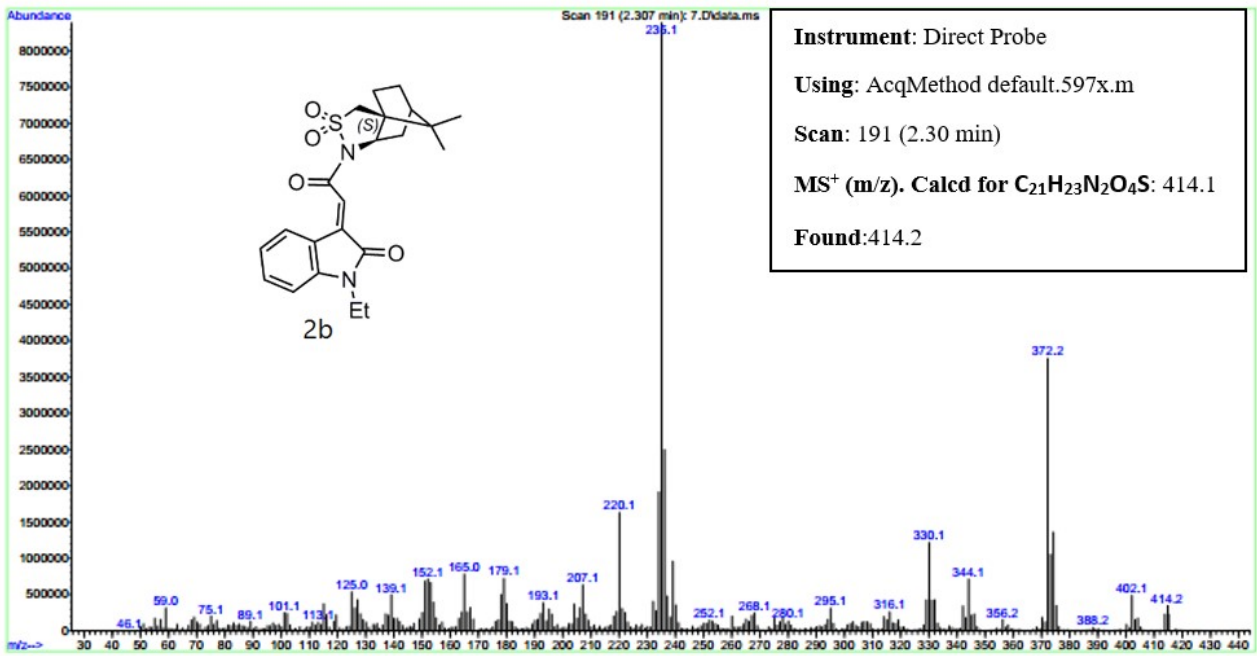
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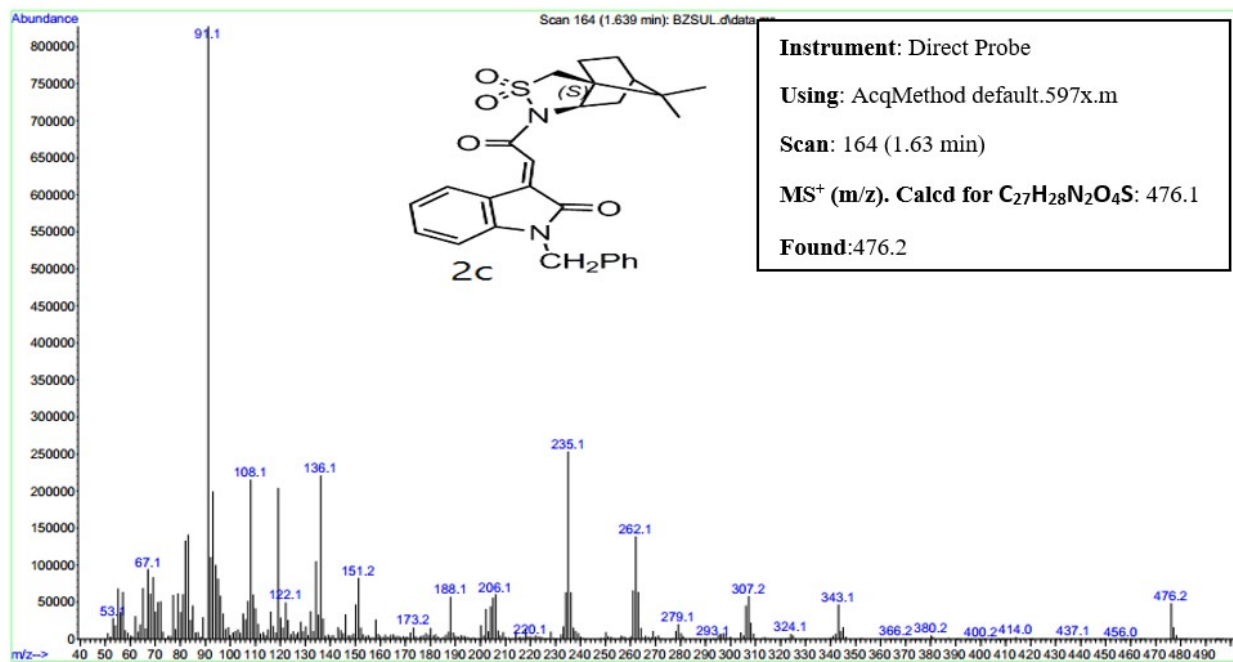
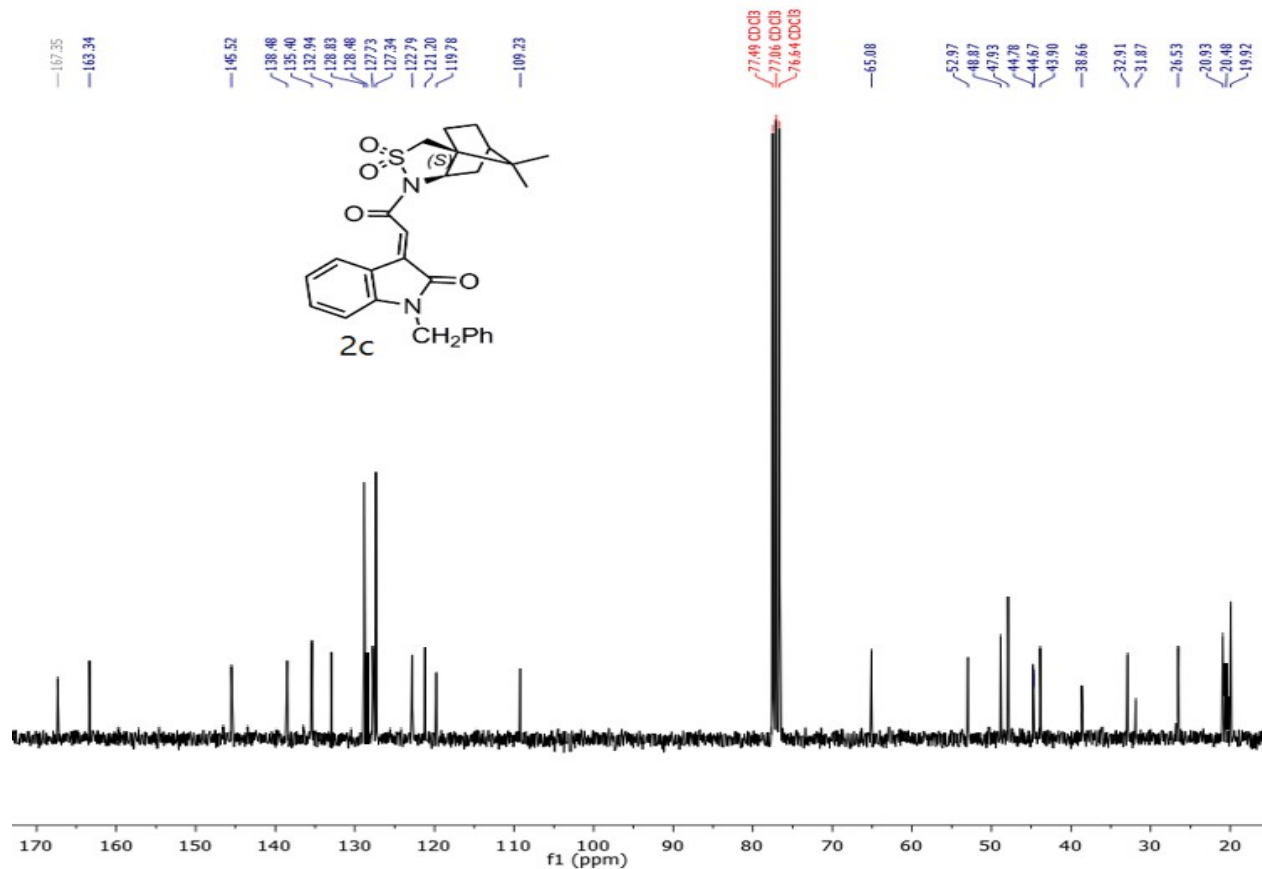


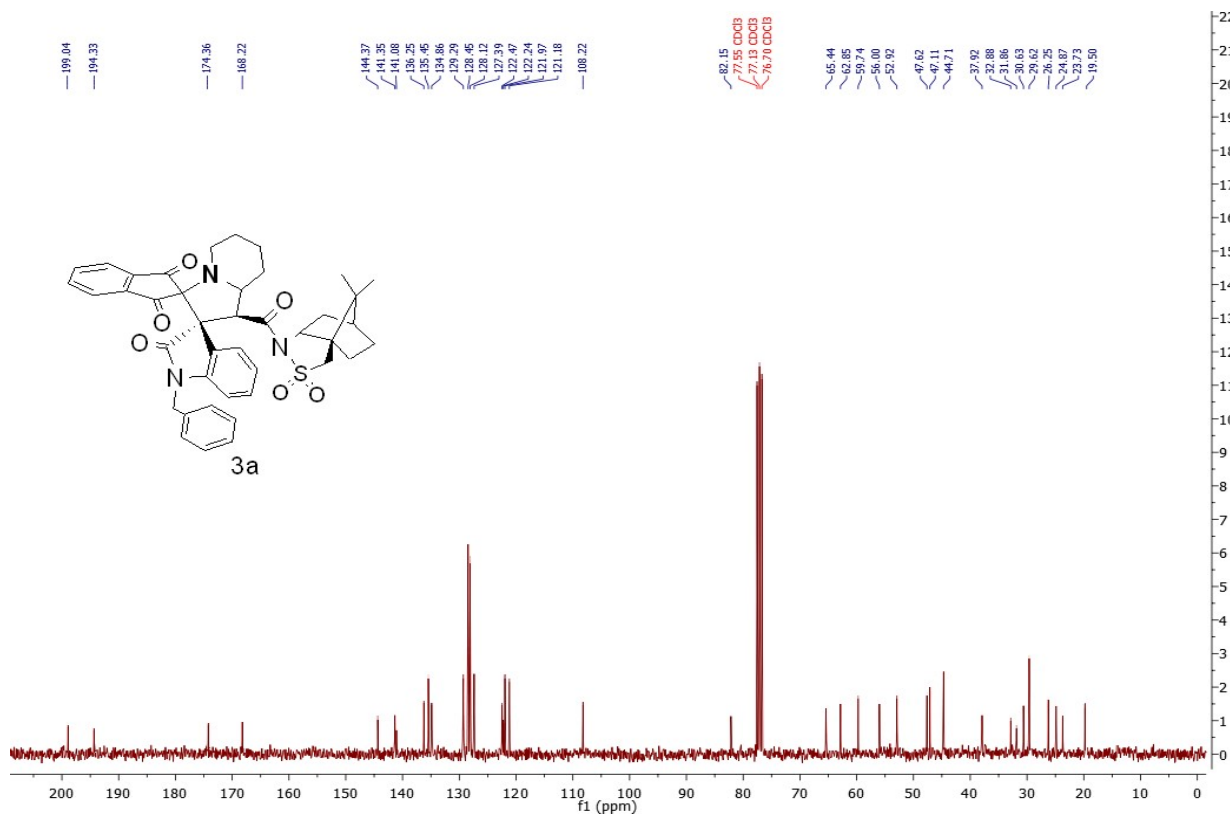
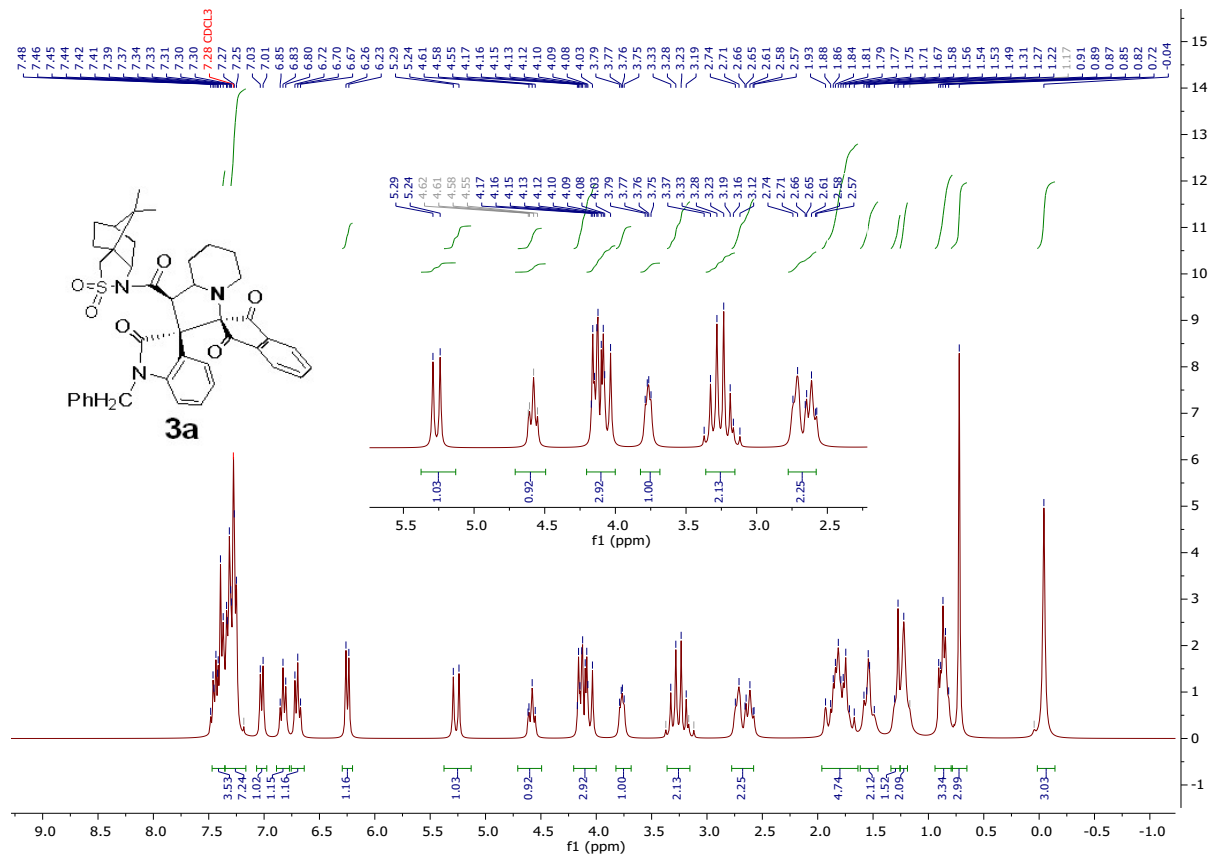
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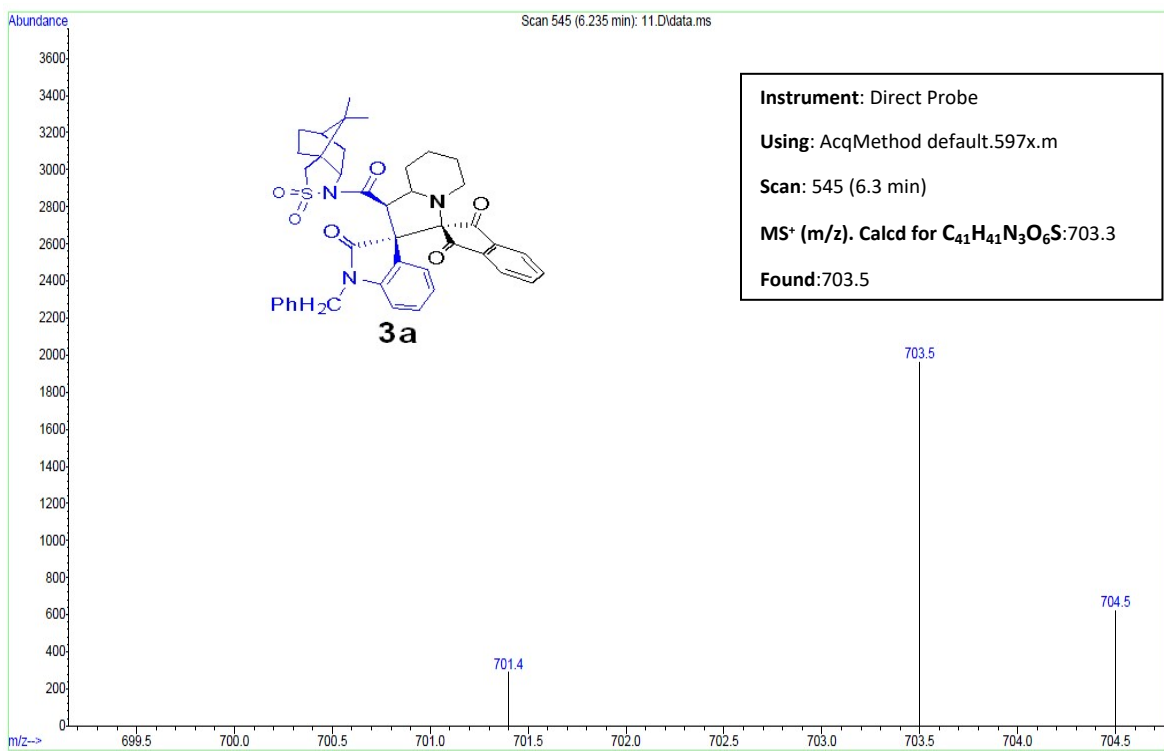
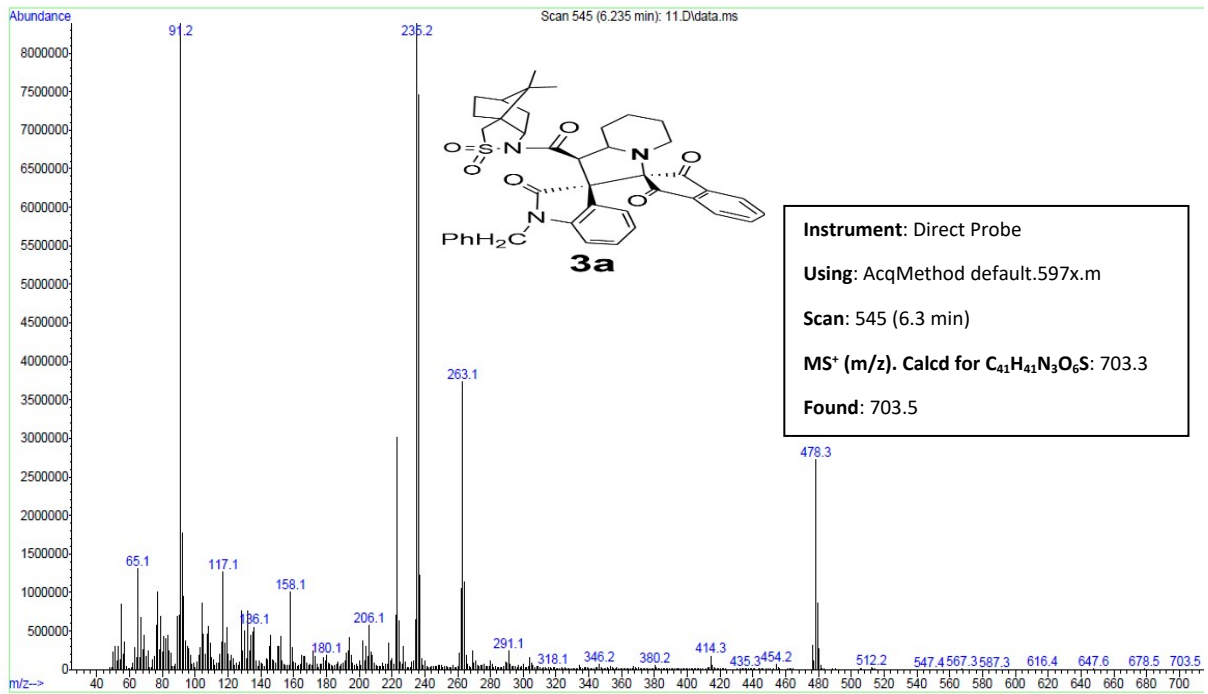
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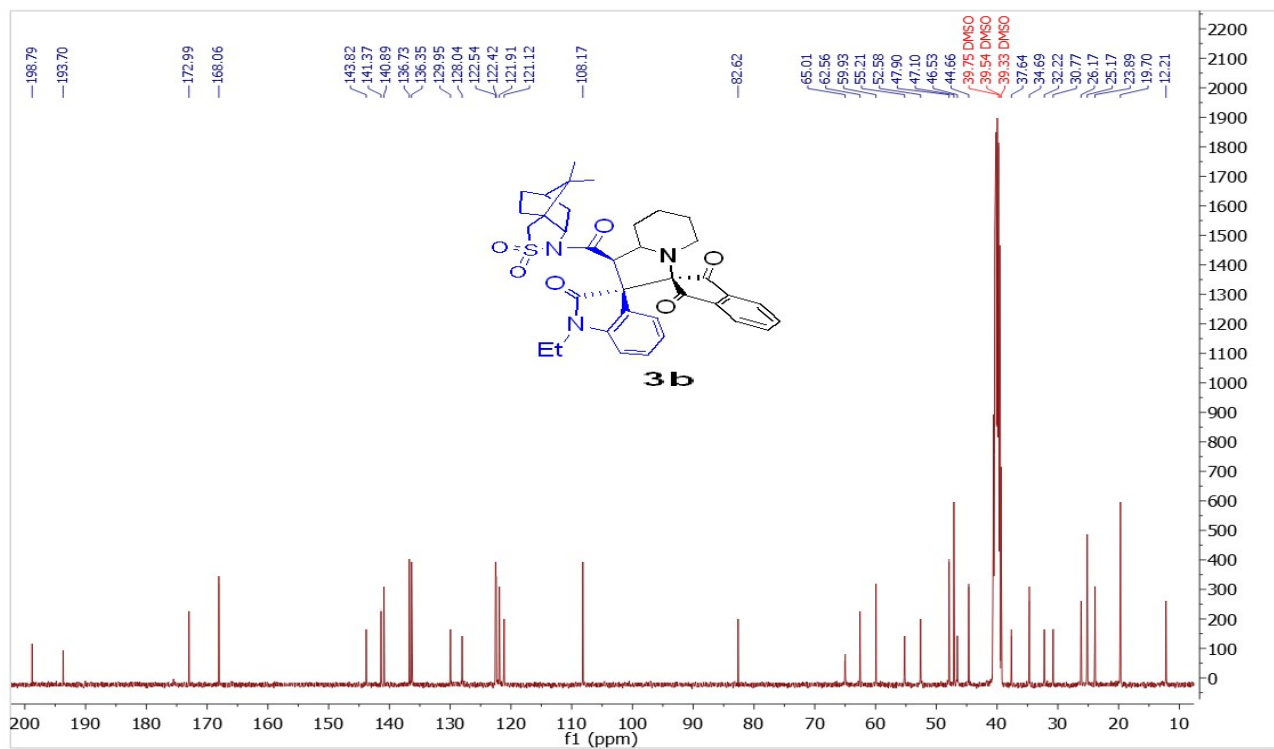
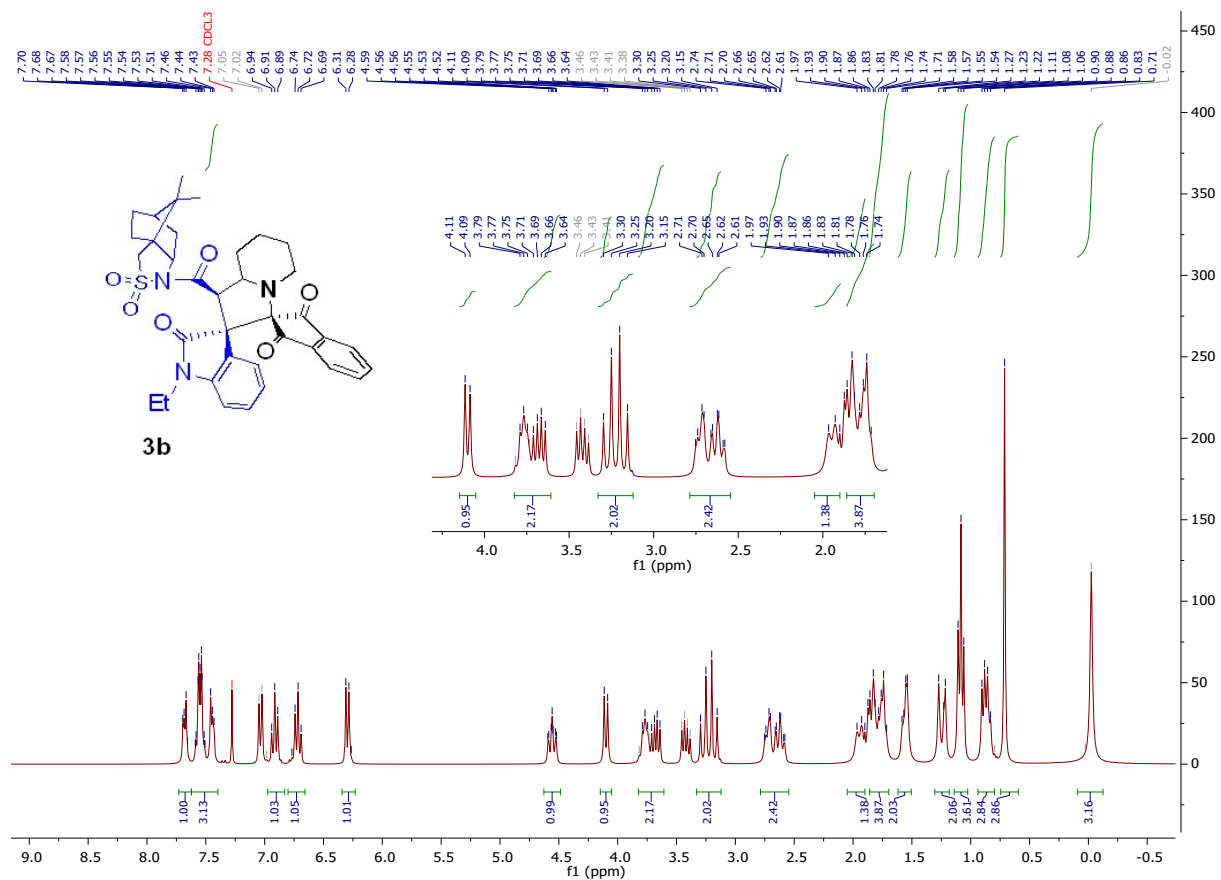


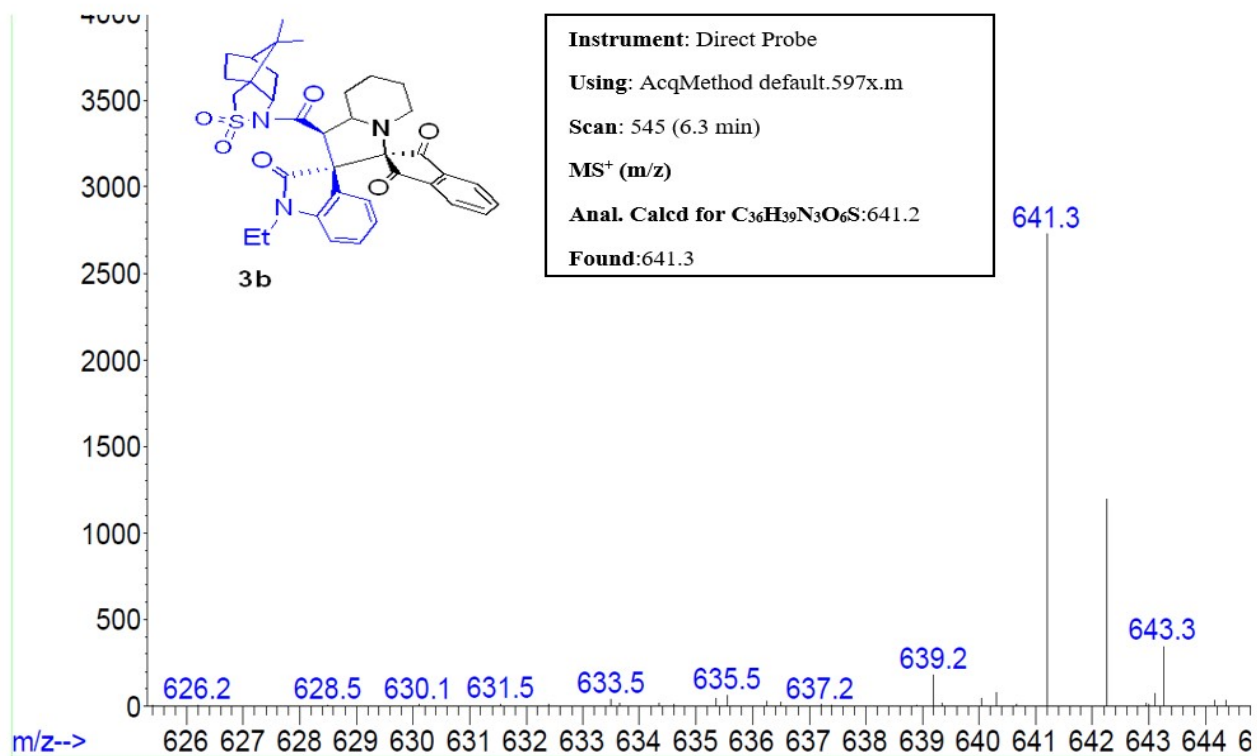
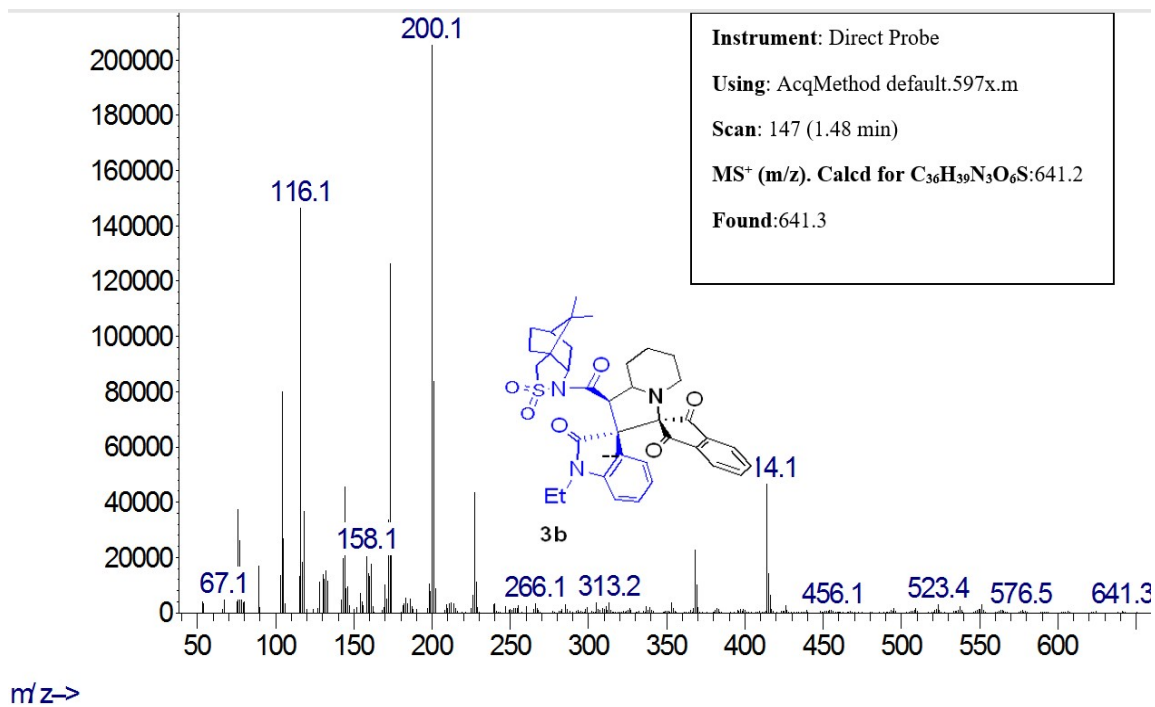


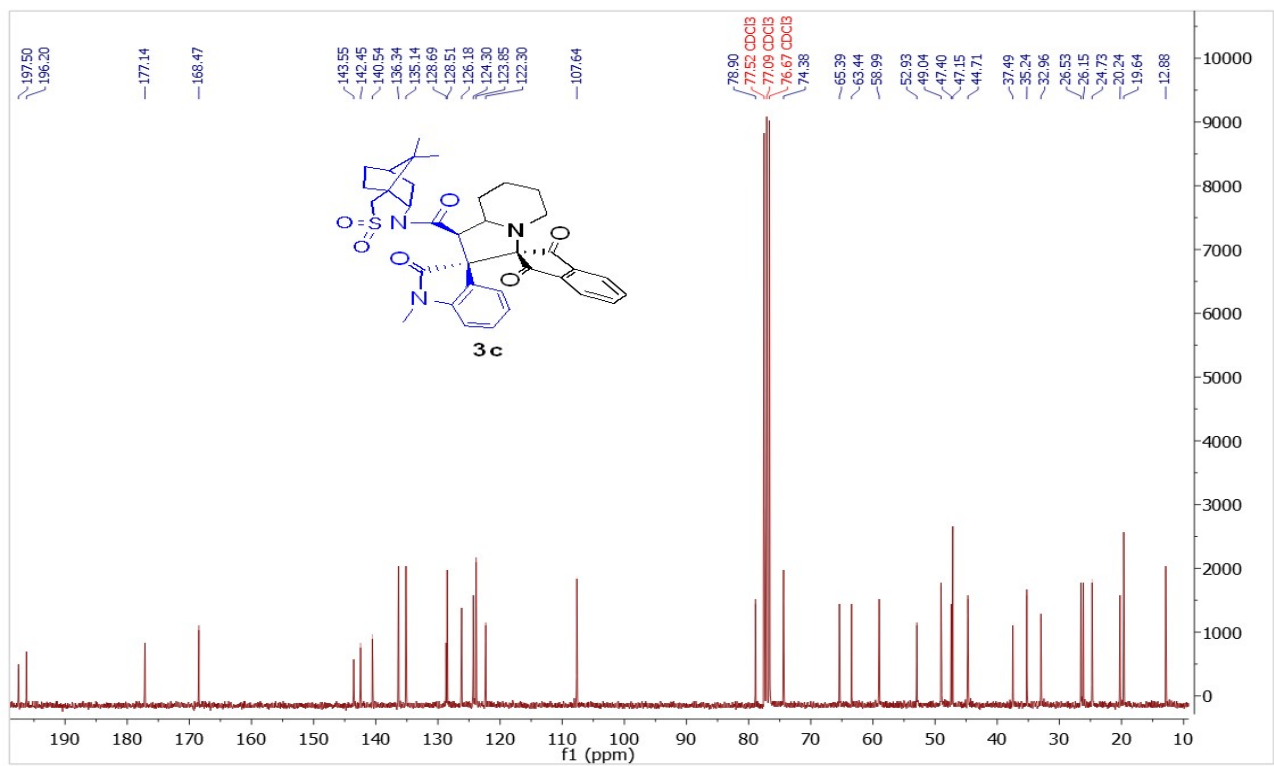
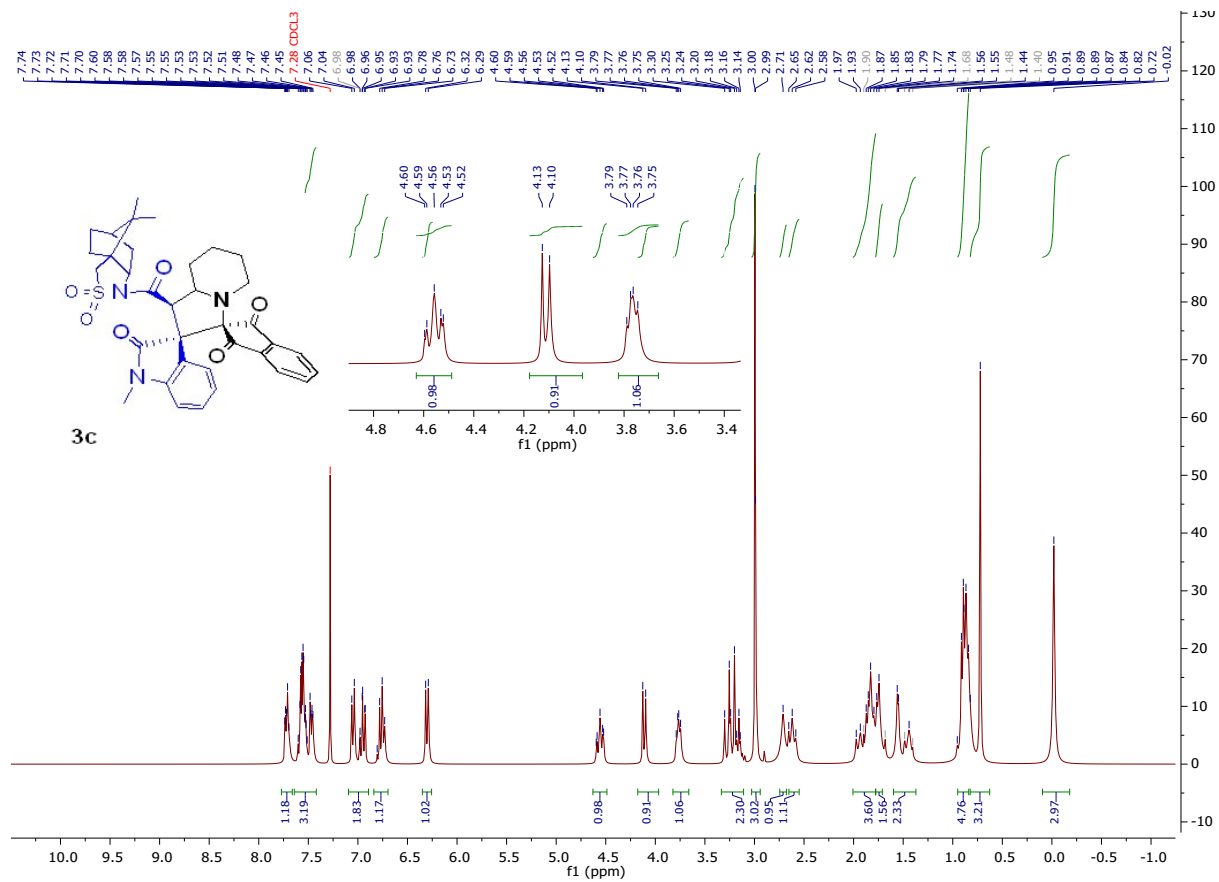


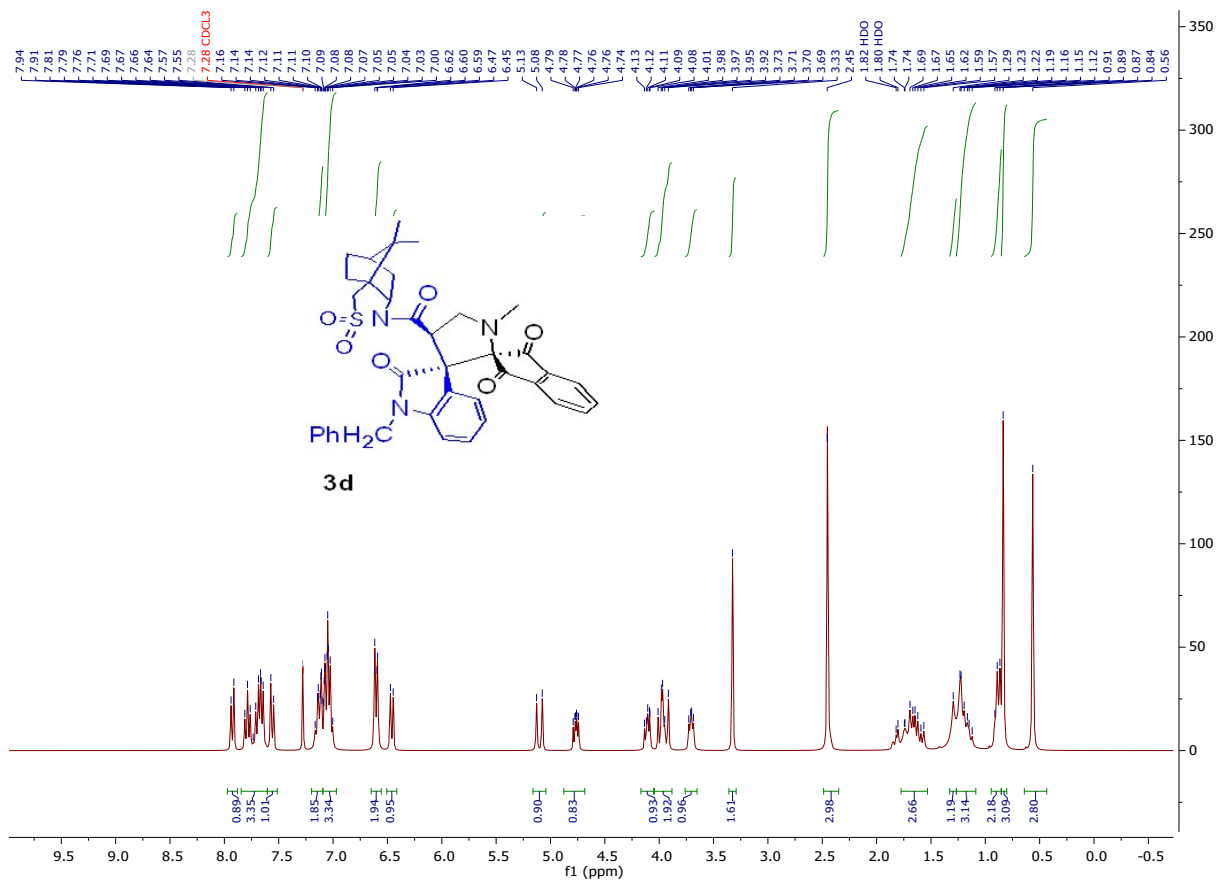
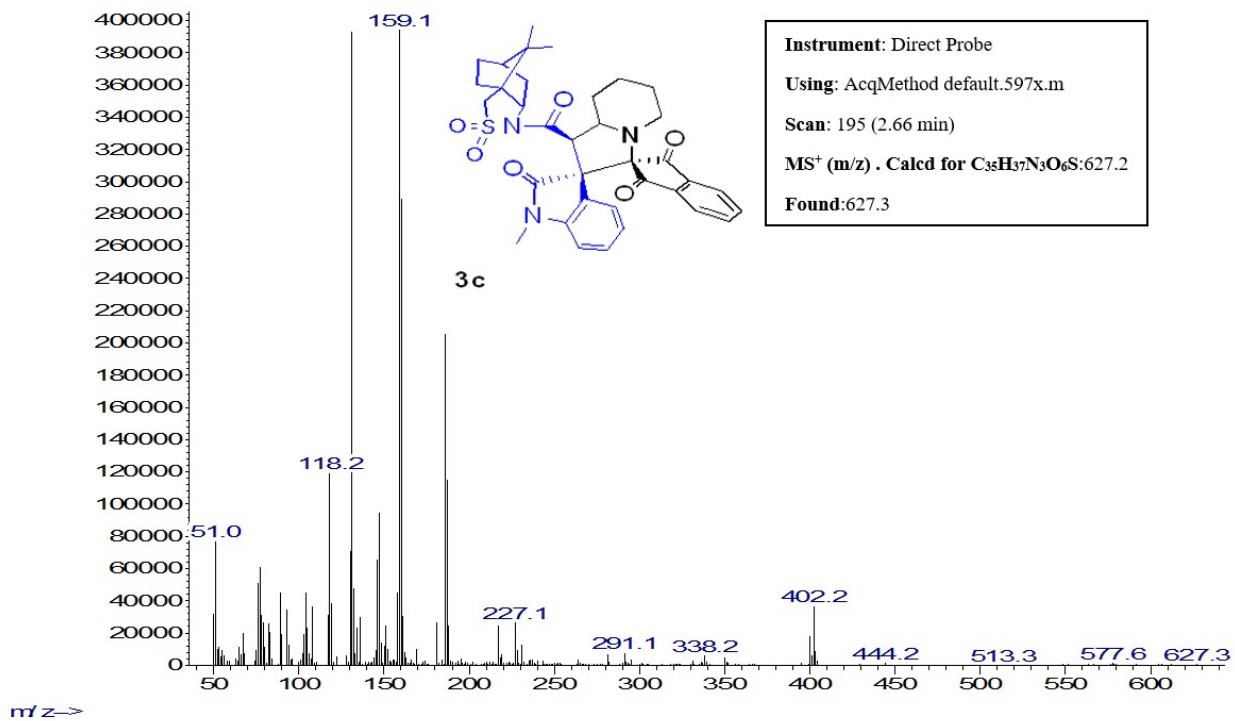


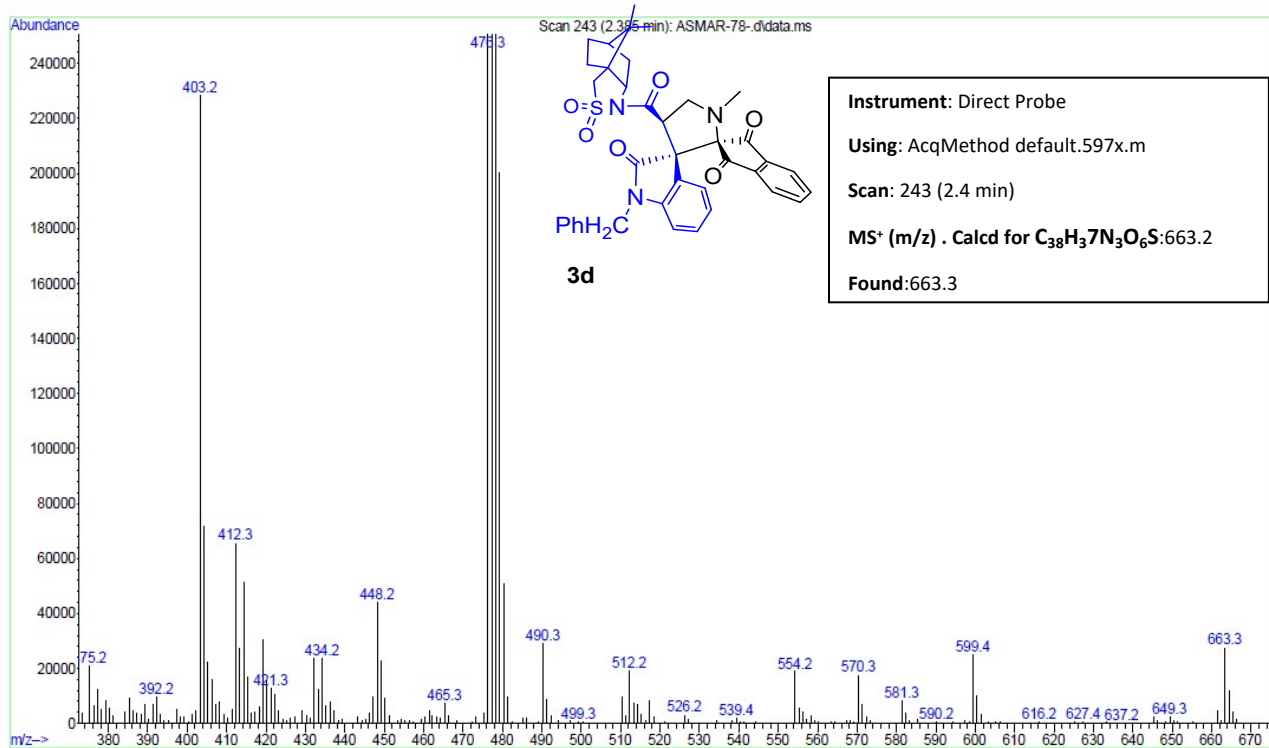
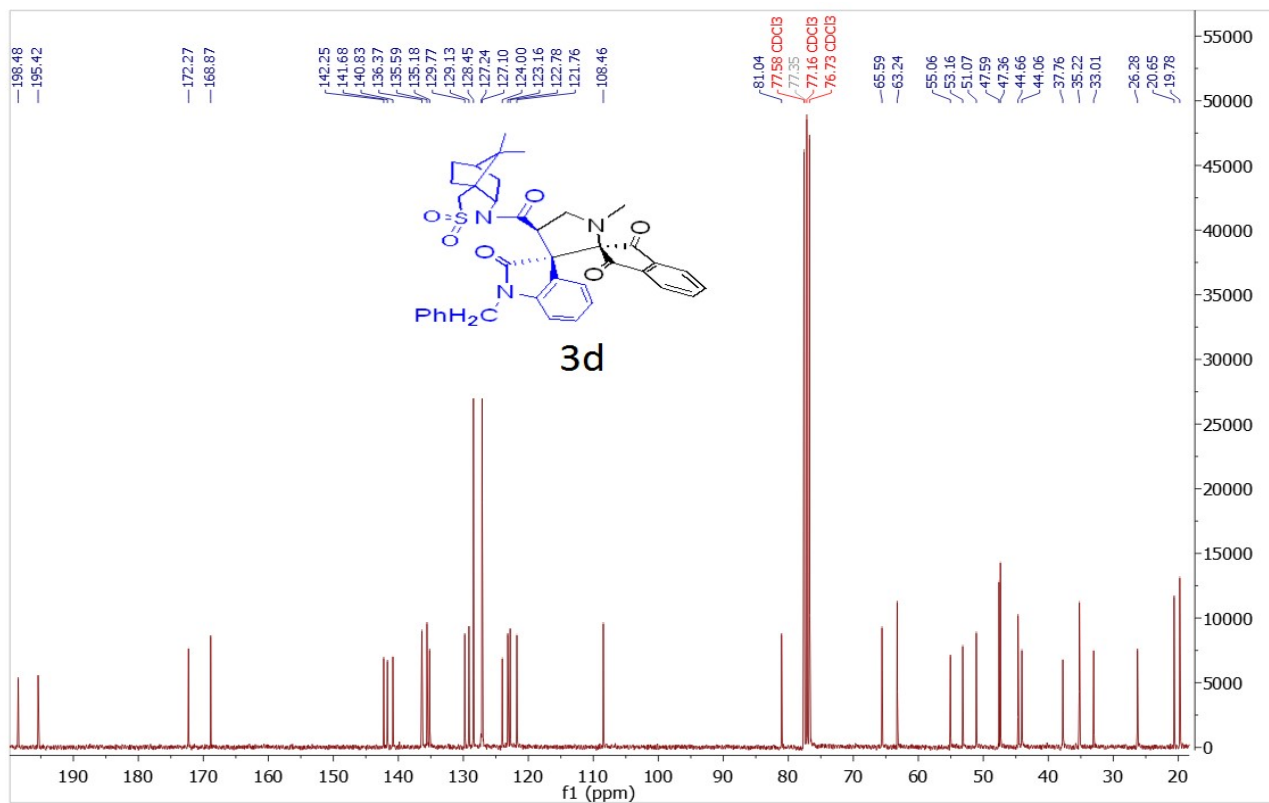


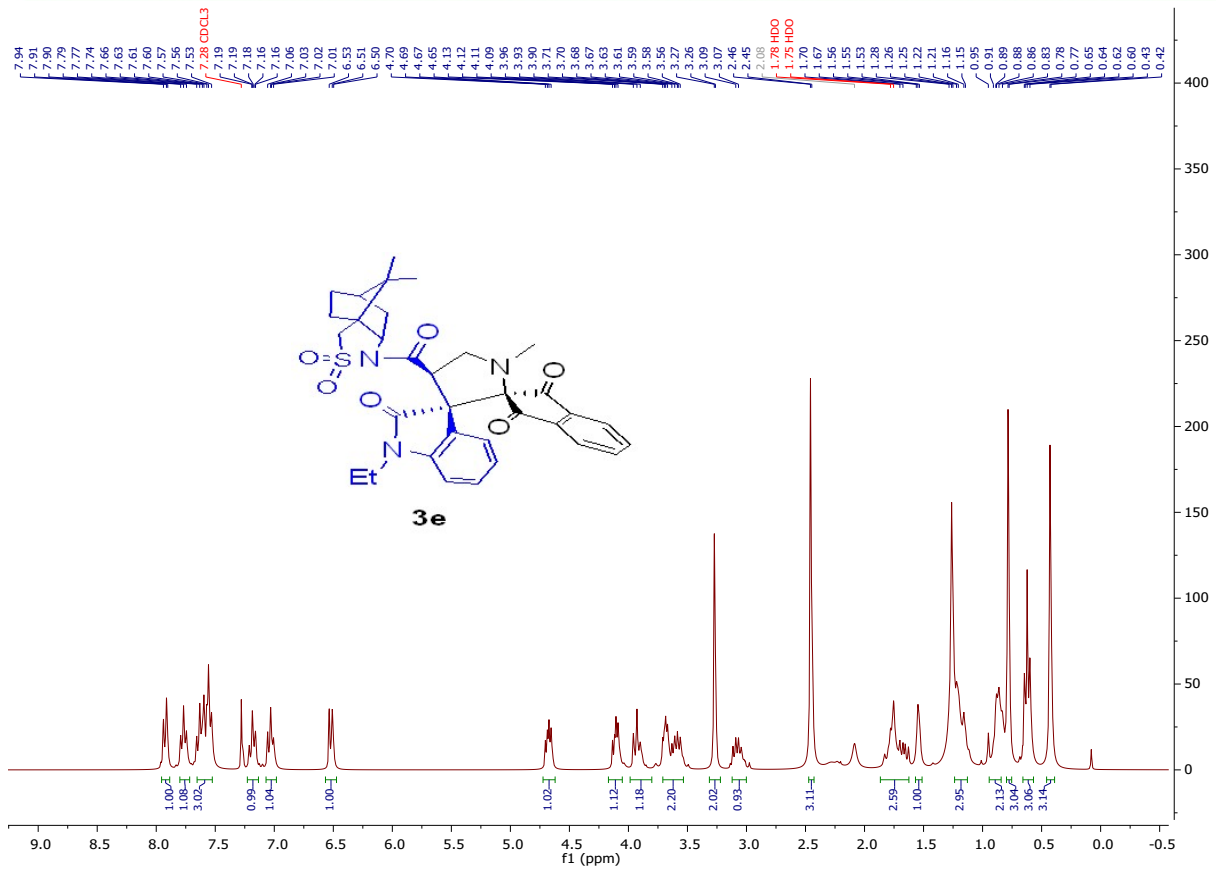
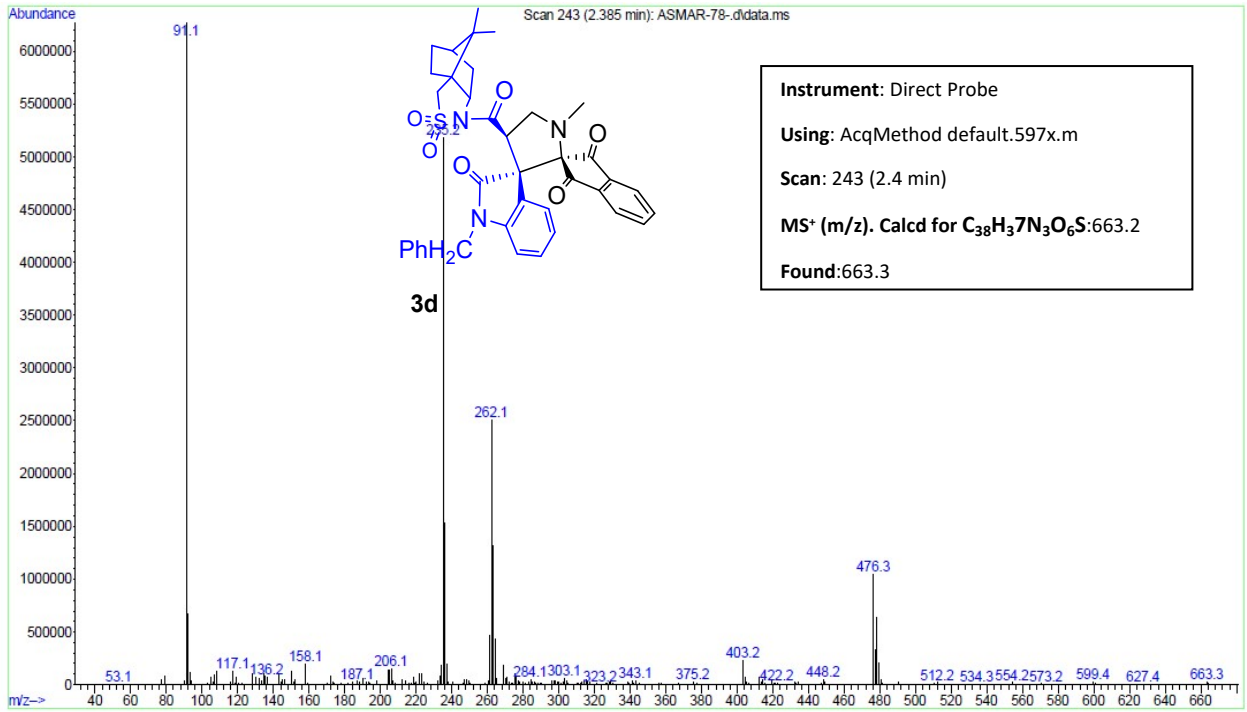


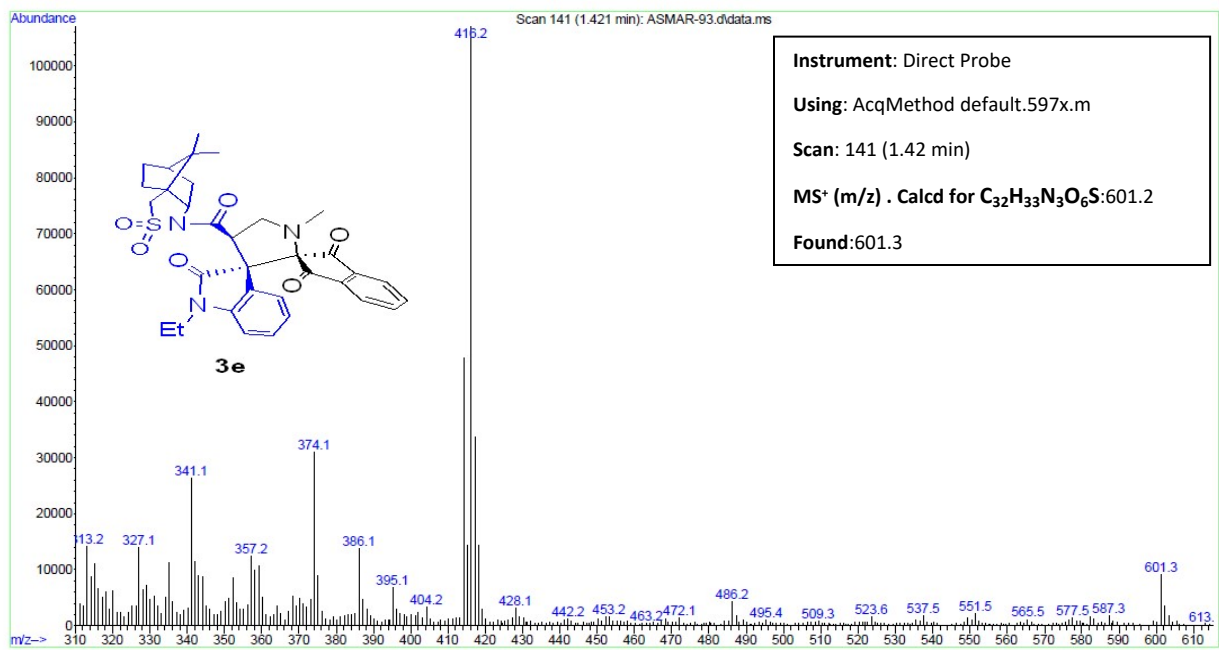
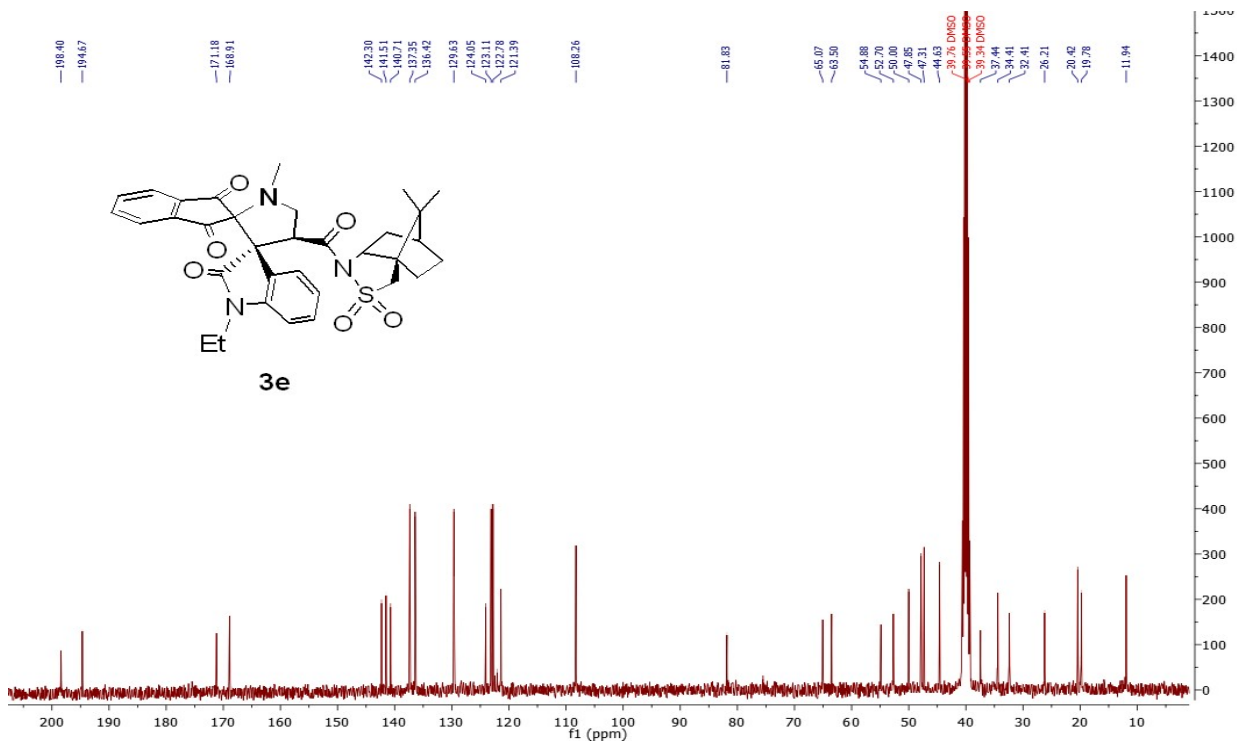




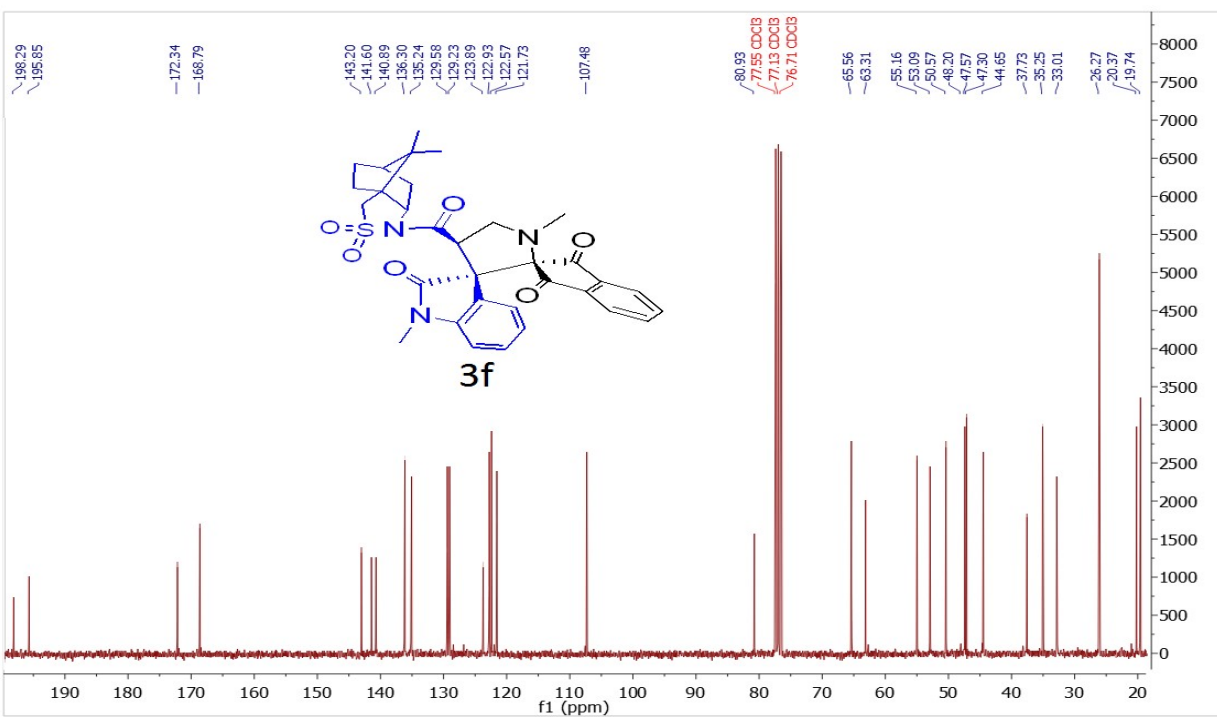
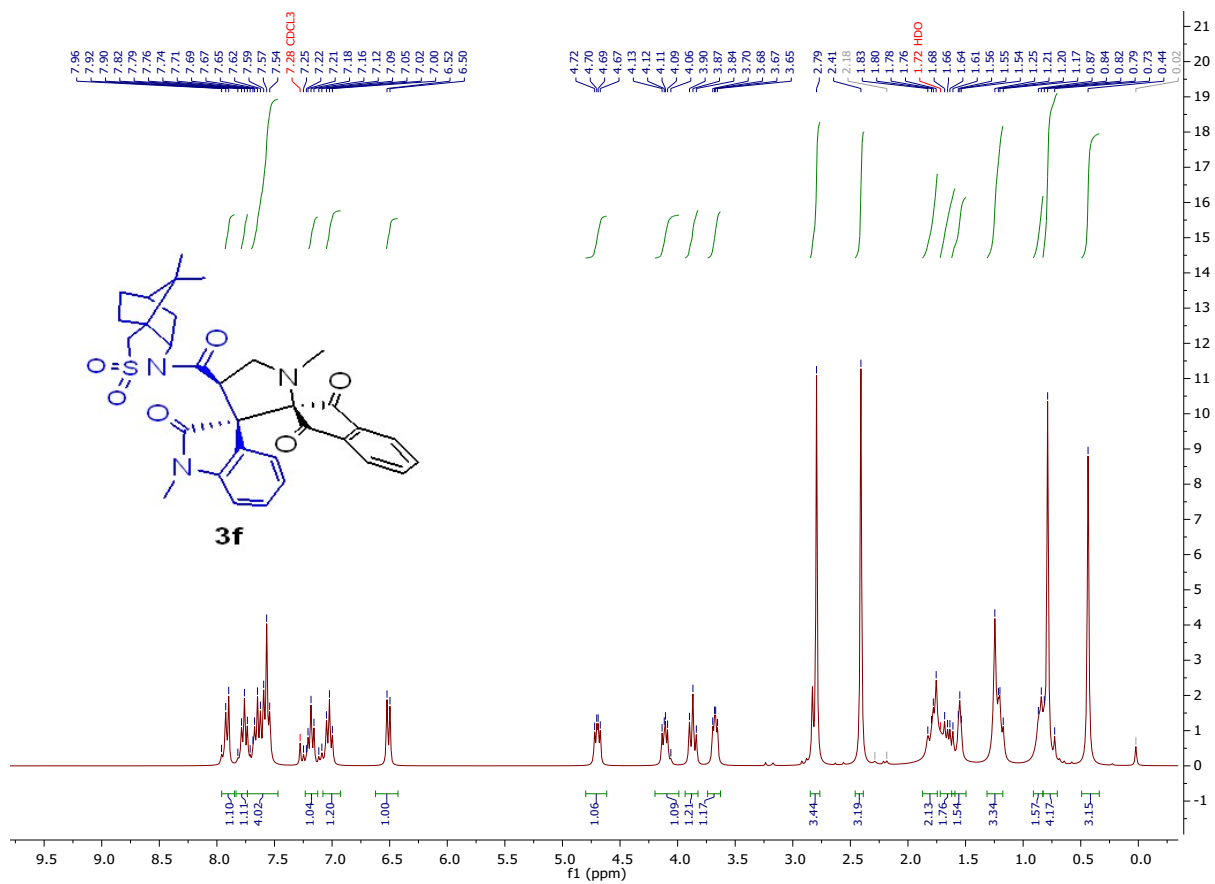


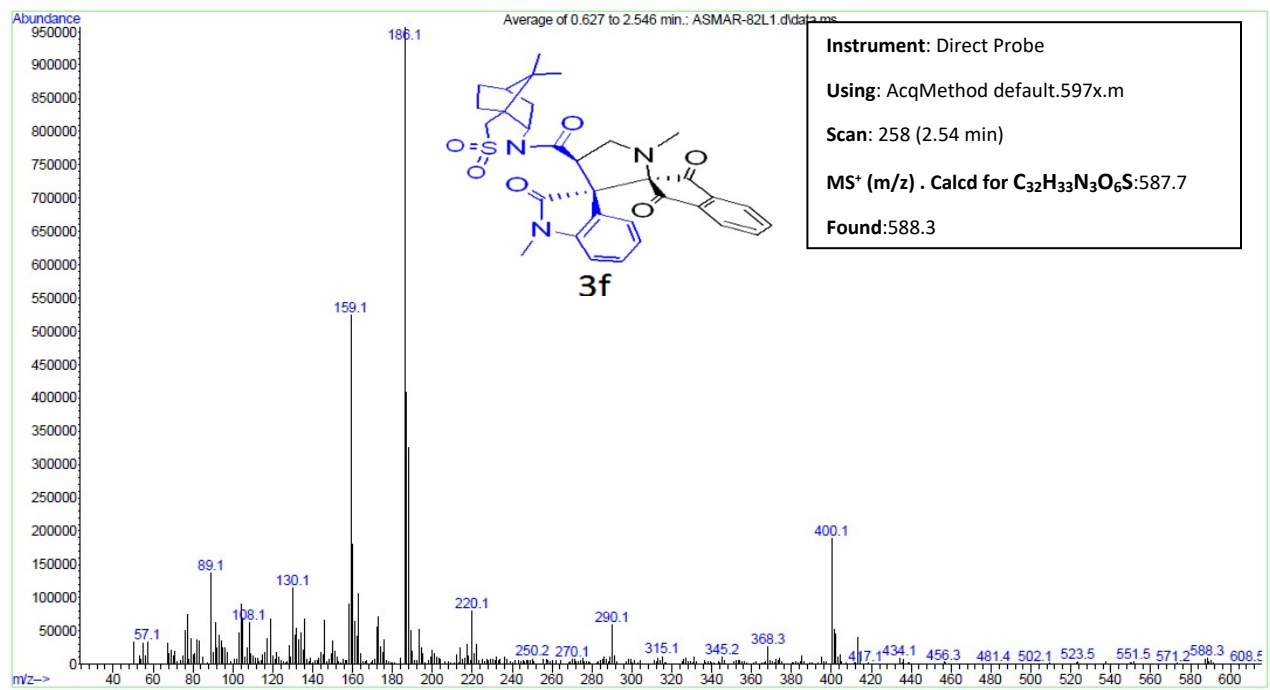
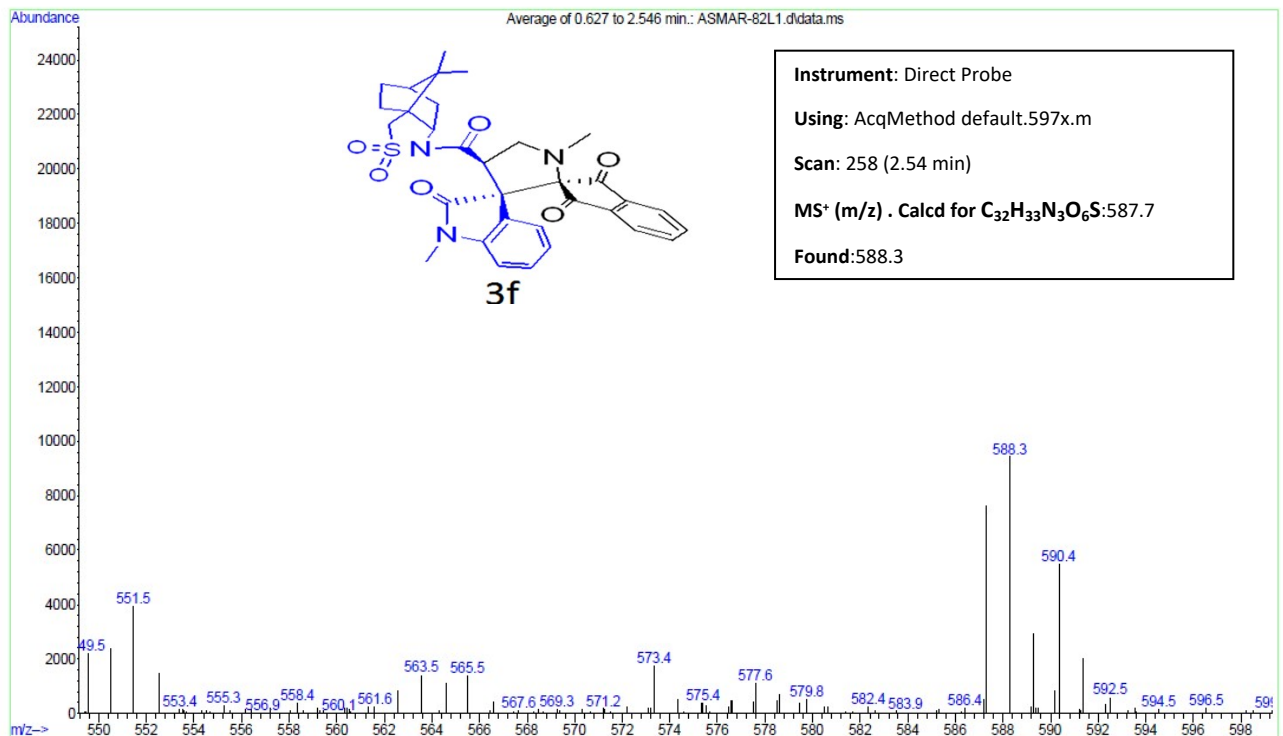


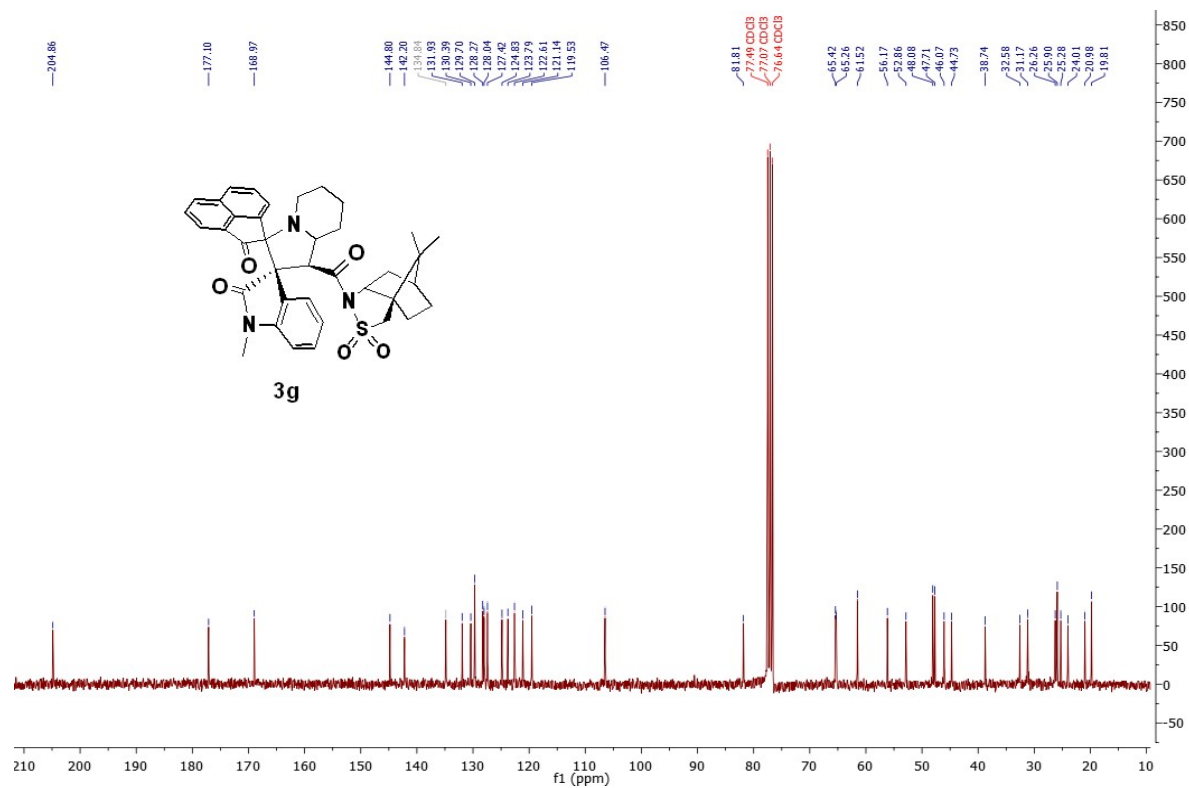
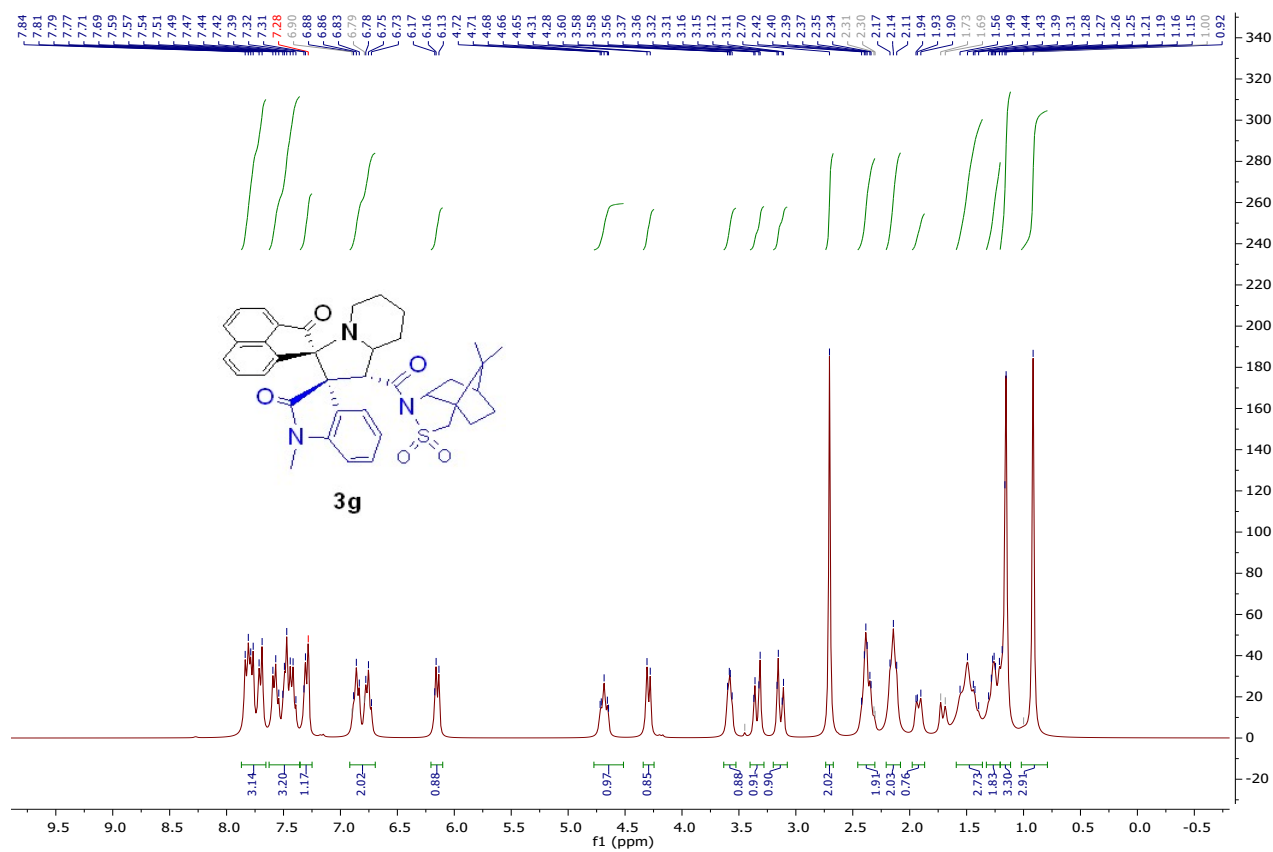


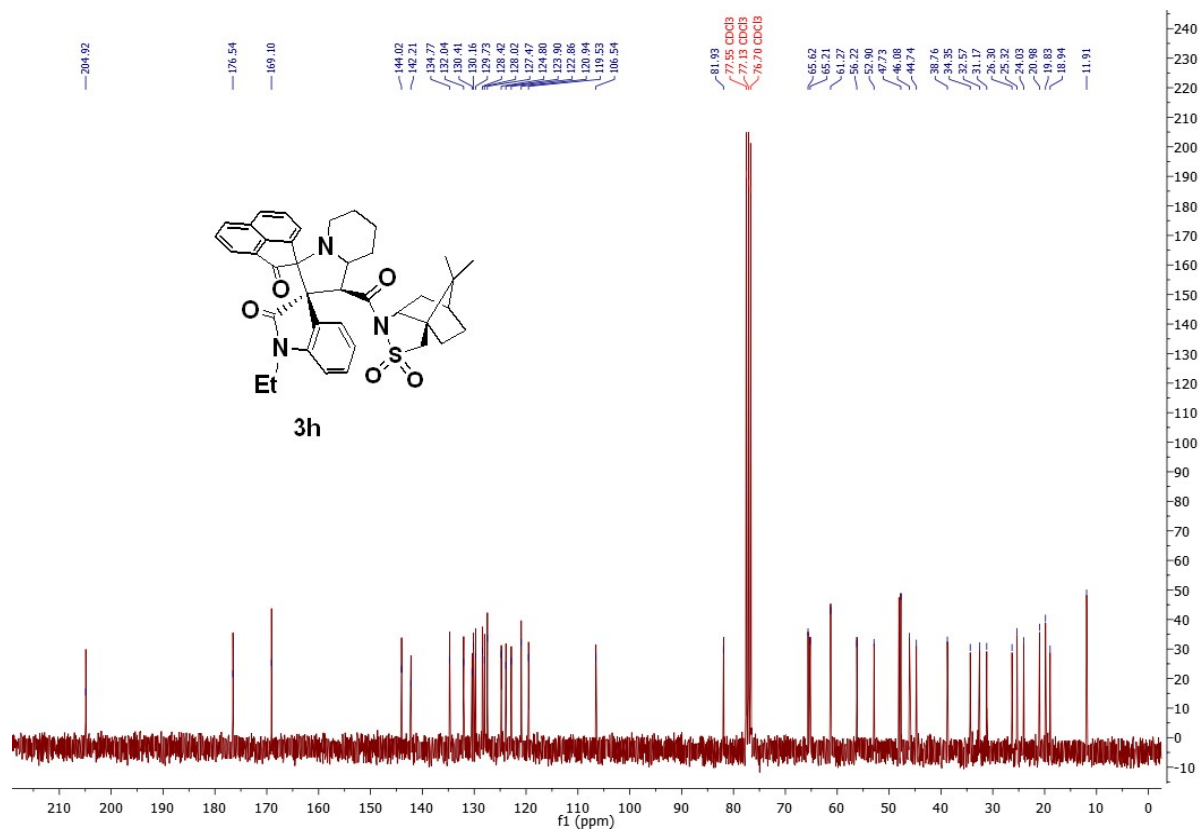
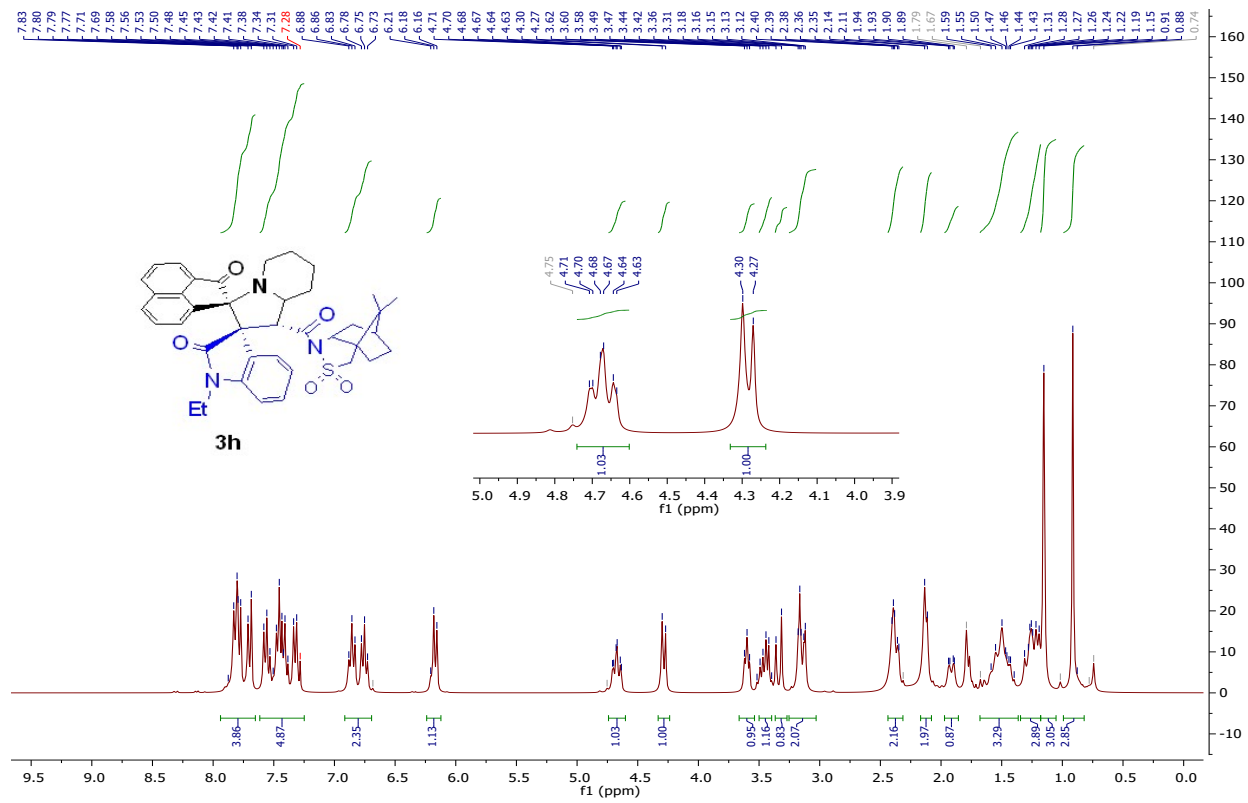


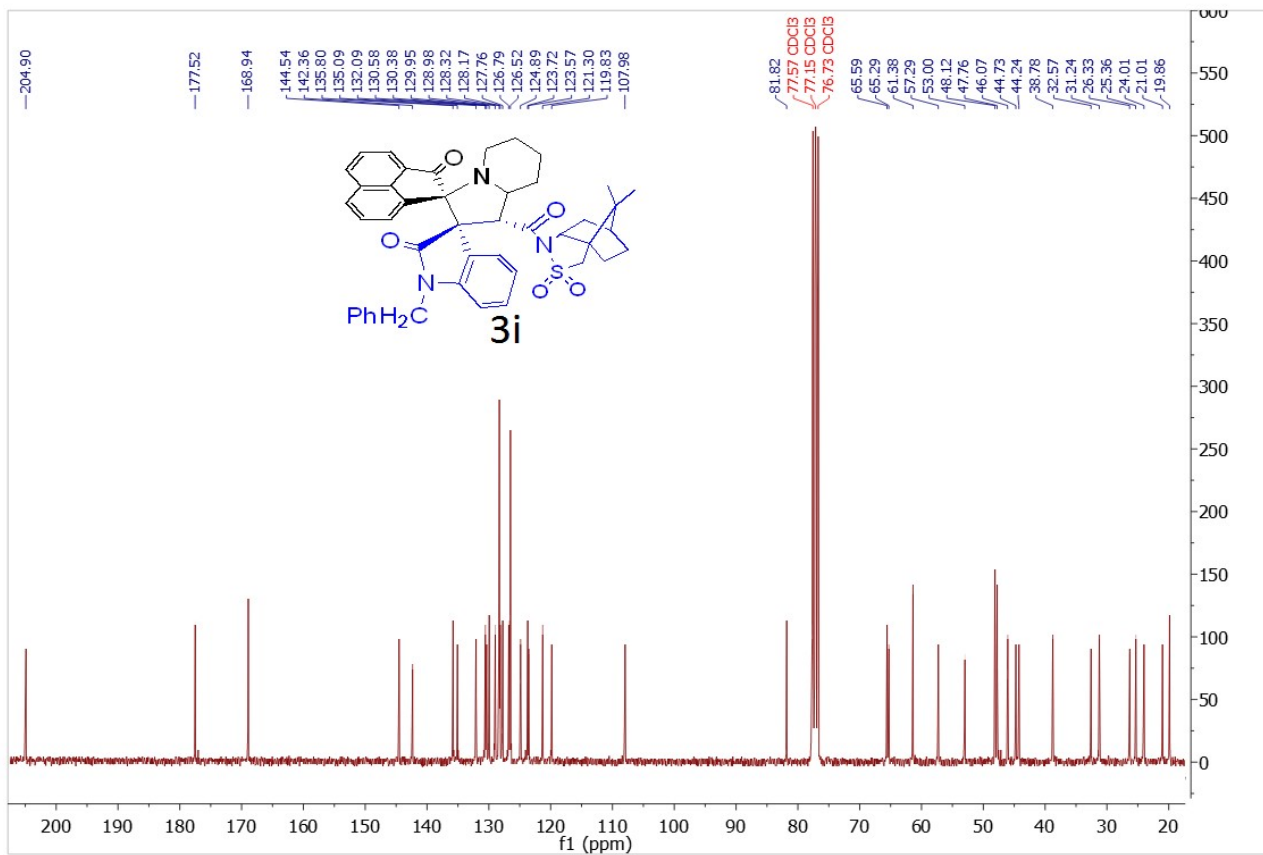
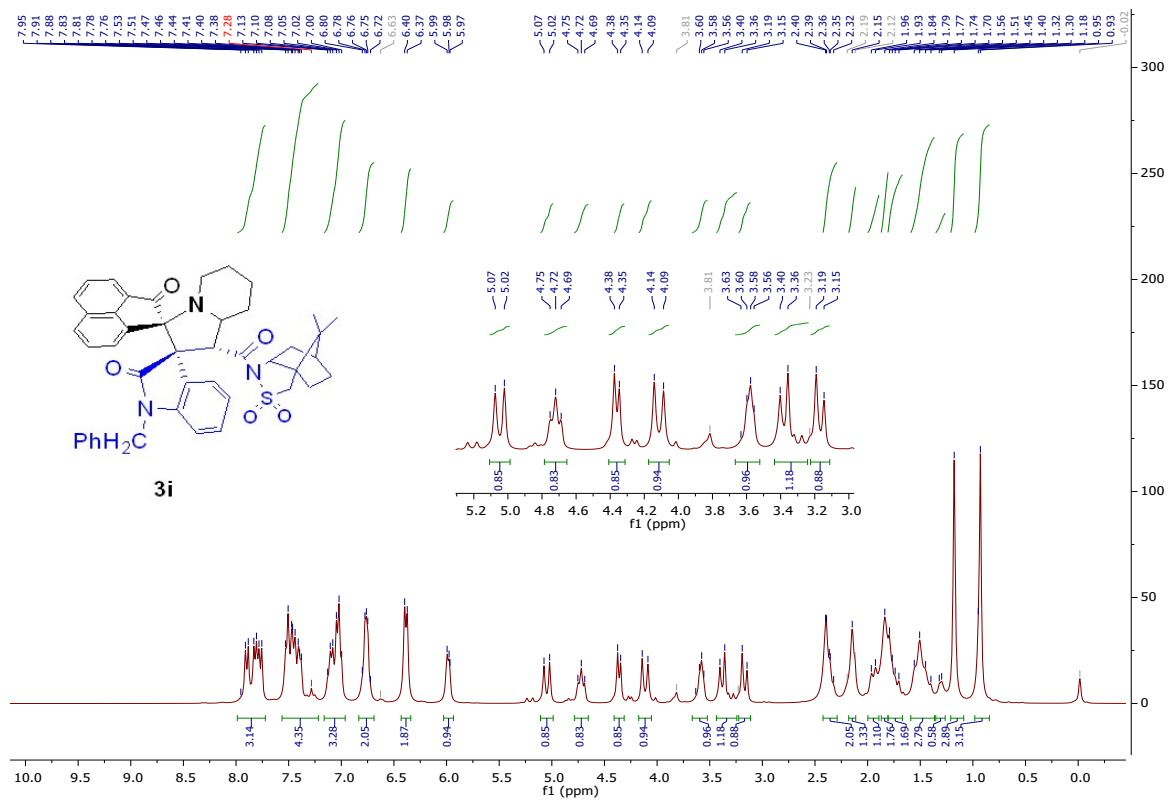


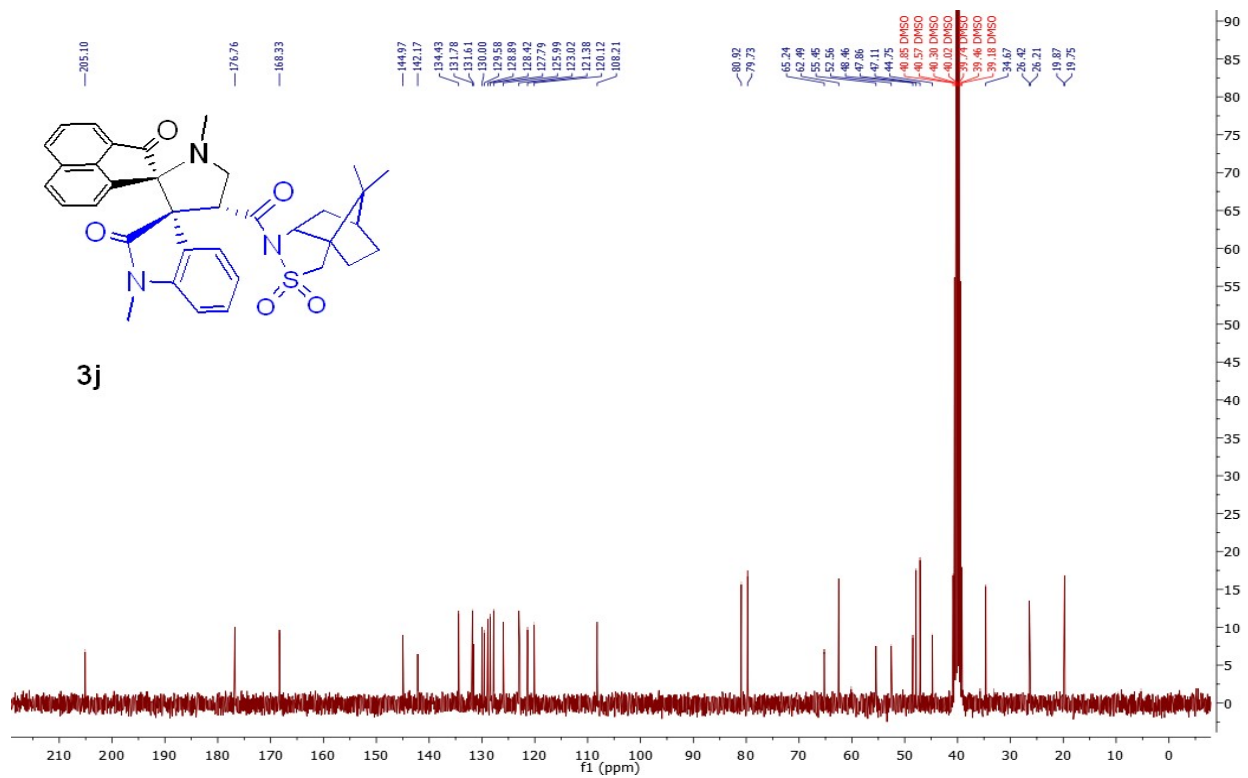
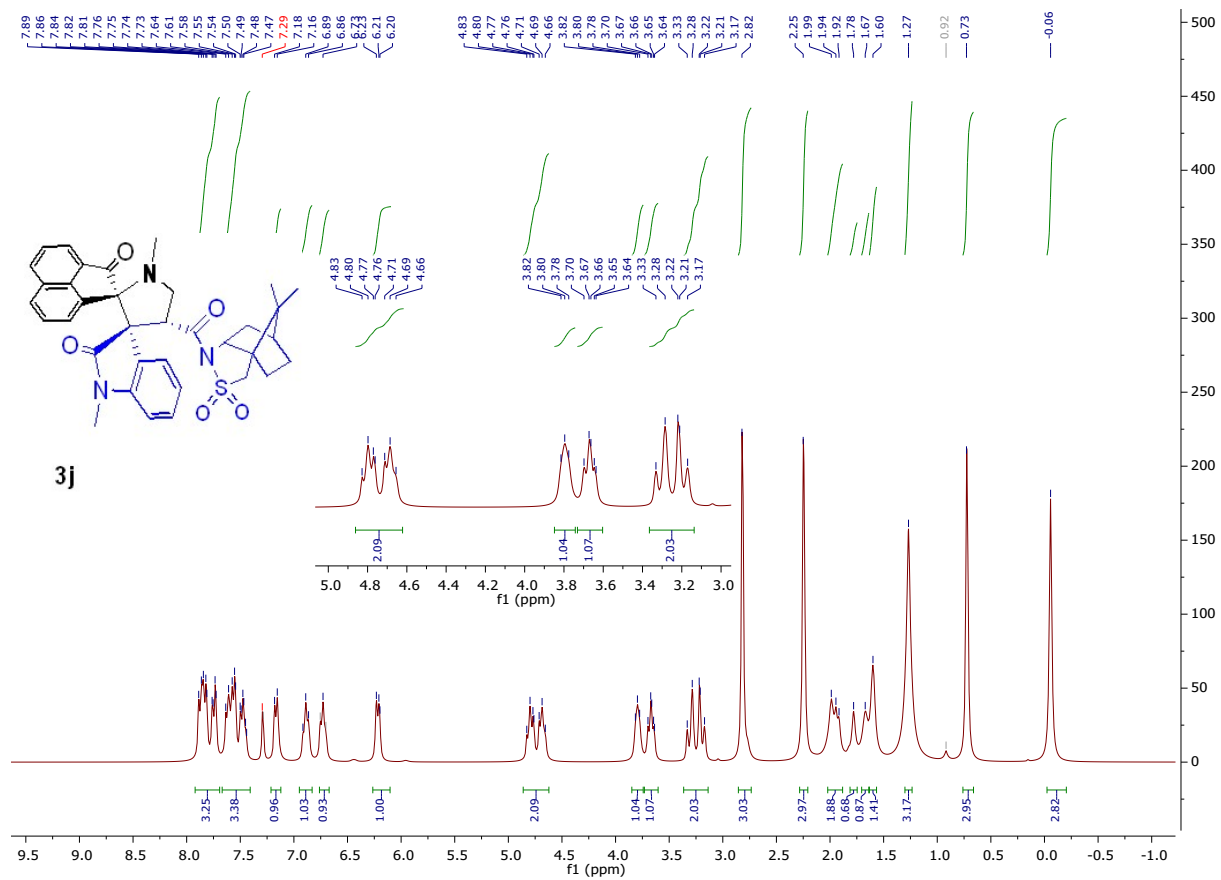


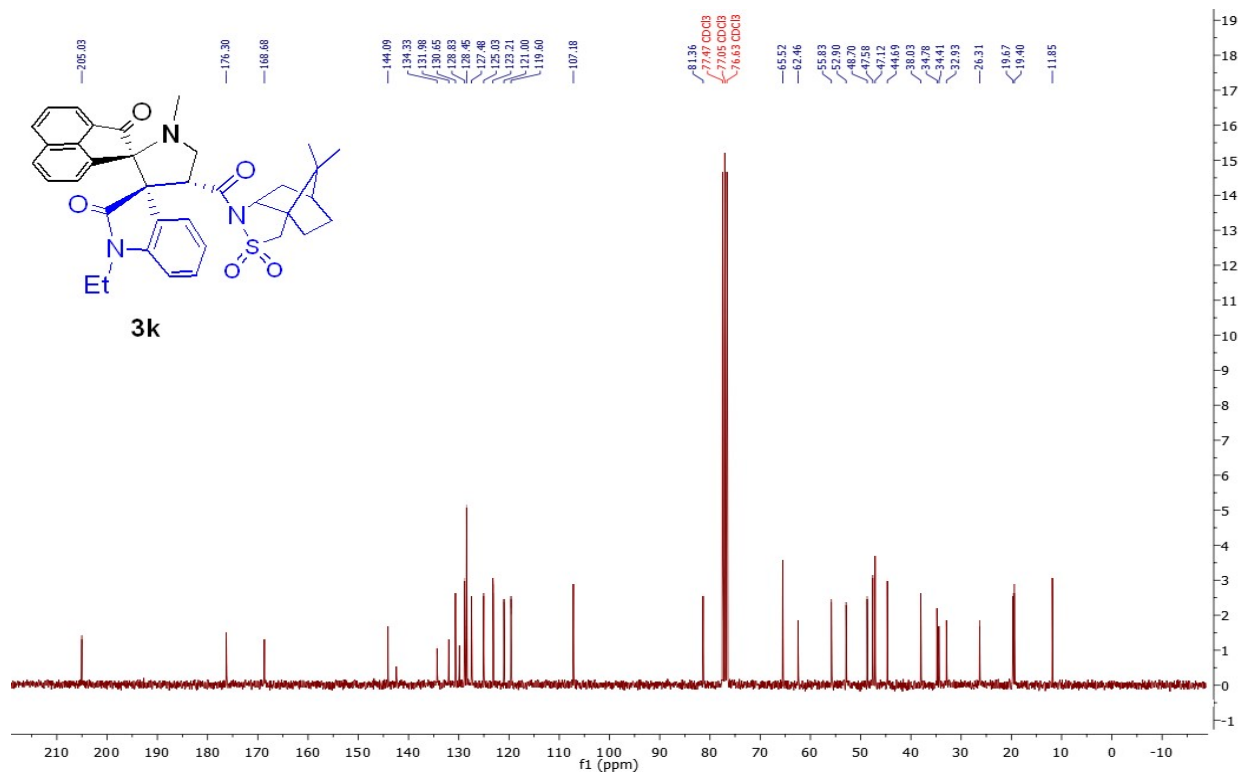
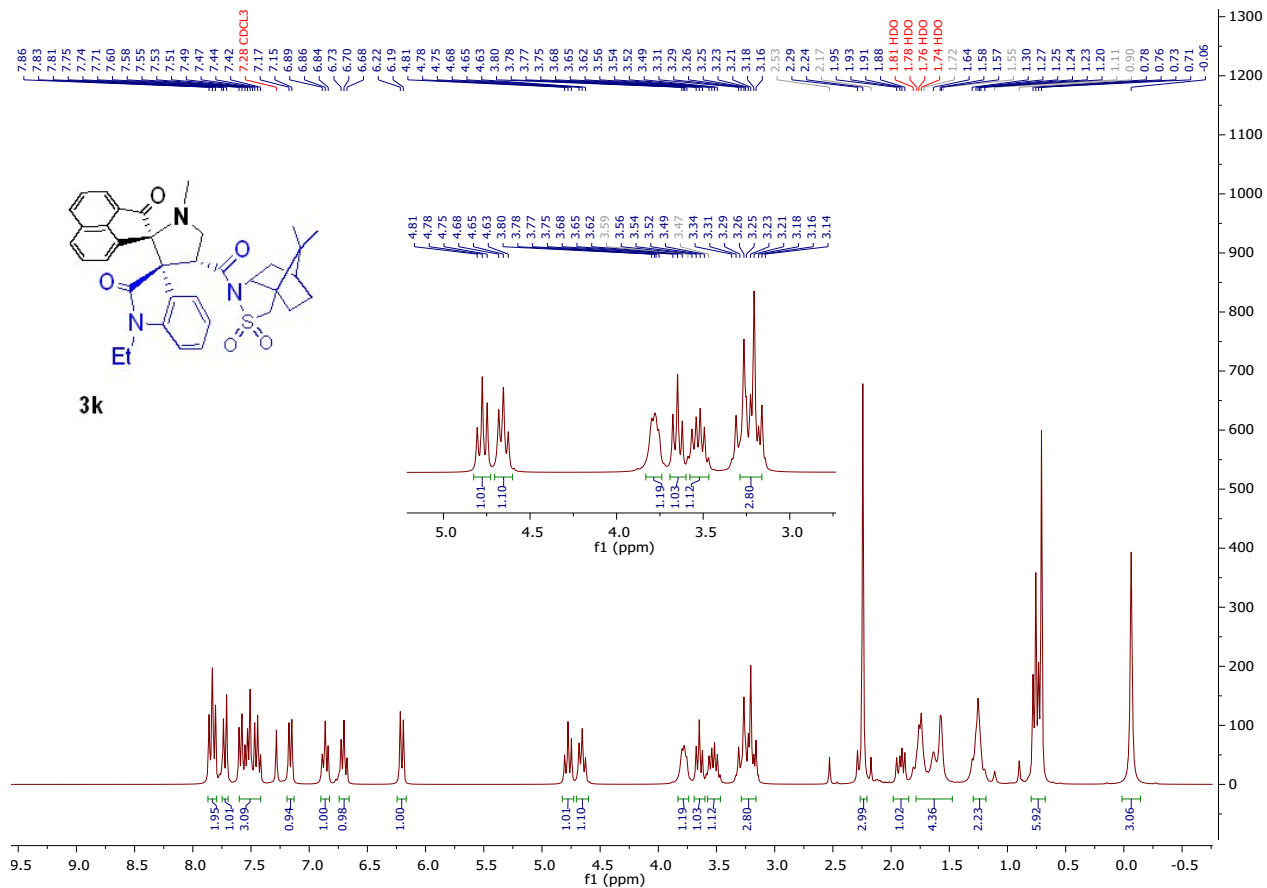


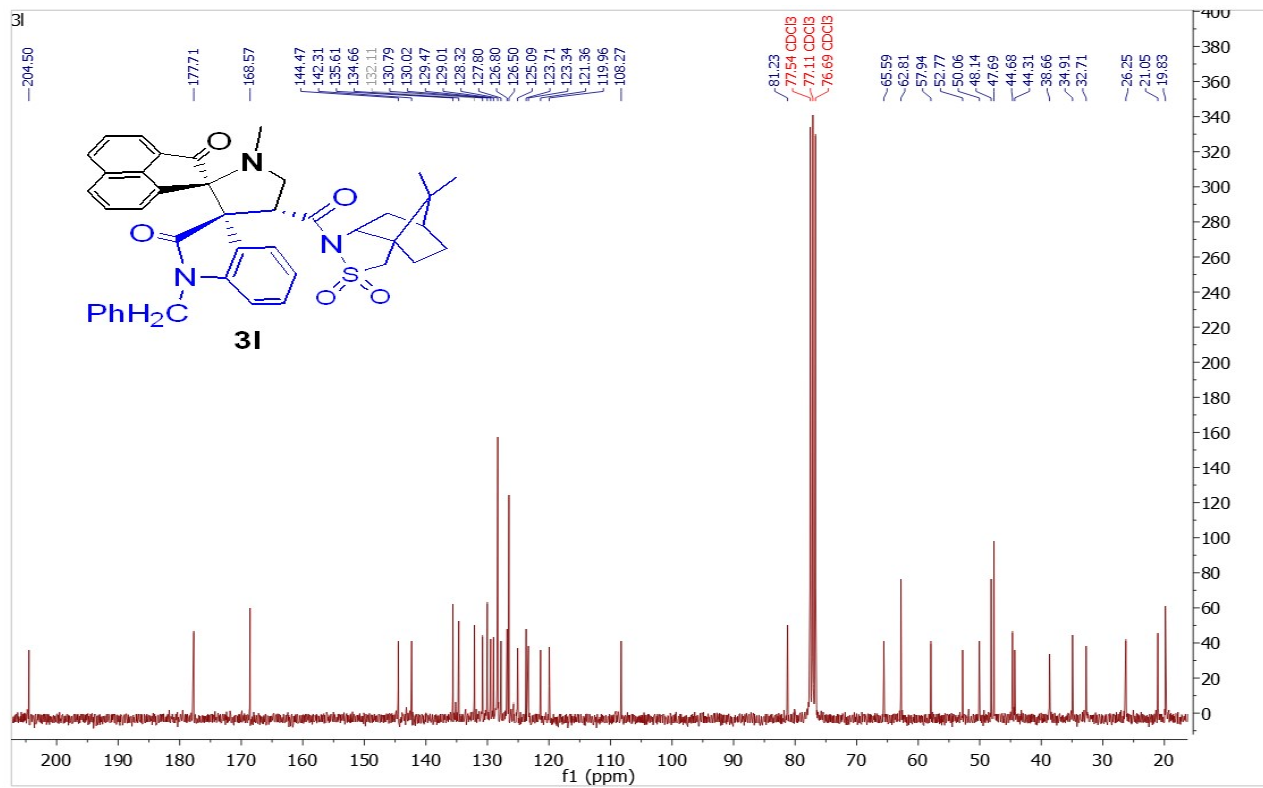
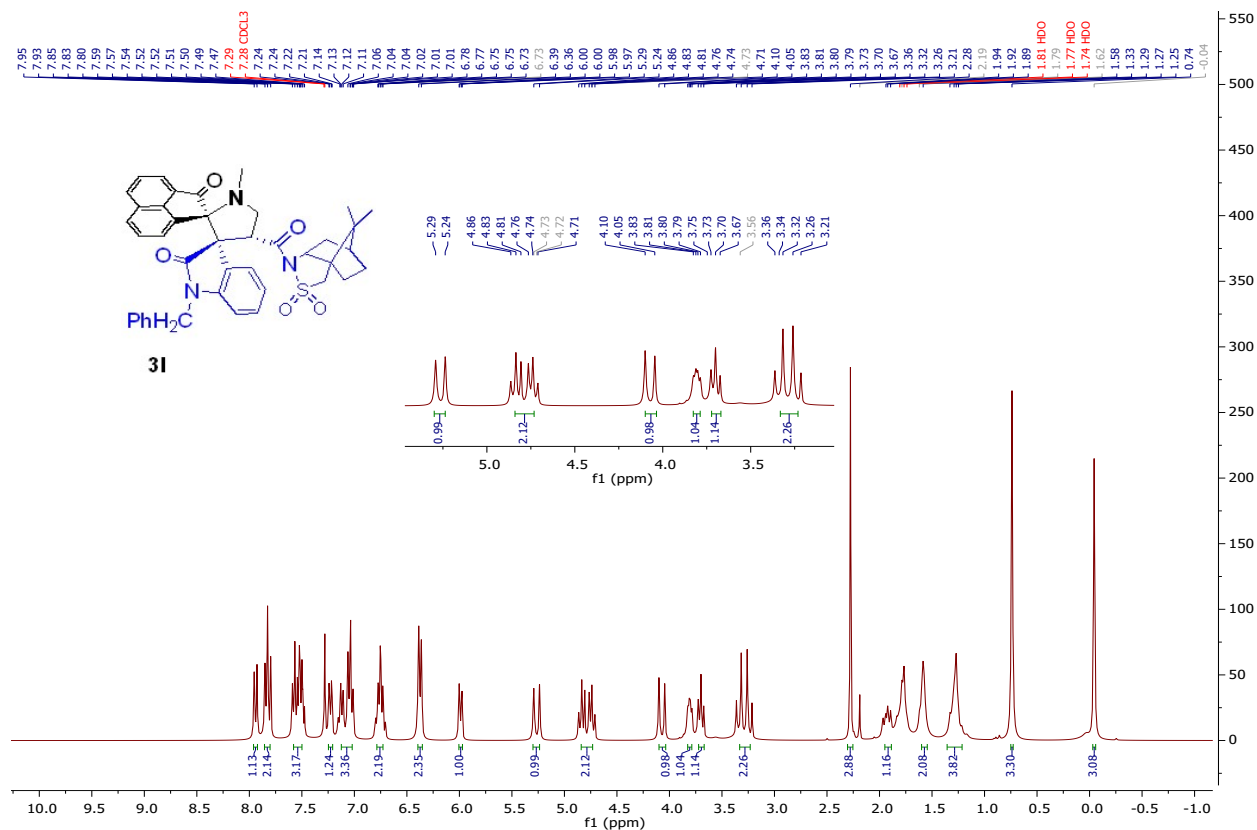




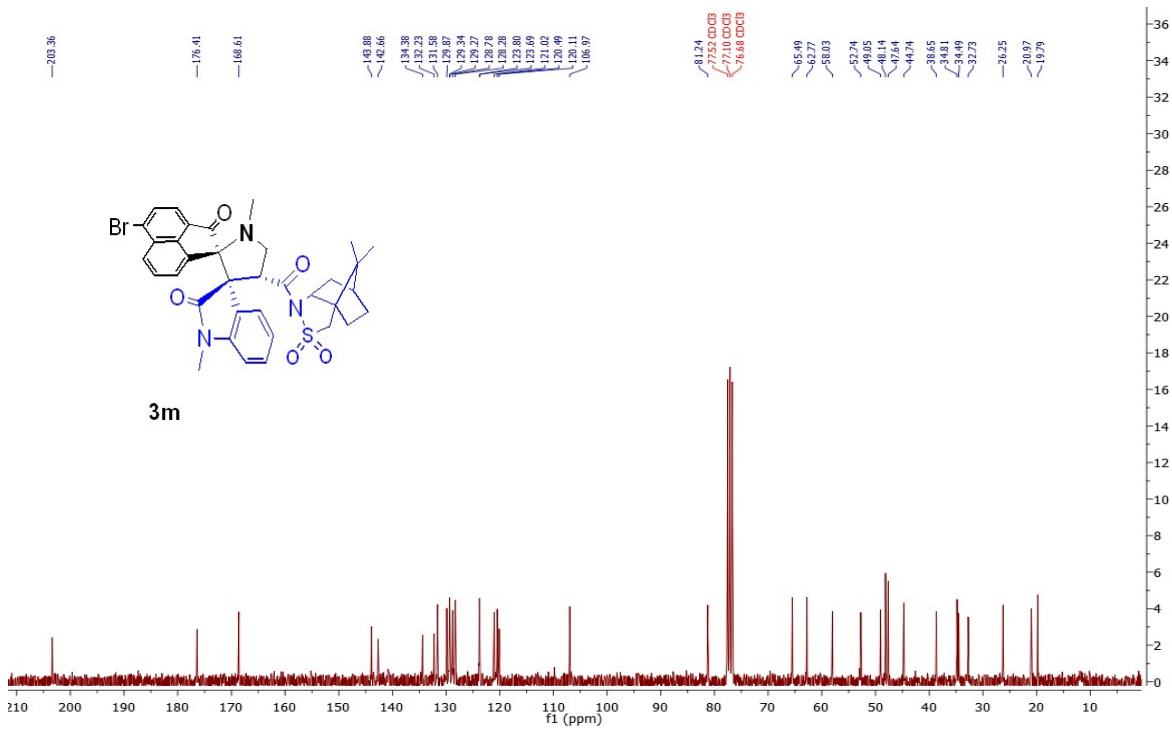
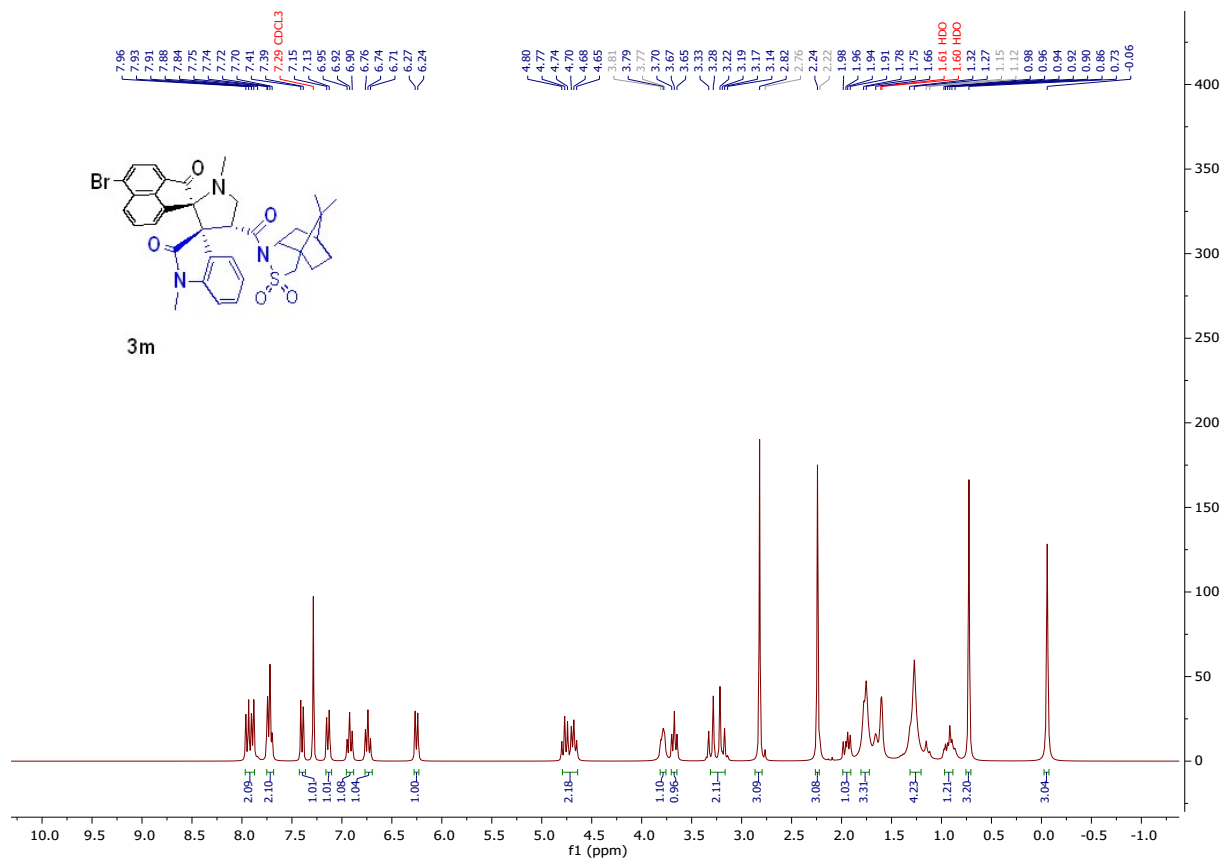


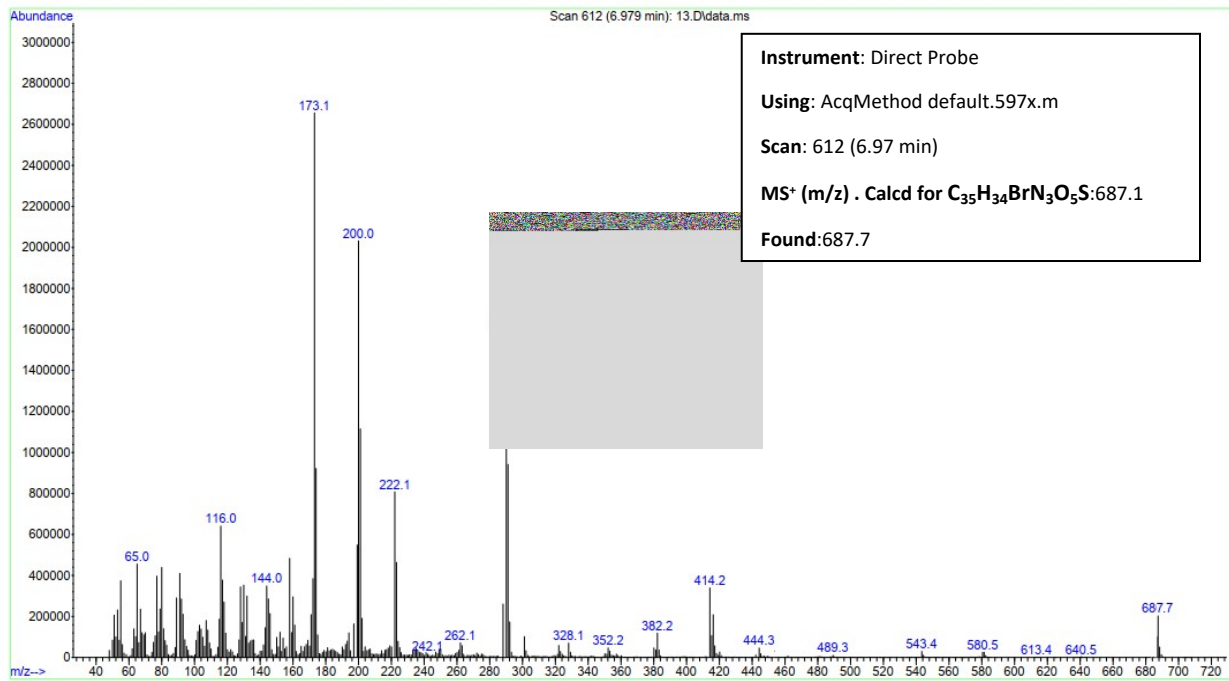
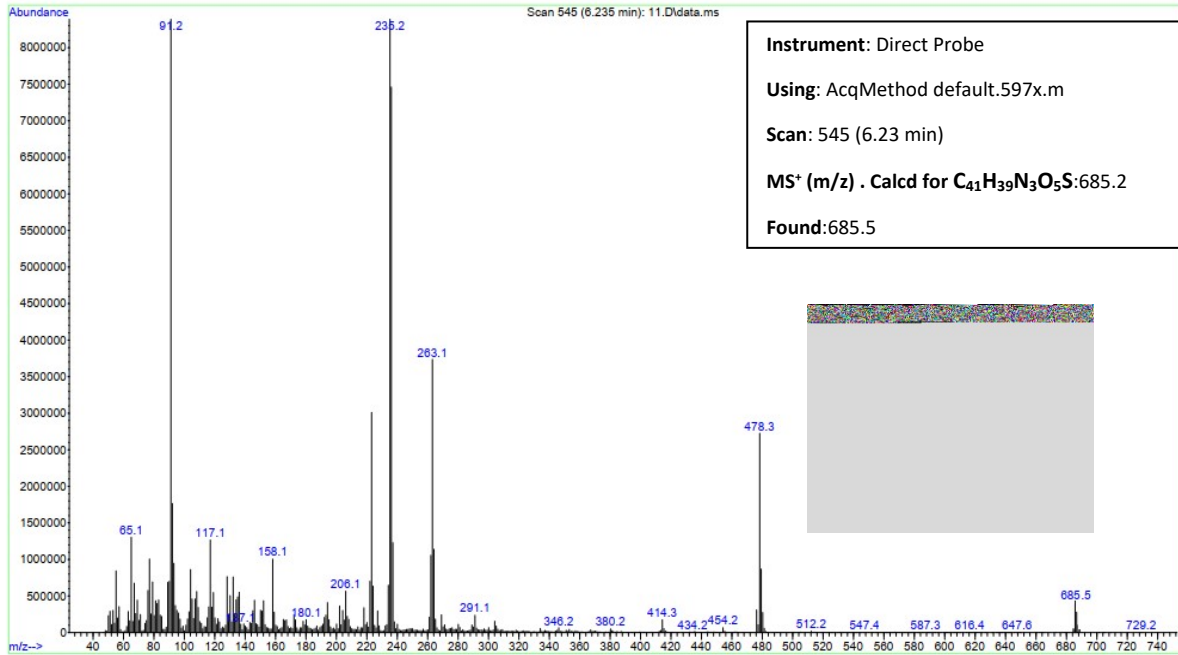


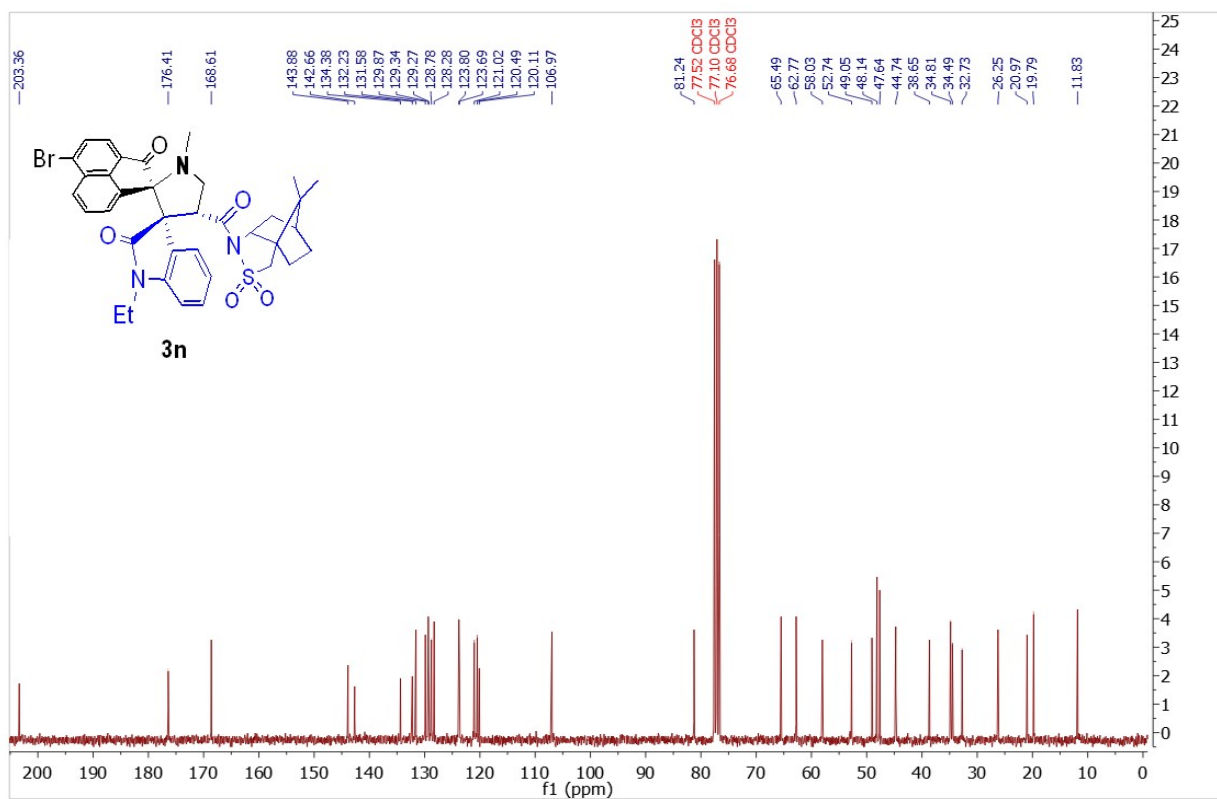
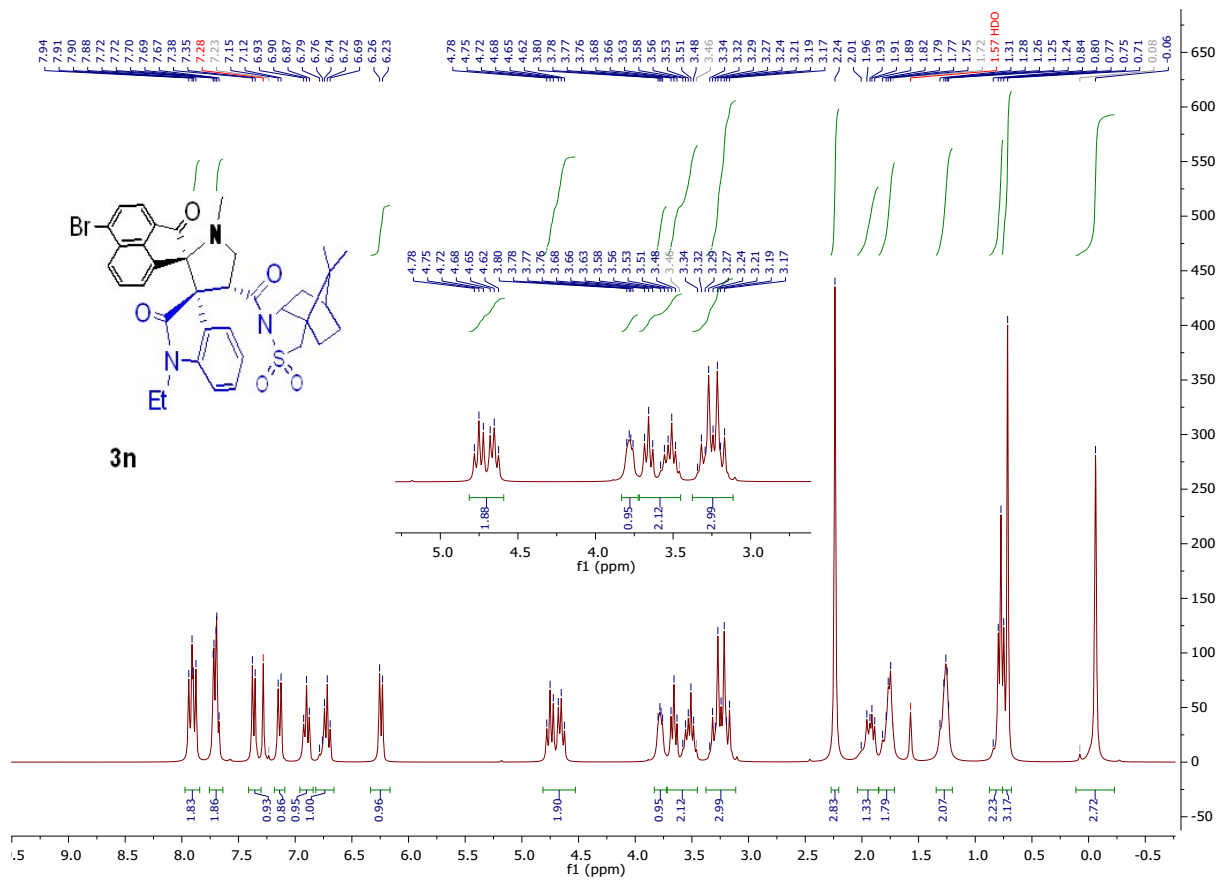


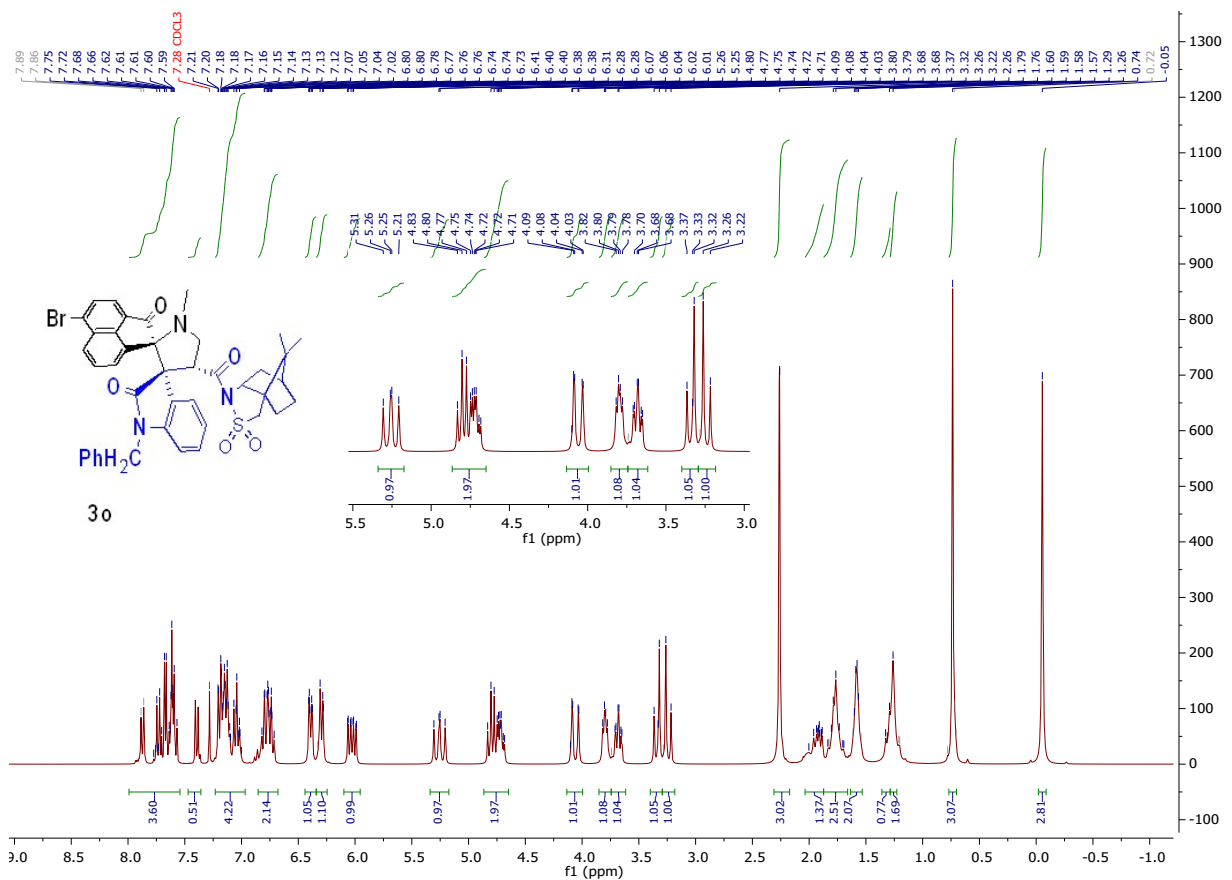
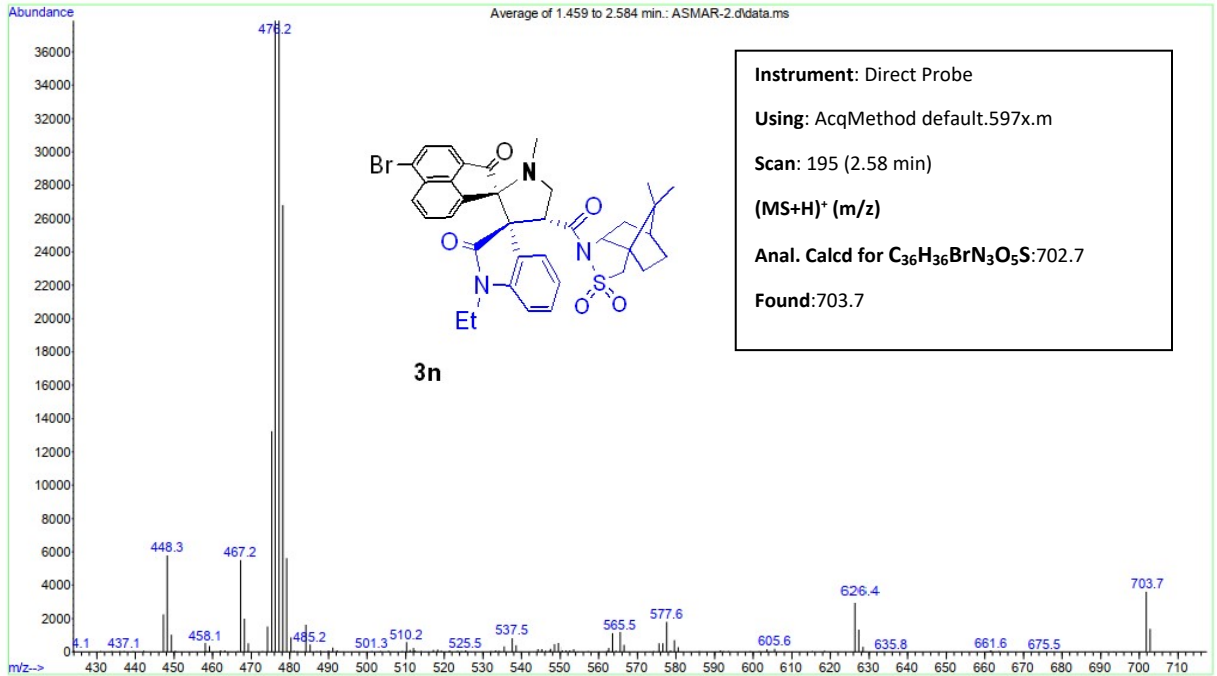


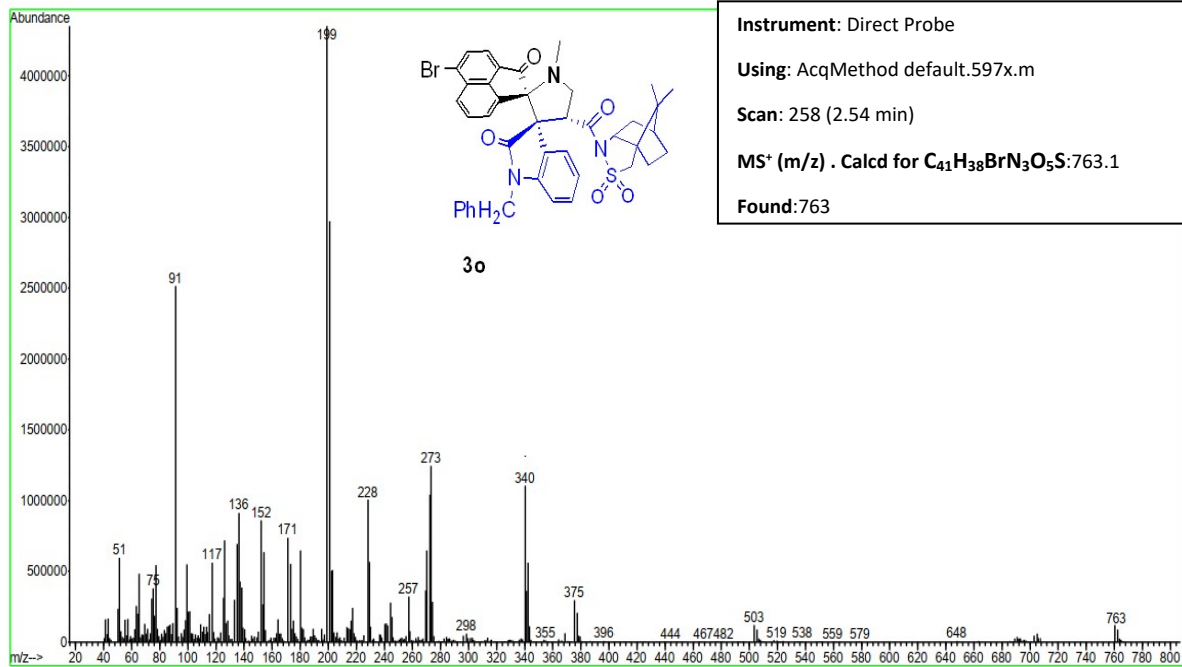
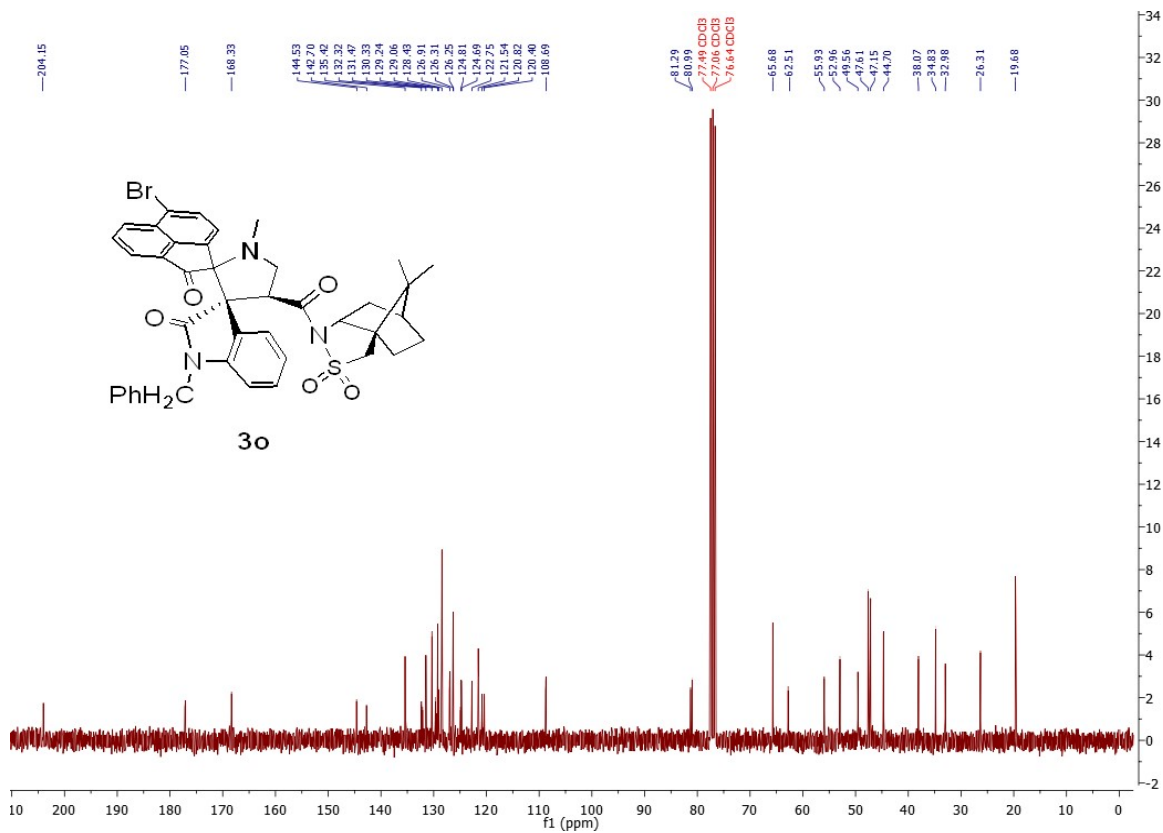


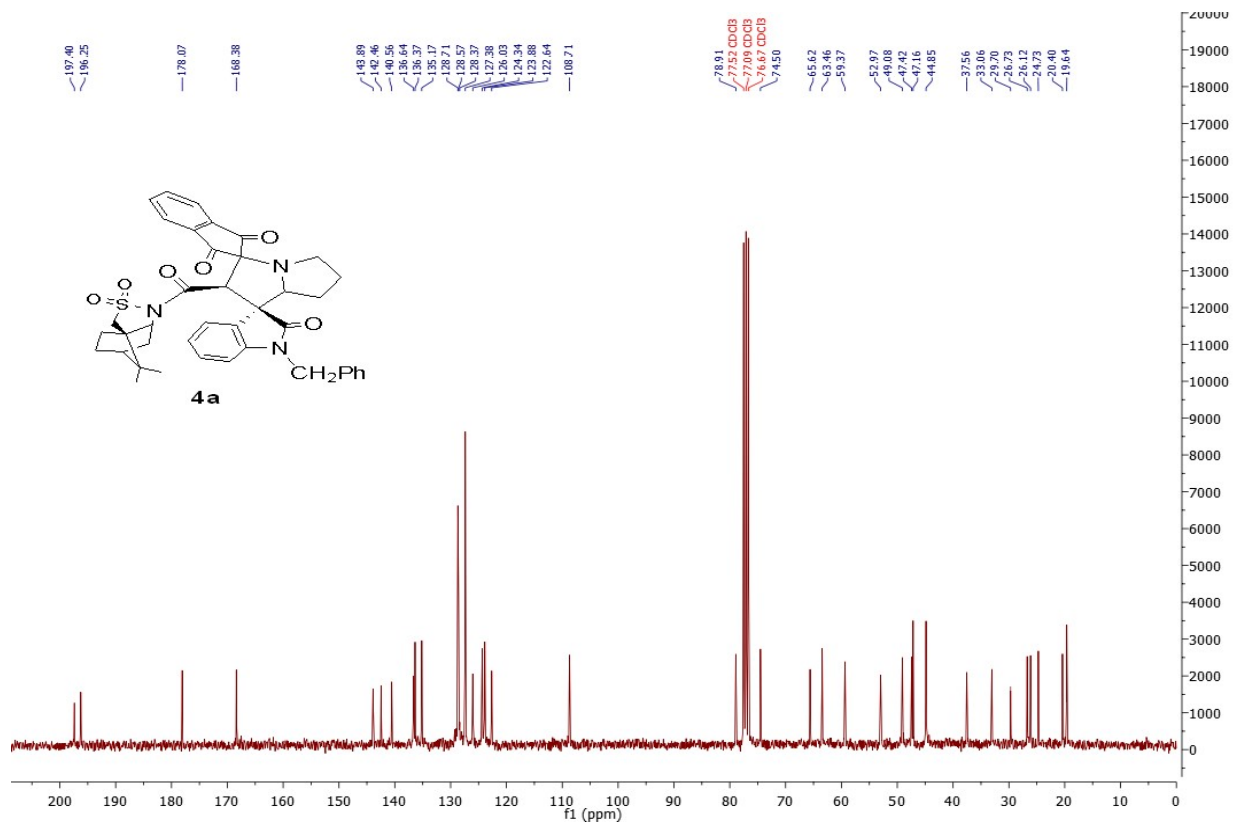
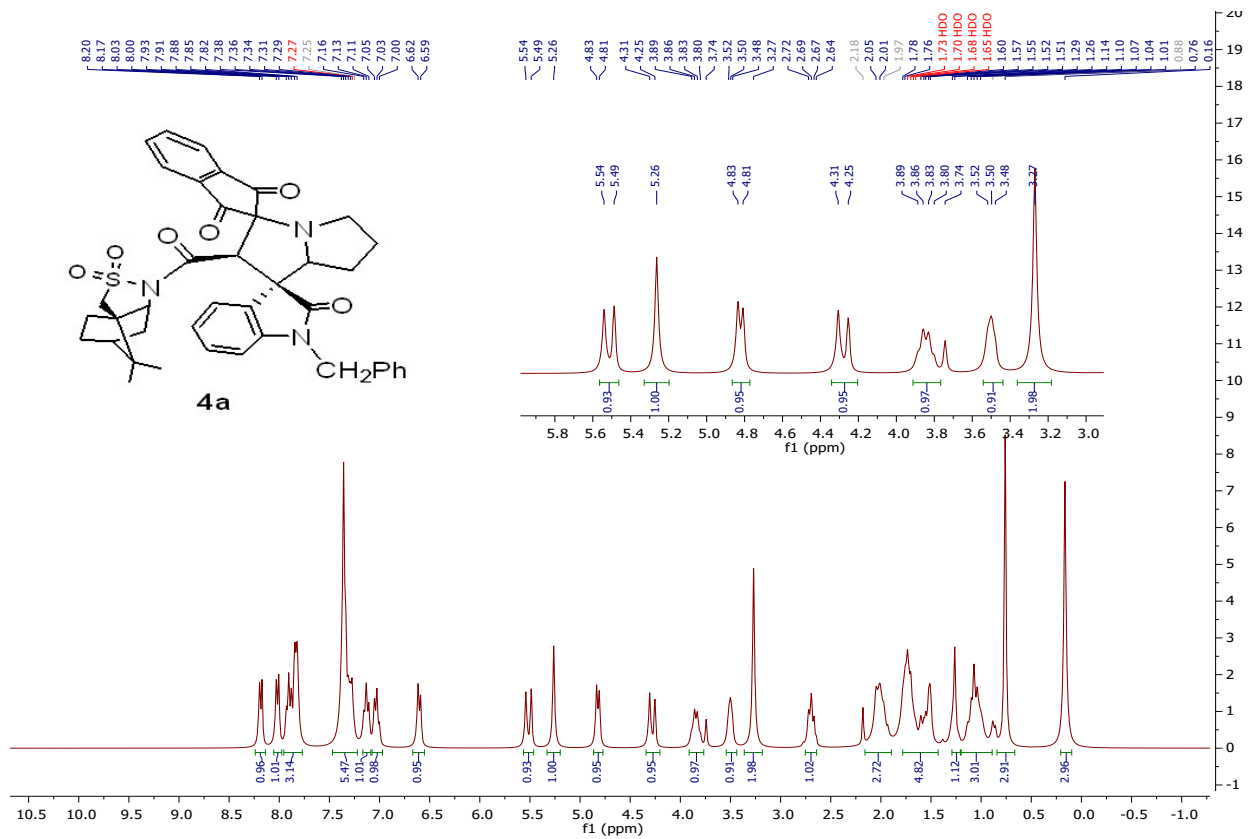


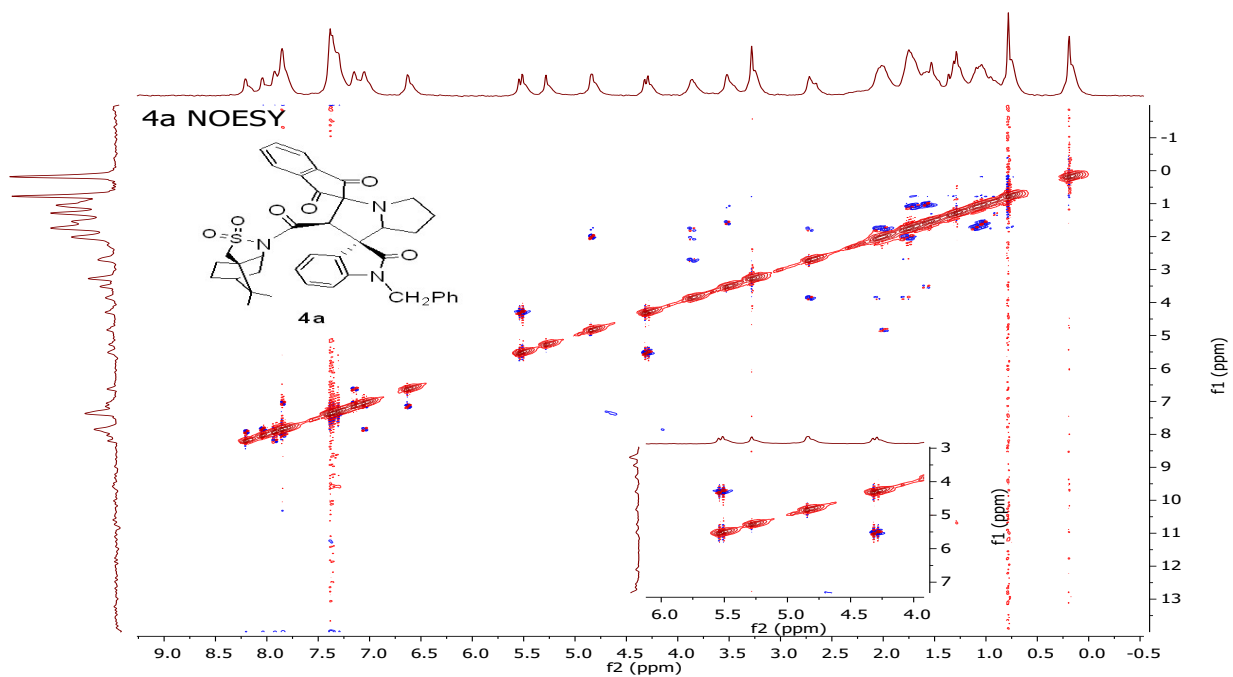
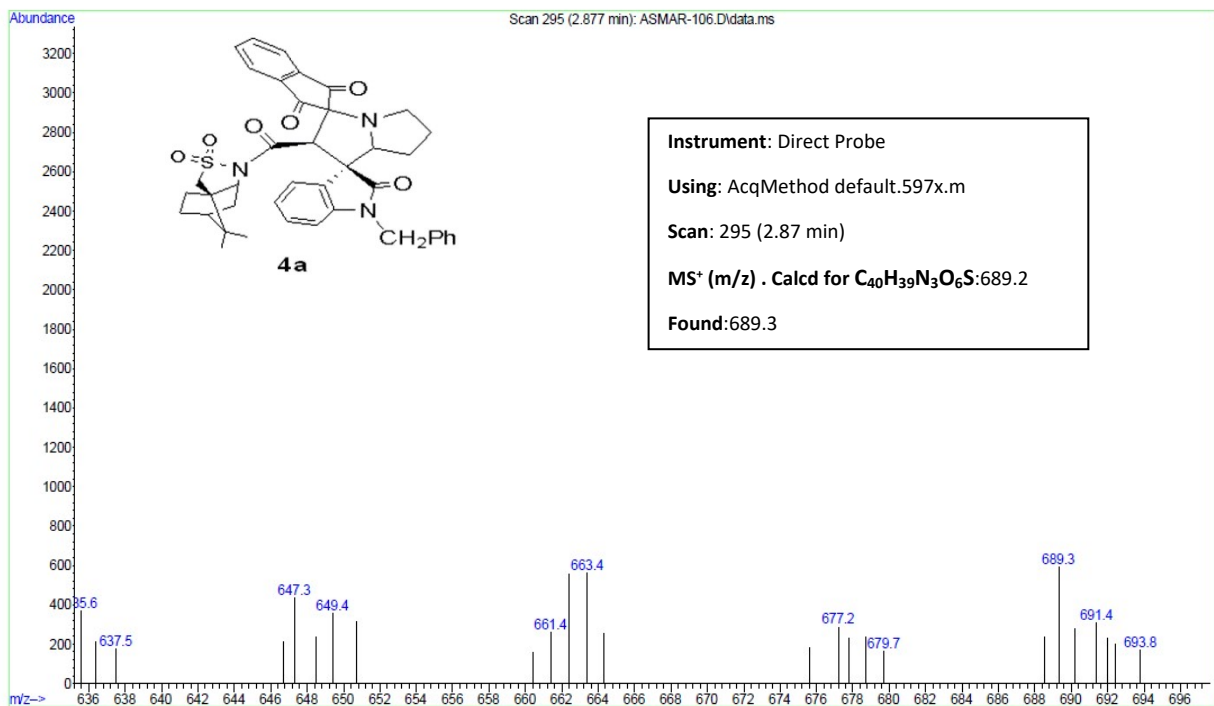


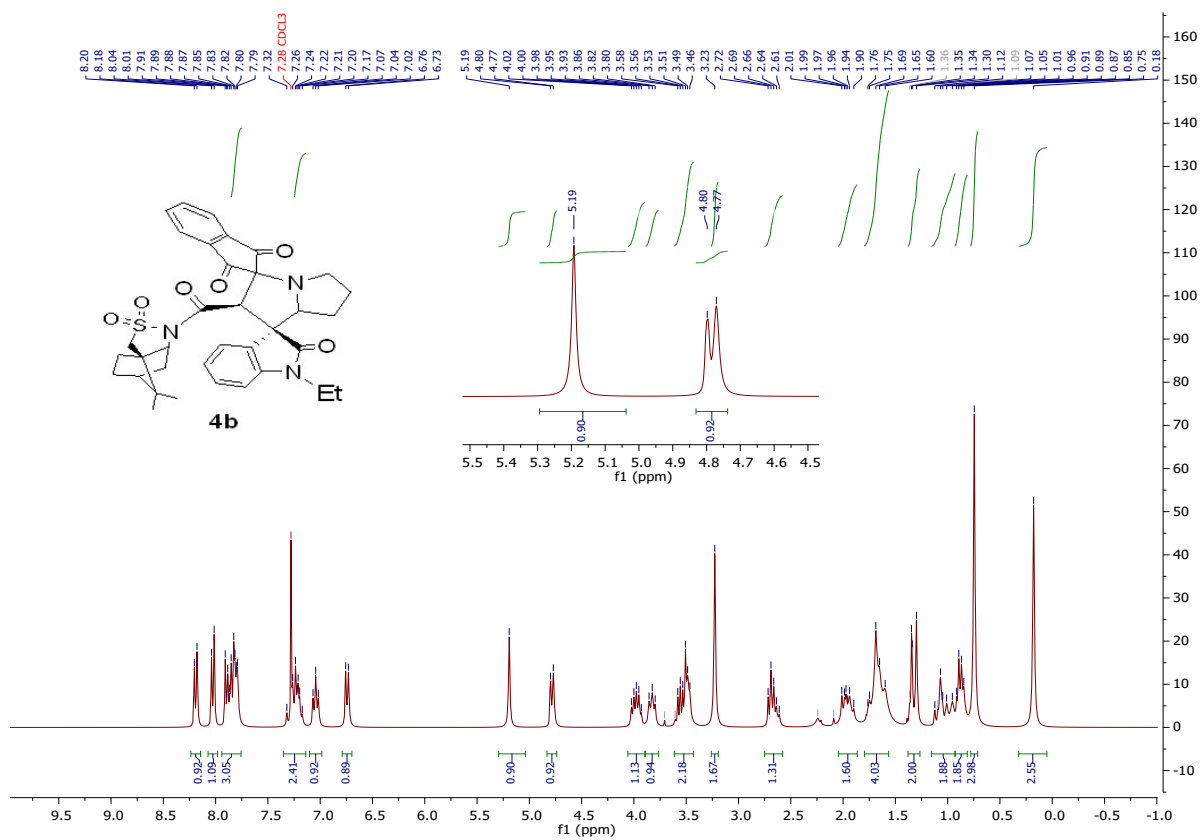
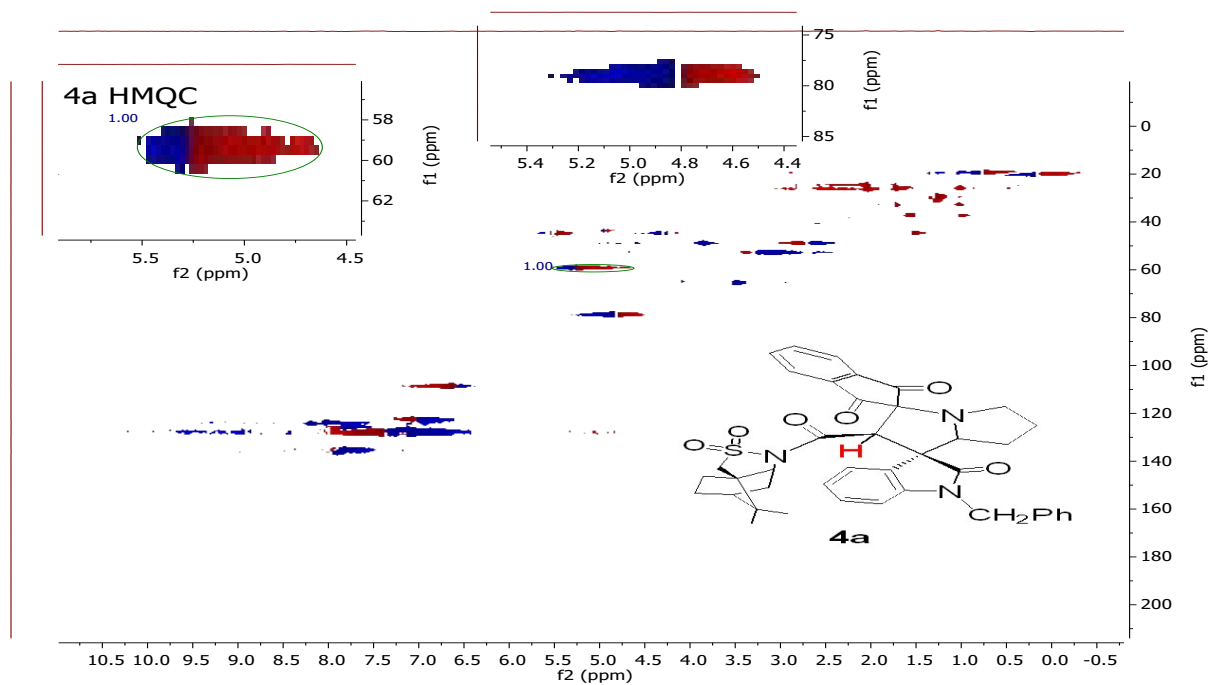




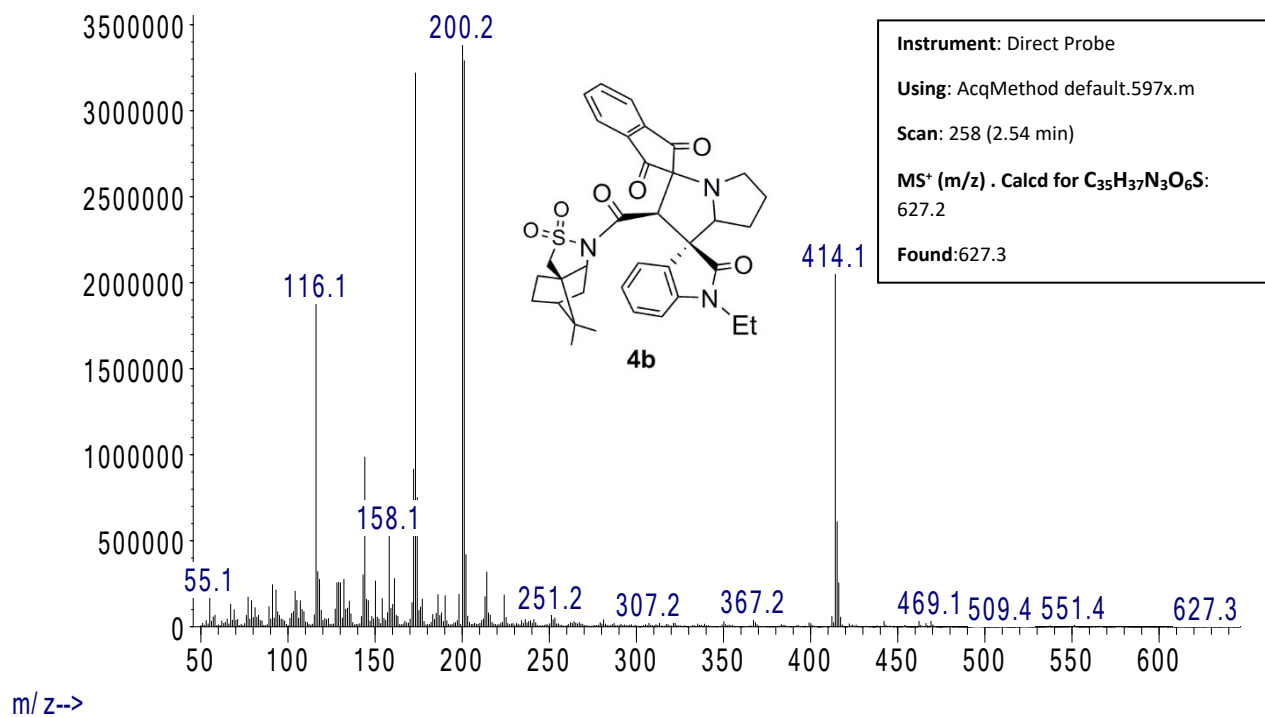
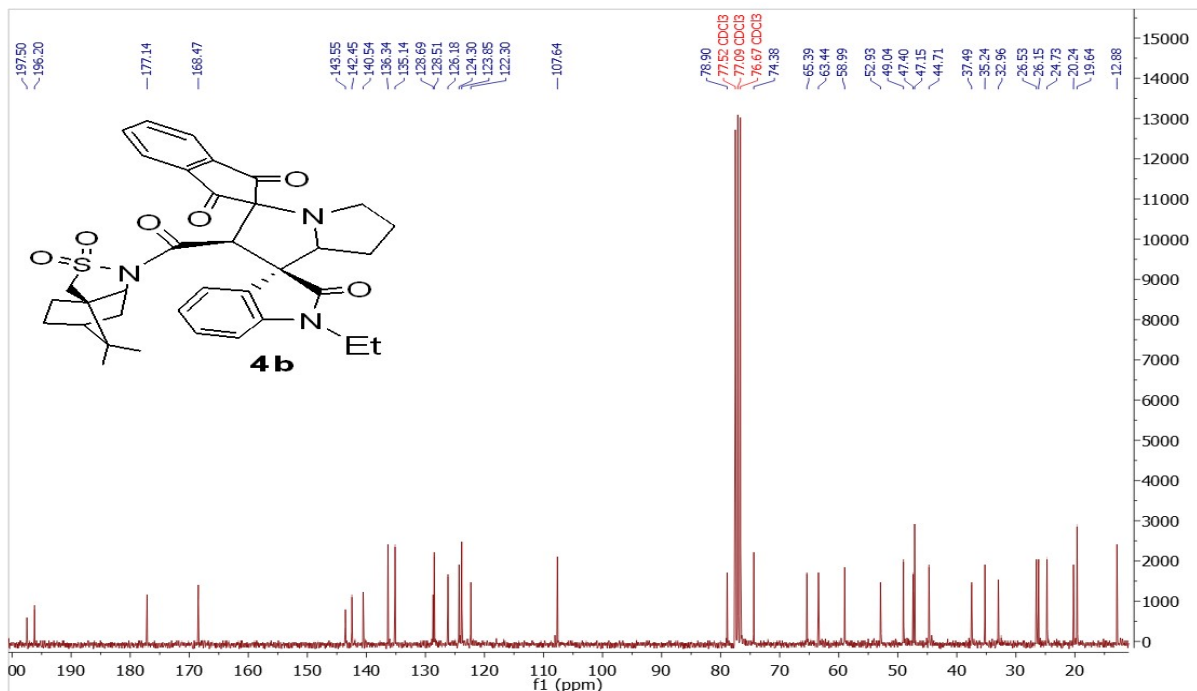


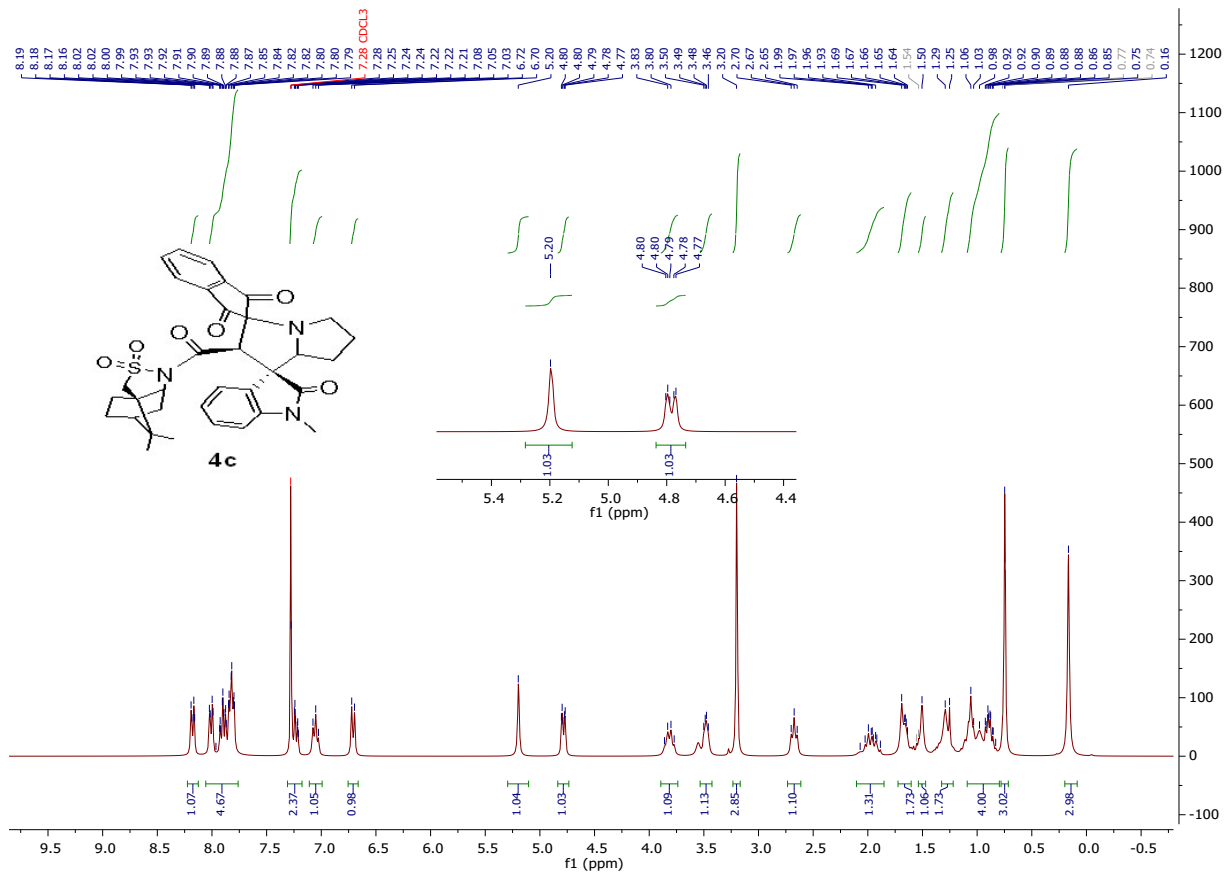
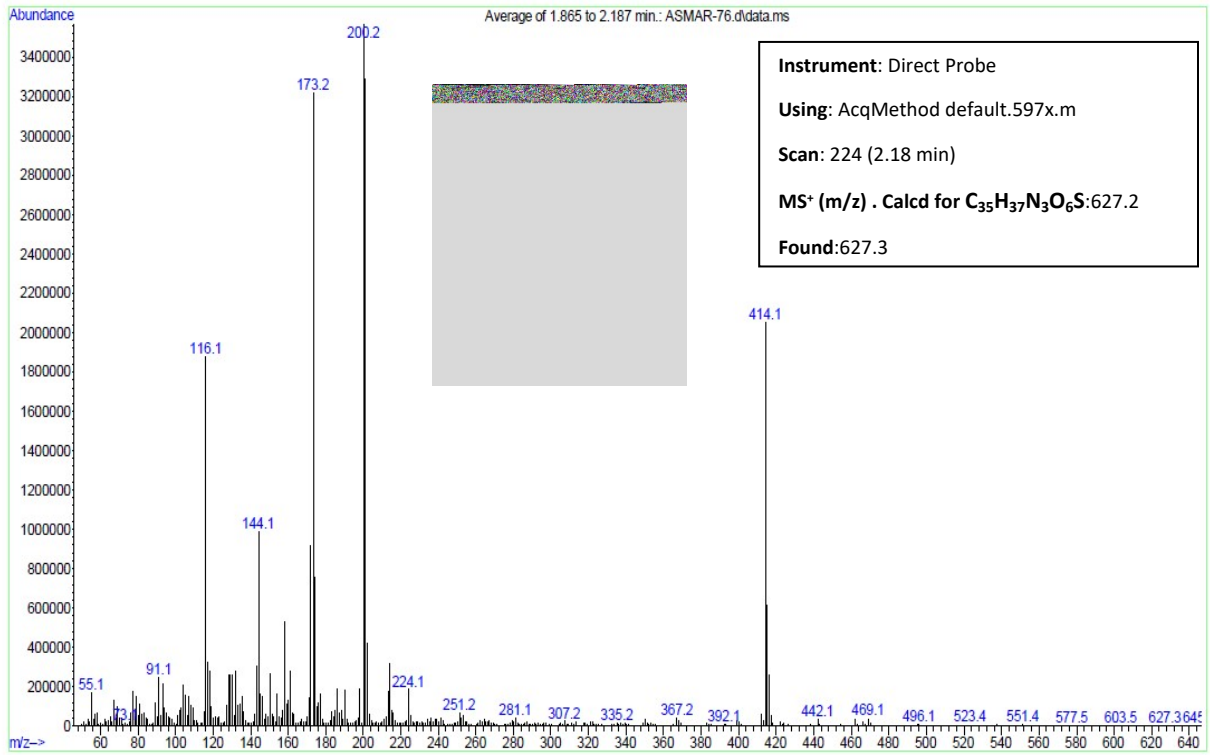


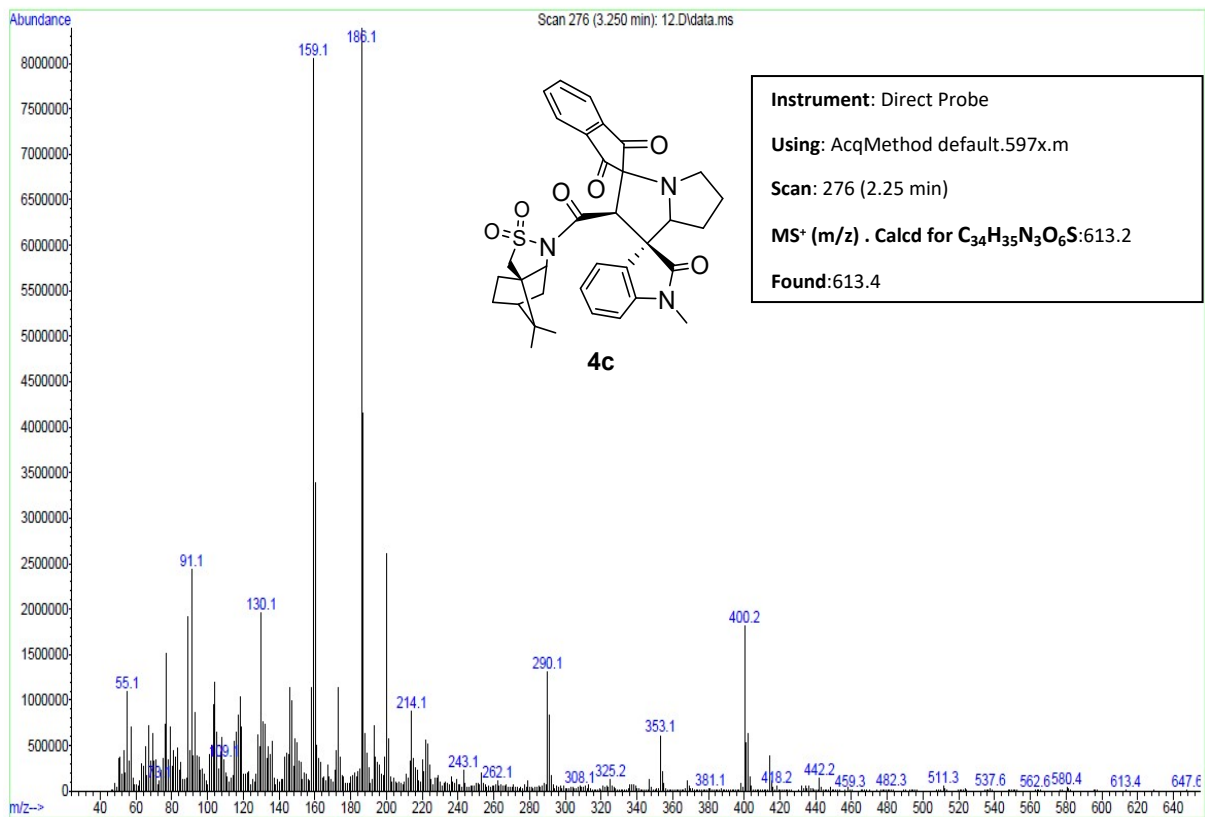
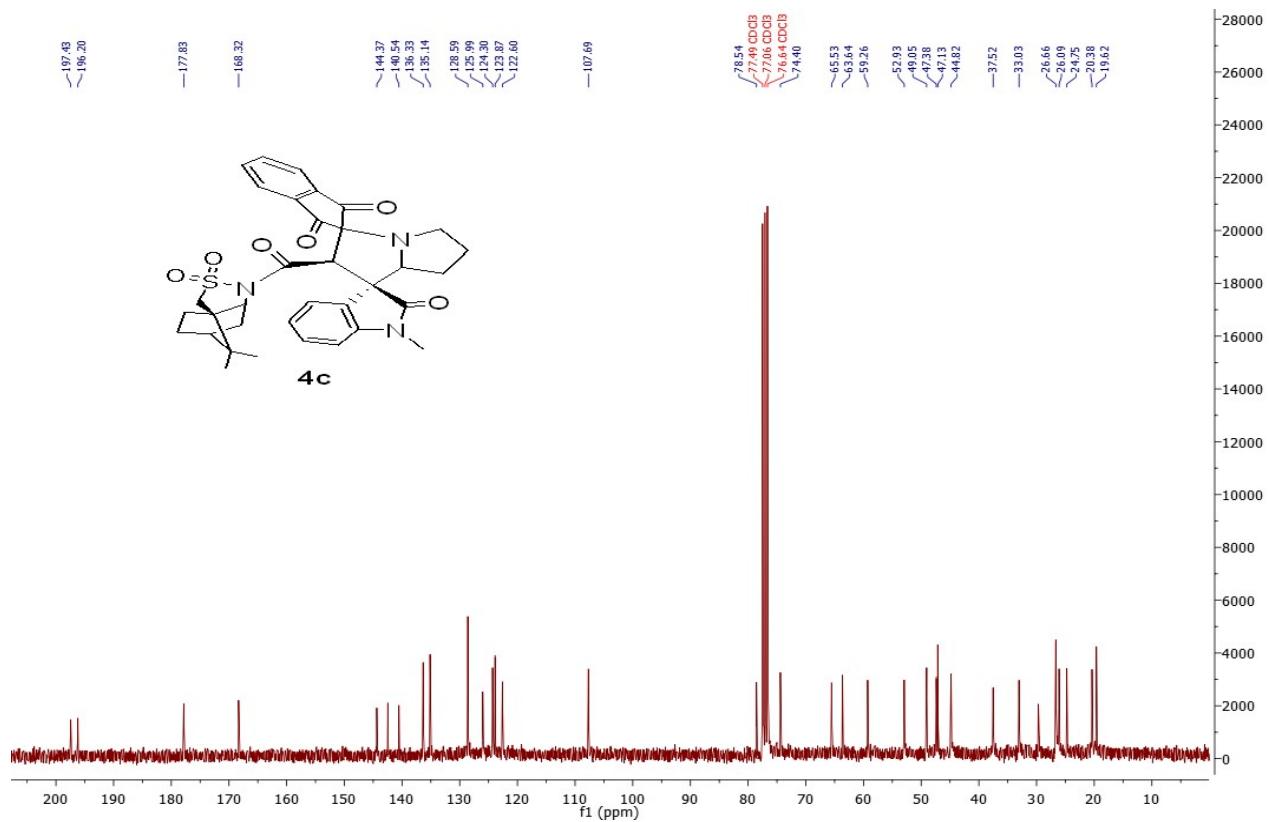


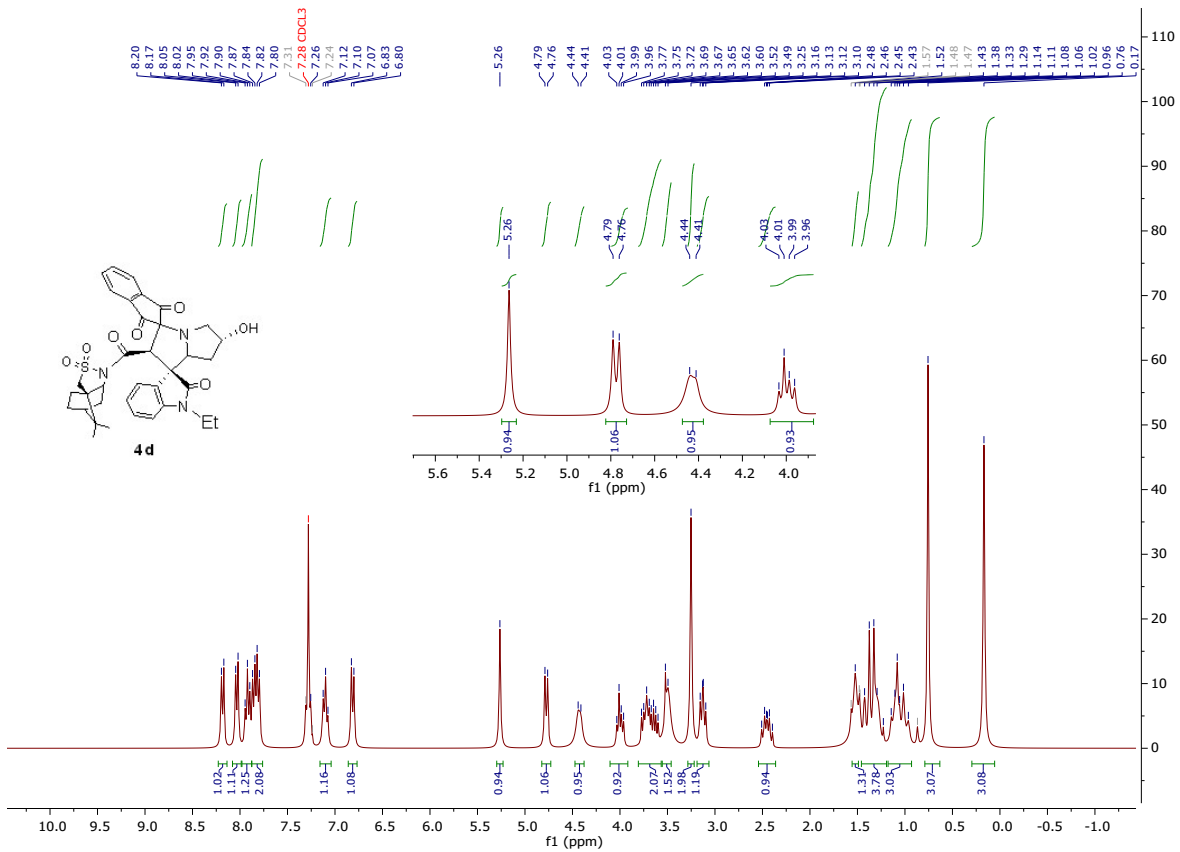
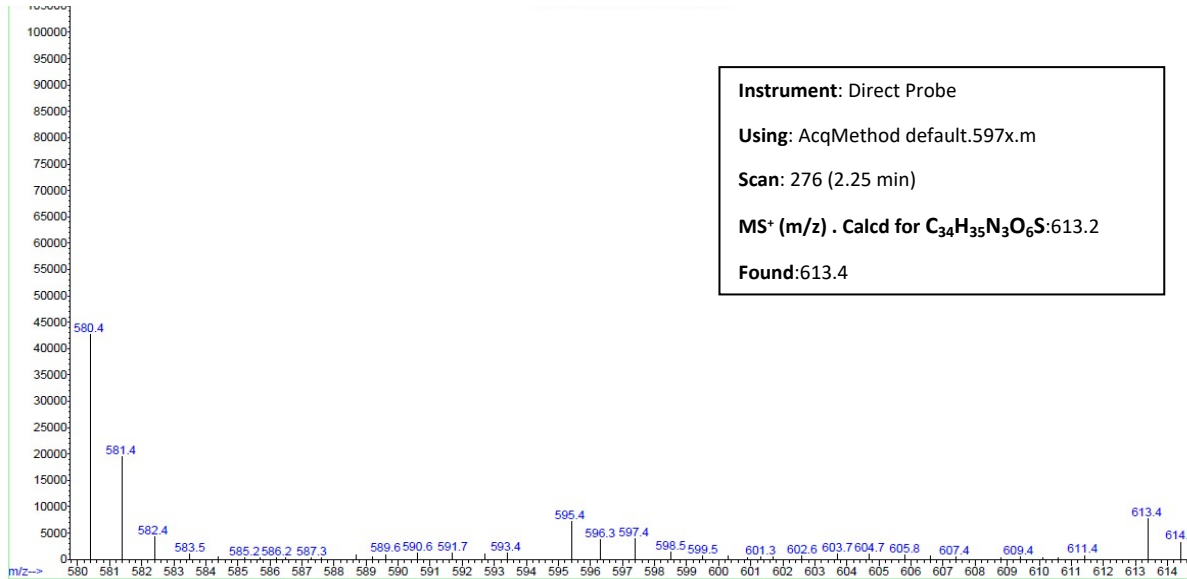


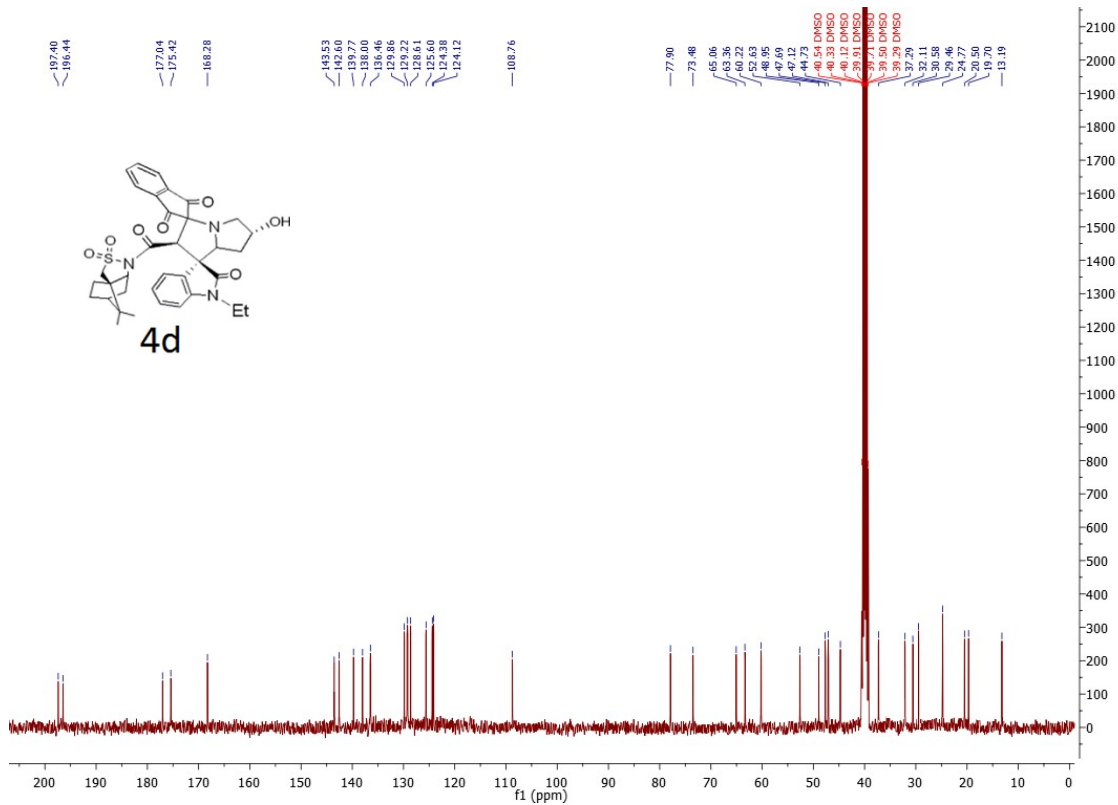




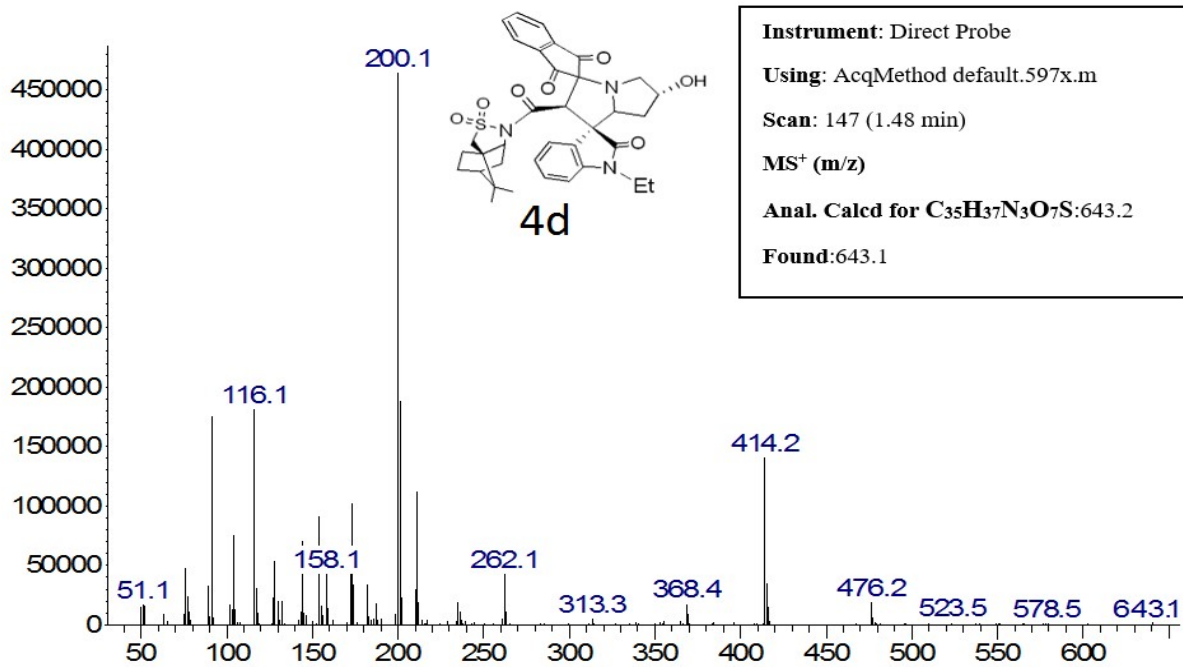




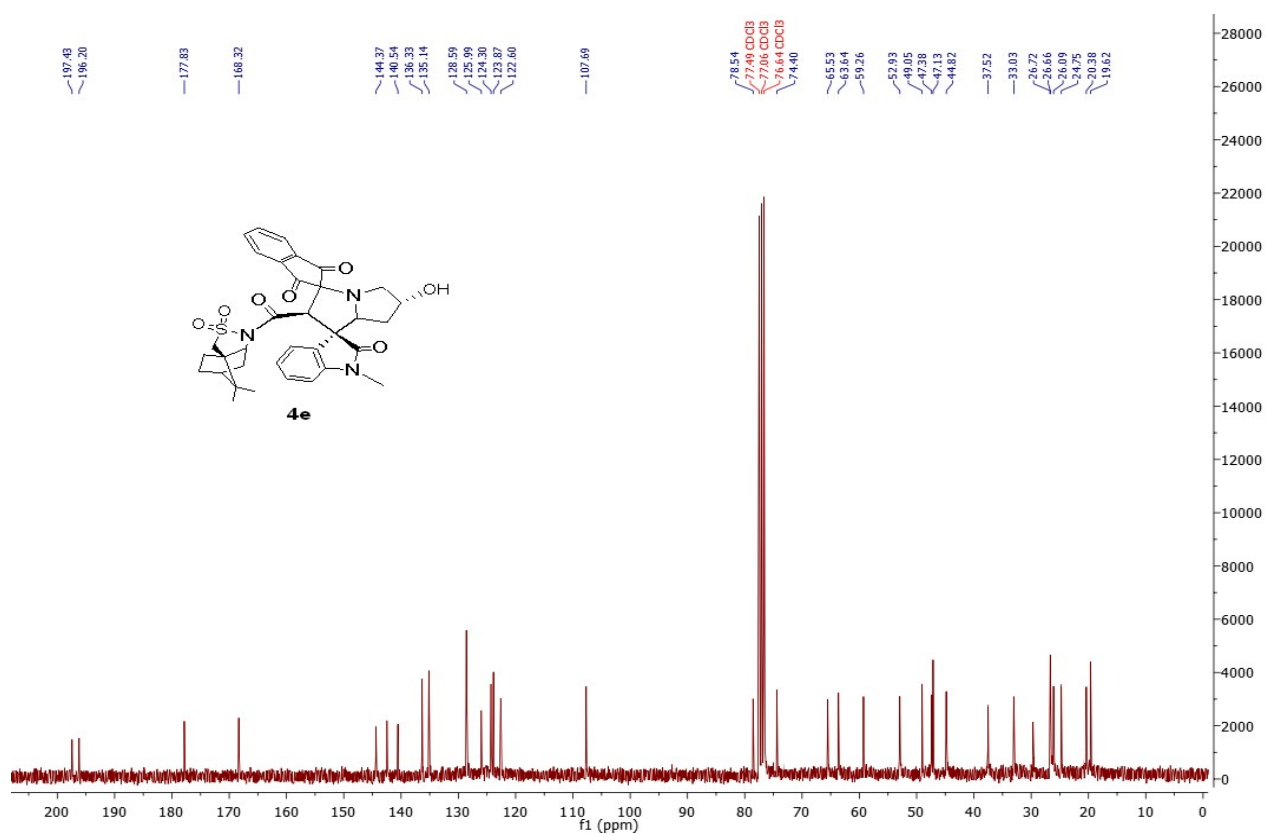
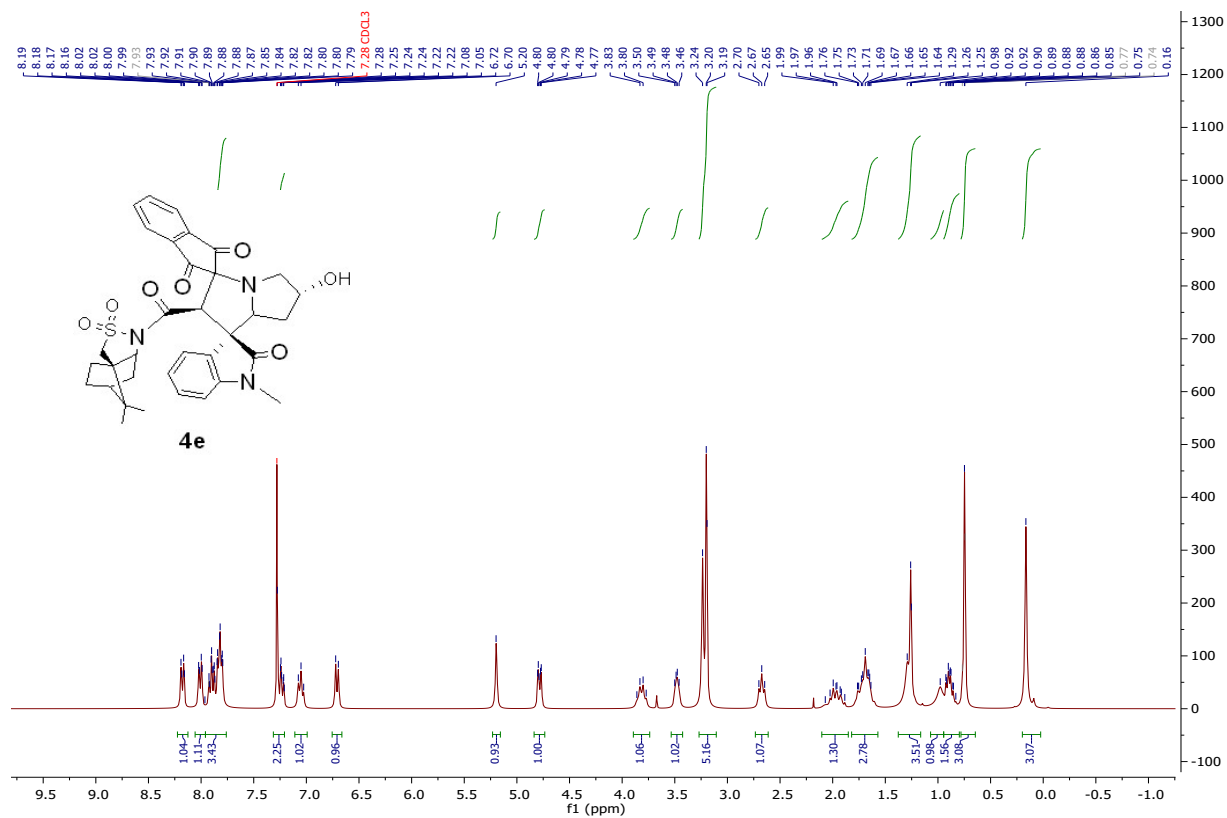


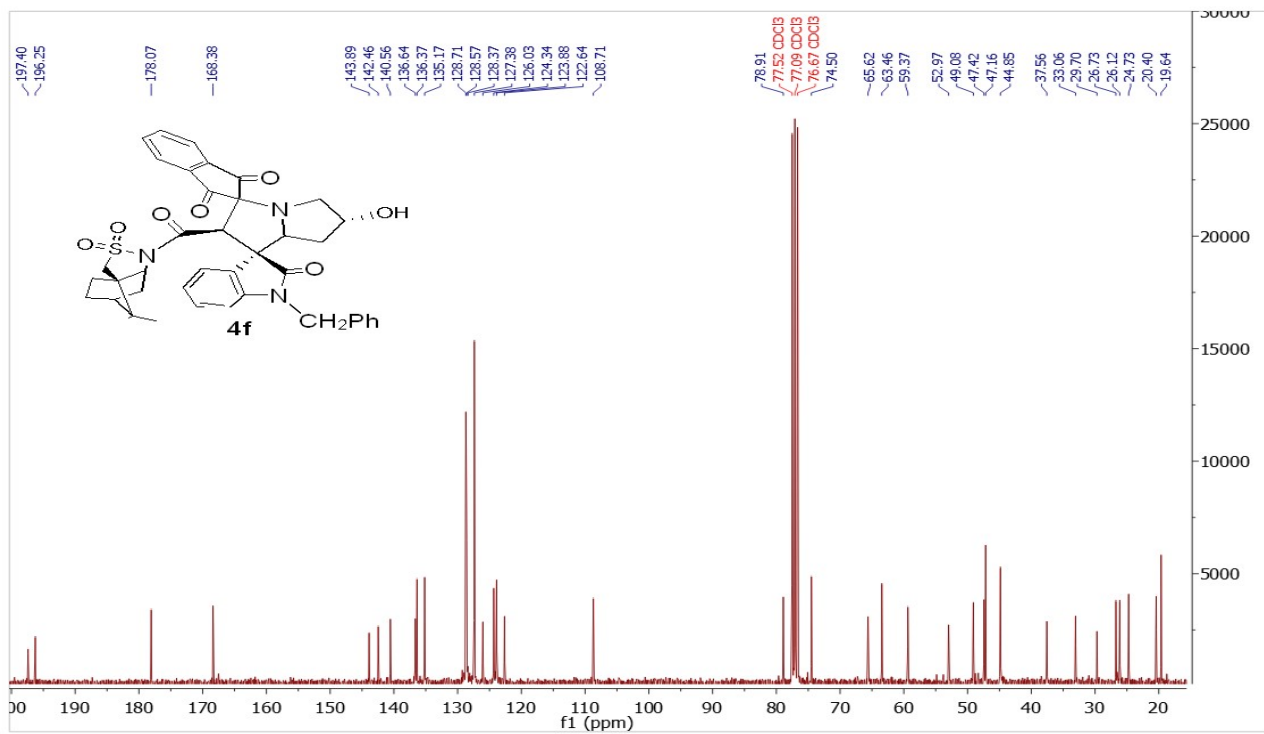
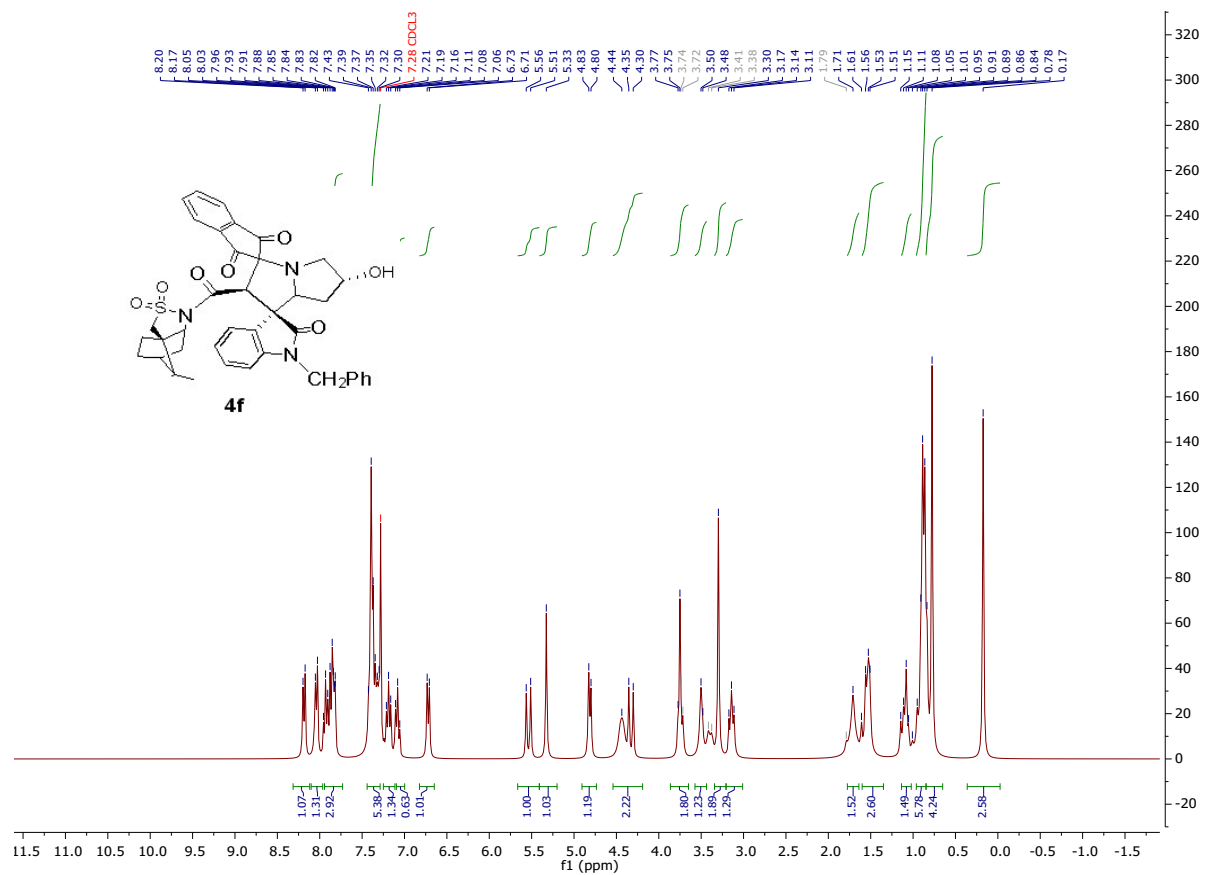


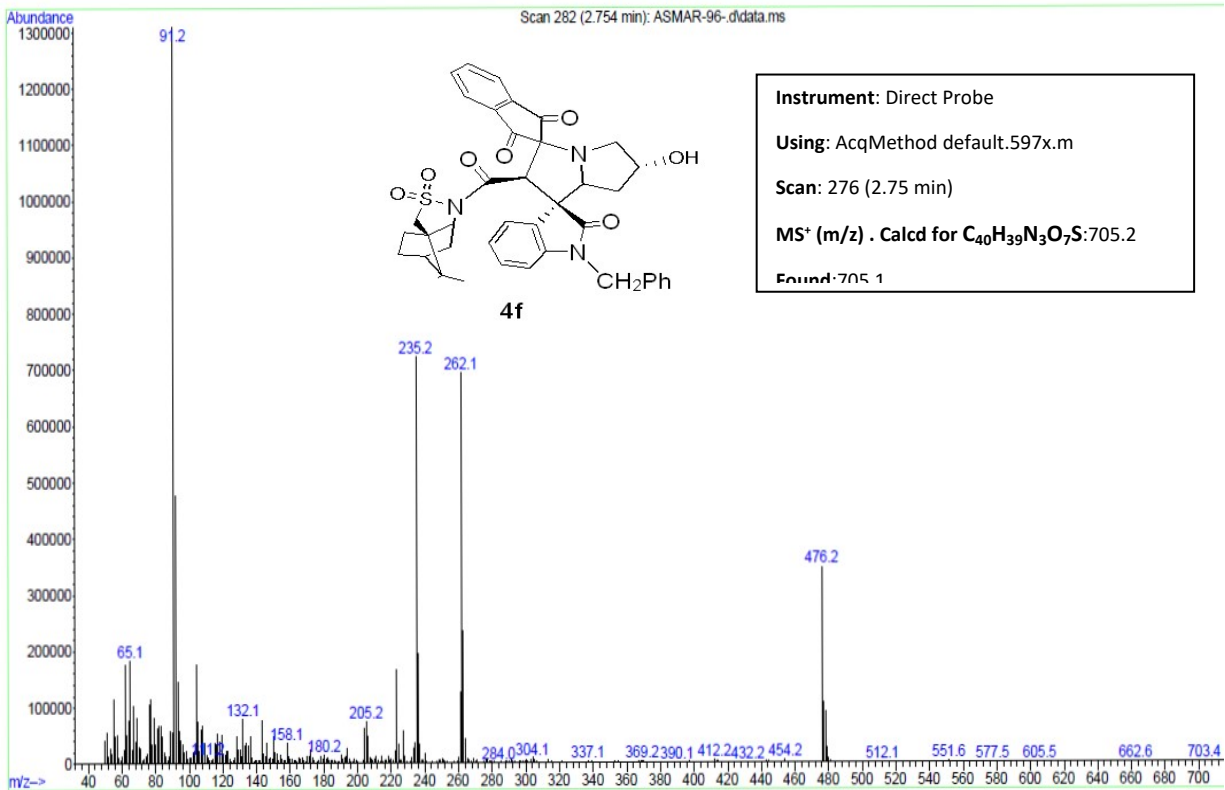
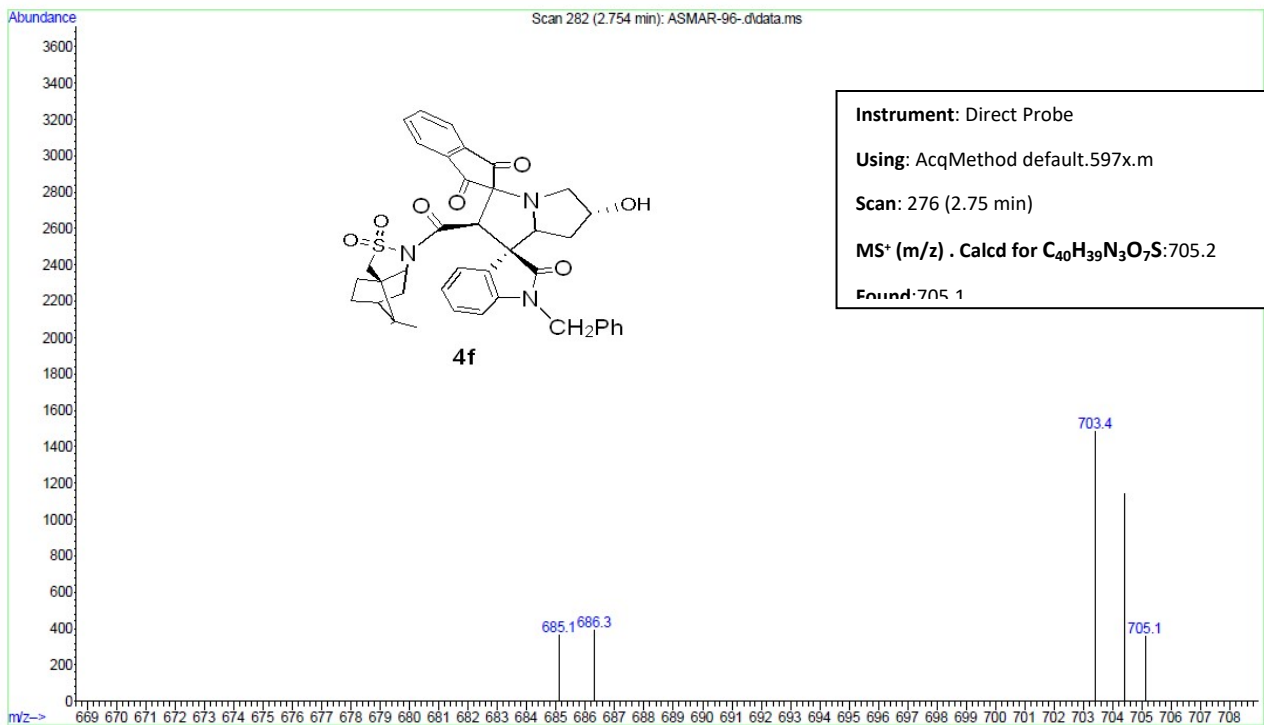
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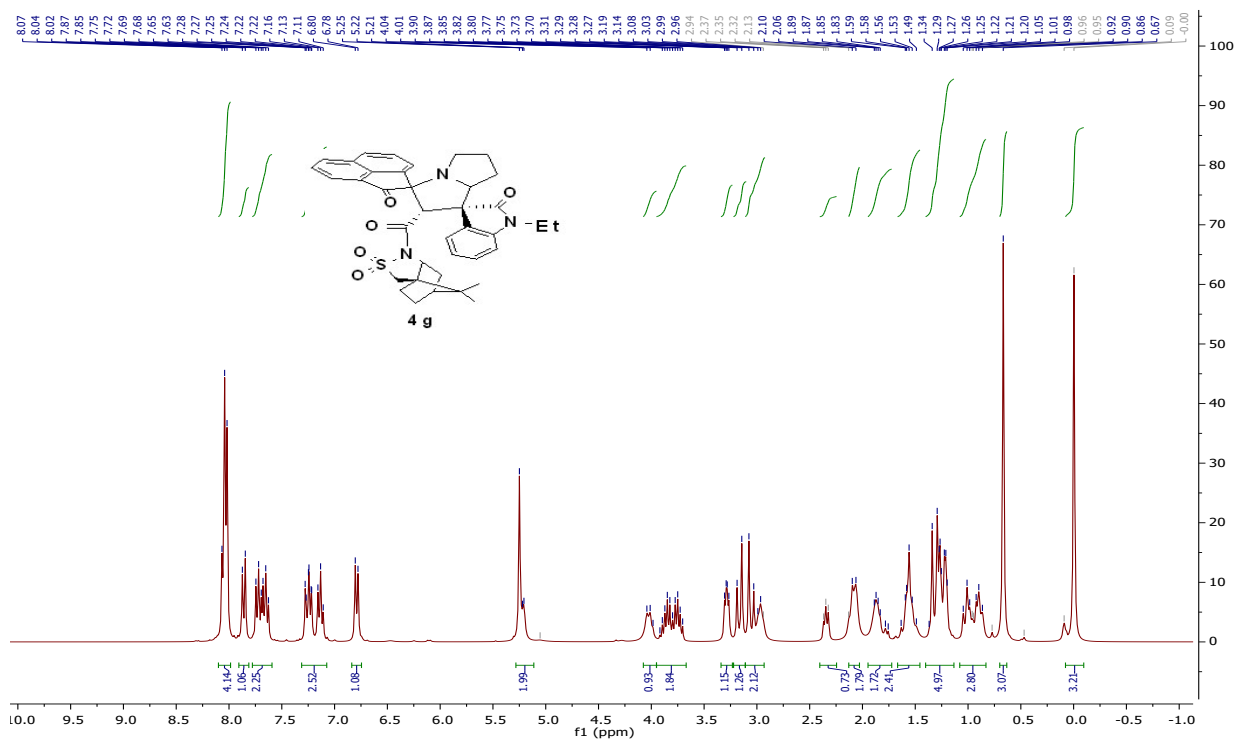
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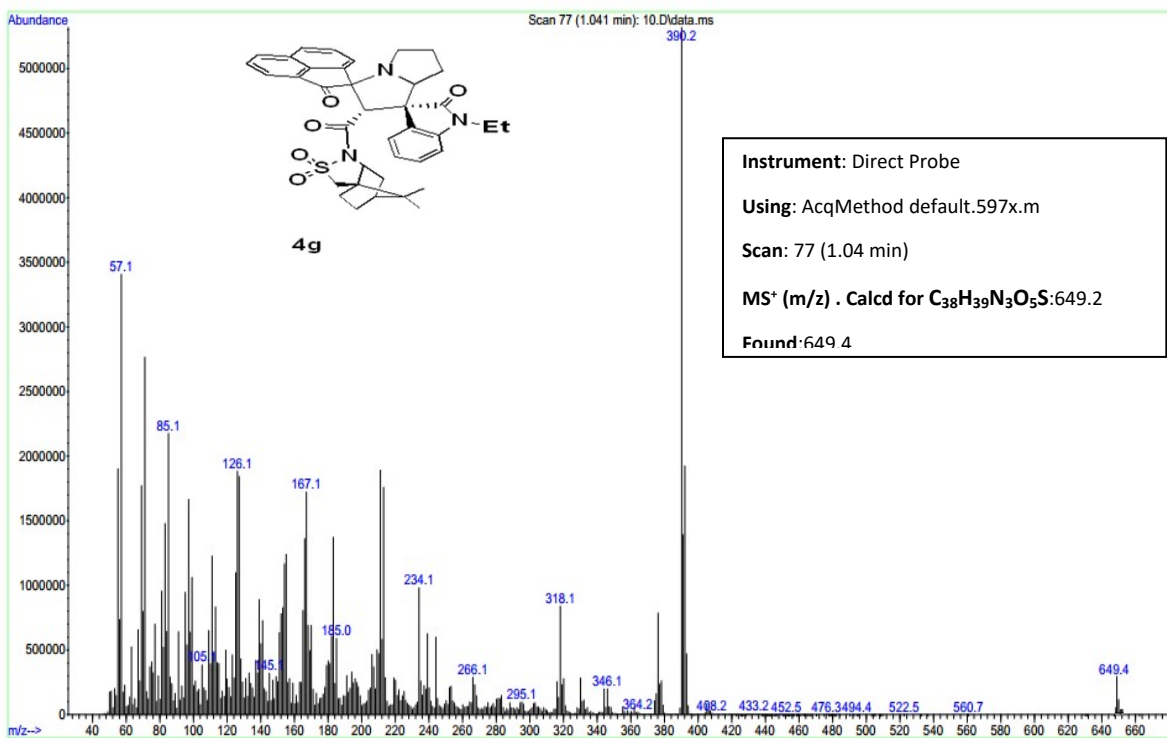
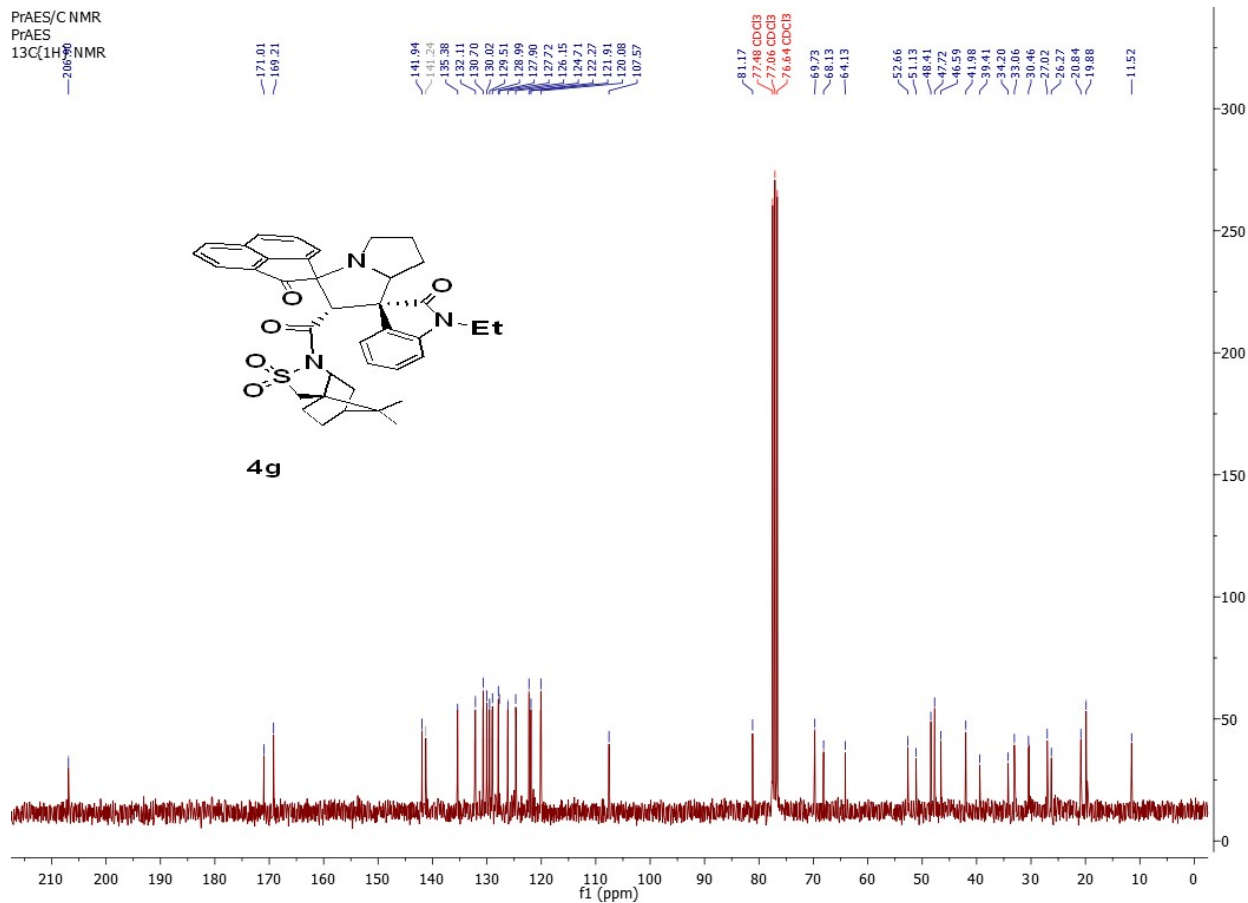


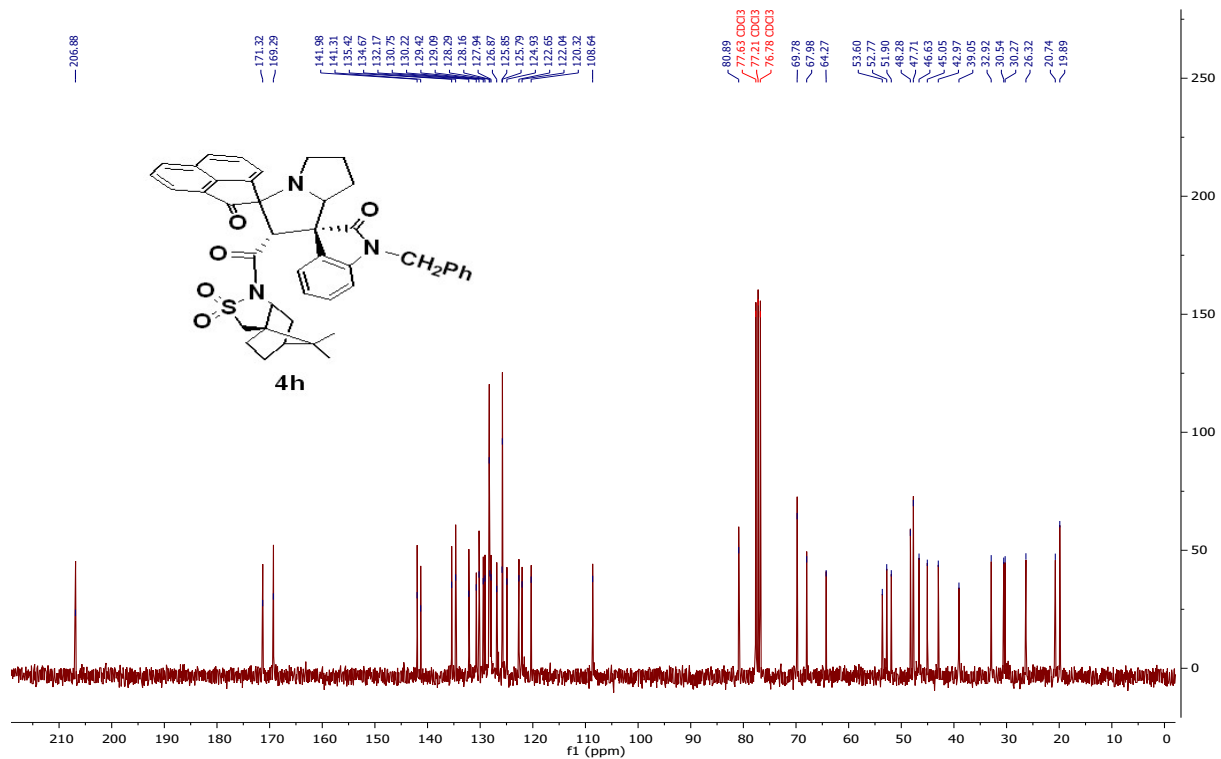
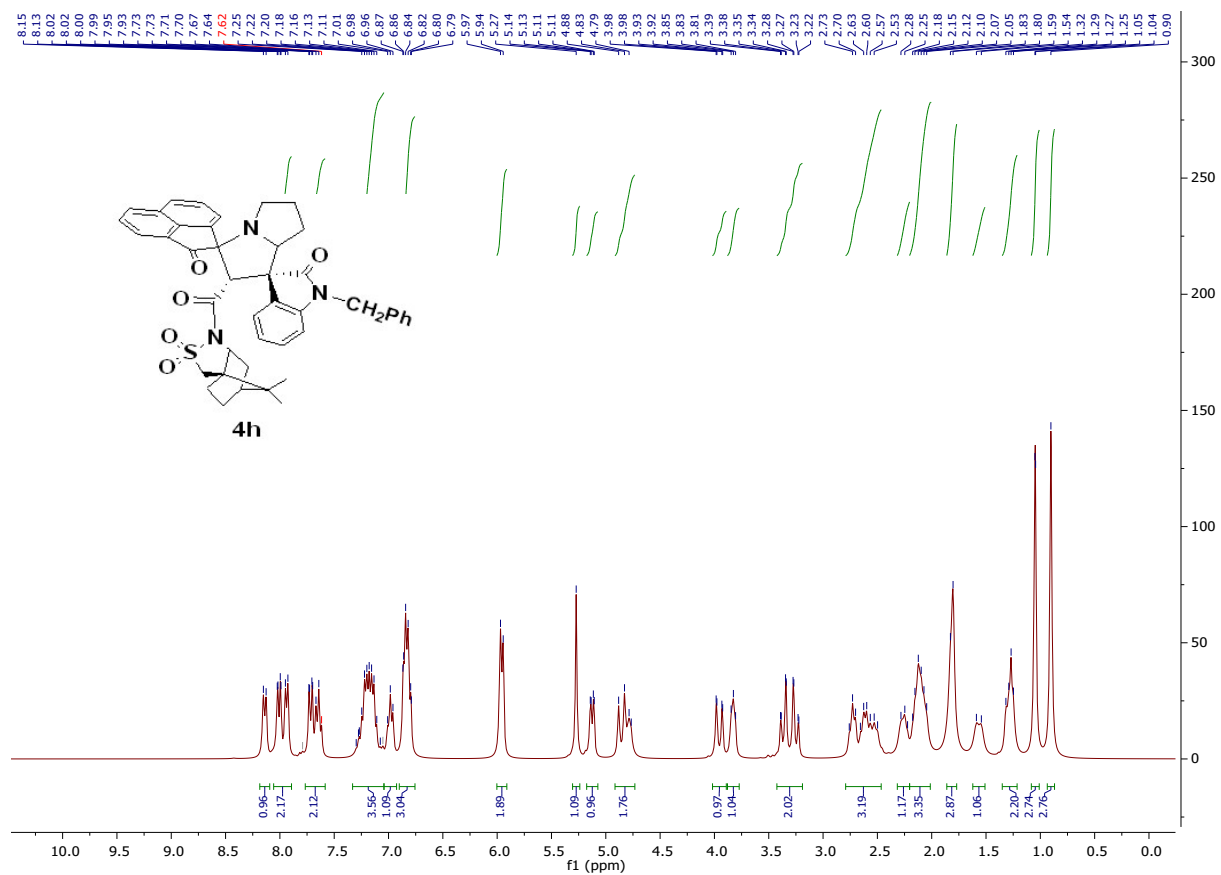


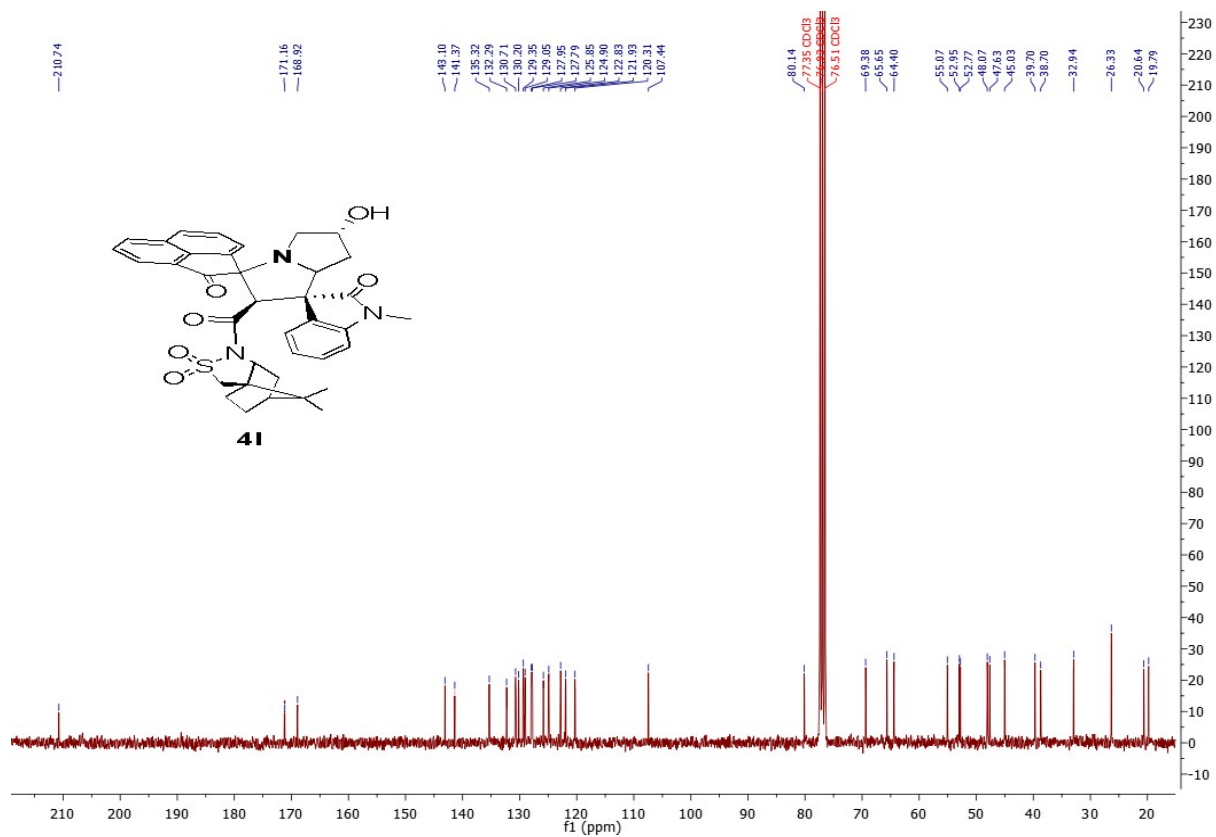
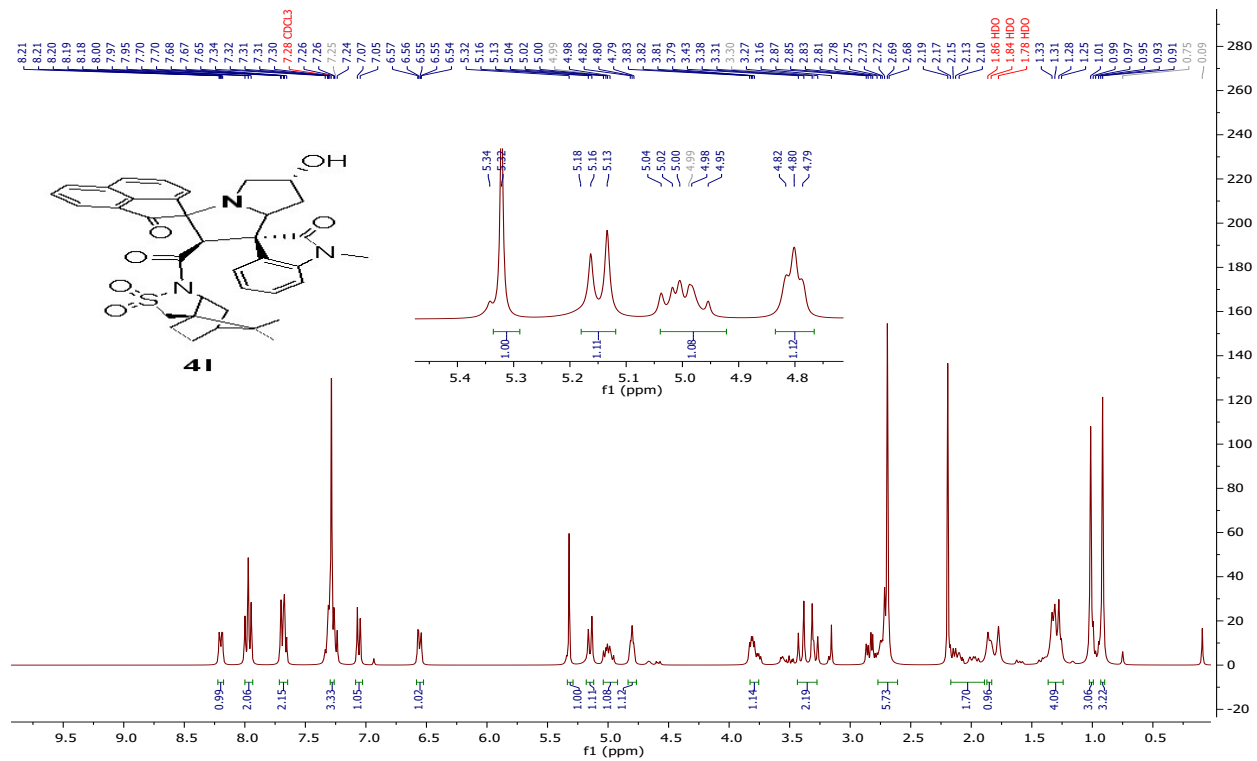


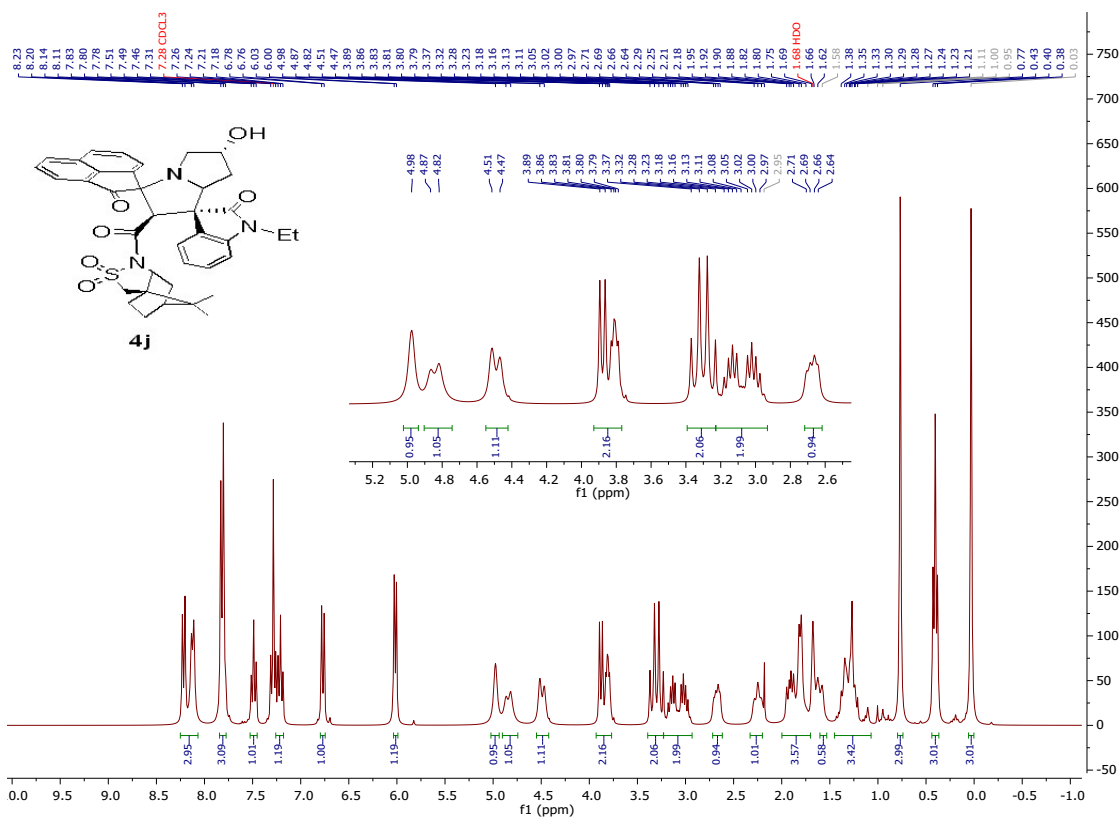
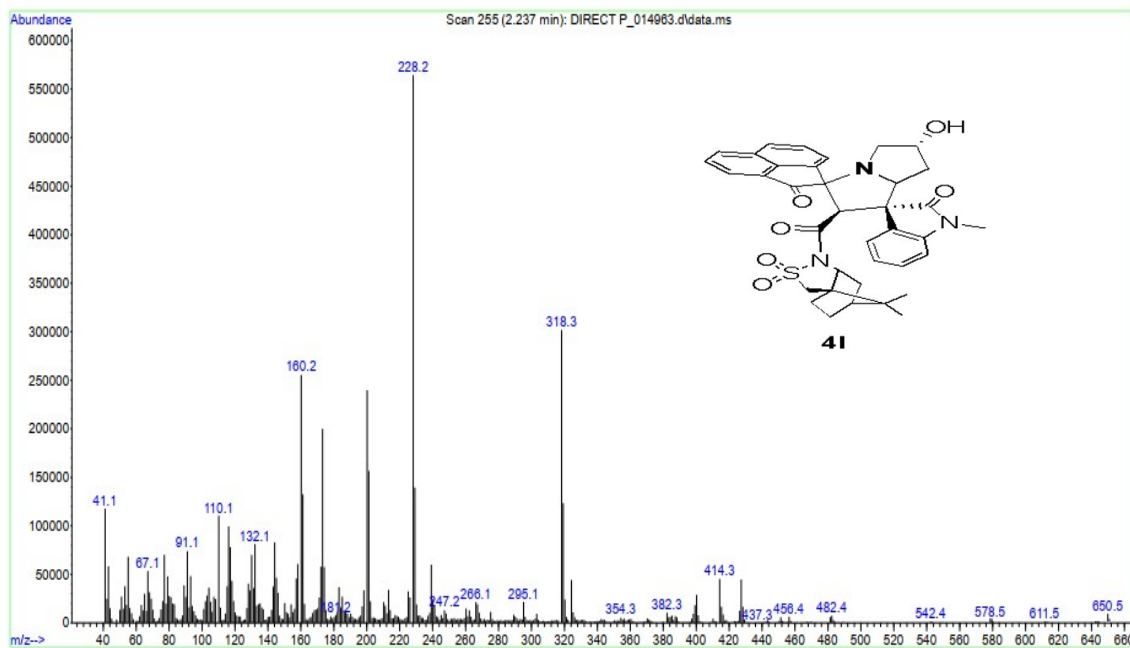


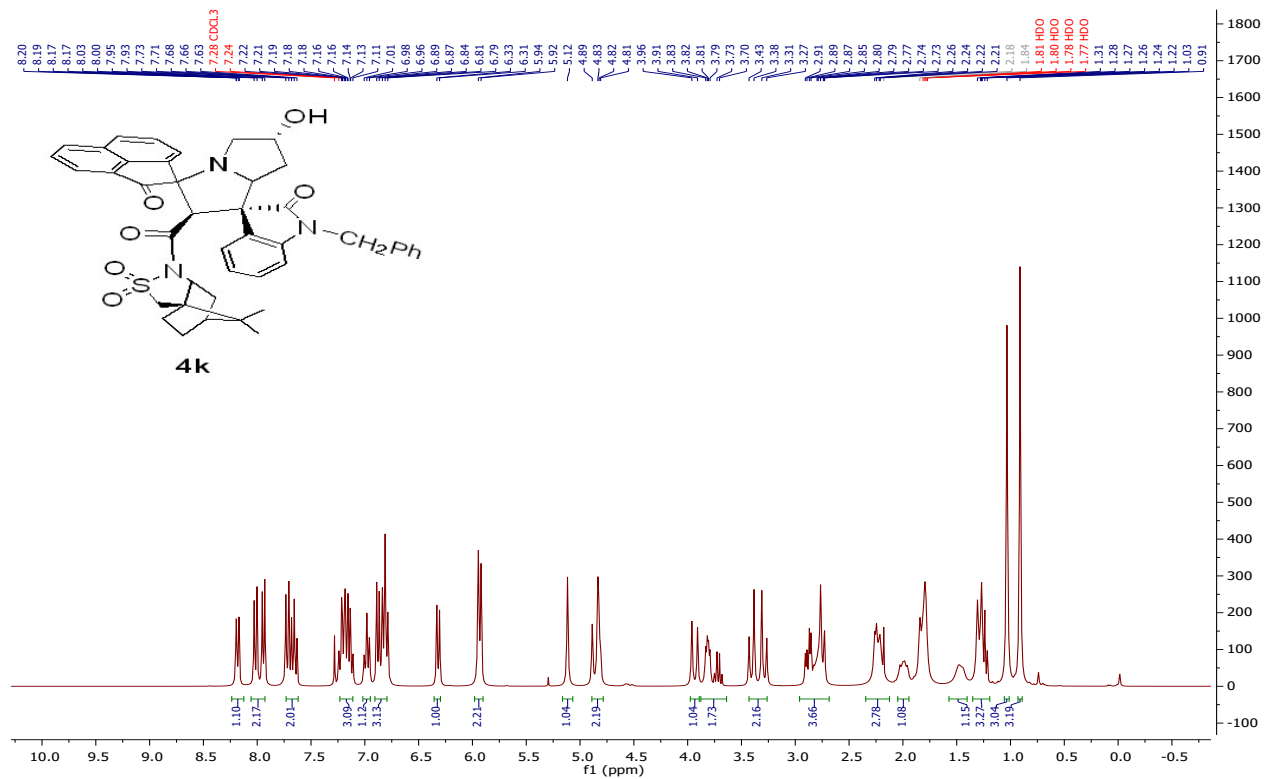
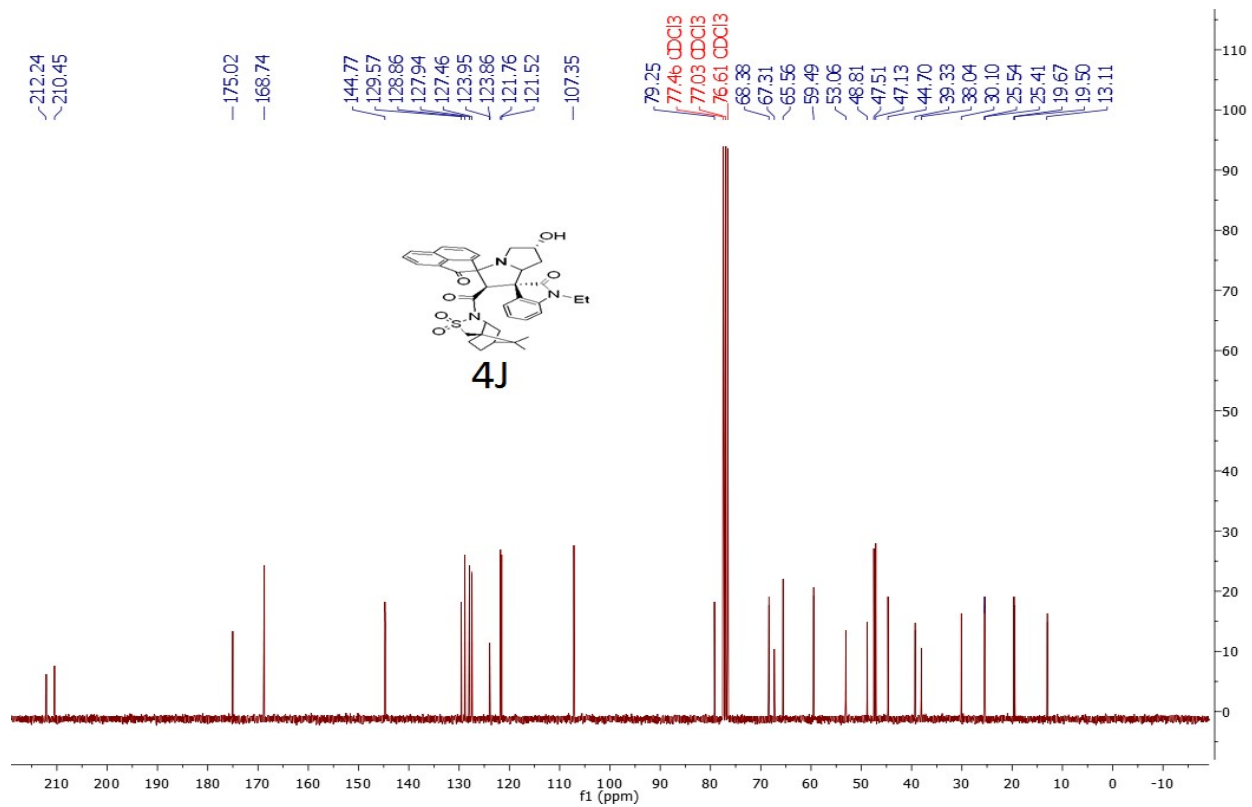
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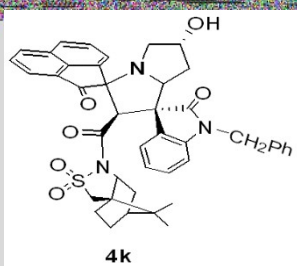
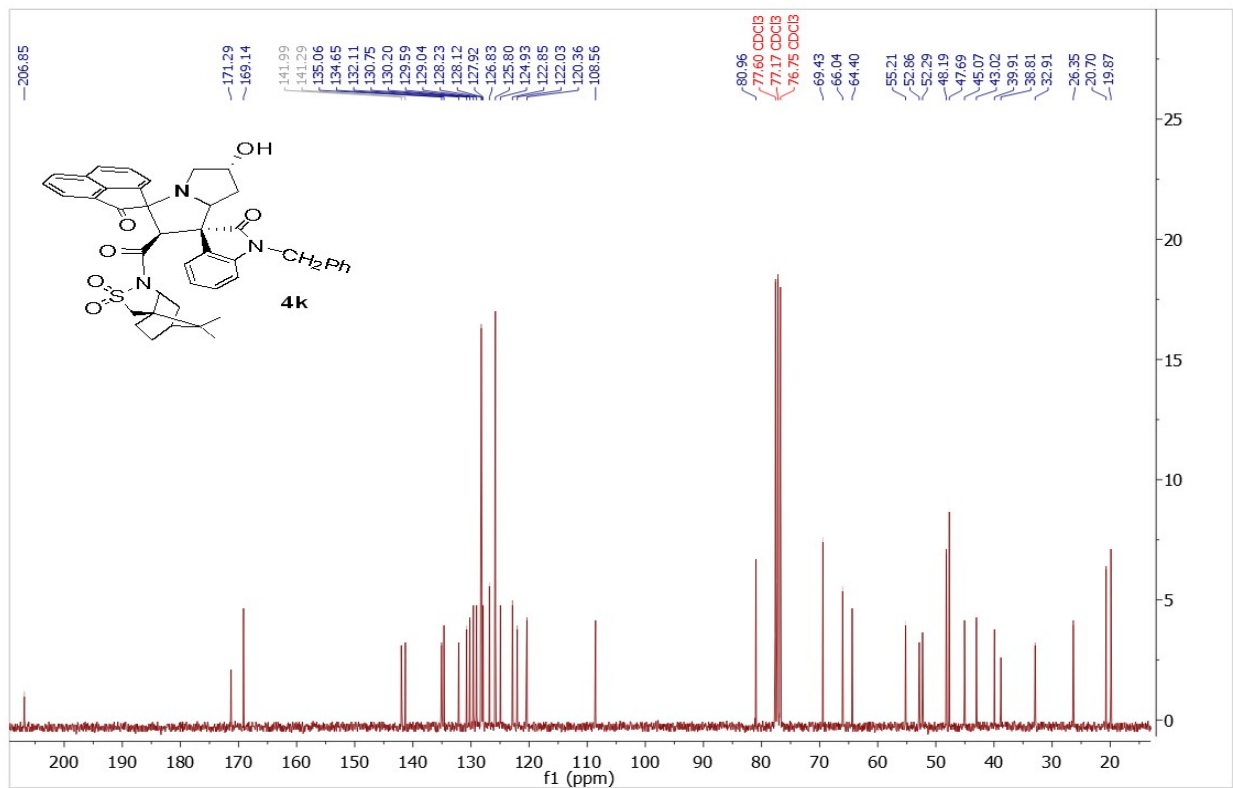












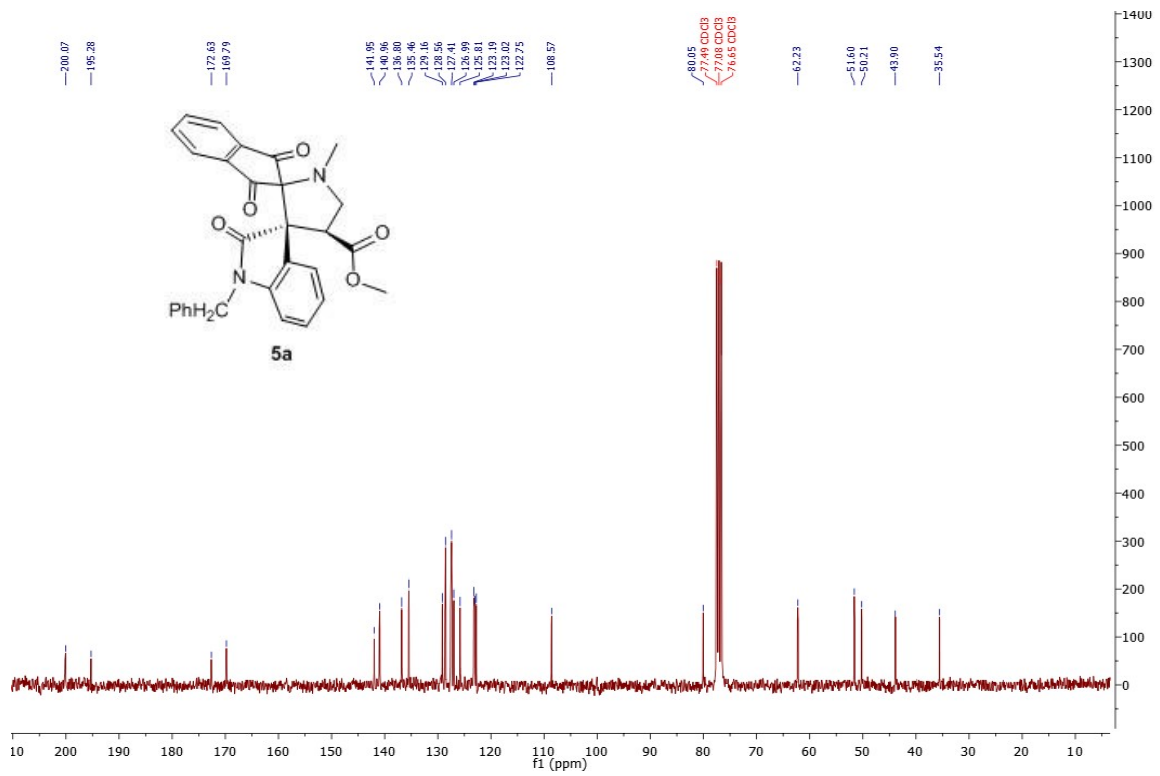
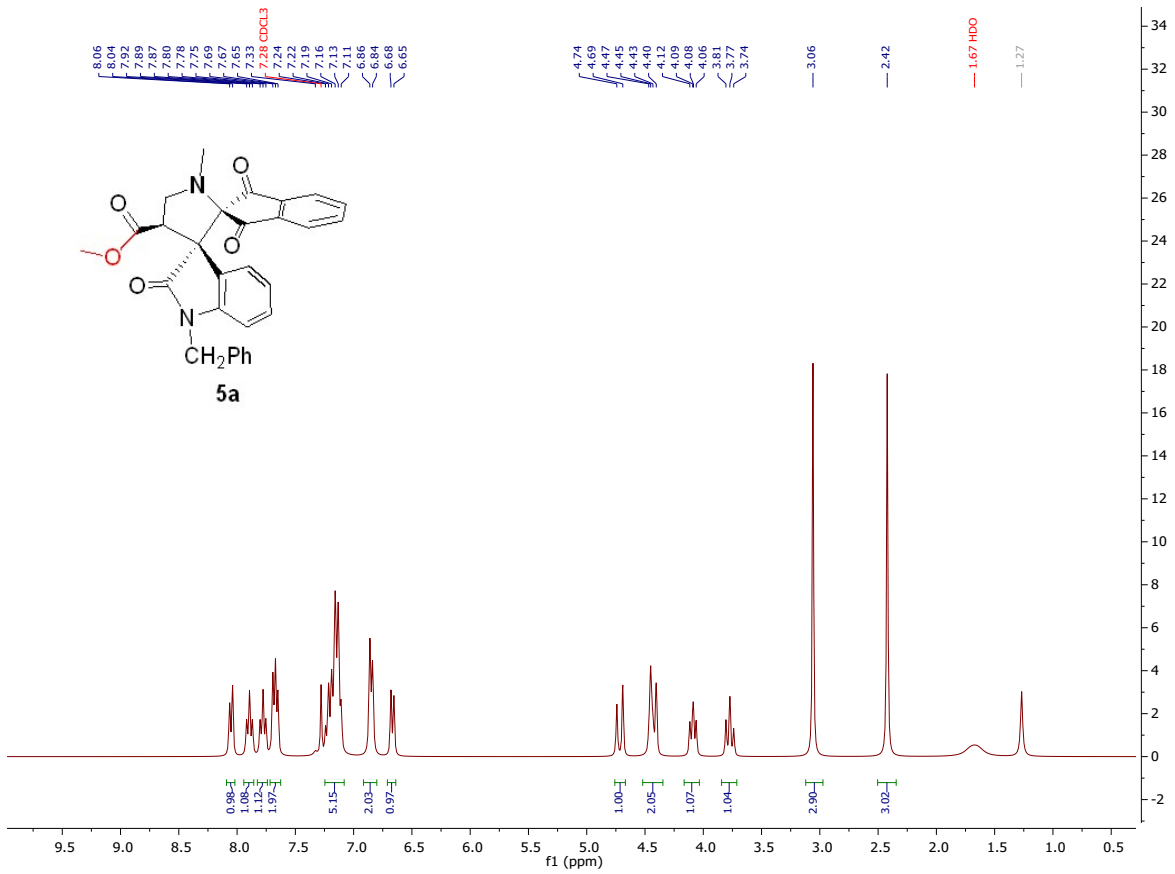
**Instrument:** Direct Probe

**Using:** AcqMethod default.597x.m

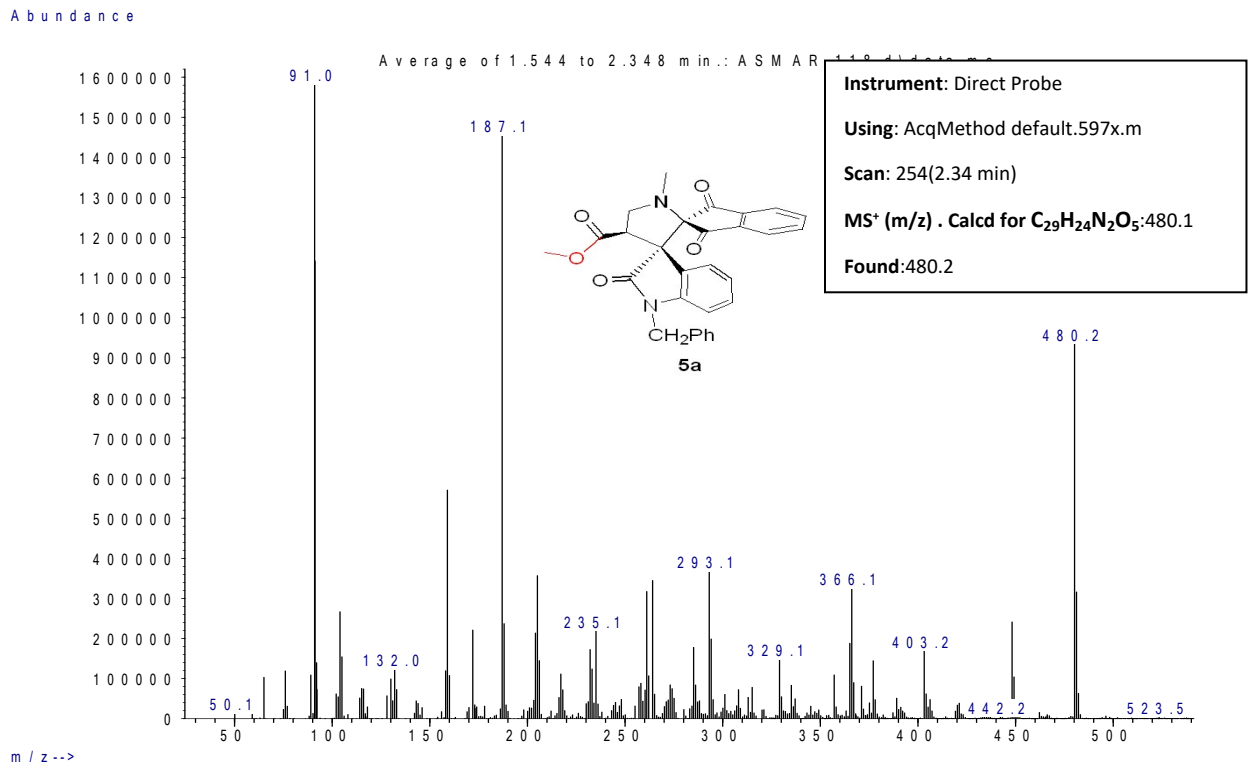
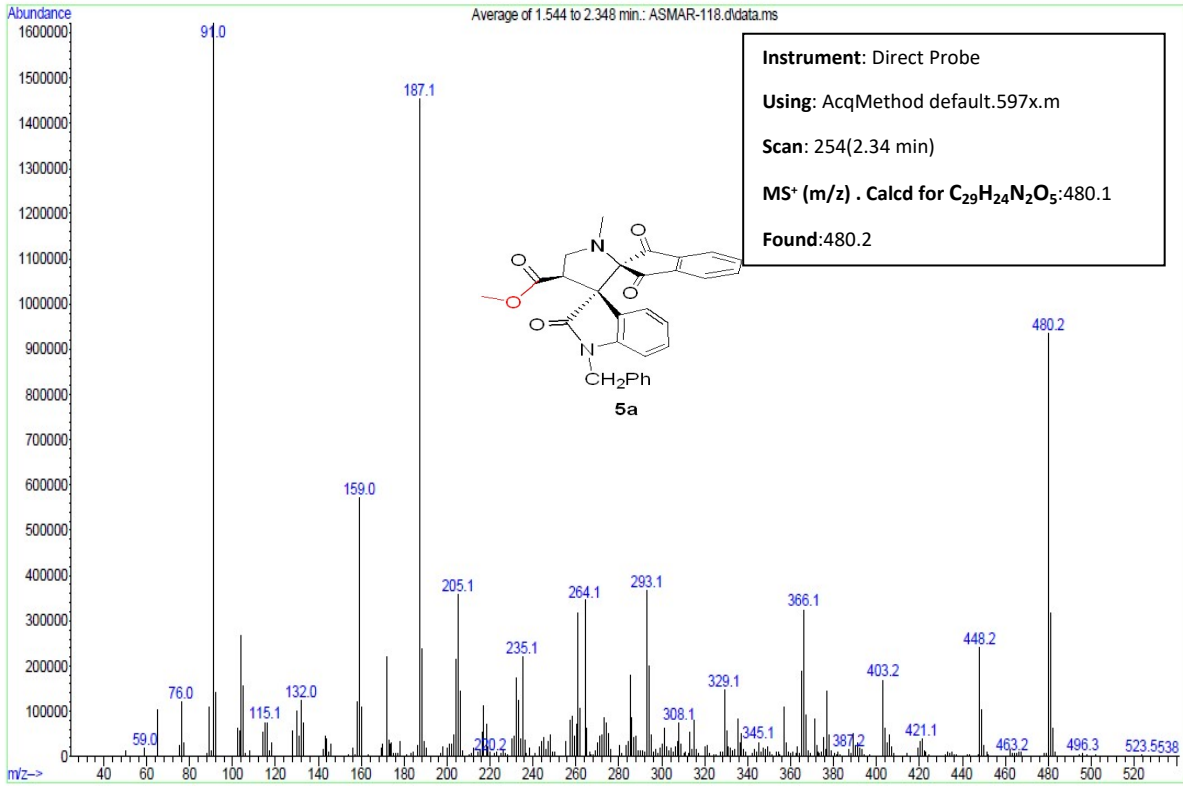
**Scan:** 171 (1.54 min)

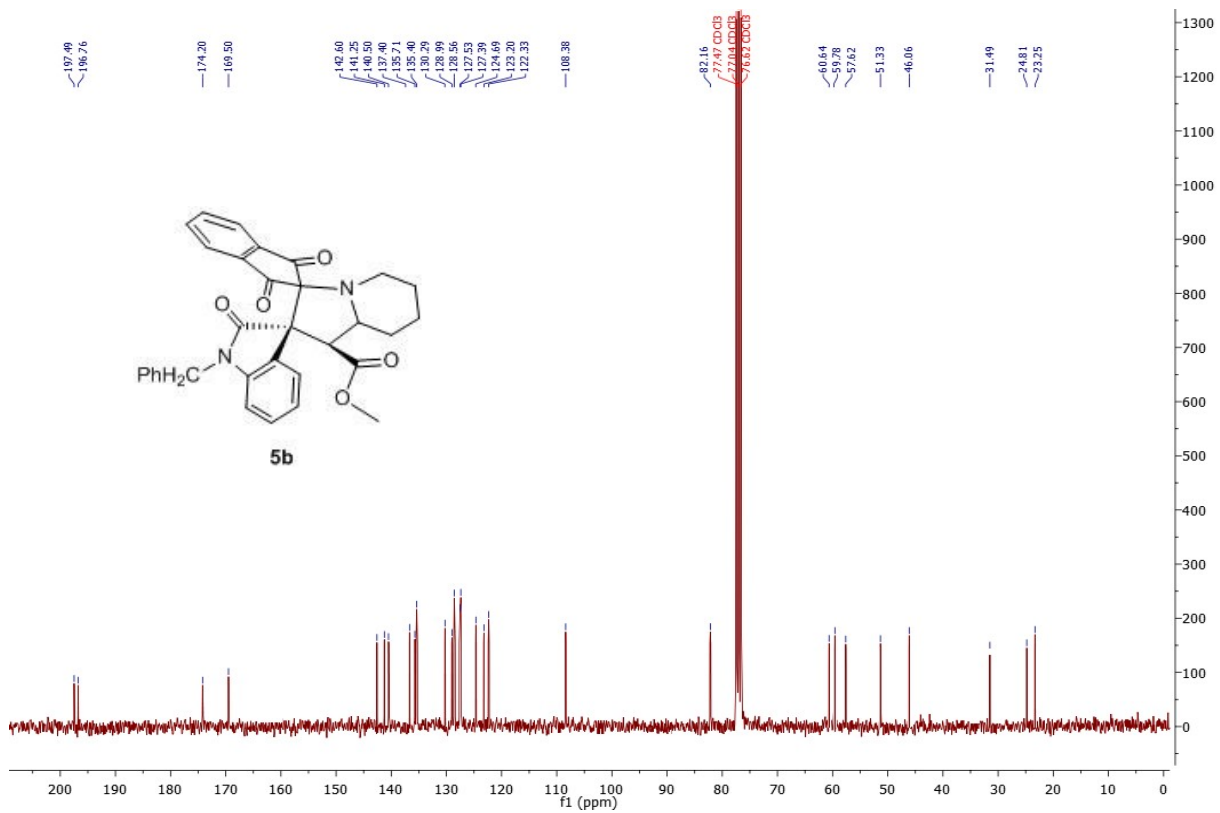
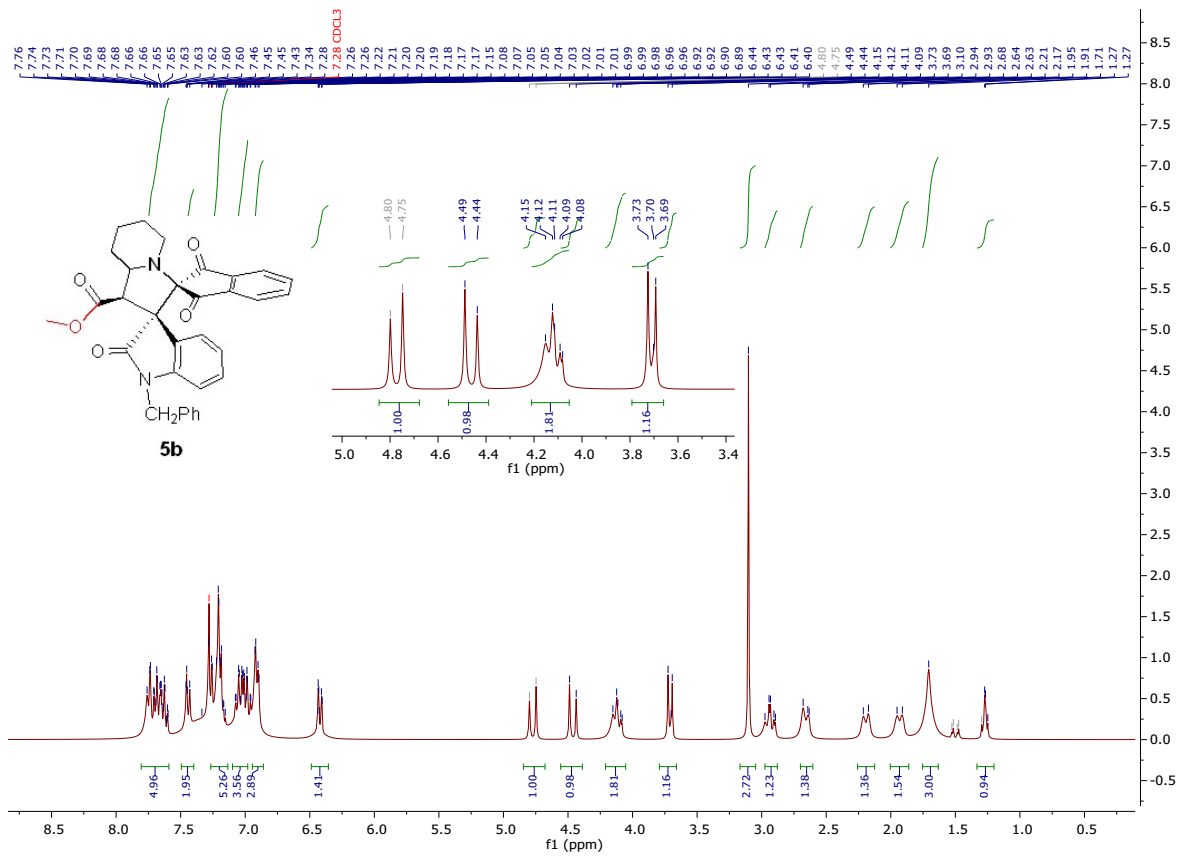
**MS<sup>+</sup> (m/z) . Calcd for C<sub>43</sub>H<sub>41</sub>N<sub>3</sub>O<sub>6</sub>S:**  
728.2

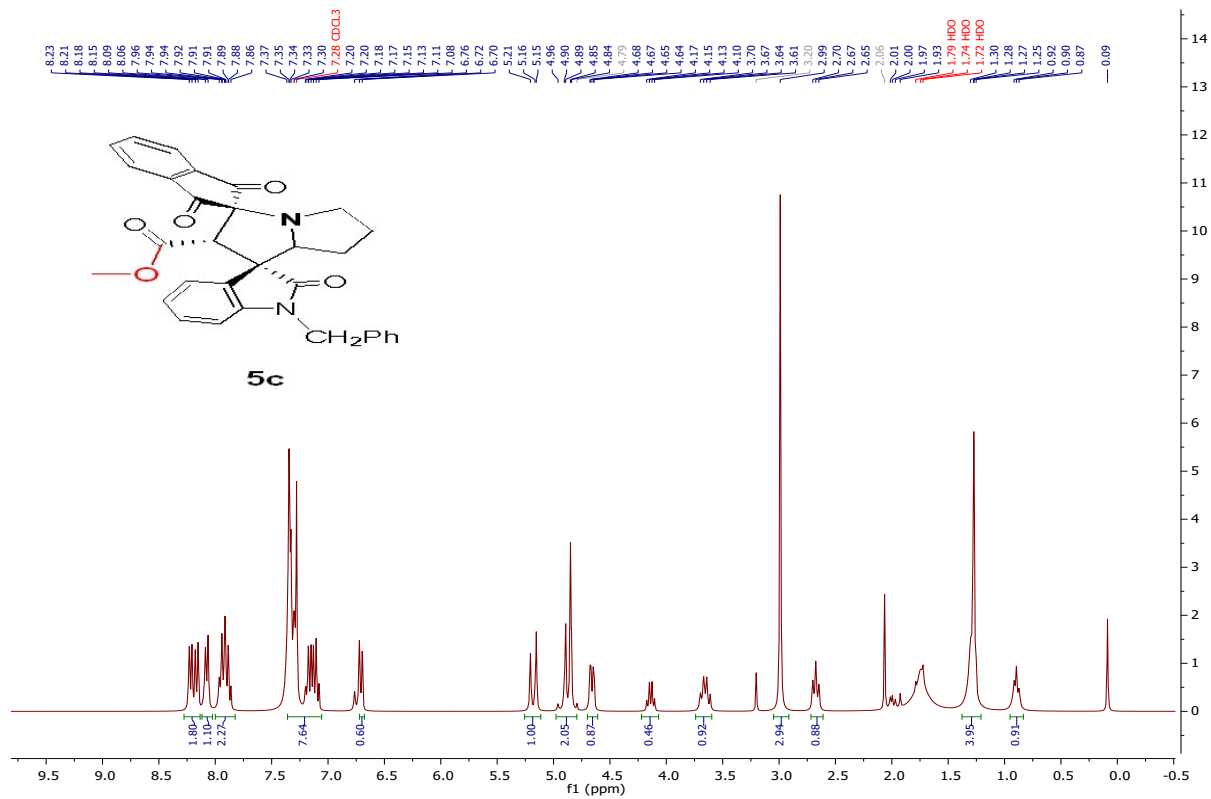
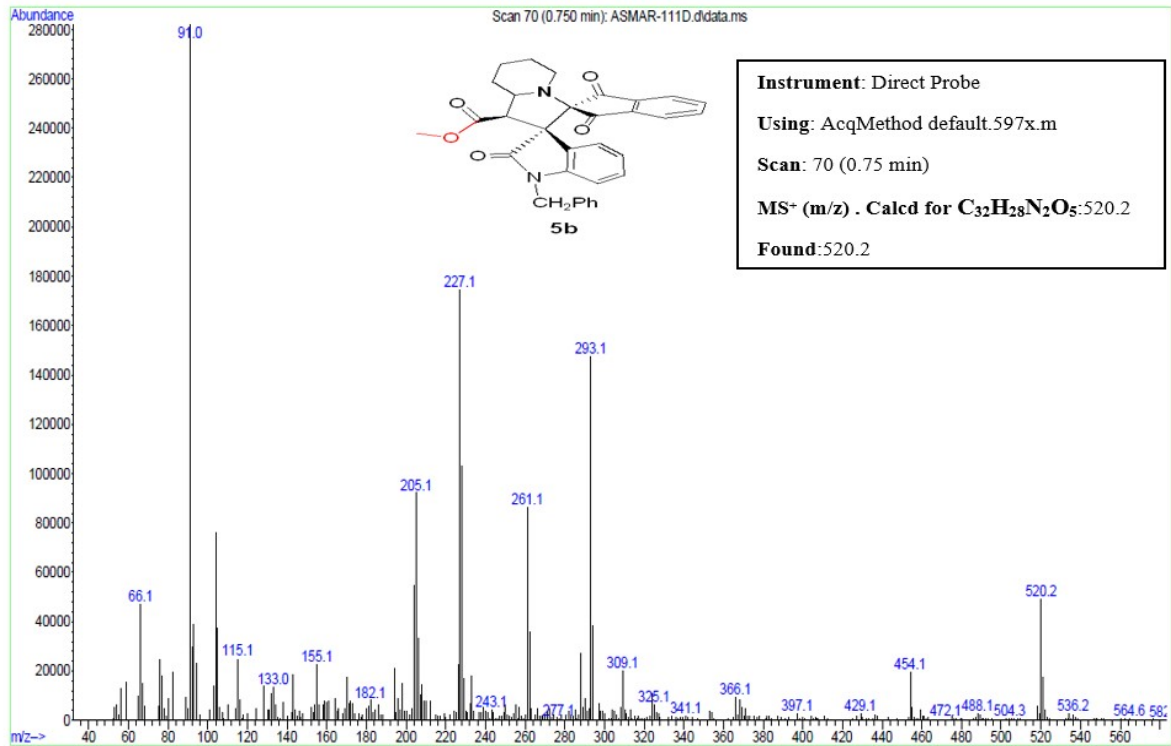
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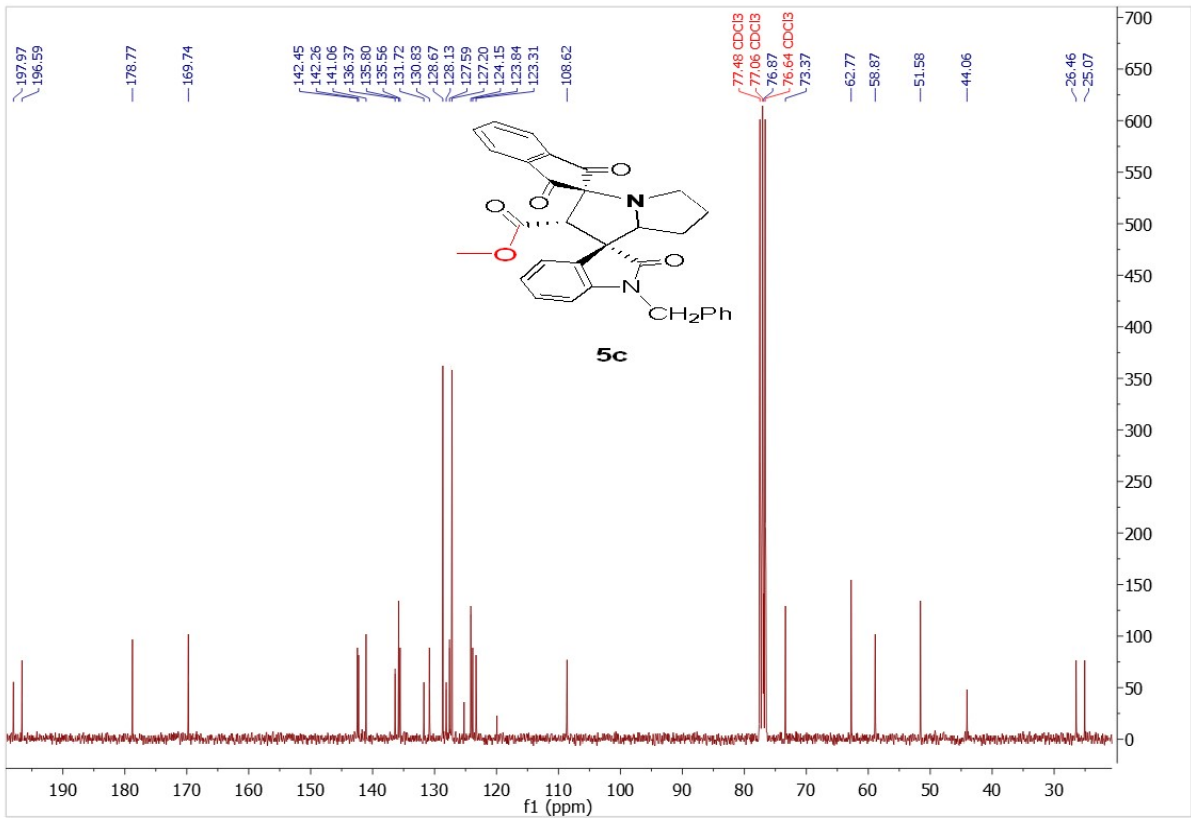




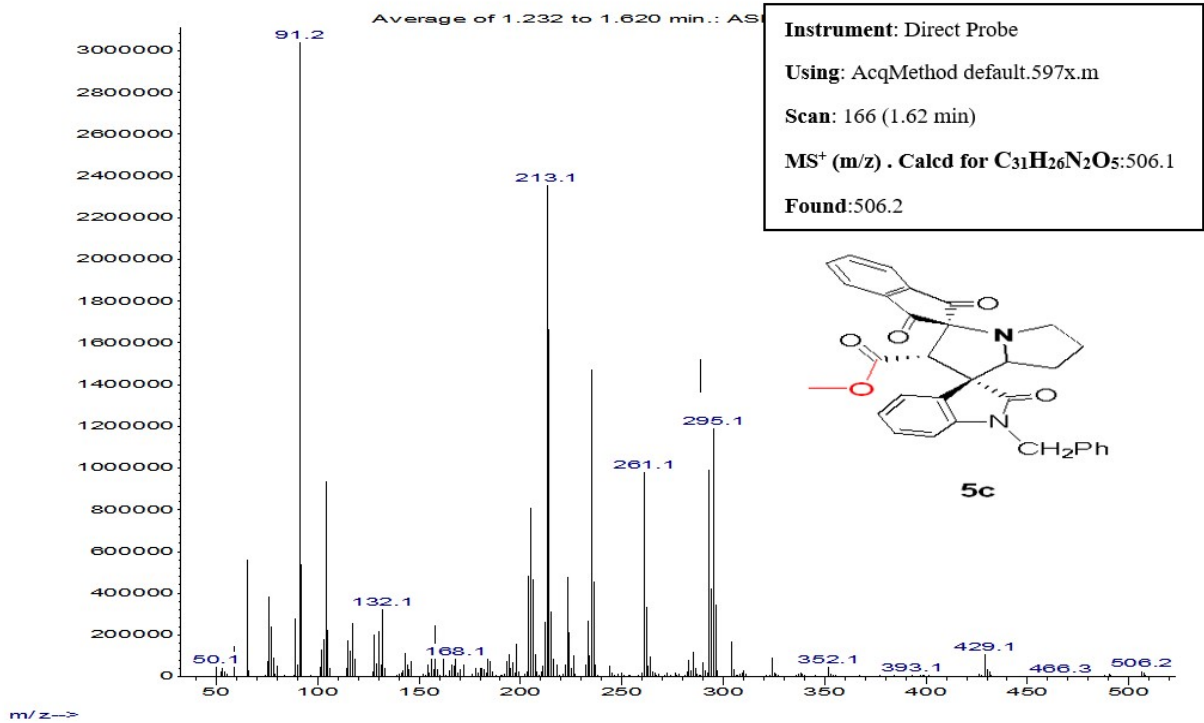


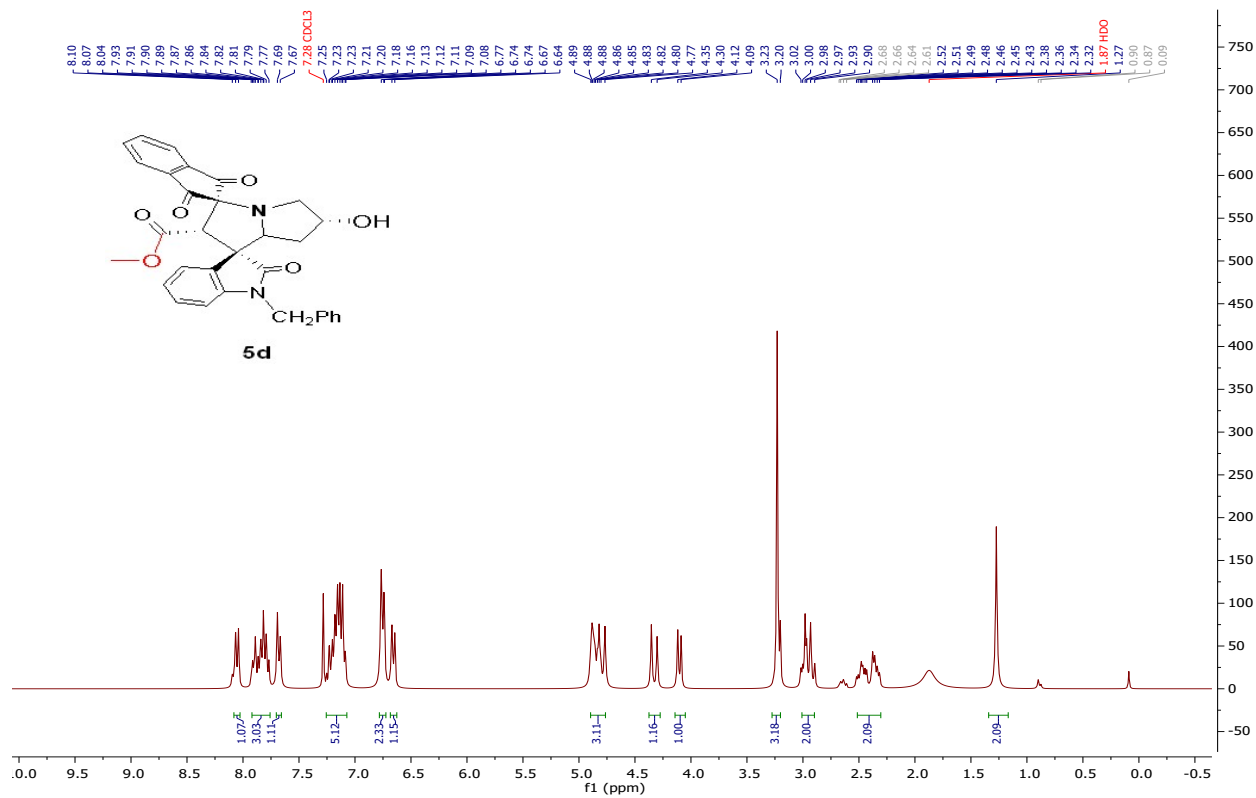
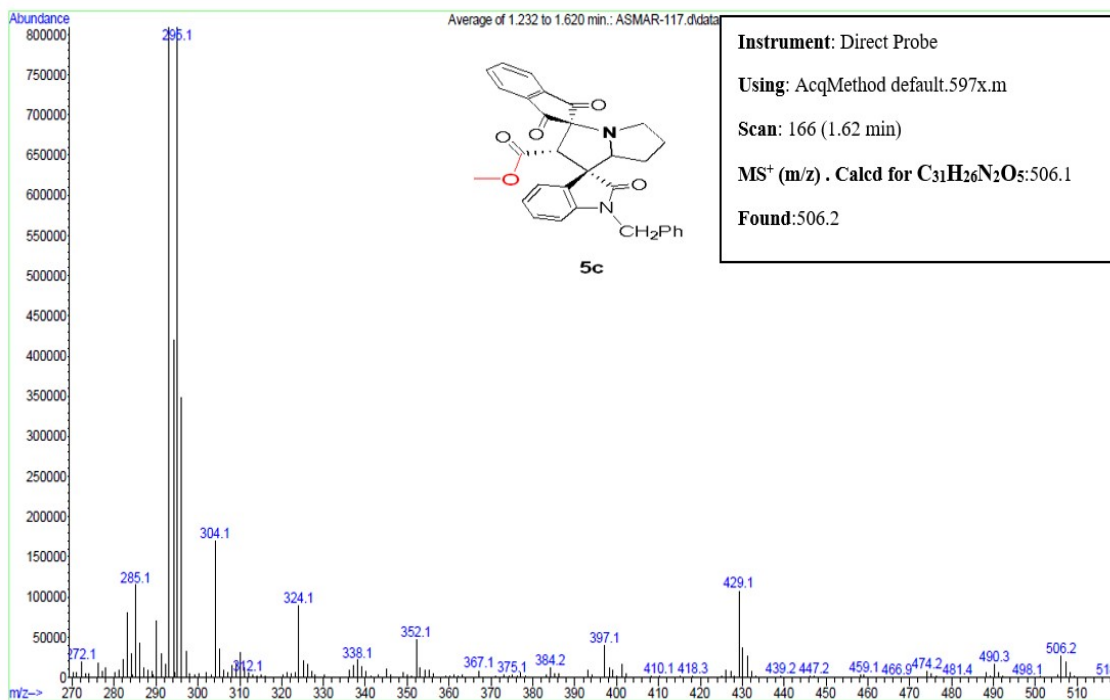


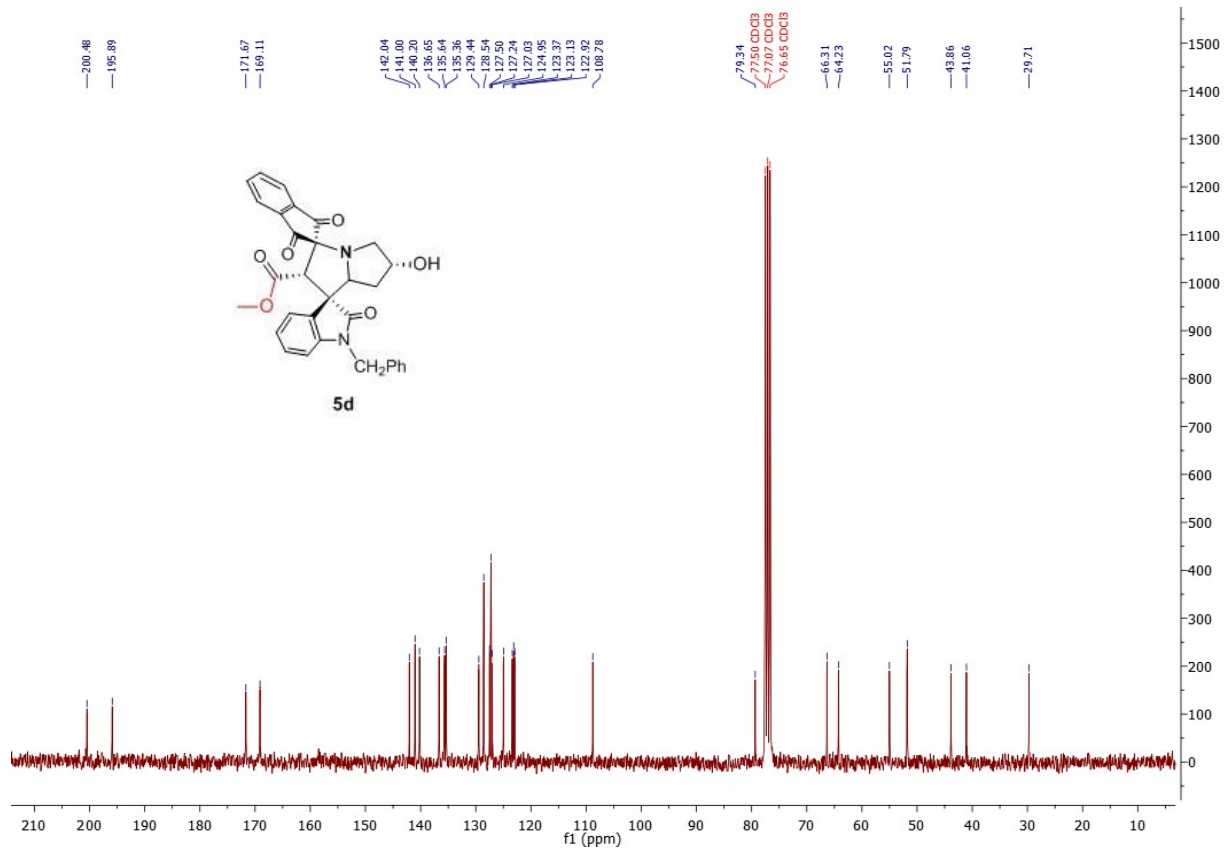


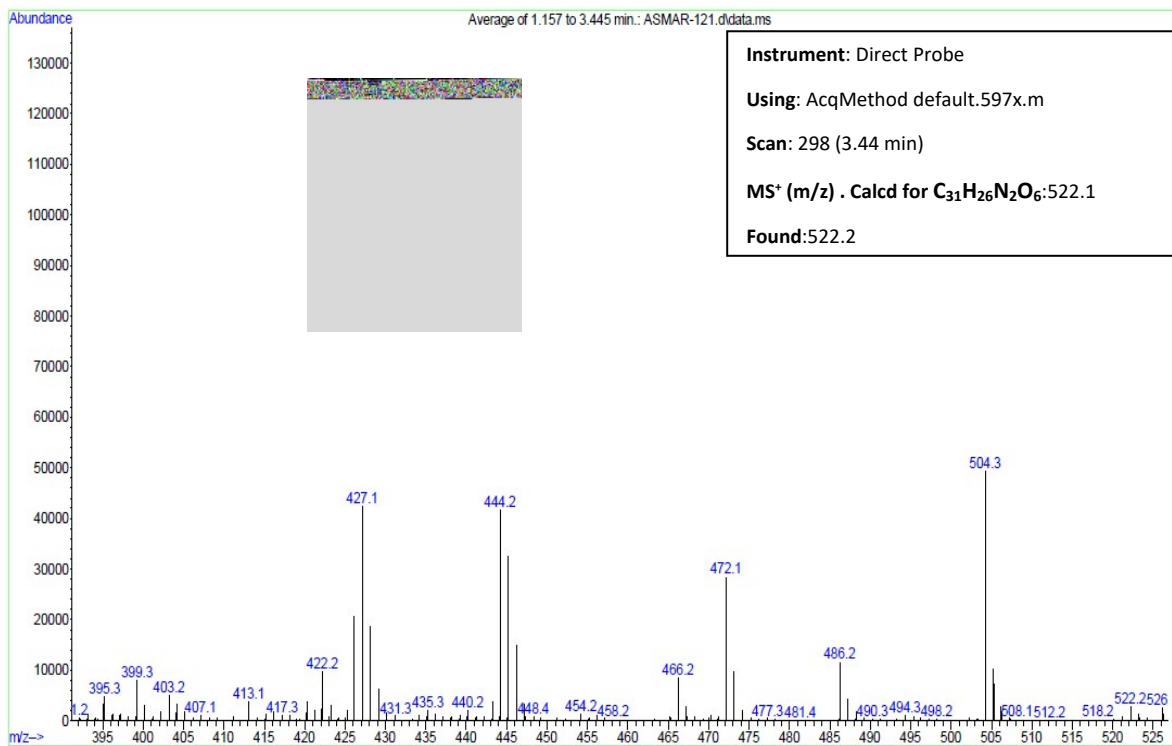
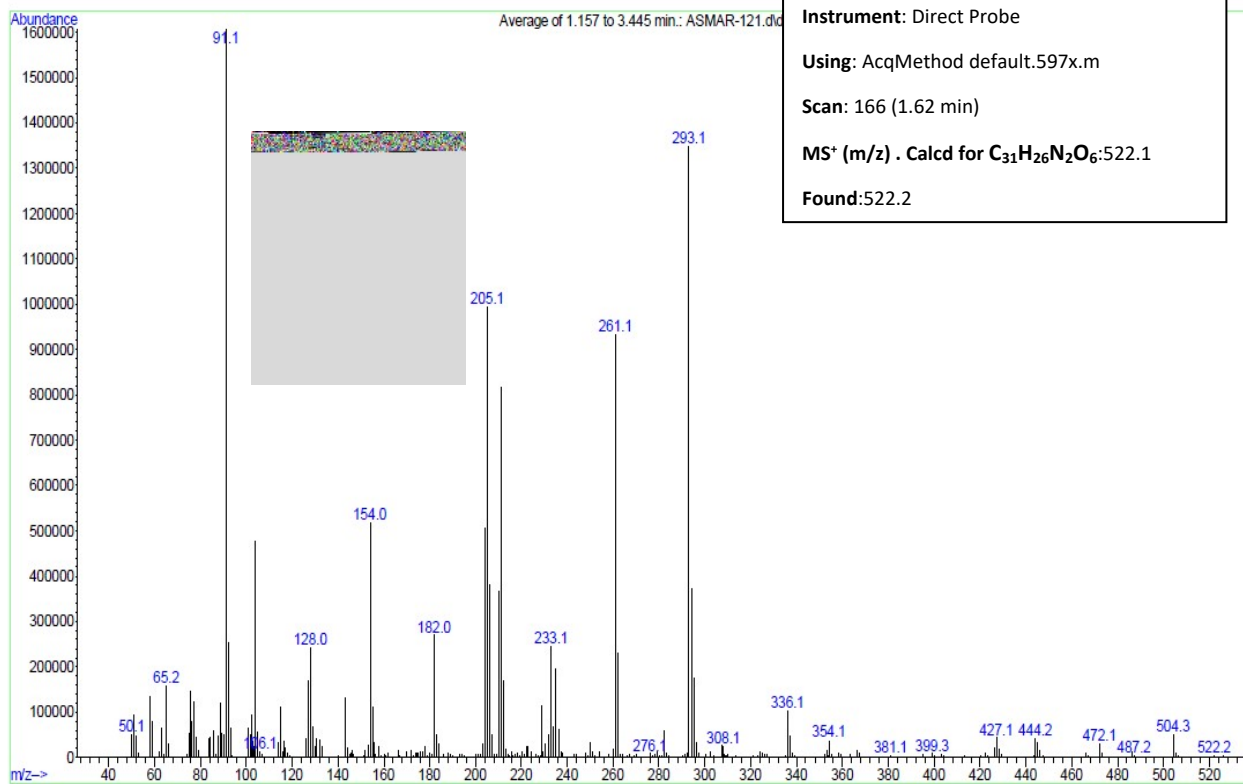


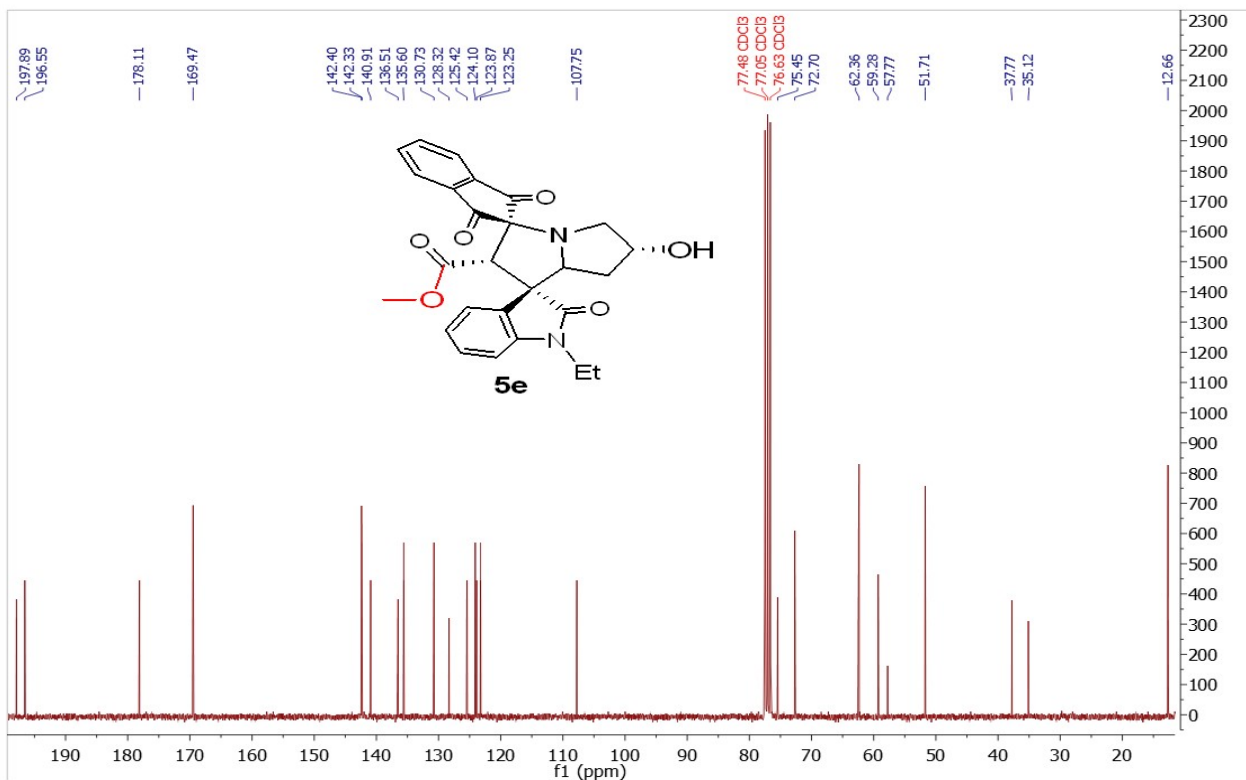
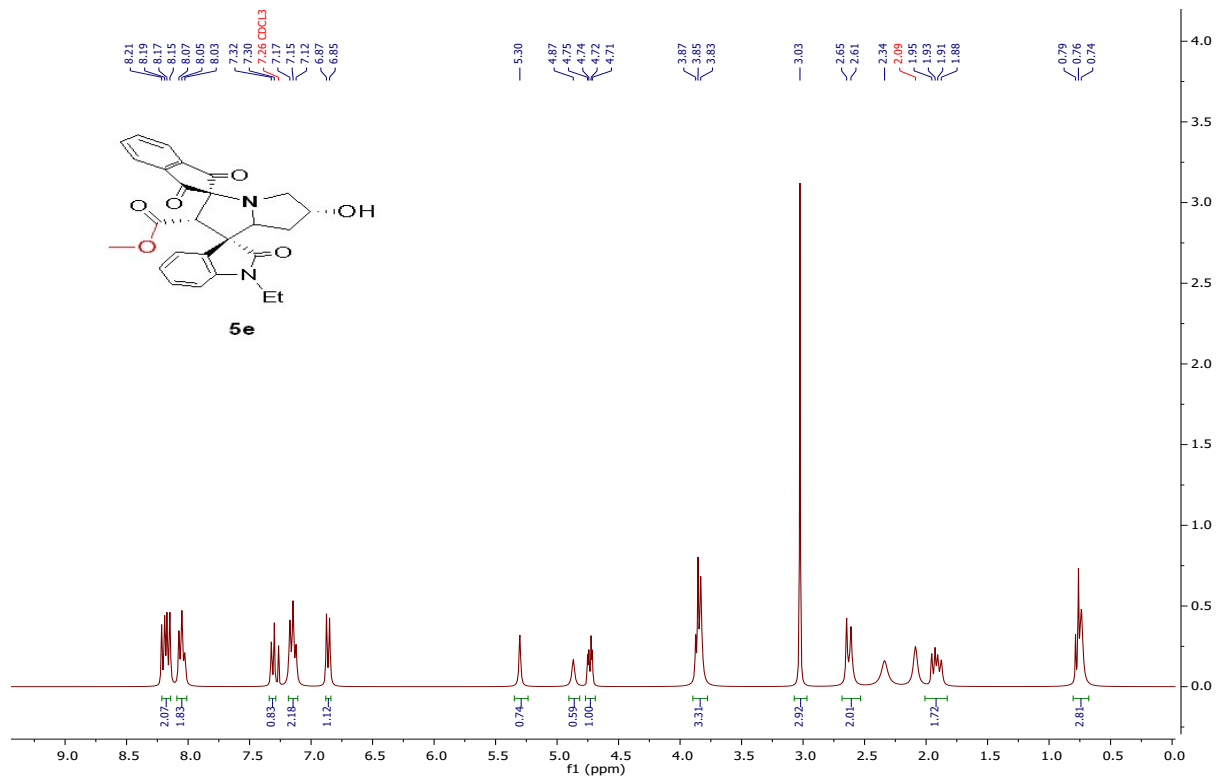
Abundance



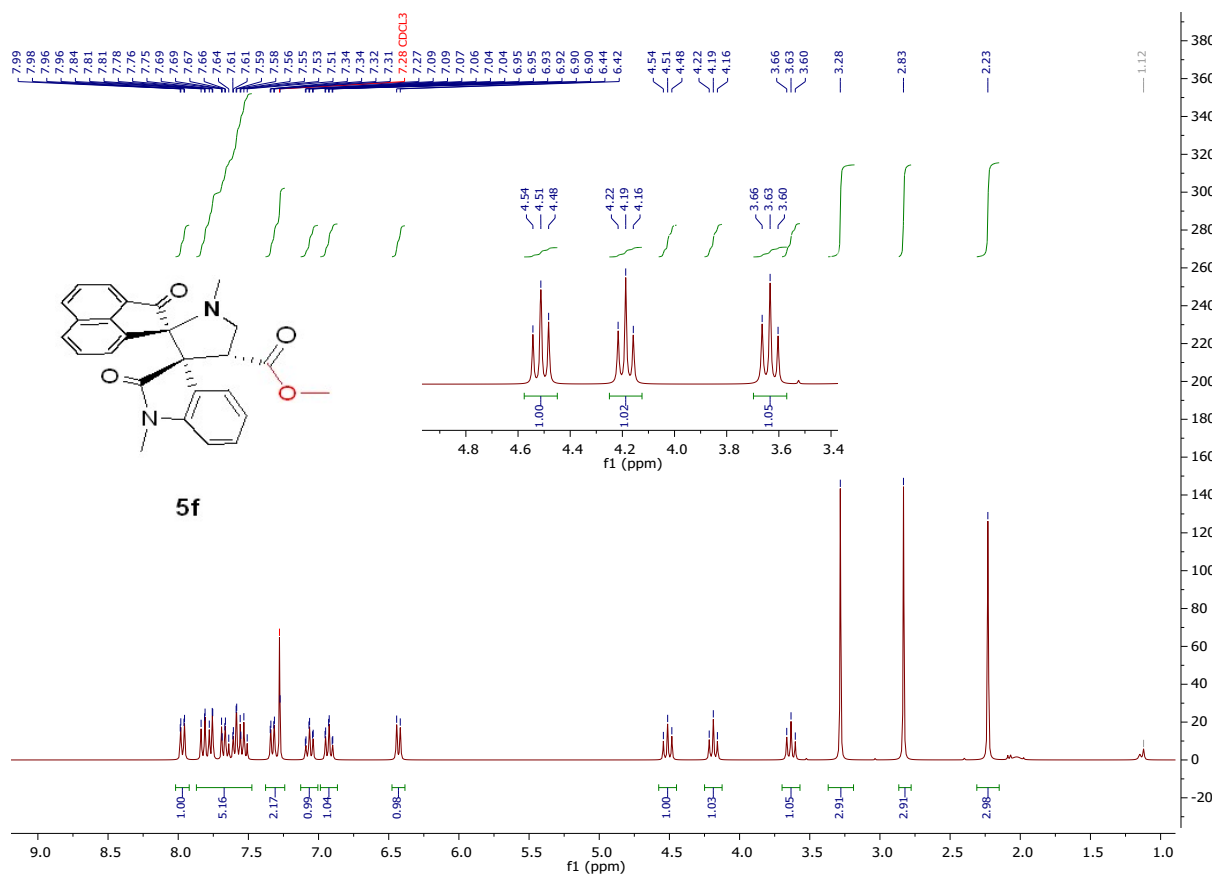
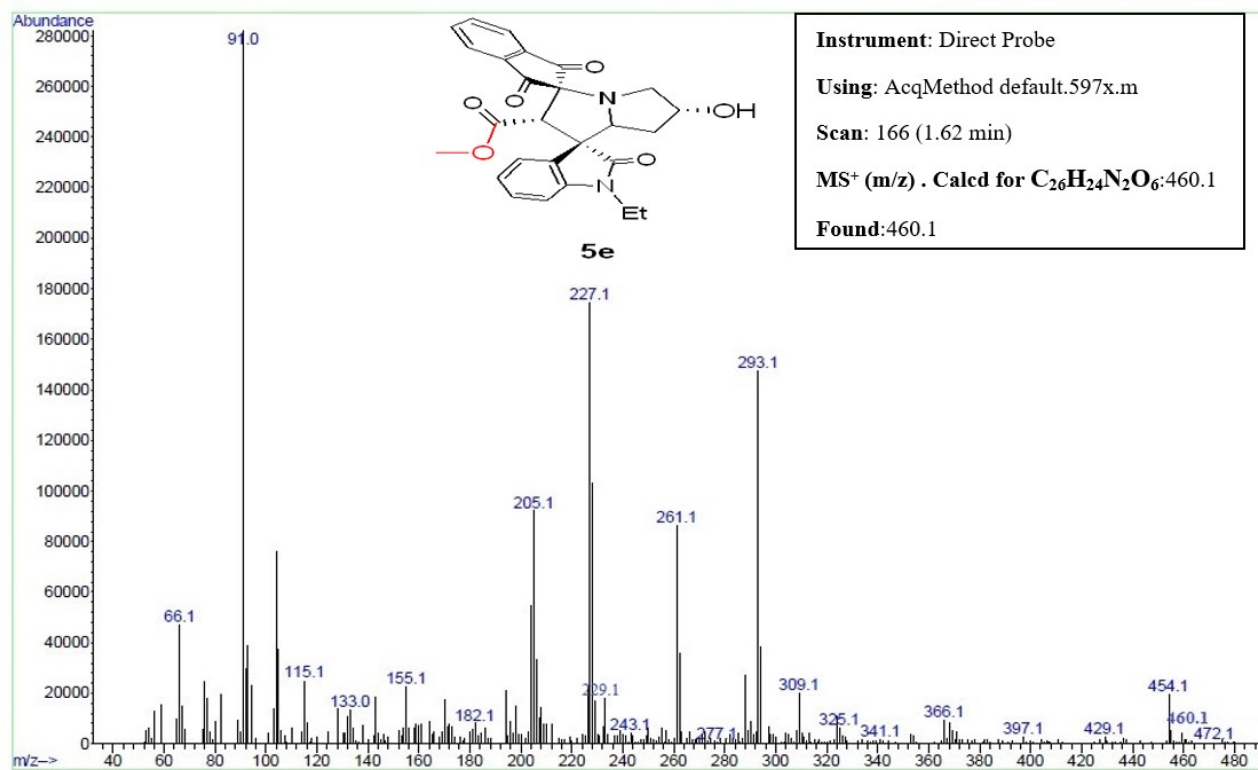


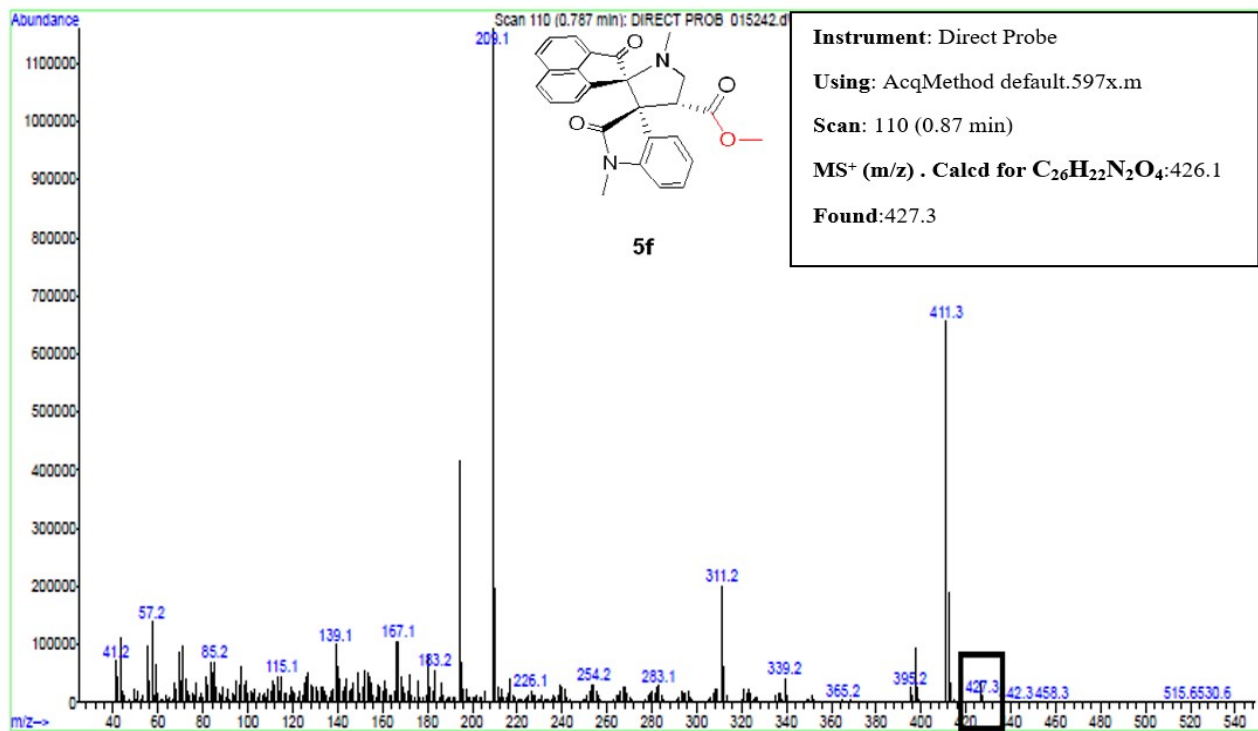
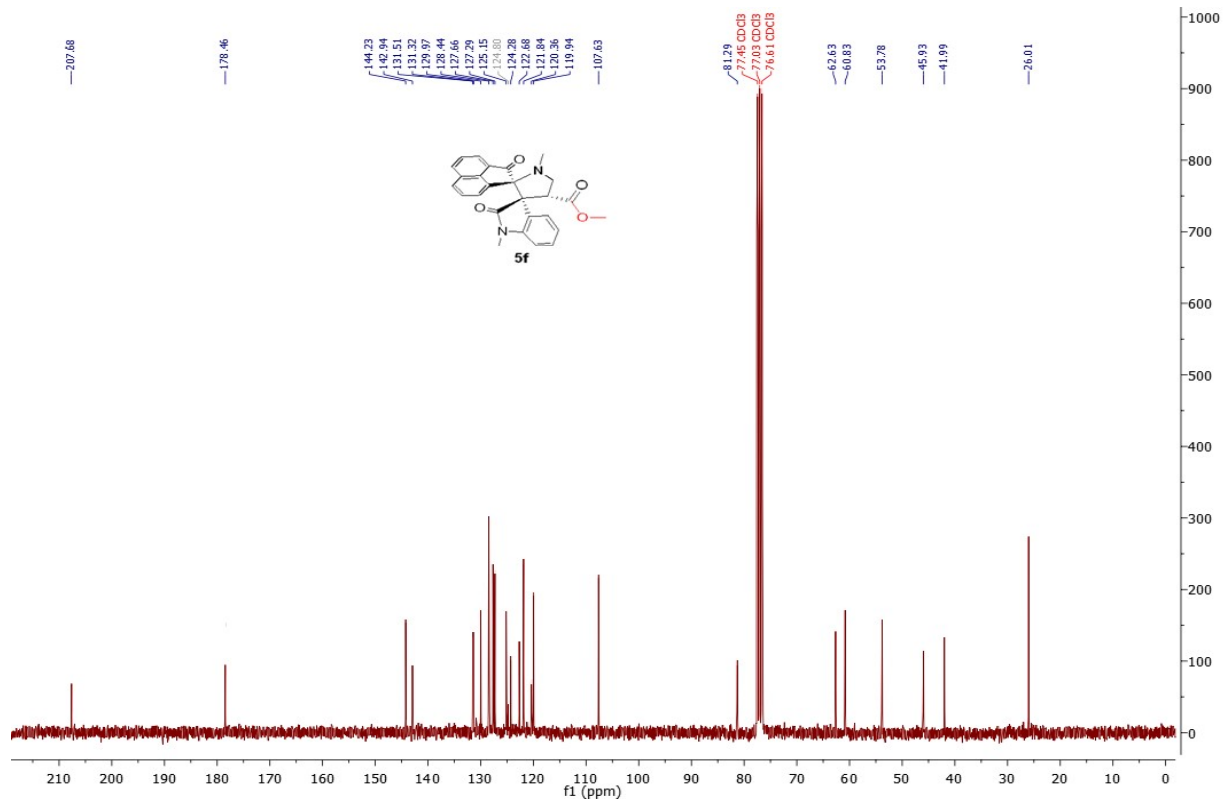


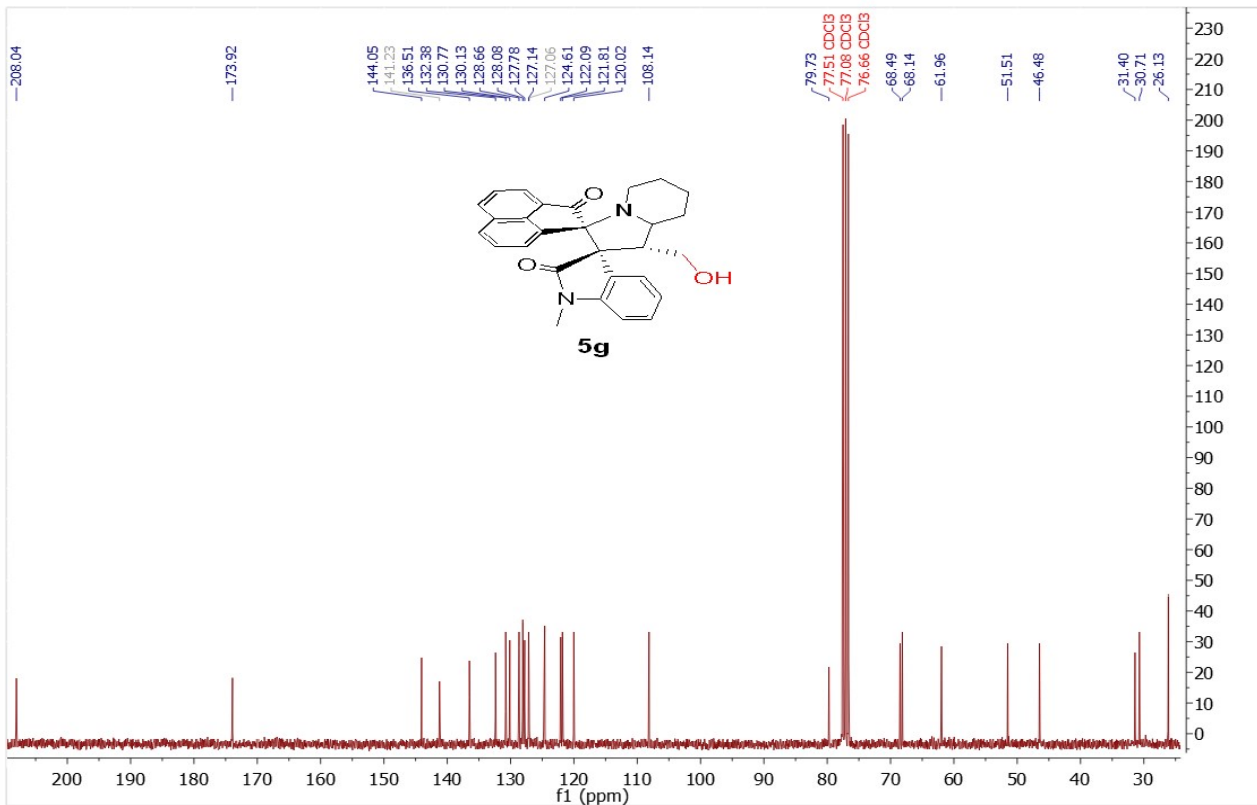
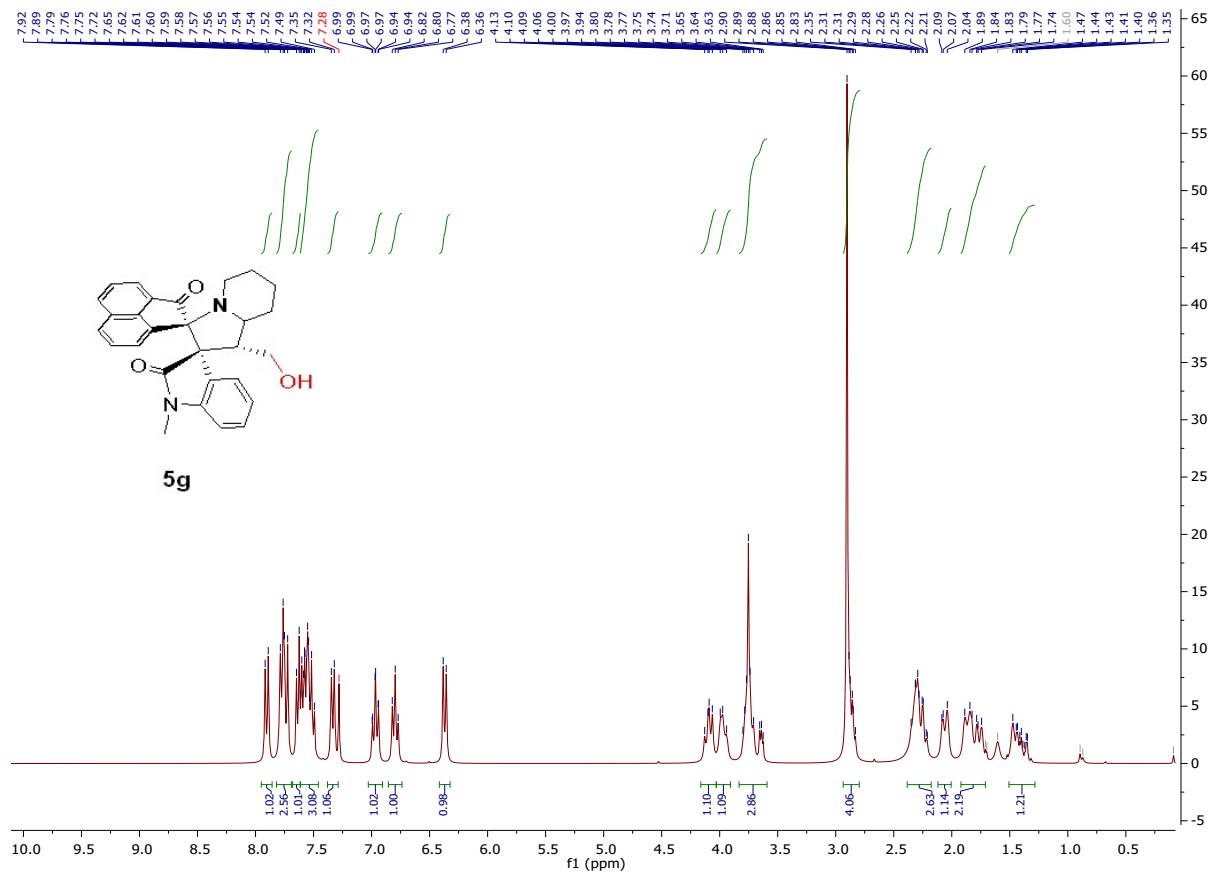


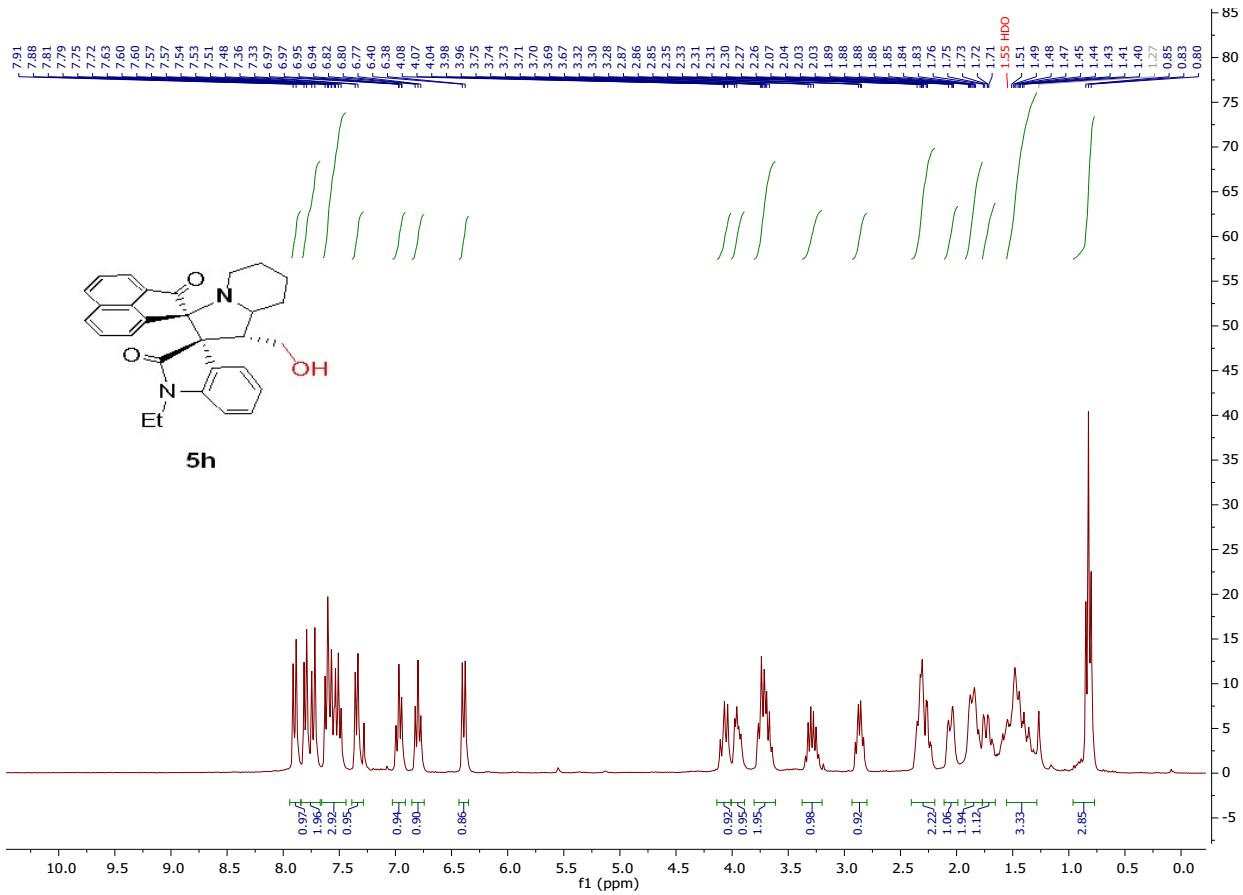
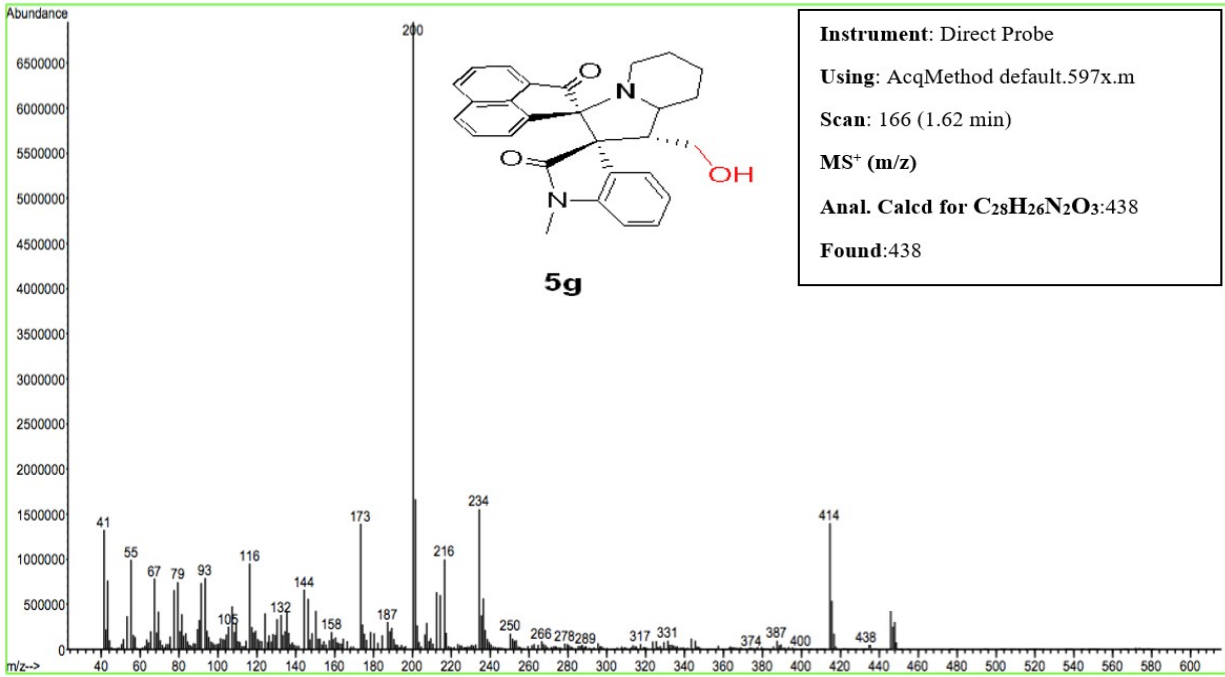


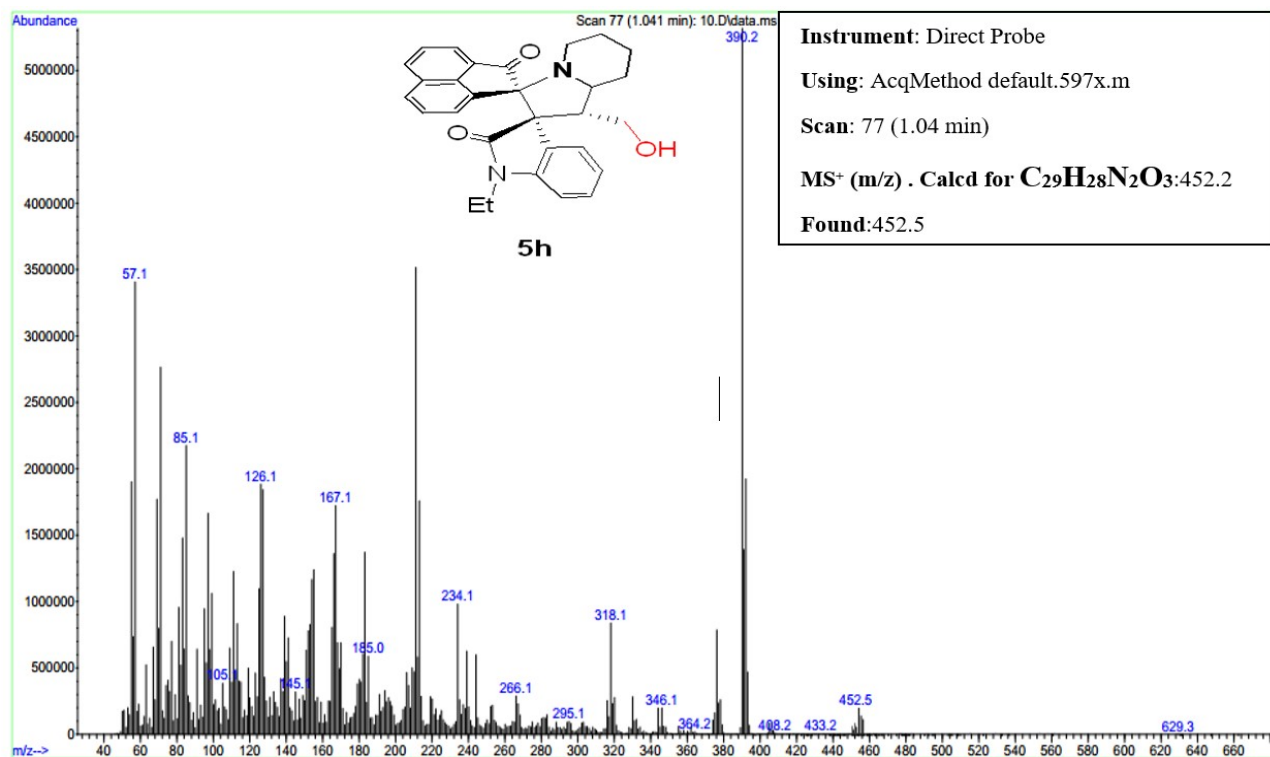
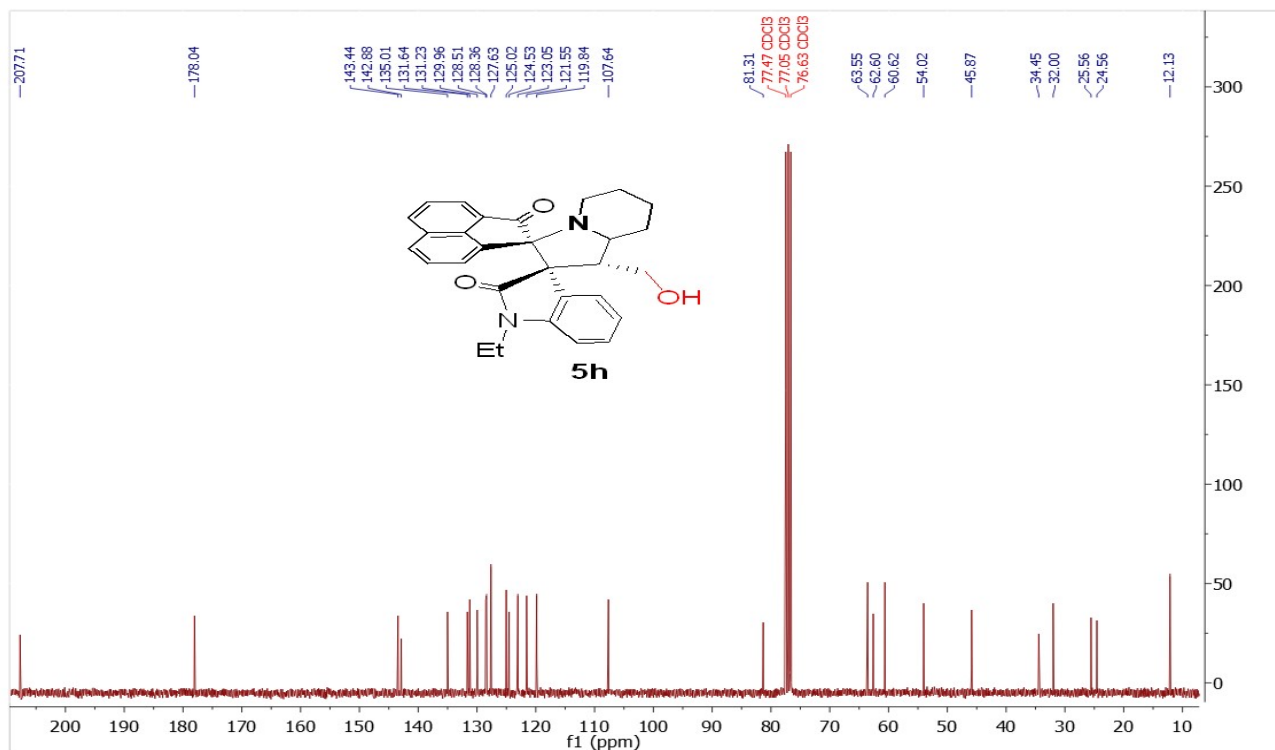


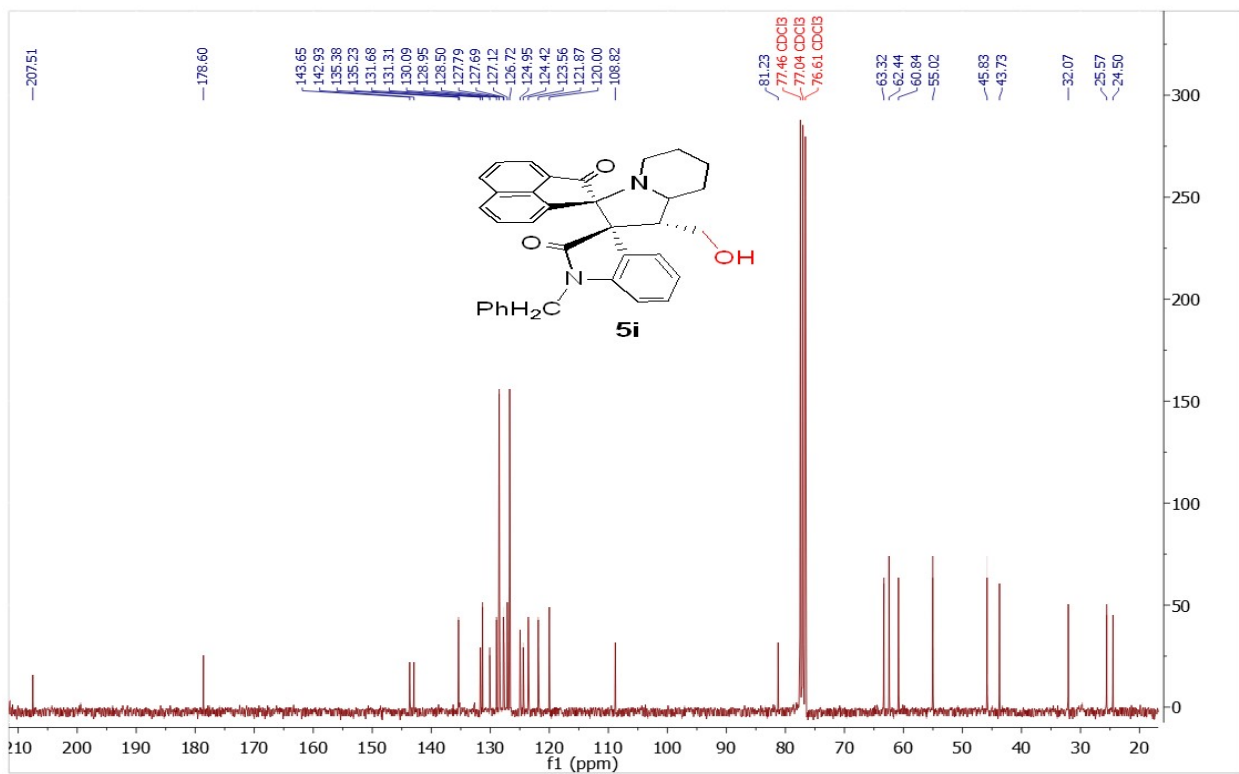
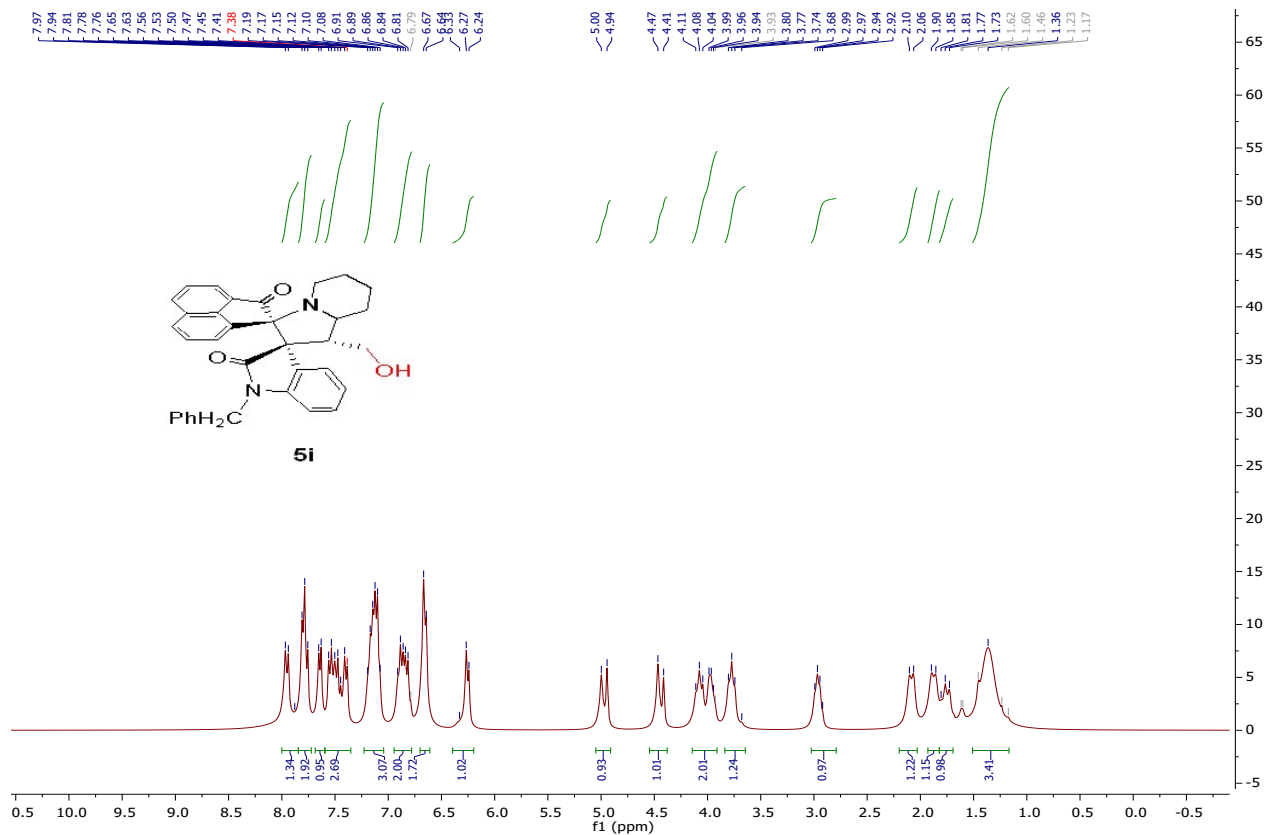


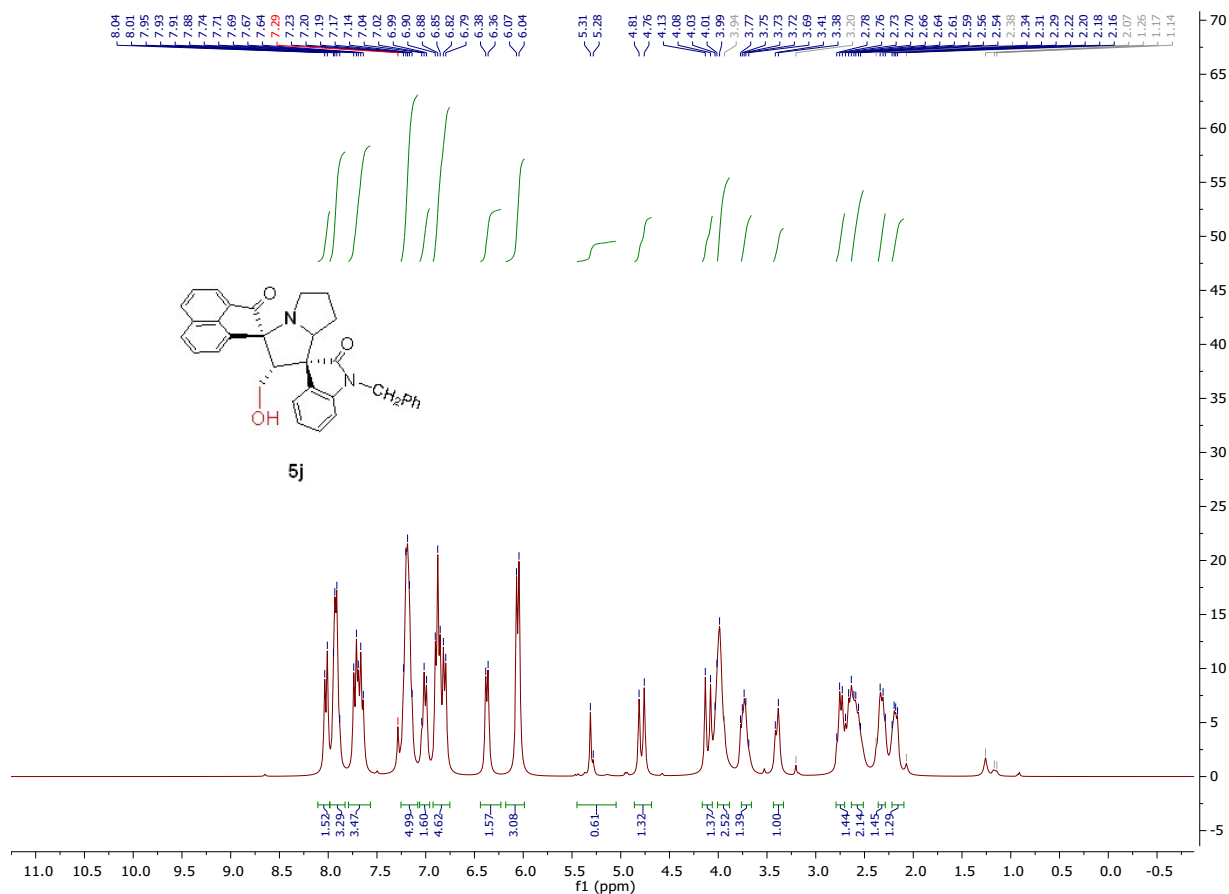
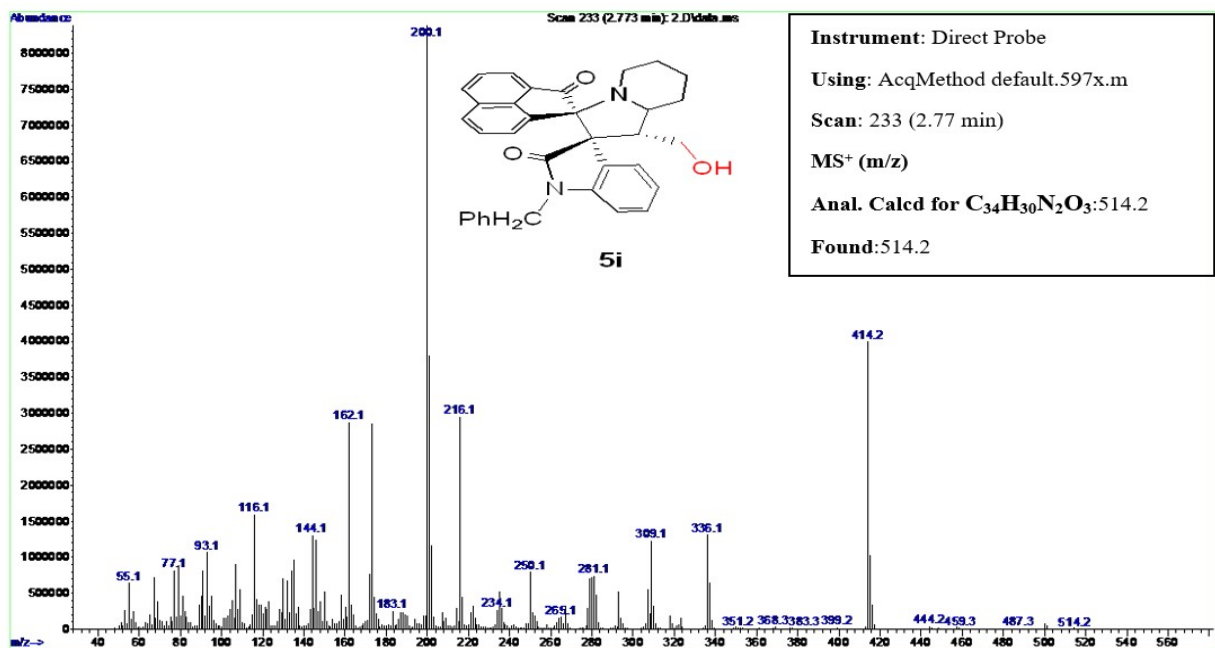


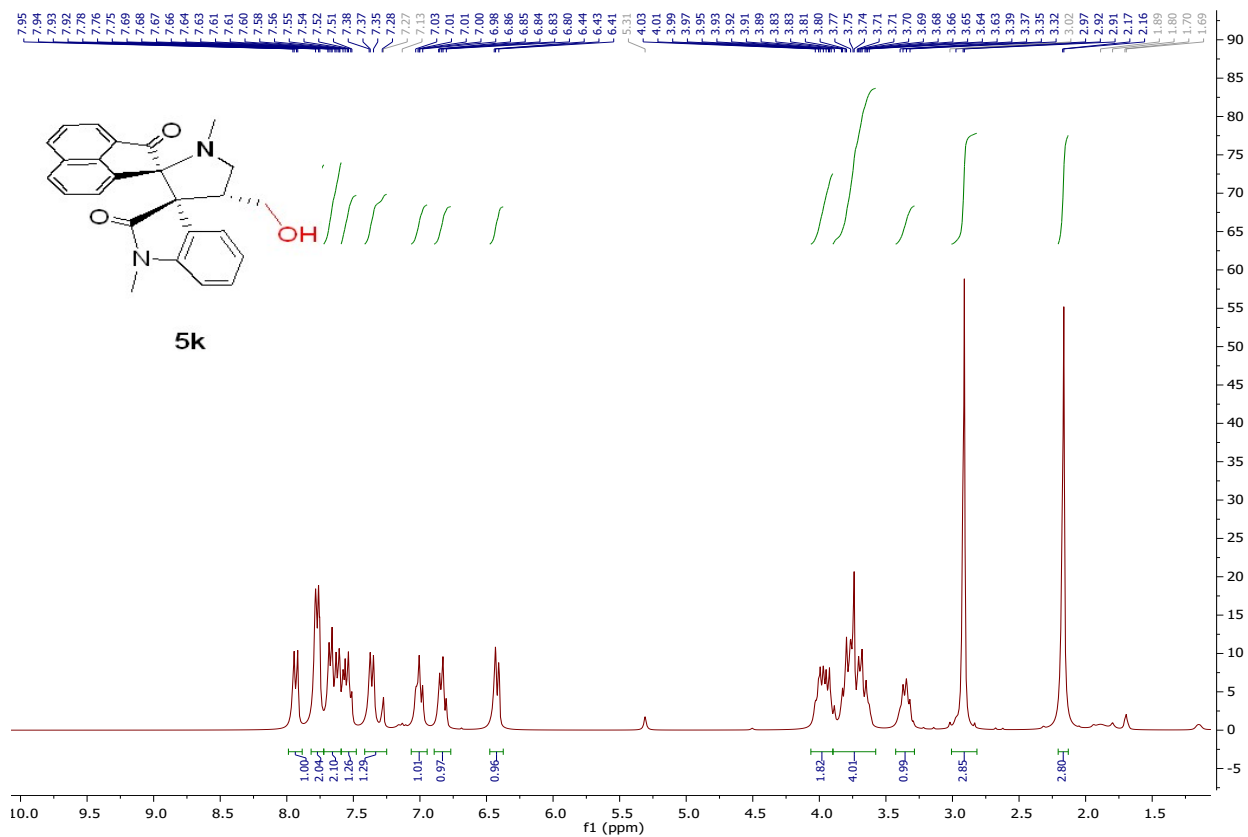
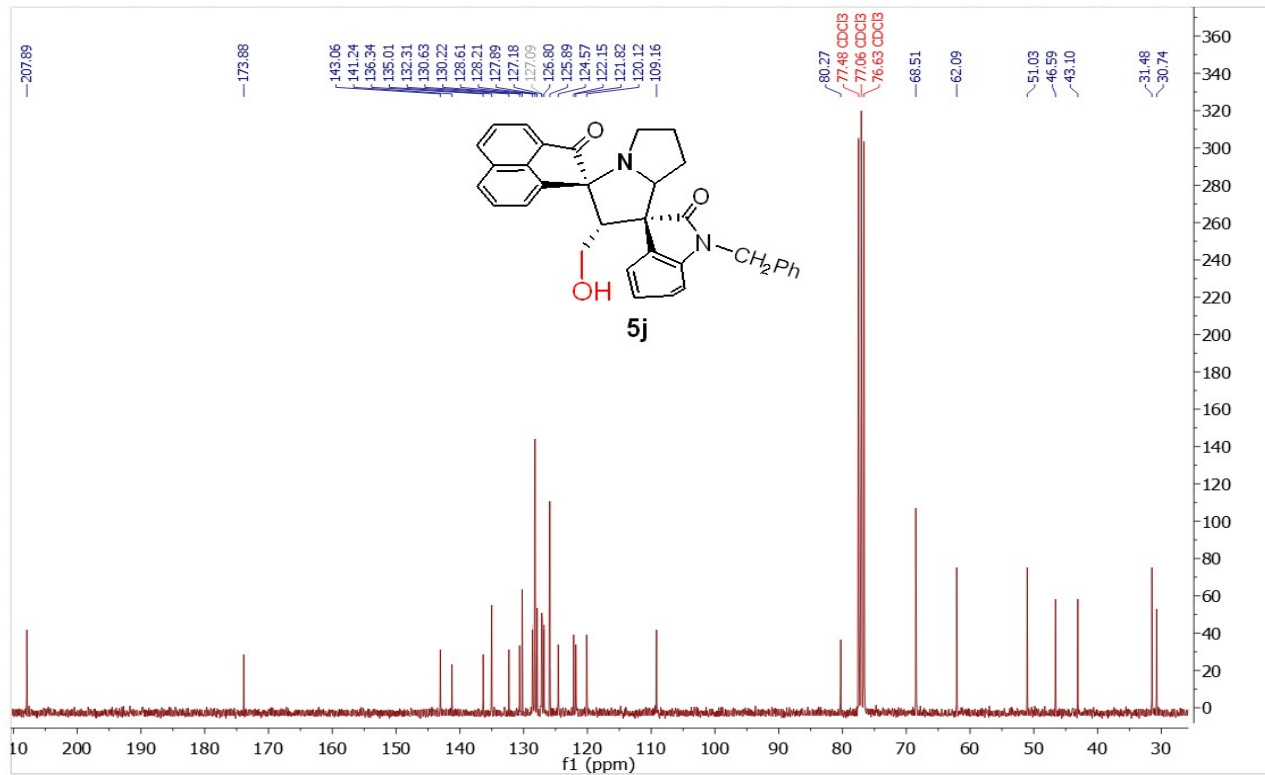




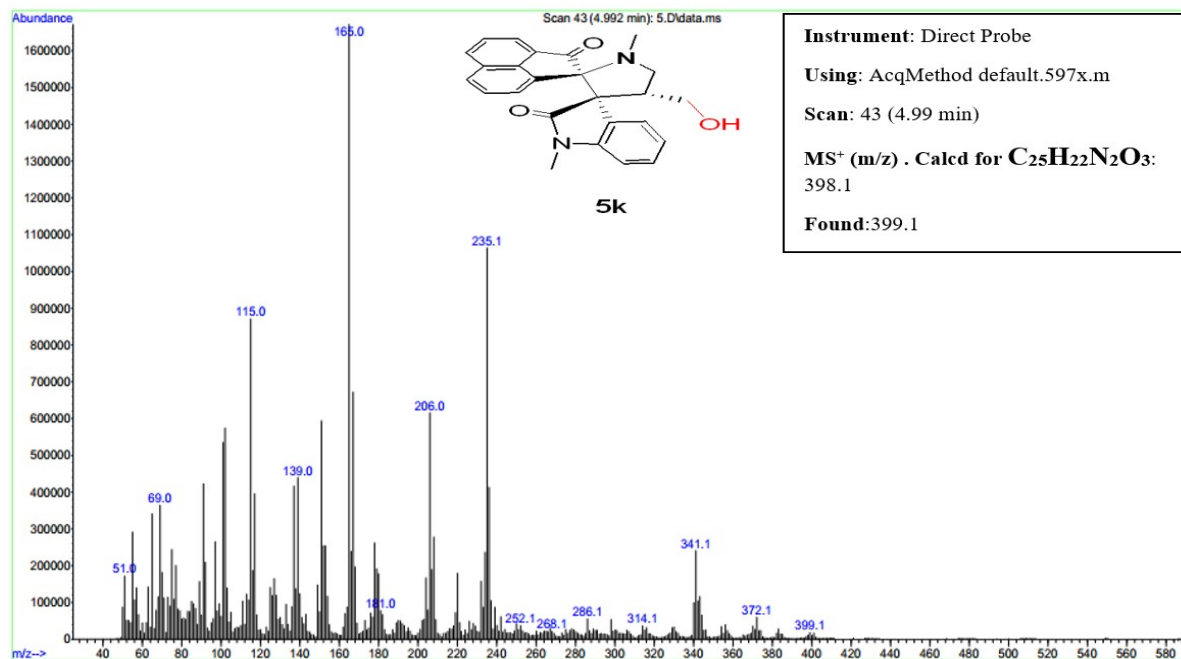
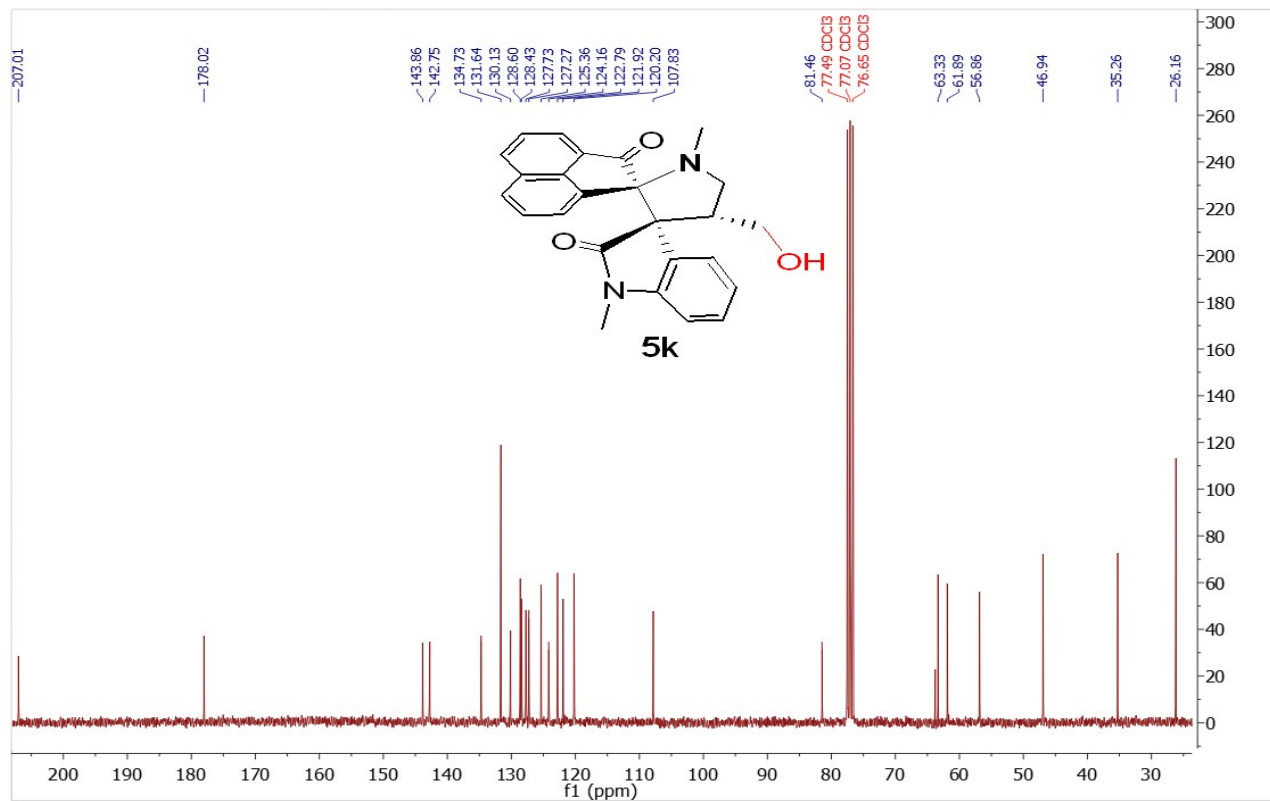


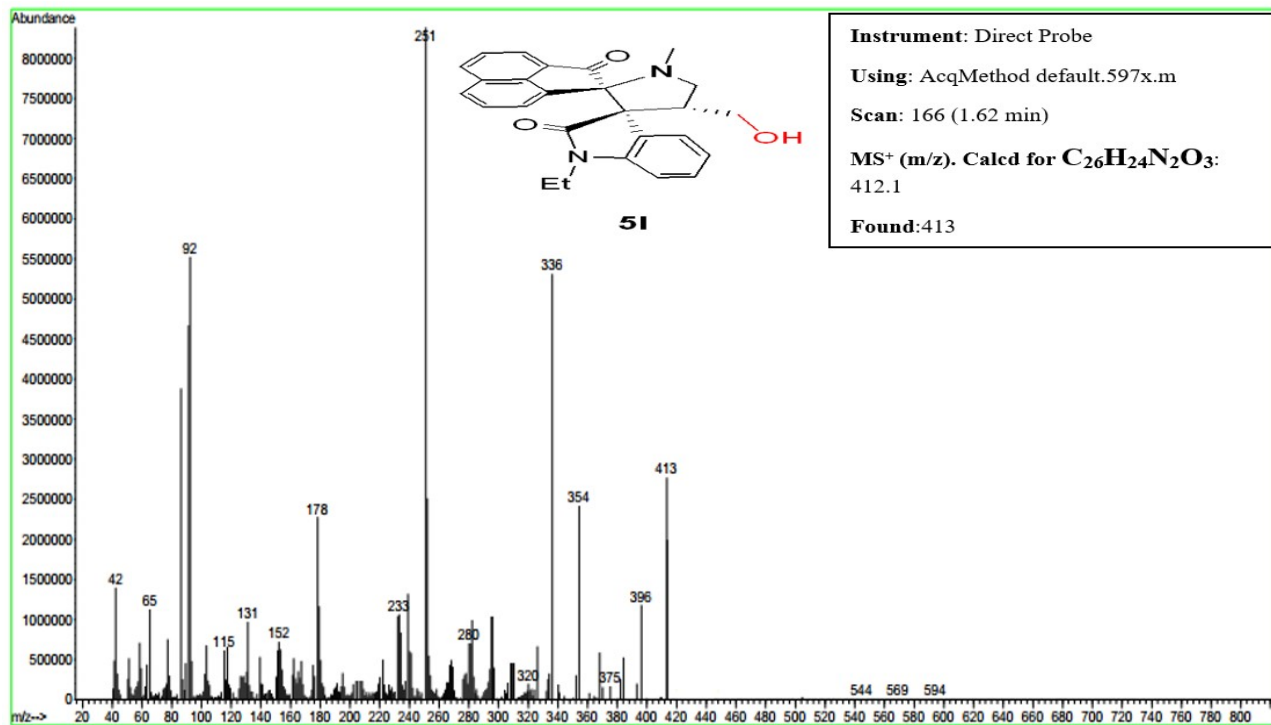
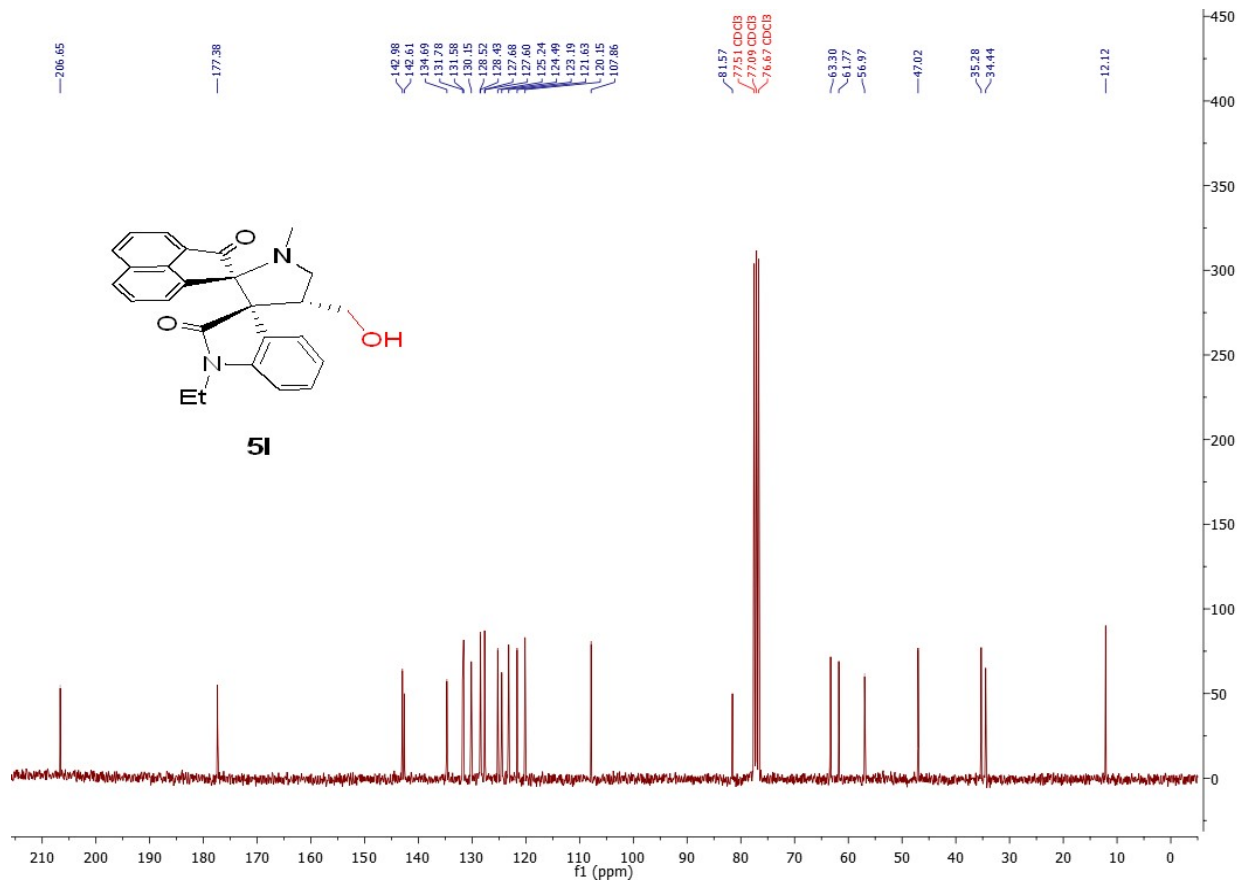


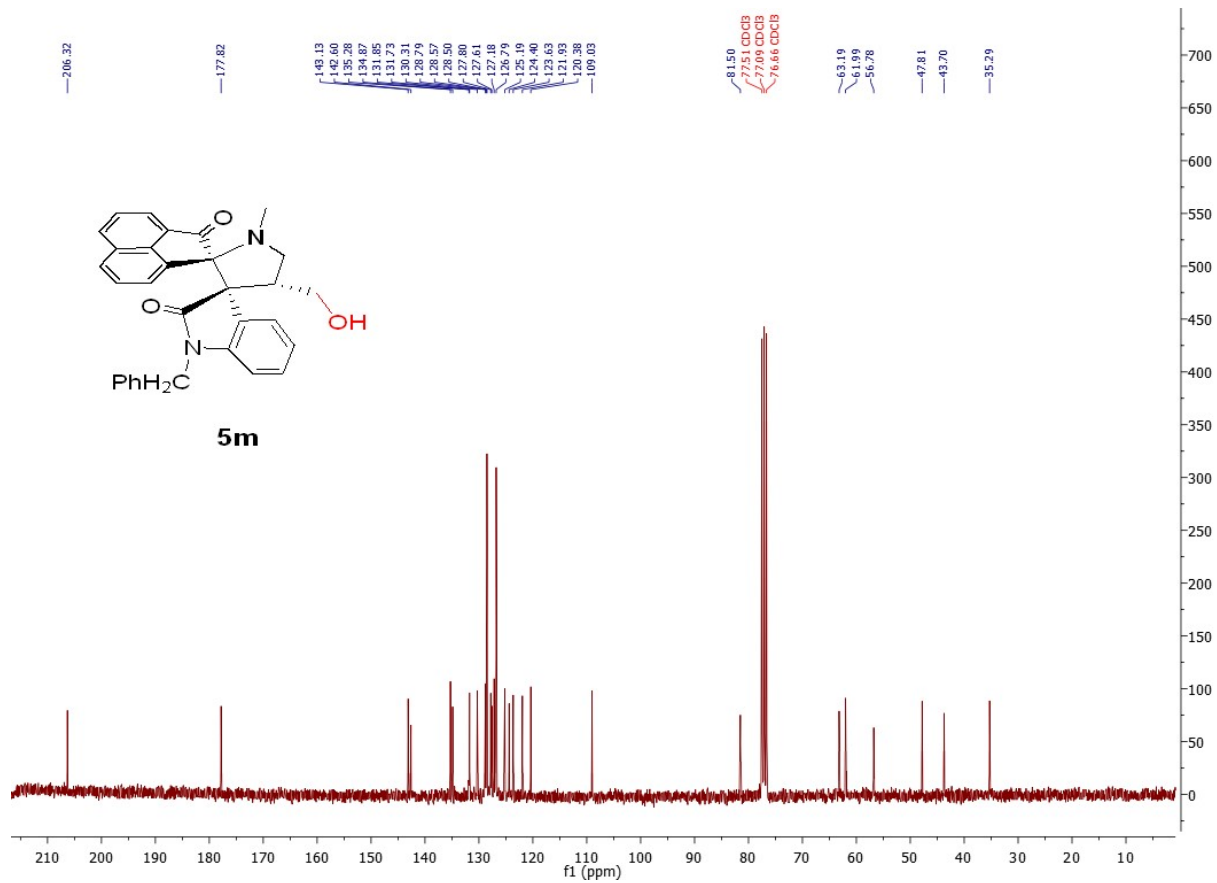
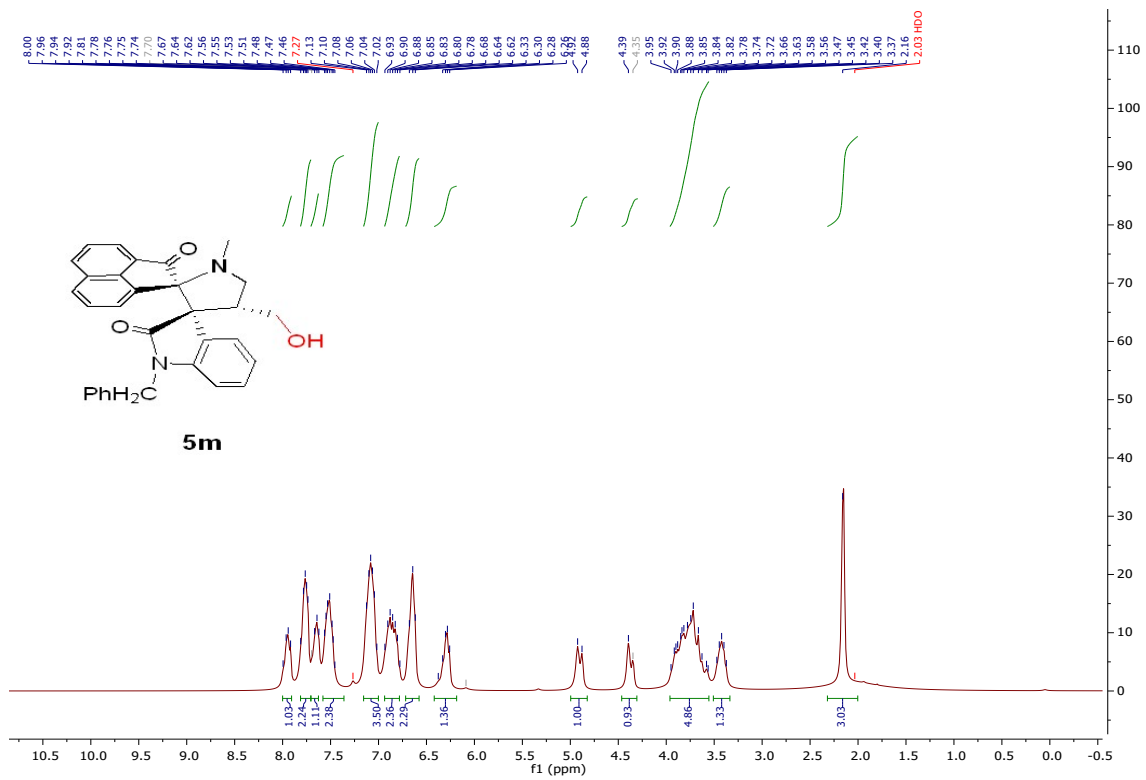


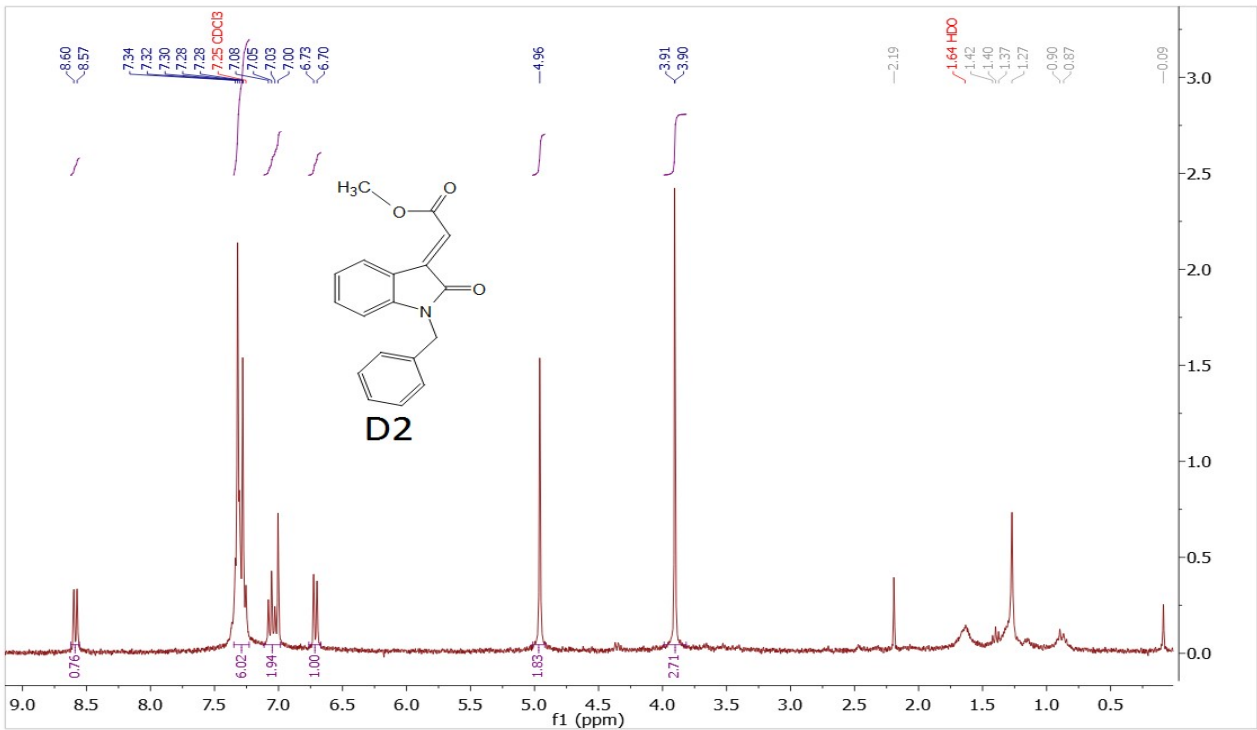
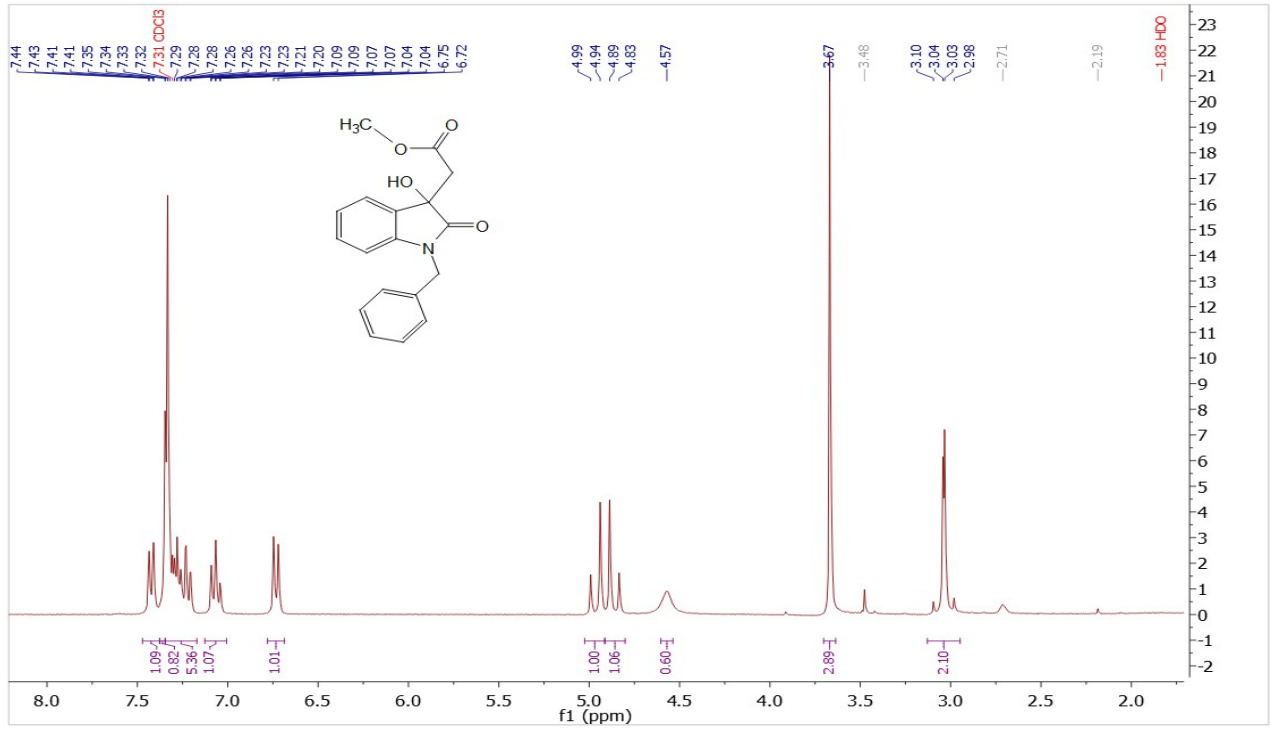


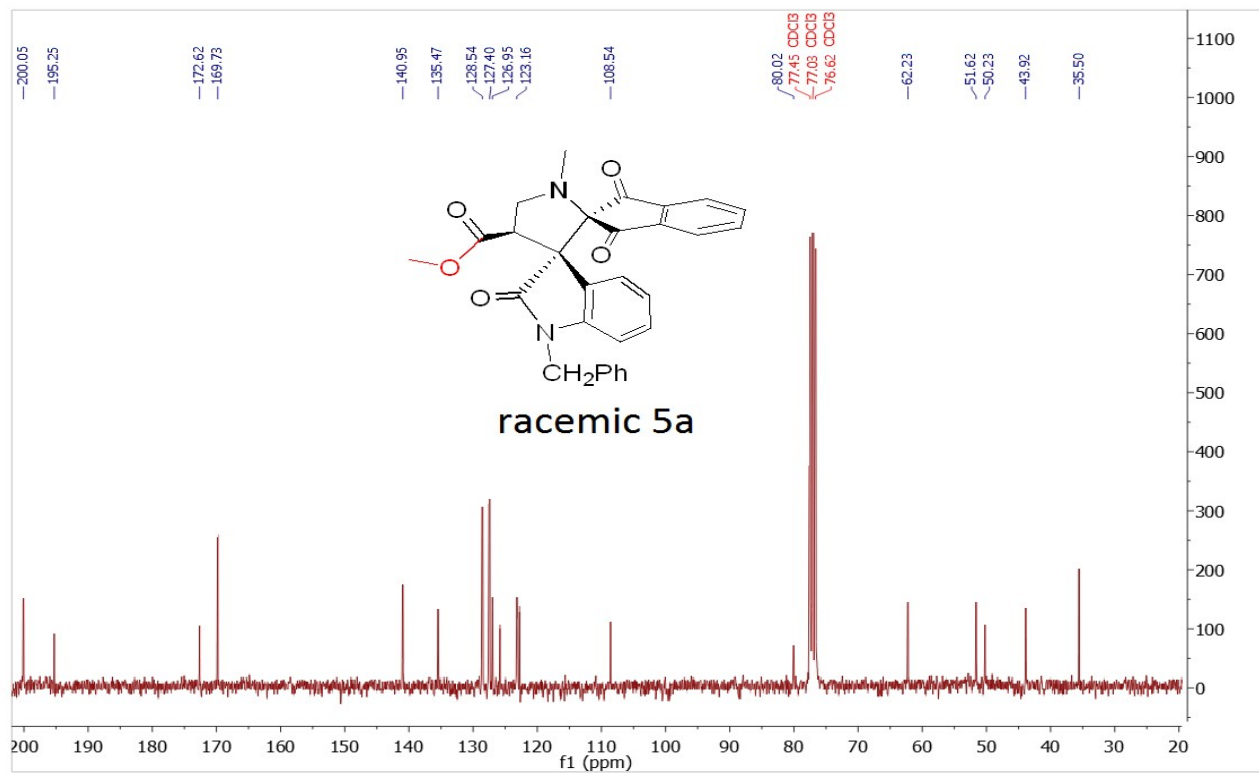
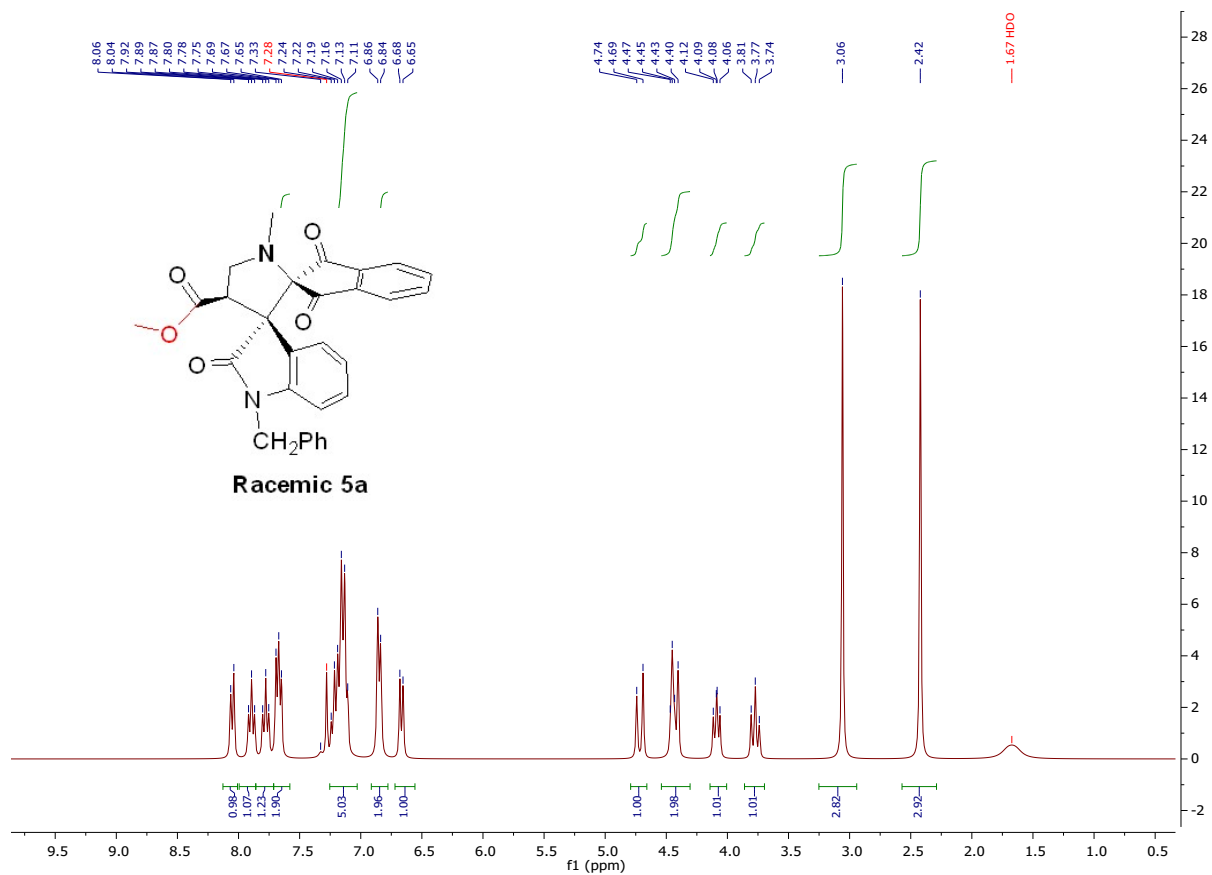


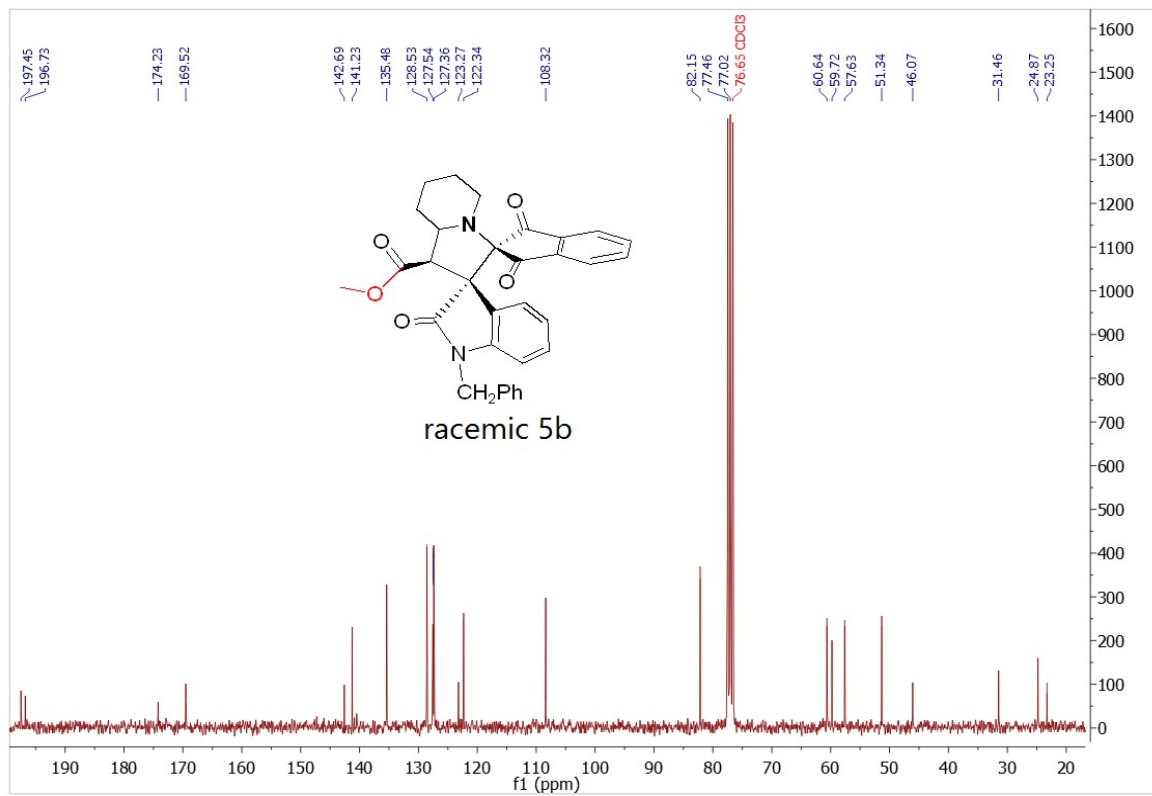
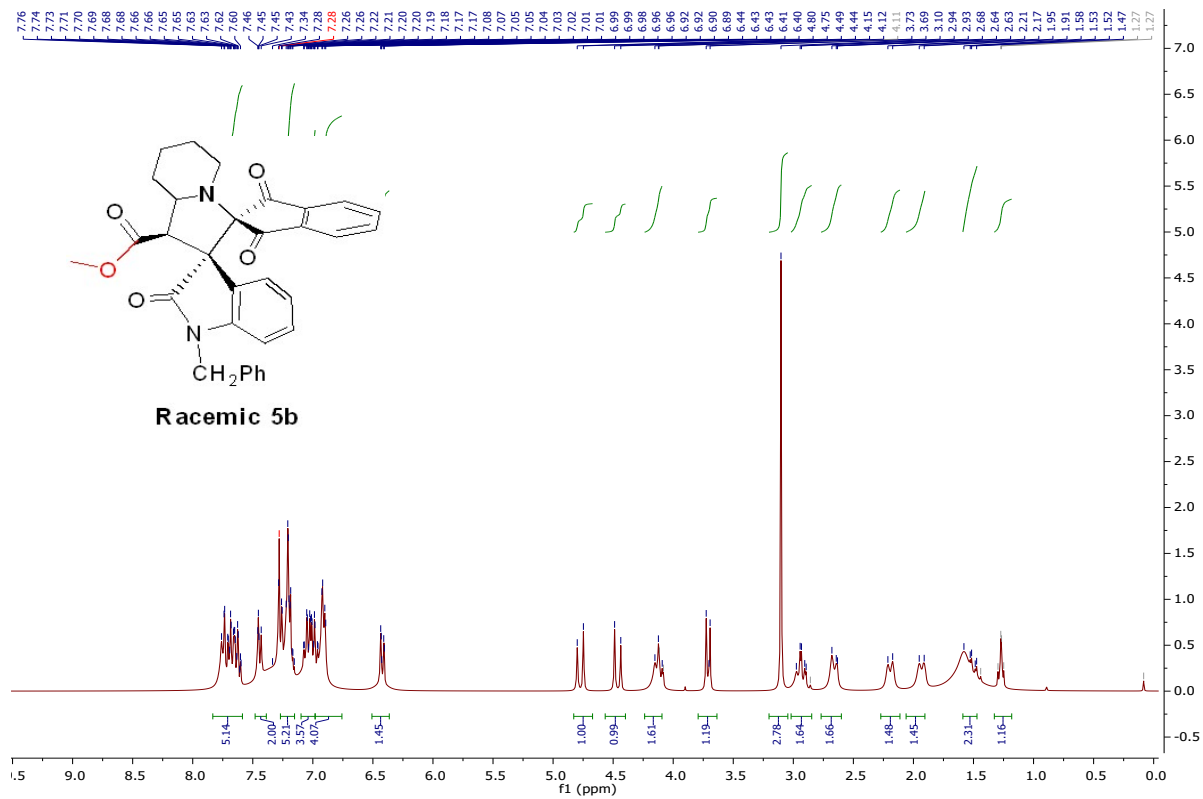


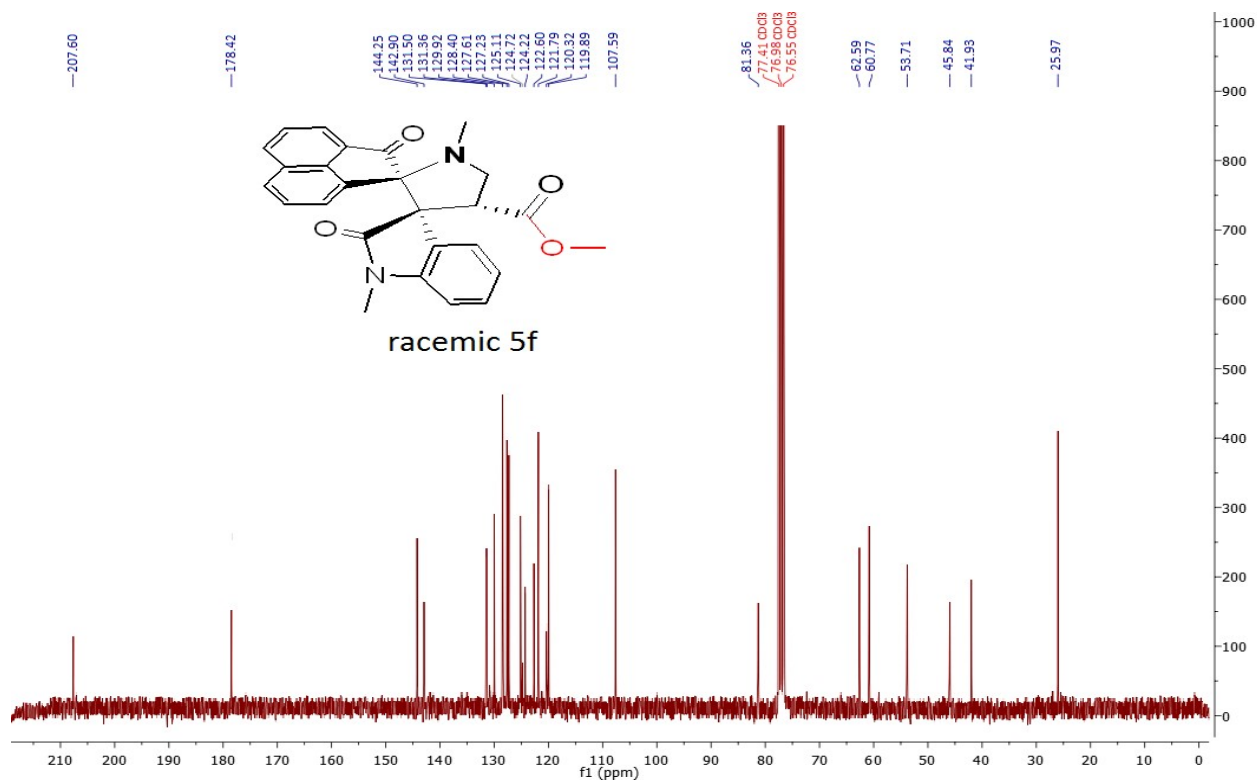
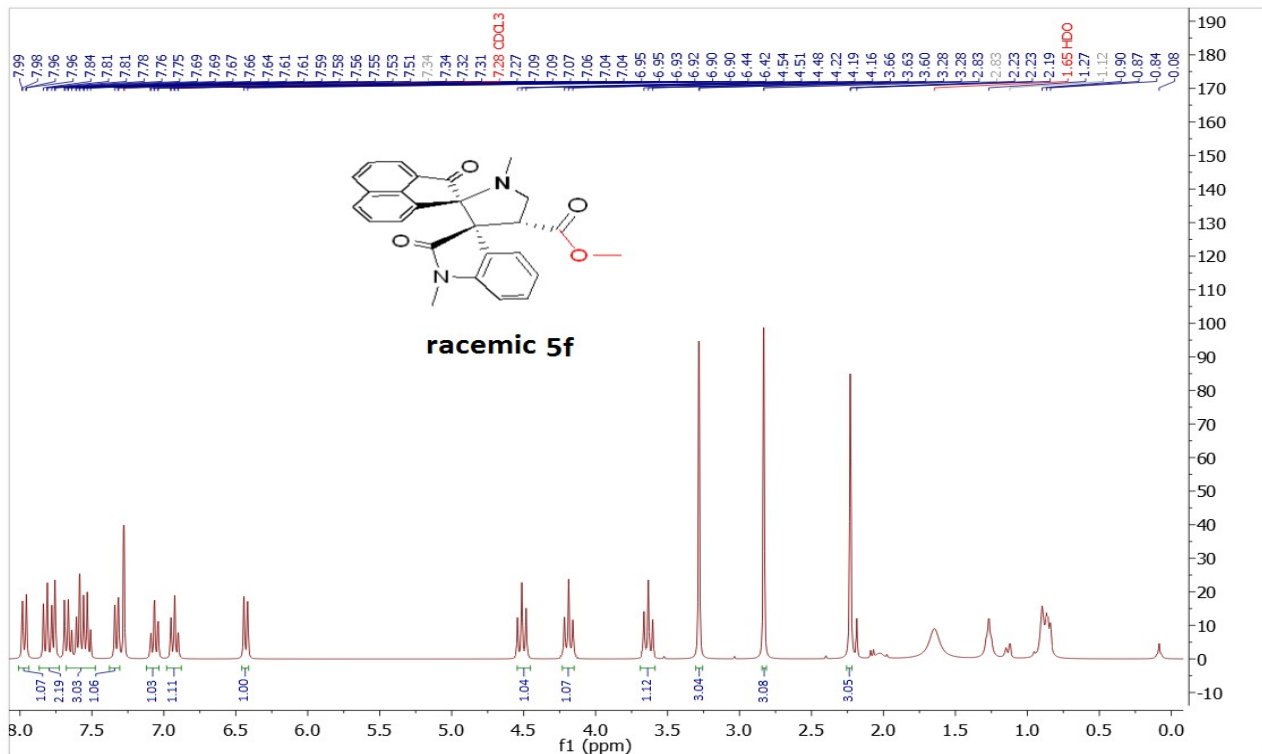


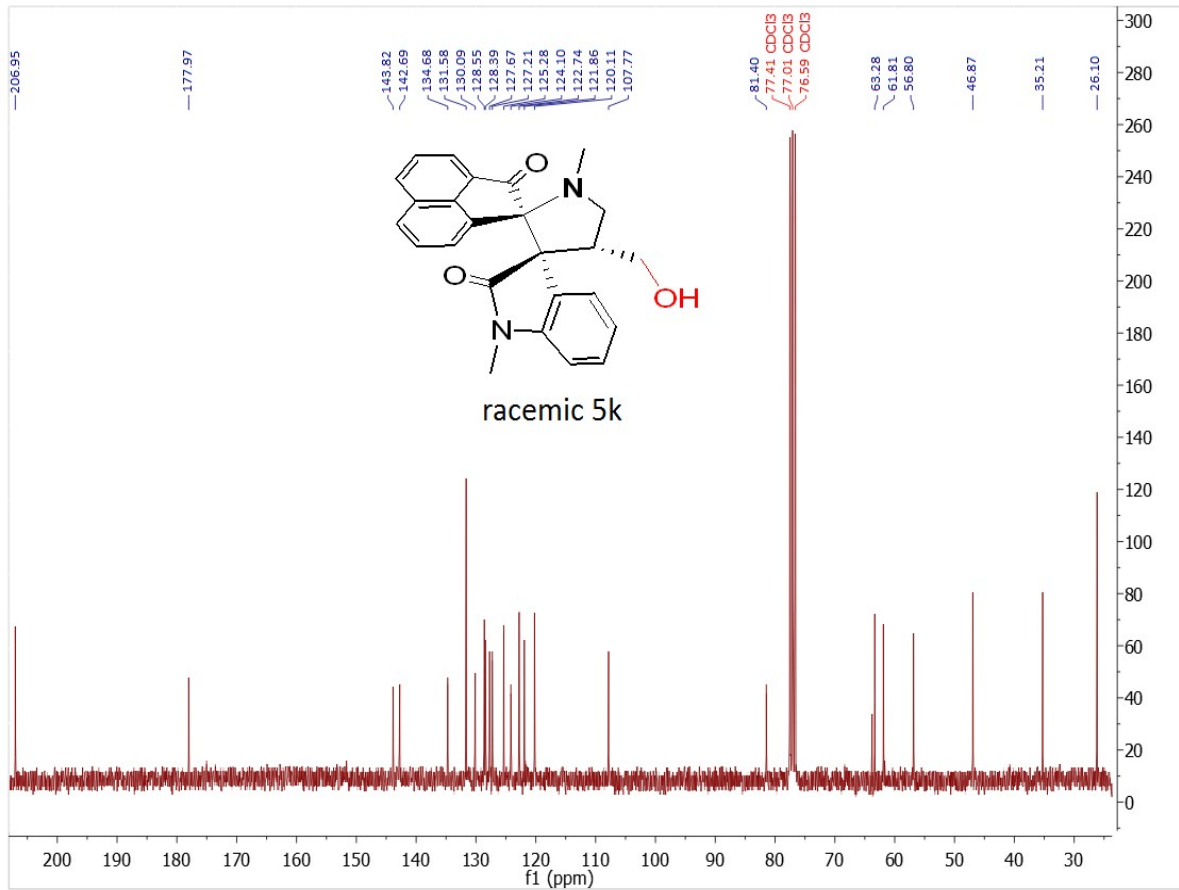




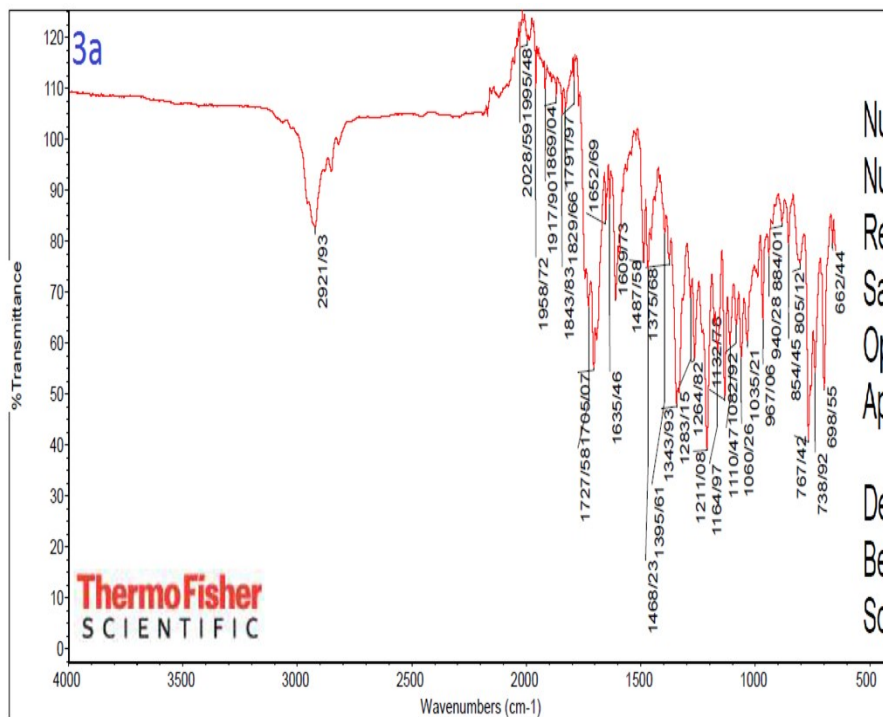






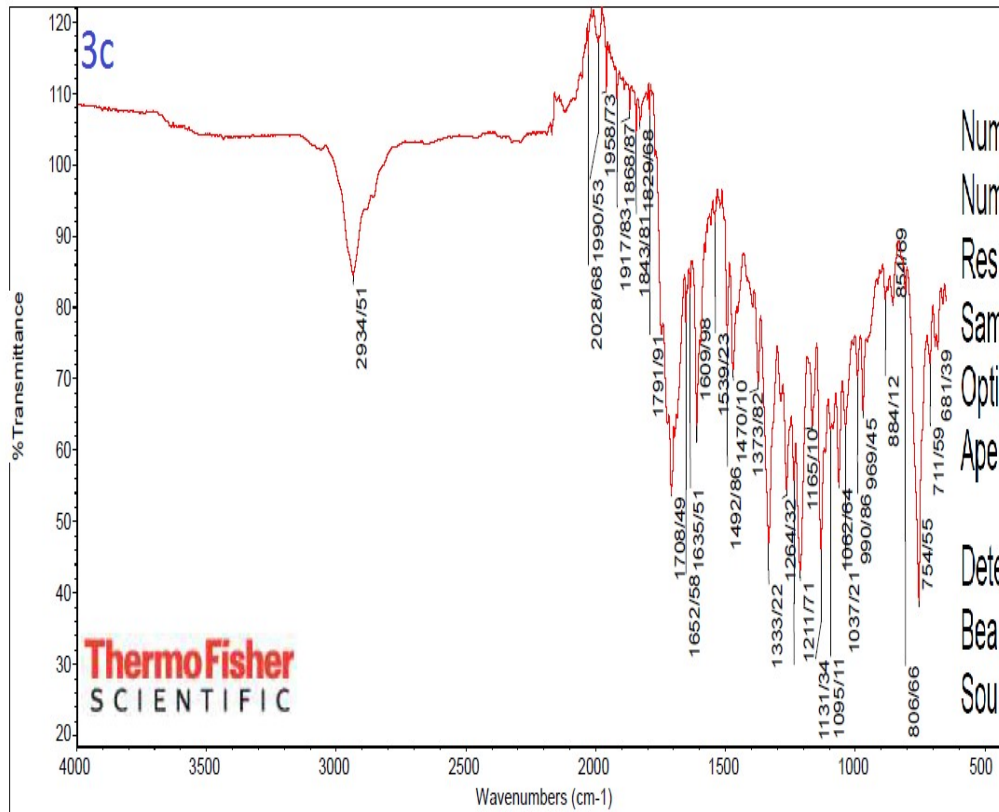
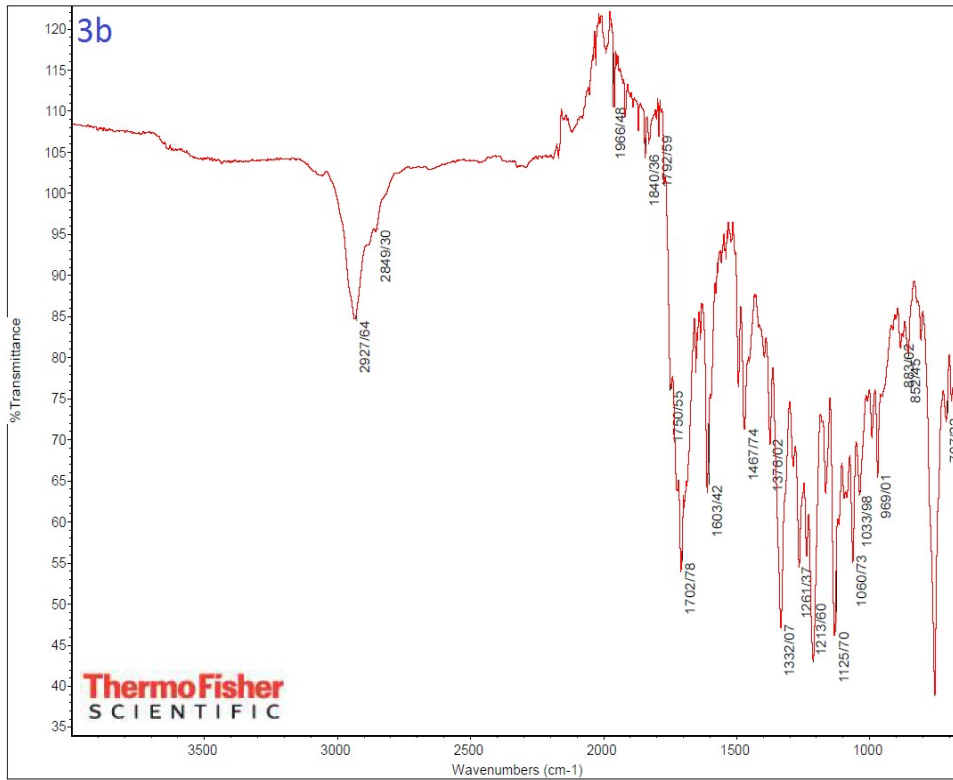


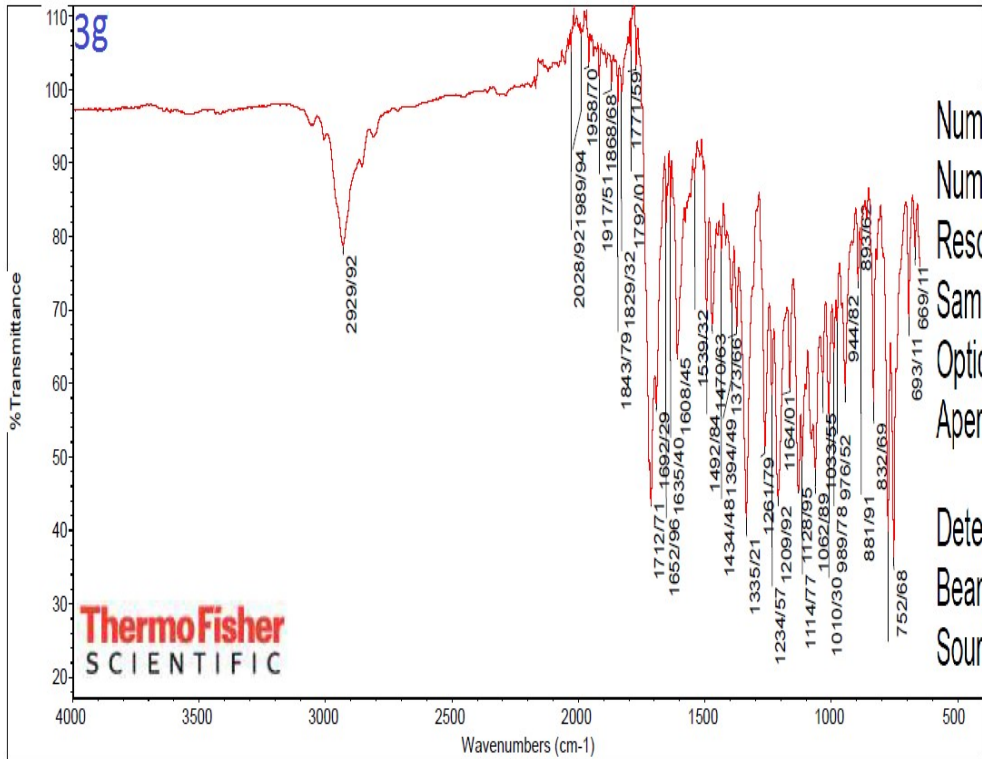
## IR spectroscopy



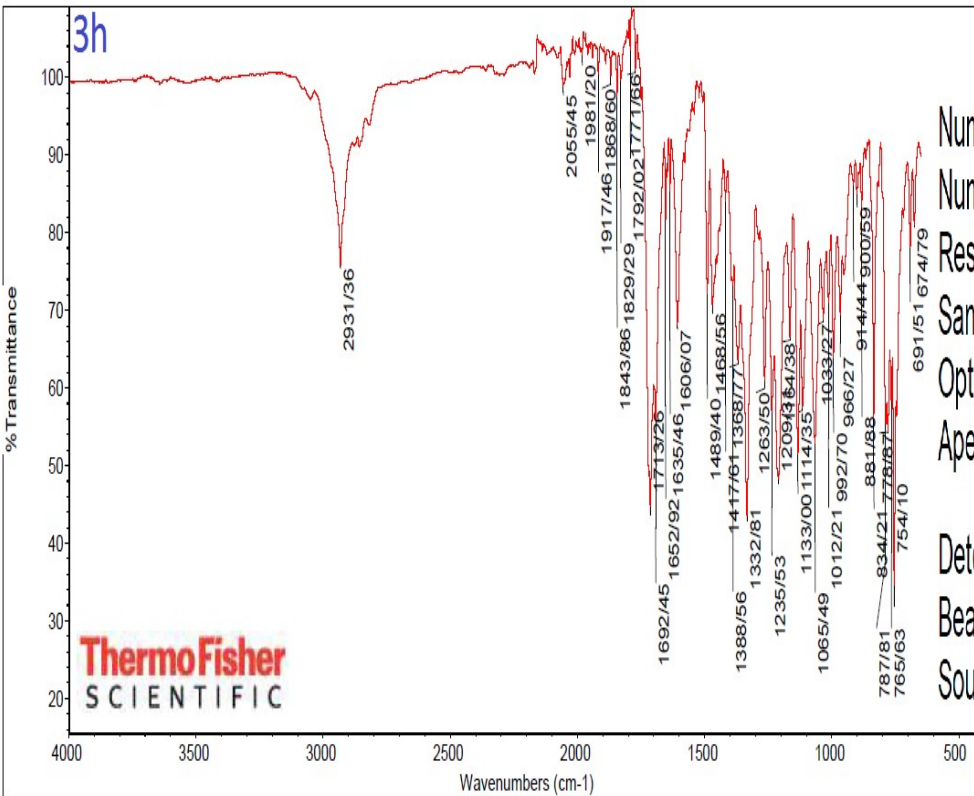
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 Number of background scans: 32  
 Resolution: 4/000  
 Sample gain: 4/0  
 Optical velocity: 0/6329  
 Aperture: 100/00  
 Detector: DTGS KBr  
 Beamsplitter: KBr  
 Source: IR



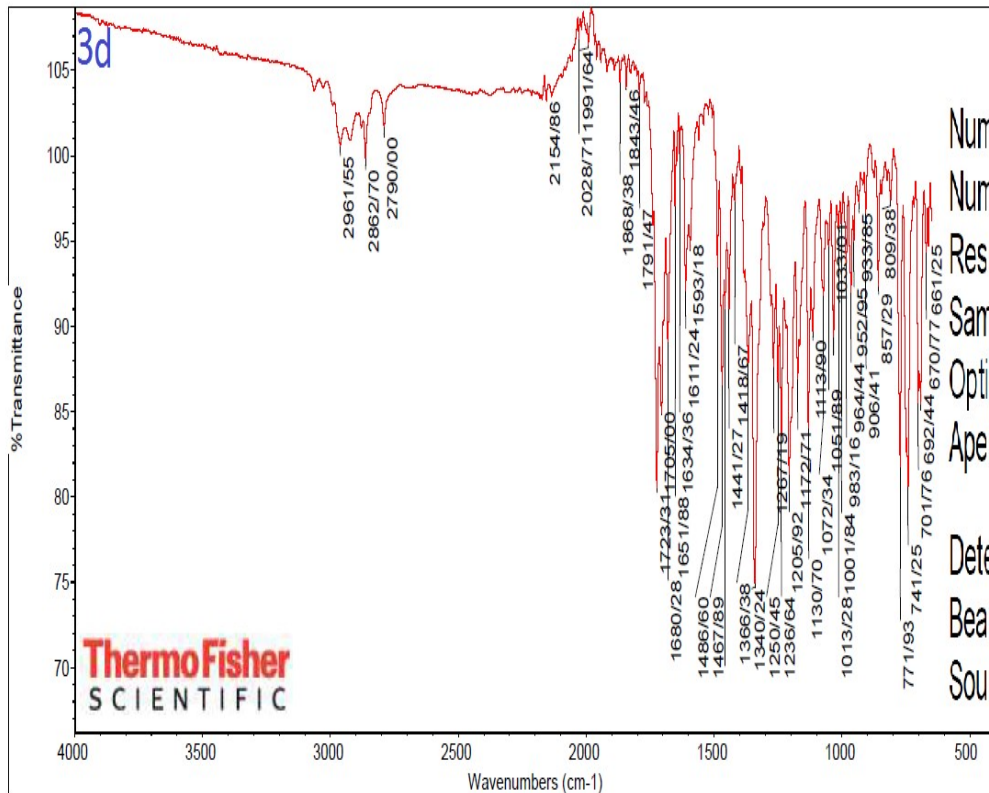
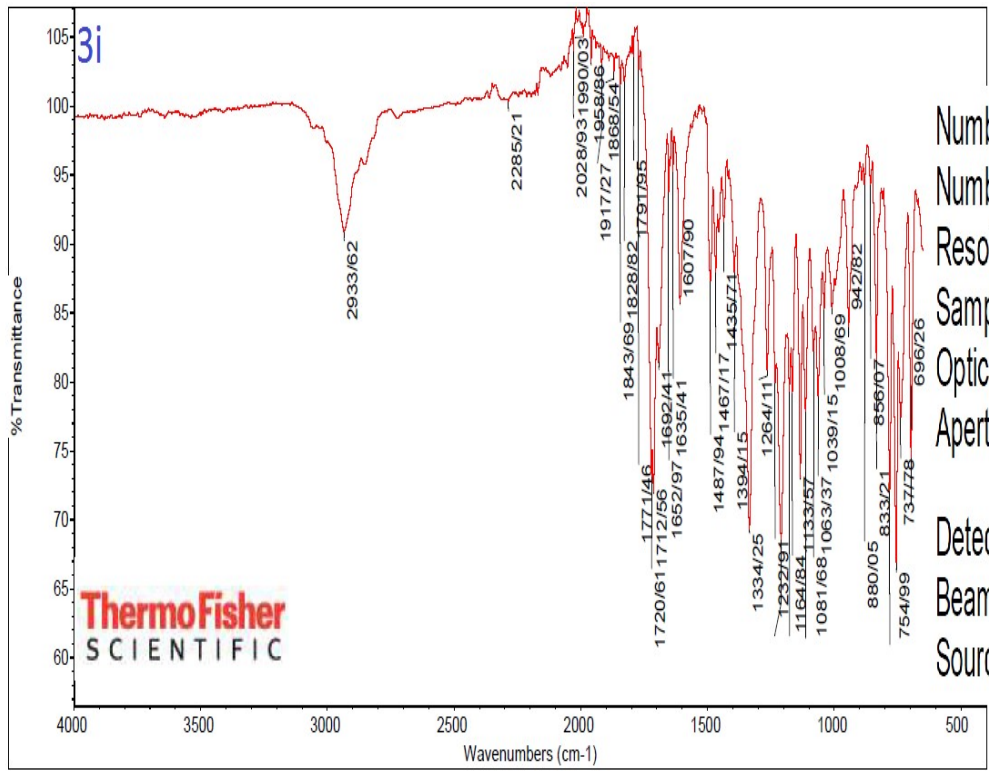


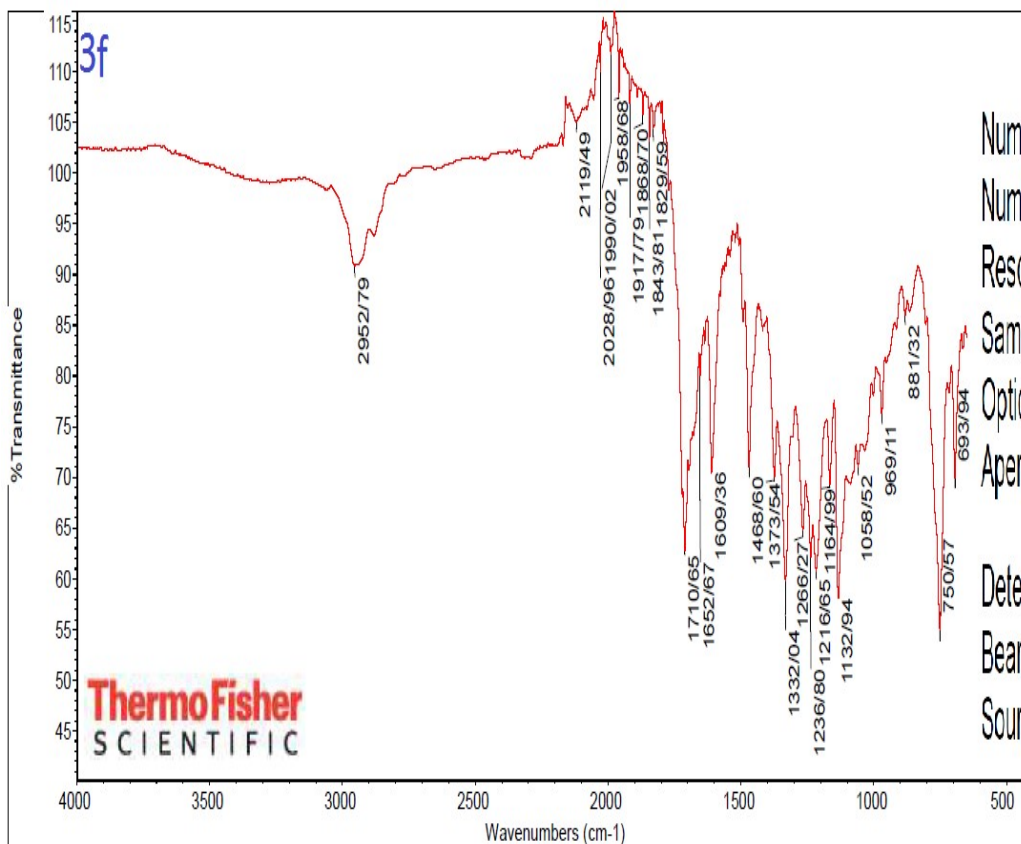
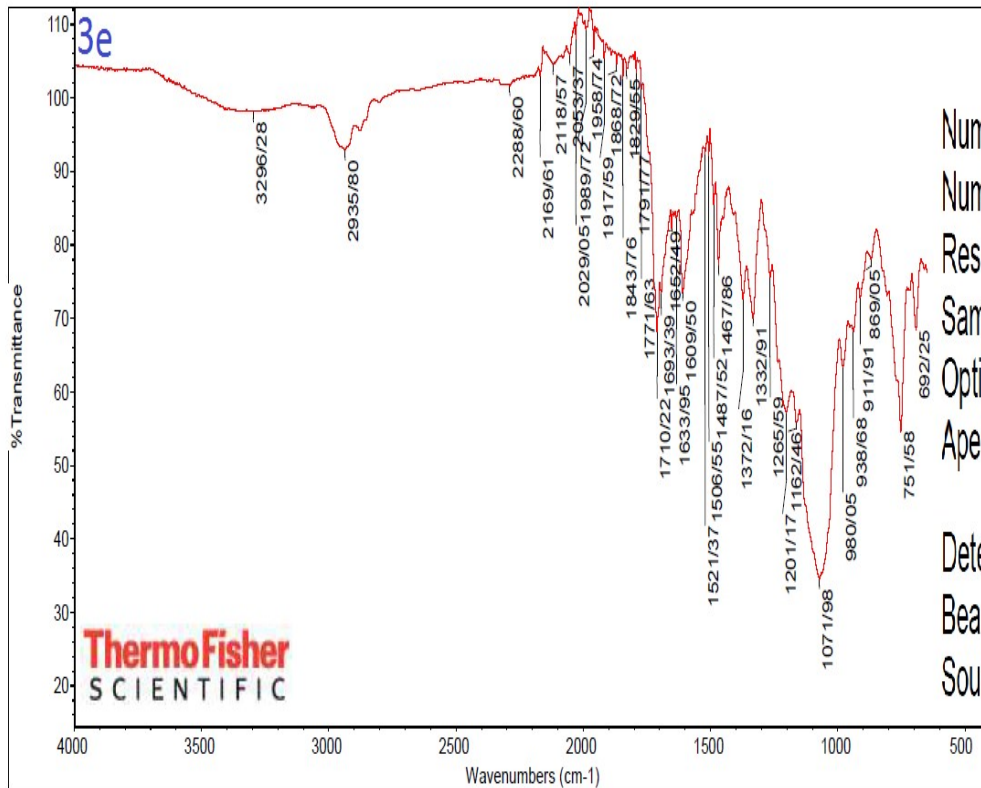


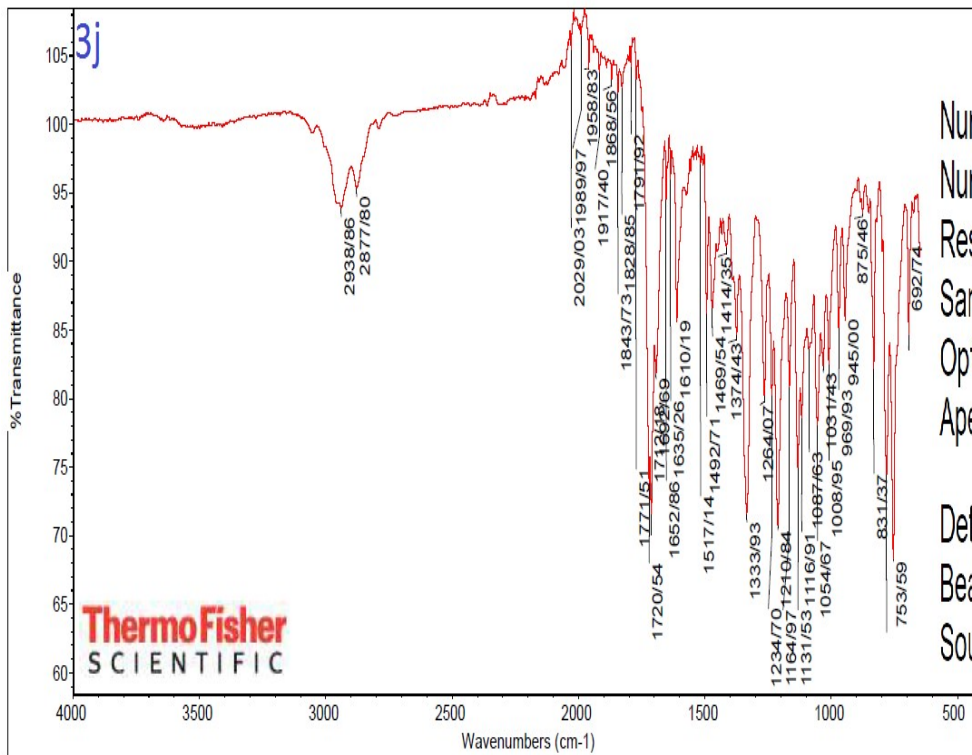
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 Detector: DTGS KBr  
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 Source: IR



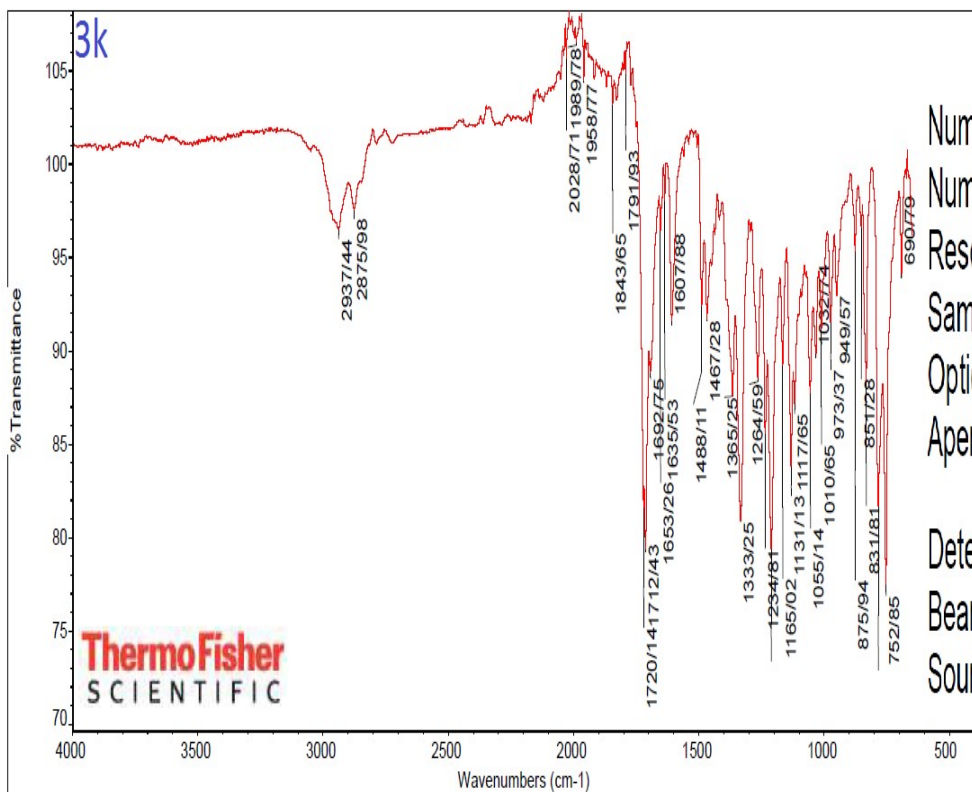
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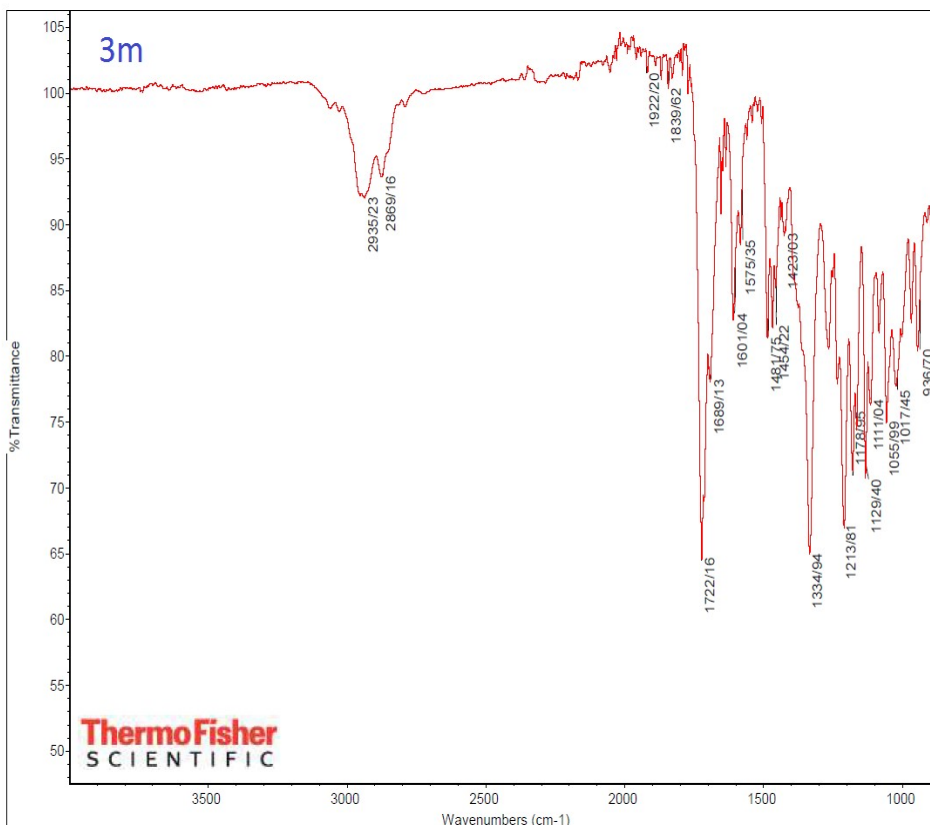
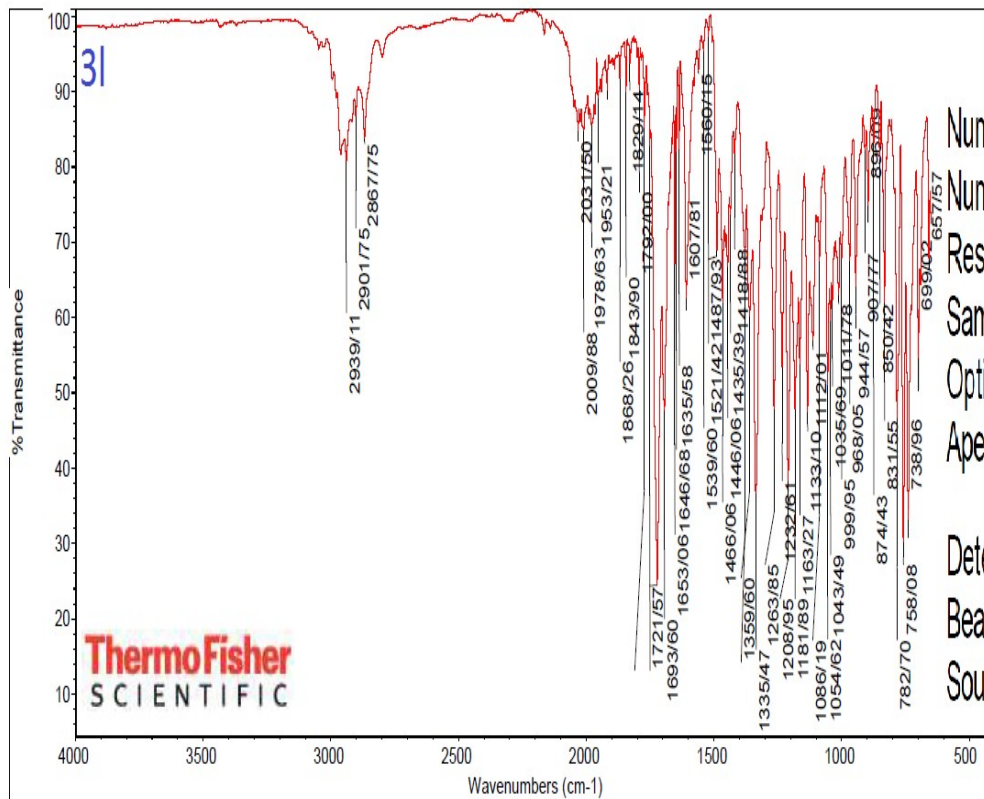


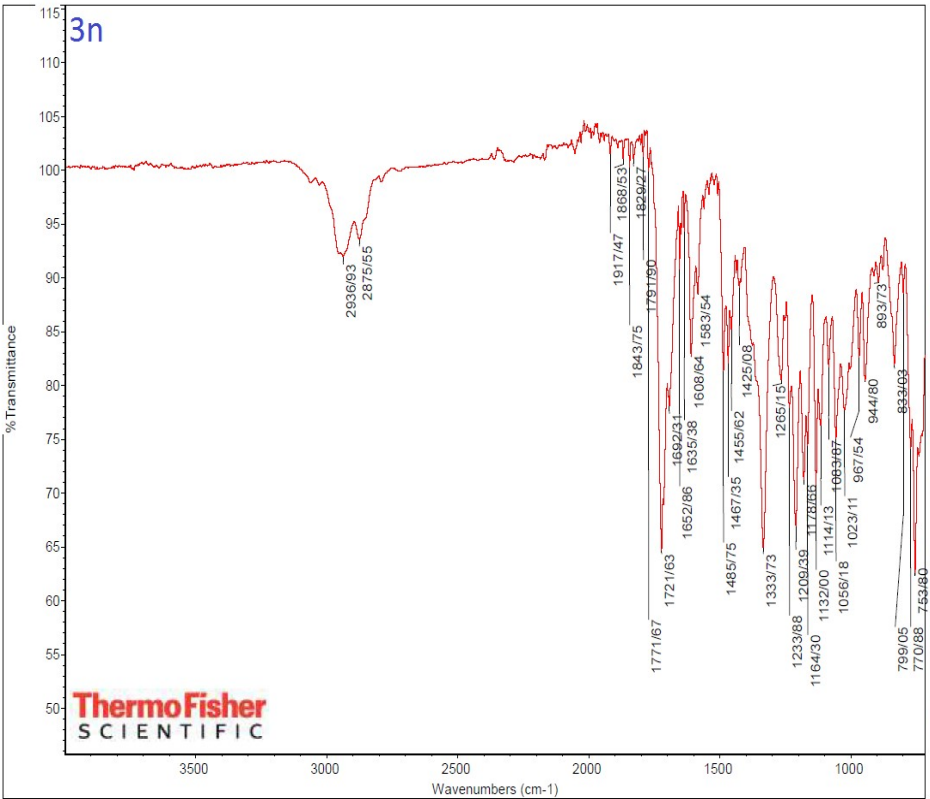


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 Optical velocity: 0/6329  
 Aperture: 100/00  
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 Source: IR

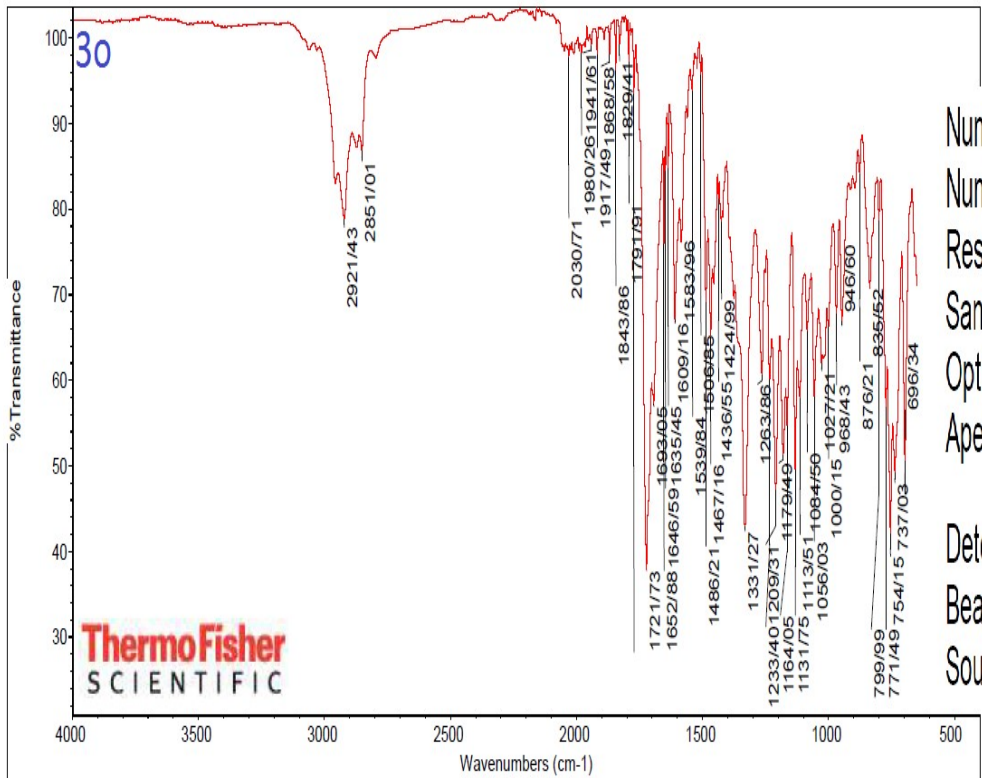


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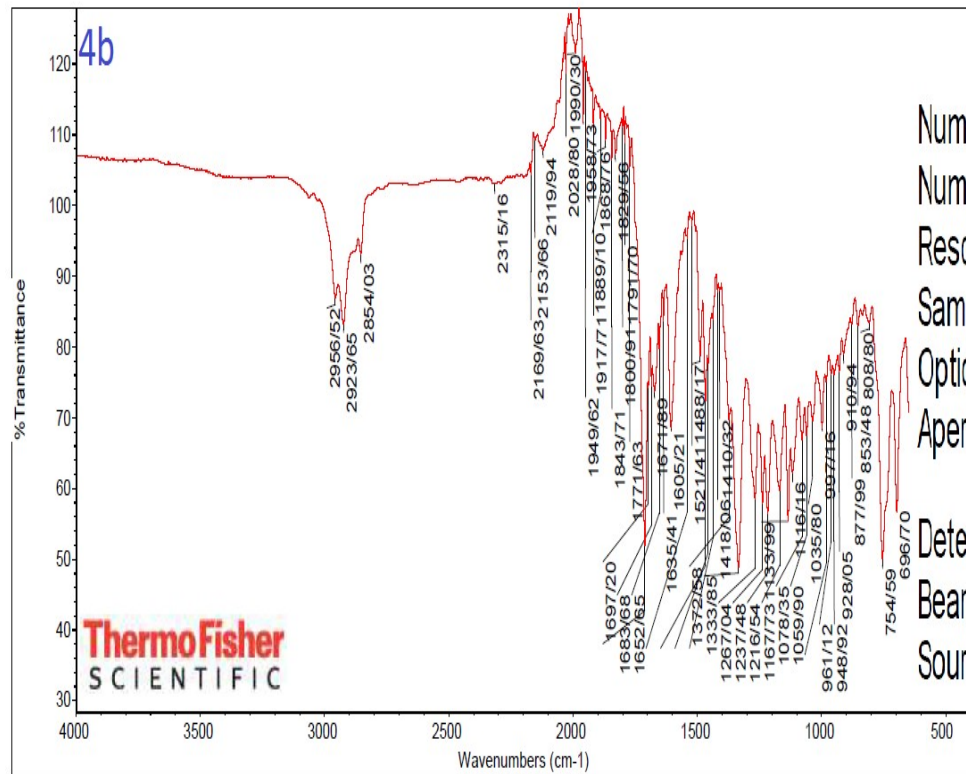
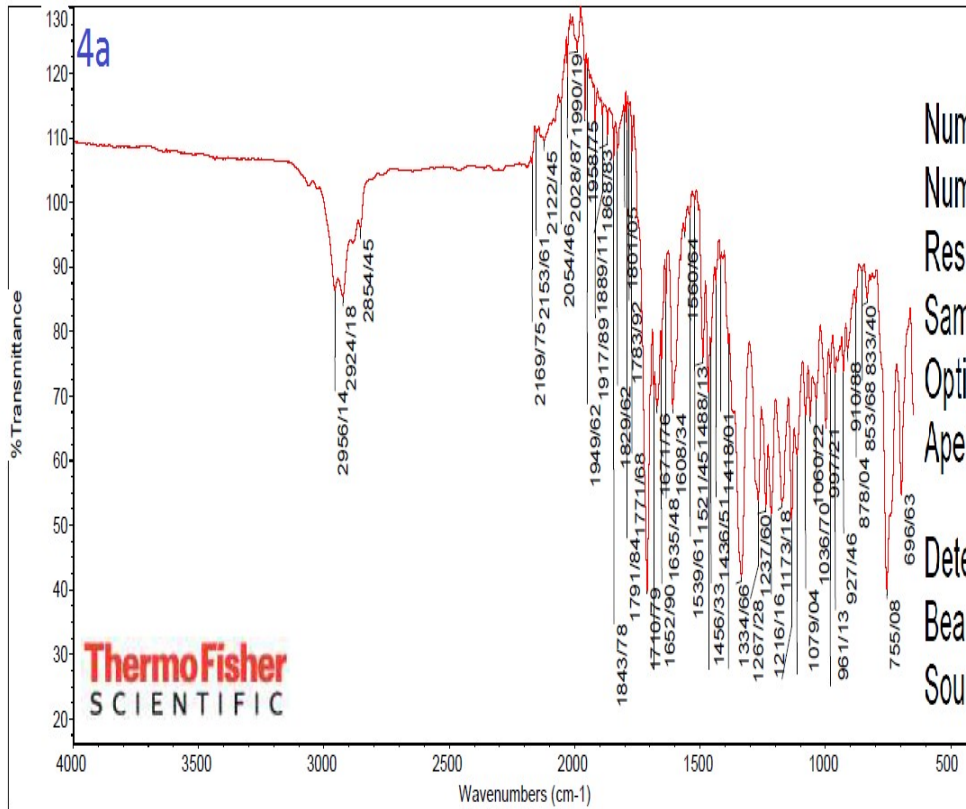




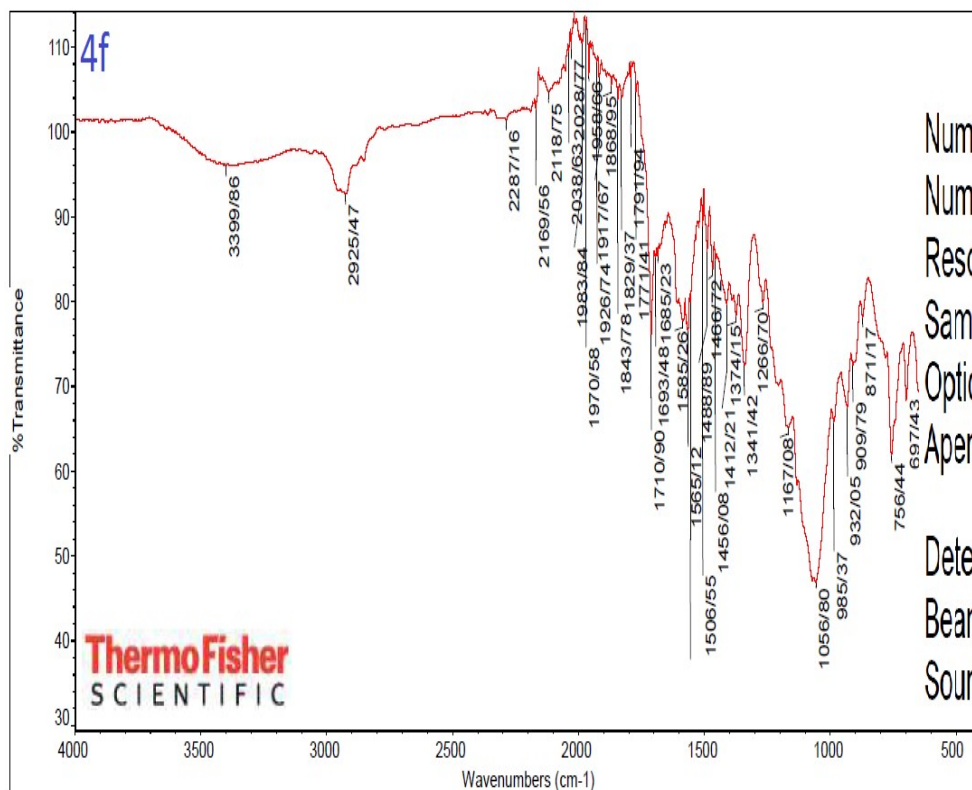
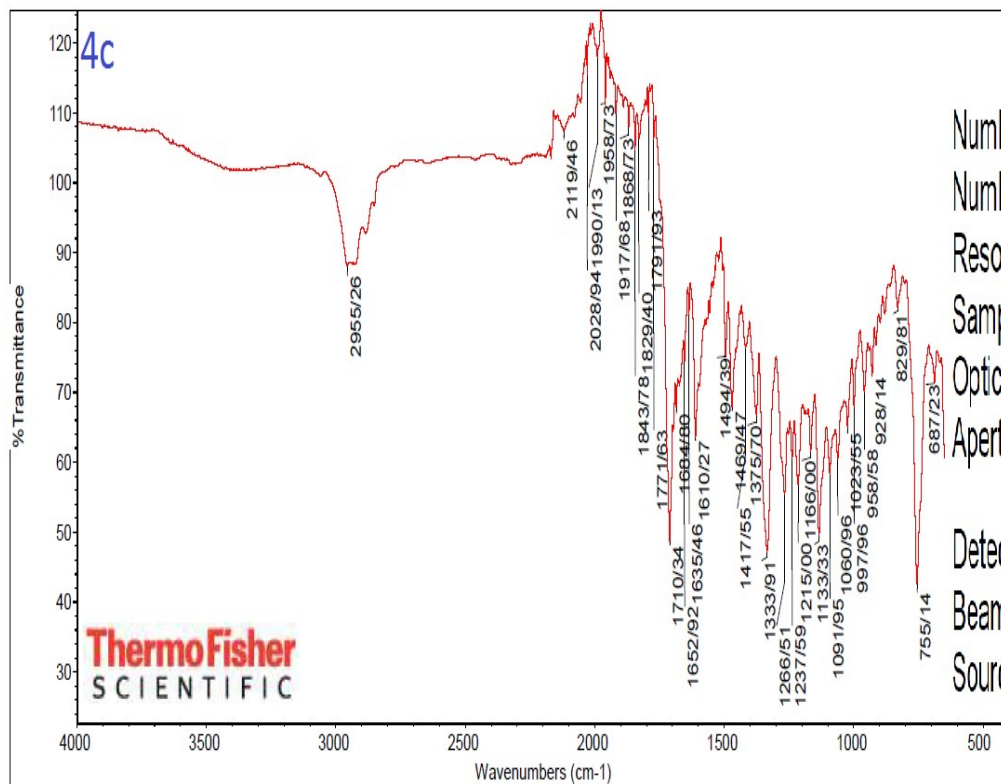
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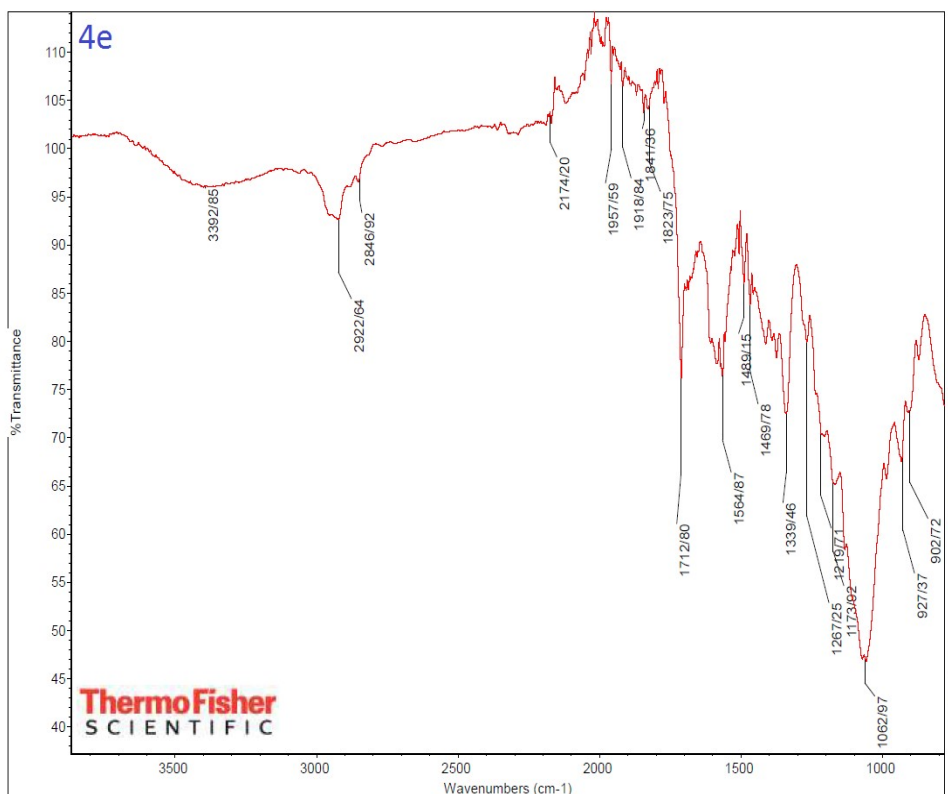
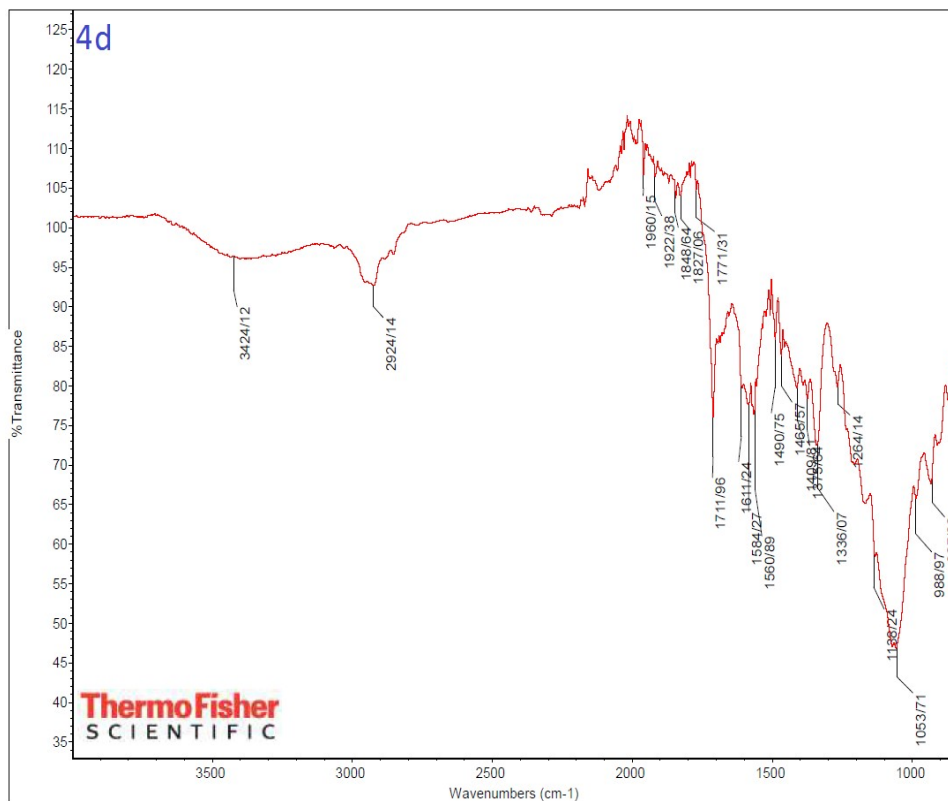


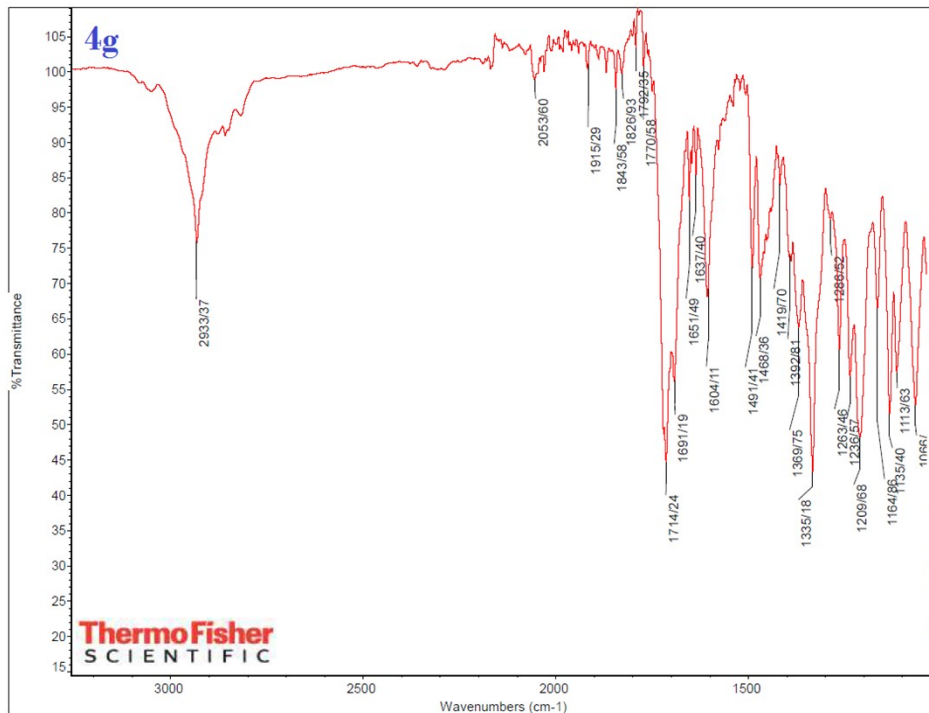
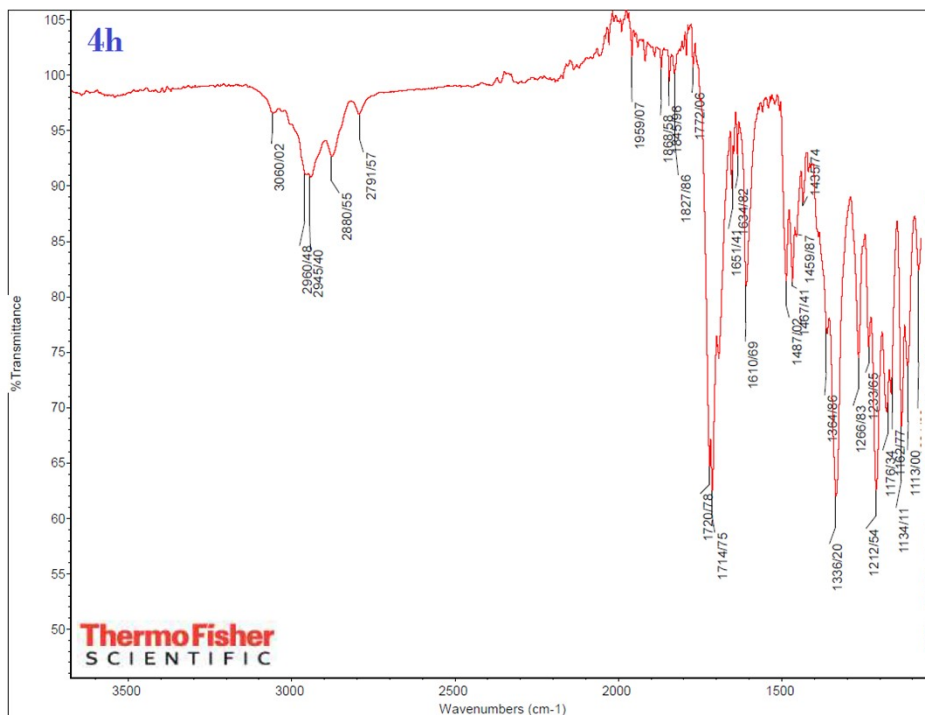
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 Beamsplitter: KBr  
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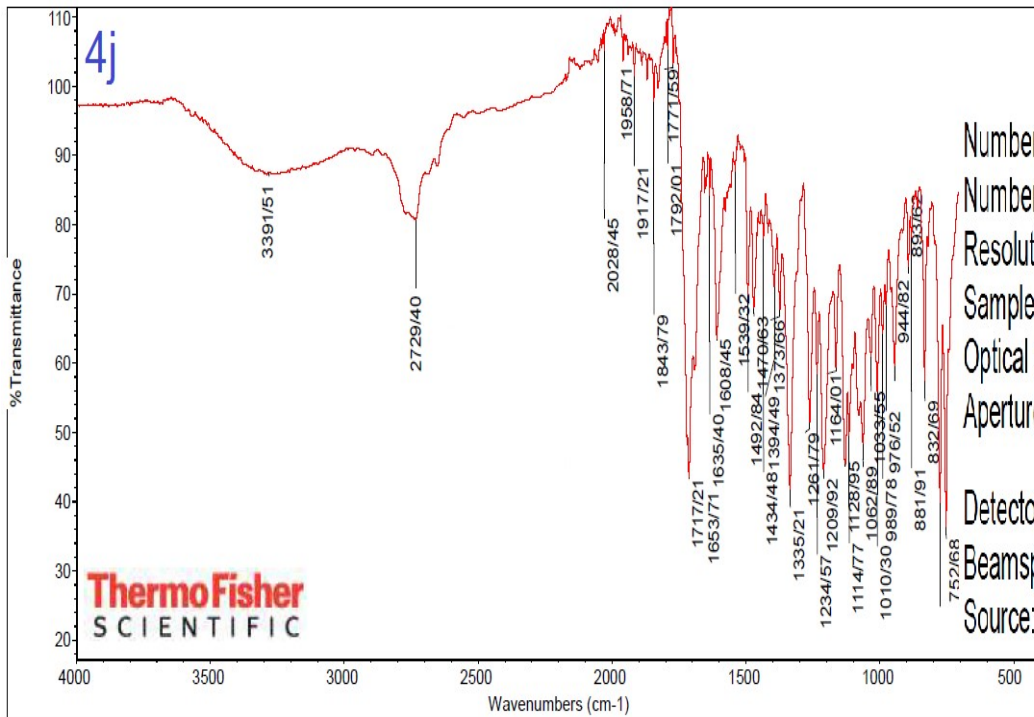
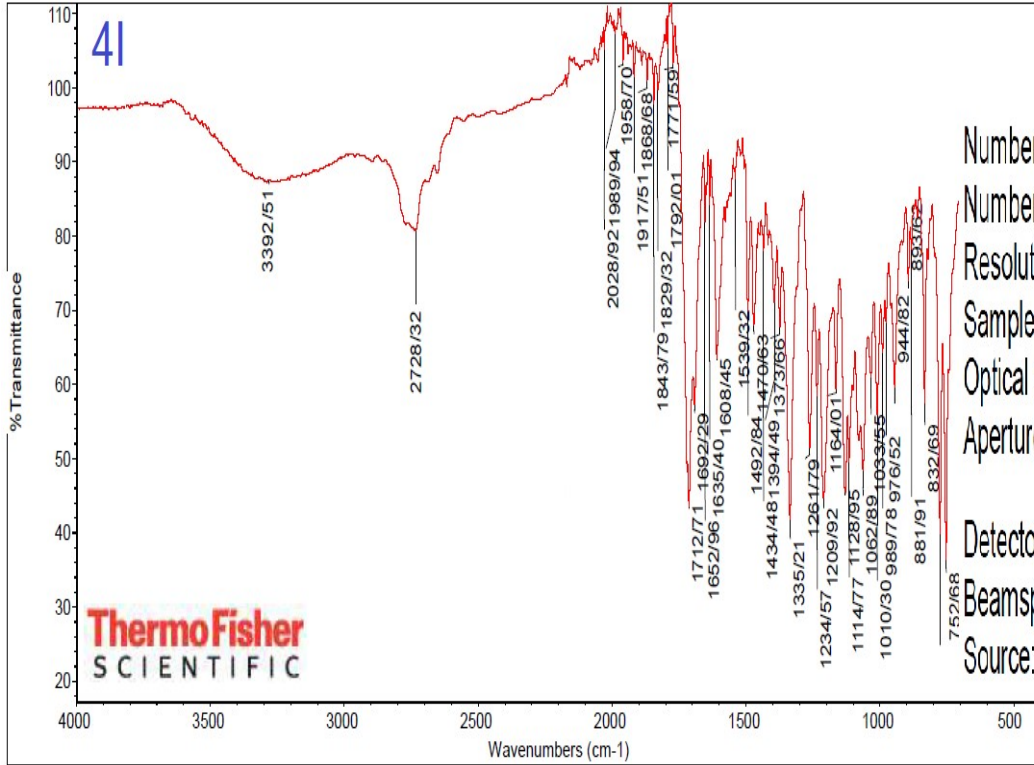


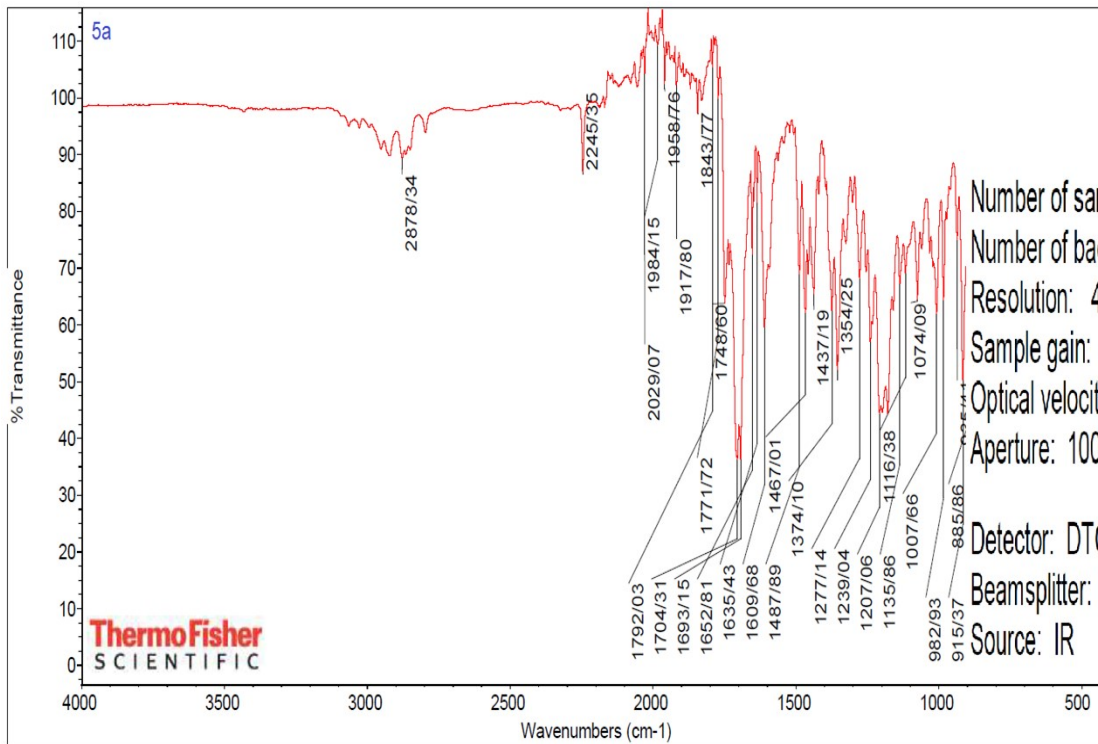
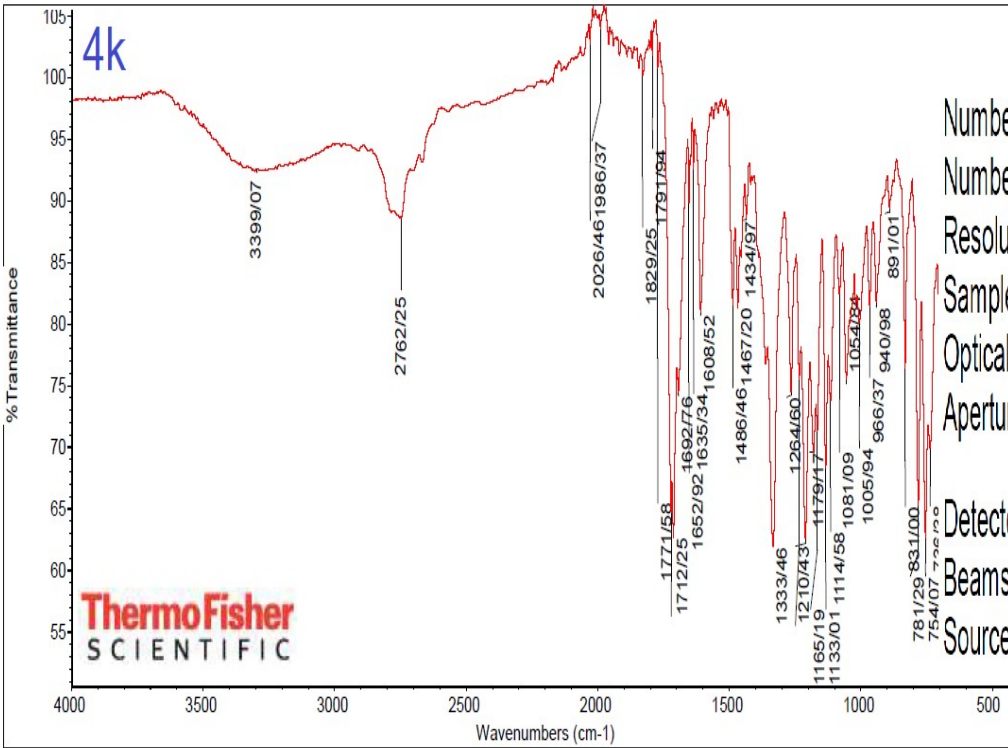


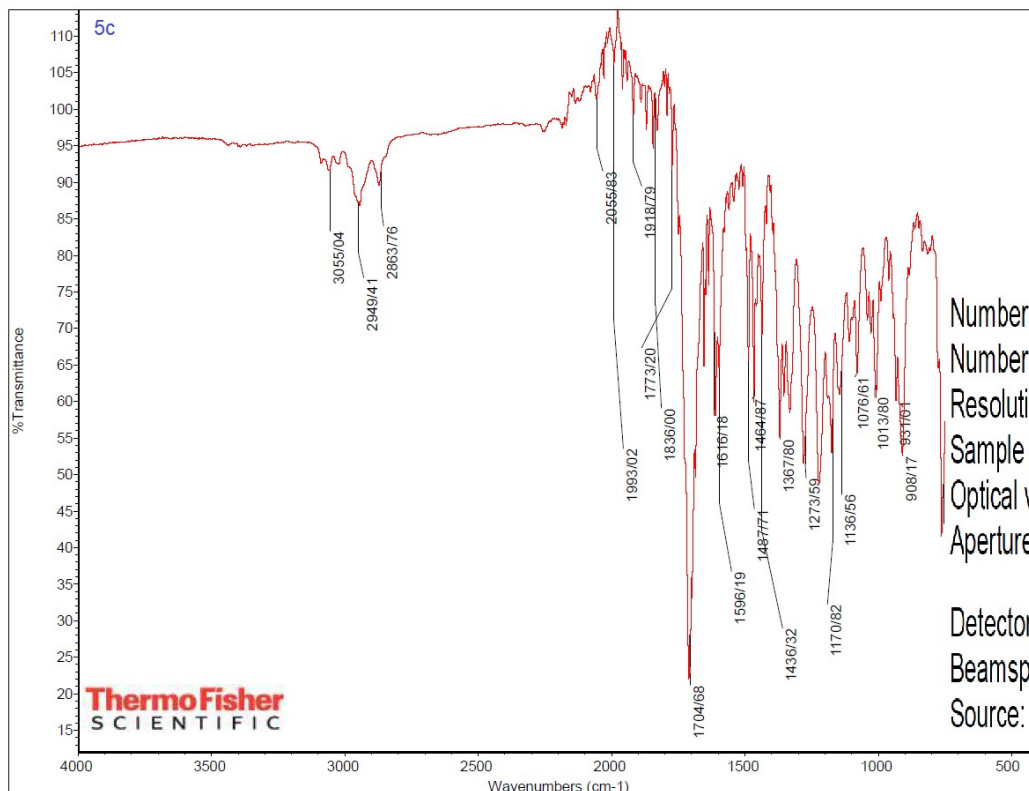
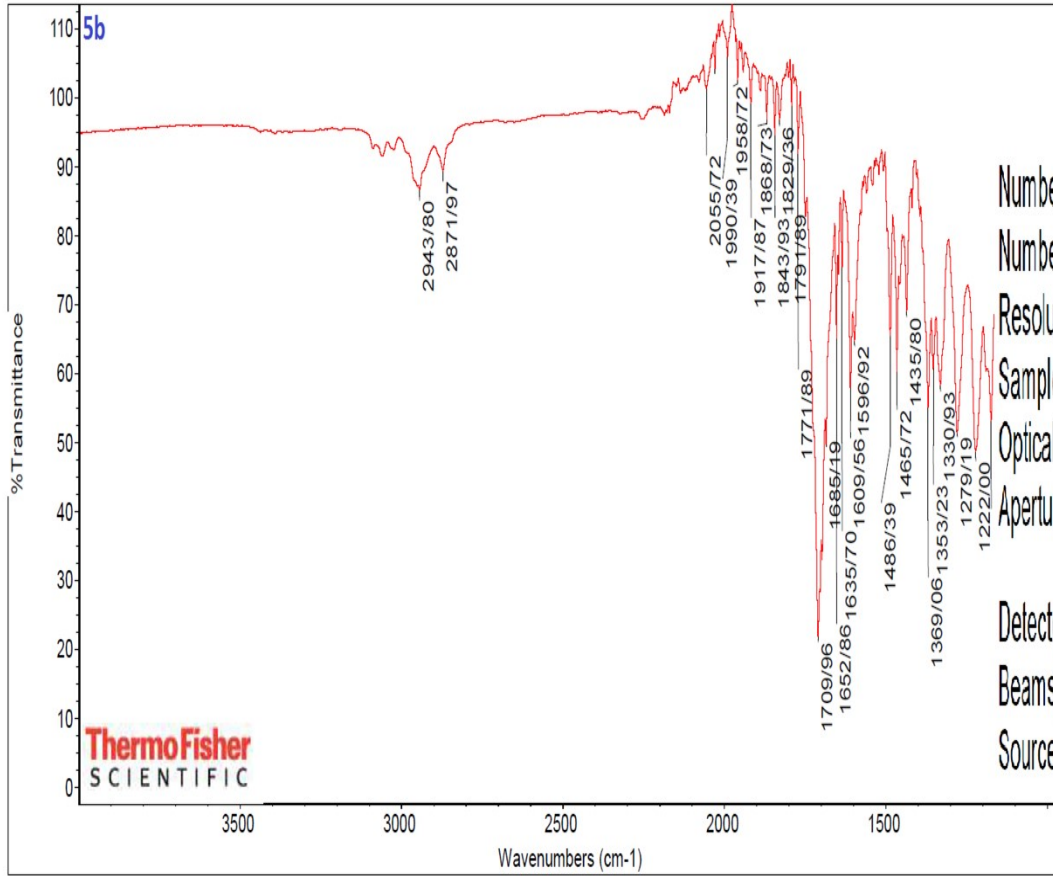


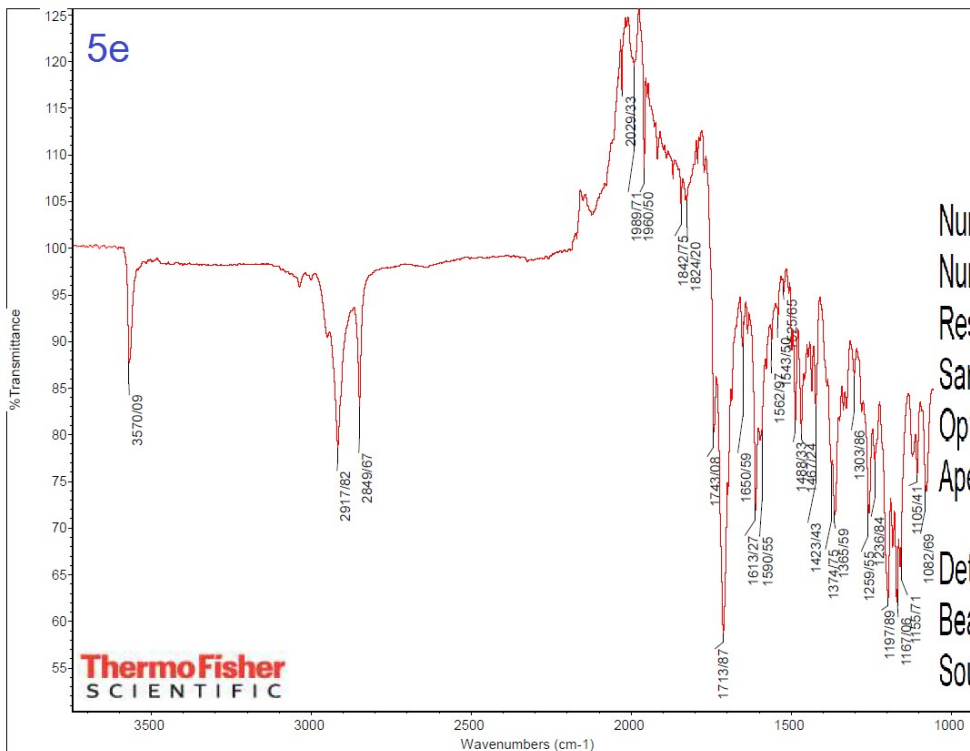
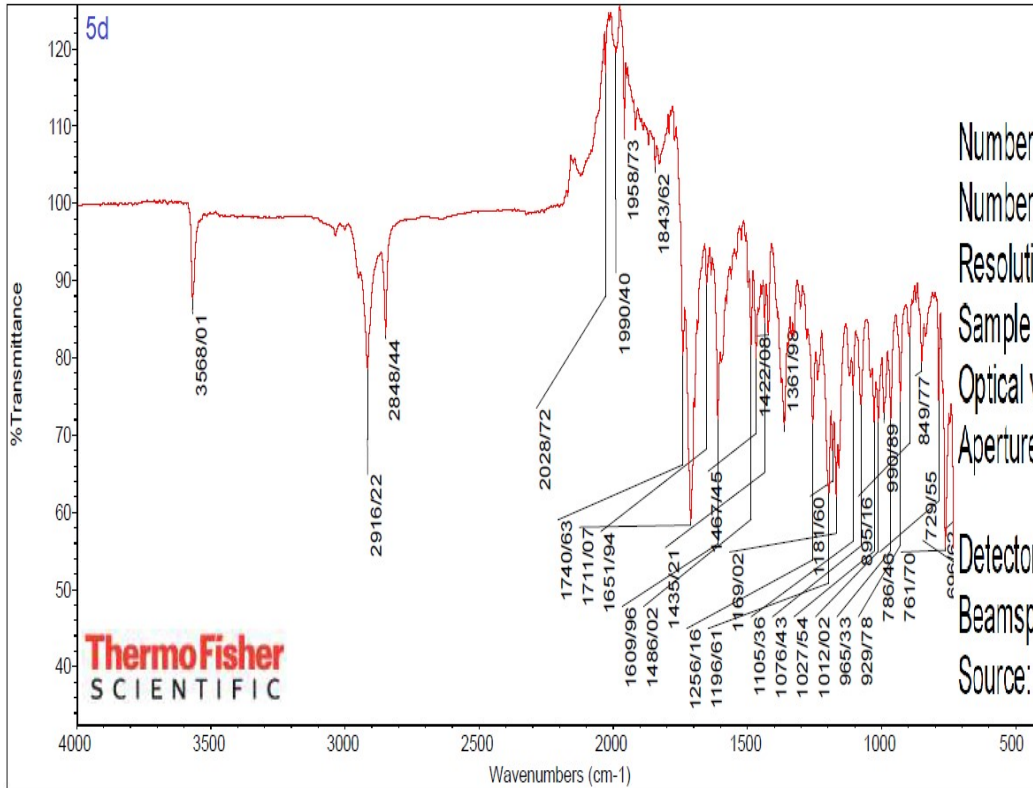


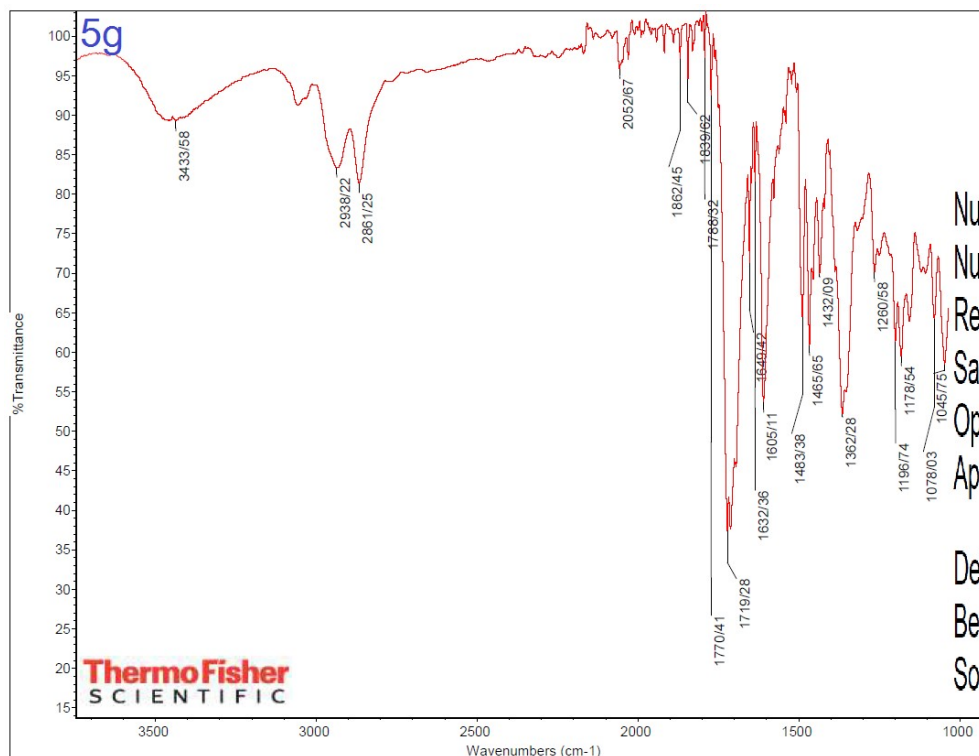
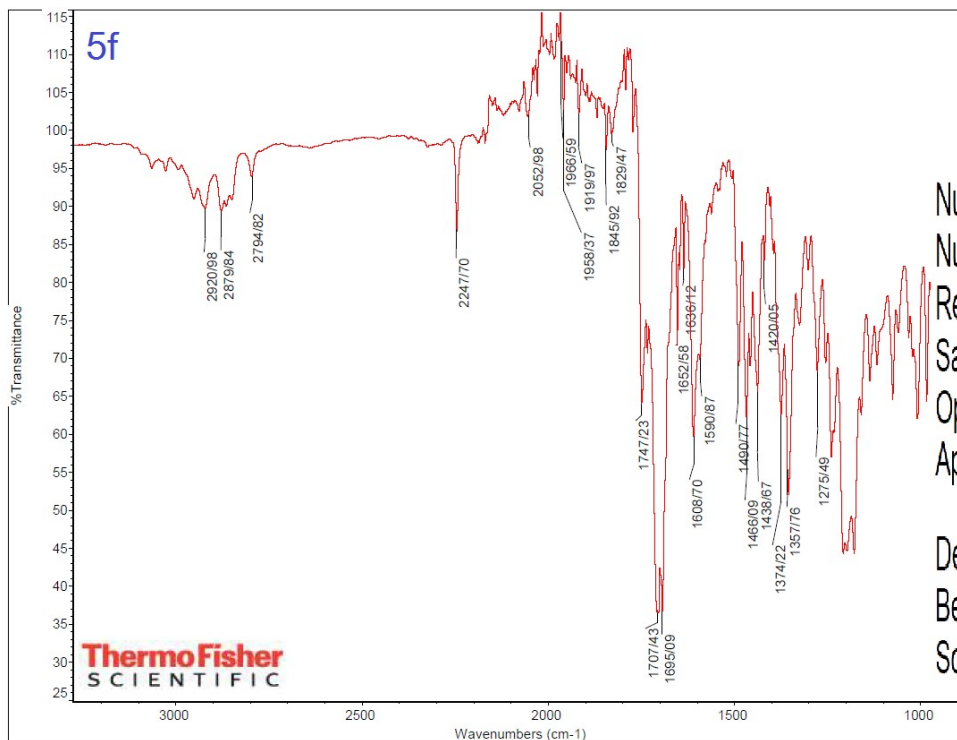




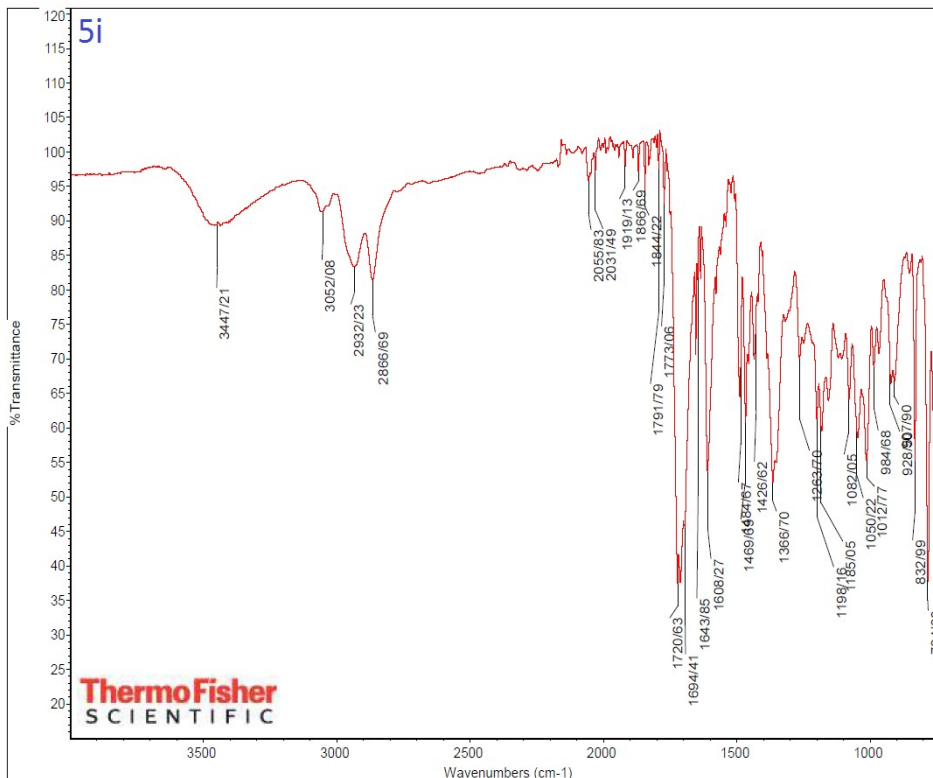
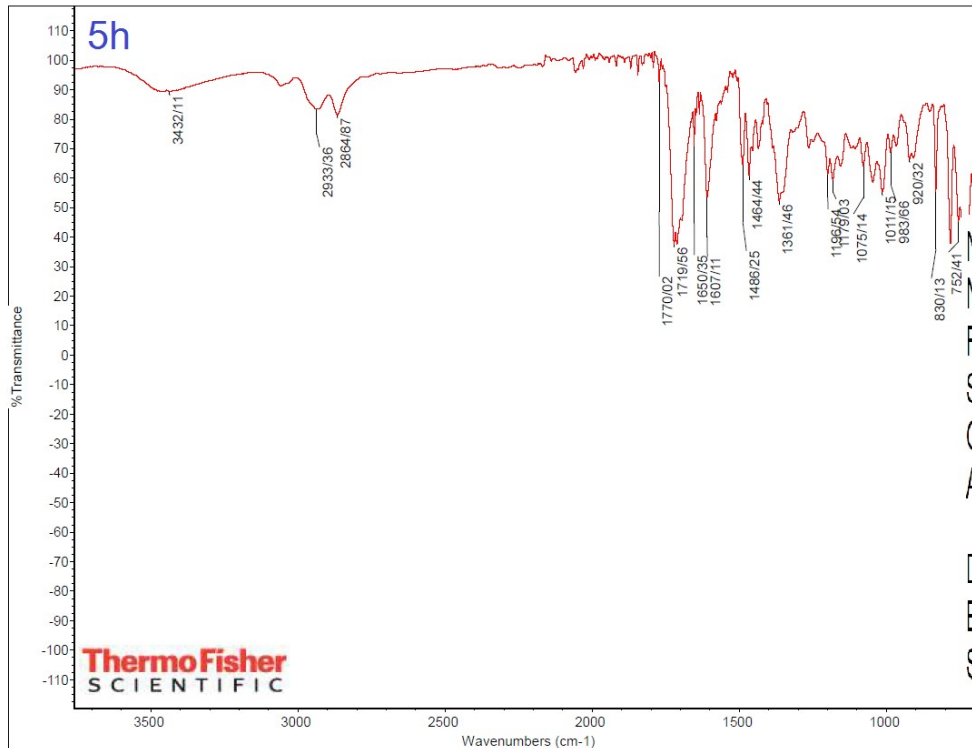


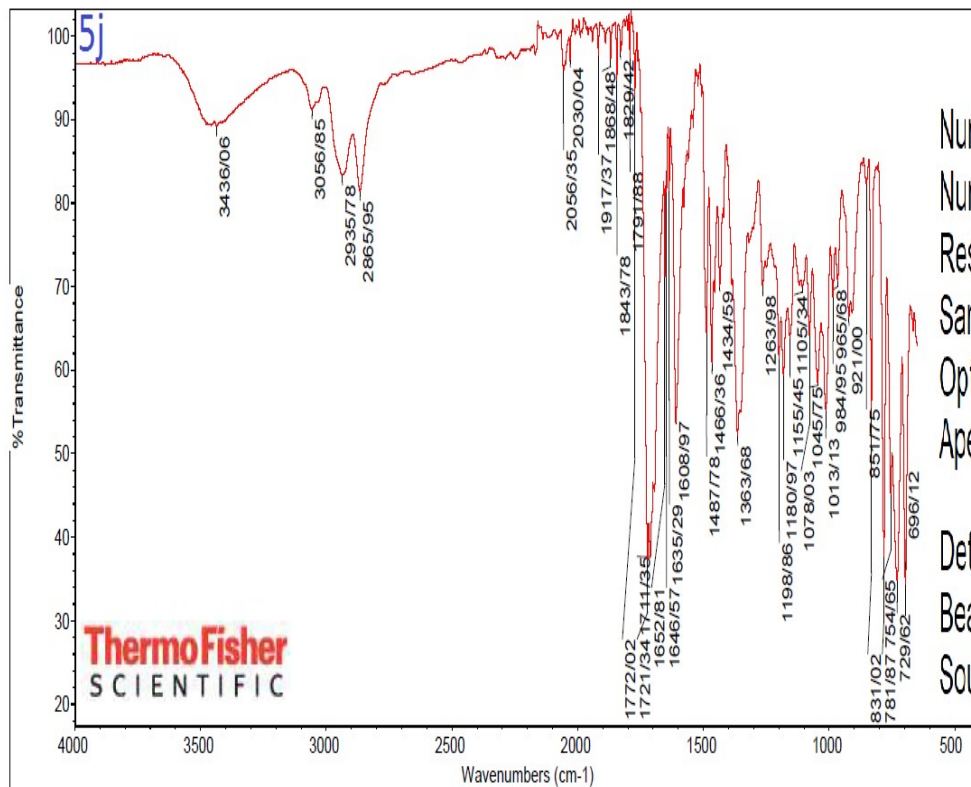




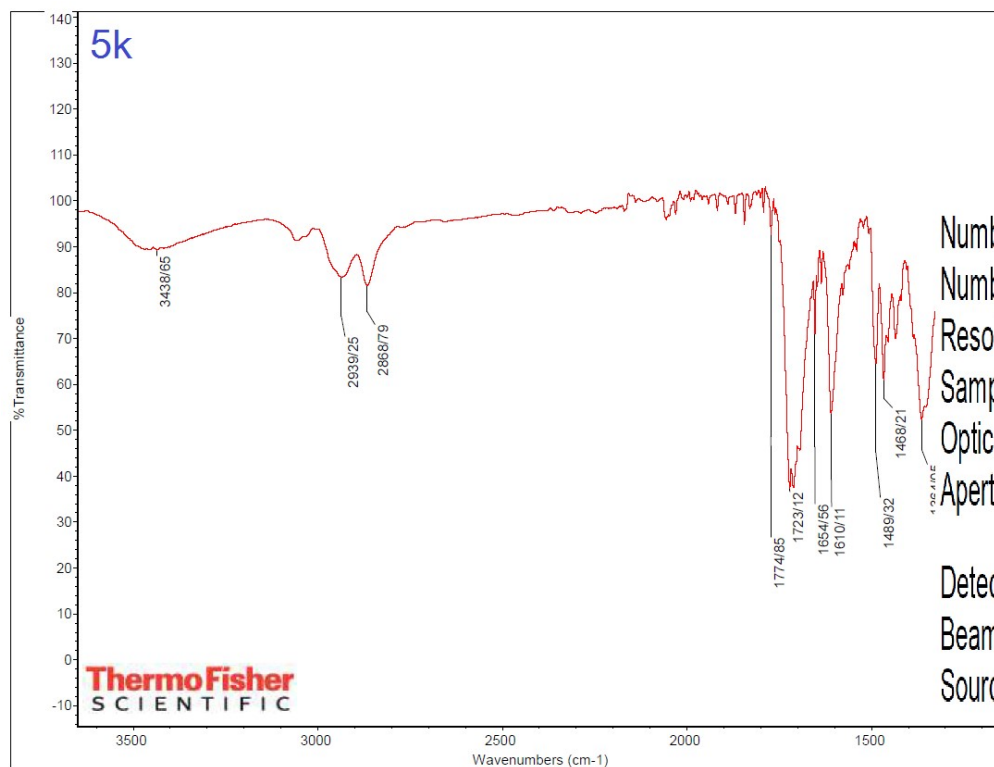




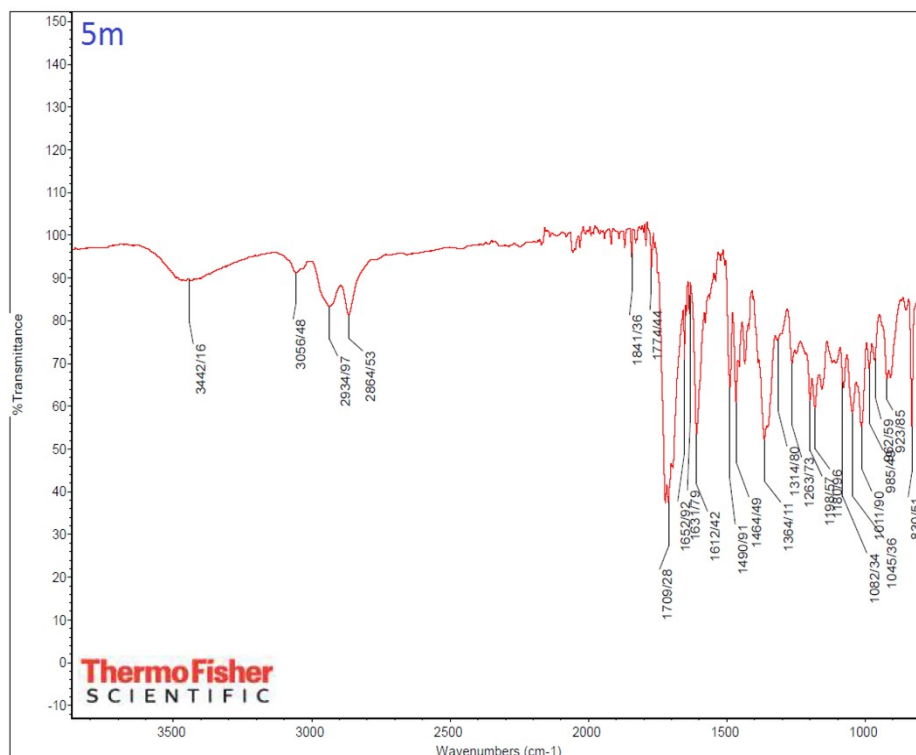
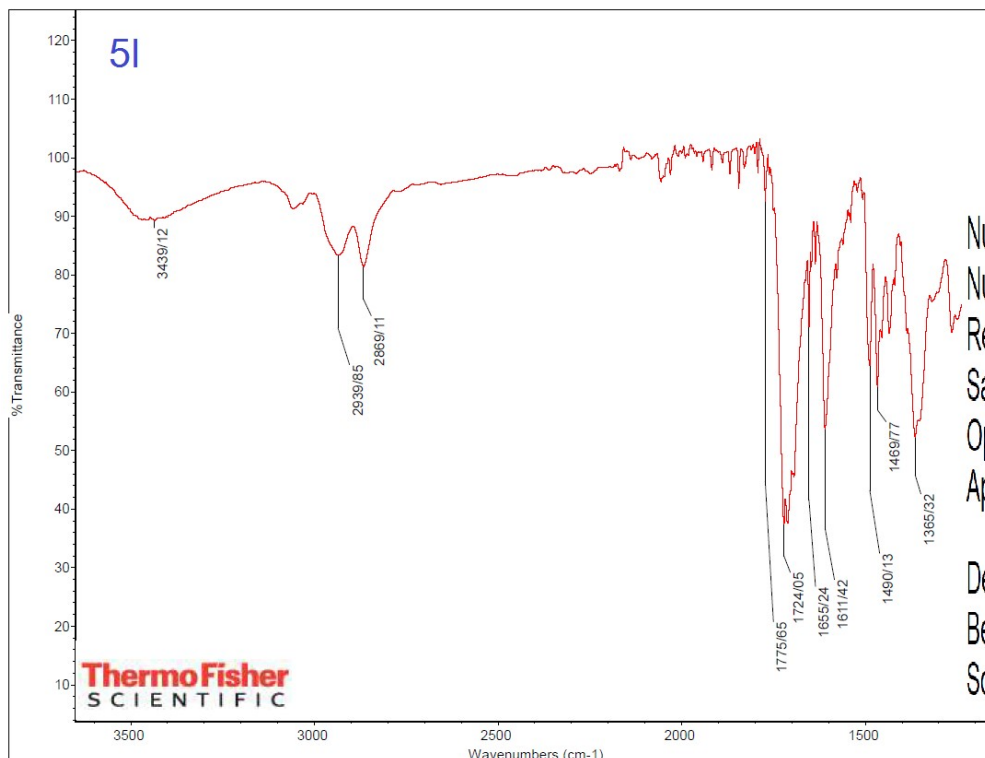




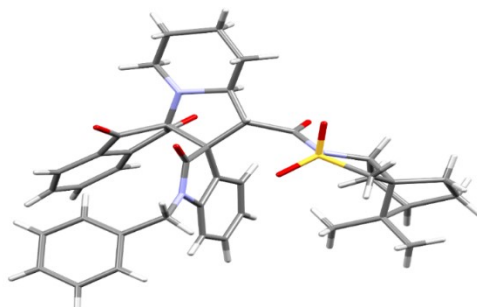
Number of sample scans: 32  
 Number of background scans: 32  
 Resolution: 4/000  
 Sample gain: 4/0  
 Optical velocity: 0/6329  
 Aperture: 100/00  
 Detector: DTGS KBr  
 Beamsplitter: KBr  
 Source: IR



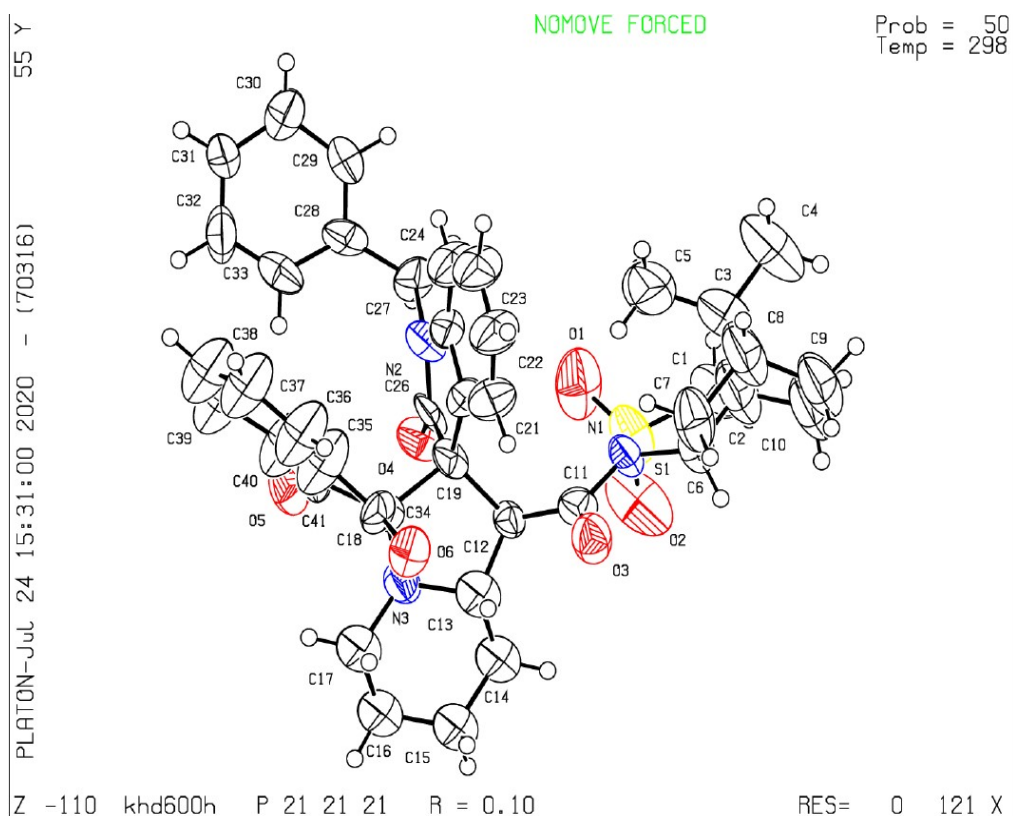
Number of sample scans: 32  
 Number of background scans: 32  
 Resolution: 4/000  
 Sample gain: 4/0  
 Optical velocity: 0/6329  
 Aperture: 100/00  
 Detector: DTGS KBr  
 Beamsplitter: KBr  
 Source: IR



2. the X-ray data for compound **3a**:



According to the specific chiral center in the chiral auxiliary ((1*S*)-(-)-2,10-Camphorsultam), the Absolute Configuration of compound **3a** was determined with X-Ray:



**Atomic coordinates (  $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **3a**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.**

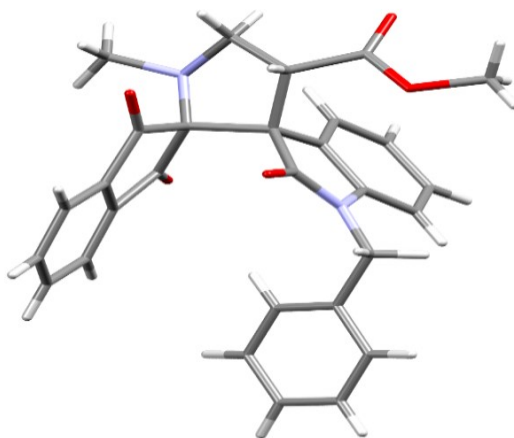
	x	y	z	U(eq)
S(1)	1523(4)	8670(2)	1399(1)	78(1)
O(3)	3318(9)	6815(4)	1208(3)	78(2)
N(1)	2689(8)	8024(4)	1202(3)	54(2)
N(3)	2284(9)	6415(5)	2999(3)	62(2)
C(18)	3577(11)	6780(6)	3108(4)	53(3)
C(20)	4822(10)	7778(5)	2444(4)	51(3)
C(34)	4823(11)	6347(6)	2961(4)	56(3)
N(2)	3994(9)	8660(5)	3076(3)	58(2)
C(25)	5120(11)	8453(6)	2724(4)	54(3)
O(5)	2913(9)	7186(5)	4153(3)	87(3)
O(4)	1834(8)	8248(4)	3257(3)	66(2)
C(11)	2806(10)	7339(6)	1499(4)	53(3)
C(12)	2392(9)	7244(5)	2161(4)	44(2)
O(6)	4954(8)	5887(4)	2555(3)	69(2)
C(26)	2938(12)	8179(6)	3038(4)	55(3)
C(27)	3828(11)	9418(6)	3361(4)	61(3)
C(41)	3804(12)	6997(6)	3777(4)	66(3)
C(6)	2993(11)	8082(6)	525(4)	62(3)
C(19)	3475(10)	7507(5)	2658(3)	49(3)
C(40)	5178(17)	6902(9)	3904(6)	112(2)
O(2)	242(9)	8329(6)	1386(5)	122(4)
C(31)	6352(13)	9750(7)	4965(5)	74(3)
C(13)	2012(13)	6470(8)	2327(5)	92(2)
C(21)	5812(12)	7460(7)	2028(5)	72(3)
C(22)	7017(12)	7828(8)	1966(5)	80(2)
C(17)	2172(13)	5639(8)	3252(5)	92(2)
C(28)	4743(11)	9507(6)	3935(4)	56(3)
C(14)	554(13)	6235(8)	2234(5)	92(2)
O(1)	1949(11)	9044(5)	1934(3)	117(4)
C(29)	5488(12)	10144(7)	3989(4)	70(3)

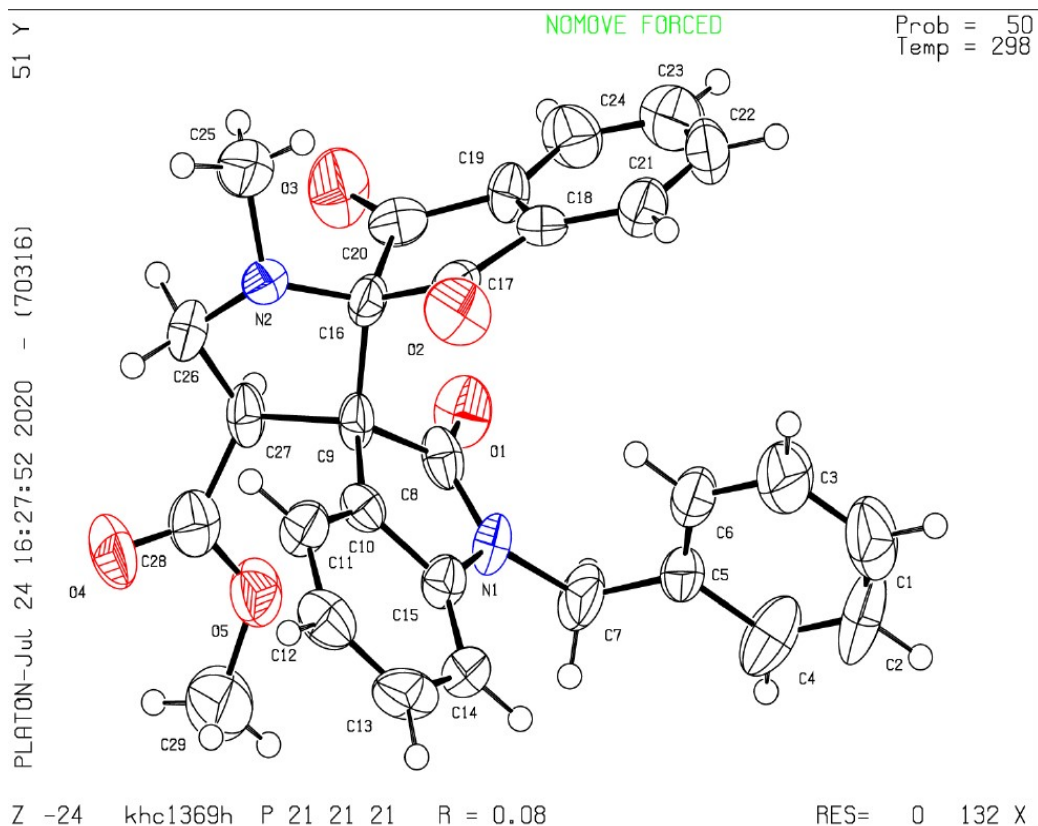
C(35)	5787(15)	6537(9)	3418(6)	112(2)
C(33)	4803(15)	8993(6)	4424(5)	86(4)
C(30)	6402(14)	10288(8)	4500(5)	90(4)
C(1)	1670(14)	9222(7)	714(5)	93(4)
C(24)	6277(11)	8810(8)	2638(5)	80(2)
C(23)	7191(11)	8489(8)	2244(5)	80(2)
C(7)	4471(14)	7926(8)	369(5)	93(4)
C(2)	2760(20)	8880(9)	325(6)	120(3)
C(32)	5567(16)	9108(8)	4928(5)	93(5)
C(16)	668(13)	5424(8)	3156(5)	92(2)
C(39)	5848(15)	7083(8)	4492(6)	112(2)
C(15)	306(14)	5479(7)	2499(5)	92(2)
C(3)	4240(15)	9262(8)	388(6)	93(4)
C(10)	2611(17)	8834(9)	-354(5)	120(3)
C(9)	4022(15)	8636(9)	-615(5)	120(3)
C(8)	4850(19)	8623(9)	3(5)	120(3)
C(38)	7258(15)	6951(8)	4435(6)	112(2)
C(36)	7180(15)	6366(9)	3444(6)	112(2)
C(37)	7867(15)	6621(8)	3941(6)	112(2)
C(5)	4751(15)	9294(8)	1049(6)	111(5)
C(4)	4350(20)	10046(10)	97(8)	164(8)

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### 3. The X-ray data for compound **5a**

The Absolute Configuration of compound **5a** was determined with X-Ray:





**Atomic coordinates (  $\times 10^4$  ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 5a.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.**

	x	y	z	$U(\text{eq})$
O(4)	2043(6)	-2588(4)	8145(2)	70(2)
N(1)	5475(6)	1204(4)	8488(2)	43(1)
O(5)	2086(6)	-467(5)	8273(2)	64(1)
C(15)	6041(8)	366(5)	8151(2)	39(2)
O(1)	4144(6)	1036(4)	9167(2)	59(1)
N(2)	5871(7)	-2903(4)	9042(2)	46(2)
C(5)	7281(9)	3164(5)	8508(2)	49(2)
C(10)	5895(7)	-911(5)	8308(2)	35(2)
C(17)	8085(8)	-1200(6)	9122(2)	41(2)
O(3)	4360(7)	-1433(5)	9802(2)	80(2)

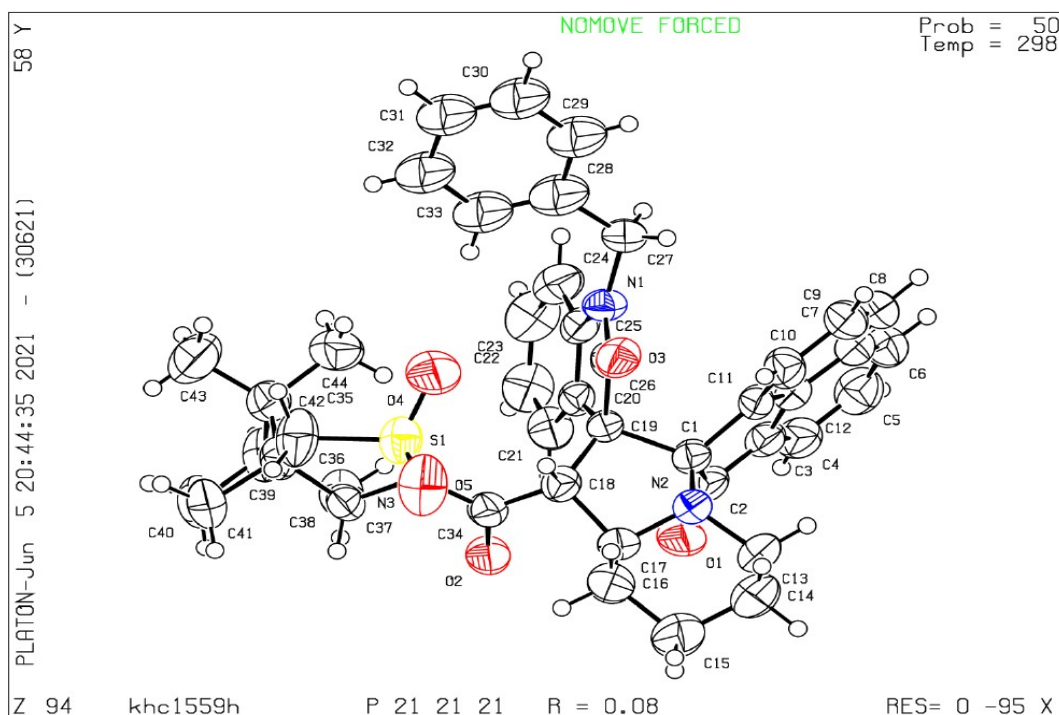
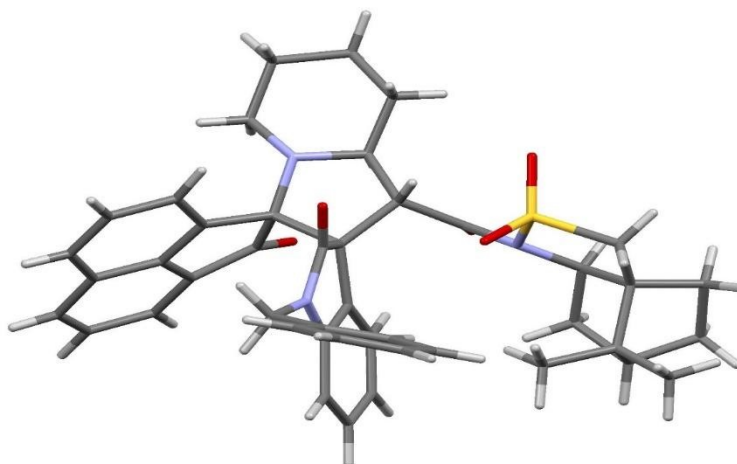
C(12)	6969(8)	-1606(7)	7614(2)	54(2)
C(9)	5123(7)	-890(5)	8761(2)	36(2)
C(8)	4800(7)	576(6)	8838(3)	41(2)
O(2)	9119(6)	-1570(4)	8863(2)	64(1)
C(7)	5498(9)	2605(5)	8454(3)	61(2)
C(14)	6606(8)	674(6)	7742(2)	49(2)
C(28)	2437(8)	-1688(7)	8378(3)	53(2)
C(25)	6539(10)	-3796(6)	9376(2)	75(2)
C(16)	6195(8)	-1547(5)	9136(2)	38(2)
C(21)	9855(9)	439(6)	9583(3)	62(2)
C(18)	8405(8)	-281(6)	9500(2)	44(2)
C(19)	6974(9)	-199(6)	9769(2)	46(2)
C(13)	7057(8)	-332(8)	7460(2)	59(2)
C(20)	5631(9)	-1074(6)	9605(2)	49(2)
C(26)	4065(9)	-3047(6)	8932(2)	63(2)
C(11)	6371(8)	-1901(6)	8030(2)	46(2)
C(4)	7568(11)	4446(6)	8398(3)	78(3)
C(6)	8638(10)	2496(7)	8661(3)	78(3)
C(3)	10240(11)	3011(9)	8708(3)	103(3)
C(27)	3464(7)	-1720(5)	8790(2)	41(2)
C(22)	9770(11)	1238(7)	9963(3)	73(3)
C(23)	8352(14)	1291(7)	10229(3)	83(3)
C(24)	6946(11)	564(7)	10141(3)	63(2)
C(1)	10467(12)	4299(9)	8605(3)	86(3)
C(29)	1139(11)	-257(8)	7868(3)	112(4)
C(2)	9129(13)	4988(8)	8453(3)	91(3)

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#### 4. The X-ray data for compound **3f**:

The Absolute Configuration of compound **3f** was determined with X-Ray:



**Atomic coordinates (  $\times 10^4$  ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$  ) for **3f**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U_{ij}$  tensor.**

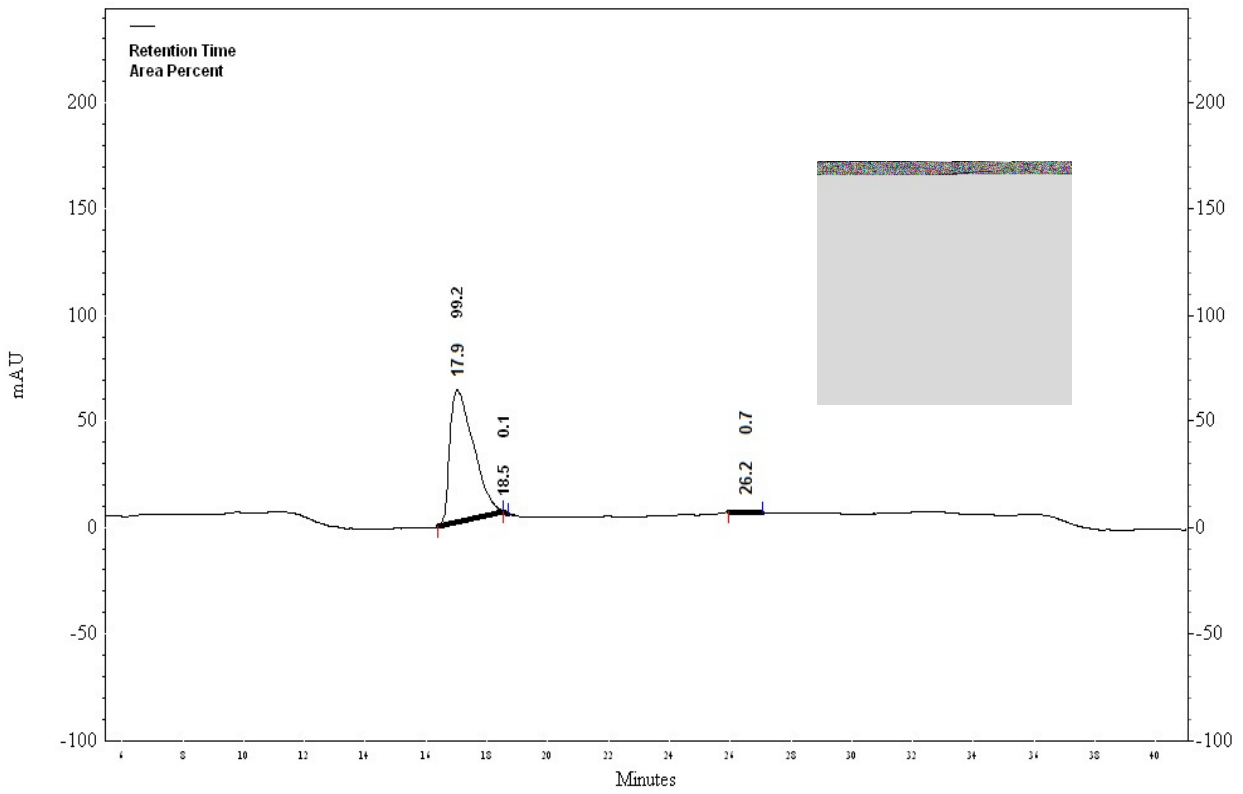
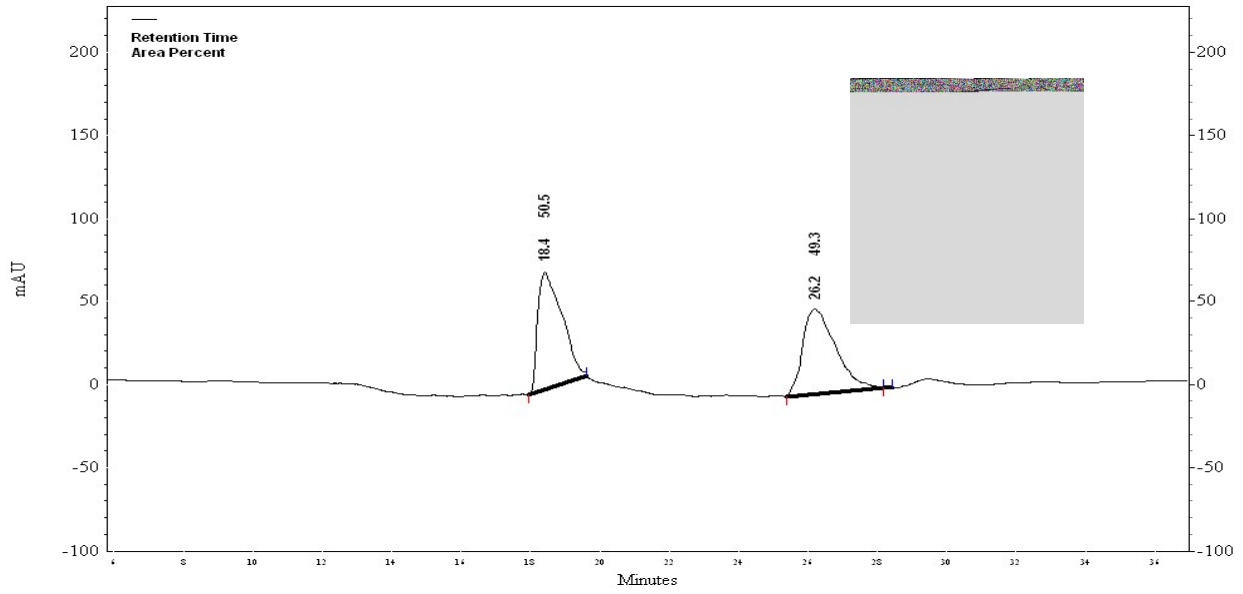
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	x	y	z	U(eq)
C(41)	4051(8)	4741(7)	3410(2)	86(2)
S(1)	4807(2)	6323(1)	2265(1)	64(1)
O(3)	4039(4)	7433(3)	1009(1)	62(1)
N(3)	3938(4)	5147(3)	2192(1)	51(1)
O(1)	2478(4)	3161(3)	723(1)	72(1)
C(19)	3040(5)	5596(4)	1122(1)	49(1)
N(2)	4563(5)	4871(3)	612(1)	54(1)
C(26)	3097(5)	6879(4)	1080(1)	48(1)
C(1)	3235(6)	5105(4)	629(2)	52(1)
O(2)	3746(5)	3544(3)	1813(1)	73(1)
N(1)	1880(4)	7269(3)	1116(1)	53(1)
C(20)	1734(5)	5425(4)	1303(1)	48(1)
C(3)	1327(5)	4388(4)	238(2)	53(1)
C(25)	1059(6)	6441(4)	1277(2)	54(1)
C(10)	3312(6)	6809(5)	71(2)	62(1)
C(12)	1677(5)	5446(4)	61(1)	50(1)
C(17)	4960(6)	4389(4)	1038(2)	58(1)
C(11)	2768(5)	5876(4)	253(1)	50(1)
C(34)	3968(5)	4532(5)	1800(2)	55(1)
C(2)	2306(6)	4077(4)	556(2)	56(1)
C(13)	5035(7)	4237(5)	230(2)	74(2)
C(21)	1073(6)	4502(5)	1473(2)	63(2)
O(4)	4145(5)	7237(3)	2073(2)	87(2)
C(6)	-51(6)	5374(6)	-456(2)	68(2)
O(5)	6066(5)	6145(5)	2125(1)	95(2)
C(7)	1018(6)	5948(5)	-294(2)	61(1)
C(36)	3753(6)	5428(5)	2987(2)	62(1)
C(22)	-147(7)	4622(6)	1615(2)	77(2)
C(9)	2646(7)	7354(5)	-281(2)	66(2)
C(8)	1561(7)	6956(5)	-453(2)	68(2)
C(4)	284(6)	3843(5)	66(2)	68(2)
C(14)	6432(7)	4178(7)	238(2)	89(2)
C(15)	6957(8)	3723(8)	683(2)	106(3)

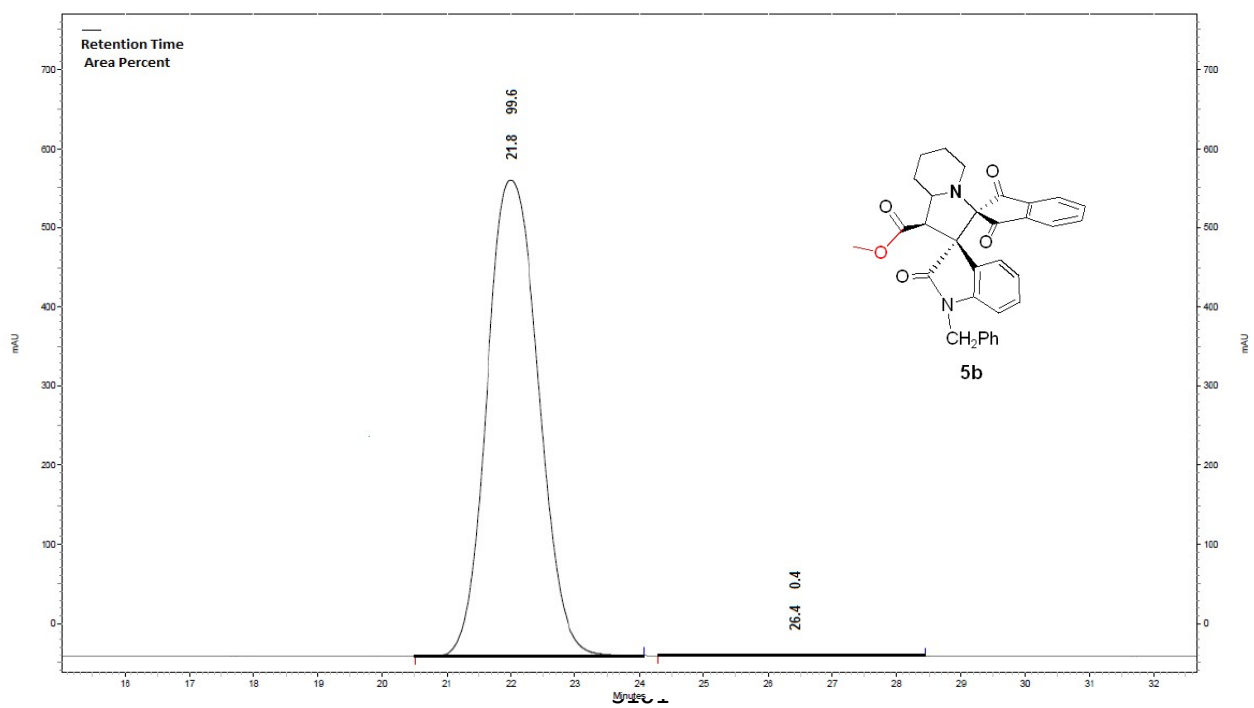
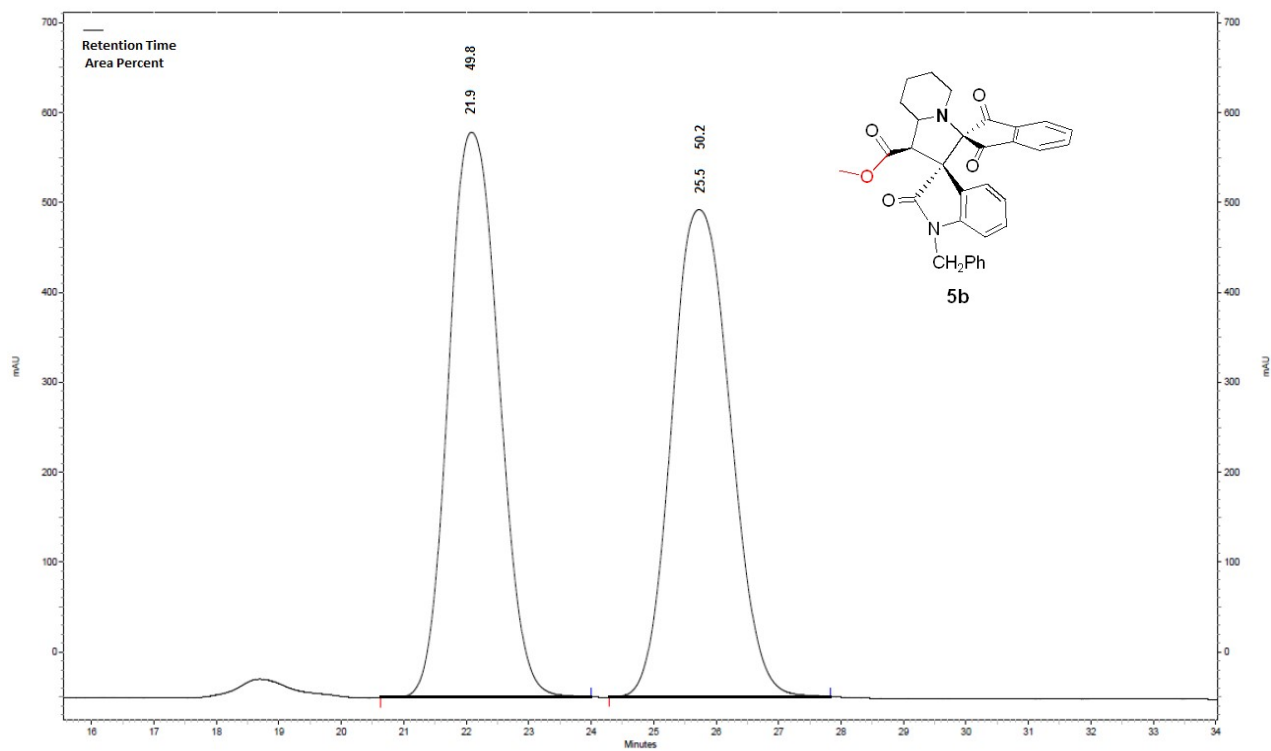
C(5)	-392(7)	4359(6)	-279(2)	78(2)
C(24)	-177(7)	6562(6)	1415(2)	74(2)
C(16)	6358(6)	4399(7)	1065(2)	78(2)
C(18)	4239(5)	5153(4)	1367(2)	51(1)
C(35)	4689(7)	6324(6)	2861(2)	84(2)
C(38)	2396(7)	4019(5)	2667(2)	73(2)
C(37)	3697(6)	4547(5)	2619(2)	61(1)
C(42)	2335(7)	5749(5)	3059(2)	70(2)
C(23)	-778(7)	5636(7)	1582(2)	85(2)
C(40)	2780(9)	4092(7)	3476(2)	96(3)
C(39)	1937(8)	4510(6)	3110(2)	79(2)
C(28)	1675(8)	9259(6)	1354(3)	90(1)
C(33)	1778(8)	9001(6)	1792(3)	90(1)
C(27)	1528(7)	8393(4)	992(2)	68(2)
C(30)	1837(8)	11191(6)	1552(3)	90(1)
C(44)	1668(7)	6348(7)	2671(2)	89(2)
C(31)	1895(8)	10918(6)	1975(3)	90(1)
C(43)	2116(10)	6462(7)	3478(2)	114(3)
C(29)	1708(8)	10379(5)	1235(3)	90(1)
C(32)	1879(8)	9821(5)	2113(3)	90(1)

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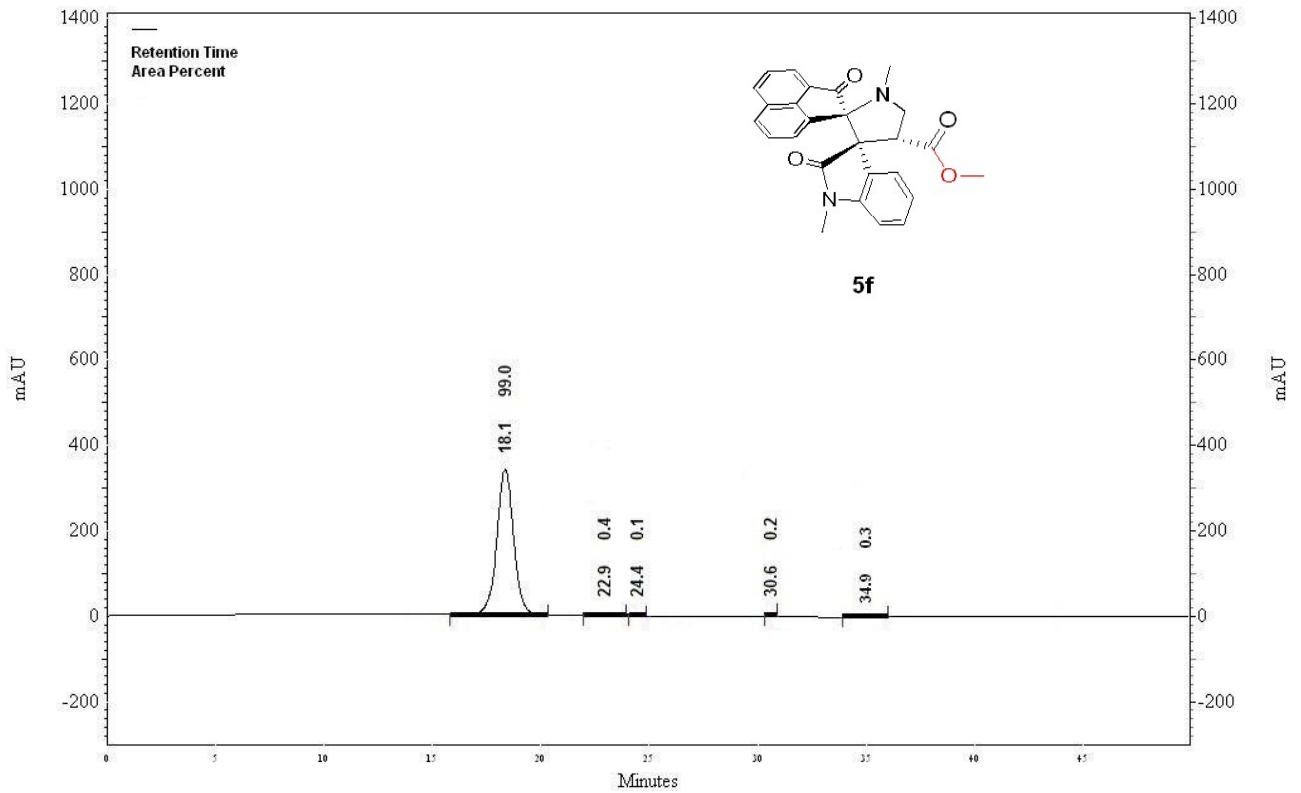
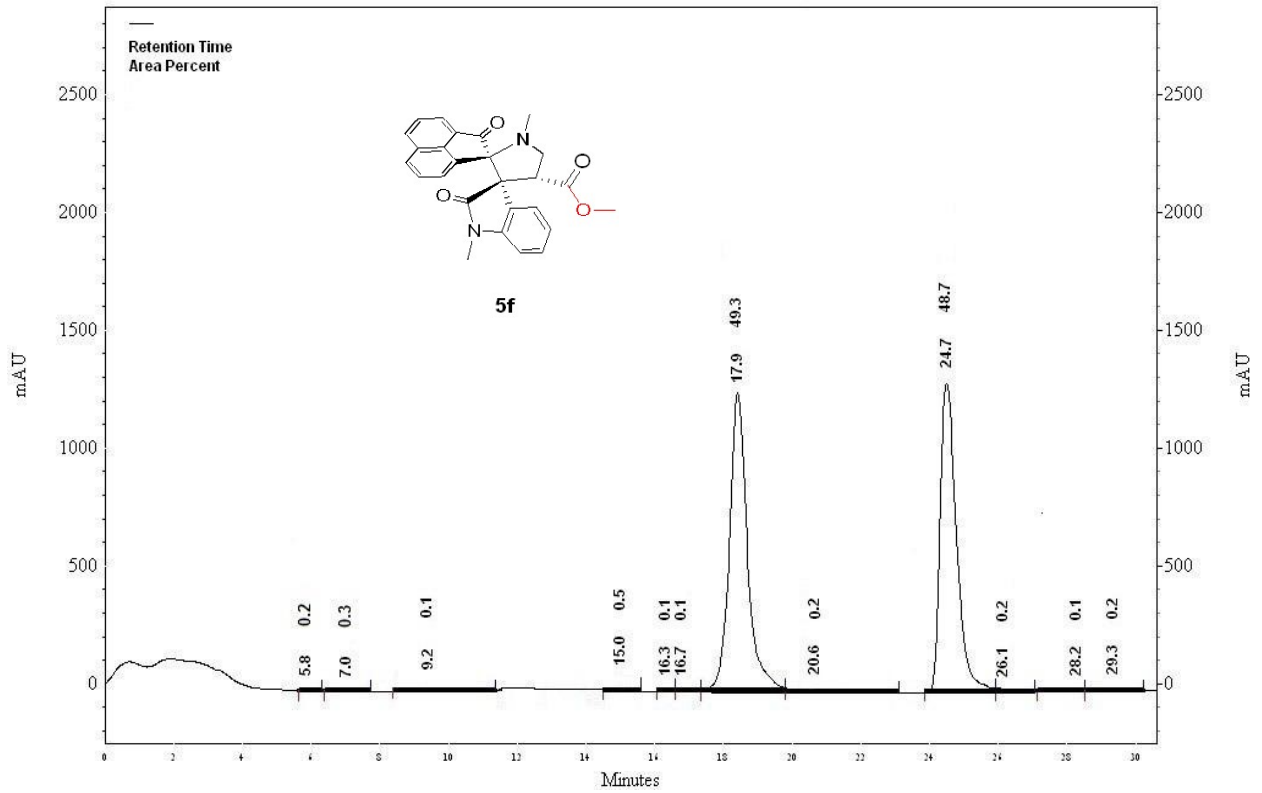
## 5. HPLC Chromatograms: 5a



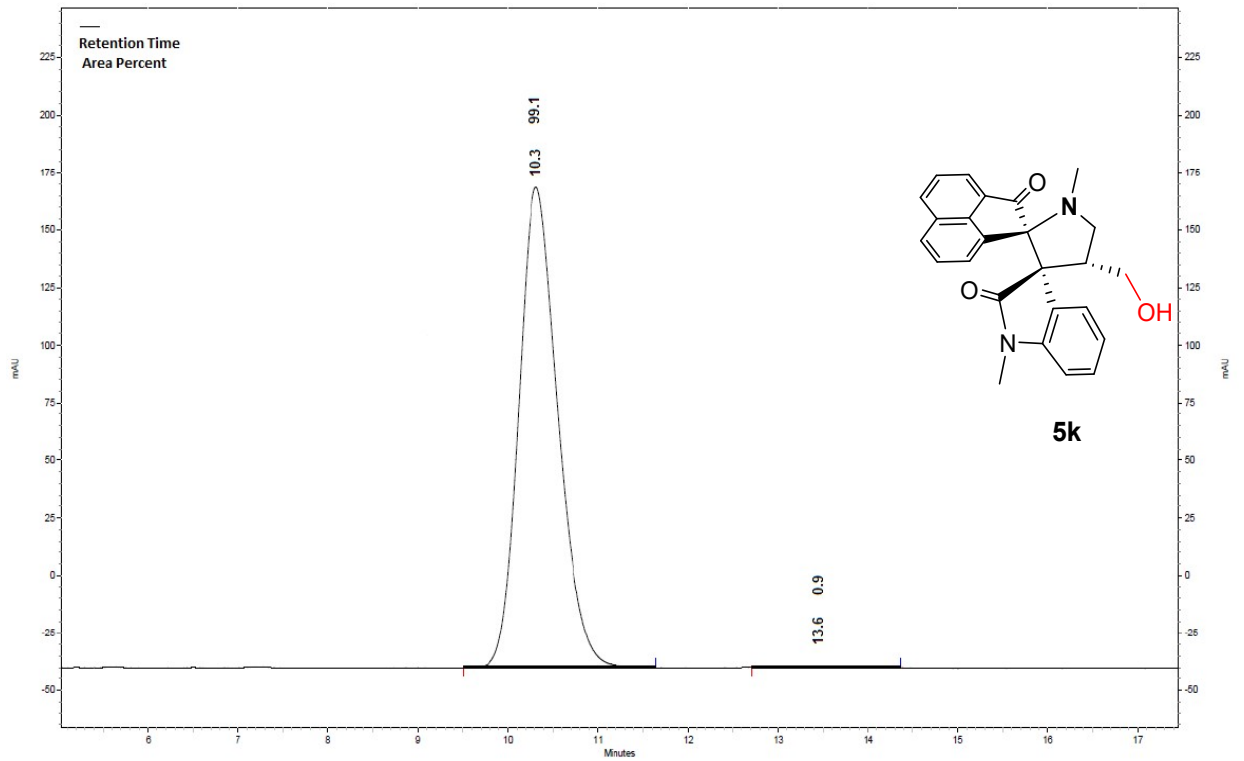
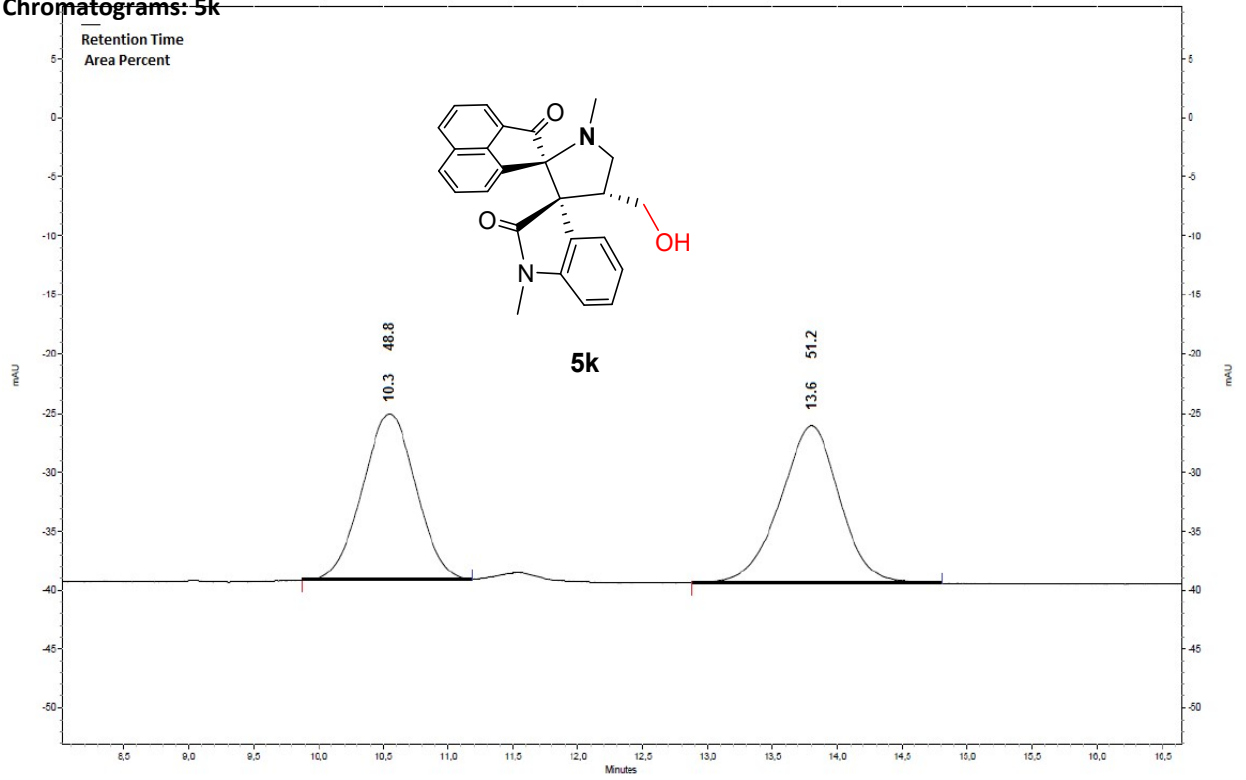
## HPLC Chromatograms: 5b



# HPLC Chromatograms: 5f



# HPLC Chromatograms: 5k



## 6. SDE test and result

HPLC conditions:

**Column:** Chiralpak AD-H, **Eluent:** 10-20-30% i-PrOH/hexane, **Flow:** 0.5 mL/min, **Detection:** UV, 210 nm

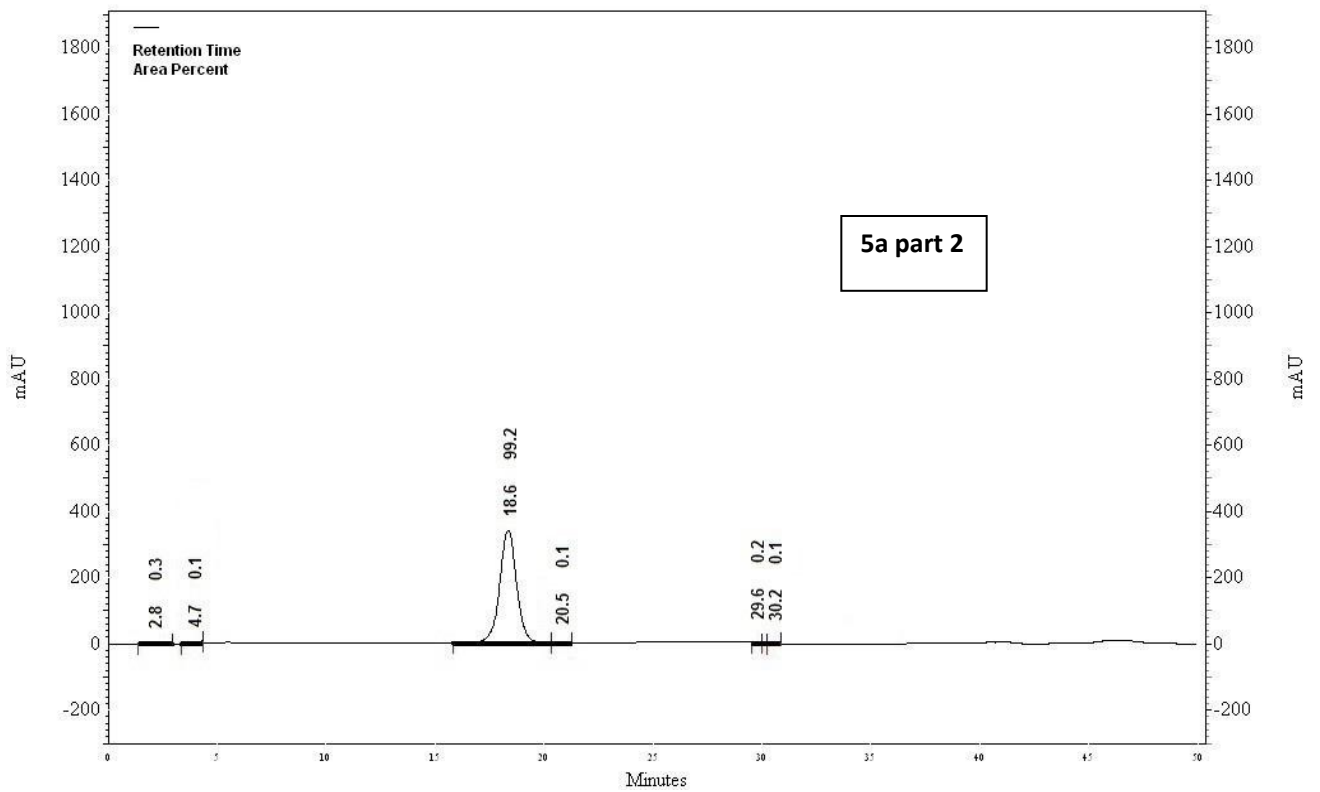
**Table1:** Achiral flash chromatography on SiO<sub>2</sub>; Eluent: 10-20-30% i-PrOH/hexane

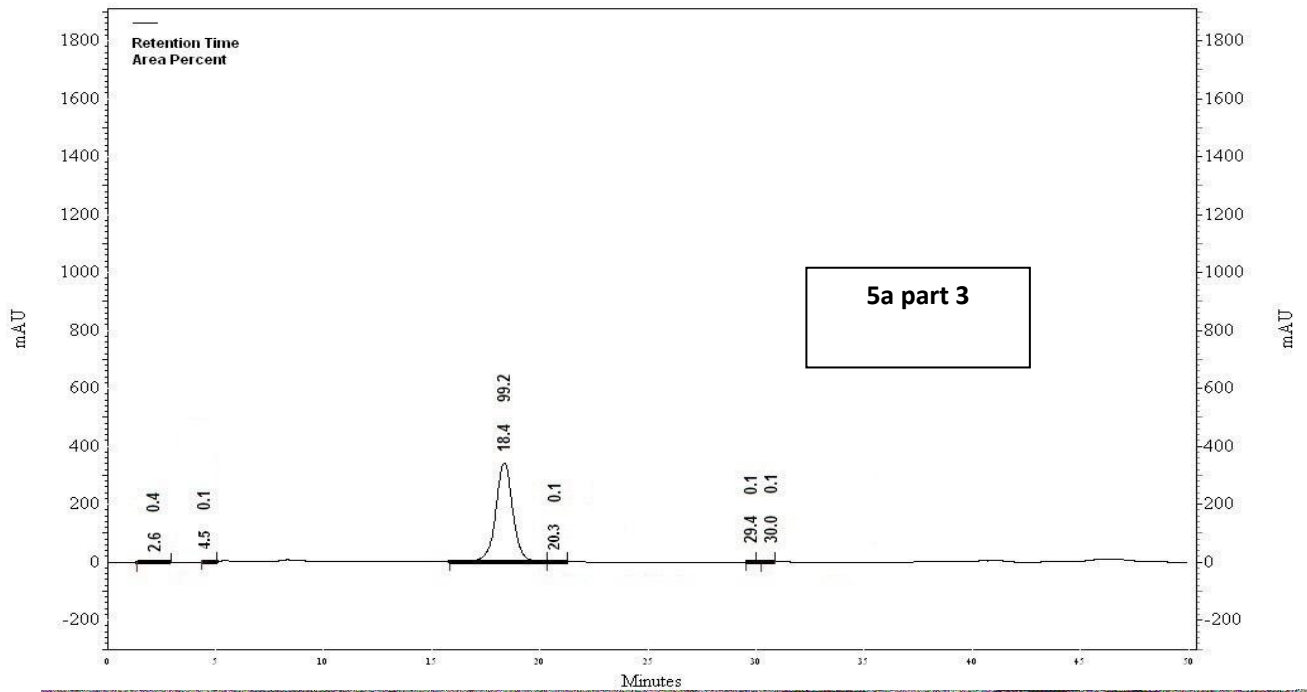
<b>Compound</b>	<b>Part 1</b>	<b>Part 2</b>	<b>Part 3</b>
<b>5a</b>	99.2% ee	99.2% ee	99.2% ee
<b>5b</b>	99.6% ee	99.6% ee	99.6% ee
<b>5k</b>	99.1% ee	99.1% ee	99.1% ee

SDE test was performed to confirm the enantiomeric purity results. Thus, we conducted the SDE test via achiral flash chromatography in order to confirm that the values of enantiomeric excess that were obtained were reliable. After performing the appropriate test, we found that no SDE phenomenon was present in our case.



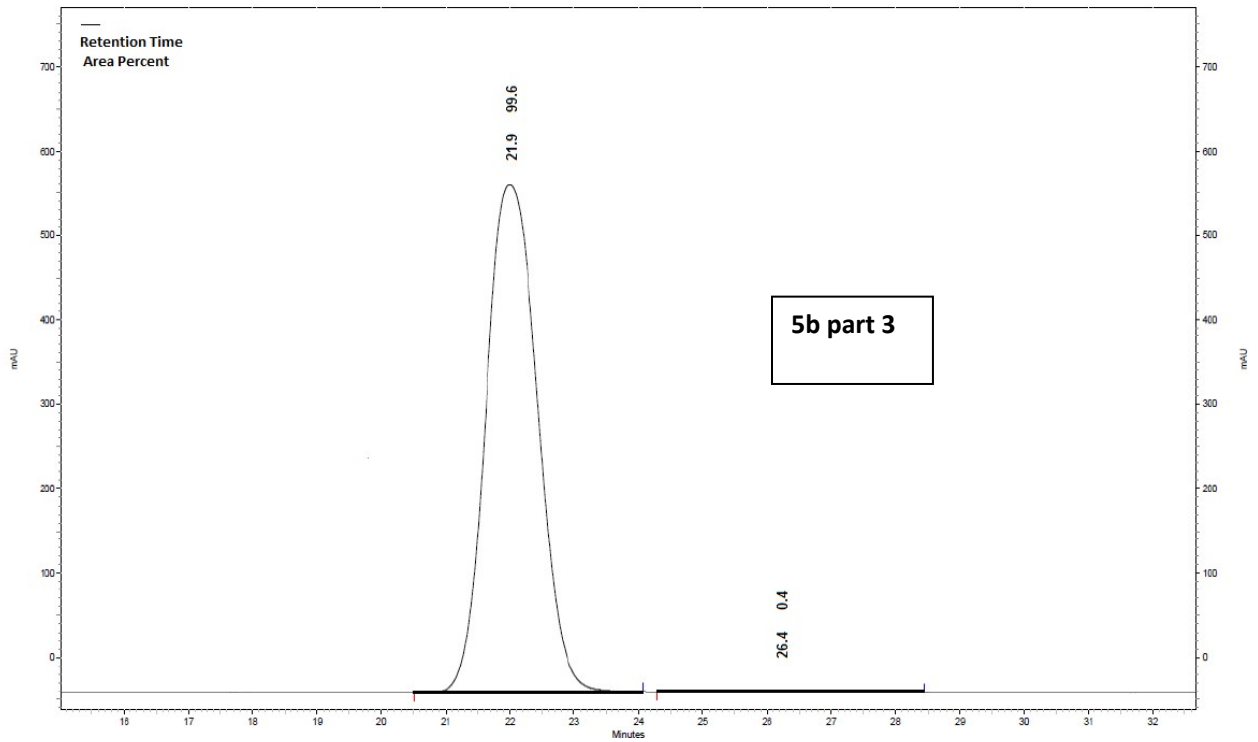
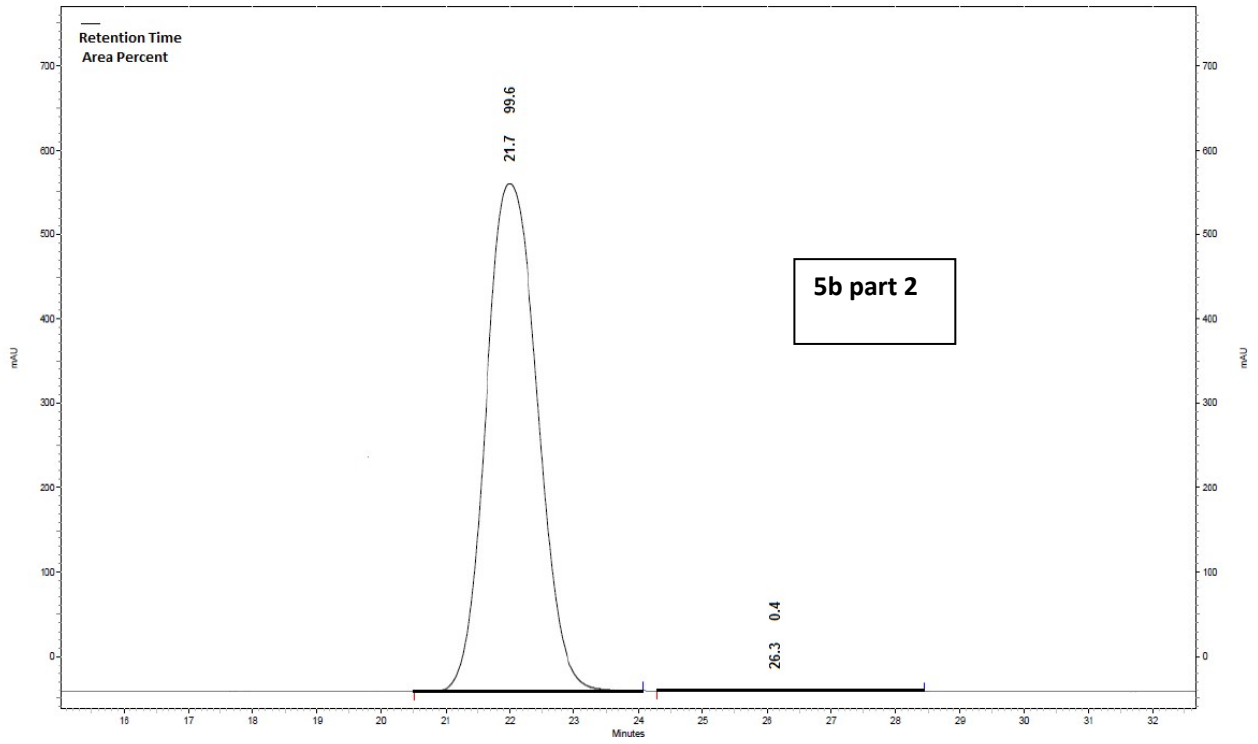
5a



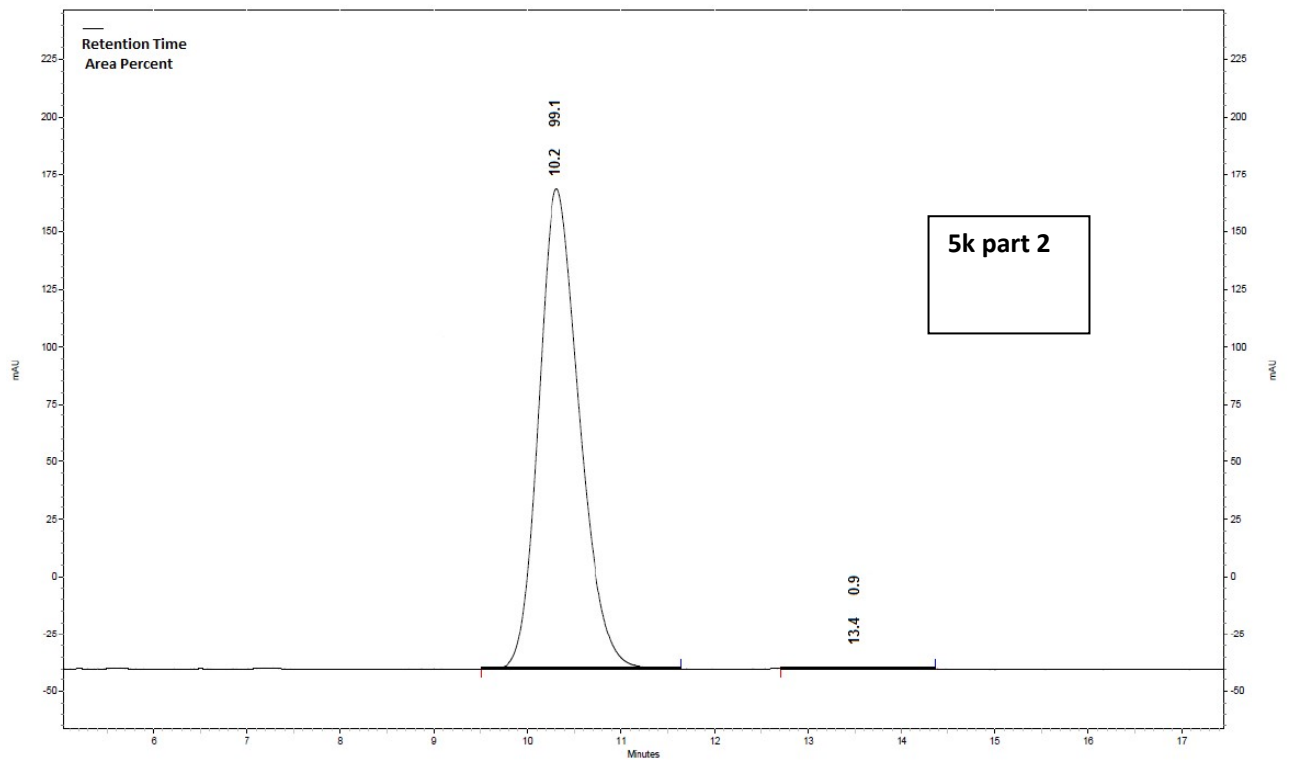


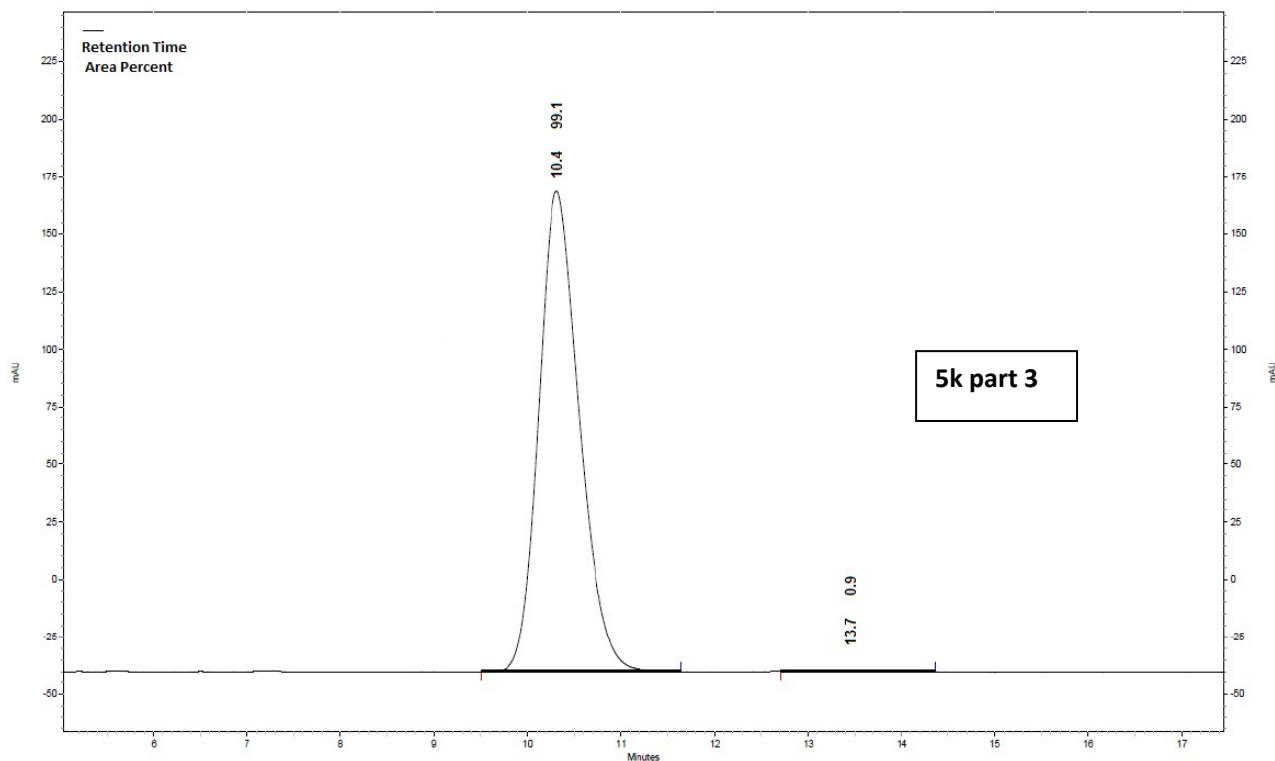
5b





5k





## 7- Computational details

The quantum chemical calculations were carried out by using the Gaussian 09 suite of programs at the M06-2x<sup>1</sup> functional together with 6-31G(d,p) basis set which has been proven helpful for investigating the selectivity and mechanism of cycloaddition reactions<sup>2</sup>. All calculations were performed in methanol solvent at 298.15K through using the polarisable continuum model (PCM) developed by Tomasi et al.<sup>3,4</sup> in the framework of the self-consistent reaction field (SCRF)<sup>5</sup>. In addition, transition states (TSs) were optimised using Bery analytical gradient without any symmetrical restriction was used for optimising.<sup>6,7</sup> The frequency was calculated to confirm that the TSs had only one imaginary frequency. Further, intrinsic reaction coordinate (IRC) was computed for approving that the TSs connected the corresponding reactants and products.<sup>8,9</sup> The global electrophilicity index,  $\omega$ , is defined as the stabilisation energy of a molecule when attracting some electrons and expressed as  $\omega = \mu^2 / (2\eta)^4$ , in which  $\mu$  and  $\eta$  illustrate electronic chemical potential and chemical hardness, respectively. The electronic chemical potential,  $\mu$ , represents the mean value of the one-electron energies of frontier molecular orbitals (HOMO and LUMO), while chemical hardness,  $\eta$ , reflects their difference ( $\mu = (E_{\text{HOMO}} + E_{\text{LUMO}}) / 2$  and  $\eta = (E_{\text{LUMO}} - E_{\text{HOMO}}) / 2$ ).<sup>5</sup> Furthermore, global nucleophilicity index,  $N$ , refers to the difference between the HOMO energies of reactants and those of tetracyanoethylene (TCE) as a reference ( $N = E_{\text{HOMO}} - E_{\text{TCE}}$ ).<sup>10</sup>

The electron density transferred from nucleophile to electrophile at the TSs as a measure of the reaction polarity was determined through computing global electron density transfer (GEDT).<sup>11</sup> GEDT values are higher than 0.2 and near 0.0e for polar and non-polar processes, respectively.<sup>11</sup> The natural bond orbital (NBO)<sup>12</sup> and noncovalent interaction (NCI) analyses were implemented, the first of which was carried out for all possible TSs by using NCI PLOT program.<sup>13</sup>

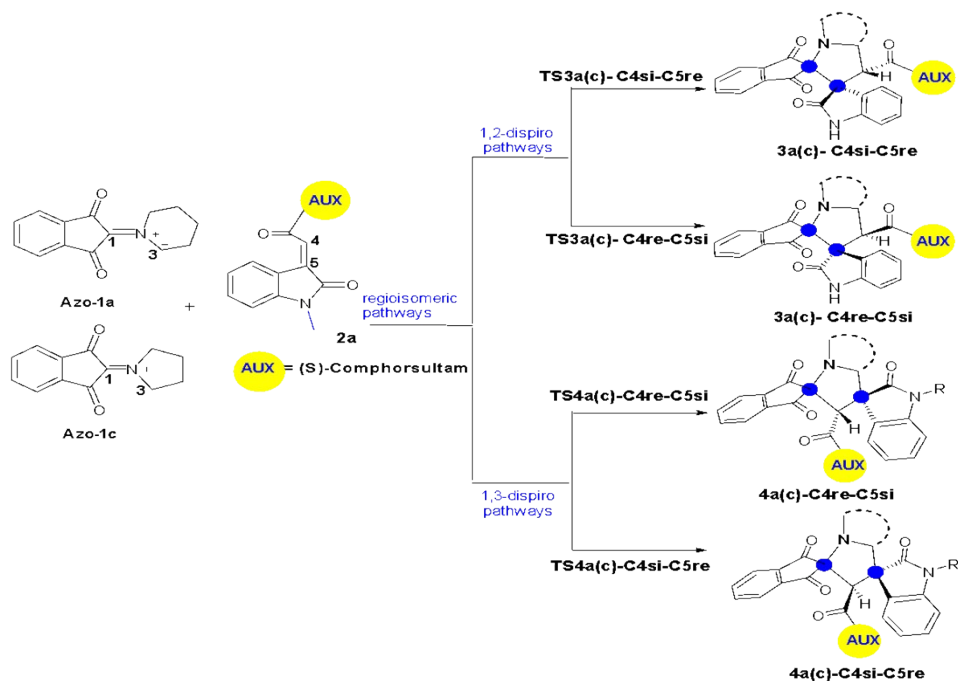
#### Density-functional theory (DFT) analysis based on the global reactivity indices, as well as the prediction of regiochemistry by using local indices

As summarised in Table S1, the calculated electrophilicity indices of the reactants at B3LYP/6-31G (d) are higher than 1.5 eV, which reflects their strong electrophilicity<sup>14</sup>. They could be classified as strong nucleophiles due to the nucleophilicity indices above 3.0. However, the highest electrophilic index was observed in **2a** and its electronic chemical potential ( $\mu = -4.11$  eV) and nucleophilicity ( $N = 3.33$  eV) were lower than those of **Azo-1a** and **Azo-1c**. Thus, the products of 32CA reactions were generated through the nucleophilic attack of azomethine ylides **1a** and **1c** on **2a**. The values indicated that the direction of the electron flux was from **Azo-1a** and **Azo-1c** to **2a**.

Parr functions are one of the best reliable local indices for predicting the regioselectivity of the polar cycloaddition reactions<sup>15</sup>. The nucleophilic  $P_k^-$  and electrophilic  $P_k^+$  Parr indices are respectively considered as the Mulliken atomic spin density of the radical cations and anions of reactants. Regarding the polar reactions, the most favourable regioisomeric pathways include the interaction between the most electrophilic center with the most nucleophilic one of the corresponding reactants. Further, local electrophilicity and nucleophilicity indices are defined as  $\omega_k = \omega \cdot P_k^+$  and  $N_k = N \cdot P_k^-$ <sup>16</sup>, respectively.

As shown in Scheme S3, two regioisomeric pathways are possible for each of the studied 32CA reactions, leading to 1,2-dispiro (**3a** or **3c**) and 1,3-dispiro products (**4a** or **4c**). Therefore, Parr functions, and local electrophilicity and nucleophilicity indices were calculated to examine the observed regioselectivity of the 32CA reactions between **Azo-1a** and **Azo-1c** with **2a**. (Figure S1). displays the selected atomic spin density (ASD) maps of the reactants. Based on the obtained nucleophilic Parr functions and local nucleophilicity analysis, the most nucleophile atom was the C1 atoms of **Azo-1a** and **Azo-1c** (Scheme S3, Table S1). However, C4 was determined as the most electrophilic center of **2a** by considering electrophilic Parr function and local electrophilicity analysis. Accordingly, the most favourable electrophile–nucleophile interactions occurred during the nucleophilic attack of C1 atom in Azomethine ylides **1a** and **1c** to the electrophilic center of **2a** (C4 atom) in both reactions, leading to the formation of 1,3-dispiro regioisomers **4a** and **4c** (Scheme S3). Thus, the predicted regioisomeric pathway was consistent with the experimental result of the 32CA reaction between **Azo-1c** and **2a**, while it was not in line with that of the reaction between **Azo-1a** and **2a**. The regioselectivity of the 32CA reactions is under the control of both electronic and steric factors. However, the prediction of regioselectivity through

analysing the local indices of separate reactants is based on the electronic effects without considering the steric ones. Therefore, the energy profiles of the possible reaction pathways were evaluated.



**Scheme S3.** Regio- and stereoisomeric pathways of the 32CA reaction of the **Azo-1a** and **Azo-1c** with **2a**.

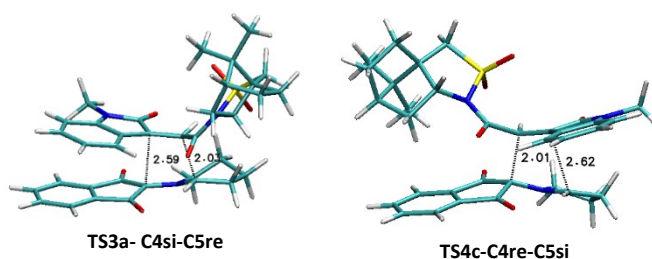
**Table S1.** Calculated global electrophilicity index ( $\omega$ ), electronic chemical potential ( $\mu$ ), chemical hardness ( $\eta$ ), and nucleophilicity index ( $N$ ), as well as electrophilic  $P^+$  and nucleophilic  $P^-$  Parr functions, local nucleophilicity  $N_k$  and local electrophilicity  $\omega_k$  indices of **Azo-1a** and **Azo-1c** with dipole **2a**, in eV, at B3LYP/6-31G(d).

Species	$\mu$	$\eta$	$\omega$	$N$	$k$	$P_k^+$	$P_k^-$	$\omega_k$	$N_k$
<b>Azo-1a</b>	<b>-3.44</b>	3.78	1.56	<b>3.79</b>	C1	0.050	<b>0.635</b>	0.078	<b>2.407</b>
					C3	0.091	0.243	0.142	0.921
<b>2a</b>	-4.11	3.36	<b>2.50</b>	3.33	C4	<b>0.263</b>	0.270	<b>0.658</b>	0.899
					C5	0.186	0.051	0.465	0.170
<b>Azo-1c</b>	<b>-3.49</b>	3.80	1.60	<b>3.73</b>	C1	0.038	<b>0.611</b>	0.061	<b>2.280</b>
					C3	0.103	0.229	0.165	0.854

## Assessing the activation energies of the 32CA reaction between Azo-1a and Azo-1c with dipolarophile 2a

The possible regio- and stereoisomeric pathways for the studied 32CA reactions are shown in Scheme 3 and Table S1. The stereochemistries of the chiral atoms of **2a** fragments in TSs and products are considered similar to the X-ray data of **3a**. Therefore, among the several possible pathways, two regioisomeric pathways **3** and **4**, and two stereoisomeric pathways with respect to the two new chiral centers in **2a** fragment are evaluated for each reaction.

Based on analysing the stationary points of the 32CA reactions between **Azo-1a** and **Azo-1c** with **2a** in methanol (solvent), the activation energies and entropies in terms of the separate reactants are negative at M06-2X, while the activation free energies are positive which reported in Table 7<sup>17</sup>. Then, the precomplexes were optimised and the activation parameters were calculated with respect to the generation of the TSs from the corresponding precomplexes. The favored transition structures corresponding to the 32CA reaction of the **Azo-1a** and **Azo-1c** with **2a**, namely **TS3a-C4si-C5re** and **TS4c-C4re-C5si** are shown in Figure S5, and all optimized structures are represented in supporting information (Figures S2 and S3).



**Figure S5.** The favored transition structures corresponding to the 32CA reaction of the **Azo-1a** and **Azo-1c** with **2a** at M06-2X/6-31G (d, p)

GEDT as a powerful tool for determining the polarity of the reactions<sup>11</sup> was computed for the possible pathways of the studied reactions (Table S2). As demonstrated, the TSs **4a** and **4c** are more polar than the TSs **3a** and **3c**, and charge flows from **Azo** fragments to **2a** fragment in the TSs, which were consistent with the results of local indices.

Table S2 represents the kinetic parameters calculated at M06-2X/6-31G (d, p) in methanol as solvent, and the thermodynamic parameters are shown in the supporting information (Table S2). The most kinetically favoured pathway for the 32CA reaction of **Azo-1c** and **2a** includes **TS4c-C4re-C5si** with  $E_a=8.02$  kcal.mol<sup>-1</sup>, which exhibits the highest GEDT value because of interacting the more nucleophilic center of **Azo-1c** with the more electrophilic center of **2a**. Furthermore, **3a-C4si-C5re** is determined as the most kinetically favourable product for the reaction of **Azo-1a** and **2a**. Therefore, the energy analysis of two 32CA reactions was in agreement with the experimental observations. However, a small difference is observed between the activation



parameters related to the two regioisomeric pathways of each reaction. Thus, it can predict poor to moderate selectivity, which was not in line with the experimental results. As shown in Table S1, all possible reactions progress exothermically between -15.39 and -29.93 for the 32CA reaction of **Azo-1a**, as well as -7.63 and -18.07 for that of **Azo-1c**.

**Table S2.** The calculated kinetic parameters (in kcal/mol) of the 32CA reaction of **Azo-1a**, **Azo-1c** and dipolarophile **2a** at M06-2X/6-31G(d,p) level of theory in methanol.

Structure	$E_a$	$\Delta H^\#$	$\Delta G^\#$	$\Delta G^\#$ <sup>*(a)</sup>	GEDT
<b>TS3a-C4si-C5re</b> (experimental product)	9.35	9.17	10.94	10.58	0.21
<b>TS3a-C4re-C5si</b>	15.58	14.86	17.02	15.68	0.20
<b>TS4a-C4si-C5re</b>	10.58	9.62	13.65	19.69	0.36
<b>TS4a-C4re-C5si</b>	10.19	9.60	11.29	13.10	0.43
<b>TS3c-C4si-C5re</b>	9.83	8.73	11.31	12.76	0.20
<b>TS3c-C4re-C5si</b>	14.68	13.85	16.82	15.09	0.21
<b>TS4c-C4si-C5re</b>	15.52	15.14	14.59	16.56	0.39
<b>TS4c-C4re-C5si</b> (experimental product)	8.02	7.51	9.84	9.29	0.43

(a) Relative to separate reactants

### NCI topological analysis of the TSs

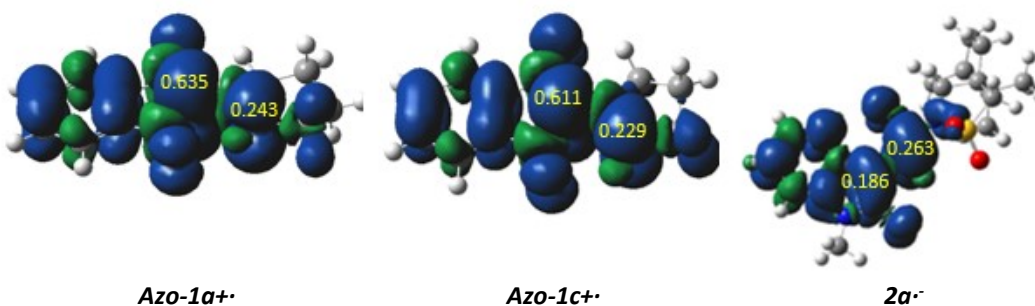
The favoured and unflavoured NCI and RDG plots of the possible TSs were assessed to study the regioselectivity of the 32CA reactions between **Azo-1a** and **Azo-1c** with **2a** (please see Figures S4 and S5 in supporting information pages 112-113)<sup>12</sup>. As depicted, blue, green, and red colours denote strong attractive, weak favourable or unfavourable van der Waals, and strong repulsive interactions, respectively. Additionally, the single blue surfaces in the NCI plot of the TSs **3a** are related to the strong attractive interactions between the C1 of **Azo-1a** and C5 of dipolarophile **2a**, while these strong interactions in TSs **4a** are associated with the noncovalent interaction between C3 and C5. Further, the green surfaces between the aromatic rings of **Azo-1a** and dipolarophile **2a** in TSs **3a** support weak van der Waals interactions. Considering the strongest attractive interaction with three steep slopes in the RDG plot and large extended green surface in the NCI plot, **TS3a-C4si-C5re** was more stable than the other TSs. This issue was consistent with the experimental observations, as well as the results of energy path analysis.

The NCI gradient isosurfaces and RDG plots for the TSs of the 32CA reaction between **Azo-1c** and **2a** were shown in Figure S5. The strong and attractive interactions between the carbon atoms of **Azo-1c** and **2a**, which shown with a single blue surface in the NCI plots and a steep slope in the RDG maps, in all TSs are nearly similar.

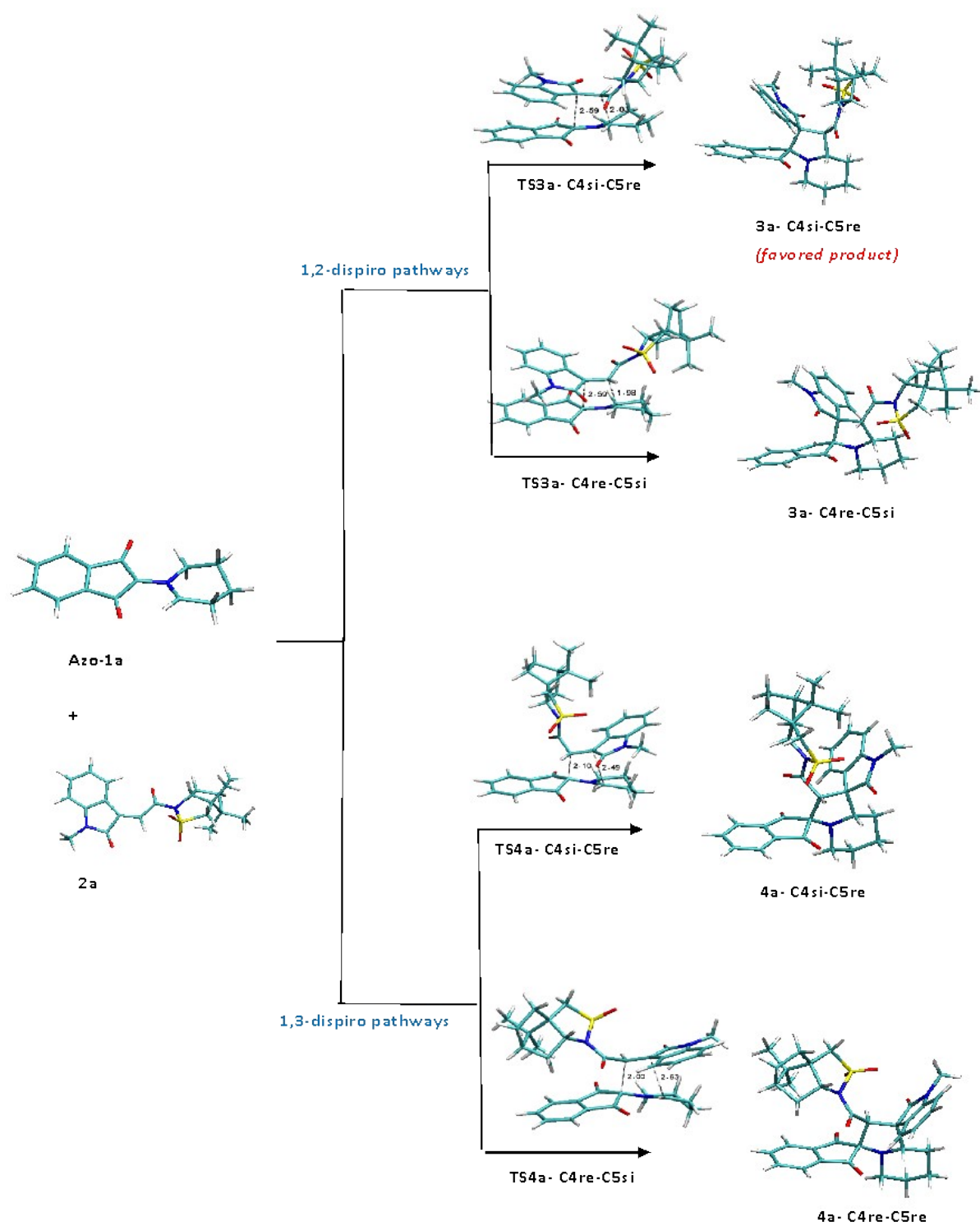
However, the less repulsive interaction was observed in the **TS4c-C4re-C5si**, which is the most favourable product based on the experimental results, global and local reactivity indices and energy path analysis. The repulsive interaction in **TS3c-C4si-C5re** is higher than the others (Figure S3), therefore despite the more extended green surface between the aromatic parts of **Azo-1c**

and **2a**, the pyrrolidine ring closing can be hard, as the corresponding product is not formed in the experimental observation.

In summary, DFT analysis shows that the steric and electronic effects controlled the regioselectivities of these reactions. Thus, the local indices analysis is not reliable alone for predicting regioselectivity. However, based on GEDT calculations, adding an electron-withdrawing group to **2a** can be expected to lower the activation energies. The quantum mechanical calculations of the possible transition states and NCI taking place in them are very useful tools for studying cycloaddition reaction mechanisms. The strong attractive and repulsive interactions responsible for observed stereoselectivity can be detected by NCI analysis. Our results align with the previous reports.<sup>13</sup>

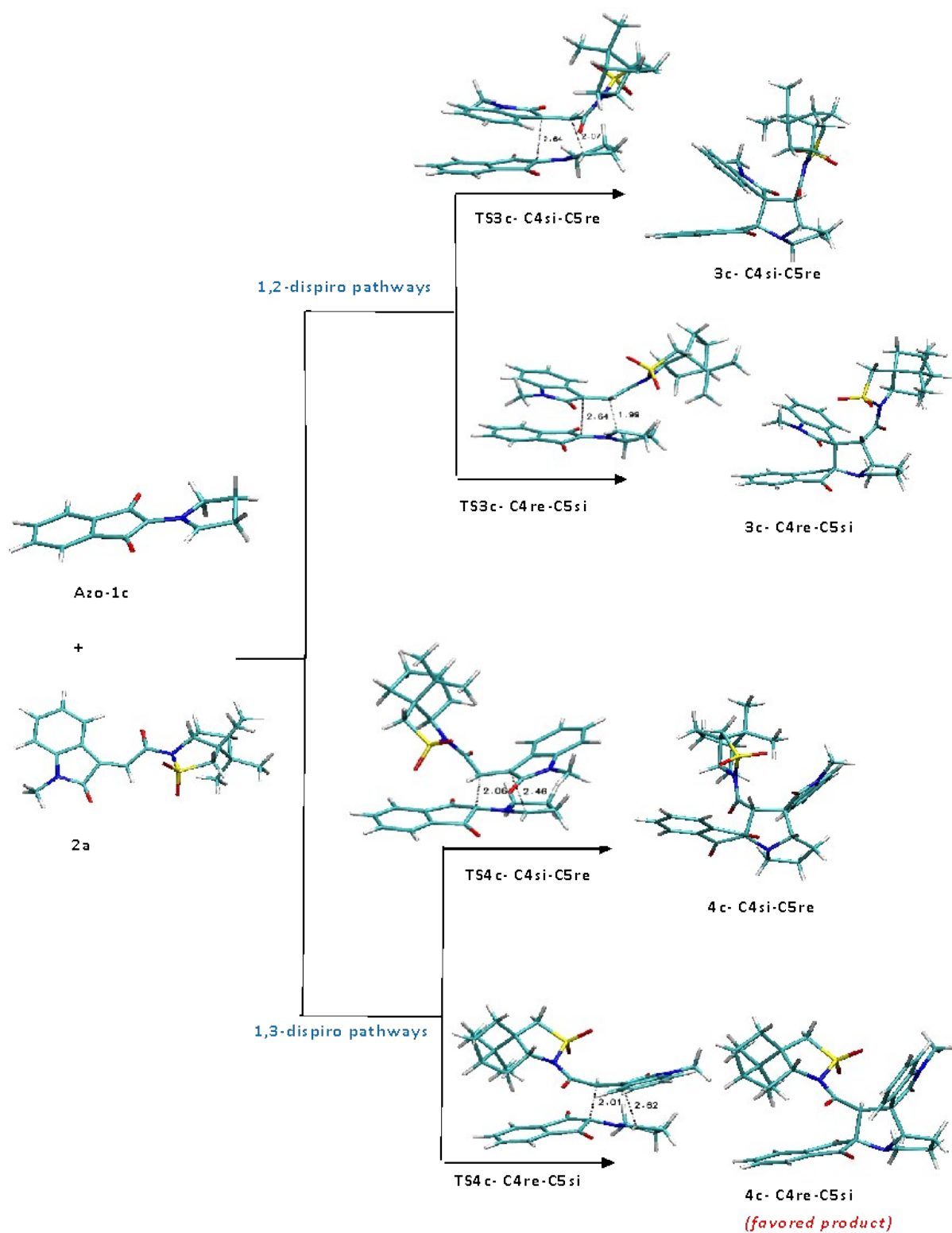


**Figure S1.** Atomic spin density (ASD) maps of the radical anion and the local electrophilic Parr function values of **2a** and radical cation and the local nucleophilic Parr function values of **Azo-1a** and **Azo-1c** at B3LP/6-31G(d,p).



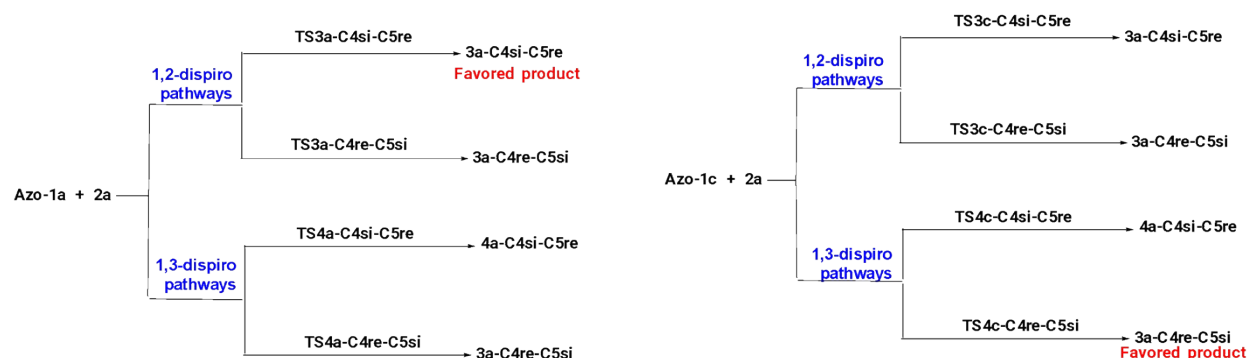
**Figure S2.** The optimized structures corresponding to the 32CA reaction of the **Azo-1a** and **2a** at M06-2X/6-31G (d, p)

9. Figure S3



**Figure S3.** The optimized structures corresponding to the 32CA reaction of the **Azo-1c** and **2a** at M06-2X/6-31G (d, p)

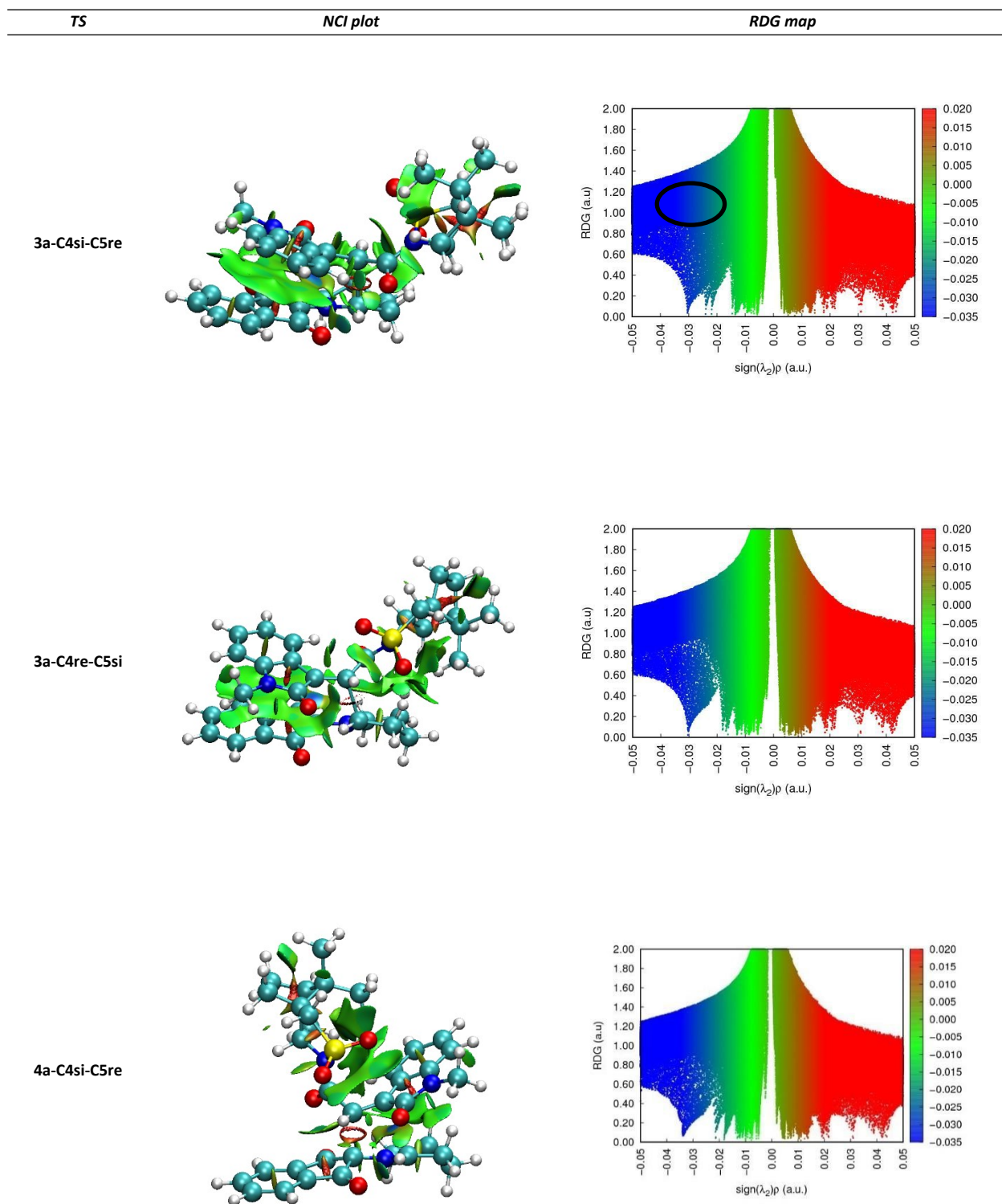
10. Table S3: The calculated thermodynamic and kinetic parameters (in kcal/mol) of the 32CA reaction of **Azo-1a**, **Azo-1c** and dipolraphile **2a** at M06-2X/6-31G(d,p) level of theory in methanol.

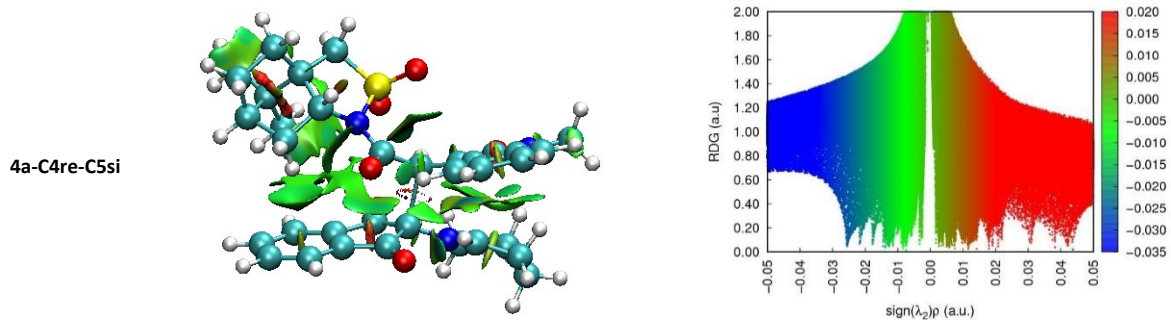


Structure	$E_a$	$\Delta H^\ddagger$	$\Delta G^\ddagger$	$\Delta G^\ddagger$ <sup>(a)</sup>	$\Delta E_{rxn}$	$\Delta H$	$\Delta G$	GEDT
<b>3a-C4si-C5re</b> (experimental product)	9.35	9.17	10.94	10.58	-23.66	-24.80	-21.31	0.21
<b>3a-C4re-C5si</b>	15.58	14.86	17.02	15.68	-14.54	-15.39	-13.84	0.20
<b>4a-C4si-C5re</b>	10.58	9.62	13.65	19.69	-28.50	-29.93	-24.84	0.36
<b>4a-C4re-C5si</b>	10.19	9.60	11.29	13.10	-21.81	-22.81	-20.36	0.43
<b>3c-C4si-C5re</b>	9.83	8.73	11.31	12.76	-17.06	-18.07	-14.62	0.20
<b>3c-C4re-C5si</b>	14.68	13.85	16.82	15.09	-6.45	-7.63	-4.45	0.21
<b>4c-C4si-C5re</b>	15.52	15.14	14.59	16.56	-12.04	-13.23	-10.01	0.39
<b>4c-C4re-C5si</b> (experimental product)	8.02	7.51	9.84	9.29	-14.80	-15.92	-12.78	0.43

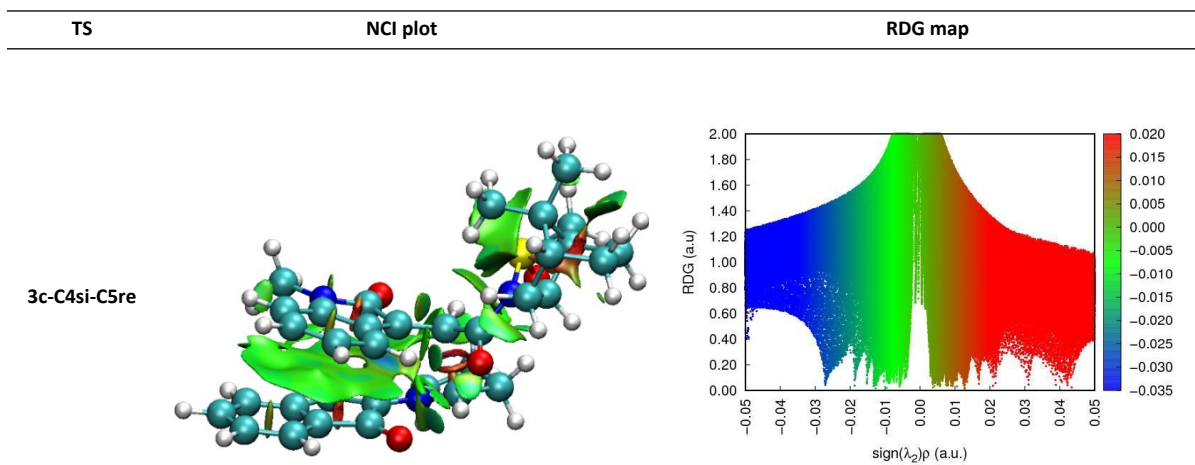
(b) Relative to separate reactants

## 11. NCI topological analysis of the TSs

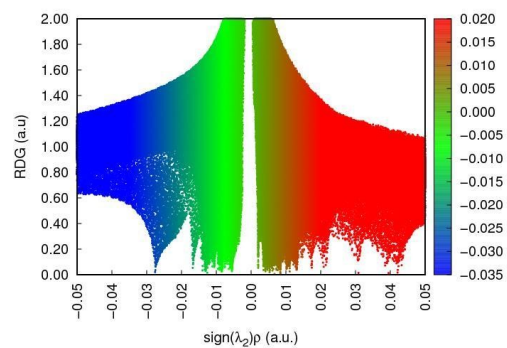
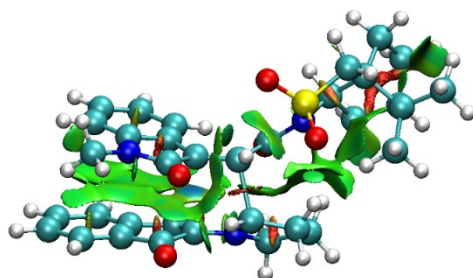




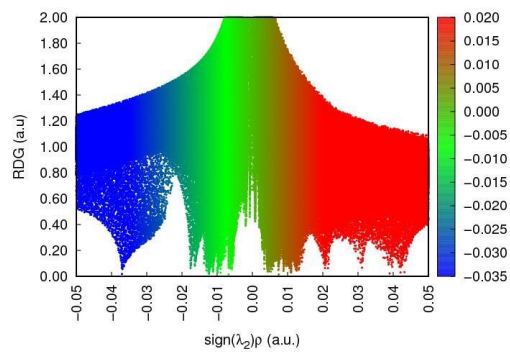
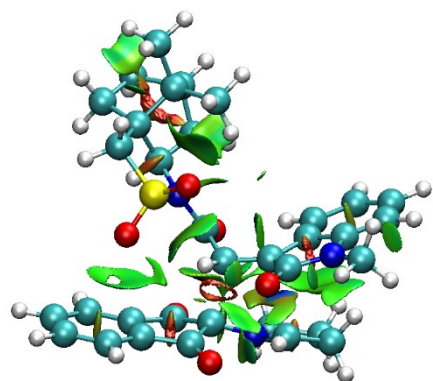
**Figure 7.** NCI gradient isosurfaces, represented at an isovalue of 0.5 a.u. and plots of the RDG versus the electron-density multiplied by the sign of the second Hessian eigenvalue for TSs **3a** and **4a** at the M06-2X/6-31G(d,p) level of theory.



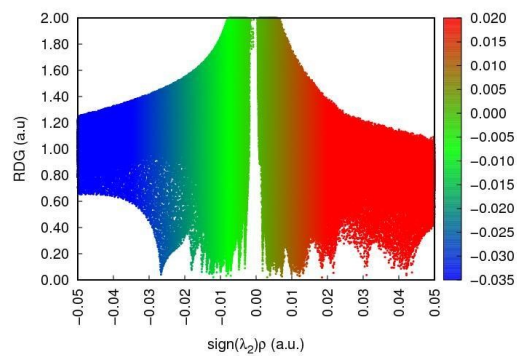
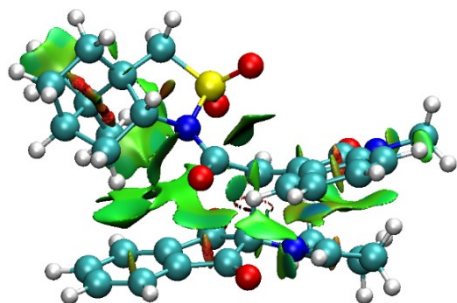
3c-C4re-C5si



4c-C4si-C5re



4c-C4re-C5si



**Figure 8.** NCI gradient isosurfaces, represented at an isovalue of 0.5 a.u. and plots of the RDG versus the electron-density multiplied by the sign of the second Hessian eigenvalue for TSs **3c** and **4c** at the M06-2X/6-31G(d,p) level of theory.

## 12. coordinates and energies



**TS3c-C4re-C5si****E=-2329.6759578**

N	-0.93866400	2.08153000	-0.96451300
C	-2.17253600	1.69419000	-0.58659600
C	-3.19343700	1.14268400	-1.48278700
O	-2.27239200	2.51741200	1.69532400
O	-3.12520800	0.95654200	-2.68977600
C	-2.77018400	1.95713000	0.73430100
C	-4.12876500	1.33950500	0.68290800
C	-0.21792700	1.33721700	-1.83566300
H	-0.77753600	0.79113300	-2.59071100
C	-0.13353800	3.13760000	-0.30426700
H	-0.13899500	2.97646000	0.77181500
H	-0.60883800	4.09558600	-0.52840800
C	1.07098300	2.04612400	-2.14828400
H	1.89698400	1.34176300	-2.28507400
H	0.95384200	2.60201400	-3.08398900
C	-4.38452500	0.88452300	-0.61164300
C	1.25707300	2.98996800	-0.94211400
H	1.66640500	3.95541000	-1.23834900
H	1.93917500	2.54653200	-0.21709400
C	-5.05312600	1.18583300	1.70278000
H	-4.83519600	1.53686400	2.70606500
C	-6.25709000	0.55065100	1.39317500
H	-7.00319300	0.40360300	2.16701400
C	-5.58404200	0.26733000	-0.93005900
H	-5.77924900	-0.07900800	-1.94029000
C	-6.51895000	0.09906700	0.09484200
H	-7.46474000	-0.38904100	-0.11693100
S	2.81684500	-1.58894000	-1.10735200
O	0.84457900	0.67967600	1.25830700
N	2.42275400	-0.36268300	0.02801700
C	-1.87870300	-0.97974600	0.92556300
N	-3.06540400	-2.01511200	-0.75741600
C	-3.02280800	-1.75619300	0.61265800
O	-1.69784200	-1.57067100	-2.57359900
C	1.10723900	0.03440600	0.25637400
C	0.08593000	-0.31904900	-0.76575500
H	0.42869600	-0.83565900	-1.65932100
C	-1.96930000	-1.47391000	-1.38279500
C	-4.07188200	-2.80852300	-1.42269900
H	-3.89407700	-2.73287400	-2.49527400
H	-5.06768200	-2.42245000	-1.18800800
C	3.41017000	-0.27592600	1.12245000
H	3.04698500	-0.90789900	1.94013300
C	-1.18542200	-0.74541200	-0.34112900
O	1.96712500	-2.75527100	-0.89346000
C	-1.67900600	-0.60048700	2.25452300
H	-0.83237500	0.01718300	2.52096800
C	-2.59387000	-1.01322100	3.22602300
H	-2.43695200	-0.71961300	4.25860800
O	2.82504500	-0.99225500	-2.43936300

C	4.47548800	-1.89026900	-0.46732400
H	4.43044700	-2.89160300	-0.03326200
H	5.15014600	-1.88559100	-1.32688400
C	-3.93573700	-2.17001300	1.56822100
H	-4.80181100	-2.76369400	1.29520000
C	-3.70457500	-1.78720800	2.89085100
H	-4.40415400	-2.09102500	3.66281300
C	3.77610700	1.14067300	1.63302500
H	3.46024000	1.27437600	2.66921900
H	3.29119200	1.91665900	1.04212900
C	4.75616000	-0.81136000	0.56217600
C	5.50261100	0.47853800	0.09445600
C	5.56977000	-1.23106500	1.80065900
H	4.98556300	-1.88651600	2.45153500
H	6.46983200	-1.77720700	1.50995800
C	5.90515500	0.14192900	2.45633100
H	5.45774000	0.24265500	3.44838900
H	6.98308900	0.27373800	2.57065200
C	5.30782500	1.16962300	1.46694600
H	5.73830500	2.17069300	1.54840400
C	4.86671900	1.22125200	-1.08628200
H	5.39178300	2.16936000	-1.23838700
H	3.80749400	1.44167200	-0.95477700
H	4.96661100	0.63696700	-2.00732900
C	6.96834000	0.23041100	-0.27877300
H	7.03690700	-0.41120800	-1.16419000
H	7.55626200	-0.23018900	0.51528200
H	7.44267800	1.18299600	-0.53275800
H	-4.01121700	-3.85627500	-1.11415500

### TS3c-C4si-C5re

**E=-2329.6778082**

N	-2.25712300	1.96650400	-1.02547500
C	-1.01407300	1.84424400	-0.40792800
C	-0.86996000	2.32159300	1.00334500
O	0.45491200	2.15251700	-2.32082700
O	-1.73224000	2.34831100	1.85888100
C	0.22321200	2.26973400	-1.13319900
C	1.16010100	2.79771400	-0.10153600
C	-3.37547000	1.64479200	-0.42387300
H	-3.40613300	1.54824500	0.65259300
C	-2.42008600	2.08508900	-2.50223400
H	-2.00763500	1.17980500	-2.95066900
H	-1.86603100	2.95320800	-2.85452300
C	-4.53678300	1.65333200	-1.35863300
H	-4.91448700	0.63040400	-1.46855100
H	-5.35455800	2.26197800	-0.96632900
C	0.53557400	2.80158500	1.14524100
C	2.46384800	3.25142400	-0.26032700
H	2.93207200	3.26129800	-1.23895800

C	-3.93905500	2.19911100	-2.67066600
H	-4.27763900	1.63556900	-3.53916000
H	-4.22239000	3.24430000	-2.80496300
C	3.13853600	3.68711000	0.87961100
H	4.15830400	4.04762200	0.79656800
C	1.20300600	3.22576700	2.28540100
H	0.71233800	3.21581400	3.25276600
C	2.51865400	3.66549300	2.13646800
H	3.07227400	4.00507700	3.00535400
S	1.26344900	-1.96499200	-1.41363000
O	0.28897800	-0.11425400	1.76384600
N	1.36901900	-0.95616800	-0.02570000
C	-2.82839000	-1.01199500	1.32637000
N	-4.17441000	-1.71010500	-0.39369900
C	-4.03948100	-1.66636100	0.99066100
O	-2.96599900	-0.98023800	-2.23138100
C	0.24519400	-0.40565000	0.58143700
C	-0.93149600	-0.15655200	-0.30297700
H	-0.73045500	-0.27464000	-1.36903400
C	-3.09089000	-1.10240100	-1.00852800
C	-5.28747300	-2.29205700	-1.10590800
H	-5.10666600	-2.14067800	-2.17019200
H	-6.22638400	-1.80625500	-0.82299300
C	2.53124700	-1.27310100	0.81828900
H	2.19960900	-1.96529500	1.59975900
C	-2.19760100	-0.64678000	0.06225500
O	0.18788700	-2.93210900	-1.22429900
C	-2.52777400	-0.81662300	2.67389700
H	-1.62784100	-0.28369900	2.95361300
C	-3.40590100	-1.30373000	3.64603500
H	-3.17045300	-1.15695500	4.69517900
O	1.22529900	-1.13449100	-2.61055900
C	2.87993100	-2.73603400	-1.16969800
H	2.66057500	-3.75967100	-0.85687700
H	3.37401900	-2.73990100	-2.14427900
C	-4.91939200	-2.14943000	1.94729700
H	-5.83860600	-2.65036200	1.66119000
C	-4.58193100	-1.96437800	3.29078300
H	-5.24998300	-2.33199000	4.06289900
C	3.26858400	-0.05016200	1.41390300
H	3.18886500	-0.03113300	2.50274900
H	2.84118000	0.88025100	1.03389100
C	3.59445800	-1.93373700	-0.09722100
C	4.50323100	-0.74061100	-0.53702300
C	4.51799000	-2.70682000	0.86205700
H	3.94164100	-3.35642400	1.52584600
H	5.21650900	-3.33935600	0.31000100
C	5.24470300	-1.55199000	1.61710300
H	5.00860700	-1.55027400	2.68435900
H	6.32920400	-1.63920300	1.52442000
C	4.71288400	-0.27316800	0.92533100
H	5.35737600	0.60193500	1.04436900
C	3.84572200	0.30147300	-1.44787800

H	4.50846400	1.16982400	-1.52820900
H	2.87272000	0.65067000	-1.10281100
H	3.70733800	-0.10354400	-2.45559400
C	5.79095700	-1.18657100	-1.23992400
H	5.55815100	-1.69750900	-2.18082400
H	6.41544800	-1.85160200	-0.64320800
H	6.38978700	-0.30569900	-1.48997000
H	-5.36596200	-3.36332900	-0.89909300

### TS4c-C4si-C5re

**E=-2329.6688366**

S	2.06065300	0.46965900	1.47253500
O	0.20425200	-0.18166400	-1.82001100
N	1.62016300	-0.11665700	-0.07353700
N	-2.87757100	1.21583300	-1.07935600
C	-1.74065000	1.88141800	-0.66030200
C	-2.01632300	-1.93254800	-0.15114600
C	-1.80613300	2.81223600	0.51186500
N	-3.00872000	-1.97286600	1.91802600
C	-2.82133700	-2.68641600	0.73878400
O	-0.73480600	2.35257600	-2.83849300
O	-2.30607100	0.05454100	2.78857000
C	0.35859800	0.02445800	-0.62761200
C	-0.76389600	0.34177000	0.30817600
H	-0.49576300	0.87751900	1.21753100
O	-2.65141500	2.85005800	1.38285300
C	-2.33351600	-0.76483200	1.87418500
C	-3.76372300	-2.43426300	3.05921500
H	-3.71851100	-1.65200500	3.81652400
H	-3.33515000	-3.35662400	3.46189000
C	-0.81834700	2.53583800	-1.64154000
C	2.76816700	-0.46381900	-0.92327100
H	2.97100900	0.39116700	-1.57760900
C	-1.71396300	-0.67378600	0.53614200
C	-0.01408400	3.50937500	-0.84623200
O	1.78777900	1.90204100	1.53806800
C	-3.66560200	0.61432900	-0.21054100
H	-3.70355900	0.97487700	0.80967800
C	-1.72830800	-2.47821100	-1.40293200
H	-1.11963200	-1.93307000	-2.11385300
C	-2.23030200	-3.74121400	-1.73417900
H	-2.00163700	-4.16211500	-2.70777600
C	-3.02070800	0.66433200	-2.45248000
H	-2.09186200	0.14333300	-2.69331300
H	-3.14188800	1.49280800	-3.14956300
C	-4.67278300	-0.26022400	-0.87122500
H	-4.65079500	-1.26035100	-0.42400600
H	-5.67934700	0.13908600	-0.71398700
O	1.46735200	-0.37627300	2.50059900
C	-0.60872100	3.69216500	0.40133200

C	3.82498800	0.15754400	1.25130900
H	4.27269700	1.14400800	1.10876300
H	4.18430700	-0.28544000	2.18329900
C	-3.32795000	-3.93749300	0.41859700
H	-3.94226000	-4.48868200	1.12306000
C	-3.01977800	-4.46128200	-0.83936600
H	-3.40202500	-5.43764300	-1.11832900
C	2.64649800	-1.78130700	-1.73142300
H	2.61906000	-1.58205300	-2.80427700
H	1.73068000	-2.31577900	-1.47192300
C	3.96409400	-0.73281400	0.03011500
C	-4.24858600	-0.25834400	-2.35825000
H	-5.05532700	0.11039800	-2.99172500
H	-3.98904900	-1.26476200	-2.68803000
C	1.12792600	4.20757200	-1.21141800
H	1.57978600	4.06563400	-2.18752700
C	3.94068200	-2.28415500	0.22936800
C	5.21872100	-0.53583800	-0.83955500
H	5.19052000	0.42553300	-1.35896400
H	6.12529600	-0.55275300	-0.23073300
C	5.13962800	-1.75612500	-1.80607500
H	5.00550000	-1.44591800	-2.84566000
H	6.05067100	-2.35648800	-1.76116400
C	3.91035500	-2.54626200	-1.29630300
H	3.90723400	-3.60039600	-1.58480200
C	1.66465300	5.09503400	-0.27866900
H	2.55937700	5.65684900	-0.52526500
C	-0.08843900	4.58153000	1.32929400
H	-0.56174700	4.71886700	2.29568900
C	1.06371800	5.28117400	0.97238000
H	1.50443500	5.98329900	1.67218100
C	2.73550900	-2.85312600	0.98892500
H	2.74218200	-3.94360400	0.89259500
H	1.76735400	-2.49076800	0.64261500
H	2.80820700	-2.61464100	2.05453000
C	5.19318300	-2.82346800	0.93008300
H	5.25994200	-2.43575100	1.95266100
H	6.12563300	-2.58368000	0.41873500
H	5.12564600	-3.91311200	1.00169200
H	-4.80670800	-2.61620500	2.78436900

#### TS4c-C4re-C5si

**E=-2329.68488**

S	2.96730200	1.44256600	0.95027300
O	1.10772300	-0.29642100	-1.92284700
N	2.54555000	0.38706300	-0.32787600
N	-1.87717400	2.34951300	-1.03609200
C	-2.77046400	1.34545000	-0.90577100
C	-1.25718600	-1.27607100	0.28812400
C	-2.79917600	0.15365300	-1.76367600

N	-2.44341000	-0.35084800	2.02884000
C	-2.22973100	-1.51294000	1.29101400
O	-4.32640500	2.20199200	0.75662000
O	-1.54467800	1.78954700	2.05298500
C	1.27248300	0.29635800	-0.87026400
C	0.16460000	0.91313100	-0.08568000
H	0.42117500	1.74577100	0.56518200
O	-2.05654100	-0.14218600	-2.68767400
C	-1.61942300	0.66179600	1.58103700
C	-3.39181500	-0.20160900	3.10819600
H	-3.42635300	0.85657300	3.36661200
H	-3.08891800	-0.78452700	3.98256700
C	-3.95757500	1.34878100	-0.03599800
C	3.70371900	-0.17289000	-1.04018300
H	3.87004400	0.43452700	-1.93632600
C	-0.85071000	0.11208000	0.42844400
C	-4.62423800	0.03056200	-0.27266800
O	2.63697700	2.81529000	0.57045500
C	-0.64513800	2.14752900	-1.54131100
H	-0.52794400	1.37809500	-2.29565800
C	-0.92820500	-2.30249400	-0.59764400
H	-0.21821800	-2.12308300	-1.39614000
C	-1.54300900	-3.54612100	-0.44419400
H	-1.29183200	-4.35302300	-1.12436900
C	-2.01546900	3.69170000	-0.40466500
H	-2.48010200	3.58613600	0.57121900
H	-2.65810800	4.28943200	-1.05817800
C	0.11892500	3.44265200	-1.51655800
H	1.18619000	3.29044700	-1.34187100
H	-0.00258300	3.95516400	-2.47807600
O	2.41101900	0.94498700	2.20164600
C	-3.95070400	-0.66440400	-1.27806700
C	4.74229600	1.14734600	0.80819800
H	5.14730900	2.05503200	0.35453000
H	5.12282400	1.03555900	1.82648800
C	-2.84820100	-2.74355100	1.44671500
H	-3.59202000	-2.90527700	2.21972900
C	-2.48558100	-3.76246200	0.56355200
H	-2.95495500	-4.73637700	0.65869100
C	3.63411600	-1.68293900	-1.38368000
H	3.59215700	-1.83780200	-2.46332400
H	2.74455500	-2.14273500	-0.94960600
C	4.91376800	-0.07784500	-0.07101000
C	-0.57302500	4.20125400	-0.37300500
H	-0.52280800	5.28371000	-0.48994100
H	-0.11168500	3.93307900	0.58153000
C	-5.71735300	-0.52486700	0.37430700
H	-6.24240500	0.02323700	1.15049800
C	4.95832300	-1.48467900	0.61102100
C	6.15526600	-0.11798400	-0.98001900
H	6.08411600	0.62631600	-1.77729600
H	7.06412100	0.09503600	-0.41317700
C	6.12402100	-1.58431200	-1.50793600

H	5.97206800	-1.62583500	-2.58965600
H	7.06012500	-2.10309600	-1.29120000
C	4.93229300	-2.21936500	-0.75173700
H	4.97311700	-3.30975400	-0.69077500
C	-6.11586300	-1.80762000	-0.01181700
H	-6.96514700	-2.27476400	0.47580800
C	-4.34456000	-1.93047500	-1.67480400
H	-3.80318400	-2.46170900	-2.45044500
C	-5.43955200	-2.50043400	-1.02127900
H	-5.77203300	-3.49601300	-1.29623600
C	3.78205800	-1.82882200	1.53332300
H	3.83529300	-2.89173300	1.78976700
H	2.79813600	-1.63498500	1.10587300
H	3.84790900	-1.25978100	2.46585500
C	6.23593200	-1.72157800	1.42472900
H	6.29133300	-1.02272600	2.26682600
H	7.15482600	-1.62372600	0.84639800
H	6.21476600	-2.73179000	1.84419400
H	-4.38302700	-0.52918100	2.78238000

### TS3a-C4si-C5re

**E=-2368.9773161**

S	2.96987900	1.25774300	1.01087400
O	1.08744300	-0.60171100	-1.77909600
N	2.54372800	0.17479800	-0.24459500
N	-1.72432900	2.28007900	-0.94693300
C	-2.68097900	1.31930900	-0.82801900
C	-1.41418600	-1.43126400	0.26387300
C	-2.82549000	0.17584700	-1.75447000
N	-2.54971900	-0.51551400	2.04275200
C	-2.40641700	-1.65225400	1.25170000
O	-4.20441300	2.17819400	0.89063200
O	-1.51824900	1.55833900	2.17439000
C	1.25931000	0.03289000	-0.75142200
C	0.15497900	0.68358100	0.00542300
H	0.43651400	1.46796600	0.70185900
O	-2.13361200	-0.13843500	-2.71114200
C	-1.66109600	0.46299400	1.64543800
C	-3.49035800	-0.35684900	3.12734800
H	-4.49528800	-0.62616100	2.79089900
H	-3.47479800	0.69287400	3.42004900
C	-3.87824300	1.35970000	0.04404100
C	3.69828700	-0.34757700	-0.99192300
H	3.79934400	0.25143700	-1.90366900
C	-0.92727300	-0.07598200	0.46536000
C	-4.64329700	0.11391500	-0.26030900
O	2.56886900	2.61461700	0.64231100
C	-0.52337100	1.91237200	-1.45665700
H	-0.57402400	1.07248300	-2.13902400
C	-1.14796200	-2.43671300	-0.66696800

H	-0.41975000	-2.26903900	-1.45066100
C	-1.84333800	-3.64311400	-0.57318100
H	-1.63980600	-4.43257600	-1.28885600
C	-1.87217800	3.58543400	-0.24685500
H	-2.52759400	3.42418700	0.60327200
H	-2.36110800	4.26832400	-0.95083200
C	0.52744200	2.94566900	-1.78393400
H	1.50599400	2.48858300	-1.60728700
H	0.46991300	3.12170500	-2.86378800
O	2.48270700	0.74171900	2.28355900
C	-4.02937000	-0.57665600	-1.30121400
C	4.74936400	1.04151700	0.79963200
H	5.09234800	1.96398700	0.32512300
H	5.17445100	0.95583100	1.80274300
C	-3.10501000	-2.84561700	1.34796600
H	-3.86208200	-2.99359400	2.11079700
C	-2.80488900	-3.84410600	0.41951800
H	-3.33713200	-4.78872000	0.46773300
C	3.68616600	-1.86416500	-1.31281600
H	2.84238300	-2.35985200	-0.83023500
H	3.59977700	-2.03638100	-2.38718500
C	4.94331200	-0.18143900	-0.07753100
C	-0.52253300	4.13463000	0.18282100
H	-0.69245400	5.10827000	0.65062600
H	-0.09071600	3.47999000	0.94564500
C	-5.77558400	-0.38590700	0.36530900
H	-6.25505800	0.16266100	1.16994300
C	0.40696500	4.27320400	-1.01697800
H	1.39664700	4.60369200	-0.69583300
H	0.00307400	5.04327100	-1.68223400
C	5.09043000	-1.57589300	0.61445000
C	6.14350200	-0.16983600	-1.04114400
H	7.06533600	0.09161400	-0.51715500
H	6.00115700	0.56266800	-1.83977900
C	6.15927200	-1.64114800	-1.55607700
H	7.12932900	-2.11121400	-1.38179800
H	5.95732900	-1.70048800	-2.62874400
C	5.03797100	-2.32695300	-0.73832600
H	5.13745500	-3.41310400	-0.66936100
C	-6.27094400	-1.61316000	-0.08159800
H	-7.15277300	-2.03816000	0.38642000
C	-4.51741600	-1.78897700	-1.75905300
H	-4.01937100	-2.31967300	-2.56353200
C	-5.65014900	-2.30564700	-1.12750100
H	-6.05786800	-3.25865000	-1.44813800
C	3.97604300	-1.96337500	1.59390600
H	4.08723300	-3.02066700	1.85494900
H	2.96611700	-1.81551400	1.21173300
H	4.06094200	-1.38362700	2.51833100
C	6.41470800	-1.73999400	1.36931700
H	6.47931000	-1.02251500	2.19494800
H	7.29951600	-1.61370500	0.74515900
H	6.45892900	-2.74152800	1.80733600



H -3.21708100 -0.98220200 3.98201400

**TS3a-C4re-C5si**

**E=-2368.9701081**

S -2.74045100 -1.19278900 1.61992800  
O -0.82147700 0.04271600 -1.44360200  
N -2.38145400 -0.46105600 0.10776900  
N 0.91103200 2.24163000 -0.03696800  
C 2.15052400 1.70898800 -0.19825400  
C 1.90575900 -1.35490900 -0.45135700  
C 3.18659800 1.65349100 0.84579400  
N 3.10862600 -1.56327900 1.50325100  
C 3.05166200 -1.92474000 0.15747800  
O 2.28932600 1.38776200 -2.61554800  
O 1.76325800 -0.36291700 2.95669800  
C -1.07442700 -0.15581700 -0.26609600  
C -0.05428700 -0.03870000 0.80775800  
H -0.39606500 -0.15100500 1.83469900  
O 3.12753600 2.04636400 2.00203900  
C 2.02254100 -0.79478700 1.83957400  
C 4.12531300 -1.98940300 2.43596000  
H 3.94148700 -1.47555900 3.37927400  
H 5.11594700 -1.72039200 2.05839500  
C 2.76580800 1.34786000 -1.49441000  
C -3.37009700 -0.81583500 -0.92988800  
H -2.99540900 -1.70398200 -1.45032000  
C 1.22789400 -0.58412800 0.59081600  
C 4.13171000 0.84608500 -1.16364900  
O -1.86380700 -2.33936900 1.83210700  
C 0.24823900 1.89236100 1.10124000  
H 0.92182600 1.66065600 1.92142100  
C 1.69102200 -1.58897000 -1.81068200  
H 0.84383400 -1.13975300 -2.31085600  
C 2.59378800 -2.38934100 -2.51448300  
H 2.42629300 -2.57289300 -3.57052600  
C 0.23765900 2.89826700 -1.18675800  
H 0.30926900 2.23153500 -2.04326600  
H 0.82265200 3.79891800 -1.39676900  
C -1.02878800 2.60906500 1.49767200  
H -1.85763600 1.89115100 1.51794200  
H -0.91007600 2.96259500 2.52536100  
O -2.75653500 -0.15417800 2.64492200  
C 4.38539000 1.03934900 0.19276100  
C -4.39722200 -1.73510600 1.15808800  
H -4.33756800 -2.82539200 1.12650400  
H -5.06668600 -1.42036100 1.96230800  
C 3.95235900 -2.72017000 -0.53080100  
H 4.82059500 -3.14150500 -0.03511700  
C 3.70652300 -2.94838400 -1.88598300  
H 4.39591300 -3.56295800 -2.45578000

C	-3.76500400	0.29672600	-1.93366900
H	-3.28571800	1.24310000	-1.68740300
H	-3.46229900	0.03133200	-2.94826900
C	-4.70262700	-1.12015100	-0.19508500
C	-1.20781000	3.25968800	-0.87958700
H	-1.53007200	4.00494200	-1.61081000
H	-1.83694300	2.37525200	-1.01870400
C	5.06462800	0.26033500	-2.00356100
H	4.84590000	0.11035500	-3.05565800
C	-1.36012300	3.75957800	0.54984300
H	-2.37796600	4.11148200	0.73530900
H	-0.68137300	4.60185600	0.72580600
C	-5.46467600	0.24369000	-0.23274400
C	-5.51896300	-1.98179900	-1.17679400
H	-6.40449100	-2.39630200	-0.69009200
H	-4.92639600	-2.82230500	-1.54717700
C	-5.88904200	-0.95687200	-2.28994300
H	-6.97089000	-0.88866500	-2.42177200
H	-5.45931400	-1.22858100	-3.25741000
C	-5.29552500	0.37141700	-1.76717300
H	-5.74089700	1.26521900	-2.21091900
C	6.27624300	-0.14156500	-1.43955800
H	7.03045600	-0.61265400	-2.06113800
C	5.59177800	0.65606600	0.75811600
H	5.78544300	0.81220800	1.81481800
C	6.53574000	0.05394800	-0.07799700
H	7.48750400	-0.26752200	0.33239600
C	-4.83009500	1.38633000	0.56965000
H	-5.39405300	2.30655300	0.38815100
H	-3.78644400	1.57919800	0.31972100
H	-4.87638900	1.17723700	1.64380900
C	-6.92108600	0.13423300	0.23216200
H	-6.96659300	-0.11638400	1.29779800
H	-7.50482900	-0.60869000	-0.31161700
H	-7.41543700	1.10200800	0.10615100
H	4.08137400	-3.07096500	2.59297900

#### TS4a-C4re-C5si

**E=-2368.9730097**

N	-2.34599700	1.91576200	-0.60096800
C	-1.02271200	1.79175000	-0.12706100
C	-0.75481000	2.19602200	1.29712000
O	0.31626500	2.23198000	-2.12852100
O	-1.52395200	2.16228900	2.23738400
C	0.14478600	2.29851900	-0.92621600
C	-0.80471700	-0.19637800	-0.25677900
C	1.15036200	2.80154000	0.05092100
C	-3.31250200	1.44995000	0.14877100
H	-3.04078300	1.14572300	1.14879100
C	-2.57165400	2.36976200	-2.00346500

H	-1.83912800	1.85048000	-2.61783500
H	-2.34120600	3.43905100	-2.02050300
C	-4.75682300	1.52280900	-0.21731700
H	-5.09026400	0.49384500	-0.41991100
H	-5.30616500	1.84721700	0.67137500
C	0.64144400	2.71438900	1.34306200
C	-3.98415500	2.08783800	-2.49083700
H	-4.14176600	2.67437600	-3.39923400
H	-4.05665300	1.02740100	-2.75188100
C	2.42262100	3.30259900	-0.19584500
H	2.80129000	3.38002800	-1.20957900
C	-5.01326100	2.42371300	-1.42010500
H	-6.02944700	2.27350500	-1.78977000
H	-4.92155400	3.47397600	-1.12194700
C	3.18396000	3.69630800	0.90409100
H	4.18237900	4.09289800	0.75321700
C	1.39457200	3.09588500	2.44443800
H	0.99200400	3.01475100	3.44839800
C	2.67886300	3.58648700	2.20704800
H	3.29810900	3.89550800	3.04244100
C	-2.01750600	-0.83582700	0.04919600
C	-2.60937000	-1.40867700	1.25029900
C	-2.90533100	-1.16484700	-1.06694200
C	-3.80595300	-2.04746100	0.83638800
C	-2.28925000	-1.40333300	2.60763100
N	-3.96167800	-1.89212600	-0.53827300
O	-2.78306300	-0.87380800	-2.26128500
C	-4.65175800	-2.69446900	1.72410800
H	-1.39841600	-0.89130600	2.95108200
C	-3.13433100	-2.05700200	3.50919500
C	-5.05655600	-2.41415300	-1.32130700
H	-5.55984000	-3.17947000	1.38058300
C	-4.29560600	-2.69671700	3.07599000
H	-2.88401800	-2.05948300	4.56514900
H	-4.89597100	-2.09959700	-2.35264000
H	-6.01313100	-2.01961500	-0.96489200
H	-5.08470100	-3.50671800	-1.27420700
H	-4.93766100	-3.19585600	3.79441800
H	-0.61405400	-0.16717100	-1.33124100
C	0.40069100	-0.46639000	0.58350000
O	0.45928900	-0.26062200	1.78330300
N	1.52725400	-0.93146100	-0.08458100
S	1.42531800	-1.84354000	-1.53902500
C	2.72156700	-1.25631200	0.70889000
O	0.38611400	-2.85761800	-1.39986900
O	1.33806000	-0.93281800	-2.67319900
C	3.06992100	-2.57706600	-1.37658600
H	2.43501100	-2.00488500	1.45530700
C	3.42963600	-0.04367900	1.35871400
C	3.78385900	-1.82276300	-0.26949400
H	2.88792800	-3.62471700	-1.12543200
H	3.54273800	-2.50400100	-2.35895900
H	2.96601200	0.89127900	1.03553300

H	3.36895300	-0.08494000	2.44817600
C	4.87006900	-0.19215400	0.83308400
C	4.64557500	-0.57622000	-0.65101400
C	4.75257300	-2.62339200	0.61972600
C	5.45376700	-1.49387500	1.43538900
H	5.49047000	0.69362600	0.99382800
C	3.93506100	0.49532200	-1.48423700
C	5.93309100	-0.93348300	-1.40324300
H	5.46164300	-3.19242200	0.01453300
H	4.21351500	-3.33539300	1.24983700
H	6.53891400	-1.53924100	1.32235800
H	5.23512100	-1.56638500	2.50394300
H	4.55745300	1.39632900	-1.50986900
H	2.95079200	0.77587700	-1.10996400
H	3.80493800	0.15249100	-2.51590900
H	6.49157700	-0.01730900	-1.61740200
H	5.69907200	-1.40206900	-2.36561100
H	6.59627700	-1.60377700	-0.85620700

#### TS4a-C4si-C5re

**E=-2368.9629382**

N	-3.10562600	-0.60796900	-0.74160700
C	-2.69412600	0.68781300	-0.39636300
C	-3.28699600	1.36248400	0.80458600
O	-2.54619300	1.68559100	-2.64633600
O	-3.81981800	0.84962400	1.77083000
C	-2.58180700	1.77232300	-1.43581000
C	-0.86780700	0.27594600	0.55037400
C	-2.63293100	3.06085300	-0.68226500
C	-3.18396800	-1.49882500	0.22469700
H	-3.19681300	-1.10812300	1.23328800
C	-3.11219400	-1.00724300	-2.17873200
H	-2.23209600	-0.56016500	-2.63710500
H	-3.98870600	-0.53450600	-2.62877000
C	-3.56136100	-2.92854700	0.00613800
H	-2.66472200	-3.54016500	0.18947500
H	-4.28341600	-3.20536700	0.77967000
C	-3.06749400	2.82387200	0.61716200
C	-3.12961600	-2.51536900	-2.37743700
H	-3.41079600	-2.70490300	-3.41625200
H	-2.12056800	-2.91738300	-2.22933600
C	-2.36721500	4.34544600	-1.13255000
H	-2.03711300	4.52063100	-2.15097200
C	-4.08663300	-3.18437900	-1.40115200
H	-4.15472300	-4.25787500	-1.58785200
H	-5.09258200	-2.76374700	-1.50850000
C	-2.54133900	5.39278500	-0.22767000
H	-2.34007500	6.41182900	-0.54078000
C	-3.25167600	3.85960700	1.52322300
H	-3.59598900	3.66213500	2.53285400

C	-2.97817500	5.15387300	1.08188300
H	-3.10684900	5.99149300	1.75902400
C	-0.75753900	-1.11577000	0.62864300
C	-0.13155800	-2.01135800	-0.32660400
C	-0.95969600	-1.88034900	1.86771000
C	0.01297400	-3.25937600	0.31871000
C	0.29566600	-1.86395000	-1.64330700
N	-0.49154900	-3.16297100	1.61274000
O	-1.46033500	-1.51543000	2.92937100
C	0.57755300	-4.35423900	-0.31899100
H	0.17987000	-0.91425500	-2.16047800
C	0.87246100	-2.95982500	-2.29419200
C	-0.49984300	-4.23072400	2.58414100
H	0.68542900	-5.30784200	0.18752900
C	1.01029200	-4.18423600	-1.63924800
H	1.21255400	-2.85608100	-3.31920900
H	-0.96531900	-3.84198300	3.48956100
H	0.51901900	-4.55840800	2.81045100
H	-1.07621600	-5.08499100	2.21642800
H	1.45784600	-5.02392800	-2.16065700
H	-1.06586500	0.76280600	1.50643000
C	0.19853100	0.97959700	-0.25736100
O	0.02326500	1.62155600	-1.27484500
N	1.49764700	0.80823400	0.21174700
S	1.88972600	0.38909000	1.83437500
C	2.58400200	1.51752700	-0.48469800
O	1.04059700	1.15996600	2.73860000
O	1.93180700	-1.05581200	2.00877900
C	3.55751400	1.07783500	1.75950700
H	2.33921700	2.58489100	-0.46809200
C	2.89860300	1.03579000	-1.92164300
C	3.89813600	1.24025200	0.29102600
H	3.49815500	2.03513500	2.28346500
H	4.20275300	0.38834500	2.30892500
H	2.33729800	0.12785100	-2.15602700
H	2.63636600	1.79504400	-2.66086600
C	4.41429100	0.76920200	-1.84468400
C	4.54800700	0.04495600	-0.48183700
C	4.82977000	2.40781200	-0.08306300
C	5.11978000	2.12265400	-1.58771000
H	4.80839300	0.21629400	-2.70120000
C	3.80503400	-1.29512800	-0.41700400
C	5.99667700	-0.23301100	-0.06407800
H	5.74008000	2.39184900	0.52032400
H	4.34188100	3.37153700	0.08439300
H	6.19298400	2.05992700	-1.77962900
H	4.71897800	2.90615100	-2.23632300
H	4.20191100	-1.95526400	-1.19616100
H	2.72544700	-1.22566700	-0.55466500
H	3.97628100	-1.77978500	0.54881400
H	6.04277700	-0.52732700	0.99038000
H	6.67070600	0.61197200	-0.20719300
H	6.38649800	-1.07035100	-0.65071000

**Precomplex3a-C4si-C5re****E=-2368.991904**

S	3.18345300	1.17762000	1.07644200
O	1.08982300	-1.15014000	-1.16602300
N	2.67946300	-0.05277100	-0.00323900
N	-1.63119100	2.14168000	-1.04526400
C	-2.72755000	1.26593900	-0.97020000
C	-1.60780300	-1.54837500	0.63498500
C	-2.86708600	0.09906600	-1.81239900
N	-2.84430200	-0.29580300	2.13231800
C	-2.78326100	-1.49667700	1.41689700
O	-4.20927300	2.28019600	0.69266900
O	-1.51960500	1.59162700	2.31072100
C	1.35400700	-0.39543400	-0.24307800
C	0.33993000	0.20183200	0.65007400
H	0.56736300	1.14492400	1.14204900
O	-2.11602900	-0.34428400	-2.68272600
C	-1.74757300	0.47922100	1.86714600
C	-3.92217800	0.10156100	3.01066000
H	-4.87699000	0.03126800	2.48498700
H	-3.74521900	1.13789000	3.29447200
C	-3.90616500	1.42950000	-0.14410700
C	3.73856000	-0.50552600	-0.91868800
H	3.59102300	0.01314600	-1.87263000
C	-0.86764600	-0.32000300	0.92287900
C	-4.79313500	0.25626300	-0.47274800
O	2.54732800	2.44139500	0.70591500
C	-0.54692800	1.82935000	-1.68977100
H	-0.53236400	0.84043500	-2.13567000
C	-1.38183200	-2.64999400	-0.18605200
H	-0.49893500	-2.68623500	-0.81114700
C	-2.31740400	-3.68612800	-0.19459000
H	-2.15376400	-4.54862500	-0.83124300
C	-1.75166200	3.44770100	-0.33156100
H	-2.30190500	3.24249200	0.58255900
H	-2.36393300	4.09314300	-0.96916500
C	0.62631000	2.72900600	-1.87838300
H	1.48177400	2.24371200	-1.38915300
H	0.86060400	2.73516300	-2.94898500
O	3.00498100	0.72022600	2.44778900
C	-4.17696500	-0.53166000	-1.44001200
C	4.90600800	1.15644500	0.53914000
H	5.02828700	2.06718800	-0.05191800
H	5.51601900	1.21257800	1.44410500
C	-3.71635500	-2.51922700	1.41989900
H	-4.61702200	-2.45864600	2.02098900
C	-3.46269600	-3.62059400	0.59912500
H	-4.18134500	-4.43351900	0.57173600
C	3.87169500	-2.03605600	-1.12667600

H	3.20867900	-2.58251400	-0.45462100
H	3.61003300	-2.31604700	-2.14861900
C	5.09725400	-0.10845900	-0.27673900
C	-0.39111000	4.05506200	-0.04720200
H	-0.55105300	5.04389700	0.38988700
H	0.13092500	3.44422900	0.69829600
C	-6.02392800	-0.08505000	0.05532200
H	-6.50716600	0.54530600	0.79599600
C	0.43418500	4.13751500	-1.32446800
H	1.40809200	4.59441800	-1.13649300
H	-0.08885200	4.76102300	-2.05761400
C	5.55742300	-1.40624900	0.46397600
C	6.08594200	-0.04028800	-1.45435800
H	7.04514400	0.37488400	-1.13789000
H	5.70177800	0.59526600	-2.25631700
C	6.20309400	-1.53968600	-1.86480900
H	7.24285600	-1.87288500	-1.85460900
H	5.81404100	-1.71910800	-2.87048600
C	5.35675000	-2.27807100	-0.79935000
H	5.61343100	-3.33355700	-0.67948300
C	-6.62380800	-1.26609500	-0.40425200
H	-7.58857500	-1.56735900	-0.00899300
C	-4.75805200	-1.69445800	-1.90527900
H	-4.26085100	-2.30575900	-2.65167500
C	-5.99934100	-2.05943900	-1.36644400
H	-6.48428900	-2.97058900	-1.70188700
C	4.70650500	-1.83187400	1.66635400
H	5.00219300	-2.84131100	1.96942800
H	3.63257900	-1.83718500	1.48115900
H	4.88553600	-1.16567800	2.51615000
C	7.00878200	-1.34317700	0.95393700
H	7.12985900	-0.55208200	1.70225000
H	7.73727400	-1.17020300	0.16163400
H	7.26639500	-2.28910800	1.43946700
H	-3.94624800	-0.53199600	3.90151500

### Precomplex3a-C4re-C5si

**E=-2368.994705**

S	3.10829400	0.35704200	-1.79832200
O	1.02356400	-1.84204000	0.52571600
N	2.60927400	-0.55658800	-0.43674700
N	-1.25005500	2.02229500	1.04139300
C	-2.45078400	1.28485900	1.10803800
C	-1.92208100	-1.52875300	-0.81467600
C	-3.66823400	1.67502200	0.44367600
N	-3.08557700	0.02379400	-2.07179500
C	-3.14719100	-1.22797900	-1.45133600
O	-1.90218000	-0.59024000	2.58051700
O	-1.49609800	1.68876300	-2.27733500
C	1.27752800	-0.91310200	-0.22341200

C	0.26488600	-0.08386100	-0.90524500
H	0.57568800	0.87183500	-1.32398000
O	-3.90104100	2.64083000	-0.28984300
C	-1.85843500	0.59483800	-1.87829500
C	-4.17015000	0.65605100	-2.79031500
H	-3.85127500	1.66754200	-3.03759200
H	-5.05876200	0.70439600	-2.15680700
C	-2.65613100	0.06619700	1.86310100
C	3.66916500	-1.42430100	0.09689900
H	3.51082100	-2.42666100	-0.31548400
C	-1.02711700	-0.40482800	-1.08977500
C	-4.08740300	-0.32732200	1.60829400
O	2.47783500	-0.16985000	-3.00367100
C	-1.09303200	3.01988100	0.22592700
H	-1.93822400	3.23792400	-0.41505600
C	-1.80258800	-2.71745000	-0.09749200
H	-0.88010300	-2.94472400	0.41935200
C	-2.89087400	-3.59004800	-0.05333600
H	-2.80924900	-4.51757400	0.50250200
C	-0.16754400	1.59342300	1.97405100
H	-0.14718400	0.50554000	1.94171400
H	-0.50214100	1.88325300	2.97443700
C	0.14457500	3.84610500	0.13176700
H	0.65861100	3.54122600	-0.79237900
H	-0.16100000	4.88520600	-0.02183700
O	2.91418100	1.77357700	-1.50076200
C	-4.68656700	0.62371700	0.78773500
C	4.84078000	-0.14823600	-1.70897800
H	4.97866000	-0.81817100	-2.56090100
H	5.43940900	0.75604800	-1.84383900
C	-4.23211400	-2.08703600	-1.41886400
H	-5.16612800	-1.83434700	-1.90861200
C	-4.08310900	-3.27951600	-0.70783100
H	-4.91982700	-3.96879400	-0.65410200
C	3.80212400	-1.47069400	1.63856800
H	3.15086800	-0.72932100	2.10781600
H	3.52440000	-2.45146000	2.02867800
C	5.03295200	-0.84270500	-0.37262300
C	1.18247000	2.19545300	1.63136300
H	1.85335100	2.00044100	2.47265300
H	1.60425500	1.69338600	0.75291900
C	-4.77965600	-1.43382400	2.05653400
H	-4.29750400	-2.17334200	2.68792800
C	1.06781800	3.68306300	1.33232500
H	2.04753400	4.11431700	1.11529100
H	0.65454300	4.21148300	2.19829400
C	5.51965400	0.01420700	0.83965700
C	6.00092800	-2.03851800	-0.32775600
H	6.96488900	-1.78044800	-0.77142600
H	5.60231200	-2.89243800	-0.88112700
C	6.11353500	-2.30114700	1.20565100
H	7.15444500	-2.28354000	1.53484500
H	5.70162200	-3.27469600	1.48398000



C	5.29533900	-1.14758700	1.83876200
H	5.56402400	-0.92731400	2.87483800
C	-6.11537500	-1.57197600	1.65264100
H	-6.68974600	-2.43276500	1.97989300
C	-6.00509800	0.50563700	0.39161400
H	-6.46915300	1.25895500	-0.23816100
C	-6.71870400	-0.61745600	0.83504800
H	-7.75543700	-0.74533900	0.54078400
C	4.69228000	1.26913300	1.12867900
H	4.98118500	1.67710300	2.10281400
H	3.61910100	1.09169700	1.14127100
H	4.88590700	2.04006300	0.37527500
C	6.98093000	0.46322100	0.72444700
H	7.11828900	1.11038900	-0.14899500
H	7.69388700	-0.35792000	0.64905400
H	7.24682900	1.05172100	1.60755500
H	-4.39983800	0.10200600	-3.70443600

### Precomplex4a-C4re-C5si

**E=-2368.988964**

N	-2.58789500	1.97106700	-0.23913600
C	-1.22444300	2.24083000	-0.05683900
C	-0.68434400	2.60605800	1.23033600
O	-0.27944800	2.11859500	-2.29546300
O	-1.24007500	2.64474900	2.32596200
C	-0.23110200	2.36734600	-1.08926000
C	-0.68230100	-0.76156800	-0.53230200
C	1.00924900	2.86813400	-0.38639100
C	-3.30269500	1.45827000	0.71570300
H	-2.75207900	1.12851200	1.58986500
C	-3.18080200	2.39629900	-1.53899400
H	-2.52286100	1.98718900	-2.30584700
H	-3.10043300	3.48693900	-1.55768500
C	-4.79157800	1.38443900	0.70288000
H	-5.07483000	0.32406100	0.64595200
H	-5.13677700	1.72415000	1.68521700
C	0.74560000	2.99967600	0.97662400
C	-4.61802300	1.93369700	-1.70731700
H	-5.04114900	2.47175500	-2.55891900
H	-4.63254700	0.86831200	-1.95863700
C	2.24067300	3.20517000	-0.91482300
H	2.43468600	3.10894700	-1.97867500
C	-5.41649400	2.18643600	-0.43429200
H	-6.46260100	1.90034400	-0.56080900
H	-5.39368100	3.25369700	-0.18897100
C	3.22514700	3.67206400	-0.03109700
H	4.20460200	3.94280400	-0.41291700
C	1.70532300	3.45977100	1.85704600
H	1.48846200	3.55852300	2.91593700
C	2.96258500	3.79516100	1.33293000

H	3.74197000	4.15785600	1.99531900
C	-1.92230600	-1.17905200	-0.24915800
C	-2.60043800	-1.73660600	0.92480200
C	-2.95443300	-1.15131700	-1.35281900
C	-3.91768200	-2.03547400	0.51896400
C	-2.21174900	-1.99780800	2.23452700
N	-4.10765200	-1.67360600	-0.82184900
O	-2.81152200	-0.73344600	-2.48942700
C	-4.85084700	-2.58736000	1.38069600
H	-1.20949300	-1.75670100	2.56683700
C	-3.14068200	-2.56116300	3.11270600
C	-5.33650700	-1.85500500	-1.56415900
H	-5.86145500	-2.80751000	1.05468500
C	-4.43760400	-2.84940200	2.69068200
H	-2.85011700	-2.76925200	4.13627200
H	-5.14992500	-1.53618700	-2.58959600
H	-6.14262600	-1.25115800	-1.13538400
H	-5.63304400	-2.90687400	-1.55785000
H	-5.14574000	-3.28133900	3.38996500
H	-0.47217500	-0.43810700	-1.55151300
C	0.43444600	-0.71743600	0.44622000
O	0.32221900	-0.31359100	1.59068300
N	1.67153900	-1.11585700	-0.03857800
S	1.80477100	-2.26331700	-1.30896500
C	2.82781100	-1.12127000	0.86626200
O	0.89884400	-3.37679500	-1.04749500
O	1.68262900	-1.57691400	-2.58873400
C	3.51150900	-2.72050400	-0.92389100
H	2.58299000	-1.76009400	1.72187800
C	3.31543500	0.27679500	1.31105700
C	4.02996800	-1.69485600	0.06850800
H	3.44411400	-3.72515300	-0.49989400
H	4.05057200	-2.75025800	-1.87394300
H	2.76507500	1.05906100	0.78450100
H	3.16939800	0.42998600	2.38250900
C	4.80131400	0.24281900	0.90805100
C	4.75205600	-0.42579800	-0.48844700
C	5.01810700	-2.18097300	1.14392600
C	5.49632900	-0.83647000	1.77487000
H	5.28436000	1.22343400	0.93689100
C	3.98035300	0.36408300	-1.54990900
C	6.13328800	-0.72474400	-1.08396400
H	5.84270100	-2.73978100	0.69610400
H	4.52662700	-2.84075500	1.86347600
H	6.58391900	-0.74650900	1.73674400
H	5.19965600	-0.75030400	2.82349700
H	4.48610100	1.32054500	-1.71951400
H	2.94388400	0.57670300	-1.28839100
H	3.97459700	-0.18101700	-2.49963200
H	6.58423700	0.20876000	-1.43369100
H	6.04321000	-1.38580600	-1.95316800
H	6.82995400	-1.18517400	-0.38322200

**Precomplex4a-C4si-C5re****E=-2368.979023**

N	3.32481600	-0.12518100	-0.89599200
C	2.84499300	-1.40117200	-0.56919800
C	2.93036900	-1.97671900	0.74618600
O	2.07249500	-2.28427300	-2.70973300
O	3.36957300	-1.49733400	1.79605800
C	2.27457700	-2.35460500	-1.50007500
C	0.36581500	-0.27653500	1.19322200
C	1.96683100	-3.58177900	-0.68042800
C	3.89853000	0.65597300	-0.02594000
H	3.94172500	0.26981800	0.98815300
C	3.13540700	0.29657900	-2.31653300
H	2.10237200	0.05421800	-2.56386900
H	3.77263700	-0.35714600	-2.91609700
C	4.54511400	1.95924500	-0.36288700
H	3.91863500	2.76742400	0.03972400
H	5.48681800	2.00432700	0.19350900
C	2.34543600	-3.35676300	0.63884500
C	3.44245100	1.76455300	-2.54649400
H	3.48480000	1.92683900	-3.62635600
H	2.62595400	2.38037500	-2.15342800
C	1.40347800	-4.77954500	-1.07335600
H	1.11251100	-4.94661100	-2.10562300
C	4.74419700	2.15303700	-1.86015800
H	5.01073300	3.19018100	-2.07282700
H	5.56331900	1.51862700	-2.21632800
C	1.22019100	-5.76469100	-0.09240800
H	0.77935300	-6.71830400	-0.36456100
C	2.16943700	-4.31736000	1.61626800
H	2.46830500	-4.12945700	2.64274700
C	1.59563700	-5.53716300	1.23130500
H	1.44212900	-6.31645100	1.97075500
C	0.85645600	0.95066600	1.00363300
C	0.64528200	1.92445900	-0.06757900
C	1.70808100	1.64065600	2.04076600
C	1.27592400	3.11547100	0.33913400
C	0.01754900	1.85683600	-1.30354200
N	1.88912600	2.93038500	1.58390000
O	2.12103600	1.19115000	3.09210200
C	1.26331500	4.25559800	-0.44934800
H	-0.42693700	0.92800200	-1.64950000
C	-0.01456500	3.00199700	-2.10580400
C	2.59433900	3.95542900	2.32169700
H	1.74898000	5.17125000	-0.12990000
C	0.59411900	4.18121400	-1.67693000
H	-0.50902100	2.96843200	-3.07012500
H	2.94091000	3.50723600	3.25226000
H	1.92806500	4.79296400	2.54355900
H	3.45441900	4.32230400	1.75348600

H	0.56324500	5.05994100	-2.31232900
H	0.66517500	-0.85400700	2.06446200
C	-0.66801100	-0.85797500	0.27720000
O	-0.44072700	-1.67768500	-0.59004500
N	-1.95235000	-0.36337900	0.45420500
S	-2.43476700	0.42371900	1.90781600
C	-3.06796100	-0.99875600	-0.26480700
O	-1.90889200	-0.32232800	3.04630700
O	-2.13030600	1.84502900	1.82558100
C	-4.19517000	0.09564900	1.67496200
H	-3.05281000	-2.06377500	-0.00986900
C	-3.10908900	-0.79312900	-1.79864200
C	-4.38007500	-0.33093300	0.23038800
H	-4.43134400	-0.70236200	2.38302700
H	-4.72372000	1.01087500	1.95221200
H	-2.35112700	-0.07577800	-2.12010400
H	-2.92663100	-1.73002600	-2.32793100
C	-4.53476300	-0.24909100	-2.01053700
C	-4.67393500	0.76358900	-0.84662900
C	-5.48155200	-1.36738000	-0.05589000
C	-5.52898900	-1.36768900	-1.61397400
H	-4.70402200	0.16546900	-3.00740500
C	-3.68033000	1.92890500	-0.90585600
C	-6.07175800	1.38082300	-0.72312600
H	-6.43285000	-1.05871800	0.38309300
H	-5.22606700	-2.34270800	0.36608600
H	-6.53627900	-1.15876100	-1.98001200
H	-5.22520200	-2.33119700	-2.03158000
H	-3.83932700	2.48689700	-1.83474400
H	-2.63266100	1.63138600	-0.86702200
H	-3.84834300	2.61727900	-0.07172300
H	-6.18026500	1.89936400	0.23596700
H	-6.88477600	0.65961000	-0.80907500
H	-6.20698300	2.12739100	-1.51141900

### Precomplex3c-C4si-C5re

E= -2329.693076

S	3.18748300	1.39570900	0.83208800
O	1.14340000	-1.14538500	-1.20670100
N	2.70800700	0.05682100	-0.11844500
N	-1.80693000	2.25042000	-1.12813700
C	-2.83033800	1.32043000	-1.03963700
C	-1.53048000	-1.43330700	0.65647200
C	-2.86211900	0.10633700	-1.81528000
N	-2.76681700	-0.09936600	2.08157600
C	-2.68570900	-1.35271300	1.46506400
O	-4.35525200	2.32539300	0.56506000
O	-1.49825800	1.83504800	2.06892600
C	1.38677800	-0.30217500	-0.35922300
C	0.35789100	0.36862300	0.46525400

H	0.56832300	1.36018100	0.86033100
O	-2.05583800	-0.30496500	-2.64923100
C	-1.70470500	0.68521500	1.71918300
C	-3.82737400	0.32900200	2.96667400
H	-3.66618000	1.38444900	3.18097100
H	-3.80929900	-0.24905100	3.89461700
C	-4.01299900	1.44281400	-0.21937600
C	3.78710000	-0.49180600	-0.95431700
H	3.66204700	-0.08213600	-1.96250000
C	-0.82642900	-0.16084800	0.81566700
C	-4.80721400	0.18919400	-0.48524200
O	2.55462300	2.61017100	0.31973300
C	-0.69002200	2.11293000	-1.77704800
H	-0.50539700	1.19965700	-2.32972900
C	-1.29163500	-2.59137300	-0.07899400
H	-0.42474400	-2.65262700	-0.72409800
C	-2.19315300	-3.65217700	0.02435300
H	-2.01914600	-4.55871300	-0.54482200
C	-1.90849200	3.59392400	-0.47953400
H	-2.33475600	3.46903500	0.51141800
H	-2.58417100	4.19197900	-1.09764000
C	0.16394000	3.33286100	-1.69487400
H	1.21558200	3.08521700	-1.53991900
H	0.08211100	3.89385600	-2.63506700
O	2.98726000	1.08722300	2.24181100
C	-4.12586000	-0.60060500	-1.41216500
C	4.91976400	1.32494800	0.33236300
H	5.04899700	2.16097400	-0.35924000
H	5.51362300	1.49065000	1.23461000
C	-3.58581600	-2.39853900	1.57770700
H	-4.47191700	-2.31510600	2.19740100
C	-3.31913000	-3.55546400	0.84227100
H	-4.01258200	-4.38838600	0.90103100
C	3.92310200	-2.03558900	-0.98874100
H	3.68629000	-2.42730700	-1.97954700
H	3.24303900	-2.50505700	-0.27657800
C	5.13068700	-0.02422900	-0.32889300
C	-0.46140900	4.08261400	-0.50697000
H	-0.39815600	5.16610600	-0.60335700
H	0.04207400	3.77947300	0.41530800
C	-6.00908700	-0.22043700	0.06055600
H	-6.54162000	0.40632900	0.76992900
C	5.57140000	-1.23126600	0.56247300
C	6.14692400	-0.08649500	-1.48317900
H	5.78203800	0.45525200	-2.35946400
H	7.09894800	0.36307700	-1.19290400
C	6.27225700	-1.62195800	-1.72125500
H	5.90752000	-1.91287100	-2.70984900
H	7.31109300	-1.95047000	-1.64899200
C	5.39974600	-2.23825100	-0.60094800
H	5.65191200	-3.27355000	-0.35815200
C	-6.51460800	-1.46654000	-0.33670800
H	-7.45402600	-1.82086000	0.07519000

C	-4.61598300	-1.82697800	-1.81420700
H	-4.07120400	-2.43791500	-2.52699800
C	-5.82793400	-2.25758100	-1.25684200
H	-6.23976800	-3.21971100	-1.54421700
C	4.69167300	-1.52511000	1.78330400
H	4.97734000	-2.49684400	2.19866900
H	3.62240500	-1.54923700	1.57435500
H	4.85270300	-0.77229300	2.56113800
C	7.01058300	-1.11206000	1.07723900
H	7.11392100	-0.24337100	1.73695500
H	7.75815400	-1.02552700	0.28854400
H	7.25595600	-1.99848100	1.66968000
H	-4.79622800	0.20656300	2.47688600

### Precomplex4c-C4si-C5re

**-2329.694194**

S	1.86675200	-0.24528100	1.83639400
O	-0.27424400	-1.24857800	-1.21616300
N	1.31541900	-0.81426700	0.31538400
N	-2.10900300	1.78398300	-1.04998200
C	-0.78110400	2.08583800	-0.78454900
C	-3.22629400	-1.56206400	-0.07894800
C	-0.35944000	2.87743400	0.34557000
N	-4.52581900	-0.65949600	1.60621200
C	-4.53496300	-1.42462200	0.43524800
O	0.36475100	1.26463000	-2.76528000
O	-2.92135800	0.41118400	2.87594000
C	-0.01329900	-0.89435500	-0.07689100
C	-1.03976000	-0.52640000	0.92375600
H	-0.74732600	0.07286600	1.78210100
O	-1.02809700	3.29047800	1.29144800
C	-3.24944100	-0.26673300	1.91943400
C	-5.69398000	-0.32929800	2.39316400
H	-5.35716200	0.25889700	3.24590900
H	-6.18668800	-1.23864000	2.74642500
C	0.31850600	1.86350400	-1.69415300
C	2.38257700	-0.98128500	-0.68868800
H	2.29181300	-0.14181300	-1.38632100
C	-2.34611500	-0.82302400	0.83227000
C	1.50503100	2.53770800	-1.05338800
O	1.26512200	1.04760200	2.14247700
C	-3.13359500	2.04425700	-0.29770600
H	-2.97856300	2.52689000	0.66007500
C	-3.03029600	-2.31443600	-1.23572800
H	-2.03522100	-2.43571600	-1.64100900
C	-4.13608000	-2.88889700	-1.86678600
H	-3.99143800	-3.47102800	-2.76993700
C	-2.48732800	1.08482500	-2.31227200
H	-1.96360700	0.12655100	-2.31156200
H	-2.11538900	1.68045200	-3.14557300

C	-4.43092800	1.68999300	-0.93610200
H	-5.04193600	1.06551100	-0.27745900
H	-5.00453900	2.60592700	-1.11640000
O	1.70429100	-1.29536400	2.83443600
C	1.10836400	3.14209500	0.13643800
C	3.57196200	-0.05106700	1.29021500
H	3.66749500	1.01414100	1.05043600
H	4.21018800	-0.30660100	2.13973500
C	-5.64158200	-1.97827600	-0.18732300
H	-6.63957600	-1.84946800	0.21680100
C	-5.42121200	-2.71511500	-1.35457000
H	-6.26855000	-3.16061400	-1.86521700
C	2.44193000	-2.32445300	-1.45847700
H	2.18073300	-2.18165300	-2.50867000
H	1.74537400	-3.05230200	-1.03997300
C	3.73893200	-0.93461900	0.06824600
C	-4.01867600	0.97532700	-2.24183600
H	-4.47825700	1.44630600	-3.11039200
H	-4.32632700	-0.07161100	-2.22257600
C	2.80855300	2.62454400	-1.50824700
H	3.09754200	2.16928700	-2.45147000
C	4.12567100	-2.44220800	0.24820600
C	4.76391900	-0.47197000	-0.98307100
H	4.43903000	0.45034700	-1.46891100
H	5.73481700	-0.27431200	-0.52330400
C	4.80902500	-1.69204200	-1.95096300
H	4.42532500	-1.43949000	-2.94320200
H	5.82971700	-2.05781400	-2.08105000
C	3.91081400	-2.74297800	-1.25518000
H	4.11920100	-3.77406200	-1.55215900
C	3.73002100	3.32538300	-0.71860400
H	4.76233300	3.41051200	-1.04270600
C	2.00656700	3.83803300	0.92303300
H	1.69130900	4.29547100	1.85523300
C	3.33322600	3.92142700	0.48060300
H	4.06472300	4.45992300	1.07432400
C	3.23557300	-3.28415800	1.16967100
H	3.45632700	-4.34227800	0.99378500
H	2.16602400	-3.13320800	1.02579700
H	3.45239200	-3.06656500	2.21893500
C	5.56792300	-2.64625600	0.72741800
H	5.71158600	-2.19824700	1.71698600
H	6.32178300	-2.23179900	0.05778600
H	5.76683400	-3.71763900	0.82554000
H	-6.40291200	0.25845700	1.80281600

**Precomplex4c-C4re-C5si**

**E=2329.697515**

N	-2.12419600	1.96170200	-1.32316500
C	-0.96569000	2.17260300	-0.59123800
C	-0.94642300	2.24536500	0.84786000
O	0.71064400	2.55067900	-2.31027600
O	-1.86454000	2.05067300	1.64242300
C	0.32364500	2.51371000	-1.14459000
C	1.18749100	2.84690100	0.04725300
C	-3.32991700	1.84378300	-0.85644700
H	-3.49111700	1.90464100	0.21357600
C	-2.06803400	1.80844000	-2.80458900
H	-1.50410100	0.89515800	-3.00642200
H	-1.51661800	2.65295600	-3.21303400
C	-4.35662300	1.69398600	-1.92409700
H	-4.91413900	0.76129500	-1.79828200
H	-5.08371100	2.50890400	-1.85134100
C	0.45590800	2.64877700	1.21779500
C	2.49177200	3.30583900	0.08190300
H	3.04522100	3.47403300	-0.83638400
C	-3.53965800	1.72954500	-3.23353700
H	-3.71448500	0.83108800	-3.82310600
H	-3.80797400	2.59863700	-3.83426700
C	3.06674400	3.54199200	1.33768200
H	4.08840500	3.90231000	1.40230200
C	1.01599500	2.86796900	2.46233600
H	0.44069400	2.70323800	3.36781200
C	2.34277000	3.31659700	2.50955500
H	2.81334100	3.50086000	3.46988300
S	1.46200500	-2.20134900	-1.38889200
O	0.22380100	-0.49222700	1.78469500
N	1.42035800	-1.20282900	0.00488100
C	-2.96008800	-1.09334400	1.42514700
N	-4.47193300	-1.41788100	-0.29144600
C	-4.30384300	-1.37507500	1.09982700
O	-3.11384200	-1.12610200	-2.13805300
C	0.22377700	-0.82904700	0.61344400
C	-0.97057200	-0.86471500	-0.25777700
H	-0.81323900	-0.86825000	-1.33473200
C	-3.28581200	-1.17355300	-0.92977300
C	-5.71642900	-1.71679700	-0.96619900
H	-5.52263900	-1.69234400	-2.03867600
H	-6.47894700	-0.97470200	-0.71355000
C	2.62785900	-1.33451600	0.83354800
H	2.42005700	-2.07858000	1.61064500
C	-2.24304300	-0.98336300	0.15306600
O	0.56827400	-3.33989200	-1.19959600
C	-2.59382600	-0.97439200	2.76205700
H	-1.57417100	-0.72144100	3.01890800
C	-3.56635400	-1.16546700	3.74639600
H	-3.29223000	-1.07679500	4.79181000
O	1.25664700	-1.37251200	-2.57161200
C	3.18592400	-2.70034000	-1.17929100



H	3.13957200	-3.75135300	-0.88455700
H	3.66144600	-2.60627800	-2.15864100
C	-5.27855900	-1.56326600	2.06419300
H	-6.30612500	-1.78143300	1.79504200
C	-4.88495900	-1.45770500	3.40180300
H	-5.62565200	-1.59907100	4.18206600
C	3.16873400	-0.01573200	1.43179100
H	3.10167600	-0.01700300	2.52181500
H	2.59125300	0.83422800	1.06678200
C	3.77290000	-1.80888400	-0.10017700
C	4.47372700	-0.48334300	-0.53927600
C	4.81909800	-2.43141100	0.84261800
H	4.36137700	-3.16706300	1.50896900
H	5.60177400	-2.94321200	0.27848700
C	5.36417000	-1.17943500	1.59693300
H	5.14823800	-1.22221500	2.66763000
H	6.44710800	-1.09197100	1.48694900
C	4.62298100	0.00196200	0.92435100
H	5.11673300	0.97013600	1.04557800
C	3.64696700	0.43842900	-1.44095900
H	4.18239200	1.38497500	-1.56632500
H	2.64994900	0.66520400	-1.06423400
H	3.52882700	-0.00652400	-2.43459900
C	5.80772700	-0.71491100	-1.25974600
H	5.64576100	-1.23618600	-2.20984600
H	6.53291300	-1.28855400	-0.68247900
H	6.26260900	0.25176100	-1.49578400
H	-6.07391200	-2.71035700	-0.68344100

### Precomplex3c-C4re-C5si

**-2329.699006**

N	-1.23610900	-1.89702500	-1.35023100
C	-2.41197200	-1.15333500	-1.33726700
C	-3.64516200	-1.62839300	-0.77222100
O	-1.76085600	0.89675400	-2.46814400
O	-3.88895800	-2.70369800	-0.21995900
C	-2.56563700	0.17203800	-1.88691600
C	-3.99695500	0.55098800	-1.60322400
C	-1.02928000	-3.03277600	-0.76140900
H	-1.82829700	-3.48906200	-0.19248900
C	-0.04729600	-1.43599700	-2.12521600
H	0.11287200	-0.37842900	-1.92083000
H	-0.29557100	-1.54524600	-3.18374100
C	0.34167400	-3.56257400	-0.99924200
H	0.80613600	-3.88384100	-0.06284500
H	0.28744900	-4.44028800	-1.65392100
C	-4.63585700	-0.51137400	-0.96260700
C	1.06879400	-2.36931900	-1.64764600
H	1.71853100	-2.67054700	-2.46939600
H	1.68312800	-1.87219000	-0.89451700

C	-4.65964900	1.72980300	-1.87833400
H	-4.14901500	2.55301500	-2.36801400
C	-6.00345800	1.82806700	-1.48932300
H	-6.55378800	2.74300800	-1.68404700
C	-5.96276000	-0.43026600	-0.58588900
H	-6.45801600	-1.26604900	-0.10038000
C	-6.64499500	0.76524100	-0.85567000
H	-7.68712400	0.86479200	-0.56972500
S	3.15599400	-0.73454400	1.68735400
O	1.04034200	1.84022000	-0.15981000
N	2.63012400	0.38089800	0.49655800
C	-1.90104700	1.28644300	1.05645400
N	-3.08312100	-0.46304700	1.99848700
C	-3.13685500	0.87801200	1.60688300
O	-1.49571800	-2.14144200	1.92939900
C	1.29711600	0.78280100	0.39157500
C	0.28685300	-0.15385100	0.91998300
H	0.59754100	-1.16775800	1.16751800
C	-1.85165800	-0.99305600	1.72738300
C	-4.17942900	-1.20927900	2.57584400
H	-3.84933000	-2.24127500	2.68433500
H	-5.04588700	-1.17794000	1.91112700
C	3.68216700	1.33396300	0.10883100
H	3.55648400	2.23329800	0.72157800
C	-1.00822700	0.13054700	1.14371600
O	2.59030500	-0.37062400	2.98195800
C	-1.77168700	2.58591500	0.56923700
H	-0.83986500	2.90383900	0.12268400
C	-2.86217100	3.45188900	0.65920600
H	-2.77239100	4.46421900	0.28099500
O	2.90985500	-2.08932400	1.20134200
C	4.89907100	-0.26969600	1.59178500
H	5.10819200	0.22819300	2.54142300
H	5.46843300	-1.19987300	1.52366200
C	-4.22456200	1.72872300	1.70537600
H	-5.16721000	1.39199100	2.12259300
C	-4.06686200	3.02861900	1.22099500
H	-4.90570400	3.71546200	1.27260100
C	3.75832400	1.68713300	-1.39711100
H	3.51359000	2.73729000	-1.56603500
H	3.05259800	1.08662400	-1.97488000
C	5.04738000	0.65215800	0.39417700
C	5.44617500	0.02094700	-0.97880100
C	6.05008700	1.81364100	0.52034300
H	5.69605200	2.56496600	1.23077500
H	7.01981100	1.45849100	0.87544000
C	6.12061700	2.34260300	-0.94463200
H	5.74769000	3.36668200	-1.02784200
H	7.14691200	2.33911900	-1.31754800
C	5.22588800	1.35563300	-1.73339100
H	5.43576700	1.32325300	-2.80533600
C	4.55829500	-1.12934100	-1.46096700
H	4.85111300	-1.40802900	-2.47820300

H	3.49696500	-0.88821400	-1.47249200
H	4.68796200	-2.01250900	-0.82601700
C	6.89118400	-0.48930700	-1.01526500
H	7.02144800	-1.32477500	-0.31841200
H	7.63615500	0.26863400	-0.77265600
H	7.11588400	-0.86622200	-2.01741700
H	-4.44908300	-0.79839400	3.55242500

### 3a-C4si-C5re

**E=-2369.031573**

S	2.39954000	1.18266500	1.47048100
O	0.92090500	1.50719200	-2.04355100
N	2.10379700	0.99354600	-0.20323600
N	-2.58755200	2.05838700	-0.07950300
C	-2.54640300	0.62412000	-0.09909400
C	-0.54418900	-1.03061000	-0.09912200
C	-2.79842400	-0.07353500	-1.45986000
N	-0.92079800	-1.23778700	2.15828000
C	-0.52607200	-1.90648500	0.99513200
O	-4.05124000	0.38768900	1.82939300
O	-1.24436700	0.96820300	2.74943800
C	0.93440900	1.39420600	-0.83146300
C	-0.29443400	1.62127900	0.03438500
H	-0.01008900	2.08181900	0.98507500
O	-2.46234400	0.34707800	-2.54515100
C	-1.08447100	0.10359500	1.91544900
C	-0.76371300	-1.77908300	3.49090700
H	-1.06430500	-1.00631700	4.19714500
H	0.28242100	-2.04858500	3.66685900
C	-3.60810200	-0.05694700	0.79652500
C	3.32958000	0.80075700	-0.99524100
H	3.59622200	1.77107800	-1.42752600
C	-1.06033600	0.30487200	0.38106600
C	-4.00629400	-1.32179300	0.13014200
O	2.14181000	2.56365200	1.86928800
C	-1.32194900	2.53113600	-0.64772700
H	-1.28819400	2.35396700	-1.73250300
C	-0.18663700	-1.49038300	-1.35817400
H	-0.19793800	-0.82169300	-2.21330800
C	0.18732900	-2.83111900	-1.50725900
H	0.47447400	-3.20151200	-2.48527900
C	-3.76114700	2.70025600	-0.66546500
H	-4.65705100	2.28644500	-0.19100100
H	-3.82537100	2.50310700	-1.74958000
C	-1.16048200	4.01932800	-0.37500900
H	-1.11327700	4.17428800	0.71029900
H	-0.22031200	4.37565500	-0.80935900
O	1.69260100	0.12886100	2.19014400
C	-3.54569200	-1.32639300	-1.18732900
C	4.17604900	0.88578500	1.35504700
H	4.63456700	1.86689800	1.49889600

H	4.43776900	0.22452500	2.18488300
C	-0.15958300	-3.23792100	0.86595800
H	-0.14833200	-3.90570400	1.72040800
C	0.19451100	-3.68811400	-0.40936300
H	0.48560500	-4.72525700	-0.54026100
C	3.28083200	-0.30382700	-2.07933000
H	2.35664100	-0.88058500	-2.00562200
H	3.33083900	0.12554100	-3.08168900
C	4.43652600	0.30625100	-0.02246900
C	-3.67313900	4.20585600	-0.41909000
H	-4.52883100	4.70068600	-0.88775700
H	-3.73353500	4.38635500	0.66014400
C	-4.74585000	-2.38428000	0.64131100
H	-5.10616200	-2.36825000	1.66432600
C	-2.35811000	4.77471600	-0.96018600
H	-2.28345200	5.84233900	-0.73457900
H	-2.34460100	4.67491500	-2.05347400
C	4.41787800	-1.24781200	-0.18490800
C	5.76064800	0.68653800	-0.70895500
H	6.61073000	0.51312600	-0.04555500
H	5.77285500	1.74299900	-0.98892300
C	5.77216100	-0.27294000	-1.93820500
H	6.68490100	-0.87178500	-1.96461900
H	5.71518300	0.27400600	-2.88306600
C	4.51609600	-1.15391900	-1.72714200
H	4.55230200	-2.11389200	-2.24843300
C	-4.99430800	-3.46073000	-0.20447200
H	-5.56003900	-4.31153900	0.15978600
C	-3.79965700	-2.39644500	-2.03954500
H	-3.43487400	-2.39038000	-3.06123300
C	-4.52615000	-3.46720500	-1.52811700
H	-4.73924100	-4.32327000	-2.15937400
C	3.16044200	-1.95687700	0.32888300
H	3.16311500	-2.99227900	-0.02766800
H	2.21947100	-1.50252700	0.01716400
H	3.15844100	-1.98469100	1.42386500
C	5.61589500	-1.94176700	0.47399000
H	5.60928500	-1.77661500	1.55728700
H	6.58396000	-1.61799600	0.09105500
H	5.54007000	-3.02110200	0.31176200
H	-1.39621000	-2.65988300	3.62126500

### 3a-C4re-C5si

**E=-2369.020783**

S	-2.54014800	-1.52567400	-1.20684900
O	-1.04669800	1.81202700	-0.15574700
N	-2.34801500	-0.00170300	-0.43756300
N	1.52132200	-1.24849500	1.51228200
C	2.36325800	-0.72760000	0.47536600
C	1.56315900	1.66535200	0.86348400

C	2.72414400	-1.68812600	-0.68705400
N	2.21571400	2.31897600	-1.24045900
C	2.03394400	2.73226500	0.08934500
O	4.01216000	0.22969800	2.01880700
O	1.89773700	0.37973800	-2.44732400
C	-1.10190400	0.60068600	-0.22626900
C	0.10850200	-0.30453900	-0.12979200
H	0.15565600	-0.84514300	-1.08331400
O	2.00219600	-2.55671700	-1.12340700
C	1.87390600	1.00982600	-1.40243900
C	2.66565500	3.17586000	-2.31575800
H	2.69642800	2.57570800	-3.22425300
H	3.66378500	3.56476800	-2.09863800
C	3.75190500	-0.24975000	0.94022500
C	-3.48610900	0.90198100	-0.69809100
H	-3.20902800	1.53913000	-1.54463700
C	1.45476200	0.45317100	-0.03181500
C	4.71085900	-0.54176300	-0.15609900
O	-1.63696700	-1.61439200	-2.35168700
C	0.15076200	-1.37304500	1.00267400
H	0.00856700	-2.35629300	0.52908800
C	1.34167500	1.84796700	2.21618900
H	1.02076200	1.01526300	2.83131000
C	1.56737400	3.11275500	2.77325200
H	1.39256900	3.27020200	3.83205000
C	1.93961500	-2.38230600	2.32023700
H	2.98107200	-2.23883900	2.62307300
H	1.87227400	-3.32845800	1.75476000
C	-0.80804300	-1.29322900	2.18419600
H	-0.71731600	-0.31730300	2.67674500
H	-1.83744000	-1.41294600	1.84101100
O	-2.46918200	-2.58818800	-0.21077000
C	4.12099200	-1.39289500	-1.09302300
C	-4.23416000	-1.22497000	-1.75702500
H	-4.15856100	-1.09159000	-2.83877200
H	-4.80101600	-2.13105400	-1.52964800
C	2.26828700	3.99041400	0.61850100
H	2.62892400	4.80652000	0.00175000
C	2.02000800	4.16635200	1.98389100
H	2.19039300	5.14014500	2.43117800
C	-3.96867100	1.74805100	0.50506400
H	-3.43799000	1.46532300	1.41696900
H	-3.79010200	2.81122600	0.33409800
C	-4.71557600	0.02384400	-1.04367000
C	1.02805800	-2.42563800	3.54884400
H	1.26223900	-3.30662800	4.15403000
H	1.23908800	-1.53800300	4.15662800
C	6.03145400	-0.12259500	-0.29099600
H	6.48370300	0.53095500	0.44723200
C	-0.45279200	-2.43344600	3.15042600
H	-1.08242400	-2.38366000	4.04352800
H	-0.68348100	-3.38440900	2.65133700
C	-5.46532500	-0.13027200	0.31874400

C	-5.65841600	0.95596000	-1.82750100
H	-6.49191800	0.39798500	-2.25959300
H	-5.13207900	1.44756900	-2.64961400
C	-6.12899200	1.94912800	-0.72190500
H	-7.21783300	1.96368400	-0.64024500
H	-5.80409300	2.97256900	-0.92626700
C	-5.46956000	1.39912400	0.56586500
H	-5.95954400	1.71835600	1.48906400
C	6.73928100	-0.56999200	-1.40181700
H	7.76892200	-0.25994900	-1.54423200
C	4.82882600	-1.85073000	-2.19968900
H	4.36237500	-2.51412700	-2.92001700
C	6.14518800	-1.42401400	-2.34452400
H	6.72789100	-1.75675800	-3.19684700
C	-4.73381000	-0.93588300	1.39590800
H	-5.28505500	-0.85614600	2.33813200
H	-3.71307700	-0.60163900	1.57511700
H	-4.69124500	-1.99593900	1.12523500
C	-6.86112100	-0.74792700	0.17669200
H	-6.78855900	-1.78104500	-0.18108600
H	-7.52114200	-0.20463600	-0.49970400
H	-7.34453400	-0.77853200	1.15768300
H	1.97421600	4.01161100	-2.45099900

#### 4a-C4si-C5re

E=-2369.028907

N	-3.08233200	-1.04628500	-0.25107700
C	-2.51052200	0.26461200	-0.05974300
C	-3.16337000	1.18036100	1.00584100
O	-2.82641900	0.68672800	-2.46153700
O	-3.53542900	0.81555800	2.09939200
C	-2.68126100	1.11924800	-1.34339900
C	-1.05253400	-0.00762500	0.46262900
C	-2.88956300	2.52737600	-0.90892900
C	-2.37683800	-1.99907400	0.58962400
H	-2.61928600	-1.85315600	1.65846200
C	-4.53659400	-1.15855600	-0.21045900
H	-4.95917500	-0.42005400	-0.90068500
H	-4.92514800	-0.94152600	0.79873800
C	-2.72313600	-3.42672200	0.19393100
H	-2.36814300	-3.60950800	-0.82635800
H	-2.21306500	-4.12889000	0.86269300
C	-3.20865300	2.55488800	0.45072900
C	-4.94138500	-2.57155000	-0.62451900
H	-6.02822500	-2.67211700	-0.55338600
H	-4.65865700	-2.72589100	-1.67221200
C	-2.87681400	3.69224700	-1.66851700
H	-2.63962700	3.66178700	-2.72653500
C	-4.24261900	-3.61321300	0.25301200
H	-4.51177400	-4.62442400	-0.06476000

H	-4.58286900	-3.49929200	1.29056800
C	-3.17216200	4.88858700	-1.02144200
H	-3.16244700	5.81823100	-1.58048100
C	-3.51942400	3.74791000	1.09853800
H	-3.77181500	3.75578700	2.15352900
C	-3.49089000	4.91663500	0.34541500
H	-3.72169800	5.86648400	0.81561000
C	-0.91035200	-1.56242600	0.41003100
C	-0.18846000	-2.08473600	-0.80175800
C	-0.08285000	-2.13245900	1.57194100
C	0.92090400	-2.81948400	-0.36405900
C	-0.42907800	-1.91727200	-2.15504100
N	0.96668000	-2.82988700	1.03757300
O	-0.36000800	-2.02992200	2.75164200
C	1.80666900	-3.41125700	-1.25240800
H	-1.28318500	-1.33071200	-2.48426800
C	0.45340600	-2.51006000	-3.06728500
C	1.95677700	-3.51969900	1.83336700
H	2.66349600	-3.97908300	-0.90533200
C	1.55047400	-3.24323100	-2.61804100
H	0.28365800	-2.39531100	-4.13228400
H	1.77204600	-3.26230400	2.87563100
H	2.96068700	-3.19254100	1.55136000
H	1.87680200	-4.60207200	1.69880100
H	2.22518500	-3.69370900	-3.33880100
H	-0.99985600	0.27930500	1.51936600
C	0.03478100	0.69756900	-0.32977100
O	-0.14684400	1.12267800	-1.45328100
N	1.32270800	0.74285200	0.20344400
S	1.64781900	1.00561400	1.87455000
C	2.34527600	1.35694300	-0.66792400
O	0.59903400	1.86242600	2.42116500
O	1.90506600	-0.26396800	2.53533700
C	3.18572700	1.91188800	1.59781600
H	1.93226800	2.30450600	-1.02677100
C	2.83487600	0.47516600	-1.83960200
C	3.61910900	1.60255000	0.17681300
H	2.93009300	2.96568800	1.73446700
H	3.87961600	1.58762800	2.37679700
H	2.43357400	-0.53966400	-1.75355700
H	2.51731300	0.88147000	-2.80209900
C	4.36457200	0.52172500	-1.64803100
C	4.51247700	0.35258100	-0.11437700
C	4.37536100	2.71504100	-0.57368000
C	4.82233100	1.98320900	-1.87552200
H	4.90724600	-0.21448200	-2.24637200
C	3.98980100	-0.98792800	0.41002600
C	5.95122500	0.49646500	0.39473300
H	5.22698900	3.07192900	0.00961900
H	3.72598200	3.57304300	-0.76558400
H	5.90329600	2.04890000	-2.01549200
H	4.35260300	2.41039100	-2.76538200
H	4.54937900	-1.79913800	-0.06959500

H	2.92802500	-1.15497800	0.22547100
H	4.14814000	-1.06326800	1.49046500
H	5.96408200	0.59385500	1.48602400
H	6.48827900	1.34730300	-0.02496400
H	6.51494000	-0.40703500	0.14354900

#### 4a-C4re-C5si

#### E=-2369.030013

N	-2.54196300	1.76179700	-0.80711900
C	-1.19807500	1.73263900	-0.29113400
C	-0.95835900	2.38277100	1.09393900
O	-0.12749000	2.41683700	-2.38300500
O	-1.74836500	2.42005400	2.01122700
C	-0.14399400	2.43354300	-1.17468000
C	-0.90077100	0.20151600	-0.32225400
C	0.84812700	3.06375800	-0.26921800
C	-3.28099900	0.71065400	-0.10322200
H	-3.47004600	1.01364100	0.93998500
C	-3.23232200	3.04984500	-0.80579500
H	-2.61554100	3.77429900	-1.34836400
H	-3.37667800	3.42482600	0.22168800
C	-4.62224700	0.46665500	-0.78050000
H	-4.44710500	0.11284400	-1.80181300
H	-5.17259500	-0.30940800	-0.23658700
C	0.37770900	3.03688800	1.04547500
C	-4.58944300	2.88393700	-1.48758900
H	-5.12707000	3.83612700	-1.45909900
H	-4.42399300	2.62546700	-2.53957500
C	2.09085700	3.60958100	-0.58400200
H	2.44383200	3.62769100	-1.60989100
C	-5.40965100	1.78113800	-0.81189400
H	-6.36109600	1.64058600	-1.33253200
H	-5.64639900	2.08520300	0.21612800
C	2.85757600	4.11270700	0.46234100
H	3.83501700	4.53671300	0.25870400
C	1.13669000	3.54957100	2.09246500
H	0.76567200	3.52072600	3.11132700
C	2.38539500	4.08212800	1.78458200
H	3.00898000	4.48194900	2.57710600
C	-2.27654100	-0.47896200	-0.04072400
C	-2.44390900	-1.31701100	1.19972400
C	-2.52391700	-1.50963300	-1.16406900
C	-2.80114100	-2.61453100	0.81346100
C	-2.36543200	-0.98931400	2.54251100
N	-2.87060900	-2.69725300	-0.58258200
O	-2.42191900	-1.30249500	-2.35951200
C	-3.05394900	-3.61564900	1.73918300
H	-2.09651700	0.01965600	2.84123100
C	-2.61811800	-1.98526300	3.49317300
C	-3.04846700	-3.92538400	-1.32377200



H	-3.32564500	-4.61889300	1.42919800
C	-2.95131400	-3.27747600	3.09228900
H	-2.55241600	-1.74950600	4.54969500
H	-3.00491600	-3.67709900	-2.38351900
H	-4.01587200	-4.37776200	-1.09261100
H	-2.24813800	-4.63047900	-1.08100800
H	-3.14145900	-4.03899900	3.84164300
H	-0.66158000	-0.00585700	-1.36981600
C	0.25670600	-0.16581200	0.58489200
O	0.30390100	0.15026200	1.75938300
N	1.35377500	-0.76273100	-0.00811900
S	1.20887300	-1.81622300	-1.35484000
C	2.54785500	-1.02339200	0.80564300
O	0.12243700	-2.75222400	-1.07734000
O	1.14340700	-1.03937300	-2.58536600
C	2.83352000	-2.57372500	-1.12371800
H	2.26081300	-1.68494200	1.62980100
C	3.28302900	0.24244500	1.31191300
C	3.58172600	-1.70270400	-0.12827600
H	2.63157000	-3.57577300	-0.73735300
H	3.29180100	-2.63736000	-2.11342300
H	2.82078200	1.14788000	0.90776500
H	3.25006300	0.31179000	2.40100800
C	4.70902500	0.02341600	0.76941400
C	4.44210500	-0.50898800	-0.66101500
C	4.56548100	-2.41393700	0.81883300
C	5.29873000	-1.21282600	1.48992600
H	5.33990700	0.91457900	0.82040700
C	3.72948100	0.49378000	-1.57715900
C	5.70427400	-0.95950500	-1.40598900
H	5.25224900	-3.05563600	0.26279900
H	4.03400100	-3.04548900	1.53530700
H	6.37952900	-1.28105900	1.35042900
H	5.11167000	-1.16989700	2.56598200
H	4.37518900	1.36837600	-1.71048900
H	2.76746300	0.84391200	-1.20240500
H	3.55465900	0.05605400	-2.56486700
H	5.43745600	-1.50709600	-2.31666100
H	6.36656700	-1.59287100	-0.81563800
H	6.27586800	-0.07895900	-1.71398900

### 3c-C4si-C5re

**E=-2329.725331**

S	2.38975000	1.52983000	0.96100600
O	0.90156700	0.72424100	-2.46801100
N	2.07349300	0.79687600	-0.54987900
N	-2.57351200	2.18876700	-1.00517500
C	-2.59958600	0.84362200	-0.49795100
C	-0.74040500	-0.89647200	0.14359000
C	-2.80776000	-0.15776000	-1.66405800

N	-1.11086700	-0.31662000	2.33551600
C	-0.77083100	-1.35876000	1.46740100
O	-4.11961300	1.05254800	1.44178800
O	-1.33889100	1.96922600	2.15675600
C	0.92440500	1.03414800	-1.29141100
C	-0.26966900	1.62675800	-0.56369300
H	0.07266100	2.31835200	0.21006600
O	-2.31648400	-0.06879800	-2.76549900
C	-1.20963100	0.86877400	1.65714100
C	-1.00095200	-0.39408200	3.77568400
H	-1.25792300	0.58496400	4.17786100
H	0.02414100	-0.64986100	4.06131600
C	-3.73366400	0.43621800	0.47452600
C	3.27926600	0.26807300	-1.20626300
H	3.61566500	1.01707900	-1.93119700
C	-1.14852500	0.55836400	0.14600000
C	-4.25408600	-0.88295800	0.03866400
O	2.24996100	2.98015800	0.85068200
C	-1.21253600	2.41287300	-1.51697700
H	-1.10802600	2.00611900	-2.52325800
C	-0.41737200	-1.77447900	-0.88153400
H	-0.38093700	-1.43204900	-1.91079000
C	-0.13151200	-3.10870600	-0.56701100
H	0.12654800	-3.80137400	-1.36068900
C	-2.97785600	3.34410900	-0.15761100
H	-3.23520600	3.03117400	0.85213300
H	-3.85733300	3.81332000	-0.61283300
C	-1.02071500	3.92470100	-1.44760500
H	0.03671200	4.20233100	-1.42463600
H	-1.47911300	4.39398500	-2.32323100
O	1.59879600	0.85320700	1.98368900
C	-3.72100800	-1.22864600	-1.19939100
C	4.13587000	1.07320400	1.00135100
H	4.67423800	2.00770700	0.82722400
H	4.34031500	0.70533100	2.01001300
C	-0.49008300	-2.67572500	1.79803700
H	-0.51487500	-3.01627300	2.82741600
C	-0.17199100	-3.54868200	0.75333100
H	0.05263800	-4.58554300	0.98141400
C	3.14600100	-1.12944300	-1.86005700
H	3.22851200	-1.06573500	-2.94672300
H	2.18006200	-1.57886000	-1.62147400
C	4.34902800	0.05064500	-0.09914100
C	-1.77725600	4.29981600	-0.16834000
H	-2.08246600	5.34785000	-0.14811000
H	-1.15447800	4.10792700	0.71013800
C	-5.15481200	-1.71461100	0.69801000
H	-5.56812100	-1.43283500	1.66045400
C	4.21128200	-1.46179800	0.26799000
C	5.69616400	0.08120700	-0.84260200
H	5.78732800	0.97805100	-1.46061200
H	6.53239400	0.08019800	-0.14007300
C	5.63200400	-1.23401000	-1.67781600

H	5.61508800	-1.03425500	-2.75250300
H	6.49646400	-1.87118700	-1.47988700
C	4.31275000	-1.89938400	-1.21370600
H	4.27441200	-2.97865800	-1.38208800
C	-5.49542300	-2.91159600	0.07624200
H	-6.19062900	-3.58985200	0.55916500
C	-4.06120800	-2.42139100	-1.82934300
H	-3.63783800	-2.67996000	-2.79405300
C	-4.95462100	-3.26112500	-1.17168800
H	-5.24281100	-4.20254900	-1.62699400
C	2.90458800	-1.85999200	0.96182600
H	2.82781000	-2.95211400	0.98230900
H	2.00087700	-1.47372700	0.48947700
H	2.90224700	-1.50965300	1.99984900
C	5.35441200	-1.97989900	1.14872600
H	5.36378700	-1.46059900	2.11358800
H	6.34327100	-1.87530500	0.70169000
H	5.19553600	-3.04243400	1.35567100
H	-1.68906600	-1.14459400	4.17088600

### 3c-C4re-C5si

**E=-2329.672668**

N	-1.76023900	2.65935400	-0.03024200
C	-2.42171200	1.39108000	-0.05424400
C	-3.37785100	1.27869900	-1.27085500
O	-3.29367200	1.37027000	2.25276900
O	-3.31054100	1.91188700	-2.29494200
C	-3.37814200	1.02711700	1.09751800
C	-4.43668600	0.16561900	0.50588800
C	-0.58652500	2.51691900	-0.89101900
H	-0.91351400	2.55451900	-1.93287100
C	-1.30349600	3.22037700	1.25518200
H	-0.89186900	2.45611200	1.92053400
H	-2.13994200	3.70120000	1.76605900
C	0.31310600	3.70723200	-0.53331500
H	1.36806200	3.42799400	-0.49963100
H	0.20746800	4.48111900	-1.29647000
C	-4.43991700	0.31053400	-0.88175100
C	-0.20869900	4.20989700	0.83467500
H	-0.62474000	5.21522000	0.73044100
H	0.58315700	4.24653500	1.58474400
C	-5.33893600	-0.67584800	1.14861800
H	-5.33062800	-0.77934900	2.22887100
C	-6.23575100	-1.38359200	0.35312500
H	-6.94718300	-2.05975800	0.81572500
C	-5.34474400	-0.38035300	-1.67971100
H	-5.34032800	-0.25993900	-2.75814600
C	-6.23882400	-1.23743200	-1.04294600
H	-6.95271900	-1.80382800	-1.63200500
S	2.05506000	-1.12732800	-1.26835100

O	1.26022200	1.62205300	1.26971700
N	2.20466900	0.14356500	-0.12989700
C	-1.15191700	-0.62749200	1.07341500
N	-2.00110700	-1.96713400	-0.59085700
C	-1.65323800	-1.90114400	0.76017000
O	-1.70771700	-0.62307400	-2.43519300
C	1.15464200	0.97134500	0.24552900
C	-0.04100900	1.05597400	-0.68287600
H	0.23490600	0.66800000	-1.66609100
C	-1.66442000	-0.81271600	-1.23307400
C	-2.38959800	-3.17717000	-1.27909500
H	-2.56963400	-2.91962300	-2.32264300
H	-3.30449100	-3.58275500	-0.83913200
C	3.33963300	-0.03330100	0.78971600
H	2.94986400	-0.48534600	1.70874800
C	-1.26254100	0.23616700	-0.17020900
O	0.89028700	-1.93952000	-0.92648000
C	-0.75152000	-0.36668300	2.37607700
H	-0.36789100	0.60693700	2.65607300
C	-0.83648600	-1.38236600	3.33528300
H	-0.51589000	-1.18234300	4.35212600
O	2.12309000	-0.58405600	-2.61950800
C	3.58696200	-1.95286300	-0.78600500
H	3.27161100	-2.84841600	-0.24425000
H	4.09681600	-2.23599600	-1.71071000
C	-1.75397300	-2.91815500	1.69647900
H	-2.14014300	-3.89552300	1.42671900
C	-1.33335400	-2.63857000	2.99900600
H	-1.39775800	-3.41425700	3.75549300
C	4.17534000	1.23560200	1.09339600
H	4.07991400	1.52694000	2.14152300
H	3.84216600	2.07852400	0.48400600
C	4.35297400	-0.97707600	0.08856500
C	5.36660500	0.00054600	-0.59107400
C	5.19496900	-1.57458400	1.23059800
H	4.55698100	-2.00240700	2.00877300
H	5.84444300	-2.37318200	0.86401600
C	6.00705800	-0.33662000	1.71834900
H	5.75549800	-0.06231900	2.74673300
H	7.08177300	-0.53033900	1.68763600
C	5.60066100	0.78001100	0.72652300
H	6.32092000	1.59965800	0.65820400
C	4.81531300	0.85616800	-1.73795200
H	5.55393700	1.62388200	-1.99309500
H	3.87256200	1.35700400	-1.51501700
H	4.65452800	0.24271600	-2.63076100
C	6.61767600	-0.70198800	-1.13154300
H	6.35200300	-1.39995300	-1.93427500
H	7.17658700	-1.25671200	-0.37660400
H	7.29371600	0.04380600	-1.56211100
H	-1.59138400	-3.92386600	-1.21758800

**4c-C4si-C5re****E=-2329.717411**

S	-0.97055300	-1.34546100	1.54442600
O	0.23342200	-0.51669600	-1.99589500
N	-0.91907300	-1.00885500	-0.13287000
N	2.94007200	1.60527800	-1.02830900
C	2.68025500	0.26755300	-0.56829000
C	-0.38854000	2.31368500	-0.26556200
C	3.60189500	-0.15083000	0.60883100
N	-0.42789300	2.75740900	1.99152200
C	-1.10601400	2.91788800	0.78090000
O	2.98728900	-0.85349800	-2.75272100
O	1.43918500	1.60823200	2.70203900
C	0.17347400	-0.46027000	-0.78137900
C	1.21946600	0.24314100	0.07083500
H	1.28186400	-0.24960000	1.04490700
O	4.14407600	0.58815900	1.39322700
C	0.69266200	1.99403600	1.82216900
C	-0.99169900	3.06473200	3.28681700
H	-0.26488100	2.76431400	4.04050800
H	-1.92184700	2.50663600	3.43240200
C	2.95419600	-0.89517400	-1.54755400
C	-1.93206600	-1.74745800	-0.90692400
H	-1.44319700	-2.63620800	-1.32037400
C	0.89040100	1.74764000	0.31458500
C	3.30768400	-2.07290100	-0.70533300
O	0.18559100	-2.15716600	1.91608500
C	2.24373000	2.48384100	-0.09214200
H	2.82680600	2.55458300	0.82895700
C	-0.90817500	2.36653900	-1.55117600
H	-0.39293000	1.89504800	-2.38091400
C	-2.13012300	3.01537700	-1.77323400
H	-2.53975300	3.05007000	-2.77688900
C	2.45673800	1.94966000	-2.38592700
H	1.56466900	1.36810600	-2.64699000
H	3.22366100	1.70335200	-3.12126900
C	2.11298500	3.81949600	-0.81745100
H	1.19752800	4.34507500	-0.53621300
H	2.95686100	4.45738500	-0.54748000
O	-1.17735800	-0.09480200	2.26557300
C	3.70145500	-1.63485900	0.55931300
C	-2.45809200	-2.36273500	1.45791600
H	-2.10854400	-3.38625500	1.61213700
H	-3.09685100	-2.05571800	2.28981600
C	-2.31256500	3.57141700	0.58158600
H	-2.84718000	4.02883500	1.40704700
C	-2.81740500	3.61229200	-0.72072000
H	-3.76163600	4.11301900	-0.90829100
C	-2.67790400	-0.95063800	-2.00629700
H	-2.42986500	-1.32858300	-2.99993000

H	-2.40805100	0.10656200	-1.97328100
C	-3.06123400	-2.14435400	0.08263000
C	2.15966600	3.45861700	-2.32059300
H	2.93999100	4.03107900	-2.82557800
H	1.21434400	3.68467900	-2.81897300
C	3.35589400	-3.41861800	-1.05202400
H	3.06324800	-3.74912200	-2.04284100
C	-4.12475800	-1.01201700	-0.08942700
C	-3.75876200	-3.34904700	-0.57443900
H	-3.03570300	-4.11947900	-0.85430100
H	-4.47734400	-3.80686400	0.10885100
C	-4.45664800	-2.68970400	-1.80259500
H	-4.05839100	-3.06527200	-2.74881900
H	-5.53061400	-2.88742400	-1.80068900
C	-4.15349500	-1.18195000	-1.62809600
H	-4.84949800	-0.52308700	-2.15352000
C	3.78537700	-4.31761100	-0.07937200
H	3.82406700	-5.37745200	-0.30715800
C	4.15316800	-2.52561200	1.52660600
H	4.46857400	-2.17407100	2.50304900
C	4.17915800	-3.87706300	1.19300500
H	4.51489800	-4.60473400	1.92401000
C	-3.69864500	0.38334800	0.37863400
H	-4.43758200	1.11546700	0.03656100
H	-2.72270200	0.70671700	0.01503700
H	-3.66922800	0.43113100	1.47260600
C	-5.45837900	-1.32369200	0.59915700
H	-5.32434800	-1.39215100	1.68454600
H	-5.92855700	-2.24706100	0.26011000
H	-6.16060000	-0.50597100	0.41144900
H	-1.18993900	4.13535700	3.37514800

#### 4c-C4re-C5si

E=-2329.723671

N	-2.36807400	2.34385500	-0.80161600
C	-1.03603800	2.00972700	-0.35114500
C	-0.73880700	2.64966900	1.02674800
O	0.28093800	2.33343900	-2.39909600
O	-1.53516500	2.81728100	1.92099700
C	0.16364800	2.47786900	-1.20391400
C	1.18957600	3.01941500	-0.28030200
C	-3.25951700	1.38605100	-0.13507600
H	-3.43896500	1.71762100	0.88919900
C	-2.63228100	2.22799500	-2.25298600
H	-2.12888000	1.36178700	-2.69541400
H	-2.28721000	3.12821500	-2.76557100
C	-4.54256500	1.37521200	-0.97787100
H	-4.92348900	0.36126000	-1.11789300
H	-5.32405400	1.94298600	-0.47022500
C	0.67702100	3.10450500	1.01284600

C	2.50486800	3.37904000	-0.56704000
H	2.88990600	3.30998500	-1.57907900
C	-4.15147400	2.04603100	-2.31622800
H	-4.43258900	1.43894800	-3.17831600
H	-4.64723400	3.01514600	-2.40785800
C	3.29663100	3.81440800	0.49070300
H	4.32868200	4.09568600	0.31116500
C	1.46189100	3.54762200	2.07207600
H	1.05616800	3.60601200	3.07626900
C	2.78085700	3.89535800	1.79468400
H	3.42629000	4.23616300	2.59718800
S	0.77051900	-1.93410700	-1.27030600
O	0.19690500	0.27636700	1.75469100
N	1.08546700	-0.84828200	0.02056000
C	-2.74663300	-0.70144800	1.28962000
N	-3.38636000	-2.11879300	-0.39501200
C	-3.29345600	-1.95576900	0.99199800
O	-2.80863000	-0.91202700	-2.26472800
C	0.09163800	-0.07463600	0.59359100
C	-1.00073100	0.43361000	-0.32272500
H	-0.79721000	0.14213700	-1.35819800
C	-2.89112200	-1.02994600	-1.05375600
C	-3.77485700	-3.34470900	-1.05445000
H	-3.71962800	-3.17062300	-2.12828800
H	-4.79566500	-3.62198300	-0.77990400
C	2.23781600	-1.24486300	0.84040400
H	1.86784300	-1.82728000	1.69093100
C	-2.46289400	0.01844900	-0.00503200
O	-0.43233100	-2.69274300	-0.93659300
C	-2.61227400	-0.30449300	2.60945400
H	-2.19611900	0.66996100	2.84565600
C	-3.00317600	-1.18849900	3.62254500
H	-2.89657800	-0.89553100	4.66133100
O	0.79545700	-1.21933300	-2.53975000
C	2.27676700	-2.90063100	-1.01750700
H	1.94323100	-3.84510300	-0.58040900
H	2.70553100	-3.07453300	-2.00713800
C	-3.68445100	-2.84716500	1.97916100
H	-4.10181200	-3.81754300	1.73293300
C	-3.52506300	-2.44107400	3.30785400
H	-3.82019300	-3.11577600	4.10488500
C	3.15006100	-0.07823600	1.29385700
H	3.14518900	0.02902900	2.38040200
H	2.81187700	0.86986300	0.86602500
C	3.15464000	-2.09827100	-0.07131700
C	4.16207900	-1.05597500	-0.66227200
C	4.04562100	-2.89947700	0.89585900
H	3.44260100	-3.41902400	1.64497900
H	4.62584100	-3.65479900	0.36150600
C	4.95166100	-1.78700500	1.50527700
H	4.79516800	-1.67630000	2.58134900
H	6.00949500	-2.00993200	1.35185600
C	4.52327400	-0.51059700	0.74275700

H	5.27027000	0.28740300	0.75047100
C	3.58045700	0.00016500	-1.61058800
H	4.34371700	0.76347500	-1.79558300
H	2.68882700	0.50291600	-1.23537900
H	3.32005200	-0.44936100	-2.57371300
C	5.33790300	-1.70480100	-1.40201600
H	4.98458300	-2.23724700	-2.29192600
H	5.91090100	-2.40704800	-0.79643300
H	6.02483900	-0.92467600	-1.74332700
H	-3.09073000	-4.15265200	-0.77954700

### Azo-1a

**E=-746.219206**

N	1.62656200	0.01255300	-0.11252100
C	0.21868200	-0.01334600	-0.11437900
C	-0.57718100	1.17463400	0.02846200
O	-0.32302100	-2.37755800	-0.32604100
O	-0.22054400	2.35117300	0.11423300
C	-0.60907700	-1.18709000	-0.18682000
C	-2.02713600	-0.67984900	-0.07347200
C	2.28796300	1.05126700	-0.51312900
H	1.69521000	1.85070700	-0.94298000
C	2.30870700	-1.17789300	0.47157000
H	1.77537600	-2.04553100	0.08543200
H	2.13589700	-1.12011900	1.55060600
C	3.76458900	1.21177700	-0.39484300
H	4.16803300	1.19725500	-1.41679200
H	3.95570600	2.22166600	-0.01698600
C	-2.00894300	0.70681700	0.06222100
C	3.78982300	-1.20683900	0.14096500
H	4.24688100	-2.01597900	0.71540900
H	3.92762900	-1.44003700	-0.92087000
C	-3.21401400	-1.38526800	-0.08998100
H	-3.21837300	-2.46544800	-0.19773500
C	4.42474600	0.13978400	0.46641300
H	5.50096400	0.12711100	0.28391000
H	4.27285400	0.36930700	1.52654600
C	-4.40616000	-0.65773100	0.03917100
H	-5.35746600	-1.18009200	0.03181000
C	-3.17548100	1.43485800	0.18903300
H	-3.15055800	2.51508900	0.29309300
C	-4.38737200	0.72912900	0.17737500
H	-5.32444400	1.26777200	0.27514300



**2a****E=-1622.747202**

S	1.44275700	-1.51887400	0.87472700
O	-0.31395800	1.66567000	-0.25901800
N	1.14872100	-0.01055300	0.11482900
C	-3.41195200	0.80102400	-0.02595200
N	-4.70199400	-1.09189800	-0.33984400
C	-4.72479000	0.28358600	-0.08713900
O	-3.06660900	-2.68902600	-0.66495800
C	-0.13566700	0.46654500	-0.12746300
C	-1.18996800	-0.55910900	-0.27901700
H	-0.88267700	-1.58823800	-0.45524700
C	-3.41427300	-1.54328700	-0.44772300
C	-5.87233900	-1.93150900	-0.46978300
H	-5.52638700	-2.94793300	-0.65472700
H	-6.49159700	-1.59856700	-1.30691800
C	2.24342700	0.95094000	0.30179200
H	1.99260200	1.58335200	1.16061900
C	-2.51219300	-0.33508700	-0.24345700
O	0.59595100	-1.63402700	2.05731400
C	-3.22967600	2.15931700	0.22123300
H	-2.23140700	2.57388700	0.25940900
C	-4.35167600	2.96994400	0.40671500
H	-4.21845500	4.02862800	0.59946200
O	1.36022200	-2.58234900	-0.11945800
C	3.14872200	-1.13668600	1.32479900
H	3.13240600	-0.99269900	2.40785100
H	3.74364100	-2.01786800	1.07280900
C	-5.84510500	1.07649900	0.08968100
H	-6.84496000	0.65996500	0.03696100
C	-5.63705200	2.43582400	0.34018800
H	-6.49595500	3.08371900	0.48270300
C	2.60991400	1.80197800	-0.93954100
H	2.39940000	2.85924000	-0.76768400
H	2.03393000	1.48615400	-1.81144100
C	3.52908800	0.12504500	0.57081000
C	4.18433000	-0.01469500	-0.84230900
C	4.48688200	1.09942600	1.27900200
H	4.00081100	1.57832400	2.13304900
H	5.37068800	0.57905500	1.65471000
C	4.83825900	2.09979300	0.13608700
H	4.48621300	3.11123300	0.35547800
H	5.91719500	2.15864000	-0.02121900
C	4.11456400	1.51131400	-1.09875900
H	4.52732300	1.83986400	-2.05596600
C	3.41278900	-0.86062000	-1.86197100
H	3.87519700	-0.73695000	-2.84644800
H	2.35671800	-0.60645700	-1.95033700
H	3.47055800	-1.92191000	-1.59972700
C	5.60912000	-0.57846700	-0.79344800
H	5.60225300	-1.60322200	-0.40568600
H	6.29828100	0.00588100	-0.18328400

H	6.01747900	-0.61954800	-1.80763500
H	-6.46371800	-1.90821800	0.44923800

### Azo-1c

**E=-706.923636**

N	1.90545600	0.07320700	0.01671600
C	0.51656300	0.02774500	0.00486900
C	-0.30900700	1.20221500	-0.00503200
O	0.04829800	-2.35557600	0.02835800
O	0.02456900	2.38902900	-0.01002900
C	-0.28224600	-1.17131300	0.01312600
C	-1.71340100	-0.69110900	0.00242700
C	2.65585000	1.13071800	0.02056700
H	2.19397800	2.10995500	0.00453200
C	2.71246600	-1.18123400	0.09610500
H	2.29982200	-1.90777500	-0.59929400
H	2.59799500	-1.57026500	1.11072100
C	4.10773600	0.80027500	0.09878500
H	4.69989500	1.40562700	-0.59062100
H	4.47123100	1.01471200	1.11167100
C	-1.72971700	0.70326600	-0.00851000
C	4.12867900	-0.70342800	-0.22778000
H	4.87821900	-1.24914700	0.34413800
H	4.33242900	-0.84884600	-1.29035100
C	-2.88349100	-1.42467200	0.00340200
H	-2.85999100	-2.50987000	0.01278300
C	-4.09502800	-0.71895700	-0.00812900
H	-5.03377400	-1.26341100	-0.00785300
C	-2.91680600	1.40939100	-0.02023500
H	-2.91998400	2.49483600	-0.02918400
C	-4.11132100	0.67492600	-0.01981600
H	-5.06261600	1.19716400	-0.02885600

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