10.1071/CH19524_AC

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Supplementary Material

Phenol as a Modulator in the Chemical Reactivity of TCT: Rules of the Game II

Rotimi Sheyi,[A] *Anamika Sharma,*[A,B] *Ayman El-Faham,*[C,D] *Beatriz G. de la Torre,*[B] *and Fernando Albericio*[A,C,E,F]

[A]Peptide Science Laboratory, School of Chemistry and Physics, University of KwaZulu-Natal, Durban 4001, South Africa.

[B]KwaZulu-Natal Research Innovation and Sequencing Platform (KRISP), School of Laboratory Medicine and Medical Sciences, College of Health Sciences, University of KwaZulu-Natal, Durban 4041, South Africa.

[C]Department of Chemistry, College of Science, King Saud University, PO Box 2455, Riyadh 11451, Saudi Arabia.

[D]Department of Chemistry, Faculty of Science, Alexandria University, PO Box 426, Alexandria 21321, Egypt.

[E]CIBER-BBN (Networking Centre on Bioengineering, Biomaterials and Nanomedicine) and Department of Organic Chemistry, University of Barcelona, 08028 Barcelona, Spain.

[F]Corresponding author. Email: albericio@ukzn.ac.za

I. Chromatogram and spectra for derivatives

Figure S1. HPLC of **2**

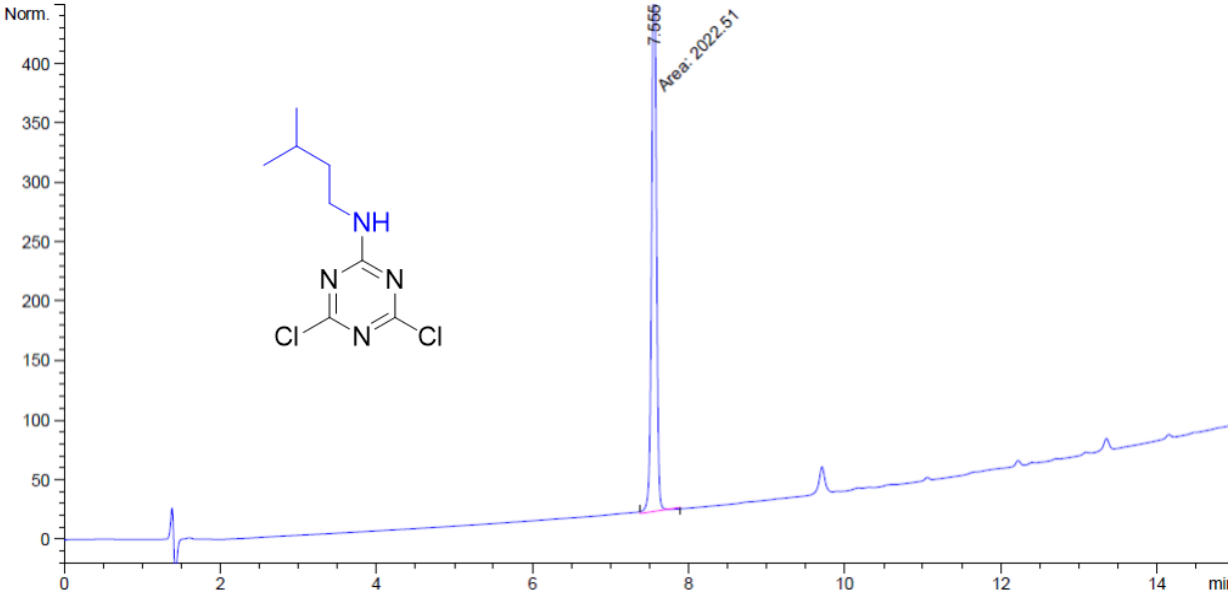


Figure S2. ^{1}H NMR of **2**

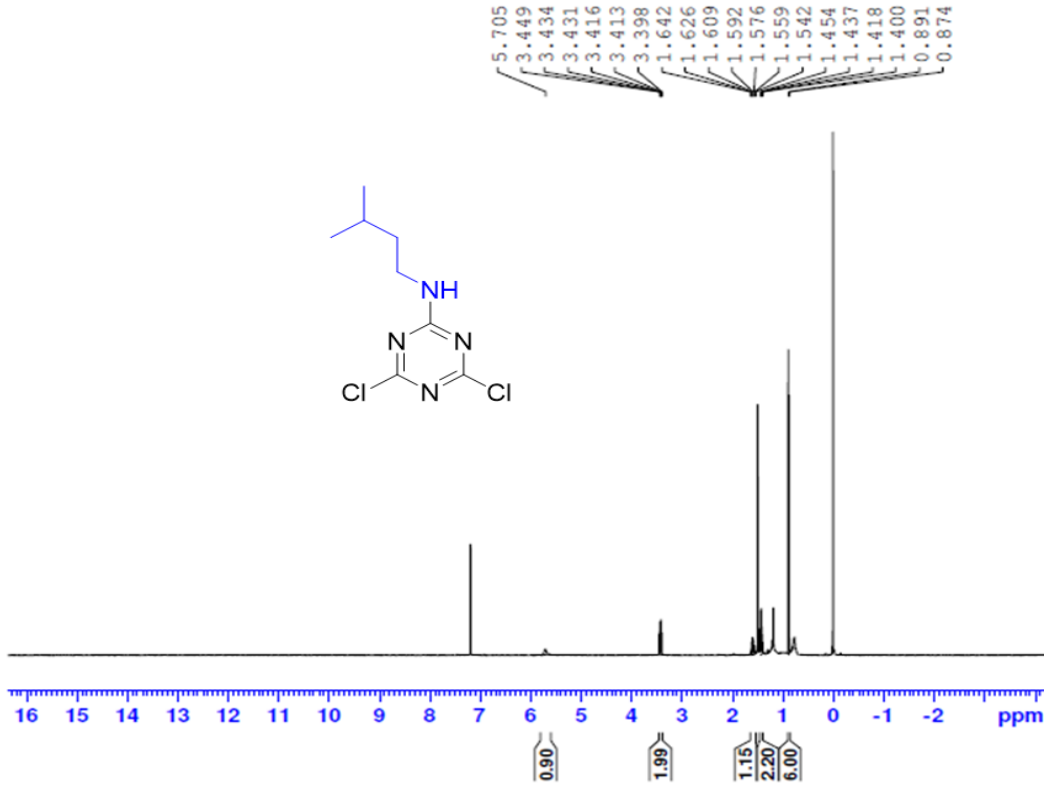


Figure S3. ^{13}C NMR of **2**

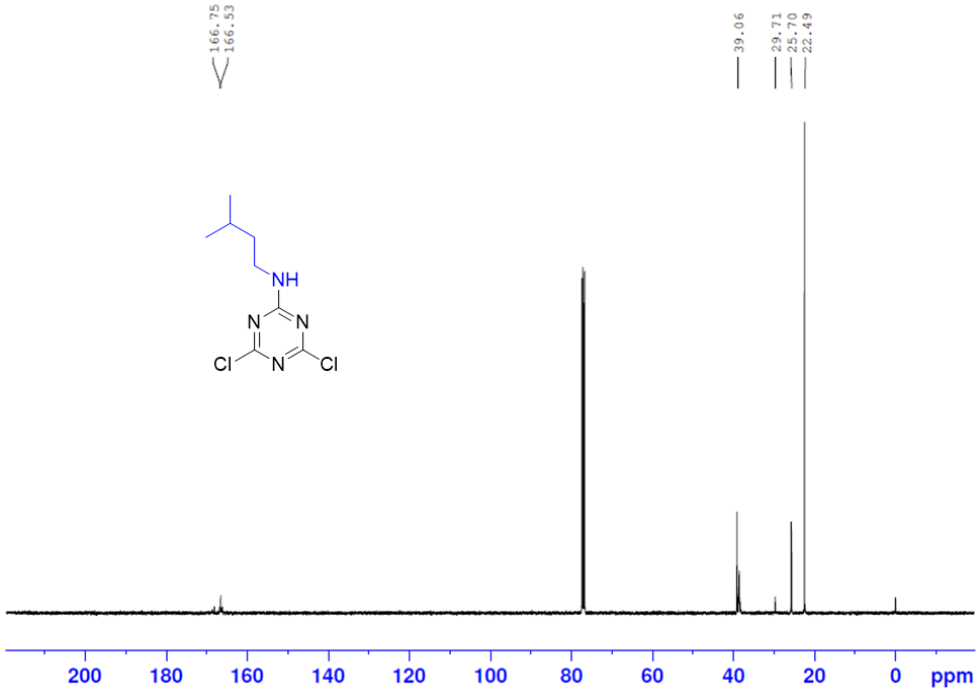


Figure S4. HPLC of **3**

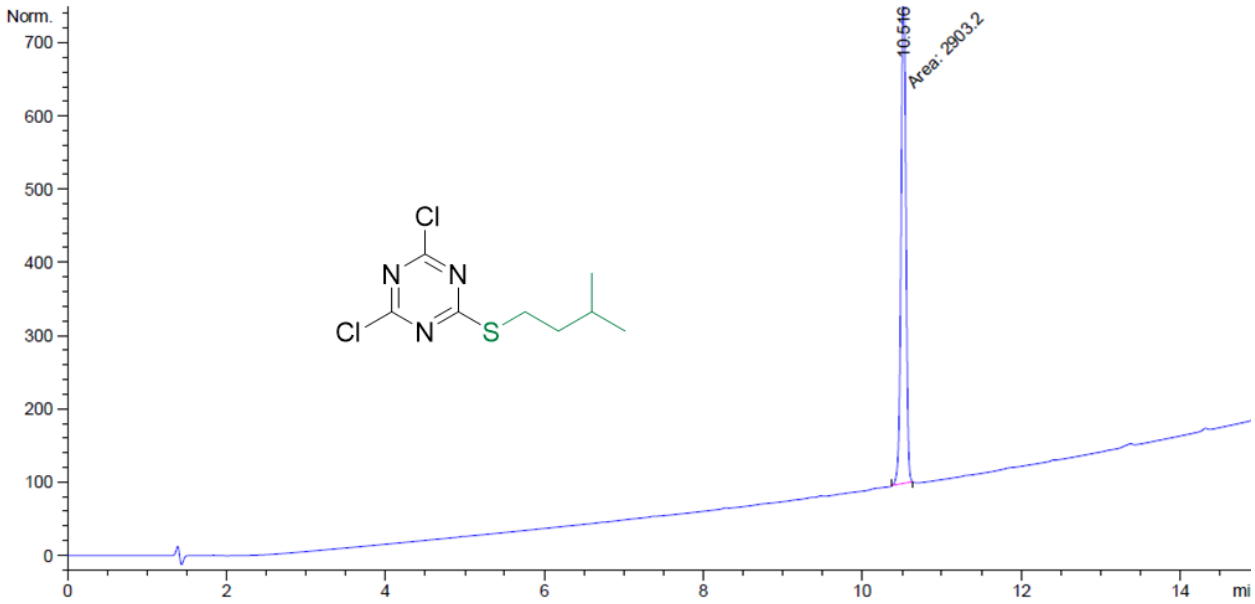


Figure S5. ^{1}H NMR of **3**

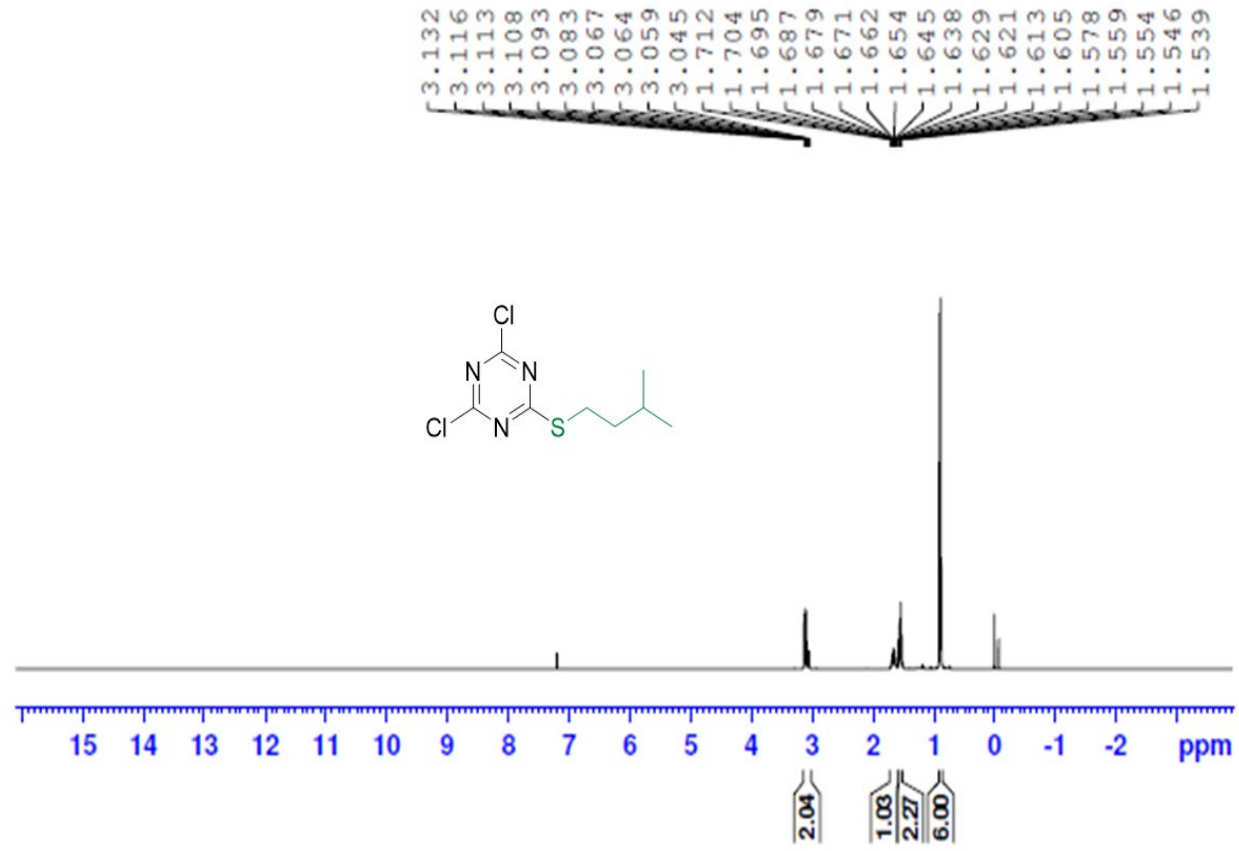


Figure S6. ^{13}C NMR of **3**

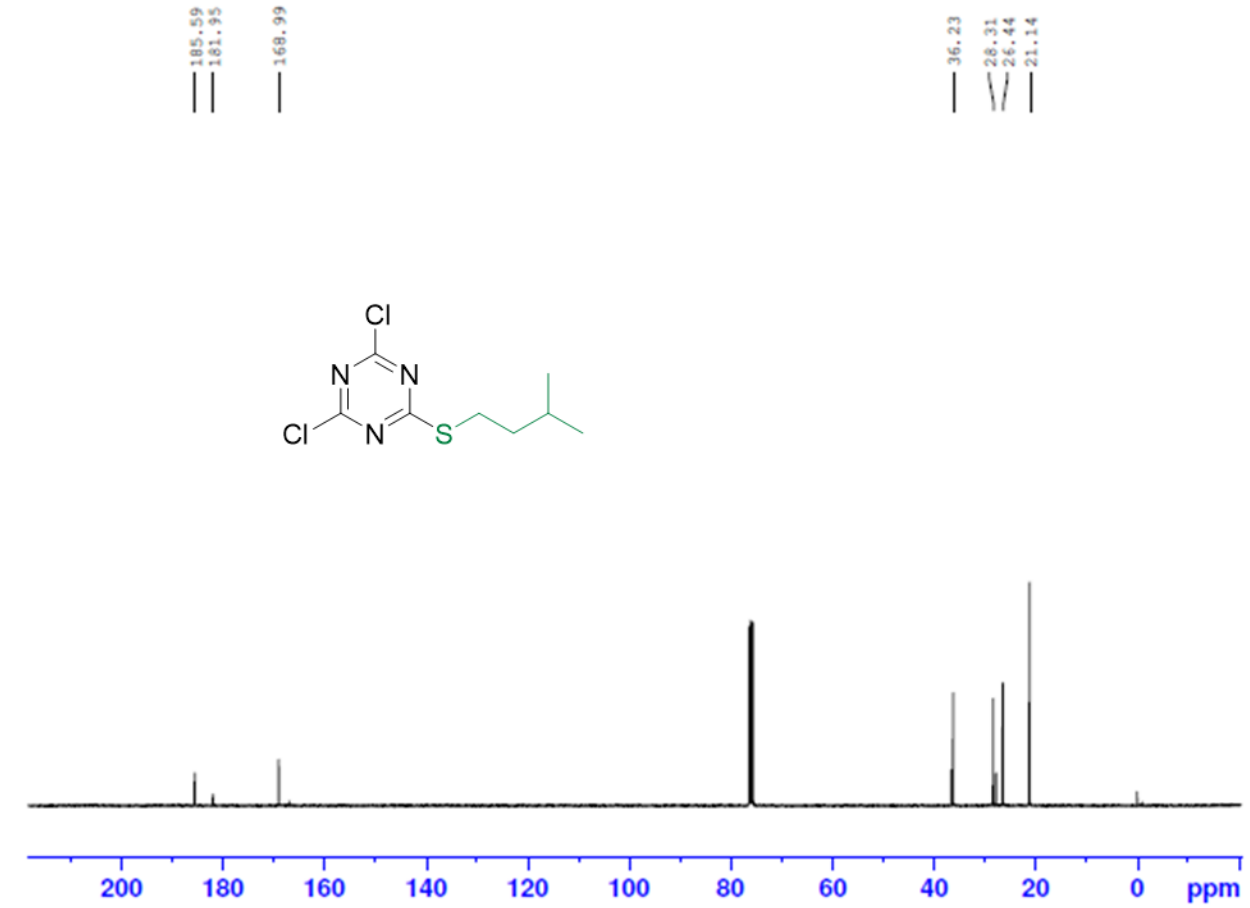


Figure S7. HPLC of **4**

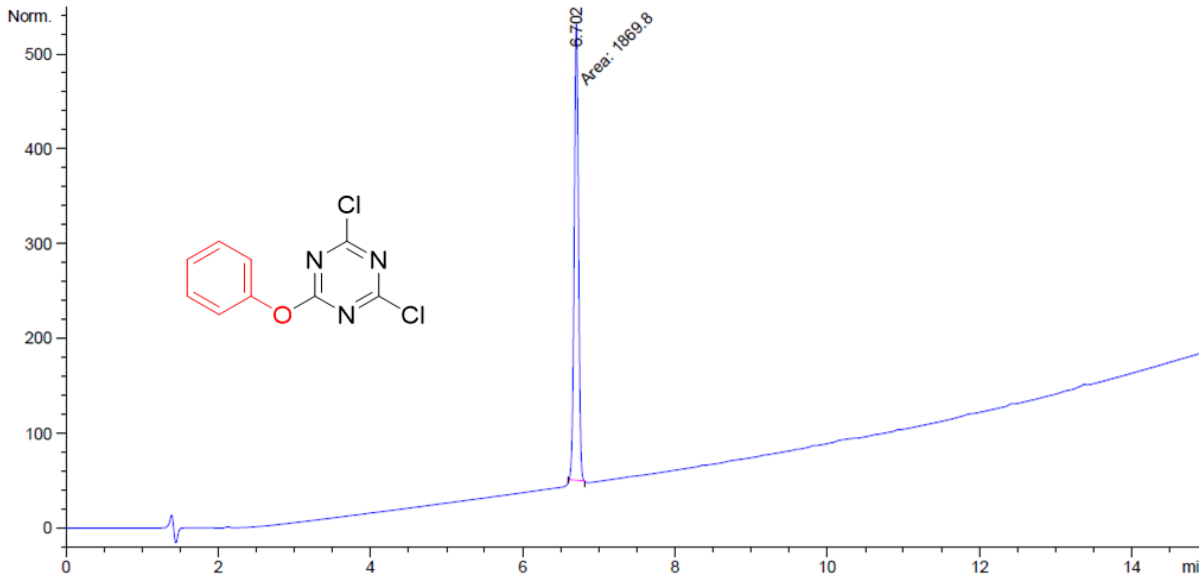


Figure S8. ^{1}H NMR of **4**

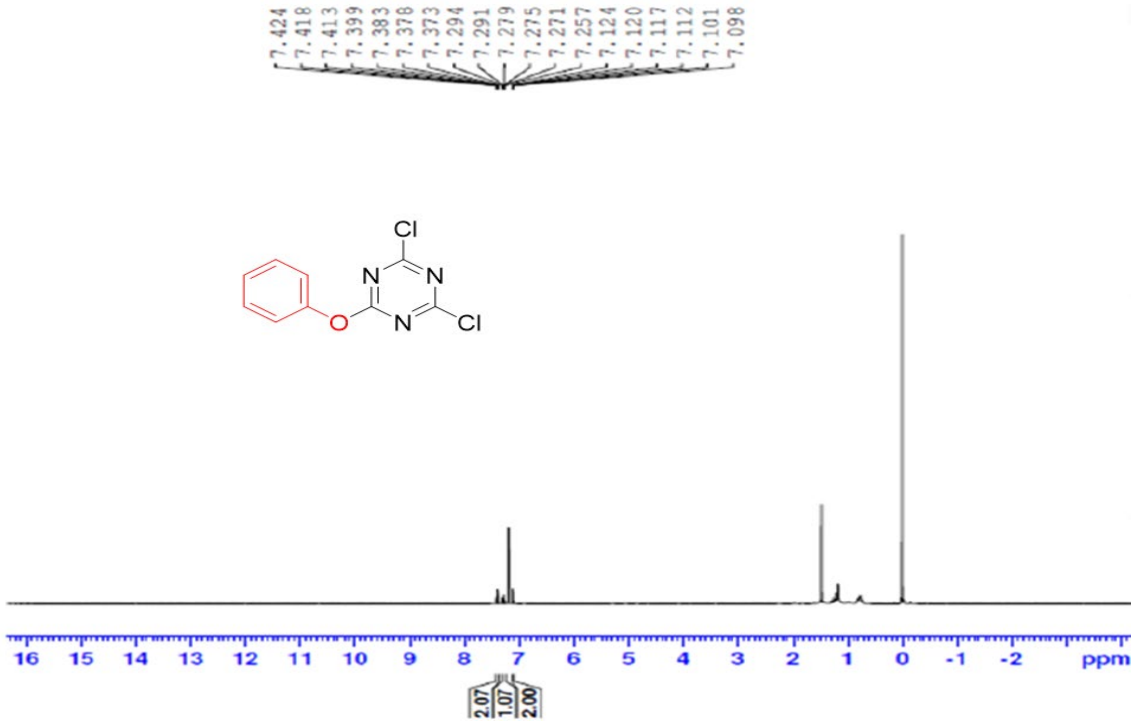


Figure S9. ^{13}C NMR of **4**

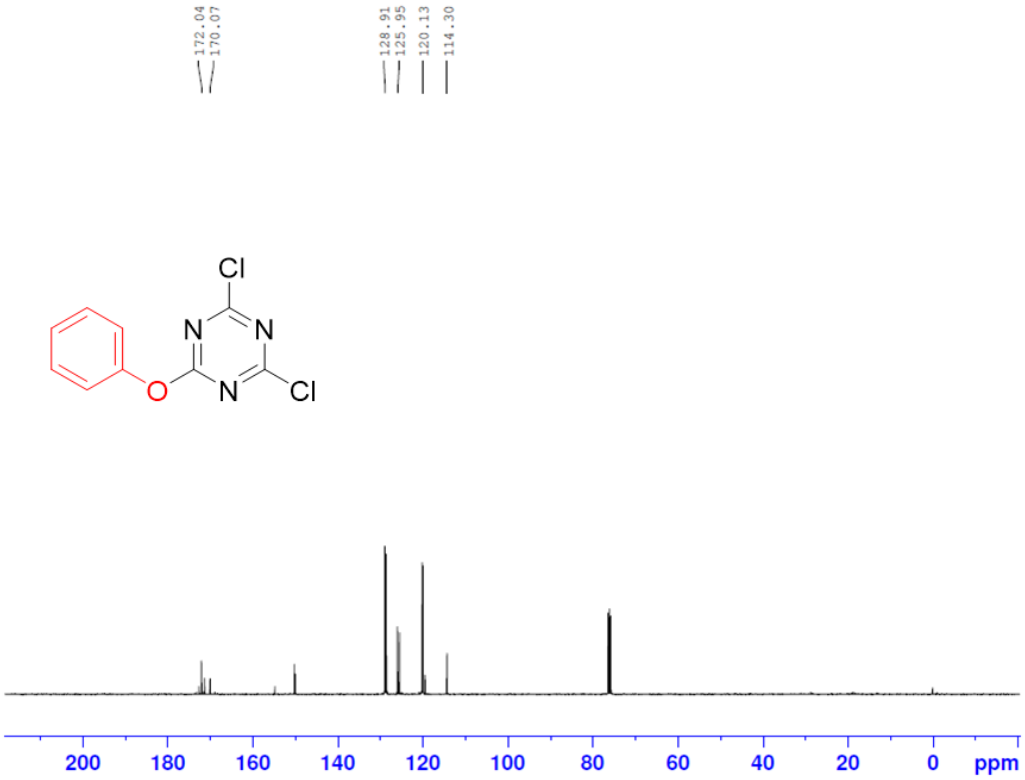


Figure S10. HPLC of **5**

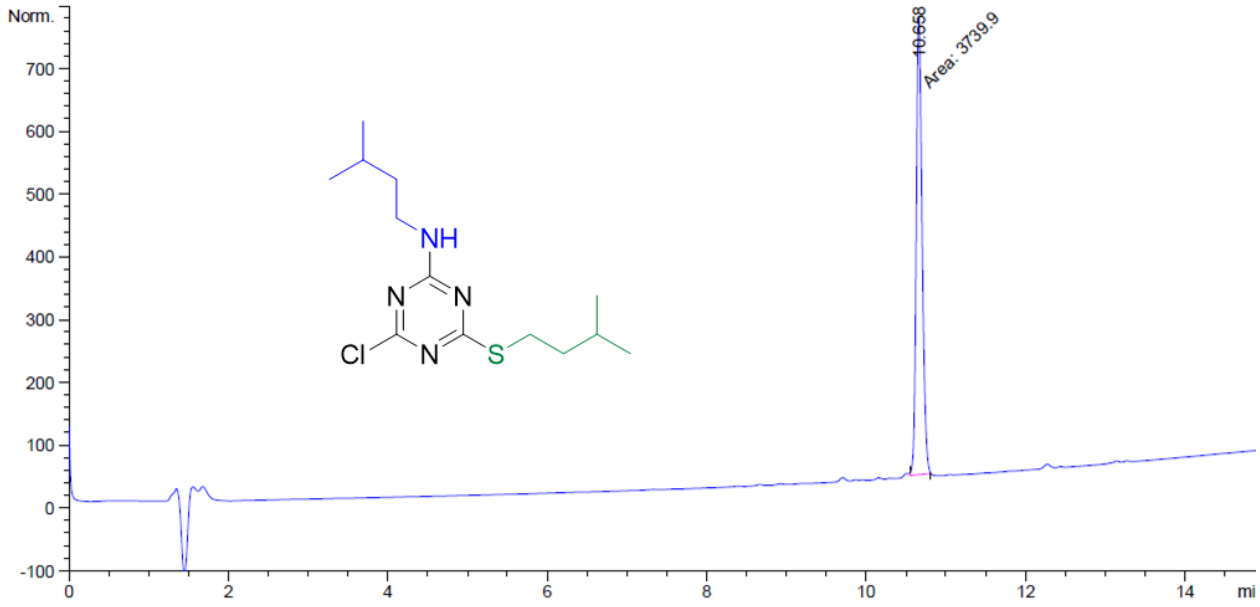


Figure S11. ^{1}H NMR of **5**

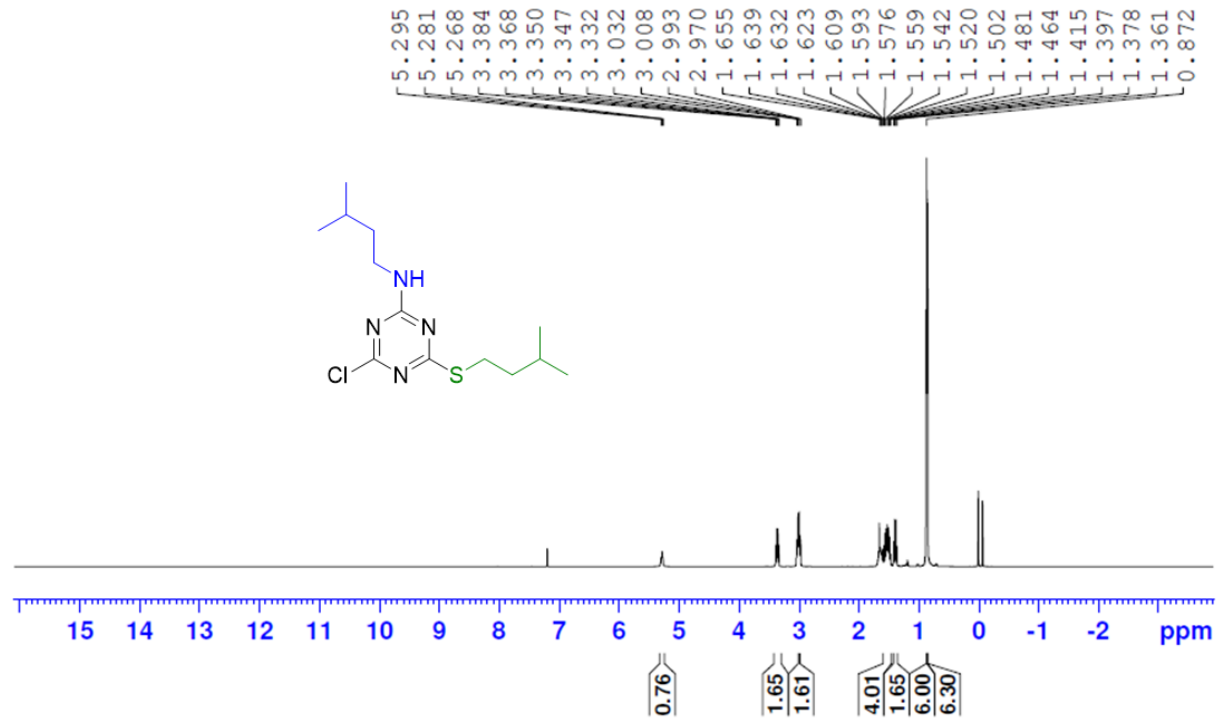


Figure S12. ^{13}C NMR of **5**

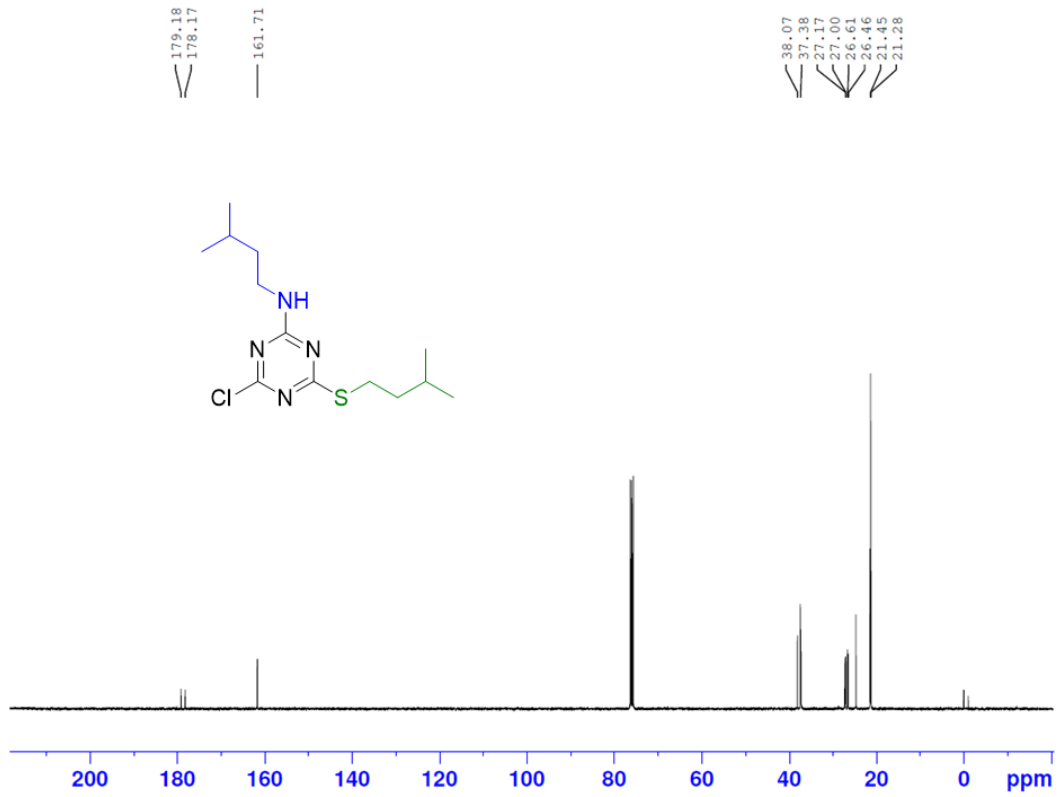


Figure S13. HPLC of **6**

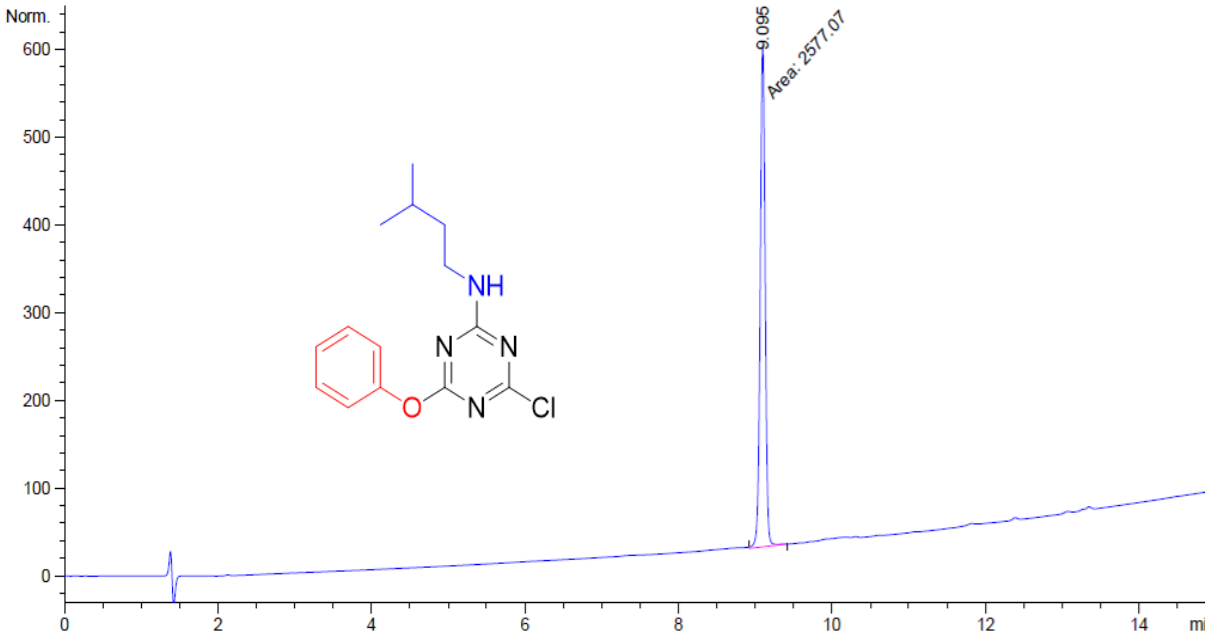


Figure S14. ^{1}H NMR of **6**

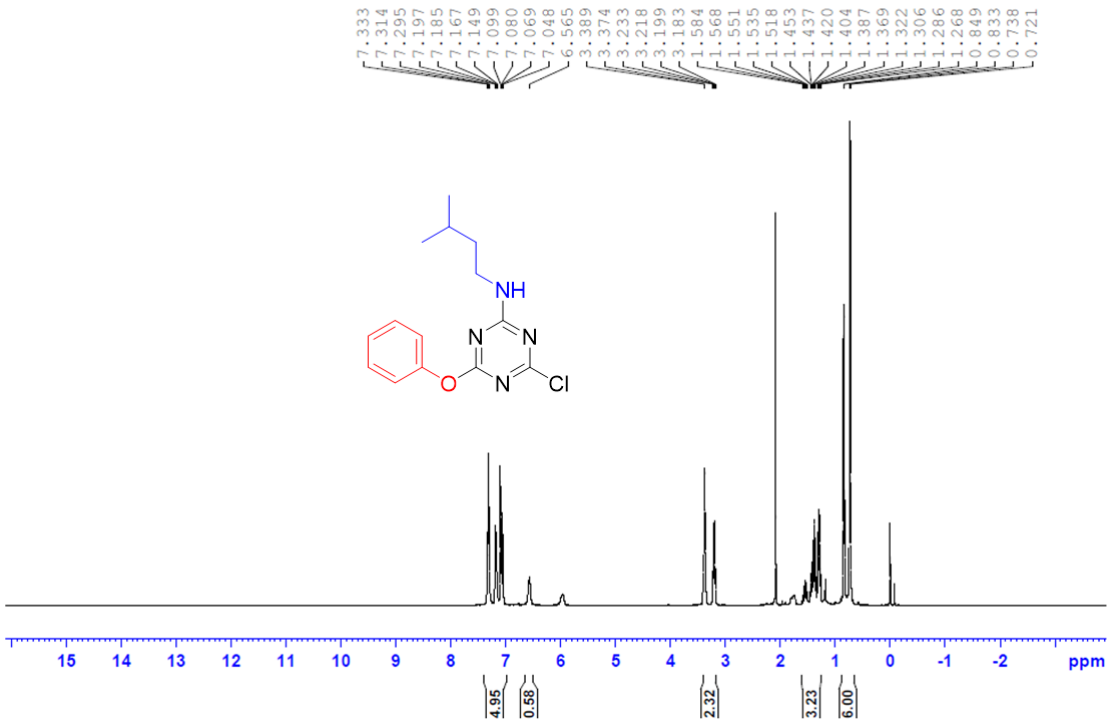


Figure S15. ^{13}C NMR of **6**

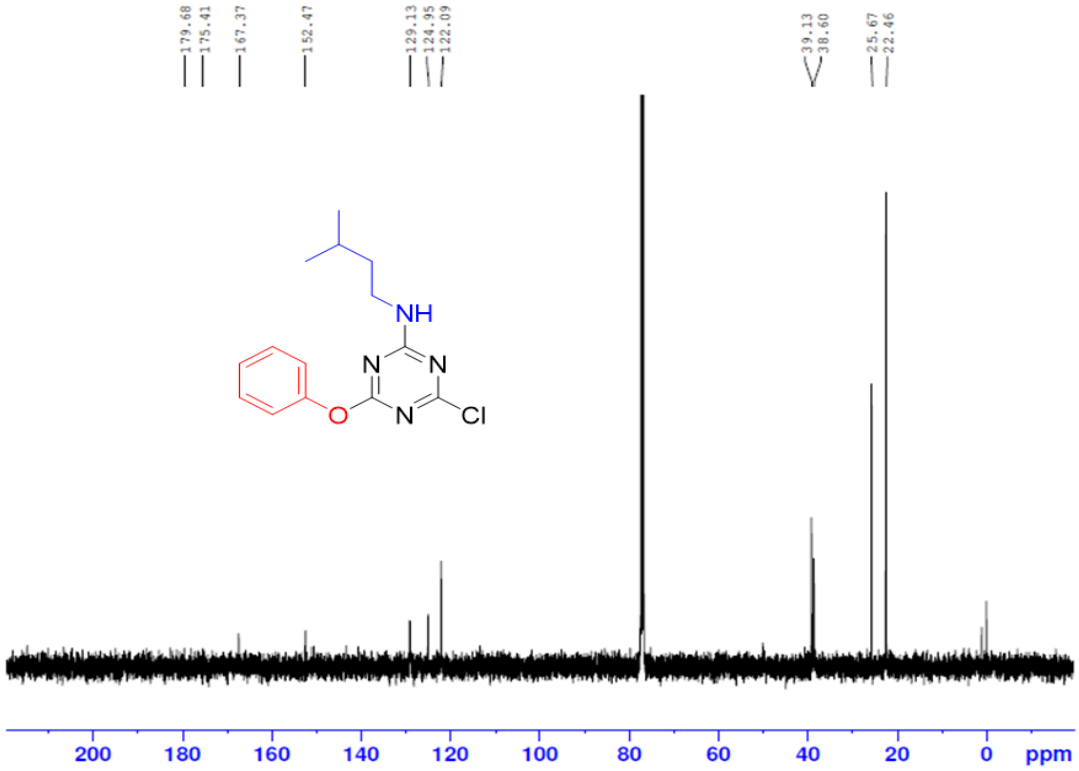


Figure S16. HPLC of **7**

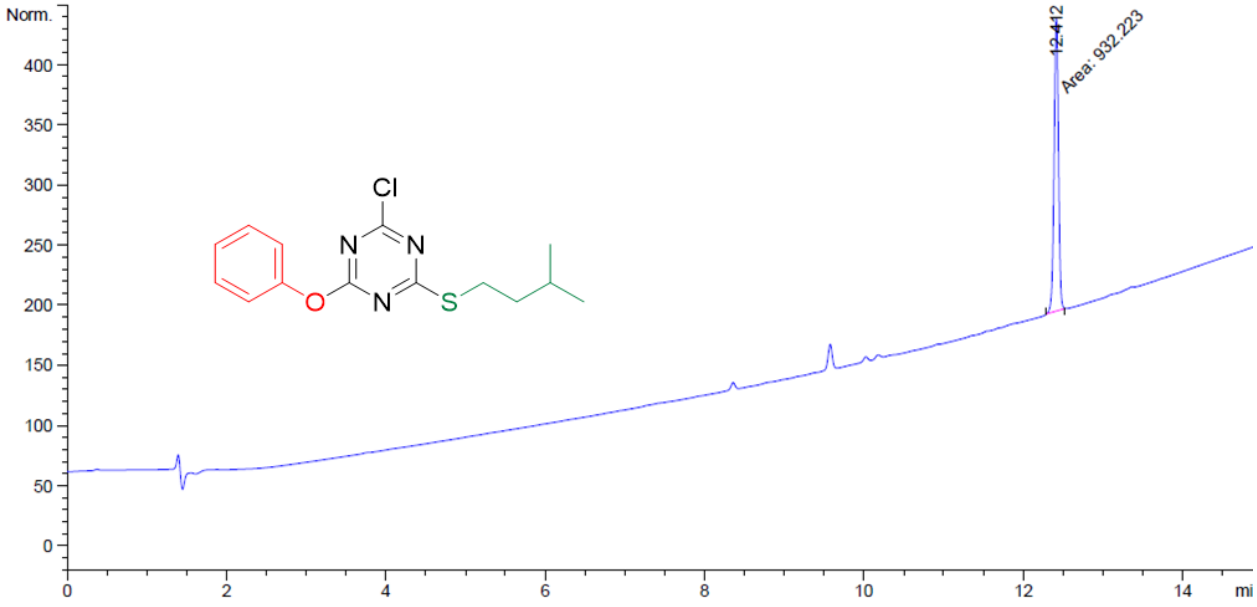


Figure S17. ^{1}H NMR of **7**

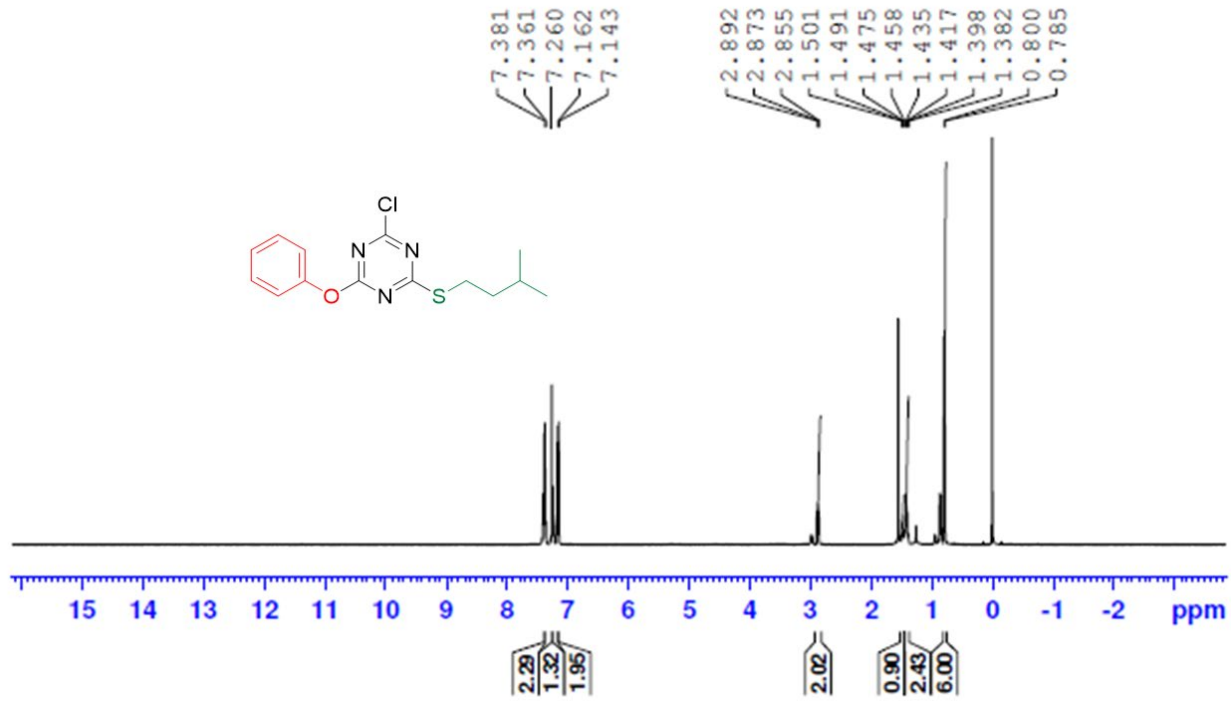


Figure S18. ^{13}C NMR of **7**

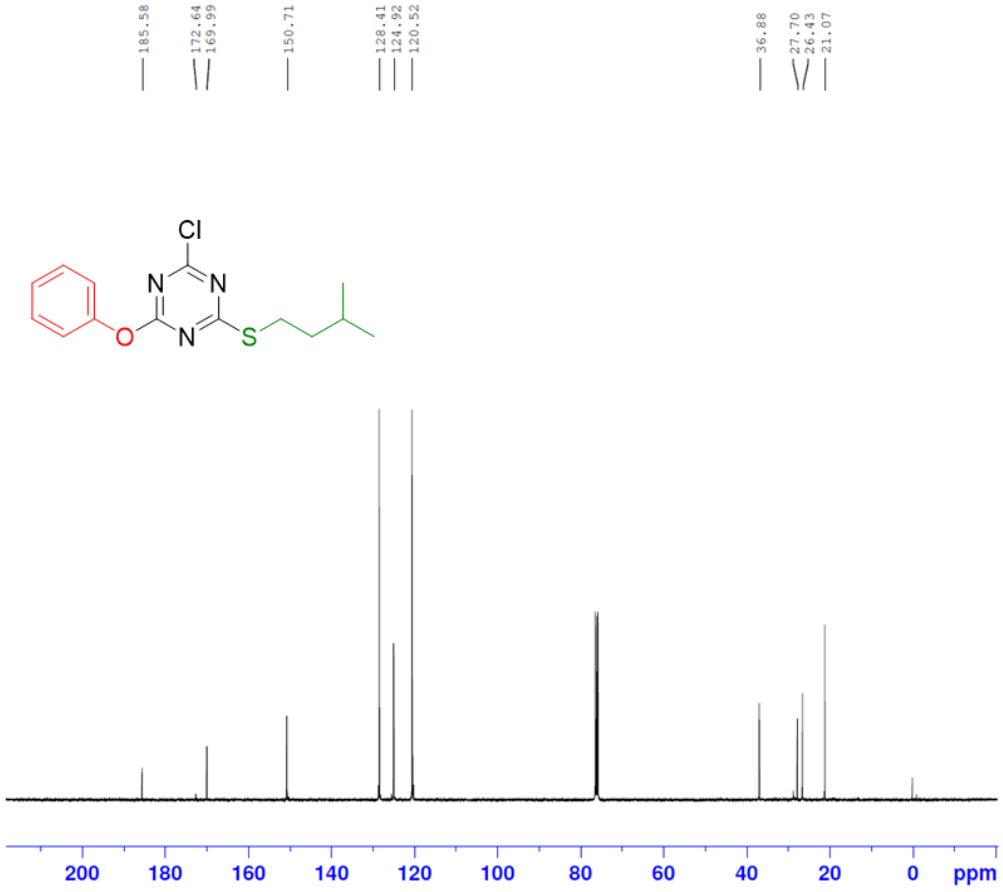


Figure S19. HPLC of **8**

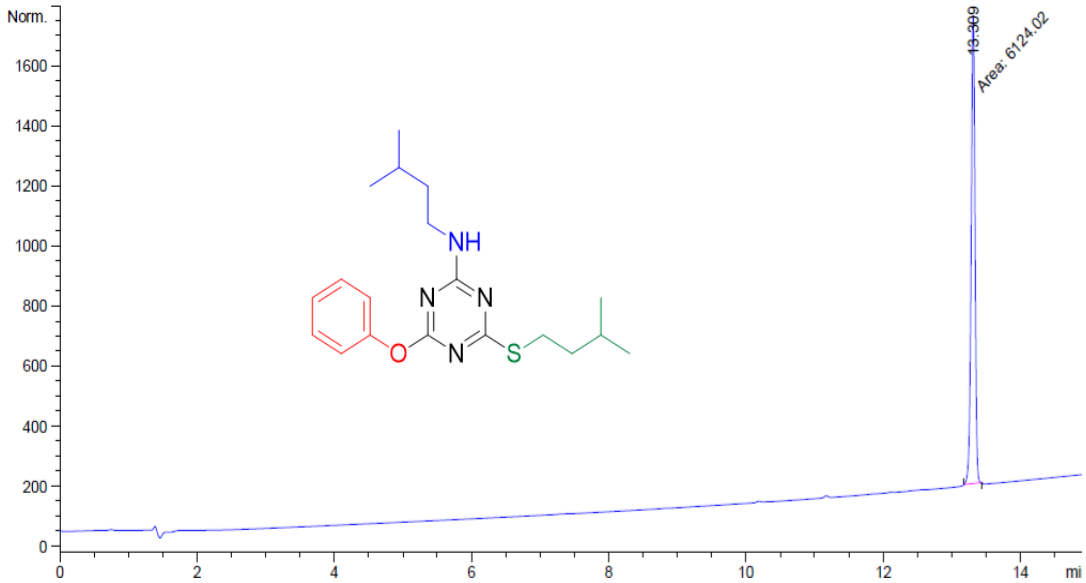


Figure S20. ^{1}H NMR of **8**

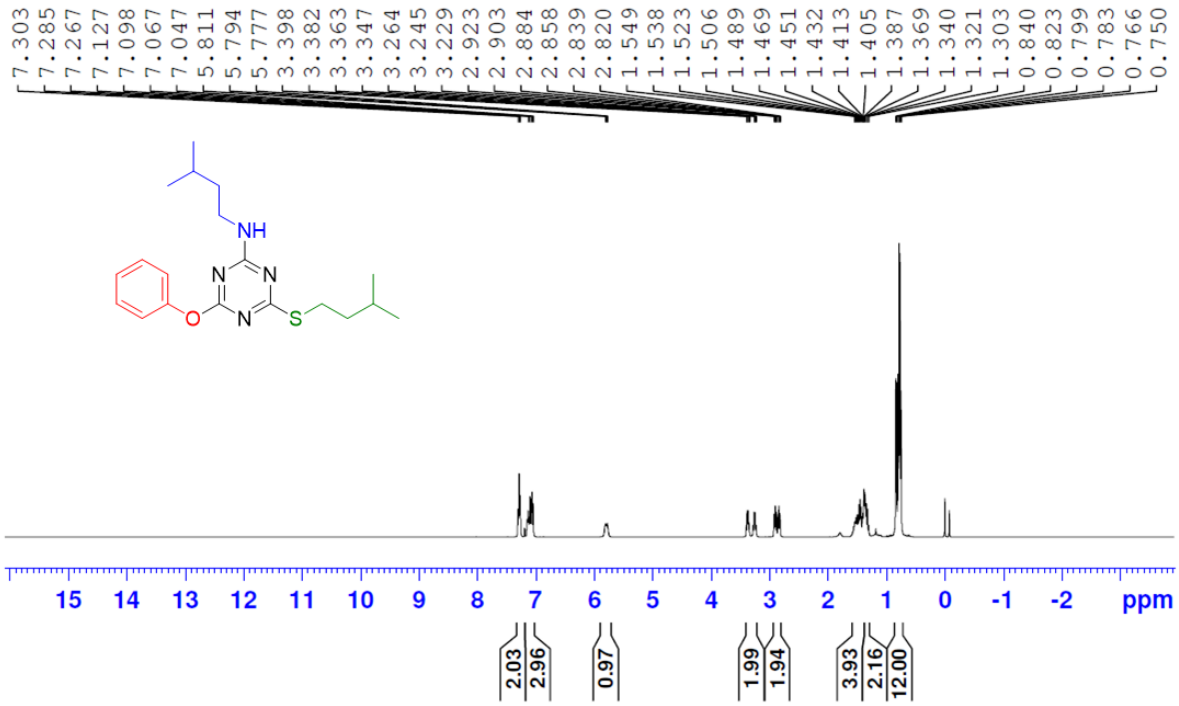
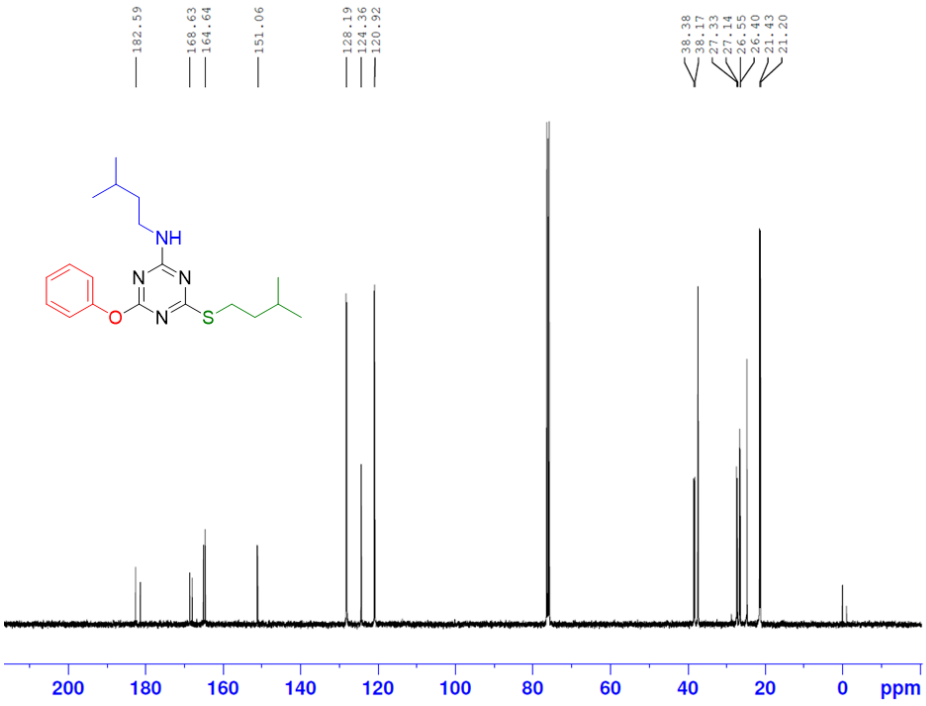


Figure S21. ^{13}C NMR of **8**



Cartesian co-ordinates for the NBO calculations

1. **Optimized Co-ordinates of 1 for NBO calculations**

b3lyp/6-311++g(d,p) pop=(nbo,savenbo) geom=connectivity

Title Card Required

0 1

C	1.27012700	-0.16535400	-0.00003900
C	-0.77814500	-1.01726200	0.00001100
C	-0.49180600	1.18253700	0.00006400
Cl	-1.15664700	2.78037700	-0.00007600
Cl	-1.82980500	-2.39171400	0.00000200
Cl	2.98629300	-0.38858700	0.00005600
N	0.83176700	1.08718400	0.00000400
N	-1.35730100	0.17665000	0.00001300
N	0.52577000	-1.26395100	-0.00000500

1 6 1.0 7 1.5 9 1.5
2 5 1.0 8 1.5 9 1.5
3 4 1.0 7 1.5 8 1.5
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2. **Optimized Co-ordinates of 2 for NBO calculations**

b3lyp/6-311++g(d,p) pop=(nbo,savenbo) geom=connectivity

Title Card Required

0 1

C	2.66253600	0.67681700	-0.10054300
C	1.55298100	-1.22955200	0.02799200
C	0.49210300	0.69350500	0.44250400
Cl	4.15296000	1.53064400	-0.40855800
N	1.62210300	1.40919600	0.21584900
N	2.72150600	-0.64929700	-0.21747300
N	0.41654900	-0.65219100	0.35251600
N	-0.60456900	1.38714800	0.78393000
H	-0.48731600	2.38997700	0.78757300
C	-1.93189700	0.81660700	1.00500700
H	-1.79045600	-0.20551000	1.35170800

H	-2.40048300	1.38316300	1.81547600
C	-2.81374900	0.85659900	-0.25007000
H	-2.33489800	0.26354900	-1.03803200
H	-2.85411400	1.88984200	-0.61511400
C	-4.25038500	0.34898000	-0.02478500
H	-4.67906000	0.91833200	0.81206800
C	-5.11121500	0.62566800	-1.26543800
H	-4.72670400	0.08315300	-2.13577700
H	-6.14517900	0.30682300	-1.10667200
H	-5.12350800	1.69078500	-1.51493100
C	-4.29468600	-1.14193500	0.34258000
H	-3.84664800	-1.75042700	-0.45021200
H	-3.76018900	-1.36036300	1.27052500
H	-5.32723600	-1.47689500	0.47543900
Cl	1.52660100	-2.97044100	-0.10081200

1 4 1.0 5 2.0 6 1.5
2 6 1.5 7 2.0 26 1.0
3 5 1.5 7 1.5 8 1.5
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8 9 1.0 10 1.0
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16 17 1.0 18 1.0 22 1.0
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18 19 1.0 20 1.0 21 1.0
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22 23 1.0 24 1.0 25 1.0
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3. Optimized Co-ordinates of 3 for NBO calculations

b3lyp/6-311++g(d,p) pop=(nbo,savenbo) geom=connectivity

Title Card Required

0 1

C	-1.91990500	1.27675100	0.07190000
C	-2.97313400	-0.66708200	-0.04279100
C	-0.74073500	-0.61868000	0.01124400
Cl	-1.97019300	3.01533600	0.14998700
N	-0.72002200	0.72099600	0.07470400
N	-3.09057400	0.65868700	0.01617900
N	-1.85779100	-1.36597400	-0.05004600
C	2.02020100	-0.19421200	0.10300300
H	1.85240700	0.48546900	-0.73059000
H	1.86111800	0.35504000	1.03189800
C	3.40976600	-0.83366800	0.06228700
H	3.54972700	-1.35496300	-0.89241000
H	3.47968200	-1.59413900	0.84790000
C	4.55807900	0.17784500	0.25801600
H	4.37919400	0.70296200	1.20594800
C	5.89606600	-0.56461600	0.37853700
H	6.12402600	-1.11237700	-0.54225500
H	6.71731000	0.13410400	0.56036000
H	5.88137000	-1.28550300	1.20105600
C	4.61796000	1.22626900	-0.86237100
H	4.75778600	0.74620300	-1.83732900
H	3.71038800	1.83287000	-0.91414800
H	5.45731300	1.90973000	-0.70712200
Cl	-4.46195800	-1.56252000	-0.11789300
S	0.75282200	-1.52680400	0.00414400

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2 6 1.5 7 2.0 24 1.0
3 5 1.5 7 1.5 25 1.0
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8 9 1.0 10 1.0 11 1.0 25 1.0
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11 12 1.0 13 1.0 14 1.0
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14 15 1.0 16 1.0 20 1.0
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16 17 1.0 18 1.0 19 1.0
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20 21 1.0 22 1.0 23 1.0
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4. Optimized Co-ordinates of 4 for NBO calculations

b3lyp/6-311++g(d,p) pop=(nbo,savenbo) geom=connectivity

Title Card Required

0 1

C	1.36540900	1.24195700	-0.00006300
C	0.29787000	-0.70897500	0.00001000
C	2.51750700	-0.64707200	0.00000700
Cl	1.32084900	2.97943100	-0.00013000
Cl	4.04882200	-1.46814100	0.00007700
O	-0.80288700	-1.45620800	0.00001200
C	-2.07228900	-0.84310300	-0.00000400
C	-2.69628200	-0.59714700	1.21391100
C	-2.69651200	-0.59760100	-1.21387100
C	-3.98599100	-0.06931000	1.20737400
H	-2.18155200	-0.81746200	2.14102600
C	-3.98622700	-0.06975600	-1.20725600
H	-2.18193300	-0.81830400	-2.14097700
C	-4.63059000	0.19608900	0.00006400
H	-4.48637800	0.13060500	2.14763200
H	-4.48679700	0.12979800	-2.14749600
H	-5.63427000	0.60464100	0.00008100
N	2.56716700	0.68339600	-0.00005300
N	0.19772400	0.62142500	-0.00005300
N	1.43971700	-1.40511300	0.00003500

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2 6 1.5 19 1.5 20 1.5
3 5 1.0 18 1.5 20 2.0
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7 8 1.5 9 1.5
8 10 1.5 11 1.0
9 12 1.5 13 1.0
10 14 1.5 15 1.0

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14 17 1.0
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5. Optimized Co-ordinates of 5 for NBO calculations

b3lyp/6-311++g(d,p) pop=(nbo,savenbo) geom=connectivity

Title Card Required

0 1

C	0.12956000	1.51771100	-0.21629500
C	1.40189900	-0.31490200	-0.27524300
C	-0.84313200	-0.48337900	-0.17361600
Cl	-0.00751100	3.26831000	-0.20641800
N	-1.01239600	0.85348600	-0.16340000
N	1.35249400	1.03884200	-0.27822500
N	0.32100200	-1.11772100	-0.22642600
C	-3.64299500	-0.31713500	-0.06105900
H	-3.47895600	0.33947600	0.79129100
H	-3.60192900	0.28585600	-0.96894700
C	-4.96406300	-1.08271600	0.03996600
H	-4.98977400	-1.65459400	0.97571000
H	-5.01896000	-1.81411800	-0.77418600
C	-6.21130800	-0.17810200	-0.03242800
H	-6.14654500	0.40185900	-0.96297300
C	-7.48129500	-1.03749700	-0.10330100
H	-7.59595000	-1.64097300	0.80380400
H	-8.37387500	-0.41295400	-0.20068100
H	-7.45517300	-1.72051400	-0.95741600
C	-6.29073200	0.81137700	1.13899900
H	-6.32059900	0.27848300	2.09607500
H	-5.43872900	1.49507900	1.16227400
H	-7.19664000	1.42046000	1.07092700
S	-2.25856300	-1.52938800	-0.11382900
C	3.88935200	-0.22670500	-0.44273100
H	4.10461800	-0.02431700	-1.50036700
H	3.79566200	0.73776100	0.05425400
C	5.01067300	-1.06909200	0.16822300
H	4.98652500	-2.06986900	-0.28269100

H	4.81671500	-1.20422700	1.23944100
C	6.42040700	-0.48117100	-0.02851500
H	6.57060900	-0.32975800	-1.10620800
C	7.48340900	-1.47681500	0.45612600
H	7.39948800	-2.43676400	-0.06195800
H	8.49183100	-1.09055900	0.28351300
H	7.38038100	-1.66642900	1.53009200
C	6.59080900	0.87631200	0.66921700
H	5.90261700	1.63164900	0.28217600
H	6.41537400	0.78396000	1.74676900
H	7.60623200	1.25790300	0.53059600
N	2.60691200	-0.91249200	-0.31637800
H	2.58019300	-1.92059700	-0.36618800

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6. Optimized Co-ordinates of 6 for NBO calculations

b3lyp/6-311++g(d,p) pop=(nbo,savenbo) geom=connectivity

Title Card Required

0 1

C	-0.89307200	2.08325500	0.06335700
C	-0.91586100	-0.12435000	-0.13597000
C	1.02979900	0.97956600	-0.20728400
Cl	-1.76708000	3.58730400	0.27507900
O	-1.54787500	-1.30761100	-0.18612800
C	-2.94557900	-1.35966400	-0.06932500
C	-3.50931700	-1.55560500	1.18366800
C	-3.72055400	-1.31741700	-1.22001900
C	-4.89177400	-1.69831600	1.28535300
H	-2.87266100	-1.59442900	2.05904800
C	-5.10200500	-1.46107500	-1.10732200
H	-3.24543900	-1.17374500	-2.18270500
C	-5.68934400	-1.64973600	0.14293300
H	-5.34389900	-1.84912800	2.25887600
H	-5.71790100	-1.42648100	-1.99860200
H	-6.76415000	-1.76132700	0.22630600
N	0.40885700	2.17951200	-0.04276300
N	-1.63903600	0.98589000	0.03033500
N	0.40075500	-0.20413800	-0.26554700
N	2.37039200	1.01799000	-0.30899400
H	2.77118900	1.94469300	-0.30612800
C	3.23535000	-0.13353200	-0.54478500
H	2.72852500	-1.00795500	-0.13980700
H	3.35170100	-0.29921800	-1.62412600
C	4.60495100	0.07853700	0.10360800
H	4.47749000	0.17534100	1.18873600
H	5.01799400	1.03295400	-0.24839500
C	5.62535300	-1.03442000	-0.19774800
H	5.70382600	-1.12802600	-1.28955400

C	7.01010400	-0.64508500	0.33854300
H	6.98999600	-0.53376700	1.42811500
H	7.75415700	-1.40937800	0.09752600
H	7.35360900	0.30231600	-0.08729000
C	5.19094800	-2.39597000	0.36465300
H	5.06186400	-2.34415800	1.45142200
H	4.24946900	-2.74427800	-0.06718200
H	5.94681100	-3.15858500	0.15724800

1 4 1.0 17 2.0 18 1.5
2 5 1.5 18 1.5 19 1.5
3 17 1.5 19 1.5 20 1.5
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5 6 1.0
6 7 1.5 8 1.5
7 9 1.5 10 1.0
8 11 1.5 12 1.0
9 13 1.5 14 1.0
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11 13 1.5 15 1.0
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13 16 1.0
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20 21 1.0 22 1.0
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22 23 1.0 24 1.0 25 1.0
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25 26 1.0 27 1.0 28 1.0
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28 29 1.0 30 1.0 34 1.0
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30 31 1.0 32 1.0 33 1.0
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34 35 1.0 36 1.0 37 1.0
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7. Optimized Co-ordinates of 7 for NBO calculations

b3lyp/6-311++g(d,p) pop=(nbo,savenbo) geom=connectivity

Title Card Required

0 1

C	-0.49754600	1.23455600	0.09259100
C	-1.55426500	-0.71513600	-0.01616200
C	0.68063800	-0.65534300	0.02712000
Cl	-0.55342900	2.98001200	0.17000100
N	0.70482200	0.68878600	0.09091400
N	-1.66439000	0.61769100	0.04248800
N	-0.42163200	-1.40641400	-0.02796400
C	3.44552400	-0.21068400	0.10560200
H	3.26004200	0.47846900	-0.71617700
H	3.29882300	0.32694300	1.04331900
C	4.83951100	-0.83789000	0.03470900
H	4.97110200	-1.33796600	-0.93255500
H	4.92498200	-1.61490700	0.80257300
C	5.98357800	0.17650500	0.23823400
H	5.81588400	0.67612700	1.20191700
C	7.32901500	-0.55794700	0.31867600
H	7.54712200	-1.07840700	-0.62021400
H	8.14792500	0.14180900	0.50763600
H	7.33183000	-1.30148300	1.12098500
C	6.01835200	1.25391200	-0.85541400
H	6.14449800	0.79979400	-1.84464600
H	5.10582100	1.85479200	-0.87635100
H	6.85598700	1.93889900	-0.69672600
S	2.18796000	-1.55224000	0.01109600
O	-2.66415300	-1.45875900	-0.07135300
C	-3.92741100	-0.84220000	-0.05622200
C	-4.53965700	-0.58146800	1.16157600
C	-4.56763300	-0.60610400	-1.26421700
C	-5.82811300	-0.05133800	1.16488100
H	-4.01449400	-0.79131800	2.08527800
C	-5.85659300	-0.07627600	-1.24886900
H	-4.06284200	-0.83658700	-2.19435800
C	-6.48701700	0.20293600	-0.03735900
H	-6.31697400	0.15979500	2.10888900
H	-6.36746900	0.11475700	-2.18547500
H	-7.48997600	0.61341100	-0.02976100

1 4 1.0 5 2.0 6 2.0

2 6 1.5 7 1.5 25 1.5
3 5 1.5 7 1.5 24 1.0
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8 9 1.0 10 1.0 11 1.0 24 1.0
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27 29 1.5 30 1.0
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29 33 1.5 34 1.0
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31 33 1.5 35 1.0
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33 36 1.0
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