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Supporting Information

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10 4-Amino-4*H*-1,2,4-triazol-1-ium 3-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide **(9c)**
a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA, e. HRMS, f. C, H, N analysis.

11 3-Amino-1*H*-1,2,4-triazol-4-ium 3-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide **(9d)**
a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA, e. C, H, N analysis

12 3,5-Diamino-1*H*-1,2,4-triazol-4-ium 3-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide **(9e)**
a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA, e. C, H, N analysis

13 5-(1*H*-Tetrazol-1-yl)-1*H*-1,2,4-triazol-3-amine **(10)**
a. ^{1}HNMR, b. D_2O exchange ^{1}H c. ^{13}CNMR, d. DEPT, e. DSC-TGA, f. HRMS and g. C, H, N analysis

14 Diaminomethaniminium 3-amino-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide **(10a)**
a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA, d. HRMS and e. C, H, N analysis

15 (Hydrazinylcarbonyl)hydrazonium 3-mino-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide **(10b)**
a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA, d. HRMS, e. C, H, N analysis

16 3-Amino-1*H*-1,2,4-triazol-4-ium 3-amino-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide **(10d)**
a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA, e. C, H, N analysis

17 3,5-Diamino-1*H*-1,2,4-triazol-4-ium 3-amino-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide **(10e)**
a. ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA, e. HRMS, f. C, H, N analysis

18 1-(3-Azido-1*H*-1,2,4-triazol-5-yl)-1*H*-tetrazole **(11)**
a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA, d. HRMS, e. C, H, N analysis

19 3,5-Diamino-1*H*-1,2,4-triazol-4-ium 3-azido-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide **(11e)**

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a . ^{1}HNMR, b. ^{13}CNMR, c. DEPT, d. DSC-TGA, e. C, H, N analysis

20 3-Azido-1*H*-1,2,4-triazol-5-amine **(12)**

a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA, d. HRMS, e. C, H, N analysis

21 Diaminomethaniminium 5-amino-3-azido-1,2,4-triazol-1-ide **(12a)**

a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA, d. HRMS and e. C, H, N analysis

22 3,5-Diamino-1*H*-1,2,4-triazol-4-ium 5-amino-3-azido-1,2,4-triazol-1-ide **(12e)**

a. ^{1}HNMR, b. ^{13}CNMR, c. DSC-TGA, d. HRMS, e. C, H, N analysis

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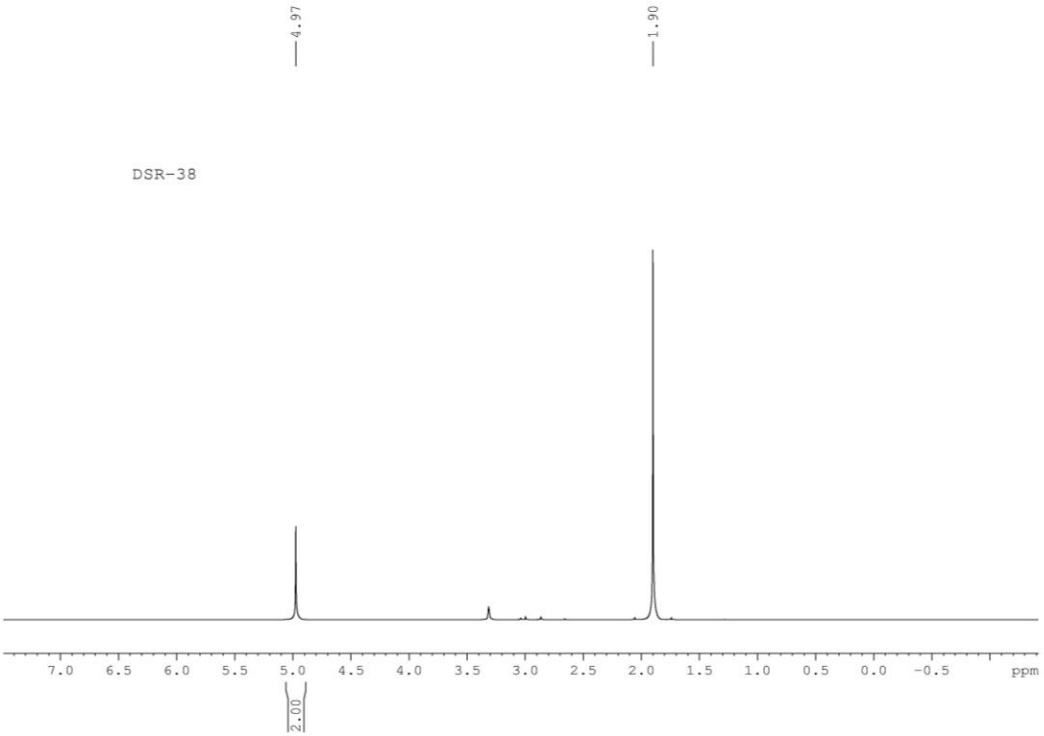
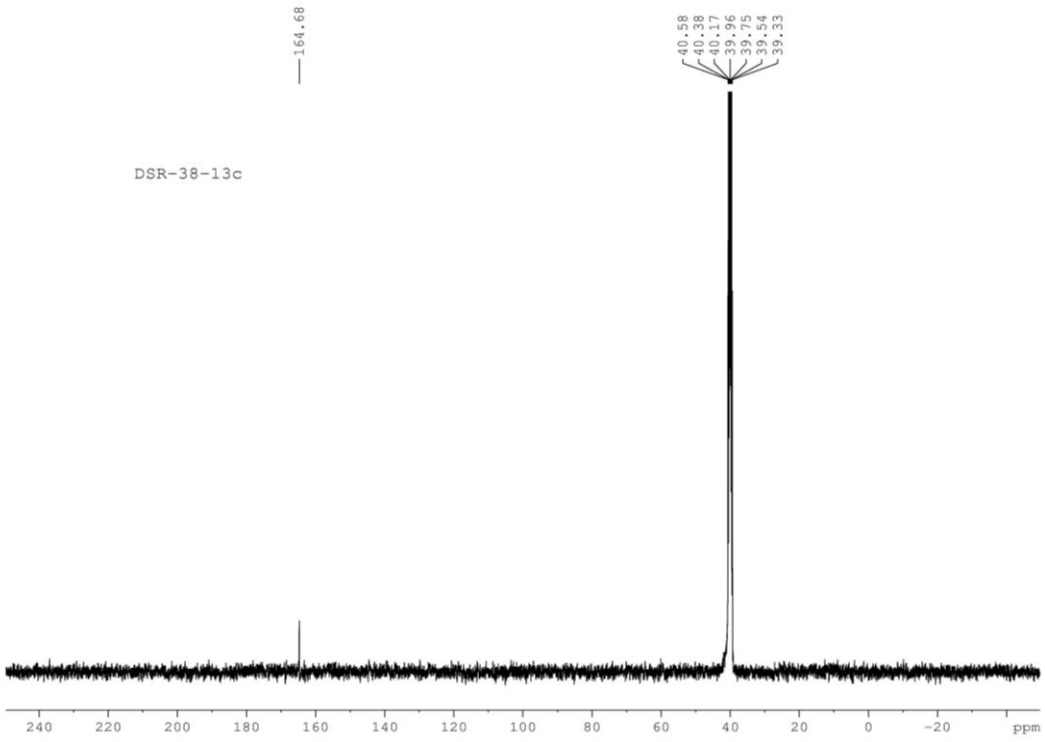
1. 1*H*-Tetrazol-5-amine (1)

a. ^{1}H NMR



b. ^{13}C NMR



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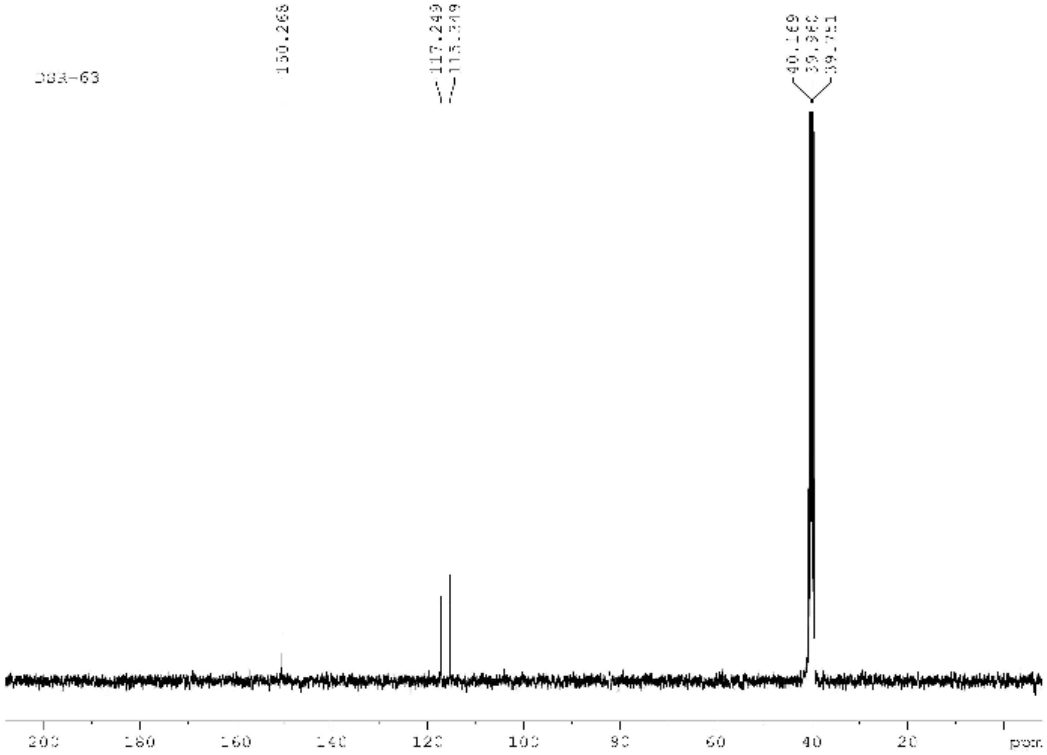
2. 2-Azido-1*H*-imidazole-4,5-dicarbonitrile (4)

a. ^{13}C NMR



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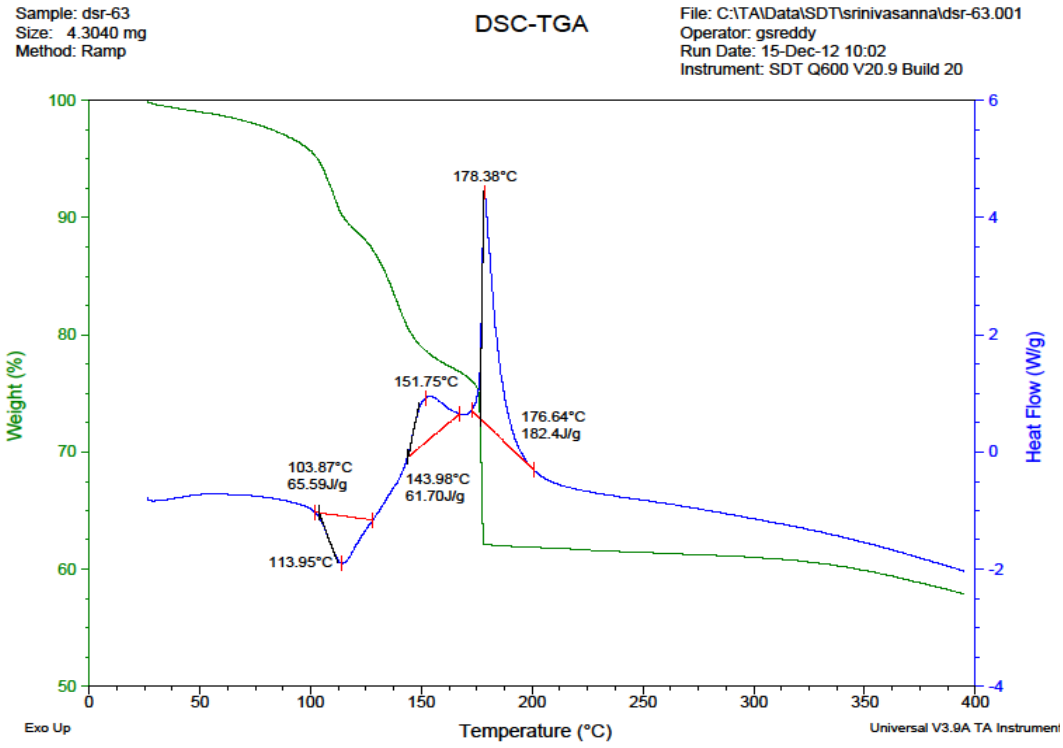

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c. C H N analysis

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Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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Chromatogram filename:	UNK-15022013-5.dat
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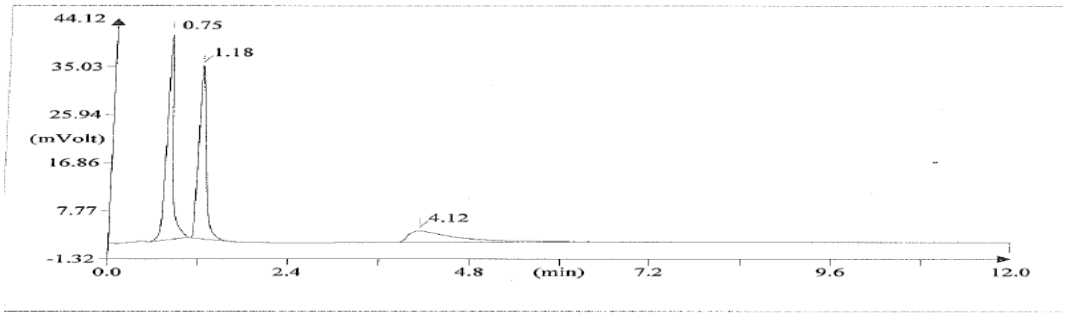

Element Name	Element %	Ret. Time
Nitrogen	61. 52	0. 75
Carbon	37. 62	1. 18
Hydrogen	0. 71	4. 12

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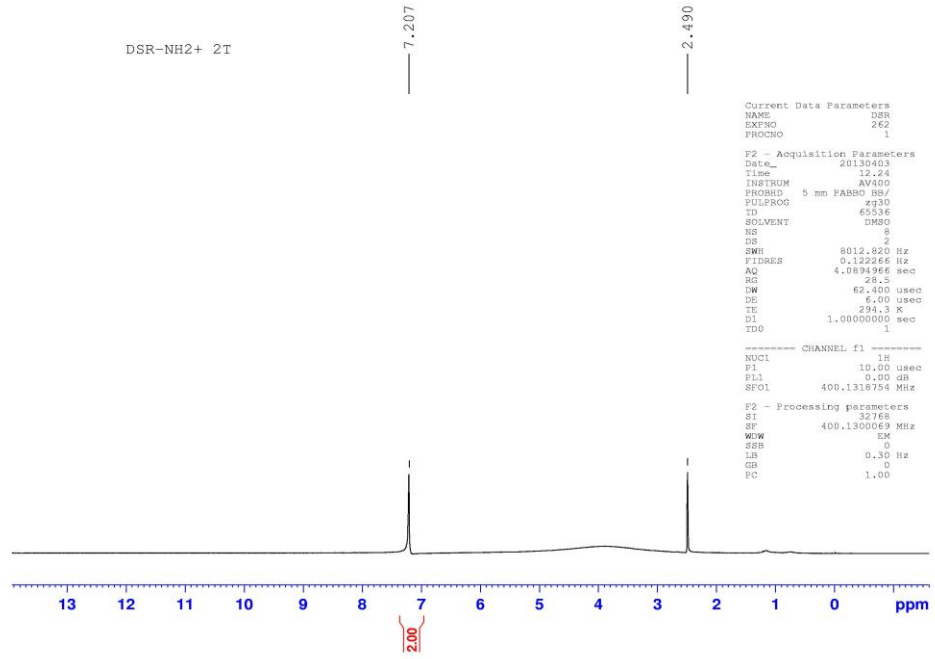
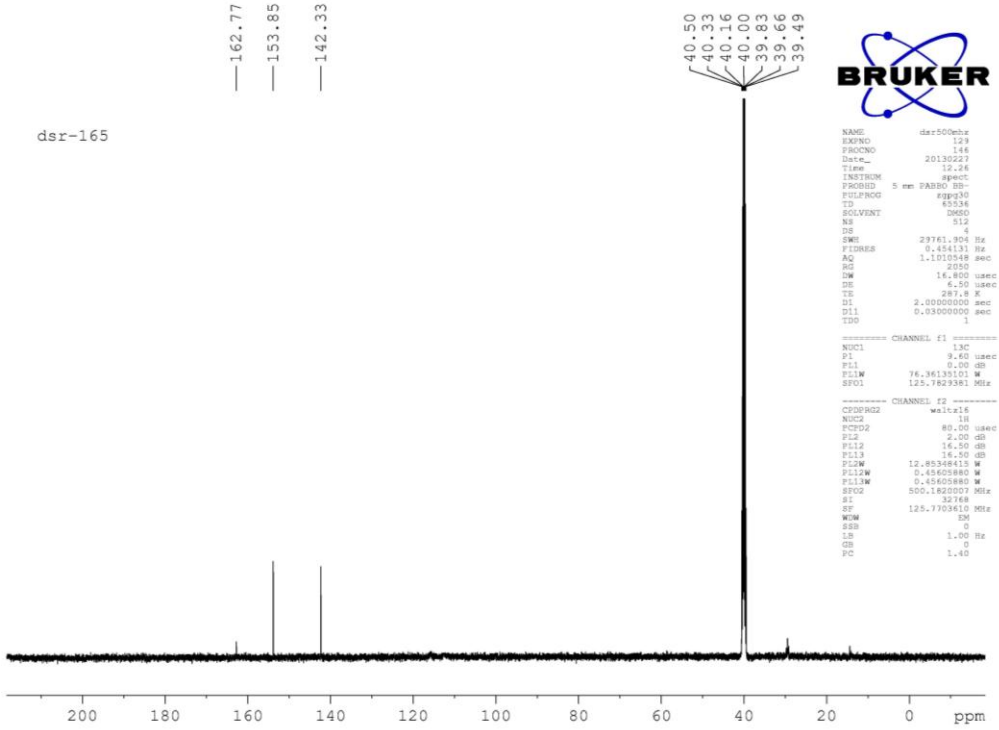
3. 4,5-Di(1*H*-tetrazol-5-yl)-1*H*-imidazol-2-amine(5)

a. ^{1}H NMR



b. ^{13}C NMR



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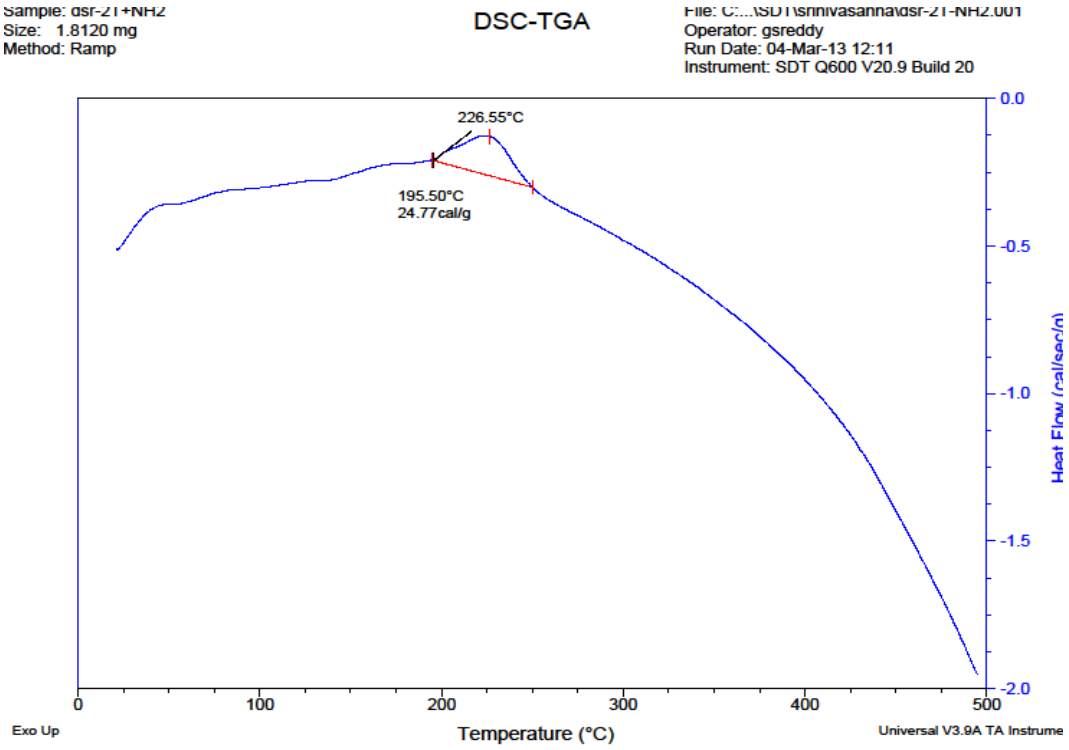
c. TG-DTA measurement



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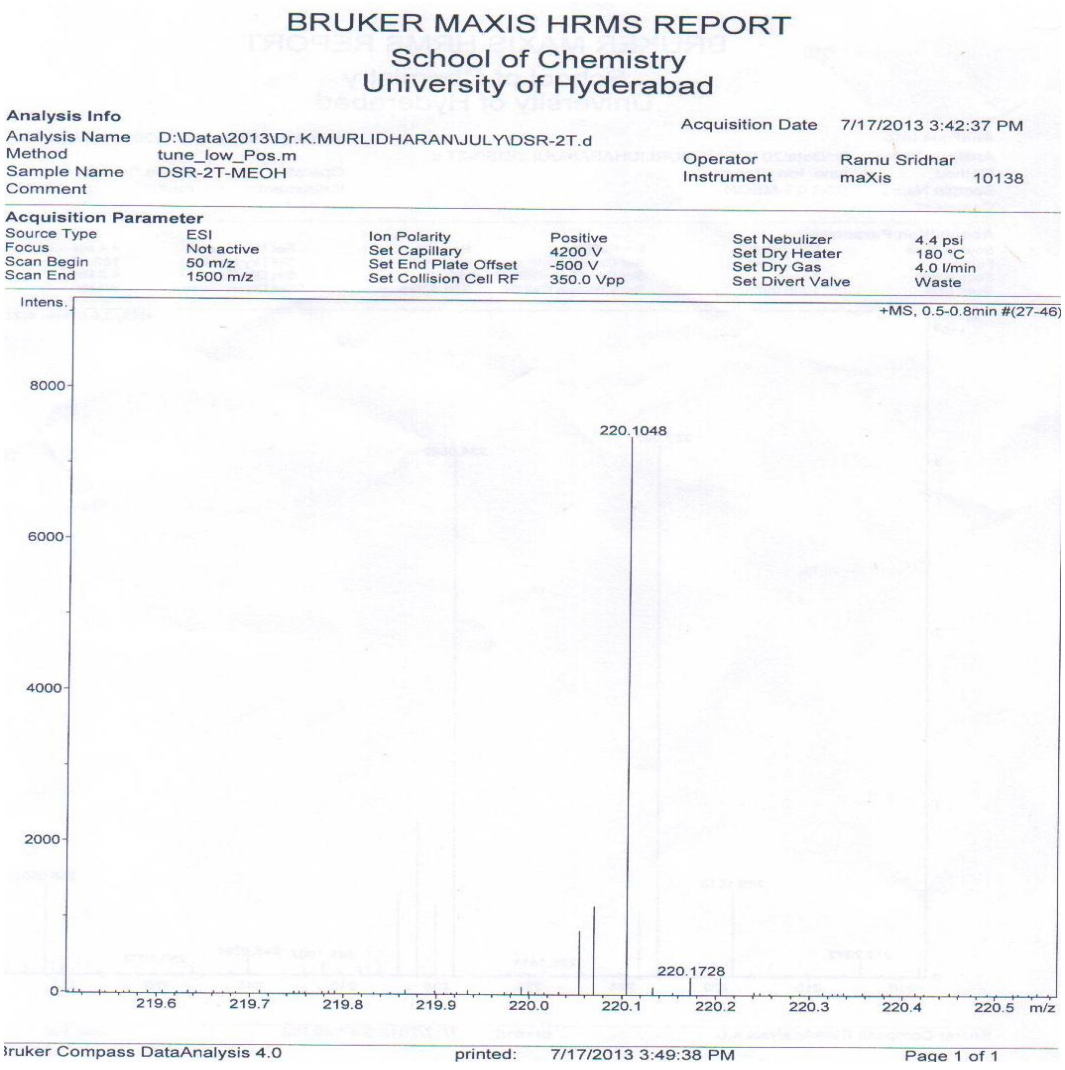
d.HRMS



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e. C H N analysis

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Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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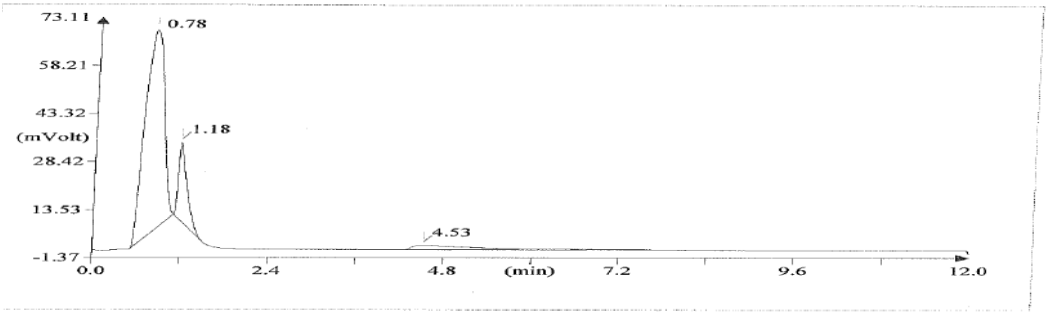

Element Name	Element %	Ret. Time
Nitrogen	70. 21	0. 78
Carbon	27. 51	1. 18
Hydrogen	2. 36	4. 53

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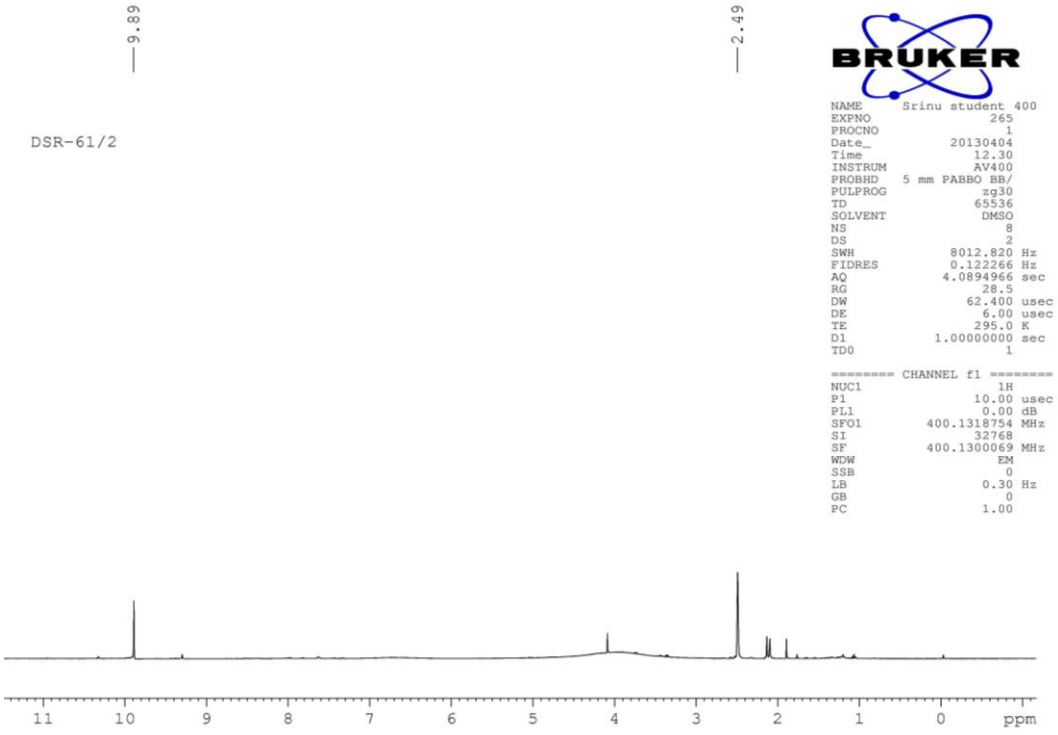
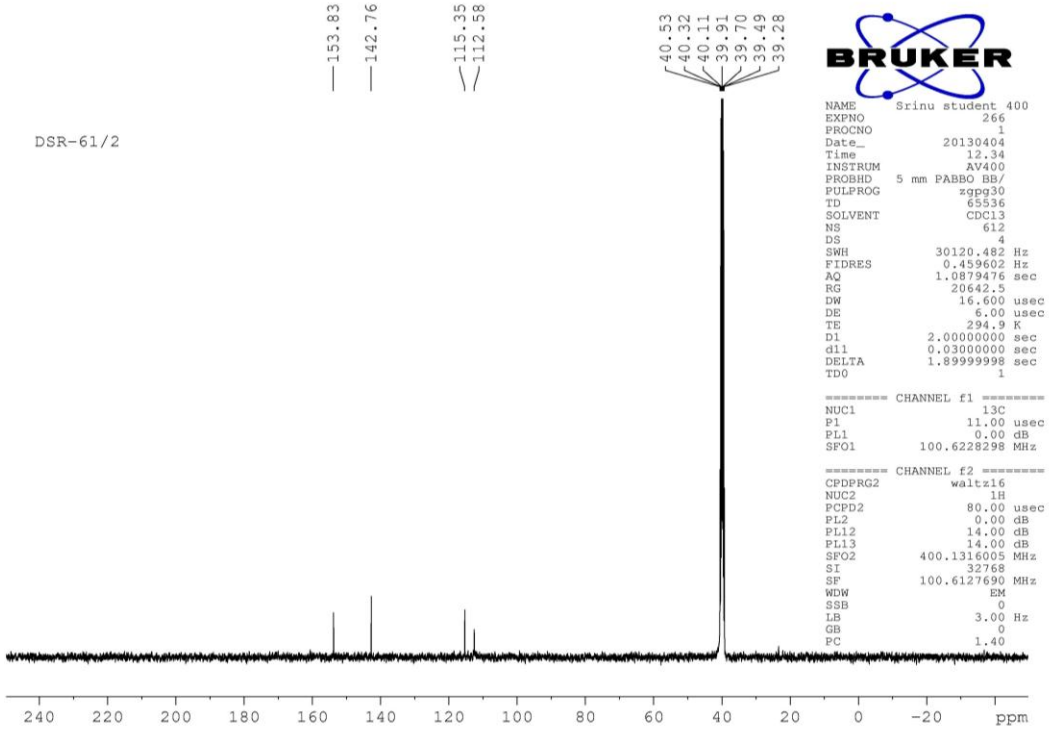
4. 2-(1*H*-Tetrazol-1-yl)-1*H*-imidazole-4,5-dicarbonitrile(6)

a. ^{1}H NMR



b. ^{13}C NMR



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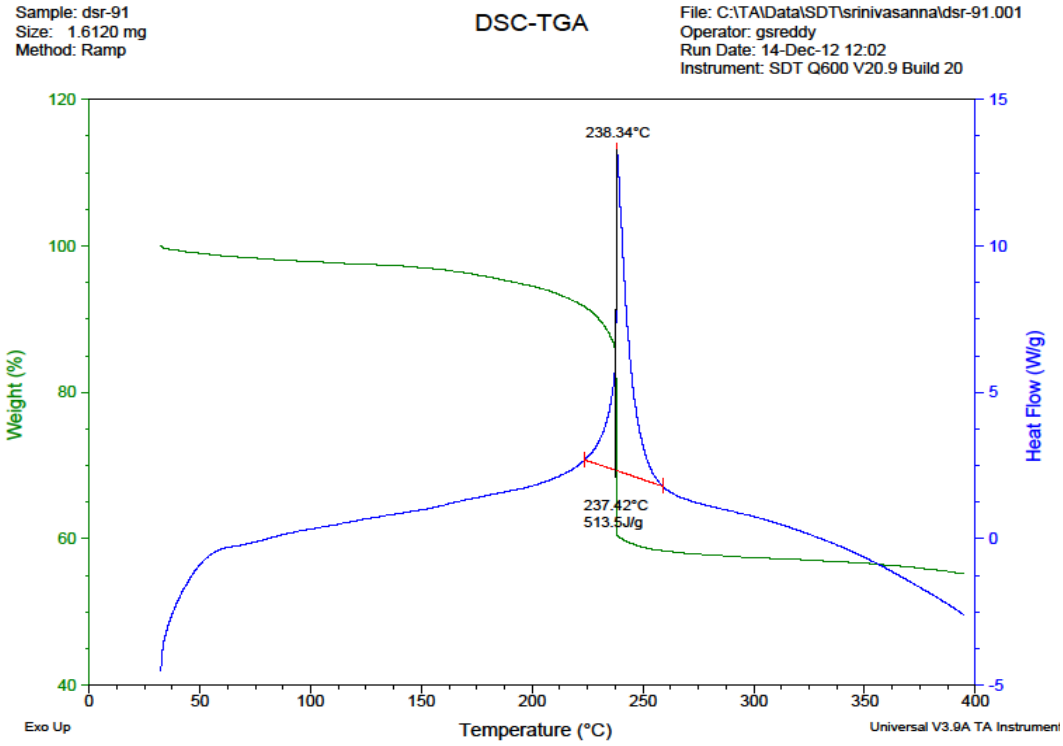
c. TG-DTA measurement



d.HRMS

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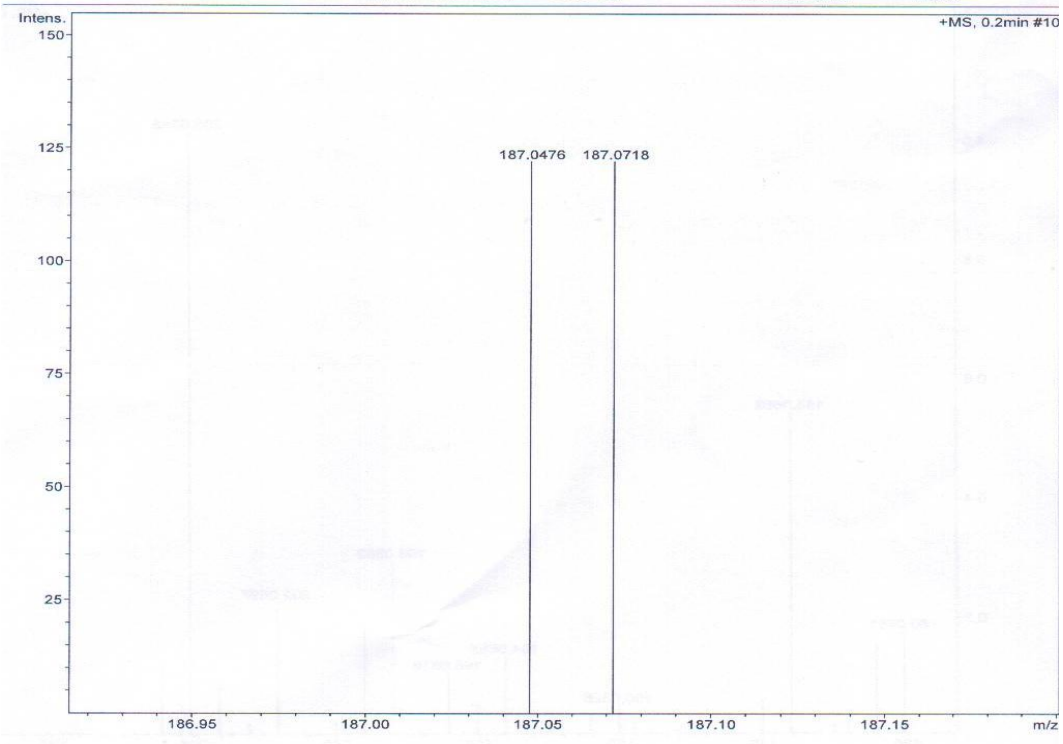
Analysis Info

Analysis Name	D:\Data\2013\Dr.K.MURLIDHARAN\JULY\DSR-61.d	Acquisition Date	7/31/2013 2:33:05 PM
Method	tune_low_Pos.m	Operator	Ramu Sridhar
Sample Name	DSR-61-MEOH	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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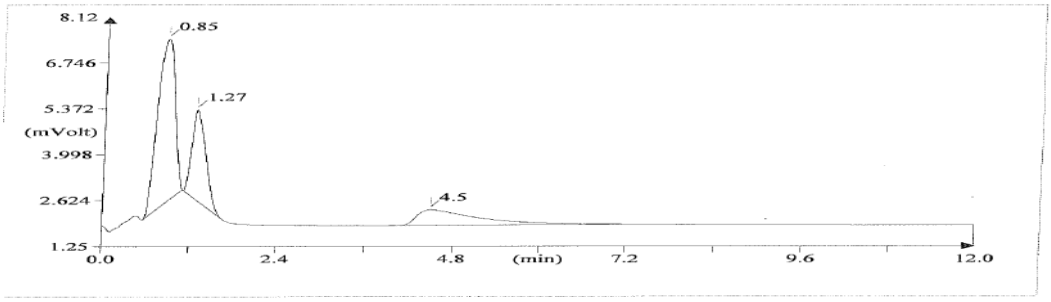
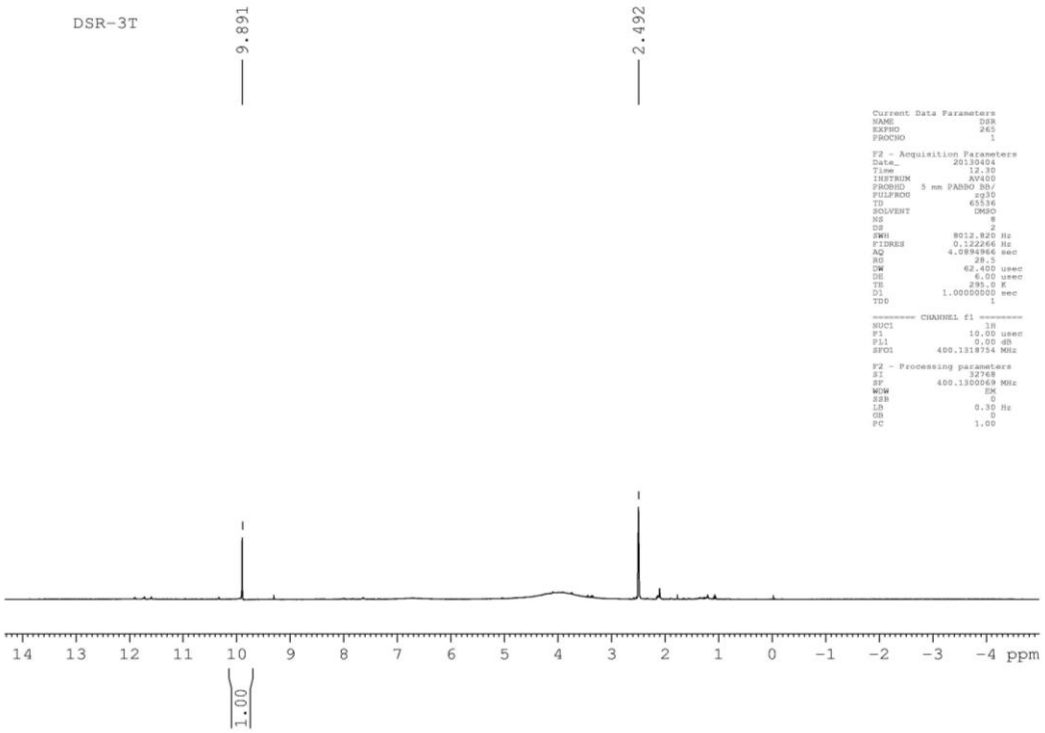
Sample weight:	.612



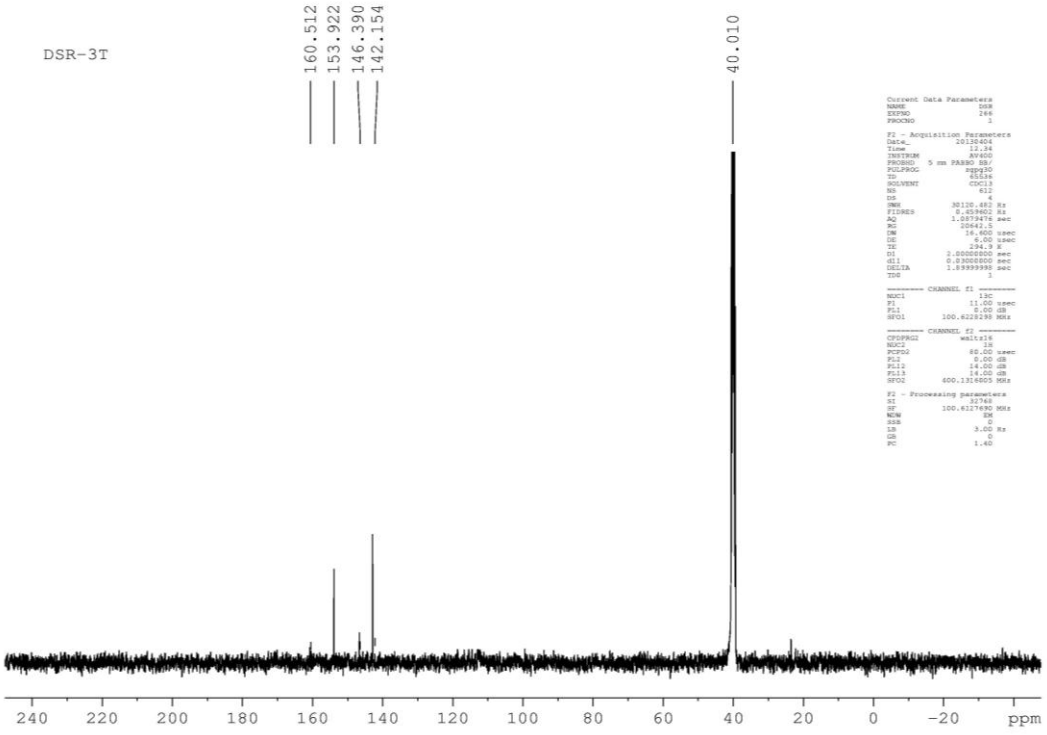
Element Name	Element %	Ret. Time
Nitrogen	60. 36	0. 85
Carbon	38. 65	1. 27
Hydrogen	1. 16	4. 50

5. 5, 5'-(2-(1*H*-Tetrazol-1-yl)-1*H*-imidazole-4,5-diyl)bis(1*H*-tetrazole) (7)

a. ^{1}H NMR



b. ^{13}C NMR



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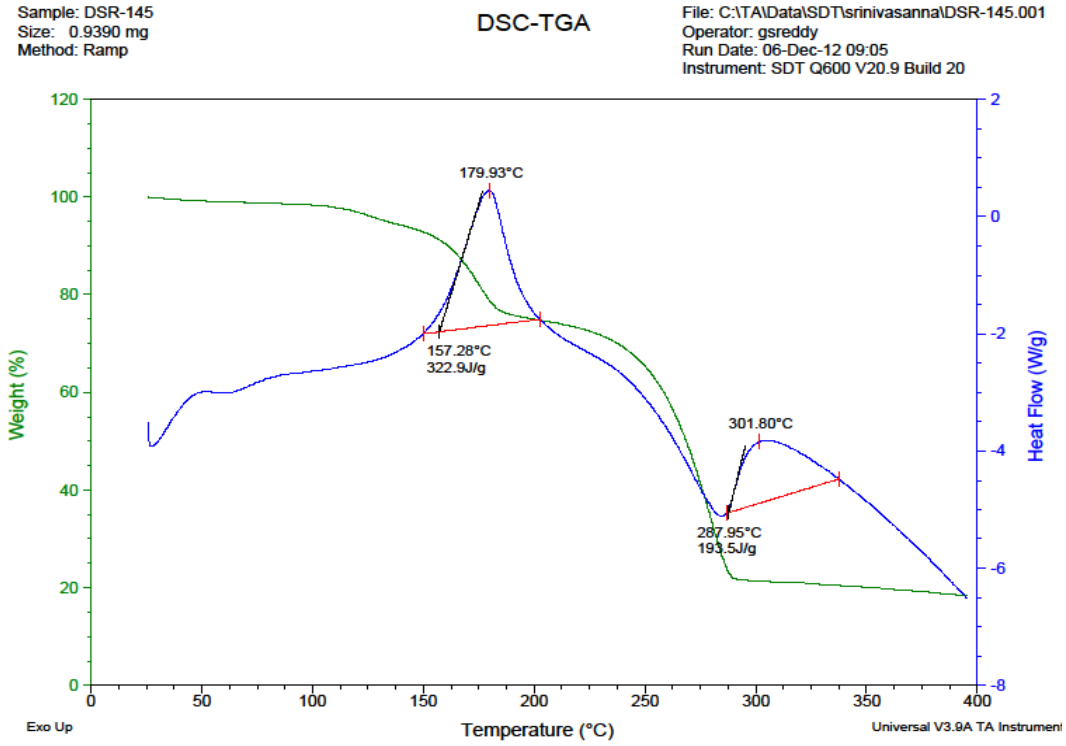
c. TG-DTA measurement



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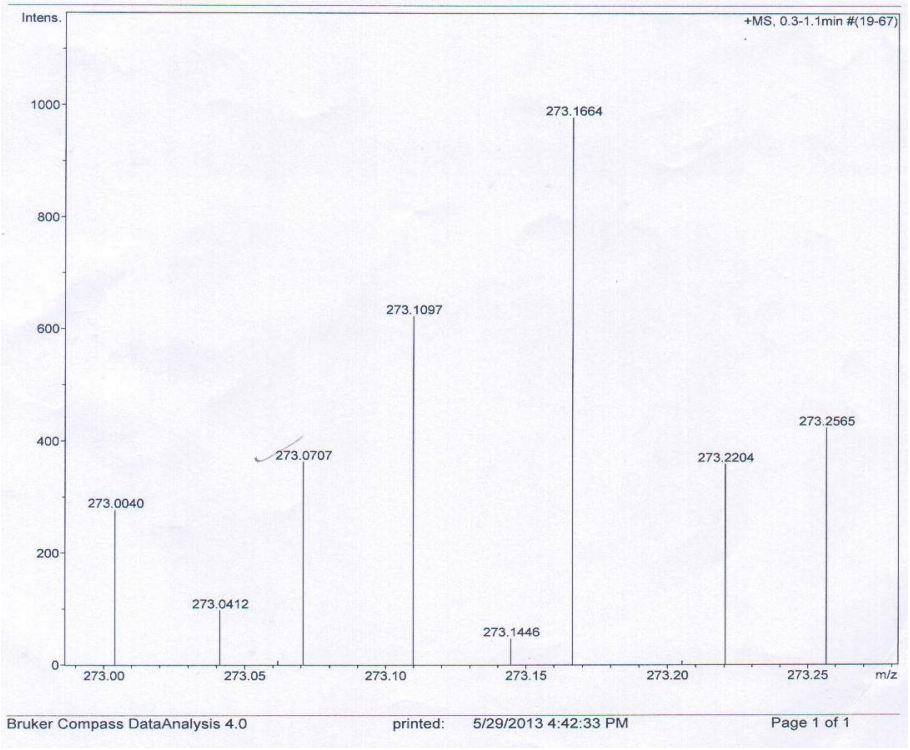
Analysis Info

Analysis Name	D:\Data\2013\Dr.K.MURLIDHARAN\MAY\DSR-7-37.d	Acquisition Date	5/29/2013 3:04:58 PM
Method	tune_low.m	Operator	Ramu Sridhar
Sample Name	DSR-7-37-MEOH	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	200 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1800 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



Bruker Compass DataAnalysis 4.0 printed: 5/29/2013 4:42:33 PM Page 1 of 1

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e. C H N analysis

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Method filename: E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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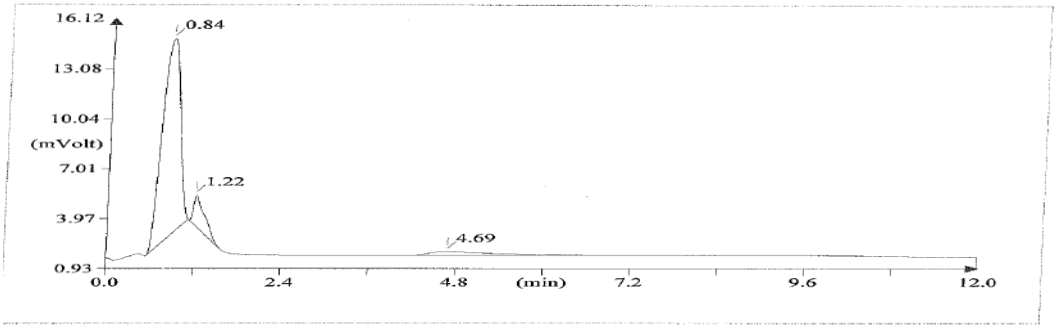
Analysis type: UnkNown
Chromatogram filename: UNK-15022013-1.dat
Sample weight: .786



Element Name	Element %	Ret. Time
Nitrogen	72. 15	0. 84
Carbon	26. 35	1. 22
Hydrogen	1. 41	4. 69

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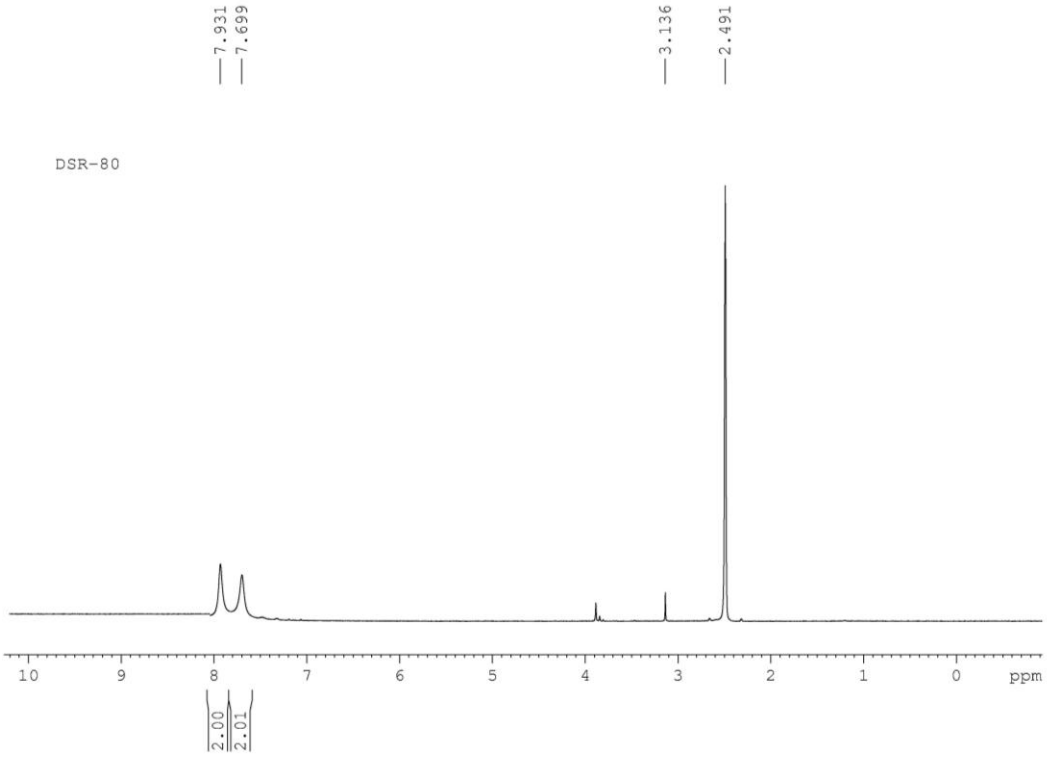
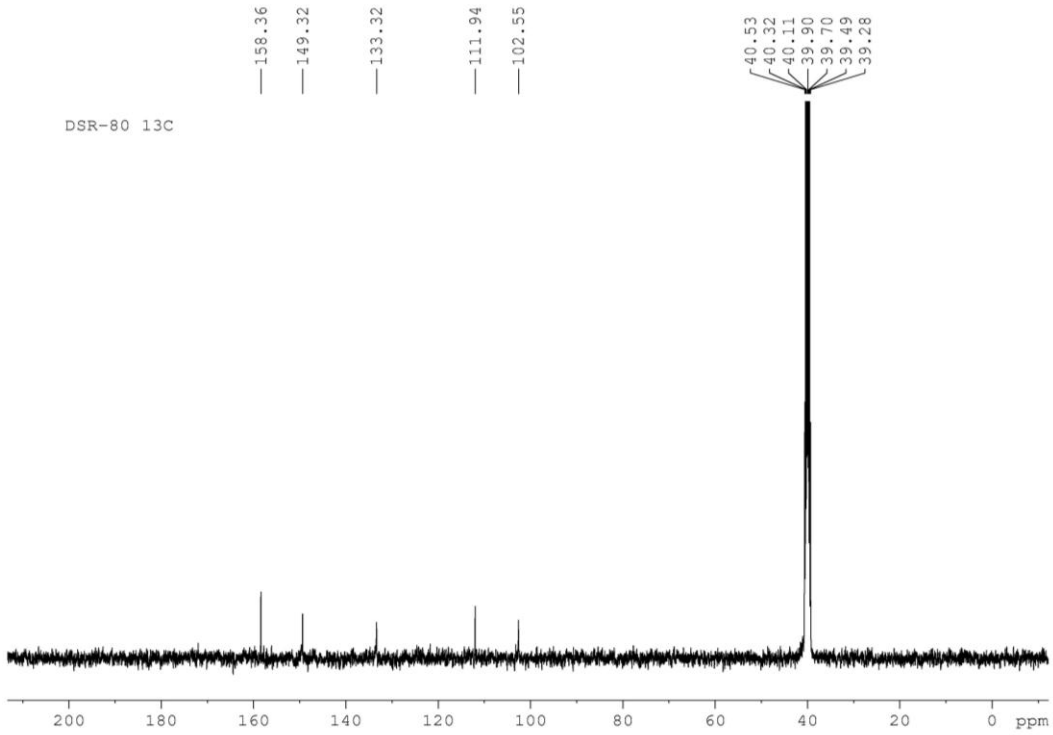
6. 2-Amino-5-cyano-1*H*-imidazole-4-carboxamide (8)

a. ^{1}H NMR



b. ^{13}C NMR



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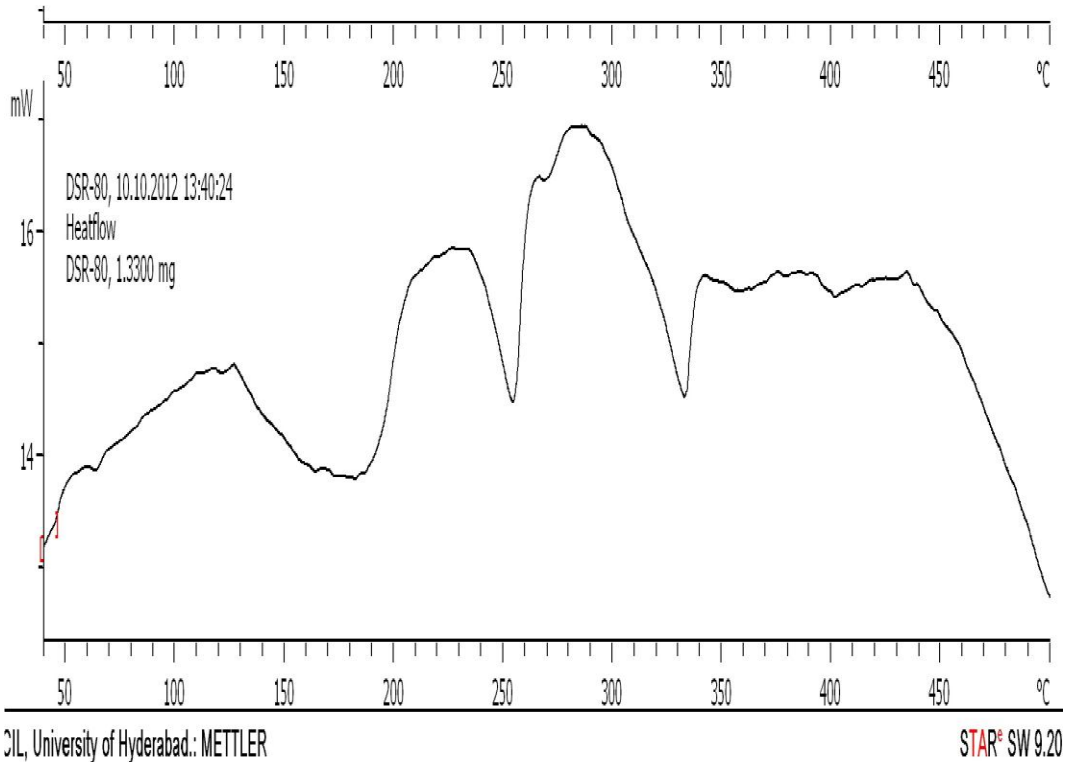
c. TG-DTA measurement



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d. HRMS

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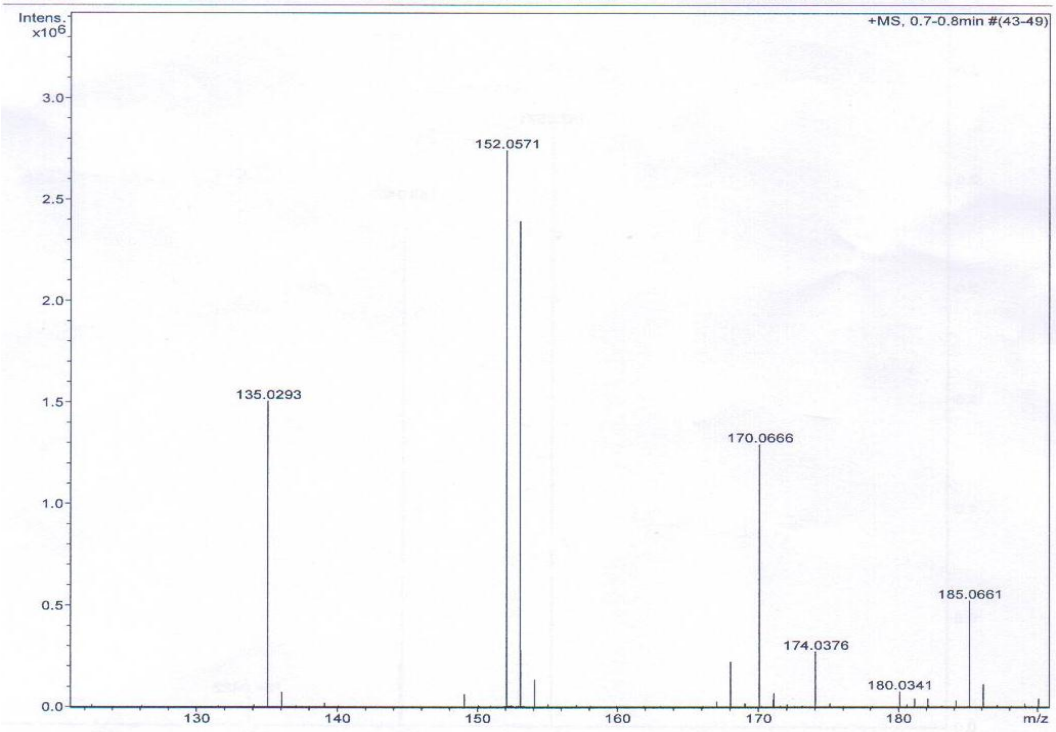
Analysis Info

Analysis Name	D:\Data\2013\Dr.K.MURLIDHARAN\JULY\DSR-80.d	Acquisition Date	7/9/2013 4:31:32 PM
Method	tune_low_Pos-R2.m	Operator	Ramu Sridhar
Sample Name	DSR-80-MEOH	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2580 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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Method filename:	C:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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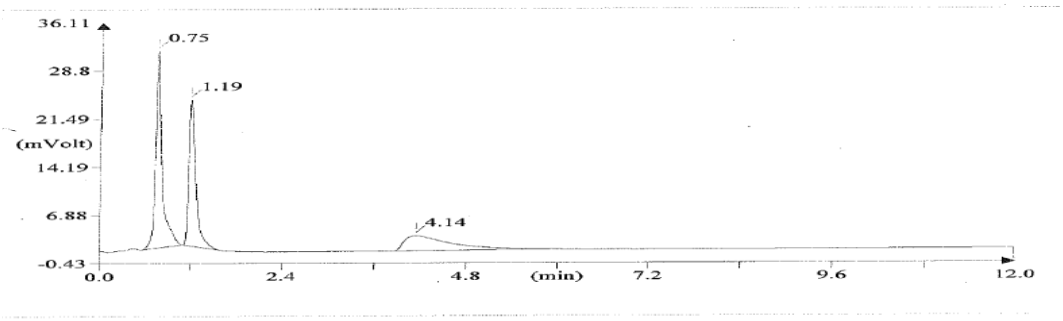

Element Name	Element %	Ret. Time
Nitrogen	46. 23	0. 75
Carbon	39. 62	1. 19
Hydrogen	3. 38	4. 14

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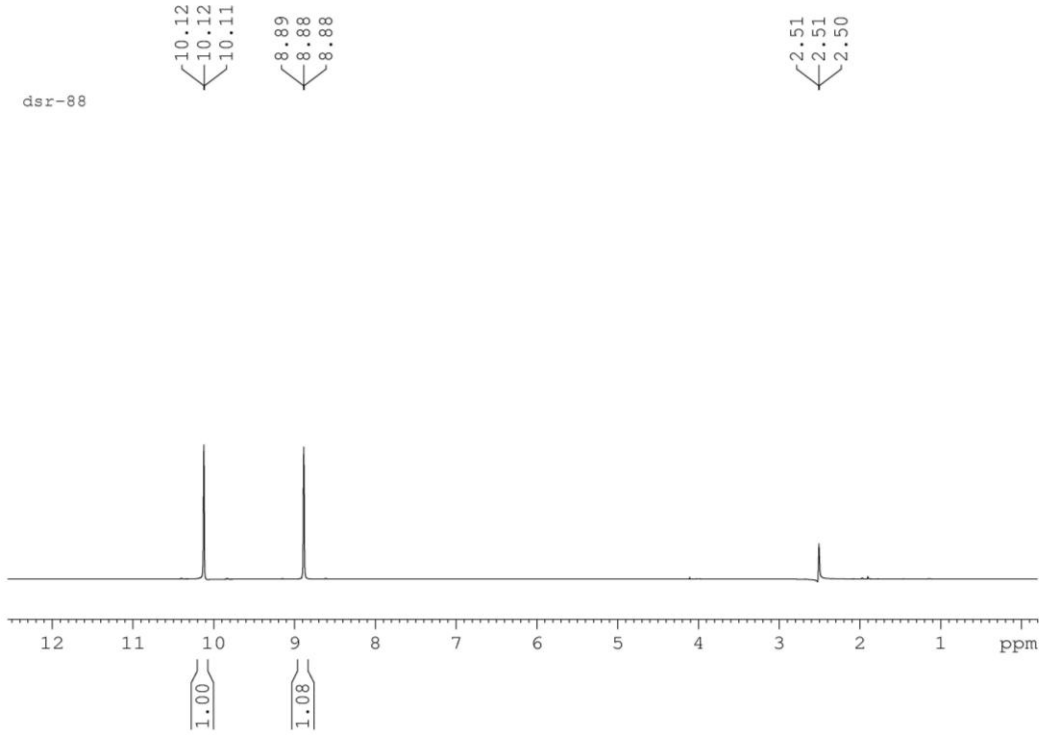
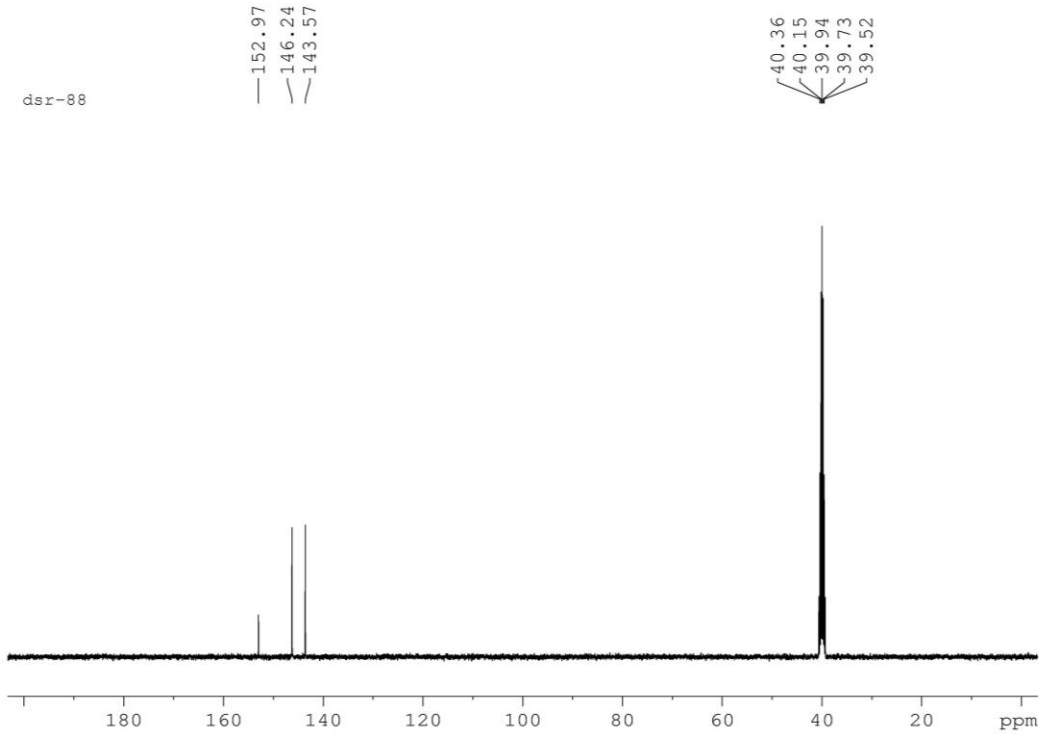
7. 1-(1*H*-1,2,4-Triazol-3-yl)-1*H*-tetrazole (9)

a. ^{1}H NMR



b. ^{13}C NMR



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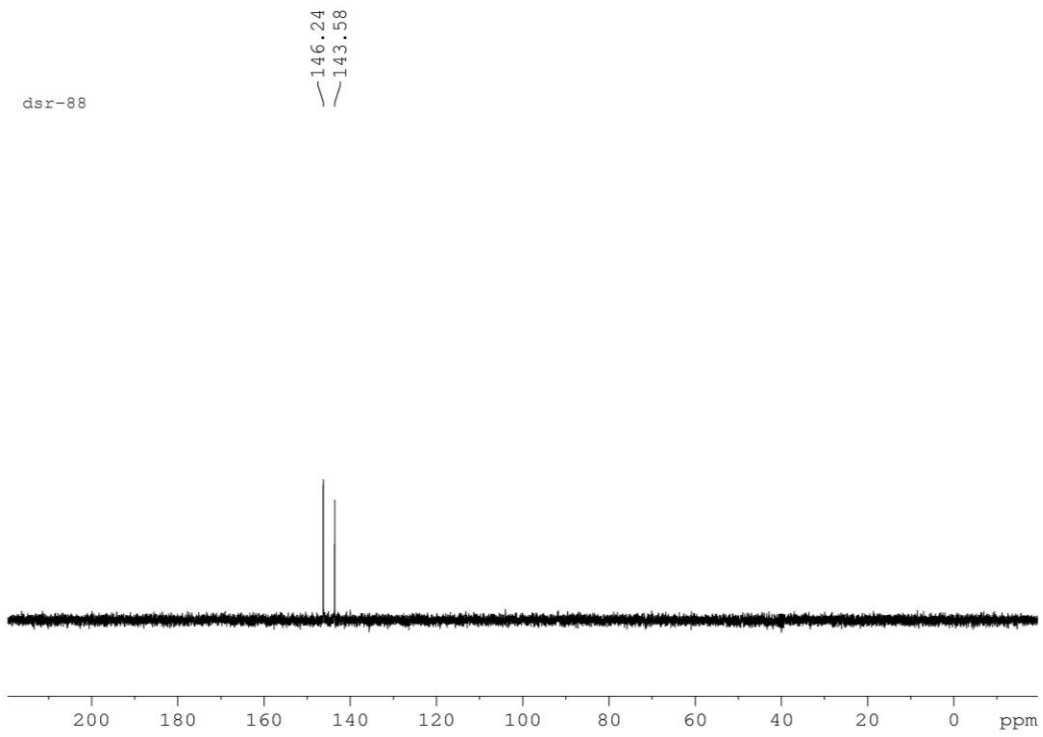
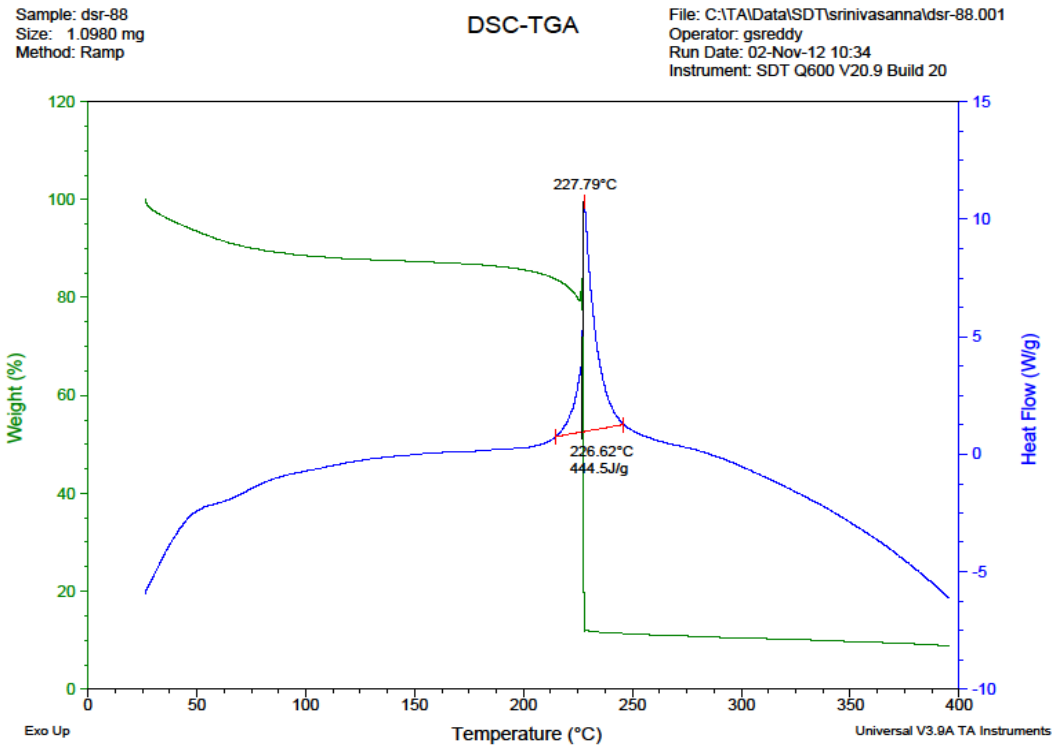
c. DEPT



d. TG-DTA measurement



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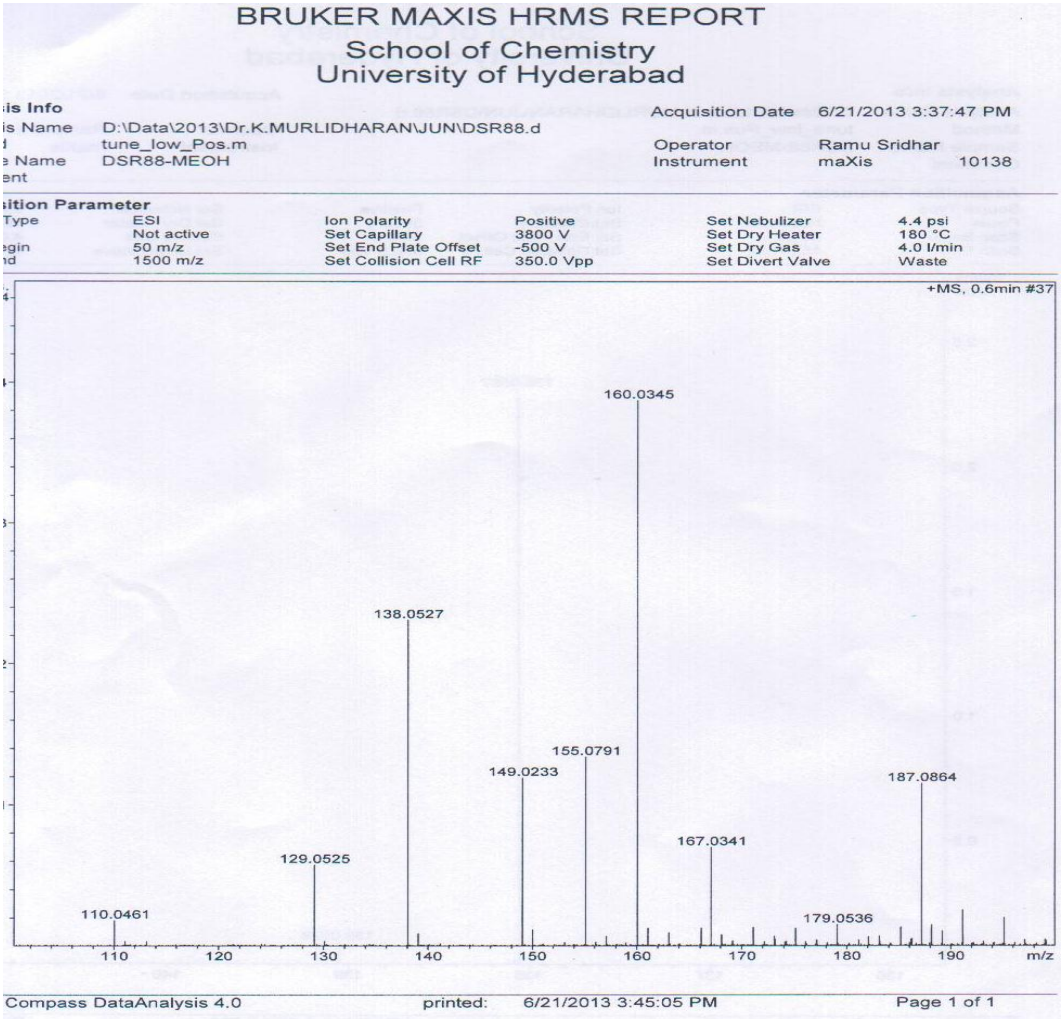
e. HRMS



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f. C H N analysis

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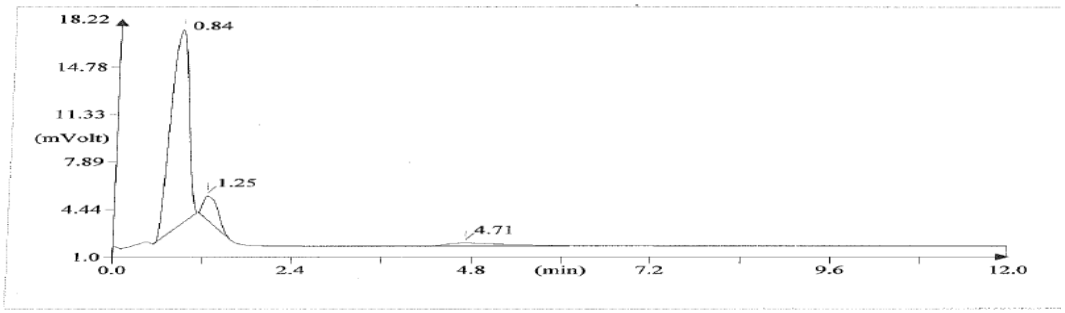

Element Name	Element %	Ret. Time
Nitrogen	72. 21	0. 84
Carbon	26. 58	1. 25
Hydrogen	1. 42	4. 71

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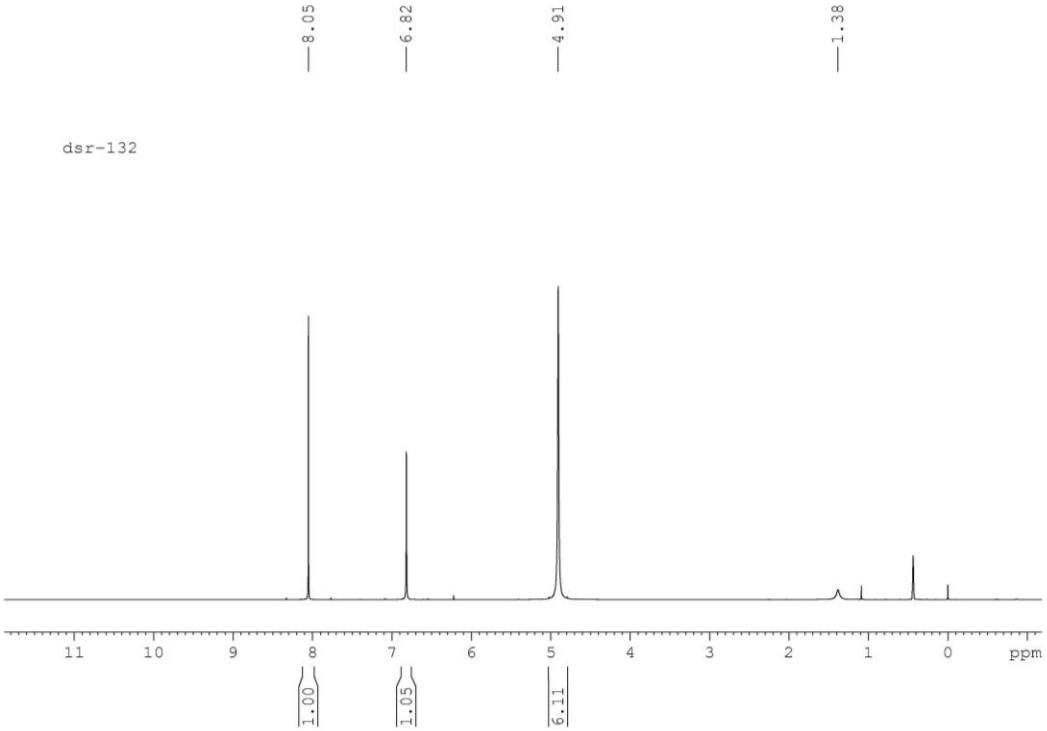
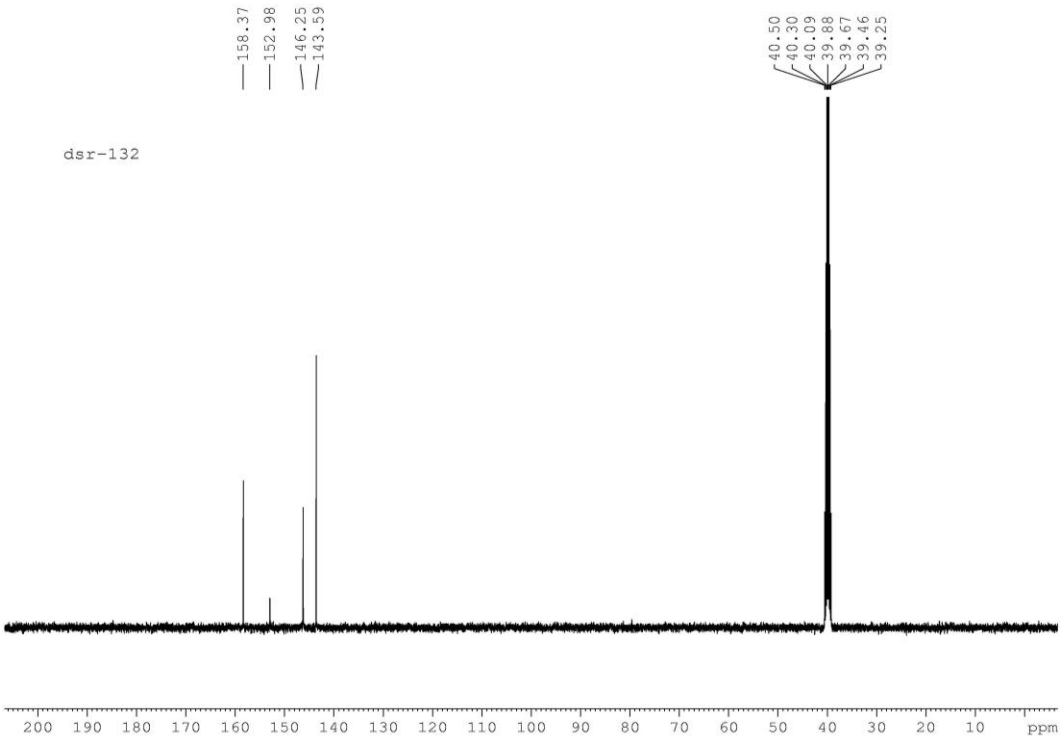
8. Diaminomethaniminium 3-(1H-tetrazol-1-yl)-1,2,4-triazol-1-ide (9a)

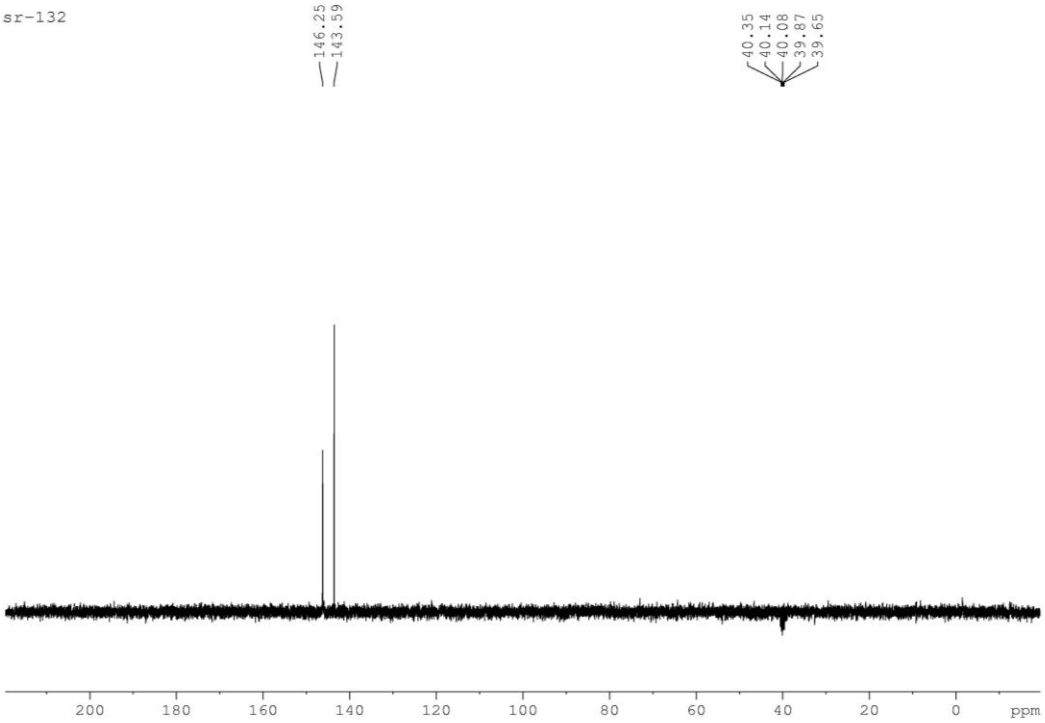
a. ^{1}H NMR



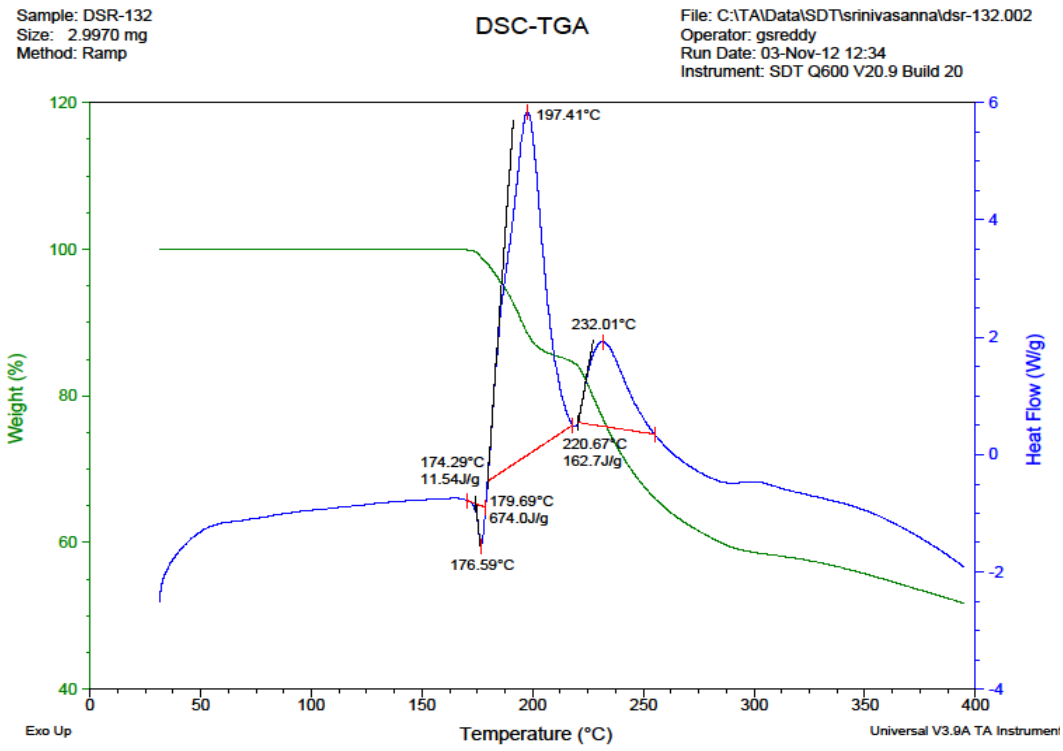
b. ^{13}C NMR



c. DEPT



d. TG-DTA measurement



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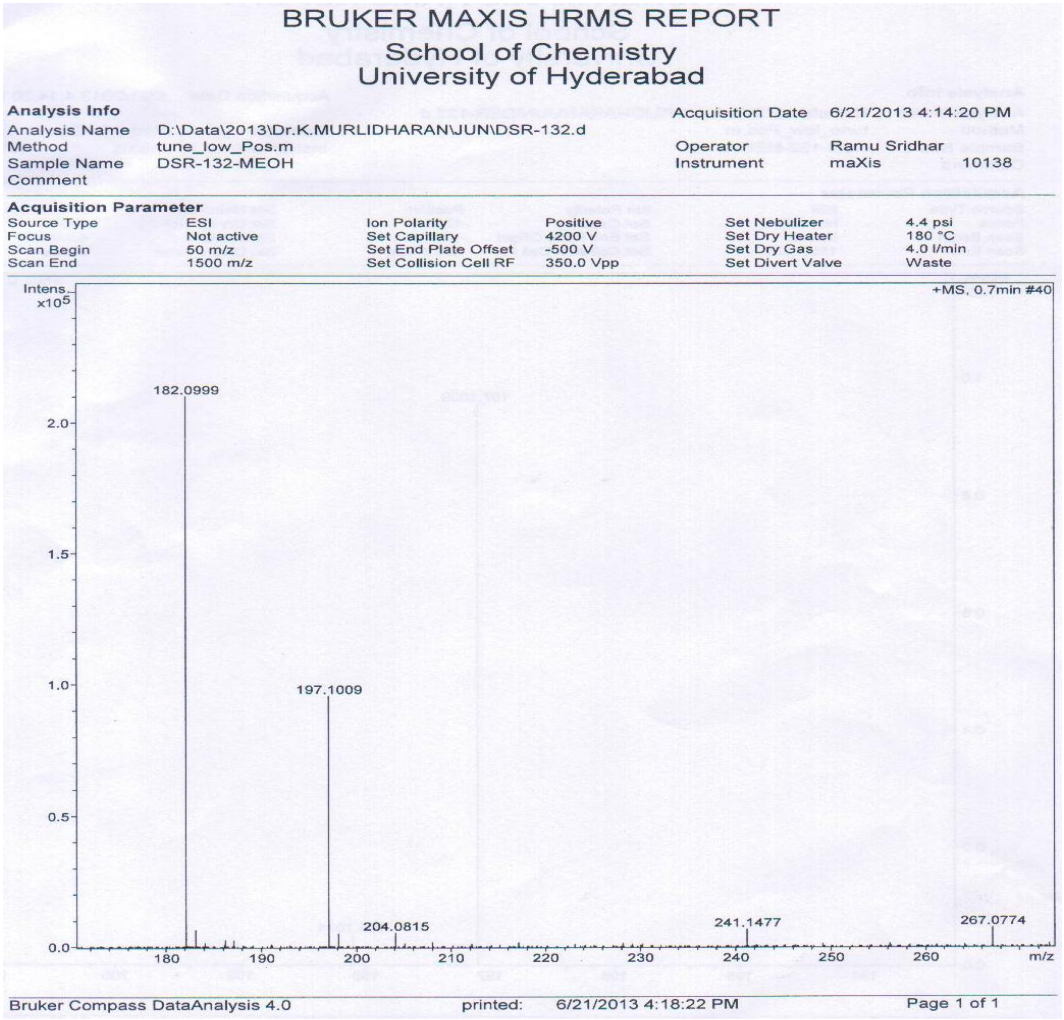
e. HRMS



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f. C H N analysis

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Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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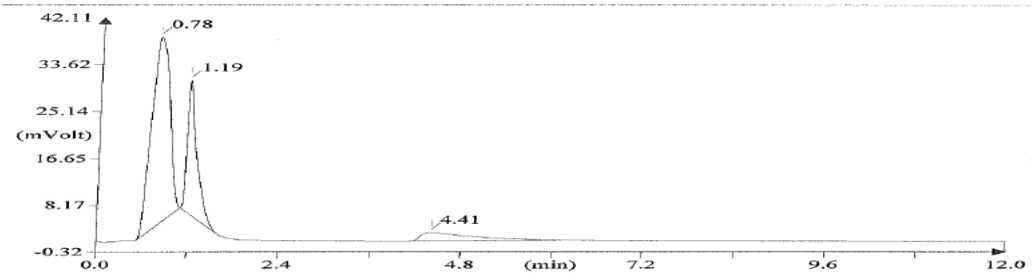
Chromatogram filename:	UNK-20022013-17.dat
Sample weight:	1.481



Element Name	Element %	Ret. Time
Nitrogen	71. 52	0. 78
Carbon	24. 56	1. 19
Hydrogen	4. 06	4. 41

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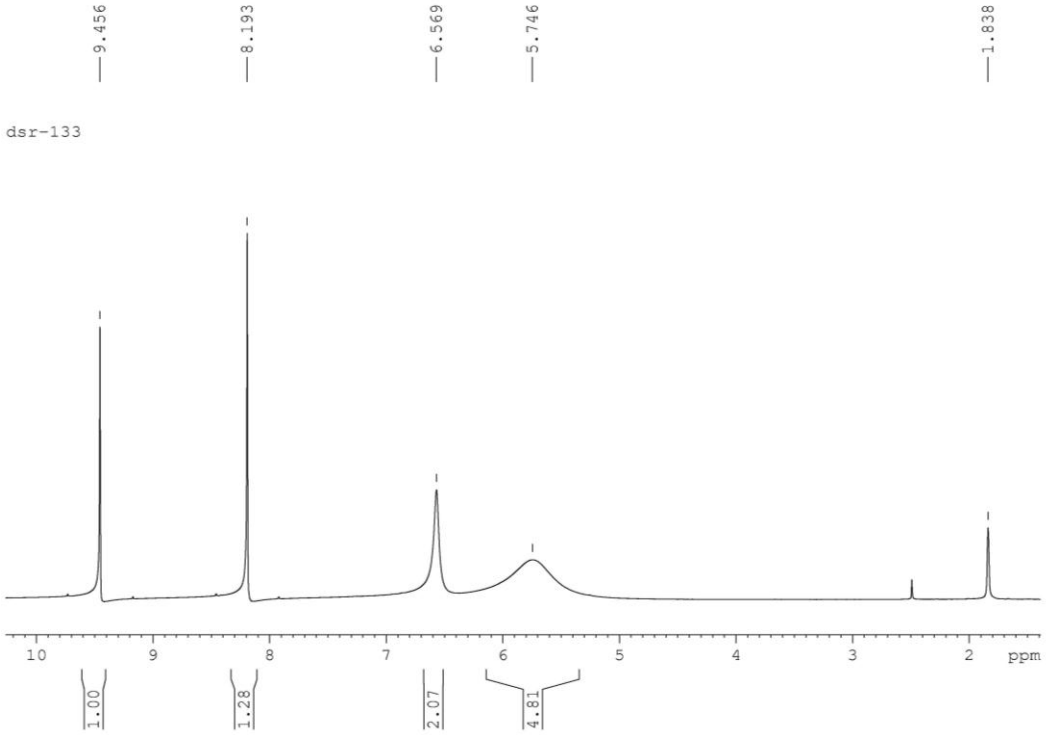
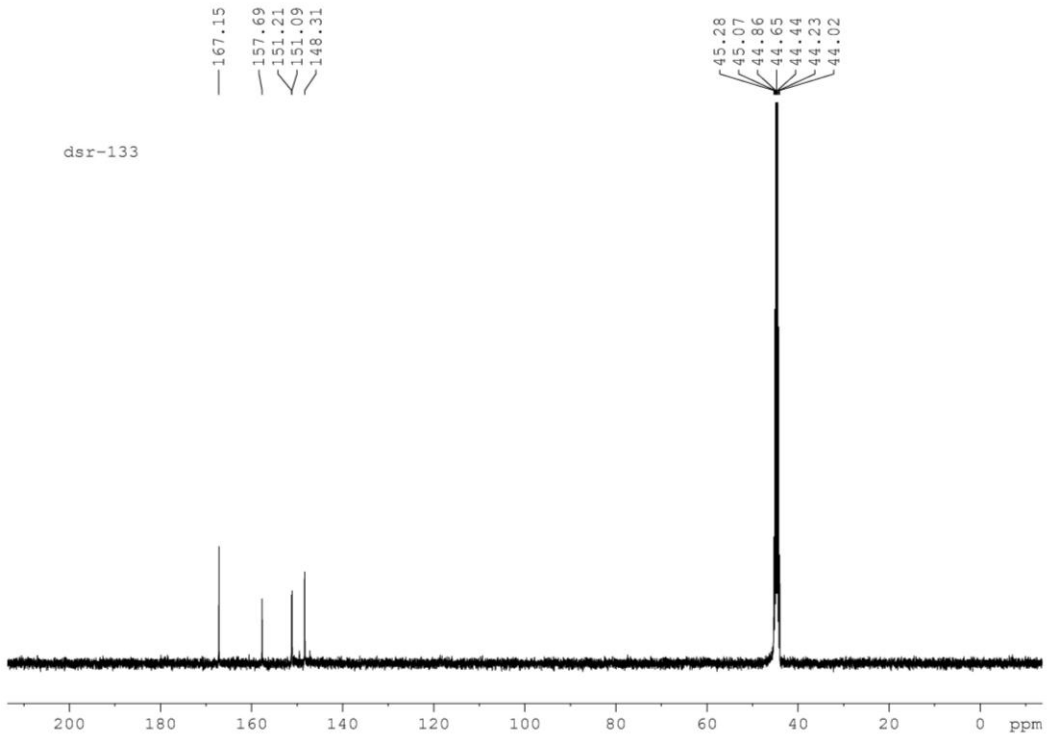
9. (Hydrazinylcarbonyl)hydrazinium 3-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide (9b)

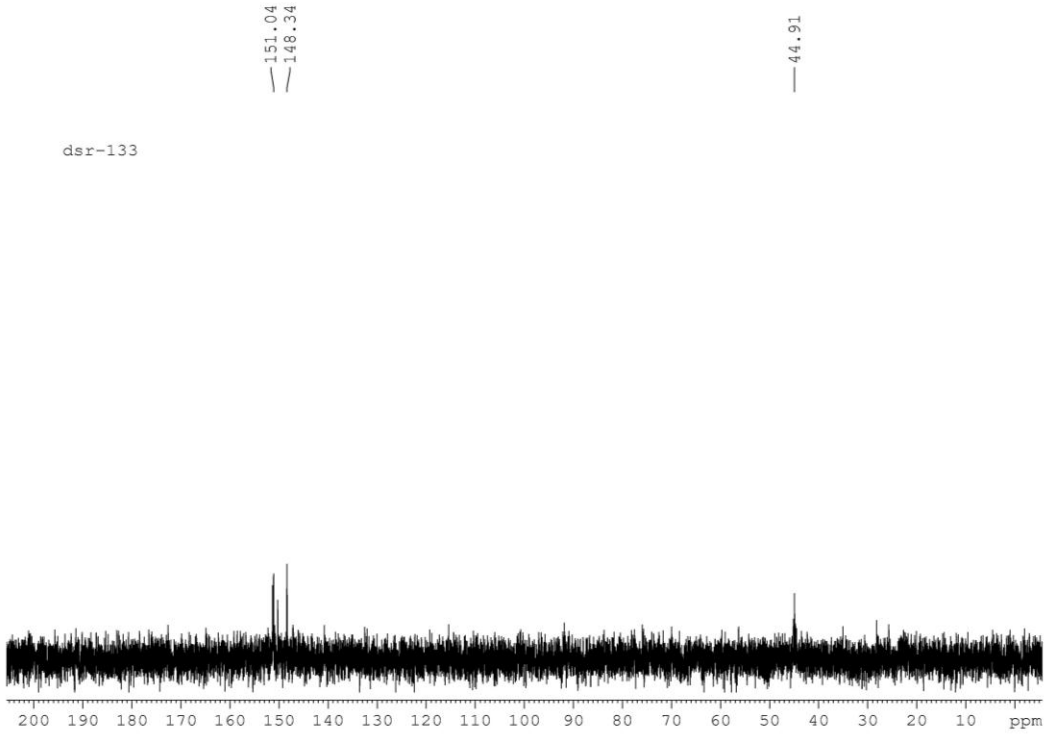
a. ^{1}H NMR



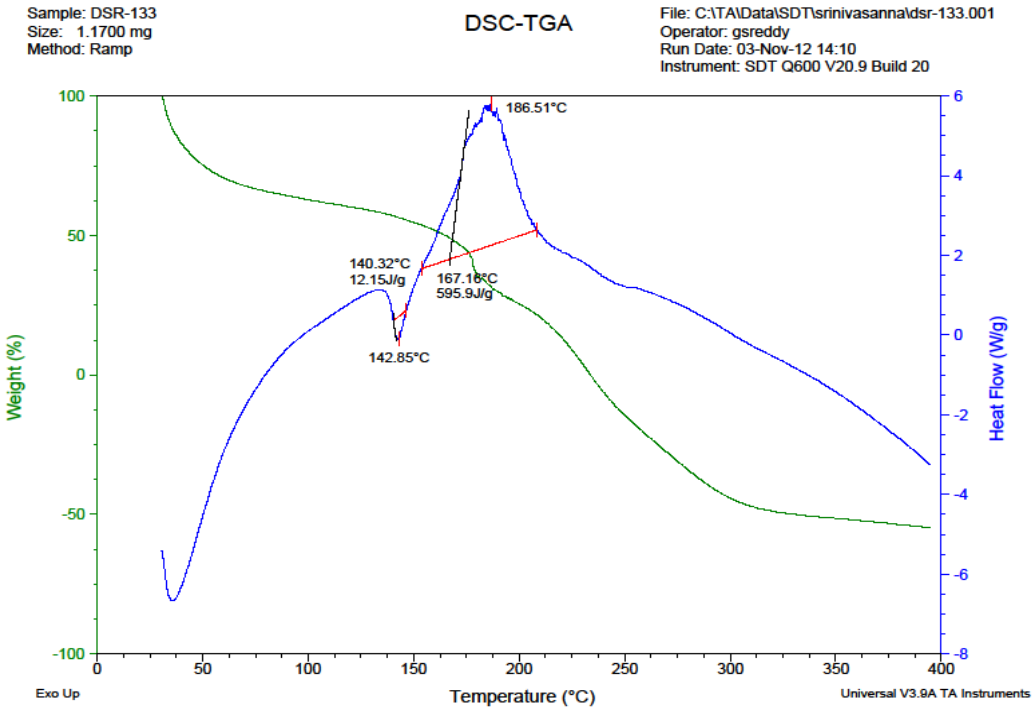
b. ^{13}C NMR



c. DEPT



d. TG-DTA measurement



e. C H N analysis

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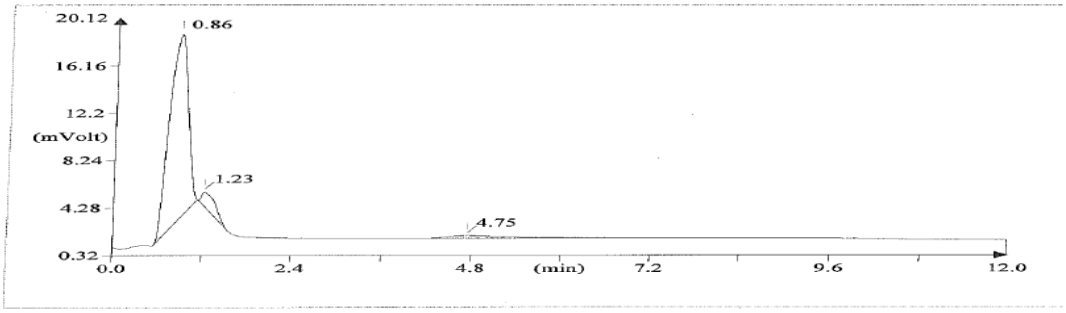
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	DSR-133 (# 102)
Analysis type:	UnkNown
Chromatogram filename:	UNK-20022013-22.dat
Sample weight:	.973



Element Name	Element %	Ret. Time
Nitrogen	67. 72	0. 86
Carbon	21. 06	1. 23
Hydrogen	3. 91	4. 75

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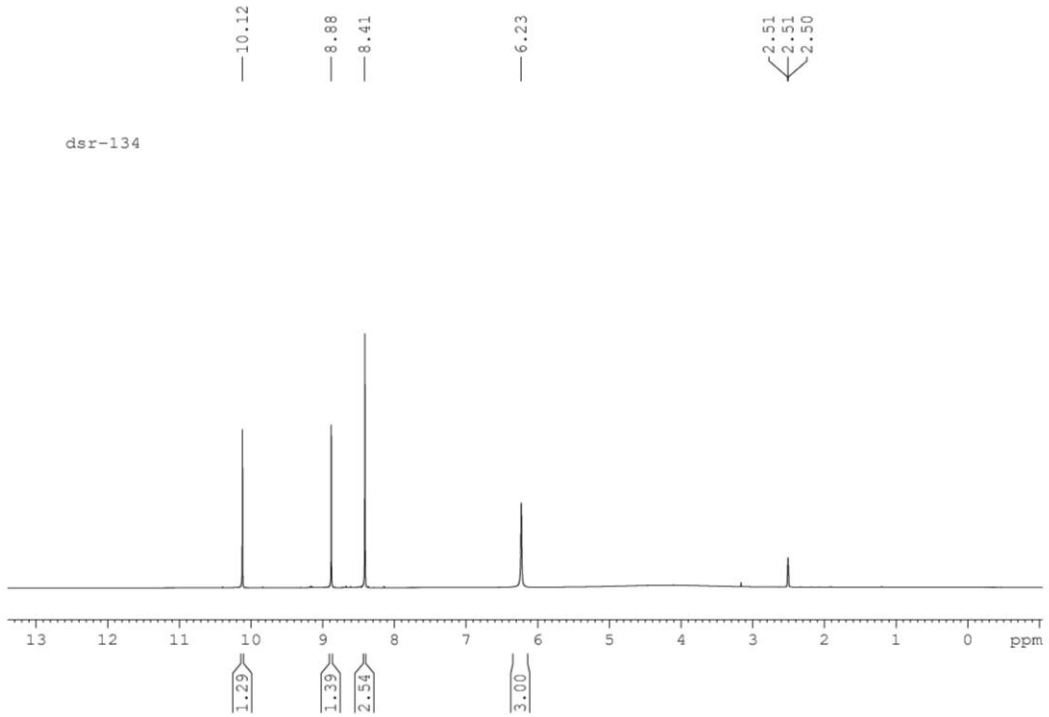
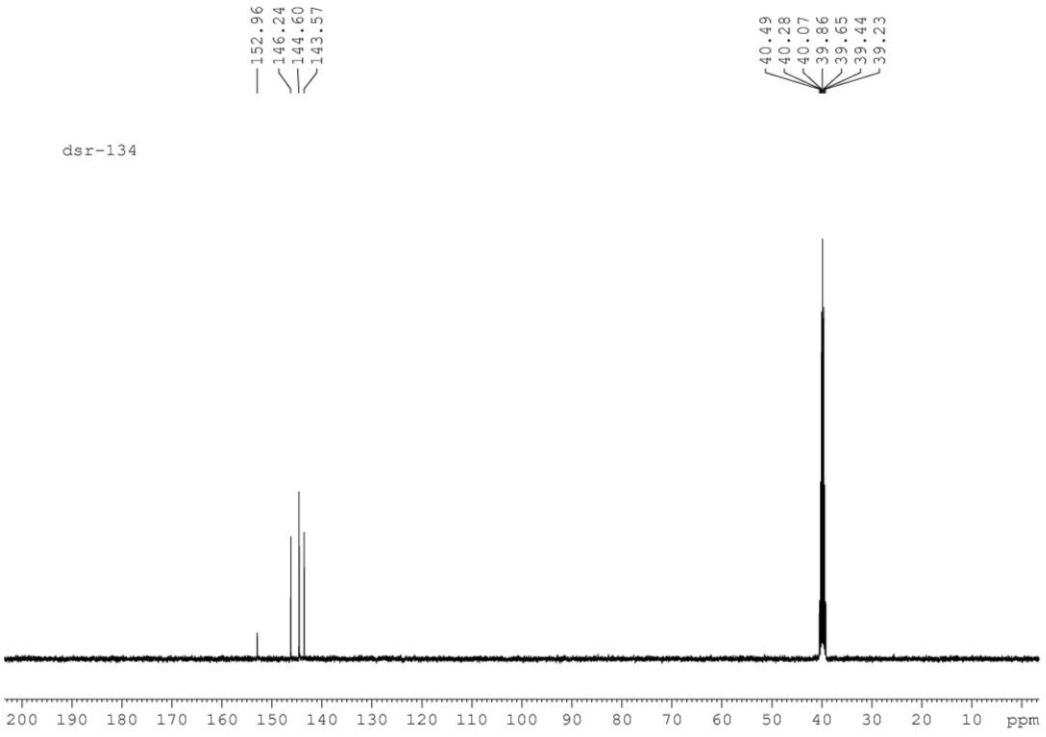
10. 4-Amino-4*H*-1,2,4-triazol-1-ium 3-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide (9c)

a. ^{1}H NMR



b. ^{13}C NMR



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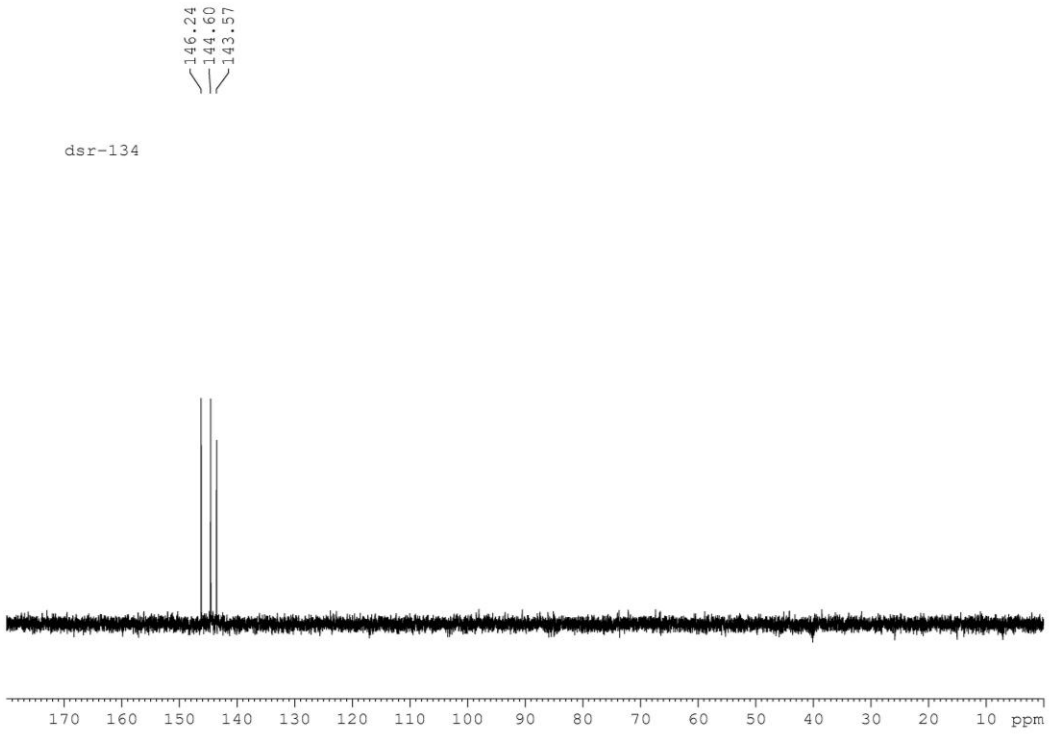
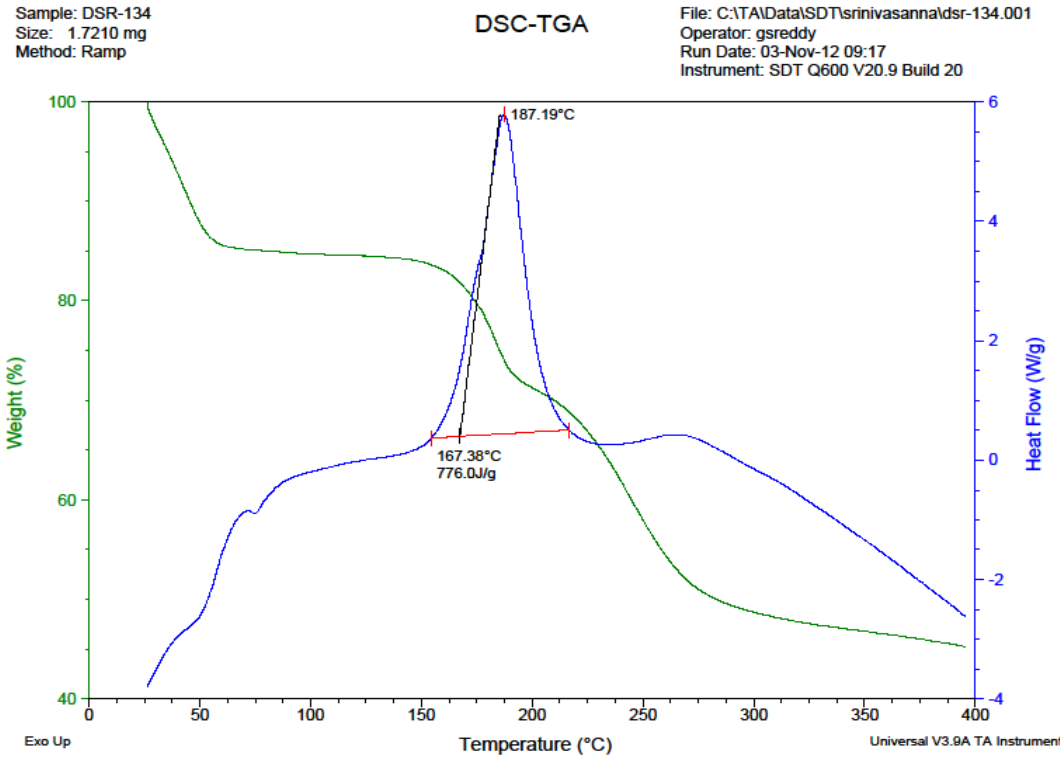
c. DEPT



d. TG-DTA measurement



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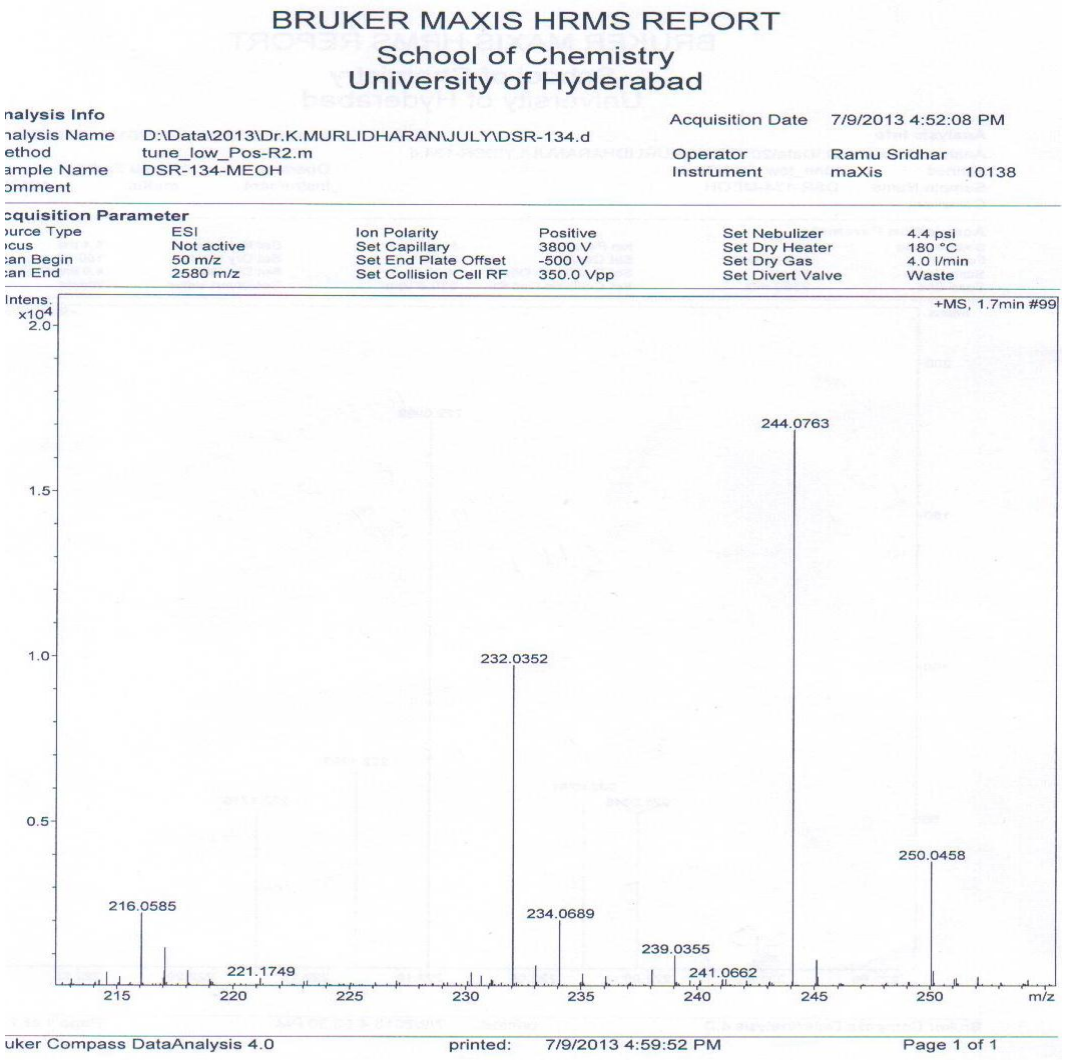
e. HRMS



f. C H N analysis

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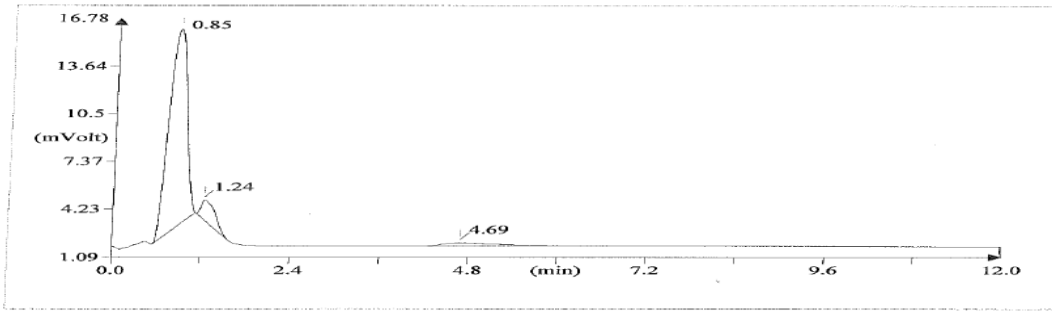
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	DSR-134 (# 104)
Analysis type:	UnkNown
Chromatogram filename:	UNK-20022013-24.dat
Sample weight:	.955



Element Name	Element %	Ret. Time
Nitrogen	69. 51	0. 85
Carbon	27. 06	1. 24
Hydrogen	3. 25	4. 89

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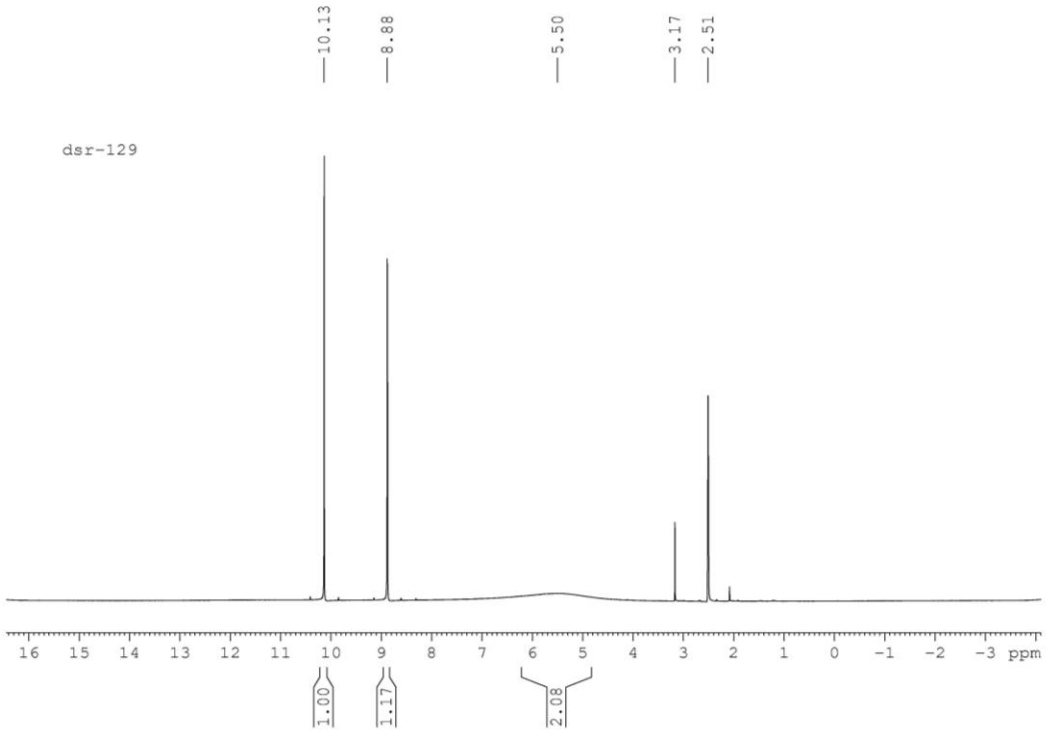
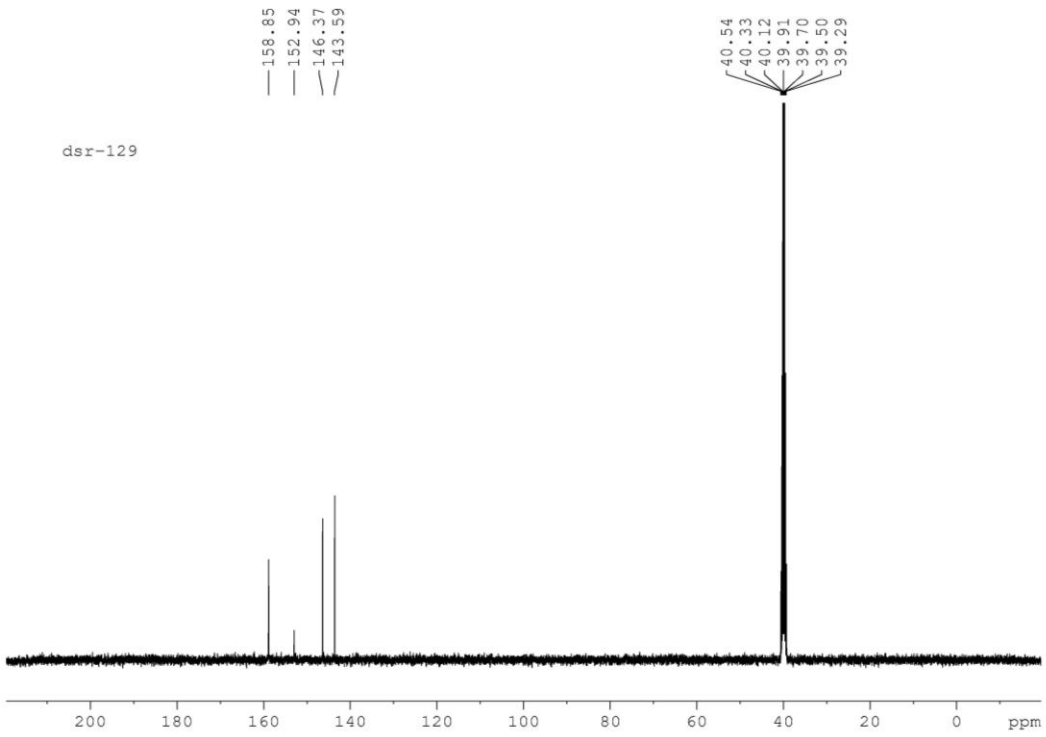
11. 3-Amino-1*H*-1,2,4-triazol-4-ium 3-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide (9d)

a. ^{1}H NMR



b. ^{13}C NMR



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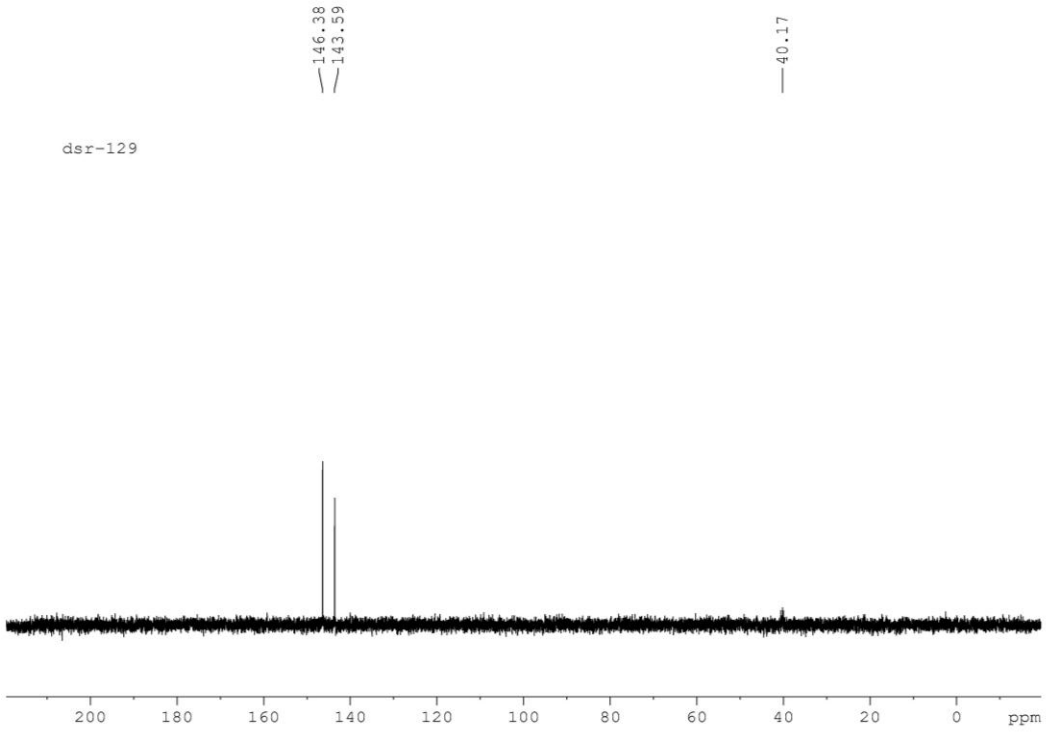
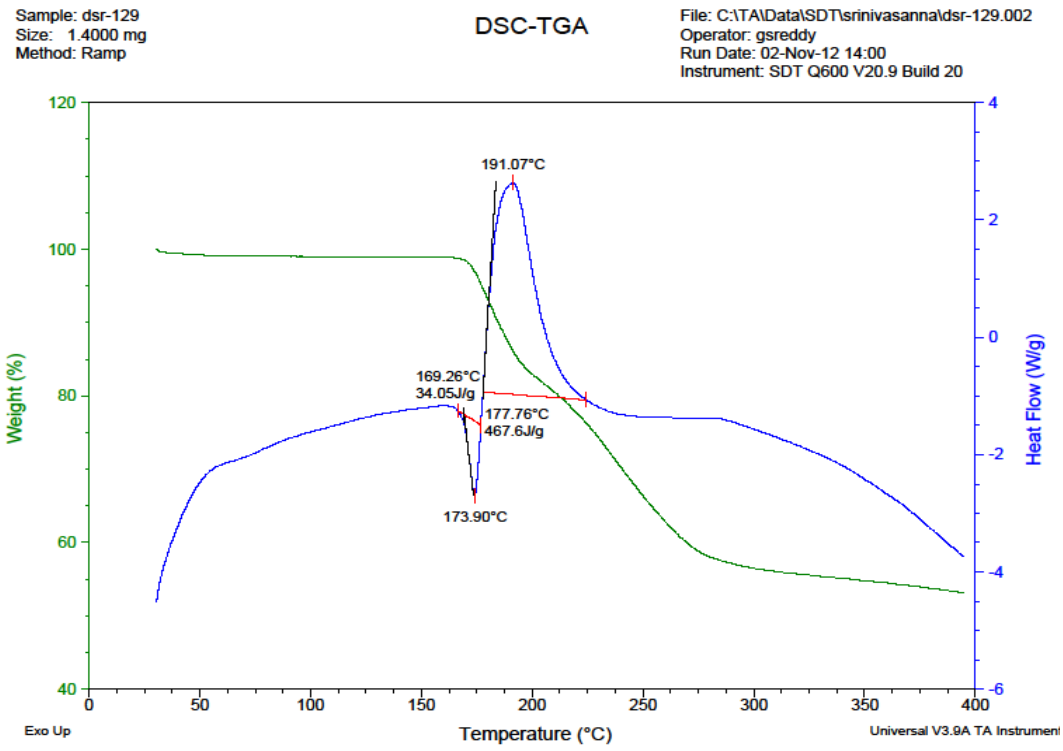
c. DEPT



d. TG-DTA measurement



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e. C H N analysis

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Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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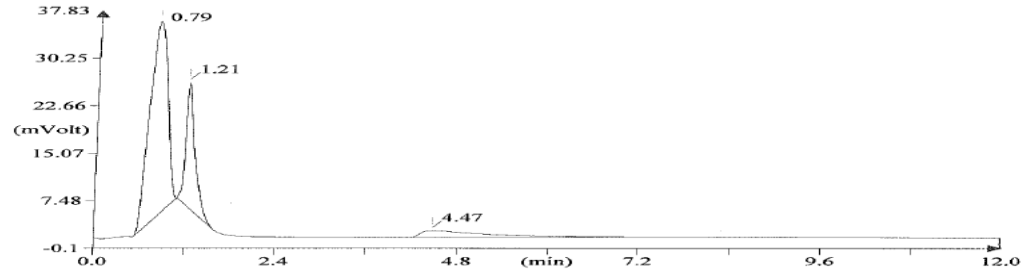
Analysis type:	UnkNown
Chromatogram filename:	UNK-20022013-16.dat
Sample weight:	1.472



Element Name	Element %	Ret. Time
Nitrogen	69. 52	0. 79
Carbon	27. 06	1. 21
Hydrogen	3. 24	4. 47

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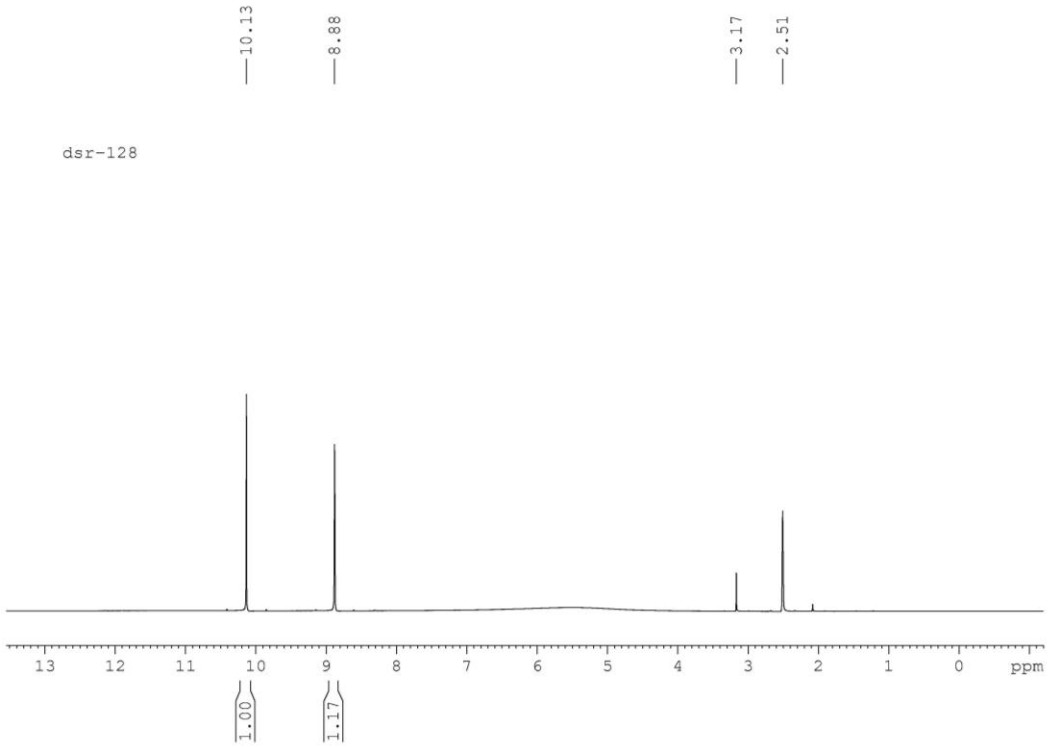
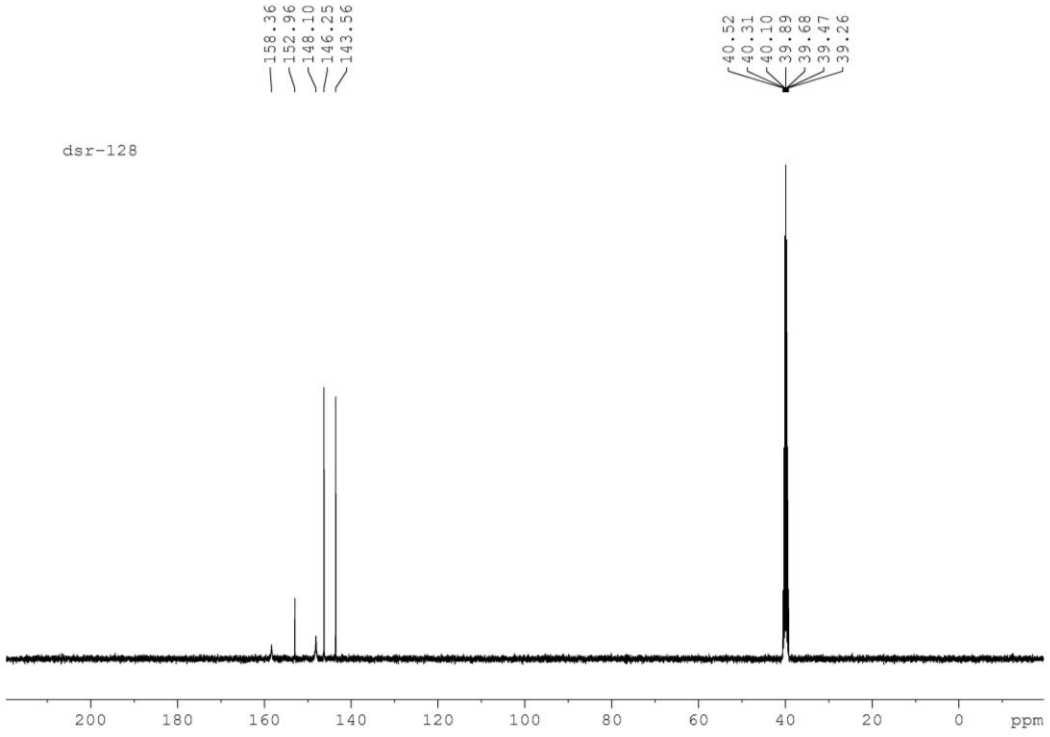
12. 3,5-Diamino-1*H*-1,2,4-triazol-4-ium 3-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide (9e)

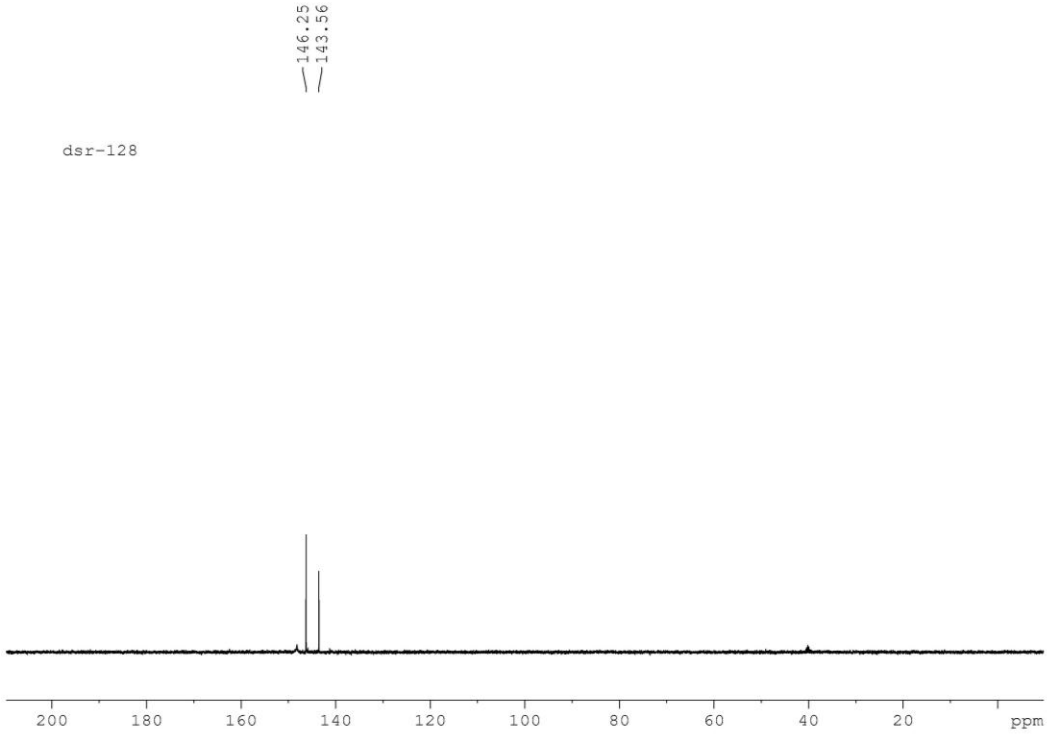
a. ^{1}H NMR



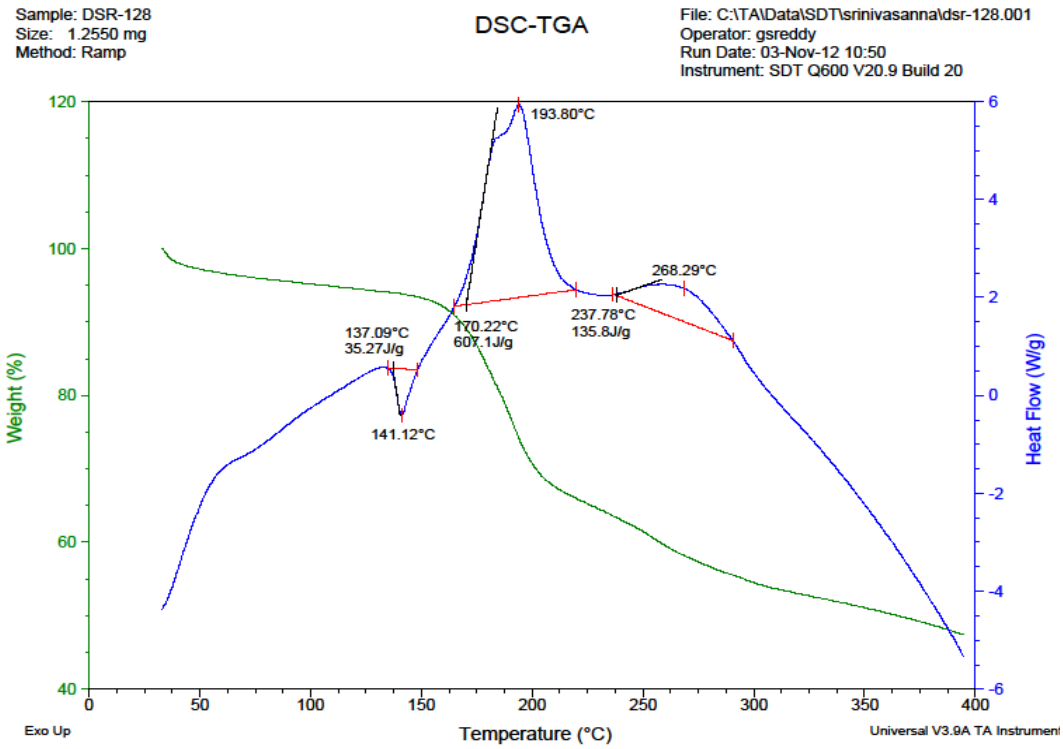
b. ^{13}C NMR



c. DEPT



d. TG-DTA measurement



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e. C H N analysis

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ethod filename: E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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nalysis type: UnkNown
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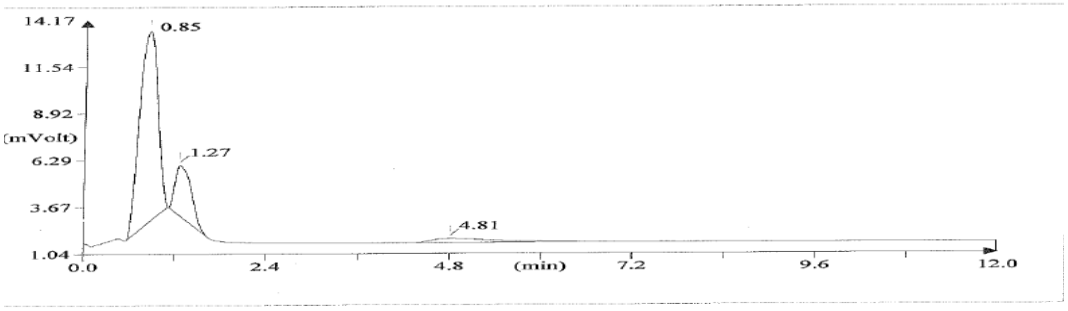
mple weight: .731



Element Name	Element %	Ret. Time
Nitrogen	71. 32	0. 85
Carbon	25. 51	1. 27
Hydrogen	3. 36	4. 81

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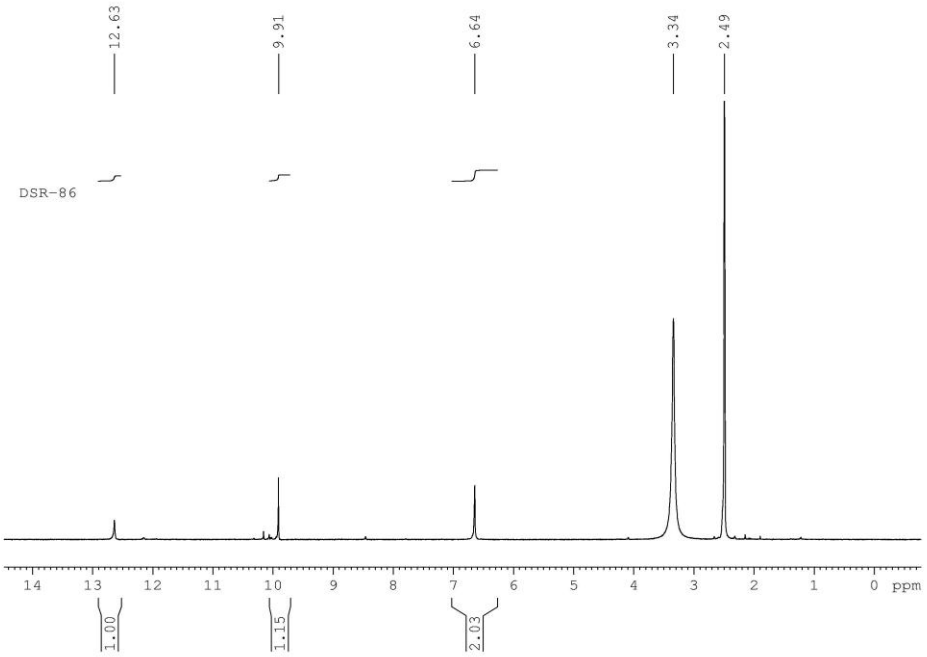
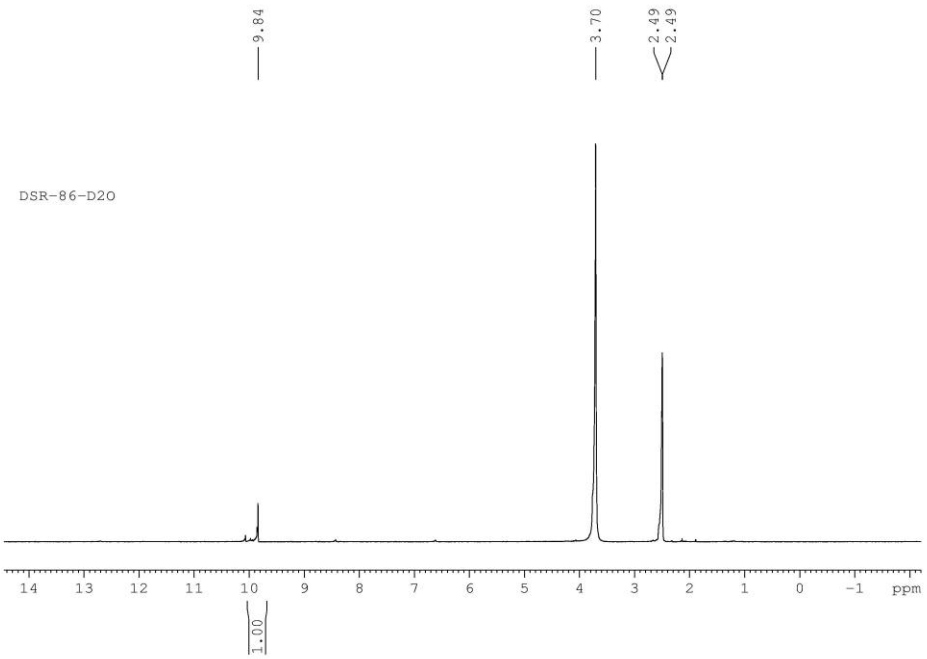
13. 5-(1*H*-Tetrazol-1-yl)-1*H*-1,2,4-triazol-3-amine (10)

a. ^{1}H NMR



b. ^{1}H NMR (D_2O exchange)



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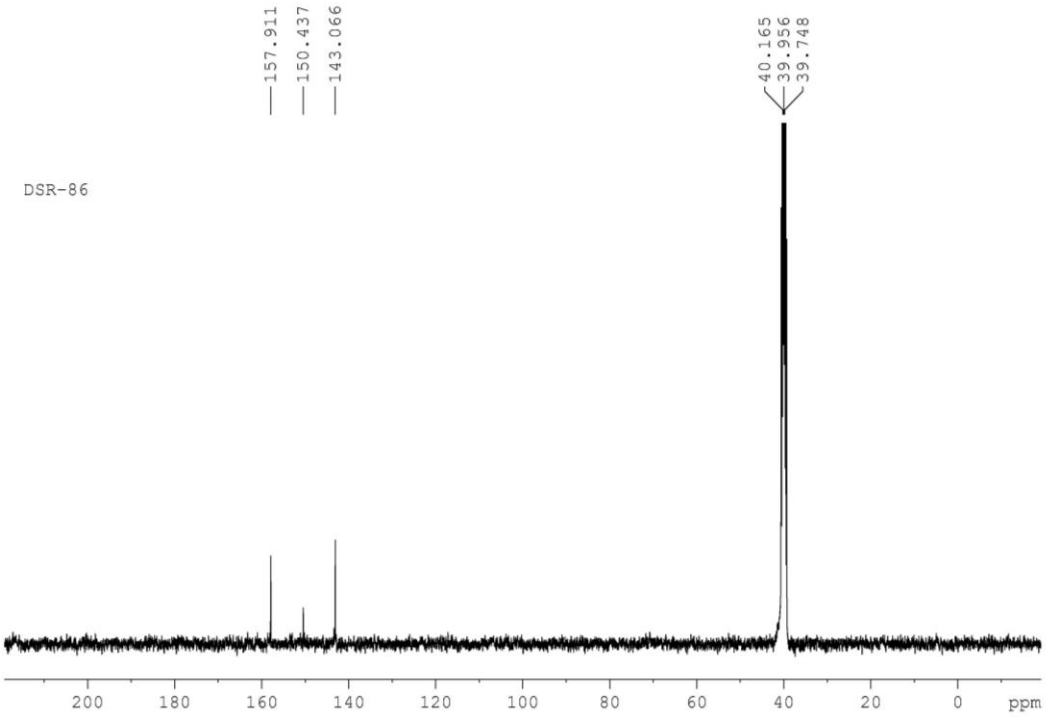
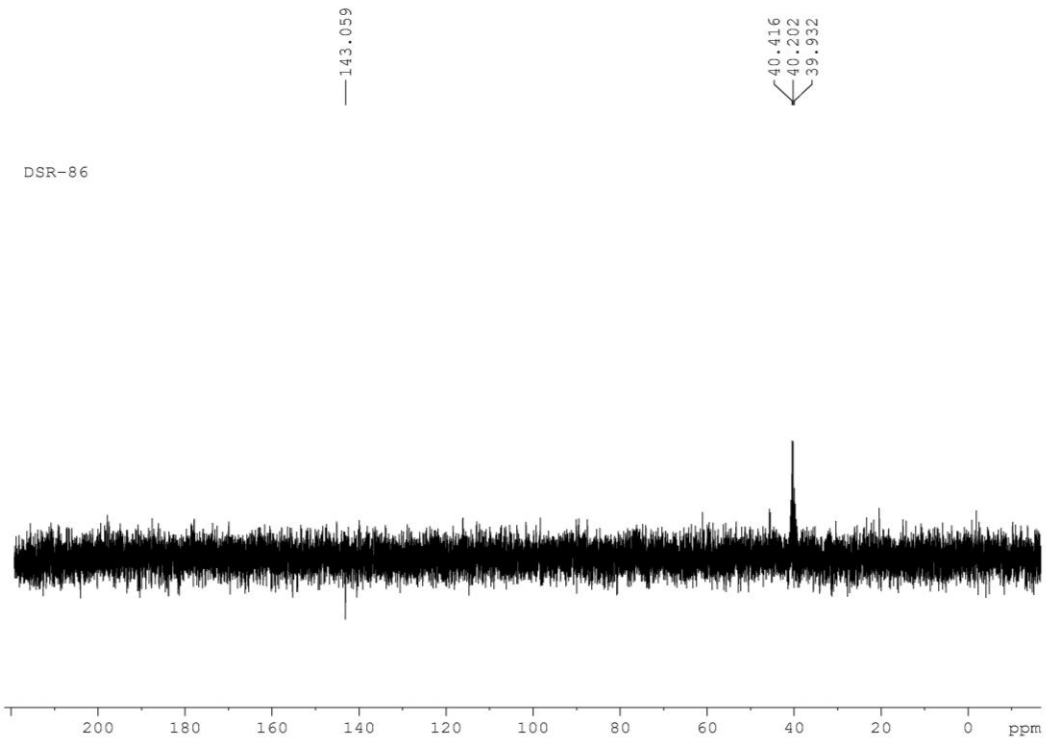
c. ^{13}C NMR



d. DEPT



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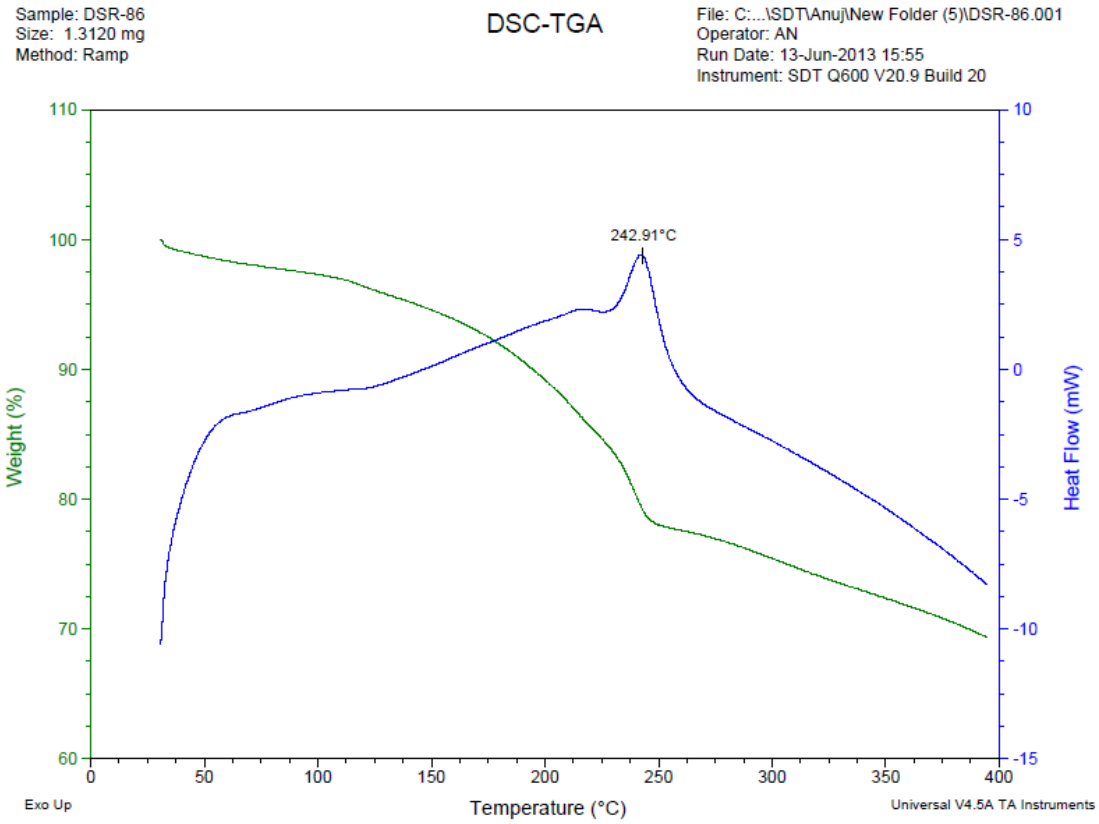
e. TG-DTA measurement



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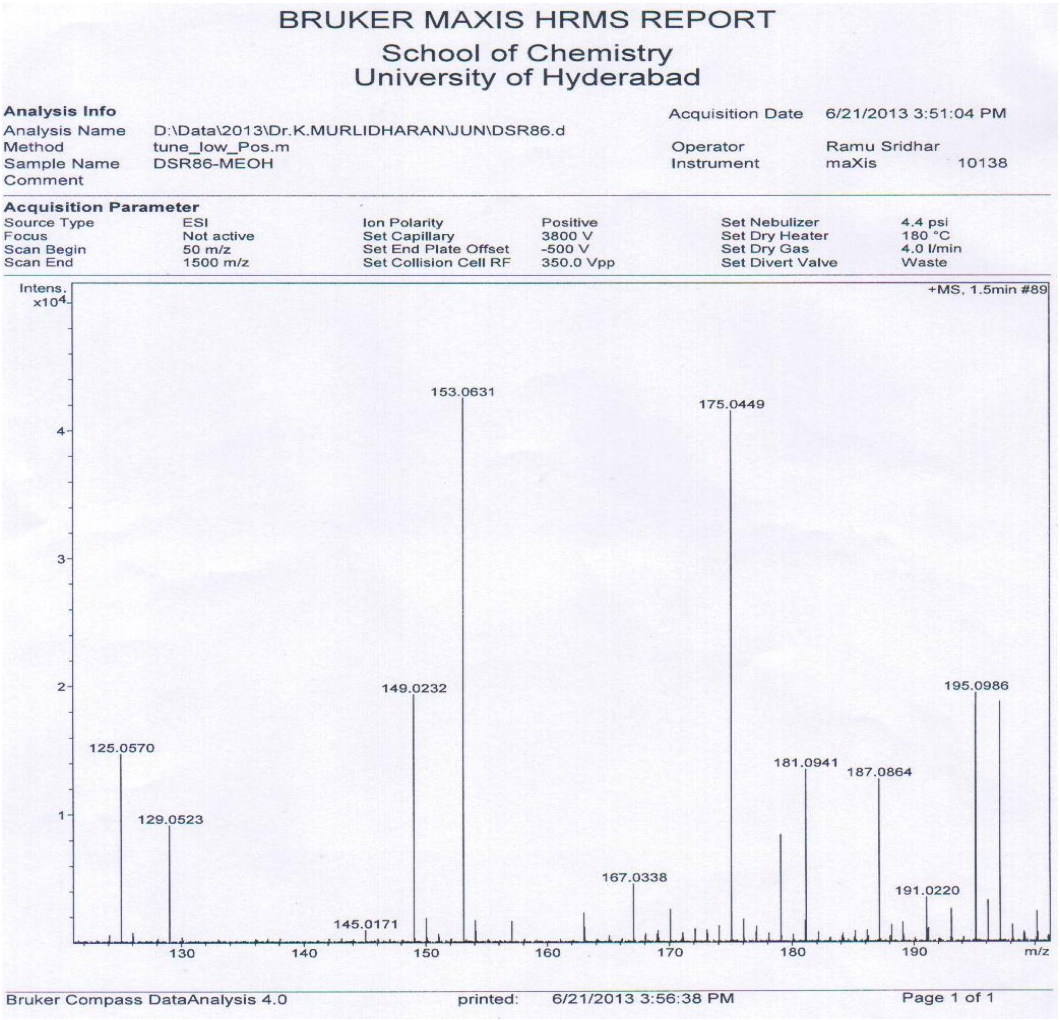
e. HRMS



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g. C H N analysis

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Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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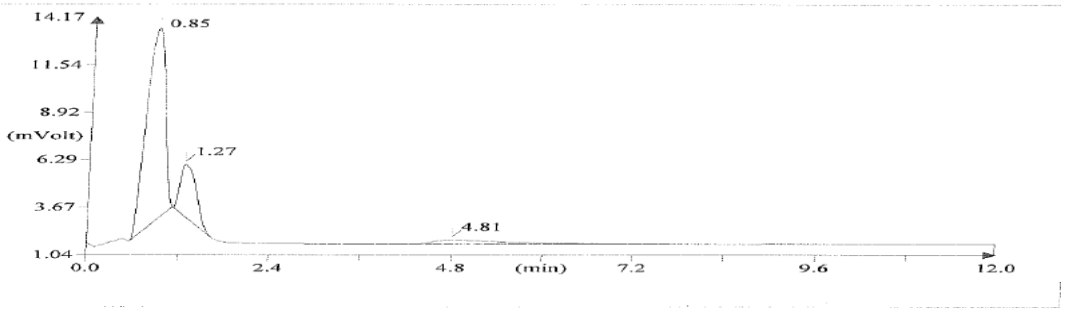

Element Name	Element %	Ret. Time
Nitrogen	73. 45	0. 85
Carbon	23. 76	1. 27
Hydrogen	2. 58	4. 81

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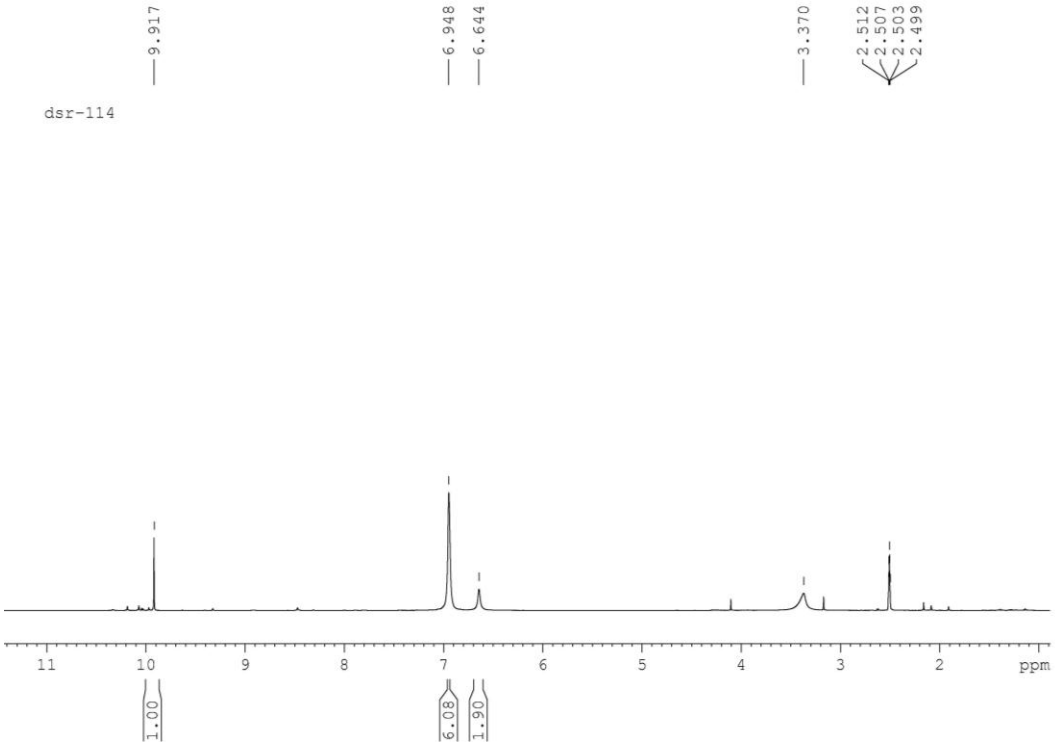
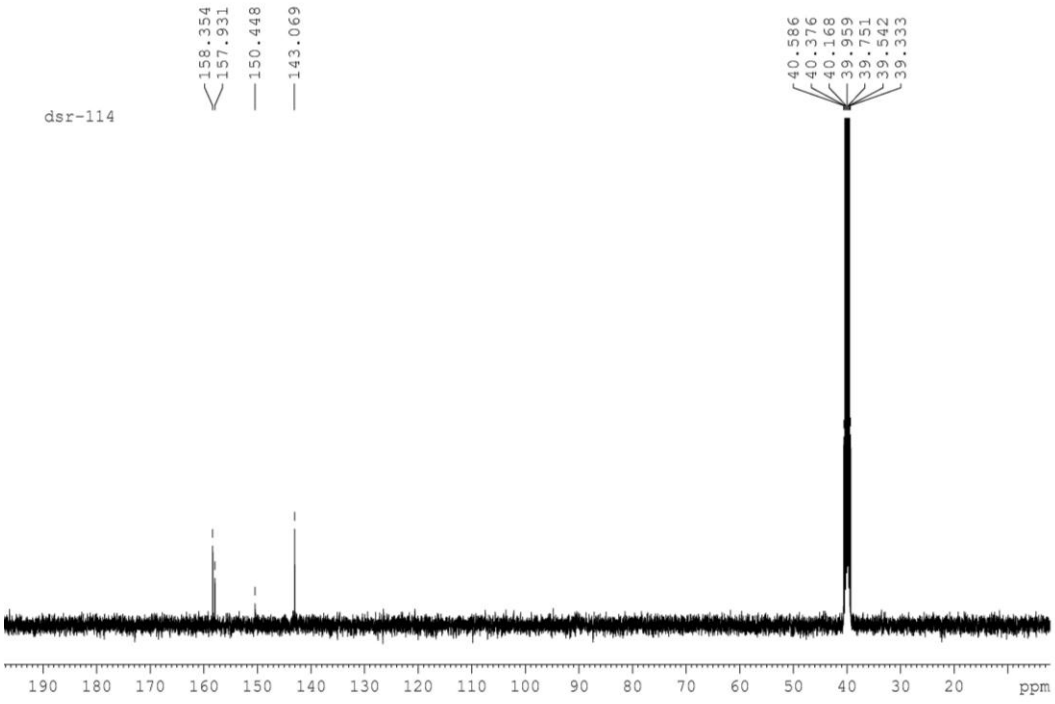
14. Diaminomethaniminium 3-amino-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide (10a)

a. ^{1}H NMR



b. ^{13}C NMR



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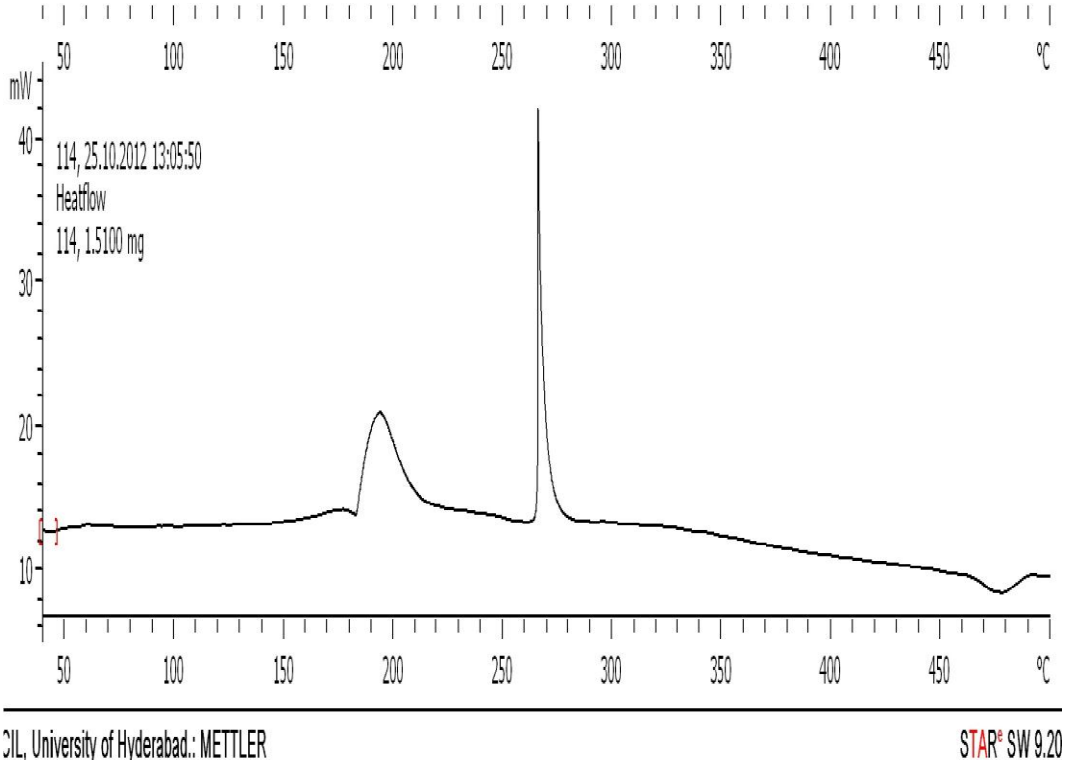
c. TG-DTA measurement



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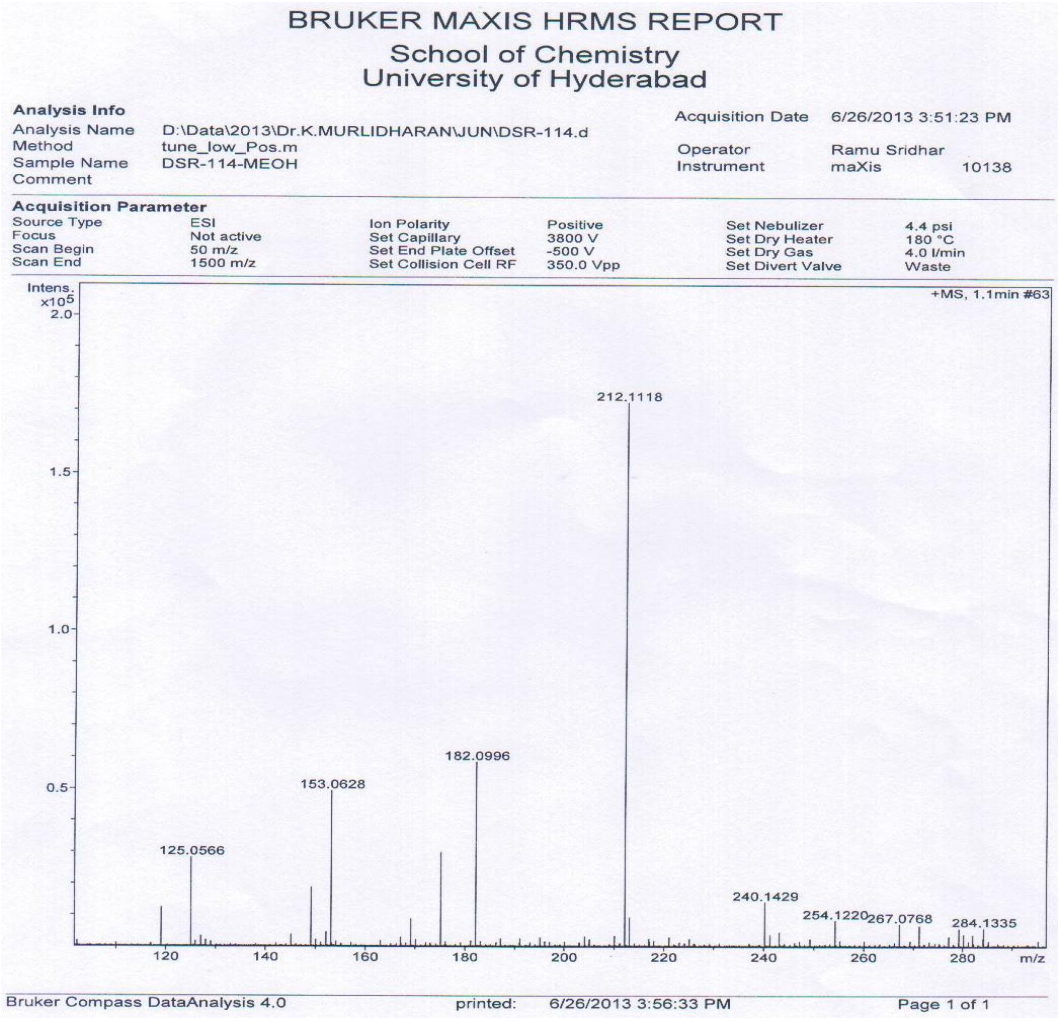
d. HRMS



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e. C H N analysis

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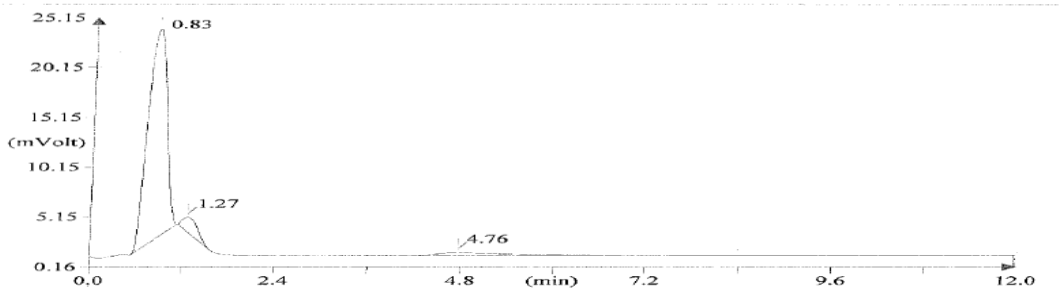
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_e:
Sample ID:	DSR-114 (# 31)
Analysis type:	UnkNown
Chromatogram filename:	UNK-15102012-31.dat
Sample weight:	.315



Element Name	Element %	Ret. Time
Nitrogen	72. 85	0. 83
Carbon	22. 61	1. 27
Hydrogen	4. 41	4. 76

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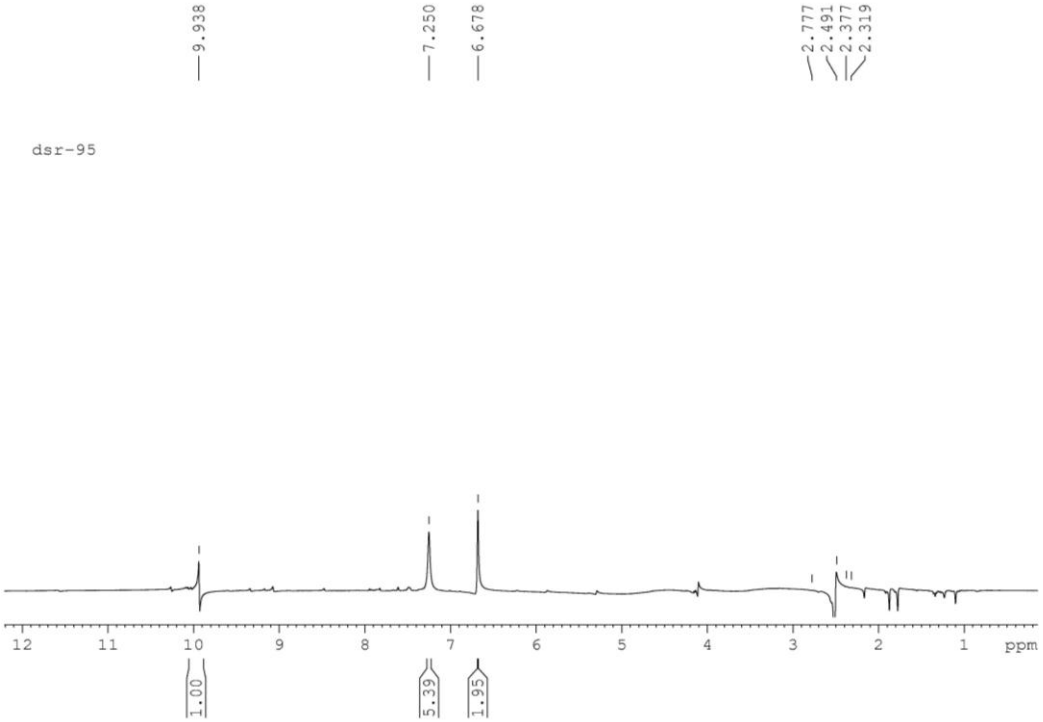
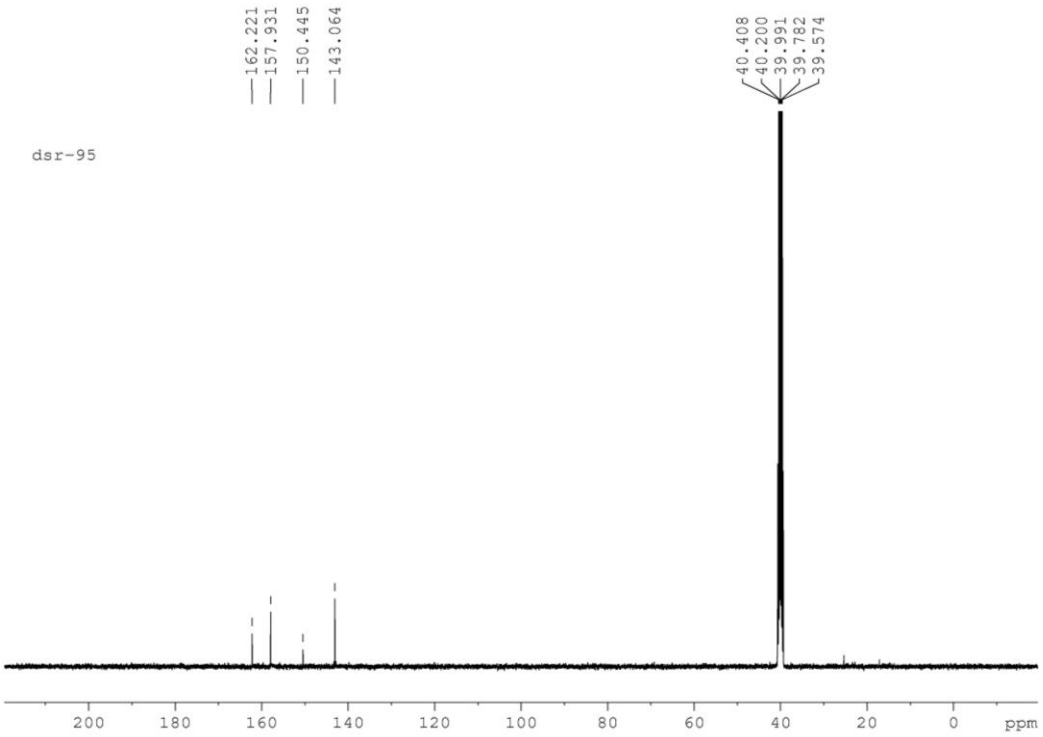
15. (Hydrazinylcarbonyl)hydrazonium 3-mino-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide (10b)

a. ^{1}H NMR



b. ^{13}C NMR



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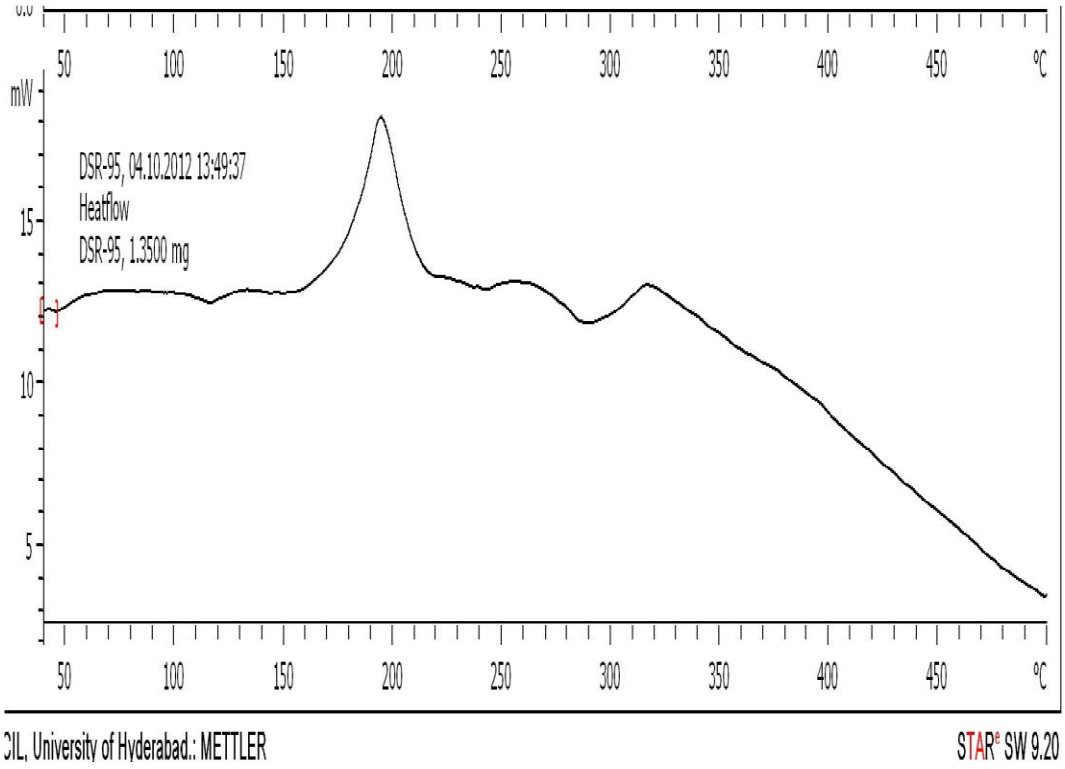
c. TG-DTA measurement



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d.HRMS

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University of Hyderabad

nalysis Info

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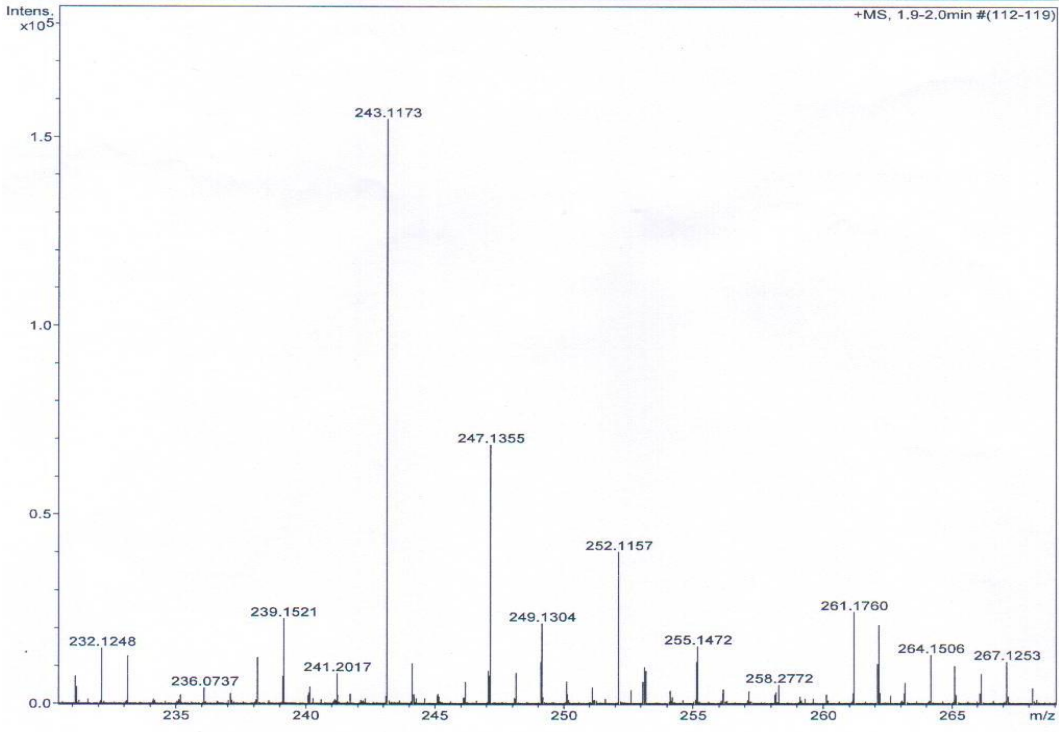
ample Name	DSR-95-MEOH	Instrument	maXis 10138
omment			

cquisition Parameter

ource Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
ocus	Not active	Set Capillary	4200 V	Set Dry Heater	180 °C
can Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
can End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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e. C H N analysis

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Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
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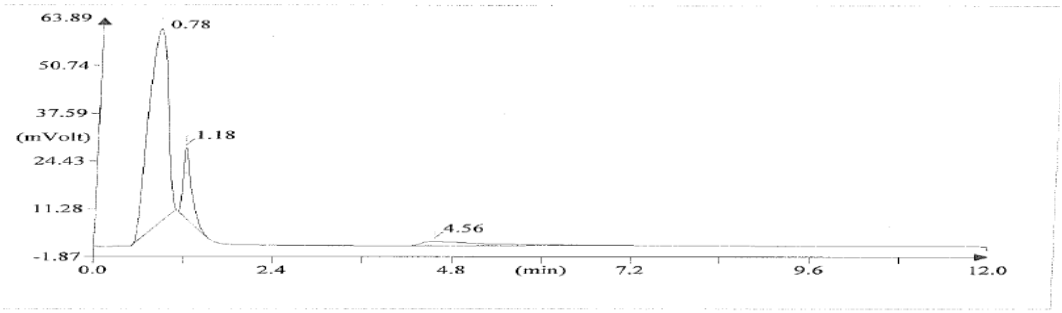

Element Name	Element %	Ret. Time
Nitrogen	69. 28	0. 78
Carbon	19. 69	1. 18
Hydrogen	4. 23	4. 56

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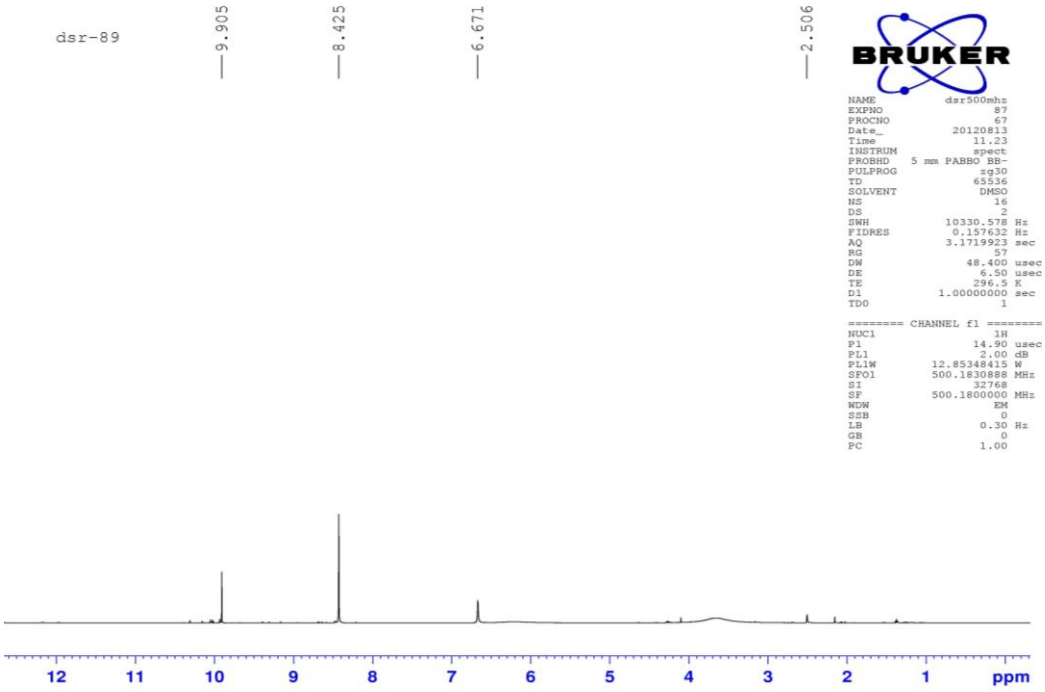
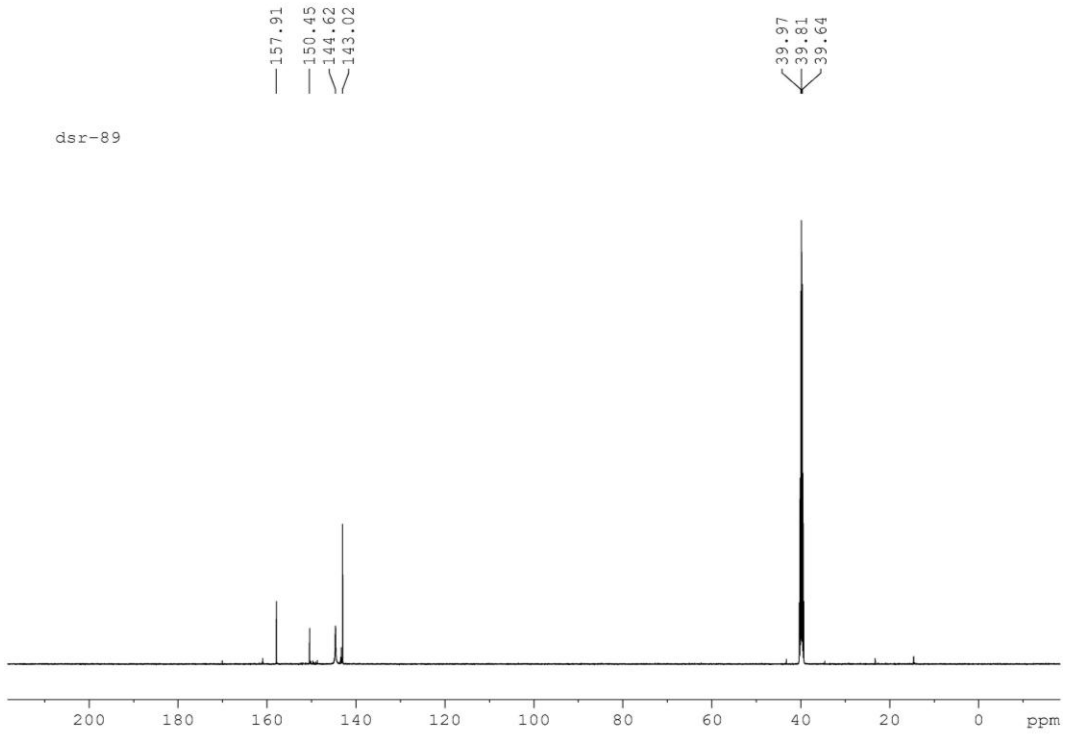
16. 3-Amino-1*H*-1,2,4-triazol-4-ium 3-amino-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide (10d)

a. ^{1}H NMR



b. ^{13}C NMR



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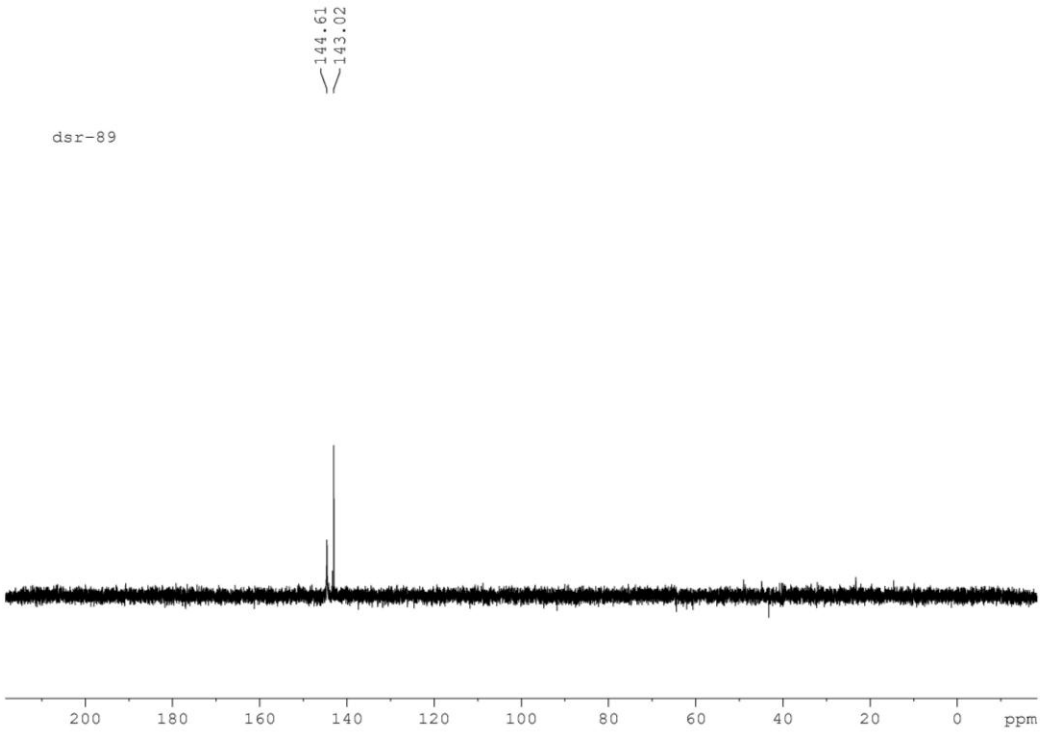
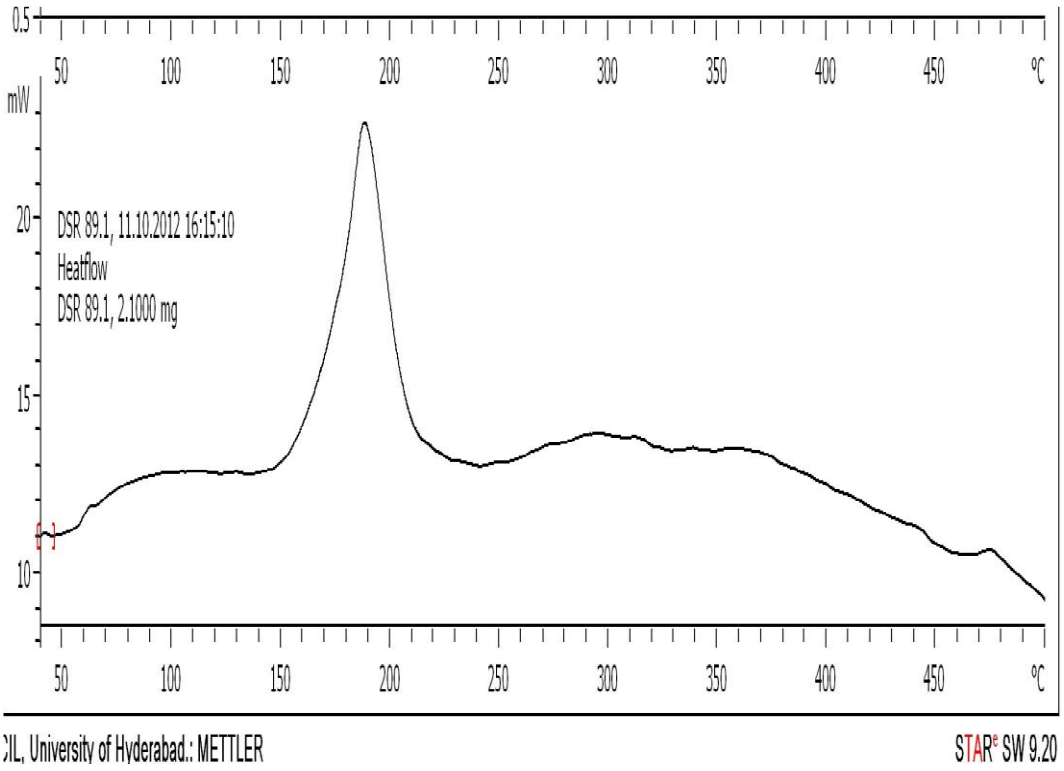
c. DEPT



d. TG-DTA measurement



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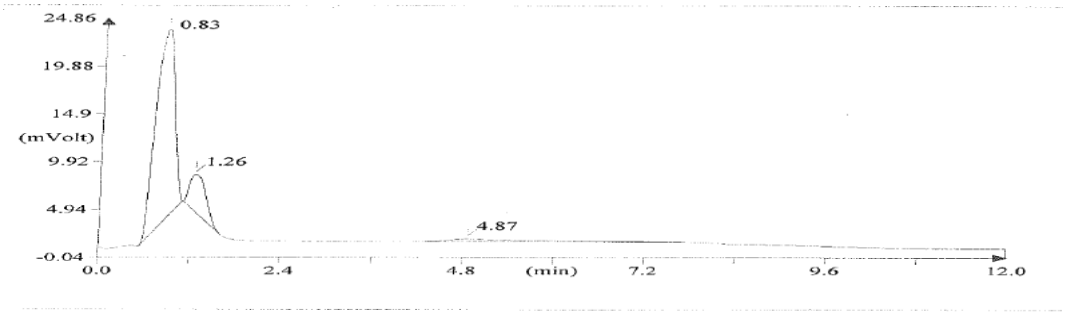
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	DSR-89 (# 16)
Analysis type:	UnkNown
Chromatogram filename:	UNK-15102012-16.dat
Sample weight:	.315



Element Name	Element %	Ret. Time
Nitrogen	70. 69	0. 83
Carbon	25. 15	1. 26
Hydrogen	3. 76	4. 87

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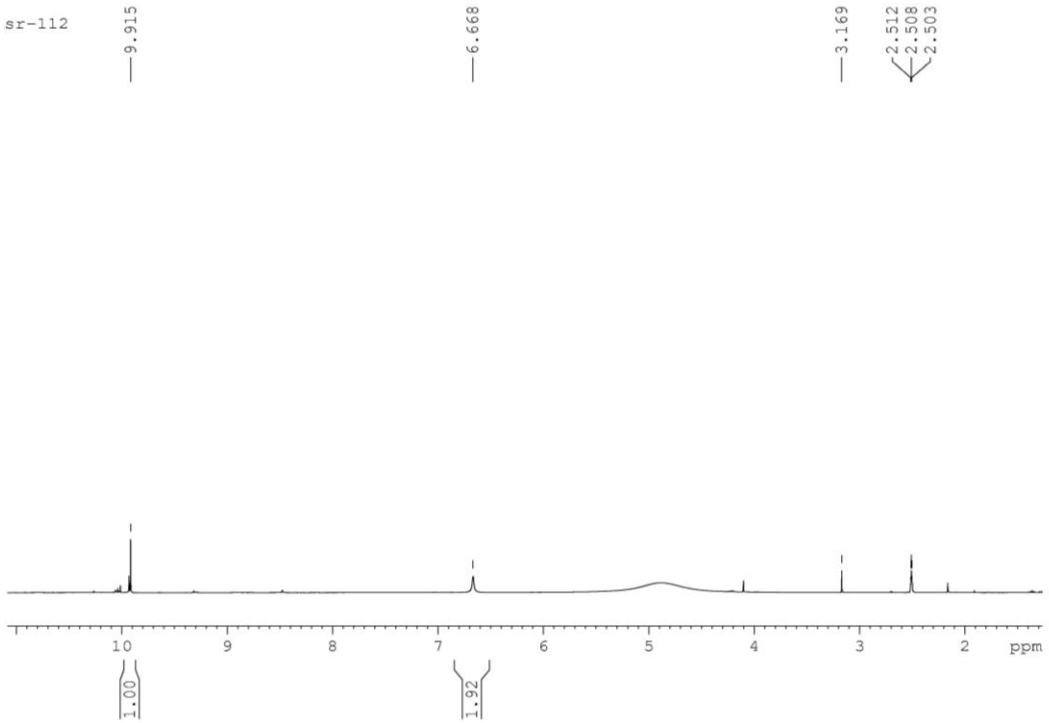
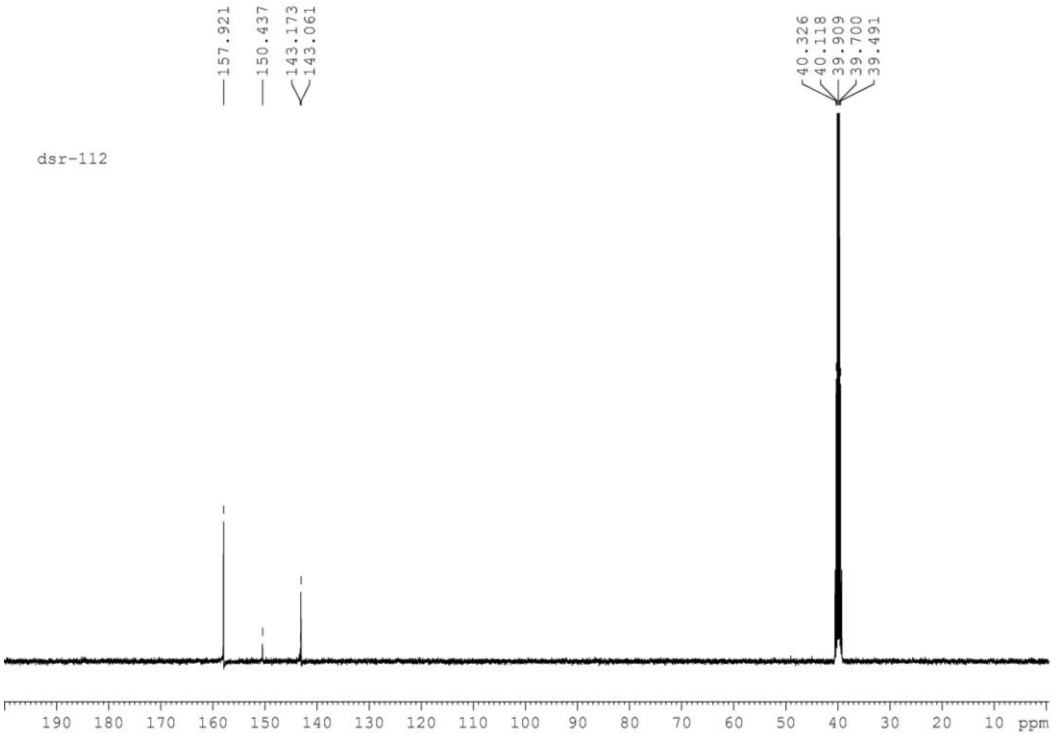
17. 3,5-Diamino-1*H*-1,2,4-triazol-4-ium 3-amino-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide (10e)

a. ^{1}H NMR



b. ^{13}C NMR



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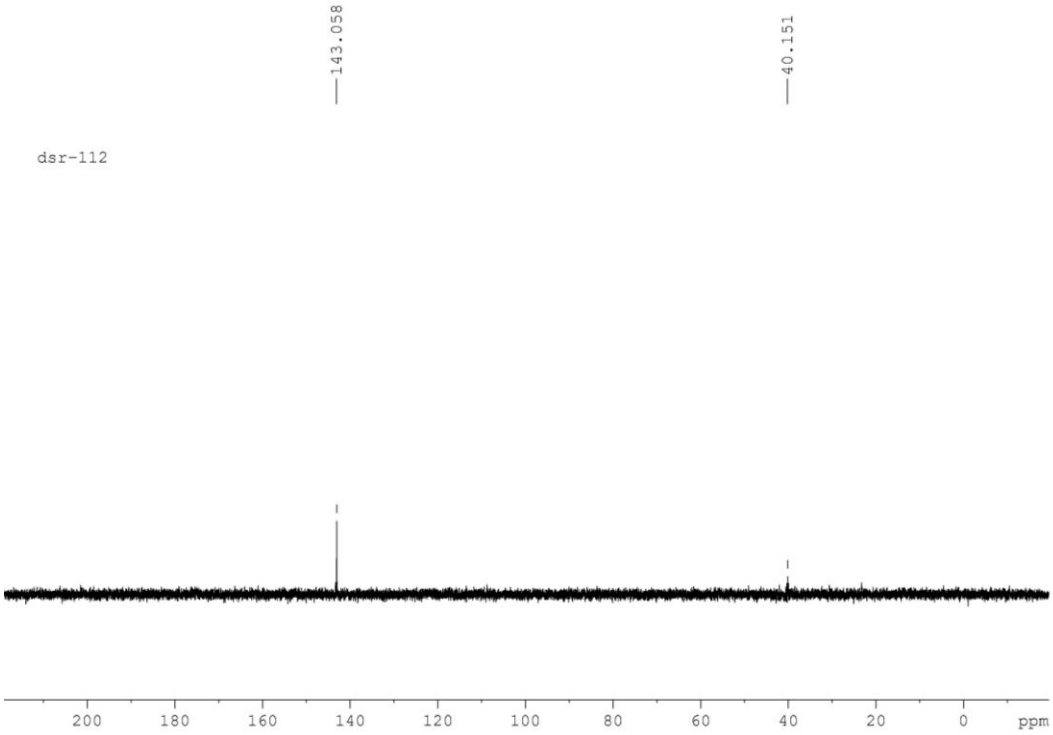
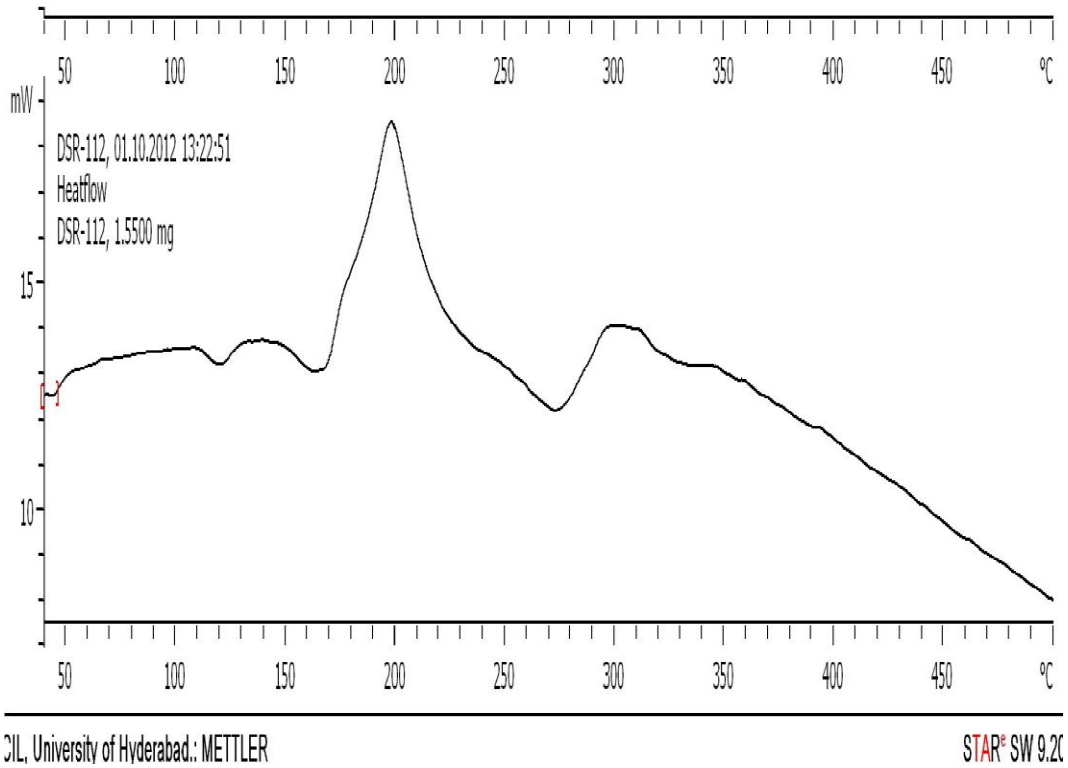
c. DEPT



d. TG-DTA measurement



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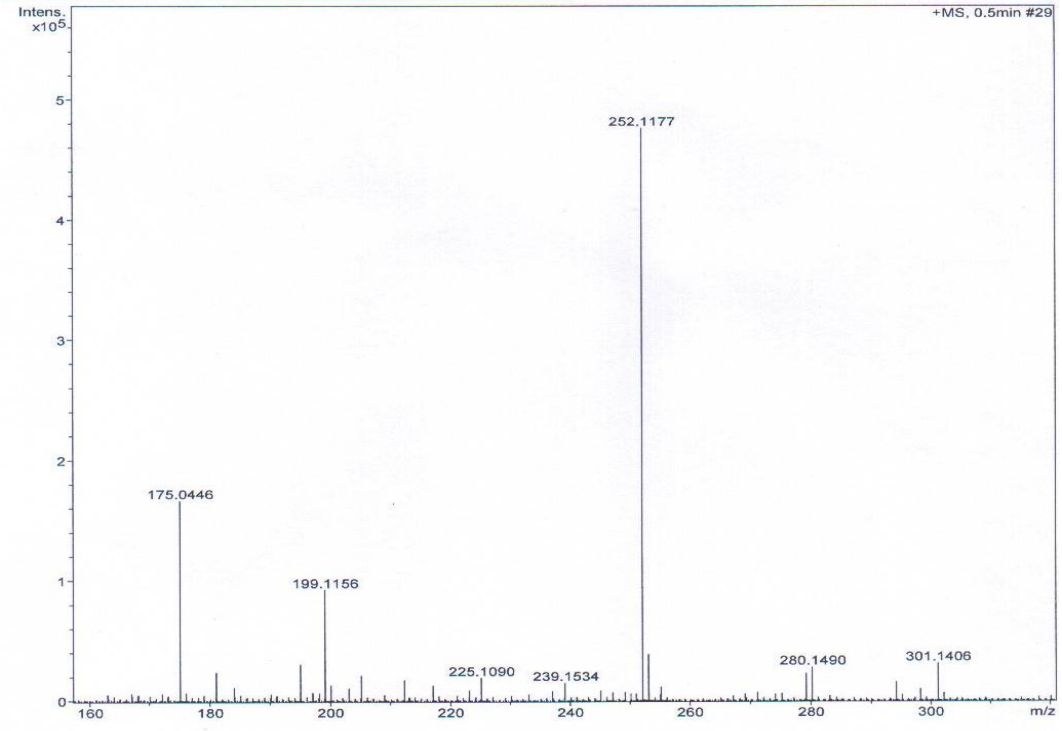
Analysis Info

Analysis Name	D:\Data\2013\Dr.K.MURLIDHARAN\JULY\DSR-112.d	Acquisition Date	7/15/2013 1:56:43 PM
Method	tune_low_Pos.m	Operator	Ramu Sridhar
Sample Name	DSR-112-MEOH	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	4200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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f. C H N analysis

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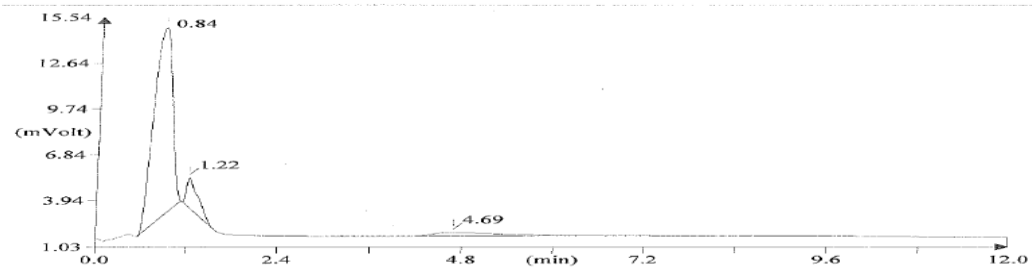
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	DSR-112 (# 36)
Analysis type:	UnkNown
Chromatogram filename:	UNK-15102012-36.dat
Sample weight:	.296



Element Name	Element %	Ret. Time
Nitrogen	72. 65	0. 84
Carbon	24. 12	1. 22
Hydrogen	3. 21	4. 69

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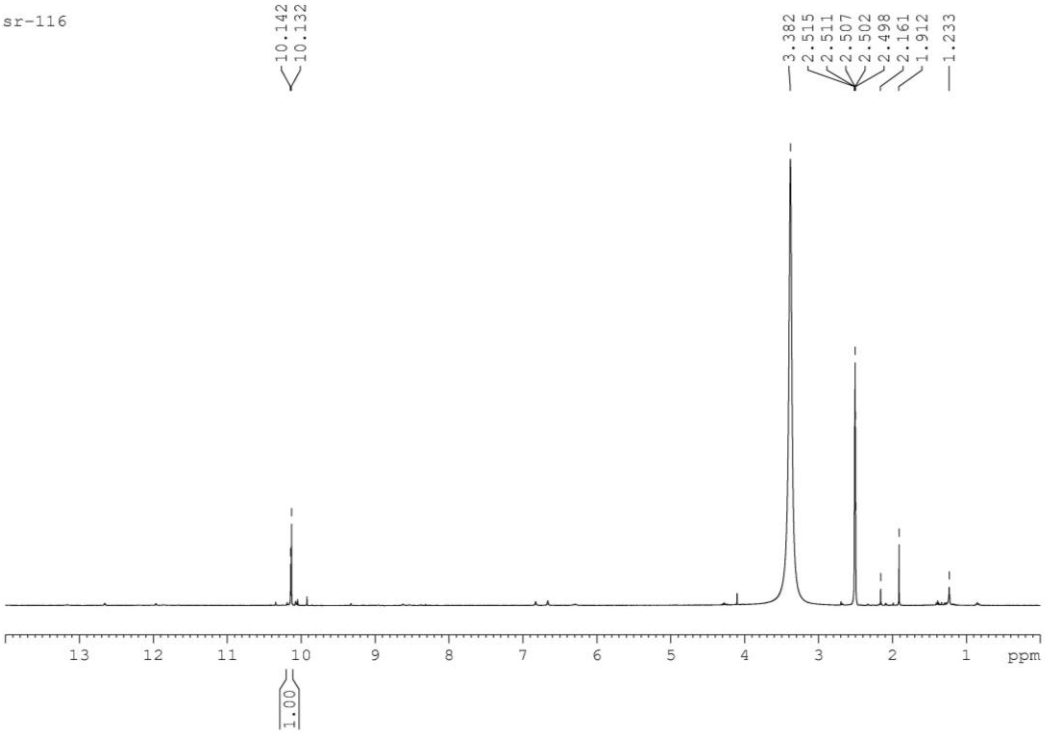
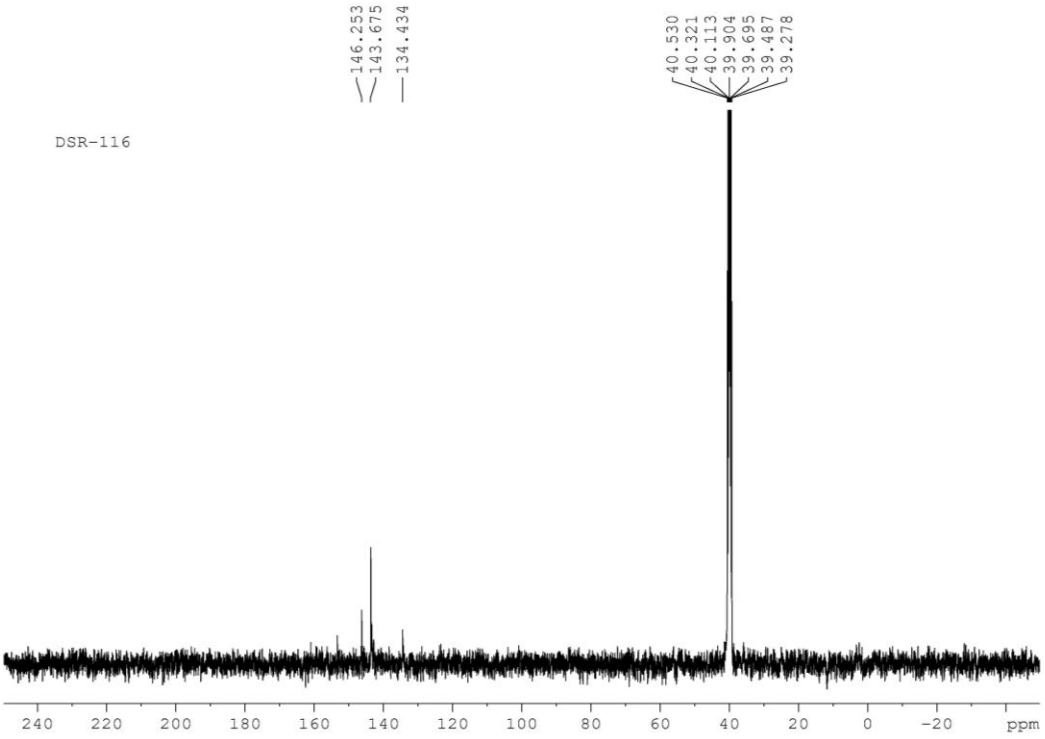
18. 1-(3-Azido-1*H*-1,2,4-triazol-5-yl)-1*H*-tetrazole (11)

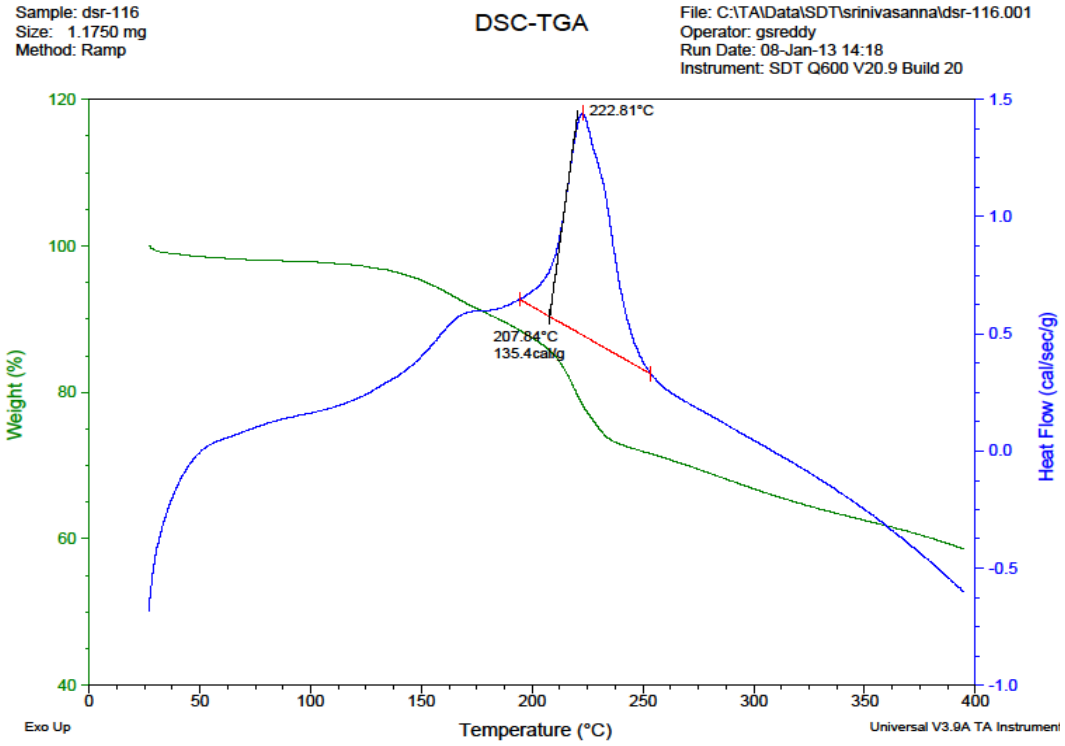
a. ^{1}H NMR



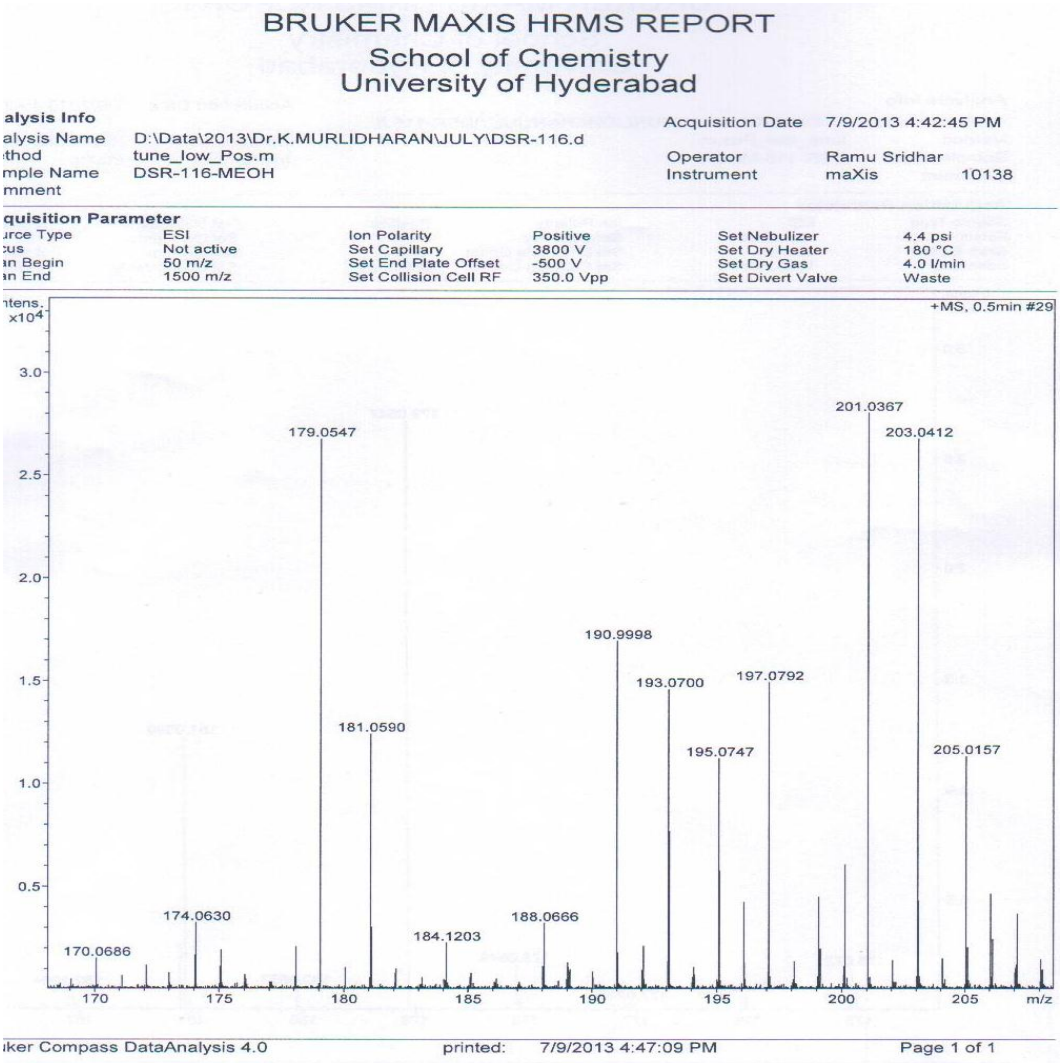
b. ^{13}C NMR



c. TG-DTA measurement



d. HRMS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alysis Info
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thod tune_low_Pos.m
mple Name DSR-116-MEOH
mment
Acquisition Date 7/9/2013 4:42:45 PM
Operator Ramu Sridhar
Instrument maXis 10138
quisition Parameter
urce Type ESI
cus Not active
an Begin 50 m/z
an End 1500 m/z
Ion Polarity Positive
Set Capillary 3800 V
Set End Plate Offset -500 V
Set Collision Cell RF 350.0 Vpp
Set Nebulizer 4.4 psi
Set Dry Heater 180 °C
Set Dry Gas 4.0 l/min
Set Divert Valve Waste
ntens.
x10^4
+MS, 0.5min #29
3.0
2.5
2.0
1.5
1.0
0.5
179.0547
201.0367
203.0412
190.9998
193.0700
197.0792
181.0590
195.0747
205.0157
174.0630
188.0666
184.1203
170.0686
170
175
180
185
190
195
200
205
m/z
ker Compass DataAnalysis 4.0
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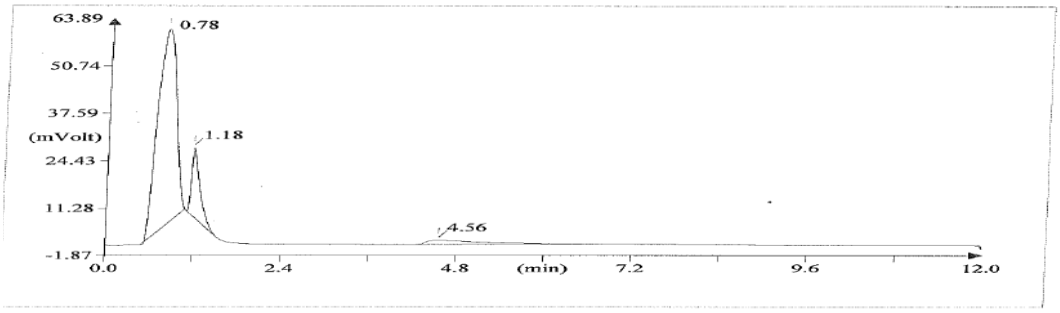
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	DSR-116 (# 100)
Analysis type:	UnkNown
Chromatogram filename:	UNK-20022013-20.dat
Sample weight:	1.683



Element Name	Element %	Ret. Time
Nitrogen	78. 54	0. 78
Carbon	20. 32	1. 18
Hydrogen	1. 18	4. 56

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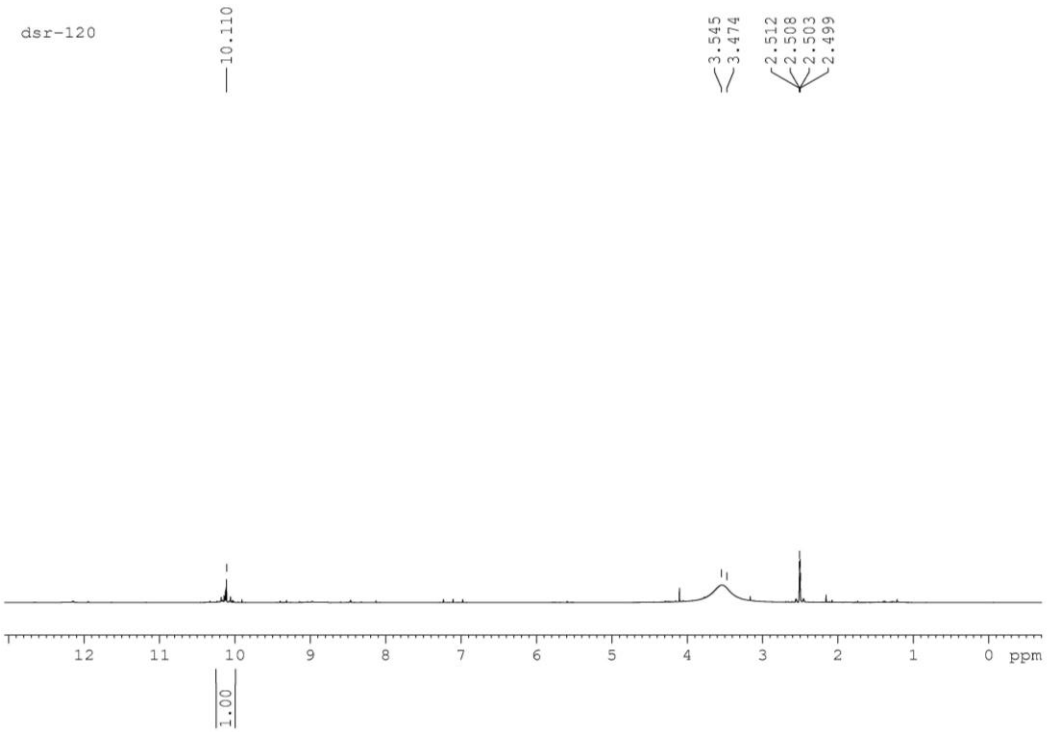
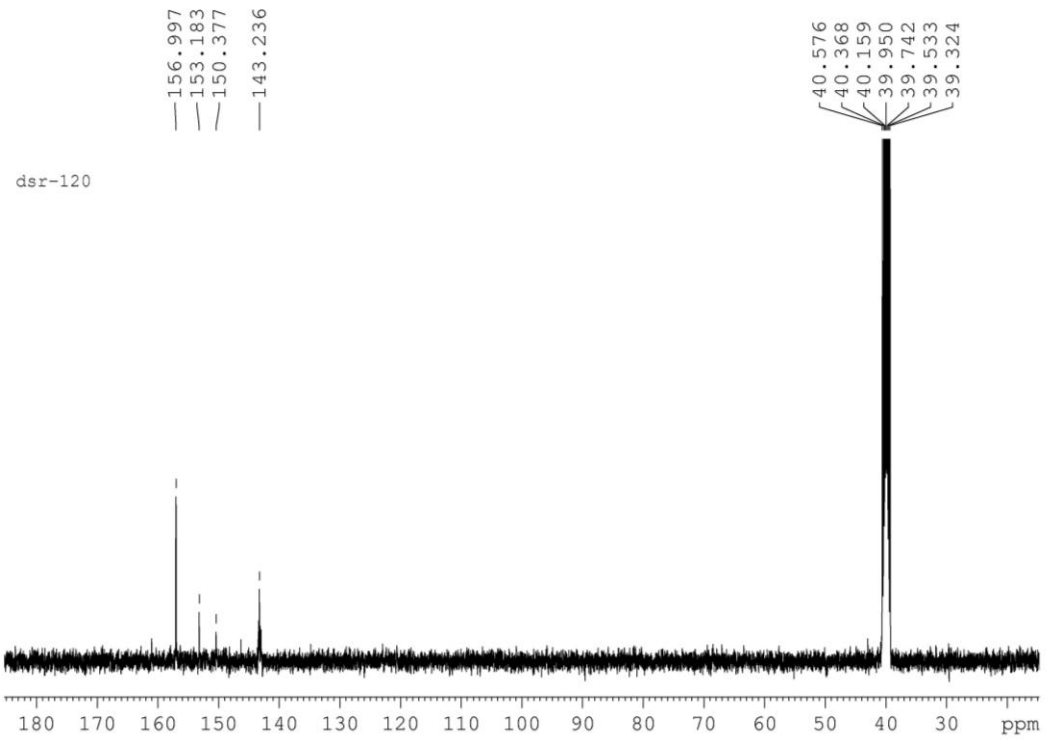
19. 3,5-Diamino-1*H*-1,2,4-triazol-4-ium 3-azido-5-(1*H*-tetrazol-1-yl)-1,2,4-triazol-1-ide (11e)

a. ^{1}H NMR



b. ^{13}C NMR



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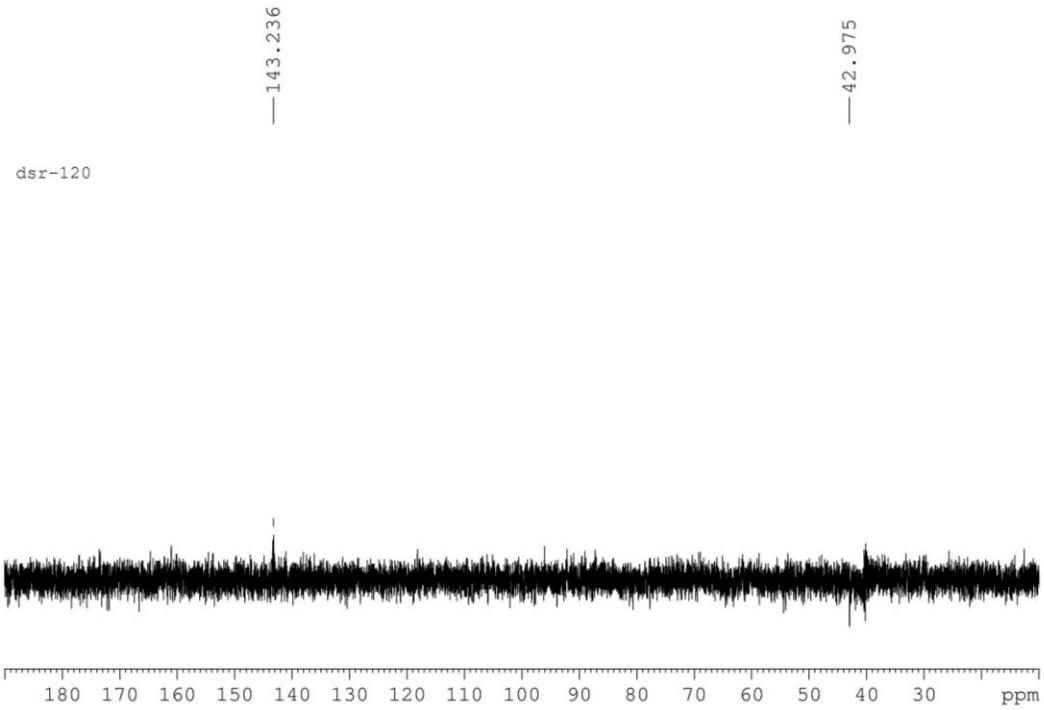
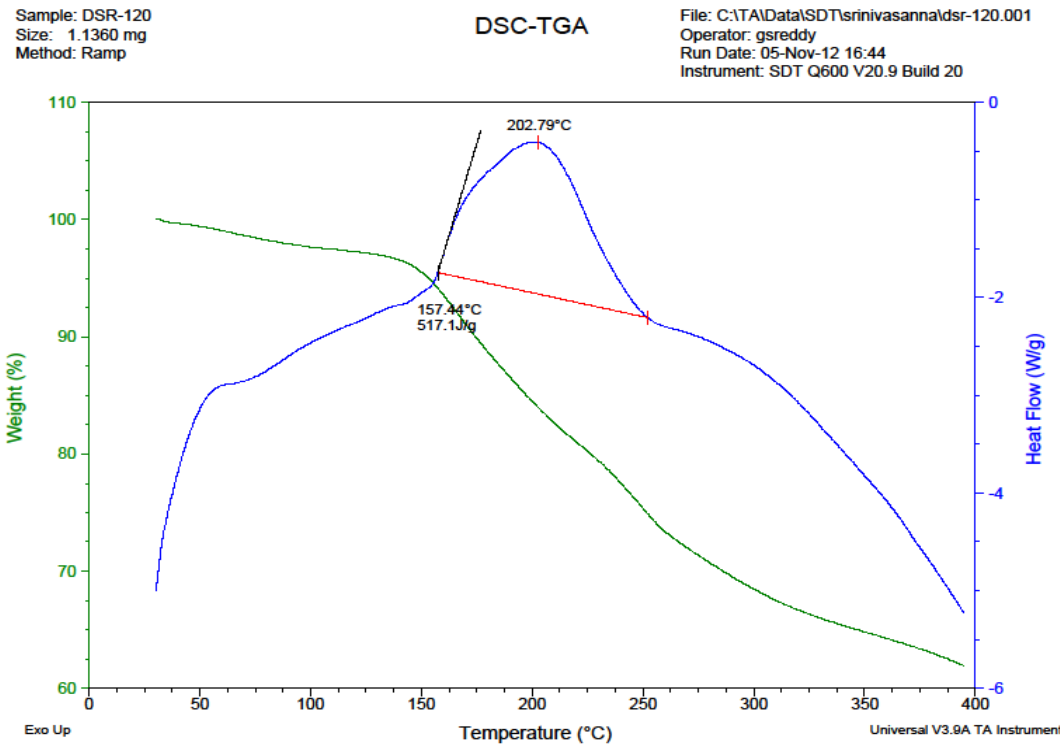


d. TG-DTA measurement



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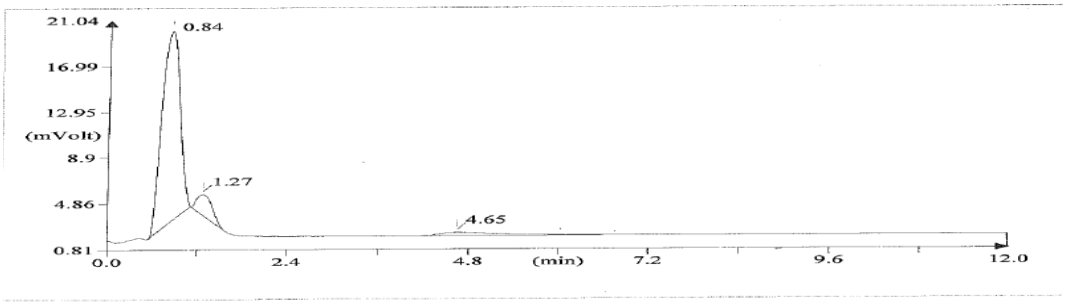
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_ex
Sample ID:	DSR-120 (# 94)
Analysis type:	UnkNown
Chromatogram filename:	UNK-20022013-14.dat
Sample weight:	.981



Element Name	Element %	Ret. Time
Nitrogen	75. 63	0. 84
Carbon	21. 52	1. 27
Hydrogen	2. 58	4. 65

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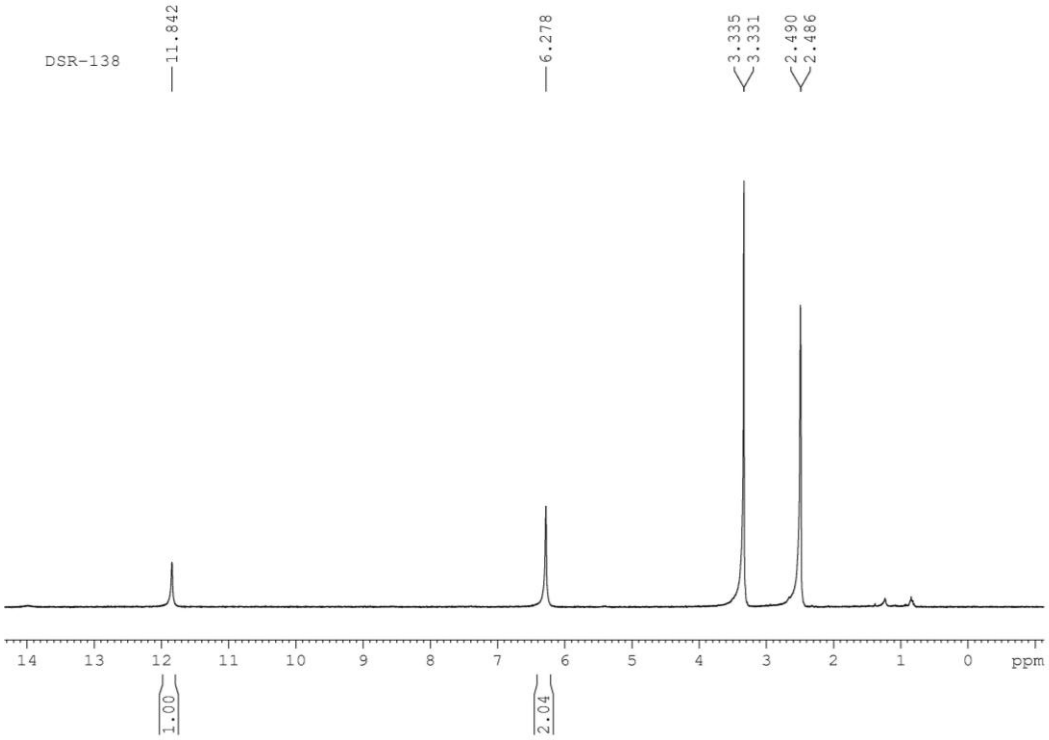
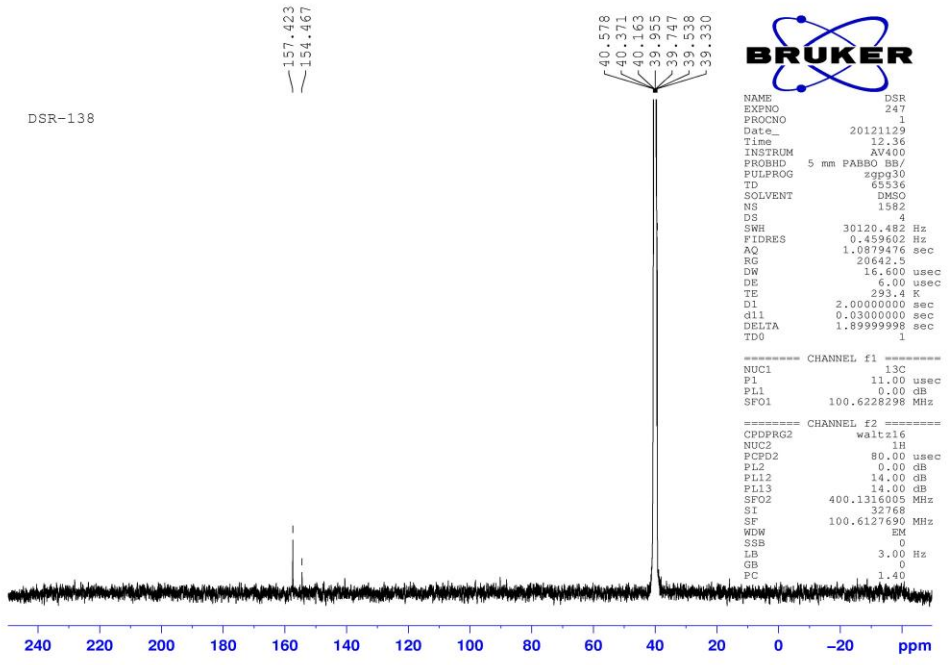
20. 3-Azido-1*H*-1,2,4-triazol-5-amine (12)

a. ^{1}H NMR



b. ^{13}C NMR



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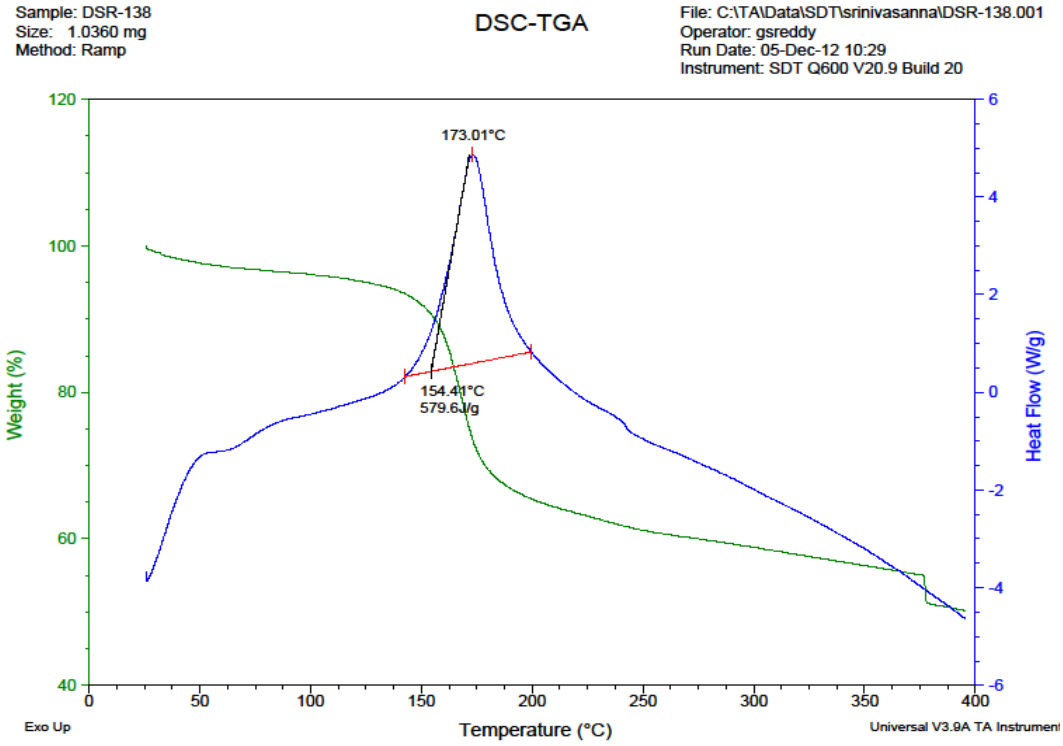
c . TG-DTA measurement



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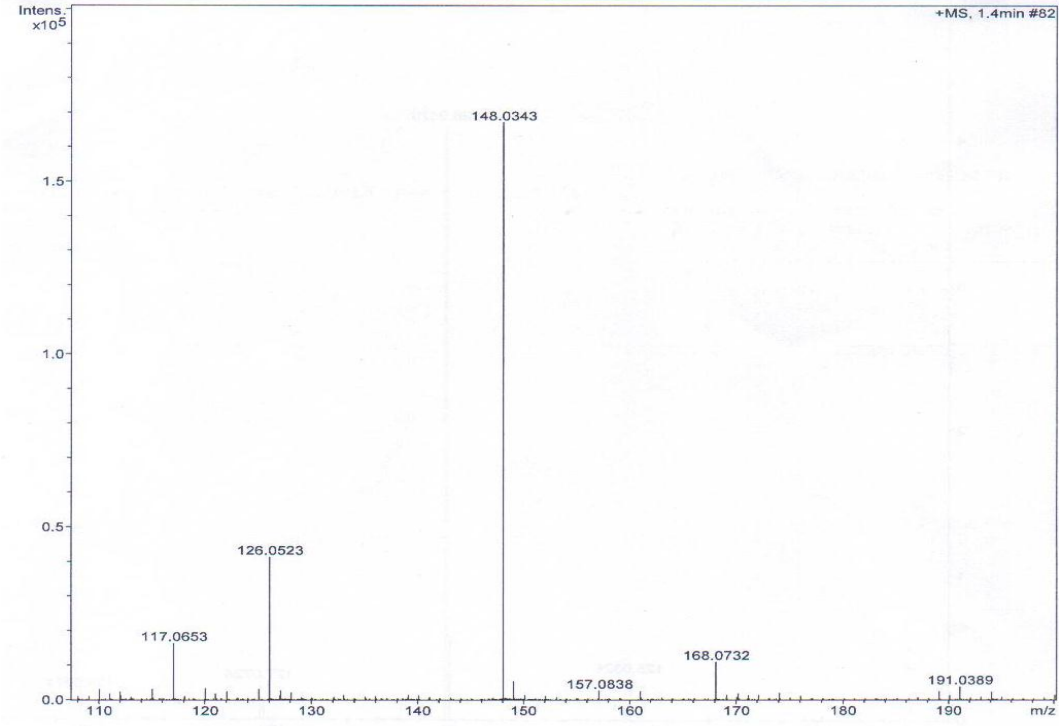
Analysis Info

Analysis Name	D:\Data\2013\Dr.K.MURLIDHARAN\JULY\DSR-138.d	Acquisition Date	7/31/2013 2:19:30 PM
Method	tune_low_Pos.m	Operator	Ramu Sridhar
Sample Name	DSR-138-MEOH	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	4.4 psi
Focus	Not active	Set Capillary	3800 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	350.0 Vpp	Set Divert Valve	Waste



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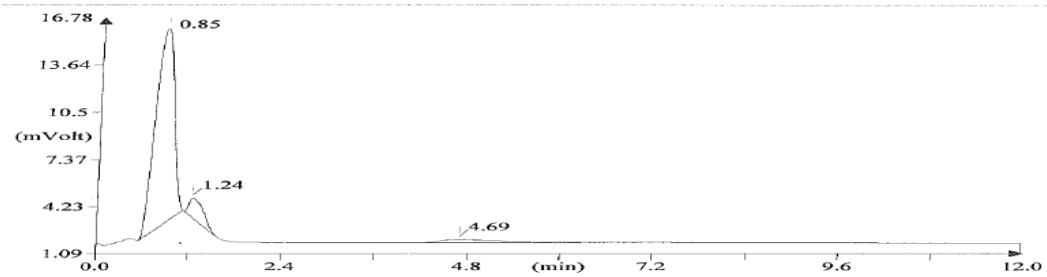
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_e
Sample ID:	DSR-138 (# 45)
Analysis type:	UnkNown
Chromatogram filename:	UNK-06022013-15.dat
Sample weight:	.792



Element Name	Element %	Ret. Time
Nitrogen	78. 21	0. 85
Carbon	19. 12	1. 24
Hydrogen	2. 46	4. 49

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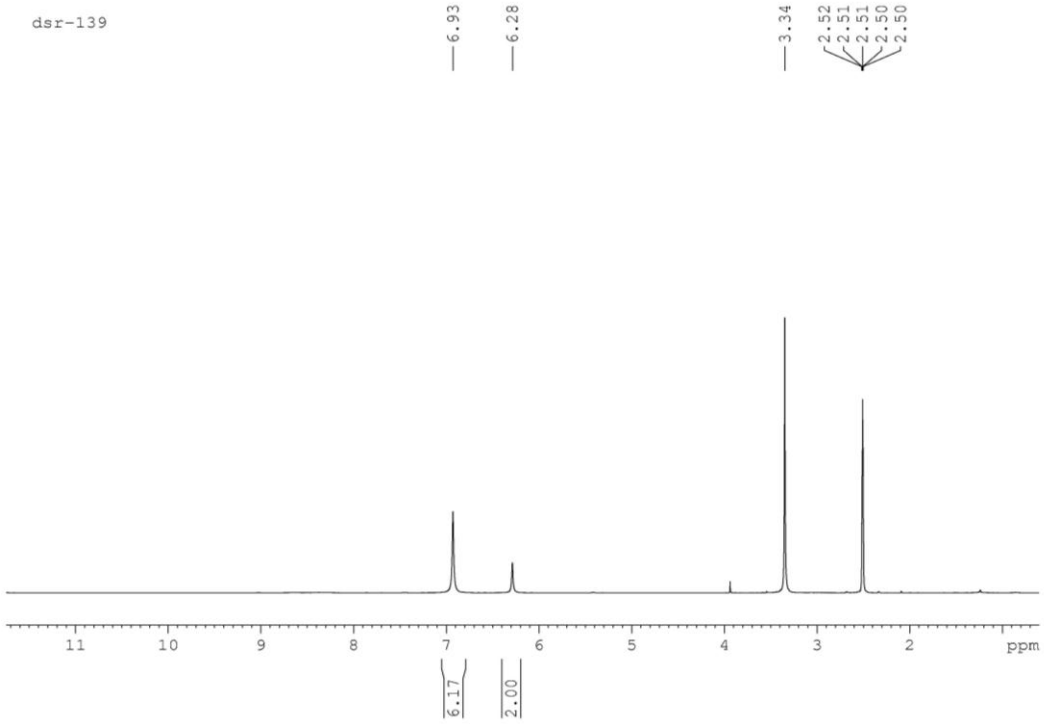
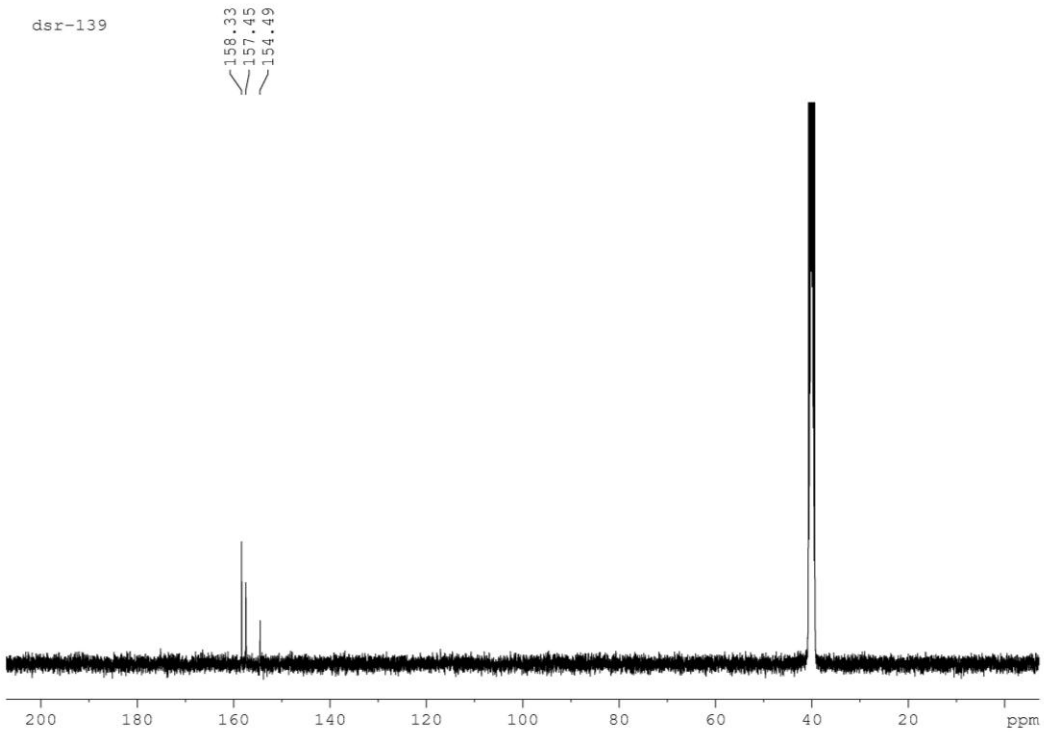
21. Diaminomethaniminium 5-amino-3-azido-1,2,4-triazol-1-ide (12a)

a. ^{1}H NMR



b. ^{13}C NMR



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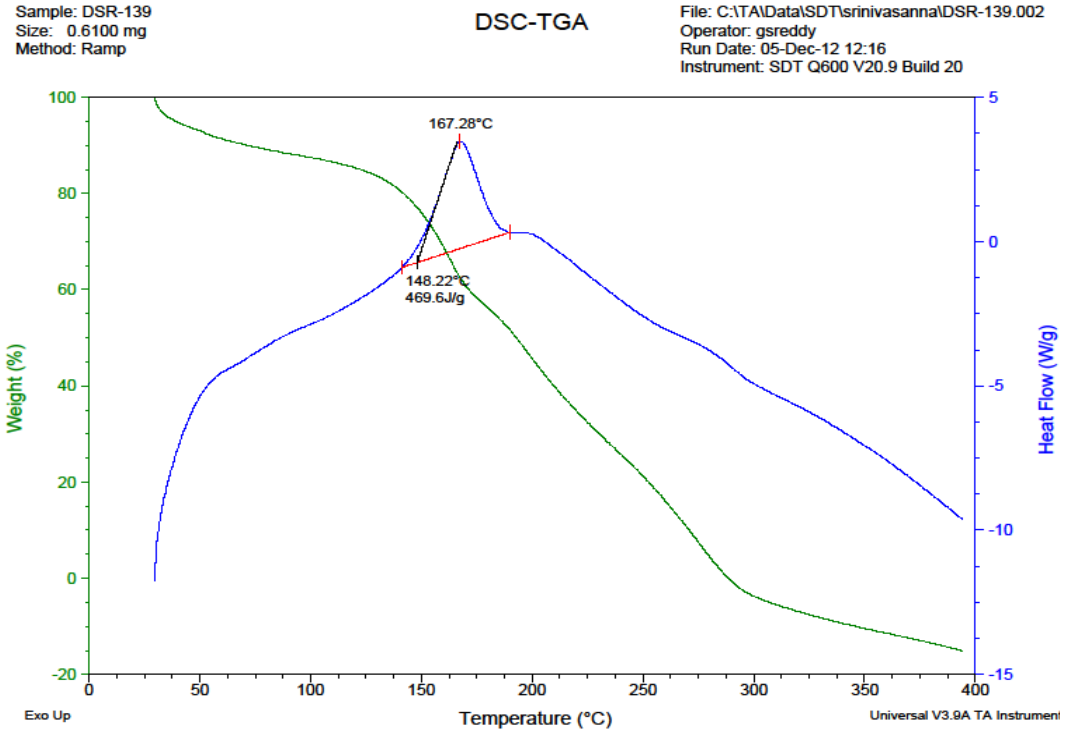
c. TG-DTA measurement



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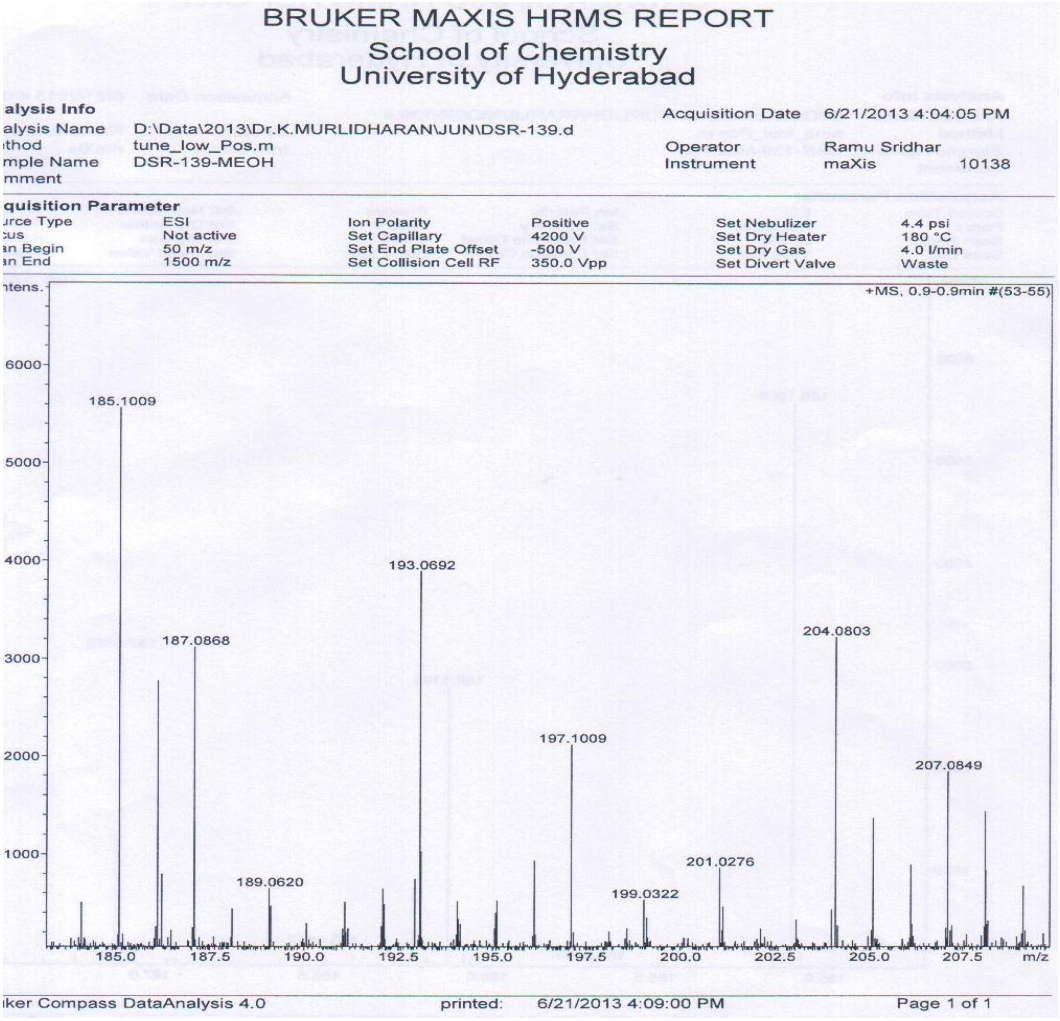

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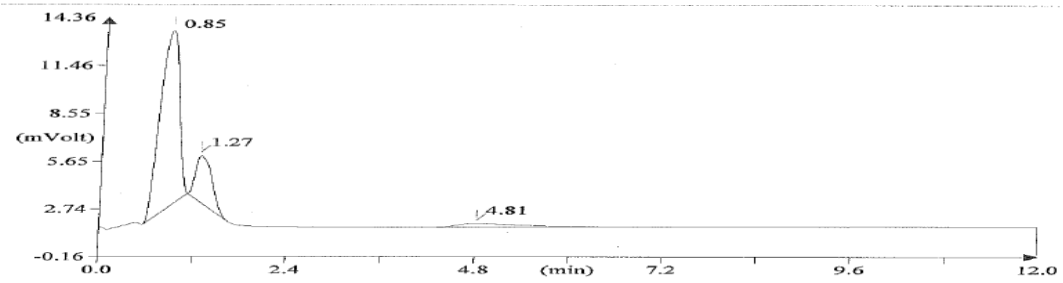
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_
Sample ID:	DSR-139 (# 46)
Analysis type:	UnkNown
Chromatogram filename:	UNK-06022013-16.dat
Sample weight:	.763



Element Name	Element %	Ret. Time
Nitrogen	76. 21	0. 85
Carbon	19. 46	1. 27
Hydrogen	4. 31	4. 81

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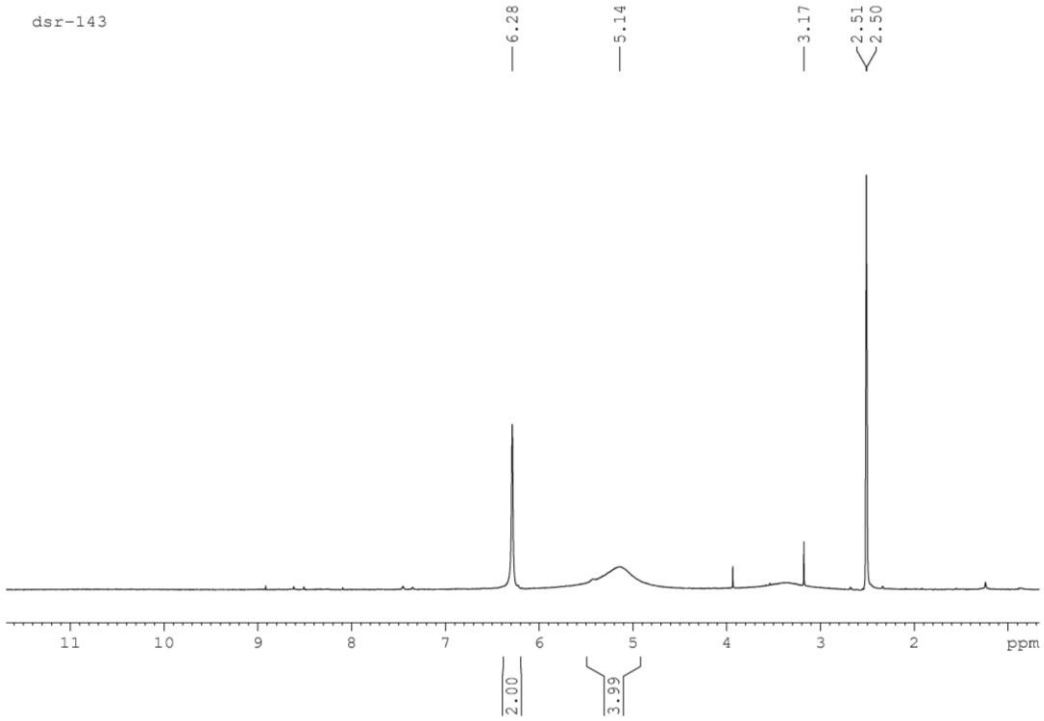
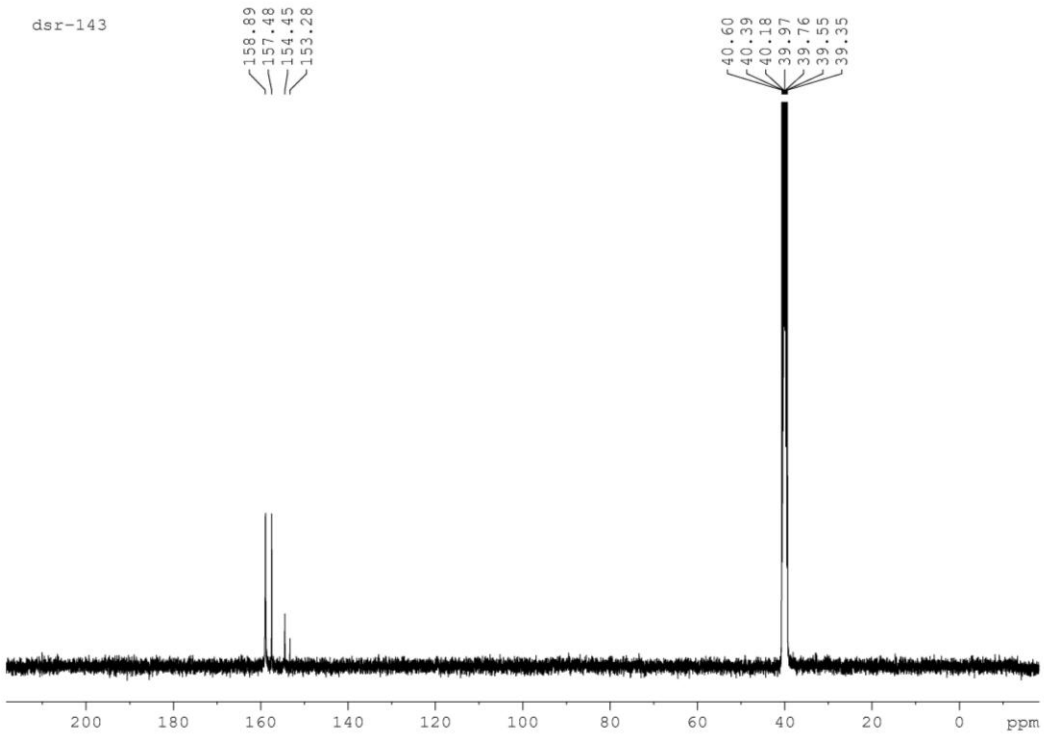
22. 3,5-Diamino-1*H*-1,2,4-triazol-4-ium 5-amino-3-azido-1,2,4-triazol-1-ide (12e)

a. ^{1}H NMR



b. ^{13}C NMR



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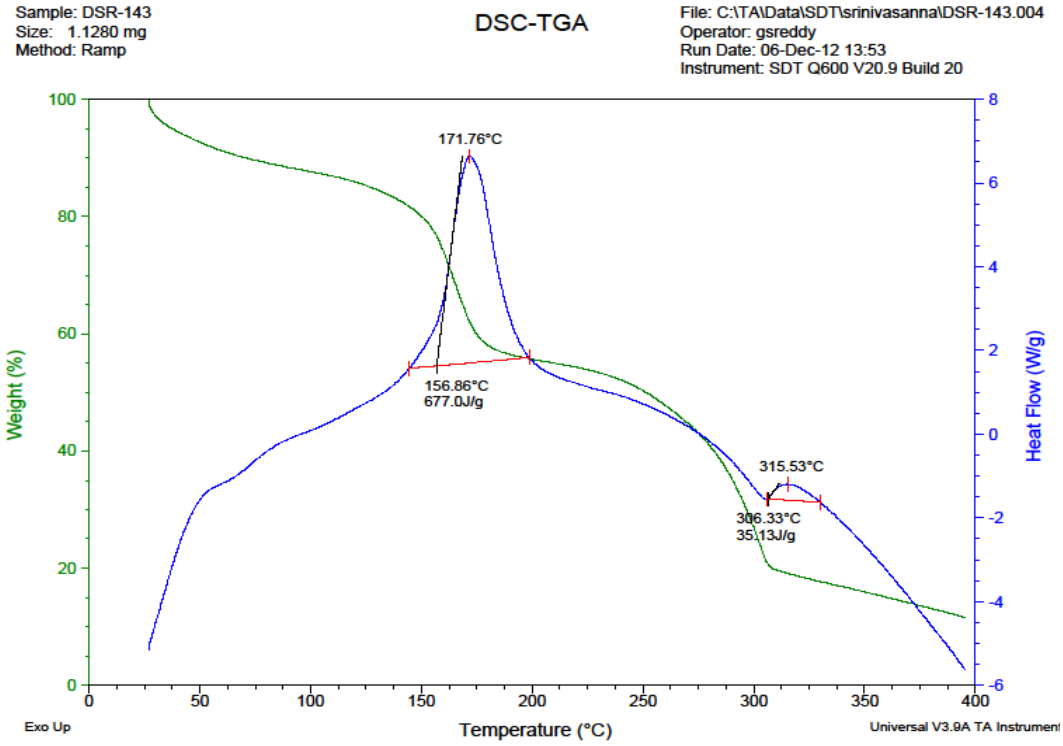
c. TG-DTA measurement



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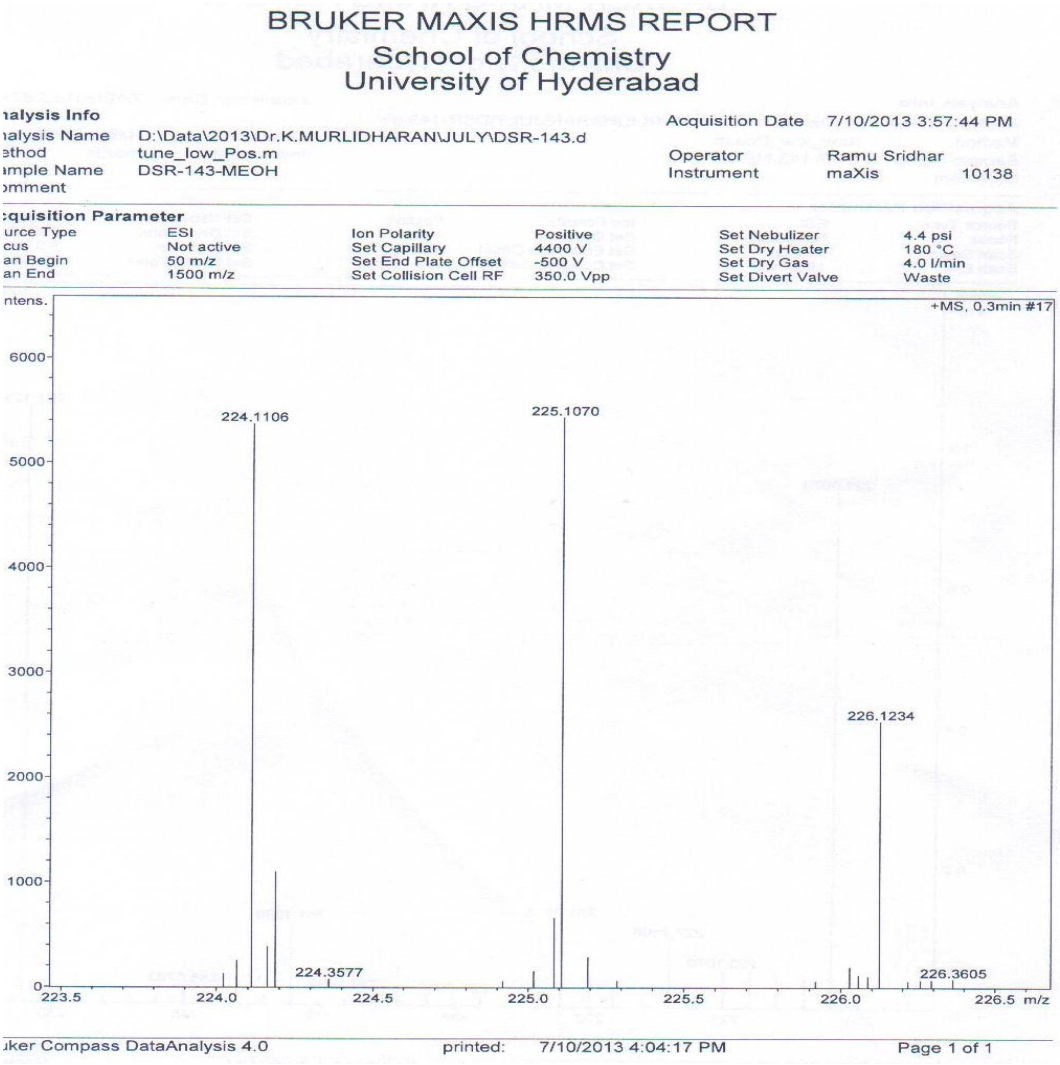

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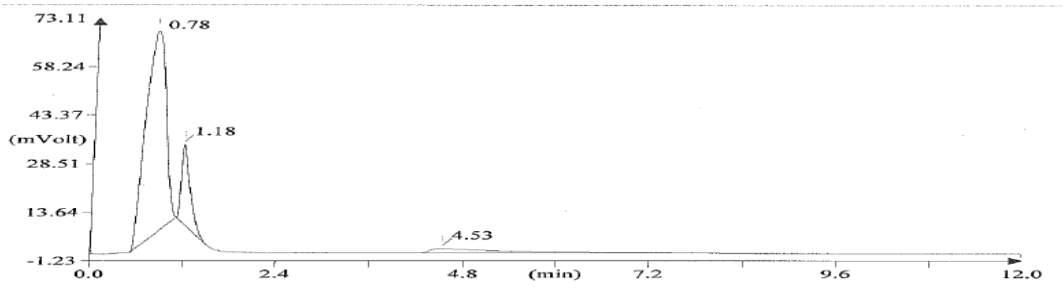
Method filename:	E:\Program Files\Thermo Finnigan\Eager 300 for EA1112\DATA\Sys_data_e
Sample ID:	DSR-143 (# 42)
Analysis type:	UnkNown
Chromatogram filename:	UNK-06022013-12.dat
Sample weight:	1.912



Element Name	Element %	Ret. Time
Nitrogen	74. 85	0. 78
Carbon	21. 37	1. 18
Hydrogen	3. 65	4. 53

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Table 1. Calculated total energy (E_0), zero point energy (ZPE) and thermal correction (ΔH_T) at B3PW91/6-31G(d,p) level for selective nonionic compounds and their molecular surface properties.

Comp.	E_0 (a.u.)	ZPE (a.u.)	ΔH_T (a.u.)	A ($Å^2$)	σ^2_{tot} (kcal/mol)	ν
5	-795.27592	0.1445	0.0130	217.21	702.91	0.20
7	-996.87609	0.1547	0.0152	255.88	534.86	0.18
9	-499.02838	0.0878	0.0078	151.34	432.26	0.22
10	-554.35787	0.1046	0.0093	166.32	235.98	0.23
11	-662.54621	0.0908	0.0105	186.37	213.53	0.22
12	-460.94548	0.0805	0.0085	147.58	402.34	0.16

A: Area of the isosurface of 0.001 electrons/$bohr^3$ electronic density. ν: Degree of balance between the positive and negative surface potentials. σ^2_{tot}: Measure of variability of the electrostatic potential.