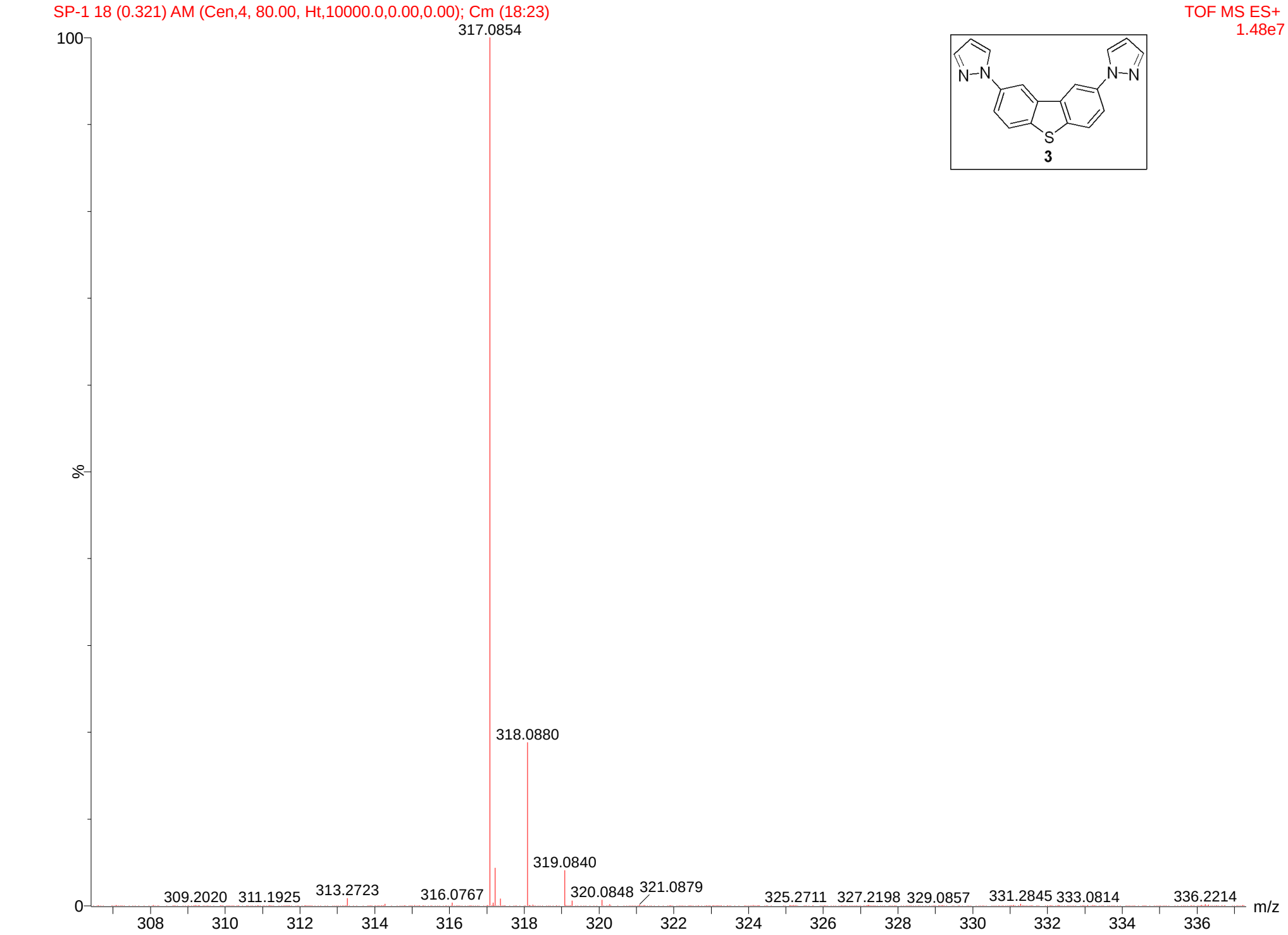
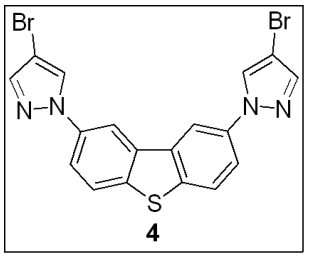
Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SP-2 20 (0.355) AM (Cen,4, 80.00, Ht,10000.0,0.00,0.00); Cm (20:25)

TOF MS ES+
2.25e5




**4**

100

%

0

474.9042
468.3891
476.9021
472.9060
467.4079
451.3604
496.4235
495.4415
495.3901
457.1346
457.3478
479.3938
453.3949
497.4260
489.3186
501.3772
445.2892
458.1376
446.2725
463.3411
480.3978
485.3561
493.4253
502.3805
455.3399
447.3337
460.3295
483.3681

445 450 455 460 465 470 475 480 485 490 495 500 505

m/z

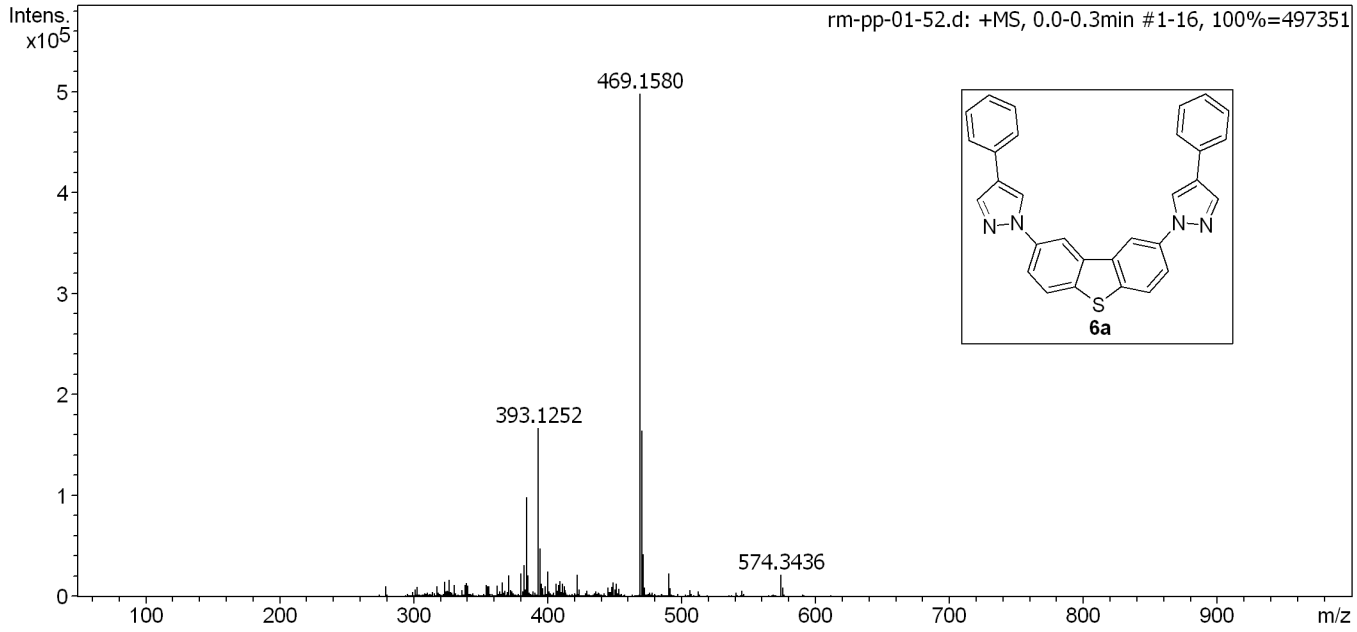
# DEPARTMENT OF CHEMISTRY,I.I.T.(B)

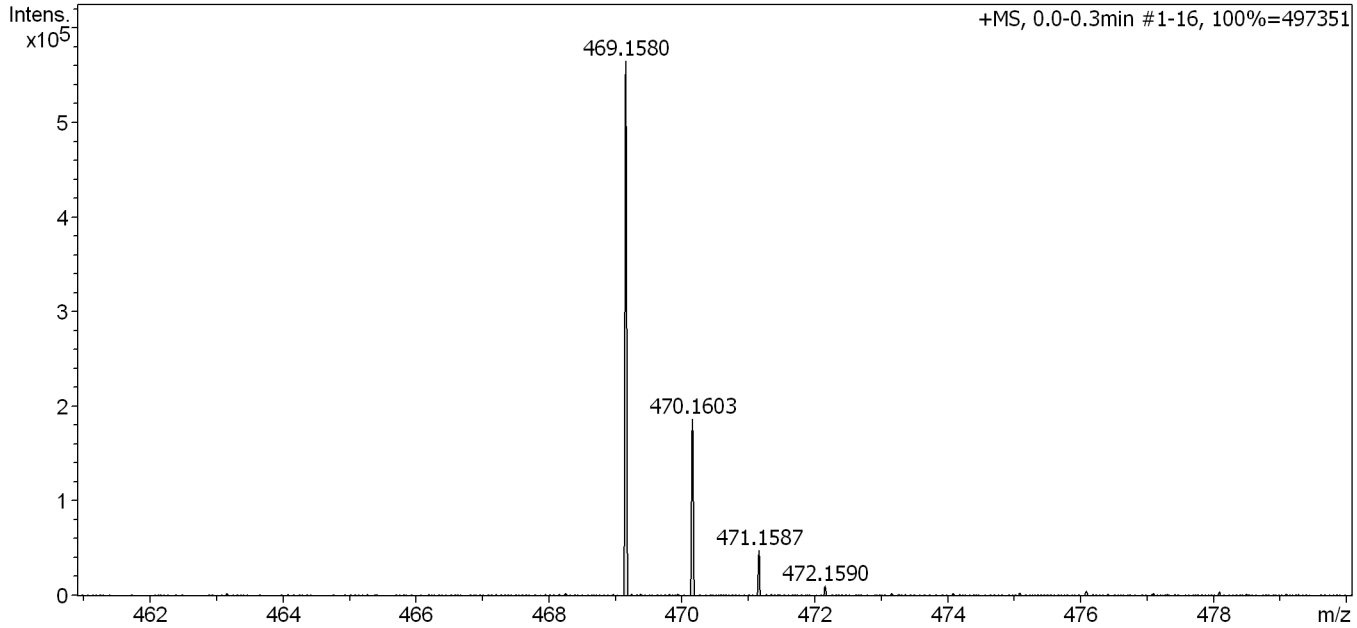
**Analysis Info**

| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\JULY-19\rm-pp-01-52.d | Acquisition Date | 7/30/2019 5:58:26 PM |
| Method | Tune_pos_1000a_NAF-05-07-2019.m | Operator | PG OUT |
| Sample Name | rm-pp-01-52 | Instrument | maXis impact 282001.00081 |
| Comment | lrms | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4000 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 | 1000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |



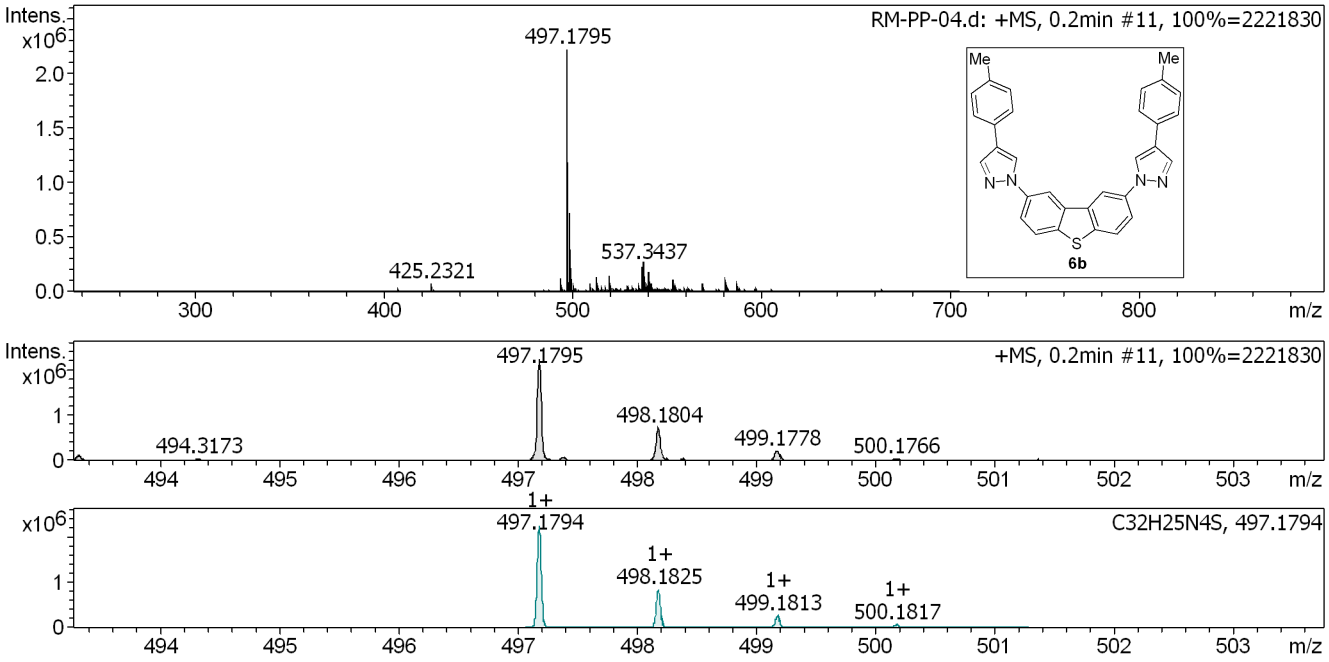
# DEPARTMENT OF CHEMISTRY, I.I.T.(B)

**Analysis Info**

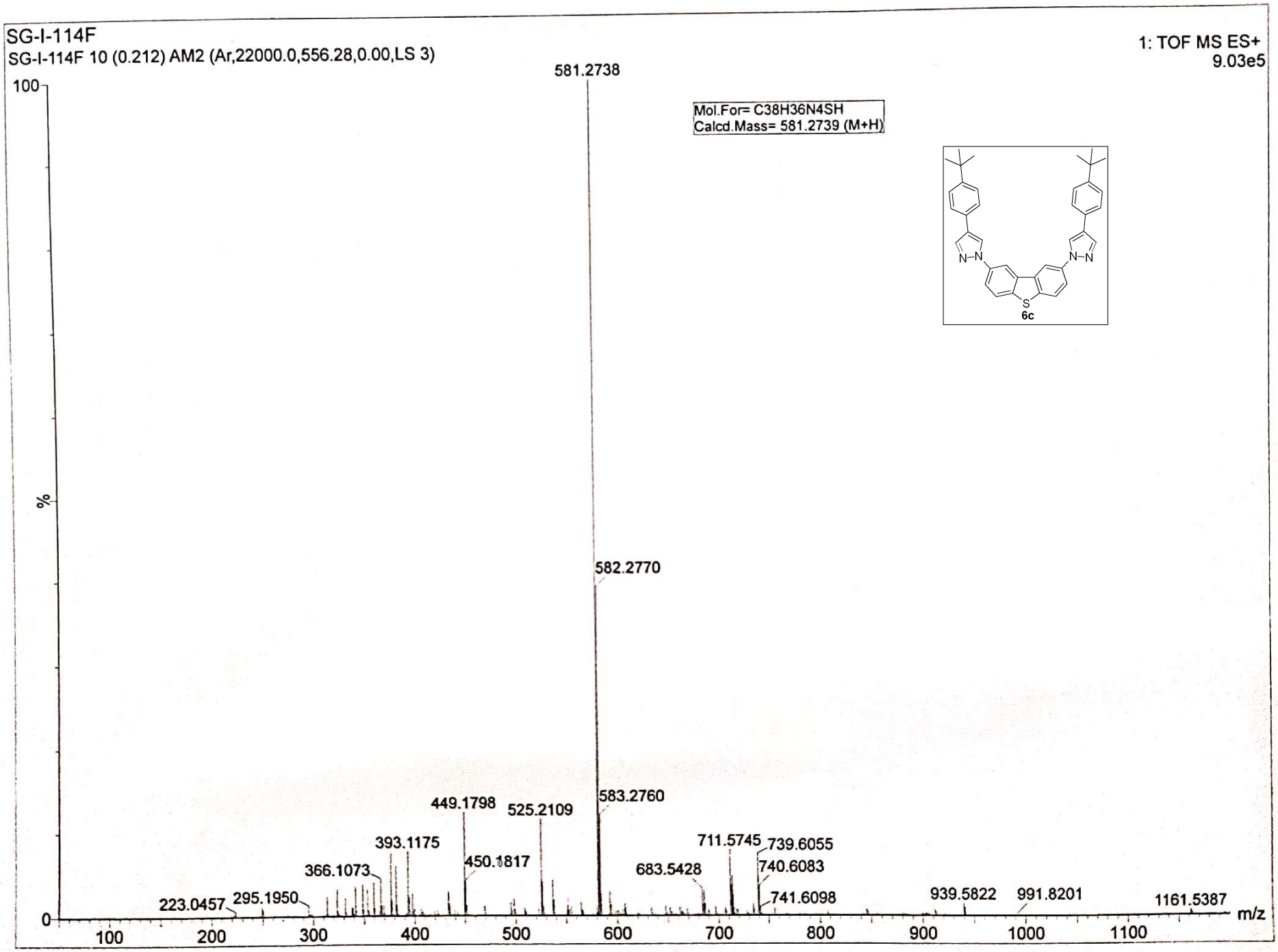
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\AUG-19\RM-PP-04.d | Acquisition Date | 8/13/2019 3:57:57 PM |
| Method | Tune_pos_1000a_NAF-05-07-2019.m | Operator | INN out |
| Sample Name | RM-PP-04 | Instrument | maXis impact 282001.00081 |
| Comment | C32H24N4S | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4000 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 | 700 m/z | Set Collision Cell RF | 1200.0 Vpp | Set Divert Valve | Source |

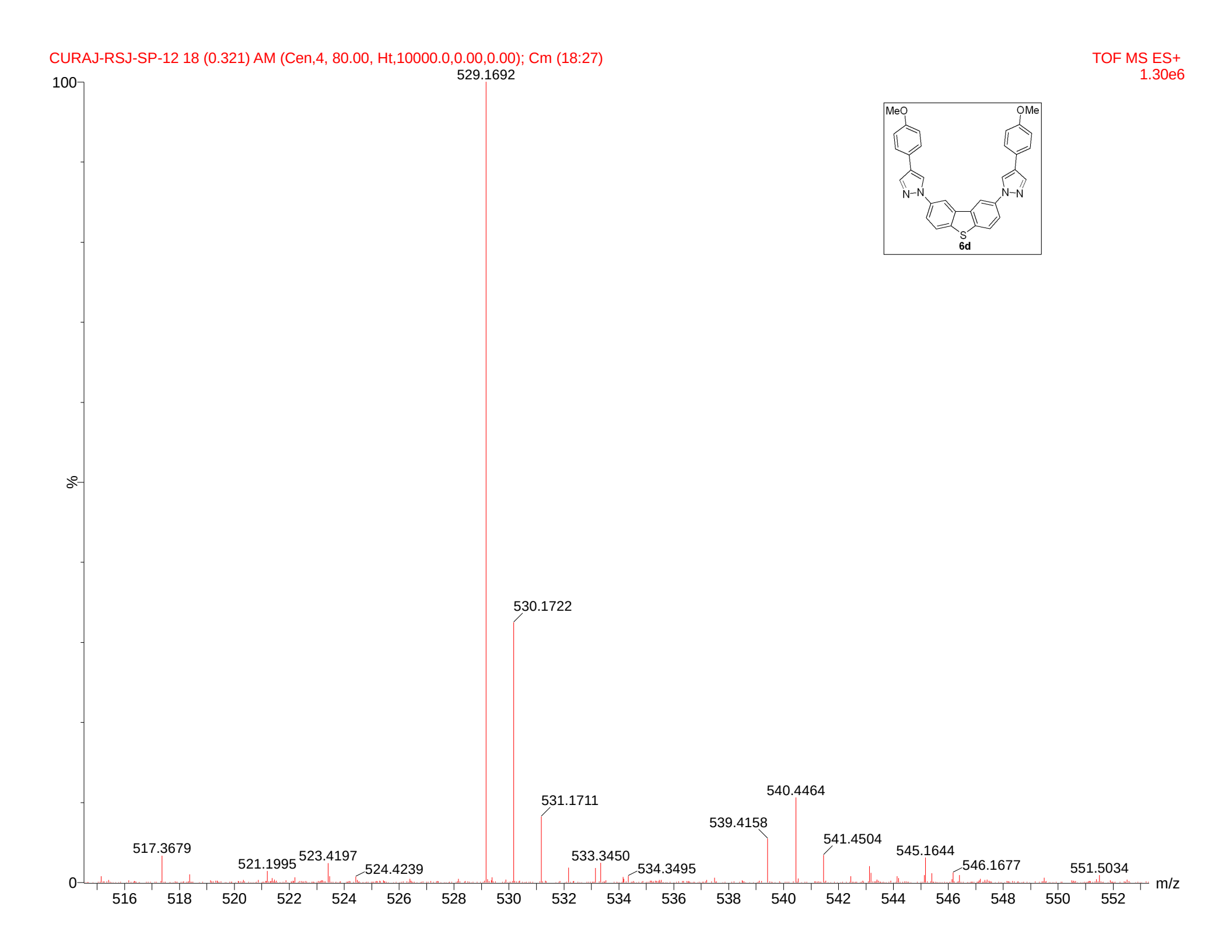



| Meas. m/z | # | Ion Formula | m/z | err [ppm] | mSigma | # Sigma | Score | rdb | e⁻ Conf | N-Rule |
|---|---|---|---|---|---|---|---|---|---|---|
| 497.1795 | 1 | C32H25N4S | 497.1794 | 0.0 | 22.4 | 1 | 100.00 | 22.5 | even | ok |



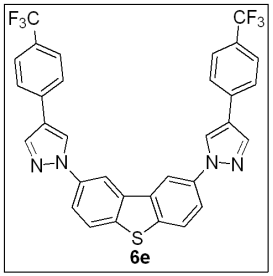
CURAJ-RSJ-SP-12 18 (0.321) AM (Cen,4, 80.00, Ht,10000.0,0.00,0.00); Cm (18:27)

TOF MS ES+
1.30e6



SP-4 17 (0.304) AM (Cen,4, 80.00, Ht,10000.0,0.00,0.00); Cm (17:21)

TOF MS ES+
3.05e5




6e

100

%

0

600.4677
605.1227
601.4712
606.1257
602.4738
606.4240
611.4733
621.3980
613.3939
622.4019
589.4274
590.4302
607.5652
617.2559
618.2595
624.6295
594.2239
599.5038
603.5339

588 590 592 594 596 598 600 602 604 606 608 610 612 614 616 618 620 622 624

m/z

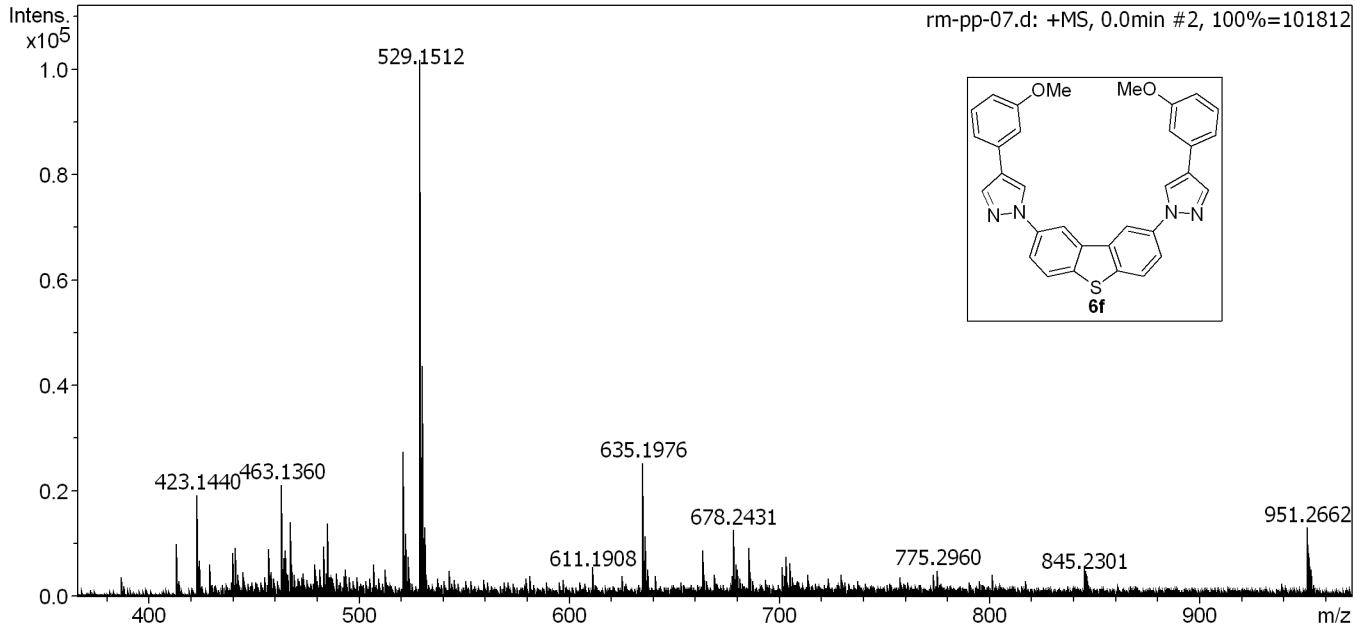
# DEPARTMENT OF CHEMISTRY,I.I.T.(B)

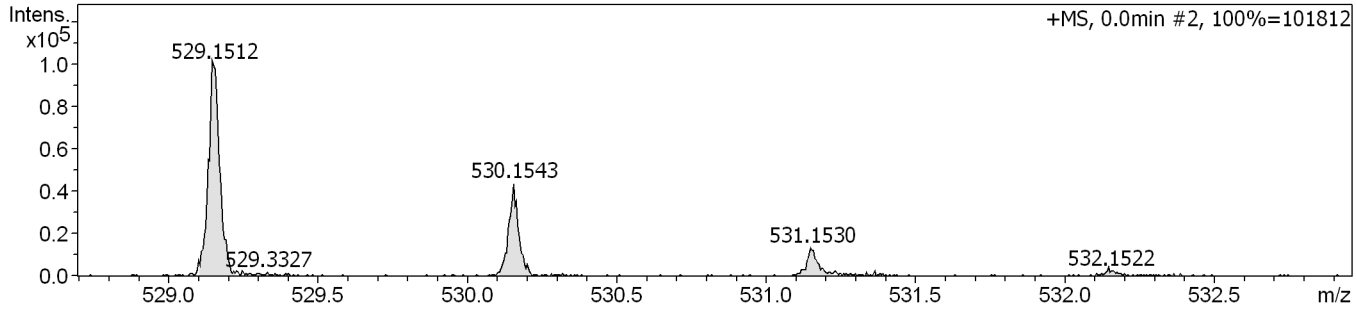
**Analysis Info**

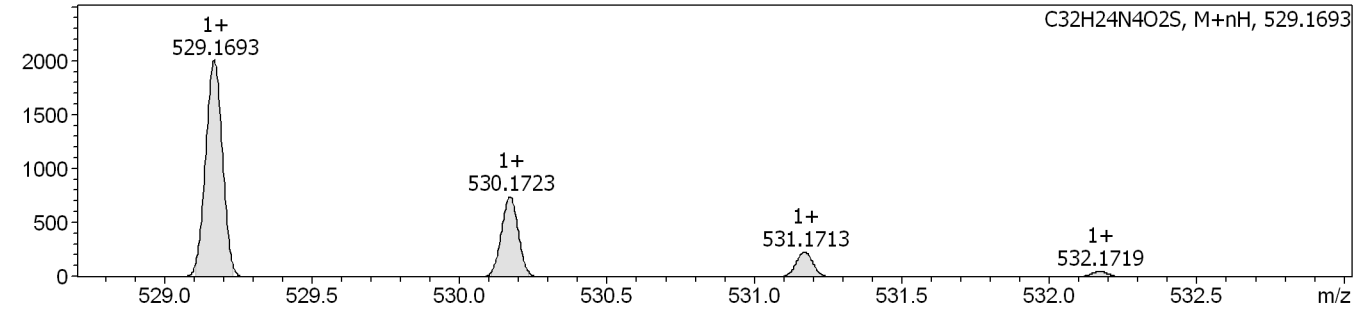
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\AUG-19\rm-pp-07.d | Acquisition Date | 8/8/2019 1:43:35 PM |
| Method | Tune_pos_NAICSI-1000a.m | Operator | PG SRD IN |
| Sample Name | rm-pp-07 | Instrument | maXis impact 282001.00081 |
| Comment | LRMS | | |

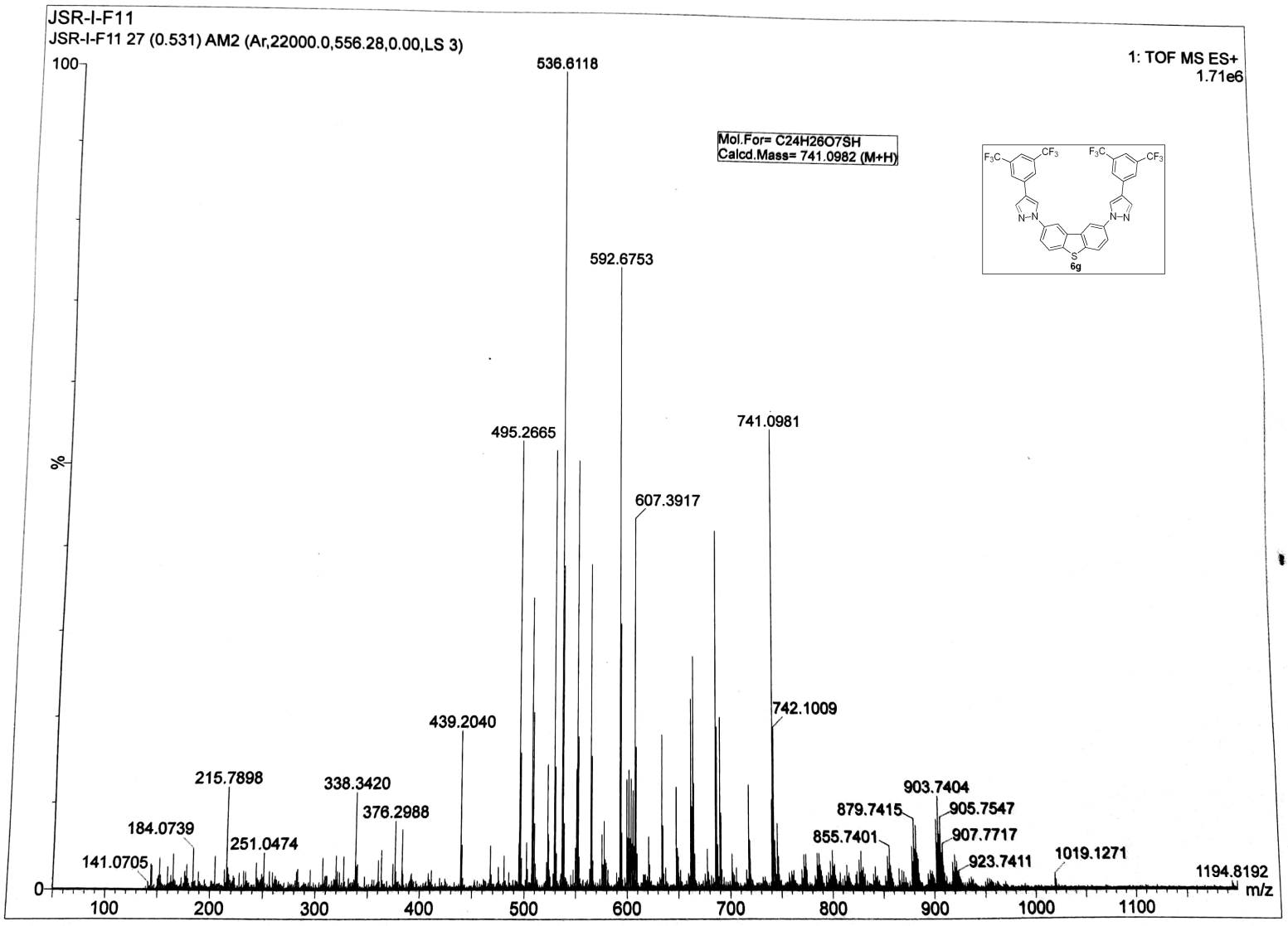
**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.3 Bar |
| Focus | Active | Set Capillary | 4500 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 | 1000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |



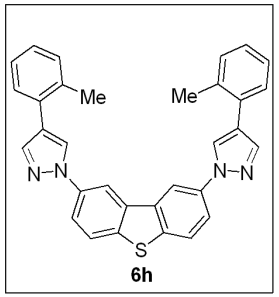





CURAJ-RSJ-SP-13 19 (0.338) AM (Cen,4, 80.00, Ht,10000.0,0.00,0.00); Cm (19:26)

TOF MS ES+
3.06e6




**6h**

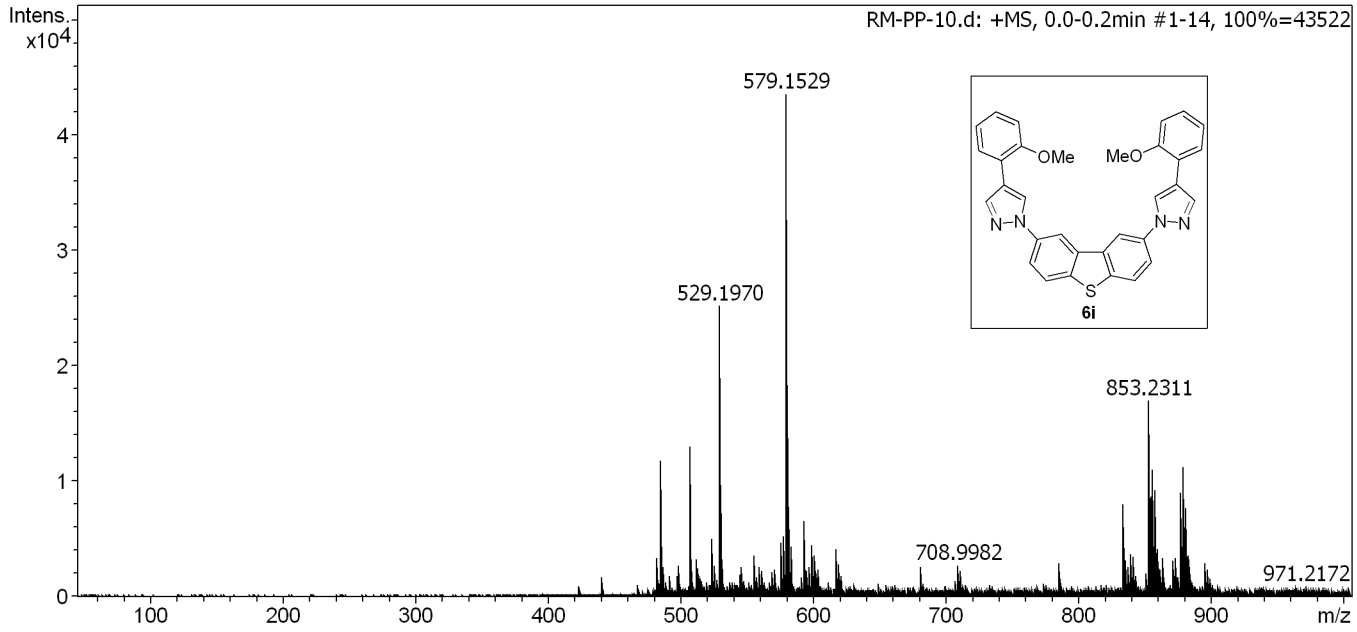
# DEPARTMENT OF CHEMISTRY,I.I.T.(B)

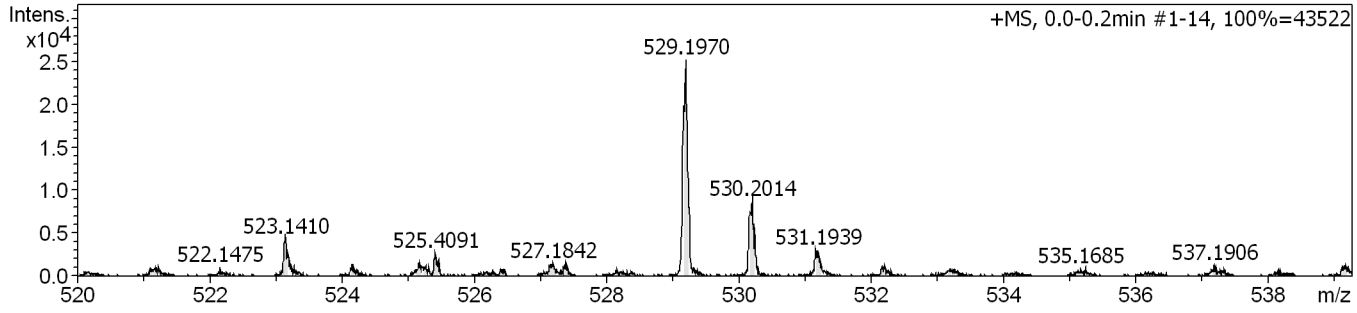
**Analysis Info**

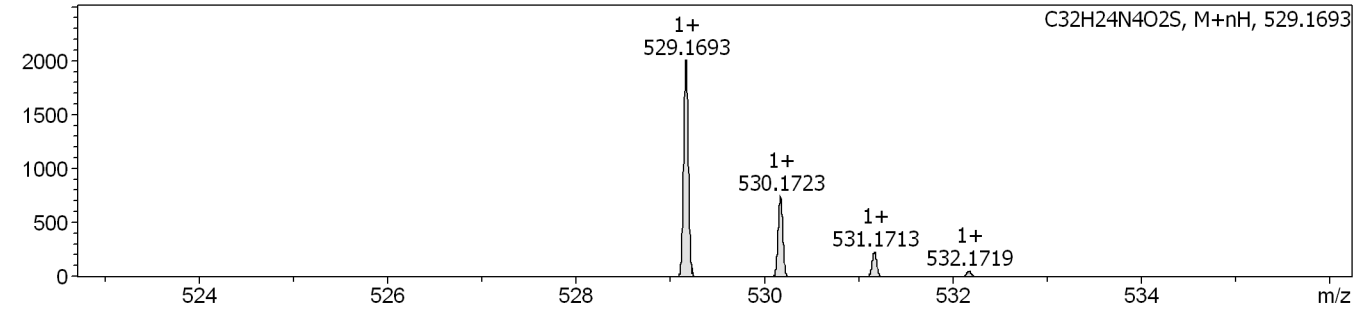
| | | | |
|---|---|---|---|
| Analysis Name | D:\Data\AUG-19\RM-PP-10.d | Acquisition Date | 8/6/2019 7:24:39 PM |
| Method | Tune_pos_1000a_NAF-05-07-2019.m | Operator | PG SRD IN |
| Sample Name | RM-PP-10 | Instrument | maXis impact 282001.00081 |
| Comment | LRMS | | |

**Acquisition Parameter**

| | | | | | |
|---|---|---|---|---|---|
| Source Type | ESI | Ion Polarity | Positive | Set Nebulizer | 0.4 Bar |
| Focus | Active | Set Capillary | 4000 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 | 1000 m/z | Set Charging Voltage | 2000 V | Set Divert Valve | Source |
| | | Set Corona | 0 nA | Set APCI Heater | 0 °C |



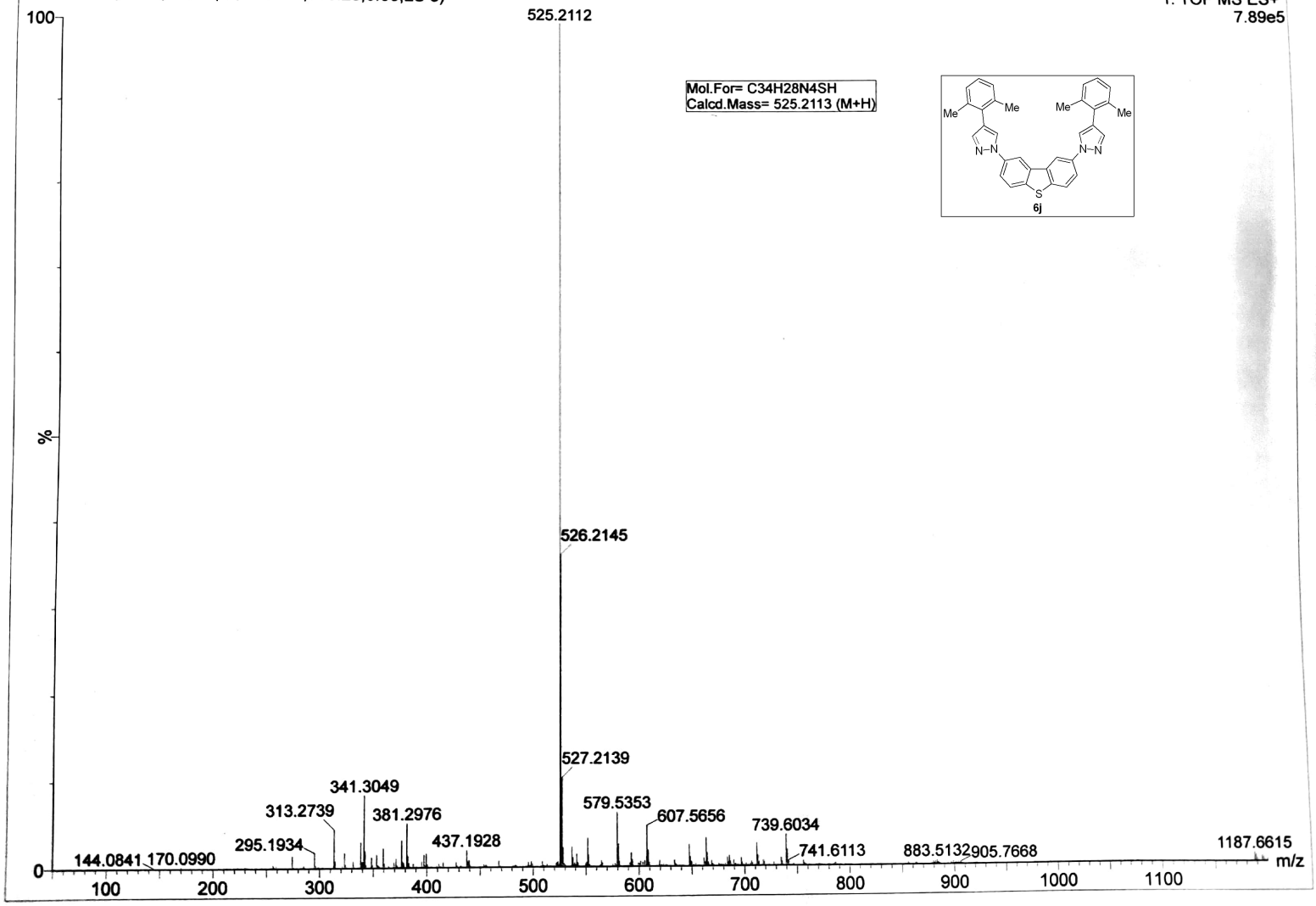



SG-I-78

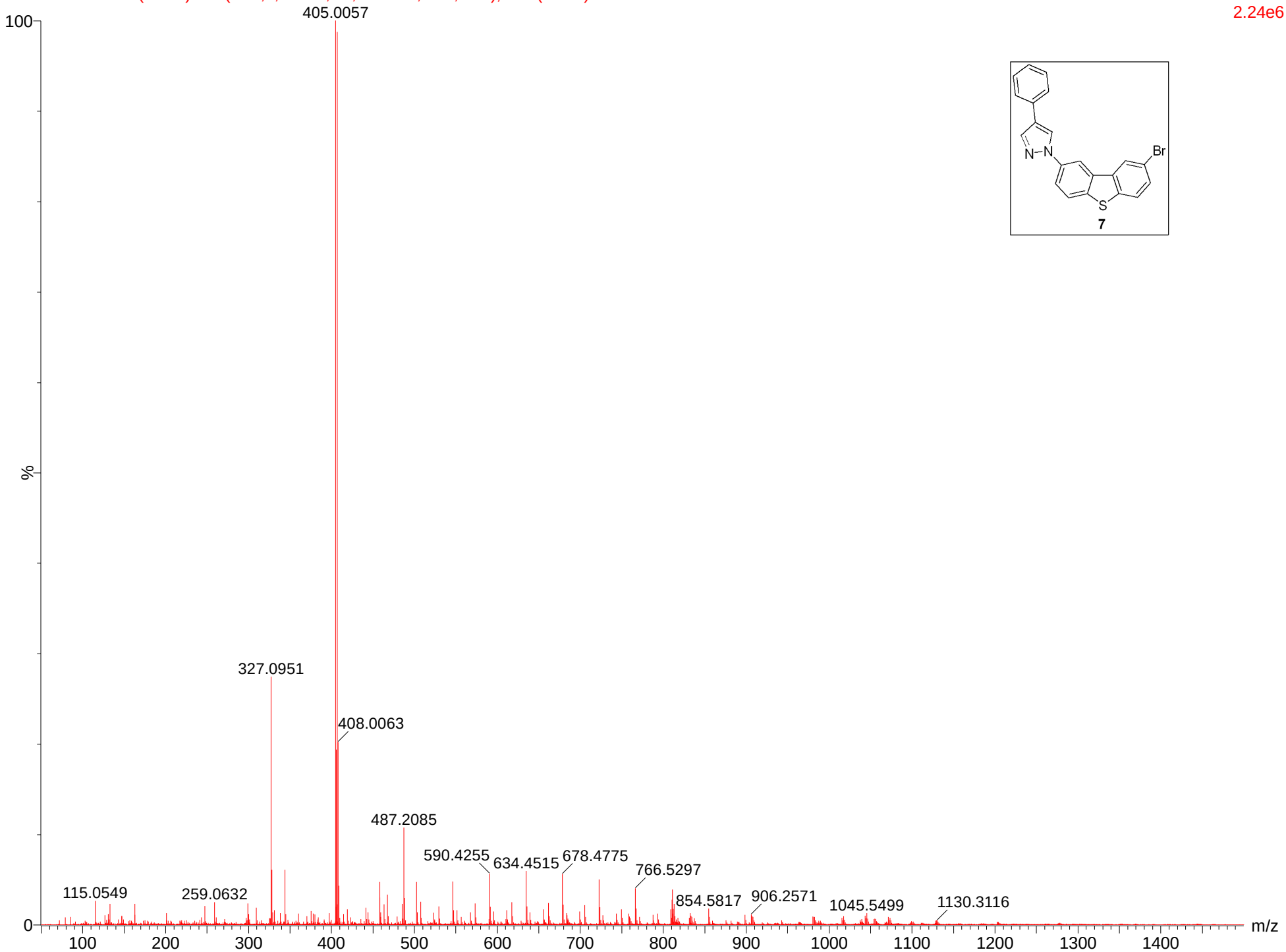
SG-I-78 18 (0.360) AM2 (Ar,22000.0,556.28,0.00,LS 3)

1: TOF MS ES+
7.89e5



CURAJ-RSJ-7 12 (0.220) AM (Cen,4, 80.00, Ht,10000.0,0.00,0.00); Cm (12:15)

TOF MS ES+
2.24e6



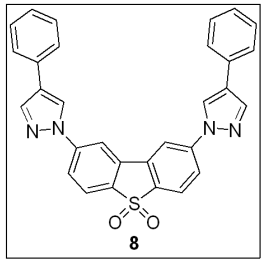




**7**

SP-6 15 (0.271) AM (Cen,4, 80.00, Ht,10000.0,0.00,0.00); Cm (15:22)

TOF MS ES+
2.67e4




8

100

%

0

501.1382

501.8242

500.8264

502.1407

502.8264

503.0678

502.7529

503.1447

504.7527

503.8305

504.0062

504.6211

504.9295

505.0638

500.1336

500.7464

501.7545

502.1806

503.7564

504.2154

500

501

502

503

504

505

m/z