Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supporting Information

Improvement of D-π-A organic dye-based dye-sensitized solar cell performance by simple triphenylamine donor substitutions on the π-linker of the dye

T. Sudyoadsuk,[a] A. Thangthong,[a] N. Prachumrak,[a] P. Nalaoh,[a] S. Jungsuttiwong,[b] R. Daengngern,[c] S. Namuangruk,[c] P. Pattanasattaya[a] and V. Promarak[a]*

[a] Department of Material Science and Engineering, School of Molecular Science and Engineering, Vidyasirimedhi Institute of Science and Technology, Wangchan, Rayong 21210, Thailand

[b] Department of Chemistry, Faculty of Science, Ubon Ratchathani University, Ubon Ratchathani 34190, Thailand

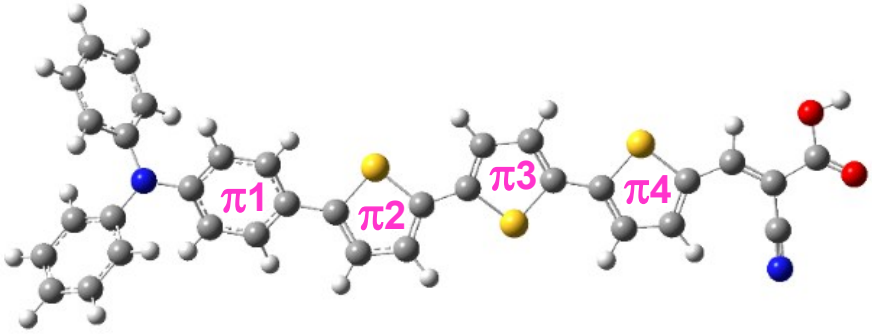
[c] NANOTEC, National Science and Technology Development Agency, Pathum Thani 12120, Thailand

*e-mail: vinich.p@vistec.ac.th

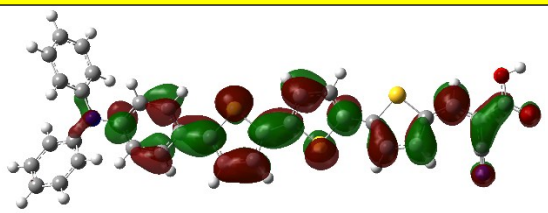
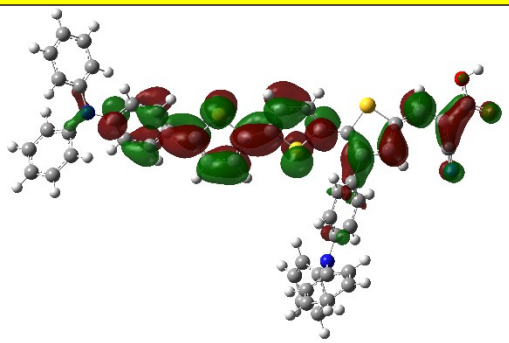
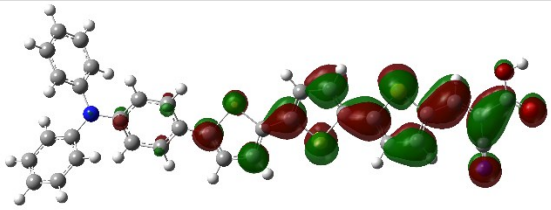
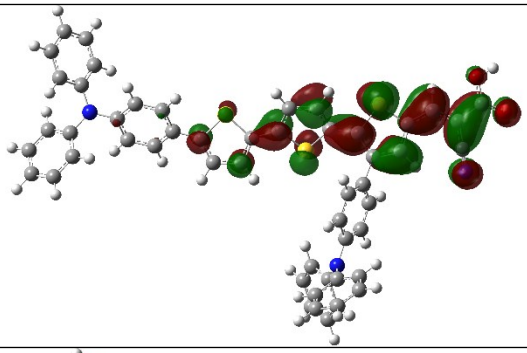
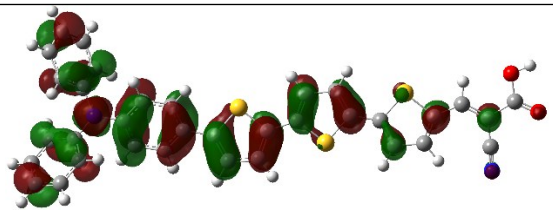
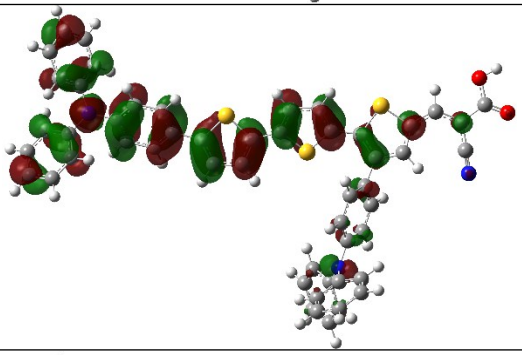
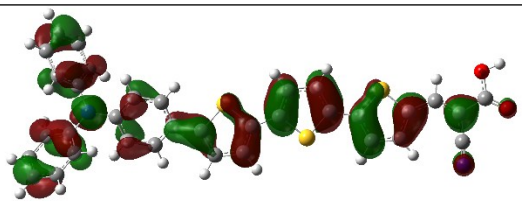
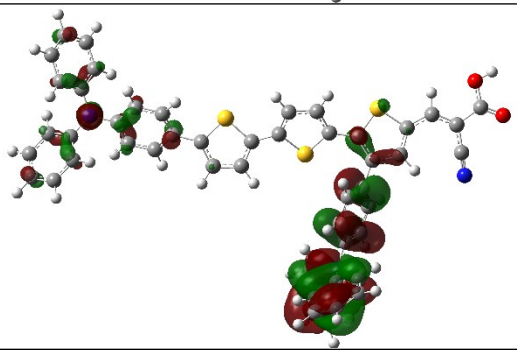
……

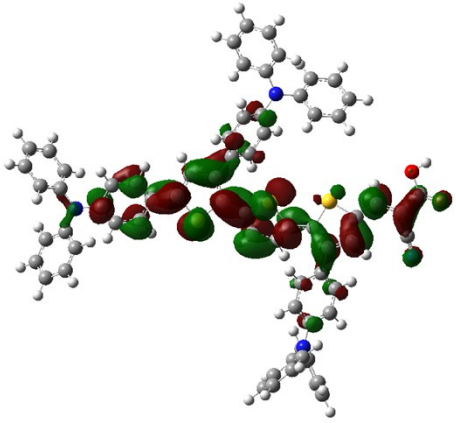
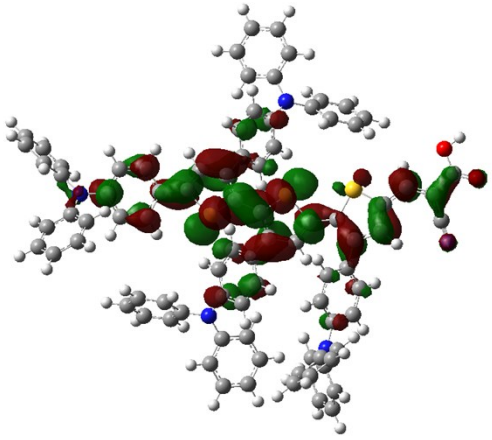
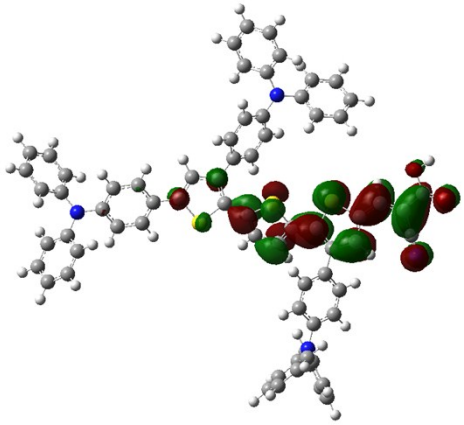
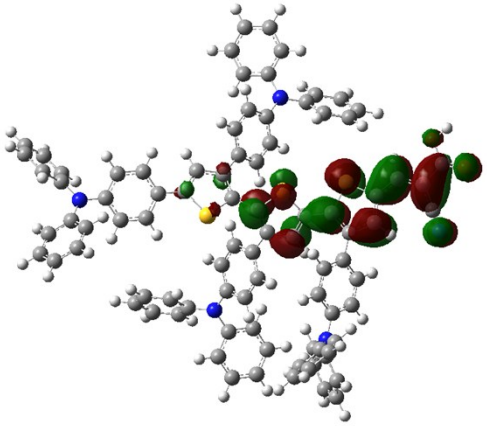
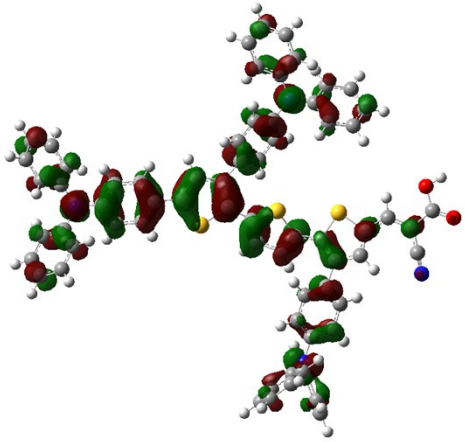
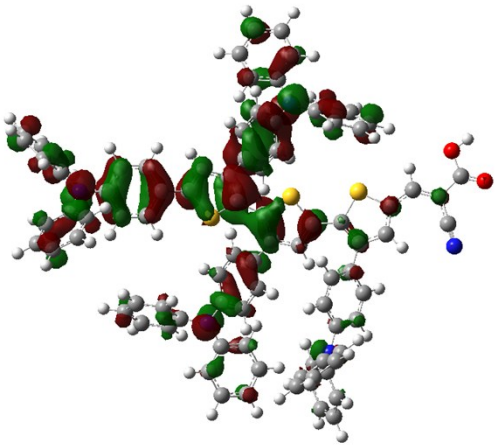
1. Quantum chemical calculation results

Table S1. The optimized geometry parameters, dihedral angles (in degree), of the dyes computed at B3LYP/6-31G(d,p) level.



Dye	Dihedral angle (°) / intergroup			
	π 1-π2	π2-π3	π3-π4	π3-A
T1	-24.30	10.75	-4.91	0.27
T2	-24.30	16.01	-28.05	3.03
T3	-24.35	37.82	-29.94	3.69
T4	-26.81	55.37	-30.71	3.37
Note: π1 = Triphenylamine, π2-π4 = Thiophenes, and A = Cyanoacrylic acid				

	T1	T2
L+1		
L		
H		
H-1		

	T3	T4
L+1		
L		
H		

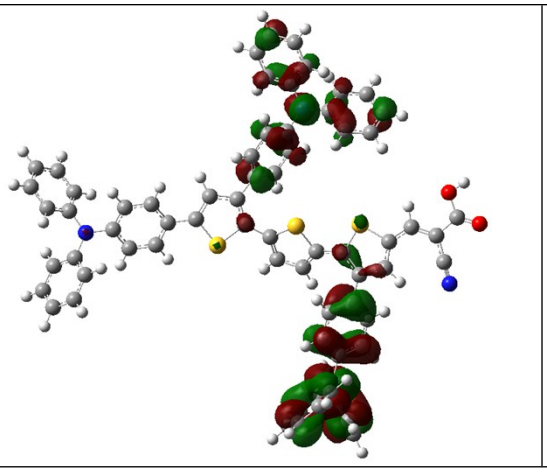
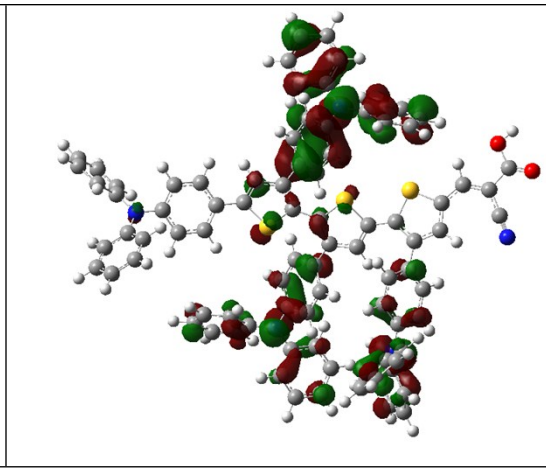
H-1		

Figure S1. HOMO and LUMO of the dyes calculated by B3LYP/6-31G(d,p) level.

Table S2. Excitation energy (E_{ex}), oscillator strength (*f*) and transition composition of the dyes calculated by TD-CAM-B3LYP/6-31G(d,p) in CH_2Cl_2 solvent.

Dyes	Transition	E_{ex}, eV (nm)	*f*	Composition H=HOMO, L=LUMO, …
T1	$S_0 \rightarrow S_1$	2.56 (485)	2.0919	0.53 (H→L)+0.40 (H-1→L)
	$S_0 \rightarrow S_3$	3.79 (327)	0.2045	0.40 (H→L)+0.26 (H-1→L+1)
	$S_0 \rightarrow S_4$	4.10 (302)	0.3119	0.38 (H-1→L+1)+0.33 (H→L+1)
T2	$S_0 \rightarrow S_1$	2.62 (473)	1.8779	0.53 (H→L)+0.36 (H-2→L)
	$S_0 \rightarrow S_2$	3.23 (384)	0.1609	0.64 (H-1→L)
	$S_0 \rightarrow S_3$	3.47 (357)	0.1672	0.46 (H→L+1) + 0.36 (H-2→L)
	$S_0 \rightarrow S_5$	3.97 (312)	0.6677	0.35 (H→L+2) + 0.34 (H-1→L+1)
T3	$S_0 \rightarrow S_1$	2.62 (474)	1.3284	0.55 (H→L)+0.33 (H-3→L)
	$S_0 \rightarrow S_3$	3.41 (364)	0.5260	0.57 (H-2→L)+0.28 (H-3→L)
	$S_0 \rightarrow S_4$	3.49 (355)	0.1797	0.43 (H→L+1)+0.34 (H-3→L)
	$S_0 \rightarrow S_5$	3.76 (330)	0.3260	0.35 (H→L)+0.32 (H→L+1)
	$S_0 \rightarrow S_6$	3.96 (313)	1.1369	0.36 (H→L+2)
T4	$S_0 \rightarrow S_1$	2.75 (451)	1.1432	0.51 (H→L)+0.37 (H-4→L)
	$S_0 \rightarrow S_3$	3.40 (364)	0.2165	0.54 (H-1→L)+0.26 (H-2→L)
	$S_0 \rightarrow S_4$	3.50 (354)	0.4442	0.40 (H→L+1)+0.31 (H-4→L)
	$S_0 \rightarrow S_5$	3.57 (348)	0.4432	0.34 (H-2→L)+0.33 (H-3→L)
	$S_0 \rightarrow S_6$	3.77 (329)	0.3166	0.34 (H→L)+0.31 (H→L+1)
	$S_0 \rightarrow S_7$	3.96 (313)	1.2051	0.0.29 (H-2→L+1)+0.26 (H→L+2)
	$S_0 \rightarrow S_8$	4.02 (309)	0.1792	0.32 (H-3→L+1)+0.24 (H→L+3)

2. Fluorescence property

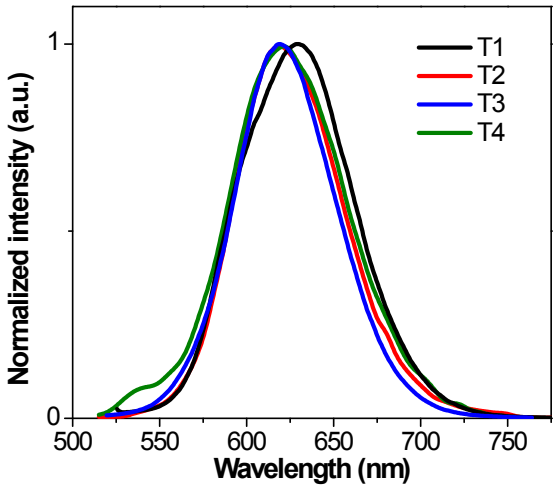


Figure S2. Photoluminescence spectra of dyes **T1-4** in CH_2Cl_2 solution.

3. IMVS/IMPS plots

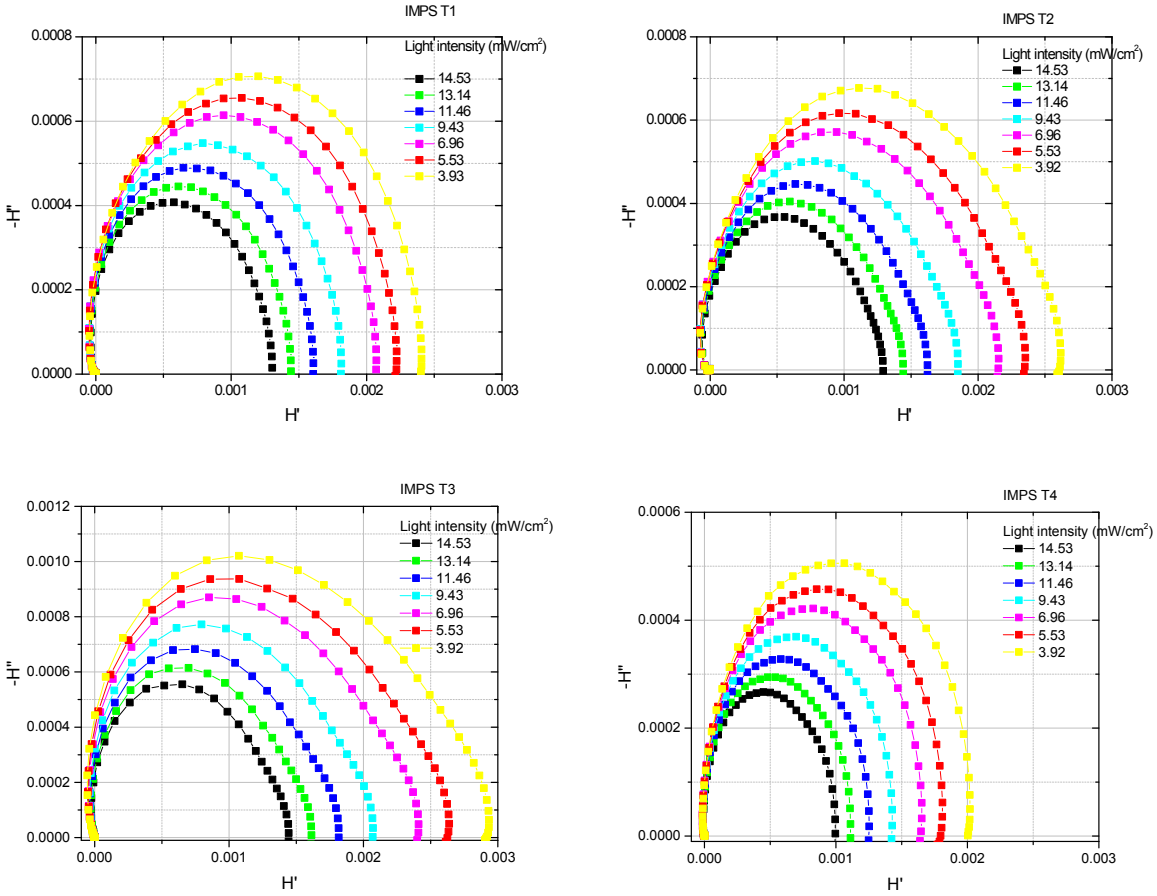


Figure S3 IMPS Nyquist plots of DSSCs based on dyes **T1-T4** at different light intensities

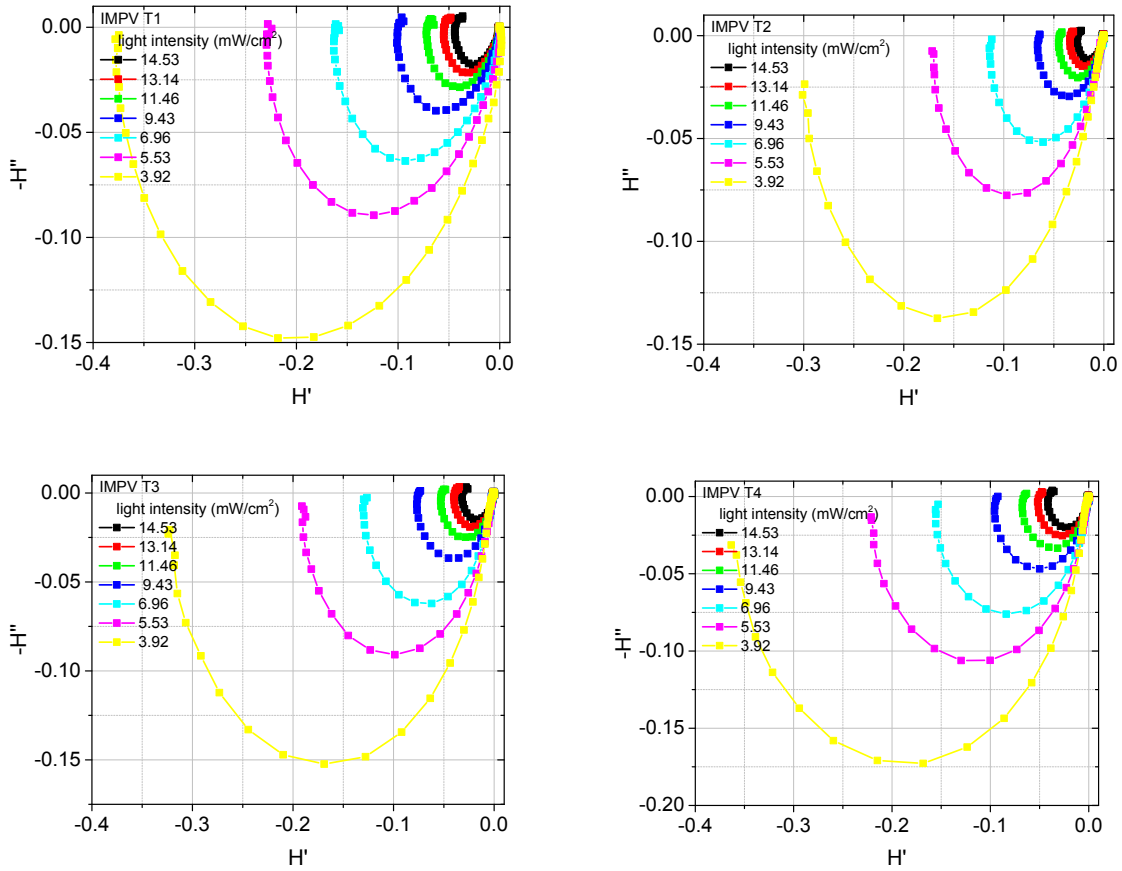
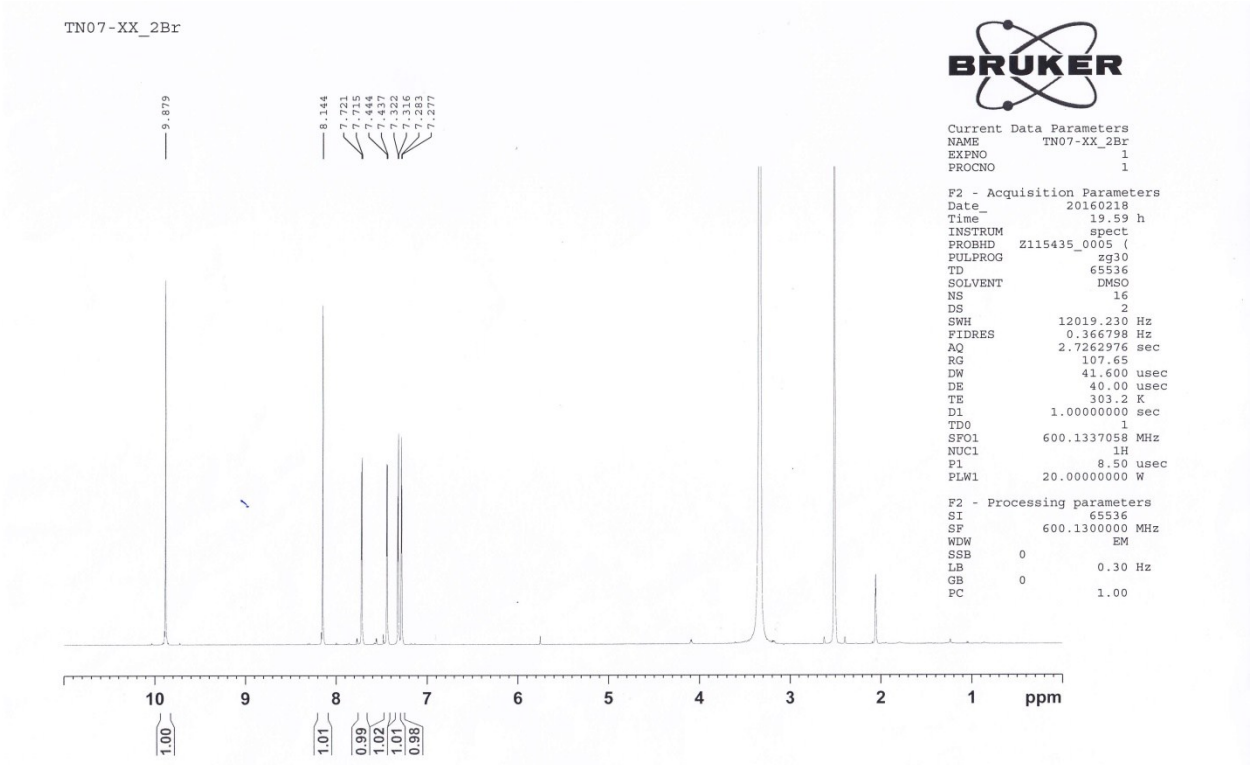
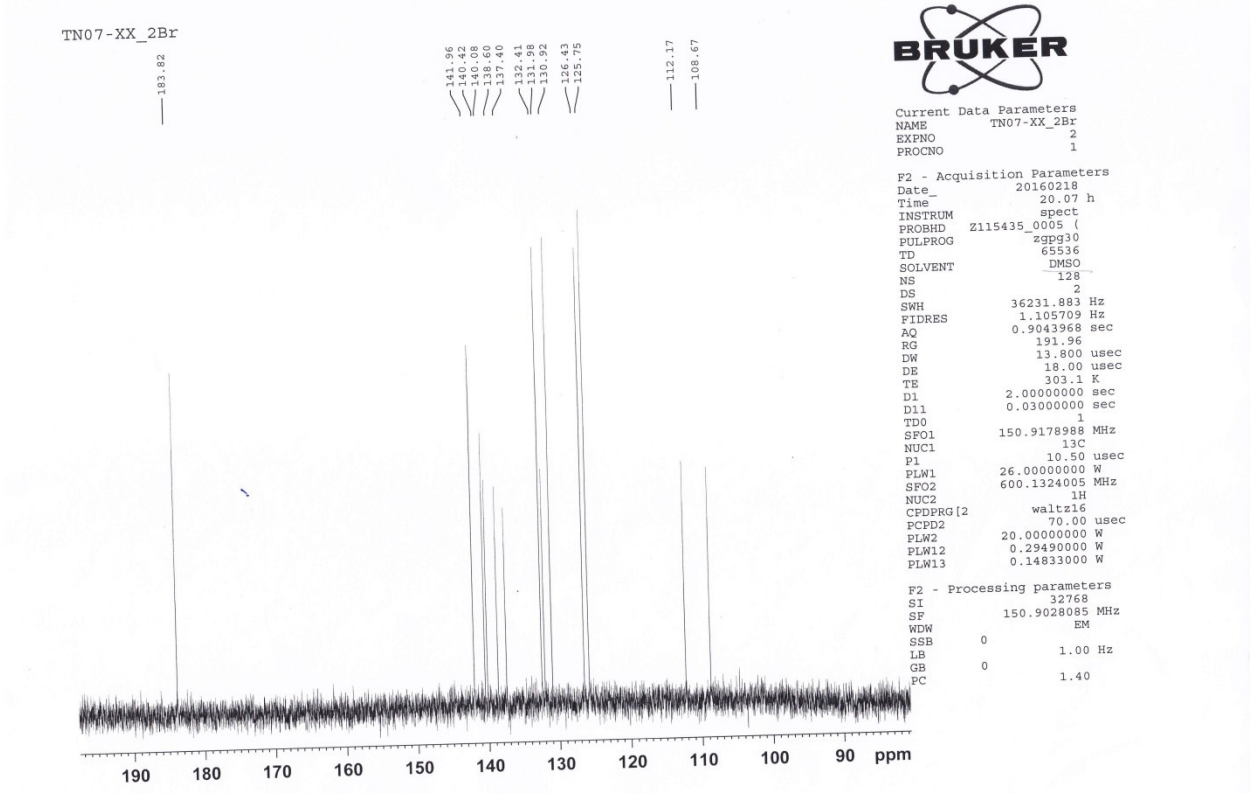


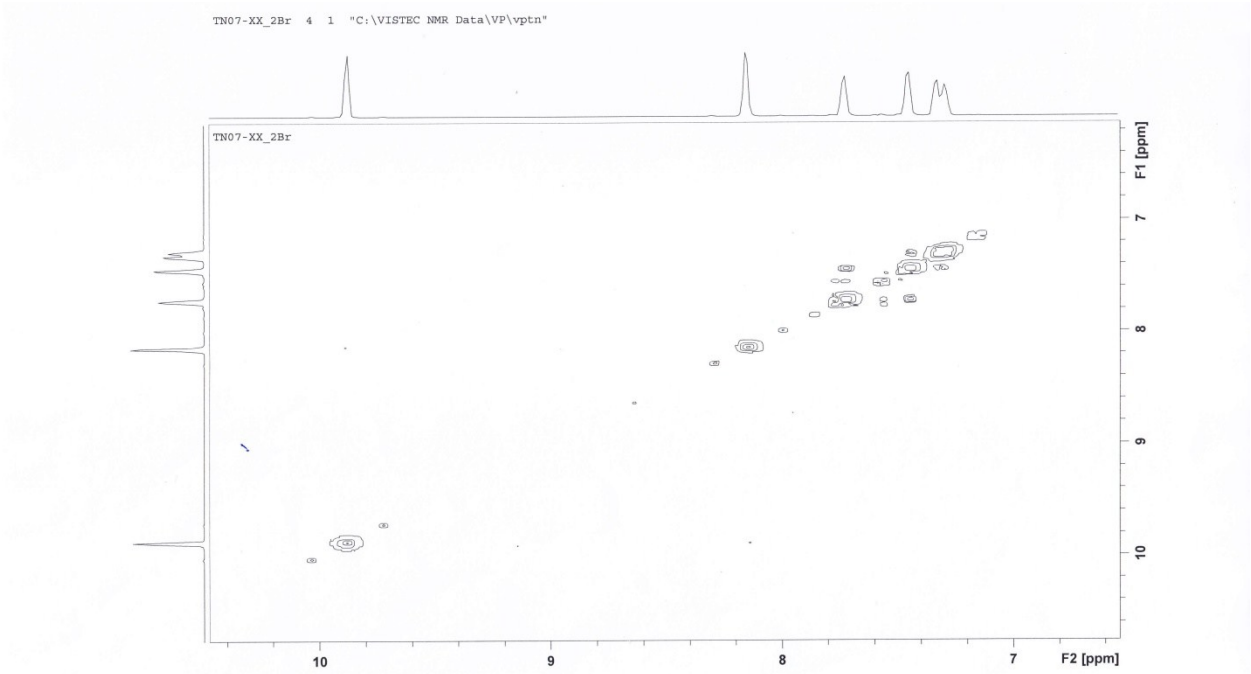
Figure S4 IMVS Nyquist plots of DSSCs based on dyes **T1-T4** at different light intensities

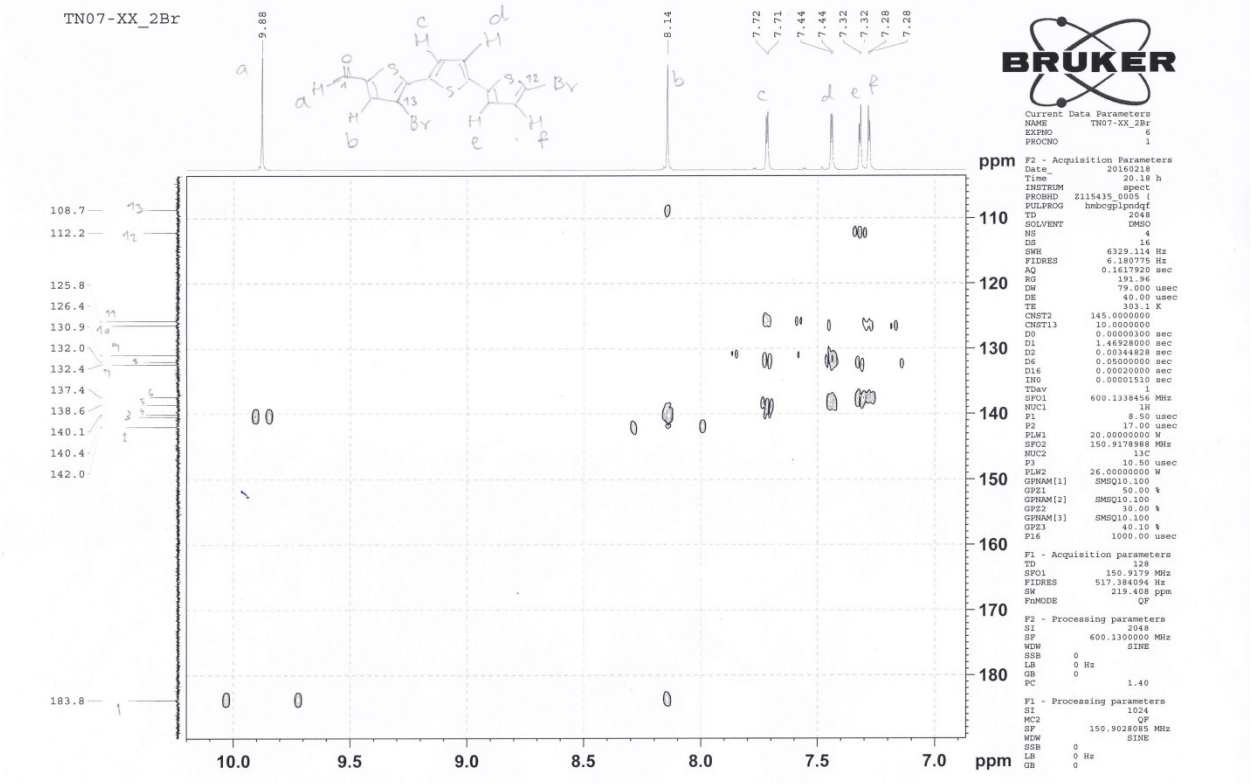
4. NMR and APCI-Q-TOF/MALDI-TOF spectra

Compound 3









BRUKER

Current Data Parameters
NAME TN07-XX_2Br
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160218
Time 20.18 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG hmbcgplpndqf
TD 2048
SOLVENT DMSO
NS 4
DS 16
SWH 6329.114 Hz
FIDRES 6.180775 Hz
AQ 0.1617920 sec
RG 191.96
DW 79.000 usec
DE 40.00 usec
TE 303.1 K
CNST2 145.0000000
CNST13 10.0000000
D0 0.00000300 sec
D1 1.46928000 sec
D2 0.00344828 sec
D6 0.05000000 sec
D16 0.00020000 sec
IN0 0.00001510 sec
TDav 1
SFO1 600.1338456 MHz
NUC1 1H
P1 8.50 usec
P2 17.00 usec
PLW1 20.00000000 W
SFO2 150.9178988 MHz
NUC2 13C
P3 10.50 usec
PLW2 26.00000000 W
GPNAM[1] SMSQ10.100
GPZ1 50.00 %
GPNAM[2] SMSQ10.100
GPZ2 10.00 %
GPNAM[3] SMSQ10.100
GPZ3 40.10 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 150.9179 MHz
FIDRES 517.384094 Hz
SW 219.408 ppm
FnMODE QF

F2 - Processing parameters
SI 2048
SF 600.1300000 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 150.9028085 MHz
WDW SINE
SSB 0
LB 0 Hz
GB 0

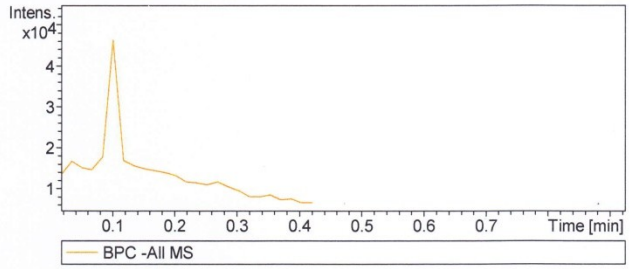
Q-ToF MS Report | Frontier Research Center@VISTEC

Analysis Info

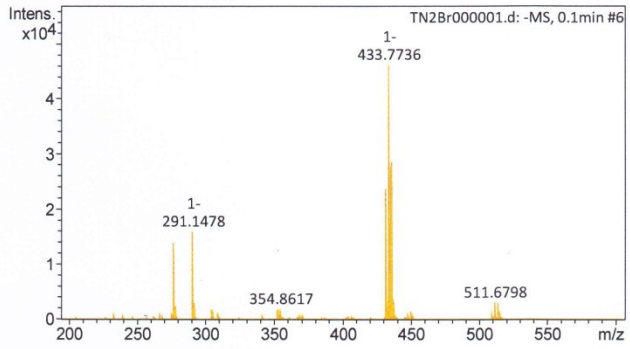
Analysis Name	D:\Data\VISTEC Data QTOF\Vinich\A-monrat\TN2Br000001.d	Acquisition Date	10/14/2016 10:38:33 AM
Method	APCI_DirectProbe.m	Operator	VISTEC_Scientist
Sample Name	TN2Br m/z = 433.7927	Instrument	compact 8255754.20068
Comment			

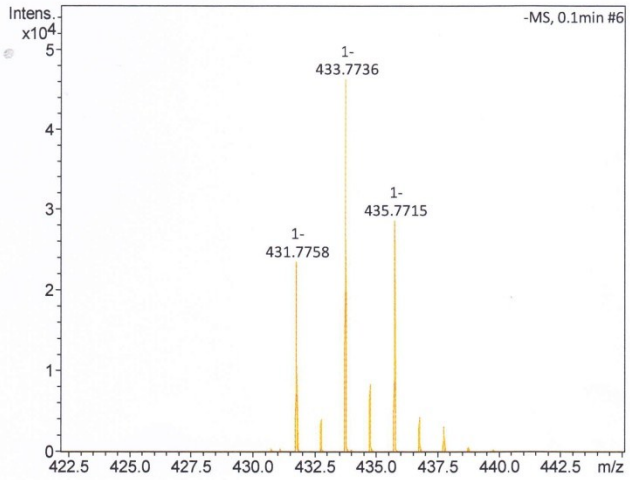
Acquisition Parameter

Source Type	APCI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	200 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	2000 nA	Set APCI Heater	450 °C

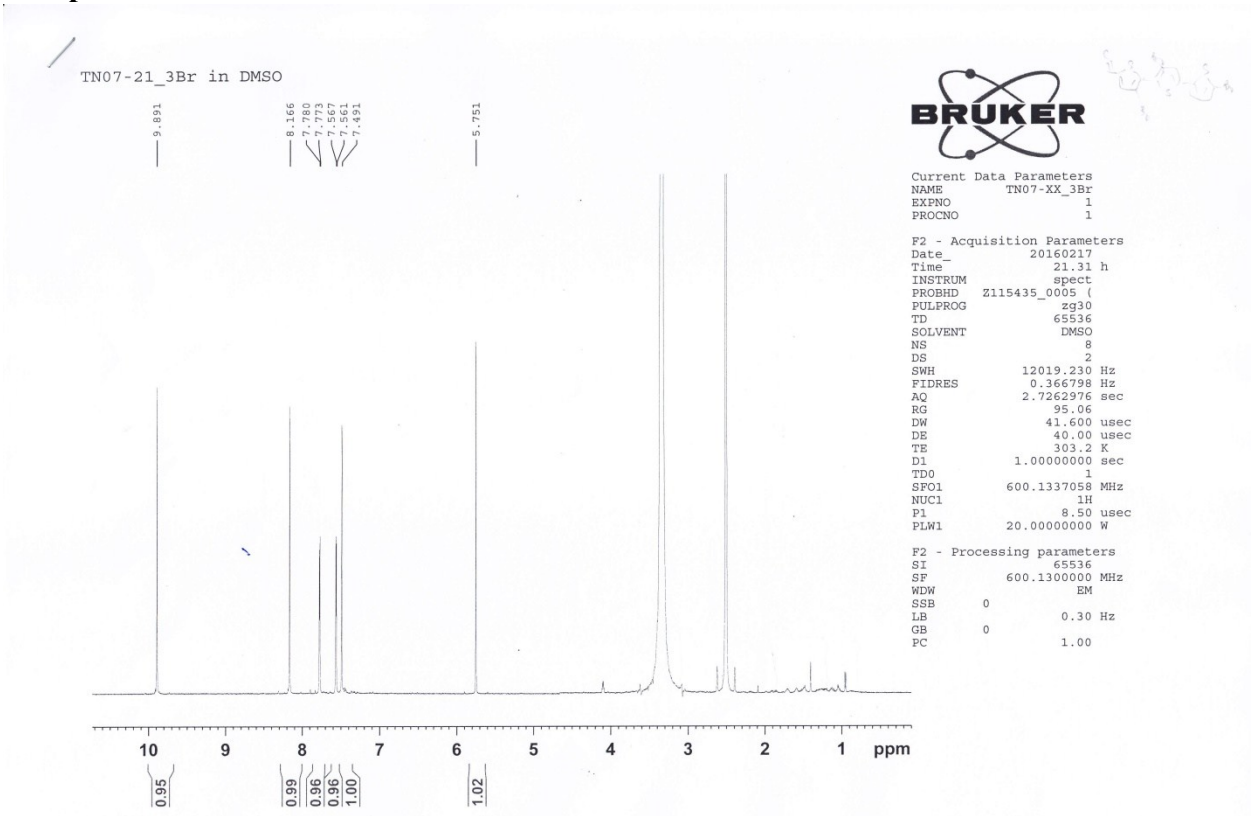


#	m/z	I
1	431.7758	23568
2	432.7771	4037
3	433.7736	46281
4	434.7762	8499
5	435.7715	28678
6	436.7746	4296
7	437.7681	3235



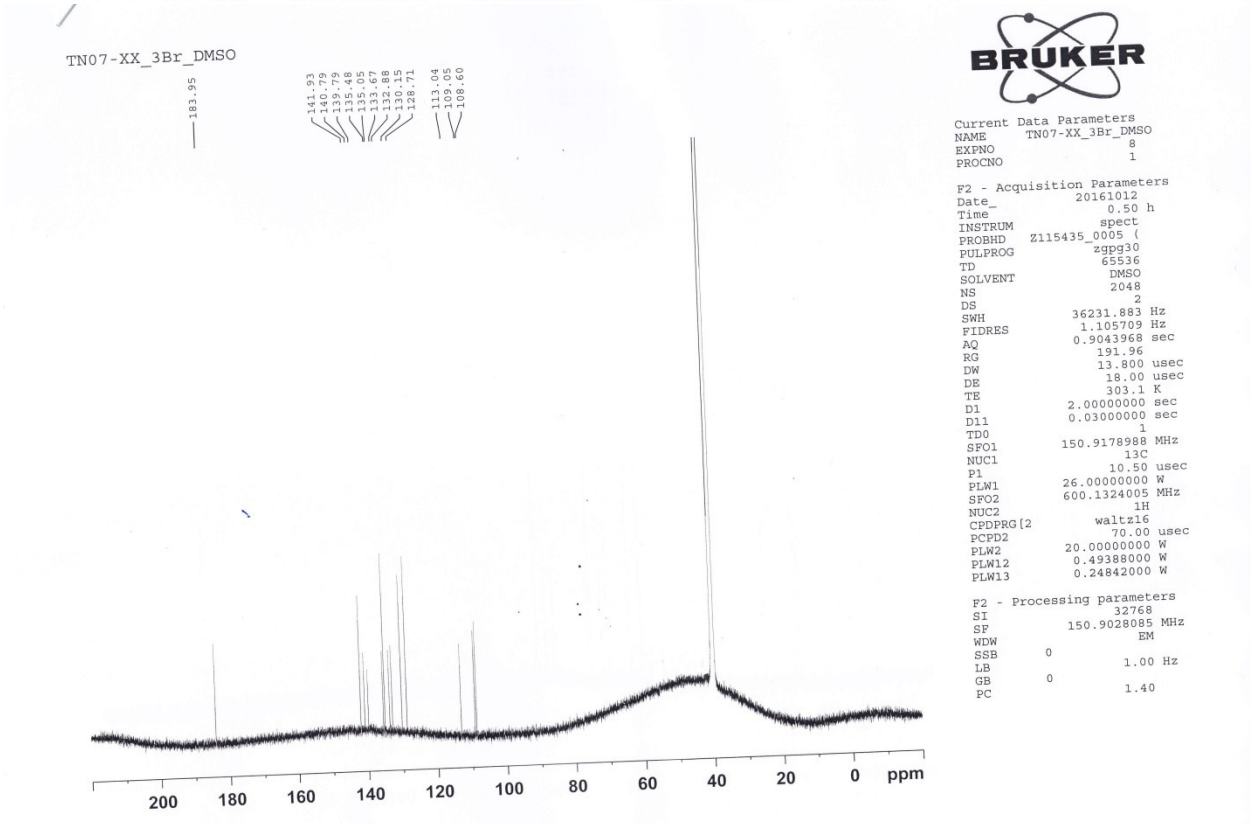


Compound 4



BRUKER

```
Current Data Parameters
NAME          TN07-XX_3Br
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160217
Time                21.31 h
INSTRUM             spect
PROBHD    Z115435_0005 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     2
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ             2.7262976 sec
RG                 95.06
DW                41.600 usec
DE                40.00 usec
TE                303.2 K
D1            1.00000000 sec
TD0                    1
SFO1          600.1337058 MHz
NUC1                  1H
P1                  8.50 usec
PLW1         20.00000000 W

F2 - Processing parameters
SI                 65536
SF            600.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



BRUKER

```
Current Data Parameters
NAME       TN07-XX_3Br_DMSO
EXPNO                     8
PROCNO                    1

F2 - Acquisition Parameters
Date_            20161012
Time                0.50 h
INSTRUM             spect
PROBHD    Z115435_0005 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  2048
DS                     2
SWH            36231.883 Hz
FIDRES          1.105709 Hz
AQ             0.9043968 sec
RG                 191.96
DW                13.800 usec
DE                18.00 usec
TE                303.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1          150.9178988 MHz
NUC1                  13C
P1                10.50 usec
PLW1         26.00000000 W
SFO2          600.1324005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2               70.00 usec
PLW2         20.00000000 W
PLW12         0.49388000 W
PLW13         0.24842000 W

F2 - Processing parameters
SI                 32768
SF            150.9028085 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

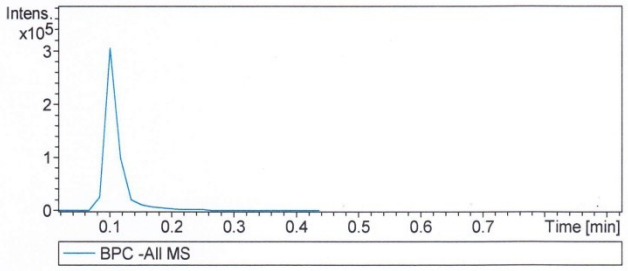
Q-ToF MS Report | Frontier Research Center@VISTEC

Analysis Info

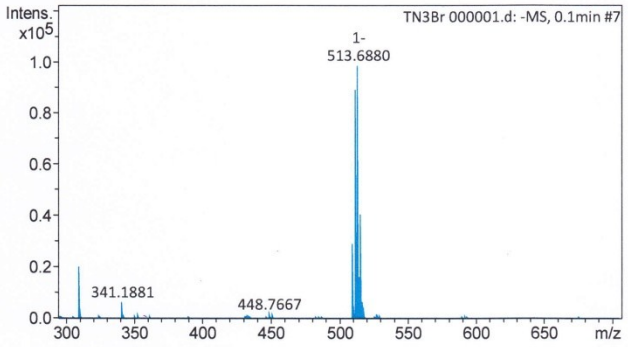
Analysis Name	D:\Data\VISTEC Data QTOF\Vinich\A-monrat\TN3Br 000001.d	Acquisition Date	10/14/2016 10:49:21 AM
Method	APCI_DirectProbe.m	Operator	VISTEC_Scientist
Sample Name	TN3Br m/z = 511.7032	Instrument	compact 8255754.20068
Comment			

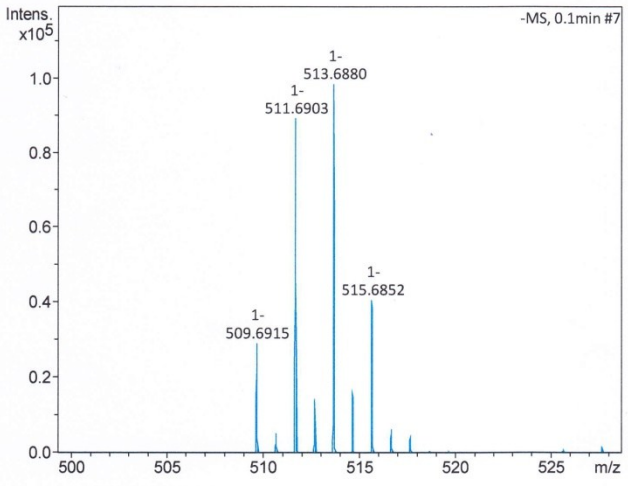
Acquisition Parameter

Source Type	APCI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	300 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	700 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	2000 nA	Set APCI Heater	450 °C

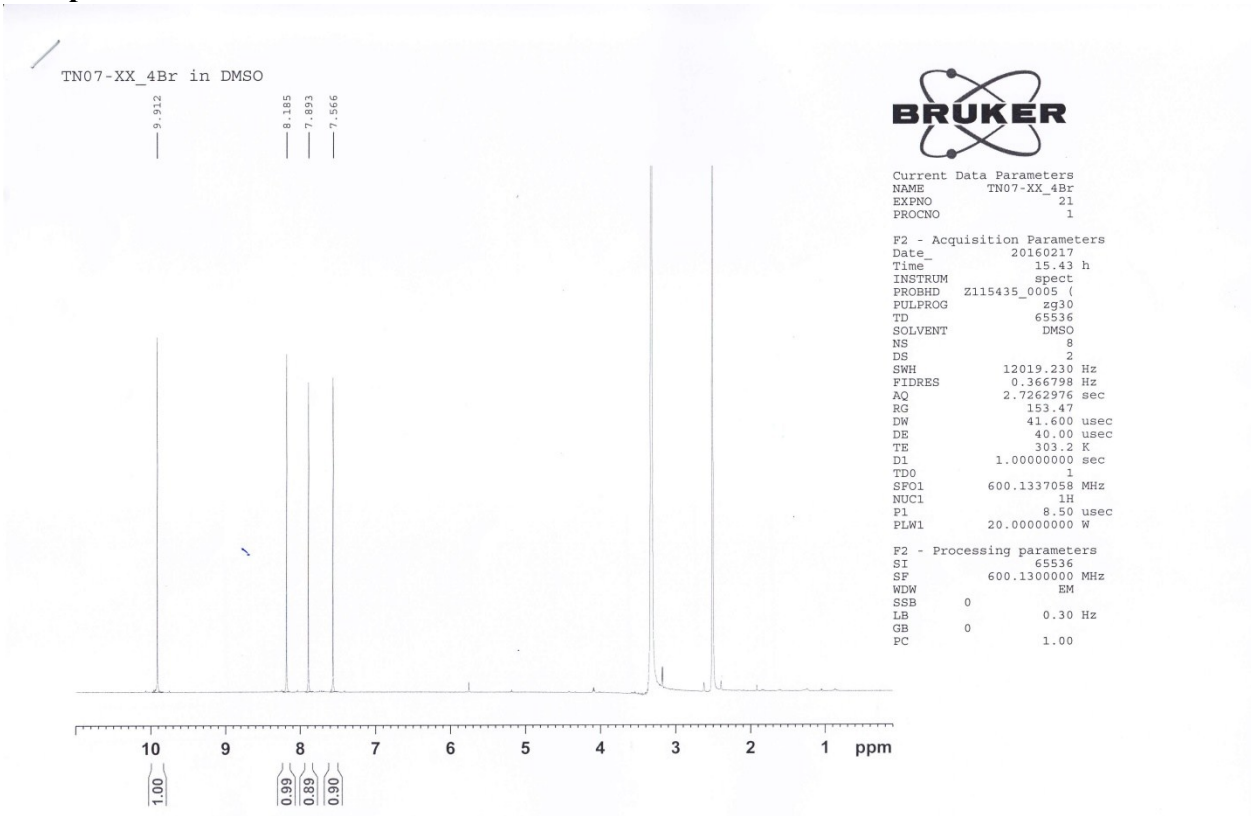


#	m/z	I
1	509.6915	29055
2	510.6926	5245
3	511.6903	89229
4	512.6923	14421
5	513.6880	98559
6	514.6902	16060
7	515.6852	40652
8	516.6891	6362
9	517.6807	4310



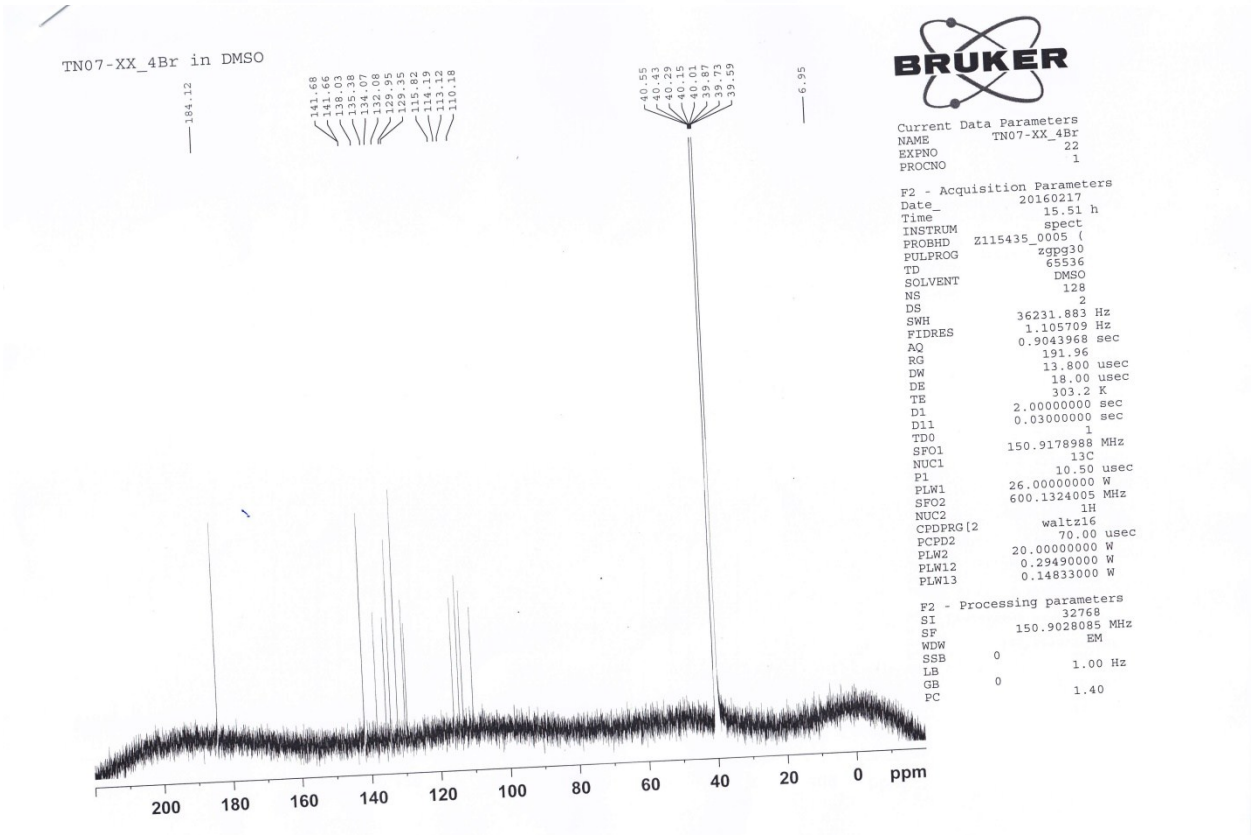


Compound 5



BRUKER

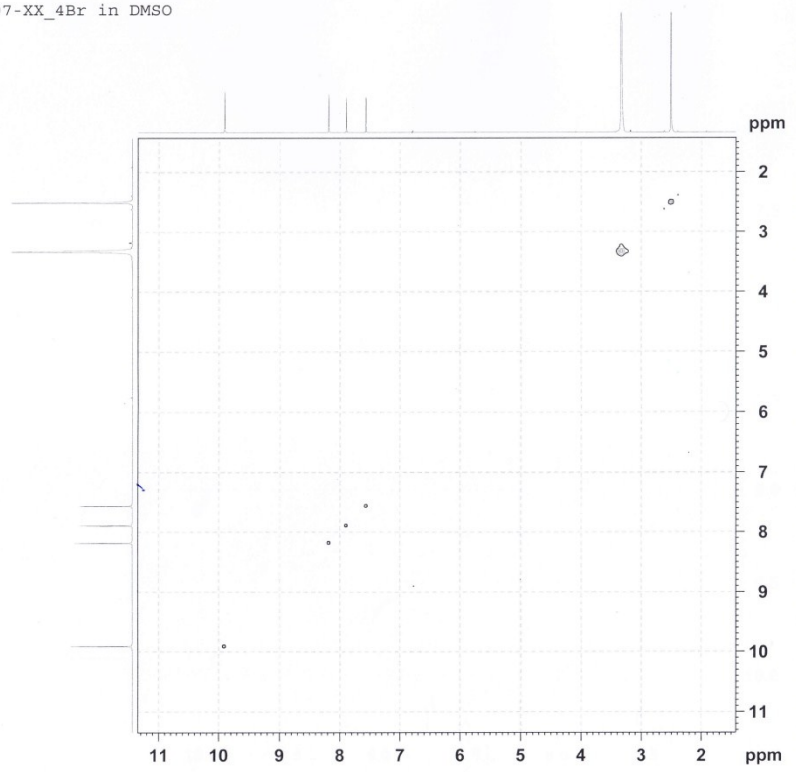
```
Current Data Parameters
NAME          TN07-XX_4Br
EXPNO                  21
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160217
Time               15.43 h
INSTRUM             spect
PROBHD    Z115435_0005 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     2
SWH            12019.230 Hz
FIDRES          0.366798 Hz
AQ              2.7262976 sec
RG                153.47
DW                41.600 usec
DE                40.00 usec
TE                303.2 K
D1             1.00000000 sec
TD0                    1
SFO1           600.1337058 MHz
NUC1                  1H
P1                  8.50 usec
PLW1          20.00000000 W

F2 - Processing parameters
SI                 65536
SF            600.1300000 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



BRUKER

```
Current Data Parameters
NAME          TN07-XX_4Br
EXPNO                  22
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160217
Time               15.51 h
INSTRUM             spect
PROBHD    Z115435_0005 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   128
DS                     2
SWH            36231.883 Hz
FIDRES          1.105709 Hz
AQ              0.9043968 sec
RG                191.96
DW                13.800 usec
DE                18.00 usec
TE                303.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1           150.9178988 MHz
NUC1                  13C
P1                 10.50 usec
PLW1          26.00000000 W
SFO2           600.1324005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              70.00 usec
PLW2          20.00000000 W
PLW12          0.29490000 W
PLW13          0.14833000 W

F2 - Processing parameters
SI                 32768
SF            150.9028085 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

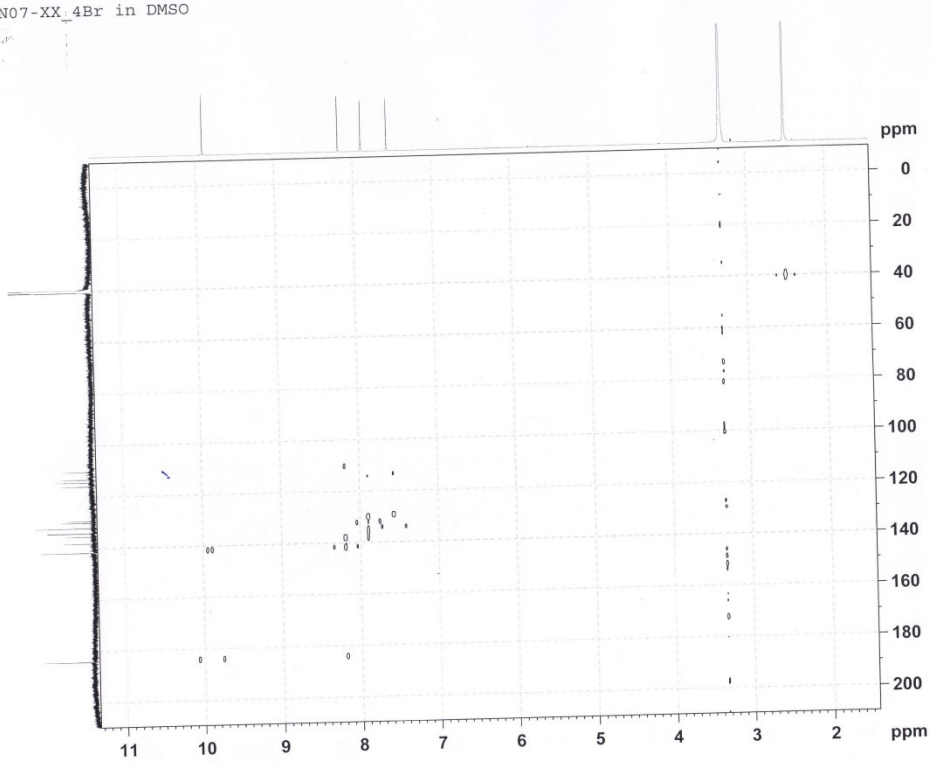
TN07-XX_4Br in DMSO



BRUKER

```
Current Data Parameters
NAME          TN07-XX_4Br
EXPNO                  25
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160217
Time               16.34 h
INSTRUM              spect
PROBHD    Z115435_0005 (
PULPROG       cosygpppqf
TD                   2048
SOLVENT               DMSO
NS                       1
DS                      16
SWH             5952.381 Hz
FIDRES          5.812872 Hz
AQ              0.1720320 sec
RG                   59.53
DW                 84.000 usec
DE                 40.00 usec
TE                 303.1 K
D0              0.00000300 sec
D1              1.95904005 sec
D11             0.03000000 sec
D12             0.00002000 sec
D13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00016800 sec
TDav                     1
SFO1          600.1338329 MHz
NUC1                    1H
P0                   8.50 usec
P1                   8.50 usec
P17               2500.00 usec
PLW1         20.00000000 W
PLW10         2.31200004 W
GPNAM[1]      SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1            600.1338 MHz
FIDRES          93.005951 Hz
SW                9.918 ppm
FnMODE                  QF

F2 - Processing parameters
SI                     1024
SF            600.1300000 MHz
WDW                   QSINE
SSB          0
LB           0 Hz
GB           0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2                      QF
SF            600.1300000 MHz
WDW                   QSINE
SSB          0
LB           0 Hz
GB           0
```

TN07-XX_4Br in DMSO



BRUKER

```
Current Data Parameters
NAME          TN07-XX_4Br
EXPNO                  27
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160217
Time               17.17 h
INSTRUM              spect
PROBHD    Z115435_0005 (
PULPROG     hmbcgplpndqf
TD                   2048
SOLVENT               DMSO
NS                       8
DS                      16
SWH             5952.381 Hz
FIDRES          5.812872 Hz
AQ              0.1720320 sec
RG                  191.96
DW                 84.000 usec
DE                 40.00 usec
TE                 303.1 K
CNST2         145.0000000
CNST13         10.0000000
D0              0.00000300 sec
D1              1.95904005 sec
D2              0.00344828 sec
D6              0.05000000 sec
D16             0.00020000 sec
IN0             0.00001510 sec
TDav                     1
SFO1          600.1338329 MHz
NUC1                    1H
P1                   8.50 usec
P2                  17.00 usec
PLW1         20.00000000 W
SFO2          150.9178988 MHz
NUC2                    13C
P3                  10.50 usec
PLW2         26.00000000 W
GPNAM[1]      SMSQ10.100
GPZ1                50.00 %
GPNAM[2]      SMSQ10.100
GPZ2                30.00 %
GPNAM[3]      SMSQ10.100
GPZ3                40.10 %
P16               1000.00 usec

F1 - Acquisition parameters
TD                     128
SFO1            150.9179 MHz
FIDRES          517.384094 Hz
SW                219.408 ppm
FnMODE                  QF

F2 - Processing parameters
SI                     2048
SF            600.1300000 MHz
WDW                   SINE
SSB          0
LB           0 Hz
GB           0
PC                     1.40

F1 - Processing parameters
SI                     1024
MC2                      QF
SF            150.9028085 MHz
WDW                   SINE
SSB          0
LB           0 Hz
GB           0
```

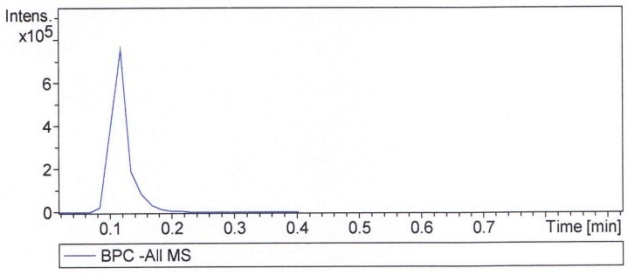
Q-ToF MS Report | Frontier Research Center@VISTEC

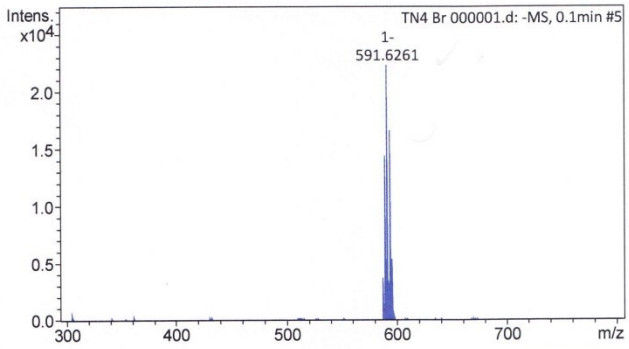
Analysis Info

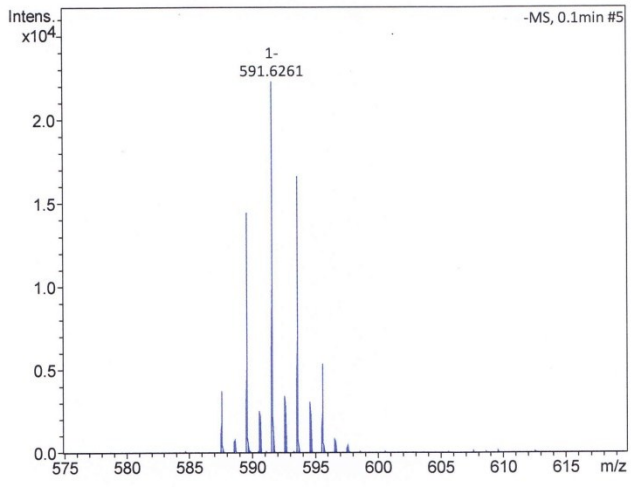
Analysis Name	D:\Data\VISTEC Data QTOF\Vinich\A-monrat\TN4 Br 000001.d	Acquisition Date	10/14/2016 12:56:55 PM
Method	APCI_DirectProbe.m	Operator	VISTEC_Scientist
Sample Name	TN4 Br m/z = 591.6117	Instrument	compact 8255754.20068
Comment			

Acquisition Parameter

Source Type	APCI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	300 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	800 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	2000 nA	Set APCI Heater	450 °C

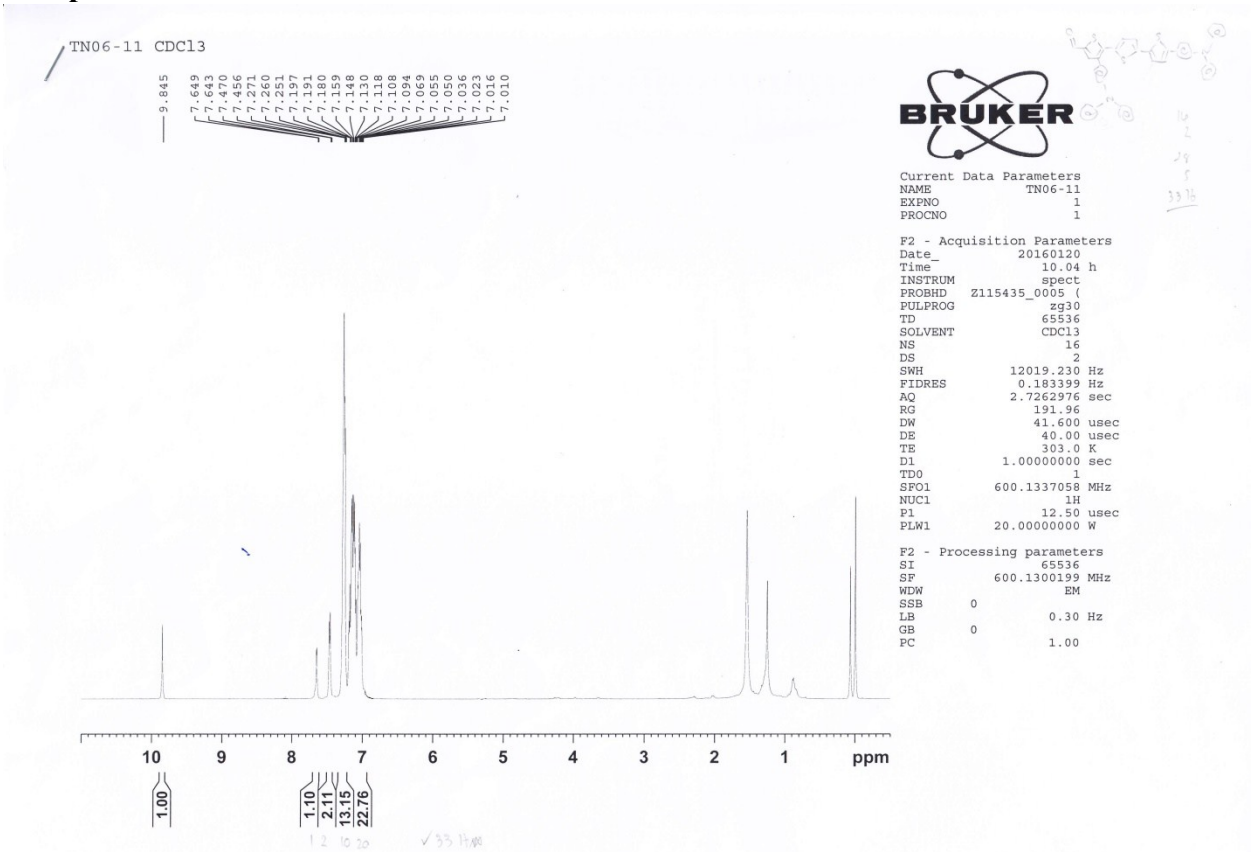


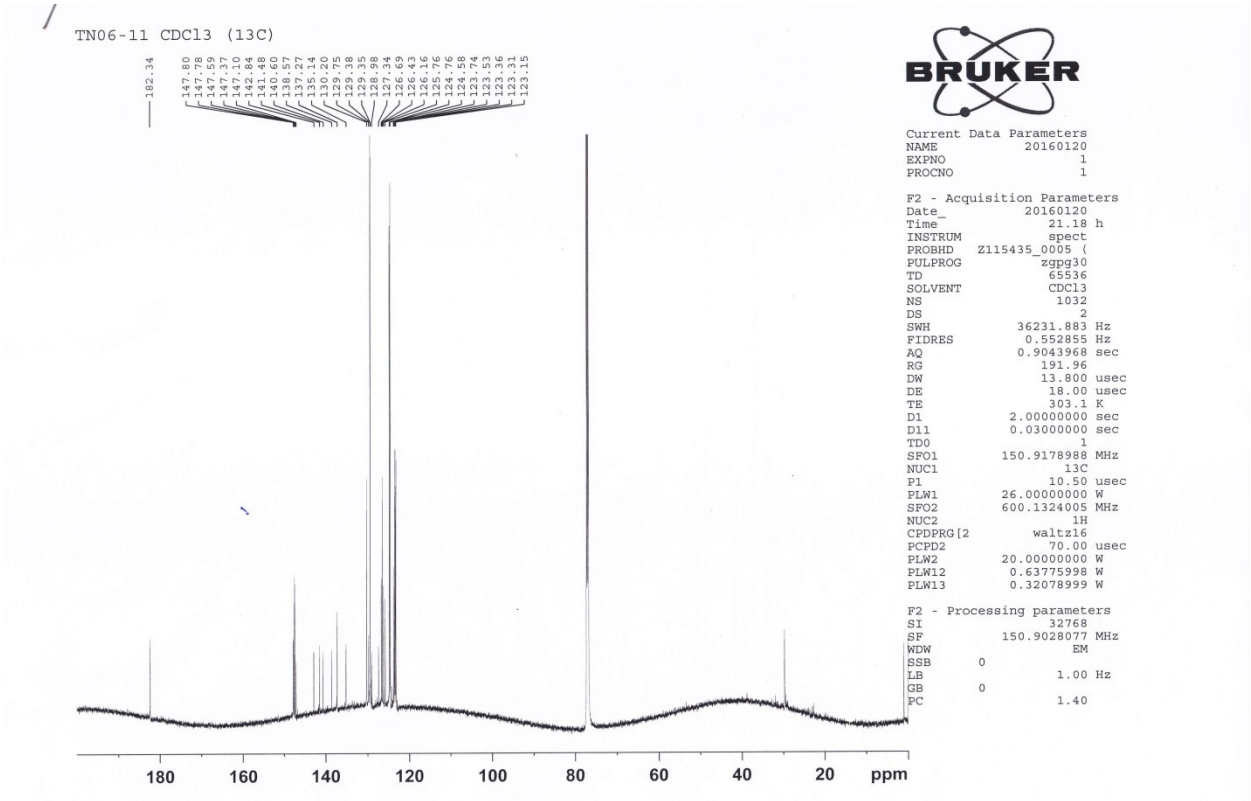




#	m/z	I
1	305.1848	517
2	306.1854	202
3	341.2057	226
4	361.2142	281
5	430.7775	231
6	432.7770	181
7	509.7075	132
8	510.7030	146
9	511.7078	127
10	512.6990	120
11	513.7160	171
12	515.4973	104
13	526.6998	141
14	528.7066	109
15	551.9753	115
16	587.6295	3750
17	588.6390	804
18	589.6289	14421
19	590.6311	2584
20	591.6261	22287
21	592.6277	3441
22	593.6238	16599
23	594.6266	3090
24	595.6217	5381
25	596.6228	805
26	597.6134	518
27	607.6285	142
28	609.6340	159
29	640.2624	109
30	669.5304	181

Compound 7


TN06-11 CDCl3
9.845
7.649
7.643
7.470
7.456
7.271
7.260
7.251
7.197
7.191
7.180
7.159
7.148
7.130
7.118
7.108
7.094
7.069
7.055
7.050
7.036
7.023
7.016
7.010
BRUKER
Current Data Parameters
NAME TN06-11
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160120
Time 10.04 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 191.96
DW 41.600 usec
DE 40.00 usec
TE 303.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P1 12.50 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1300199 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.10
2.11
13.15
22.76


TN06-11 CDCl3 (13C)
182.34
147.80
147.78
147.59
147.37
147.10
142.84
141.48
140.60
139.57
135.14
130.20
129.75
129.38
129.35
128.98
127.34
126.69
126.43
126.16
125.76
124.76
124.58
123.74
123.53
123.36
123.31
123.15
BRUKER
Current Data Parameters
NAME 20160120
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160120
Time 21.18 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1032
DS 2
SWH 36231.883 Hz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 18.00 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 10.50 usec
PLW1 26.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 20.00000000 W
PLW12 0.63775998 W
PLW13 0.32078999 W
F2 - Processing parameters
SI 32768
SF 150.9028077 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
160
140
120
100
80
60
40
20
ppm

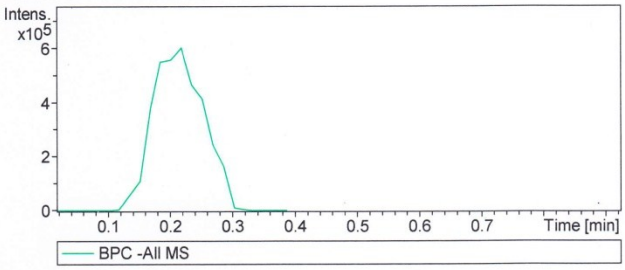
Q-ToF MS Report | Frontier Research Center@VISTEC

Analysis Info

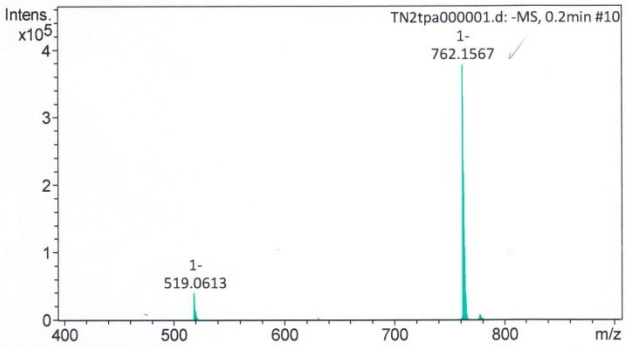
Analysis Name	D:\Data\VISTEC Data QTOF\Vinich\A-monrat\TN2tpa000001.d	Acquisition Date	10/14/2016 10:42:04 AM
Method	APCI_DirectProbe.m	Operator	VISTEC_Scientist
Sample Name	TN2tpa m/z = 762.1833	Instrument	compact 8255754.20068
Comment			

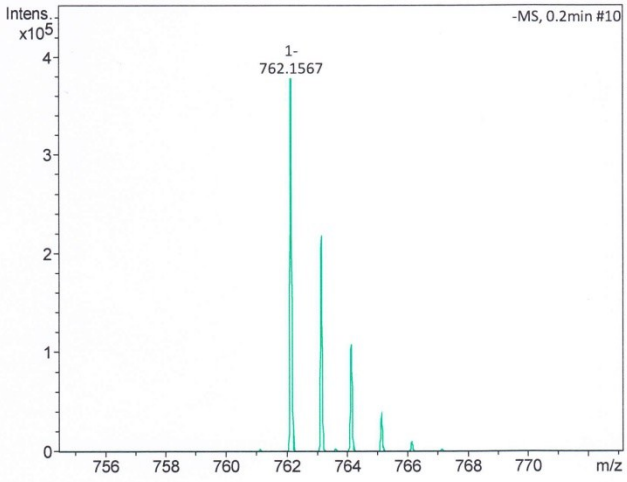
Acquisition Parameter

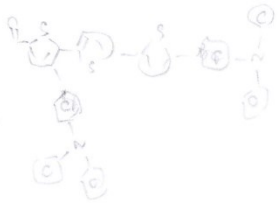
Source Type	APCI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	400 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	900 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	2000 nA	Set APCI Heater	450 °C



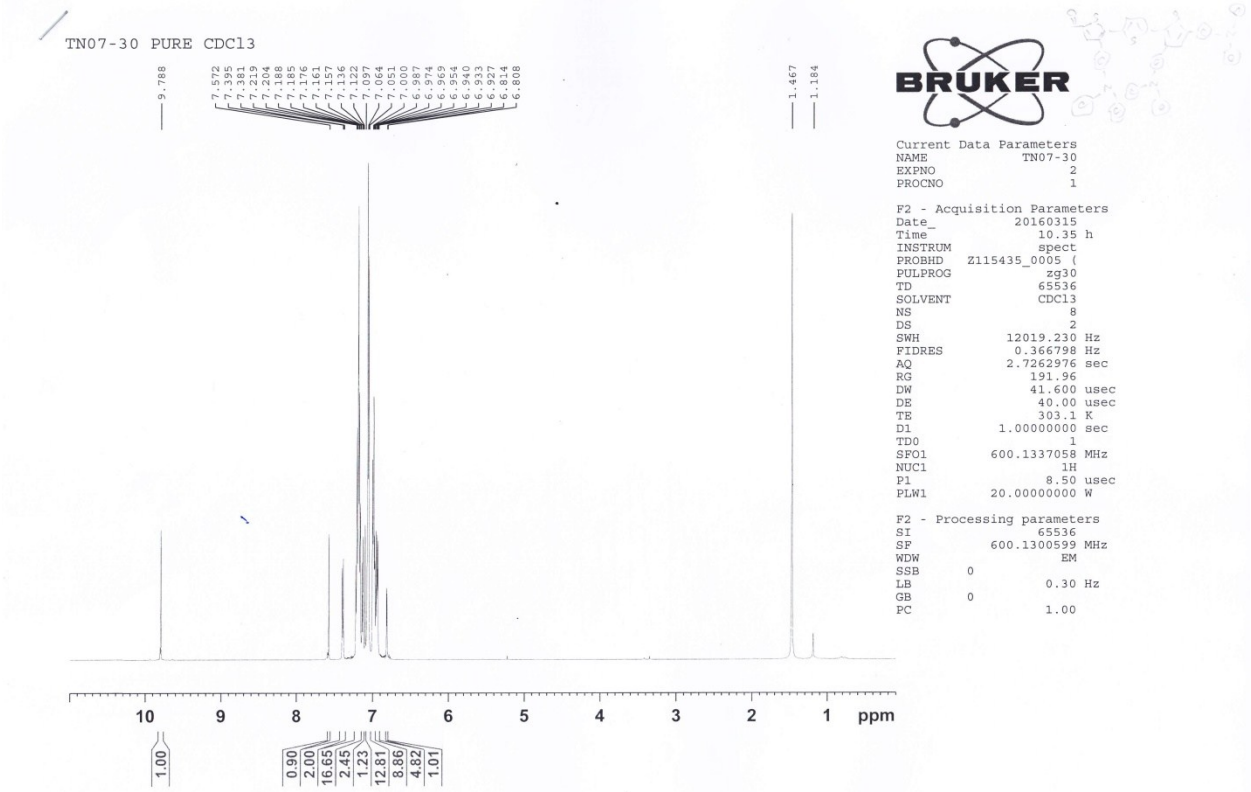
#	m/z	I
1	762.1567	377847
2	763.1599	218769
3	764.1583	108607
4	765.1576	39173
5	766.1573	10338

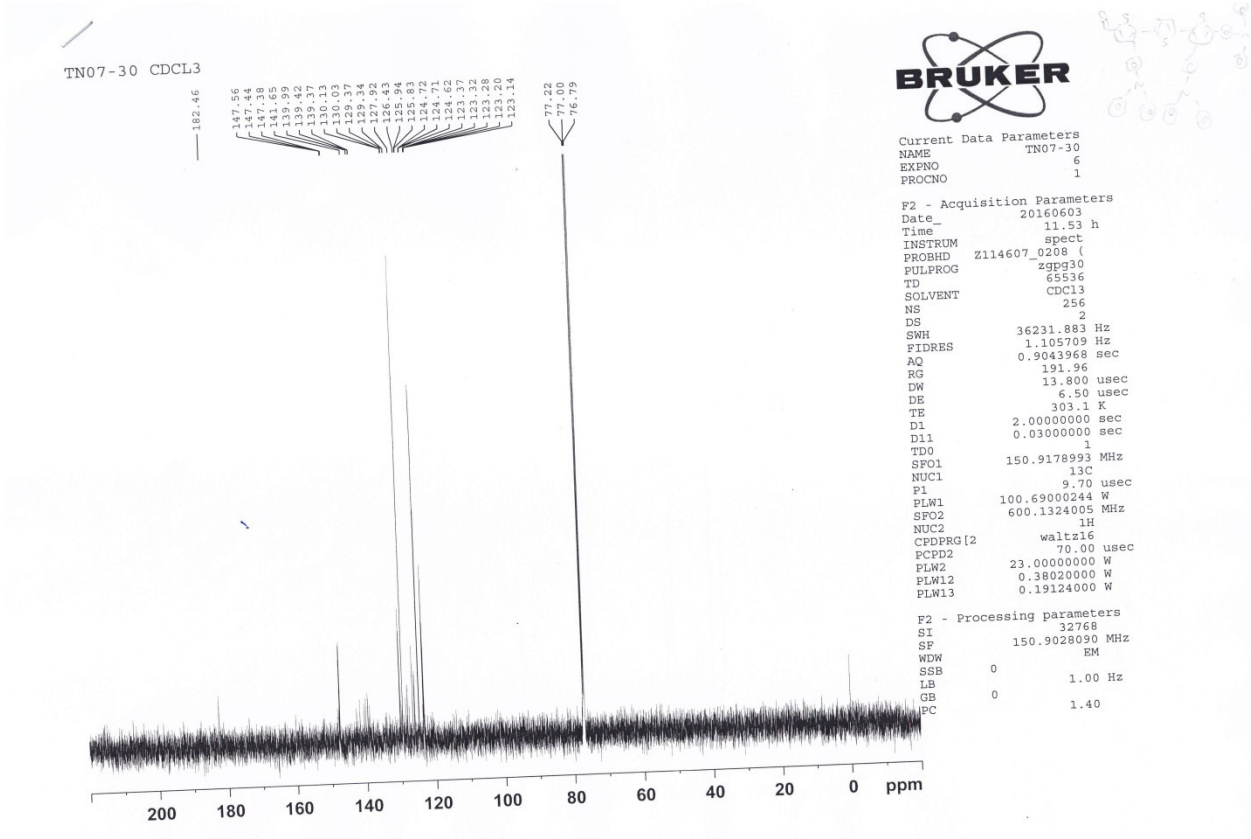






Compound 8


TN07-30 PURE CDCl3
9.788
7.572
7.395
7.381
7.219
7.204
7.188
7.185
7.176
7.161
7.157
7.116
7.122
7.097
7.064
7.051
7.000
6.987
6.974
6.969
6.954
6.940
6.933
6.927
6.814
6.808
1.467
1.184
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.90
2.00
16.65
2.45
1.23
12.81
8.86
4.82
1.01
BRUKER
Current Data Parameters
NAME TN07-30
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160315
Time 10.35 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 191.96
DW 41.600 usec
DE 40.00 usec
TE 303.1 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P1 8.50 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1300599 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


TN07-30 CDCL3
182.46
147.56
147.44
147.38
141.65
139.59
139.42
139.37
130.13
130.03
129.37
129.34
127.92
126.43
125.94
125.83
124.72
124.71
124.62
123.37
123.32
123.28
123.20
123.14
77.22
77.00
76.79
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME TN07-30
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160603
Time 11.53 h
INSTRUM spect
PROBHD Z114607_0208 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 2
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 6.50 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178993 MHz
NUC1 13C
P1 9.70 usec
PLW1 100.69000244 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 23.00000000 W
PLW12 0.38020000 W
PLW13 0.19124000 W
F2 - Processing parameters
SI 32768
SF 150.9028090 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

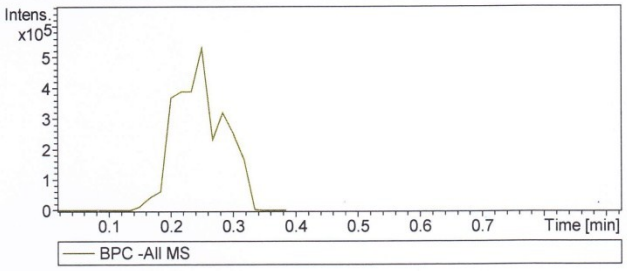
Q-ToF MS Report | Frontier Research Center@VISTEC

Analysis Info

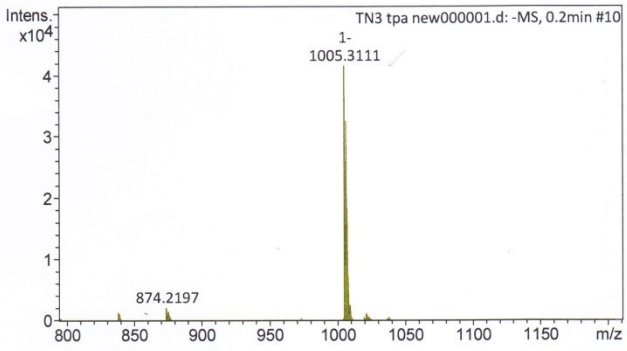
Analysis Name	D:\Data\VISTEC Data QTOF\Vinich\A-monrat\TN3 tpa new000001.d	Acquisition Date	10/14/2016 12:54:33 PM
Method	APCI_DirectProbe.m	Operator	VISTEC_Scientist
Sample Name	TN4 tpa new m/z = 1005.2881	Instrument	compact 8255754.20068
Comment			

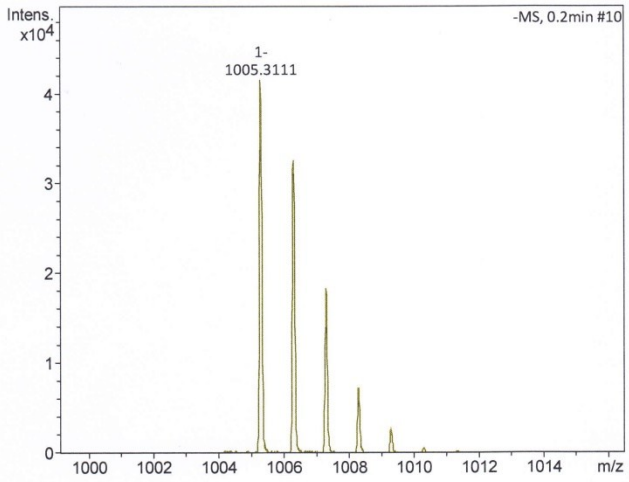
Acquisition Parameter

Source Type	APCI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	800 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1200 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	2000 nA	Set APCI Heater	450 °C

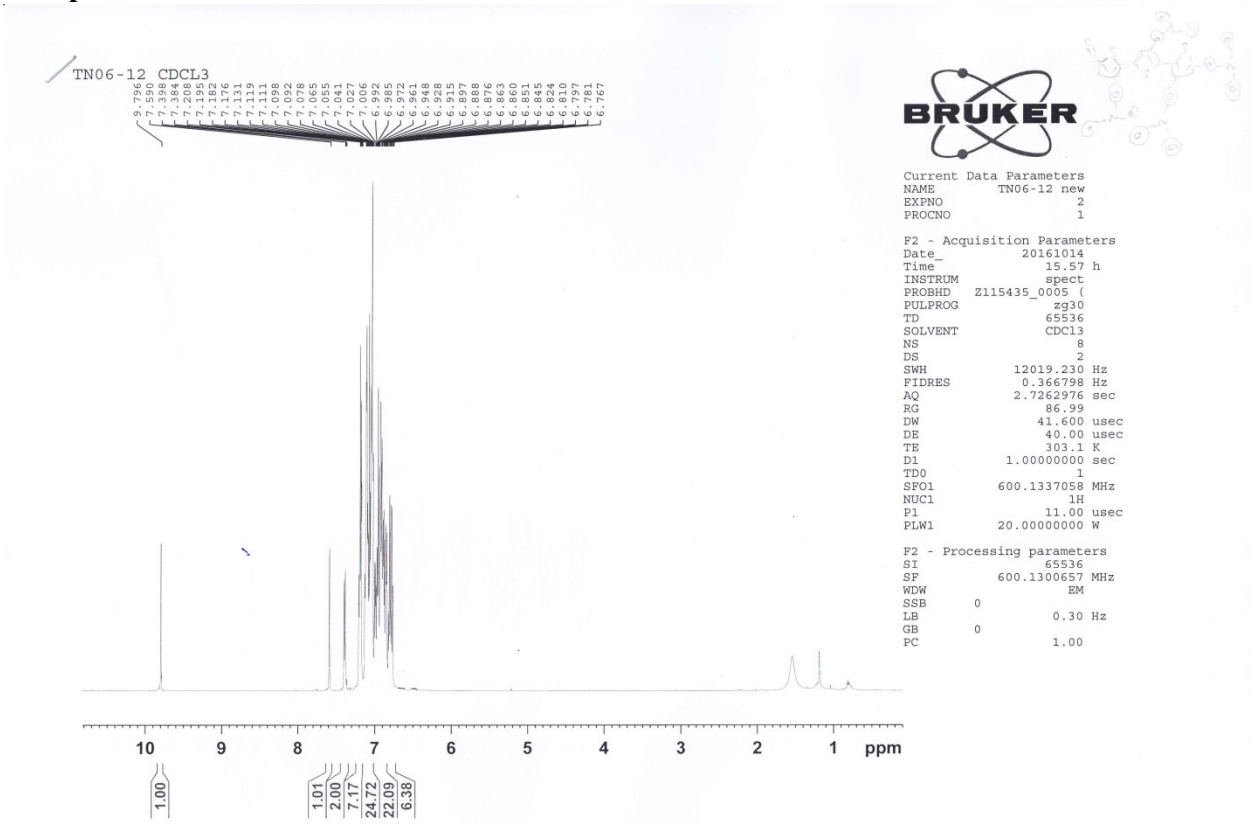


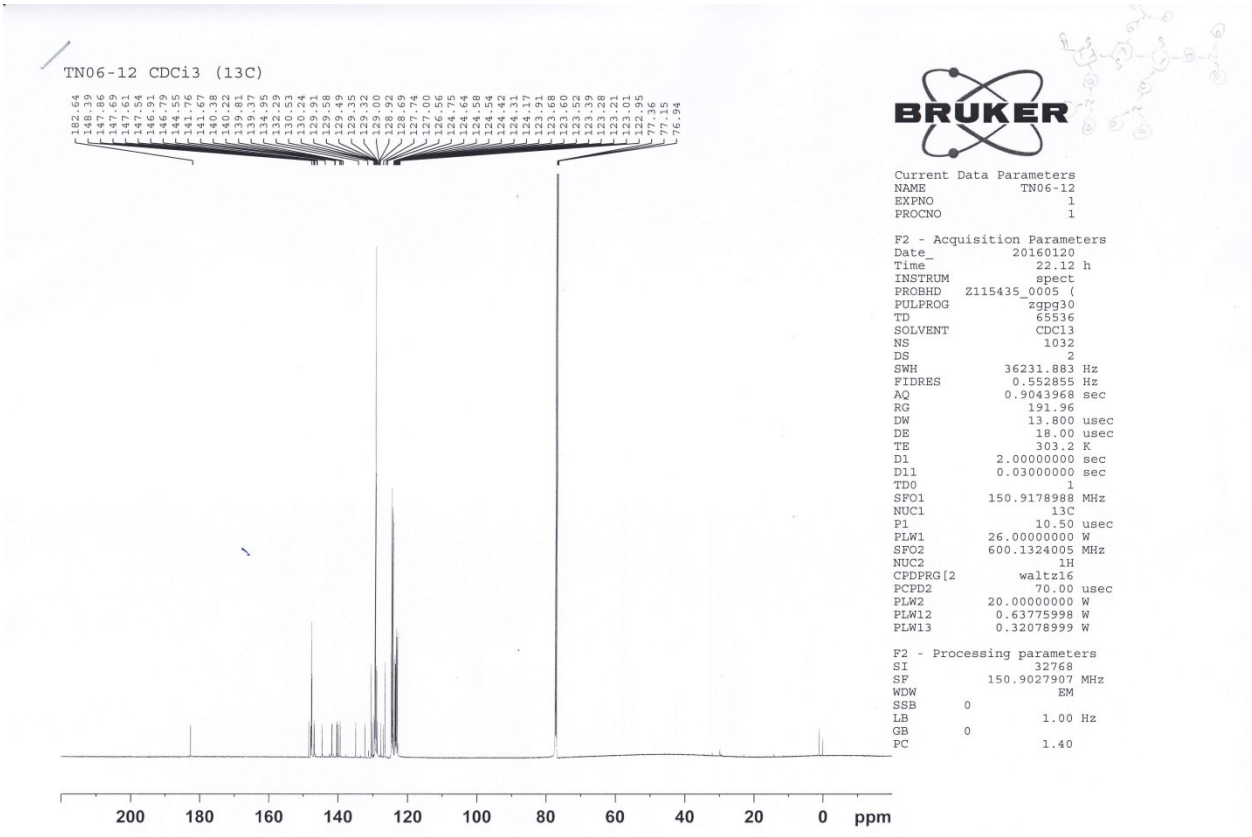
#	m/z	I
1	1005.3111	41543
2	1006.3154	32638
3	1007.3159	18332
4	1008.3170	7269
5	1009.3122	2515





Compound 9


TN06-12 CDCL3
9.796
7.590
7.398
7.384
7.208
7.195
7.182
7.176
7.131
7.119
7.111
7.098
7.092
7.078
7.065
7.055
7.041
7.027
7.006
6.992
6.985
6.972
6.941
6.928
6.915
6.897
6.888
6.876
6.863
6.860
6.831
6.815
6.824
6.810
6.797
6.781
6.767
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
2.00
7.17
24.72
22.09
6.38
BRUKER
Current Data Parameters
NAME TN06-12 new
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161014
Time 15.57 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 86.99
DW 41.600 usec
DE 40.00 usec
TE 303.1 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P1 11.00 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1300657 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


TN06-12 CDCi3 (13C)
182.64
148.39
147.86
147.69
147.61
147.54
146.91
146.79
144.55
141.76
141.67
140.38
140.22
139.81
139.37
134.95
132.29
130.53
130.34
129.81
129.58
129.49
129.35
129.32
129.00
128.92
128.69
127.74
127.00
126.56
124.75
124.64
124.58
124.54
124.42
124.31
124.17
123.91
123.68
123.60
123.52
123.39
123.28
123.21
123.01
122.95
77.36
77.15
76.94
200
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME TN06-12
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160120
Time 22.12 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1032
DS 2
SWH 36231.883 Hz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 18.00 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 10.50 usec
PLW1 26.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 20.00000000 W
PLW12 0.63775998 W
PLW13 0.32078999 W
F2 - Processing parameters
SI 32768
SF 150.9027907 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

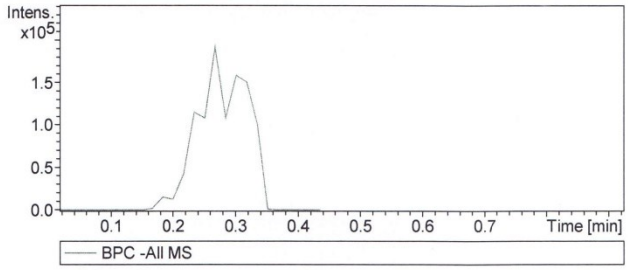
Q-ToF MS Report | Frontier Research Center@VISTEC

Analysis Info

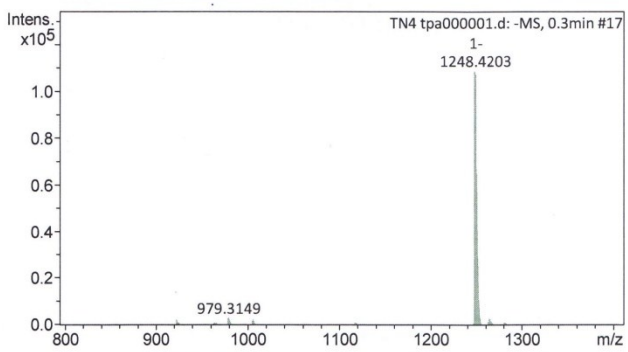
Analysis Name	D:\Data\VISTEC Data QTOF\Vinich\A-monrat\TN4 tpa000001.d	Acquisition Date	10/14/2016 1:43:16 PM
Method	APCI_DirectProbe.m	Operator	VISTEC_Scientist
Sample Name	TN 4tpa m/z = 1248.3929	Instrument	compact 8255754.20068
Comment			

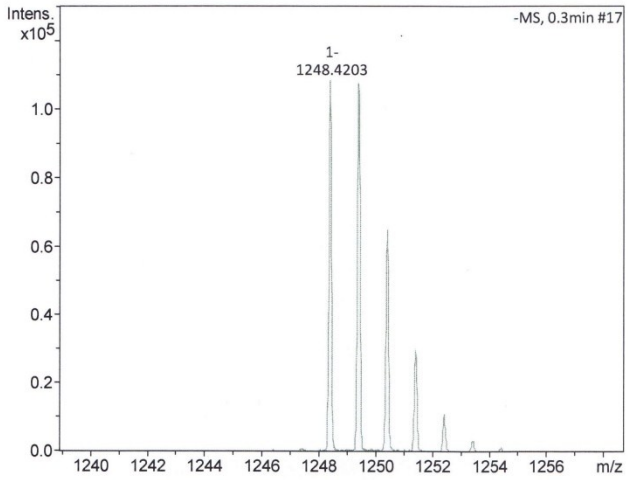
Acquisition Parameter

Source Type	APCI	Ion Polarity	Negative	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4000 V	Set Dry Heater	220 °C
Scan Begin	800 m/z	Set End Plate Offset	-500 V	Set Dry Gas	5.0 l/min
Scan End	1400 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	2000 nA	Set APCI Heater	450 °C

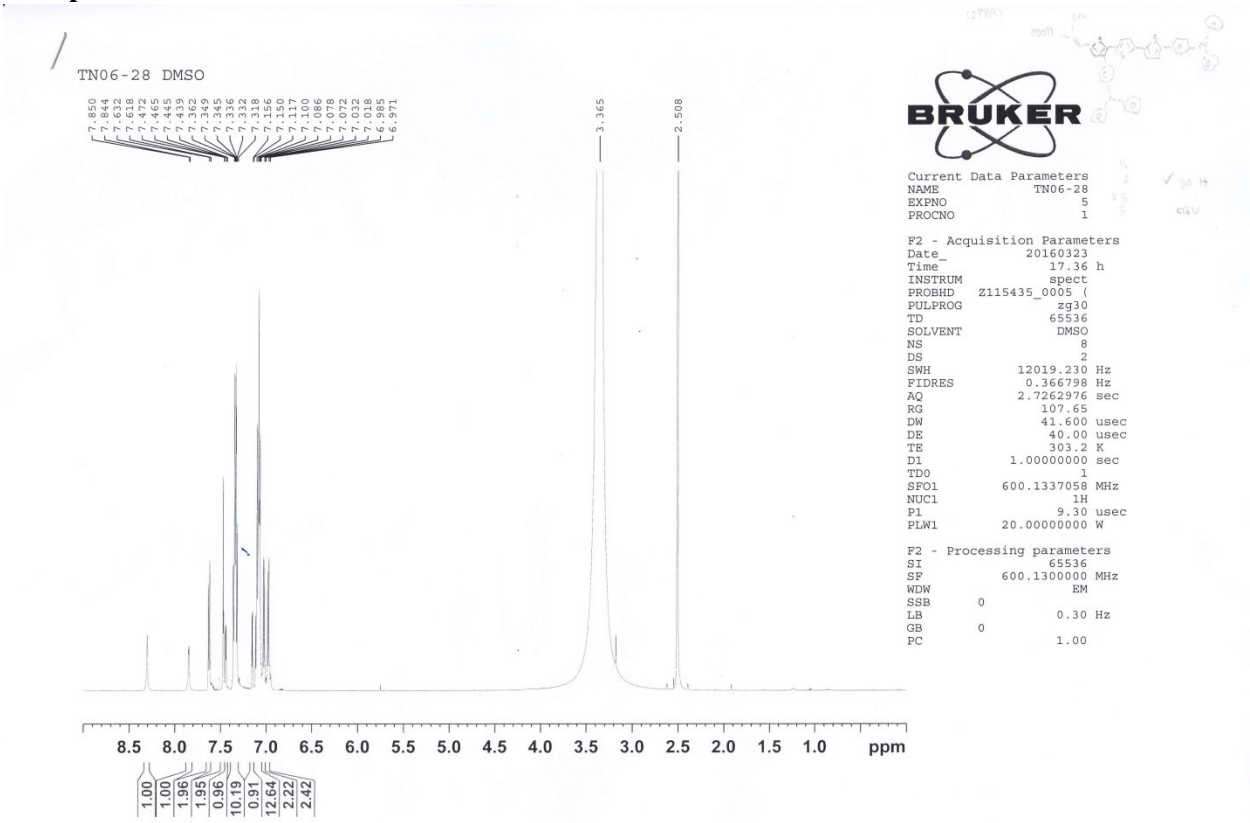


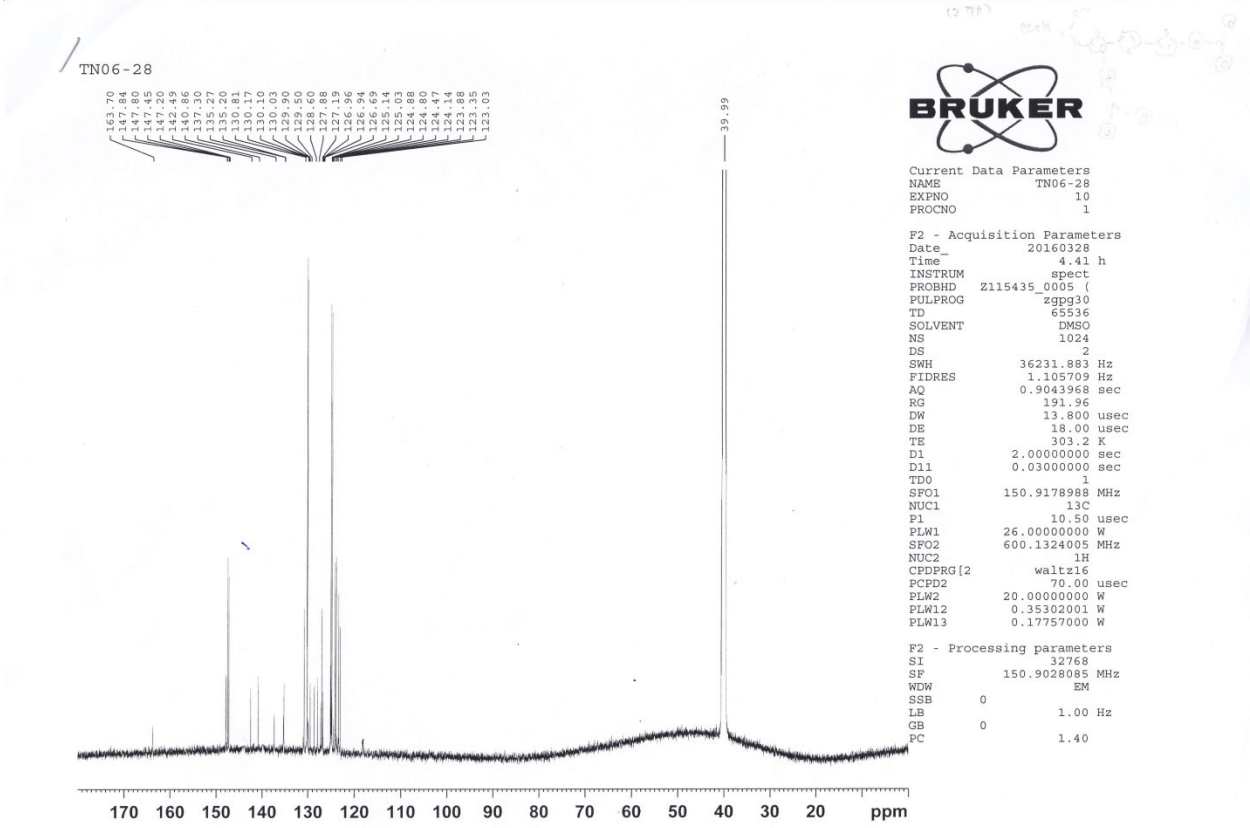
#	m/z	I
1	1248.4203	108465
2	1249.4229	107447
3	1250.4250	64999
4	1251.4236	28881
5	1252.4235	10822
6	1253.4267	3131





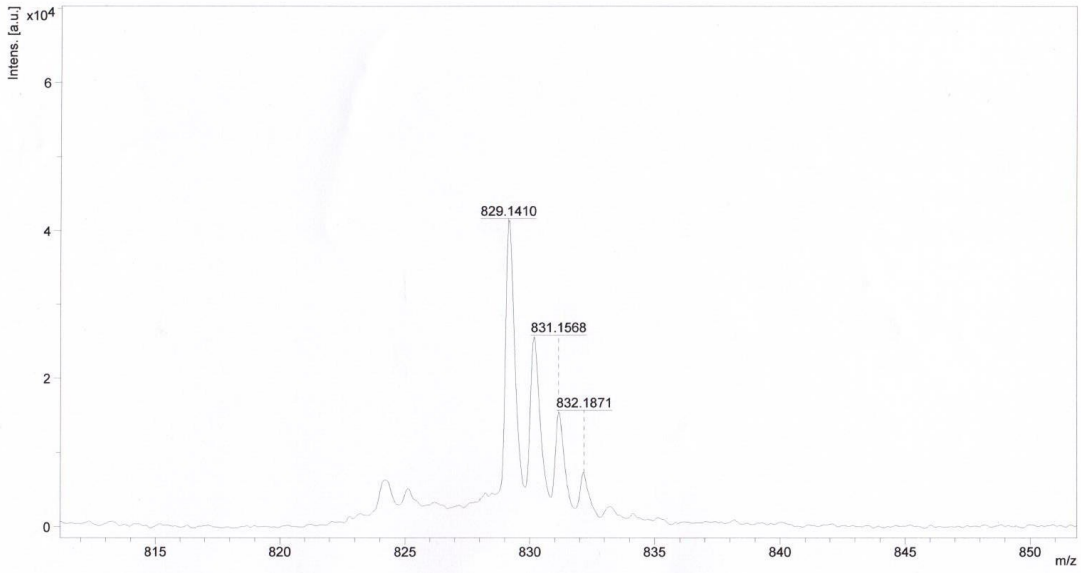
Compound T2


TN06-28 DMSO
7.850
7.844
7.632
7.618
7.472
7.465
7.445
7.439
7.362
7.349
7.345
7.336
7.332
7.318
7.156
7.150
7.117
7.100
7.086
7.078
7.072
7.022
7.018
6.985
6.971
3.365
2.508
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
1.00
1.96
1.95
0.96
10.19
0.91
12.64
2.22
2.42
BRUKER
Current Data Parameters
NAME TN06-28
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160323
Time 17.36 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 107.65
DW 41.600 usec
DE 40.00 usec
TE 303.2 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P1 9.30 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


TN06-28
163.70
147.84
147.80
147.45
147.20
142.49
140.86
137.30
135.27
135.20
130.81
130.17
130.10
130.03
129.90
129.50
128.60
127.88
127.19
126.96
126.94
126.69
125.14
125.03
124.88
124.80
124.47
124.14
123.88
123.35
123.03
39.99
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm
BRUKER
Current Data Parameters
NAME TN06-28
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160328
Time 4.41 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 2
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 18.00 usec
TE 303.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 10.50 usec
PLW1 26.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 20.00000000 W
PLW12 0.35302001 W
PLW13 0.17757000 W
F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

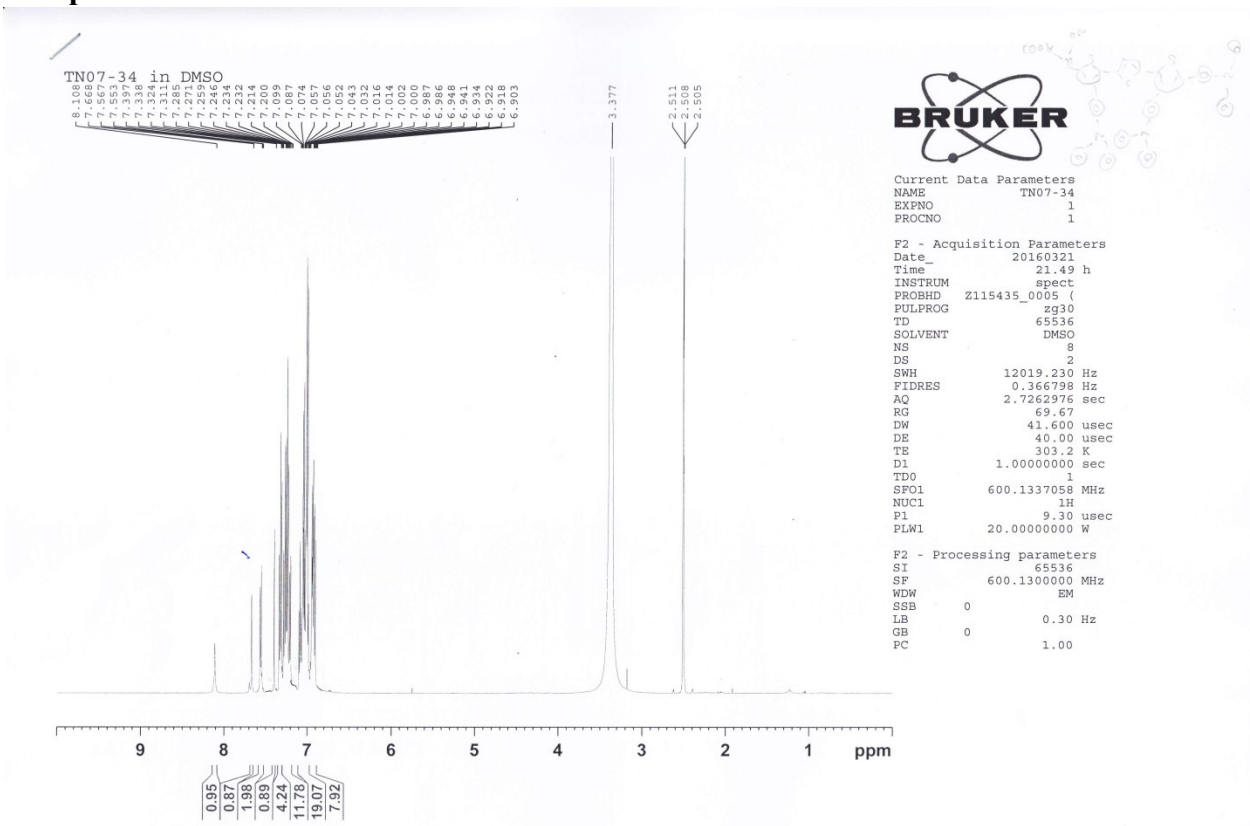
D:\Data\MSE\POSD\A-monrat\TN06-28-new\0_F5\1\1SLin

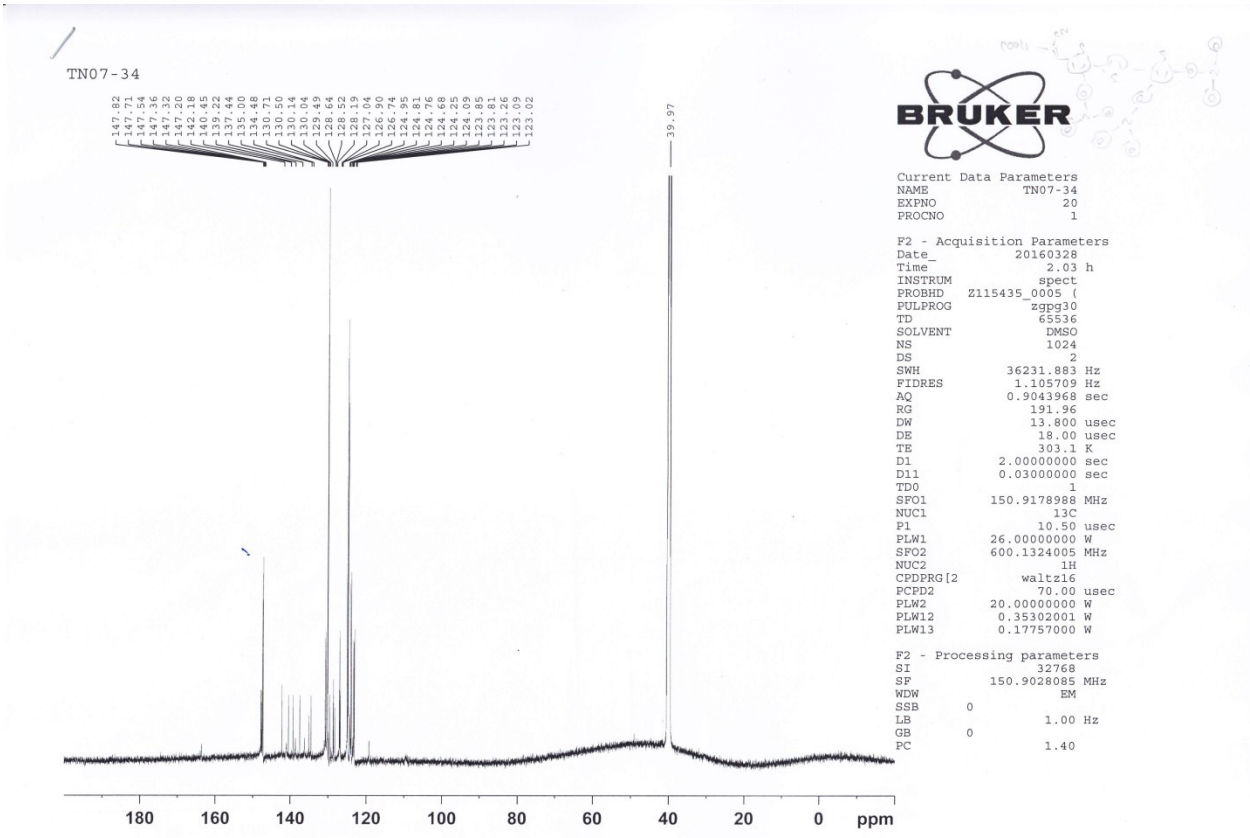
Comment 1 829.1891
Comment 2



Bruker Daltonics flexAnalysis printed: 10/14/2016 5:10:29 PM

Compound T3

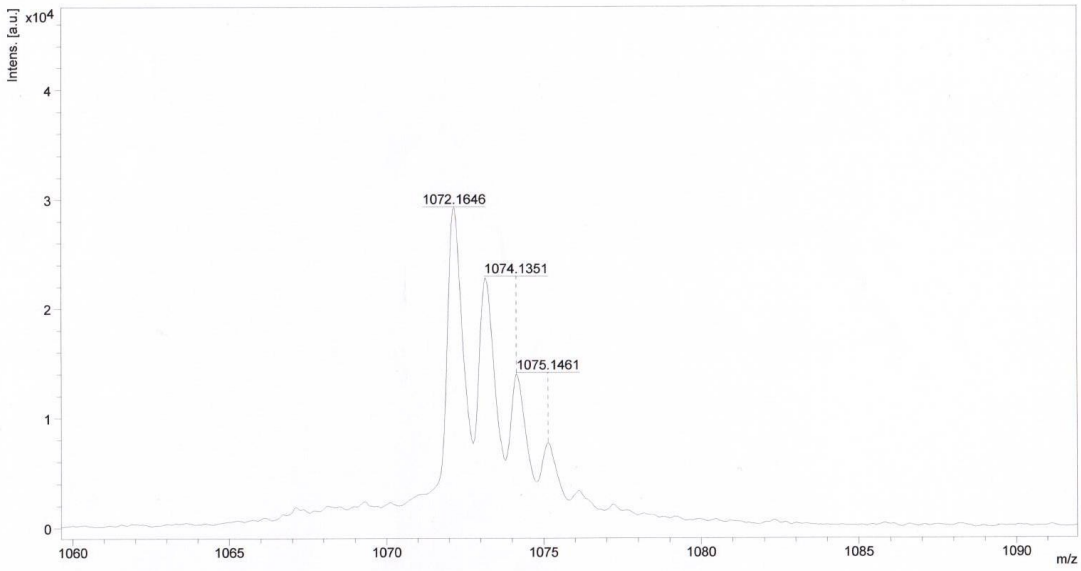

TN07-34 in DMSO
8.108
7.668
7.567
7.553
7.397
7.338
7.324
7.311
7.285
7.271
7.259
7.246
7.234
7.232
7.214
7.200
7.099
7.087
7.074
7.057
7.056
7.052
7.043
7.032
7.016
7.014
7.002
7.000
6.987
6.986
6.948
6.941
6.934
6.922
6.918
6.903
3.377
2.511
2.508
2.505
9
8
7
6
5
4
3
2
1
ppm
0.95
0.87
1.98
0.89
4.24
11.78
19.07
7.92
BRUKER
Current Data Parameters
NAME TN07-34
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160321
Time 21.49 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 69.67
DW 41.600 usec
DE 40.00 usec
TE 303.2 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P1 9.30 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


TN07-34
147.82
147.71
147.54
147.36
147.32
147.20
142.18
140.45
139.02
137.44
135.00
134.48
130.71
130.50
130.14
130.04
129.49
128.64
128.50
128.19
127.04
126.90
126.74
124.95
124.81
124.76
124.68
124.25
124.09
123.85
123.81
123.26
123.09
123.02
39.97
180
160
140
120
100
80
60
40
20
0
ppm
BRUKER
Current Data Parameters
NAME TN07-34
EXPNO 20
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160328
Time 2.03 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 2
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 18.00 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 10.50 usec
PLW1 26.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 20.00000000 W
PLW12 0.35302001 W
PLW13 0.17757000 W
F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

D:\Data\MSE\POSD\A-monrat\TN07-34-new\0_F9\1\1SLin

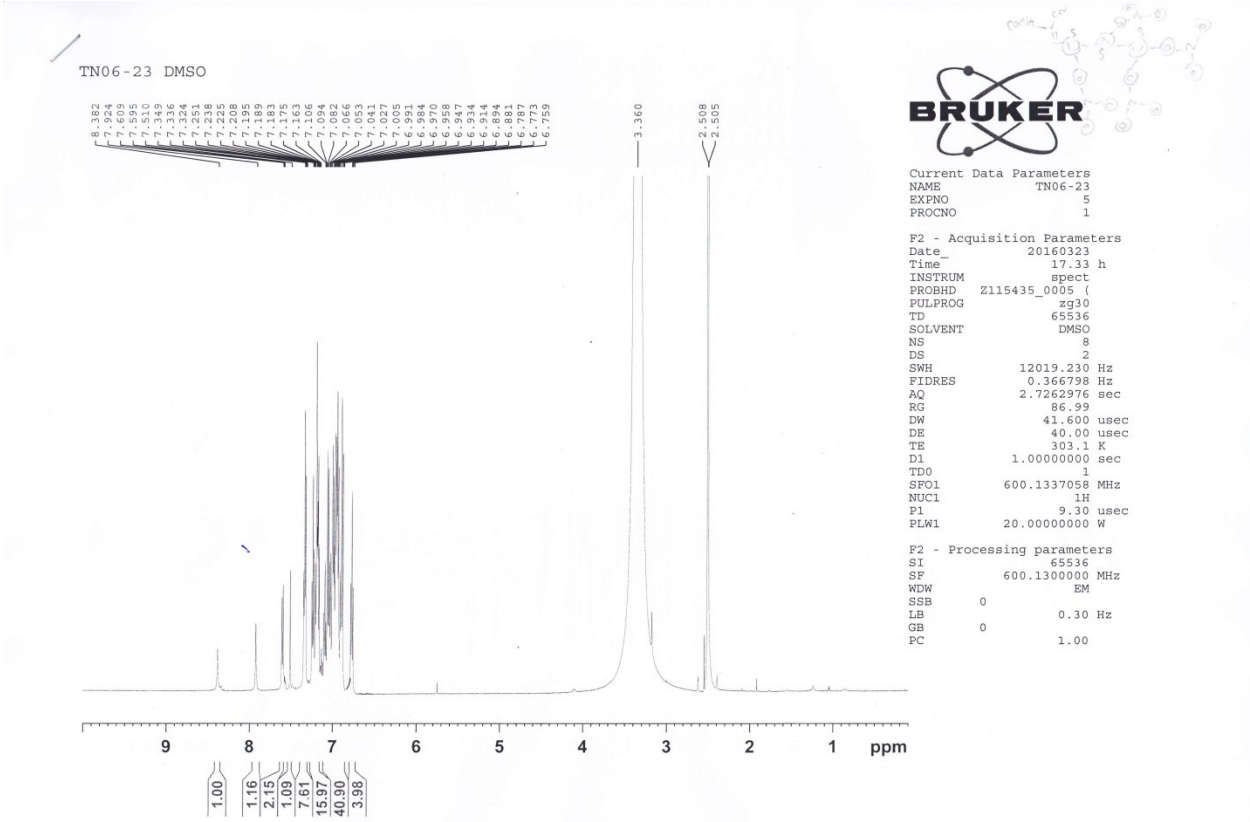
Comment 1 1072.2939

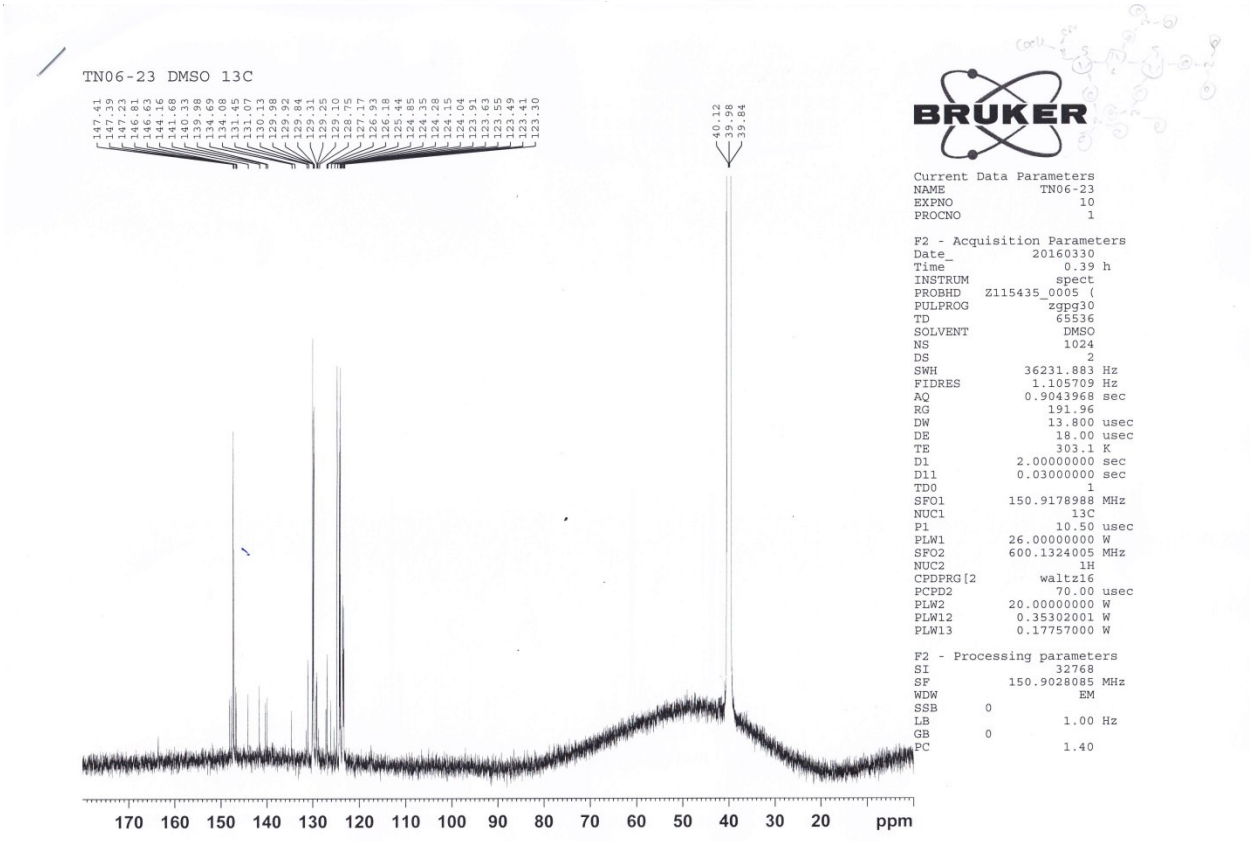
Comment 2



Bruker Daltonics flexAnalysis printed: 10/14/2016 5:14:01 PM

Compound T4

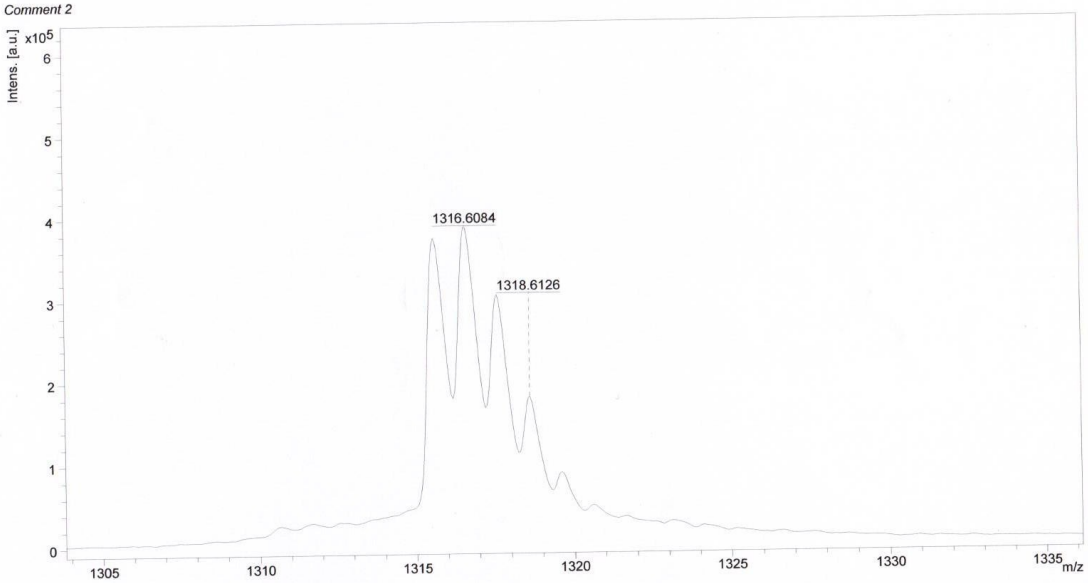

TN06-23 DMSO
8.382
7.924
7.609
7.595
7.515
7.349
7.336
7.324
7.251
7.238
7.225
7.208
7.195
7.189
7.183
7.175
7.163
7.106
7.094
7.082
7.066
7.053
7.041
7.027
7.005
6.991
6.984
6.970
6.958
6.947
6.934
6.914
6.881
6.864
6.787
6.773
6.759
3.360
2.508
2.505
9
8
7
6
5
4
3
2
1
ppm
1.00
1.16
2.15
1.09
7.61
15.97
40.90
3.98
BRUKER
Current Data Parameters
NAME TN06-23
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160323
Time 17.33 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 2.7262976 sec
RG 86.99
DW 41.600 usec
DE 40.00 usec
TE 303.1 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P1 9.30 usec
PLW1 20.00000000 W
F2 - Processing parameters
SI 65536
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


TN06-23 DMSO 13C
147.41
147.39
147.23
146.81
146.63
144.16
140.33
139.98
134.69
134.08
131.45
131.07
130.33
129.98
129.92
129.84
129.31
129.25
129.10
128.75
127.17
126.93
126.18
125.44
124.85
124.35
124.28
124.15
124.04
123.91
123.63
123.55
123.49
123.41
123.30
40.12
39.98
39.84
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm
BRUKER
Current Data Parameters
NAME TN06-23
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160330
Time 0.39 h
INSTRUM spect
PROBHD Z115435_0005 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 2
SWH 36231.883 Hz
FIDRES 1.105709 Hz
AQ 0.9043968 sec
RG 191.96
DW 13.800 usec
DE 18.00 usec
TE 303.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 150.9178988 MHz
NUC1 13C
P1 10.50 usec
PLW1 26.00000000 W
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 20.00000000 W
PLW12 0.35302001 W
PLW13 0.17757000 W
F2 - Processing parameters
SI 32768
SF 150.9028085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

D:\Data\MSE\POSD\A-monrat\TN06-23\0_F1\1\1SLin

Comment 1 1315.3987

Comment 2



Bruker Daltonics flexAnalysis

printed: 10/14/2016 5:12:03 PM