Electronic Supplementary Material (ESI) for Analytical Methods.

Highly Emissive Salicylidene Schiff bases (SASBs) in solution and its application in the Detection of Chemical Warfare Agent Mimic Diethylchlorophosphate

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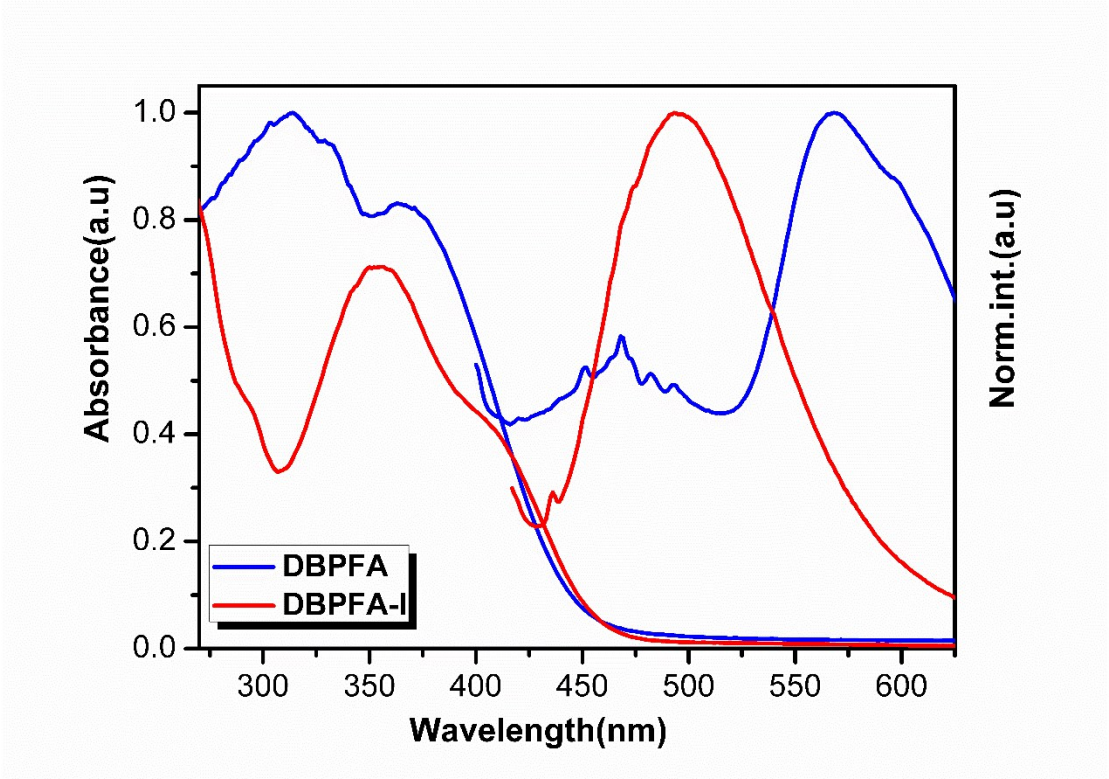


Figure S1. The absorption and emission spectra of DBPFA and DBPFA-I

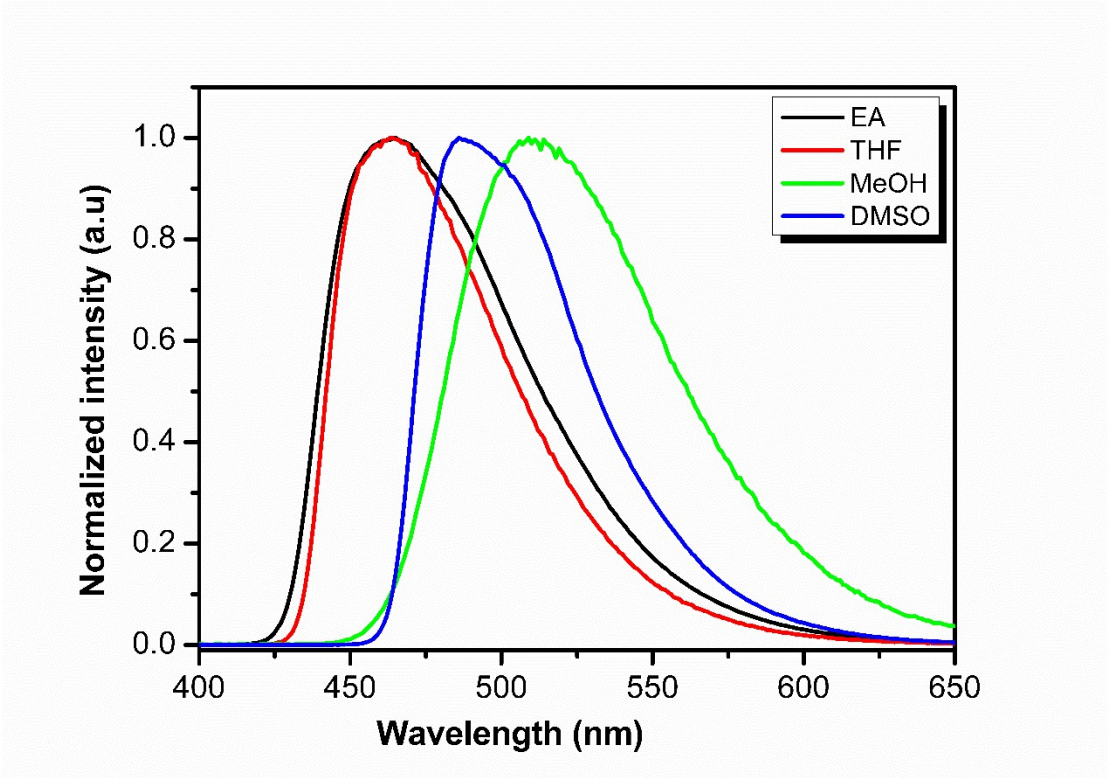


Figure S2. The emission spectra of DBPFA-I in different solvents such as EA, THF, MeOH and DMSO.

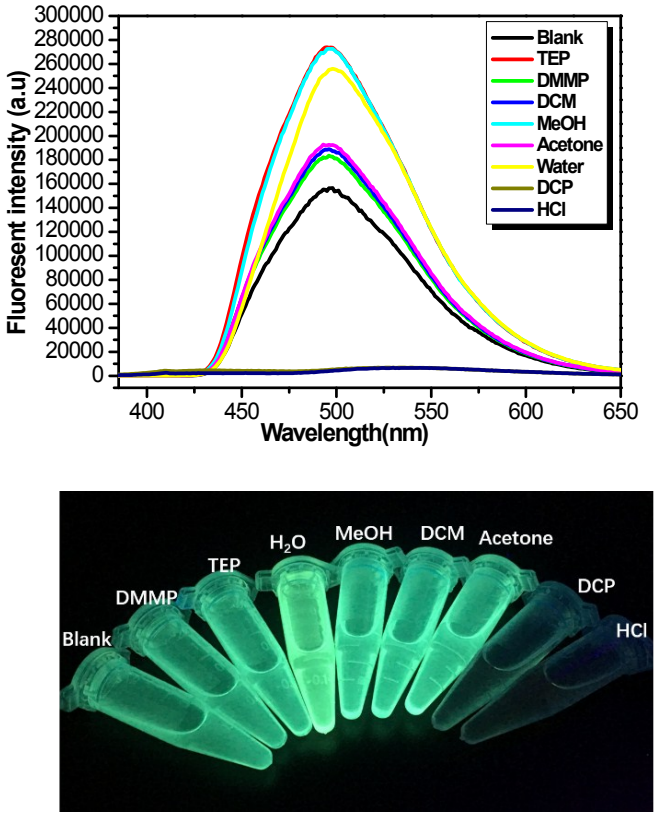


Figure S3. The emission spectra of DBPFA-I and fluorescence image under the excitation of a mobile UV lamp at a wavelength of 365 nm in different analytes such as TEP, DMMP, DCM, MeOH, Acetone, Water, DCP and HCl.

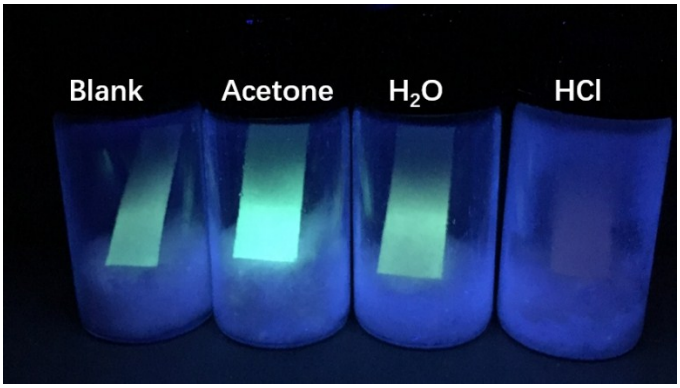
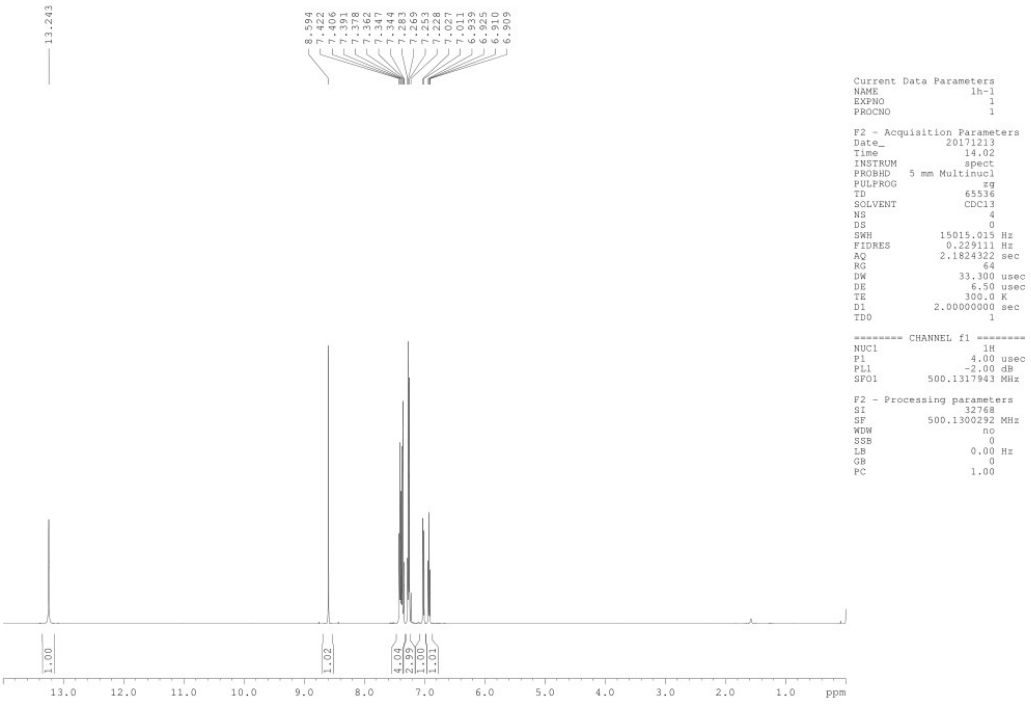
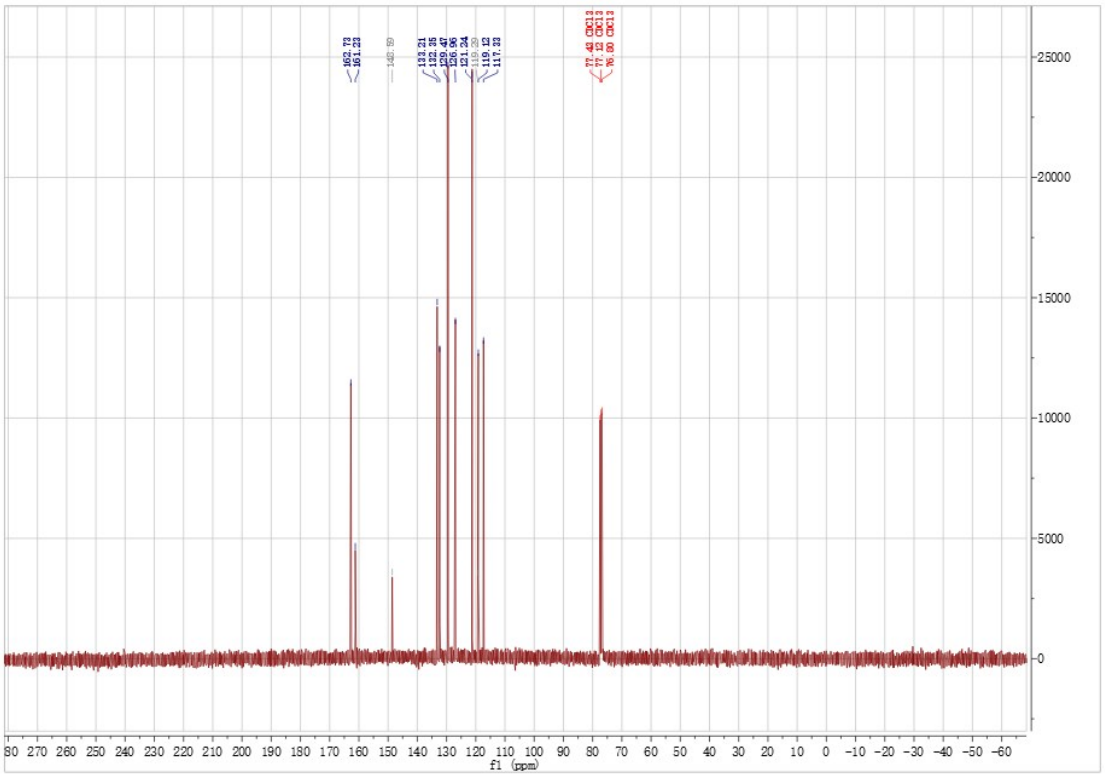


Figure S4. The fluorescence image of DBPFA-I under the excitation of a mobile UV lamp at a wavelength of 365 nm in different analytes such as Acetone, H_2O and HCl.



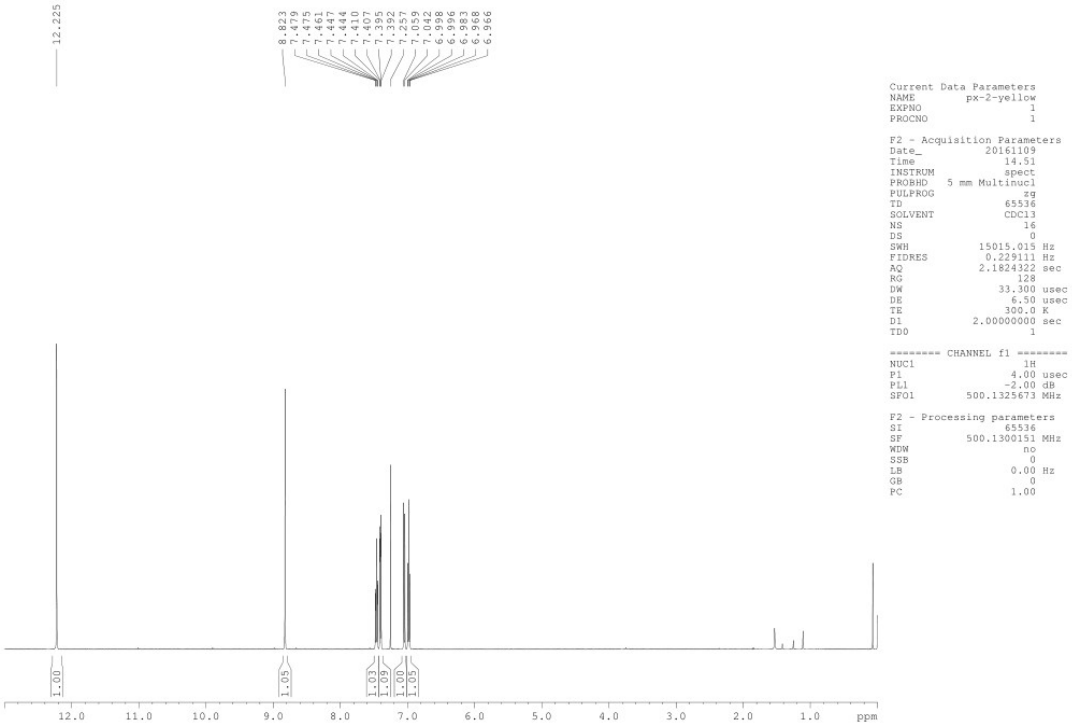


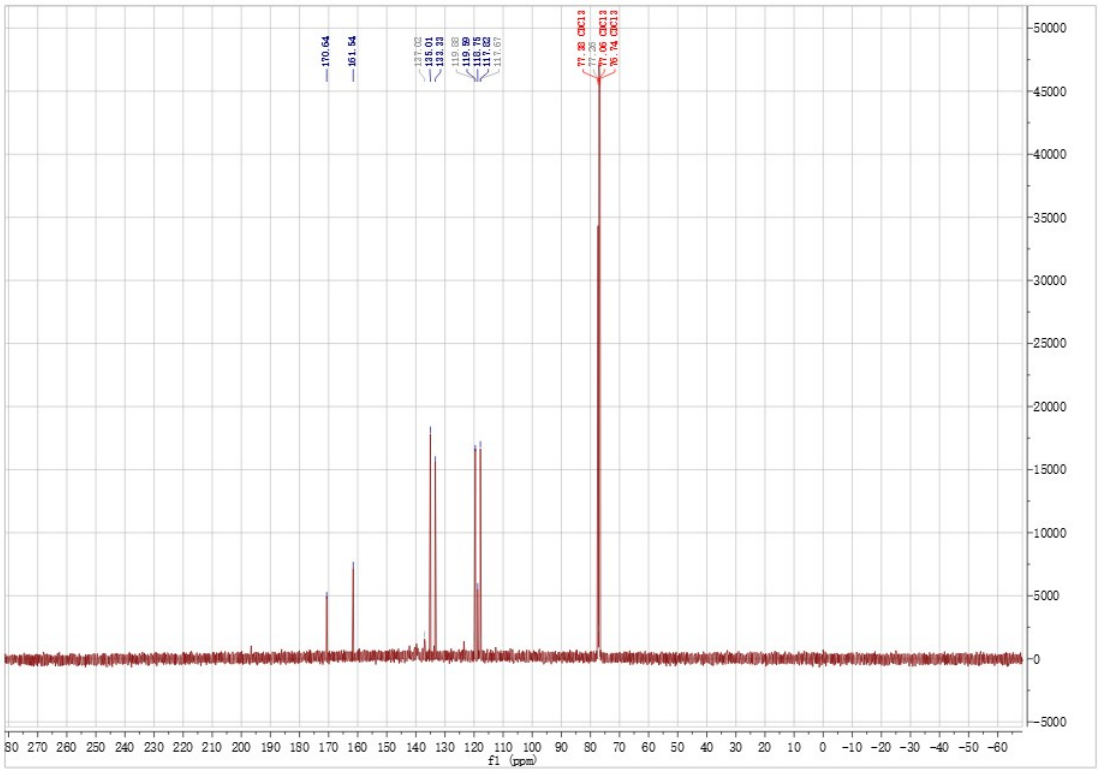
Elemental composition search on mass 198.09

m/z= 193.09-203.09

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
198.0912	198.0913	-0.66	8.5	$C_{13}H_{12}ON$

The ^{1}HNMR, ^{13}CNMR and HRMS of SB1



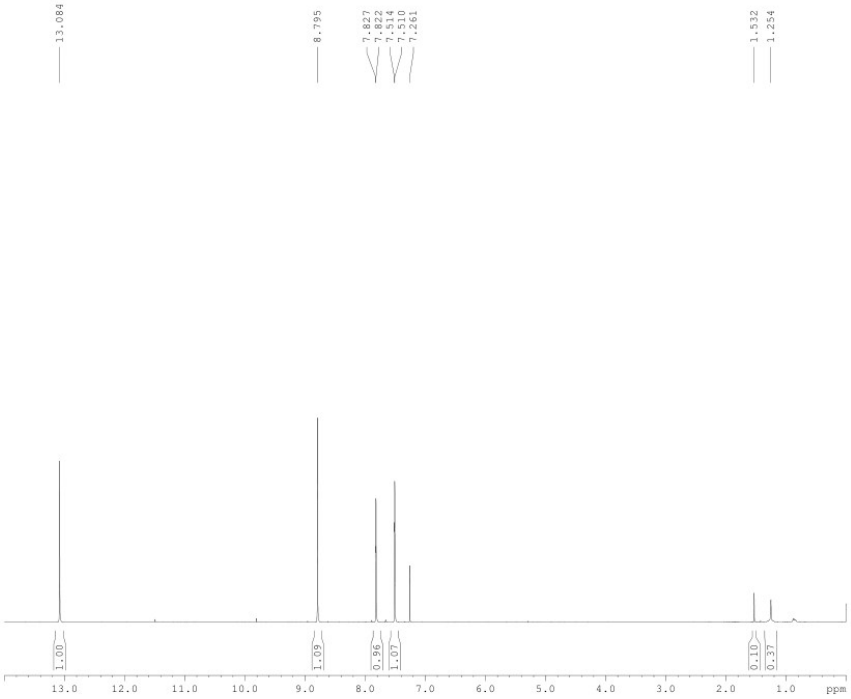


Elemental composition search on mass 288.04

m/z= 283.04-293.04

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
288.0440	288.0440	0.12	7.0	$C_{12}H_{10}O_6F_2$
	288.0442	-0.70	8.5	$C_{13}H_7ONF_5$
	288.0431	3.27	12.5	$C_{16}H_6NF_4$
	288.0429	4.09	11.0	$C_{15}H_9O_5F$
	288.0427	4.78	7.5	$C_{10}H_8O_5N_3F_2$

The ^{1}HNMR, ^{13}CNMR and HRMS of SB2

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PROCNO                   1

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PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       0
SWH             15015.015 Hz
FIDRES          0.229111 Hz
AQ              2.1824322 sec
RG                     128
DW                33.300 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   1H
P1                 4.00 usec
PL1               -2.00 dB
SFO1          500.1313130 MHz

F2 - Processing parameters
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SSB                      0
LB                  0.00 Hz
GB                       0
PC                    1.00
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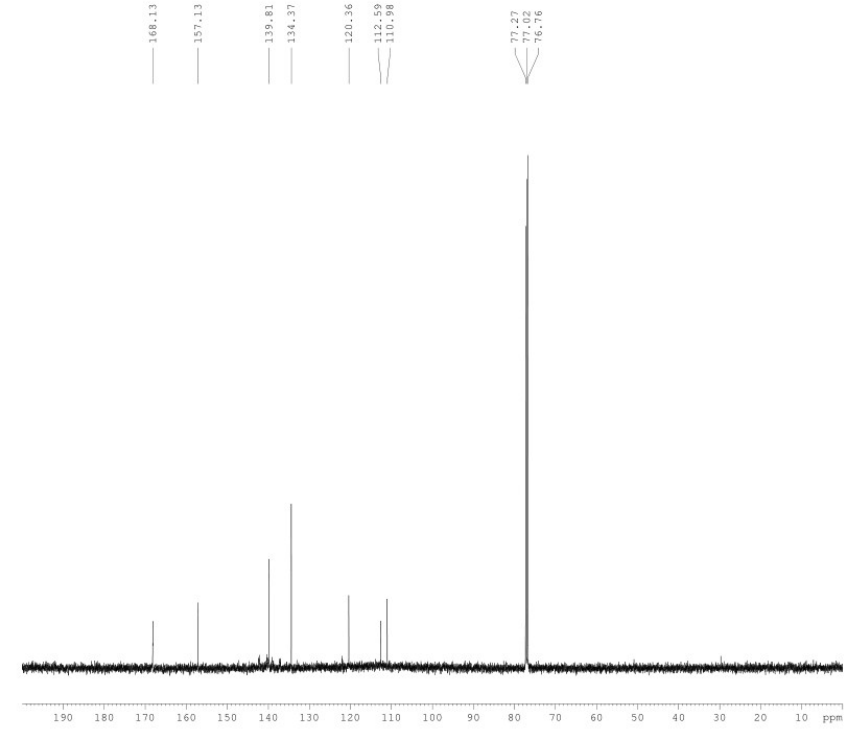


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PROCNO                   1

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TD                   65536
SOLVENT              CDCl3
NS                     402
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FIDRES          0.669245 Hz
AQ              0.7471718 sec
RG                   32768
DW                11.400 usec
DE                 6.50 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                  13C
P1                10.30 usec
PL1               -6.00 dB
SFO1          125.7666449 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             80.00 usec
PL12              18.00 dB
PL13              17.00 dB
PL2               120.00 dB
SFO2          500.1320005 MHz

F2 - Processing parameters
SI                   32768
SF            125.7577884 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
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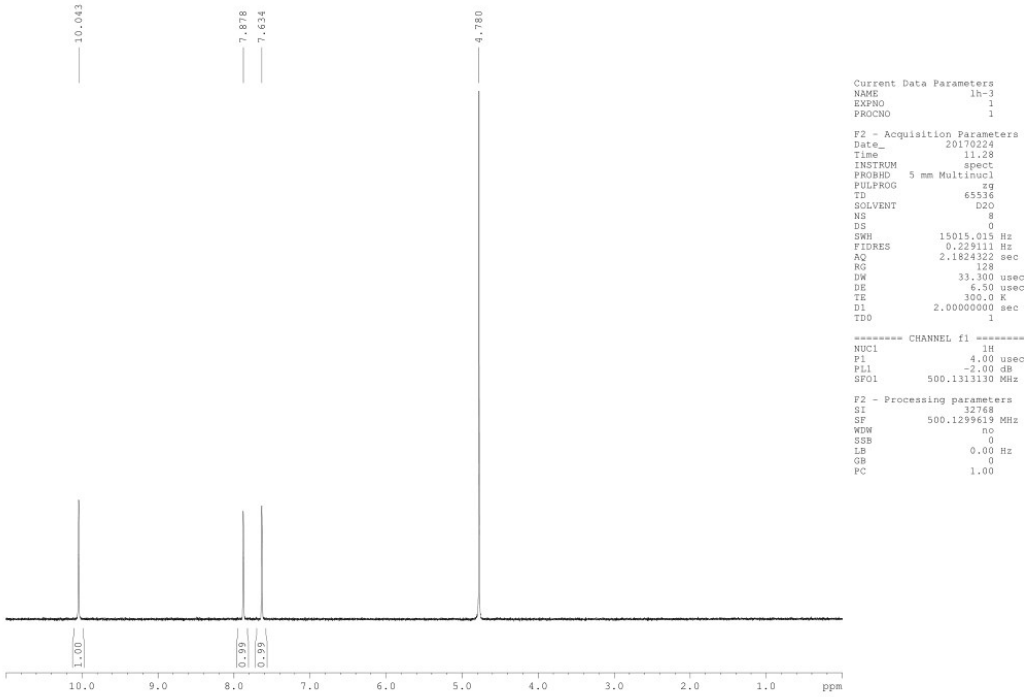
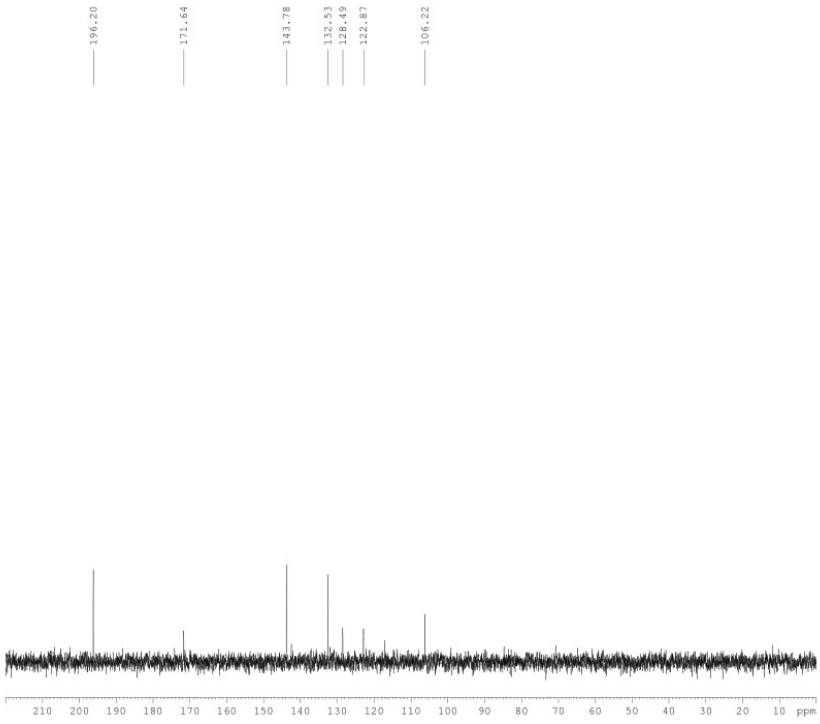
Elemental composition search on mass 443.87

m/z= 438.87-448.87

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
443.8658	443.8653	1.20	8.5	$C_{13}H_5ONBr_2F_5$
	443.8666	-1.73	15.5	$C_{18}H_5O_2NBr_2F$
	443.8650	1.73	7.0	$C_{12}H_8O_6Br_2F_2$
	443.8641	3.78	12.5	$C_{16}H_4NBr_2F_4$
	443.8677	-4.31	11.5	$C_{15}H_6O_3NBr_2F_2$
	443.8639	4.31	11.0	$C_{15}H_7O_5Br_2F$
	443.8637	4.76	7.5	$C_{10}H_6O_5N_3Br_2F_2$

The ^{1}HNMR, ^{13}CNMR and HRMS of DBPFA



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PROCNO                   1

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PULPROG          zgpg30
TD                65536
SOLVENT             D2O
NS                 1042
DS                    0
SWH           43859.648 Hz
FIDRES            0.669245 Hz
AQ             0.7471718 sec
RG                32768
DW               11.400 usec
DE                6.50 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.30 usec
PL1                -6.00 dB
SFO1         125.7666449 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL12               18.00 dB
PL13               17.00 dB
PL2               120.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                32768
SF           125.7574556 MHz
WDW                  EM
SSB                   0
LB                 3.00 Hz
GB                    0
PC                 1.40
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Elemental composition search on mass 443.87

m/z= 438.87-448.87

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
443.8650	443.8650	-0.02	7.0	$C_{12}H_8O_6Br_2F_2$
	443.8653	-0.56	8.5	$C_{13}H_5ONBr_2F_5$
	443.8641	2.02	12.5	$C_{16}H_4NBr_2F_4$
	443.8639	2.55	11.0	$C_{15}H_7O_5Br_2F$
	443.8637	3.00	7.5	$C_{10}H_6O_5N_3Br_2F_2$
	443.8666	-3.49	15.5	$C_{18}H_5O_2NBr_2F$

The ^{1}HNMR, ^{13}CNMR and HR MS of DBPFA-I

Table S1

Literature results summary on the detection of DCP in solution.

Some materials	A range of DCP concentration	Limit of detection	Fluorescence signal	Reaction time	reference
dRB-AE	25-250 ppm	Not given	chromogenic	20 min	1
o-OH	25-500 ppm	Not given	chromogenic	10min	2
RB-AE	0.1-3 mg/L	0.71 μg/L	chromogenic	20min	3
NA-p1	1-45 μM	21 nM	enhancing	10 min	4
NTBT	45-400 μM	17 nM	chromogenic	Not given	5
Comp. 3	0.25-3.0 μM	0.14 ppm	enhancing	Not given	6
PQ	0. 5 mM-0.01 M	14.9 μM	quenching	Not given	7
RTU	10 μM-180 μM	0.142 μM	chromogenic	Not given	8
DBPFA-I	0.27- 29.7 μM	1.94 nM	quenching	10s	This work

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Table S2 Detail methodology and parameters of Dmol^3

Dmol^3	
Task	Geometry Optimization
Properties	Optics, Orbitals
Energy	1.0^{-5}Ha
Max. force	0.002Ha/Å
Max, displacement	0.005 Å
Max, interactions	50
Max, step size	0.3 Å
Functional	GGA, BLYP
Integration accuracy	fine
SCF tolerance	fine
Core treatment	All Electron
Basis set	DNP+
Basis file	4.4
Orbital cut off quality	fine
Run in parallel on	12ores