

Electronic Supplementary Information for Energetic Materials with
Fluorinated Four-membered Heterocyclic Ring: 3, 3'-Difluoroazetidine
(DFAZ) Salts

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Figure S1 single-crystal X-ray structure (a) and crystal packing (b) of compound 2

Figure S2 single-crystal X-ray structure (a) and crystal packing (b) of compound 3

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Figure S4 single-crystal X-ray structure (a) and crystal packing (b) of compound 5

Figure S5 single-crystal X-ray structure (a) and crystal packing (b) of compound 6

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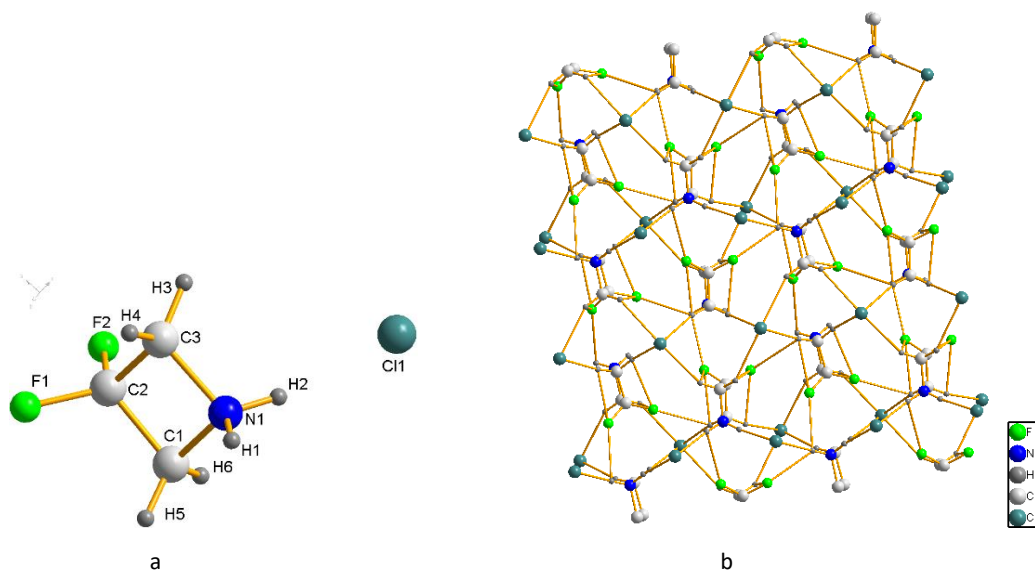


Figure S1 single-crystal X-ray structure (a) and crystal packing (b) of compound 2

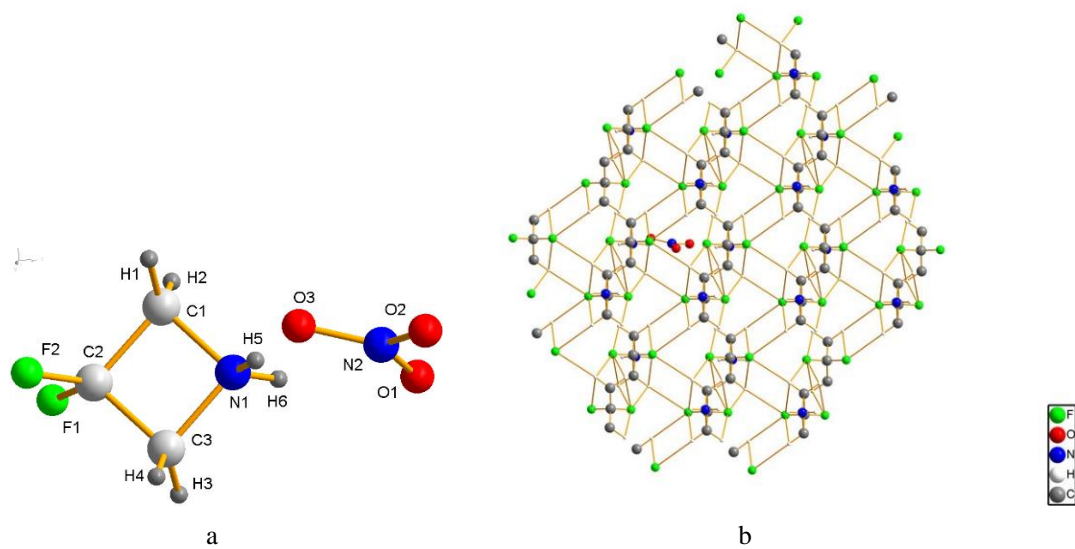
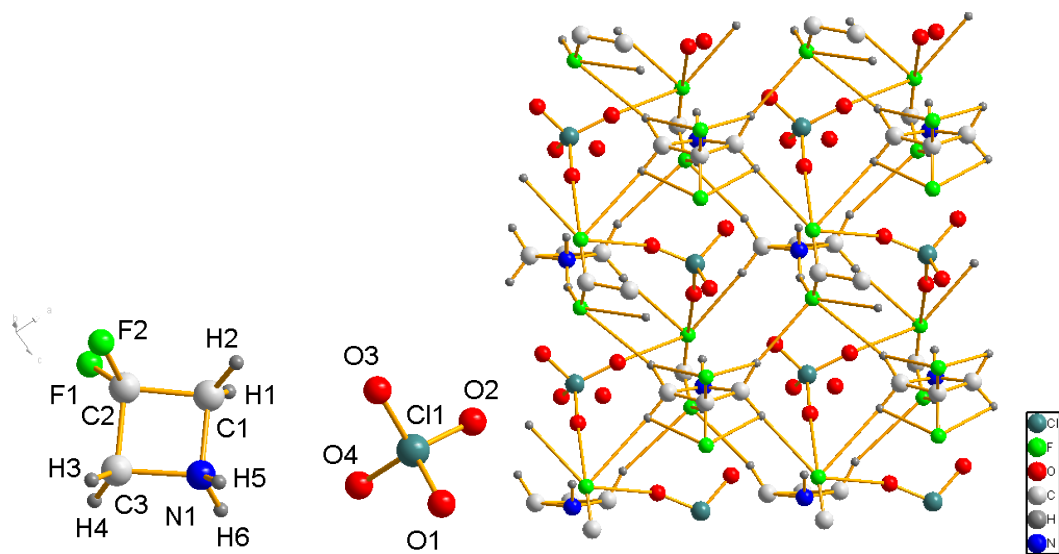


Figure S2 single-crystal X-ray structure (a) and crystal packing (b) of compound 3



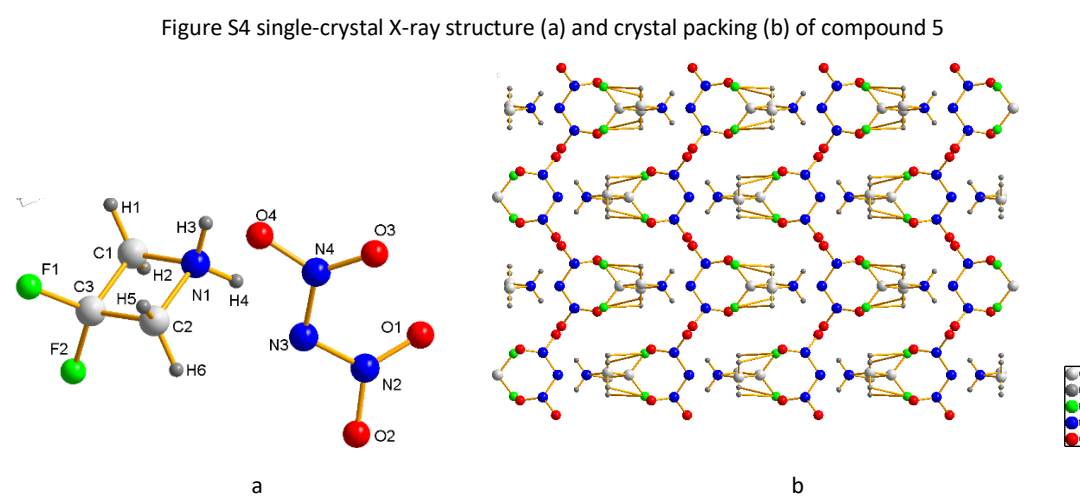
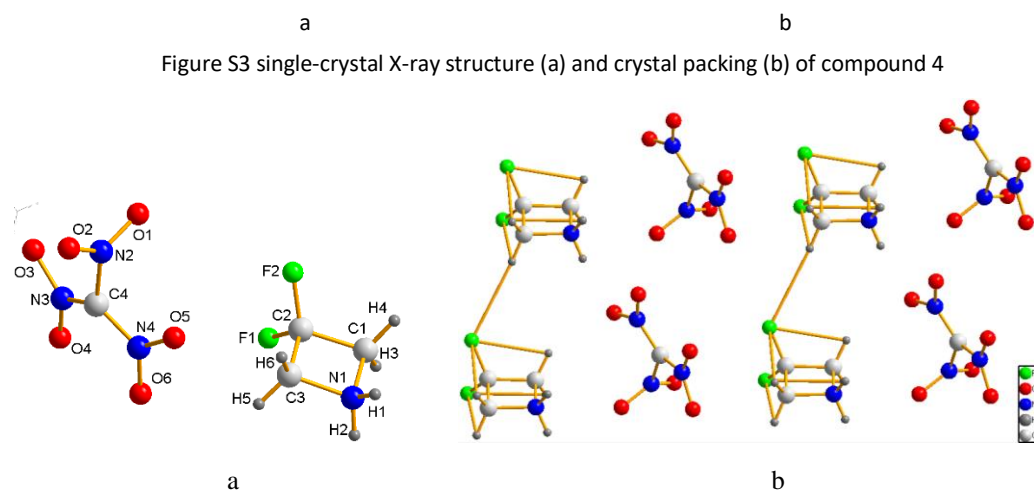


Figure S5 single-crystal X-ray structure (a) and crystal packing (b) of compound 6

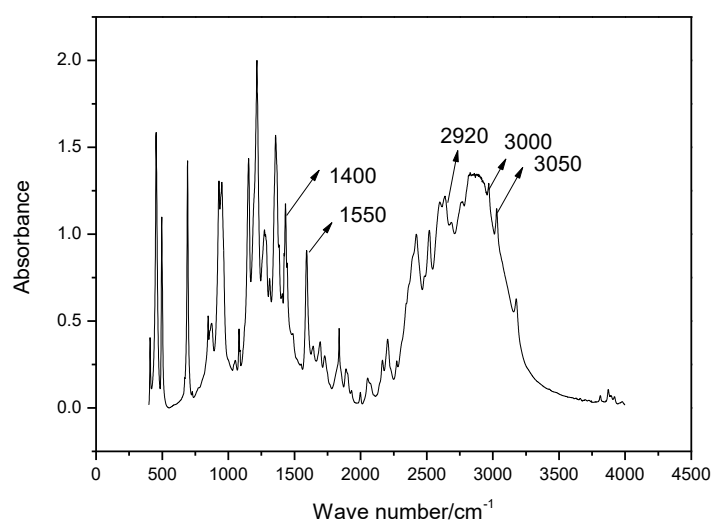


Figure S6 IR spectra of compound 2

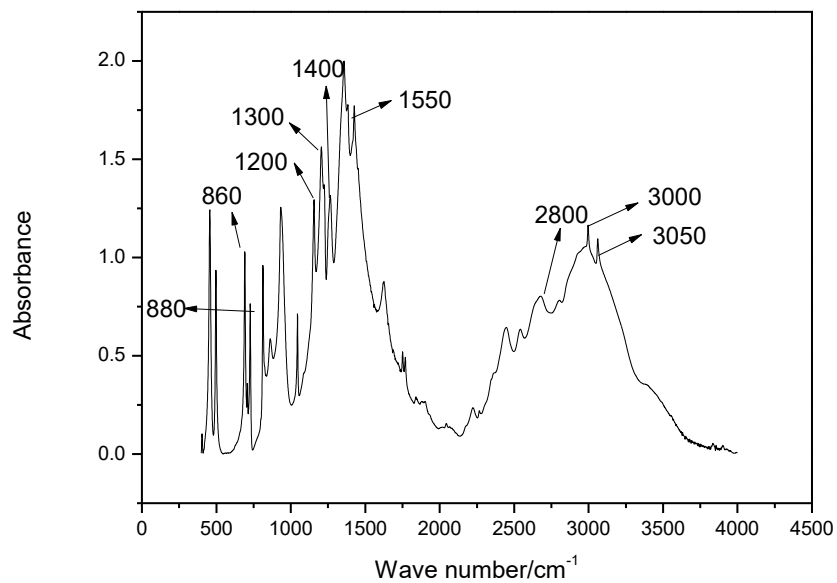


Figure S7 IR spectra of compound 3

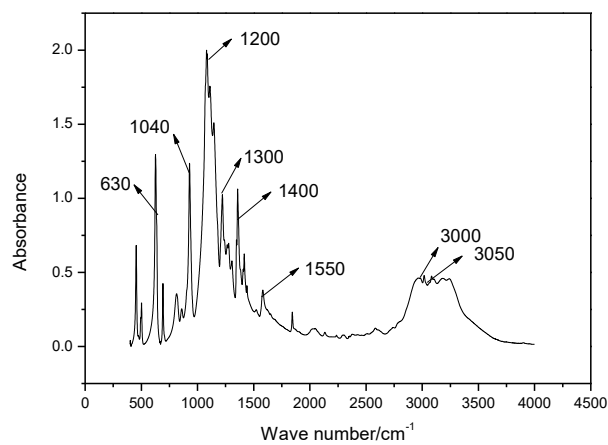


Figure S8 IR spectra of compound 4

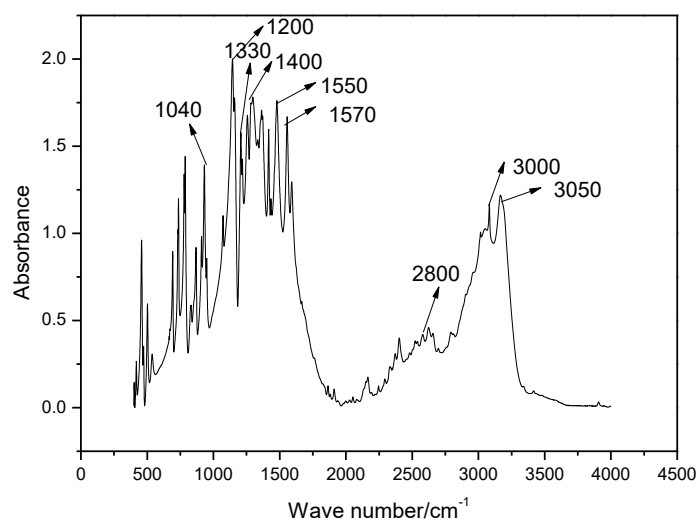


Figure S9 IR spectra of compound 5

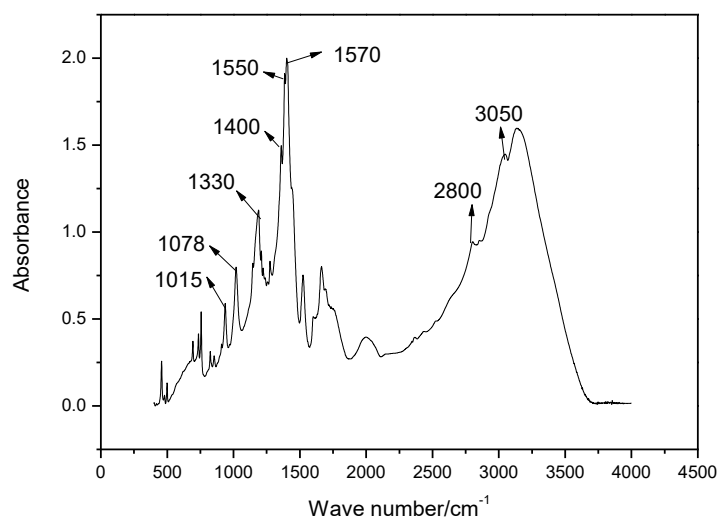


Figure S10 IR spectra of compound 6

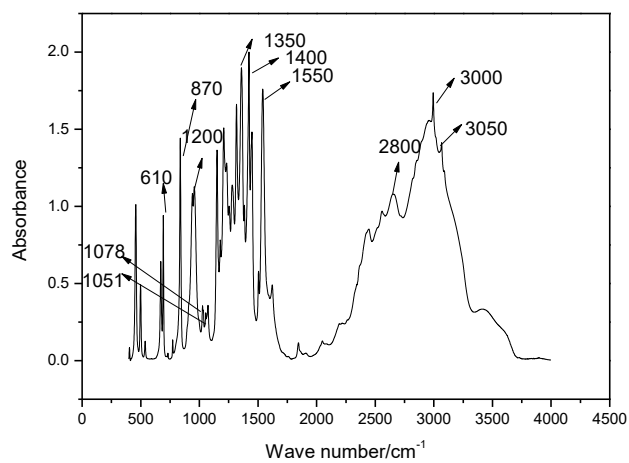


Figure S11 IR spectra of compound 7

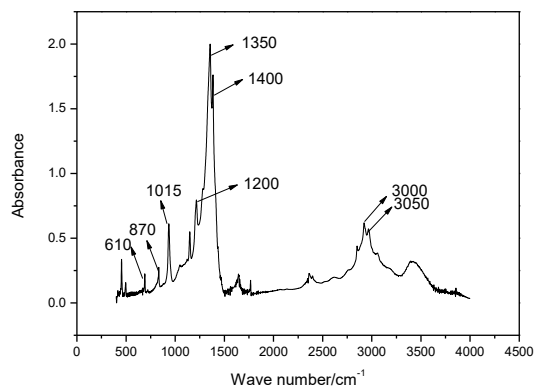


Figure S12 IR spectra of compound 8

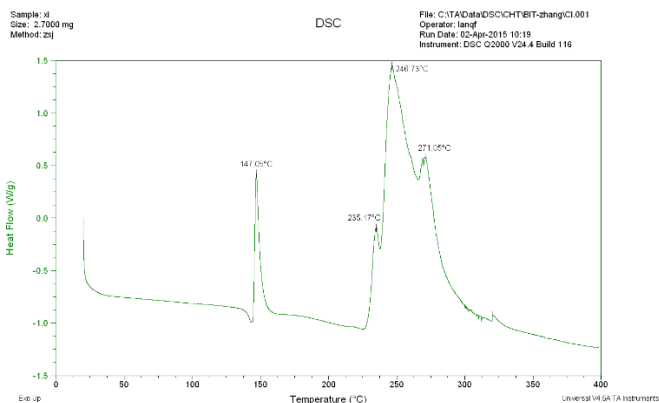


Figure S13 differential scanning calorimeter of compound 2

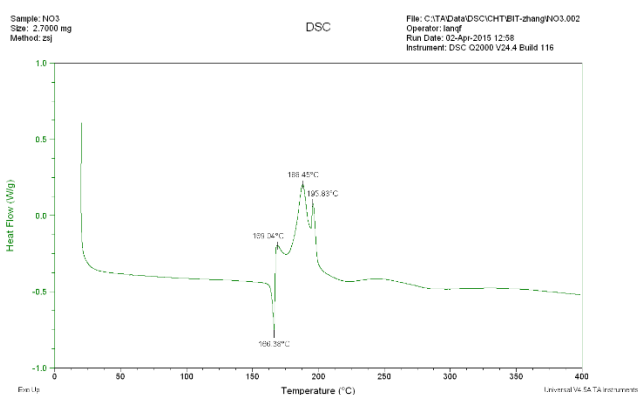


Figure S14 differential scanning calorimeter of compound 3

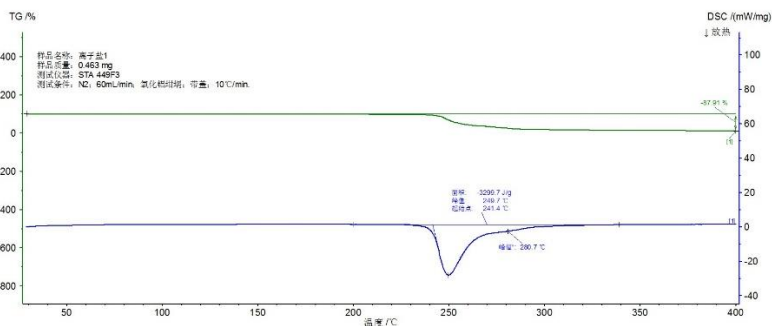


Figure S15 differential scanning calorimeter of compound 4

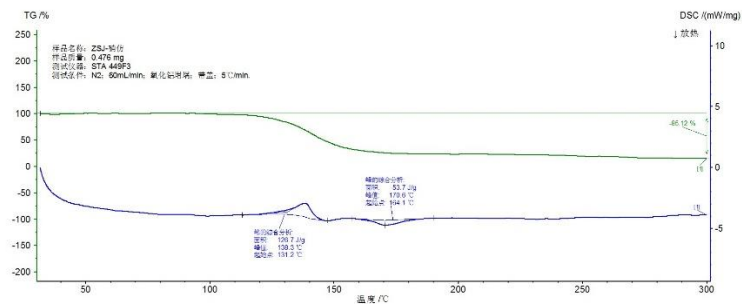


Figure S16 differential scanning calorimeter of compound 5

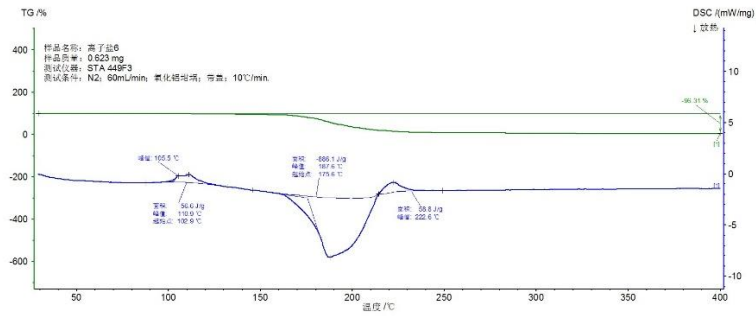


Figure S17 differential scanning calorimeter of compound 6

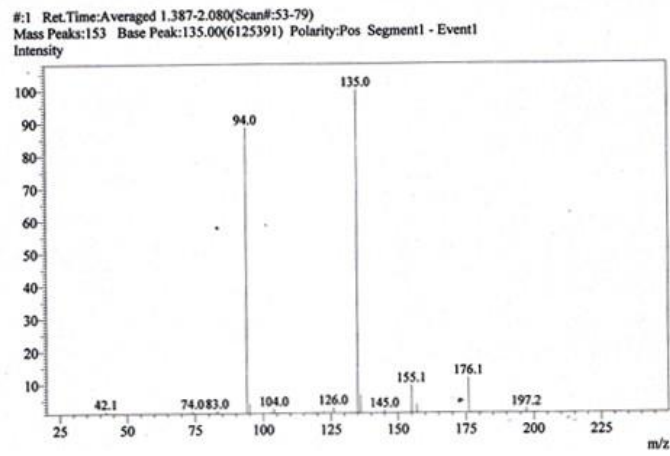


Figure S18 mass spectra of compound 2

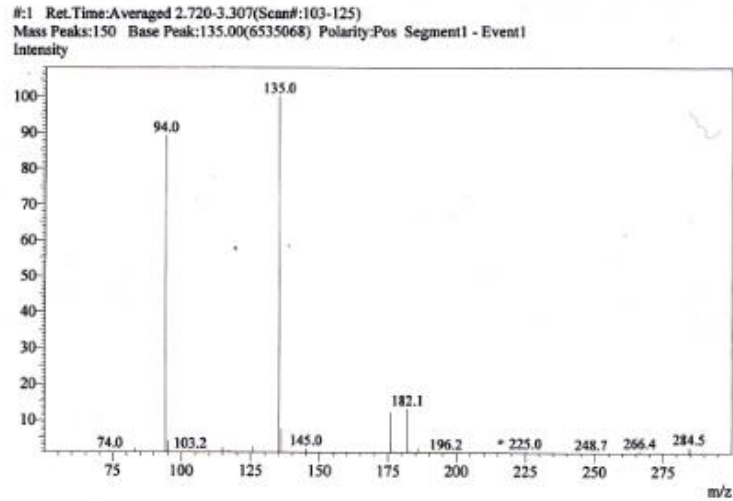


Figure S19 mass spectra of compound 3

ESI-MS Spectrum, 1

#1 Ret.Time:Averaged 1.813-2.293(Scan#:69-87)
Mass Peaks:161 Base Peak:94.0(2042354) Polarity:Pos Segment1 - Event1
Intensity

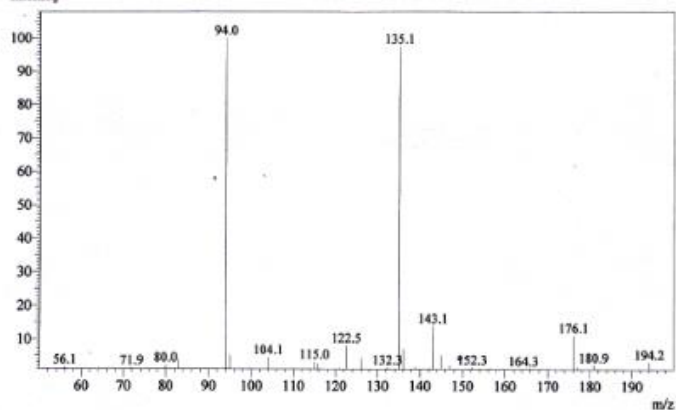


Figure S20 mass spectra of compound 4 (MS Screening mode for cations)

#2 Ret.Time:Averaged 1.840-2.320(Scan#:70-88)
Mass Peaks:316 Base Peak:98.95(110232) Polarity:Neg Segment1 - Event2
Intensity

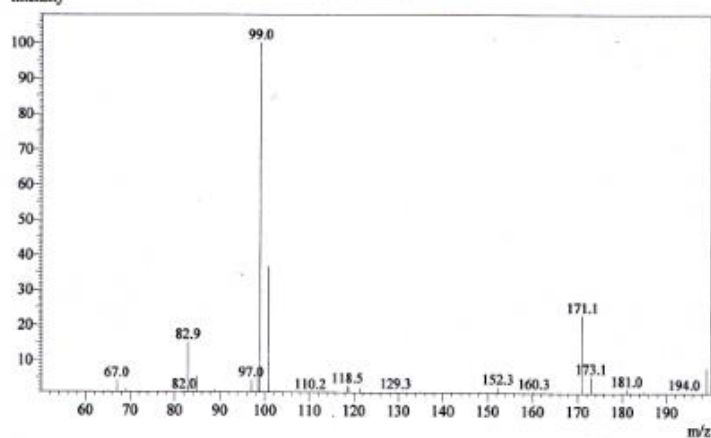


Figure S21 mass spectra of compound 4 (MS Screening mode for anions)

#1 Ret.Time:Averaged 1.333-1.867(Scan#:51-71)
Mass Peaks:133 Base Peak:135.05(3221419) Polarity:Pos Segment1 - Event1
Intensity

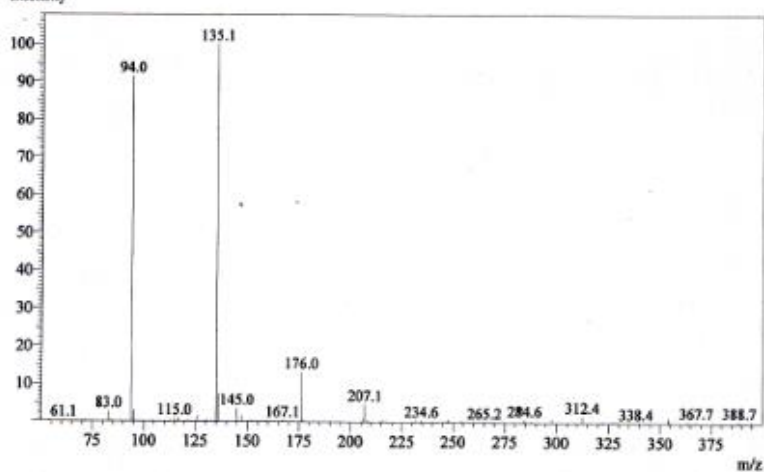


Figure S22 mass spectra of compound 5 (MS Screening mode for cations)

#2 Ret.Time:Averaged 1.360-1.893(Scan#:52-72)
Mass Peaks:252 Base Peak:149.95(1606258) Polarity:Neg Segment1 - Event2

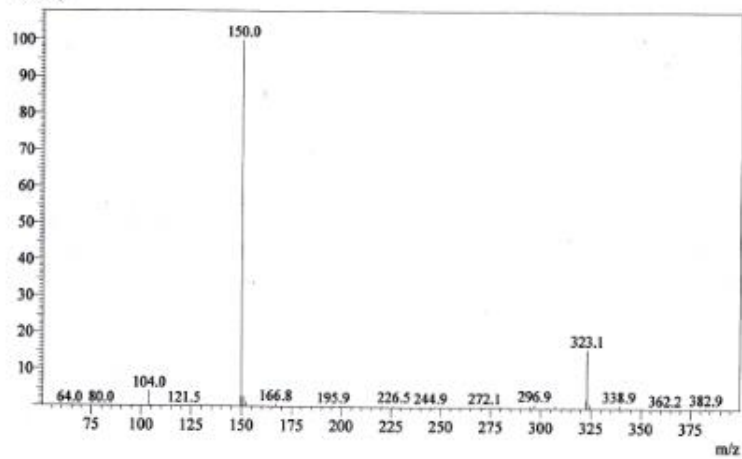


Figure S23 mass spectra of compound 5 (MS Screening mode for anions)

ESI-MS Spectrum, 6

#1 Ret.Time:Averaged 1.333-2.080(Scan#:51-79)
Mass Peaks:212 Base Peak:135.05(3269941) Polarity:Pos Segment1 - Event1

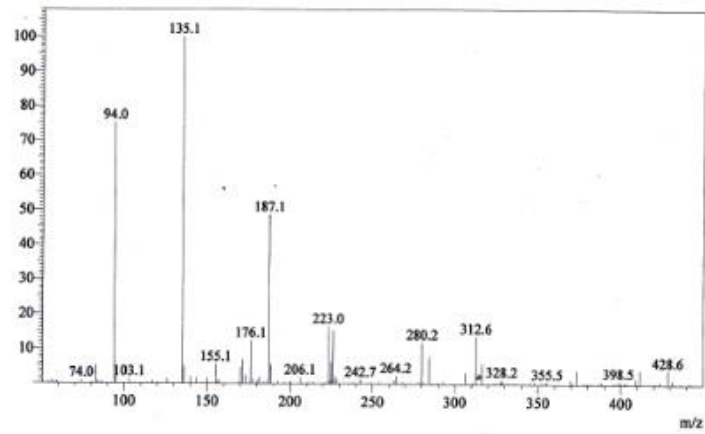


Figure S24 mass spectra of compound 6