```
Get["QUADRUPOLE"];

(*
 One-dimensional phase-modulated shifted-antiecho MQMAS of a spin I = 5/2,
 Three-pulse sequence,
 -3 Q antiecho amplitude optimization with the first pulse,
 Coherence transfer pathway 0 Q → -3 Q → 1 Q → -1 Q,
 Wolfram Mathematica 5.0,
 Author: R. HAJJAR
 *)

(*------------ Nucleus ------------*)
quadrupoleSpin = 2.5;
larmorFrequencyMhz = 208.61889974; (* Al-27 with 800 MHz NMR spectrometer *)

(*----- Quadrupole interaction ----*)
quadrupoleOrder = 2;
QCCMHz = 5;       η = 1;

(*--- Rotor Euler angles in PAS ---*)
αPR = 0;      βPR = 0;       γPR = 0;

(*----------- Parameters ----------*)
startOperator = Iz;
ωRFkHz = 100;   (* strong RF pulse strength in kHz unit *)
ωRF3kHz = 10;   (* weak RF pulse strength in kHz unit *)
spinRatekHz = 15;
powderFile = "rep100_simp";
numberOfGammaAngles = 10;
t1 = 4;    (* the first-pulse duration in microsecond unit *)
t2 = 1.75;  (* the second-pulse duration in microsecond unit *)
t3 = 15;   (* the third-pulse duration in microsecond unit *)
Δt = 0.25;  (* pulse duration increment in microsecond unit *)
np = t1 / Δt; (* number increment of the first-pulse duration *)

(*--------- Pulse sequence ---------*)
coherence1 = {-3};    (* -3 Q coherences *)
coherence2 = {1};     (* 1 Q coherences *)
detectelt = {{4, 3}}; (* central-transition matrix element of a spin 5/2 *)

fsimulation := (
  acq0;
  For [p = 1, p ≤ np, p++, {
     pulse[Δt, ωRFkHz];  (* first pulse *)
        store[2];
       filterCoh[coherence1];  (* -3 Q coherence pathway selection *)
     pulse[t2, ωRFkHz]; (* second pulse *)
        filterCoh[coherence2];  (* 1 Q coherence pathway selection *)
     pulse[t3, ωRF3kHz]; (* third pulse *)
       acq[p];
       recall[2];
   }];
 );
```

```
(*--- Execute, plot, and save simulation
  in "shifted_antiecho_P1" file ----------------*)
run;
tabgraph["shifted_antiecho_P1"];

(* ------------------------------------ *)
```

Rang	t (μs)	intensity
0	0	0.
1	0.25	0.0000105992132
2	0.5	0.0002468808041
3	0.75	0.001546198597
4	1.	0.005391445548
5	1.25	0.01267681527
6	1.5	0.02296717639
7	1.75	0.03476298089
8	2.	0.04623975947
9	2.25	0.05593179647
10	2.5	0.0630882312
11	2.75	0.06779514524
12	3.	0.0707672482
13	3.25	0.0727797922
14	3.5	0.07435445986
15	3.75	0.07574033171
16	4.	0.07664773228