

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091018\
 Data File : BG036627.D
 Acq On : 10 Sep 2018 16:27
 Operator : JU/SJ
 Sample : J4830-07
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 090618-TIPC-E-D-M

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.621	391	397	407	rBV	341007	542137	12.05%	2.913%
2	7.207	660	667	677	rBV	217923	379651	8.44%	2.040%
3	7.583	723	731	740	rBV	611709	1054065	23.42%	5.664%
4	8.053	805	811	818	rBV	192639	336540	7.48%	1.809%
5	8.376	857	866	875	rBV	812328	1431758	31.81%	7.694%
6	9.216	1001	1009	1021	rBV	707446	1244356	27.65%	6.687%
7	10.862	1281	1289	1297	rVB	283741	502552	11.17%	2.701%
8	13.306	1697	1705	1721	rBV	1952265	3091439	68.69%	16.613%
9	14.122	1839	1844	1851	rBV	125416	186024	4.13%	1.000%
10	14.681	1932	1939	1947	rBV2	467059	770118	17.11%	4.139%
11	15.967	2153	2158	2163	rBV	79921	99530	2.21%	0.535%
12	16.161	2185	2191	2206	rBV	909686	1405204	31.22%	7.551%
13	17.424	2399	2406	2416	rBV	612851	963855	21.42%	5.180%
14	20.027	2843	2849	2859	rBV	3402263	4500440	100.00%	24.185%
15	21.684	3125	3131	3142	rBV2	620811	1081631	24.03%	5.813%
16	23.376	3413	3419	3428	rVB	49739	98867	2.20%	0.531%
17	24.898	3668	3678	3696	rBV	272339	920406	20.45%	4.946%

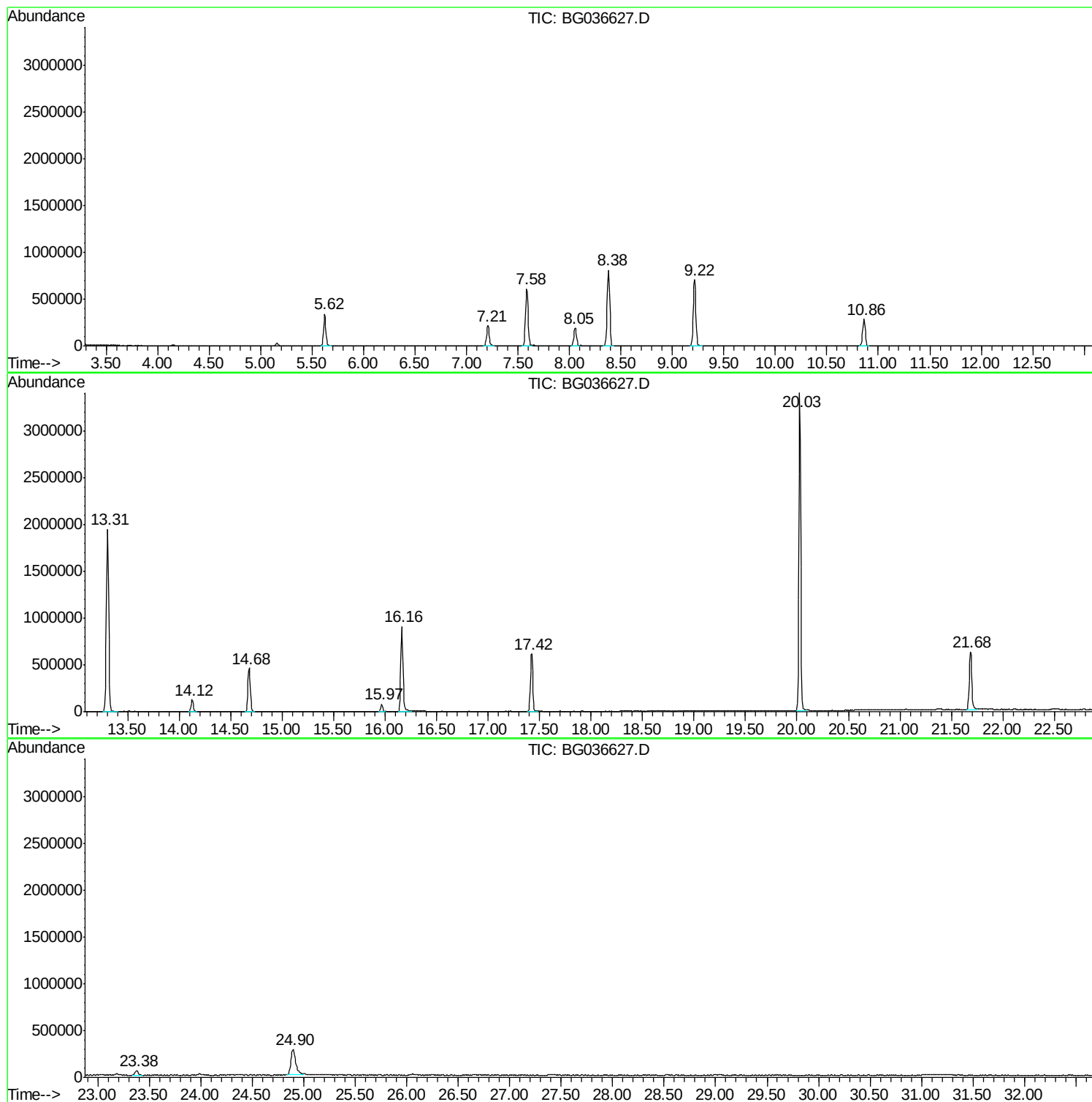
Sum of corrected areas: 18608573

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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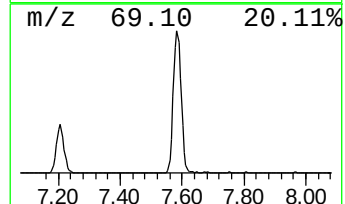
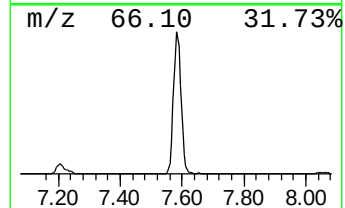
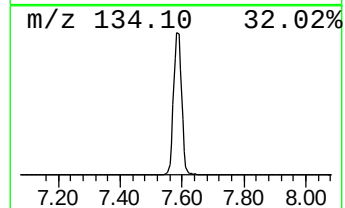
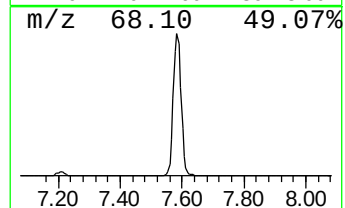
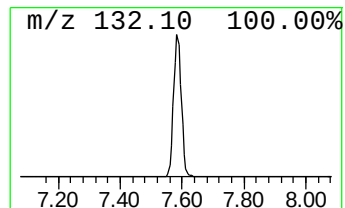
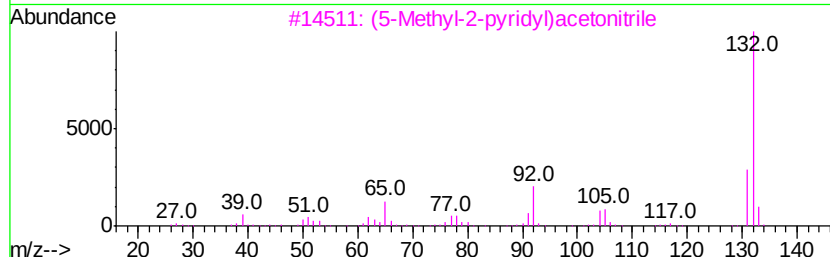
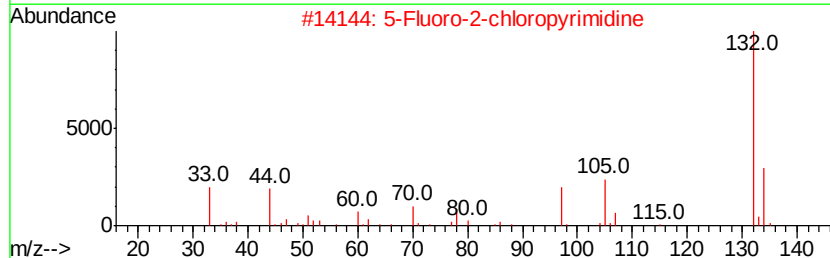
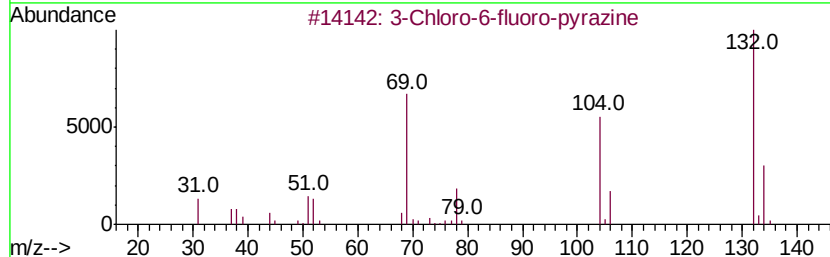
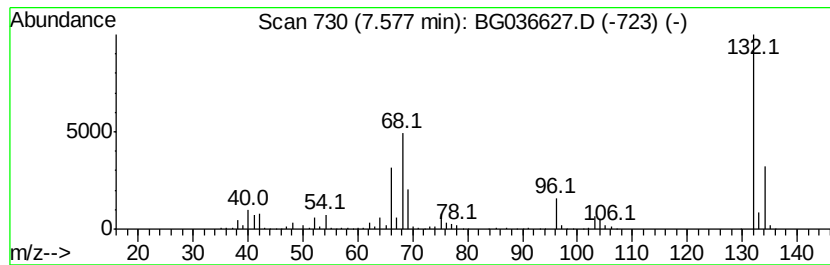
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	62.64 ng	1054070	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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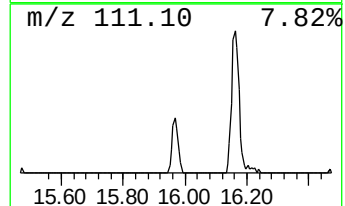
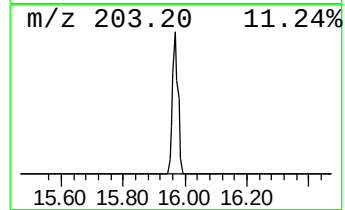
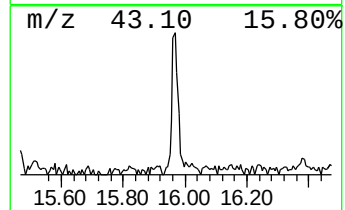
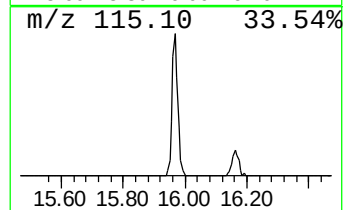
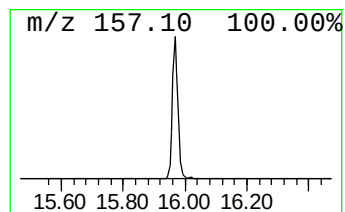
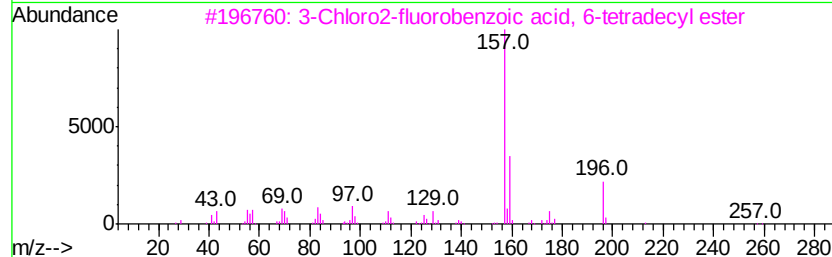
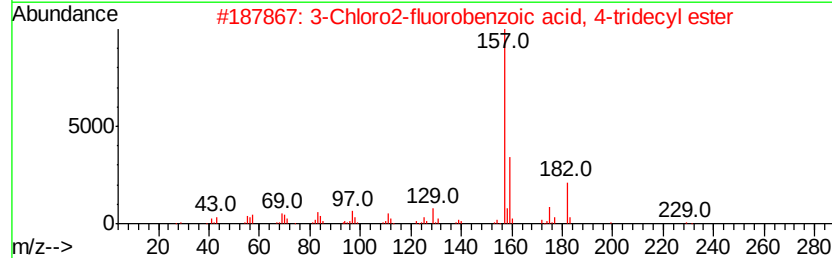
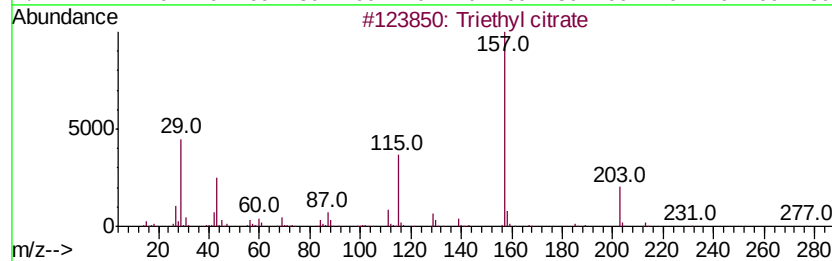
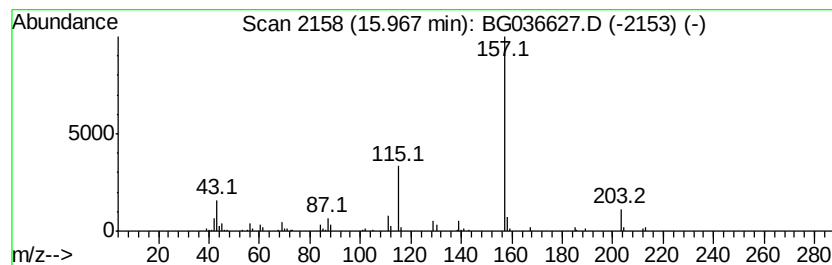
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Peak Number 3 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.58 ng	99530	Acenaphthene-d10	14.68
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triethyl citrate	276 C12H20O7	000077-93-0 52
2		3-Chloro2-fluorobenzoic acid, 4-...	356 C20H30ClF02	1000338-64-4 40
3		3-Chloro2-fluorobenzoic acid, 6-...	370 C21H32ClF02	1000338-64-9 40
4		O-Acetylcitric acid triethyl ester	318 C14H22O8	000077-89-4 39
5		Piperazine-1-carboxylic acid, 4-...	362 C14H19ClN2O5S	1000303-79-9 33



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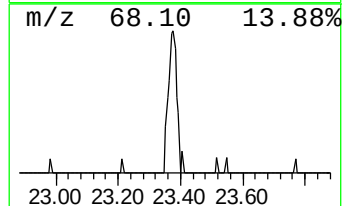
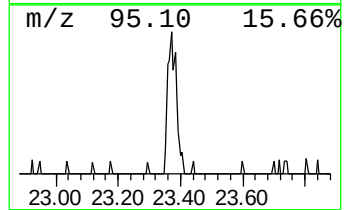
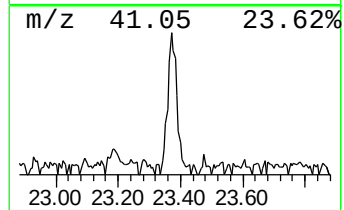
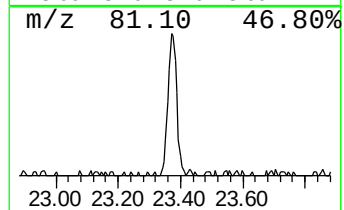
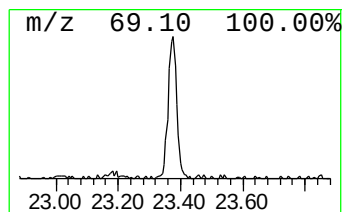
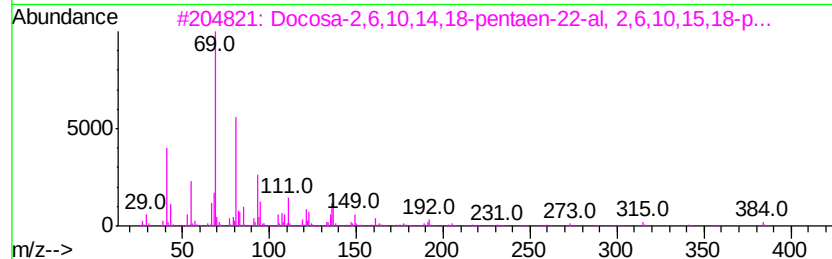
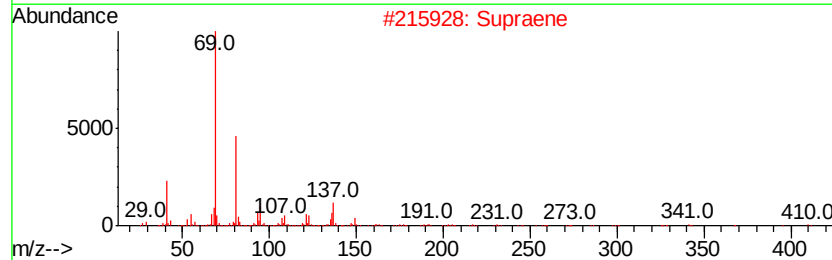
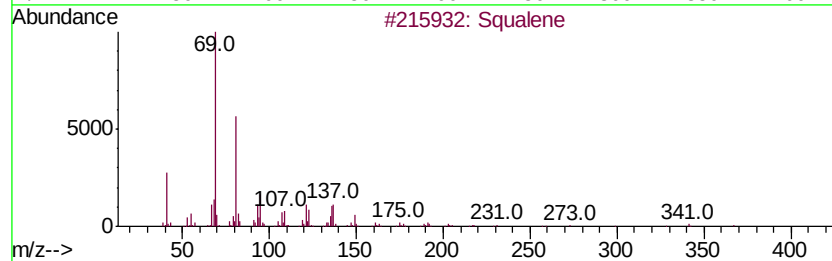
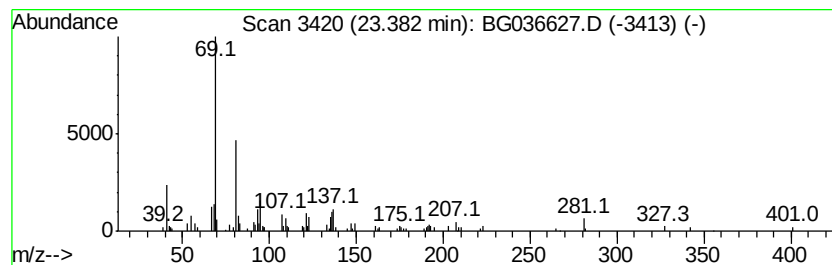
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Peak Number 4 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.38	2.15 ng	98867	Perylene-d12	24.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	87
2		Supraene	410	C30H50	007683-64-9	87
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	86
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5		trans-Farnesol	222	C15H26O	000106-28-5	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.58	7.58	62.6	ng	1054070	1	8.05	336540	20.0
Triethyl citrate	15.97	2.6	ng	99530	3	14.68	770118	20.0
Squalene	23.38	2.1	ng	98867	6	24.90	920406	20.0