

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092118\
 Data File : BG036896.D
 Acq On : 22 Sep 2018 16:11
 Operator : JU/SJ
 Sample : J5019-06
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 091918-DBRI-E-U-S

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BG092018.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	5.150	313	317	327	rBV2	29431	49503	1.20%	0.322%
2	5.614	390	396	416	rBV	179693	358353	8.68%	2.331%
3	7.206	660	667	691	rBV	110795	274439	6.65%	1.786%
4	7.577	723	730	745	rBV	371258	725709	17.58%	4.721%
5	8.047	803	810	823	rBV	119342	234237	5.68%	1.524%
6	8.370	857	865	886	rBV	533366	1010834	24.49%	6.577%
7	9.210	999	1008	1032	rBV	458330	968647	23.47%	6.302%
8	10.849	1281	1287	1298	rBV	167042	343516	8.32%	2.235%
9	13.293	1696	1703	1719	rBV	1465182	2484803	60.21%	16.166%
10	14.122	1839	1844	1853	rBV	26455	43040	1.04%	0.280%
11	14.674	1931	1938	1952	rBB2	314921	556484	13.48%	3.621%
12	16.161	2184	2191	2203	rBV	793319	1318518	31.95%	8.578%
13	17.418	2399	2405	2420	rBV	461264	749744	18.17%	4.878%
14	20.027	2842	2849	2865	rBV	2837015	4127027	100.00%	26.851%
15	21.684	3124	3131	3143	rBV	493684	869665	21.07%	5.658%
16	23.164	3378	3383	3393	rVB4	22312	42857	1.04%	0.279%
17	23.358	3409	3416	3424	rVB	113218	215949	5.23%	1.405%
18	23.969	3514	3520	3529	rVB3	24590	51403	1.25%	0.334%
19	24.892	3667	3677	3693	rVB2	297951	886788	21.49%	5.769%
20	26.031	3864	3871	3882	rVB5	19769	58830	1.43%	0.383%

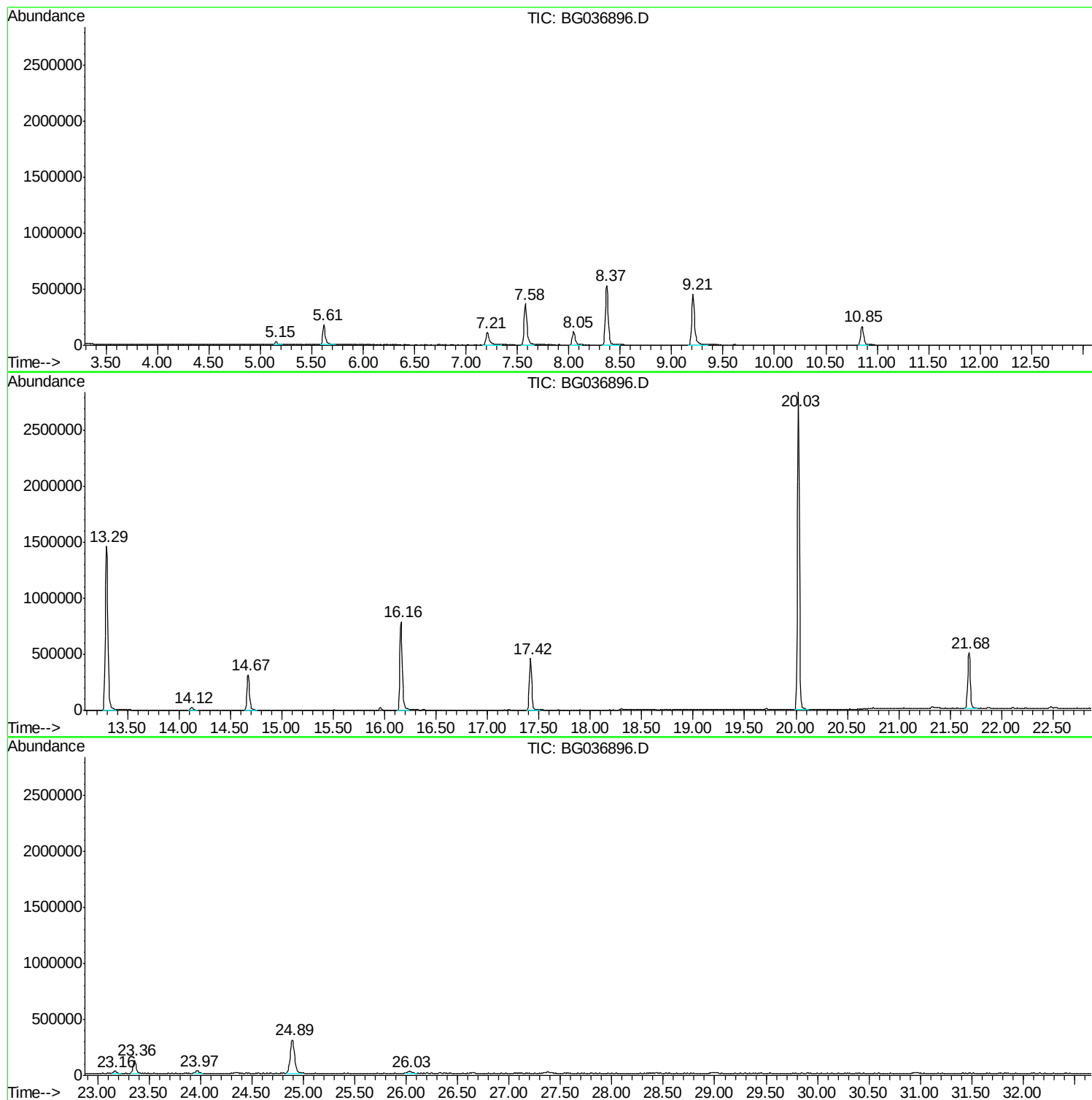
Sum of corrected areas: 15370346

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG092018.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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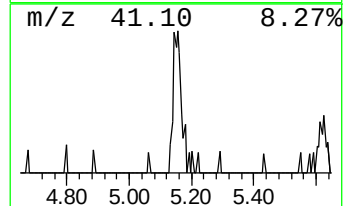
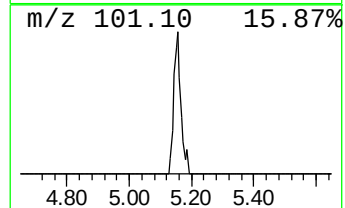
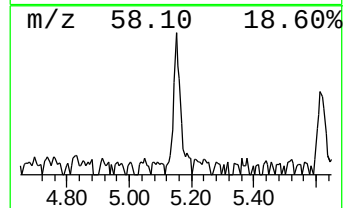
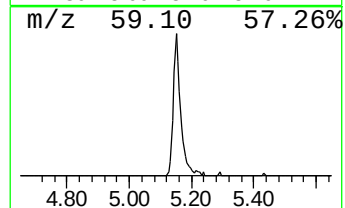
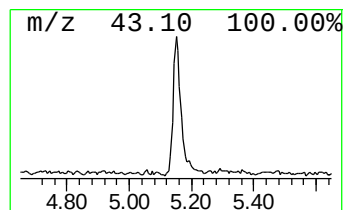
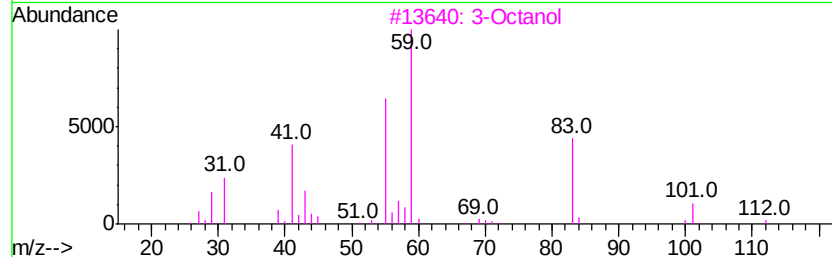
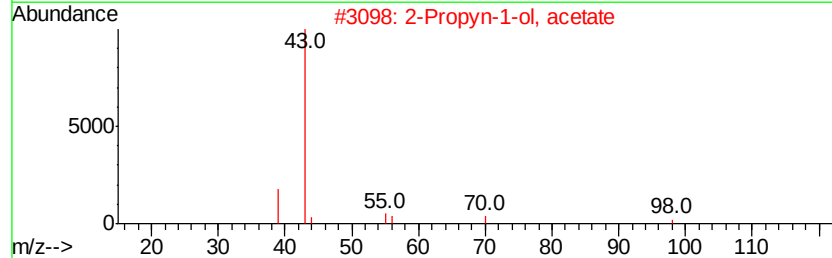
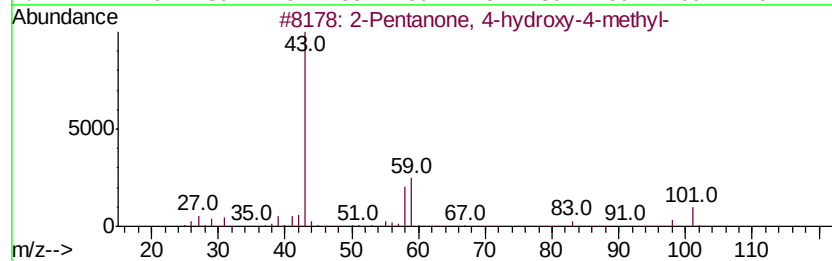
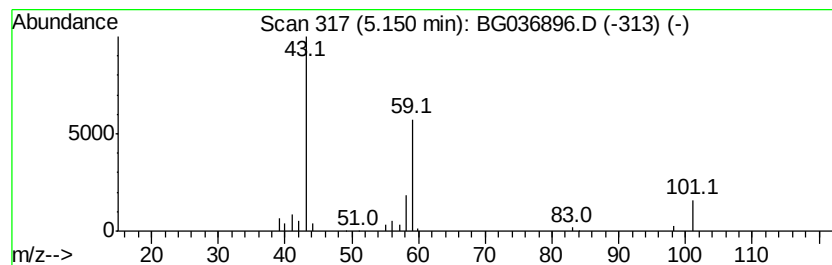
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	4.23 ng	49503	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
3		3-Octanol	130	C8H18O	000589-98-0	9
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5		5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9



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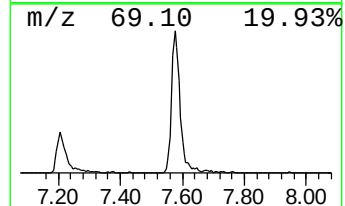
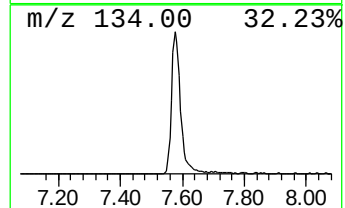
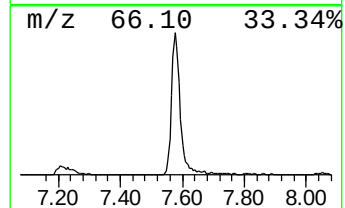
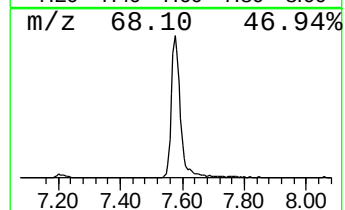
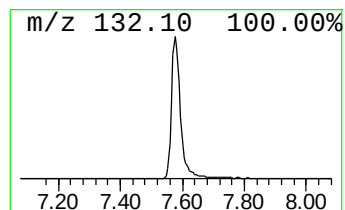
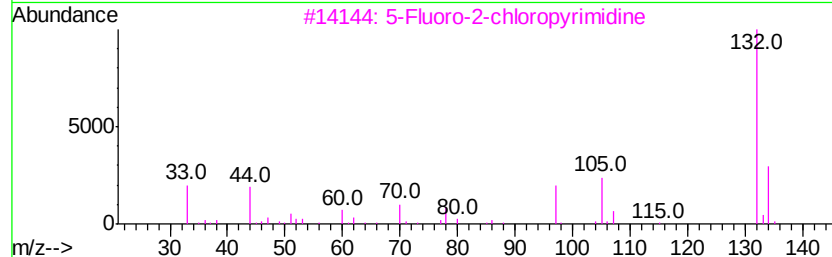
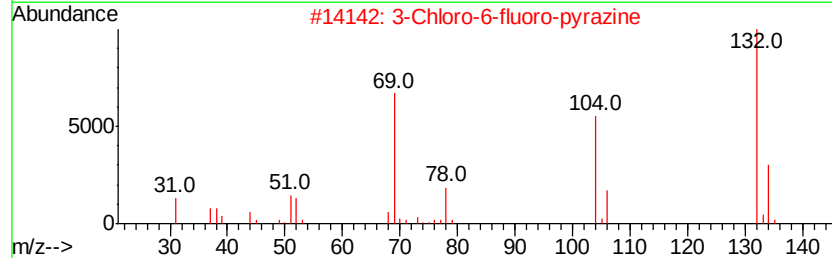
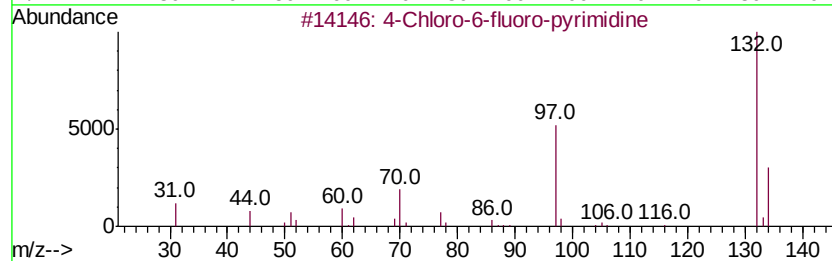
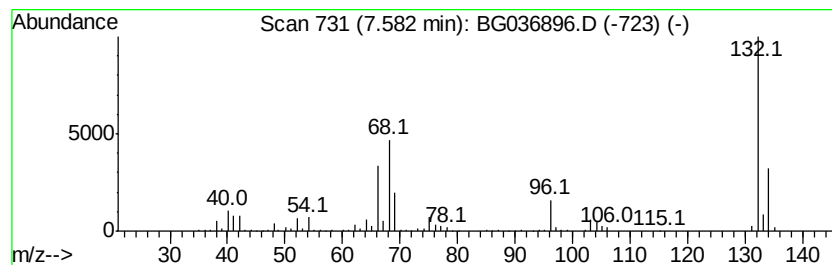
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Peak Number 2 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	61.96 ng	725709	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10



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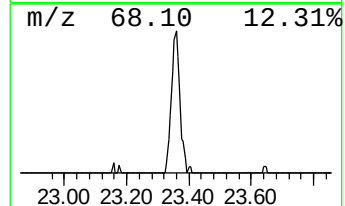
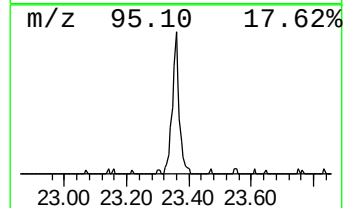
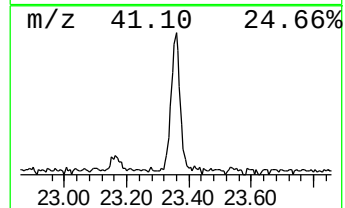
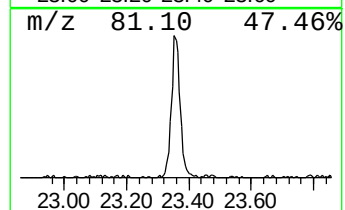
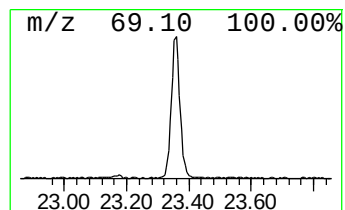
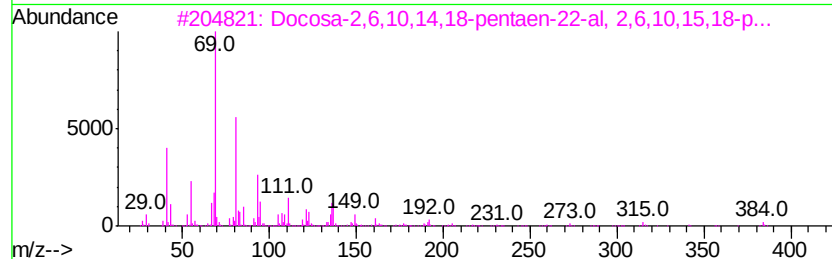
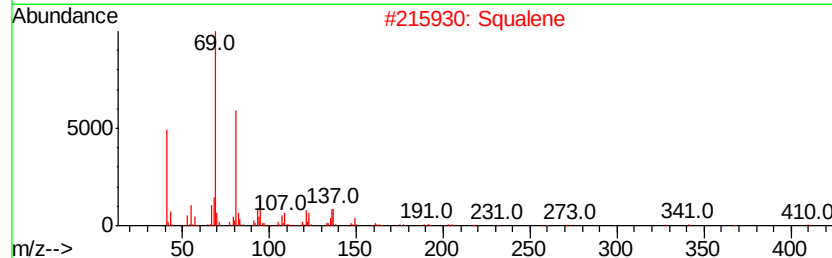
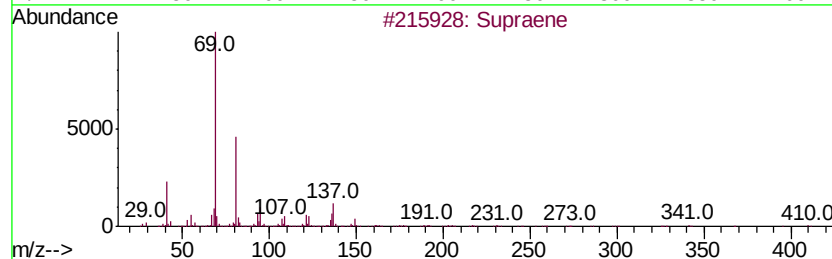
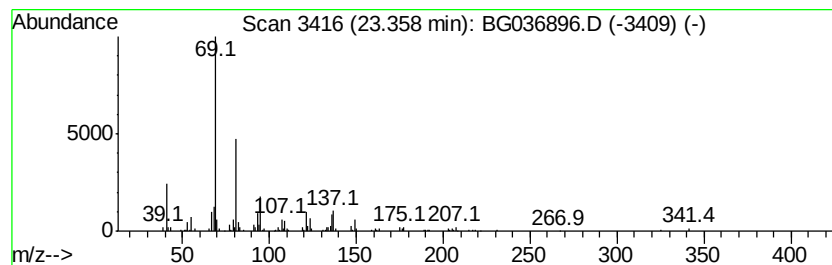
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Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.36	4.87 ng	215949	Perylene-d12	24.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	91
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.15	4.2	ng	49503	1	8.05	234237	20.0
unknown7.58	7.58	62.0	ng	725709	1	8.05	234237	20.0
Supraene	23.36	4.9	ng	215949	6	24.89	886788	20.0