

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062618\
 Data File : BG035421.D
 Acq On : 26 Jun 2018 22:09
 Operator : JU/SJ
 Sample : J3688-03
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EPE-109-6(70-72)

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-BG060718.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	5.159	312	318	328	rVB	66065	106164	3.17%	0.603%
2	5.629	388	398	410	rBV	743355	1220552	36.43%	6.936%
3	7.210	659	667	680	rBV	815970	1432730	42.77%	8.142%
4	7.585	723	731	741	rBV	758927	1307452	39.03%	7.430%
5	8.050	803	810	818	rBV	164429	278563	8.32%	1.583%
6	8.373	856	865	873	rBV	560635	974134	29.08%	5.536%
7	9.213	1000	1008	1020	rBV	453644	841472	25.12%	4.782%
8	10.852	1280	1287	1296	rVB	208902	375604	11.21%	2.134%
9	13.295	1696	1703	1712	rBV	1351232	2054310	61.32%	11.674%
10	14.118	1837	1843	1854	rBV	191278	287296	8.58%	1.633%
11	14.670	1931	1937	1948	rVB2	359384	593293	17.71%	3.371%
12	16.156	2180	2190	2200	rBV	1183671	1802286	53.80%	10.242%
13	16.368	2222	2226	2235	rBV	23068	37029	1.11%	0.210%
14	17.413	2398	2404	2415	rBV	535948	805947	24.06%	4.580%
15	18.295	2548	2554	2560	rBV2	90493	131111	3.91%	0.745%
16	19.558	2766	2769	2774	rBV4	30692	40437	1.21%	0.230%
17	20.022	2842	2848	2855	rBV	2553450	3349956	100.00%	19.036%
18	21.326	3066	3070	3079	rBV7	20244	46095	1.38%	0.262%
19	21.678	3123	3130	3138	rBV	572532	925532	27.63%	5.259%
20	23.358	3410	3416	3423	rVB	84308	145078	4.33%	0.824%
21	24.897	3667	3678	3688	rBV2	292162	842581	25.15%	4.788%

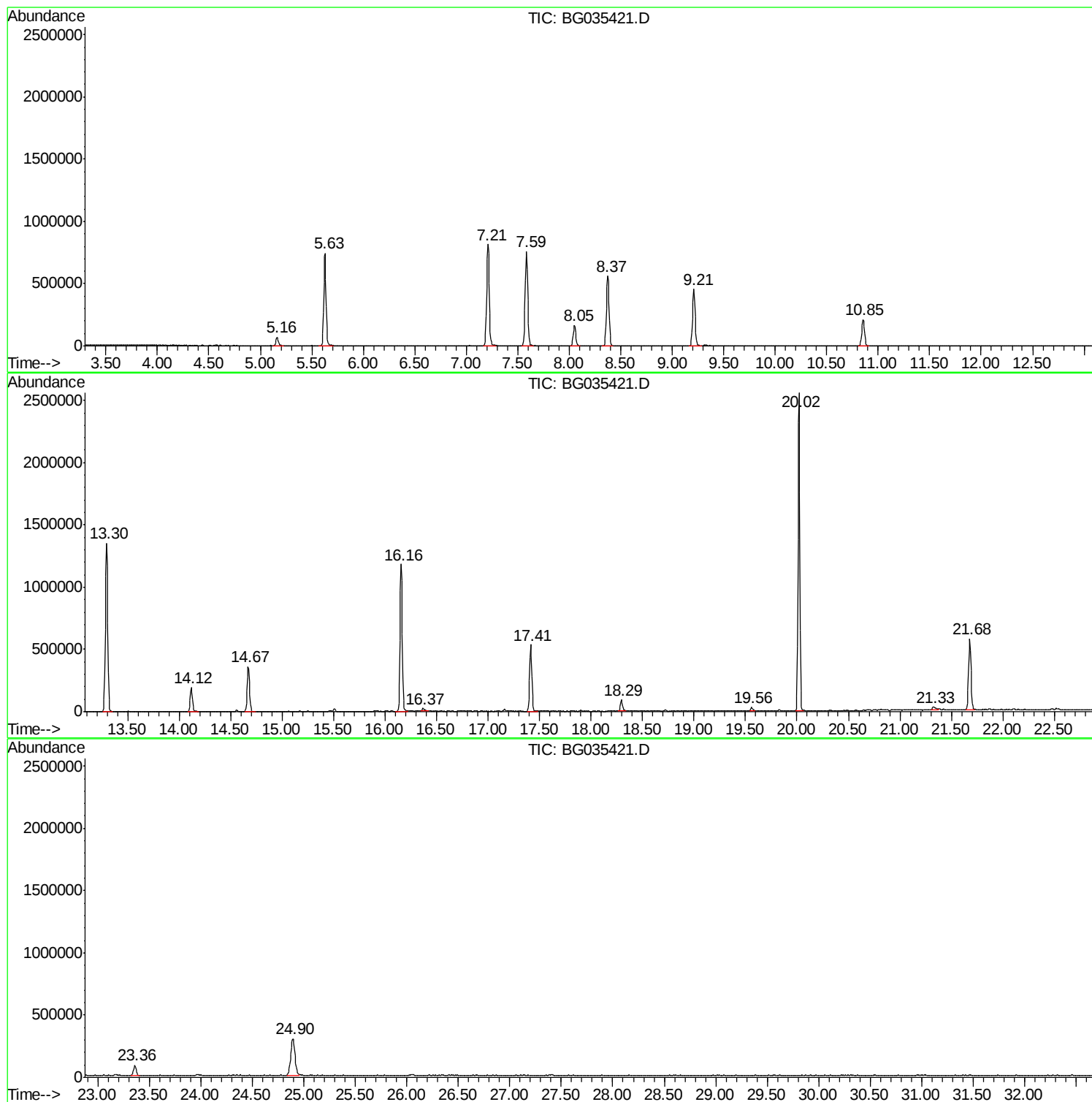
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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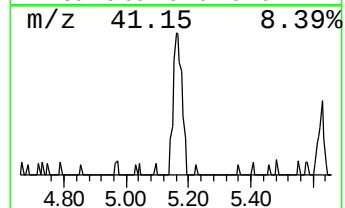
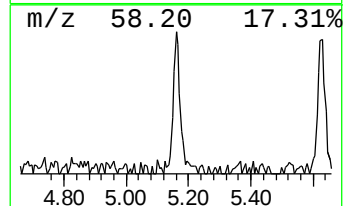
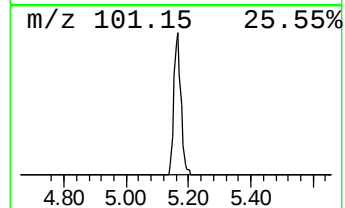
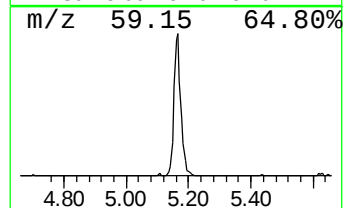
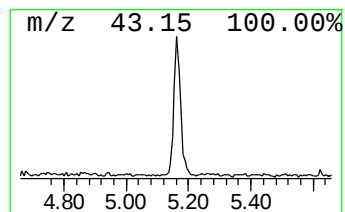
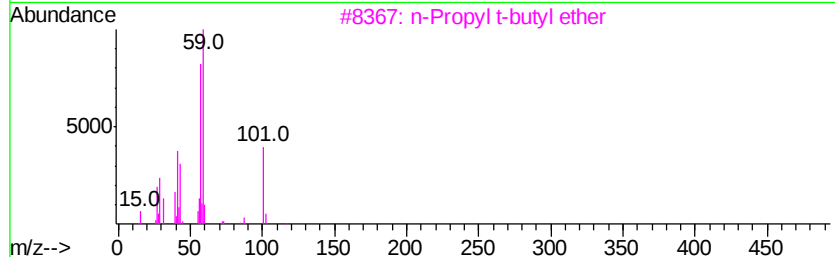
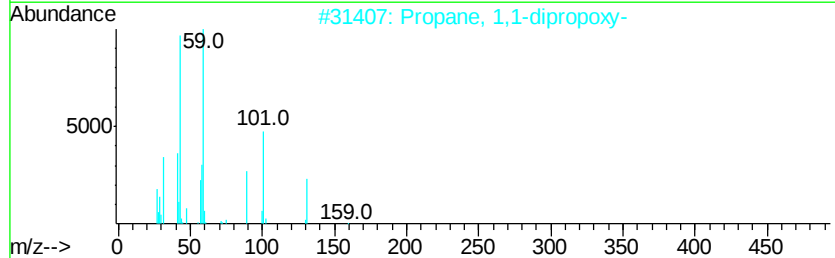
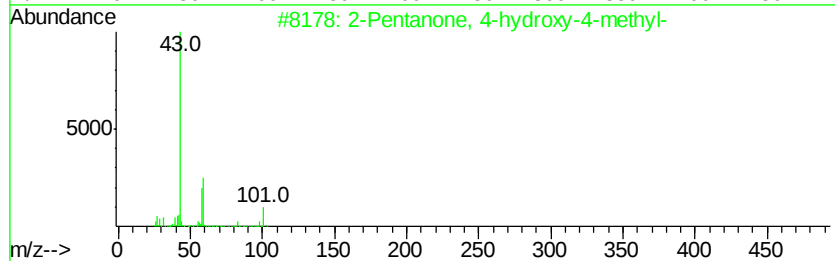
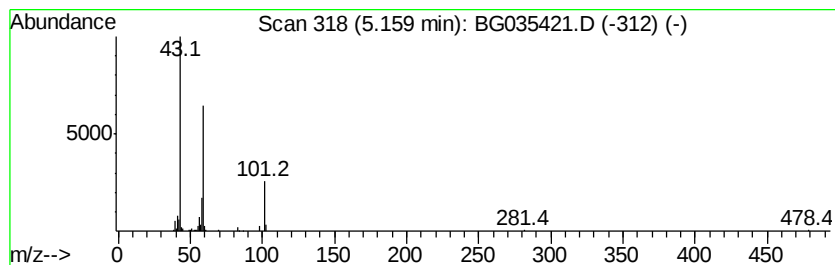
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	7.62 ng	106164	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	39
3			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4			1,2-Butanediol	90	C4H10O2	000584-03-2	32
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32



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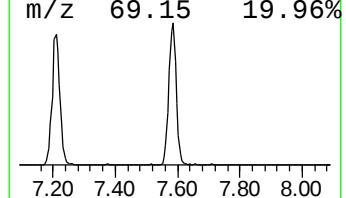
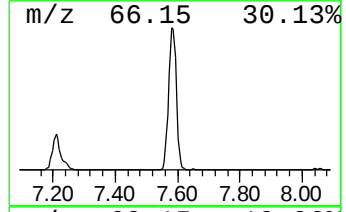
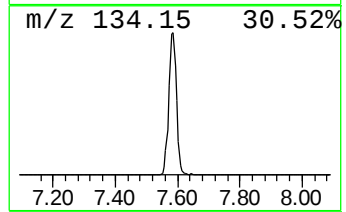
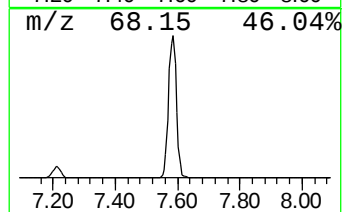
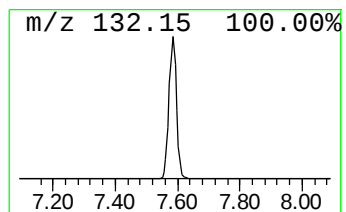
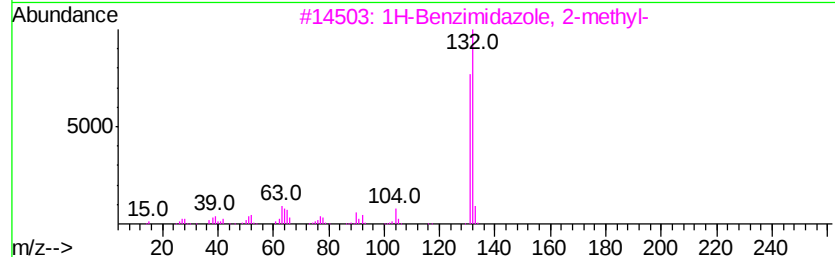
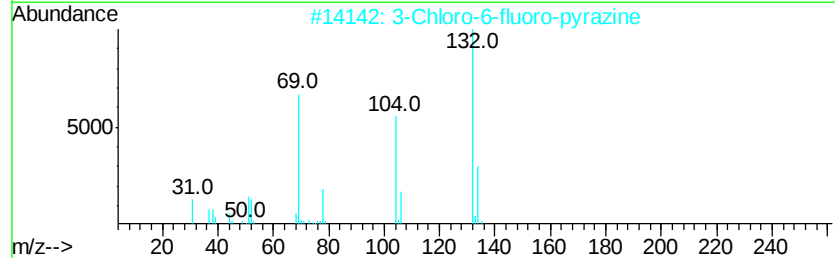
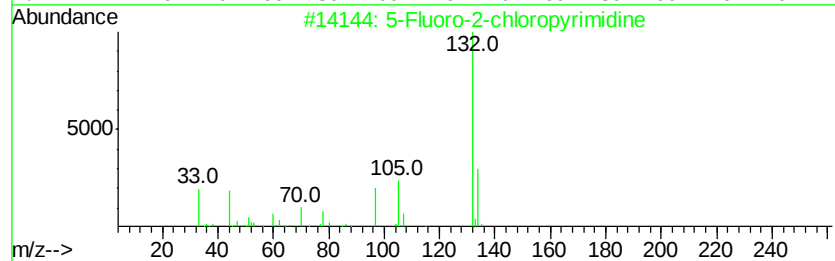
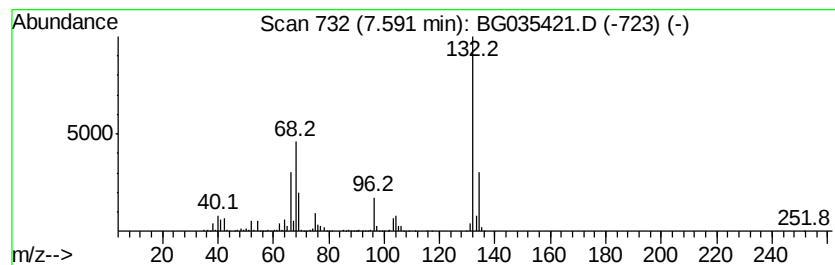
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	93.87 ng	1307450	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10



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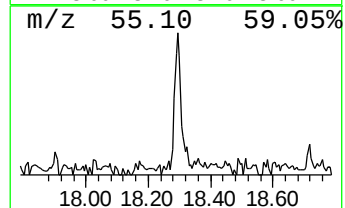
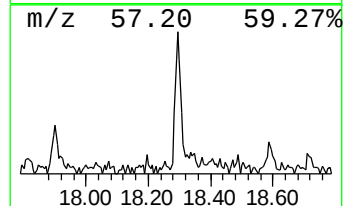
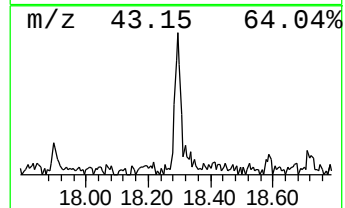
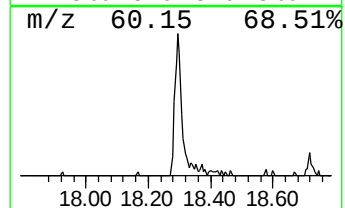
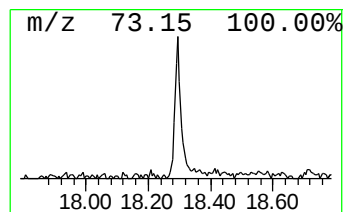
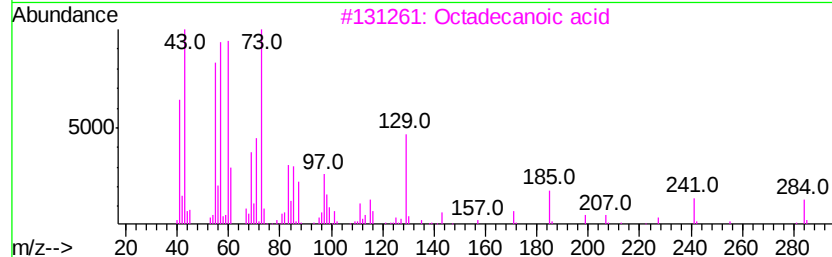
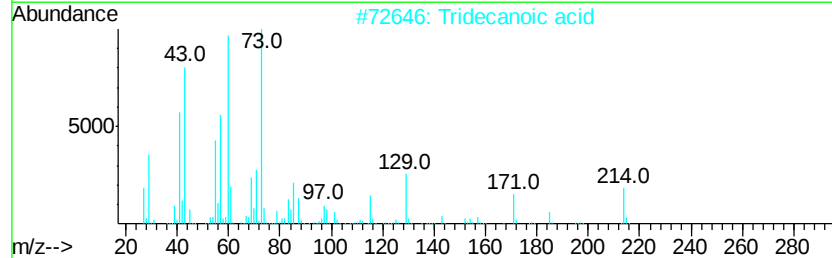
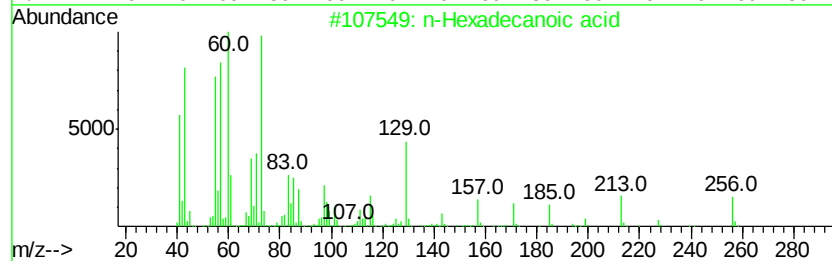
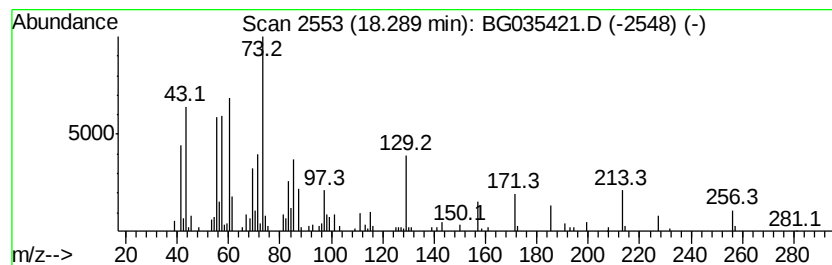
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.29	3.25 ng	131111	Phenanthrene-d10	17.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	64
3	Octadecanoic acid	284	C18H36O2	000057-11-4	53
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5	l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	43



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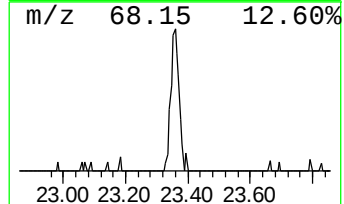
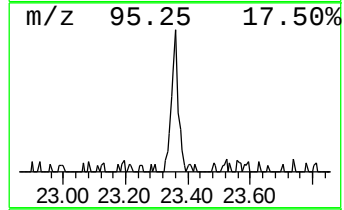
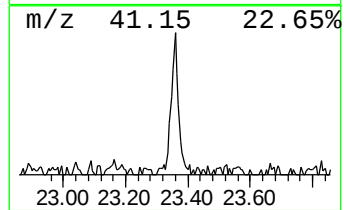
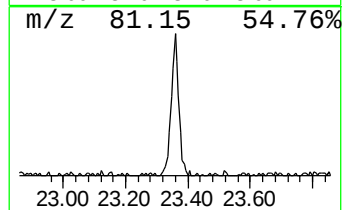
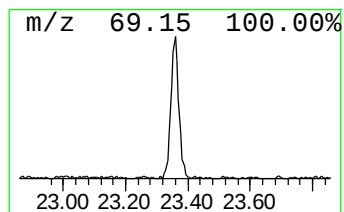
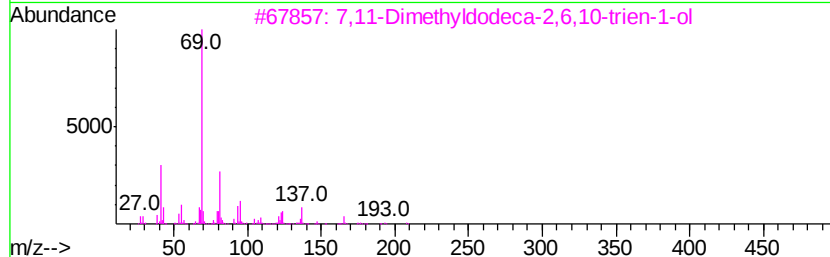
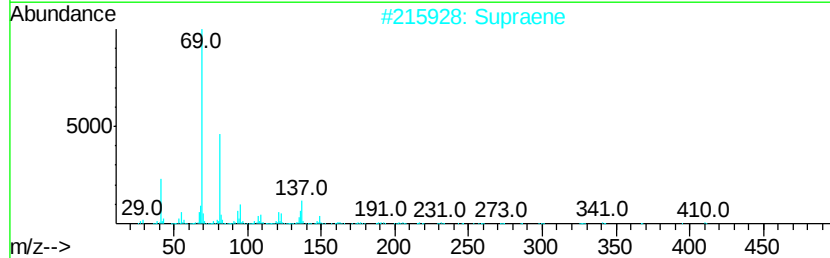
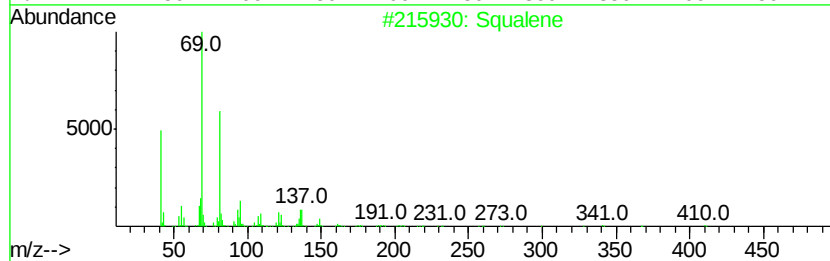
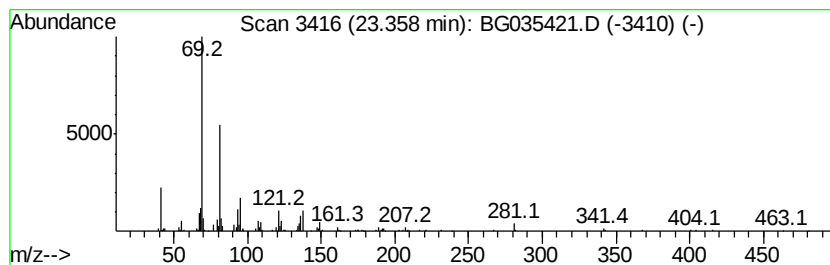
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.36	3.44 ng	145078	Perylene-d12	24.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	83
2		Supraene	410	C30H50	007683-64-9	83
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5		6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.16	7.6	ng	106164	1	8.05	278563	20.0
unknown7.59	7.59	93.9	ng	1307450	1	8.05	278563	20.0
n-Hexadecanoic acid	18.29	3.3	ng	131111	4	17.41	805947	20.0
Squalene	23.36	3.4	ng	145078	6	24.90	842581	20.0