

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091418\
 Data File : BG036705.D
 Acq On : 14 Sep 2018 13:15
 Operator : JU/SJ
 Sample : J4866-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DPT-SB-E1-180911

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-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	5.156	312	318	327	rVB	36853	55434	2.15%	0.300%
2	5.620	389	397	410	rBV	777513	1222194	47.42%	6.623%
3	7.207	659	667	677	rBV	815603	1403215	54.45%	7.605%
4	7.583	723	731	738	rBV	770060	1310248	50.84%	7.101%
5	8.053	804	811	818	rBV	250646	432101	16.77%	2.342%
6	8.376	857	866	874	rBV	581937	999728	38.79%	5.418%
7	9.210	1000	1008	1017	rBV	485252	861089	33.41%	4.667%
8	10.855	1277	1288	1298	rBV	365637	663535	25.75%	3.596%
9	13.300	1695	1704	1710	rBV	1352806	2068533	80.26%	11.210%
10	14.122	1838	1844	1855	rBV	313942	454464	17.63%	2.463%
11	14.674	1931	1938	1947	rVB2	554041	910706	35.34%	4.935%
12	16.161	2184	2191	2204	rBV	940032	1442839	55.99%	7.819%
13	17.418	2398	2405	2412	rBV	700568	1058118	41.06%	5.734%
14	18.300	2551	2555	2562	rBV	90884	150363	5.83%	0.815%
15	19.569	2768	2771	2779	rBV5	27914	56592	2.20%	0.307%
16	20.027	2843	2849	2858	rBV	1879024	2577148	100.00%	13.966%
17	21.572	3107	3112	3117	rVB	192190	274019	10.63%	1.485%
18	21.684	3124	3131	3138	rBV2	641613	1084611	42.09%	5.878%
19	21.872	3161	3163	3168	rVB4	21578	30984	1.20%	0.168%
20	23.153	3375	3381	3383	rBV3	39494	75430	2.93%	0.409%
21	23.364	3412	3417	3426	rVB2	63387	129563	5.03%	0.702%
22	23.969	3516	3520	3532	rVB2	35714	86047	3.34%	0.466%
23	24.892	3666	3677	3692	rBV2	344045	1105450	42.89%	5.991%

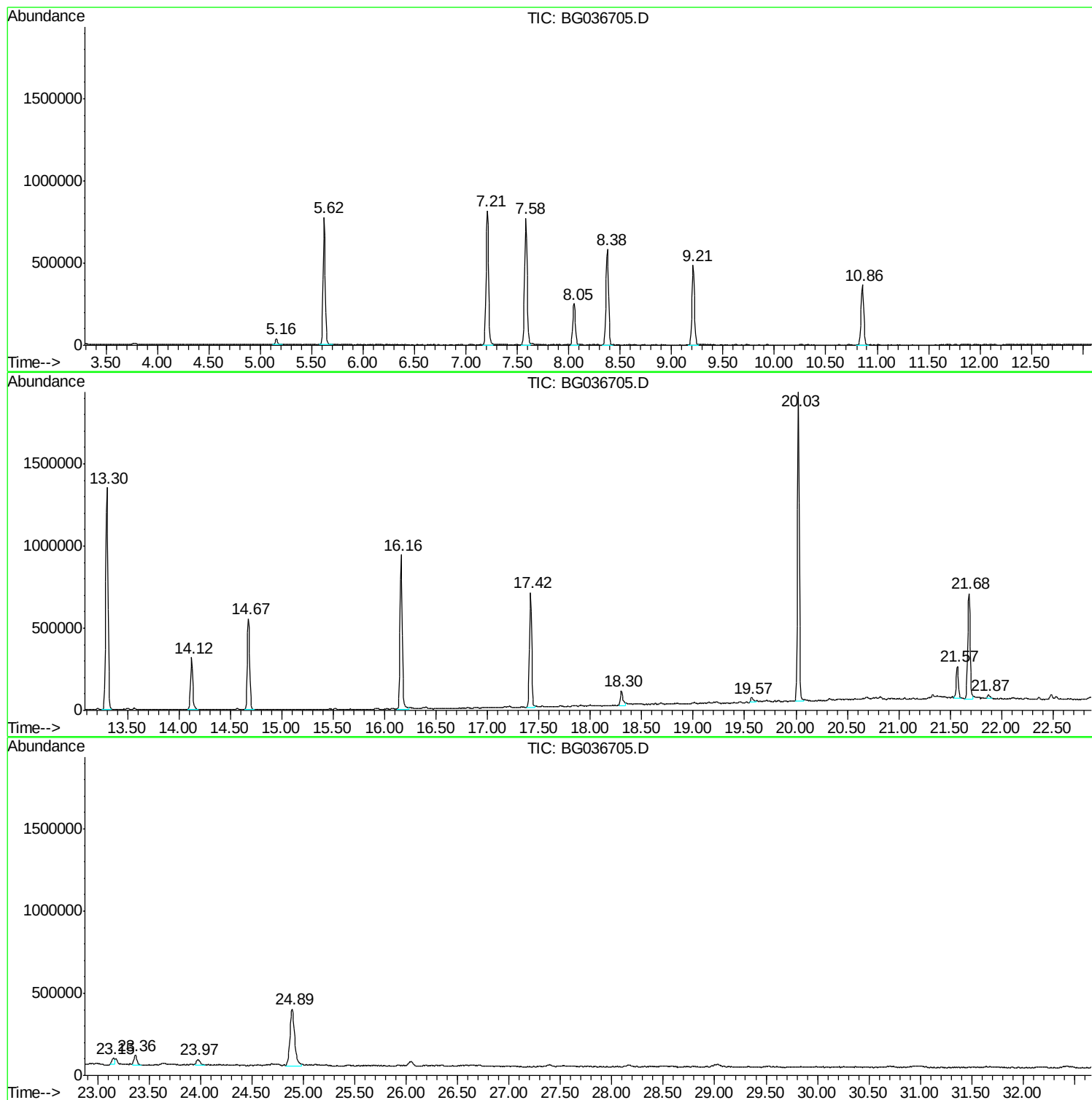
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TIC Library : C:\Database\NIST11.L
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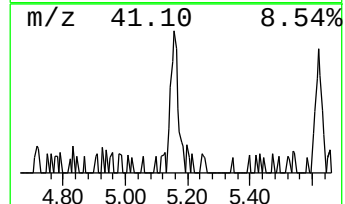
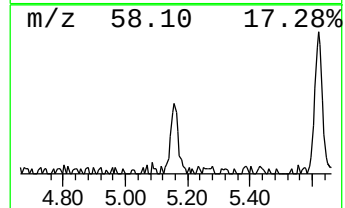
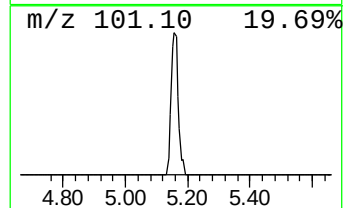
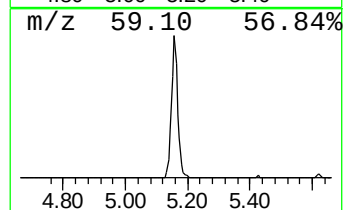
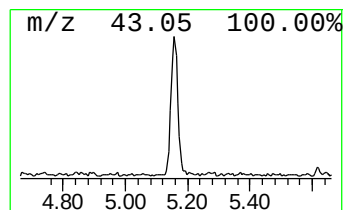
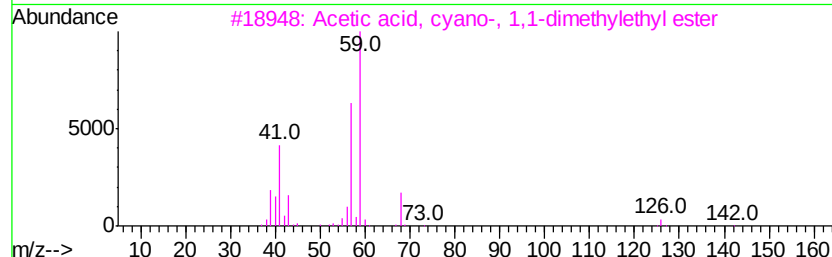
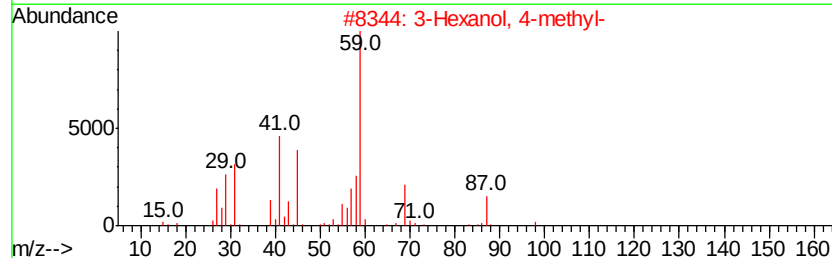
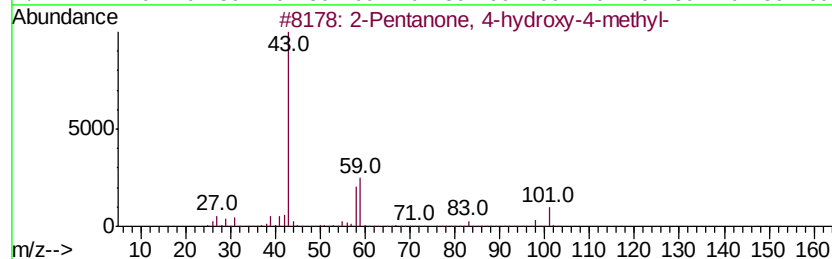
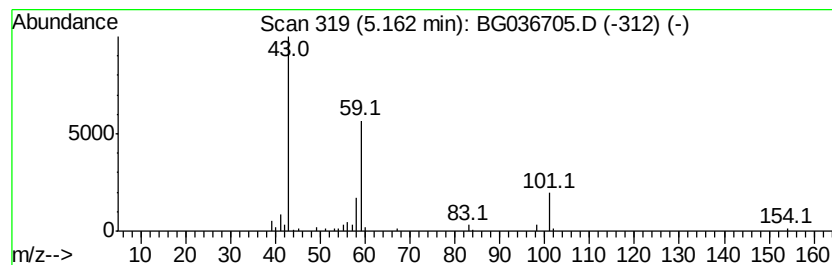
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	2.57 ng	55434	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			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5			Acetone	58	C3H6O	000067-64-1	9



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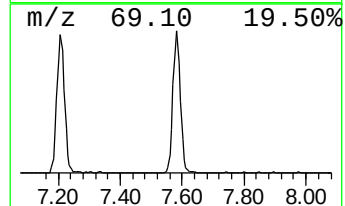
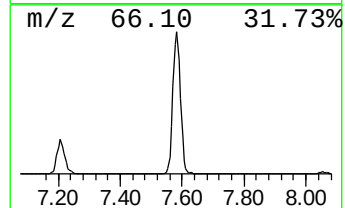
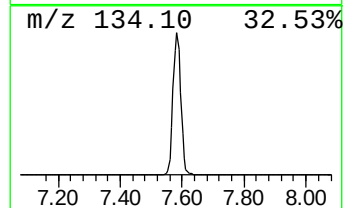
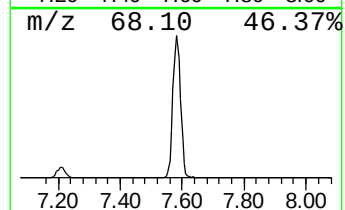
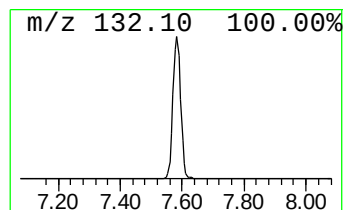
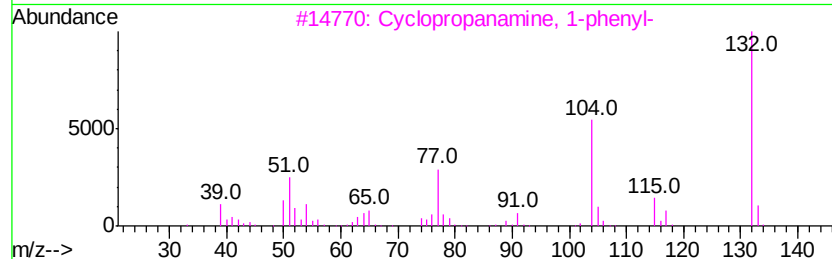
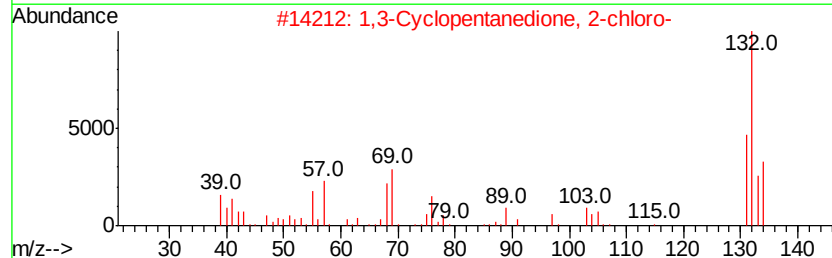
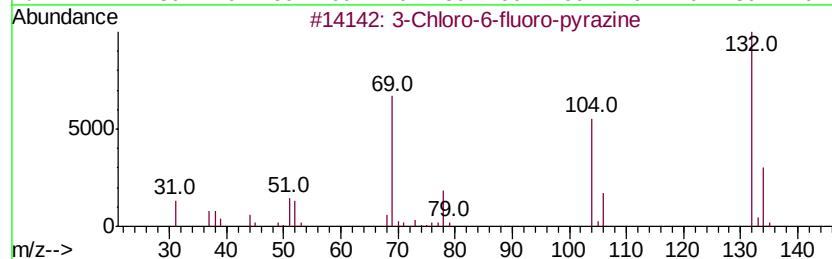
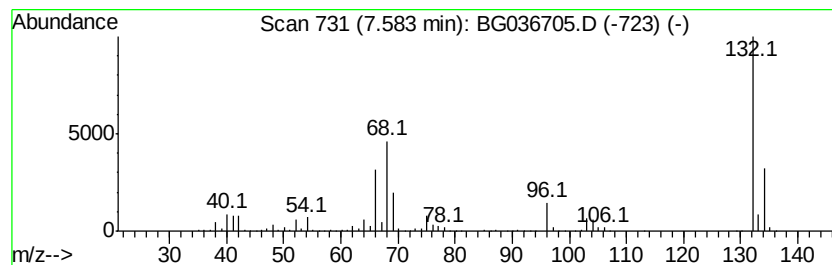
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Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	60.65 ng	1310250	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		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
3		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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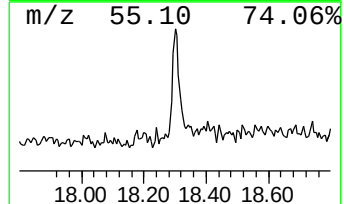
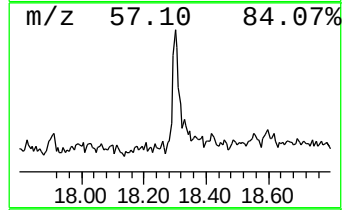
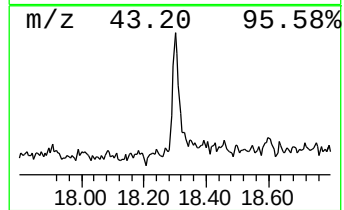
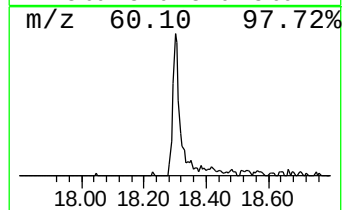
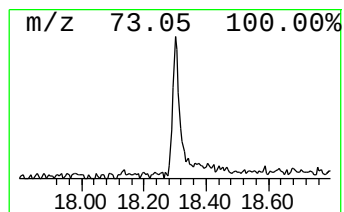
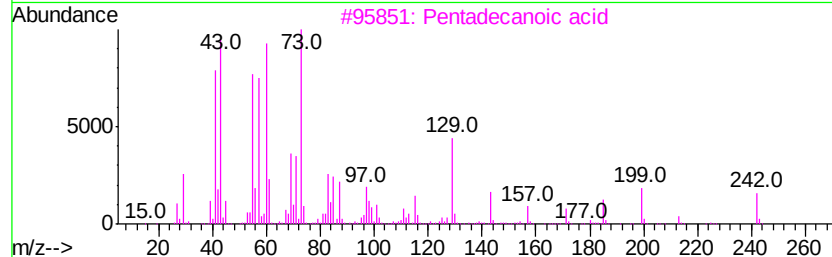
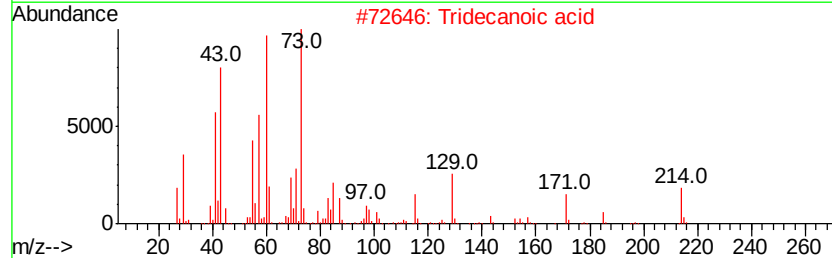
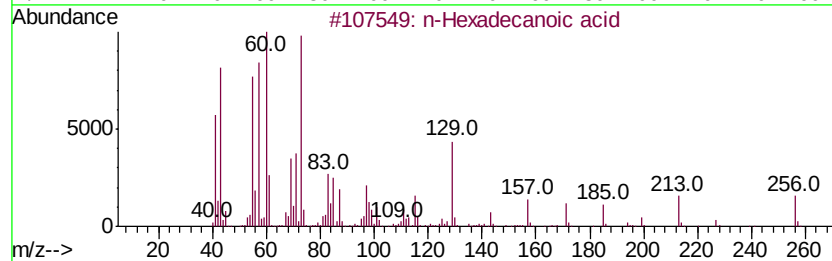
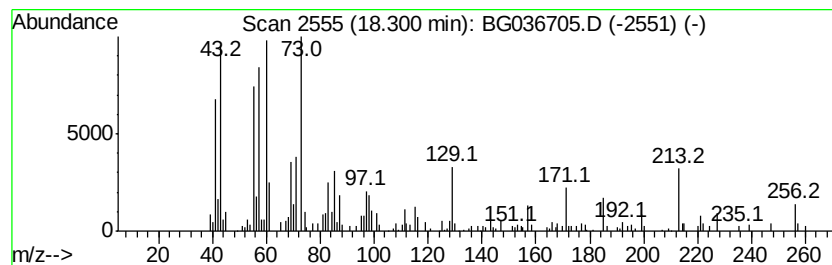
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.30	2.84 ng	150363	Phenanthrene-d10		17.42
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



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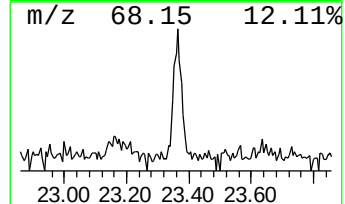
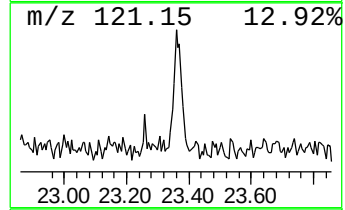
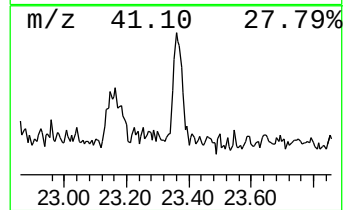
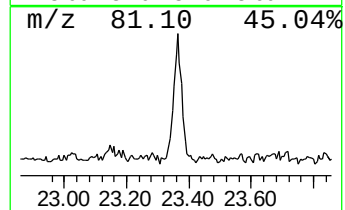
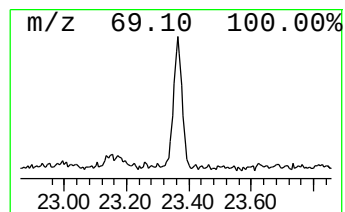
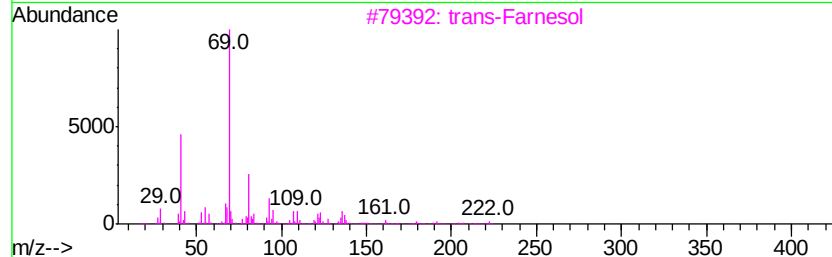
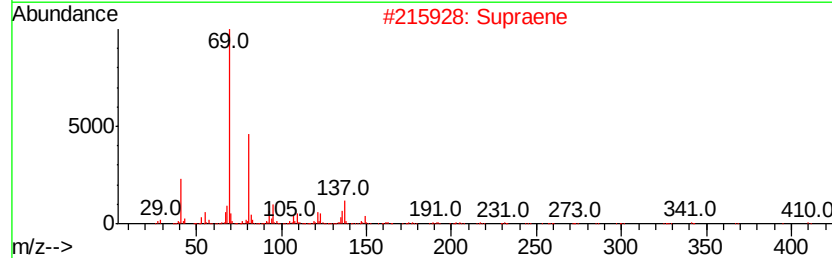
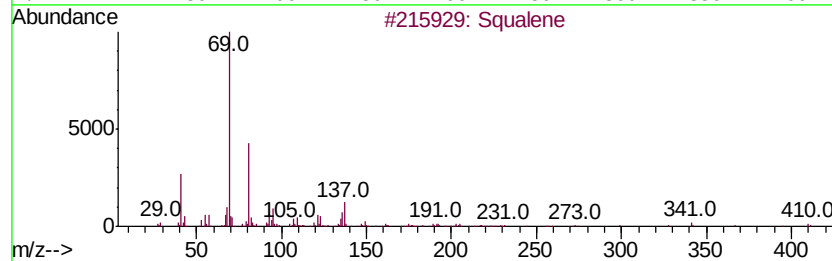
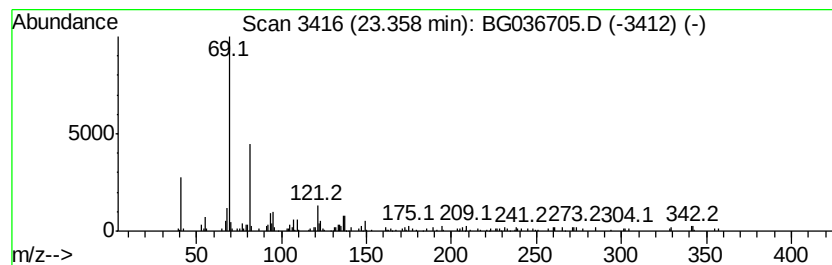
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.36	2.34 ng	129563	Perylene-d12	24.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	86
2		Supraene	410	C30H50	007683-64-9	72
3		trans-Farnesol	222	C15H26O	000106-28-5	70
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.16	2.6	ng	55434	1	8.05	432101	20.0
unknown7.58	7.58	60.6	ng	1310250	1	8.05	432101	20.0
n-Hexadecanoic acid	18.30	2.8	ng	150363	4	17.42	1058120	20.0
Squalene	23.36	2.3	ng	129563	6	24.89	1105450	20.0