

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071516\
 Data File : BG023120.D
 Acq On : 15 Jul 2016 19:30
 Operator : UM/SJ
 Sample : H4018-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 D8-B3(6-12)C

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:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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	3.039	29	34	54	rBV	6445665	9936395	100.00%	15.709%
2	5.219	399	405	412	rBV2	288464	453539	4.56%	0.717%
3	5.701	480	487	499	rBV	2249699	3701908	37.26%	5.853%
4	7.311	753	761	770	rBV	2567464	4498680	45.27%	7.112%
5	7.681	814	824	833	rBV	2401090	4169626	41.96%	6.592%
6	8.151	898	904	911	rBV	392373	664807	6.69%	1.051%
7	8.480	952	960	967	rBV	1622459	2900564	29.19%	4.586%
8	9.326	1094	1104	1112	rBV	1617535	2919554	29.38%	4.616%
9	10.977	1378	1385	1393	rBV	557679	1054476	10.61%	1.667%
10	13.416	1793	1800	1819	rBV	4178451	6708577	67.52%	10.606%
11	14.238	1932	1940	1946	rBV	597219	896050	9.02%	1.417%
12	14.802	2028	2036	2043	rBV2	993977	1716848	17.28%	2.714%
13	16.289	2282	2289	2303	rBV	3936657	6327939	63.68%	10.004%
14	16.483	2318	2322	2329	rVB3	66221	115334	1.16%	0.182%
15	17.552	2497	2504	2512	rBV2	1364250	2144833	21.59%	3.391%
16	18.416	2646	2651	2661	rBV3	196927	291332	2.93%	0.461%
17	19.685	2861	2867	2873	rBV3	98439	156096	1.57%	0.247%
18	20.155	2941	2947	2953	rBV	6999850	9511539	95.72%	15.038%
19	21.477	3167	3172	3178	rBV10	82174	218192	2.20%	0.345%
20	21.853	3229	3236	3252	rBV2	1483275	2573285	25.90%	4.068%
21	23.580	3525	3530	3536	rVB2	107278	216629	2.18%	0.342%
22	25.231	3801	3811	3823	rBV2	673806	2075167	20.88%	3.281%

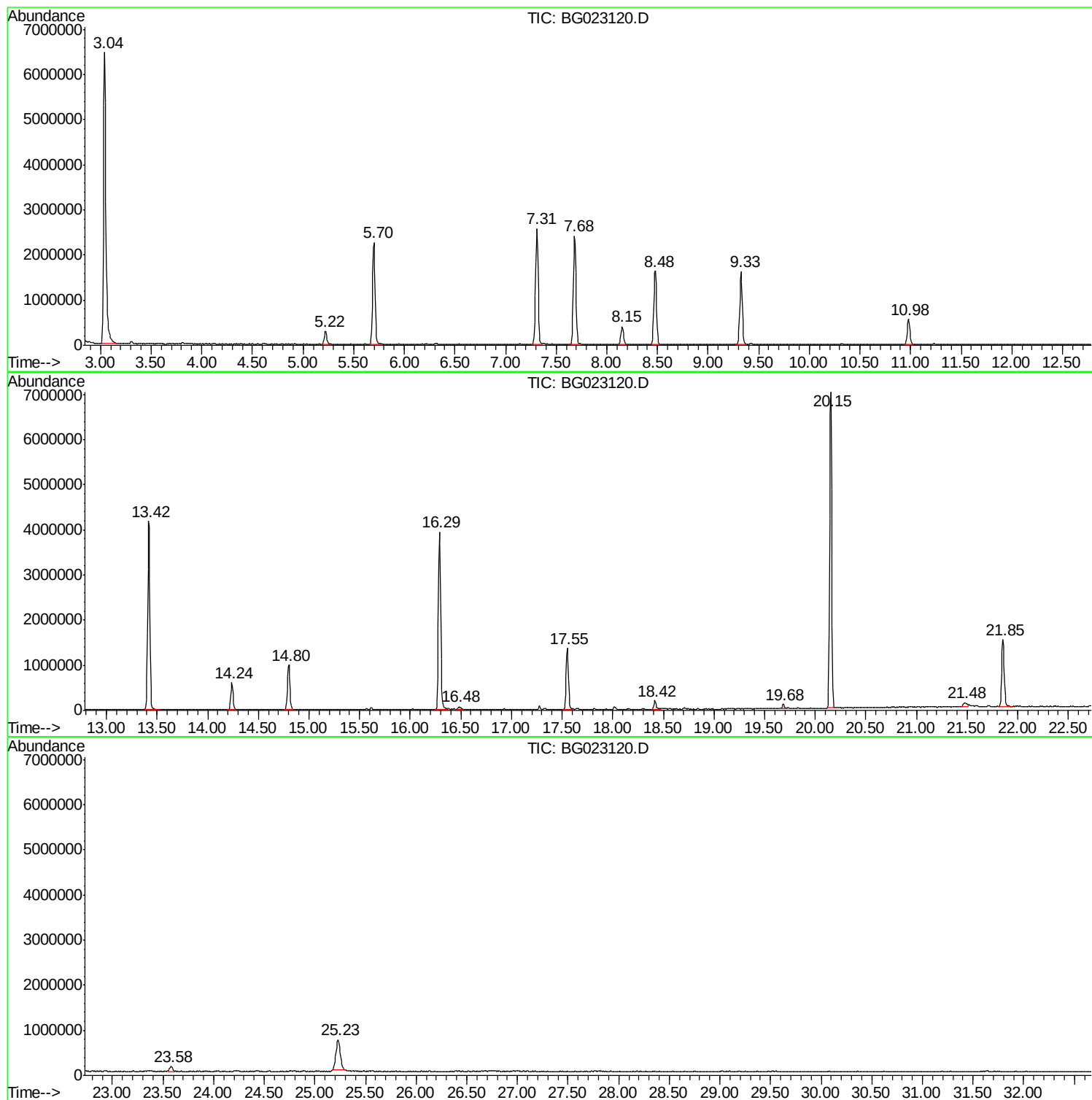
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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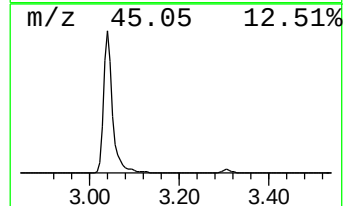
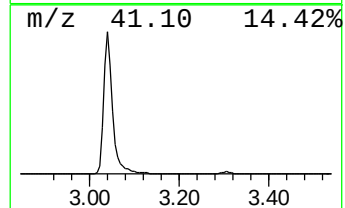
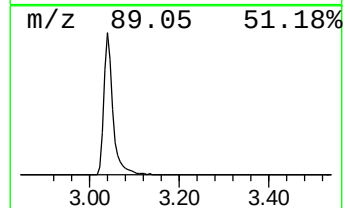
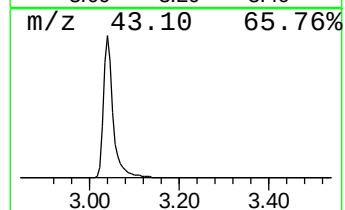
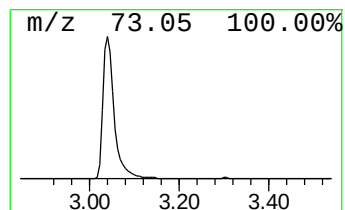
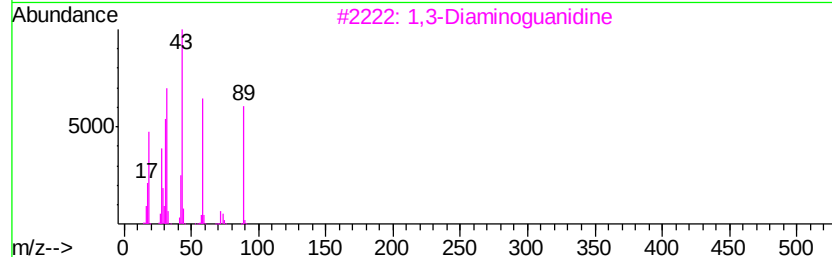
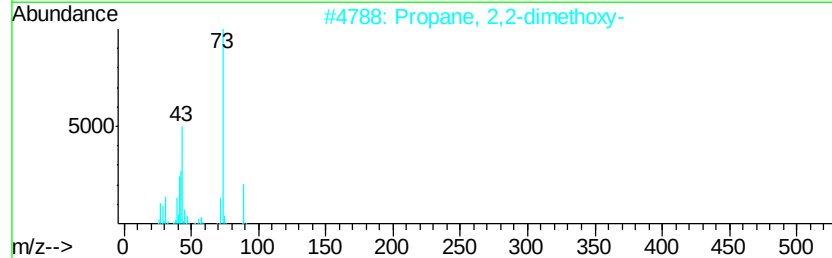
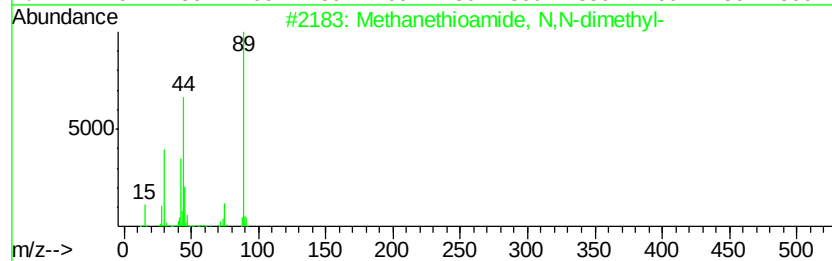
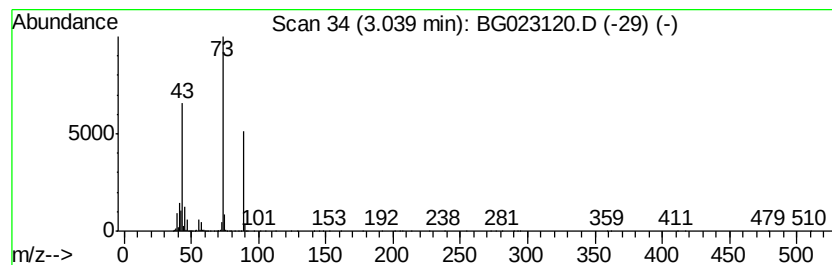
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	298.93 ng	9936400	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	47
2		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
3		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9



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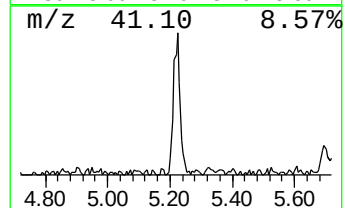
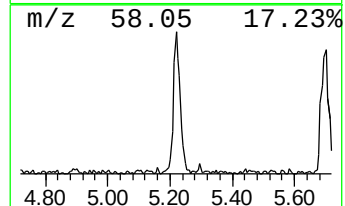
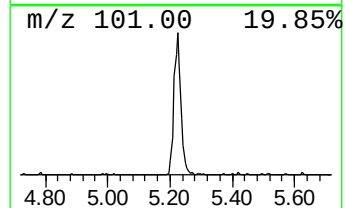
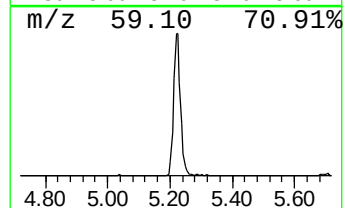
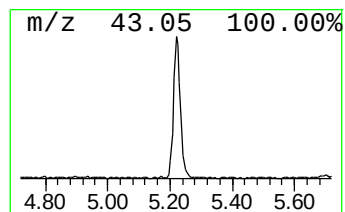
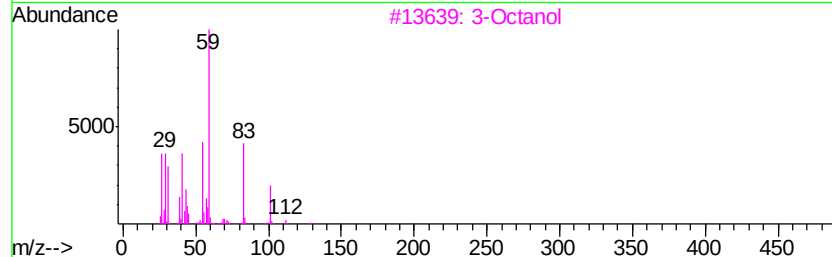
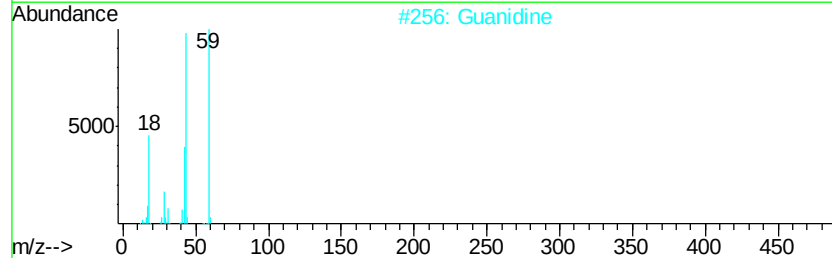
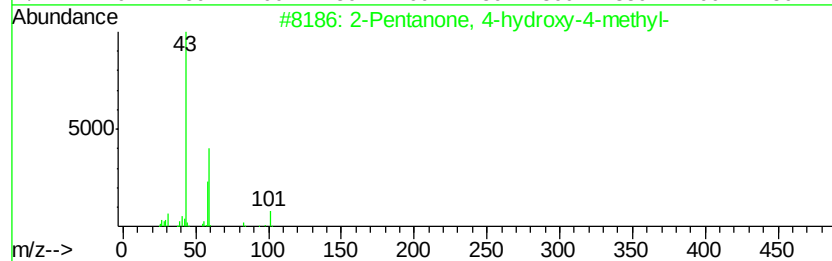
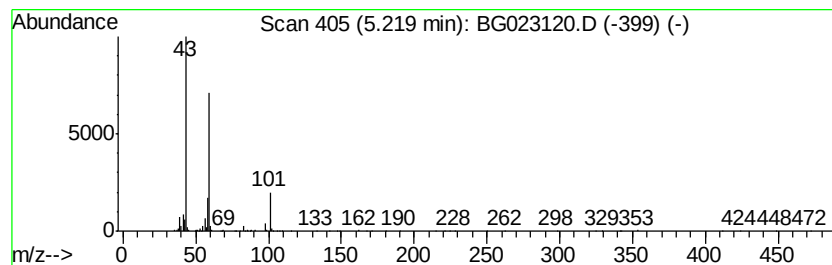
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	13.64 ng	453539	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Guanidine	59	CH5N3	000113-00-8	43
3		3-Octanol	130	C8H18O	000589-98-0	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Dimethadione	129	C5H7NO3	000695-53-4	33



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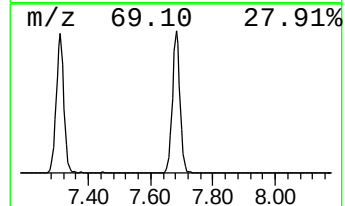
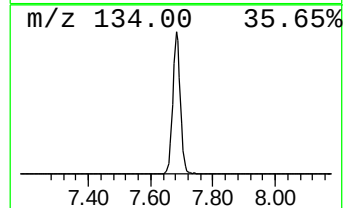
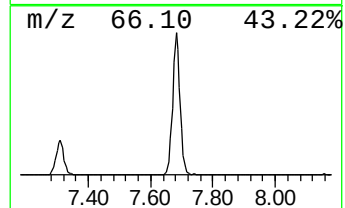
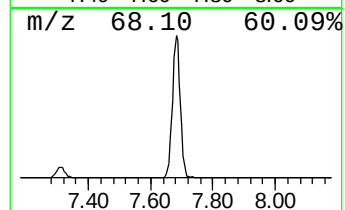
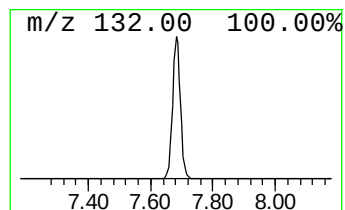
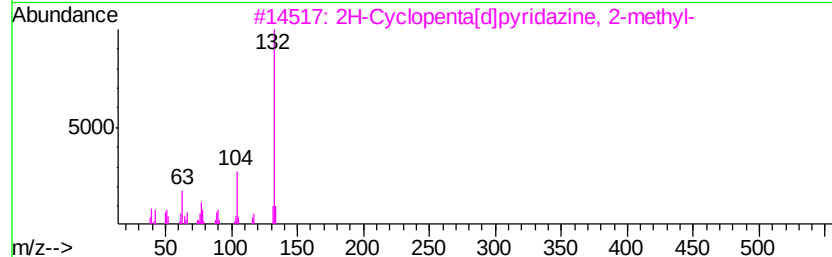
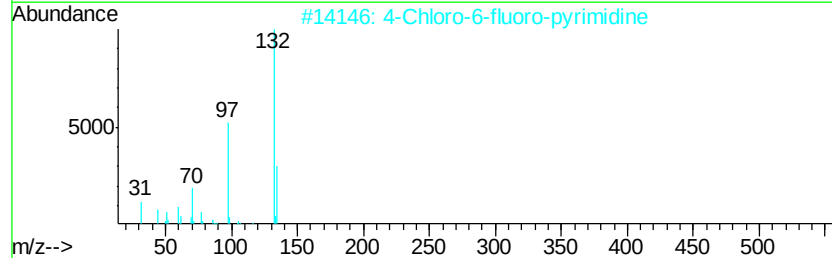
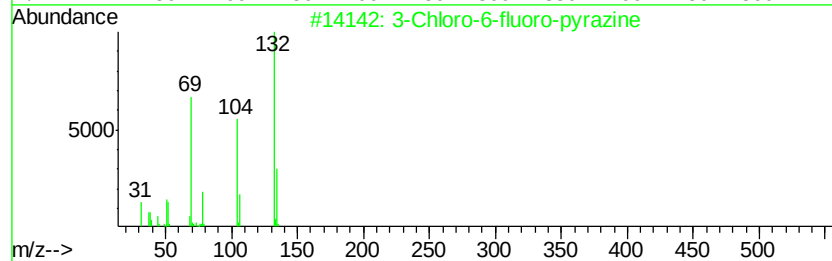
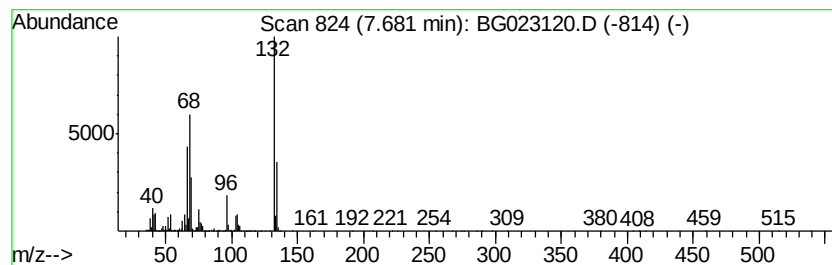
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Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	125.44 ng	4169630	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	18
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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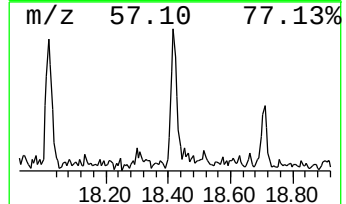
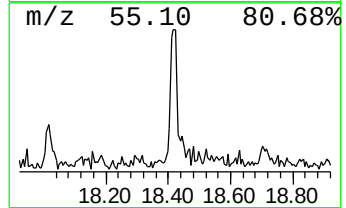
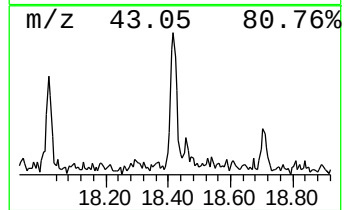
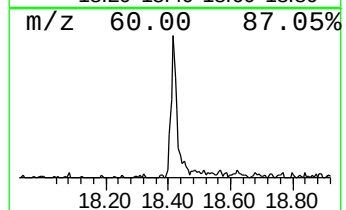
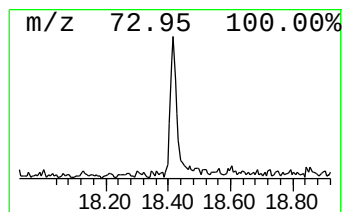
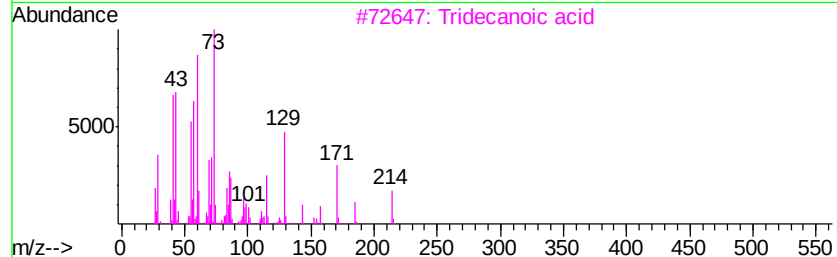
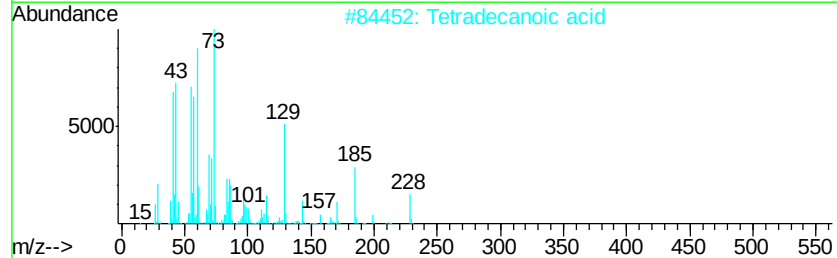
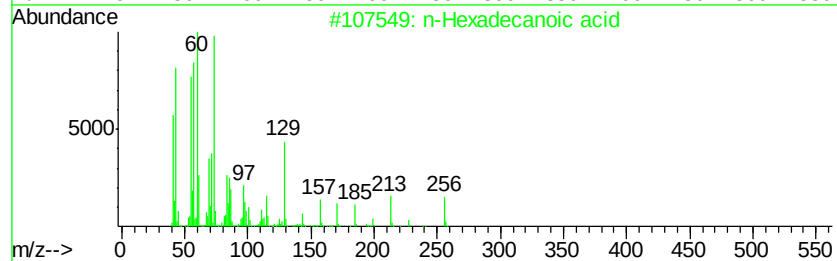
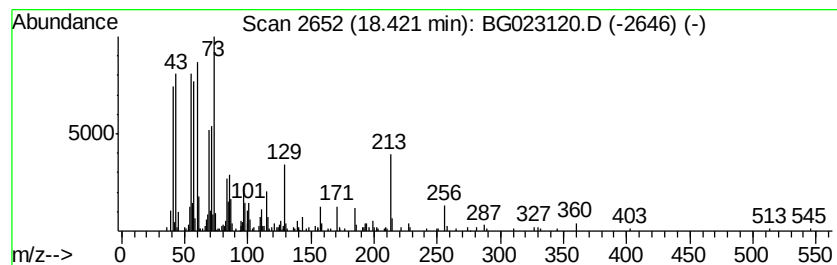
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.42	2.72 ng	291332	Phenanthrene-d10		17.55
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59



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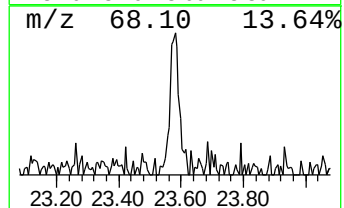
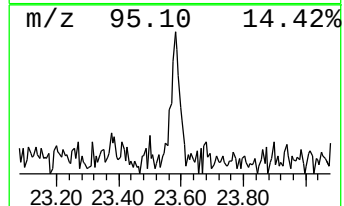
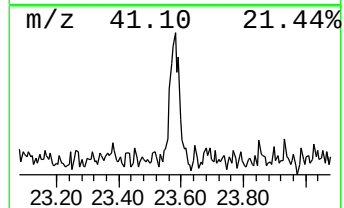
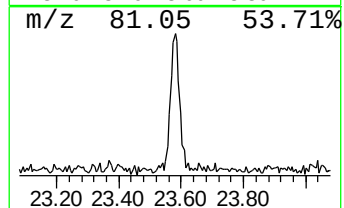
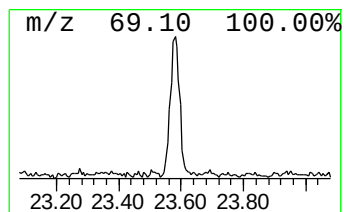
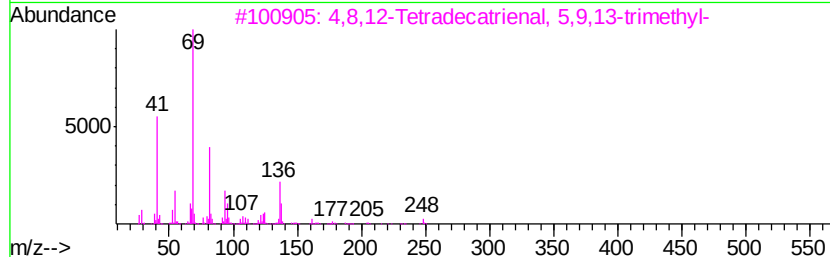
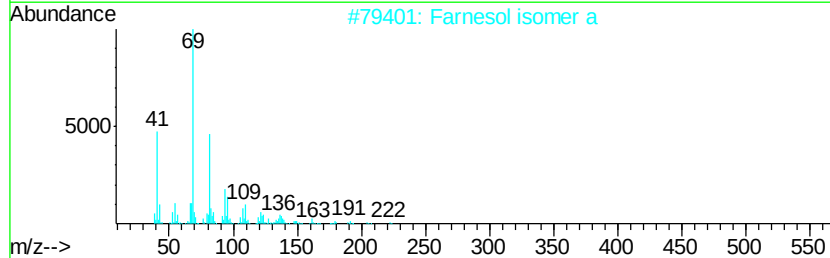
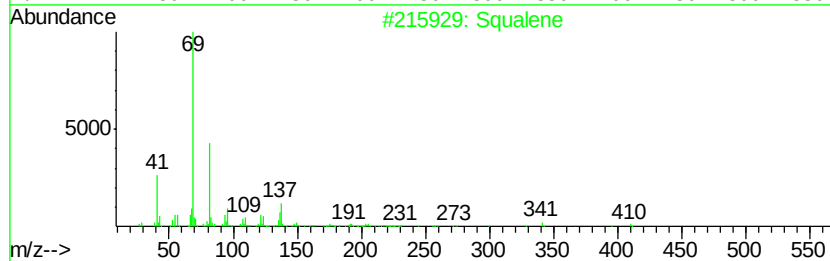
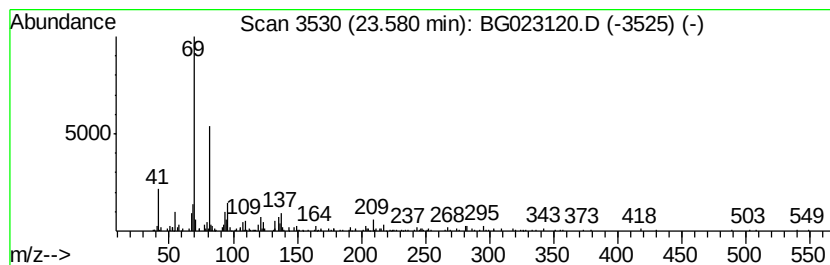
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Peak Number 6 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.58	2.09 ng	216629	Perylene-d12	25.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	000111-02-4	72
2	Farnesol isomer a	222 C15H26O	1000108-92-4	72
3	4,8,12-Tetradecatrienal, 5,9,13-...	248 C17H28O	066408-55-7	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	72
5	Supraene	410 C30H50	007683-64-9	64



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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2-Pentanone, 4-hy...	5.22	13.6	ng	453539	1	8.15	664807	20.0
unknown7.68	7.68	125.4	ng	4169630	1	8.15	664807	20.0
n-Hexadecanoic acid	18.42	2.7	ng	291332	4	17.55	2144830	20.0
Squalene	23.58	2.1	ng	216629	6	25.23	2075170	20.0