

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071216\
 Data File : BG023047.D
 Acq On : 12 Jul 2016 22:06
 Operator : UM/SJ
 Sample : H3975-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LOCATION-22A-9-11

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	49	rVB	2046867	2860694	30.46%	5.293%
2	5.224	400	406	415	rBV	359520	593934	6.32%	1.099%
3	5.694	480	486	499	rBV	1850372	3073544	32.73%	5.687%
4	7.304	752	760	772	rBV	2195322	3954624	42.11%	7.317%
5	7.680	816	824	836	rBV	2035012	3553296	37.83%	6.575%
6	8.156	898	905	911	rBV	391064	702868	7.48%	1.301%
7	8.479	949	960	967	rBV	1468999	2549358	27.14%	4.717%
8	9.326	1096	1104	1114	rVB	1441640	2573524	27.40%	4.762%
9	10.982	1378	1386	1394	rVB	650844	1169018	12.45%	2.163%
10	13.421	1793	1801	1810	rBV	3985365	6457171	68.75%	11.948%
11	14.237	1932	1940	1947	rBV	766162	1140329	12.14%	2.110%
12	14.801	2030	2036	2044	rBV2	1142026	1918583	20.43%	3.550%
13	16.294	2284	2290	2302	rBV	3748542	5745695	61.18%	10.632%
14	16.488	2319	2323	2333	rBV2	82112	137129	1.46%	0.254%
15	17.287	2454	2459	2462	rBV	75176	99199	1.06%	0.184%
16	17.557	2499	2505	2519	rBV2	1468000	2334251	24.85%	4.319%
17	18.427	2646	2653	2660	rBV2	188564	262633	2.80%	0.486%
18	20.160	2942	2948	2954	rBV	7021336	9391943	100.00%	17.378%
19	21.476	3167	3172	3180	rBV4	148920	358877	3.82%	0.664%
20	21.864	3231	3238	3246	rVB	1554635	2719489	28.96%	5.032%
21	25.248	3805	3814	3827	rVB3	822612	2447893	26.06%	4.529%

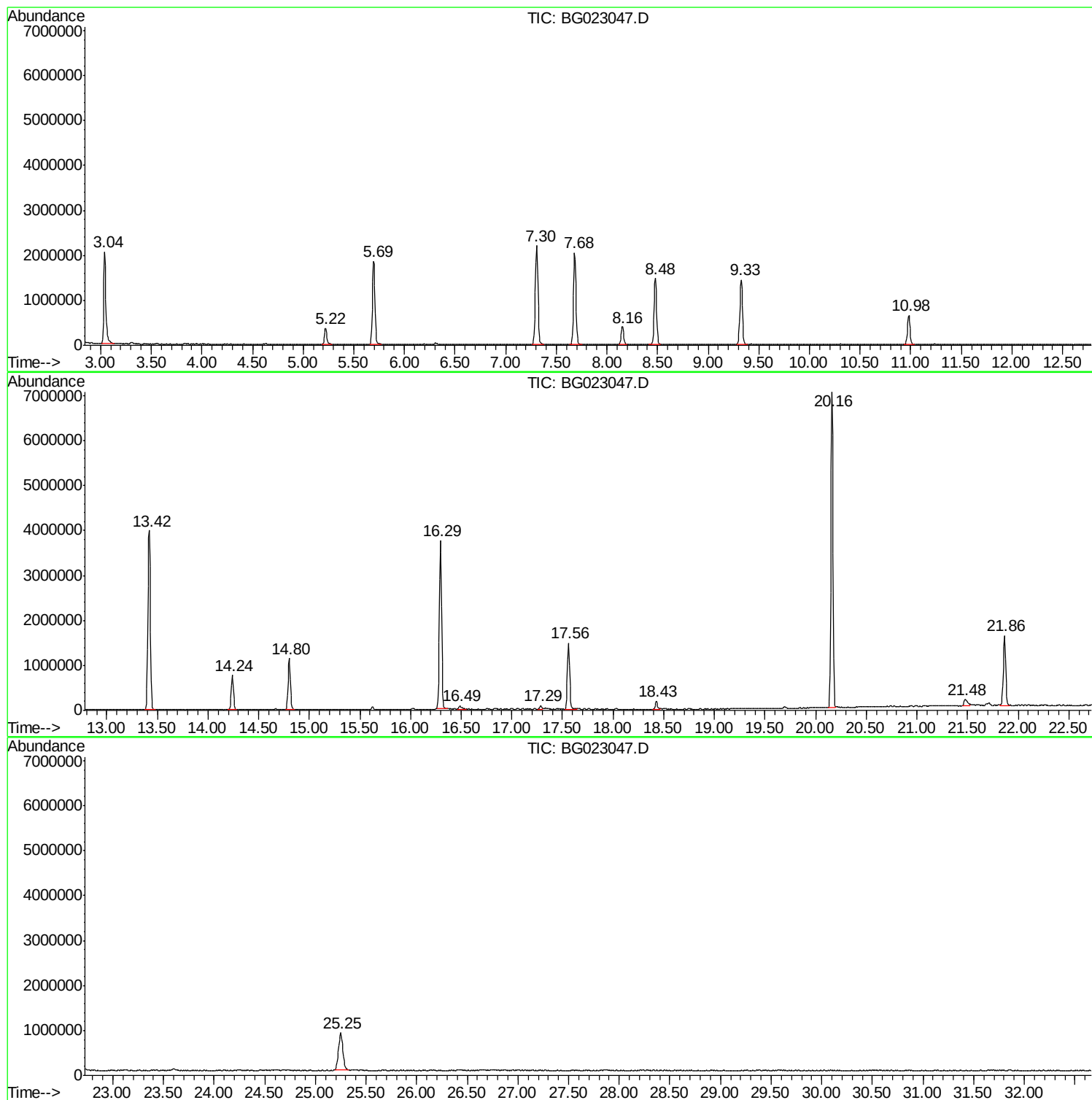
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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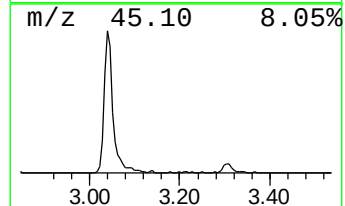
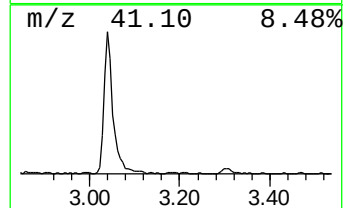
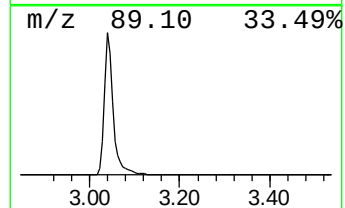
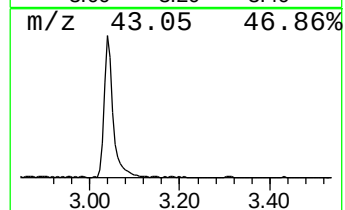
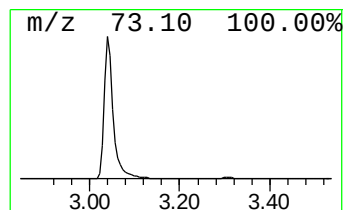
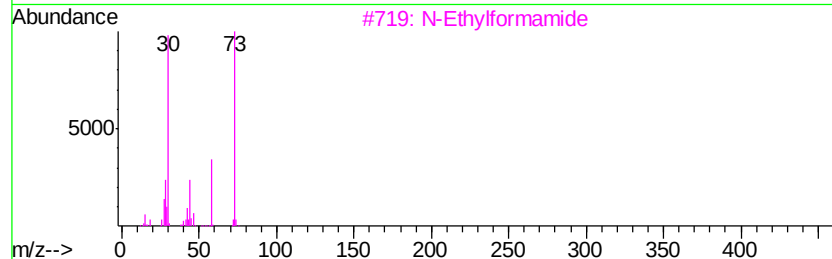
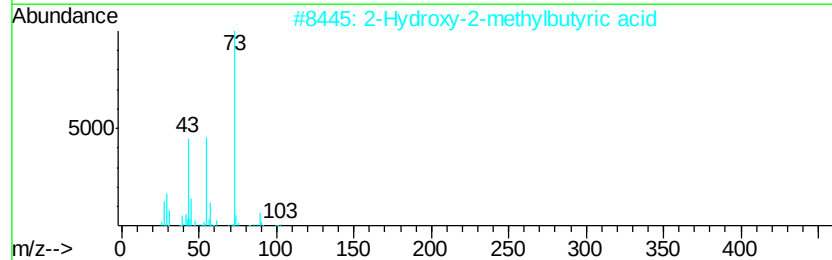
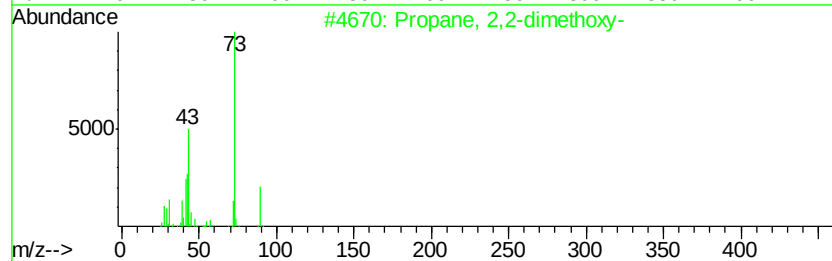
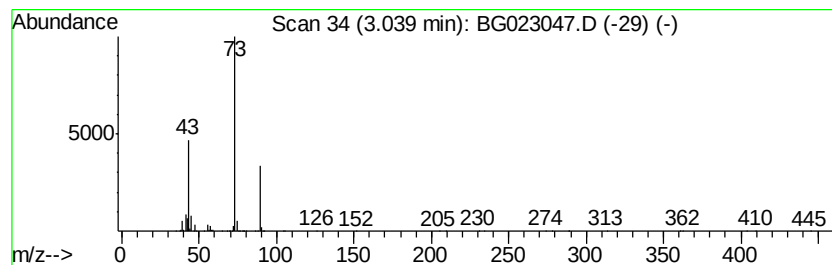
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.04	81.40 ng	2860690	1,4-Dichlorobenzene-d4	8.16	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	28
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5	1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9



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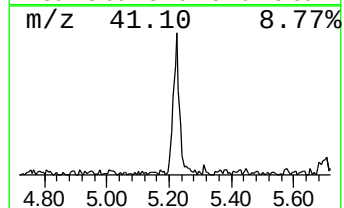
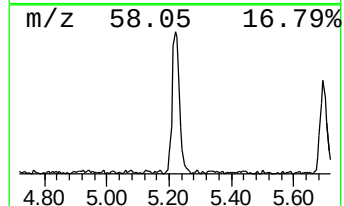
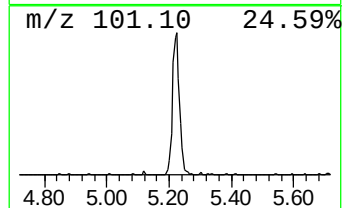
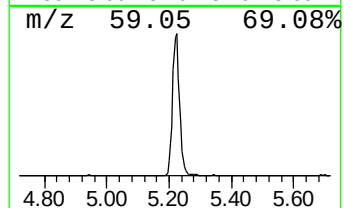
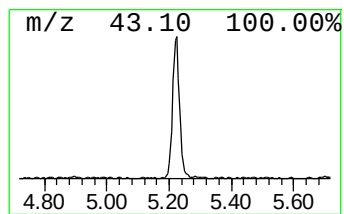
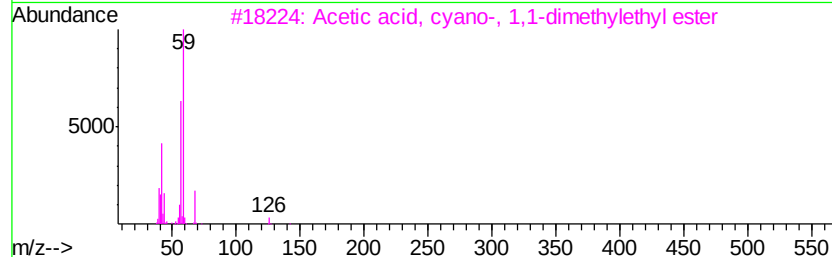
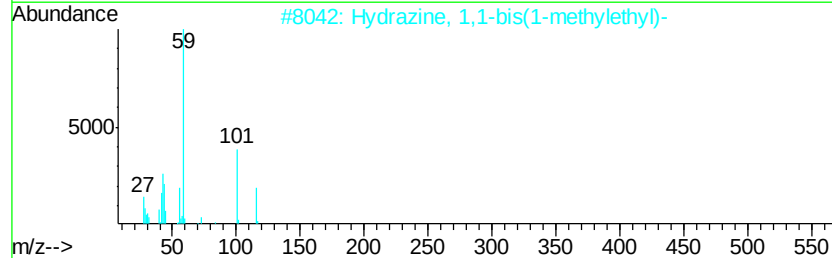
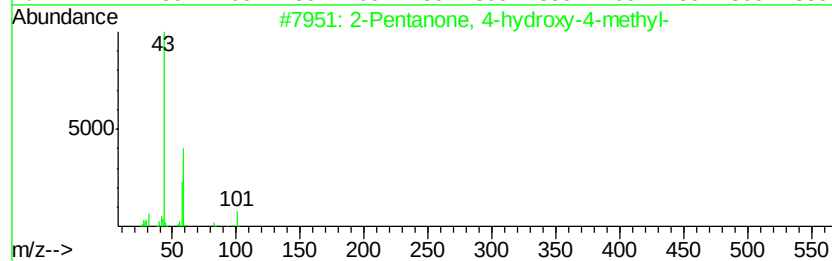
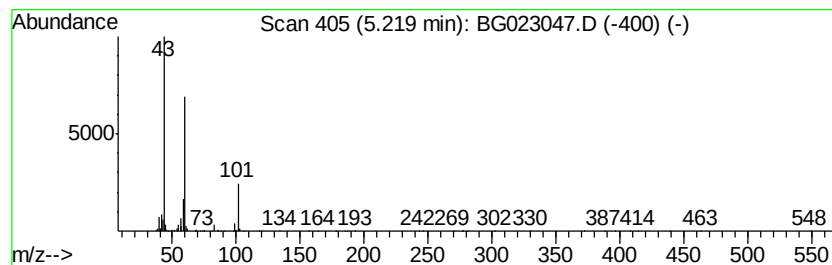
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	16.90 ng	593934	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	32
4		Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	25
5		Acetic acid, chloro-, 1,1-dimeth...	150	C6H11ClO2	000107-59-5	23



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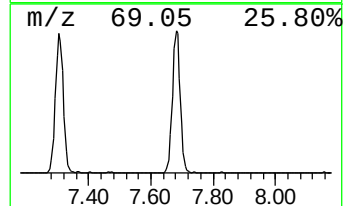
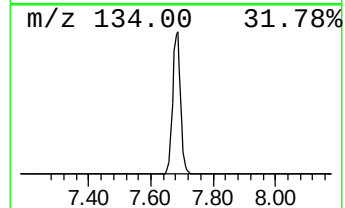
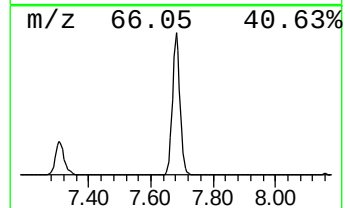
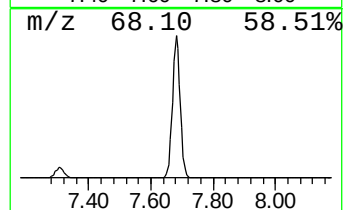
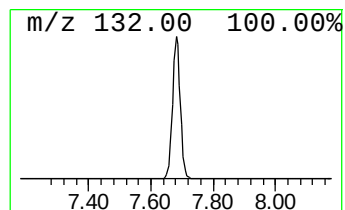
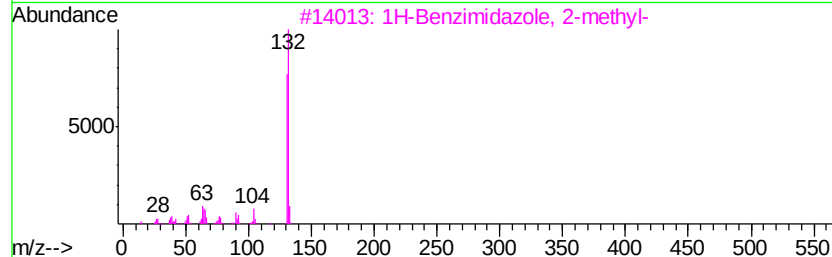
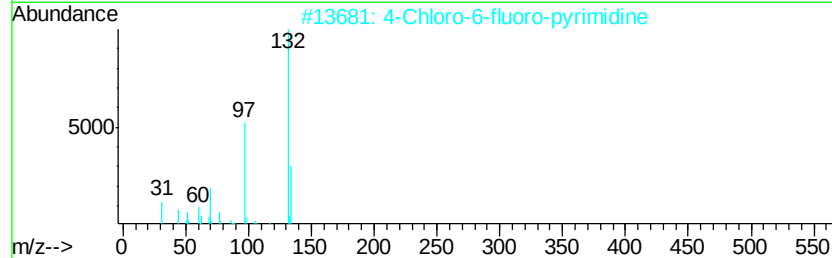
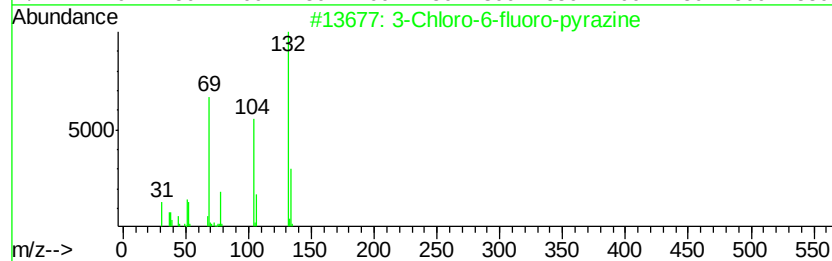
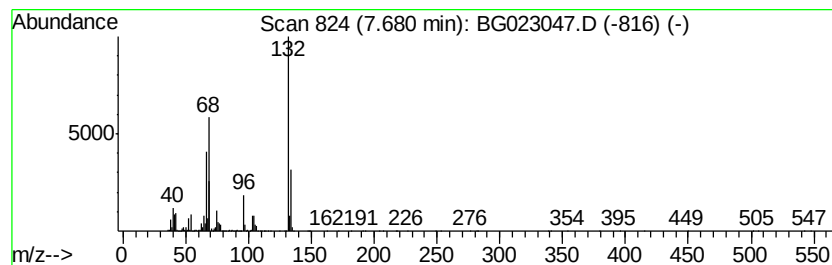
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Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	101.11 ng	3553300	1,4-Dichlorobenzene-d4	8.16

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		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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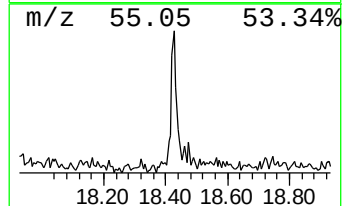
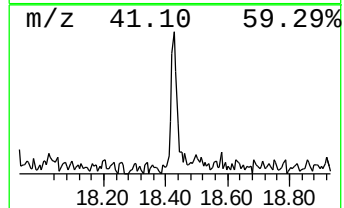
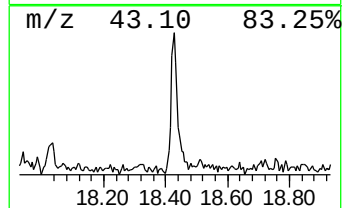
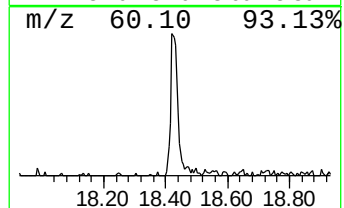
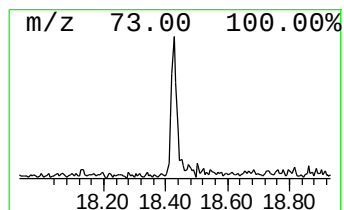
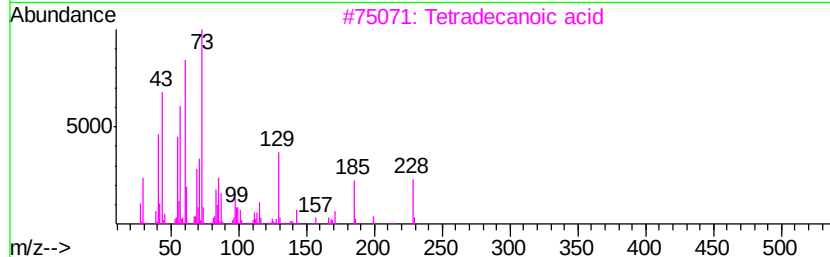
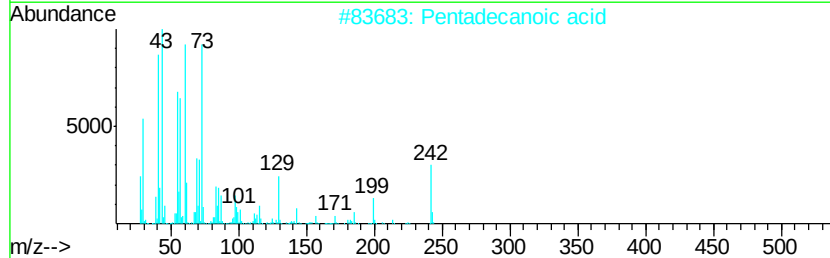
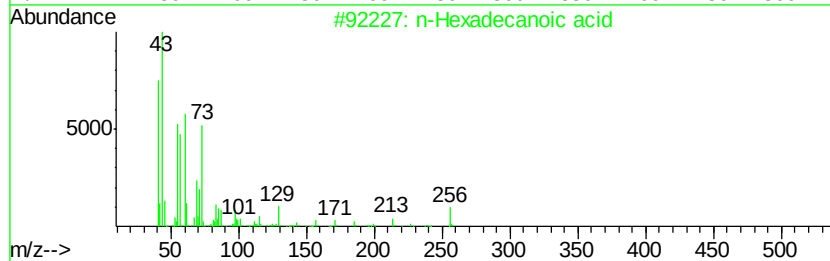
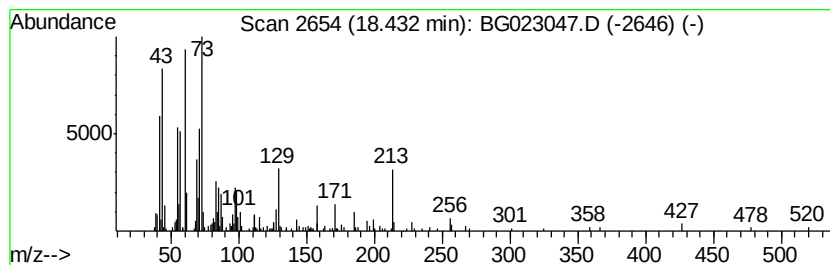
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	2.25 ng	262633	Phenanthrene-d10	17.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	50
5		Tridecanoic acid	214	C13H26O2	000638-53-9	49



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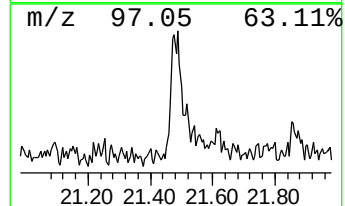
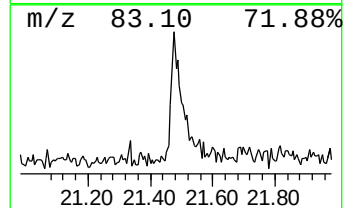
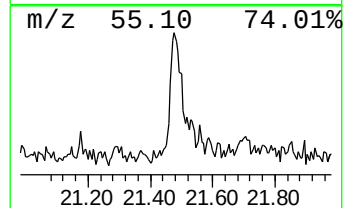
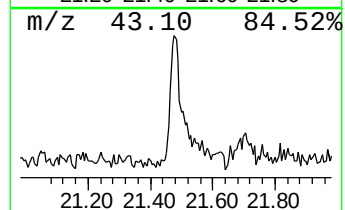
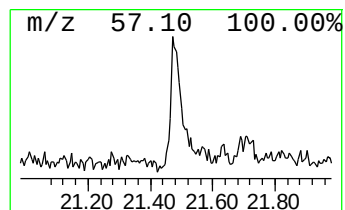
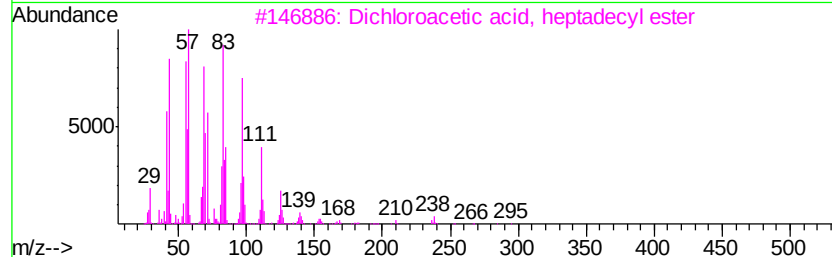
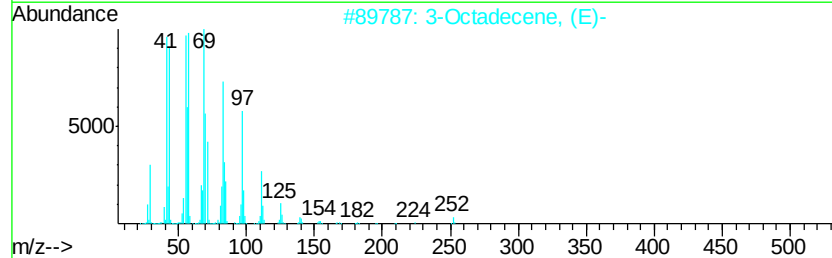
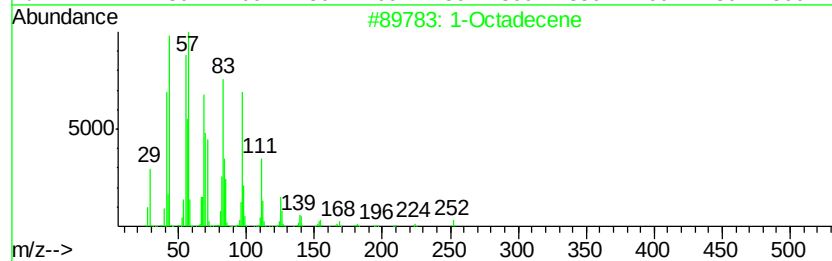
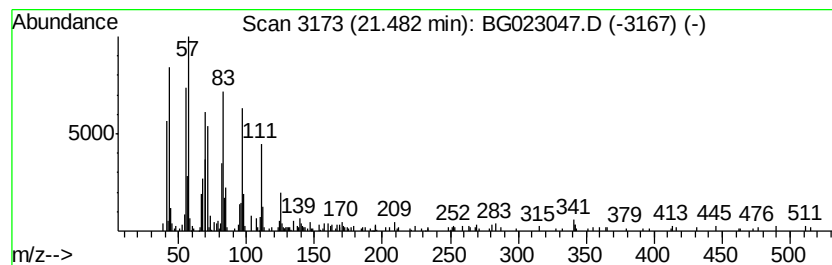
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Peak Number 6 1-Octadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.48	2.64 ng	358877	Chrysene-d12	21.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	95
2	3-Octadecene, (E)-	252	C18H36	007206-19-1	93
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	90
5	1-Hexacosanol	382	C26H54O	000506-52-5	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	3.04	81.4	ng	2860690	1	8.16	702868	20.0
2-Pentanone, 4-hy...	5.22	16.9	ng	593934	1	8.16	702868	20.0
unknown7.68	7.68	101.1	ng	3553300	1	8.16	702868	20.0
n-Hexadecanoic acid	18.43	2.3	ng	262633	4	17.56	2334250	20.0
1-Octadecene	21.48	2.6	ng	358877	5	21.86	2719490	20.0