

Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022923.D
Acq On : 8 Jul 2016 9:25
Operator : UM/SJ
Sample : H3900-03
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-3

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	3.043	31	35	40	rBV	160798	218874	2.52%	0.471%
2	5.223	401	406	413	rVB	121839	187109	2.16%	0.402%
3	5.699	479	487	497	rBV	1625955	2679303	30.90%	5.760%
4	7.303	753	760	772	rBV	1903644	3304402	38.11%	7.103%
5	7.679	814	824	834	rBV	1705042	3005139	34.66%	6.460%
6	8.149	897	904	912	rBV	382876	681232	7.86%	1.464%
7	8.478	952	960	967	rBV	1232297	2126278	24.52%	4.571%
8	9.324	1097	1104	1114	rVB	1164844	2075808	23.94%	4.462%
9	10.981	1378	1386	1394	rVB	583081	1048514	12.09%	2.254%
10	13.419	1791	1801	1809	rBV	3243813	5222057	60.23%	11.226%
11	14.236	1932	1940	1947	rBV	446540	678497	7.83%	1.459%
12	14.800	2029	2036	2043	rBV2	1037822	1717351	19.81%	3.692%
13	16.292	2280	2290	2298	rBV	3417043	5314694	61.29%	11.425%
14	16.486	2318	2323	2330	rVB2	70642	119874	1.38%	0.258%
15	17.280	2452	2458	2463	rBV2	74571	103036	1.19%	0.221%
16	17.556	2498	2505	2514	rBV2	1536842	2371181	27.35%	5.097%
17	18.419	2647	2652	2658	rBV2	211732	300266	3.46%	0.645%
18	19.689	2863	2868	2873	rBV7	58819	100485	1.16%	0.216%
19	20.153	2941	2947	2954	rBV	6321601	8670745	100.00%	18.639%
20	21.451	3164	3168	3173	rBV2	177620	279277	3.22%	0.600%
21	21.845	3228	3235	3244	rBV2	1645883	2848405	32.85%	6.123%
22	23.343	3482	3490	3497	rBV2	398822	824889	9.51%	1.773%
23	25.194	3795	3805	3817	rVB2	870720	2640943	30.46%	5.677%

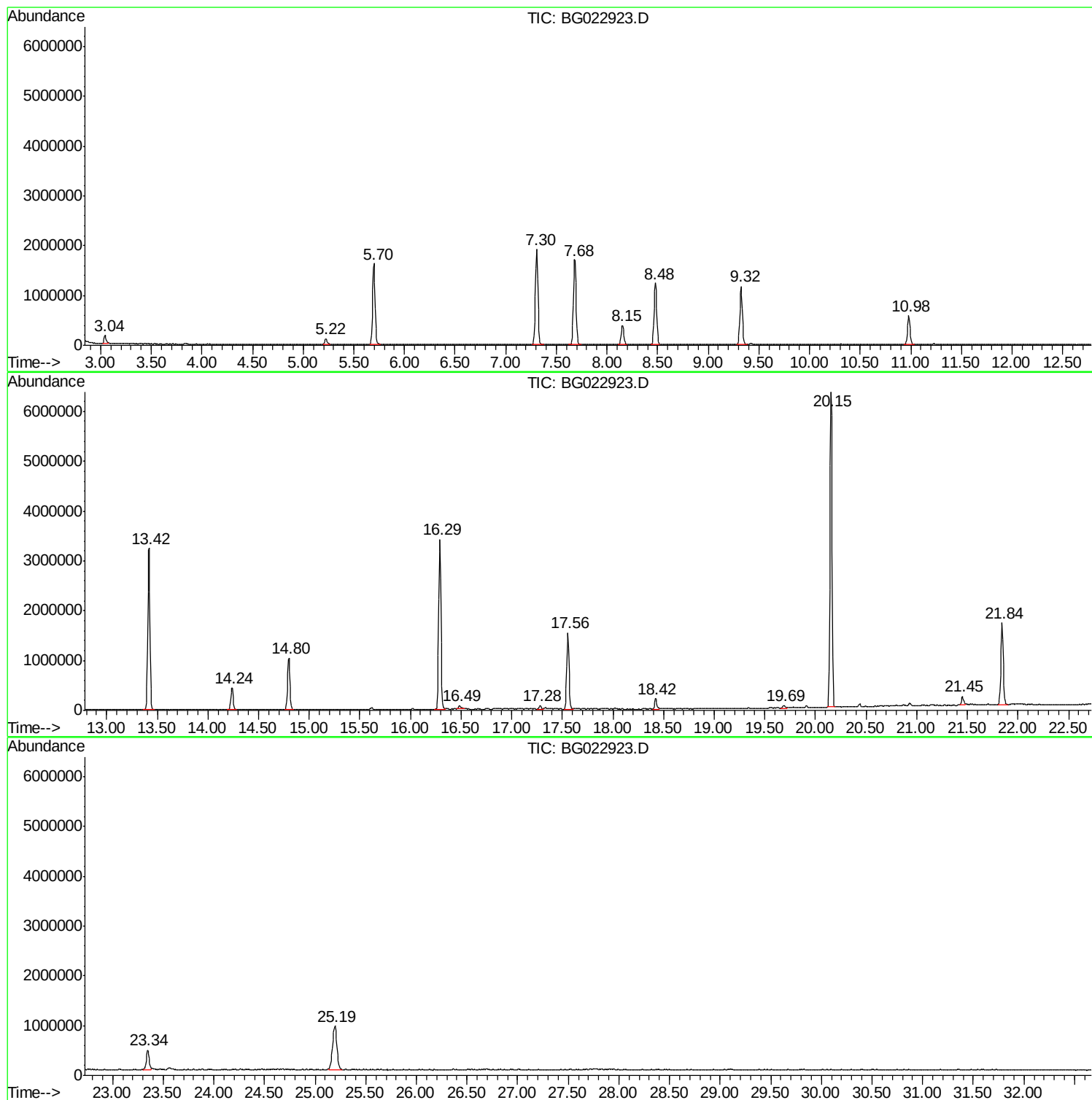
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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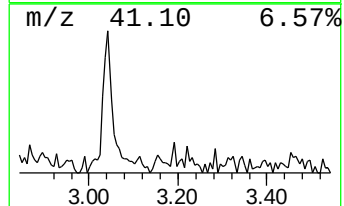
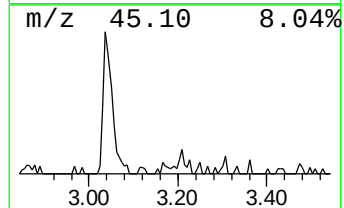
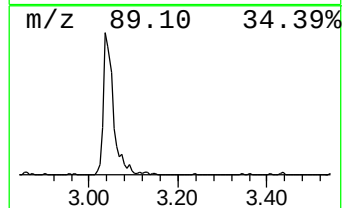
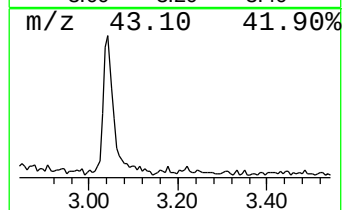
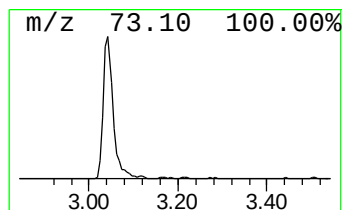
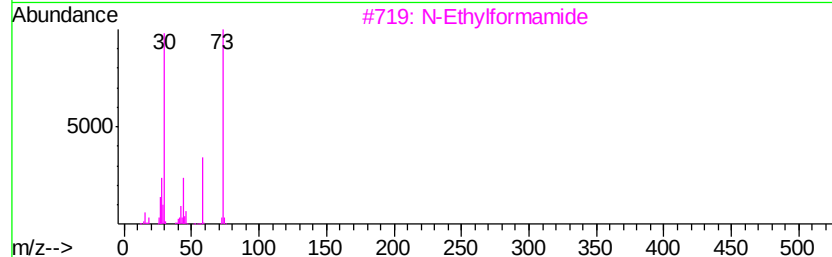
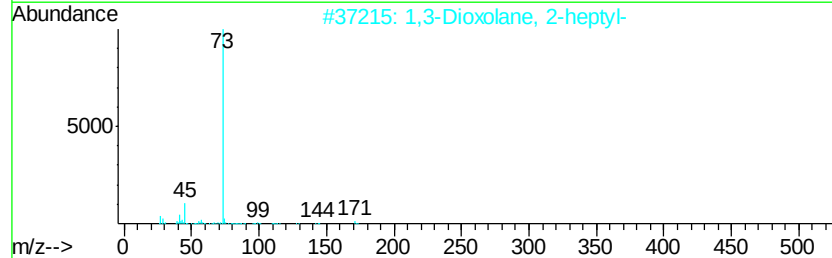
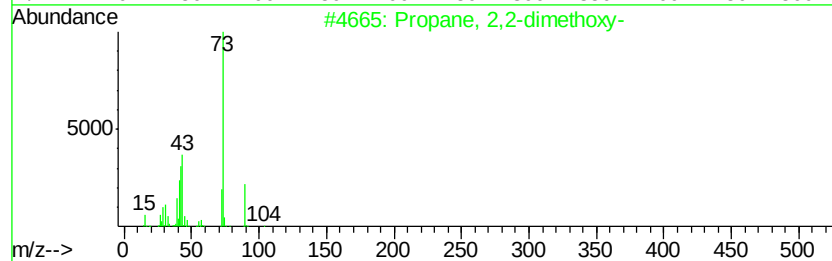
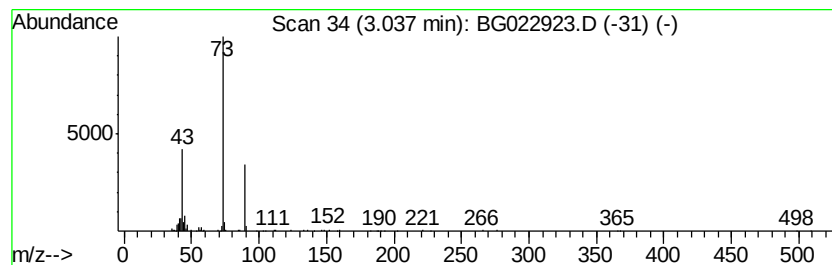
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.04 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	6.43 ng	218874	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	42
2		1,3-Dioxolane, 2-heptyl-	172	C10H20O2	004359-57-3	9
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	4



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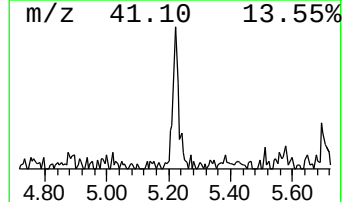
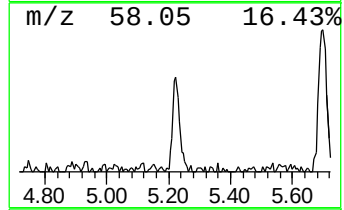
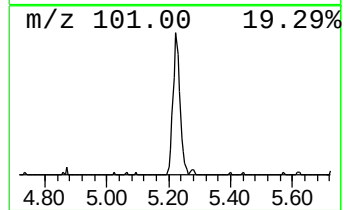
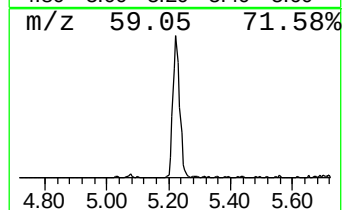
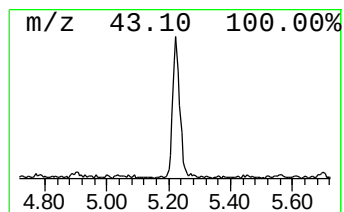
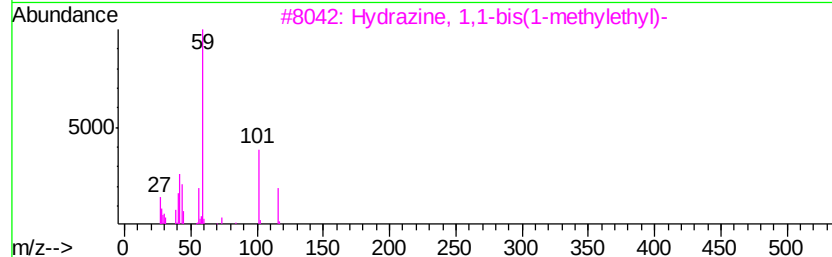
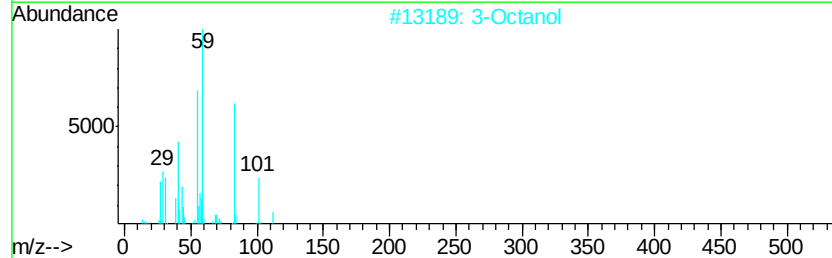
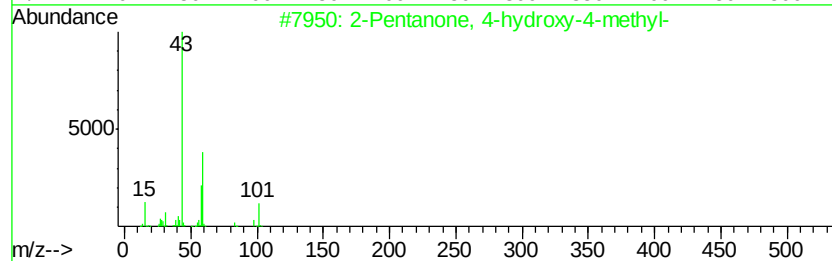
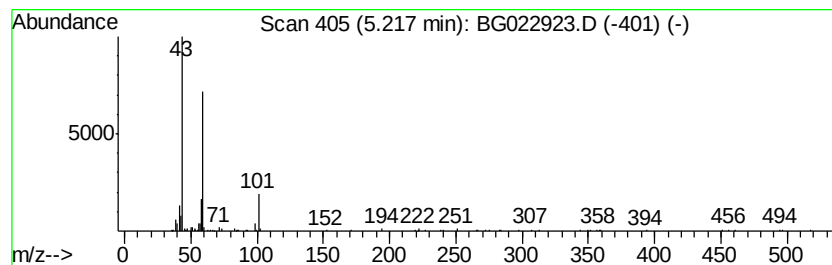
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	5.49 ng	187109	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	59
2		3-Octanol	130	C8H18O	000589-98-0	40
3		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	38
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	36



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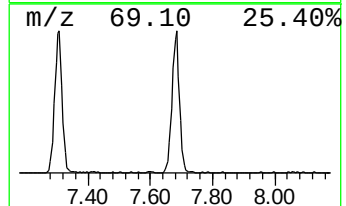
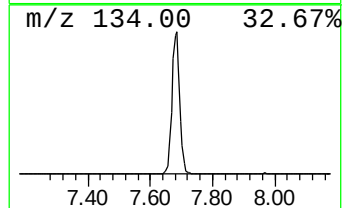
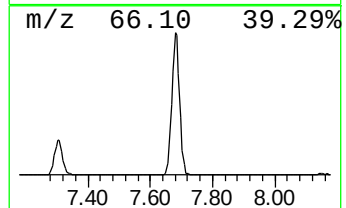
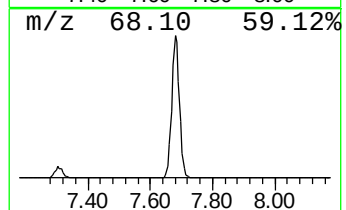
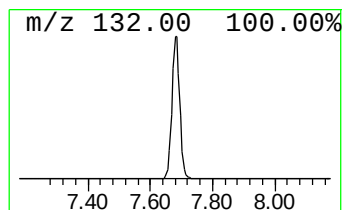
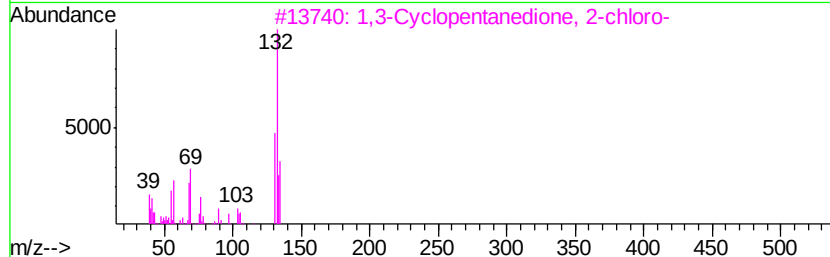
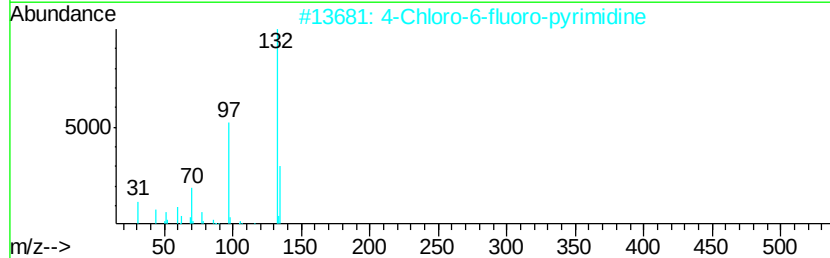
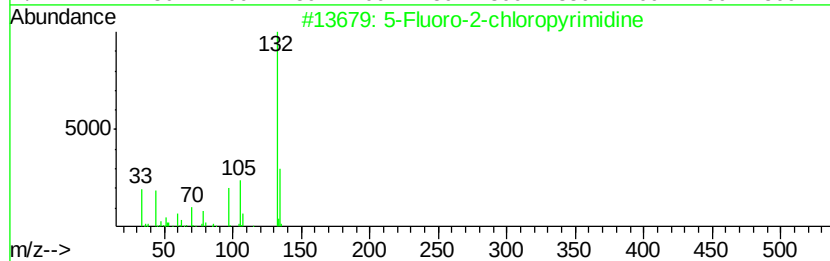
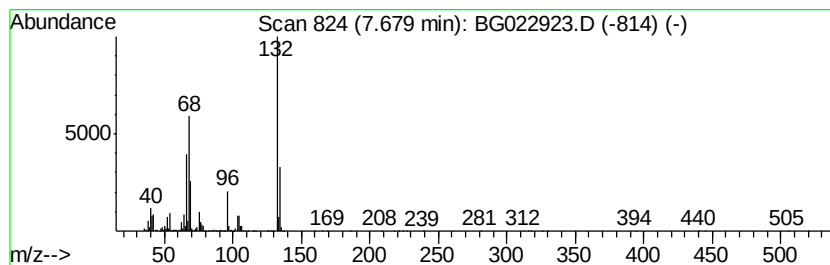
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Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	88.23 ng	3005140	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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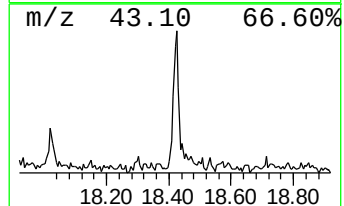
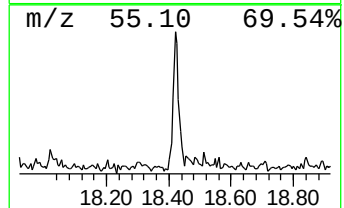
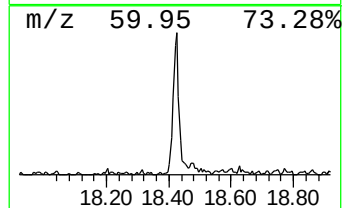
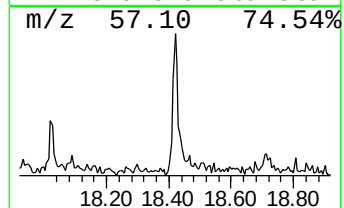
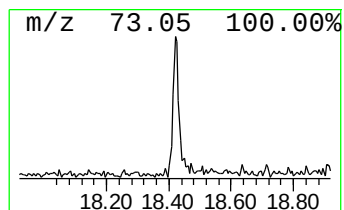
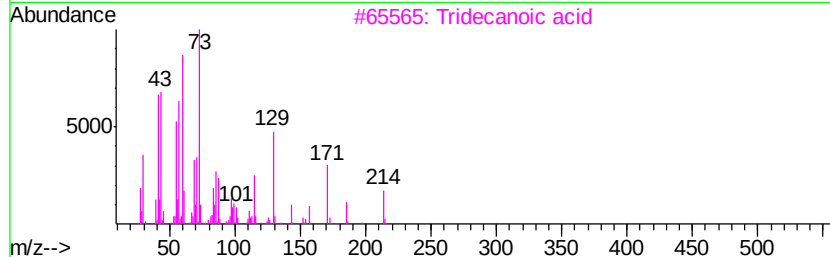
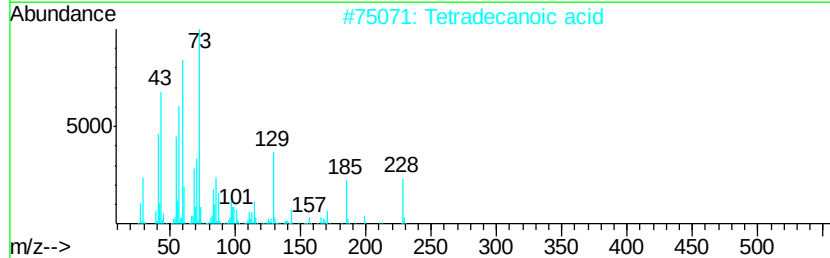
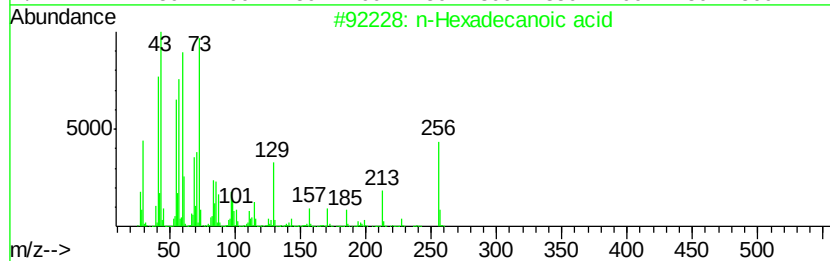
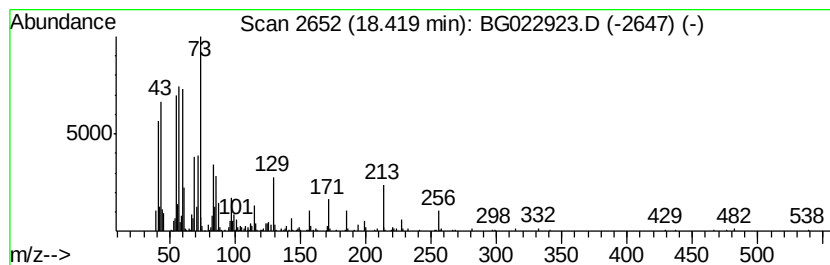
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.42	2.53 ng	300266	Phenanthrene-d10	17.56	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59



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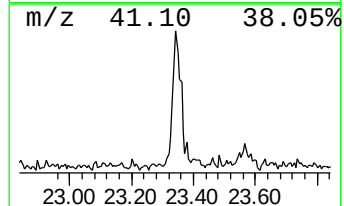
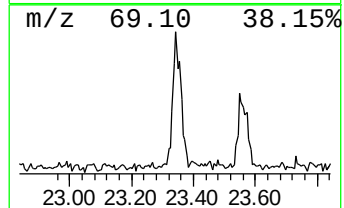
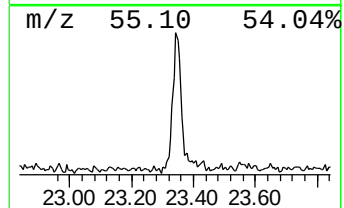
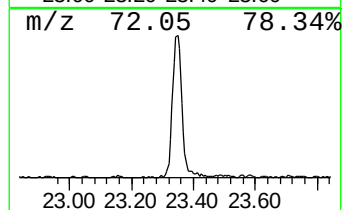
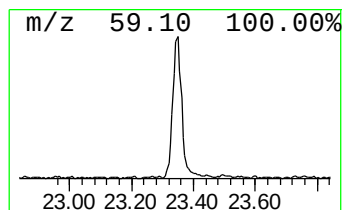
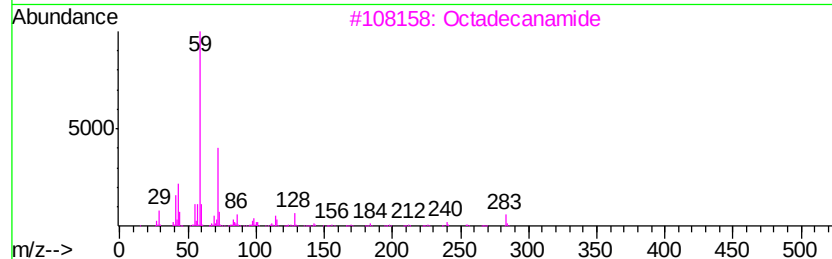
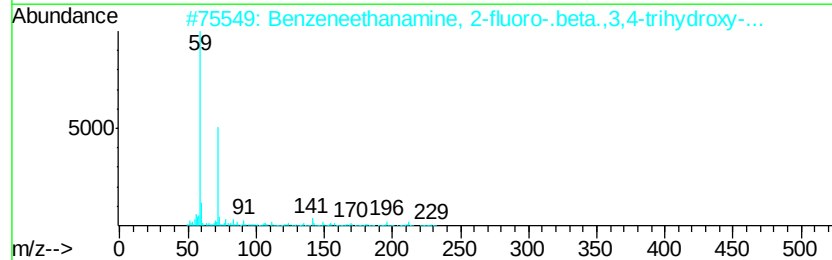
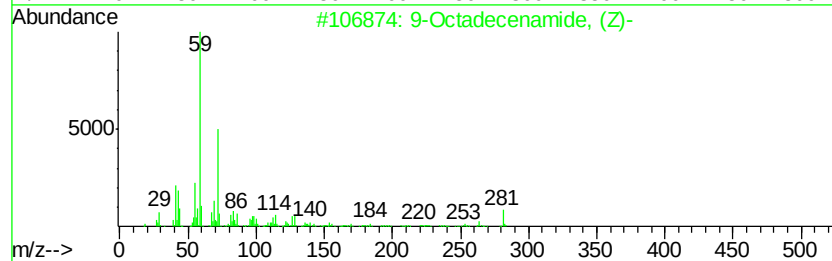
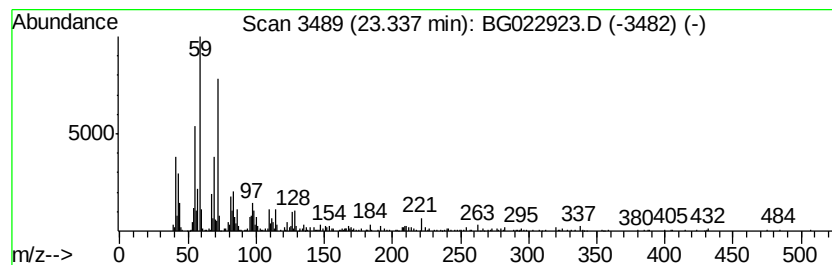
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Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.34	5.79 ng	824889	Chrysene-d12	21.84

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	81
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	52
3		Octadecanamide	283	C18H37NO	000124-26-5	47
4		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	42
5		Dodecanamide	199	C12H25NO	001120-16-7	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.04	3.04	6.4	ng	218874	1	8.15	681232	20.0
2-Pentanone, 4-hy...	5.22	5.5	ng	187109	1	8.15	681232	20.0
unknown7.68	7.68	88.2	ng	3005140	1	8.15	681232	20.0
n-Hexadecanoic acid	18.42	2.5	ng	300266	4	17.56	2371180	20.0
9-Octadecenamide,...	23.34	5.8	ng	824889	5	21.84	2848410	20.0