

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071416\
 Data File : BG023097.D
 Acq On : 14 Jul 2016 12:10
 Operator : UM/SJ
 Sample : H3996-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B7-B2(5-12)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	3.037	29	34	53	rBV	7072475	11267536	100.00%	17.344%
2	5.222	400	406	413	rBV	250180	389928	3.46%	0.600%
3	5.698	480	487	500	rBV	2227193	3587423	31.84%	5.522%
4	7.308	753	761	772	rBV	2517147	4442749	39.43%	6.839%
5	7.684	816	825	835	rBV	2334973	4038616	35.84%	6.217%
6	8.154	898	905	911	rBV	402573	690616	6.13%	1.063%
7	8.477	953	960	970	rVB	1486584	2683559	23.82%	4.131%
8	9.329	1096	1105	1116	rBV	1495781	2777058	24.65%	4.275%
9	10.980	1377	1386	1394	rBV	612326	1142553	10.14%	1.759%
10	13.419	1793	1801	1808	rBV	4016914	6563924	58.26%	10.104%
11	14.241	1935	1941	1947	rBV	555466	850744	7.55%	1.310%
12	14.805	2028	2037	2044	rBV2	1143815	1942712	17.24%	2.990%
13	16.298	2280	2291	2305	rBV	3996350	6485194	57.56%	9.983%
14	17.279	2454	2458	2462	rBV	115516	133837	1.19%	0.206%
15	17.555	2499	2505	2519	rBV2	1538534	2475145	21.97%	3.810%
16	18.019	2580	2584	2591	rVB2	103250	148480	1.32%	0.229%
17	18.419	2647	2652	2658	rBV2	187519	281131	2.50%	0.433%
18	20.158	2942	2948	2954	rBV	7132008	9685441	85.96%	14.909%
19	21.862	3230	3238	3245	rBV2	1604998	2751037	24.42%	4.235%
20	25.240	3801	3813	3828	rBV2	795603	2627676	23.32%	4.045%

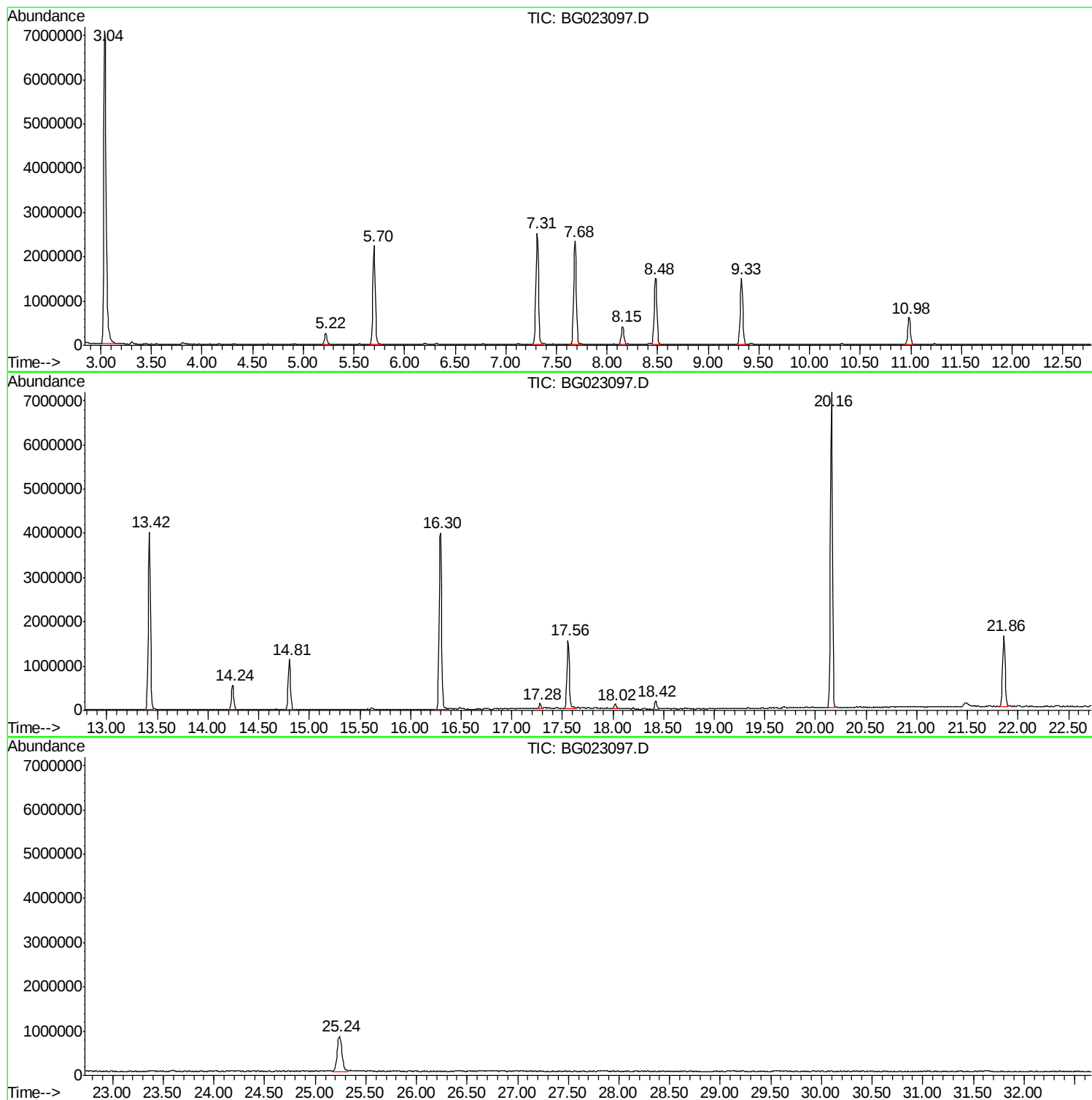
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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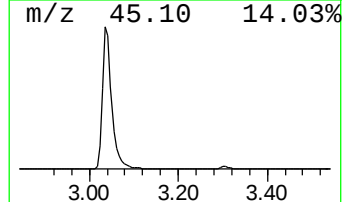
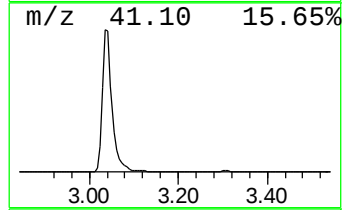
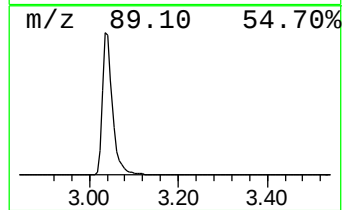
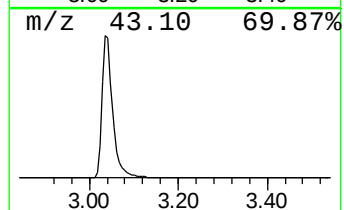
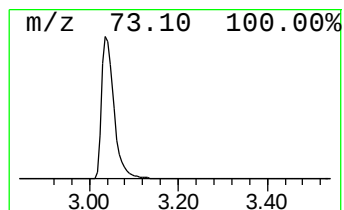
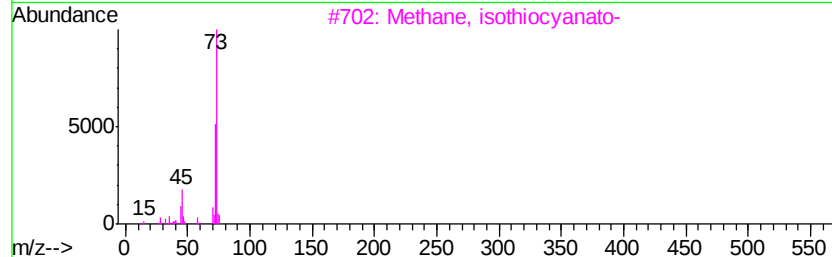
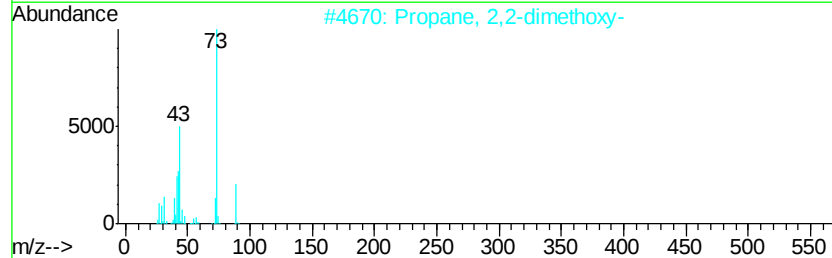
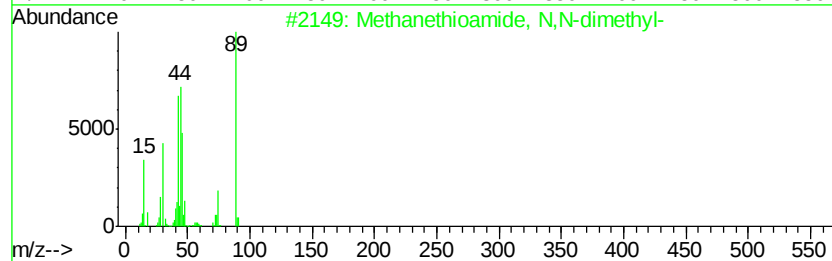
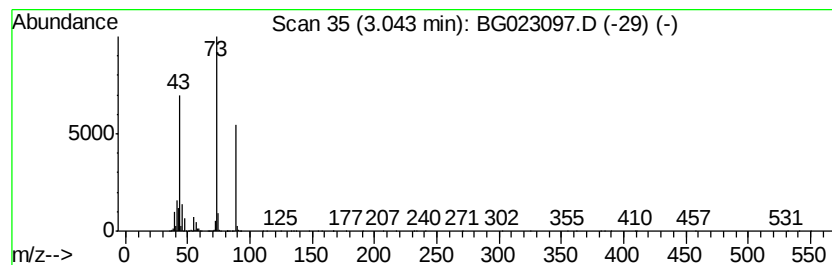
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	326.30 ng	11267500	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	38
3		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	12
4		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
5		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9



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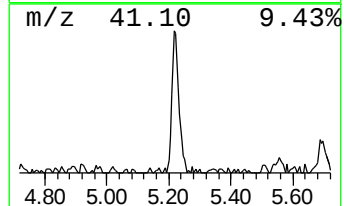
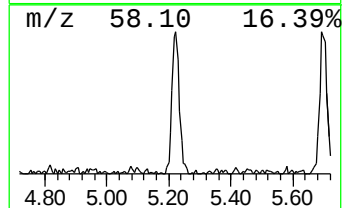
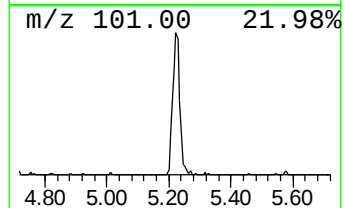
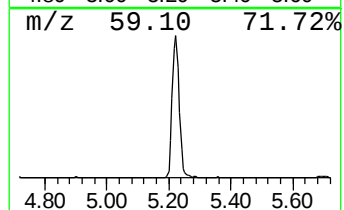
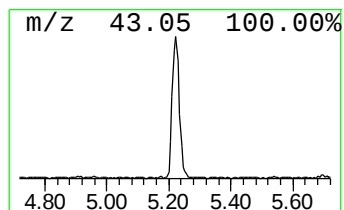
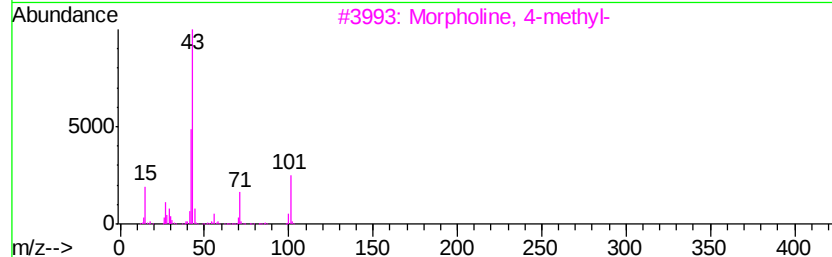
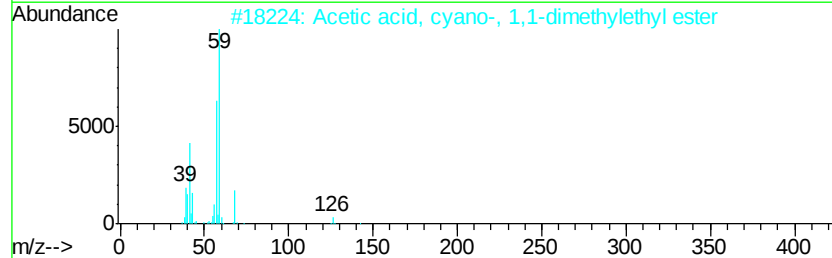
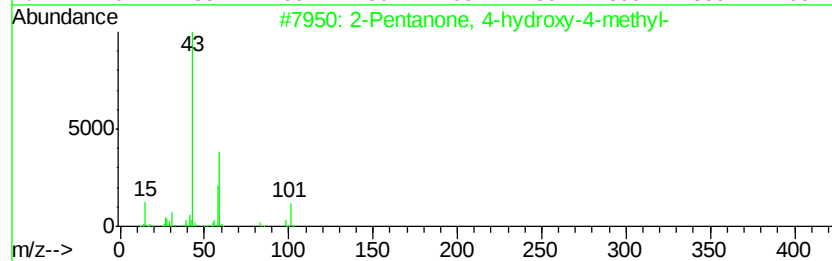
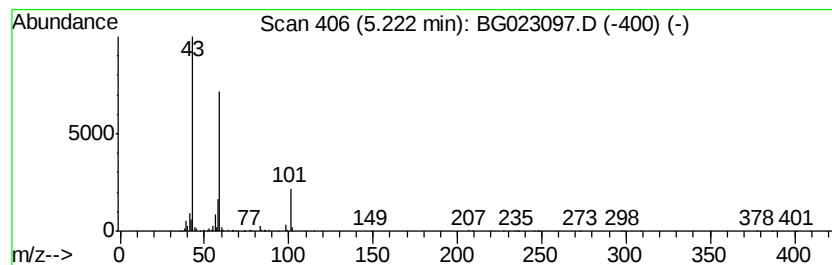
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	11.29 ng	389928	1,4-Dichlorobenzene-d4	8.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	12	
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
5	Hexanamide	115	C6H13NO	000628-02-4	9	



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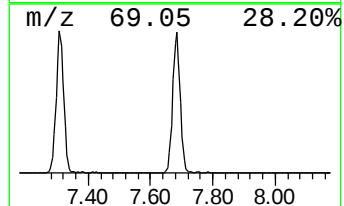
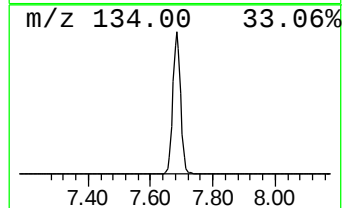
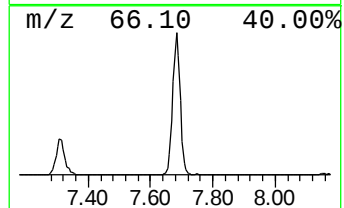
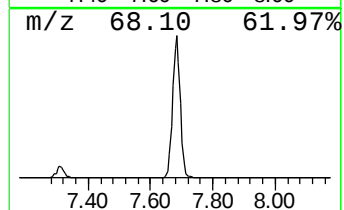
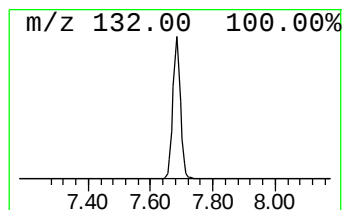
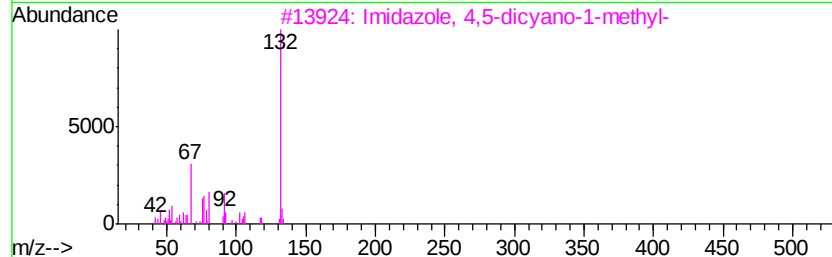
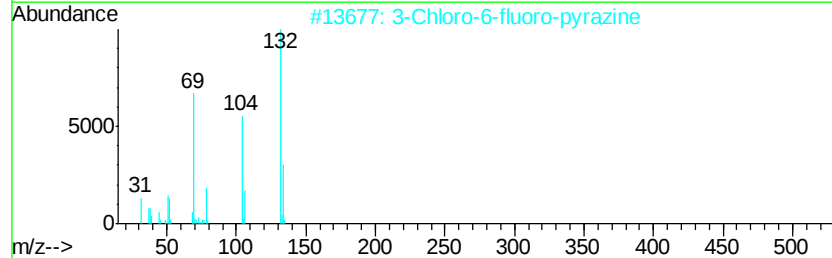
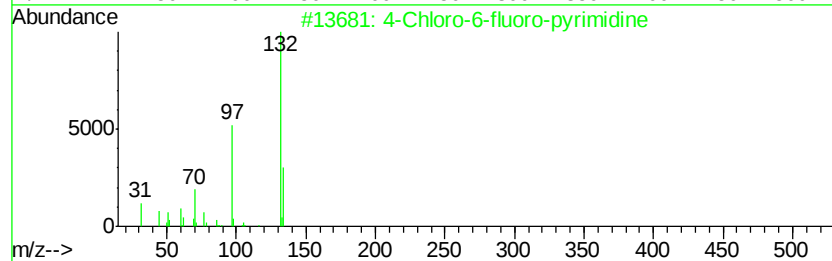
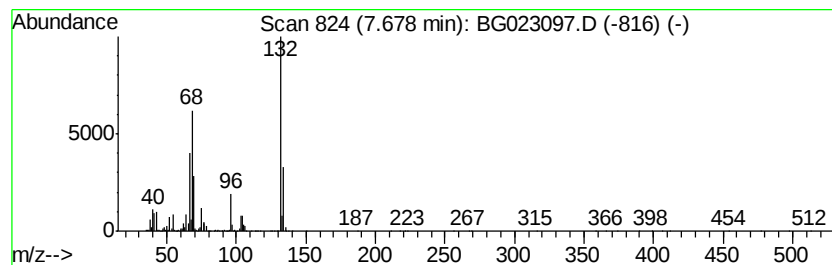
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Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	116.96 ng	4038620	1,4-Dichlorobenzene-d4	8.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	11
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	10
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10



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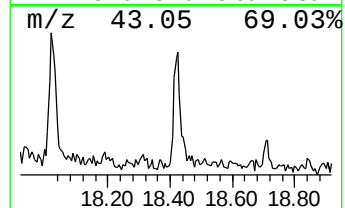
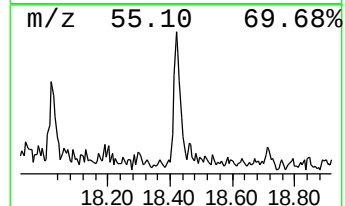
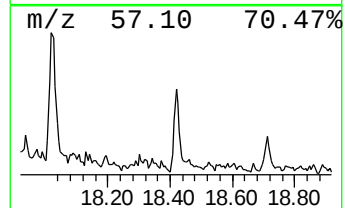
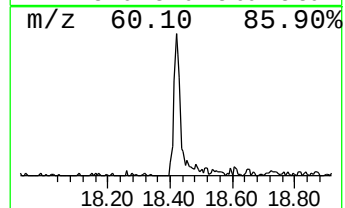
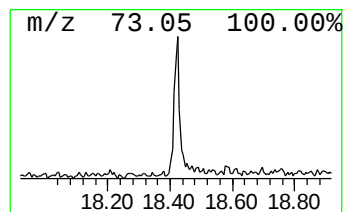
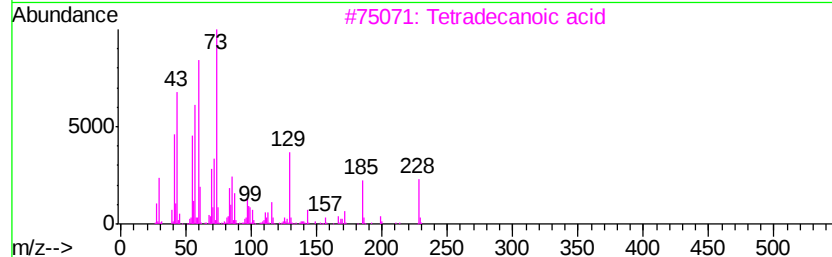
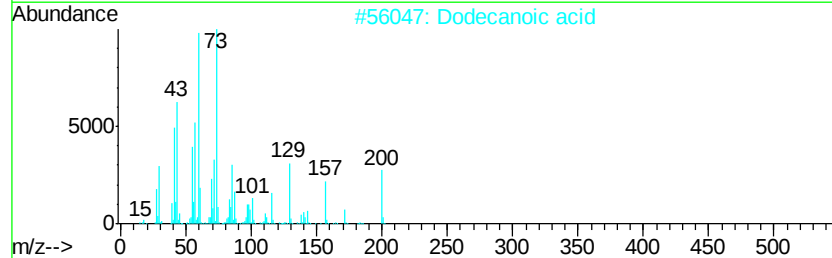
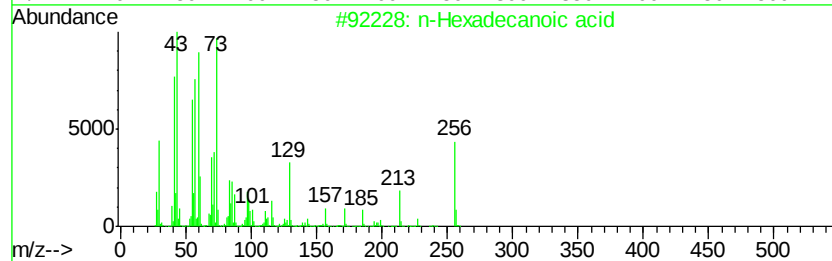
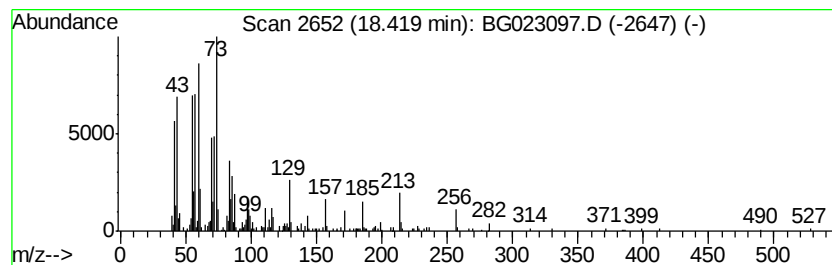
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	2.27 ng	281131	Phenanthrene-d10	17.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91	
2	Dodecanoic acid	200	C12H24O2	000143-07-7	81	
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64	
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64	
5	n-Decanoic acid	172	C10H20O2	000334-48-5	59	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.04	3.04	326.3	ng	11267500	1	8.15	690616	20.0
2-Pentanone, 4-hy...	5.22	11.3	ng	389928	1	8.15	690616	20.0
unknown7.68	7.68	117.0	ng	4038620	1	8.15	690616	20.0
n-Hexadecanoic acid	18.42	2.3	ng	281131	4	17.56	2475150	20.0