

Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
 Data File : BG023317.D
 Acq On : 28 Jul 2016 21:46
 Operator : UM/SJ
 Sample : H4205-20
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-40-14.0-15.0

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-BG072616.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	3.004	23	28	47	rVB	7134107	11535967	100.00%	13.847%
2	5.195	395	401	408	rBV	585343	888547	7.70%	1.067%
3	5.671	475	482	492	rBV	3003677	4849976	42.04%	5.822%
4	7.286	749	757	772	rBV	3100818	5659897	49.06%	6.794%
5	7.662	812	821	833	rBV	3072304	5383298	46.67%	6.462%
6	8.132	895	901	909	rBV	629287	1079243	9.36%	1.295%
7	8.461	947	957	965	rBV	2202818	3820455	33.12%	4.586%
8	9.313	1094	1102	1112	rBV	1988608	3567668	30.93%	4.283%
9	10.975	1377	1385	1392	rBV	920846	1704418	14.77%	2.046%
10	13.419	1792	1801	1810	rBV	5018817	8125869	70.44%	9.754%
11	14.247	1935	1942	1949	rBV	1296261	1891398	16.40%	2.270%
12	14.806	2030	2037	2046	rVB2	1687443	2771678	24.03%	3.327%
13	15.628	2172	2177	2183	rVB2	61221	117143	1.02%	0.141%
14	16.303	2281	2292	2304	rBV	4840109	7735574	67.06%	9.286%
15	16.497	2320	2325	2332	rBV	85017	175015	1.52%	0.210%
16	17.572	2500	2508	2518	rBV2	2254365	3547124	30.75%	4.258%
17	18.442	2651	2656	2662	rBV4	114374	212019	1.84%	0.255%
18	19.717	2866	2873	2879	rBV8	58633	128645	1.12%	0.154%
19	19.857	2893	2897	2902	rVB	433915	525988	4.56%	0.631%
20	19.969	2912	2916	2921	rVB	109361	117406	1.02%	0.141%
21	20.181	2945	2952	2959	rBV	7731051	11082511	96.07%	13.303%
22	20.897	3070	3074	3082	rBV	316033	406622	3.52%	0.488%
23	21.890	3236	3243	3252	rVB	2384961	3950008	34.24%	4.741%
24	23.441	3500	3507	3511	rBV6	57634	121287	1.05%	0.146%
25	25.303	3812	3824	3835	rBV2	1296184	3909838	33.89%	4.693%

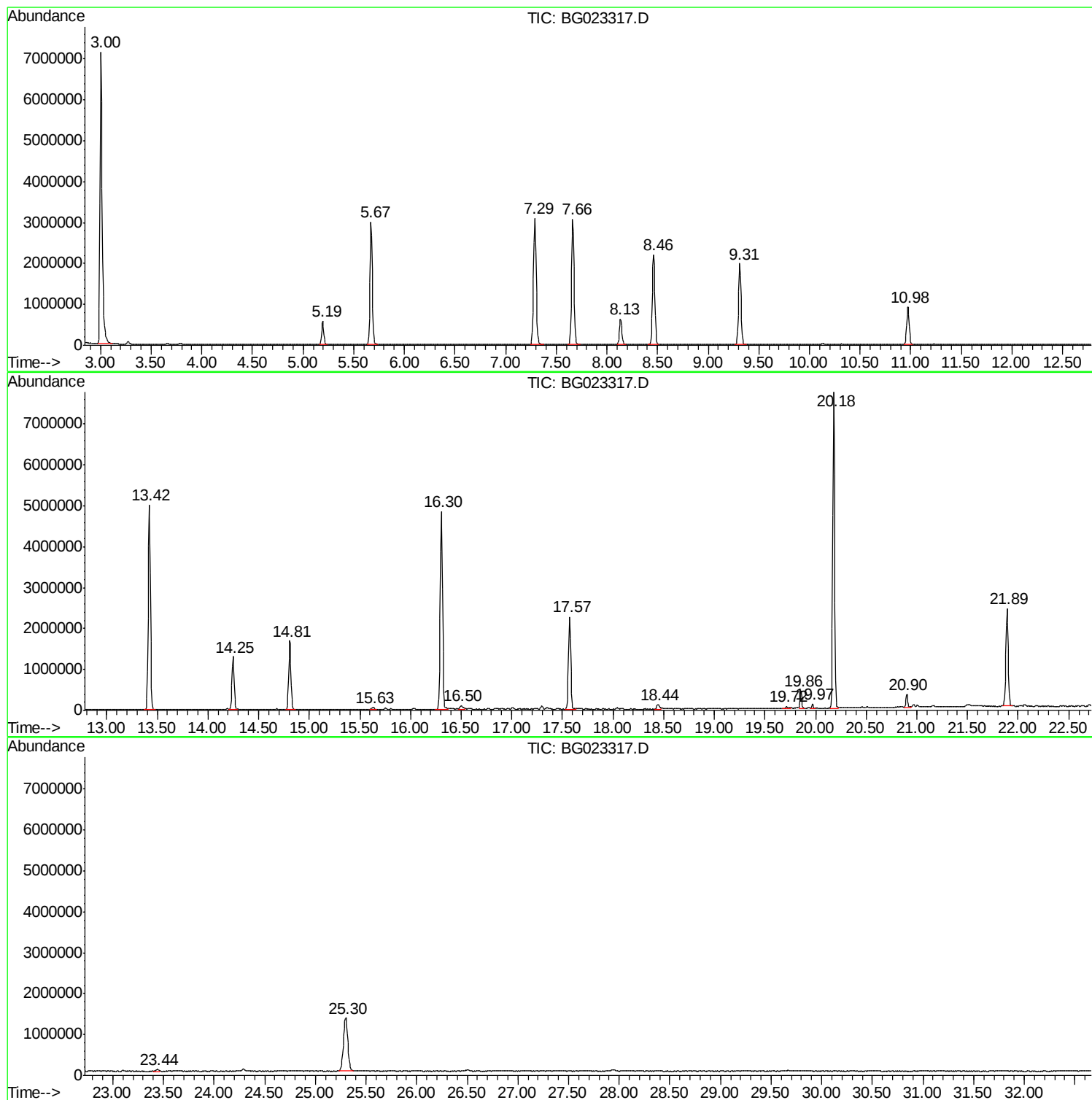
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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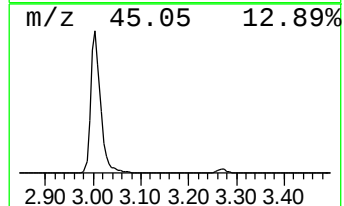
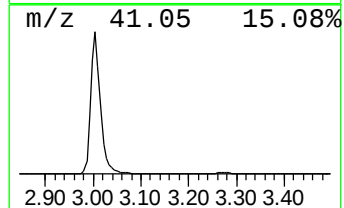
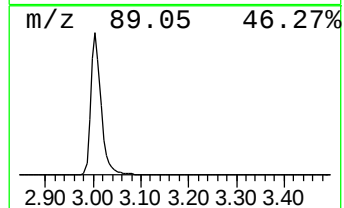
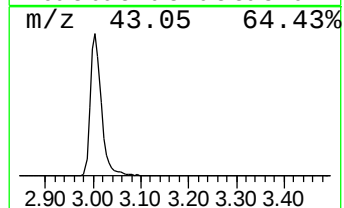
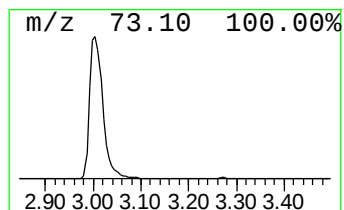
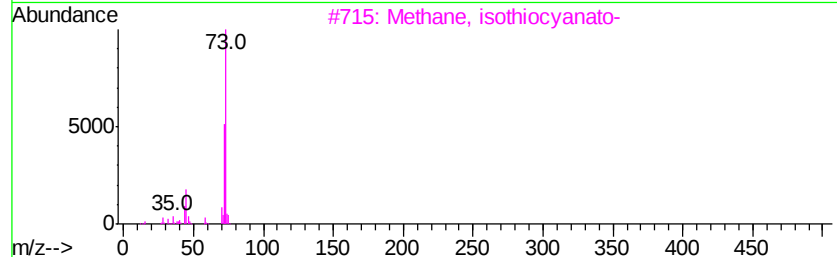
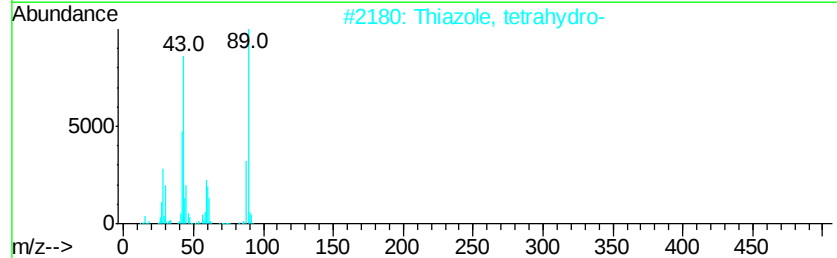
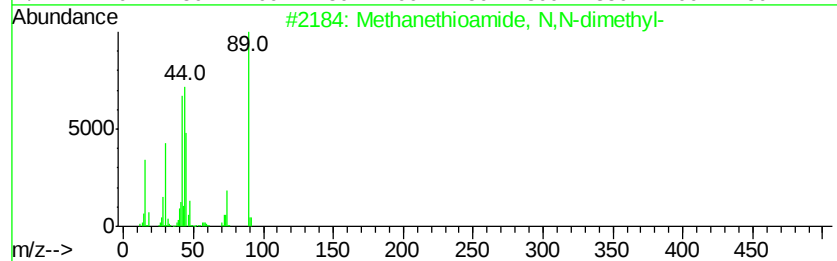
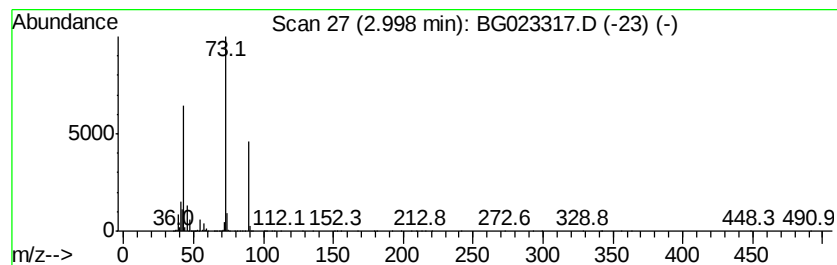
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	213.78 ng	11536000	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	47
2		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	23
3		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
5		Thiopropionamide	89	C3H7NS	000631-58-3	9



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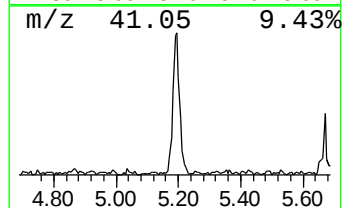
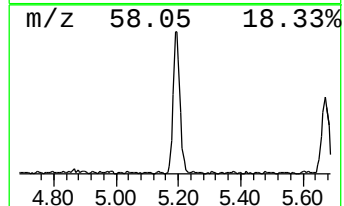
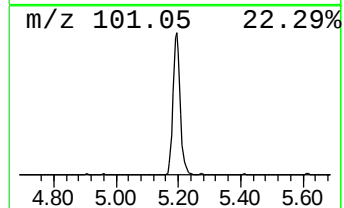
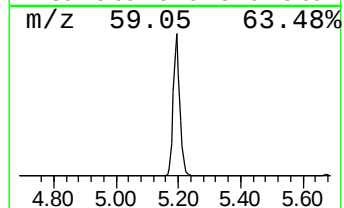
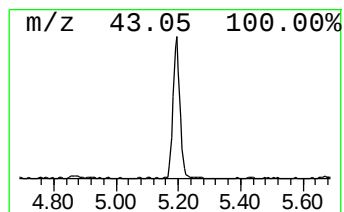
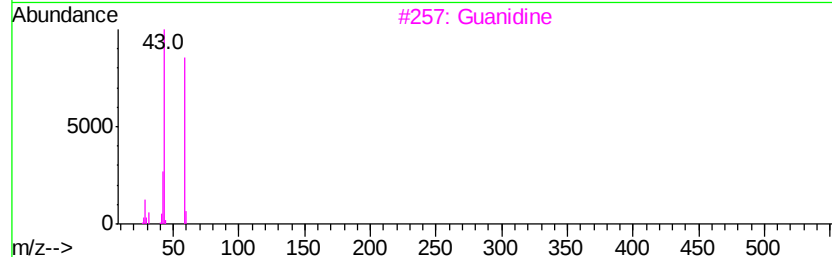
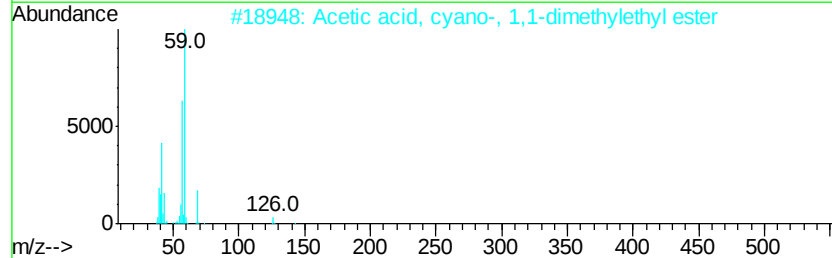
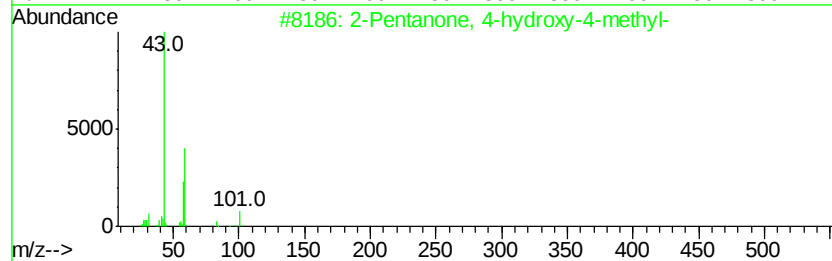
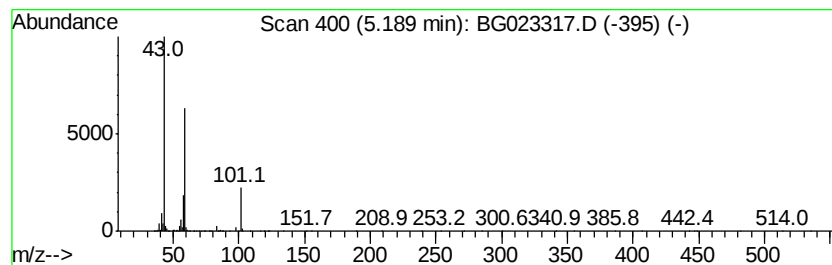
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	16.47 ng	888547	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Guanidine	59	CH5N3	000113-00-8	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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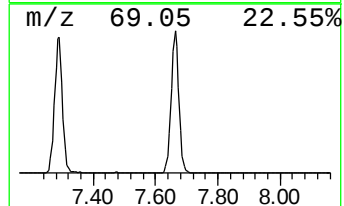
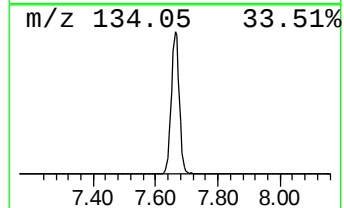
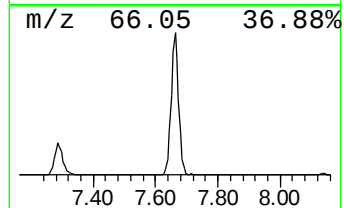
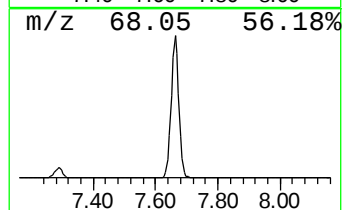
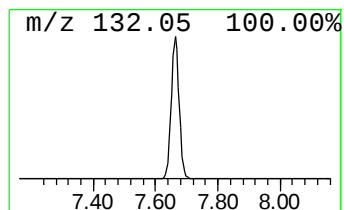
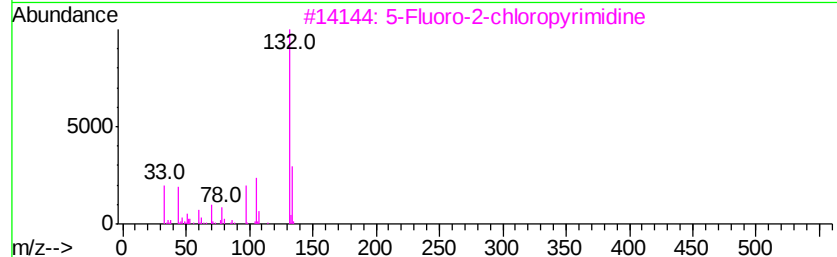
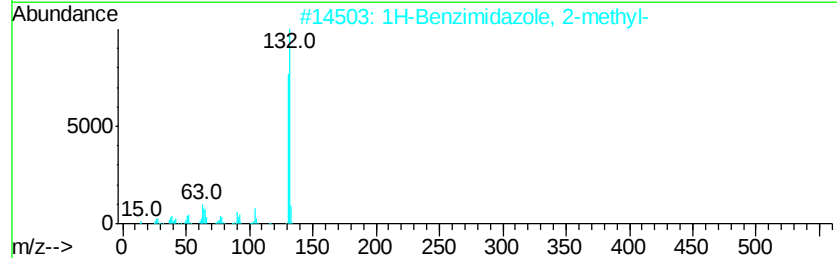
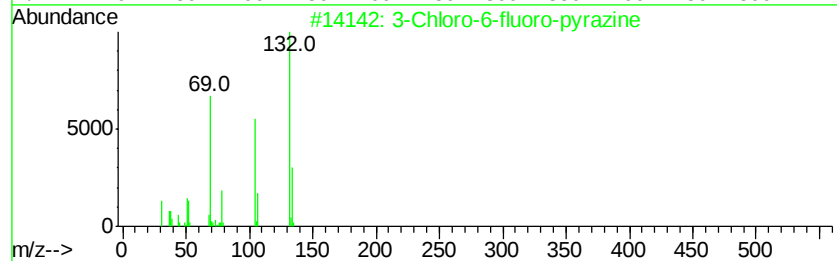
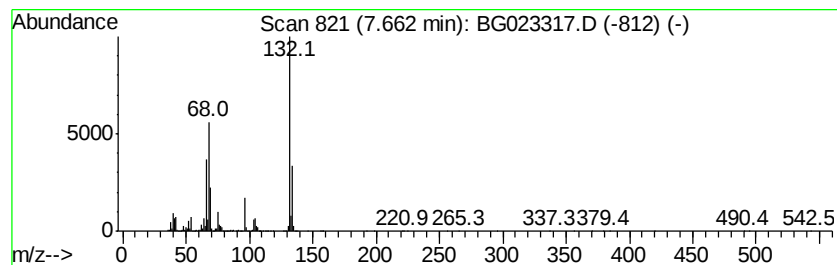
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Peak Number 3 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	99.76 ng	5383300	1,4-Dichlorobenzene-d4	8.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	12
4	2-Cyclohexen-1-one			96	C6H8O	000930-68-7	11
5	Cyclopropanamine, 1-phenyl-			133	C9H11N	1000351-26-2	10



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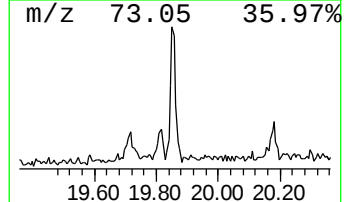
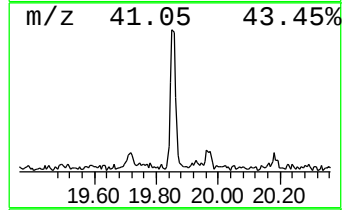
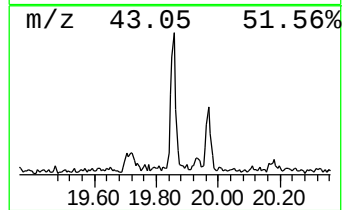
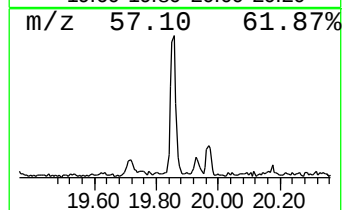
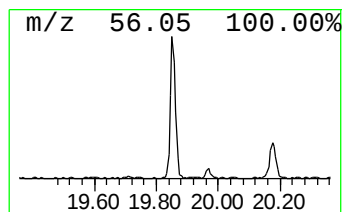
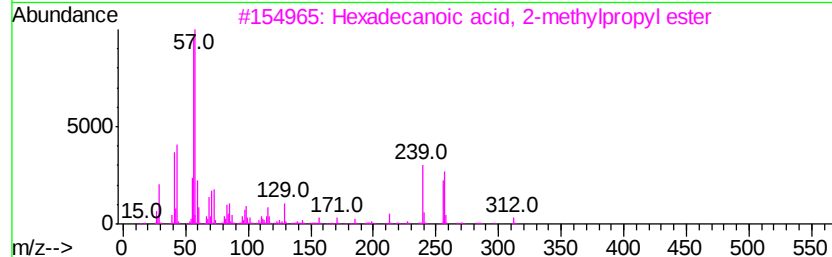
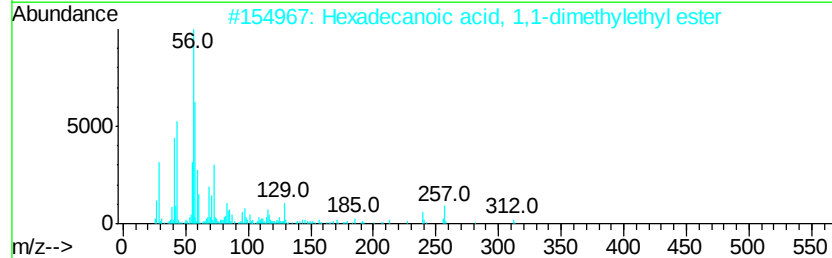
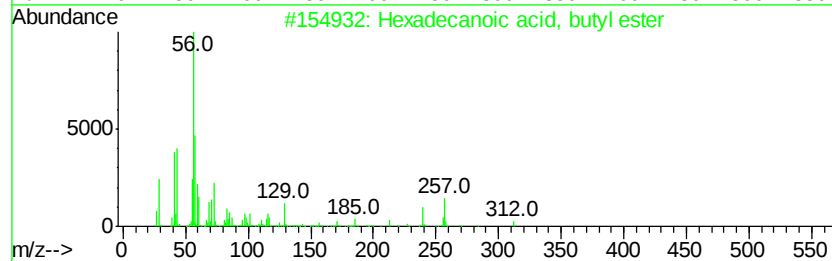
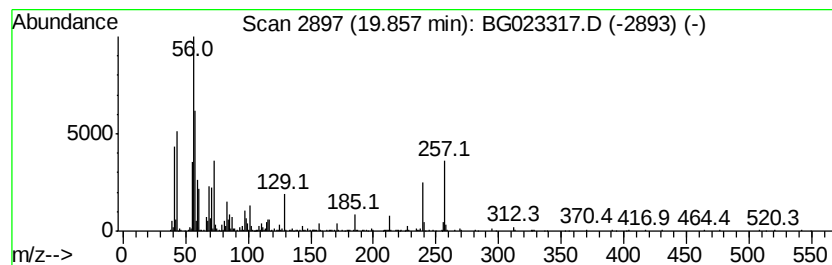
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Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.86	2.66 ng	525988	Chrysene-d12	21.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	92
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	46
4		Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	40
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	27



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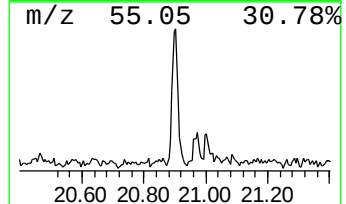
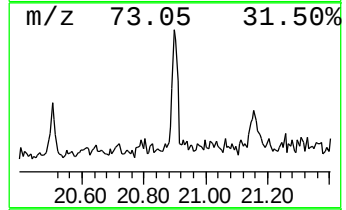
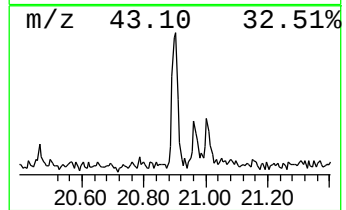
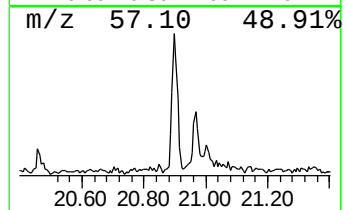
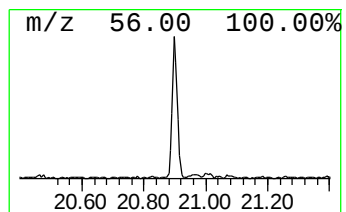
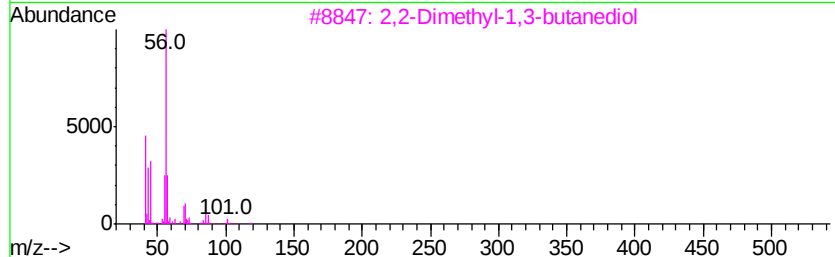
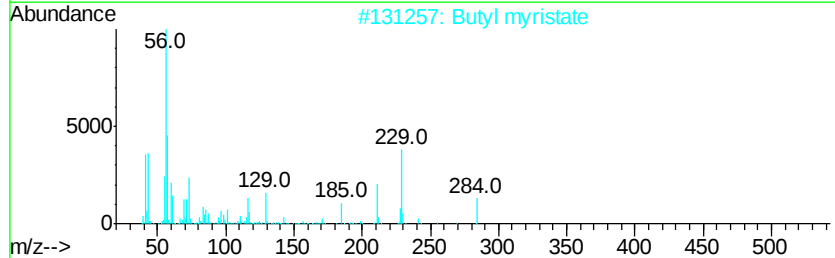
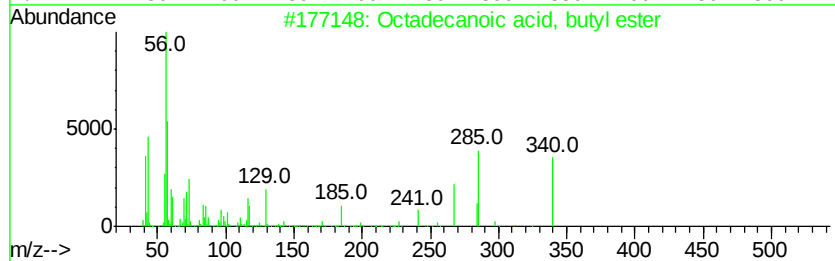
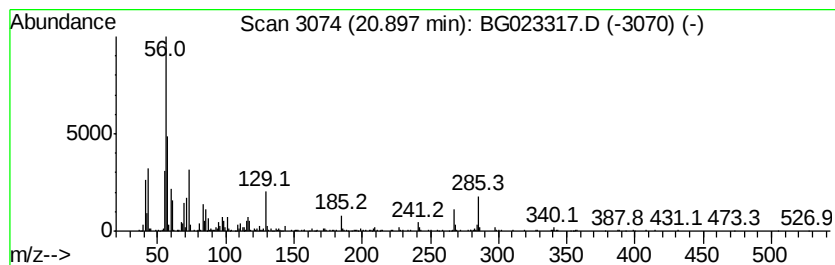
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.90	2.06 ng	406622	Chrysene-d12	21.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Butyl myristate	284	C18H36O2	000110-36-1	64
3		2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	38
4		Chloromethyl 2-chloroundecanoate	268	C12H22Cl2O2	080418-88-8	32
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.00	3.00	213.8	ng	11536000	1	8.13	1079240	20.0
2-Pentanone, 4-hy...	5.19	16.5	ng	888547	1	8.13	1079240	20.0
unknown7.66	7.66	99.8	ng	5383300	1	8.13	1079240	20.0
Hexadecanoic acid...	19.86	2.7	ng	525988	5	21.89	3950010	20.0
Octadecanoic acid...	20.90	2.1	ng	406622	5	21.89	3950010	20.0