

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
 Data File : BG022439.D
 Acq On : 19 Jun 2016 1:18
 Operator : UM/SJ
 Sample : H3514-07
 Misc :
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S5-B3(0-8)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-BG060616.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	2.873	3	6	26	rVB	1766111	2734495	100.00%	19.751%
2	5.106	379	386	395	rVB2	32903	61909	2.26%	0.447%
3	5.605	464	471	487	rBV	426833	825983	30.21%	5.966%
4	7.233	739	748	762	rBV	489010	974104	35.62%	7.036%
5	7.579	799	807	822	rBV	545020	1043911	38.18%	7.540%
6	8.044	879	886	899	rVB	89079	166196	6.08%	1.200%
7	8.367	932	941	951	rBV	418337	800176	29.26%	5.780%
8	9.219	1077	1086	1103	rBV	292647	615934	22.52%	4.449%
9	10.864	1358	1366	1378	rBV	134698	276319	10.10%	1.996%
10	13.302	1773	1781	1795	rBV	983917	1717959	62.83%	12.409%
11	14.125	1915	1921	1933	rBV	79479	134712	4.93%	0.973%
12	14.683	2008	2016	2025	rBV2	234635	393413	14.39%	2.842%
13	16.175	2263	2270	2284	rBV	591687	1006979	36.83%	7.273%
14	17.427	2476	2483	2497	rBV	240474	418052	15.29%	3.020%
15	19.695	2865	2869	2875	rVB	47562	63739	2.33%	0.460%
16	19.812	2885	2889	2899	rBV4	11859	29454	1.08%	0.213%
17	20.024	2919	2925	2934	rBV	1181048	1715382	62.73%	12.390%
18	20.735	3042	3046	3051	rVB2	38794	53233	1.95%	0.384%
19	21.692	3201	3209	3223	rBV	209417	414146	15.15%	2.991%
20	24.930	3752	3760	3786	rVB2	113809	398822	14.58%	2.881%

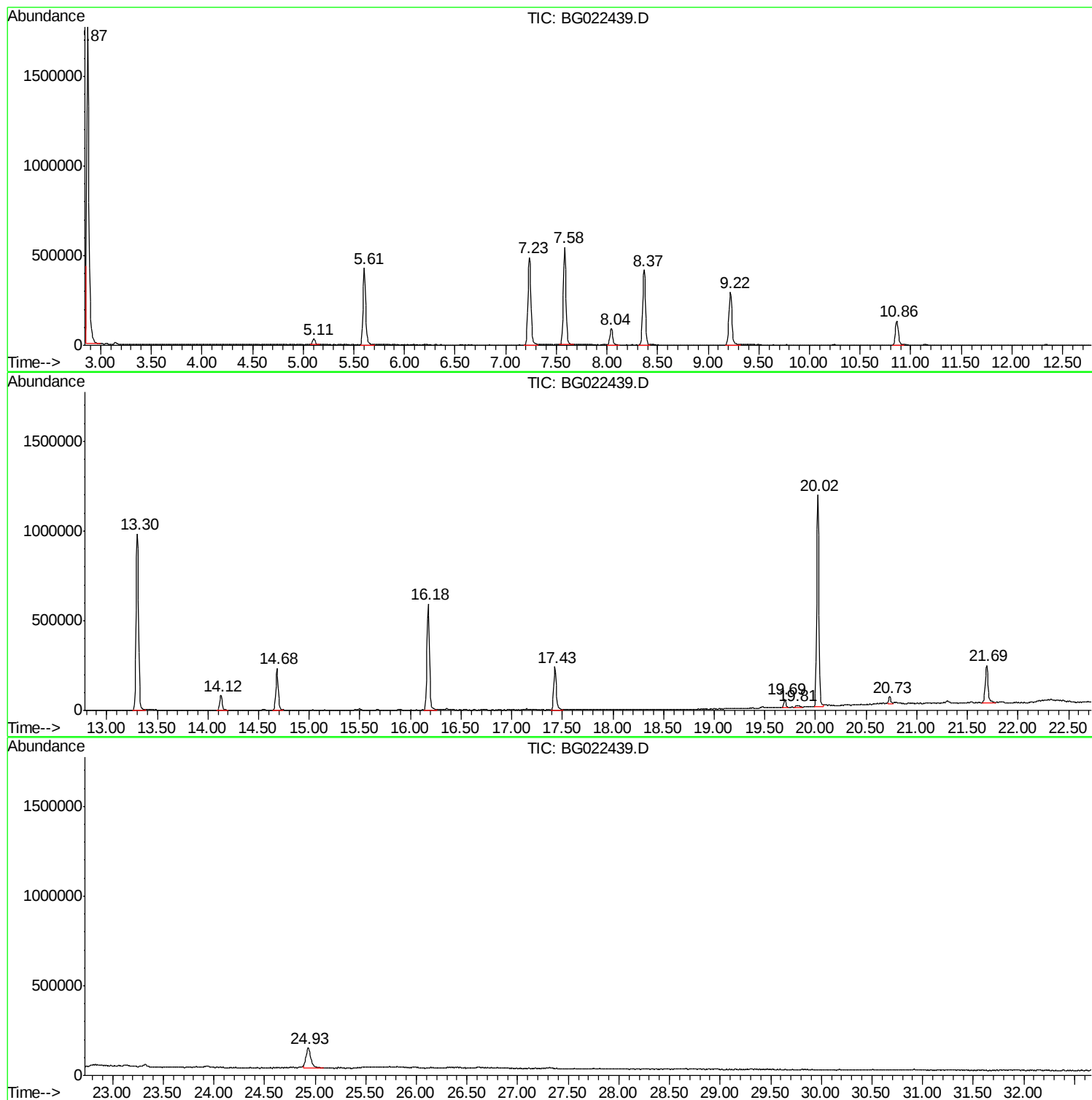
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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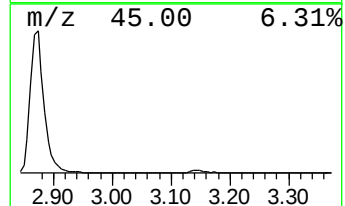
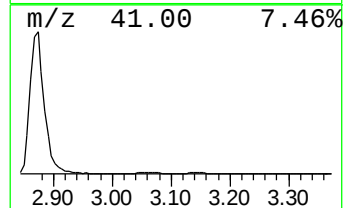
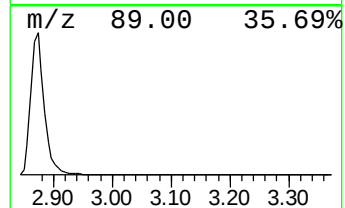
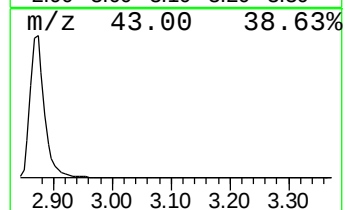
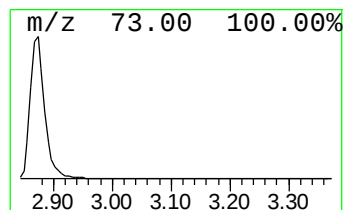
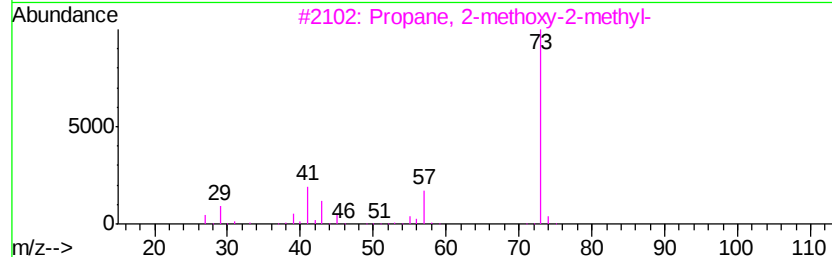
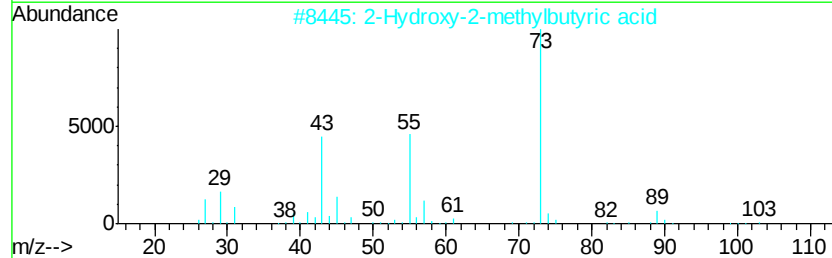
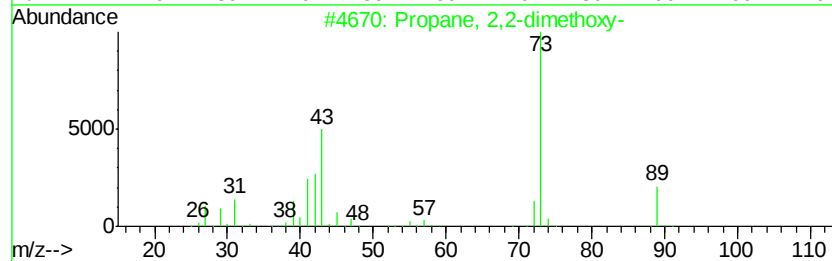
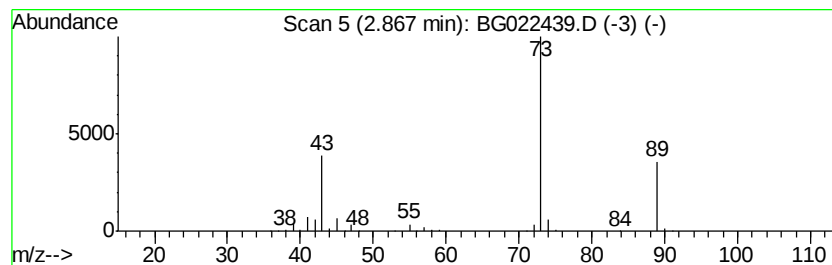
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	329.07 ng	2734500	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	64
2		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	28
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7



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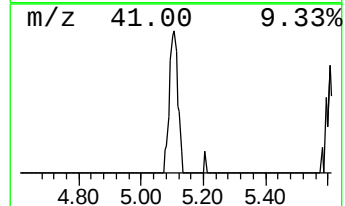
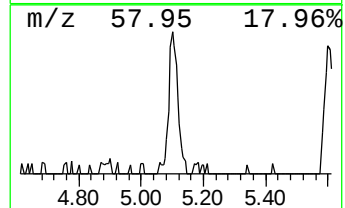
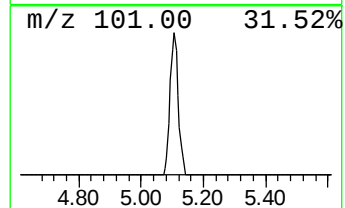
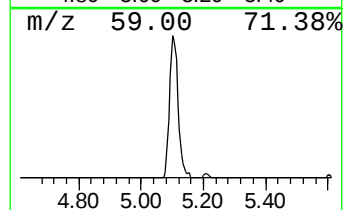
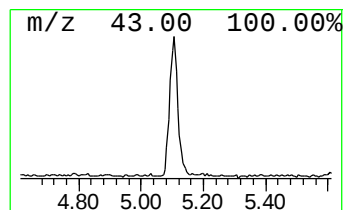
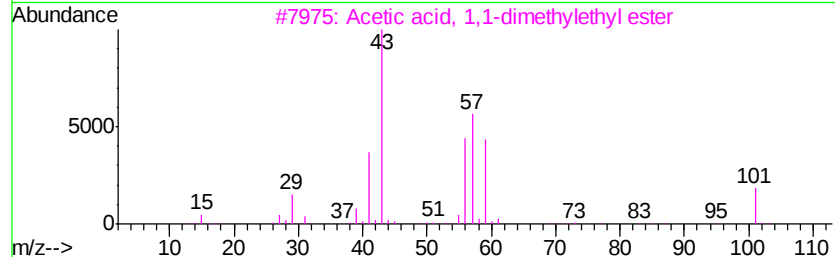
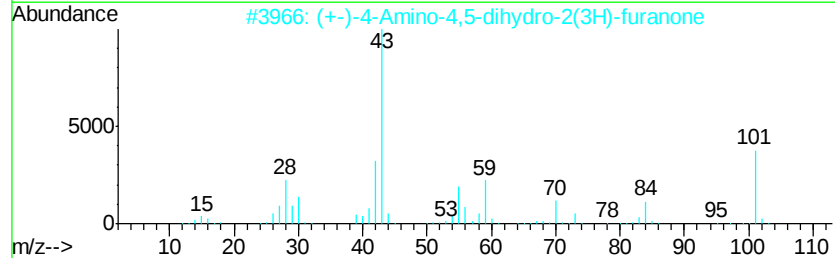
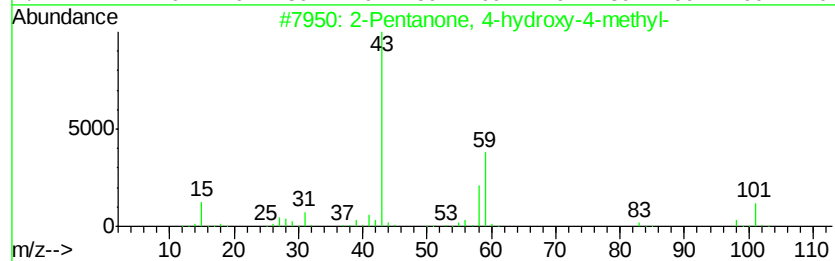
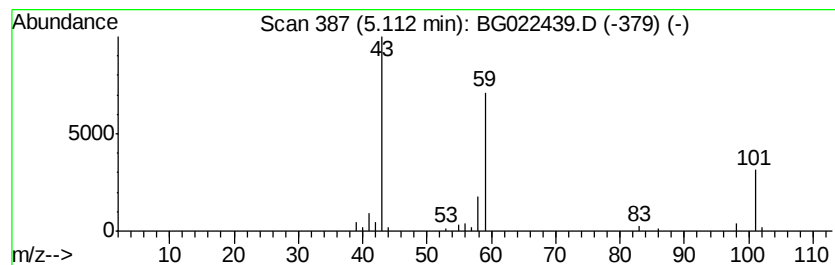
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	7.45 ng	61909	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	38
3		Acetic acid, 1,1-dimethylethyl ester	116	C6H12O2	000540-88-5	38
4		3-Hexanol	102	C6H14O	000623-37-0	25
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25



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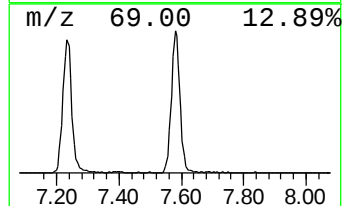
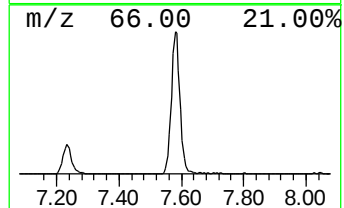
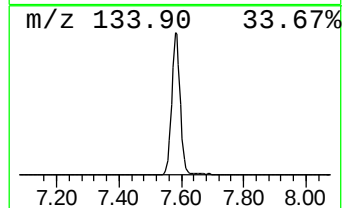
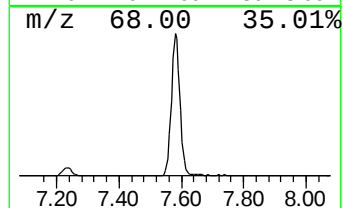
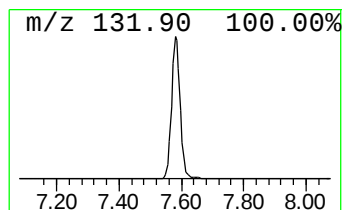
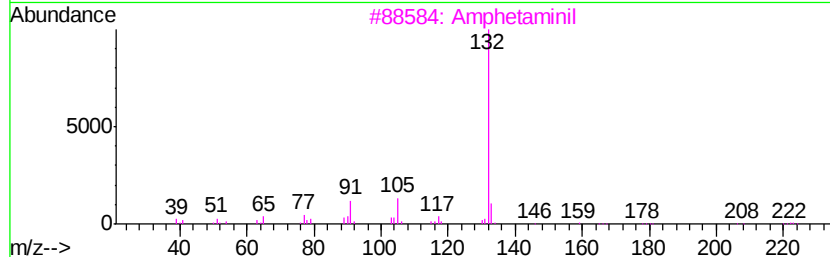
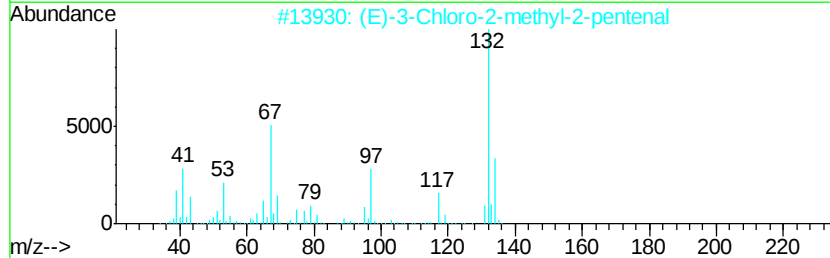
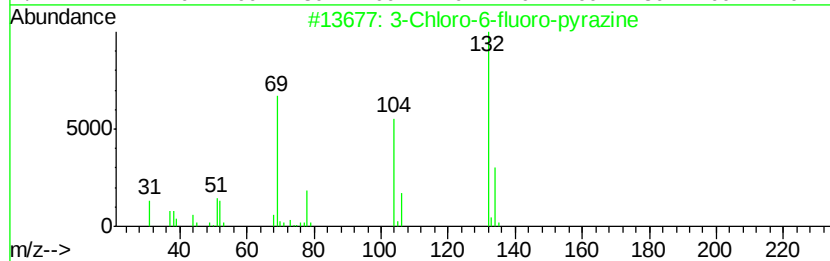
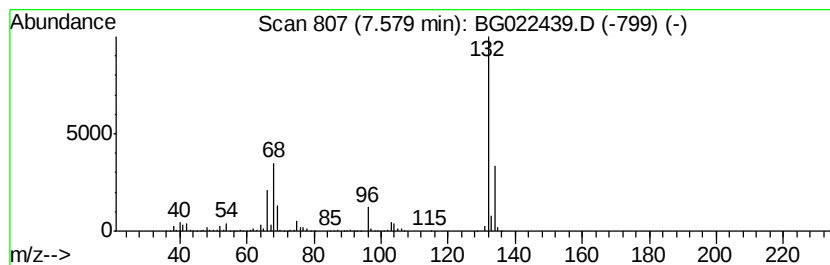
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Peak Number 3 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	125.62 ng	1043910	1,4-Dichlorobenzene-d4	8.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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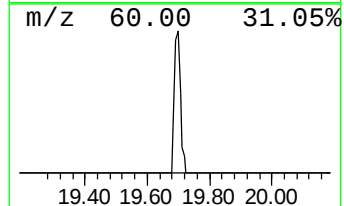
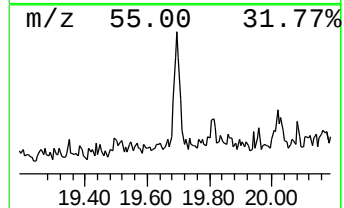
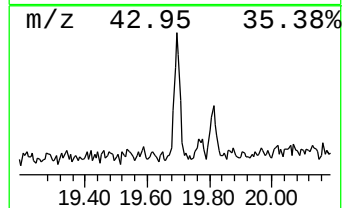
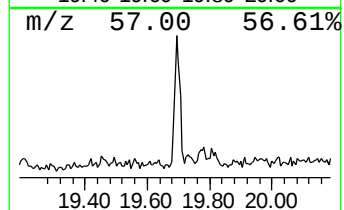
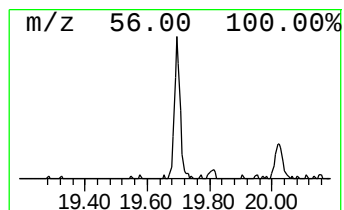
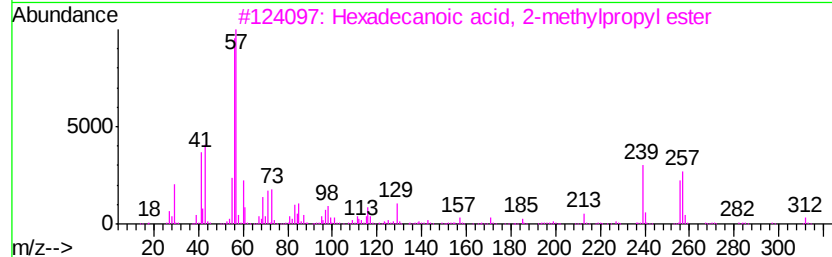
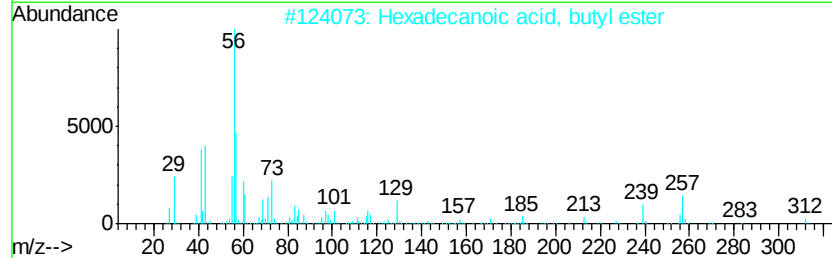
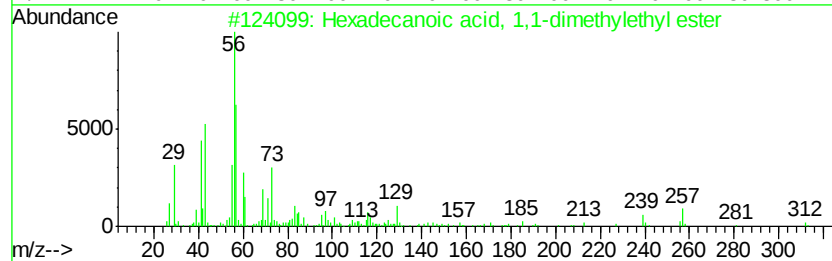
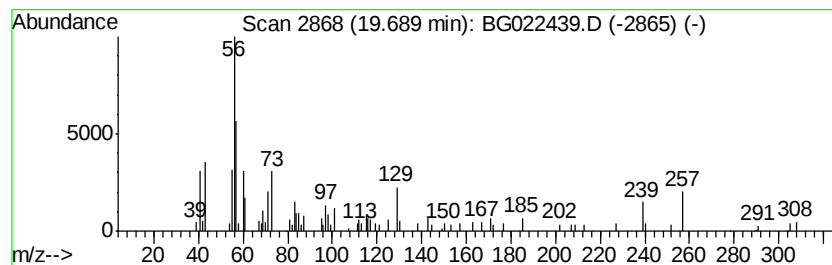
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	3.08 ng	63739	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	86
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	35



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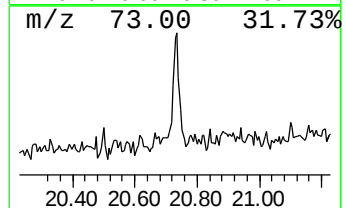
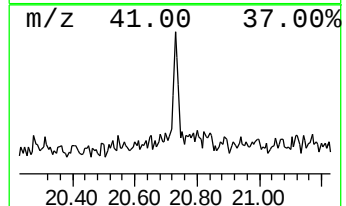
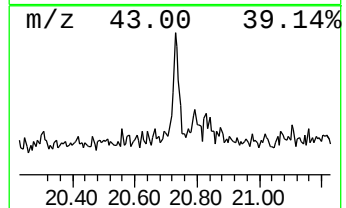
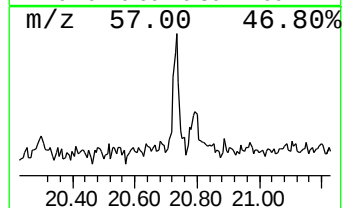
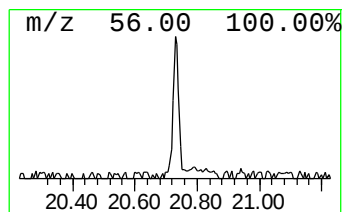
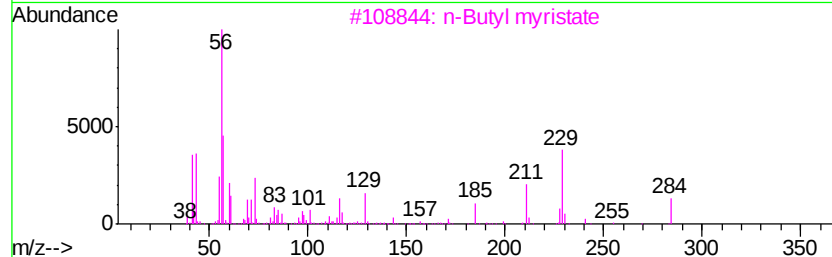
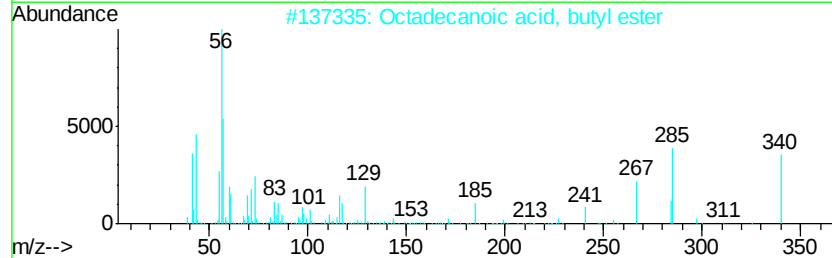
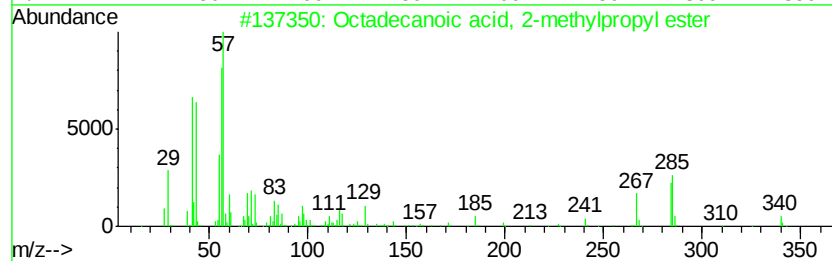
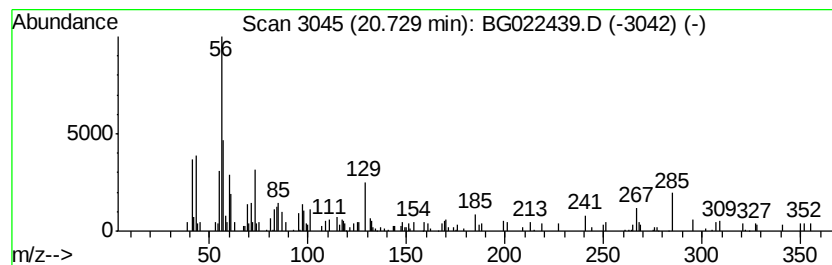
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Peak Number 6 Octadecanoic acid, 2-methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.73	2.57 ng	53233	Chrysene-d12	21.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	83
2		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	80
3		n-Butyl myristate	284	C18H36O2	000110-36-1	53
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Cyclohexanol, 2-amino-, cis-	115	C6H13NO	000931-15-7	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	2.87	329.1	ng	2734500	1	8.04	166196	20.0
2-Pentanone, 4-hy...	5.11	7.5	ng	61909	1	8.04	166196	20.0
unknown7.58	7.58	125.6	ng	1043910	1	8.04	166196	20.0
Hexadecanoic acid...	19.69	3.1	ng	63739	5	21.69	414146	20.0
Octadecanoic acid...	20.73	2.6	ng	53233	5	21.69	414146	20.0