

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061616\
 Data File : BG022388.D
 Acq On : 17 Jun 2016 5:40
 Operator : UM/SJ
 Sample : H3569-19
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-11-COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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	2.881	3	7	26	rVB	1098131	1751633	100.00%	15.182%
2	3.028	26	32	48	rVV	88301	196849	11.24%	1.706%
3	5.113	381	387	396	rVB	18817	34982	2.00%	0.303%
4	5.619	465	473	486	rBV	310365	619157	35.35%	5.367%
5	7.246	742	750	768	rBV	341823	718919	41.04%	6.231%
6	7.593	801	809	826	rBV	388901	757344	43.24%	6.564%
7	8.051	880	887	895	rBV	97248	186802	10.66%	1.619%
8	8.374	935	942	953	rBV	300865	601483	34.34%	5.213%
9	9.232	1079	1088	1104	rBV	195899	441698	25.22%	3.828%
10	10.871	1360	1367	1379	rBV	143281	320696	18.31%	2.780%
11	13.316	1775	1783	1803	rBV	689982	1295523	73.96%	11.229%
12	14.138	1916	1923	1939	rBV	126905	230248	13.14%	1.996%
13	14.690	2010	2017	2029	rBV2	253633	464717	26.53%	4.028%
14	15.507	2151	2156	2161	rVB	25669	35443	2.02%	0.307%
15	15.912	2216	2225	2229	rBV4	8842	20060	1.15%	0.174%
16	16.189	2265	2272	2287	rBV	380747	729345	41.64%	6.322%
17	16.365	2297	2302	2318	rVB	29928	58342	3.33%	0.506%
18	17.158	2432	2437	2442	rBV2	13667	20863	1.19%	0.181%
19	17.440	2476	2485	2500	rBV2	250485	492425	28.11%	4.268%
20	17.898	2558	2563	2571	rBV4	10444	18285	1.04%	0.158%
21	19.849	2887	2895	2901	rVB	9203	21208	1.21%	0.184%
22	20.037	2921	2927	2944	rBV	985789	1476844	84.31%	12.801%
23	21.312	3139	3144	3154	rBV4	46189	99747	5.69%	0.865%
24	21.706	3205	3211	3226	rBV	230443	486676	27.78%	4.218%
25	23.169	3454	3460	3467	rBV10	9871	21364	1.22%	0.185%
26	24.984	3756	3769	3788	rVB2	119107	436569	24.92%	3.784%

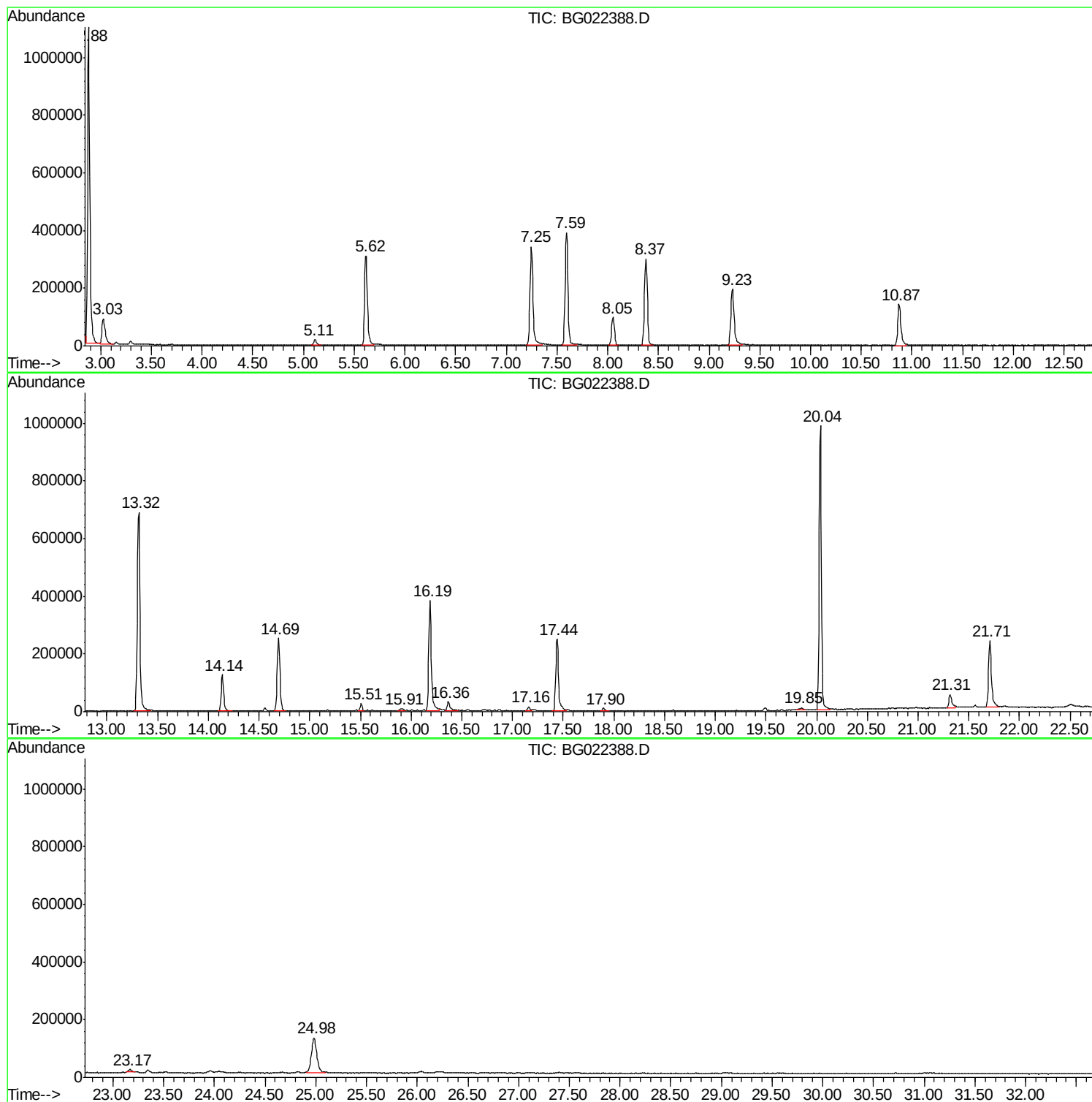
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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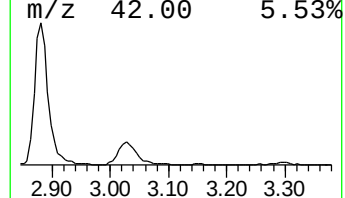
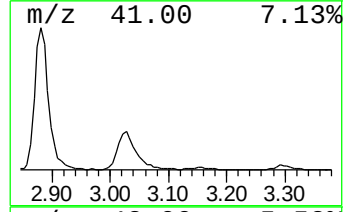
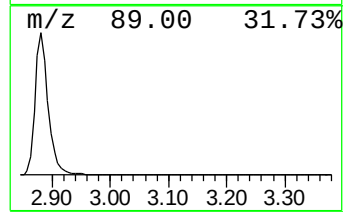
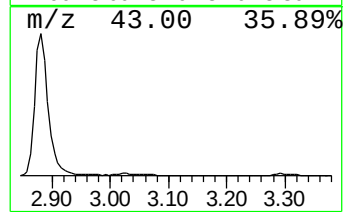
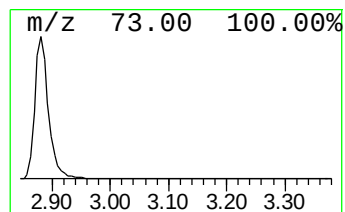
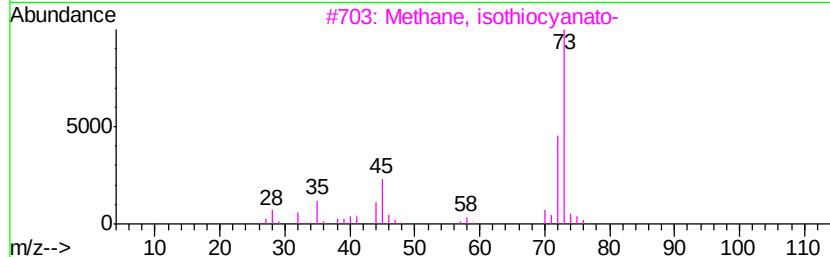
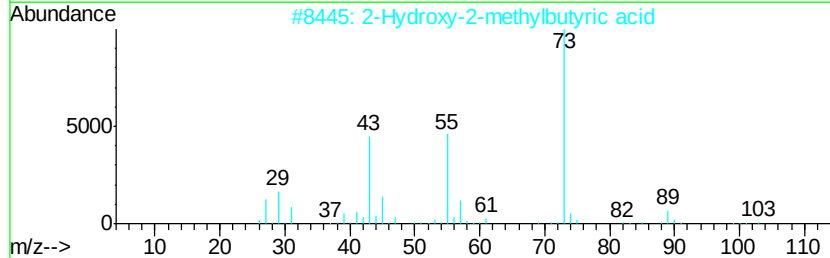
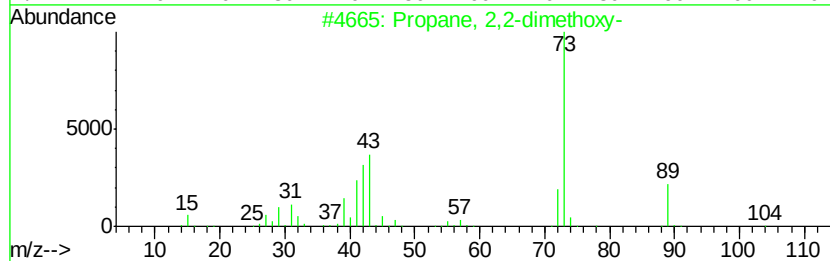
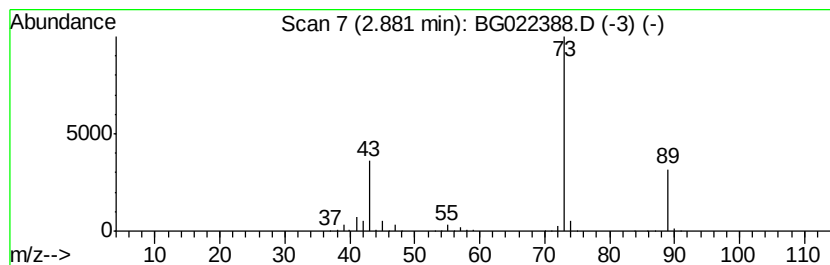
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.88 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	187.54 ng	1751630	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	28
3			Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7
4			N-Ethylformamide	73	C3H7NO	000627-45-2	7
5			1,3,5-Trioxane	90	C3H6O3	000110-88-3	4



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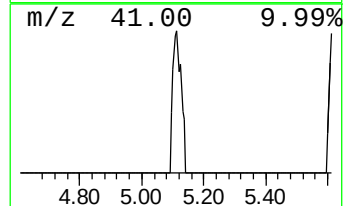
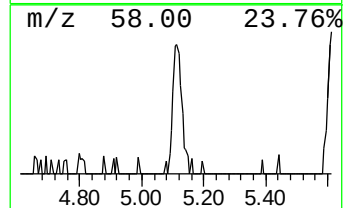
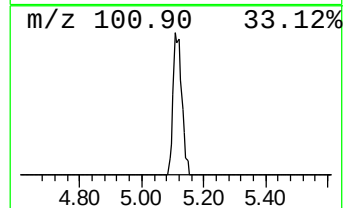
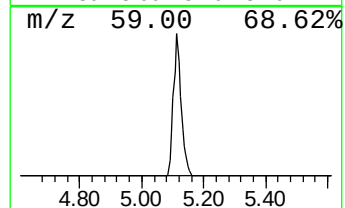
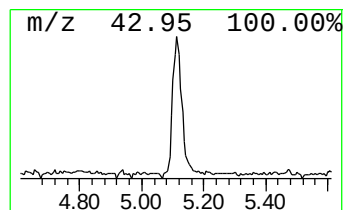
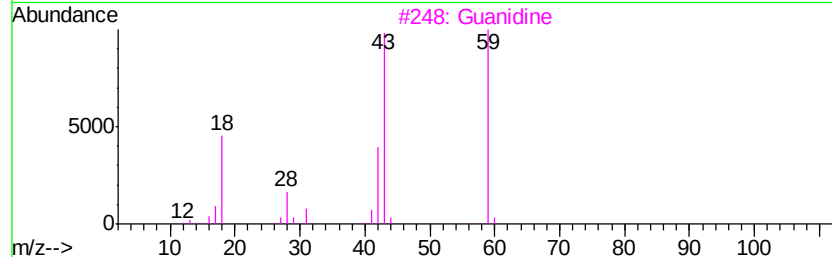
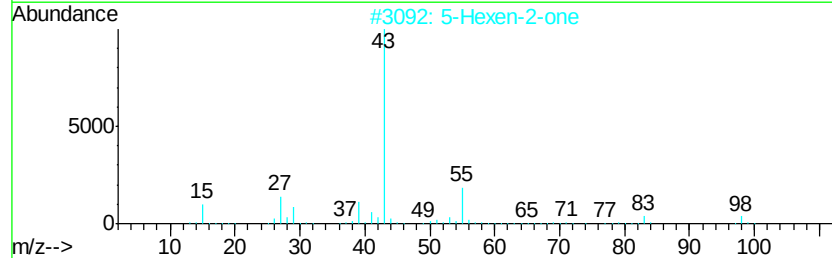
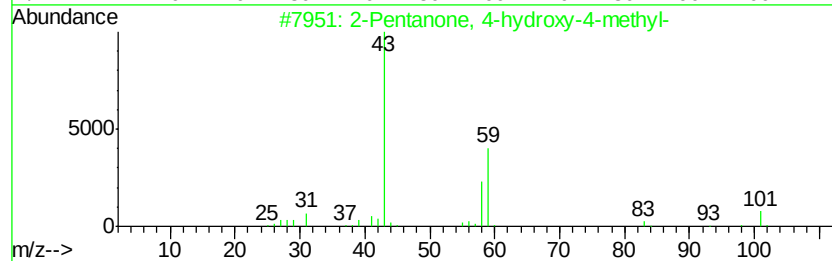
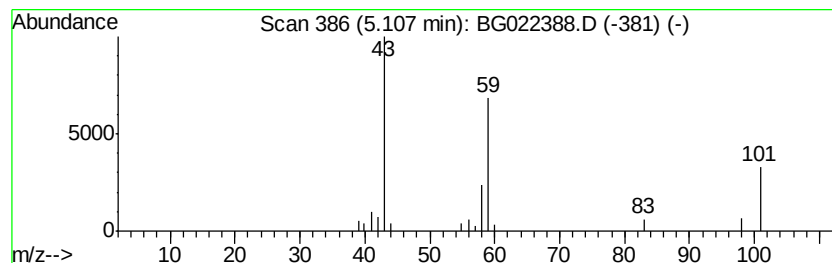
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	3.75 ng	34982	1,4-Dichlorobenzene-d4	8.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Guanidine	59	CH5N3	000113-00-8	9
4		2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	9
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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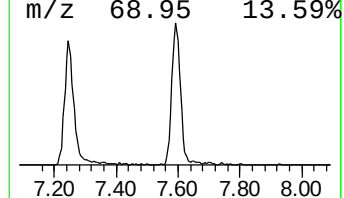
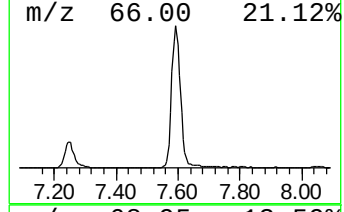
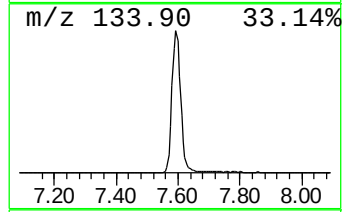
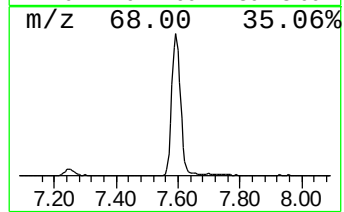
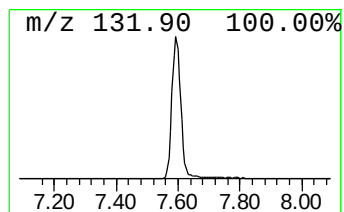
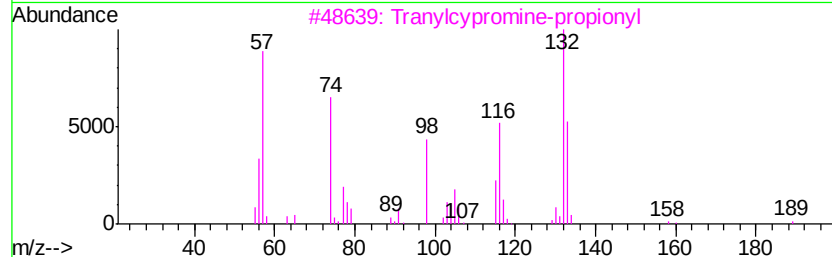
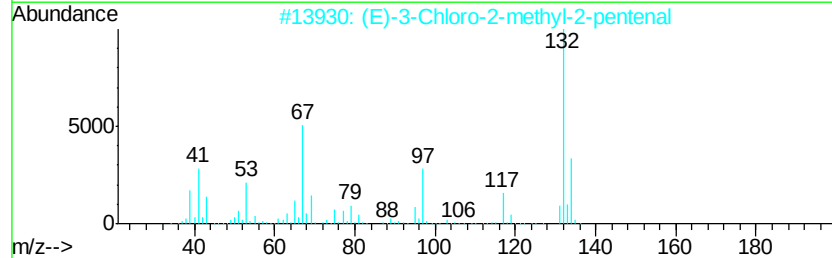
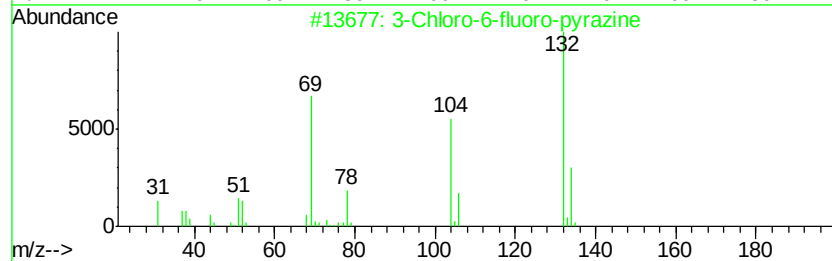
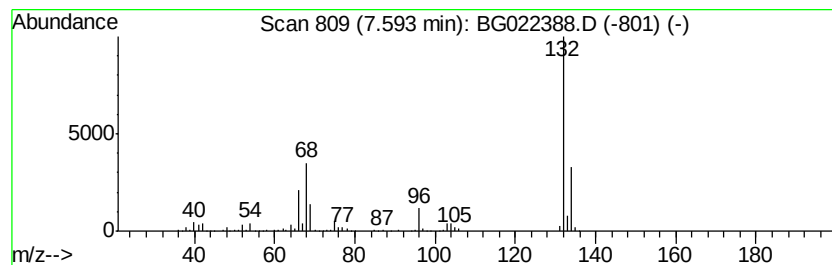
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	81.09 ng	757344	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Amphetaminil	250	C17H18N2	017590-01-1	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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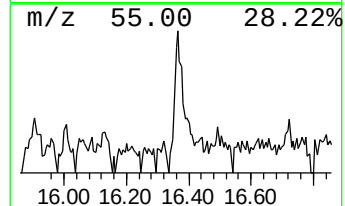
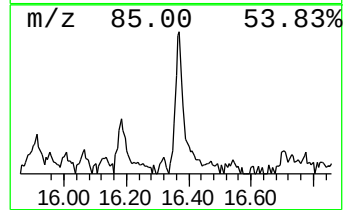
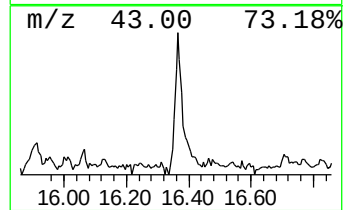
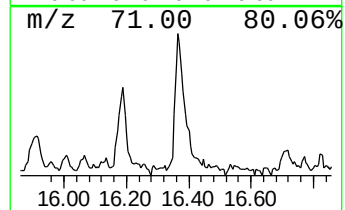
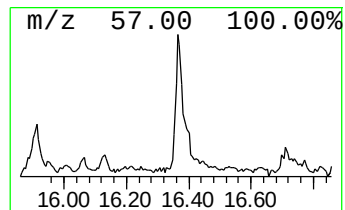
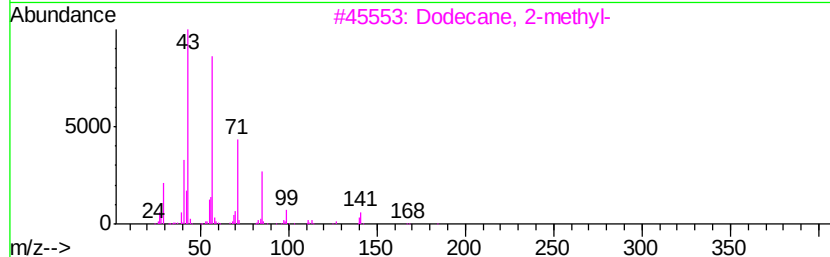
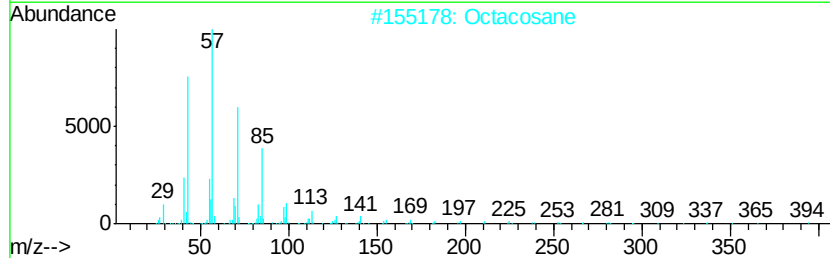
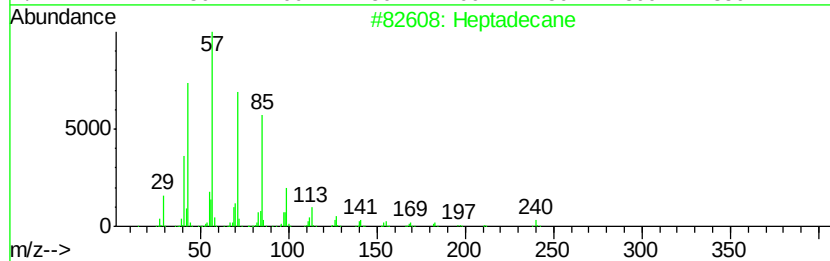
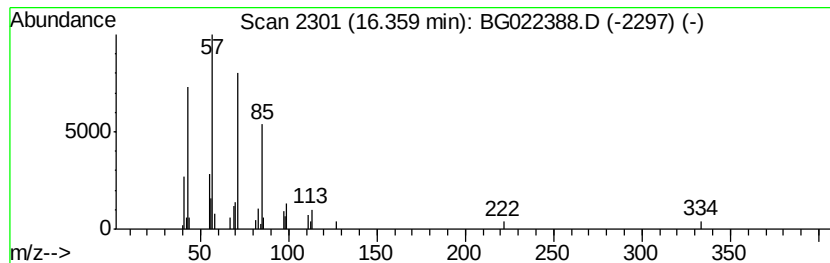
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.36	2.37 ng	58342	Phenanthrene-d10	17.44	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	78
4	Eicosane	282	C20H42	000112-95-8	72
5	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	64



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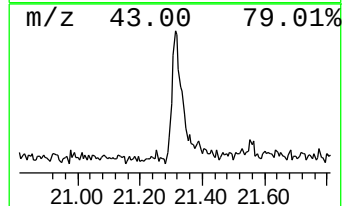
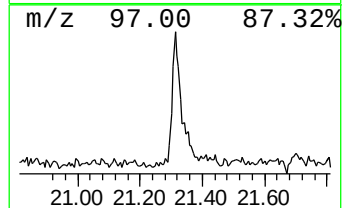
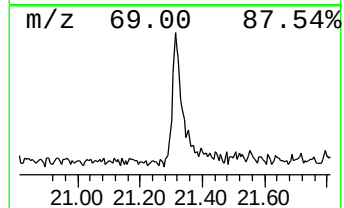
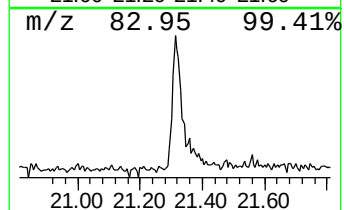
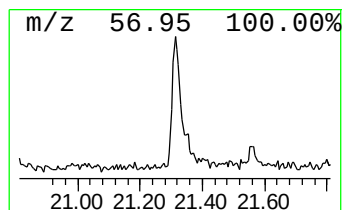
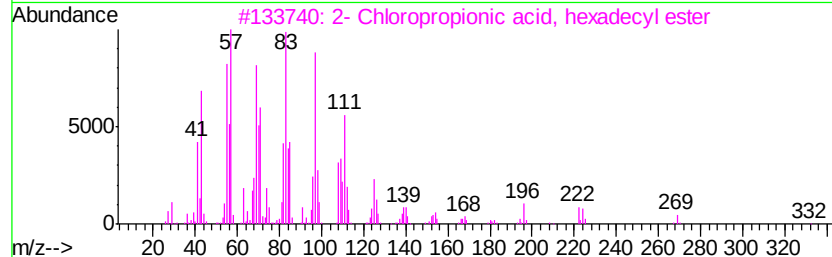
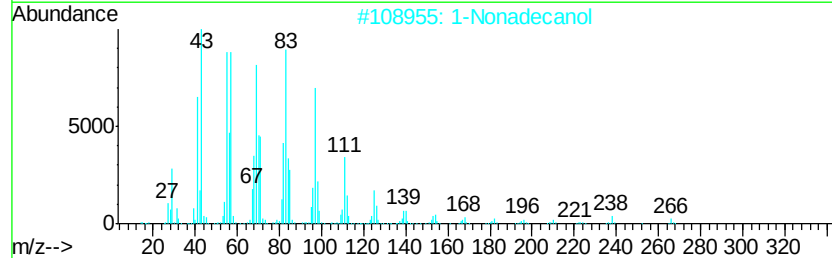
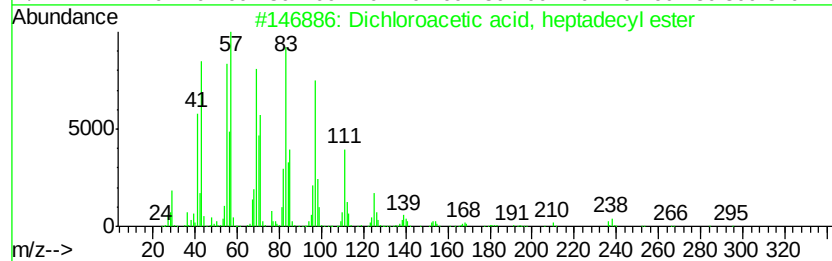
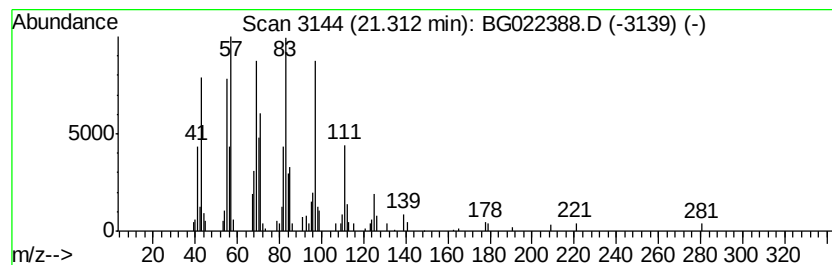
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	4.10 ng	99747	Chrysene-d12	21.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2		1-Nonadecanol	284	C19H40O	001454-84-8	91
3		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4		1-Octadecanol	270	C18H38O	000112-92-5	91
5		Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
unknown2.88	2.88	187.5	ng	1751630	1	8.05	186802	20.0
2-Pentanone, 4-hy...	5.11	3.8	ng	34982	1	8.05	186802	20.0
unknown7.59	7.59	81.1	ng	757344	1	8.05	186802	20.0
Heptadecane	16.36	2.4	ng	58342	4	17.44	492425	20.0
Dichloroacetic ac...	21.31	4.1	ng	99747	5	21.71	486676	20.0