

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051415\
 Data File : BG017146.D
 Acq On : 14 May 2015 18:24
 Operator : TP/IZ
 Sample : G2225-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DCW-WW-141-51215

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-BG051315.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	2.794	14	18	27	rVB	149862	240389	5.17%	1.144%
2	2.876	27	32	38	rBV	627799	765063	16.46%	3.642%
3	4.815	358	362	368	rVB	105730	136628	2.94%	0.650%
4	5.297	438	444	453	rBV	495919	712769	15.33%	3.393%
5	6.901	711	717	730	rVB	326343	505088	10.86%	2.404%
6	7.248	769	776	784	rBV	960708	1462946	31.47%	6.964%
7	7.706	849	854	862	rVB	216096	325377	7.00%	1.549%
8	8.023	900	908	917	rBV	841959	1352599	29.10%	6.439%
9	8.869	1044	1052	1060	rBV	750274	1247474	26.83%	5.938%
10	10.497	1321	1329	1336	rBV	277395	477441	10.27%	2.273%
11	12.982	1744	1752	1758	rBV	1884192	2772634	59.64%	13.198%
12	13.816	1890	1894	1902	rVB	81908	117991	2.54%	0.562%
13	14.363	1979	1987	1994	rBV2	441131	675652	14.53%	3.216%
14	15.855	2232	2241	2250	rBV	1738082	2428731	52.24%	11.561%
15	17.107	2443	2454	2460	rBV	627101	859965	18.50%	4.094%
16	18.011	2602	2608	2617	rBV2	95851	148635	3.20%	0.708%
17	18.875	2750	2755	2757	rBV2	48493	63315	1.36%	0.301%
18	19.292	2822	2826	2833	rBV3	60107	83720	1.80%	0.399%
19	19.745	2896	2903	2909	rBV	3801372	4648886	100.00%	22.130%
20	20.385	3008	3012	3016	rBV	73194	75484	1.62%	0.359%
21	21.008	3114	3118	3125	rBV2	79906	120611	2.59%	0.574%
22	21.290	3161	3166	3172	rBV	739201	907989	19.53%	4.322%
23	23.558	3544	3552	3561	rVB2	441087	878191	18.89%	4.180%

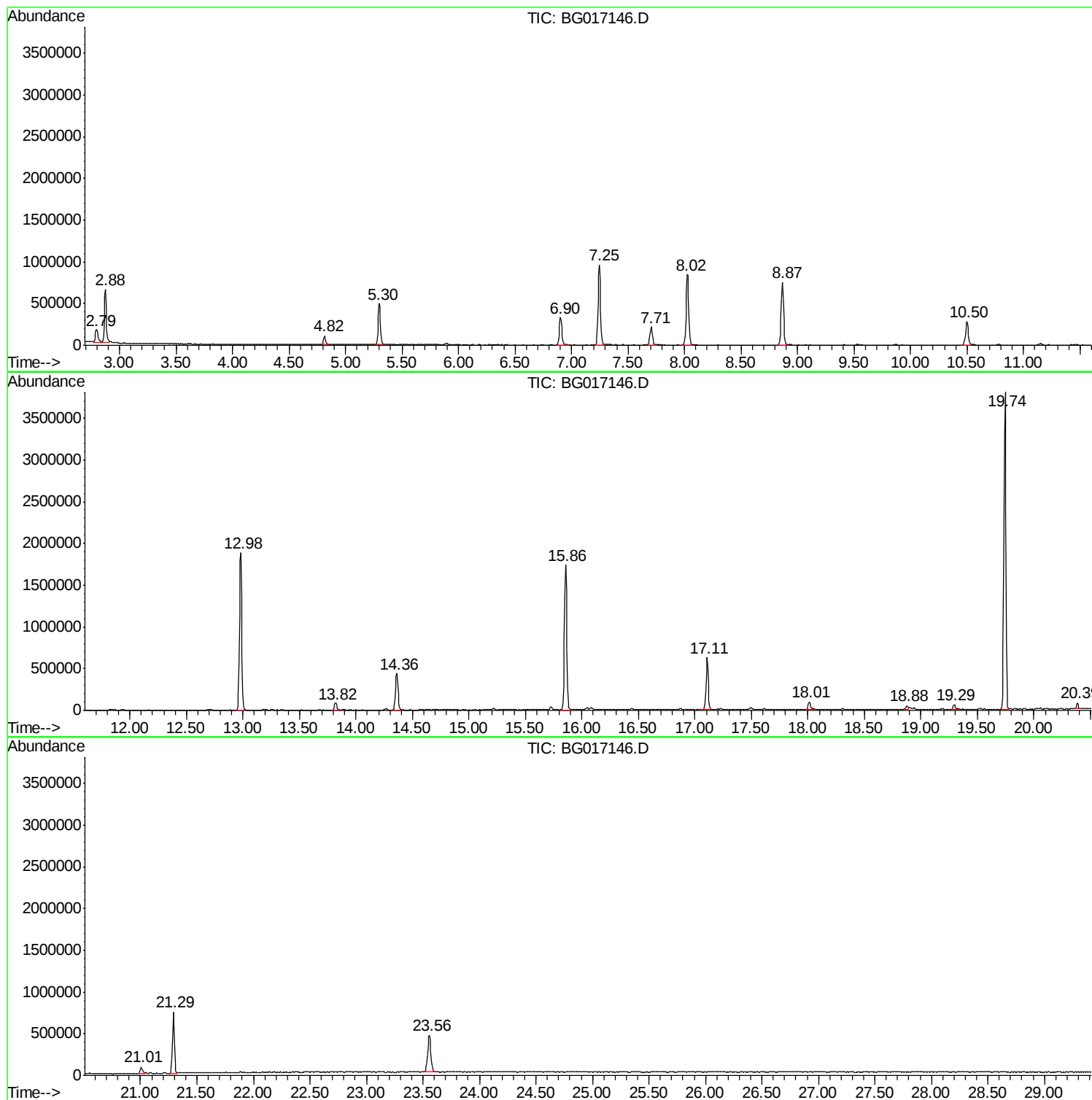
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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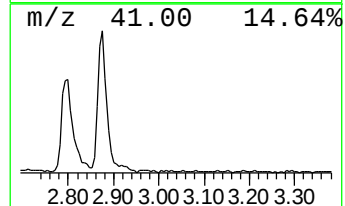
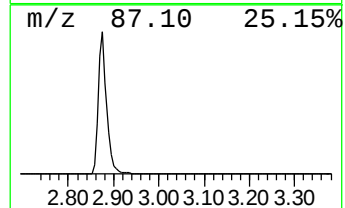
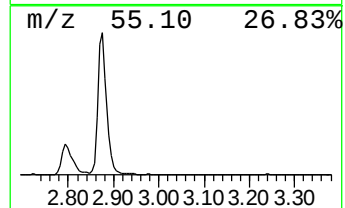
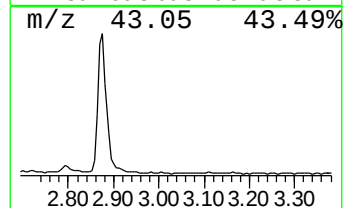
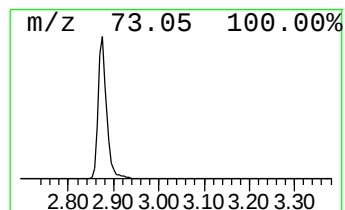
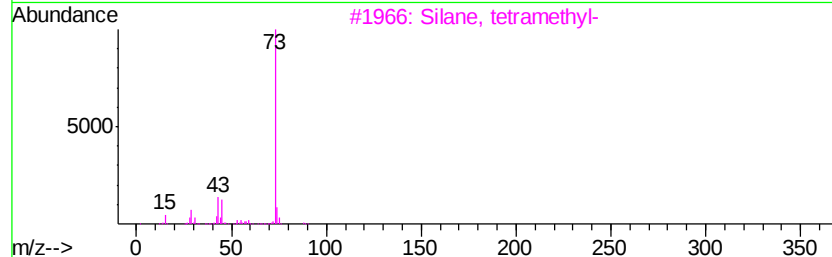
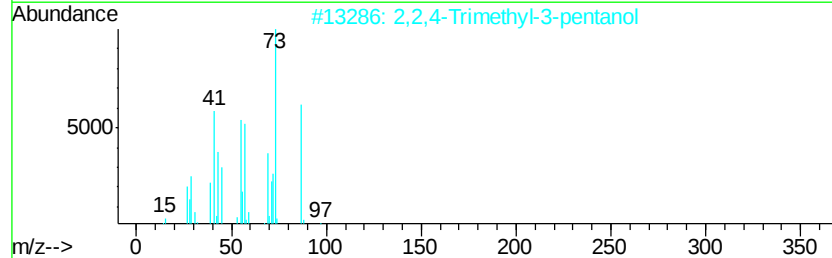
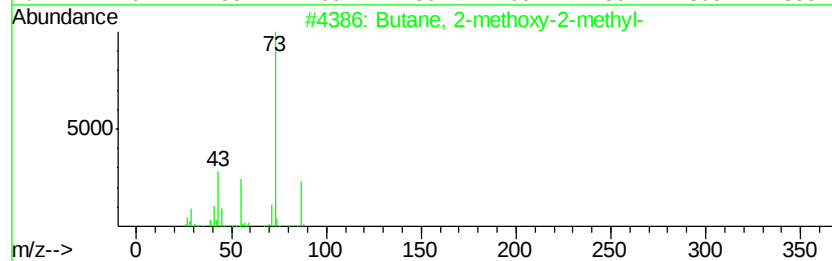
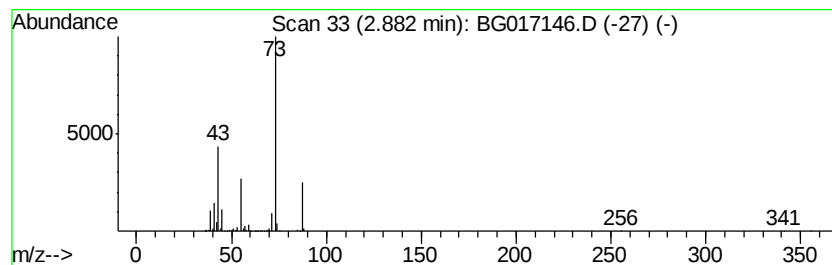
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	47.03 ng	765063	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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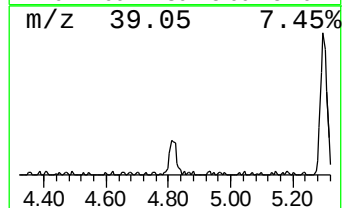
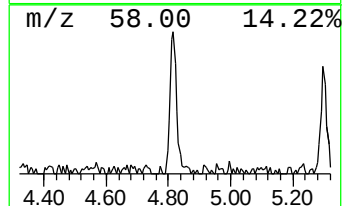
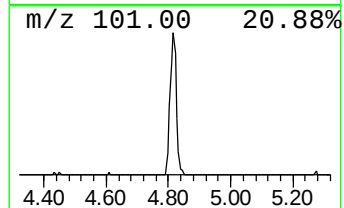
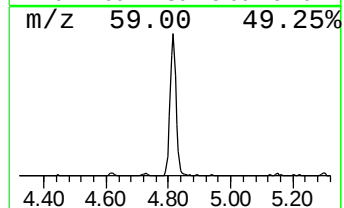
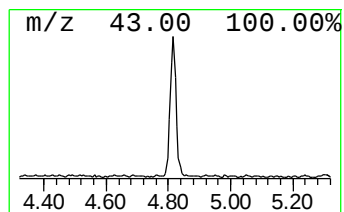
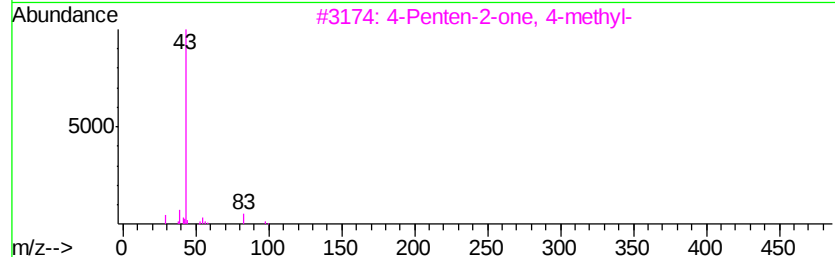
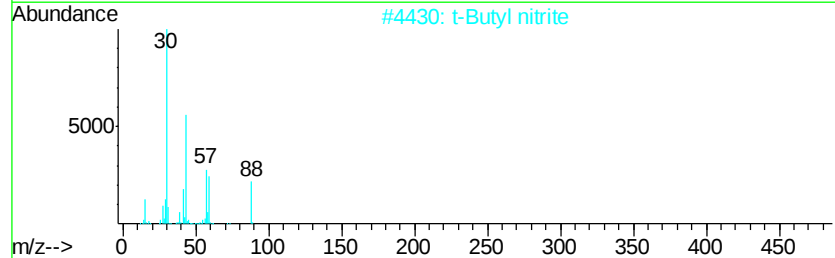
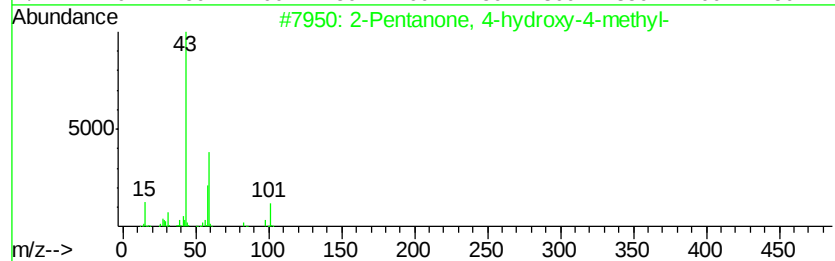
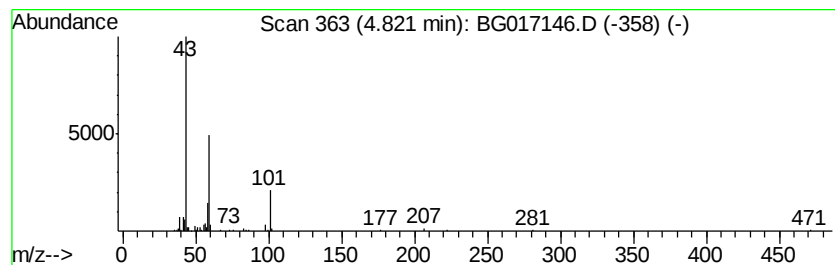
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.82	8.40 ng	136628	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		t-Butyl nitrite	103	C4H9NO2	000540-80-7	45
3		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9



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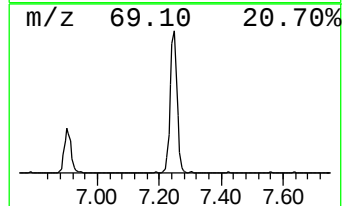
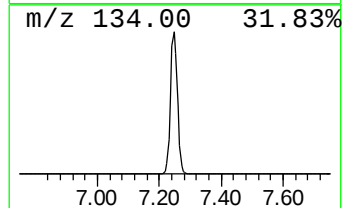
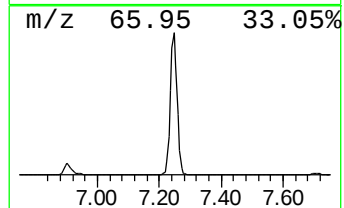
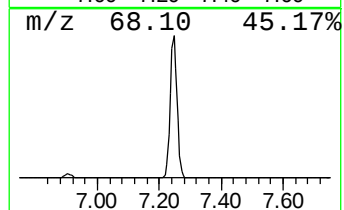
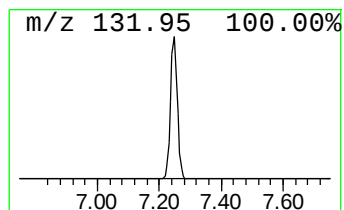
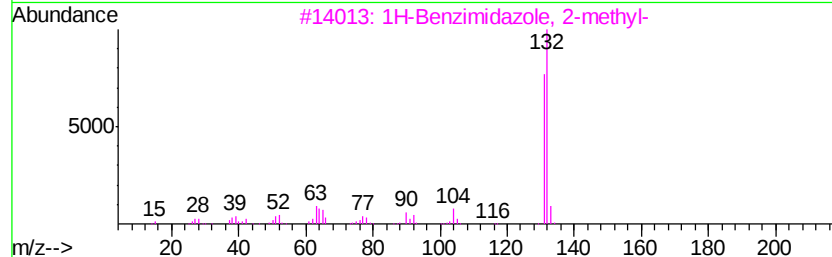
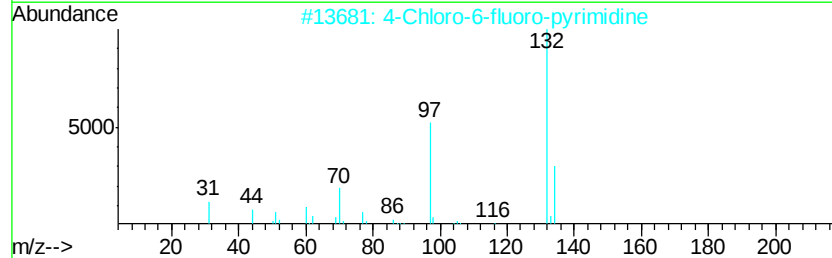
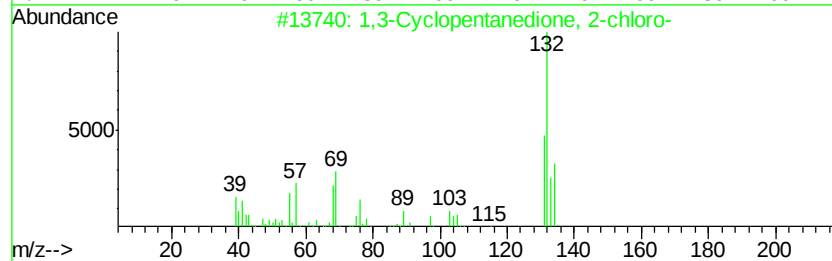
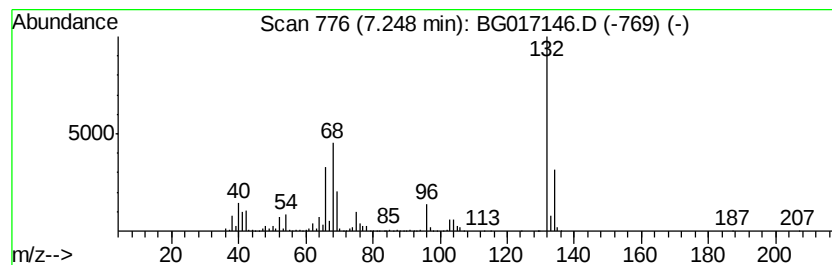
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.25 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.25	89.92 ng	1462950	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	35
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		5-Aminoindole	132	C8H8N2	005192-03-0	22



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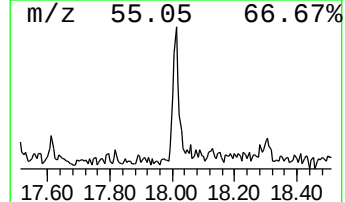
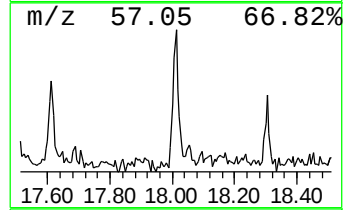
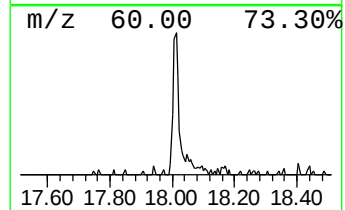
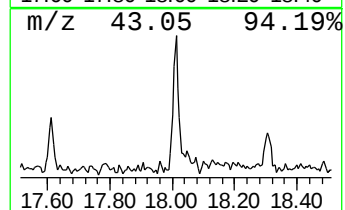
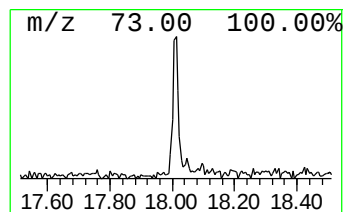
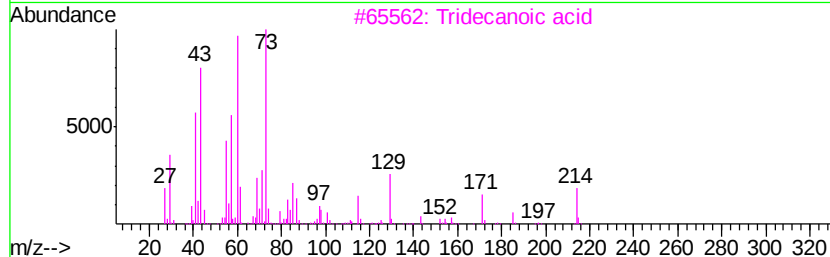
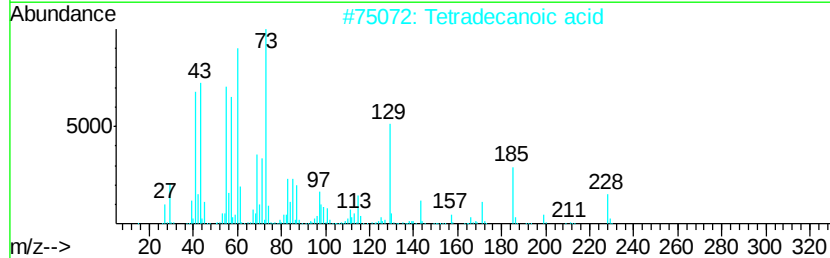
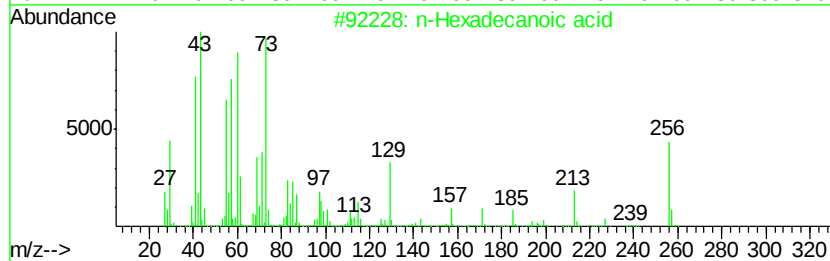
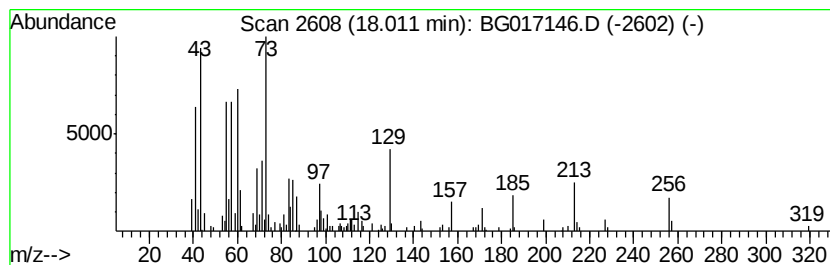
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.01	3.46 ng	148635	Phenanthrene-d10	17.11	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47



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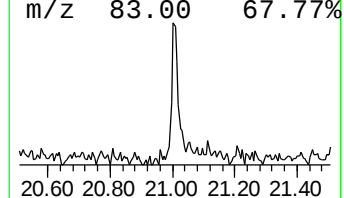
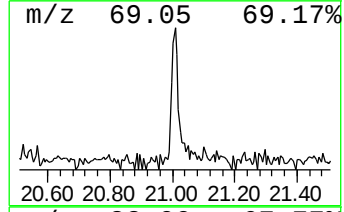
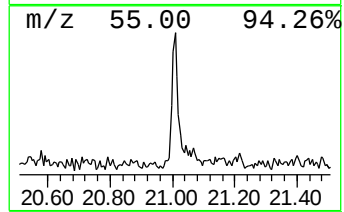
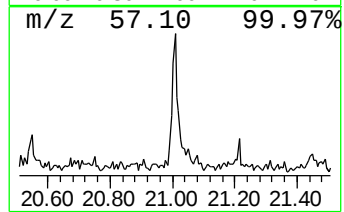
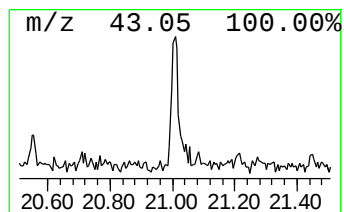
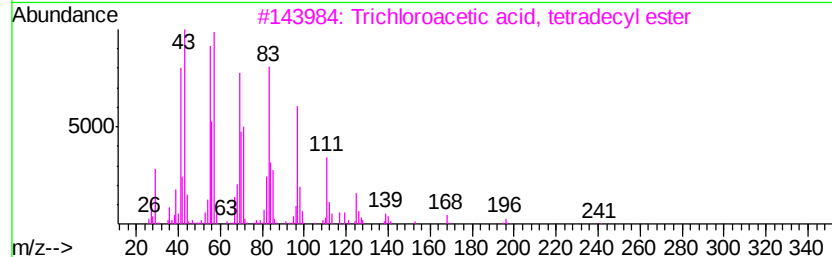
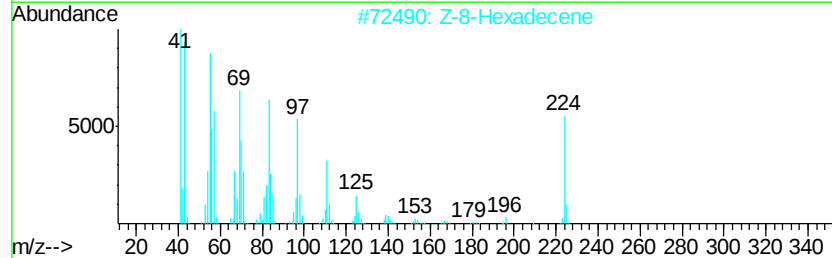
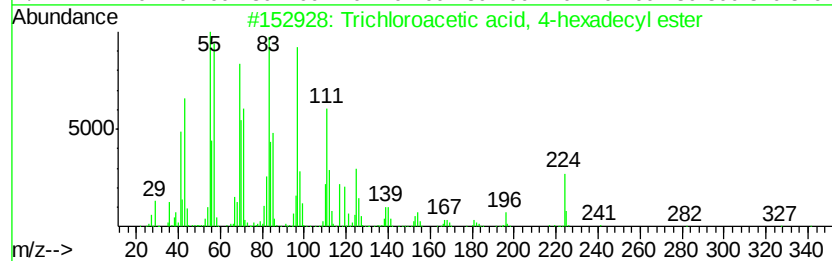
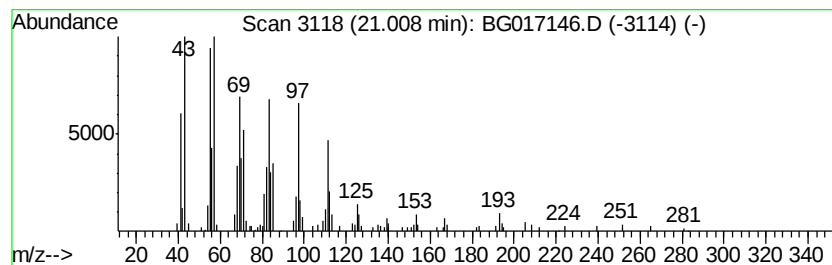
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Trichloroacetic acid, 4-hex... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.01	2.66 ng	120611	Chrysene-d12	21.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, 4-hexadecy...	386	C18H33Cl3O2	1000282-92-4	91
2			Z-8-Hexadecene	224	C16H32	1000130-87-5	90
3			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87
4			Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	87
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.88	47.0	ng	765063	1	7.71	325377	20.0
2-Pentanone, 4-hy...	4.82	8.4	ng	136628	1	7.71	325377	20.0
unknown7.25	7.25	89.9	ng	1462950	1	7.71	325377	20.0
n-Hexadecanoic acid	18.01	3.5	ng	148635	4	17.11	859965	20.0
Trichloroacetic a...	21.01	2.7	ng	120611	5	21.29	907989	20.0