

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061115\
 Data File : BF079920.D
 Acq On : 12 Jun 2015 4:50
 Operator : TP/IZ
 Sample : G2573-03
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S3

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_F\METHODS\8270-BF061115.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	2.170	85	86	93	rVV	170592	241420	3.78%	0.734%
2	2.284	93	96	98	rVV	4381993	6393033	100.00%	19.448%
3	2.353	98	102	123	rVB	698542	1646130	25.75%	5.008%
4	2.707	130	133	141	rVB	296936	458936	7.18%	1.396%
5	5.621	384	388	397	rBV	187184	253541	3.97%	0.771%
6	6.010	419	422	424	rBV	2293822	2241083	35.06%	6.817%
7	6.993	506	508	510	rBV	2659473	2238821	35.02%	6.811%
8	7.164	520	523	525	rBV	2097416	2337666	36.57%	7.111%
9	7.393	541	543	545	rVB	506981	400226	6.26%	1.218%
10	7.553	555	557	559	rBV	2193773	1769057	27.67%	5.382%
11	7.953	589	592	594	rBV	1295959	1332177	20.84%	4.053%
12	8.685	654	656	658	rVB	736085	581297	9.09%	1.768%
13	9.759	748	750	753	rVB	3229244	2904117	45.43%	8.834%
14	10.148	782	784	786	rBV	249642	191075	2.99%	0.581%
15	10.456	809	811	814	rBV	724903	708022	11.07%	2.154%
16	11.256	878	881	883	rBV	2037321	1896571	29.67%	5.769%
17	11.965	941	943	945	rBV	1035284	876417	13.71%	2.666%
18	13.634	1086	1089	1091	rBV	3359914	4193651	65.60%	12.757%
19	14.639	1175	1177	1181	rBV	149811	218250	3.41%	0.664%
20	14.868	1194	1197	1199	rBV	912262	1016472	15.90%	3.092%
21	16.731	1357	1360	1373	rVB	590762	974736	15.25%	2.965%

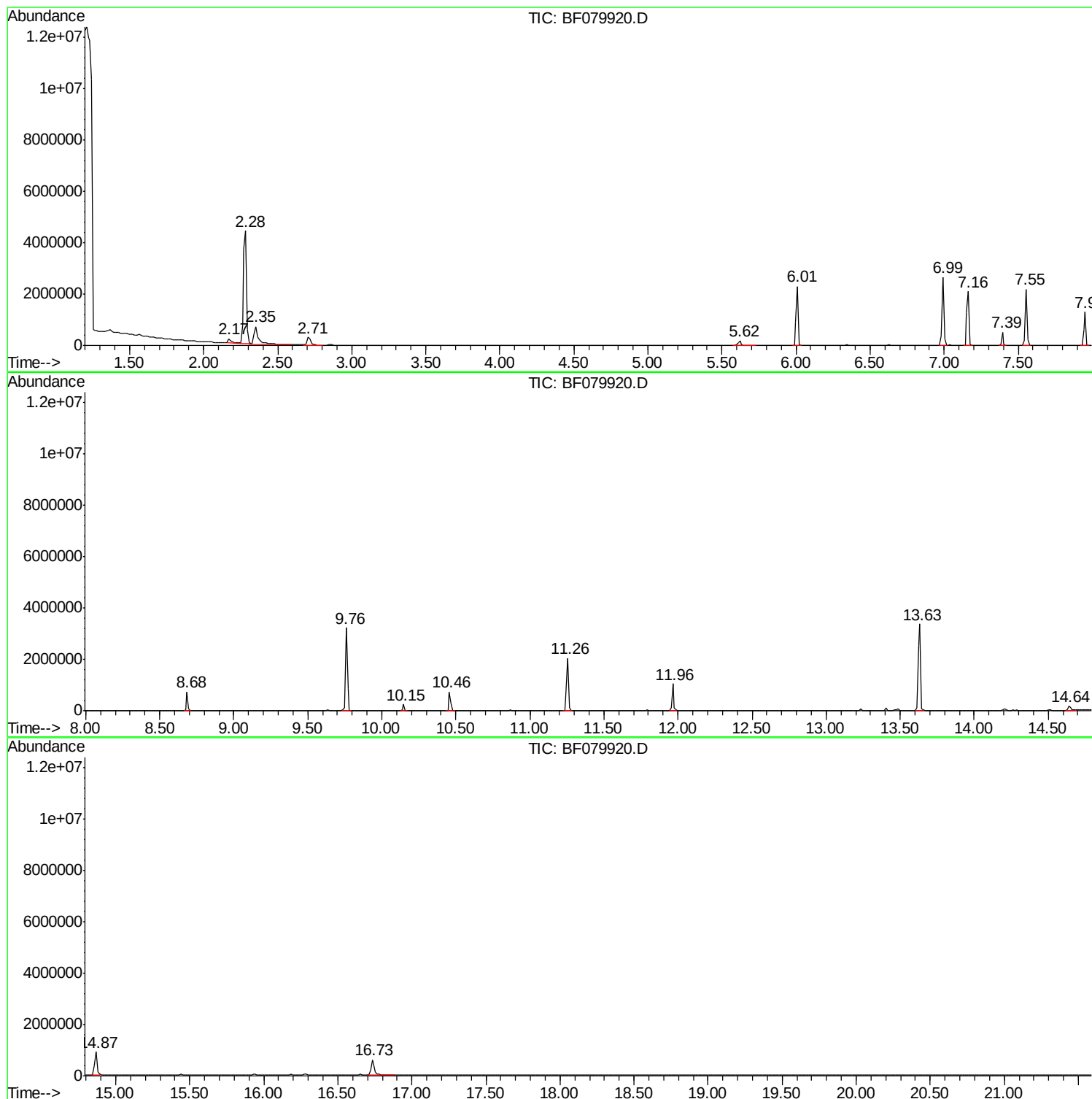
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF061115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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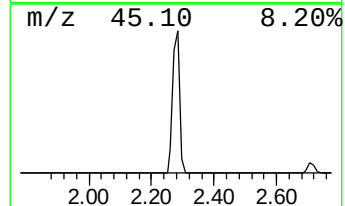
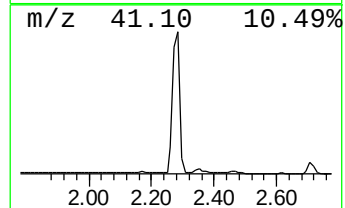
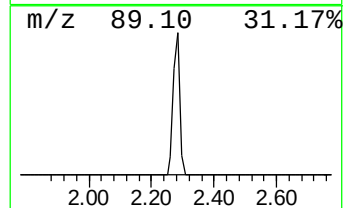
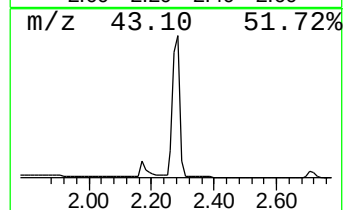
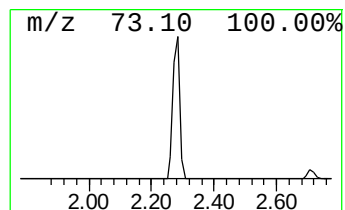
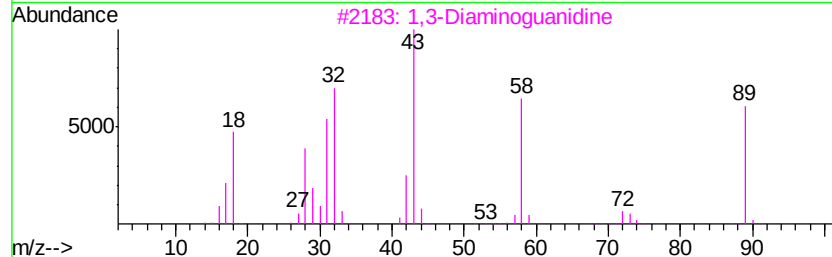
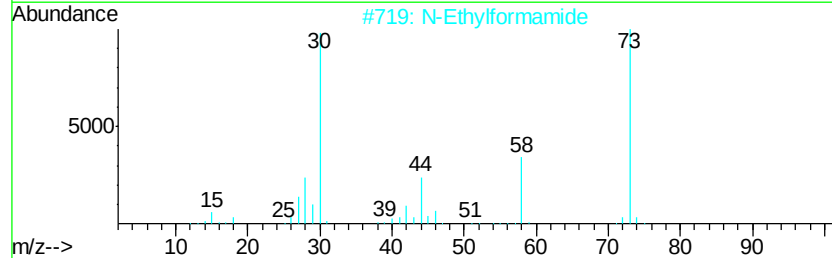
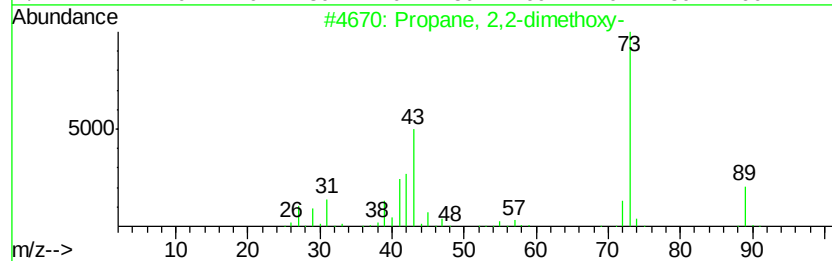
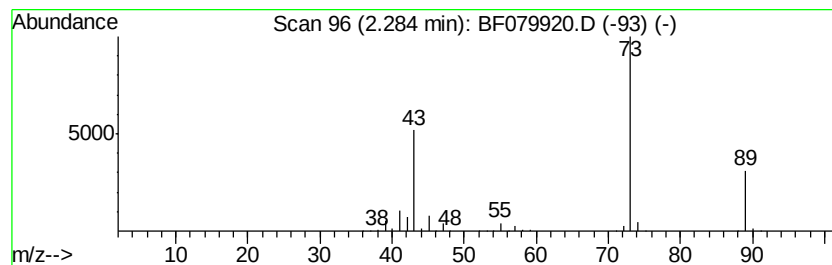
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.28	319.47 ng	6393030	1,4-Dichlorobenzene-d4	7.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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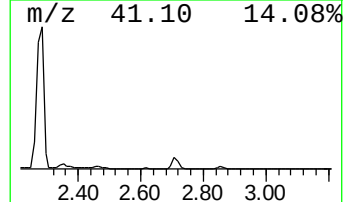
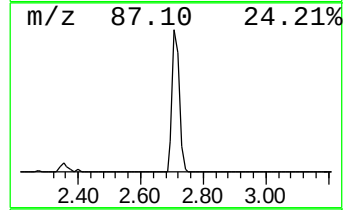
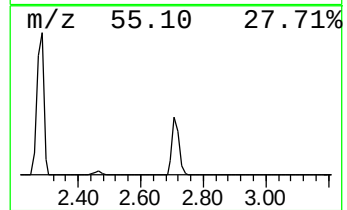
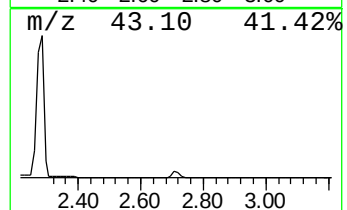
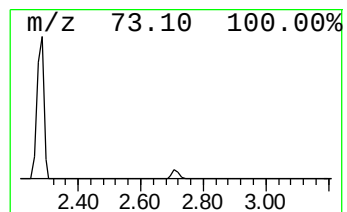
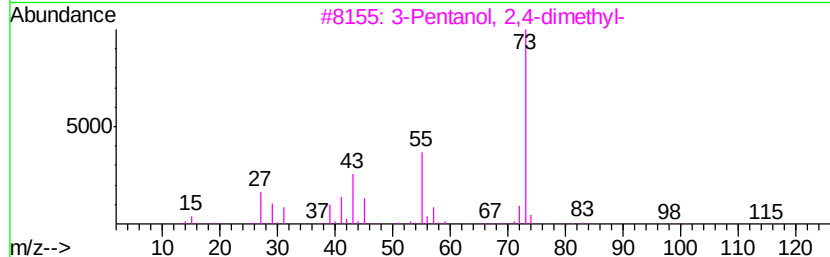
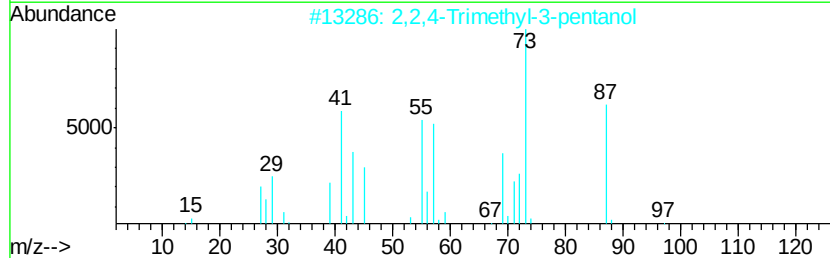
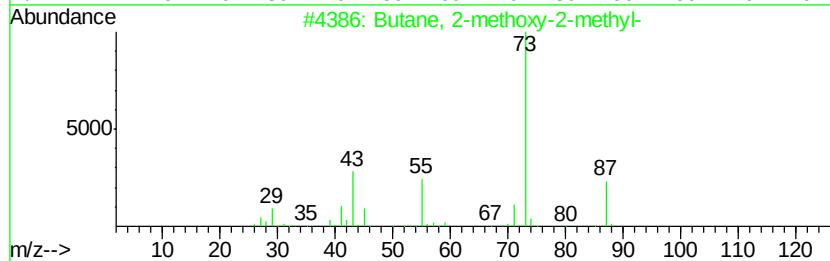
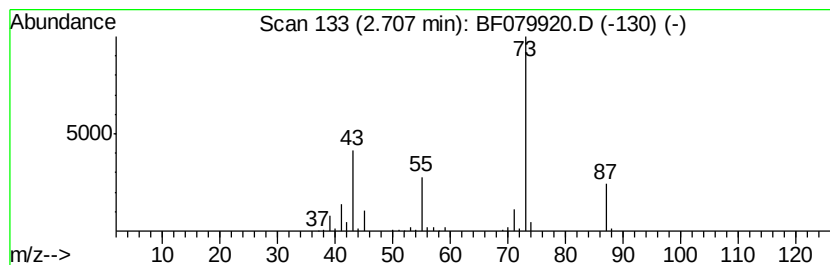
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Peak Number 4 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.71	22.93 ng	458936	1,4-Dichlorobenzene-d4	7.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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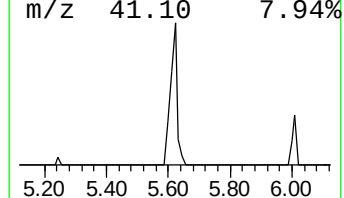
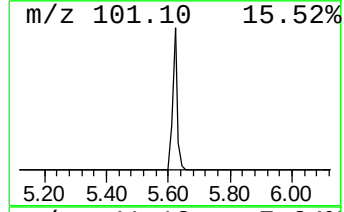
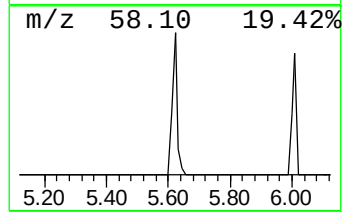
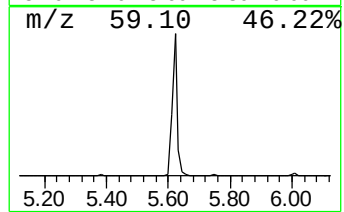
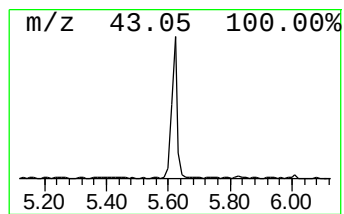
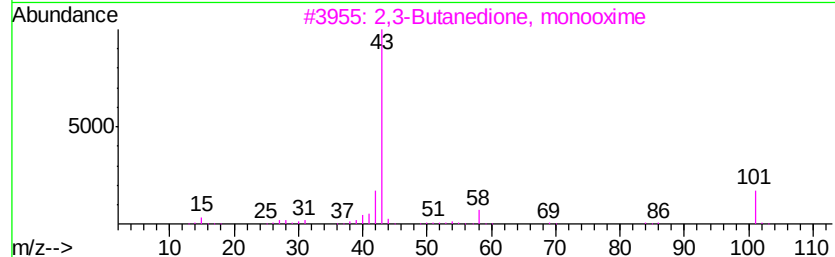
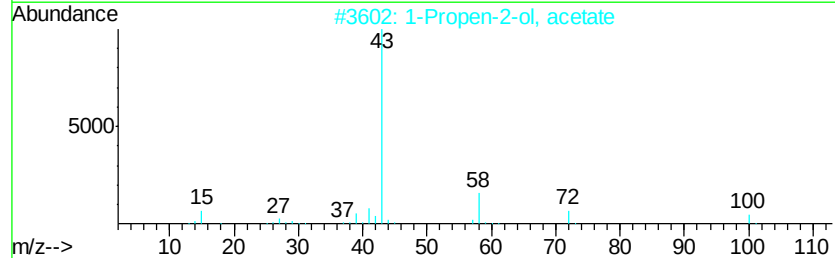
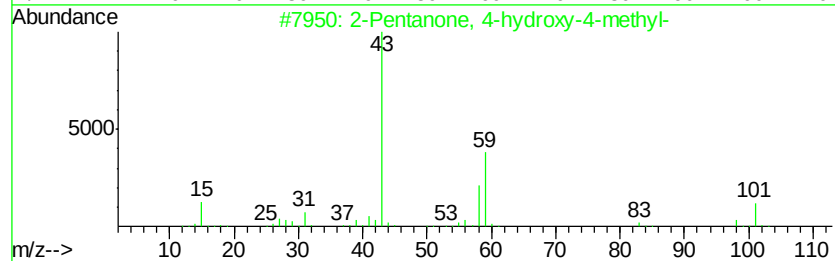
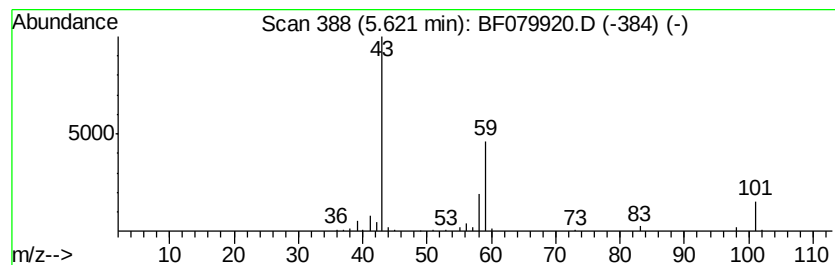
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.62	12.67 ng	253541	1,4-Dichlorobenzene-d4	7.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83		
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		
4	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9		
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		



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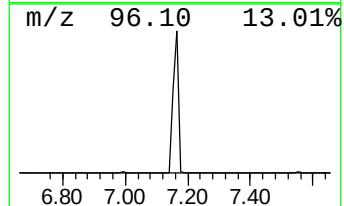
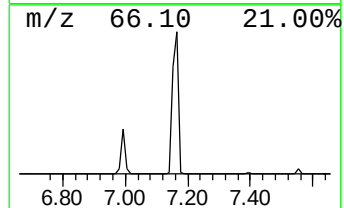
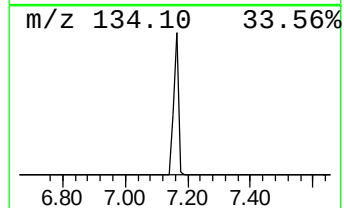
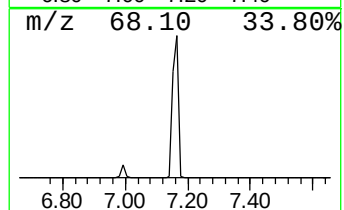
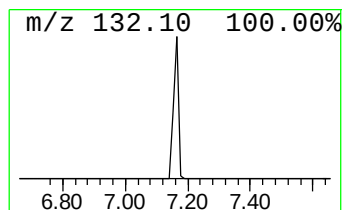
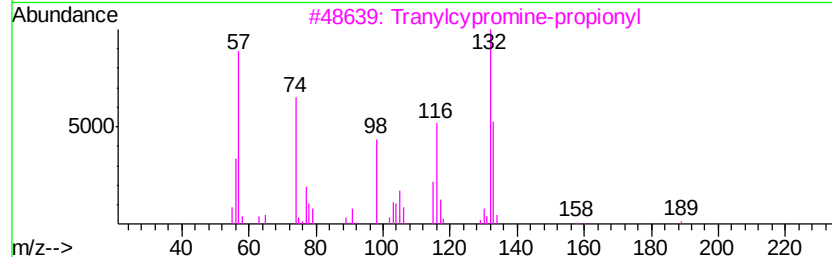
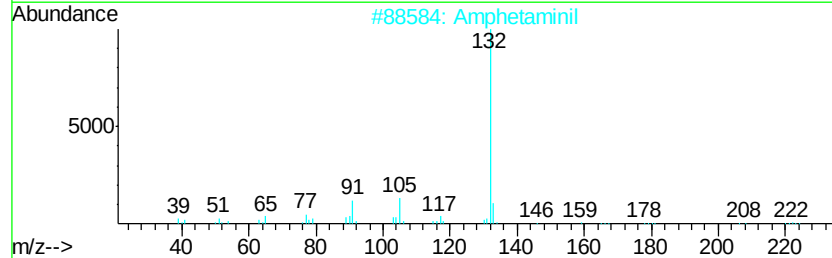
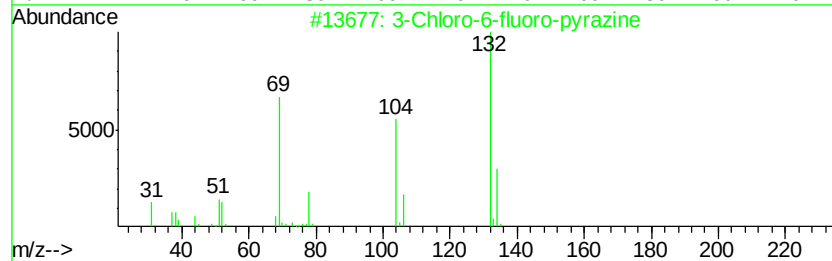
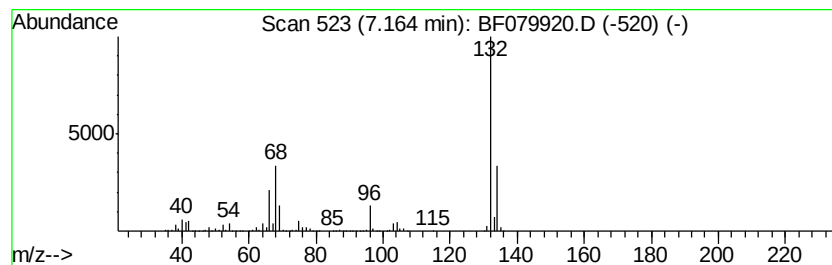
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown7.16 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	116.82 ng	2337670	1,4-Dichlorobenzene-d4	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	Amphetaminil	250	C17H18N2	017590-01-1	12
3	Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
5	Xenon	132	Xe	007440-63-3	9



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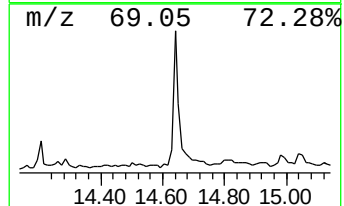
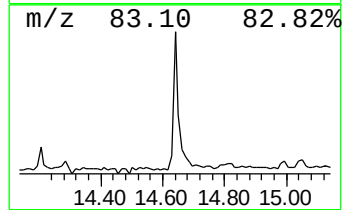
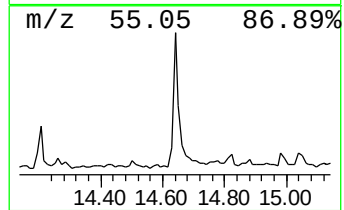
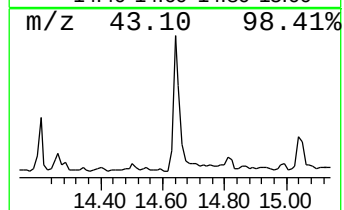
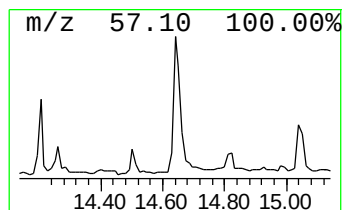
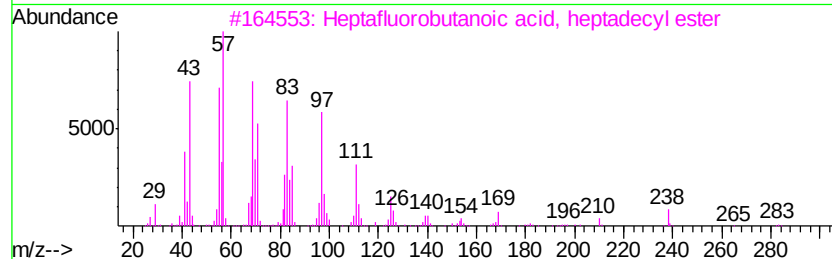
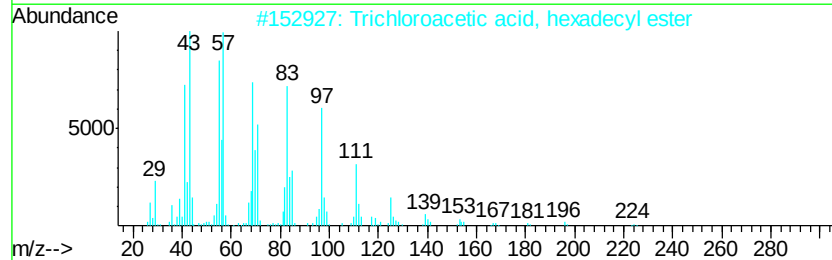
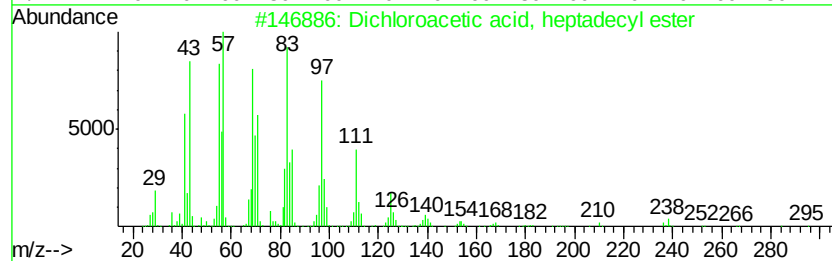
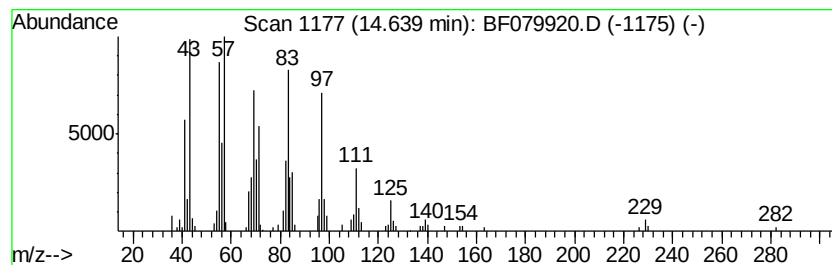
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	4.29 ng	218250	Chrysene-d12	14.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
4		1-Docosene	308	C22H44	001599-67-3	91
5		1-Tetracosanol	354	C24H50O	000506-51-4	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.28	2.28	319.5	ng	6393030	1	7.39	400226	20.0
Butane, 2-methoxy...	2.71	22.9	ng	458936	1	7.39	400226	20.0
2-Pentanone, 4-hy...	5.62	12.7	ng	253541	1	7.39	400226	20.0
unknown7.16	7.16	116.8	ng	2337670	1	7.39	400226	20.0
Dichloroacetic ac...	14.64	4.3	ng	218250	5	14.87	1016470	20.0