

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112120\
 Data File : BF122434.D
 Acq On : 21 Nov 2020 22:20
 Operator : JU/CG
 Sample : L4868-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 KENS-B3-112020-8-10

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122434.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	11	15	24	rVB	271657	362927	5.64%	0.941%
2	2.993	148	154	162	rVB	68547	114007	1.77%	0.296%
3	5.081	503	509	517	rBV	885383	1134618	17.63%	2.942%
4	5.487	573	578	582	rBV	4123368	4250079	66.04%	11.019%
5	5.875	641	644	648	rBV	154611	125364	1.95%	0.325%
6	6.493	744	749	764	rBV	3838428	4559642	70.86%	11.821%
7	6.863	808	812	815	rBV	1385566	1121260	17.42%	2.907%
8	7.422	902	907	911	rBV	2761363	2865133	44.52%	7.428%
9	8.145	1026	1030	1034	rBV	1421672	1448104	22.50%	3.754%
10	9.228	1208	1214	1217	rBV	5588434	5199988	80.81%	13.482%
11	9.622	1276	1281	1290	rVB	236763	242392	3.77%	0.628%
12	9.904	1325	1329	1340	rVB	1882653	1739850	27.04%	4.511%
13	10.698	1459	1464	1479	rBV	3255261	3411707	53.02%	8.845%
14	11.392	1578	1582	1589	rBV	1985940	1818391	28.26%	4.714%
15	12.986	1848	1853	1856	rBV	6490936	6435169	100.00%	16.684%
16	13.892	2002	2007	2022	rBV	170768	310976	4.83%	0.806%
17	14.039	2028	2032	2041	rBV	2056595	1862564	28.94%	4.829%
18	15.515	2277	2283	2288	rBV	1210508	1568776	24.38%	4.067%

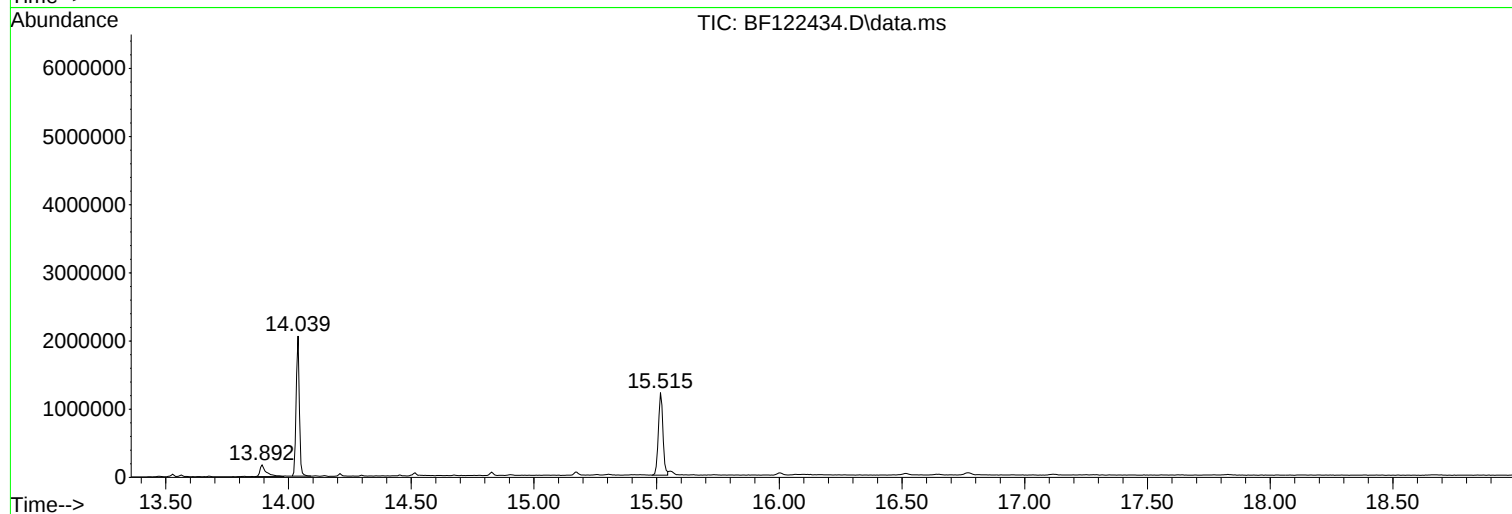
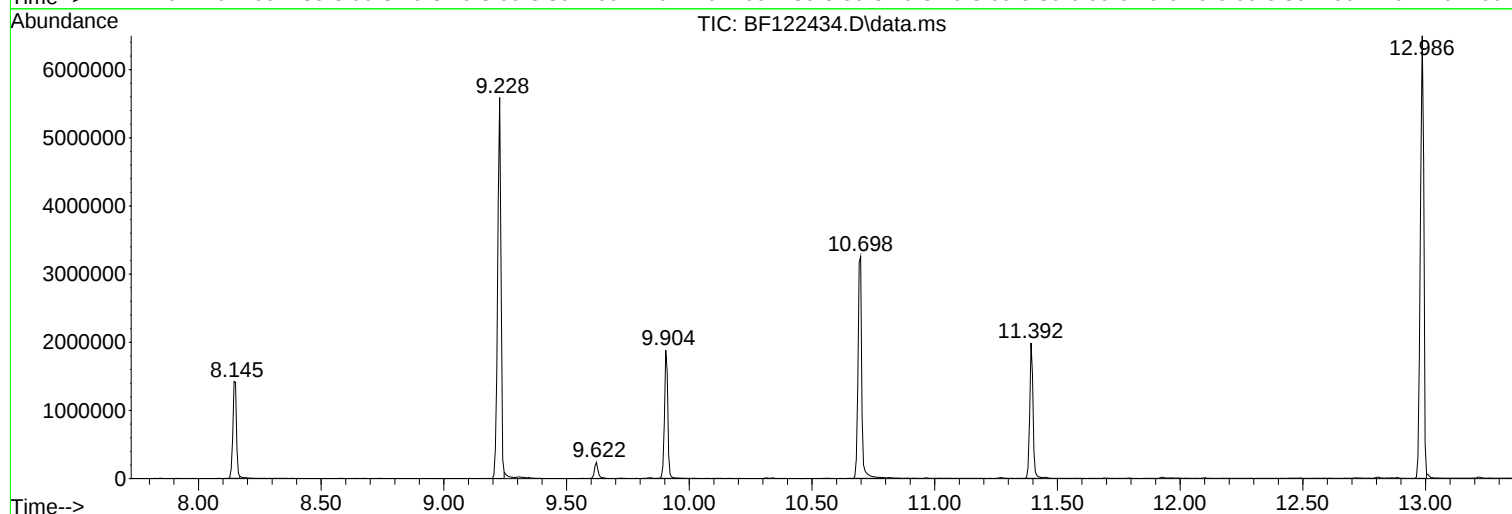
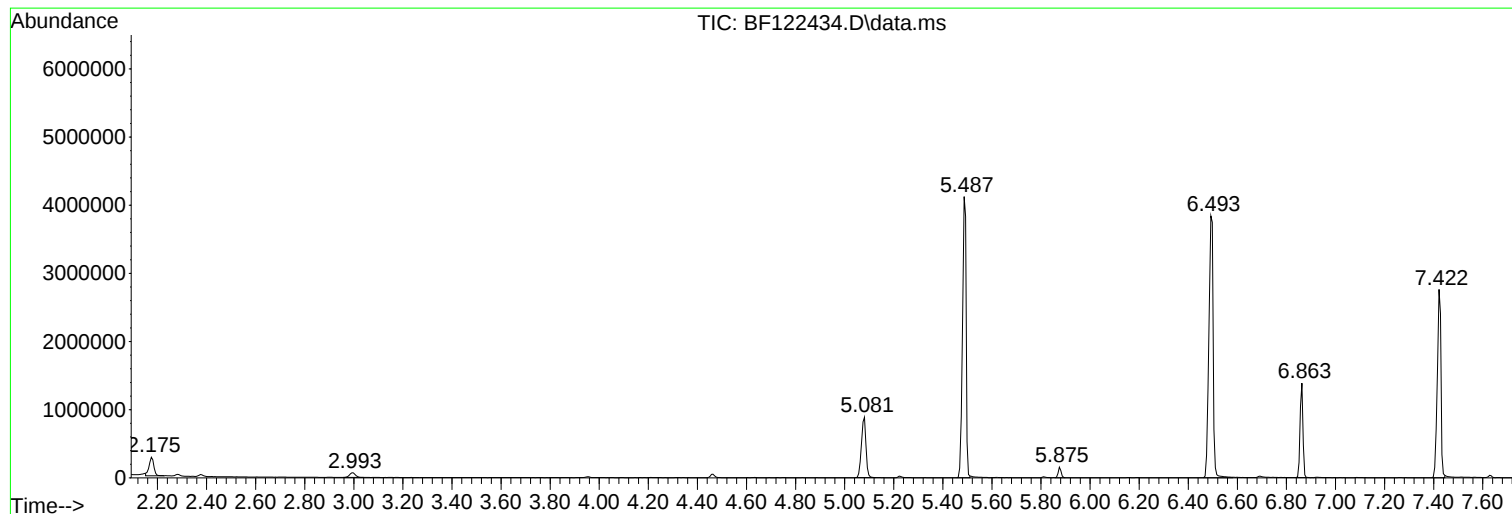
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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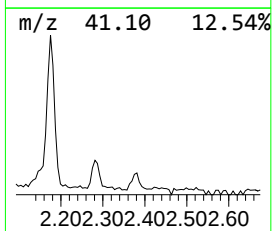
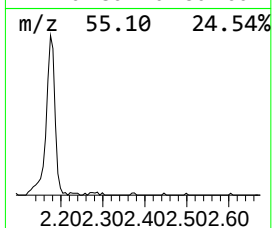
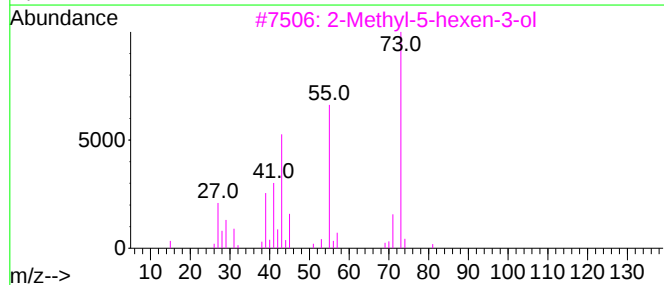
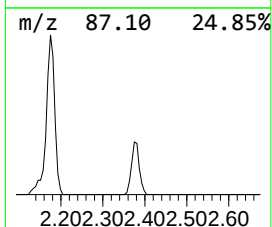
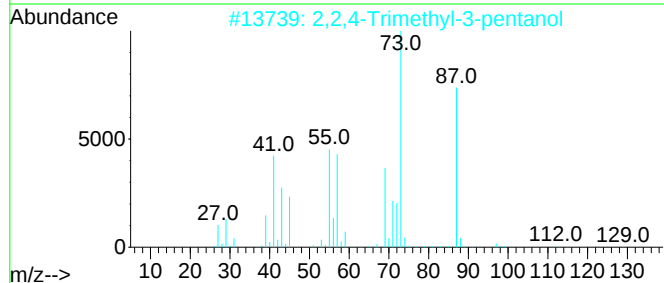
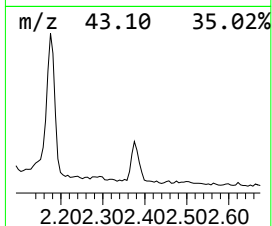
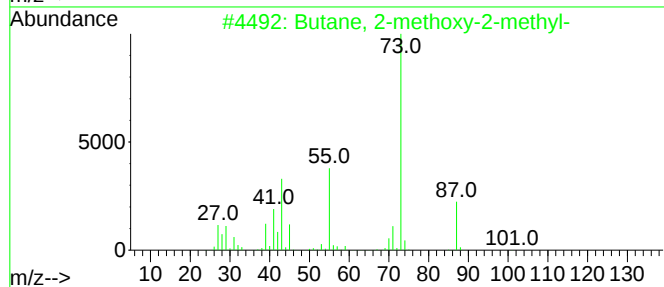
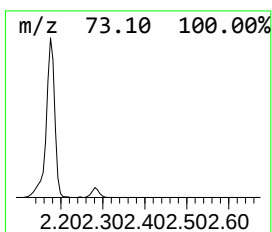
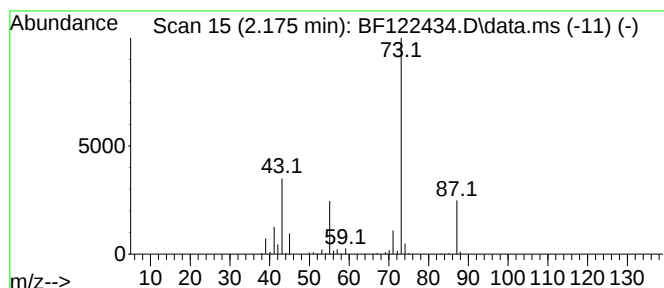
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	6.47 ng	362927	1,4-Dichlorobenzene-d4	6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		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		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17



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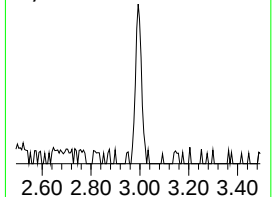
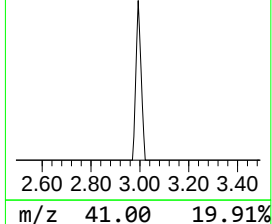
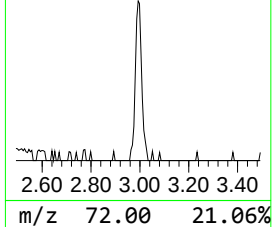
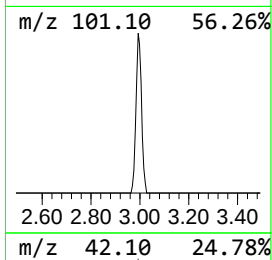
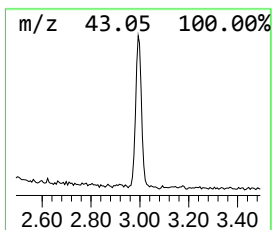
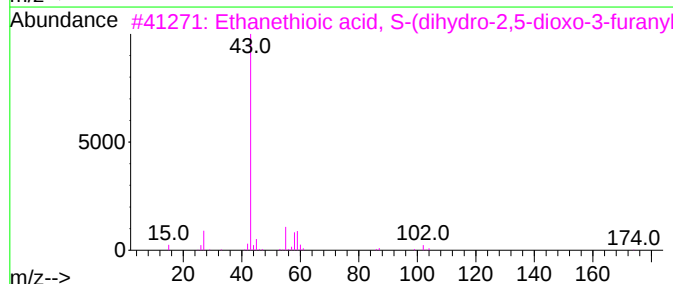
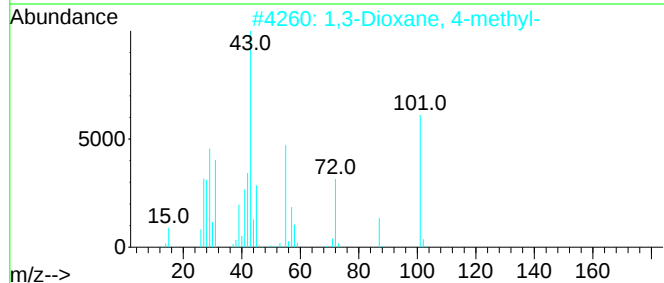
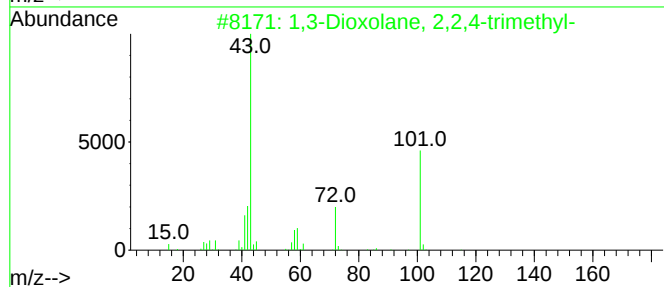
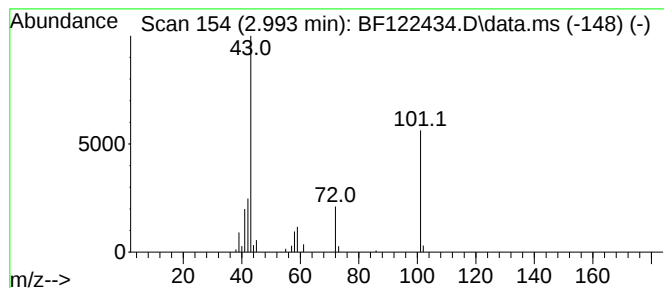
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.993	2.03 ng	114007	1,4-Dichlorobenzene-d4	6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	90
2		1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	72
3		Ethanethioic acid, S-(dihydro-2,...	174	C6H6O4S	006953-60-2	10
4		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9



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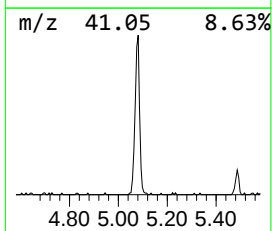
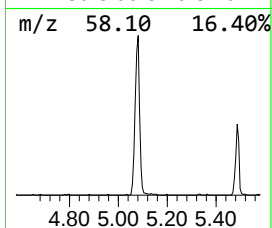
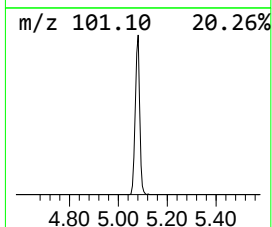
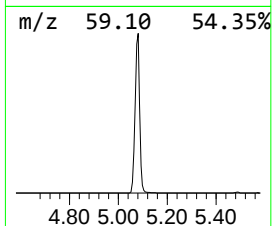
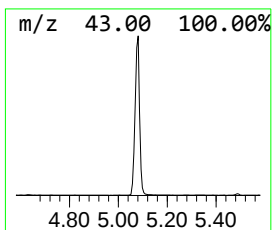
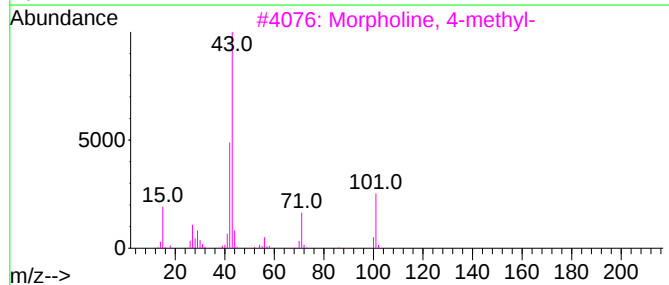
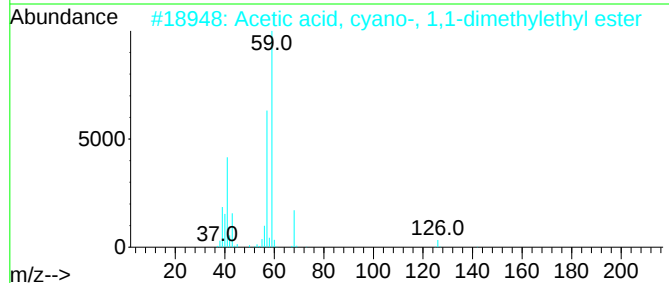
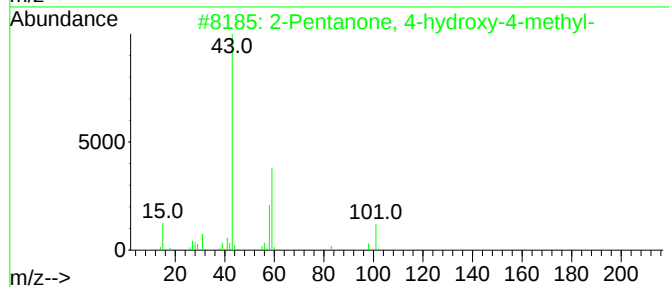
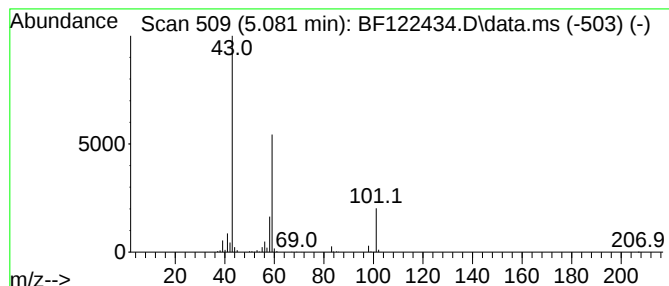
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.081	20.24 ng	1134620	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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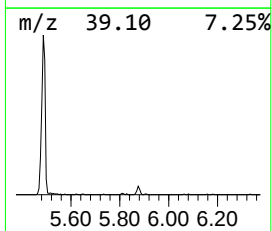
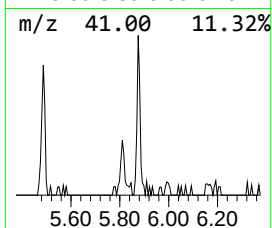
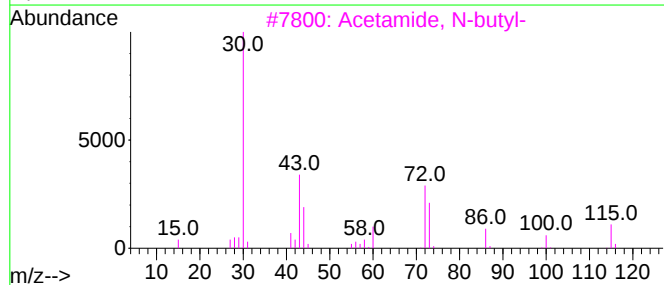
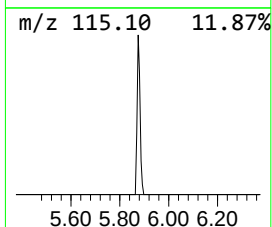
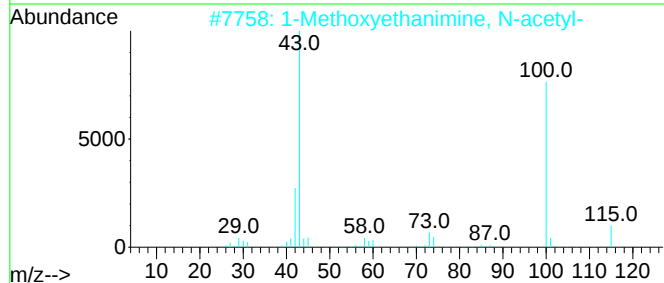
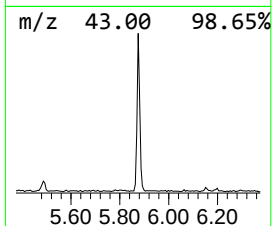
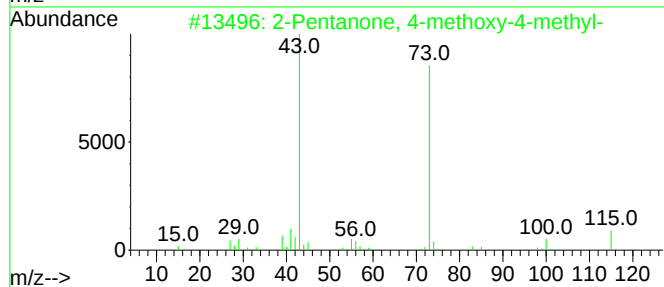
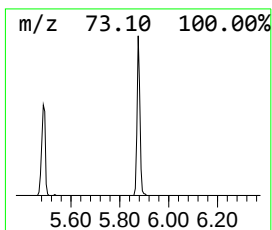
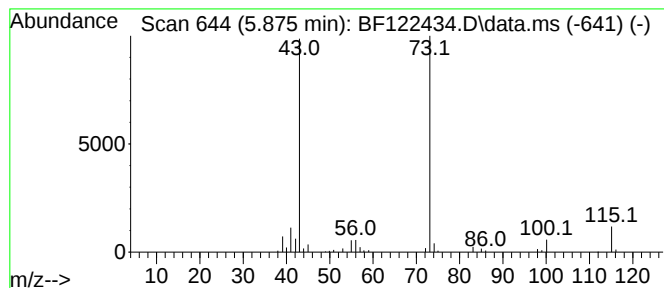
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown5.875 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.875	2.24 ng	125364	1,4-Dichlorobenzene-d4	6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	28
3		Acetamide, N-butyl-	115	C6H13NO	001119-49-9	9
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9



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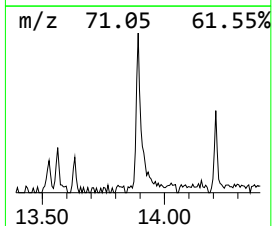
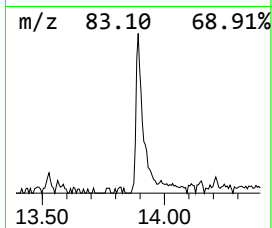
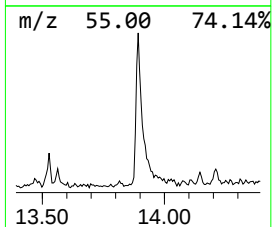
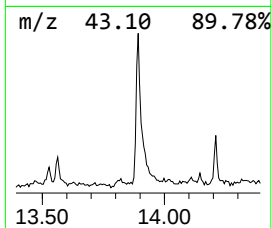
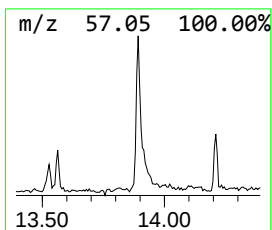
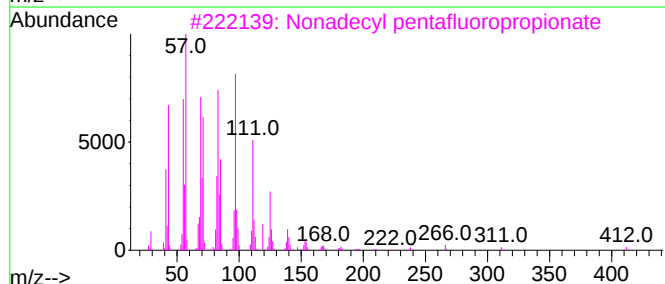
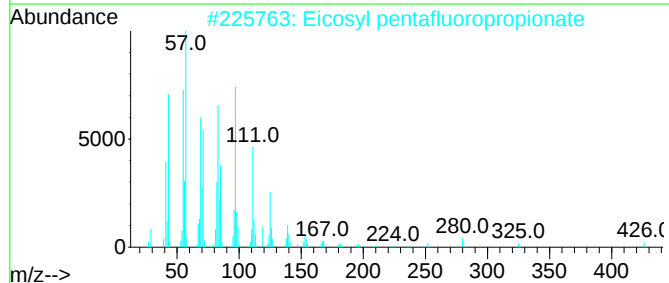
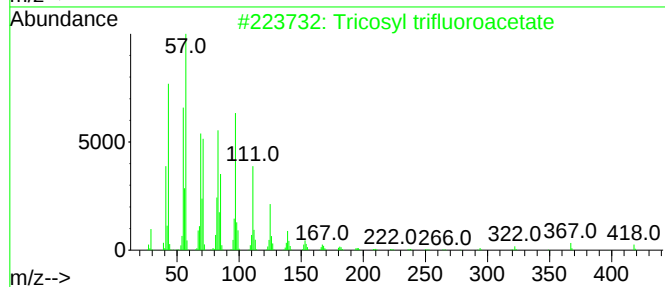
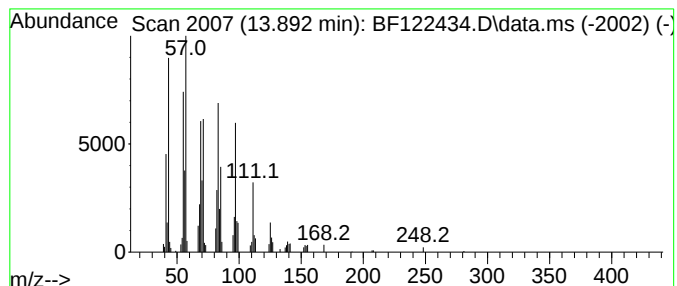
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tricosyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	3.34 ng	310976	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
3			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
5			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	87



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.175	6.5	ng	362927	1	6.863	1121260	20.0
1,3-Dioxolane, ...	2.993	2.0	ng	114007	1	6.863	1121260	20.0
2-Pentanone, 4-...	5.081	20.2	ng	1134620	1	6.863	1121260	20.0
unknown5.875	5.875	2.2	ng	125364	1	6.863	1121260	20.0
Tricosyl triflu...	13.892	3.3	ng	310976	5	14.039	1862560	20.0