

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051515\
 Data File : BF079284.D
 Acq On : 15 May 2015 22:03
 Operator : TP/IZ
 Sample : G2234-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW7

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-BF043015.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	1.461	21	24	27	rVB	155317	219092	11.07%	1.438%
2	1.621	36	38	41	rVV	461635	578787	29.24%	3.800%
3	1.678	41	43	51	rVV	54209	129450	6.54%	0.850%
4	1.793	51	53	84	rVB	969875	1969522	99.51%	12.931%
5	4.947	327	329	339	rBV	27325	43108	2.18%	0.283%
6	5.461	372	374	377	rBV	517365	578476	29.23%	3.798%
7	6.742	484	486	488	rBV	421201	377452	19.07%	2.478%
8	6.890	496	499	501	rBV	1068354	1171853	59.21%	7.694%
9	7.176	522	524	526	rBV	378032	331978	16.77%	2.180%
10	7.359	538	540	543	rBV	1065108	1072387	54.18%	7.041%
11	7.873	582	585	587	rBV	836685	890578	45.00%	5.847%
12	8.753	659	662	664	rBV	496951	450147	22.74%	2.955%
13	9.508	726	728	730	rBV	27724	32311	1.63%	0.212%
14	10.102	777	780	782	rBV	2100493	1882343	95.11%	12.359%
15	10.605	822	824	827	rBV	34873	33937	1.71%	0.223%
16	10.925	850	852	855	rBV	562586	515196	26.03%	3.383%
17	11.908	935	938	940	rBV	1040417	1205128	60.89%	7.912%
18	12.651	1001	1003	1005	rVB2	19081	28658	1.45%	0.188%
19	12.765	1011	1013	1016	rBV	563156	530210	26.79%	3.481%
20	13.131	1042	1045	1048	rBV	25564	53531	2.70%	0.351%
21	14.148	1132	1134	1142	rBV	44673	106815	5.40%	0.701%
22	14.765	1185	1188	1190	rBV	1877363	1979187	100.00%	12.994%
23	15.977	1292	1294	1300	rBV3	16296	40012	2.02%	0.263%
24	16.080	1300	1303	1305	rBV	421039	517621	26.15%	3.398%
25	17.908	1460	1463	1466	rBV	315995	493272	24.92%	3.239%

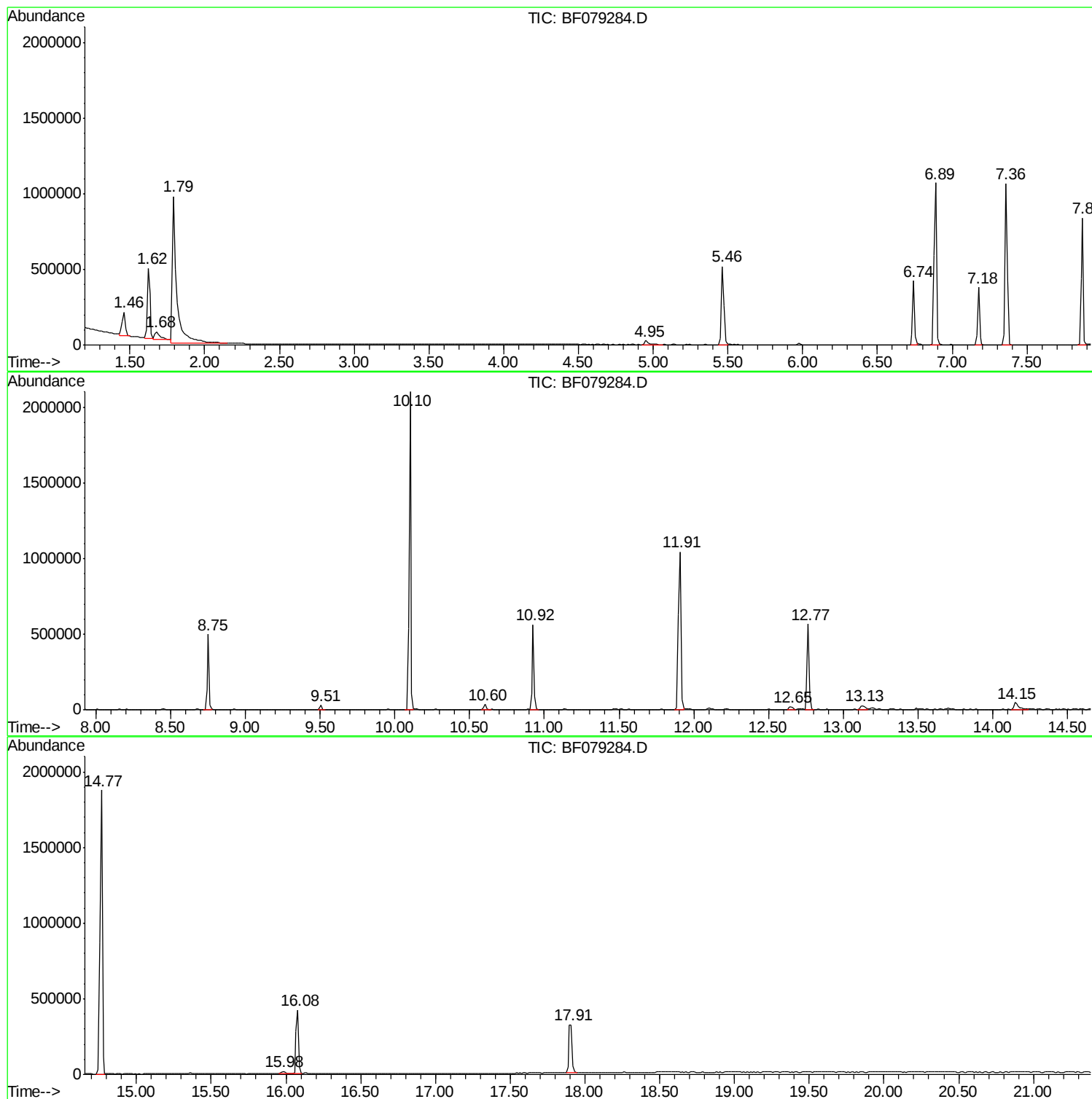
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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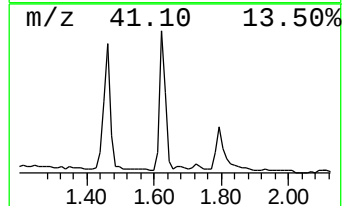
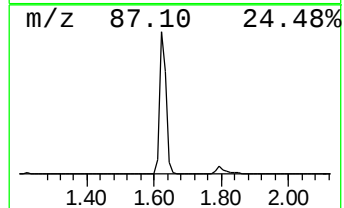
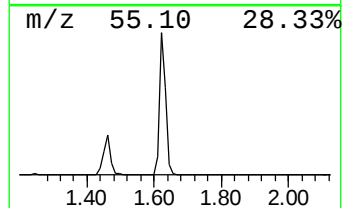
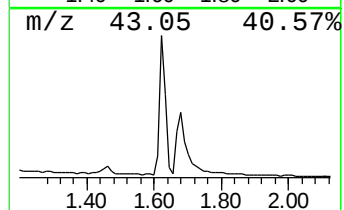
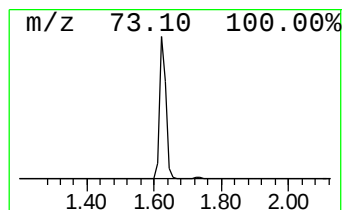
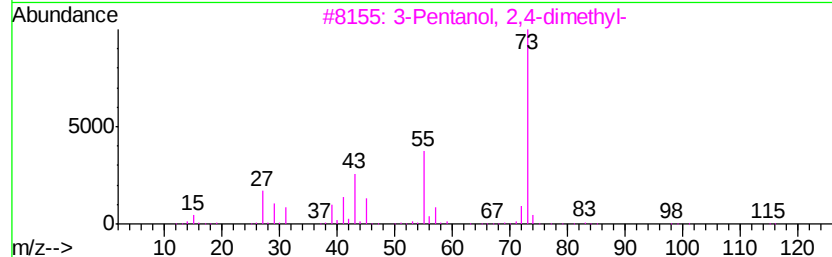
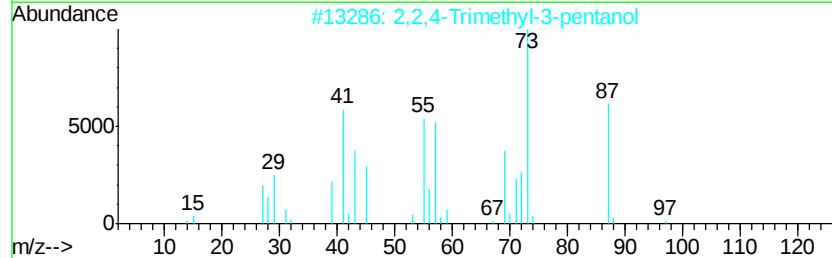
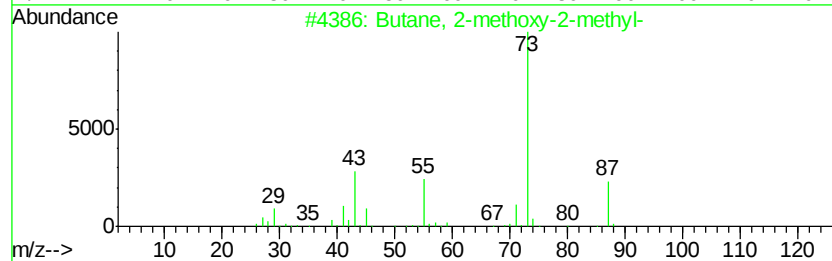
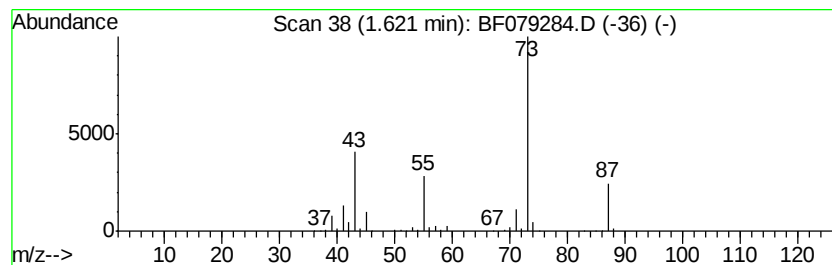
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF043015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.62	34.87 ng	578787	1,4-Dichlorobenzene-d4	7.18

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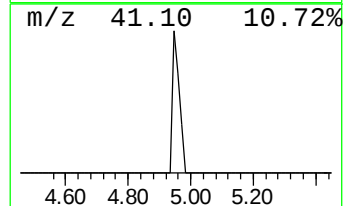
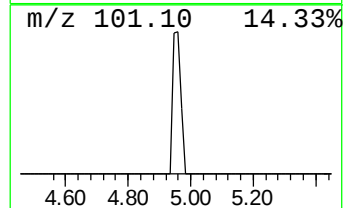
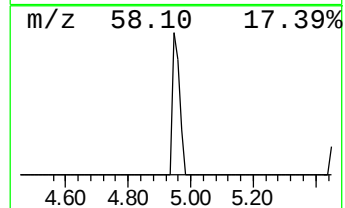
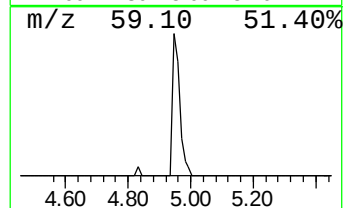
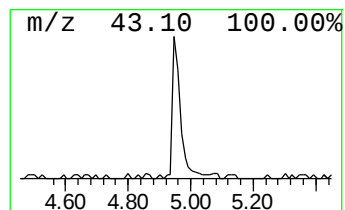
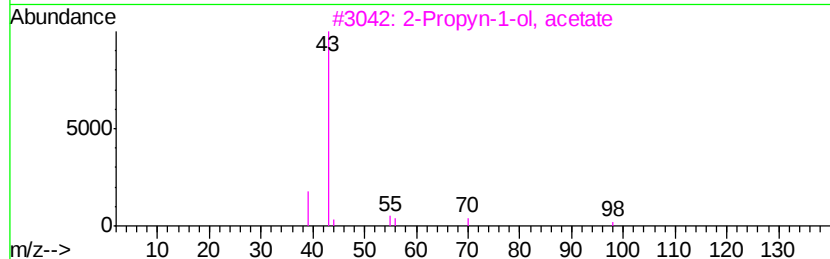
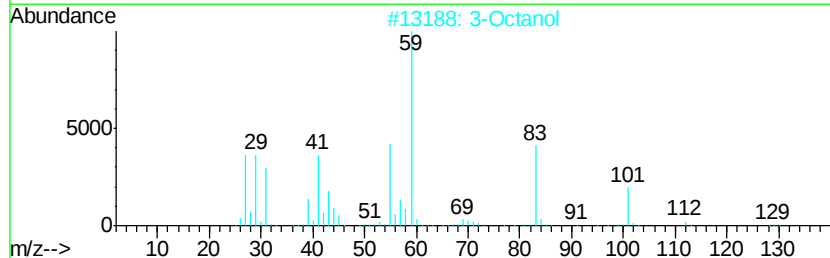
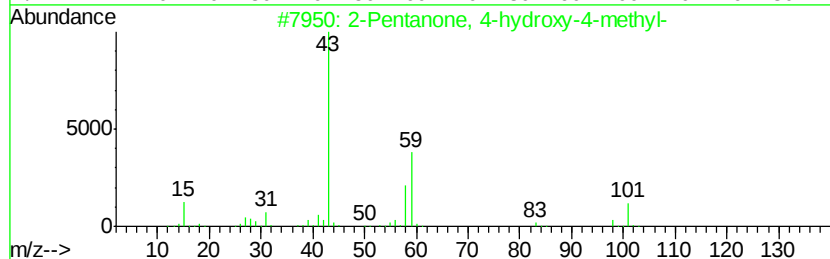
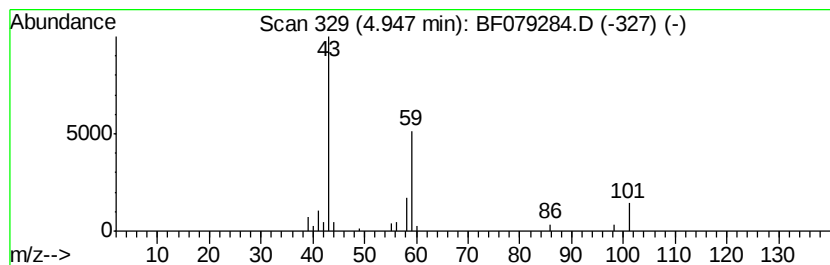
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	2.60 ng	43108	1,4-Dichlorobenzene-d4	7.18

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2	Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72	
2	3	Octanol	130	C8H18O	000589-98-0	28	
3	2	Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9	
4		Pentanamide	101	C5H11NO	000626-97-1	9	
5	2	Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	9	



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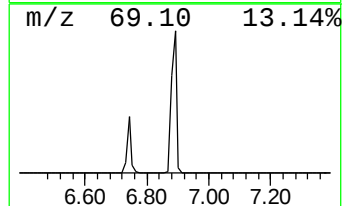
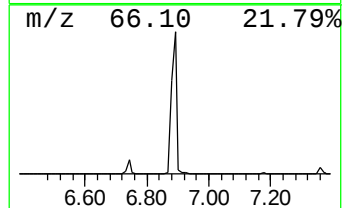
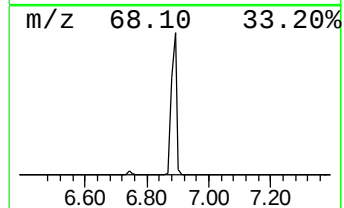
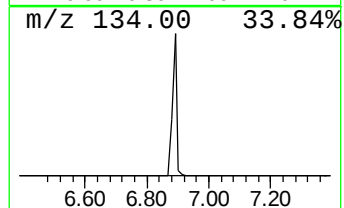
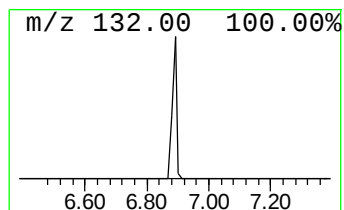
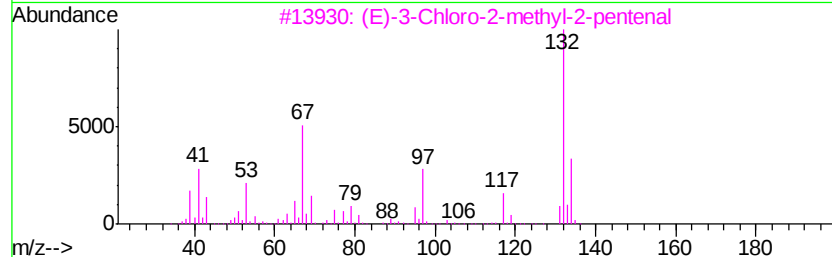
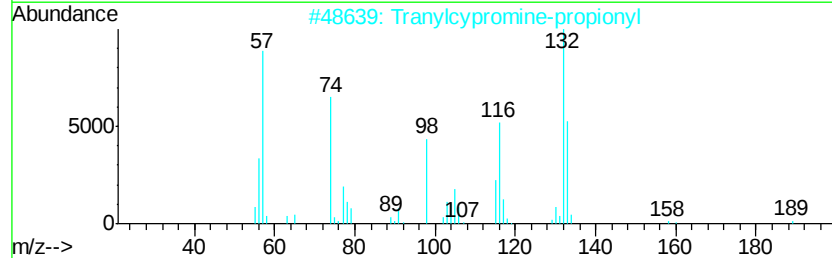
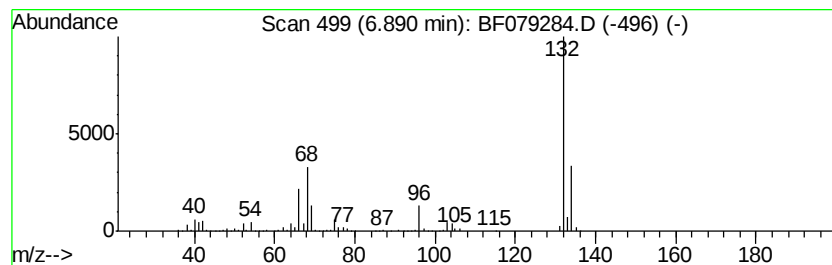
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.89 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.89	70.60 ng	1171850	1,4-Dichlorobenzene-d4	7.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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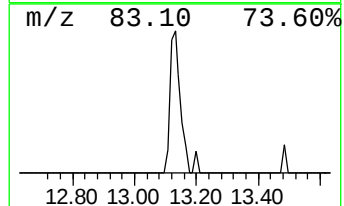
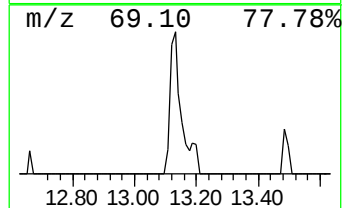
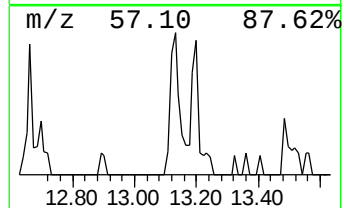
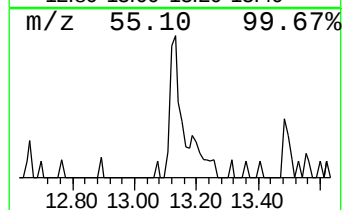
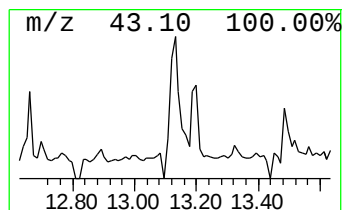
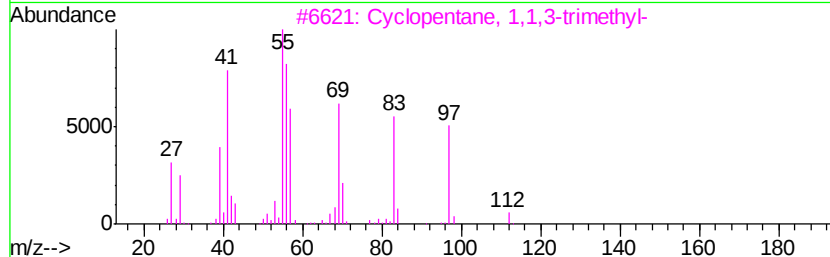
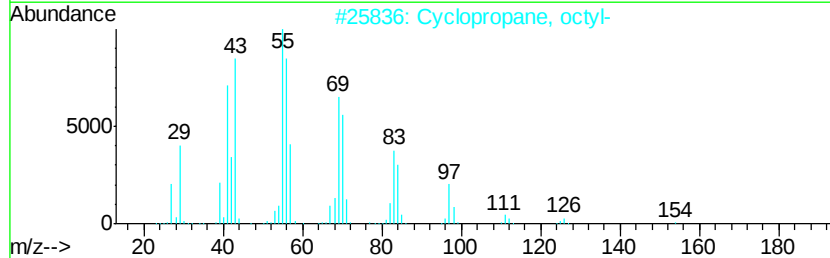
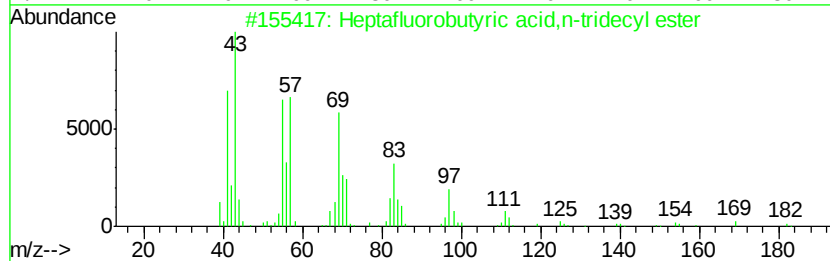
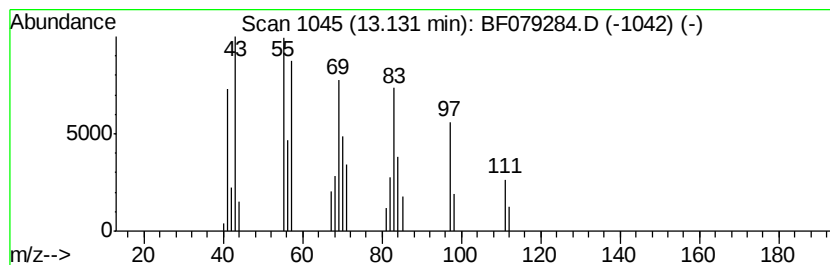
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Peak Number 8 Heptafluorobutyric acid,n-t... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	2.02 ng	53531	Phenanthrene-d10	12.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid,n-tridec...	396	C17H27F7O2	1000216-78-9	86
2		Cyclopropane, octyl-	154	C11H22	001472-09-9	59
3		Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	50
4		Cyclopentane, 1-ethyl-2-methyl-	112	C8H16	003726-46-3	49
5		Acetic acid, trifluoro-, decyl e...	254	C12H21F3O2	000333-88-0	47



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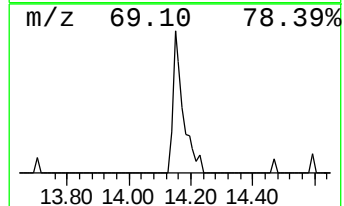
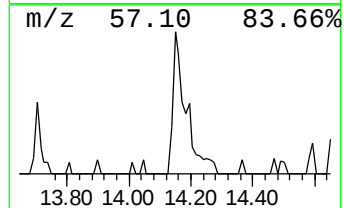
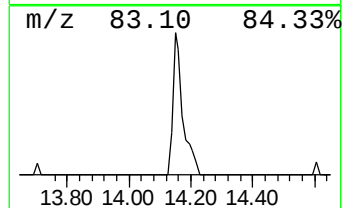
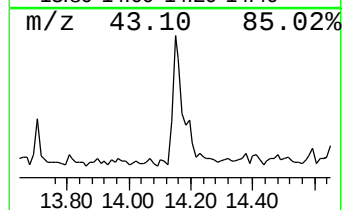
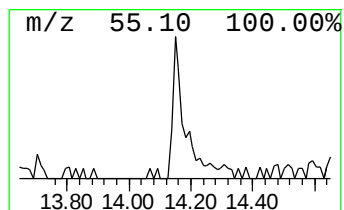
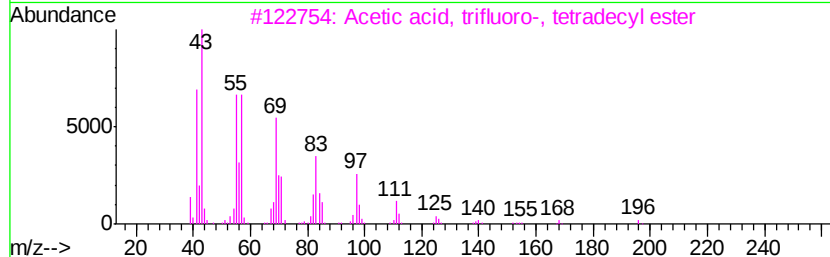
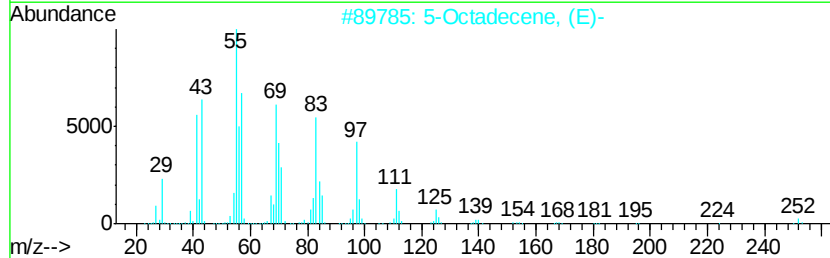
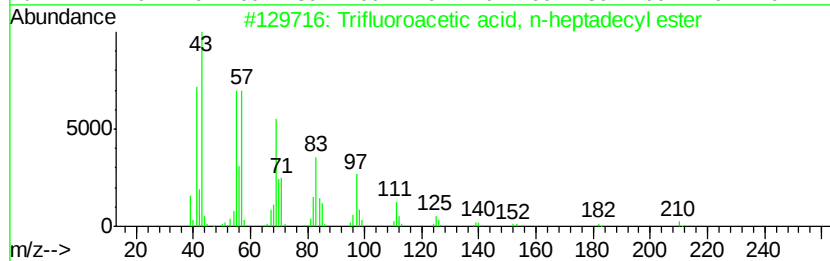
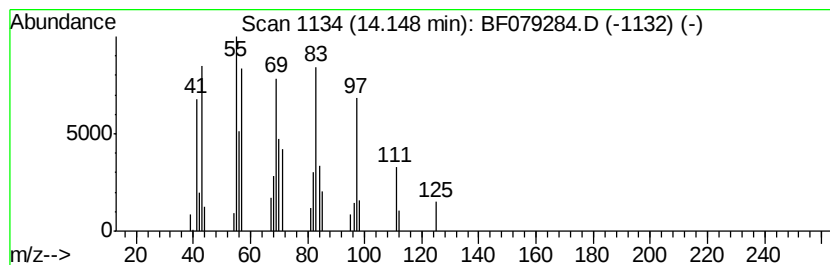
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Trifluoroacetic acid, n-hep... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.15	4.03 ng	106815	Phenanthrene-d10	12.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
2		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
3		Acetic acid, trifluoro-, tetradec...	310	C16H29F3O2	006222-02-2	72
4		Heptafluorobutyric acid, n-tridec...	396	C17H27F7O2	1000216-78-9	59
5		Cyclopentane, 1-ethyl-2-methyl-, ...	112	C8H16	000930-89-2	46



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	1.62	34.9	ng	578787	1	7.18	331978	20.0
2-Pentanone, 4-hy...	4.95	2.6	ng	43108	1	7.18	331978	20.0
unknown6.89	6.89	70.6	ng	1171850	1	7.18	331978	20.0
Heptafluorobutyri...	13.13	2.0	ng	53531	4	12.77	530210	20.0
Trifluoroacetic a...	14.15	4.0	ng	106815	4	12.77	530210	20.0