

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100317\
 Data File : BF099038.D
 Acq On : 3 Oct 2017 18:58
 Operator : SJ/JU
 Sample : I5496-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PAMT-COMP-A

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-BF092317.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	2.151	7	11	30	rVB	477082	731595	9.74%	3.288%
2	4.475	402	406	413	rVB	116705	126972	1.69%	0.571%
3	5.133	506	518	521	rBV	3182907	7509517	100.00%	33.752%
4	5.486	574	578	586	rVB	224025	186775	2.49%	0.839%
5	6.486	745	748	759	rVB2	290202	316935	4.22%	1.424%
6	6.633	770	773	777	rBV	596913	513816	6.84%	2.309%
7	6.869	810	813	817	rBV	1168161	1046939	13.94%	4.706%
8	7.027	836	840	843	rVB	1339141	1083907	14.43%	4.872%
9	7.427	904	908	912	rBV	905946	870482	11.59%	3.912%
10	8.151	1027	1031	1035	rBV	1505673	1436867	19.13%	6.458%
11	9.227	1209	1214	1217	rBV	1948001	1659737	22.10%	7.460%
12	9.616	1277	1280	1283	rBV	239582	183266	2.44%	0.824%
13	9.910	1325	1330	1334	rBV	1752246	1576822	21.00%	7.087%
14	10.327	1394	1401	1404	rBV2	87816	86371	1.15%	0.388%
15	10.692	1460	1463	1470	rVB	201366	154149	2.05%	0.693%
16	10.804	1479	1482	1491	rVB	121490	132281	1.76%	0.595%
17	11.398	1578	1583	1586	rBV	1684346	1520440	20.25%	6.834%
18	12.974	1847	1851	1854	rBV	1476594	1231335	16.40%	5.534%
19	13.862	1998	2002	2010	rBV2	87060	106513	1.42%	0.479%
20	14.033	2027	2031	2035	rVB	1098818	962749	12.82%	4.327%
21	15.509	2276	2282	2289	rBV	618944	811630	10.81%	3.648%

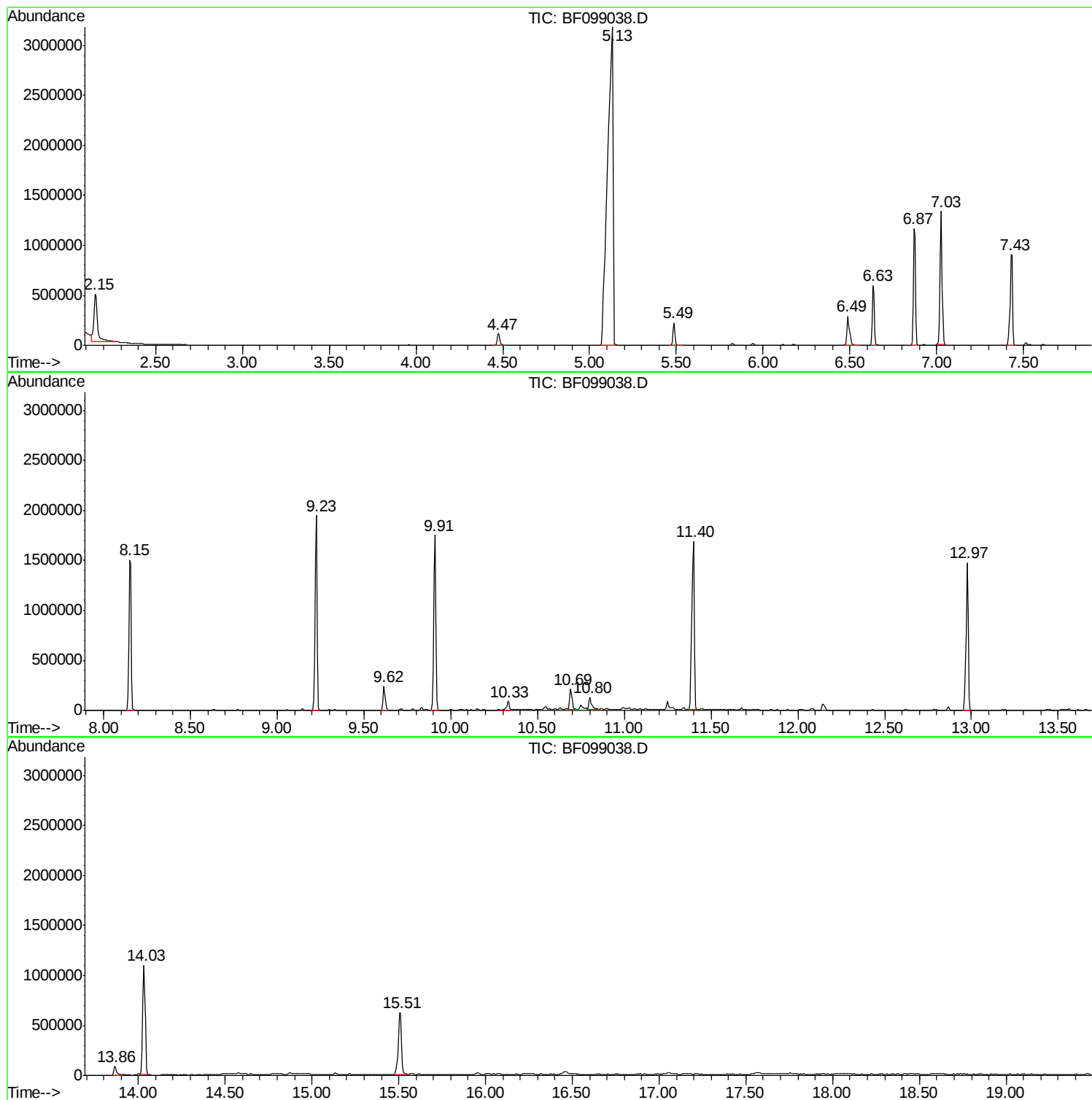
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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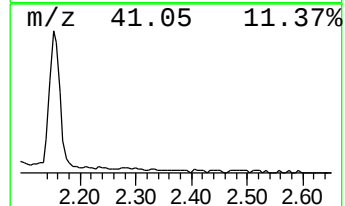
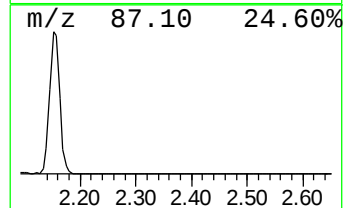
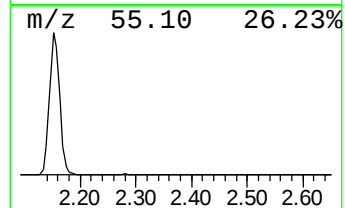
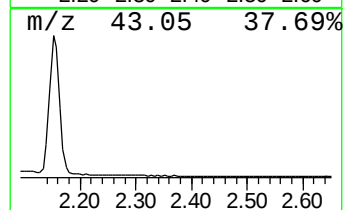
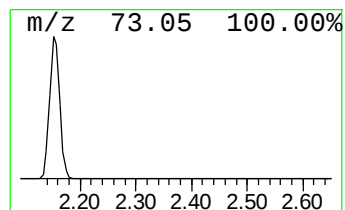
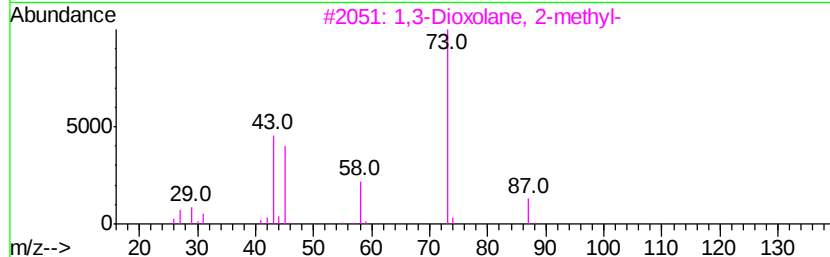
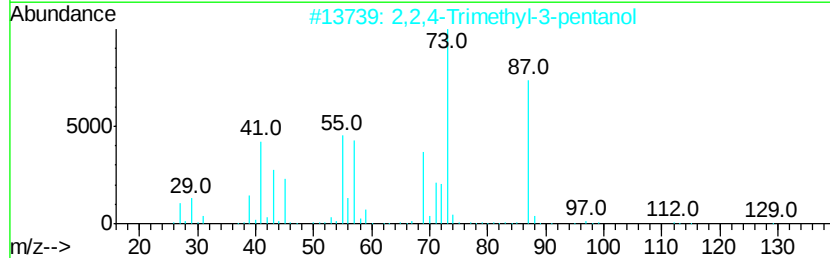
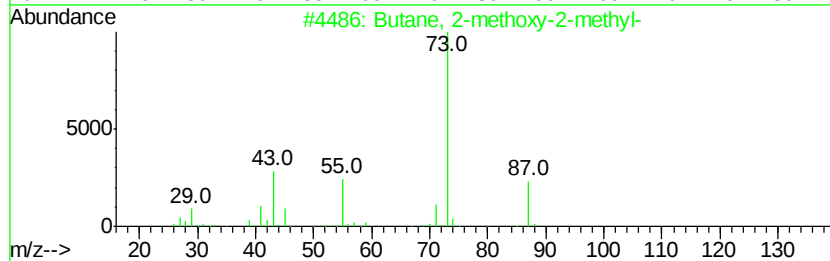
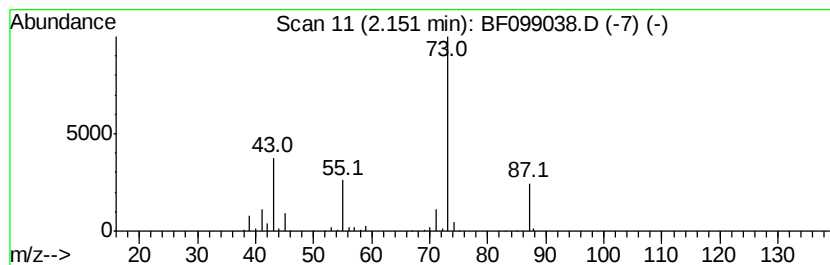
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.15	13.98 ng	731595	1,4-Dichlorobenzene-d4	6.87

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		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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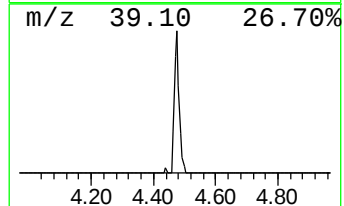
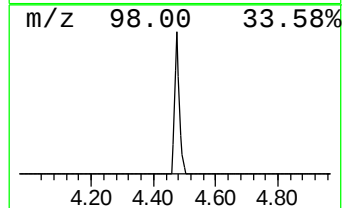
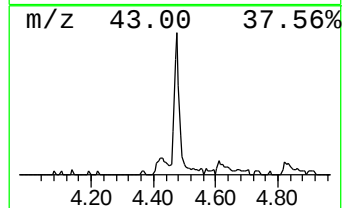
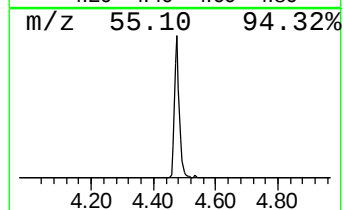
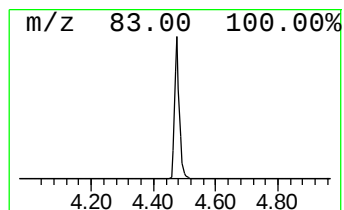
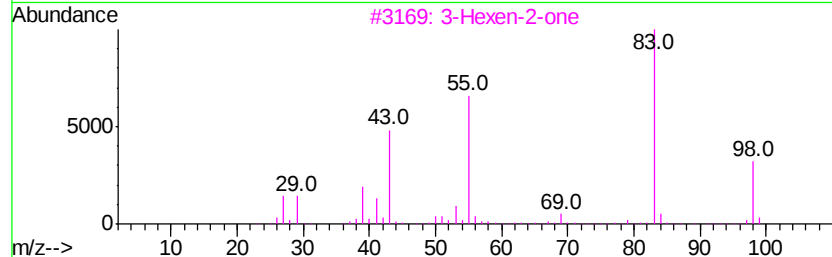
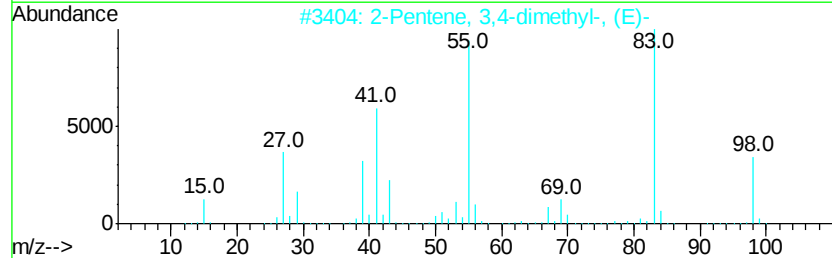
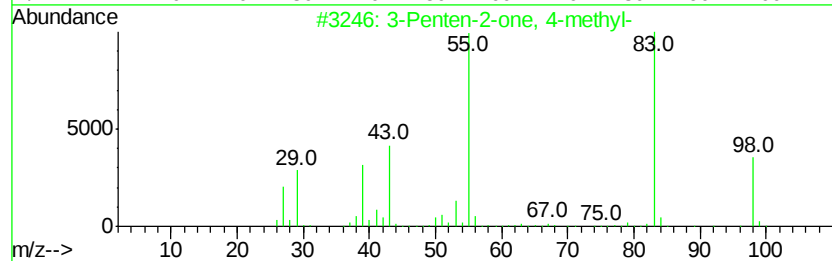
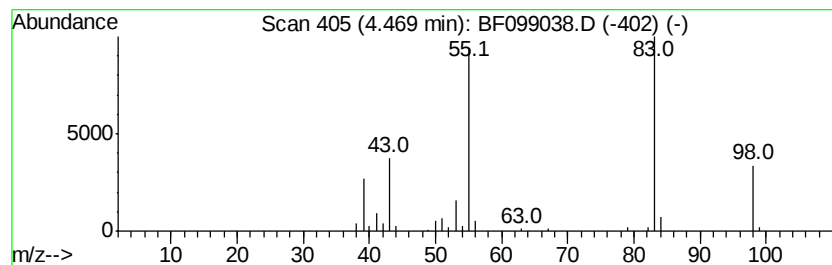
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	2.43 ng	126972	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3		3-Hexen-2-one	98	C6H10O	000763-93-9	87
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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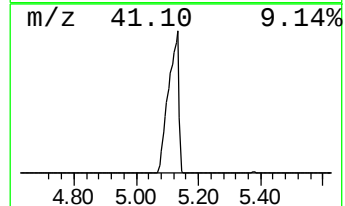
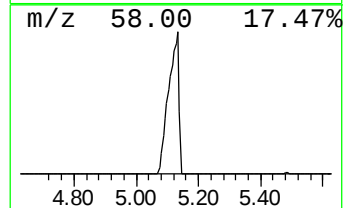
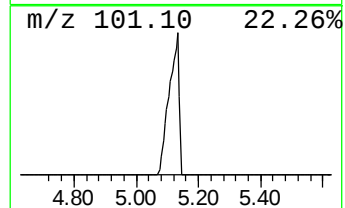
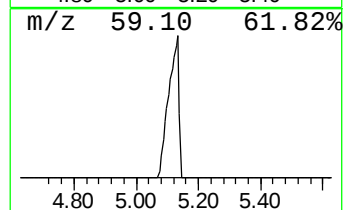
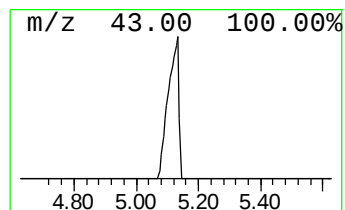
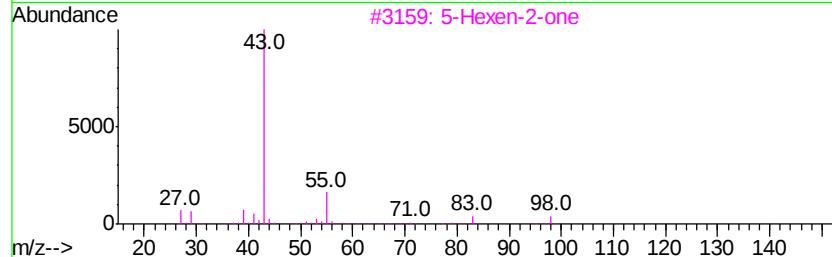
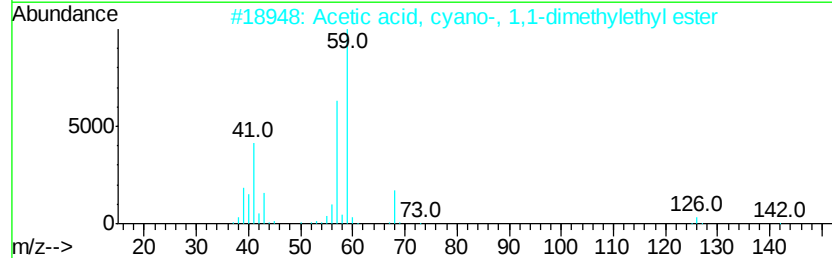
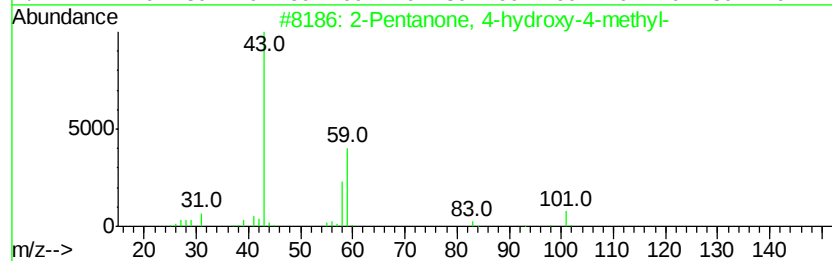
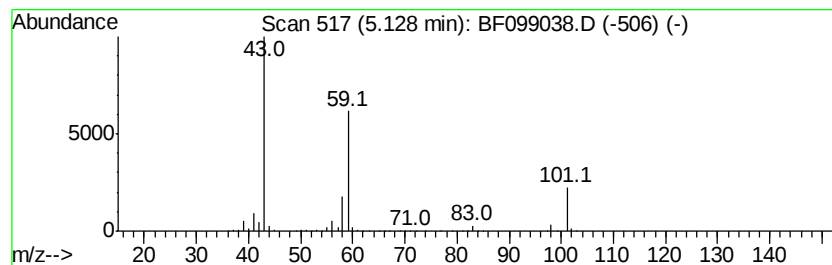
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	143.46 ng	7509520	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		1,2-Butanediol	90	C4H10O2	000584-03-2	9



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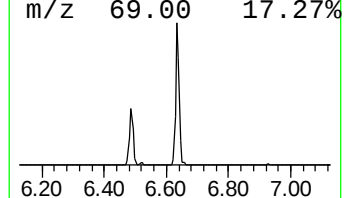
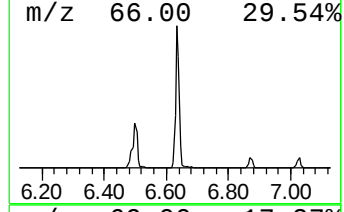
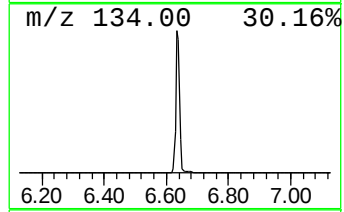
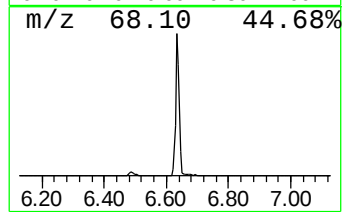
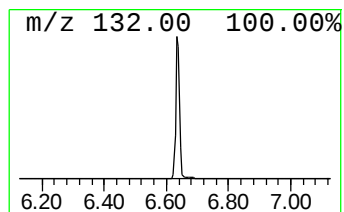
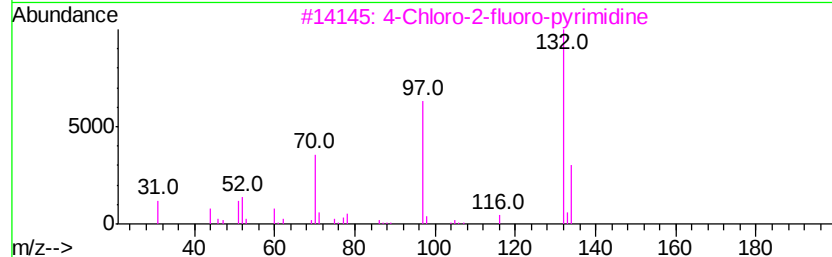
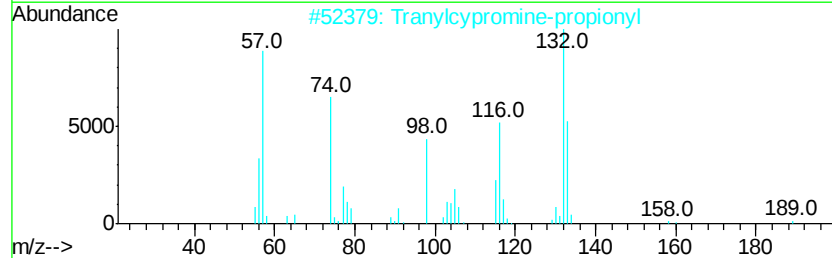
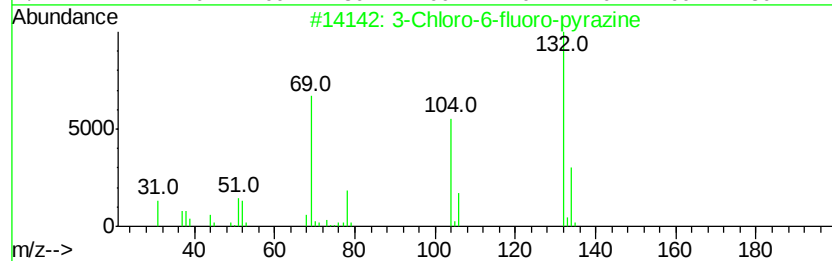
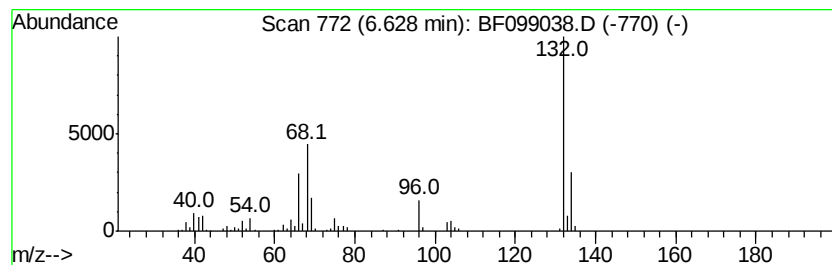
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown6.63 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	9.82 ng	513816	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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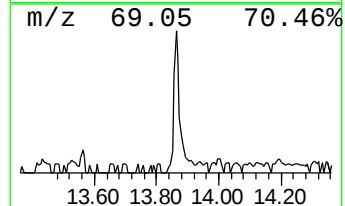
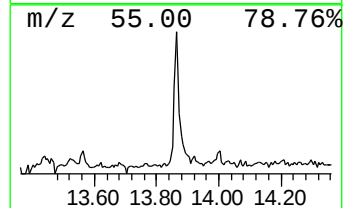
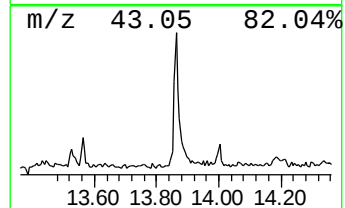
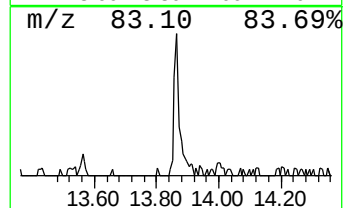
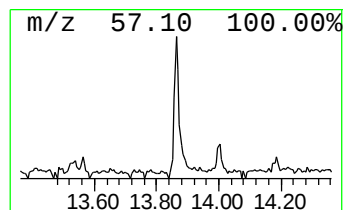
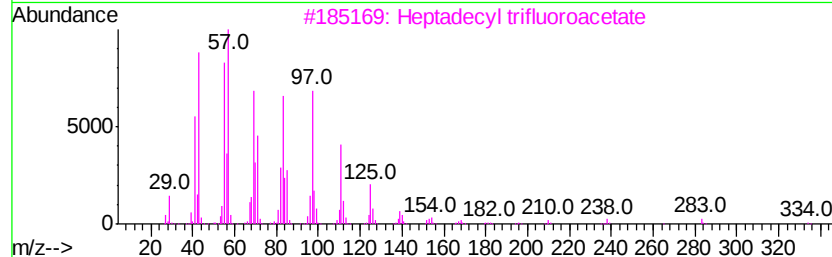
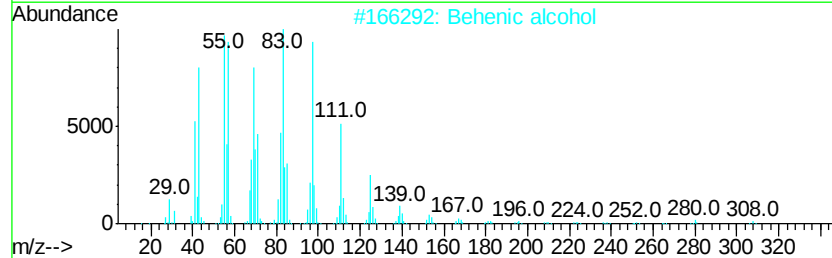
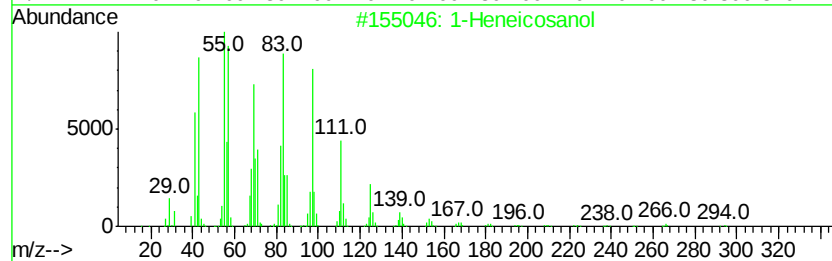
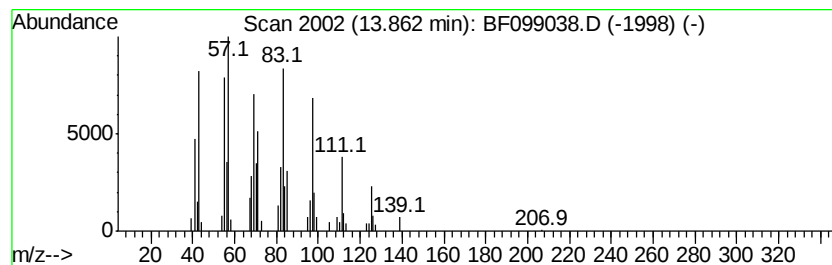
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.86	2.21 ng	106513	Chrysene-d12	14.03	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	Octacosanol	410	C28H58O	000557-61-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.15	14.0	ng	731595	1	6.87	1046940	20.0
3-Penten-2-one, 4...	4.47	2.4	ng	126972	1	6.87	1046940	20.0
2-Pentanone, 4-hy...	5.13	143.5	ng	7509520	1	6.87	1046940	20.0
unknown6.63	6.63	9.8	ng	513816	1	6.87	1046940	20.0
1-Heneicosanol	13.86	2.2	ng	106513	5	14.03	962749	20.0