

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101416\
 Data File : BF090576.D
 Acq On : 14 Oct 2016 18:23
 Operator : UM/SJ
 Sample : H5260-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BRANE-1.5

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.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	5.103	240	242	251	rBV	596053	919007	20.44%	2.461%
2	5.526	277	279	300	rBV	3381527	3787039	84.23%	10.140%
3	6.554	366	369	371	rBV	3189610	3675276	81.75%	9.841%
4	6.691	378	381	383	rBV	2576964	3840588	85.43%	10.284%
5	6.920	399	401	412	rBV	872357	1073109	23.87%	2.873%
6	7.069	412	414	417	rBV	2252982	2867444	63.78%	7.678%
7	7.480	448	450	466	rBV	2043662	2643617	58.80%	7.079%
8	8.200	511	513	516	rBV	1129654	1381413	30.73%	3.699%
9	8.326	522	524	534	rVB2	19110	59525	1.32%	0.159%
10	9.286	605	608	610	rBV	4243513	4495835	100.00%	12.038%
11	9.675	640	642	647	rBV	269846	252459	5.62%	0.676%
12	9.892	659	661	663	rVB	59535	51199	1.14%	0.137%
13	9.960	665	667	669	rBV	1959612	1669222	37.13%	4.469%
14	10.395	701	705	706	rBV	116217	111842	2.49%	0.299%
15	10.612	721	724	727	rBV	41141	66352	1.48%	0.178%
16	10.749	733	736	745	rBV	2207342	2471307	54.97%	6.617%
17	10.863	745	746	753	rVB	121058	171266	3.81%	0.459%
18	11.309	783	785	787	rBV	36744	53571	1.19%	0.143%
19	11.446	795	797	811	rBV	1271022	1521625	33.85%	4.074%
20	13.035	934	936	949	rBV	3489728	3782612	84.14%	10.128%
21	13.481	960	975	990	rBV4	39851	335698	7.47%	0.899%
22	13.926	1012	1014	1022	rBV	72655	129454	2.88%	0.347%
23	14.086	1026	1028	1040	rVV	737495	990303	22.03%	2.652%
24	15.469	1146	1149	1153	rVV5	29278	82101	1.83%	0.220%
25	15.549	1153	1156	1166	rVB	565038	915200	20.36%	2.451%

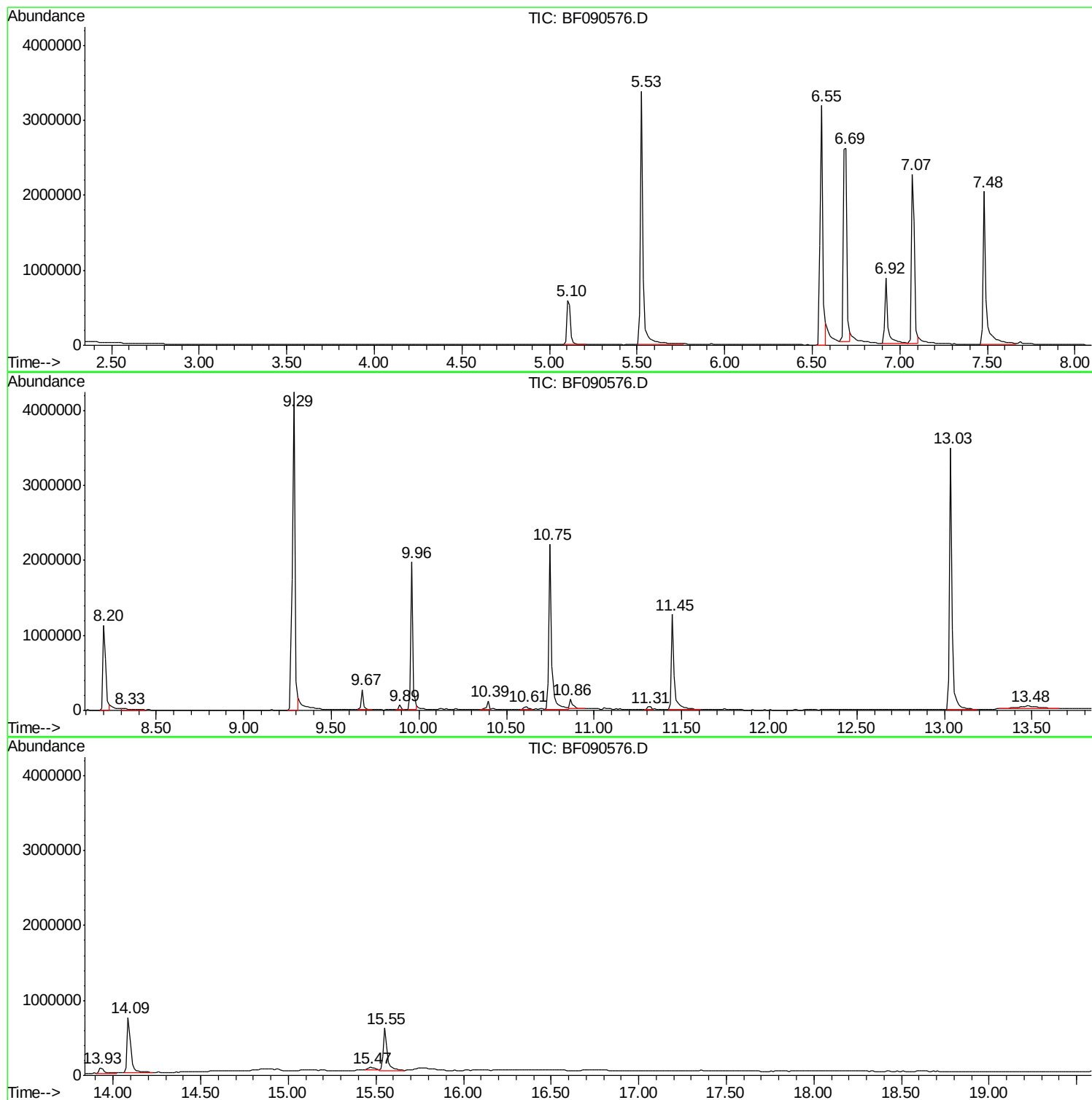
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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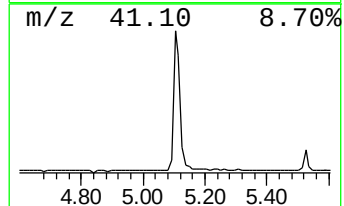
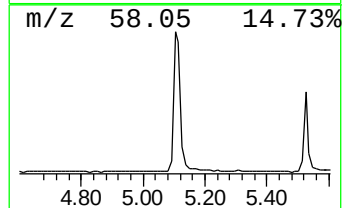
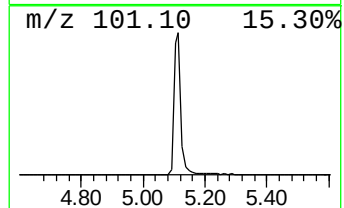
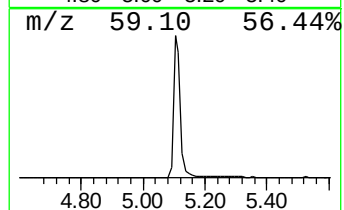
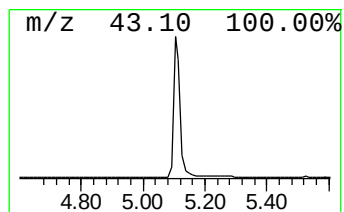
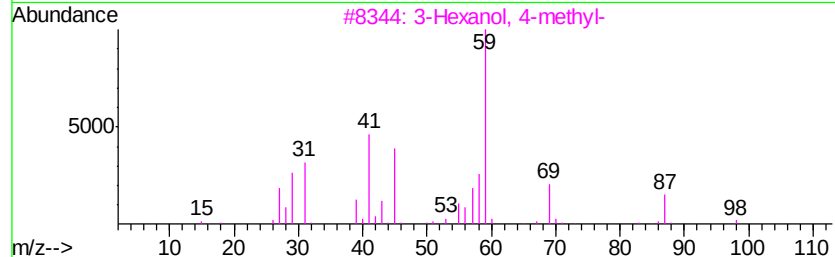
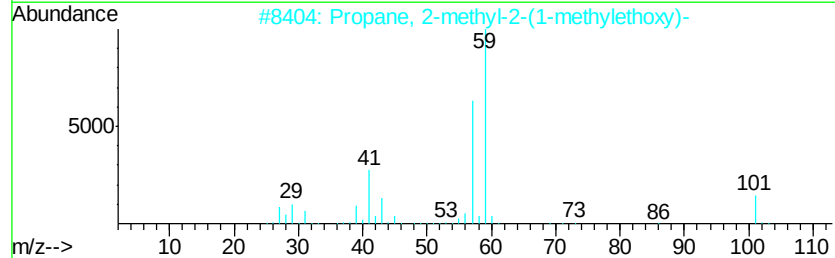
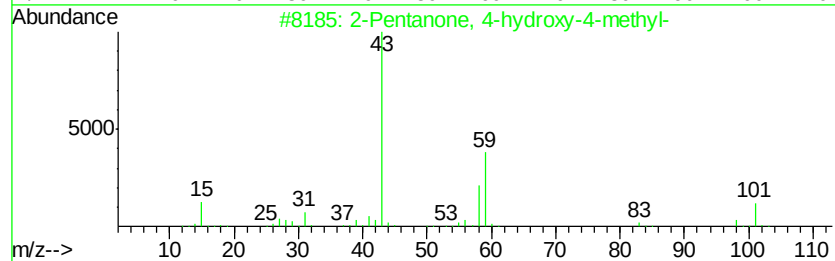
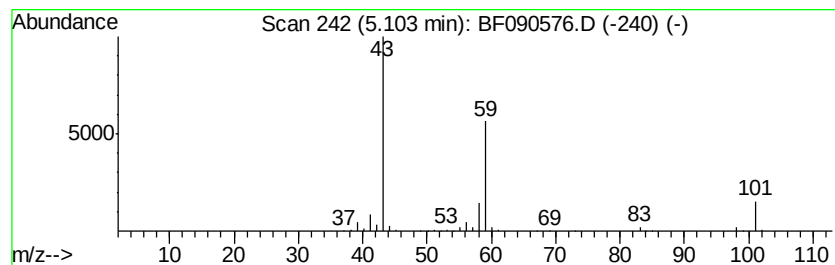
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	17.13 ng	919007	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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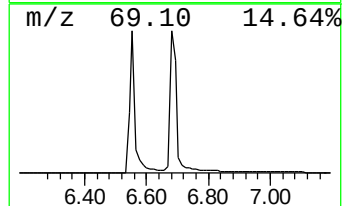
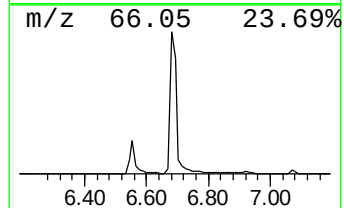
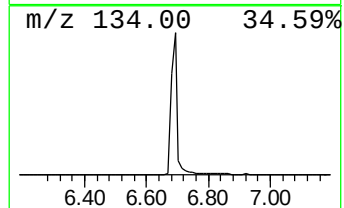
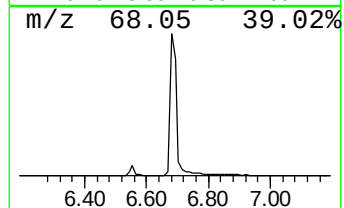
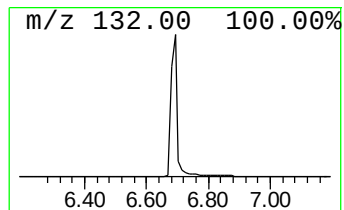
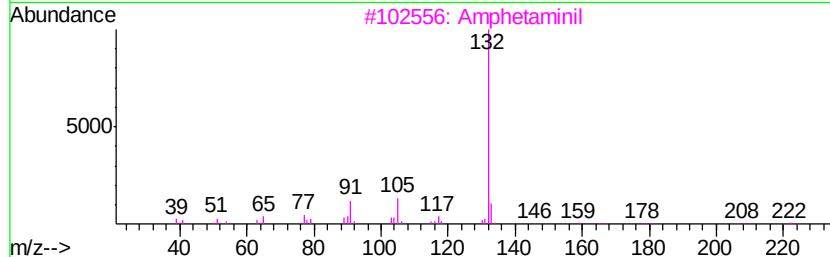
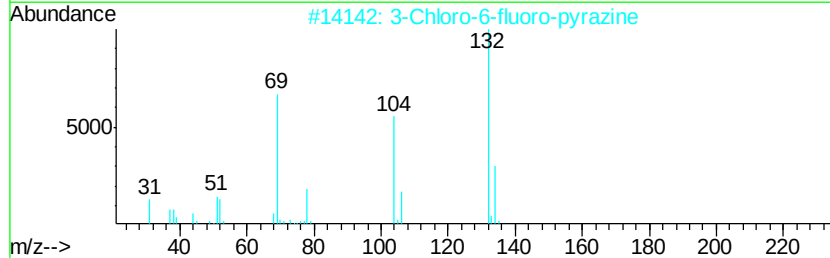
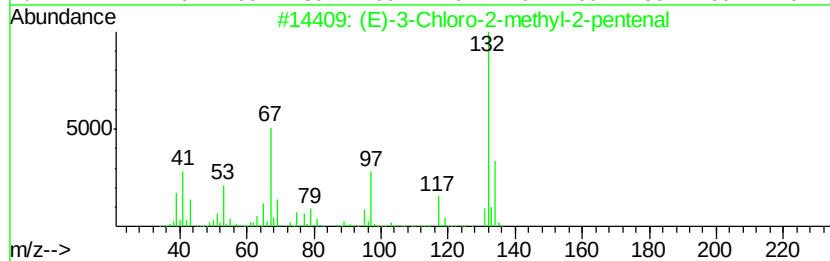
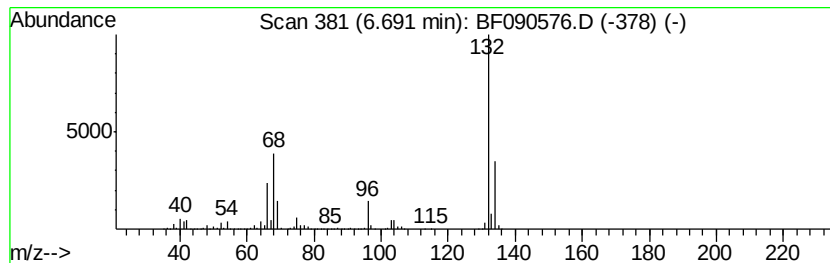
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	71.58 ng	3840590	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Amphetaminil	250	C17H18N2	017590-01-1	10
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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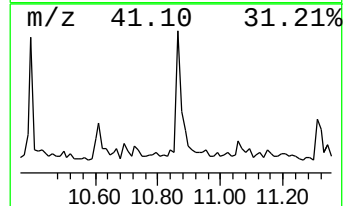
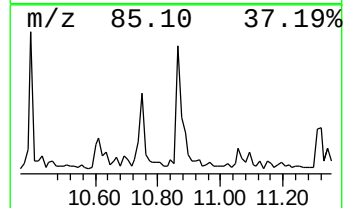
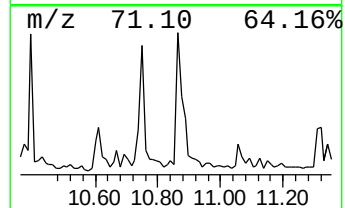
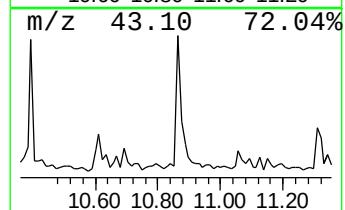
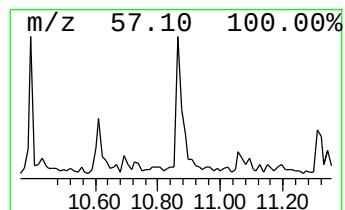
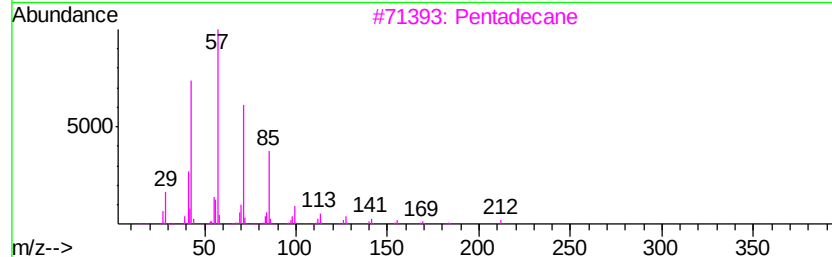
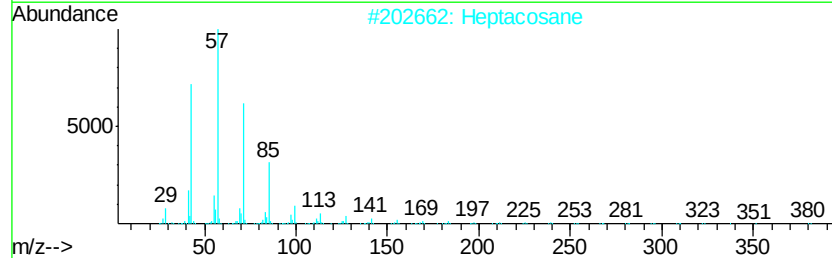
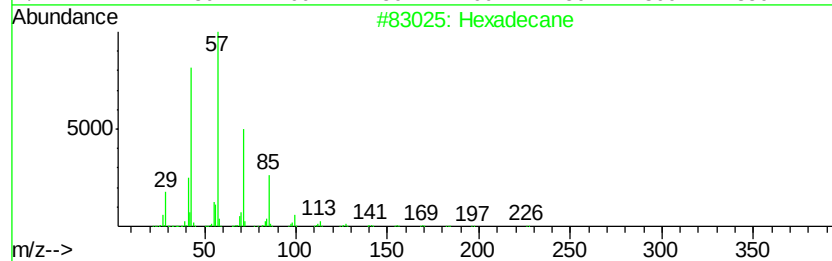
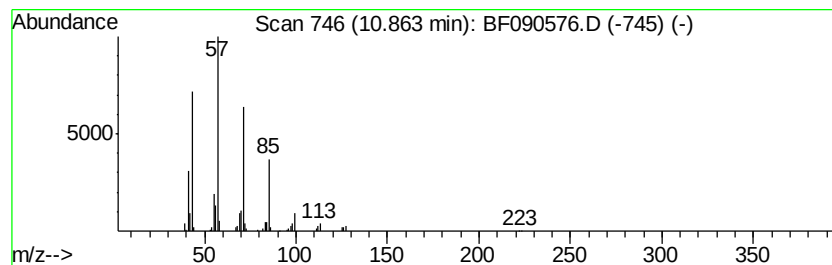
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Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.86	2.25 ng	171266	Phenanthrene-d10	11.45	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptacosane	380	C27H56	000593-49-7	90
3	Pentadecane	212	C15H32	000629-62-9	78
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
5	Nonadecane	268	C19H40	000629-92-5	59



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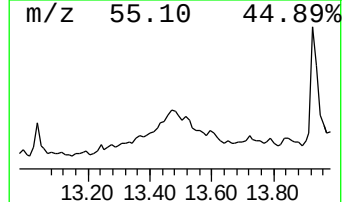
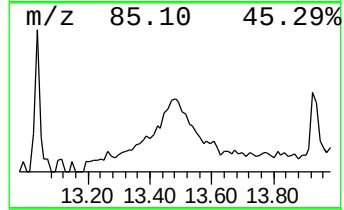
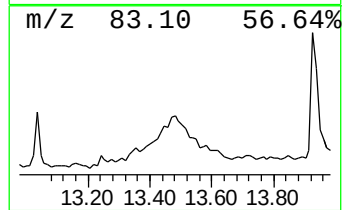
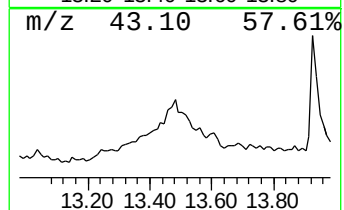
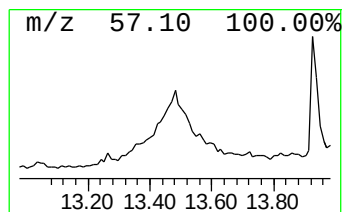
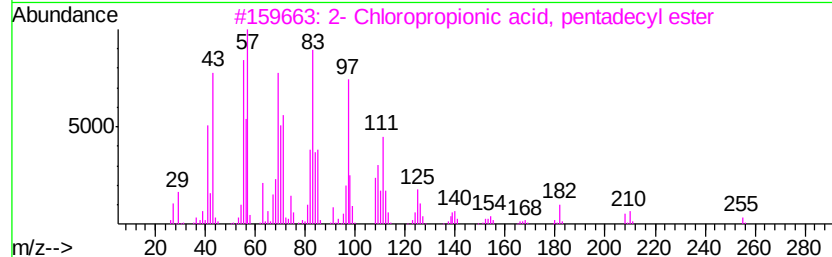
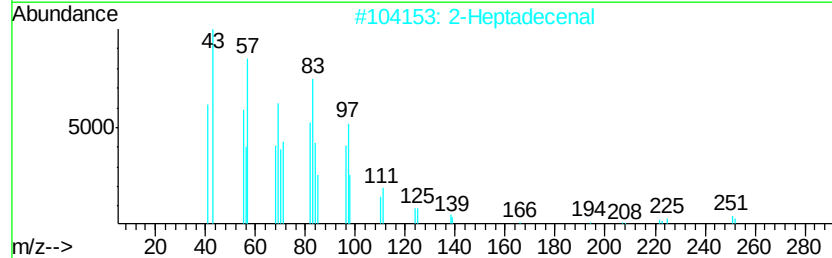
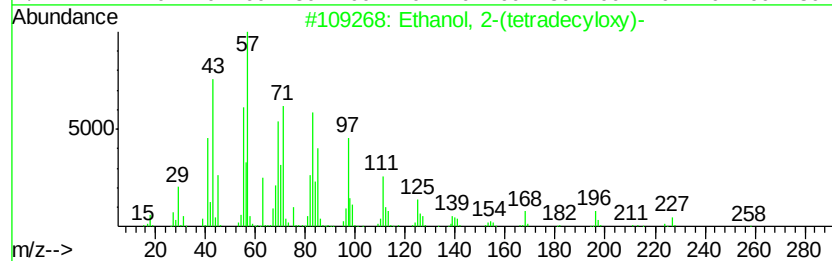
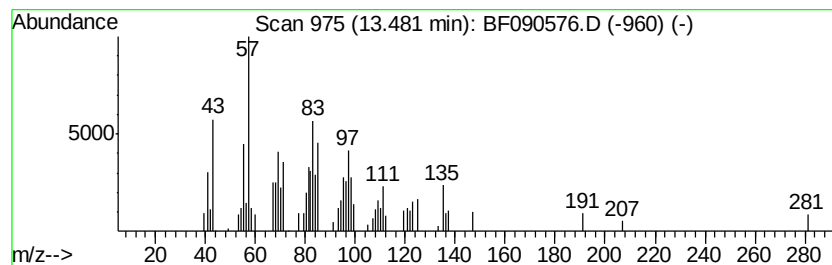
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethanol, 2-(tetradecyloxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.48	6.78 ng	335698	Chrysene-d12	14.09		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	52
2		2-Heptadecenal	252	C17H32O	1000143-48-6	46
3		2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	43
4		n-Pentadecanol	228	C15H32O	000629-76-5	43
5		1-Tetradecanol	214	C14H30O	000112-72-1	38



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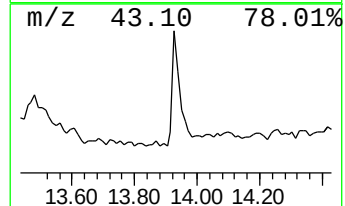
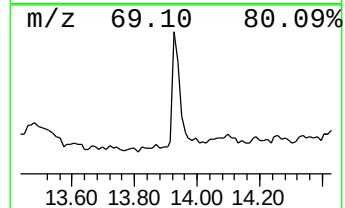
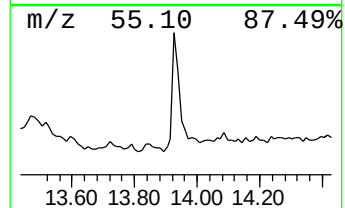
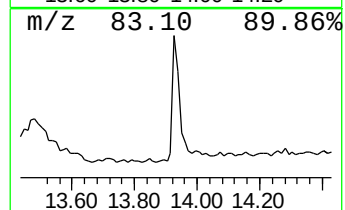
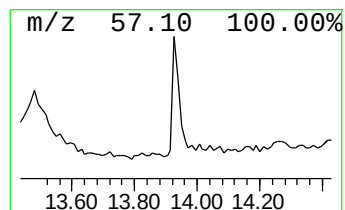
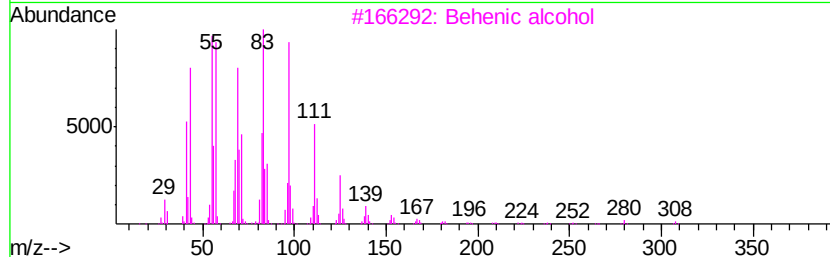
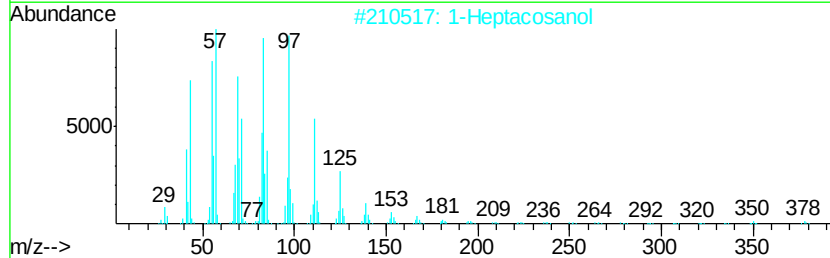
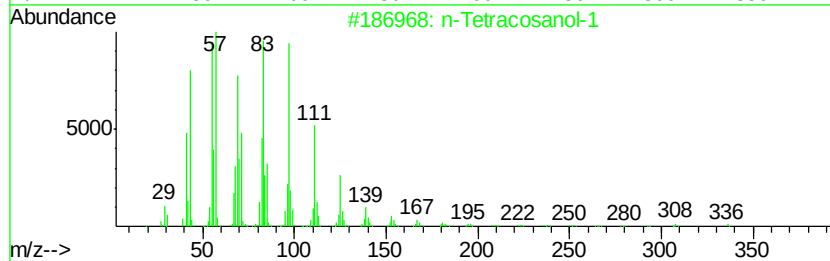
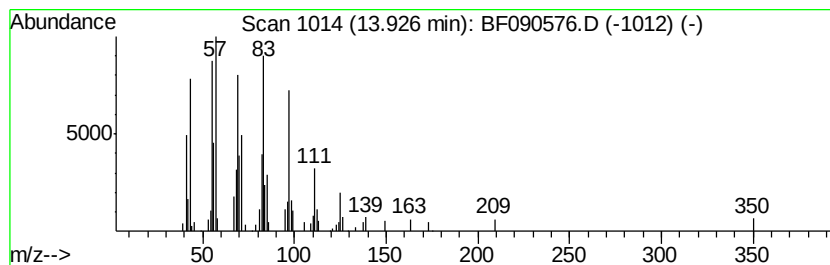
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	2.61 ng	129454	Chrysene-d12	14.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2		1-Heptacosanol	396	C27H56O	002004-39-9	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	17.1	ng	919007	1	6.92	1073110	20.0
unknown6.69	6.69	71.6	ng	3840590	1	6.92	1073110	20.0
Hexadecane	10.86	2.3	ng	171266	4	11.45	1521630	20.0
Ethanol, 2-(tetra...	13.48	6.8	ng	335698	5	14.09	990303	20.0
n-Tetracosanol-1	13.93	2.6	ng	129454	5	14.09	990303	20.0