

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031117\
 Data File : BF093573.D
 Acq On : 11 Mar 2017 17:58
 Operator : SJ/MA
 Sample : I2215-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 E2-V4-BASE

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-BF030717.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	4.287	208	210	218	rVB	102114	163884	2.30%	0.276%
2	4.881	260	262	277	rBV	893813	1803062	25.25%	3.039%
3	5.327	298	301	319	rBV	4736779	6874511	96.28%	11.585%
4	5.716	333	335	340	rBV	72402	93313	1.31%	0.157%
5	6.390	391	394	401	rBV	5378324	7140035	100.00%	12.032%
6	6.493	401	403	406	rVB	5333020	5380838	75.36%	9.068%
7	6.722	421	423	429	rVB	1110054	1221947	17.11%	2.059%
8	6.870	434	436	439	rBV	3982189	4496981	62.98%	7.578%
9	7.293	471	473	476	rBV	3270216	4141369	58.00%	6.979%
10	8.002	533	535	538	rBV	1546273	1691286	23.69%	2.850%
11	9.087	627	630	632	rBV	4894591	6439484	90.19%	10.852%
12	9.488	662	665	667	rBV	1224835	1294213	18.13%	2.181%
13	9.590	671	674	679	rVB2	70200	124317	1.74%	0.209%
14	9.716	680	685	686	rBV2	110168	244494	3.42%	0.412%
15	9.750	686	688	691	rVB	1697258	1776766	24.88%	2.994%
16	10.162	721	724	725	rBV	71890	92233	1.29%	0.155%
17	10.185	725	726	728	rVB	140507	104859	1.47%	0.177%
18	10.550	755	758	765	rBV	3091609	3382028	47.37%	5.699%
19	10.653	765	767	770	rVV	171665	198021	2.77%	0.334%
20	10.790	774	779	786	rBV	131979	503827	7.06%	0.849%
21	11.099	804	806	808	rBV	174256	165188	2.31%	0.278%
22	11.236	816	818	824	rBV	1926460	2143110	30.02%	3.612%
23	11.476	837	839	842	rBV3	60819	117265	1.64%	0.198%
24	11.522	842	843	846	rVB	149627	170112	2.38%	0.287%
25	11.773	864	865	868	rBV	331675	319466	4.47%	0.538%
26	11.853	871	872	877	rVB2	62550	99351	1.39%	0.167%
27	11.933	877	879	881	rBV	128157	110273	1.54%	0.186%
28	12.459	923	925	928	rBV	257450	381494	5.34%	0.643%
29	12.676	942	944	948	rVB	267413	415775	5.82%	0.701%
30	12.825	954	957	959	rBV	4670477	4962109	69.50%	8.362%
31	13.019	970	974	975	rBV2	45045	88231	1.24%	0.149%
32	13.717	1033	1035	1037	rBV	137333	140084	1.96%	0.236%
33	13.877	1046	1049	1055	rBV	1476533	1730381	24.23%	2.916%
34	14.894	1136	1138	1140	rBV	85234	137527	1.93%	0.232%

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35	15.168	1160	1162	1166	rVB	54743	77119	1.08%	0.130%
36	15.225	1166	1167	1169	rBV	64905	93042	1.30%	0.157%
37	15.271	1169	1171	1180	rVB	613616	1022045	14.31%	1.722%

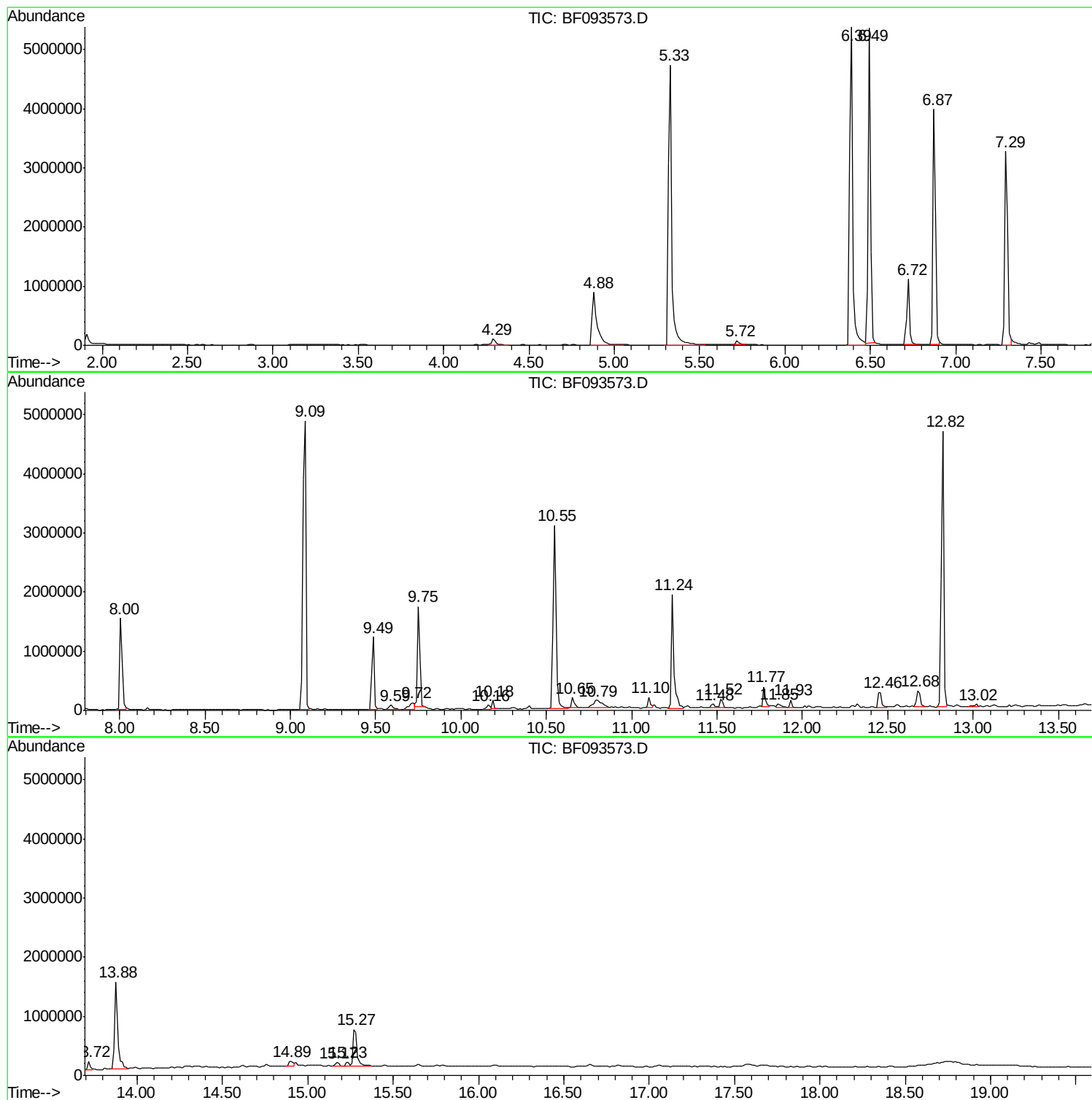
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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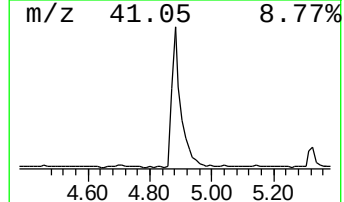
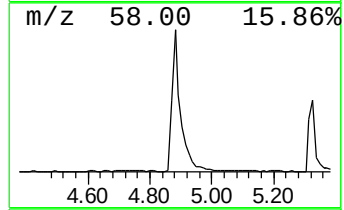
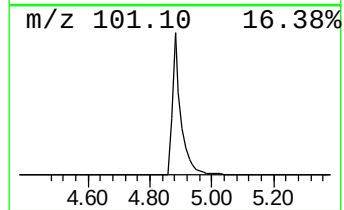
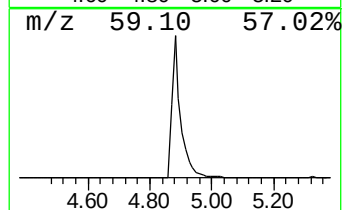
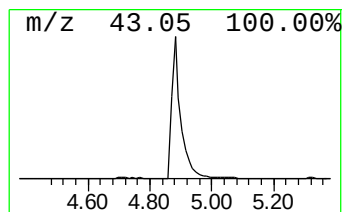
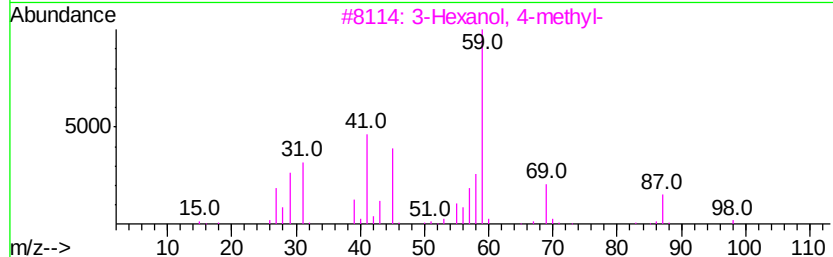
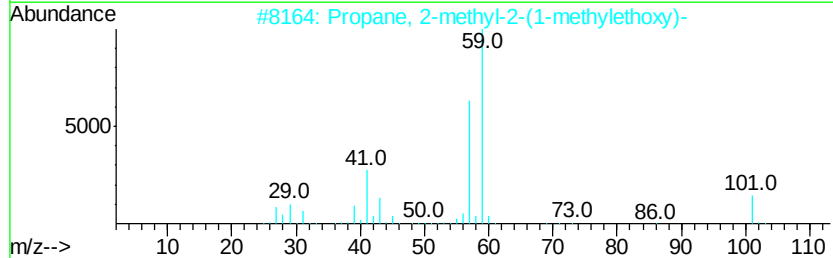
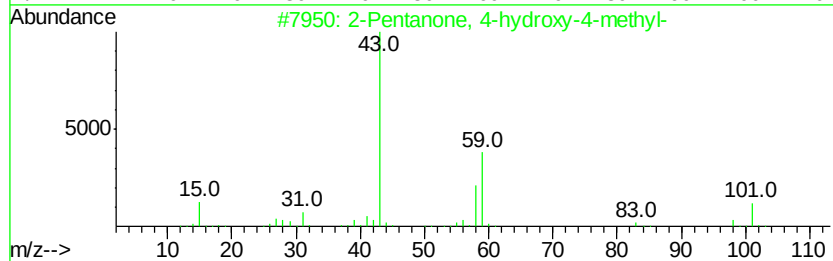
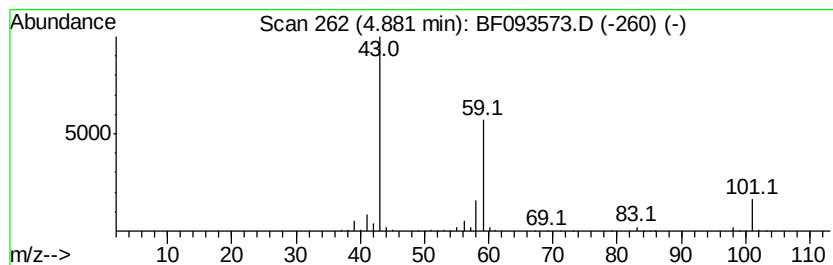
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	29.51 ng	1803060	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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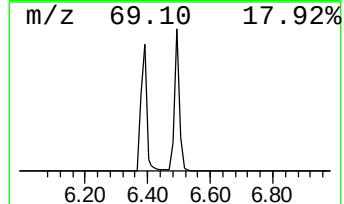
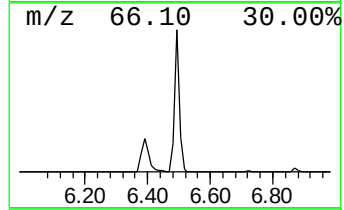
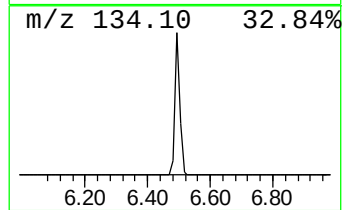
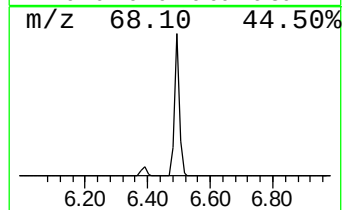
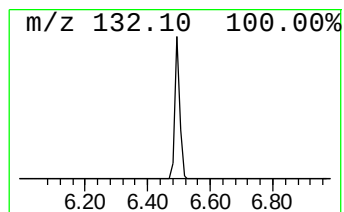
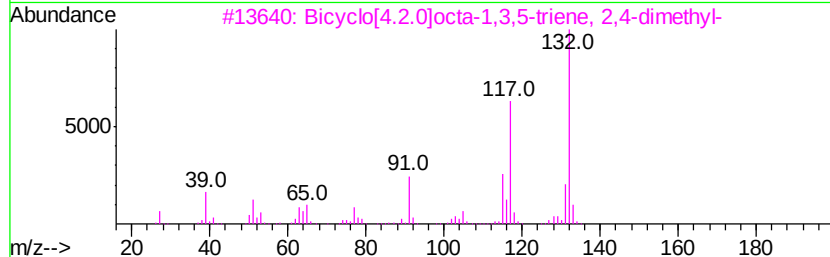
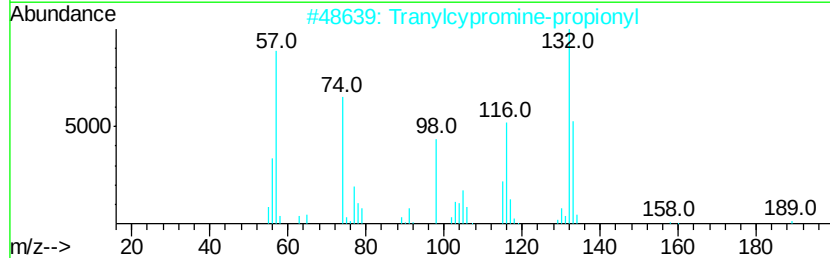
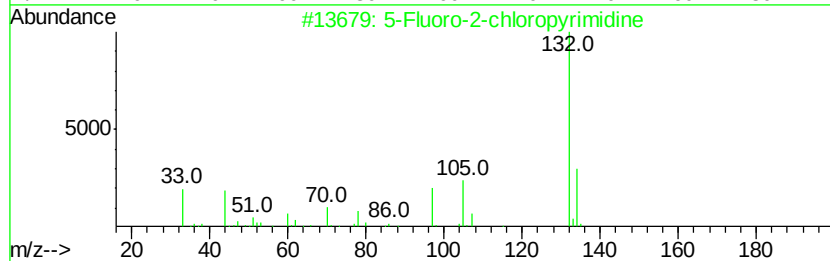
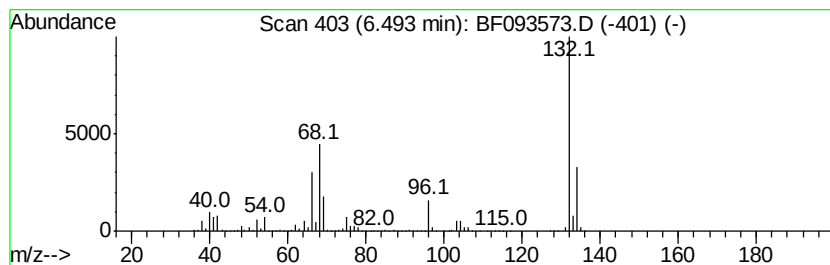
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Peak Number 3 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	88.07 ng	5380840	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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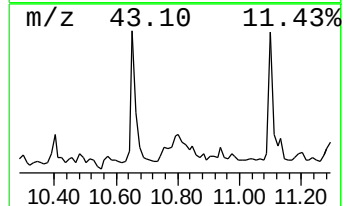
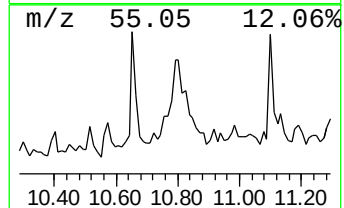
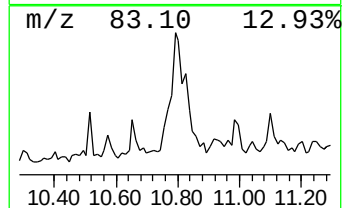
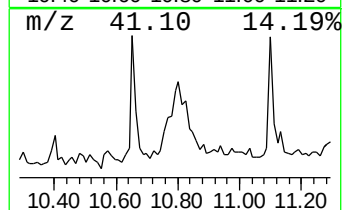
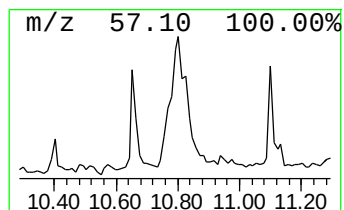
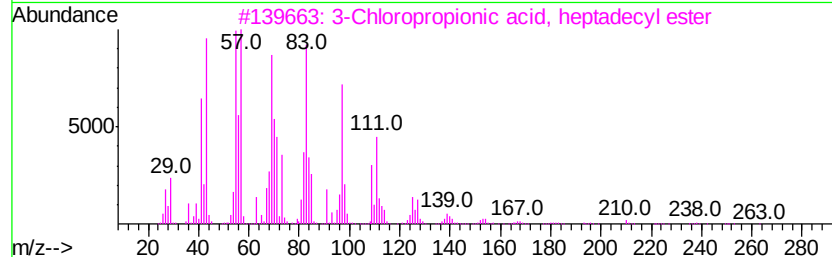
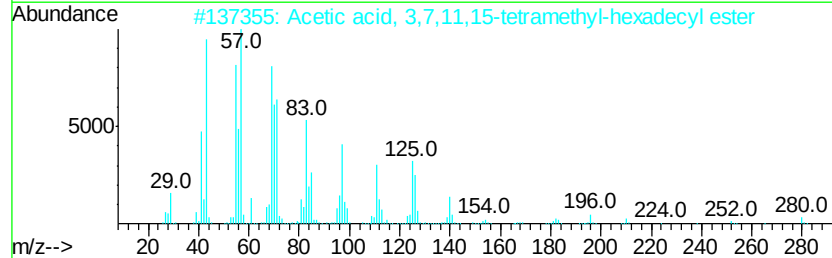
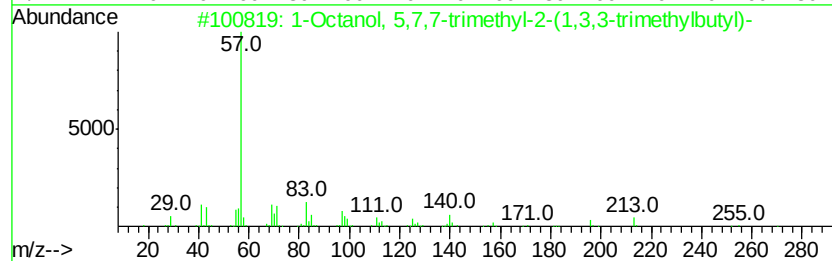
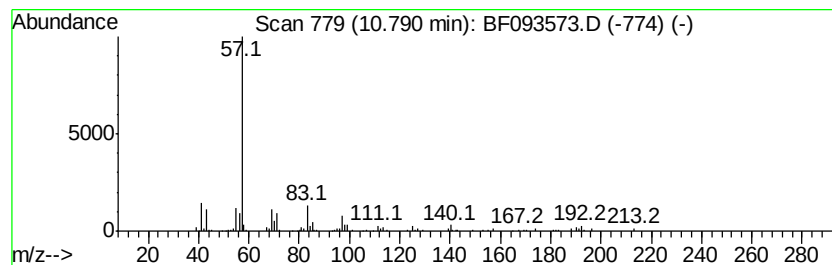
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Peak Number 5 1-Octanol, 5,7,7-trimethyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.79	4.70 ng	503827	Phenanthrene-d10	11.24		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 5,7,7-trimethyl-2-(1,...	270	C18H38O	036400-98-3	86	
2	Acetic acid, 3,7,11,15-tetrameth...	340	C22H44O2	1000193-63-0	59	
3	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	59	
4	3-Propionyloxytridecane	256	C16H32O2	1000245-62-5	53	
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	53	



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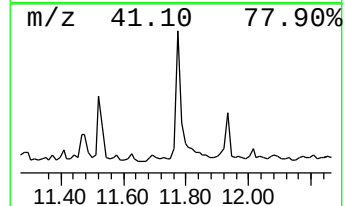
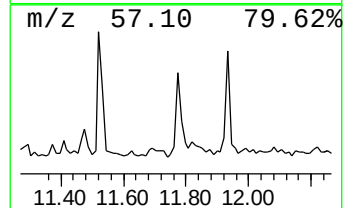
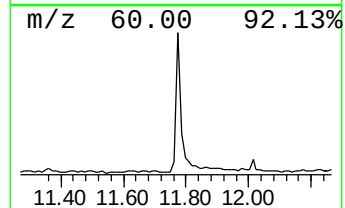
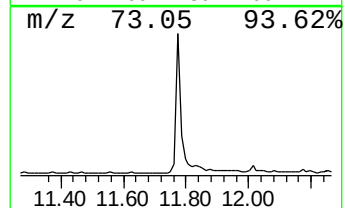
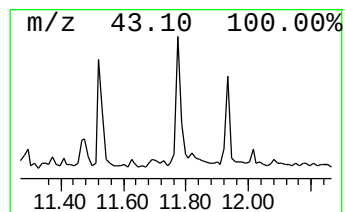
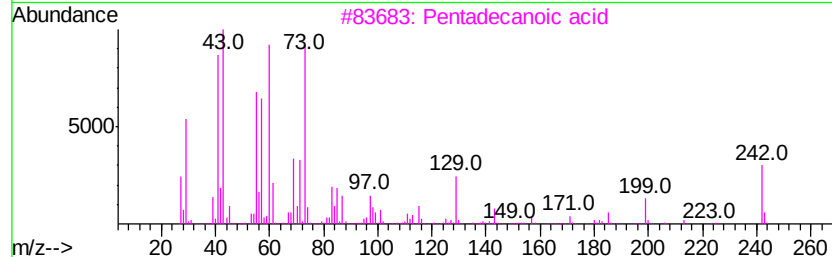
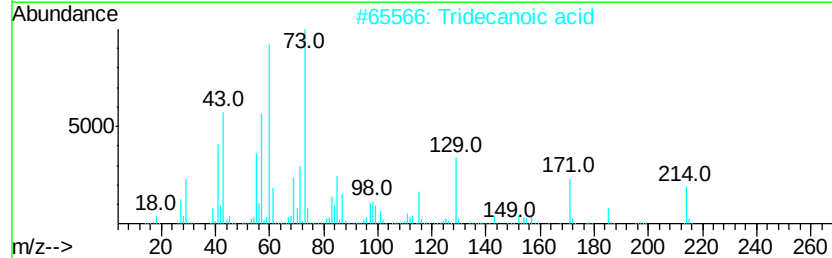
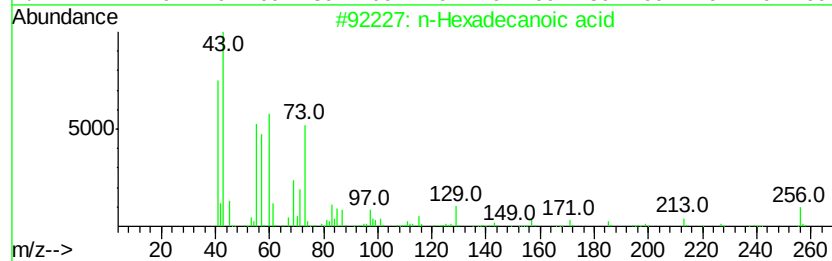
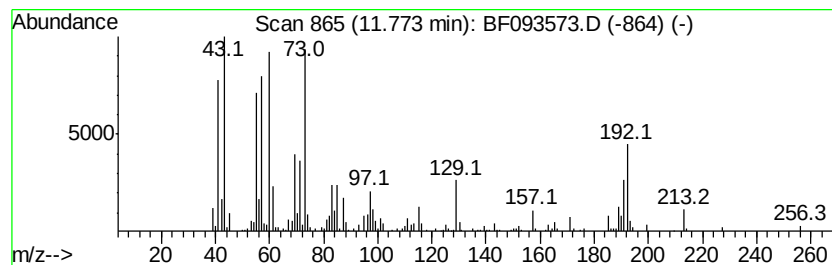
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.77	2.98 ng	319466	Phenanthrene-d10		11.24
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.88	29.5	ng	1803060	1	6.72	1221950	20.0
unknown6.49	6.49	88.1	ng	5380840	1	6.72	1221950	20.0
1-Octanol, 5,7,7-...	10.79	4.7	ng	503827	4	11.24	2143110	20.0
n-Hexadecanoic acid	11.77	3.0	ng	319466	4	11.24	2143110	20.0