

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011617\
 Data File : BF092302.D
 Acq On : 16 Jan 2017 23:17
 Operator : UM/SJ
 Sample : I1162-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-45-COMP

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-BF122116.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	4.679	250	253	270	rBV	1352710	2235572	42.74%	4.817%
2	5.159	292	295	311	rBV	3398422	4981882	95.24%	10.734%
3	6.233	386	389	391	rBV	4720531	5230785	100.00%	11.270%
4	6.336	396	398	400	rBV	5035270	4661372	89.11%	10.043%
5	6.565	415	418	420	rBV	1118348	1150397	21.99%	2.479%
6	6.713	429	431	434	rBV	2970565	3493304	66.78%	7.526%
7	7.136	465	468	470	rBV	3201791	2991021	57.18%	6.444%
8	7.845	528	530	533	rBV	1261741	1500134	28.68%	3.232%
9	8.930	622	625	627	rBV	5356329	5047884	96.50%	10.876%
10	9.331	658	660	662	rBV	486946	425077	8.13%	0.916%
11	9.548	677	679	681	rBV	57754	54846	1.05%	0.118%
12	9.593	681	683	685	rBV	2005076	1715800	32.80%	3.697%
13	10.039	721	722	724	rVB	73180	85371	1.63%	0.184%
14	10.382	750	752	755	rBV	3014598	3043347	58.18%	6.557%
15	10.519	762	764	767	rBV	92609	137758	2.63%	0.297%
16	10.954	801	802	804	rBV	62366	84480	1.62%	0.182%
17	11.068	810	812	815	rBV	1821378	1662371	31.78%	3.582%
18	11.628	859	861	865	rBV2	166180	212898	4.07%	0.459%
19	12.405	927	929	934	rBV2	45336	62718	1.20%	0.135%
20	12.497	934	937	940	rVB2	67885	68405	1.31%	0.147%
21	12.657	948	951	953	rBV	4552758	4336896	82.91%	9.344%
22	13.194	996	998	1001	rBV2	42129	58375	1.12%	0.126%
23	13.571	1029	1031	1039	rBV	157149	319942	6.12%	0.689%
24	13.697	1039	1042	1045	rBV	1493363	1427085	27.28%	3.075%
25	15.045	1158	1160	1163	rBV	877627	1032261	19.73%	2.224%
26	15.445	1192	1195	1198	rVB	49305	63493	1.21%	0.137%
27	15.857	1228	1231	1238	rVB2	44097	88349	1.69%	0.190%
28	16.326	1269	1272	1275	rBV	30371	60128	1.15%	0.130%
29	16.886	1318	1321	1326	rVB	28238	66718	1.28%	0.144%
30	17.548	1375	1379	1384	rBV3	20806	59534	1.14%	0.128%
31	18.337	1445	1448	1456	rVB5	17959	55528	1.06%	0.120%

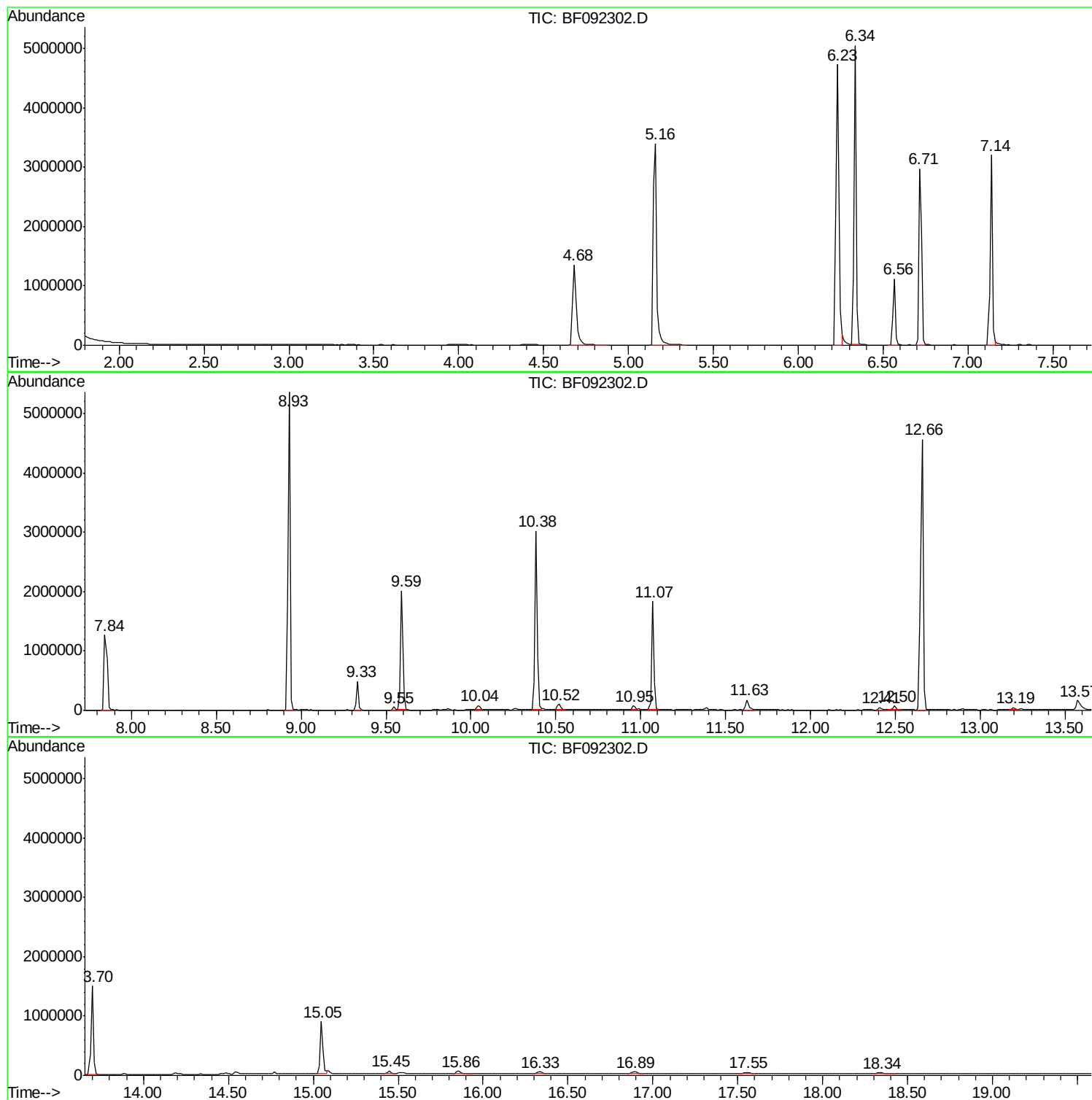
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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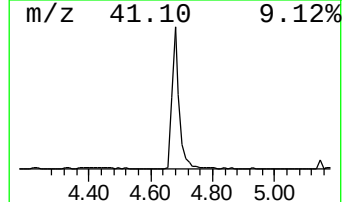
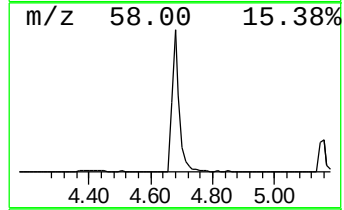
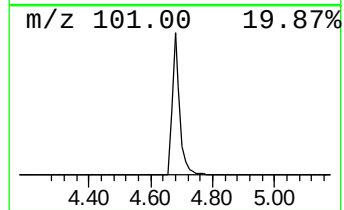
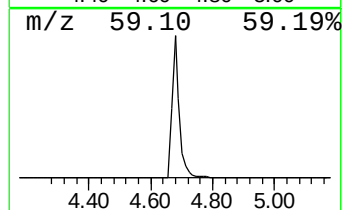
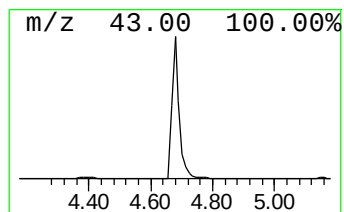
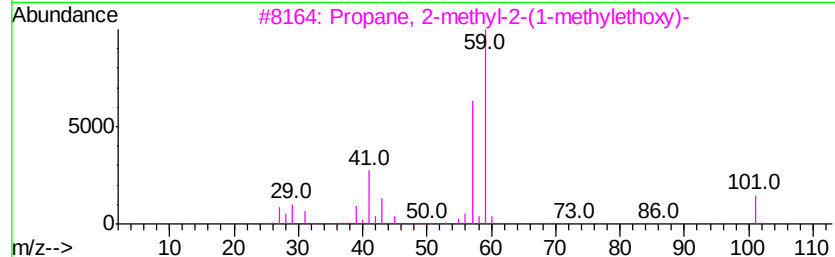
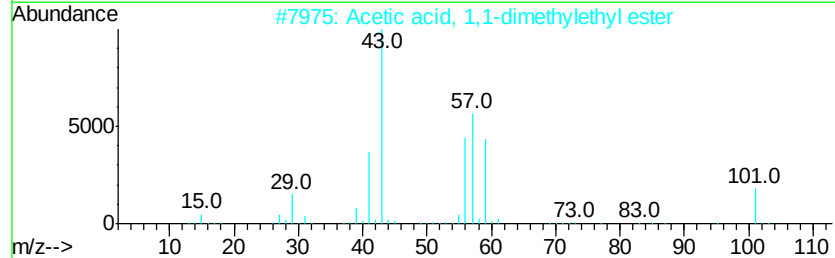
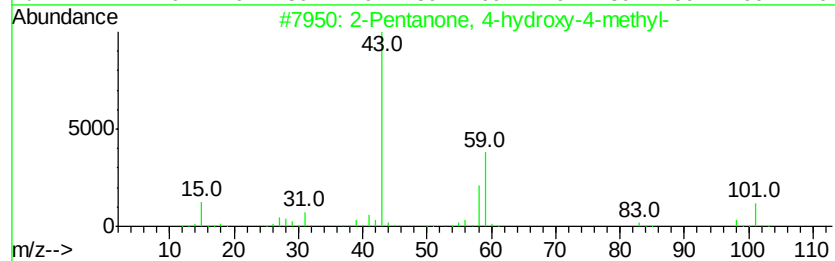
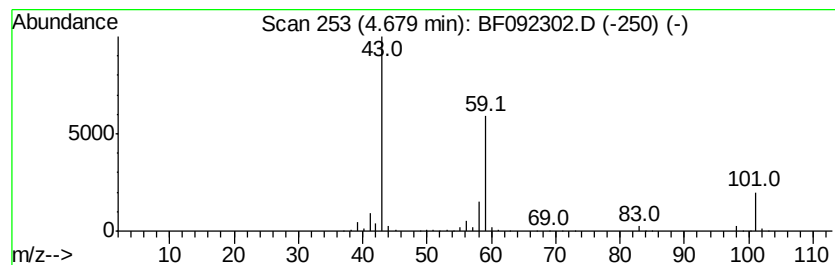
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.68	38.87 ng	2235570	1,4-Dichlorobenzene-d4	6.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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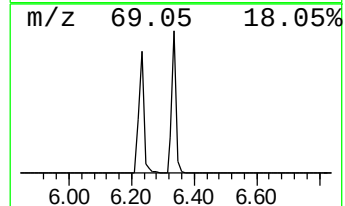
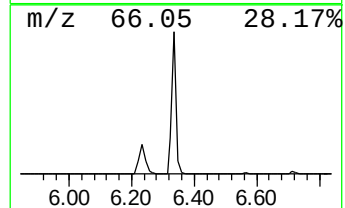
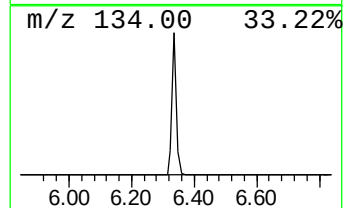
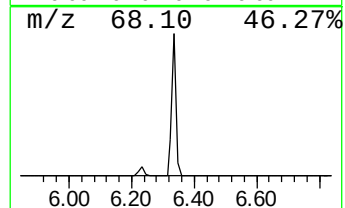
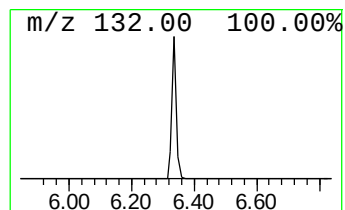
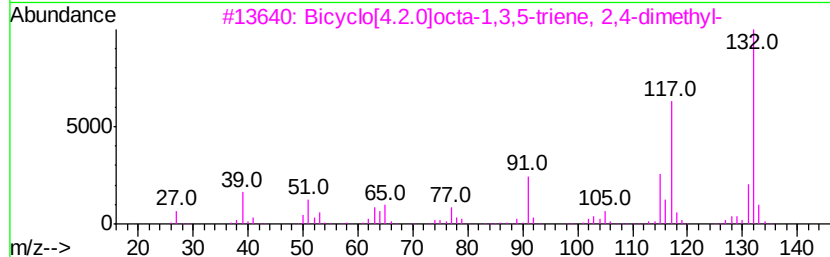
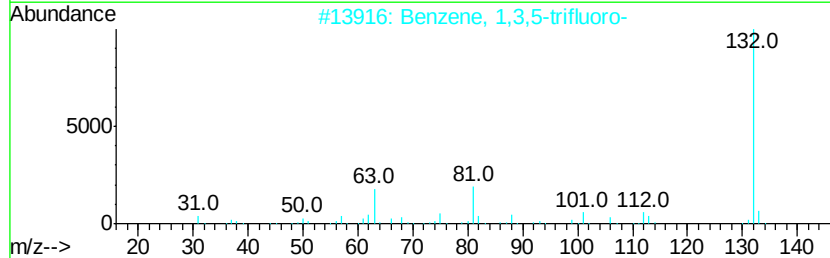
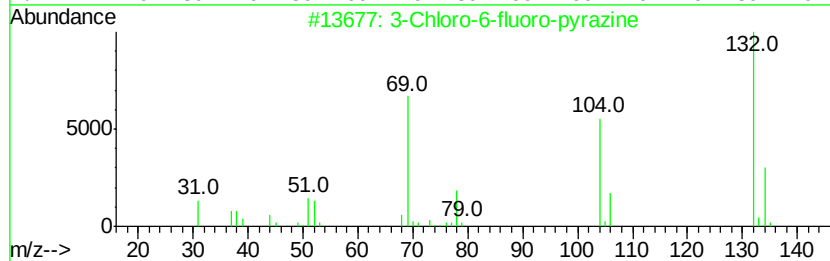
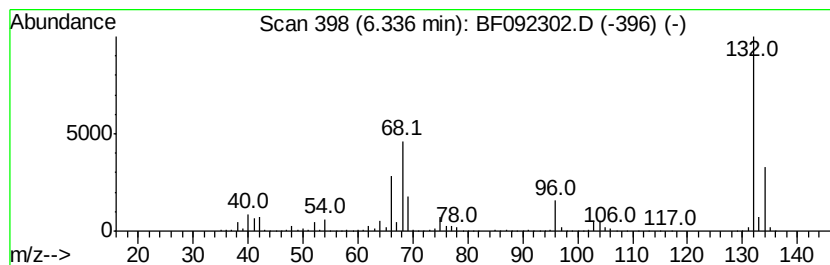
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Peak Number 2 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	81.04 ng	4661370	1,4-Dichlorobenzene-d4	6.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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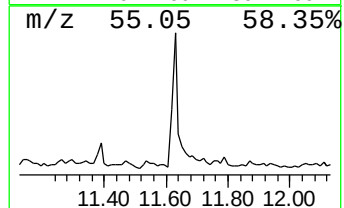
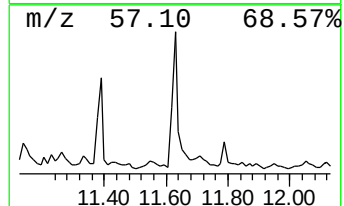
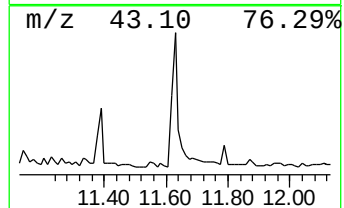
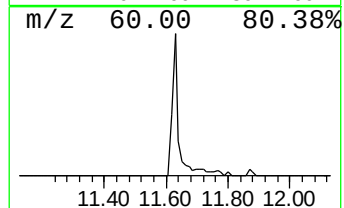
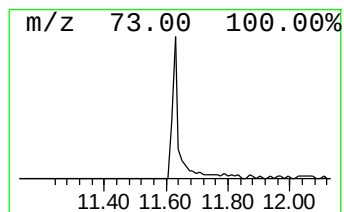
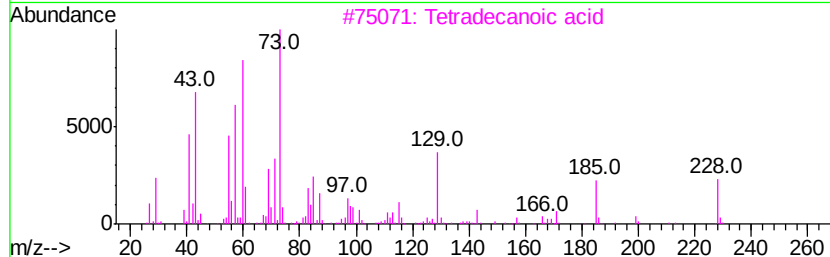
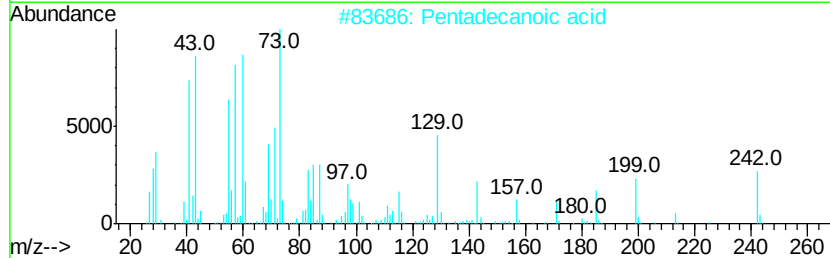
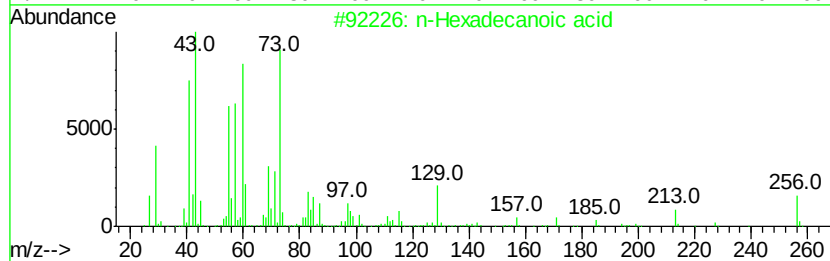
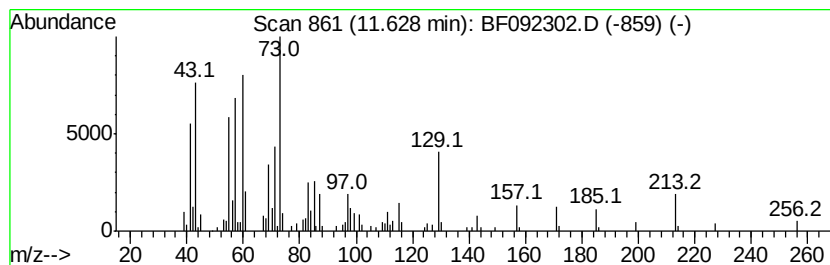
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.63	2.56 ng	212898	Phenanthrene-d10		11.07
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tridecanoic acid	214	C13H26O2	000638-53-9	72



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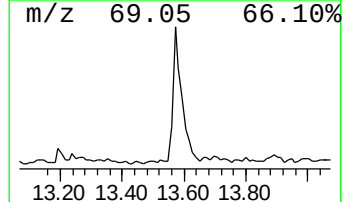
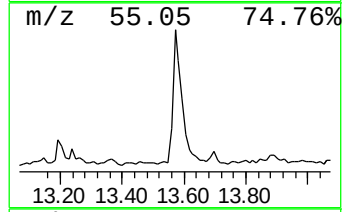
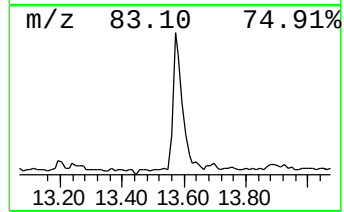
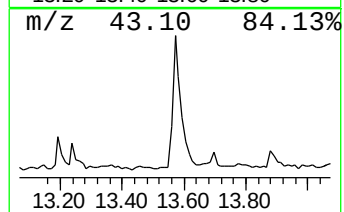
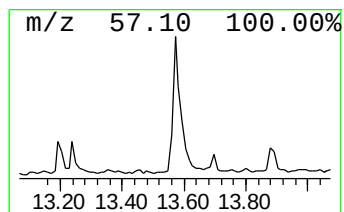
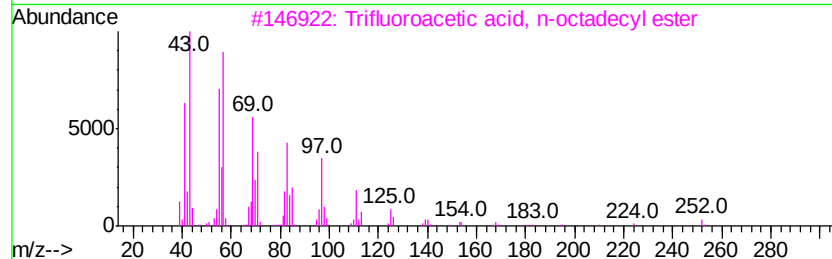
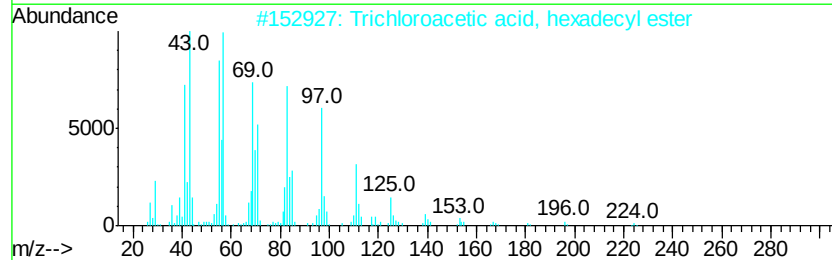
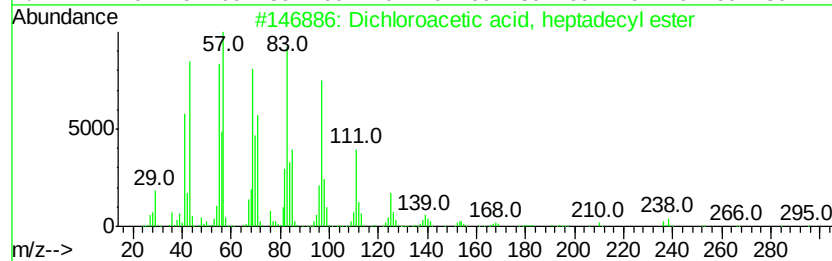
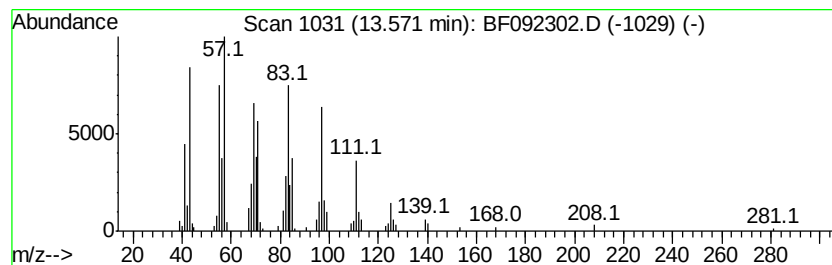
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	4.48 ng	319942	Chrysene-d12	13.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		Trifluoroacetic acid, n-octadecyl ...	366	C20H37F3O2	079392-43-1	91
4		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.68	38.9	ng	2235570	1	6.56	1150400	20.0
unknown6.34	6.34	81.0	ng	4661370	1	6.56	1150400	20.0
n-Hexadecanoic acid	11.63	2.6	ng	212898	4	11.07	1662370	20.0
Dichloroacetic ac...	13.57	4.5	ng	319942	5	13.70	1427090	20.0