

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031116\
 Data File : BF085412.D
 Acq On : 12 Mar 2016 11:16
 Operator : UM/SJ
 Sample : H1731-14
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-25-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-BF030316.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	5.144	248	250	260	rVB	215740	316209	6.86%	0.877%
2	5.544	282	285	287	rBV	3588279	3924995	85.15%	10.881%
3	6.573	371	375	377	rBV	3304576	4609333	100.00%	12.778%
4	6.710	384	387	389	rBV	3408102	4515000	97.95%	12.516%
5	6.939	404	407	409	rBV	865043	906091	19.66%	2.512%
6	7.099	418	421	423	rBV	2531837	3385928	73.46%	9.386%
7	7.499	453	456	459	rBV	2364001	2602469	56.46%	7.214%
8	7.590	461	464	466	rBV	39332	60549	1.31%	0.168%
9	8.219	517	519	522	rBV	1234473	1101190	23.89%	3.053%
10	9.305	611	614	616	rBV	3699754	4173229	90.54%	11.569%
11	9.693	646	648	650	rBV	963752	803320	17.43%	2.227%
12	9.910	665	667	669	rVB	123108	104580	2.27%	0.290%
13	9.979	671	673	675	rVB	1345263	1121773	24.34%	3.110%
14	10.413	707	711	712	rBV	116931	172466	3.74%	0.478%
15	10.631	727	730	731	rBV	57807	81068	1.76%	0.225%
16	10.768	739	742	745	rBV	2197742	2158178	46.82%	5.983%
17	10.882	748	752	757	rBV	187777	240189	5.21%	0.666%
18	11.328	789	791	793	rBV	101329	90843	1.97%	0.252%
19	11.465	801	803	805	rBV	1138922	971060	21.07%	2.692%
20	11.991	845	849	851	rBV	52722	65520	1.42%	0.182%
21	13.054	939	942	944	rBV	3155944	2848229	61.79%	7.896%
22	13.945	1018	1020	1025	rBV	114141	139173	3.02%	0.386%
23	14.105	1031	1034	1036	rBV	919755	816114	17.71%	2.262%
24	14.951	1106	1108	1110	rVB	53532	59756	1.30%	0.166%
25	15.568	1159	1162	1165	rBV	504455	668262	14.50%	1.853%
26	16.540	1243	1247	1251	rBV3	20171	48276	1.05%	0.134%
27	17.626	1338	1342	1348	rVB7	34633	89565	1.94%	0.248%

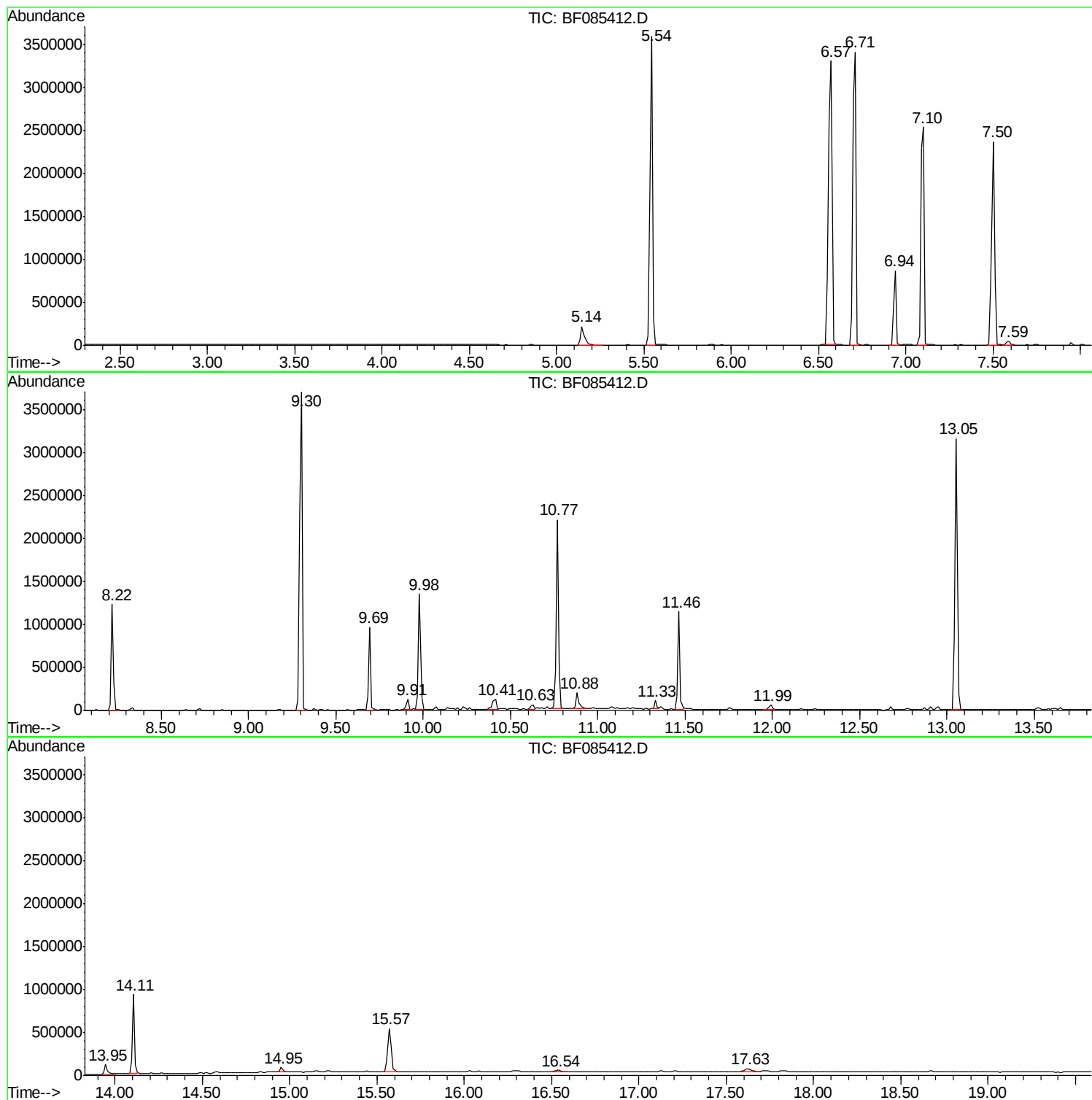
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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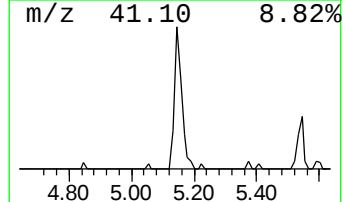
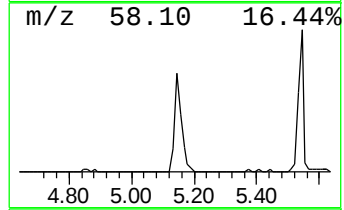
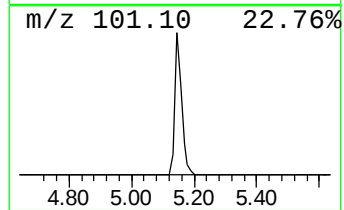
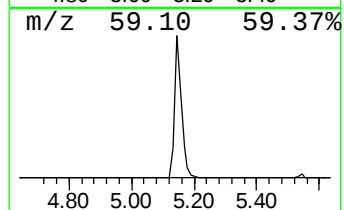
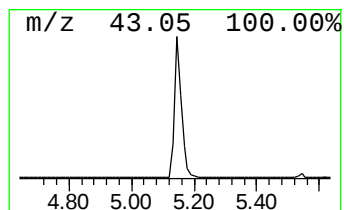
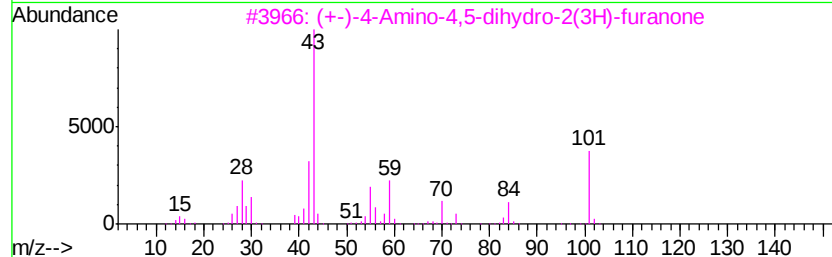
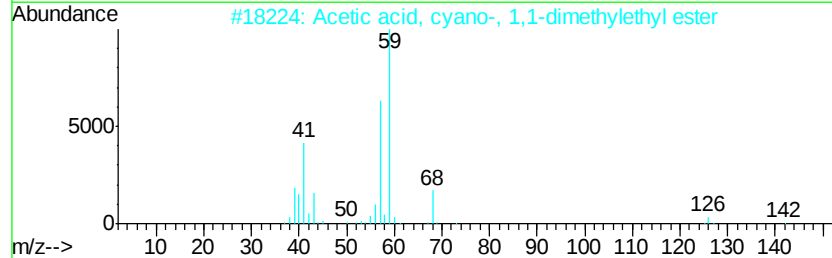
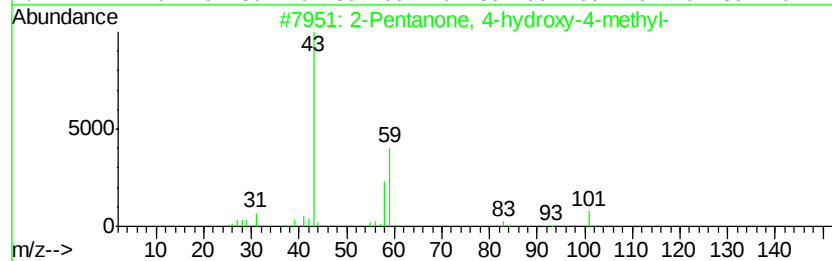
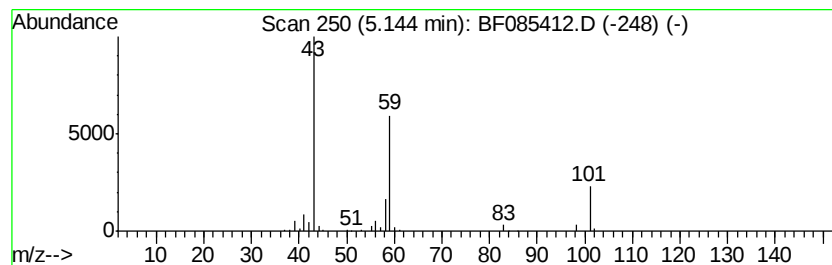
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.14	6.98 ng	316209	1,4-Dichlorobenzene-d4	6.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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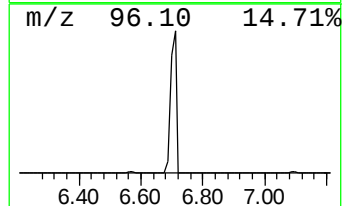
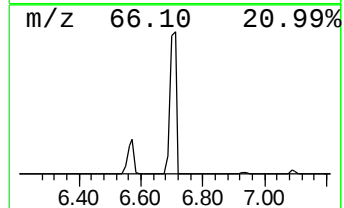
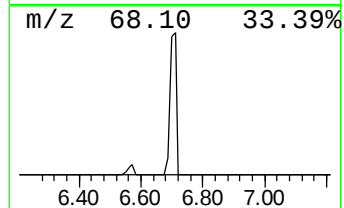
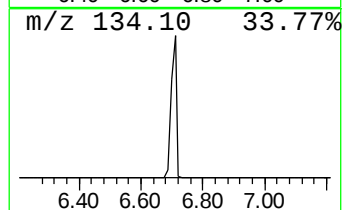
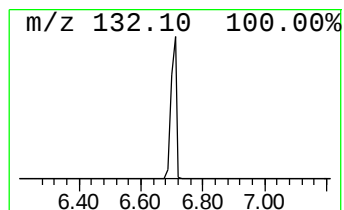
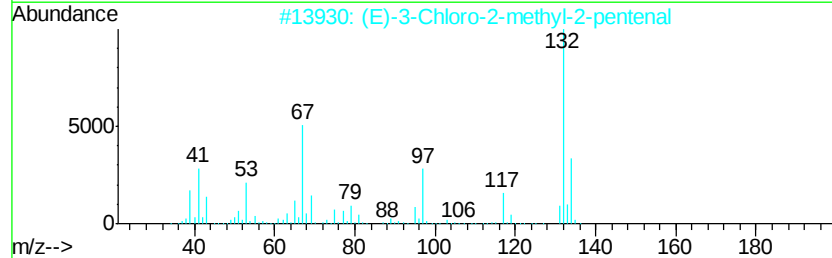
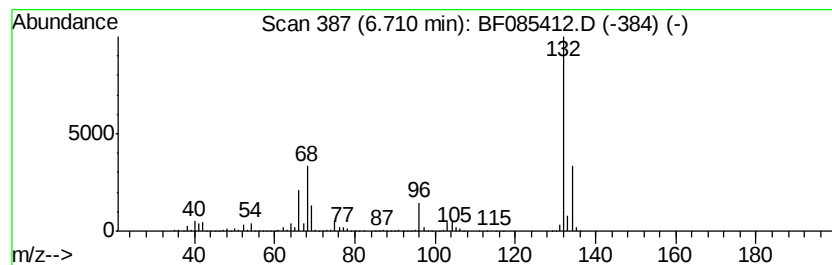
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.71 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	99.66 ng	4515000	1,4-Dichlorobenzene-d4	6.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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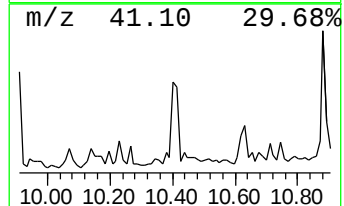
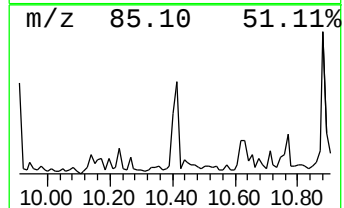
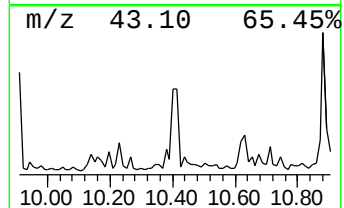
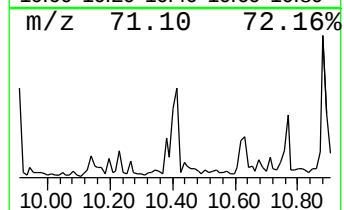
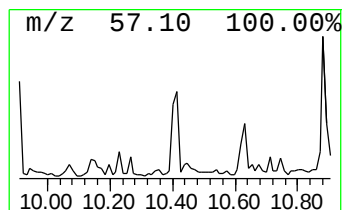
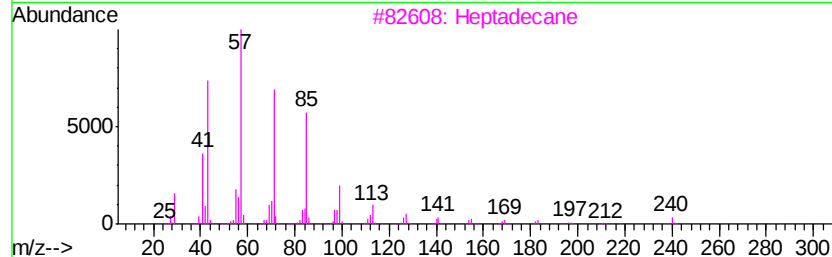
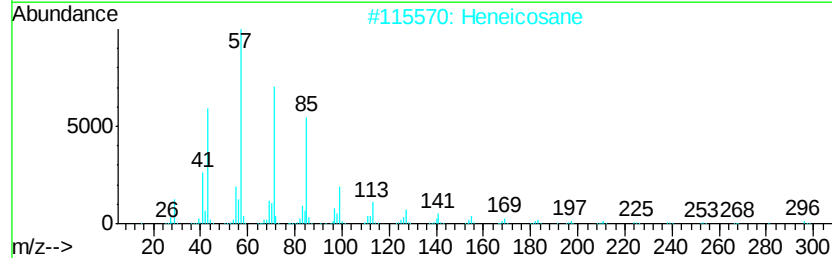
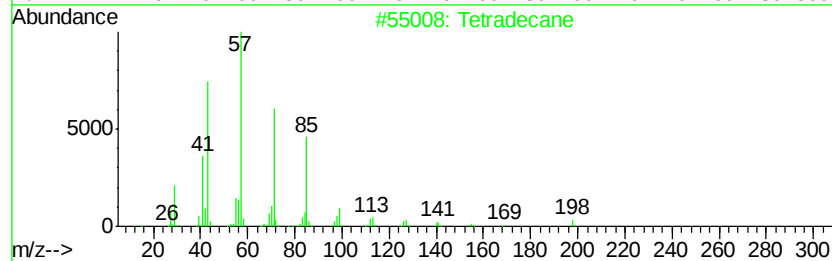
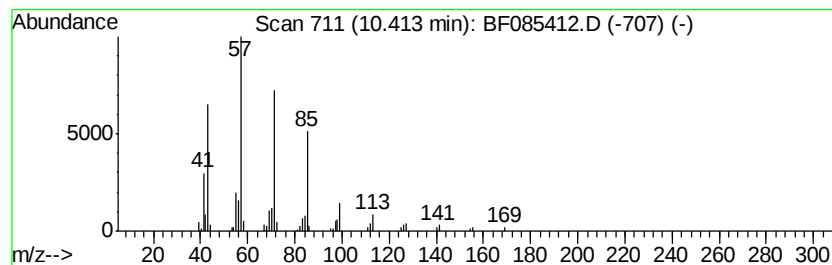
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.41	3.07 ng	172466	Acenaphthene-d10		9.98
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane	240	C17H36	000629-78-7	91
4	Pentadecane	212	C15H32	000629-62-9	91
5	Hexadecane	226	C16H34	000544-76-3	90



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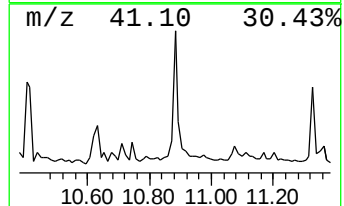
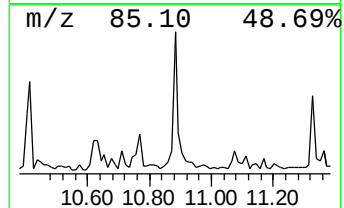
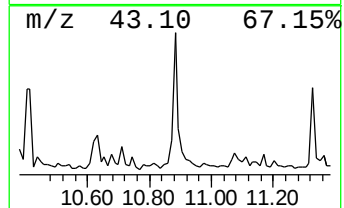
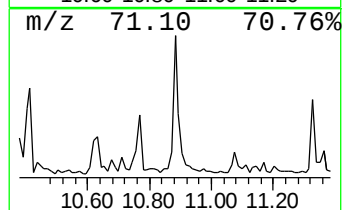
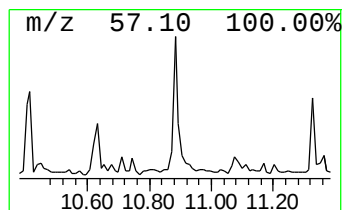
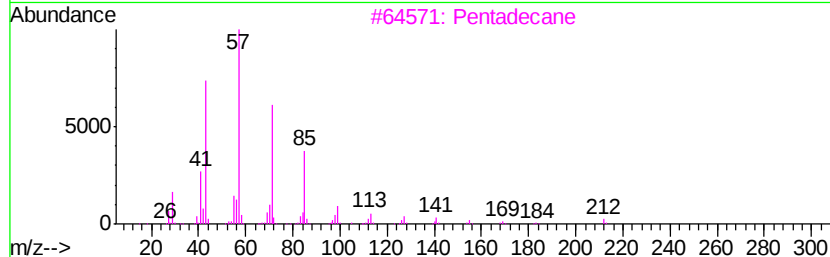
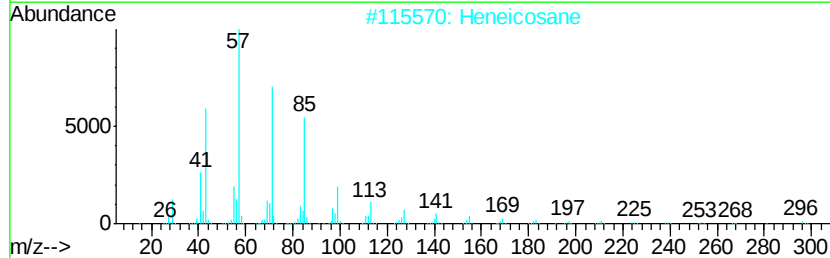
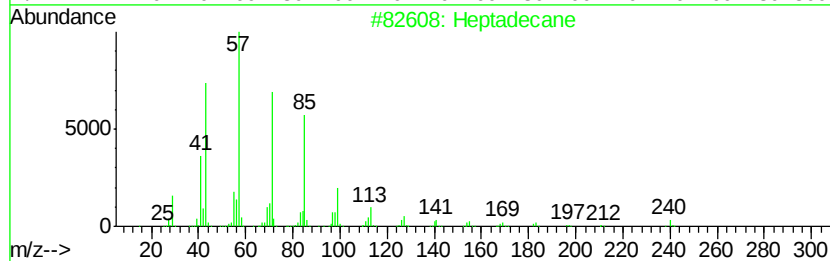
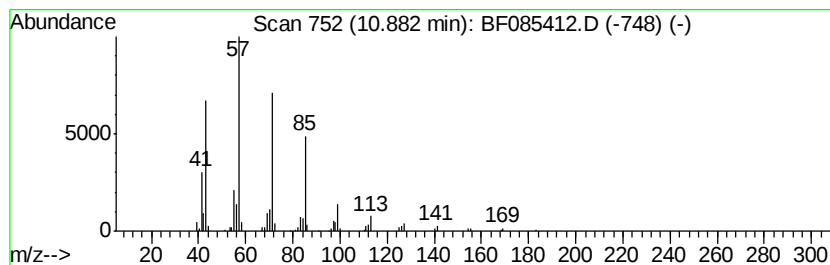
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	4.95 ng	240189	Phenanthrene-d10	11.46

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Pentadecane		212	C15H32	000629-62-9	91
4	Decane, 2,3,5-trimethyl-		184	C13H28	062238-11-3	90
5	Hexadecane		226	C16H34	000544-76-3	90



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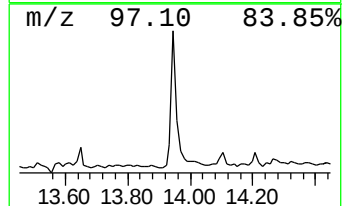
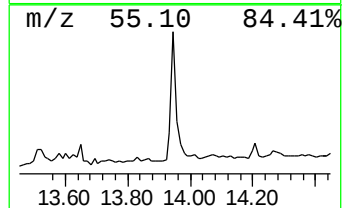
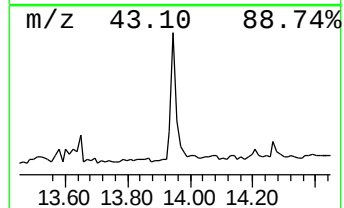
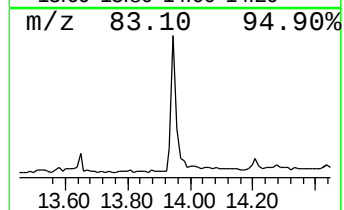
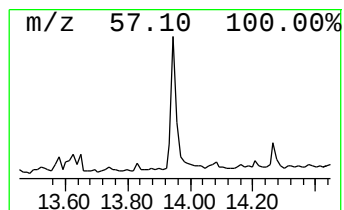
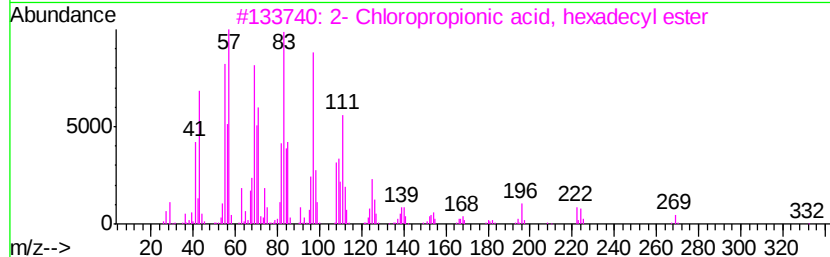
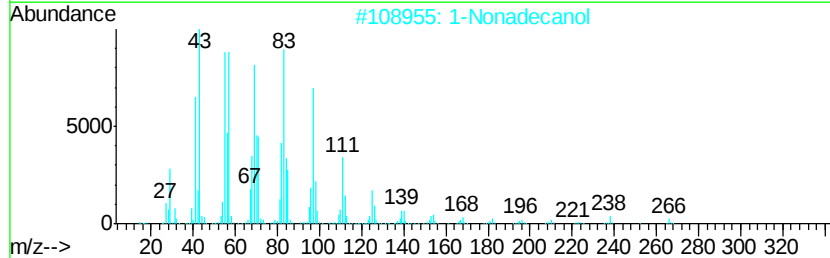
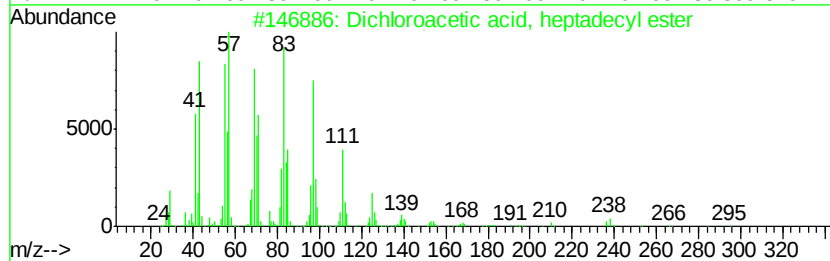
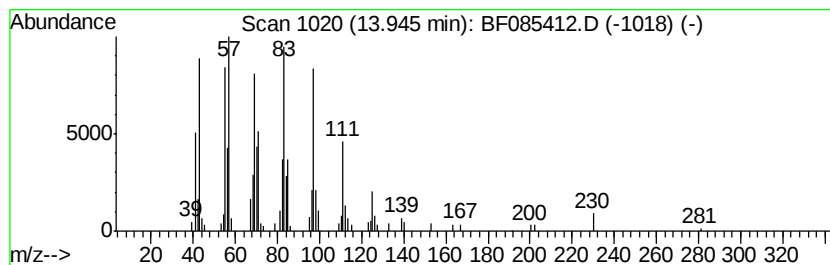
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.41 ng	139173	Chrysene-d12	14.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		1-Nonadecanol	284	C19H40O	001454-84-8	95
3		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	94
4		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	7.0	ng	316209	1	6.94	906091	20.0
unknown6.71	6.71	99.7	ng	4515000	1	6.94	906091	20.0
Tetradecane	10.41	3.1	ng	172466	3	9.98	1121770	20.0
Heptadecane	10.88	5.0	ng	240189	4	11.46	971060	20.0
Dichloroacetic ac...	13.95	3.4	ng	139173	5	14.11	816114	20.0