

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
 Data File : BF096514.D
 Acq On : 6 Jul 2017 6:05
 Operator : SJ/MA
 Sample : I3975-06
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B7-10-12

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-BF070117.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	4.910	475	480	493	rVB	320832	497471	15.30%	1.938%
2	5.334	546	552	555	rBV	3077580	3225581	99.20%	12.566%
3	6.357	717	726	729	rBV	2966136	3251542	100.00%	12.667%
4	6.487	743	748	751	rBV	3163550	3078655	94.68%	11.994%
5	6.710	783	786	790	rBV	766665	682436	20.99%	2.659%
6	6.869	809	813	817	rVB	2331466	2320276	71.36%	9.039%
7	7.275	876	882	885	rBV	2104023	2019063	62.10%	7.866%
8	7.375	894	899	904	rBV	41884	49922	1.54%	0.194%
9	7.710	953	956	959	rBV	32949	34684	1.07%	0.135%
10	7.992	1000	1004	1008	rBV	973328	818528	25.17%	3.189%
11	9.075	1183	1188	1191	rBV	2839527	2523080	77.60%	9.829%
12	9.469	1250	1255	1258	rBV	1315499	1065680	32.77%	4.152%
13	9.745	1298	1302	1306	rBV	702776	653004	20.08%	2.544%
14	10.192	1376	1378	1381	rVB	47820	39839	1.23%	0.155%
15	10.533	1432	1436	1449	rBV	1355439	1252888	38.53%	4.881%
16	10.663	1455	1458	1466	rVB	48662	55564	1.71%	0.216%
17	11.116	1531	1535	1537	rBV2	35239	33232	1.02%	0.129%
18	11.227	1550	1554	1558	rBV	684791	555581	17.09%	2.164%
19	12.651	1789	1796	1803	rBV2	29217	48161	1.48%	0.188%
20	12.816	1819	1824	1827	rBV	2181796	2072181	63.73%	8.073%
21	13.298	1900	1906	1913	rBV	85308	99176	3.05%	0.386%
22	13.721	1974	1978	1987	rBV	188230	224303	6.90%	0.874%
23	13.863	1998	2002	2005	rBV	667128	634566	19.52%	2.472%
24	15.268	2237	2241	2246	rVB	356861	433272	13.33%	1.688%

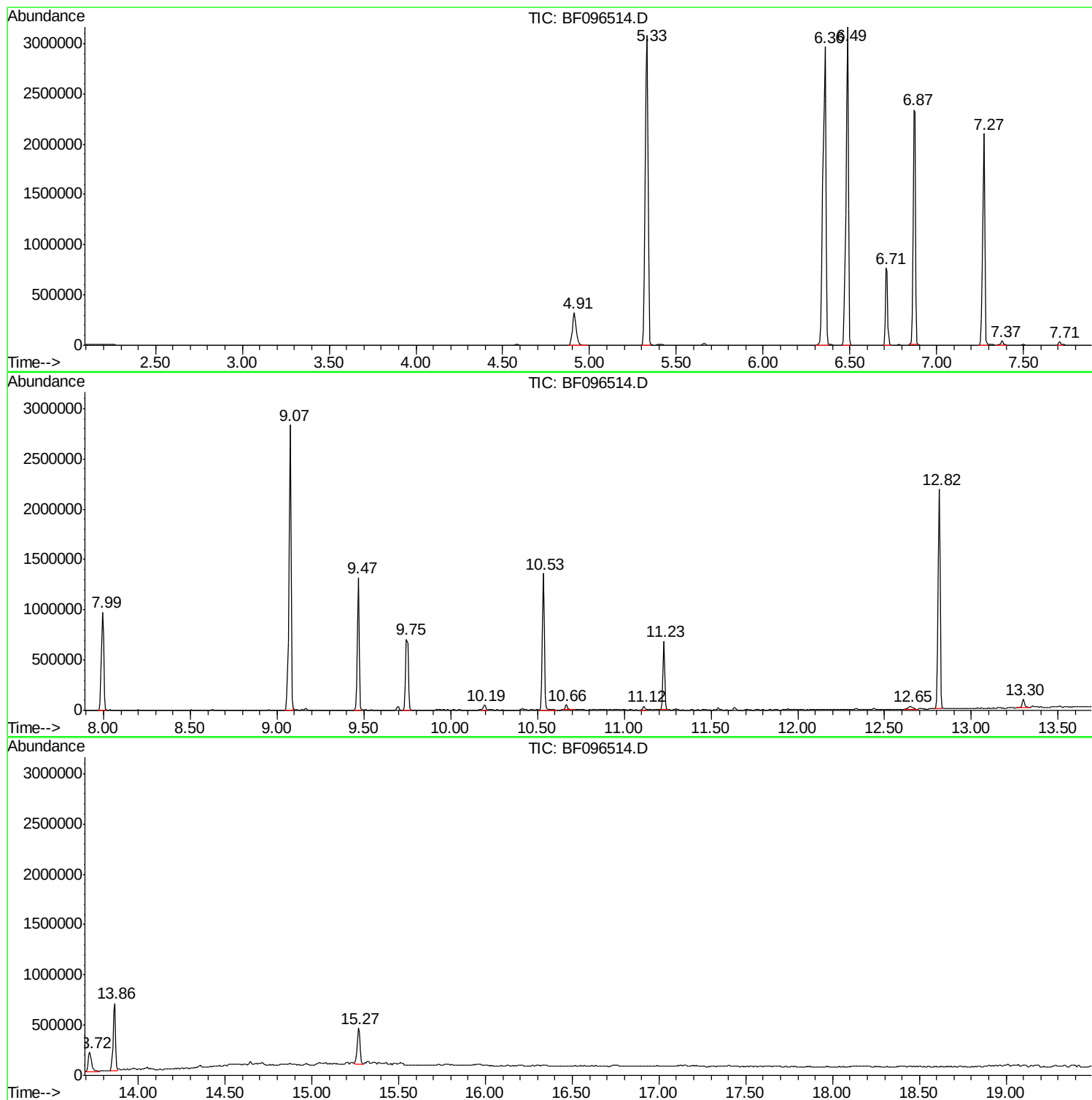
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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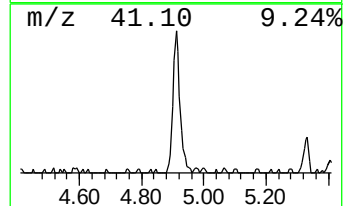
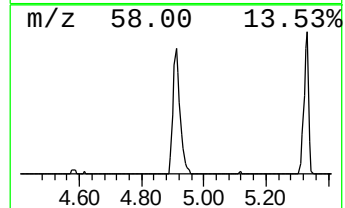
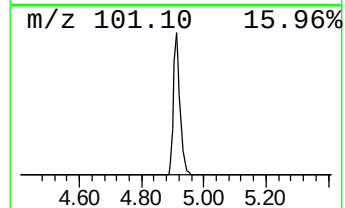
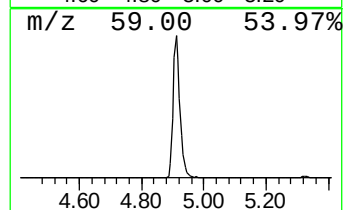
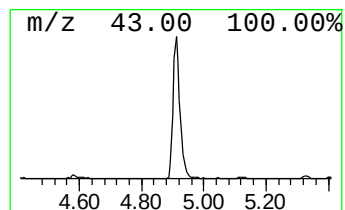
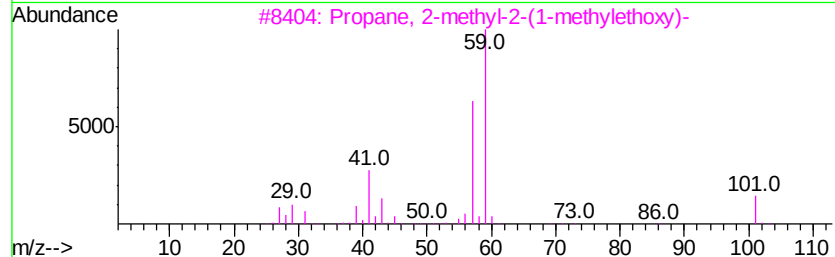
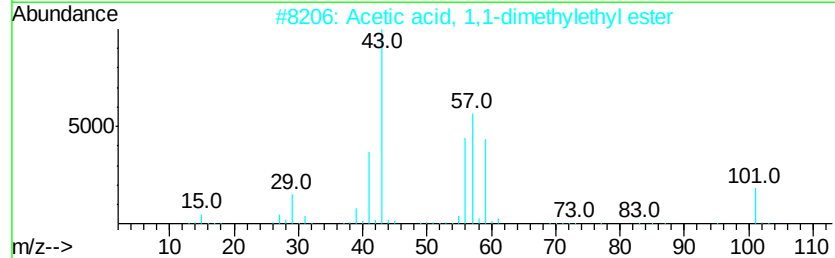
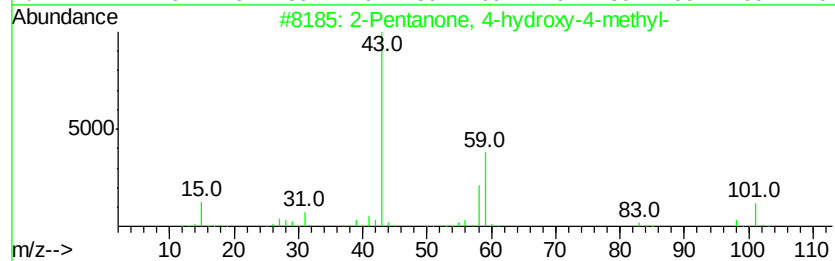
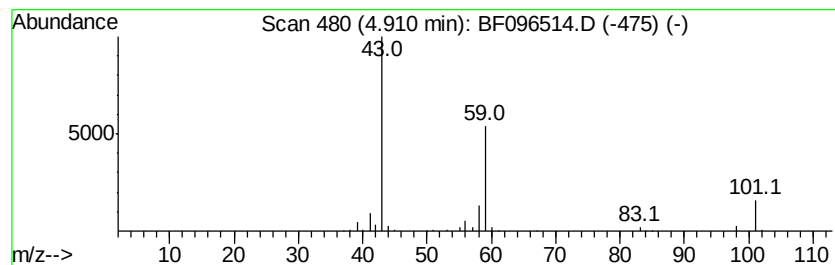
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.91	14.58 ng	497471	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
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	36
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32



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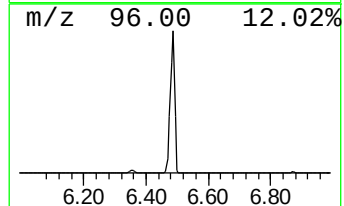
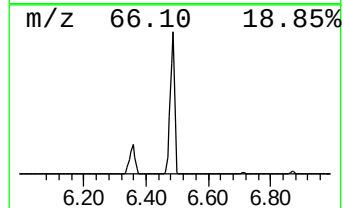
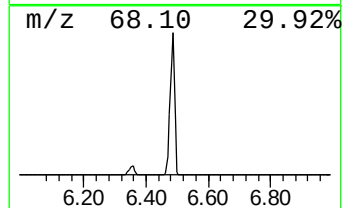
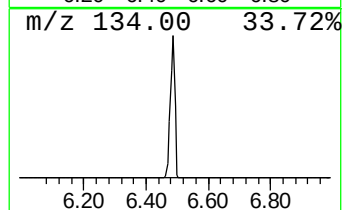
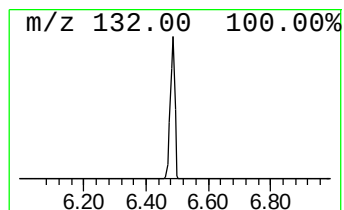
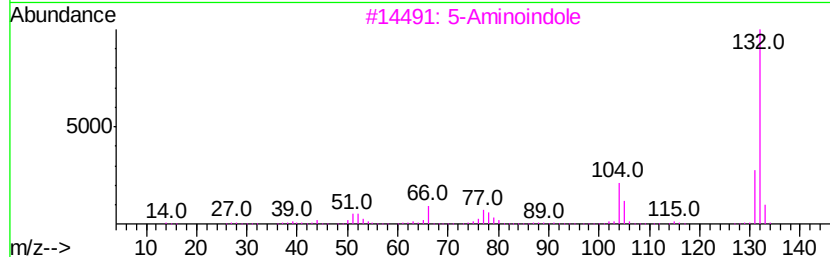
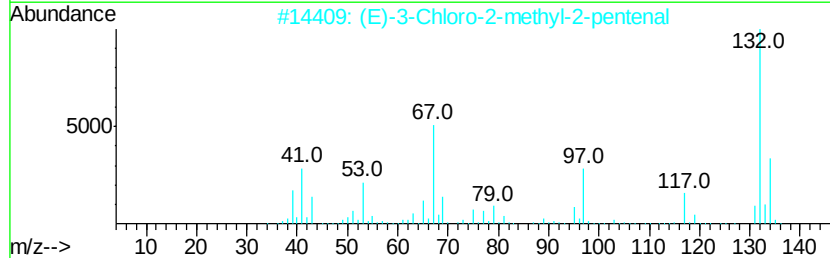
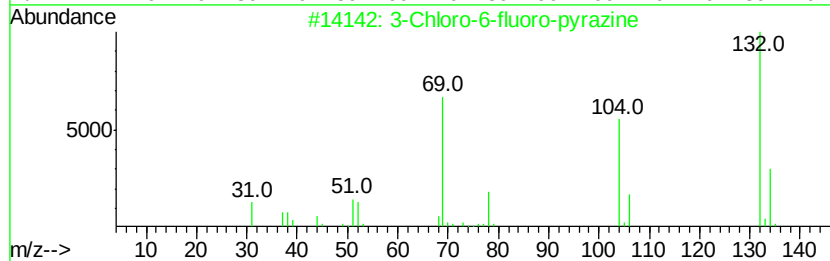
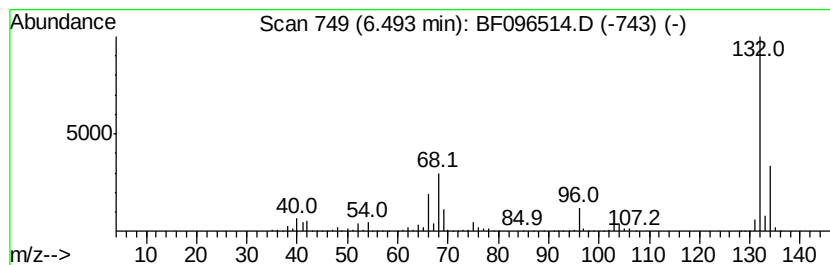
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	90.23 ng	3078660	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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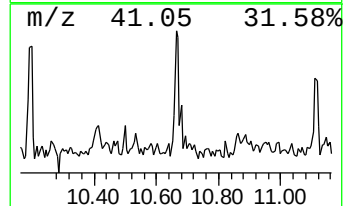
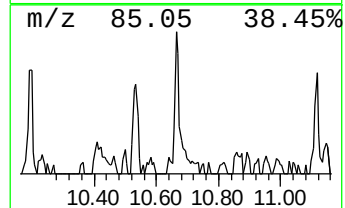
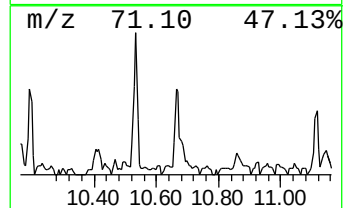
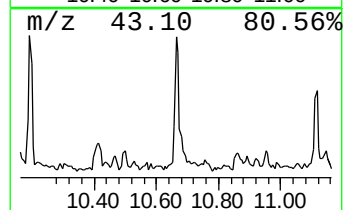
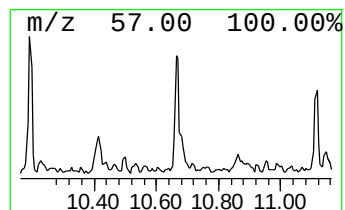
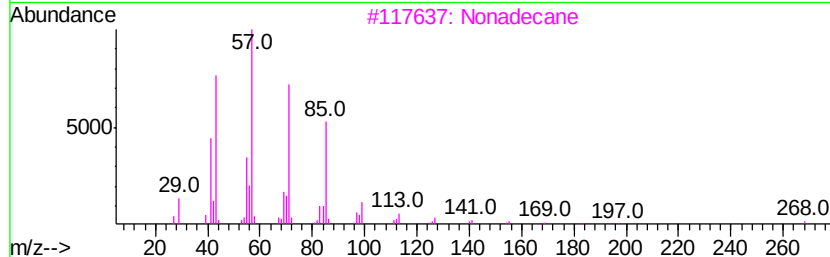
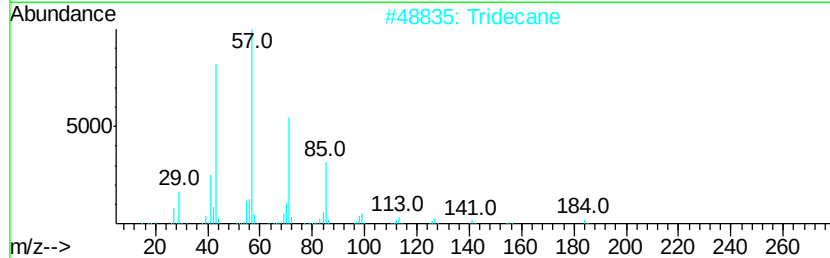
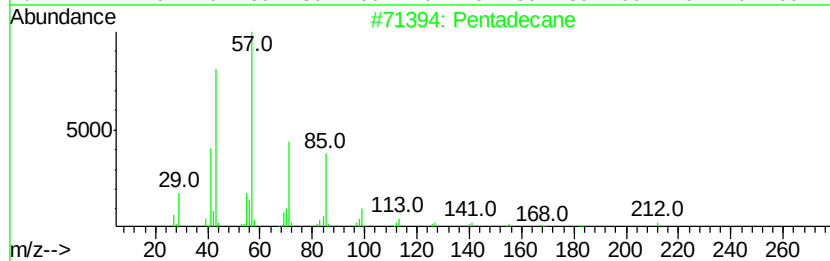
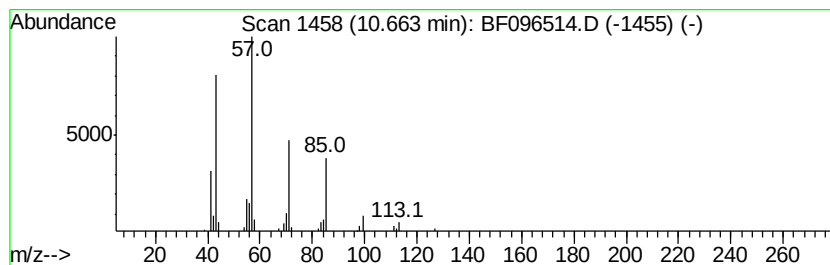
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Peak Number 4 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.66	2.00 ng	55564	Phenanthrene-d10		11.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	90
2	Tridecane	184	C13H28	000629-50-5	90
3	Nonadecane	268	C19H40	000629-92-5	86
4	Heptadecane	240	C17H36	000629-78-7	83
5	Tetradecane	198	C14H30	000629-59-4	83



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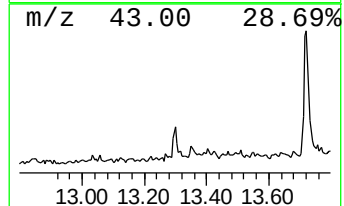
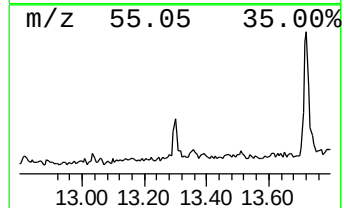
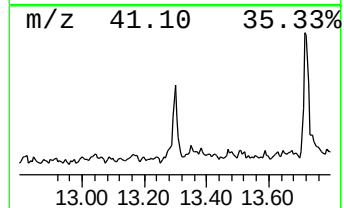
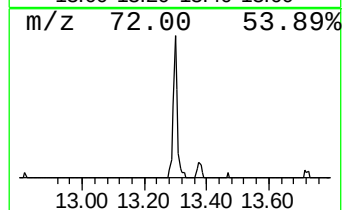
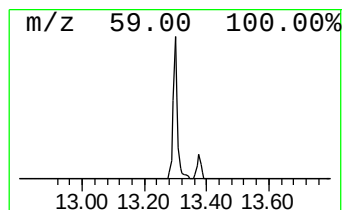
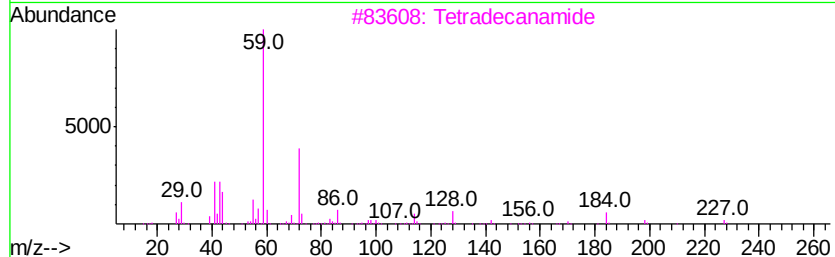
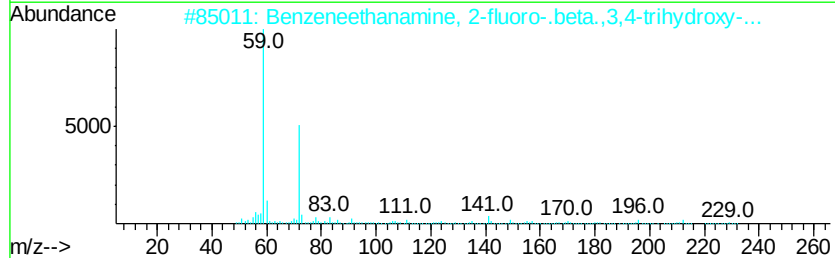
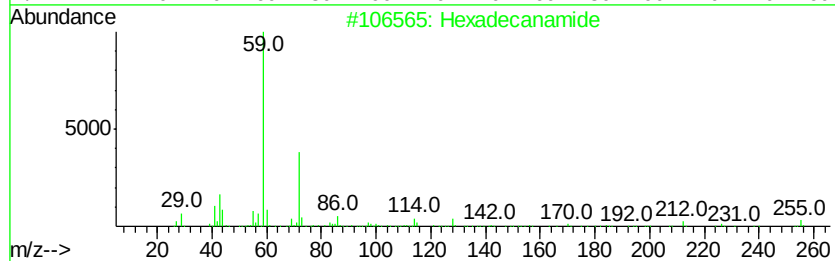
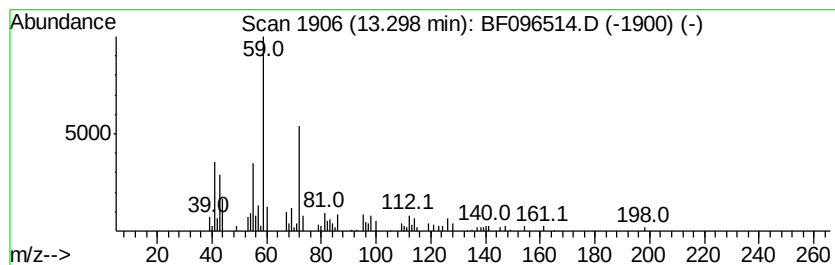
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanamide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.30	3.13 ng	99176	Chrysene-d12		13.86	
Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanamide	255	C16H33NO	000629-54-9	72
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
3		Tetradecanamide	227	C14H29NO	000638-58-4	64
4		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	62
5		Nonanamide	157	C9H19NO	001120-07-6	53



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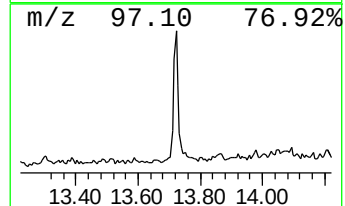
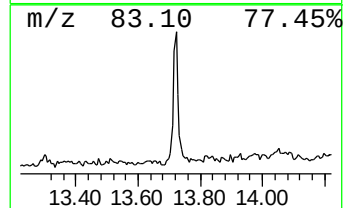
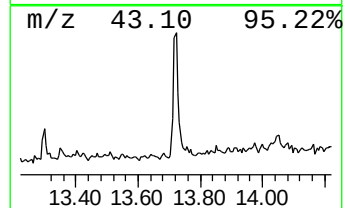
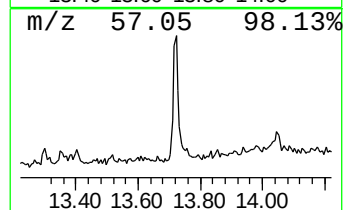
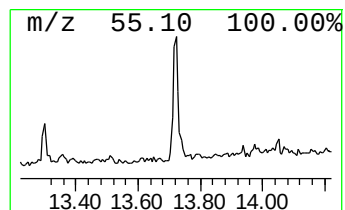
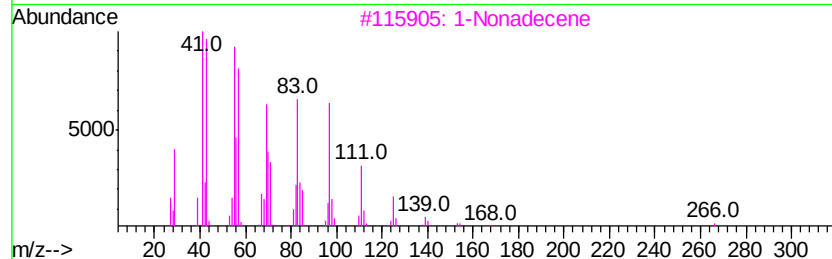
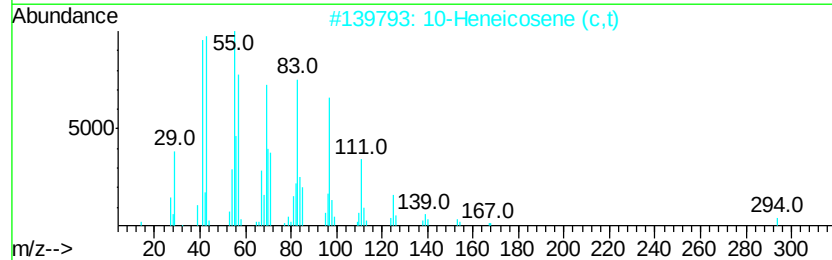
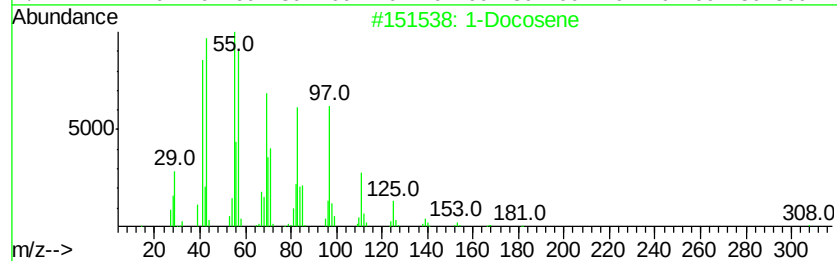
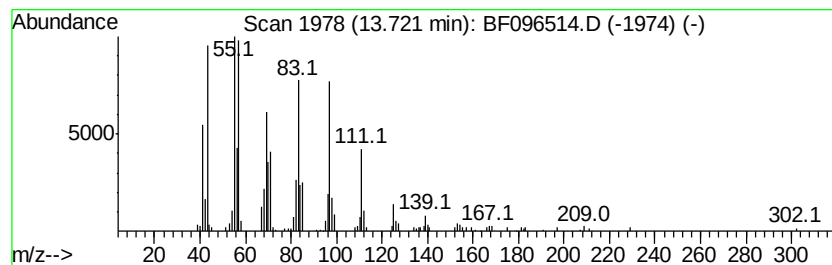
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.72	7.07 ng	224303	Chrysene-d12	13.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	10-Heneicosene (c,t)	294	C21H42	095008-11-0	94
3	1-Nonadecene	266	C19H38	018435-45-5	90
4	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	87
5	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.91	14.6	ng	497471	1	6.72	682436	20.0
unknown6.49	6.49	90.2	ng	3078660	1	6.72	682436	20.0
Pentadecane	10.66	2.0	ng	55564	4	11.23	555581	20.0
Hexadecanamide	13.30	3.1	ng	99176	5	13.86	634566	20.0
1-Docosene	13.72	7.1	ng	224303	5	13.86	634566	20.0