

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071917\
 Data File : BF096876.D
 Acq On : 19 Jul 2017 18:07
 Operator : SJ/JU
 Sample : I4254-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-12019/72-11985/72-12016-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-BF071317.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	2.869	147	150	161	rBV	22599	58336	1.73%	0.199%
2	4.775	470	474	487	rVB	219375	365305	10.81%	1.243%
3	5.204	541	547	550	rBV	2912532	3234129	95.66%	11.009%
4	6.245	718	724	732	rBV	2834046	3380745	100.00%	11.508%
5	6.363	738	744	747	rBV	3008257	3158808	93.44%	10.753%
6	6.586	778	782	785	rBV	779725	635361	18.79%	2.163%
7	6.745	804	809	812	rBV	2484838	2313087	68.42%	7.874%
8	7.151	872	878	881	rBV	1816700	2078504	61.48%	7.075%
9	7.869	995	1000	1003	rBV	1015696	900843	26.65%	3.066%
10	8.951	1177	1184	1187	rBV	2910832	3285117	97.17%	11.183%
11	9.280	1235	1240	1242	rBV	45226	43060	1.27%	0.147%
12	9.339	1246	1250	1254	rVB	413011	392198	11.60%	1.335%
13	9.616	1292	1297	1301	rBV	1100666	982424	29.06%	3.344%
14	9.716	1310	1314	1321	rBV4	31944	38471	1.14%	0.131%
15	10.069	1371	1374	1377	rVB	48678	39953	1.18%	0.136%
16	10.404	1423	1431	1435	rBV	1811935	2056182	60.82%	6.999%
17	10.539	1450	1454	1461	rBV	58407	64072	1.90%	0.218%
18	10.986	1526	1530	1533	rBV	63153	56232	1.66%	0.191%
19	11.092	1543	1548	1551	rBV	1211801	1062649	31.43%	3.617%
20	11.116	1551	1552	1555	rVV	122959	65537	1.94%	0.223%
21	11.169	1555	1561	1565	rVB3	36735	38780	1.15%	0.132%
22	11.592	1627	1633	1636	rBV2	46308	50837	1.50%	0.173%
23	11.621	1636	1638	1640	rVV	47949	44084	1.30%	0.150%
24	11.669	1643	1646	1648	rVV	52508	51213	1.51%	0.174%
25	11.698	1648	1651	1654	rVV	57268	67347	1.99%	0.229%
26	12.145	1720	1727	1729	rBV	38459	52159	1.54%	0.178%
27	12.298	1749	1753	1759	rBV	66386	64247	1.90%	0.219%
28	12.521	1787	1791	1794	rBV2	82911	91901	2.72%	0.313%
29	12.592	1798	1803	1810	rVB4	31642	39313	1.16%	0.134%
30	12.680	1810	1818	1822	rBV	2407956	2800824	82.85%	9.534%
31	13.239	1906	1913	1917	rBV2	27832	45673	1.35%	0.155%
32	13.586	1968	1972	1978	rBV2	152473	176938	5.23%	0.602%
33	13.721	1989	1995	1998	rBV	936043	990232	29.29%	3.371%
34	14.715	2161	2164	2172	rVB2	18473	34416	1.02%	0.117%

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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

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35	15.092	2223	2228	2233	rBV	471430	542583	16.05%	1.847%
36	15.557	2304	2307	2314	rVB6	21424	37378	1.11%	0.127%
37	15.956	2369	2375	2382	rVB9	17455	38308	1.13%	0.130%

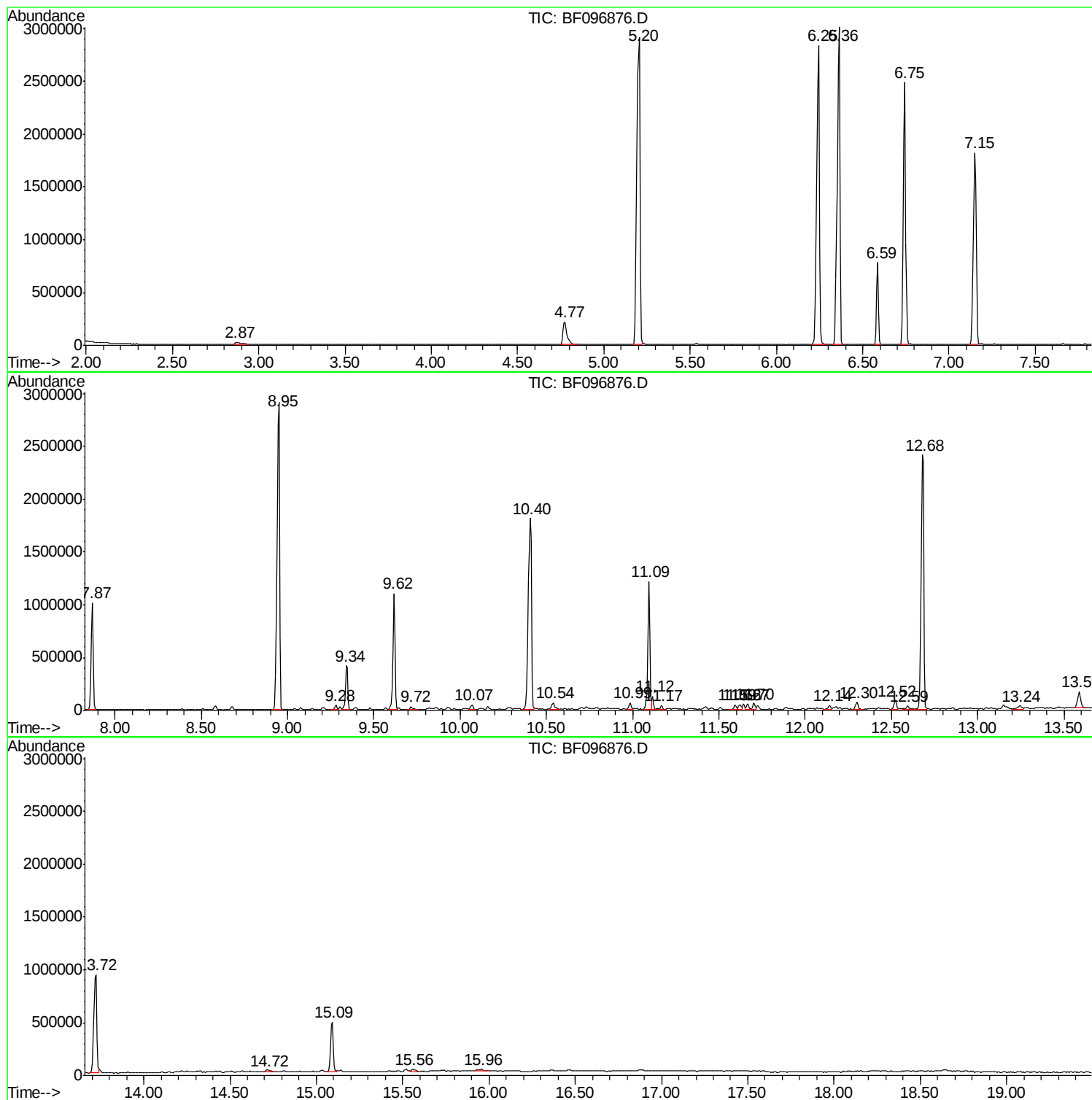
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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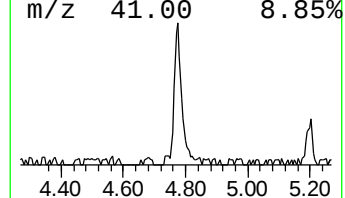
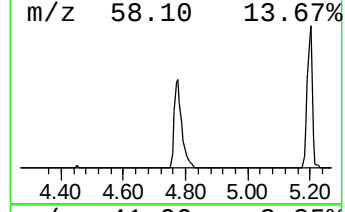
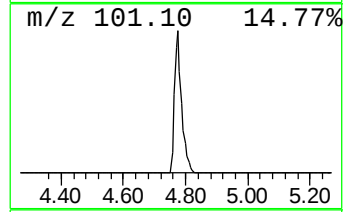
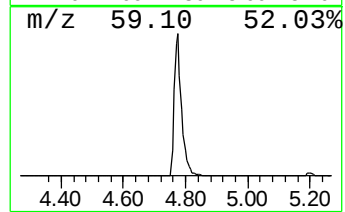
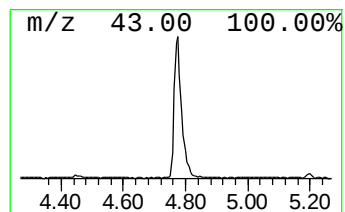
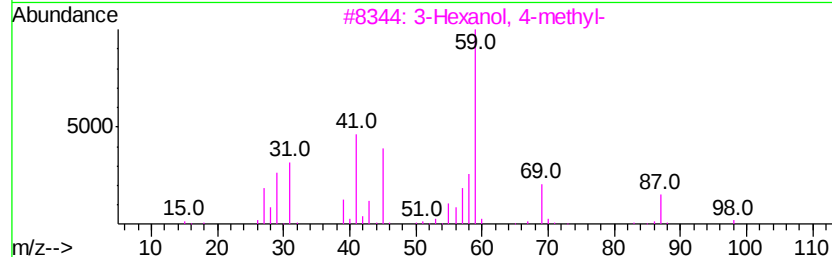
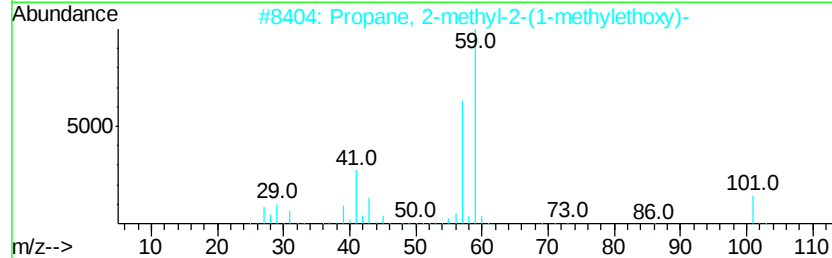
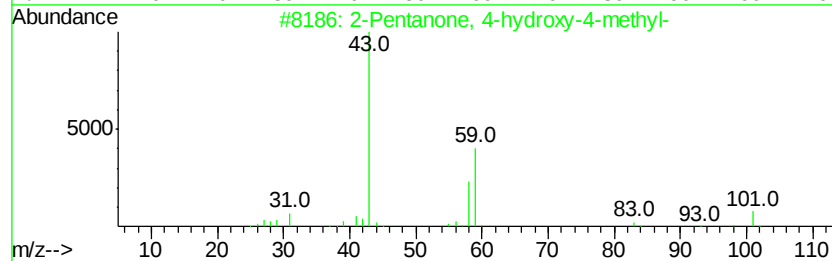
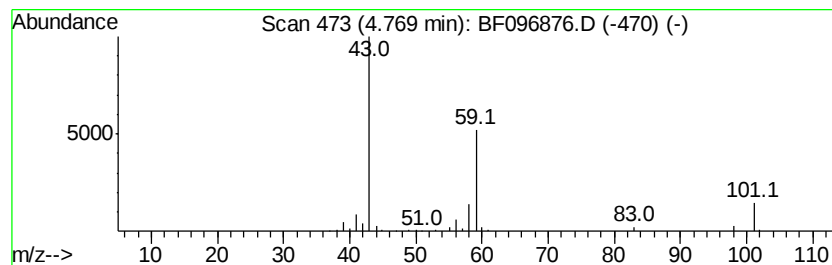
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	11.50 ng	365305	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	32
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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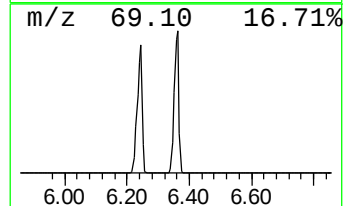
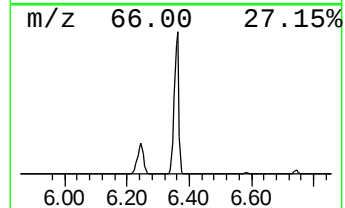
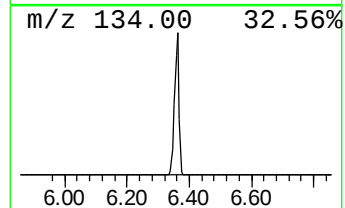
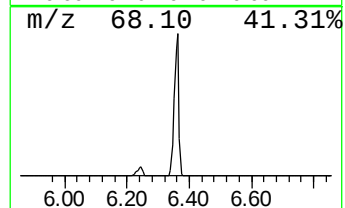
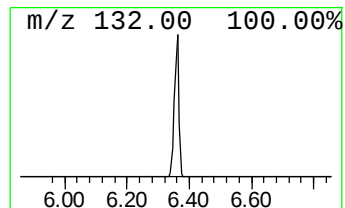
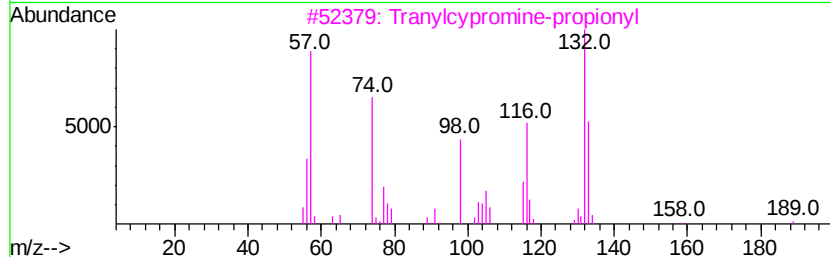
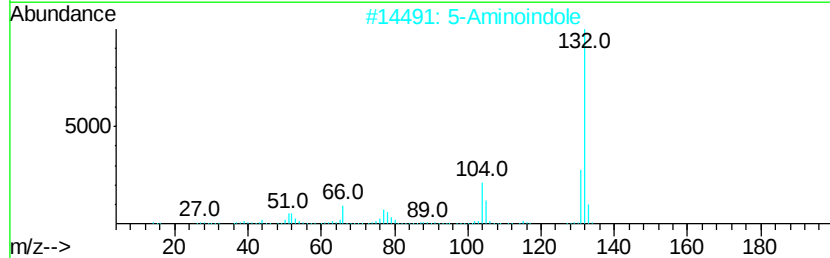
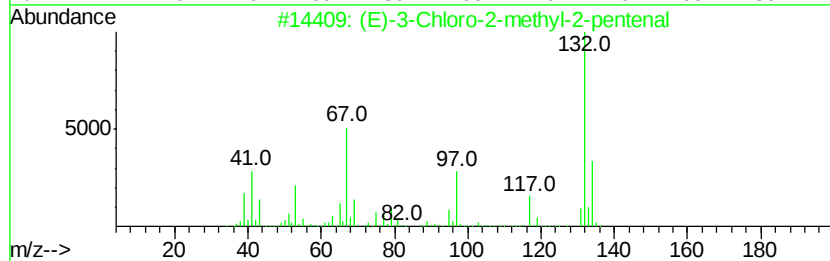
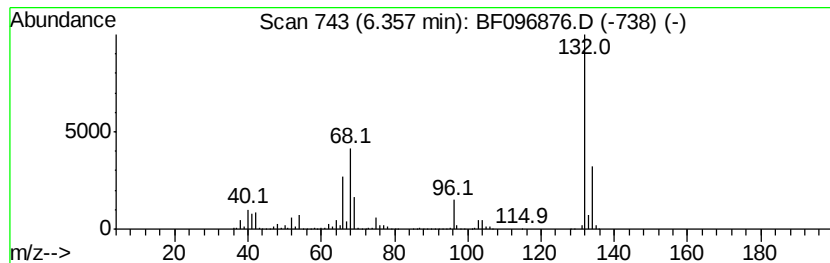
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Peak Number 2 unknown6.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	99.43 ng	3158810	1,4-Dichlorobenzene-d4	6.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		Imidazole, 4,5-dicvano-1-methyl-	132	C6H4N4	019485-35-9	9
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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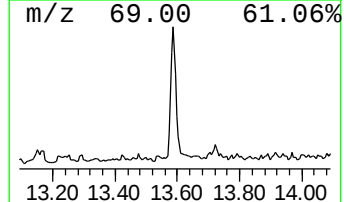
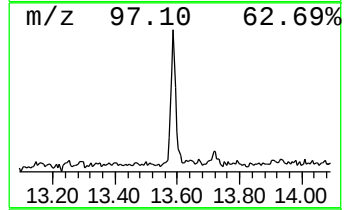
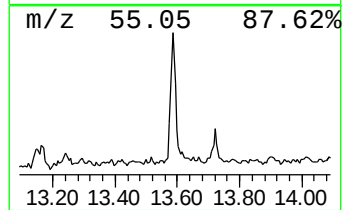
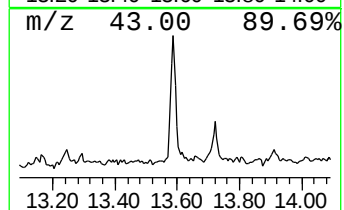
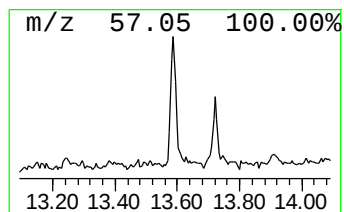
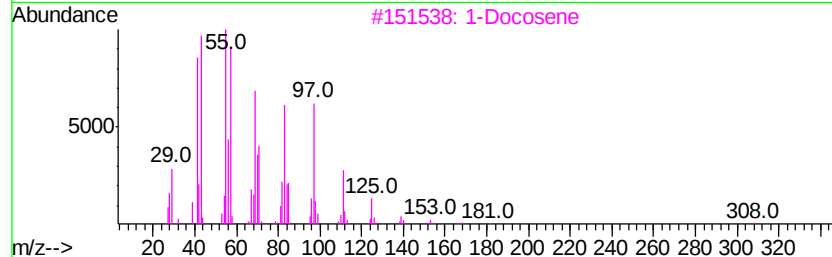
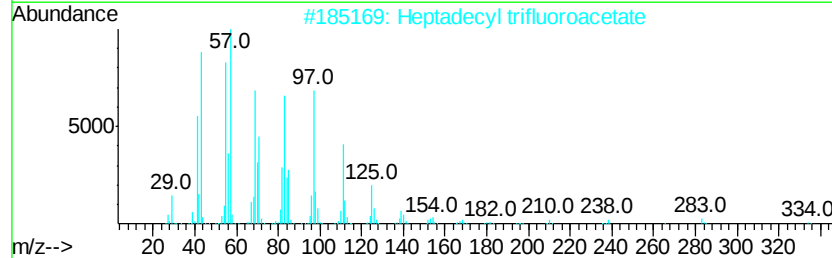
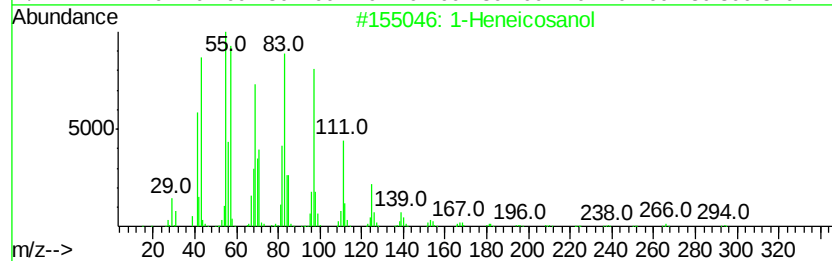
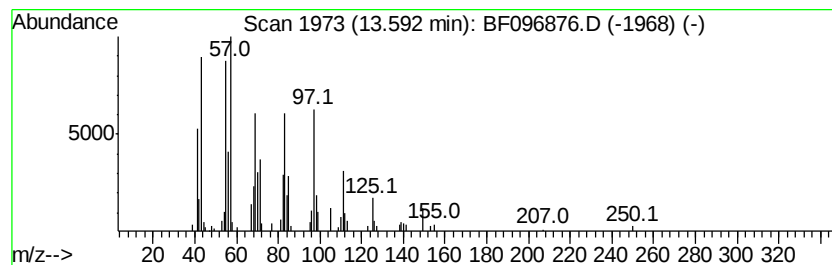
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.59	3.57 ng	176938	Chrysene-d12		13.72		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3			1-Docosene	308	C22H44	001599-67-3	91
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.77	11.5	ng	365305	1	6.59	635361	20.0
unknown6.36	6.36	99.4	ng	3158810	1	6.59	635361	20.0
1-Heneicosanol	13.59	3.6	ng	176938	5	13.72	990232	20.0