

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072017\
 Data File : BF096921.D
 Acq On : 20 Jul 2017 22:29
 Operator : SJ/JU
 Sample : I4317-01
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1-TP-1-2-3-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	4.734	463	467	480	rVB	194909	284626	12.56%	1.556%
2	5.175	538	542	558	rBV	2201399	2265786	100.00%	12.388%
3	6.222	715	720	736	rBV	1858256	2075379	91.60%	11.347%
4	6.339	736	740	743	rBV	2144312	1997275	88.15%	10.920%
5	6.569	775	779	783	rBV	630917	506849	22.37%	2.771%
6	6.728	801	806	809	rBV	1547641	1489766	65.75%	8.145%
7	7.133	870	875	878	rBV	1327379	1235027	54.51%	6.752%
8	7.851	993	997	1000	rBV	823092	676273	29.85%	3.697%
9	8.927	1175	1180	1183	rBV	2165850	2041222	90.09%	11.160%
10	9.322	1244	1247	1253	rBV	214552	187515	8.28%	1.025%
11	9.598	1290	1294	1298	rBV2	793864	664752	29.34%	3.634%
12	10.051	1367	1371	1374	rVB	44896	36638	1.62%	0.200%
13	10.380	1423	1427	1435	rVB	991732	1001018	44.18%	5.473%
14	10.521	1448	1451	1460	rBV	50665	61941	2.73%	0.339%
15	11.074	1541	1545	1547	rBV	625213	524956	23.17%	2.870%
16	11.098	1547	1549	1553	rVB	41450	34088	1.50%	0.186%
17	12.280	1746	1750	1756	rVB	129716	113593	5.01%	0.621%
18	12.504	1783	1788	1792	rBV	124015	113477	5.01%	0.620%
19	12.657	1810	1814	1818	rVB	1334259	1324759	58.47%	7.243%
20	13.568	1963	1969	1975	rBV3	91285	111773	4.93%	0.611%
21	13.698	1987	1991	1994	rBV	560749	558845	24.66%	3.055%
22	13.721	1994	1995	2002	rVB	55521	48727	2.15%	0.266%
23	14.556	2133	2137	2140	rVB2	26733	29184	1.29%	0.160%
24	14.692	2157	2160	2163	rBV	74375	98864	4.36%	0.541%
25	14.792	2173	2177	2185	rVB2	27780	46433	2.05%	0.254%
26	14.956	2201	2205	2209	rVB	40603	45145	1.99%	0.247%
27	15.009	2211	2214	2219	rBV	38833	43749	1.93%	0.239%
28	15.068	2219	2224	2228	rBV	463288	511476	22.57%	2.796%
29	15.492	2293	2296	2300	rBV4	23894	28698	1.27%	0.157%
30	15.539	2300	2304	2310	rVB8	20602	36884	1.63%	0.202%
31	16.333	2434	2439	2442	rBV2	17716	30645	1.35%	0.168%
32	16.427	2449	2455	2461	rBV4	19667	38921	1.72%	0.213%
33	17.021	2552	2556	2564	rVB9	13209	25832	1.14%	0.141%

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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-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

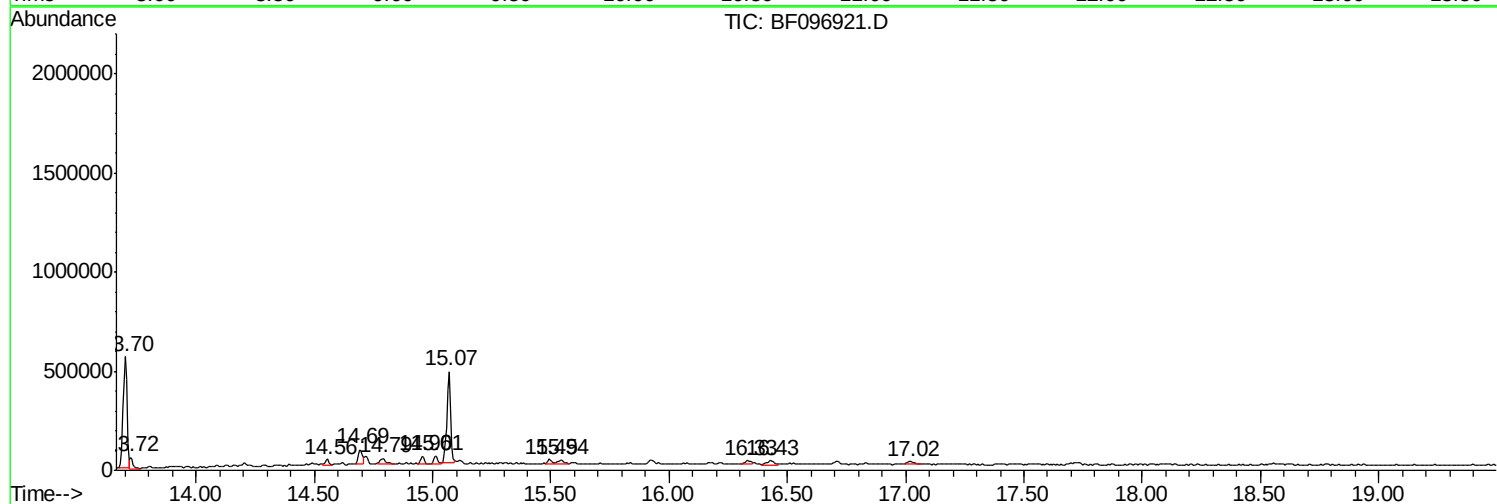
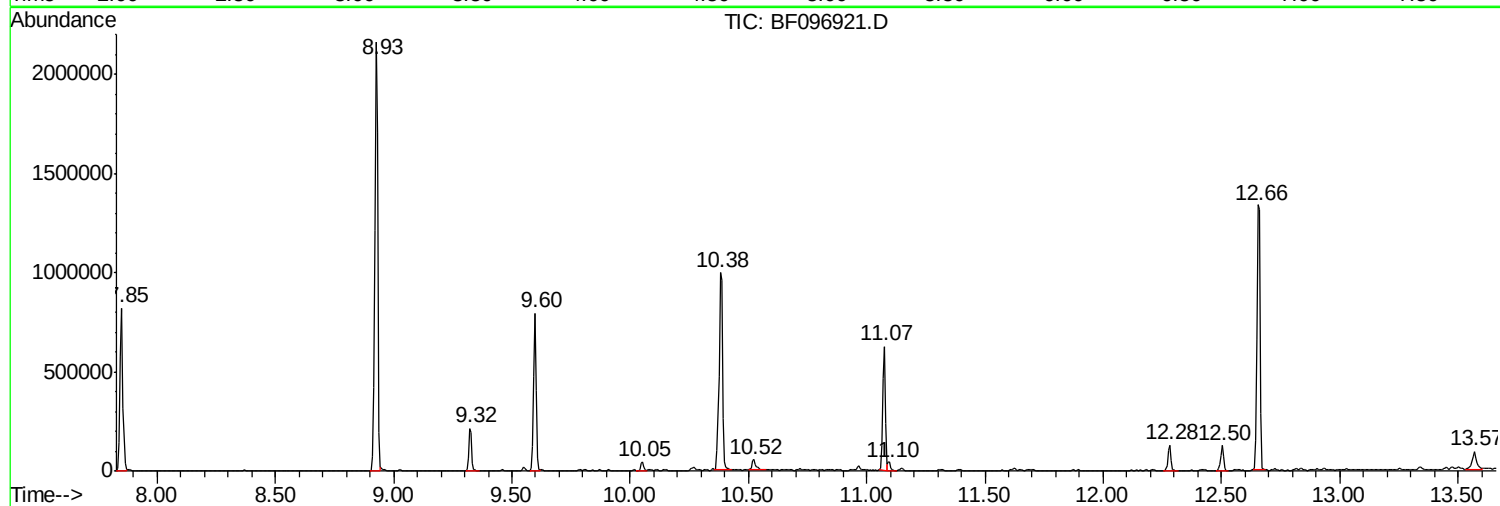
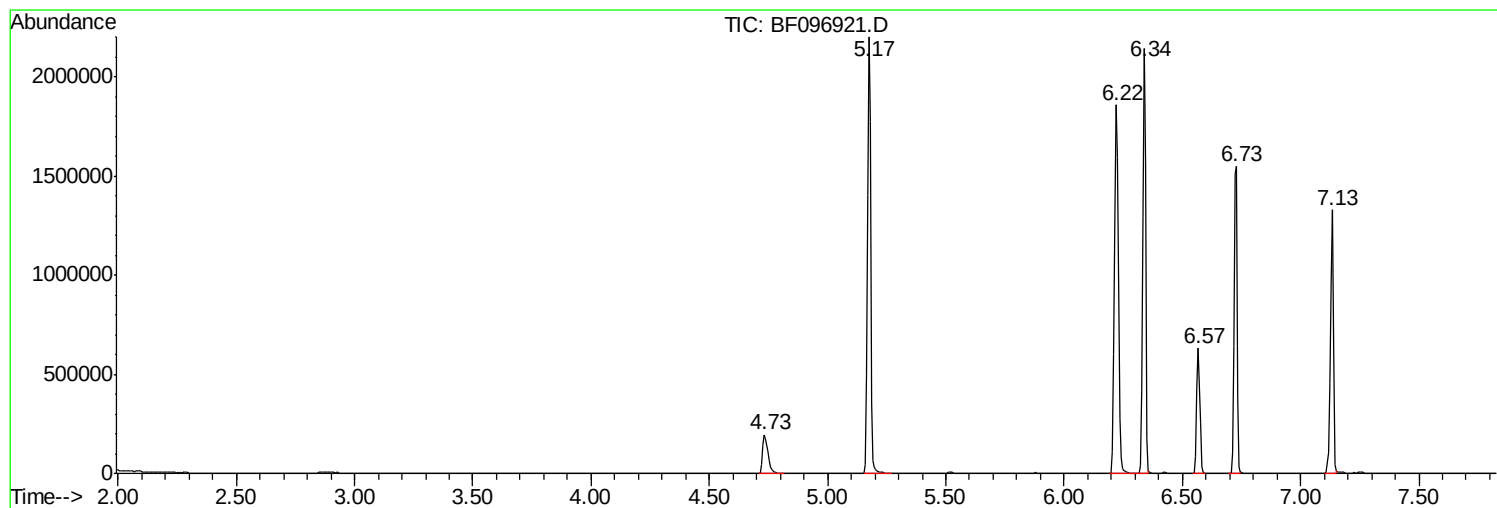
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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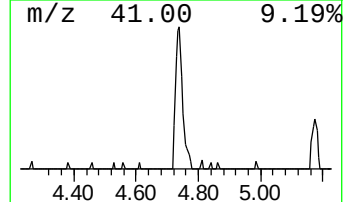
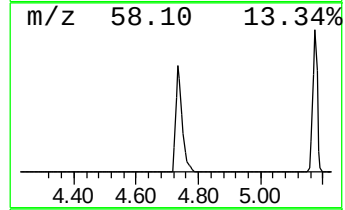
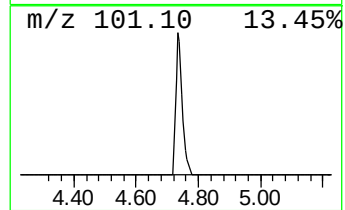
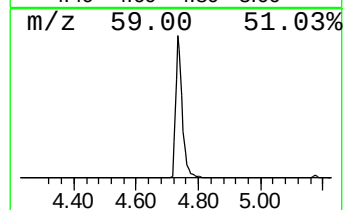
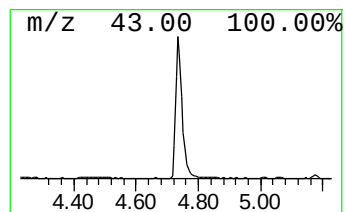
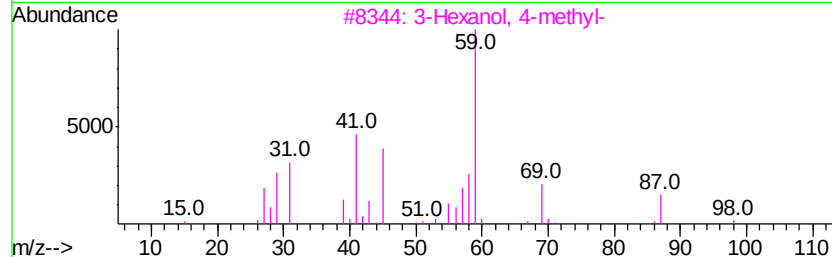
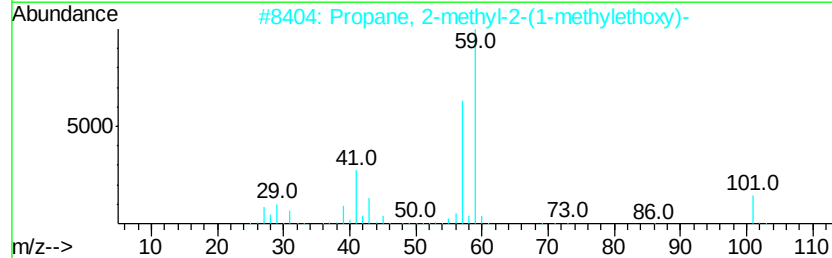
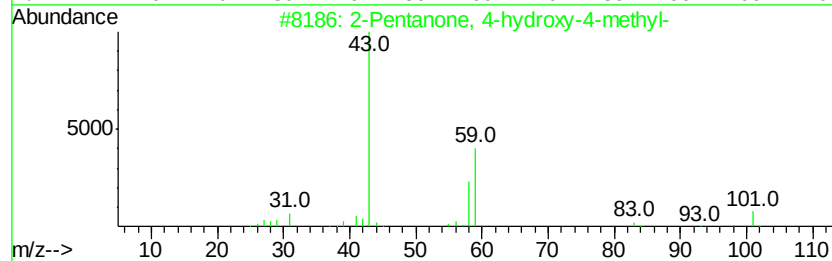
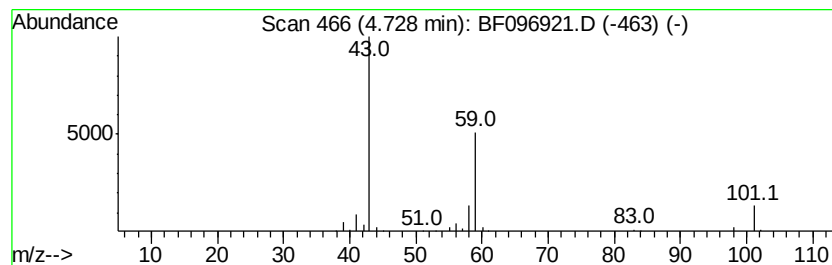
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	11.23 ng	284626	1,4-Dichlorobenzene-d4	6.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
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	23



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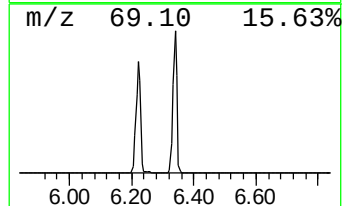
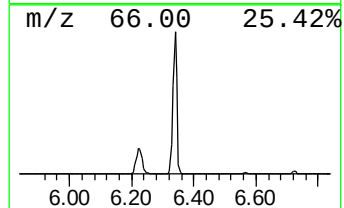
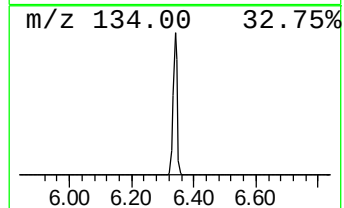
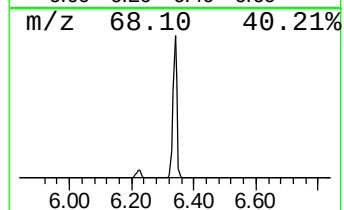
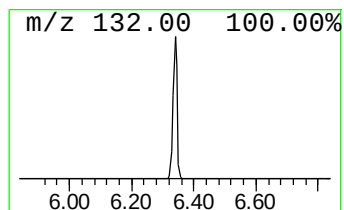
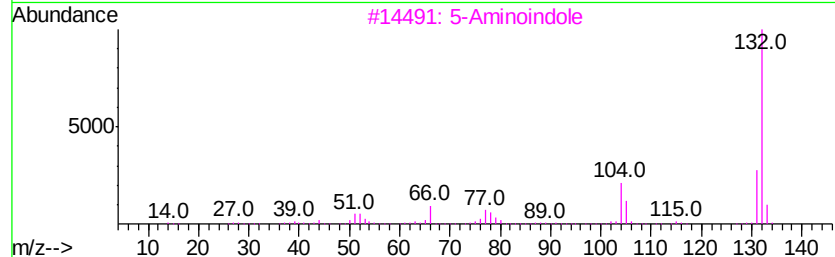
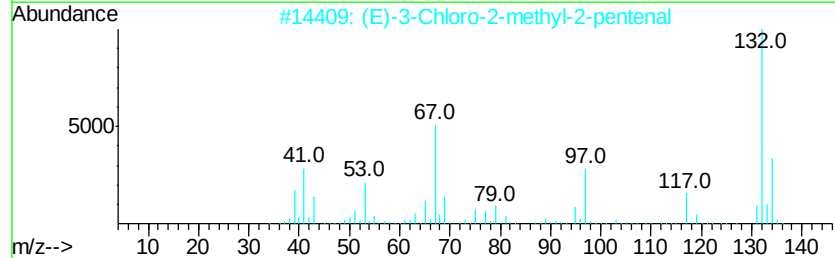
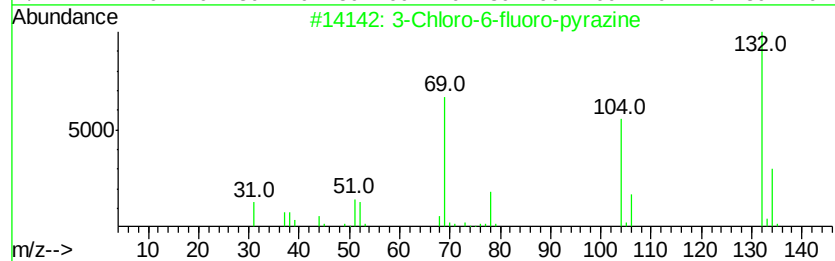
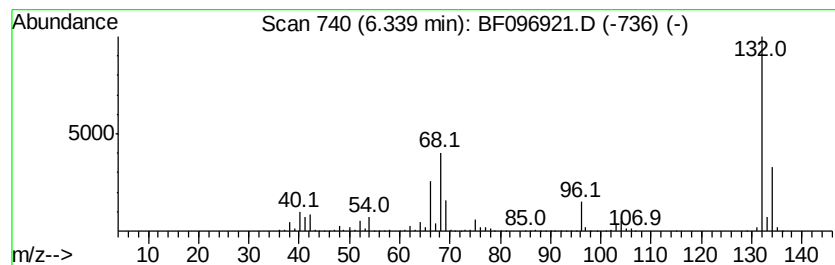
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Peak Number 2 unknown6.34 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	78.81 ng	1997280	1,4-Dichlorobenzene-d4	6.57

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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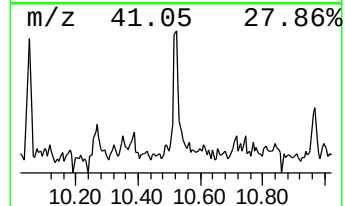
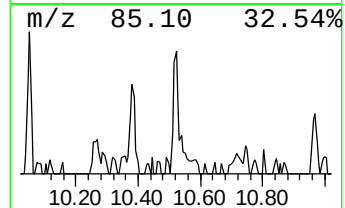
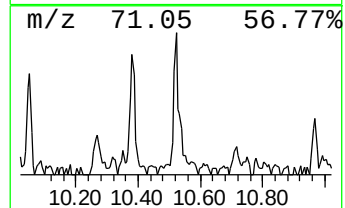
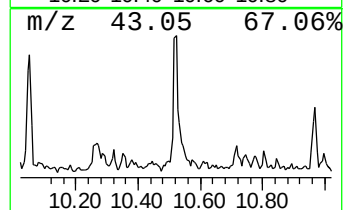
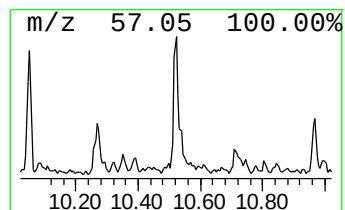
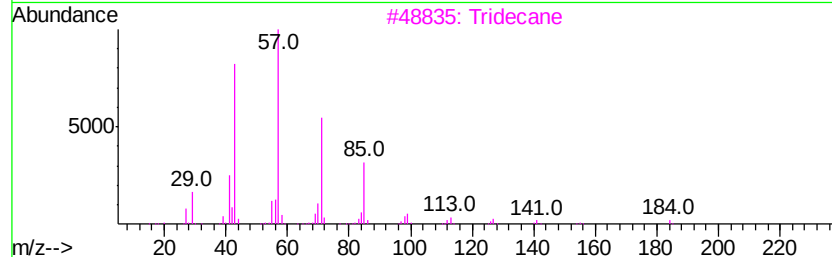
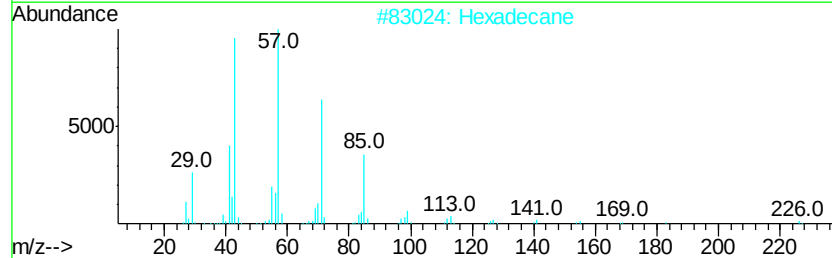
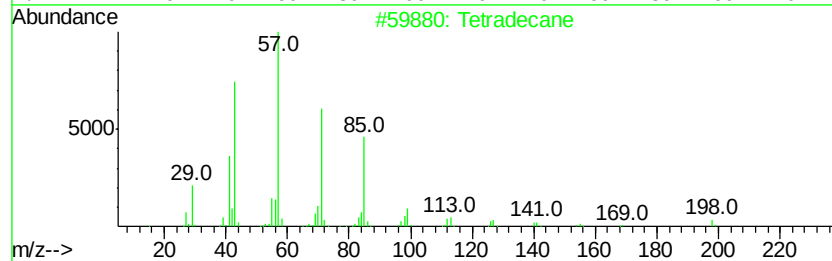
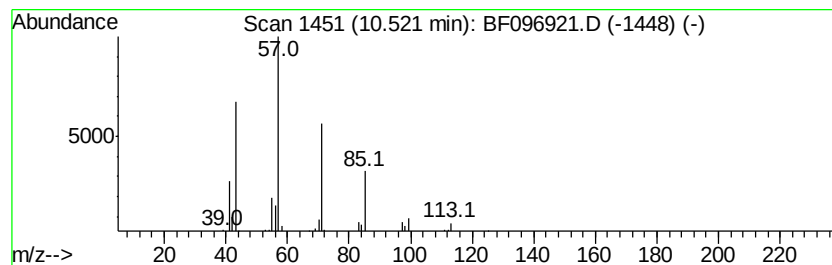
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Tetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.52	2.36 ng	61941	Phenanthrene-d10		11.07
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	86
2	Hexadecane	226	C16H34	000544-76-3	86
3	Tridecane	184	C13H28	000629-50-5	78
4	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	64
5	Octane, 2,3,7-trimethyl-	156	C11H24	062016-34-6	53



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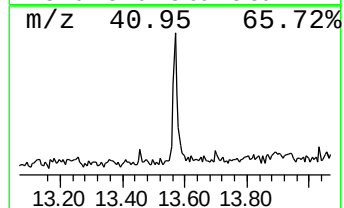
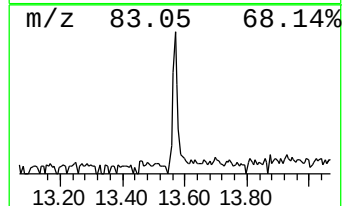
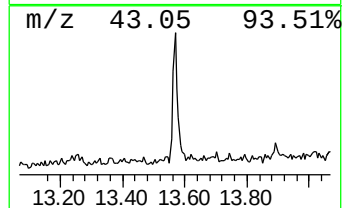
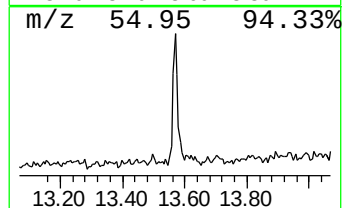
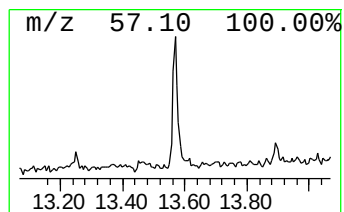
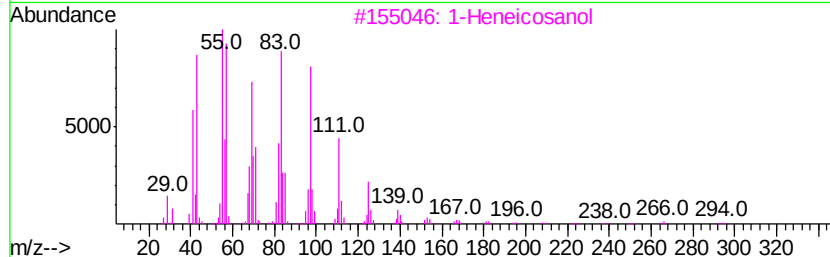
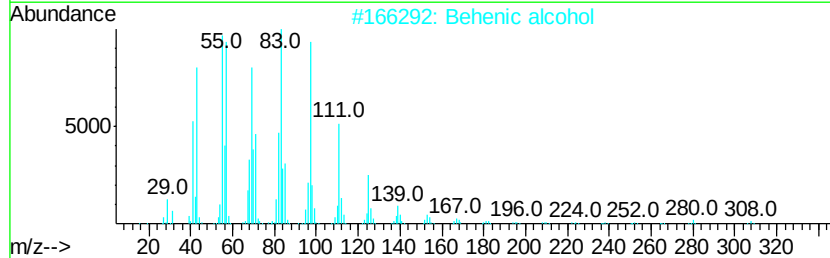
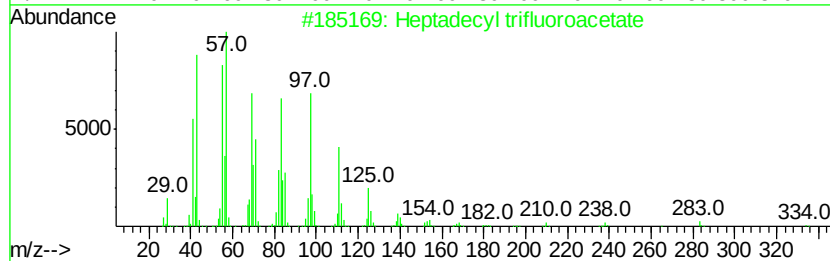
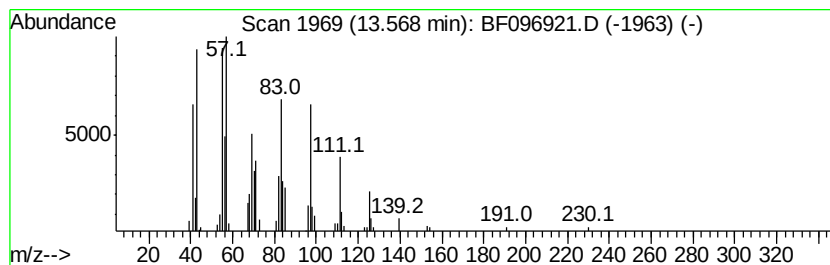
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	4.00 ng	111773	Chrysene-d12	13.70

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	93
5		1-Docosene	308	C22H44	001599-67-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.73	11.2	ng	284626	1	6.57	506849	20.0
unknown6.34	6.34	78.8	ng	1997280	1	6.57	506849	20.0
Tetradecane	10.52	2.4	ng	61941	4	11.07	524956	20.0
Heptadecyl triflu...	13.57	4.0	ng	111773	5	13.70	558845	20.0