

Data Path : Z:\HPCHEM1\BNA F\DATA\BF092717\
 Data File : BF098859.D
 Acq On : 27 Sep 2017 13:21
 Operator : SJ/JU
 Sample : I5396-04
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PAMT-COMP-A-DUP

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-BF092317.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	2.222	20	23	44	rVB2	140353	346019	10.08%	1.093%
2	4.028	325	330	336	rVB	46069	54879	1.60%	0.173%
3	5.146	516	520	531	rVB	527523	670568	19.54%	2.119%
4	5.540	581	587	590	rBV	3187125	3299532	96.13%	10.425%
5	6.540	751	757	760	rBV	3152635	3432482	100.00%	10.845%
6	6.687	777	782	785	rBV	3374766	3395720	98.93%	10.729%
7	6.916	817	821	824	rBV	910775	813459	23.70%	2.570%
8	7.069	843	847	850	rBV	2725249	2398441	69.87%	7.578%
9	7.475	911	916	919	rBV	2216420	2040241	59.44%	6.446%
10	8.192	1034	1038	1042	rBV	1254024	1114336	32.46%	3.521%
11	9.269	1216	1221	1224	rBV	3757647	3426658	99.83%	10.827%
12	9.657	1283	1287	1290	rBV	685468	565798	16.48%	1.788%
13	9.951	1333	1337	1341	rVB	1499470	1243798	36.24%	3.930%
14	10.375	1406	1409	1412	rVB	72500	59691	1.74%	0.189%
15	10.739	1466	1471	1474	rBV	2249114	2139103	62.32%	6.759%
16	10.845	1486	1489	1494	rBV	94202	87706	2.56%	0.277%
17	11.292	1562	1565	1568	rBV	53294	41047	1.20%	0.130%
18	11.439	1586	1590	1593	rBV	1403190	1209681	35.24%	3.822%
19	11.951	1674	1677	1682	rBV	46165	45235	1.32%	0.143%
20	13.021	1854	1859	1862	rBV	3147894	2875280	83.77%	9.085%
21	13.904	2006	2009	2017	rBV	289027	277263	8.08%	0.876%
22	14.074	2034	2038	2042	rBV	940565	802382	23.38%	2.535%
23	14.539	2113	2117	2123	rBV3	52001	70857	2.06%	0.224%
24	15.192	2224	2228	2230	rBV	42369	46798	1.36%	0.148%
25	15.568	2286	2292	2302	rVB	596987	783203	22.82%	2.475%
26	16.027	2365	2370	2375	rBV	52836	76109	2.22%	0.240%
27	16.080	2375	2379	2385	rVV8	23983	41676	1.21%	0.132%
28	16.545	2453	2458	2465	rVB2	38629	64469	1.88%	0.204%
29	17.162	2557	2563	2570	rVB	37025	80701	2.35%	0.255%
30	17.886	2679	2686	2693	rVB3	31061	76559	2.23%	0.242%
31	18.739	2825	2831	2839	rVB3	26871	69265	2.02%	0.219%

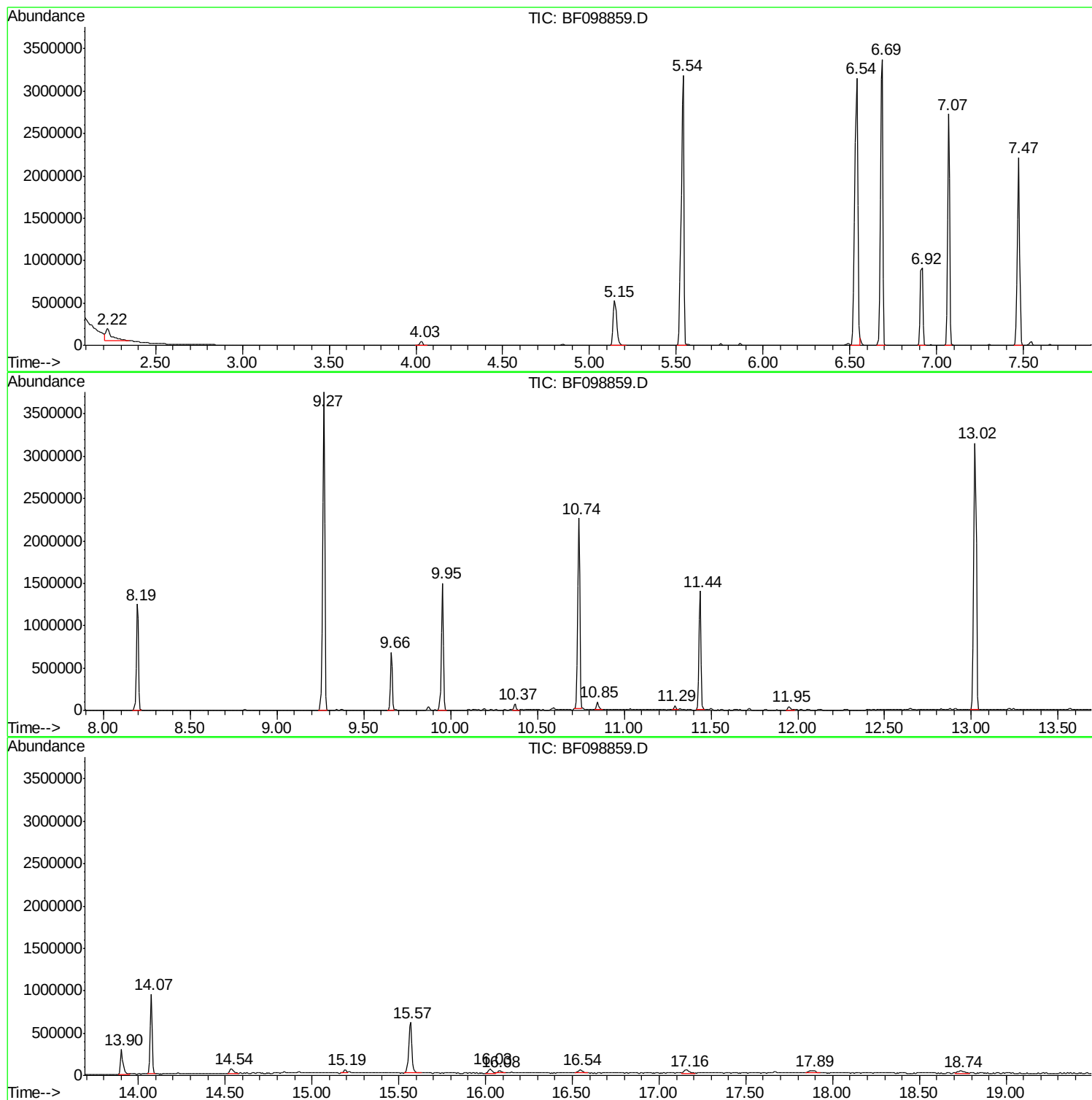
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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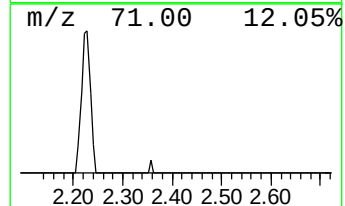
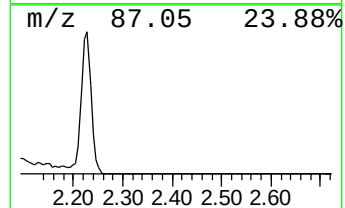
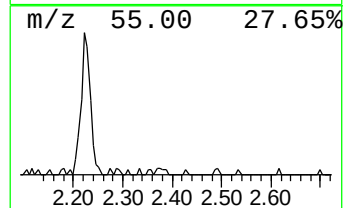
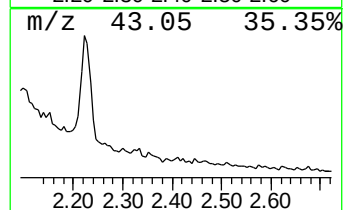
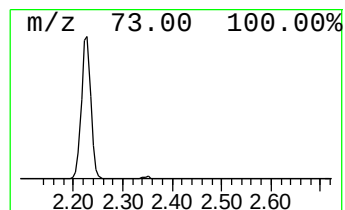
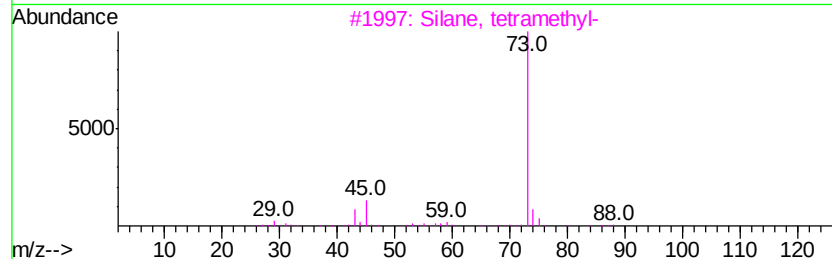
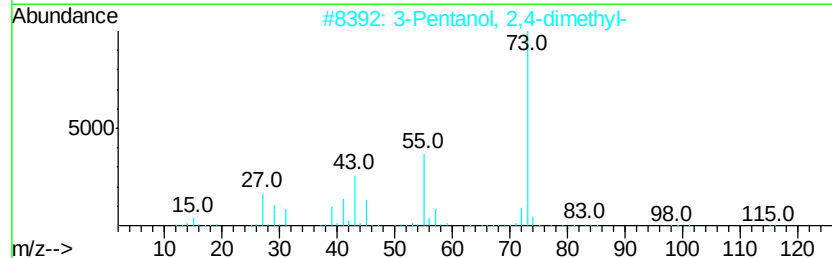
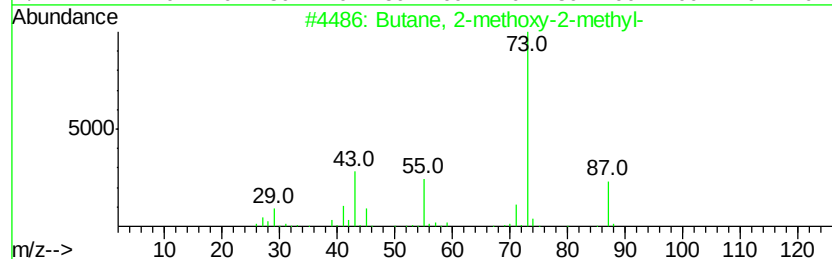
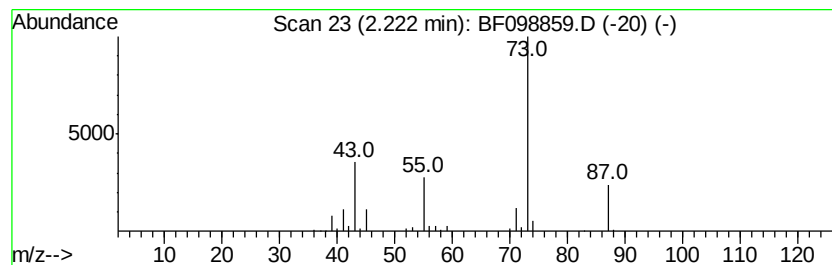
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	8.51 ng	346019	1,4-Dichlorobenzene-d4	6.92

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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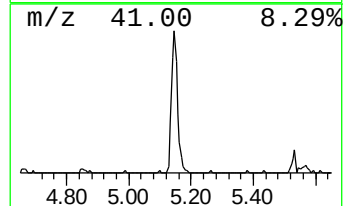
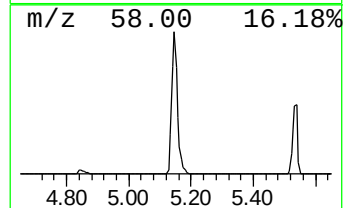
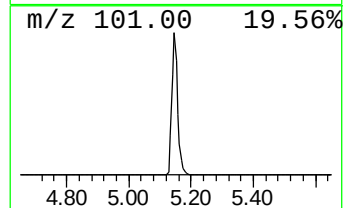
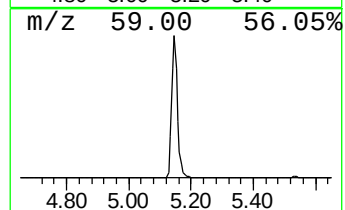
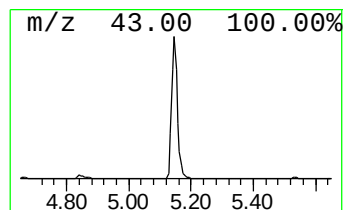
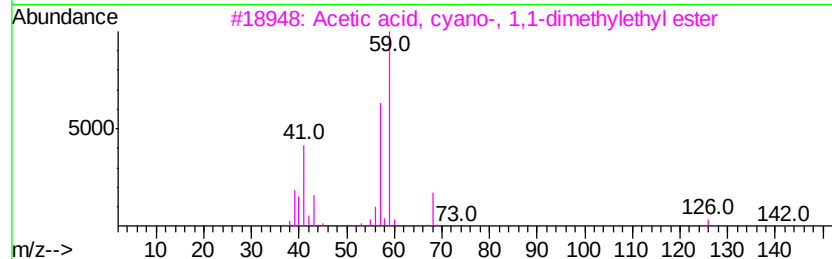
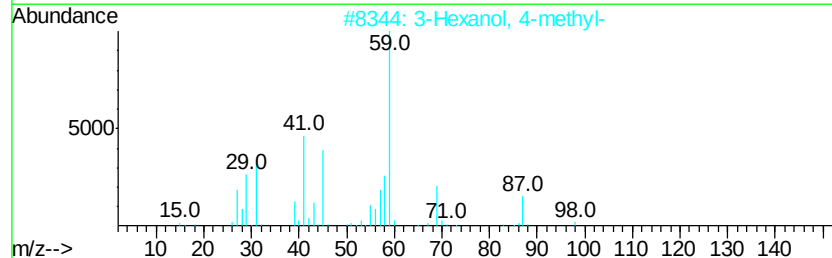
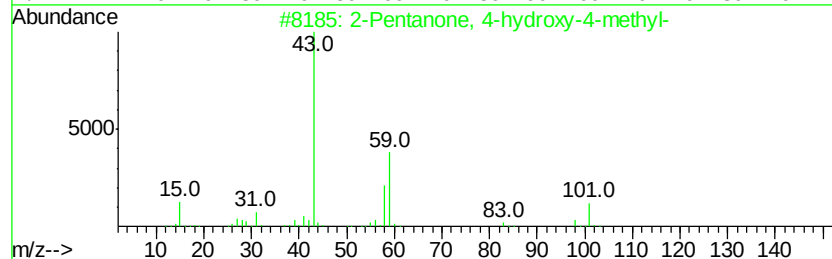
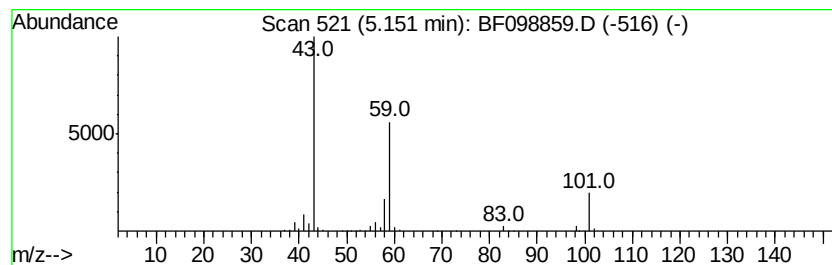
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.15	16.49 ng	670568	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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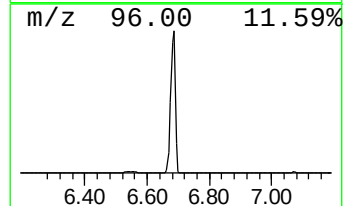
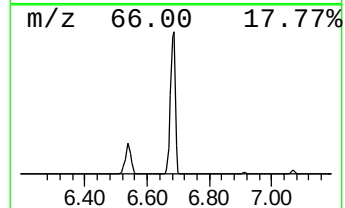
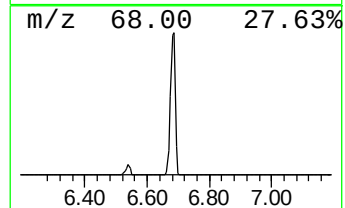
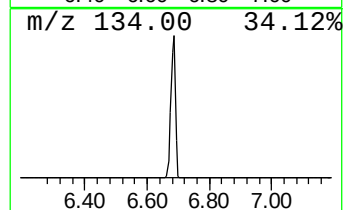
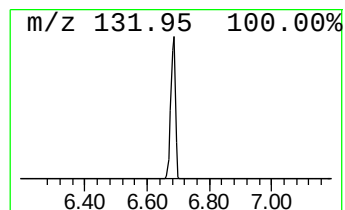
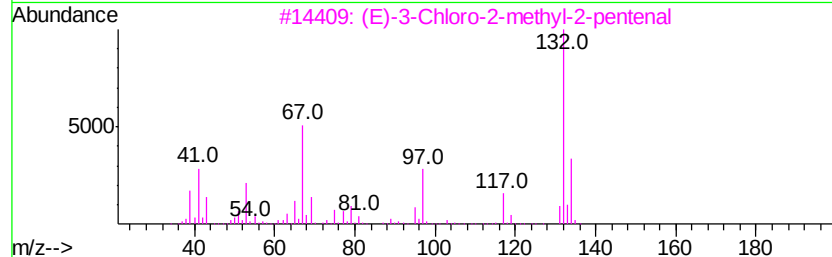
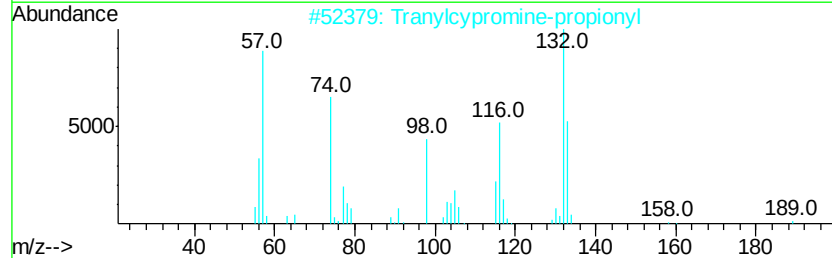
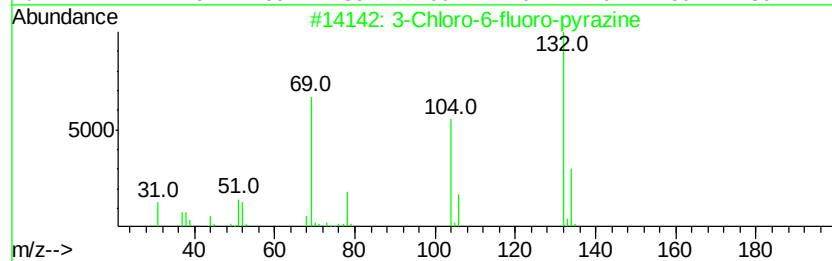
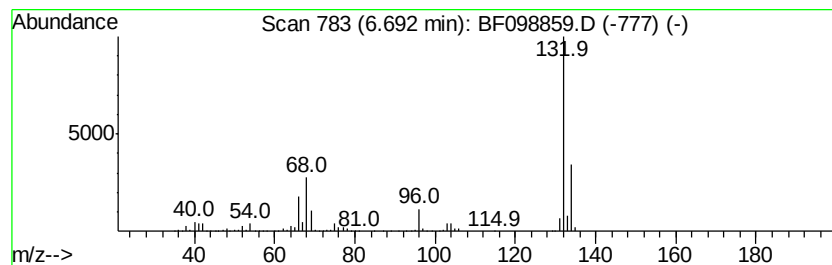
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Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	83.49 ng	3395720	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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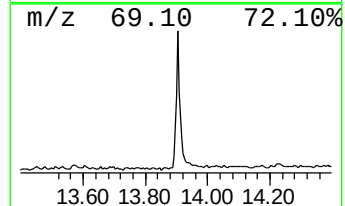
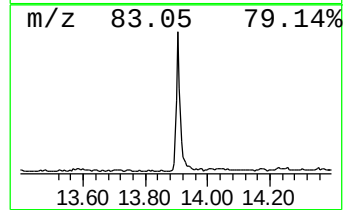
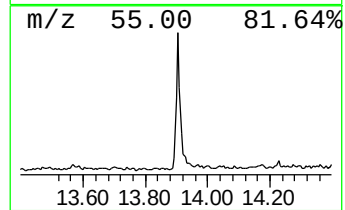
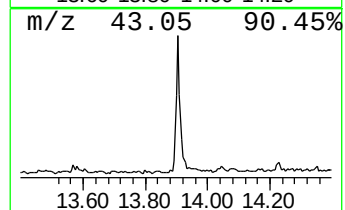
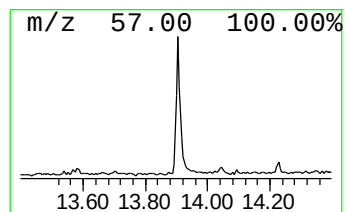
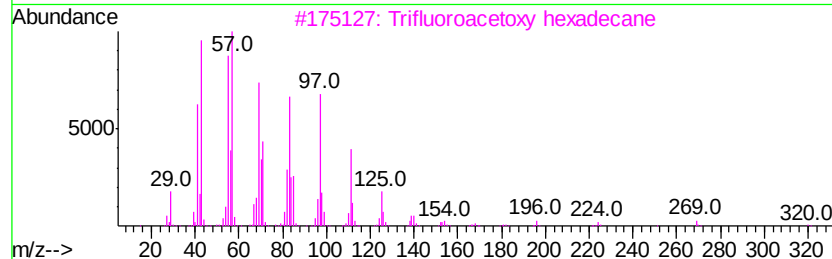
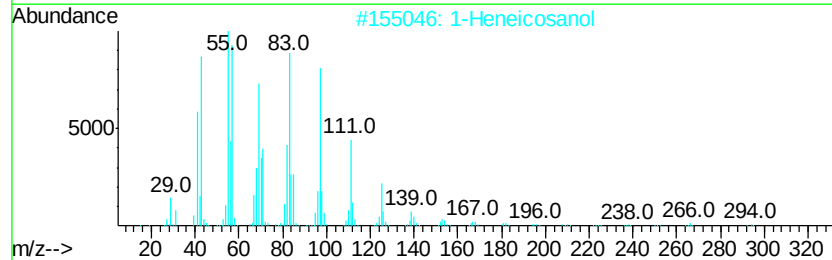
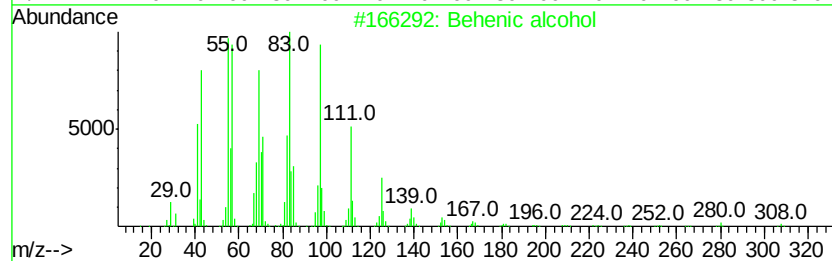
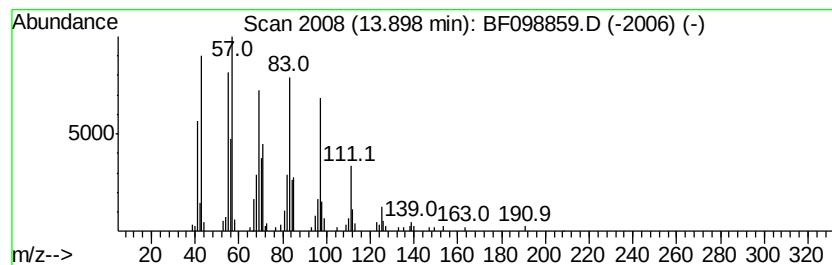
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.90	6.91 ng	277263	Chrysene-d12	14.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93



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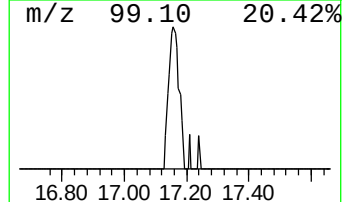
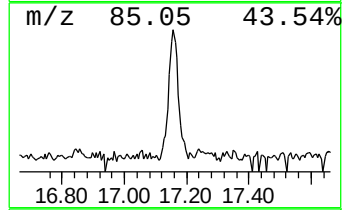
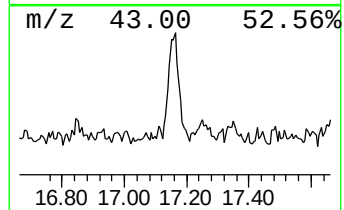
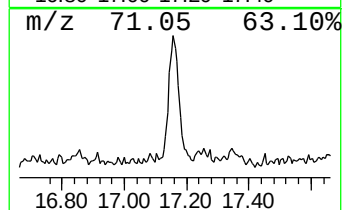
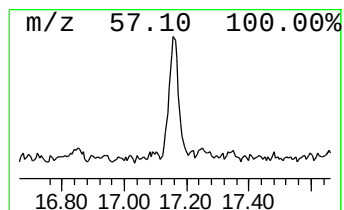
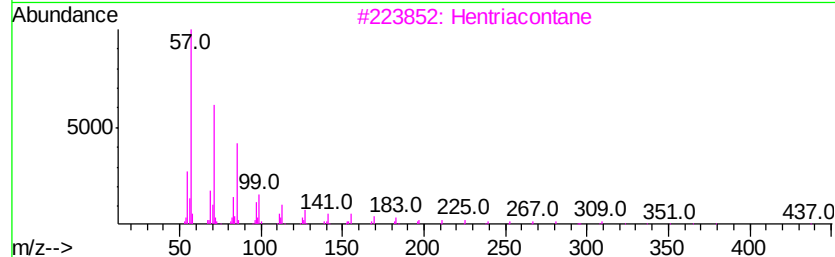
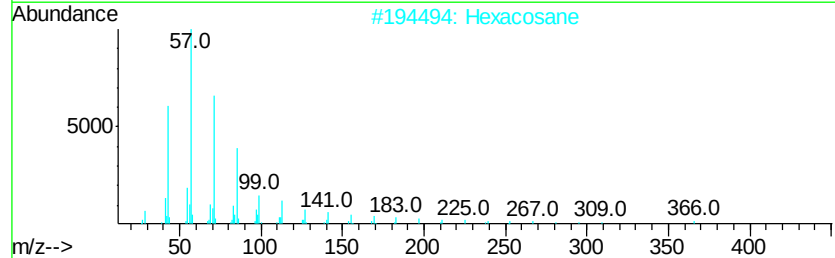
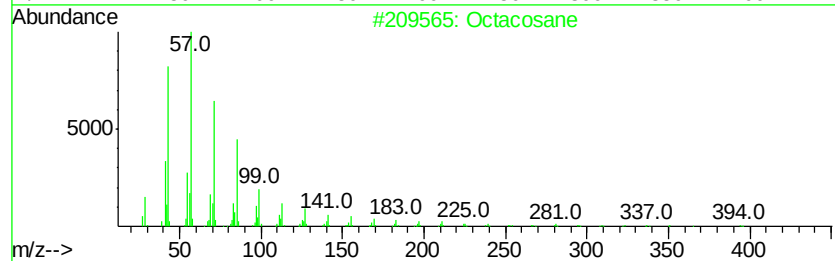
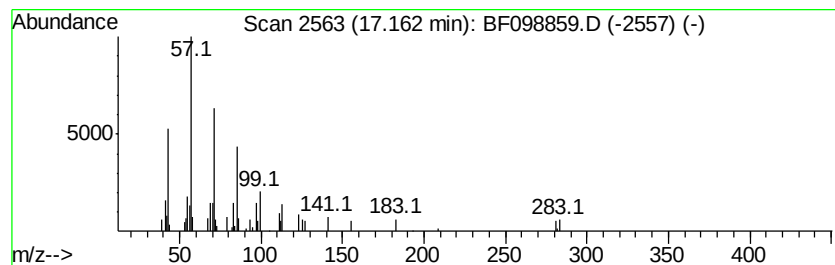
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Octacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.16	2.06 ng	80701	Perylene-d12	15.57

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	87
2	Hexacosane		366	C26H54	000630-01-3	86
3	Hentriacontane		437	C31H64	000630-04-6	86
4	Pentacosane		352	C25H52	000629-99-2	86
5	Heneicosane		296	C21H44	000629-94-7	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.22	8.5	ng	346019	1	6.92	813459	20.0
2-Pentanone, 4-hy...	5.15	16.5	ng	670568	1	6.92	813459	20.0
unknown6.69	6.69	83.5	ng	3395720	1	6.92	813459	20.0
Behenic alcohol	13.90	6.9	ng	277263	5	14.07	802382	20.0
Octacosane	17.16	2.1	ng	80701	6	15.57	783203	20.0