

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080415\
 Data File : BF080852.D
 Acq On : 4 Aug 2015 22:23
 Operator : TP/UM
 Sample : G3088-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DIN46-EFFLUENT-072315

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-BF080415.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	4.361	196	199	203	rBV	106827	162366	7.06%	1.169%
2	5.001	253	255	258	rBV	445408	465134	20.22%	3.349%
3	5.413	289	291	294	rVB	520127	591924	25.73%	4.262%
4	5.836	326	328	330	rBB	30263	37516	1.63%	0.270%
5	5.984	339	341	344	rBV	39514	34440	1.50%	0.248%
6	6.441	379	381	384	rBV	411062	366190	15.92%	2.637%
7	6.590	391	394	396	rBV	1044379	1125841	48.93%	8.107%
8	6.819	412	414	417	rBV	430594	464346	20.18%	3.344%
9	6.979	425	428	430	rBB	1493261	1387589	60.31%	9.991%
10	7.390	460	464	466	rBV	1252446	1635677	71.09%	11.778%
11	8.030	518	520	524	rBV	36412	31593	1.37%	0.227%
12	8.099	524	526	529	rBV	429367	589862	25.64%	4.247%
13	9.185	617	621	623	rBV	2264807	2300735	100.00%	16.566%
14	9.573	653	655	657	rVB	71424	54539	2.37%	0.393%
15	9.859	677	680	682	rBV	521705	585946	25.47%	4.219%
16	10.636	745	748	751	rBV	777028	790511	34.36%	5.692%
17	10.762	758	759	764	rVB	31750	39792	1.73%	0.287%
18	11.208	796	798	800	rBV	29649	31350	1.36%	0.226%
19	11.333	807	809	811	rBV	650359	542814	23.59%	3.909%
20	11.505	822	824	827	rVB	53624	44718	1.94%	0.322%
21	11.871	854	856	858	rBV	75328	73969	3.22%	0.533%
22	12.922	945	948	950	rBV	1823929	1745112	75.85%	12.566%
23	13.962	1036	1039	1041	rBV	431917	402120	17.48%	2.895%
24	14.259	1056	1065	1070	rBV5	4955	31264	1.36%	0.225%
25	14.808	1111	1113	1116	rBV	48326	47162	2.05%	0.340%
26	15.368	1159	1162	1165	rBV	275616	305385	13.27%	2.199%

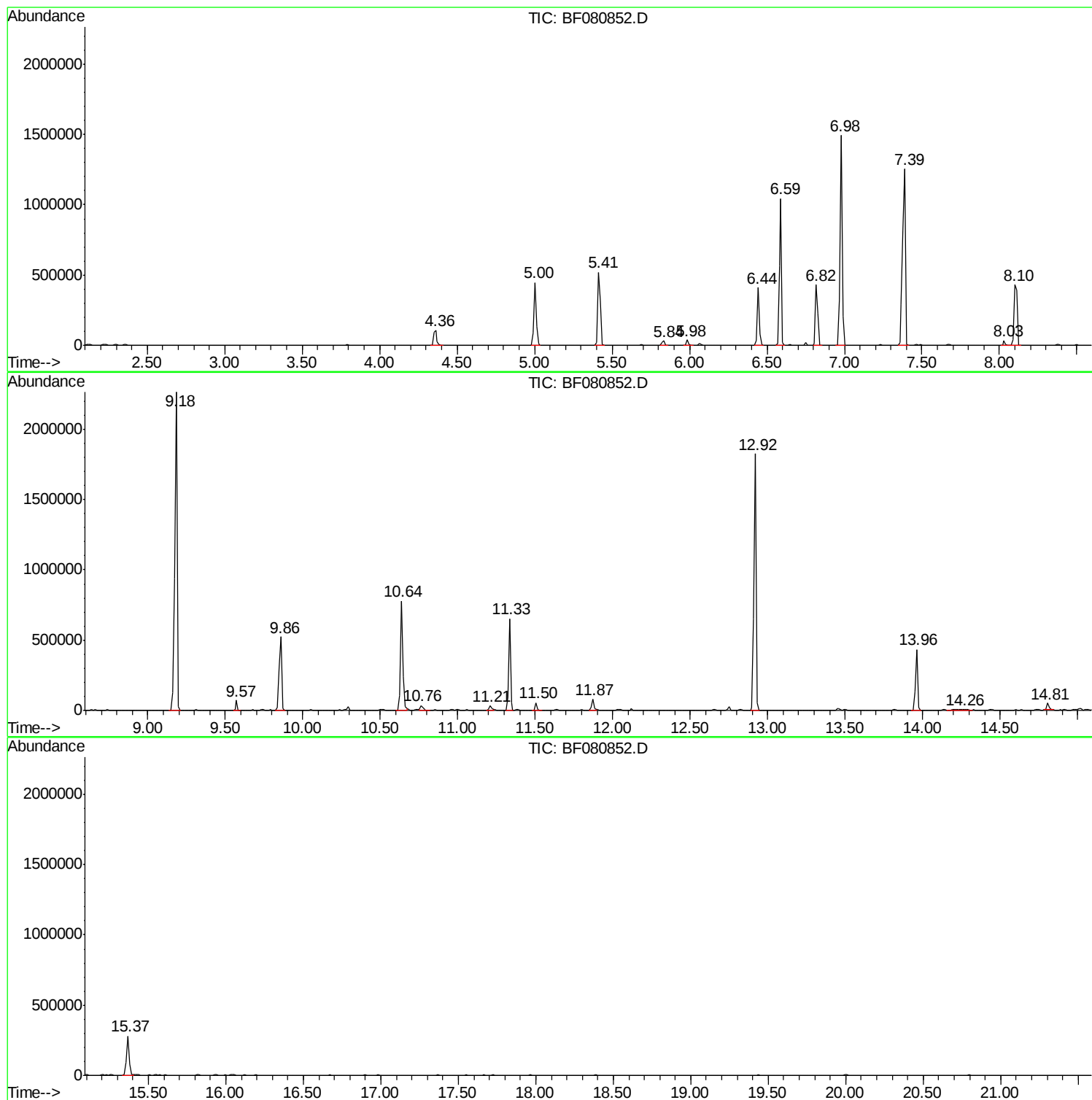
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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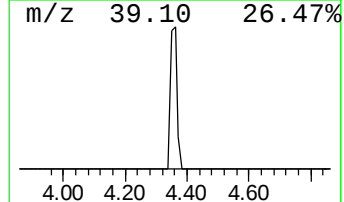
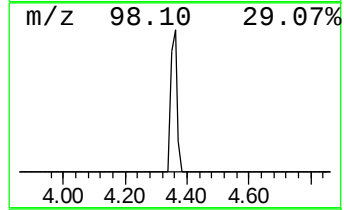
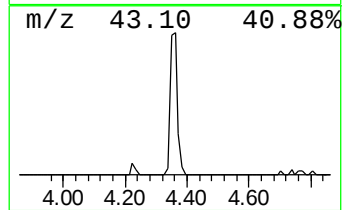
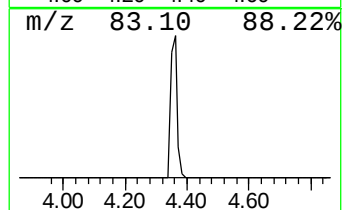
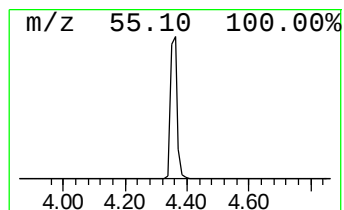
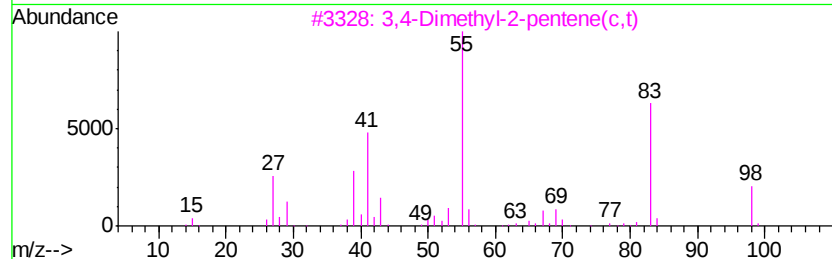
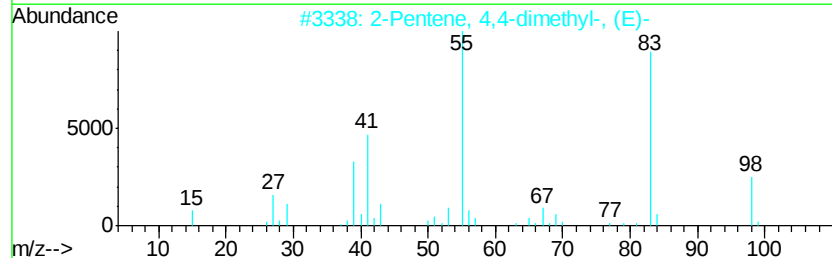
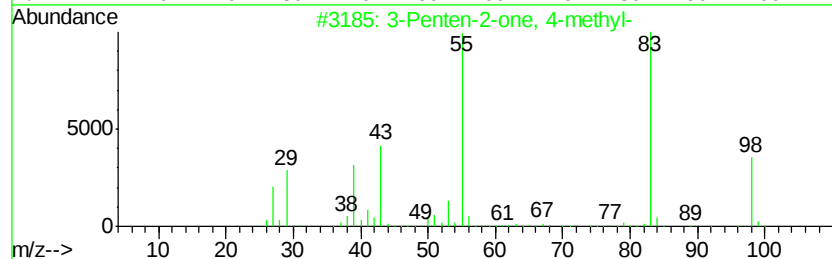
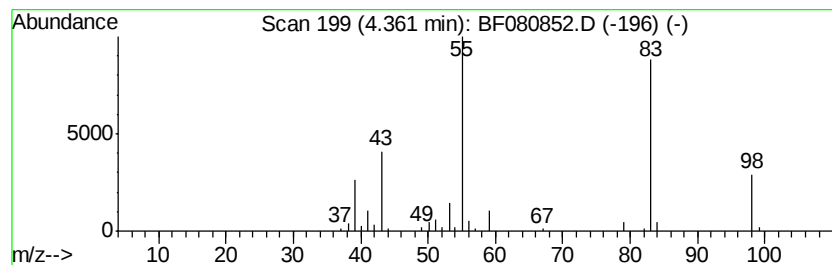
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.36	6.99 ng	162366	1,4-Dichlorobenzene-d4	6.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80
3			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	72
4			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	64
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	64



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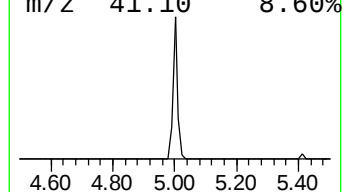
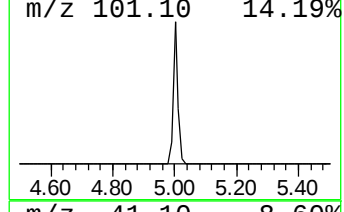
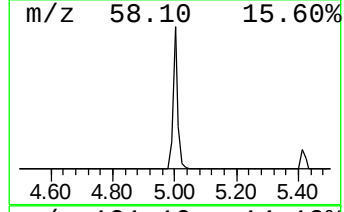
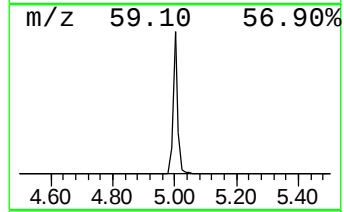
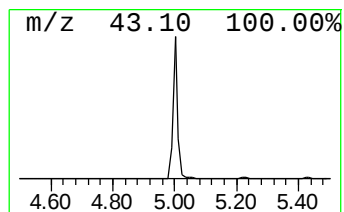
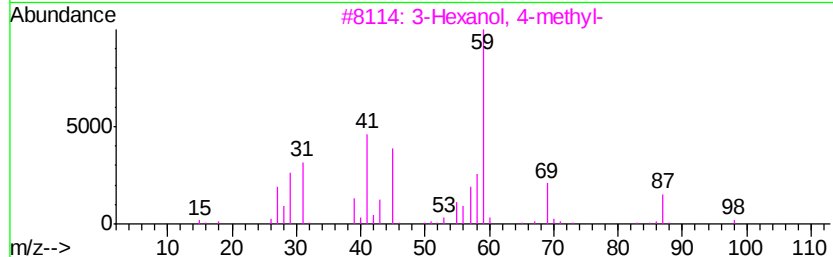
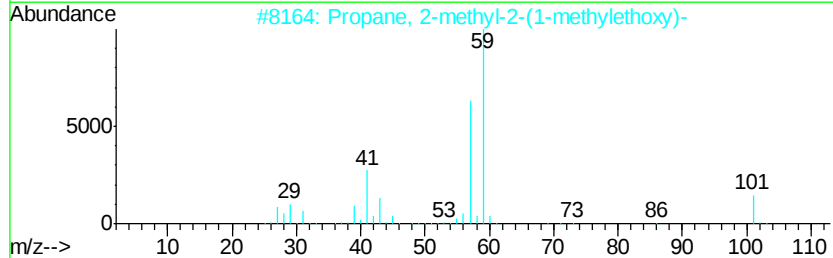
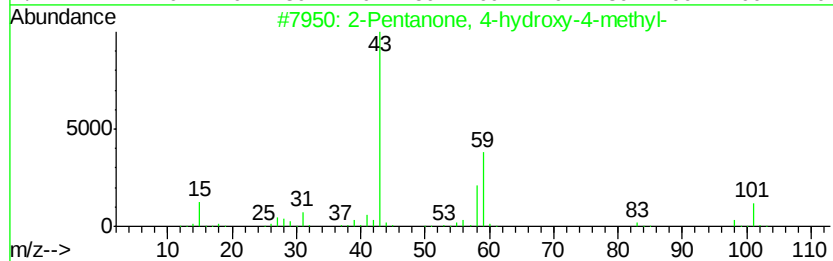
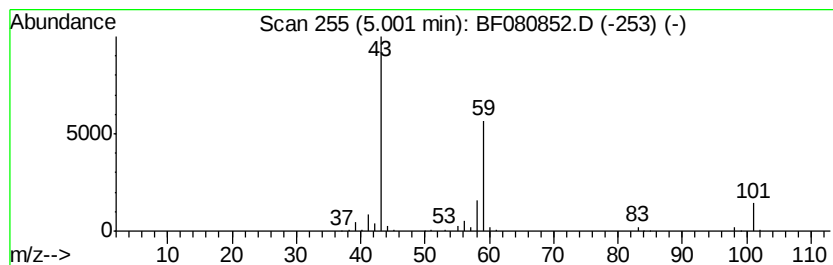
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	20.03 ng	465134	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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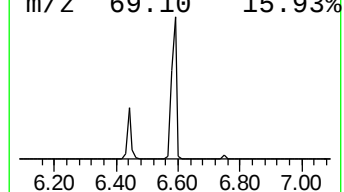
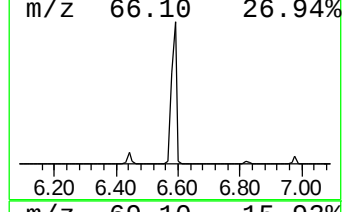
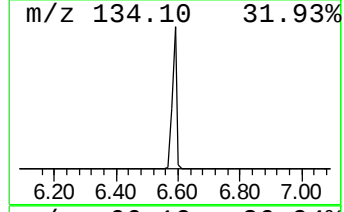
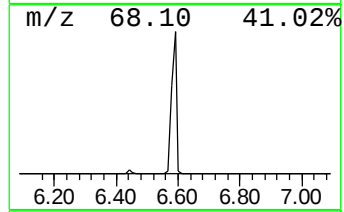
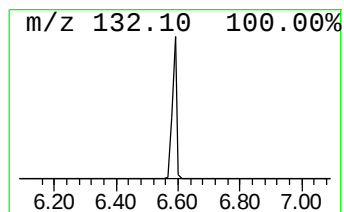
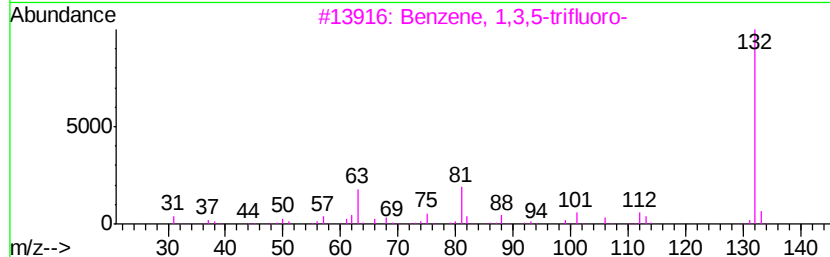
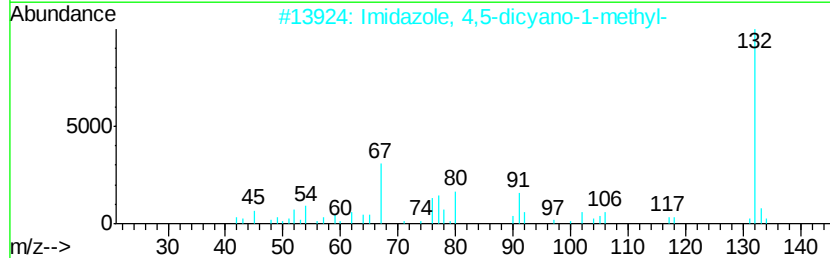
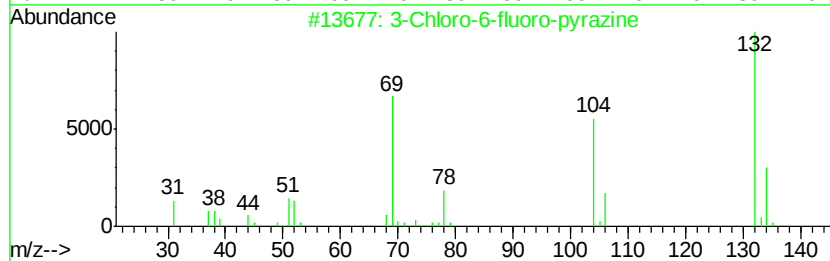
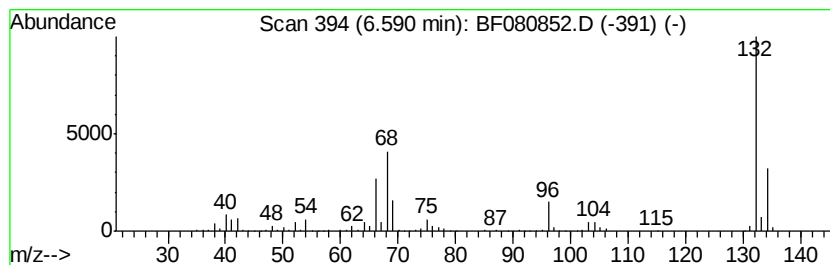
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.59 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	48.49 ng	1125840	1,4-Dichlorobenzene-d4	6.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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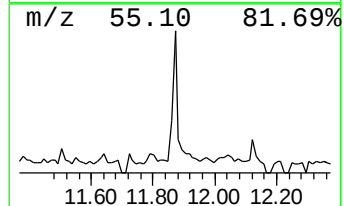
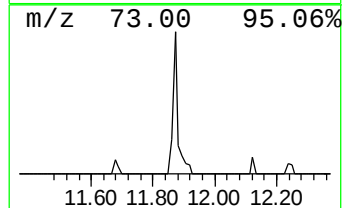
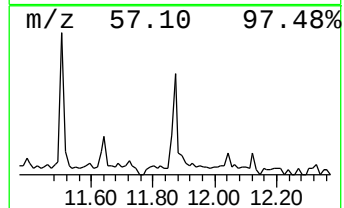
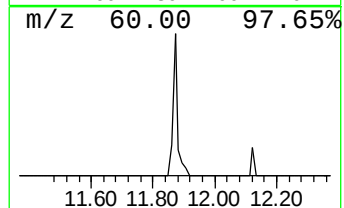
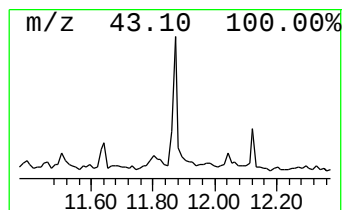
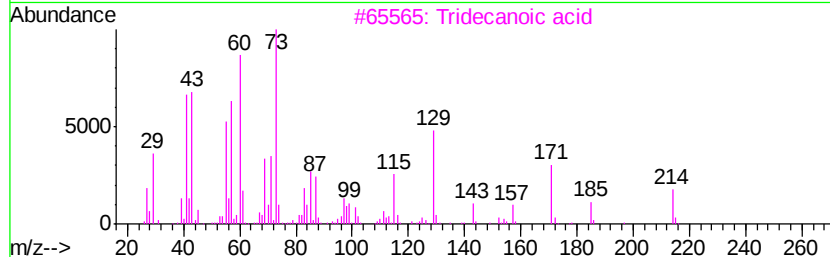
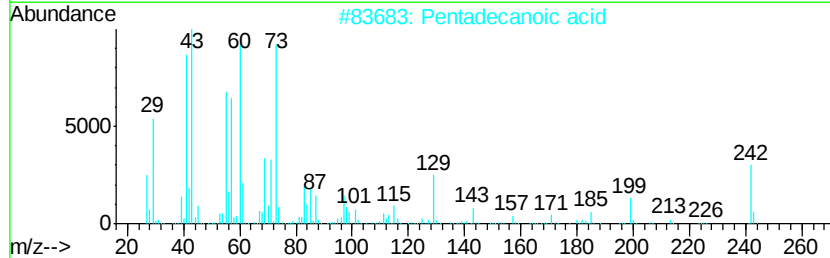
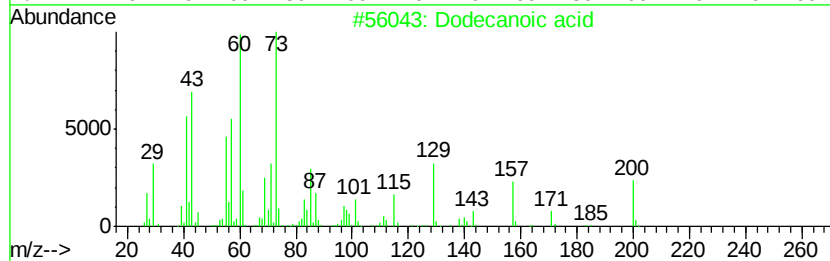
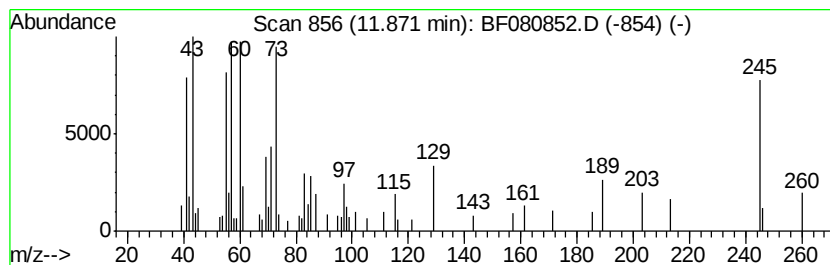
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown11.87 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	2.73 ng	73969	Phenanthrene-d10	11.33

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecanoic acid	200	C12H24O2	000143-07-7	38
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	38
3		Tridecanoic acid	214	C13H26O2	000638-53-9	38
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	38
5		Benzoic acid, 3-[(1,2-dihydro-2-...	245	C12H11N3O3	145820-05-9	38



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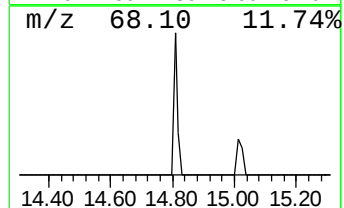
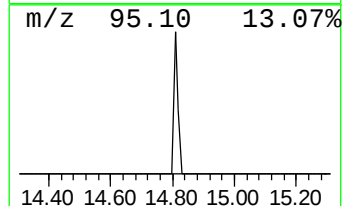
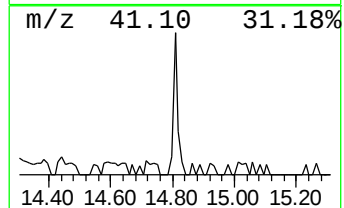
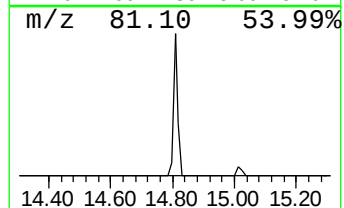
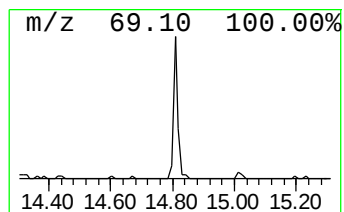
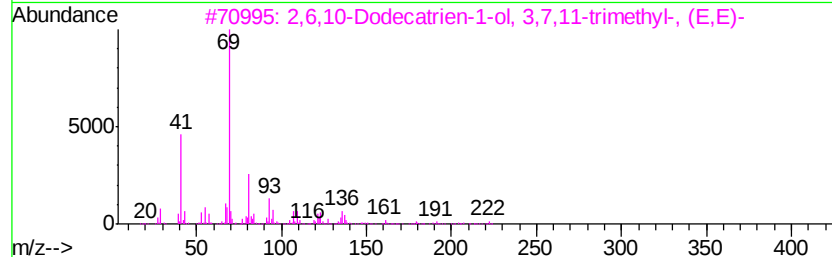
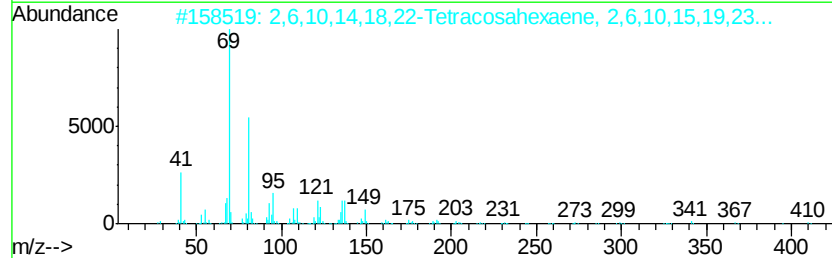
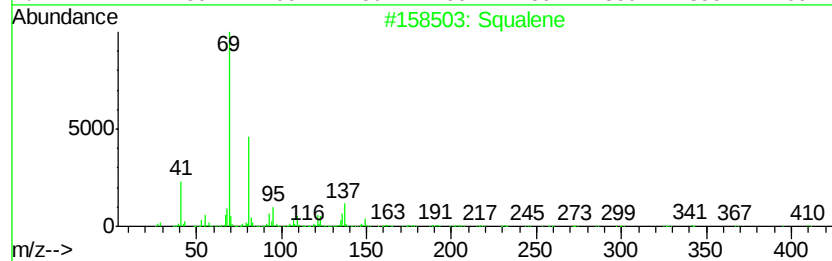
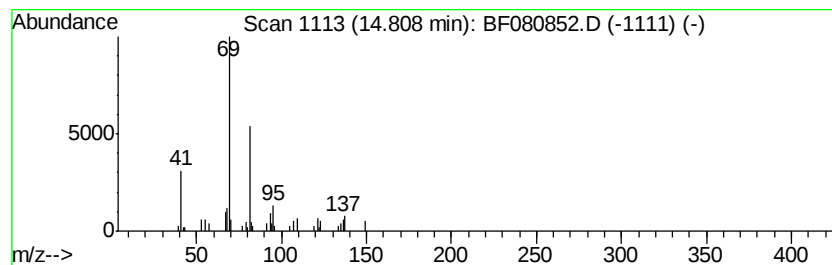
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	3.09 ng	47162	Perylene-d12	15.37

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	78
4		1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	64
5		Farnesol isomer a	222	C15H26O	1000108-92-4	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.36	7.0	ng	162366	1	6.82	464346	20.0
2-Pentanone, 4-hy...	5.00	20.0	ng	465134	1	6.82	464346	20.0
unknown6.59	6.59	48.5	ng	1125840	1	6.82	464346	20.0
unknown11.87	11.87	2.7	ng	73969	4	11.33	542814	20.0
Squalene	14.81	3.1	ng	47162	6	15.37	305385	20.0