

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF090817\
 Data File : BF098349.D
 Acq On : 8 Sep 2017 14:38
 Operator : SJ/JU
 Sample : I5110-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1

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-BF081517.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	4.216	358	362	370	rBV	46870	66349	2.40%	0.277%
2	4.881	471	475	487	rVB	152828	235011	8.49%	0.979%
3	5.298	540	546	549	rBV	2280548	2473063	89.39%	10.306%
4	6.334	716	722	738	rBV	2177099	2706887	97.84%	11.281%
5	6.457	738	743	746	rBV	2386088	2494372	90.16%	10.395%
6	6.681	777	781	784	rBV	720864	565863	20.45%	2.358%
7	6.840	803	808	811	rBV	2004833	1937176	70.02%	8.073%
8	7.251	872	878	881	rBV	1576340	1607005	58.08%	6.697%
9	7.963	994	999	1002	rBV	892113	761160	27.51%	3.172%
10	9.039	1177	1182	1186	rBV	2642396	2766702	100.00%	11.530%
11	9.439	1246	1250	1253	rBV	293803	254846	9.21%	1.062%
12	9.716	1292	1297	1301	rBV	986965	853210	30.84%	3.556%
13	10.510	1426	1432	1435	rBV	1624300	1675392	60.56%	6.982%
14	10.622	1448	1451	1460	rVB	51606	55758	2.02%	0.232%
15	11.198	1545	1549	1551	rBV	1020963	852200	30.80%	3.552%
16	11.222	1551	1553	1556	rVV	120585	92355	3.34%	0.385%
17	11.269	1557	1561	1566	rVB	28280	31397	1.13%	0.131%
18	12.404	1751	1754	1758	rVB	175014	155540	5.62%	0.648%
19	12.633	1786	1793	1796	rBV	154296	157816	5.70%	0.658%
20	12.786	1814	1819	1822	rBV	2203106	2155464	77.91%	8.983%
21	13.474	1933	1936	1940	rVB2	28401	29730	1.07%	0.124%
22	13.680	1967	1971	1979	rVB	203120	218459	7.90%	0.910%
23	13.833	1991	1997	1999	rBV	607515	668171	24.15%	2.785%
24	13.857	1999	2001	2007	rVB	66374	61490	2.22%	0.256%
25	14.310	2075	2078	2082	rBV2	28692	36380	1.31%	0.152%
26	14.839	2164	2168	2171	rBV	61253	79733	2.88%	0.332%
27	14.916	2178	2181	2183	rBV2	27092	28090	1.02%	0.117%
28	14.939	2183	2185	2189	rVB3	27467	28392	1.03%	0.118%
29	15.121	2212	2216	2221	rBV	35917	47755	1.73%	0.199%
30	15.174	2222	2225	2230	rBV	46433	55646	2.01%	0.232%
31	15.239	2231	2236	2239	rBV	473963	557185	20.14%	2.322%
32	15.663	2304	2308	2312	rBV	38210	54058	1.95%	0.225%
33	15.710	2313	2316	2322	rVB5	28584	42207	1.53%	0.176%
34	16.121	2382	2386	2390	rBV3	21773	32388	1.17%	0.135%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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35	16.586	2462	2465	2472	rVB2	24967	38725	1.40%	0.161%
36	16.662	2474	2478	2485	rVB3	29715	51832	1.87%	0.216%
37	16.992	2529	2534	2539	rVB	17314	30708	1.11%	0.128%
38	17.104	2548	2553	2559	rBV9	15860	36912	1.33%	0.154%

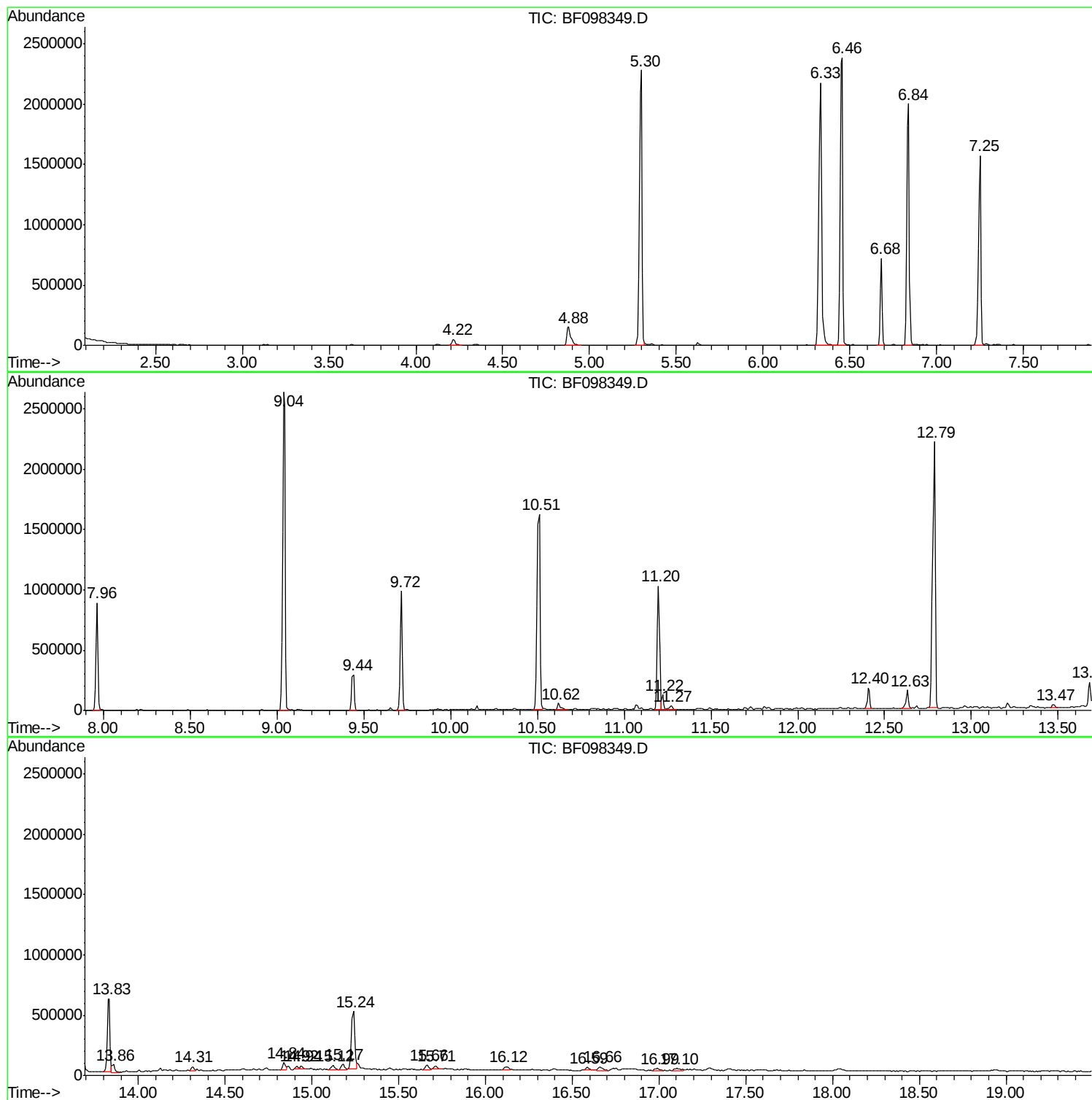
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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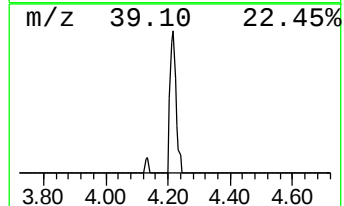
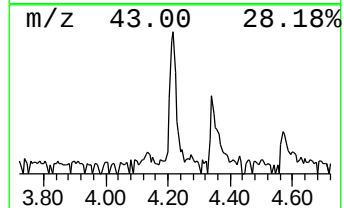
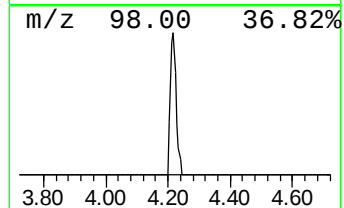
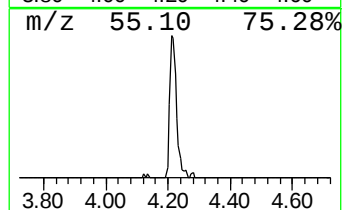
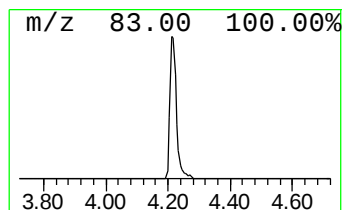
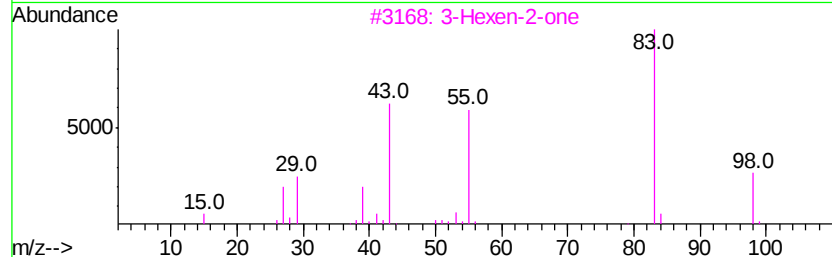
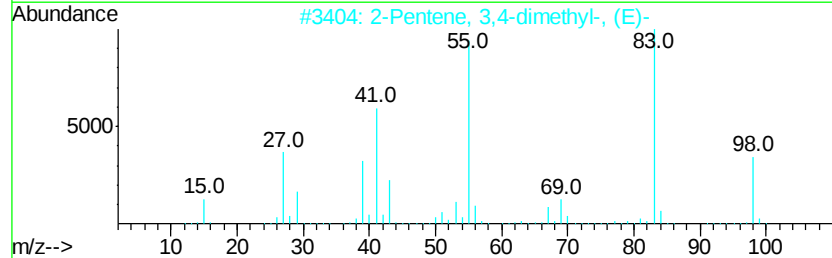
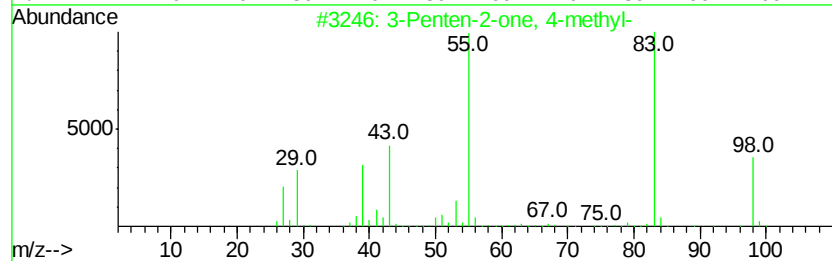
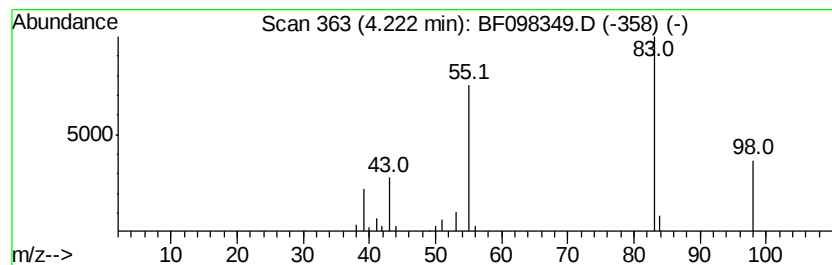
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.22	2.35 ng	66349	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3		3-Hexen-2-one	98	C6H10O	000763-93-9	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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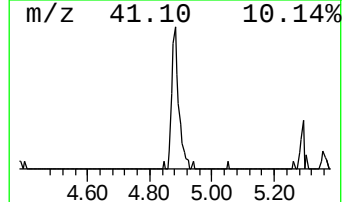
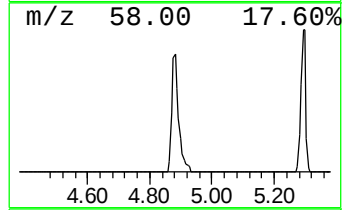
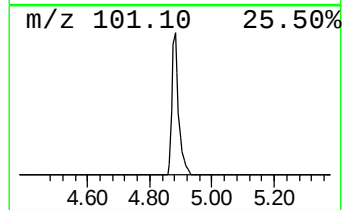
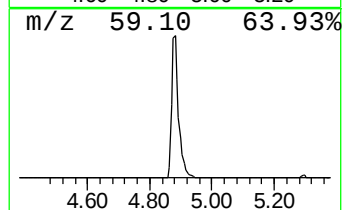
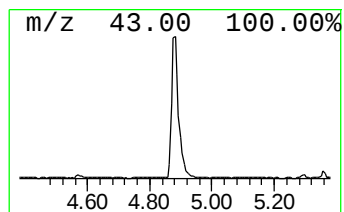
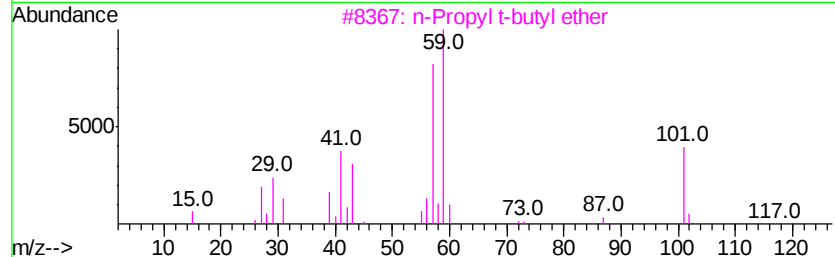
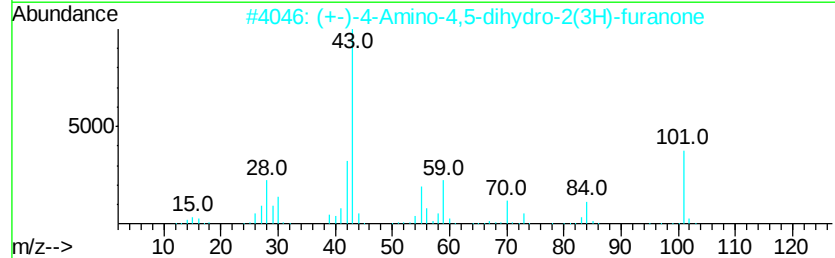
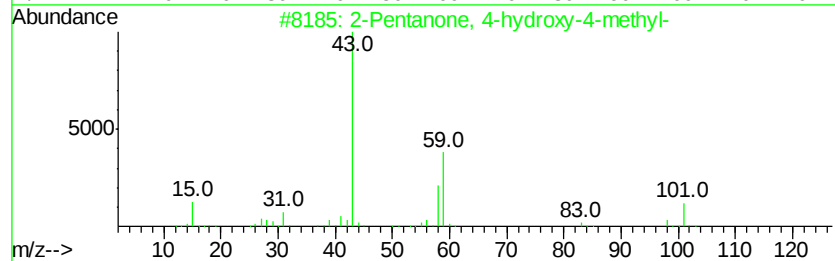
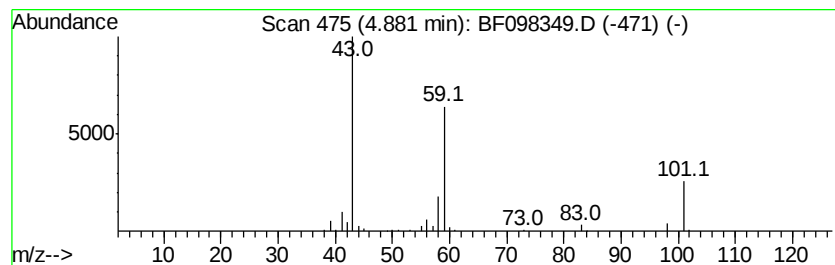
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	8.31 ng	235011	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	37
3		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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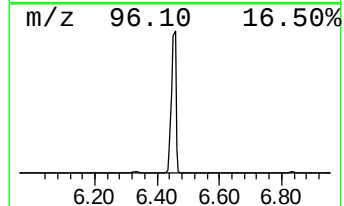
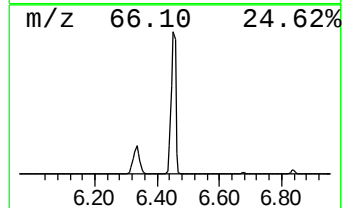
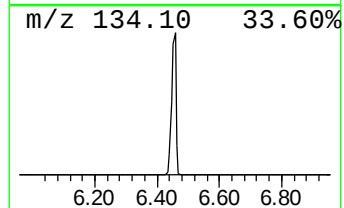
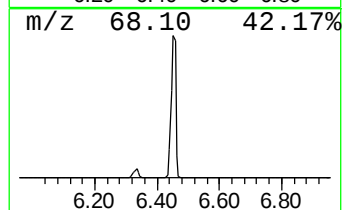
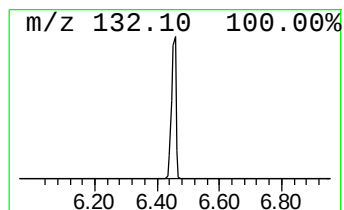
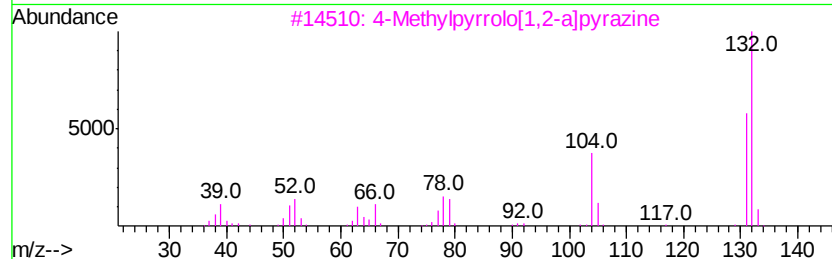
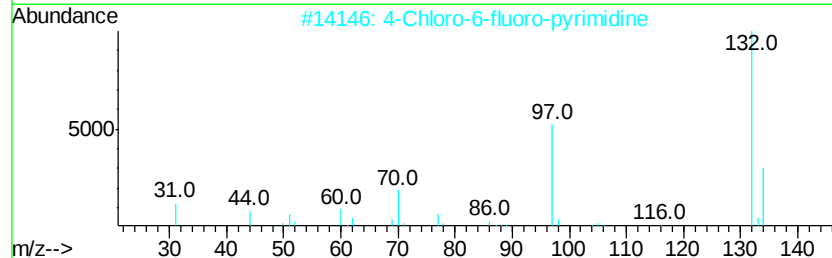
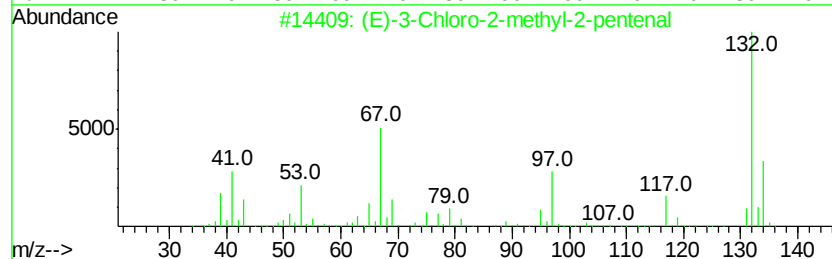
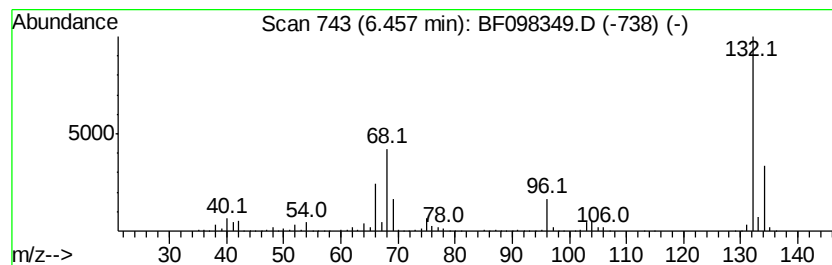
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	88.16 ng	2494370	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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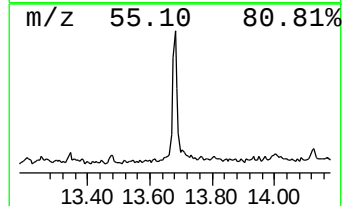
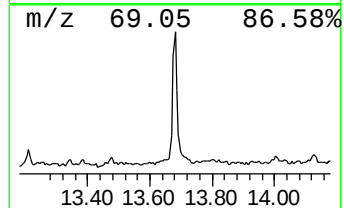
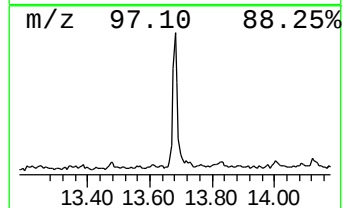
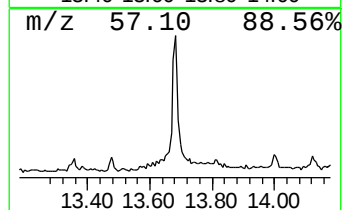
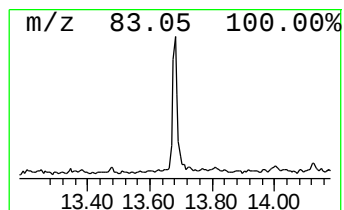
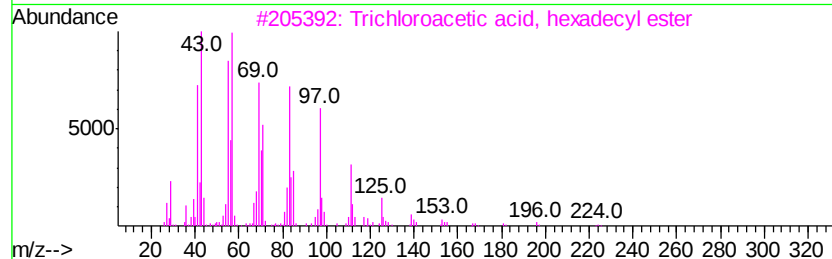
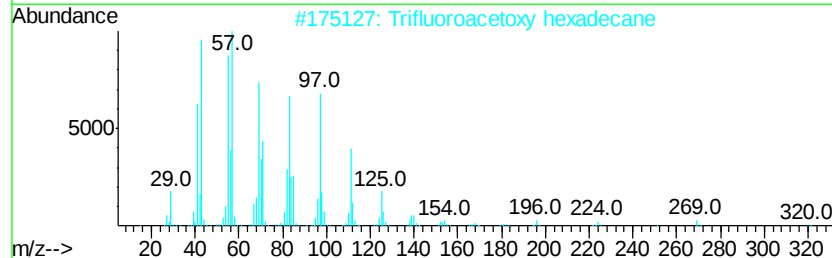
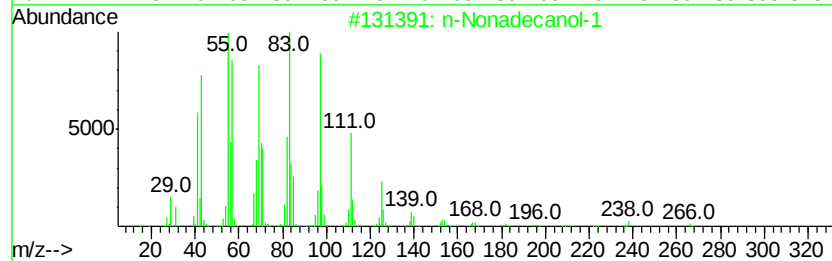
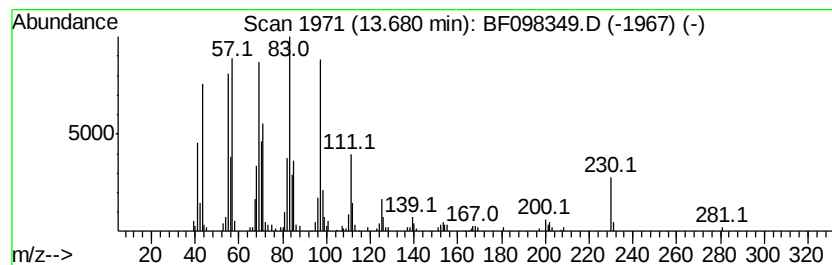
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Peak Number 5 n-Nonadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	6.54 ng	218459	Chrysene-d12	13.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.22	2.4	ng	66349	1	6.68	565863	20.0
2-Pentanone, 4-hy...	4.88	8.3	ng	235011	1	6.68	565863	20.0
unknown6.46	6.46	88.2	ng	2494370	1	6.68	565863	20.0
n-Nonadecanol-1	13.68	6.5	ng	218459	5	13.83	668171	20.0