

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051017\
 Data File : BF095066.D
 Acq On : 10 May 2017 20:38
 Operator : SJ/MA
 Sample : I3049-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DRUM-M4935

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-BF050217.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	4.990	515	519	535	rBV	120899	245142	10.00%	1.620%
2	5.643	626	630	661	rBV	978394	1903299	77.64%	12.580%
3	7.248	899	903	918	rBV	970276	1614204	65.85%	10.669%
4	7.366	918	923	934	rVB	1359089	1926480	78.59%	12.734%
5	7.701	976	980	989	rBV	381868	430698	17.57%	2.847%
6	7.889	1007	1012	1016	rBV	187919	326596	13.32%	2.159%
7	7.936	1016	1020	1035	rVB	1340203	1748909	71.35%	11.560%
8	8.601	1129	1133	1152	rBV	892150	1223184	49.90%	8.085%
9	9.725	1320	1324	1342	rBV	486055	686551	28.01%	4.538%
10	11.501	1621	1626	1635	rBV	2082814	2451340	100.00%	16.203%
11	12.160	1730	1738	1740	rBV7	32628	78294	3.19%	0.518%
12	12.195	1740	1744	1748	rVV	129334	180157	7.35%	1.191%
13	12.324	1762	1766	1772	rBV2	260494	324293	13.23%	2.143%
14	12.413	1777	1781	1789	rVV5	93615	150390	6.14%	0.994%
15	12.554	1801	1805	1809	rBV2	518959	672727	27.44%	4.447%
16	13.107	1897	1899	1905	rVB5	63841	83060	3.39%	0.549%
17	13.866	2024	2028	2041	rBV	411677	1083828	44.21%	7.164%

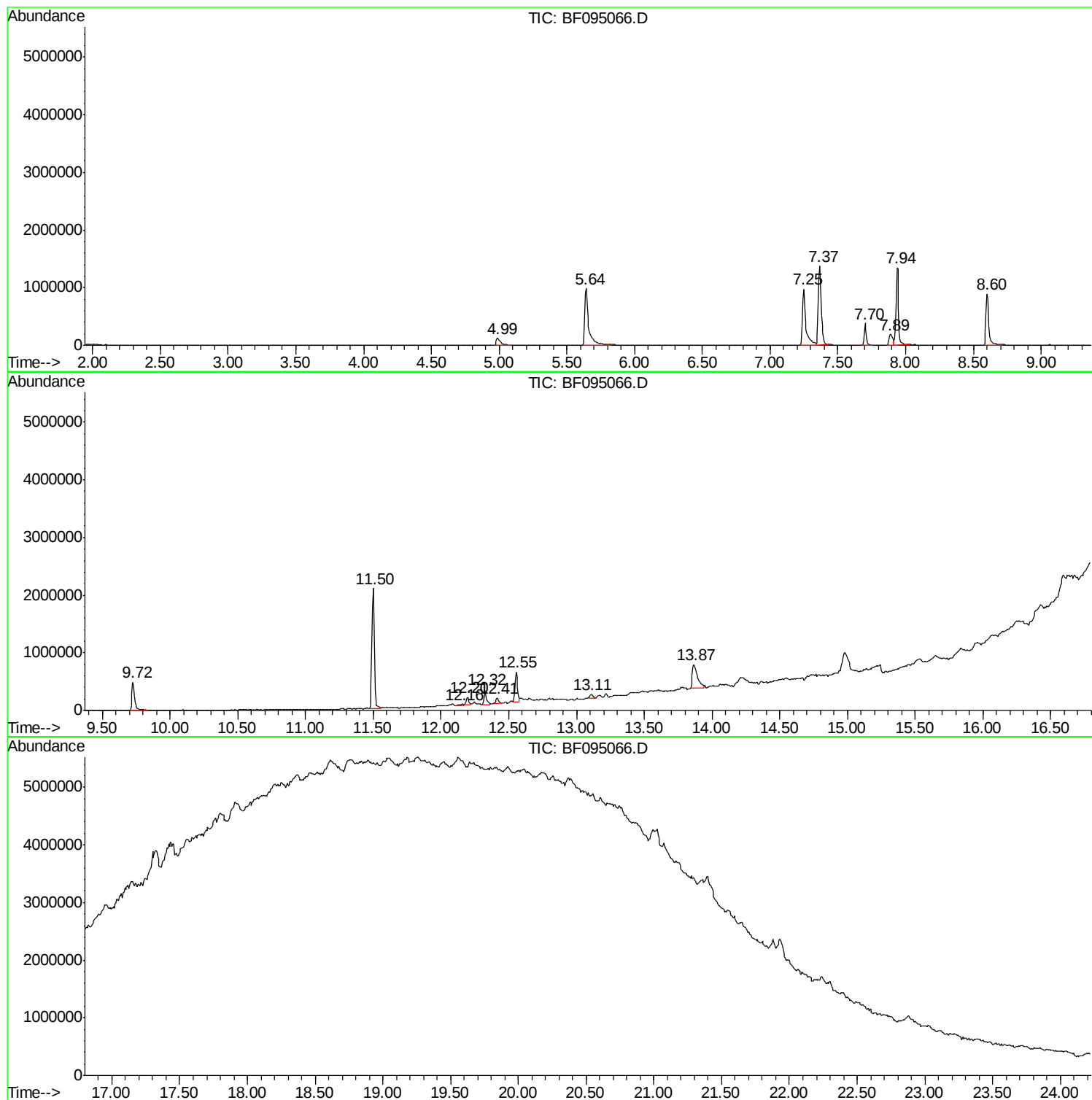
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Data Path : Z:\HPCHEM1\BNA F\DATA\BF051017\
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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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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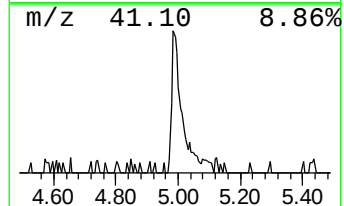
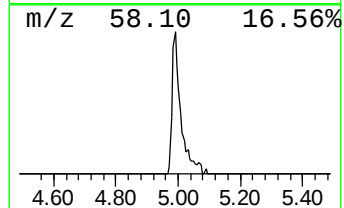
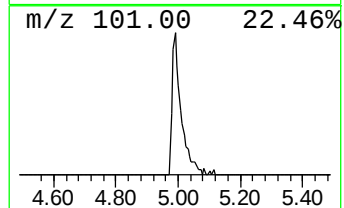
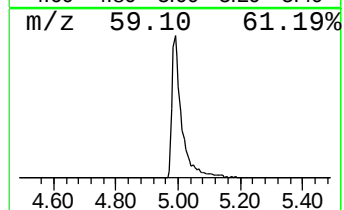
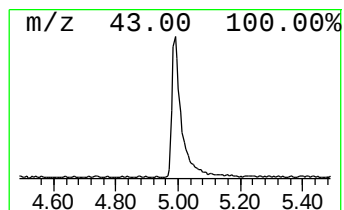
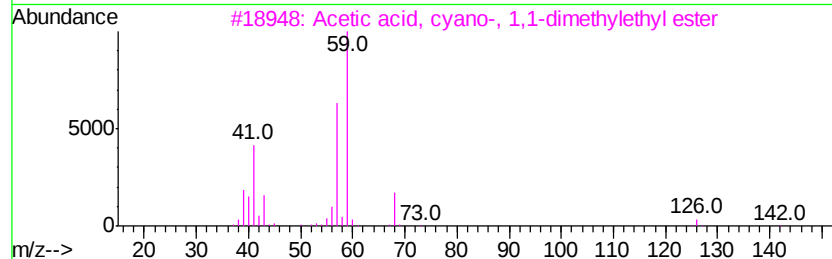
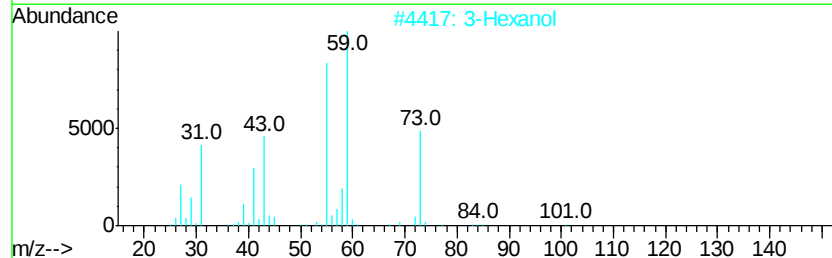
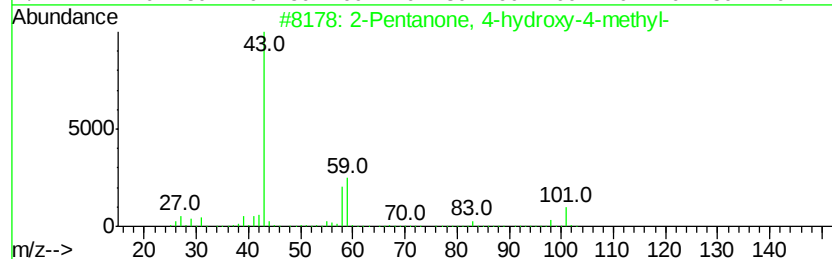
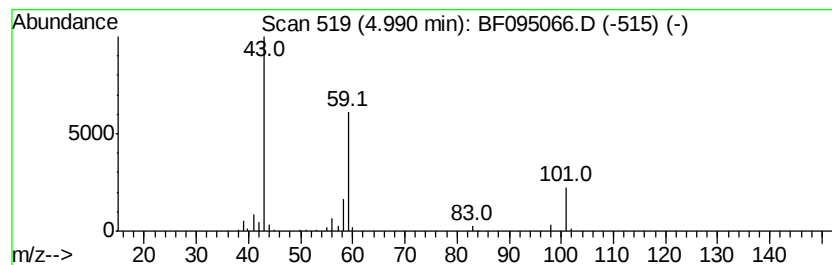
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	11.38 ng	245142	1,4-Dichlorobenzene-d4	7.70

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	102	C6H14O	000623-37-0	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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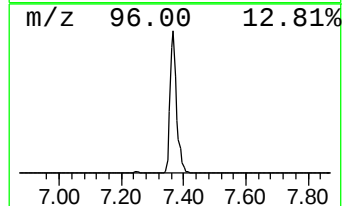
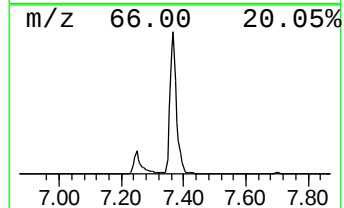
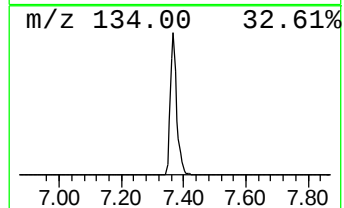
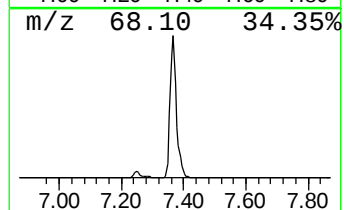
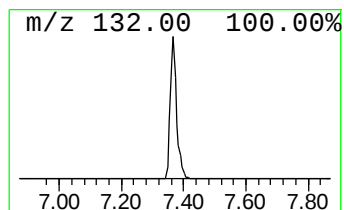
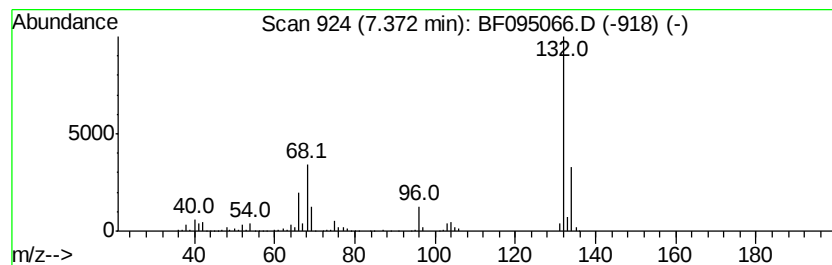
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	89.46 ng	1926480	1,4-Dichlorobenzene-d4	7.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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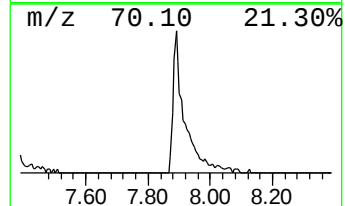
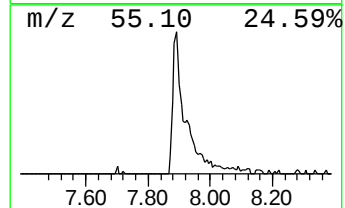
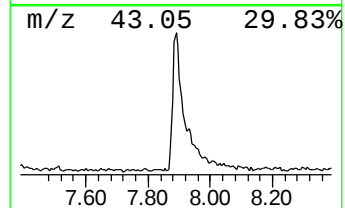
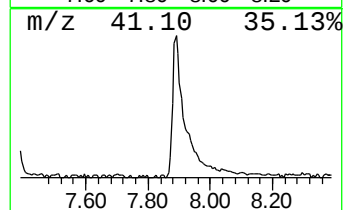
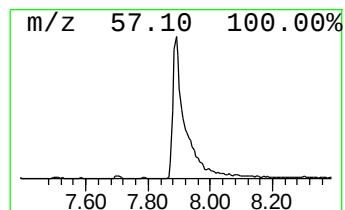
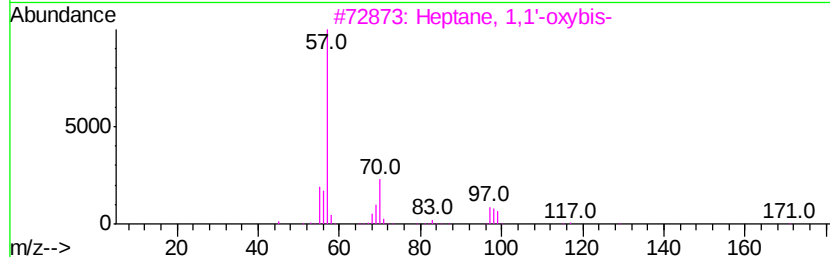
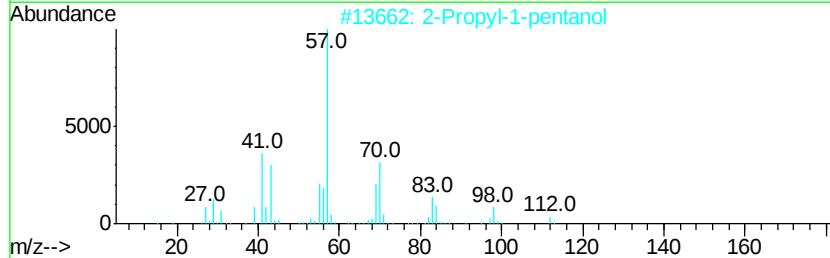
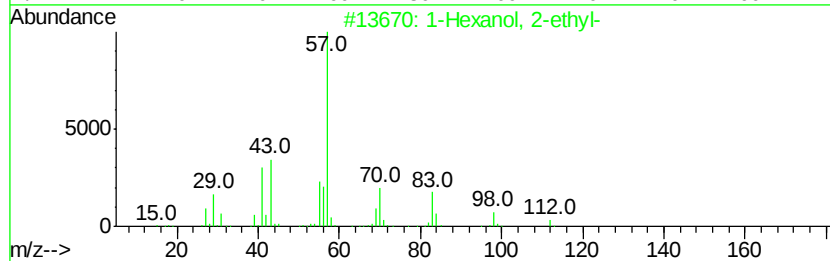
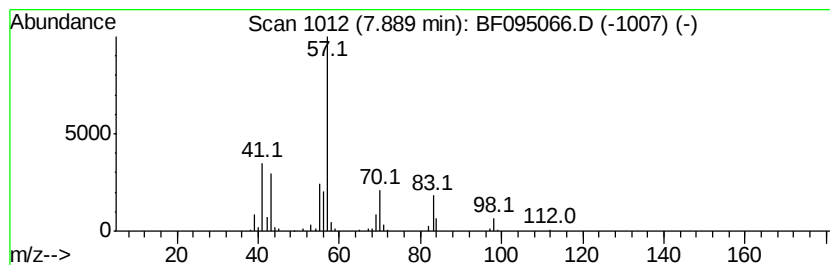
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.89	15.17 ng	326596	1,4-Dichlorobenzene-d4	7.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	72
3		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
4		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	53
5		1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	50



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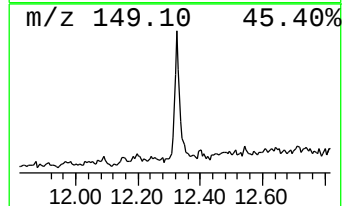
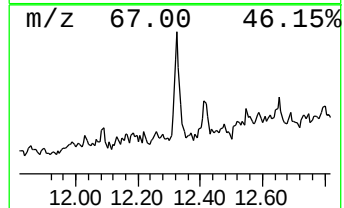
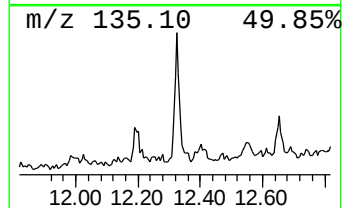
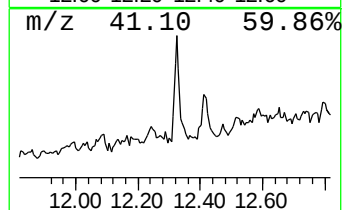
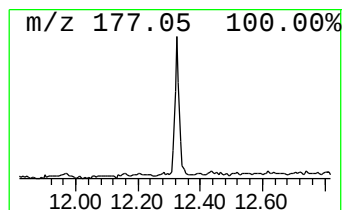
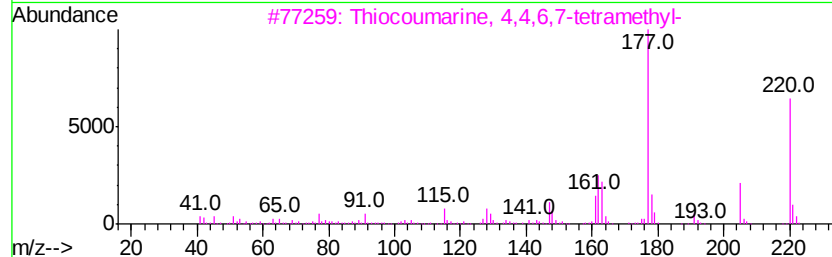
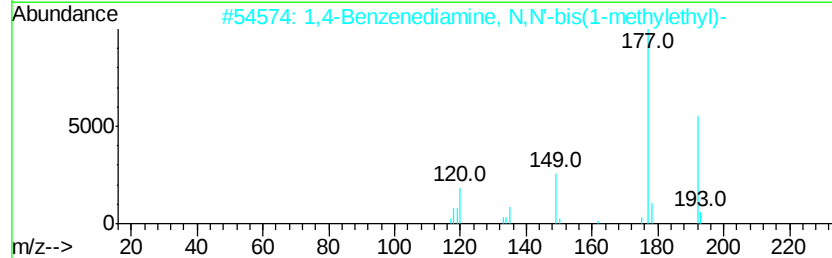
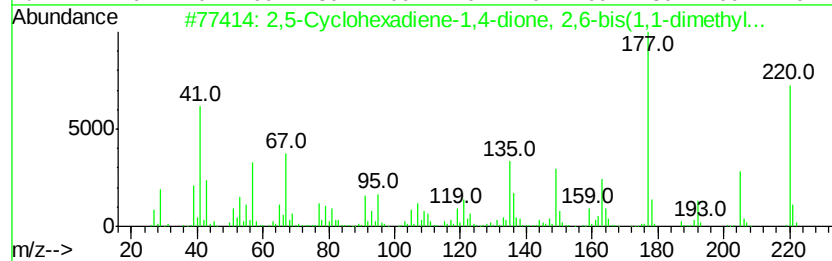
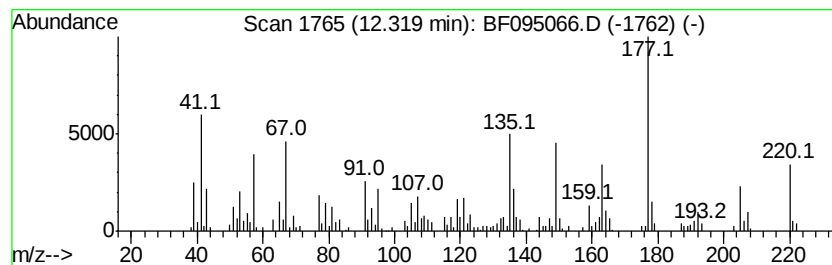
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Peak Number 5 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	9.64 ng	324293	Acenaphthene-d10	12.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2		1,4-Benzenediamine, N,N'-bis(1-m...	192	C12H20N2	004251-01-8	46
3		Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	43
4		trans-.beta.-Ionone	192	C13H20O	000079-77-6	42
5		3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	38



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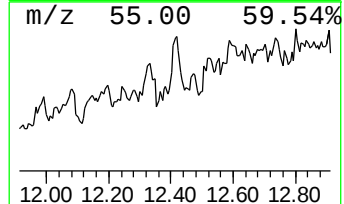
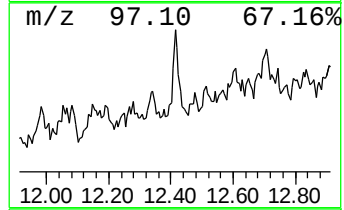
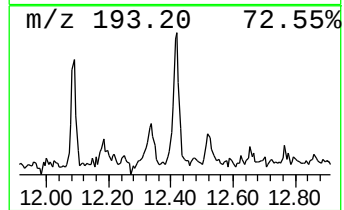
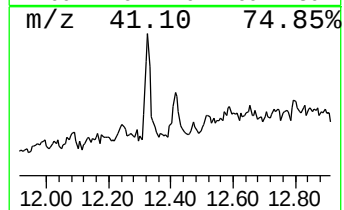
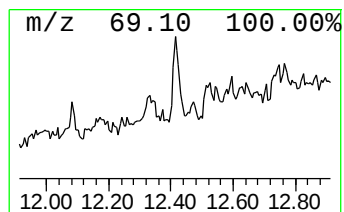
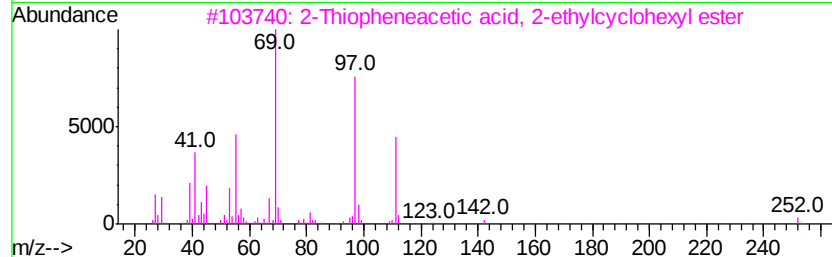
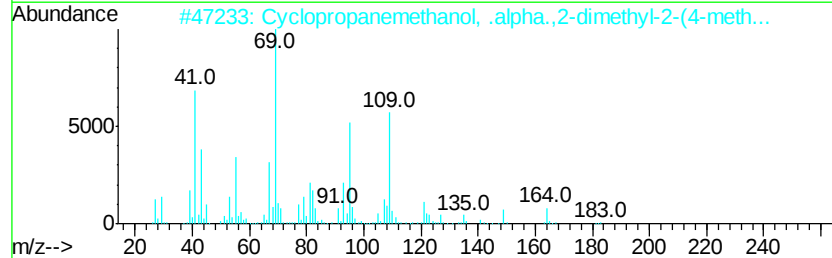
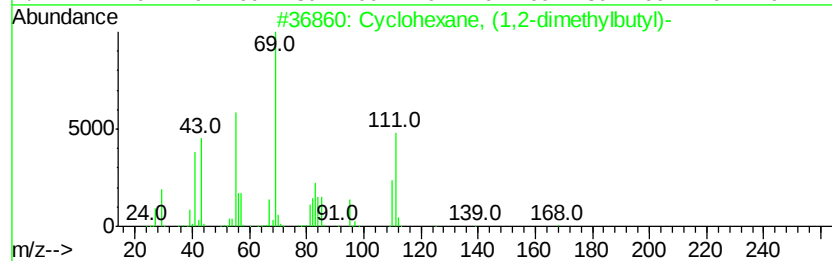
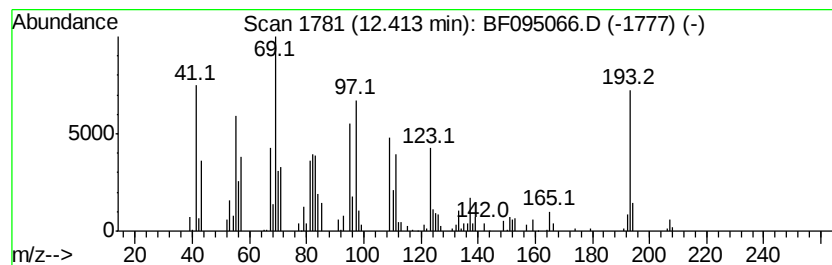
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown12.41 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	4.47 ng	150390	Acenaphthene-d10	12.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, (1,2-dimethylbutyl)-	168	C12H24	061142-37-8	35
2		Cyclopropanemethanol, .alpha.,2-...	182	C12H22O	121959-70-4	35
3		2-Thiopheneacetic acid, 2-ethylc...	252	C14H20O2S	1000278-96-1	35
4		Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	27
5		2-Butenedioic acid (Z)-, monodod...	284	C16H28O4	002424-61-5	27



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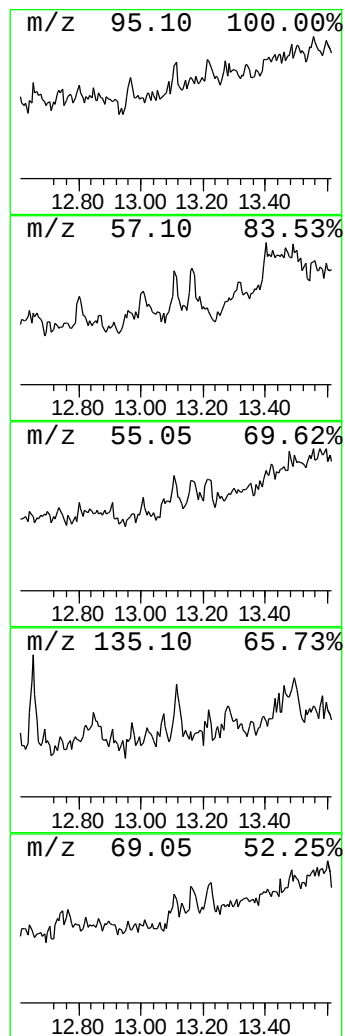
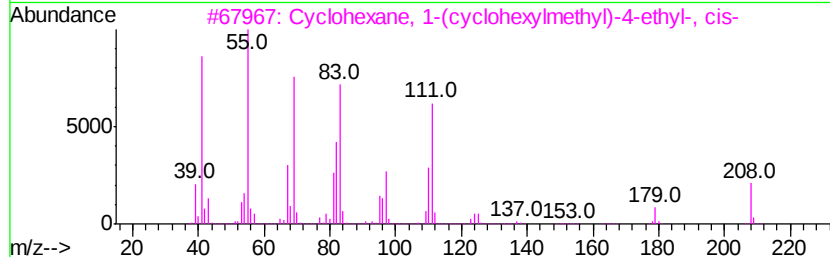
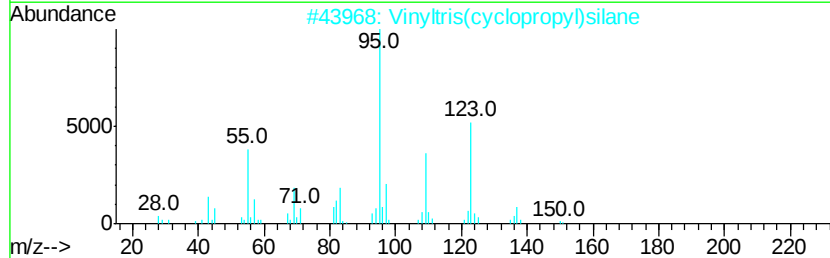
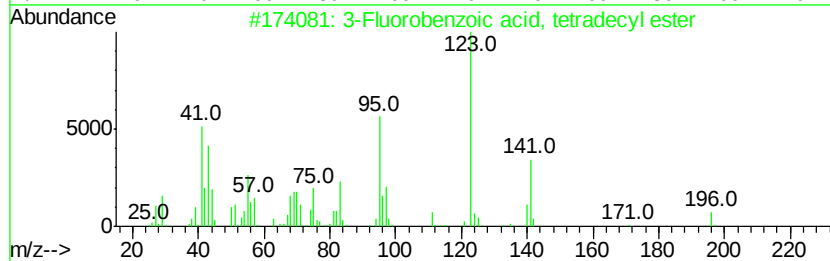
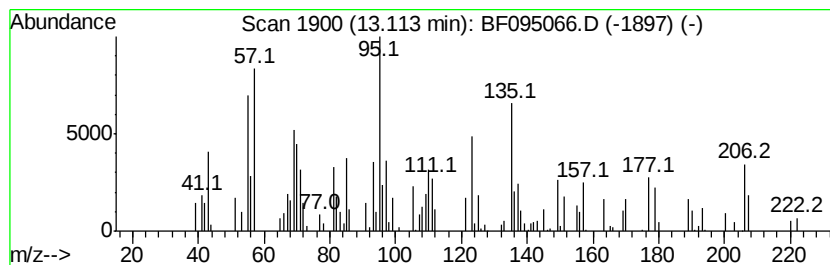
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Peak Number 7 unknown13.11 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.11	2.47 ng	83060	Acenaphthene-d10	12.55	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Fluorobenzoic acid, tetradecyl...	336	C21H33F02	1000279-01-5	38
2	Vinyltris(cyclopropyl)silane	178	C11H18Si	1000109-97-3	35
3	Cyclohexane, 1-(cyclohexylmethyl)...	208	C15H28	054934-95-1	25
4	4-(3-Hydroxy-2,6,6-trimethylcyclo...	222	C14H22O2	097306-57-5	25
5	Epicedrol	222	C15H26O	1000156-22-8	18



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.99	11.4	ng	245142	1	7.70	430698	20.0
unknown7.37	7.37	89.5	ng	1926480	1	7.70	430698	20.0
1-Hexanol, 2-ethyl-	7.89	15.2	ng	326596	1	7.70	430698	20.0
2,5-Cyclohexadien...	12.32	9.6	ng	324293	3	12.55	672727	20.0
unknown12.41	12.41	4.5	ng	150390	3	12.55	672727	20.0
unknown13.11	13.11	2.5	ng	83060	3	12.55	672727	20.0