

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080615\
 Data File : BF080900.D
 Acq On : 6 Aug 2015 21:03
 Operator : TP/UM
 Sample : G3196-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-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-BF080615.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	4.293	191	193	195	rBB	16791	24447	1.33%	0.195%
2	4.956	249	251	254	rBV	366597	378959	20.61%	3.026%
3	5.390	286	289	291	rBV	360130	474067	25.78%	3.786%
4	5.802	324	325	328	rBB	20438	21875	1.19%	0.175%
5	6.430	378	380	382	rBV	369876	339856	18.48%	2.714%
6	6.567	390	392	394	rBV	954445	785622	42.73%	6.274%
7	6.807	411	413	415	rBV	421346	353764	19.24%	2.825%
8	6.967	424	427	429	rVB	935607	1015906	55.25%	8.113%
9	7.367	459	462	465	rVB	820268	858580	46.70%	6.857%
10	8.088	523	525	528	rBV	378498	419691	22.83%	3.352%
11	9.173	617	620	622	rBV	1883600	1769433	96.24%	14.131%
12	9.288	628	630	637	rVB	12913	20874	1.14%	0.167%
13	9.562	652	654	656	rVB	184327	144219	7.84%	1.152%
14	9.848	676	679	681	rBV	450350	498867	27.13%	3.984%
15	10.259	713	715	716	rBV	17709	19349	1.05%	0.155%
16	10.282	716	717	719	rVB	26922	20146	1.10%	0.161%
17	10.625	745	747	750	rBV	739246	735651	40.01%	5.875%
18	10.751	757	758	763	rBV	33538	46696	2.54%	0.373%
19	11.196	796	797	799	rBV	38781	42570	2.32%	0.340%
20	11.322	806	808	810	rBV	657804	550076	29.92%	4.393%
21	11.631	828	835	841	rBV	75806	234259	12.74%	1.871%
22	11.859	853	855	857	rBV	37652	35753	1.94%	0.286%
23	12.031	868	870	872	rBV	28006	22689	1.23%	0.181%
24	12.111	875	877	882	rVB	203631	172056	9.36%	1.374%
25	12.454	902	907	916	rBV4	79256	433012	23.55%	3.458%
26	12.739	929	932	934	rBV	20077	20181	1.10%	0.161%
27	12.797	934	937	941	rVB3	12222	27909	1.52%	0.223%
28	12.911	944	947	949	rBV	1944901	1838656	100.00%	14.684%
29	13.151	965	968	969	rBV	18263	24684	1.34%	0.197%
30	13.357	984	986	992	rVB	41344	49161	2.67%	0.393%
31	13.448	992	994	996	rVV	18134	26010	1.41%	0.208%
32	13.482	996	997	1001	rVB	16553	20586	1.12%	0.164%
33	13.951	1035	1038	1040	rVB	643112	589423	32.06%	4.707%
34	15.357	1158	1161	1164	rBV	434616	506565	27.55%	4.046%

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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-BF080615.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

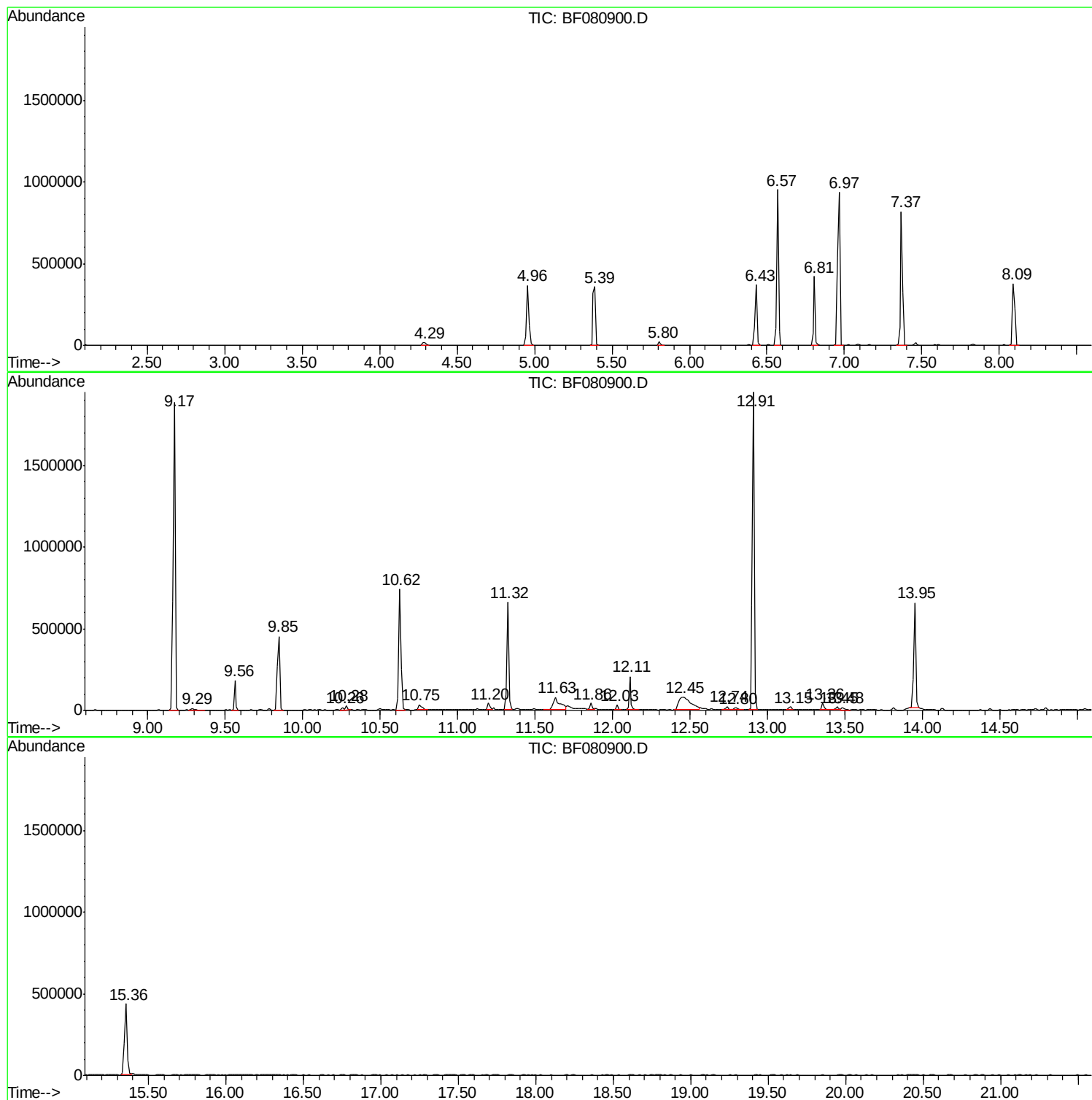
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF080615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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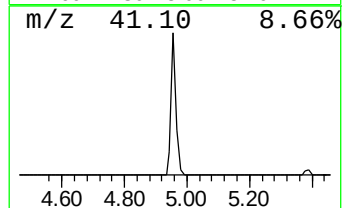
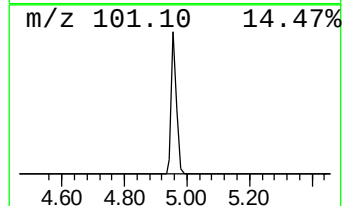
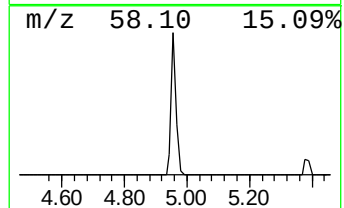
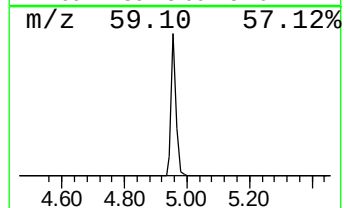
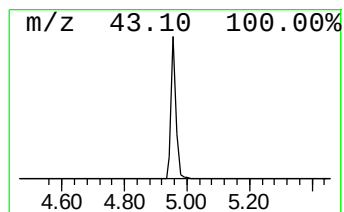
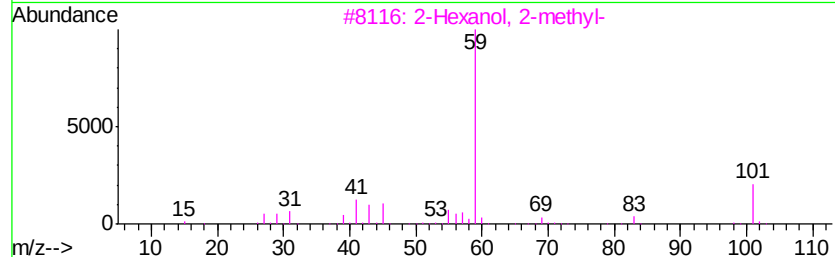
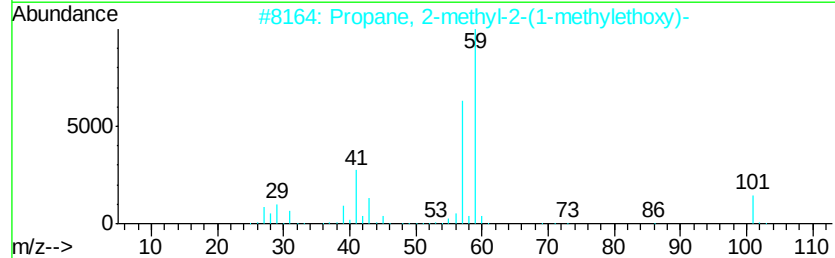
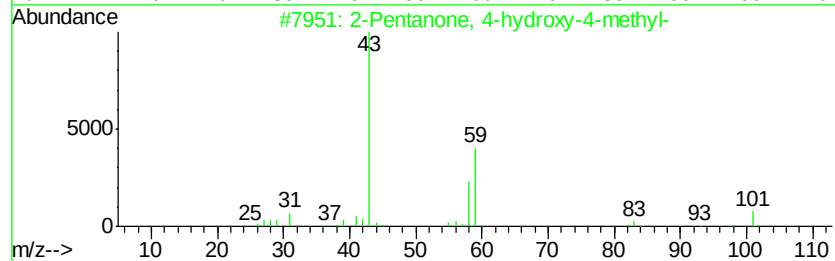
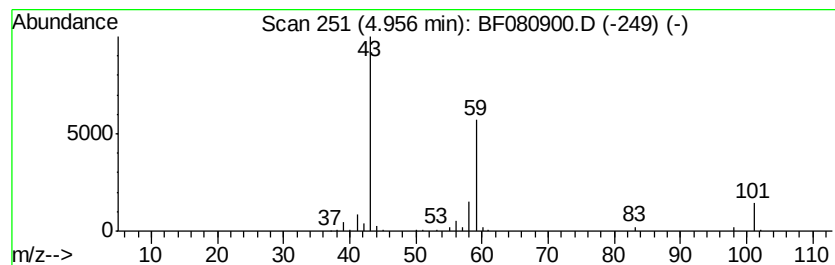
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF080615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.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.
4.96	21.42 ng	378959	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	25



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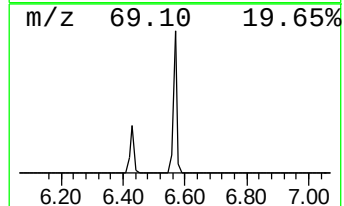
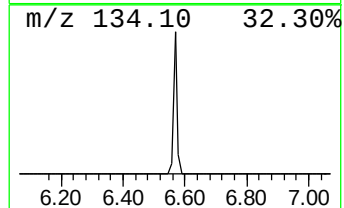
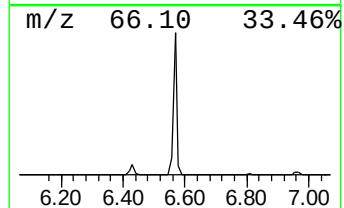
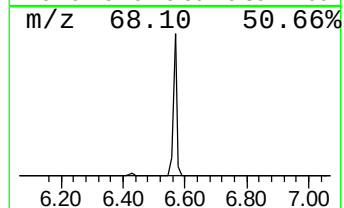
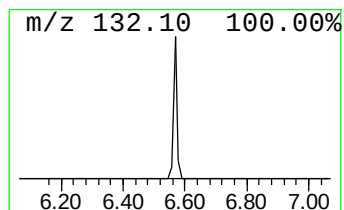
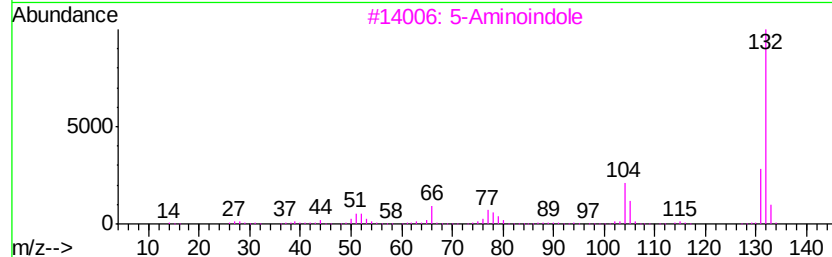
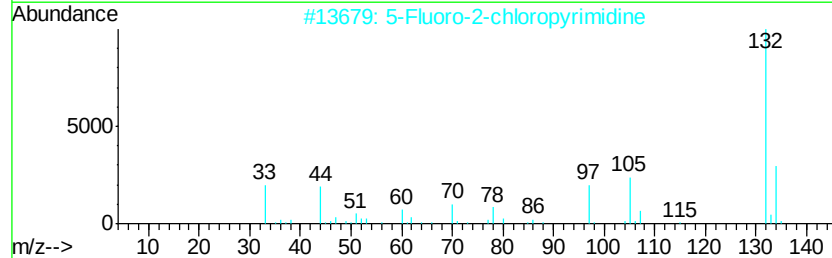
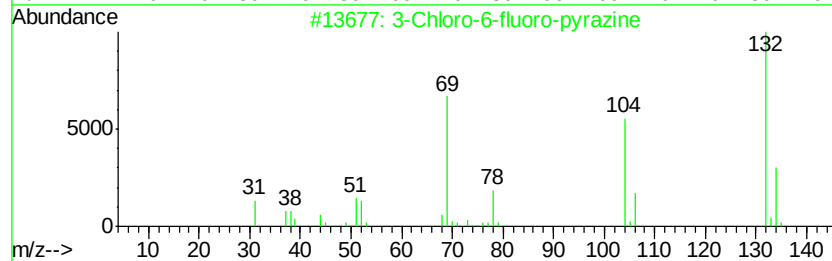
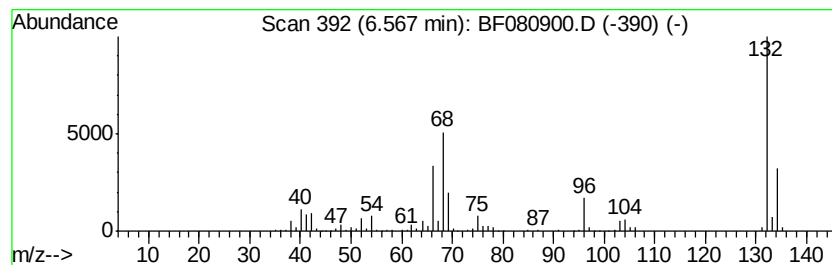
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	44.42 ng	785622	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	27
4		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
5		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10



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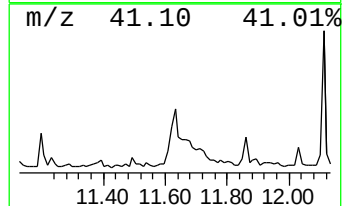
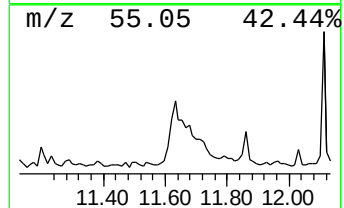
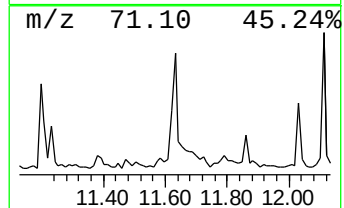
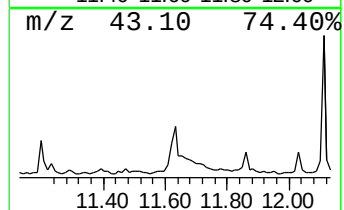
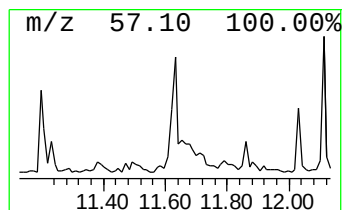
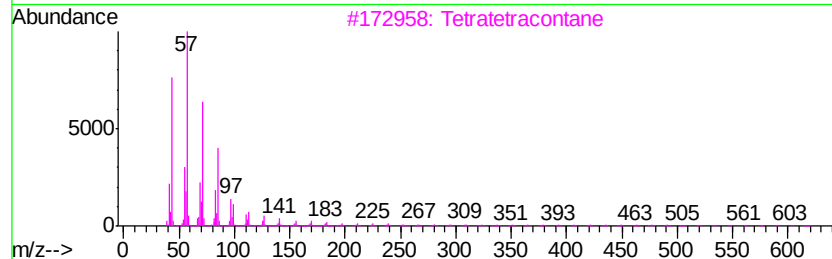
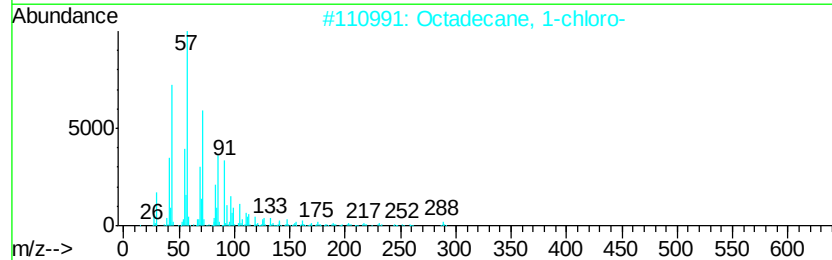
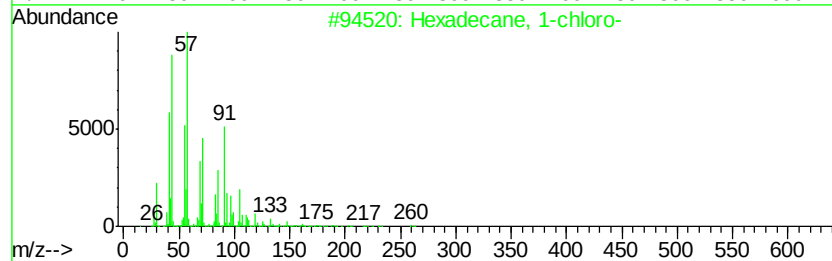
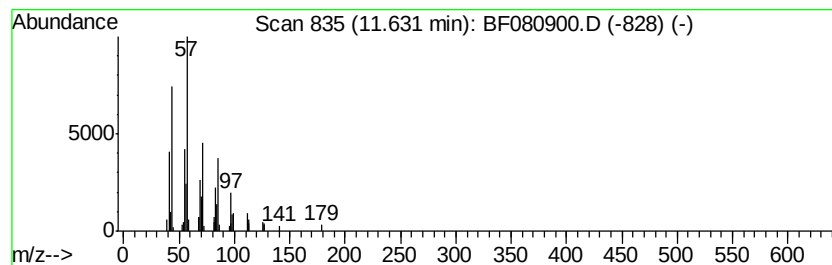
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane, 1-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.63	8.52 ng	234259	Phenanthrene-d10	11.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	90
2	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	80
3	Tetratetracontane	619	C44H90	007098-22-8	72
4	Dodecane	170	C12H26	000112-40-3	52
5	Decane	142	C10H22	000124-18-5	52



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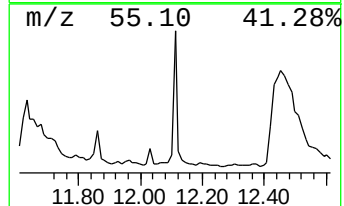
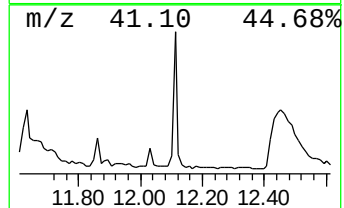
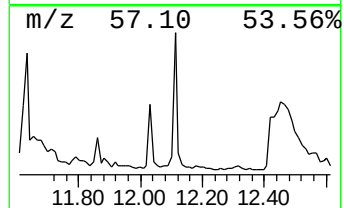
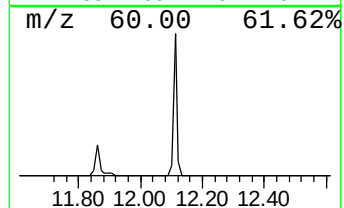
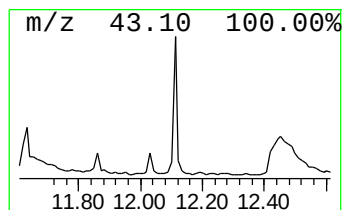
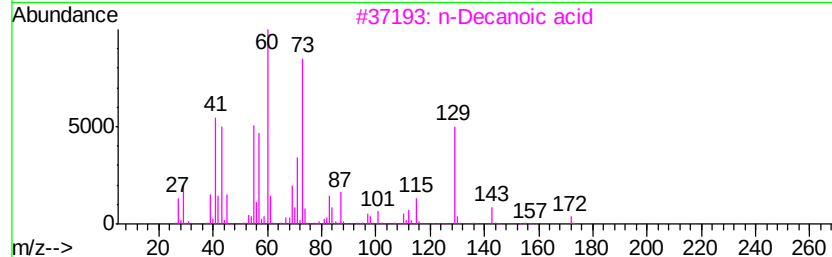
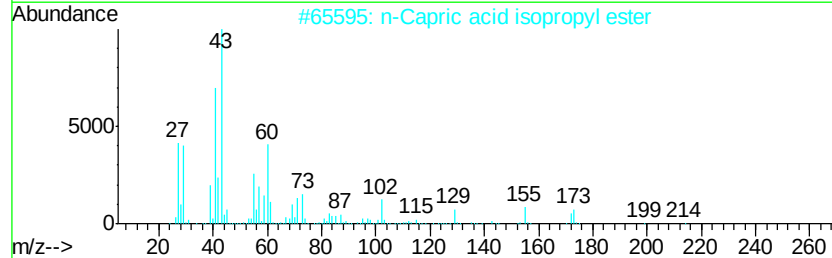
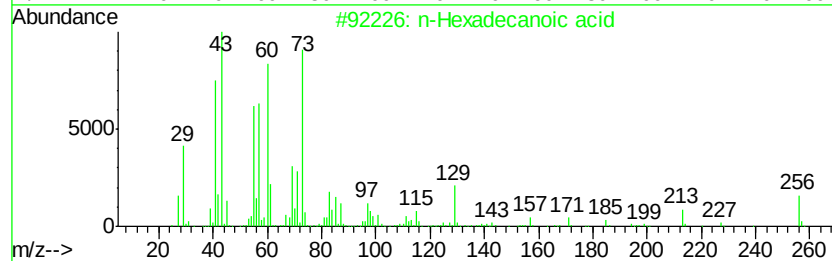
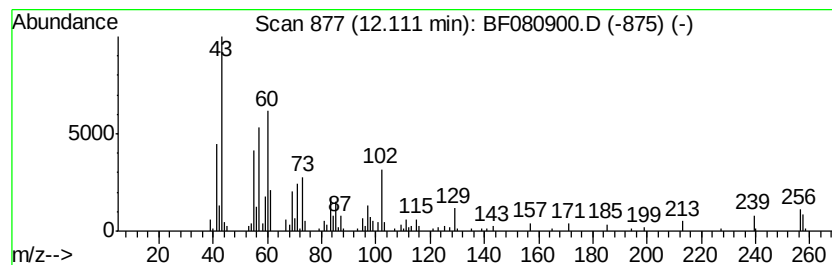
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	6.26 ng	172056	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	38
4	Undecanoic acid	186	C11H22O2	000112-37-8	38
5	Amyl Nitrite	117	C5H11NO2	000110-46-3	22



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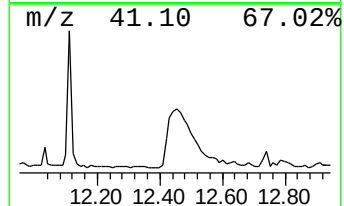
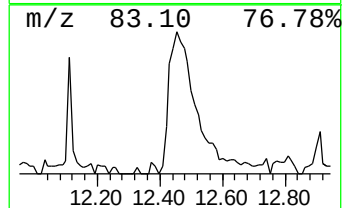
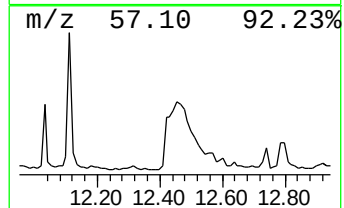
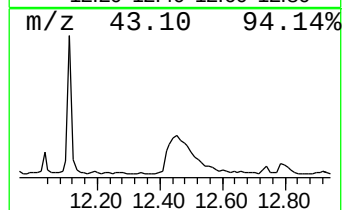
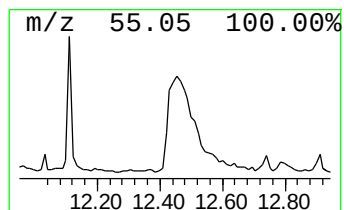
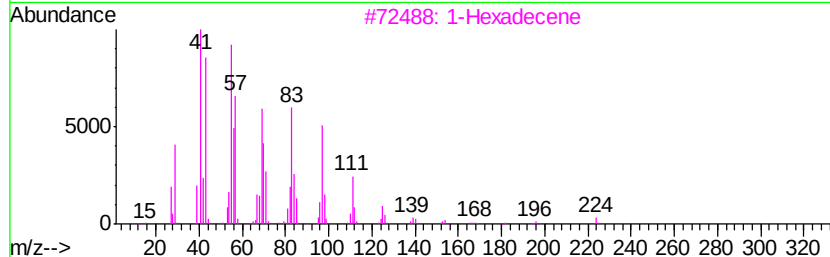
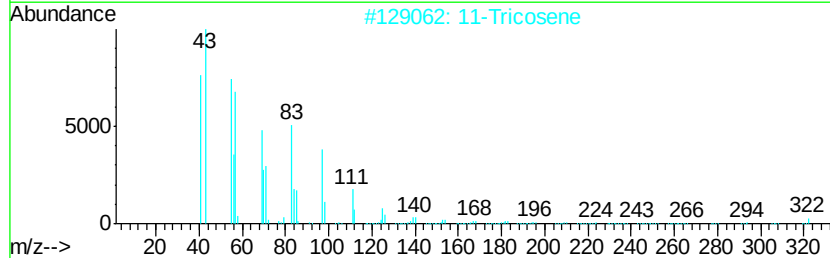
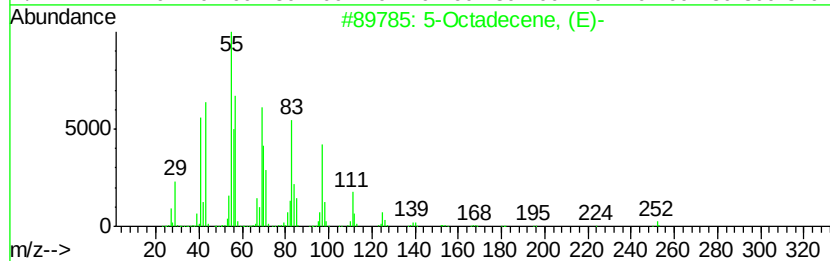
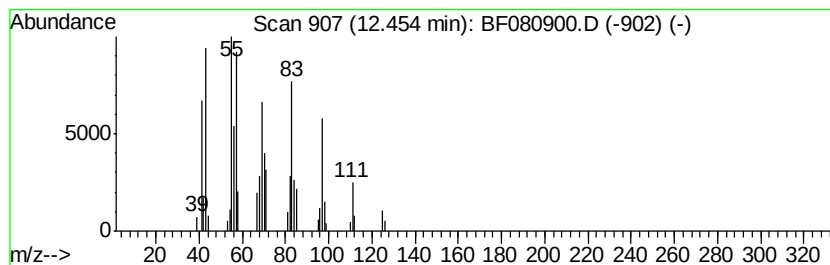
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 5-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.45	15.74 ng	433012	Phenanthrene-d10	11.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2		11-Tricosene	322	C23H46	052078-56-5	91
3		1-Hexadecene	224	C16H32	000629-73-2	91
4		1-Hexadecanol	242	C16H34O	036653-82-4	90
5		9-Octadecene, (E)-	252	C18H36	007206-25-9	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	21.4	ng	378959	1	6.81	353764	20.0
unknown6.57	6.57	44.4	ng	785622	1	6.81	353764	20.0
Hexadecane, 1-chl...	11.63	8.5	ng	234259	4	11.32	550076	20.0
n-Hexadecanoic acid	12.11	6.3	ng	172056	4	11.32	550076	20.0
5-Octadecene, (E)-	12.45	15.7	ng	433012	4	11.32	550076	20.0