

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093614.D
 Acq On : 13 Mar 2017 18:23
 Operator : SJ/MA
 Sample : I2174-24
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-77

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-BF030717.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	2.401	43	45	61	rVB	67348	186672	3.98%	0.466%
2	4.150	195	198	206	rVB	55011	91113	1.94%	0.228%
3	4.401	218	220	228	rBV	38586	83321	1.78%	0.208%
4	4.859	258	260	281	rBV	1045827	1856162	39.61%	4.638%
5	5.316	298	300	326	rBV	2749783	4550778	97.11%	11.371%
6	5.716	332	335	346	rVB	47693	98798	2.11%	0.247%
7	6.367	390	392	400	rBV	3013553	4222430	90.11%	10.551%
8	6.482	400	402	405	rVB	4391355	4316654	92.12%	10.786%
9	6.710	420	422	433	rVB	944799	991889	21.17%	2.478%
10	6.859	433	435	438	rBV	3243892	3365985	71.83%	8.411%
11	7.282	470	472	486	rBV	2710743	3095445	66.06%	7.735%
12	8.002	532	535	546	rVB	1238937	1357642	28.97%	3.392%
13	9.076	627	629	632	rBV	3597018	4686080	100.00%	11.709%
14	9.762	687	689	691	rBV	1101383	1386992	29.60%	3.466%
15	10.551	756	758	761	rBV	2156472	2516011	53.69%	6.287%
16	11.248	817	819	824	rBV	1415354	1348487	28.78%	3.370%
17	12.836	955	958	960	rBV	3933011	4024460	85.88%	10.056%
18	13.899	1049	1051	1057	rVB	621543	843704	18.00%	2.108%
19	15.305	1171	1174	1183	rVB	479681	759436	16.21%	1.898%
20	15.682	1204	1207	1210	rBV	47277	69729	1.49%	0.174%
21	16.128	1243	1246	1253	rVB	49231	90264	1.93%	0.226%
22	16.643	1288	1291	1295	rBV	34309	78085	1.67%	0.195%

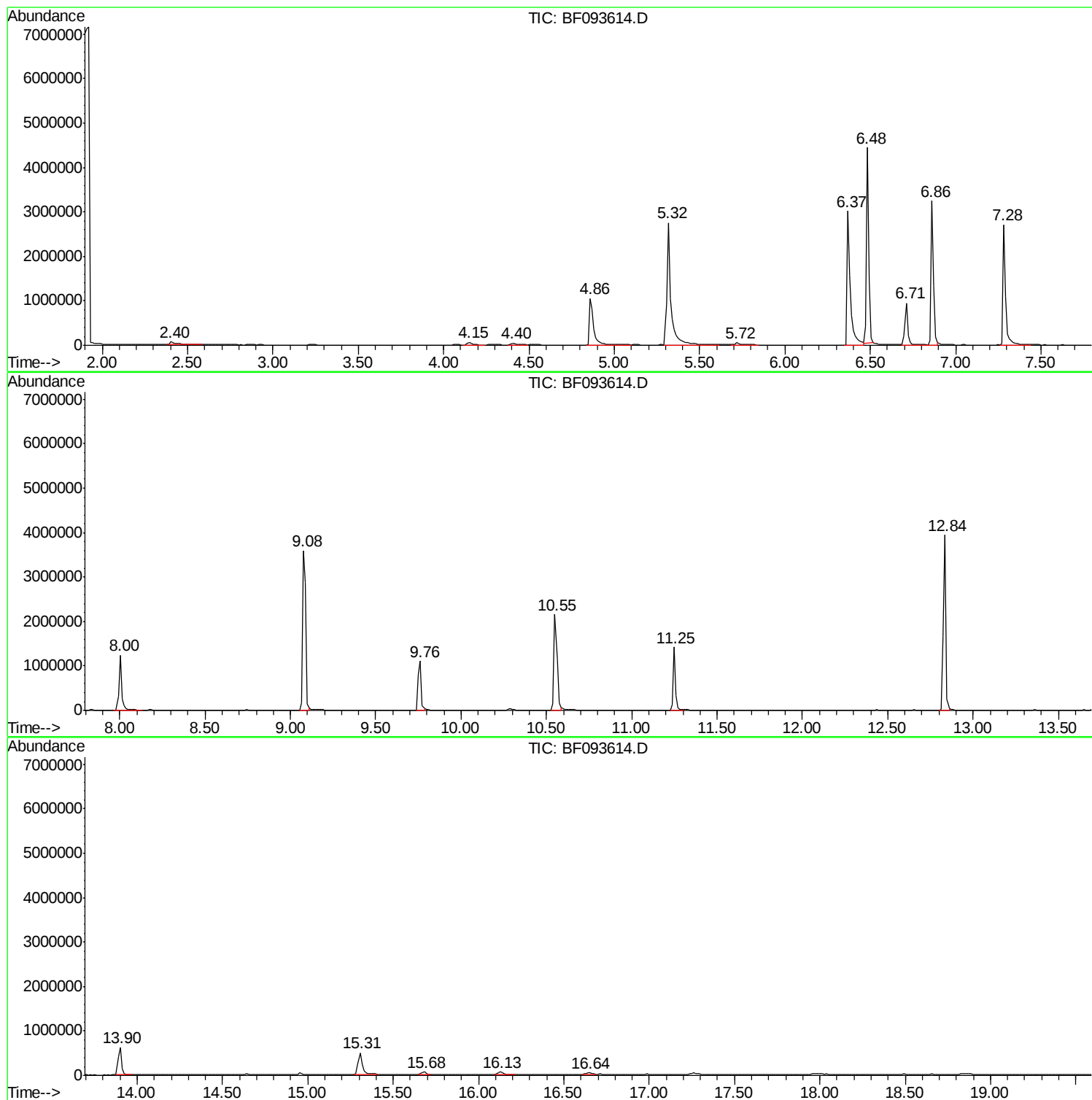
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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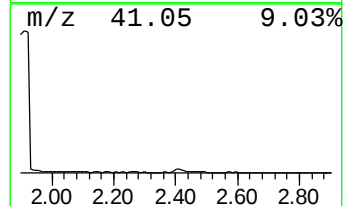
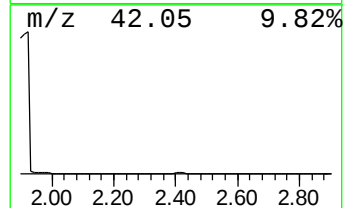
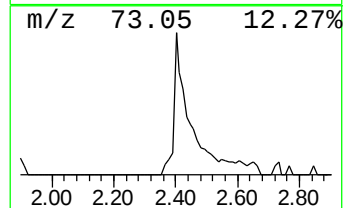
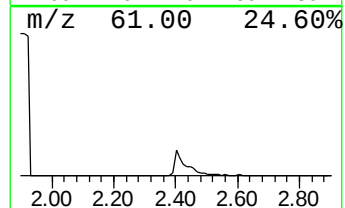
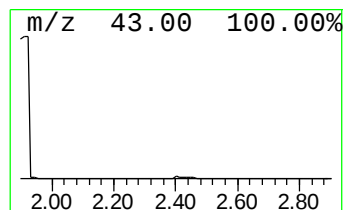
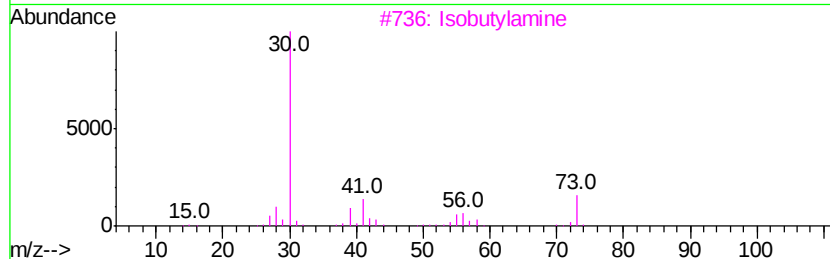
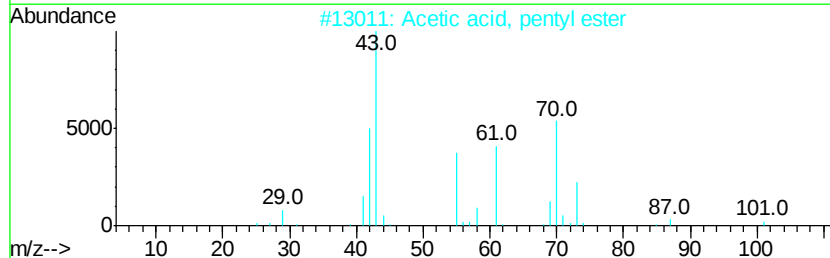
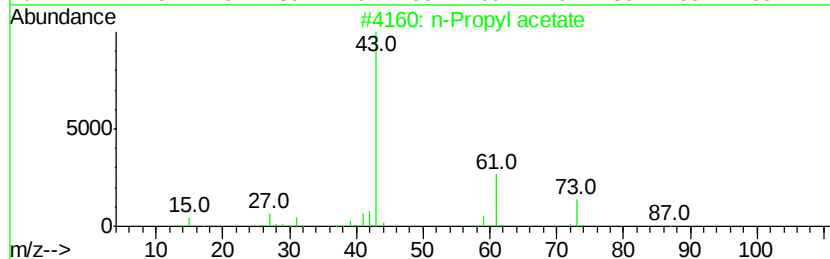
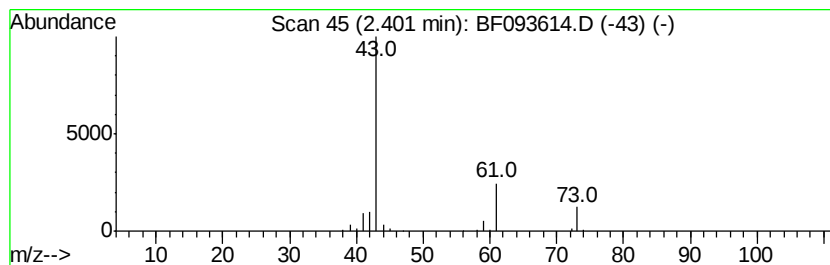
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.40	3.76 ng	186672	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	9
3		Isobutylamine	73	C4H11N	000078-81-9	7
4		Methylglyoxal	72	C3H4O2	000078-98-8	7
5		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7



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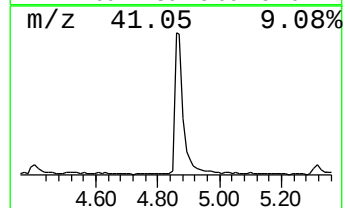
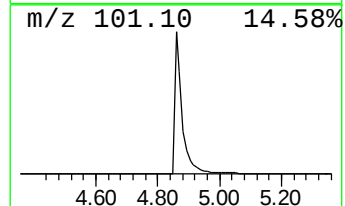
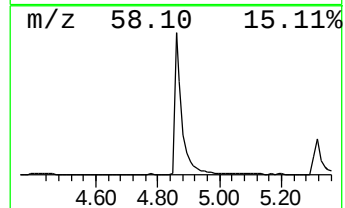
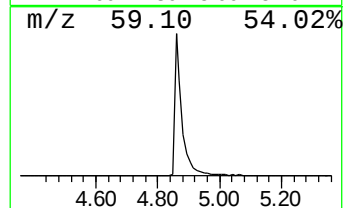
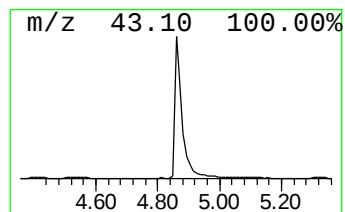
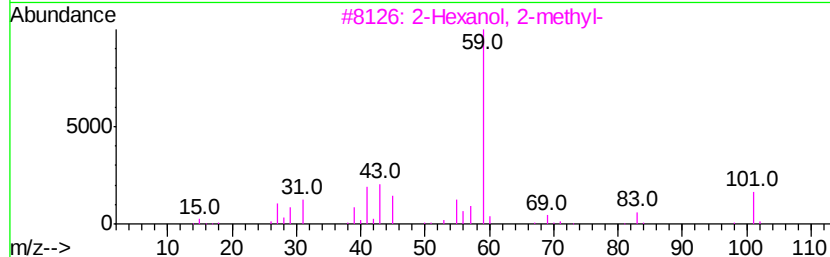
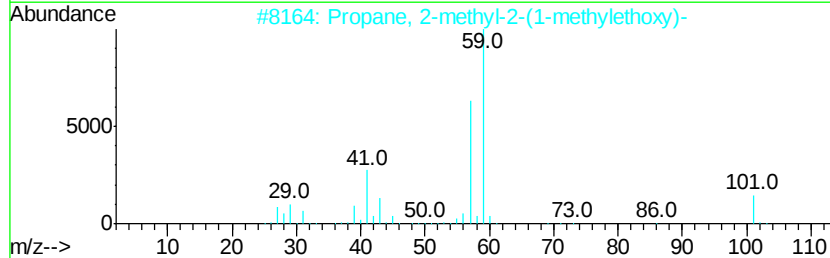
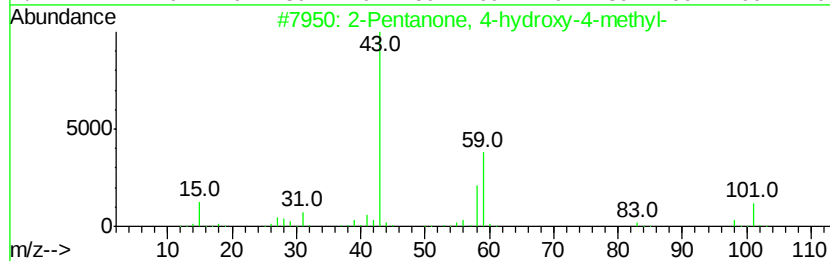
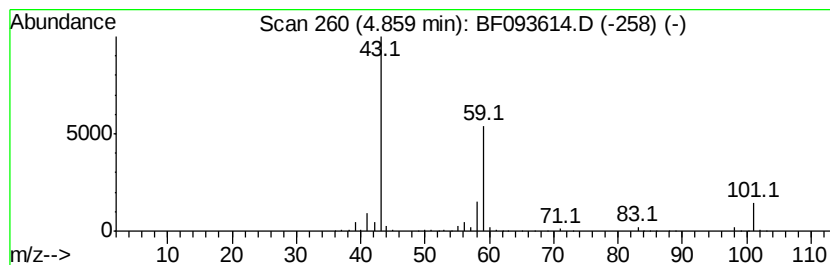
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	37.43 ng	1856160	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
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	32



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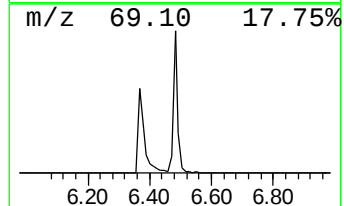
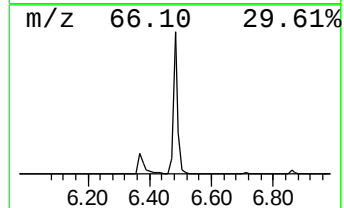
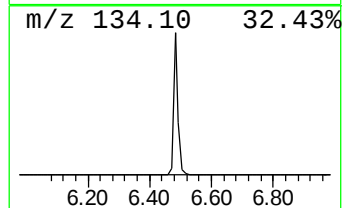
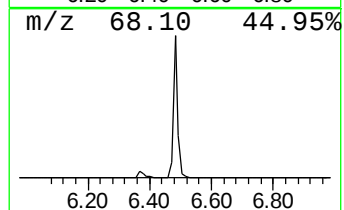
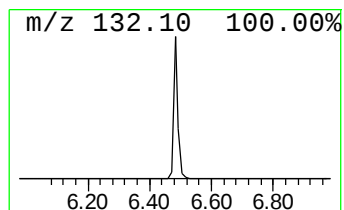
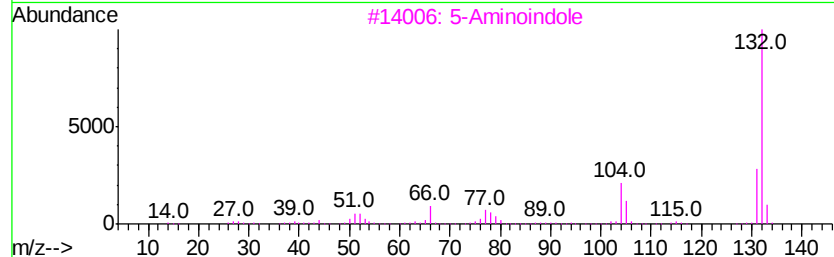
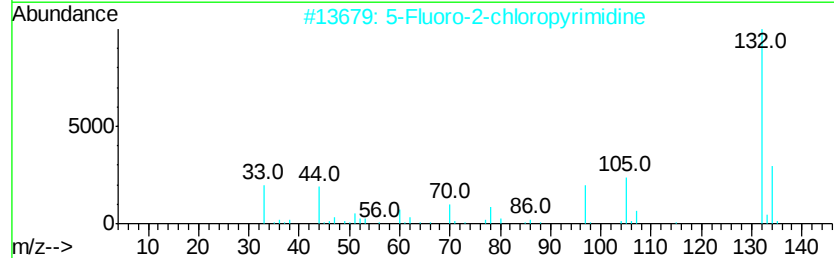
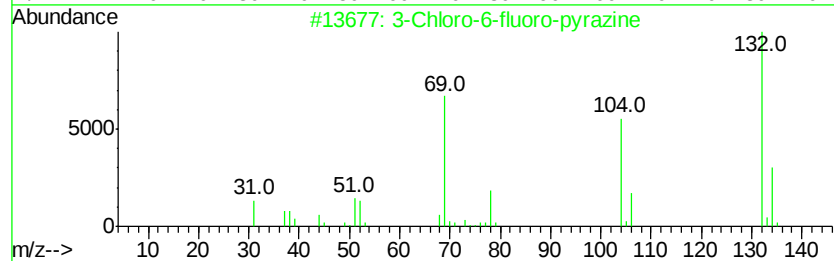
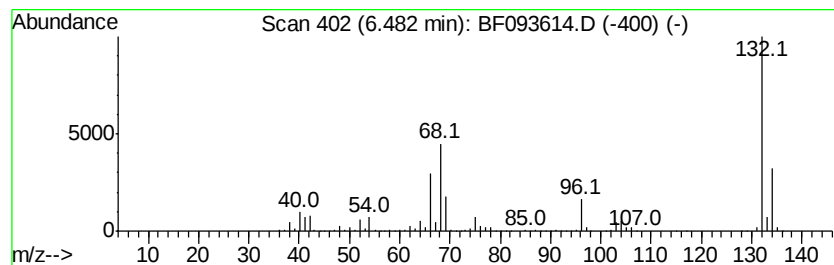
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Peak Number 3 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	87.04 ng	4316650	1,4-Dichlorobenzene-d4	6.71

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	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Xenon	132	Xe	007440-63-3	9



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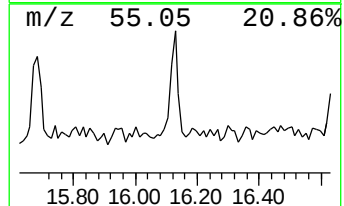
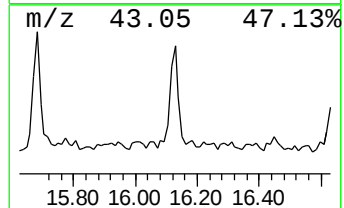
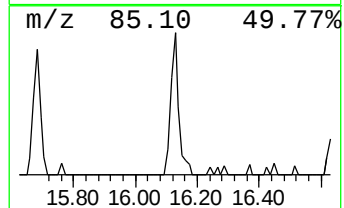
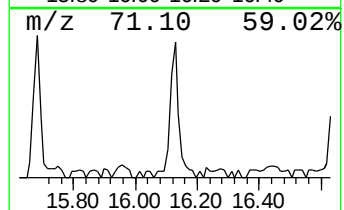
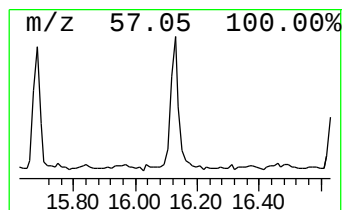
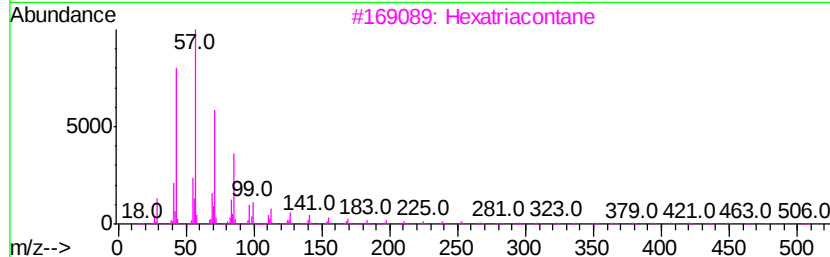
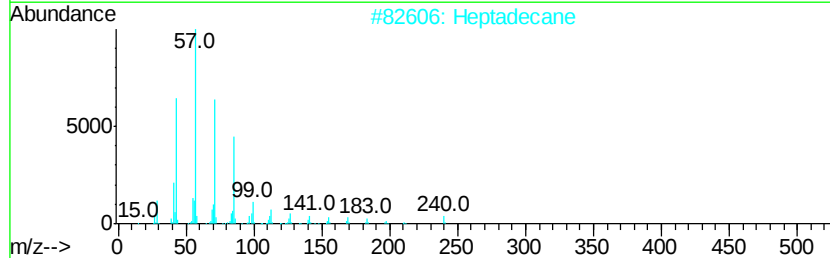
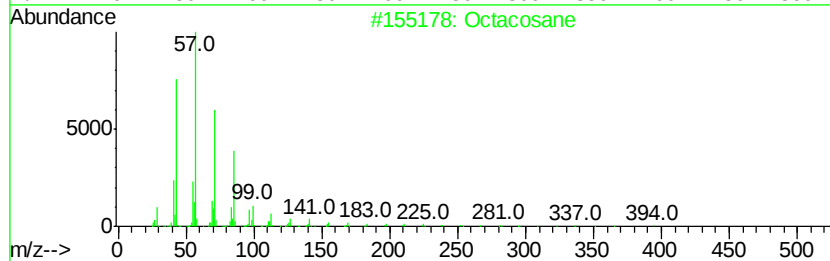
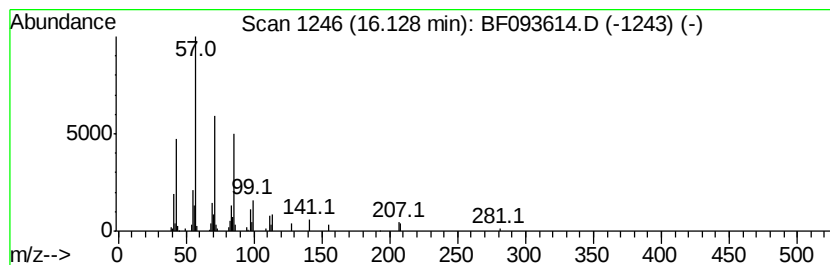
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Octacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	2.38 ng	90264	Perylene-d12	15.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	87
2	Heptadecane		240	C17H36	000629-78-7	80
3	Hexatriacontane		507	C36H74	000630-06-8	80
4	Nonadecane		268	C19H40	000629-92-5	80
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	80



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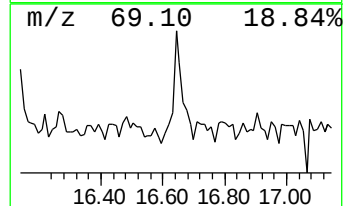
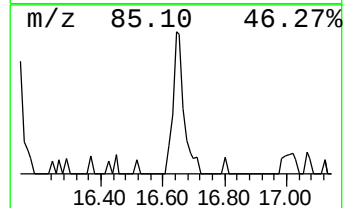
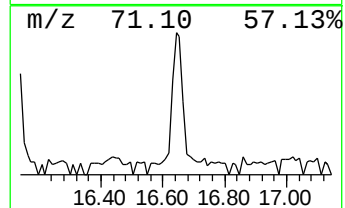
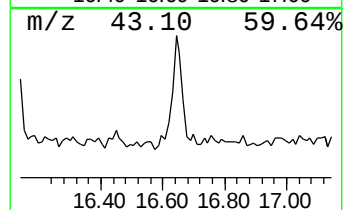
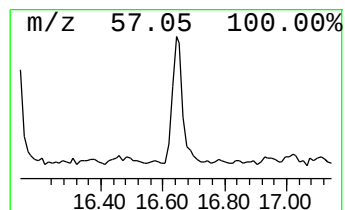
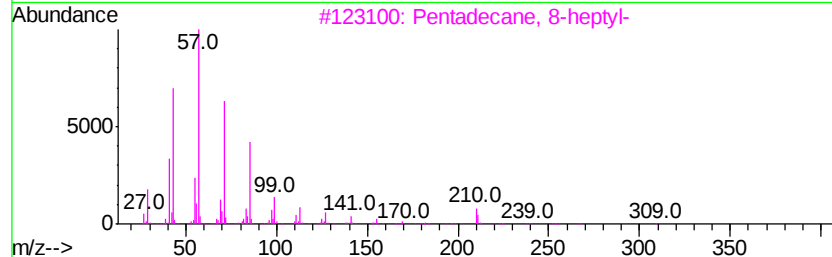
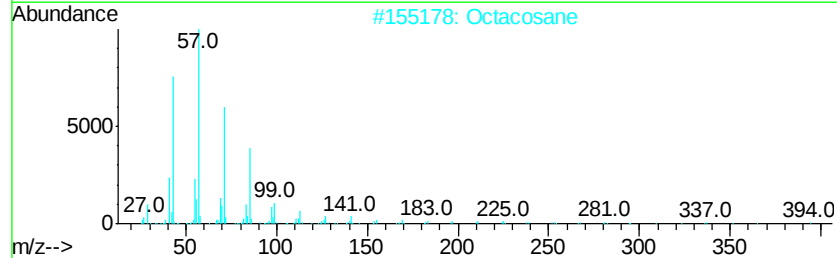
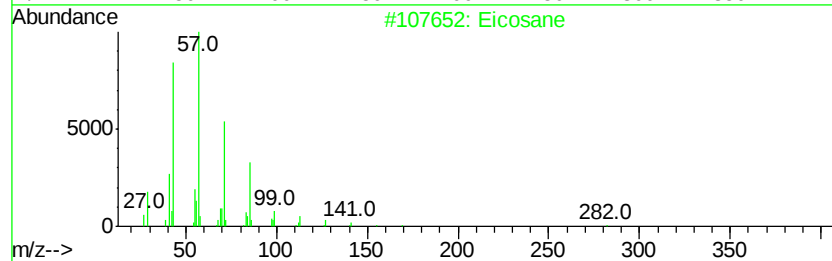
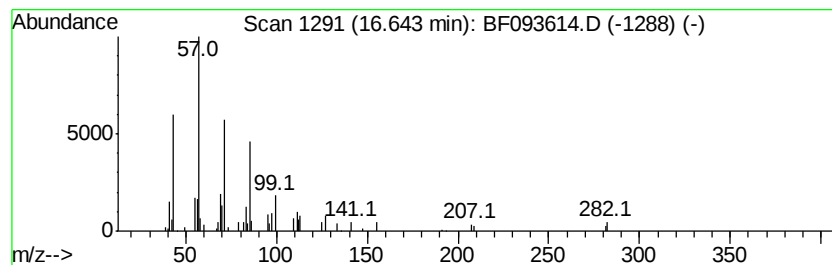
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	2.06 ng	78085	Perylene-d12	15.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	91
2	Octacosane		394	C28H58	000630-02-4	80
3	Pentadecane, 8-heptyl-		310	C22H46	071005-15-7	72
4	Tetracosane		338	C24H50	000646-31-1	72
5	Heptadecane		240	C17H36	000629-78-7	72



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.40	3.8	ng	186672	1	6.71	991889	20.0
2-Pentanone, 4-hy...	4.86	37.4	ng	1856160	1	6.71	991889	20.0
unknown6.48	6.48	87.0	ng	4316650	1	6.71	991889	20.0
Octacosane	16.13	2.4	ng	90264	6	15.31	759436	20.0
Eicosane	16.64	2.1	ng	78085	6	15.31	759436	20.0