

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121416\
 Data File : BF091590.D
 Acq On : 14 Dec 2016 18:01
 Operator : UM/SJ
 Sample : H5974-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-16R

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-BF120916.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	4.956	248	251	253	rBV	813887	1013692	13.20%	1.906%
2	5.390	286	289	291	rBV	3568900	3231680	42.07%	6.077%
3	6.430	378	380	382	rBV	2701582	2381372	31.00%	4.478%
4	6.556	389	391	394	rBV	3947816	5138362	66.90%	9.662%
5	6.796	409	412	414	rBV	1483733	1601587	20.85%	3.012%
6	6.944	423	425	428	rVB	3733456	4420352	57.55%	8.312%
7	7.356	458	461	463	rBV	4092600	3921533	51.05%	7.374%
8	8.076	522	524	527	rBV	2420353	2106392	27.42%	3.961%
9	9.162	616	619	621	rBV	7108248	7681104	100.00%	14.444%
10	9.745	668	670	675	rVB2	37376	92507	1.20%	0.174%
11	9.836	675	678	680	rBV	1801747	2361807	30.75%	4.441%
12	10.270	713	716	718	rBV	113070	122449	1.59%	0.230%
13	10.613	744	746	749	rBV2	3493887	4634397	60.34%	8.715%
14	10.739	756	757	762	rVB	114062	164737	2.14%	0.310%
15	11.185	794	796	802	rVB2	78435	140351	1.83%	0.264%
16	11.311	805	807	809	rVV	2787672	2359616	30.72%	4.437%
17	11.848	852	854	858	rBV2	208158	252483	3.29%	0.475%
18	12.636	921	923	925	rBV	122674	143247	1.86%	0.269%
19	12.728	929	931	934	rVB	386970	354965	4.62%	0.667%
20	12.899	943	946	949	rBV	7138692	7051888	91.81%	13.260%
21	13.437	991	993	994	rBV	211820	216846	2.82%	0.408%
22	13.471	994	996	1001	rVB4	57097	109621	1.43%	0.206%
23	13.802	1022	1025	1029	rBV3	104037	197268	2.57%	0.371%
24	13.939	1035	1037	1040	rBV	2152748	2001106	26.05%	3.763%
25	15.345	1157	1160	1163	rBV	1013691	1480639	19.28%	2.784%

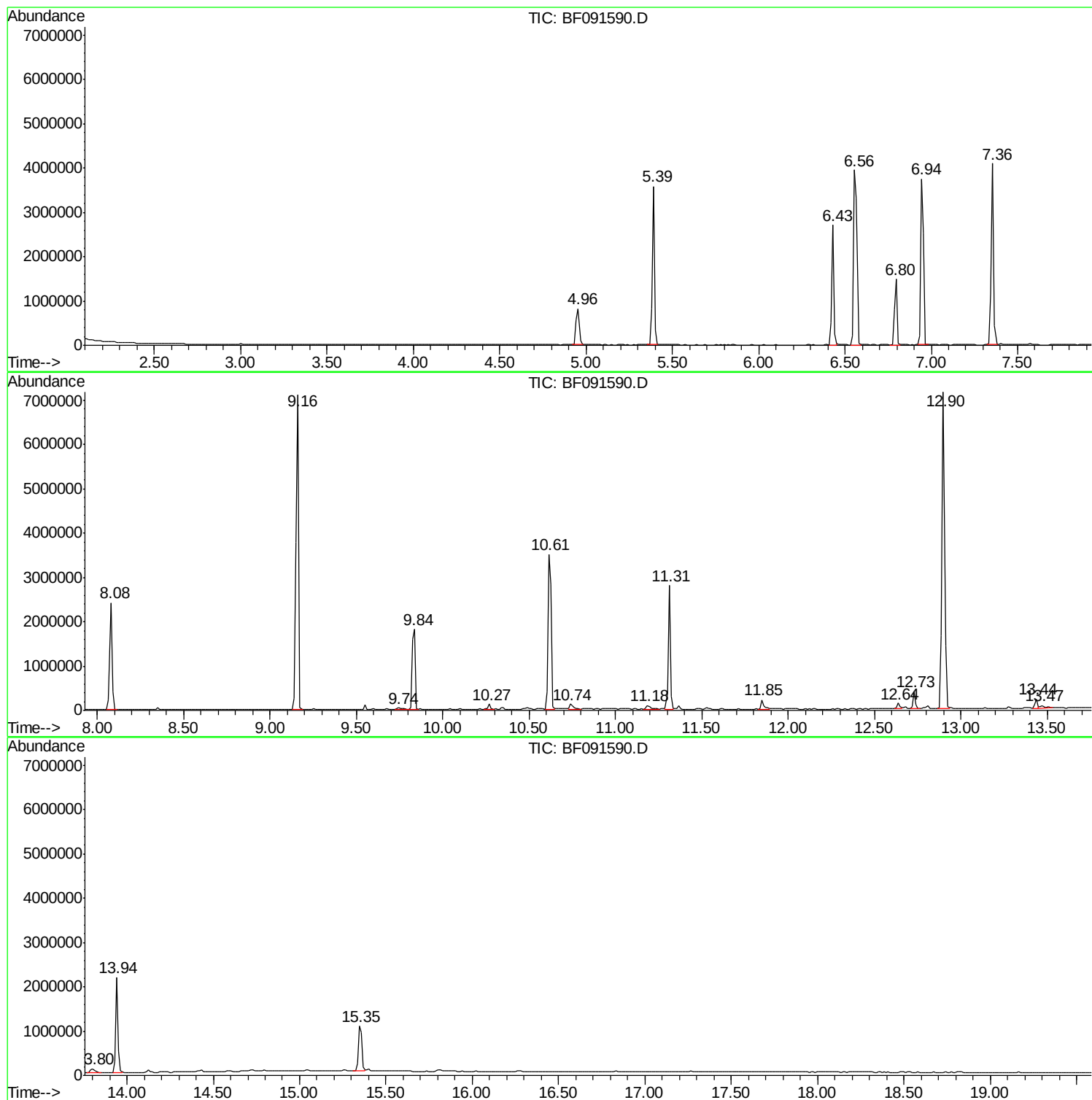
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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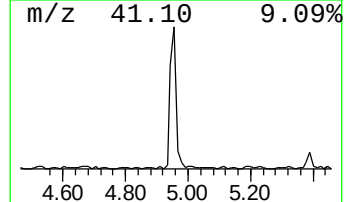
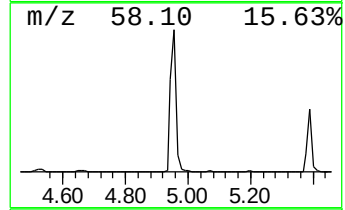
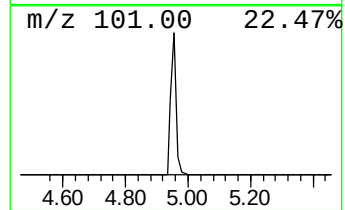
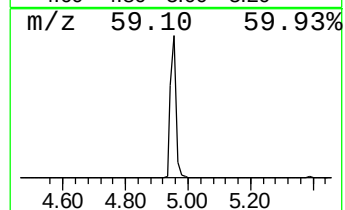
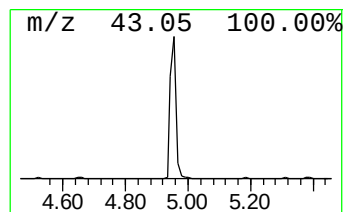
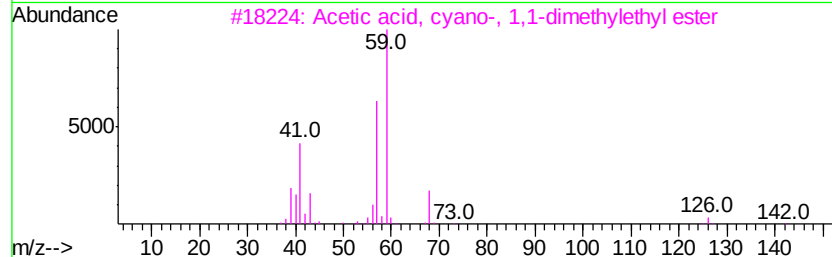
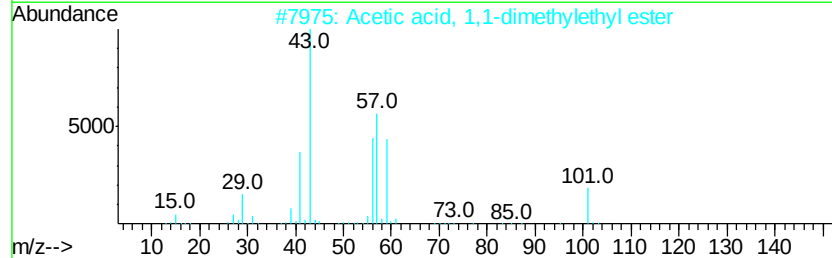
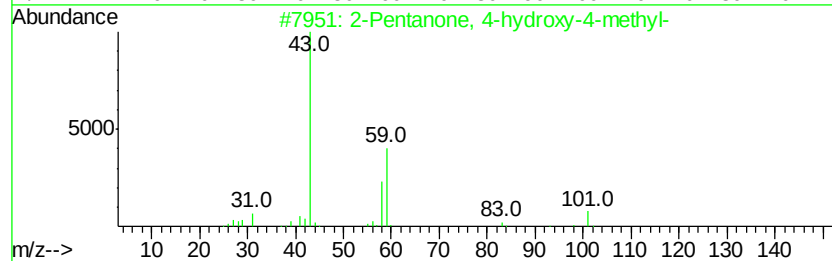
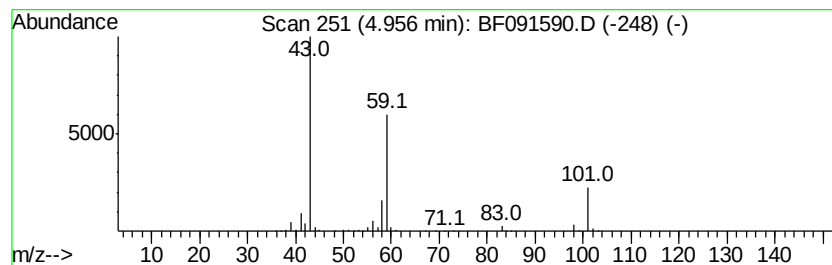
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	12.66 ng	1013690	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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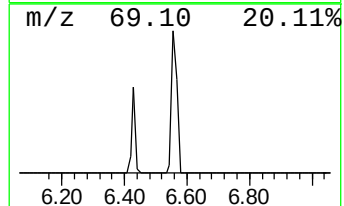
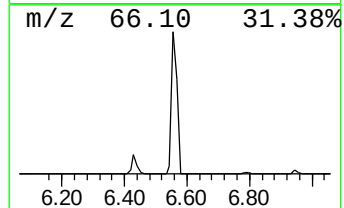
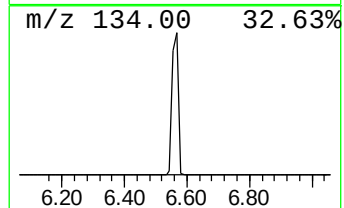
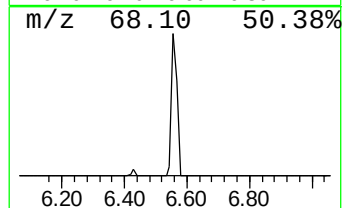
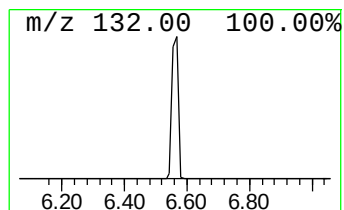
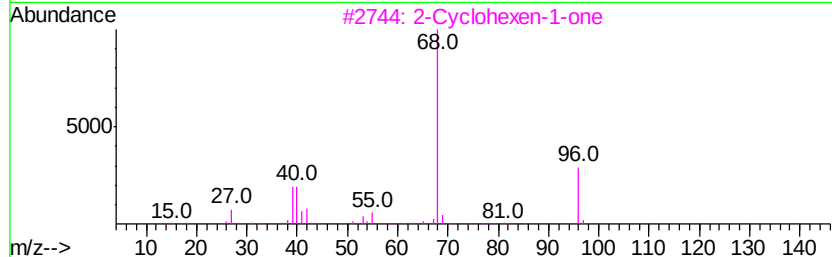
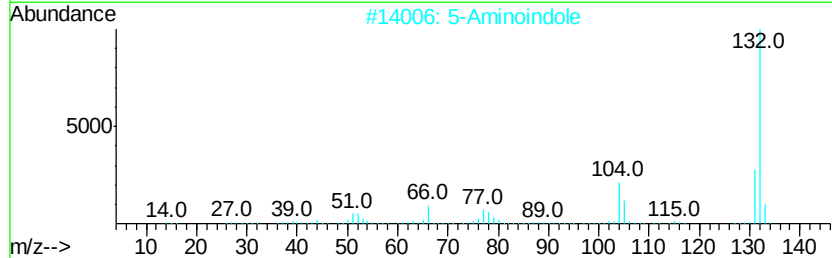
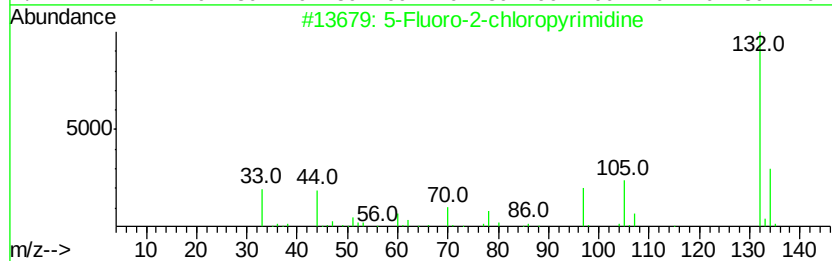
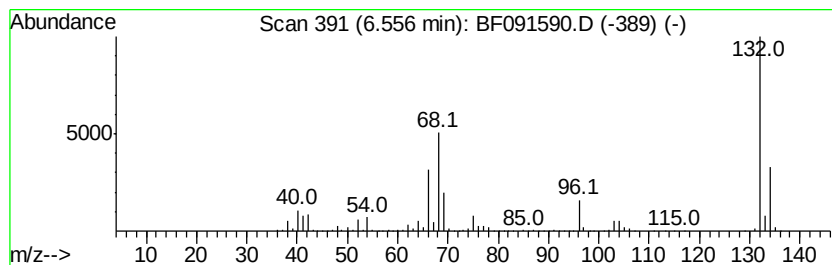
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Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	64.17 ng	5138360	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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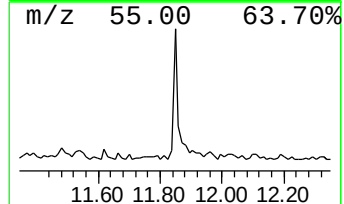
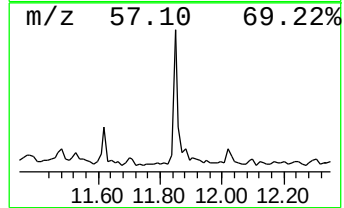
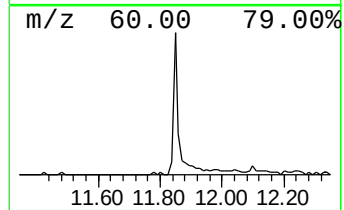
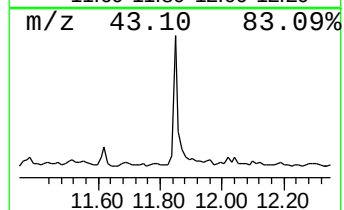
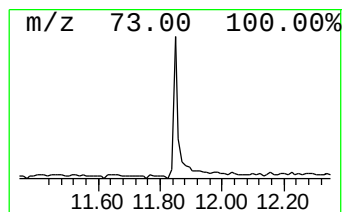
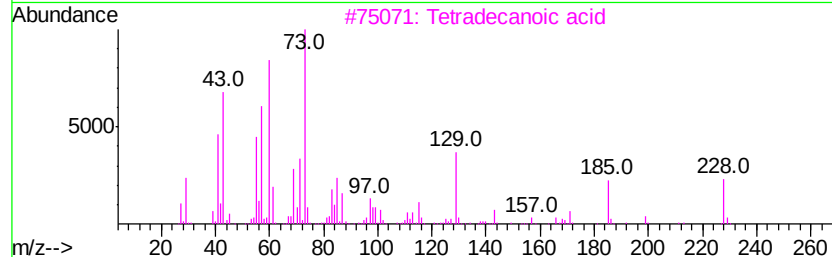
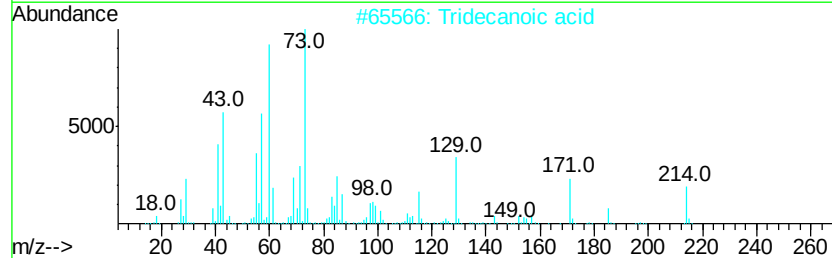
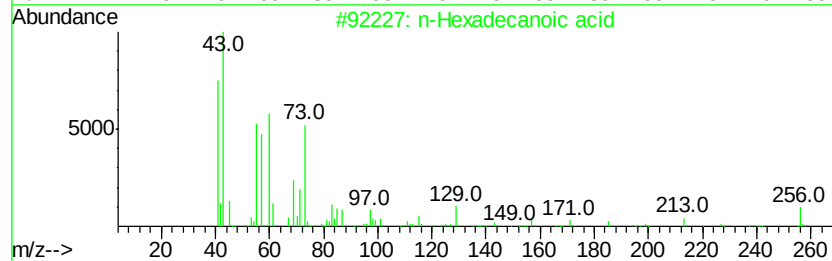
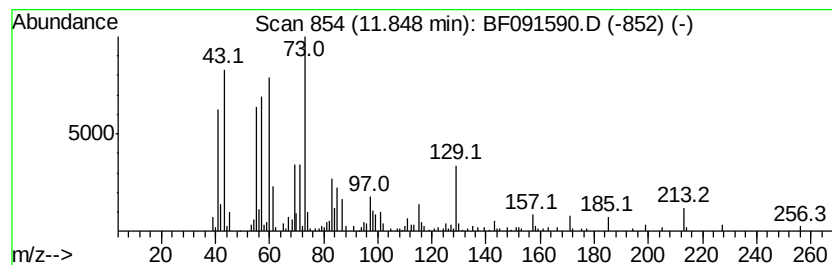
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.85	2.14 ng	252483	Phenanthrene-d10		11.31
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	72



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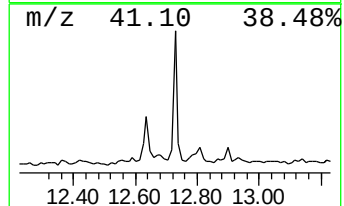
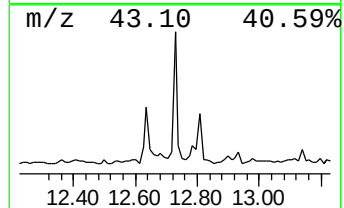
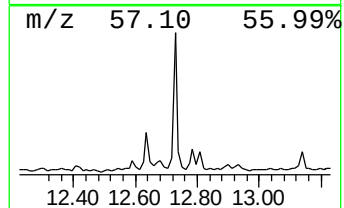
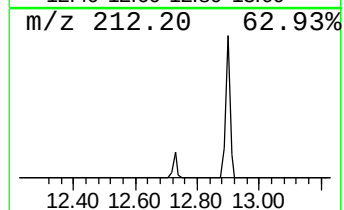
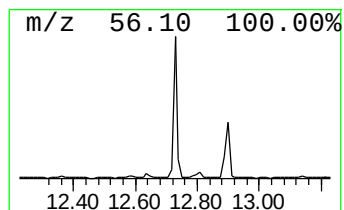
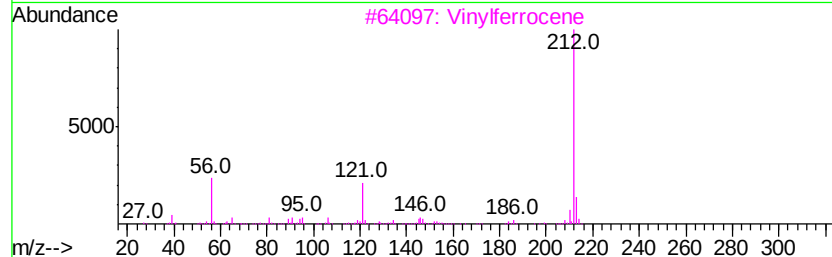
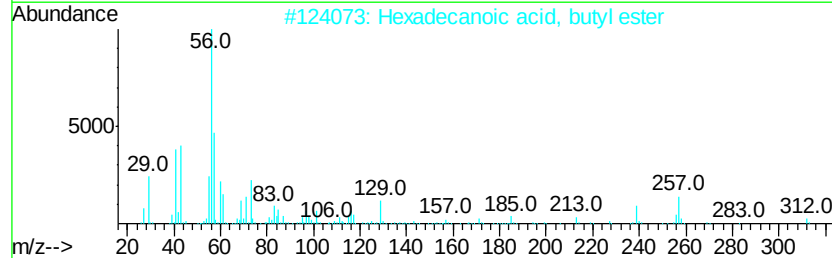
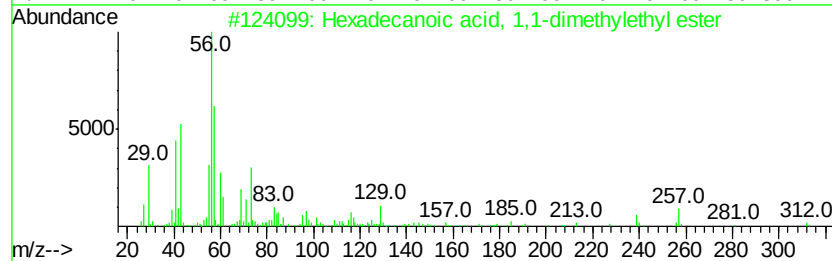
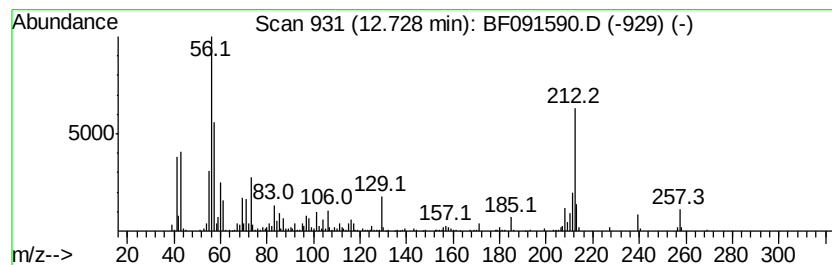
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	3.55 ng	354965	Chrysene-d12	13.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	55
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	49
3		Vinylferrocene	212	C12H12Fe	001271-51-8	46
4		Benzene, 1-chloro-3-(phenylethyn...	212	C14H9Cl	051624-34-1	35
5		1,2-Dihydroacenaphthylen-1,2-dio...	212	C12H8N2O2	001932-08-7	25



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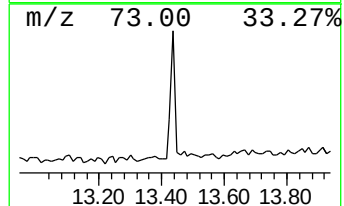
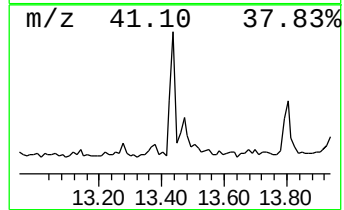
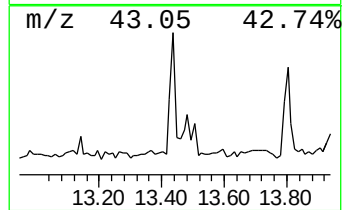
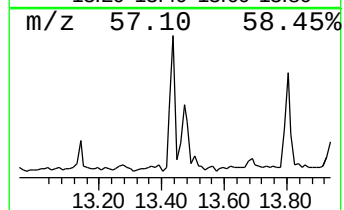
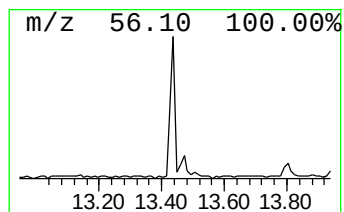
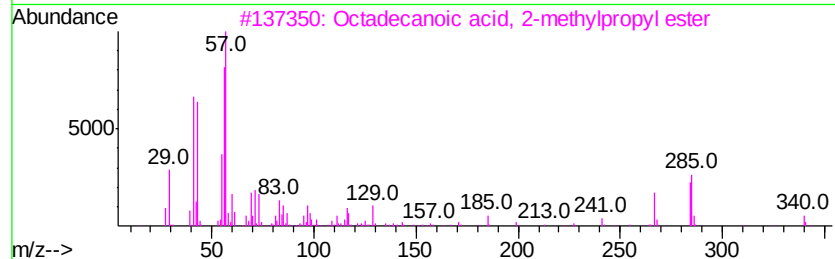
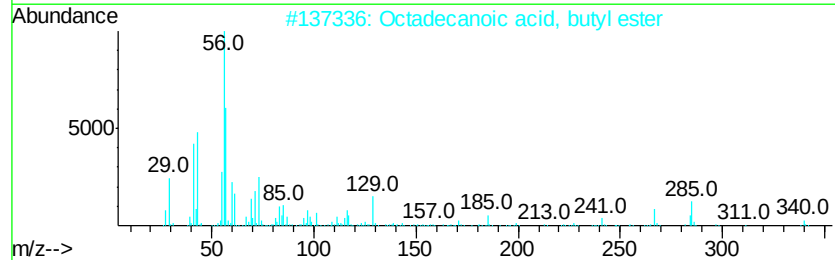
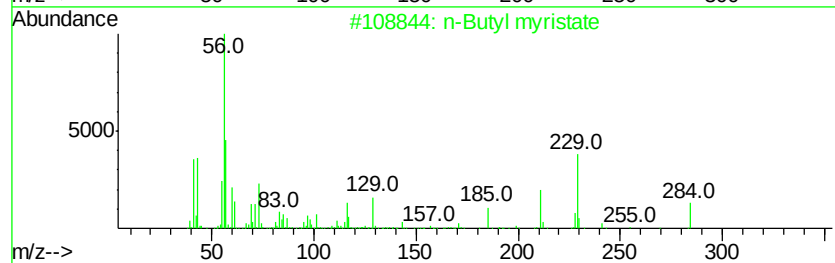
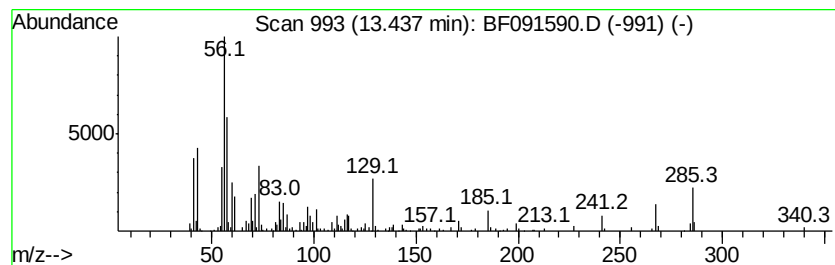
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Peak Number 6 n-Butyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.44	2.17 ng	216846	Chrysene-d12	13.94	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl myristate	284	C18H36O2	000110-36-1	64
2	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	55
3	Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	32
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.96	12.7	ng	1013690	1	6.80	1601590	20.0
unknown6.56	6.56	64.2	ng	5138360	1	6.80	1601590	20.0
n-Hexadecanoic acid	11.85	2.1	ng	252483	4	11.31	2359620	20.0
Hexadecanoic acid...	12.73	3.5	ng	354965	5	13.94	2001110	20.0
n-Butyl myristate	13.44	2.2	ng	216846	5	13.94	2001110	20.0