

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011217\
 Data File : BF092233.D
 Acq On : 13 Jan 2017 4:18
 Operator : UM/SJ
 Sample : I1131-05
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SW-002

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-BF122116.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	3.990	182	184	190	rBV	29211	58618	1.17%	0.127%
2	4.733	245	249	261	rBV	1277062	2402221	47.82%	5.189%
3	5.190	287	289	292	rBV	3187251	4597918	91.53%	9.932%
4	6.264	380	383	390	rBV	4473604	5023138	100.00%	10.850%
5	6.367	390	392	395	rVV	4706834	4837600	96.31%	10.449%
6	6.596	410	412	414	rBV	1004841	995869	19.83%	2.151%
7	6.756	423	426	428	rBV	3334702	4406506	87.72%	9.518%
8	7.167	459	462	464	rBV	3200475	3264950	65.00%	7.052%
9	7.304	472	474	480	rBV	48675	64626	1.29%	0.140%
10	7.876	522	524	527	rBV	1332671	1568032	31.22%	3.387%
11	8.962	616	619	621	rBV	5120945	4971655	98.98%	10.739%
12	9.362	651	654	656	rBV	1013362	859467	17.11%	1.856%
13	9.625	675	677	679	rBV	1269244	1312421	26.13%	2.835%
14	10.082	711	717	718	rBV3	59074	104641	2.08%	0.226%
15	10.413	744	746	749	rBV2	2037752	2878181	57.30%	6.217%
16	10.550	756	758	761	rBV	100417	125125	2.49%	0.270%
17	10.996	795	797	798	rBV2	66512	68216	1.36%	0.147%
18	11.099	804	806	811	rBV2	870099	1323807	26.35%	2.859%
19	11.179	811	813	815	rVB	70107	64776	1.29%	0.140%
20	11.351	825	828	832	rBV2	35877	77332	1.54%	0.167%
21	11.659	852	855	858	rBV2	175198	202274	4.03%	0.437%
22	11.716	858	860	866	rVB2	46151	67166	1.34%	0.145%
23	12.311	910	912	914	rBV	321599	281914	5.61%	0.609%
24	12.539	929	932	934	rBV2	249637	354761	7.06%	0.766%
25	12.688	943	945	948	rVB	2679254	3395242	67.59%	7.334%
26	13.236	990	993	994	rBV	56136	62285	1.24%	0.135%
27	13.602	1022	1025	1033	rBV2	175108	307991	6.13%	0.665%
28	13.728	1033	1036	1040	rBV	836606	1083639	21.57%	2.341%
29	14.585	1108	1111	1113	rVB	83437	93950	1.87%	0.203%
30	14.722	1121	1123	1128	rBV	104366	208481	4.15%	0.450%
31	14.814	1128	1131	1133	rBV2	33484	54787	1.09%	0.118%
32	14.985	1144	1146	1148	rBV	60359	65643	1.31%	0.142%
33	15.042	1148	1151	1153	rBV	73995	97525	1.94%	0.211%
34	15.088	1153	1155	1158	rBV	697805	878329	17.49%	1.897%

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ALS Vial : 28 Sample Multiplier: 1

Instrument :
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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

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35	15.568	1193	1197	1199	rBV4	30083	72030	1.43%	0.156%
36	16.334	1261	1264	1268	rBV	36180	64453	1.28%	0.139%

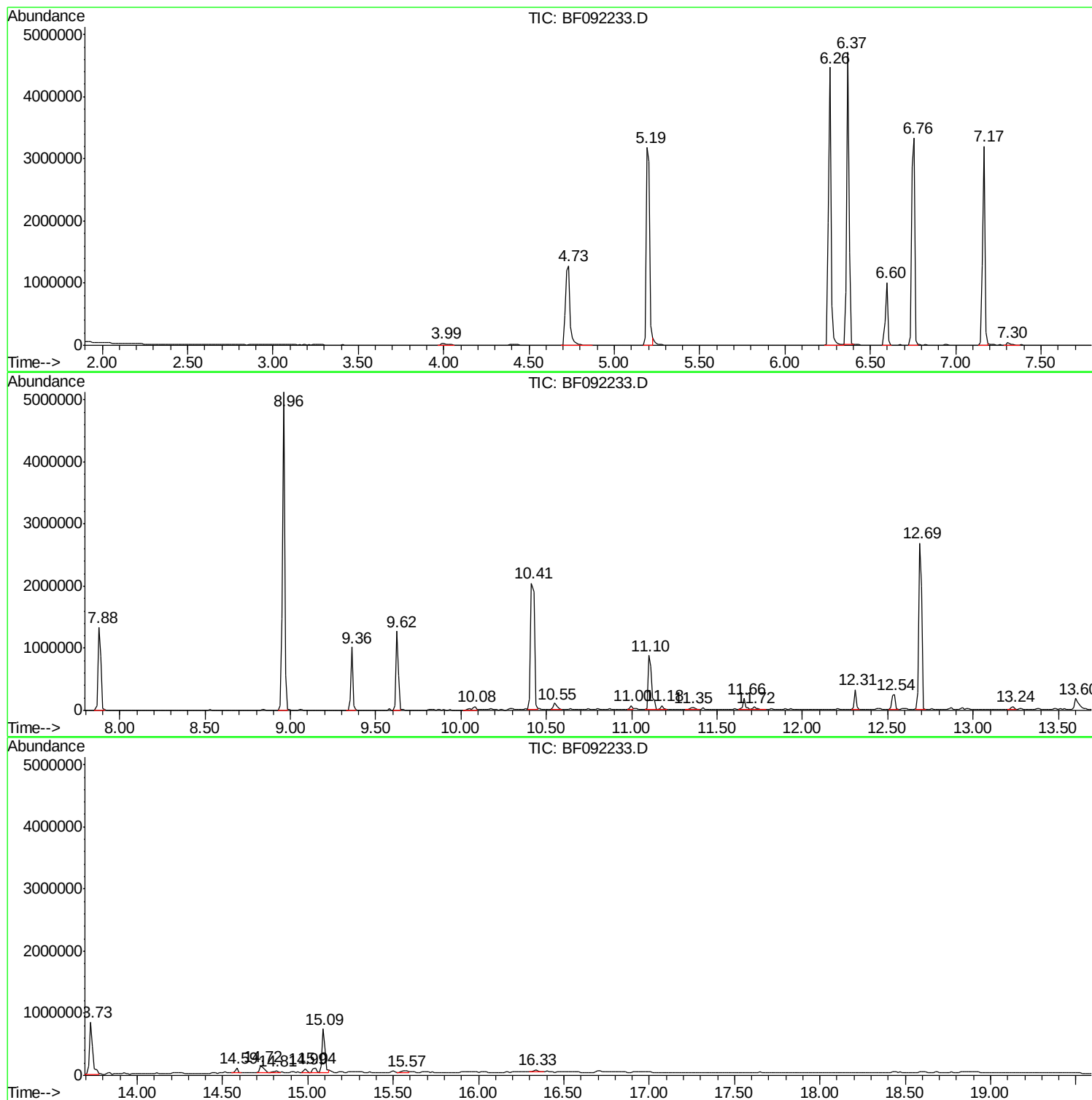
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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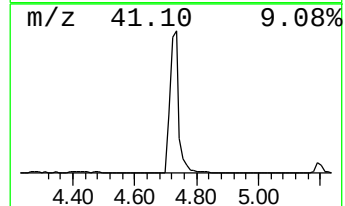
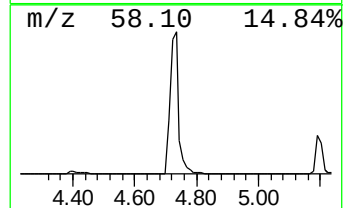
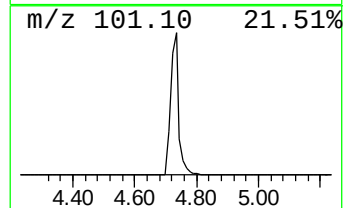
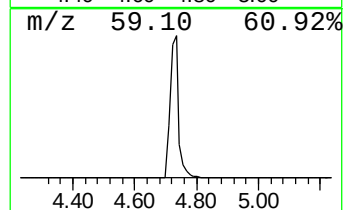
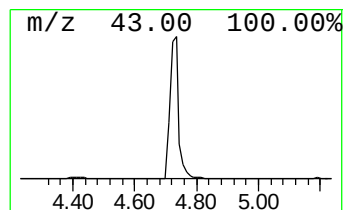
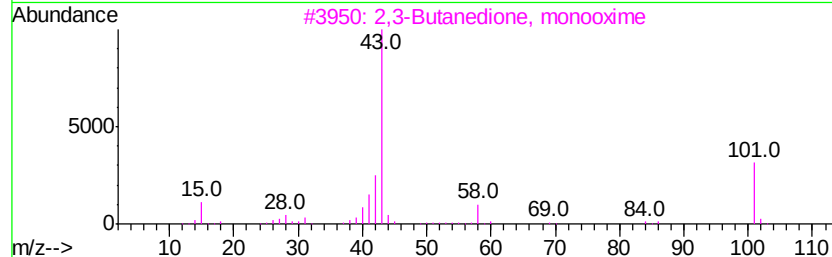
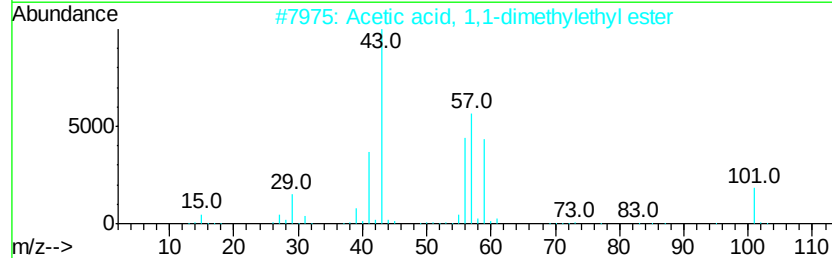
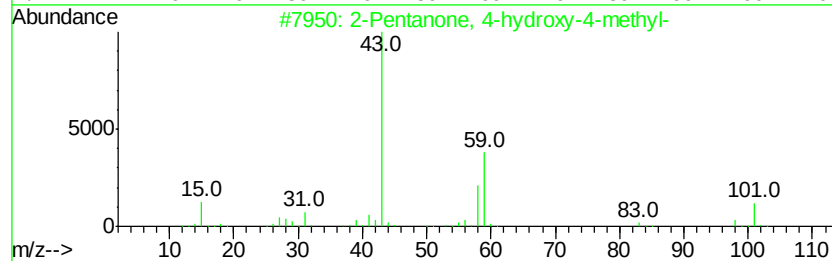
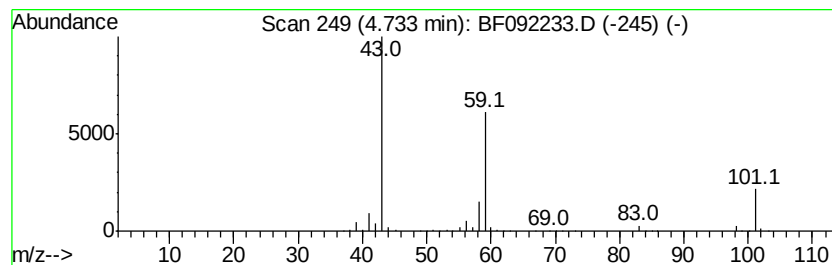
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	48.24 ng	2402220	1,4-Dichlorobenzene-d4	6.60

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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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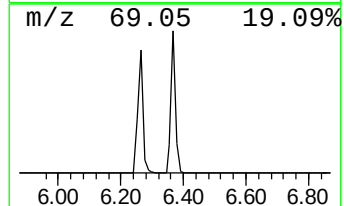
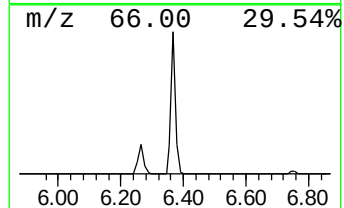
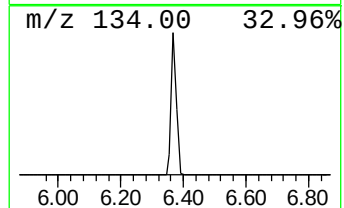
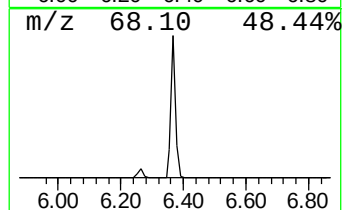
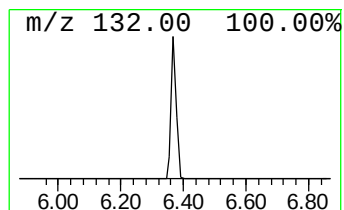
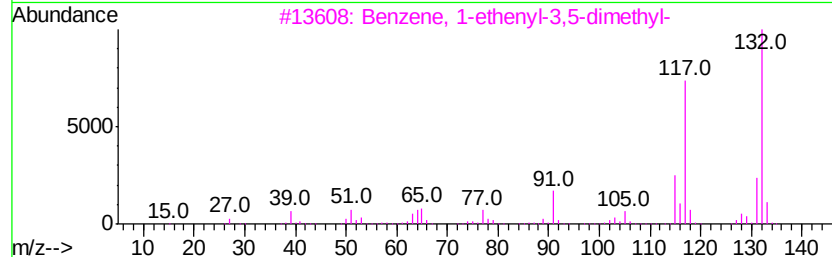
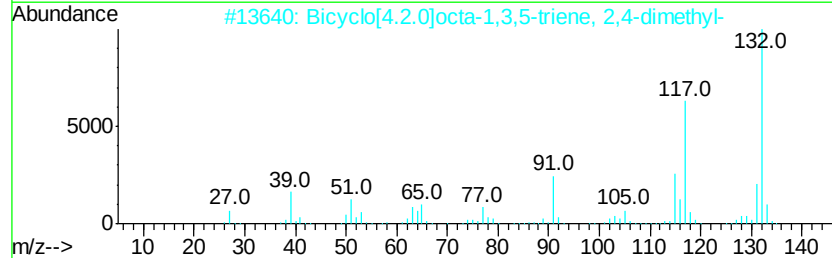
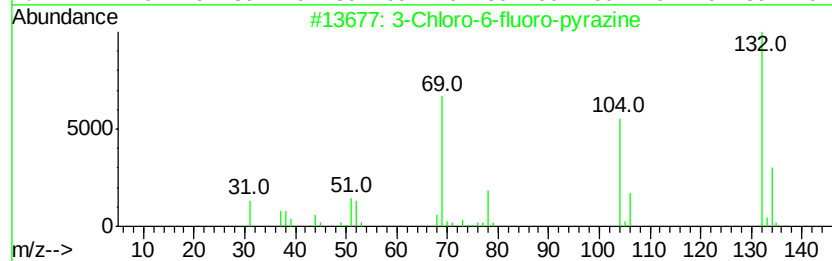
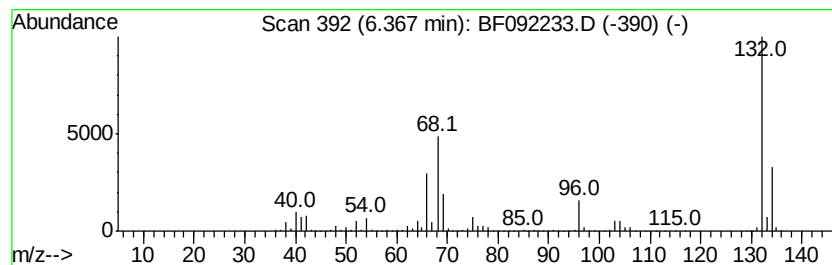
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.37	97.15 ng	4837600	1,4-Dichlorobenzene-d4	6.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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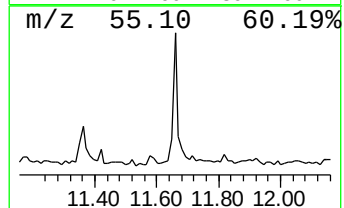
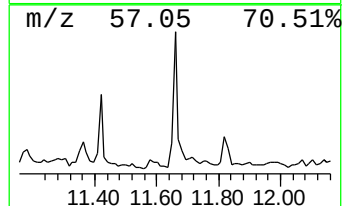
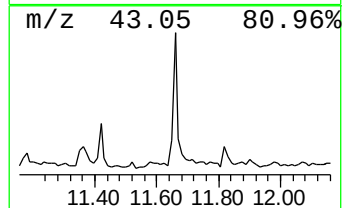
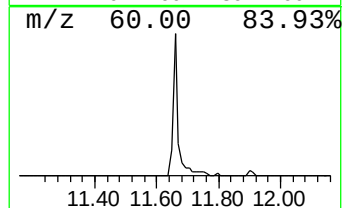
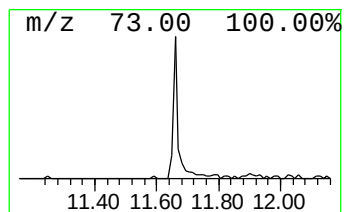
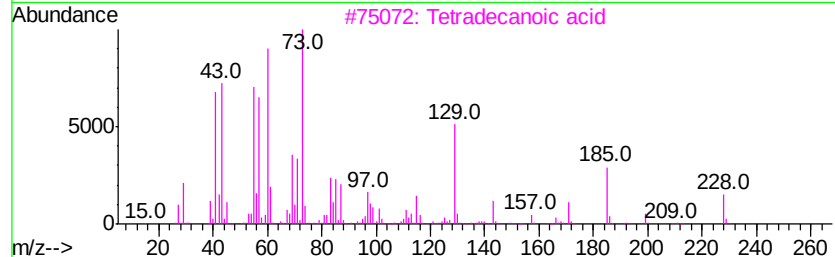
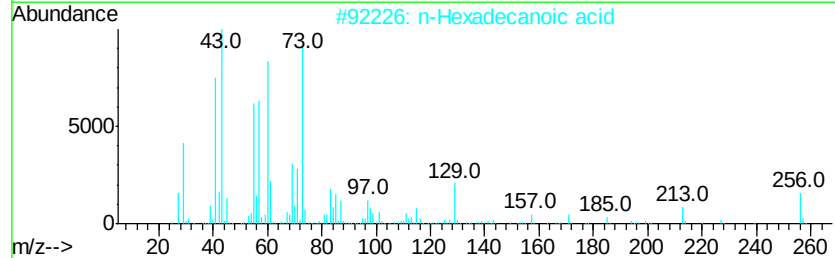
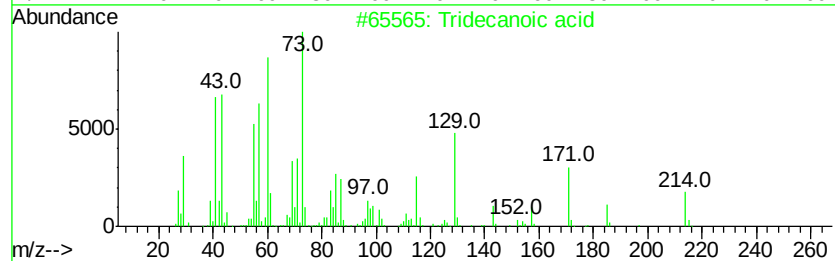
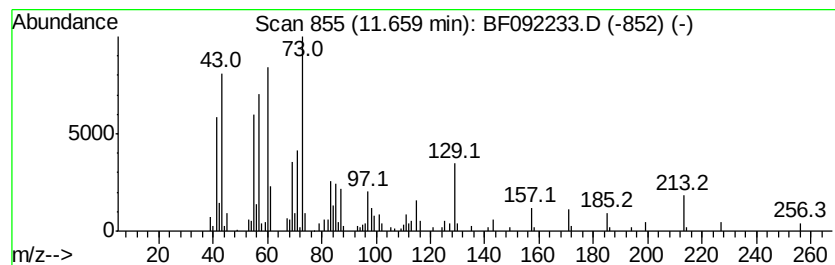
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	3.06 ng	202274	Phenanthrene-d10	11.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	30
5	Propyl 4,4-dimethyl-3-oxopentanoate	186	C10H18O3	077067-73-3	11



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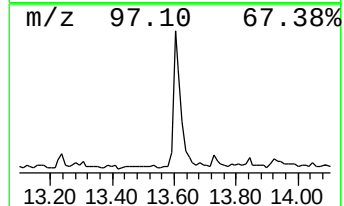
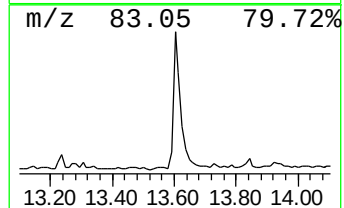
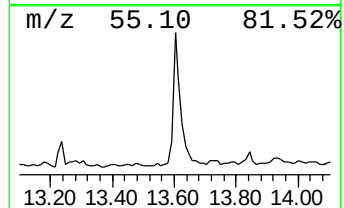
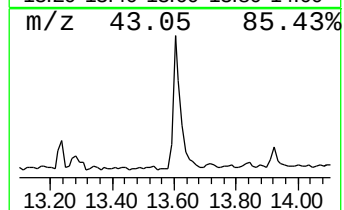
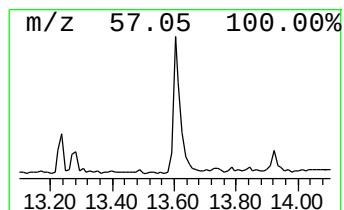
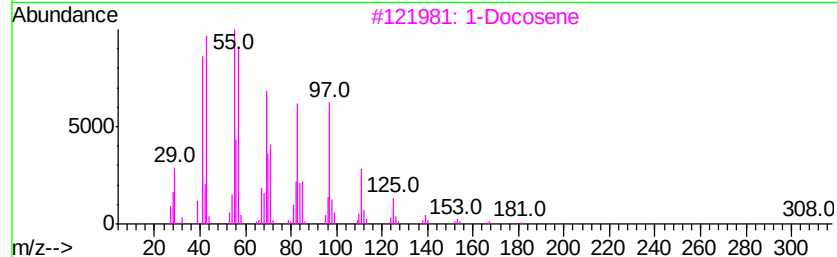
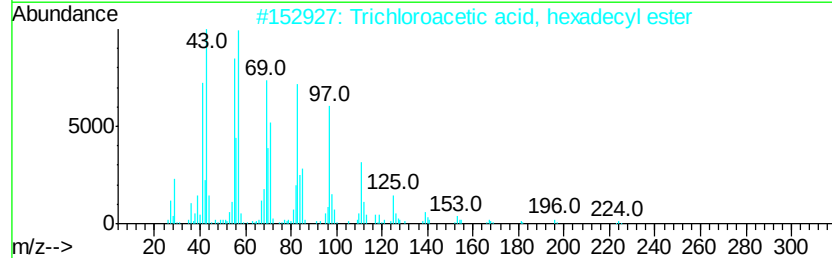
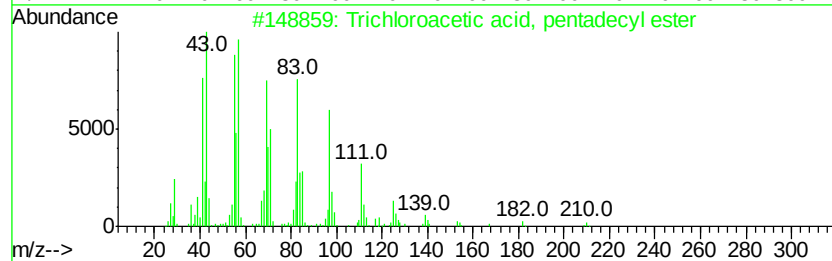
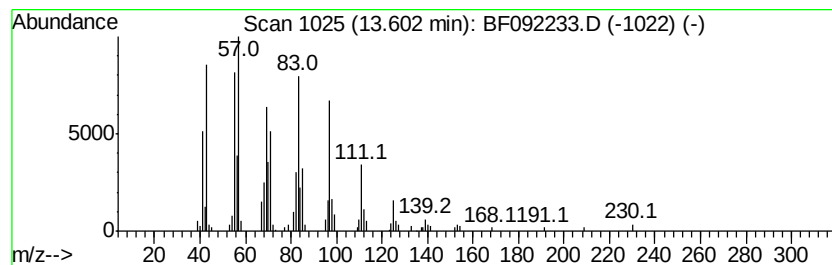
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.60	5.68 ng	307991	Chrysene-d12	13.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		1-Docosene	308	C22H44	001599-67-3	91
4		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5		1-Tetracosanol	354	C24H50O	000506-51-4	91



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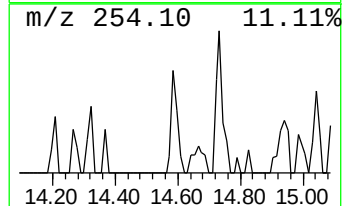
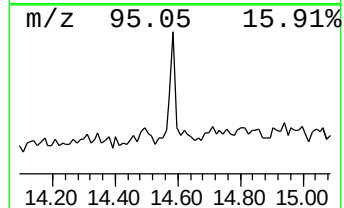
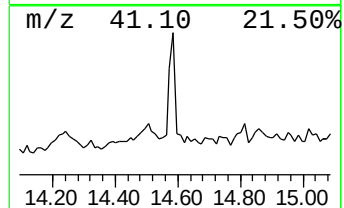
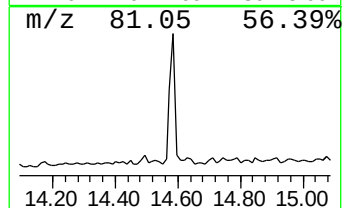
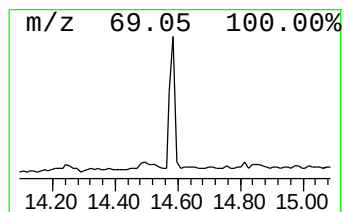
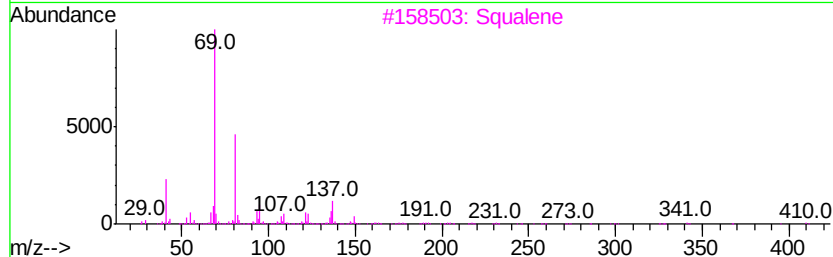
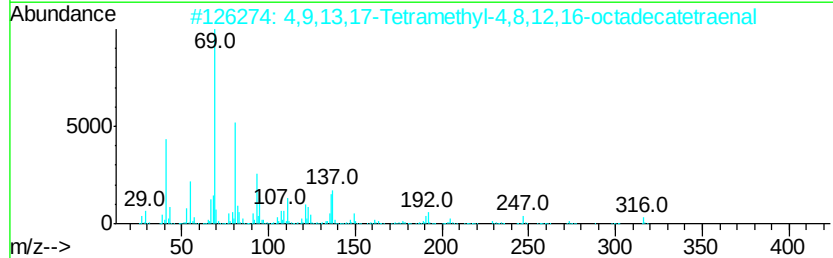
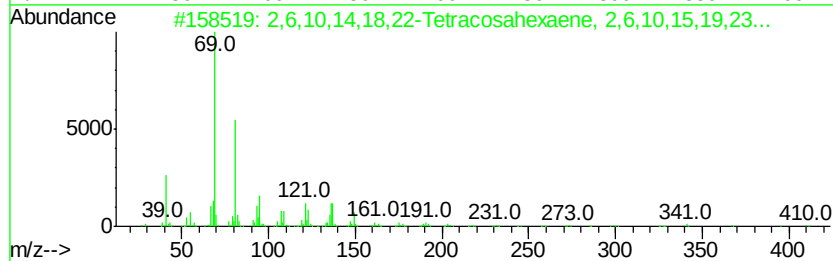
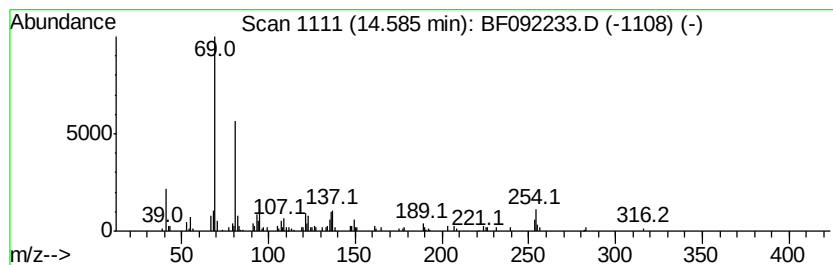
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Peak Number 6 2,6,10,14,18,22-Tetracosae... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.14 ng	93950	Perylene-d12	15.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87		
2	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	87		
3	Squalene	410	C30H50	007683-64-9	83		
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76		
5	.beta.-d-Mannofuranoside, 0-geranyl	316	C16H28O6	1000154-77-2	72		



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ClientSampleId :
SW-002

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.73	48.2	ng	2402220	1	6.60	995869	20.0
unknown6.37	6.37	97.2	ng	4837600	1	6.60	995869	20.0
Tridecanoic acid	11.66	3.1	ng	202274	4	11.10	1323810	20.0
Trichloroacetic a...	13.60	5.7	ng	307991	5	13.73	1083640	20.0
2,6,10,14,18,22-T...	14.59	2.1	ng	93950	6	15.09	878329	20.0