

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
 Data File : BF085678.D
 Acq On : 23 Mar 2016 00:24
 Operator : UM/SJ
 Sample : H1864-02
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PZ-3

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-BF031816.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	5.007	235	238	244	rBV	103478	134069	3.12%	0.464%
2	5.419	272	274	277	rBV	1028215	1437812	33.44%	4.976%
3	6.459	363	365	367	rBV	1155039	986221	22.93%	3.413%
4	6.596	374	377	380	rBV	2647407	2556412	59.45%	8.848%
5	6.824	395	397	400	rBV	580054	760541	17.69%	2.632%
6	6.984	409	411	414	rVB	2489723	2555683	59.43%	8.845%
7	7.396	444	447	450	rBV	1996243	2161267	50.26%	7.480%
8	7.487	453	455	458	rBV	40023	60841	1.41%	0.211%
9	8.116	507	510	512	rBV	1251988	1087312	25.29%	3.763%
10	9.190	601	604	607	rBV	3086589	4300179	100.00%	14.883%
11	9.590	636	639	640	rBV	264419	265507	6.17%	0.919%
12	9.865	661	663	666	rBV	1178441	1203811	27.99%	4.166%
13	10.299	697	701	703	rBV3	53775	75953	1.77%	0.263%
14	10.665	729	733	735	rBV2	2069158	2865962	66.65%	9.919%
15	10.768	740	742	747	rVB3	54517	126305	2.94%	0.437%
16	11.225	779	782	783	rBV	47028	69187	1.61%	0.239%
17	11.351	791	793	795	rBV	1492479	1292209	30.05%	4.472%
18	11.694	820	823	825	rBV	110152	101345	2.36%	0.351%
19	11.876	837	839	850	rVV2	176008	291669	6.78%	1.009%
20	12.585	898	901	906	rBV7	19009	60235	1.40%	0.208%
21	12.665	906	908	915	rVV	152578	195246	4.54%	0.676%
22	12.939	929	932	934	rBV	4079937	4269739	99.29%	14.777%
23	13.522	979	983	985	rBV	63258	76597	1.78%	0.265%
24	13.831	1008	1010	1018	rBV	194548	265758	6.18%	0.920%
25	13.979	1021	1023	1026	rBV	1051770	1019324	23.70%	3.528%
26	15.397	1144	1147	1150	rBV	538645	674789	15.69%	2.335%

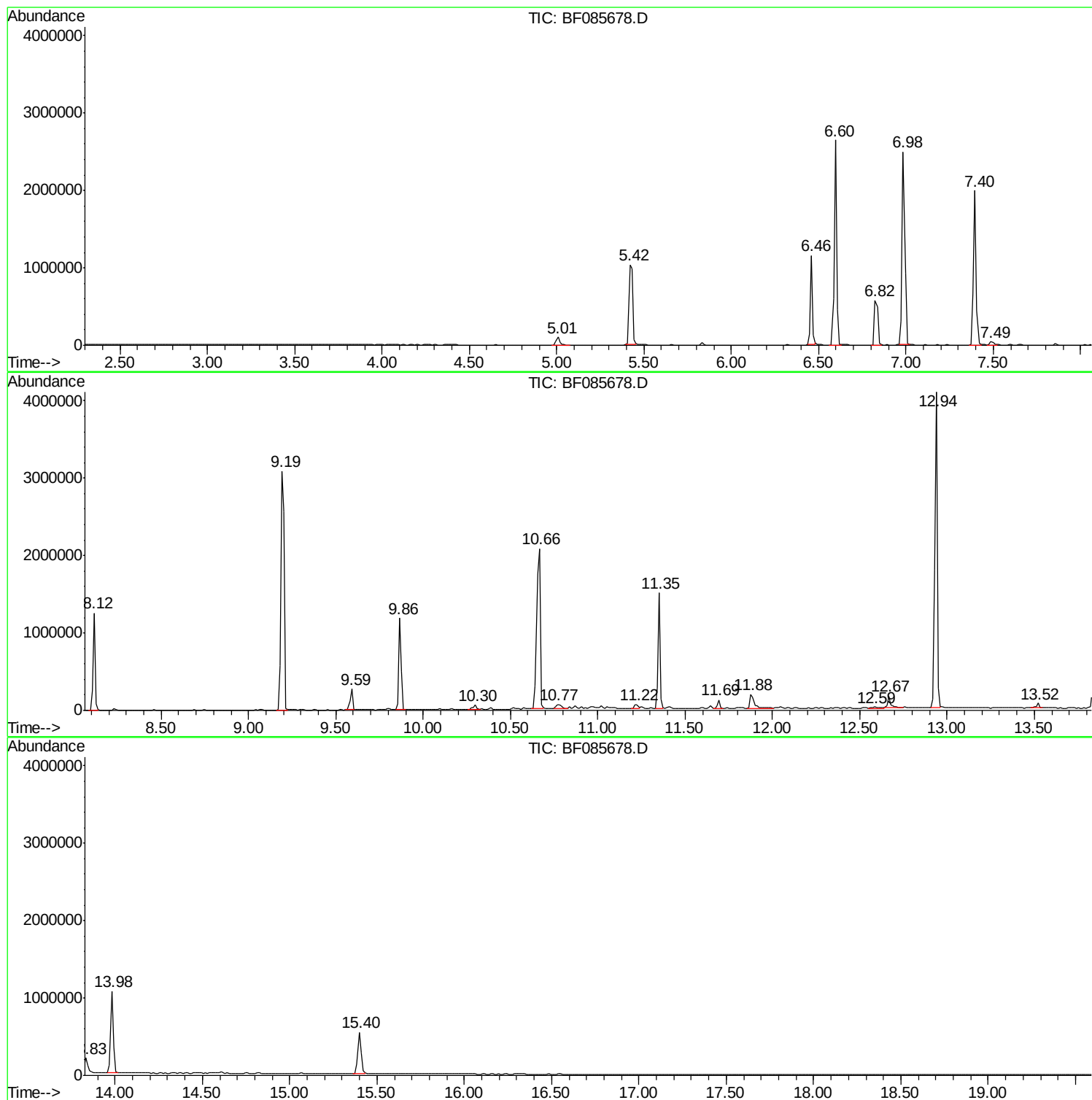
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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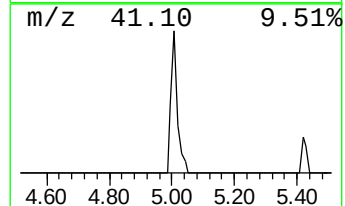
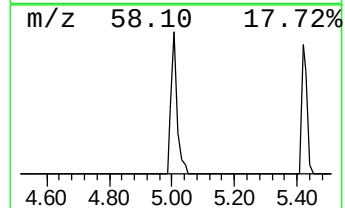
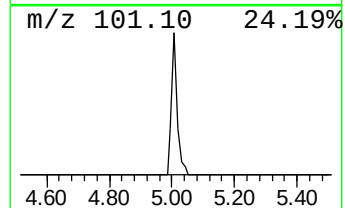
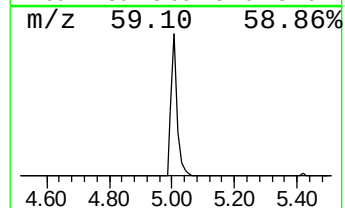
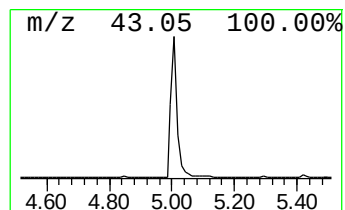
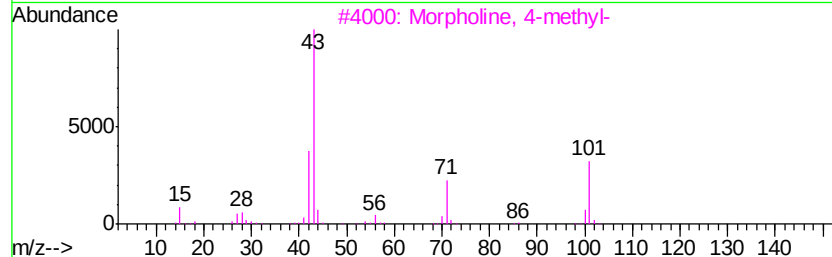
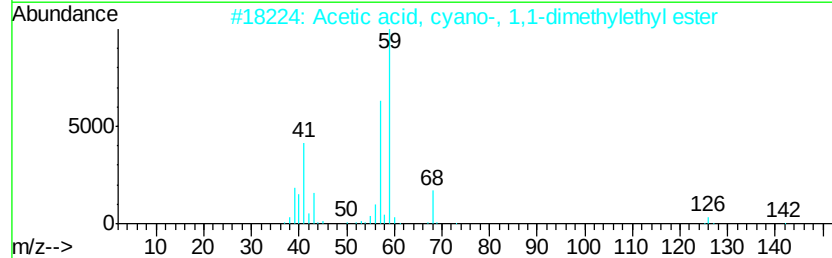
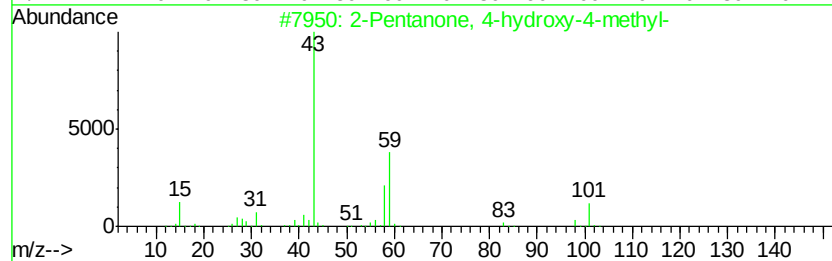
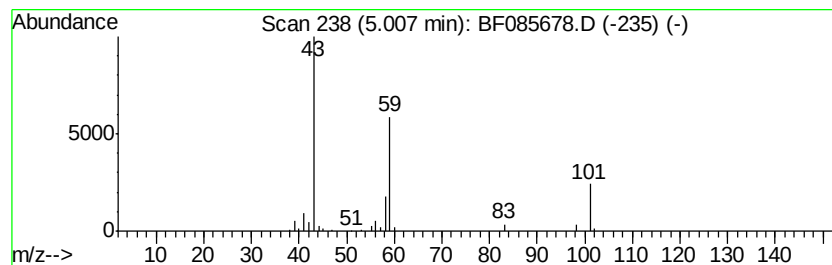
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	3.53 ng	134069	1,4-Dichlorobenzene-d4	6.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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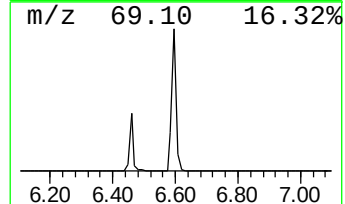
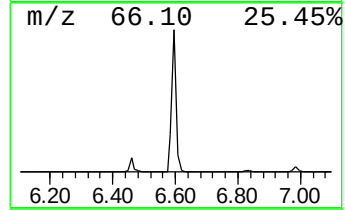
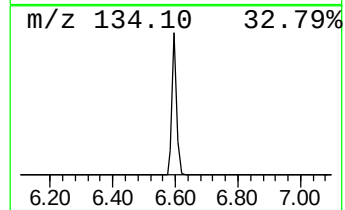
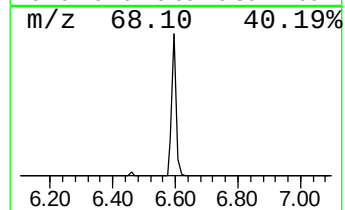
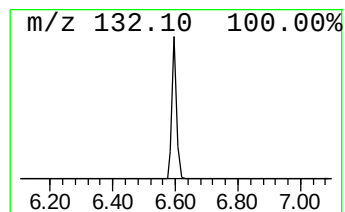
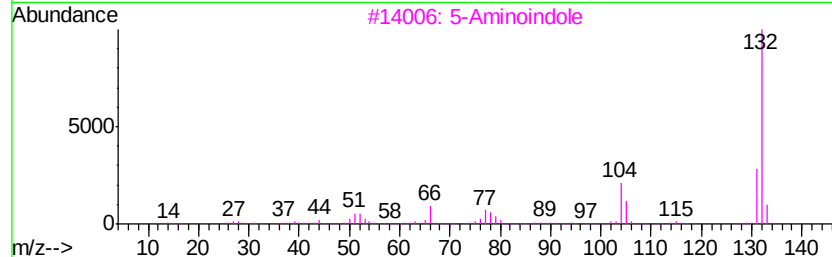
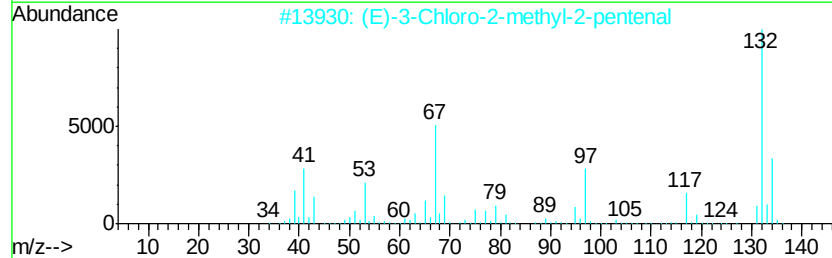
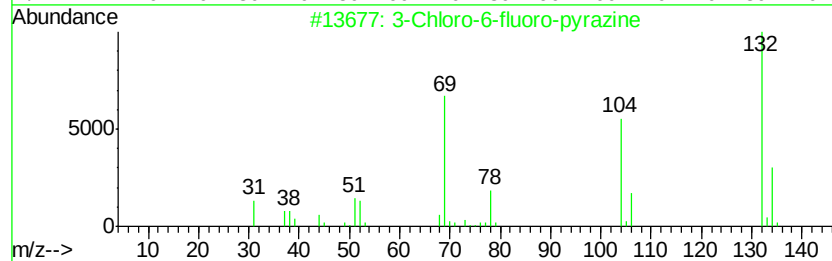
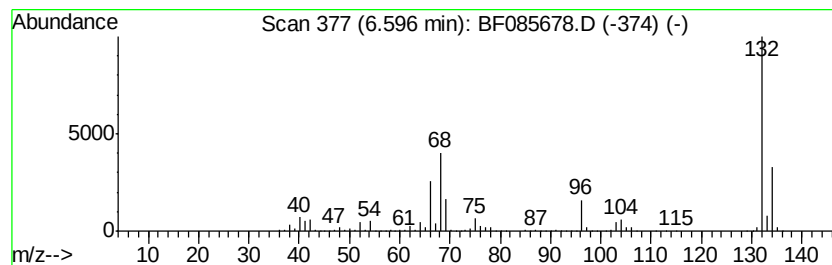
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	67.23 ng	2556410	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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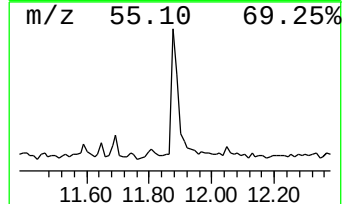
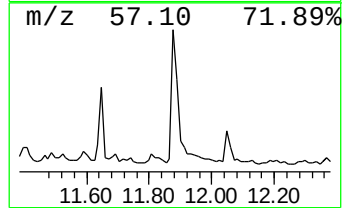
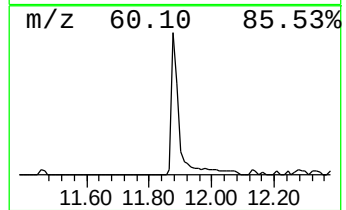
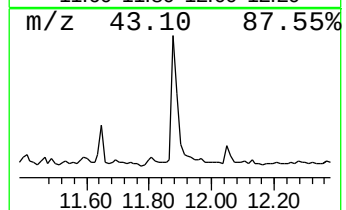
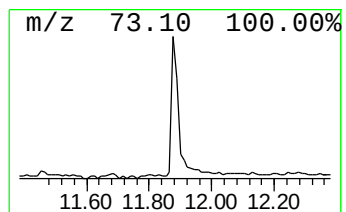
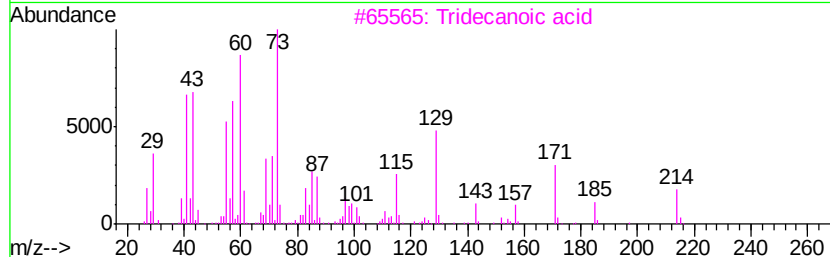
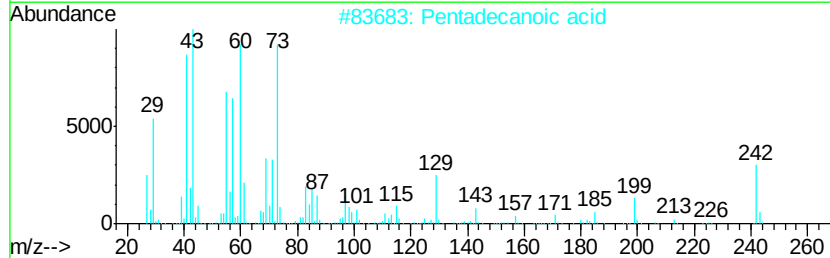
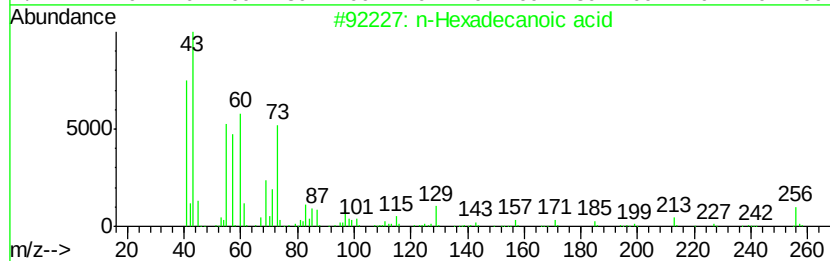
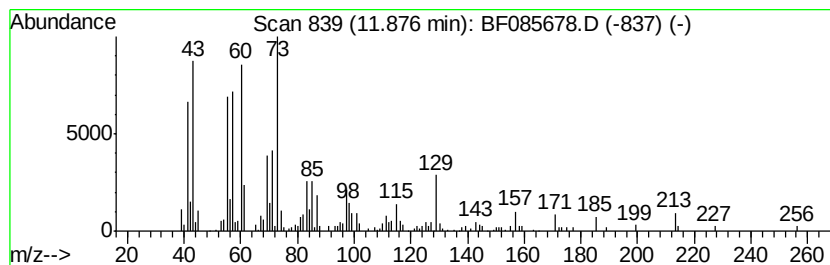
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.88	4.51 ng	291669	Phenanthrene-d10	11.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	n-Decanoic acid	172	C10H20O2	000334-48-5	25
5	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	11



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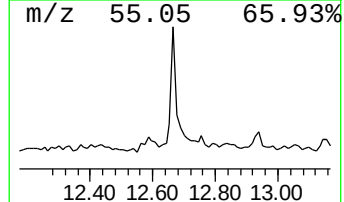
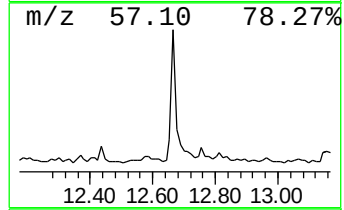
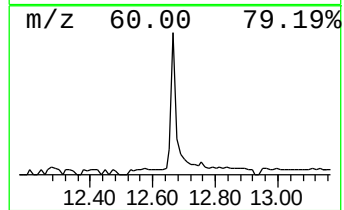
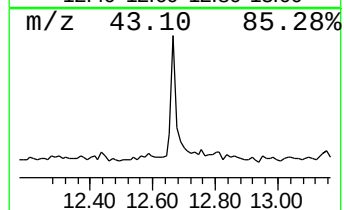
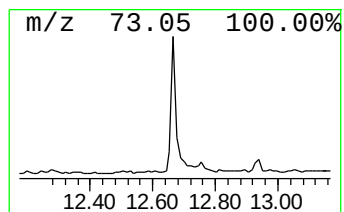
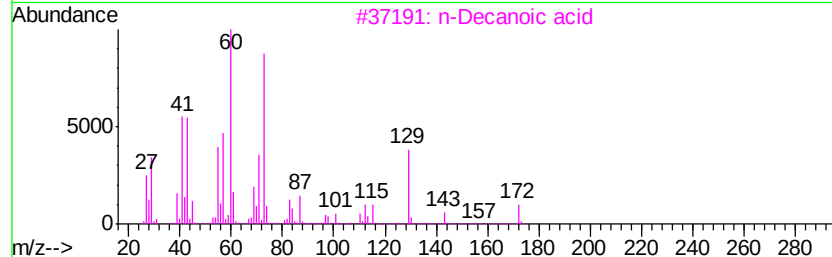
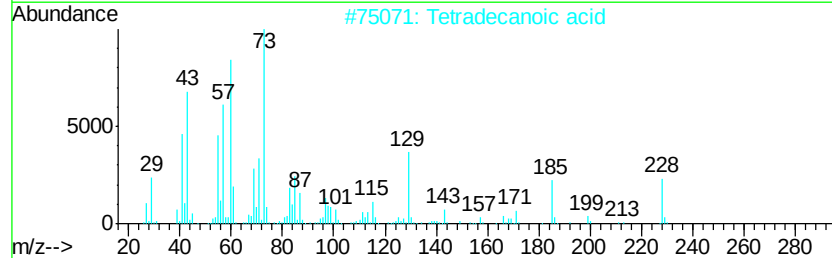
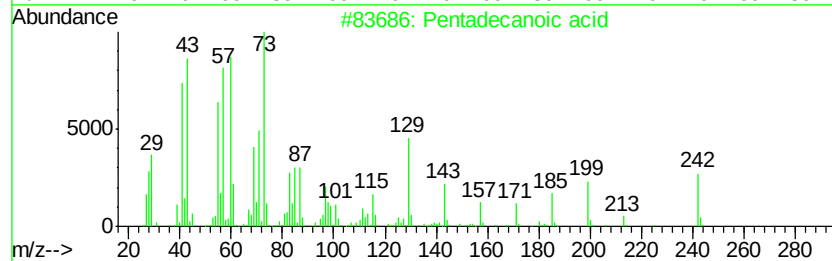
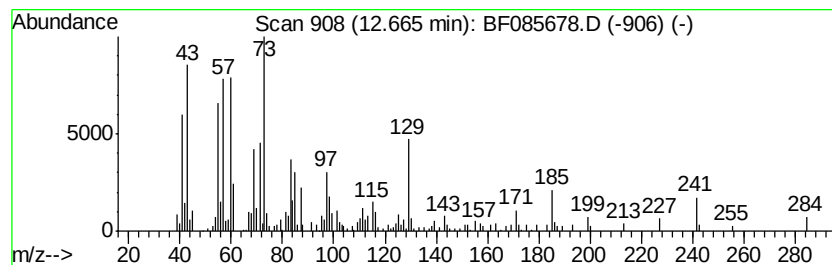
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.67	3.83 ng	195246	Chrysene-d12		13.98
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	n-Decanoic acid	172	C10H20O2	000334-48-5	76
4	Undecanoic acid	186	C11H22O2	000112-37-8	46
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	18



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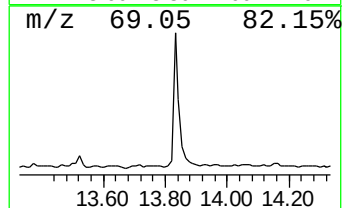
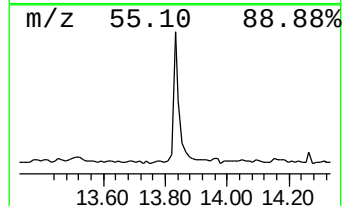
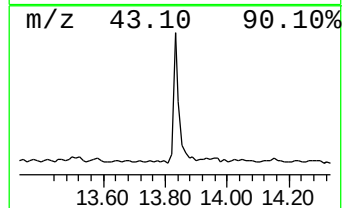
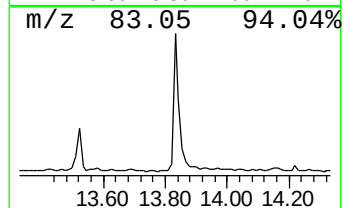
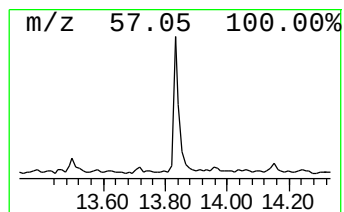
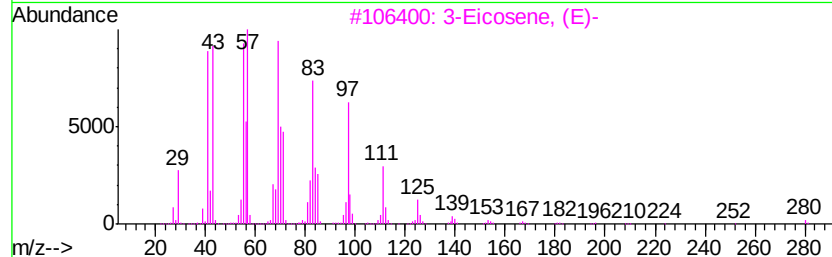
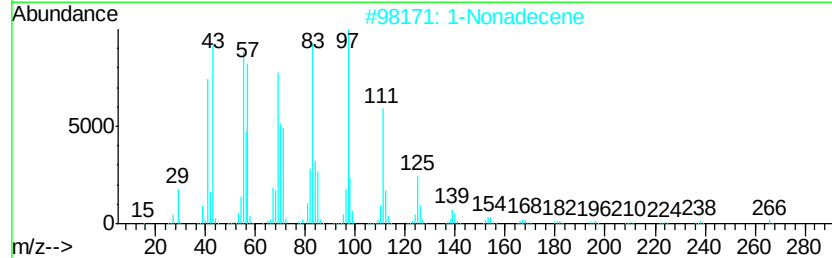
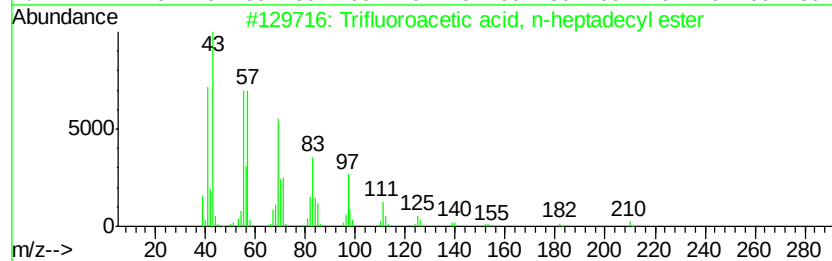
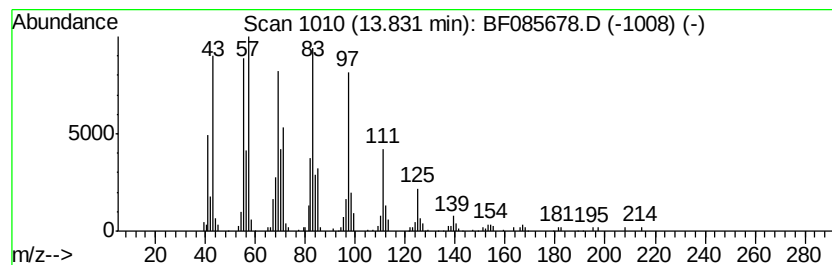
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ClientSampled :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetic acid, n-hep... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.83	5.21 ng	265758	Chrysene-d12	13.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
5	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91



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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...	5.01	3.5	ng	134069	1	6.84	760541	20.0
unknown6.60	6.60	67.2	ng	2556410	1	6.84	760541	20.0
n-Hexadecanoic acid	11.88	4.5	ng	291669	4	11.35	1292210	20.0
Pentadecanoic acid	12.67	3.8	ng	195246	5	13.98	1019320	20.0
Trifluoroacetic a...	13.83	5.2	ng	265758	5	13.98	1019320	20.0