

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062317\
 Data File : BF096173.D
 Acq On : 23 Jun 2017 22:36
 Operator : SJ/MA
 Sample : I3852-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G-33-0-1.5

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-BF060517.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	1.540	7	9	41	rVB	360296	699523	44.36%	5.471%
2	3.310	306	310	334	rBV2	83565	259565	16.46%	2.030%
3	4.416	490	498	517	rBV	498115	1120693	71.07%	8.764%
4	5.216	631	634	652	rBV2	30277	124091	7.87%	0.970%
5	6.839	907	910	922	rBV	381291	854164	54.17%	6.680%
6	6.928	922	925	943	rVB	344339	768819	48.76%	6.012%
7	7.257	978	981	994	rBV	284100	390703	24.78%	3.055%
8	7.492	1017	1021	1043	rBV	776047	1123879	71.27%	8.789%
9	8.186	1135	1139	1158	rBV	445122	805840	51.11%	6.302%
10	9.292	1323	1327	1342	rBV	359868	539910	34.24%	4.222%
11	9.392	1342	1344	1353	rVB	11707	16346	1.04%	0.128%
12	10.386	1505	1513	1518	rBV	10767	15910	1.01%	0.124%
13	11.074	1625	1630	1640	rBV	1243500	1576831	100.00%	12.331%
14	11.298	1663	1668	1674	rVB2	21551	27779	1.76%	0.217%
15	11.774	1744	1749	1754	rBV	200823	273038	17.32%	2.135%
16	11.969	1776	1782	1788	rBV5	6588	15792	1.00%	0.123%
17	12.110	1801	1806	1812	rBV2	433191	554649	35.17%	4.338%
18	12.157	1812	1814	1822	rVB2	40965	56255	3.57%	0.440%
19	12.968	1946	1952	1957	rBV	43112	54776	3.47%	0.428%
20	13.327	2005	2013	2017	rBV5	17937	33362	2.12%	0.261%
21	13.739	2079	2083	2085	rBV	45537	56669	3.59%	0.443%
22	14.468	2203	2207	2210	rVV	33979	41187	2.61%	0.322%
23	14.504	2210	2213	2218	rVV	342243	476565	30.22%	3.727%
24	14.545	2218	2220	2229	rVB	54893	86341	5.48%	0.675%
25	14.768	2251	2258	2265	rBV7	13190	27831	1.76%	0.218%
26	15.157	2320	2324	2327	rBV	26634	33074	2.10%	0.259%
27	15.374	2357	2361	2365	rVV	14408	17125	1.09%	0.134%
28	15.480	2375	2379	2383	rBV3	12258	20381	1.29%	0.159%
29	15.527	2383	2387	2396	rVB6	16831	37298	2.37%	0.292%
30	15.768	2424	2428	2432	rBV3	29650	39975	2.54%	0.313%
31	15.986	2462	2465	2471	rBV8	10620	20039	1.27%	0.157%
32	16.139	2486	2491	2494	rBV4	18845	32942	2.09%	0.258%
33	16.180	2494	2498	2501	rVB5	15355	22276	1.41%	0.174%
34	16.321	2519	2522	2523	rBV2	29138	28760	1.82%	0.225%

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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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.345	2523	2526	2531	rVB	99427	127501	8.09%	0.997%
36	16.645	2573	2577	2585	rBV	127573	171240	10.86%	1.339%
37	16.833	2606	2609	2611	rBV2	23016	25475	1.62%	0.199%
38	16.898	2614	2620	2628	rVB	854017	1077907	68.36%	8.430%
39	17.262	2679	2682	2686	rBV4	25353	36635	2.32%	0.286%
40	17.303	2687	2689	2692	rVB2	27118	26343	1.67%	0.206%
41	17.609	2738	2741	2746	rVB2	64669	69916	4.43%	0.547%
42	17.751	2763	2765	2767	rVB	32506	20915	1.33%	0.164%
43	18.168	2831	2836	2841	rVB2	55531	118010	7.48%	0.923%
44	18.245	2845	2849	2854	rBV2	381924	510806	32.39%	3.995%
45	19.927	3131	3135	3143	rVB	276984	349991	22.20%	2.737%

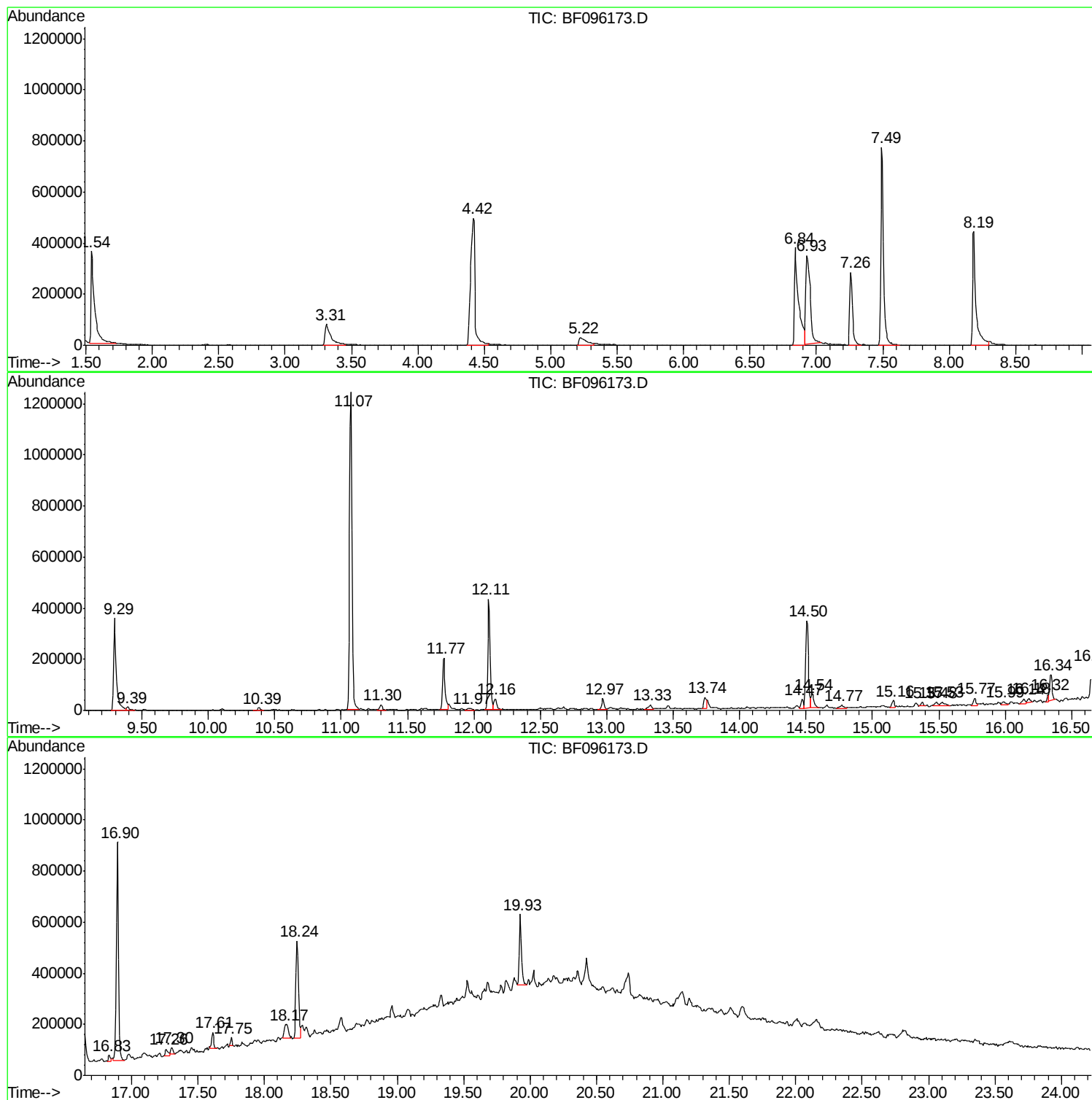
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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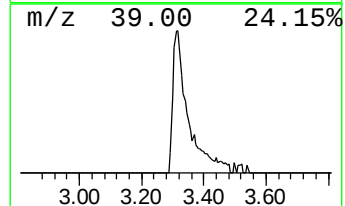
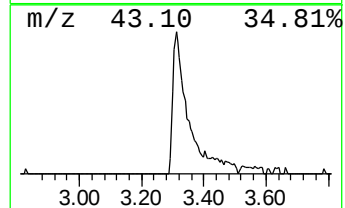
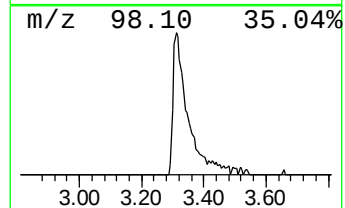
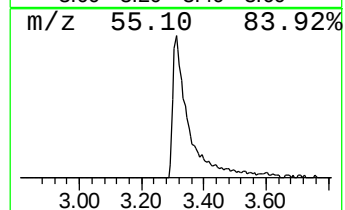
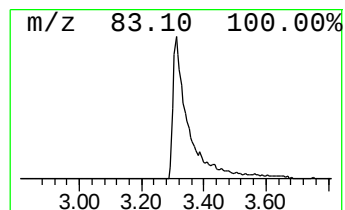
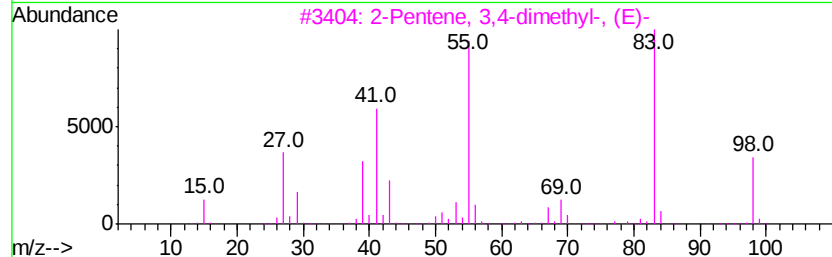
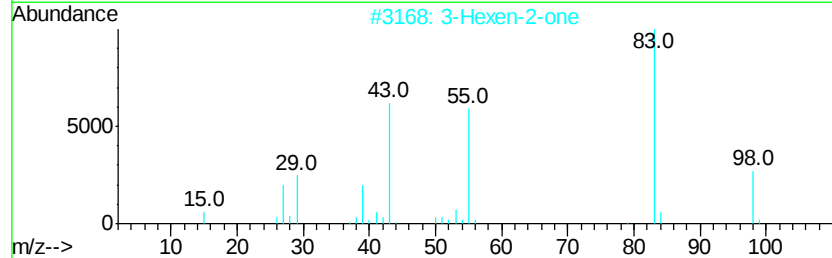
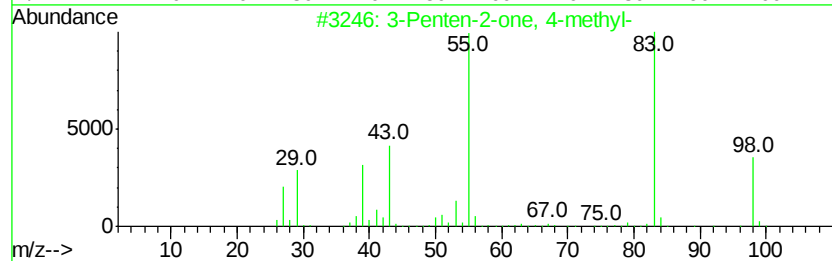
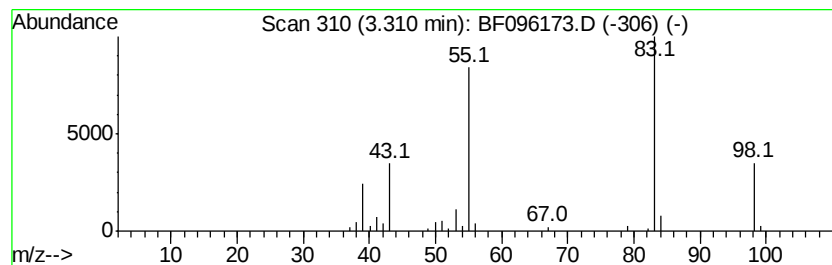
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.31	13.29 ng	259565	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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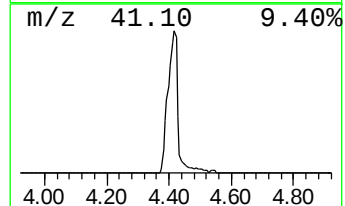
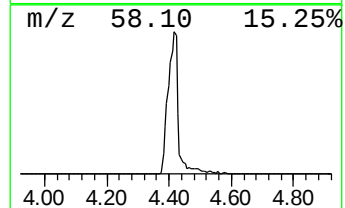
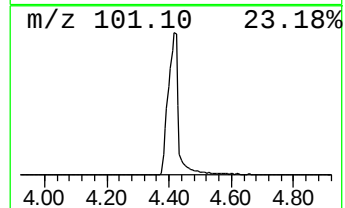
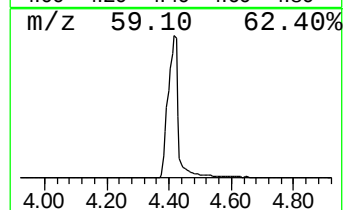
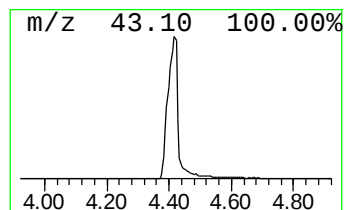
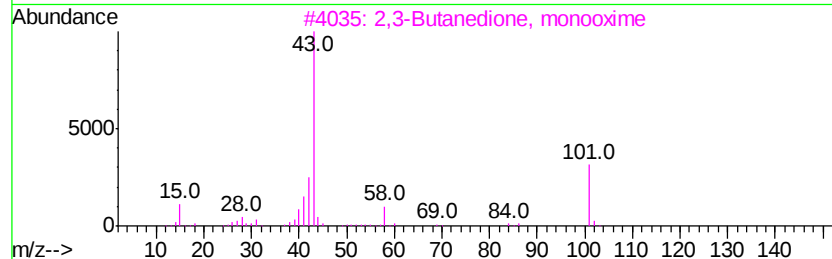
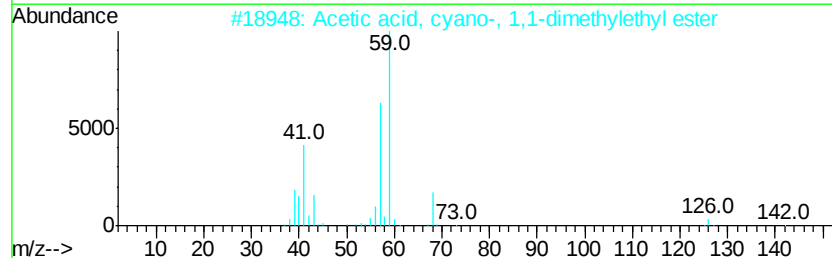
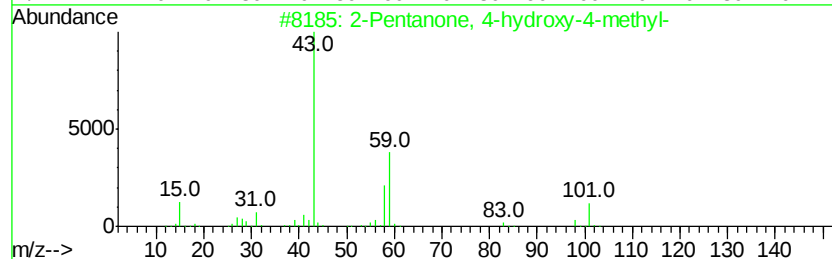
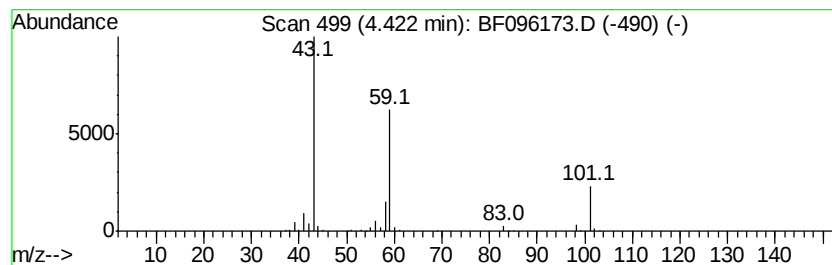
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.42	57.37 ng	1120690	1,4-Dichlorobenzene-d4	7.26

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, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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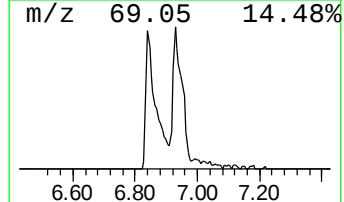
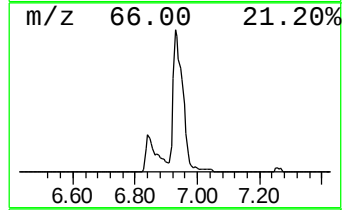
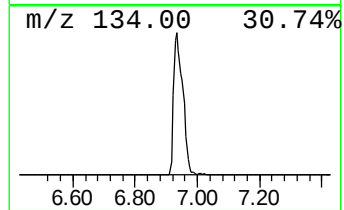
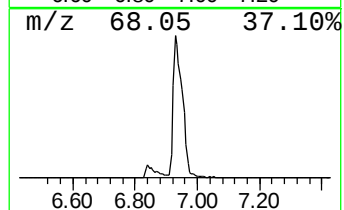
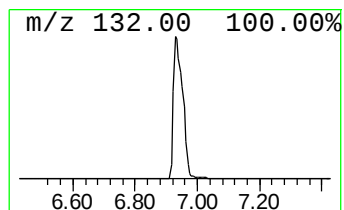
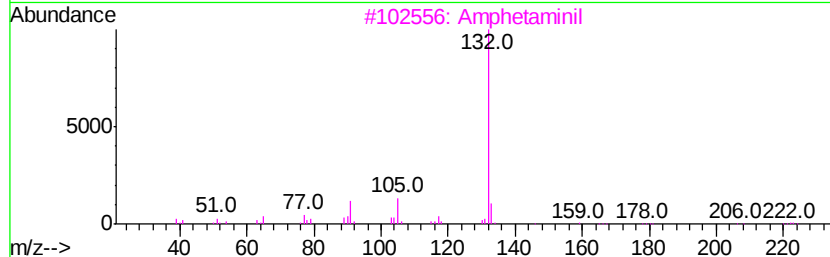
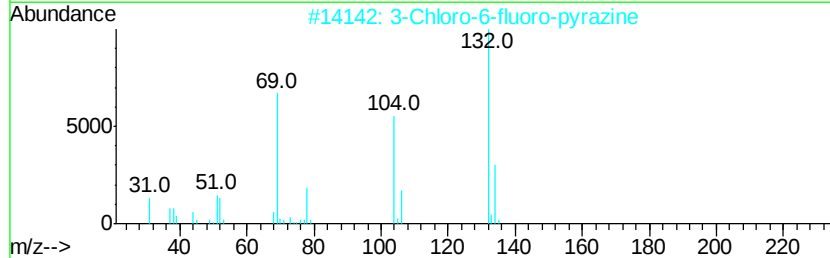
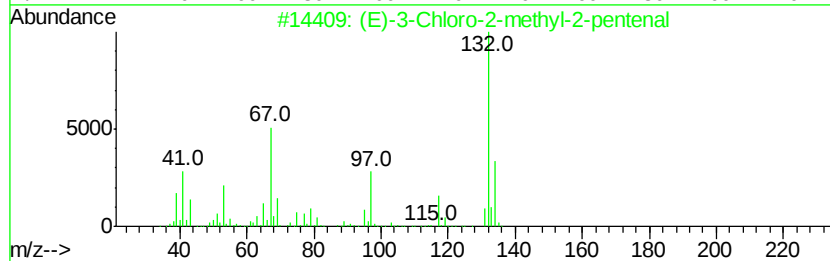
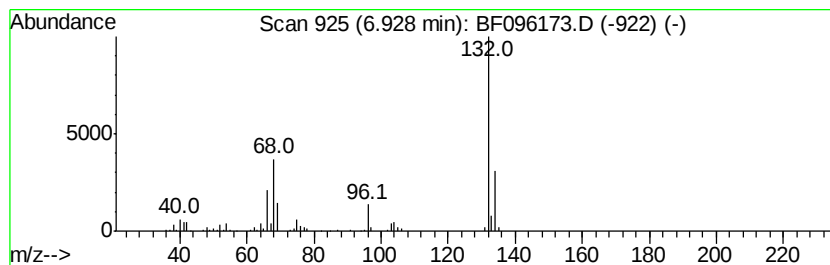
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown6.93 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	39.36 ng	768819	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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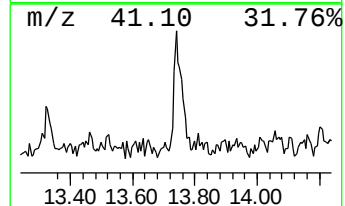
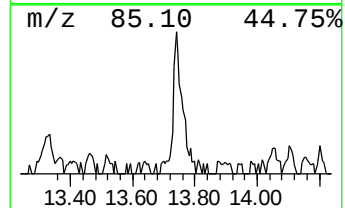
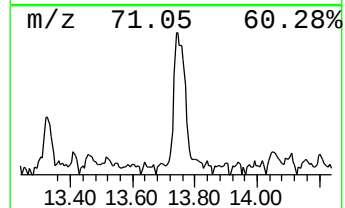
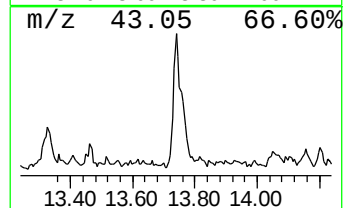
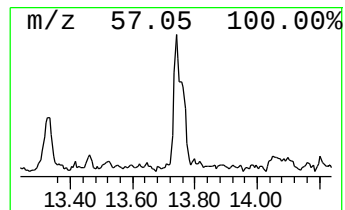
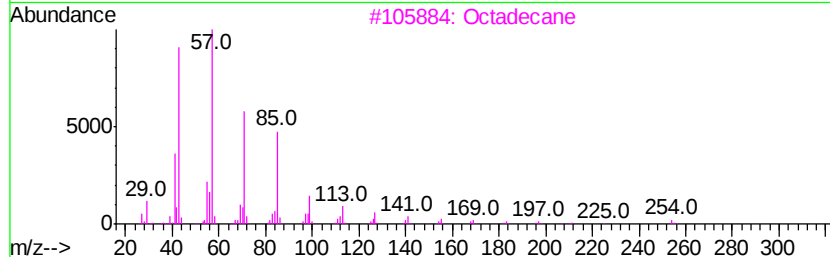
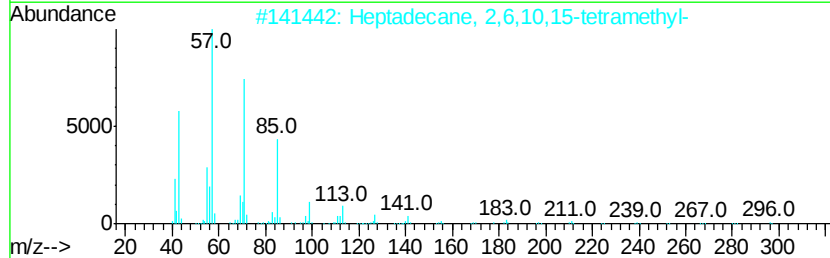
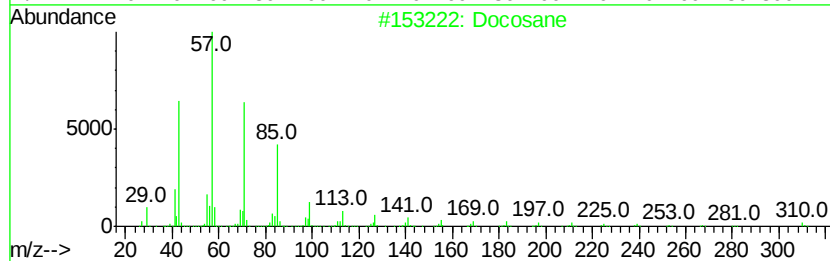
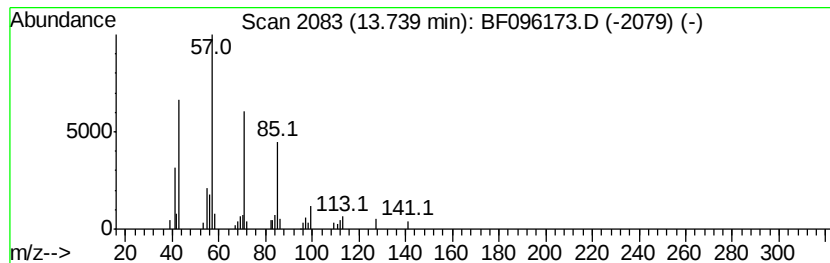
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Docosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	2.38 ng	56669	Phenanthrene-d10	14.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	90
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Tetracosane	338	C24H50	000646-31-1	83
5	Undecane, 2,10-dimethyl-	184	C13H28	017301-27-8	78



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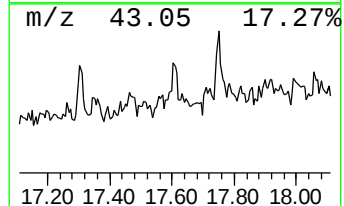
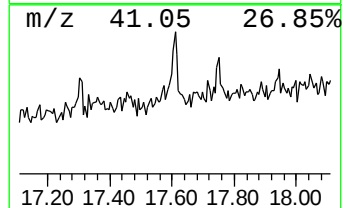
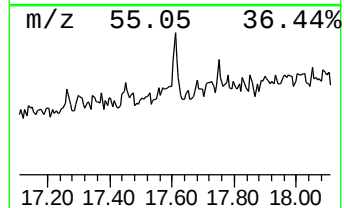
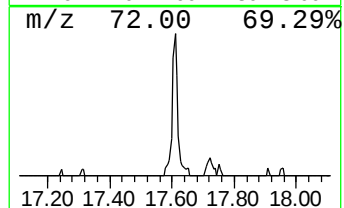
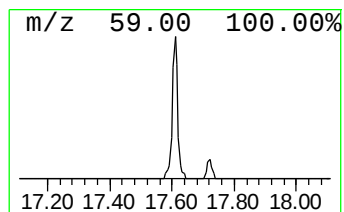
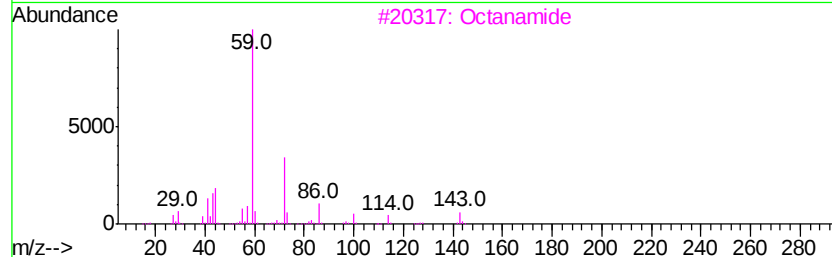
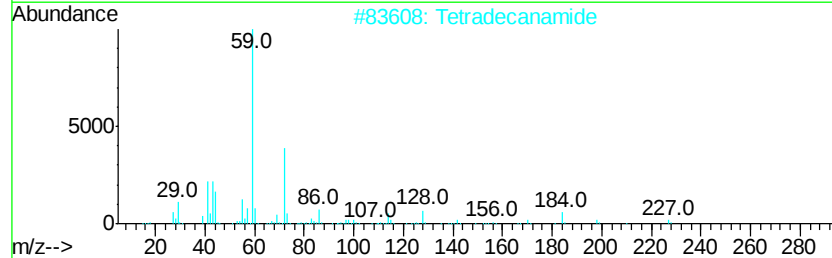
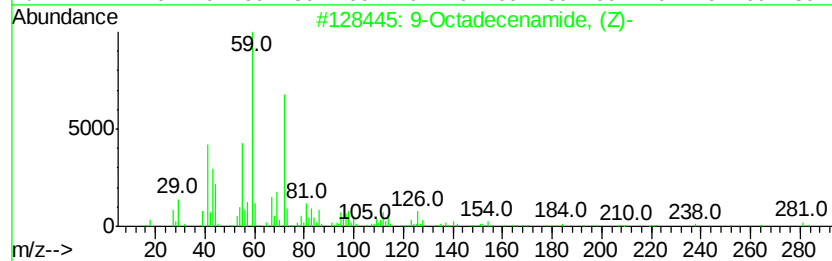
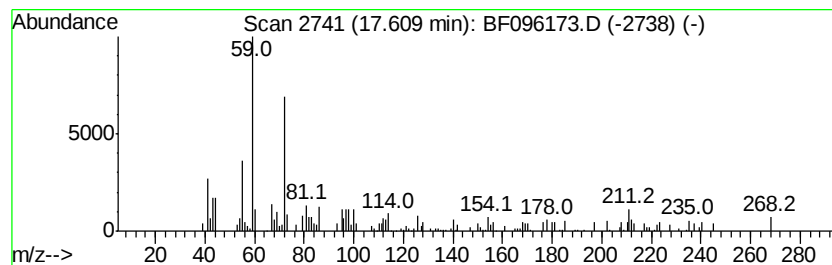
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.61	2.74 ng	69916	Chrysene-d12	18.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
2		Tetradecanamide	227	C14H29NO	000638-58-4	64
3		Octanamide	143	C8H17NO	000629-01-6	59
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
Data File : BF096173.D
Acq On : 23 Jun 2017 22:36
Operator : SJ/MA
Sample : I3852-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

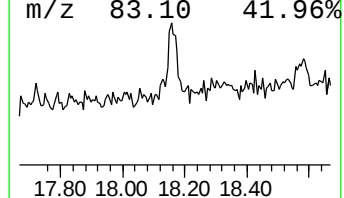
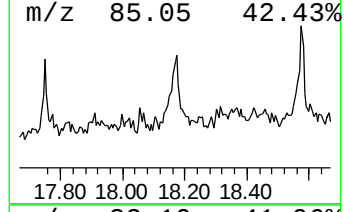
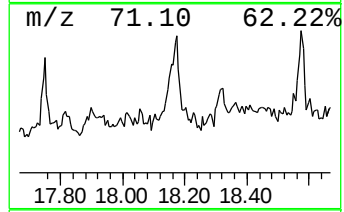
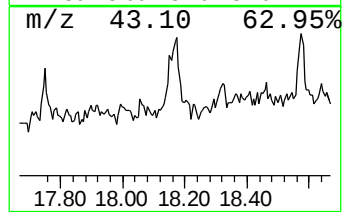
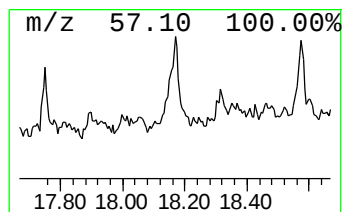
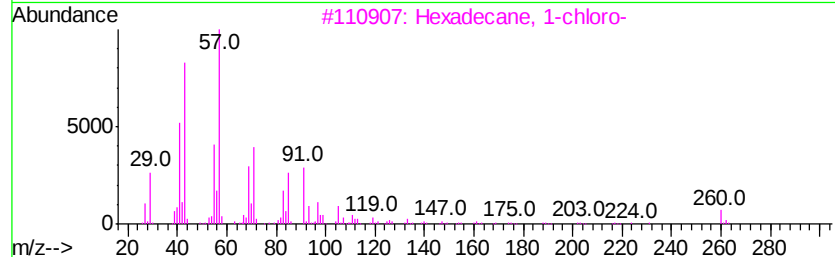
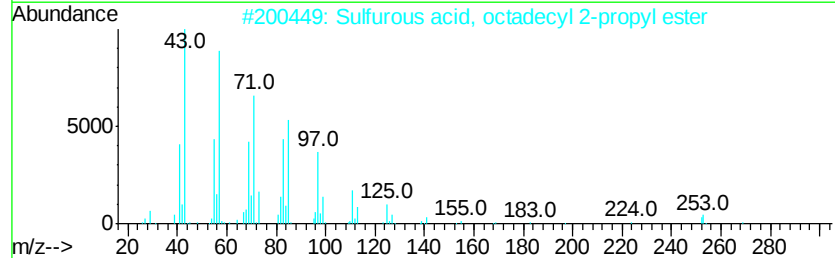
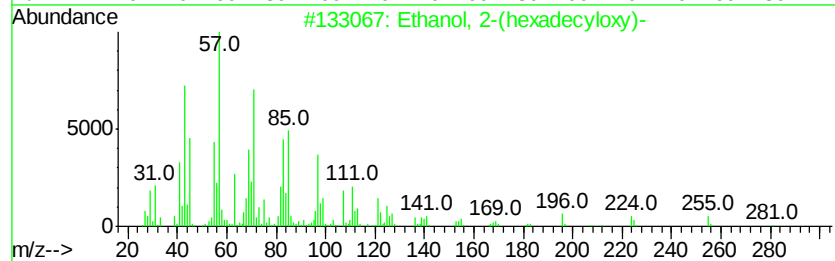
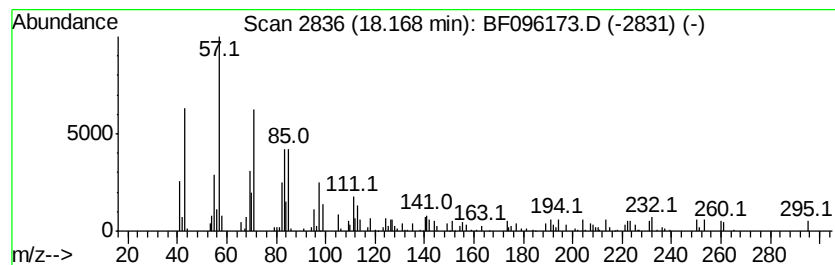
Instrument :
BNA_F
ClientSampleId :
G-33-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Ethanol, 2-(hexadecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.17	4.62 ng	118010	Chrysene-d12	18.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	72
2	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	64
3	Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	62
4	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	53
5	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062317\
Data File : BF096173.D
Acq On : 23 Jun 2017 22:36
Operator : SJ/MA
Sample : I3852-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-33-0-1.5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.31	13.3	ng	259565	1	7.26	390703	20.0
2-Pentanone, 4-hy...	4.42	57.4	ng	1120690	1	7.26	390703	20.0
unknown6.93	6.93	39.4	ng	768819	1	7.26	390703	20.0
Docosane	13.74	2.4	ng	56669	4	14.50	476565	20.0
9-Octadecenamide,...	17.61	2.7	ng	69916	5	18.24	510806	20.0
Ethanol, 2-(hexad...	18.17	4.6	ng	118010	5	18.24	510806	20.0