

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
 Data File : BM015891.D
 Acq On : 11 Jul 2018 16:31
 Operator : SJ/JU
 Sample : J3906-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 CB-7-8-6-ST-WW-2@2.75

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:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.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	5.316	340	345	360	rVB	291819	452947	8.70%	1.175%
2	5.798	420	427	440	rBV	2449723	3636328	69.81%	9.433%
3	7.445	700	707	723	rBV	2351350	3965809	76.14%	10.288%
4	7.816	763	770	783	rBV	2582059	4135669	79.40%	10.728%
5	8.292	845	851	858	rBV	427248	690680	13.26%	1.792%
6	8.616	899	906	917	rBV	1699134	2737204	52.55%	7.100%
7	9.481	1046	1053	1068	rBV	1418166	2353454	45.18%	6.105%
8	11.122	1324	1332	1343	rBV	496246	858426	16.48%	2.227%
9	13.539	1736	1743	1752	rBV	3046039	4271907	82.02%	11.082%
10	14.357	1877	1882	1890	rBV	411107	585517	11.24%	1.519%
11	14.916	1970	1977	1988	rVB2	665864	1017195	19.53%	2.639%
12	16.392	2222	2228	2242	rBV	2695940	3716474	71.35%	9.641%
13	17.639	2434	2440	2453	rBV	776225	1131180	21.72%	2.934%
14	18.480	2577	2583	2593	rBV	259967	376768	7.23%	0.977%
15	19.309	2719	2724	2727	rBV	43330	58042	1.11%	0.151%
16	19.727	2791	2795	2803	rBV	102111	134071	2.57%	0.348%
17	20.203	2870	2876	2884	rBV	4265630	5208618	100.00%	13.511%
18	20.950	3000	3003	3008	rBV	52353	62265	1.20%	0.162%
19	21.415	3077	3082	3092	rBV2	238936	492307	9.45%	1.277%
20	21.503	3093	3097	3103	rVV	202656	245804	4.72%	0.638%
21	21.745	3134	3138	3144	rBV	813231	1095574	21.03%	2.842%
22	21.845	3152	3155	3158	rVB	65054	70601	1.36%	0.183%
23	22.297	3229	3232	3235	rBV2	56834	61318	1.18%	0.159%
24	22.786	3312	3315	3322	rVB4	67569	96756	1.86%	0.251%
25	24.144	3539	3546	3555	rBV2	549568	1094797	21.02%	2.840%

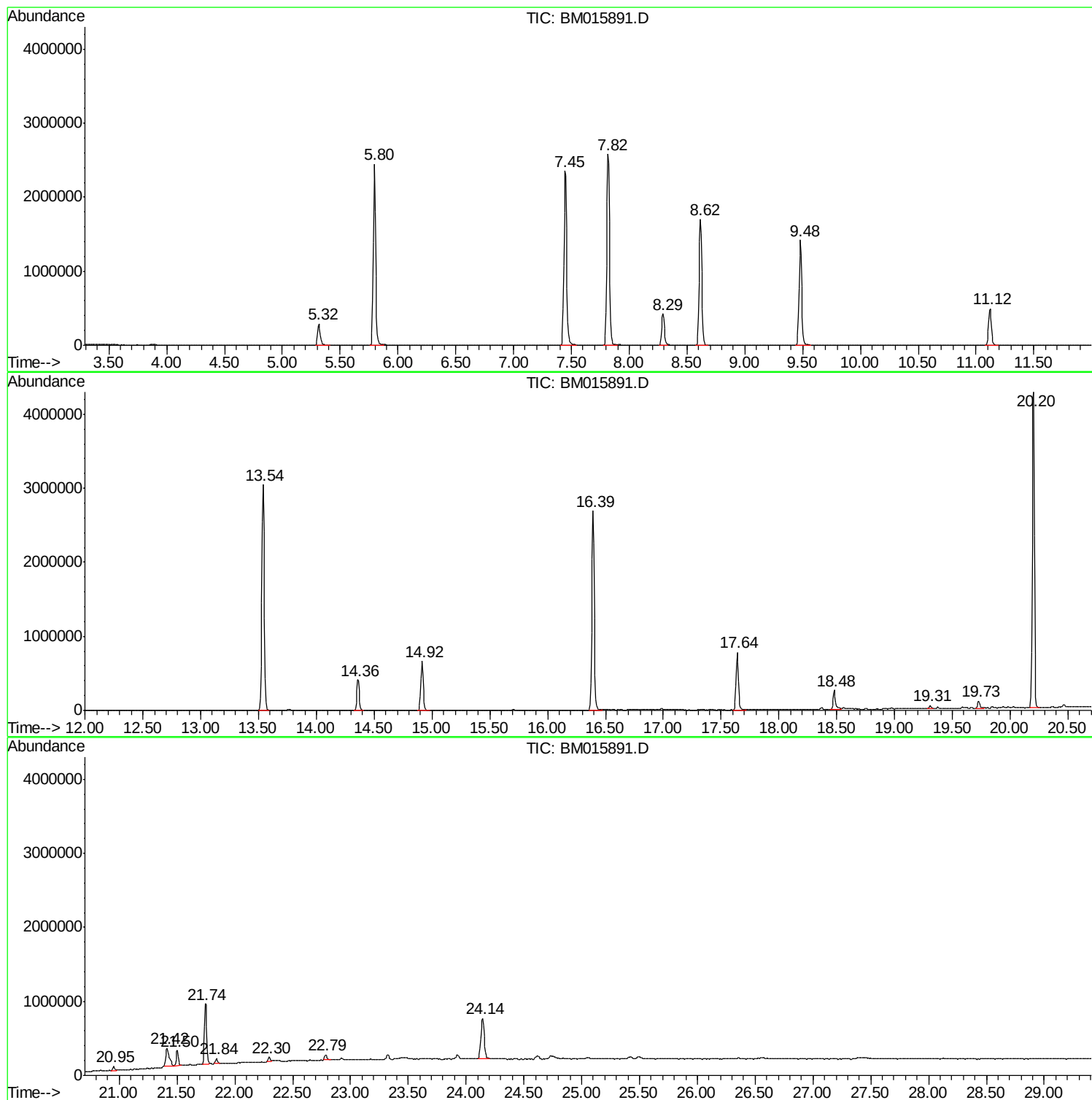
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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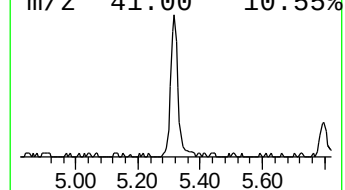
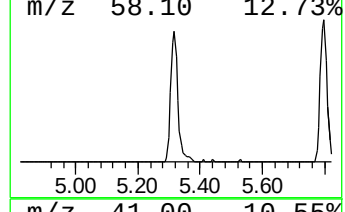
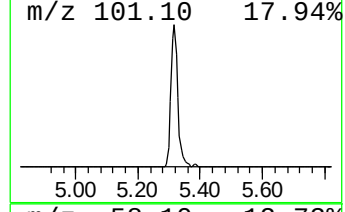
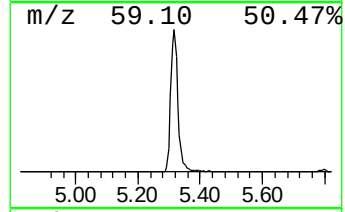
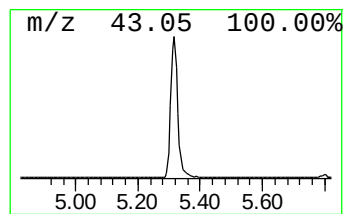
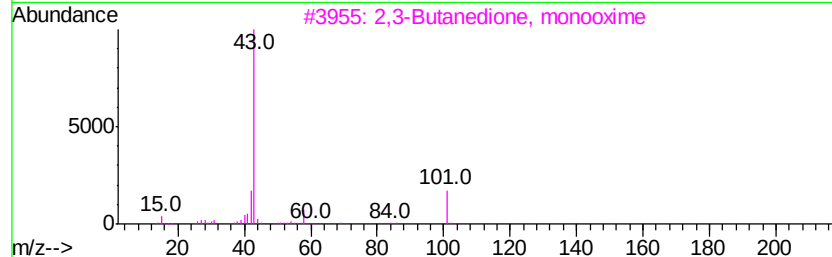
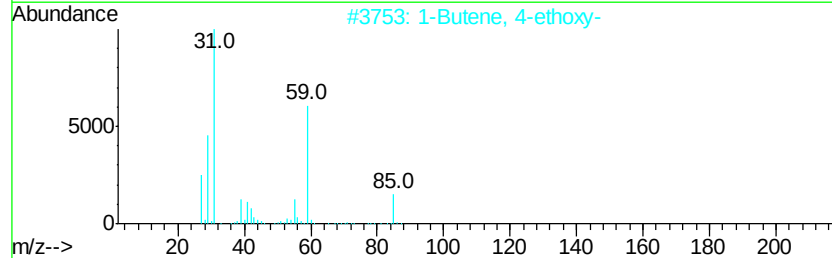
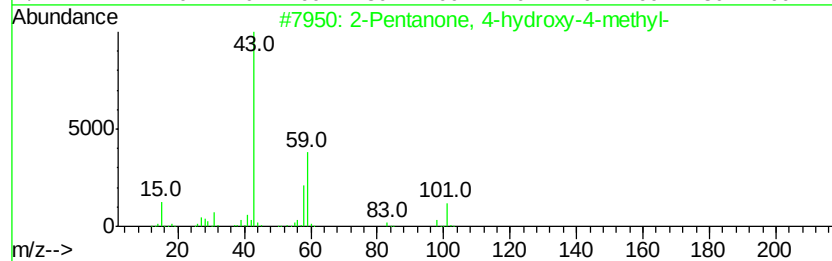
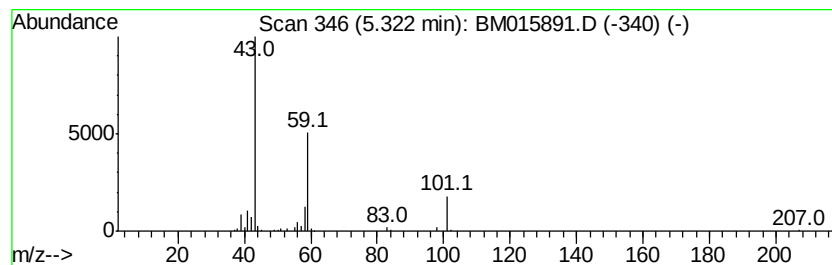
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	13.12 ng	452947	1,4-Dichlorobenzene-d4	8.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4			Butane	58	C4H10	000106-97-8	9
5			Propylamine	59	C3H9N	000107-10-8	9



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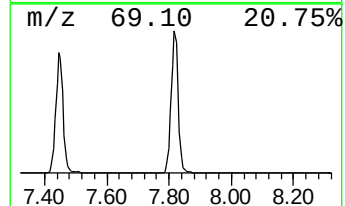
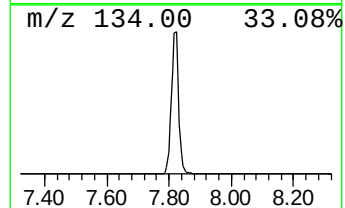
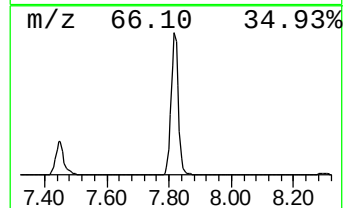
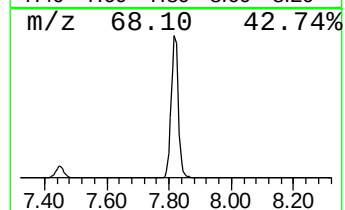
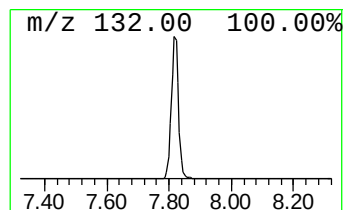
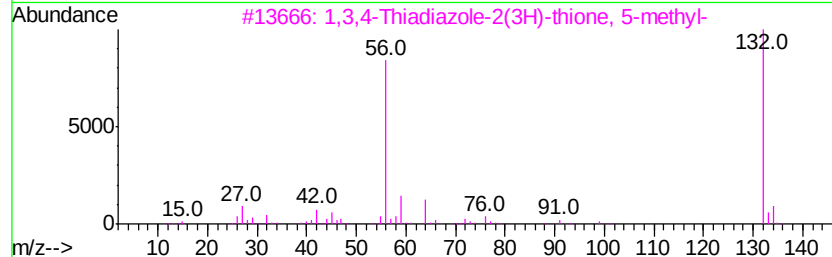
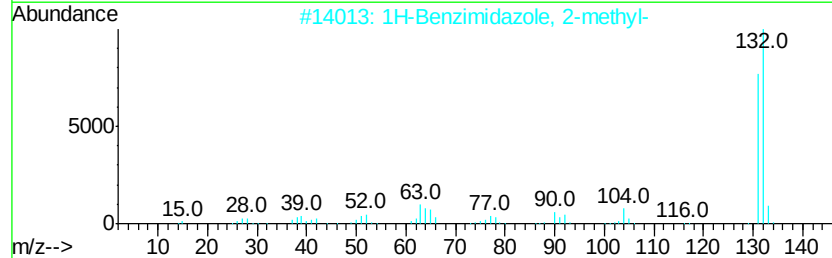
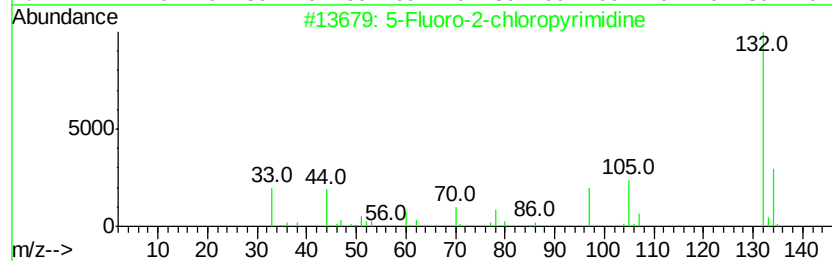
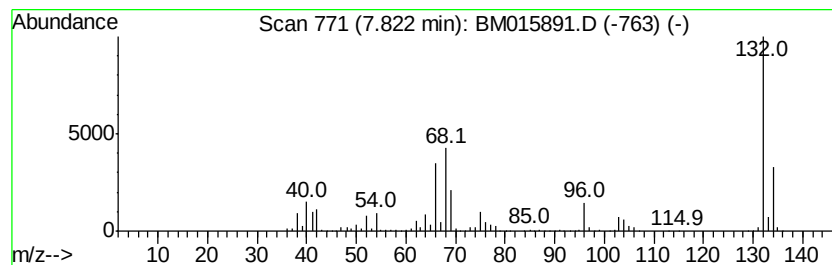
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Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	119.76 ng	4135670	1,4-Dichlorobenzene-d4	8.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	23
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22



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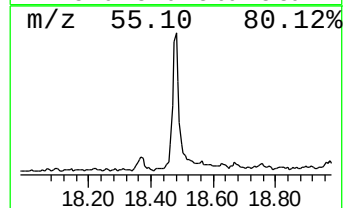
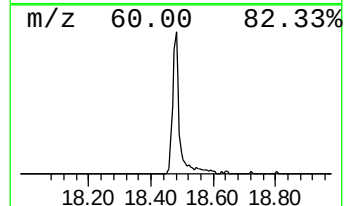
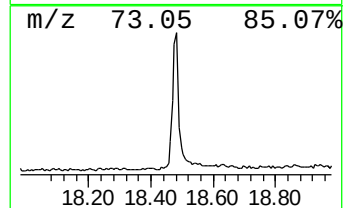
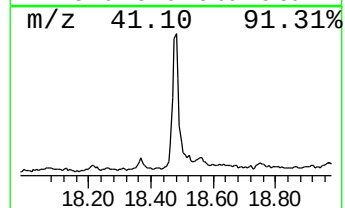
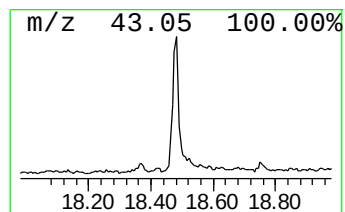
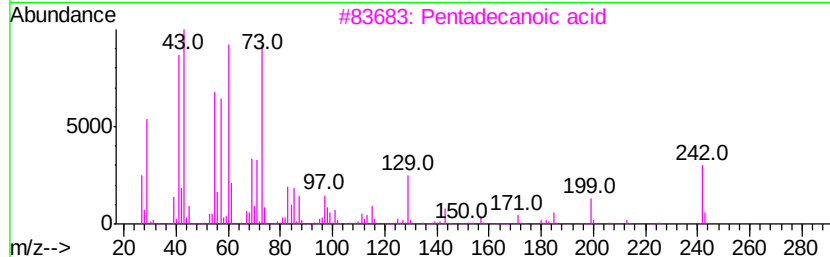
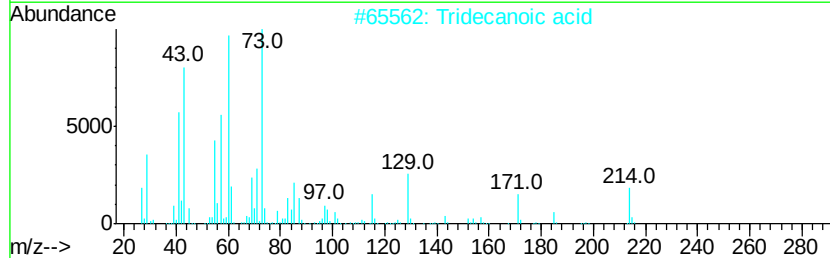
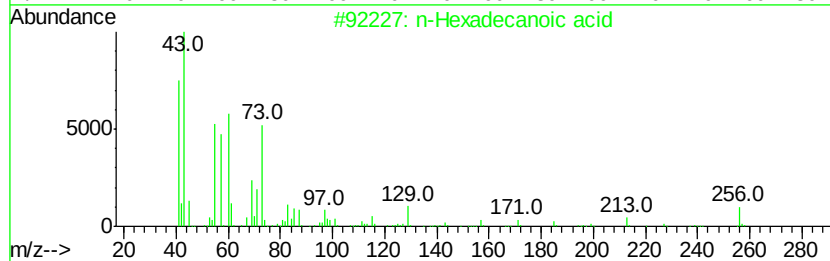
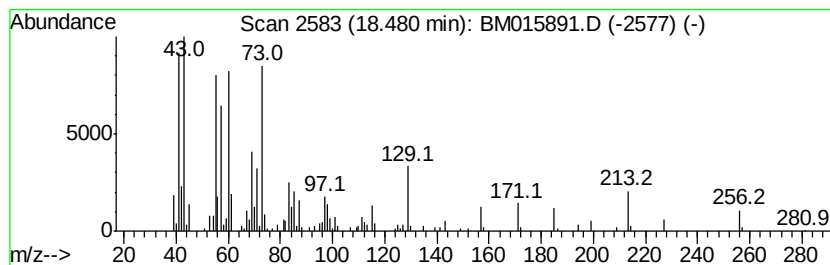
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.48	6.66 ng	376768	Phenanthrene-d10	17.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	74
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



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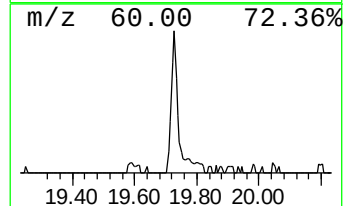
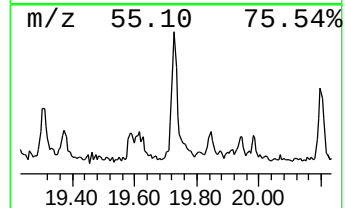
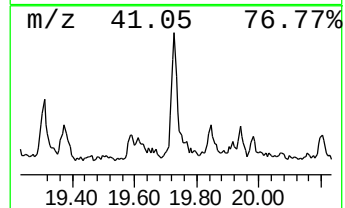
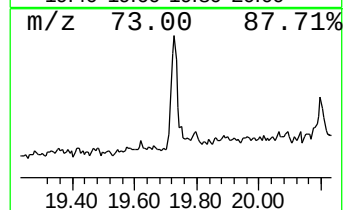
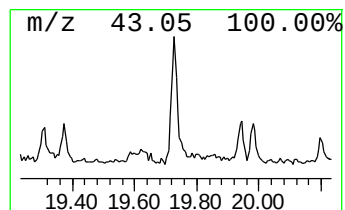
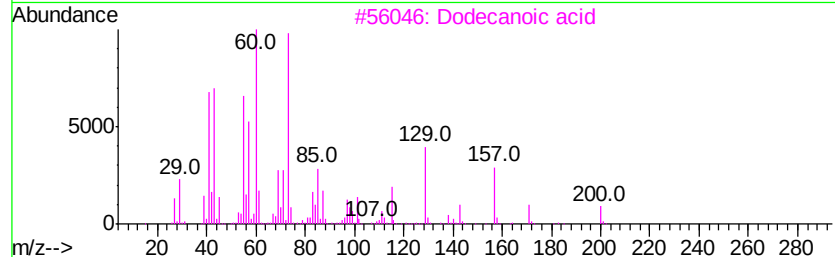
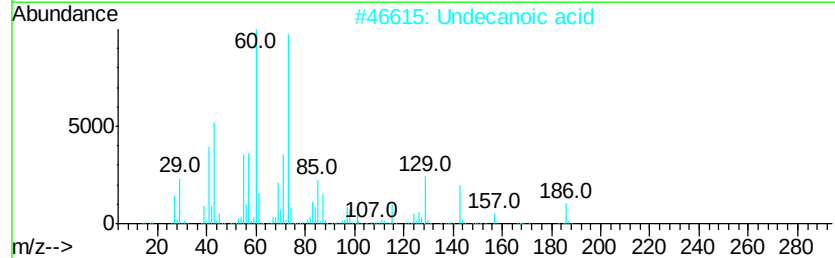
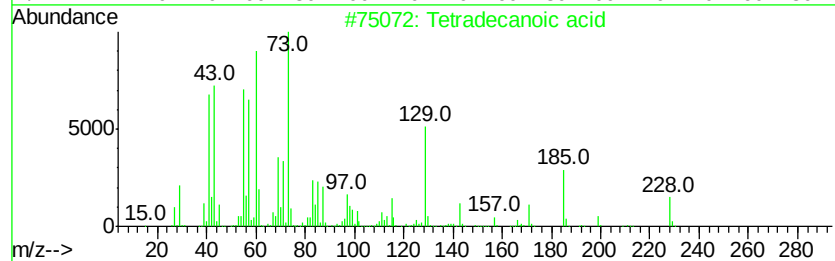
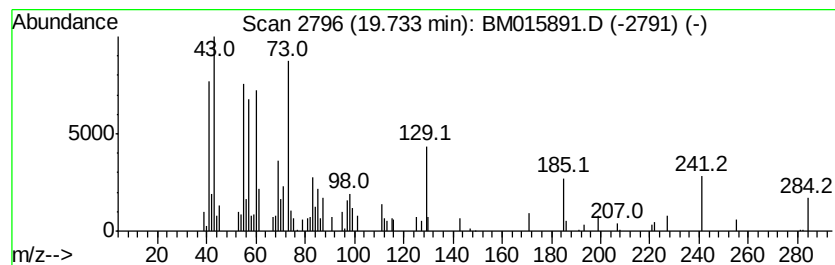
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Peak Number 5 Tetradecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	2.45 ng	134071	Chrysene-d12	21.74

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	76
2		Undecanoic acid	186	C11H22O2	000112-37-8	50
3		Dodecanoic acid	200	C12H24O2	000143-07-7	49
4		Tridecanoic acid	214	C13H26O2	000638-53-9	43
5		n-Decanoic acid	172	C10H20O2	000334-48-5	38



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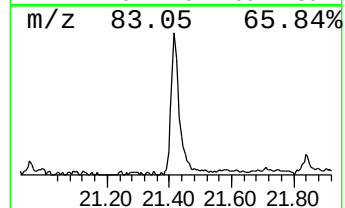
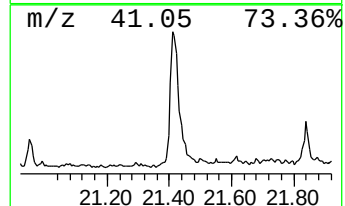
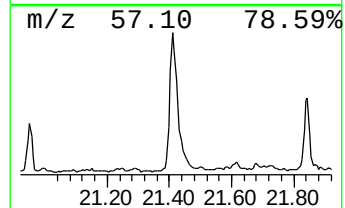
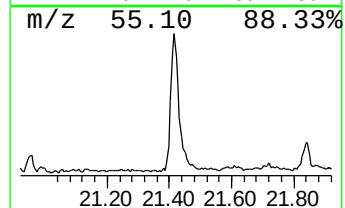
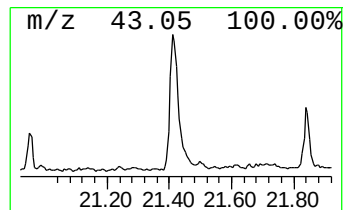
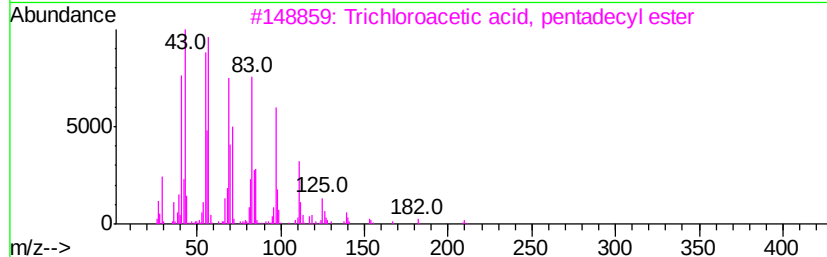
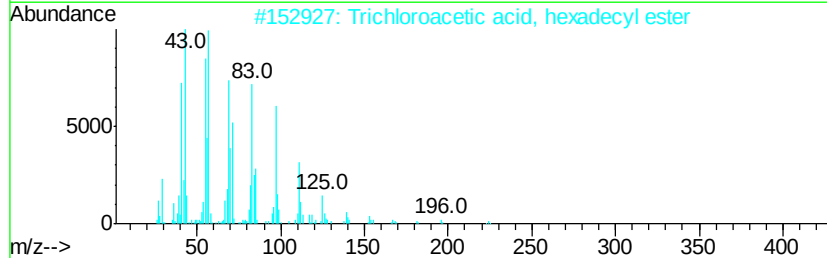
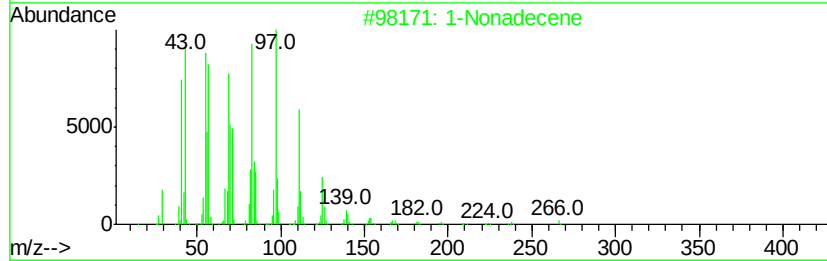
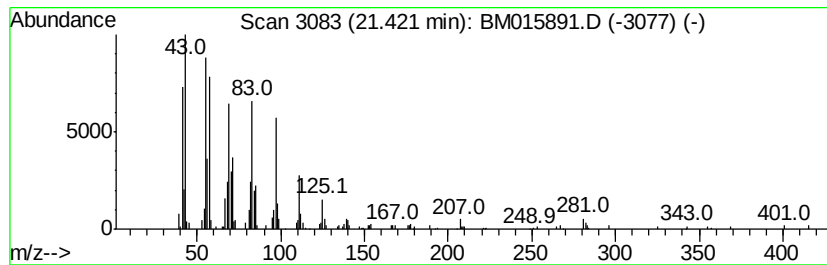
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Peak Number 6 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.42	8.99 ng	492307	Chrysene-d12	21.74	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	96
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
4	1-Tricosene	322	C23H46	018835-32-0	90
5	Cyclooctacosane	392	C28H56	000297-24-5	90



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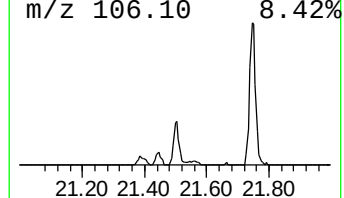
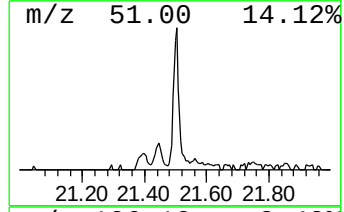
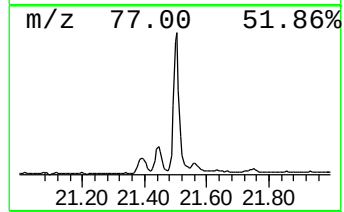
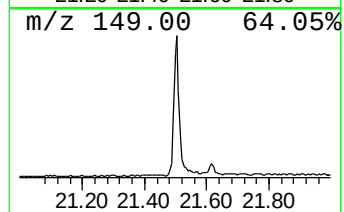
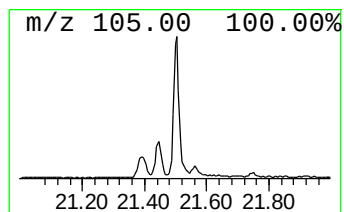
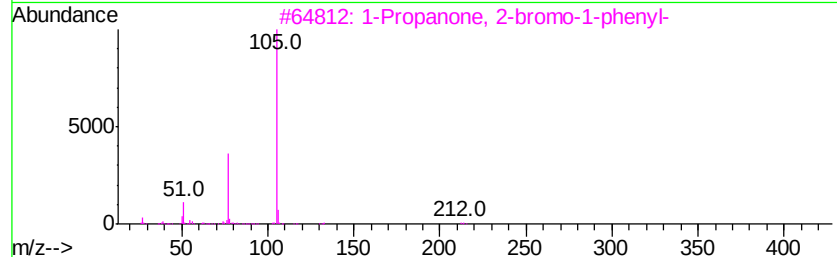
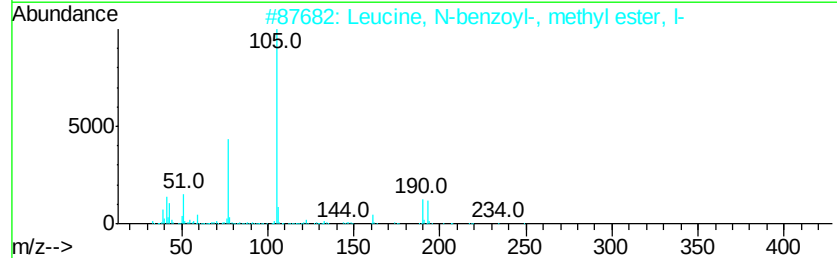
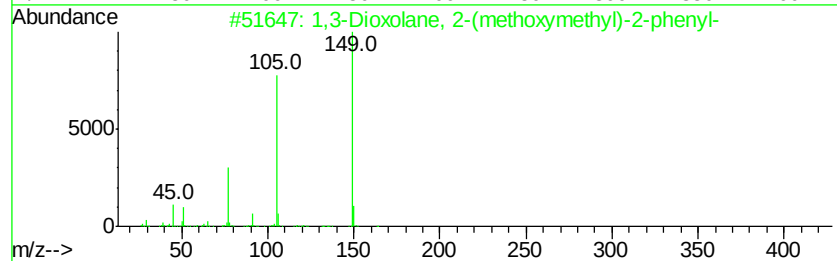
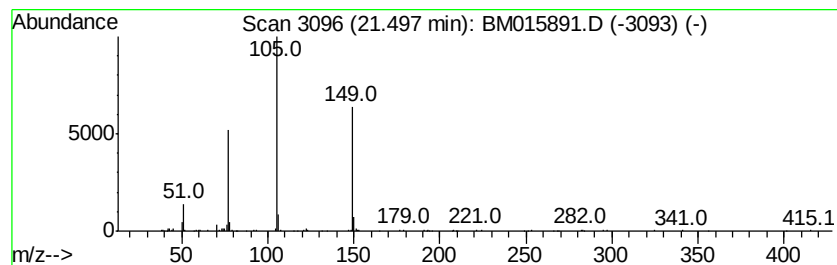
Instrument :
BNA_M
ClientSampleId :
CB-7-8-6-ST-WW-2@2.75

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM070518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
21.50	4.49 ng	245804	Chrysene-d12	21.74		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83	
2	Leucine, N-benzoyl-, methyl este...	249	C14H19NO3	003005-60-5	53	
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47	
4	4'-Nitrobenzanilide	242	C13H10N2O3	003393-96-2	47	
5	Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	47	



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM071118\
Data File : BM015891.D
Acq On : 11 Jul 2018 16:31
Operator : SJ/JU
Sample : J3906-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
CB-7-8-6-ST-WW-2@2.75

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.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...	5.32	13.1	ng	452947	1	8.29	690680	20.0
unknown7.82	7.82	119.8	ng	4135670	1	8.29	690680	20.0
n-Hexadecanoic acid	18.48	6.7	ng	376768	4	17.64	1131180	20.0
Tetradecanoic acid	19.73	2.5	ng	134071	5	21.74	1095570	20.0
1-Nonadecene	21.42	9.0	ng	492307	5	21.74	1095570	20.0
1,3-Dioxolane, 2-...	21.50	4.5	ng	245804	5	21.74	1095570	20.0