

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
 Data File : BP002320.D
 Acq On : 29 May 2020 18:02
 Operator : CG/JU
 Sample : L2773-17 2X
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 NM33-COMP-2020-0-6

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_P\METHODS\8270-BP052720.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	4.528	272	279	290	rBV3	56525	240589	2.51%	0.299%
2	5.222	390	397	415	rBV	3152425	4633744	48.26%	5.751%
3	6.787	656	663	676	rBV	3229911	5125498	53.38%	6.361%
4	7.605	793	802	812	rBV	1247030	1919385	19.99%	2.382%
5	7.922	848	856	865	rBV	2801119	4458413	46.43%	5.533%
6	8.746	984	996	1011	rBV	2127042	3534881	36.81%	4.387%
7	10.375	1265	1273	1289	rBV	1610747	2728210	28.41%	3.386%
8	12.869	1688	1697	1715	rBV	4934021	7515033	78.26%	9.327%
9	13.710	1833	1840	1849	rBV	389888	570332	5.94%	0.708%
10	14.251	1925	1932	1939	rBV	2339144	3542602	36.89%	4.397%
11	15.745	2177	2186	2198	rBV	3489892	5105884	53.17%	6.337%
12	16.404	2293	2298	2308	rBV2	161330	280452	2.92%	0.348%
13	17.004	2394	2400	2404	rBV	2844120	3963240	41.27%	4.919%
14	17.045	2404	2407	2413	rVB	428693	577379	6.01%	0.717%
15	17.140	2419	2423	2429	rVB	127933	182286	1.90%	0.226%
16	17.410	2464	2469	2475	rBV	91249	138248	1.44%	0.172%
17	17.881	2545	2549	2553	rVV	69702	99179	1.03%	0.123%
18	17.934	2553	2558	2566	rVV2	246429	365567	3.81%	0.454%
19	18.069	2576	2581	2585	rBV2	93021	155396	1.62%	0.193%
20	18.898	2718	2722	2727	rBV2	144922	205006	2.13%	0.254%
21	18.998	2733	2739	2742	rBV	1554300	1945121	20.26%	2.414%
22	19.028	2742	2744	2751	rVB	935752	1012754	10.55%	1.257%
23	19.381	2796	2804	2813	rBV	818495	1261829	13.14%	1.566%
24	19.592	2832	2840	2850	rVB	7482066	9602450	100.00%	11.917%
25	20.239	2946	2950	2953	rBV2	163713	195875	2.04%	0.243%
26	20.281	2953	2957	2962	rVB	392993	454408	4.73%	0.564%
27	20.851	3051	3054	3065	rVB3	631490	966391	10.06%	1.199%
28	21.104	3091	3097	3101	rBV2	3372586	4844257	50.45%	6.012%
29	21.139	3101	3103	3112	rVB	406631	522705	5.44%	0.649%
30	21.733	3200	3204	3209	rBV2	431821	601107	6.26%	0.746%
31	22.410	3316	3319	3330	rVB3	162498	257900	2.69%	0.320%
32	22.651	3356	3360	3364	rBV	329862	654417	6.82%	0.812%
33	22.698	3364	3368	3371	rVV2	1121670	1652670	17.21%	2.051%
34	22.733	3371	3374	3384	rVB	556031	874646	9.11%	1.085%

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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:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.216	3451	3456	3460	rBV	293955	505170	5.26%	0.627%
36	23.310	3467	3472	3488	rVB2	2177211	4269409	44.46%	5.299%
37	23.574	3512	3517	3524	rVB	322586	556142	5.79%	0.690%
38	23.922	3569	3576	3582	rBV	1627781	3199625	33.32%	3.971%
39	23.992	3583	3588	3601	rVB	568443	1184802	12.34%	1.470%
40	25.674	3869	3874	3882	rVB3	287951	673878	7.02%	0.836%

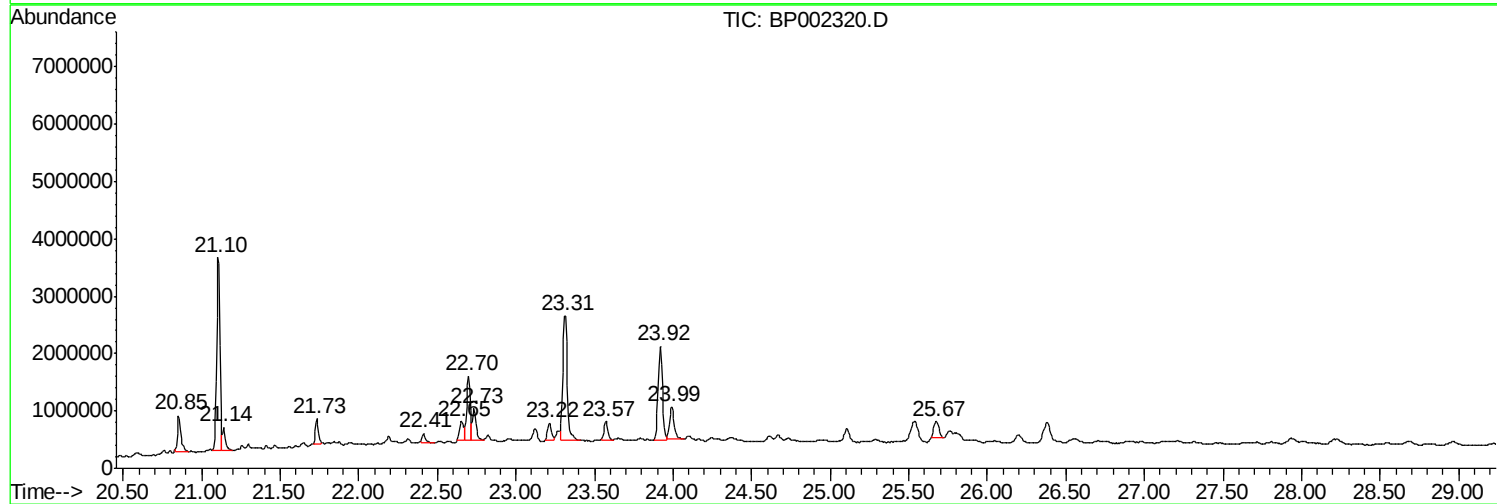
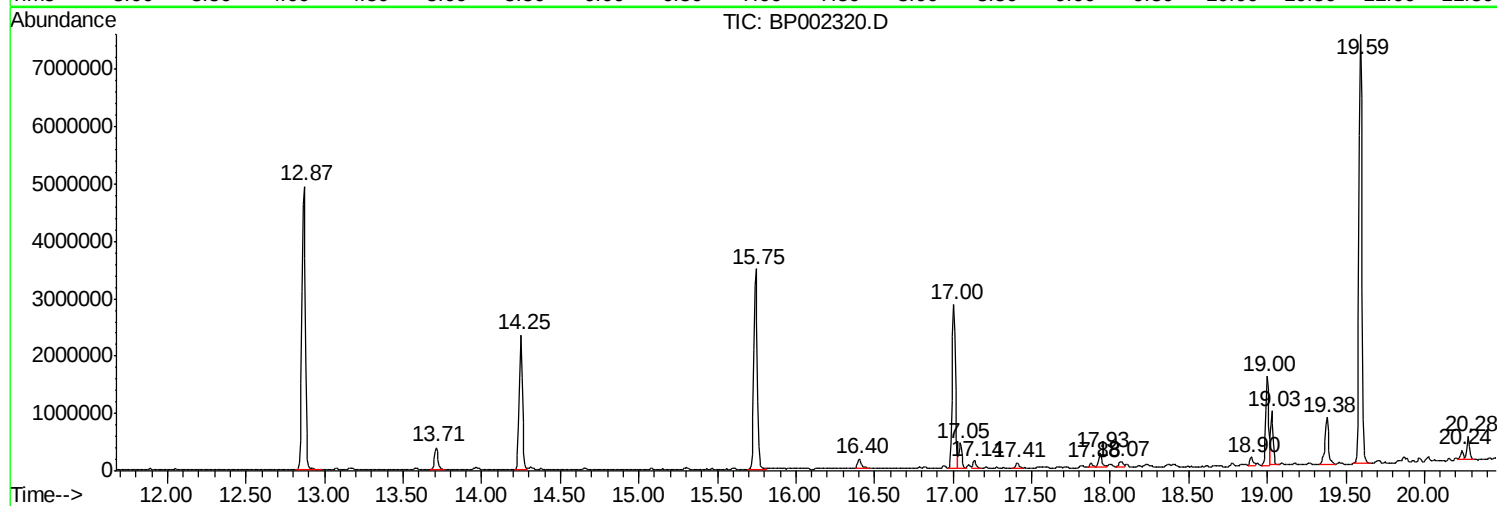
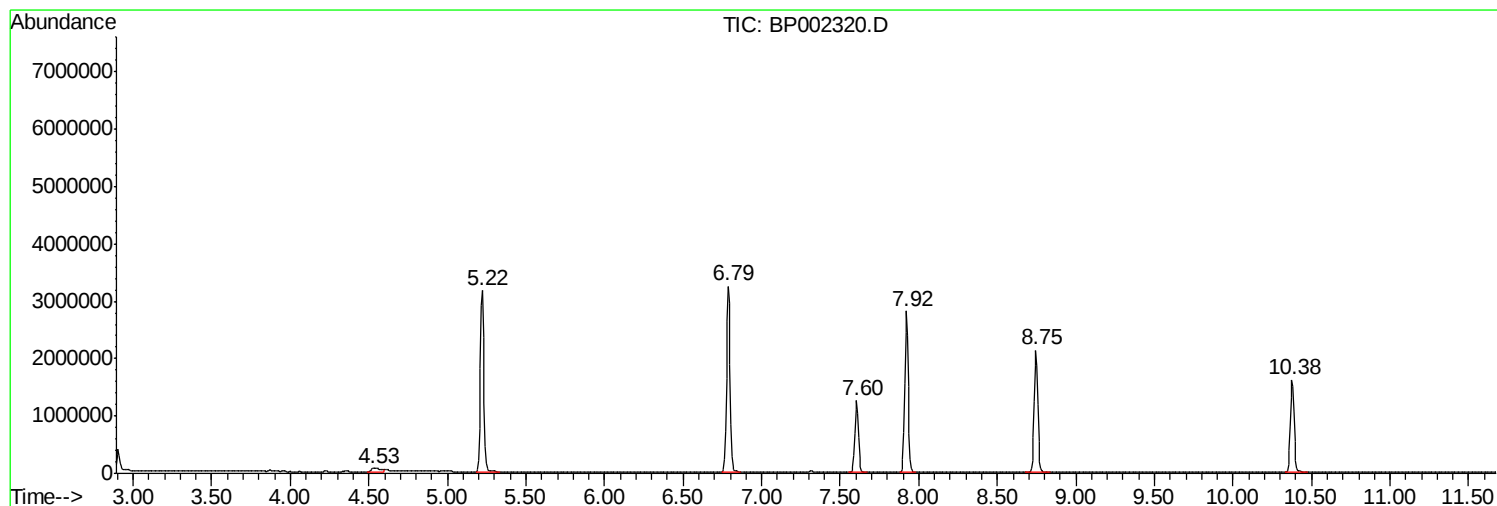
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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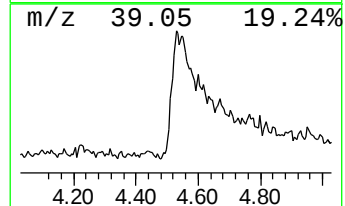
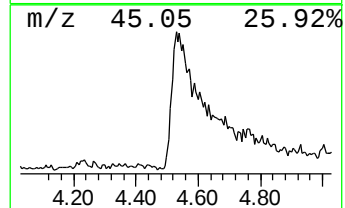
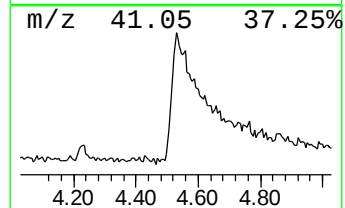
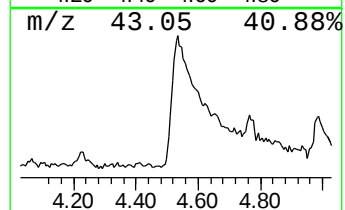
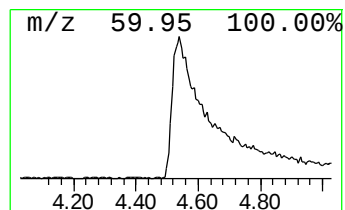
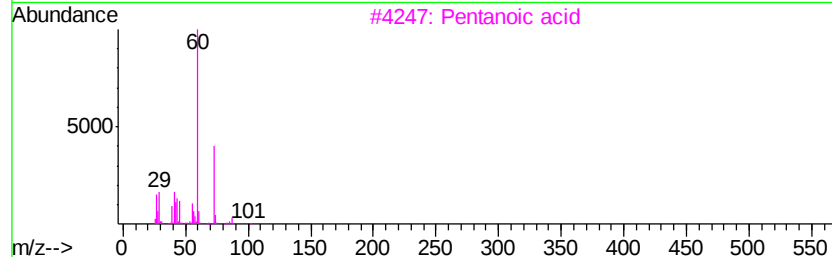
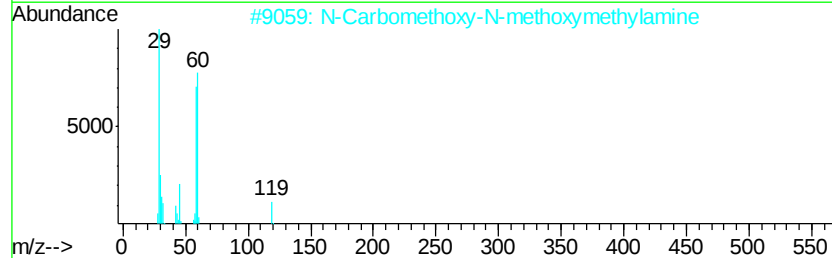
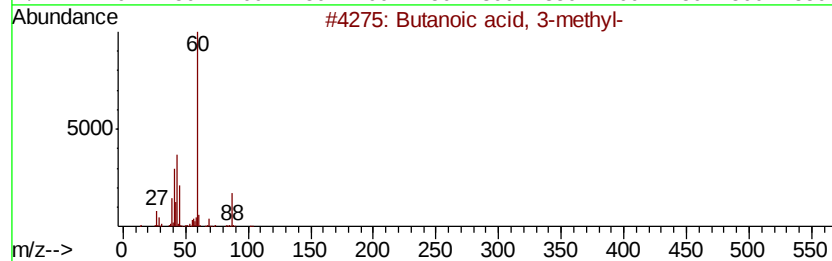
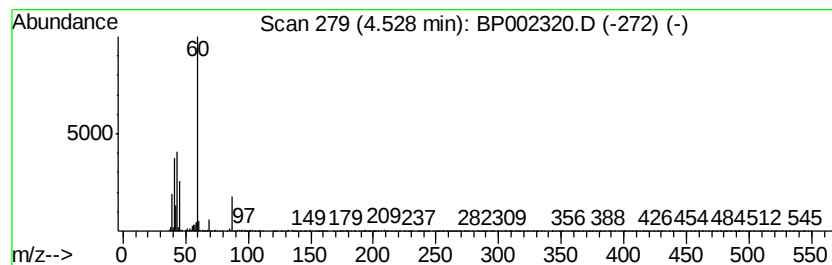
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.53	2.51 ng	240589	1,4-Dichlorobenzene-d4	7.60	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	90
2	N-Carbomethoxy-N-methoxymethylamine	119	C4H9NO3	153654-07-0	50
3	Pentanoic acid	102	C5H10O2	000109-52-4	45
4	Formic acid hydrazide	60	CH4N2O	000624-84-0	9
5	Urea, N-methyl-N-nitroso-	103	C2H5N3O2	000684-93-5	9



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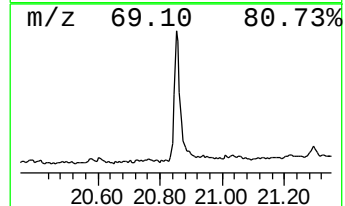
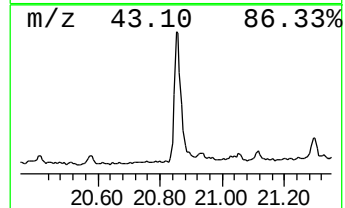
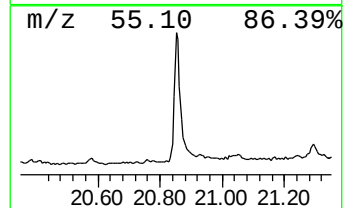
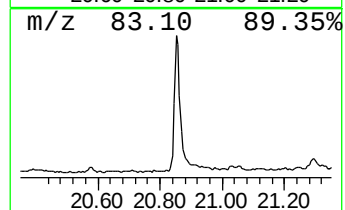
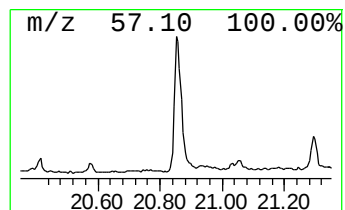
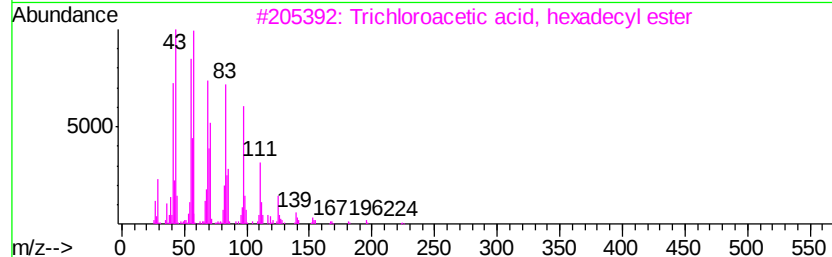
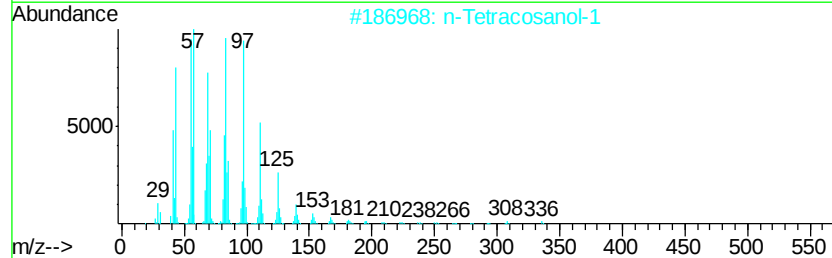
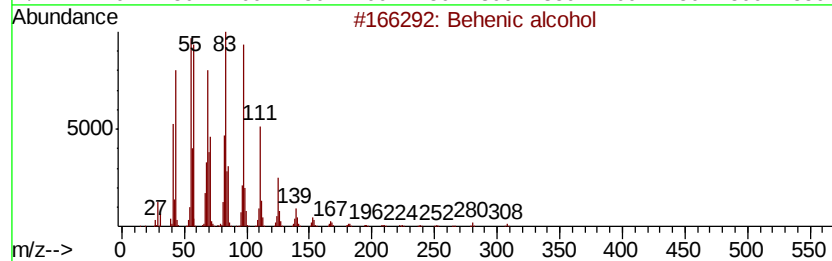
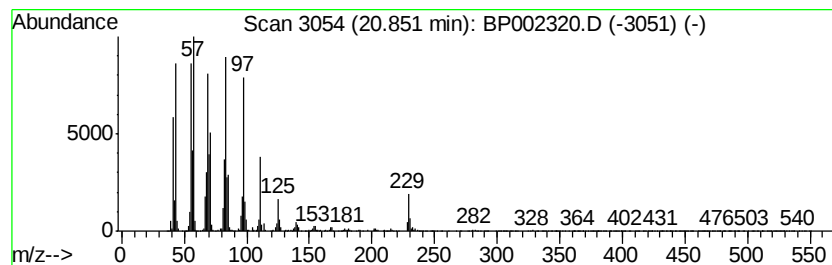
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	3.99 ng	966391	Chrysene-d12	21.10
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 94
2		n-Tetracosanol-1	354 C24H50O	000506-51-4 94
3		Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1 91
4		1-Heneicosanol	312 C21H44O	015594-90-8 91
5		1-Heneicosyl formate	340 C22H44O2	077899-03-7 91



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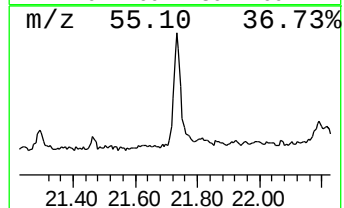
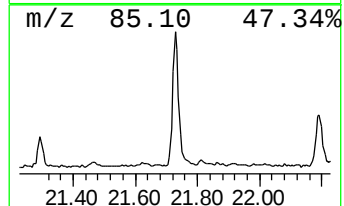
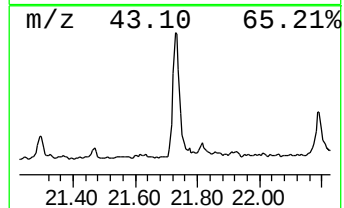
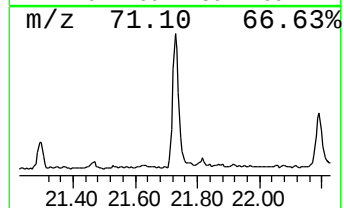
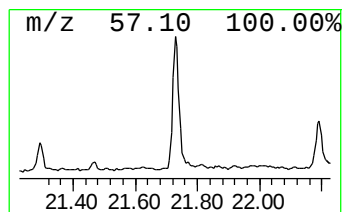
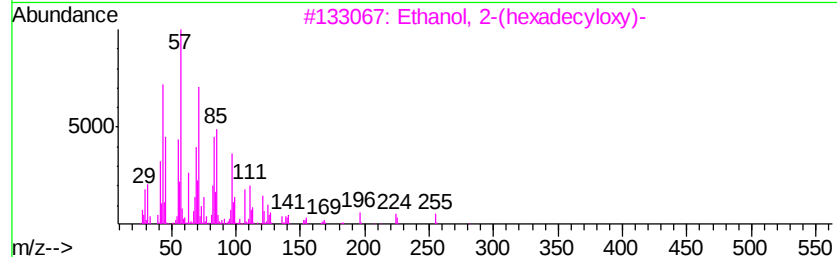
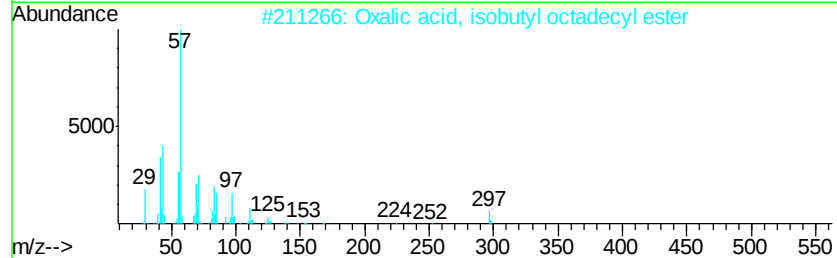
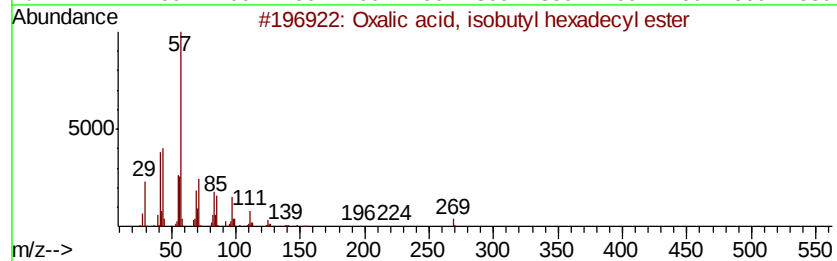
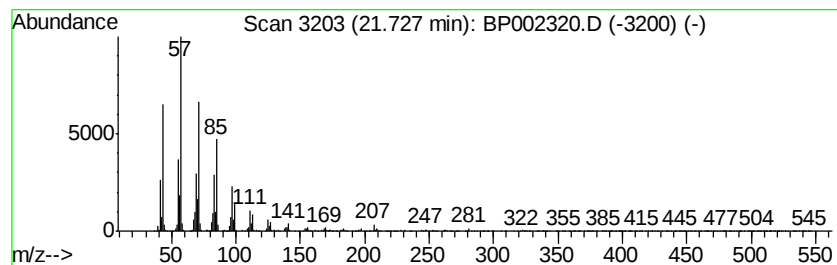
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Oxalic acid, isobutyl hexadecyl... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.73	2.48 ng	601107	Chrysene-d12	21.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91	
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91	
3	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	91	
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91	
5	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91	



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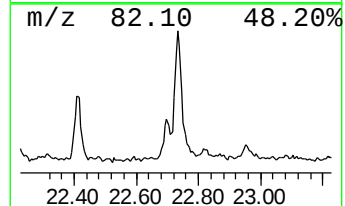
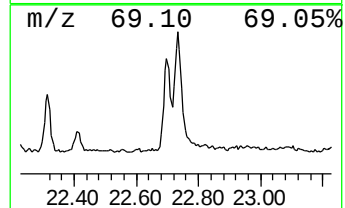
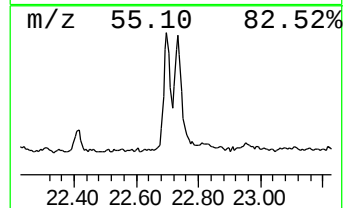
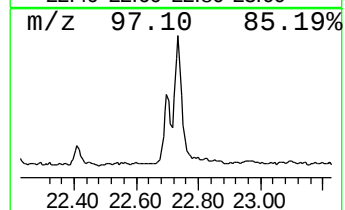
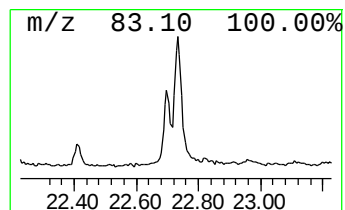
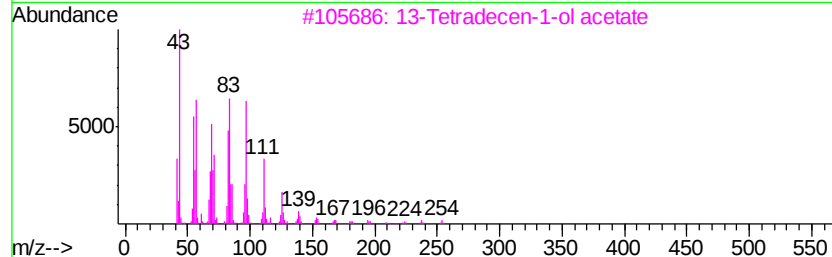
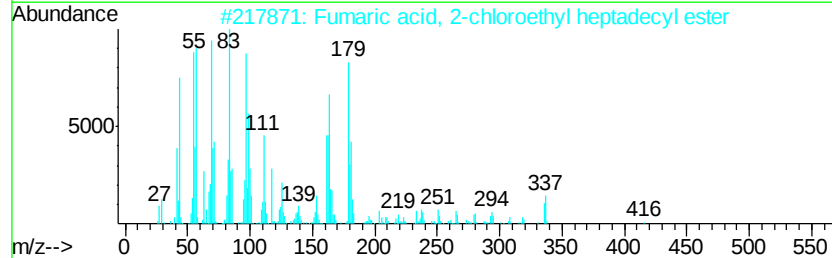
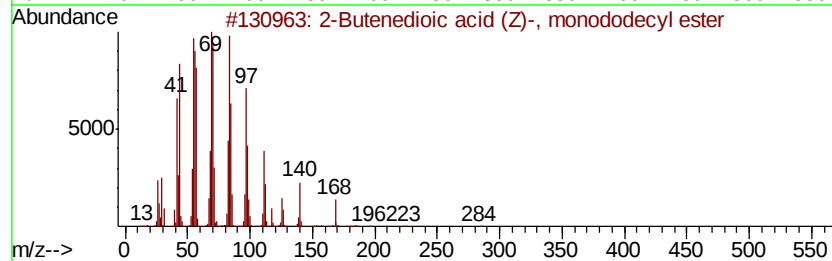
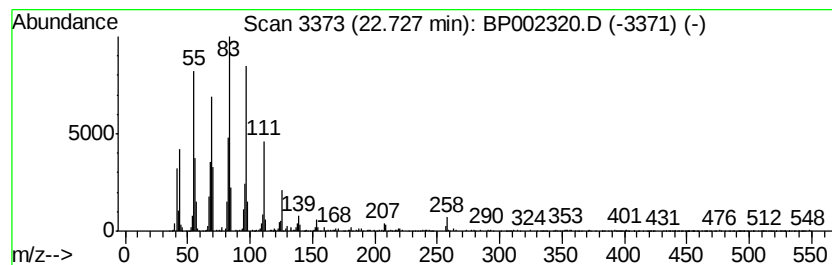
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 2-Butenedioic acid (Z)-, mo... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.73	4.10 ng	874646	Perylene-d12	23.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butenedioic acid (Z)-, monodod...	284	C16H28O4	002424-61-5	91
2		Fumaric acid, 2-chloroethyl hept...	416	C23H41ClO4	1000330-62-3	86
3		13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	74
4		1-Octadecanol	270	C18H38O	000112-92-5	68
5		1-Eicosanol	298	C20H42O	000629-96-9	58



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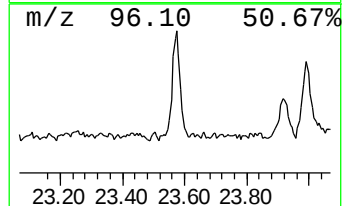
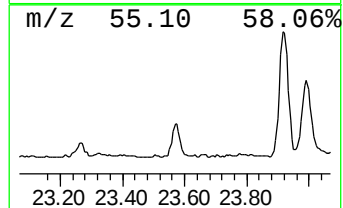
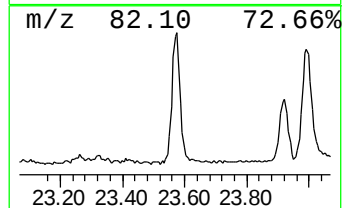
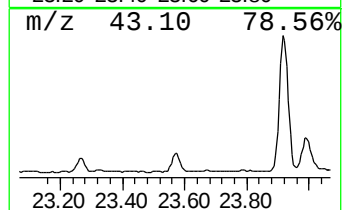
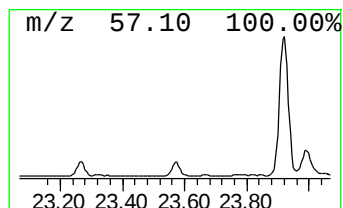
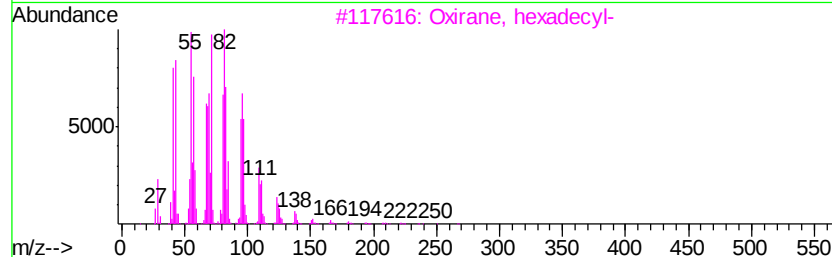
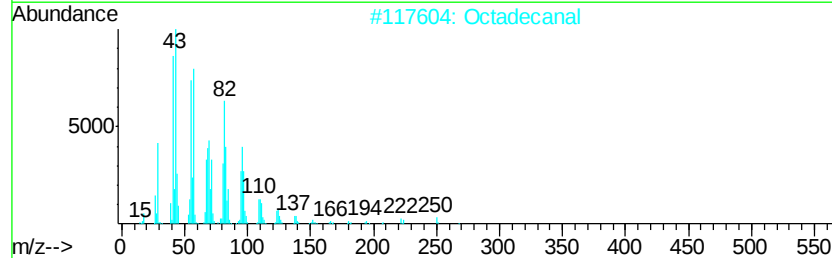
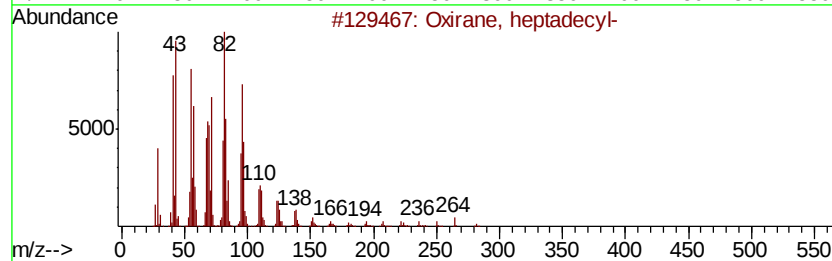
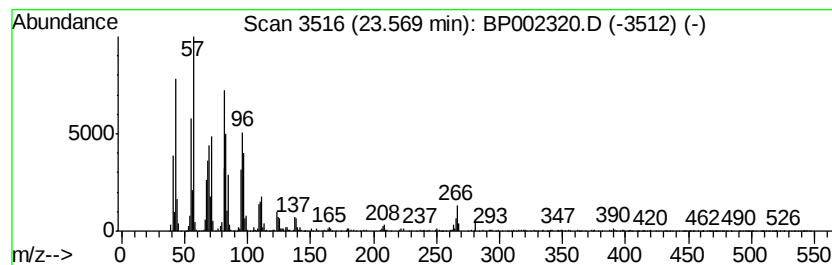
Instrument :
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 ClientSampleId :
 NM33-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP052720.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 6 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.57	2.61 ng	556142	Perylene-d12		23.31	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	87
2		Octadecanal	268	C18H36O	000638-66-4	86
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	68
4		(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	64
5		Olean-12-ene-3,16,21,22,28-pento...	572	C35H56O6	020089-98-9	56



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002320.D
Acq On : 29 May 2020 18:02
Operator : CG/JU
Sample : L2773-17 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NM33-COMP-2020-0-6

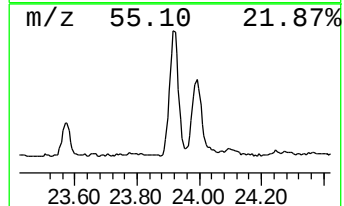
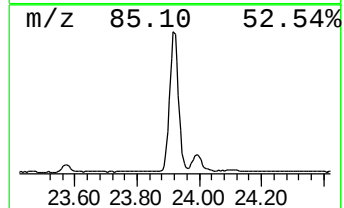
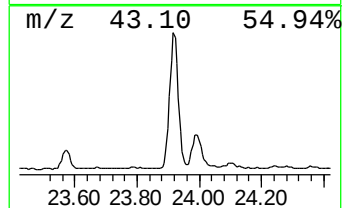
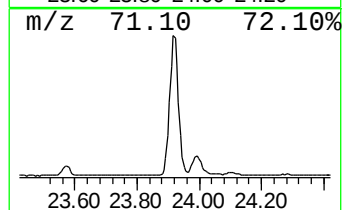
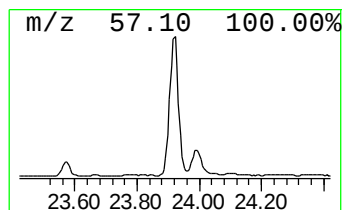
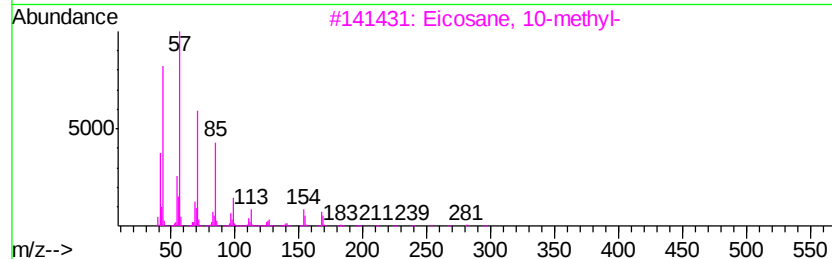
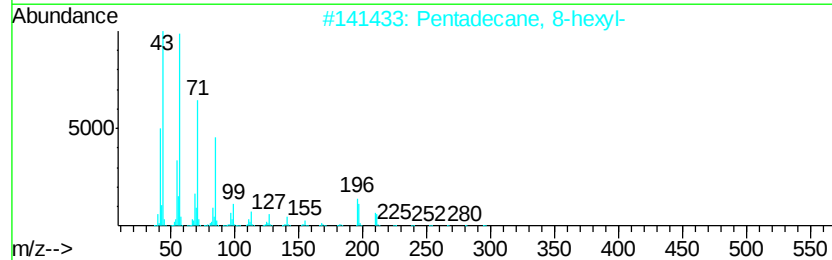
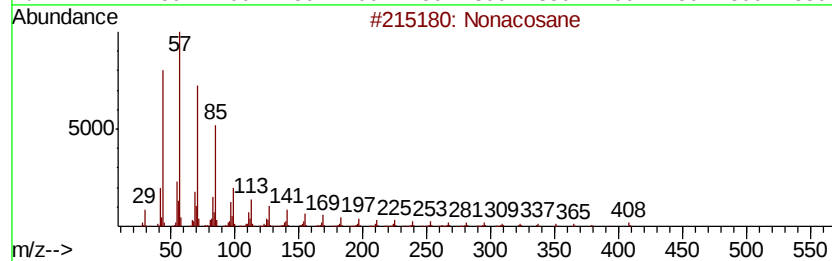
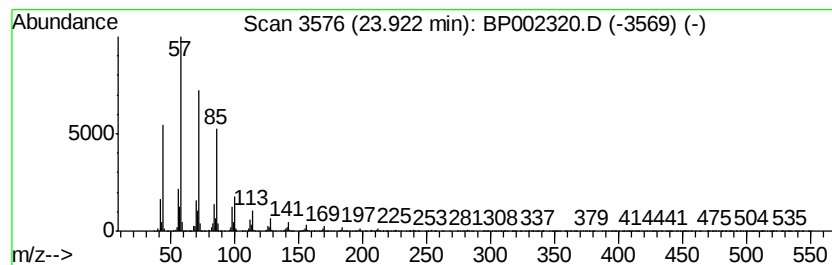
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	14.99 ng	3199630	Perylene-d12	23.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonacosane	408	C29H60	000630-03-5	95
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
3		Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
4		Hexacosane	366	C26H54	000630-01-3	91
5		Heneicosane	296	C21H44	000629-94-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002320.D
Acq On : 29 May 2020 18:02
Operator : CG/JU
Sample : L2773-17 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

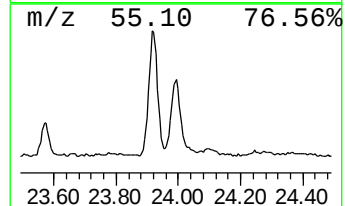
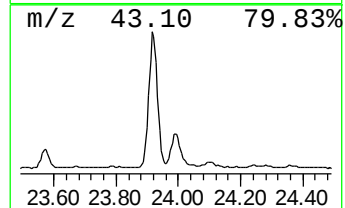
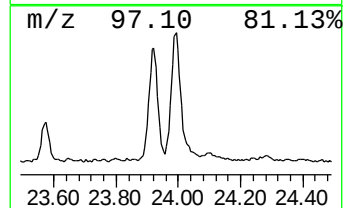
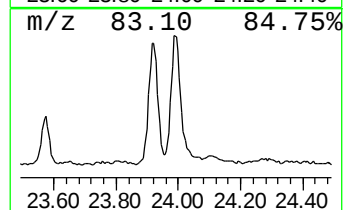
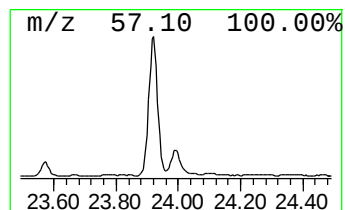
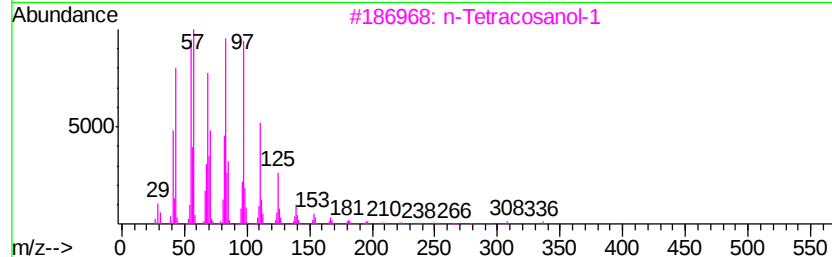
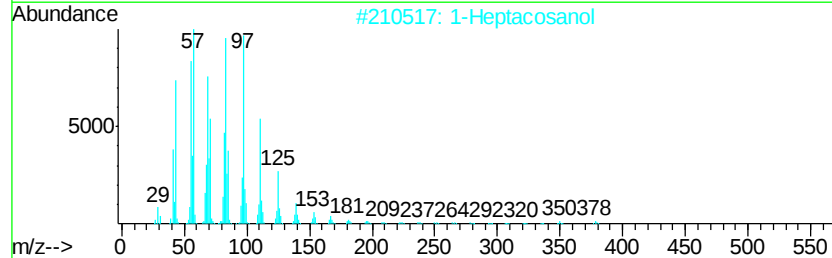
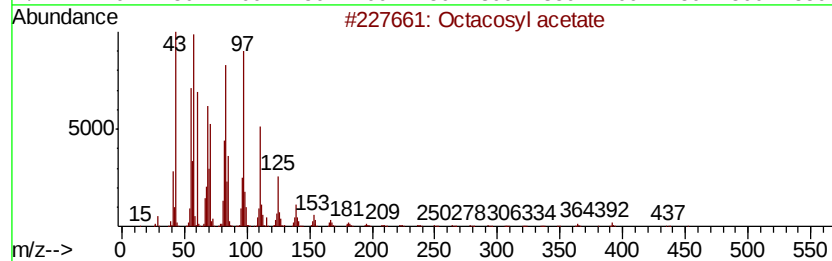
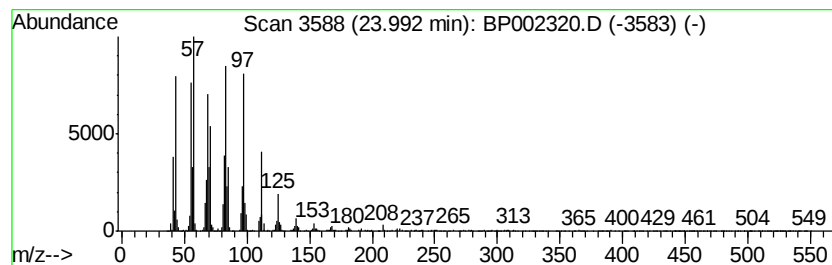
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
23.99	5.55 ng	1184800	Perylene-d12		23.31
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl acetate	452	C30H60O2	018206-97-8	95
2	1-Heptacosanol	396	C27H56O	002004-39-9	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	Octacosanol	410	C28H58O	000557-61-9	91
5	Behenic alcohol	326	C22H46O	000661-19-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
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Sample : L2773-17 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NM33-COMP-2020-0-6

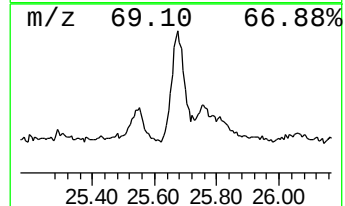
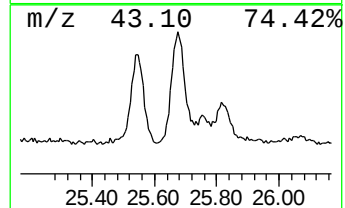
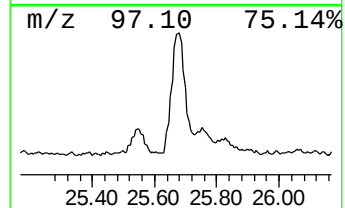
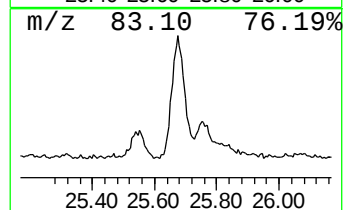
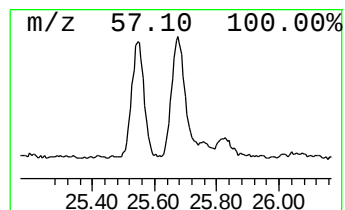
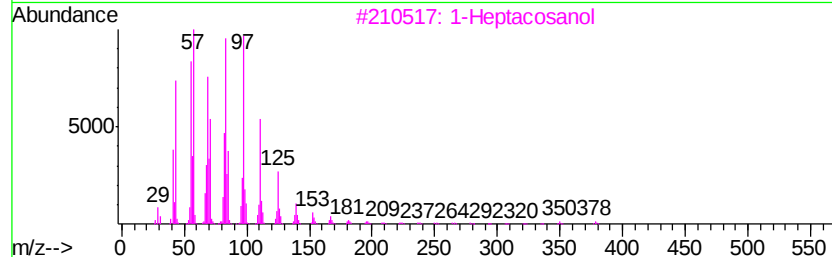
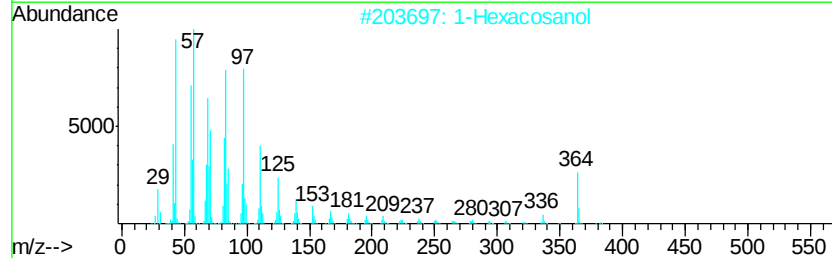
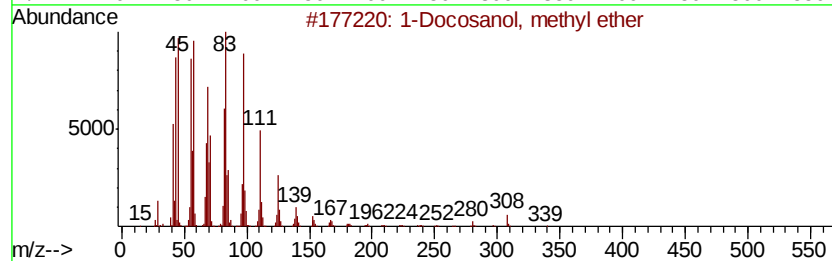
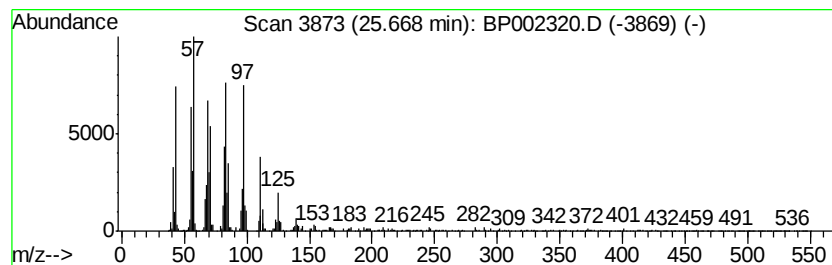
Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Docosanol, methyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.67	3.16 ng	673878	Perylene-d12	23.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	93
2		1-Hexacosanol	382	C26H54O	000506-52-5	91
3		1-Heptacosanol	396	C27H56O	002004-39-9	90
4		Heptadecafluorononanoic acid, he...	702	C26H35F17O2	1000356-03-3	90
5		1-Heneicosanol	312	C21H44O	015594-90-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP052920\
Data File : BP002320.D
Acq On : 29 May 2020 18:02
Operator : CG/JU
Sample : L2773-17 2X
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
NM33-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP052720.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
Butanoic acid, 3-...	4.53	2.5	ng	240589	1	7.60	1919390	20.0
Behenic alcohol	20.85	4.0	ng	966391	5	21.10	4844260	20.0
Oxalic acid, isob...	21.73	2.5	ng	601107	5	21.10	4844260	20.0
2-Butenedioic aci...	22.73	4.1	ng	874646	6	23.31	4269410	20.0
Oxirane, heptadecyl-	23.57	2.6	ng	556142	6	23.31	4269410	20.0
Nonacosane	23.92	15.0	ng	3199630	6	23.31	4269410	20.0
Octacosyl acetate	23.99	5.5	ng	1184800	6	23.31	4269410	20.0
1-Docosanol, meth...	25.67	3.2	ng	673878	6	23.31	4269410	20.0