

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP052920\
 Data File : BP002327.D
 Acq On : 29 May 2020 22:01
 Operator : CG/JU
 Sample : L2744-11 2X
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 NM79-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	4.540	274	281	302	rBV2	84550	506475	6.45%	0.568%
2	5.222	391	397	407	rBV	2605849	3812497	48.54%	4.273%
3	6.793	654	664	678	rBV	2670605	4252792	54.14%	4.767%
4	7.604	795	802	810	rBV	1438166	2263474	28.82%	2.537%
5	7.922	849	856	865	rBV	2268739	3631022	46.23%	4.070%
6	8.746	989	996	1012	rBV	1711374	2804726	35.71%	3.144%
7	10.381	1266	1274	1287	rBV	1911082	3251203	41.39%	3.644%
8	12.051	1552	1558	1569	rBV3	37427	105885	1.35%	0.119%
9	12.869	1690	1697	1715	rBV	4228087	6171555	78.57%	6.917%
10	13.710	1834	1840	1850	rBV	500961	821588	10.46%	0.921%
11	13.969	1879	1884	1892	rVB	59299	116656	1.49%	0.131%
12	14.251	1925	1932	1939	rBV	2871599	4359465	55.50%	4.886%
13	15.163	2078	2087	2095	rBV2	138656	206936	2.63%	0.232%
14	15.745	2178	2186	2195	rBV	2891552	4196584	53.43%	4.704%
15	15.910	2209	2214	2219	rBV4	63746	101086	1.29%	0.113%
16	16.404	2289	2298	2303	rBV4	171236	301574	3.84%	0.338%
17	16.945	2386	2390	2393	rBV2	68648	94748	1.21%	0.106%
18	17.010	2395	2401	2405	rVV	3387169	4776423	60.81%	5.353%
19	17.051	2405	2408	2413	rVV	308842	416837	5.31%	0.467%
20	17.104	2413	2417	2420	rVV2	66488	99269	1.26%	0.111%
21	17.139	2420	2423	2428	rVB	128978	175642	2.24%	0.197%
22	17.410	2465	2469	2478	rBV3	145232	205693	2.62%	0.231%
23	17.822	2534	2539	2543	rBV3	72324	125665	1.60%	0.141%
24	17.880	2545	2549	2554	rVV2	253250	378859	4.82%	0.425%
25	17.939	2554	2559	2566	rVV2	678147	1012699	12.89%	1.135%
26	17.998	2567	2569	2575	rVV2	80311	124792	1.59%	0.140%
27	18.069	2577	2581	2585	rVV3	79406	115813	1.47%	0.130%
28	18.416	2636	2640	2646	rVB6	78990	130437	1.66%	0.146%
29	18.780	2698	2702	2707	rBV3	68719	109122	1.39%	0.122%
30	18.904	2719	2723	2727	rBV2	194960	282829	3.60%	0.317%
31	19.004	2734	2740	2743	rBV	2360886	2984257	37.99%	3.345%
32	19.033	2743	2745	2749	rVB	755418	774267	9.86%	0.868%
33	19.180	2767	2770	2775	rBV3	67184	86082	1.10%	0.096%
34	19.386	2797	2805	2808	rBV	695869	1096784	13.96%	1.229%

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 Peak separation: 5

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35	19.592	2835	2840	2851	rVB	5934796	7854735	100.00%	8.804%
36	19.933	2895	2898	2901	rBV	97661	90414	1.15%	0.101%
37	20.027	2911	2914	2917	rVB2	81610	96014	1.22%	0.108%
38	20.245	2947	2951	2954	rBV	225636	258446	3.29%	0.290%
39	20.280	2954	2957	2961	rVB3	136166	152936	1.95%	0.171%
40	20.416	2978	2980	2984	rVB	90625	81972	1.04%	0.092%
41	20.857	3048	3055	3066	rBV5	771879	1452358	18.49%	1.628%
42	21.110	3092	3098	3102	rBV	3829304	5344261	68.04%	5.990%
43	21.145	3102	3104	3111	rVB	396366	465755	5.93%	0.522%
44	21.298	3127	3130	3137	rVB2	218405	264715	3.37%	0.297%
45	21.733	3200	3204	3214	rVB	816025	1208469	15.39%	1.354%
46	22.192	3279	3282	3290	rVB	244707	359529	4.58%	0.403%
47	22.415	3316	3320	3325	rVB	417180	541303	6.89%	0.607%
48	22.657	3357	3361	3364	rBV	330138	591833	7.53%	0.663%
49	22.698	3364	3368	3372	rVV	1360391	2296163	29.23%	2.574%
50	22.733	3372	3374	3384	rVB	1060565	1533007	19.52%	1.718%
51	23.215	3453	3456	3461	rBV	247104	387672	4.94%	0.435%
52	23.268	3462	3465	3468	rVV	264476	436612	5.56%	0.489%
53	23.315	3468	3473	3490	rVB	2525866	4987565	63.50%	5.590%
54	23.574	3512	3517	3525	rVB	885051	1483979	18.89%	1.663%
55	23.921	3570	3576	3583	rBV	2535096	5001177	63.67%	5.605%
56	23.992	3583	3588	3603	rVB	1388555	2844619	36.22%	3.188%
57	26.380	3989	3994	4011	rVB2	546157	1593761	20.29%	1.786%

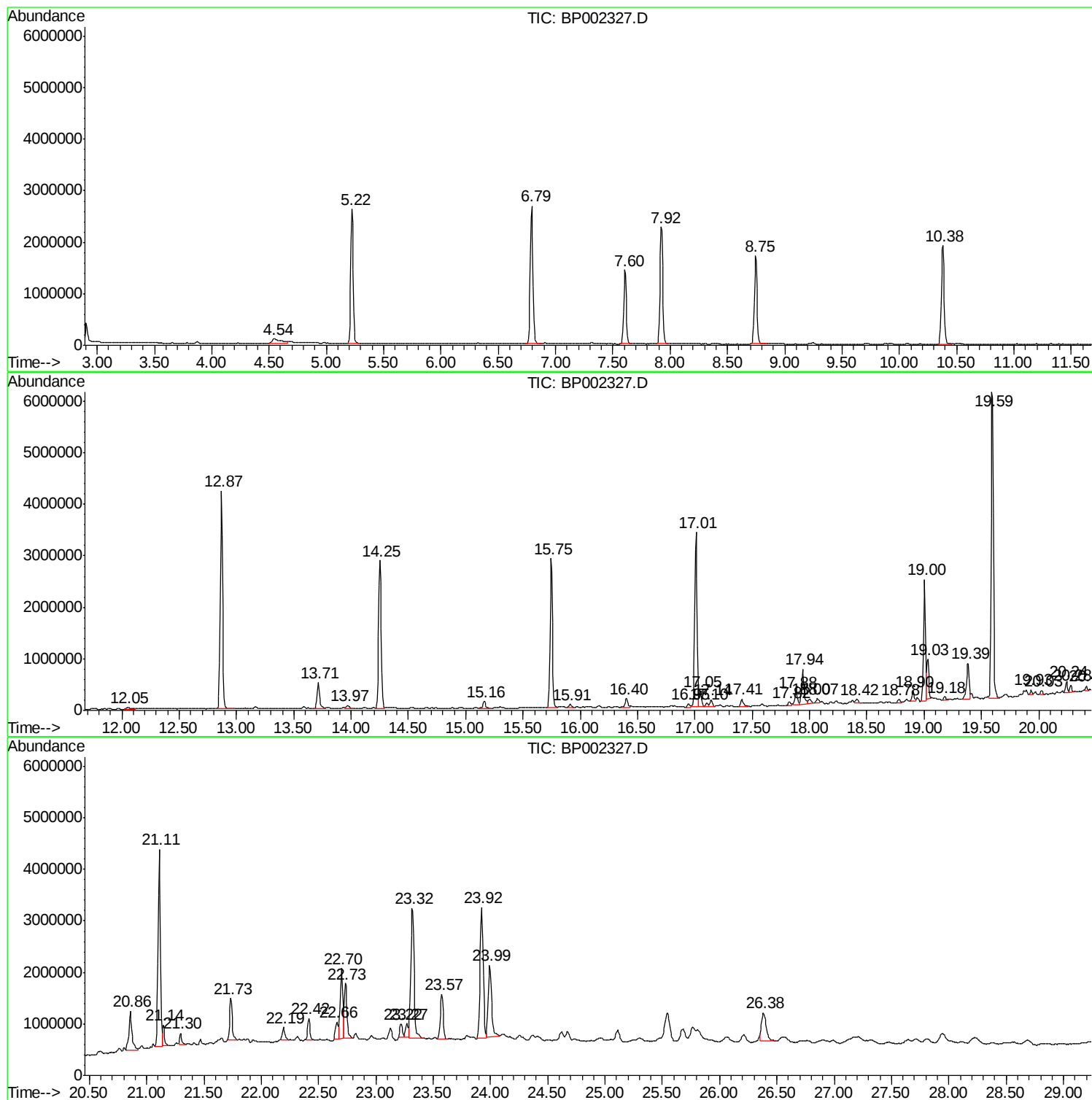
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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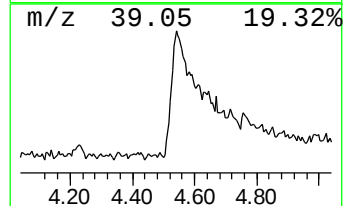
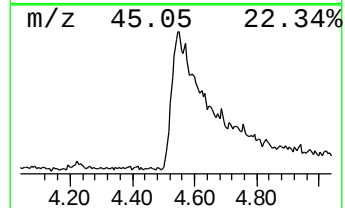
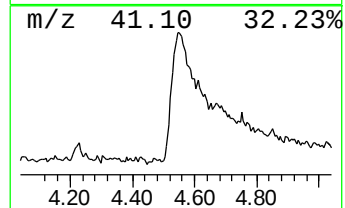
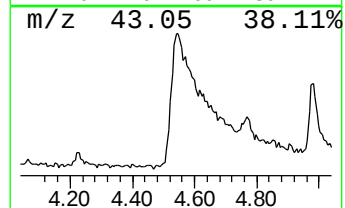
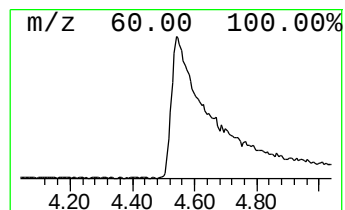
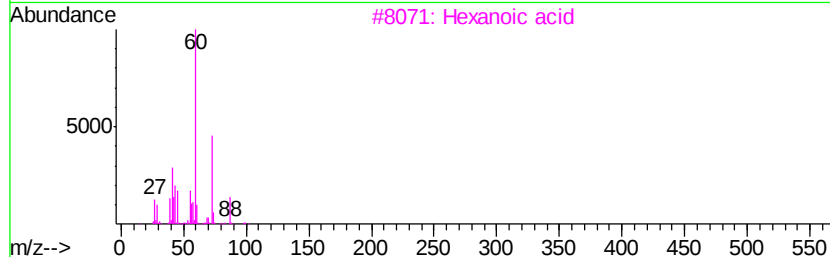
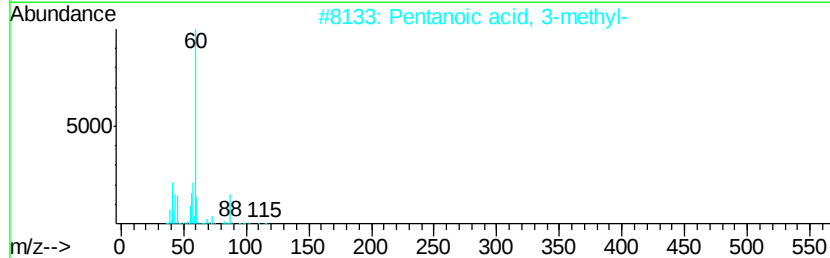
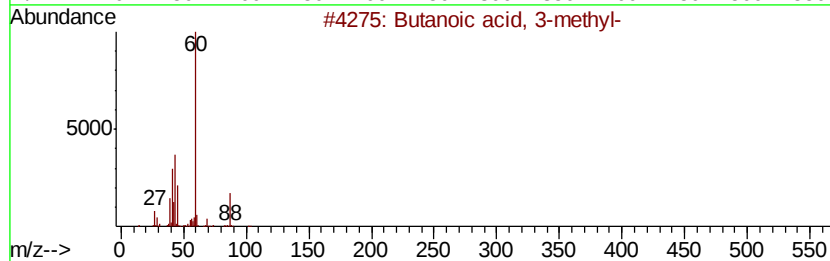
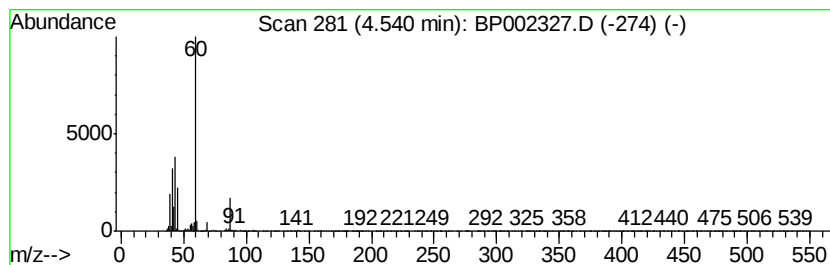
Instrument :
BNA_P
ClientSampleId :
NM79-COMP-2020-0-6

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 1 Butanoic acid, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.54	4.48 ng	506475	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	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	64
3	Hexanoic acid	116	C6H12O2	000142-62-1	40
4	N-Carbomethoxy-N-methoxymethylamine	119	C4H9NO3	153654-07-0	39
5	Pentanoic acid	102	C5H10O2	000109-52-4	38



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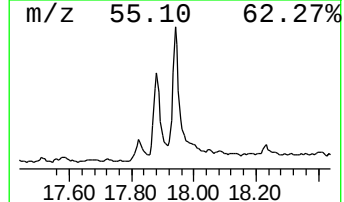
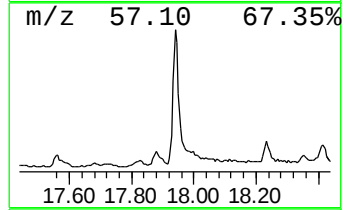
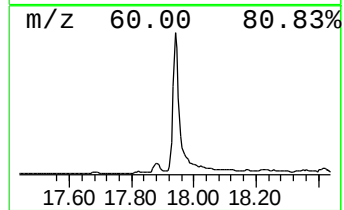
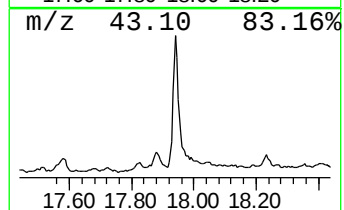
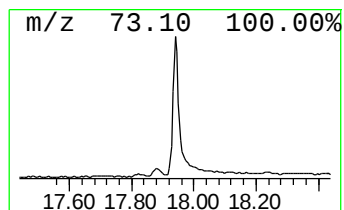
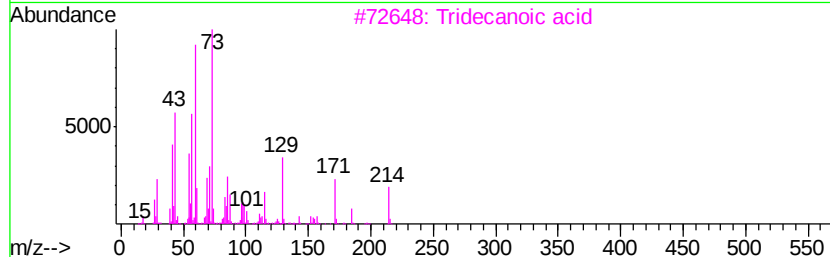
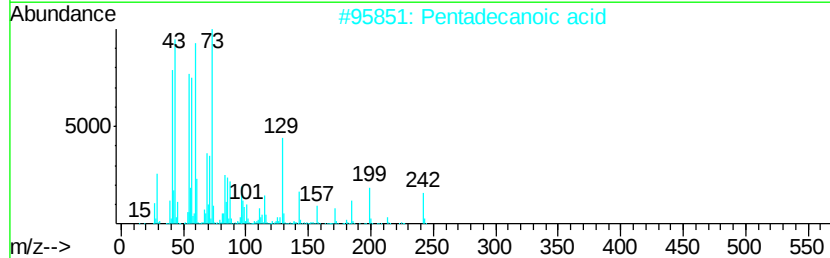
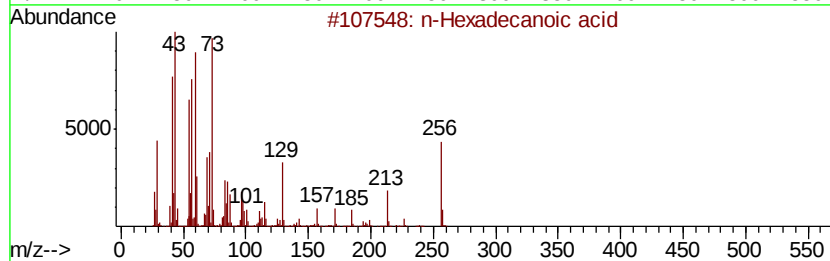
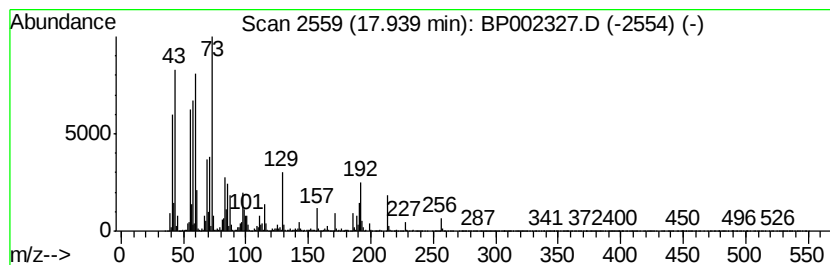
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.94	4.24 ng	1012700	Phenanthrene-d10	17.01	
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	68
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47



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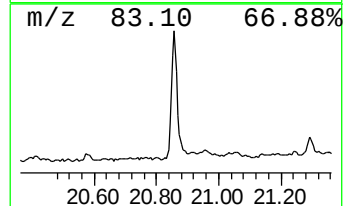
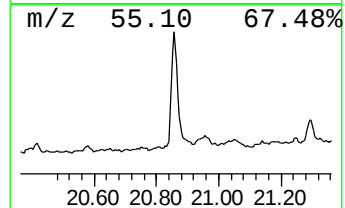
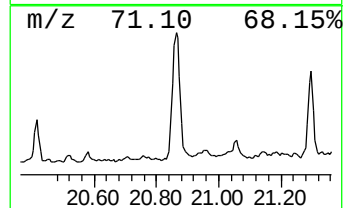
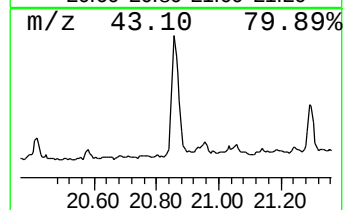
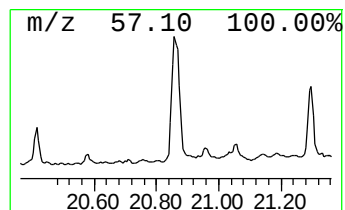
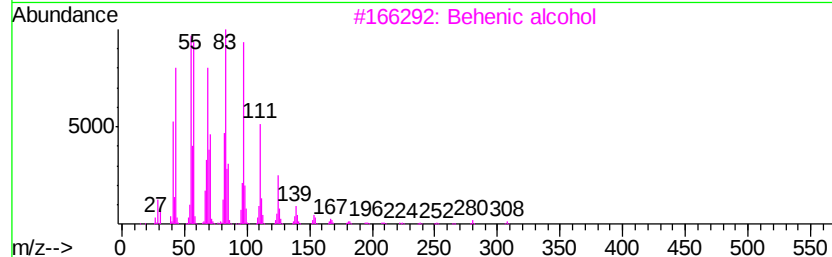
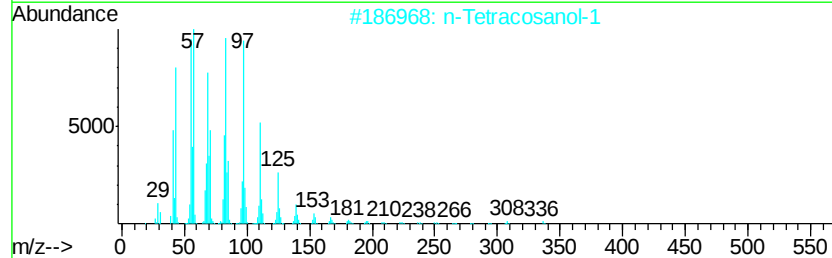
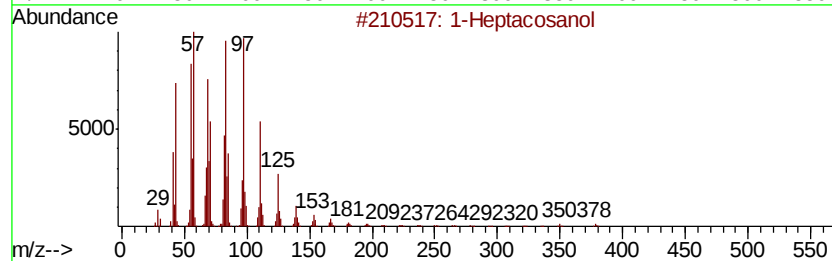
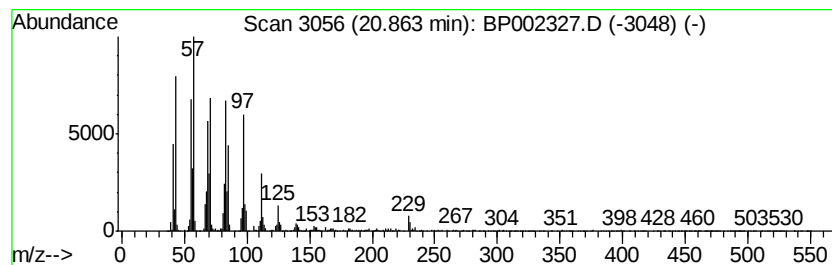
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Heptacosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	5.44 ng	1452360	Chrysene-d12	21.11
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Heptacosanol	396 C27H56O	002004-39-9	94
2	n-Tetracosanol-1	354 C24H50O	000506-51-4	94
3	Behenic alcohol	326 C22H46O	000661-19-8	94
4	17-Pentatriacontene	491 C35H70	006971-40-0	94
5	Dichloroacetic acid, heptadecyl ...	366 C19H36Cl2O2	1000282-98-2	94



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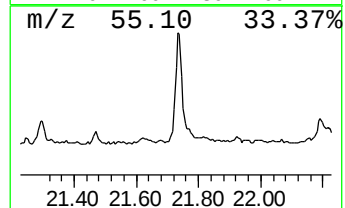
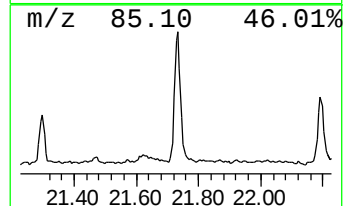
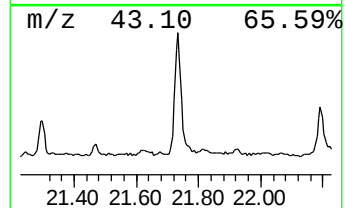
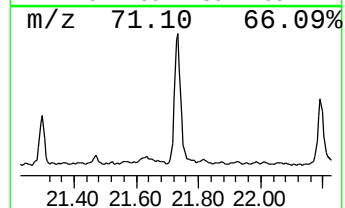
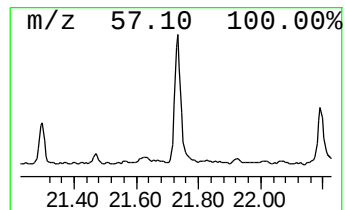
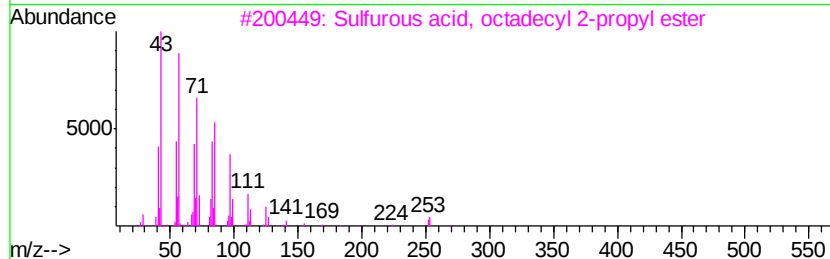
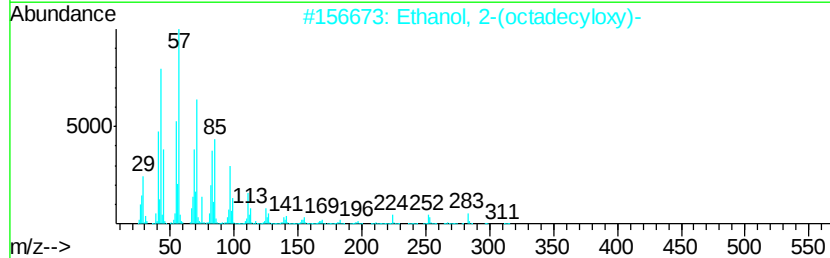
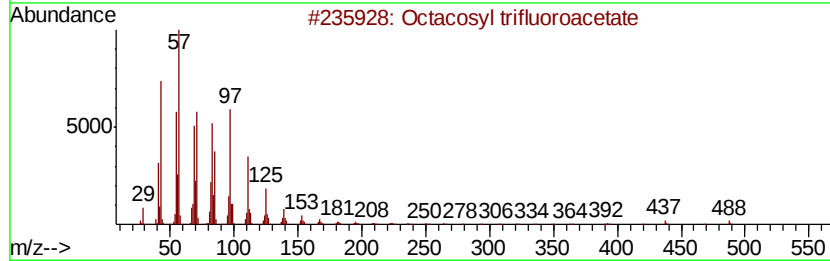
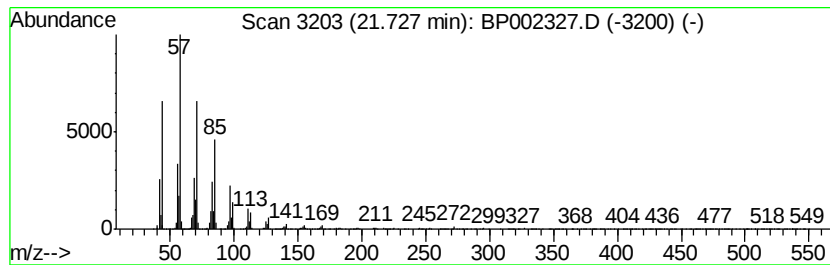
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TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.73	4.52 ng	1208470	Chrysene-d12	21.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
2		Ethanol, 2-(octadecyloxy)-	314	C20H42O2	002136-72-3	87
3		Sulfurous acid, octadecyl 2-propyl...	376	C21H44O3S	1000309-12-7	83
4		Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	81
5		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	74



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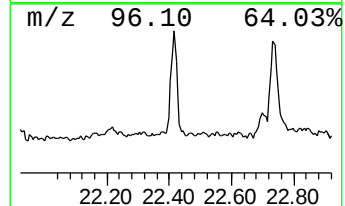
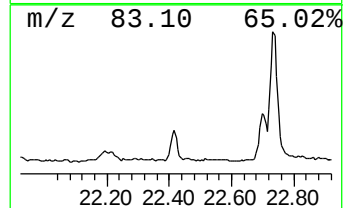
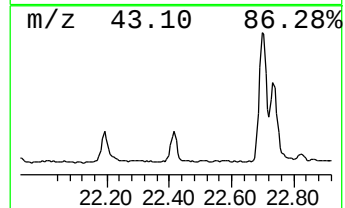
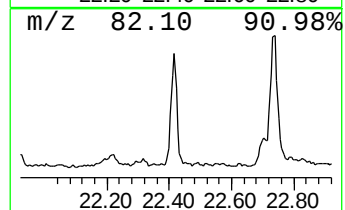
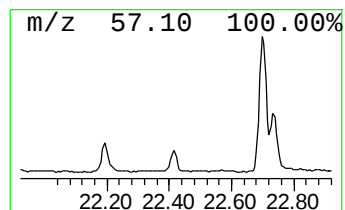
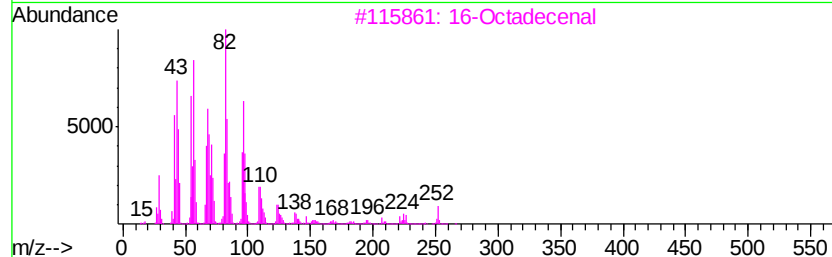
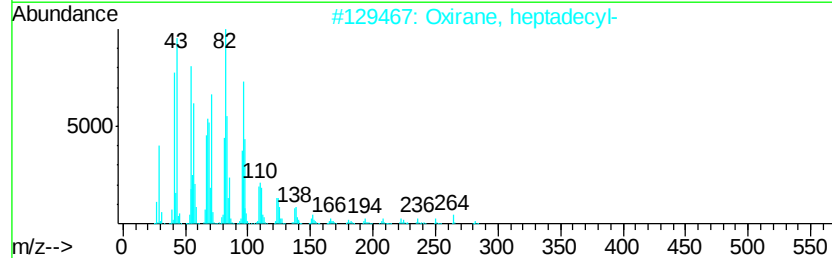
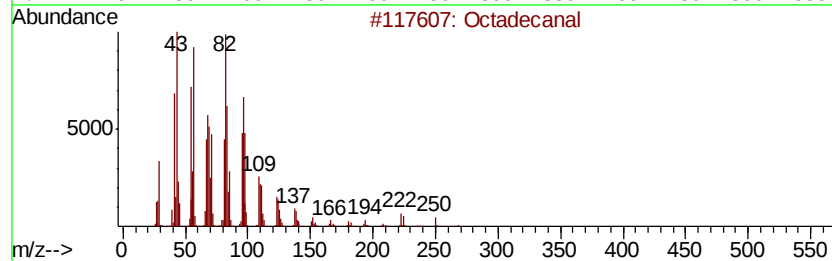
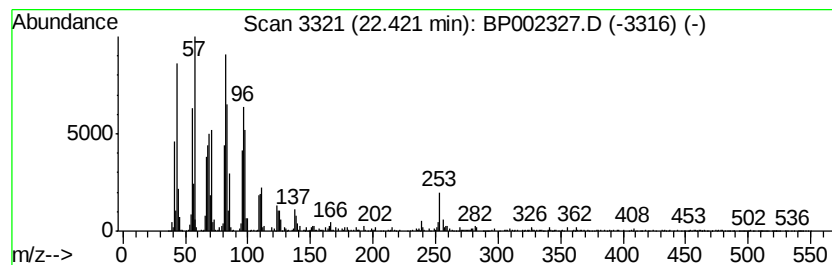
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NM79-COMP-2020-0-6

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 Octadecanal Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.42	2.17 ng	541303	Perylene-d12	23.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	96
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
3	16-Octadecenal	266	C18H34O	056554-87-1	93
4	13-Octadecenal	266	C18H34O	056554-90-6	91
5	14-Octadecenal	266	C18H34O	056554-89-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002327.D
Acq On : 29 May 2020 22:01
Operator : CG/JU
Sample : L2744-11 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

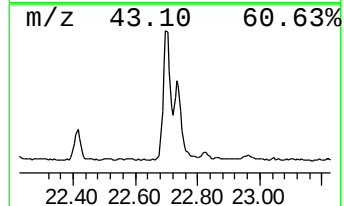
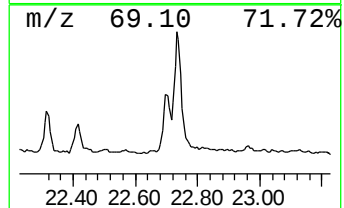
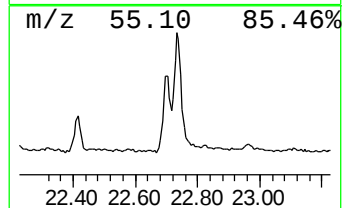
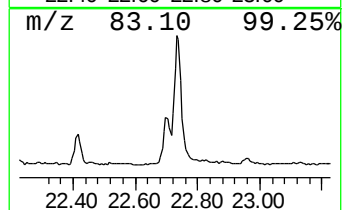
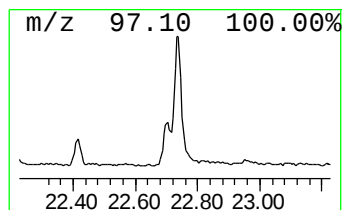
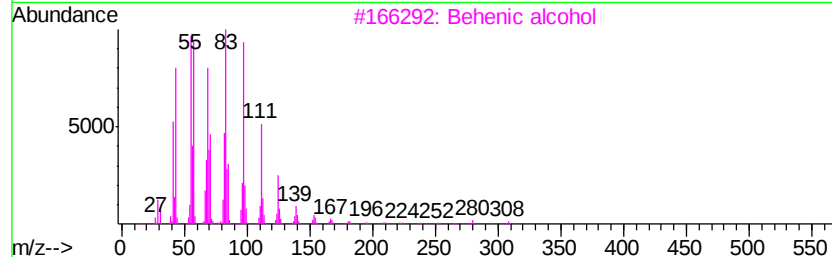
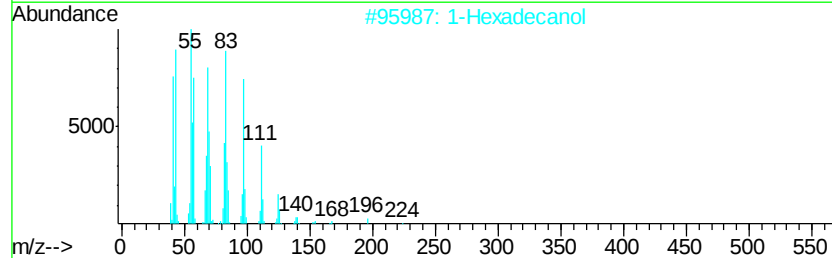
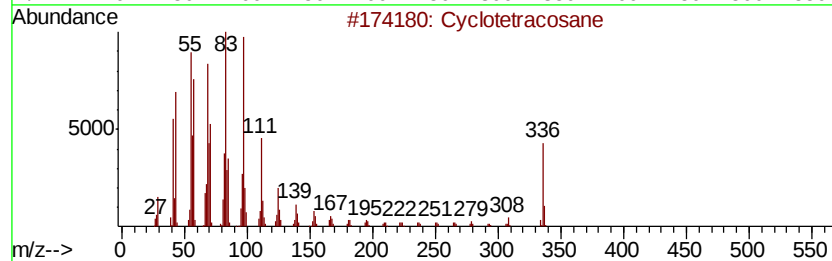
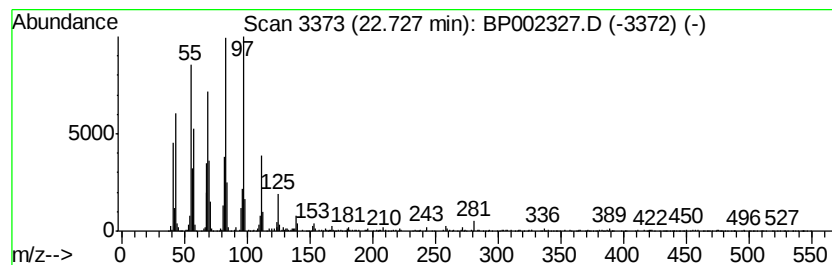
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ClientSampleId :
NM79-COMP-2020-0-6

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 7 Cyclotetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.73	6.15 ng	1533010	Perylene-d12	23.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	93
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	83
5	Octacosanol	410	C28H58O	000557-61-9	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
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Acq On : 29 May 2020 22:01
Operator : CG/JU
Sample : L2744-11 2X
Misc :
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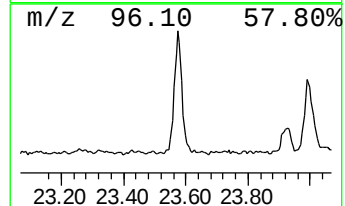
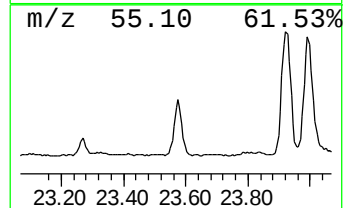
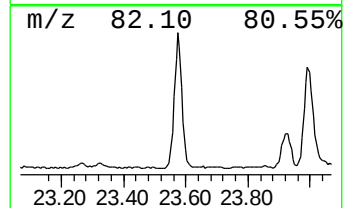
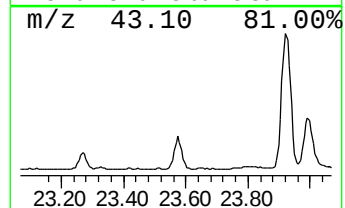
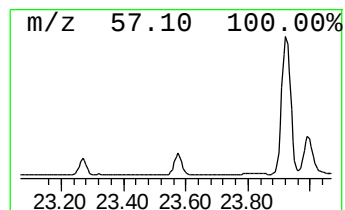
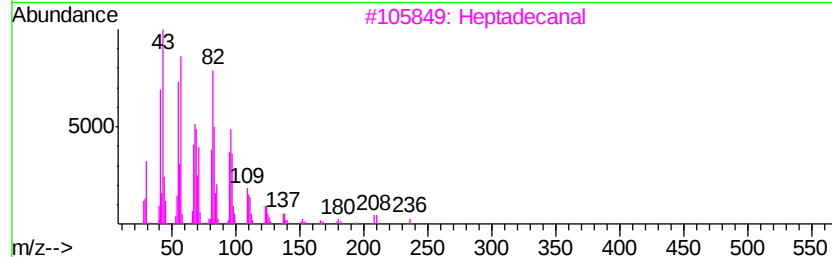
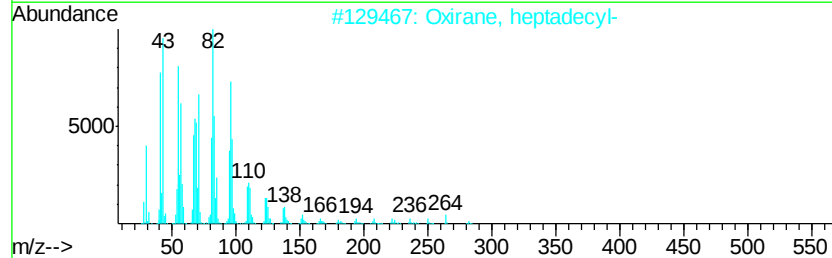
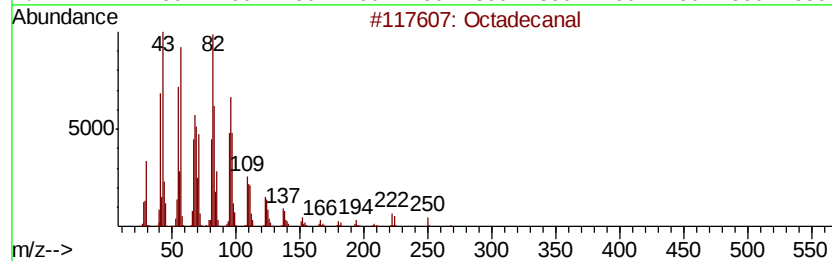
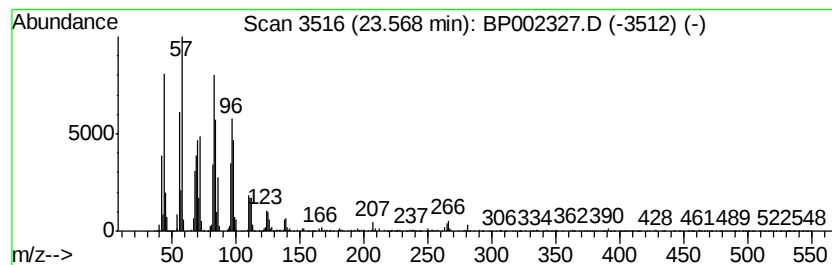
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Oxirane, heptadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.57	5.95 ng	1483980	Perylene-d12	23.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	96
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	94
3	Heptadecanal	254	C17H34O	1000376-70-0	92
4	Tetracosanal	352	C24H48O	057866-08-7	91
5	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002327.D
Acq On : 29 May 2020 22:01
Operator : CG/JU
Sample : L2744-11 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NM79-COMP-2020-0-6

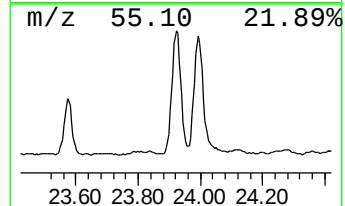
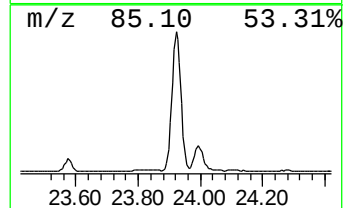
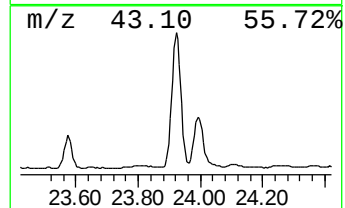
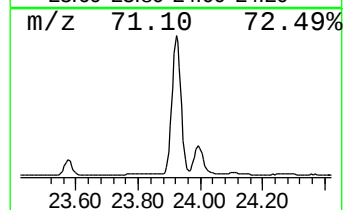
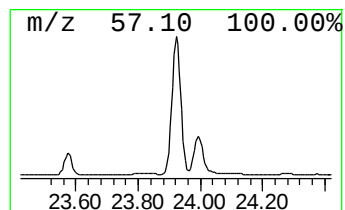
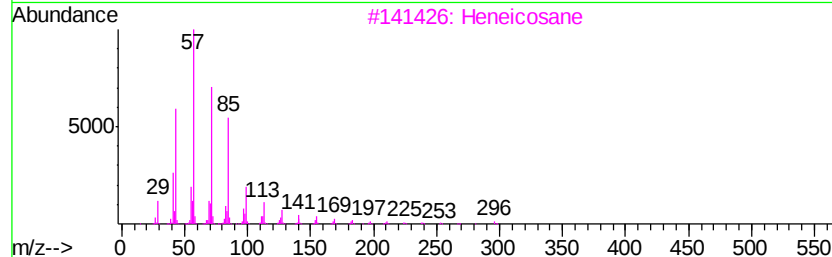
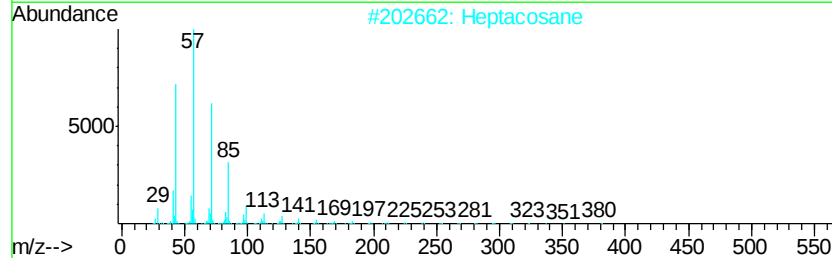
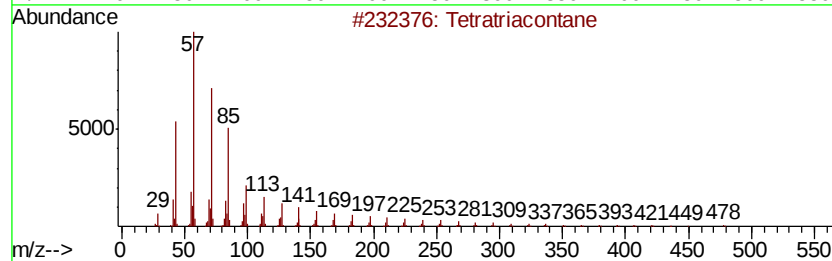
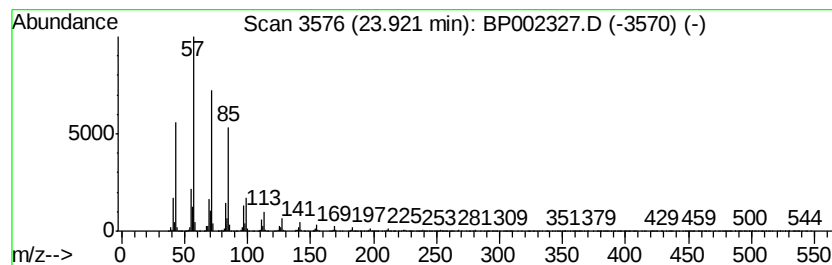
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetratriacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	20.05 ng	5001180	Perylene-d12	23.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratriacontane	479	C34H70	014167-59-0	95
2		Heptacosane	380	C27H56	000593-49-7	93
3		Heneicosane	296	C21H44	000629-94-7	91
4		Octacosane	394	C28H58	000630-02-4	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002327.D
Acq On : 29 May 2020 22:01
Operator : CG/JU
Sample : L2744-11 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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NM79-COMP-2020-0-6

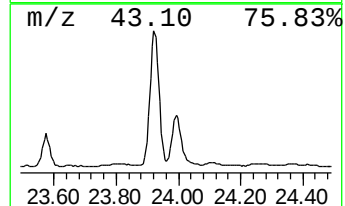
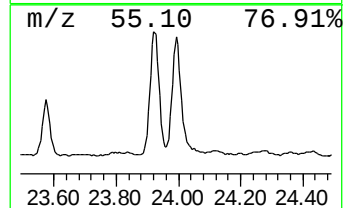
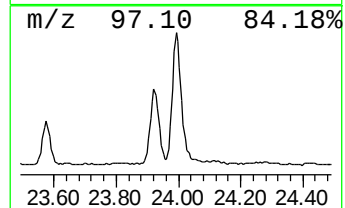
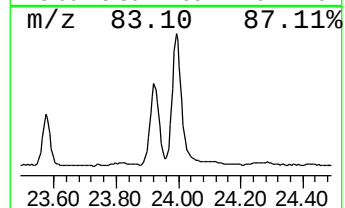
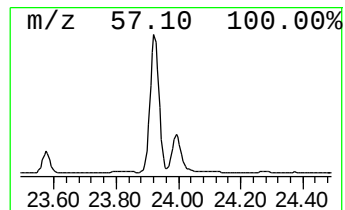
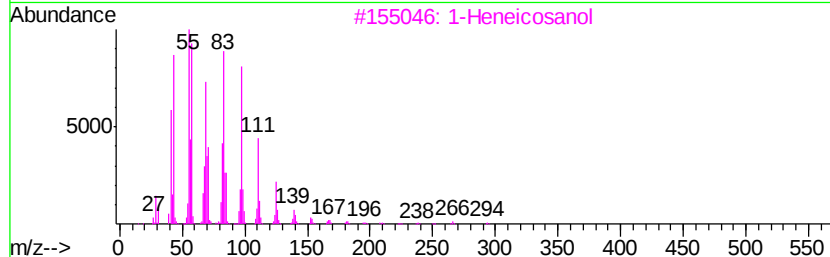
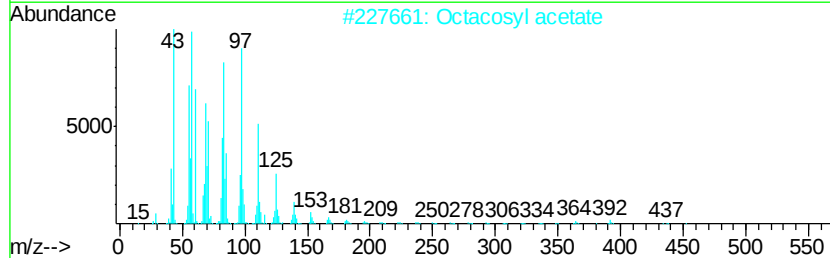
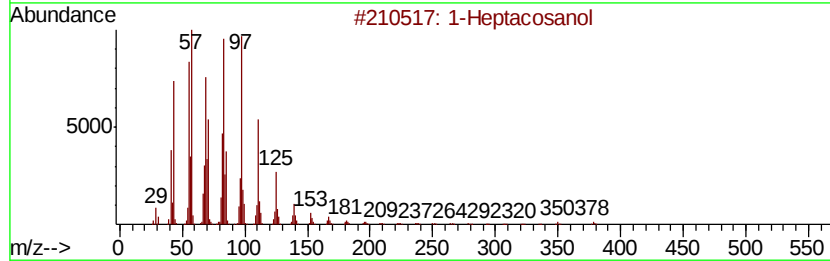
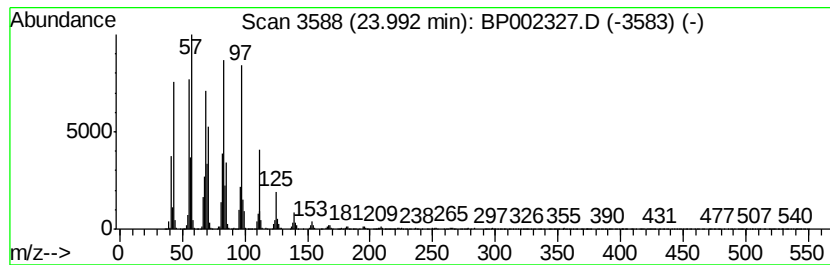
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.99	11.41 ng	2844620	Perylene-d12	23.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptacosanol	396	C27H56O	002004-39-9	95
2		Octacosyl acetate	452	C30H60O2	018206-97-8	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		1-Hexacosanol	382	C26H54O	000506-52-5	91
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
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Acq On : 29 May 2020 22:01
Operator : CG/JU
Sample : L2744-11 2X
Misc :
ALS Vial : 15 Sample Multiplier: 1

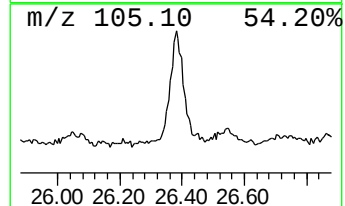
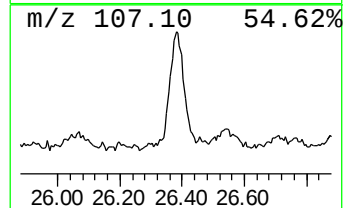
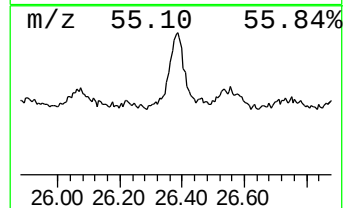
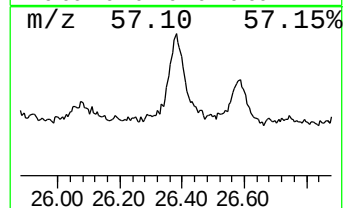
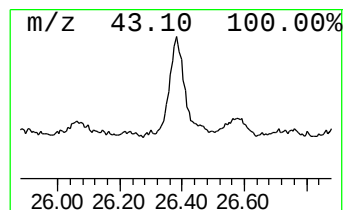
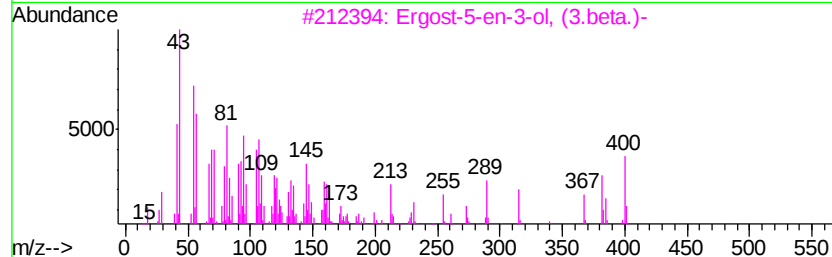
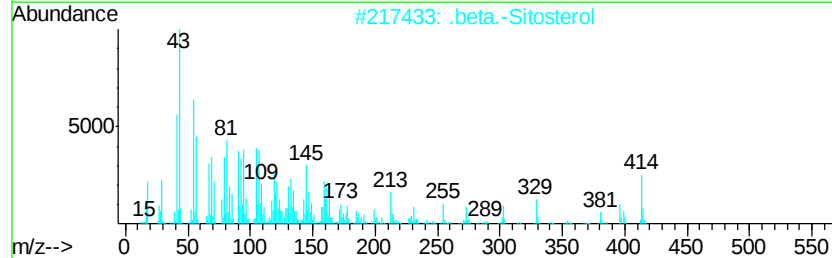
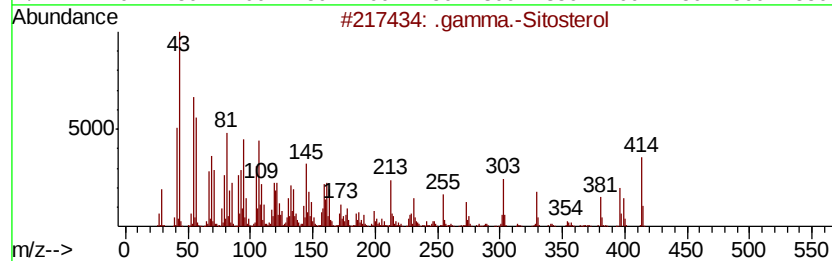
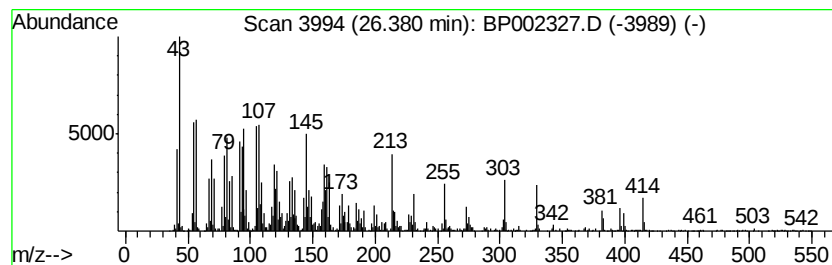
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .gamma.-Sitosterol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
26.38	6.39 ng	1593760	Perylene-d12		23.32	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Sitosterol	414	C29H50O	000083-47-6	91
2		.beta.-Sitosterol	414	C29H50O	000083-46-5	86
3		Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	43
4		Campesterol	400	C28H48O	000474-62-4	38
5		.beta.-d-Lyxofuranoside, phenyl,...	306	C15H19BO6	128902-53-4	15



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP052920\
 Data File : BP002327.D
 Acq On : 29 May 2020 22:01
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 ALS Vial : 15 Sample Multiplier: 1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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n-Hexadecanoic acid	17.94	4.2	ng	1012700	4	17.01	4776420	20.0
1-Heptacosanol	20.86	5.4	ng	1452360	5	21.11	5344260	20.0
Octacosyl trifluo...	21.73	4.5	ng	1208470	5	21.11	5344260	20.0
Octadecanal	22.42	2.2	ng	541303	6	23.32	4987570	20.0
Cyclotetracosane	22.73	6.2	ng	1533010	6	23.32	4987570	20.0
Oxirane, heptadecyl-	23.57	6.0	ng	1483980	6	23.32	4987570	20.0
Tetratriacontane	23.92	20.1	ng	5001180	6	23.32	4987570	20.0
Octacosyl acetate	23.99	11.4	ng	2844620	6	23.32	4987570	20.0
.gamma.-Sitosterol	26.38	6.4	ng	1593760	6	23.32	4987570	20.0