

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
 Data File : BP002325.D
 Acq On : 29 May 2020 20:52
 Operator : CG/JU
 Sample : L2745-07 2X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 NM86-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	294	rBV2	61114	277320	4.03%	0.354%
2	5.222	391	397	409	rBV	2311670	3353518	48.73%	4.287%
3	6.793	653	664	677	rBV	2333746	3721060	54.08%	4.757%
4	7.605	794	802	812	rBV	1351864	2103584	30.57%	2.689%
5	7.922	848	856	864	rBV	2057799	3315368	48.18%	4.238%
6	8.746	988	996	1010	rBV	1600506	2567833	37.32%	3.282%
7	10.381	1266	1274	1289	rVB	1760747	3000541	43.60%	3.836%
8	12.045	1551	1557	1570	rBV	66620	191761	2.79%	0.245%
9	12.869	1689	1697	1709	rBV	3798169	5580521	81.10%	7.134%
10	13.716	1834	1841	1850	rBV	313268	521528	7.58%	0.667%
11	13.969	1879	1884	1892	rVB	64902	124582	1.81%	0.159%
12	14.251	1925	1932	1940	rBV2	2743396	4067043	59.10%	5.199%
13	14.957	2046	2052	2058	rBV	69339	91915	1.34%	0.117%
14	15.745	2179	2186	2197	rBV	2582617	3655483	53.12%	4.673%
15	15.910	2209	2214	2220	rVB3	55229	92206	1.34%	0.118%
16	16.404	2293	2298	2302	rBV2	107352	167677	2.44%	0.214%
17	16.445	2302	2305	2315	rVB2	42323	74746	1.09%	0.096%
18	16.945	2386	2390	2394	rBV2	57943	88915	1.29%	0.114%
19	17.004	2395	2400	2405	rVV	2938492	4329857	62.92%	5.535%
20	17.045	2405	2407	2413	rVV	323129	436891	6.35%	0.558%
21	17.098	2413	2416	2419	rVV2	57978	81346	1.18%	0.104%
22	17.139	2419	2423	2428	rVB	139384	199757	2.90%	0.255%
23	17.410	2464	2469	2475	rBV3	92363	144189	2.10%	0.184%
24	17.580	2495	2498	2505	rVB3	49164	82628	1.20%	0.106%
25	17.822	2533	2539	2545	rBV	190572	383202	5.57%	0.490%
26	17.880	2545	2549	2554	rVV2	213848	335133	4.87%	0.428%
27	17.939	2554	2559	2567	rVV2	600395	890445	12.94%	1.138%
28	18.069	2577	2581	2585	rBV2	90380	137593	2.00%	0.176%
29	18.410	2636	2639	2645	rVB4	64616	108917	1.58%	0.139%
30	18.780	2698	2702	2707	rBV	73168	110880	1.61%	0.142%
31	18.898	2719	2722	2727	rBV2	177368	264344	3.84%	0.338%
32	19.004	2734	2740	2742	rBV	1514713	1883110	27.37%	2.407%
33	19.033	2742	2745	2749	rVB	860654	1079336	15.69%	1.380%
34	19.180	2767	2770	2774	rBV	83067	106396	1.55%	0.136%

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Sampling : 1
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35	19.380	2797	2804	2808	rBV	884238	1293648	18.80%	1.654%
36	19.592	2835	2840	2848	rVB	5488789	6881289	100.00%	8.796%
37	19.927	2895	2897	2901	rVB	64024	70984	1.03%	0.091%
38	20.027	2910	2914	2918	rVB3	112741	157623	2.29%	0.201%
39	20.239	2947	2950	2953	rBV	139815	147768	2.15%	0.189%
40	20.280	2953	2957	2960	rVV	261975	270896	3.94%	0.346%
41	20.416	2977	2980	2984	rBV	123692	128049	1.86%	0.164%
42	20.857	3051	3055	3066	rVB5	1025286	1516476	22.04%	1.939%
43	21.110	3092	3098	3102	rBV2	3570260	5179675	75.27%	6.621%
44	21.145	3102	3104	3111	rVB	464969	544018	7.91%	0.695%
45	21.298	3127	3130	3134	rVB2	311840	351624	5.11%	0.449%
46	21.468	3156	3159	3164	rBV2	136008	152396	2.21%	0.195%
47	21.733	3200	3204	3213	rVB2	774225	1117280	16.24%	1.428%
48	22.192	3279	3282	3290	rVB	528833	696592	10.12%	0.890%
49	22.416	3317	3320	3325	rVB	256260	349342	5.08%	0.447%
50	22.657	3357	3361	3364	rBV	383056	699452	10.16%	0.894%
51	22.698	3364	3368	3372	rVV	1338642	2121267	30.83%	2.712%
52	22.733	3372	3374	3385	rVB3	472568	720923	10.48%	0.922%
53	23.127	3437	3441	3449	rVB	320808	573021	8.33%	0.732%
54	23.221	3452	3457	3461	rBV	378284	663150	9.64%	0.848%
55	23.268	3461	3465	3468	rVV	486531	775948	11.28%	0.992%
56	23.321	3468	3474	3480	rVB2	2136852	3976685	57.79%	5.083%
57	23.574	3515	3517	3523	rVB	267501	365572	5.31%	0.467%
58	23.921	3570	3576	3583	rBV	1895701	3635360	52.83%	4.647%
59	23.992	3584	3588	3601	rVB2	611939	1181590	17.17%	1.510%
60	26.380	3990	3994	4009	rVB4	403330	1089031	15.83%	1.392%

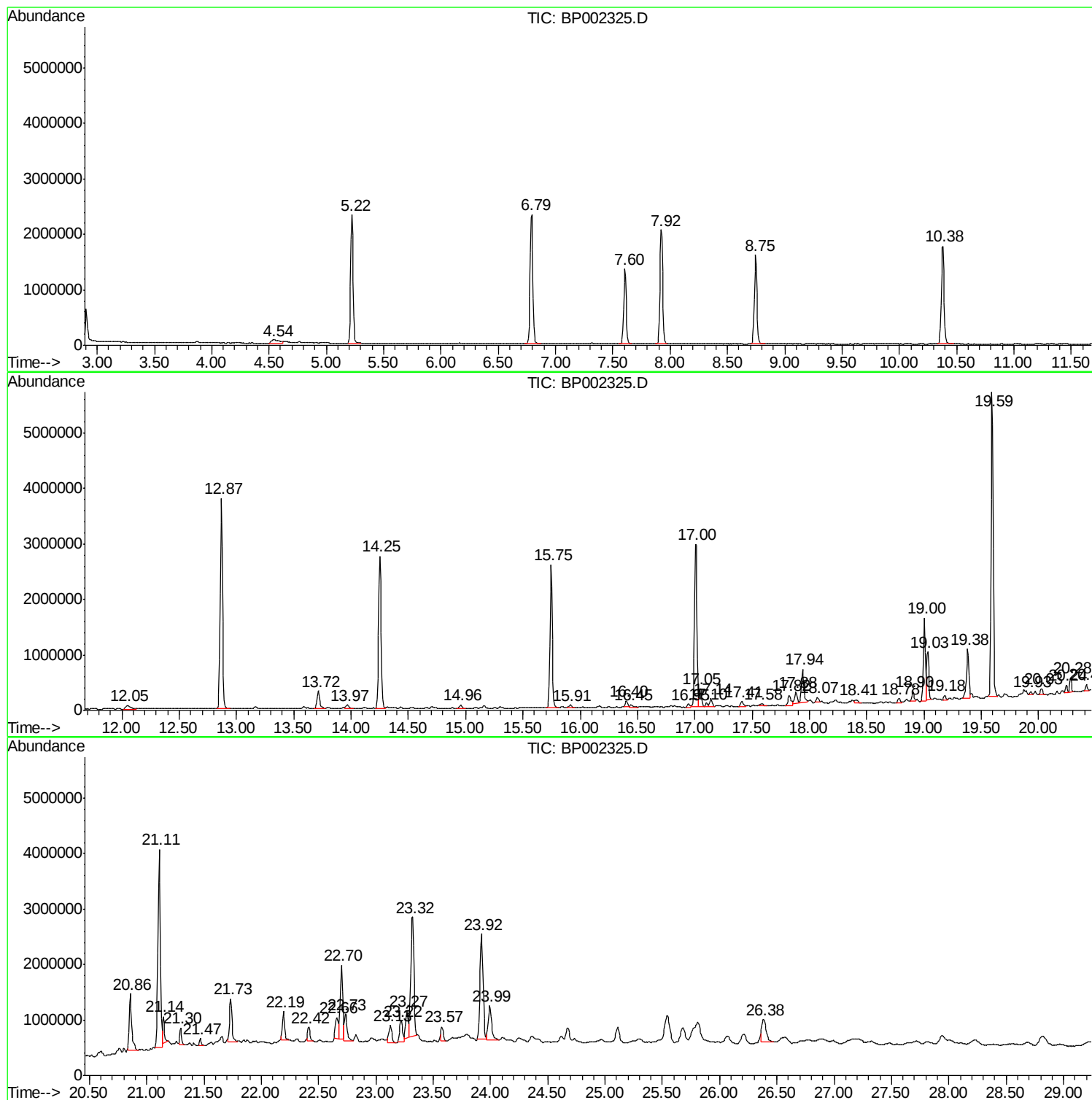
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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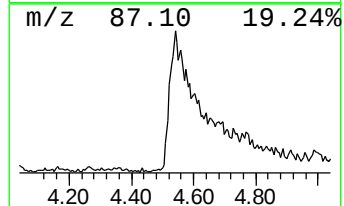
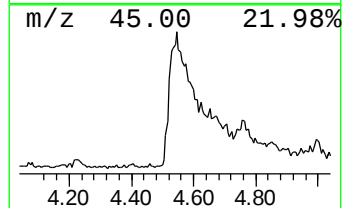
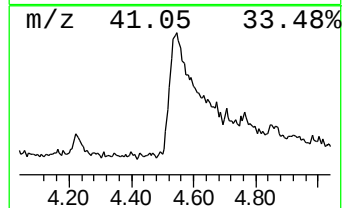
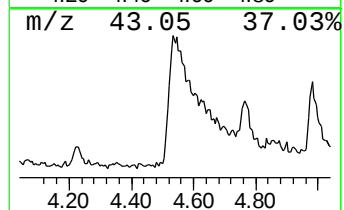
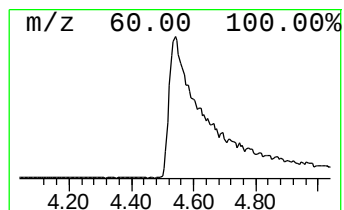
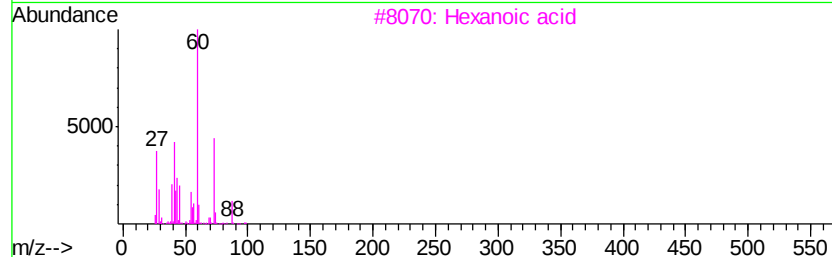
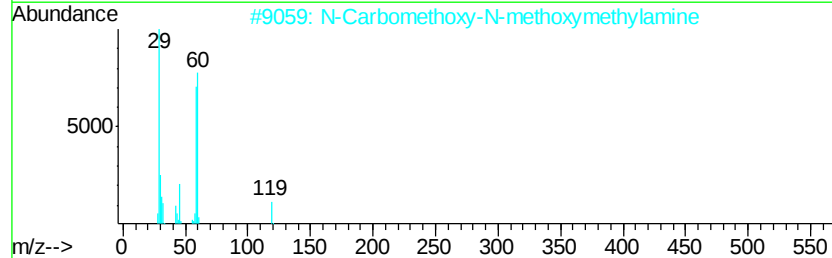
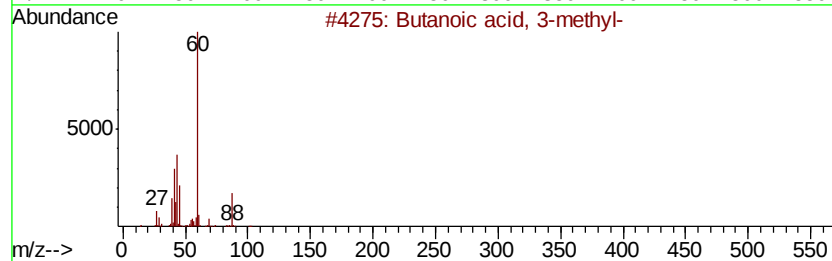
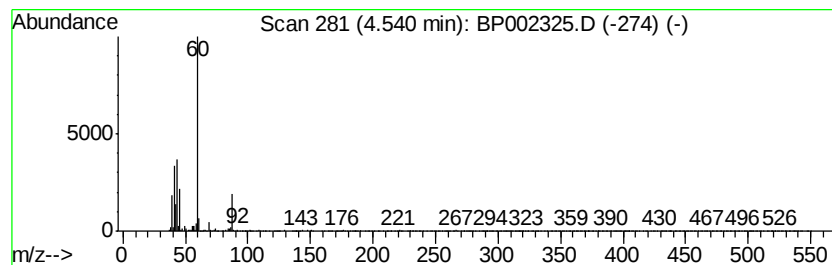
Quant Method : Z:\SVOASRV\HPCHEM1\BNA P\METHODS\8270-BP052720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	2.64 ng	277320	1,4-Dichlorobenzene-d4	7.60

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	86
2		N-Carbomethoxy-N-methoxymethylamine	119	C4H9NO3	153654-07-0	45
3		Hexanoic acid	116	C6H12O2	000142-62-1	38
4		Formic acid hydrazide	60	CH4N2O	000624-84-0	9
5		Pentanoic acid	102	C5H10O2	000109-52-4	9



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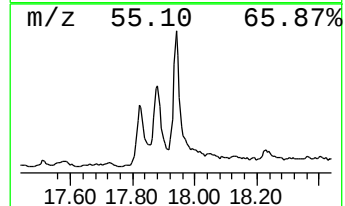
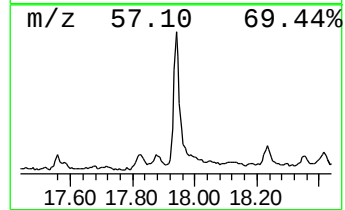
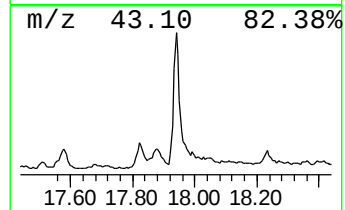
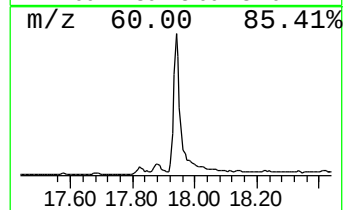
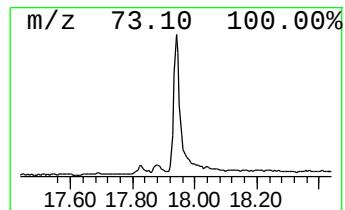
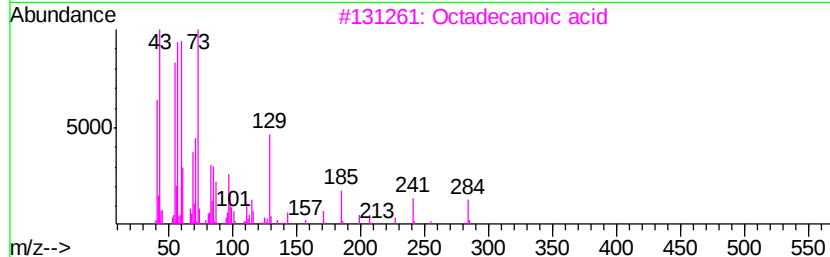
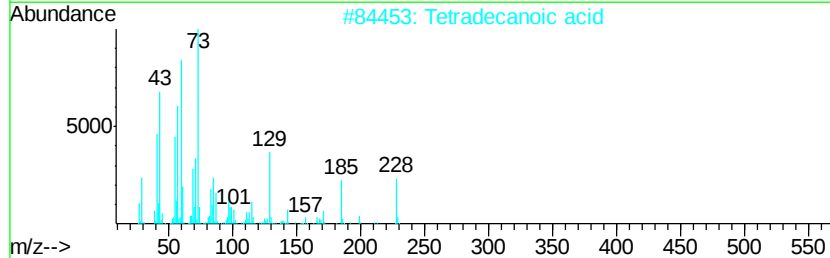
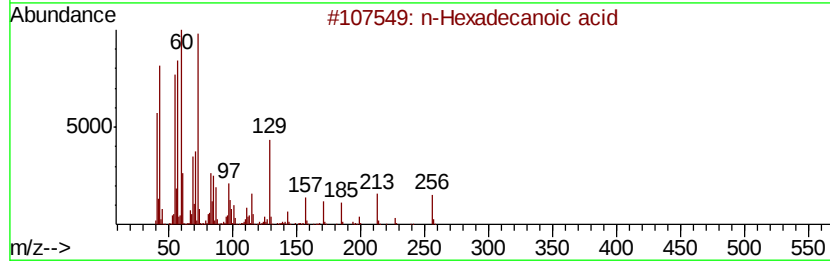
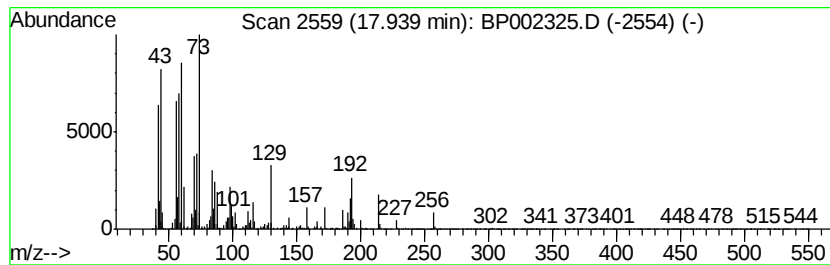
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.94	4.11 ng	890445	Phenanthrene-d10		17.00
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	83
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	68



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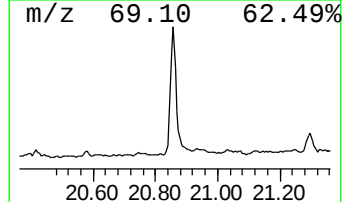
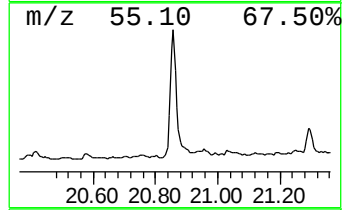
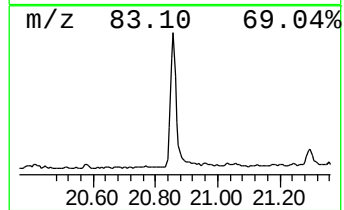
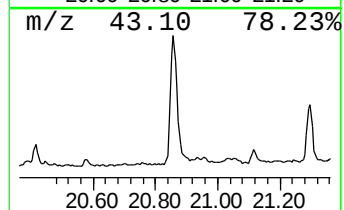
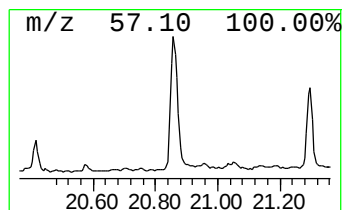
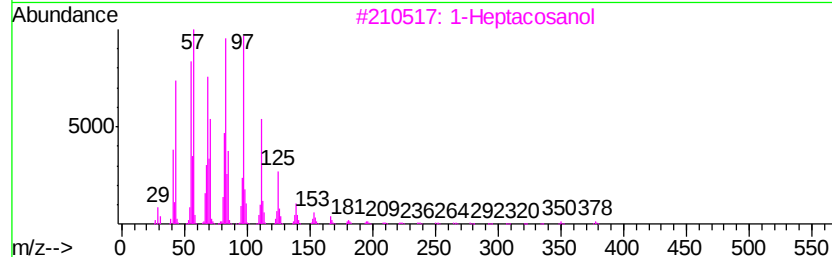
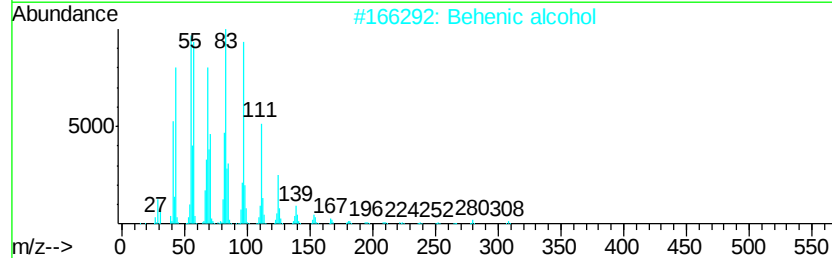
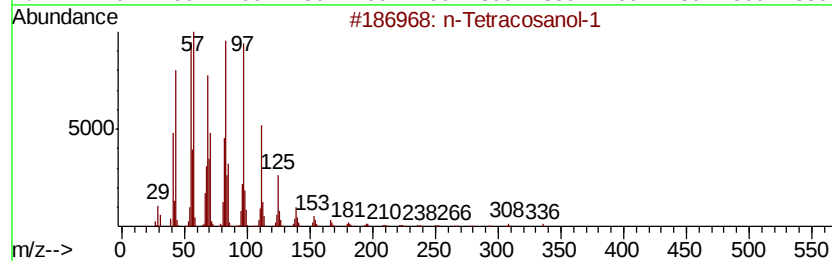
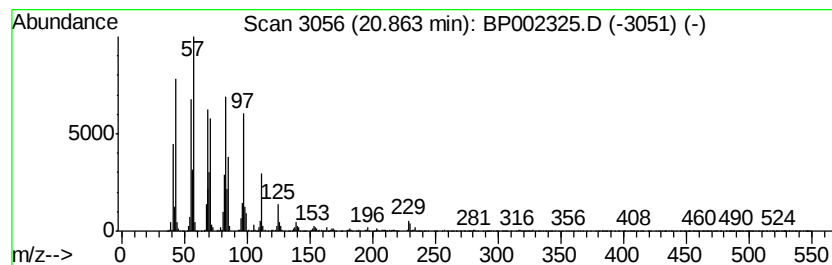
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.86	5.86 ng	1516480	Chrysene-d12	21.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94	
2	Behenic alcohol	326	C22H46O	000661-19-8	94	
3	1-Heptacosanol	396	C27H56O	002004-39-9	91	
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91	
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91	



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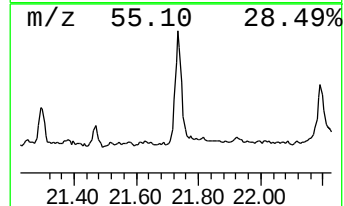
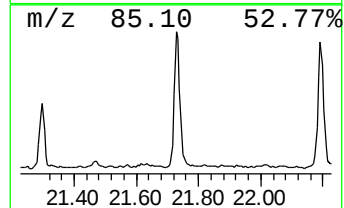
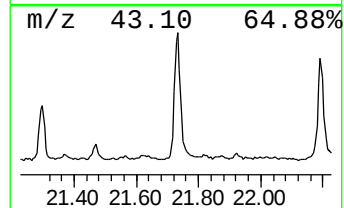
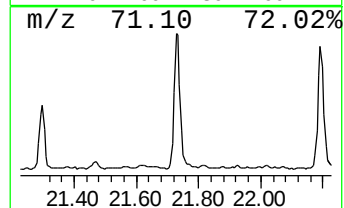
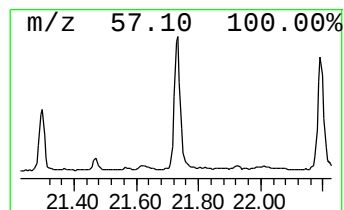
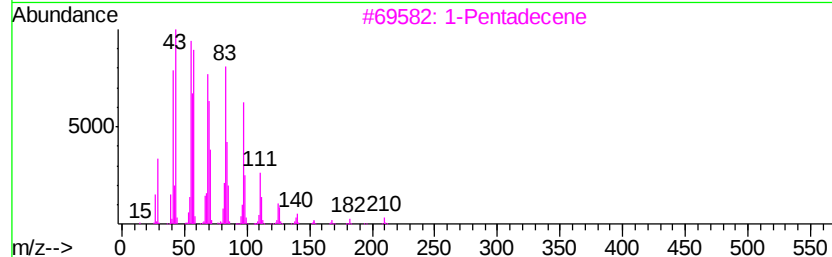
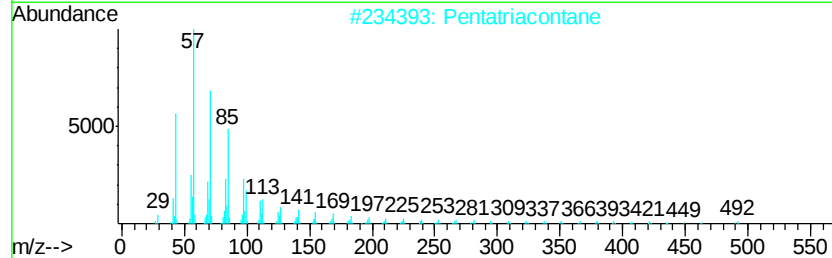
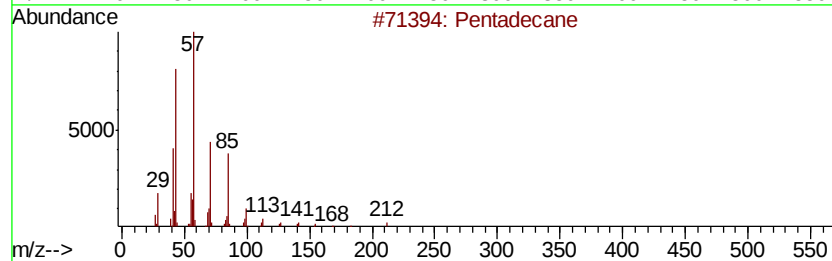
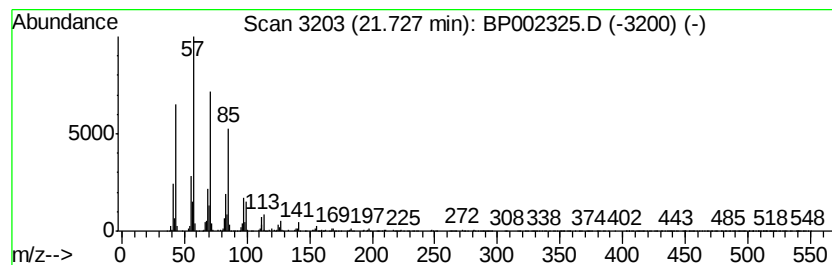
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.73	4.31 ng	1117280	Chrysene-d12	21.11	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	93
2	Pentatriacontane	493	C35H72	000630-07-9	91
3	1-Pentadecene	210	C15H30	013360-61-7	70
4	Heptadecane	240	C17H36	000629-78-7	68
5	Nonadecane	268	C19H40	000629-92-5	68



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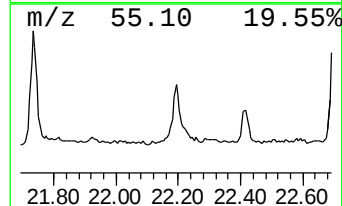
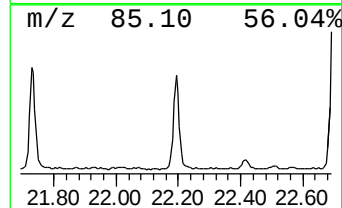
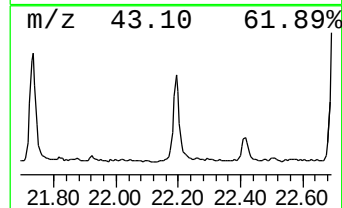
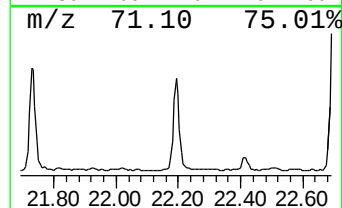
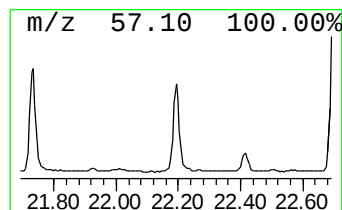
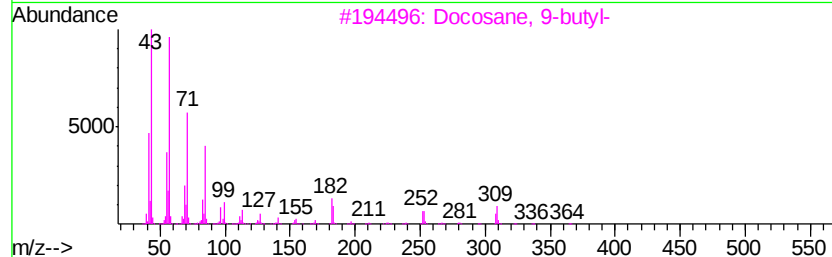
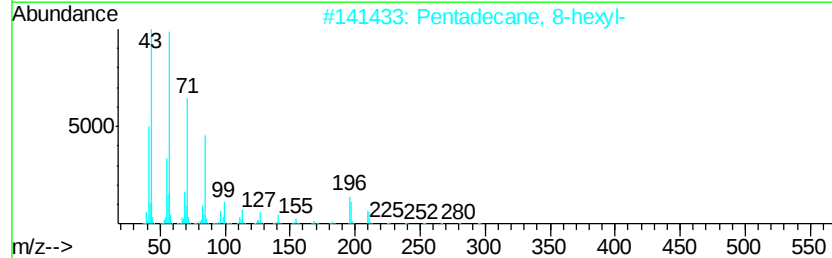
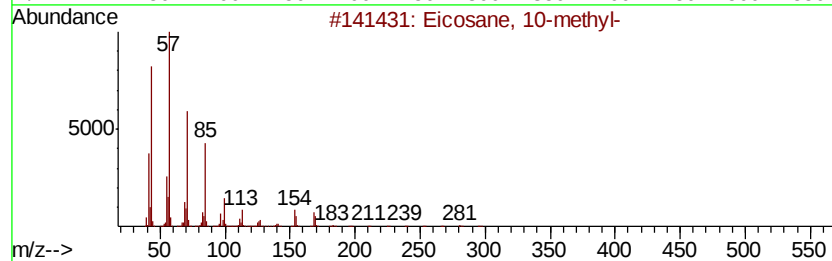
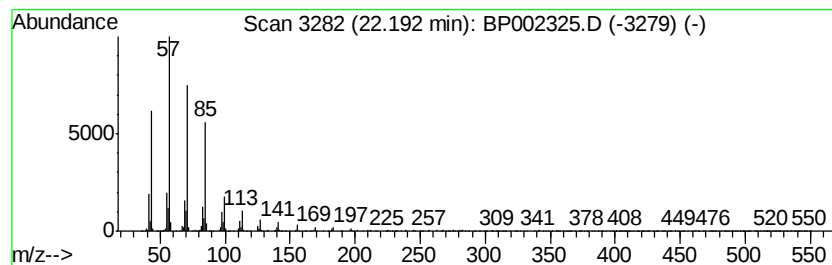
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane, 10-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
22.19	2.69 ng	696592	Chrysene-d12		21.11
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	94
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
3	Docosane, 9-butyl-	366	C26H54	055282-14-9	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002325.D
Acq On : 29 May 2020 20:52
Operator : CG/JU
Sample : L2745-07 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

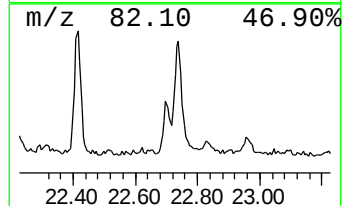
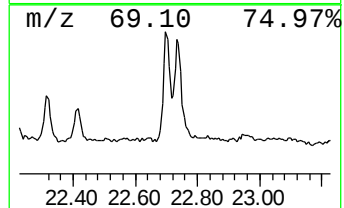
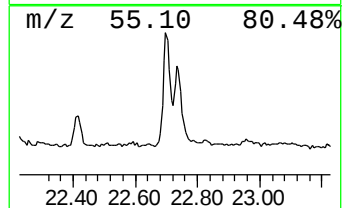
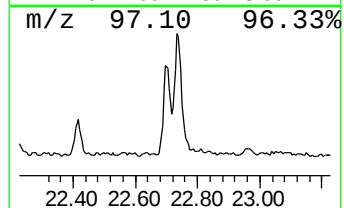
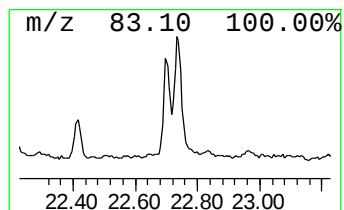
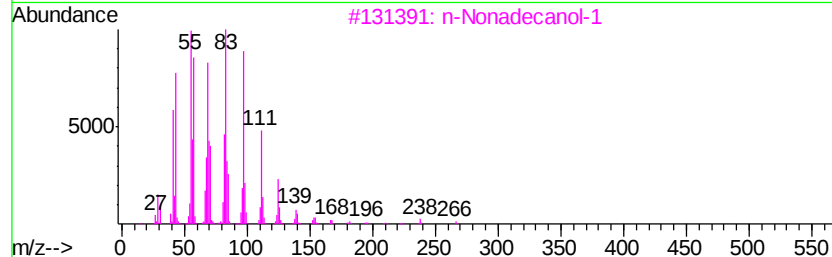
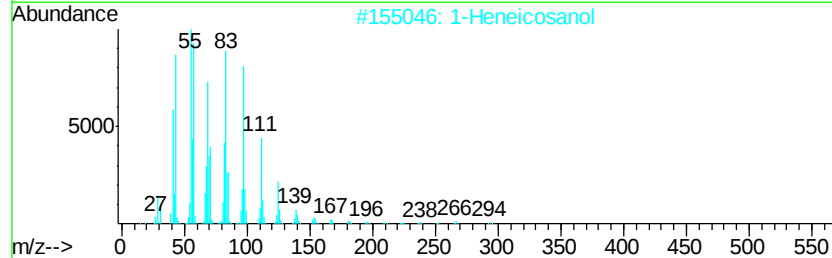
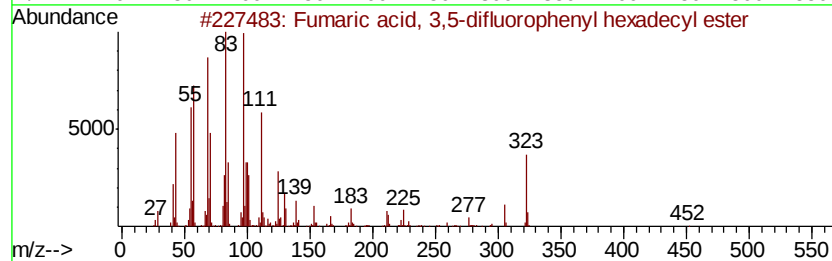
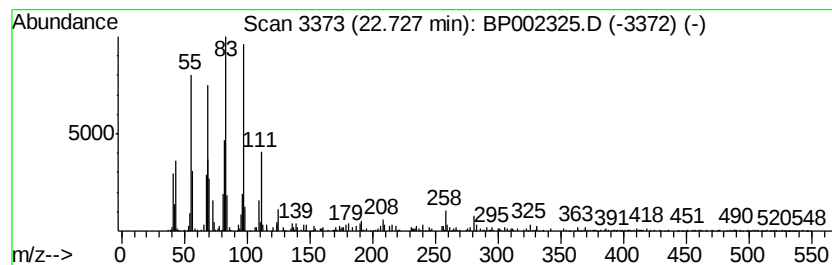
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ClientSampleId :
NM86-COMP-2020-0-6

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 Fumaric acid, 3,5-difluorop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
22.73	3.63 ng	720923	Perylene-d12	23.32		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fumaric acid, 3,5-difluorophenyl...	452	C26H38F2O4	1000339-38-1	91	
2	1-Heneicosanol	312	C21H44O	015594-90-8	91	
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	83	
4	Fumaric acid, hexadecyl 2,4,6-tr...	518	C26H37Cl3O4	1000348-27-9	64	
5	1-Hexadecanethiol	258	C16H34S	002917-26-2	64	



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002325.D
Acq On : 29 May 2020 20:52
Operator : CG/JU
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Instrument :
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ClientSampleId :
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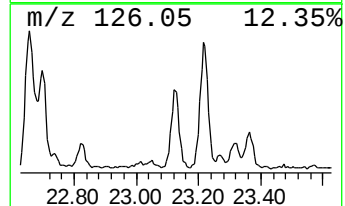
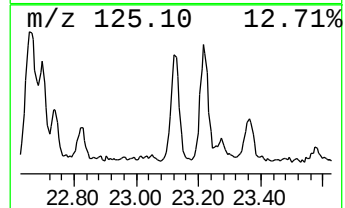
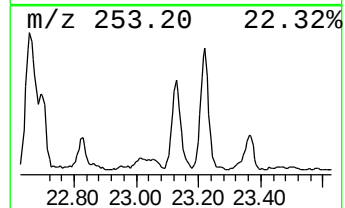
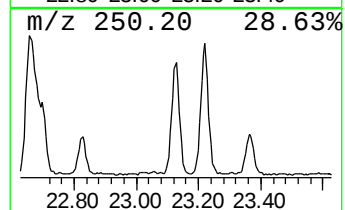
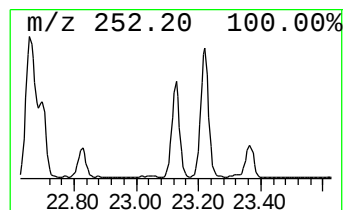
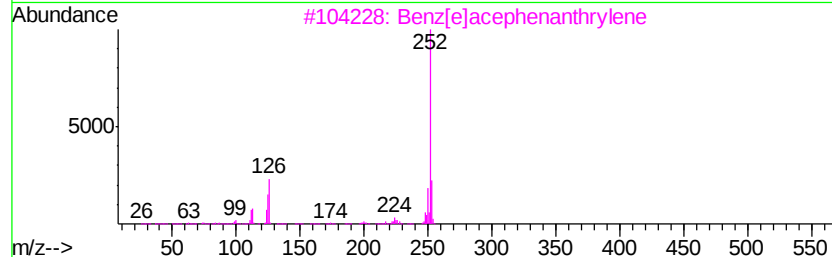
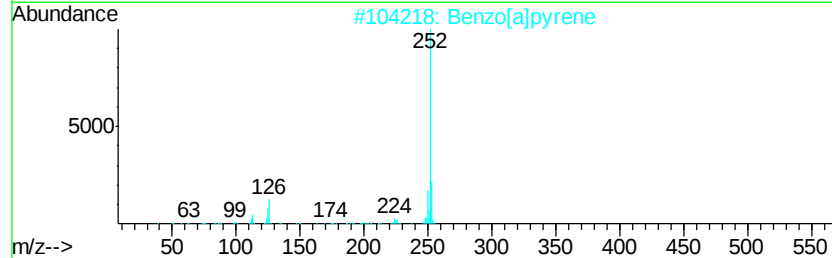
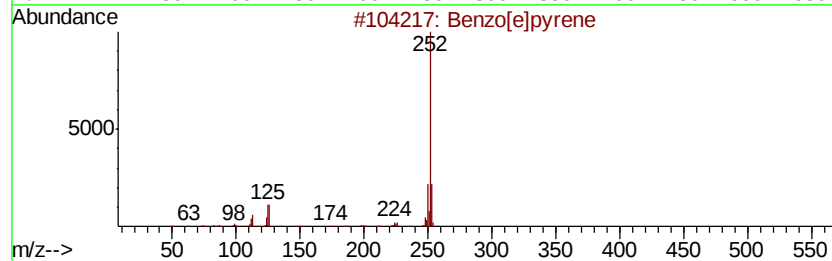
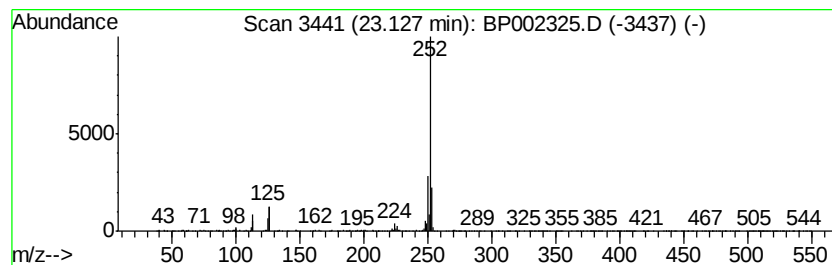
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzo[e]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.13	2.88 ng	573021	Perylene-d12	23.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzo[e]pyrene	252	C20H12	000192-97-2	99
2		Benzo[a]pyrene	252	C20H12	000050-32-8	96
3		Benz[e]acephenanthrylene	252	C20H12	000205-99-2	95
4		Perylene	252	C20H12	000198-55-0	95
5		Benzo[k]fluoranthene	252	C20H12	000207-08-9	94



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002325.D
Acq On : 29 May 2020 20:52
Operator : CG/JU
Sample : L2745-07 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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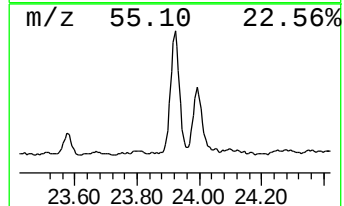
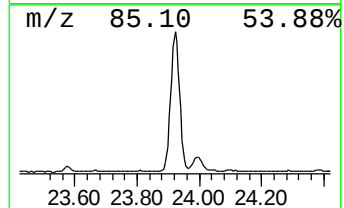
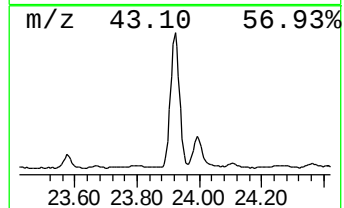
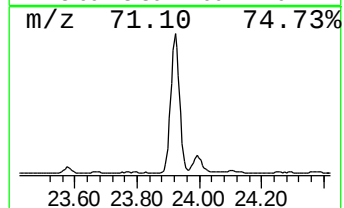
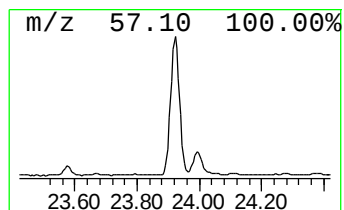
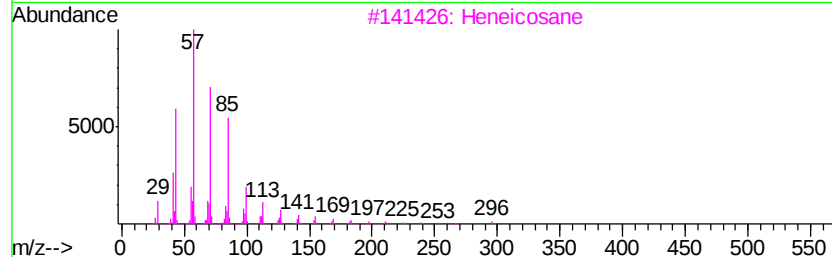
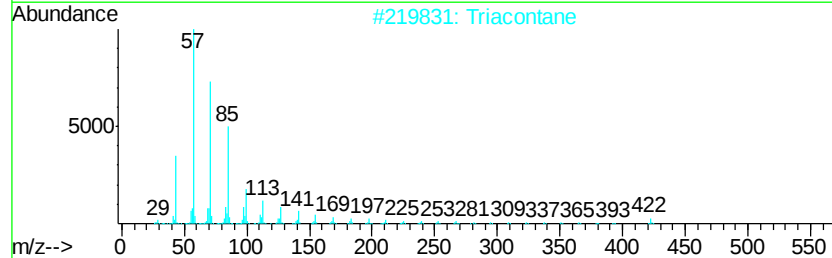
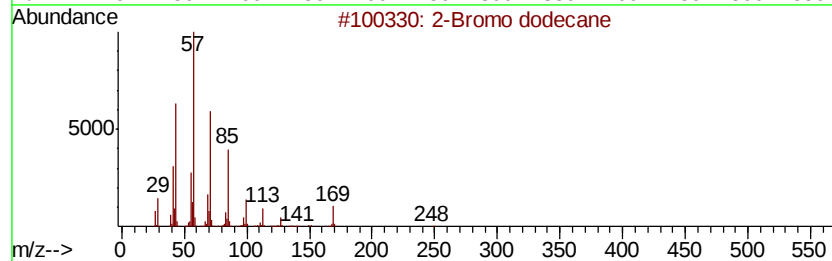
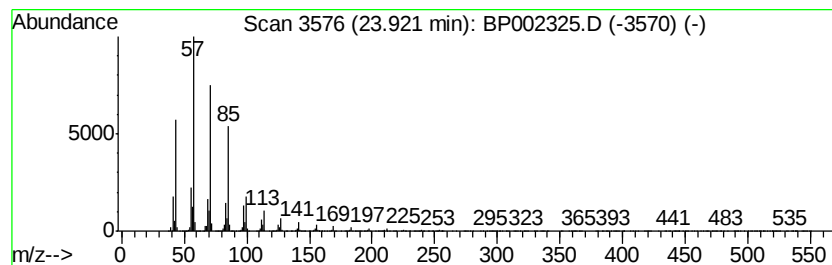
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Bromo dodecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	18.28 ng	3635360	Perylene-d12	23.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromo dodecane		248	C12H25Br	013187-99-0	94
2	triacontane		422	C30H62	000638-68-6	94
3	Heneicosane		296	C21H44	000629-94-7	91
4	Pentadecane, 8-hexyl-		296	C21H44	013475-75-7	91
5	Hexacosane		366	C26H54	000630-01-3	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
Data File : BP002325.D
Acq On : 29 May 2020 20:52
Operator : CG/JU
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
NM86-COMP-2020-0-6

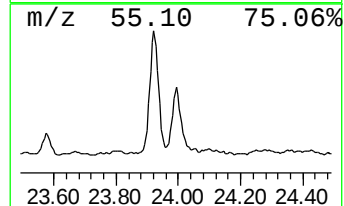
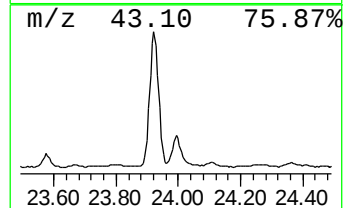
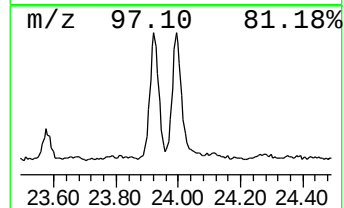
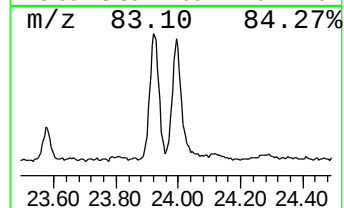
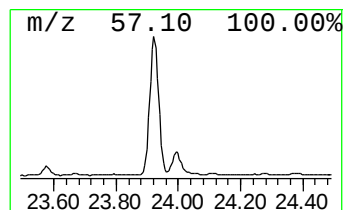
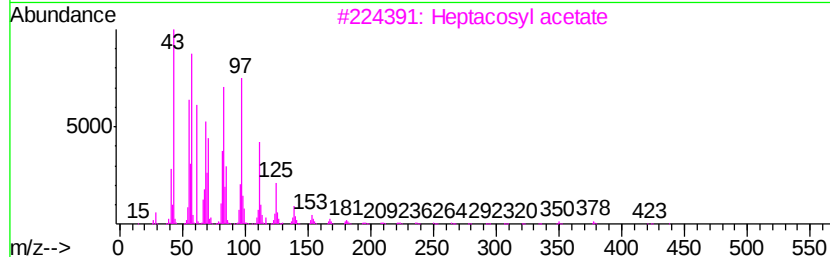
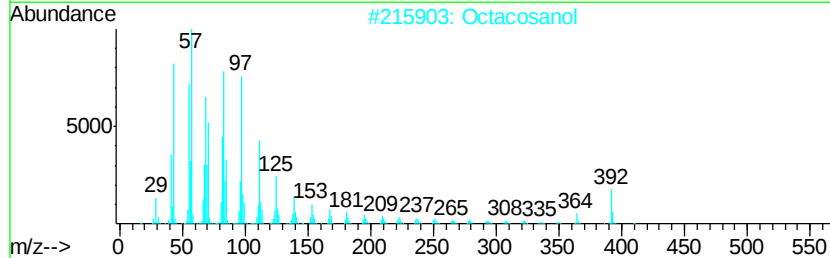
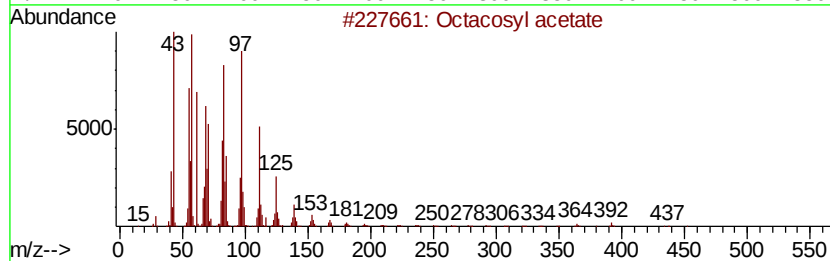
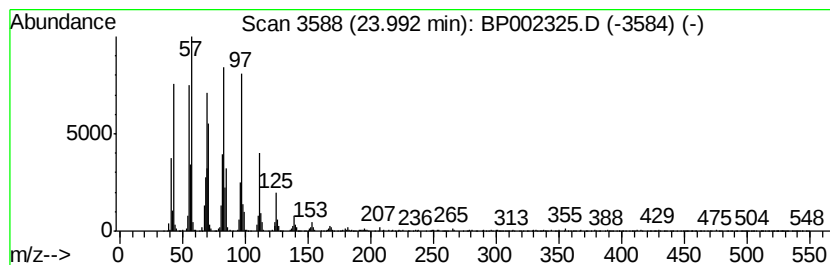
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	5.94 ng	1181590	Perylene-d12	23.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl acetate	452	C30H60O2	018206-97-8	97
2			Octacosanol	410	C28H58O	000557-61-9	94
3			Heptacosyl acetate	438	C29H58O2	1000351-78-2	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
5			1-Heptacosanol	396	C27H56O	002004-39-9	93



Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP052920\
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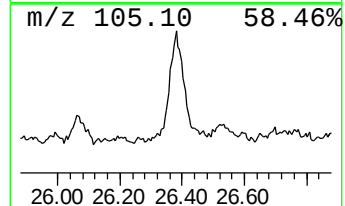
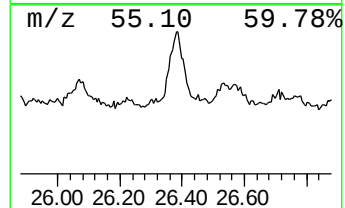
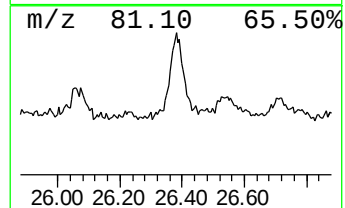
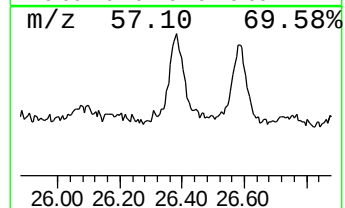
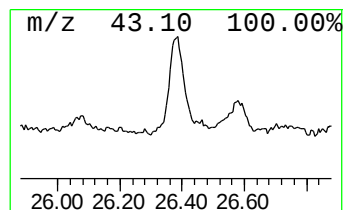
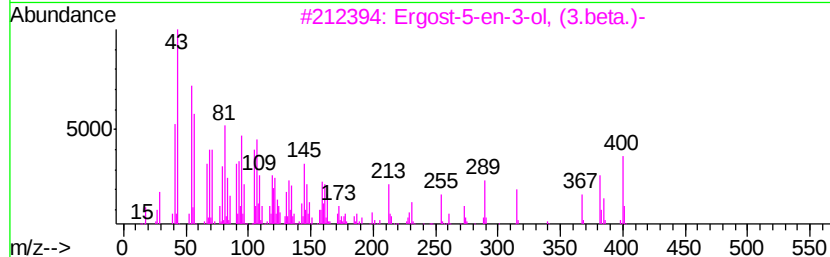
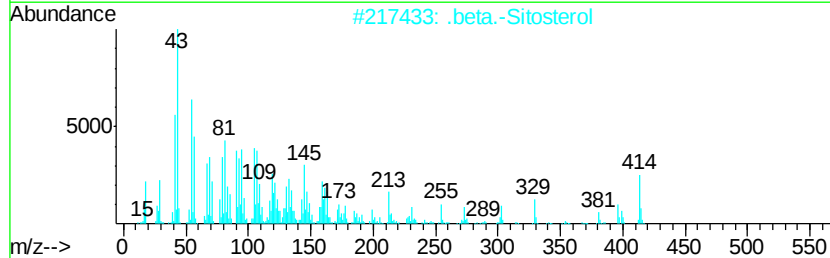
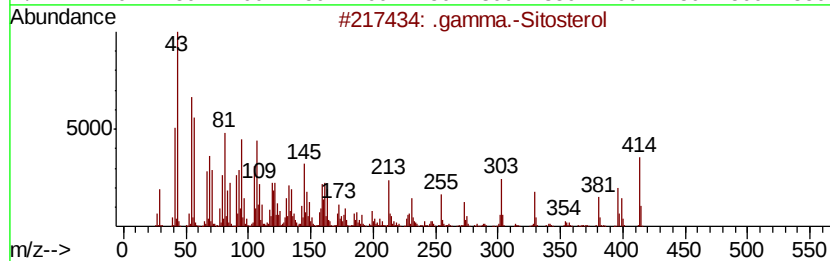
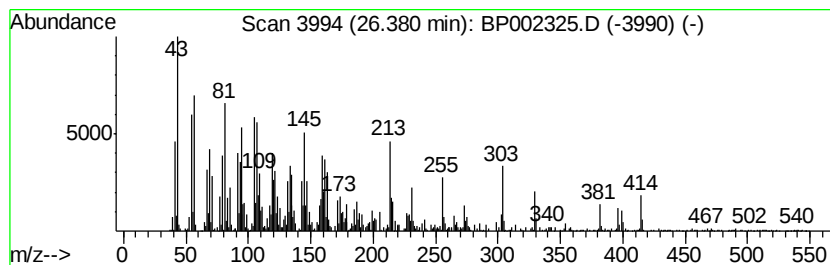
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 .gamma.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.38	5.48 ng	1089030	Perylene-d12	23.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	98
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	95
3	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	68
4	26-Hydroxycholesterol	402	C27H46O2	013095-61-9	52
5	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP052920\
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 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-...	4.54	2.6	ng	277320	1	7.60	2103580	20.0
n-Hexadecanoic acid	17.94	4.1	ng	890445	4	17.00	4329860	20.0
n-Tetracosanol-1	20.86	5.9	ng	1516480	5	21.11	5179680	20.0
Pentadecane	21.73	4.3	ng	1117280	5	21.11	5179680	20.0
Eicosane, 10-methyl-	22.19	2.7	ng	696592	5	21.11	5179680	20.0
Fumaric acid, 3,5...	22.73	3.6	ng	720923	6	23.32	3976690	20.0
Benzo[e]pyrene	23.13	2.9	ng	573021	6	23.32	3976690	20.0
2-Bromo dodecane	23.92	18.3	ng	3635360	6	23.32	3976690	20.0
Octacosyl acetate	23.99	5.9	ng	1181590	6	23.32	3976690	20.0
.gamma.-Sitosterol	26.38	5.5	ng	1089030	6	23.32	3976690	20.0