

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052620\
 Data File : BG045468.D
 Acq On : 26 May 2020 22:19
 Operator : CG/JU
 Sample : L2744-12
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NMDUP01-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_G\METHODS\8270-BG051520.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	3.115	3	4	15	rVB	147012	181557	4.00%	0.531%
2	5.564	412	421	437	rBV	973249	1680152	37.03%	4.913%
3	7.180	689	696	707	rBV	1123077	1973100	43.49%	5.770%
4	7.961	821	829	838	rBV	314098	548800	12.10%	1.605%
5	8.284	876	884	893	rBV	953494	1685034	37.14%	4.928%
6	9.124	1018	1027	1036	rBV	723057	1338829	29.51%	3.915%
7	9.201	1036	1040	1046	rVB2	31573	49296	1.09%	0.144%
8	10.769	1299	1307	1314	rBV	413096	783091	17.26%	2.290%
9	13.225	1717	1725	1738	rBV	2062452	3372559	74.33%	9.863%
10	14.053	1858	1866	1873	rBV	269670	414089	9.13%	1.211%
11	14.605	1949	1960	1966	rBV	703517	1169439	25.77%	3.420%
12	14.670	1966	1971	1977	rVB2	35566	58763	1.30%	0.172%
13	15.005	2022	2028	2036	rBV2	23176	47116	1.04%	0.138%
14	16.097	2205	2214	2227	rBV	1610375	2626629	57.89%	7.681%
15	17.172	2392	2397	2405	rVB	23545	46712	1.03%	0.137%
16	17.354	2417	2428	2431	rBV	825907	1312076	28.92%	3.837%
17	17.396	2431	2435	2441	rVB	345418	527994	11.64%	1.544%
18	17.484	2446	2450	2457	rVB	34481	58320	1.29%	0.171%
19	17.760	2494	2497	2509	rVB2	30469	63070	1.39%	0.184%
20	18.230	2573	2577	2579	rVV	47589	74865	1.65%	0.219%
21	18.259	2579	2582	2590	rVB2	100149	211482	4.66%	0.618%
22	18.424	2604	2610	2614	rBV3	51335	93335	2.06%	0.273%
23	18.723	2657	2661	2664	rBV	30518	45754	1.01%	0.134%
24	18.758	2664	2667	2674	rVB3	43413	66807	1.47%	0.195%
25	19.146	2728	2733	2740	rBV6	27537	55151	1.22%	0.161%
26	19.269	2749	2754	2762	rBV5	44372	100914	2.22%	0.295%
27	19.346	2762	2767	2772	rBV2	325946	471780	10.40%	1.380%
28	19.405	2772	2777	2783	rVB	526711	771731	17.01%	2.257%
29	19.763	2828	2838	2846	rBV	454293	809864	17.85%	2.368%
30	19.839	2847	2851	2856	rVB4	31999	51400	1.13%	0.150%
31	19.969	2866	2873	2883	rVB	3210638	4537381	100.00%	13.269%
32	20.092	2888	2894	2900	rBV3	38405	95240	2.10%	0.279%
33	20.256	2913	2922	2929	rBV4	78942	191465	4.22%	0.560%
34	20.415	2943	2949	2954	rBV2	54633	89766	1.98%	0.263%

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 Smoothing : ON
 Sampling : 1
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	20.609	2978	2982	2985	rVV2	58175	92496	2.04%	0.270%
36	20.650	2986	2989	2995	rVB3	69066	89472	1.97%	0.262%
37	21.014	3048	3051	3059	rVB	54335	93430	2.06%	0.273%
38	21.267	3090	3094	3102	rVV3	289522	556337	12.26%	1.627%
39	21.337	3104	3106	3114	rVB2	54225	90175	1.99%	0.264%
40	21.607	3144	3152	3157	rBV2	849605	1760574	38.80%	5.149%
41	21.654	3157	3160	3168	rVB	211707	341850	7.53%	1.000%
42	21.807	3182	3186	3192	rBV4	69494	106882	2.36%	0.313%
43	22.324	3272	3274	3280	rVB	41627	61841	1.36%	0.181%
44	22.412	3284	3289	3305	rVB7	105383	330734	7.29%	0.967%
45	23.088	3400	3404	3410	rVB2	67737	114837	2.53%	0.336%
46	23.763	3512	3519	3526	rBV	155571	467101	10.29%	1.366%
47	23.875	3533	3538	3545	rVB3	173641	357873	7.89%	1.047%
48	23.940	3545	3549	3558	rBV8	56142	132814	2.93%	0.388%
49	24.462	3632	3638	3649	rVB2	93945	273400	6.03%	0.800%
50	24.609	3656	3663	3674	rVB	127983	335185	7.39%	0.980%
51	24.762	3679	3689	3708	rVV	477986	1596680	35.19%	4.669%
52	25.314	3775	3783	3790	rVB8	86197	245605	5.41%	0.718%
53	25.913	3875	3885	3896	rVB2	338730	1071390	23.61%	3.133%
54	26.031	3899	3905	3923	rVB6	121067	473001	10.42%	1.383%

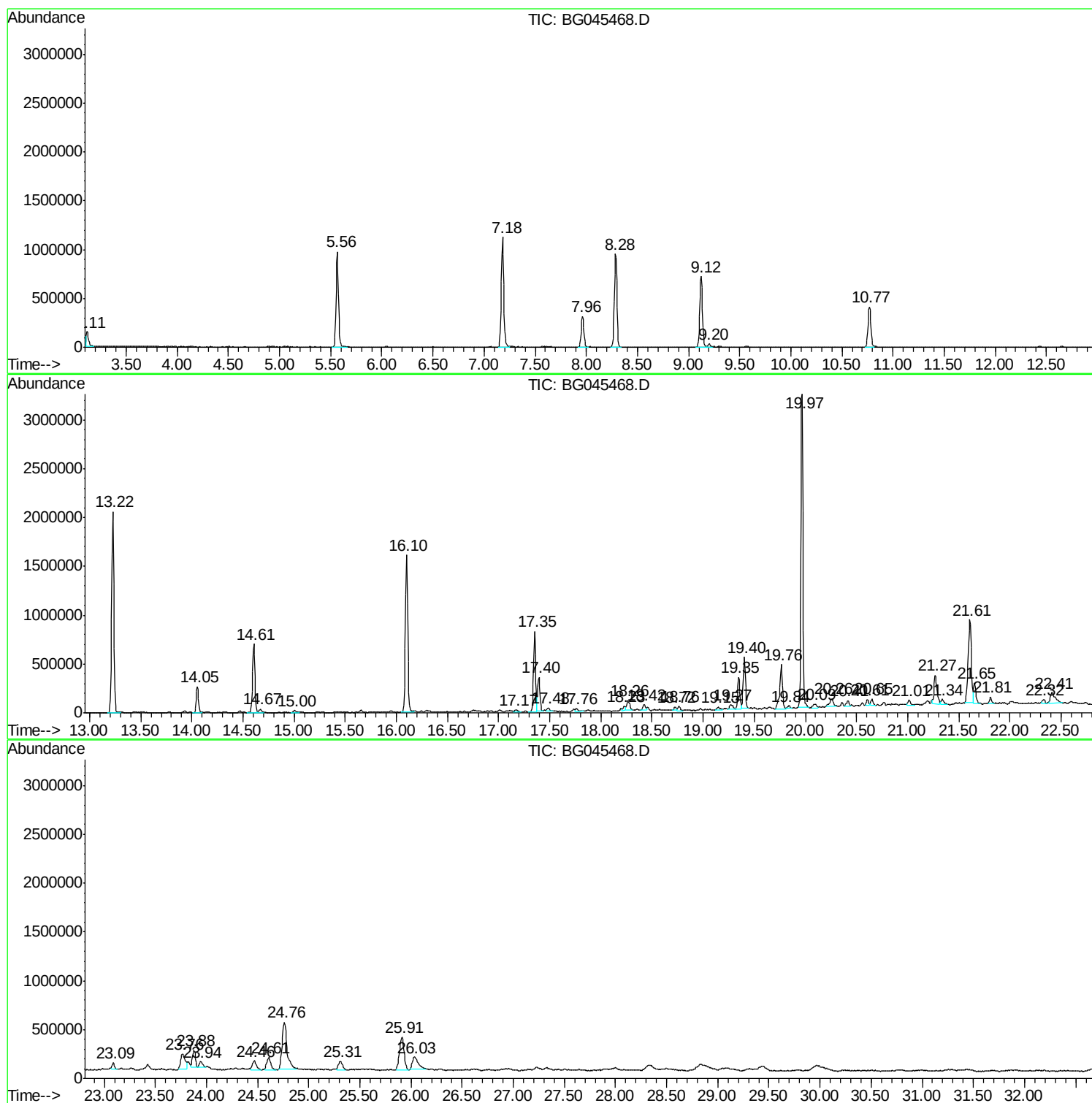
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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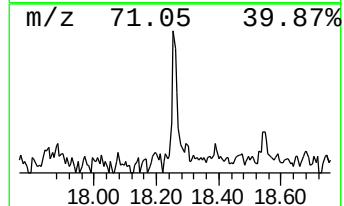
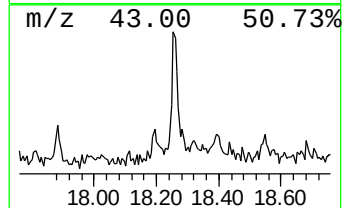
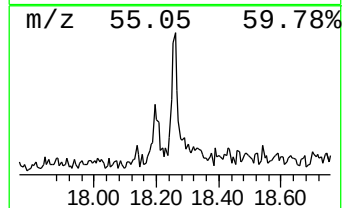
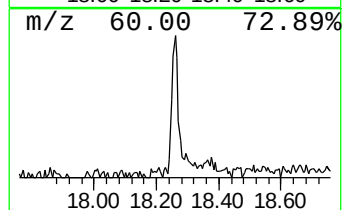
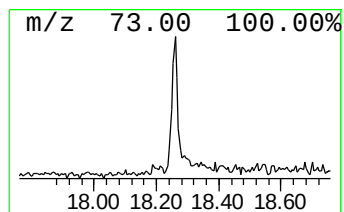
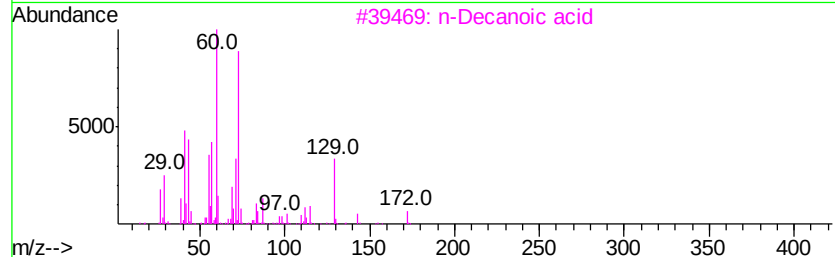
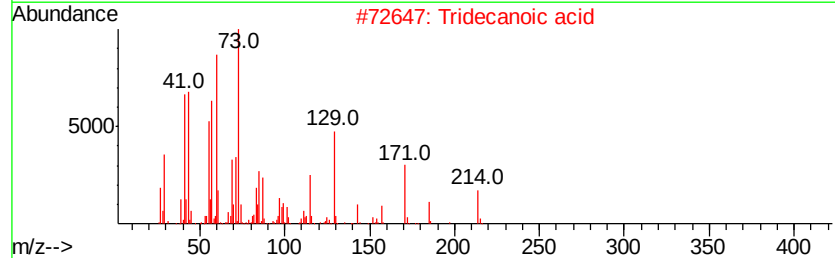
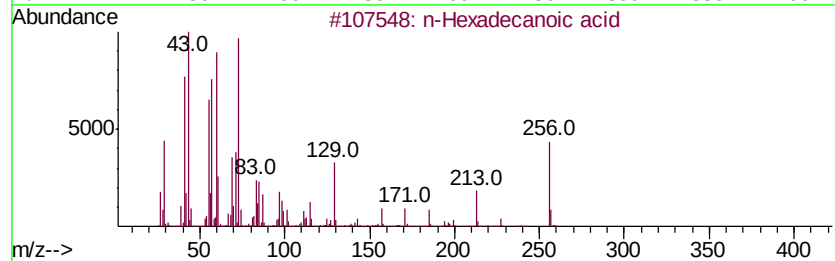
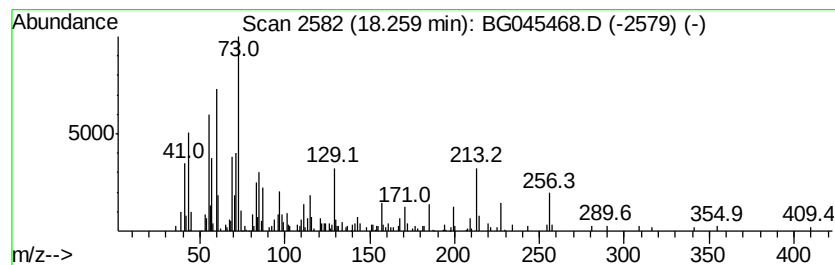
Instrument :
BNA_G
ClientSampleId :
NMDUP01-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.26	3.22 ng	211482	Phenanthrene-d10	17.35
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Hexadecanoic acid	256 C16H32O2	000057-10-3	83
2	Tridecanoic acid	214 C13H26O2	000638-53-9	64
3	n-Decanoic acid	172 C10H20O2	000334-48-5	50
4	Tetradecanoic acid	228 C14H28O2	000544-63-8	43
5	Dodecanoic acid	200 C12H24O2	000143-07-7	38



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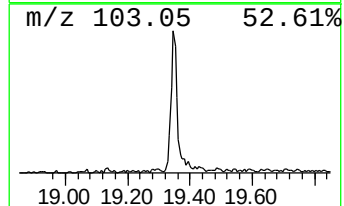
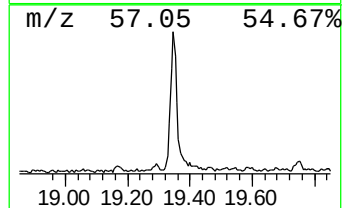
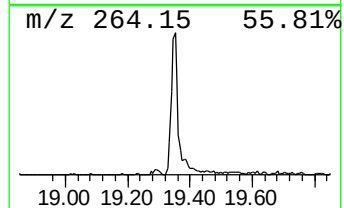
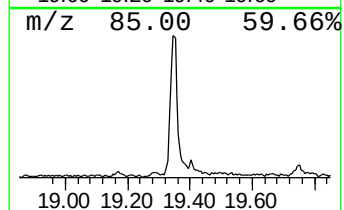
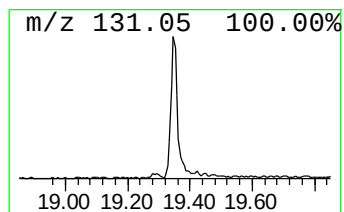
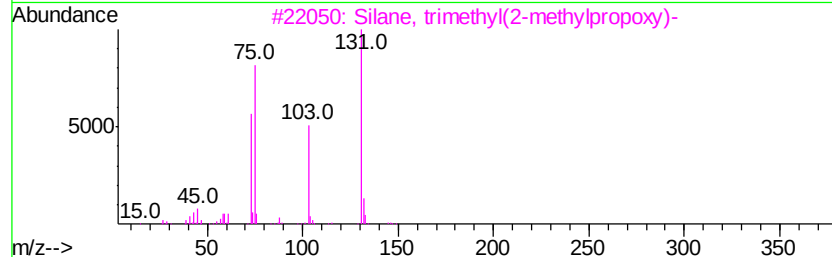
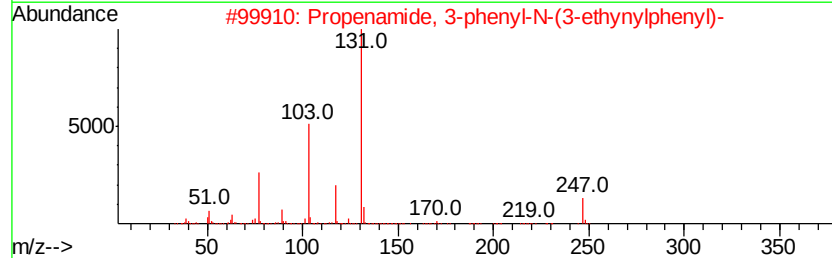
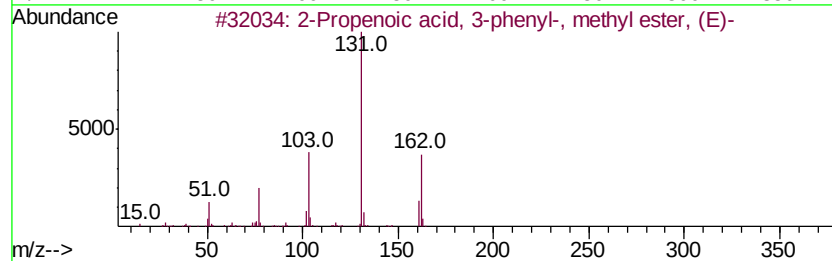
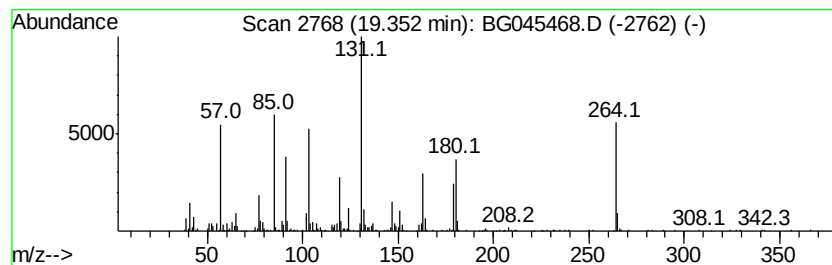
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown19.35 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.35	7.19 ng	471780	Phenanthrene-d10	17.35	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, 3-phenyl-, met...	162	C10H10O2	001754-62-7	30
2	Propenamide, 3-phenyl-N-(3-ethyn...	247	C17H13NO	294667-02-0	25
3	Silane, trimethyl(2-methylpropoxy)-	146	C7H18OSi	018269-50-6	22
4	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	22
5	2-Propenal, 3-(2-methoxyphenyl)-	162	C10H10O2	001504-74-1	22



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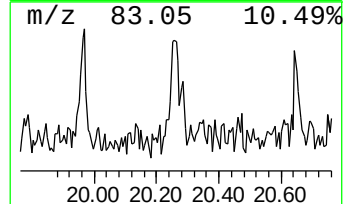
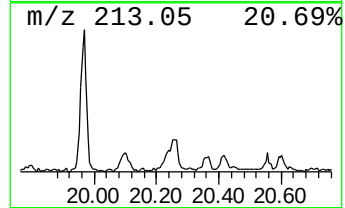
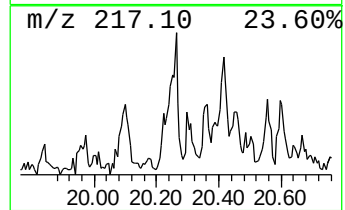
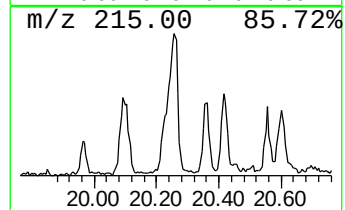
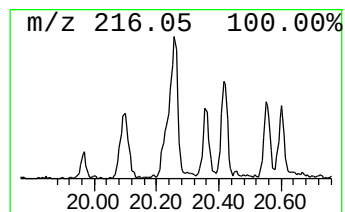
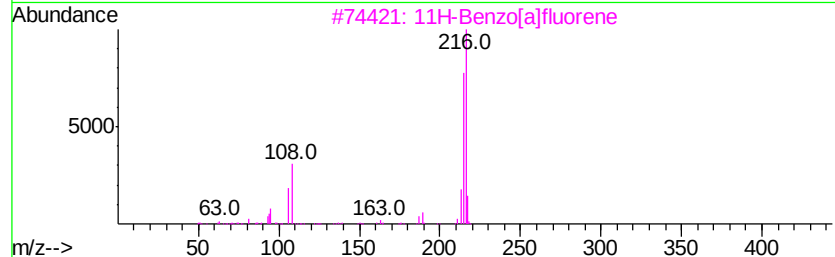
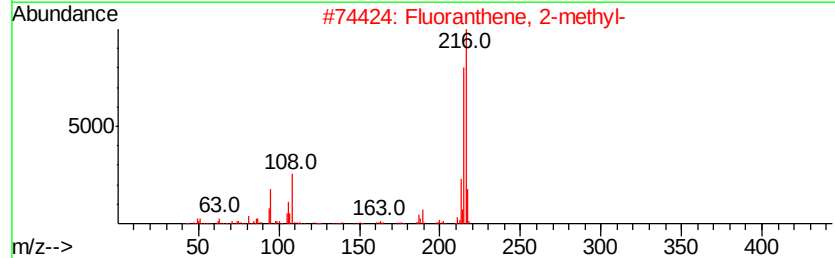
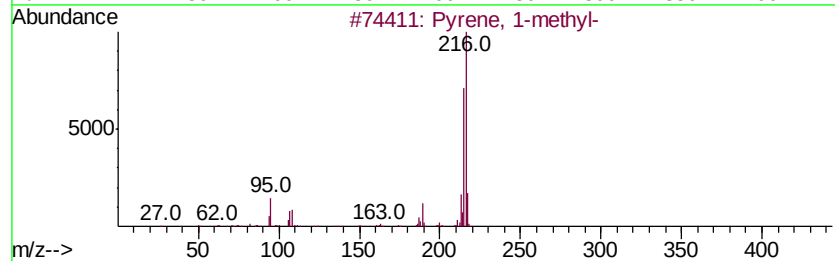
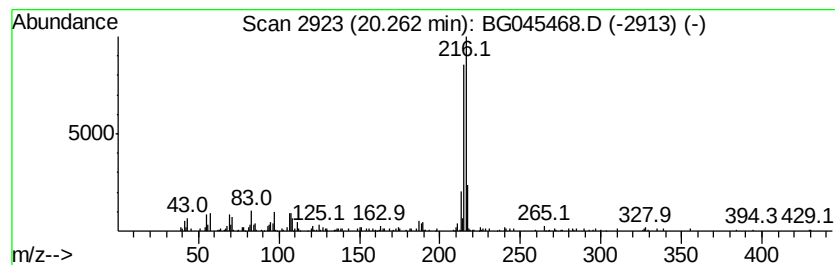
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pyrene, 1-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.26	2.18 ng	191465	Chrysene-d12	21.61
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Pyrene, 1-methyl-	216 C17H12	002381-21-7 93
2		Fluoranthene, 2-methyl-	216 C17H12	033543-31-6 87
3		11H-Benzo[a]fluorene	216 C17H12	000238-84-6 87
4		7H-Benzo[c]fluorene	216 C17H12	000205-12-9 86
5		11H-Benzo[b]fluorene	216 C17H12	000243-17-4 86



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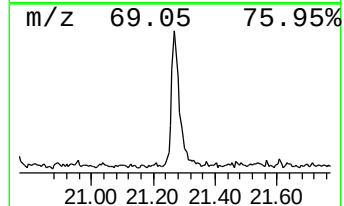
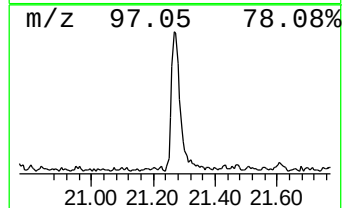
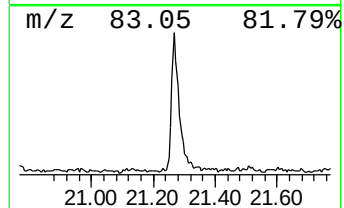
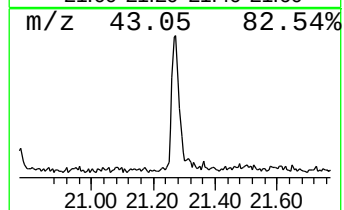
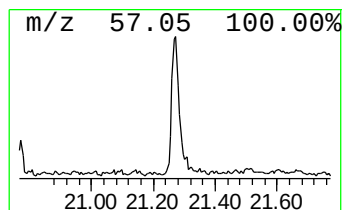
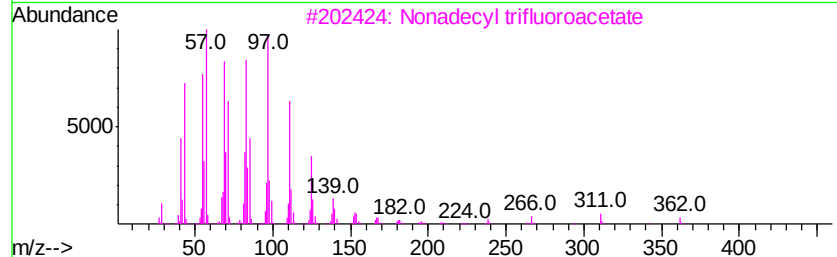
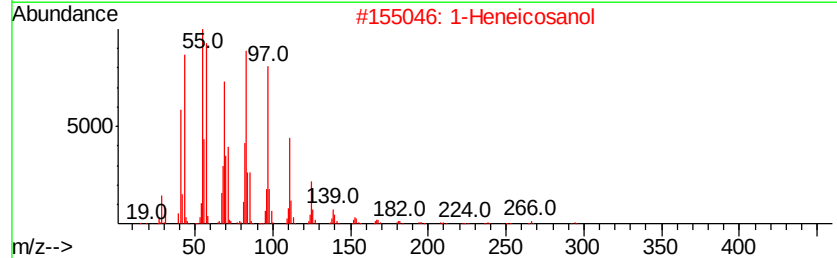
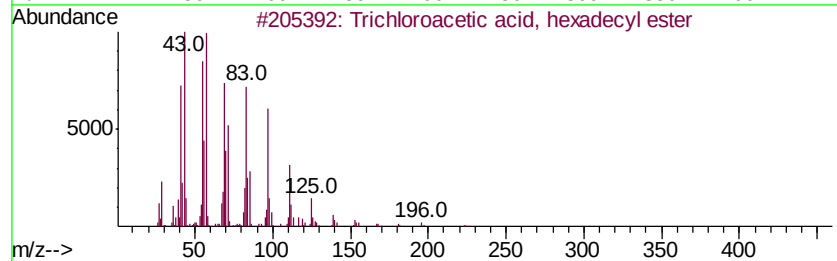
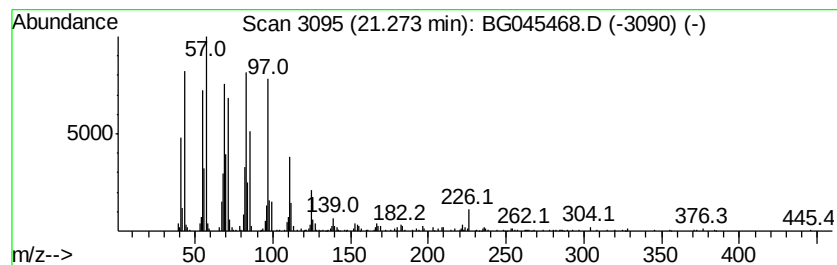
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.27	6.32 ng	556337	Chrysene-d12	21.61	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	90
3	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	83
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	81



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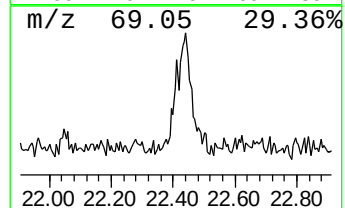
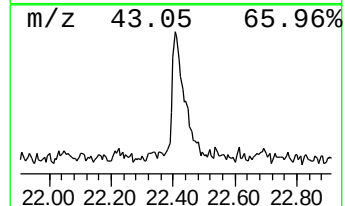
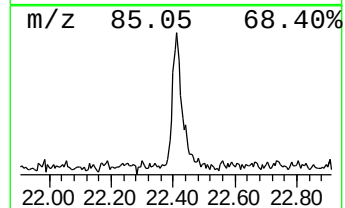
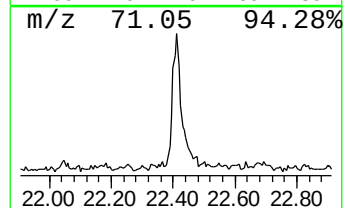
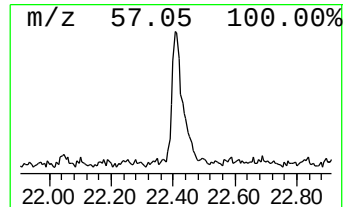
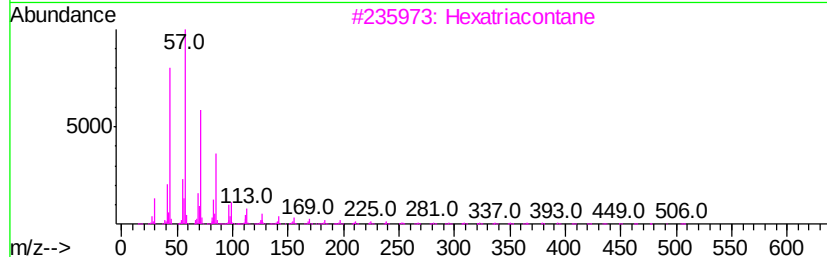
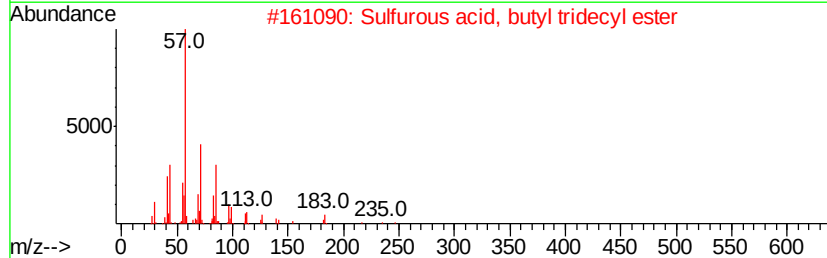
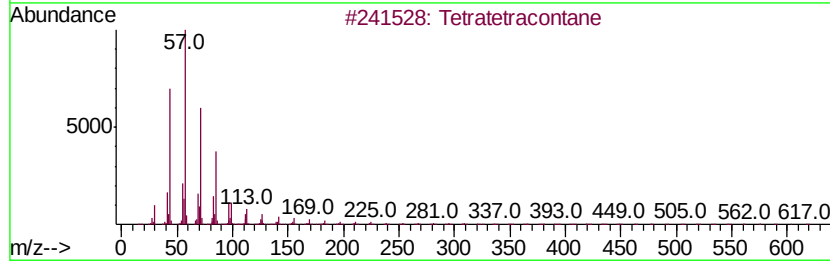
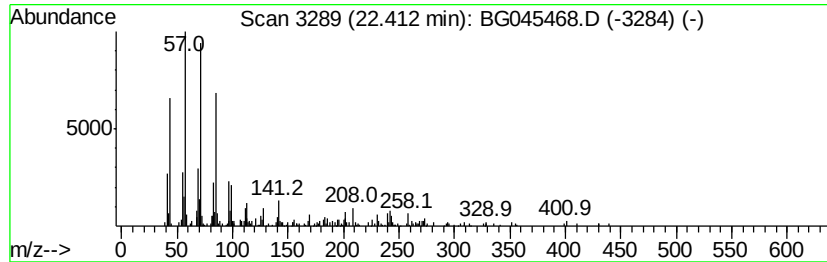
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.41	3.76 ng	330734	Chrysene-d12	21.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetratetracontane	619	C44H90	007098-22-8	83
2		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
3		Hexatriacontane	507	C36H74	000630-06-8	80
4		Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
5		Hexadecane	226	C16H34	000544-76-3	76



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052620\
Data File : BG045468.D
Acq On : 26 May 2020 22:19
Operator : CG/JU
Sample : L2744-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NMDUP01-COMP-2020-0-6

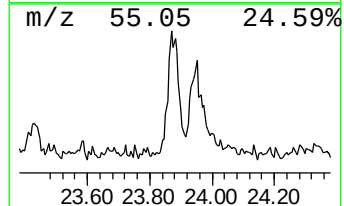
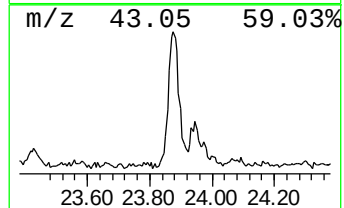
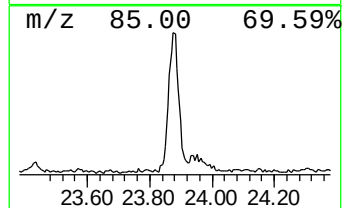
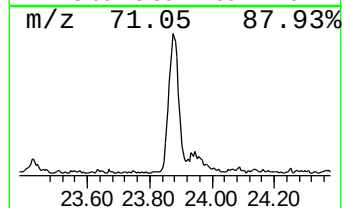
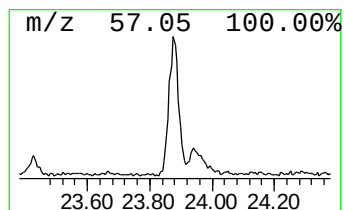
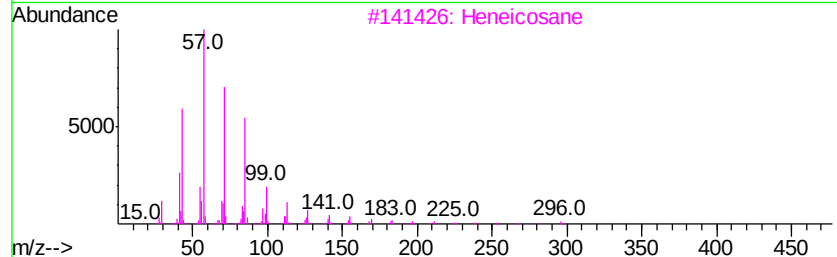
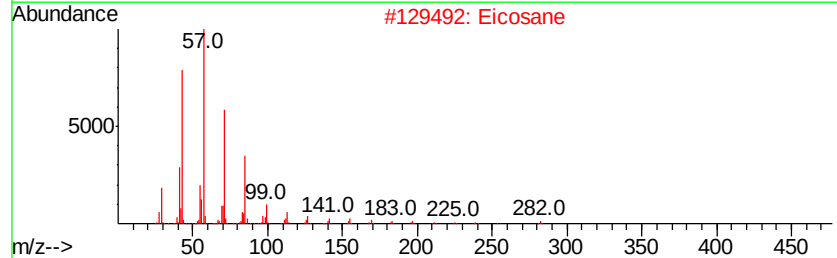
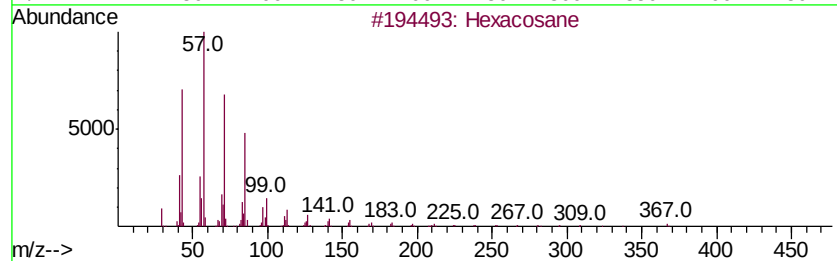
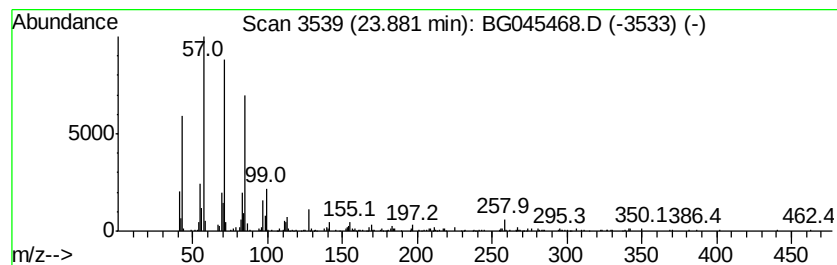
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.88	4.48 ng	357873	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Eicosane	282	C20H42	000112-95-8	90
3		Heneicosane	296	C21H44	000629-94-7	87
4		Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	86
5		Octacosane	394	C28H58	000630-02-4	80



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052620\
Data File : BG045468.D
Acq On : 26 May 2020 22:19
Operator : CG/JU
Sample : L2744-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

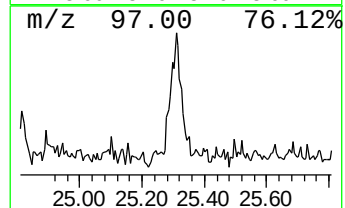
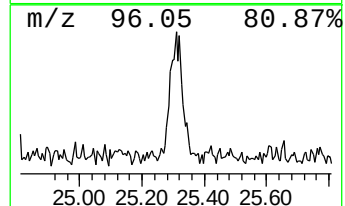
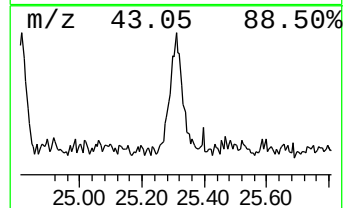
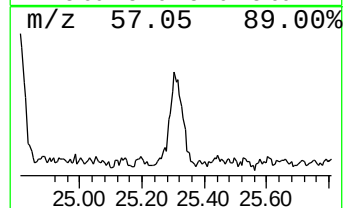
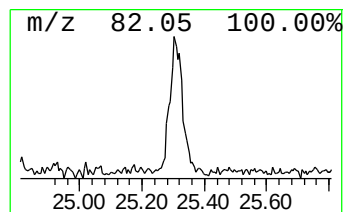
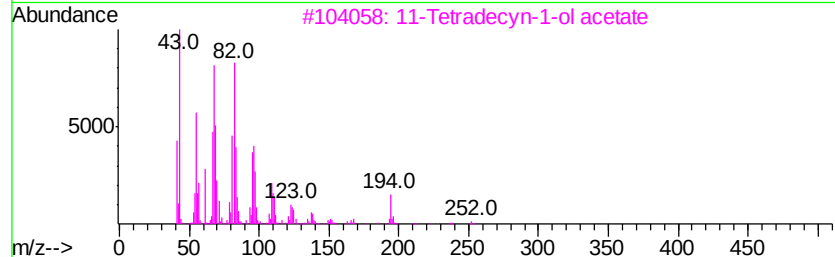
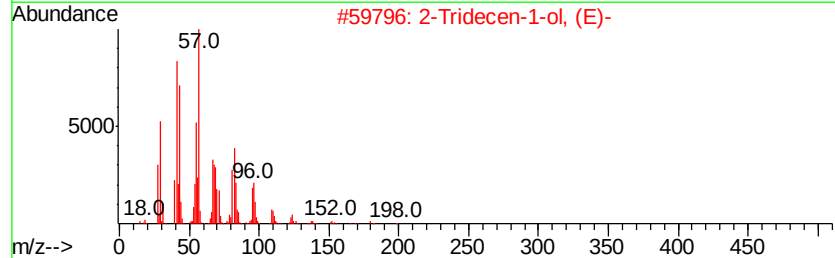
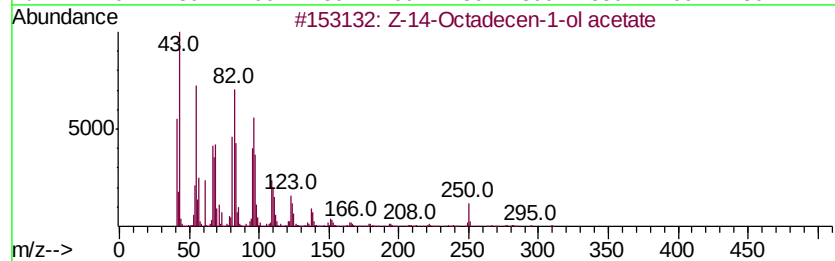
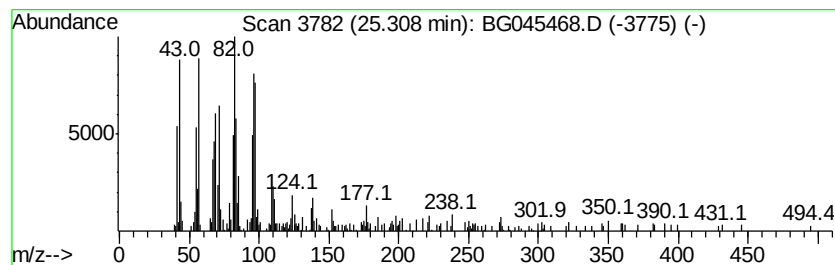
Instrument :
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ClientSampleId :
NMDUP01-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Z-14-Octadecen-1-ol acetate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.		
25.31	3.08 ng	245605	Perylene-d12		24.76		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Z-14-Octadecen-1-ol acetate	310	C20H38O2	1000131-07-6	93
2			2-Tridecen-1-ol, (E)-	198	C13H26O	074962-98-4	83
3			11-Tetradecyn-1-ol acetate	252	C16H28O2	033925-72-3	78
4			Heptadecanal	254	C17H34O	1000376-70-0	70
5			Oxirane, tetradecyl-	240	C16H32O	007320-37-8	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052620\
Data File : BG045468.D
Acq On : 26 May 2020 22:19
Operator : CG/JU
Sample : L2744-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NMDUP01-COMP-2020-0-6

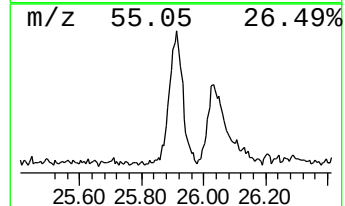
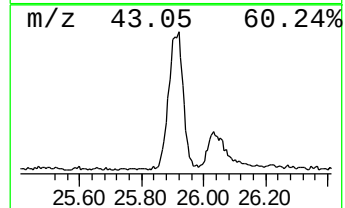
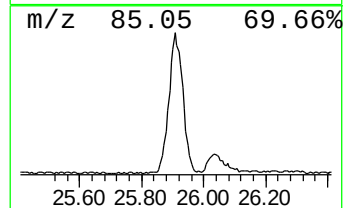
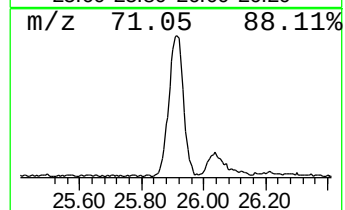
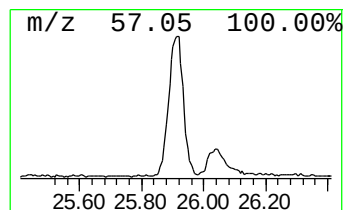
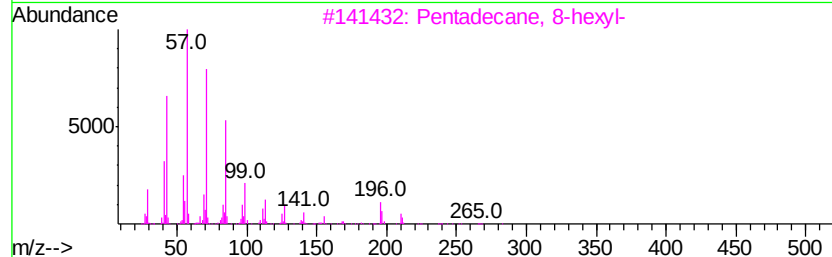
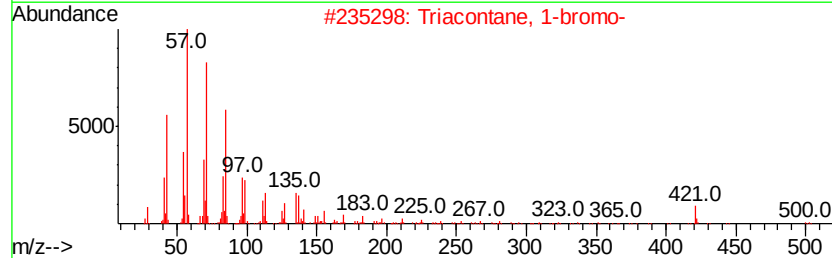
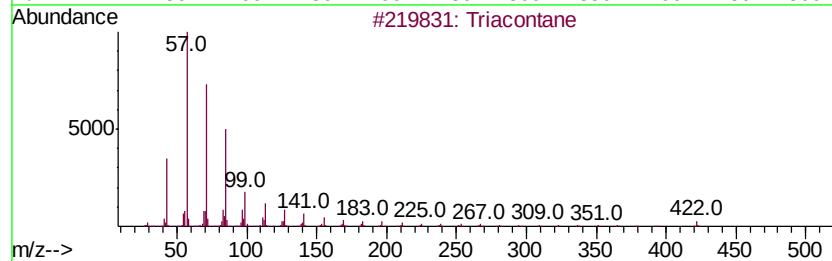
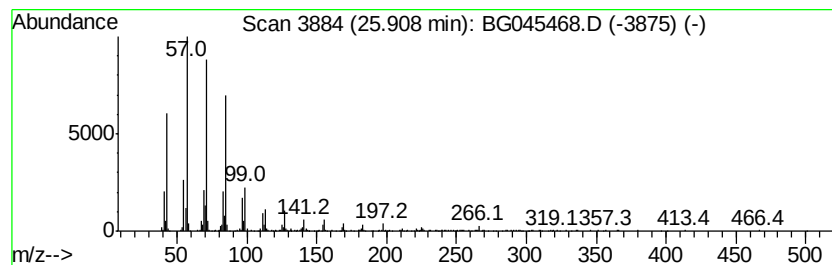
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Triacontane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.91	13.42 ng	1071390	Perylene-d12	24.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Triacontane	422	C30H62	000638-68-6	91
2		Triacontane, 1-bromo-	500	C30H61Br	004209-22-7	91
3		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
4		Heneicosane	296	C21H44	000629-94-7	87
5		Docosane	310	C22H46	000629-97-0	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG052620\
Data File : BG045468.D
Acq On : 26 May 2020 22:19
Operator : CG/JU
Sample : L2744-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

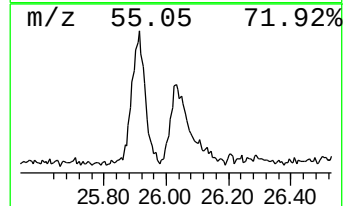
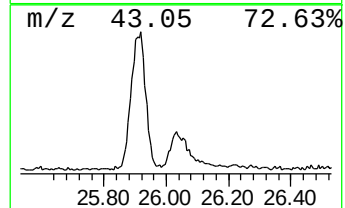
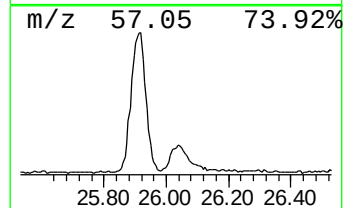
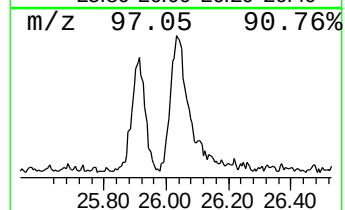
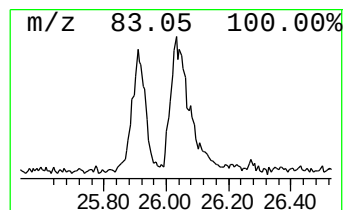
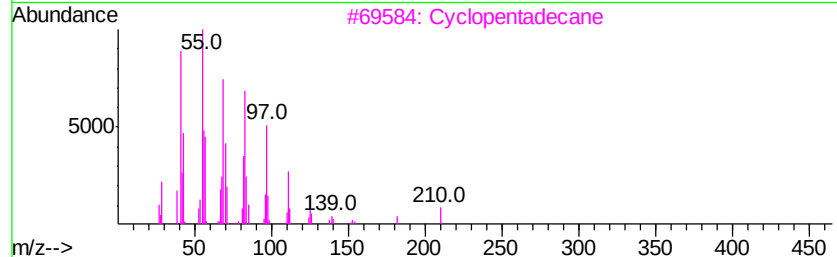
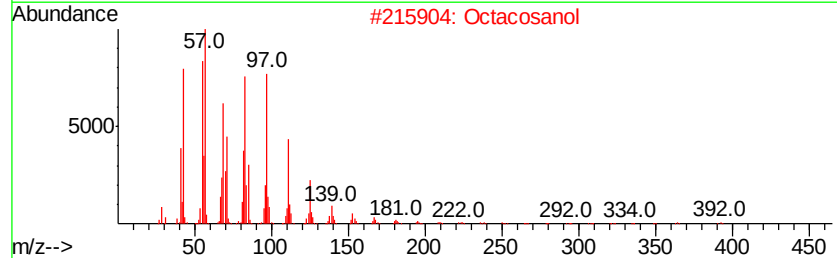
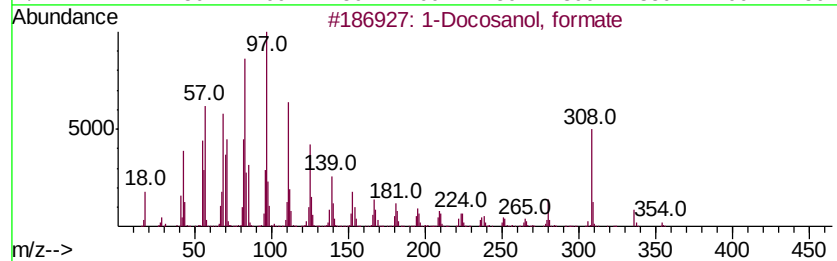
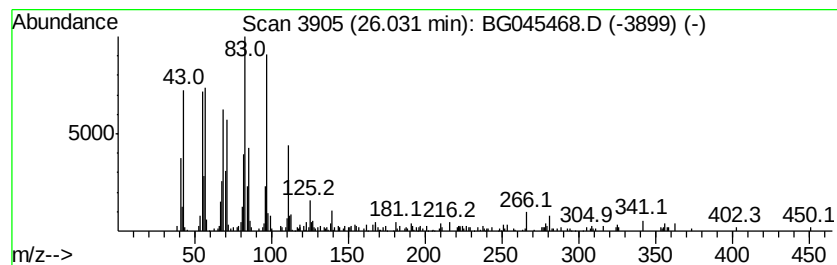
Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG051520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 1-Docosanol, formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.03	5.92 ng	473001	Perylene-d12	24.76
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Docosanol, formate	354 C23H46O2	015155-62-1	93
2	Octacosanol	410 C28H58O	000557-61-9	91
3	Cyclopentadecane	210 C15H30	000295-48-7	70
4	1-Pentadecene	210 C15H30	013360-61-7	64
5	Docosyl trifluoroacetate	422 C24H45F3O2	1000351-75-5	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG052620\
Data File : BG045468.D
Acq On : 26 May 2020 22:19
Operator : CG/JU
Sample : L2744-12
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
NMDUP01-COMP-2020-0-6

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG051520.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
n-Hexadecanoic acid	18.26	3.2	ng	211482	4	17.35	1312080	20.0
unknown19.35	19.35	7.2	ng	471780	4	17.35	1312080	20.0
Pyrene, 1-methyl-	20.26	2.2	ng	191465	5	21.61	1760570	20.0
Trichloroacetic a...	21.27	6.3	ng	556337	5	21.61	1760570	20.0
Tetratetracontane	22.41	3.8	ng	330734	5	21.61	1760570	20.0
Hexacosane	23.88	4.5	ng	357873	6	24.76	1596680	20.0
Z-14-Octadecen-1-...	25.31	3.1	ng	245605	6	24.76	1596680	20.0
Triacontane	25.91	13.4	ng	1071390	6	24.76	1596680	20.0
1-Docosanol, formate	26.03	5.9	ng	473001	6	24.76	1596680	20.0