

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
 Data File : BG048861.D
 Acq On : 23 Apr 2021 13:31
 Operator : CG/JU
 Sample : M2107-08
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-31-0-2.0

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_G\METHODS\8270-BG041421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048861.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.120	298	303	310	rVB2	19310	33102	1.63%	0.275%
2	5.608	378	386	395	rBV	638528	1003092	49.31%	8.336%
3	6.989	615	621	626	rBV3	20395	31653	1.56%	0.263%
4	7.224	653	661	670	rBV	648160	1122491	55.18%	9.329%
5	8.052	794	802	810	rBV	113682	190286	9.35%	1.581%
6	9.227	993	1002	1008	rBV	425411	741874	36.47%	6.165%
7	10.878	1276	1283	1290	rBV	146620	261453	12.85%	2.173%
8	13.334	1693	1701	1707	rBV	1032305	1588942	78.11%	13.205%
9	14.157	1831	1841	1847	rBV4	20933	46089	2.27%	0.383%
10	14.697	1926	1933	1942	rVB3	372606	797963	39.23%	6.632%
11	15.361	2041	2046	2050	rVB2	20930	26672	1.31%	0.222%
12	15.596	2080	2086	2092	rBV3	26668	42452	2.09%	0.353%
13	16.207	2182	2190	2199	rBV	796506	1166899	57.36%	9.698%
14	17.470	2399	2405	2411	rBV	275066	404434	19.88%	3.361%
15	18.299	2542	2546	2551	rBV6	42418	68412	3.36%	0.569%
16	18.358	2551	2556	2561	rVV5	25846	48020	2.36%	0.399%
17	19.380	2726	2730	2734	rVB6	13605	20989	1.03%	0.174%
18	19.451	2738	2742	2747	rBV4	33389	51597	2.54%	0.429%
19	19.521	2751	2754	2758	rVV2	26895	47924	2.36%	0.398%
20	19.885	2813	2816	2822	rVB	20570	36263	1.78%	0.301%
21	20.085	2844	2850	2855	rBV	1628022	2034173	100.00%	16.905%
22	20.349	2890	2895	2897	rBV5	12944	21601	1.06%	0.180%
23	20.373	2897	2899	2904	rVB6	20962	26677	1.31%	0.222%
24	20.872	2979	2984	2987	rBV7	15239	23199	1.14%	0.193%
25	21.384	3066	3071	3077	rBV	159238	242478	11.92%	2.015%
26	21.765	3130	3136	3150	rVB	244363	437629	21.51%	3.637%
27	22.200	3206	3210	3214	rVB7	21187	32461	1.60%	0.270%
28	22.594	3269	3277	3286	rVB4	123720	287558	14.14%	2.390%
29	23.281	3390	3394	3398	rBV7	14472	22895	1.13%	0.190%
30	23.475	3422	3427	3435	rVB2	40958	87199	4.29%	0.725%
31	23.646	3452	3456	3461	rVB7	21603	33504	1.65%	0.278%
32	24.116	3528	3536	3543	rBV2	88657	197200	9.69%	1.639%
33	24.180	3543	3547	3554	rBV7	35634	68820	3.38%	0.572%
34	25.091	3692	3702	3712	rVB2	148753	416144	20.46%	3.458%
35	25.637	3791	3795	3805	rVB2	27201	71443	3.51%	0.594%
36	26.278	3895	3904	3913	rVB3	94845	299280	14.71%	2.487%

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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_G\METHODS\8270-BG041421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

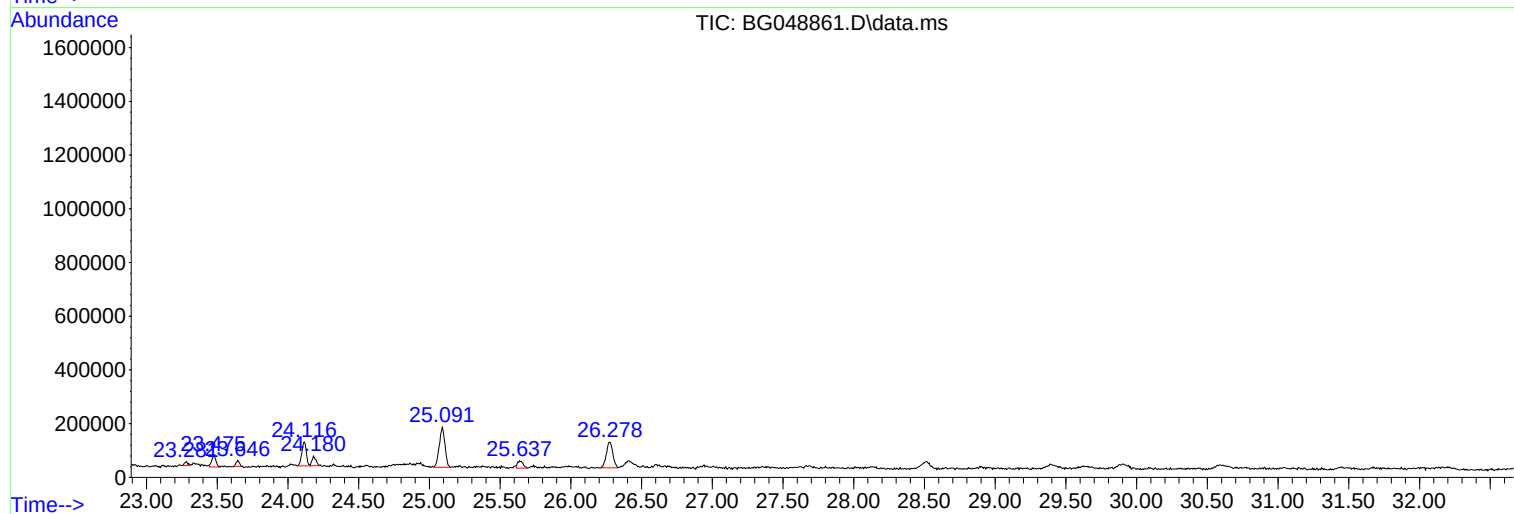
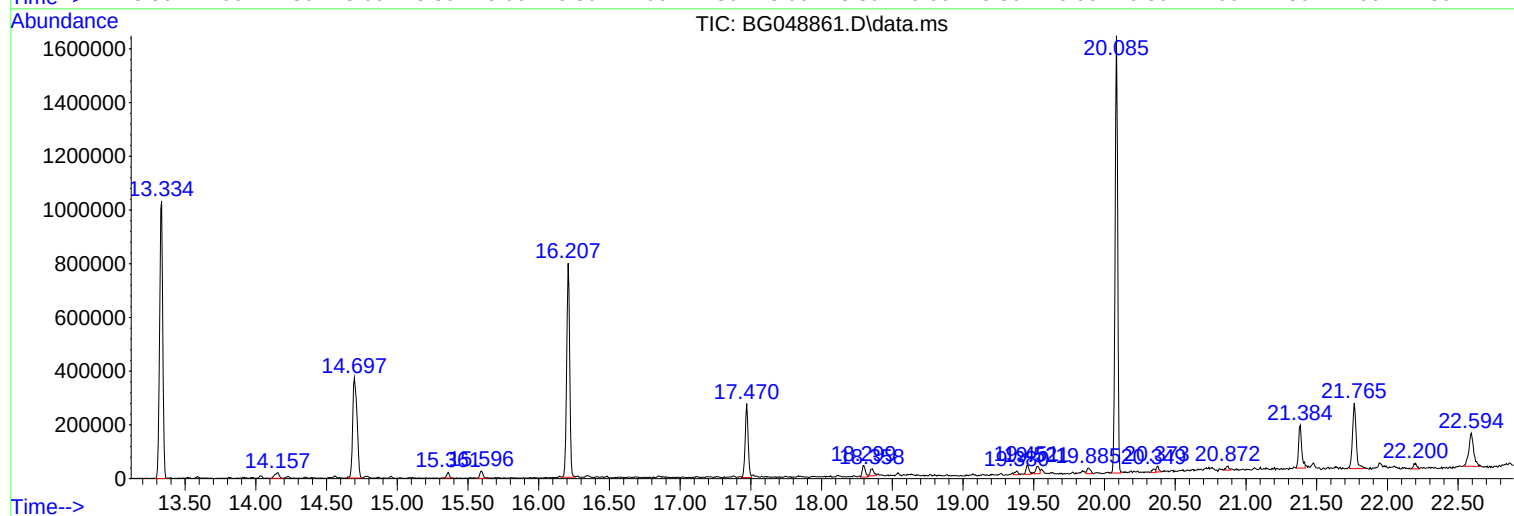
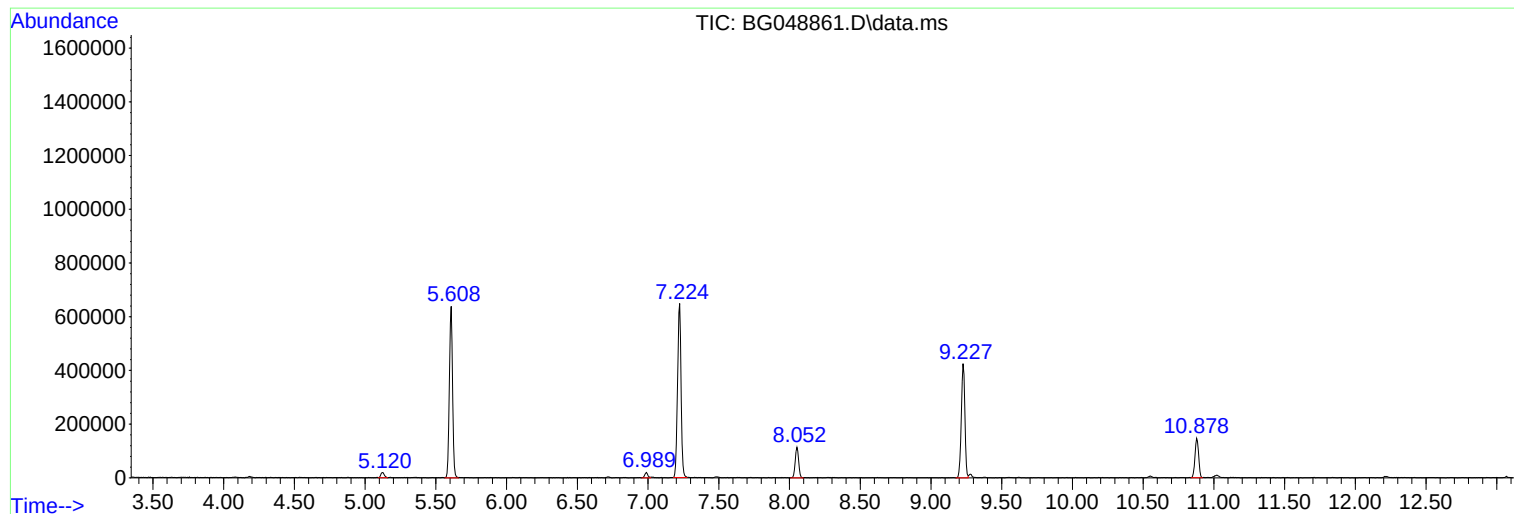
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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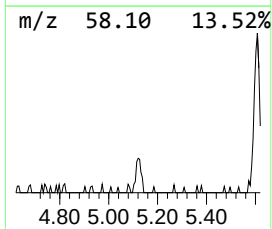
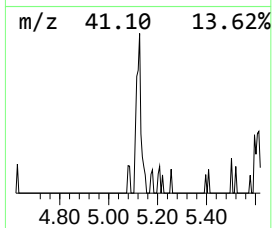
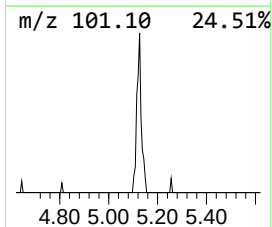
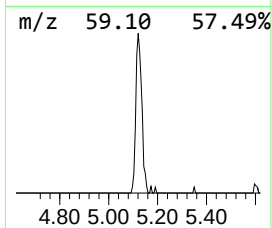
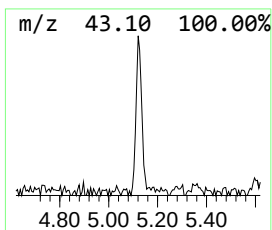
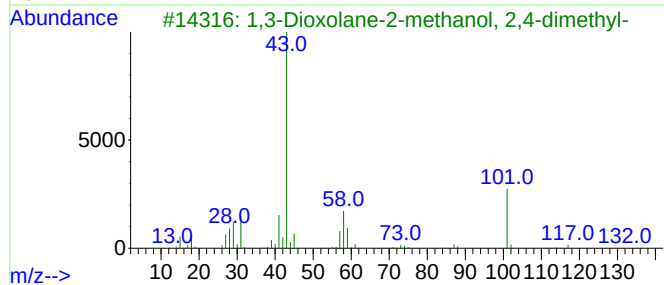
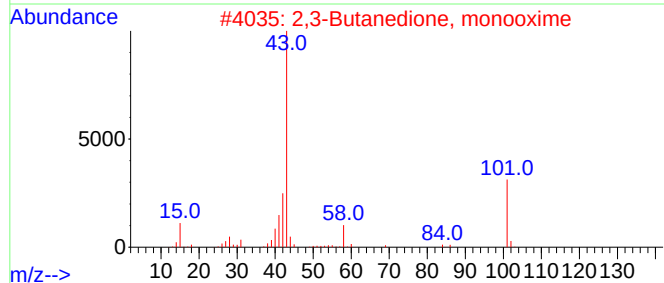
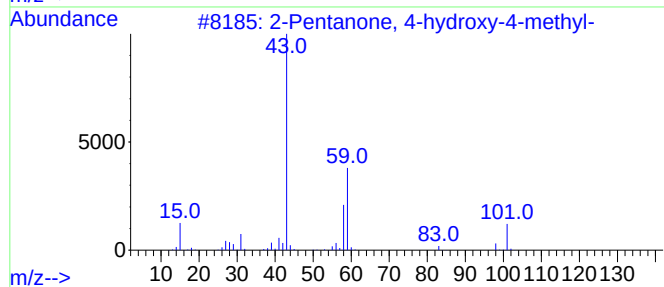
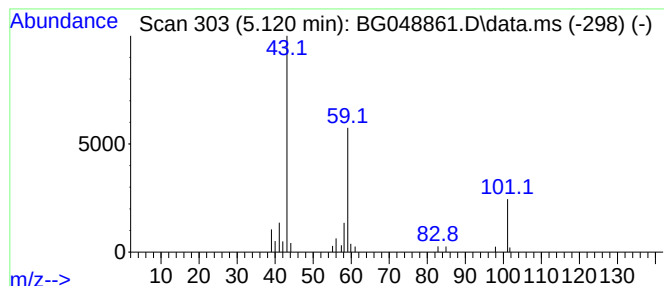
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.120	3.48 ng	33102	1,4-Dichlorobenzene-d4	8.052

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32		
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17		
5	Propylamine	59	C3H9N	000107-10-8	9		



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Instrument :
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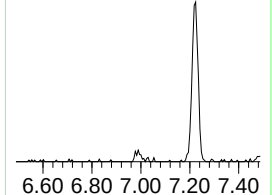
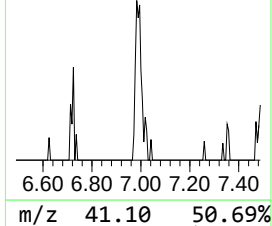
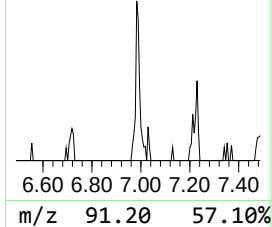
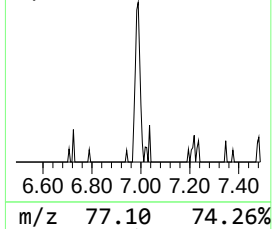
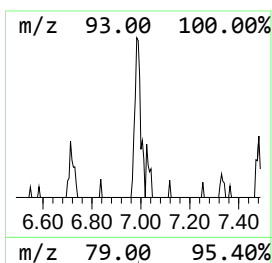
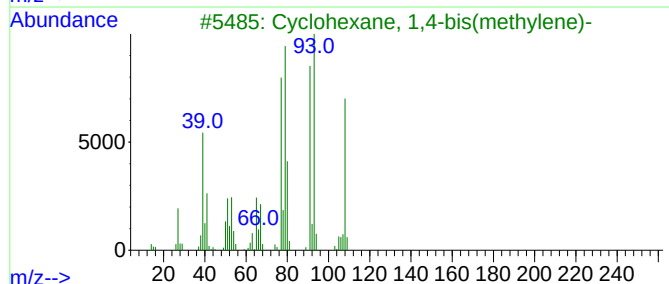
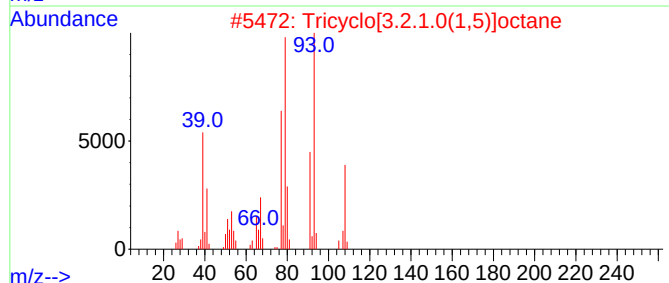
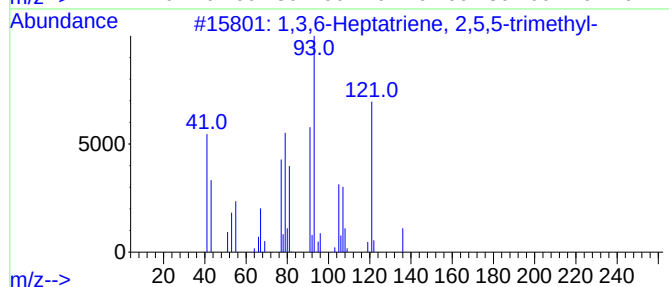
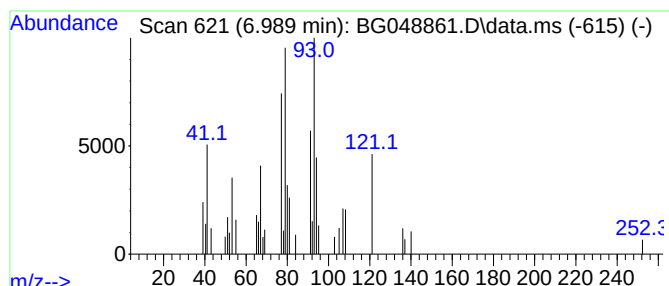
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3,6-Heptatriene, 2,5,5-tr... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.989	3.33 ng	31653	1,4-Dichlorobenzene-d4	8.052

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	029548-02-5	72	
2	Tricyclo[3.2.1.0(1,5)]octane	108	C8H12	019074-25-0	68	
3	Cyclohexane, 1,4-bis(methylene)-	108	C8H12	004982-20-1	60	
4	Bicyclo[3.1.0]hex-3-en-2-one, 5-...	136	C9H12O	036262-12-1	55	
5	7-Pentadecen-5-yne, (Z)-	206	C15H26	074744-49-3	53	



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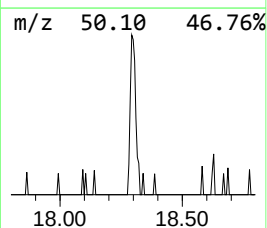
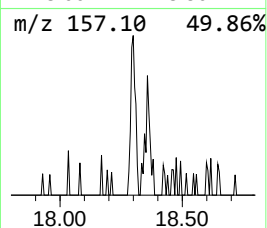
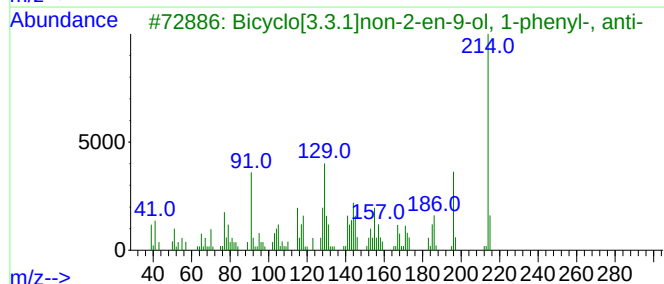
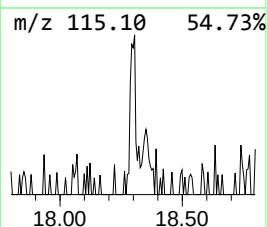
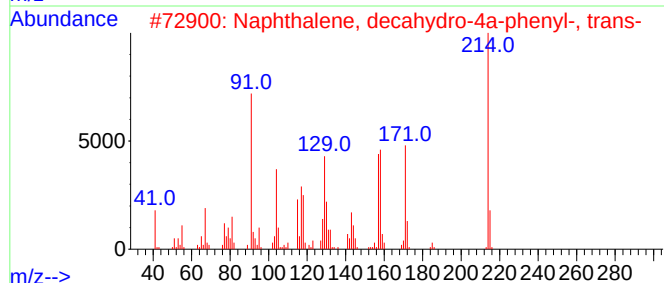
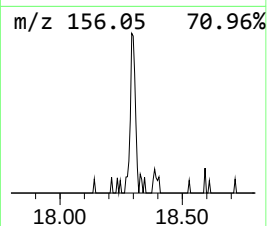
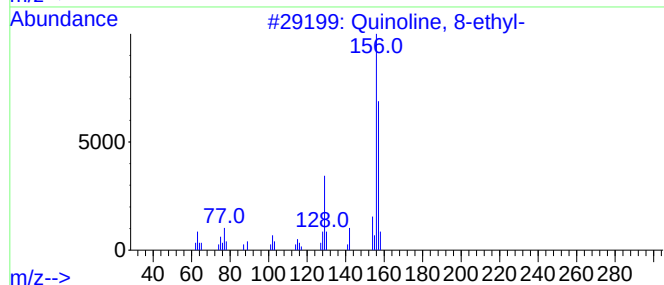
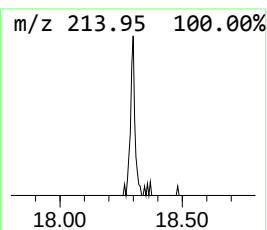
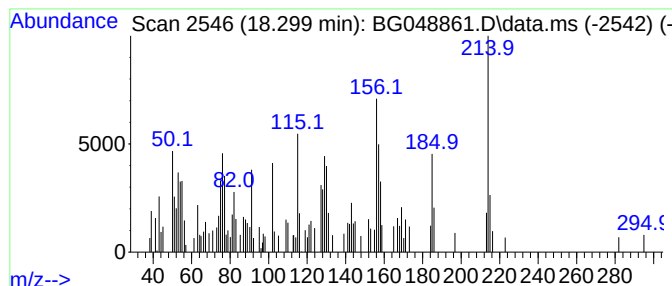
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown18.29 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.299	3.38 ng	68412	Phenanthrene-d10	17.471

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Quinoline, 8-ethyl-	157	C11H11N	019655-56-2	38
2			Naphthalene, decahydro-4a-phenyl...	214	C16H22	027863-63-4	35
3			Bicyclo[3.3.1]non-2-en-9-ol, 1-p...	214	C15H18O	042541-41-3	18
4			Ethyldiphenylphosphine	214	C14H15P	000607-01-2	15
5			4'-Fluoro-2-hydroxystilbene	214	C14H11FO	1000147-76-7	14



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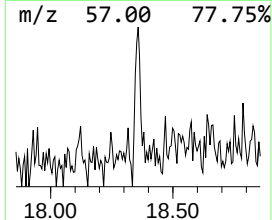
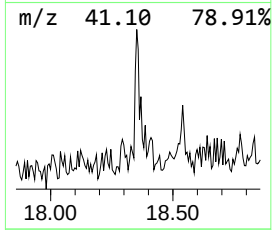
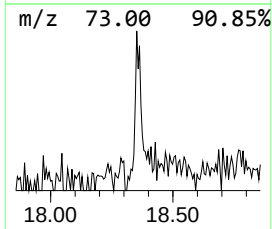
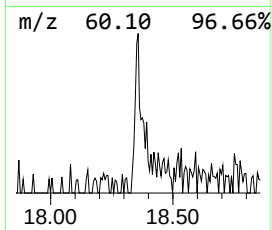
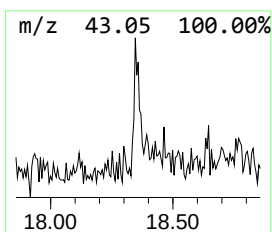
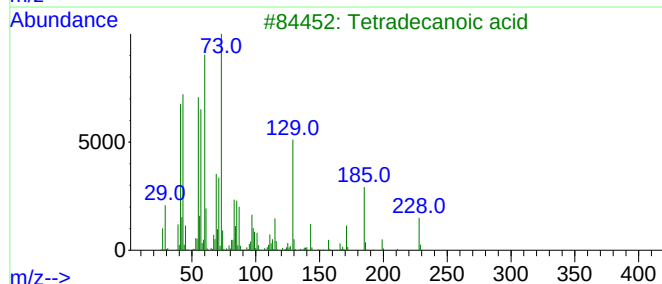
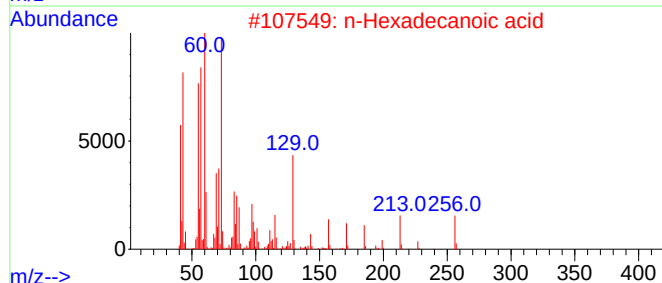
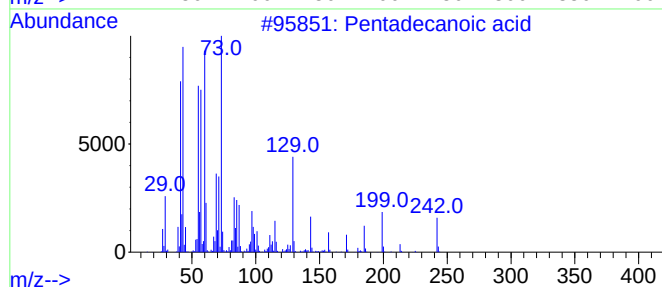
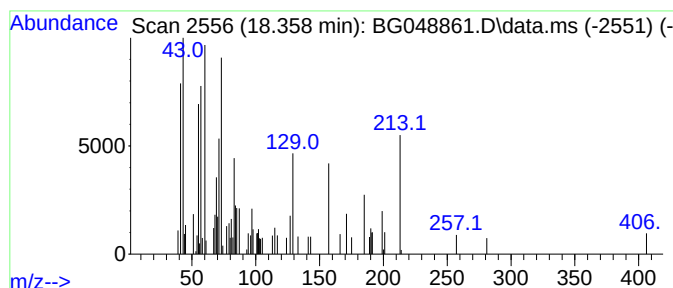
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TIC Library : C:\Database\NIST11.L
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Peak Number 4 unknown18.35 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.358	2.37 ng	48020	Phenanthrene-d10	17.471	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4	Dodecanoic acid	200	C12H24O2	000143-07-7	37
5	Tridecanoic acid	214	C13H26O2	000638-53-9	35



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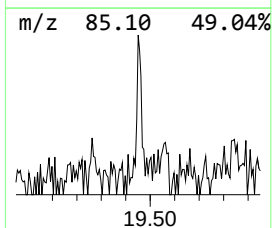
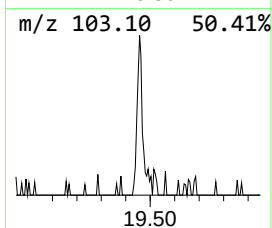
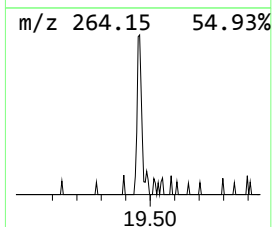
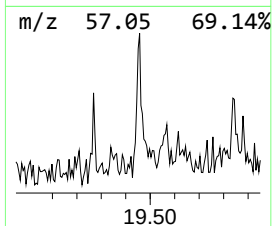
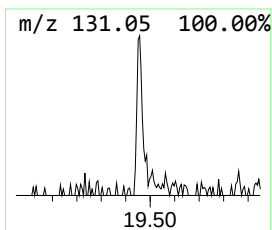
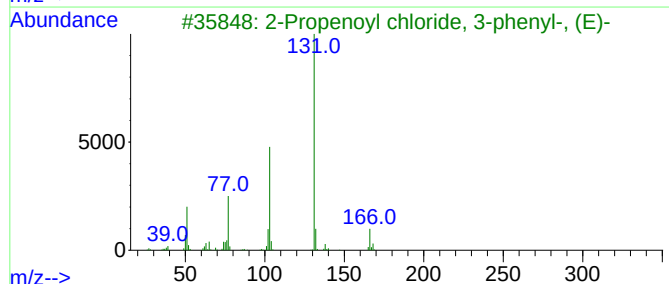
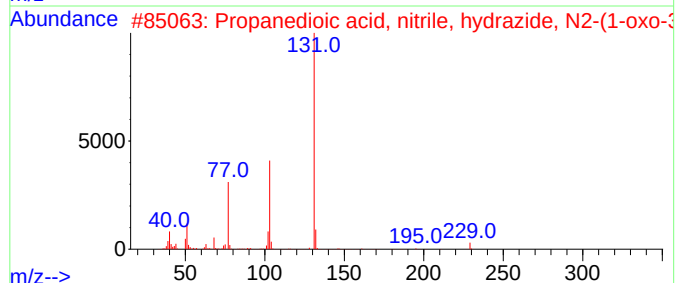
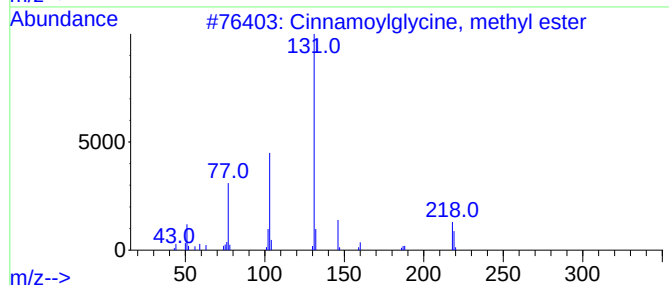
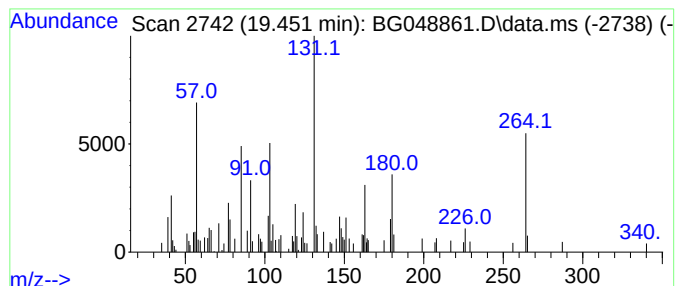
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown19.45 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	2.55 ng	51597	Phenanthrene-d10	17.471

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cinnamoylglycine, methyl ester	219	C12H13NO3	040778-04-9	35
2			Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	35
3			2-Propenoyl chloride, 3-phenyl-,...	166	C9H7ClO	017082-09-6	27
4			Vinyl trans-cinnamate	174	C11H10O2	017719-70-9	27
5			2-Propenamide, N-(1-methylethyl)...	265	C18H19NO	055044-37-6	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048861.D
Acq On : 23 Apr 2021 13:31
Operator : CG/JU
Sample : M2107-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

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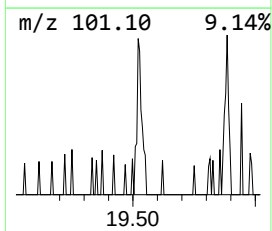
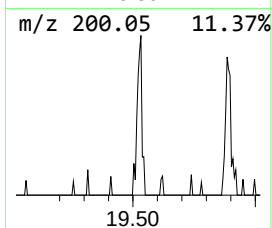
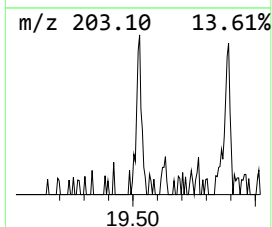
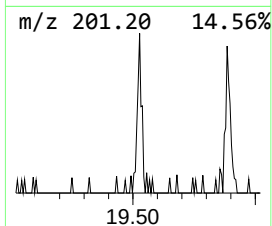
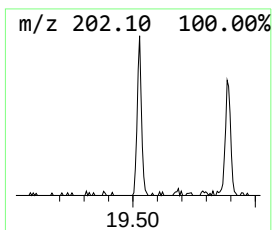
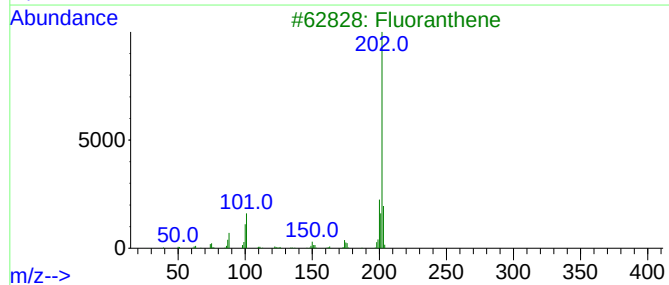
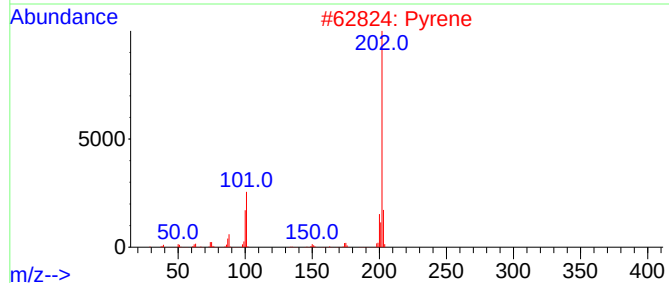
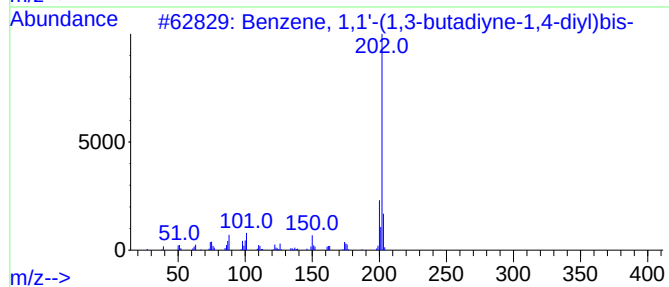
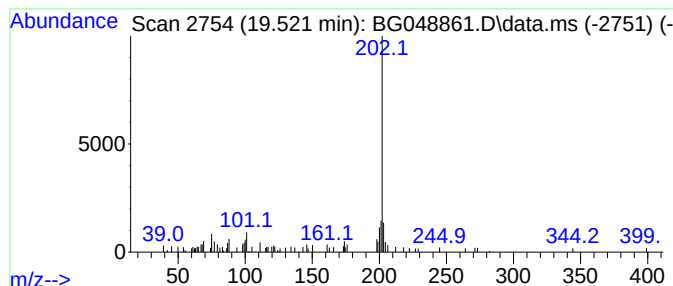
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.521	2.37 ng	47924	Phenanthrene-d10	17.471

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	81
2			Pyrene	202	C16H10	000129-00-0	72
3			Fluoranthene	202	C16H10	000206-44-0	72
4			Pyrimidine, 4-methoxy-6-(2-hydro...	202	C11H10N2O2	097630-79-0	59
5			3H-Benzo[4,5]furo[3,2-d]pyrimidi...	202	C10H6N2O5	062208-70-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048861.D
Acq On : 23 Apr 2021 13:31
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Sample : M2107-08
Misc :
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Instrument :
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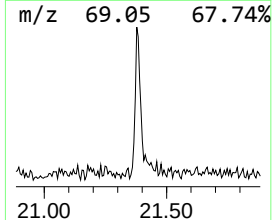
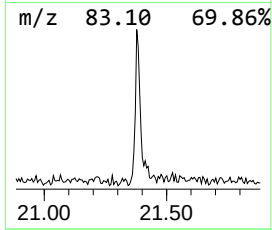
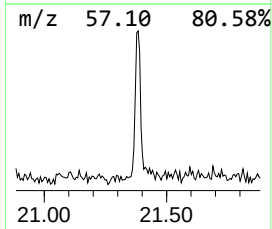
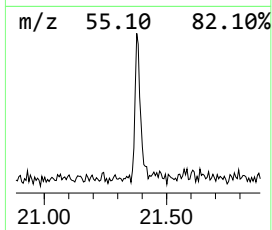
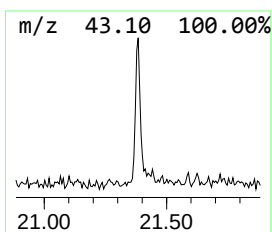
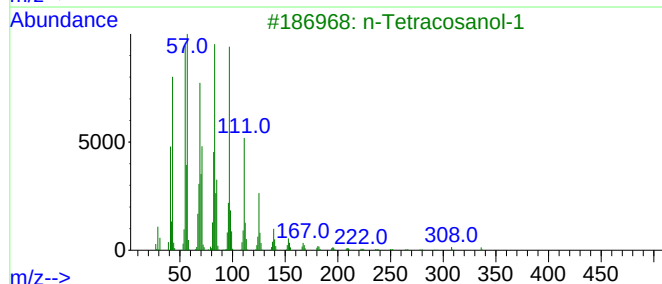
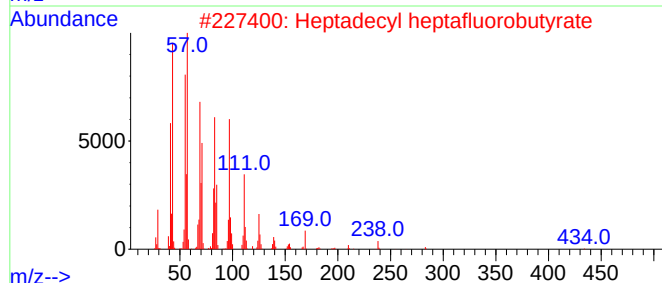
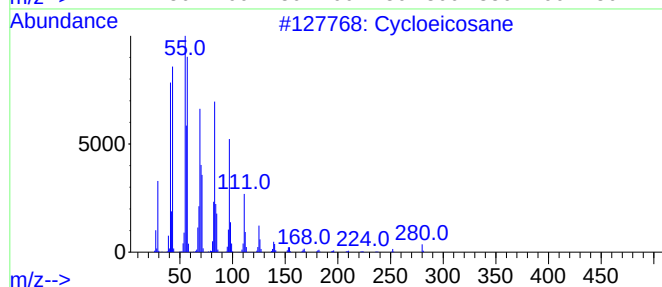
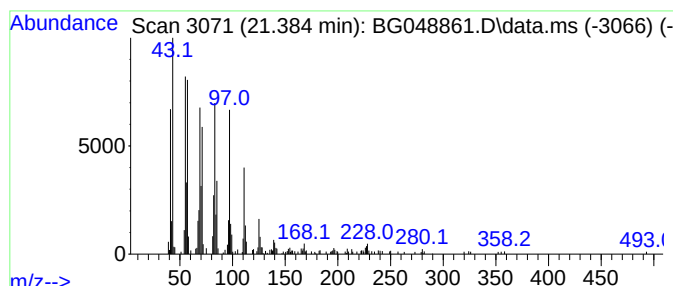
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.384	11.08 ng	242478	Chrysene-d12	21.765

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloeicosane	280	C20H40	000296-56-0	97
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4			Behenic alcohol	326	C22H46O	000661-19-8	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048861.D
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Operator : CG/JU
Sample : M2107-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

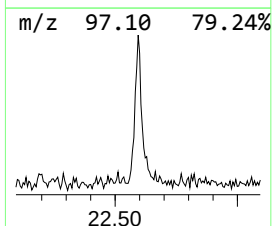
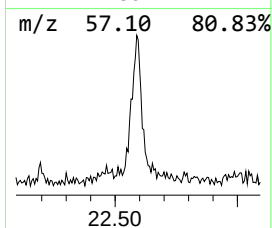
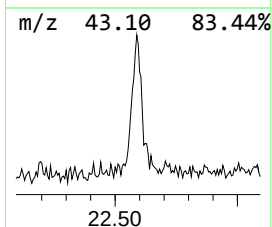
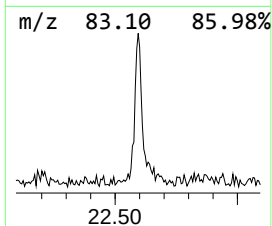
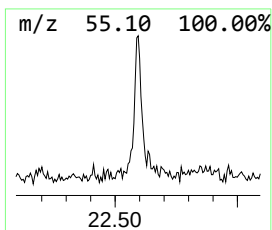
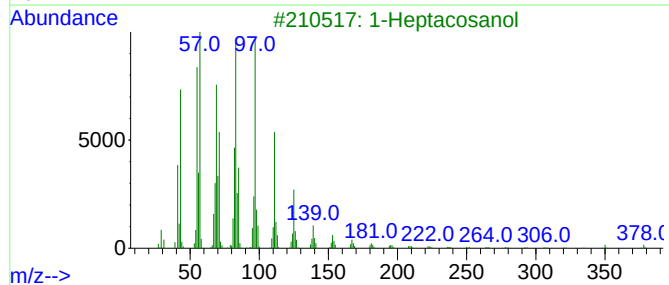
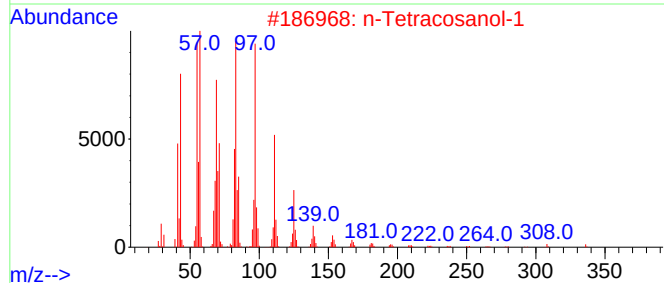
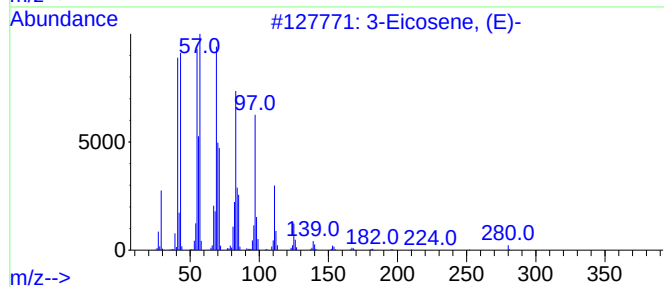
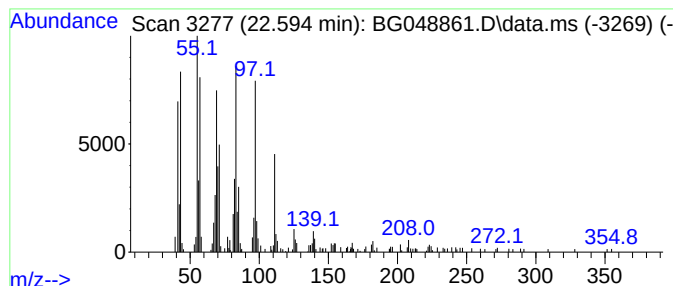
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.594	13.14 ng	287558	Chrysene-d12		21.765	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-		280	C20H40	074685-33-9	91
2	n-Tetracosanol-1		354	C24H50O	000506-51-4	90
3	1-Heptacosanol		396	C27H56O	002004-39-9	87
4	Octacosanol		410	C28H58O	000557-61-9	86
5	Behenic alcohol		326	C22H46O	000661-19-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048861.D
Acq On : 23 Apr 2021 13:31
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Sample : M2107-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

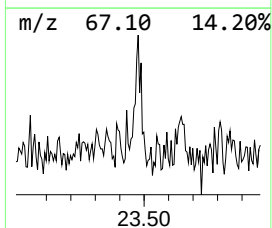
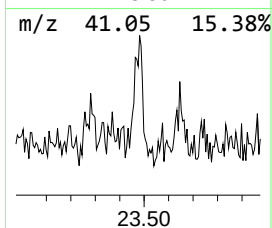
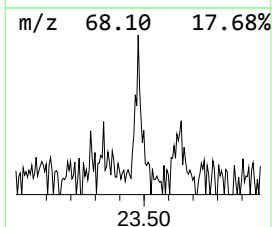
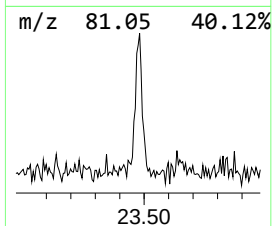
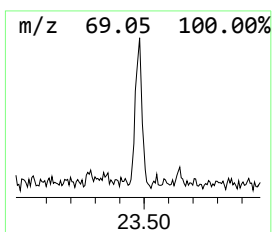
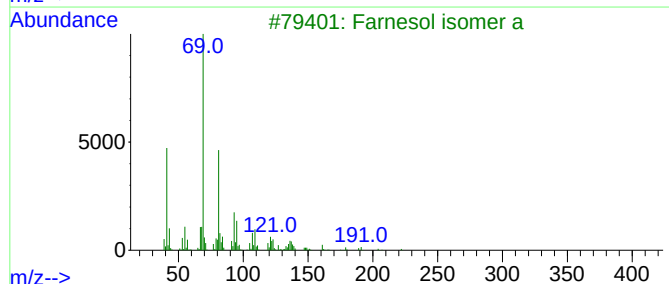
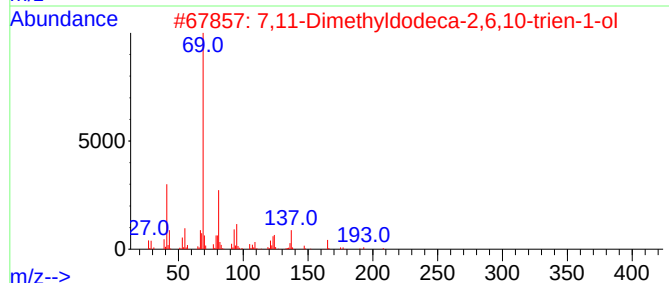
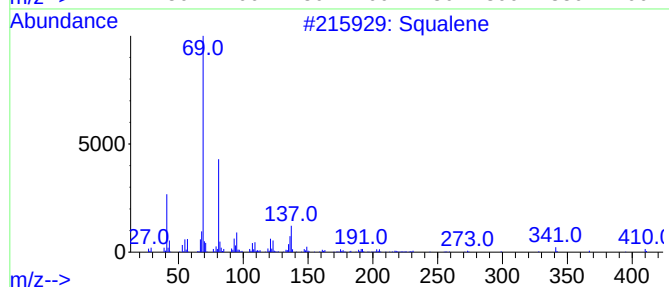
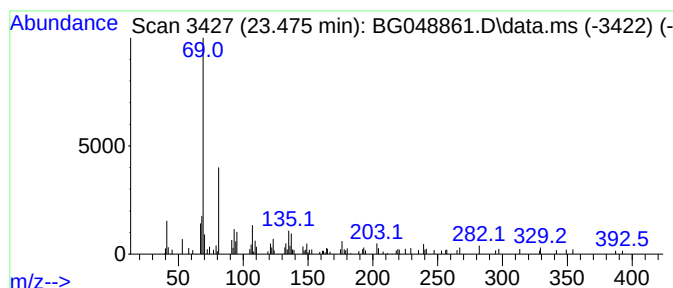
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.475	4.19 ng	87199	Perylene-d12	25.091	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	59
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
3	Farnesol isomer a	222	C15H26O	1000108-92-4	59
4	2,6,10-Undecatrien-8-ol, 2,6-dim...	194	C13H22O	1000163-48-4	53
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048861.D
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Operator : CG/JU
Sample : M2107-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

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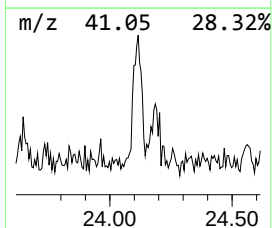
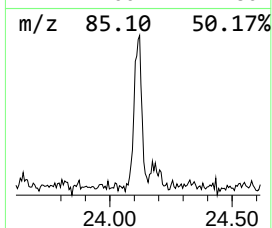
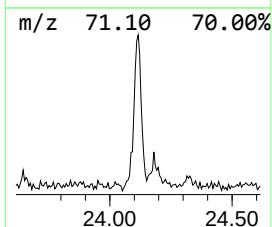
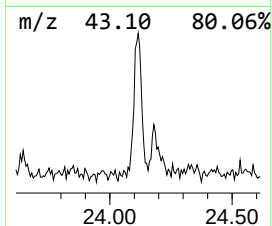
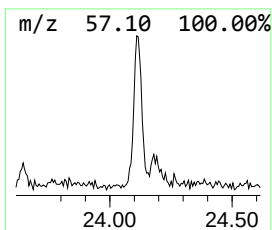
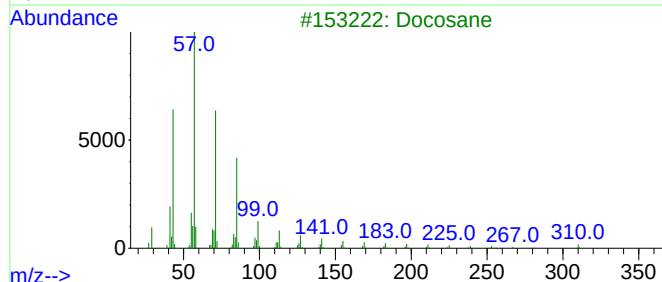
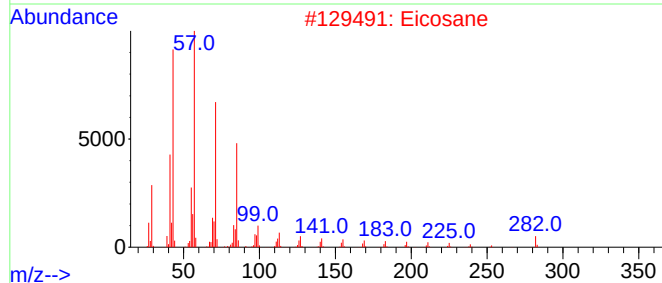
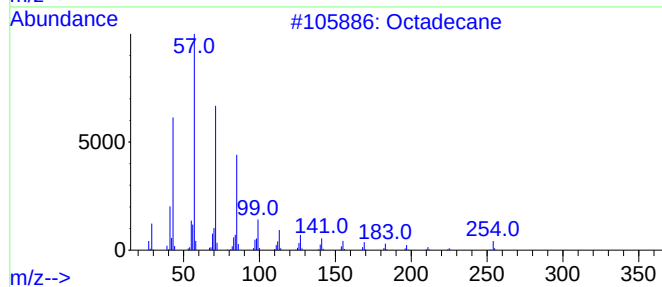
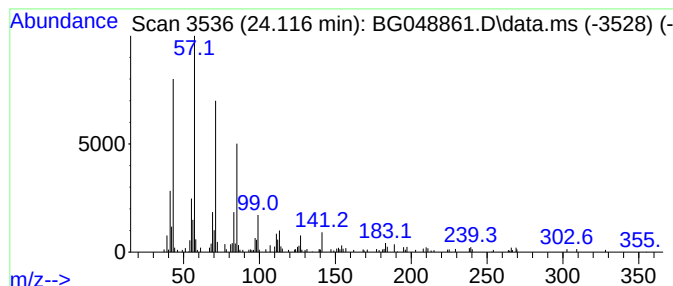
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Octadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.116	9.48 ng	197200	Perylene-d12	25.091

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	93
2			Eicosane	282	C20H42	000112-95-8	87
3			Docosane	310	C22H46	000629-97-0	87
4			Triacontane	422	C30H62	000638-68-6	87
5			Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
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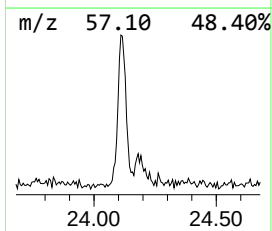
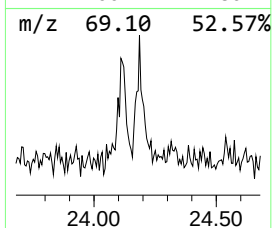
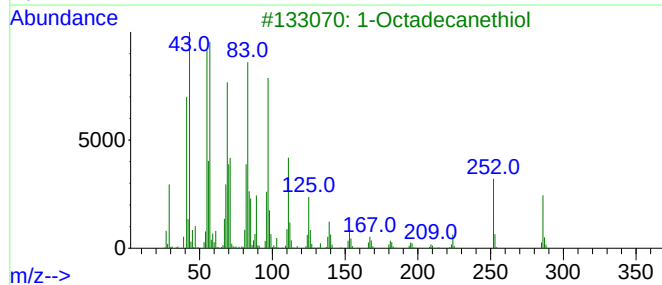
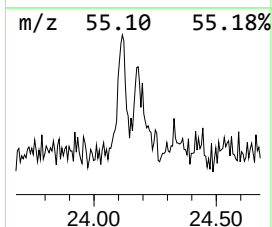
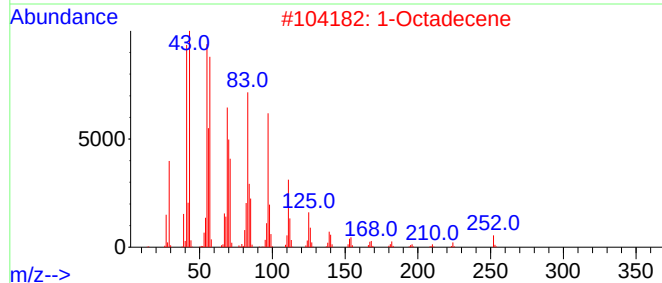
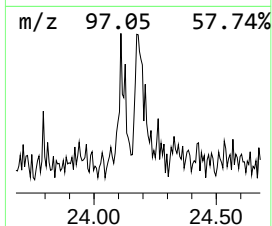
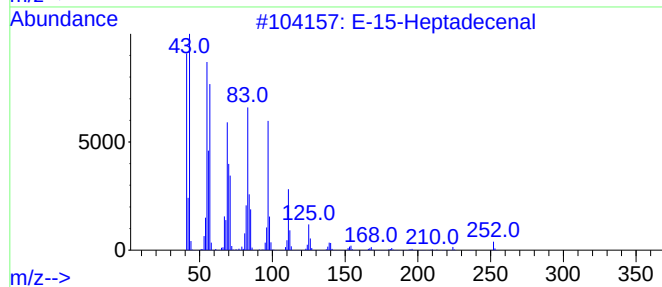
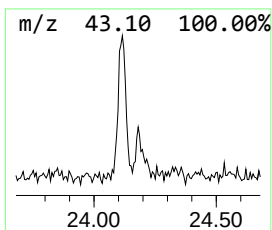
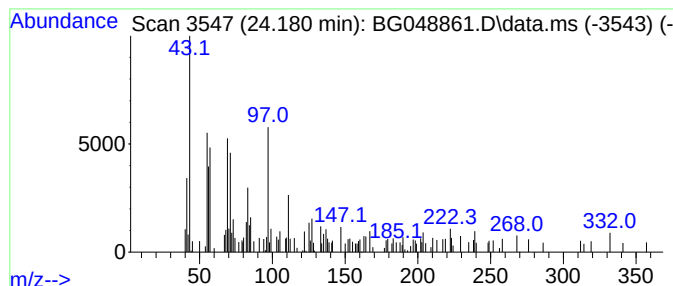
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 E-15-Heptadecenal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.180	3.31 ng	68820	Perylene-d12	25.091

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		E-15-Heptadecenal	252	C17H32O	1000130-97-9	58
2		1-Octadecene	252	C18H36	000112-88-9	50
3		1-Octadecanethiol	286	C18H38S	002885-00-9	50
4		1-Hexadecanethiol	258	C16H34S	002917-26-2	50
5		Cycloheptane, methyl-	112	C8H16	004126-78-7	46



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048861.D
Acq On : 23 Apr 2021 13:31
Operator : CG/JU
Sample : M2107-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

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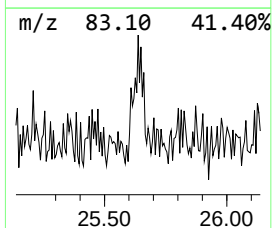
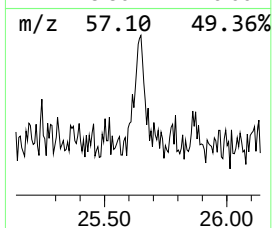
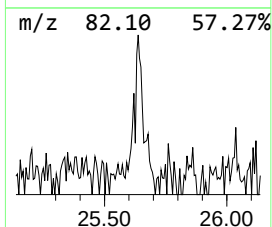
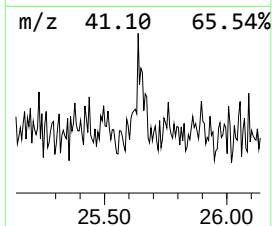
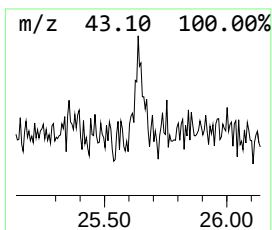
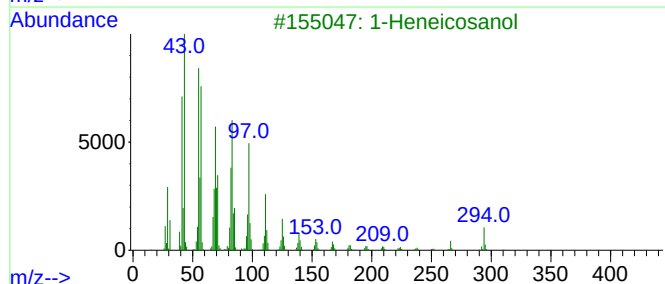
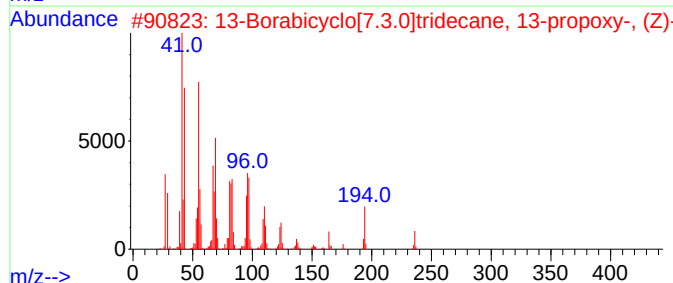
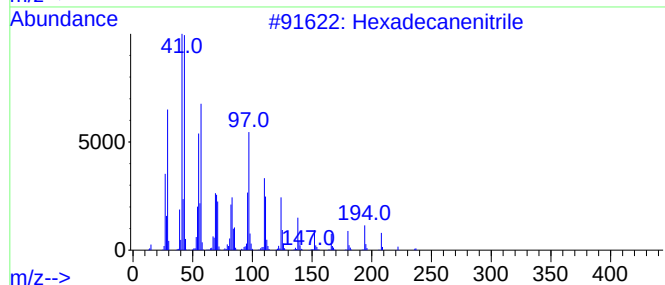
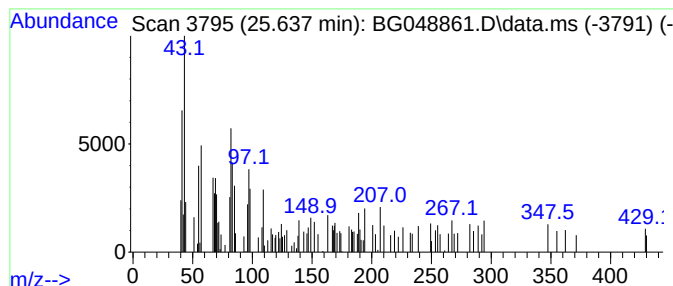
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown25.63 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.637	3.43 ng	71443	Perylene-d12	25.091

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanenitrile	237	C16H31N	000629-79-8	14
2			13-Borabicyclo[7.3.0]tridecane, ...	236	C15H29BO	1000156-41-7	13
3			1-Heneicosanol	312	C21H44O	015594-90-8	12
4			Pentadecanenitrile	223	C15H29N	018300-91-9	10
5			Cyclooctaneacetic acid, 2-oxo-	184	C10H16O3	019144-09-3	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048861.D
Acq On : 23 Apr 2021 13:31
Operator : CG/JU
Sample : M2107-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

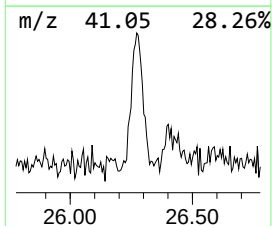
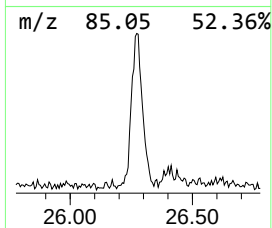
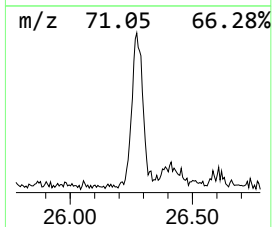
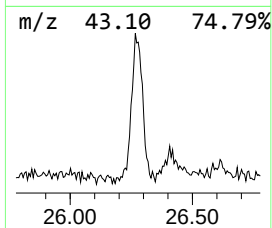
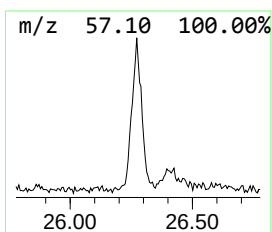
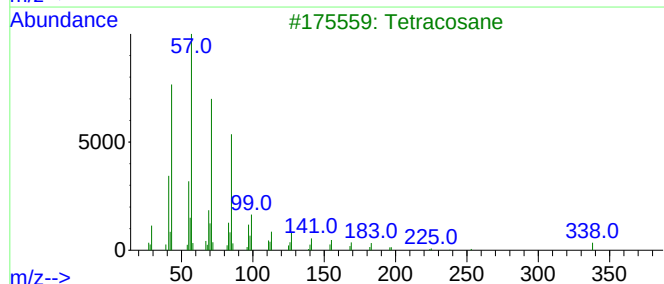
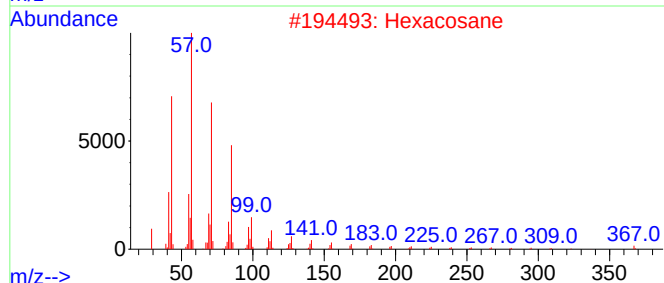
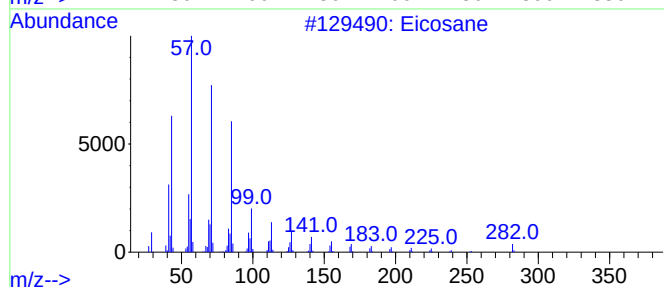
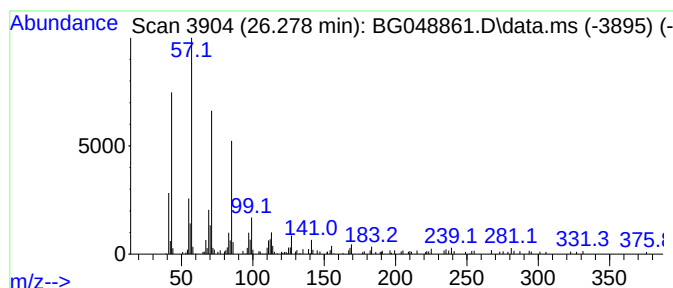
Instrument :
BNA_G
ClientSampleId :
SB-31-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Eicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.278	14.38 ng	299280	Perylene-d12	25.091	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Hexacosane	366	C26H54	000630-01-3	90
3	Tetracosane	338	C24H50	000646-31-1	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
Data File : BG048861.D
Acq On : 23 Apr 2021 13:31
Operator : CG/JU
Sample : M2107-08
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-31-0-2.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.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
2-Pentanone, 4-...	5.120	3.5	ng	33102	1	8.052	190286	20.0
1,3,6-Heptatrie...	6.989	3.3	ng	31653	1	8.052	190286	20.0
unknown18.29	18.299	3.4	ng	68412	4	17.471	404434	20.0
unknown18.35	18.358	2.4	ng	48020	4	17.471	404434	20.0
unknown19.45	19.451	2.5	ng	51597	4	17.471	404434	20.0
Benzene, 1,1'-(...	19.521	2.4	ng	47924	4	17.471	404434	20.0
Cycloeicosane	21.384	11.1	ng	242478	5	21.765	437629	20.0
3-Eicosene, (E)-	22.594	13.1	ng	287558	5	21.765	437629	20.0
Squalene	23.475	4.2	ng	87199	6	25.091	416144	20.0
Octadecane	24.116	9.5	ng	197200	6	25.091	416144	20.0
E-15-Heptadecenal	24.180	3.3	ng	68820	6	25.091	416144	20.0
unknown25.63	25.637	3.4	ng	71443	6	25.091	416144	20.0
Eicosane	26.278	14.4	ng	299280	6	25.091	416144	20.0