

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
 Data File : BG048498.D
 Acq On : 25 Mar 2021 12:21
 Operator : CG/JU
 Sample : M1779-02
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-3B1-(3.0-3.5)

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-BG031821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048498.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.177	308	313	318	rBV2	27082	42351	1.47%	0.265%
2	5.653	385	394	402	rBV	683852	1116188	38.64%	6.975%
3	7.251	658	666	680	rBV	721923	1256384	43.49%	7.851%
4	8.097	804	810	817	rVB	167293	286814	9.93%	1.792%
5	9.267	999	1009	1018	rVB	459473	817408	28.30%	5.108%
6	10.924	1282	1291	1299	rBV	221461	394697	13.66%	2.467%
7	13.362	1699	1706	1714	rVB	1131662	1749757	60.57%	10.934%
8	14.184	1842	1846	1850	rVB	23523	32551	1.13%	0.203%
9	14.743	1934	1941	1947	rBV	348555	547623	18.96%	3.422%
10	14.960	1971	1978	1979	rBV2	19149	36566	1.27%	0.229%
11	15.530	2053	2075	2076	rBV2	84690	289982	10.04%	1.812%
12	15.589	2081	2085	2086	rVV2	29202	43429	1.50%	0.271%
13	16.229	2187	2194	2202	rVB	1083516	1572879	54.45%	9.829%
14	17.492	2402	2409	2415	rBV	455252	684593	23.70%	4.278%
15	17.786	2444	2459	2468	rBV	35638	164670	5.70%	1.029%
16	18.368	2552	2558	2568	rBV	246334	364048	12.60%	2.275%
17	19.355	2718	2726	2736	rVB3	73189	199033	6.89%	1.244%
18	19.637	2770	2774	2782	rVB3	77573	100886	3.49%	0.630%
19	20.101	2847	2853	2859	rVB	2231722	2888602	100.00%	18.051%
20	20.407	2899	2905	2912	rVB	91648	199328	6.90%	1.246%
21	20.606	2933	2939	2949	rVB2	85652	172476	5.97%	1.078%
22	21.288	3049	3055	3062	rVB2	93246	193384	6.69%	1.208%
23	21.411	3071	3076	3085	rBV3	182690	359295	12.44%	2.245%
24	21.494	3086	3090	3095	rVB	82898	122367	4.24%	0.765%
25	21.652	3115	3117	3124	rVB6	18969	29191	1.01%	0.182%
26	21.781	3133	3139	3145	rBV	468175	779282	26.98%	4.870%
27	21.981	3169	3173	3177	rBV6	29581	43315	1.50%	0.271%
28	22.293	3222	3226	3235	rVB4	91041	197312	6.83%	1.233%
29	22.604	3272	3279	3283	rBV8	44550	93468	3.24%	0.584%
30	23.491	3425	3430	3441	rVB5	72830	209764	7.26%	1.311%
31	24.167	3541	3545	3550	rVB5	31329	62176	2.15%	0.389%
32	24.942	3672	3677	3678	rBV5	26624	42156	1.46%	0.263%
33	25.113	3695	3706	3722	rVB	285621	910225	31.51%	5.688%

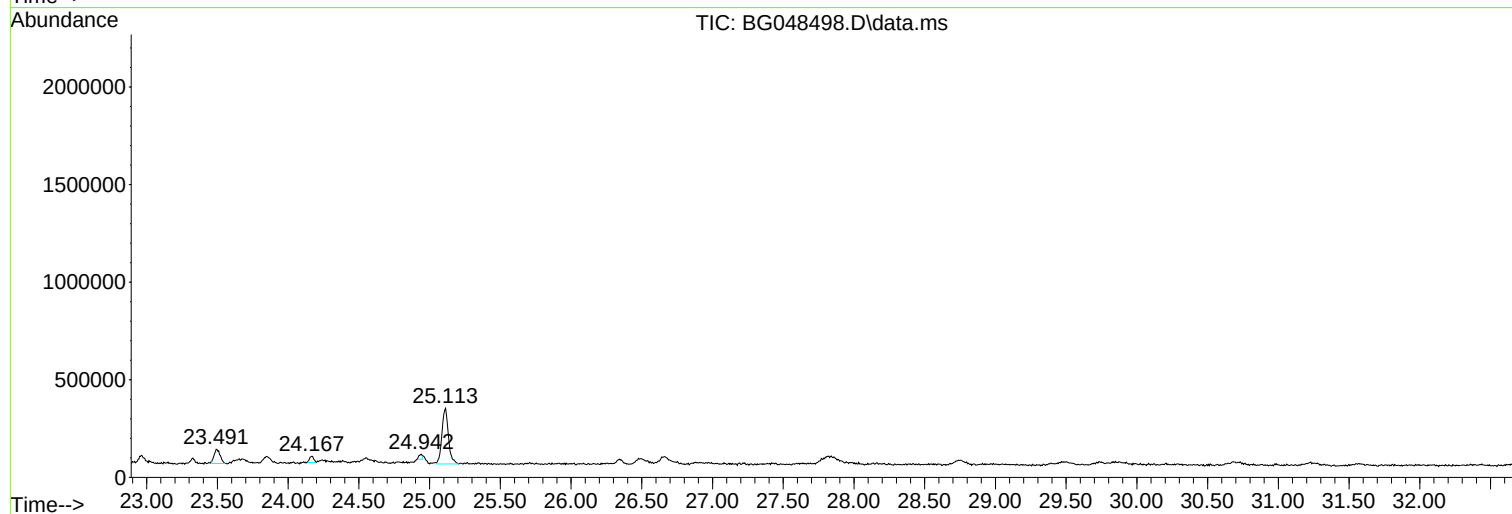
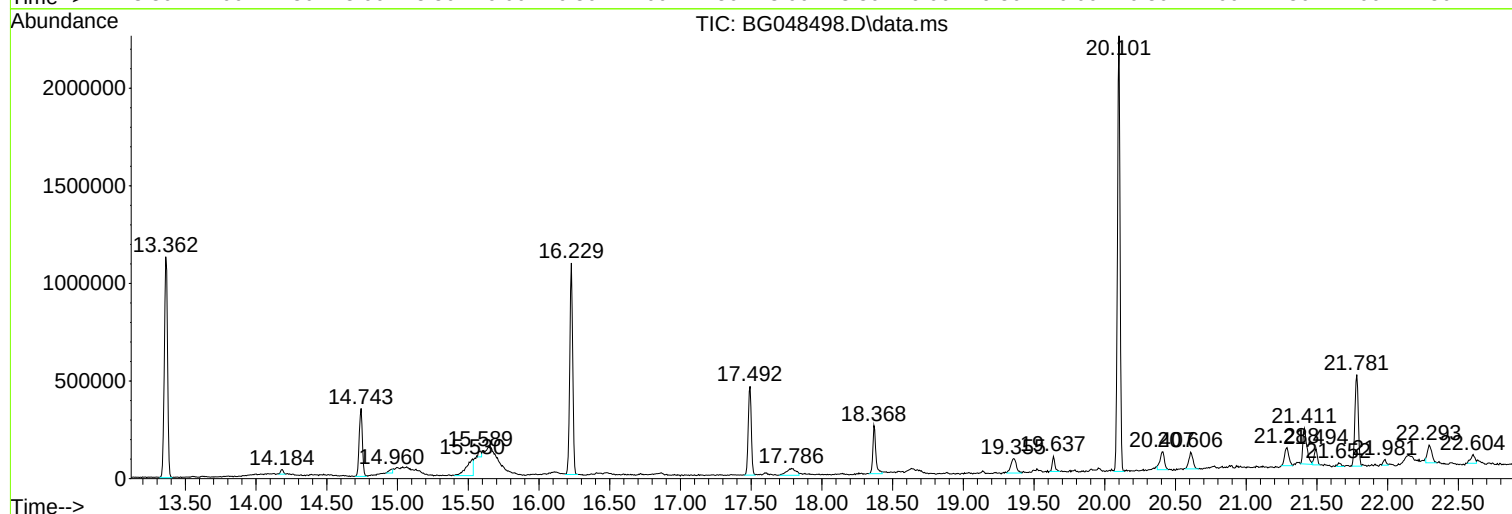
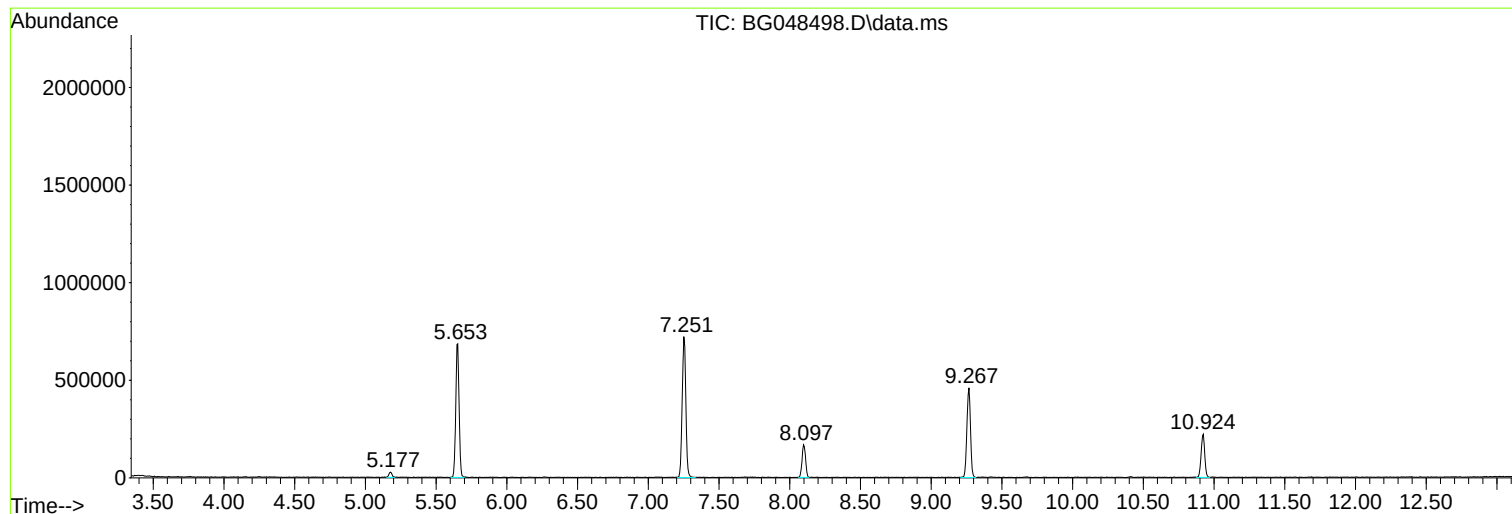
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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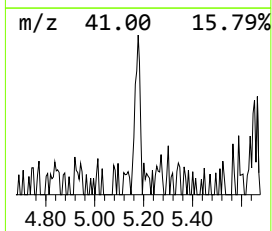
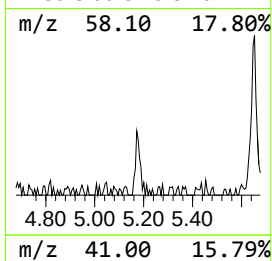
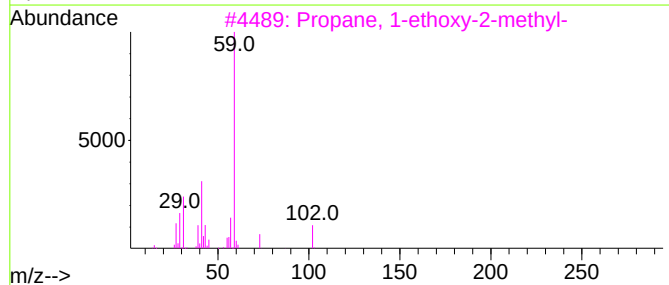
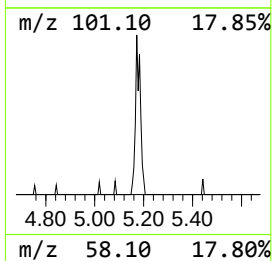
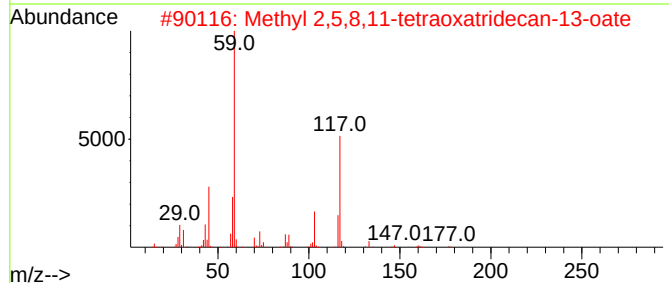
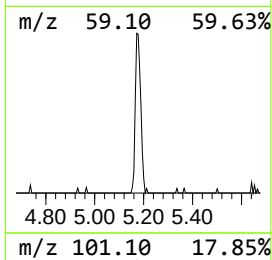
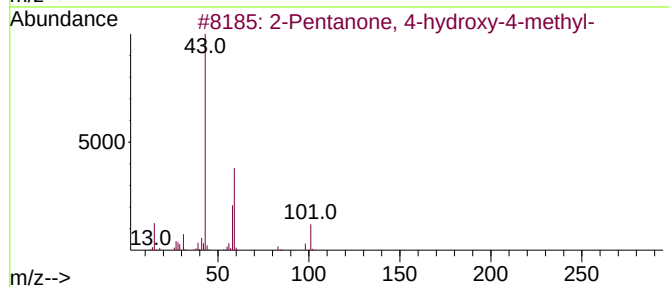
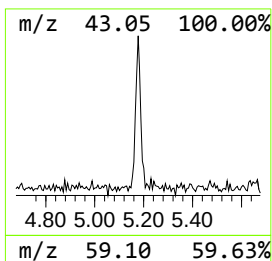
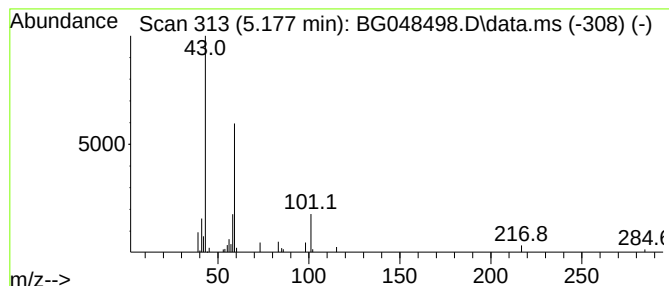
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.177	2.95 ng	42351	1,4-Dichlorobenzene-d4	8.097

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	37		
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35		
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	27		
5	3-Octanol	130	C8H18O	000589-98-0	25		



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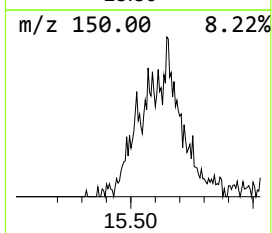
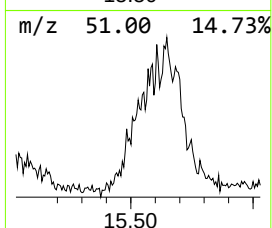
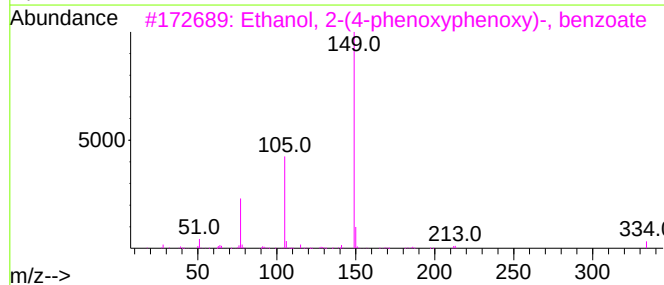
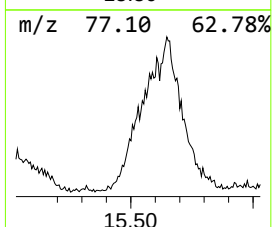
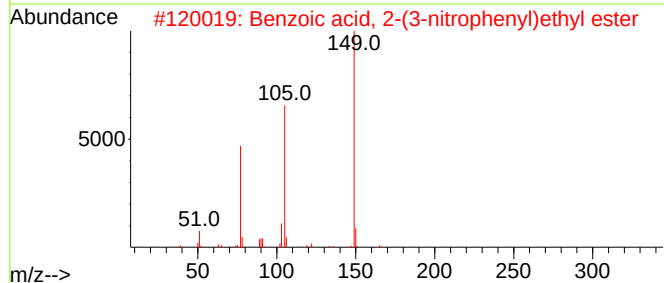
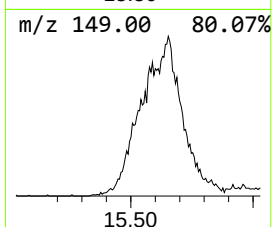
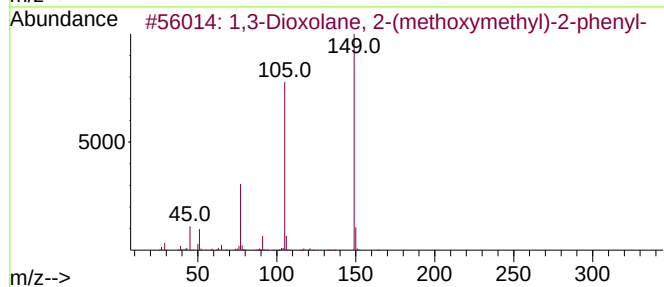
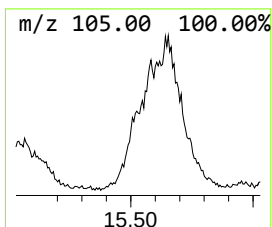
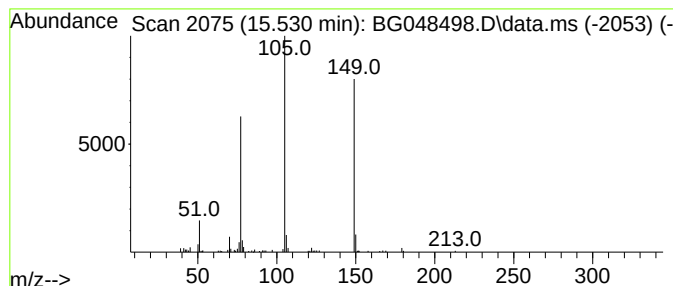
Instrument :
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Peak Number 2 1,3-Dioxolane, 2-(methoxyme... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.530	10.59 ng	289982	Acenaphthene-d10		14.743	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-(methoxymethyl)...		194	C11H14O3	1000156-71-2	83
2	Benzoic acid, 2-(3-nitrophenyl)e...		271	C15H13NO4	1000368-22-4	78
3	Ethanol, 2-(4-phenoxyphenoxy)-, ...		334	C21H18O4	055191-59-8	74
4	Diethylene glycol dibenzoate		314	C18H18O5	000120-55-8	74
5	Benzoic acid, 2-(4-nitrophenoxy)...		287	C15H13NO5	1000368-92-7	74



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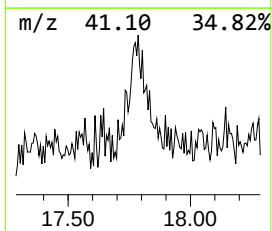
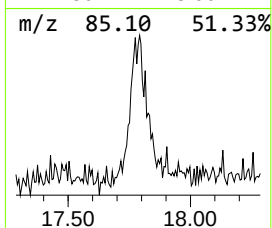
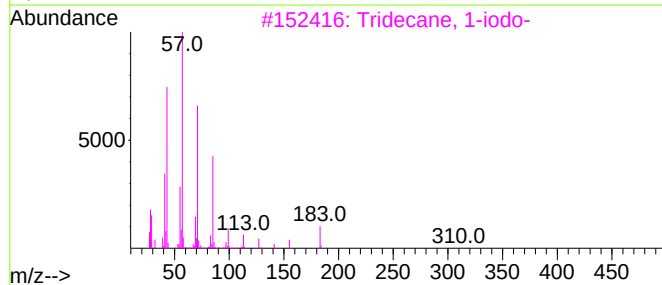
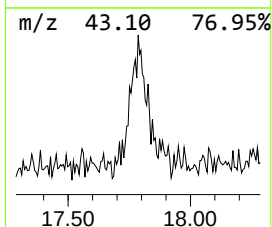
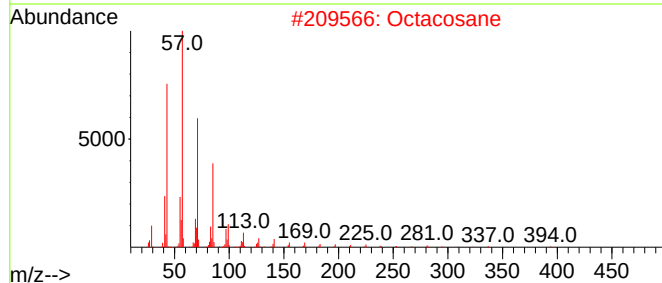
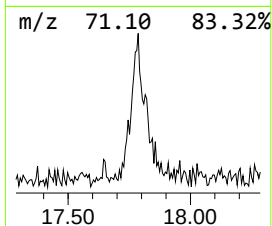
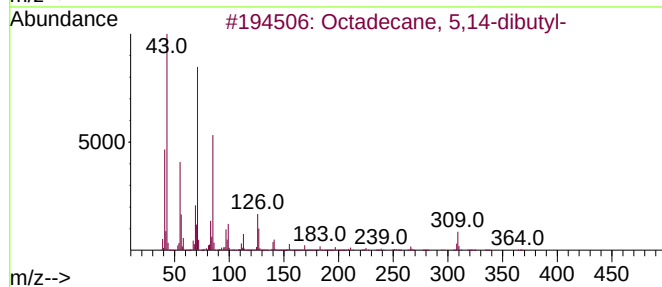
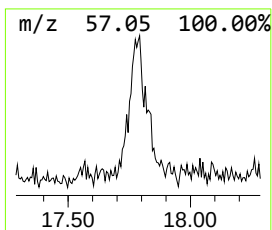
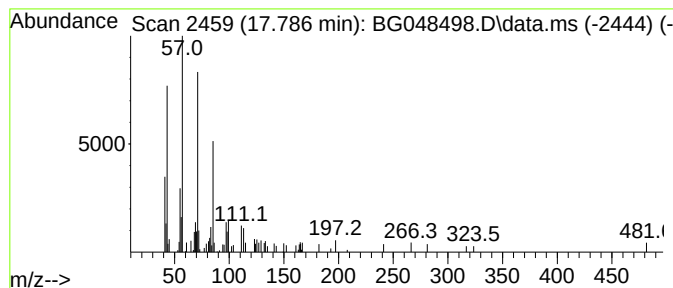
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Peak Number 3 Octadecane, 5,14-dibutyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.786	4.81 ng	164670	Phenanthrene-d10	17.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	80
2			Octacosane	394	C28H58	000630-02-4	72
3			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	64
5			Tritriacontane	465	C33H68	000630-05-7	64



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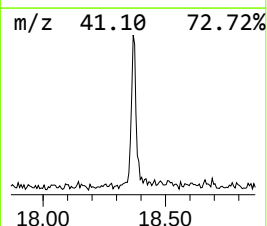
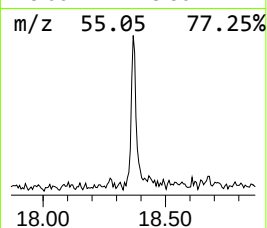
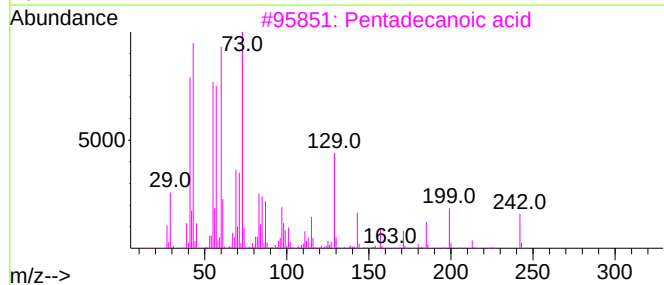
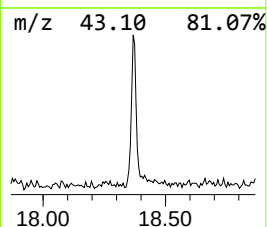
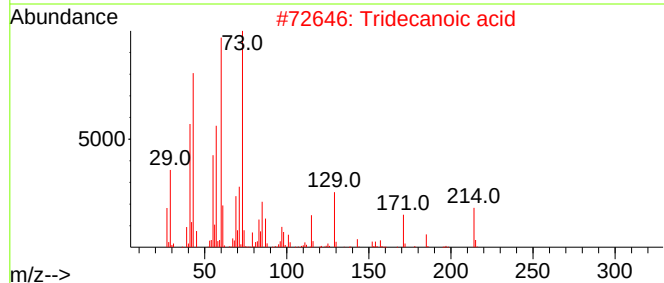
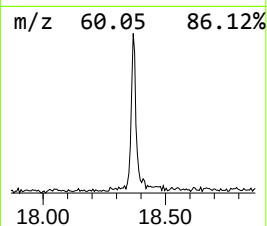
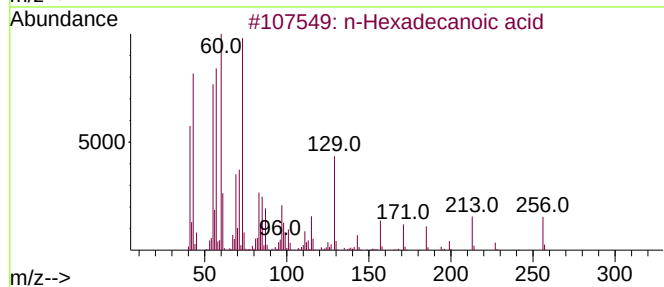
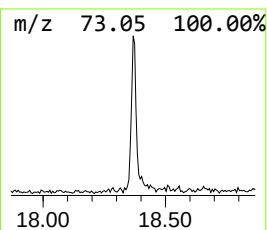
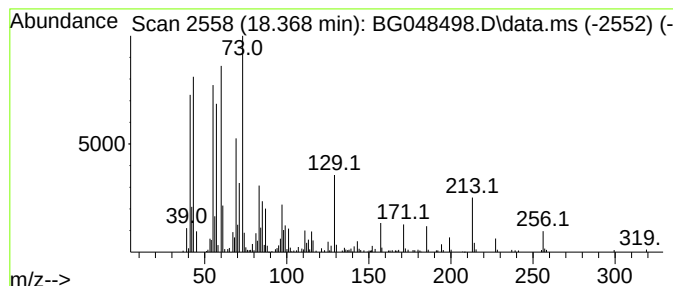
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.368	10.64 ng	364048	Phenanthrene-d10	17.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5			Octadecanoic acid	284	C18H36O2	000057-11-4	81



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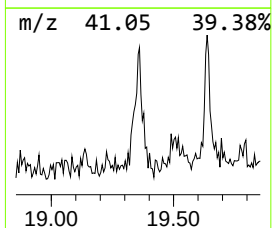
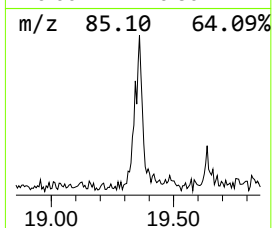
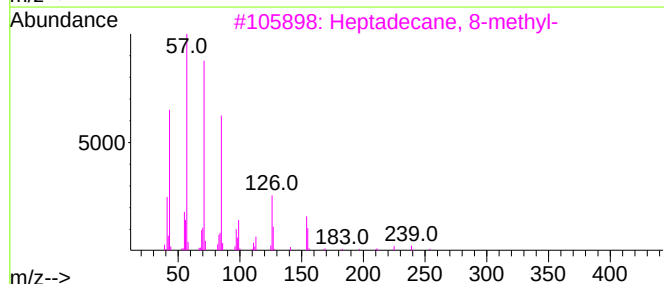
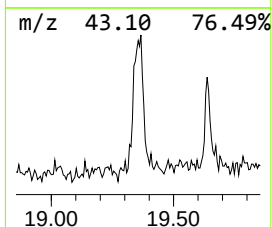
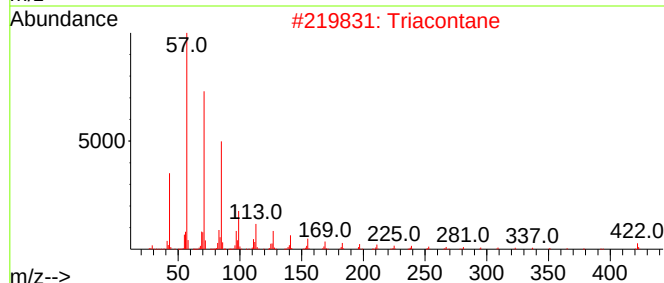
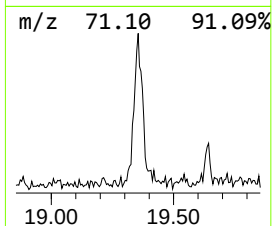
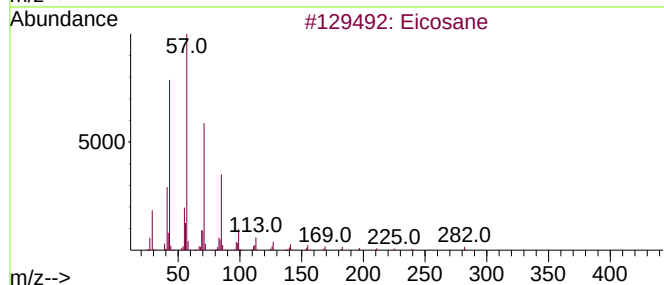
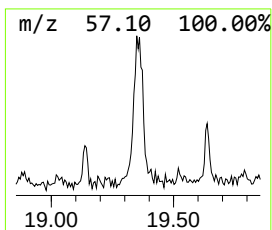
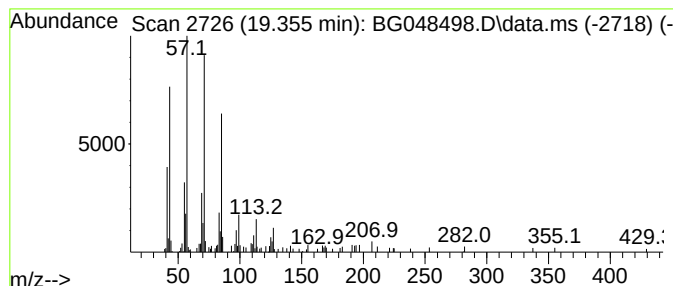
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Peak Number 5 Triacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.355	5.81 ng	199033	Phenanthrene-d10	17.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Triacontane	422	C30H62	000638-68-6	90
3			Heptadecane, 8-methyl-	254	C18H38	013287-23-5	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Hexadecane	226	C16H34	000544-76-3	86



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ALS Vial : 5 Sample Multiplier: 1

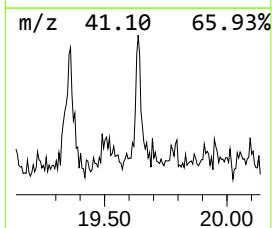
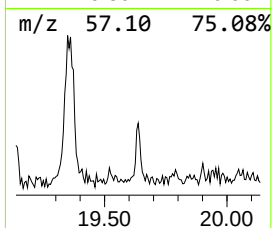
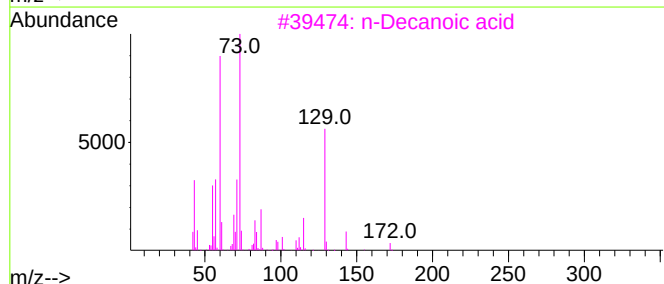
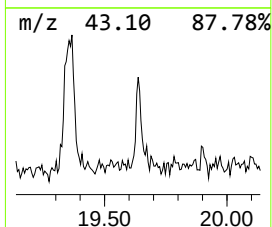
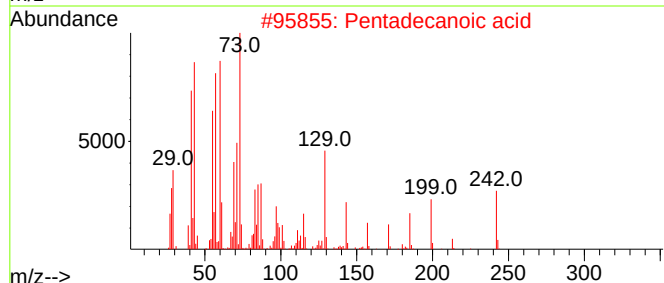
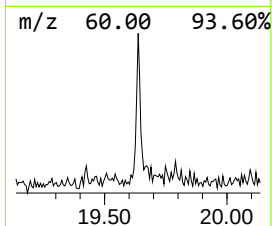
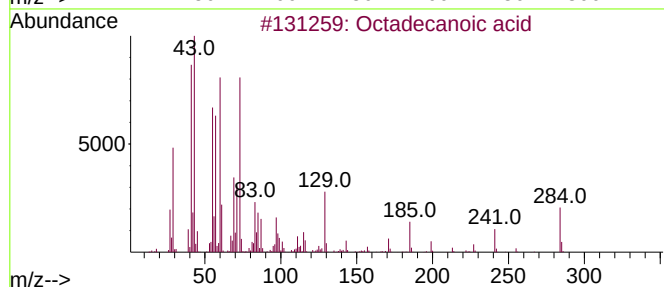
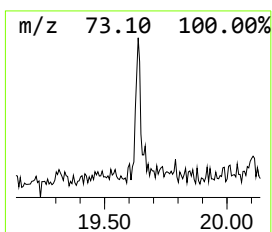
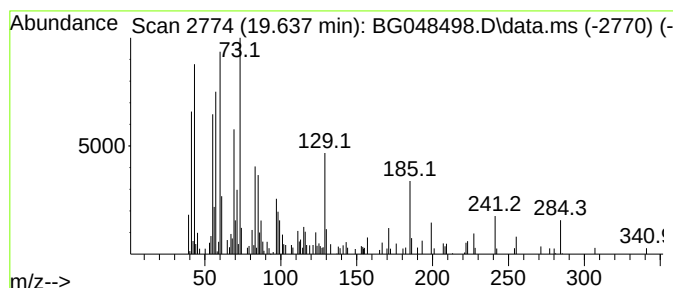
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ClientSampleId :
SB-3B1-(3.0-3.5)

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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 Octadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.637	2.95 ng	100886	Phenanthrene-d10	17.492	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3	n-Decanoic acid	172	C10H20O2	000334-48-5	55
4	Tridecanoic acid	214	C13H26O2	000638-53-9	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
Data File : BG048498.D
Acq On : 25 Mar 2021 12:21
Operator : CG/JU
Sample : M1779-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-3B1-(3.0-3.5)

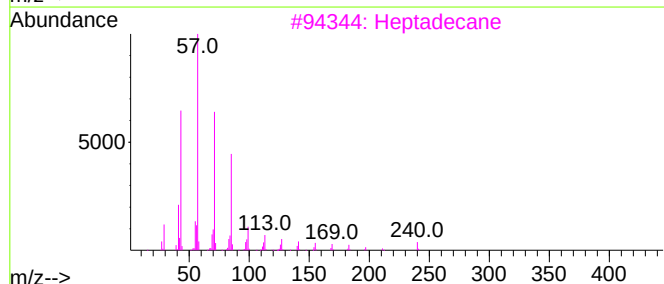
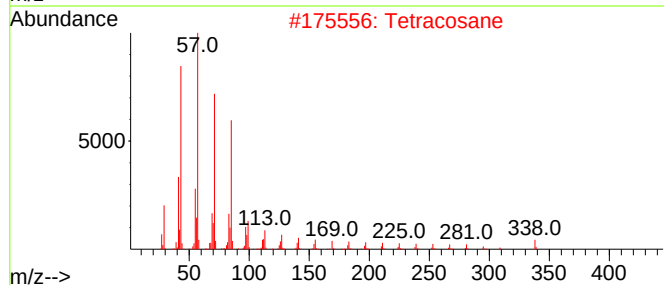
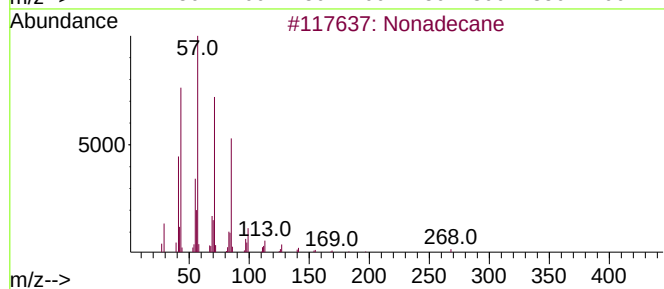
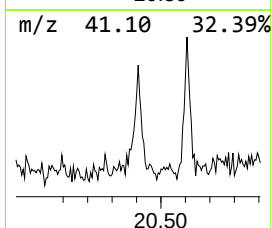
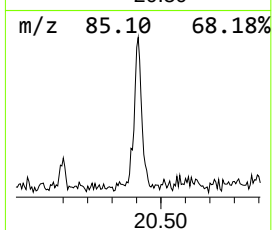
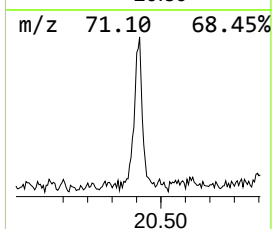
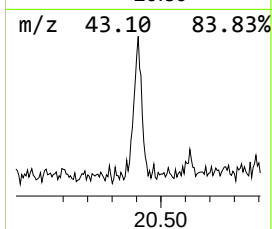
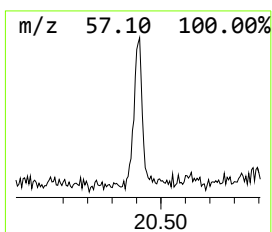
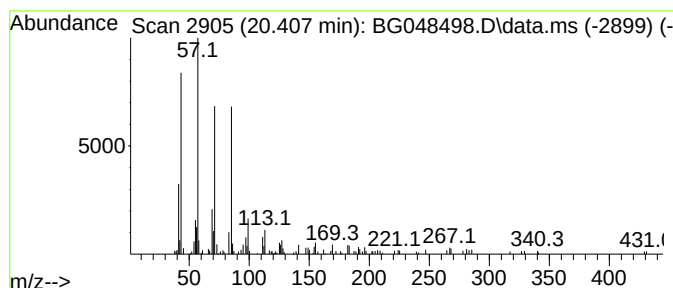
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.407	5.12 ng	199328	Chrysene-d12	21.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	90
2			Tetracosane	338	C24H50	000646-31-1	86
3			Heptadecane	240	C17H36	000629-78-7	86
4			Octacosane	394	C28H58	000630-02-4	86
5			Docosane	310	C22H46	000629-97-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
Data File : BG048498.D
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Operator : CG/JU
Sample : M1779-02
Misc :
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Instrument :
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ClientSampleId :
SB-3B1-(3.0-3.5)

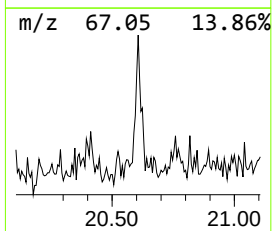
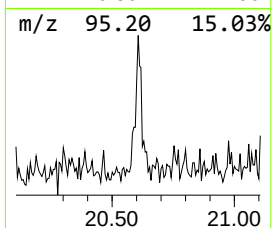
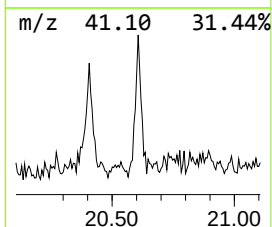
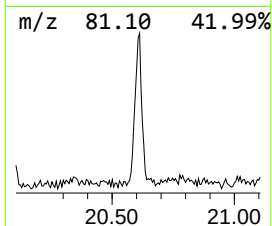
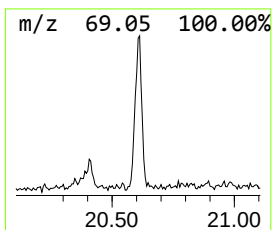
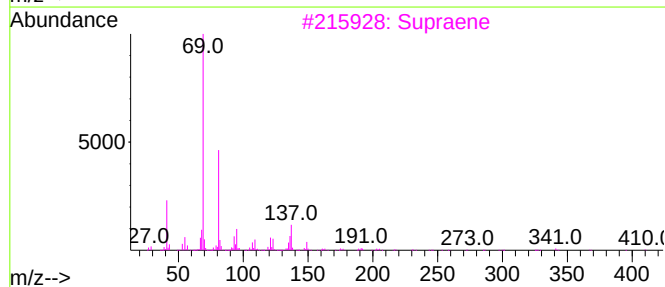
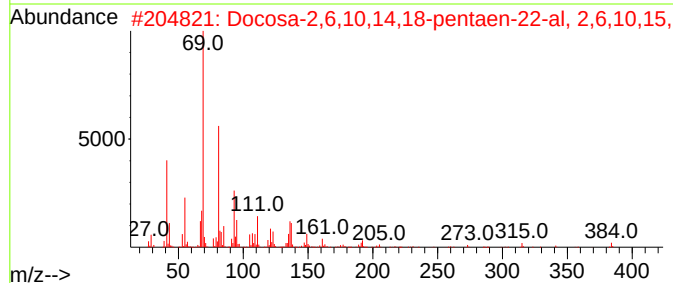
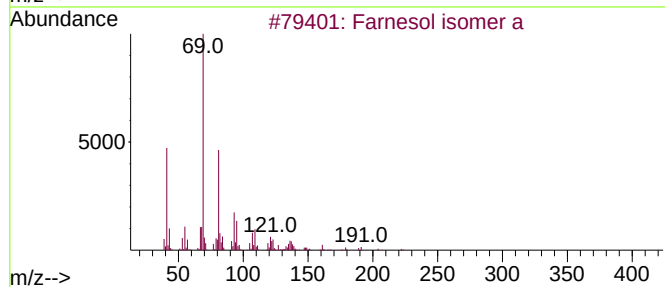
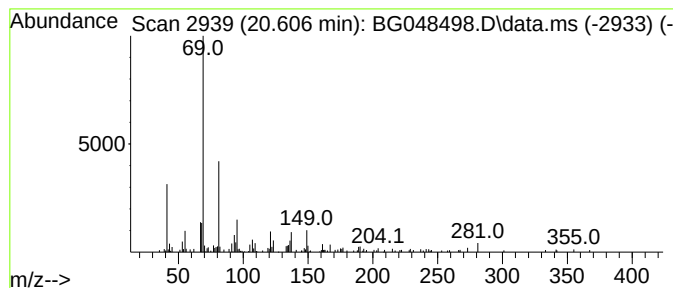
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Farnesol isomer a Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.606	4.43 ng	172476	Chrysene-d12	21.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Farnesol isomer a	222	C15H26O	1000108-92-4	76
2			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	72
3			Supraene	410	C30H50	007683-64-9	68
4			Squalene	410	C30H50	000111-02-4	64
5			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
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Acq On : 25 Mar 2021 12:21
Operator : CG/JU
Sample : M1779-02
Misc :
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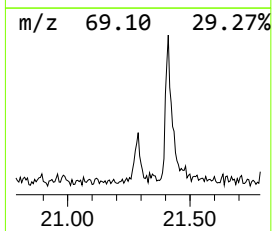
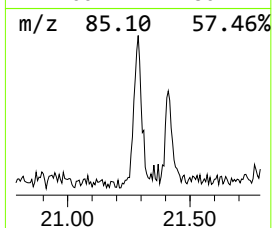
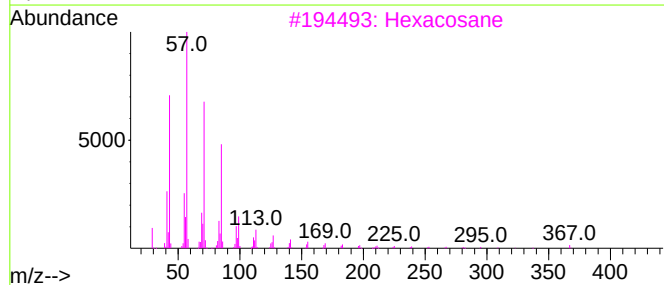
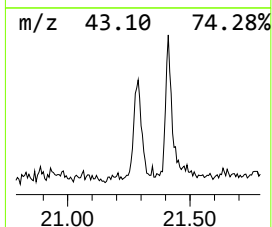
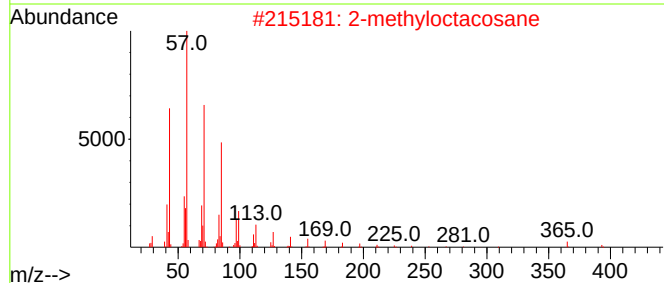
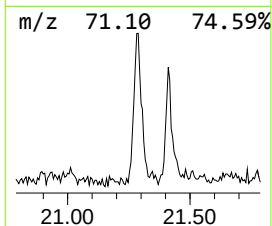
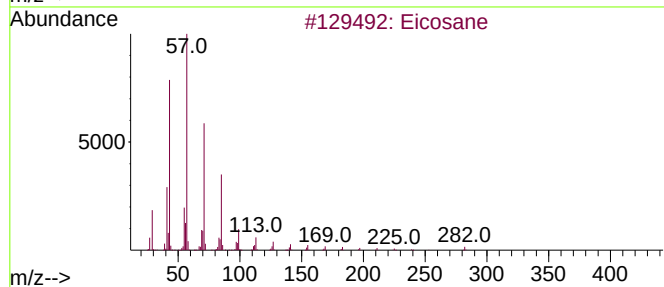
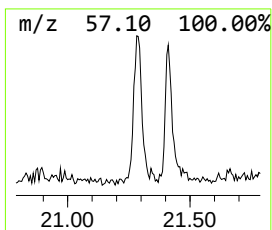
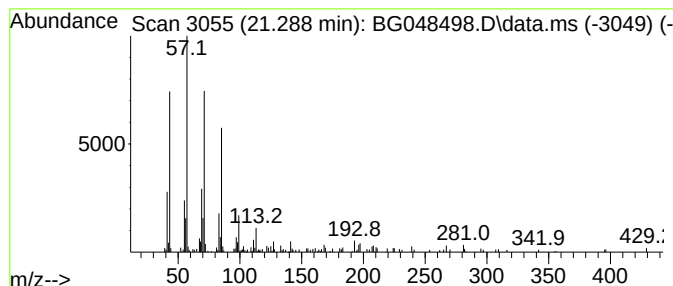
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.288	4.96 ng	193384	Chrysene-d12		21.781	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Eicosane		282	C20H42	000112-95-8	93
2	2-methyloctacosane		408	C29H60	1000376-72-8	87
3	Hexacosane		366	C26H54	000630-01-3	87
4	Eicosane, 10-methyl-		296	C21H44	054833-23-7	86
5	Tetracosane, 11-decyl-		479	C34H70	055429-84-0	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
Data File : BG048498.D
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Operator : CG/JU
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Misc :
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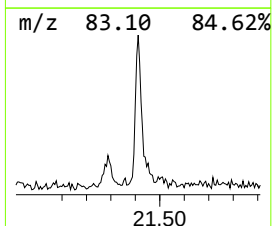
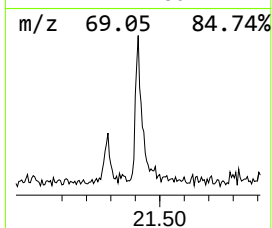
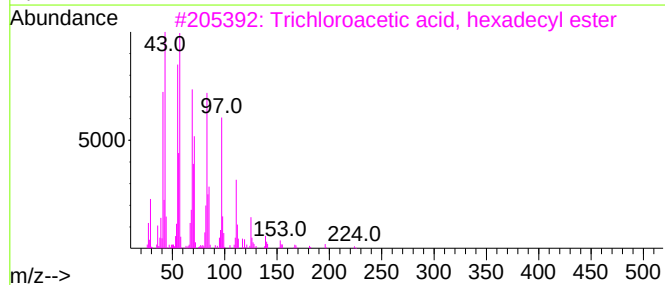
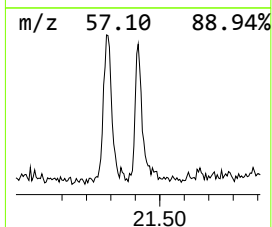
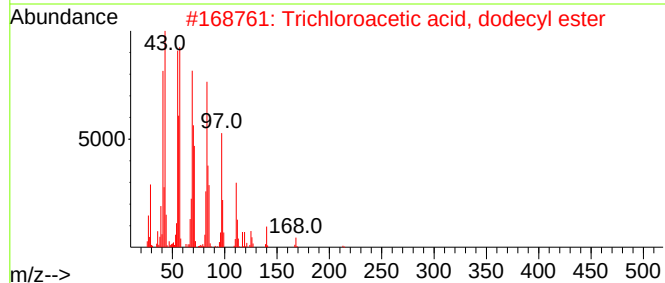
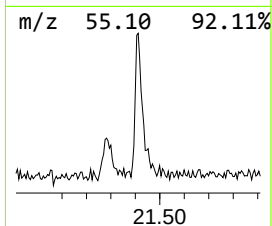
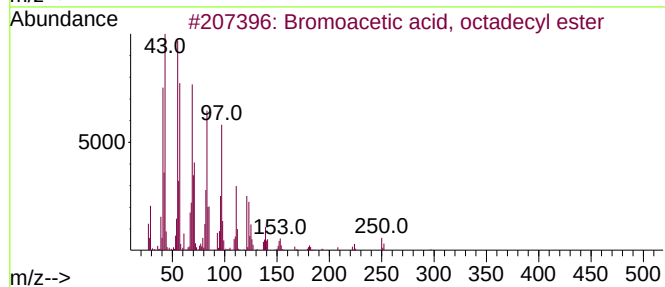
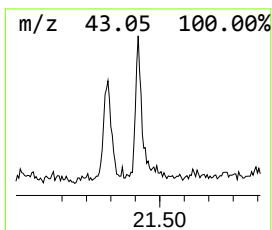
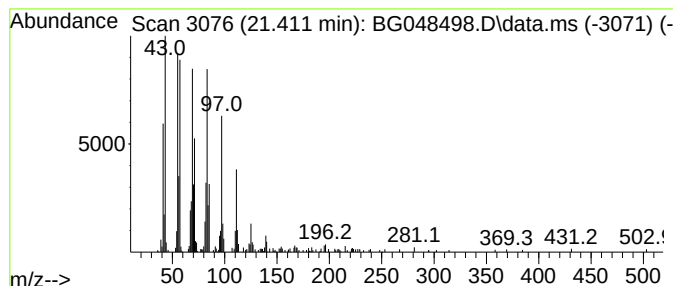
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Bromoacetic acid, octadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.411	9.22 ng	359295	Chrysene-d12	21.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
2			Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	87
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81
4			n-Heptadecanol-1	256	C17H36O	001454-85-9	64
5			Cyclooctane, 1,2-diethyl-	168	C12H24	023609-46-3	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
Data File : BG048498.D
Acq On : 25 Mar 2021 12:21
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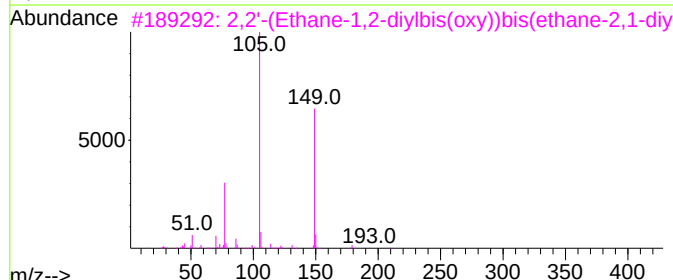
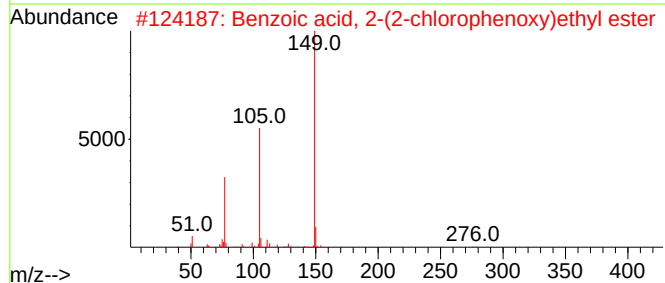
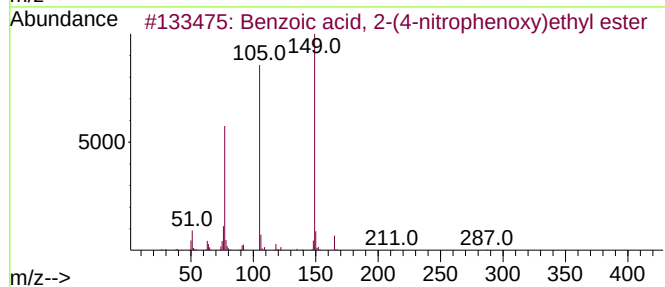
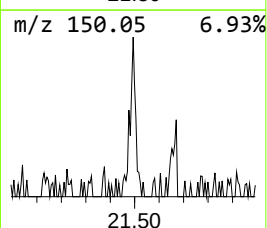
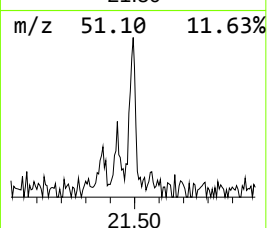
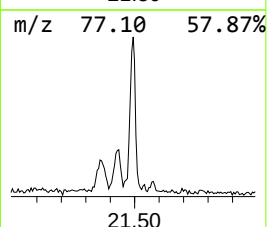
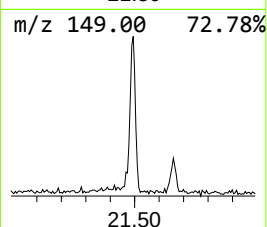
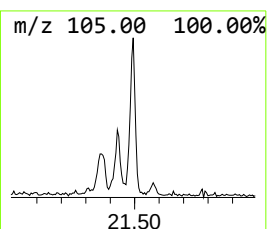
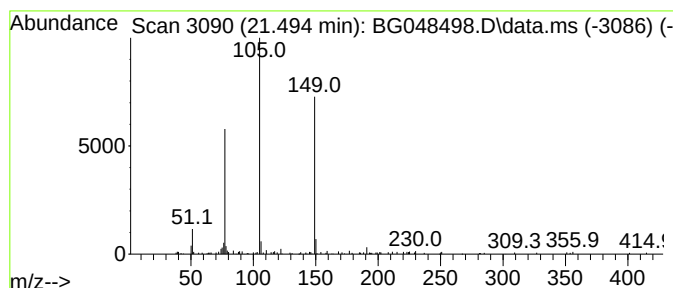
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzoic acid, 2-(4-nitrophe... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.494	3.14 ng	122367	Chrysene-d12	21.781	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
2	Benzoic acid, 2-(2-chlorophenoxy)...	276	C15H13ClO3	1000368-25-9	72
3	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	53
4	2',4'-Benzoxylidide	225	C15H15NO	006328-77-4	38
5	N-Benzoyl derivative of o-fluoro...	215	C13H10FNO	000367-97-5	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
Data File : BG048498.D
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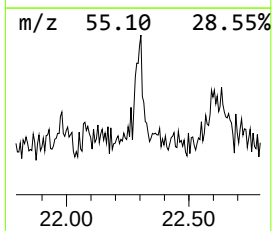
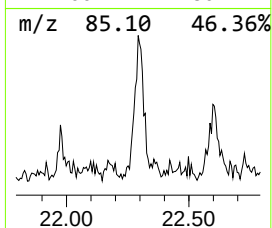
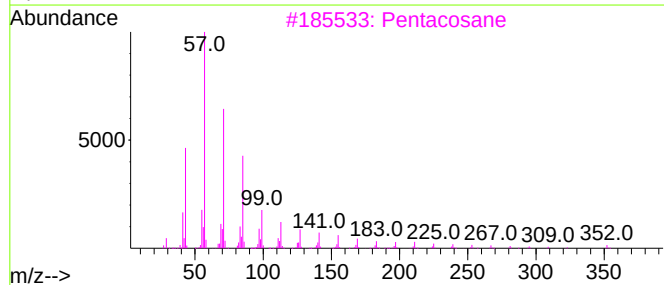
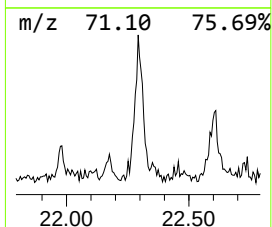
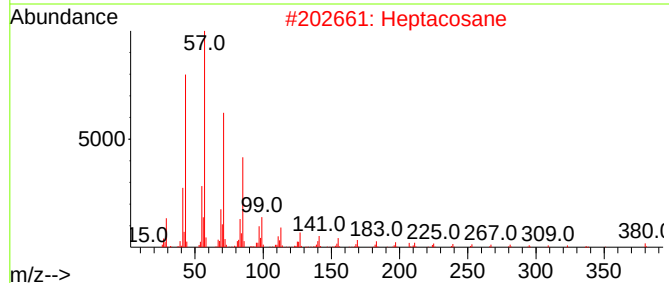
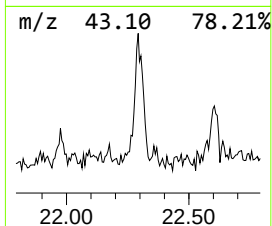
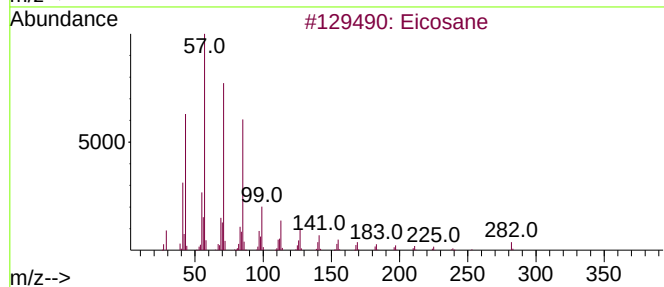
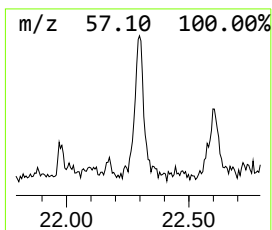
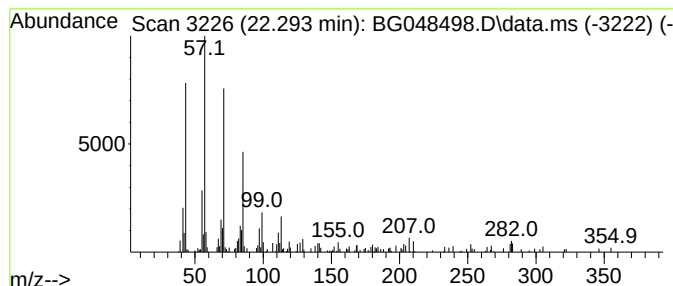
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.293	5.06 ng	197312	Chrysene-d12	21.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Heptacosane	380	C27H56	000593-49-7	86
3			Pentacosane	352	C25H52	000629-99-2	78
4			Heneicosane	296	C21H44	000629-94-7	72
5			Heneicosane, 10-methyl-	310	C22H46	013287-25-7	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
Data File : BG048498.D
Acq On : 25 Mar 2021 12:21
Operator : CG/JU
Sample : M1779-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

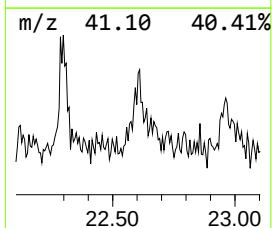
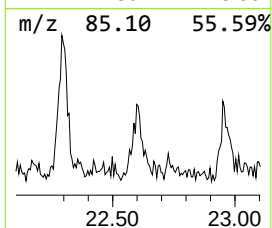
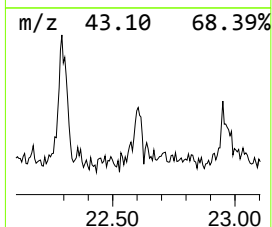
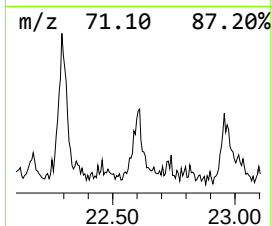
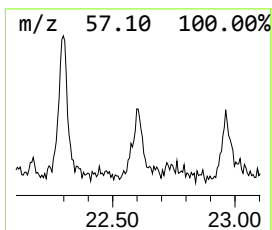
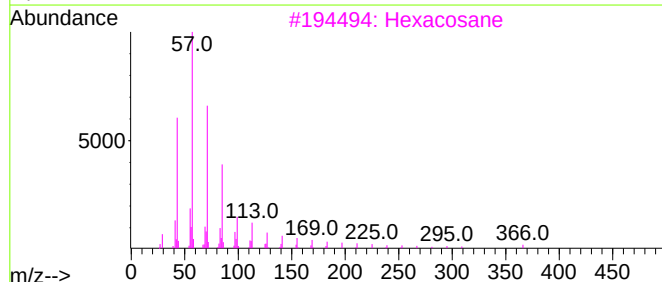
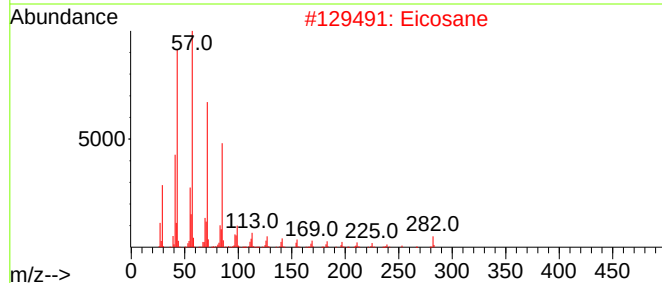
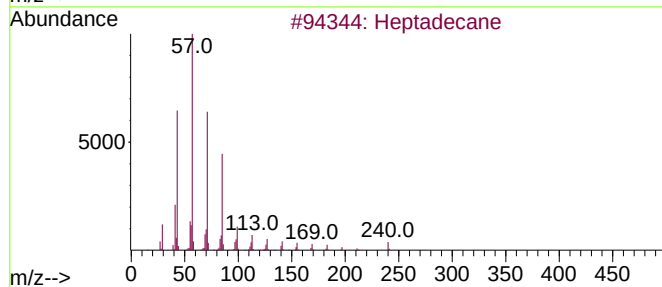
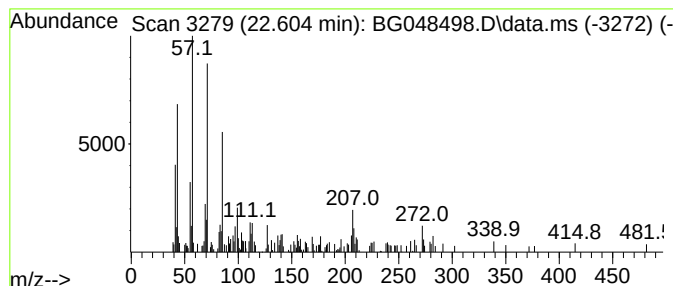
Instrument :
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ClientSampleId :
SB-3B1-(3.0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heptadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.604	2.40 ng	93468	Chrysene-d12		21.781	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	95
2	Eicosane		282	C20H42	000112-95-8	93
3	Hexacosane		366	C26H54	000630-01-3	62
4	Octacosane		394	C28H58	000630-02-4	62
5	10-Methylnonadecane		282	C20H42	056862-62-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
Data File : BG048498.D
Acq On : 25 Mar 2021 12:21
Operator : CG/JU
Sample : M1779-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

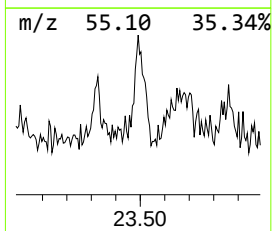
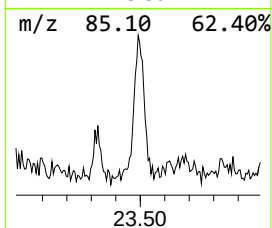
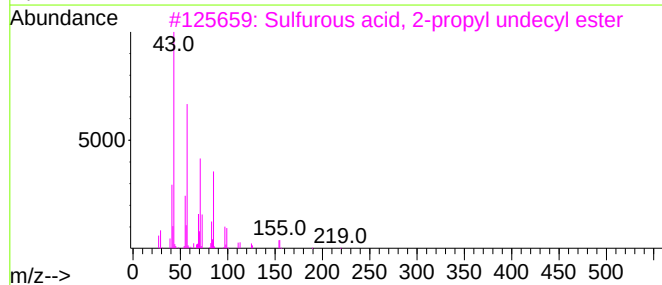
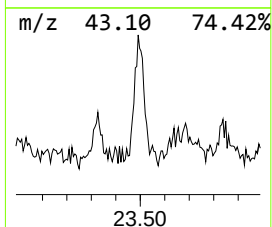
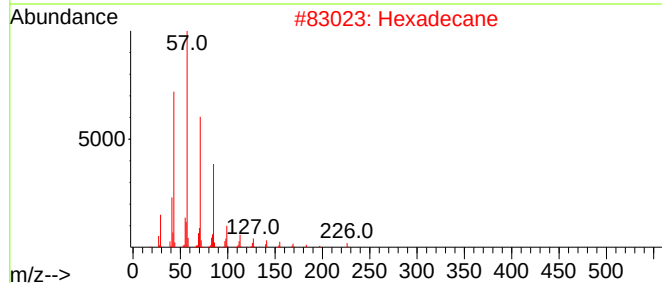
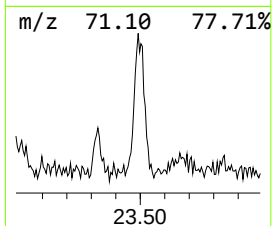
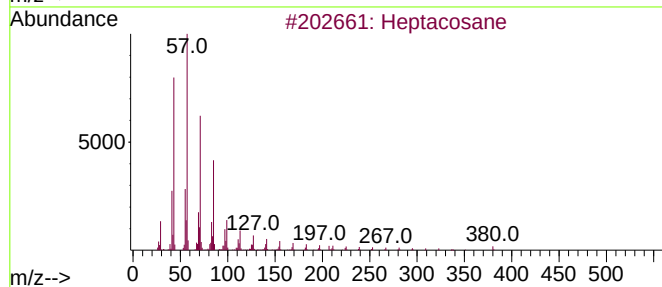
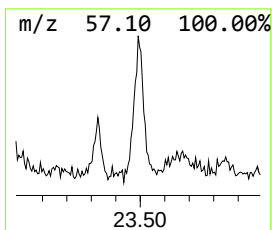
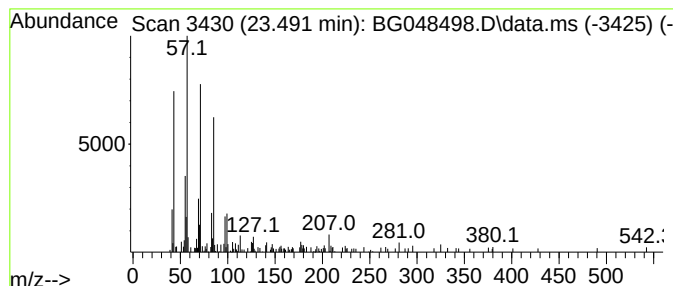
Instrument :
BNA_G
ClientSampleId :
SB-3B1-(3.0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Sulfurous acid, 2-propyl un... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.491	4.61 ng	209764	Perylene-d12	25.113	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	87
2	Hexadecane	226	C16H34	000544-76-3	81
3	Sulfurous acid, 2-propyl undecyl...	278	C14H30O3S	1000309-12-2	72
4	Hexacosane	366	C26H54	000630-01-3	72
5	Tritriacontane	465	C33H68	000630-05-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032521\
Data File : BG048498.D
Acq On : 25 Mar 2021 12:21
Operator : CG/JU
Sample : M1779-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-3B1-(3.0-3.5)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.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-...	5.177	3.0	ng	42351	1	8.097	286814	20.0
1,3-Dioxolane, ...	15.530	10.6	ng	289982	3	14.743	547623	20.0
Octadecane, 5,1...	17.786	4.8	ng	164670	4	17.492	684593	20.0
n-Hexadecanoic ...	18.368	10.6	ng	364048	4	17.492	684593	20.0
Triacotane	19.355	5.8	ng	199033	4	17.492	684593	20.0
Octadecanoic acid	19.637	3.0	ng	100886	4	17.492	684593	20.0
Nonadecane	20.407	5.1	ng	199328	5	21.781	779282	20.0
Farnesol isomer a	20.606	4.4	ng	172476	5	21.781	779282	20.0
Eicosane	21.288	5.0	ng	193384	5	21.781	779282	20.0
Bromoacetic aci...	21.411	9.2	ng	359295	5	21.781	779282	20.0
Benzoic acid, 2...	21.494	3.1	ng	122367	5	21.781	779282	20.0
Heptacosane	22.293	5.1	ng	197312	5	21.781	779282	20.0
Heptadecane	22.604	2.4	ng	93468	5	21.781	779282	20.0
Sulfurous acid,...	23.491	4.6	ng	209764	6	25.113	910225	20.0