

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
 Data File : BG056359.D
 Acq On : 19 Jan 2023 23:14
 Operator : CG/JU
 Sample : 01215-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BU-02-011823

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056359.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.316	3	5	16	rVB	98061	134446	6.16%	1.039%
2	5.343	343	350	359	rBB	123241	187265	8.59%	1.447%
3	5.825	424	432	442	rBV	407128	653996	29.99%	5.054%
4	7.447	700	708	717	rBV	415376	708304	32.48%	5.473%
5	8.304	847	854	862	rVB	135982	230192	10.55%	1.779%
6	9.479	1046	1054	1067	rBB	234682	431992	19.81%	3.338%
7	11.136	1328	1336	1344	rBV	179702	326541	14.97%	2.523%
8	13.545	1739	1746	1752	rBV	911235	1410021	64.65%	10.896%
9	14.920	1970	1980	1987	rVB	342606	549075	25.18%	4.243%
10	16.254	2202	2207	2214	rVB2	21096	34862	1.60%	0.269%
11	16.395	2225	2231	2238	rBV	644867	997657	45.74%	7.709%
12	17.658	2438	2446	2451	rBV	461467	705591	32.35%	5.452%
13	17.699	2451	2453	2459	rVB	32853	37214	1.71%	0.288%
14	18.281	2547	2552	2558	rVB	256251	314711	14.43%	2.432%
15	18.498	2585	2589	2599	rBV2	82691	148522	6.81%	1.148%
16	19.403	2738	2743	2746	rBV	884636	1127146	51.68%	8.710%
17	19.438	2746	2749	2759	rVB2	510258	730300	33.49%	5.643%
18	19.562	2766	2770	2775	rBV	120952	140184	6.43%	1.083%
19	19.691	2788	2792	2797	rVB	54156	74473	3.41%	0.575%
20	19.756	2800	2803	2810	rVB9	28257	39602	1.82%	0.306%
21	20.049	2849	2853	2860	rVB	56915	86771	3.98%	0.671%
22	20.232	2878	2884	2889	rBV	1724838	2180963	100.00%	16.853%
23	20.502	2928	2930	2934	rBV5	18857	25716	1.18%	0.199%
24	21.530	3101	3105	3114	rVB2	83017	137977	6.33%	1.066%
25	21.947	3169	3176	3182	rBV2	431871	785288	36.01%	6.068%
26	25.396	3754	3763	3773	rVB2	240206	742213	34.03%	5.735%

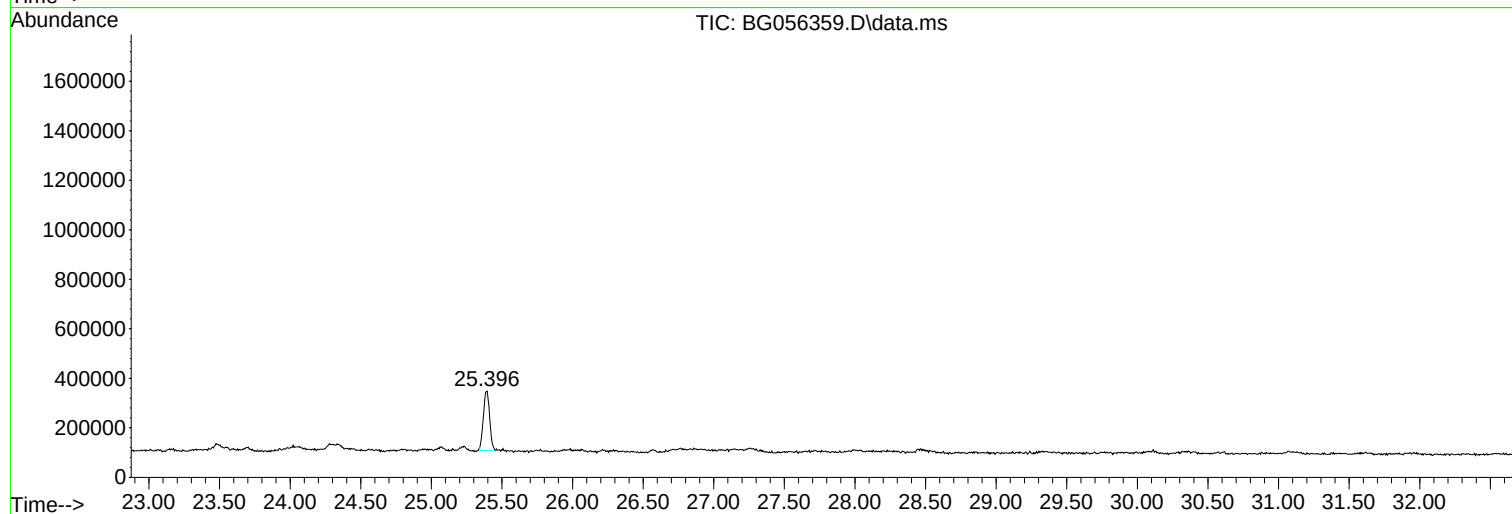
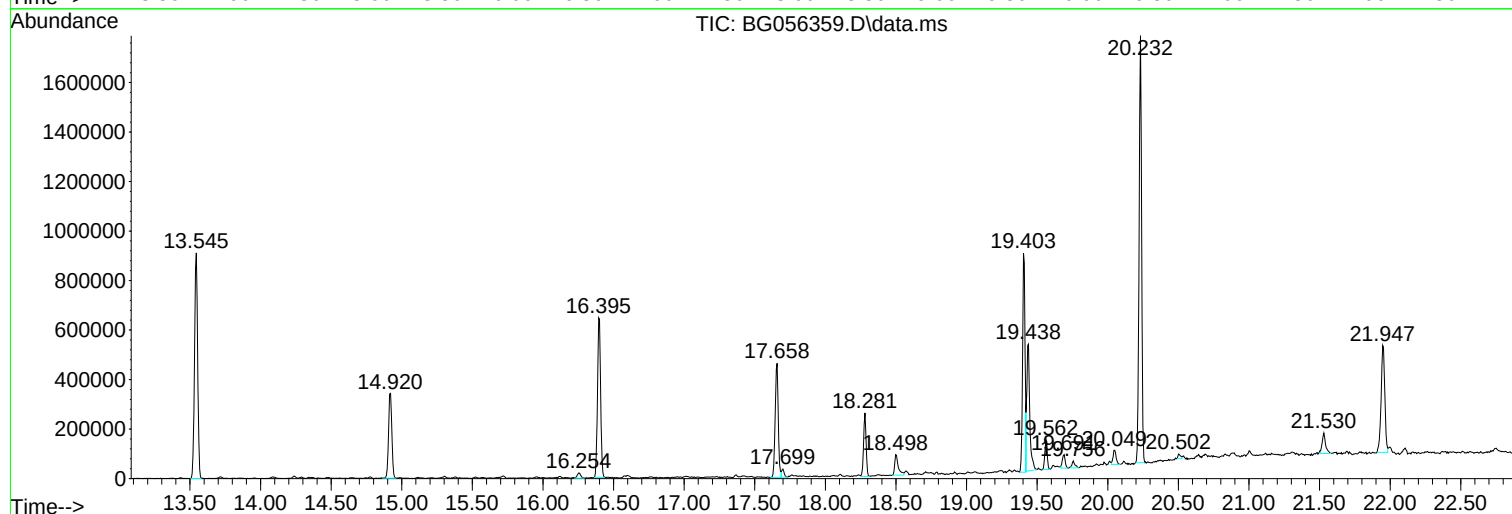
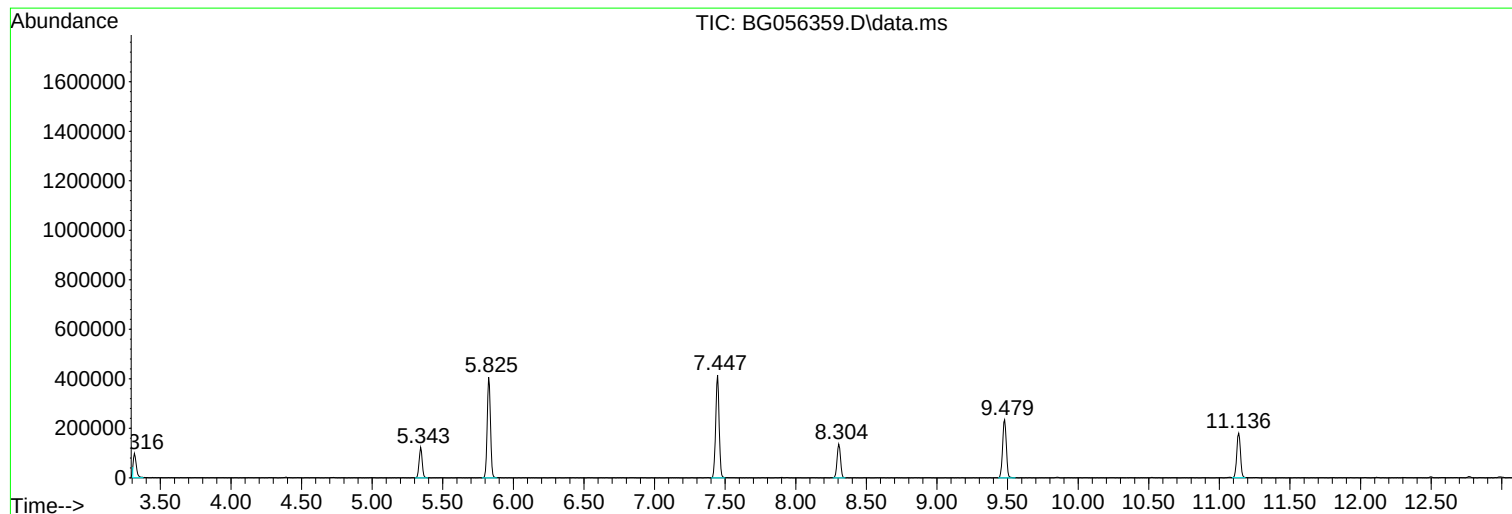
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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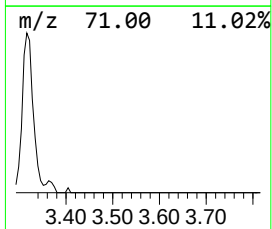
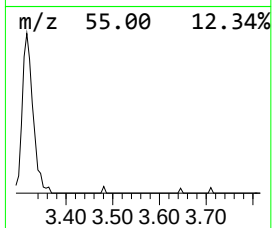
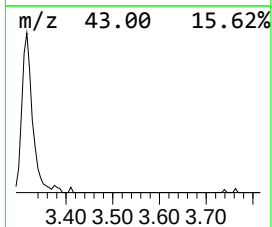
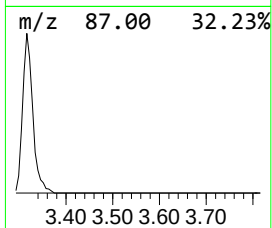
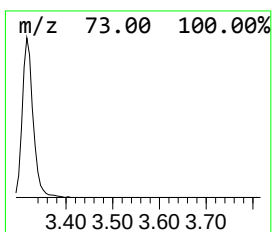
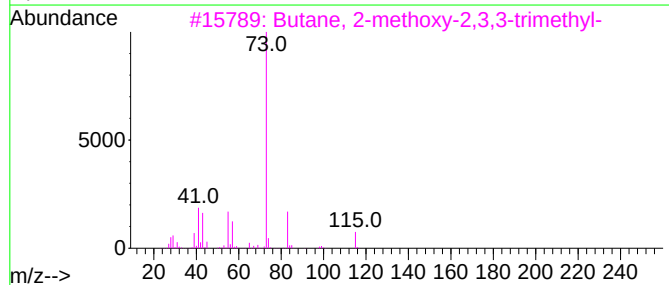
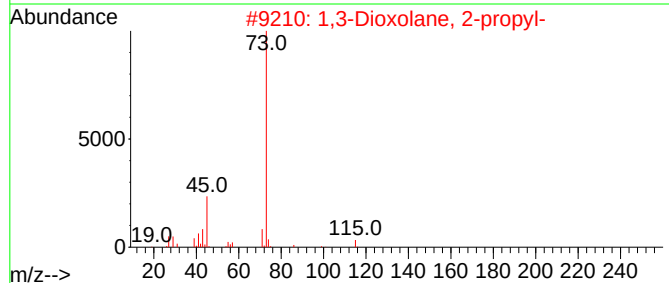
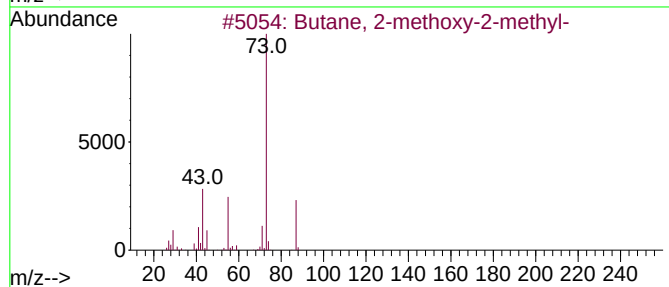
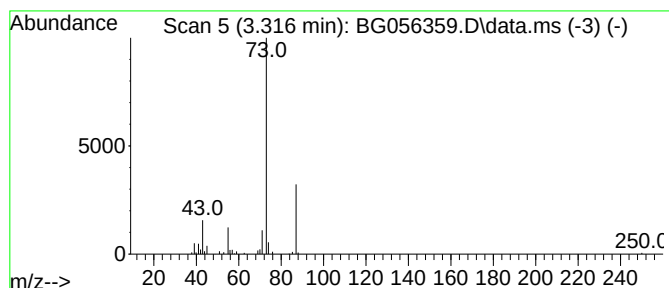
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.316	11.68 ng	134446	1,4-Dichlorobenzene-d4	8.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17
3			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			1-Cyclohexyl-3-ethoxy-butan-2-one	198	C12H22O2	074897-69-1	9



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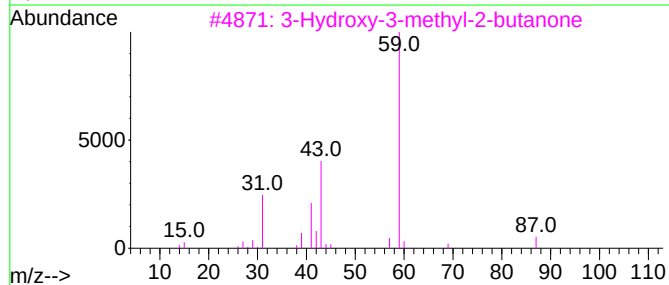
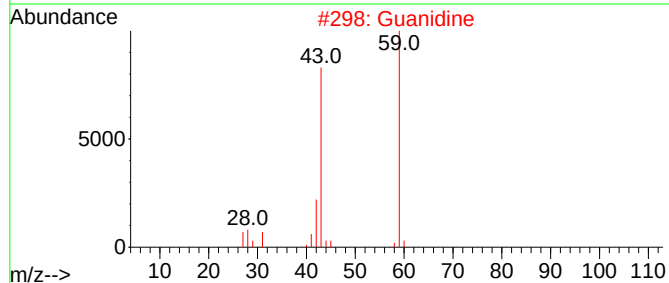
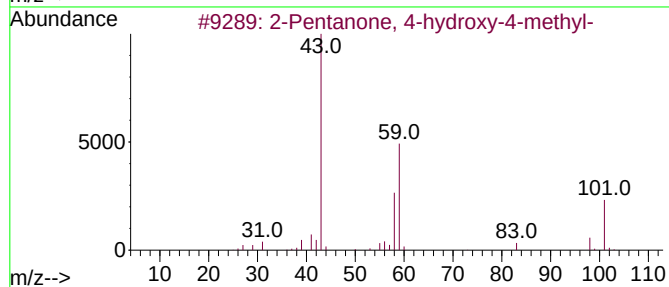
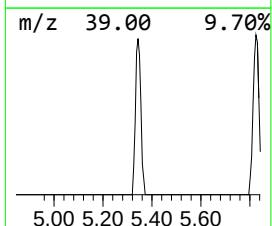
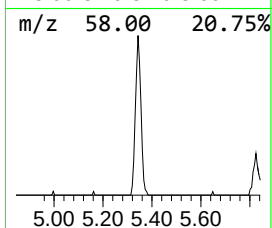
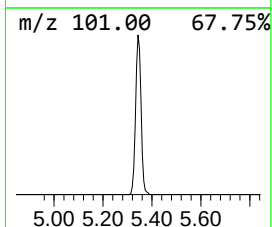
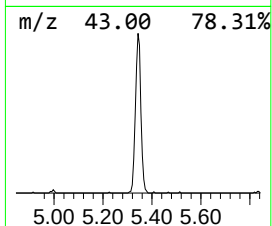
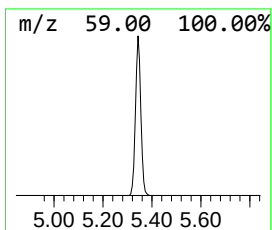
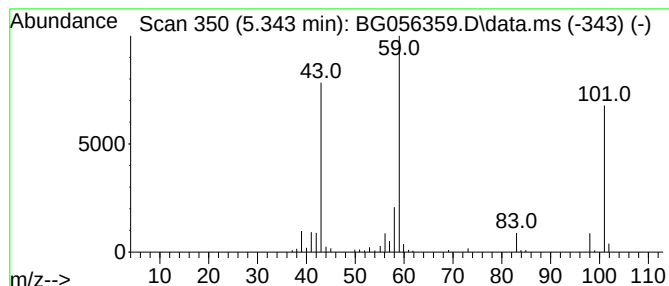
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.343	16.27 ng	187265	1,4-Dichlorobenzene-d4	8.304

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Guanidine	59	CH5N3	000113-00-8	37
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
5		1,2-Butanediol	90	C4H10O2	000584-03-2	23



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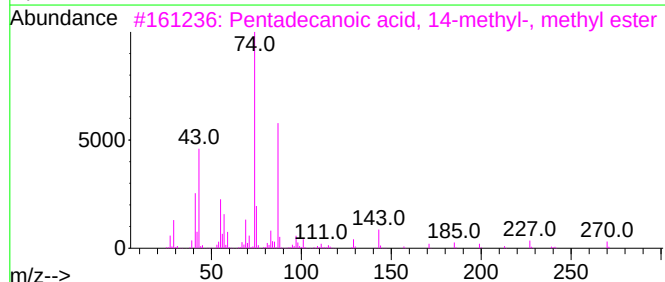
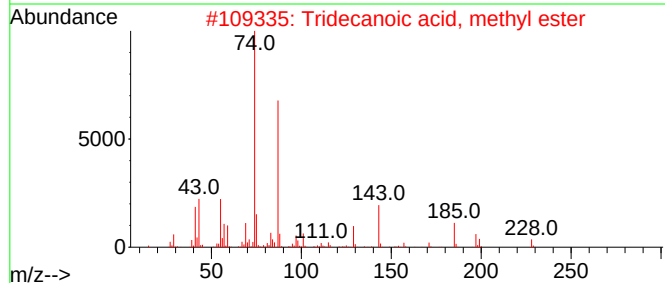
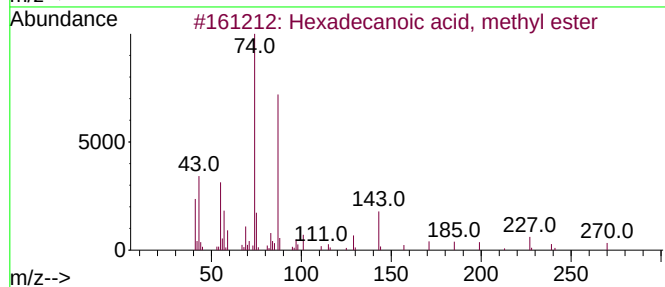
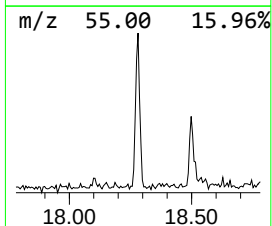
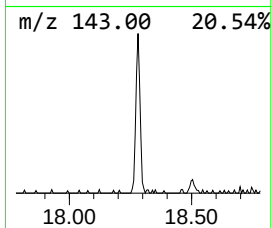
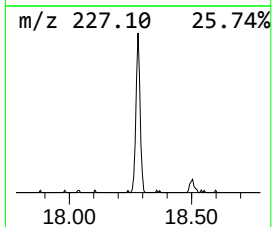
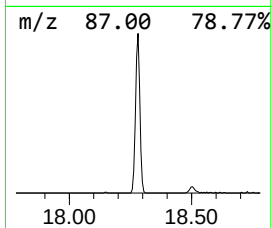
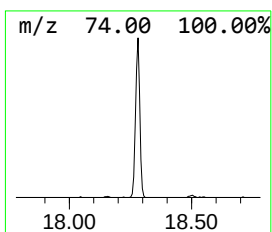
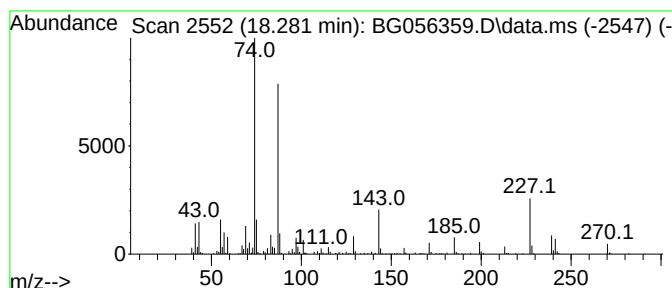
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.281	8.92 ng	314711	Phenanthrene-d10	17.658

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	91
2		Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
3		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	81
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	74
5		Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	72



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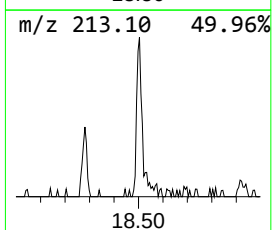
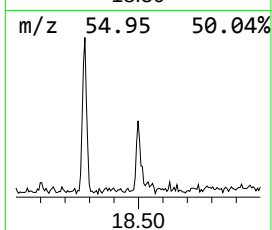
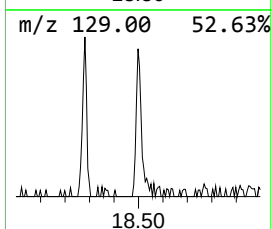
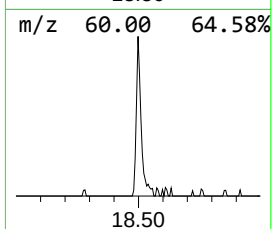
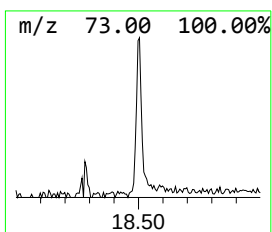
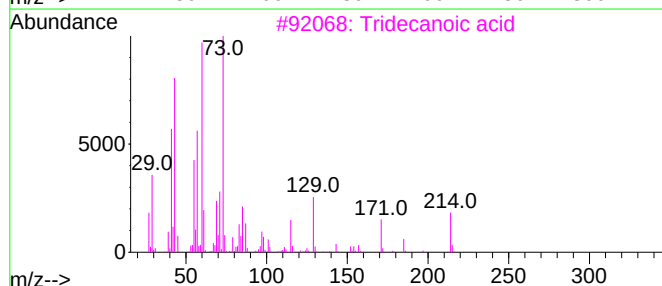
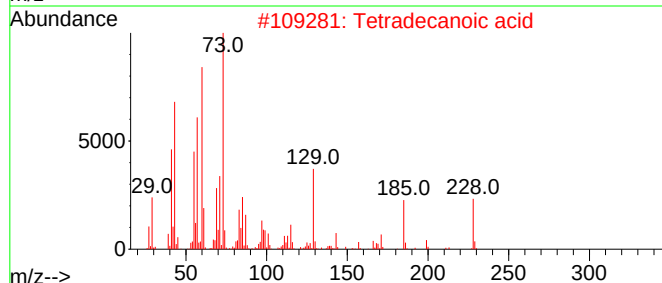
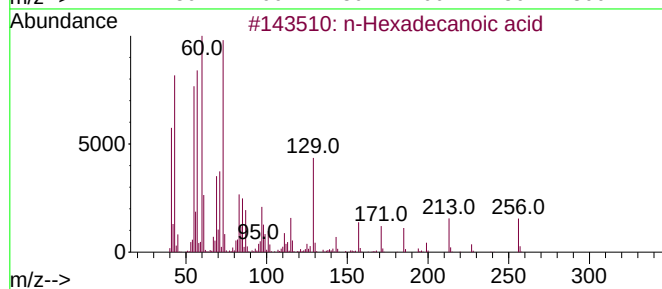
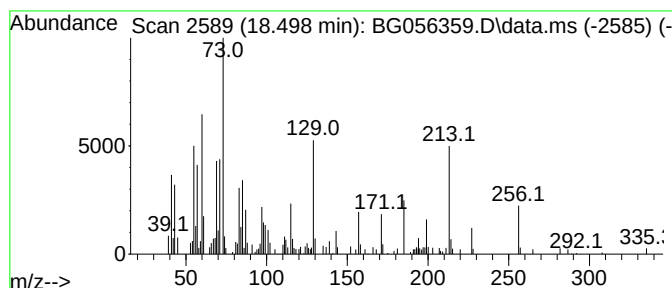
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.498	4.21 ng	148522	Phenanthrene-d10	17.658

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	92
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Dodecanoic acid	200	C12H24O2	000143-07-7	49
5			Nonanoic acid	158	C9H18O2	000112-05-0	38



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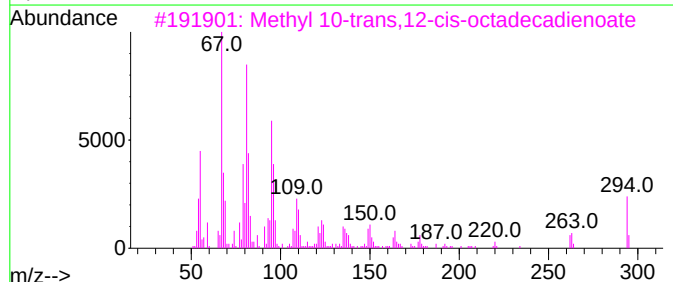
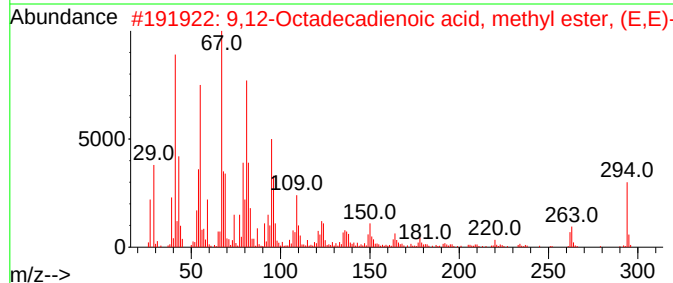
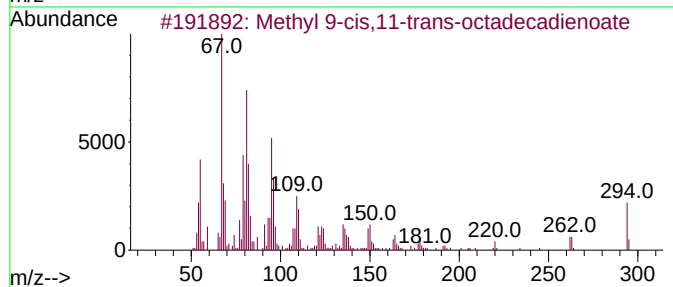
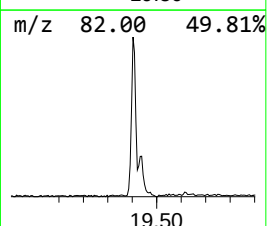
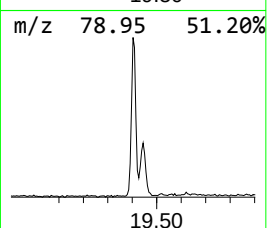
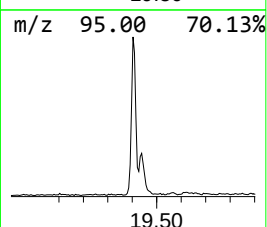
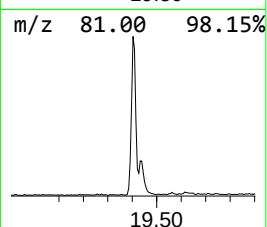
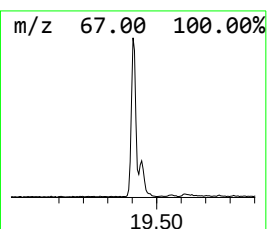
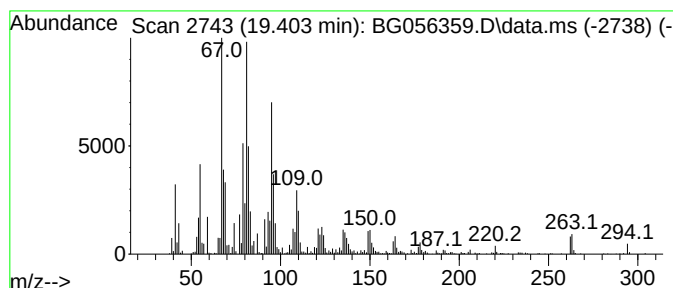
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Peak Number 5 Methyl 9-cis,11-trans-octad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.403	31.95 ng	1127150	Phenanthrene-d10	17.658	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	96
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	94
3	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	94
4	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	93
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	92



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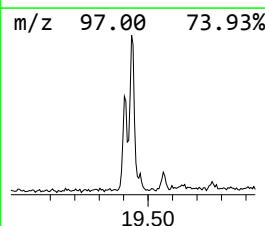
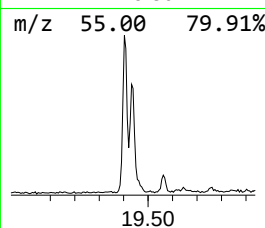
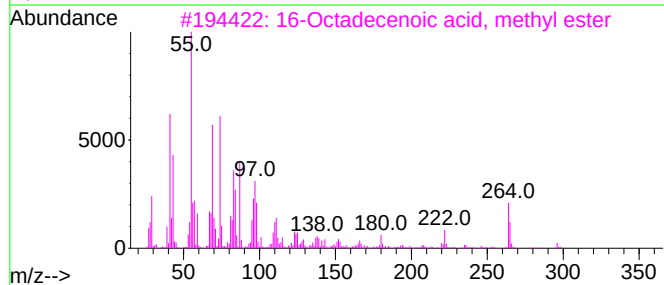
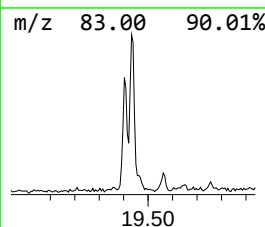
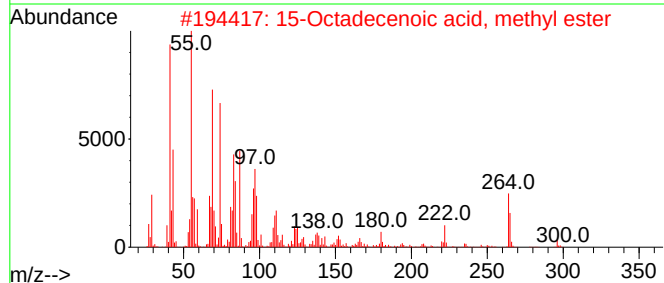
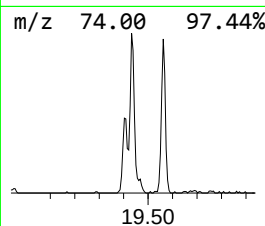
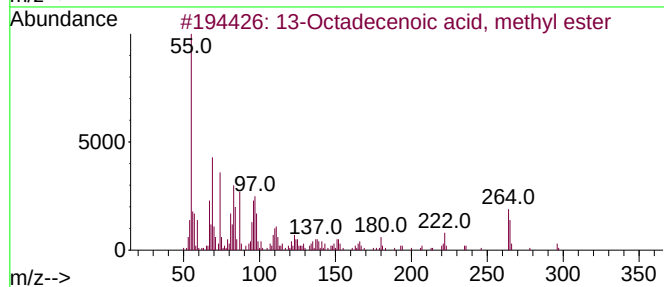
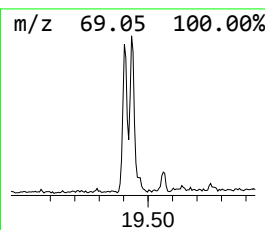
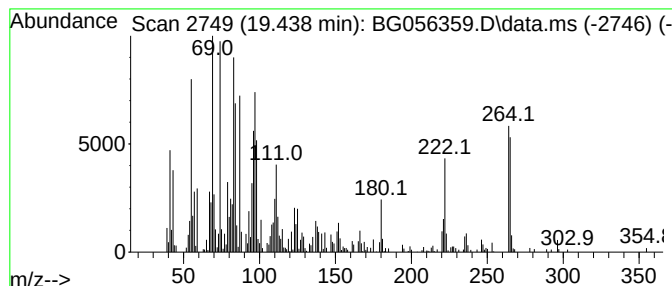
Instrument :
BNA_G
ClientSampleId :
BU-02-011823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 13-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.438	20.70 ng	730300	Phenanthrene-d10	17.658	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	98
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	98
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	97
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	95
5	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056359.D
Acq On : 19 Jan 2023 23:14
Operator : CG/JU
Sample : 01215-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-02-011823

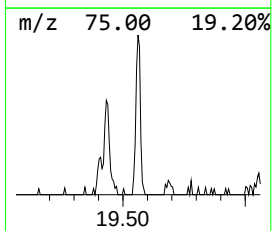
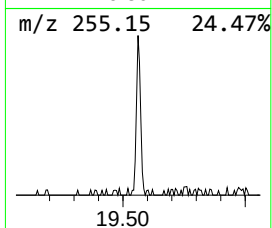
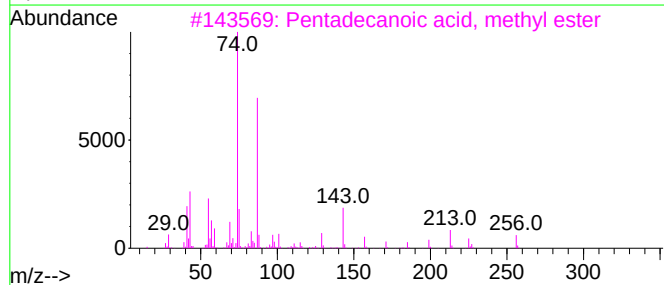
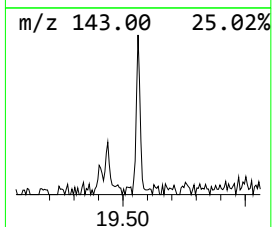
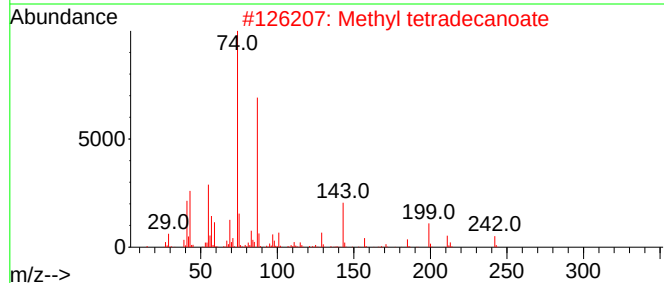
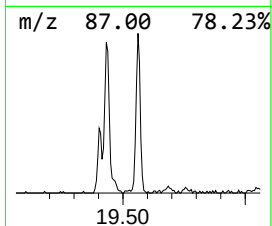
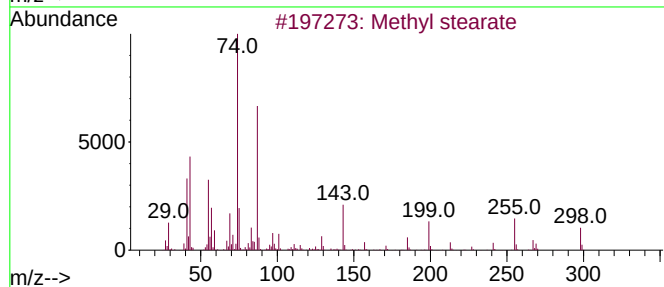
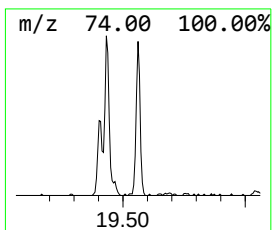
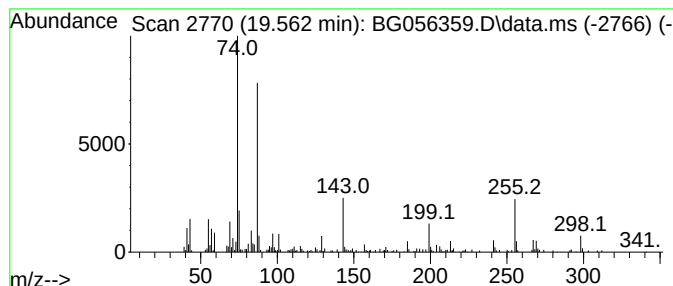
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.562	3.97 ng	140184	Phenanthrene-d10	17.658

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
3			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	90
5			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056359.D
Acq On : 19 Jan 2023 23:14
Operator : CG/JU
Sample : 01215-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

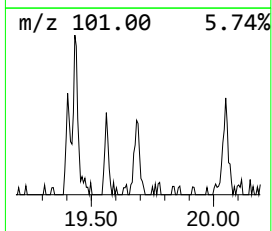
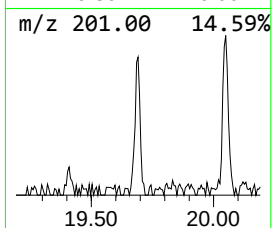
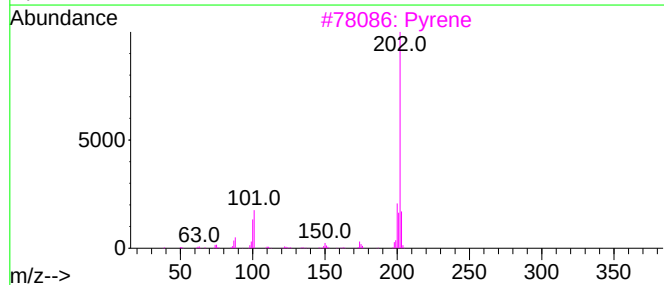
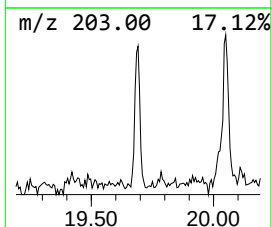
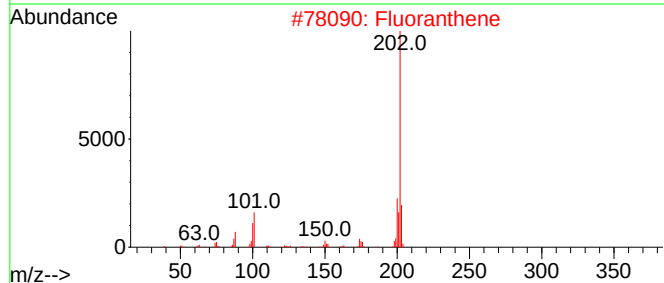
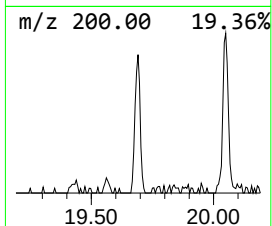
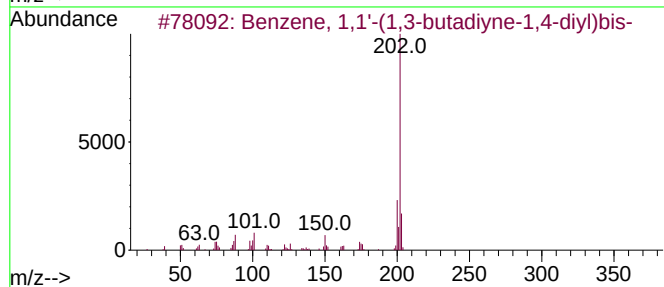
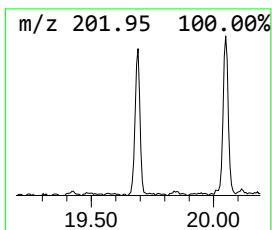
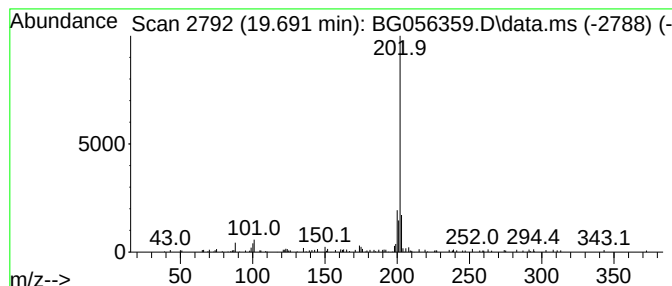
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.691	2.11 ng	74473	Phenanthrene-d10	17.658	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
2	Fluoranthene	202	C16H10	000206-44-0	76
3	Pyrene	202	C16H10	000129-00-0	76
4	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	38
5	2-[Methyl(trifluoroacetyl)amino]...	315	C11H7F6NO3	1000452-81-9	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056359.D
Acq On : 19 Jan 2023 23:14
Operator : CG/JU
Sample : 01215-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-02-011823

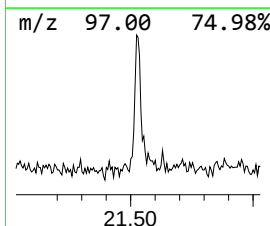
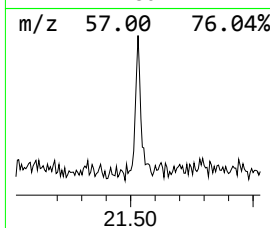
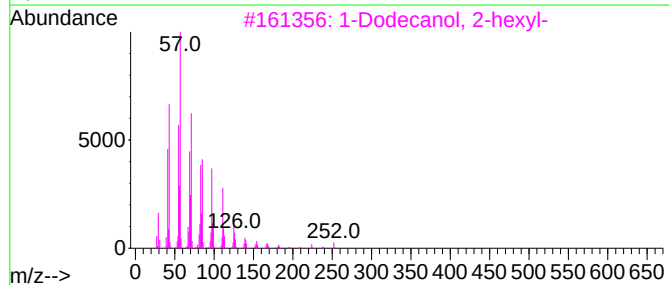
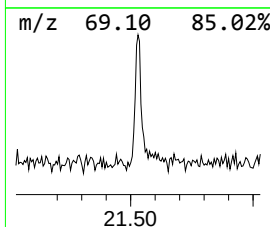
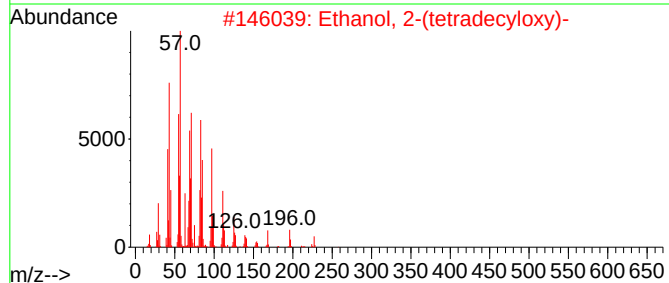
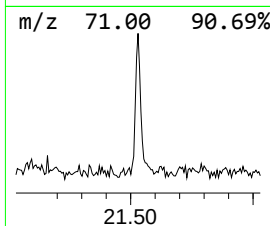
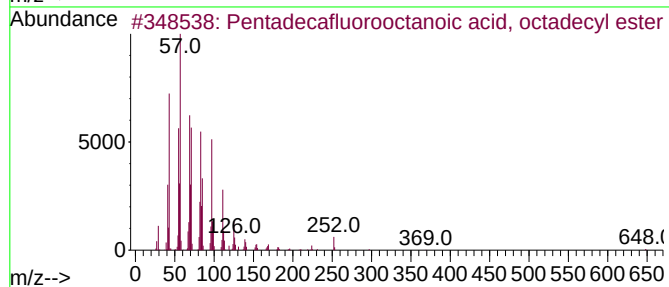
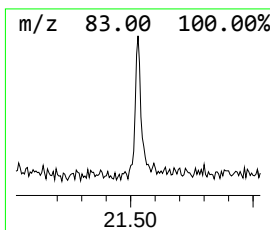
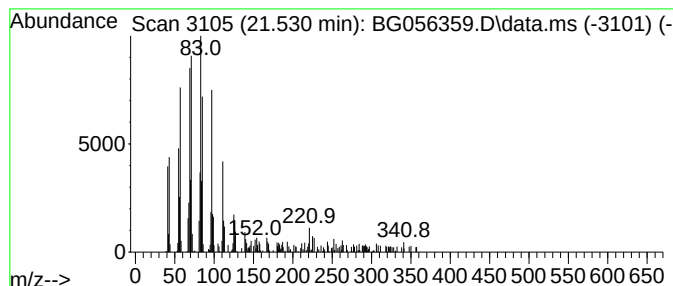
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Pentadecafluorooctanoic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.530	3.51 ng	137977	Chrysene-d12	21.947

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	64
3			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	64
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	62
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011923\
Data File : BG056359.D
Acq On : 19 Jan 2023 23:14
Operator : CG/JU
Sample : 01215-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-02-011823

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.316	11.7	ng	134446	1	8.304	230192	20.0
2-Pentanone, 4-...	5.343	16.3	ng	187265	1	8.304	230192	20.0
Hexadecanoic ac...	18.281	8.9	ng	314711	4	17.658	705591	20.0
n-Hexadecanoic ...	18.498	4.2	ng	148522	4	17.658	705591	20.0
Methyl 9-cis,11...	19.403	31.9	ng	1127150	4	17.658	705591	20.0
13-Octadecenoic...	19.438	20.7	ng	730300	4	17.658	705591	20.0
Methyl stearate	19.562	4.0	ng	140184	4	17.658	705591	20.0
Benzene, 1,1'-(...	19.691	2.1	ng	74473	4	17.658	705591	20.0
Pentadecafluoro...	21.530	3.5	ng	137977	5	21.947	785288	20.0