

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060822\
 Data File : BG053848.D
 Acq On : 8 Jun 2022 11:41
 Operator : CG/JU
 Sample : N3194-04
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-3

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-BG060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053848.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.192	301	307	312	rBV	10968	19450	1.11%	0.200%
2	5.656	379	386	401	rVB	331710	558058	31.98%	5.741%
3	7.242	647	656	666	rBV	331452	595027	34.10%	6.121%
4	8.088	793	800	809	rBV	72461	131636	7.54%	1.354%
5	9.246	989	997	1006	rBV	197187	373649	21.41%	3.844%
6	10.903	1271	1279	1287	rVB	98496	186549	10.69%	1.919%
7	13.341	1686	1694	1704	rBV	581168	953352	54.63%	9.808%
8	14.710	1921	1927	1934	rVB	168062	272749	15.63%	2.806%
9	16.197	2173	2180	2190	rBV	536212	889437	50.97%	9.150%
10	17.454	2388	2394	2399	rBV	242003	387090	22.18%	3.982%
11	17.495	2399	2401	2407	rVB	15653	20393	1.17%	0.210%
12	18.265	2524	2532	2533	rBV5	22905	43564	2.50%	0.448%
13	18.341	2535	2545	2563	rVB3	136869	447195	25.63%	4.601%
14	19.058	2661	2667	2673	rVB5	15956	35838	2.05%	0.369%
15	19.499	2737	2742	2747	rBV	43987	87280	5.00%	0.898%
16	19.610	2749	2761	2783	rVB	230964	813487	46.62%	8.369%
17	19.863	2796	2804	2813	rVB	32661	67174	3.85%	0.691%
18	20.063	2831	2838	2843	rBV	1281027	1745114	100.00%	17.953%
19	20.509	2908	2914	2924	rBV	46187	89612	5.14%	0.922%
20	21.291	3041	3047	3054	rBV	50592	101392	5.81%	1.043%
21	21.373	3055	3061	3071	rVV5	49061	89675	5.14%	0.923%
22	21.490	3077	3081	3091	rVB8	12363	24540	1.41%	0.252%
23	21.725	3112	3121	3127	rBV	281324	546299	31.30%	5.620%
24	22.178	3192	3198	3207	rVB2	60504	133116	7.63%	1.369%
25	23.200	3364	3372	3383	rBV3	41446	123305	7.07%	1.269%
26	23.459	3413	3416	3423	rVB2	16864	33157	1.90%	0.341%
27	23.964	3494	3502	3505	rBV4	13132	37787	2.17%	0.389%
28	24.411	3569	3578	3589	rVB5	34445	128504	7.36%	1.322%
29	24.722	3622	3631	3640	rVB5	25295	91328	5.23%	0.940%
30	24.834	3645	3650	3659	rVB3	12522	34225	1.96%	0.352%
31	24.992	3667	3677	3687	rBV2	162103	493635	28.29%	5.078%
32	25.815	3808	3817	3818	rBV6	24543	49473	2.83%	0.509%
33	28.647	4285	4299	4302	rBV6	30759	117407	6.73%	1.208%

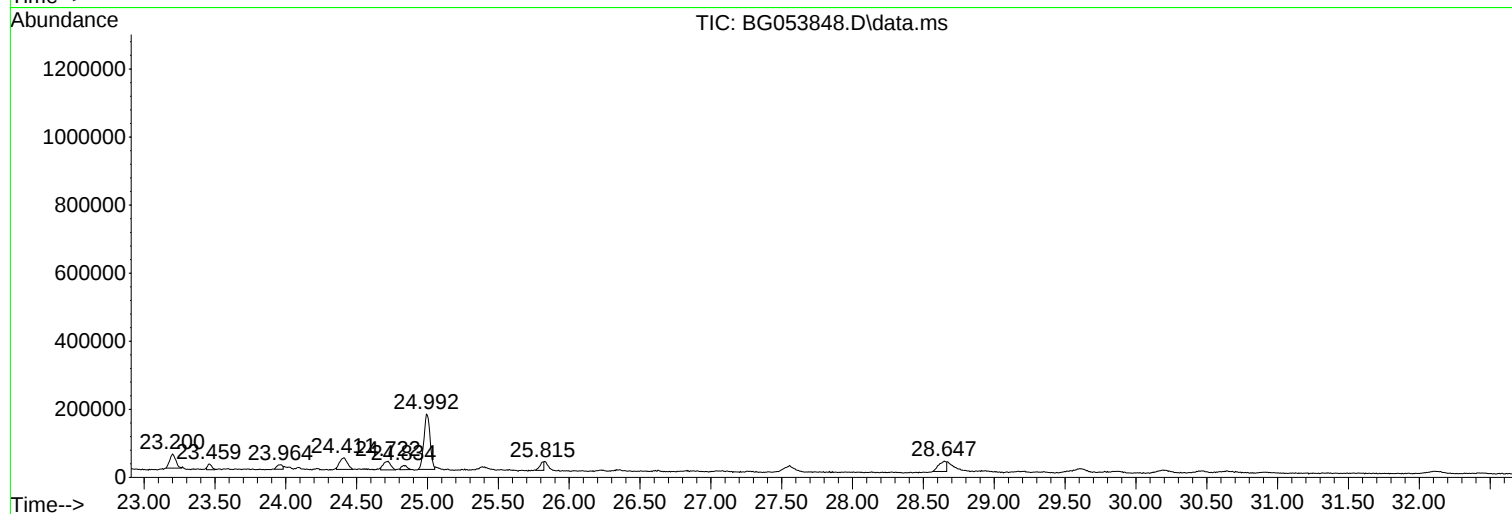
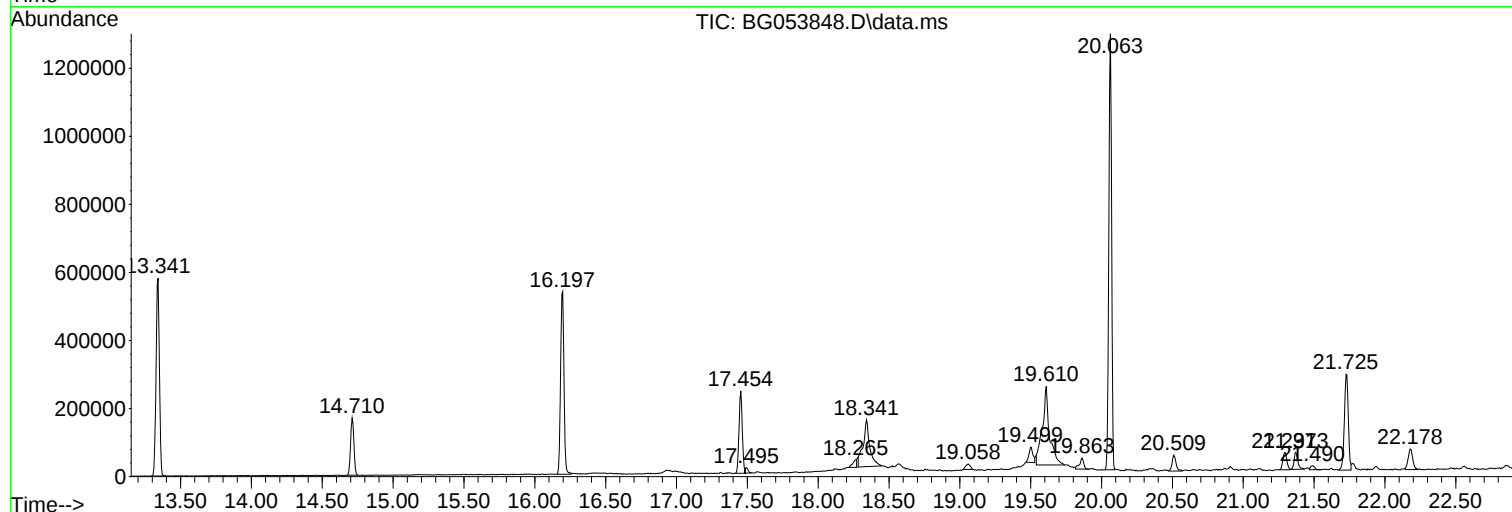
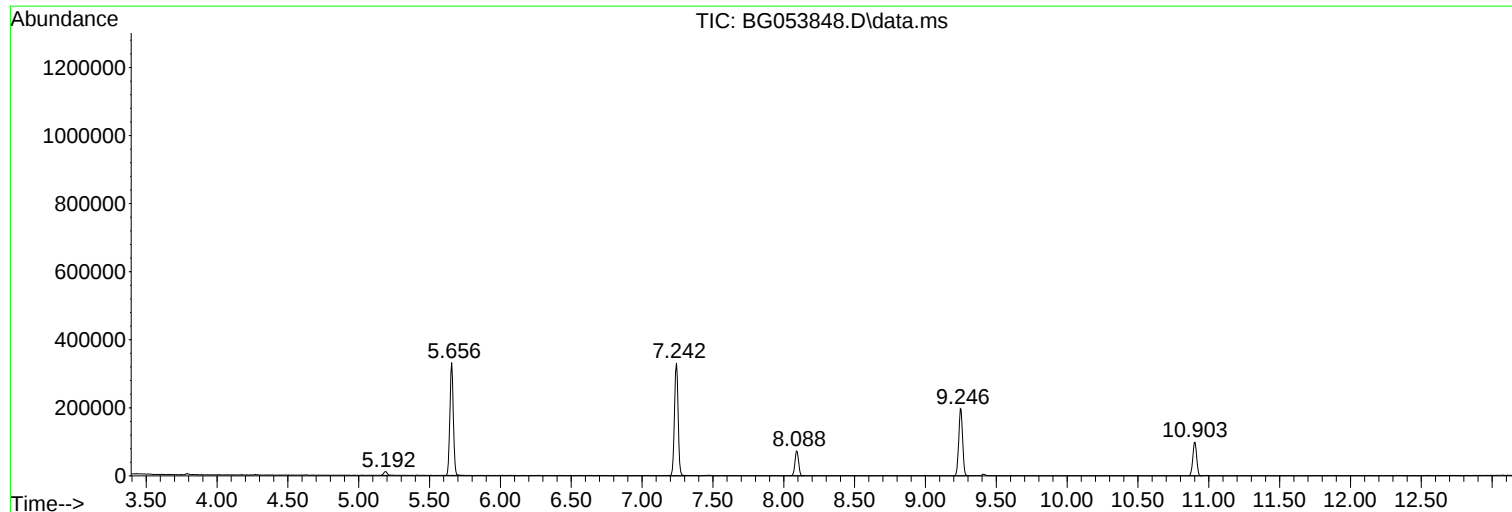
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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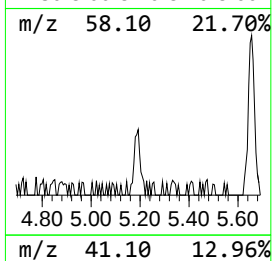
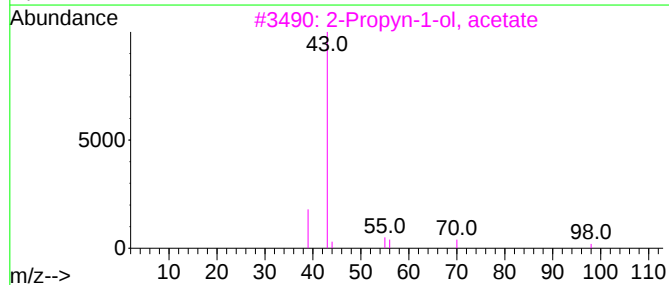
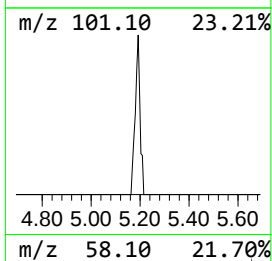
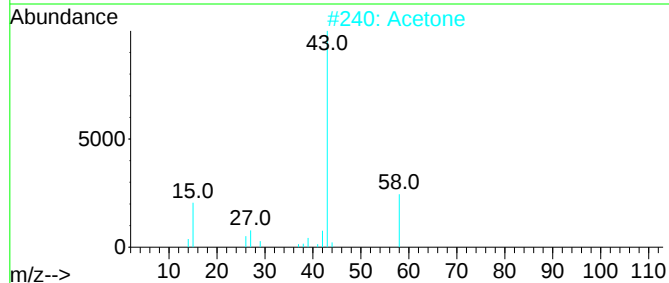
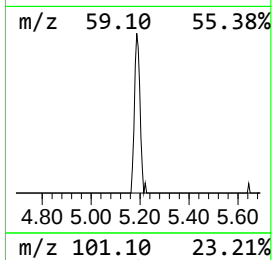
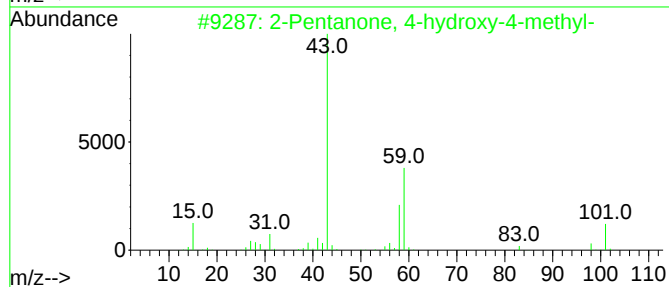
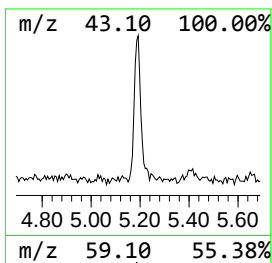
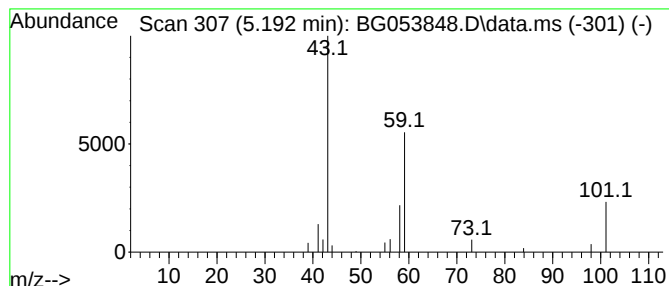
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.192	2.96 ng	19450	1,4-Dichlorobenzene-d4	8.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetone	58	C3H6O	000067-64-1	9
3			2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
4			1,3,4-Oxadiazole, 2-(acetyloxy)-...	172	C7H12N2O3	066398-57-0	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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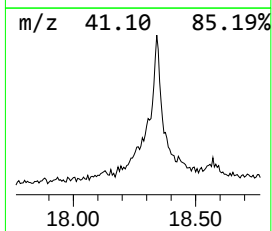
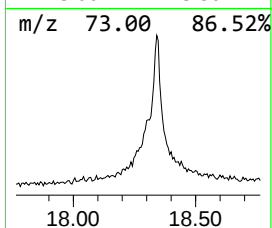
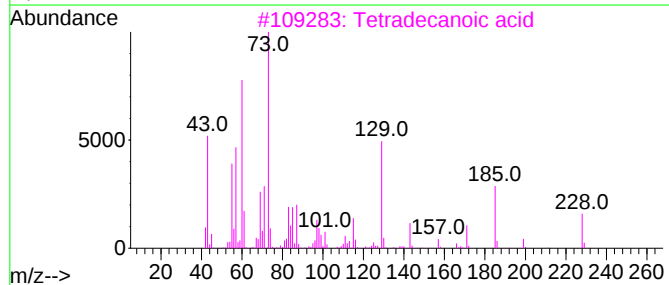
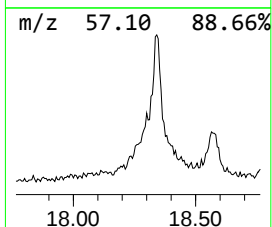
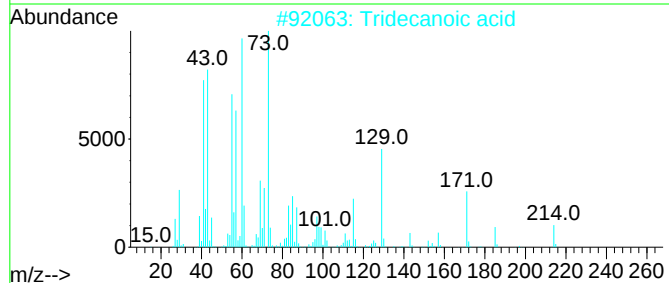
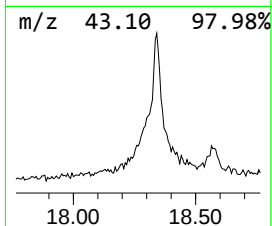
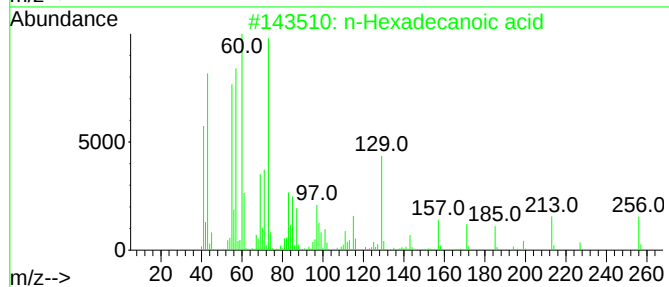
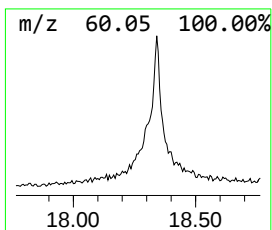
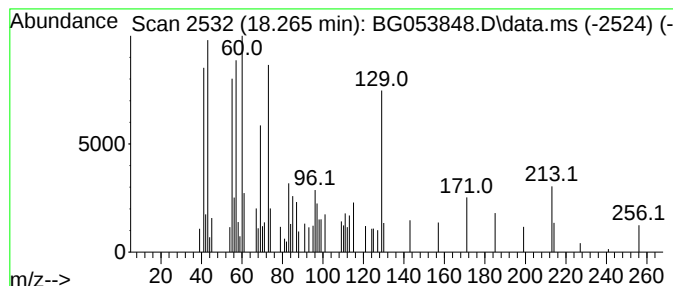
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Tridecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.265	2.25 ng	43564	Phenanthrene-d10	17.454

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	52
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	43



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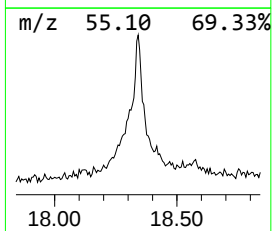
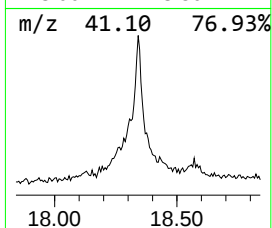
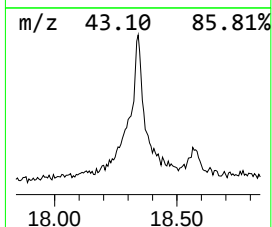
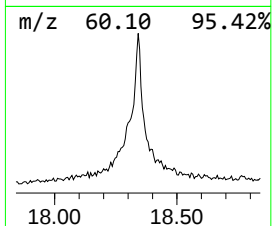
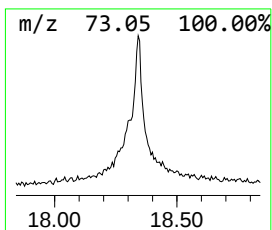
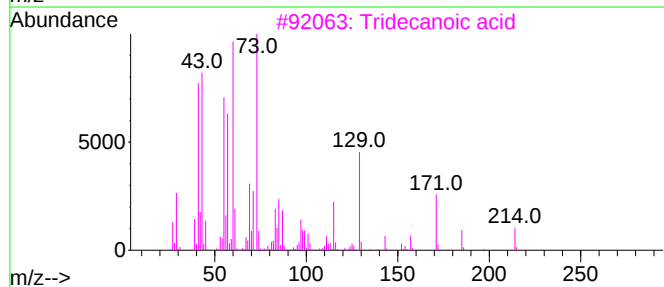
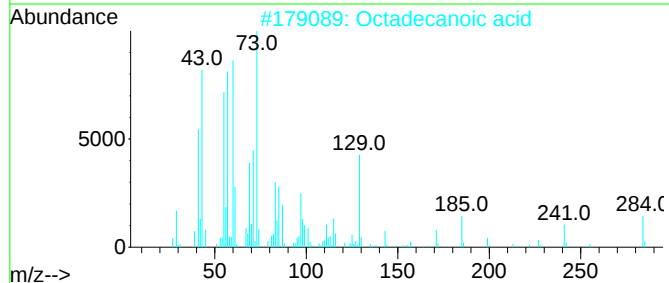
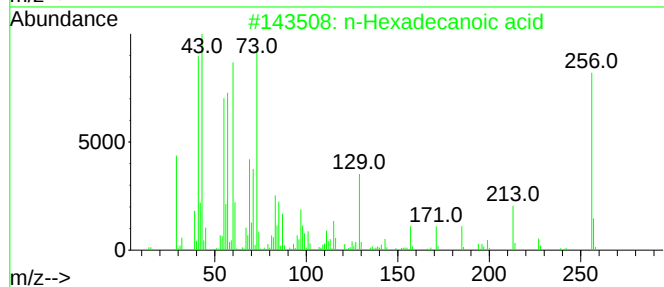
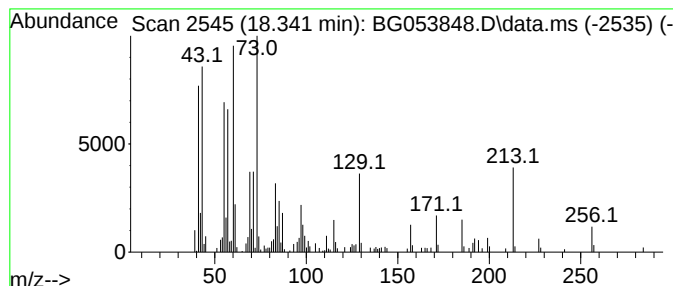
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.341	23.11 ng	447195	Phenanthrene-d10	17.454

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Octadecanoic acid	284	C18H36O2	000057-11-4	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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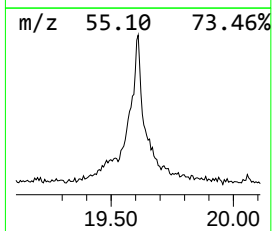
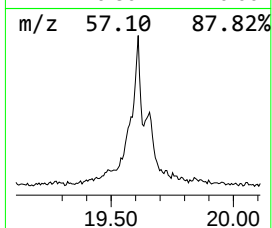
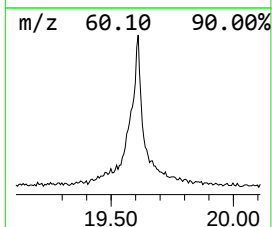
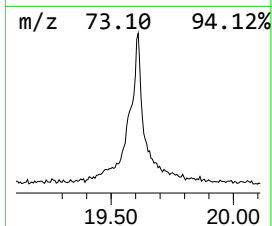
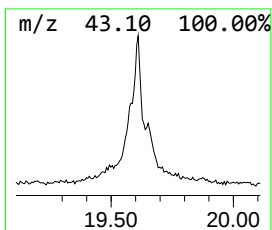
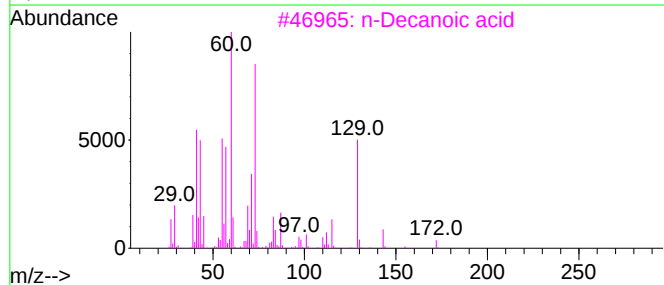
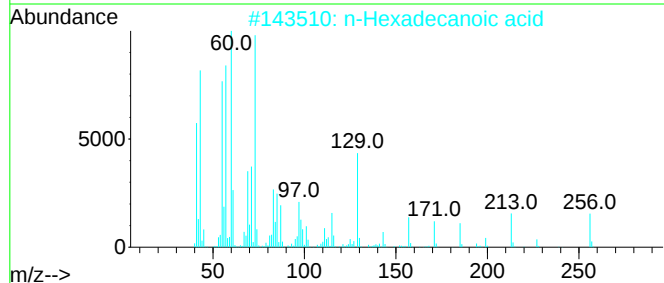
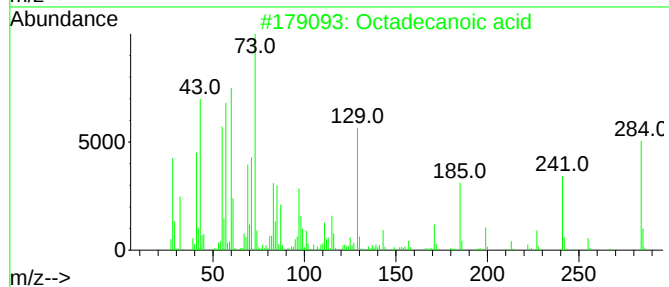
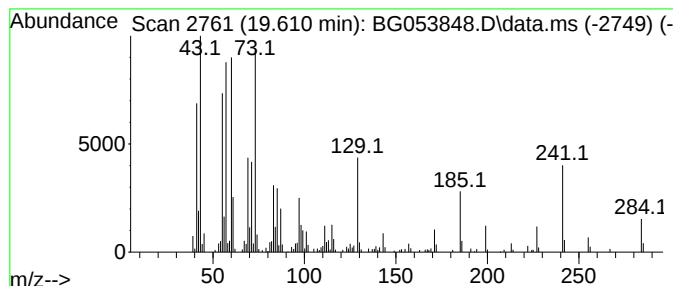
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Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.610	29.78 ng	813487	Chrysene-d12	21.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3			n-Decanoic acid	172	C10H20O2	000334-48-5	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	74



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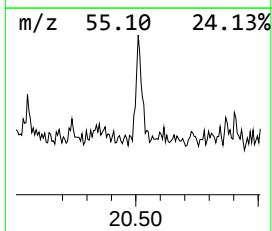
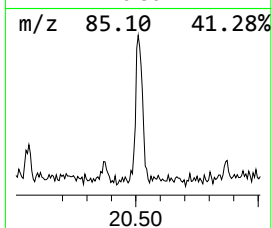
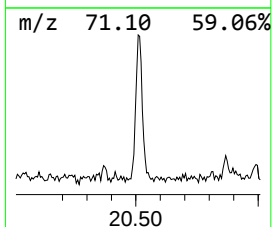
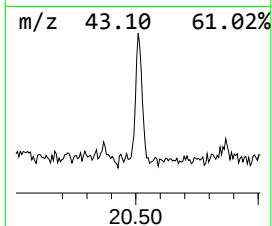
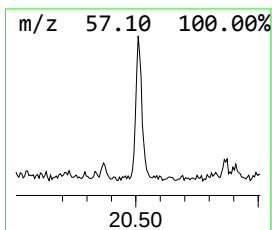
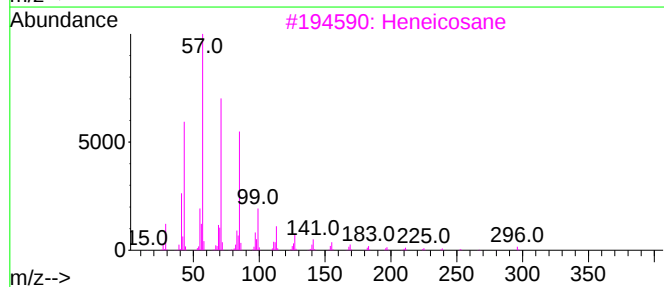
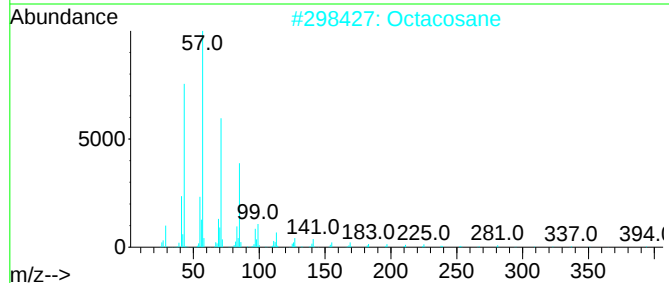
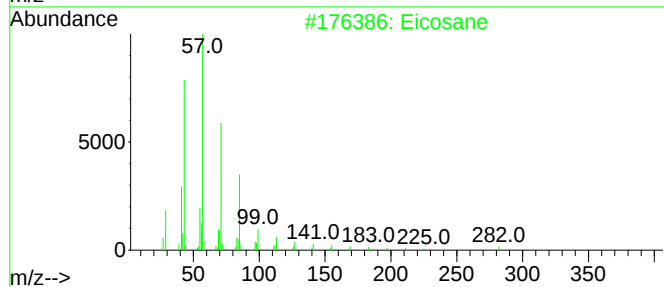
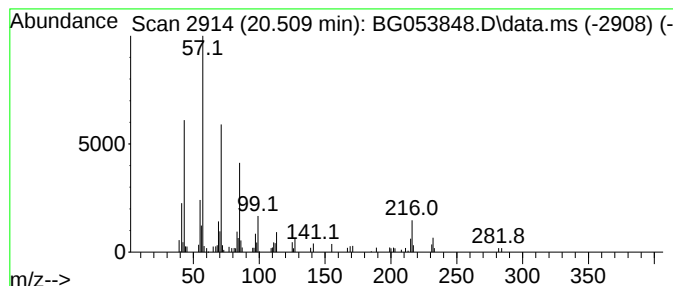
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Peak Number 6 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.509	3.28 ng	89612	Chrysene-d12	21.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Octacosane	394	C28H58	000630-02-4	87
3			Heneicosane	296	C21H44	000629-94-7	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Pentacosane	352	C25H52	000629-99-2	87



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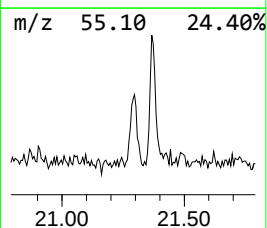
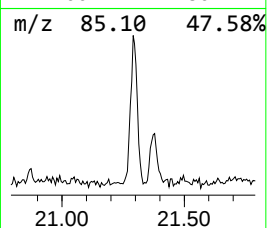
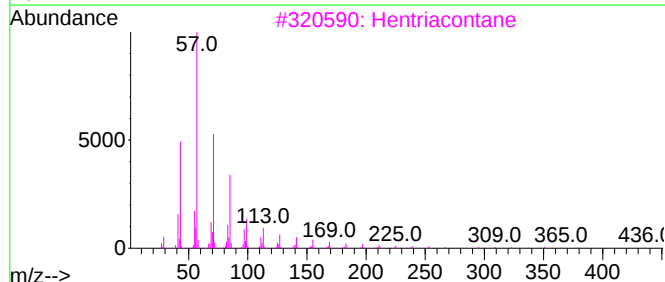
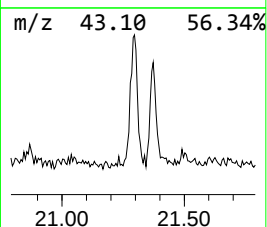
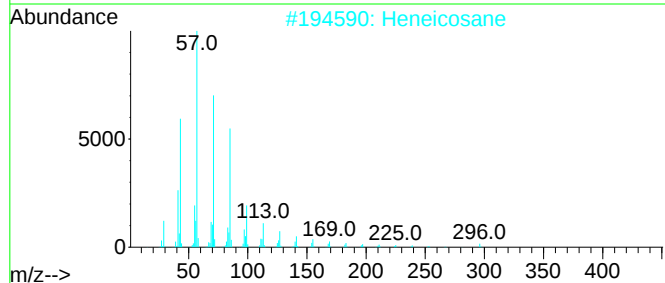
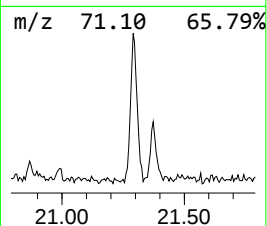
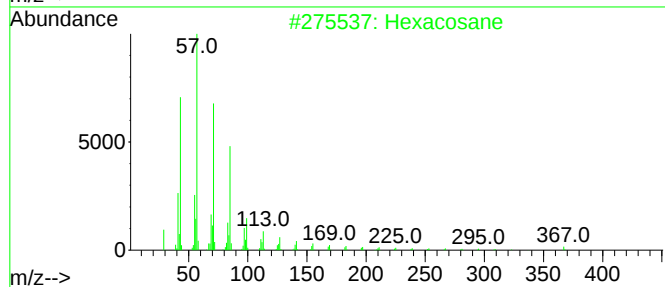
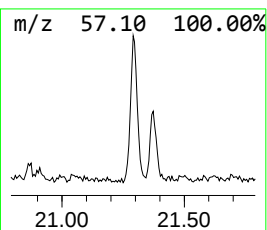
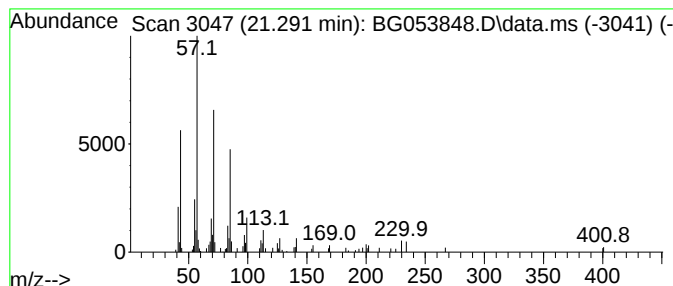
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.291	3.71 ng	101392	Chrysene-d12	21.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Heneicosane	296	C21H44	000629-94-7	87
3			Hentriacontane	437	C31H64	000630-04-6	83
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
5			Tridecane, 3-methyl-	198	C14H30	006418-41-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060822\
Data File : BG053848.D
Acq On : 8 Jun 2022 11:41
Operator : CG/JU
Sample : N3194-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-3

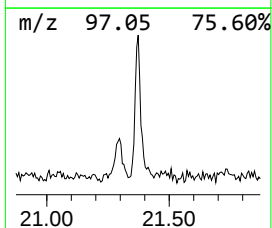
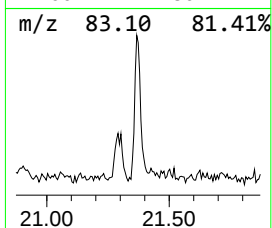
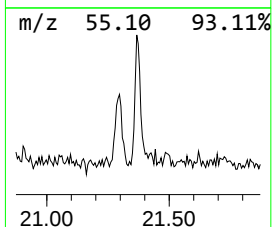
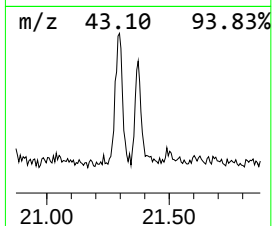
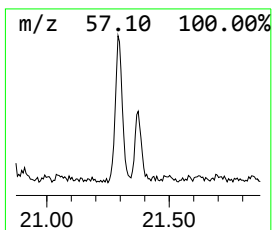
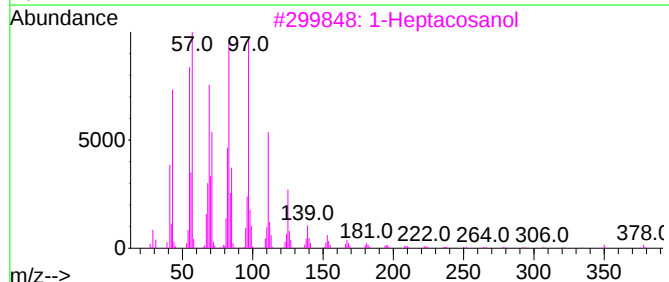
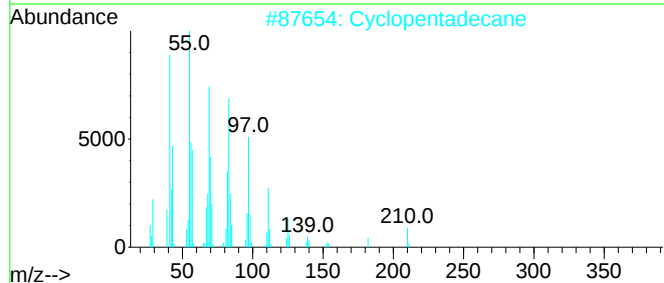
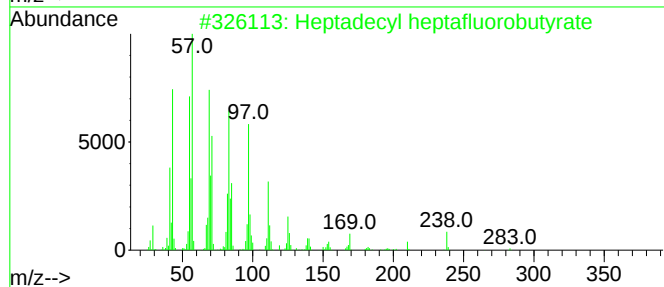
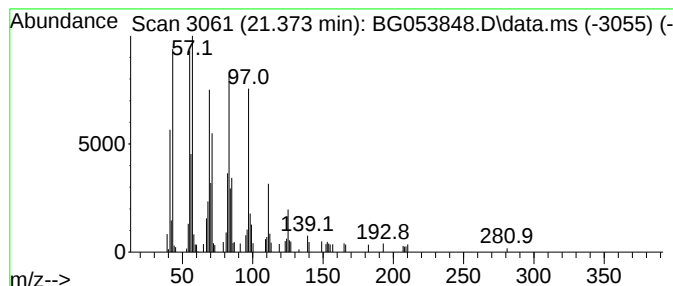
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.373	3.28 ng	89675	Chrysene-d12	21.725

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Cyclopentadecane	210	C15H30	000295-48-7	93
3		1-Heptacosanol	396	C27H56O	002004-39-9	91
4		1-Tetracosene	336	C24H48	010192-32-2	90
5		1-Hexacosene	364	C26H52	018835-33-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060822\
Data File : BG053848.D
Acq On : 8 Jun 2022 11:41
Operator : CG/JU
Sample : N3194-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-3

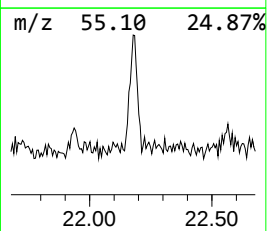
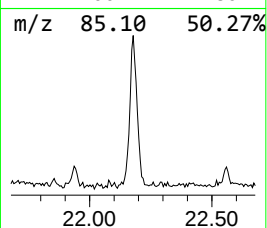
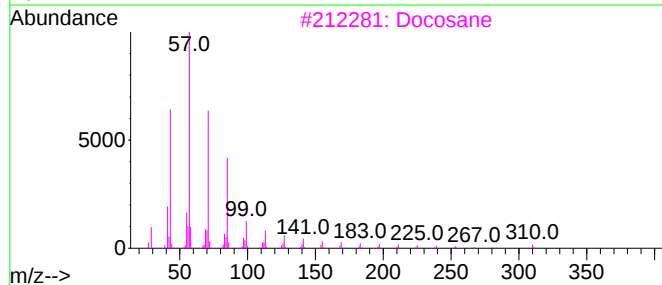
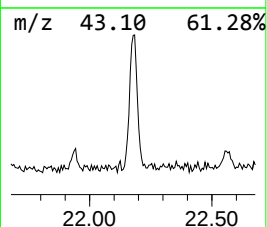
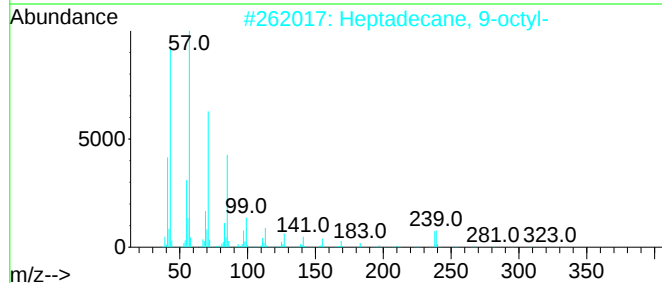
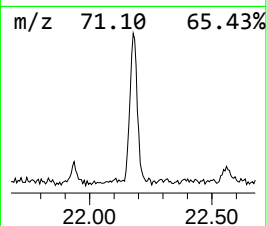
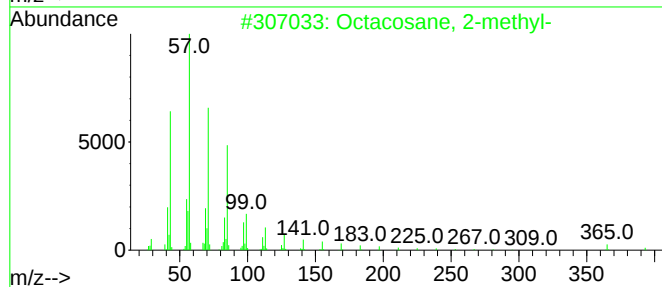
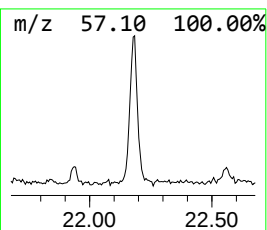
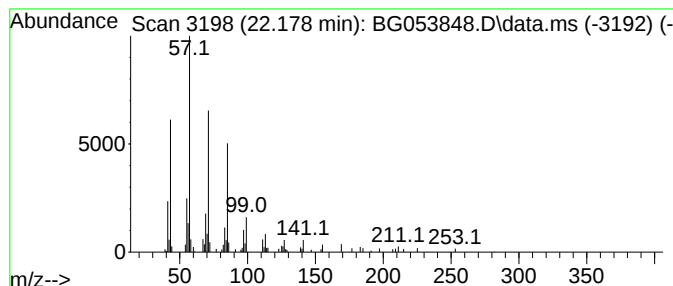
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octacosane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.178	4.87 ng	133116	Chrysene-d12	21.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3			Docosane	310	C22H46	000629-97-0	91
4			Eicosane	282	C20H42	000112-95-8	90
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060822\
Data File : BG053848.D
Acq On : 8 Jun 2022 11:41
Operator : CG/JU
Sample : N3194-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-3

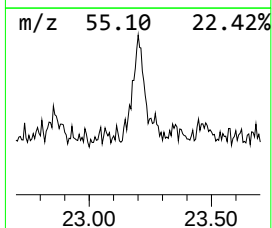
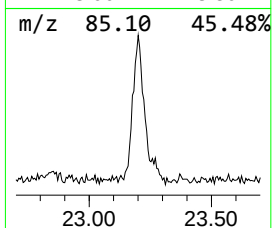
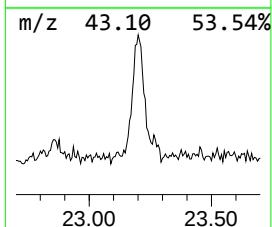
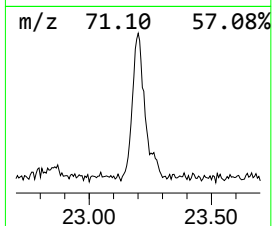
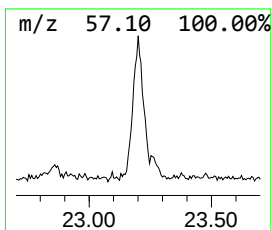
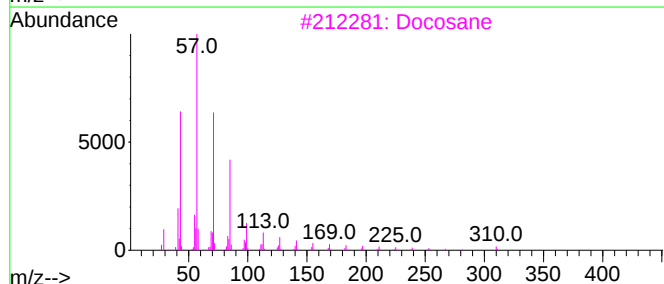
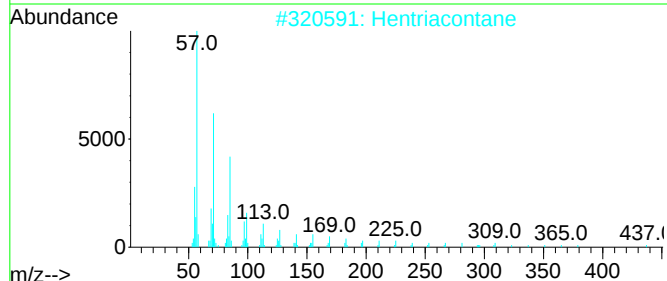
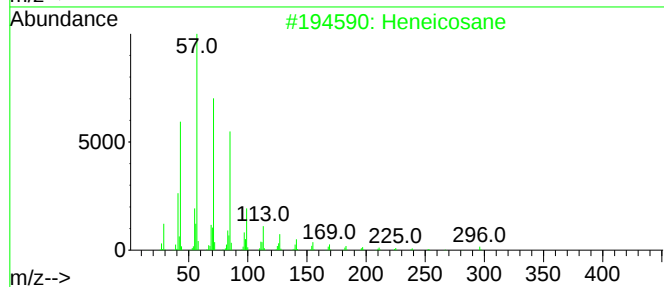
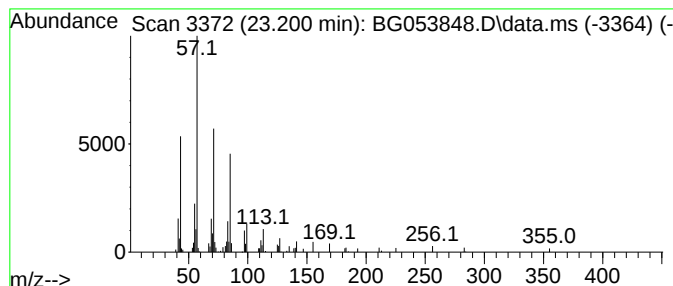
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.200	4.51 ng	123305	Chrysene-d12	21.725

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	91
2		Hentriacontane	437	C31H64	000630-04-6	91
3		Docosane	310	C22H46	000629-97-0	91
4		Triacontane	422	C30H62	000638-68-6	91
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060822\
Data File : BG053848.D
Acq On : 8 Jun 2022 11:41
Operator : CG/JU
Sample : N3194-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

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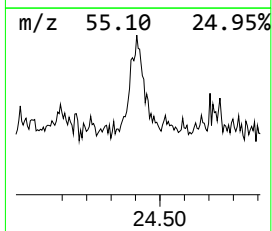
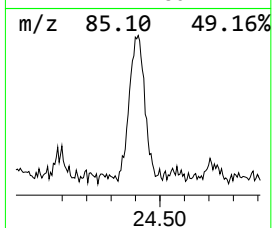
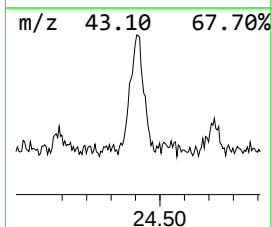
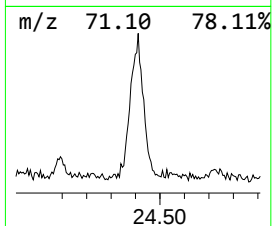
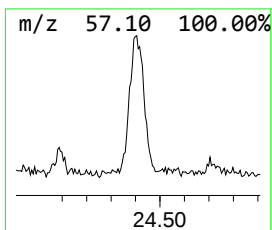
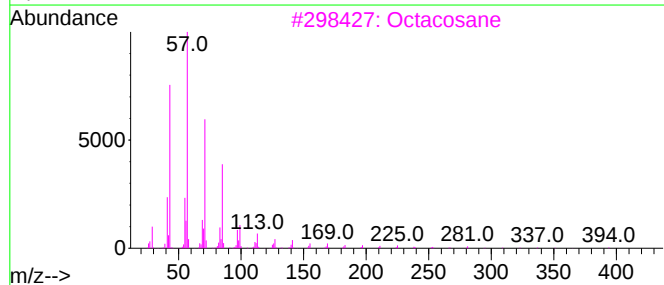
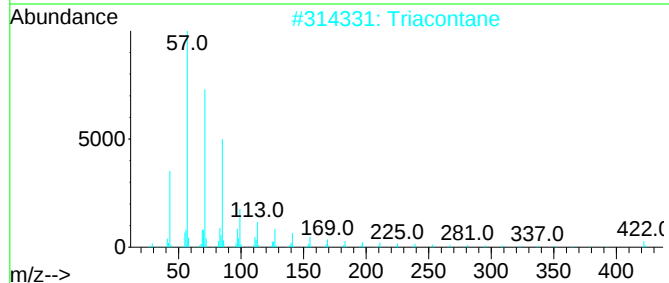
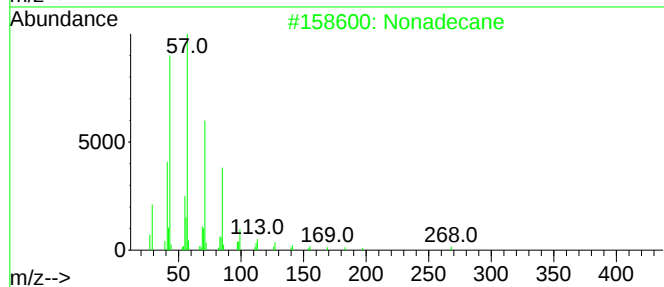
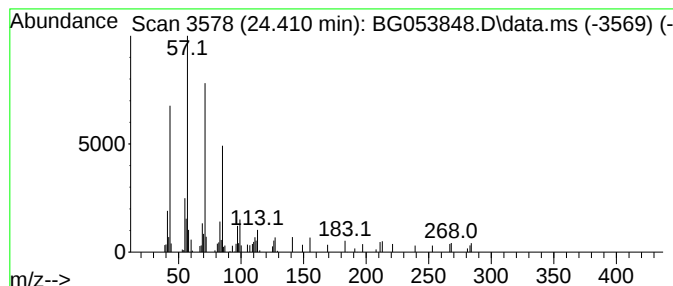
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Nonadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.410	5.21 ng	128504	Perylene-d12	24.992

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Nonadecane	268	C19H40	000629-92-5	93
2		Triacontane	422	C30H62	000638-68-6	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060822\
Data File : BG053848.D
Acq On : 8 Jun 2022 11:41
Operator : CG/JU
Sample : N3194-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-3

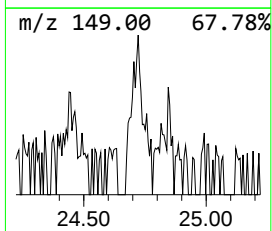
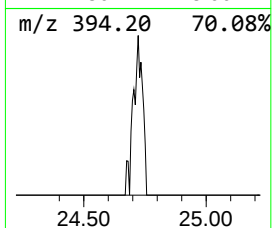
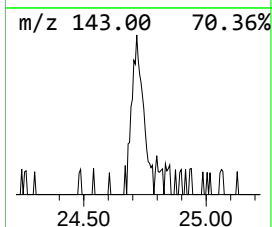
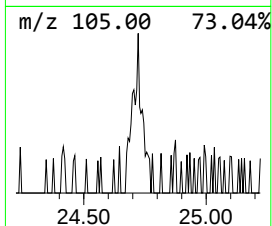
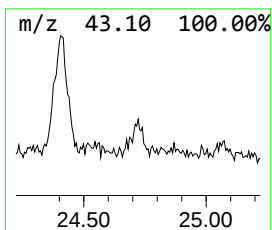
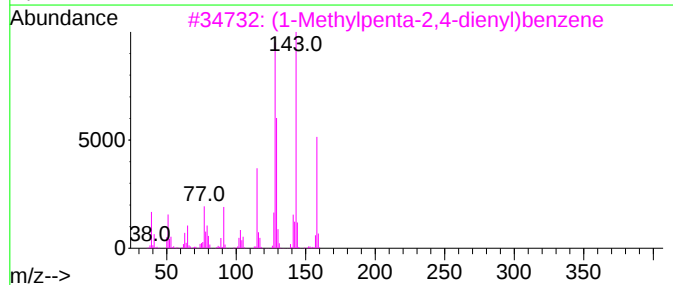
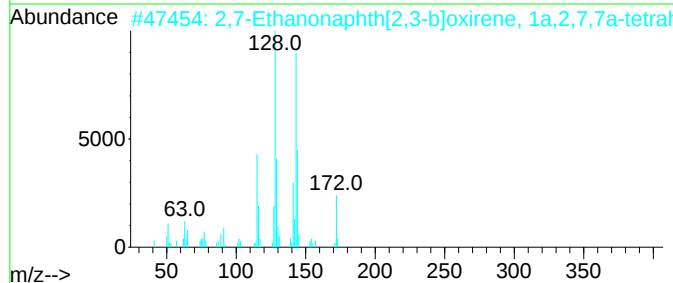
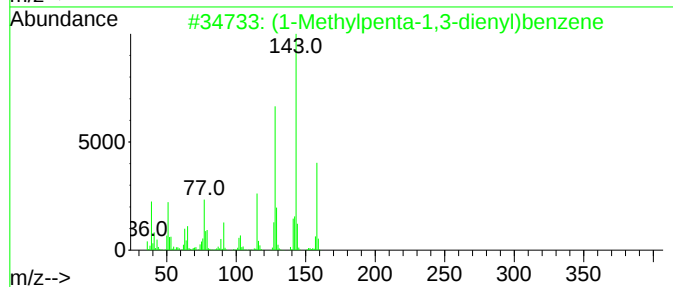
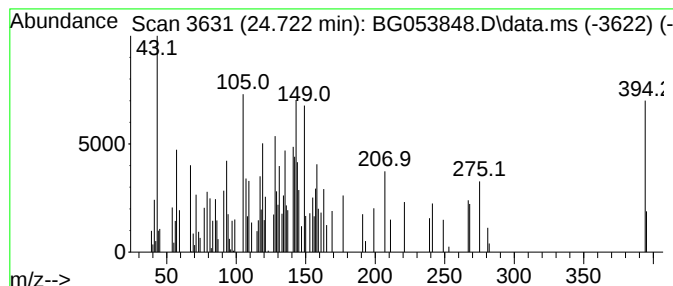
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown24.722 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.722	3.70 ng	91328	Perylene-d12	24.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1-Methylpenta-1,3-dienyl)benzene	158	C12H14	116669-49-9	14
2			2,7-Ethanonaphth[2,3-b]oxirene, ...	172	C12H12O	054515-76-3	14
3			(1-Methylpenta-2,4-dienyl)benzene	158	C12H14	1000210-01-1	10
4			Cyclohexane, 1,2,2,3-tetramethyl...	158	C7H18N2Si	036972-04-0	10
5			Pimelic acid, 4-chloro-2-methylp...	368	C20H29ClO4	1000420-05-9	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060822\
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Sample : N3194-04
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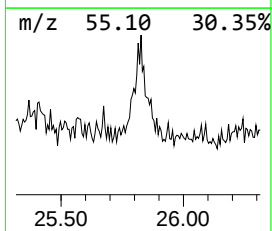
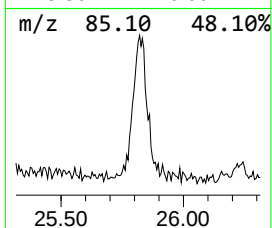
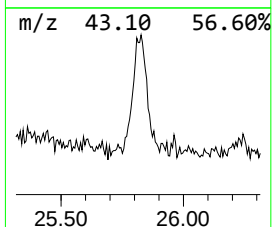
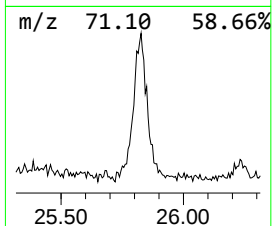
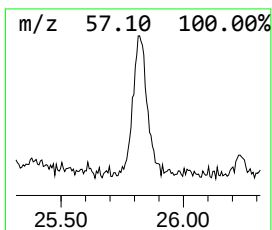
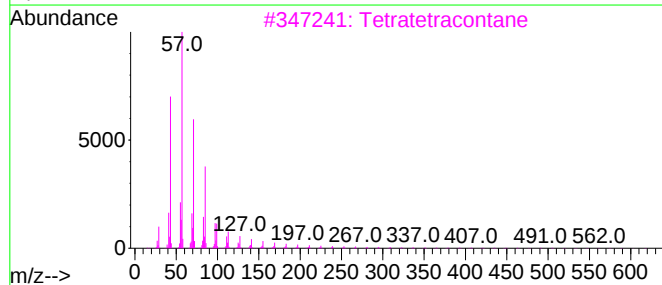
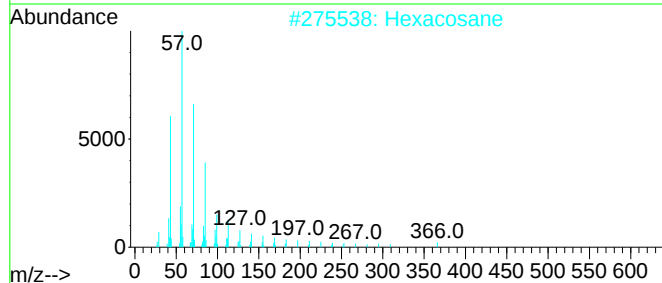
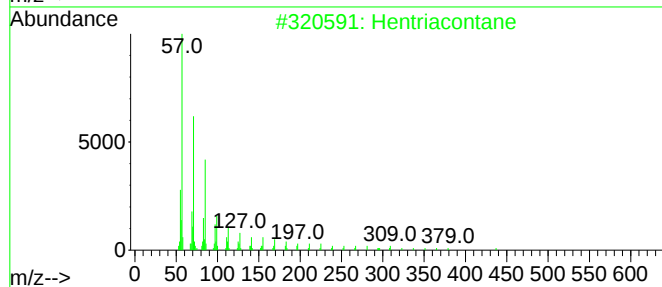
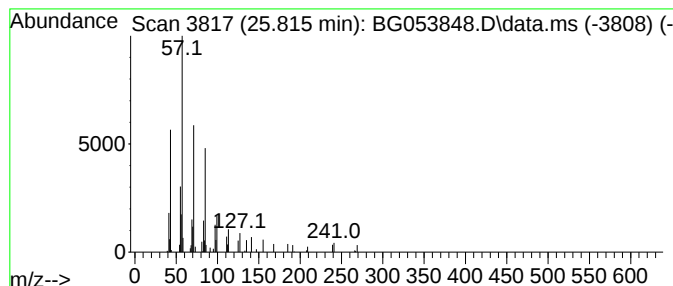
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TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Hentriacontane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
25.815	2.00 ng	49473	Perylene-d12	24.992	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Tetratetracontane	619	C44H90	007098-22-8	87
4	Pentacosane	352	C25H52	000629-99-2	87
5	Octacosane	394	C28H58	000630-02-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060822\
Data File : BG053848.D
Acq On : 8 Jun 2022 11:41
Operator : CG/JU
Sample : N3194-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-3

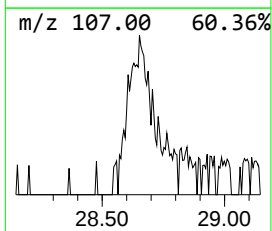
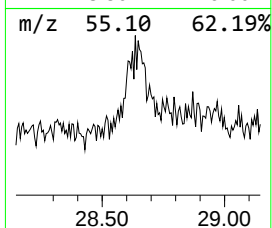
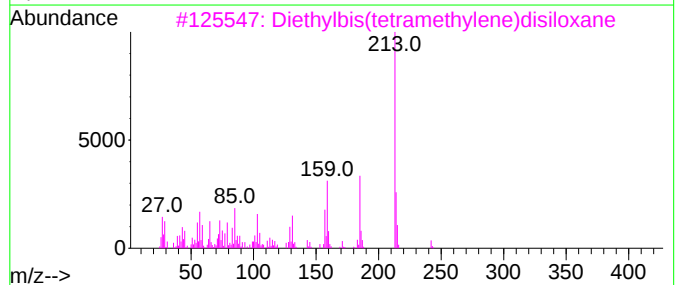
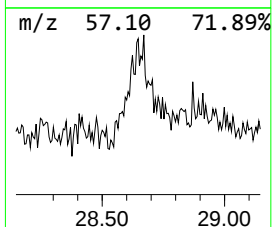
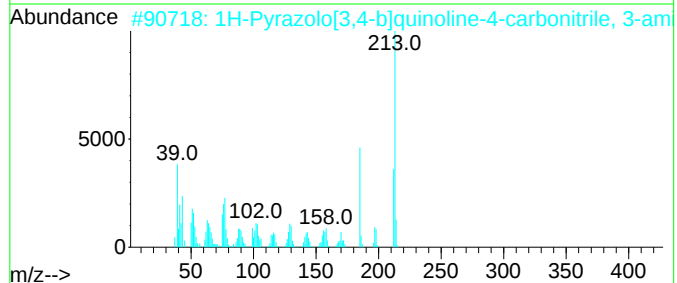
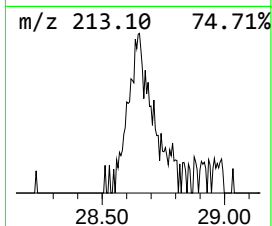
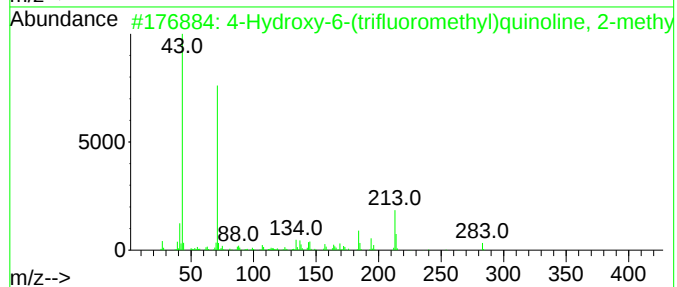
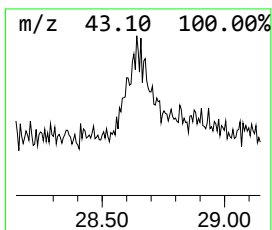
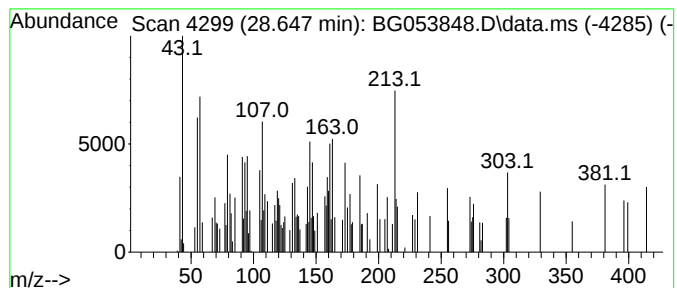
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown28.647 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.647	4.76 ng	117407	Perylene-d12	24.992

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Hydroxy-6-(trifluoromethyl)qui...	283	C14H12F3NO2	1000463-38-0	22
2			1H-Pyrazolo[3,4-b]quinoline-4-ca...	213	C11H11N5	1000351-24-9	22
3			Diethylbis(tetramethylene)disilo...	242	C12H26OSi2	018035-51-3	22
4			4-(1-Adamantyl)pyridine	213	C15H19N	060159-38-8	22
5			3-Chloro-4-fluoro-5-(trifluorome...	213	C7H4ClF4N	914225-61-9	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060822\
Data File : BG053848.D
Acq On : 8 Jun 2022 11:41
Operator : CG/JU
Sample : N3194-04
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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
2-Pentanone, 4-...	5.192	3.0	ng	19450	1	8.094	131636	20.0
Tridecanoic acid	18.265	2.3	ng	43564	4	17.454	387090	20.0
n-Hexadecanoic ...	18.341	23.1	ng	447195	4	17.454	387090	20.0
Octadecanoic acid	19.610	29.8	ng	813487	5	21.725	546299	20.0
Eicosane	20.509	3.3	ng	89612	5	21.725	546299	20.0
Hexacosane	21.291	3.7	ng	101392	5	21.725	546299	20.0
Heptadecyl hept...	21.373	3.3	ng	89675	5	21.725	546299	20.0
Octacosane, 2-m...	22.178	4.9	ng	133116	5	21.725	546299	20.0
Heneicosane	23.200	4.5	ng	123305	5	21.725	546299	20.0
Nonadecane	24.410	5.2	ng	128504	6	24.992	493635	20.0
unknown24.722	24.722	3.7	ng	91328	6	24.992	493635	20.0
Hentriacontane	25.815	2.0	ng	49473	6	24.992	493635	20.0
unknown28.647	28.647	4.8	ng	117407	6	24.992	493635	20.0