

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
 Data File : BG058565.D
 Acq On : 1 Aug 2023 16:42
 Operator : MA/JU
 Sample : 03715-13
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FIELD-BLANK

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-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058565.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.386	384	391	403	rBV	645429	1030670	44.30%	5.112%
2	6.984	654	663	681	rBV	614339	1095318	47.08%	5.432%
3	7.812	797	804	811	rBV	226987	378592	16.27%	1.878%
4	8.976	990	1002	1016	rBV	374809	669998	28.80%	3.323%
5	10.615	1273	1281	1294	rBV	312471	565399	24.30%	2.804%
6	13.082	1694	1701	1713	rBV	997625	1571298	67.54%	7.793%
7	13.917	1837	1843	1850	rBV	64008	94611	4.07%	0.469%
8	14.099	1869	1874	1897	rBV	103209	272399	11.71%	1.351%
9	14.463	1929	1936	1947	rVB	488986	777006	33.40%	3.854%
10	14.886	2004	2008	2016	rBV3	16956	37202	1.60%	0.185%
11	15.820	2159	2167	2180	rBV	579923	828320	35.60%	4.108%
12	15.950	2182	2189	2197	rBV	769727	1214866	52.22%	6.025%
13	17.207	2397	2403	2410	rBV	609938	907041	38.99%	4.498%
14	18.100	2549	2555	2570	rBV	435540	698180	30.01%	3.463%
15	19.258	2750	2752	2762	rVB7	16596	34258	1.47%	0.170%
16	19.375	2767	2772	2792	rBV	231750	403978	17.36%	2.004%
17	19.634	2813	2816	2822	rVB2	25994	32373	1.39%	0.161%
18	19.733	2824	2833	2838	rBV4	32358	113798	4.89%	0.564%
19	19.827	2843	2849	2863	rVB	1730608	2326606	100.00%	11.539%
20	20.127	2896	2900	2906	rBV	64620	75041	3.23%	0.372%
21	20.621	2979	2984	2988	rBV	95357	111611	4.80%	0.554%
22	21.102	3062	3066	3070	rBV	105666	151086	6.49%	0.749%
23	21.332	3102	3105	3110	rVB	23019	29970	1.29%	0.149%
24	21.449	3118	3125	3134	rBV2	604905	947335	40.72%	4.698%
25	21.625	3150	3155	3160	rVB	95126	128432	5.52%	0.637%
26	22.201	3247	3253	3258	rBV	85193	136187	5.85%	0.675%
27	22.560	3310	3314	3318	rBV3	16397	24550	1.06%	0.122%
28	22.853	3358	3364	3375	rVB2	85279	174978	7.52%	0.868%
29	23.035	3389	3395	3403	rVB	72195	137461	5.91%	0.682%
30	23.611	3487	3493	3501	rVB	64273	132491	5.69%	0.657%
31	24.522	3637	3648	3666	rBV	412472	1173163	50.42%	5.818%
32	25.151	3744	3755	3766	rBV	545768	1549056	66.58%	7.683%
33	25.562	3820	3825	3833	rVB3	37286	96830	4.16%	0.480%
34	26.637	3996	4008	4009	rBV3	28769	77865	3.35%	0.386%
35	26.831	4036	4041	4050	rVB8	22642	68334	2.94%	0.339%
36	31.120	4752	4771	4794	rVB3	386861	2096930	90.13%	10.400%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

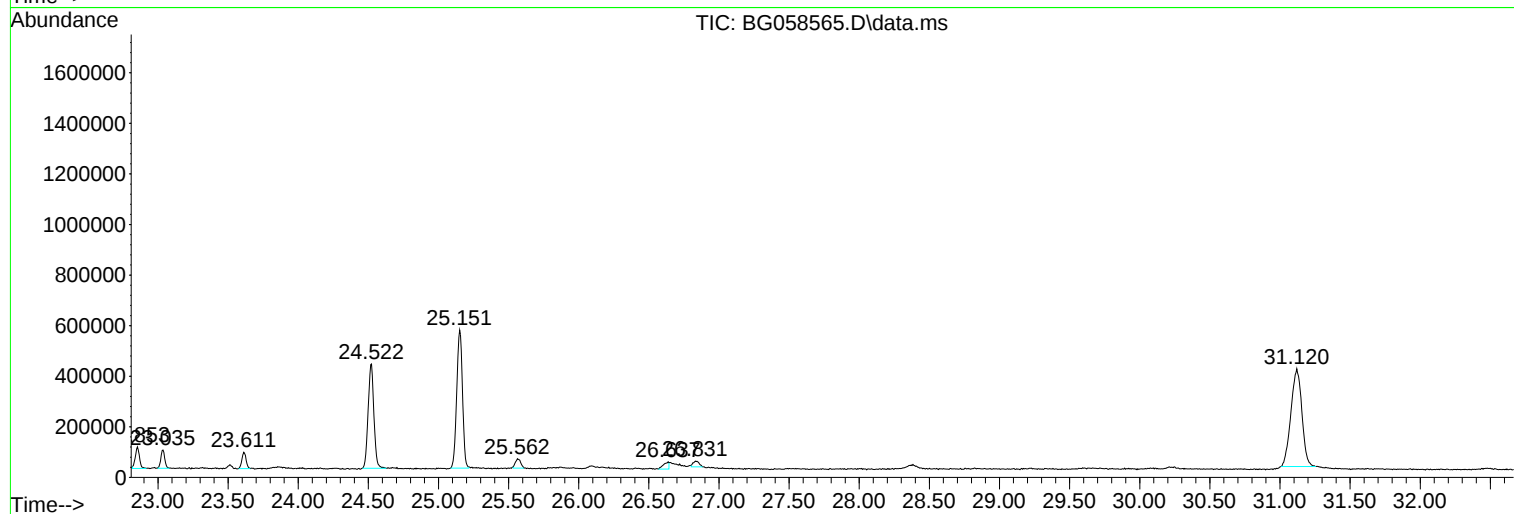
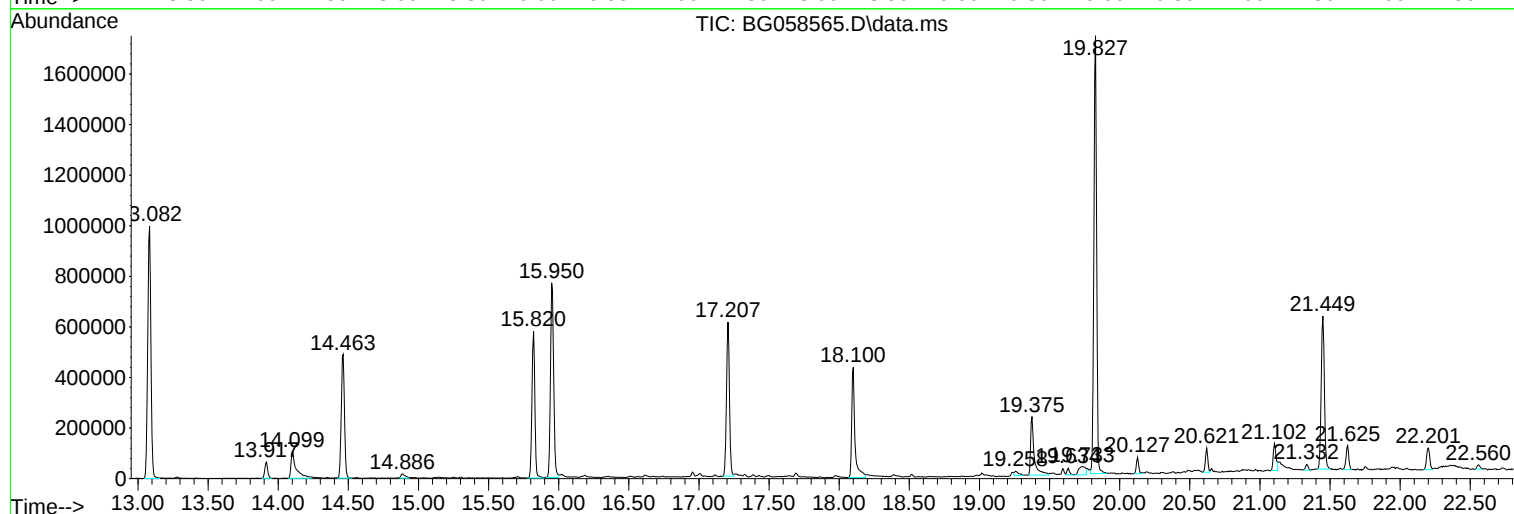
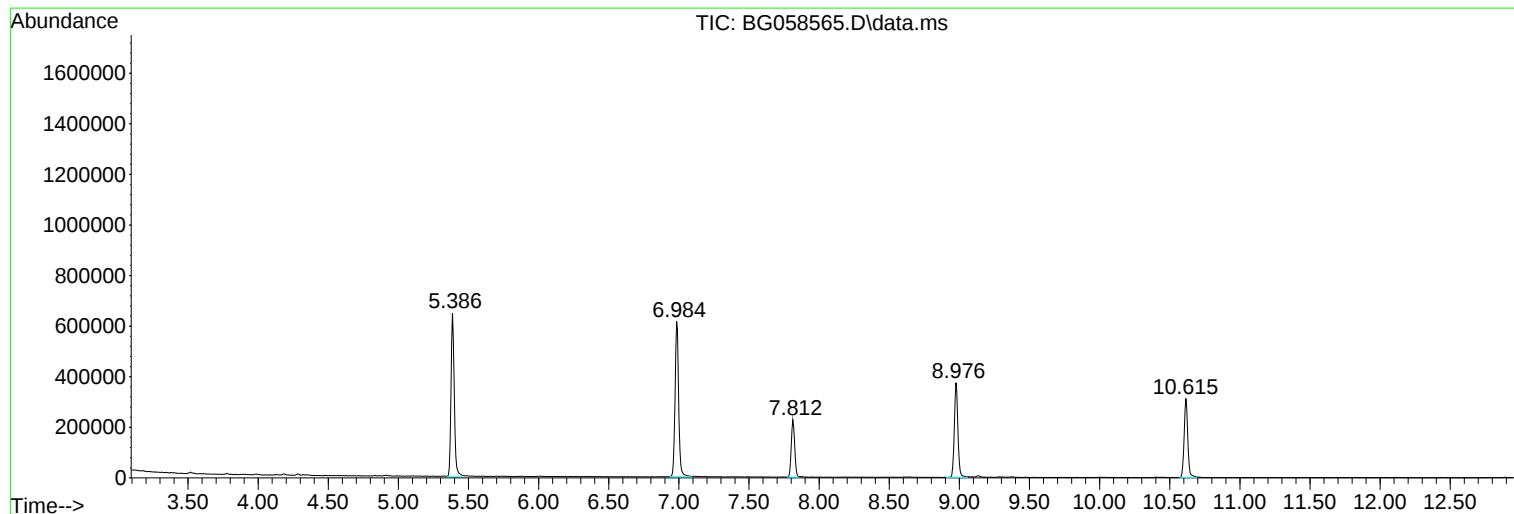
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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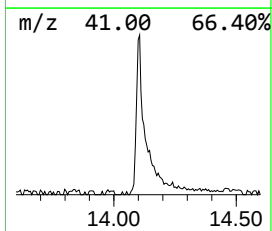
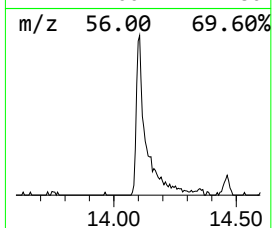
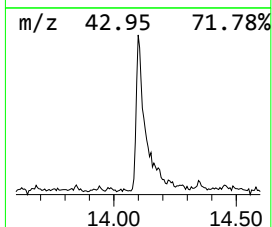
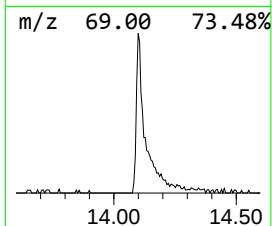
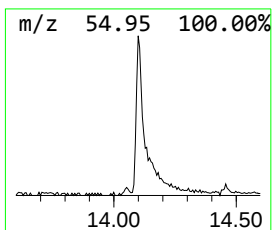
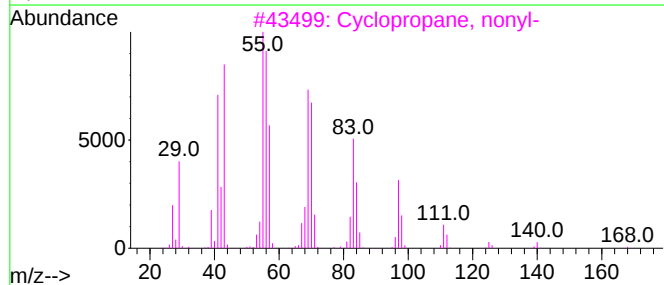
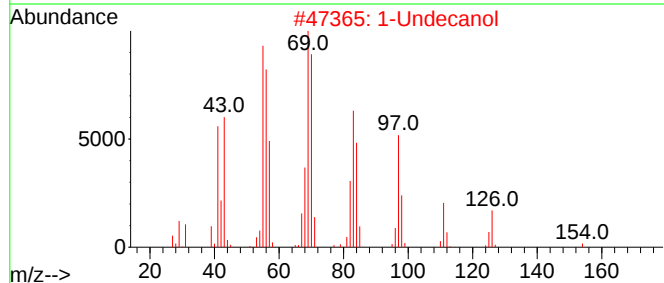
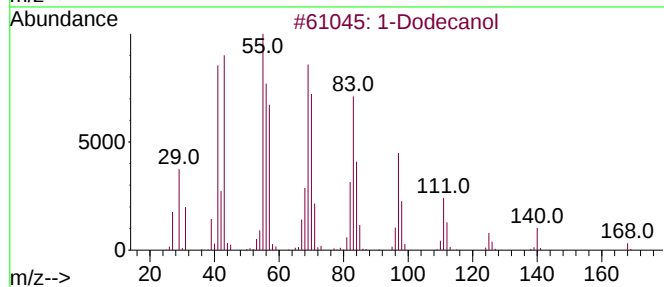
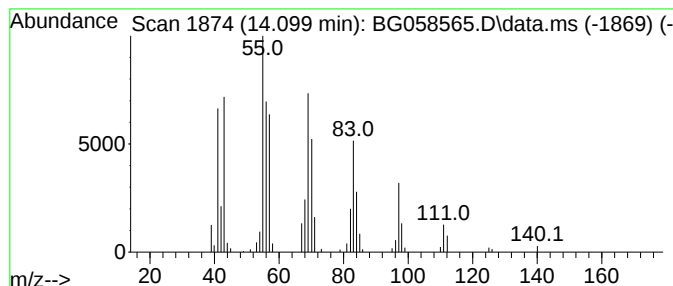
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Dodecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.099	7.01 ng	272399	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol			186	C12H26O	000112-53-8	91
2	1-Undecanol			172	C11H24O	000112-42-5	91
3	Cyclopropane, nonyl-			168	C12H24	074663-85-7	87
4	Cyclooctane, methyl-			126	C9H18	001502-38-1	78
5	Cyclopropane, 1-methyl-2-octyl-			168	C12H24	037617-26-8	72



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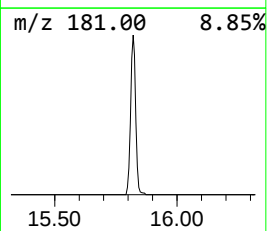
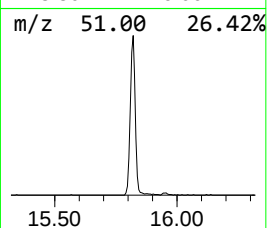
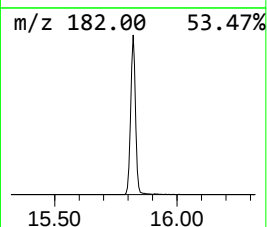
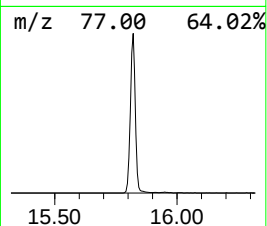
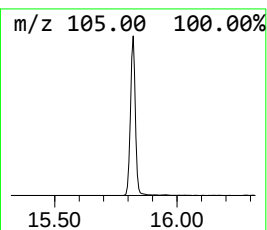
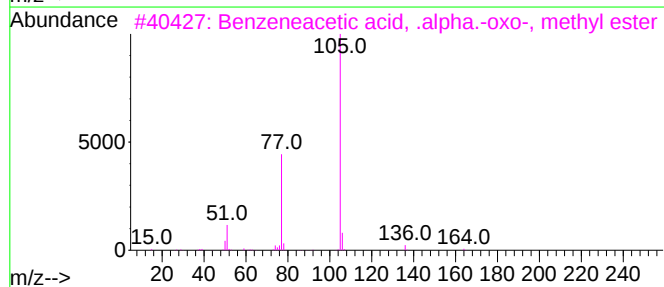
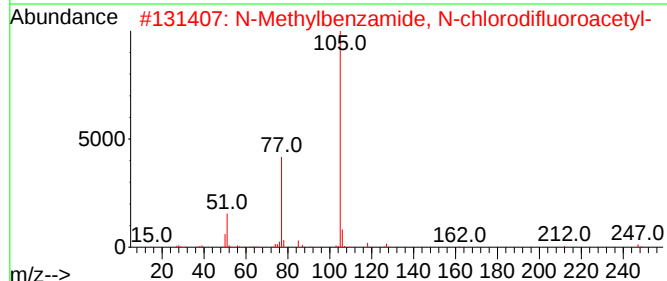
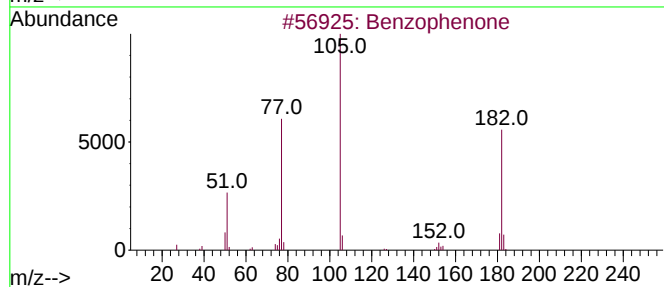
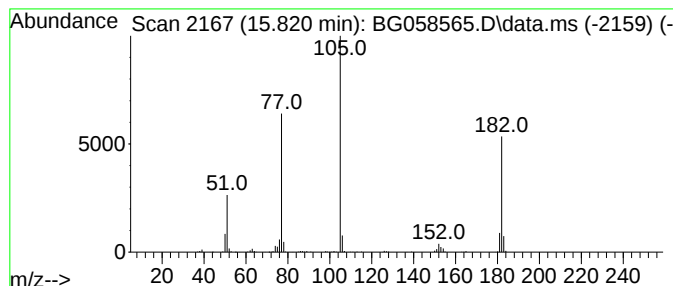
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.820	21.32 ng	828320	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			N-Methylbenzamide, N-chlorodiflu...	247	C10H8ClF2NO2	1000446-98-2	47
3			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
4			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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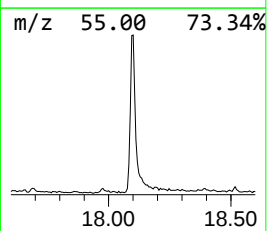
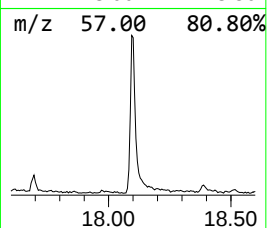
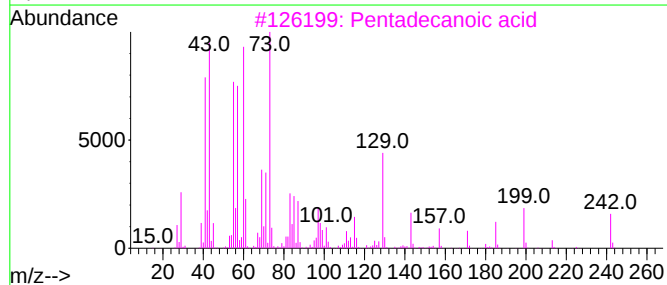
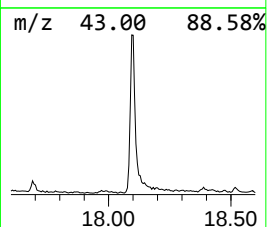
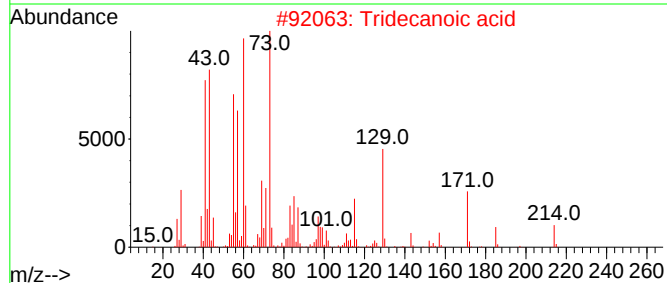
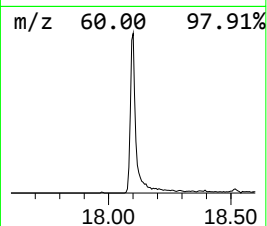
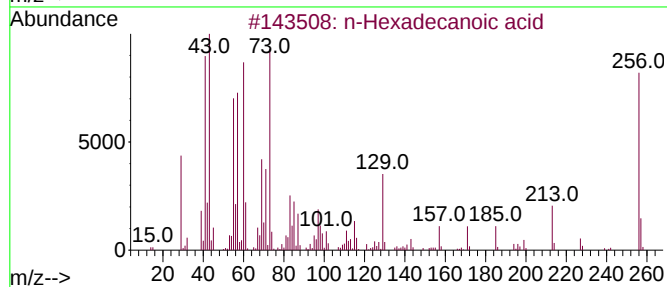
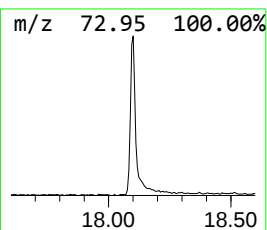
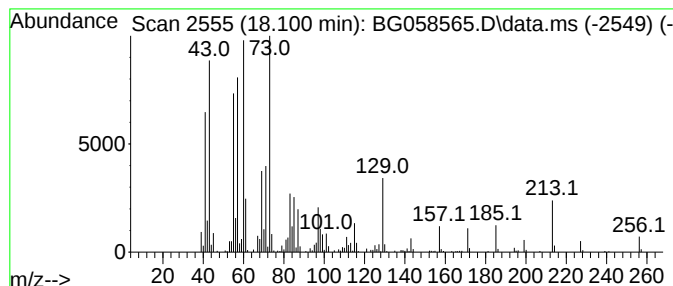
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.100	15.39 ng	698180	Phenanthrene-d10	17.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



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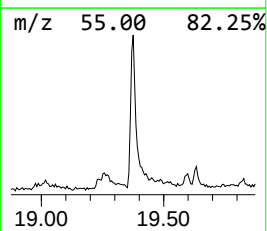
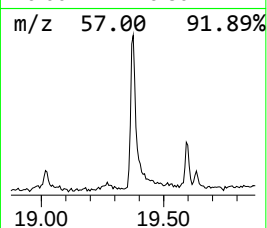
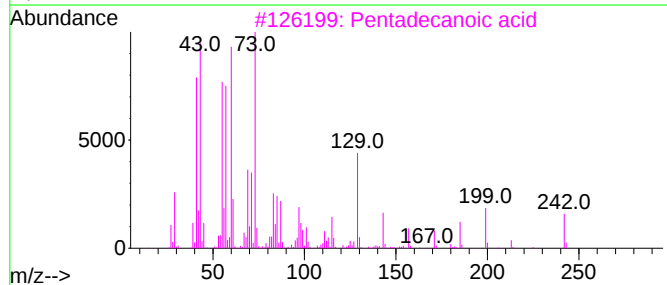
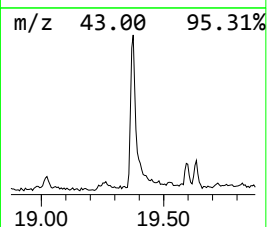
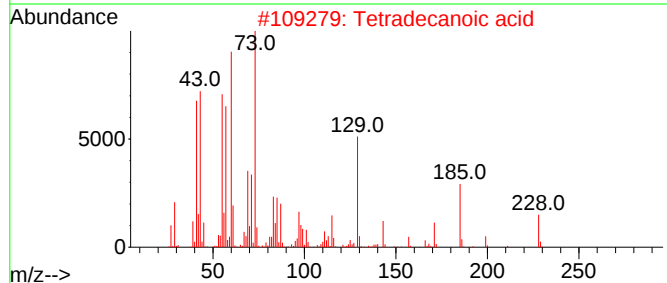
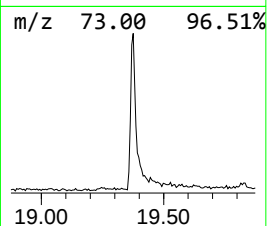
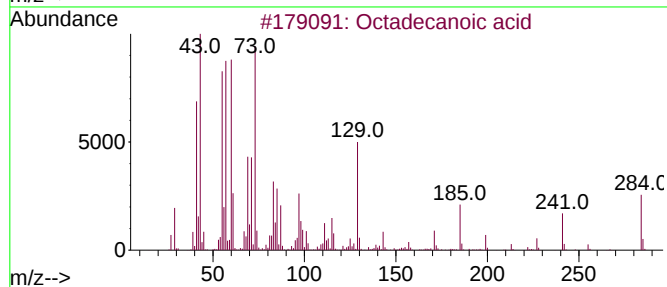
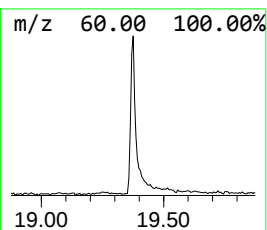
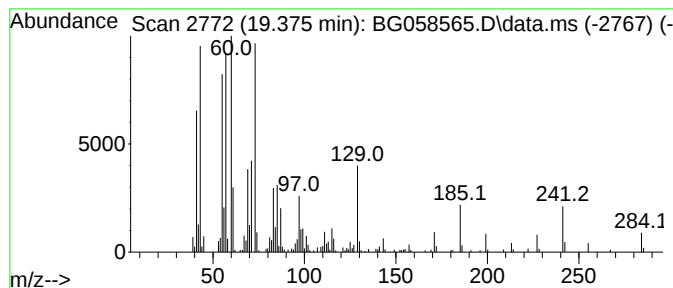
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.375	8.53 ng	403978	Chrysene-d12	21.449

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Undecanoic acid	186	C11H22O2	000112-37-8	62
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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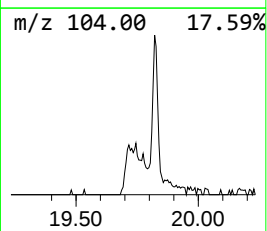
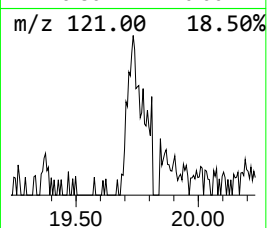
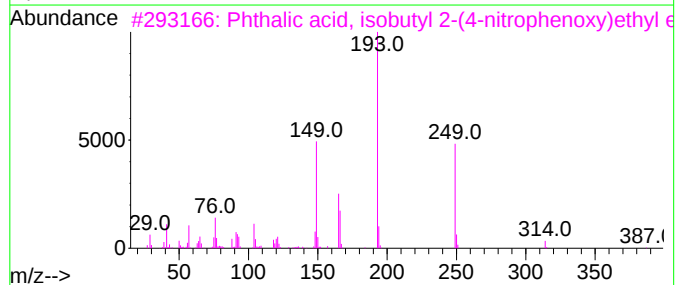
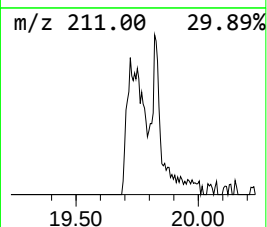
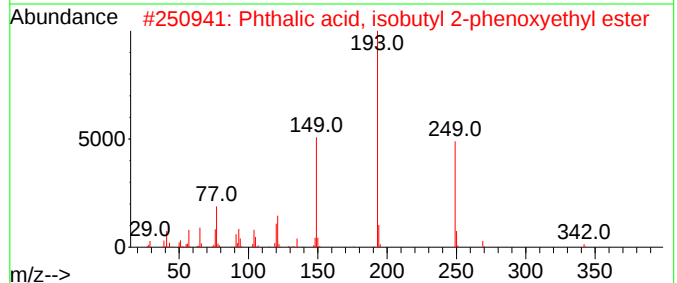
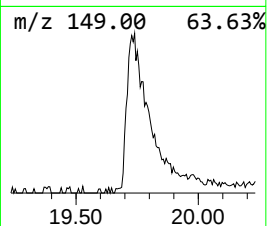
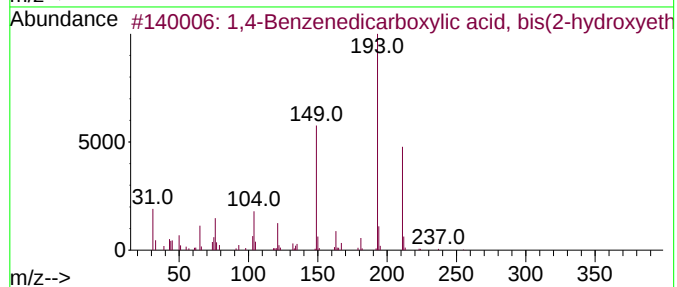
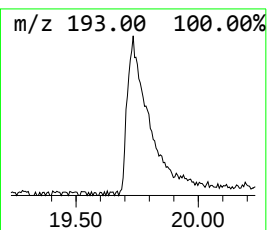
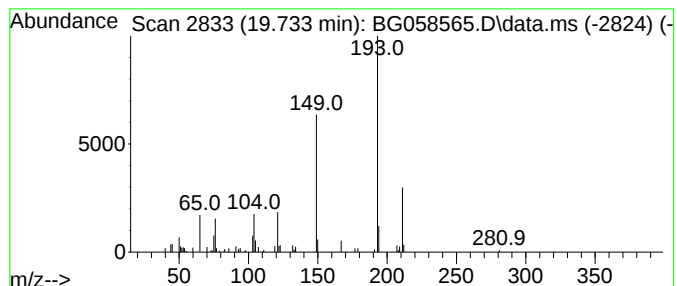
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TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.733	2.40 ng	113798	Chrysene-d12	21.449

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	254	C12H14O6	000959-26-2	83
2			Phthalic acid, isobutyl 2-phenox...	342	C20H22O5	1000382-47-9	72
3			Phthalic acid, isobutyl 2-(4-nit...	387	C20H21NO7	1000382-57-3	64
4			2,4,6-Trimethoxybenzonitrile	193	C10H11NO3	002571-54-2	47
5			2,1-benzisoxazole-4-carboxylic a...	193	C9H7NO4	1000395-98-5	43



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Acq On : 1 Aug 2023 16:42
Operator : MA/JU
Sample : 03715-13
Misc :
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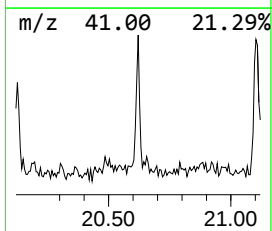
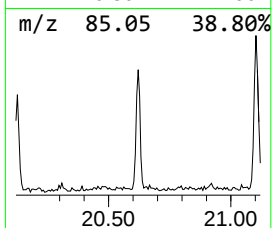
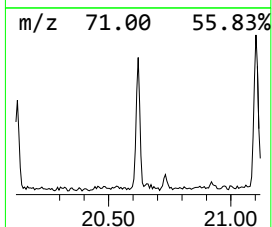
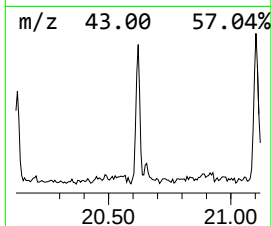
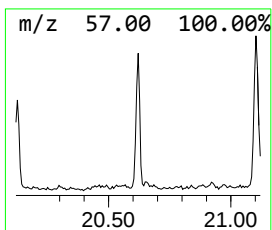
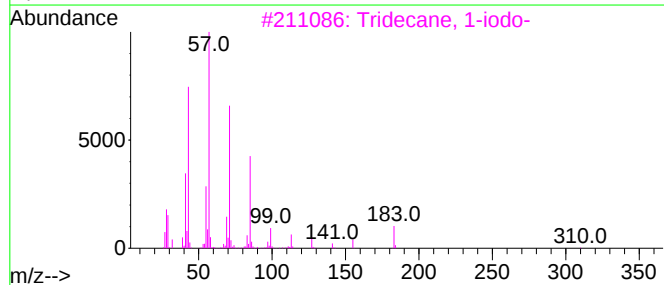
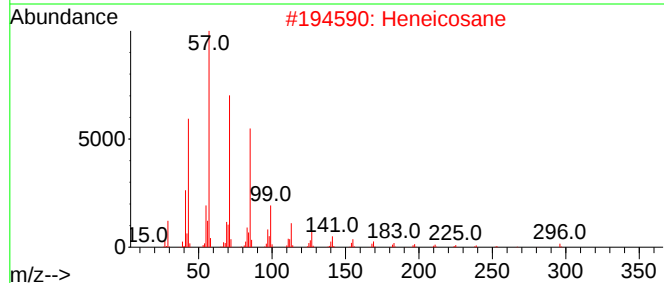
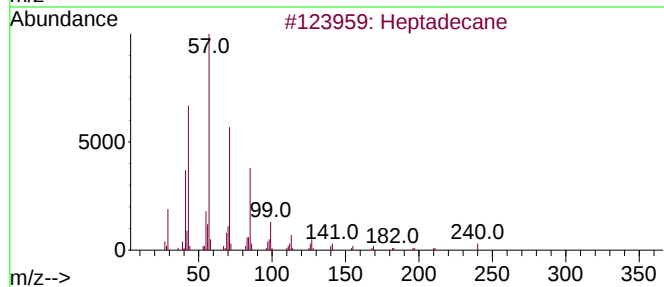
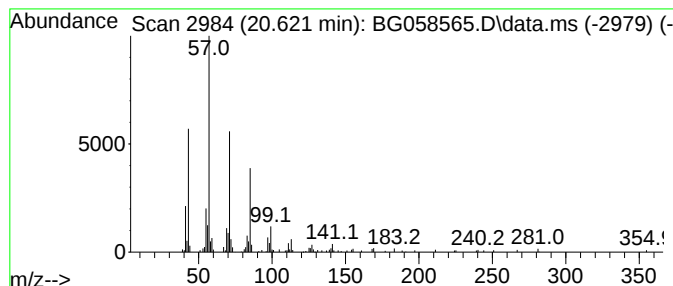
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.621	2.36 ng	111611	Chrysene-d12	21.449

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane	240	C17H36	000629-78-7	93
2		Heneicosane	296	C21H44	000629-94-7	90
3		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	86
4		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
5		Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058565.D
Acq On : 1 Aug 2023 16:42
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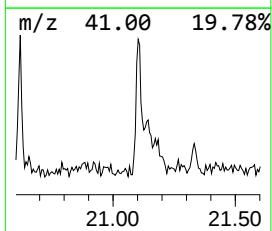
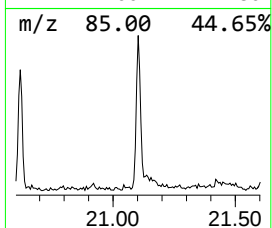
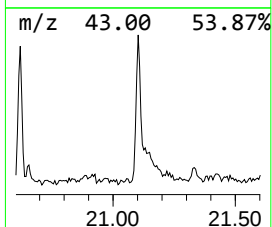
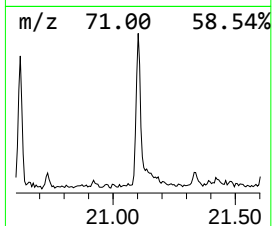
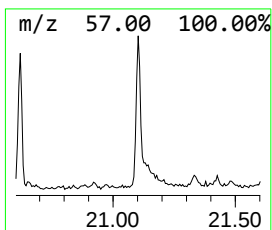
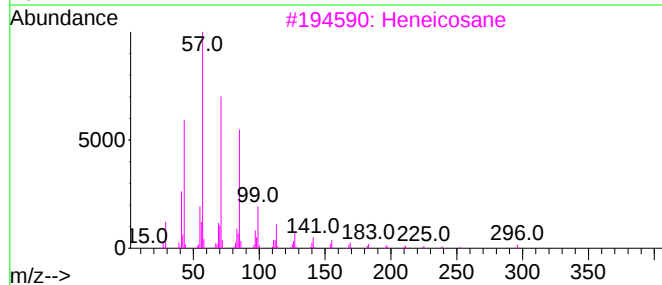
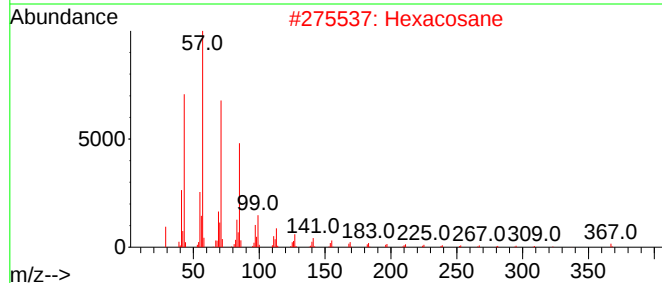
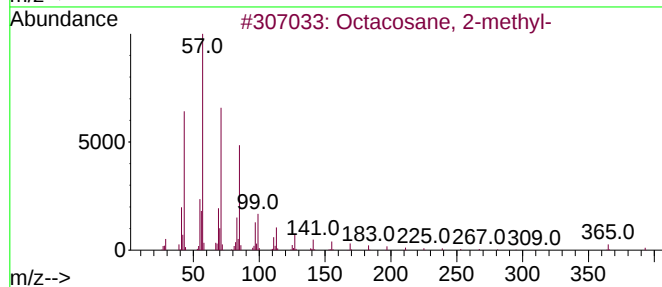
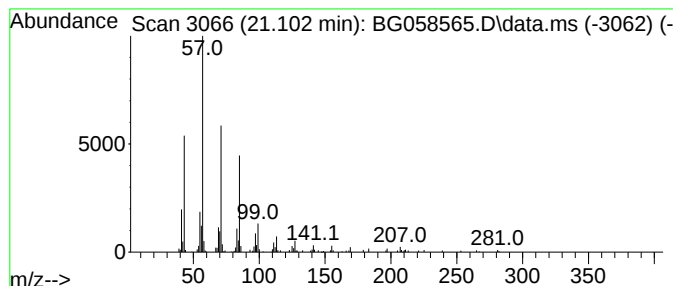
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octacosane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.102	3.19 ng	151086	Chrysene-d12	21.449

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2			Hexacosane	366	C26H54	000630-01-3	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Tetratetracontane	619	C44H90	007098-22-8	87
5			Heptacosane	380	C27H56	000593-49-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058565.D
Acq On : 1 Aug 2023 16:42
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Sample : 03715-13
Misc :
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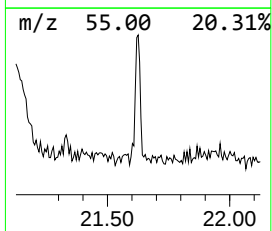
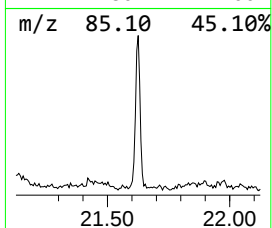
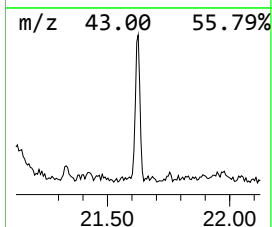
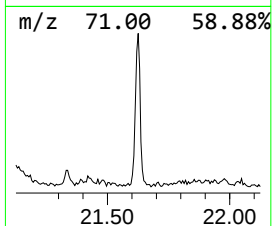
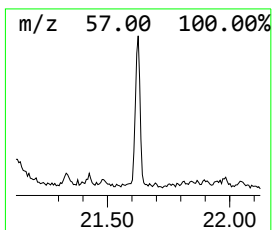
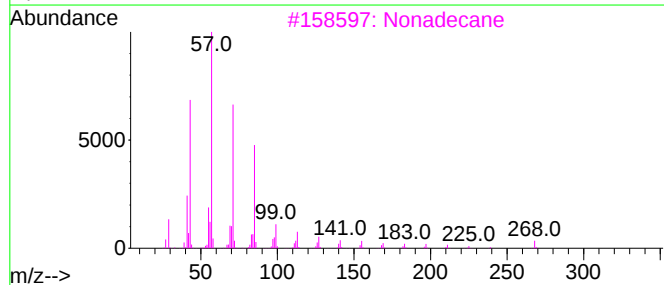
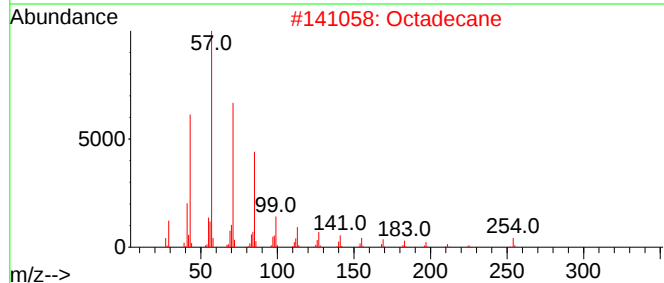
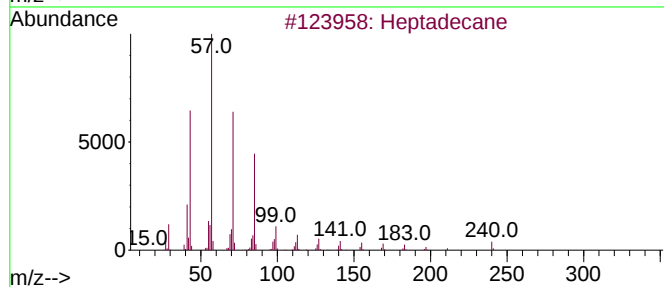
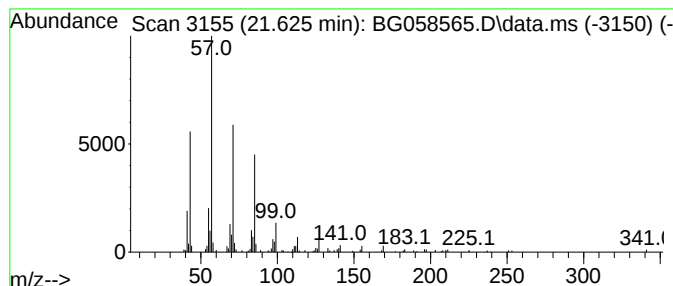
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.625	2.71 ng	128432	Chrysene-d12	21.449

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	91
2			Octadecane	254	C18H38	000593-45-3	91
3			Nonadecane	268	C19H40	000629-92-5	91
4			Pentacosane	352	C25H52	000629-99-2	90
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058565.D
Acq On : 1 Aug 2023 16:42
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Sample : 03715-13
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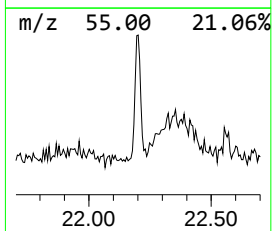
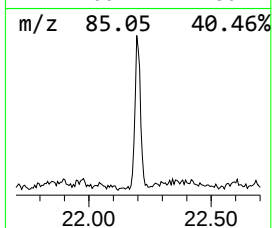
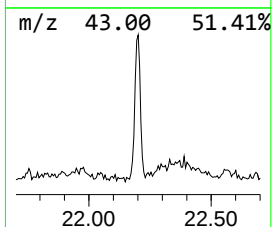
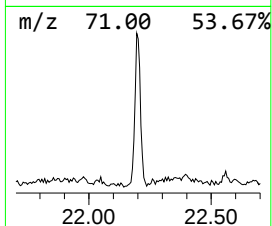
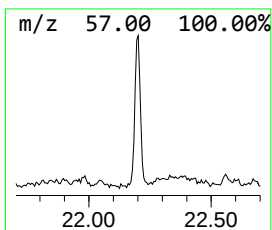
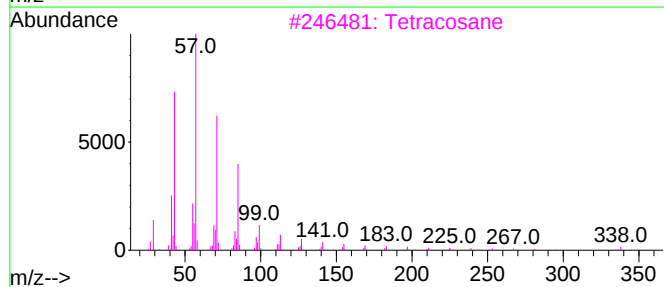
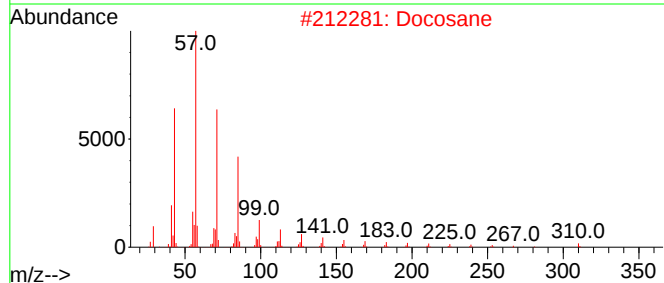
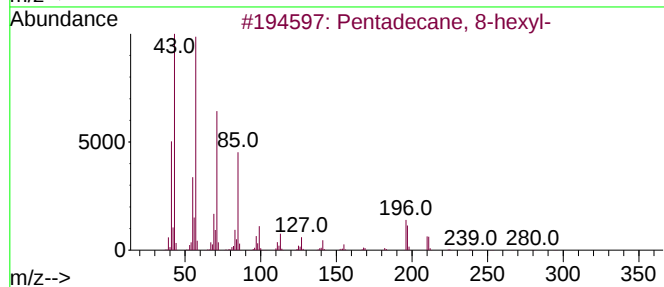
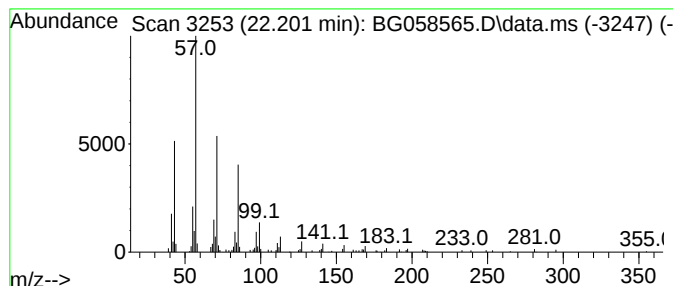
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecane, 8-hexyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.201	2.88 ng	136187	Chrysene-d12	21.449

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
2			Docosane	310	C22H46	000629-97-0	87
3			Tetracosane	338	C24H50	000646-31-1	87
4			Hexacosane	366	C26H54	000630-01-3	87
5			Eicosane	282	C20H42	000112-95-8	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058565.D
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Operator : MA/JU
Sample : 03715-13
Misc :
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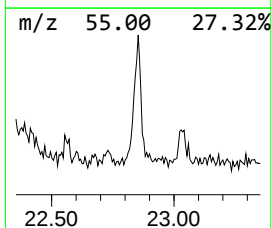
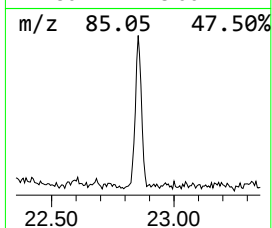
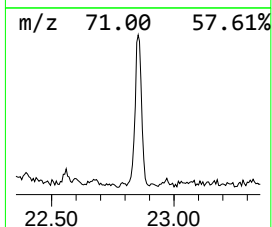
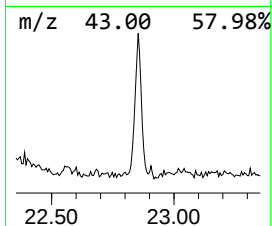
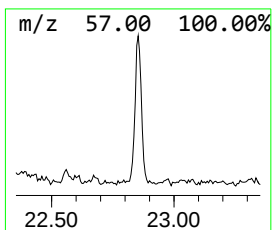
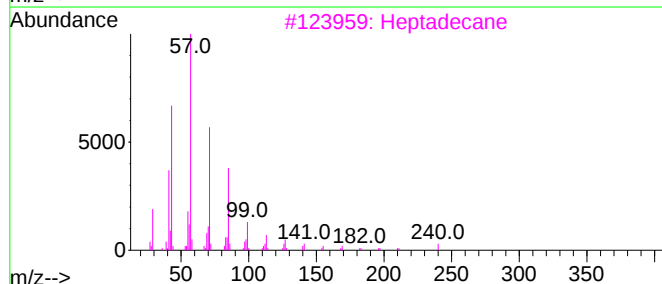
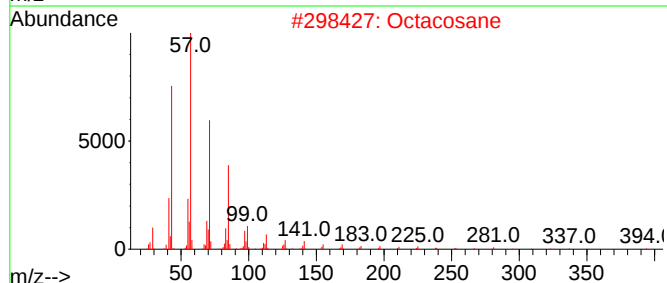
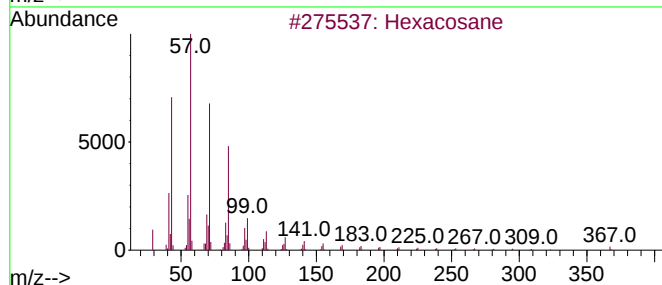
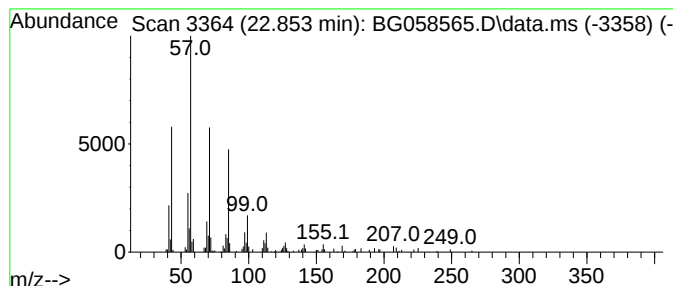
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.853	3.69 ng	174978	Chrysene-d12	21.449	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	87
3	Heptadecane	240	C17H36	000629-78-7	86
4	Octadecane	254	C18H38	000593-45-3	83
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
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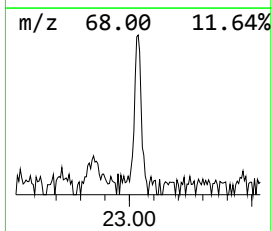
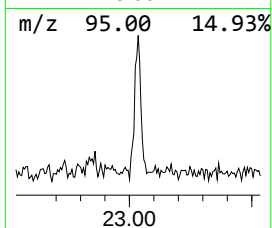
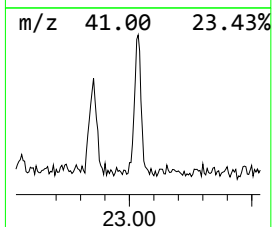
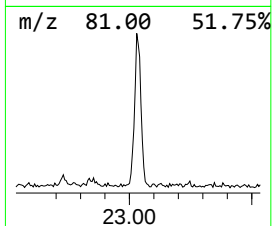
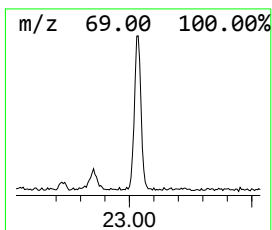
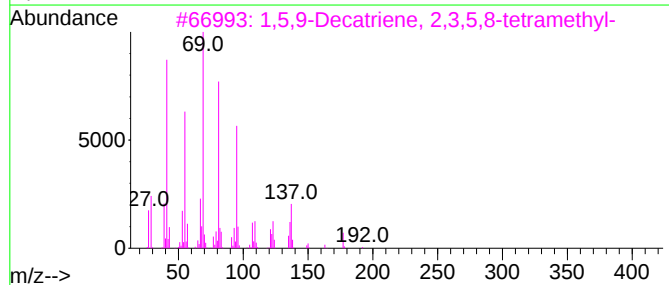
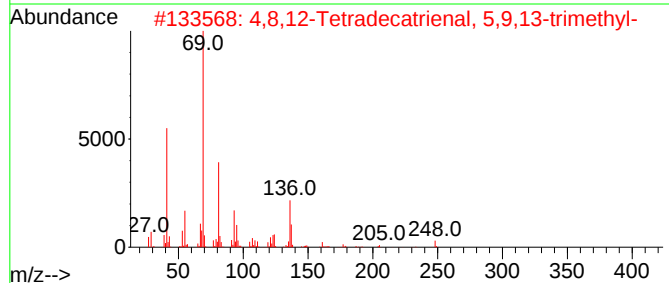
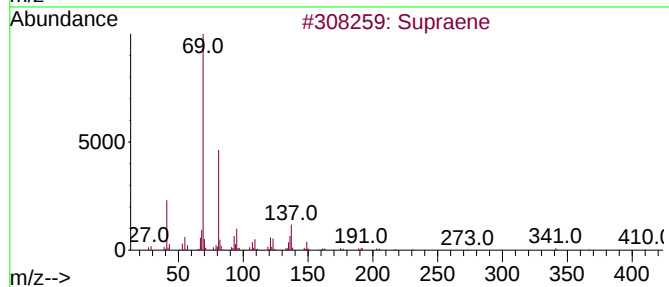
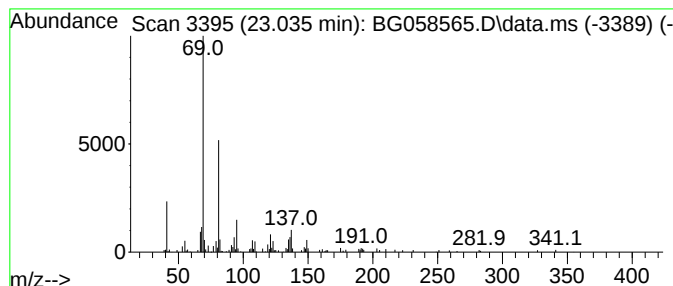
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Supraene Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.035	2.34 ng	137461	Perylene-d12	24.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
3			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	64
4			Farnesol isomer a	222	C15H26O	1000108-92-4	64
5			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058565.D
Acq On : 1 Aug 2023 16:42
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Sample : 03715-13
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ALS Vial : 14 Sample Multiplier: 1

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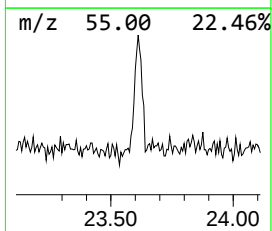
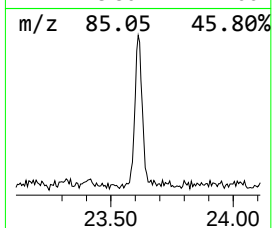
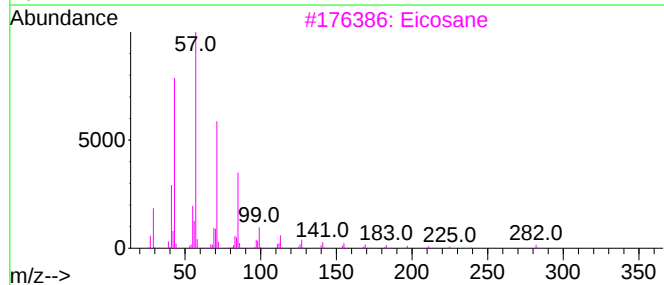
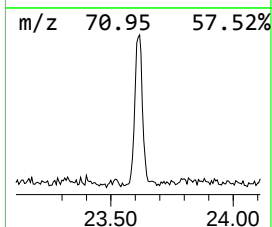
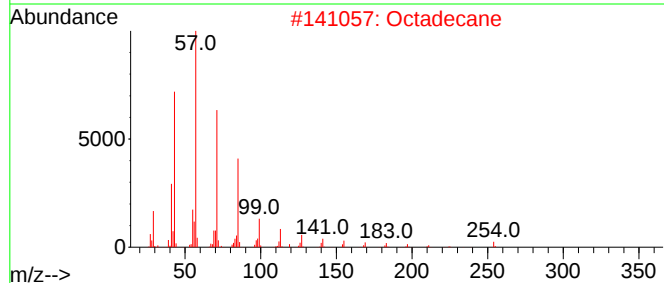
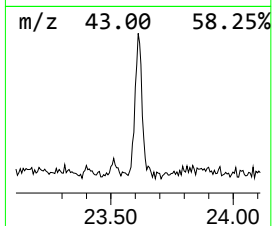
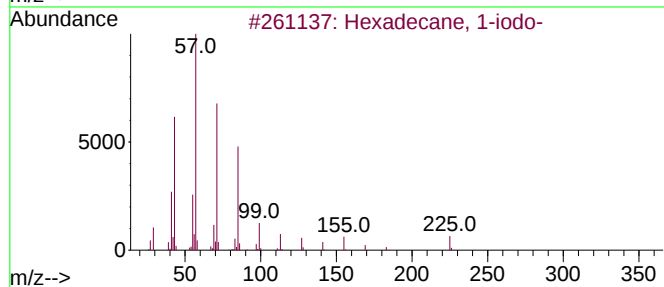
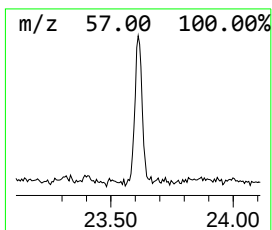
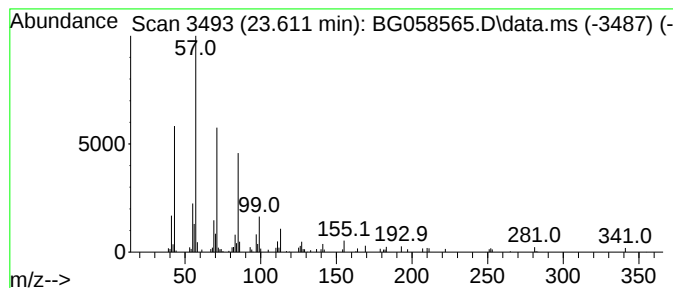
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexadecane, 1-iodo- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.611	2.26 ng	132491	Perylene-d12	24.522

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87	
2	Octadecane	254	C18H38	000593-45-3	87	
3	Eicosane	282	C20H42	000112-95-8	86	
4	Docosane	310	C22H46	000629-97-0	86	
5	Octacosane	394	C28H58	000630-02-4	86	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058565.D
Acq On : 1 Aug 2023 16:42
Operator : MA/JU
Sample : 03715-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

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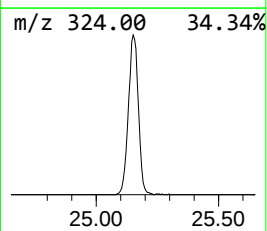
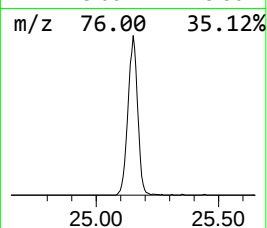
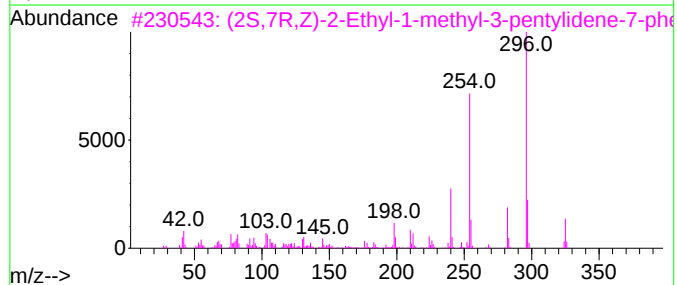
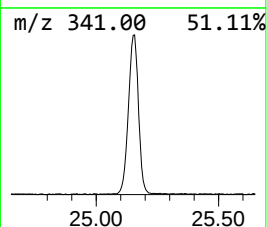
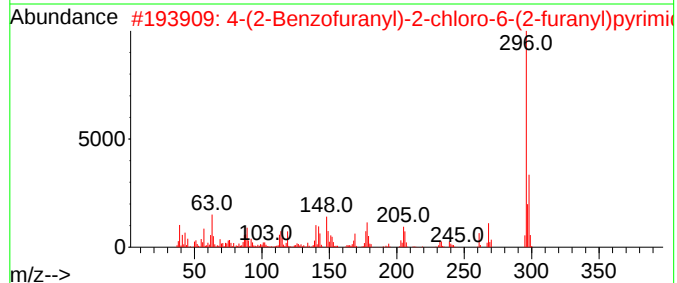
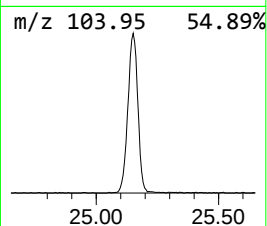
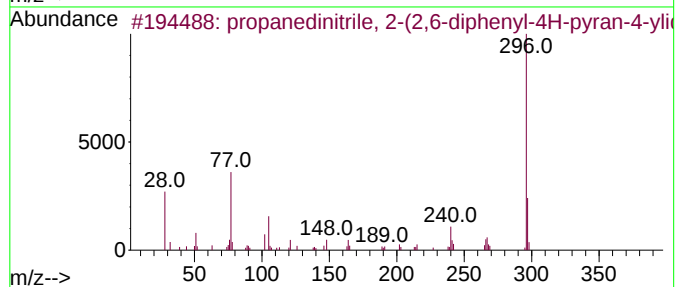
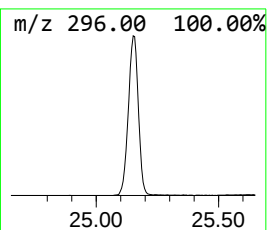
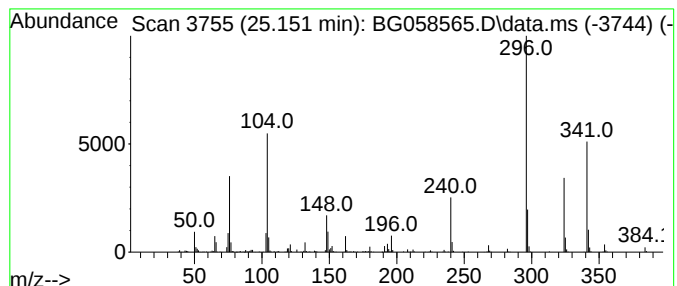
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown25.151 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.151	26.41 ng	1549060	Perylene-d12	24.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			propanedinitrile, 2-(2,6-dipheny...	296	C20H12N2O	1000402-09-2	27
2			4-(2-Benzofuranyl)-2-chloro-6-(2...	296	C16H9ClN2O2	131022-75-8	27
3			(2S,7R,Z)-2-Ethyl-1-methyl-3-pen...	325	C20H27N3O	1000482-33-2	25
4			1-Methyl-2,4,6-tris(cyclopentyl)...	296	C22H32	100325-74-4	22
5			2-(2-Quinolyl)(1,2,4)triazolo(1...	296	C19H12N4	1000241-15-8	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058565.D
Acq On : 1 Aug 2023 16:42
Operator : MA/JU
Sample : 03715-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FIELD-BLANK

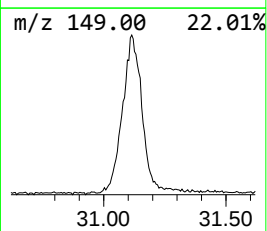
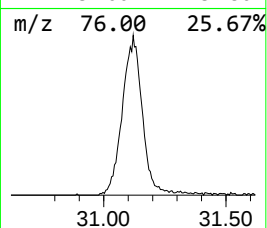
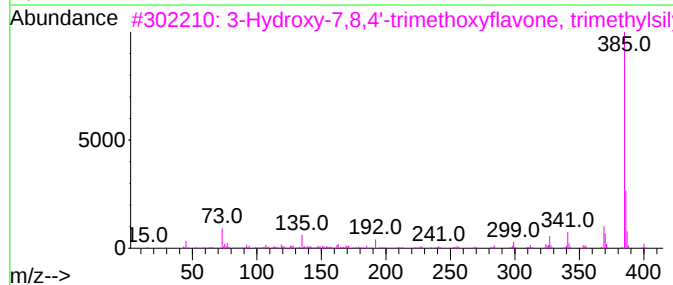
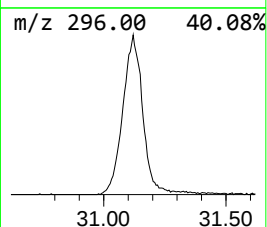
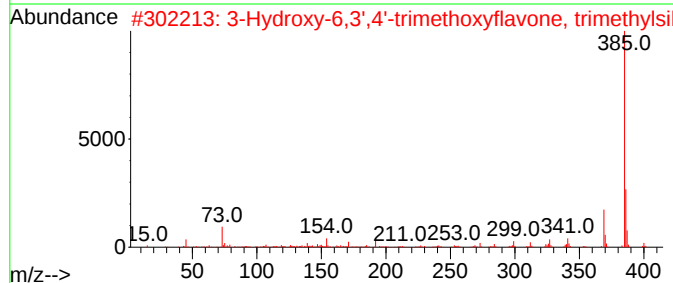
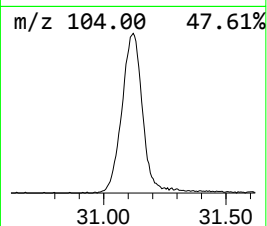
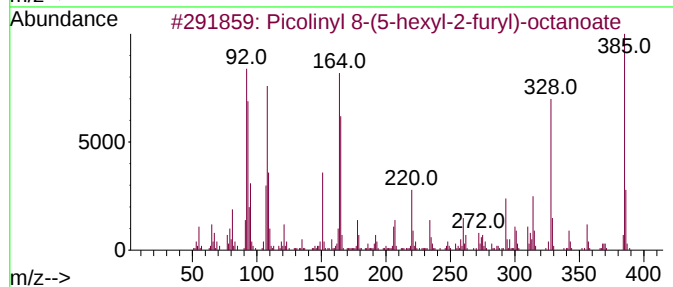
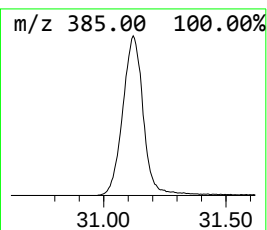
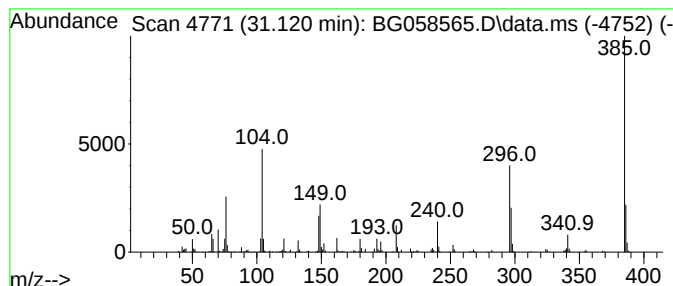
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown31.120 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
31.120	35.75 ng	2096930	Perylene-d12	24.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Picolinyl 8-(5-hexyl-2-furyl)-oc...	385	C24H35NO3	1000335-93-0	25
2			3-Hydroxy-6,3',4'-trimethoxyflav...	400	C21H24O6Si	1000448-94-7	22
3			3-Hydroxy-7,8,4'-trimethoxyflavo...	400	C21H24O6Si	1000454-18-7	12
4			2,3-Dibenzyl-5,8-dimethoxy-6-am...	385	C24H23N3O2	056393-28-3	12
5			3-Hydroxy-7,8,2'-trimethoxyflavo...	400	C21H24O6Si	1000454-19-8	10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058565.D
Acq On : 1 Aug 2023 16:42
Operator : MA/JU
Sample : 03715-13
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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
1-Dodecanol	14.099	7.0	ng	272399	3	14.463	777006	20.0
Benzophenone	15.820	21.3	ng	828320	3	14.463	777006	20.0
n-Hexadecanoic ...	18.100	15.4	ng	698180	4	17.207	907041	20.0
Octadecanoic acid	19.375	8.5	ng	403978	5	21.449	947335	20.0
1,4-Benzenedica...	19.733	2.4	ng	113798	5	21.449	947335	20.0
Heptadecane	20.621	2.4	ng	111611	5	21.449	947335	20.0
Octacosane, 2-m...	21.102	3.2	ng	151086	5	21.449	947335	20.0
Octadecane	21.625	2.7	ng	128432	5	21.449	947335	20.0
Pentadecane, 8-...	22.201	2.9	ng	136187	5	21.449	947335	20.0
Hexacosane	22.853	3.7	ng	174978	5	21.449	947335	20.0
Supraene	23.035	2.3	ng	137461	6	24.522	1173160	20.0
Hexadecane, 1-i...	23.611	2.3	ng	132491	6	24.522	1173160	20.0
unknown25.151	25.151	26.4	ng	1549060	6	24.522	1173160	20.0
unknown31.120	31.120	35.8	ng	2096930	6	24.522	1173160	20.0