

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
 Data File : BG058532.D
 Acq On : 29 Jul 2023 00:32
 Operator : MA/JU
 Sample : 03632-08
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-12-(4-6)

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: BG058532.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.909	305	310	315	rBV	20951	30856	1.35%	0.227%
2	5.385	384	391	404	rBV	810856	1266546	55.38%	9.331%
3	6.983	656	663	683	rBV	764355	1333017	58.29%	9.821%
4	7.406	730	735	745	rBV	12002	27344	1.20%	0.201%
5	7.812	795	804	811	rBV	186365	314719	13.76%	2.319%
6	8.975	995	1002	1023	rBV	464627	854428	37.36%	6.295%
7	10.614	1273	1281	1291	rBV	255394	462876	20.24%	3.410%
8	13.082	1691	1701	1711	rBV	1221759	1947468	85.16%	14.348%
9	13.347	1742	1746	1756	rBV9	12468	27568	1.21%	0.203%
10	13.805	1815	1824	1831	rBV	174386	260018	11.37%	1.916%
11	13.875	1831	1836	1840	rBV2	45716	69636	3.04%	0.513%
12	13.940	1843	1847	1851	rVB3	19258	29130	1.27%	0.215%
13	14.193	1885	1890	1896	rBV9	27209	57088	2.50%	0.421%
14	14.287	1901	1906	1913	rVB2	68251	101205	4.43%	0.746%
15	14.357	1913	1918	1924	rBV7	16679	34356	1.50%	0.253%
16	14.428	1924	1930	1931	rBV3	34859	53538	2.34%	0.394%
17	14.463	1931	1936	1943	rVB	428091	692659	30.29%	5.103%
18	14.980	2020	2024	2033	rVB9	18714	38859	1.70%	0.286%
19	15.086	2037	2042	2044	rBV3	21317	34430	1.51%	0.254%
20	15.180	2054	2058	2062	rVB5	20578	33025	1.44%	0.243%
21	15.244	2063	2069	2073	rBV4	65003	113980	4.98%	0.840%
22	15.503	2108	2113	2117	rBV5	25432	52867	2.31%	0.389%
23	15.708	2145	2148	2159	rVB2	43685	77082	3.37%	0.568%
24	15.949	2183	2189	2196	rBV	932389	1412536	61.77%	10.407%
25	16.184	2223	2229	2234	rBV3	138469	235629	10.30%	1.736%
26	16.748	2322	2325	2328	rBV	39694	55826	2.44%	0.411%
27	17.007	2365	2369	2374	rBV	114327	149541	6.54%	1.102%
28	17.207	2398	2403	2411	rBV	513428	815575	35.66%	6.009%
29	17.612	2469	2472	2478	rBV3	80996	123617	5.41%	0.911%
30	18.100	2551	2555	2560	rBV4	147779	238311	10.42%	1.756%
31	19.774	2837	2840	2844	rBV2	239111	342487	14.98%	2.523%
32	19.827	2845	2849	2854	rVB	1693507	2286934	100.00%	16.849%

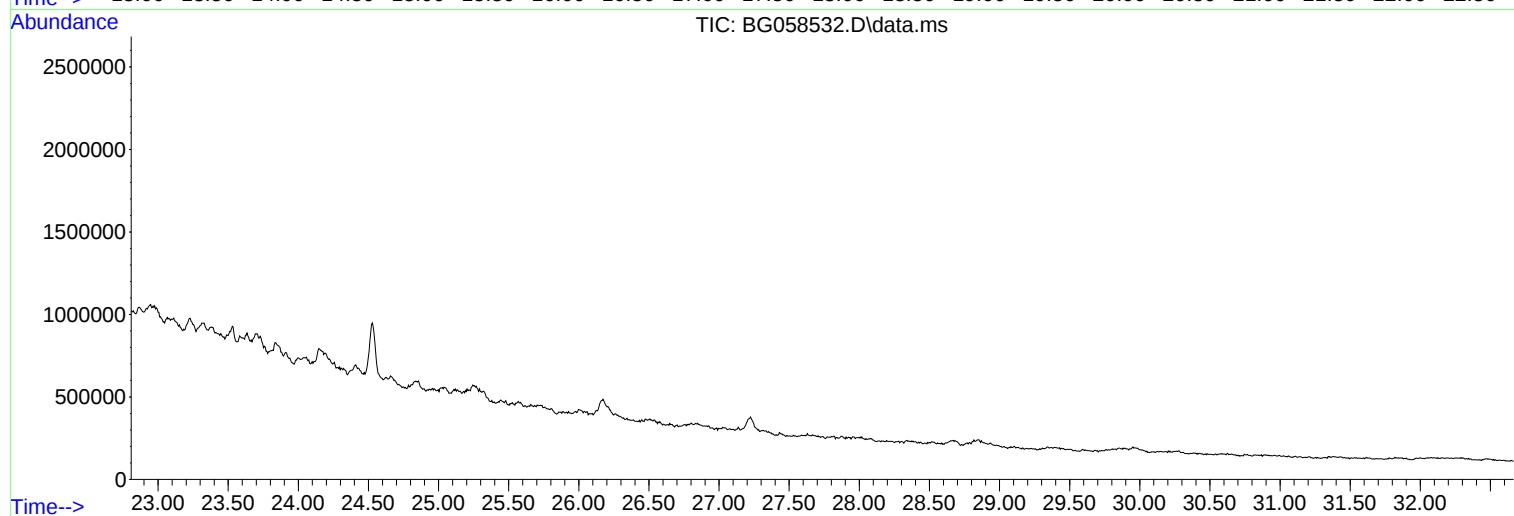
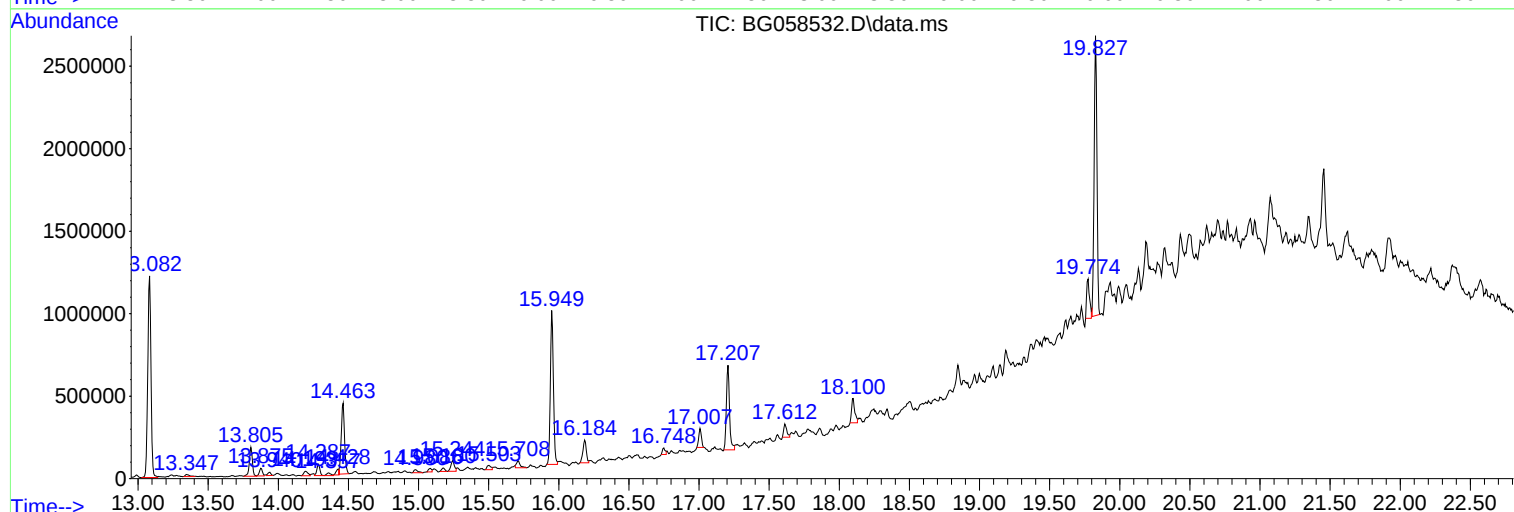
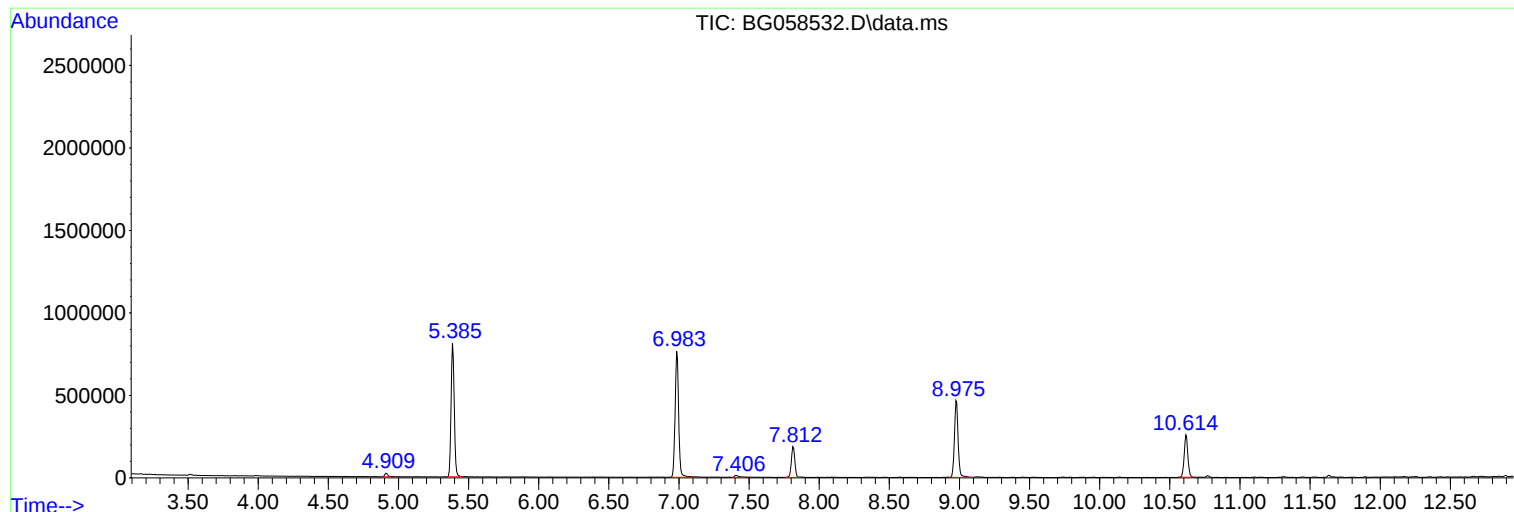
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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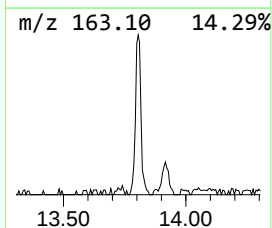
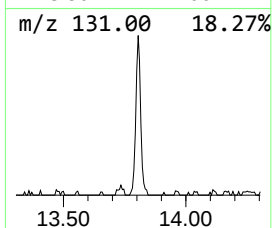
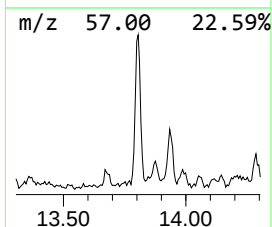
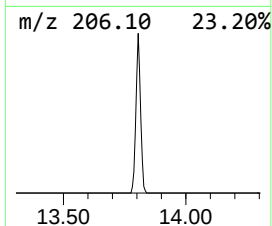
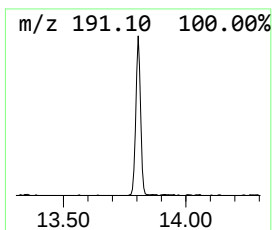
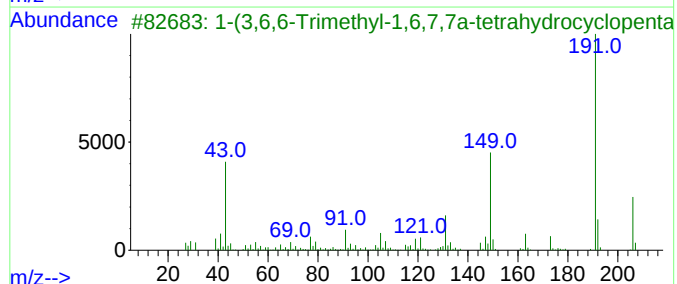
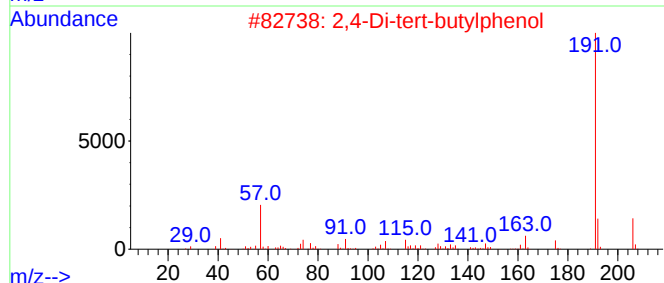
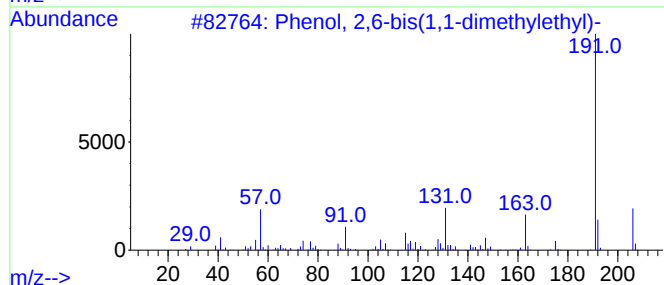
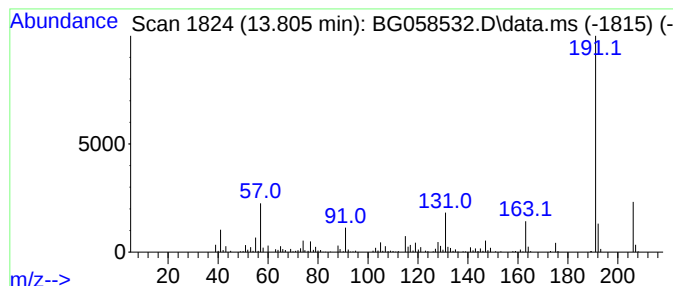
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.805	7.51 ng	260018	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	96
2			2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	86
3			1-(3,6,6-Trimethyl-1,6,7,7a-tetr...	206	C13H18O2	1000194-97-2	86
4			Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	80
5			4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	80



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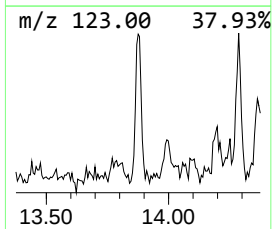
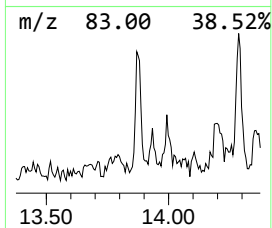
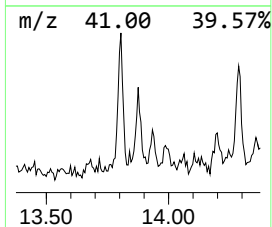
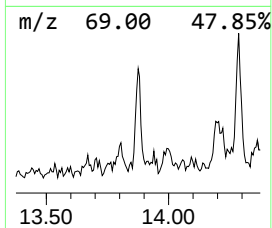
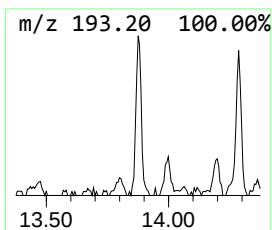
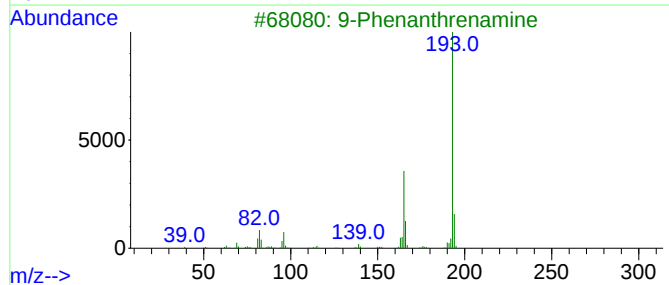
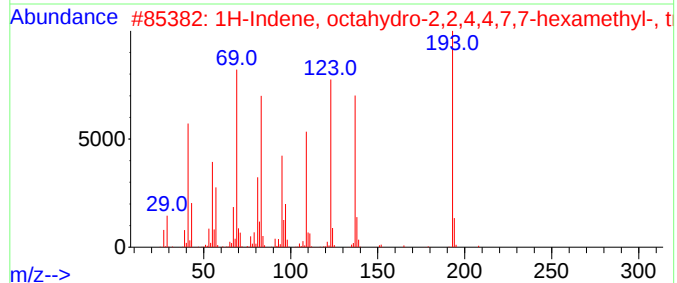
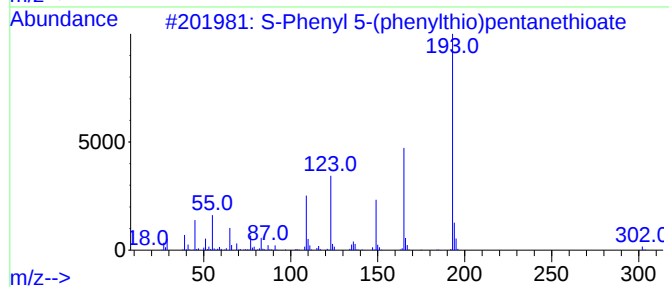
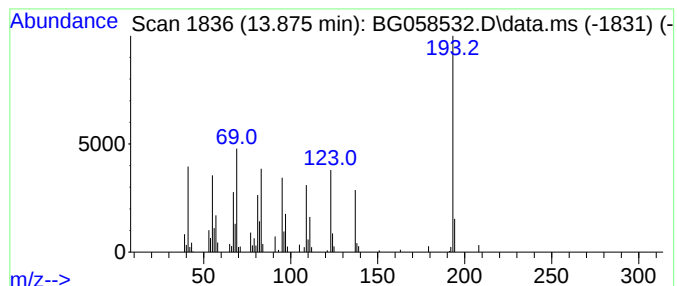
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown13.875 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.875	2.01 ng	69636	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			S-Phenyl 5-(phenylthio)pentaneth...	302	C17H18OS2	1000234-40-7	43
2			1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	42
3			9-Phenanthrenamine	193	C14H11N	000947-73-9	35
4			2-Anthracenamine	193	C14H11N	000613-13-8	35
5			Benzonitrile, 2-(4-methylphenyl)-	193	C14H11N	114772-53-1	27



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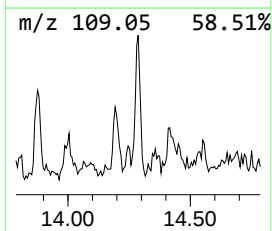
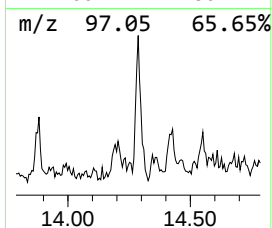
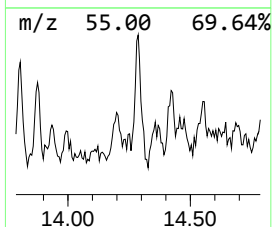
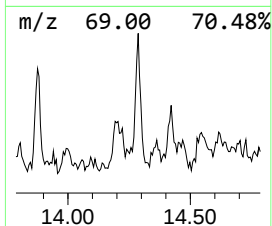
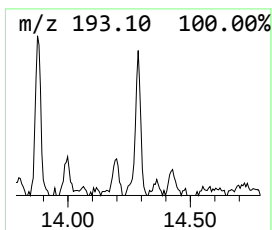
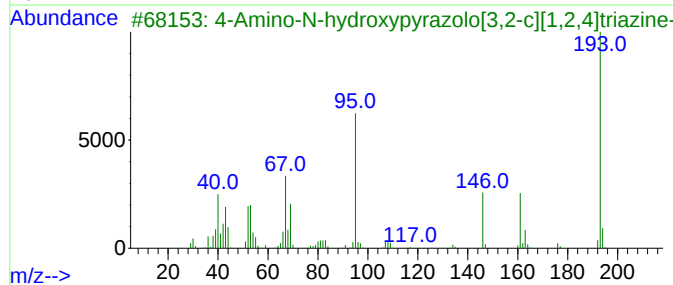
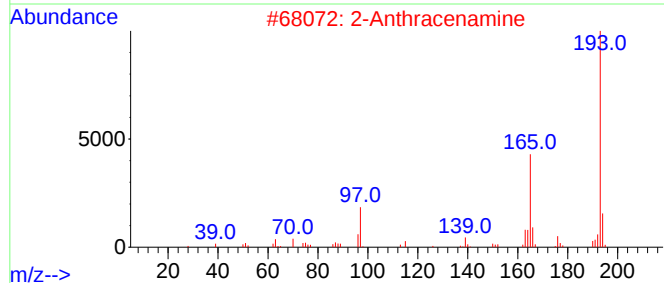
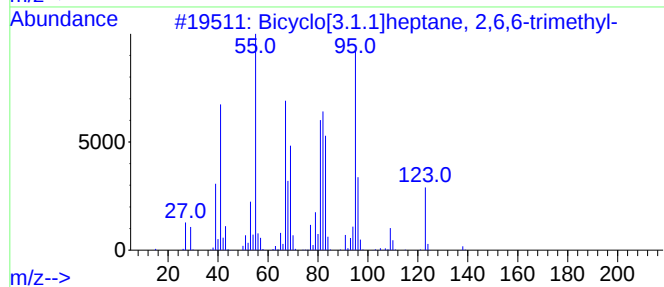
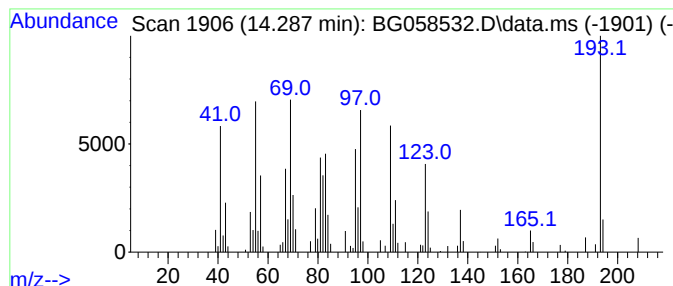
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown14.287 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.287	2.92 ng	101205	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	38
2			2-Anthracenamine	193	C14H11N	000613-13-8	30
3			4-Amino-N-hydroxypyrazolo[3,2-c]...	193	C6H7N7O	1000443-50-2	25
4			[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	18
5			(-)-trans-Pinane	138	C10H18	033626-25-4	18



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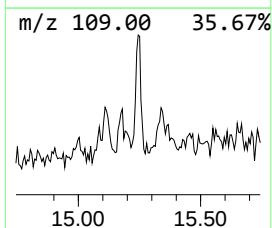
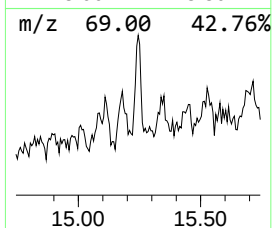
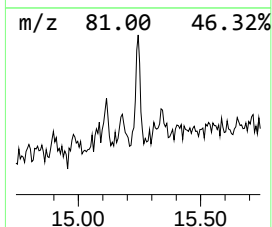
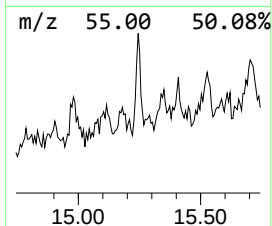
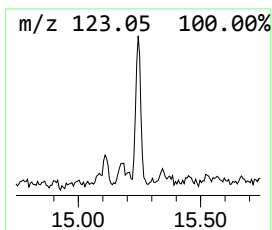
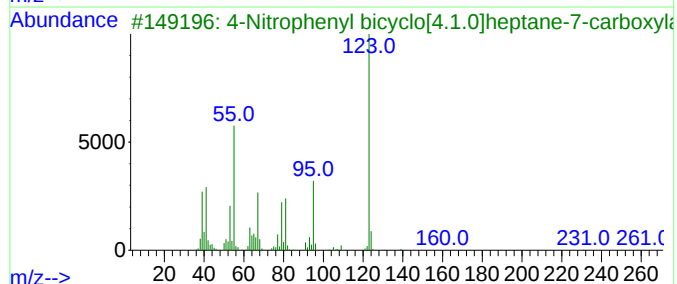
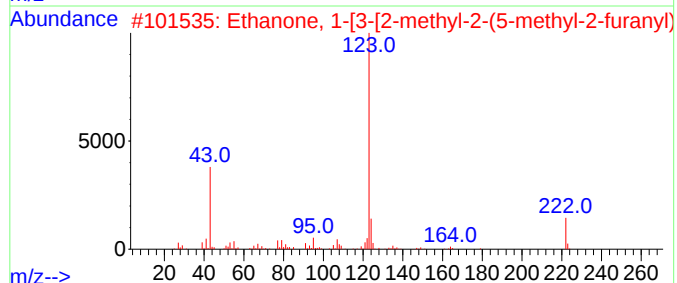
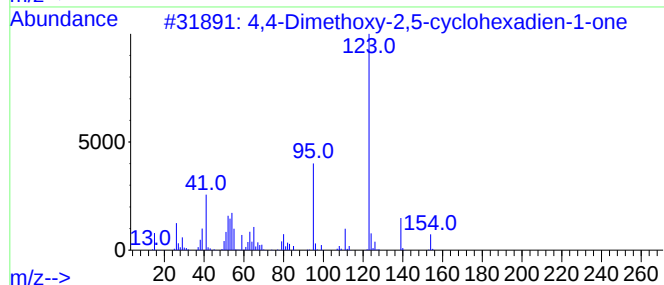
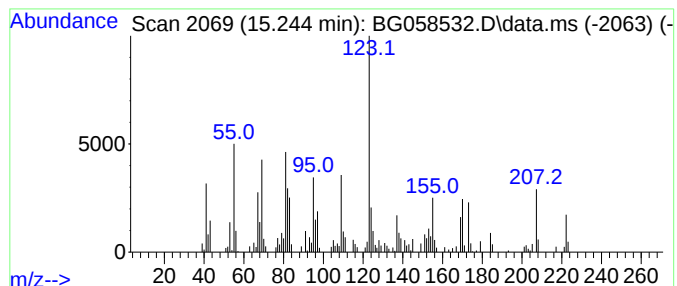
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown15.244 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.244	3.29 ng	113980	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4-Dimethoxy-2,5-cyclohexadien-...	154	C8H10O3	000935-50-2	38
2			Ethanone, 1-[3-[2-methyl-2-(5-me...	222	C13H18O3	080114-28-9	38
3			4-Nitrophenyl bicyclo[4.1.0]hept...	261	C14H15NO4	328938-65-4	35
4			N-(4-Nitro-1,8-naphthalimido)-4-...	379	C19H10FN3O5	300690-90-8	35
5			N-acetyl-3-fluorobenzamide	181	C9H8FN02	1000505-22-0	35



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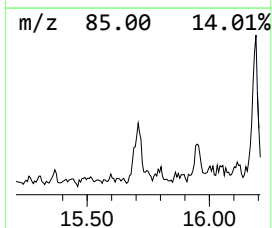
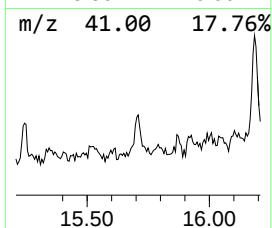
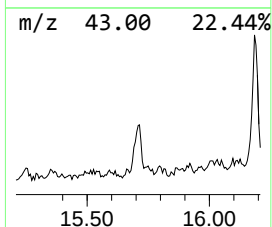
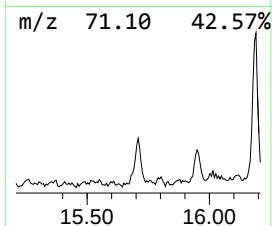
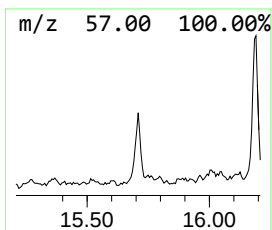
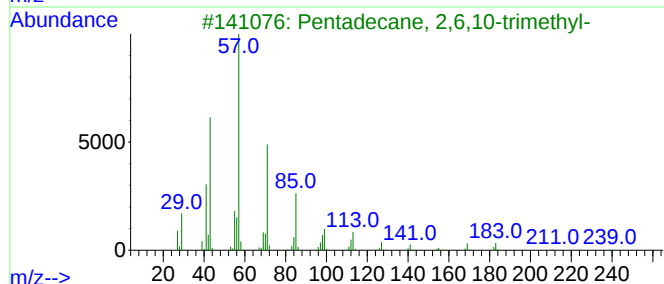
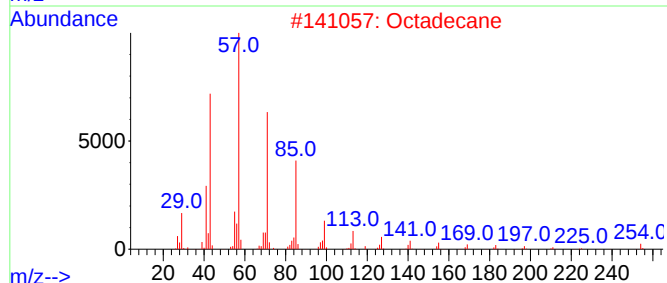
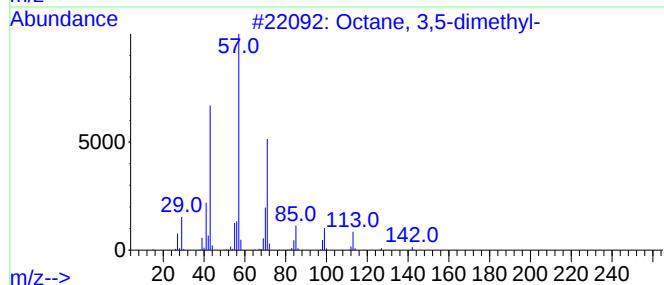
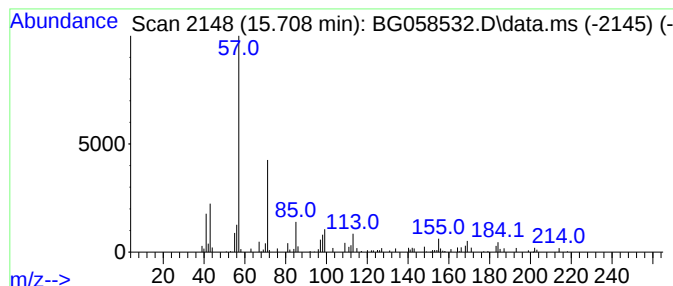
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Peak Number 5 Octane, 3,5-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.709	2.23 ng	77082	Acenaphthene-d10	14.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	72
2			Octadecane	254	C18H38	000593-45-3	59
3			Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	59
4			Heptadecane	240	C17H36	000629-78-7	59
5			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058532.D
Acq On : 29 Jul 2023 00:32
Operator : MA/JU
Sample : 03632-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-12-(4-6)

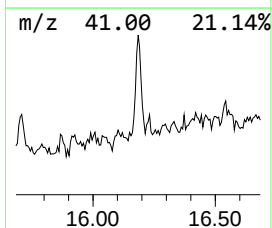
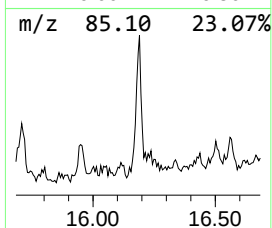
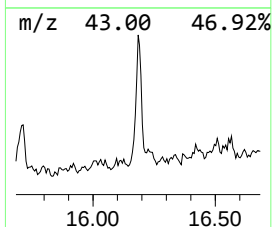
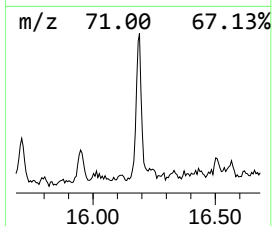
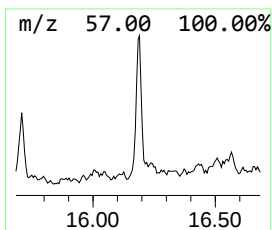
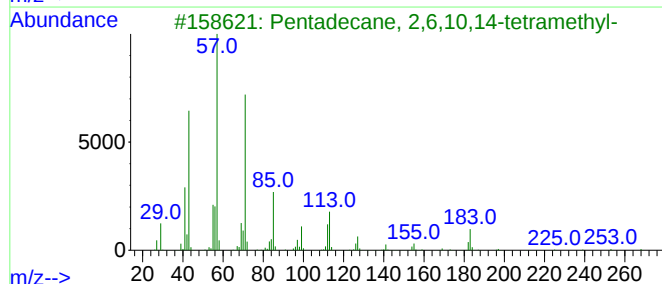
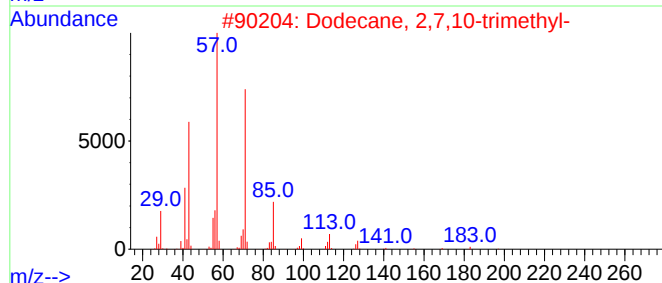
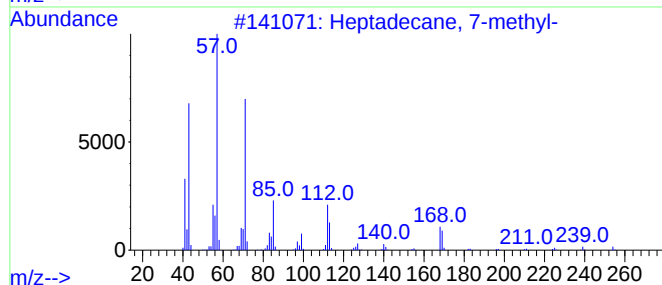
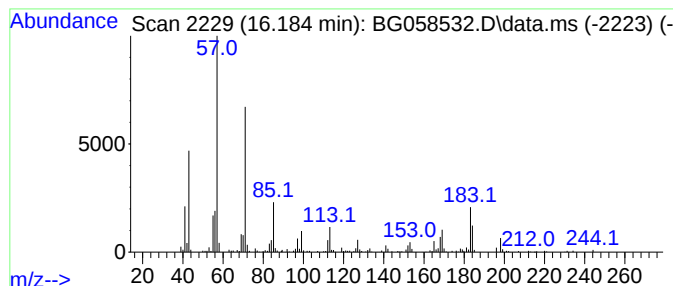
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptadecane, 7-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.184	5.78 ng	235629	Phenanthrene-d10	17.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 7-methyl-	254	C18H38	020959-33-5	64
2			Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	58
3			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	53
4			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	52
5			Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058532.D
Acq On : 29 Jul 2023 00:32
Operator : MA/JU
Sample : 03632-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-12-(4-6)

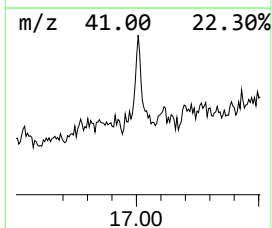
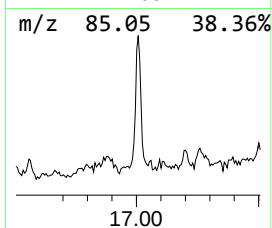
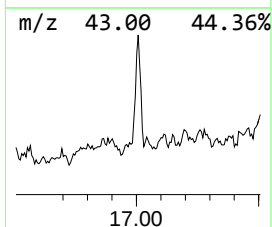
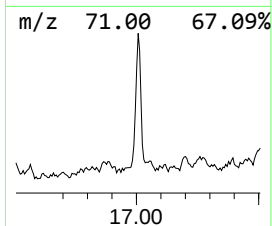
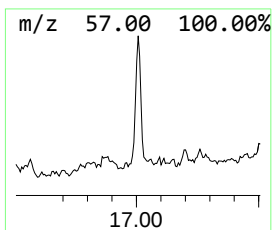
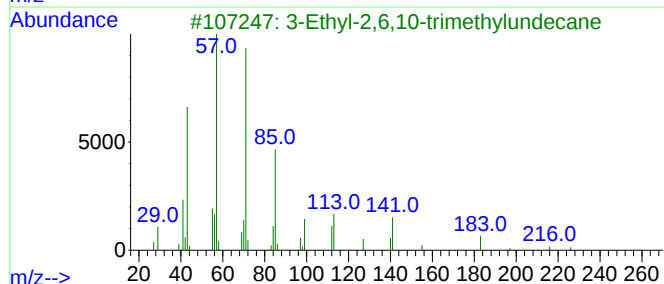
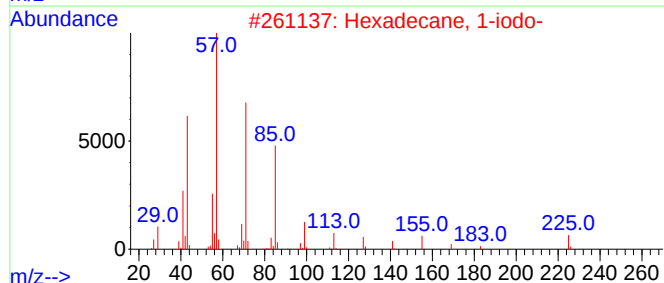
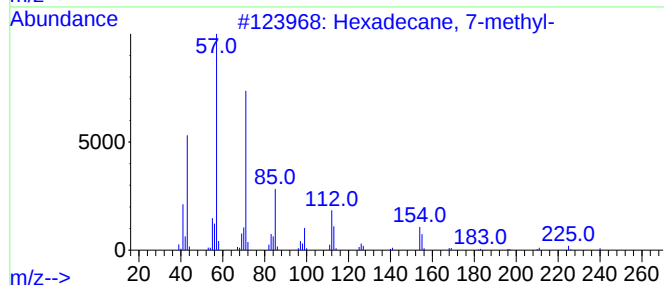
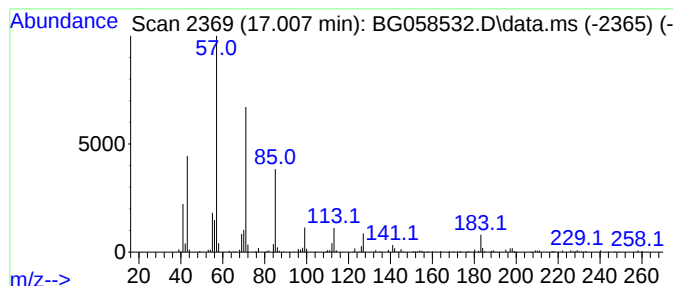
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane, 7-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.007	3.67 ng	149541	Phenanthrene-d10	17.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 7-methyl-	240	C17H36	026730-20-1	87
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
3			3-Ethyl-2,6,10-trimethylundecane	226	C16H34	1000432-25-9	81
4			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
5			Tridecane	184	C13H28	000629-50-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058532.D
Acq On : 29 Jul 2023 00:32
Operator : MA/JU
Sample : 03632-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-12-(4-6)

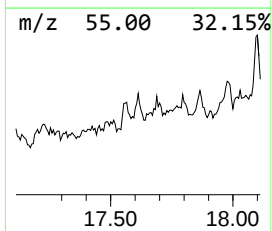
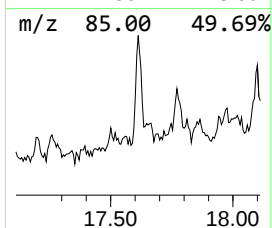
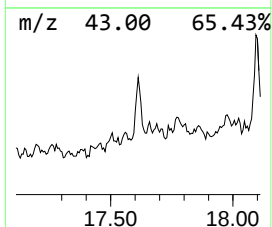
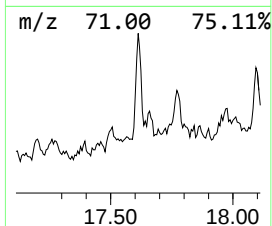
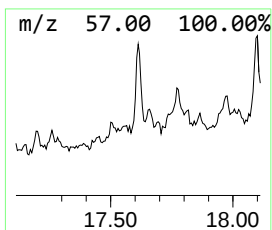
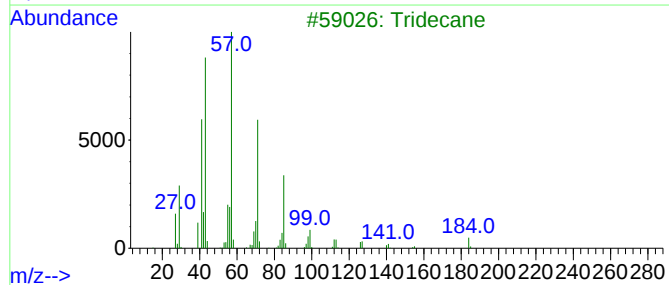
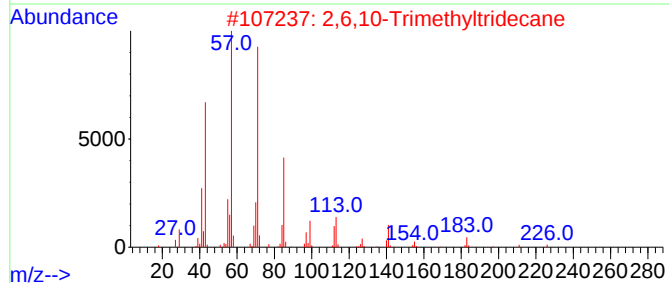
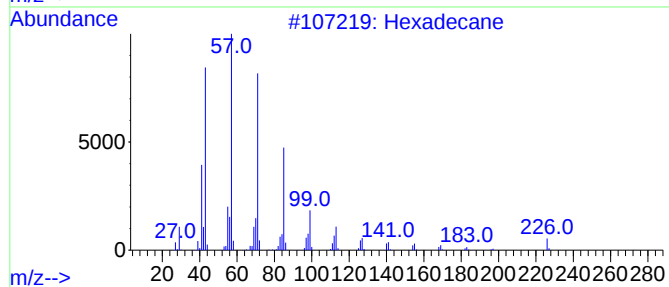
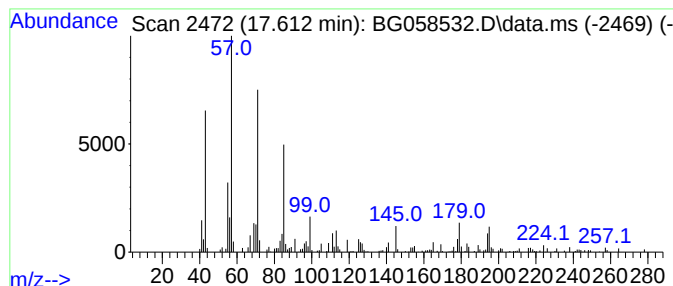
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.612	3.03 ng	123617	Phenanthrene-d10	17.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	93
2			2,6,10-Trimethyltridecane	226	C16H34	003891-99-4	86
3			Tridecane	184	C13H28	000629-50-5	81
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	74
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058532.D
Acq On : 29 Jul 2023 00:32
Operator : MA/JU
Sample : 03632-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-12-(4-6)

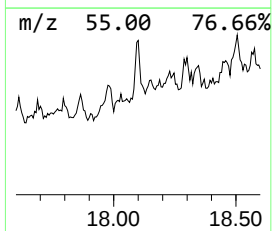
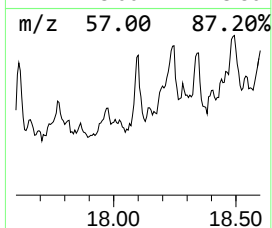
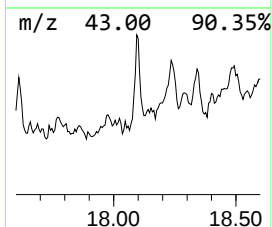
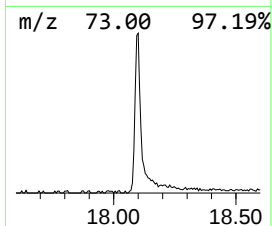
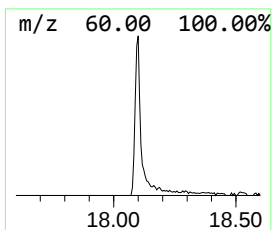
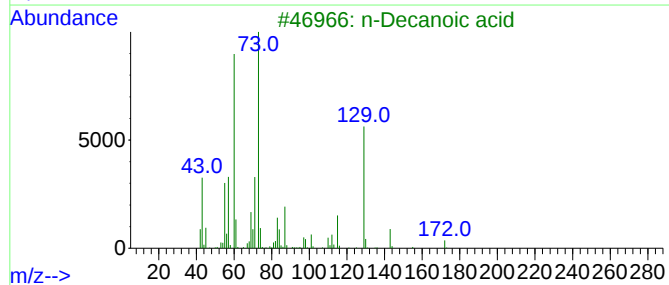
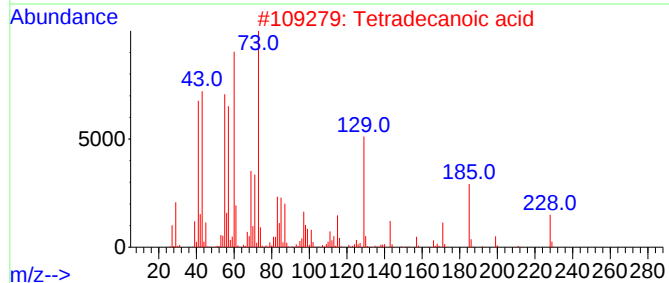
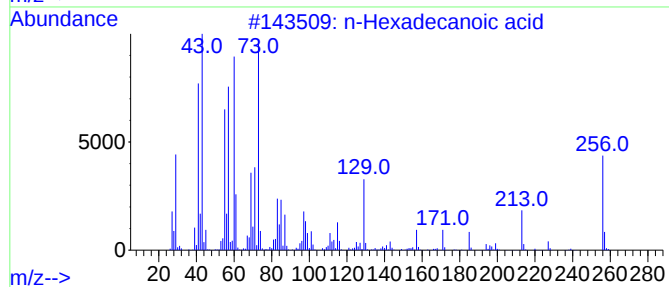
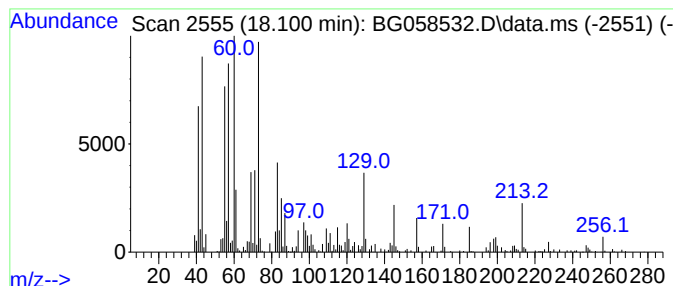
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.100	5.84 ng	238311	Phenanthrene-d10	17.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3			n-Decanoic acid	172	C10H20O2	000334-48-5	50
4			Tridecanoic acid	214	C13H26O2	000638-53-9	49
5			Dodecanoic acid	200	C12H24O2	000143-07-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058532.D
Acq On : 29 Jul 2023 00:32
Operator : MA/JU
Sample : 03632-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-12-(4-6)

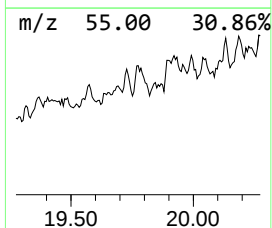
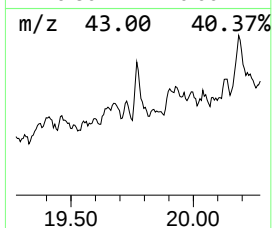
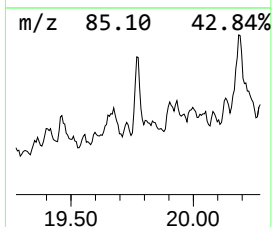
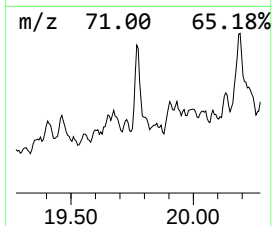
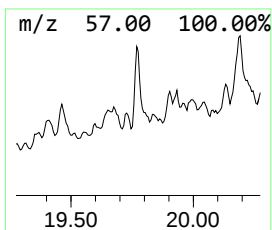
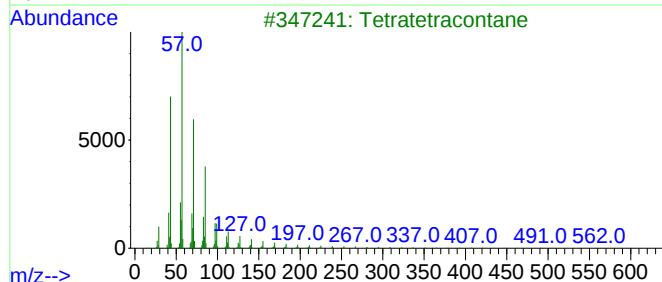
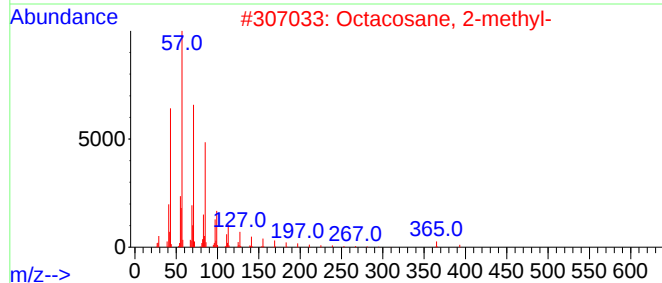
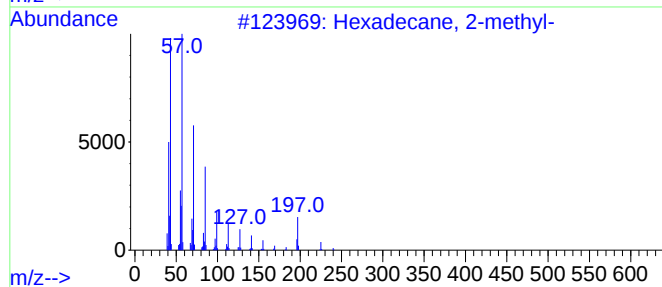
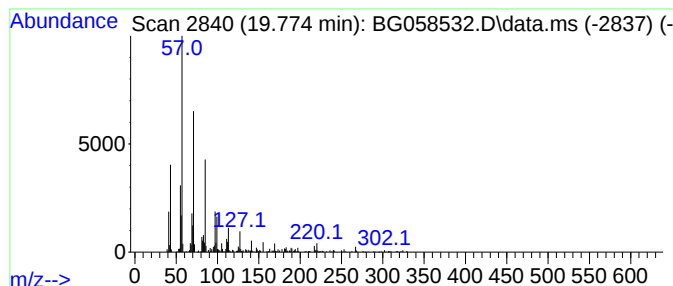
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecane, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.774	3.00 ng	342487	Chrysene-d12	21.449

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Tetratetracontane	619	C44H90	007098-22-8	91
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
5			Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072823\
Data File : BG058532.D
Acq On : 29 Jul 2023 00:32
Operator : MA/JU
Sample : 03632-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-12-(4-6)

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
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unknown13.875	13.875	2.0	ng	69636	3	14.463	692659	20.0
unknown14.287	14.287	2.9	ng	101205	3	14.463	692659	20.0
unknown15.244	15.244	3.3	ng	113980	3	14.463	692659	20.0
Octane, 3,5-dim...	15.709	2.2	ng	77082	3	14.463	692659	20.0
Heptadecane, 7-...	16.184	5.8	ng	235629	4	17.207	815575	20.0
Hexadecane, 7-m...	17.007	3.7	ng	149541	4	17.207	815575	20.0
Hexadecane	17.612	3.0	ng	123617	4	17.207	815575	20.0
n-Hexadecanoic ...	18.100	5.8	ng	238311	4	17.207	815575	20.0
Hexadecane, 2-m...	19.774	3.0	ng	342487	5	21.449	2286930	20.0