

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
 Data File : BG058575.D
 Acq On : 2 Aug 2023 12:41
 Operator : MA/JU
 Sample : 03686-14
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-22-4-6-20230721

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: BG058575.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	384	391	403	rBV	831313	1293468	48.03%	8.578%
2	6.983	655	663	674	rBV	772268	1337343	49.66%	8.869%
3	7.811	798	804	811	rVB	167331	281205	10.44%	1.865%
4	8.975	994	1002	1018	rBV	463400	831902	30.89%	5.517%
5	10.614	1271	1281	1290	rBV	238794	429800	15.96%	2.850%
6	13.082	1693	1701	1709	rBV	1186344	1883036	69.93%	12.488%
7	13.910	1835	1842	1852	rBV	151432	220418	8.19%	1.462%
8	14.457	1929	1935	1945	rBV	402524	617065	22.91%	4.092%
9	15.949	2182	2189	2207	rBV	1040832	1622384	60.25%	10.760%
10	16.954	2356	2360	2364	rBV	23553	29917	1.11%	0.198%
11	17.206	2397	2403	2410	rBV	484834	747201	27.75%	4.956%
12	17.324	2419	2423	2429	rVB2	25086	33858	1.26%	0.225%
13	17.694	2482	2486	2490	rVB2	21635	29741	1.10%	0.197%
14	18.093	2549	2554	2564	rBV	212582	342464	12.72%	2.271%
15	19.004	2700	2709	2710	rBV5	21787	51923	1.93%	0.344%
16	19.374	2767	2772	2782	rBV2	67724	134114	4.98%	0.889%
17	19.827	2843	2849	2855	rBV	2037294	2692933	100.00%	17.860%
18	20.126	2896	2900	2904	rBV	26169	32477	1.21%	0.215%
19	20.455	2953	2956	2959	rBV	29124	41103	1.53%	0.273%
20	20.614	2980	2983	2988	rBV	55050	80220	2.98%	0.532%
21	21.102	3062	3066	3069	rBV2	70056	101657	3.77%	0.674%
22	21.442	3118	3124	3131	rBV	463268	789199	29.31%	5.234%
23	21.619	3151	3154	3160	rVB	84140	115907	4.30%	0.769%
24	22.195	3248	3252	3257	rBV2	84123	140904	5.23%	0.934%
25	22.853	3359	3364	3372	rBV2	72772	137661	5.11%	0.913%
26	23.605	3489	3492	3499	rVB	59004	109037	4.05%	0.723%
27	24.515	3638	3647	3663	rBV	318387	951223	35.32%	6.309%

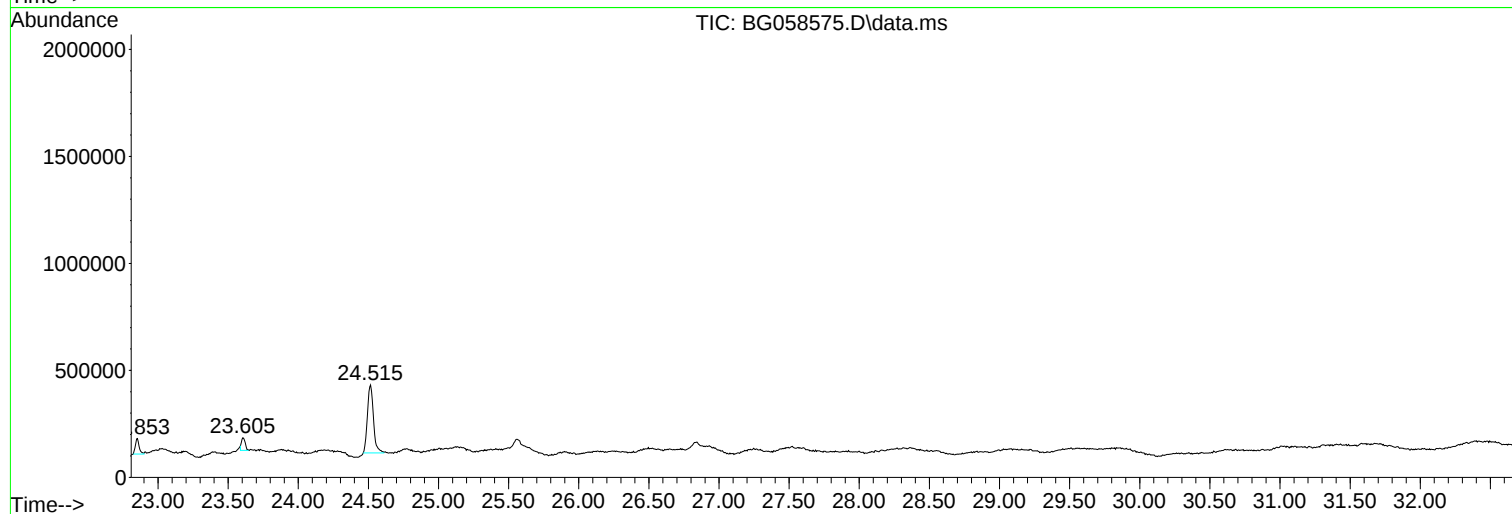
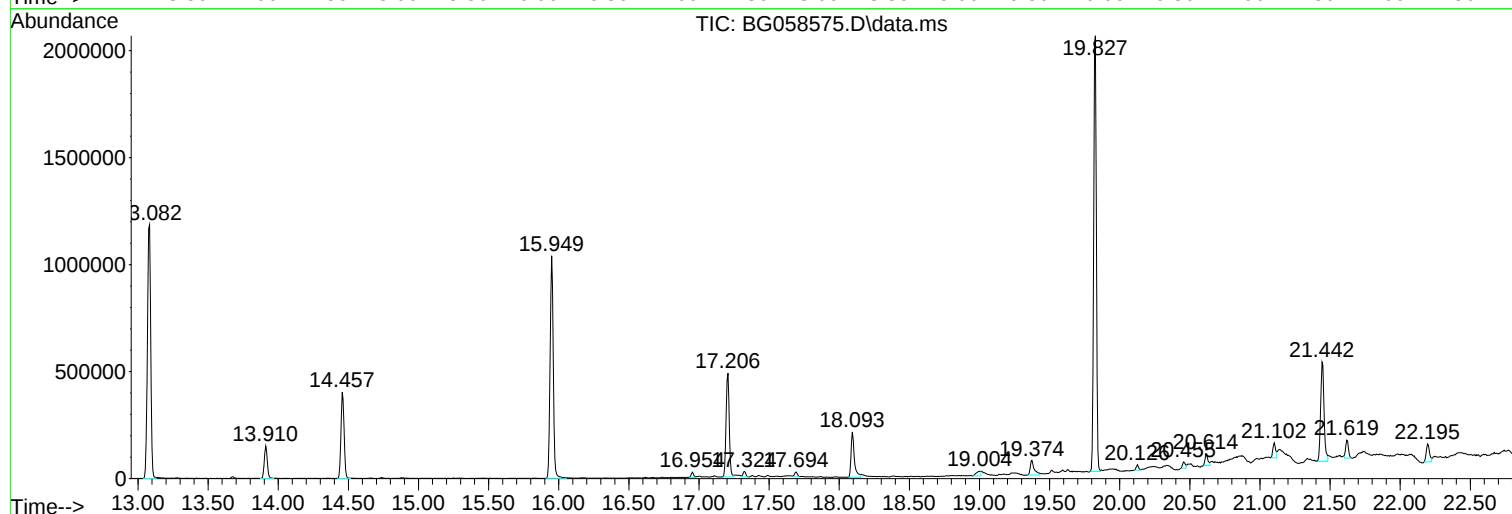
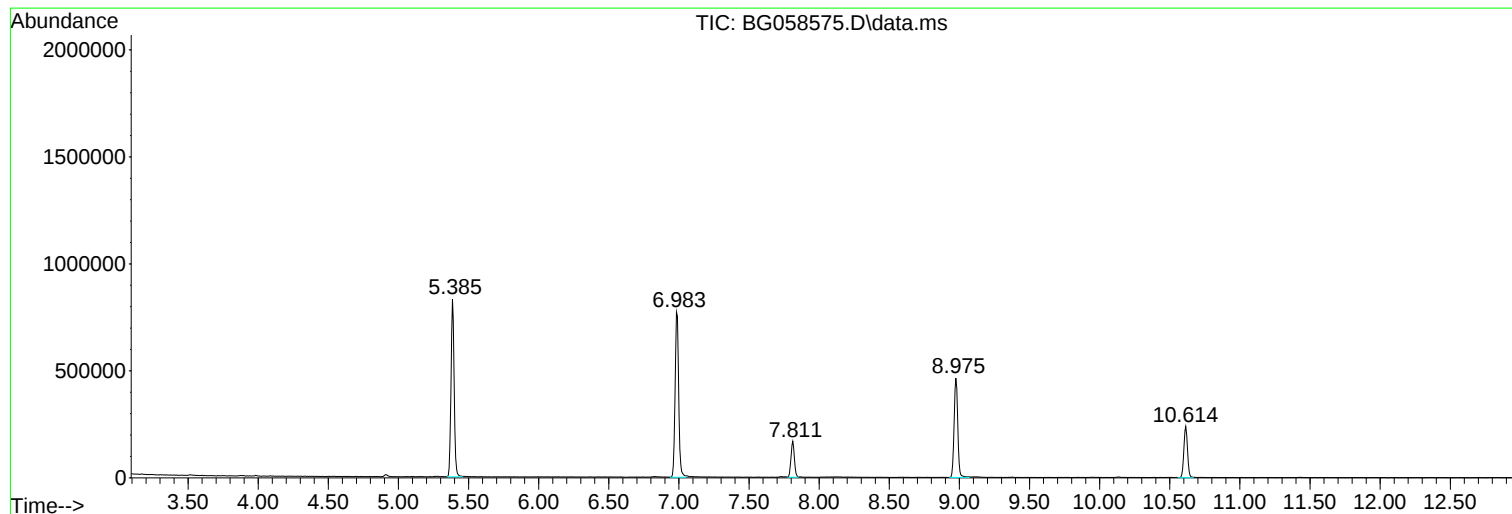
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Instrument :
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ClientSampleId :
SB-22-4-6-20230721

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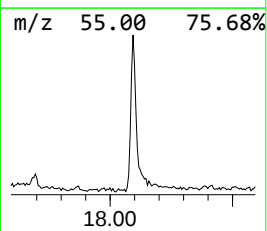
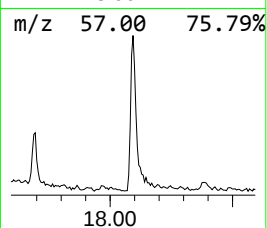
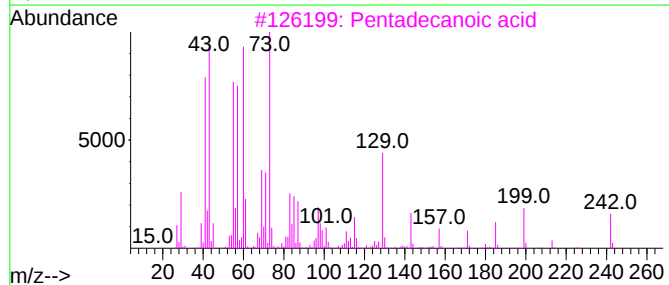
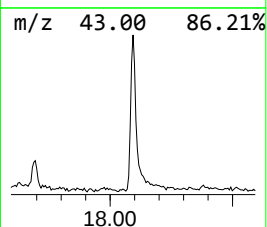
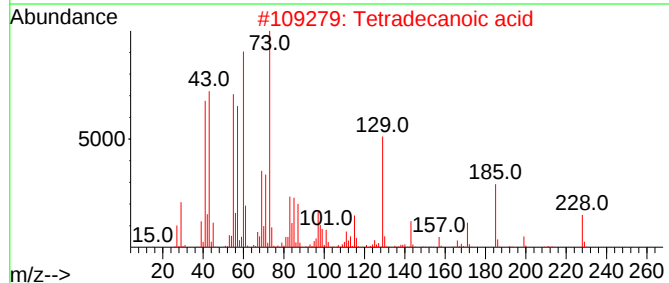
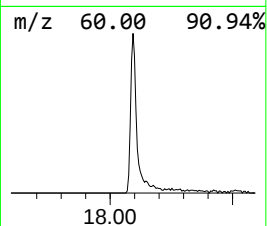
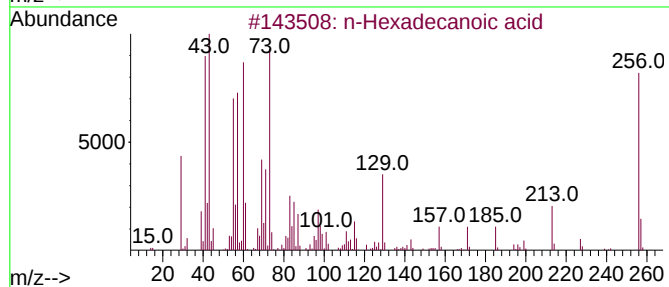
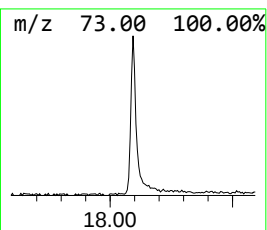
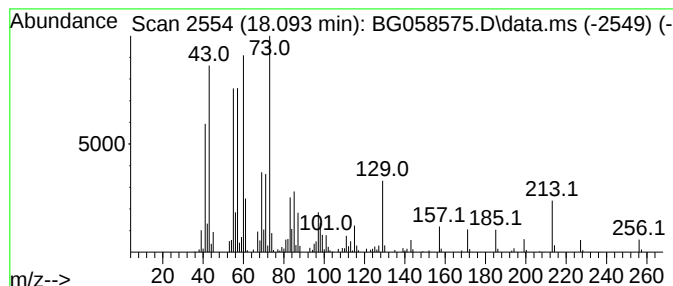
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.093	9.17 ng	342464	Phenanthrene-d10	17.206	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53



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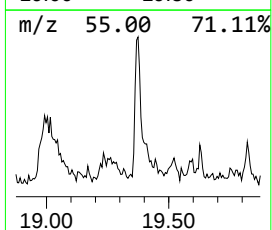
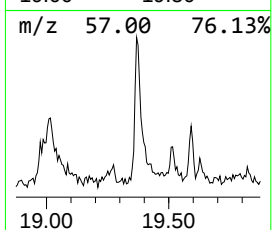
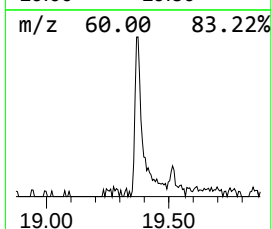
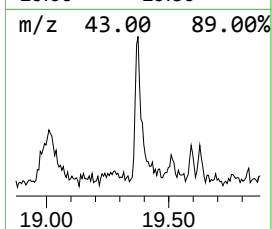
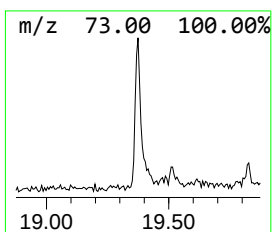
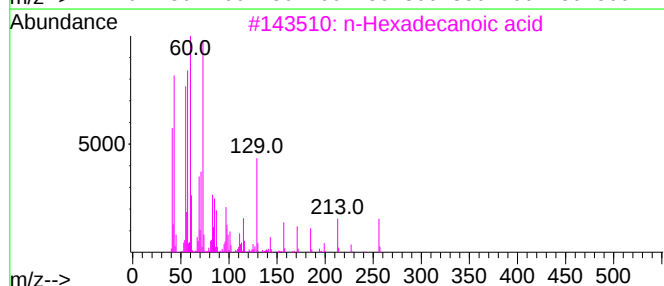
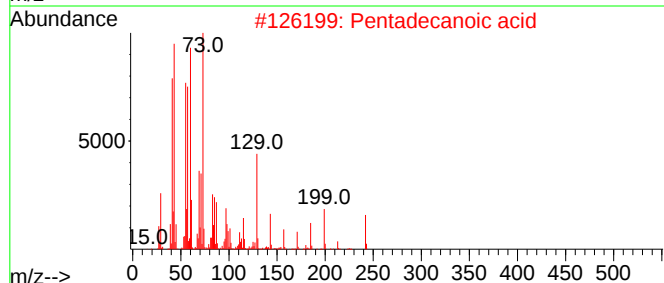
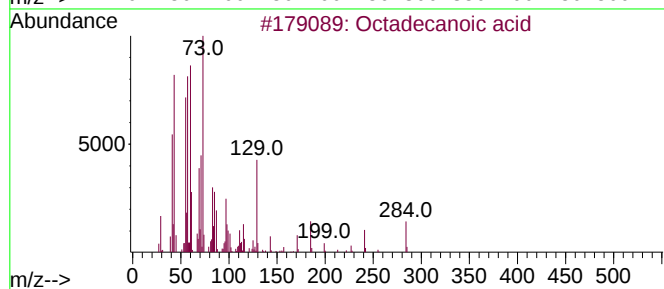
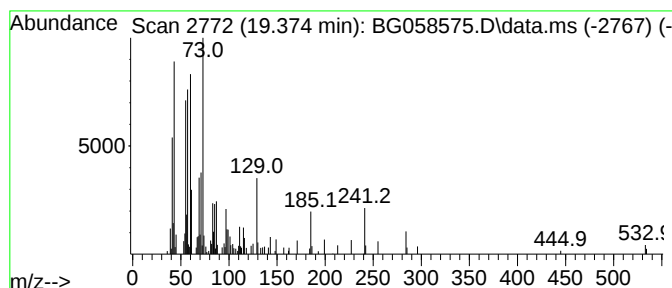
Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.374	3.40 ng	134114	Chrysene-d12	21.442	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53



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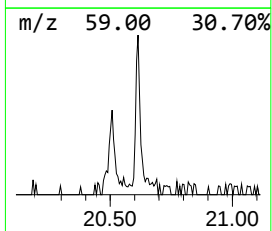
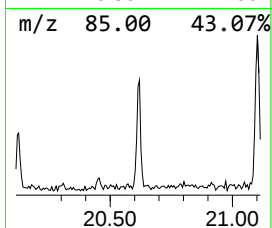
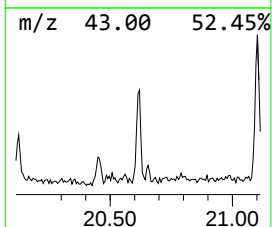
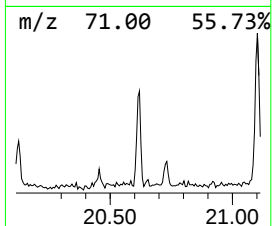
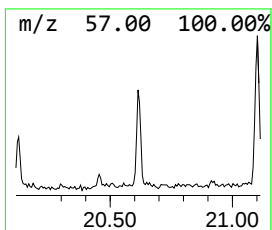
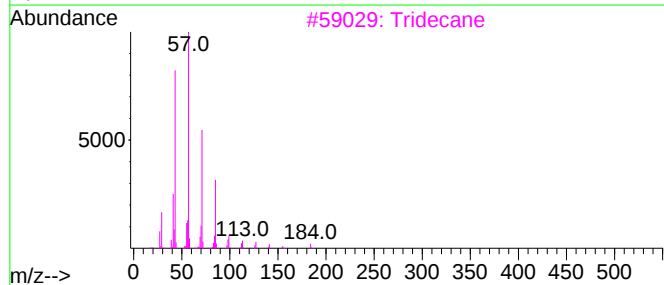
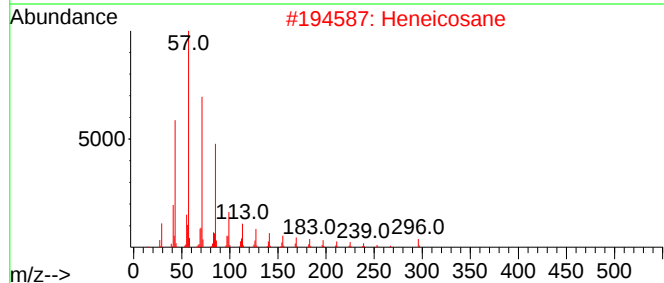
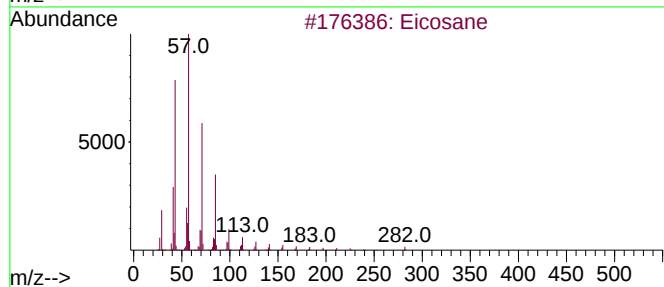
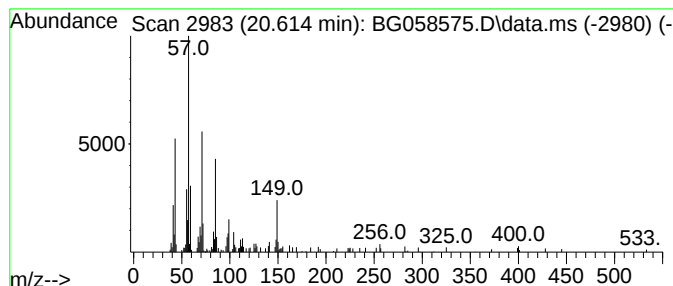
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.614	2.03 ng	80220	Chrysene-d12	21.442

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	70
2			Heneicosane	296	C21H44	000629-94-7	55
3			Tridecane	184	C13H28	000629-50-5	50
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	49
5			Hexacosane	366	C26H54	000630-01-3	46



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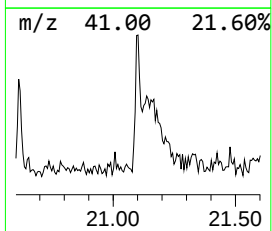
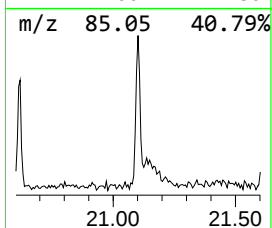
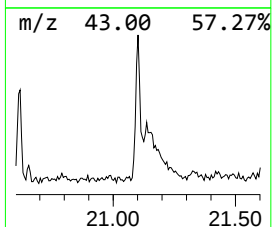
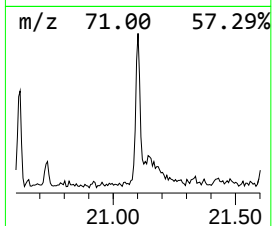
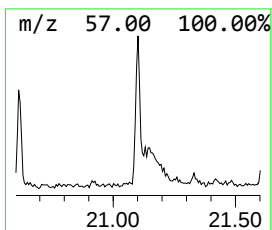
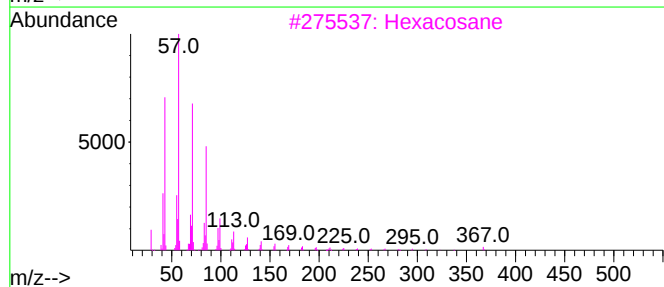
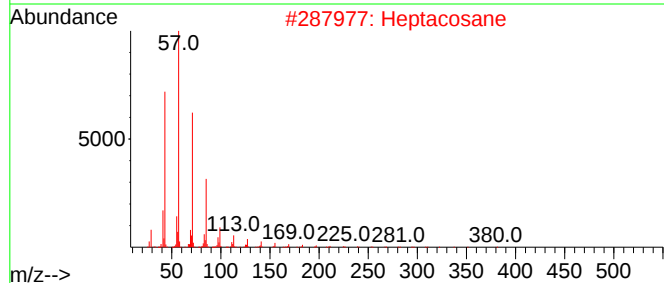
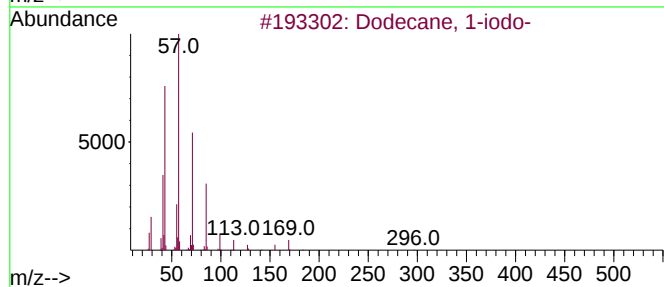
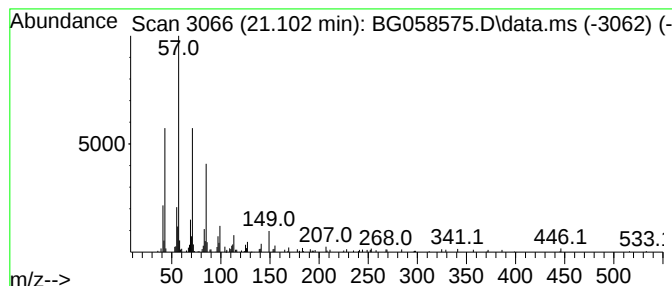
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Dodecane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.102	2.58 ng	101657	Chrysene-d12	21.442

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	81
2			Heptacosane	380	C27H56	000593-49-7	81
3			Hexacosane	366	C26H54	000630-01-3	76
4			Heneicosane	296	C21H44	000629-94-7	76
5			Pentadecane	212	C15H32	000629-62-9	74



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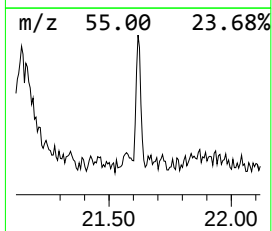
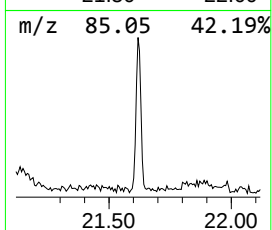
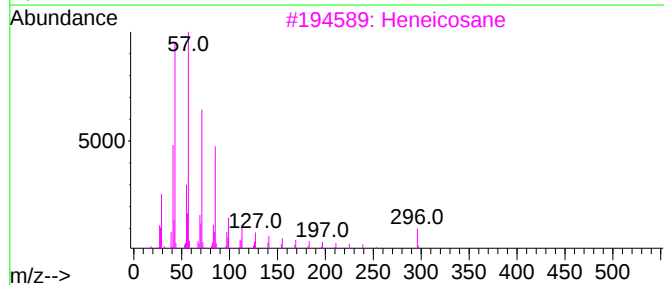
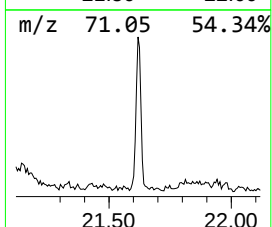
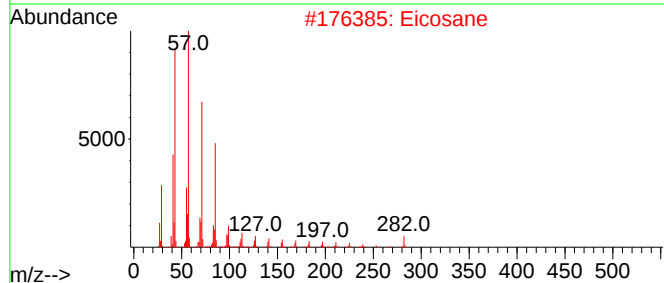
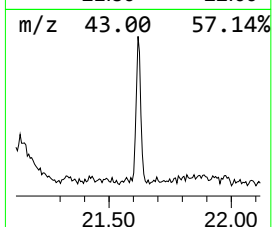
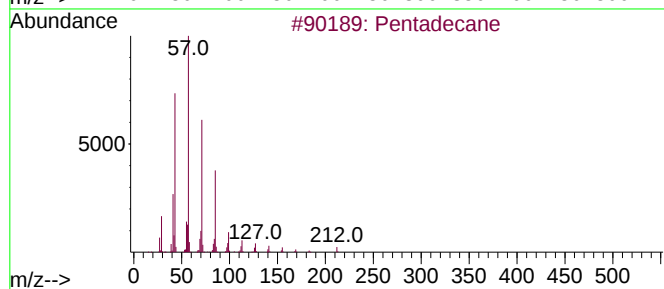
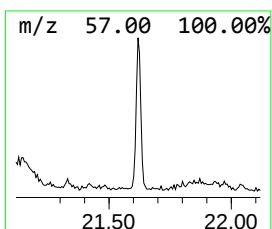
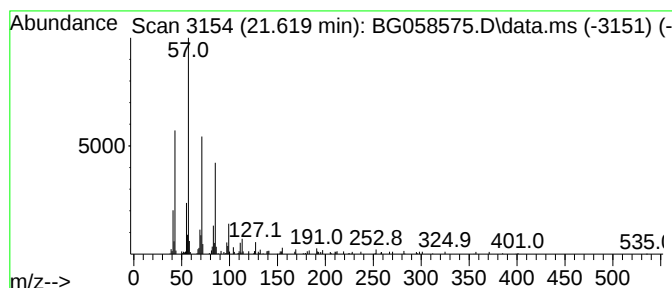
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.619	2.94 ng	115907	Chrysene-d12	21.442

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane	212	C15H32	000629-62-9	93
2			Eicosane	282	C20H42	000112-95-8	93
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane	240	C17H36	000629-78-7	83
5			Tetracosane	338	C24H50	000646-31-1	83



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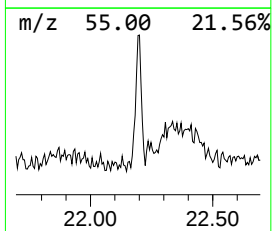
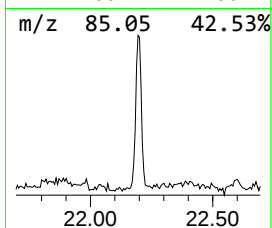
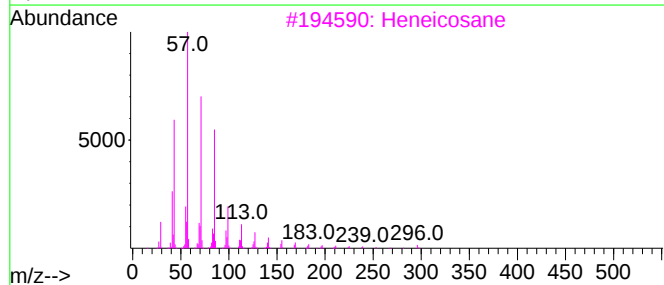
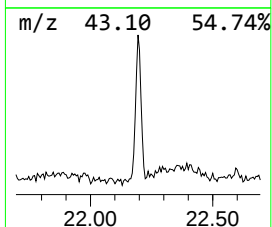
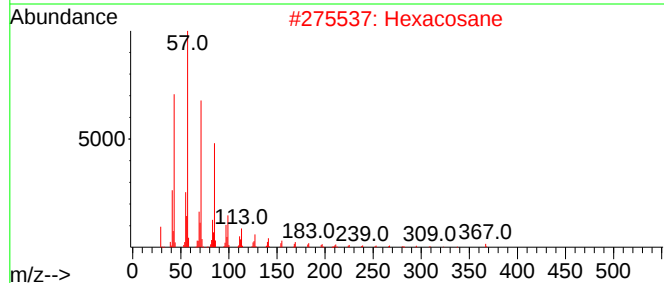
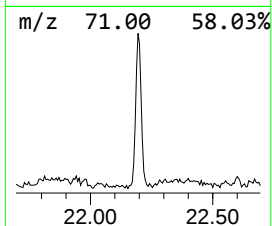
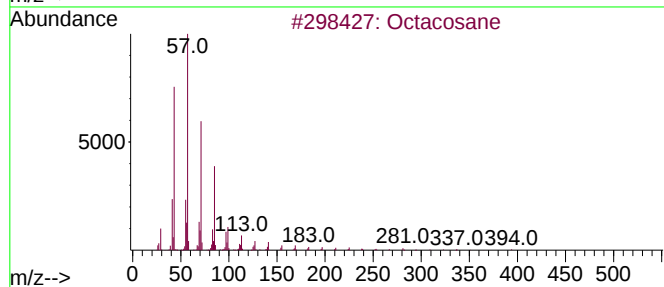
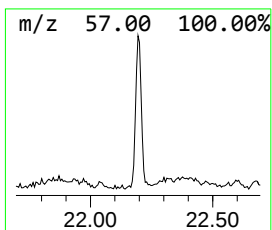
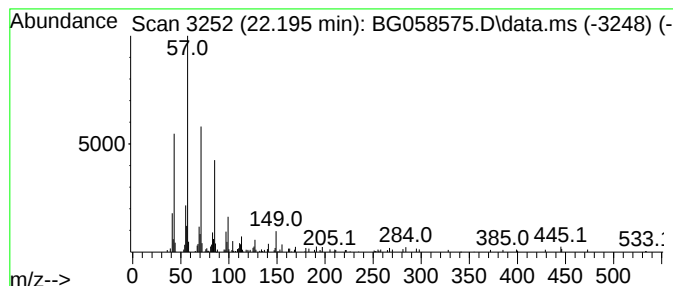
Instrument :
BNA_G
ClientSampleId :
SB-22-4-6-20230721

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 6 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.195	3.57 ng	140904	Chrysene-d12	21.442	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	76
2	Hexacosane	366	C26H54	000630-01-3	76
3	Heneicosane	296	C21H44	000629-94-7	76
4	Tetracosane	338	C24H50	000646-31-1	76
5	Pentacosane	352	C25H52	000629-99-2	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058575.D
Acq On : 2 Aug 2023 12:41
Operator : MA/JU
Sample : 03686-14
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-22-4-6-20230721

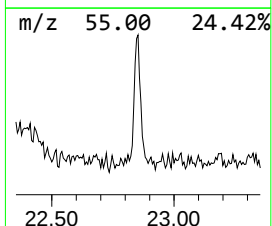
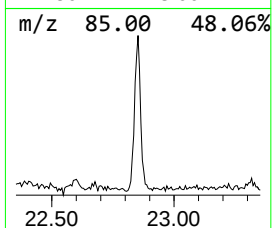
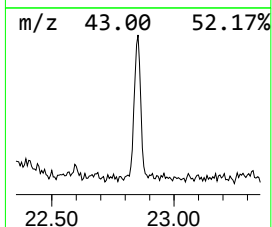
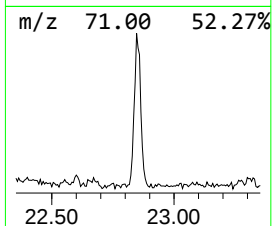
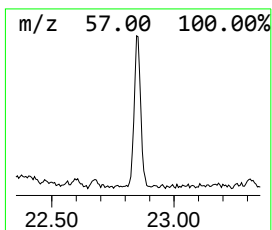
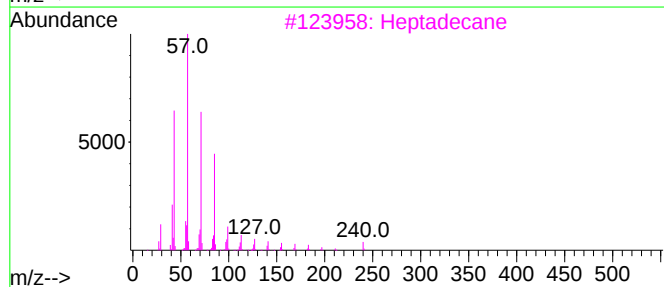
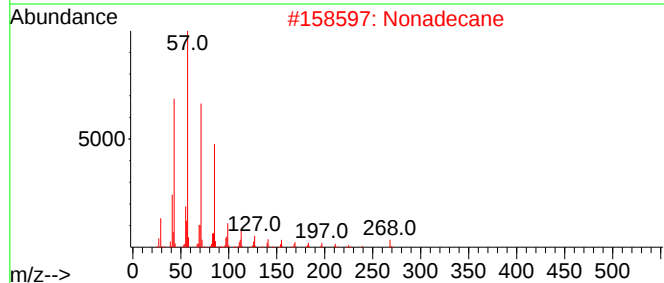
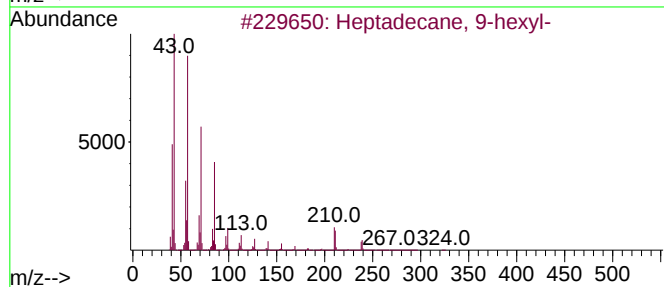
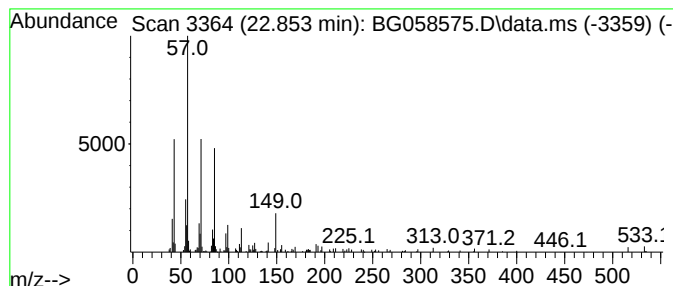
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 9-hexyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.853	3.49 ng	137661	Chrysene-d12	21.442

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	80
2			Nonadecane	268	C19H40	000629-92-5	80
3			Heptadecane	240	C17H36	000629-78-7	80
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	76
5			Hexadecane, 2-methyl-	240	C17H36	001560-92-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058575.D
Acq On : 2 Aug 2023 12:41
Operator : MA/JU
Sample : 03686-14
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-22-4-6-20230721

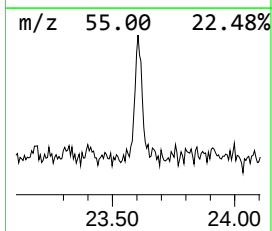
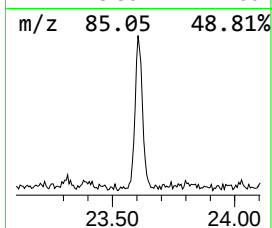
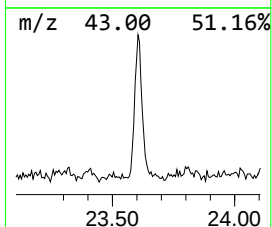
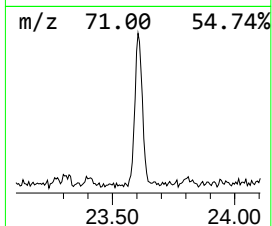
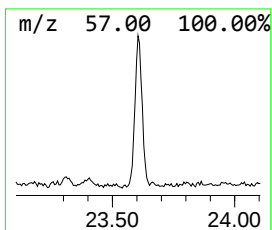
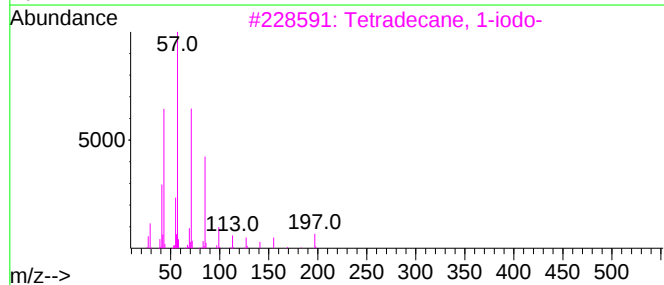
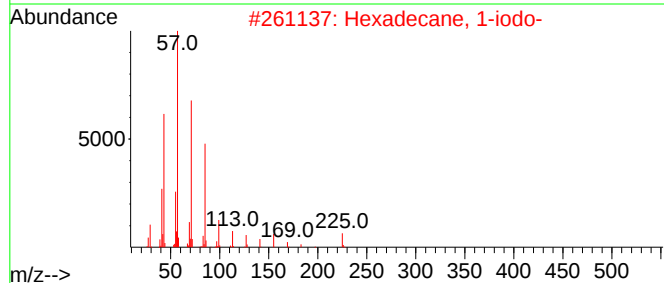
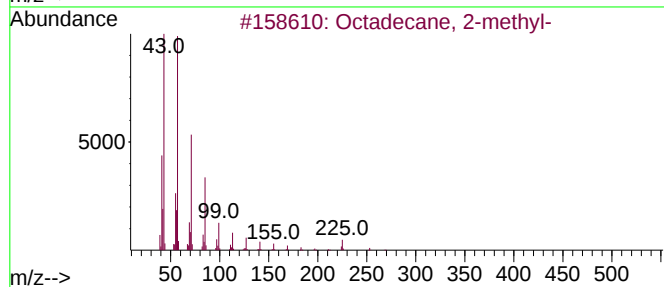
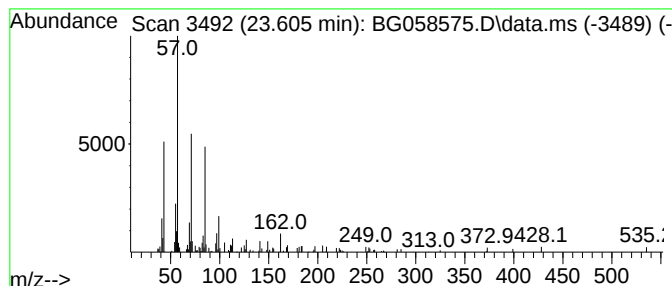
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.605	2.29 ng	109037	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane, 2-methyl-	268	C19H40	001560-88-9	83
2			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83
3			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
4			Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5			Nonadecane	268	C19H40	000629-92-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058575.D
Acq On : 2 Aug 2023 12:41
Operator : MA/JU
Sample : 03686-14
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-22-4-6-20230721

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
n-Hexadecanoic ...	18.093	9.2	ng	342464	4	17.206	747201	20.0
Octadecanoic acid	19.374	3.4	ng	134114	5	21.442	789199	20.0
Eicosane	20.614	2.0	ng	80220	5	21.442	789199	20.0
Dodecane, 1-iodo-	21.102	2.6	ng	101657	5	21.442	789199	20.0
Pentadecane	21.619	2.9	ng	115907	5	21.442	789199	20.0
Octacosane	22.195	3.6	ng	140904	5	21.442	789199	20.0
Heptadecane, 9-...	22.853	3.5	ng	137661	5	21.442	789199	20.0
Octadecane, 2-m...	23.605	2.3	ng	109037	6	24.515	951223	20.0