LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CL-01-112322

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055795.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.288	332	340	349	rBV	110882	184782	8.98%	1.272%
2	5.770	414	422	434	rBV	665543	1110337	53.95%	7.641%
3	7.386	688	697	707	rBV	641540	1149516	55.85%	7.910%
4	8.232	830	841	848	rBV	194076	336777	16.36%	2.317%
5	9.407	1033	1041	1051	rBV	401851	720537	35.01%	4.958%
6	11.064	1315	1323	1330	rBV	256007	460372	22.37%	3.168%
7	13.479	1727	1734	1744	rVB	1025302	1613658	78.41%	11.104%
8	13.661	1756	1765	1770	rBV6	11180	26615	1.29%	0.183%
9	14.307	1872	1875	1880	rVB3	15639	22781	1.11%	0.157%
10	14.413	1889	1893	1903	rVB6	10264	23218	1.13%	0.160%
11	14.583	1917	1922	1929	rBV2	18920	37592	1.83%	0.259%
12	14.854	1956	1968	1975	rBV	374272	615589	29.91%	4.236%
13	14.918	1975	1979	1984	rVB2	15717	24315	1.18%	0.167%
14	15.247	2025	2035	2042	rBV4	18187	42264	2.05%	0.291%
15	15.465	2066	2072	2075	rBV4	12755	22697	1.10%	0.156%
16	15.900	2140	2146	2152	rBV2	23671	46247	2.25%	0.318%
17	16.070	2170	2175	2179	rBV2	13492	22053	1.07%	0.152%
18	16.193	2193	2196	2202	rVB3	15264	25562	1.24%	0.176%
19	16.340	2215	2221	2229	rBV	776866	1171309	56.91%	8.060%
20	16.552	2249	2257	2263	rBV2	37569	79037	3.84%	0.544%
21	17.368	2392	2396	2401	rVV	27666	43961	2.14%	0.303%
22	17.415	2401	2404	2410	rVB	16857	24490	1.19%	0.169%
23	17.598	2429	2435	2439	rBV	450322	691187	33.58%	4.756%
24	17.639	2439	2442	2450	rVB	159870	230141	11.18%	1.584%
25	17.733	2453	2458	2462	rBV	34942	55743	2.71%	0.384%
26	17.991	2500	2502	2509	rVB	14430	24042	1.17%	0.165%
27	18.173	2530	2533	2540	rVB2	13499	20817	1.01%	0.143%
28	18.326	2554	2559	2566	rBV5	11871	24642	1.20%	0.170%
29	18.455	2577	2581	2587	rBV2	137185	252737	12.28%	1.739%
30	18.514	2588	2591	2597	rVB2	61096	99582	4.84%	0.685%
31	18.602	2602	2606	2610	rVB	17305	22956	1.12%	0.158%
32	18.661	2610	2616	2620	rBV2	57645	126198	6.13%	0.868%
33	18.955	2662	2666	2670	rBV	27248	39821	1.93%	0.274%
34	19.196	2702	2707	2711	rVB5	43120	75347	3.66%	0.518%
35	19.254	2713	2717	2720	rVV	22931	32051	1.56%	0.221%
36	19.290	2720	2723	2726	rVB3	14052	20967	1.02%	0.144%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

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-BG111622.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.366	2732	2736	2742	rBV2	65935	118195	5.74%	0.813%
38	19.636	2777	2782	2786	rBV	279812	395457	19.21%	2.721%
39	19.677	2786	2789	2793	rVV3	53014	76368	3.71%	0.526%
40	19.719	2793	2796	2802	rVB4	49226	82976	4.03%	0.571%
41	19.965	2835	2838	2839	rBV	26674	28965	1.41%	0.199%
42	20.001	2839	2844	2850	rVB	289251	440387	21.40%	3.030%
43	20.065	2852	2855	2860	rVB2	38463	51109	2.48%	0.352%
44	20.183	2870	2875	2880	rVB	1590121	2058066	100.00%	14.162%
45	21.892	3158	3166	3171	rBV3	454775	979282	47.58%	6.739%
46	25.294	3738	3745	3755	rVB2	261185	781441	37.97%	5.377%

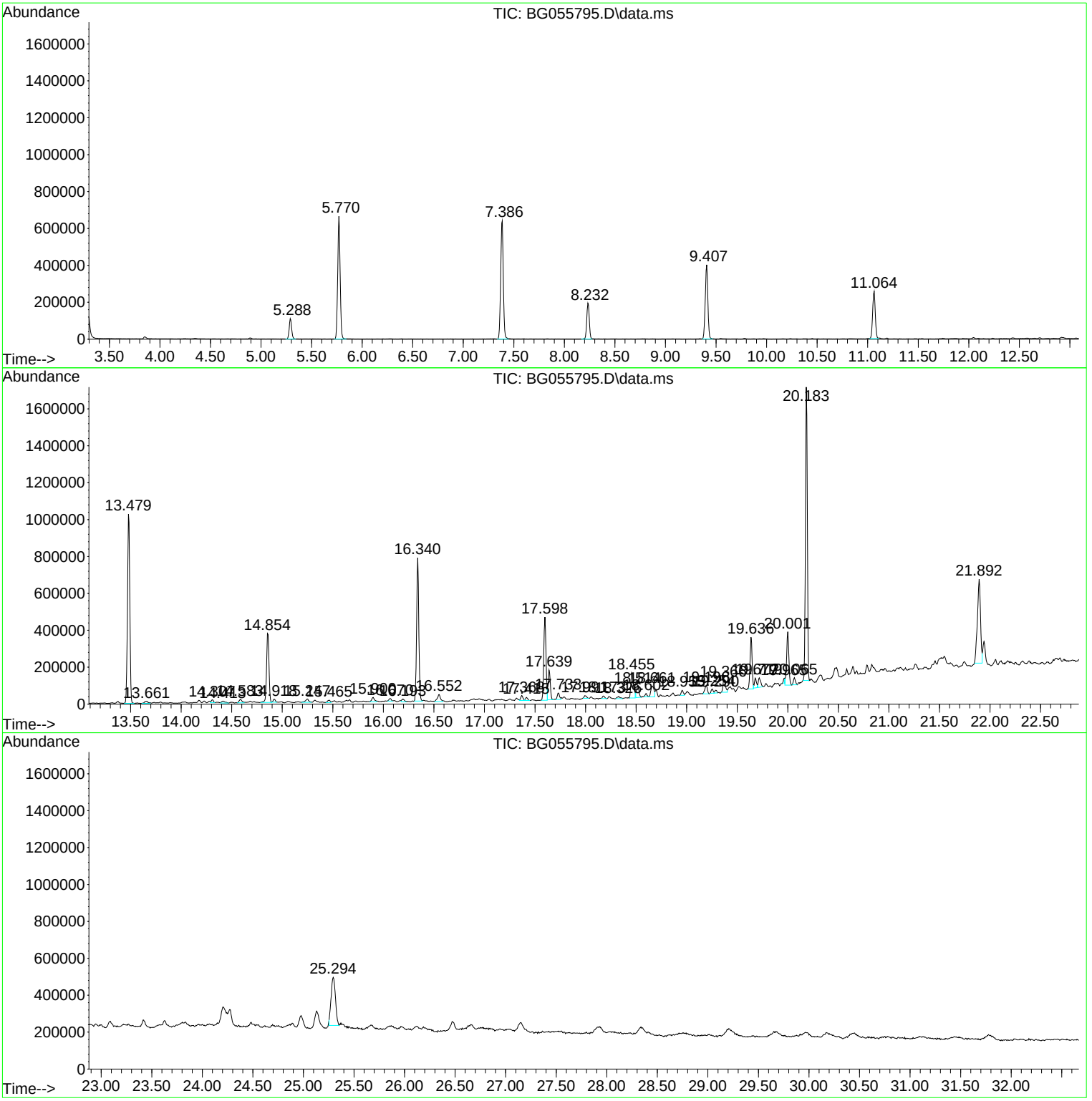
Sum of corrected areas: 14532186

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

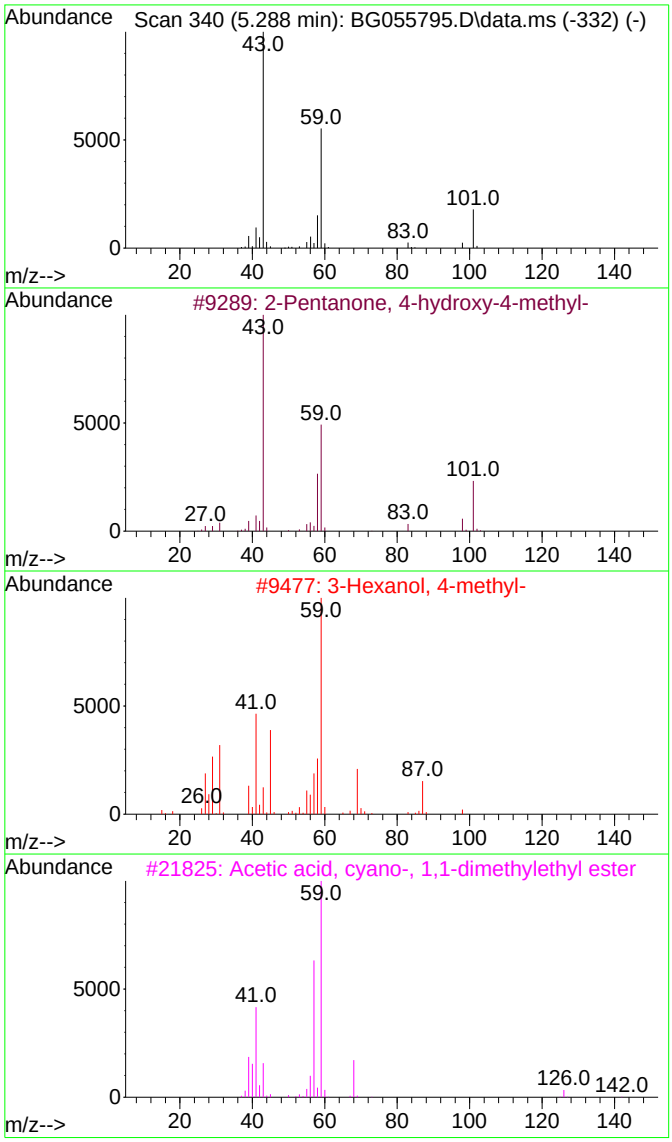
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

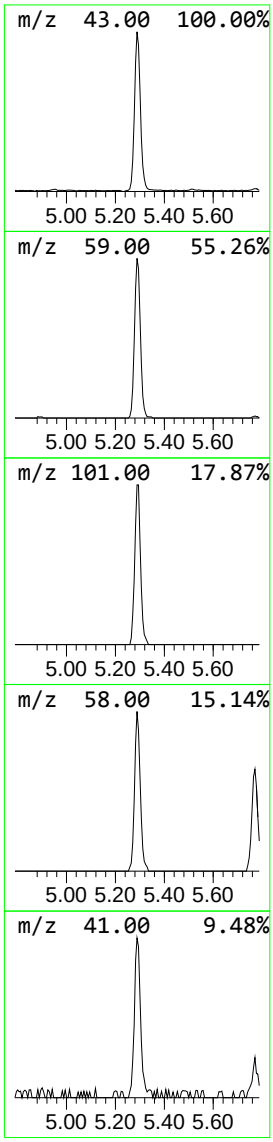
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.288	10.97 ng	184782	1,4-Dichlorobenzene-d4	8.232

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

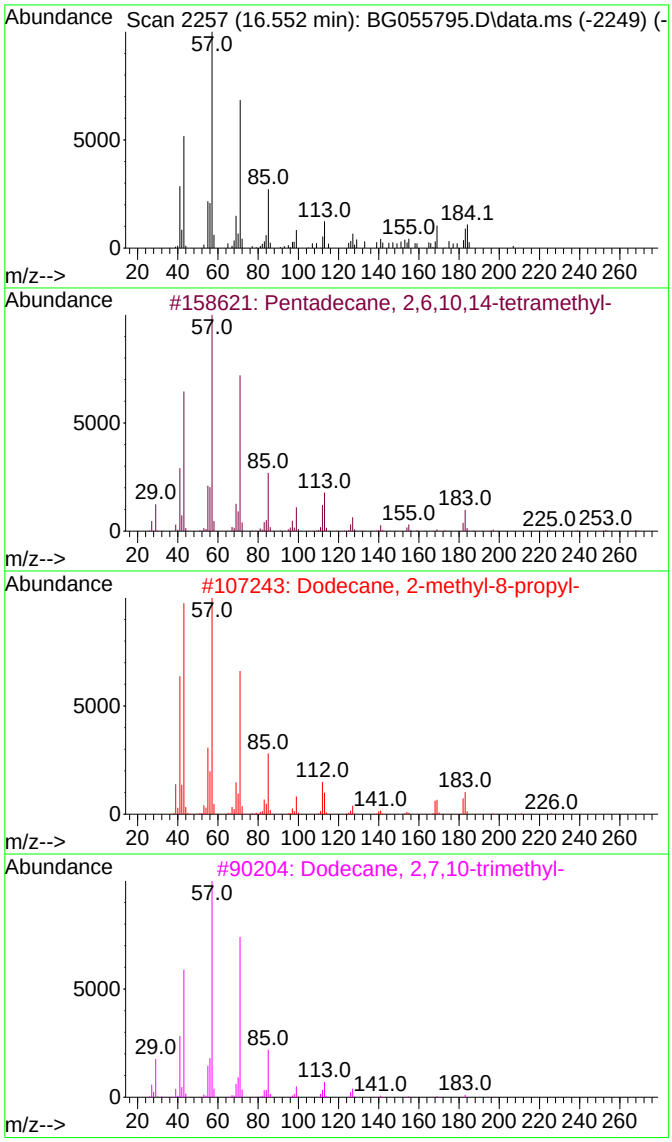
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

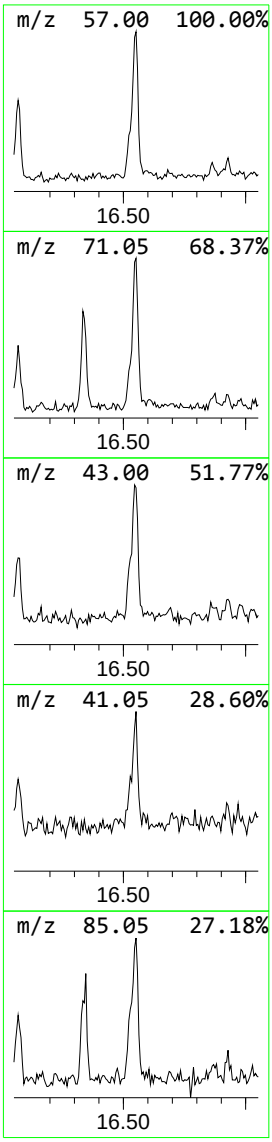
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentadecane, 2,6,10,14-tetr... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.552	2.29 ng	79037	Phenanthrene-d10	17.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	80
2	Dodecane, 2-methyl-8-propyl-	226	C16H34	055045-07-3	80
3	Dodecane, 2,7,10-trimethyl-	212	C15H32	074645-98-0	64
4	Dodecane, 2,6,10-trimethyl-	212	C15H32	003891-98-3	58
5	Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

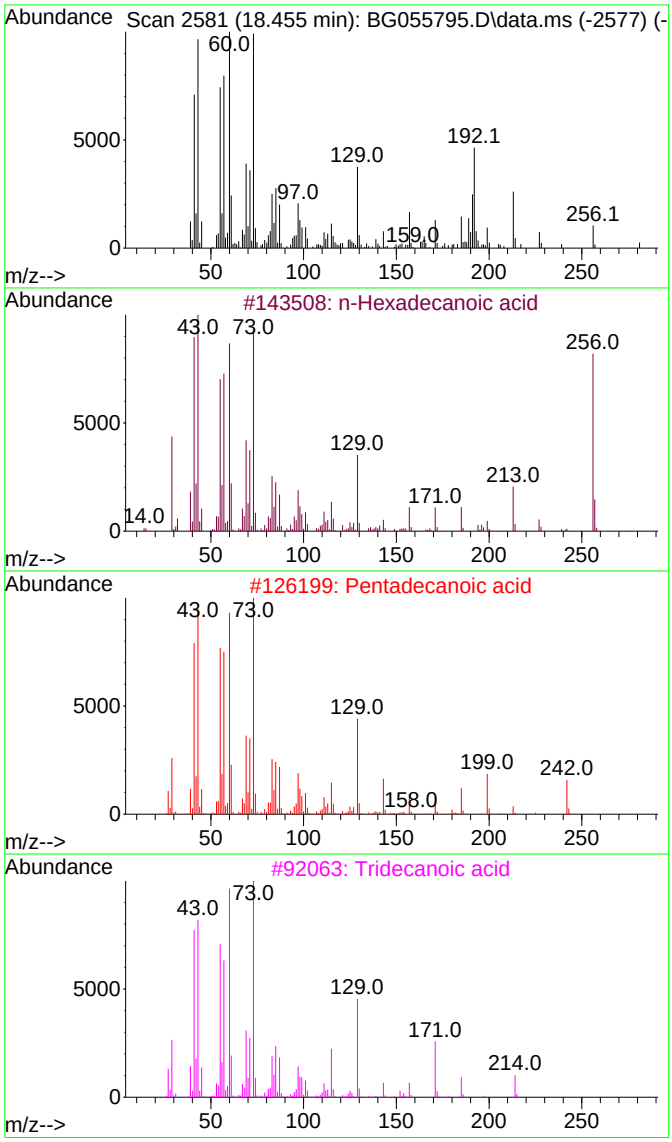
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

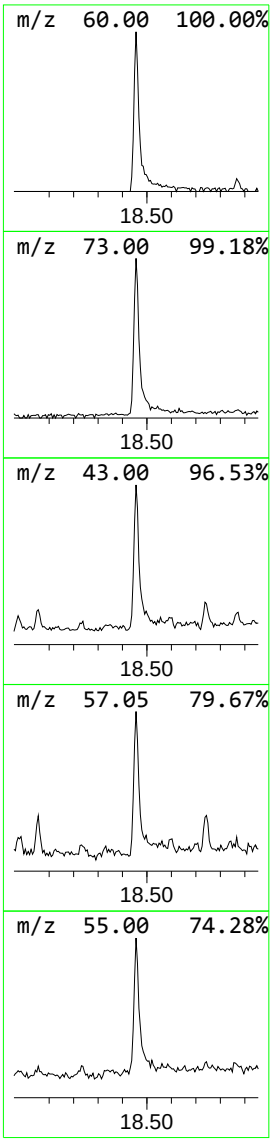
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.455	7.31 ng	252737	Phenanthrene-d10	17.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

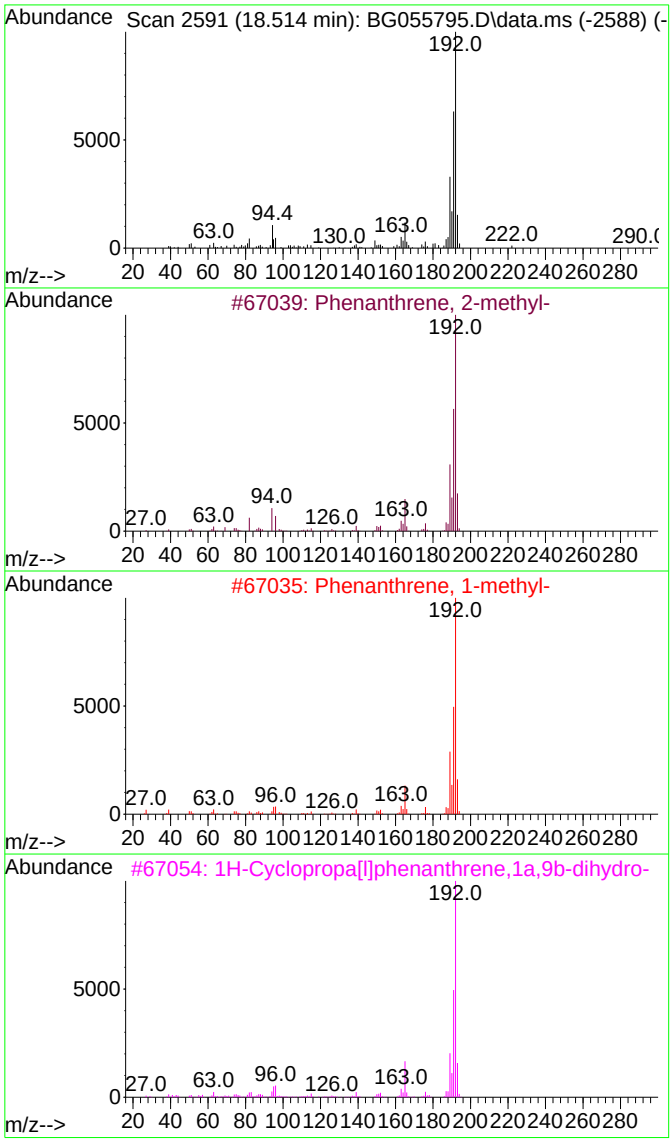
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

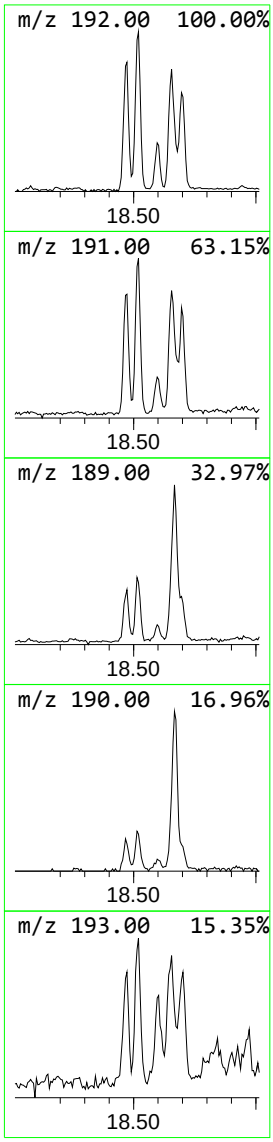
****

Peak Number 4 Phenanthrene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.514	2.88 ng	99582	Phenanthrene-d10	17.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95
2	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	93
3	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	93
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	90
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

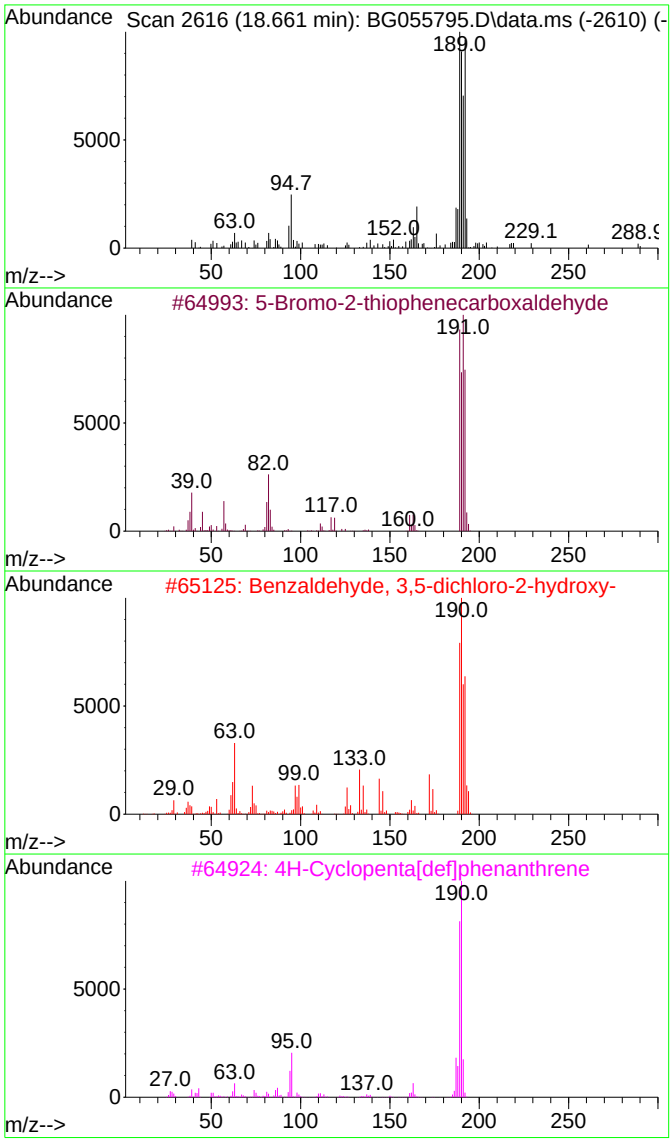
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

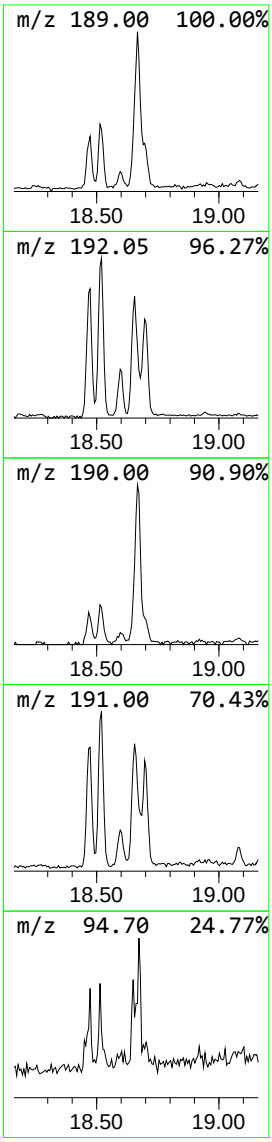
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 5-Bromo-2-thiophenecarboxal... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.661	3.65 ng	126198	Phenanthrene-d10	17.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Bromo-2-thiophenecarboxaldehyde	190	C5H3BrOS	004701-17-1	53
2	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	53
3	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	49
4	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	43
5	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	41





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

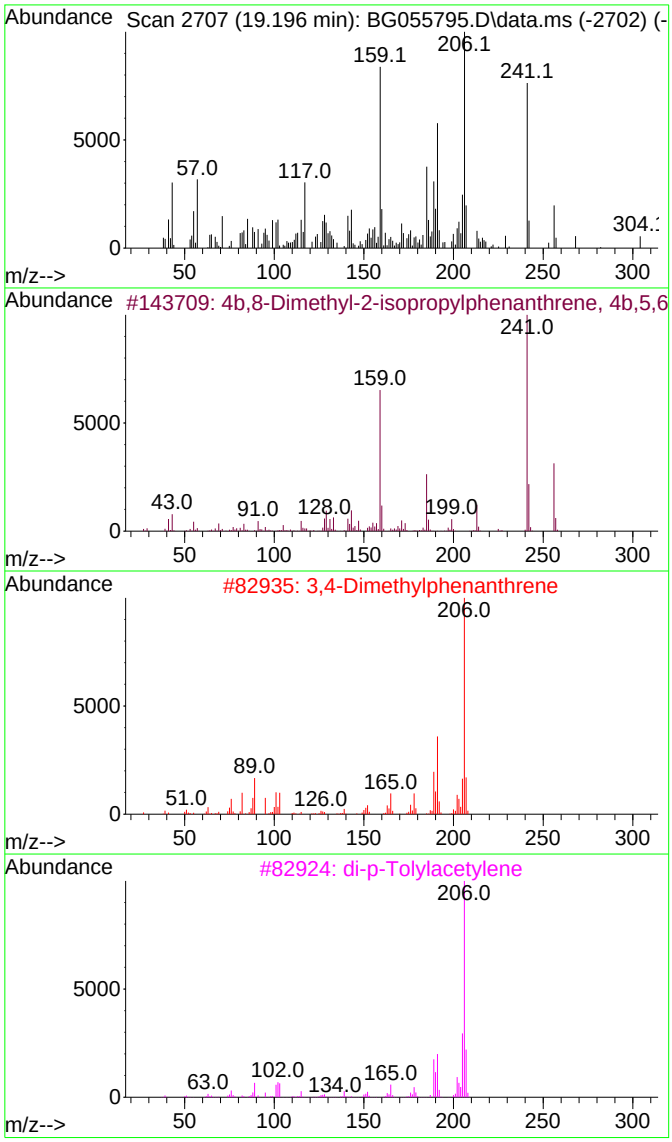
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

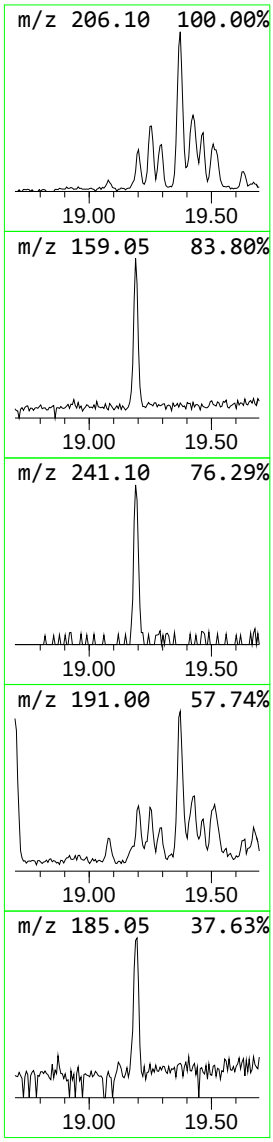
****

Peak Number 6 4b,8-Dimethyl-2-isopropylph... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.196	2.18 ng	75347	Phenanthrene-d10	17.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4b,8-Dimethyl-2-isopropylphenant...	256	C19H28	1000197-14-1	64
2	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	62
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	59
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	55
5	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

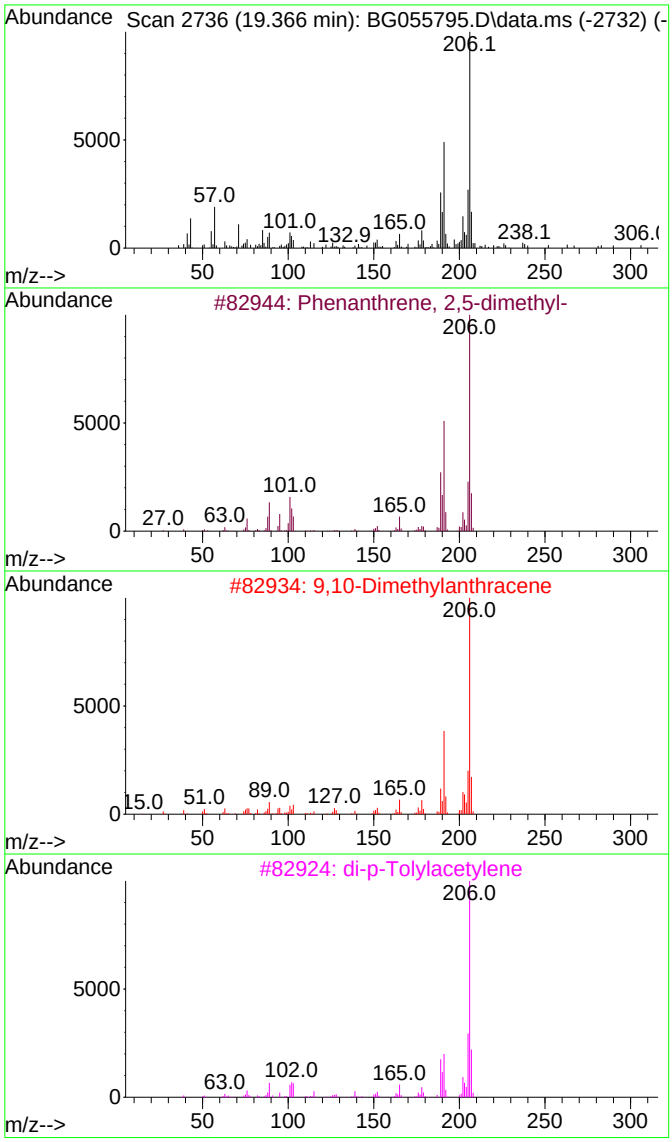
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

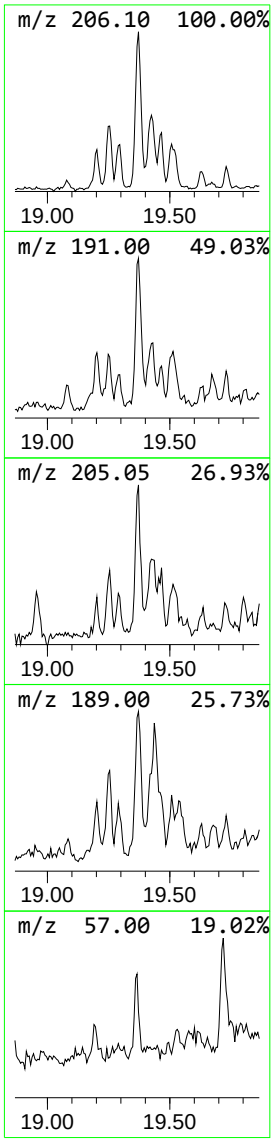
****

Peak Number 7 Phenanthrene, 2,5-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.366	3.42 ng	118195	Phenanthrene-d10	17.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	93
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	90
3	di-p-Tolylacetylene	206	C16H14	002789-88-0	90
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87
5	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

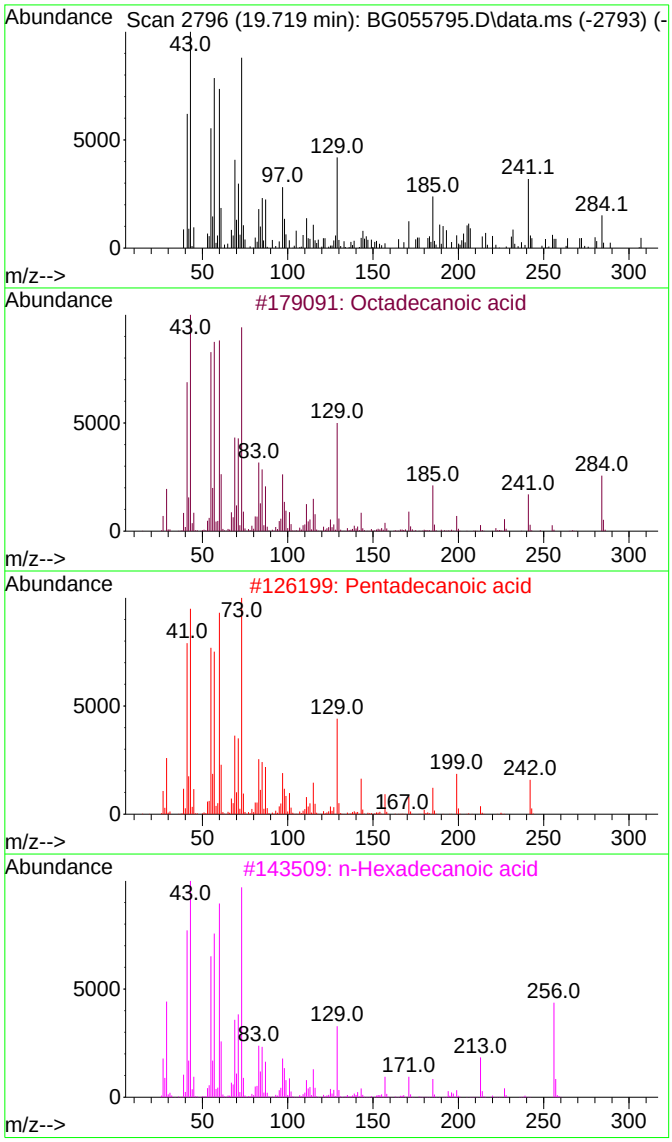
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

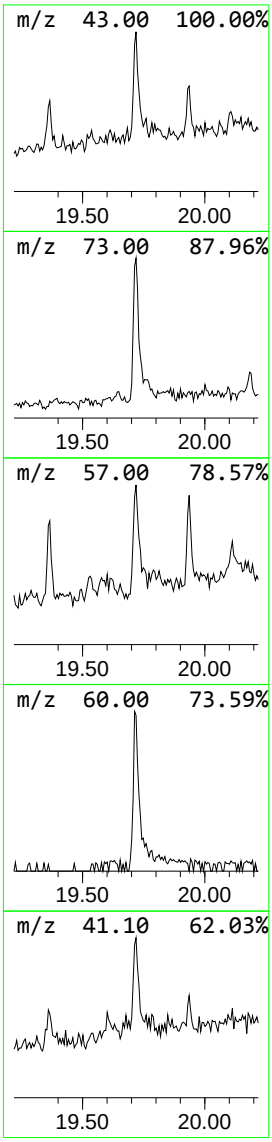
****

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.719	2.40 ng	82976	Phenanthrene-d10	17.598

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112522\
Data File : BG055795.D
Acq On : 26 Nov 2022 00:51
Operator : CG/JU
Sample : N5779-01
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CL-01-112322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111622.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-...	5.288	11.0	ng	184782	1	8.232	336777	20.0
Pentadecane, 2,...	16.552	2.3	ng	79037	4	17.598	691187	20.0
n-Hexadecanoic ...	18.455	7.3	ng	252737	4	17.598	691187	20.0
Phenanthrene, 2...	18.514	2.9	ng	99582	4	17.598	691187	20.0
5-Bromo-2-thiop...	18.661	3.6	ng	126198	4	17.598	691187	20.0
4b,8-Dimethyl-2...	19.196	2.2	ng	75347	4	17.598	691187	20.0
Phenanthrene, 2...	19.366	3.4	ng	118195	4	17.598	691187	20.0
Octadecanoic acid	19.719	2.4	ng	82976	4	17.598	691187	20.0