LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
Data File : BG055635.D
Acq On : 15 Nov 2022 23:54
Operator : CG/JU
Sample : N5431-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
20221176-COMP-11-MODIFIED-ELUTRIATE

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.689	232	238	245	rBV	17182	27404	1.07%	0.241%
2	5.306	338	343	350	rBV	47445	72961	2.86%	0.642%
3	5.782	417	424	435	rVB	288200	454707	17.83%	4.003%
4	7.392	690	698	707	rBV	211025	372748	14.62%	3.281%
5	8.256	837	845	852	rBV	134241	226810	8.90%	1.997%
6	9.425	1036	1044	1053	rVB	334367	597275	23.42%	5.258%
7	11.088	1319	1327	1334	rBV	182101	335347	13.15%	2.952%
8	13.502	1729	1738	1747	rBV	947658	1431637	56.15%	12.603%
9	14.877	1965	1972	1981	rVB	328150	511075	20.04%	4.499%
10	16.358	2217	2224	2240	rBV	886291	1388902	54.47%	12.226%
11	17.621	2431	2439	2447	rBV	450252	708809	27.80%	6.240%
12	18.256	2543	2547	2552	rVB	33516	41700	1.64%	0.367%
13	18.479	2580	2585	2596	rBV	253808	384776	15.09%	3.387%
14	19.413	2741	2744	2749	rVB2	24962	28178	1.11%	0.248%
15	19.619	2771	2779	2790	rBV2	16348	48219	1.89%	0.424%
16	19.736	2795	2799	2806	rBV	84143	137473	5.39%	1.210%
17	20.206	2873	2879	2885	rBV	1991995	2549770	100.00%	22.446%
18	21.534	3099	3105	3125	rBV4	90834	374608	14.69%	3.298%
19	21.916	3163	3170	3180	rVB2	466065	785327	30.80%	6.913%
20	23.679	3466	3470	3480	rVB3	34263	74007	2.90%	0.651%
21	25.330	3741	3751	3762	rVB2	272073	808089	31.69%	7.114%

Sum of corrected areas: 11359822

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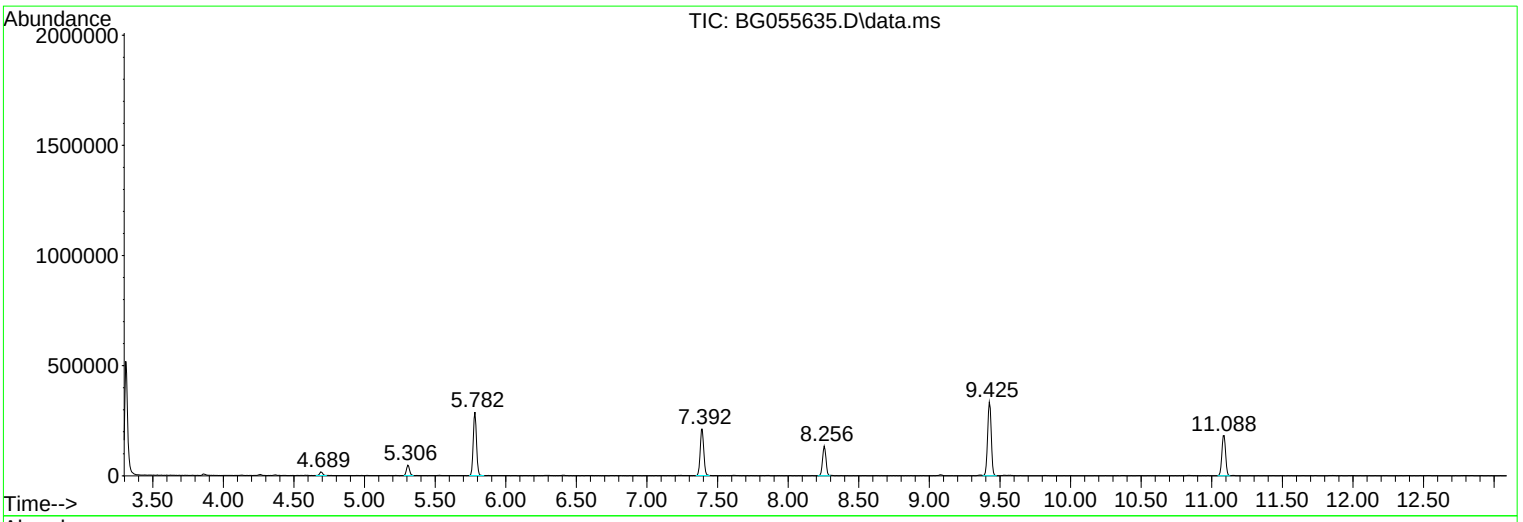
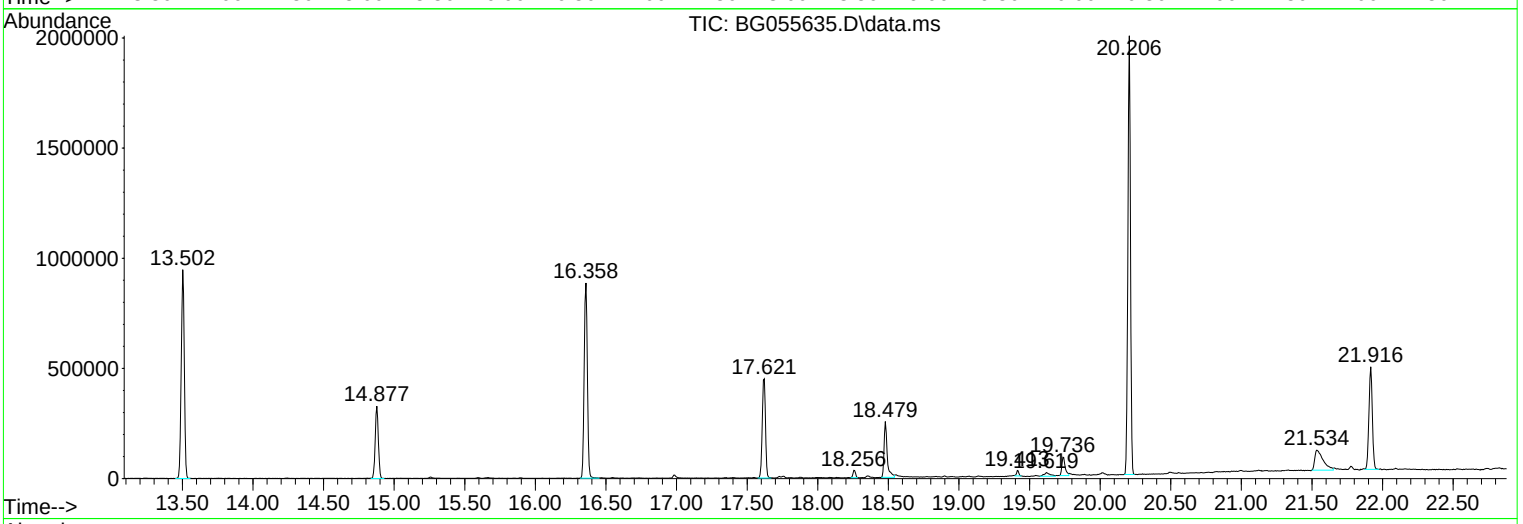
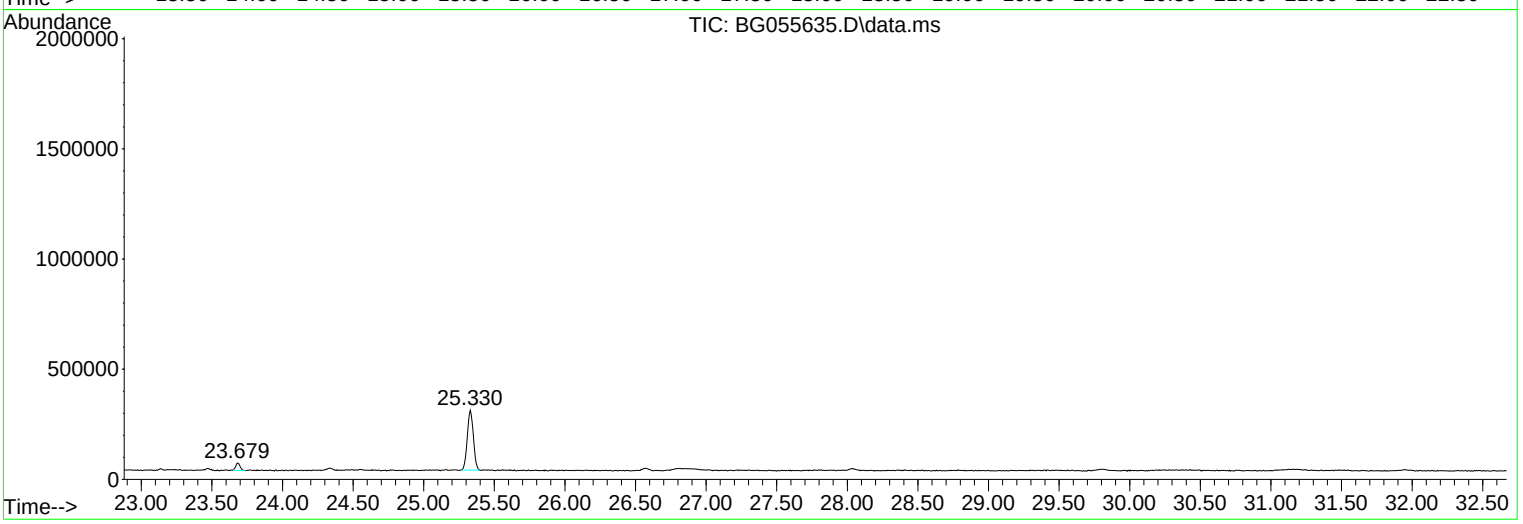
BNA_G
ClientSampleId :
20221176-COMP-11-MODIFIED-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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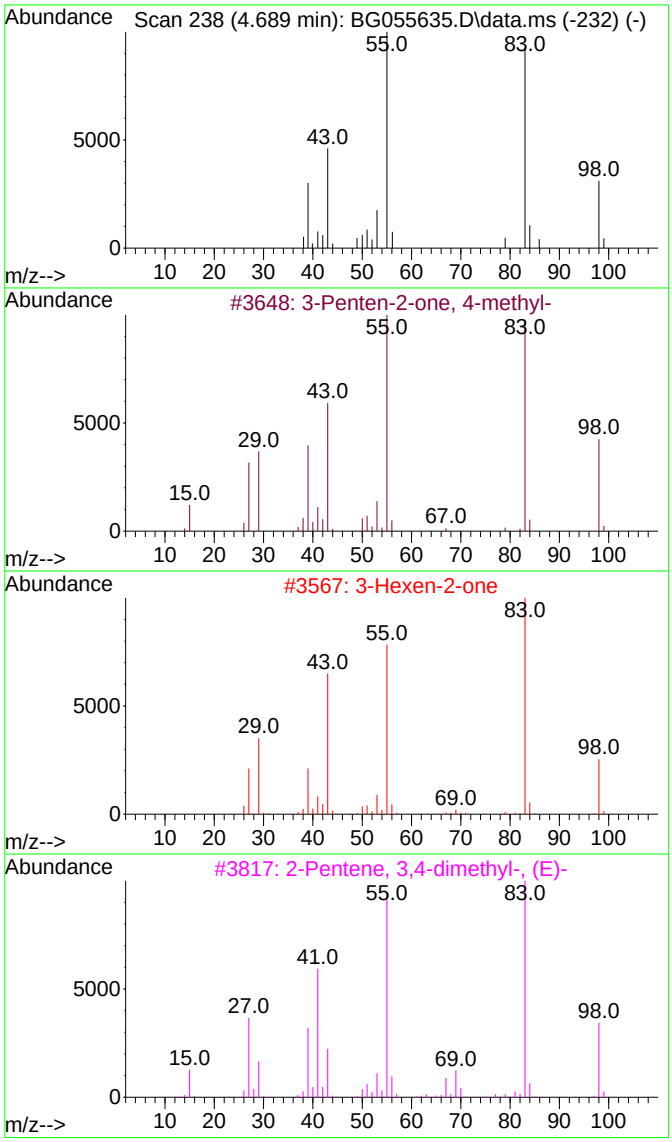
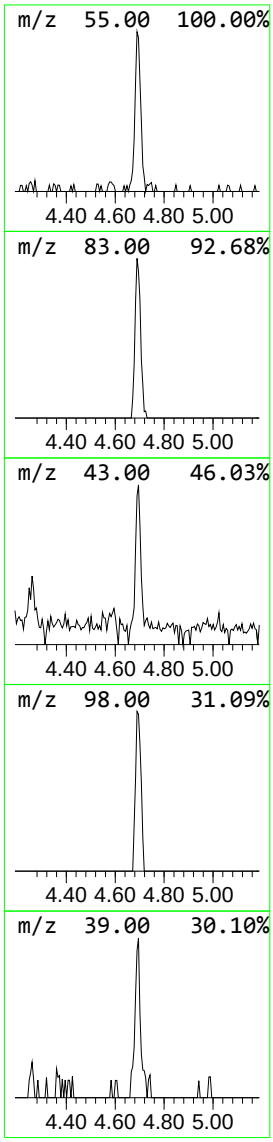
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.689	2.42 ng	27404	1,4-Dichlorobenzene-d4	8.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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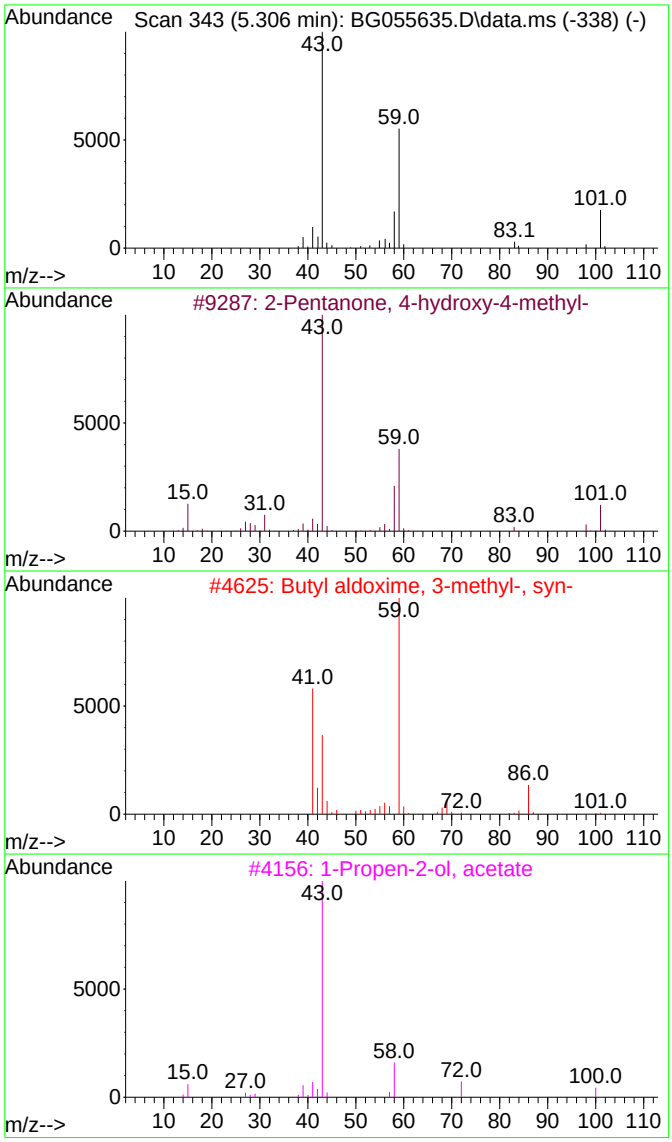
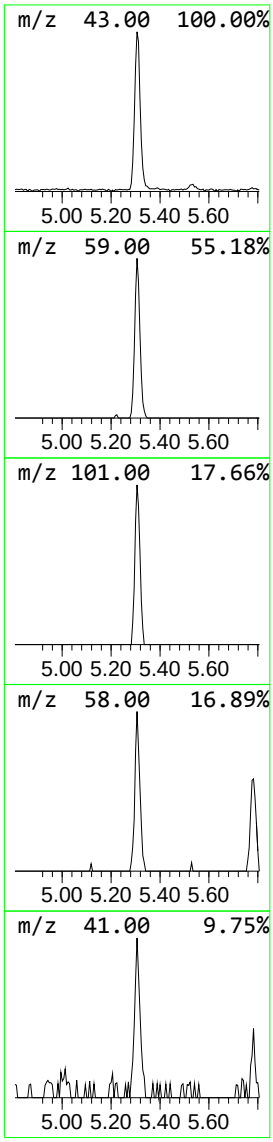
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.306	6.43 ng	72961	1,4-Dichlorobenzene-d4	8.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	Acetone	58	C3H6O	000067-64-1	12
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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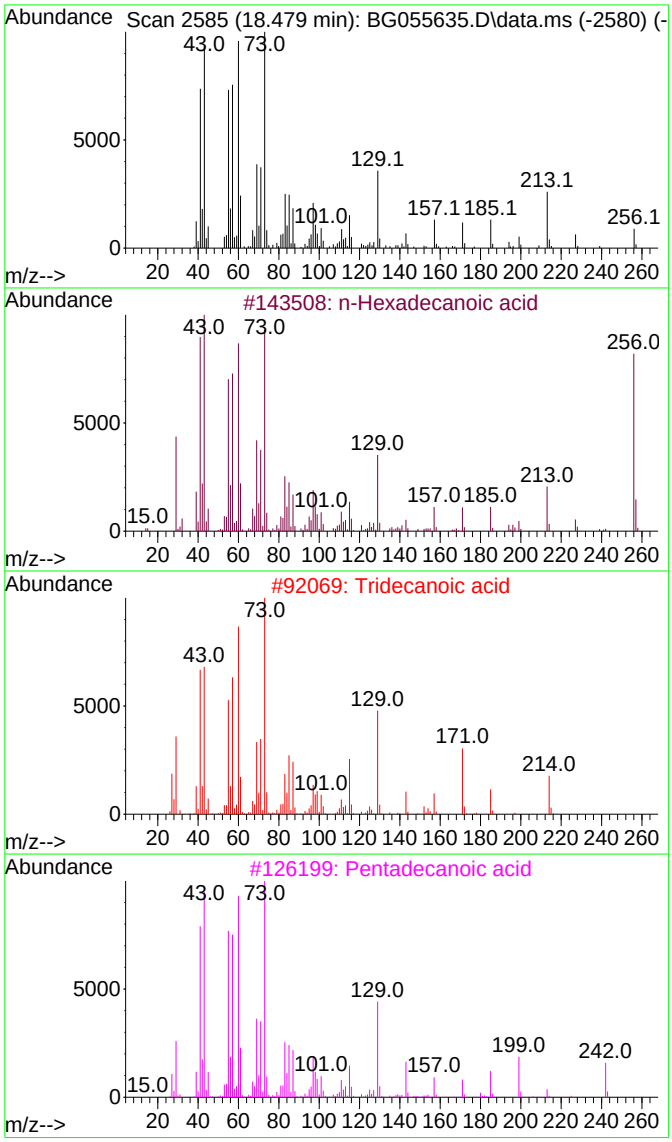
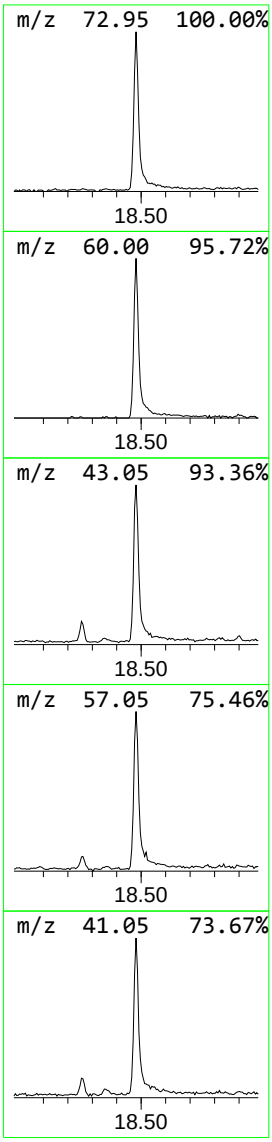
Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.479	10.86 ng	384776	Phenanthrene-d10	17.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	70





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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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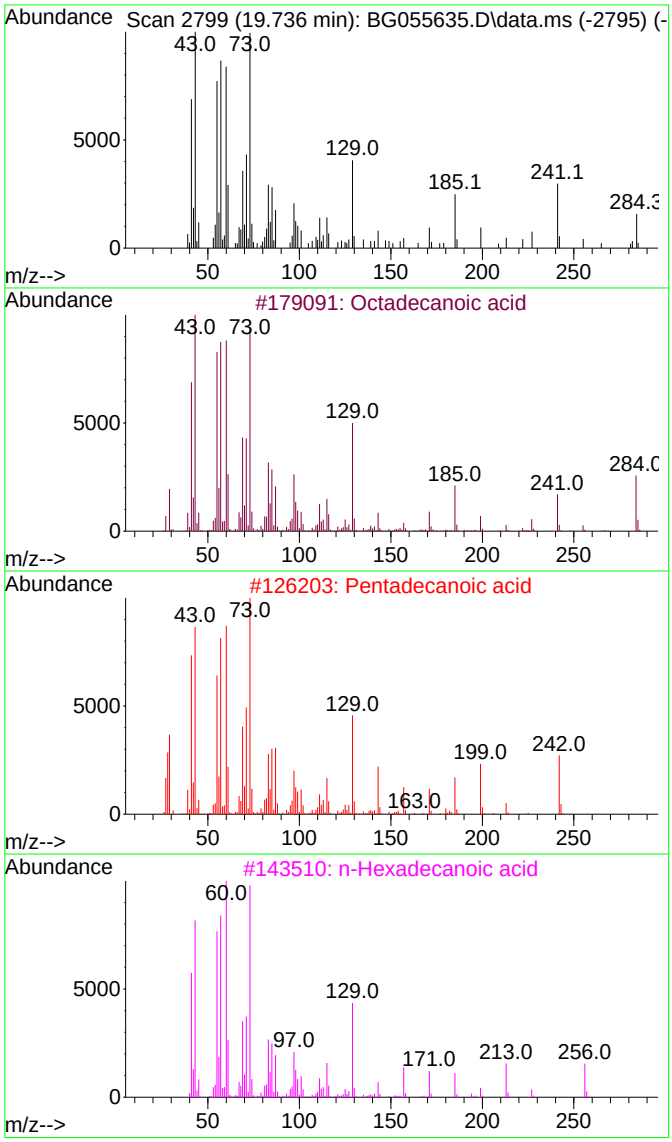
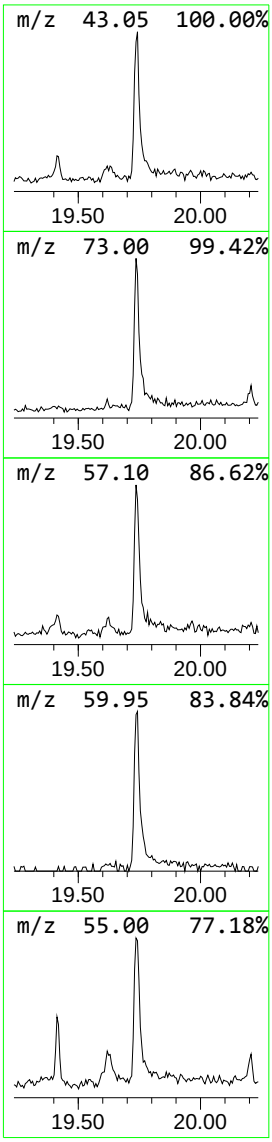
Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.736	3.88 ng	137473	Phenanthrene-d10	17.621

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	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Eicosane	282	C20H42	000112-95-8	56





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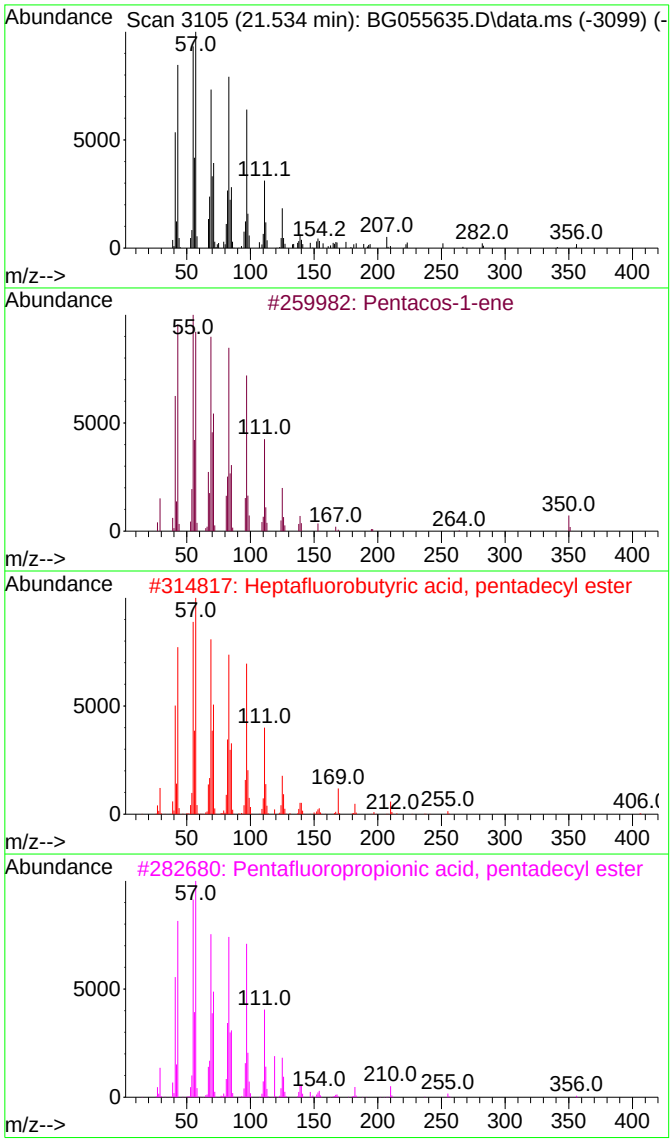
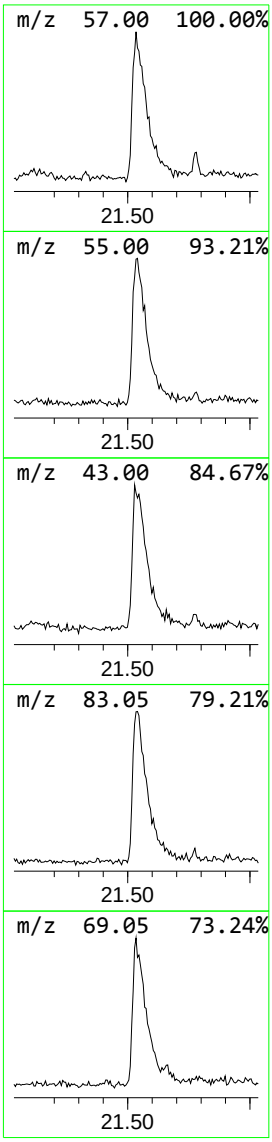
Peak Number 5 Pentacos-1-ene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.534	9.54 ng	374608	Chrysene-d12	21.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacos-1-ene	350	C25H50	016980-85-1	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4	Cyclotetracosane	336	C24H48	000297-03-0	93
5	1-Hexacosene	364	C26H52	018835-33-1	91





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.689	2.4	ng	27404	1	8.256	226810	20.0
2-Pentanone, 4-...	5.306	6.4	ng	72961	1	8.256	226810	20.0
n-Hexadecanoic ...	18.479	10.9	ng	384776	4	17.621	708809	20.0
Octadecanoic acid	19.736	3.9	ng	137473	4	17.621	708809	20.0
Pentacos-1-ene	21.534	9.5	ng	374608	5	21.916	785327	20.0