LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055986.D
Acq On : 15 Dec 2022 21:14
Operator : CG/JU
Sample : N6058-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-03-121422

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055986.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.412	16	21	29	rBB3	6707	11435	1.64%	0.369%
2	5.421	359	363	368	rBB2	5896	8942	1.28%	0.289%
3	5.897	438	444	451	rBB	55131	89971	12.88%	2.904%
4	7.507	711	718	725	rBB	57547	99687	14.27%	3.218%
5	8.383	861	867	873	rBB	39097	65714	9.41%	2.121%
6	9.552	1059	1066	1072	rBB	35323	61685	8.83%	1.991%
7	11.215	1342	1349	1356	rBB	51446	89868	12.87%	2.901%
8	13.612	1751	1757	1764	rBB	123039	188328	26.96%	6.079%
9	14.987	1985	1991	1998	rBB2	87513	136073	19.48%	4.392%
10	16.461	2236	2242	2249	rBV	128071	192041	27.49%	6.199%
11	17.725	2451	2457	2461	rBV	119934	173983	24.91%	5.616%
12	17.766	2461	2464	2470	rVB	13966	20644	2.96%	0.666%
13	18.353	2559	2564	2569	rVB	124534	161544	23.13%	5.214%
14	18.571	2597	2601	2608	rBV3	18195	34974	5.01%	1.129%
15	18.641	2609	2613	2618	rVB	9512	13806	1.98%	0.446%
16	18.782	2631	2637	2640	rBV3	10800	22393	3.21%	0.723%
17	19.035	2676	2680	2682	rBV4	4938	8000	1.15%	0.258%
18	19.481	2751	2756	2759	rBV	558805	698518	100.00%	22.547%
19	19.511	2759	2761	2770	rVB2	294843	380577	54.48%	12.285%
20	19.634	2778	2782	2787	rBV	64290	81420	11.66%	2.628%
21	19.752	2798	2802	2806	rBV	24972	36140	5.17%	1.167%
22	20.075	2855	2857	2859	rBV3	9362	9249	1.32%	0.299%
23	20.116	2860	2864	2869	rVB	30433	50296	7.20%	1.623%
24	20.298	2890	2895	2900	rBV	226372	300010	42.95%	9.684%
25	22.037	3186	3191	3197	rVB2	95304	162708	23.29%	5.252%

Sum of corrected areas: 3098006

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Instrument :
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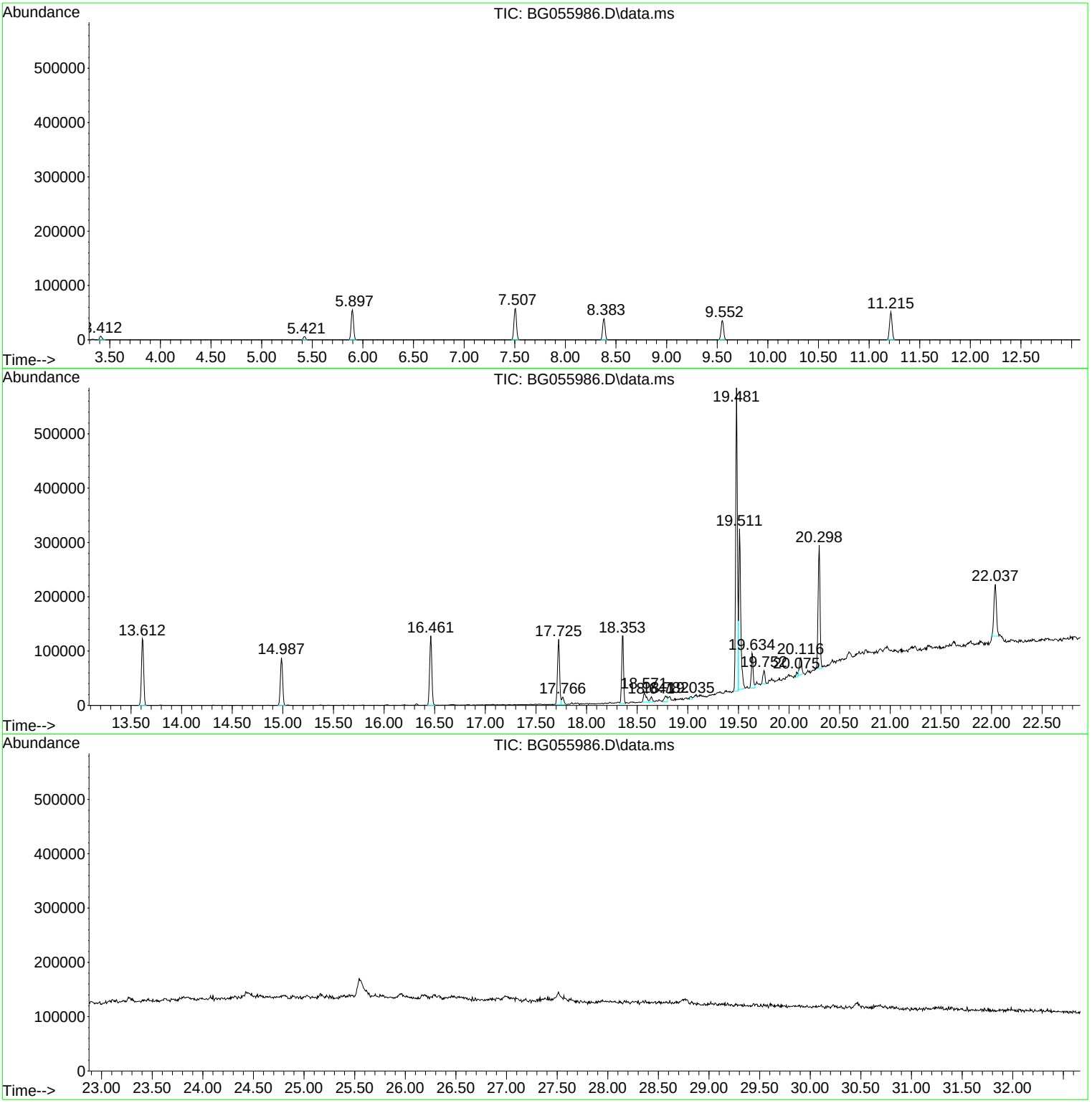
ClientSampleId :
SU-03-121422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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\BG121522\
Data File : BG055986.D
Acq On : 15 Dec 2022 21:14
Operator : CG/JU
Sample : N6058-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

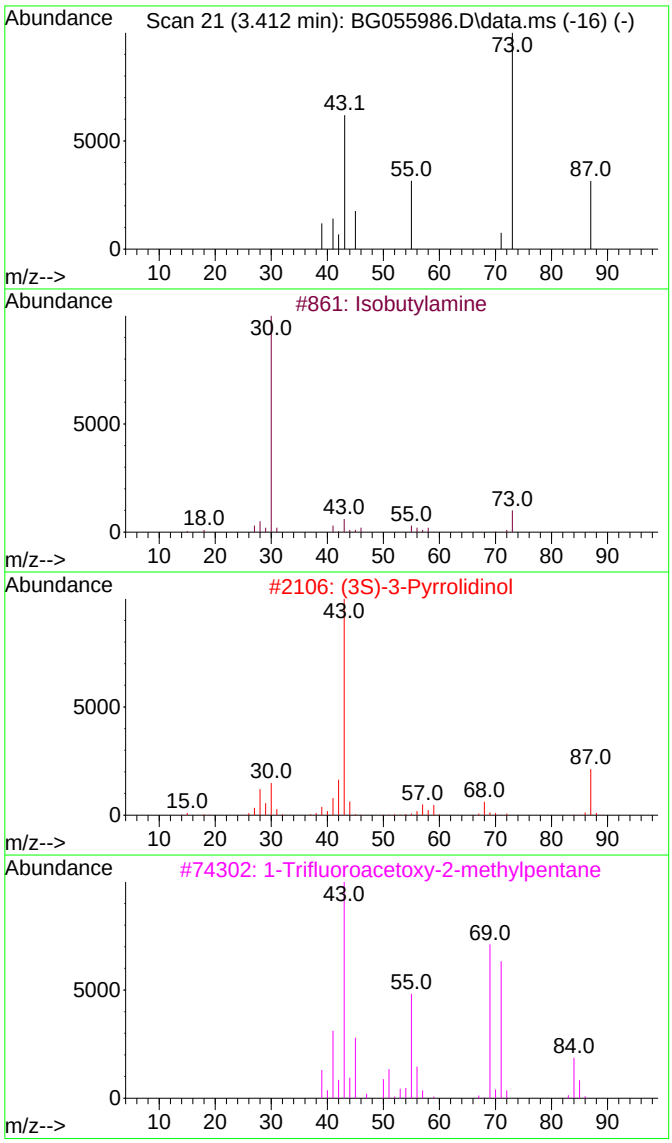
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

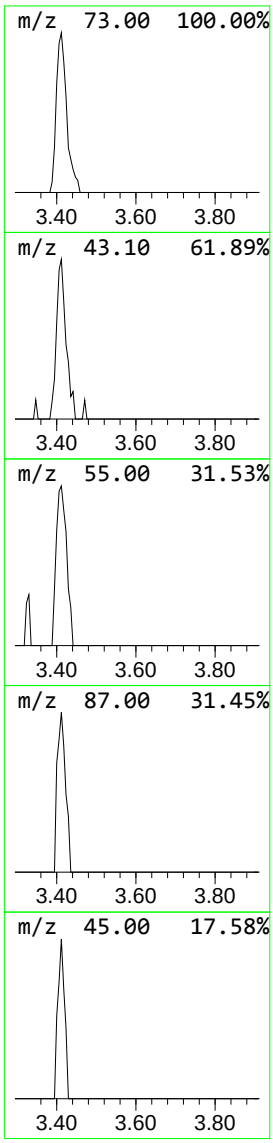
****

Peak Number 1 unknown3.412 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.412	3.48 ng	11435	1,4-Dichlorobenzene-d4	8.383

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutylamine	73	C4H11N	000078-81-9	4
2	(3S)-3-Pyrrolidinol	87	C4H9NO	100243-39-8	4
3	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	4
4	Hydroperoxide, 1-methylbutyl	104	C5H12O2	014018-58-7	4
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	4





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Data File : BG055986.D
Acq On : 15 Dec 2022 21:14
Operator : CG/JU
Sample : N6058-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-03-121422

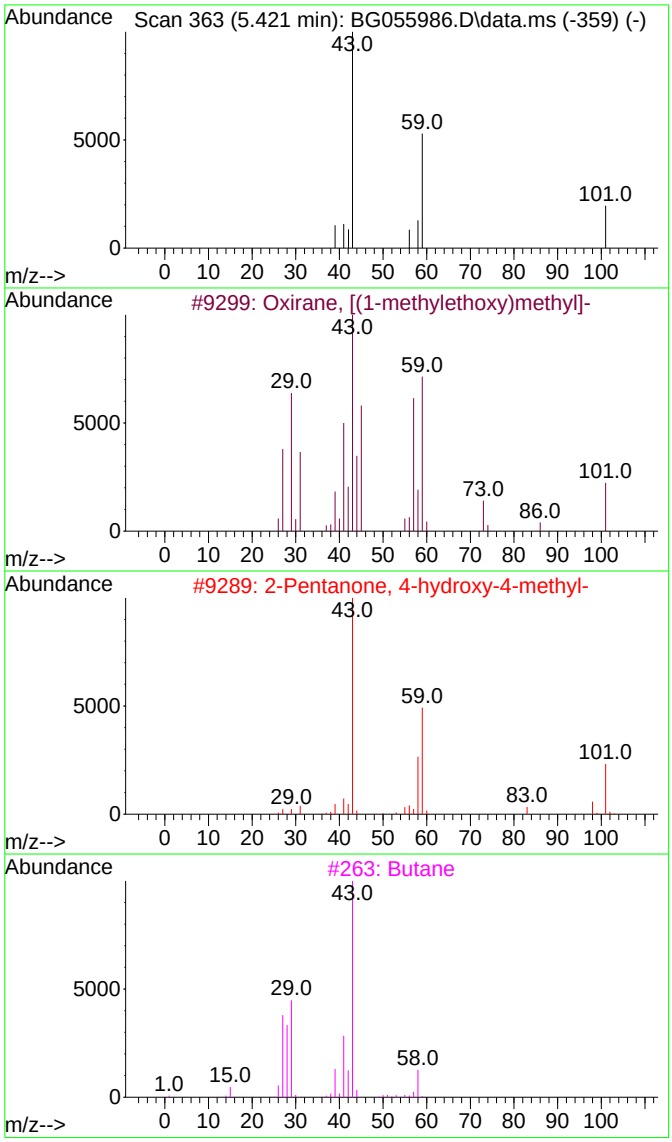
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

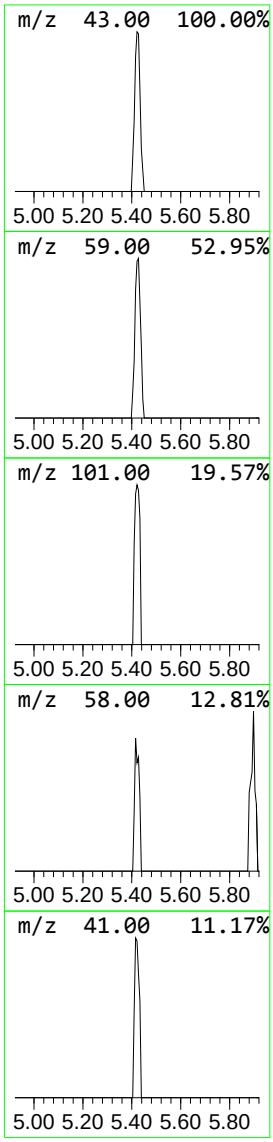
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Oxirane, [(1-methylethoxy)m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.421	2.72 ng	8942	1,4-Dichlorobenzene-d4	8.383

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	64
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
3	Butane	58	C4H10	000106-97-8	7
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055986.D
Acq On : 15 Dec 2022 21:14
Operator : CG/JU
Sample : N6058-01 2X
Misc :
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Instrument :
BNA_G
ClientSampleId :
SU-03-121422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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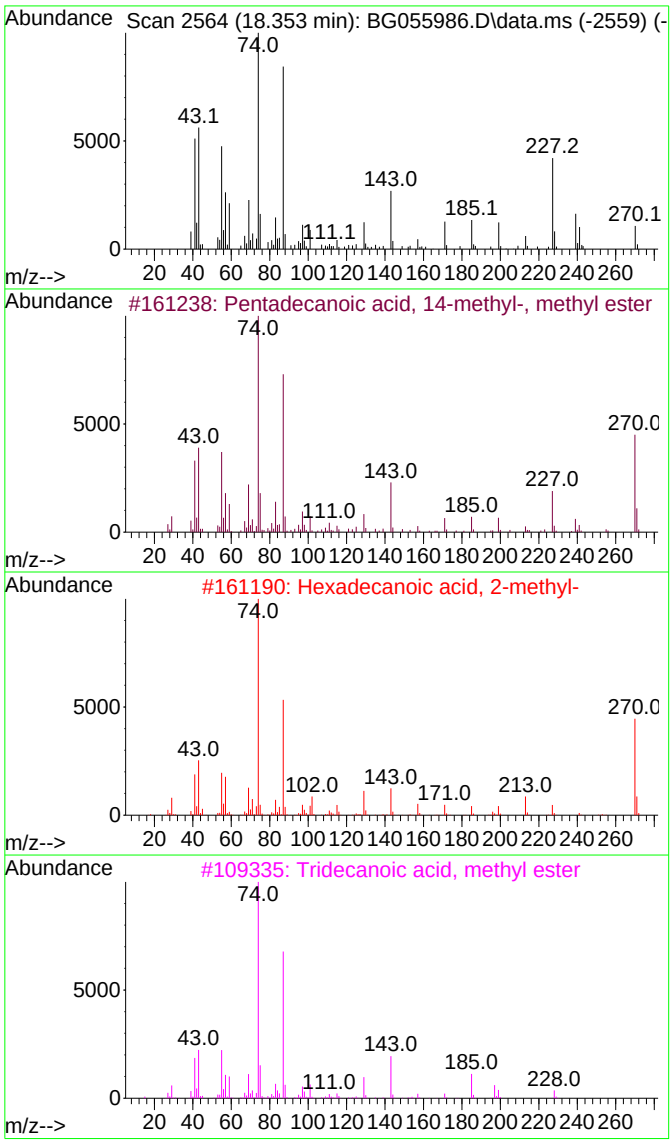
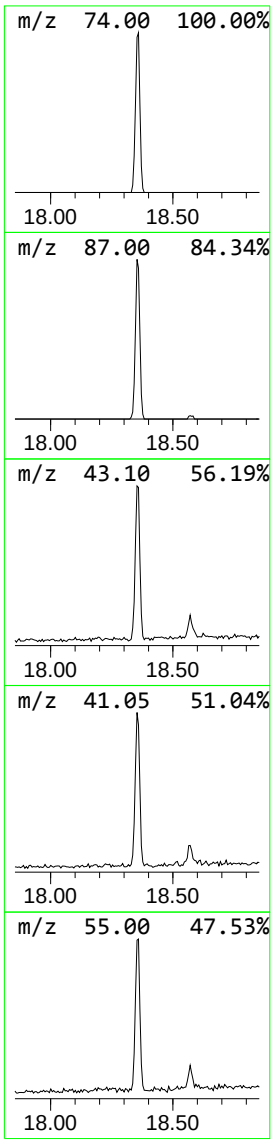
****
Peak Number 3 Pentadecanoic acid, 14-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.353	18.57 ng	161544	Phenanthrene-d10	17.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
2	Hexadecanoic acid, 2-methyl-	270	C17H34O2	027147-71-3	89
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	83
4	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	78
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	76





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Data File : BG055986.D
Acq On : 15 Dec 2022 21:14
Operator : CG/JU
Sample : N6058-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-03-121422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

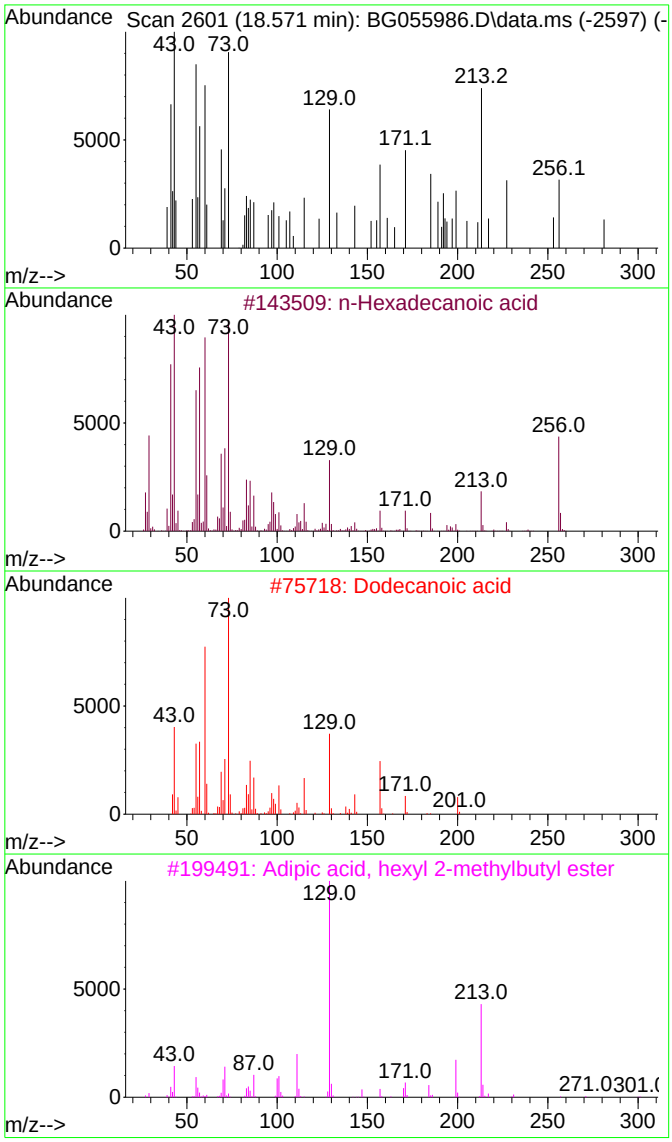
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

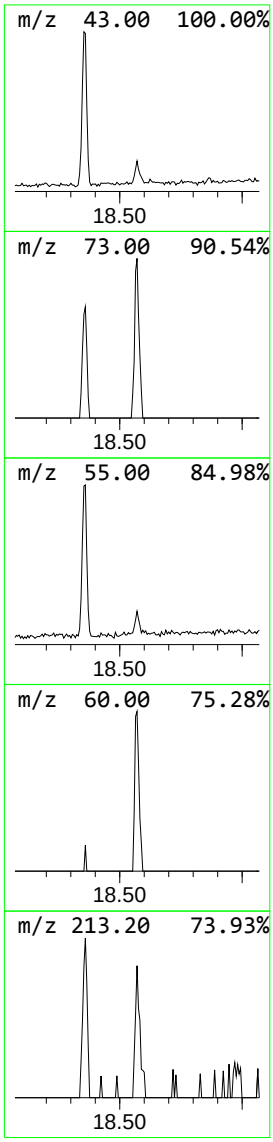
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.571	4.02 ng	34974	Phenanthrene-d10	17.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
2	Dodecanoic acid	200	C12H24O2	000143-07-7	35
3	Adipic acid, hexyl 2-methylbutyl...	300	C17H32O4	1000324-67-5	27
4	Tridecanoic acid	214	C13H26O2	000638-53-9	27
5	Chlorpropham	213	C10H12ClNO2	000101-21-3	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
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Operator : CG/JU
Sample : N6058-01 2X
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SU-03-121422

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

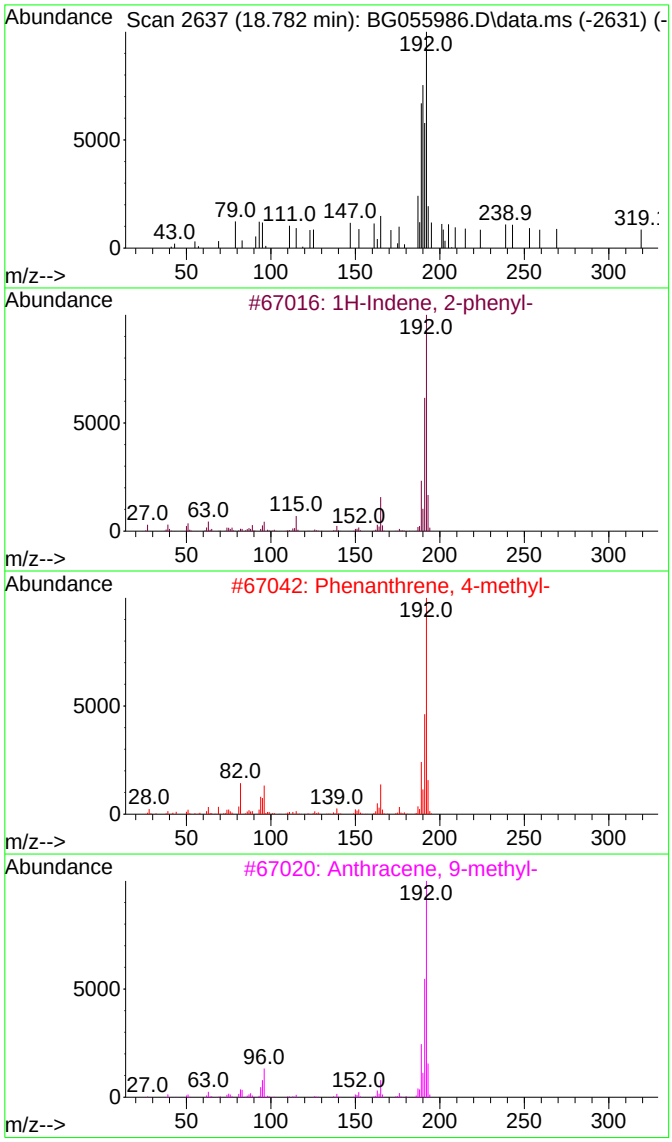
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

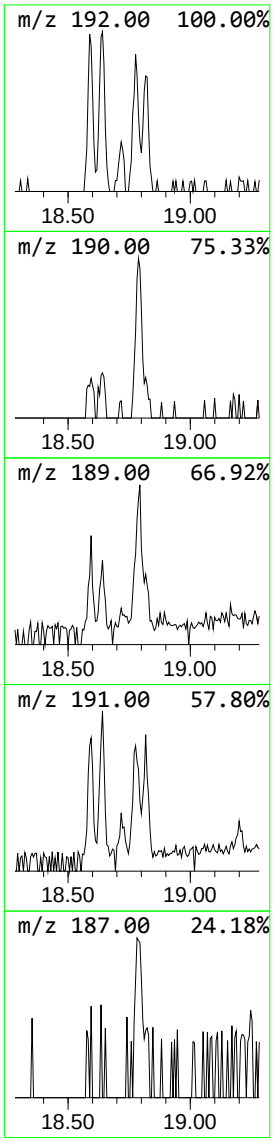
****

Peak Number 5 unknown18.782 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.782	2.57 ng	22393	Phenanthrene-d10	17.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	43
2	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	43
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	43
4	1-(9-Phenanthrenyl)-2-propanol	236	C17H16O	1000326-09-0	43
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	43





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Instrument :
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ClientSampleId :
SU-03-121422

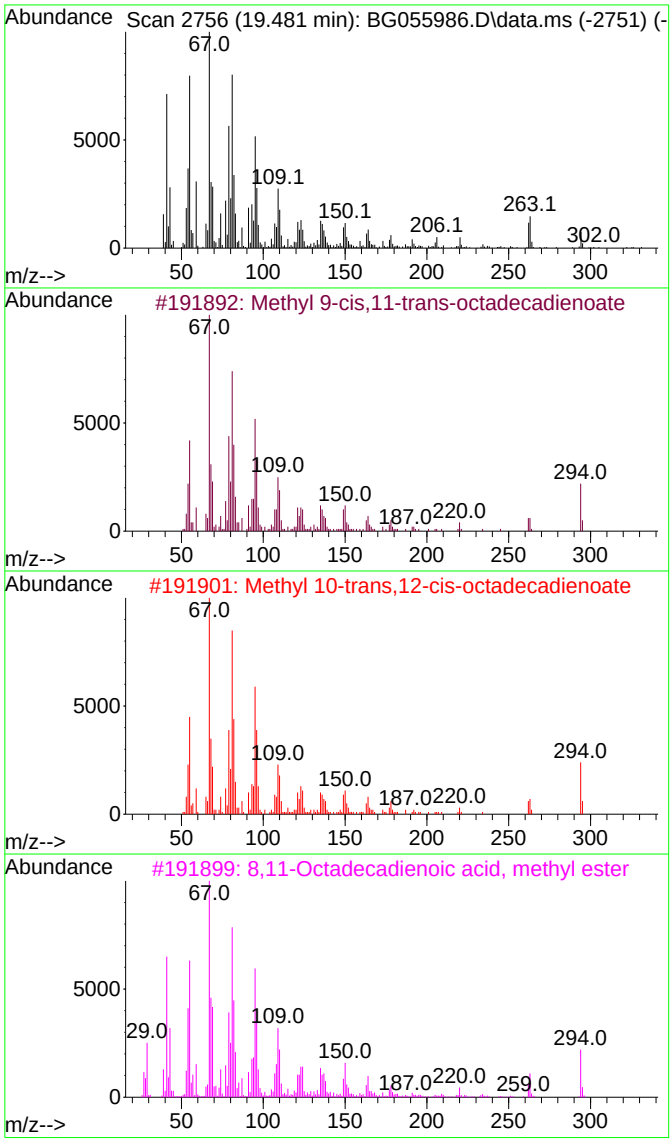
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

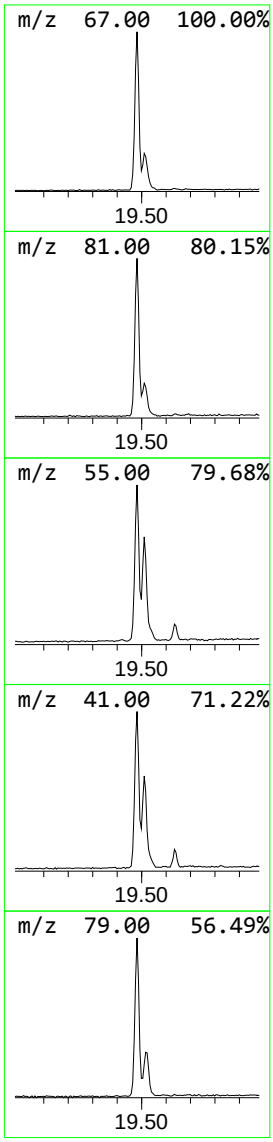
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Methyl 9-cis,11-trans-octad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.481	80.30 ng	698518	Phenanthrene-d10	17.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	98
2	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98
3	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	96
4	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	96
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	95





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Instrument :
BNA_G
ClientSampleId :
SU-03-121422

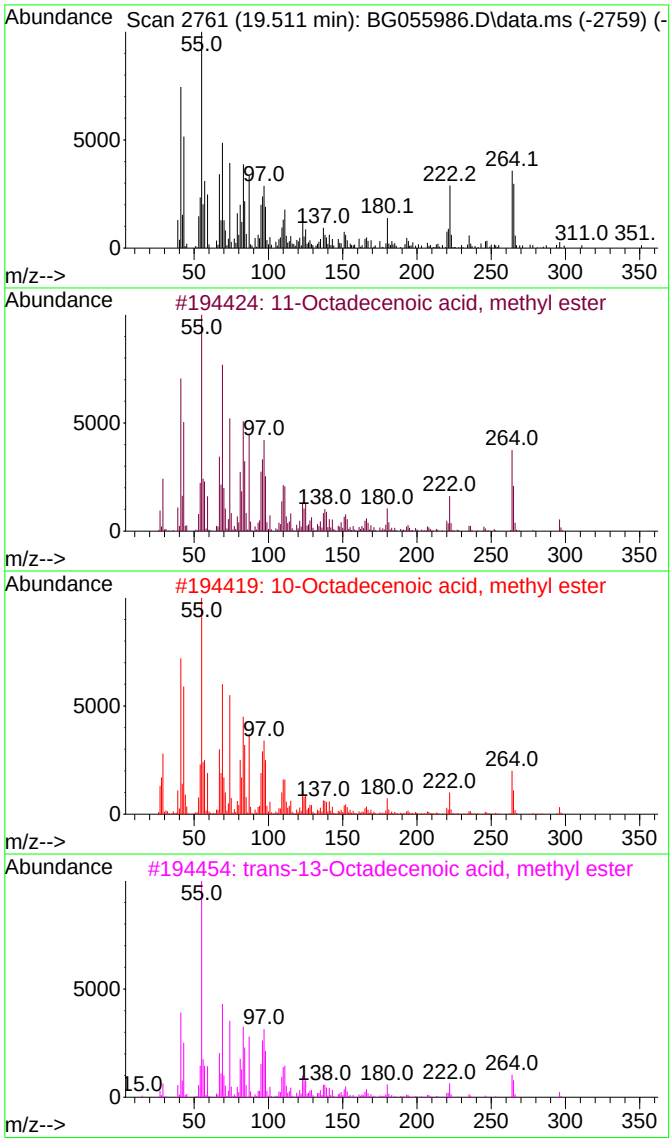
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

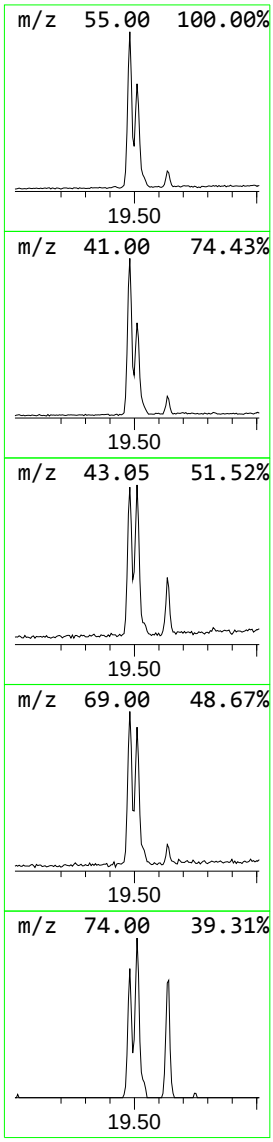
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 11-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.511	43.75 ng	380577	Phenanthrene-d10	17.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	98
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	98
3	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	98
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	96
5	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	96





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BNA_G
ClientSampleId :
SU-03-121422

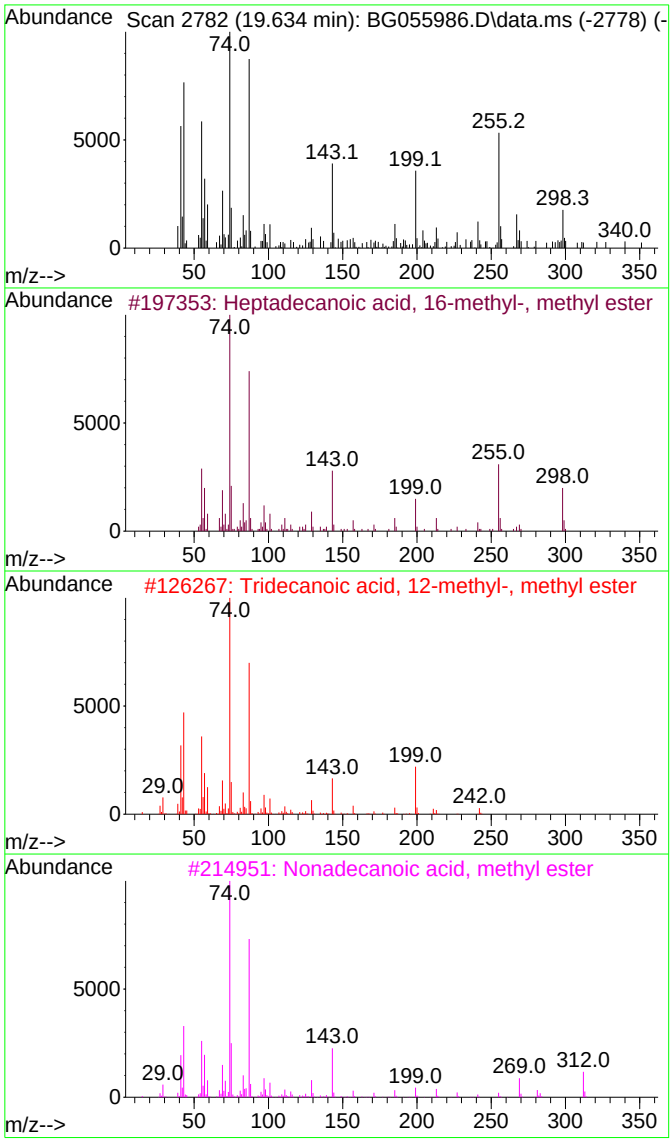
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

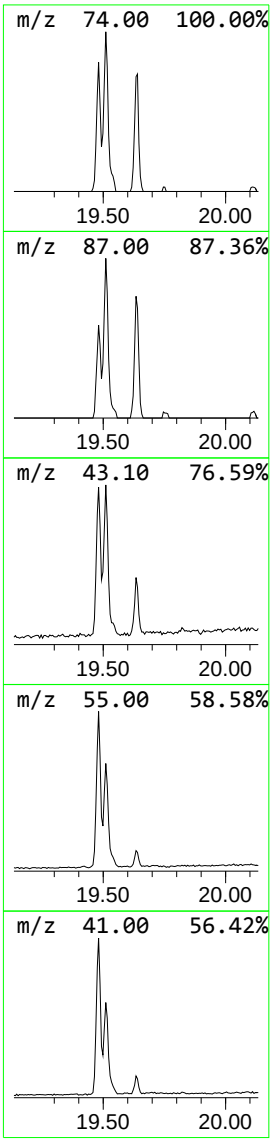
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Heptadecanoic acid, 16-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.634	9.36 ng	81420	Phenanthrene-d10	17.724

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
2	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	83
3	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	83
4	Methyl stearate	298	C19H38O2	000112-61-8	70
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	60





Tentatively Identified Compound (LSC) summary

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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
unknown3.412	3.412	3.5	ng	11435	1	8.383	65714	20.0
Oxirane, [(1-me...	5.421	2.7	ng	8942	1	8.383	65714	20.0
Pentadecanoic a...	18.353	18.6	ng	161544	4	17.724	173983	20.0
n-Hexadecanoic ...	18.571	4.0	ng	34974	4	17.724	173983	20.0
unknown18.782	18.782	2.6	ng	22393	4	17.724	173983	20.0
Methyl 9-cis,11...	19.481	80.3	ng	698518	4	17.724	173983	20.0
11-Octadecenoic...	19.511	43.8	ng	380577	4	17.724	173983	20.0
Heptadecanoic a...	19.634	9.4	ng	81420	4	17.724	173983	20.0