LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102922\
Data File : BM037280.D
Acq On : 29 Oct 2022 20:35
Operator : CG/JU
Sample : N5234-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : LSP-SS-04-15-3

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_M\Methods\8270-BM102822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037280.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.975	315	321	328	rBV	709289	1005580	7.88%	1.187%
2	5.440	393	400	416	rBV	6183969	8580310	67.24%	10.131%
3	7.046	665	673	689	rBV	5798876	9151432	71.71%	10.805%
4	7.869	806	813	820	rBV	1717118	2562488	20.08%	3.025%
5	9.040	1004	1012	1024	rBV	3526620	5642678	44.22%	6.662%
6	10.451	1244	1252	1265	rBV	142740	296620	2.32%	0.350%
7	10.669	1282	1289	1301	rBV	2165800	3606893	28.26%	4.259%
8	13.133	1700	1708	1719	rBV	8166956	12042957	94.37%	14.219%
9	14.504	1934	1941	1957	rVB	3248564	4619611	36.20%	5.454%
10	15.992	2187	2194	2211	rBV	6271693	8922934	69.92%	10.535%
11	17.245	2398	2407	2420	rBV	3581337	5019298	39.33%	5.926%
12	17.363	2423	2427	2434	rVB3	86758	135181	1.06%	0.160%
13	18.133	2554	2558	2568	rBV	320223	561708	4.40%	0.663%
14	19.415	2771	2776	2782	rBV	230654	393452	3.08%	0.465%
15	19.674	2815	2820	2826	rVB3	109368	189893	1.49%	0.224%
16	19.862	2847	2852	2859	rBV	11064777	12761585	100.00%	15.067%
17	20.662	2985	2988	2991	rVB	175376	166819	1.31%	0.197%
18	21.127	3063	3067	3076	rBV2	426714	664387	5.21%	0.784%
19	21.415	3111	3116	3126	rBV	3256100	4239579	33.22%	5.006%
20	21.562	3138	3141	3147	rBV	187220	192494	1.51%	0.227%
21	22.503	3298	3301	3305	rVB2	291998	352588	2.76%	0.416%
22	23.774	3511	3517	3534	rVB2	1822780	3587996	28.12%	4.236%

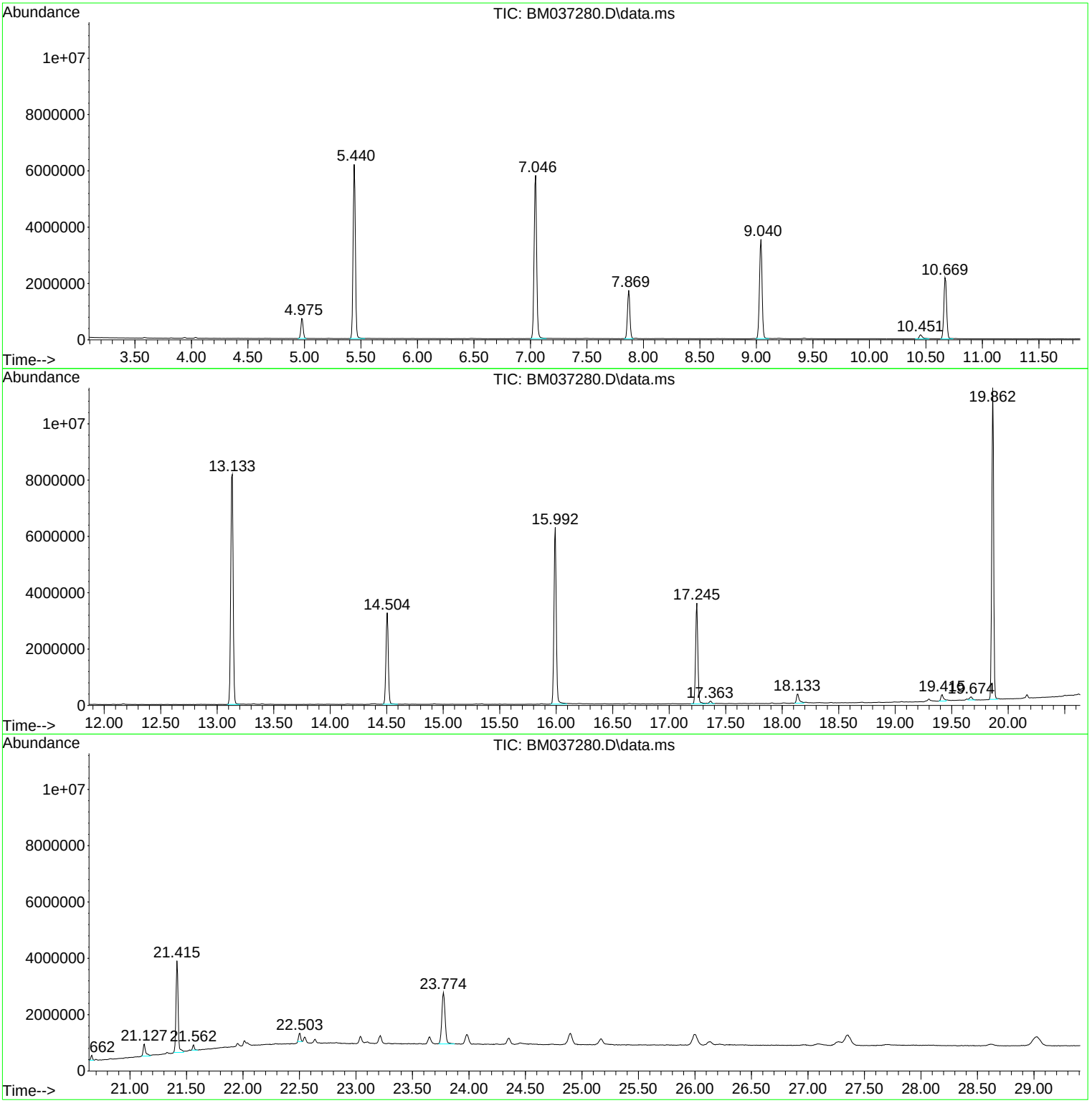
Sum of corrected areas: 84696483

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102922\
Data File : BM037280.D
Acq On : 29 Oct 2022 20:35
Operator : CG/JU
Sample : N5234-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSP-SS-04-15-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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_M\Data\BM102922\
Data File : BM037280.D
Acq On : 29 Oct 2022 20:35
Operator : CG/JU
Sample : N5234-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSP-SS-04-15-3

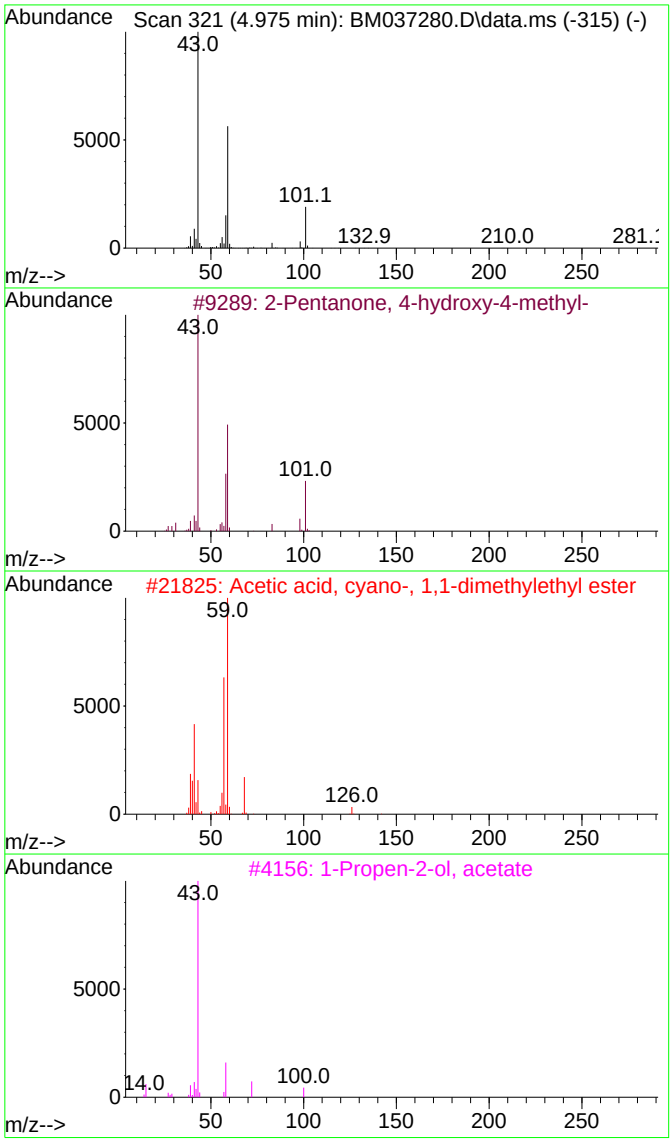
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

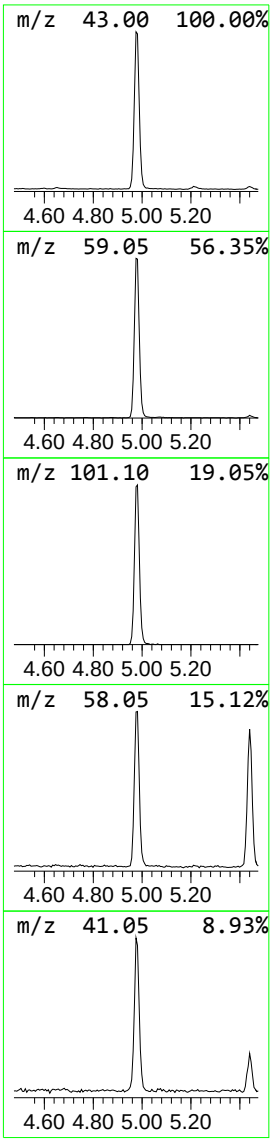
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	7.85 ng	1005580	1,4-Dichlorobenzene-d4	7.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102922\
Data File : BM037280.D
Acq On : 29 Oct 2022 20:35
Operator : CG/JU
Sample : N5234-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSP-SS-04-15-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

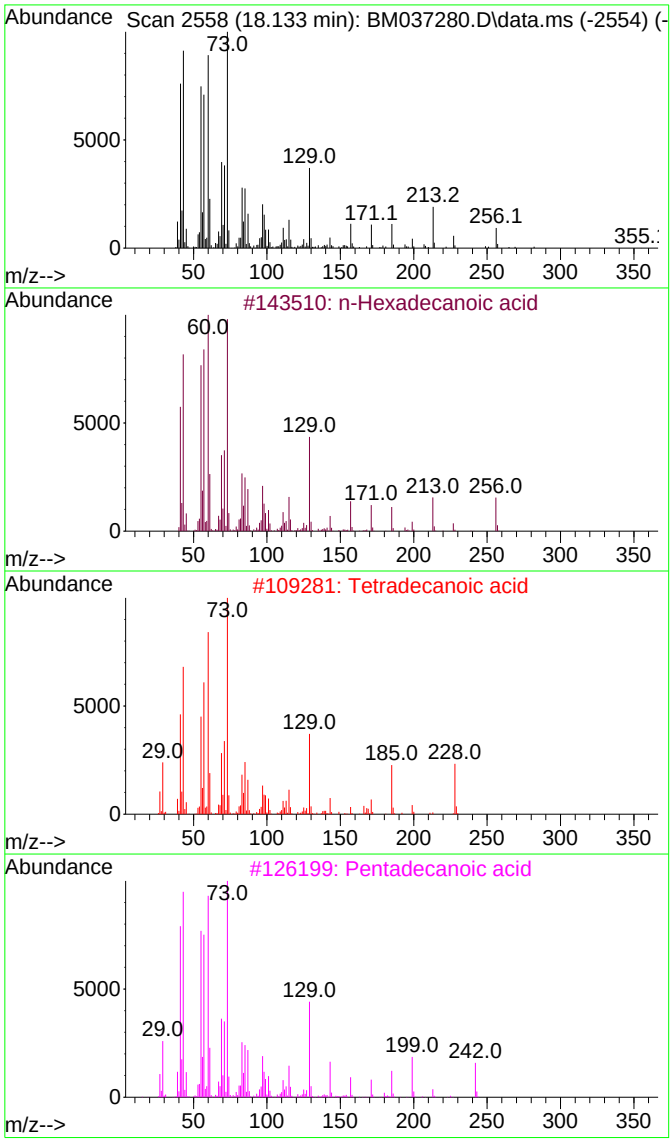
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

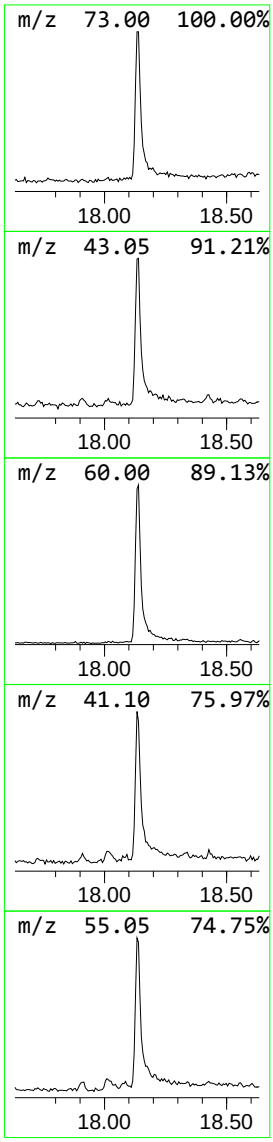
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.133	2.24 ng	561708	Phenanthrene-d10	17.245

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102922\
Data File : BM037280.D
Acq On : 29 Oct 2022 20:35
Operator : CG/JU
Sample : N5234-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSP-SS-04-15-3

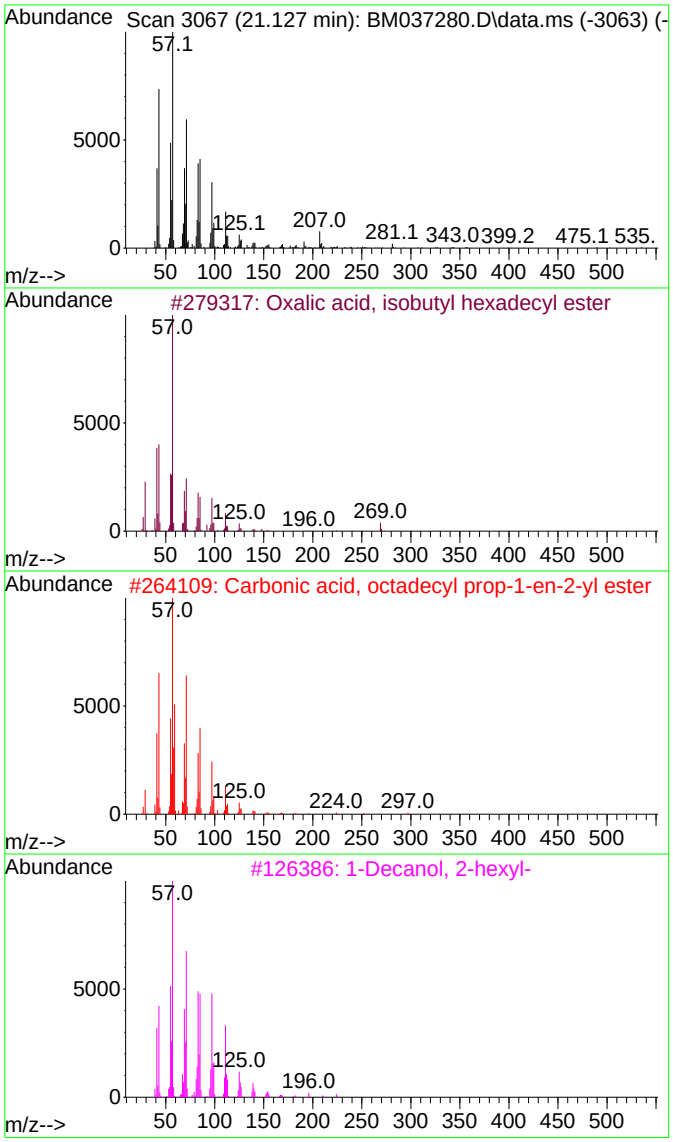
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

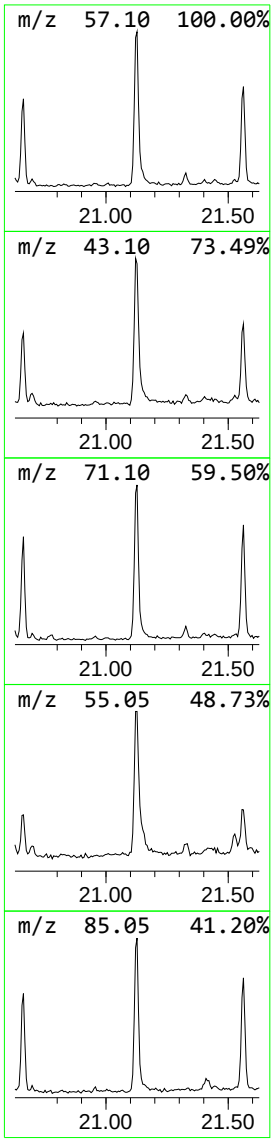
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Oxalic acid, isobutyl hexad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	3.13 ng	664387	Chrysene-d12	21.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
2	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	91
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	91
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	91
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102922\
Data File : BM037280.D
Acq On : 29 Oct 2022 20:35
Operator : CG/JU
Sample : N5234-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSP-SS-04-15-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.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-...	4.975	7.8	ng	1005580	1	7.869	2562490	20.0
n-Hexadecanoic ...	18.133	2.2	ng	561708	4	17.245	5019300	20.0
Oxalic acid, is...	21.127	3.1	ng	664387	5	21.415	4239580	20.0