LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
Data File : BM042825.D
Acq On : 17 Nov 2023 02:57
Operator : MA/JU
Sample : 05268-16
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DCKD9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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\SFAM-EPA-BM111323.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM042825.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.175	30	32	37	rVB4	7731	9904	0.32%	0.060%
2	3.628	106	109	123	rBV	21866	42917	1.40%	0.261%
3	3.804	135	139	143	rVB6	3485	5214	0.17%	0.032%
4	6.998	676	682	693	rBV3	18172	48422	1.58%	0.295%
5	7.169	706	711	727	rBV	107524	196802	6.44%	1.197%
6	7.345	736	741	756	rBV	113033	203702	6.67%	1.239%
7	7.822	816	822	839	rBV	96609	174271	5.70%	1.060%
8	8.545	940	945	964	rBV	62255	136723	4.47%	0.832%
9	9.022	1019	1026	1039	rBV	132412	264526	8.66%	1.609%
10	9.527	1087	1112	1129	rBV	506452	2124152	69.51%	12.923%
11	9.733	1141	1147	1166	rVB	116705	239521	7.84%	1.457%
12	10.098	1180	1209	1231	rBV	624531	3055916	100.00%	18.592%
13	10.263	1231	1237	1249	rBV	156284	317412	10.39%	1.931%
14	10.633	1293	1300	1309	rBV	148952	251584	8.23%	1.531%
15	10.816	1324	1331	1347	rBV	113527	273021	8.93%	1.661%
16	11.492	1429	1446	1462	rBV	428970	1254125	41.04%	7.630%
17	11.692	1478	1480	1488	rVB5	2359	4150	0.14%	0.025%
18	13.321	1753	1757	1764	rVB	11378	17496	0.57%	0.106%
19	13.821	1831	1842	1844	rBV4	43540	144342	4.72%	0.878%
20	13.898	1850	1855	1868	rVB	420793	613560	20.08%	3.733%
21	14.180	1896	1903	1916	rBV	421470	614738	20.12%	3.740%
22	14.474	1947	1953	1962	rBV	222684	327255	10.71%	1.991%
23	14.568	1966	1969	1974	rVB2	6633	9212	0.30%	0.056%
24	14.780	2000	2005	2008	rBV5	3796	7082	0.23%	0.043%
25	14.874	2020	2021	2025	rVV3	2667	3483	0.11%	0.021%
26	15.474	2116	2123	2137	rBV	547643	791363	25.90%	4.815%
27	15.621	2142	2148	2161	rVV	161378	264479	8.65%	1.609%
28	15.709	2161	2163	2168	rVV3	4288	5585	0.18%	0.034%
29	16.339	2265	2270	2276	rBV	23122	29019	0.95%	0.177%
30	17.233	2416	2422	2433	rBV	255213	378431	12.38%	2.302%
31	17.333	2433	2439	2453	rVV	576559	868161	28.41%	5.282%
32	17.856	2525	2528	2533	rVV4	2556	3494	0.11%	0.021%
33	18.086	2562	2567	2579	rBV	30441	58948	1.93%	0.359%
34	18.986	2716	2720	2724	rBV5	2952	4493	0.15%	0.027%
35	19.027	2724	2727	2730	rBV3	4572	5728	0.19%	0.035%
36	19.186	2751	2754	2757	rVV4	6124	7415	0.24%	0.045%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
Data File : BM042825.D
Acq On : 17 Nov 2023 02:57
Operator : MA/JU
Sample : 05268-16
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DCKD9

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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\SFAM-EPA-BM111323.MA.M
Title : SVOA CALIBRATION

37	19.250	2762	2765	2776	rVB5	29336	58347	1.91%	0.355%
38	19.368	2781	2785	2795	rVB4	24564	45524	1.49%	0.277%
39	19.503	2806	2808	2813	rVB5	5191	6257	0.20%	0.038%
40	19.627	2823	2829	2844	rBV	939494	1204982	39.43%	7.331%
41	20.550	2984	2986	2989	rBV3	4342	4172	0.14%	0.025%
42	21.086	3074	3077	3084	rVB7	10216	15657	0.51%	0.095%
43	21.415	3128	3133	3145	rBV	320687	472842	15.47%	2.877%
44	23.621	3500	3508	3523	rBV	649162	1325524	43.38%	8.064%
45	23.768	3527	3533	3547	rVB	264208	547111	17.90%	3.329%

Sum of corrected areas: 16437062

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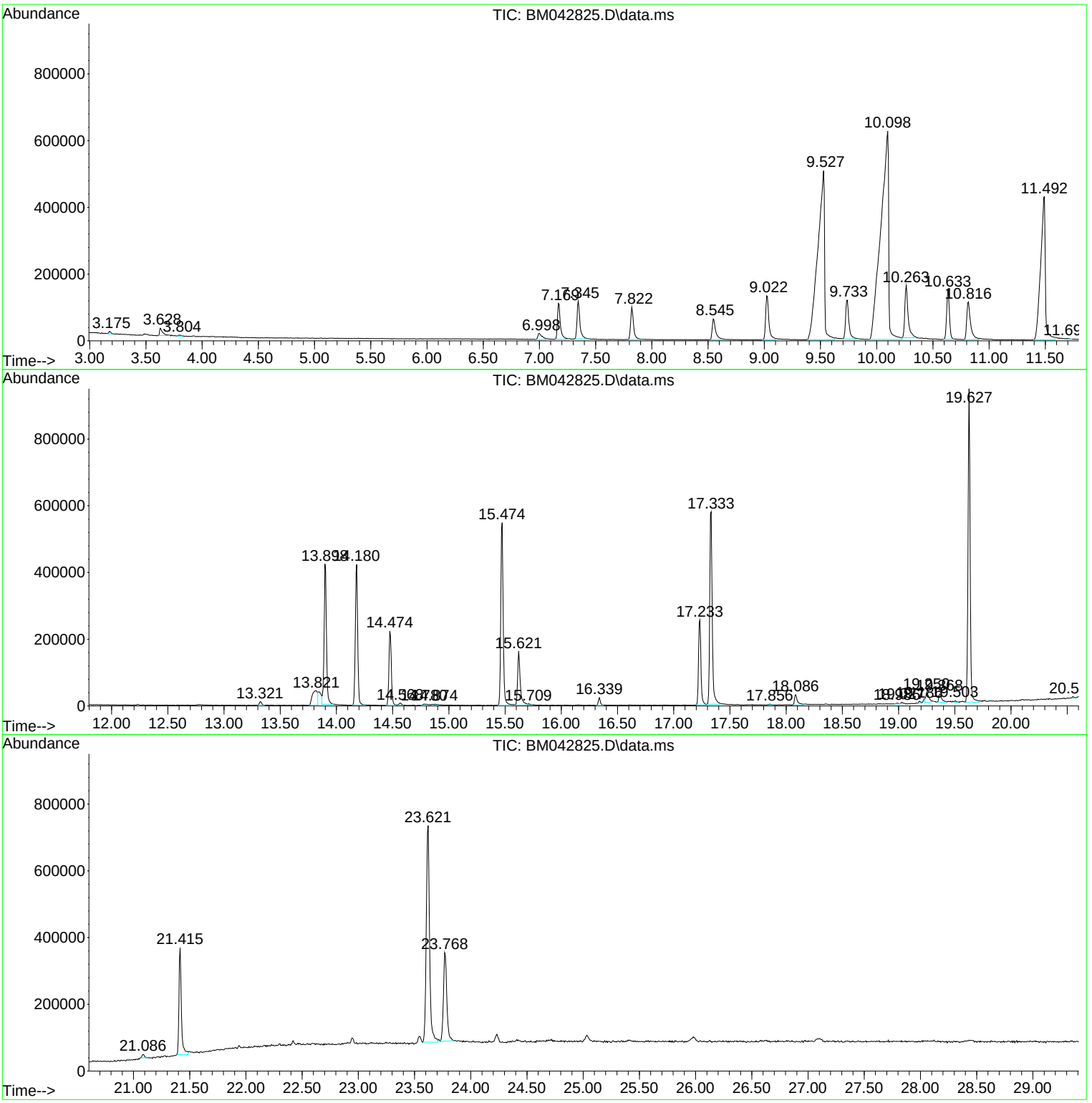
Sample : 05268-16
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DCKD9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
Data File : BM042825.D
Acq On : 17 Nov 2023 02:57
Operator : MA/JU
Sample : 05268-16
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DCKD9

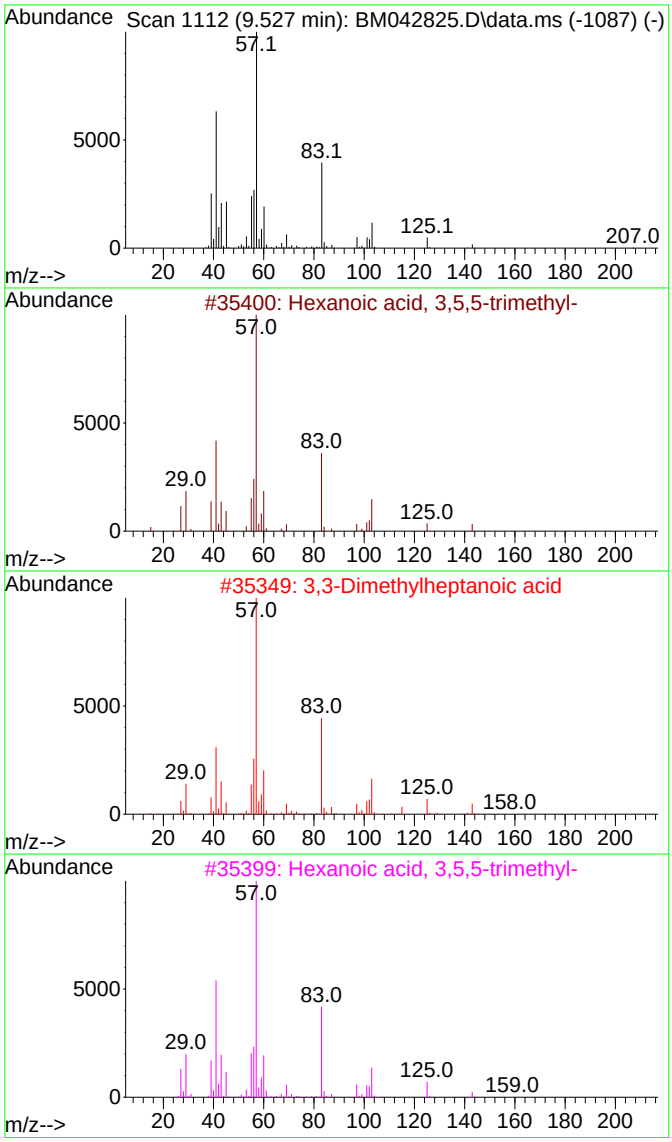
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

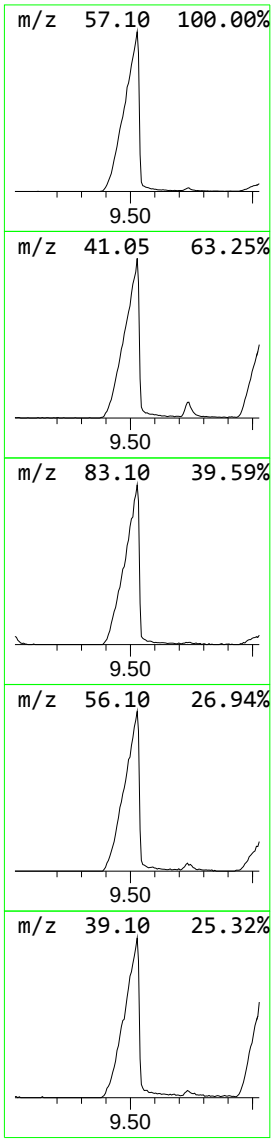
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexanoic acid, 3,5,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.527	168.86 ng/ul	2124150	Naphthalene-d8	10.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	86
2	3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	72
3	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	72
4	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	53
5	Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
Data File : BM042825.D
Acq On : 17 Nov 2023 02:57
Operator : MA/JU
Sample : 05268-16
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DCKD9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

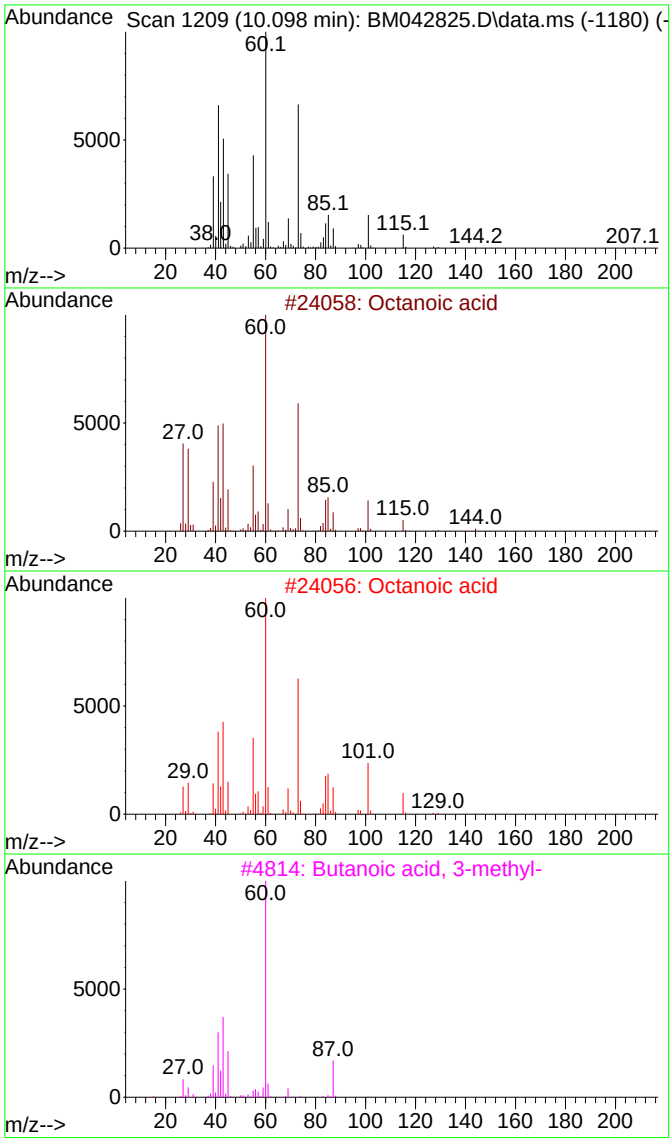
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

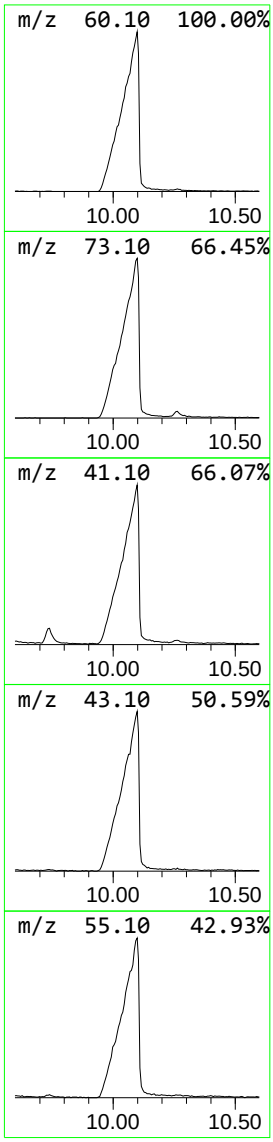
****

Peak Number 2 Octanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.098	242.93 ng/ul	3055920	Naphthalene-d8	10.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanoic acid	144	C8H16O2	000124-07-2	86
2	Octanoic acid	144	C8H16O2	000124-07-2	64
3	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
4	Hexanoic acid	116	C6H12O2	000142-62-1	53
5	Pentanoic acid	102	C5H10O2	000109-52-4	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
Data File : BM042825.D
Acq On : 17 Nov 2023 02:57
Operator : MA/JU
Sample : 05268-16
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DCKD9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

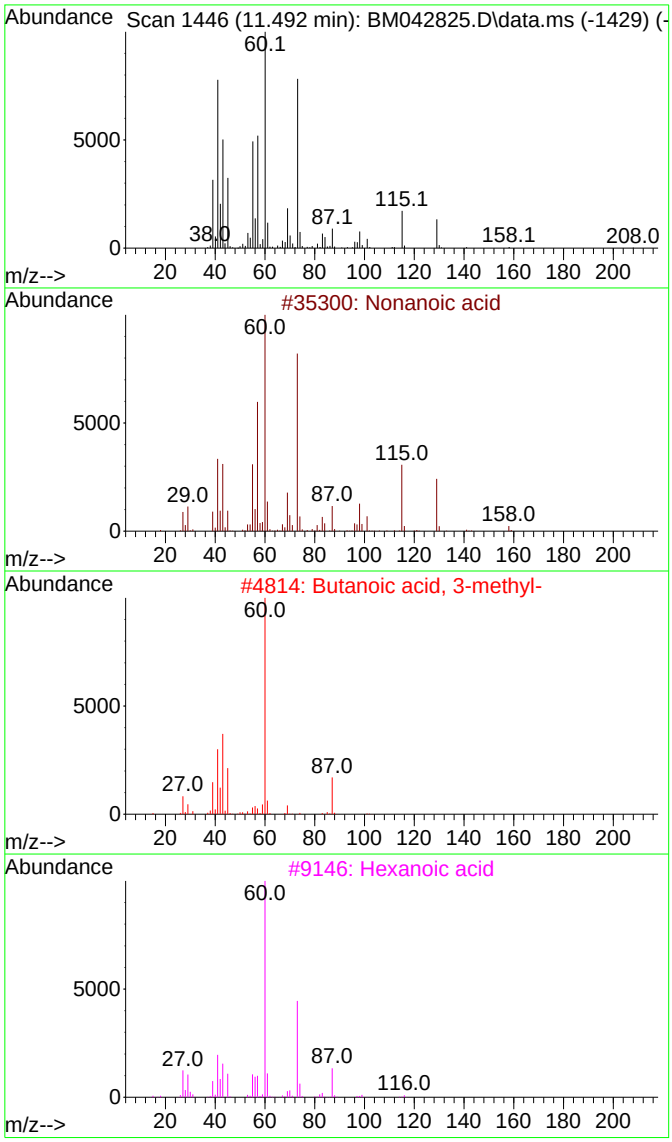
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

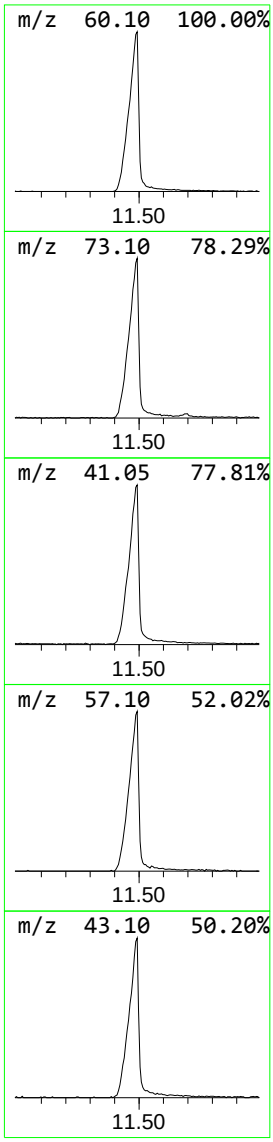
****

Peak Number 3 Nonanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.492	99.70 ng/ul	1254130	Naphthalene-d8	10.633

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	59
2	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53
3	Hexanoic acid	116	C6H12O2	000142-62-1	52
4	Hexanoic acid	116	C6H12O2	000142-62-1	50
5	Nonanoic acid	158	C9H18O2	000112-05-0	42





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
Data File : BM042825.D
Acq On : 17 Nov 2023 02:57
Operator : MA/JU
Sample : 05268-16
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DCKD9

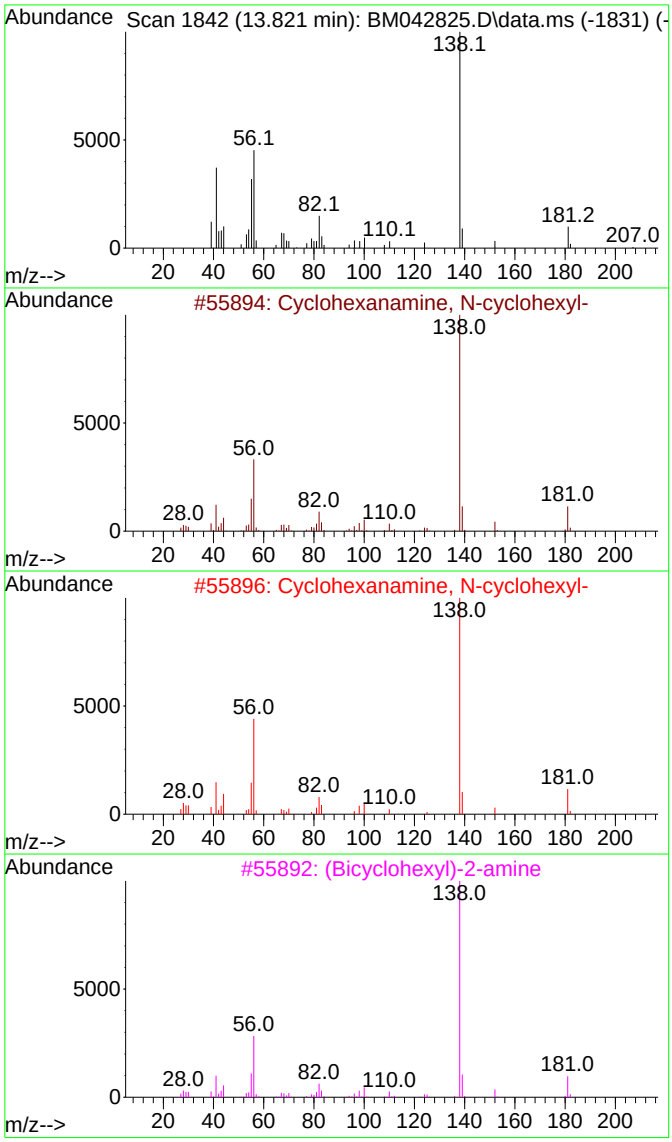
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

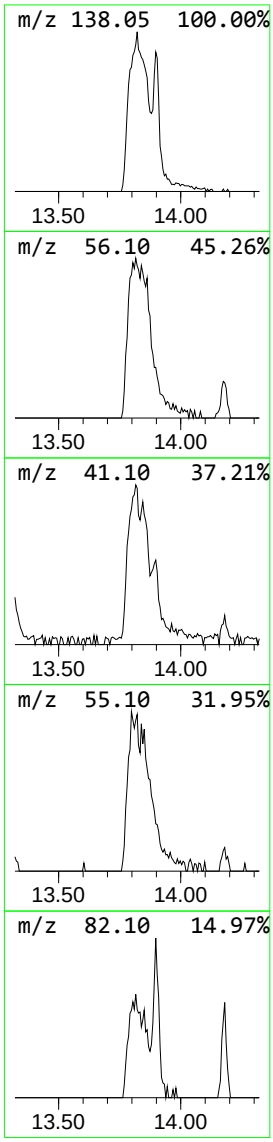
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexanamine, N-cyclohexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	8.82 ng/ul	144342	Acenaphthene-d10	14.474

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	95
2	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	94
3	(Bicyclohexyl)-2-amine	181	C12H23N	006283-14-3	91
4	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	91
5	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
Data File : BM042825.D
Acq On : 17 Nov 2023 02:57
Operator : MA/JU
Sample : 05268-16
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DCKD9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

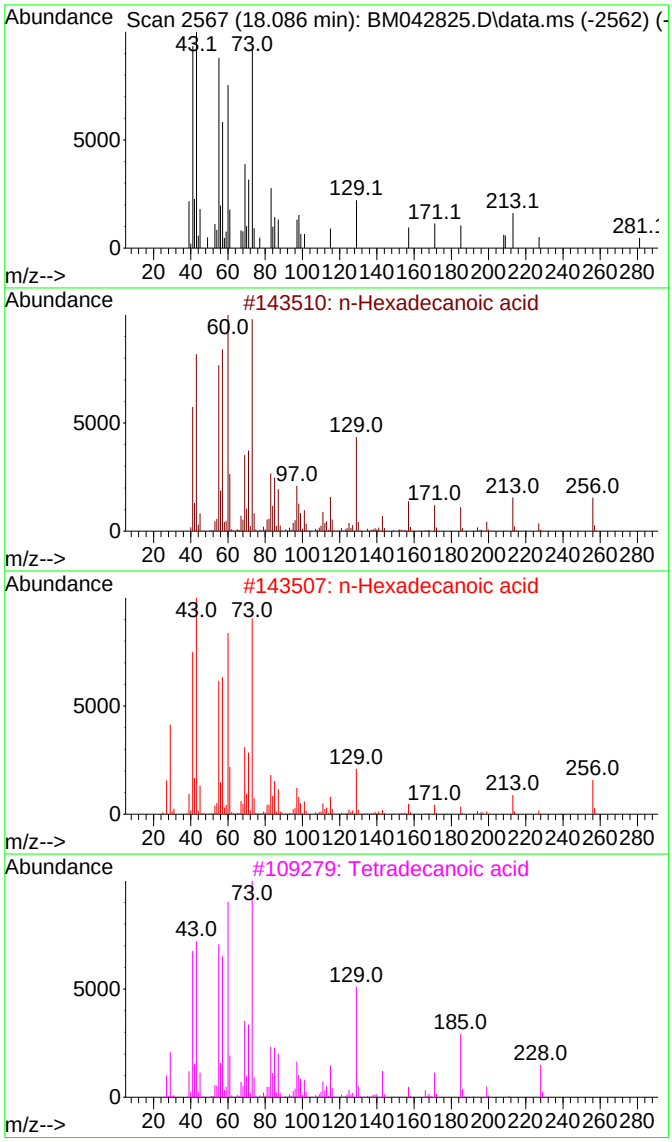
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

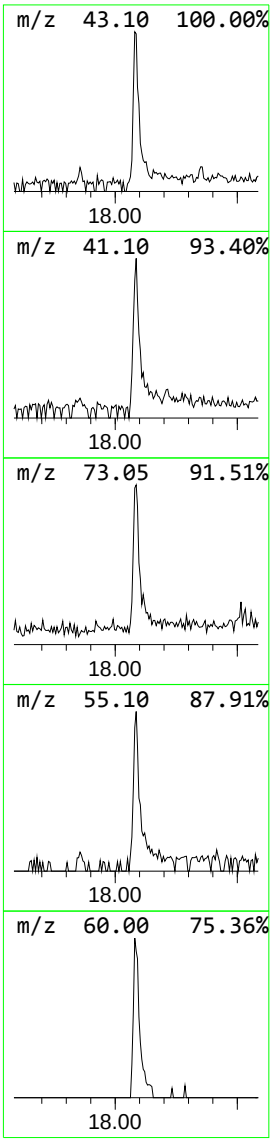
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.086	3.12 ng/ul	58948	Phenanthrene-d10	17.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58





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Instrument :
BNA_M
ClientSampleId :
DCKD9

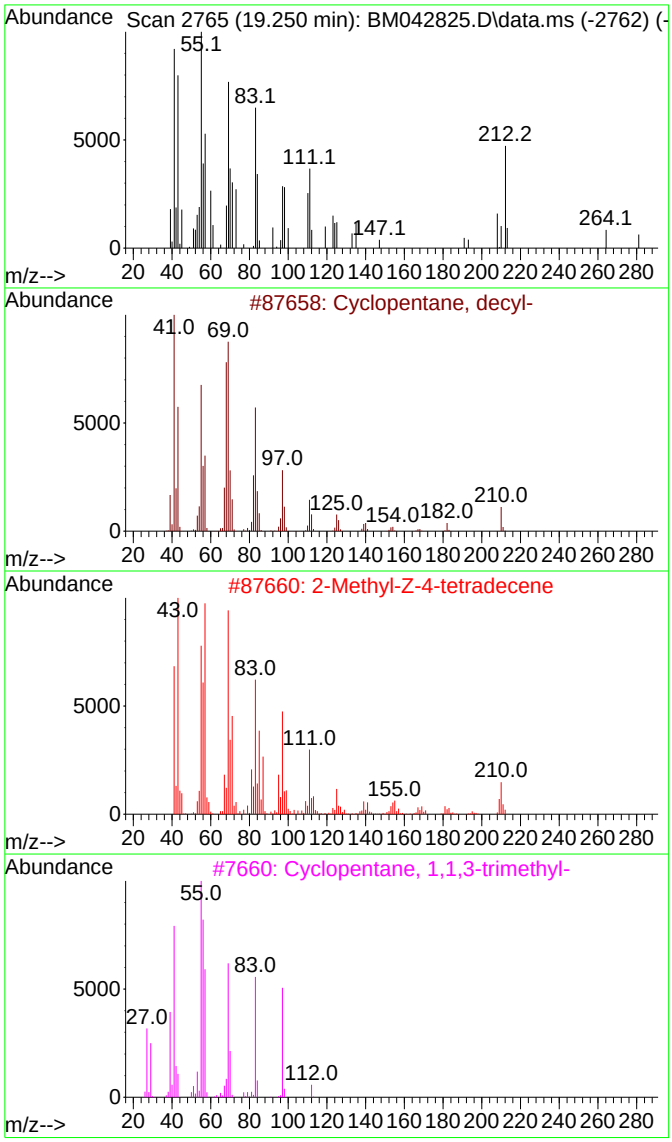
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA CALIBRATION

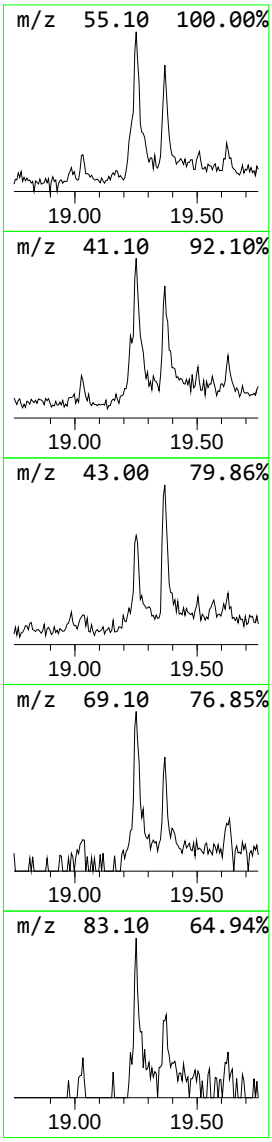
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Cyclic19.250 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.250	3.08 ng/ul	58347	Phenanthrene-d10	17.233

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, decyl-	210	C15H30	001795-21-7	64
2	2-Methyl-Z-4-tetradecene	210	C15H30	1000130-78-3	45
3	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	38
4	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	38
5	Cyclopropane, 1,1-diethyl-	98	C7H14	001003-19-6	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111323\
Data File : BM042825.D
Acq On : 17 Nov 2023 02:57
Operator : MA/JU
Sample : 05268-16
Misc :
ALS Vial : 67 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DCKD9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM111323.MA.M
Quant Title : SVOA 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
Hexanoic acid, ...	9.527	168.9	ng/ul	2124150	2	10.633	251584	20.0
Octanoic acid	10.098	242.9	ng/ul	3055920	2	10.633	251584	20.0
Nonanoic acid	11.492	99.7	ng/ul	1254130	2	10.633	251584	20.0
Cyclohexanamine...	13.821	8.8	ng/ul	144342	3	14.474	327255	20.0
n-Hexadecanoic ...	18.086	3.1	ng/ul	58948	4	17.233	378431	20.0
(DEL) Alkane: C...	19.250	3.1	ng/ul	58347	4	17.233	378431	20.0