LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111722\
Data File : BN022715.D
Acq On : 17 Nov 2022 12:11
Operator : CG/JU
Sample : PB149074BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK120

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_N\Methods\SFAM-EPA-BN111522.M
Title : SVOA CALIBRATION

Signal : TIC: BN022715.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.181	29	33	40	rVB	21585	29098	1.08%	0.106%
2	3.617	104	107	129	rBV	242650	427544	15.87%	1.550%
3	3.952	160	164	170	rVB2	5404	9174	0.34%	0.033%
4	5.052	347	351	355	rBV7	1660	3228	0.12%	0.012%
5	5.893	489	494	499	rVB8	1379	2748	0.10%	0.010%
6	6.963	671	676	677	rBV4	2754	3647	0.14%	0.013%
7	7.028	680	687	700	rVV	330037	553664	20.55%	2.008%
8	7.187	706	714	725	rBV	289745	457080	16.96%	1.658%
9	7.381	739	747	757	rBV	347074	555319	20.61%	2.014%
10	7.852	821	827	836	rVB	287538	475520	17.65%	1.724%
11	8.581	945	951	963	rVV	430254	706190	26.21%	2.561%
12	9.034	1020	1028	1041	rBV	361735	592608	21.99%	2.149%
13	9.757	1144	1151	1165	rVB	311461	505860	18.77%	1.835%
14	10.299	1237	1243	1255	rBV	418067	713958	26.49%	2.589%
15	10.675	1294	1307	1314	rBV	452891	746567	27.70%	2.707%
16	10.822	1325	1332	1345	rBV	447226	772245	28.66%	2.801%
17	11.851	1502	1507	1515	rVV7	4057	7963	0.30%	0.029%
18	12.275	1571	1579	1585	rVB4	6865	11800	0.44%	0.043%
19	12.863	1673	1679	1685	rBV9	3191	7993	0.30%	0.029%
20	13.428	1770	1775	1779	rBV5	2925	4457	0.17%	0.016%
21	13.787	1833	1836	1839	rBV3	2482	2748	0.10%	0.010%
22	13.945	1857	1863	1879	rVB	931670	1280903	47.53%	4.645%
23	14.222	1903	1910	1920	rBV	918528	1352635	50.19%	4.905%
24	14.528	1956	1962	1971	rBV	751367	1086806	40.33%	3.941%
25	14.757	1993	2001	2015	rBV	442264	704817	26.15%	2.556%
26	14.945	2028	2033	2041	rBV3	18013	27434	1.02%	0.099%
27	15.528	2125	2132	2141	rBV	1229682	1742570	64.66%	6.319%
28	15.657	2148	2154	2167	rVB	510680	692640	25.70%	2.512%
29	15.763	2169	2172	2176	rBV4	4914	6610	0.25%	0.024%
30	16.322	2261	2267	2270	rBV7	3424	6224	0.23%	0.023%
31	16.686	2325	2329	2334	rBV5	6738	10957	0.41%	0.040%
32	17.286	2425	2431	2438	rBV	940413	1336800	49.61%	4.848%
33	17.386	2442	2448	2456	rBV	1385035	1946619	72.23%	7.059%
34	17.828	2517	2523	2524	rBV5	1880	2987	0.11%	0.011%
35	17.951	2542	2544	2549	rVB6	1977	3149	0.12%	0.011%
36	18.186	2572	2584	2601	rBV	299463	534261	19.83%	1.937%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111722\
Data File : BN022715.D
Acq On : 17 Nov 2022 12:11
Operator : CG/JU
Sample : PB149074BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK120

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_N\Methods\SFAM-EPA-BN111522.M
Title : SVOA CALIBRATION

37	18.486	2631	2635	2640	rVB7	5875	9186	0.34%	0.033%
38	19.251	2762	2765	2770	rVB	15444	21066	0.78%	0.076%
39	19.322	2773	2777	2788	rBV	27546	57300	2.13%	0.208%
40	19.469	2797	2802	2814	rBV	201965	327019	12.13%	1.186%
41	19.692	2834	2840	2846	rBV	1691032	2234486	82.92%	8.103%
42	20.233	2929	2932	2936	rVB	16429	18034	0.67%	0.065%
43	20.727	3013	3016	3019	rBV3	12267	14647	0.54%	0.053%
44	21.163	3085	3090	3094	rBV	55072	92614	3.44%	0.336%
45	21.216	3096	3099	3104	rVV	75156	102533	3.80%	0.372%
46	21.274	3105	3109	3115	rVB	170818	195577	7.26%	0.709%
47	21.498	3141	3147	3153	rBV	1178964	1576206	58.49%	5.716%
48	21.616	3163	3167	3177	rBV	445066	601237	22.31%	2.180%
49	22.598	3331	3334	3338	rVB	48634	60312	2.24%	0.219%
50	23.151	3424	3428	3435	rVB3	79650	134230	4.98%	0.487%
51	23.751	3522	3530	3545	rVB2	1232951	2694851	100.00%	9.773%
52	23.904	3549	3556	3567	rVB2	811958	1634281	60.64%	5.927%
53	24.504	3654	3658	3667	rVB	110969	223818	8.31%	0.812%
54	25.357	3798	3803	3812	rVB	111742	252548	9.37%	0.916%

Sum of corrected areas: 27574768

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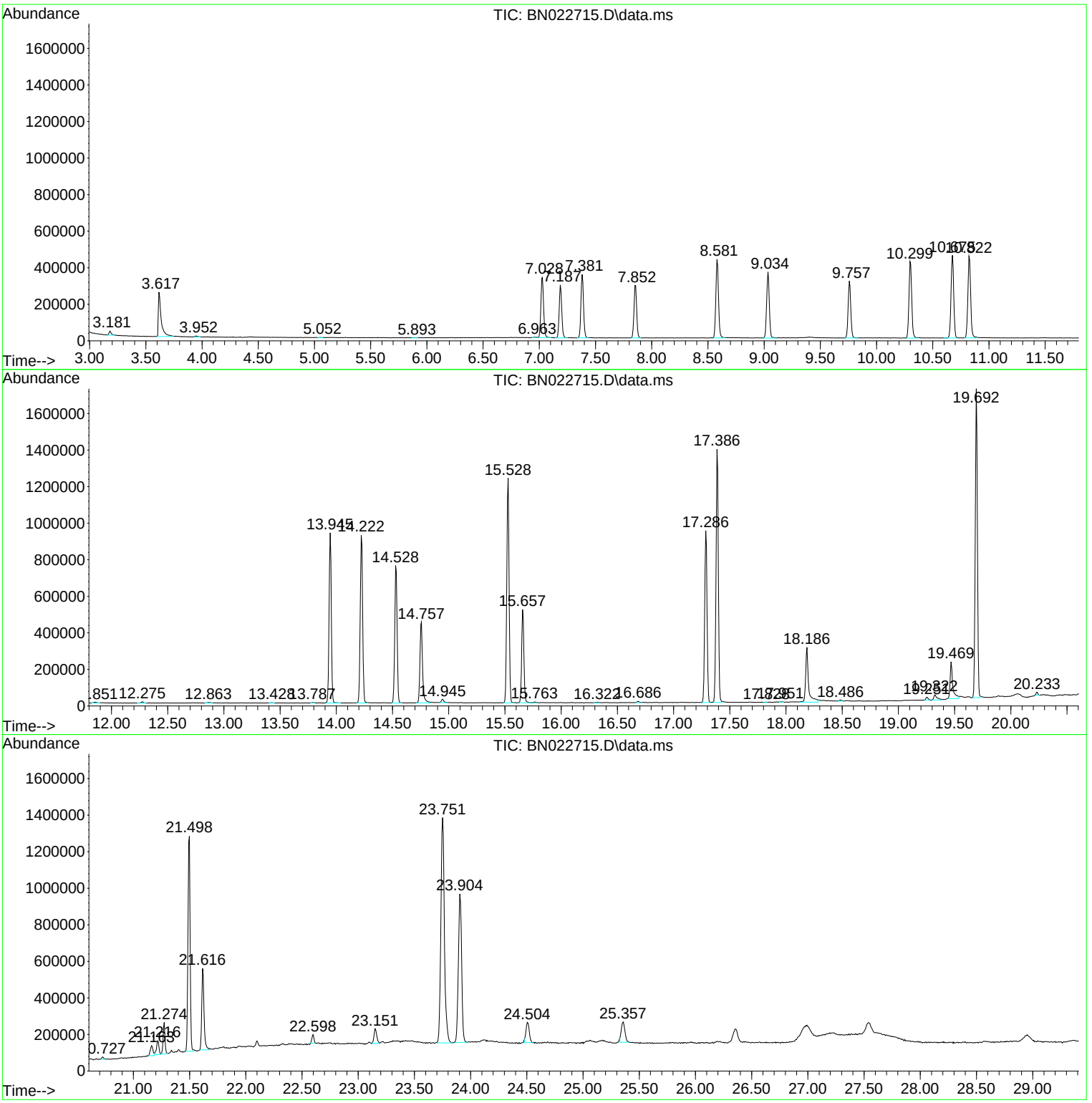
Operator : CG/JU
Sample : PB149074BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK120

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111722\
Data File : BN022715.D
Acq On : 17 Nov 2022 12:11
Operator : CG/JU
Sample : PB149074BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK120

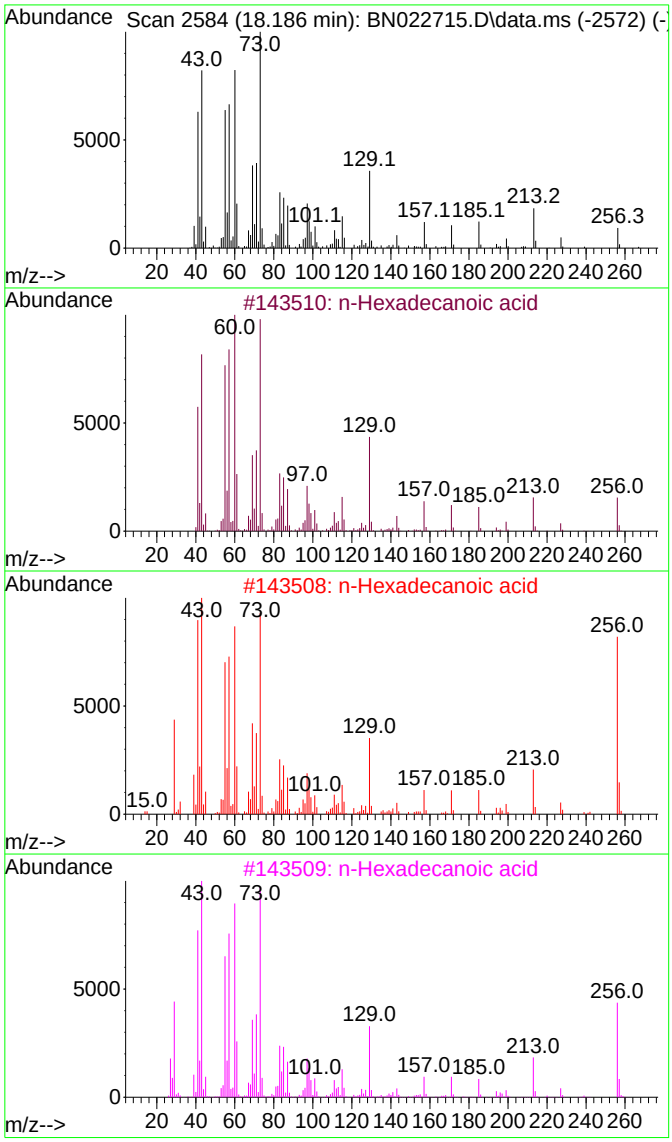
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

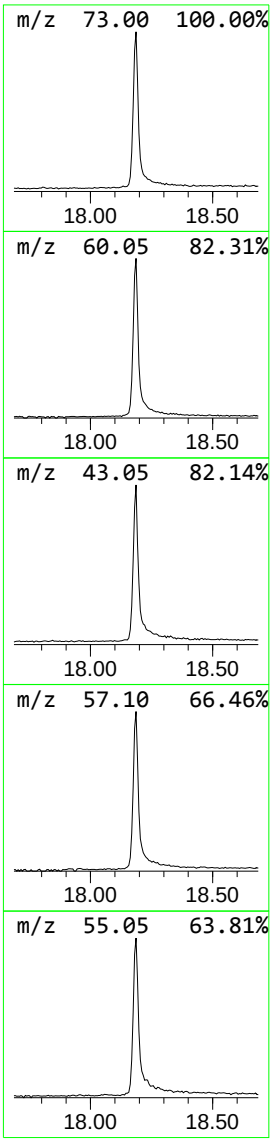
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	7.99 ng/ul	534261	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
5	Tridecanoic acid	214	C13H26O2	000638-53-9	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111722\
Data File : BN022715.D
Acq On : 17 Nov 2022 12:11
Operator : CG/JU
Sample : PB149074BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK120

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

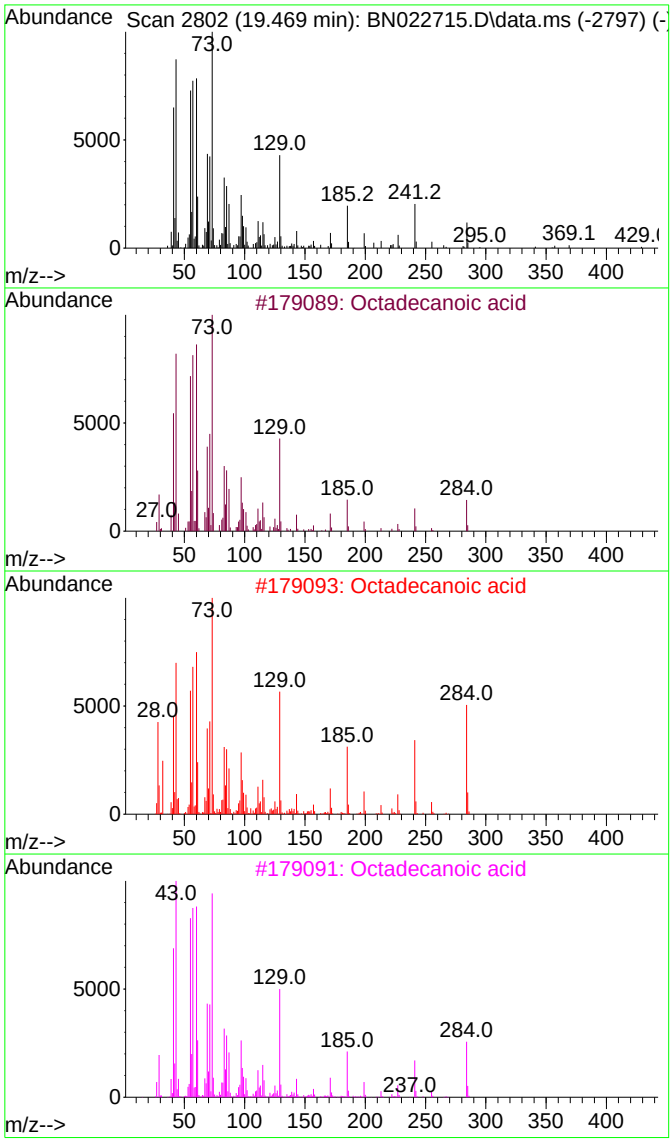
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

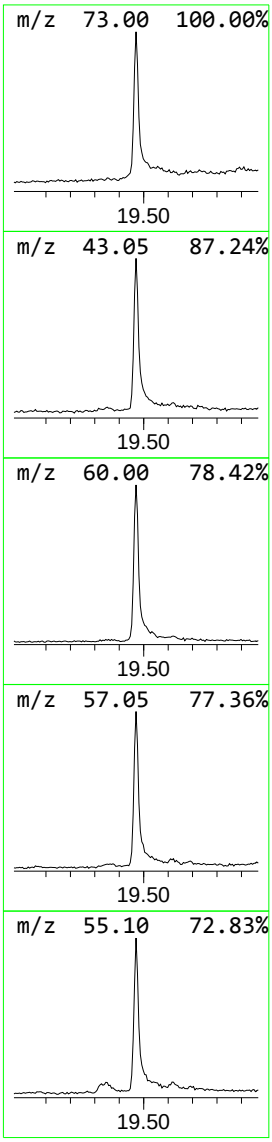
****

Peak Number 2 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.469	4.15 ng/ul	327019	Chrysene-d12	21.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	99
4	Octadecanoic acid	284	C18H36O2	000057-11-4	98
5	Octadecanoic acid	284	C18H36O2	000057-11-4	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111722\
Data File : BN022715.D
Acq On : 17 Nov 2022 12:11
Operator : CG/JU
Sample : PB149074BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK120

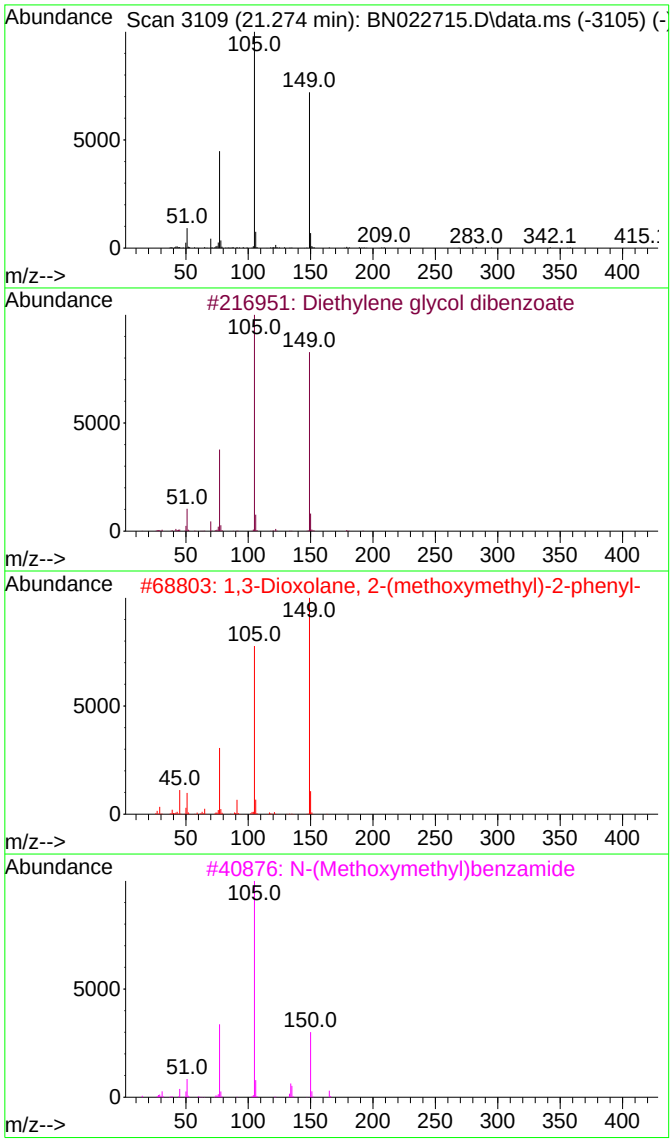
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

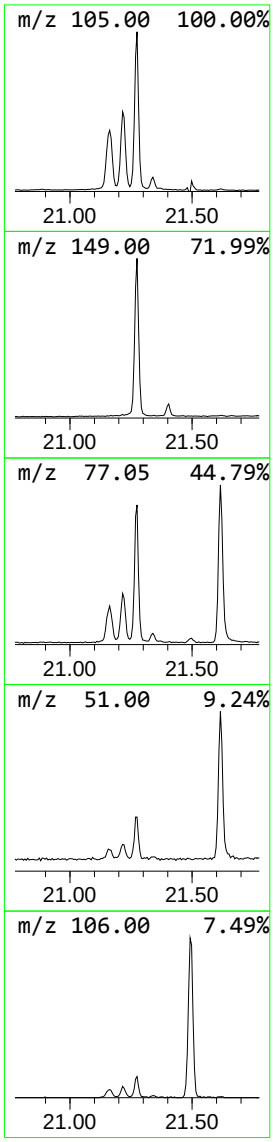
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Diethylene glycol dibenzoate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.275	2.48 ng/ul	195577	Chrysene-d12	21.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	53
3	N-(Methoxymethyl)benzamide	165	C9H11NO2	013156-28-0	50
4	Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	47
5	N-(4-Methylthiazol-2-yl)benzamide	218	C11H10N2OS	037529-67-2	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111722\
Data File : BN022715.D
Acq On : 17 Nov 2022 12:11
Operator : CG/JU
Sample : PB149074BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK120

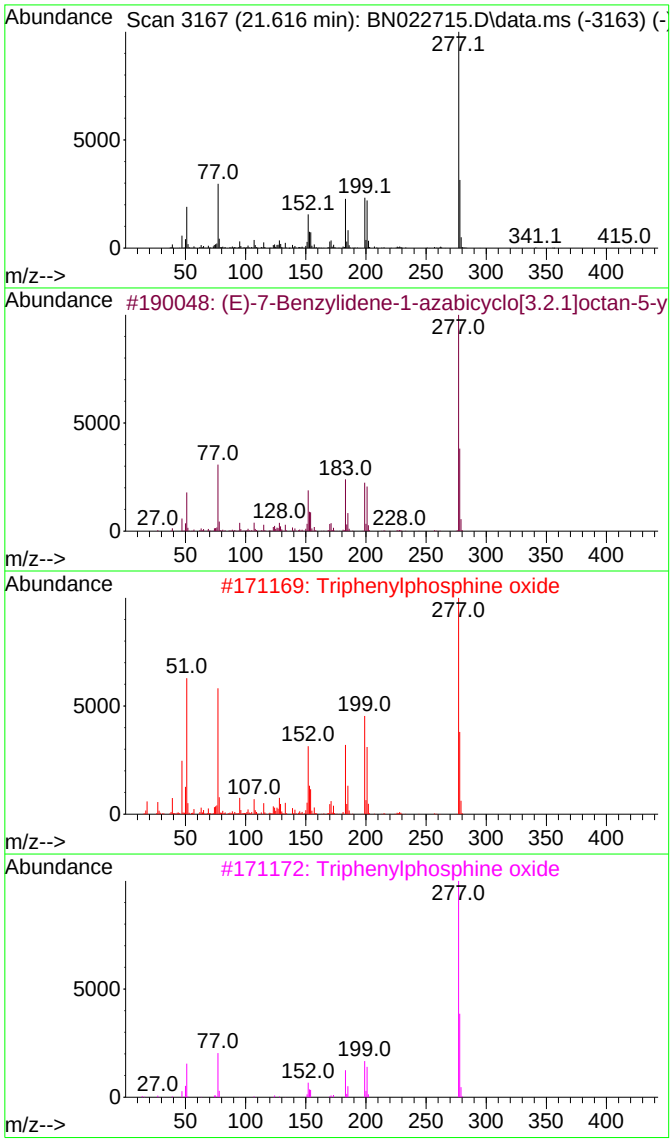
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

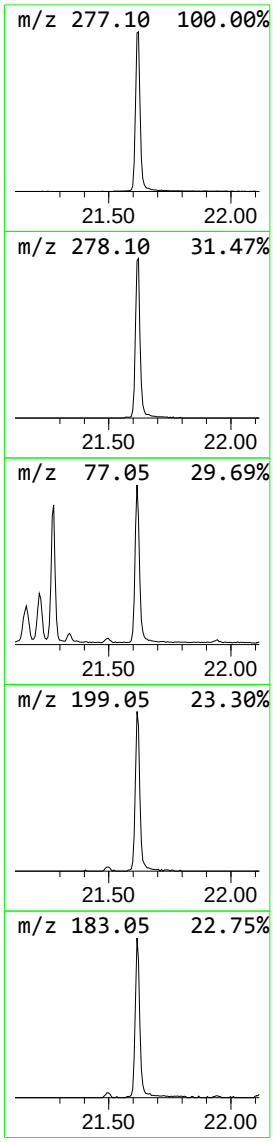
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (E)-7-Benzylidene-1-azabicy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.616	7.63 ng/ul	601237	Chrysene-d12	21.498

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	93
2	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	93
3	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	60
4	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	55
5	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50





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Acq On : 17 Nov 2022 12:11
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Instrument :
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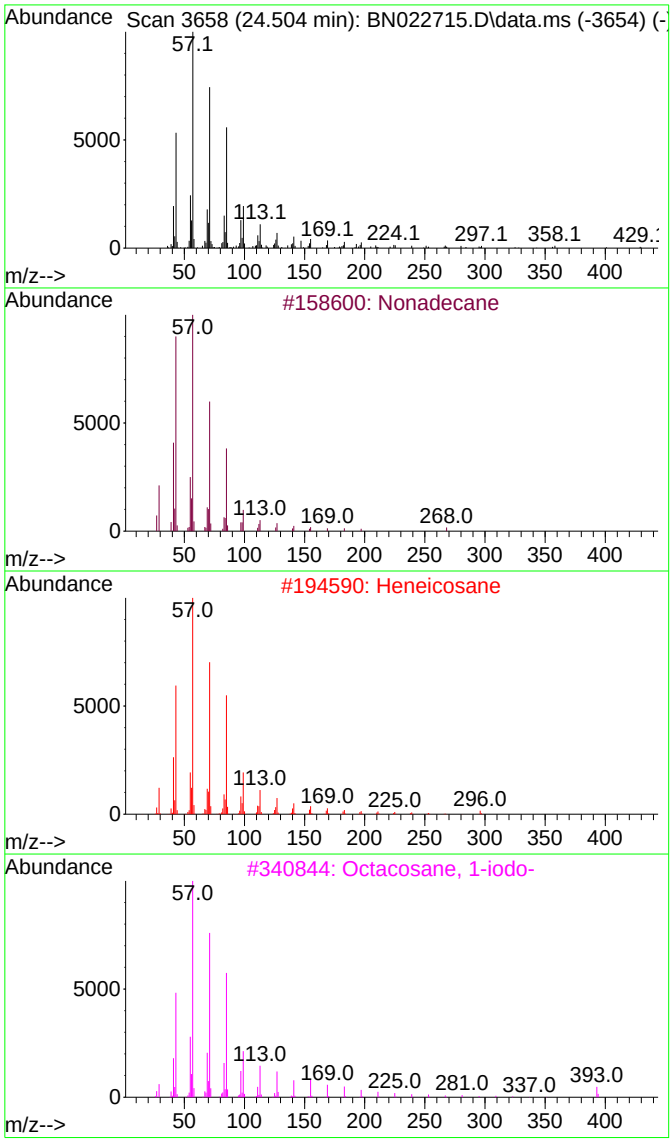
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

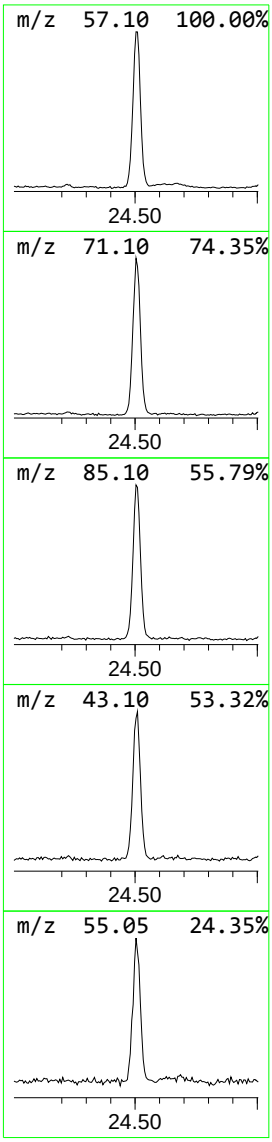
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.504	2.74 ng/ul	223818	Perylene-d12	23.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	93
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	91
4	Nonadecane	268	C19H40	000629-92-5	91
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91





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Sample : PB149074BL
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ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SBLK120

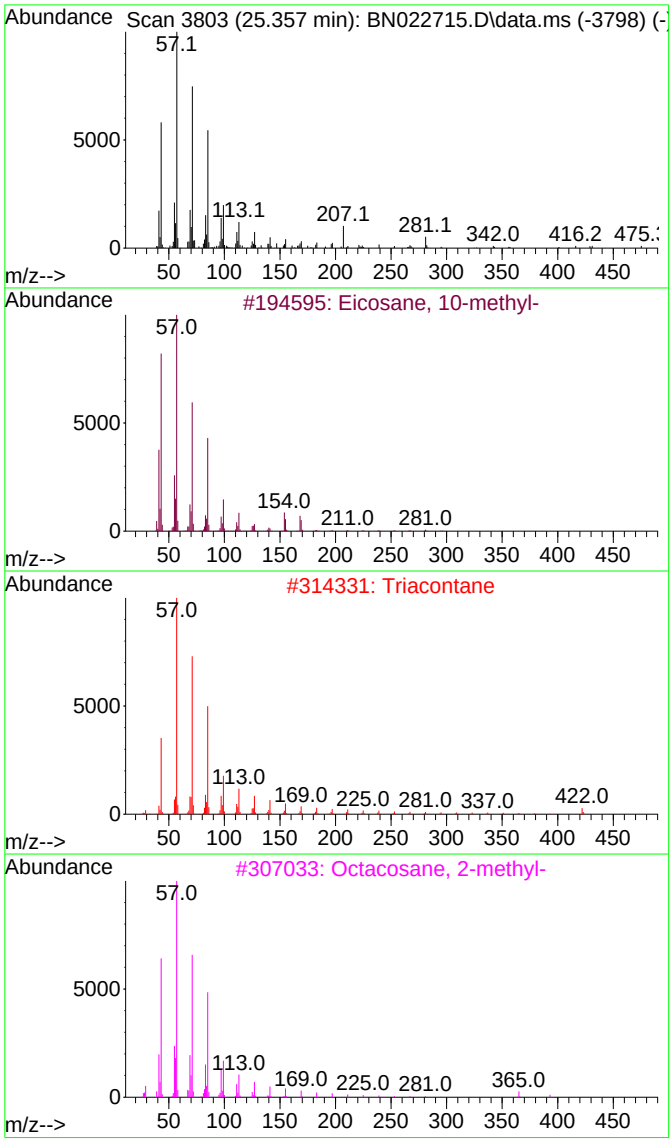
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

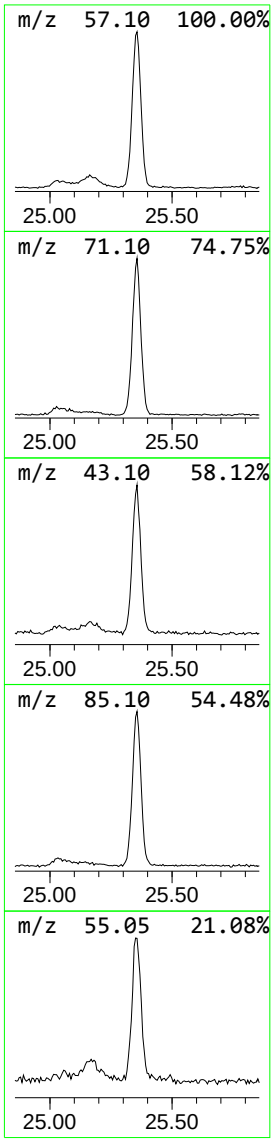
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.357	3.09 ng/ul	252548	Perylene-d12	23.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2	Triacontane	422	C30H62	000638-68-6	90
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Tetratriacontane, 2-methyl-	493	C35H72	014167-65-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN111722\
Data File : BN022715.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.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
n-Hexadecanoic ...	18.186	8.0	ng/ul	534261	4	17.286	1336800	20.0
Octadecanoic acid	19.469	4.2	ng/ul	327019	5	21.498	1576210	20.0
Diethylene glyc...	21.275	2.5	ng/ul	195577	5	21.498	1576210	20.0
(E)-7-Benzylide...	21.616	7.6	ng/ul	601237	5	21.498	1576210	20.0
(DEL) Alkane: S...	24.504	2.7	ng/ul	223818	6	23.904	1634280	20.0
(DEL) Alkane: S...	25.357	3.1	ng/ul	252548	6	23.904	1634280	20.0