

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN043024\
 Data File : BN031319.D
 Acq On : 30 Apr 2024 13:14
 Operator : MA/JU
 Sample : P2140-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 YCSQ9

Integration Parameters: LSCINT.P

Integrator: RTE

Smoother: OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0.1 % of largest Peak

Max Peaks: 100

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-BN042924.MA.M
 Title : SVOA CALIBRATION

Signal : TIC: BN031319.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.134	21	25	33	rBV	31254	40579	0.56%	0.060%
2	3.540	91	94	110	rBV	439066	688512	9.54%	1.015%
3	3.705	120	122	131	rVB10	7538	12395	0.17%	0.018%
4	3.852	143	147	151	rBV2	10081	13150	0.18%	0.019%
5	5.446	412	418	424	rBV8	4076	8471	0.12%	0.012%
6	6.793	642	647	661	rVB	216341	347774	4.82%	0.513%
7	6.957	669	675	685	rBV	980412	1481859	20.52%	2.185%
8	7.146	700	707	718	rBV	866069	1360466	18.84%	2.006%
9	7.610	780	786	793	rBV	705978	1137784	15.76%	1.678%
10	7.669	793	796	802	rVB3	22409	36312	0.50%	0.054%
11	8.322	900	907	919	rBV	708240	1125498	15.59%	1.660%
12	8.769	976	983	999	rBV	1149397	1899720	26.31%	2.801%
13	9.157	1045	1049	1057	rVB3	7945	15319	0.21%	0.023%
14	9.487	1097	1105	1121	rBV	918565	1478396	20.47%	2.180%
15	9.893	1169	1174	1179	rBV	6606	10789	0.15%	0.016%
16	10.016	1188	1195	1207	rBV	1447405	2382759	33.00%	3.513%
17	10.187	1219	1224	1236	rBV	46843	99680	1.38%	0.147%
18	10.393	1252	1259	1272	rBV	1097711	1813547	25.12%	2.674%
19	10.540	1275	1284	1295	rBV	1290733	2165062	29.98%	3.192%
20	10.769	1318	1323	1333	rBV2	12722	29920	0.41%	0.044%
21	11.645	1470	1472	1479	rVB6	5940	8725	0.12%	0.013%
22	11.987	1525	1530	1538	rVB2	26832	47967	0.66%	0.071%
23	13.075	1709	1715	1719	rBV4	10869	18037	0.25%	0.027%
24	13.157	1722	1729	1737	rVV	236385	373119	5.17%	0.550%
25	13.681	1811	1818	1831	rBV	2859356	3859794	53.46%	5.691%
26	13.957	1855	1865	1879	rBV	3118145	4713165	65.27%	6.950%
27	14.263	1910	1917	1924	rBV	1805419	2577512	35.70%	3.801%
28	14.375	1933	1936	1942	rVB7	5102	7443	0.10%	0.011%
29	14.481	1947	1954	1967	rBV	150483	297551	4.12%	0.439%
30	14.698	1986	1991	2000	rVB6	26723	46706	0.65%	0.069%
31	15.263	2080	2087	2097	rBV	3988830	5780712	80.06%	8.524%
32	15.386	2102	2108	2119	rVV	1311305	1729141	23.95%	2.550%
33	15.498	2123	2127	2134	rVB3	19393	30666	0.42%	0.045%
34	16.045	2215	2220	2227	rVB5	15181	22042	0.31%	0.033%
35	16.222	2243	2250	2257	rVB7	5109	11554	0.16%	0.017%
36	16.428	2280	2285	2287	rBV4	6134	8795	0.12%	0.013%

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Instrument :
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 ClientSampleId :
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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-BN042924.MA.M
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37	16.686	2327	2329	2335	rVB6	5843	7280	0.10%	0.011%
38	16.798	2343	2348	2351	rBV5	5116	9574	0.13%	0.014%
39	17.016	2378	2385	2392	rBV	2228523	3110297	43.08%	4.586%
40	17.116	2395	2402	2420	rVB	4453062	6325853	87.61%	9.328%
41	17.686	2493	2499	2504	rBV6	21113	27106	0.38%	0.040%
42	17.804	2516	2519	2524	rVB7	5922	9994	0.14%	0.015%
43	17.916	2532	2538	2546	rBV	355468	524369	7.26%	0.773%
44	18.263	2592	2597	2604	rBV10	9120	19572	0.27%	0.029%
45	18.404	2619	2621	2625	rVB4	6886	7862	0.11%	0.012%
46	18.851	2694	2697	2701	rVB5	8430	10593	0.15%	0.016%
47	18.980	2714	2719	2726	rBV2	61470	83623	1.16%	0.123%
48	19.051	2726	2731	2735	rBV	58350	85726	1.19%	0.126%
49	19.210	2753	2758	2769	rBV	298778	479647	6.64%	0.707%
50	19.357	2780	2783	2787	rVB3	20379	22925	0.32%	0.034%
51	19.416	2787	2793	2801	rBV	5177947	7220626	100.00%	10.647%
52	19.974	2884	2888	2890	rBV	40693	47418	0.66%	0.070%
53	20.469	2969	2972	2976	rBV2	87956	101666	1.41%	0.150%
54	20.945	3049	3053	3056	rBV	159200	197233	2.73%	0.291%
55	21.251	3099	3105	3112	rBV2	2004804	2792715	38.68%	4.118%
56	21.439	3133	3137	3143	rBV	202052	255164	3.53%	0.376%
57	21.986	3226	3230	3238	rVB	225700	342219	4.74%	0.505%
58	22.604	3328	3335	3342	rBV2	432200	853092	11.81%	1.258%
59	23.315	3451	3456	3468	rVB	279016	534604	7.40%	0.788%
60	23.945	3554	3563	3577	rVB2	2383938	5505649	76.25%	8.118%
61	24.139	3588	3596	3615	rVB	1229271	3082345	42.69%	4.545%
62	25.139	3760	3766	3777	rVB	189314	481003	6.66%	0.709%

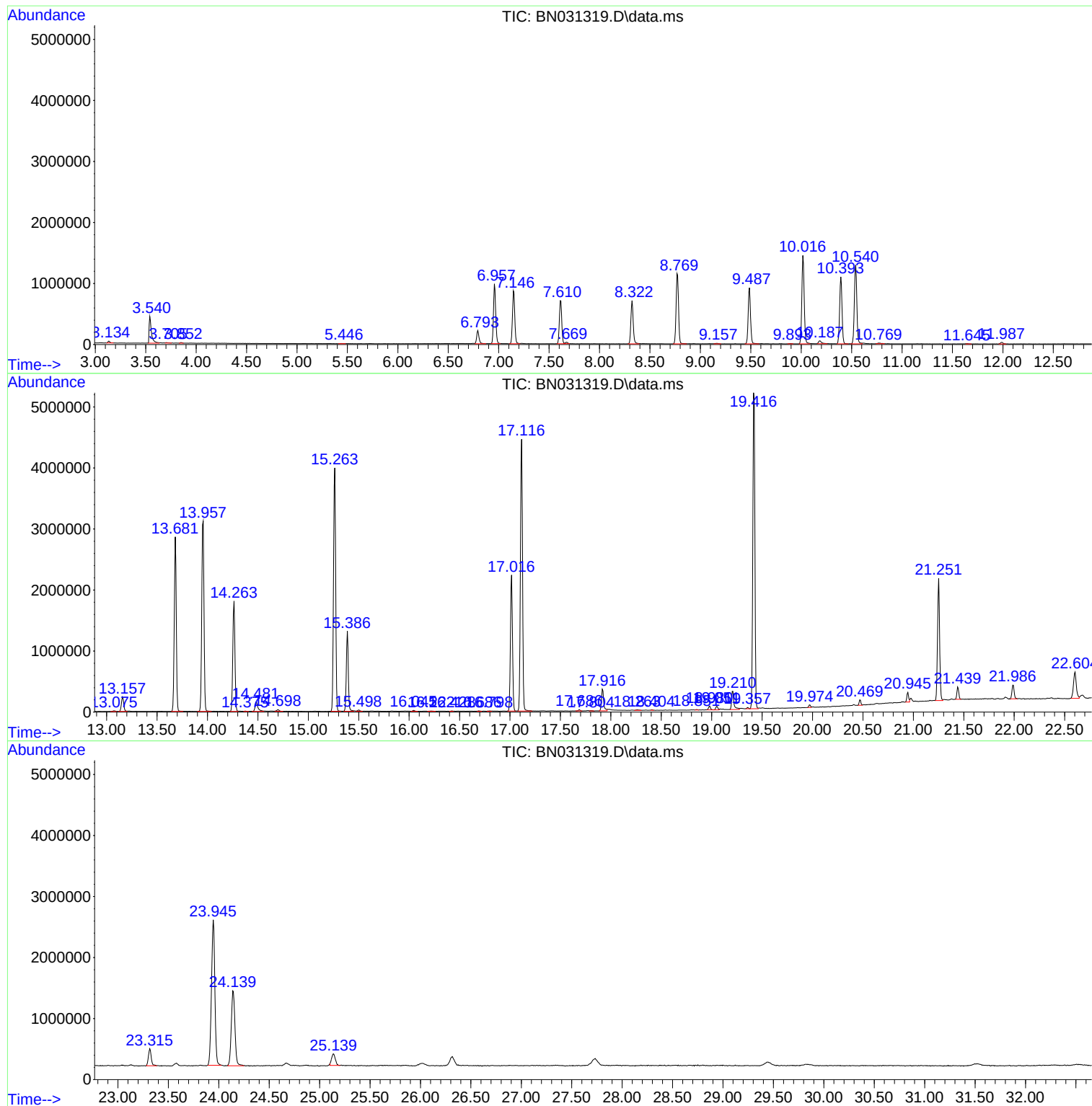
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN042924.MA.M
Quant Title : SVOA CALIBRATION

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



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Data File : BN031319.D
Acq On : 30 Apr 2024 13:14
Operator : MA/JU
Sample : P2140-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YCSQ9

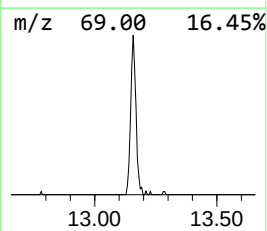
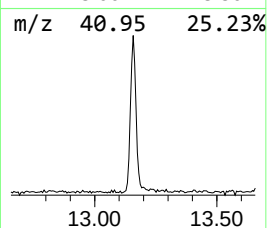
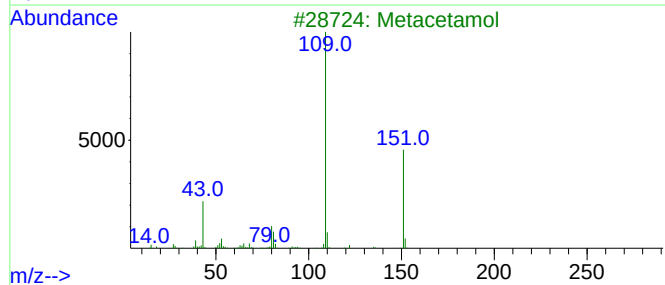
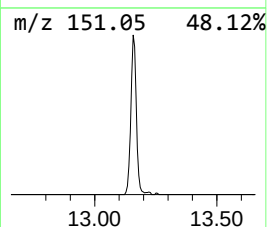
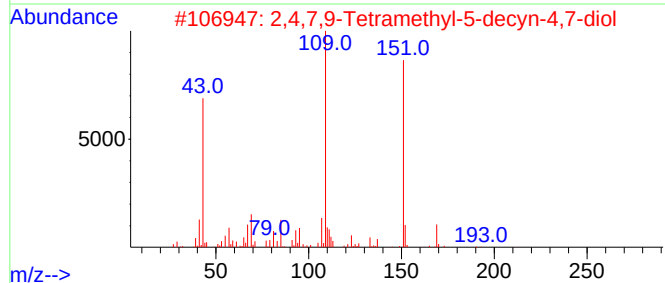
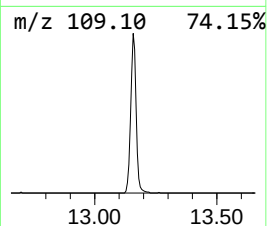
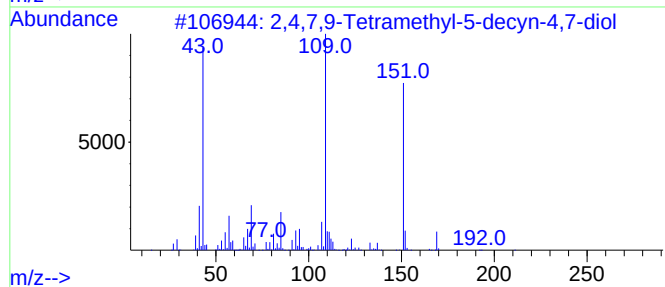
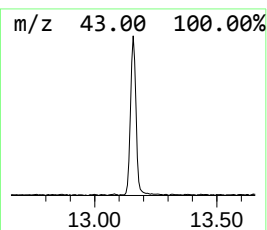
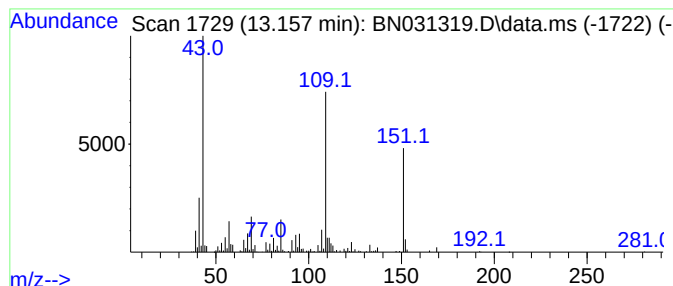
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.157	2.90 ng/ul	373119	Acenaphthene-d10	14.263

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91		
2	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91		
3	Metacetamol	151	C8H9NO2	000621-42-1	64		
4	Metacetamol	151	C8H9NO2	000621-42-1	59		
5	Acetaminophen	151	C8H9NO2	000103-90-2	59		



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Sample : P2140-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YCSQ9

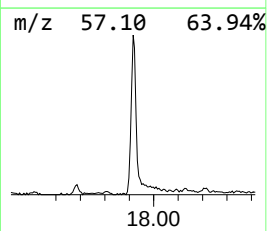
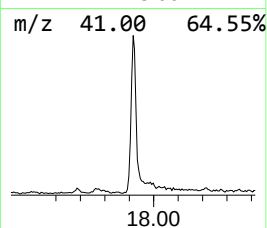
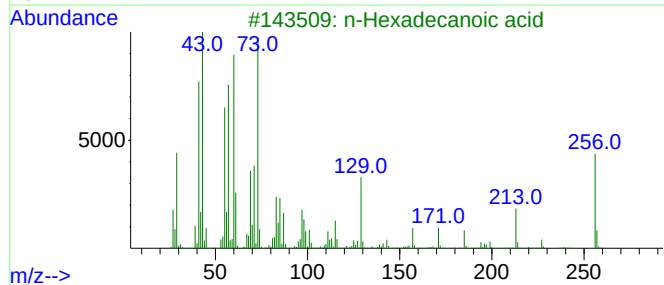
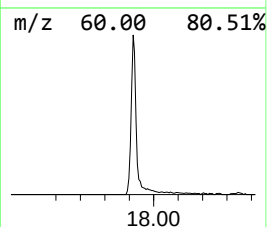
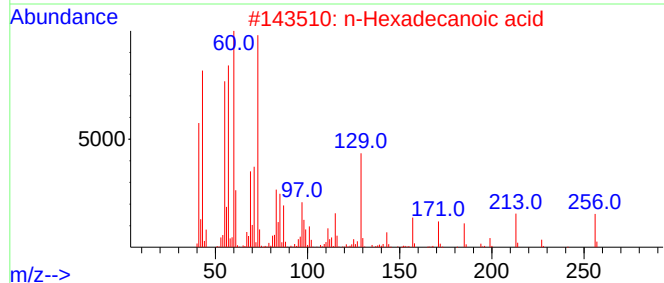
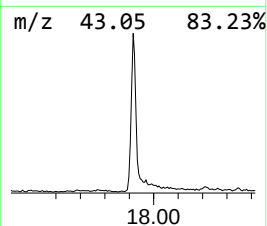
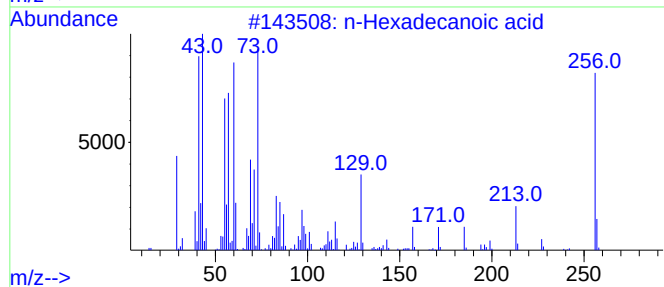
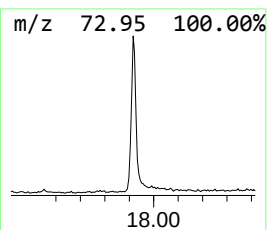
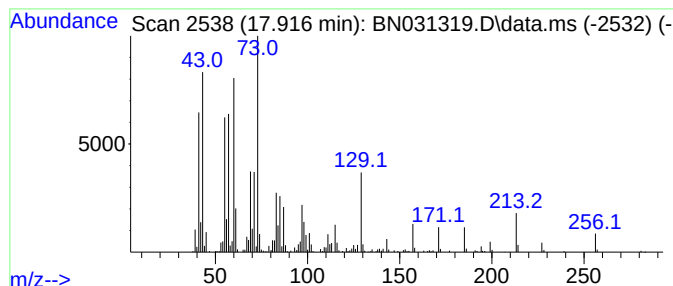
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN042924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.916	3.37 ng/ul	524369	Phenanthrene-d10	17.016

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5			Tridecanoic acid	214	C13H26O2	000638-53-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN043024\
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Sample : P2140-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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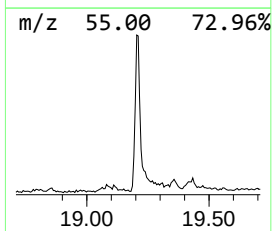
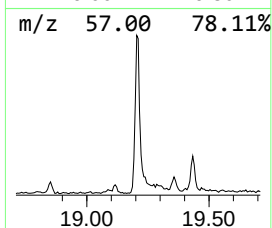
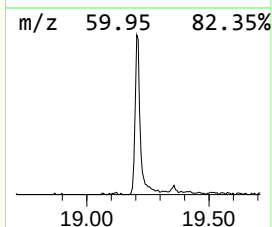
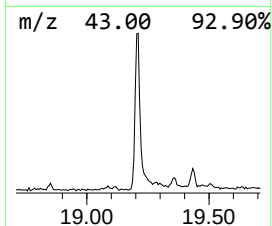
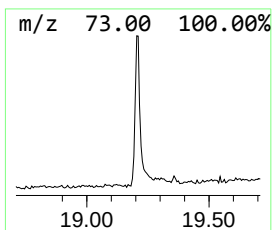
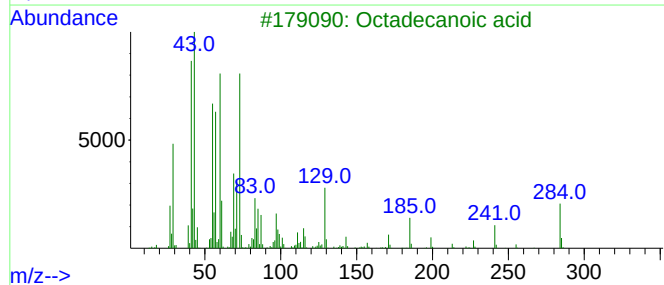
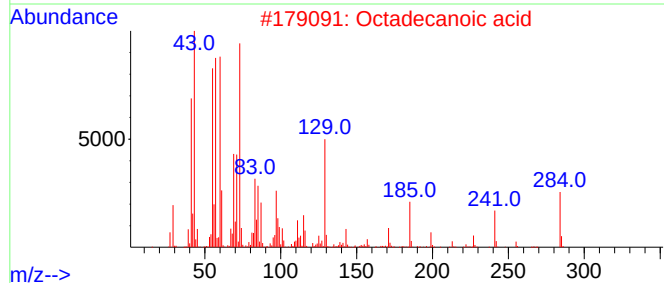
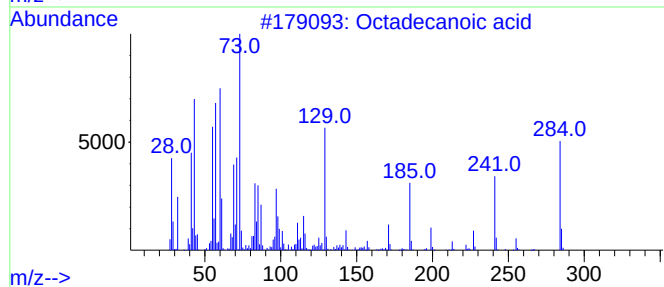
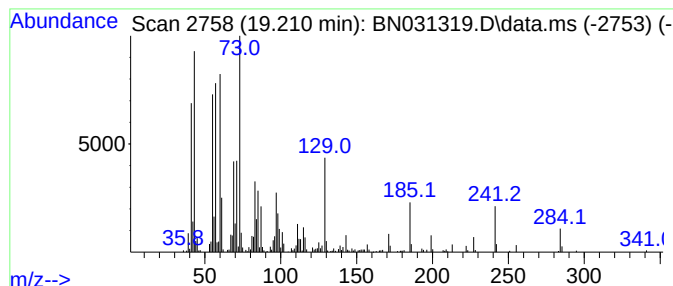
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN042924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.210	3.43 ng/ul	479647	Chrysene-d12	21.251

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



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Data File : BN031319.D
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Operator : MA/JU
Sample : P2140-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

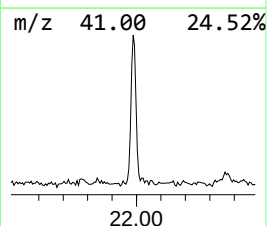
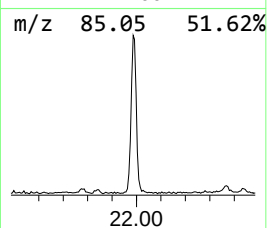
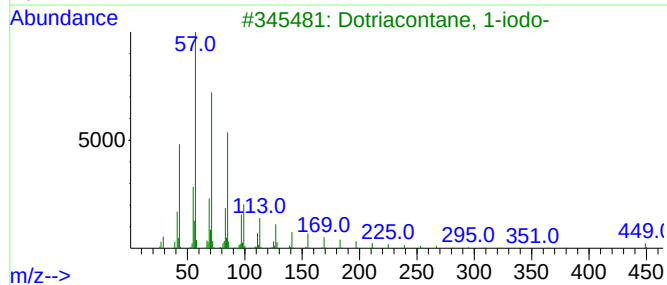
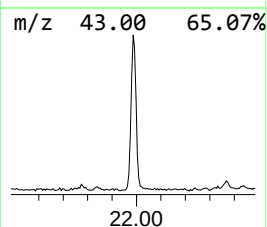
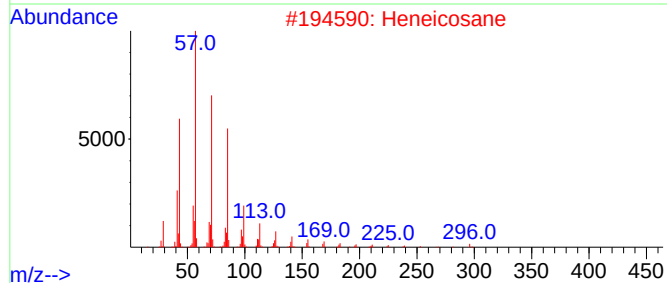
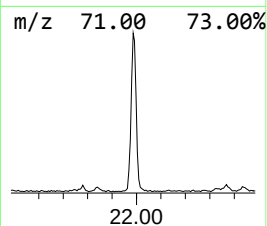
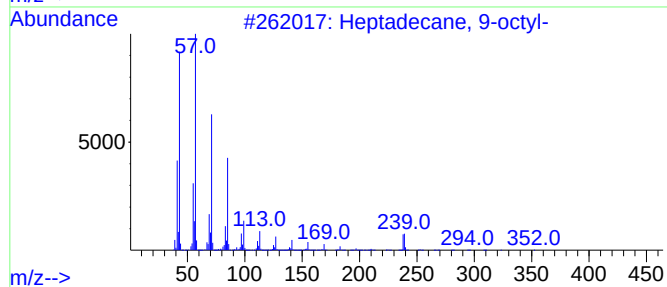
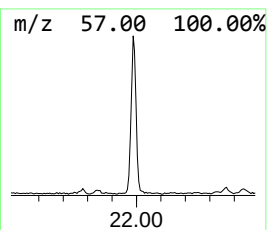
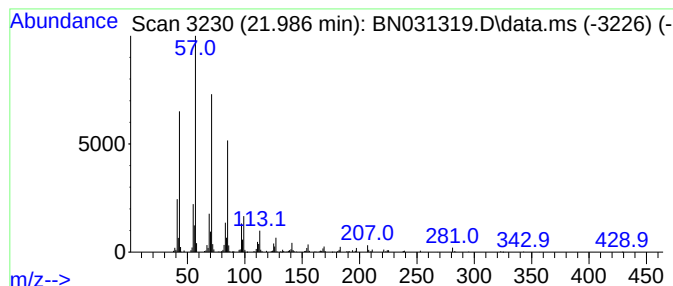
Instrument :
BNA_N
ClientSampleId :
YCSQ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN042924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.986	2.45 ng/ul	342219	Chrysene-d12		21.251	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	91
4	Eicosane, 2-methyl-		296	C21H44	001560-84-5	91
5	Octacosane, 2-methyl-		408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN043024\
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Misc :
ALS Vial : 9 Sample Multiplier: 1

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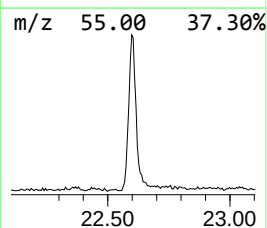
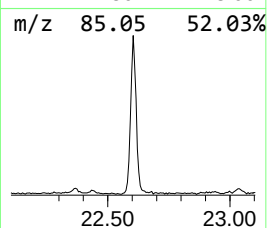
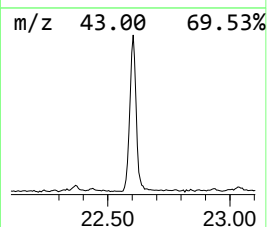
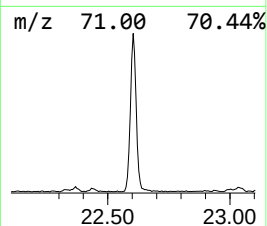
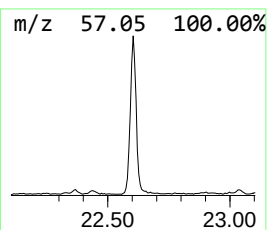
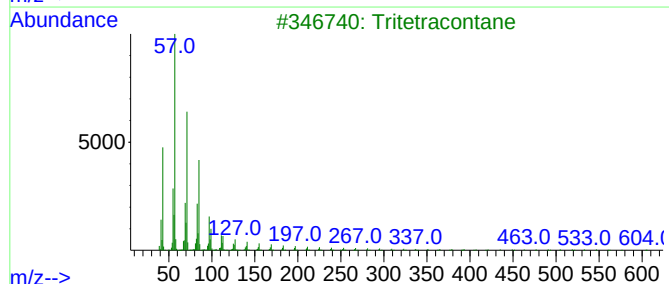
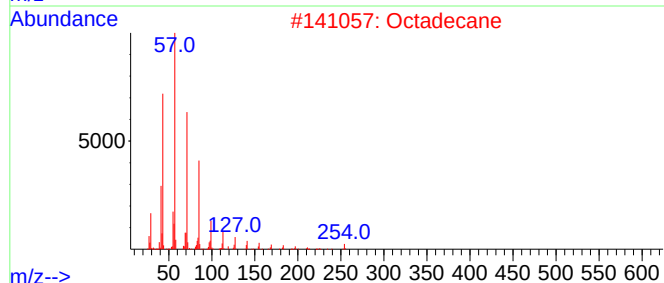
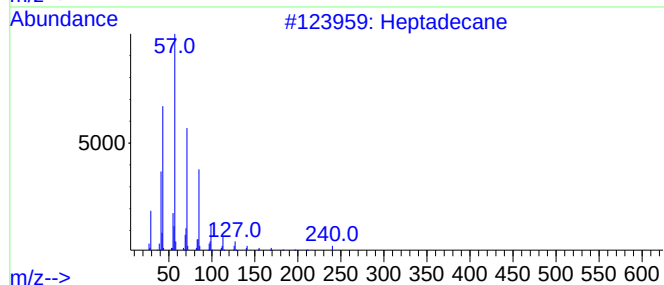
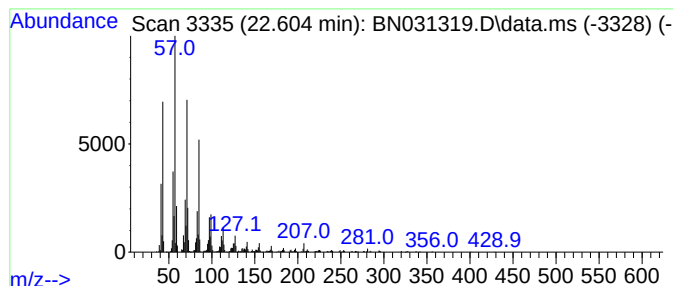
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.604	6.11 ng/ul	853092	Chrysene-d12	21.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	96
2			Octadecane	254	C18H38	000593-45-3	93
3			Tritetracontane	605	C43H88	007098-21-7	76
4			Tetracosane	338	C24H50	000646-31-1	76
5			Octacosane	394	C28H58	000630-02-4	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN043024\
Data File : BN031319.D
Acq On : 30 Apr 2024 13:14
Operator : MA/JU
Sample : P2140-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YCSQ9

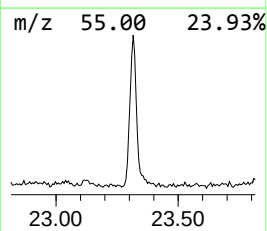
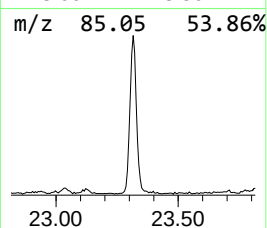
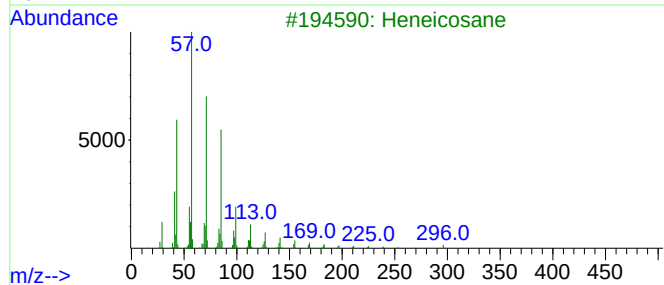
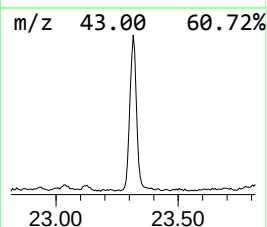
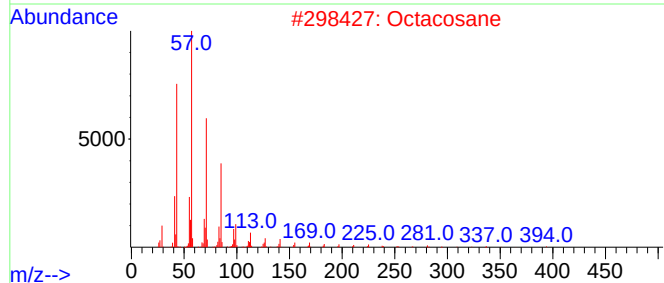
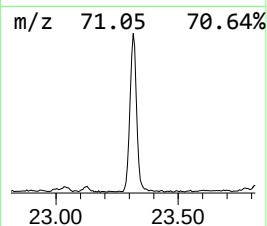
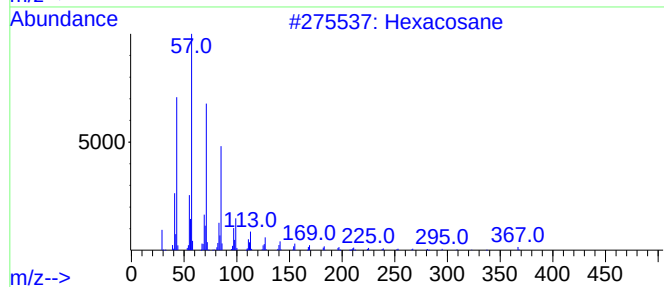
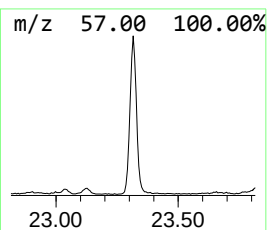
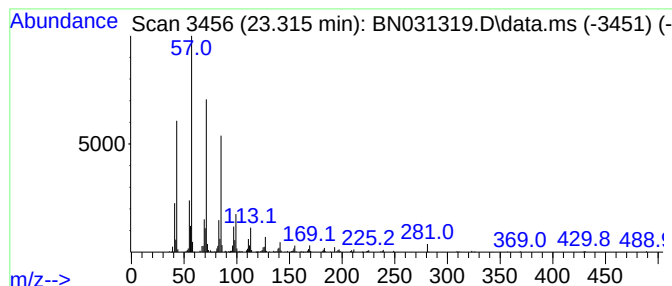
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.315	3.47 ng/ul	534604	Perylene-d12	24.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	93
2			Octacosane	394	C28H58	000630-02-4	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN043024\
Data File : BN031319.D
Acq On : 30 Apr 2024 13:14
Operator : MA/JU
Sample : P2140-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YCSQ9

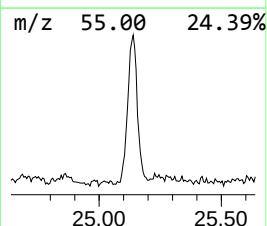
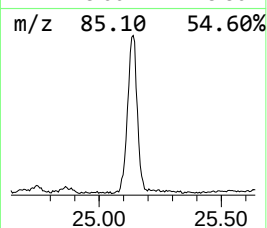
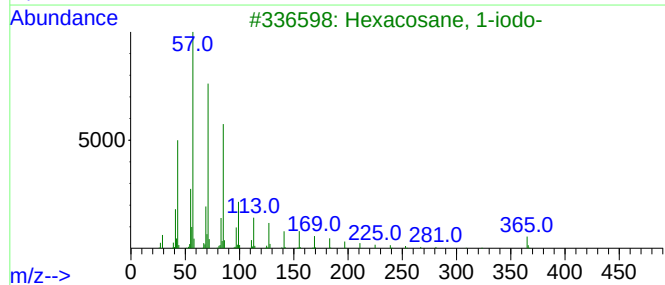
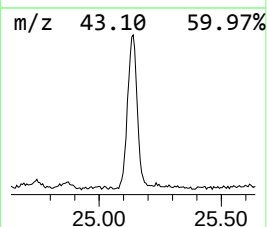
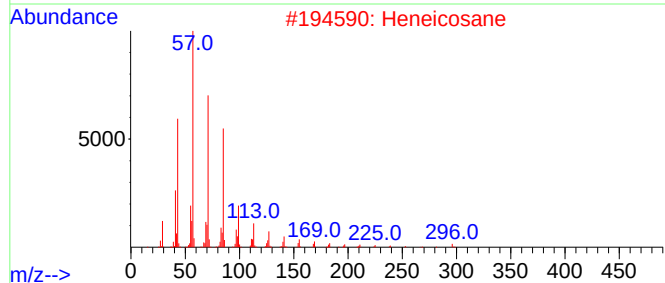
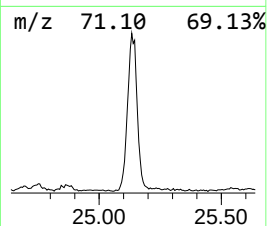
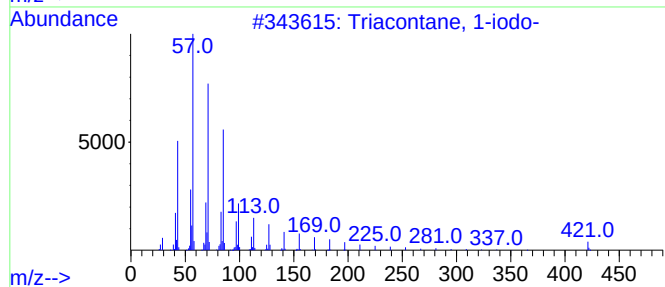
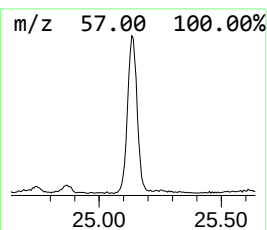
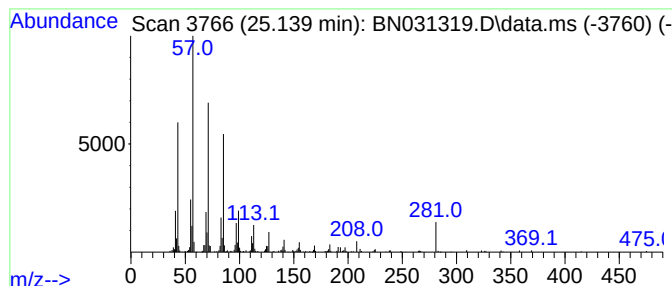
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN042924.MA.M
Quant Title : SVOA CALIBRATION

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

Peak Number 7 Triacontane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.139	3.12 ng/ul	481003	Perylene-d12	24.139

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	90
2			Heneicosane	296	C21H44	000629-94-7	90
3			Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	90
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5			Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN043024\
Data File : BN031319.D
Acq On : 30 Apr 2024 13:14
Operator : MA/JU
Sample : P2140-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
YCSQ9

Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN042924.MA.M
Quant Title : SVOA CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrame...	13.157	2.9	ng/ul	373119	3	14.263	2577510	20.0
n-Hexadecanoic ...	17.916	3.4	ng/ul	524369	4	17.016	3110300	20.0
Octadecanoic acid	19.210	3.4	ng/ul	479647	5	21.251	2792720	20.0
(DEL) Alkane: S...	21.986	2.5	ng/ul	342219	5	21.251	2792720	20.0
(DEL) Alkane: S...	22.604	6.1	ng/ul	853092	5	21.251	2792720	20.0
(DEL) Alkane: S...	23.315	3.5	ng/ul	534604	6	24.139	3082350	20.0
triacontane, 1-...	25.139	3.1	ng/ul	481003	6	24.139	3082350	20.0