

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN112122\
 Data File : BN022826.D
 Acq On : 22 Nov 2022 16:00
 Operator : CG/JU
 Sample : N5593-08
 Misc :
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 H0AD7

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: BN022826.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	29	32	43	rVB	16253	25830	1.09%	0.114%
2	3.617	105	107	124	rBV	79286	150394	6.33%	0.666%
3	3.846	142	146	152	rVB	7002	12215	0.51%	0.054%
4	3.946	159	163	168	rVB	3616	5786	0.24%	0.026%
5	4.916	323	328	335	rBV	32728	50598	2.13%	0.224%
6	7.016	678	685	693	rBV	82348	139685	5.88%	0.619%
7	7.181	706	713	724	rBV	284889	445032	18.74%	1.971%
8	7.369	739	745	755	rBV	270855	443786	18.69%	1.966%
9	7.846	819	826	834	rBV	245025	388217	16.35%	1.720%
10	8.569	942	949	963	rBV	236898	385327	16.22%	1.707%
11	9.028	1019	1027	1035	rBV	362961	606068	25.52%	2.685%
12	9.399	1087	1090	1097	rVB2	2466	3614	0.15%	0.016%
13	9.751	1143	1150	1161	rBV	300682	504474	21.24%	2.235%
14	10.287	1234	1241	1261	rBV	414932	708179	29.82%	3.137%
15	10.663	1298	1305	1313	rBV	378999	624497	26.30%	2.766%
16	10.816	1324	1331	1344	rBV	290929	532040	22.40%	2.357%
17	12.087	1544	1547	1554	rVB5	2341	3806	0.16%	0.017%
18	12.269	1572	1578	1584	rVB	4904	8631	0.36%	0.038%
19	13.334	1751	1759	1763	rVB5	1530	2654	0.11%	0.012%
20	13.934	1852	1861	1877	rBV	957839	1308820	55.11%	5.798%
21	14.210	1901	1908	1919	rBV2	1011690	1433599	60.36%	6.350%
22	14.516	1954	1960	1968	rBV	618645	863545	36.36%	3.825%
23	14.739	1993	1998	2012	rBV	68500	142569	6.00%	0.632%
24	15.351	2098	2102	2106	rBV3	1624	2410	0.10%	0.011%
25	15.510	2123	2129	2142	rBV	1252042	1832888	77.18%	8.119%
26	15.645	2146	2152	2164	rVV	509462	683910	28.80%	3.029%
27	15.751	2167	2170	2173	rVB2	4037	4866	0.20%	0.022%
28	16.298	2257	2263	2269	rBV	20802	31053	1.31%	0.138%
29	16.663	2323	2325	2331	rBV3	2724	4071	0.17%	0.018%
30	17.269	2422	2428	2436	rBV	741608	1015932	42.78%	4.500%
31	17.369	2439	2445	2456	rBV	1361346	1892327	79.68%	8.382%
32	17.633	2485	2490	2493	rBV3	1899	2415	0.10%	0.011%
33	17.663	2493	2495	2502	rVB3	1648	2787	0.12%	0.012%
34	17.939	2536	2542	2547	rBV	25356	31076	1.31%	0.138%
35	18.033	2555	2558	2563	rBV4	2376	3696	0.16%	0.016%
36	18.163	2575	2580	2591	rBV	91593	129708	5.46%	0.575%

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Stop Thrs : 0

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	18.275	2593	2599	2606	rVB	194478	258288	10.88%	1.144%
38	18.516	2637	2640	2646	rBV6	5676	8071	0.34%	0.036%
39	18.675	2662	2667	2671	rBV5	5126	7261	0.31%	0.032%
40	19.116	2740	2742	2747	rBV5	3922	4223	0.18%	0.019%
41	19.233	2758	2762	2769	rBV3	18201	24225	1.02%	0.107%
42	19.310	2771	2775	2781	rBV	19457	38837	1.64%	0.172%
43	19.445	2794	2798	2811	rBV	36517	58957	2.48%	0.261%
44	19.598	2821	2824	2826	rVB3	5134	5816	0.24%	0.026%
45	19.674	2831	2837	2847	rVV	1712682	2273867	95.74%	10.072%
46	19.751	2848	2850	2856	rVB2	8118	10965	0.46%	0.049%
47	20.645	2999	3002	3005	rBV5	7134	10169	0.43%	0.045%
48	21.192	3089	3095	3111	rBV	144810	339120	14.28%	1.502%
49	21.474	3138	3143	3151	rBV	903529	1102126	46.41%	4.882%
50	22.568	3326	3329	3332	rVB2	27885	33669	1.42%	0.149%
51	22.704	3348	3352	3360	rVB	108975	154274	6.50%	0.683%
52	23.115	3419	3422	3429	rVB2	53362	79934	3.37%	0.354%
53	23.715	3516	3524	3535	rVB	1184865	2374952	100.00%	10.520%
54	23.863	3543	3549	3560	rVB2	514374	1076745	45.34%	4.770%
55	24.462	3647	3651	3660	rVB2	70363	134229	5.65%	0.595%
56	25.298	3789	3793	3803	rVB3	64564	153333	6.46%	0.679%

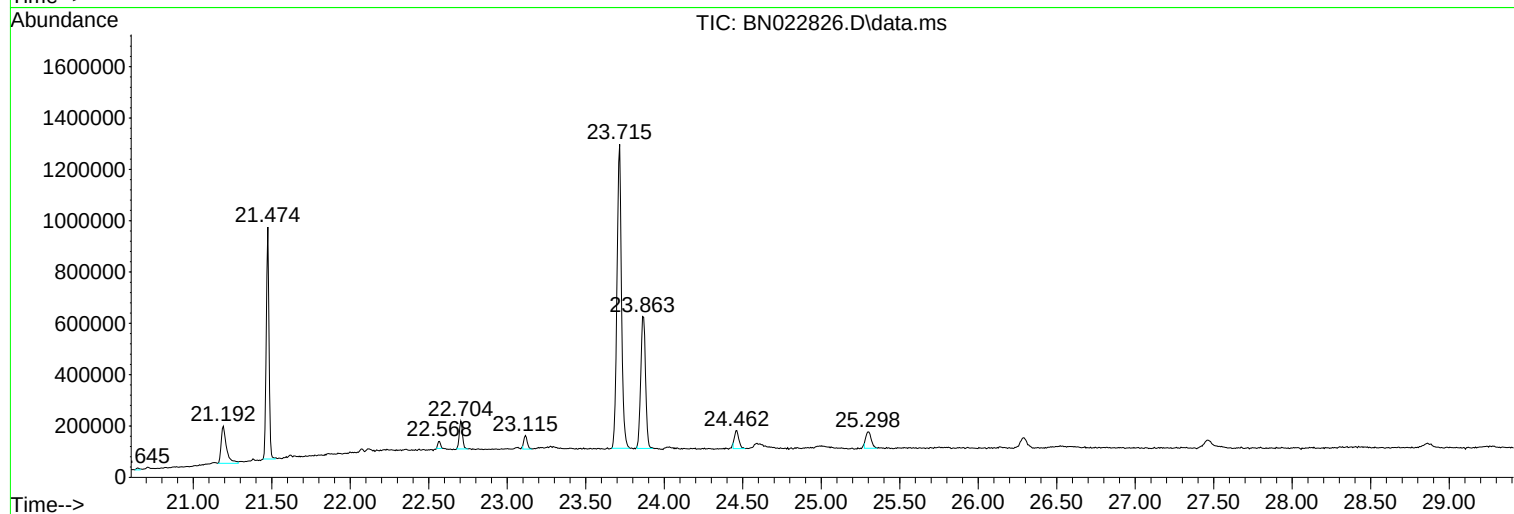
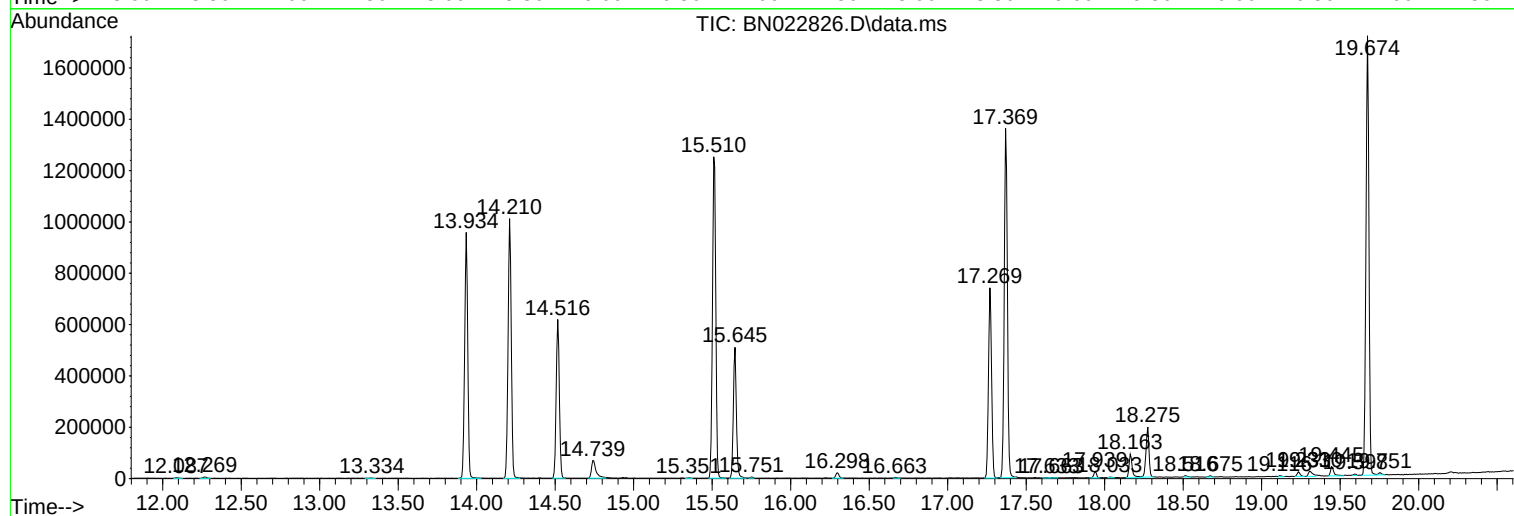
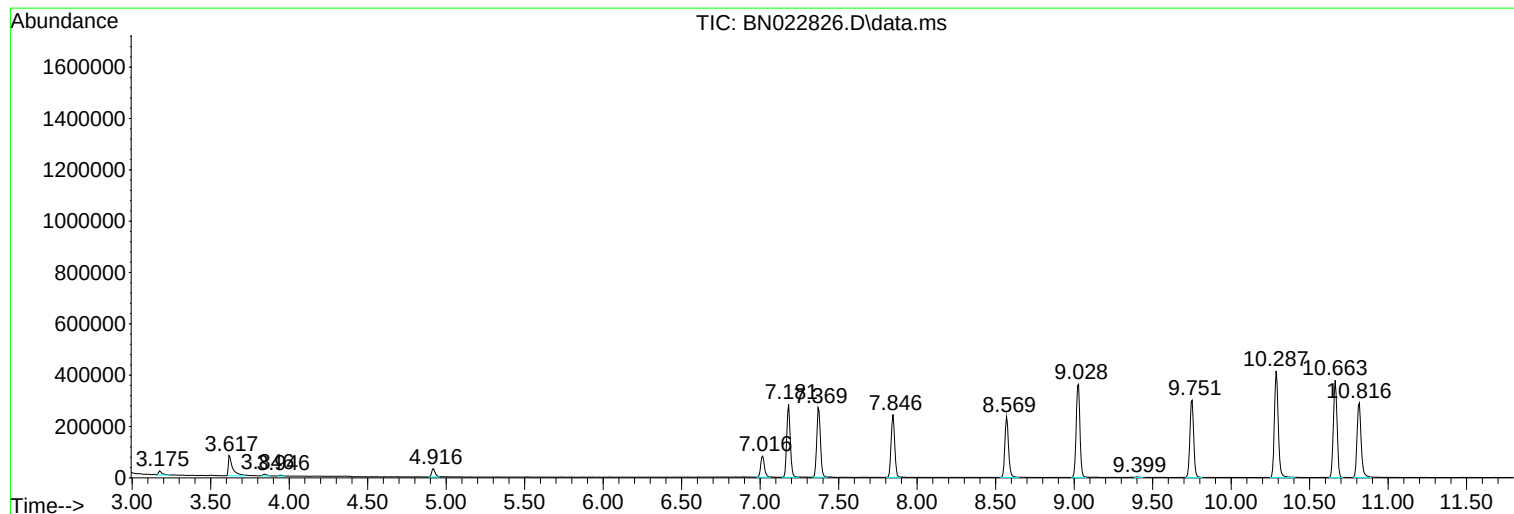
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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



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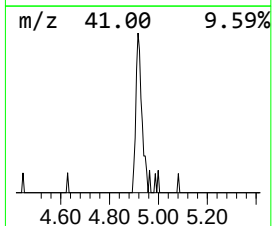
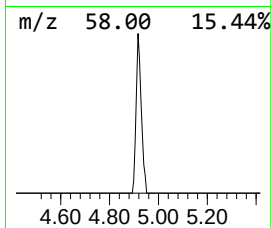
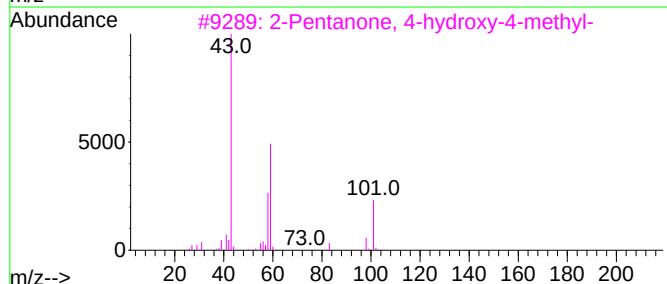
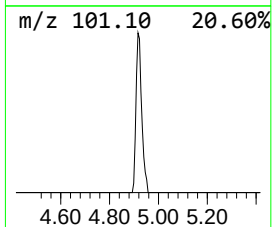
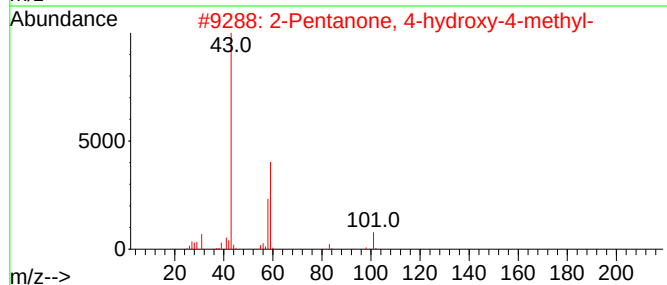
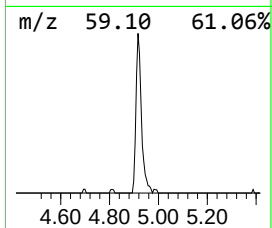
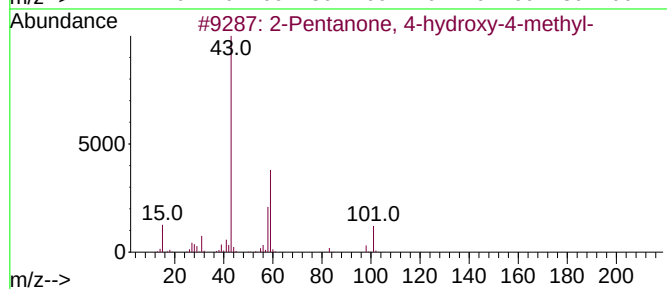
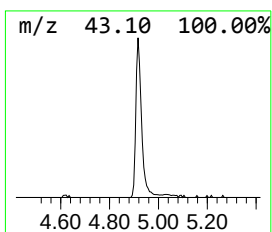
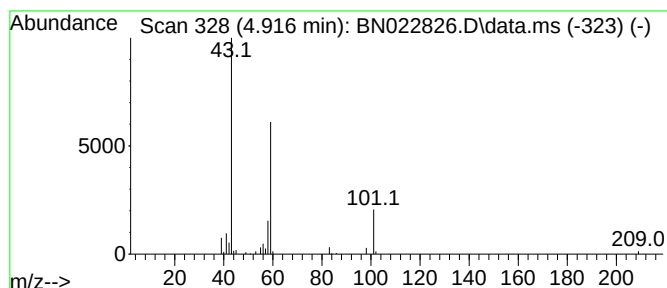
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Quant Title : SVOA CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.916	2.61 ng/ul	50598	1,4-Dichlorobenzene-d4	7.846

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	43		
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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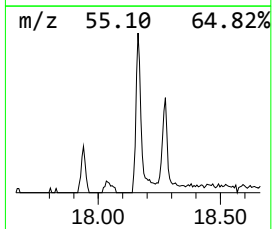
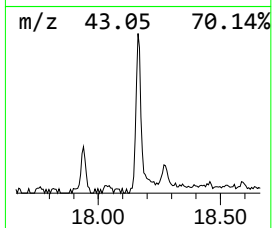
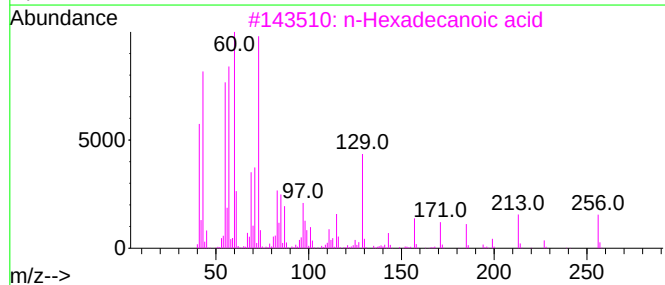
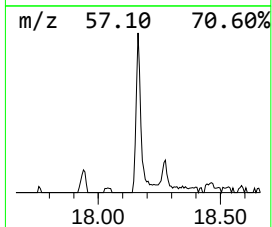
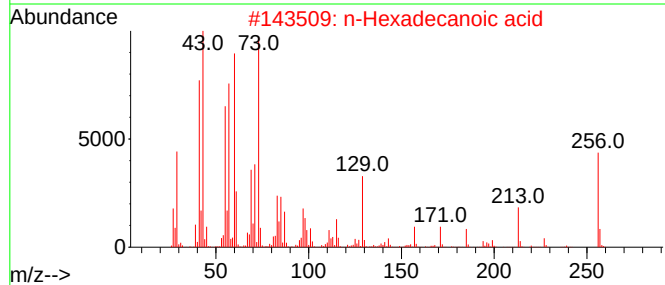
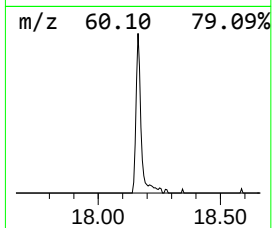
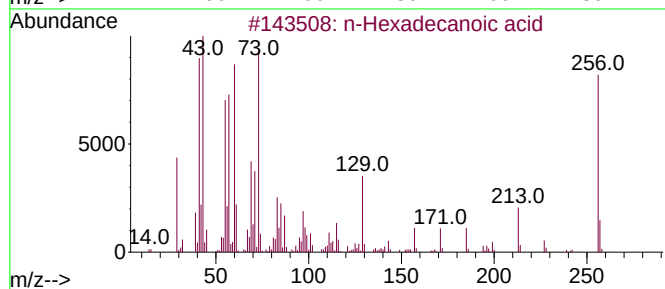
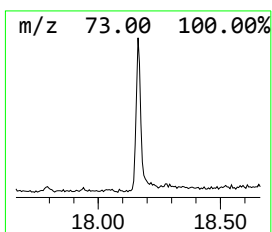
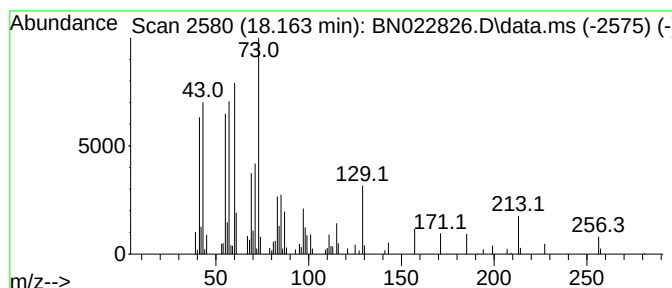
Quant Method : Z:\svoasrv\HPCHEM1\BNA_N\Methods\SFAM-EPA-BN111522.M
Quant Title : SVOA CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.163	2.55 ng/ul	129708	Phenanthrene-d10	17.269

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	98
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94



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Misc :
ALS Vial : 48 Sample Multiplier: 1

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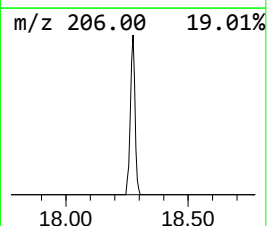
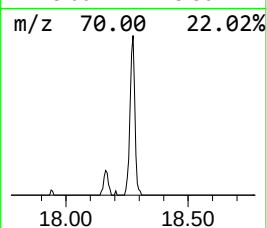
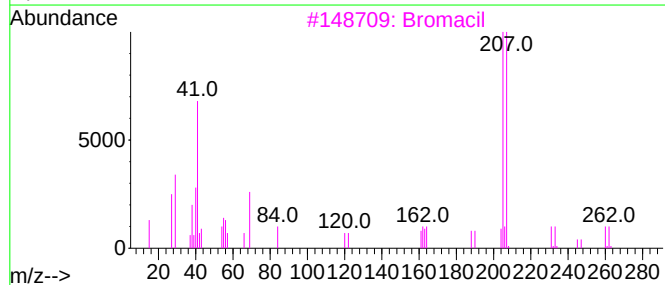
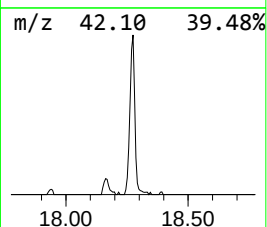
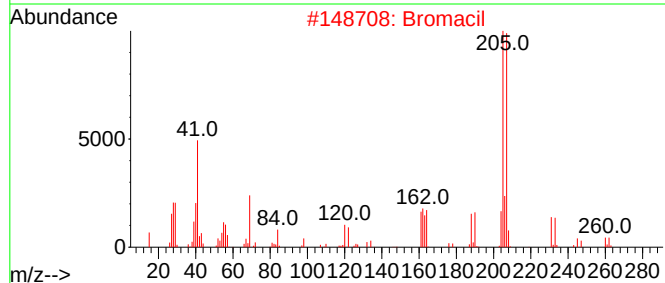
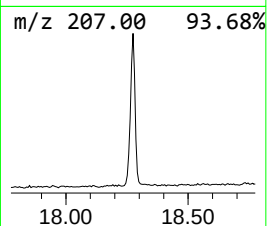
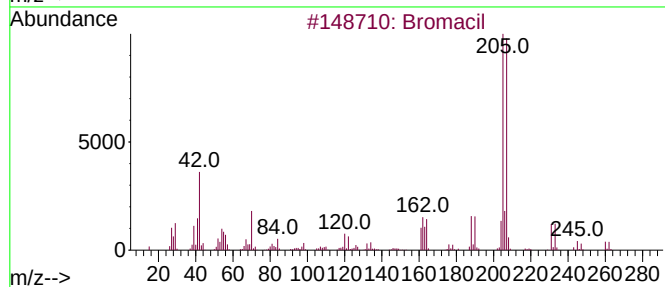
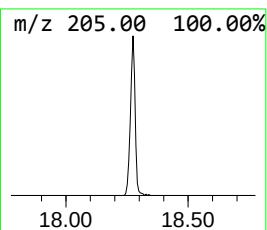
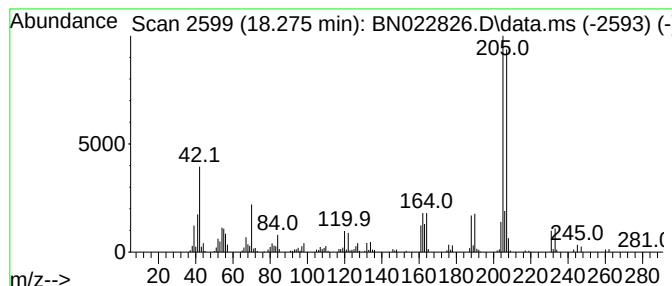
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Quant Title : SVOA CALIBRATION

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

Peak Number 3 Bromacil Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.275	5.08 ng/ul	258288	Phenanthrene-d10	17.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromacil	260	C9H13BrN2O2	000314-40-9	91
2			Bromacil	260	C9H13BrN2O2	000314-40-9	83
3			Bromacil	260	C9H13BrN2O2	000314-40-9	81
4			2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	50
5			5-Acetamido-2,4-dichlorobenzoic ...	247	C9H7Cl2NO3	050602-49-8	42



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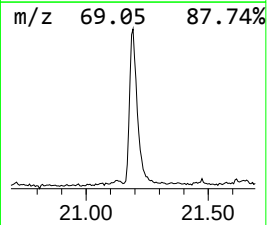
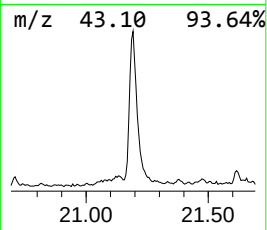
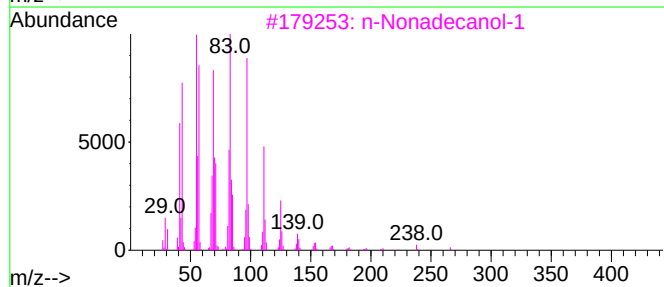
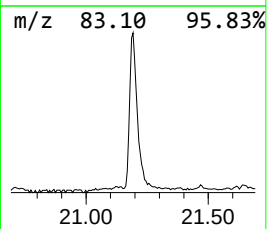
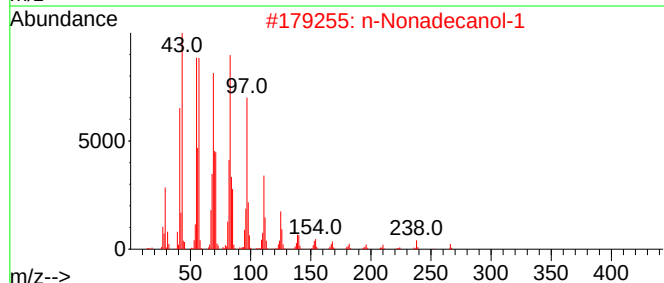
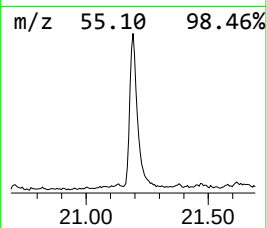
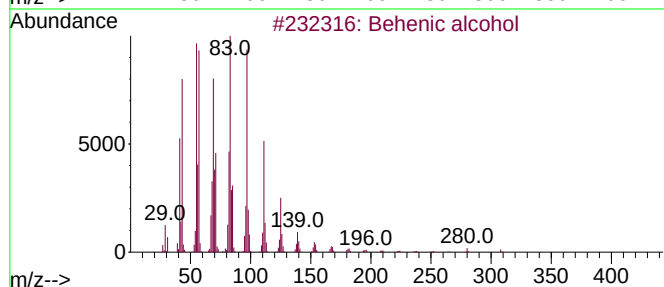
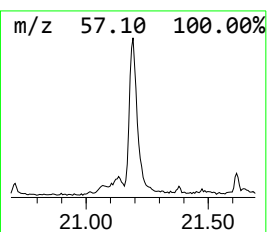
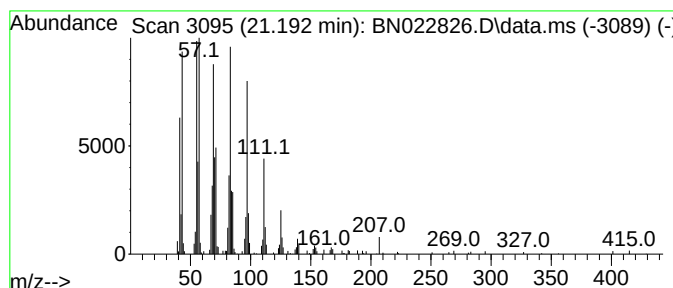
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Quant Title : SVOA CALIBRATION

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

Peak Number 4 Behenic alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.192	6.15 ng/ul	339120	Chrysene-d12	21.474

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	95
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4			1-Heneicosanol	312	C21H44O	015594-90-8	95
5			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94



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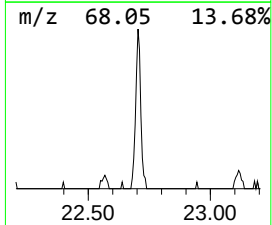
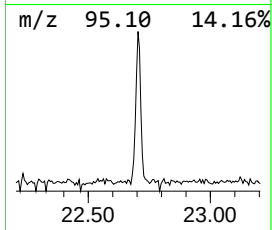
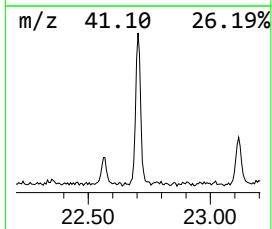
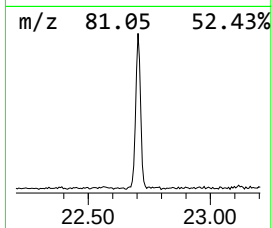
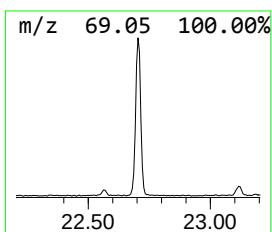
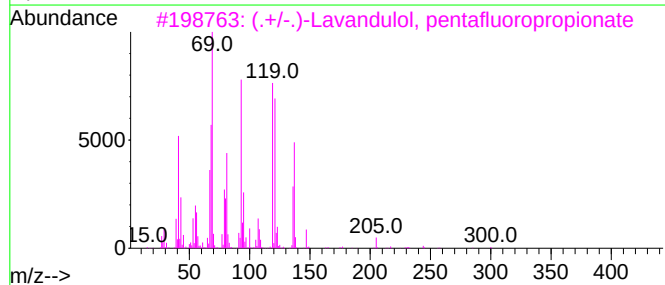
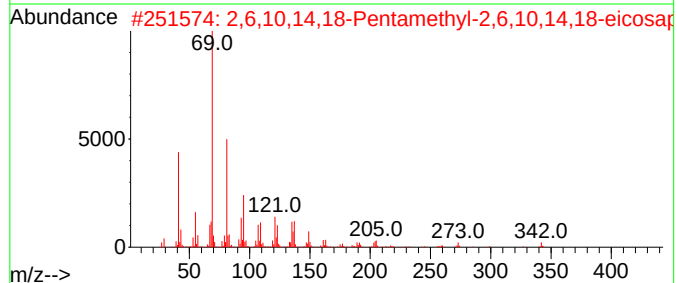
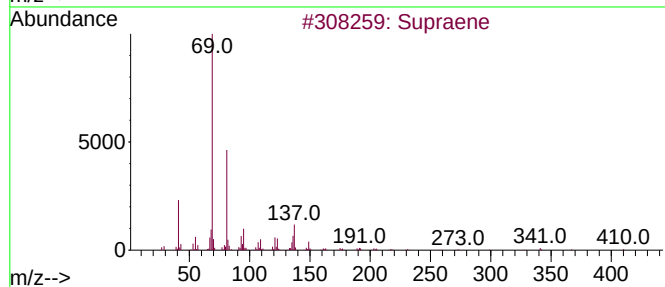
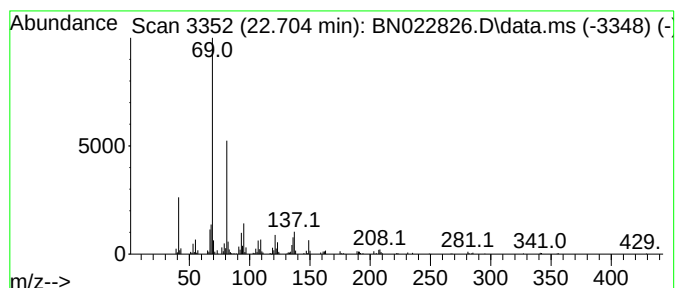
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Quant Title : SVOA CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.704	2.87 ng/ul	154274	Perylene-d12	23.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	87
3			(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	72
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5			5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN112122\
Data File : BN022826.D
Acq On : 22 Nov 2022 16:00
Operator : CG/JU
Sample : N5593-08
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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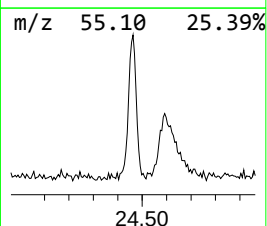
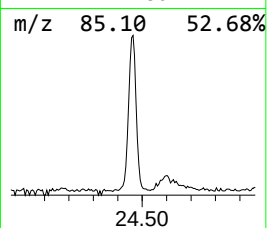
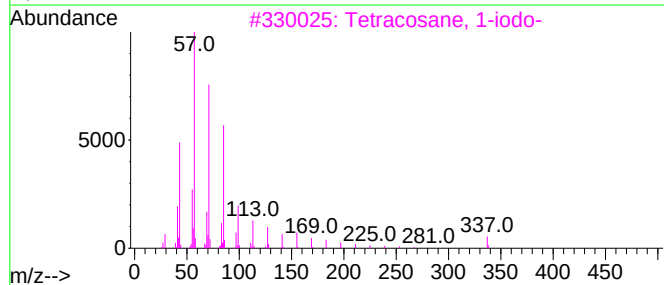
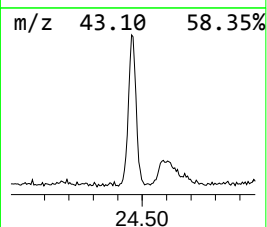
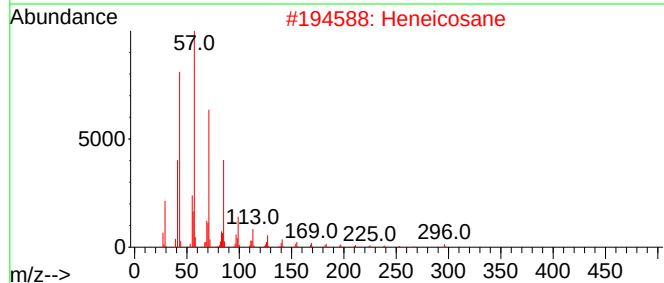
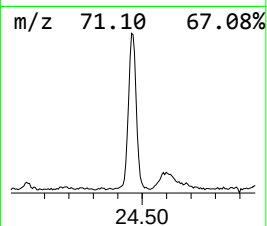
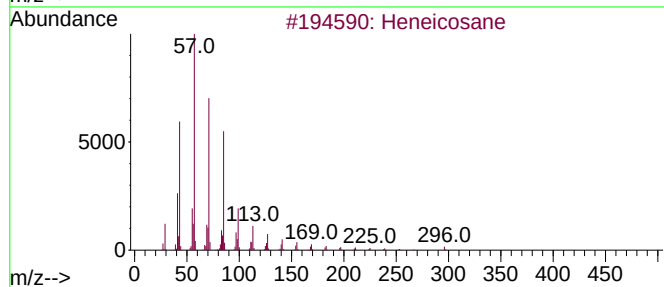
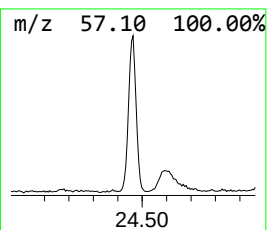
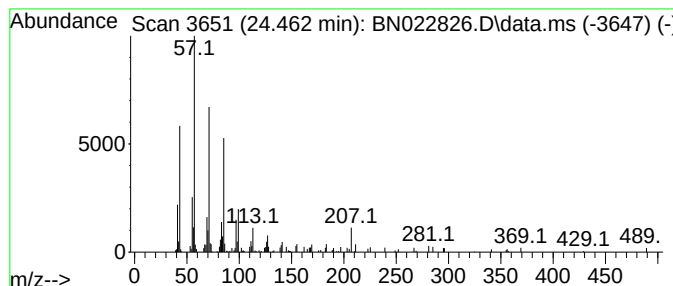
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Quant Title : SVOA CALIBRATION

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.462	2.49 ng/ul	134229	Perylene-d12	23.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	98
2			Heneicosane	296	C21H44	000629-94-7	93
3			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	83
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN112122\
Data File : BN022826.D
Acq On : 22 Nov 2022 16:00
Operator : CG/JU
Sample : N5593-08
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
H0AD7

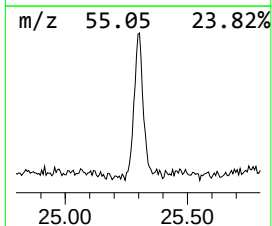
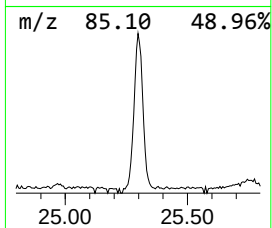
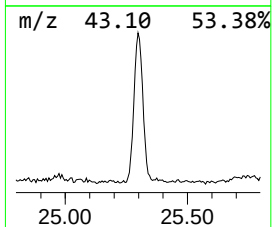
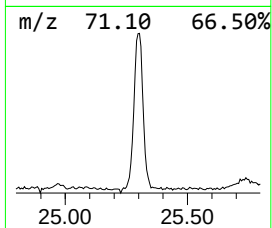
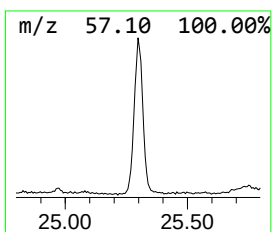
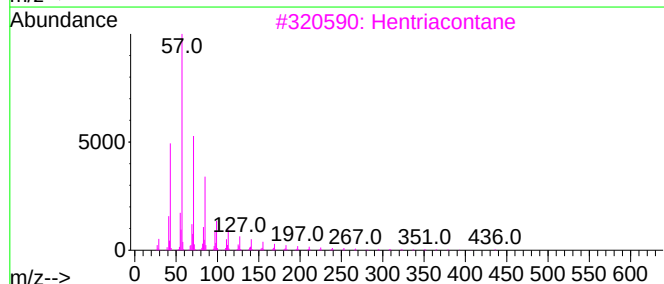
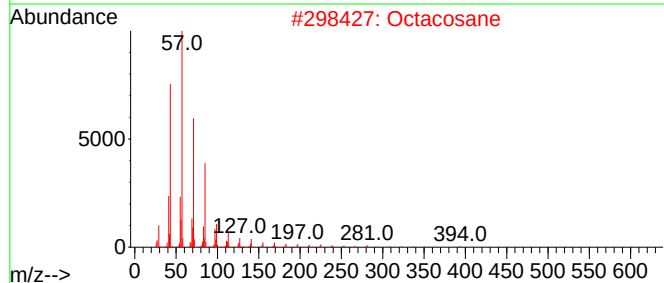
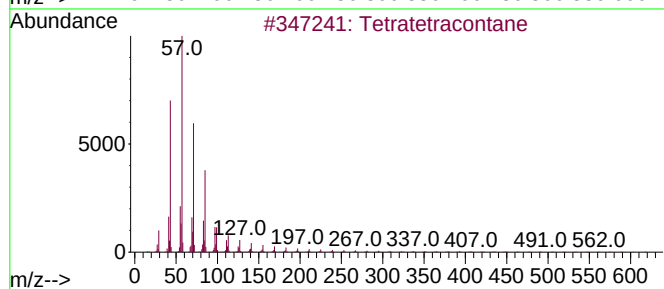
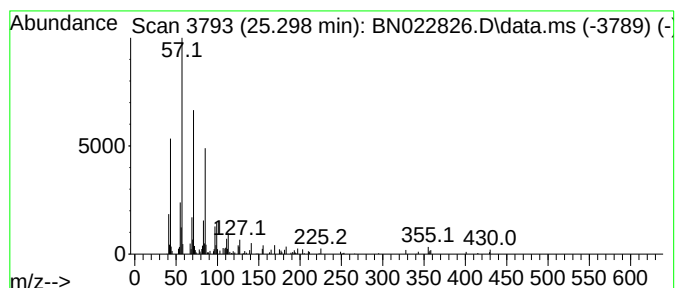
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Quant Title : SVOA CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.298	2.85 ng/ul	153333	Perylene-d12	23.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetratetracontane	619	C44H90	007098-22-8	90
2		Octacosane	394	C28H58	000630-02-4	90
3		Hentriacontane	437	C31H64	000630-04-6	90
4		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	87
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN112122\
Data File : BN022826.D
Acq On : 22 Nov 2022 16:00
Operator : CG/JU
Sample : N5593-08
Misc :
ALS Vial : 48 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
H0AD7

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.916	2.6	ng/ul	50598	1	7.846	388217	20.0
n-Hexadecanoic ...	18.163	2.5	ng/ul	129708	4	17.269	1015930	20.0
Bromacil	18.275	5.1	ng/ul	258288	4	17.269	1015930	20.0
Behenic alcohol	21.192	6.2	ng/ul	339120	5	21.474	1102130	20.0
Supraene	22.704	2.9	ng/ul	154274	6	23.863	1076750	20.0
(DEL) Alkane: S...	24.462	2.5	ng/ul	134229	6	23.863	1076750	20.0
(DEL) Alkane: S...	25.298	2.9	ng/ul	153333	6	23.863	1076750	20.0