LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
Data File : BP021101.D
Acq On : 23 Jul 2024 16:28
Operator : MA/JU
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : A4BF8

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_P\Methods\SFAM-EPA-BP071024.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BP021101.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.187	31	34	39	rVB	15489	19324	0.70%	0.063%
2	3.475	79	83	96	rBV	52107	91676	3.33%	0.299%
3	3.605	102	105	107	rBV2	6697	9149	0.33%	0.030%
4	3.628	107	109	116	rVV	19671	35093	1.28%	0.114%
5	3.699	117	121	129	rVB	36691	54043	1.97%	0.176%
6	3.911	154	157	160	rVB4	8462	9300	0.34%	0.030%
7	4.140	193	196	203	rVB6	7167	9528	0.35%	0.031%
8	4.322	224	227	238	rVB4	8090	19835	0.72%	0.065%
9	4.411	240	242	247	rVB5	4395	5350	0.19%	0.017%
10	4.464	247	251	254	rBV3	7344	10178	0.37%	0.033%
11	4.693	288	290	293	rVB4	3095	2970	0.11%	0.010%
12	4.811	306	310	318	rVB	37022	55481	2.02%	0.181%
13	4.934	324	331	339	rVB	5036	12743	0.46%	0.042%
14	5.511	424	429	431	rBV6	1902	3338	0.12%	0.011%
15	6.234	548	552	556	rVB7	2051	2933	0.11%	0.010%
16	6.634	617	620	623	rVB5	2373	3142	0.11%	0.010%
17	6.764	635	642	646	rVV3	8640	15556	0.57%	0.051%
18	6.875	654	661	673	rBV	262195	504747	18.36%	1.645%
19	7.011	678	684	697	rVB	226378	369905	13.45%	1.206%
20	7.211	711	718	728	rBV	305562	507797	18.47%	1.655%
21	7.287	728	731	747	rVB3	23771	66138	2.41%	0.216%
22	7.663	787	795	807	rBV	561271	904272	32.89%	2.948%
23	7.752	807	810	817	rVB9	6023	11289	0.41%	0.037%
24	8.099	863	869	872	rBV8	2075	3264	0.12%	0.011%
25	8.393	912	919	933	rBV	296015	519022	18.88%	1.692%
26	8.493	933	936	940	rVB3	7019	10801	0.39%	0.035%
27	8.822	985	992	1005	rBV	264728	473640	17.23%	1.544%
28	8.963	1012	1016	1021	rVB8	5302	8998	0.33%	0.029%
29	9.175	1045	1052	1055	rBV2	6778	10712	0.39%	0.035%
30	9.375	1080	1086	1096	rBV2	21823	42034	1.53%	0.137%
31	9.534	1105	1113	1129	rBV	233758	426659	15.52%	1.391%
32	10.087	1200	1207	1221	rBV	302051	657645	23.92%	2.144%
33	10.428	1257	1265	1279	rBV	716002	1269052	46.16%	4.137%
34	10.599	1286	1294	1311	rBV	222035	490719	17.85%	1.600%
35	10.987	1352	1360	1366	rBV	11640	30204	1.10%	0.098%
36	11.187	1386	1394	1405	rBV	84517	225602	8.21%	0.735%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
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Acq On : 23 Jul 2024 16:28
Operator : MA/JU
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BF8

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_P\Methods\SFAM-EPA-BP071024.MA.M
Title : SVOA CALIBRATION

37	11.263	1405	1407	1414	rVB8	4591	9908	0.36%	0.032%
38	11.646	1468	1472	1479	rVB10	2441	4597	0.17%	0.015%
39	11.922	1514	1519	1520	rBV5	2363	3004	0.11%	0.010%
40	12.034	1532	1538	1545	rVV7	5670	11118	0.40%	0.036%
41	12.316	1579	1586	1589	rBV9	1454	3215	0.12%	0.010%
42	12.804	1667	1669	1675	rVB7	1835	3089	0.11%	0.010%
43	12.887	1679	1683	1686	rBV6	3649	6120	0.22%	0.020%
44	13.087	1713	1717	1719	rBV5	3507	4740	0.17%	0.015%
45	13.193	1731	1735	1737	rVB5	3460	4469	0.16%	0.015%
46	13.263	1741	1747	1750	rBV8	4508	7544	0.27%	0.025%
47	13.634	1805	1810	1814	rVB8	3006	4805	0.17%	0.016%
48	13.716	1814	1824	1837	rBV	648258	979359	35.62%	3.193%
49	13.804	1837	1839	1844	rVB6	2472	3518	0.13%	0.011%
50	13.998	1861	1872	1886	rBV	817488	1233074	44.85%	4.020%
51	14.310	1915	1925	1934	rBV	1071973	1710873	62.22%	5.577%
52	14.504	1952	1958	1960	rBV	965457	1380296	50.20%	4.500%
53	14.528	1960	1962	1970	rVB	1068131	1578828	57.42%	5.147%
54	14.610	1970	1976	1984	rBV	125694	292899	10.65%	0.955%
55	14.716	1992	1994	1995	rBV2	4484	3932	0.14%	0.013%
56	15.110	2057	2061	2066	rBV7	5440	7268	0.26%	0.024%
57	15.328	2090	2098	2105	rBV	904172	1503837	54.69%	4.903%
58	15.392	2106	2109	2113	rVB5	13967	20295	0.74%	0.066%
59	15.487	2118	2125	2136	rBV	233759	368122	13.39%	1.200%
60	15.898	2191	2195	2205	rVB	11534	25384	0.92%	0.083%
61	16.063	2218	2223	2225	rBV6	7311	10249	0.37%	0.033%
62	16.228	2248	2251	2253	rBV4	5277	6756	0.25%	0.022%
63	16.528	2298	2302	2306	rBV6	10776	22131	0.80%	0.072%
64	16.657	2320	2324	2328	rBV7	12070	16566	0.60%	0.054%
65	16.787	2342	2346	2349	rVB5	5887	8466	0.31%	0.028%
66	16.881	2359	2362	2365	rBV5	7970	9920	0.36%	0.032%
67	17.122	2397	2403	2409	rBV	1349979	2091162	76.06%	6.817%
68	17.169	2409	2411	2416	rVV	113460	157803	5.74%	0.514%
69	17.234	2416	2422	2432	rVB	998883	1490749	54.22%	4.860%
70	17.816	2518	2521	2525	rVB2	35448	42938	1.56%	0.140%
71	18.063	2555	2563	2567	rBV	277752	408736	14.87%	1.332%
72	18.239	2590	2593	2597	rVB3	20030	29860	1.09%	0.097%
73	18.422	2621	2624	2627	rBV3	32028	45566	1.66%	0.149%
74	19.045	2727	2730	2734	rVB2	64607	87925	3.20%	0.287%
75	19.163	2747	2750	2752	rBV3	28035	39087	1.42%	0.127%
76	19.275	2764	2769	2775	rVB	431015	607429	22.09%	1.980%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
Data File : BP021101.D
Acq On : 23 Jul 2024 16:28
Operator : MA/JU
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BF8

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_P\Methods\SFAM-EPA-BP071024.MA.M
Title : SVOA CALIBRATION

77	19.398	2786	2790	2800	rVB3	135307	238830	8.69%	0.779%
78	19.622	2823	2828	2832	rBV	1395021	2094347	76.17%	6.828%
79	21.233	3098	3102	3110	rVB3	311200	497432	18.09%	1.622%
80	21.580	3154	3161	3166	rBV	1588724	2749539	100.00%	8.964%
81	24.674	3681	3687	3695	rVB	597460	1277917	46.48%	4.166%
82	24.904	3720	3726	3743	rVB	931474	2678773	97.43%	8.733%

Sum of corrected areas: 30674614

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
Data File : BP021101.D
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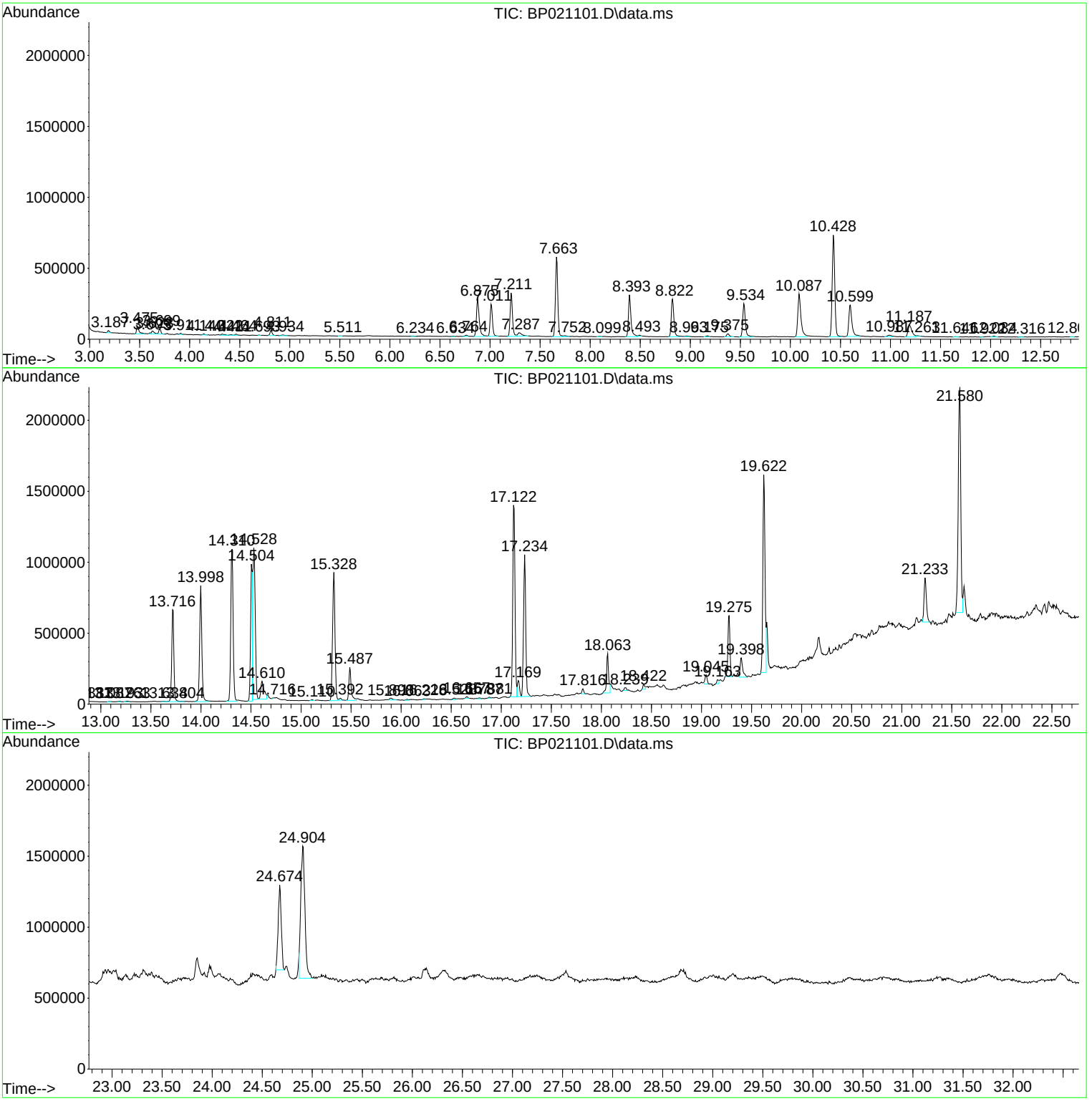
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BF8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
Data File : BP021101.D
Acq On : 23 Jul 2024 16:28
Operator : MA/JU
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BF8

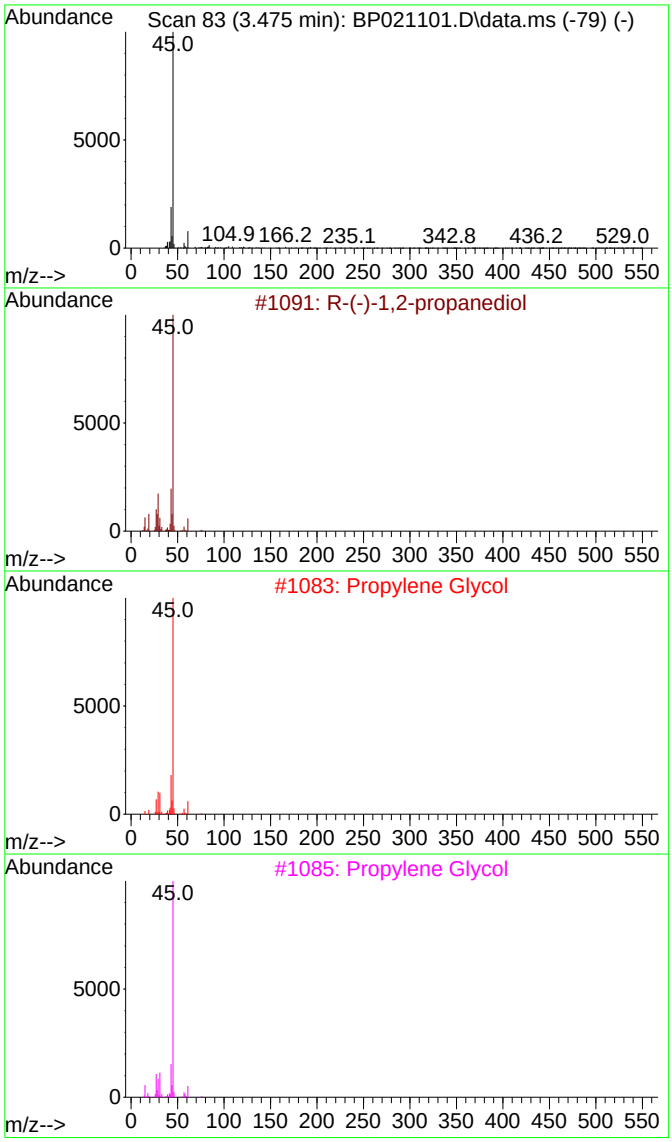
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

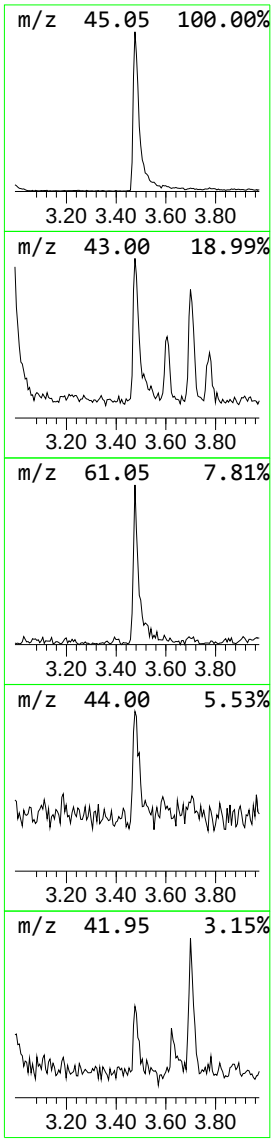
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.475	2.03 ng/ul	91676	1,4-Dichlorobenzene-d4	7.663

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
2	Propylene Glycol	76	C3H8O2	000057-55-6	64
3	Propylene Glycol	76	C3H8O2	000057-55-6	39
4	2-Hexanol	102	C6H14O	000626-93-7	39
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	39





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
Data File : BP021101.D
Acq On : 23 Jul 2024 16:28
Operator : MA/JU
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BF8

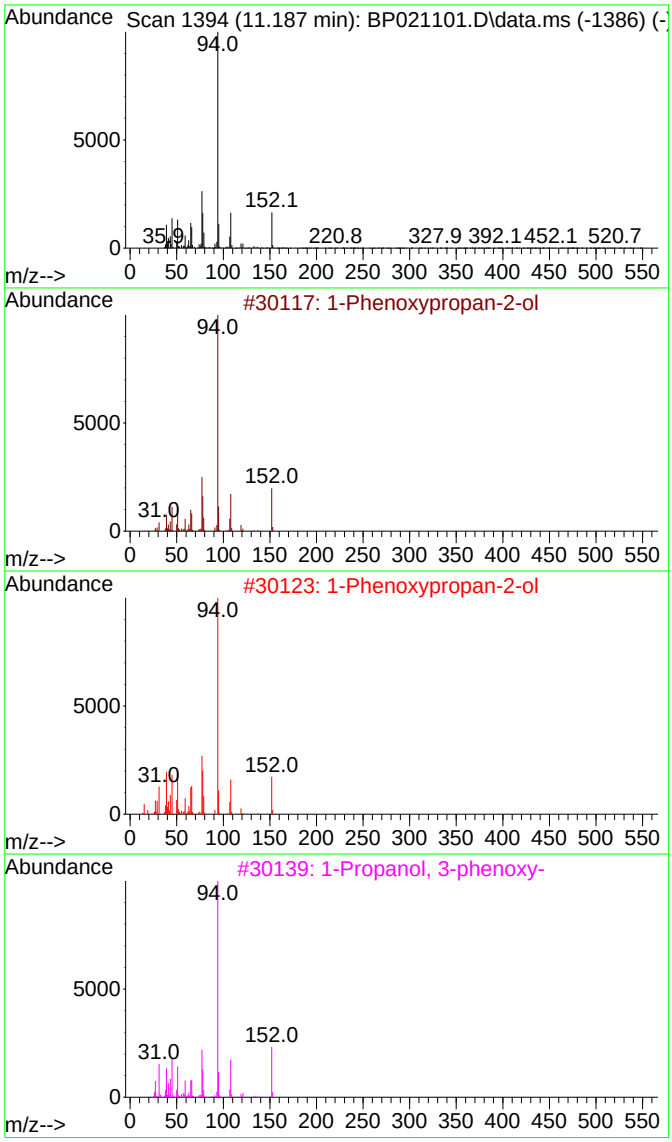
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

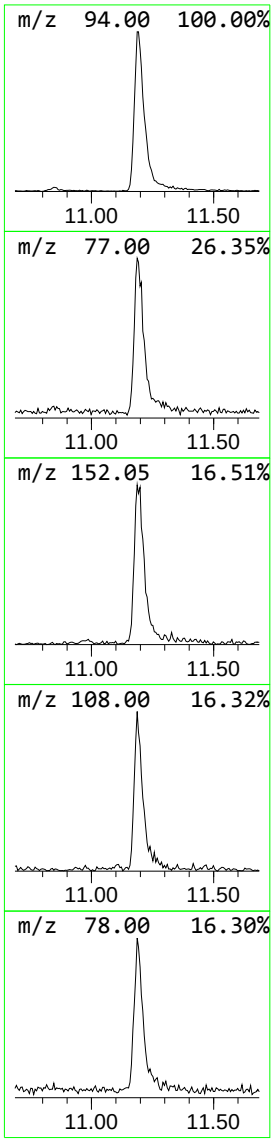
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.187	3.56 ng/ul	225602	Naphthalene-d8	10.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
3	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	94
4	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
5	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
Data File : BP021101.D
Acq On : 23 Jul 2024 16:28
Operator : MA/JU
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BF8

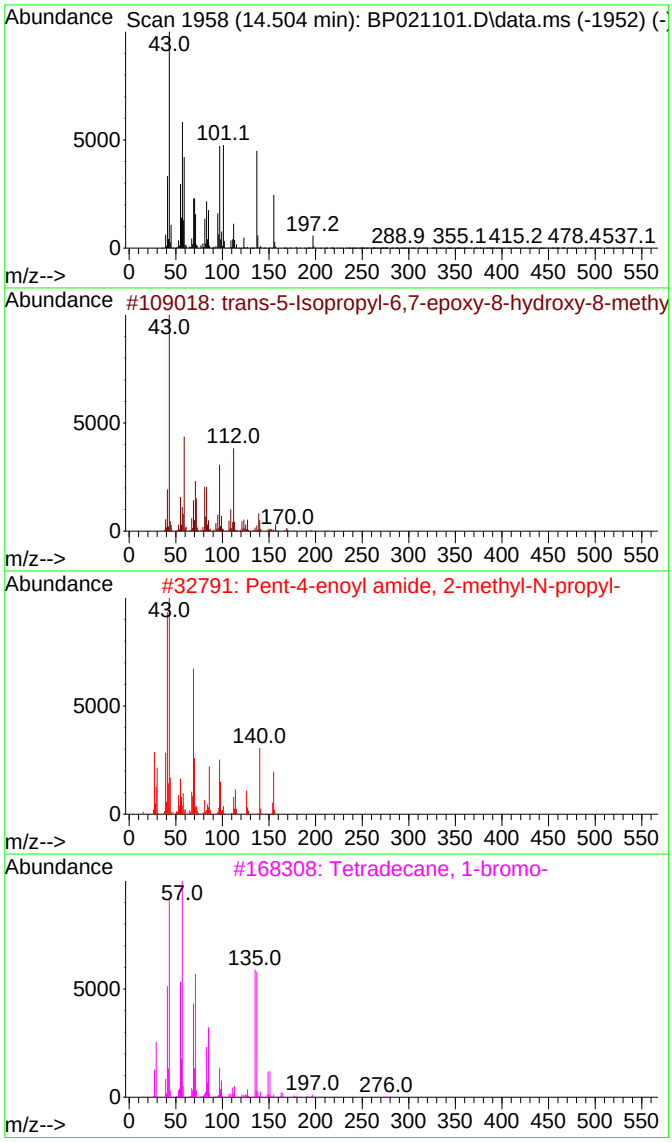
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

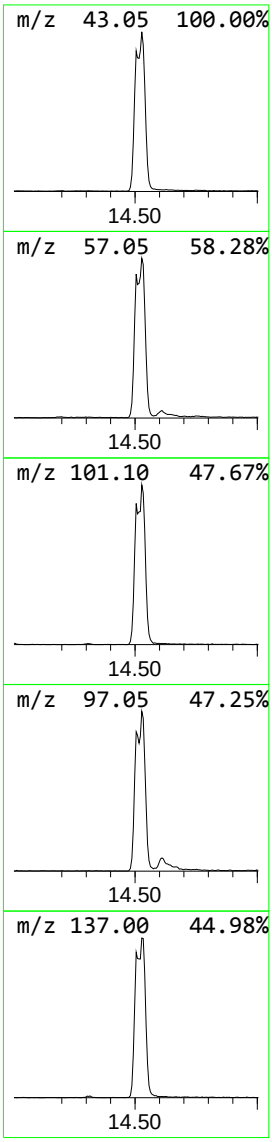
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.504	16.14 ng/ul	1380300	Acenaphthene-d10	14.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
2	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10
3	Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	10
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
5	2- Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
Data File : BP021101.D
Acq On : 23 Jul 2024 16:28
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Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

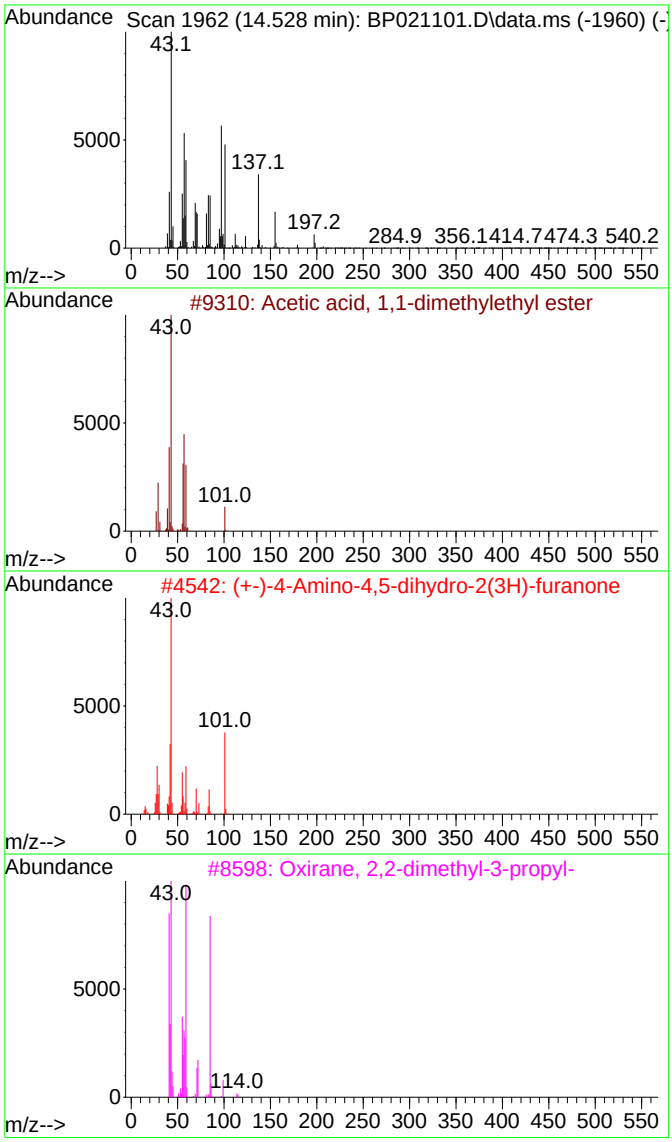
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

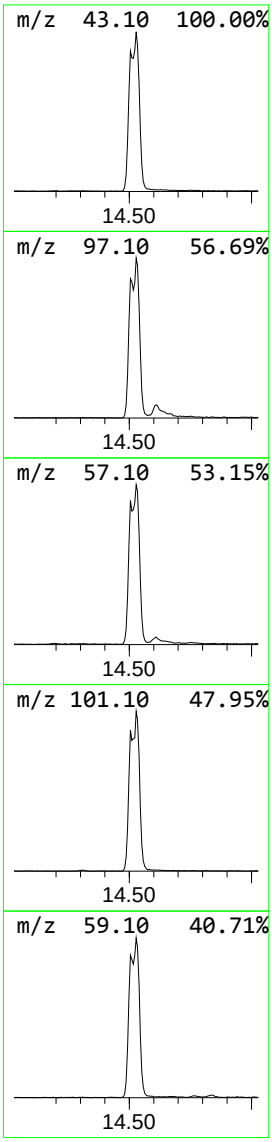
****

Peak Number 4 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.528	18.46 ng/ul	1578830	Acenaphthene-d10	14.310

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	27
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	16
3	Oxirane, 2,2-dimethyl-3-propyl-	114	C7H14O	017612-35-0	14
4	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	11
5	1,1-Dimethyl-1-silacyclo-3-pentene	112	C6H12Si	016054-12-9	11





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Data File : BP021101.D
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Operator : MA/JU
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BF8

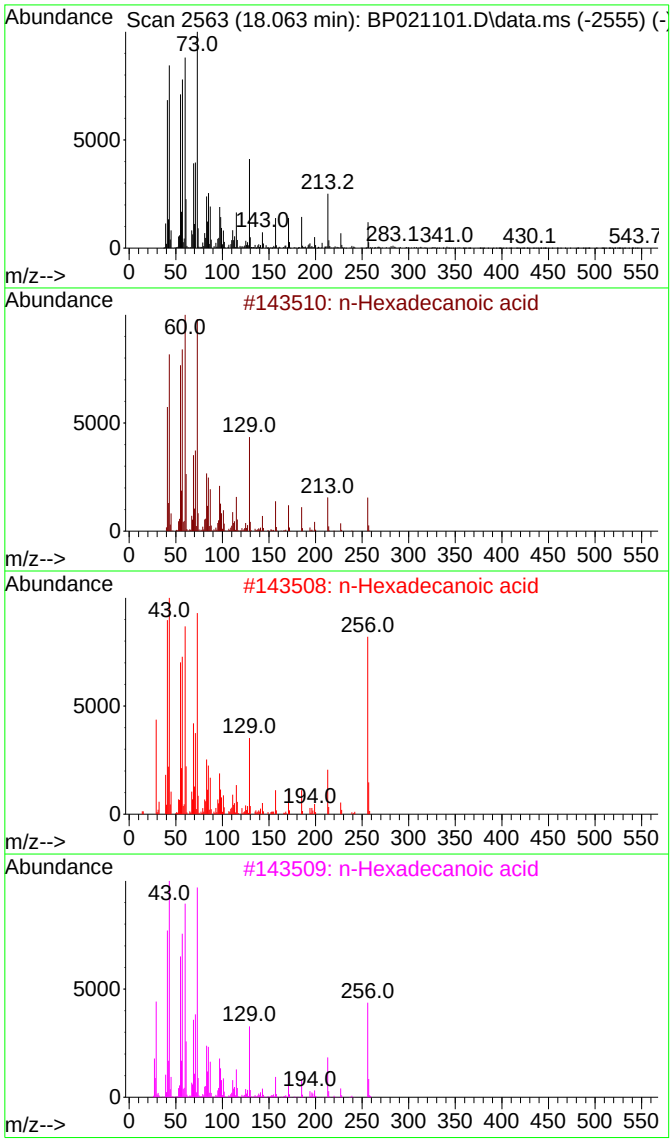
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

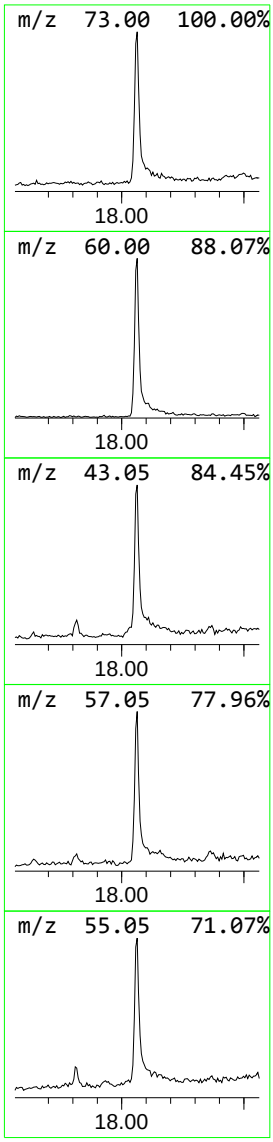
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.063	3.91 ng/ul	408736	Phenanthrene-d10	17.122

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	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
Data File : BP021101.D
Acq On : 23 Jul 2024 16:28
Operator : MA/JU
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BF8

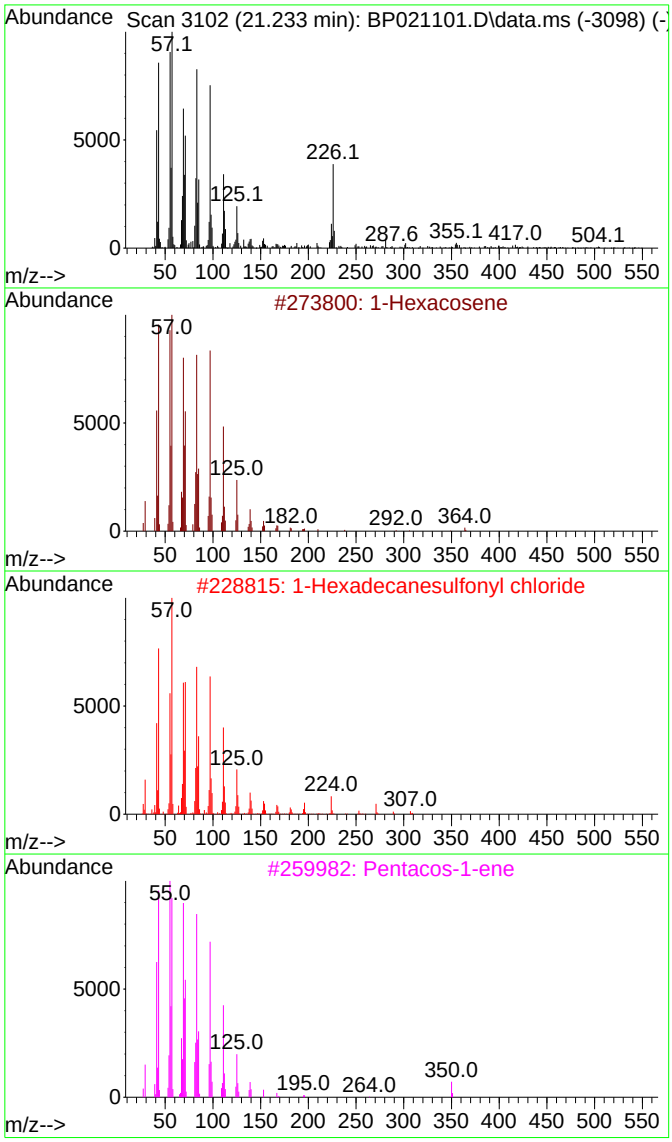
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.MA.M
Quant Title : SVOA CALIBRATION

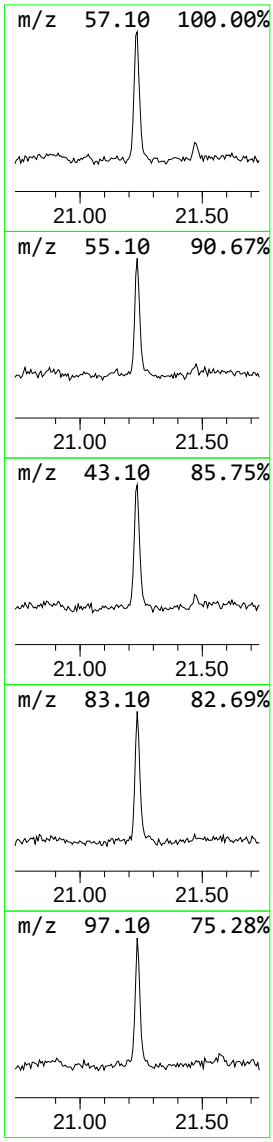
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	3.62 ng/ul	497432	Chrysene-d12	21.580

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	91
2	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	87
3	Pentacos-1-ene	350	C25H50	016980-85-1	87
4	Nonacos-1-ene	406	C29H58	018835-35-3	87
5	Cyclohexadecane	224	C16H32	000295-65-8	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP072324\
Data File : BP021101.D
Acq On : 23 Jul 2024 16:28
Operator : MA/JU
Sample : P3238-12
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
A4BF8

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP071024.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
R-(-)-1,2-propa...	3.475	2.0	ng/ul	91676	1	7.663	904272	20.0
1-Phenoxypropan...	11.187	3.6	ng/ul	225602	2	10.428	1269050	20.0
unknown-01	14.504	16.1	ng/ul	1380300	3	14.310	1710870	20.0
unknown-02	14.528	18.5	ng/ul	1578830	3	14.310	1710870	20.0
n-Hexadecanoic ...	18.063	3.9	ng/ul	408736	4	17.122	2091160	20.0
(DEL) Alkane: S...	21.233	3.6	ng/ul	497432	5	21.580	2749540	20.0