LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013157.D
Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXX3

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-BP120722.M
Title : SVOA CALIBRATION

Signal : TIC: BP013157.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.340	22	26	32	rVB	117582	150347	0.88%	0.125%
2	3.628	72	75	86	rVB	36906	56687	0.33%	0.047%
3	3.770	96	99	112	rBV	562056	845906	4.97%	0.701%
4	3.870	113	116	123	rVV	83525	118398	0.70%	0.098%
5	3.952	126	130	132	rBV3	15398	20877	0.12%	0.017%
6	3.999	134	138	142	rVB	60974	91181	0.54%	0.076%
7	4.093	151	154	159	rVB	31102	38751	0.23%	0.032%
8	5.040	309	315	323	rBV	431246	610367	3.59%	0.506%
9	5.134	328	331	337	rVB7	13177	22179	0.13%	0.018%
10	7.111	658	667	682	rBV	1808946	3002976	17.66%	2.488%
11	7.281	689	696	707	rBV	1522603	2329342	13.70%	1.930%
12	7.481	723	730	740	rVV	1884833	2901087	17.06%	2.404%
13	7.569	740	745	751	rVB3	20819	33256	0.20%	0.028%
14	7.952	802	810	818	rBV	1519866	2383872	14.02%	1.975%
15	8.663	923	931	942	rBV	1686278	2718785	15.99%	2.253%
16	8.781	946	951	960	rVB	77037	132032	0.78%	0.109%
17	9.122	1001	1009	1019	rBV	1714744	2786129	16.38%	2.308%
18	9.281	1033	1036	1041	rVB7	14263	21064	0.12%	0.017%
19	9.528	1070	1078	1086	rBV2	53890	92638	0.54%	0.077%
20	9.846	1122	1132	1145	rBV	1434524	2349169	13.81%	1.946%
21	9.993	1153	1157	1163	rVB8	8792	17100	0.10%	0.014%
22	10.387	1216	1224	1242	rBV	2121722	3545845	20.85%	2.938%
23	10.540	1246	1250	1258	rVB	8080	20457	0.12%	0.017%
24	10.769	1280	1289	1301	rBV	1967037	3300595	19.41%	2.735%
25	10.904	1304	1312	1327	rBV	1633171	2857290	16.80%	2.367%
26	11.552	1415	1422	1428	rBV	16512	39676	0.23%	0.033%
27	12.022	1496	1502	1507	rBV7	8716	17058	0.10%	0.014%
28	12.175	1524	1528	1536	rVB7	13170	20225	0.12%	0.017%
29	12.351	1553	1558	1564	rVB	37998	61280	0.36%	0.051%
30	13.410	1730	1738	1745	rVB3	36789	61694	0.36%	0.051%
31	13.481	1745	1750	1754	rBV6	12862	23306	0.14%	0.019%
32	13.916	1818	1824	1828	rBV9	13389	22582	0.13%	0.019%
33	13.998	1831	1838	1850	rVV	3261709	4706789	27.68%	3.900%
34	14.110	1854	1857	1864	rVB7	15189	27368	0.16%	0.023%
35	14.234	1874	1878	1881	rBV6	12392	21708	0.13%	0.018%
36	14.293	1881	1888	1898	rVV	3922635	5856356	34.44%	4.852%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013157.D
Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

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-BP120722.M
Title : SVOA CALIBRATION

37	14.593	1933	1939	1949	rBV	2692460	3974740	23.37%	3.293%
38	14.787	1965	1972	1986	rBV	1080240	1838446	10.81%	1.523%
39	14.893	1988	1990	1995	rVV4	27980	48995	0.29%	0.041%
40	14.951	1995	2000	2004	rVV5	29351	57717	0.34%	0.048%
41	15.010	2004	2010	2021	rVB5	59497	122172	0.72%	0.101%
42	15.387	2068	2074	2076	rBV6	12854	25534	0.15%	0.021%
43	15.434	2079	2082	2086	rVB3	15894	22927	0.13%	0.019%
44	15.587	2101	2108	2116	rBV	4937042	7149959	42.05%	5.924%
45	15.704	2122	2128	2145	rBV	1286825	1805508	10.62%	1.496%
46	15.828	2145	2149	2153	rVB4	25565	36479	0.21%	0.030%
47	15.951	2166	2170	2175	rVB	55882	79454	0.47%	0.066%
48	16.481	2256	2260	2265	rBV6	14050	18015	0.11%	0.015%
49	16.887	2324	2329	2333	rBV3	40436	60300	0.35%	0.050%
50	17.098	2361	2365	2369	rBV6	13335	18985	0.11%	0.016%
51	17.145	2369	2373	2379	rVB7	9673	19162	0.11%	0.016%
52	17.234	2383	2388	2390	rBV5	23859	36256	0.21%	0.030%
53	17.351	2402	2408	2415	rBV	3098259	4323015	25.42%	3.582%
54	17.451	2419	2425	2433	rVV	4793013	6688711	39.33%	5.542%
55	17.539	2435	2440	2447	rVB2	135177	222572	1.31%	0.184%
56	17.634	2453	2456	2460	rBV4	14408	19058	0.11%	0.016%
57	17.728	2469	2472	2480	rVB9	29768	47623	0.28%	0.039%
58	18.163	2543	2546	2551	rVB4	37607	50307	0.30%	0.042%
59	18.222	2551	2556	2566	rBV	660037	949178	5.58%	0.786%
60	18.504	2602	2604	2608	rVB5	18715	24073	0.14%	0.020%
61	18.633	2622	2626	2631	rBV	288915	326865	1.92%	0.271%
62	19.045	2694	2696	2701	rBV5	25056	34516	0.20%	0.029%
63	19.104	2702	2706	2712	rVV7	59292	110052	0.65%	0.091%
64	19.257	2729	2732	2738	rVB3	72050	96927	0.57%	0.080%
65	19.322	2738	2743	2746	rBV2	109144	197387	1.16%	0.164%
66	19.451	2761	2765	2773	rBV	178431	262666	1.54%	0.218%
67	19.680	2799	2804	2816	rBV	6403363	8664987	50.95%	7.179%
68	21.127	3046	3050	3055	rBV	1266239	1823308	10.72%	1.511%
69	21.333	3082	3085	3088	rBV	205018	225385	1.33%	0.187%
70	21.439	3098	3103	3108	rBV	3847140	4970236	29.23%	4.118%
71	23.133	3388	3391	3397	rVB2	440788	619361	3.64%	0.513%
72	23.757	3490	3497	3511	rVB2	5020327	10432300	61.35%	8.644%
73	23.916	3518	3524	3535	rVB	2810195	5770622	33.93%	4.781%
74	24.539	3626	3630	3639	rVB	625816	1211126	7.12%	1.003%
75	28.504	4294	4304	4323	rVB3	4360408	17005396	100.00%	14.090%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013157.D
Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

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-BP120722.M
Title : SVOA CALIBRATION

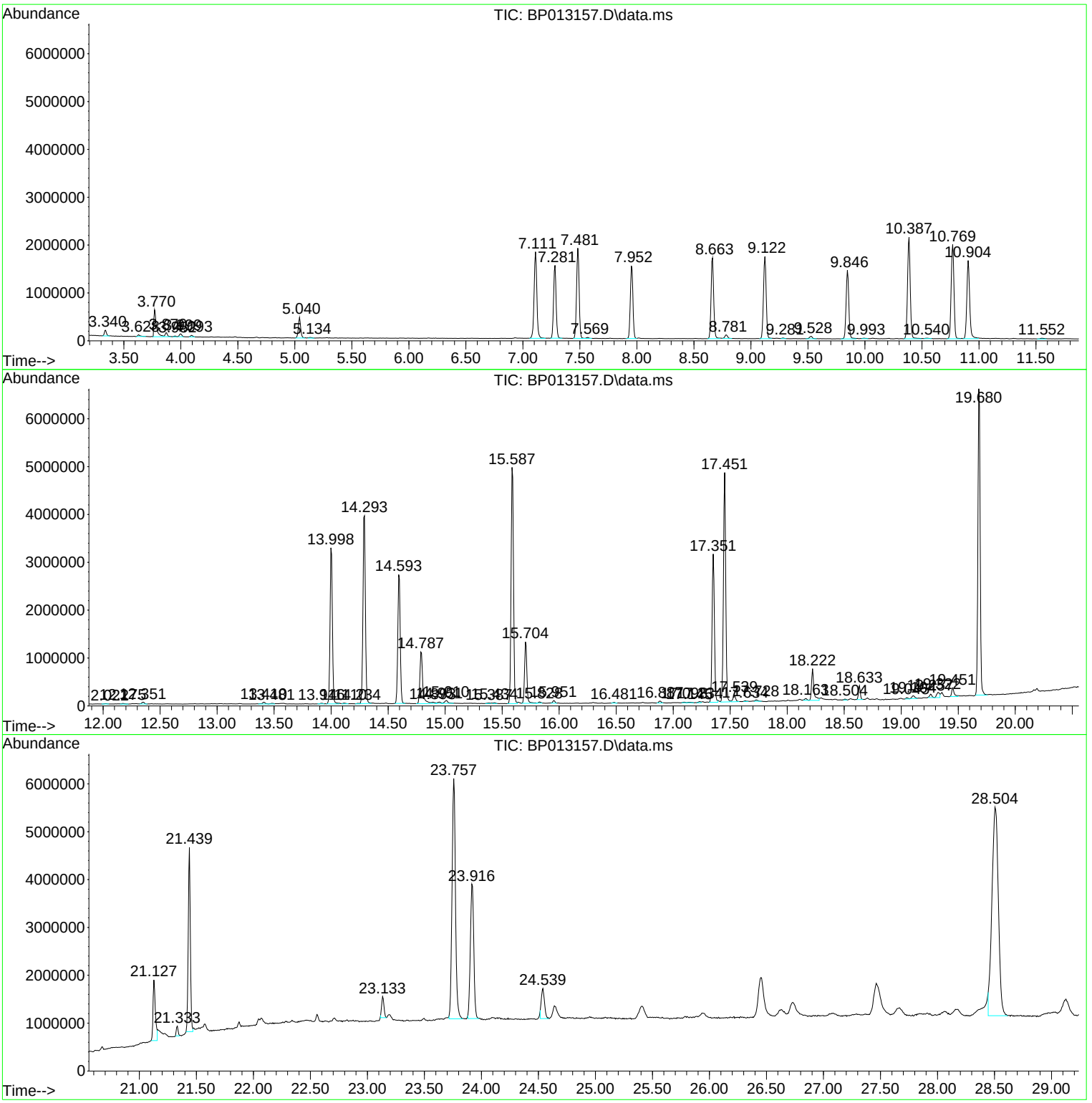
Sum of corrected areas: 120694692

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013157.D
Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013157.D
Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

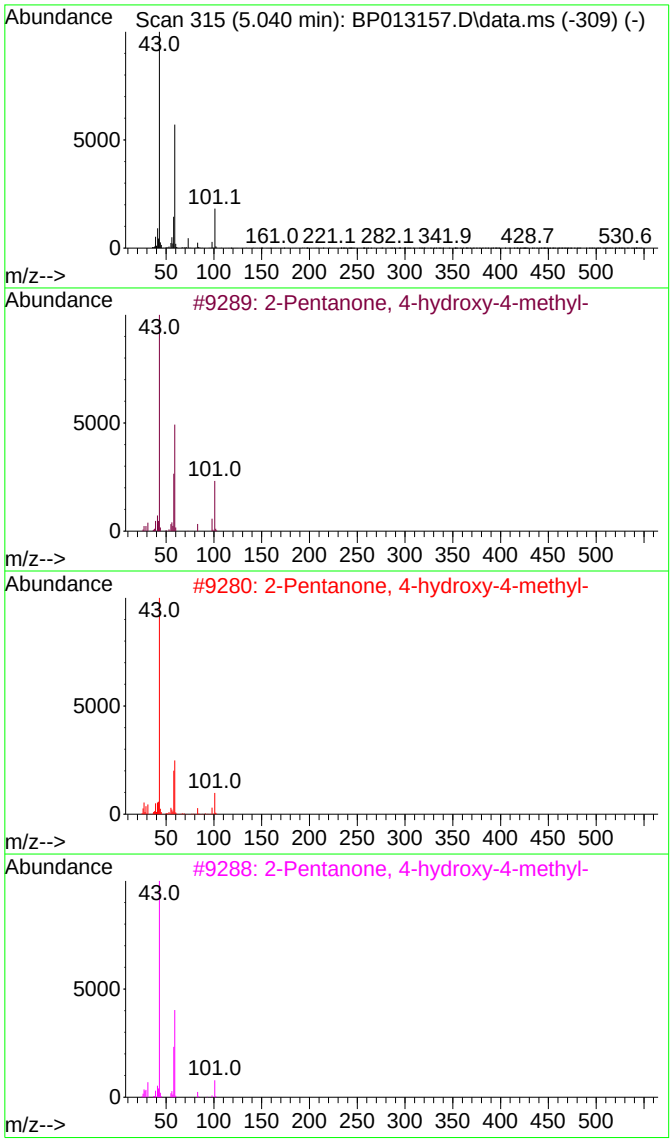
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

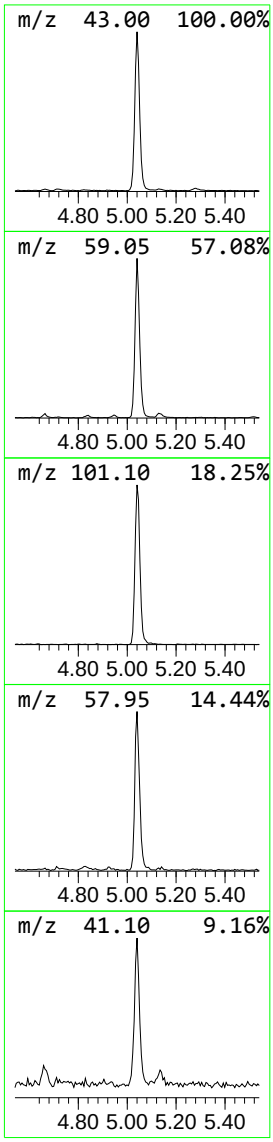
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.040	5.12 ng/ul	610367	1,4-Dichlorobenzene-d4	7.952

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
4	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013157.D
Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

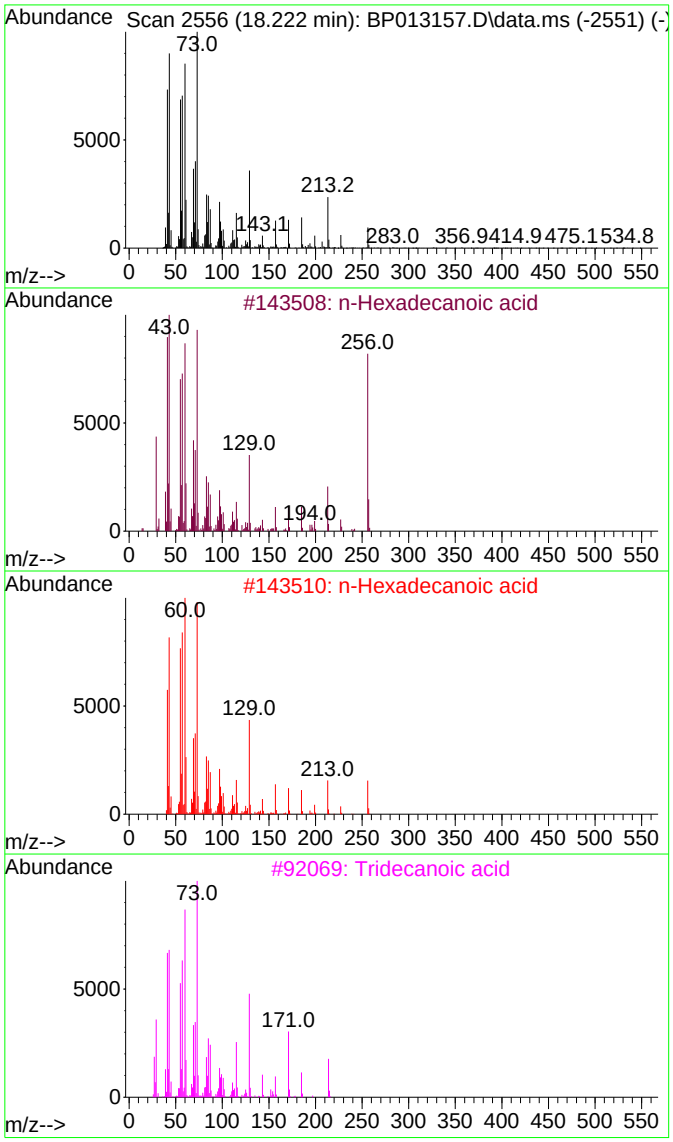
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

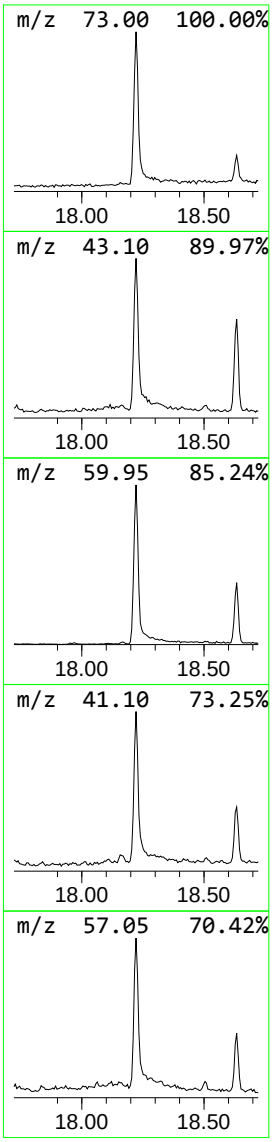
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.222	4.39 ng/ul	949178	Phenanthrene-d10	17.351

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	Tridecanoic acid	214	C13H26O2	000638-53-9	95
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
5	Tridecanoic acid	214	C13H26O2	000638-53-9	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013157.D
Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

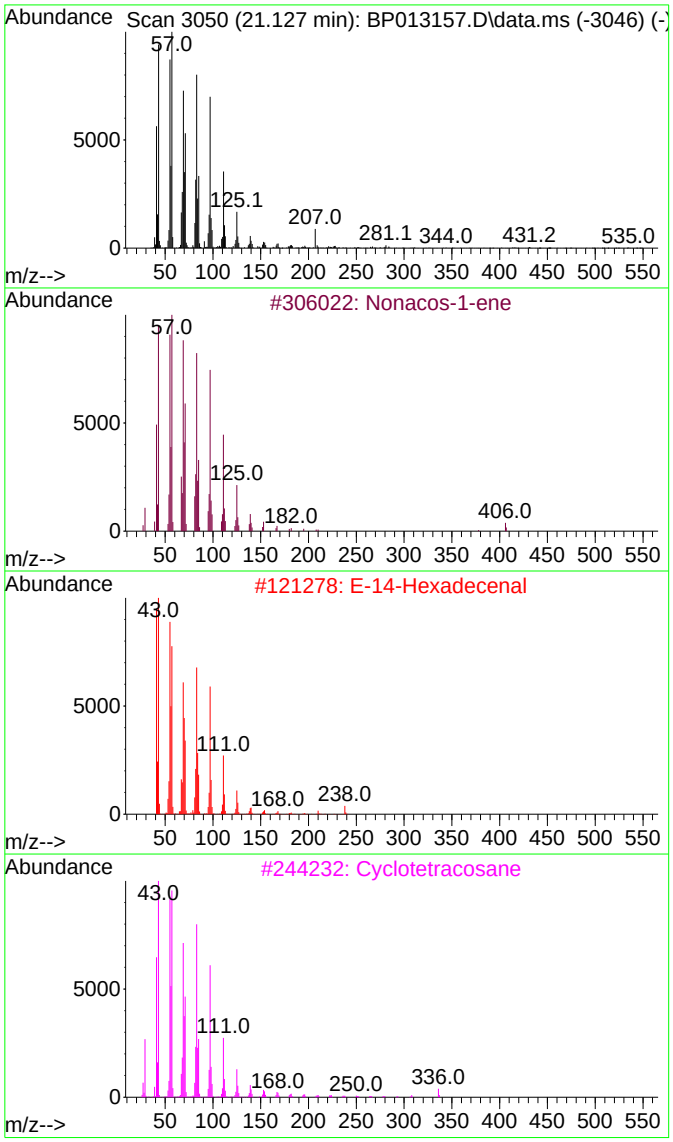
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

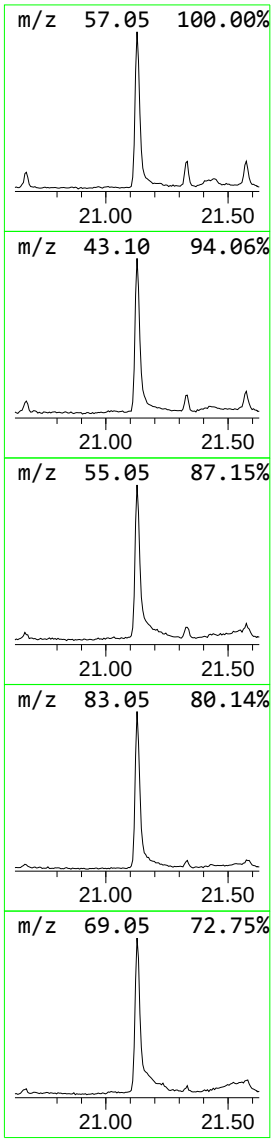
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.128	7.34 ng/ul	1823310	Chrysene-d12	21.439

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonacos-1-ene	406	C29H58	018835-35-3	98
2	E-14-Hexadecenal	238	C16H30O	330207-53-9	94
3	Cyclotetracosane	336	C24H48	000297-03-0	94
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5	Heptacos-1-ene	378	C27H54	015306-27-1	94





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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Acq On : 20 Dec 2022 09:40
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ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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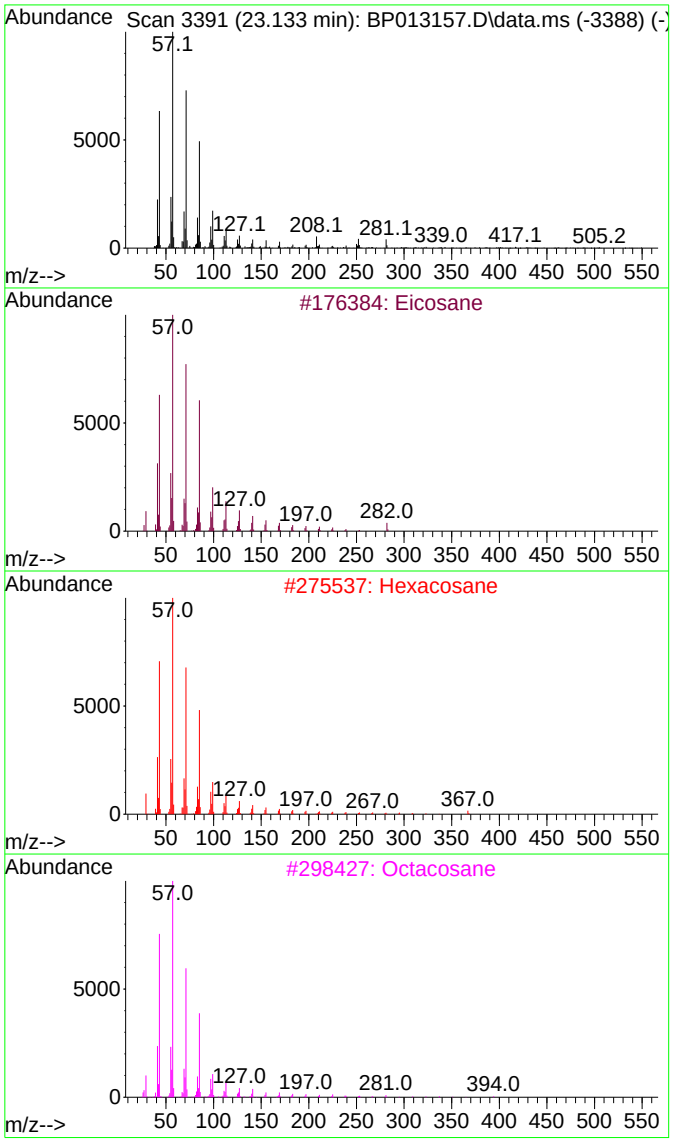
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

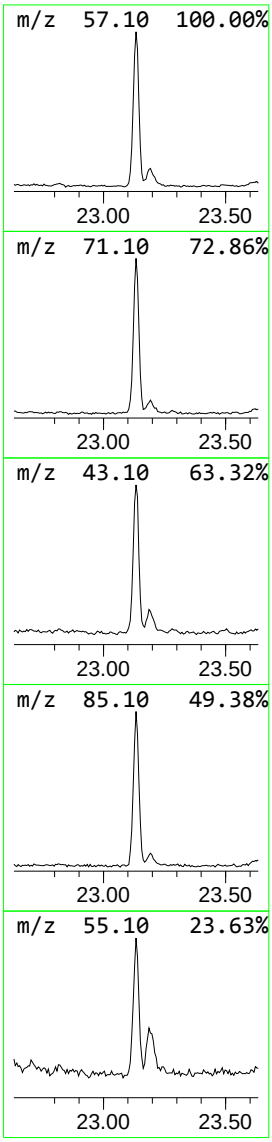
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.133	2.15 ng/ul	619361	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hexacosane	366	C26H54	000630-01-3	93
3	Octacosane	394	C28H58	000630-02-4	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
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Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

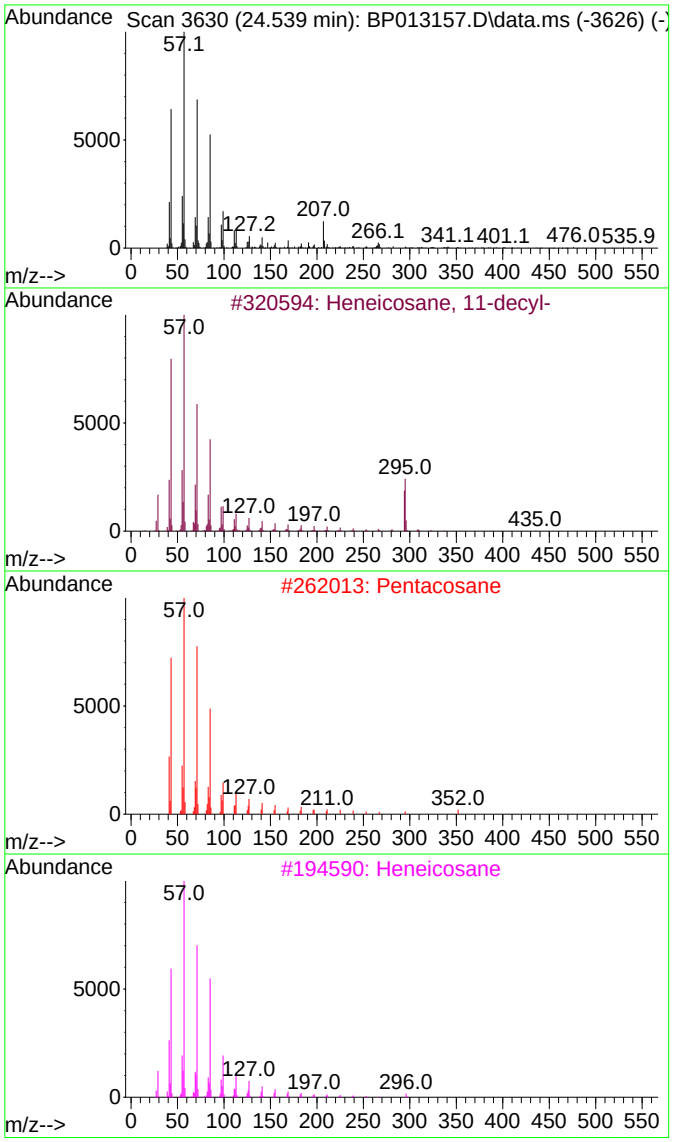
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

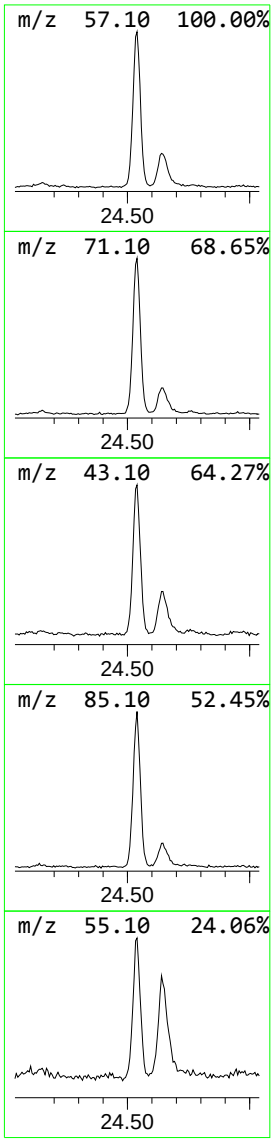
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.539	4.20 ng/ul	1211130	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	93
2	Pentacosane	352	C25H52	000629-99-2	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	87
5	Heptadecane	240	C17H36	000629-78-7	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013157.D
Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

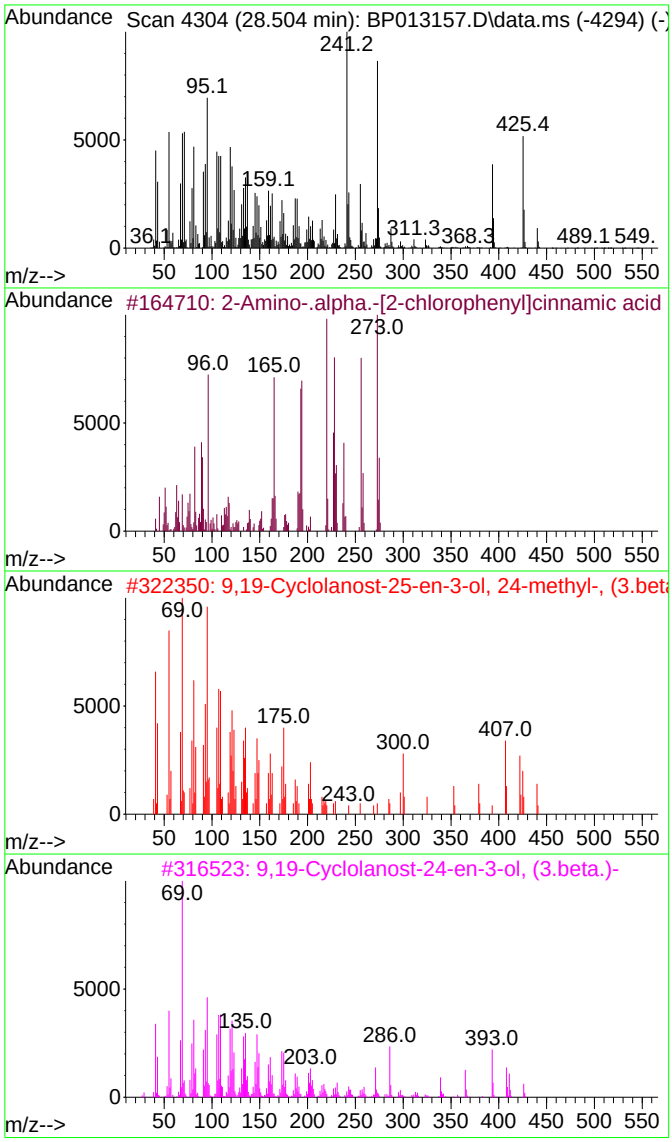
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

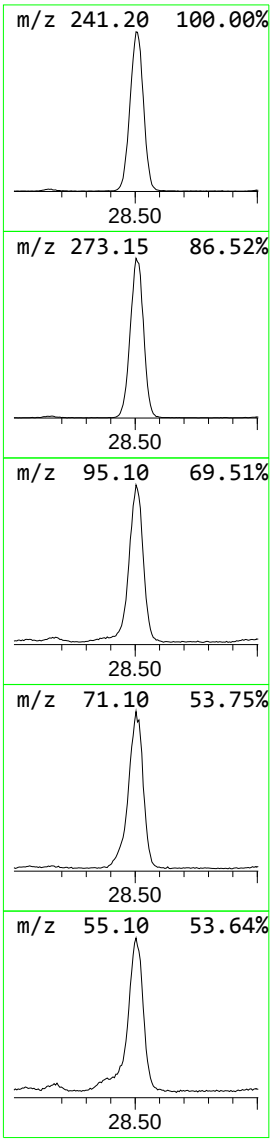
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Amino-.alpha.-[2-chloroph... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.504	58.94 ng/ul	17005400	Perylene-d12	23.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-.alpha.-[2-chlorophenyl]...	273	C15H12ClNO2	1000254-08-5	59
2	9,19-Cyclolanost-25-en-3-ol, 24-...	440	C31H52O	000511-61-5	35
3	9,19-Cyclolanost-24-en-3-ol, (3....	426	C30H50O	000469-38-5	27
4	11-Oxo-.alpha.-amyrin	440	C30H48O2	002118-90-3	25
5	Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP121922\
Data File : BP013157.D
Acq On : 20 Dec 2022 09:40
Operator : CG/JU
Sample : N6003-06
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXX3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.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
2-Pentanone, 4-...	5.040	5.1	ng/ul	610367	1	7.952	2383870	20.0
n-Hexadecanoic ...	18.222	4.4	ng/ul	949178	4	17.351	4323020	20.0
(DEL) Alkane: S...	21.128	7.3	ng/ul	1823310	5	21.439	4970240	20.0
(DEL) Alkane: S...	23.133	2.1	ng/ul	619361	6	23.916	5770620	20.0
(DEL) Alkane: S...	24.539	4.2	ng/ul	1211130	6	23.916	5770620	20.0
2-Amino-.alpha....	28.504	58.9	ng/ul	17005400	6	23.916	5770620	20.0