LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005695.D
Acq On : 03 Jun 2021 19:48
Operator : CG/JU
Sample : M2580-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B3(2-4)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270E-BP052721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005695.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.463	229	234	250	rVB	233174	321568	8.85%	1.211%
2	5.075	332	338	348	rBV	169679	246499	6.79%	0.929%
3	5.540	411	417	425	rBV	489202	709532	19.53%	2.673%
4	6.663	602	608	614	rVB2	23933	42591	1.17%	0.160%
5	7.140	682	689	697	rBV	565599	906283	24.95%	3.414%
6	7.604	762	768	771	rBV5	21631	41428	1.14%	0.156%
7	7.981	822	832	842	rBV	777072	1246758	34.33%	4.697%
8	9.146	1023	1030	1038	rVB	324342	548591	15.10%	2.067%
9	10.787	1299	1309	1315	rBV	990583	1697367	46.73%	6.394%
10	10.840	1315	1318	1326	rVB	95463	154369	4.25%	0.582%
11	12.445	1586	1591	1599	rVB	56503	91159	2.51%	0.343%
12	12.663	1621	1628	1631	rBV	28819	49094	1.35%	0.185%
13	13.234	1718	1725	1733	rBV	949199	1326915	36.53%	4.999%
14	13.439	1756	1760	1767	rVB2	37864	58166	1.60%	0.219%
15	13.769	1809	1816	1823	rBV2	24262	58762	1.62%	0.221%
16	13.934	1839	1844	1848	rBV2	27961	45100	1.24%	0.170%
17	14.057	1857	1865	1869	rBV	83630	140332	3.86%	0.529%
18	14.504	1937	1941	1947	rVB2	38312	50813	1.40%	0.191%
19	14.604	1949	1958	1964	rVV	1487210	2186341	60.19%	8.236%
20	14.669	1964	1969	1977	rVB	70993	118025	3.25%	0.445%
21	15.004	2021	2026	2032	rVB	71420	107278	2.95%	0.404%
22	15.451	2099	2102	2107	rVB	42976	51023	1.40%	0.192%
23	15.645	2130	2135	2141	rBV2	59233	88115	2.43%	0.332%
24	16.086	2204	2210	2219	rVB2	192626	307927	8.48%	1.160%
25	16.316	2244	2249	2251	rBV2	62954	95157	2.62%	0.358%
26	17.004	2362	2366	2371	rBV2	28100	36739	1.01%	0.138%
27	17.104	2380	2383	2388	rVV	50987	61220	1.69%	0.231%
28	17.163	2389	2393	2402	rVB2	60114	107556	2.96%	0.405%
29	17.345	2418	2424	2429	rBV	1743183	2610452	71.87%	9.834%
30	17.392	2429	2432	2438	rVB	441581	582094	16.03%	2.193%
31	17.480	2443	2447	2452	rVB	117002	168318	4.63%	0.634%
32	17.751	2489	2493	2500	rVB	46338	77152	2.12%	0.291%
33	17.845	2505	2509	2517	rVB3	52745	87396	2.41%	0.329%
34	18.216	2568	2572	2575	rBV	51346	70515	1.94%	0.266%
35	18.257	2576	2579	2583	rVB	75687	95575	2.63%	0.360%
36	18.333	2589	2592	2597	rBV	31481	48267	1.33%	0.182%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005695.D
Acq On : 03 Jun 2021 19:48
Operator : CG/JU
Sample : M2580-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B3(2-4)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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\8270E-BP052721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	18.392	2598	2602	2607	rVV2	95901	183269	5.05%	0.690%
38	18.433	2607	2609	2614	rVB	63648	71567	1.97%	0.270%
39	18.510	2619	2622	2625	rBV	62145	68141	1.88%	0.257%
40	18.692	2649	2653	2656	rBV	65608	85661	2.36%	0.323%
41	19.092	2718	2721	2723	rBV	53069	66207	1.82%	0.249%
42	19.345	2759	2764	2770	rBV	958163	1253023	34.50%	4.720%
43	19.698	2820	2824	2832	rVB	866603	1168835	32.18%	4.403%
44	19.892	2852	2857	2861	rVB	1648643	1951241	53.72%	7.351%
45	21.321	3097	3100	3105	rVB	325205	353526	9.73%	1.332%
46	21.416	3110	3116	3120	rBV2	2390587	3632213	100.00%	13.683%
47	23.857	3526	3531	3538	rVB2	1476843	3076801	84.71%	11.591%

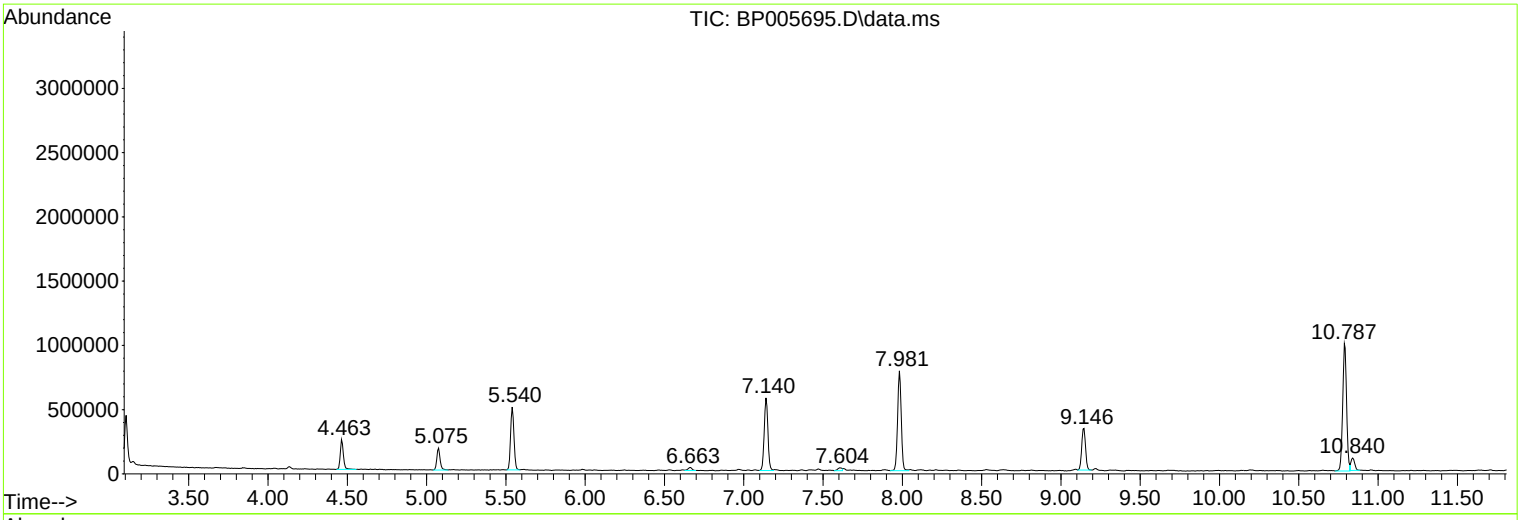
Sum of corrected areas: 26544961

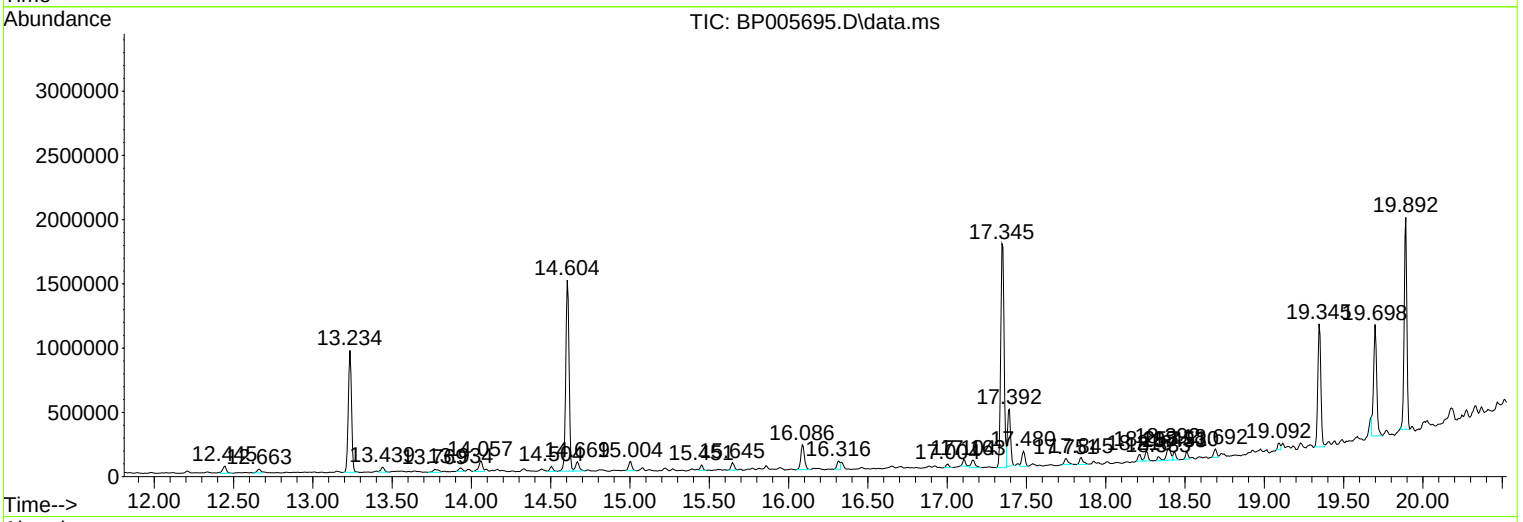
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005695.D
Acq On : 03 Jun 2021 19:48
Operator : CG/JU
Sample : M2580-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

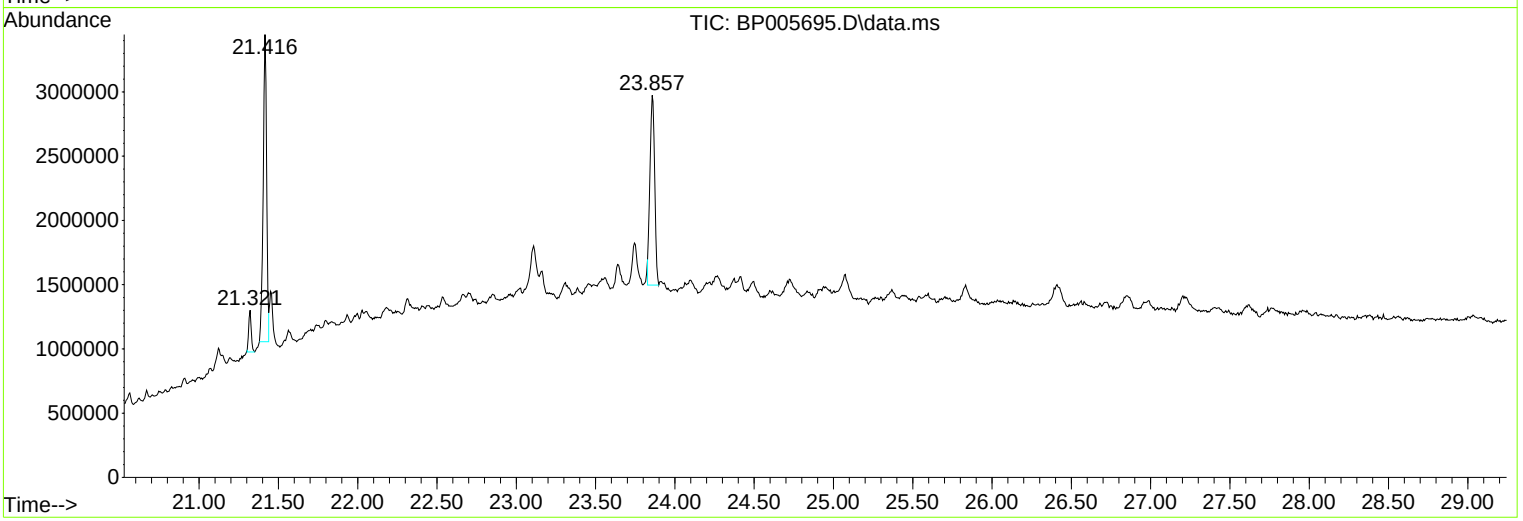
Instrument :
BNA_P
ClientSampleId :
18-B3(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005695.D
Acq On : 03 Jun 2021 19:48
Operator : CG/JU
Sample : M2580-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B3(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

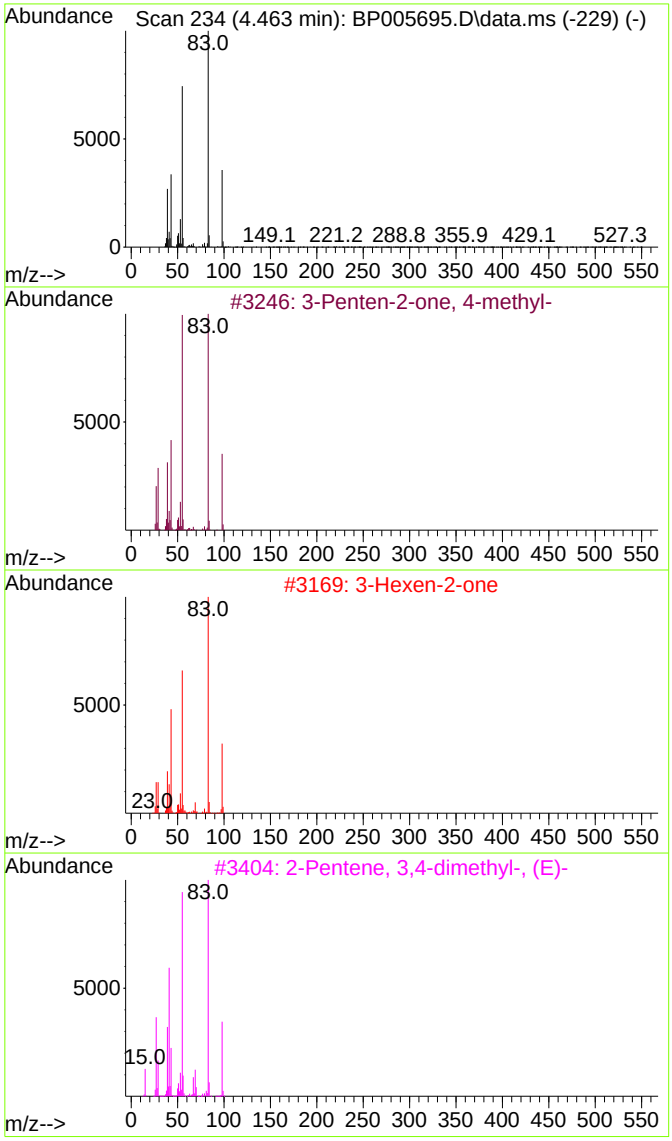
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

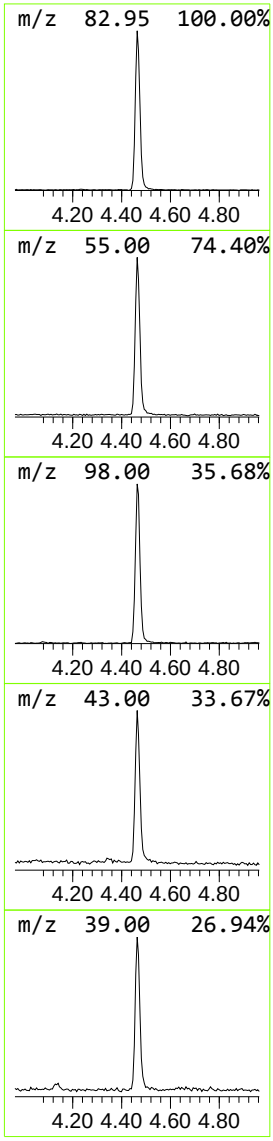
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.463	5.16 ng	321568	1,4-Dichlorobenzene-d4	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005695.D
Acq On : 03 Jun 2021 19:48
Operator : CG/JU
Sample : M2580-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B3(2-4)

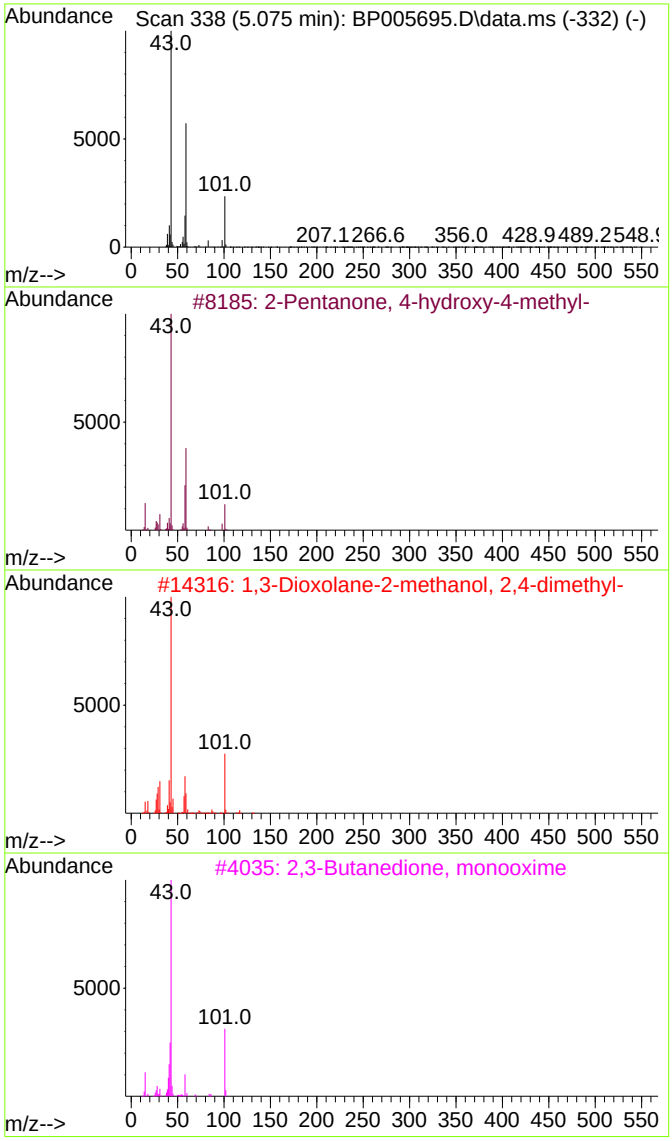
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

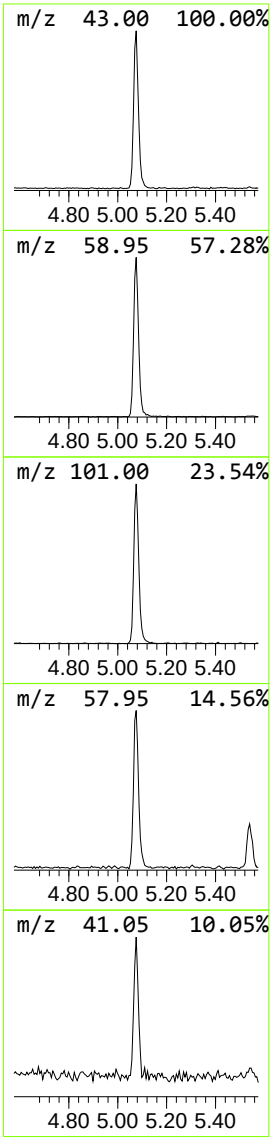
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	3.95 ng	246499	1,4-Dichlorobenzene-d4	7.981

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060321\
Data File : BP005695.D
Acq On : 03 Jun 2021 19:48
Operator : CG/JU
Sample : M2580-08 2X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B3(2-4)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.463	5.2	ng	321568	1	7.981	1246760	20.0
2-Pentanone, 4-...	5.075	4.0	ng	246499	1	7.981	1246760	20.0