LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : R-LA-37-3-WC

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-BP121120.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP004482.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.940	294	298	306	rVB	276726	398445	4.23%	0.677%
2	5.405	370	377	389	rVB	3561359	5301207	56.23%	9.007%
3	6.987	638	646	658	rBV	3405347	5734409	60.83%	9.743%
4	7.811	780	786	796	rBV	922549	1491940	15.83%	2.535%
5	8.969	975	983	992	rBV	2304393	3807450	40.39%	6.469%
6	10.605	1254	1261	1272	rBV	1180147	2055618	21.81%	3.493%
7	13.081	1673	1682	1694	rBV	5525854	8533360	90.52%	14.499%
8	13.910	1813	1823	1829	rBV	124606	198537	2.11%	0.337%
9	14.463	1907	1917	1934	rBV	1736829	2621941	27.81%	4.455%
10	15.957	2164	2171	2189	rBV	3975288	5859530	62.16%	9.956%
11	17.222	2379	2386	2396	rBV	2003529	2831225	30.03%	4.811%
12	17.510	2431	2435	2446	rVB	56668	111664	1.18%	0.190%
13	18.116	2526	2538	2545	rBV	132954	248939	2.64%	0.423%
14	18.181	2545	2549	2554	rVB	111883	146031	1.55%	0.248%
15	18.604	2616	2621	2631	rBV	67658	159509	1.69%	0.271%
16	18.857	2659	2664	2668	rBV	512187	649870	6.89%	1.104%
17	18.939	2674	2678	2686	rBV	156830	193973	2.06%	0.330%
18	19.245	2725	2730	2737	rVB4	50537	95163	1.01%	0.162%
19	19.351	2744	2748	2757	rBV2	54010	102317	1.09%	0.174%
20	19.469	2764	2768	2776	rVB	154741	191149	2.03%	0.325%
21	19.792	2817	2823	2828	rBV	7490942	9426980	100.00%	16.017%
22	19.992	2853	2857	2861	rVB	106385	125586	1.33%	0.213%
23	20.457	2932	2936	2942	rVB	244438	318787	3.38%	0.542%
24	20.533	2943	2949	2953	rBV4	63137	118897	1.26%	0.202%
25	20.663	2966	2971	2975	rBV	1232130	1430395	15.17%	2.430%
26	20.710	2975	2979	2983	rVV	296952	373235	3.96%	0.634%
27	20.769	2986	2989	2998	rVB	100364	148086	1.57%	0.252%
28	20.992	3022	3027	3030	rBV	89598	140198	1.49%	0.238%
29	21.039	3030	3035	3040	rVV2	215977	416627	4.42%	0.708%
30	21.092	3041	3044	3049	rVV	268871	375837	3.99%	0.639%
31	21.145	3050	3053	3060	rVB2	170600	245785	2.61%	0.418%
32	21.316	3077	3082	3088	rBV	2009087	2554809	27.10%	4.341%
33	22.404	3264	3267	3276	rVB2	73059	102911	1.09%	0.175%
34	22.945	3355	3359	3364	rBV3	82878	130836	1.39%	0.222%
35	23.669	3475	3482	3497	rVB2	1112905	2213367	23.48%	3.761%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R-LA-37-3-WC

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-BP121120.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

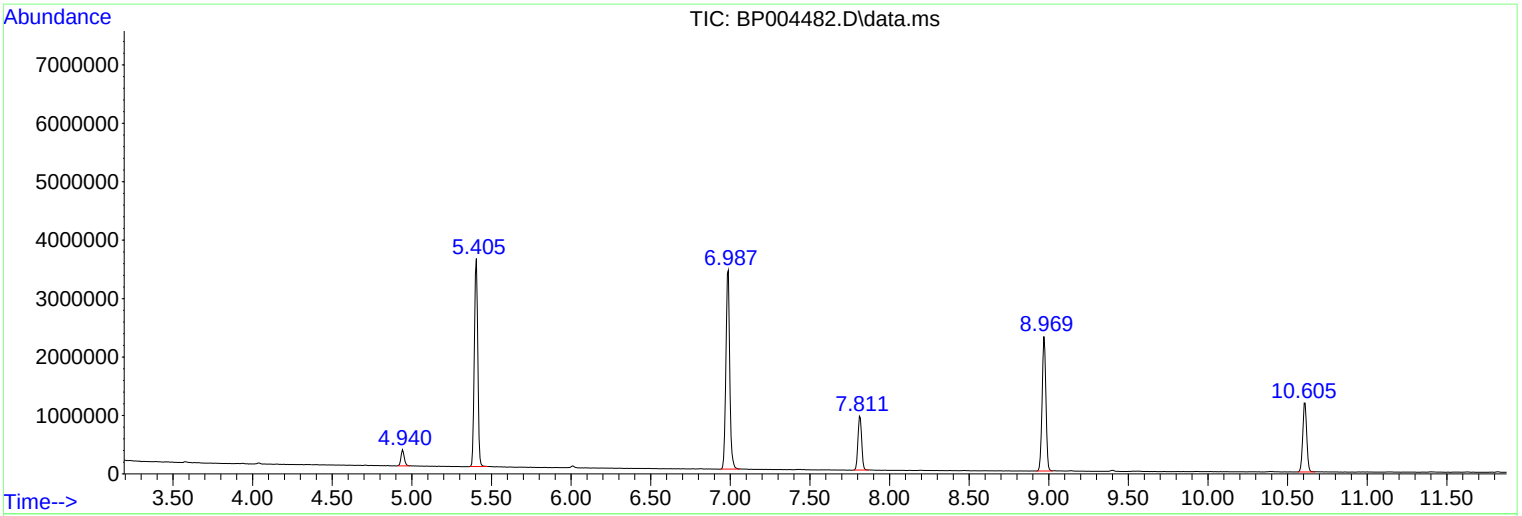
Sum of corrected areas: 58854613

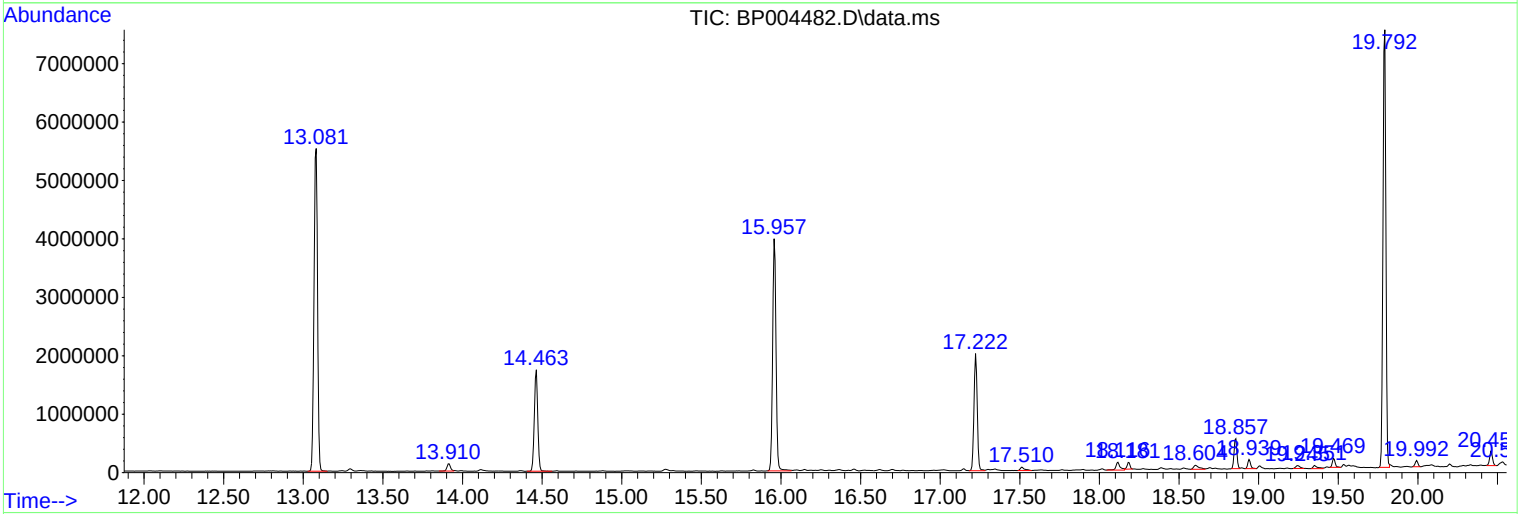
Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

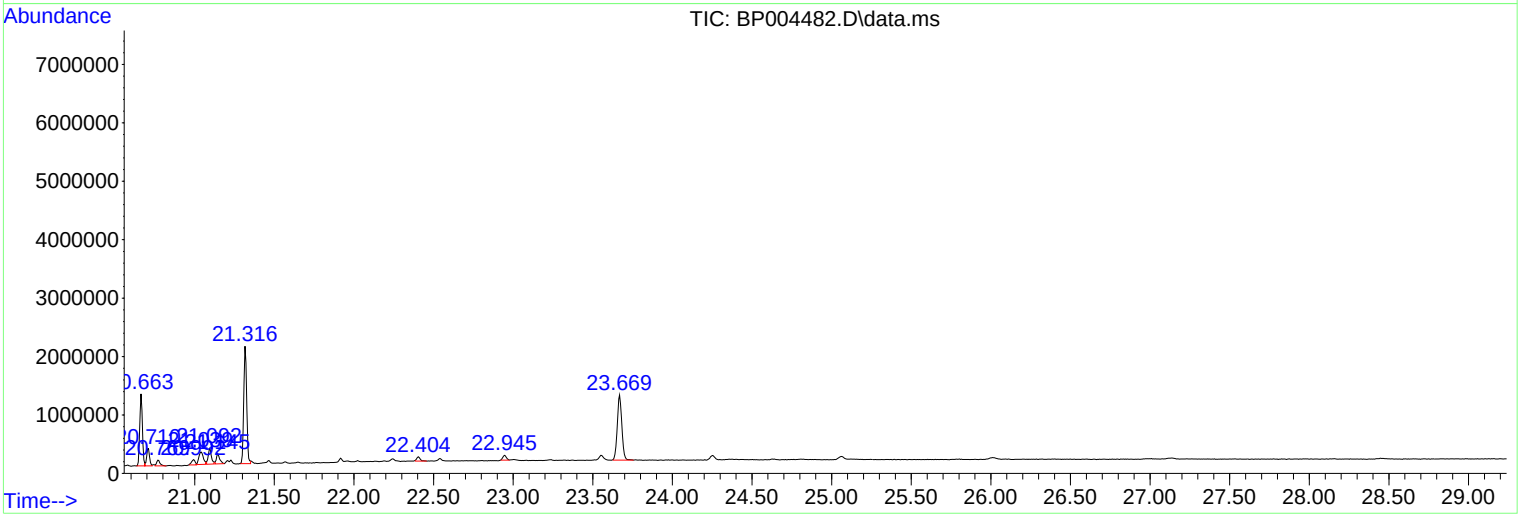
Instrument :
BNA_P
ClientSampleId :
R-LA-37-3-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.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\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R-LA-37-3-WC

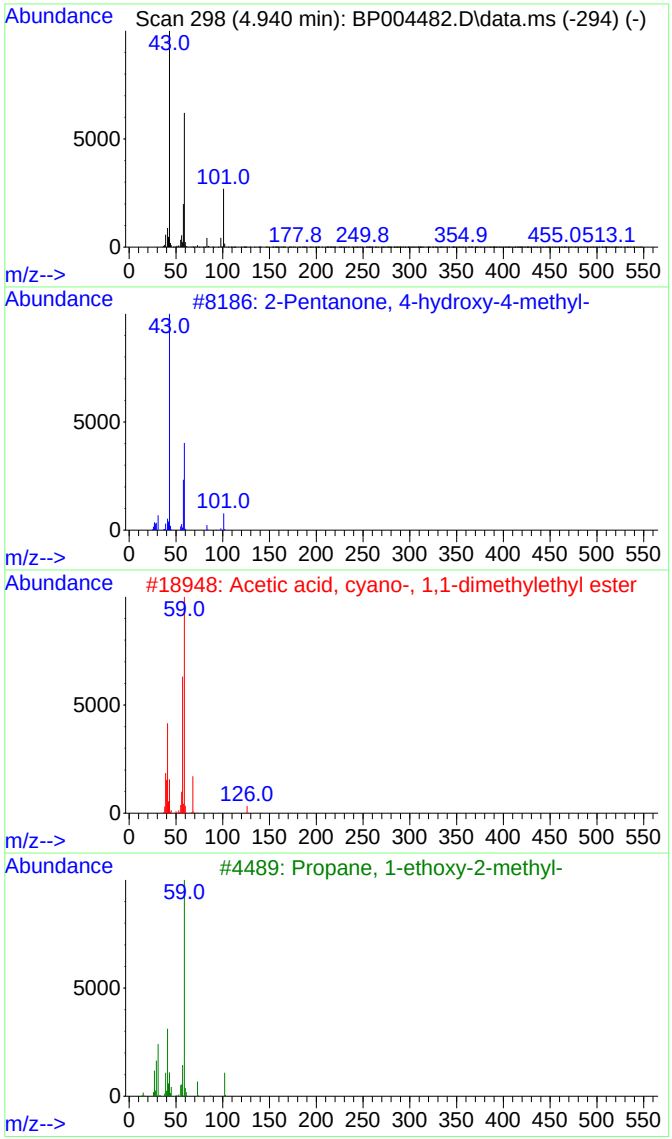
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

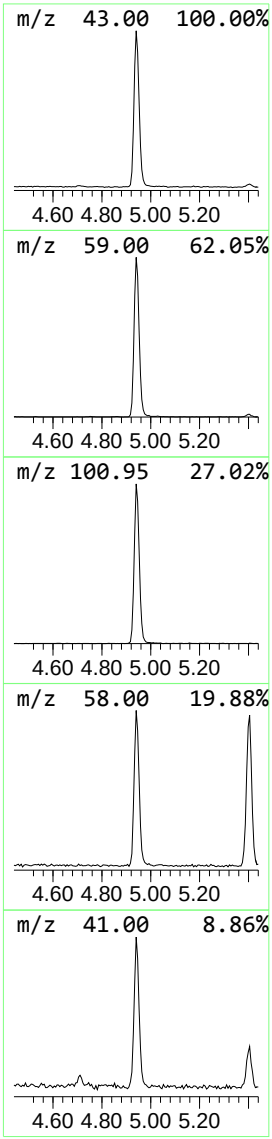
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.940	5.34 ng	398445	1,4-Dichlorobenzene-d4	7.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	16
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	16
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : R-LA-37-3-WC

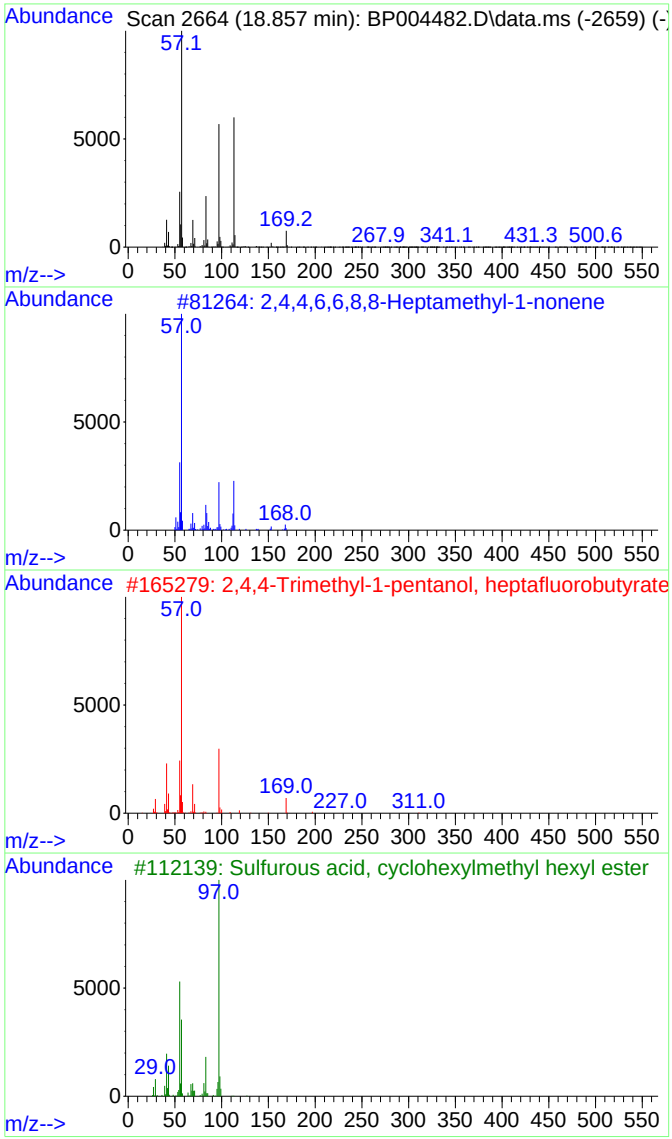
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

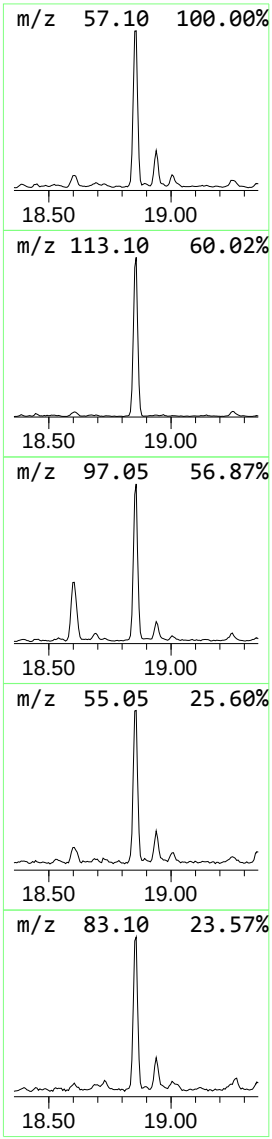
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.857	4.59 ng	649870	Phenanthrene-d10	17.222

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	59
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	37
3	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-6	35
4	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	32
5	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R-LA-37-3-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

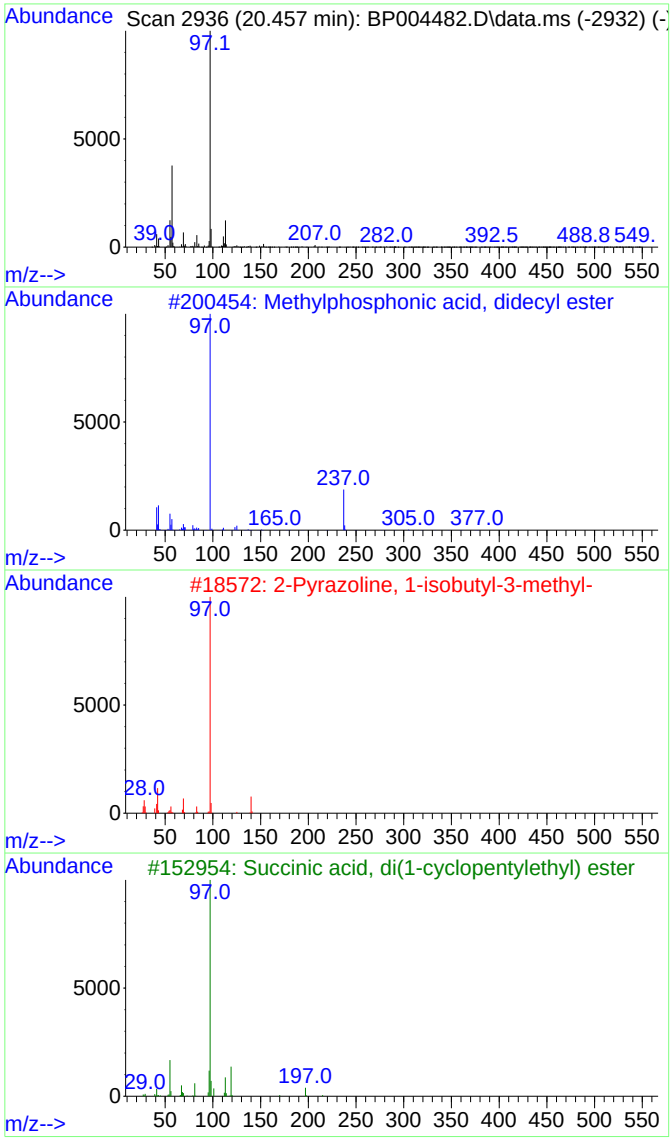
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

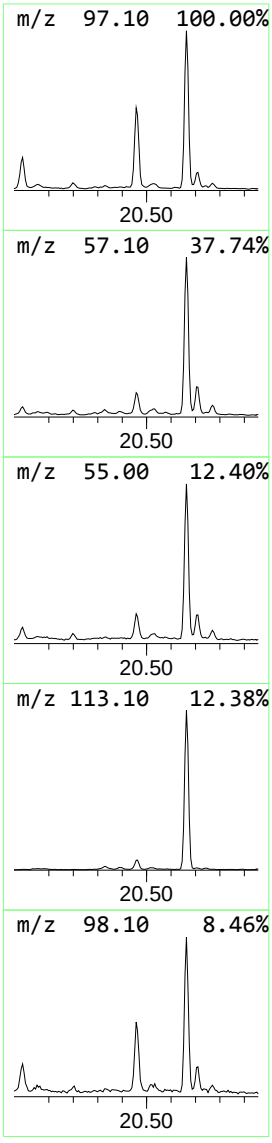
****

Peak Number 3 unknown20.45 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.457	2.50 ng	318787	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylphosphonic acid, didecyl e...	376	C21H45O3P	059651-63-7	42
2	2-Pyrazoline, 1-isobutyl-3-methyl-	140	C8H16N2	026964-53-4	42
3	Succinic acid, di(1-cyclopentyle...	310	C18H30O4	1000330-21-8	40
4	Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	38
5	1-(Trimethylsilyl)-1-propyne	112	C6H12Si	006224-91-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : R-LA-37-3-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

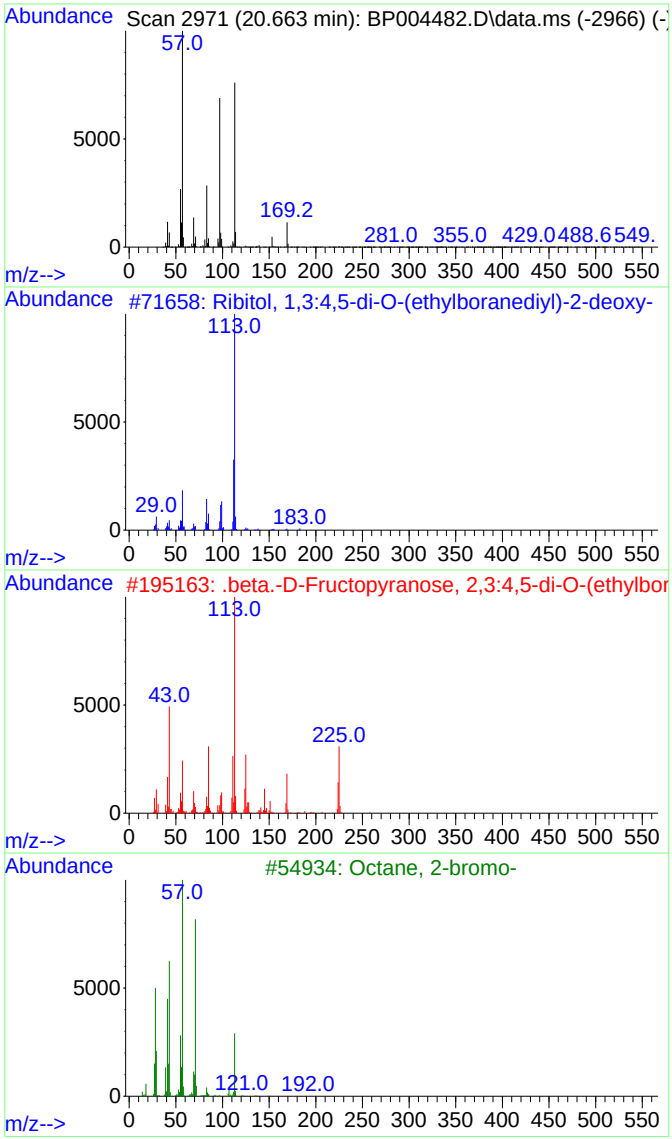
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

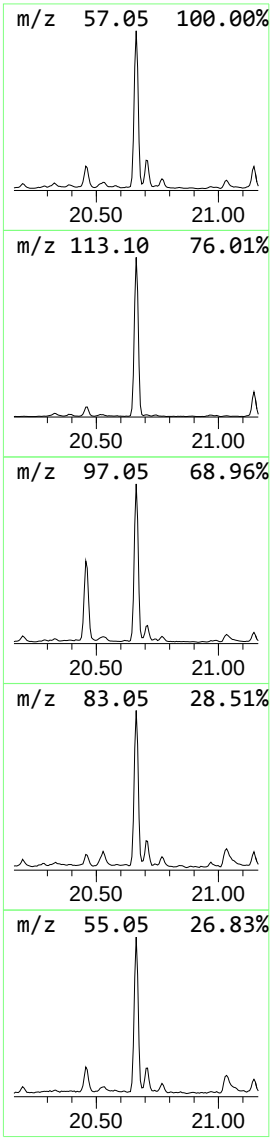
****

Peak Number 4 unknown20.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.663	11.20 ng	1430400	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ribitol, 1,3:4,5-di-O-(ethylbora...	212	C9H18B2O4	1000149-52-8	37
2	.beta.-D-Fructopyranose, 2,3:4,5...	368	C17H30B2O7	1000156-76-8	37
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	37
4	6H-Pyrido[2,3-b][1,4]benzodiazep...	351	C19H21N5O2	028797-61-7	32
5	11-Cyclopentylundecanooic acid, ...	307	C20H37NO	1000336-03-7	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R-LA-37-3-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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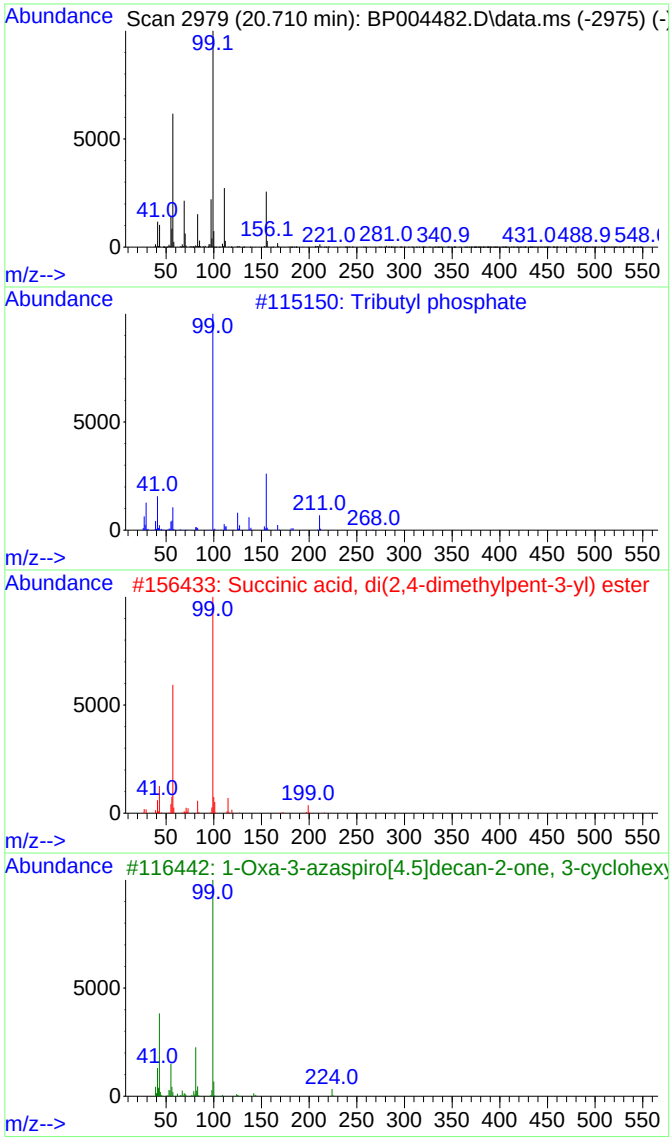
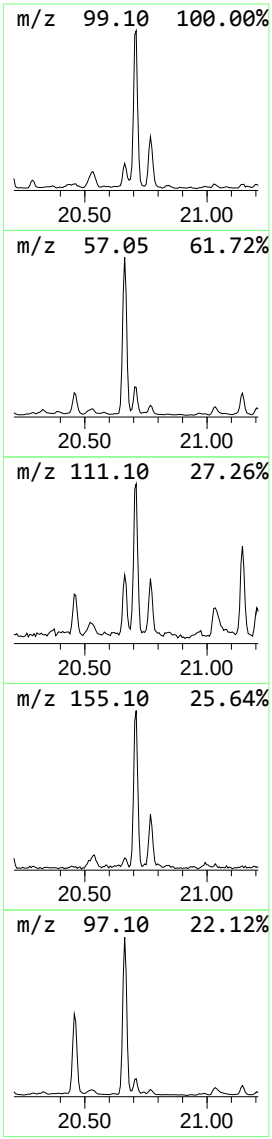
Peak Number 5 unknown20.71 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.710	2.92 ng	373235	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tributyl phosphate	266	C12H27O4P	000126-73-8	40
2	Succinic acid, di(2,4-dimethylpe...	314	C18H34O4	1000349-36-7	38
3	1-Oxa-3-azaspiro[4.5]decan-2-one...	267	C15H25NO3	341941-91-1	37
4	Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	36
5	1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	33





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : R-LA-37-3-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

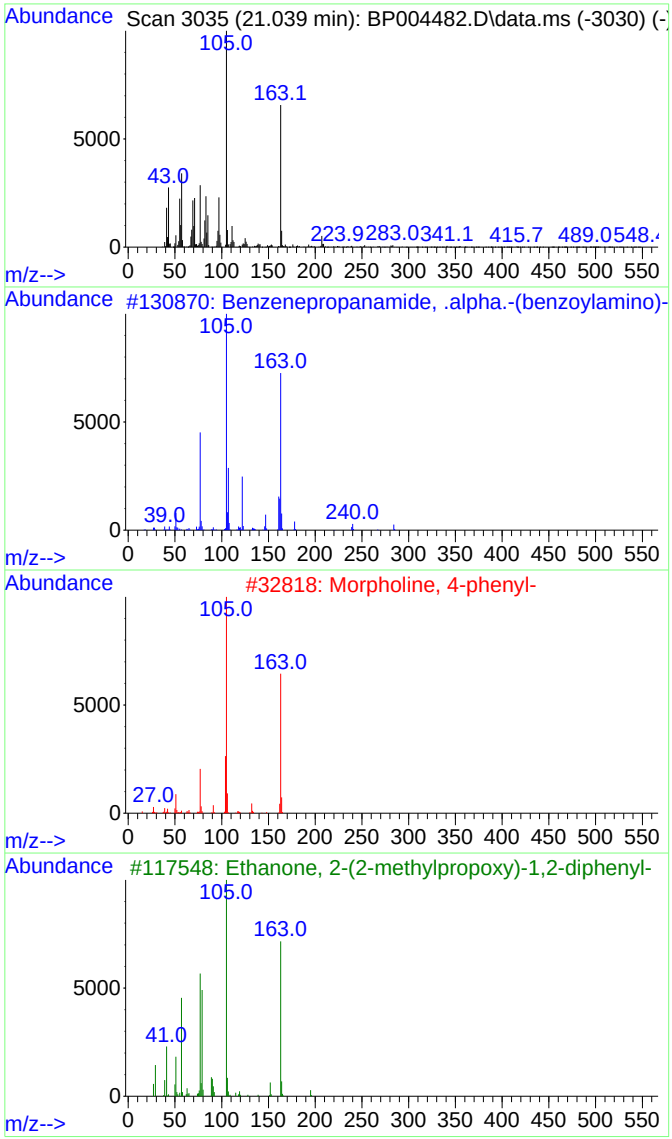
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

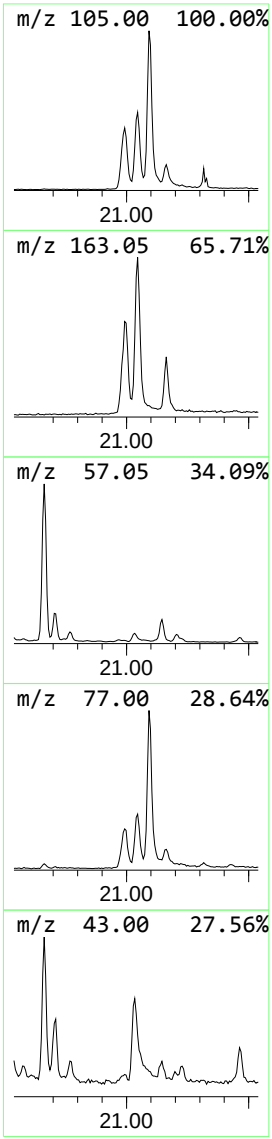
****

Peak Number 6 unknown21.03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.039	3.26 ng	416627	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	27
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	17
3	Ethanone, 2-(2-methylpropoxy)-1,...	268	C18H20O2	022499-12-3	16
4	N-(4-Formyl-phenyl)-N-methyl-for...	163	C9H9NO2	079213-80-2	12
5	Phthalic acid, methyl 4-(2-pheny...	374	C24H22O4	1000315-62-1	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
R-LA-37-3-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

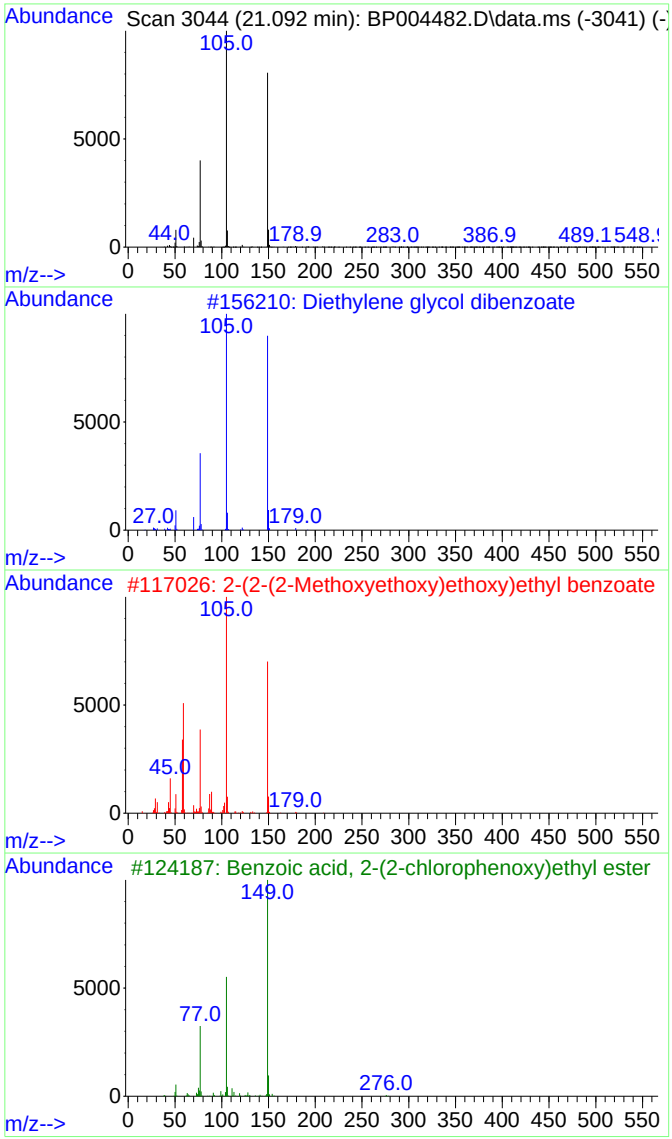
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

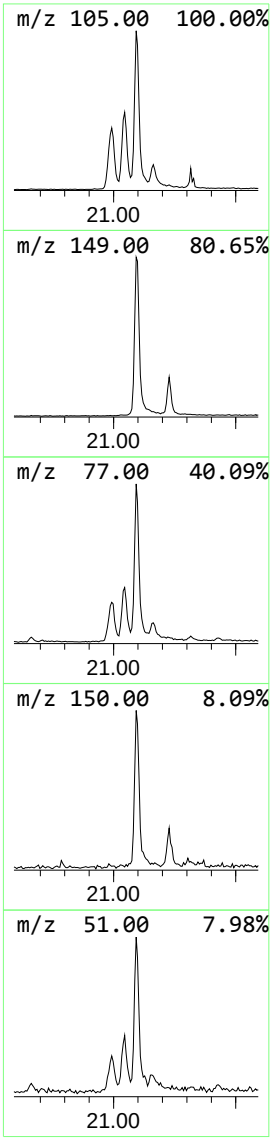
****

Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	2.94 ng	375837	Chrysene-d12	21.316

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
3	Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	72
4	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64
5	3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP010721\
Data File : BP004482.D
Acq On : 07 Jan 2021 16:22
Operator : CG/JU
Sample : M1035-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : R-LA-37-3-WC

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270E-BP121120.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
2-Pentanone, 4-...	4.940	5.3	ng	398445	1	7.811	1491940	20.0
2,4,4,6,6,8,8-H...	18.857	4.6	ng	649870	4	17.222	2831230	20.0
unknown20.45	20.457	2.5	ng	318787	5	21.316	2554810	20.0
unknown20.66	20.663	11.2	ng	1430400	5	21.316	2554810	20.0
unknown20.71	20.710	2.9	ng	373235	5	21.316	2554810	20.0
unknown21.03	21.039	3.3	ng	416627	5	21.316	2554810	20.0
Diethylene glyc...	21.092	2.9	ng	375837	5	21.316	2554810	20.0