LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005878.D
Acq On : 11 Jun 2021 19:13
Operator : CG/JU
Sample : M2625-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(210-214)

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-BP060821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.817	120	124	131	rBV	28889	40180	1.55%	0.360%
2	4.434	224	229	242	rVB	181321	255906	9.88%	2.296%
3	4.570	247	252	266	rBV2	25328	71974	2.78%	0.646%
4	5.046	328	333	340	rVB	33978	49271	1.90%	0.442%
5	5.517	407	413	431	rBV	174883	312573	12.07%	2.804%
6	7.111	675	684	699	rBV	270149	509471	19.67%	4.570%
7	7.240	701	706	724	rVB	66120	153129	5.91%	1.374%
8	7.946	819	826	833	rBV	237205	367545	14.19%	3.297%
9	8.605	931	938	948	rBV	121403	230913	8.92%	2.071%
10	9.111	1016	1024	1036	rBV	278446	484473	18.71%	4.346%
11	9.687	1116	1122	1132	rBV	23436	47282	1.83%	0.424%
12	10.552	1262	1269	1276	rBV2	18244	43880	1.69%	0.394%
13	10.752	1295	1303	1311	rBV	267200	459484	17.74%	4.122%
14	12.028	1509	1520	1529	rBV2	35727	92861	3.59%	0.833%
15	13.046	1686	1693	1703	rBV4	8965	27185	1.05%	0.244%
16	13.199	1712	1719	1734	rBV	1105991	1642740	63.44%	14.737%
17	13.998	1846	1855	1863	rBV3	34437	66874	2.58%	0.600%
18	14.569	1943	1952	1975	rBV	366042	607812	23.47%	5.452%
19	16.069	2199	2207	2222	rBV2	36392	78445	3.03%	0.704%
20	17.316	2413	2419	2434	rBV	447101	738055	28.50%	6.621%
21	19.863	2846	2852	2861	rBV	2004215	2589636	100.00%	23.231%
22	21.092	3057	3061	3069	rBV6	45371	100415	3.88%	0.901%
23	21.386	3106	3111	3121	rBV	786730	1028191	39.70%	9.224%
24	23.804	3515	3522	3535	rVB2	550565	1149111	44.37%	10.308%

Sum of corrected areas: 11147406

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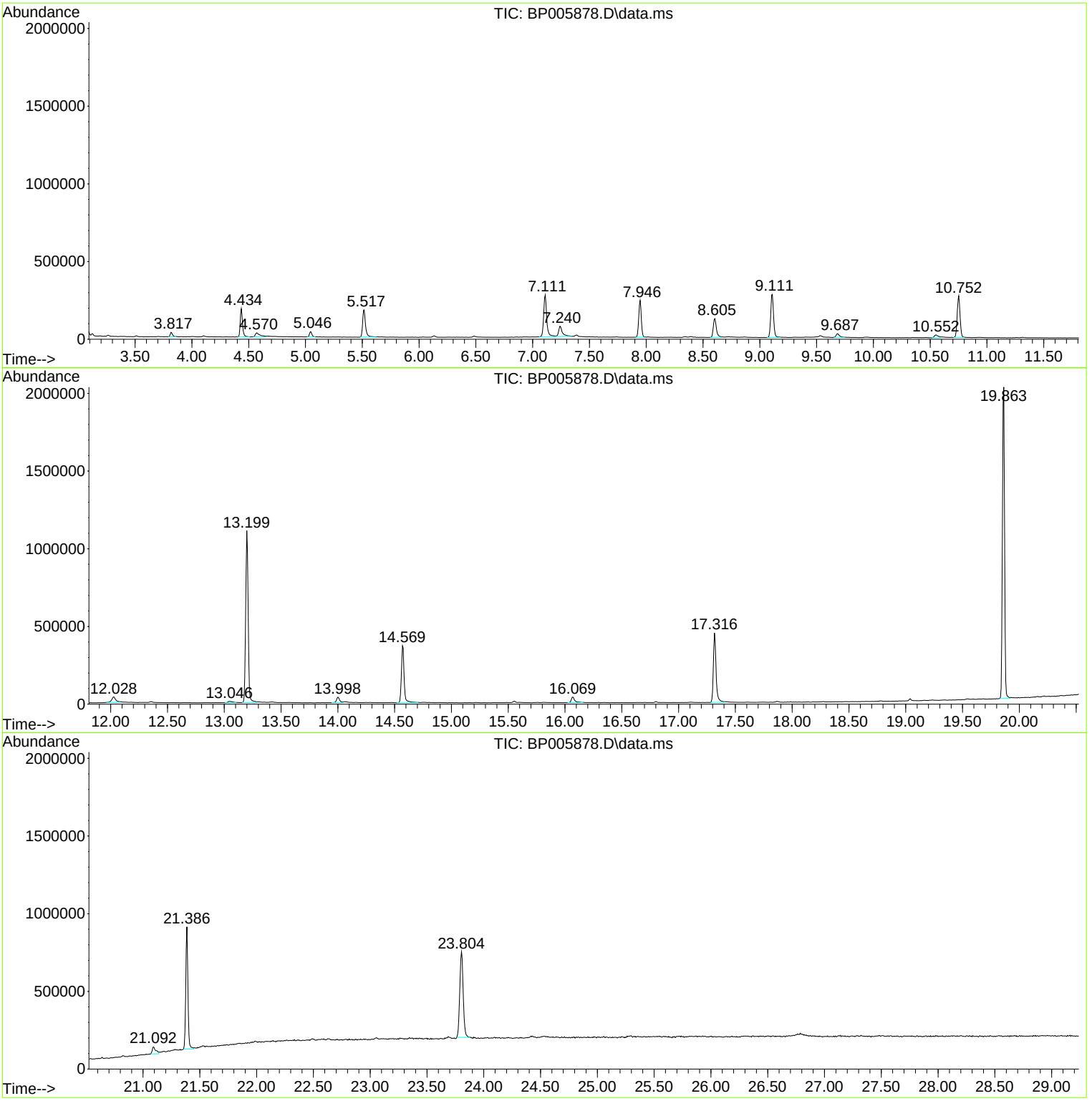
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B12(210-214)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.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\BP061121\
Data File : BP005878.D
Acq On : 11 Jun 2021 19:13
Operator : CG/JU
Sample : M2625-19
Misc :
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Instrument :
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ClientSampleId :
18-B12(210-214)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

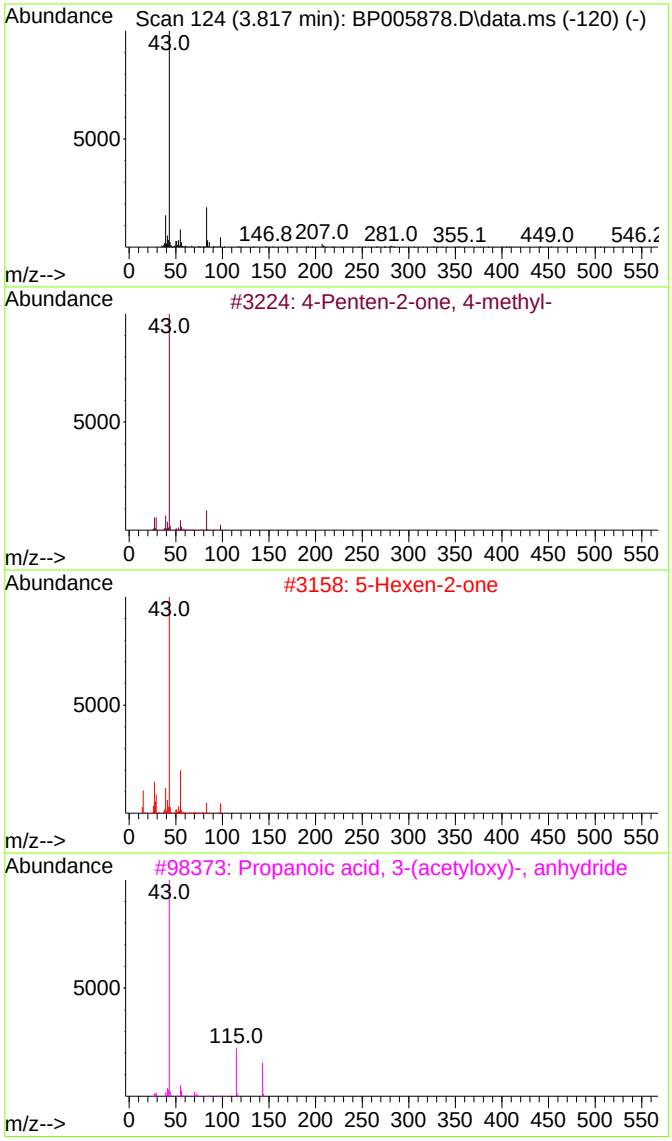
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

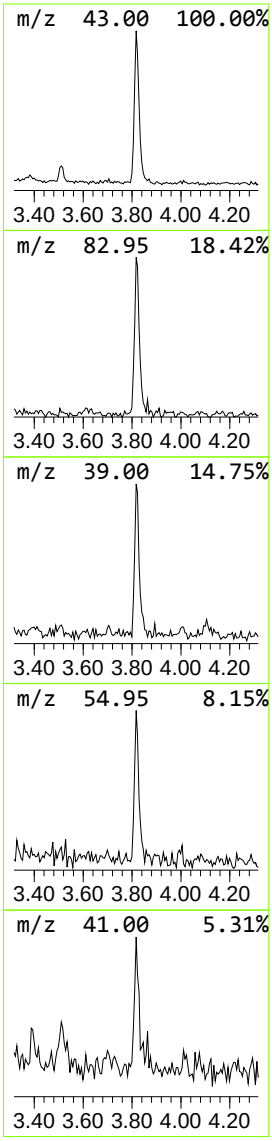
****

Peak Number 1 4-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.817	2.19 ng	40180	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	50
2	5-Hexen-2-one	98	C6H10O	000109-49-9	43
3	Propanoic acid, 3-(acetyloxy)-, ...	246	C10H14O7	055656-58-1	10
4	2-tert-Butyl-4,6-dinitrophenyl a...	282	C12H14N2O6	1000373-33-1	9
5	Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005878.D
Acq On : 11 Jun 2021 19:13
Operator : CG/JU
Sample : M2625-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(210-214)

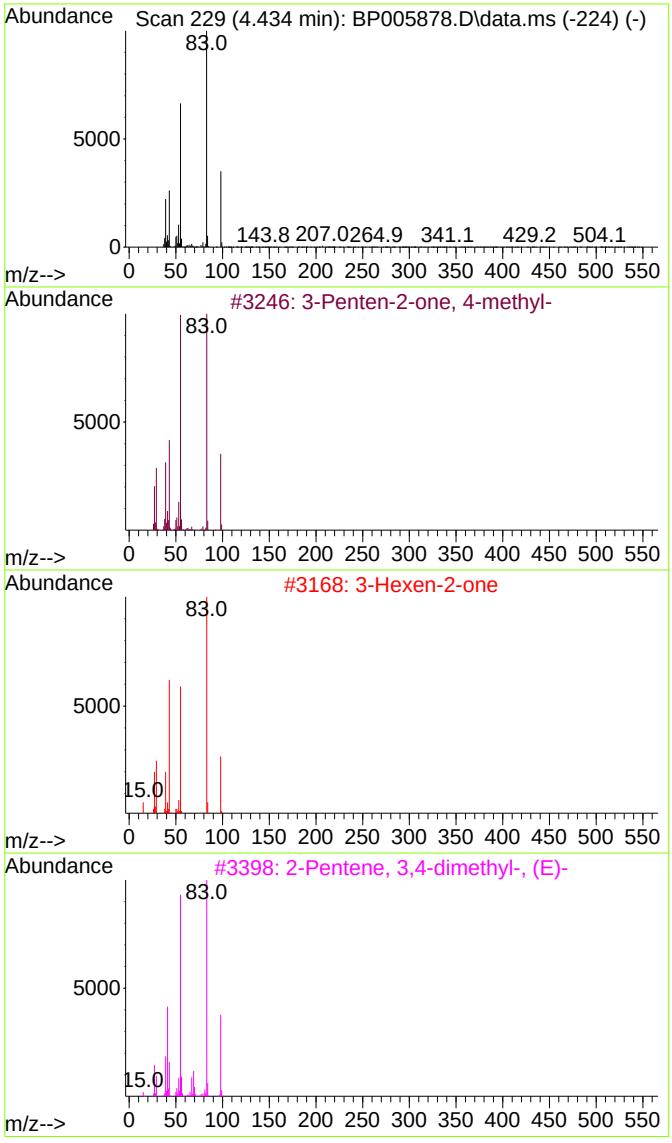
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

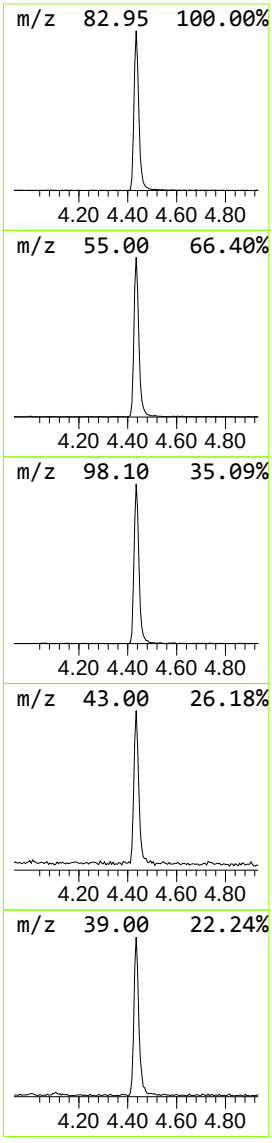
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.434	13.93 ng	255906	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005878.D
Acq On : 11 Jun 2021 19:13
Operator : CG/JU
Sample : M2625-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(210-214)

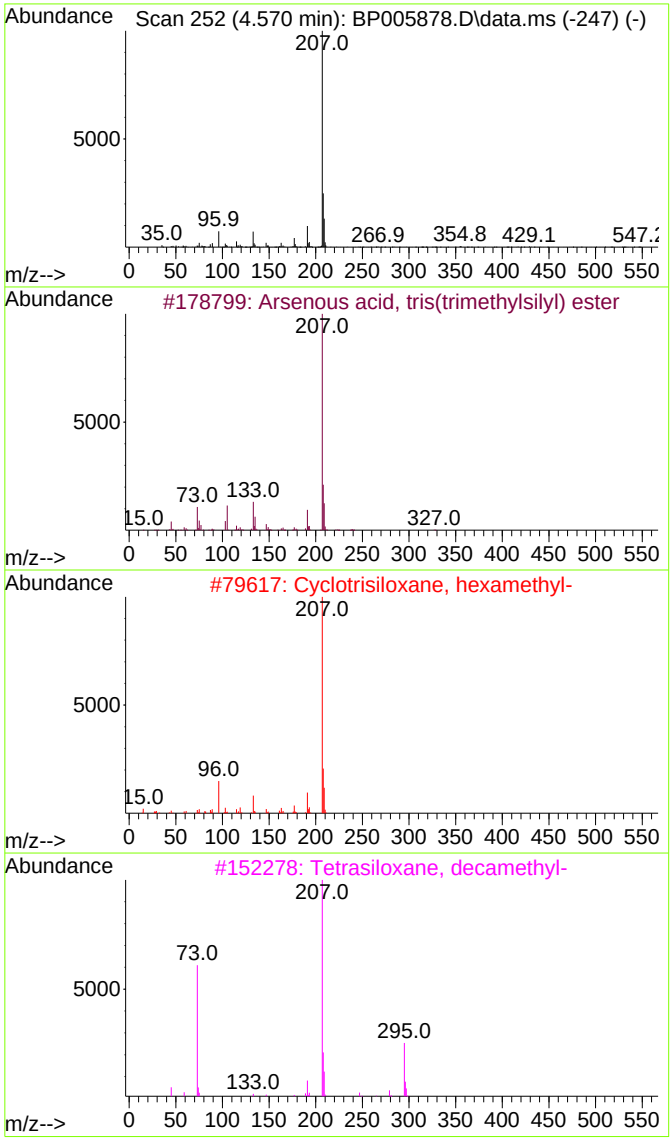
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

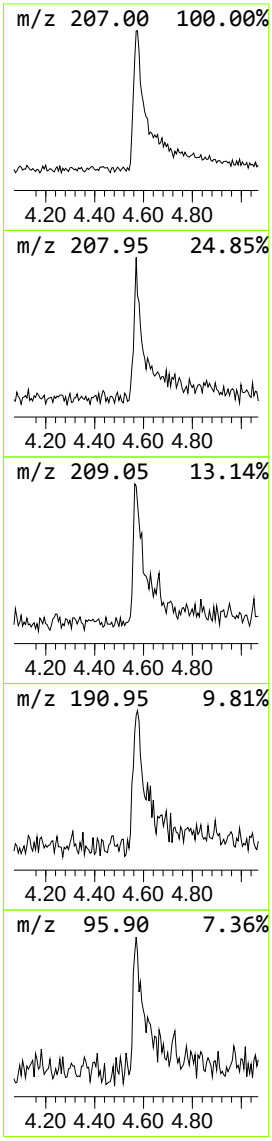
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Arsenous acid, tris(trimeth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.570	3.92 ng	71974	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Arsenous acid, tris(trimethylsil...	342	C9H27AsO3Si3	055429-29-3	78
2	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	78
3	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	78
4	2,4,6-Cycloheptatrien-1-one, 3,5...	250	C13H22OSi2	1000161-21-8	56
5	1,2-Bis(trimethylsilyl)benzene	222	C12H22Si2	017151-09-6	56





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Sample : M2625-19
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
18-B12(210-214)

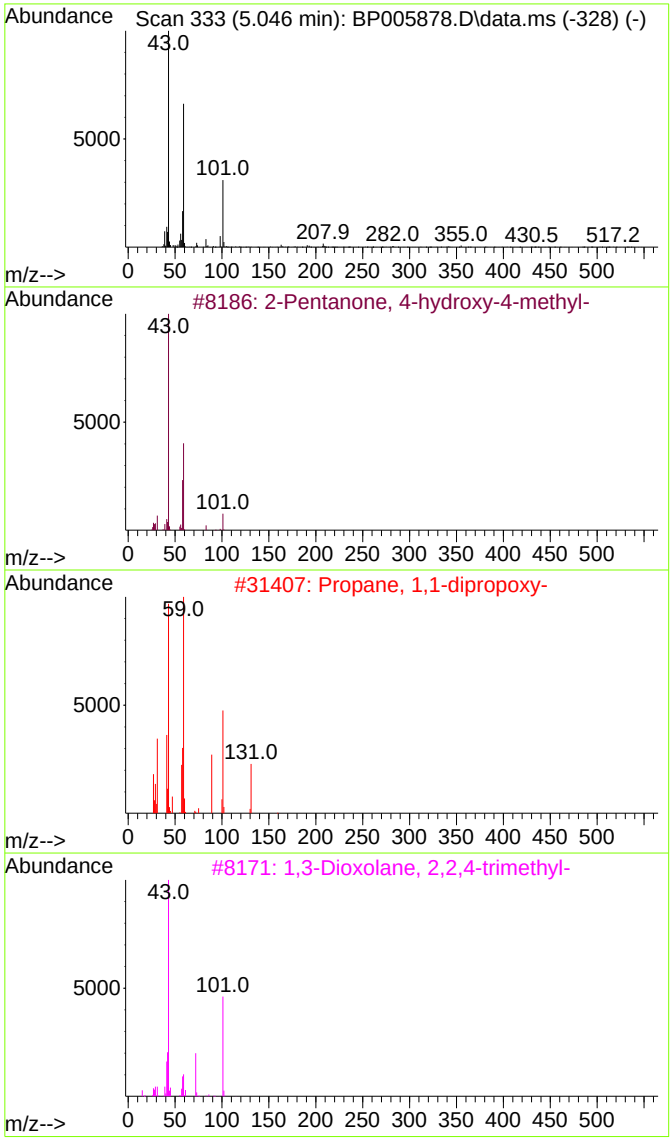
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

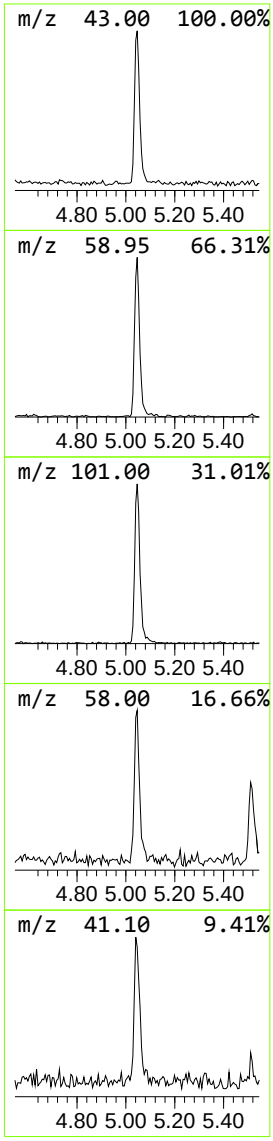
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	2.68 ng	49271	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
3	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	37
4	Dimethadione	129	C5H7NO3	000695-53-4	33
5	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28





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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(210-214)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

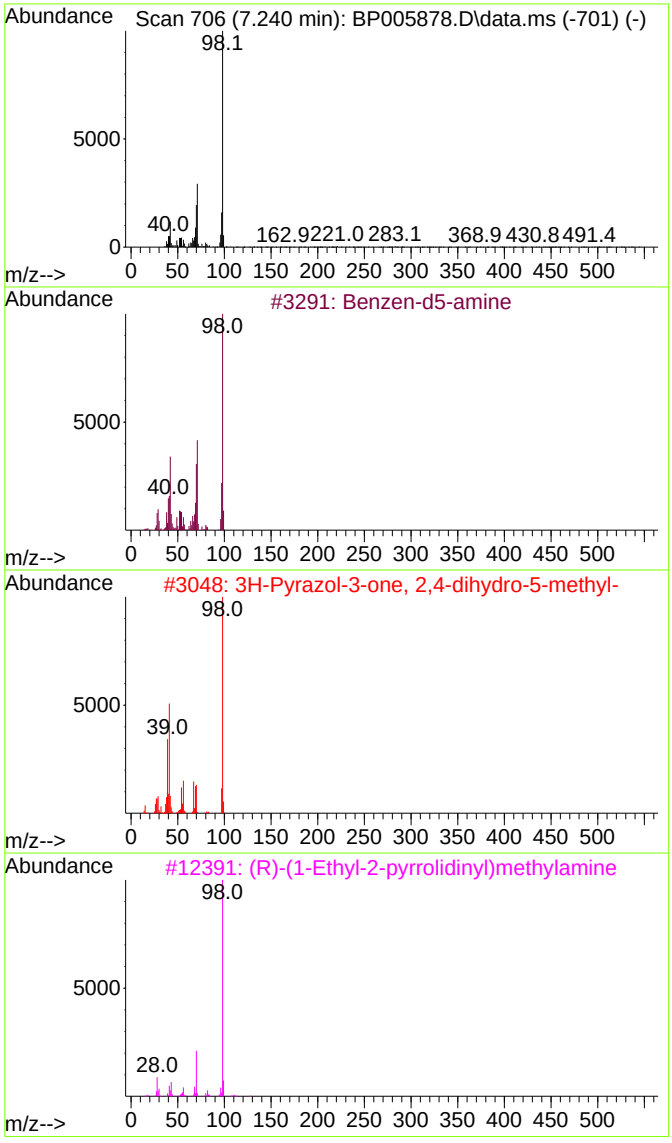
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

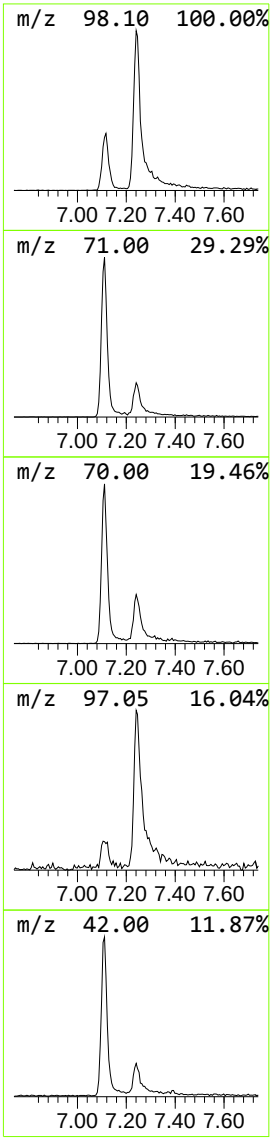
****

Peak Number 5 Benzen-d5-amine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.240	8.33 ng	153129	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzen-d5-amine	98	C6H2D5N	004165-61-1	91
2	3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	59
3	(R)-(1-Ethyl-2-pyrrolidinyl)meth...	128	C7H16N2	022795-97-7	53
4	3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	50
5	[1,3,4]Thiadiazol, 2-amino-5-(2-...	212	C9H16N4S	1000303-12-6	50





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18-B12(210-214)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
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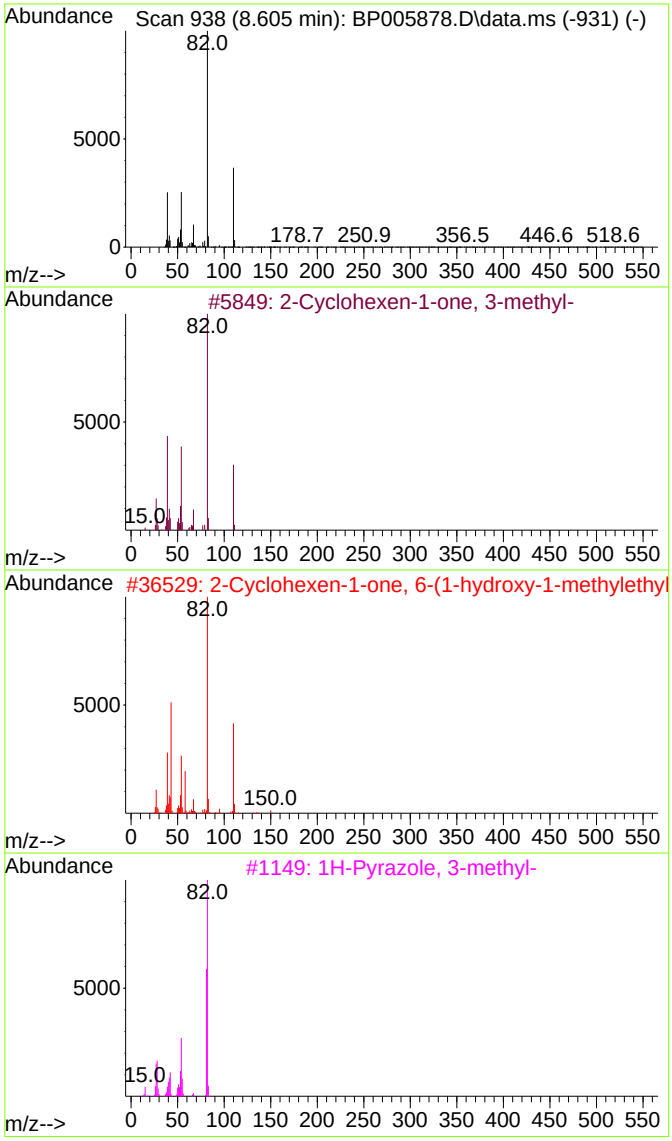
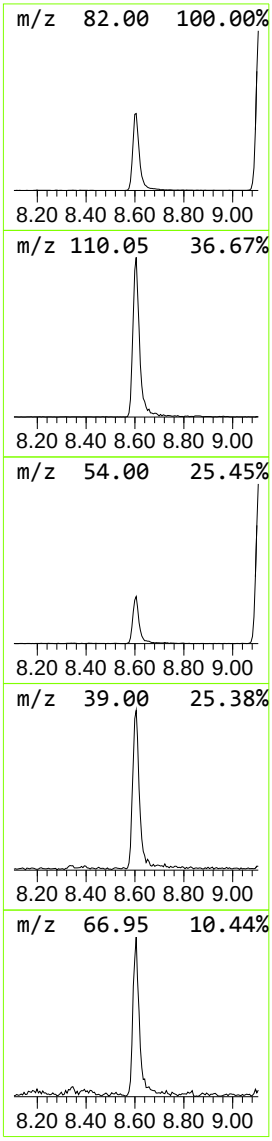
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.605	12.57 ng	230913	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	91
2	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	72
3	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	59
4	Betazole	111	C5H9N3	000105-20-4	40
5	Histamine	111	C5H9N3	000051-45-6	9





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ClientSampleId : 18-B12(210-214)

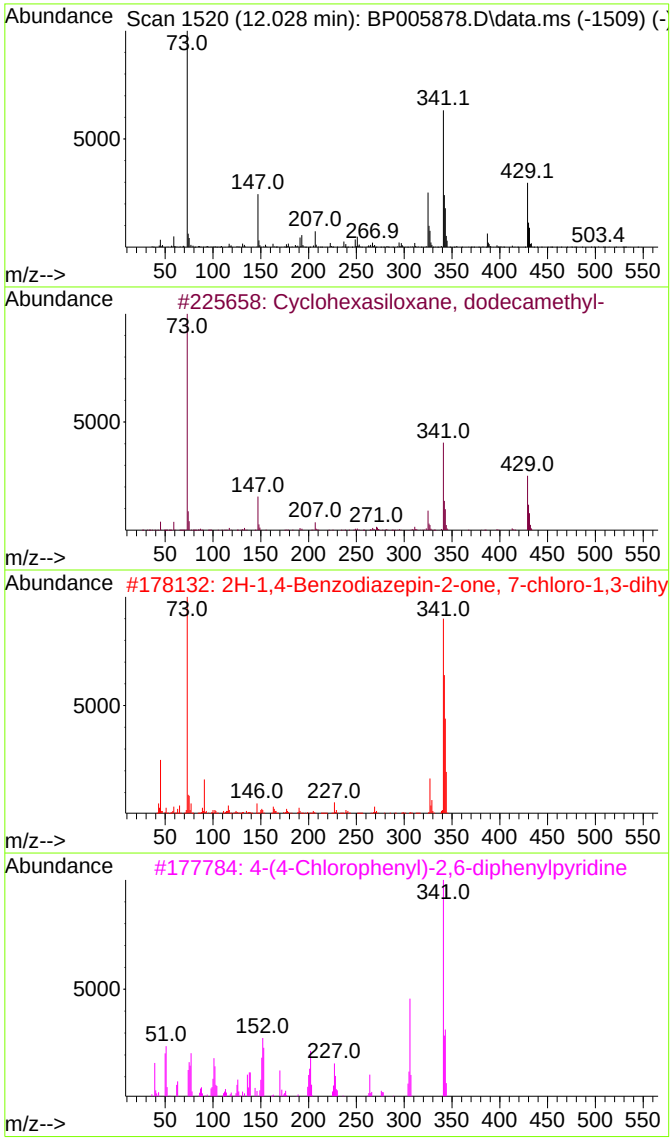
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

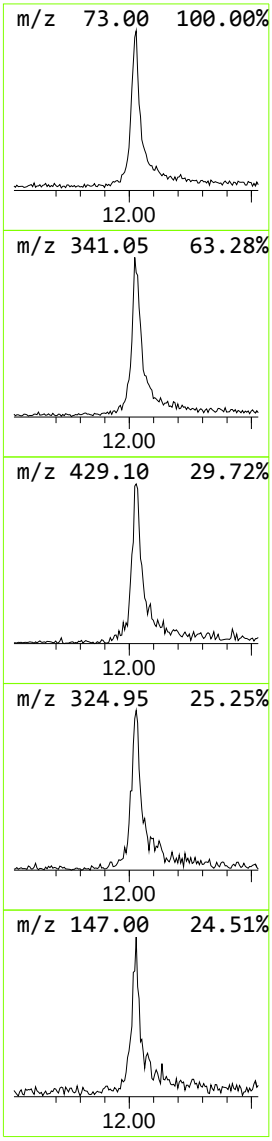
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclohexasiloxane, dodecame... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	4.04 ng	92861	Naphthalene-d8	10.752

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	83
2	2H-1,4-Benzodiazepin-2-one, 7-ch...	342	C18H19ClN2OSi	055299-24-6	27
3	4-(4-Chlorophenyl)-2,6-diphenylp...	341	C23H16ClN	001498-82-4	27
4	Acetic acid, [bis[(trimethylsily...	356	C11H29O5PSi3	053044-27-2	23
5	1,3,5,7,9-Pentaethylcyclopentasi...	370	C10H30O5Si5	017995-44-7	16





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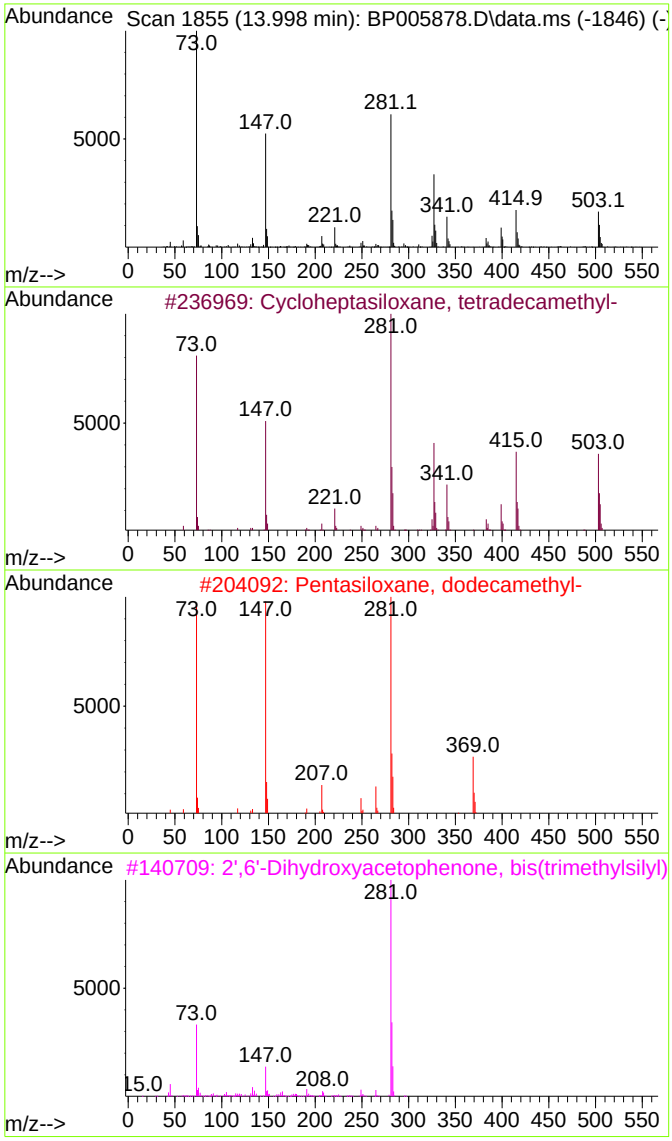
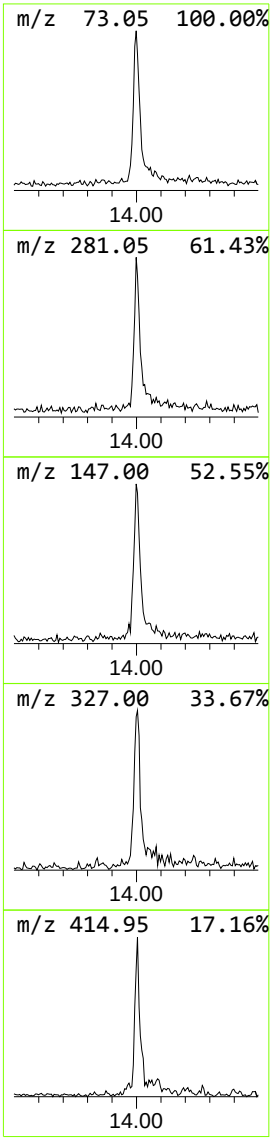
****
Peak Number 8 Cycloheptasiloxane, tetrade... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.999	2.20 ng	66874	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptasiloxane, tetradecamet...	518	C14H42O7Si7	000107-50-6	90
2	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	37
3	2',6'-Dihydroxyacetophenone, bis...	296	C14H24O3Si2	1000352-81-3	37
4	3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	32
5	Silane, [[(3.beta.,11.beta.,20S)...	638	C33H66O4Si4	032221-72-0	25





Tentatively Identified Compound (LSC) summary

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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
4-Penten-2-one,...	3.817	2.2	ng	40180	1	7.946	367545	20.0
3-Penten-2-one,...	4.434	13.9	ng	255906	1	7.946	367545	20.0
Arsenous acid, ...	4.570	3.9	ng	71974	1	7.946	367545	20.0
2-Pentanone, 4-...	5.046	2.7	ng	49271	1	7.946	367545	20.0
Benzen-d5-amine	7.240	8.3	ng	153129	1	7.946	367545	20.0
2-Cyclohexen-1-...	8.605	12.6	ng	230913	1	7.946	367545	20.0
Cyclohexasiloxa...	12.028	4.0	ng	92861	2	10.752	459484	20.0
Cycloheptasilox...	13.999	2.2	ng	66874	3	14.569	607812	20.0