LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005883.D
Acq On : 11 Jun 2021 22:03
Operator : CG/JU
Sample : M2625-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(198-202)

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: BP005883.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	% max.	% of total
1	4.587	247	255	262	rBV2	16908	61615	1.99%	0.503%
2	5.046	328	333	339	rVB	28698	39774	1.29%	0.325%
3	5.510	406	412	428	rBV	462885	727437	23.54%	5.942%
4	7.110	675	684	697	rBV	514041	943412	30.52%	7.706%
5	7.246	702	707	716	rVB2	25570	55508	1.80%	0.453%
6	7.946	819	826	835	rBV	223210	355058	11.49%	2.900%
7	8.610	931	939	952	rBV	29320	72241	2.34%	0.590%
8	9.110	1016	1024	1035	rBV	330133	572354	18.52%	4.675%
9	9.540	1091	1097	1108	rVB4	13090	32876	1.06%	0.269%
10	10.540	1261	1267	1282	rBV	27079	75859	2.45%	0.620%
11	10.751	1295	1303	1317	rVB	256570	446772	14.45%	3.649%
12	12.028	1508	1520	1537	rBV2	37792	98254	3.18%	0.803%
13	13.039	1685	1692	1705	rBV3	12147	38662	1.25%	0.316%
14	13.198	1712	1719	1739	rBV	1206807	1762426	57.02%	14.395%
15	14.004	1849	1856	1870	rBV2	30208	63180	2.04%	0.516%
16	14.569	1945	1952	1965	rBV	356334	577736	18.69%	4.719%
17	16.063	2197	2206	2217	rBV2	81776	147235	4.76%	1.203%
18	17.316	2412	2419	2434	rBV	444093	718582	23.25%	5.869%
19	19.863	2846	2852	2861	rBV	2448559	3090815	100.00%	25.245%
20	20.527	2962	2965	2971	rBV4	24376	33687	1.09%	0.275%
21	21.092	3057	3061	3070	rBV2	63591	120989	3.91%	0.988%
22	21.386	3106	3111	3118	rBV	764433	996895	32.25%	8.142%
23	23.804	3515	3522	3537	rBV2	552373	1211741	39.20%	9.897%

Sum of corrected areas: 12243108

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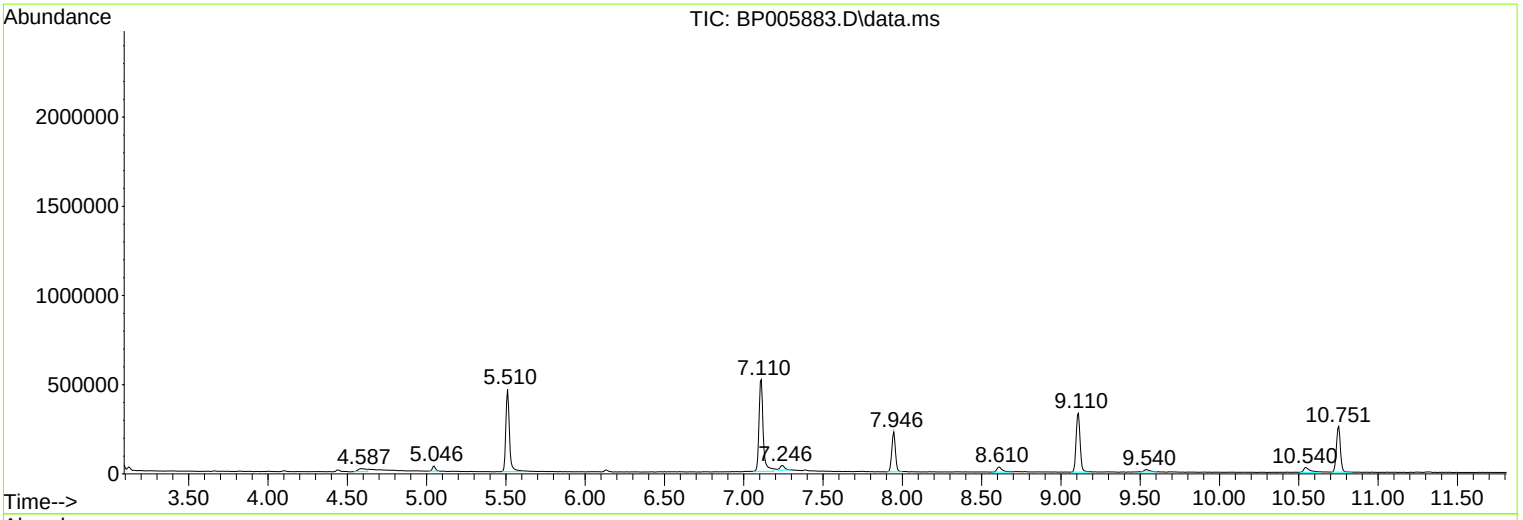
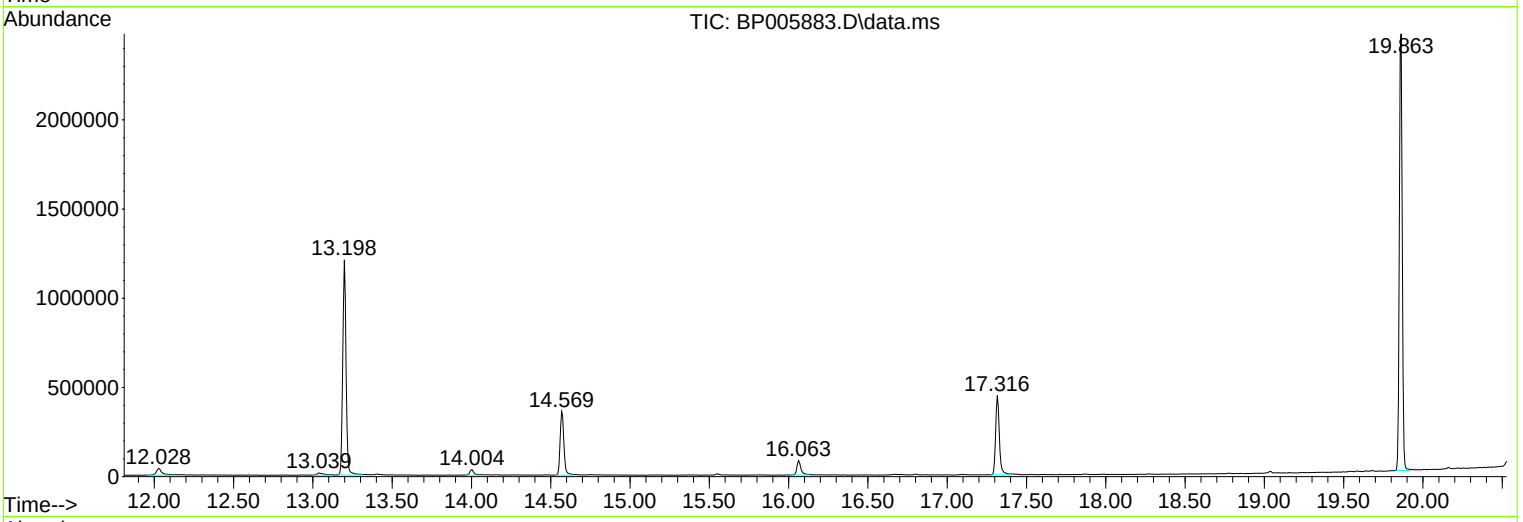
Misc :
ALS Vial : 20 Sample Multiplier: 1

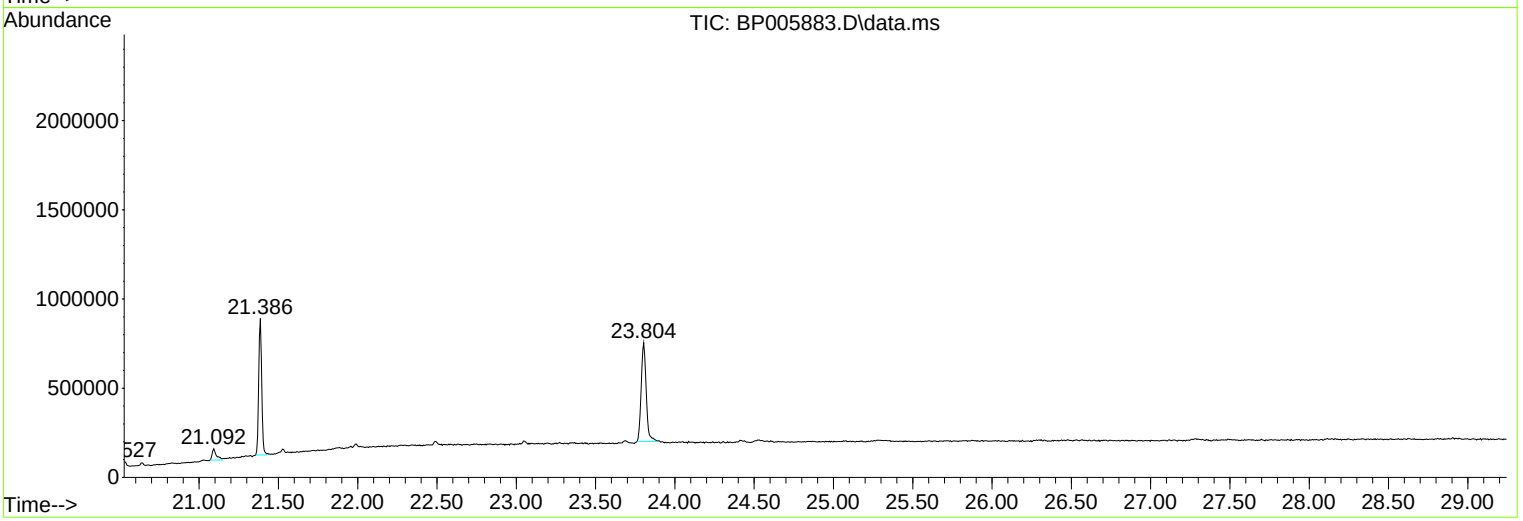
Instrument :
BNA_P
ClientSampleId :
18-B12(198-202)

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







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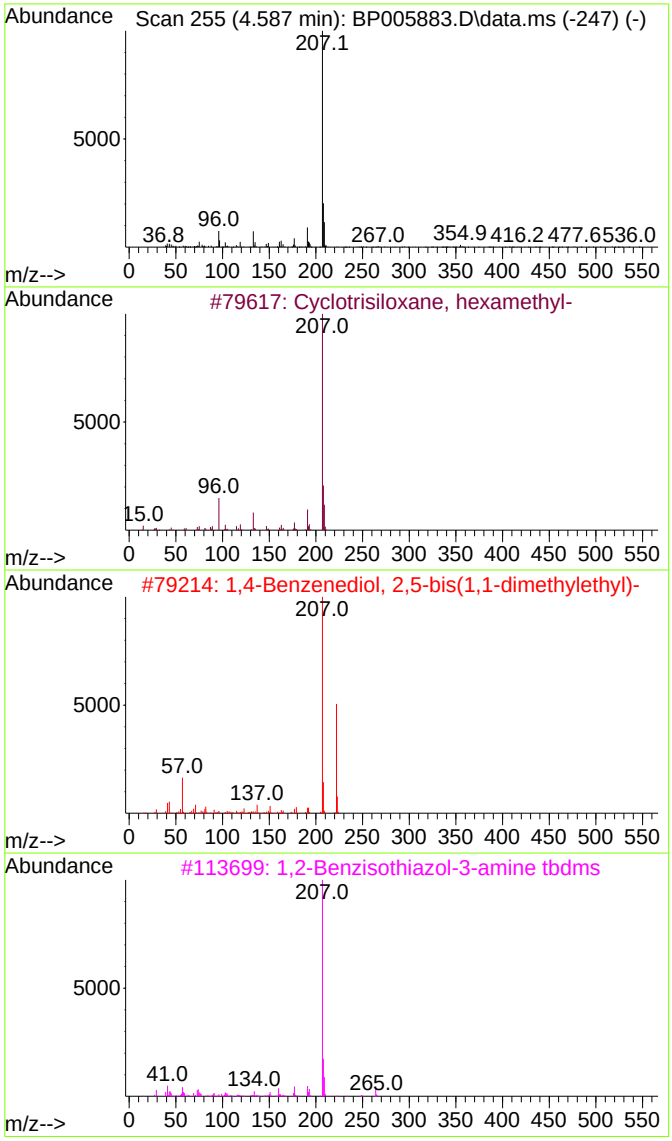
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

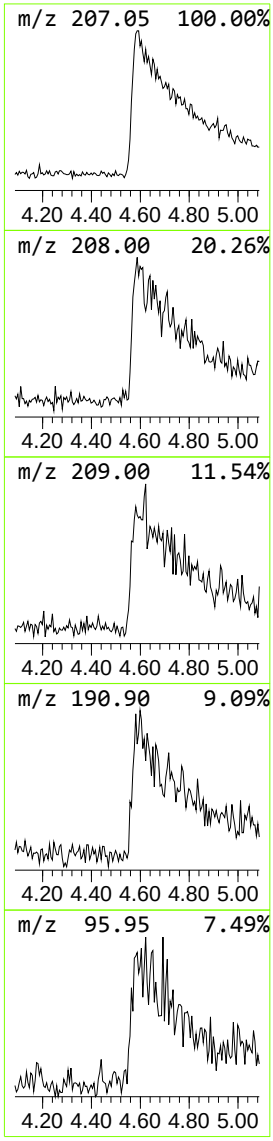
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Cyclotrisiloxane, hexamethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.587	3.47 ng	61615	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	83
2	1,4-Benzenediol, 2,5-bis(1,1-dim...	222	C14H22O2	000088-58-4	64
3	1,2-Benzisothiazol-3-amine tbdms	264	C13H20N2SSi	1000332-57-2	64
4	Tetrasiloxane, decamethyl-	310	C10H30O3Si4	000141-62-8	64
5	1,2-Benzenediol, 3,5-bis(1,1-dim...	222	C14H22O2	001020-31-1	64





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
18-B12(198-202)

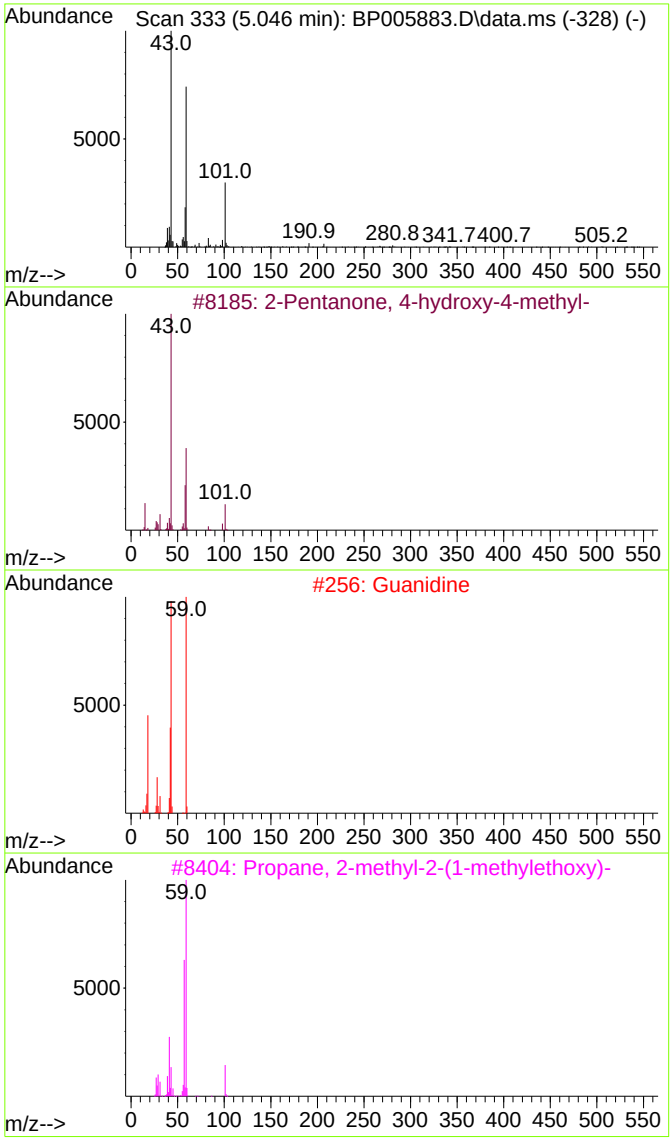
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

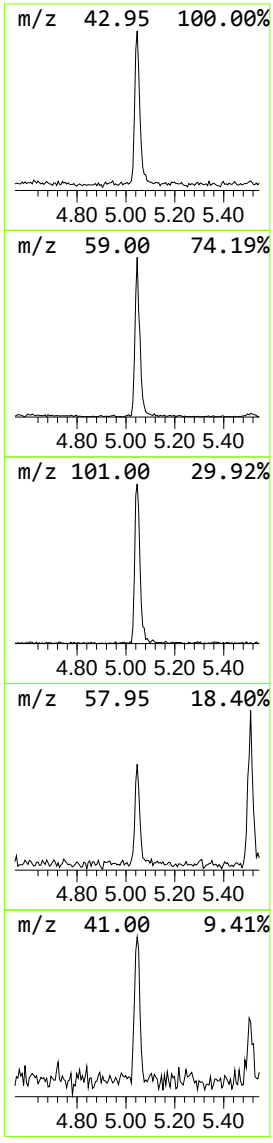
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.046	2.24 ng	39774	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	Guanidine	59	CH5N3	000113-00-8	50
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
4	Dimethadione	129	C5H7NO3	000695-53-4	38
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	37





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Data File : BP005883.D
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Operator : CG/JU
Sample : M2625-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(198-202)

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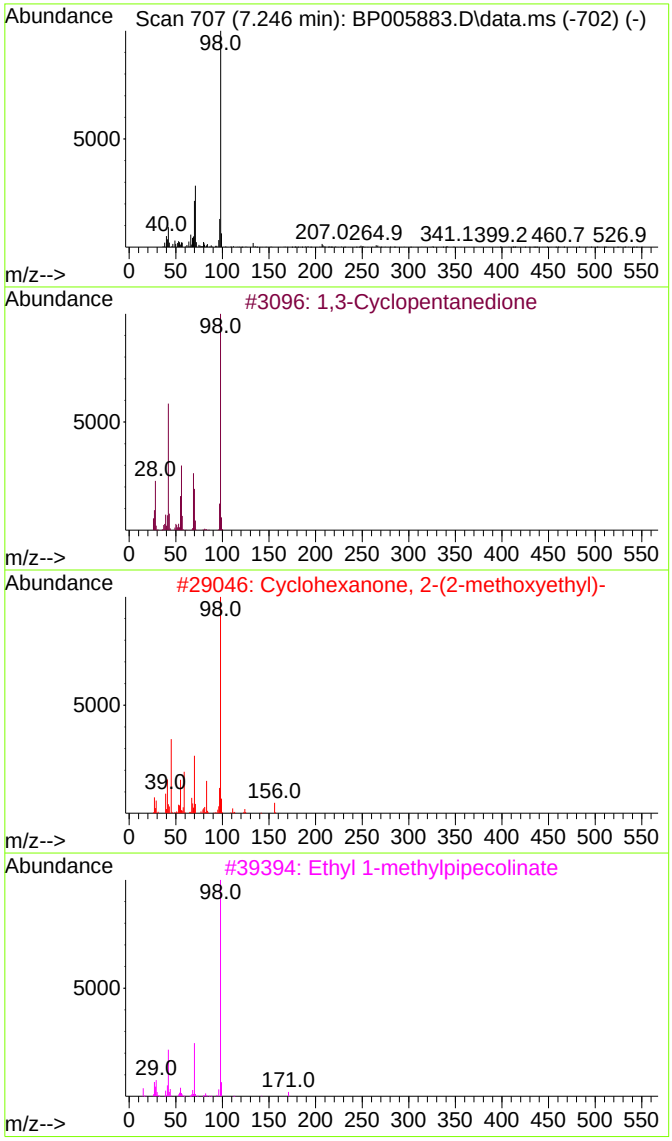
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

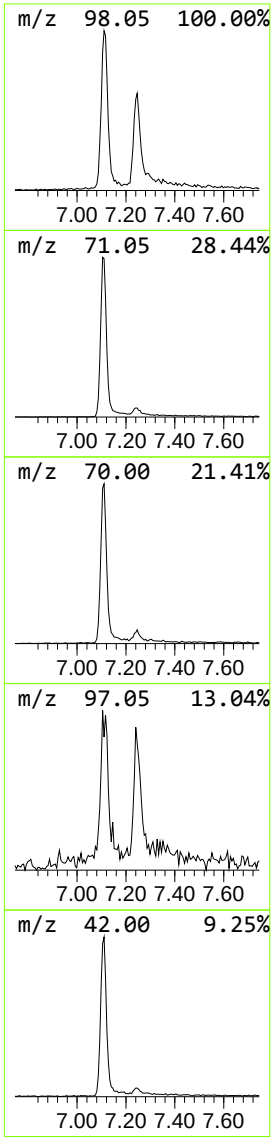
****

Peak Number 3 1,3-Cyclopentanedione Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.246	3.13 ng	55508	1,4-Dichlorobenzene-d4	7.946

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione	98	C5H6O2	003859-41-4	59
2	Cyclohexanone, 2-(2-methoxyethyl)-	156	C9H16O2	129786-15-8	59
3	Ethyl 1-methylpipecolinate	171	C9H17NO2	030727-18-5	53
4	3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	50
5	Propan-2-ol, 1-(2-methyl-4-nitro...	300	C12H20N4O3S	306326-24-9	50





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Instrument :
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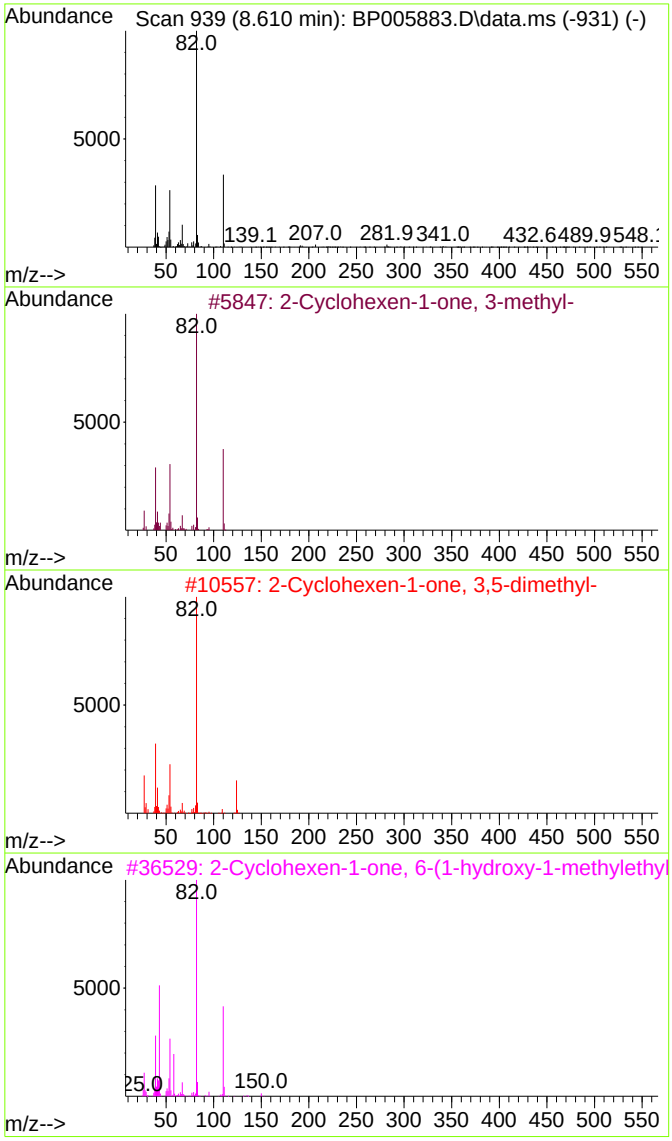
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

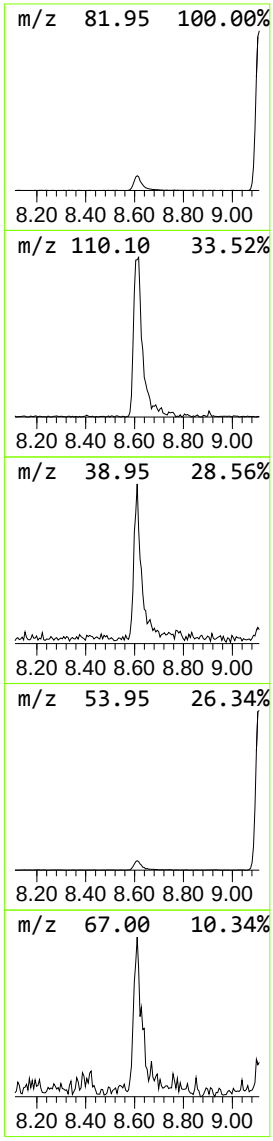
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.610	4.07 ng	72241	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	90
2	2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	59
3	2-Cyclohexen-1-one, 6-(1-hydroxy...	168	C10H16O2	087791-00-2	56
4	1H-Pyrazole, 3-methyl-	82	C4H6N2	001453-58-3	42
5	Isophorone	138	C9H14O	000078-59-1	38





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ALS Vial : 20 Sample Multiplier: 1

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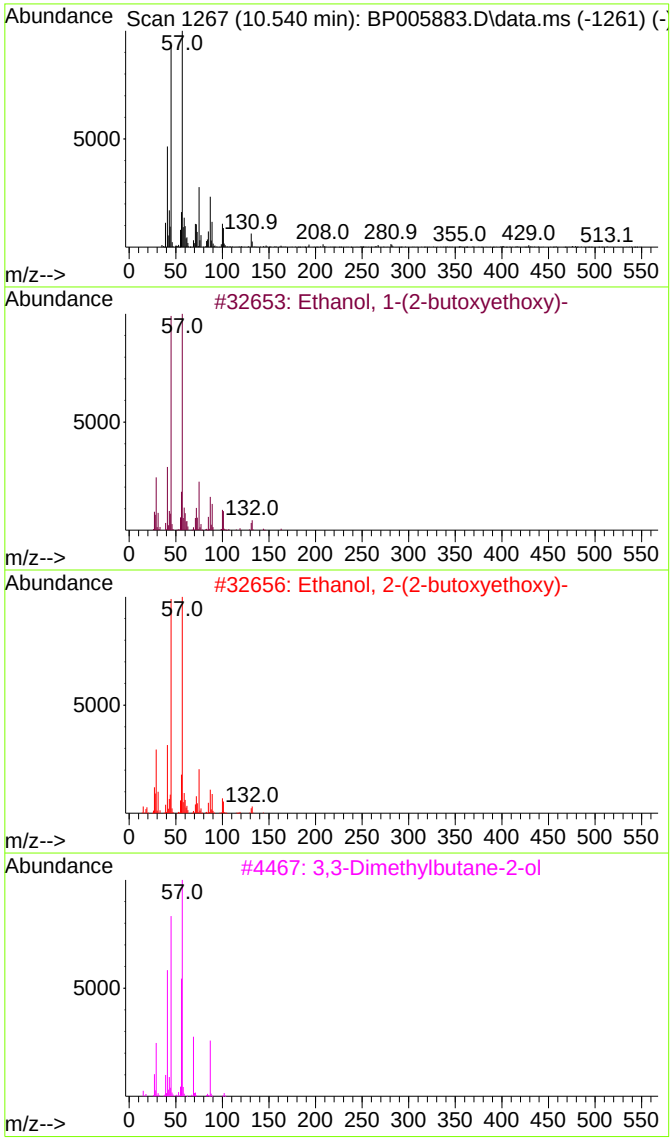
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

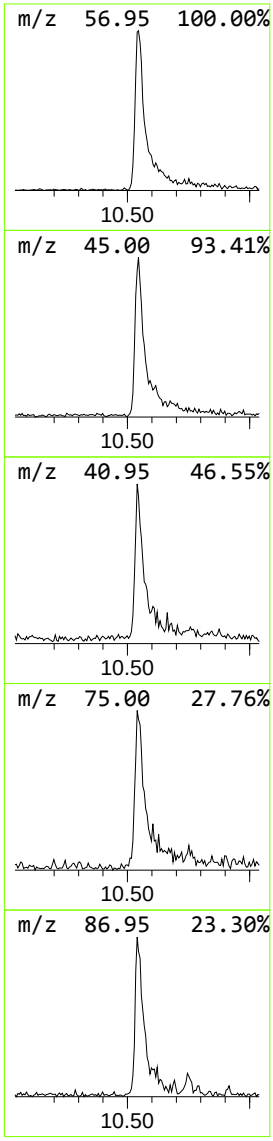
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 1-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.540	3.40 ng	75859	Naphthalene-d8	10.751

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	80
2	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	72
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	47
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	43
5	1,4,7,10,13,16-Hexaoxacyclooctad...	264	C12H24O6	017455-13-9	43





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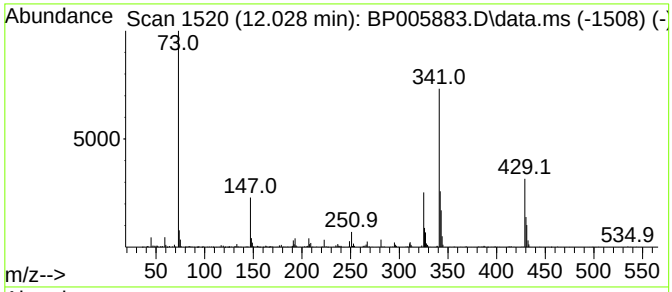
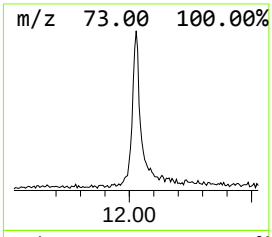
****

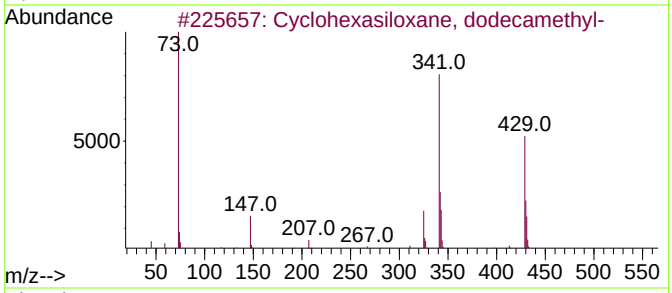
Peak Number 6 Cyclohexasiloxane, dodecame... Concentration Rank 1

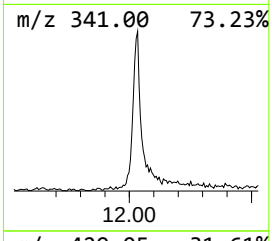
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.028	4.40 ng	98254	Naphthalene-d8	10.751

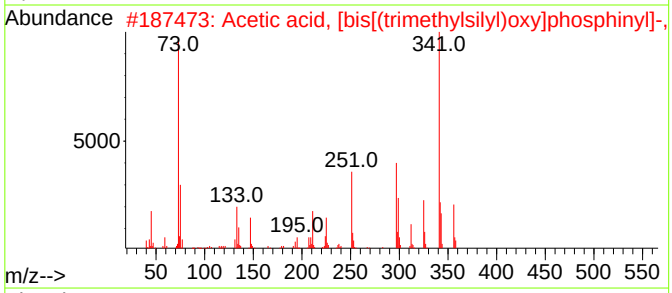
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	91
2	Acetic acid, [bis[(trimethylsily...	356	C11H29O5PSi3	053044-27-2	33
3	Purin-2,6-dione, 1,3,9-trimethyl...	341	C16H15N5O4	1000128-96-2	27
4	1-(3-Spiro-cyclopentane-3,4-dihy...	356	C25H28N2	1000301-10-2	25
5	Silane, dimethyl(dimethyl(dimeth...	476	C24H40O4Si3	1000347-25-6	25

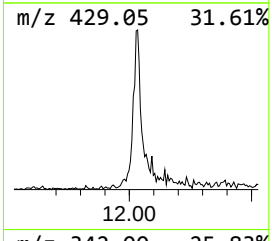


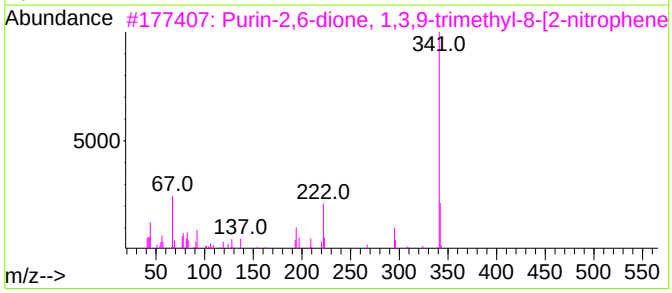


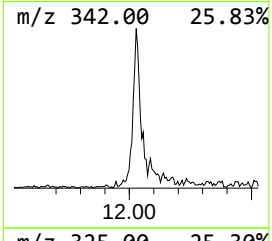


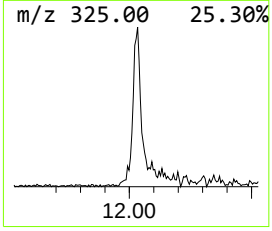












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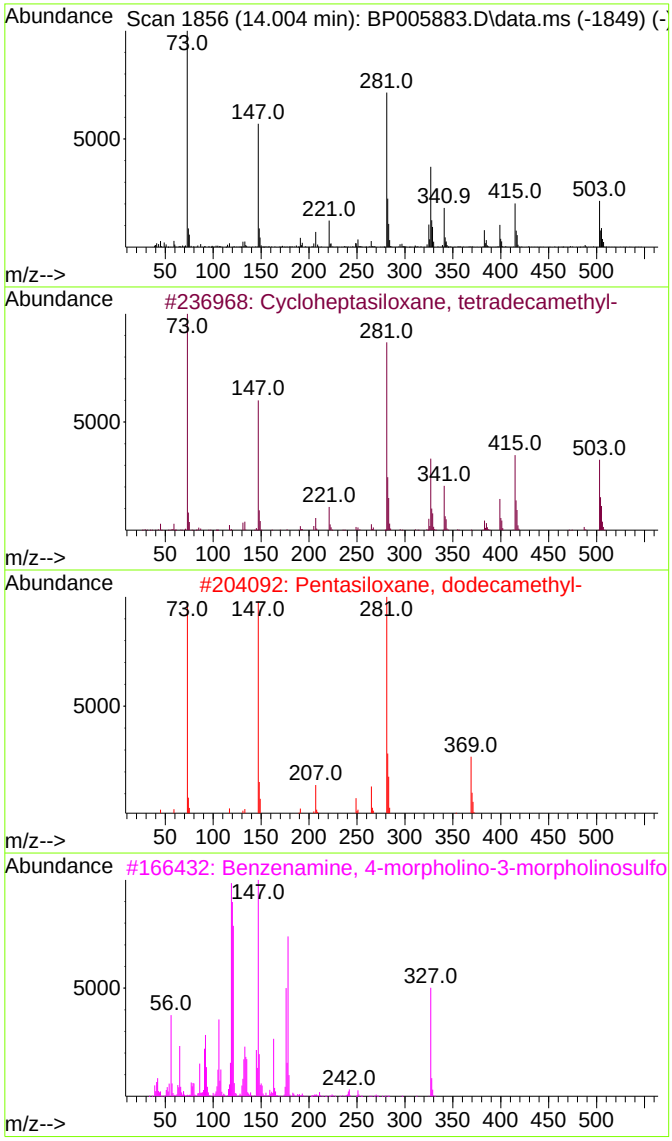
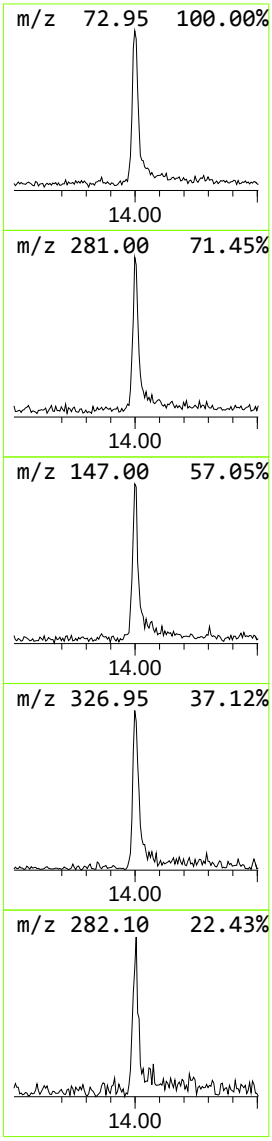
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	2.19 ng	63180	Acenaphthene-d10	14.569

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloheptasiloxane, tetradecamet...	518	C14H42O7Si7	000107-50-6	76
2	Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	32
3	Benzenamine, 4-morpholino-3-morp...	327	C14H21N3O4S	200711-95-1	18
4	2,5-Dihydroxyacetophenone, bis(t...	296	C14H24O3Si2	1000352-83-7	12
5	Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	12





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ALS Vial : 20 Sample Multiplier: 1

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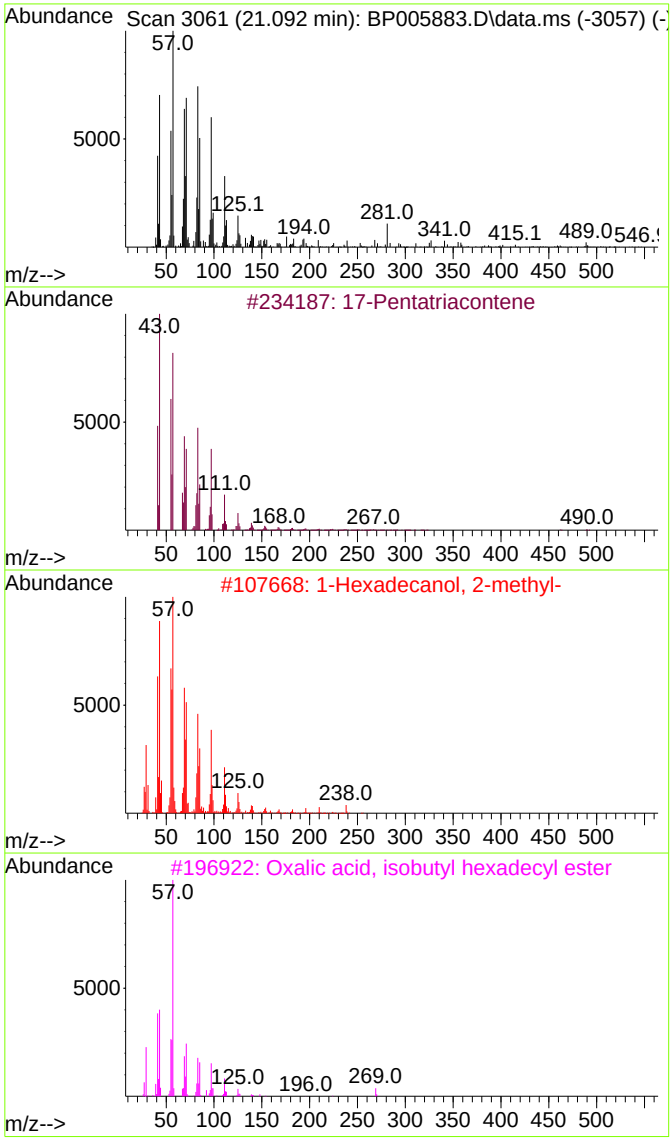
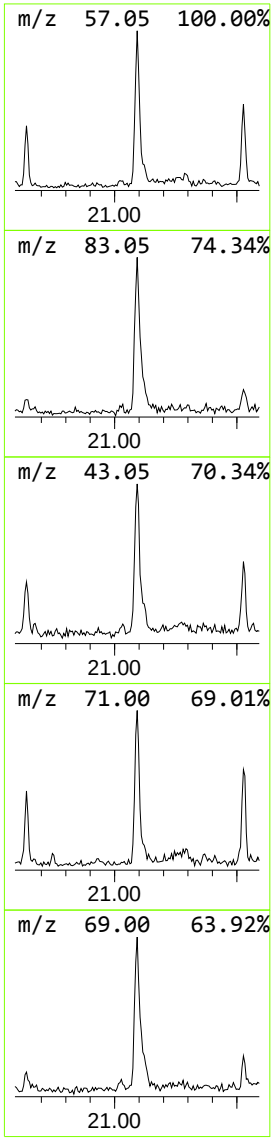
****

Peak Number 8 17-Pentatriacontene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	2.43 ng	120989	Chrysene-d12	21.386

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-Pentatriacontene	491	C35H70	006971-40-0	93
2	1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	90
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	90
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	76
5	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061121\
Data File : BP005883.D
Acq On : 11 Jun 2021 22:03
Operator : CG/JU
Sample : M2625-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 18-B12(198-202)

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Cyclotrisiloxan...	4.587	3.5	ng	61615	1	7.946	355058	20.0
2-Pentanone, 4-...	5.046	2.2	ng	39774	1	7.946	355058	20.0
1,3-Cyclopentan...	7.246	3.1	ng	55508	1	7.946	355058	20.0
2-Cyclohexen-1-...	8.610	4.1	ng	72241	1	7.946	355058	20.0
Ethanol, 1-(2-b...	10.540	3.4	ng	75859	2	10.751	446772	20.0
Cyclohexasiloxa...	12.028	4.4	ng	98254	2	10.751	446772	20.0
Cycloheptasilox...	14.004	2.2	ng	63180	3	14.569	577736	20.0
17-Pentatriacon...	21.092	2.4	ng	120989	5	21.386	996895	20.0