LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134193.D
Acq On : 10 Jul 2023 18:58
Operator : CG\JU
Sample : 03509-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WC-WWS-04

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_F\Methods\8270-BF062623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.205	3	20	24	rVB	6323501	16330544	100.00%	44.435%
2	4.204	357	360	370	rBV	78997	187808	1.15%	0.511%
3	5.481	573	577	599	rBV	2190362	2197558	13.46%	5.979%
4	5.663	603	608	618	rBV2	953851	1133473	6.94%	3.084%
5	5.869	639	643	649	rBV	207258	182788	1.12%	0.497%
6	6.104	678	683	686	rBV	1352770	1194896	7.32%	3.251%
7	6.481	743	747	750	rBV	2317401	2135387	13.08%	5.810%
8	6.840	805	808	814	rBV	814236	758427	4.64%	2.064%
9	6.951	822	827	830	rBV	350923	299502	1.83%	0.815%
10	7.004	831	836	839	rBV	1819496	1746193	10.69%	4.751%
11	7.404	900	904	907	rBV	1613002	1393632	8.53%	3.792%
12	8.122	1022	1026	1034	rBV	1229978	971226	5.95%	2.643%
13	9.198	1205	1209	1212	rBV	2666758	2101835	12.87%	5.719%
14	9.592	1273	1276	1280	rBV	373789	305089	1.87%	0.830%
15	9.881	1321	1325	1328	rBV	1275234	977804	5.99%	2.661%
16	10.669	1456	1459	1469	rBV	1037384	1023090	6.26%	2.784%
17	11.375	1575	1579	1585	rBV	1012023	852904	5.22%	2.321%
18	12.969	1846	1850	1854	rBV	1529348	1371533	8.40%	3.732%
19	13.880	2001	2005	2015	rBV4	118774	197640	1.21%	0.538%
20	14.033	2028	2031	2040	rVB	736688	693051	4.24%	1.886%
21	15.539	2282	2287	2296	rBV	501132	697371	4.27%	1.898%

Sum of corrected areas: 36751751

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134193.D
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Operator : CG\JU
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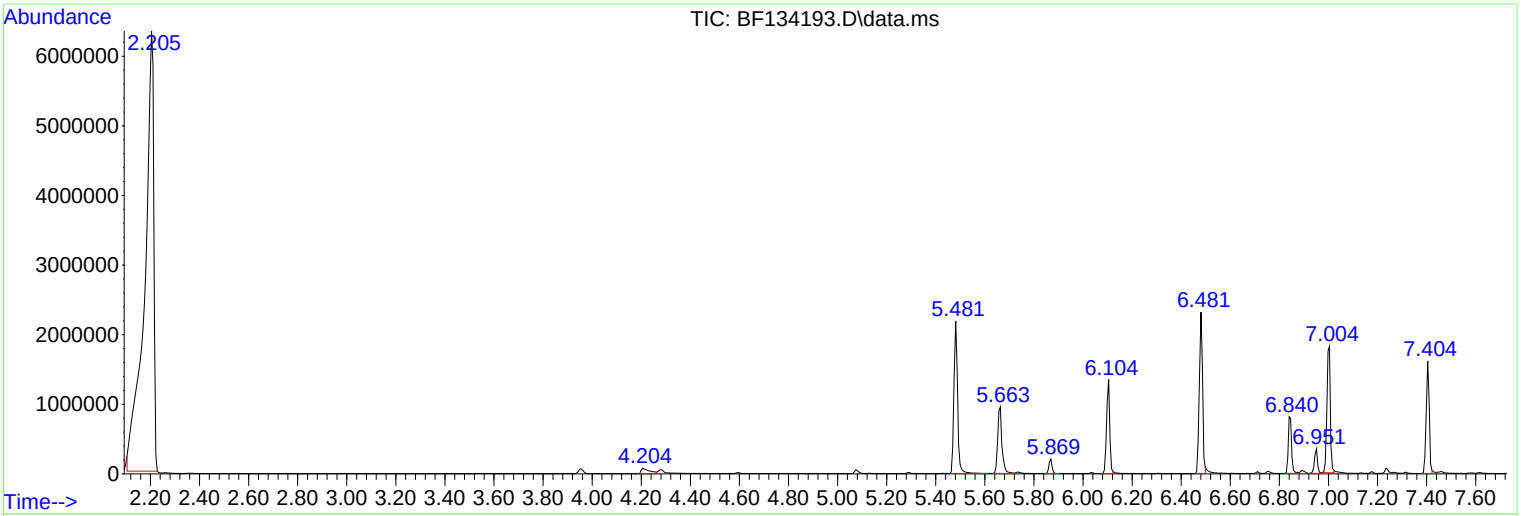
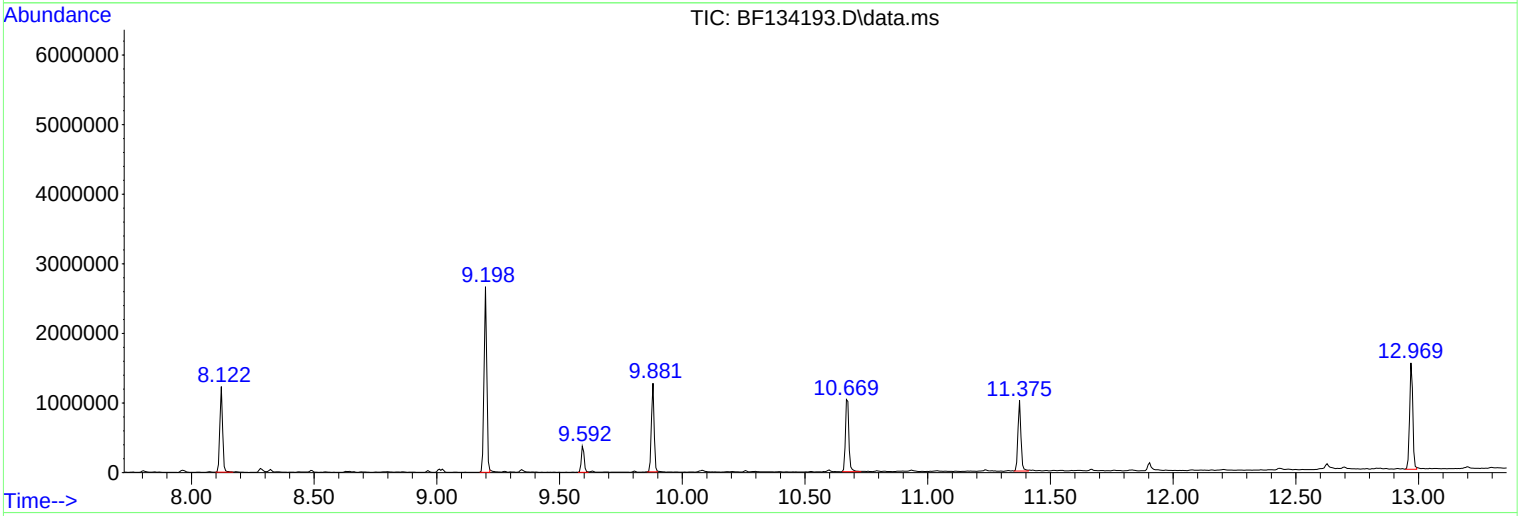
Misc :
ALS Vial : 12 Sample Multiplier: 1

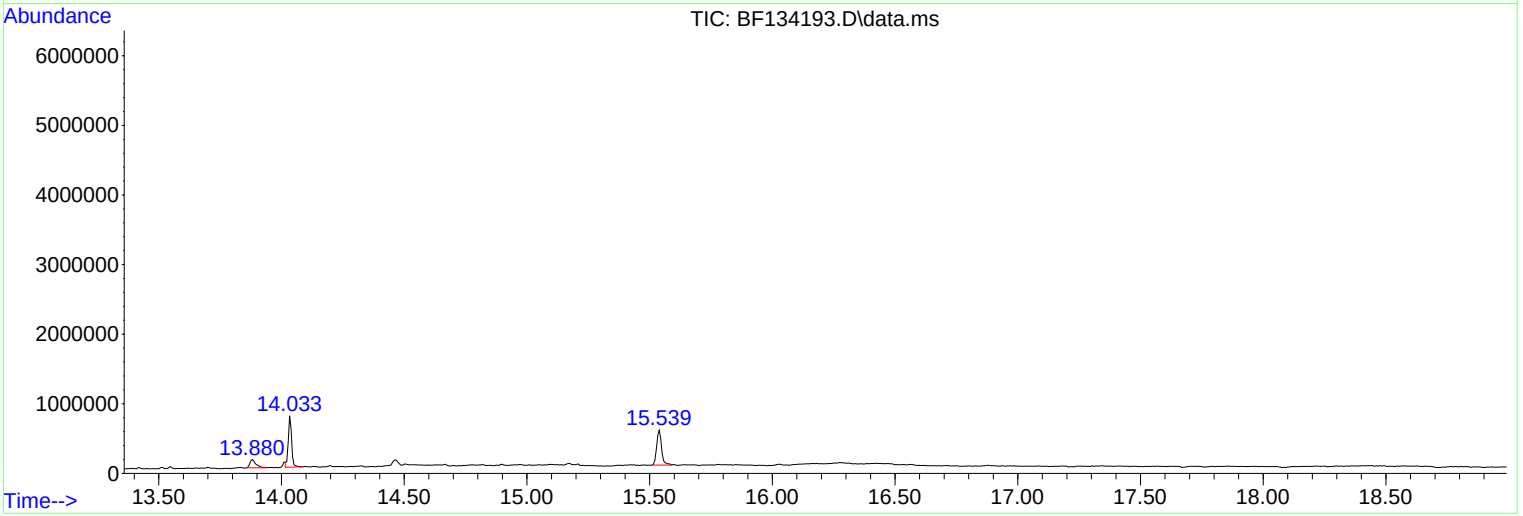
Instrument :
BNA_F
ClientSampleId :
WC-WWS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134193.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

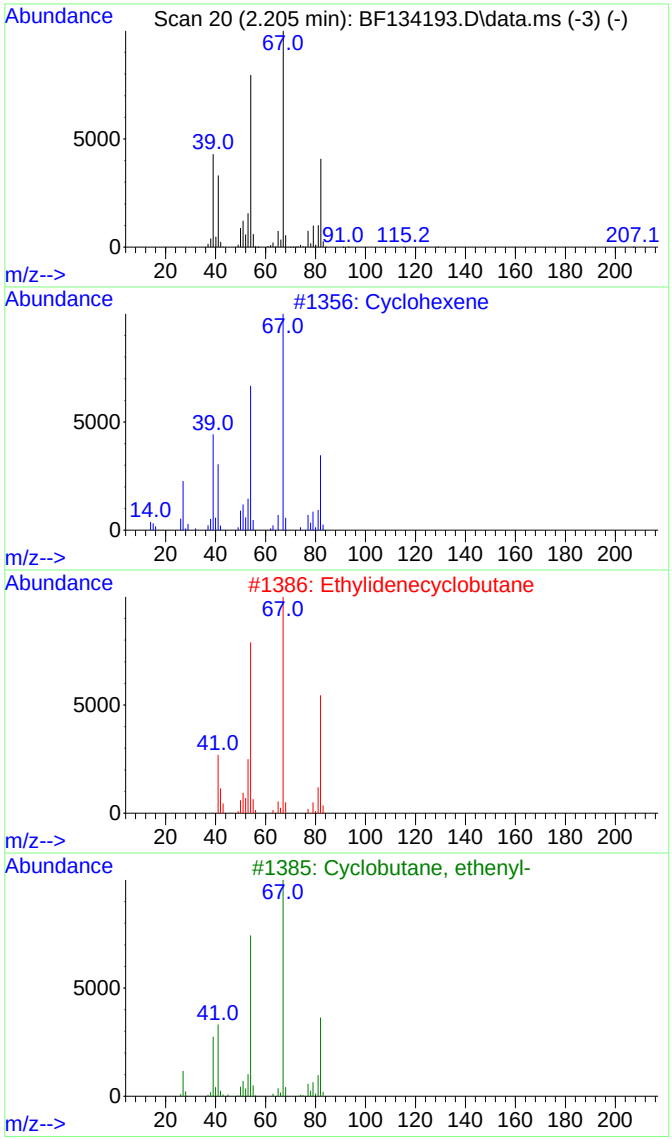
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

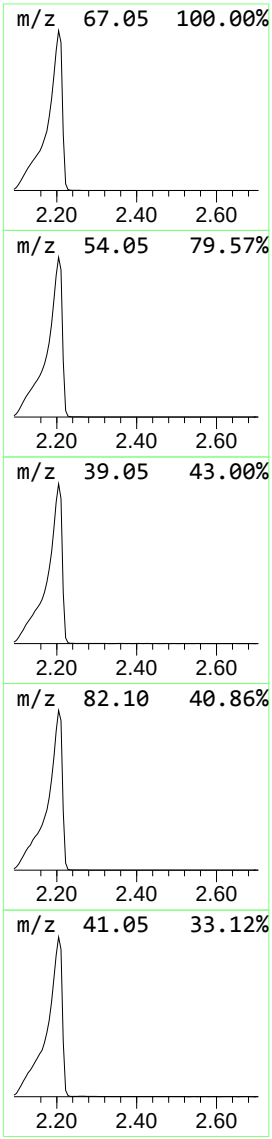
****

Peak Number 1 Cyclohexene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.205	430.64 ng	16330500	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene	82	C6H10	000110-83-8	97
2	Ethylidenecyclobutane	82	C6H10	001528-21-8	91
3	Cyclobutane, ethenyl-	82	C6H10	002597-49-1	87
4	C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	42
5	2,4-Hexadiene	82	C6H10	000592-46-1	42





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Data File : BF134193.D
Acq On : 10 Jul 2023 18:58
Operator : CG\JU
Sample : 03509-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-WWS-04

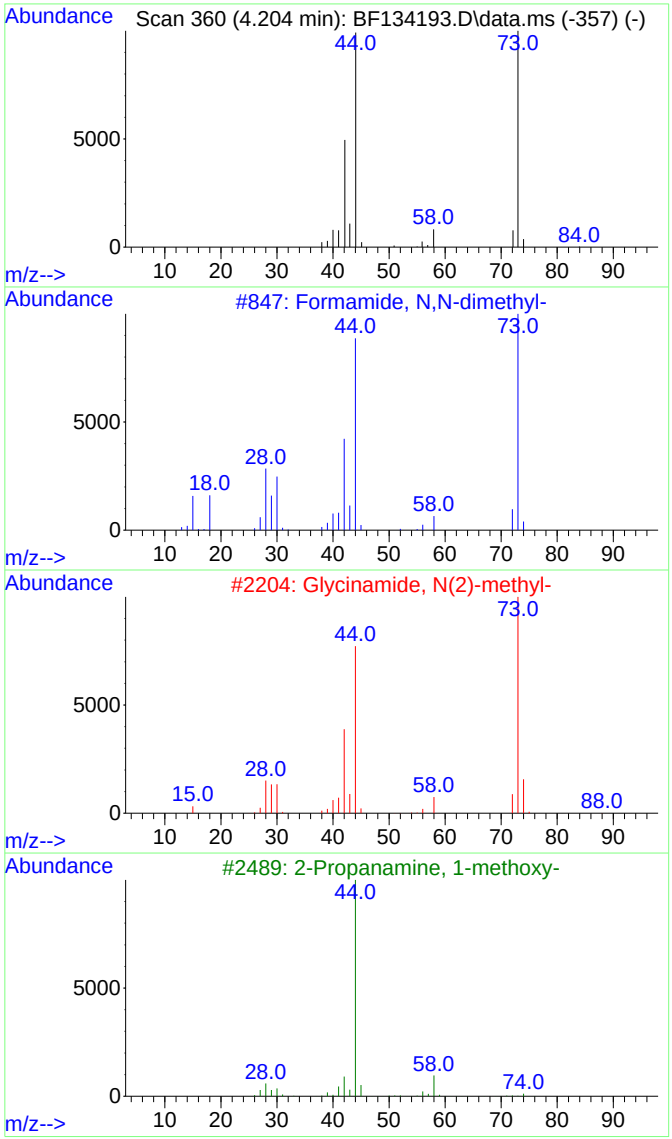
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

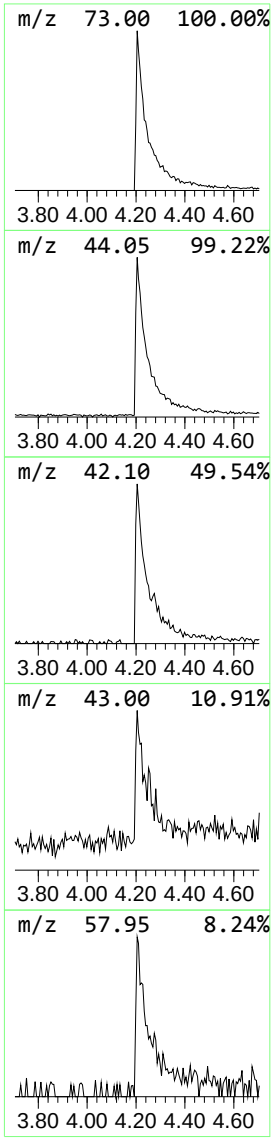
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Formamide, N,N-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.204	4.95 ng	187808	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formamide, N,N-dimethyl-	73	C3H7NO	000068-12-2	91
2	Glycinamide, N(2)-methyl-	88	C3H8N2O	1000452-55-9	83
3	2-Propanamine, 1-methoxy-	89	C4H11NO	037143-54-7	9
4	Acetonitrile-d3	44	C2D3N	002206-26-0	7
5	N-Ethylformamide	73	C3H7NO	000627-45-2	5





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134193.D
Acq On : 10 Jul 2023 18:58
Operator : CG\JU
Sample : 03509-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-WWS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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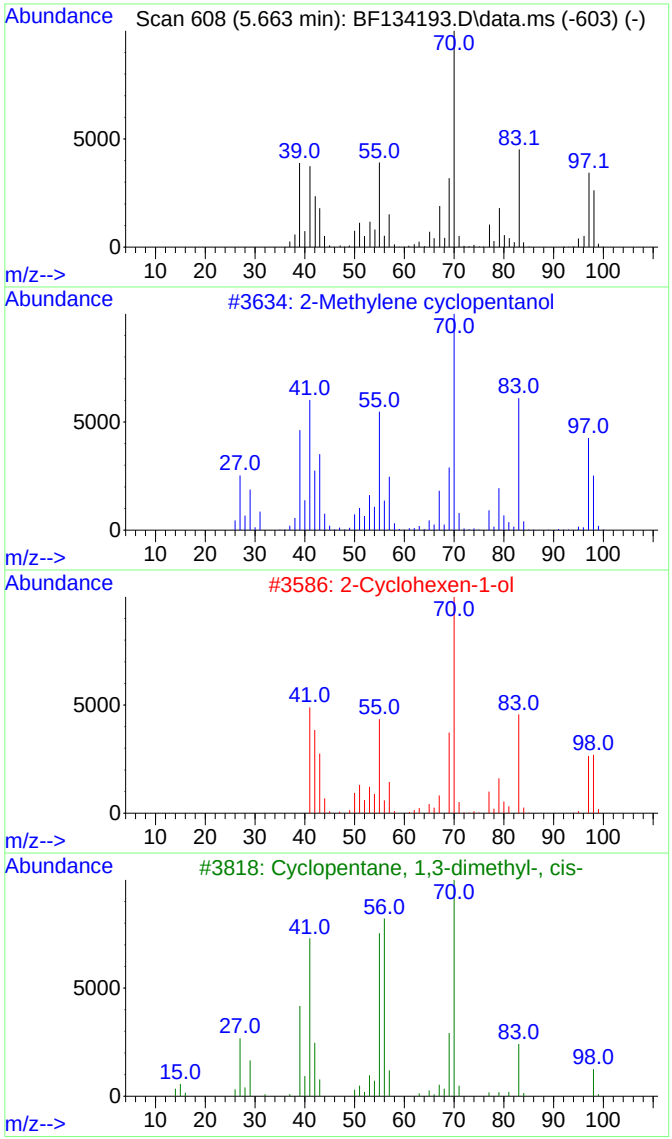
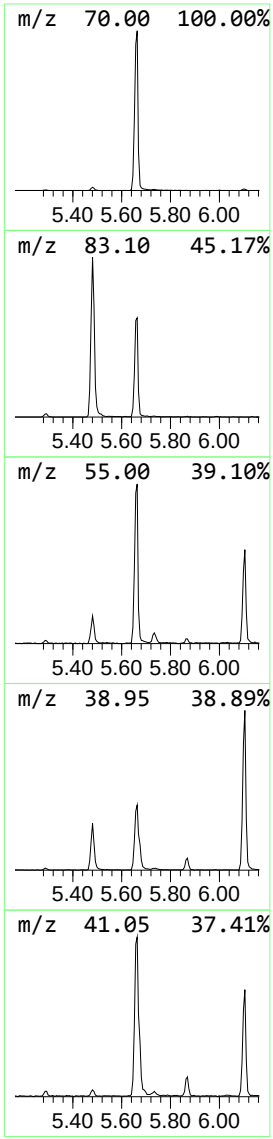
Peak Number 3 2-Methylene cyclopentanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.663	29.89 ng	1133470	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	94
2	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	87
3	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	50
4	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	38
5	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134193.D
Acq On : 10 Jul 2023 18:58
Operator : CG\JU
Sample : 03509-16
Misc :
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Instrument :
BNA_F
ClientSampleId :
WC-WWS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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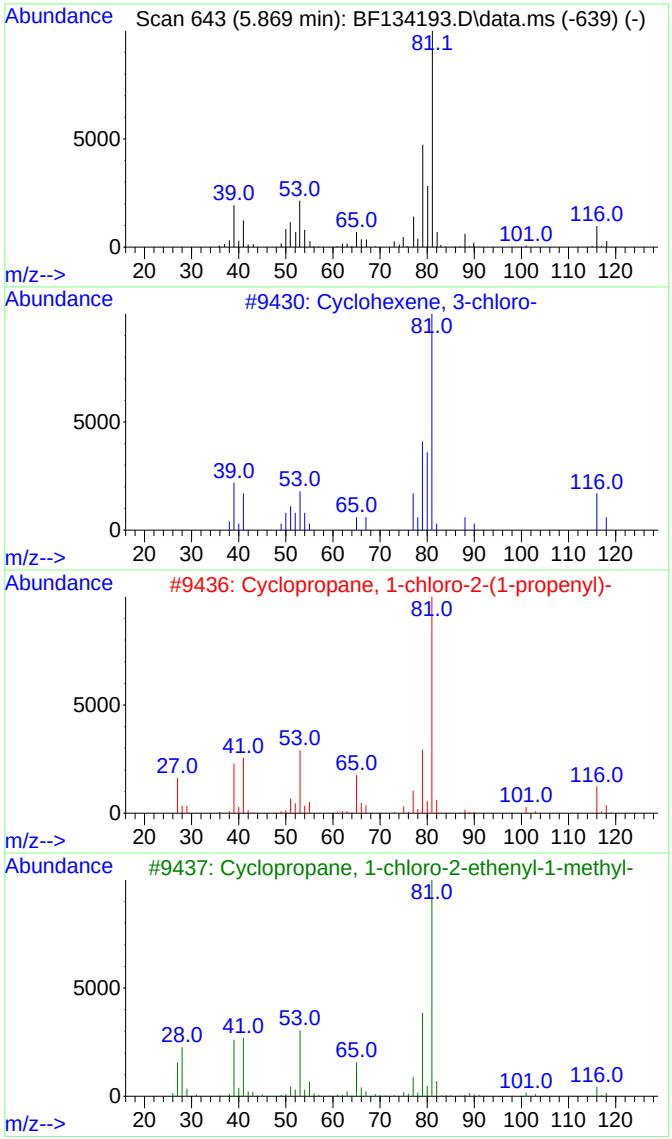
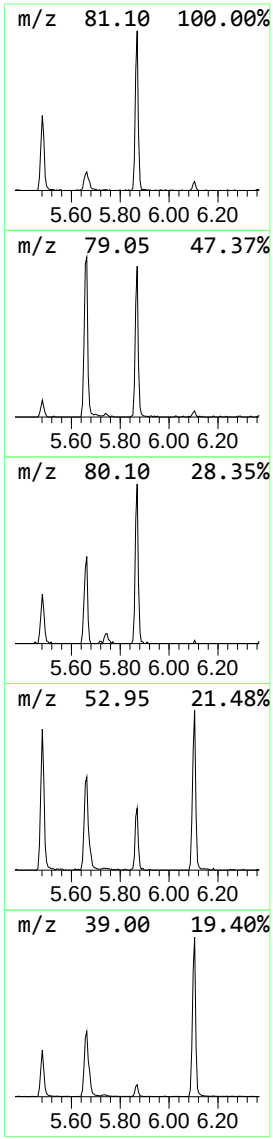
Peak Number 4 Cyclohexene, 3-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.869	4.82 ng	182788	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 3-chloro-	116	C6H9Cl	002441-97-6	83
2	Cyclopropane, 1-chloro-2-(1-prop...	116	C6H9Cl	074752-94-6	64
3	Cyclopropane, 1-chloro-2-ethenyl...	116	C6H9Cl	062337-93-3	64
4	Cyclohexene, 1-chloro-	116	C6H9Cl	000930-66-5	59
5	Cyclohexene, 3-bromo-	160	C6H9Br	001521-51-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134193.D
Acq On : 10 Jul 2023 18:58
Operator : CG\JU
Sample : 03509-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-WWS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

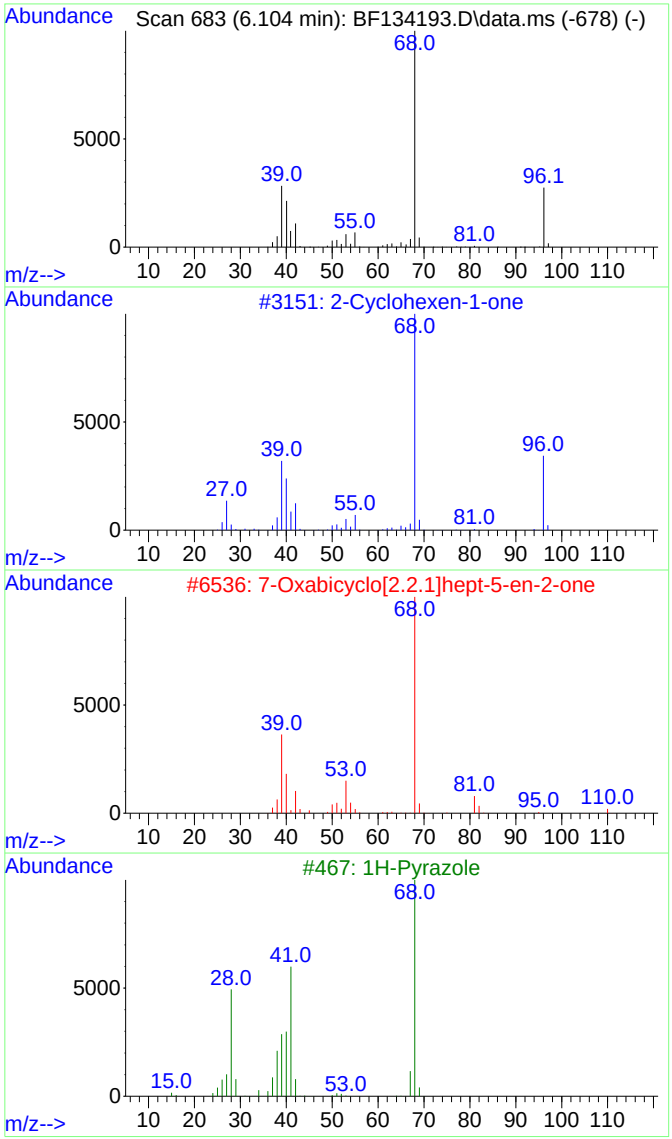
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

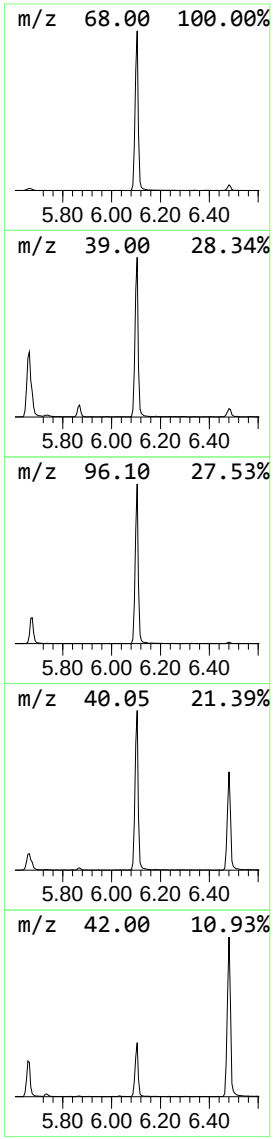
****

Peak Number 5 2-Cyclohexen-1-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.104	31.51 ng	1194900	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	91
2	7-Oxabicyclo[2.2.1]hept-5-en-2-one	110	C6H6O2	095530-78-2	42
3	1H-Pyrazole	68	C3H4N2	000288-13-1	36
4	3-Butyn-2-amine, 2-methyl-	83	C5H9N	002978-58-7	25
5	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	17





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Instrument :
BNA_F
ClientSampleId :
WC-WWS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

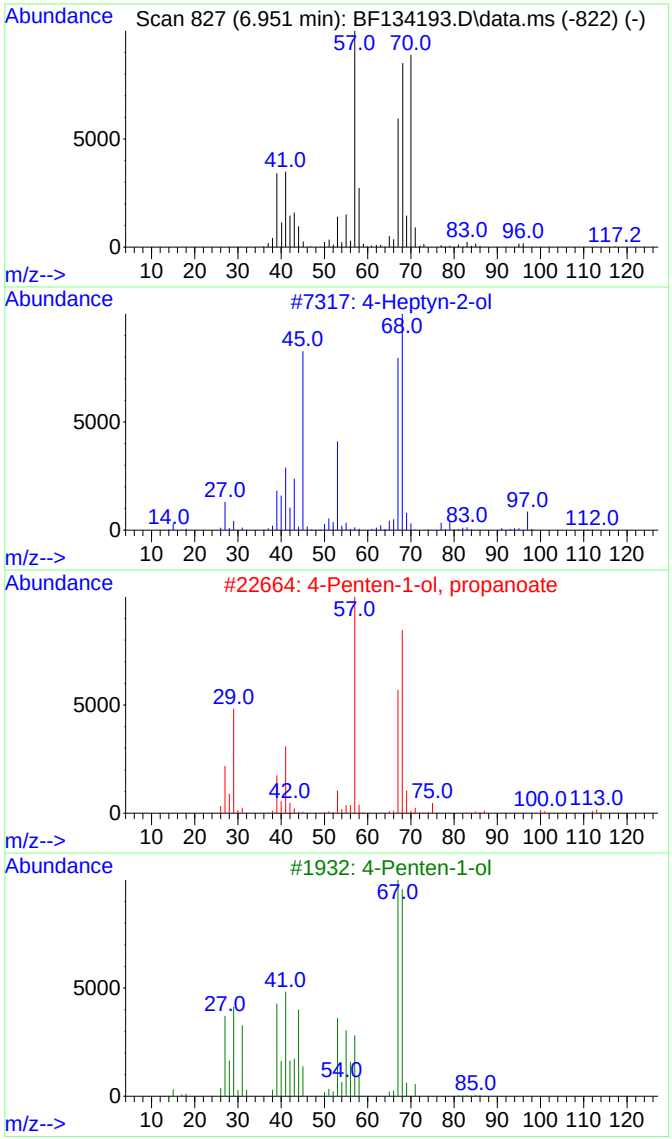
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

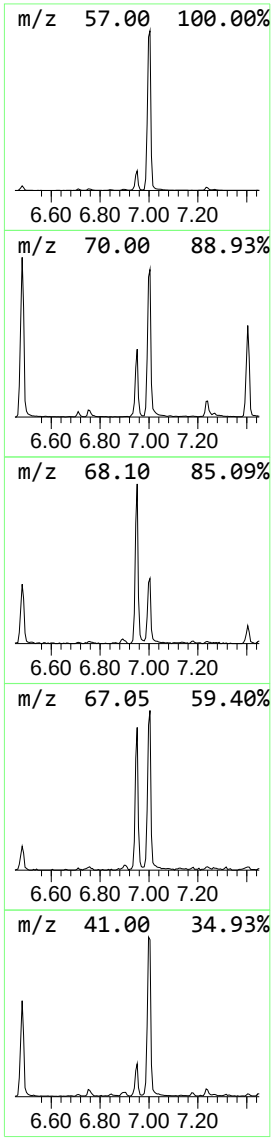
****

Peak Number 6 unknown6.951 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.951	7.90 ng	299502	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptyn-2-ol	112	C7H12O	019781-81-8	38
2	4-Penten-1-ol, propanoate	142	C8H14O2	030563-30-5	37
3	4-Penten-1-ol	86	C5H10O	000821-09-0	35
4	2,5-Dihydro-3-methyl-thiophene 1...	132	C5H8O2S	001193-10-8	35
5	1,4-Pentadiene	68	C5H8	000591-93-5	16





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Sample : 03509-16
Misc :
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BNA_F
ClientSampleId :
WC-WWS-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

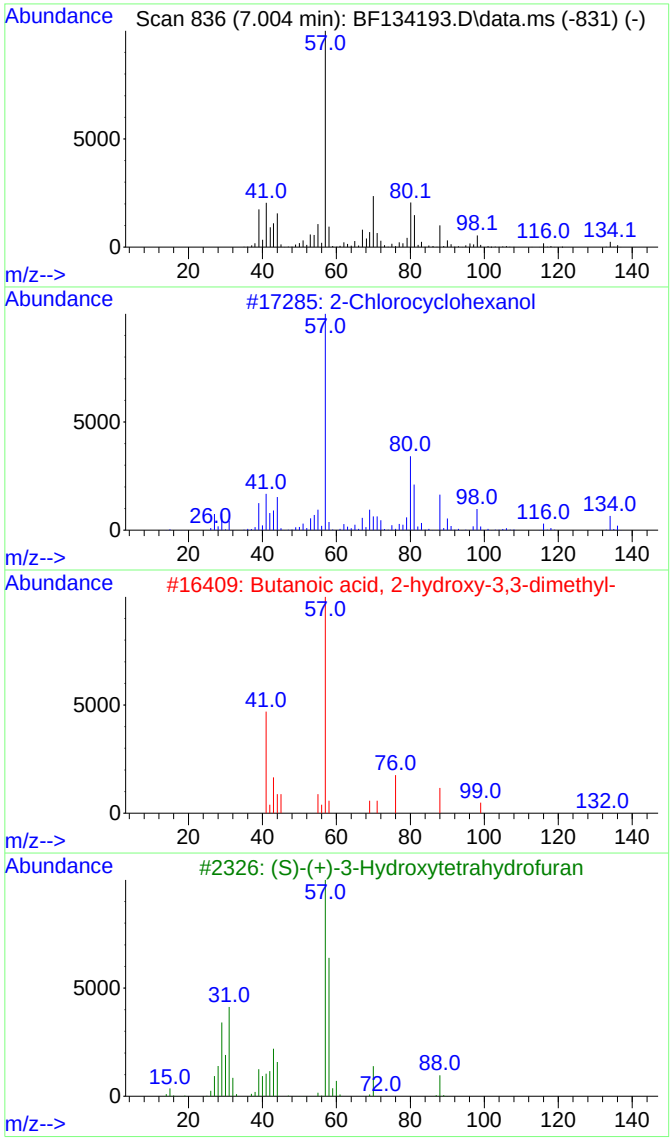
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

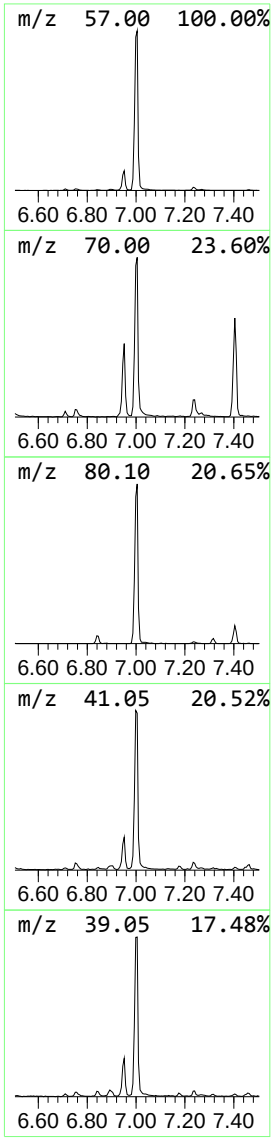
****

Peak Number 7 2-Chlorocyclohexanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.004	46.05 ng	1746190	1,4-Dichlorobenzene-d4	6.845

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	92
2	Butanoic acid, 2-hydroxy-3,3-dim...	132	C6H12O3	004026-20-4	25
3	(S)-(+)-3-Hydroxytetrahydrofuran	88	C4H8O2	086087-23-2	23
4	Cyclohexanol, 2-chloro-, trans-	134	C6H11ClO	006628-80-4	22
5	Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	17





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TIC Library : C:\Database\NIST20.L
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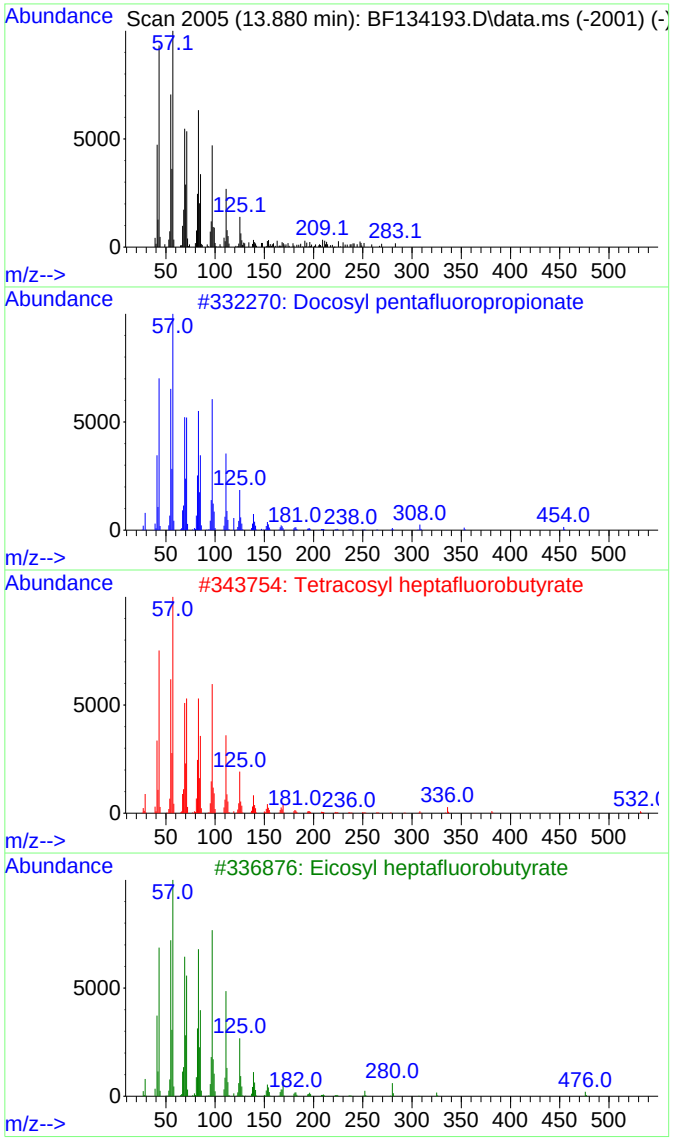
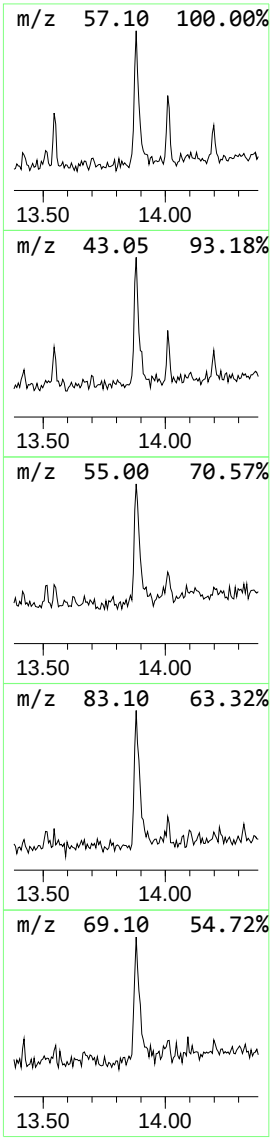
Peak Number 8 Docosyl pentafluoropropionate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	5.70 ng	197640	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
2	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
3	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
Data File : BF134193.D
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BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF062623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
Cyclohexene	2.205	430.6	ng	16330500	1	6.845	758427	20.0
Formamide, N,N-...	4.204	5.0	ng	187808	1	6.845	758427	20.0
2-Methylene cyc...	5.663	29.9	ng	1133470	1	6.845	758427	20.0
Cyclohexene, 3-...	5.869	4.8	ng	182788	1	6.845	758427	20.0
2-Cyclohexen-1-one	6.104	31.5	ng	1194900	1	6.845	758427	20.0
unknown6.951	6.951	7.9	ng	299502	1	6.845	758427	20.0
2-Chlorocyclohe...	7.004	46.0	ng	1746190	1	6.845	758427	20.0
Docosyl pentafl...	13.880	5.7	ng	197640	5	14.033	693051	20.0