LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051121\
Data File : BP005496.D
Acq On : 11 May 2021 19:06
Operator : CG/JU
Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DRUM-B-C-E

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-BP050521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005496.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.793	115	120	125	rVB8	3815	6233	1.28%	0.212%
2	4.258	194	199	202	rBV5	4305	5907	1.21%	0.201%
3	4.828	291	296	302	rBV2	7862	10509	2.16%	0.358%
4	7.152	687	691	697	rVB5	5551	8609	1.77%	0.293%
5	7.216	697	702	708	rBV6	3624	6211	1.27%	0.211%
6	7.693	775	783	790	rBV	50062	80452	16.51%	2.739%
7	7.763	790	795	805	rVV6	11220	27689	5.68%	0.943%
8	7.875	805	814	821	rVB7	8208	25794	5.29%	0.878%
9	7.993	828	834	840	rBV8	3674	7377	1.51%	0.251%
10	8.058	840	845	852	rVB2	15890	25881	5.31%	0.881%
11	8.863	975	982	996	rVB	63402	109735	22.52%	3.736%
12	9.169	1028	1034	1041	rBV9	2861	6301	1.29%	0.215%
13	10.281	1216	1223	1239	rBV	121380	191084	39.21%	6.506%
14	10.487	1252	1258	1262	rBV	49520	85500	17.54%	2.911%
15	10.534	1262	1266	1276	rVB	88861	142215	29.18%	4.842%
16	10.657	1281	1287	1294	rBV	4431	8314	1.71%	0.283%
17	10.904	1324	1329	1336	rBV2	5677	9173	1.88%	0.312%
18	12.004	1511	1516	1521	rBV3	3380	6052	1.24%	0.206%
19	12.157	1534	1542	1549	rBV2	19179	31431	6.45%	1.070%
20	12.293	1559	1565	1570	rBV4	6376	10479	2.15%	0.357%
21	12.375	1570	1579	1587	rVB2	14400	25273	5.19%	0.861%
22	12.746	1631	1642	1651	rBV3	19952	36668	7.52%	1.249%
23	12.963	1671	1679	1688	rBV	189969	277628	56.97%	9.453%
24	13.516	1766	1773	1780	rVB9	2161	5544	1.14%	0.189%
25	13.593	1780	1786	1792	rVB2	4563	7608	1.56%	0.259%
26	13.657	1792	1797	1803	rBV5	7175	14051	2.88%	0.478%
27	13.716	1803	1807	1816	rVB8	3519	6495	1.33%	0.221%
28	13.810	1816	1823	1829	rBV2	7810	12452	2.55%	0.424%
29	13.881	1829	1835	1842	rBV7	6070	11822	2.43%	0.403%
30	14.063	1862	1866	1871	rVB3	4606	6029	1.24%	0.205%
31	14.340	1905	1913	1919	rBV	87428	120363	24.70%	4.098%
32	14.404	1919	1924	1932	rVB	23408	34484	7.08%	1.174%
33	14.745	1977	1982	1988	rBV	9942	14749	3.03%	0.502%
34	15.392	2086	2092	2103	rVB	10640	17292	3.55%	0.589%
35	16.757	2320	2324	2329	rVB2	5274	7117	1.46%	0.242%
36	16.910	2345	2350	2362	rVB	121512	158040	32.43%	5.381%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051121\
Data File : BP005496.D
Acq On : 11 May 2021 19:06
Operator : CG/JU
Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DRUM-B-C-E

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-BP050521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.092	2372	2381	2385	rBV	118055	168335	34.54%	5.732%
38	17.134	2385	2388	2396	rVB	25070	36958	7.58%	1.258%
39	17.298	2411	2416	2426	rVB6	5099	9004	1.85%	0.307%
40	17.516	2447	2453	2457	rBV2	5217	7979	1.64%	0.272%
41	17.992	2531	2534	2537	rBV5	4239	4970	1.02%	0.169%
42	18.163	2555	2563	2566	rBV8	2692	5229	1.07%	0.178%
43	18.710	2652	2656	2662	rBV6	6083	9744	2.00%	0.332%
44	18.881	2679	2685	2690	rBV9	4468	7331	1.50%	0.250%
45	19.116	2719	2725	2733	rBV3	5980	11006	2.26%	0.375%
46	19.239	2740	2746	2749	rBV7	3063	5766	1.18%	0.196%
47	19.663	2812	2818	2824	rBV	416729	487365	100.00%	16.595%
48	20.598	2973	2977	2982	rBV7	8080	13076	2.68%	0.445%
49	20.898	3025	3028	3035	rBV5	17985	26555	5.45%	0.904%
50	21.186	3072	3077	3087	rBV	209352	271443	55.70%	9.243%
51	23.492	3462	3469	3477	rBV2	164885	311519	63.92%	10.607%

Sum of corrected areas: 2936841

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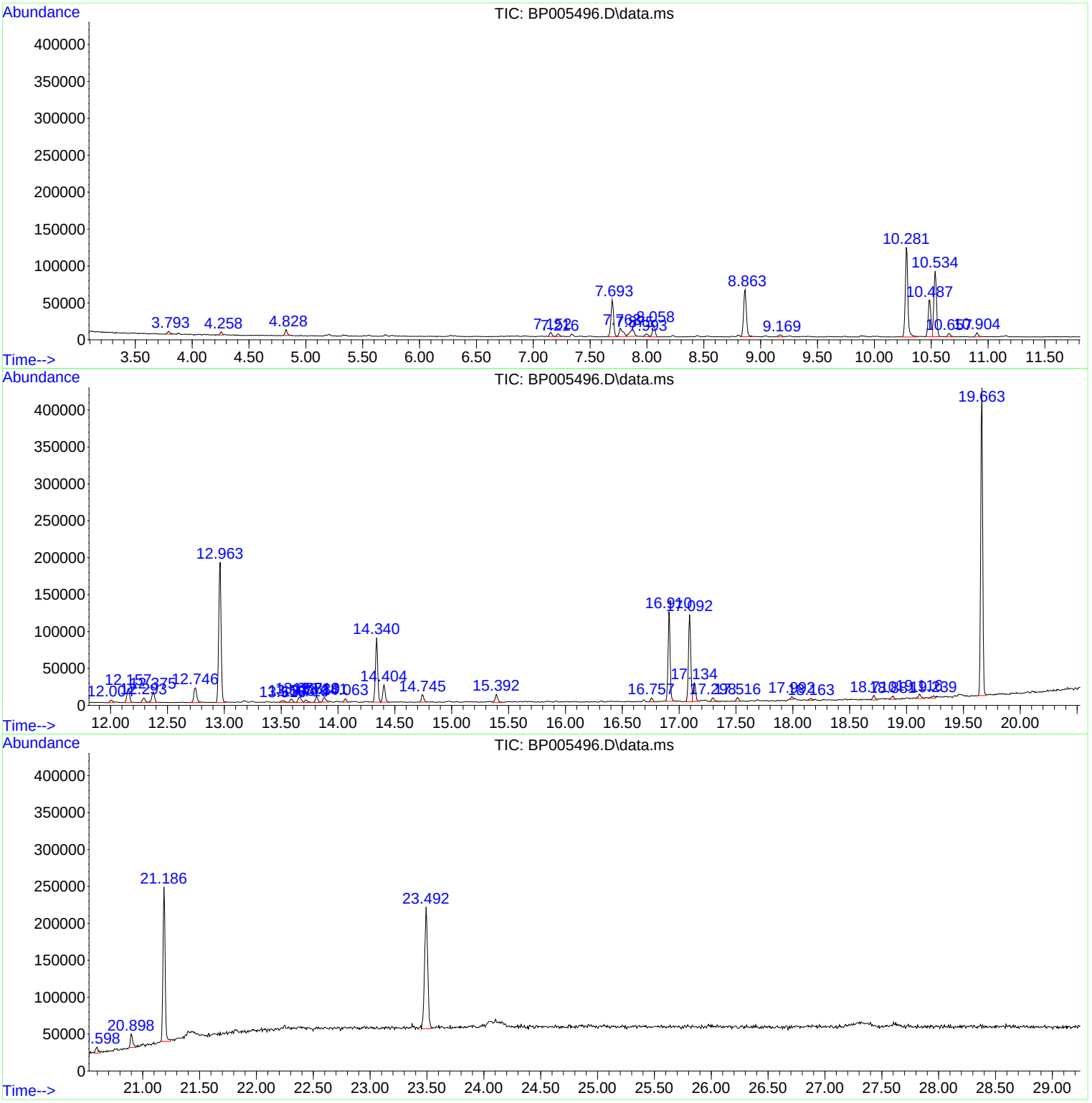
Instrument :
BNA_P
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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\BP051121\
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Operator : CG/JU
Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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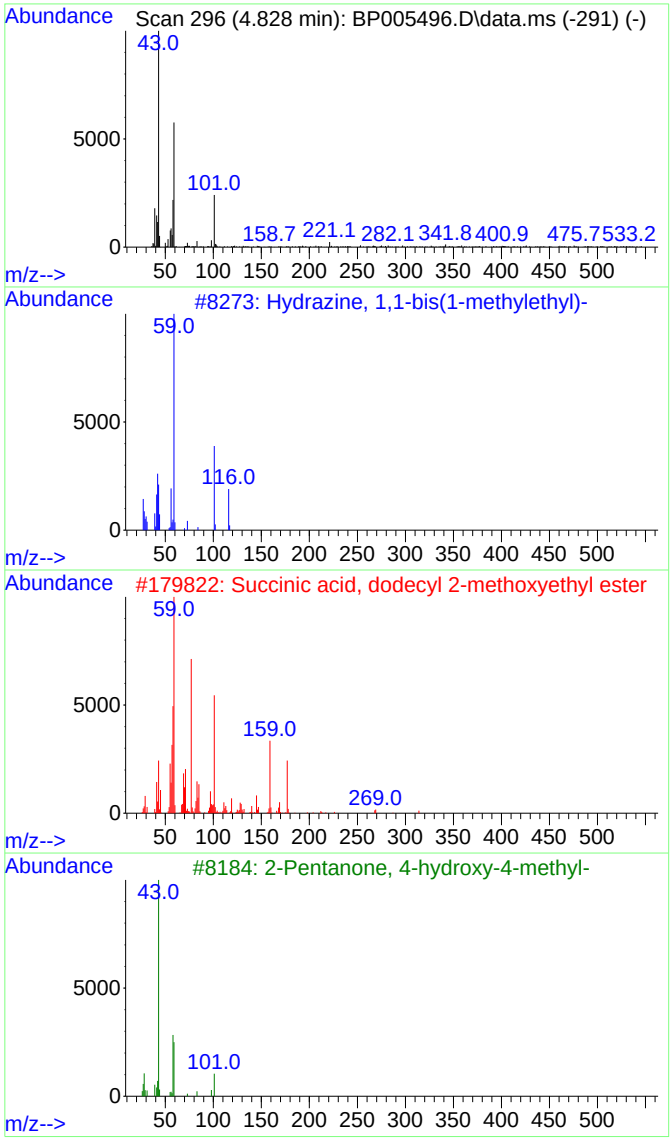
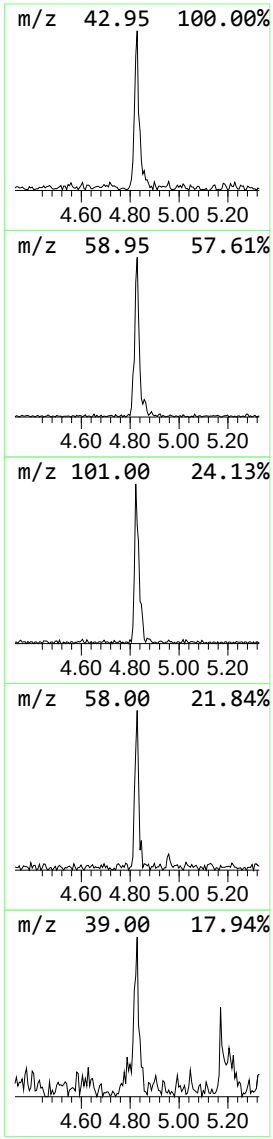
Peak Number 1 unknown4.828 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.828	2.61 ng	10509	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	45
2	Succinic acid, dodecyl 2-methoxy...	344	C19H36O5	1000325-81-2	38
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
4	Propanedioic acid, bromo-, dimet...	210	C5H7BrO4	000868-26-8	38
5	Butanoic acid, 4-iodo-, methyl e...	228	C5H9IO2	014273-85-9	32





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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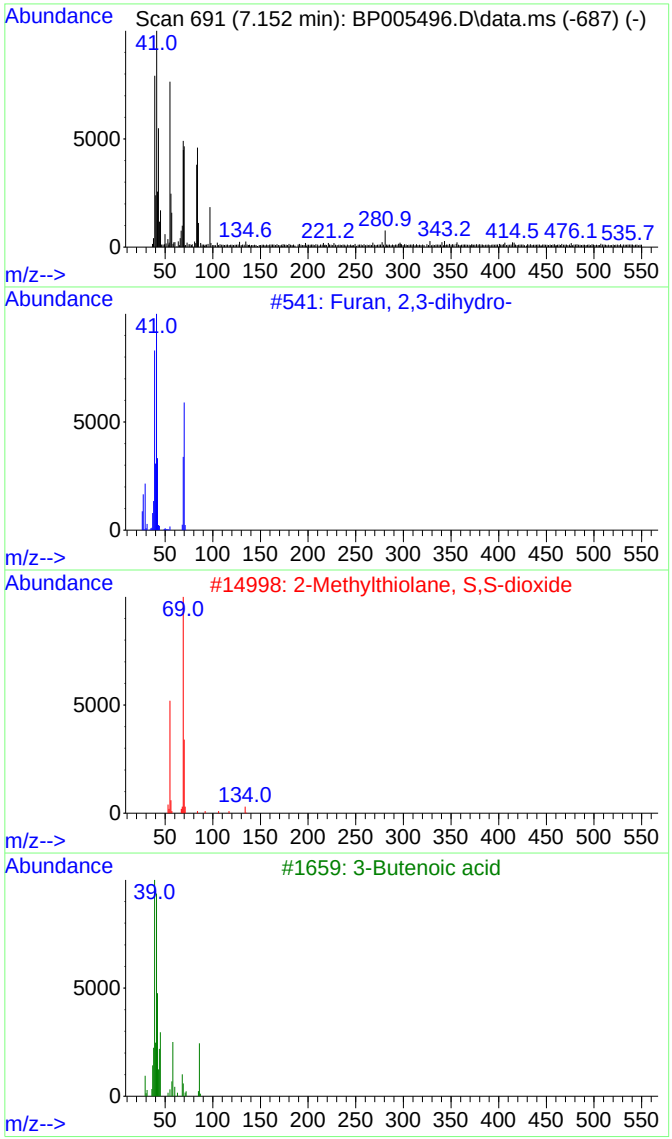
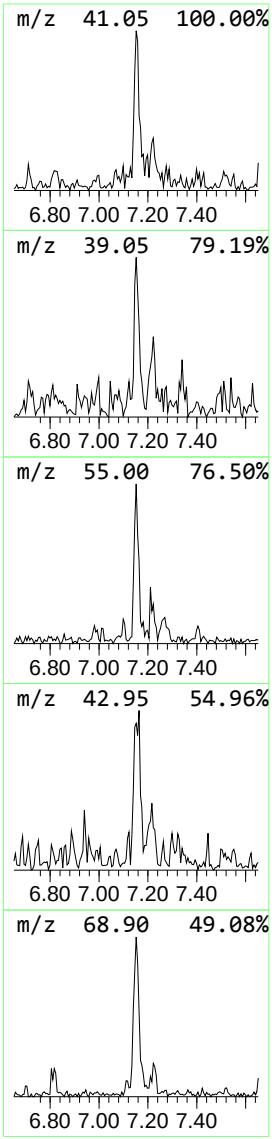
Peak Number 2 Furan, 2,3-dihydro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.152	2.14 ng	8609	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	53
2	2-Methylthiolane, S,S-dioxide	134	C5H10O2S	001003-46-9	43
3	3-Butenoic acid	86	C4H6O2	000625-38-7	42
4	Pentane, 3-methylene-	84	C6H12	000760-21-4	11
5	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051121\
Data File : BP005496.D
Acq On : 11 May 2021 19:06
Operator : CG/JU
Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

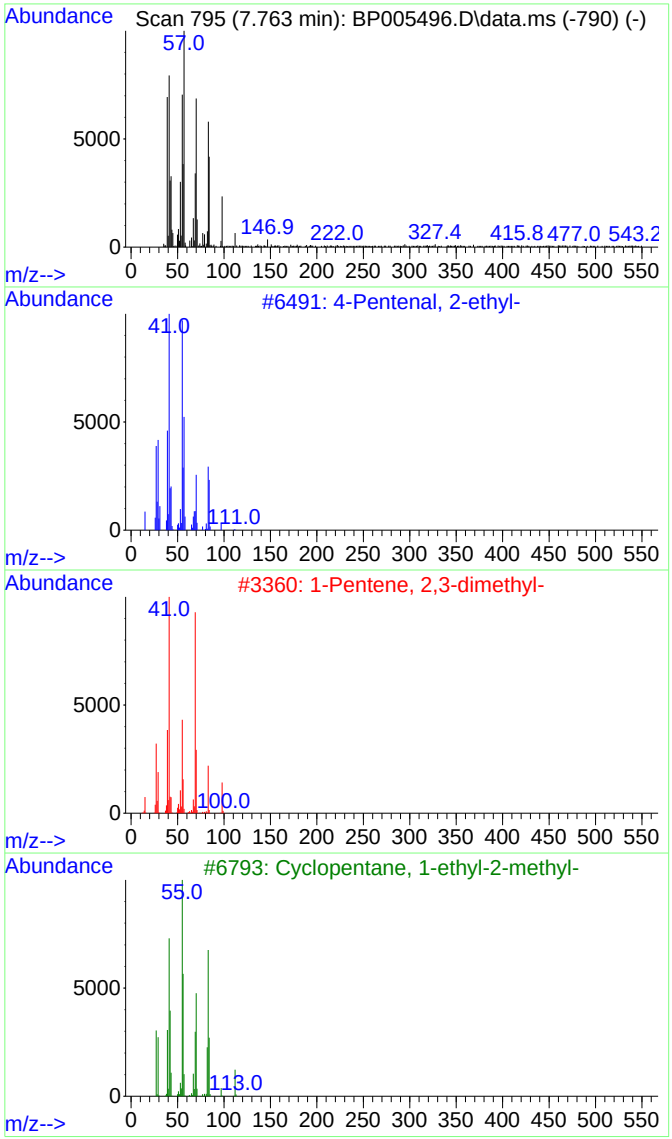
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

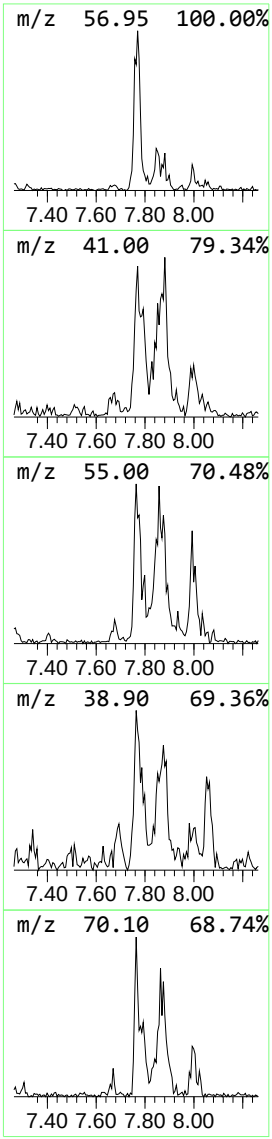
****

Peak Number 3 4-Pentenal, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.763	6.88 ng	27689	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Pentenal, 2-ethyl-	112	C7H12O	005204-80-8	53
2	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	47
3	Cyclopentane, 1-ethyl-2-methyl-	112	C8H16	003726-46-3	47
4	1,2-Cyclohexanedione	112	C6H8O2	000765-87-7	46
5	Cyclopentane, 1-ethyl-3-methyl-	112	C8H16	003726-47-4	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051121\
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Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

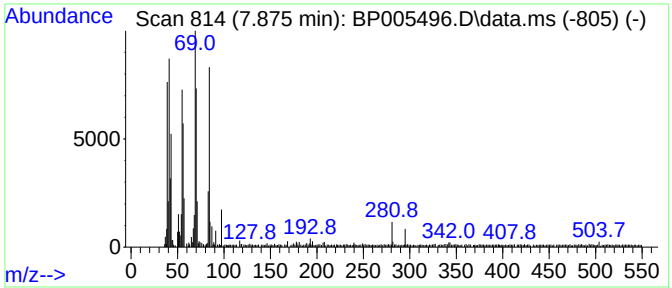
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

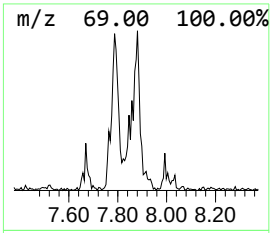
****

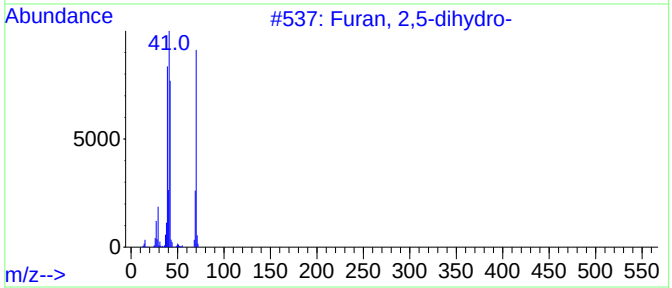
Peak Number 4 Furan, 2,5-dihydro- Concentration Rank 5

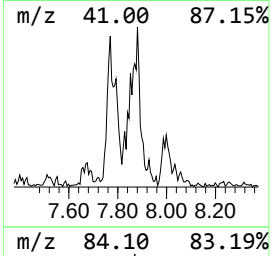
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.875	6.41 ng	25794	1,4-Dichlorobenzene-d4	7.693

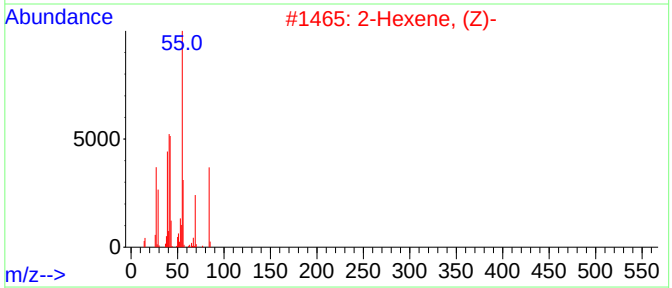
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	58
2	2-Hexene, (Z)-	84	C6H12	007688-21-3	53
3	Methacrolein	70	C4H6O	000078-85-3	53
4	Furan, 2,5-dihydro-3-methyl-	84	C5H8O	001708-31-2	53
5	2-Propenoic acid, 2-methyl-, 2-p...	124	C7H8O2	013861-22-8	53

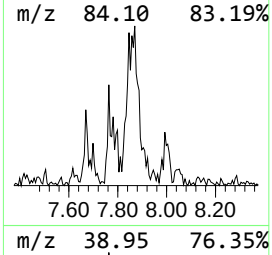


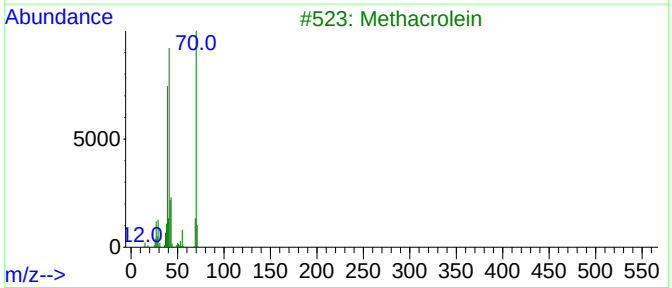


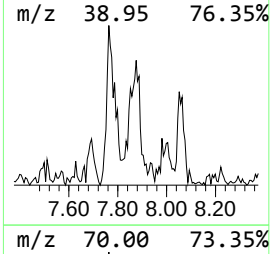


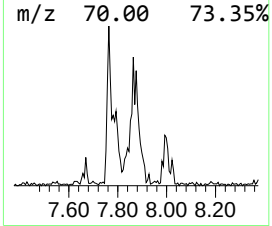












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Instrument :
BNA_P
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

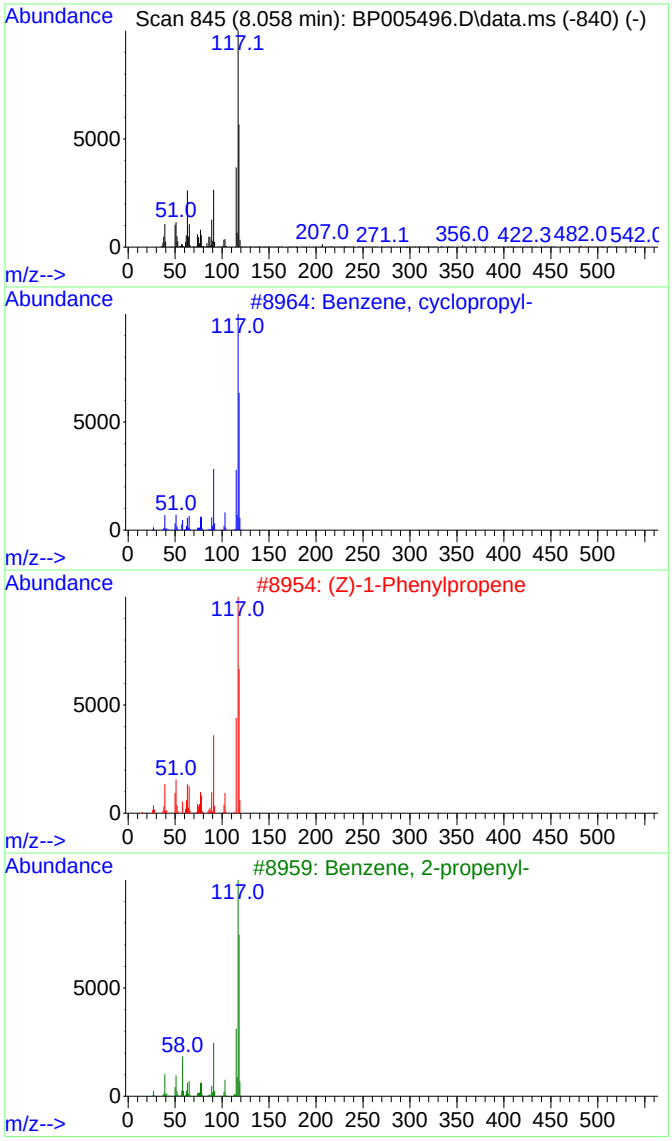
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

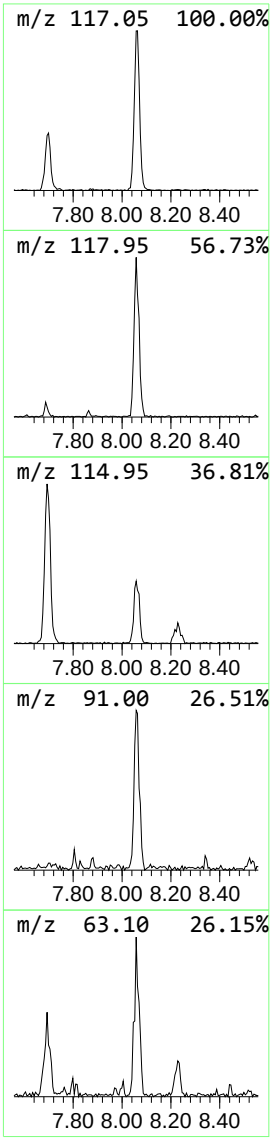
****

Peak Number 5 Benzene, cyclopropyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.058	6.43 ng	25881	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
2	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	83
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	83
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	83





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BNA_P
ClientSampleId :
DRUM-B-C-E

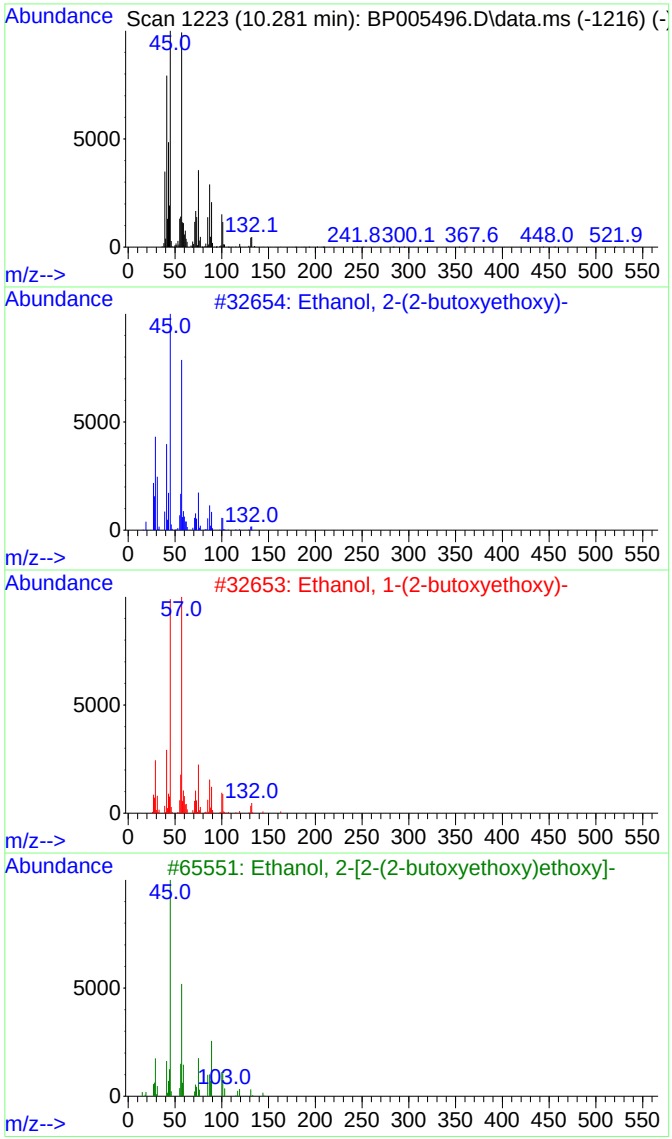
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

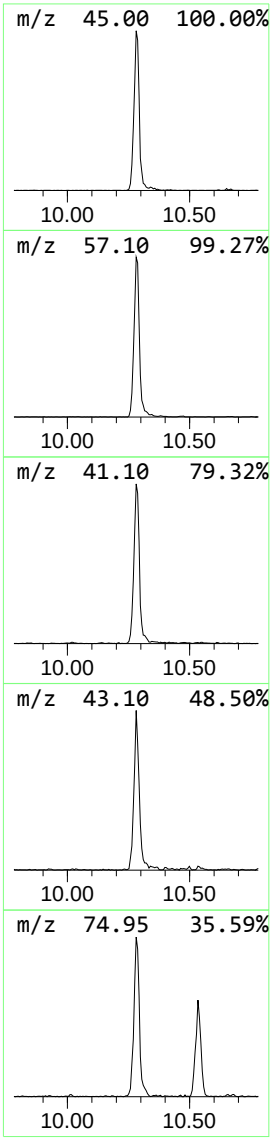
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.281	44.70 ng	191084	Naphthalene-d8	10.487

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
3	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	64
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	47
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	47





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Instrument : BNA_P
ClientSampleId : DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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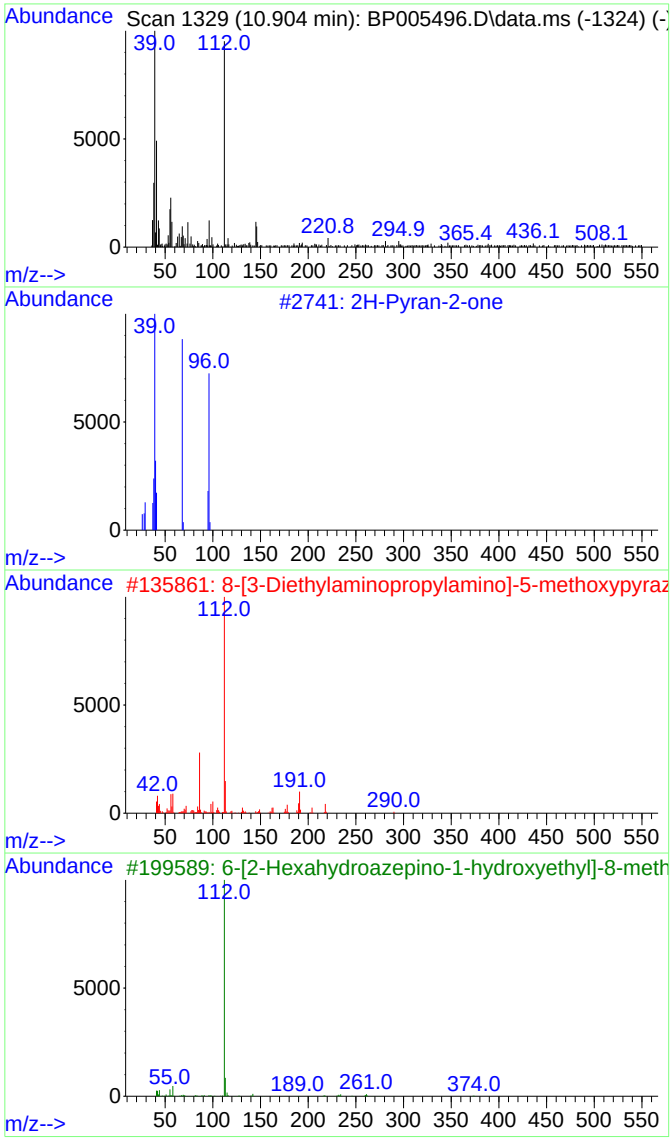
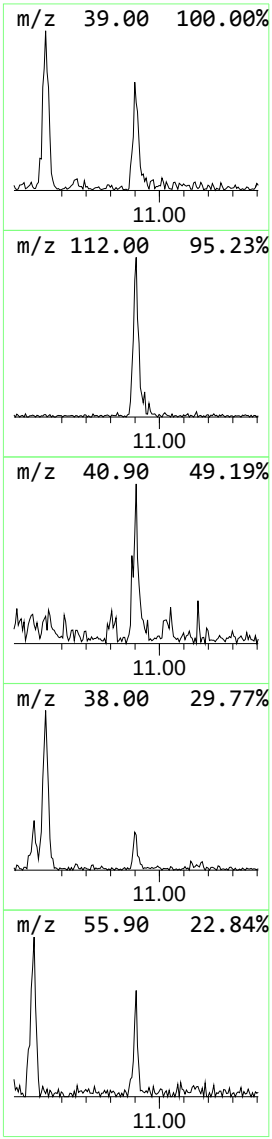
Peak Number 7 2H-Pyran-2-one Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.905	2.15 ng	9173	Naphthalene-d8	10.487

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H-Pyran-2-one	96	C5H4O2	000504-31-4	64
2	8-[3-Diethylaminopropylamino]-5-...	290	C14H22N6O	017998-27-5	40
3	6-[2-Hexahydroazepino-1-hydroxye...	374	C25H30N2O	035871-87-5	40
4	1-(4-Trimethylsilyloxycarbonylph...	333	C18H27NO3Si	1000360-39-3	40
5	Piperocaine	261	C16H23NO2	000136-82-3	40





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Data File : BP005496.D
Acq On : 11 May 2021 19:06
Operator : CG/JU
Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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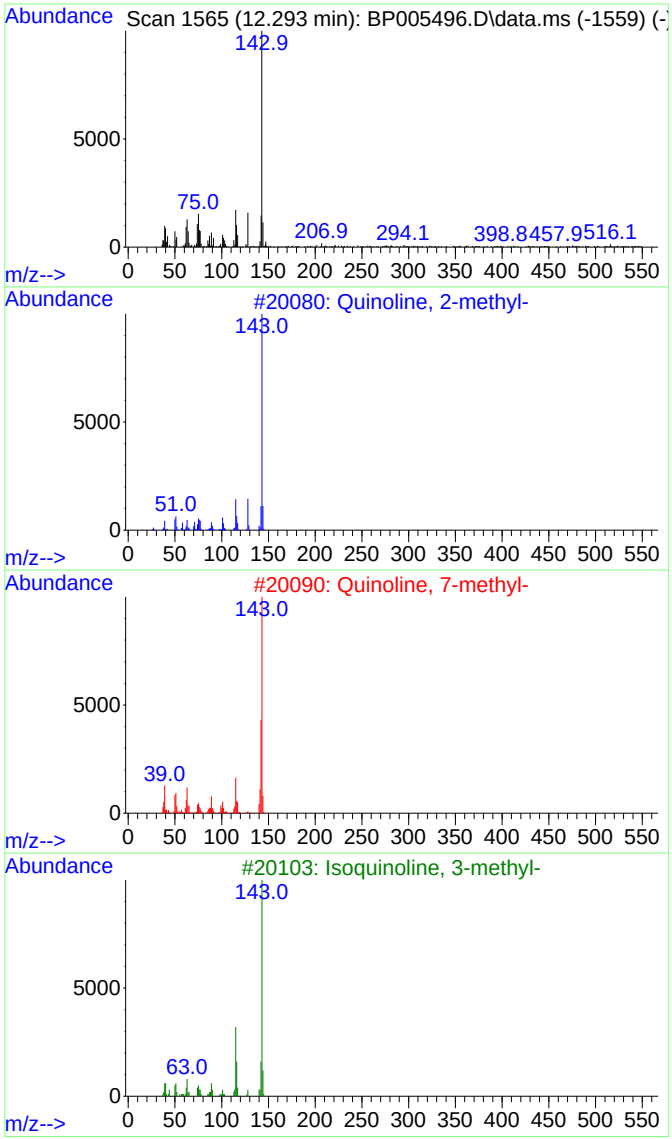
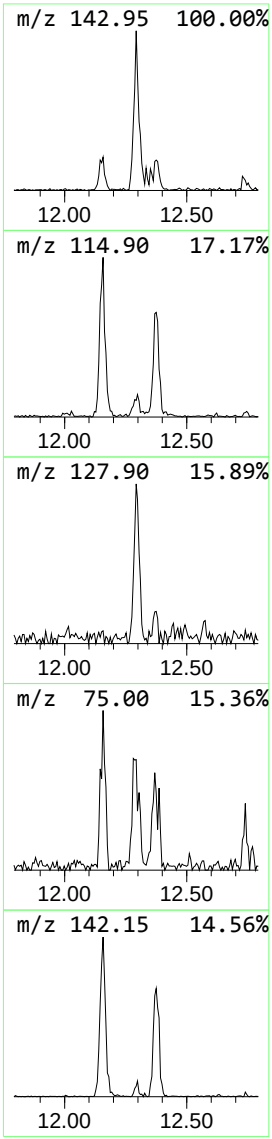
Peak Number 8 Quinoline, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.293	2.45 ng	10479	Naphthalene-d8	10.487

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline, 2-methyl-	143	C10H9N	000091-63-4	87
2	Quinoline, 7-methyl-	143	C10H9N	000612-60-2	83
3	Isoquinoline, 3-methyl-	143	C10H9N	001125-80-0	83
4	Quinoline, 6-methyl-	143	C10H9N	000091-62-3	80
5	3,5-Pyridinedicarbonitrile, 4-me...	143	C8H5N3	004574-75-8	72





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Operator : CG/JU
Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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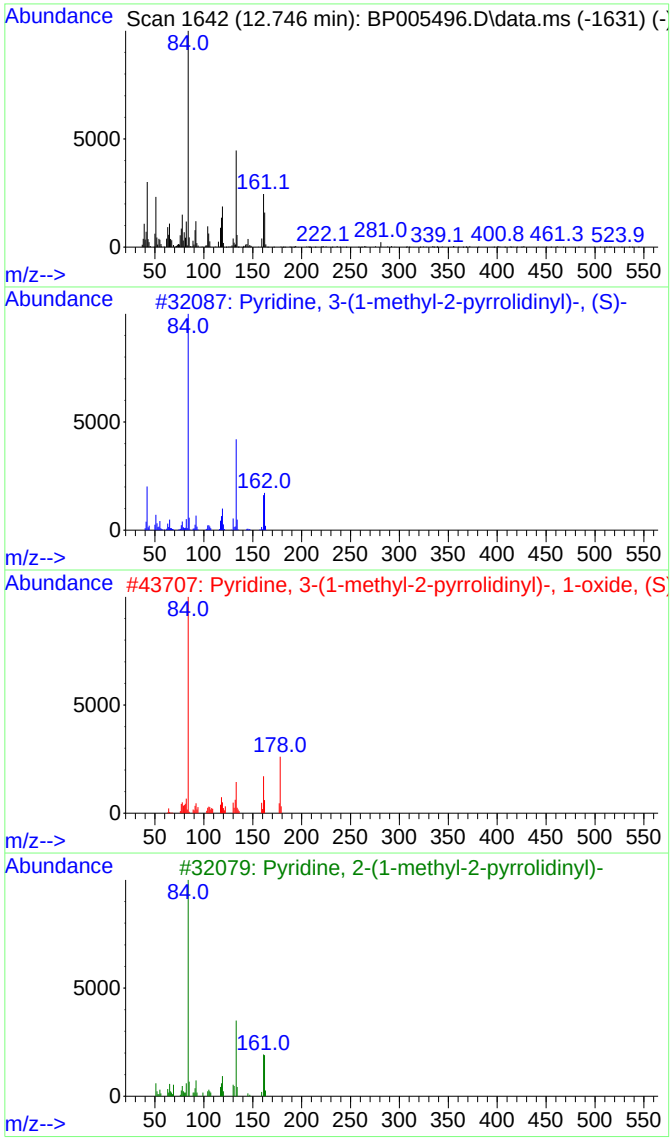
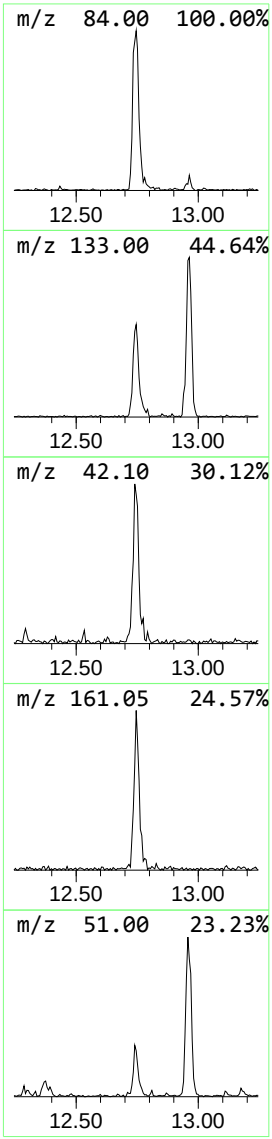
Peak Number 9 Pyridine, 3-(1-methyl-2-pyr... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.746	6.09 ng	36668	Acenaphthene-d10	14.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, 3-(1-methyl-2-pyrrolid...	162	C10H14N2	000054-11-5	59
2	Pyridine, 3-(1-methyl-2-pyrrolid...	178	C10H14N2O	002820-55-5	50
3	Pyridine, 2-(1-methyl-2-pyrrolid...	162	C10H14N2	023950-04-1	50
4	[1,2,4]Triazole-3-thione, 4-ethy...	288	C15H20N4S	1000304-75-8	32
5	Anabasine	162	C10H14N2	000494-52-0	23





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Operator : CG/JU
Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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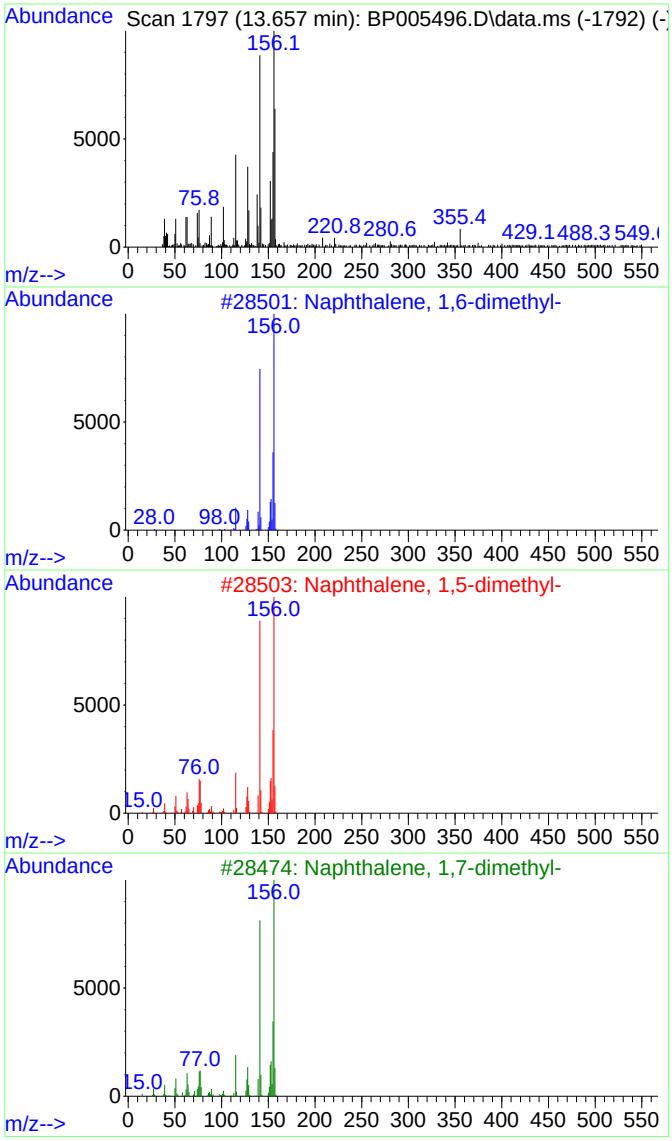
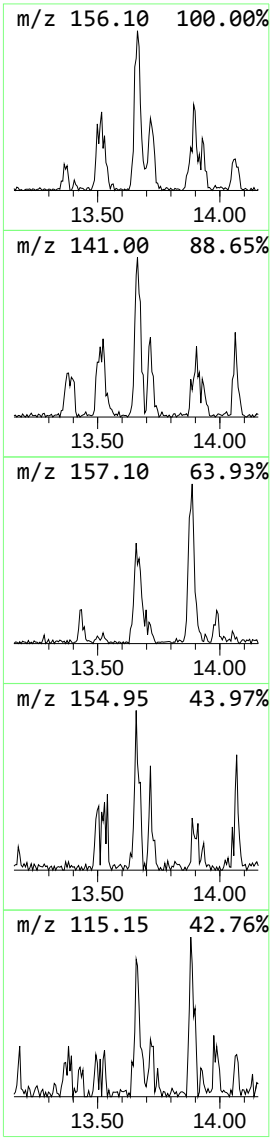
Peak Number 10 Naphthalene, 1,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.657	2.33 ng	14051	Acenaphthene-d10	14.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	74
2	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	58
3	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	58
4	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	58
5	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	58





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Operator : CG/JU
Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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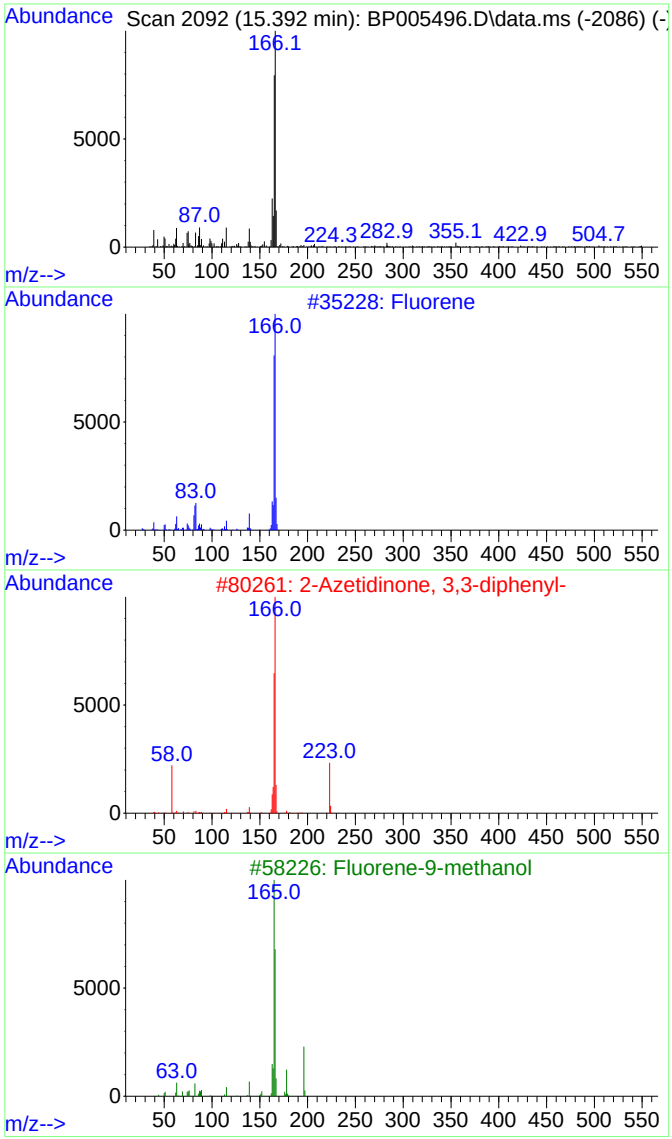
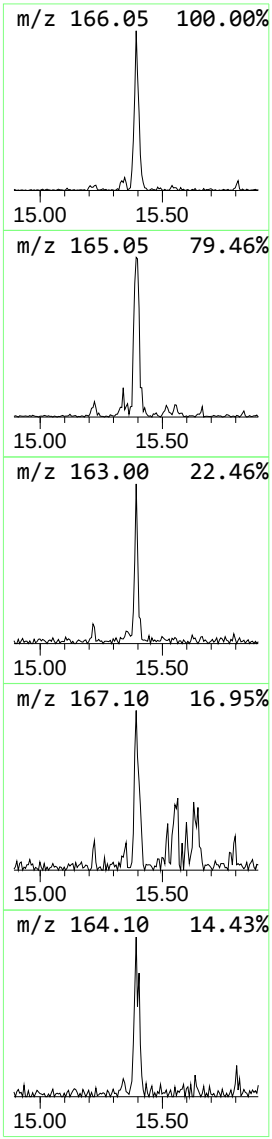
Peak Number 11 2-Azetidinone, 3,3-diphenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.393	2.87 ng	17292	Acenaphthene-d10	14.340

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluorene	166	C13H10	000086-73-7	80
2	2-Azetidinone, 3,3-diphenyl-	223	C15H13NO	015826-12-7	64
3	Fluorene-9-methanol	196	C14H12O	024324-17-2	50
4	3-Trifluoromethylbenzhydryl chlo...	270	C14H10ClF3	067240-79-3	50
5	2-Chlorofluorene	200	C13H9Cl	002523-44-6	32





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Data File : BP005496.D
Acq On : 11 May 2021 19:06
Operator : CG/JU
Sample : M2295-12 2X
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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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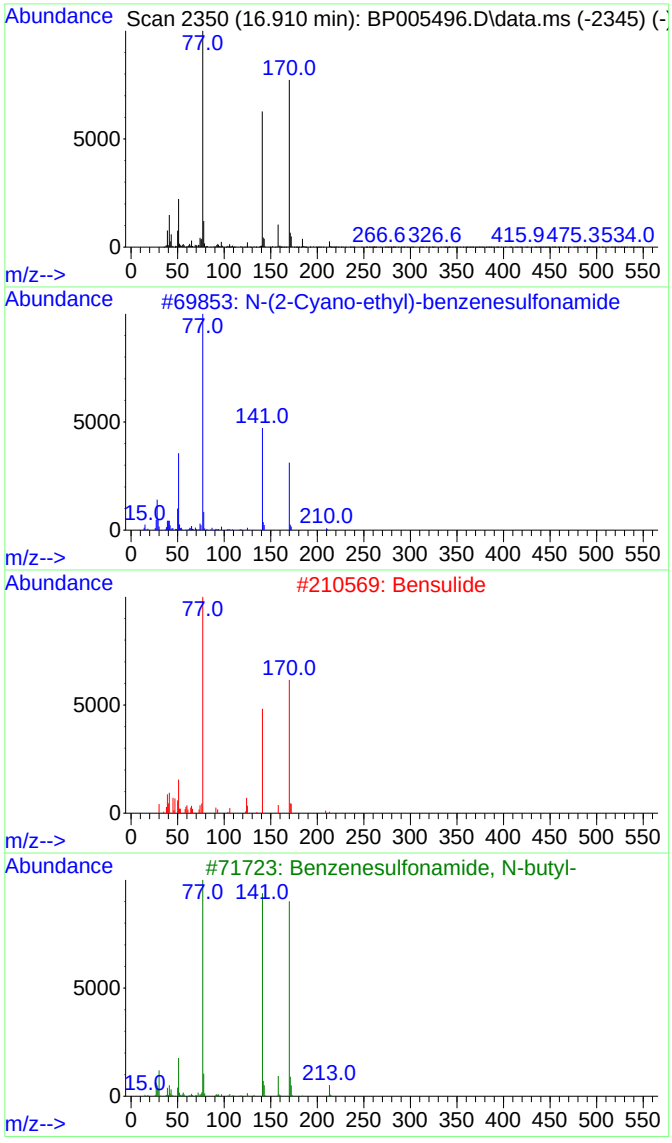
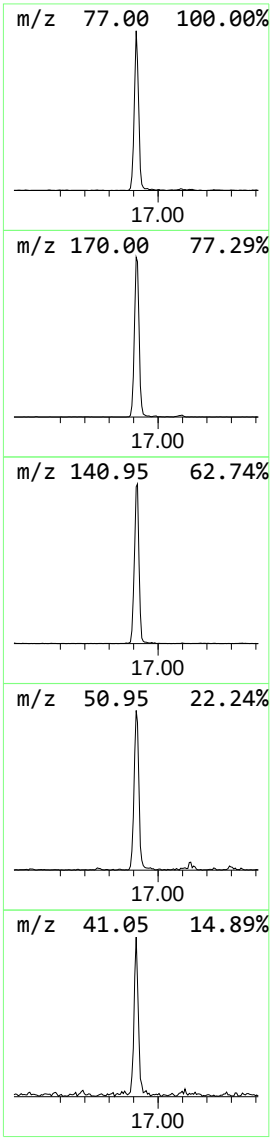
Peak Number 12 N-(2-Cyano-ethyl)-benzenesu... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.910	18.78 ng	158040	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-(2-Cyano-ethyl)-benzenesulfona...	210	C9H10N2O2S	002619-21-8	59
2	Bensulide	397	C14H24NO4PS3	000741-58-2	56
3	Benzenesulfonamide, N-butyl-	213	C10H15NO2S	003622-84-2	49
4	Benzenesulfonylamino-acetic acid...	260	C8H8N2O6S	1000301-09-0	47
5	1-[Phenylsulfonyl]-1-nitropropane	229	C9H11NO4S	021272-84-4	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP051121\
Data File : BP005496.D
Acq On : 11 May 2021 19:06
Operator : CG/JU
Sample : M2295-12 2X
Misc :
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Instrument : BNA_P
ClientSampleId : DRUM-B-C-E

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP050521.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
unknown4.828	4.828	2.6	ng	10509	1	7.693	80452	20.0
Furan, 2,3-dihy...	7.152	2.1	ng	8609	1	7.693	80452	20.0
4-Pentenal, 2-e...	7.763	6.9	ng	27689	1	7.693	80452	20.0
Furan, 2,5-dihy...	7.875	6.4	ng	25794	1	7.693	80452	20.0
Benzene, cyclop...	8.058	6.4	ng	25881	1	7.693	80452	20.0
Ethanol, 2-(2-b...	10.281	44.7	ng	191084	2	10.487	85500	20.0
2H-Pyran-2-one	10.905	2.1	ng	9173	2	10.487	85500	20.0
Quinoline, 2-me...	12.293	2.5	ng	10479	2	10.487	85500	20.0
Pyridine, 3-(1-...	12.746	6.1	ng	36668	3	14.340	120363	20.0
Naphthalene, 1,...	13.657	2.3	ng	14051	3	14.340	120363	20.0
2-Azetidinone, ...	15.393	2.9	ng	17292	3	14.340	120363	20.0
N-(2-Cyano-ethy...	16.910	18.8	ng	158040	4	17.092	168335	20.0