LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016622.D
Acq On : 01 Oct 2021 06:00
Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : SW-RR-03-(SA)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016622.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.816	77	80	88	rBV	7072	18903	5.53%	0.583%
2	4.138	113	115	123	rVB	3499	6386	1.87%	0.197%
3	4.821	185	189	196	rBV	31272	70682	20.69%	2.181%
4	4.996	205	208	211	rBV	8801	18784	5.50%	0.579%
5	5.272	234	238	246	rVB	5195	13584	3.98%	0.419%
6	6.379	354	358	367	rBV	11806	23900	7.00%	0.737%
7	6.646	383	387	392	rBV	5455	12803	3.75%	0.395%
8	6.840	403	408	418	rVB3	4893	18808	5.51%	0.580%
9	6.978	420	423	427	rBV	4172	9863	2.89%	0.304%
10	7.190	441	446	450	rBV2	2742	7580	2.22%	0.234%
11	7.264	450	454	460	rVB2	6361	15197	4.45%	0.469%
12	7.642	490	495	499	rBV	49207	103441	30.28%	3.191%
13	7.707	499	502	506	rVB	3166	5883	1.72%	0.181%
14	7.863	515	519	525	rBV	14643	29242	8.56%	0.902%
15	8.168	549	552	559	rVB	7924	17794	5.21%	0.549%
16	8.306	564	567	569	rVB2	11760	13268	3.88%	0.409%
17	8.442	574	578	581	rBV2	3807	8664	2.54%	0.267%
18	8.784	602	605	610	rBV	25788	49964	14.63%	1.541%
19	9.659	670	674	677	rVB2	5727	11067	3.24%	0.341%
20	10.191	713	716	721	rBV	23497	39985	11.71%	1.234%
21	10.406	729	733	735	rBV	105076	194048	56.80%	5.986%
22	10.457	735	737	740	rVB	159010	258541	75.68%	7.976%
23	11.205	790	796	798	rBV3	2347	6972	2.04%	0.215%
24	12.003	918	931	941	rBV2	48203	78831	23.08%	2.432%
25	12.074	941	947	959	rVB	5182	8643	2.53%	0.267%
26	12.296	991	997	1007	rVB	5918	9571	2.80%	0.295%
27	12.518	1042	1045	1047	rBV	5251	8275	2.42%	0.255%
28	12.886	1071	1074	1078	rVB	86788	152209	44.56%	4.696%
29	13.177	1094	1097	1103	rVB	8158	14837	4.34%	0.458%
30	13.812	1145	1147	1150	rBV2	4810	8375	2.45%	0.258%
31	14.269	1180	1183	1186	rBV	135653	198415	58.08%	6.121%
32	14.332	1186	1188	1192	rVB2	6296	10381	3.04%	0.320%
33	14.433	1192	1196	1198	rBV2	6101	10694	3.13%	0.330%
34	14.687	1212	1216	1219	rBV3	3239	9416	2.76%	0.290%
35	14.814	1223	1226	1230	rVB2	4428	7855	2.30%	0.242%
36	15.322	1264	1266	1268	rVB2	9190	12499	3.66%	0.386%

LSC Area Percent Report

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Acq On : 01 Oct 2021 06:00
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Misc :
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Instrument : BNA_N
ClientSampleId : SW-RR-03-(SA)

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.487	1274	1279	1282	rBV5	3998	12784	3.74%	0.394%
38	15.639	1287	1291	1295	rVV4	5395	13881	4.06%	0.428%
39	15.715	1295	1297	1299	rVV	3774	7927	2.32%	0.245%
40	15.766	1299	1301	1305	rVV2	17231	32397	9.48%	0.999%
41	15.842	1305	1307	1311	rVV4	3223	9683	2.83%	0.299%
42	15.956	1313	1316	1327	rVB	204597	341604	100.00%	10.538%
43	16.324	1342	1346	1348	rBV3	3792	10352	3.03%	0.319%
44	16.372	1348	1350	1353	rVB2	8266	15071	4.41%	0.465%
45	16.835	1386	1388	1397	rVB	6743	14209	4.16%	0.438%
46	17.017	1400	1403	1405	rBV	105474	161985	47.42%	4.997%
47	17.066	1405	1407	1410	rVV	25549	40866	11.96%	1.261%
48	17.163	1413	1415	1417	rVV2	11633	20074	5.88%	0.619%
49	17.224	1417	1420	1422	rVV	7355	16659	4.88%	0.514%
50	17.309	1425	1427	1432	rVV3	24911	65152	19.07%	2.010%
51	17.443	1434	1438	1443	rVV3	4557	16143	4.73%	0.498%
52	17.528	1443	1445	1447	rVV	6795	9700	2.84%	0.299%
53	17.601	1447	1451	1453	rVB2	4238	7849	2.30%	0.242%
54	17.954	1477	1480	1497	rVB	24169	41952	12.28%	1.294%
55	18.308	1539	1544	1548	rBV	2826	4058	1.19%	0.125%
56	18.834	1645	1650	1656	rBV2	2482	3872	1.13%	0.119%
57	19.063	1689	1696	1713	rBV	142013	204169	59.77%	6.299%
58	19.246	1727	1733	1746	rBV	22519	35478	10.39%	1.094%
59	19.460	1766	1776	1781	rBV2	9869	15794	4.62%	0.487%
60	19.559	1790	1796	1802	rVB	5073	7125	2.09%	0.220%
61	19.673	1813	1819	1834	rBV	120024	153077	44.81%	4.722%
62	20.006	1884	1886	1889	rBV2	5696	10659	3.12%	0.329%
63	20.972	1974	1977	1981	rBV2	8800	19641	5.75%	0.606%
64	21.163	1993	1995	1998	rBV	29006	38842	11.37%	1.198%
65	21.227	1998	2001	2004	rBV	142440	194466	56.93%	5.999%
66	22.109	2081	2084	2087	rVB	4685	6762	1.98%	0.209%
67	22.803	2222	2228	2233	rBV	2764	4307	1.26%	0.133%
68	23.481	2414	2426	2457	rVB	102554	198595	58.14%	6.127%
69	24.080	2595	2601	2615	rVB2	3448	6357	1.86%	0.196%
70	25.760	3076	3092	3121	rBV4	3021	10274	3.01%	0.317%
71	26.452	3281	3294	3313	rVB3	1447	4390	1.29%	0.135%

Sum of corrected areas: 3241514

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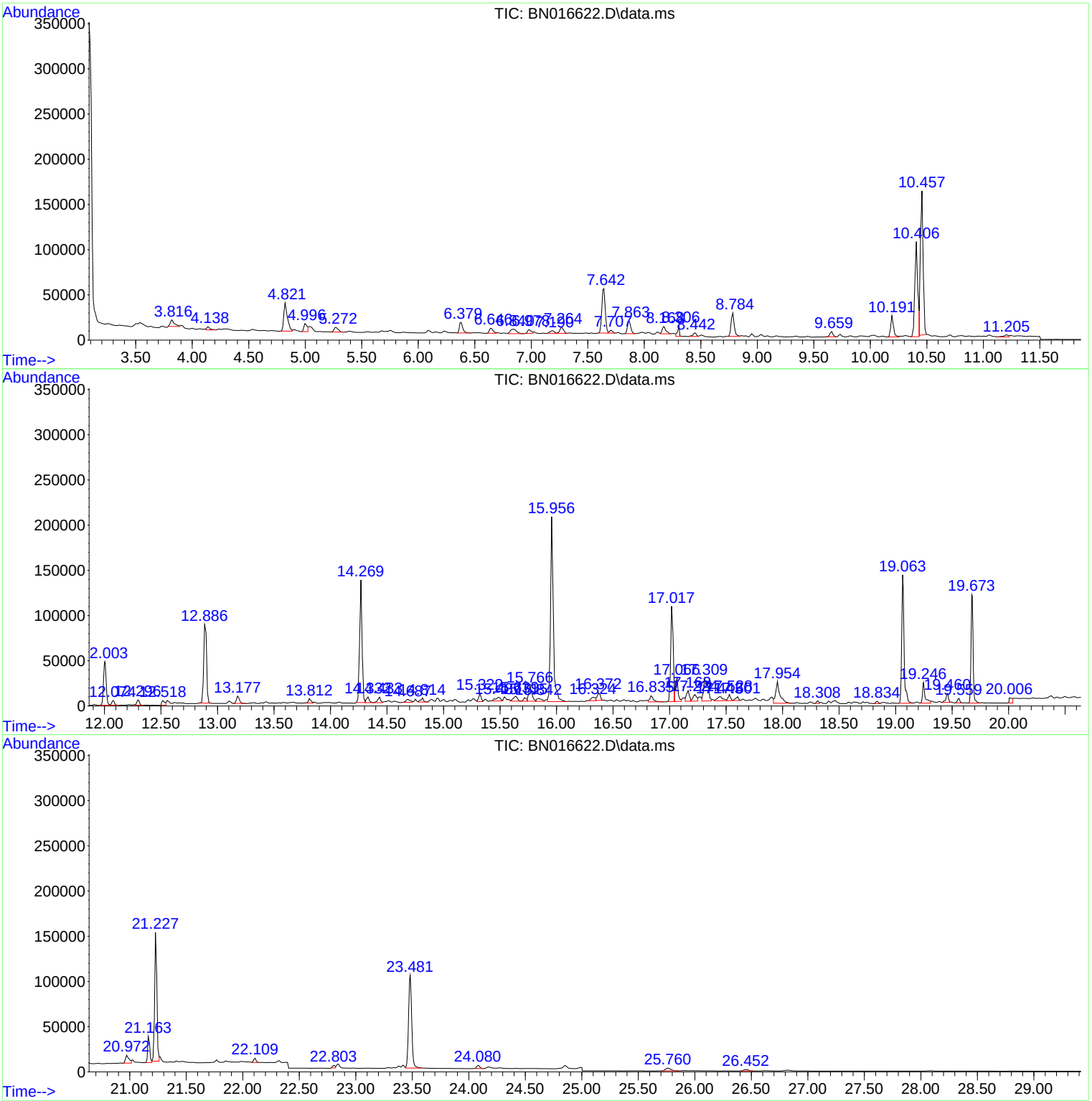
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-03-(SA)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

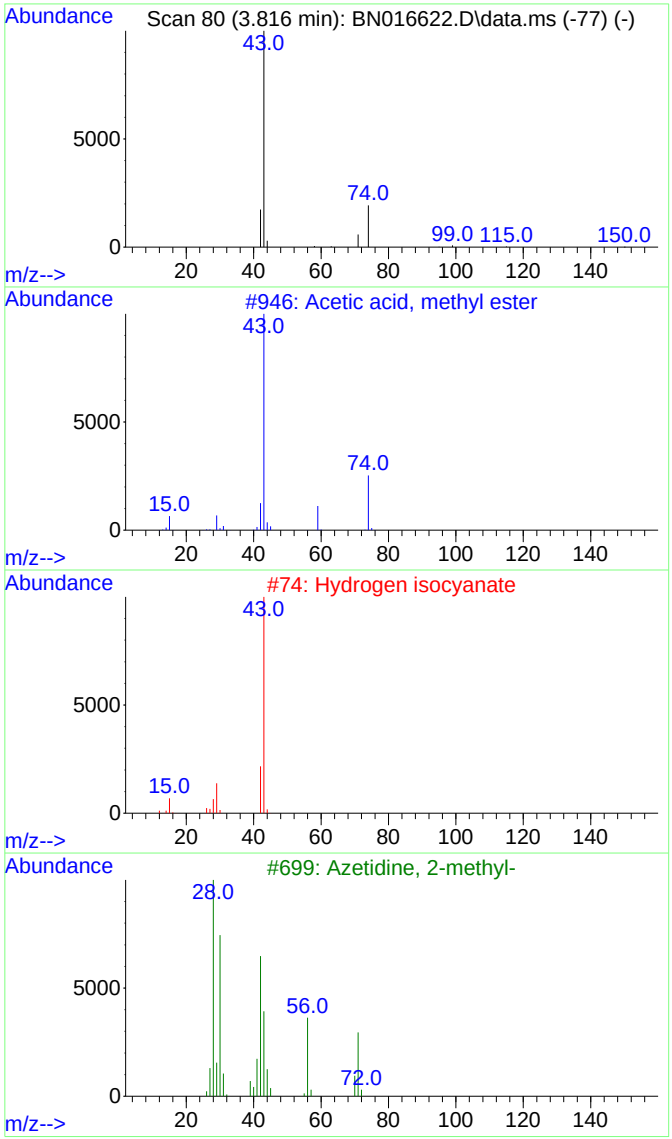
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

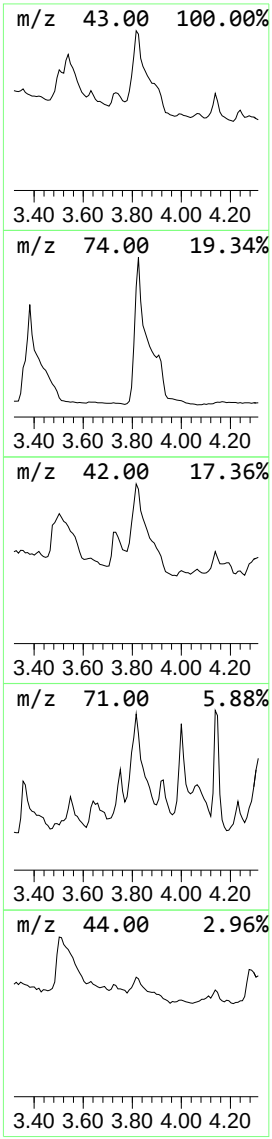
****

Peak Number 1 Acetic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.07 ng	18903	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, methyl ester	74	C3H6O2	000079-20-9	5
2	Hydrogen isocyanate	43	CHNO	000075-13-8	4
3	Azetidine, 2-methyl-	71	C4H9N	019812-49-8	4
4	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	4
5	Methoxyacetonitrile	71	C3H5NO	001738-36-9	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016622.D
Acq On : 01 Oct 2021 06:00
Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-03-(SA)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

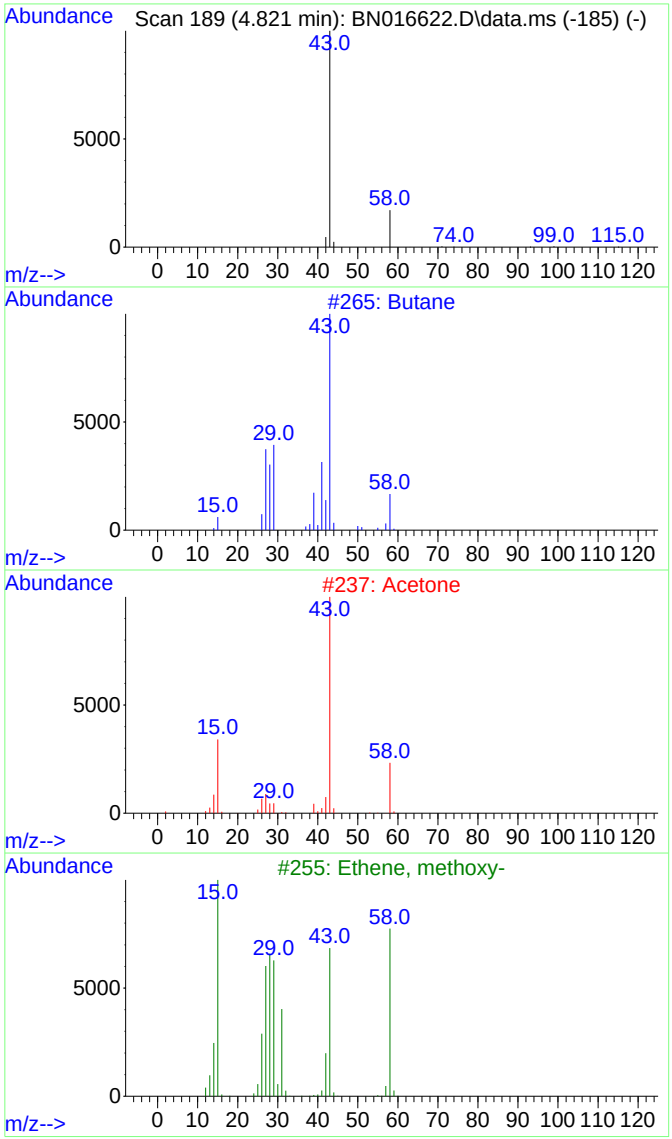
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

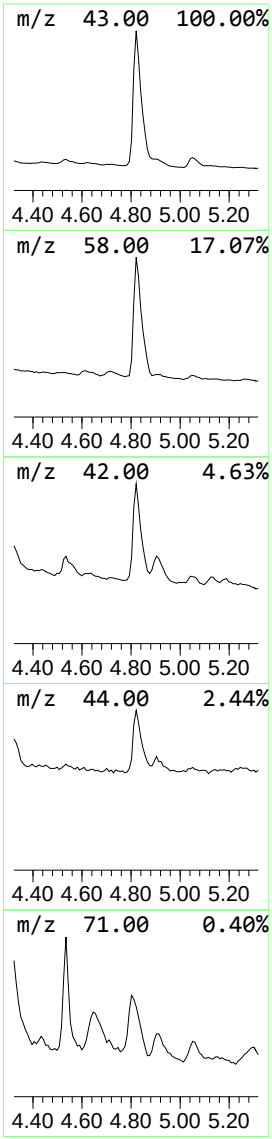
****

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.27 ng	70682	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	4
2	Acetone	58	C3H6O	000067-64-1	4
3	Ethene, methoxy-	58	C3H6O	000107-25-5	3
4	Diazene, dimethyl-	58	C2H6N2	000503-28-6	3
5	Hydrogen isocyanate	43	CHNO	000075-13-8	2





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Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-03-(SA)

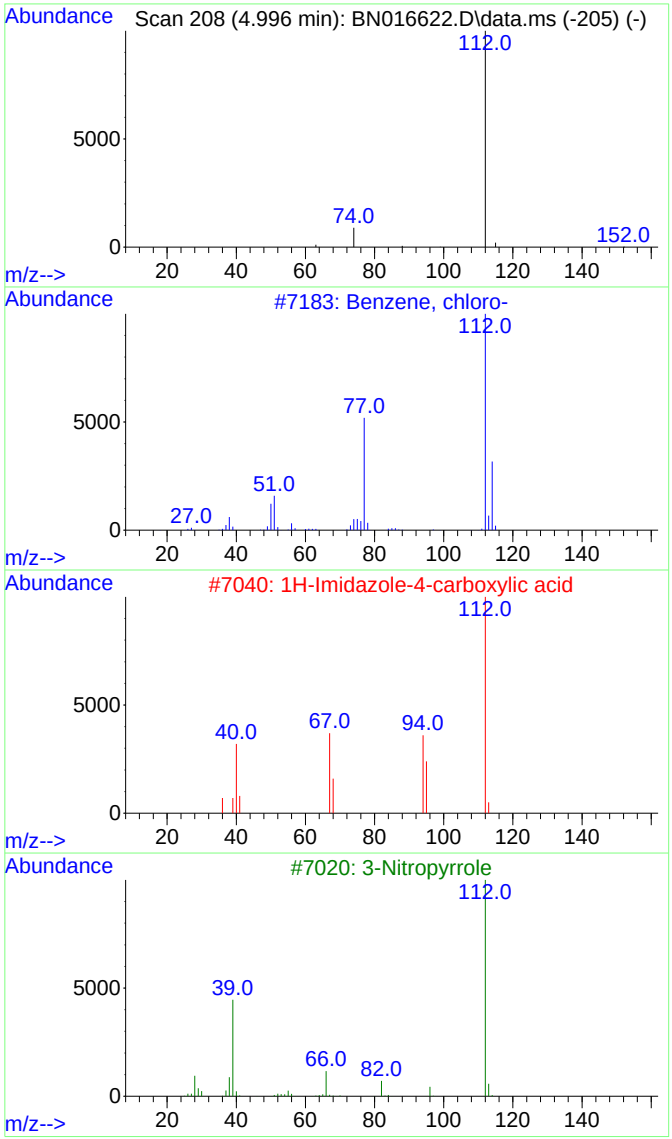
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

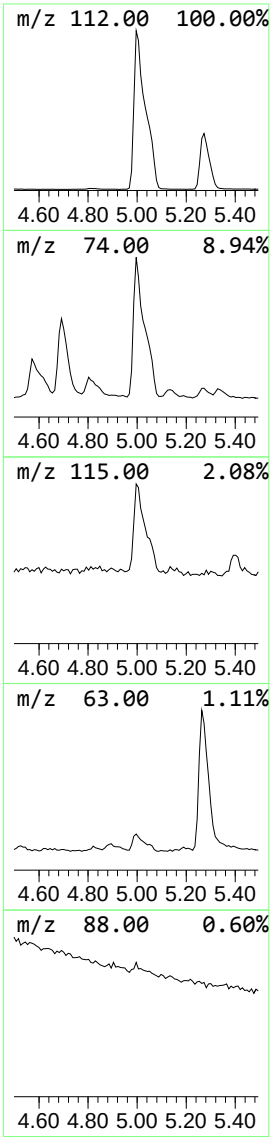
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzene, chloro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.996	0.07 ng	18784	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, chloro-	112	C6H5Cl	000108-90-7	5
2	1H-Imidazole-4-carboxylic acid	112	C4H4N2O2	001072-84-0	2
3	3-Nitropyrrole	112	C4H4N2O2	005930-94-9	2
4	Uracil	112	C4H4N2O2	000066-22-8	2
5	4H-Thiopyran-4-one	112	C5H4OS	001003-41-4	2





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Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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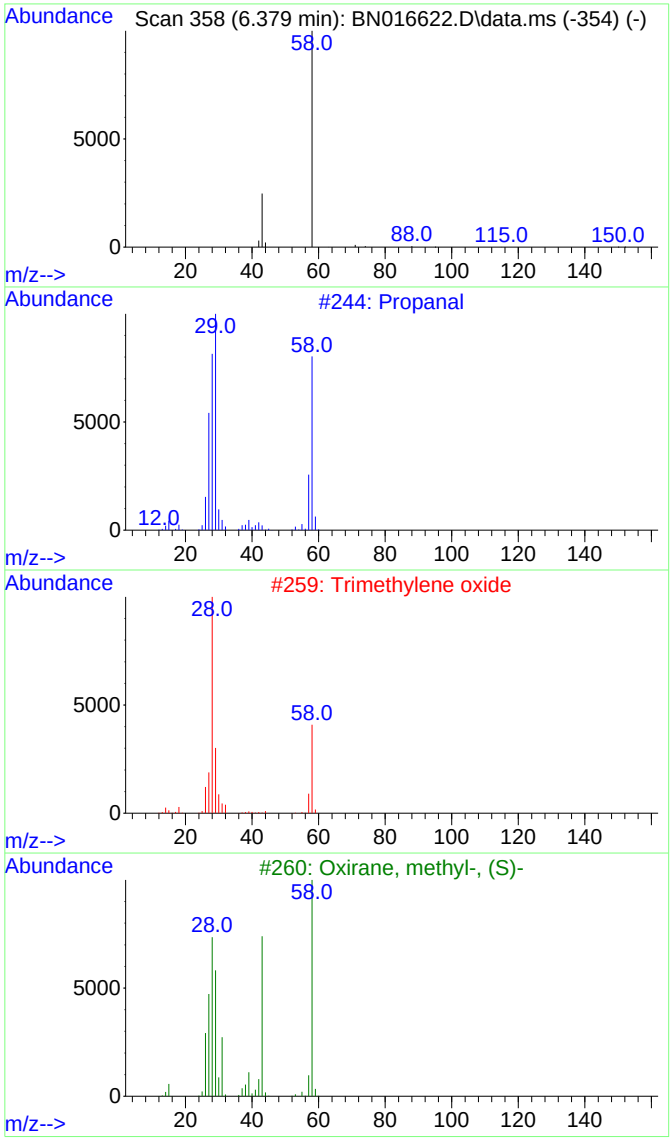
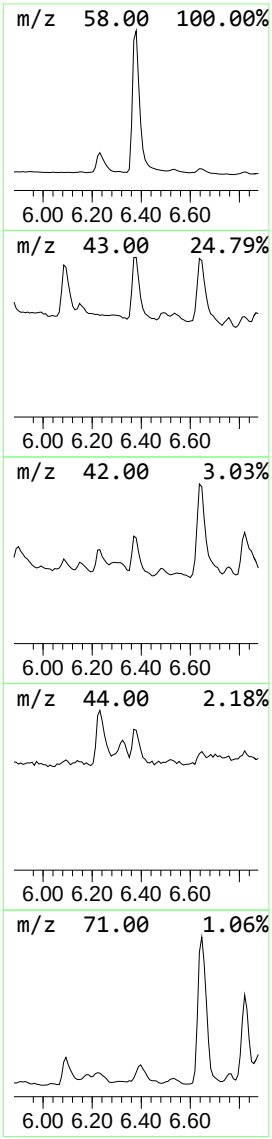
Peak Number 4 Propanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.379	0.09 ng	23900	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	3
2	Trimethylene oxide	58	C3H6O	000503-30-0	3
3	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	3
4	Propylene oxide	58	C3H6O	000075-56-9	3
5	3-Aminopentan-2-ol	103	C5H13NO	050411-28-4	2





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-03-(SA)

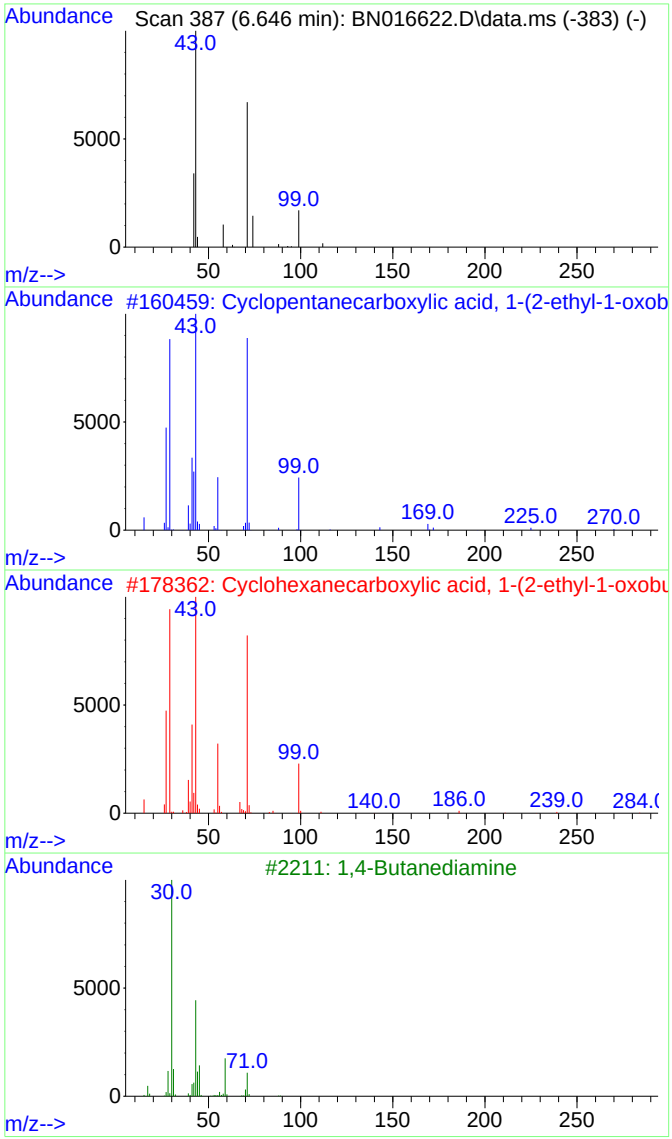
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

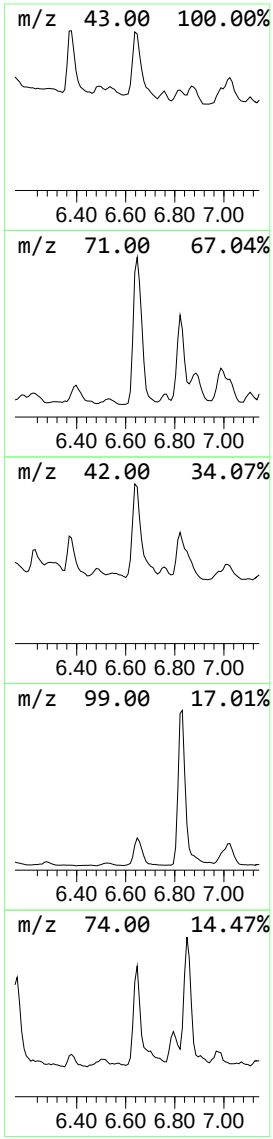
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentanecarboxylic acid... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.646	0.05 ng	12803	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanecarboxylic acid, 1-(...	270	C14H22O5	1000460-66-4	36
2	Cyclohexanecarboxylic acid, 1-(2...	284	C15H24O5	1000460-66-2	9
3	1,4-Butanediamine	88	C4H12N2	000110-60-1	5
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	5
5	2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4





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SW-RR-03-(SA)

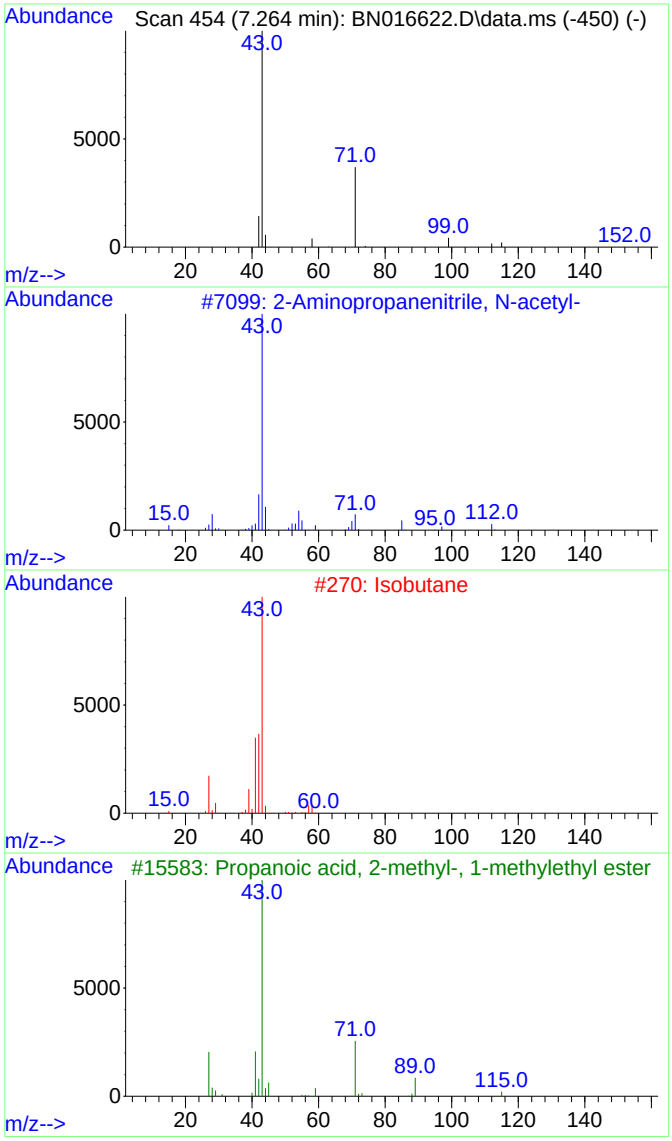
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

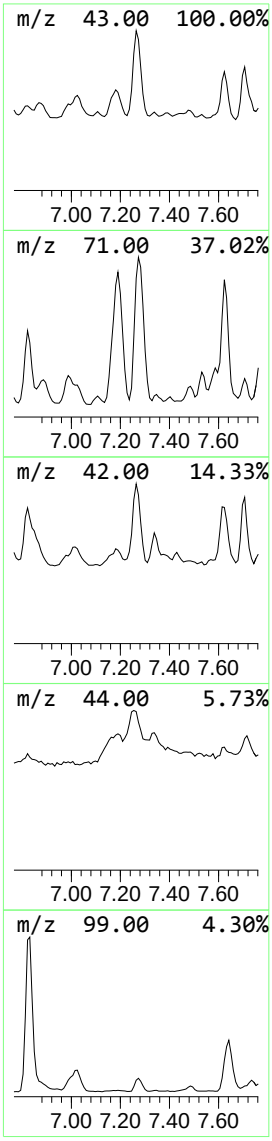
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Aminopropanenitrile, N-ac... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.06 ng	15197	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Aminopropanenitrile, N-acetyl-	112	C5H8N2O	019861-71-3	4
2	Isobutane	58	C4H10	000075-28-5	4
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	4
4	Hydrogen azide	43	HN3	007782-79-8	4
5	Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4





Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016622.D
Acq On : 01 Oct 2021 06:00
Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-03-(SA)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

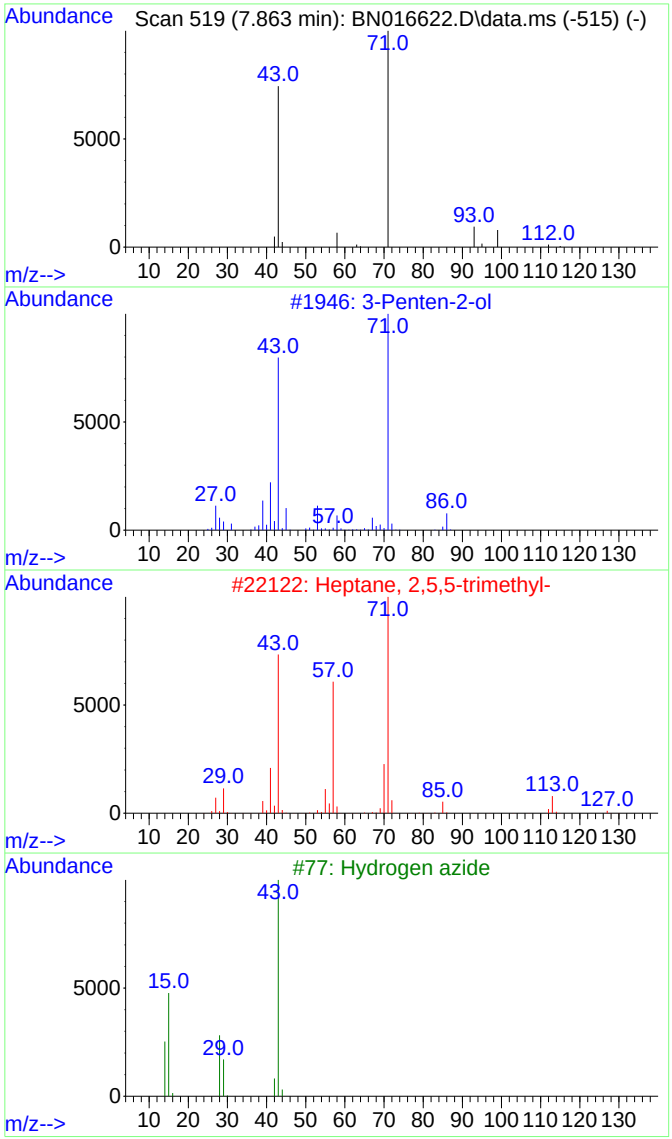
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

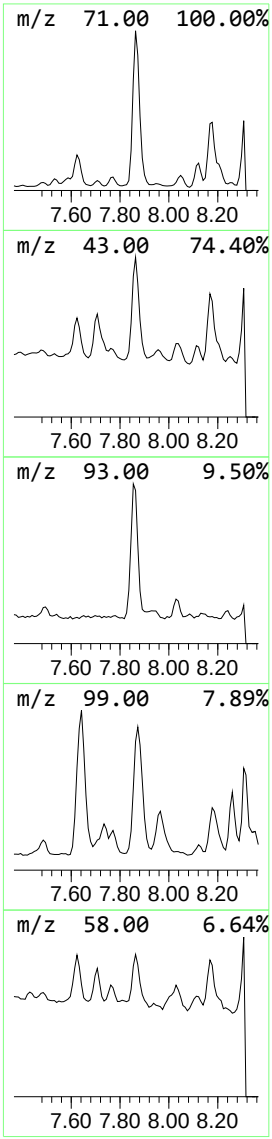
****

Peak Number 7 3-Penten-2-ol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.863	0.11 ng	29242	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-ol	86	C5H10O	001569-50-2	4
2	Heptane, 2,5,5-trimethyl-	142	C10H22	001189-99-7	4
3	Hydrogen azide	43	HN3	007782-79-8	4
4	3-Hydroxypentanedinitrile, acetate	152	C7H8N2O2	1000506-60-2	4
5	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4





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Data File : BN016622.D
Acq On : 01 Oct 2021 06:00
Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-03-(SA)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

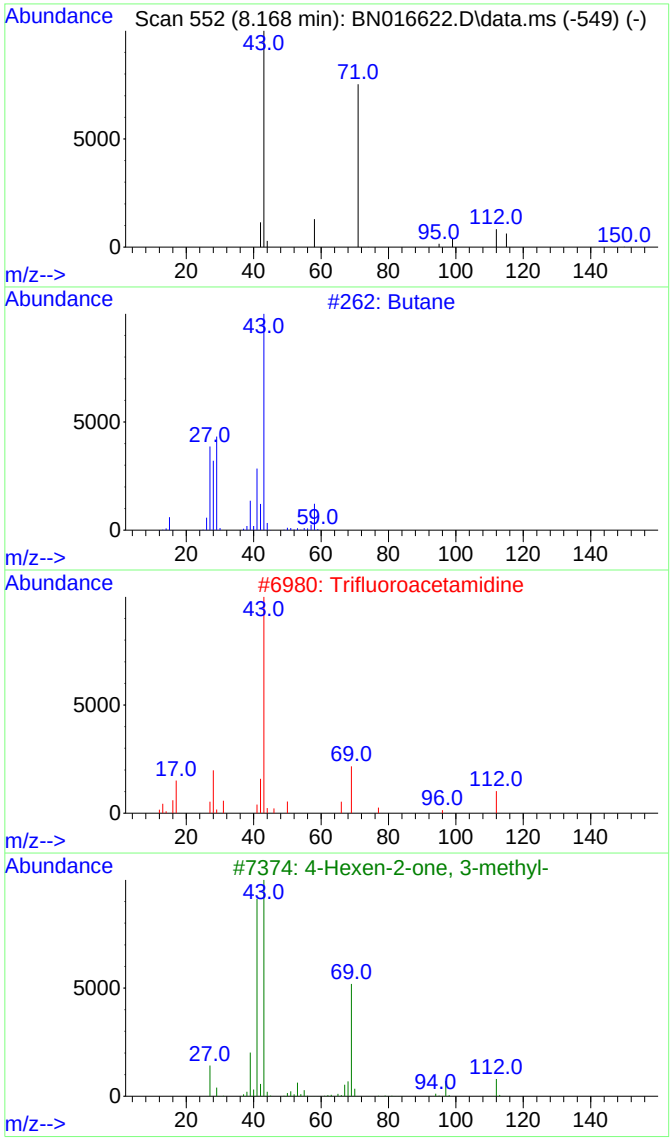
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

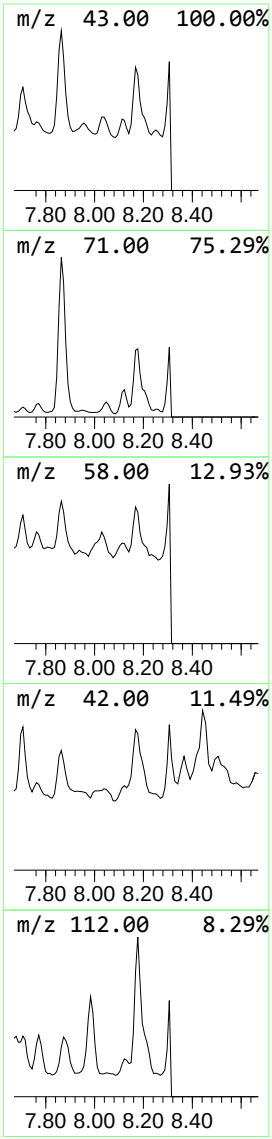
****

Peak Number 8 Butane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.07 ng	17794	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	7
2	Trifluoroacetamidine	112	C2H3F3N2	000354-37-0	7
3	4-Hexen-2-one, 3-methyl-	112	C7H12O	072189-24-3	4
4	Propanal, 2-propenylhydrazone	112	C6H12N2	019031-78-8	4
5	5-Hepten-2-one	112	C7H12O	006714-00-7	4





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Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-03-(SA)

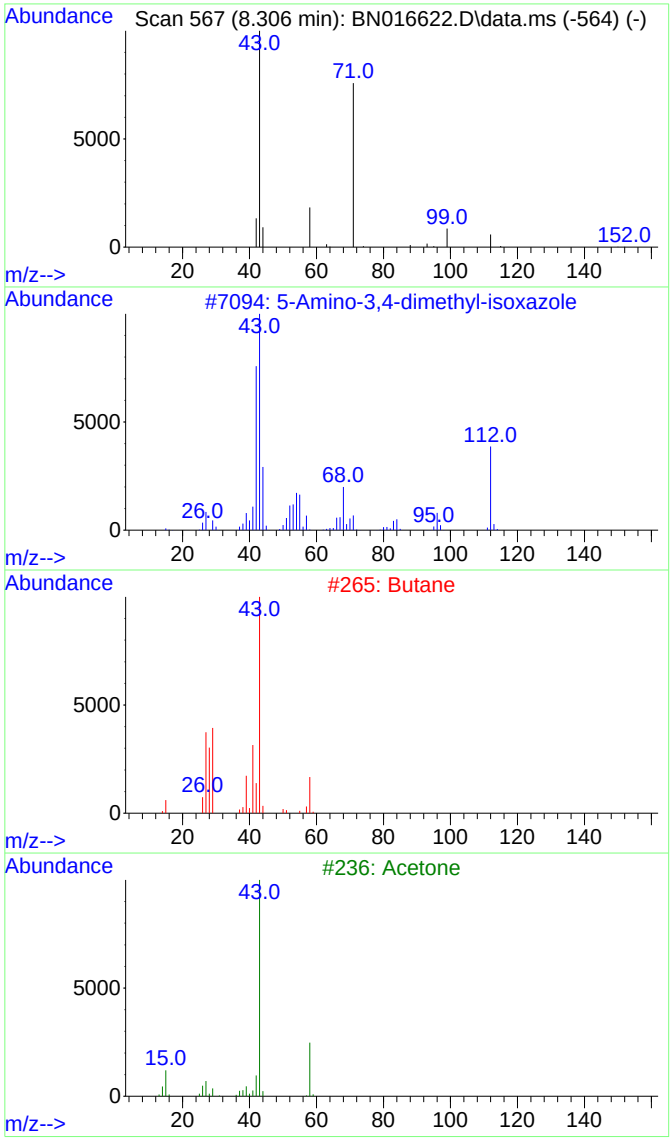
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

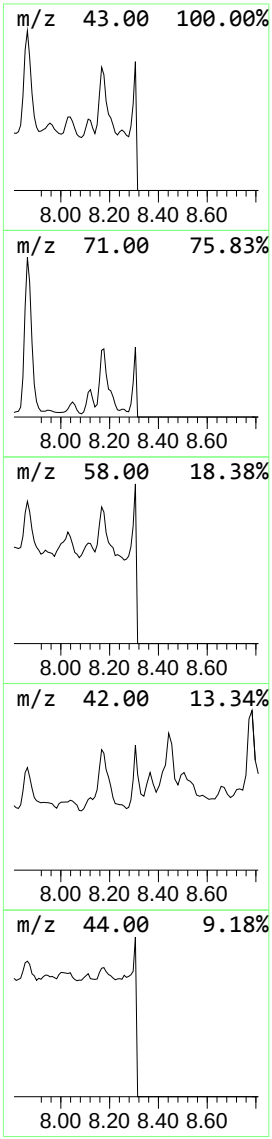
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 5-Amino-3,4-dimethyl-isoxazole Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.05 ng	13268	1,4-Dichlorobenzene-d4	7.642

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Amino-3,4-dimethyl-isoxazole	112	C5H8N2O	019947-75-2	7
2	Butane	58	C4H10	000106-97-8	5
3	Acetone	58	C3H6O	000067-64-1	5
4	Hexamethylenimine	99	C6H13N	000111-49-9	4
5	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	4





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Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-03-(SA)

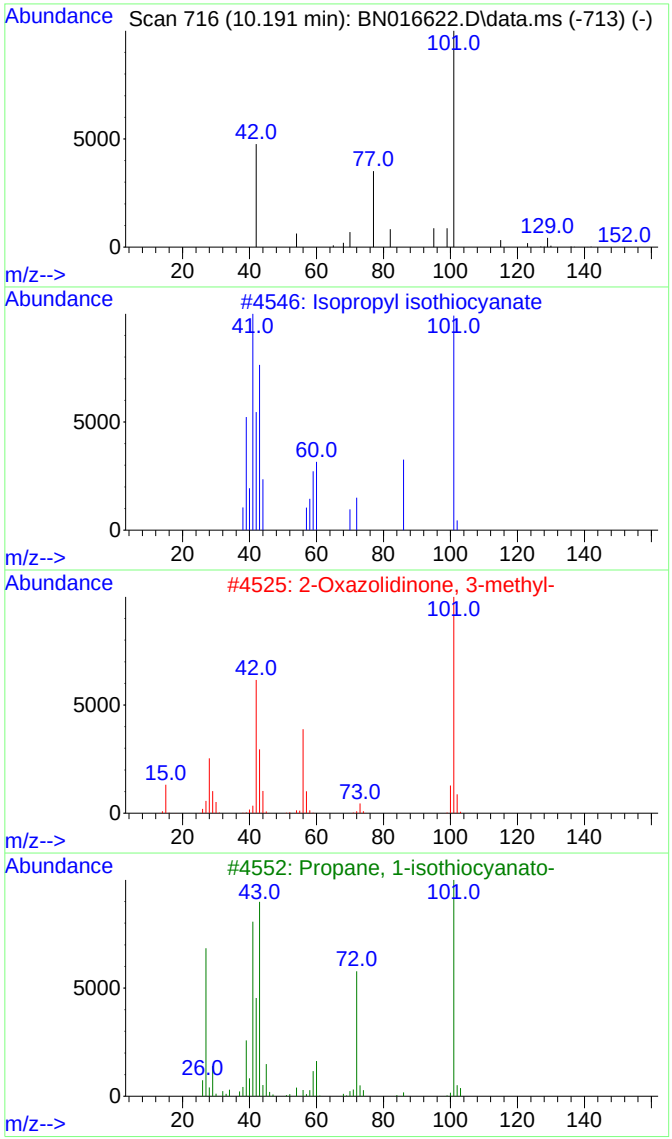
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

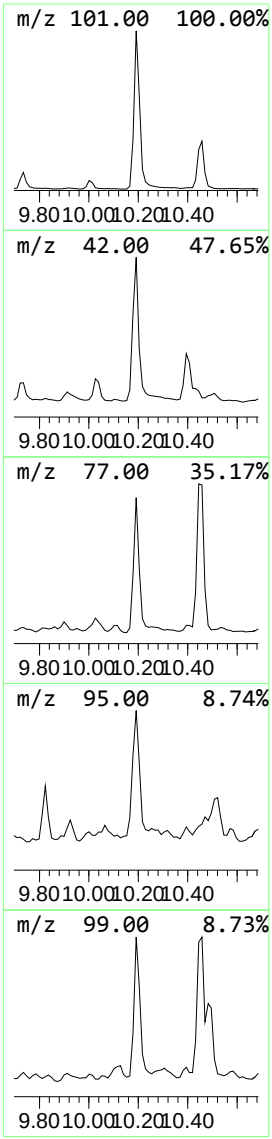
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Isopropyl isothiocyanate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.08 ng	39985	Naphthalene-d8	10.406

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	9
2	2-Oxazolidinone, 3-methyl-	101	C4H7NO2	019836-78-3	5
3	Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
4	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	4





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Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SW-RR-03-(SA)

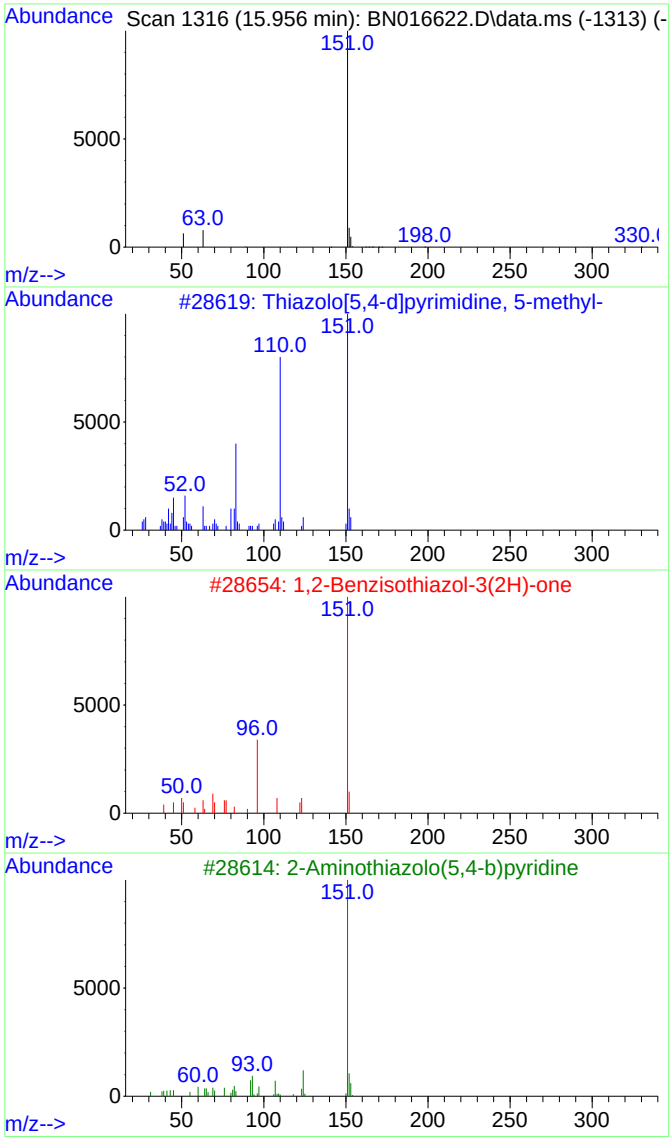
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

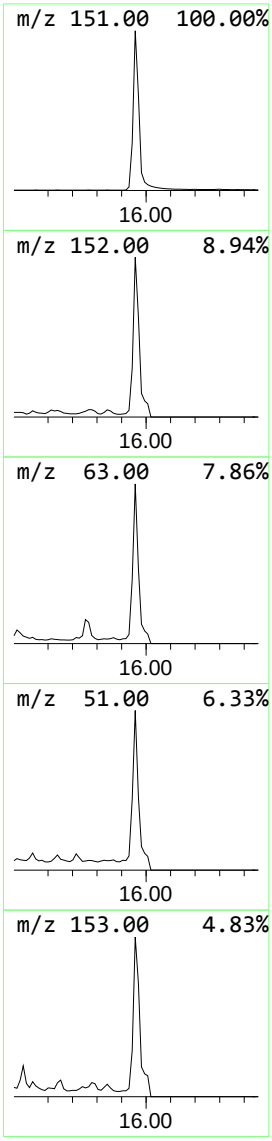
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Thiazolo[5,4-d]pyrimidine, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.956	0.84 ng	341604	Phenanthrene-d10	17.017

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazolo[5,4-d]pyrimidine, 5-met...	151	C6H5N3S	013554-89-7	9
2	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	9
3	2-Aminothiazolo(5,4-b)pyridine	151	C6H5N3S	031784-70-0	7
4	p-Toluthioamide	151	C8H9NS	002362-62-1	7
5	5-(Difluoromethyl)-1,3,4-thiadia...	151	C3H3F2N3S	025306-15-4	7





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Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

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BNA_N
ClientSampleId :
SW-RR-03-(SA)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

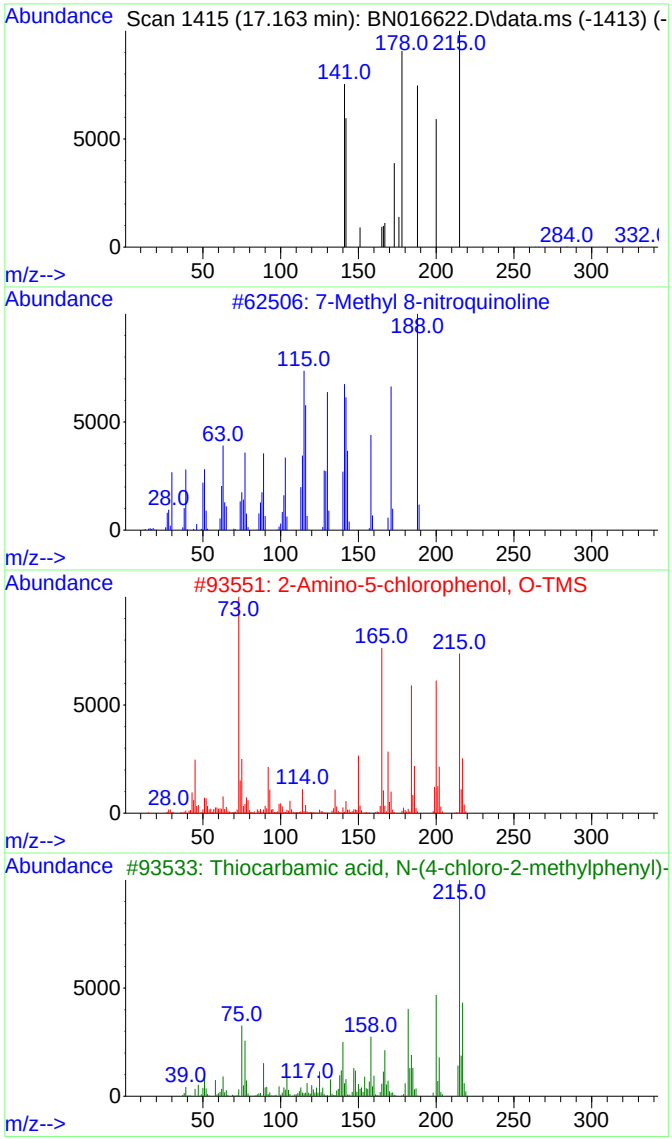
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

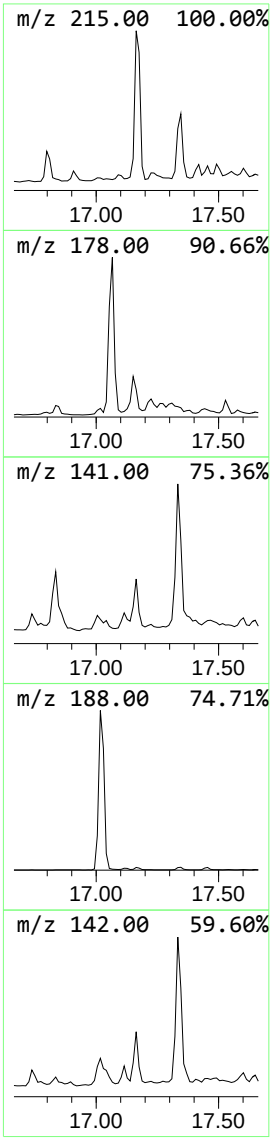
****

Peak Number 12 7-Methyl 8-nitroquinoline Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.163	0.05 ng	20074	Phenanthrene-d10	17.017

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7-Methyl 8-nitroquinoline	188	C10H8N2O2	007471-63-8	16
2	2-Amino-5-chlorophenol, O-TMS	215	C9H14ClNOSi	1000472-42-6	9
3	Thiocarbamic acid, N-(4-chloro-2...	215	C9H10ClNOS	1000266-43-5	9
4	1-Naphthaleneacethydrazide	200	C12H12N2O	034800-90-3	9
5	2-Chloro-3-(1H-pyrrol-1-yl)pyridine	178	C9H7ClN2	070291-26-8	9





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Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : SW-RR-03-(SA)

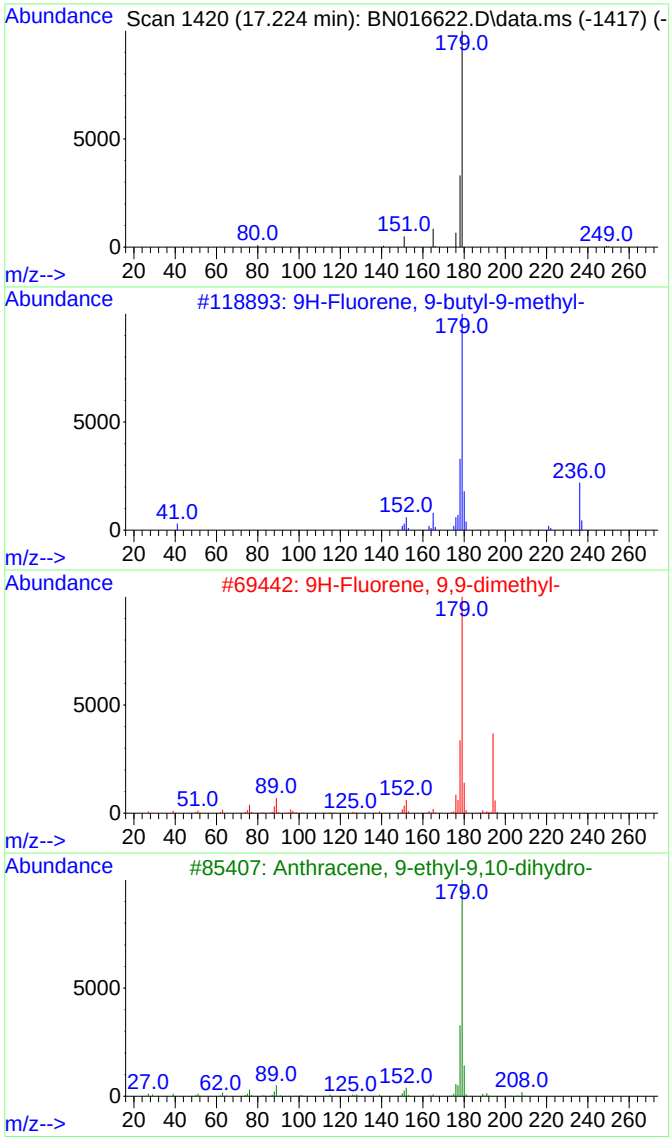
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

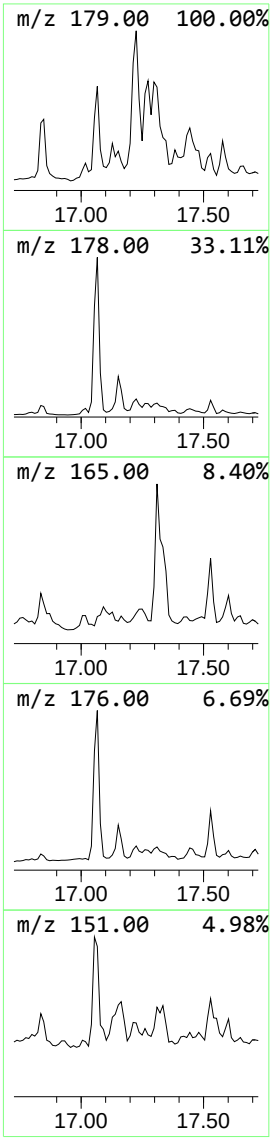
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 9H-Fluorene, 9-butyl-9-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.224	0.04 ng	16659	Phenanthrene-d10	17.017

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluorene, 9-butyl-9-methyl-	236	C18H20	042348-92-5	64
2	9H-Fluorene, 9,9-dimethyl-	194	C15H14	004569-45-3	9
3	Anthracene, 9-ethyl-9,10-dihydro-	208	C16H16	000605-82-3	9
4	4-Phenyl-1,2,3,4-tetrahydroisoqu...	209	C15H15N	075626-12-9	9
5	Ethanone, 1-(9,10-dihydro-9-anth...	222	C16H14O	054585-45-4	9





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Operator : CG/JU
Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
SW-RR-03-(SA)

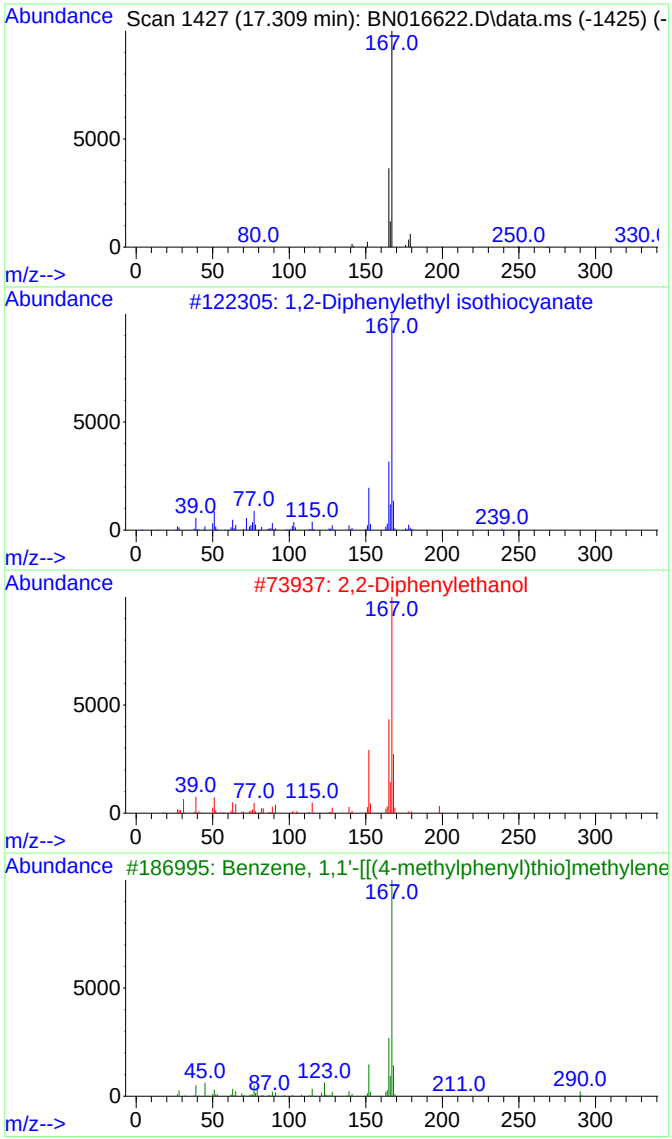
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

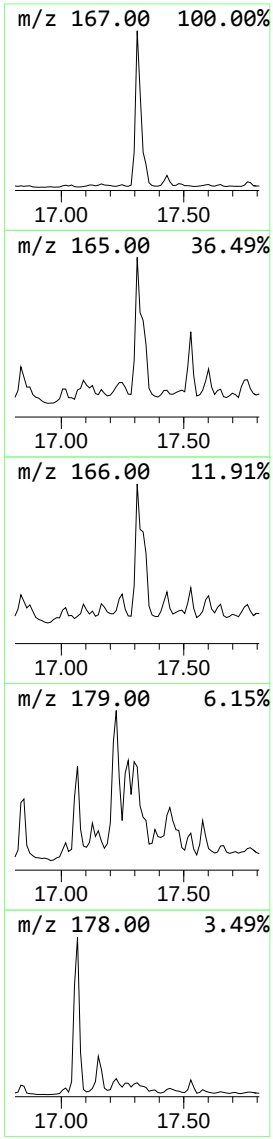
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 1,2-Diphenylethyl isothiocy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.309	0.16 ng	65152	Phenanthrene-d10	17.017

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Diphenylethyl isothiocyanate	239	C15H13NS	1010134-54-2	43
2	2,2-Diphenylethanol	198	C14H14O	001883-32-5	40
3	Benzene, 1,1'-[[(4-methylphenyl)...	290	C20H18S	032110-49-9	40
4	2-Propanone, 1,1-diphenyl-	210	C15H14O	000781-35-1	40
5	Adrafinil	289	C15H15NO3S	063547-13-7	40





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Misc :
ALS Vial : 25 Sample Multiplier: 1

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ClientSampleId :
SW-RR-03-(SA)

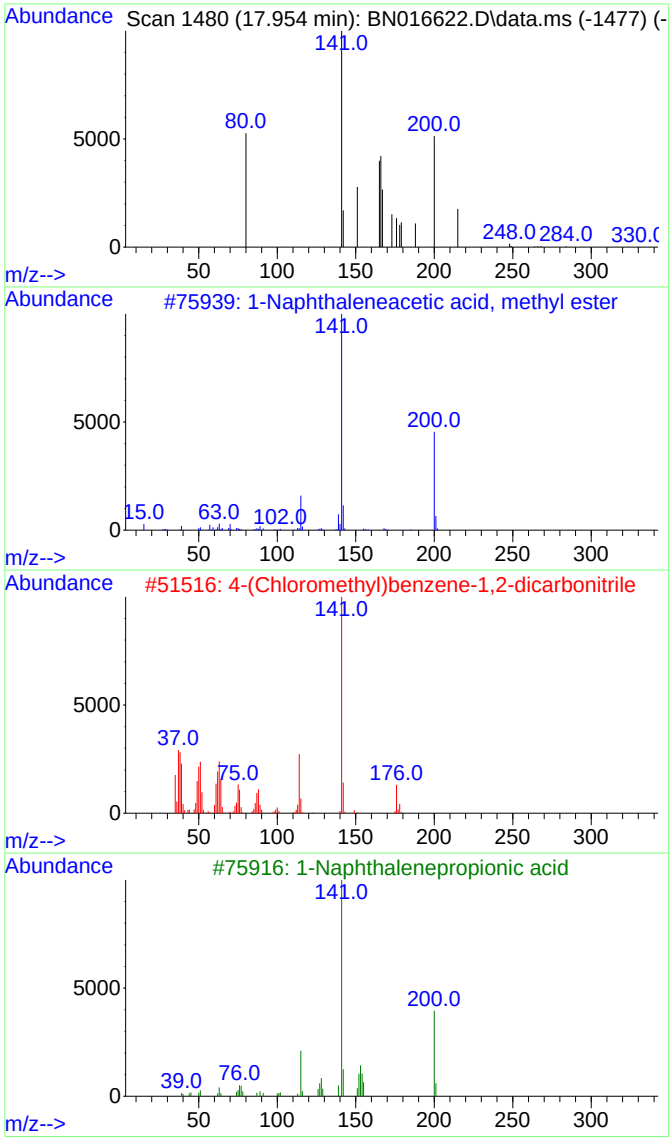
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

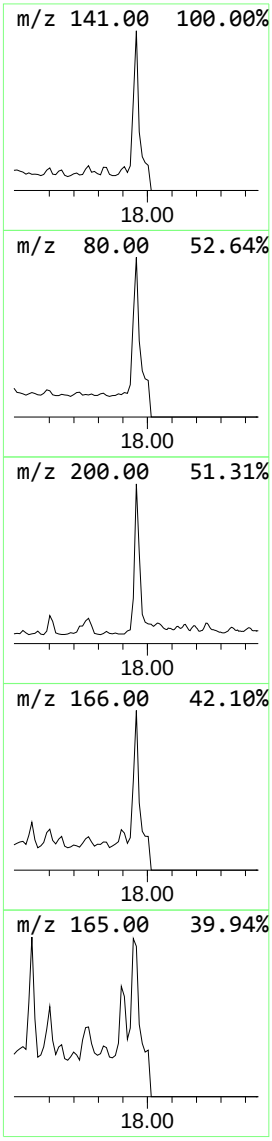
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 1-Naphthaleneacetic acid, m... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.954	0.10 ng	41952	Phenanthrene-d10	17.017

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthaleneacetic acid, methyl...	200	C13H12O2	002876-78-0	9
2	4-(Chloromethyl)benzene-1,2-dica...	176	C9H5ClN2	089927-55-9	9
3	1-Naphthalenepropionic acid	200	C13H12O2	003243-42-3	9
4	Hydrazinecarboxamide, 2-cyclopen...	141	C6H11N3O	005459-00-7	9
5	Phenylacetic acid, 2-fluoro-4,5-...	200	C9H9FO4	141523-25-3	9





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Sample : M3986-03
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_N
ClientSampleId : SW-RR-03-(SA)

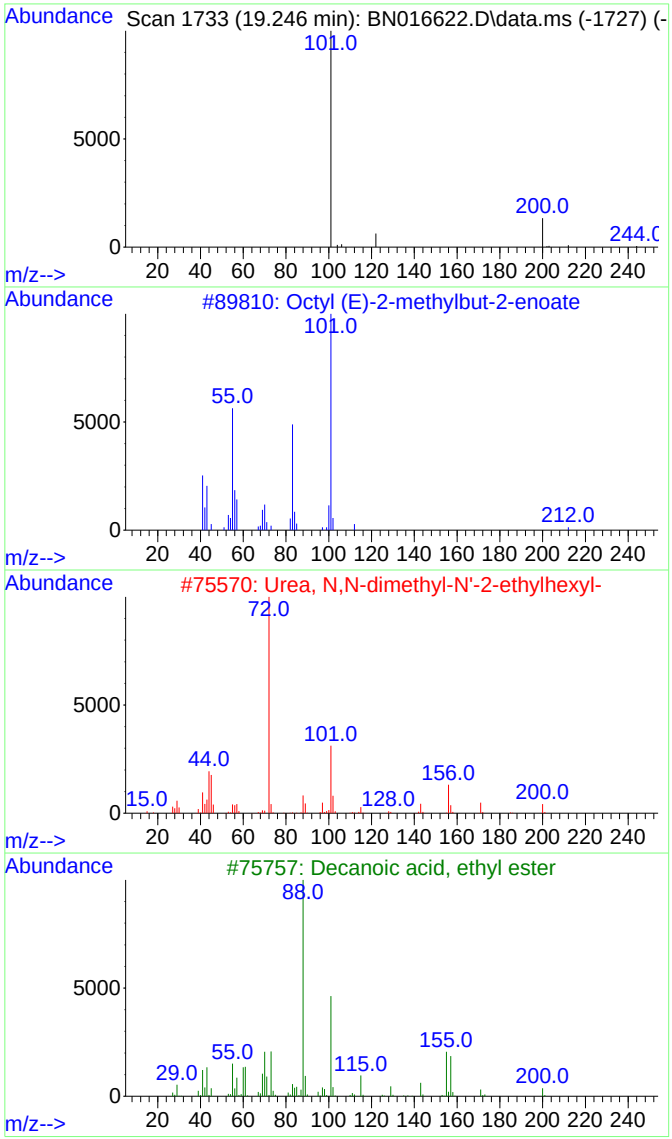
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

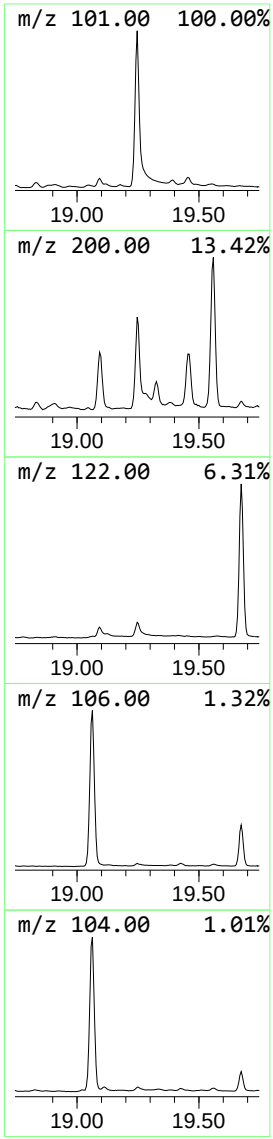
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 Octyl (E)-2-methylbut-2-enoate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.246	0.07 ng	35478	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octyl (E)-2-methylbut-2-enoate	212	C13H24O2	1000373-71-2	4
2	Urea, N,N-dimethyl-N'-2-ethylhexyl-	200	C11H24N2O	1010419-88-4	4
3	Decanoic acid, ethyl ester	200	C12H24O2	000110-38-3	4
4	Octanoic acid, 2,4,6-trimethyl-,...	200	C12H24O2	054984-07-5	4
5	Octan-2-yl (E)-2-methylbut-2-enoate	212	C13H24O2	1000373-76-0	3





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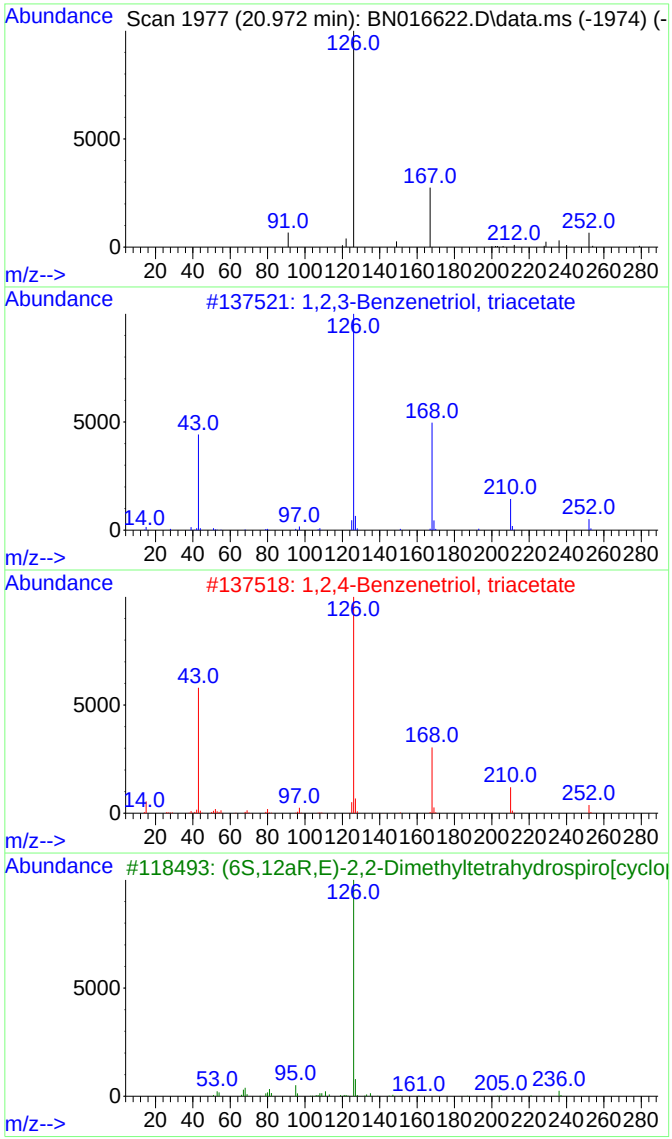
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

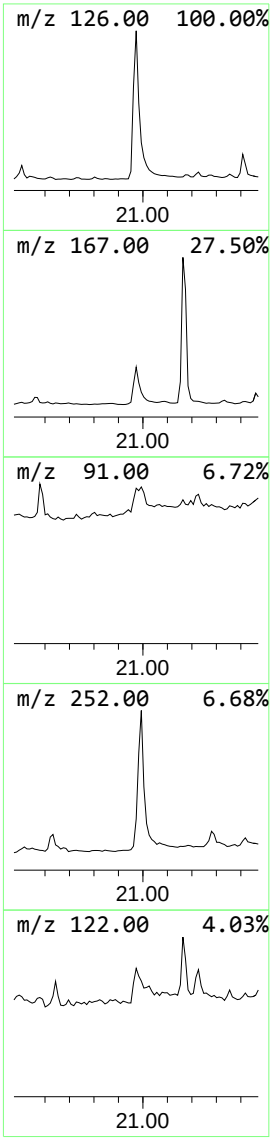
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 17 1,2,3-Benzenetriol, triacetate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.972	0.04 ng	19641	Chrysene-d12	21.227

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,3-Benzenetriol, triacetate	252	C12H12O6	000525-52-0	4
2	1,2,4-Benzenetriol, triacetate	252	C12H12O6	000613-03-6	4
3	(6S,12aR,E)-2,2-Dimethyltetrahyd...	236	C14H24N2O	155975-43-2	4
4	4(1H)-Oxopyridine-1-carboxylic a...	167	C8H9NO3	057330-83-3	4
5	Bicyclo[2.2.1]heptane-1,2-dicarb...	212	C11H16O4	1000191-44-2	4





Tentatively Identified Compound (LSC) summary

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Data File : BN016622.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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetic acid, me...	3.816	0.1	ng	18903	1	7.642	103441	0.4
Butane	4.821	0.3	ng	70682	1	7.642	103441	0.4
Benzene, chloro-	4.996	0.1	ng	18784	1	7.642	103441	0.4
Propanal	6.379	0.1	ng	23900	1	7.642	103441	0.4
Cyclopentanecar...	6.646	0.0	ng	12803	1	7.642	103441	0.4
2-Aminopropanen...	7.264	0.1	ng	15197	1	7.642	103441	0.4
3-Penten-2-ol	7.863	0.1	ng	29242	1	7.642	103441	0.4
Butane	8.168	0.1	ng	17794	1	7.642	103441	0.4
5-Amino-3,4-dim...	8.306	0.1	ng	13268	1	7.642	103441	0.4
Isopropyl isoth...	10.191	0.1	ng	39985	2	10.406	194048	0.4
Thiazolo[5,4-d]...	15.956	0.8	ng	341604	4	17.017	161985	0.4
7-Methyl 8-nitr...	17.163	0.0	ng	20074	4	17.017	161985	0.4
9H-Fluorene, 9-...	17.224	0.0	ng	16659	4	17.017	161985	0.4
1,2-Diphenyleth...	17.309	0.2	ng	65152	4	17.017	161985	0.4
1-Naphthaleneac...	17.954	0.1	ng	41952	4	17.017	161985	0.4
Octyl (E)-2-met...	19.246	0.1	ng	35478	5	21.227	194466	0.4
1,2,3-Benzenetr...	20.972	0.0	ng	19641	5	21.227	194466	0.4