LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031725\
Data File : BF141978.D
Acq On : 17 Mar 2025 13:31
Operator : RC/JU
Sample : Q1574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC1

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-BF031025.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF141978.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.487	567	577	590	rBV	604679	835083	3.27%	1.563%
2	6.498	743	749	768	rVB	577519	825590	3.23%	1.545%
3	6.881	809	814	819	rBV	448077	567019	2.22%	1.061%
4	6.939	819	824	832	rVV	324863	447029	1.75%	0.837%
5	7.434	898	908	913	rBV	414775	584598	2.29%	1.094%
6	8.157	1027	1031	1039	rVB	521954	709577	2.78%	1.328%
7	8.310	1050	1057	1068	rVB3	130222	256710	1.01%	0.480%
8	8.922	1156	1161	1166	rBV	607858	794015	3.11%	1.486%
9	9.233	1209	1214	1219	rBV	784362	994279	3.90%	1.861%
10	9.916	1324	1330	1334	rBV	713524	958031	3.75%	1.793%
11	10.698	1458	1463	1468	rBV	498187	647460	2.54%	1.212%
12	11.398	1578	1582	1584	rBV	532031	689609	2.70%	1.291%
13	11.422	1584	1586	1590	rVB	397012	456119	1.79%	0.854%
14	11.933	1669	1673	1680	rBV3	1492150	2181721	8.55%	4.083%
15	12.727	1804	1808	1814	rBV	1624377	2625854	10.29%	4.914%
16	13.868	1998	2002	2008	rBV2	2241104	4209232	16.49%	7.877%
17	14.051	2026	2033	2042	rBV	13825307	25524333	100.00%	47.766%
18	16.839	2502	2507	2521	rVB	1964853	4671523	18.30%	8.742%
19	17.392	2595	2601	2622	rVB	1902394	5458286	21.38%	10.215%

Sum of corrected areas: 53436068

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031725\
Data File : BF141978.D
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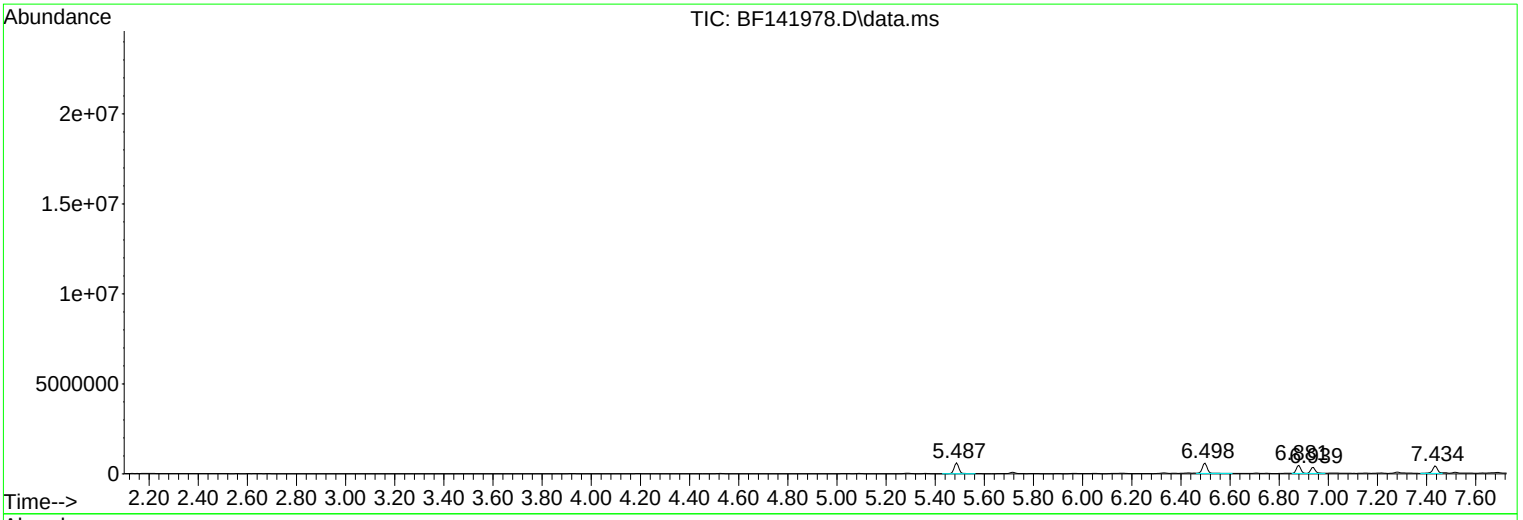
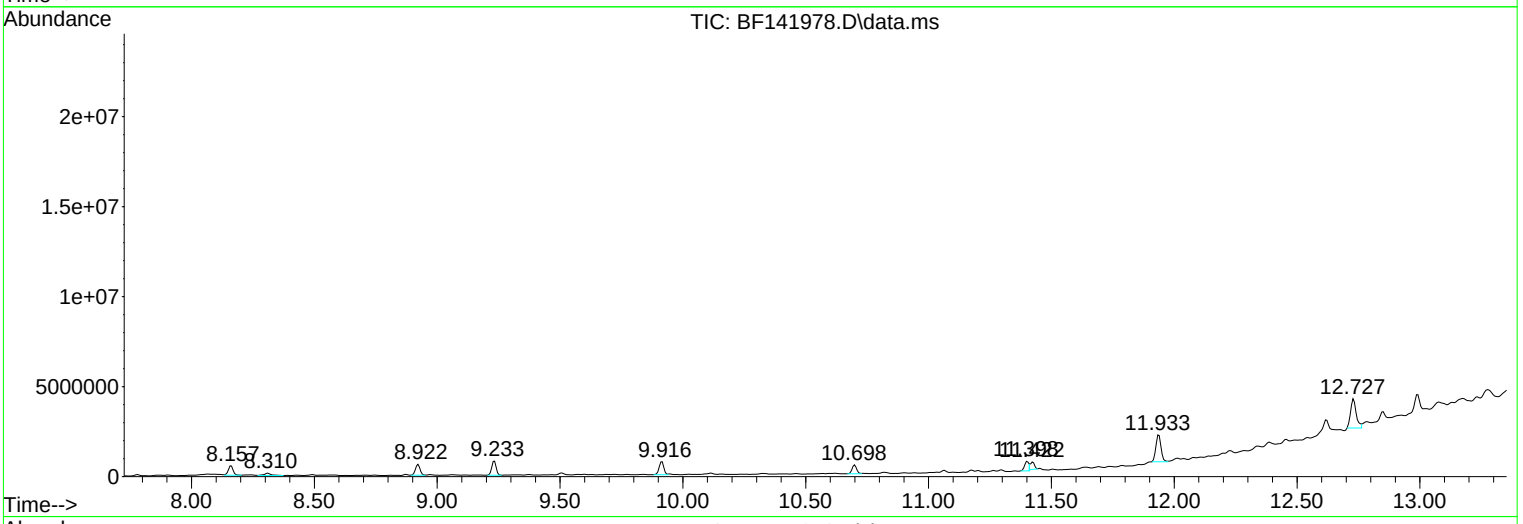
Operator : RC/JU
Sample : Q1574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

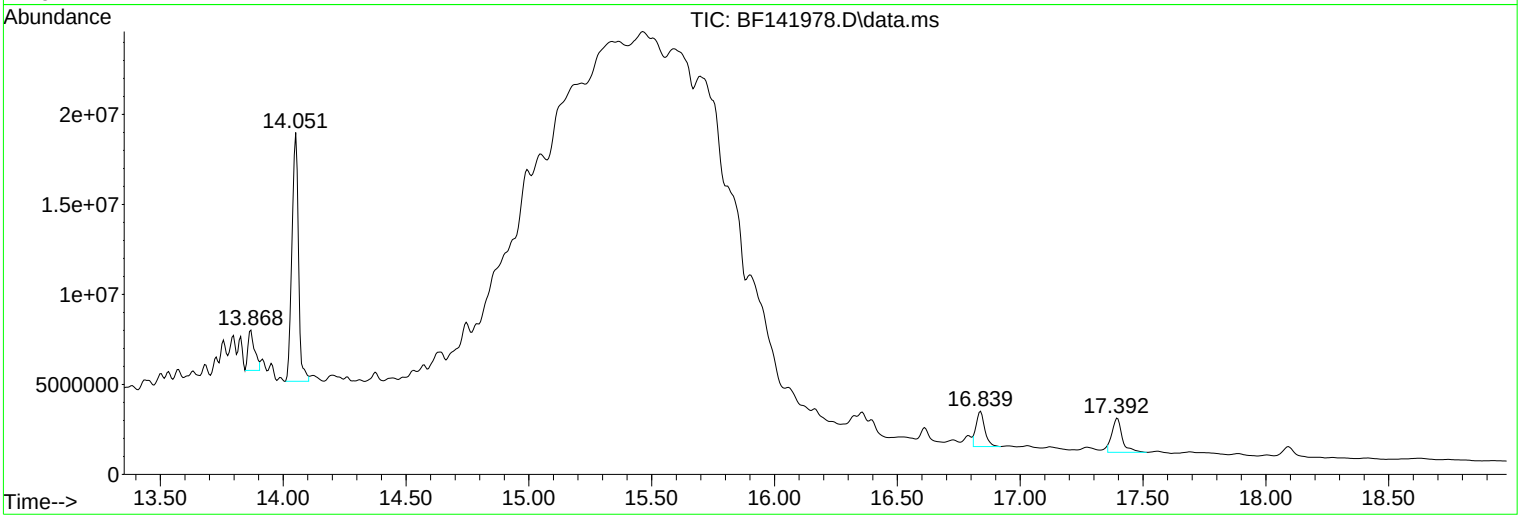
Instrument :
BNA_F
ClientSampleId :
WC1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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

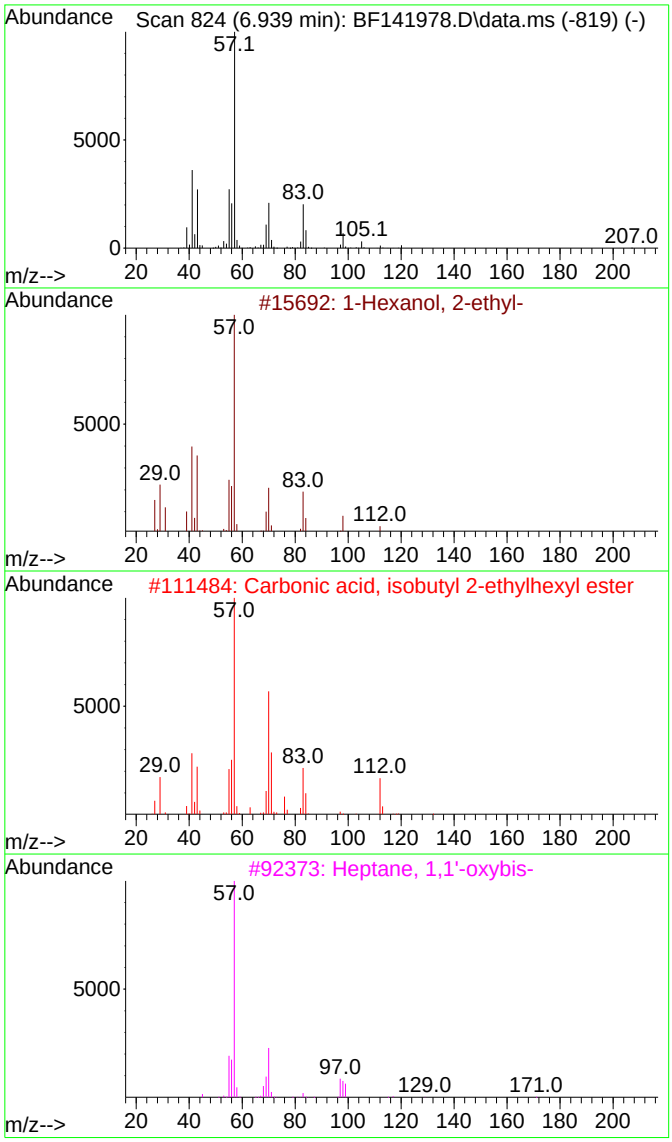
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

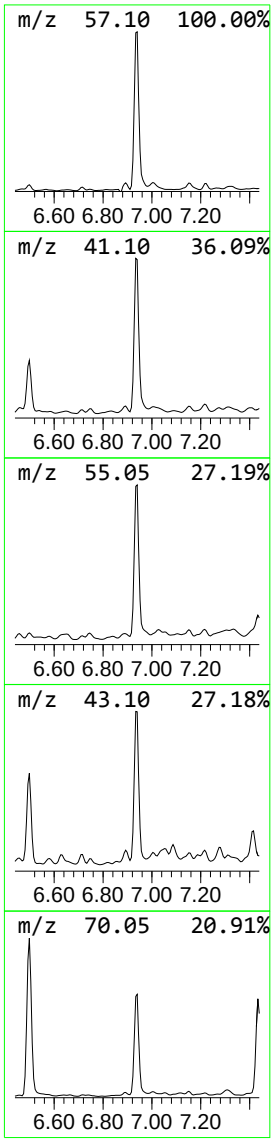
****

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.939	15.77 ng	447029	1,4-Dichlorobenzene-d4	6.881

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	53
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50





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Data File : BF141978.D
Acq On : 17 Mar 2025 13:31
Operator : RC/JU
Sample : Q1574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC1

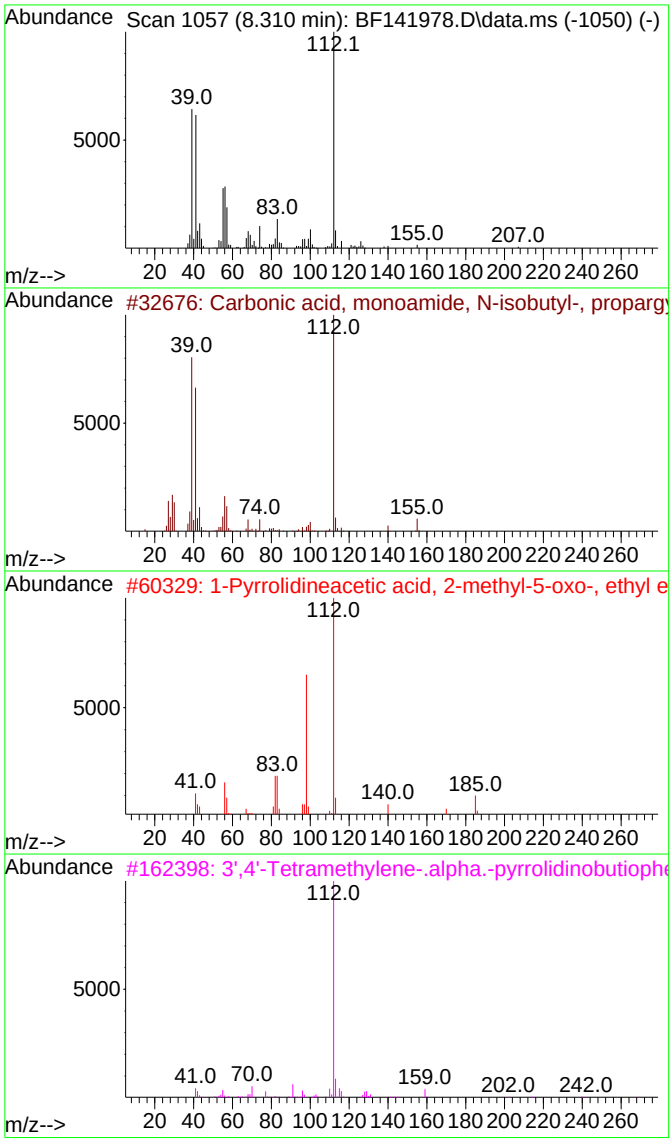
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

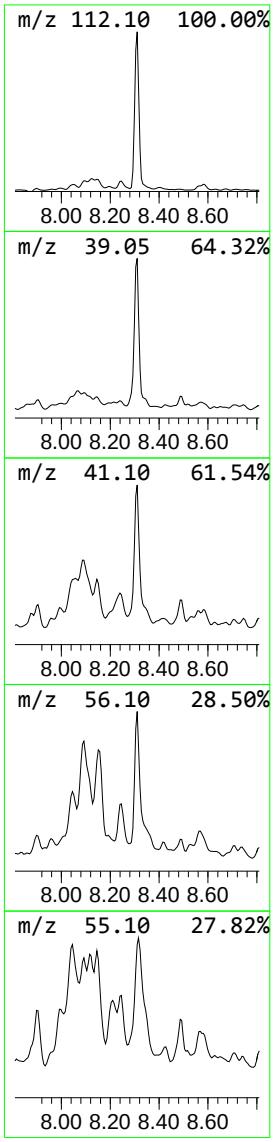
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Carbonic acid, monoamide, N... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.310	7.24 ng	256710	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, monoamide, N-isob...	155	C8H13NO2	1000420-25-2	64
2	1-Pyrrolidineacetic acid, 2-meth...	185	C9H15NO3	033927-64-9	64
3	3',4'-Tetramethylene-.alpha.-pyr...	271	C18H25NO	1000475-84-5	50
4	2-Propanol, 1-(cyclohexylamino)-	157	C9H19NO	000103-00-4	50
5	1,3-Cyclopentanedione, 2-methyl-	112	C6H8O2	000765-69-5	50





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Data File : BF141978.D
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Operator : RC/JU
Sample : Q1574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.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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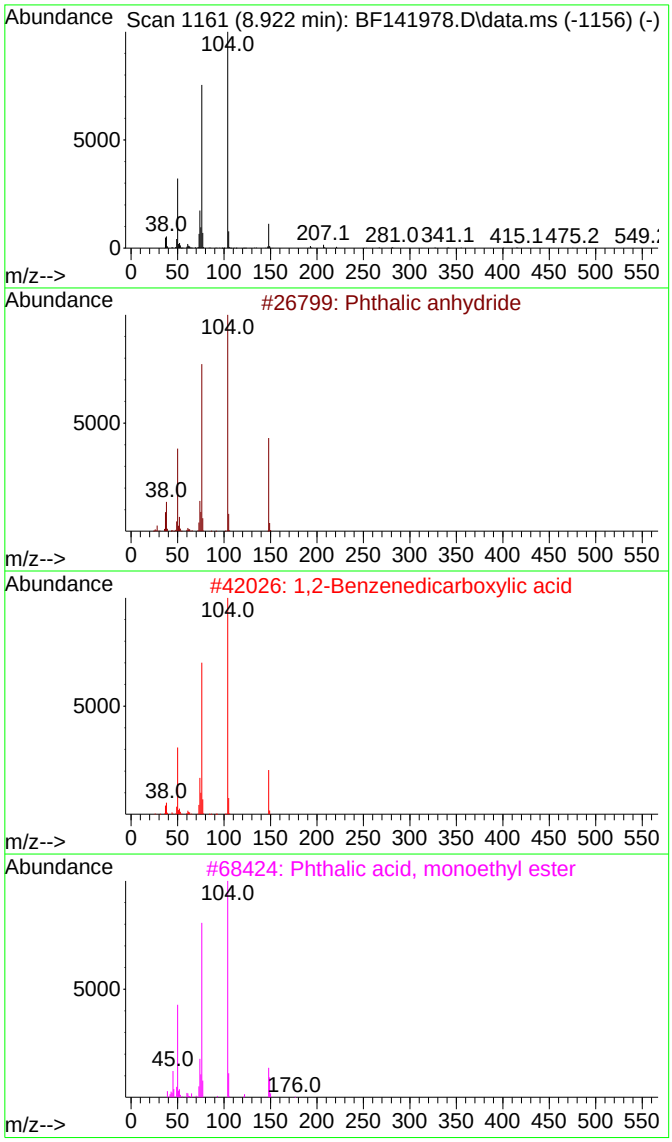
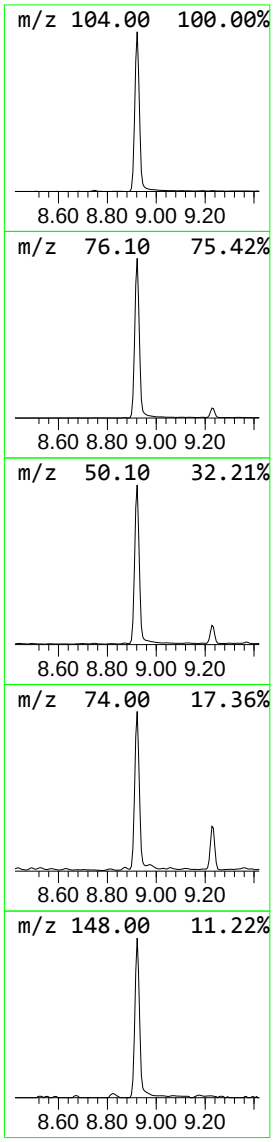
Peak Number 3 Phthalic anhydride Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.922	22.38 ng	794015	Naphthalene-d8	8.163

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	95
2	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	90
3	Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	90
4	Indan-1,2,3-trione	160	C9H4O3	000938-24-9	83
5	Ninhydrin	178	C9H6O4	000485-47-2	83





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Data File : BF141978.D
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Sample : Q1574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

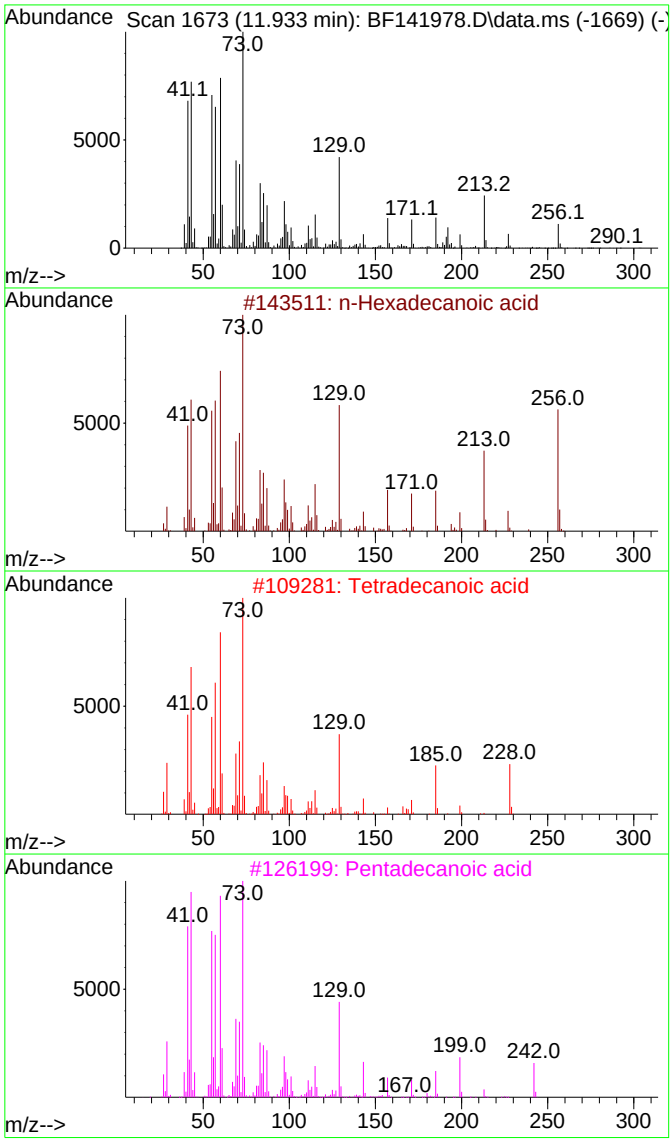
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

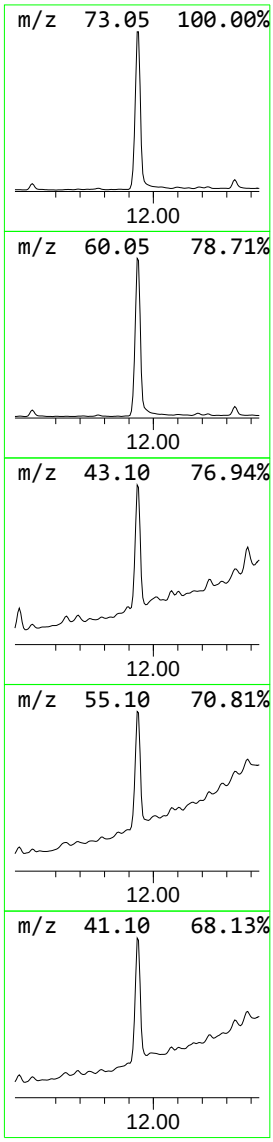
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	63.27 ng	2181720	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031725\
Data File : BF141978.D
Acq On : 17 Mar 2025 13:31
Operator : RC/JU
Sample : Q1574-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

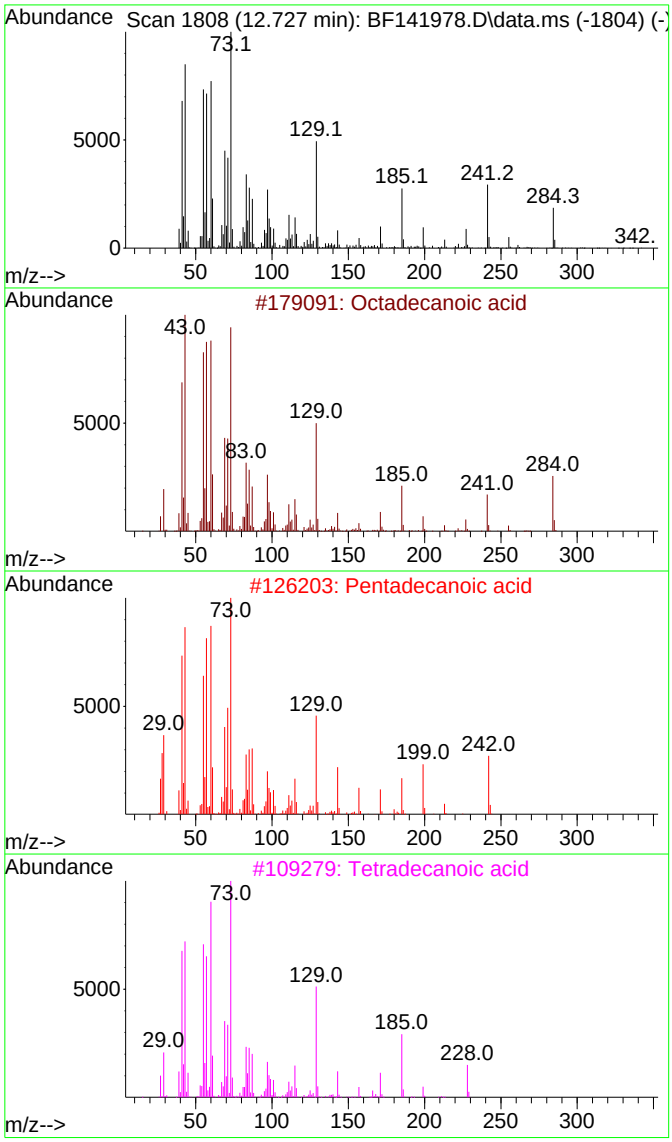
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

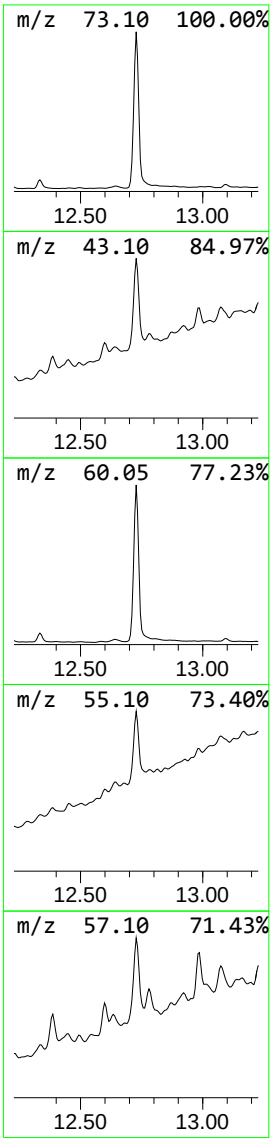
****

Peak Number 5 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.727	2.06 ng	2625850	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

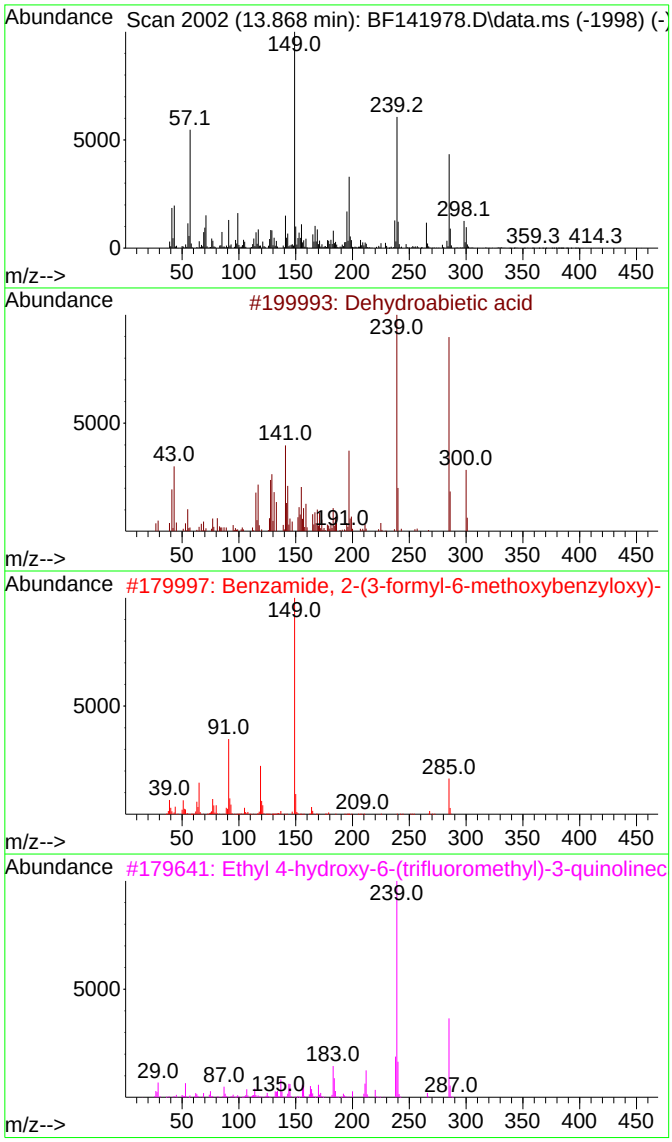
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

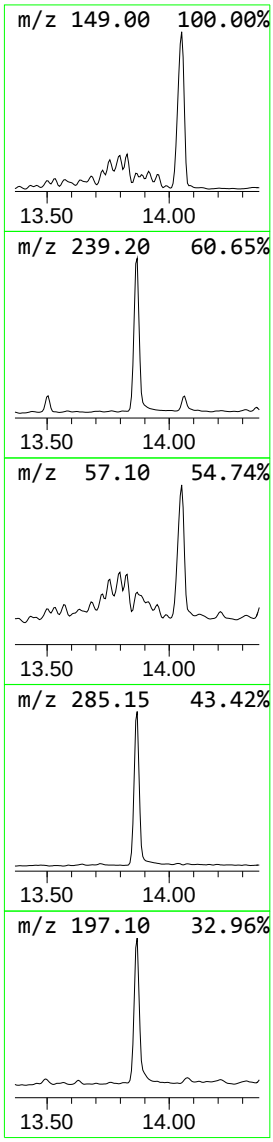
****

Peak Number 6 Dehydroabietic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.868	3.30 ng	4209230	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dehydroabietic acid	300	C20H28O2	001740-19-8	64
2	Benzamide, 2-(3-formyl-6-methoxy...	285	C16H15NO4	1000273-81-6	46
3	Ethyl 4-hydroxy-6-(trifluorometh...	285	C13H10F3NO3	026893-12-9	42
4	Ethyl 4-hydroxy-7-trifluoromethy...	285	C13H10F3NO3	000391-02-6	38
5	Phthalic acid, isohexyl isoporpy...	292	C17H24O4	1000315-00-4	35





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Instrument :
BNA_F
ClientSampleId :
WC1

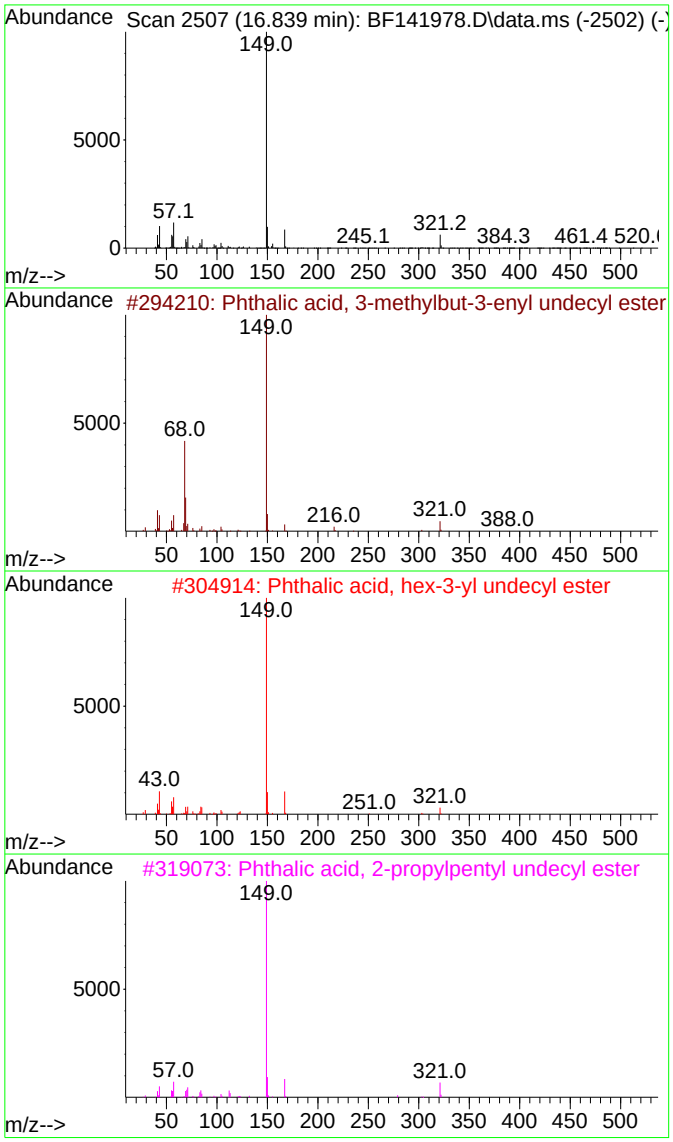
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF031025.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

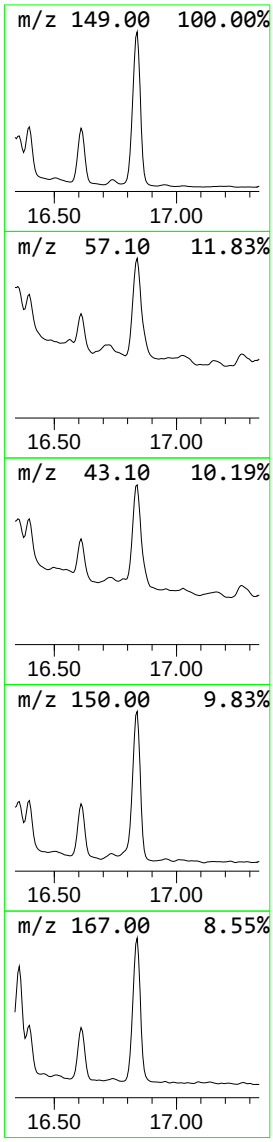
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phthalic acid, 3-methylbut-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.839	20.00 ng	4671520	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, 3-methylbut-3-eny...	388	C24H36O4	1000357-10-9	86
2	Phthalic acid, hex-3-yl undecyl ...	404	C25H40O4	1000356-96-2	86
3	Phthalic acid, 2-propylpentyl un...	432	C27H44O4	1000377-92-7	86
4	Phthalic acid, hept-3-yl nonyl e...	390	C24H38O4	1000356-99-3	80
5	Phthalic acid, 2-ethylbutyl unde...	404	C25H40O4	1000356-89-6	80





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Instrument :
BNA_F
ClientSampleId :
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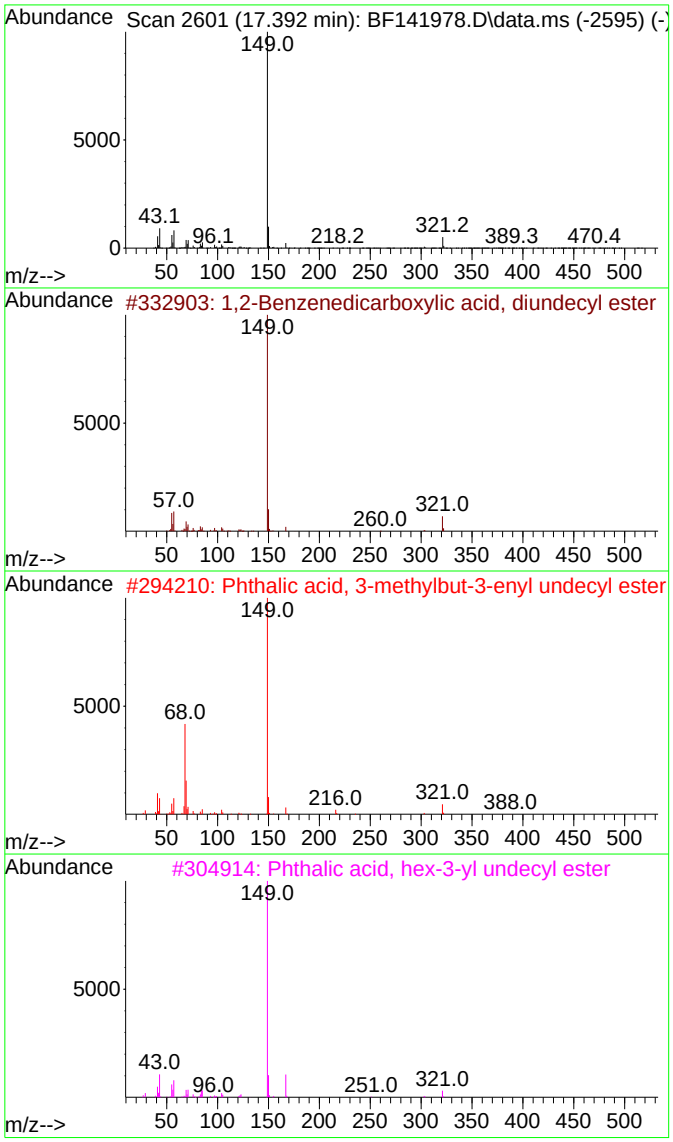
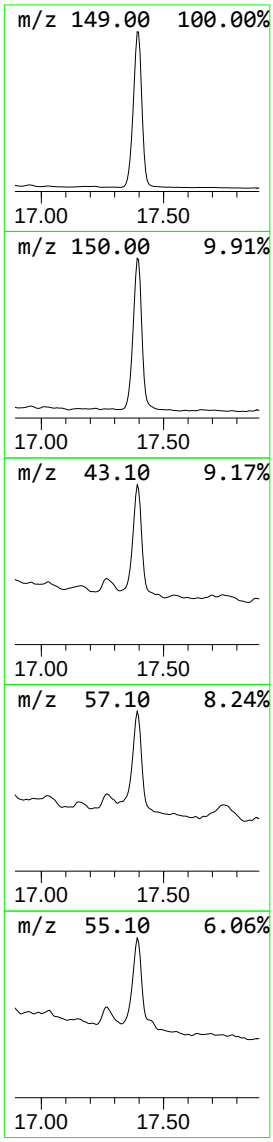
Peak Number 8 1,2-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.392	23.37 ng	5458290	Perylene-d12	15.621

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, di...	474	C30H50O4	003648-20-2	91
2	Phthalic acid, 3-methylbut-3-eny...	388	C24H36O4	1000357-10-9	90
3	Phthalic acid, hex-3-yl undecyl ...	404	C25H40O4	1000356-96-2	86
4	Phthalic acid, 2-ethylbutyl unde...	404	C25H40O4	1000356-89-6	86
5	Didecyl phthalate	446	C28H46O4	000084-77-5	80





Tentatively Identified Compound (LSC) summary

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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
1-Hexanol, 2-et...	6.939	15.8	ng	447029	1	6.881	567019	20.0
Carbonic acid, ...	8.310	7.2	ng	256710	2	8.163	709577	20.0
Phthalic anhydride	8.922	22.4	ng	794015	2	8.163	709577	20.0
n-Hexadecanoic ...	11.933	63.3	ng	2181720	4	11.398	689609	20.0
Octadecanoic acid	12.727	2.1	ng	2625850	5	14.057	25524300	20.0
Dehydroabietic ...	13.868	3.3	ng	4209230	5	14.057	25524300	20.0
Phthalic acid, ...	16.839	20.0	ng	4671520	6	15.621	4671520	20.0
1,2-Benzenedica...	17.392	23.4	ng	5458290	6	15.621	4671520	20.0