LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061522\
Data File : BP010743.D
Acq On : 15 Jun 2022 22:55
Operator : CG/JU
Sample : N3354-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-58

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-BP060722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP010743.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.416	389	396	414	rBV	962885	1471571	14.31%	4.117%
2	7.010	658	667	680	rBV	645456	1089942	10.60%	3.049%
3	7.828	799	806	815	rBV	295871	479533	4.66%	1.342%
4	8.198	863	869	878	rVB	155185	253345	2.46%	0.709%
5	8.992	998	1004	1020	rVB	1391036	2510134	24.40%	7.022%
6	9.457	1078	1083	1090	rVB	90261	141557	1.38%	0.396%
7	10.028	1170	1180	1189	rBV2	78393	155148	1.51%	0.434%
8	10.628	1270	1282	1288	rBV	431009	751879	7.31%	2.103%
9	12.510	1589	1602	1607	rBV3	70240	167710	1.63%	0.469%
10	13.092	1693	1701	1715	rBV	3729871	5489297	53.36%	15.357%
11	14.192	1883	1888	1897	rVB	81966	126039	1.23%	0.353%
12	14.469	1929	1935	1941	rBV	749265	1118586	10.87%	3.129%
13	15.963	2183	2189	2203	rVB	3721850	5360048	52.11%	14.995%
14	17.221	2398	2403	2412	rBV	1030530	1479570	14.38%	4.139%
15	17.892	2514	2517	2522	rVB	132422	155508	1.51%	0.435%
16	18.116	2551	2555	2561	rBV	145966	214123	2.08%	0.599%
17	19.027	2706	2710	2719	rVB	236585	293486	2.85%	0.821%
18	19.786	2833	2839	2847	rBV	8826142	10286551	100.00%	28.777%
19	21.021	3045	3049	3056	rBV	370943	454748	4.42%	1.272%
20	21.309	3093	3098	3105	rBV	1475404	1910932	18.58%	5.346%
21	23.703	3498	3505	3514	rVB2	876368	1835482	17.84%	5.135%

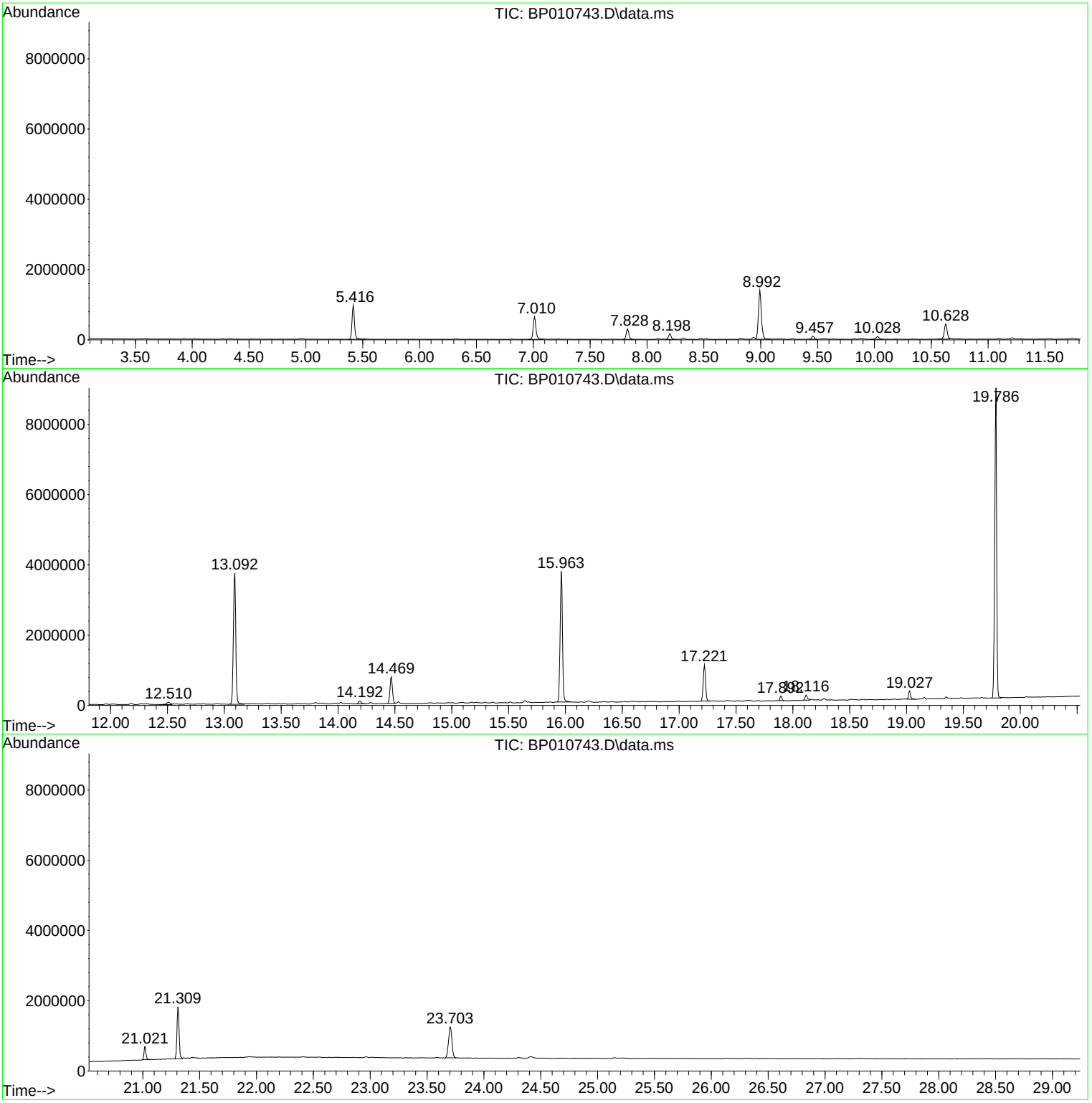
Sum of corrected areas: 35745189

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061522\
Data File : BP010743.D
Acq On : 15 Jun 2022 22:55
Operator : CG/JU
Sample : N3354-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-58

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060722.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_P\Data\BP061522\
Data File : BP010743.D
Acq On : 15 Jun 2022 22:55
Operator : CG/JU
Sample : N3354-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

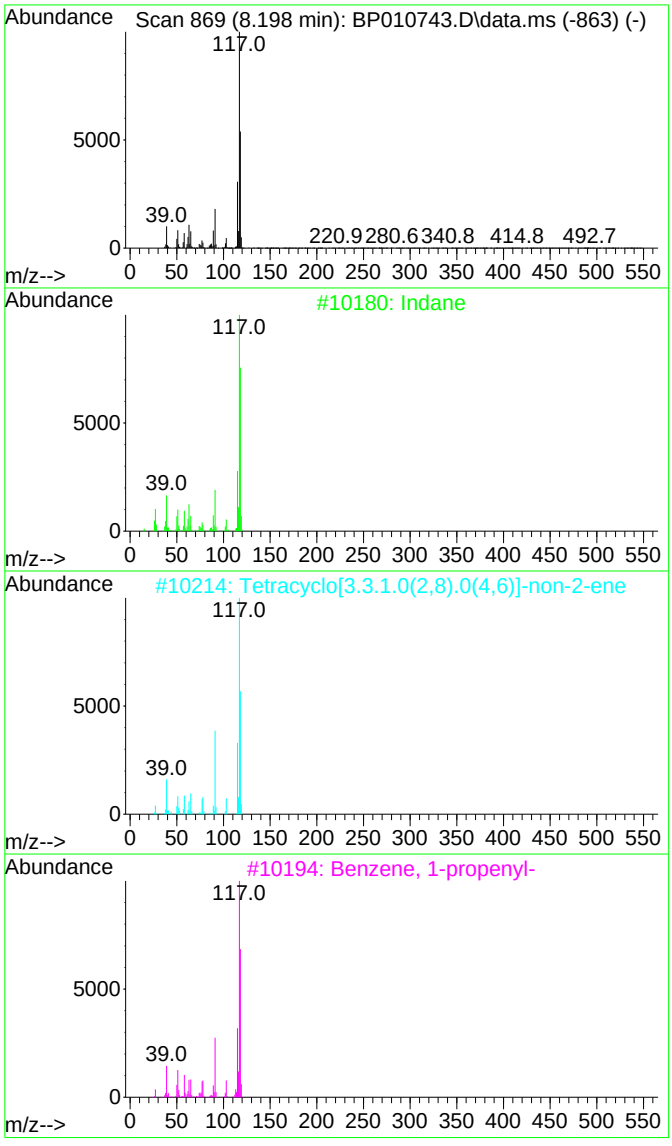
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

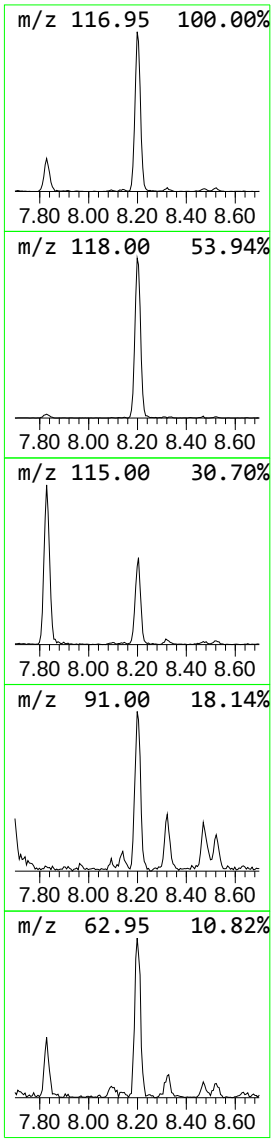
****

Peak Number 1 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.198	10.57 ng	253345	1,4-Dichlorobenzene-d4	7.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	90
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	80
3	Benzene, 1-propenyl-	118	C9H10	000637-50-3	74
4	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	72
5	Deltacyclene	118	C9H10	007785-10-6	68





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061522\
Data File : BP010743.D
Acq On : 15 Jun 2022 22:55
Operator : CG/JU
Sample : N3354-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-58

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

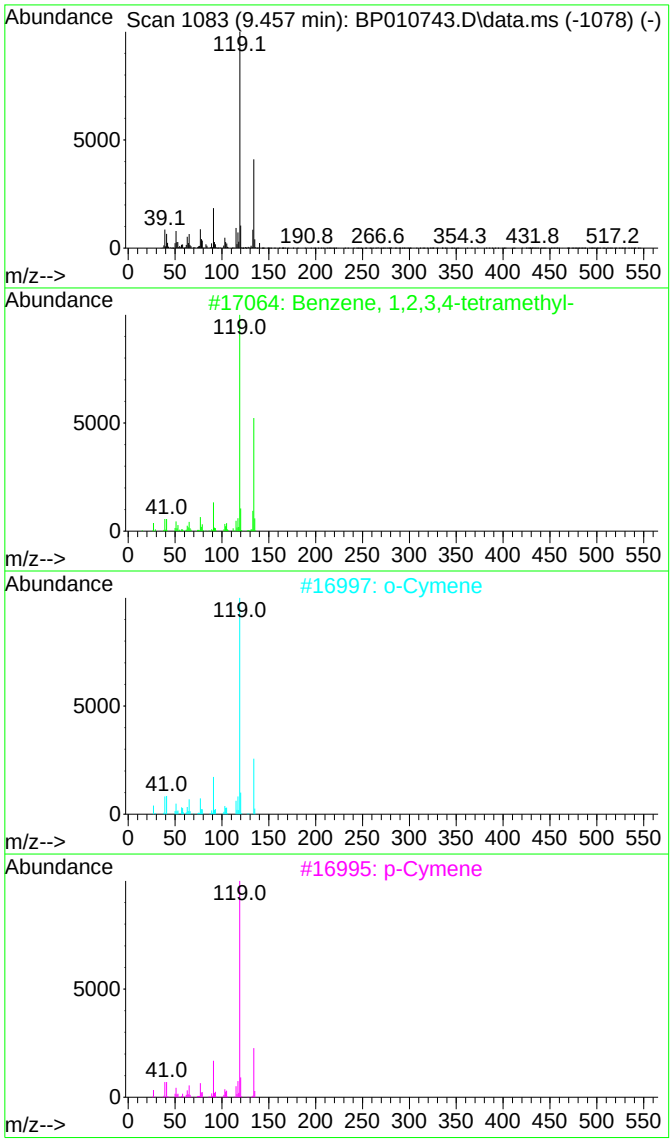
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

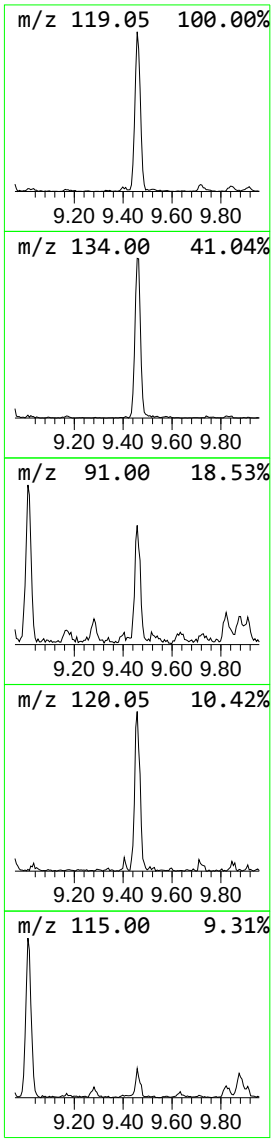
****

Peak Number 2 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.457	3.77 ng	141557	Naphthalene-d8	10.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2	o-Cymene	134	C10H14	000527-84-4	95
3	p-Cymene	134	C10H14	000099-87-6	93
4	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
5	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061522\
Data File : BP010743.D
Acq On : 15 Jun 2022 22:55
Operator : CG/JU
Sample : N3354-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-58

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

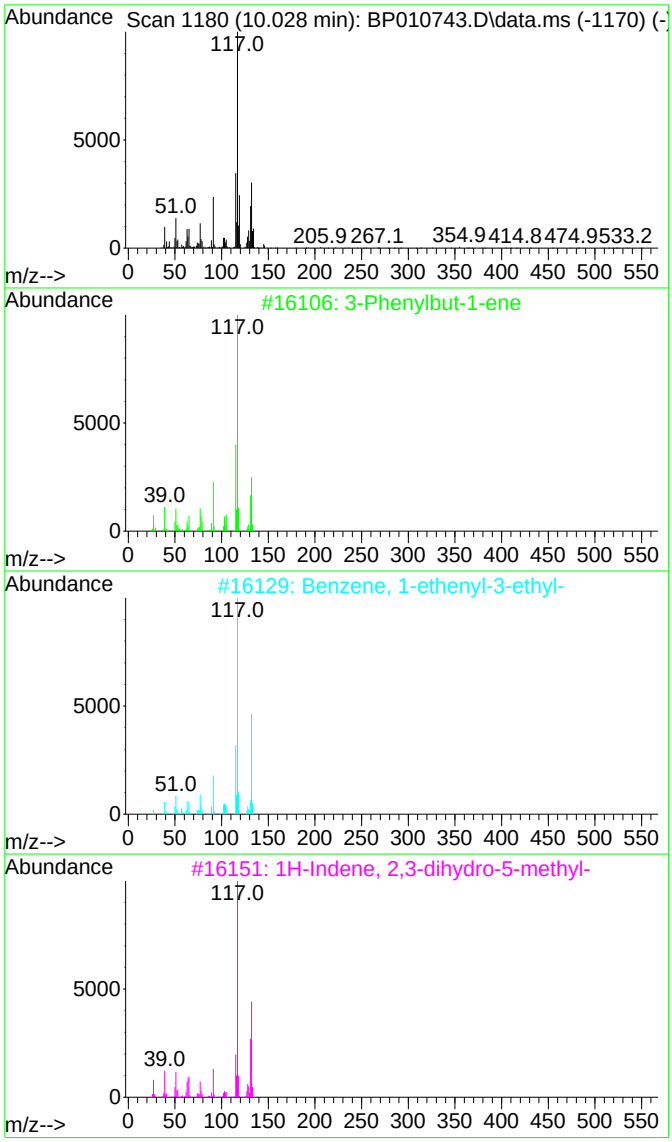
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

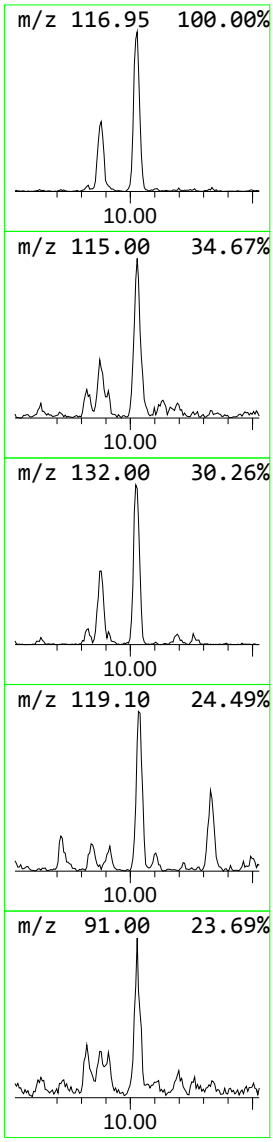
****

Peak Number 3 3-Phenylbut-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.028	4.13 ng	155148	Naphthalene-d8	10.628

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	76
3	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	72
4	Benzene, 2-ethenyl-1,3-dimethyl-	132	C10H12	002039-90-9	68
5	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061522\
Data File : BP010743.D
Acq On : 15 Jun 2022 22:55
Operator : CG/JU
Sample : N3354-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-58

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

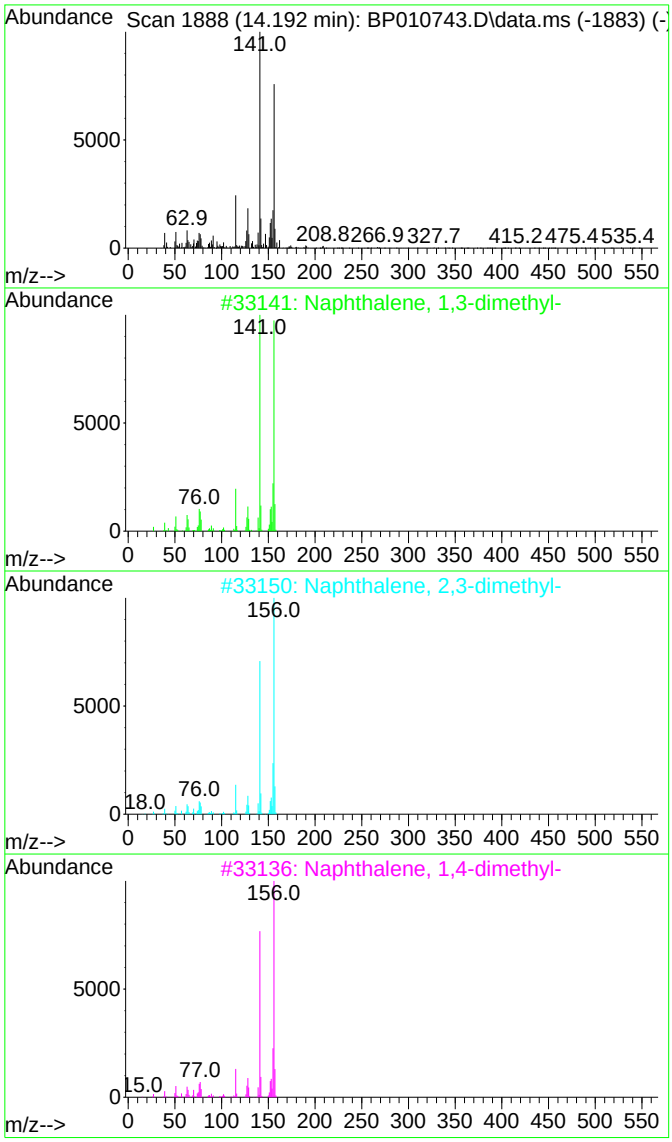
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

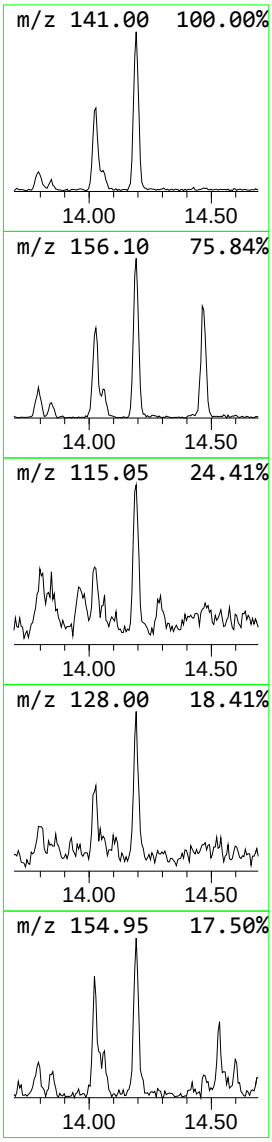
****

Peak Number 4 Naphthalene, 1,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.192	2.25 ng	126039	Acenaphthene-d10	14.469

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	95
3	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	94
4	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	93
5	Naphthalene, 1,8-dimethyl-	156	C12H12	000569-41-5	93





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Acq On : 15 Jun 2022 22:55
Operator : CG/JU
Sample : N3354-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-58

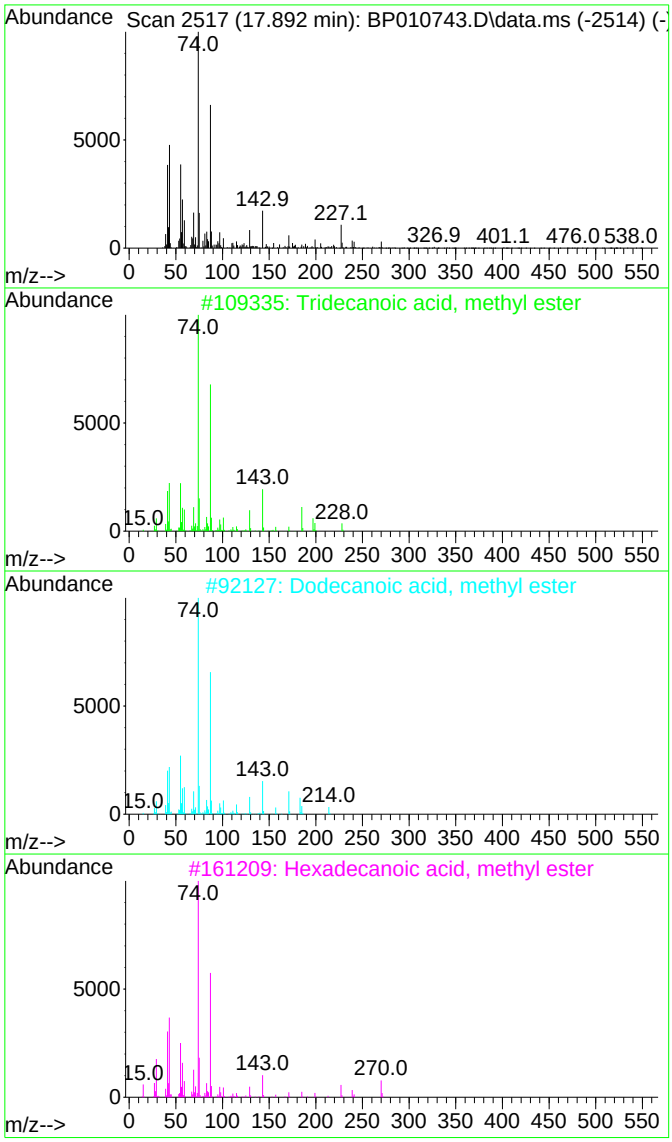
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

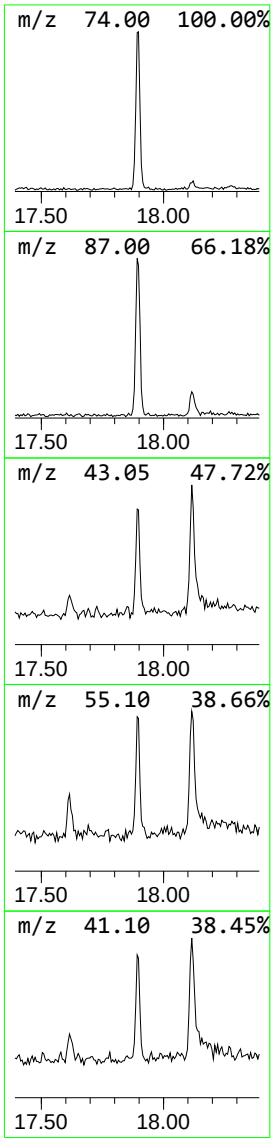
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Tridecanoic acid, methyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.892	2.10 ng	155508	Phenanthrene-d10	17.221

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
2	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	91
3	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	90
4	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	87
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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Data File : BP010743.D
Acq On : 15 Jun 2022 22:55
Operator : CG/JU
Sample : N3354-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-58

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

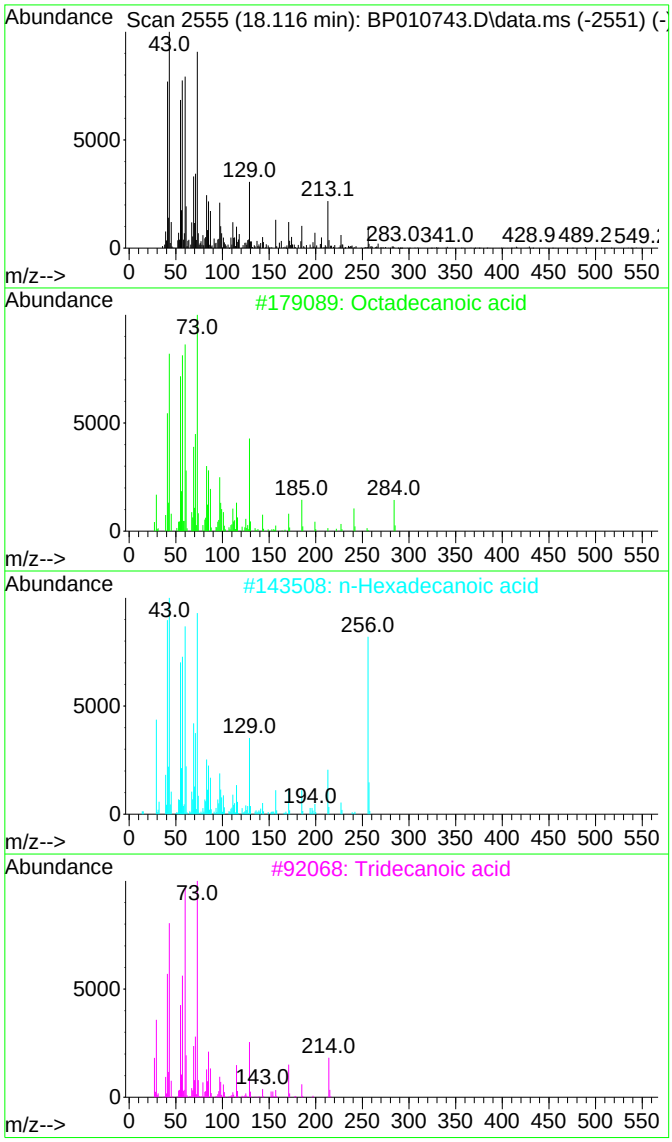
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

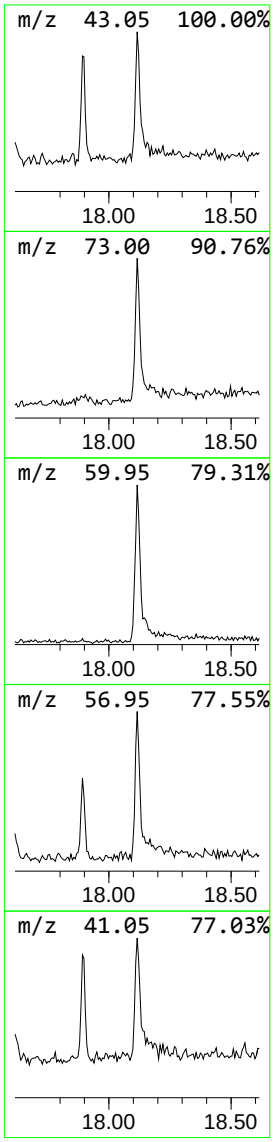
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.116	2.89 ng	214123	Phenanthrene-d10	17.221

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Data File : BP010743.D
Acq On : 15 Jun 2022 22:55
Operator : CG/JU
Sample : N3354-14
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
MW-58

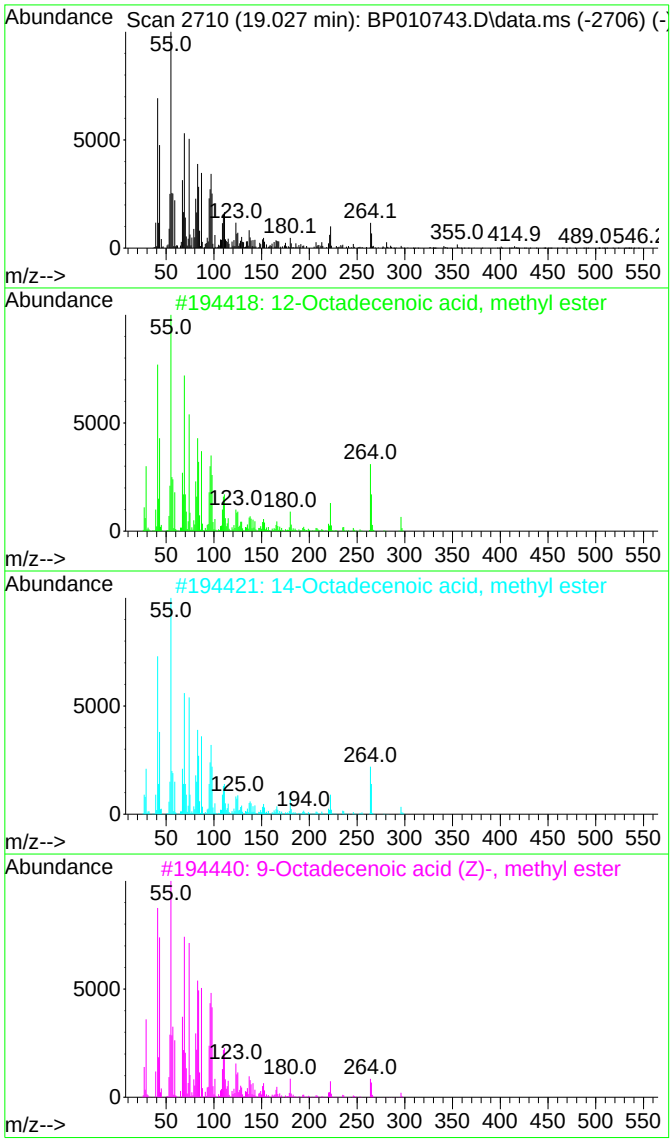
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP060722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

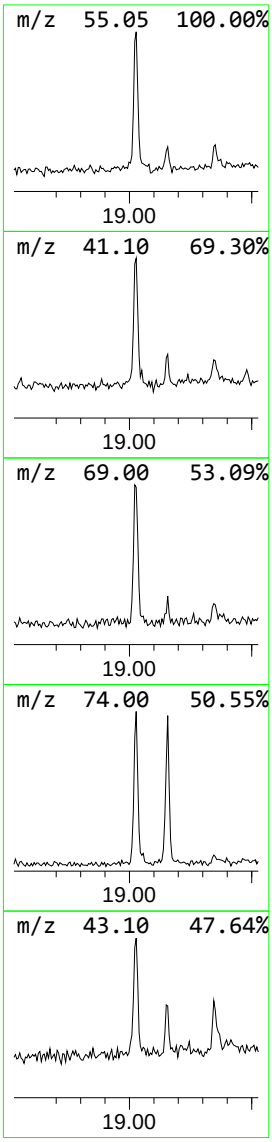
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 12-Octadecenoic acid, methy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.027	3.97 ng	293486	Phenanthrene-d10	17.221

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	98
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	98
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	96
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	94
5	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93





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ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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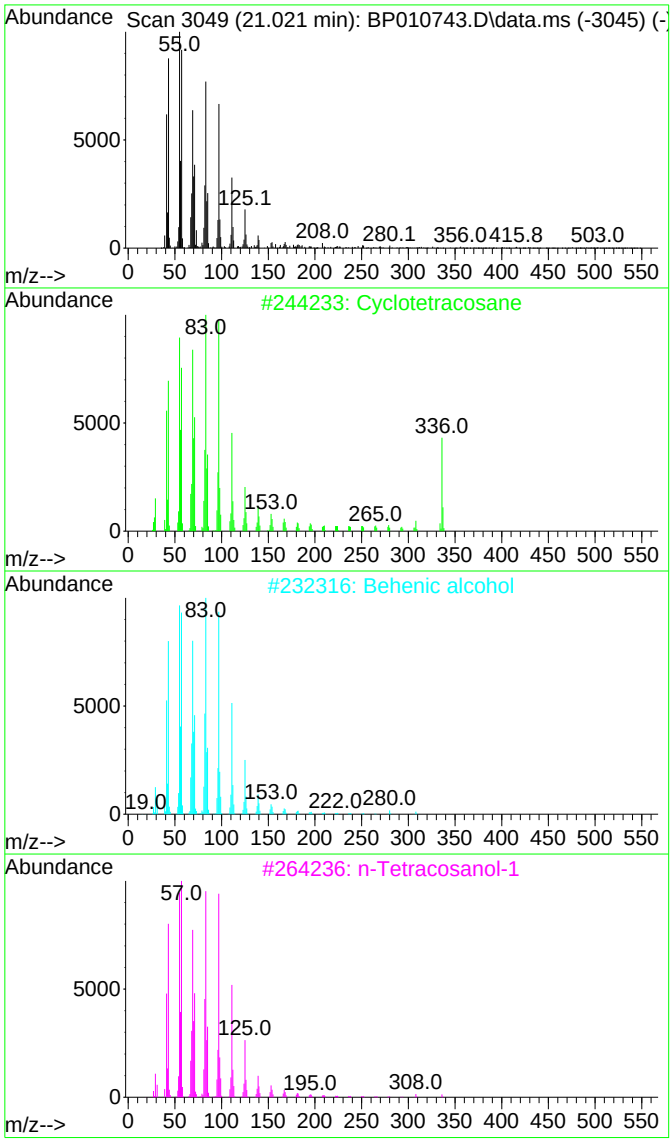
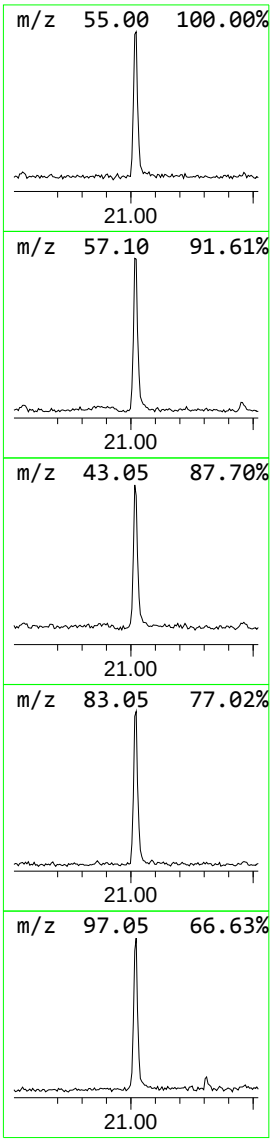
****

Peak Number 8 Cyclotetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.021	4.76 ng	454748	Chrysene-d12	21.309

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetracosane	336	C24H48	000297-03-0	96
2	Behenic alcohol	326	C22H46O	000661-19-8	93
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5	1-Octadecanol	270	C18H38O	000112-92-5	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061522\
Data File : BP010743.D
Acq On : 15 Jun 2022 22:55
Operator : CG/JU
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BNA_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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Indane	8.198	10.6	ng	253345	1	7.828	479533	20.0
Benzene, 1,2,3,...	9.457	3.8	ng	141557	2	10.628	751879	20.0
3-Phenylbut-1-ene	10.028	4.1	ng	155148	2	10.628	751879	20.0
Naphthalene, 1,...	14.192	2.3	ng	126039	3	14.469	1118590	20.0
Tridecanoic aci...	17.892	2.1	ng	155508	4	17.221	1479570	20.0
Octadecanoic acid	18.116	2.9	ng	214123	4	17.221	1479570	20.0
12-Octadecenoic...	19.027	4.0	ng	293486	4	17.221	1479570	20.0
Cyclotetracosane	21.021	4.8	ng	454748	5	21.309	1910930	20.0