LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048332.D
Acq On : 4 Mar 2021 17:25
Operator : CG/JU
Sample : M1545-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RIM-7.55

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_G\METHODS\8270-BG021021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.699	393	402	413	rBV	380400	674522	19.15%	4.034%
2	7.327	671	679	685	rBV	233125	463017	13.14%	2.769%
3	7.379	686	688	696	rVB3	45640	65088	1.85%	0.389%
4	7.632	725	731	735	rBV	35974	59928	1.70%	0.358%
5	7.679	735	739	746	rVB2	33540	51772	1.47%	0.310%
6	7.873	764	772	783	rBV2	74572	136134	3.86%	0.814%
7	8.102	806	811	819	rVB	134333	229406	6.51%	1.372%
8	9.283	1004	1012	1028	rVB	510481	953911	27.08%	5.705%
9	9.824	1096	1104	1115	rBV	1151326	2000622	56.80%	11.965%
10	10.552	1220	1228	1241	rBV9	22556	81458	2.31%	0.487%
11	10.693	1244	1252	1261	rVB6	18509	45925	1.30%	0.275%
12	10.922	1283	1291	1298	rBV	166038	319317	9.07%	1.910%
13	11.445	1372	1380	1389	rBV	492920	908770	25.80%	5.435%
14	11.669	1412	1418	1426	rVB3	29468	59846	1.70%	0.358%
15	12.074	1480	1487	1495	rBV5	25267	77041	2.19%	0.461%
16	12.315	1515	1528	1532	rBV5	18673	65260	1.85%	0.390%
17	12.961	1633	1638	1644	rBV2	57162	96172	2.73%	0.575%
18	13.355	1698	1705	1716	rVB	1225058	2057982	58.42%	12.308%
19	14.183	1841	1846	1852	rBV	21288	36159	1.03%	0.216%
20	14.736	1933	1940	1949	rVB	301771	480625	13.64%	2.875%
21	16.240	2189	2196	2207	rBV	1266651	2003926	56.89%	11.985%
22	17.485	2399	2408	2419	rBV	403750	638919	18.14%	3.821%
23	19.101	2678	2683	2689	rBV	81993	115311	3.27%	0.690%
24	20.082	2844	2850	2856	rBV	2719066	3522501	100.00%	21.067%
25	21.375	3065	3070	3080	rBV4	62029	128285	3.64%	0.767%
26	21.763	3130	3136	3144	rBV	421128	718854	20.41%	4.299%
27	25.059	3689	3697	3712	rVB2	251248	729322	20.70%	4.362%

Sum of corrected areas: 16720073

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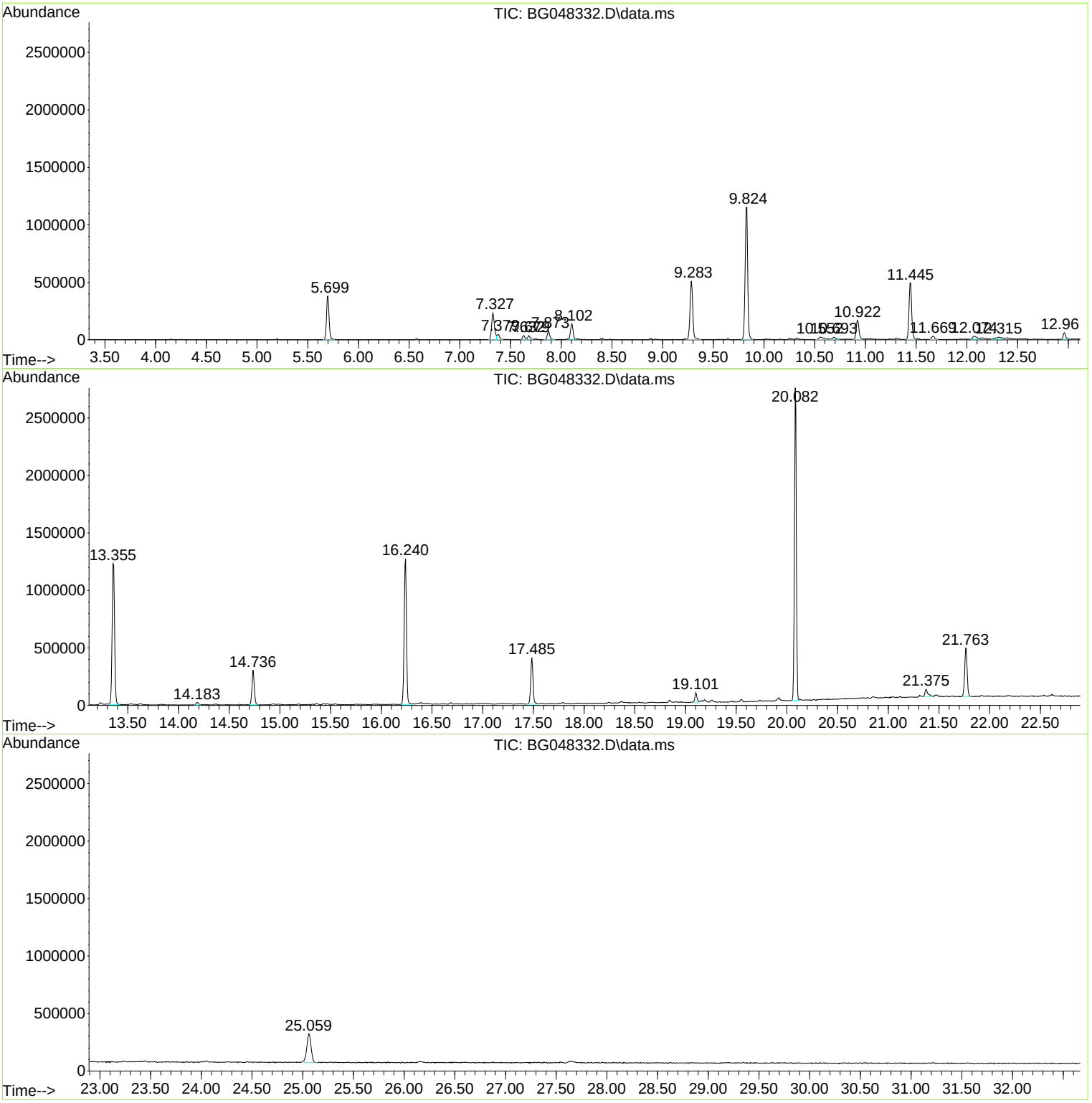
Instrument :
BNA_G
ClientSampleId :
RIM-7.55

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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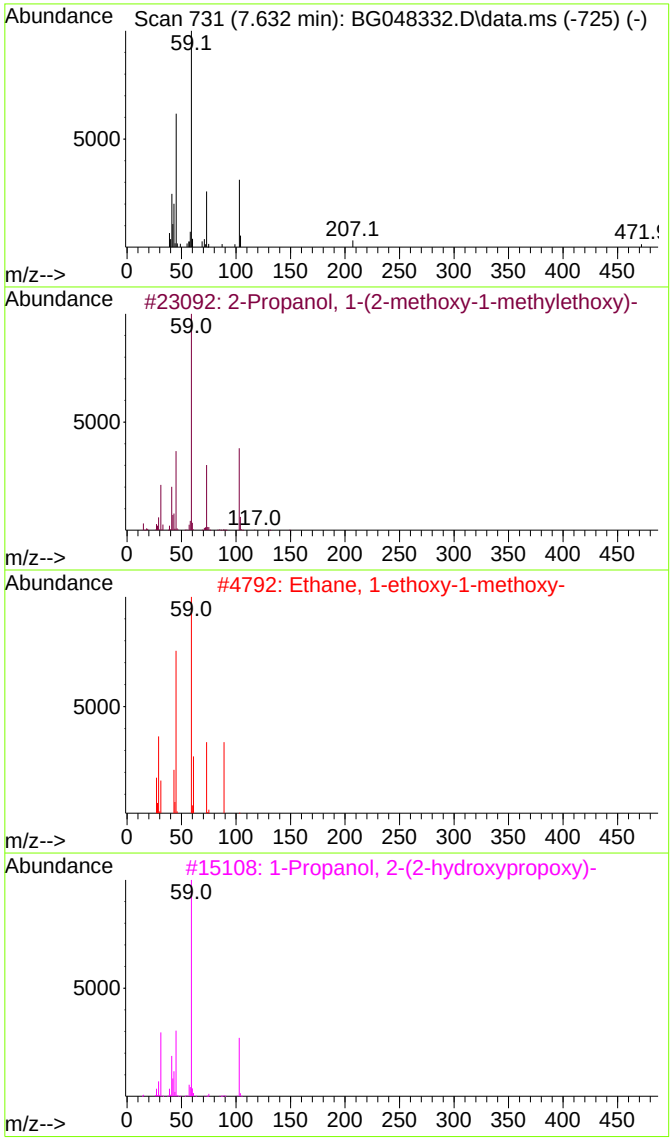
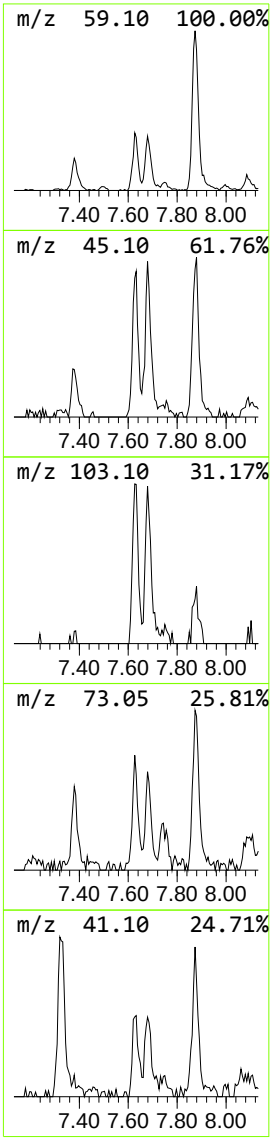
****
Peak Number 1 2-Propanol, 1-(2-methoxy-1-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.632	5.22 ng	59928	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
2	Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	59
3	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	53
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	53
5	2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	53





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Operator : CG/JU
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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RIM-7.55

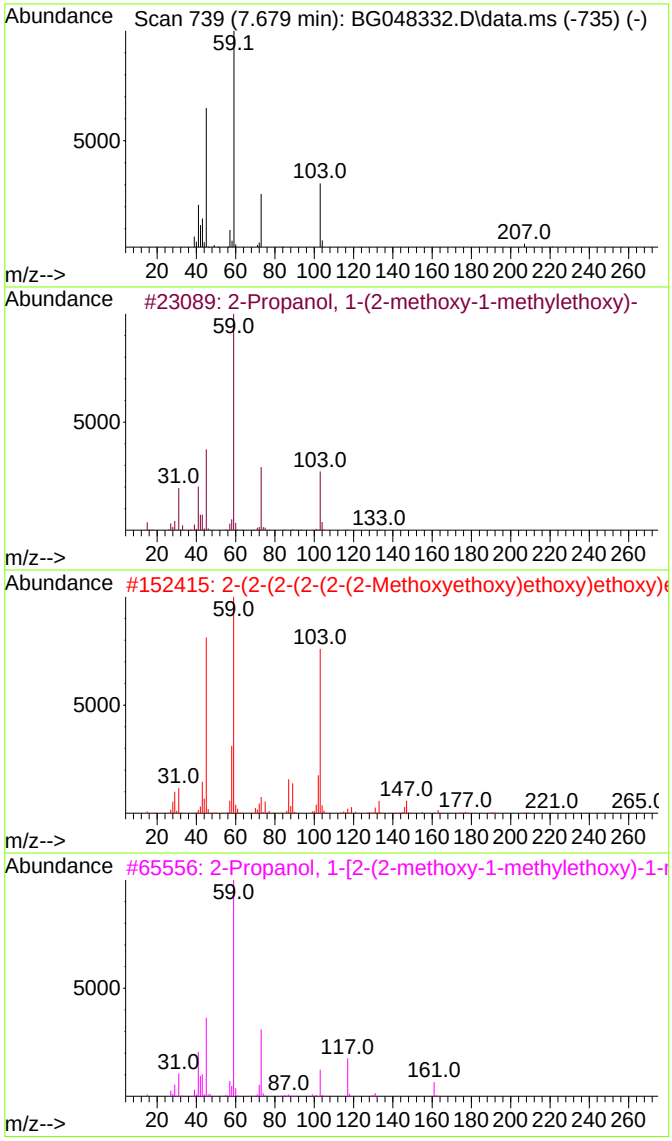
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

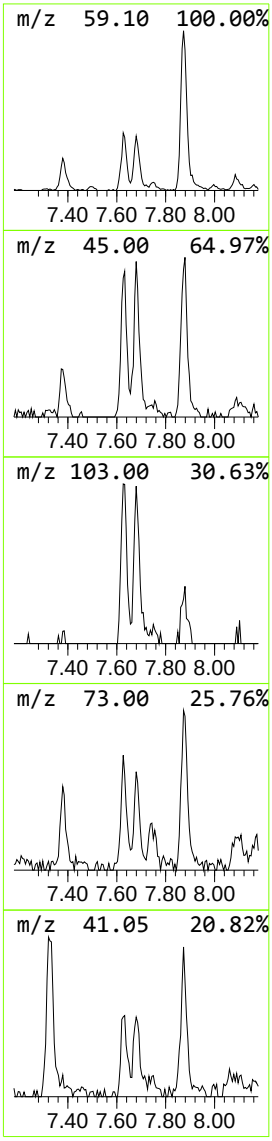
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-(2-(2-(2-(2-Methoxyeth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.679	4.51 ng	51772	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
2	2-(2-(2-(2-(2-Methoxyethoxy)e...	310	C13H26O8	1000366-93-3	59
3	2-Propanol, 1-[2-(2-methoxy-1-me...	206	C10H22O4	020324-33-8	59
4	1-Propanol, 2-(2-methoxy-1-methy...	148	C7H16O3	055956-21-3	50
5	2-(2-(2-(2-(2-Methoxyethoxy)etho...	266	C11H22O7	1000366-84-6	45





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Sample : M1545-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RIM-7.55

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
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TIC Library : C:\Database\NIST11.L
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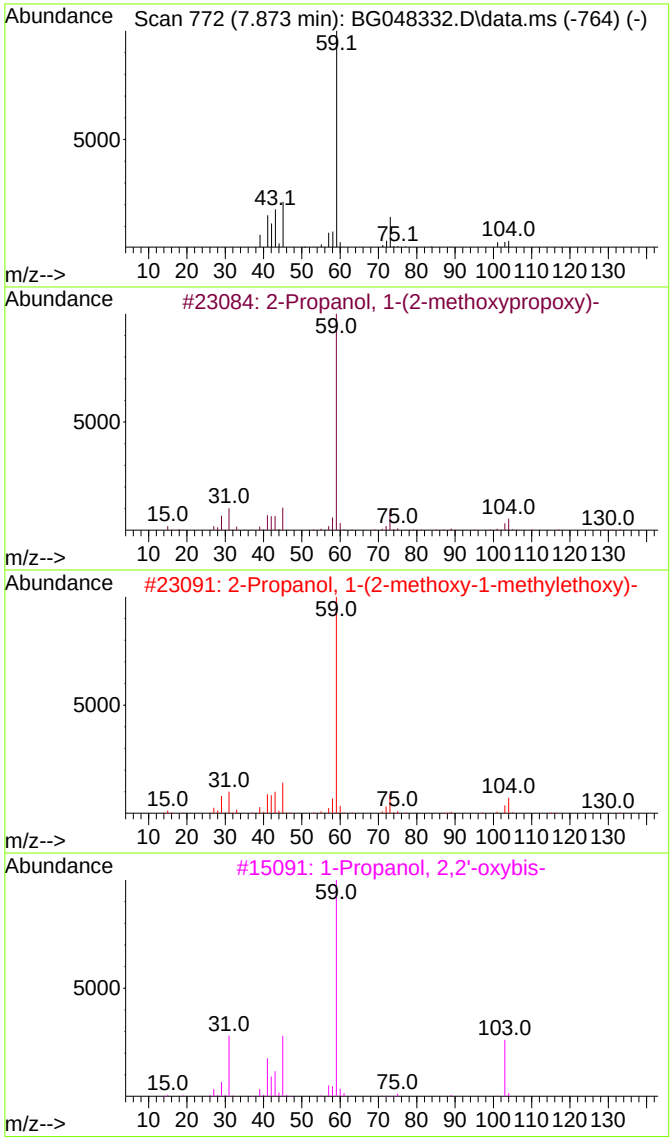
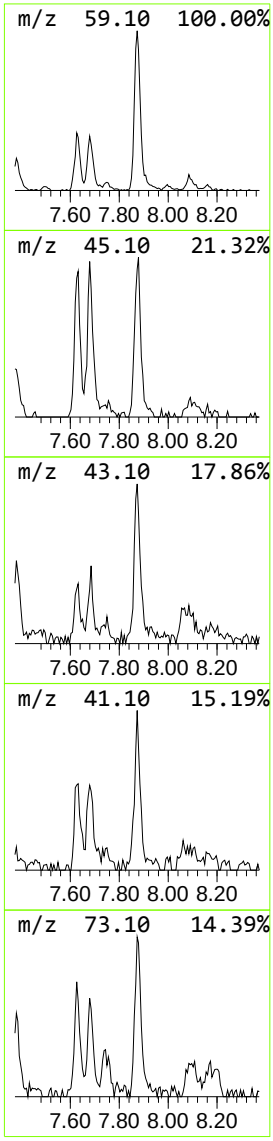
****
Peak Number 3 2-Propanol, 1-(2-methoxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.873	11.87 ng	136134	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	78
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	64
3	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	56
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	50
5	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	45





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Instrument : BNA_G
ClientSampleId : RIM-7.55

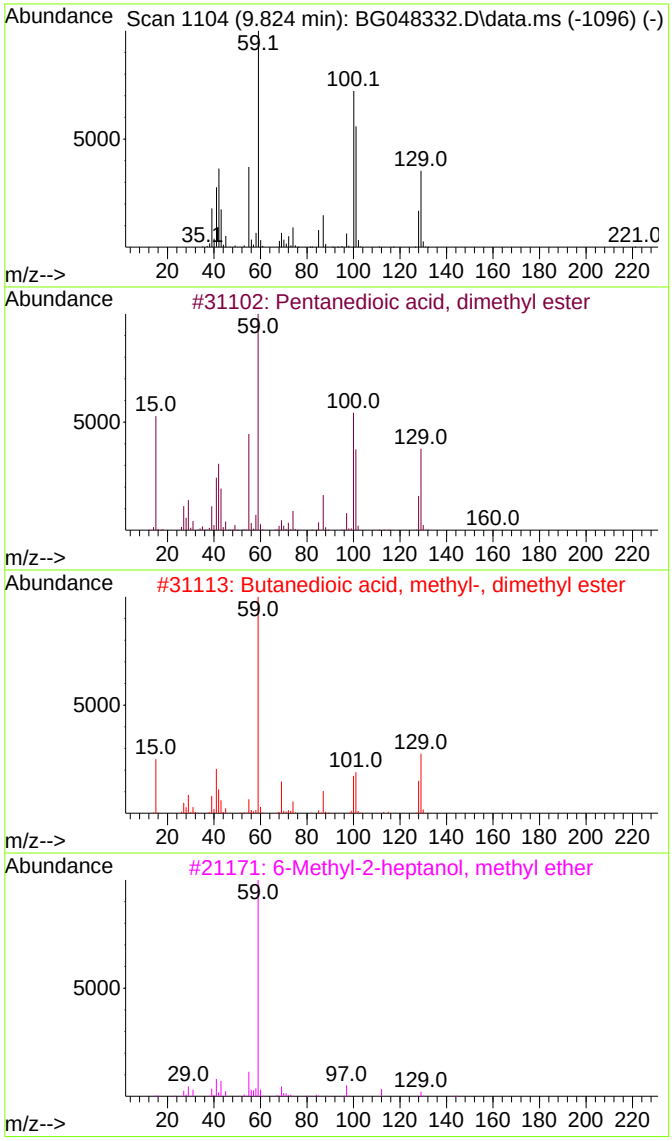
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

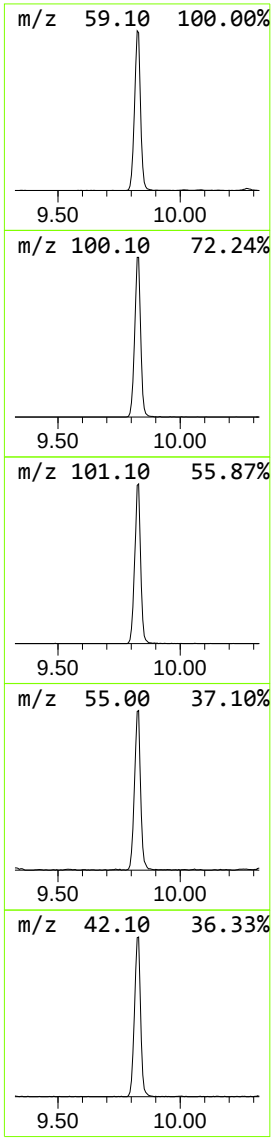
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentanedioic acid, dimethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.824	125.31 ng	2000620	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	72
2	Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	50
3	6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	22
4	1,3-Dioxane, 2-ethyl-5-methyl-	130	C7H14O2	020627-54-7	17
5	2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	12





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Sample : M1545-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RIM-7.55

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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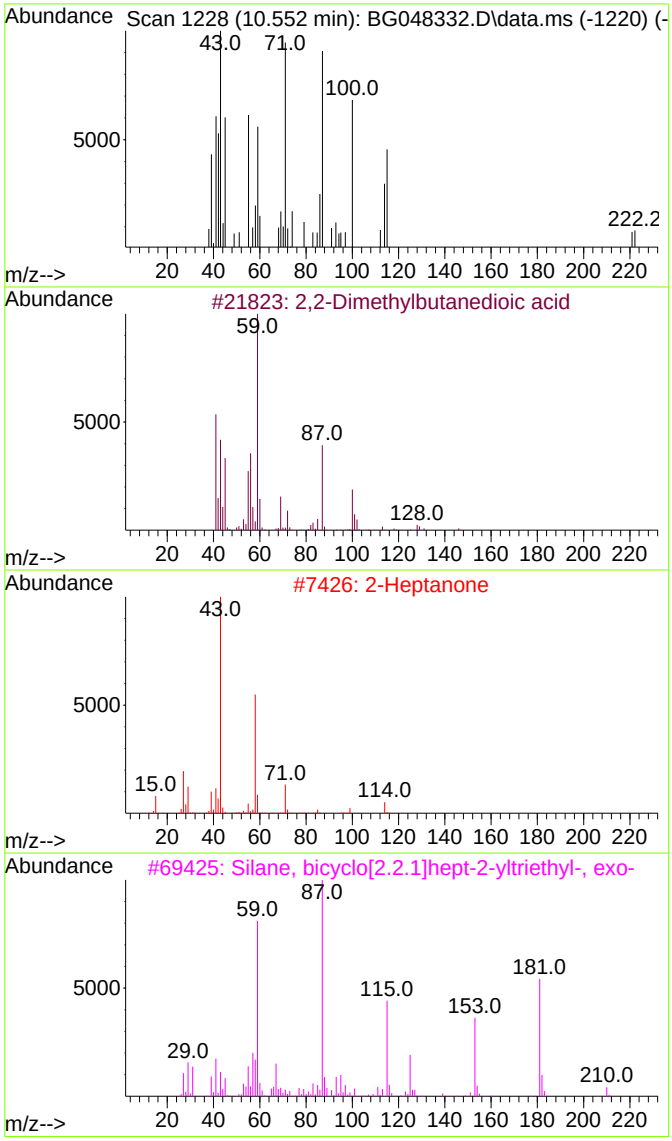
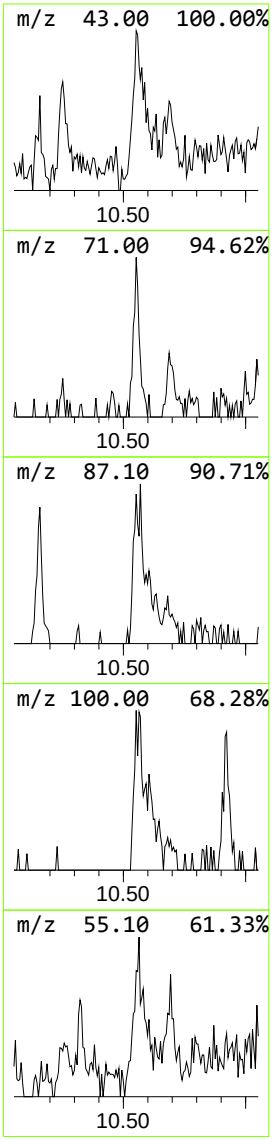
****

Peak Number 5 unknown10.552 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.552	5.10 ng	81458	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylbutanedioic acid	146	C6H10O4	000597-43-3	35
2	2-Heptanone	114	C7H14O	000110-43-0	35
3	Silane, bicyclo[2.2.1]hept-2-ylt...	210	C13H26Si	065118-97-0	27
4	Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	27
5	4-Nonanol, 4-methyl-	158	C10H22O	023418-38-4	27





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ClientSampleId :
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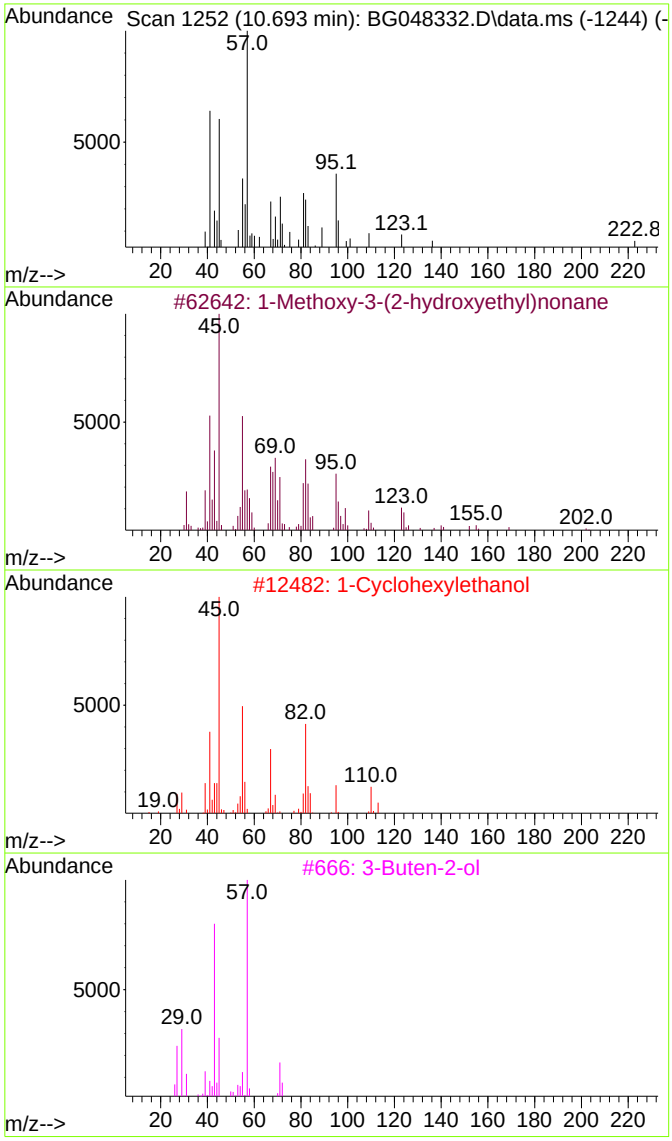
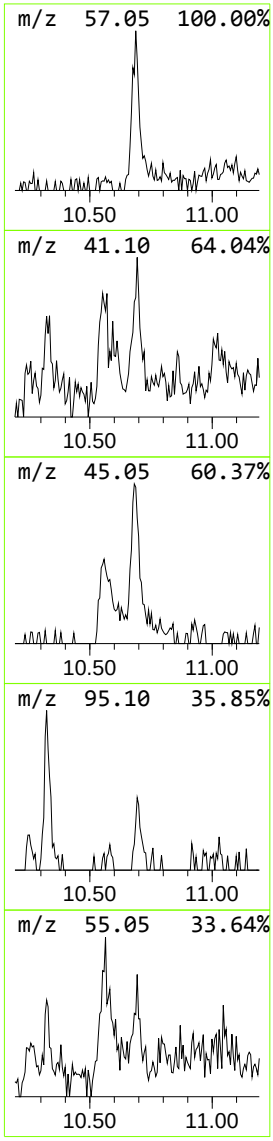
****
Peak Number 6 1-Methoxy-3-(2-hydroxyethyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.693	2.88 ng	45925	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Methoxy-3-(2-hydroxyethyl)nonane	202	C12H26O2	070928-44-8	53
2	1-Cyclohexylethanol	128	C8H16O	001193-81-3	38
3	3-Buten-2-ol	72	C4H8O	000598-32-3	27
4	trans-2-Undecen-1-ol	170	C11H22O	075039-84-8	27
5	2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	25





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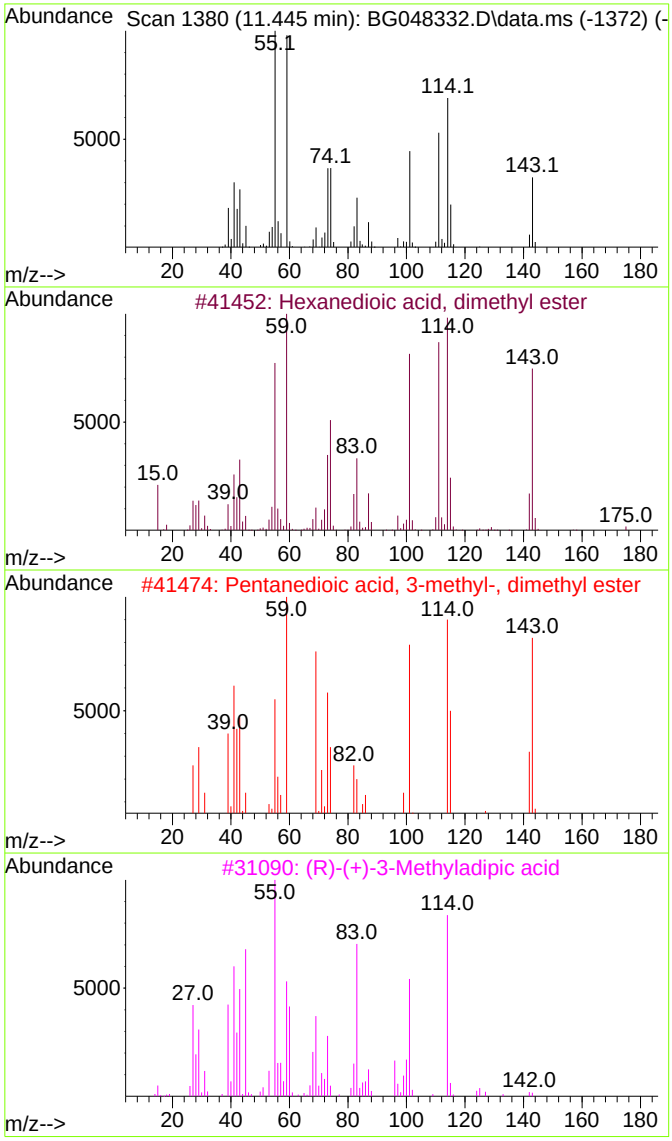
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

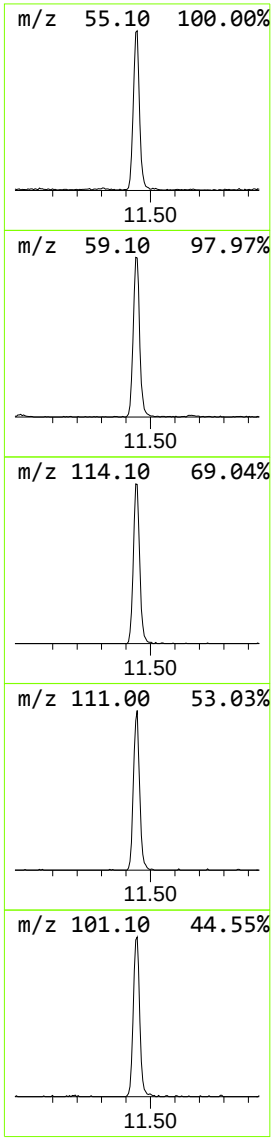
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Hexanedioic acid, dimethyl ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.445	56.92 ng	908770	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, dimethyl ester	174	C8H14O4	000627-93-0	90
2	Pentanedioic acid, 3-methyl-, di...	174	C8H14O4	019013-37-7	32
3	(R)-(+)-3-Methyladipic acid	160	C7H12O4	000623-82-5	25
4	Hydrazine, (1-methylethyl)-	74	C3H10N2	002257-52-5	18
5	Pentanedioic acid, 2-methyl-, di...	174	C8H14O4	014035-94-0	16





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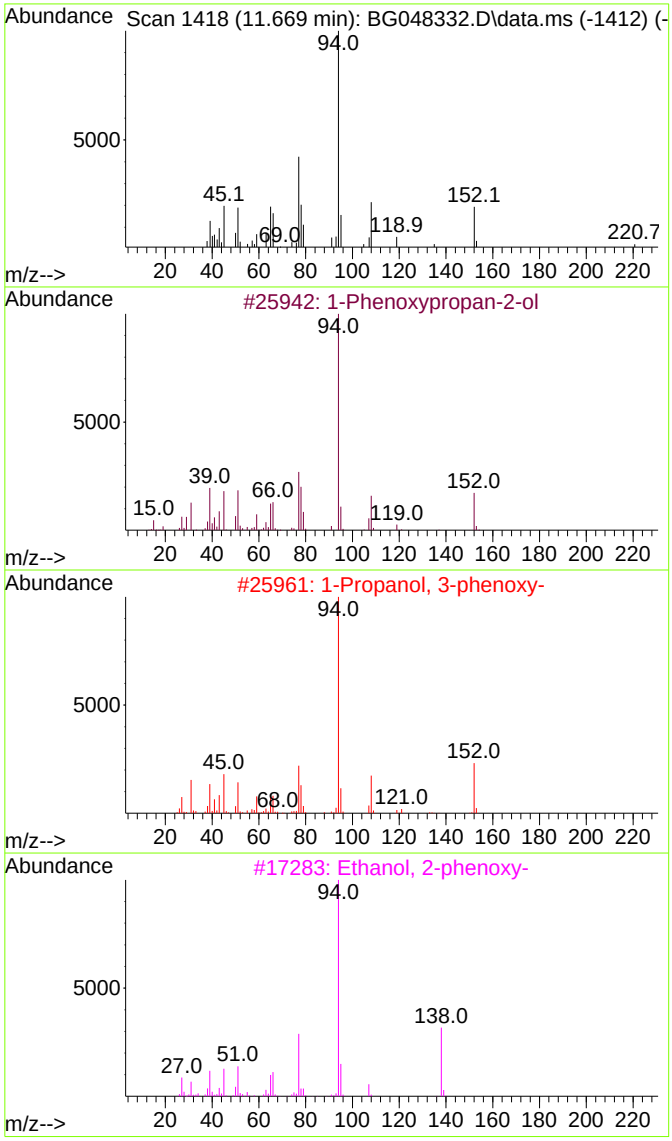
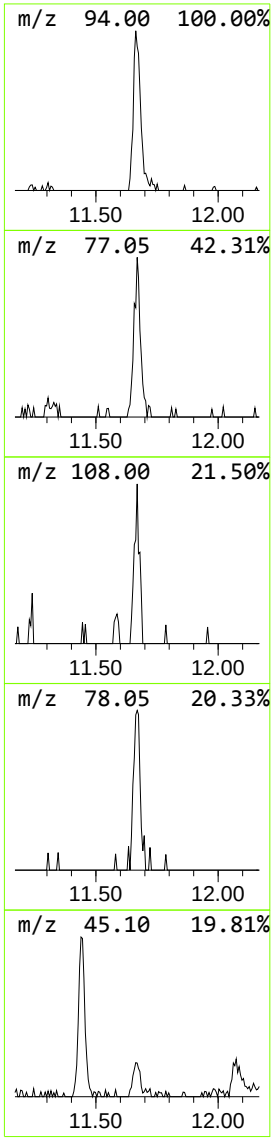
****

Peak Number 8 1-Phenoxypropan-2-ol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.669	3.75 ng	59846	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	87
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	58
3	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	53
4	2-Phenoxybutyric acid	180	C10H12O3	013794-14-4	40
5	3-Phenoxypropionic acid	166	C9H10O3	007170-38-9	38





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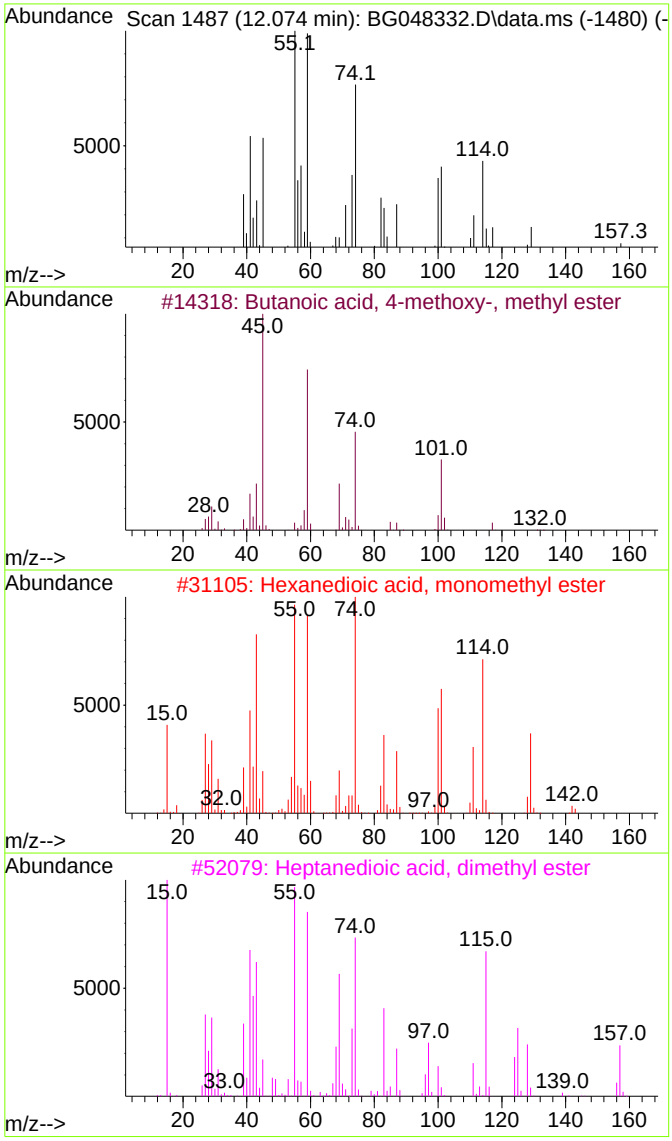
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

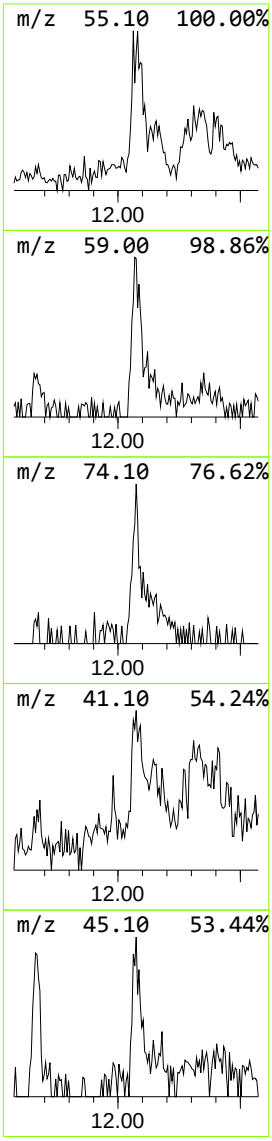
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Butanoic acid, 4-methoxy-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.074	4.83 ng	77041	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	50
2	Hexanedioic acid, monomethyl ester	160	C7H12O4	000627-91-8	42
3	Heptanedioic acid, dimethyl ester	188	C9H16O4	001732-08-7	38
4	Methyl 2-ethoxyacetate	118	C5H10O3	1000366-88-5	37
5	Ethyl ether	74	C4H10O	000060-29-7	37





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Instrument : BNA_G
ClientSampleId : RIM-7.55

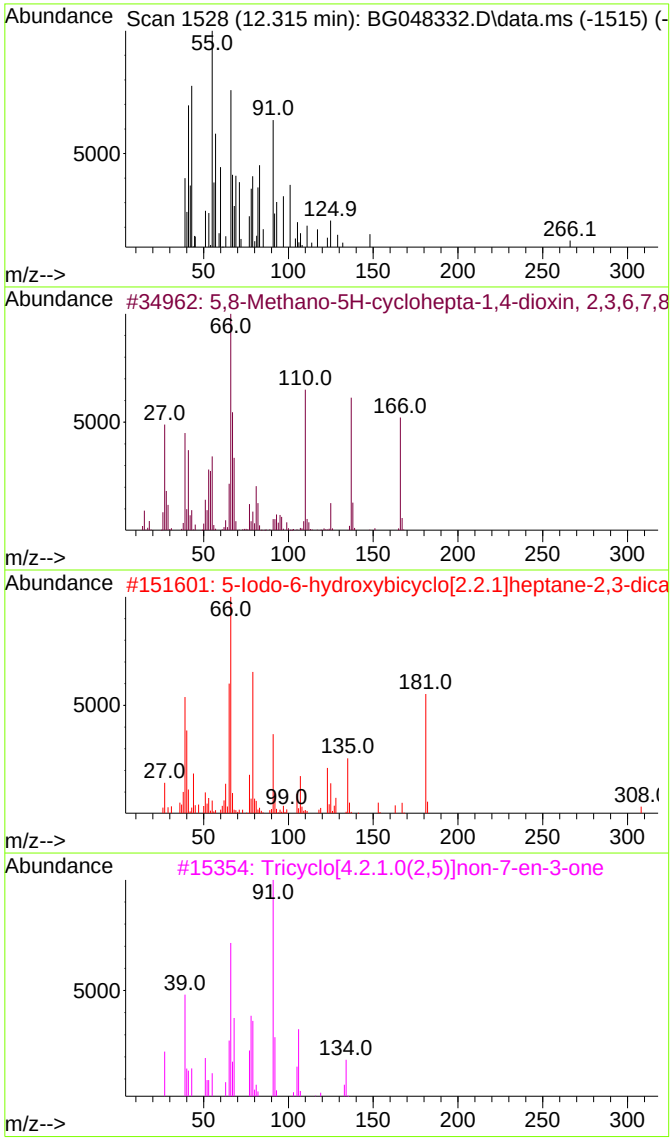
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

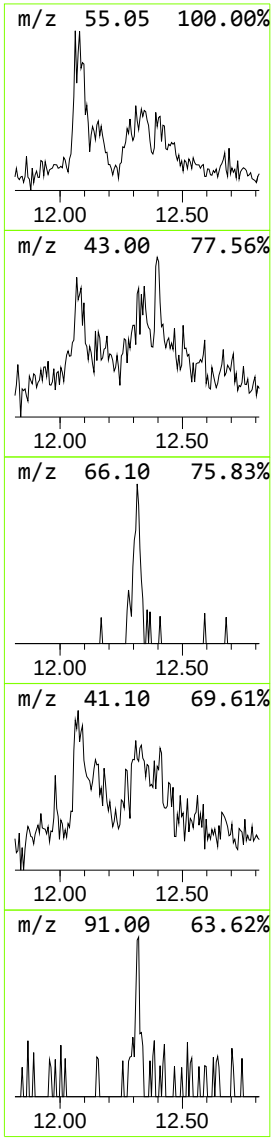
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 5,8-Methano-5H-cyclohepta-1... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.315	4.09 ng	65260	Naphthalene-d8	10.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,8-Methano-5H-cyclohepta-1,4-di...	166	C10H14O2	055956-36-0	50
2	5-Iodo-6-hydroxybicyclo[2.2.1]he...	308	C9H9IO4	015573-45-2	50
3	Tricyclo[4.2.1.0(2,5)]non-7-en-3...	134	C9H10O	035150-63-1	50
4	Tricyclo[8.2.1.0(2,9)]trideca-5,...	190	C13H18O	1000163-15-3	50
5	4,7-Methano-1H-indene-2,6-dicarb...	220	C12H12O4	037995-02-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048332.D
Acq On : 4 Mar 2021 17:25
Operator : CG/JU
Sample : M1545-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RIM-7.55

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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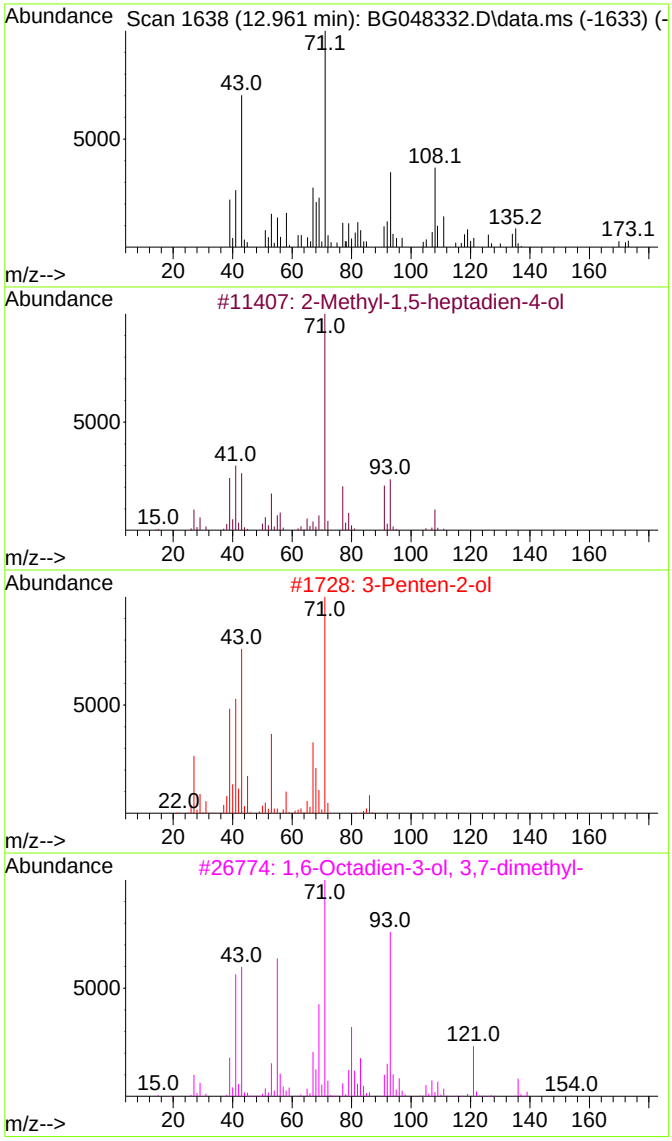
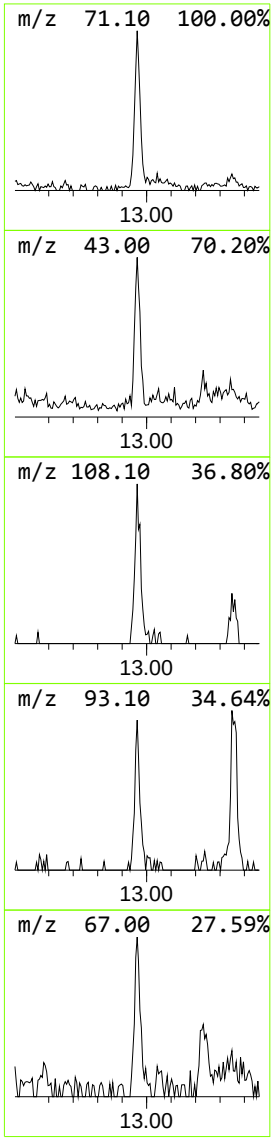
****

Peak Number 11 2-Methyl-1,5-heptadien-4-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.961	4.00 ng	96172	Acenaphthene-d10	14.736

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-1,5-heptadien-4-ol	126	C8H14O	000926-98-7	50
2	3-Penten-2-ol	86	C5H10O	001569-50-2	47
3	1,6-Octadien-3-ol, 3,7-dimethyl-	154	C10H18O	000078-70-6	47
4	1,5,7-Octatrien-3-ol, 3,7-dimethyl-	152	C10H16O	029957-43-5	38
5	Phytol	296	C20H40O	000150-86-7	38





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Data File : BG048332.D
Acq On : 4 Mar 2021 17:25
Operator : CG/JU
Sample : M1545-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RIM-7.55

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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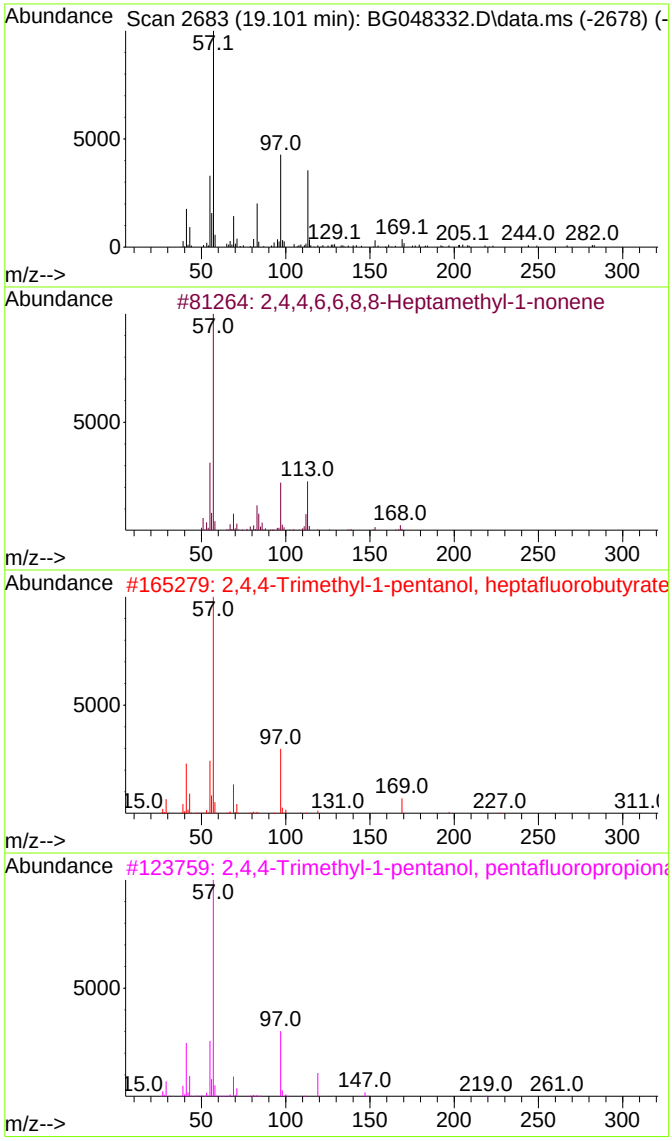
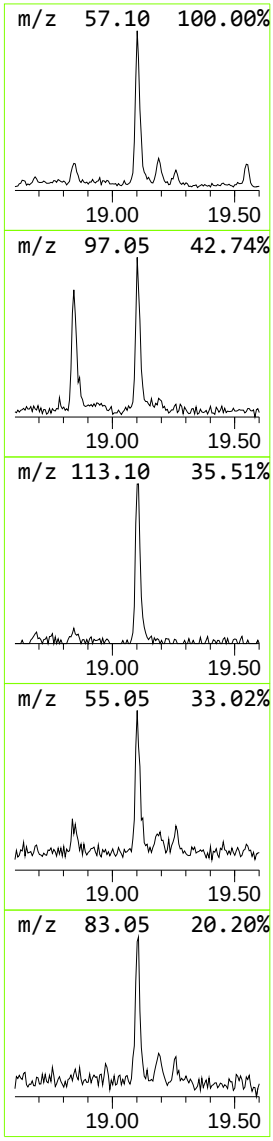
Peak Number 12 unknown19.101 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.101	3.61 ng	115311	Phenanthrene-d10	17.485

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38
2	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	37
3	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	37
4	Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	33
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32





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Data File : BG048332.D
Acq On : 4 Mar 2021 17:25
Operator : CG/JU
Sample : M1545-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RIM-7.55

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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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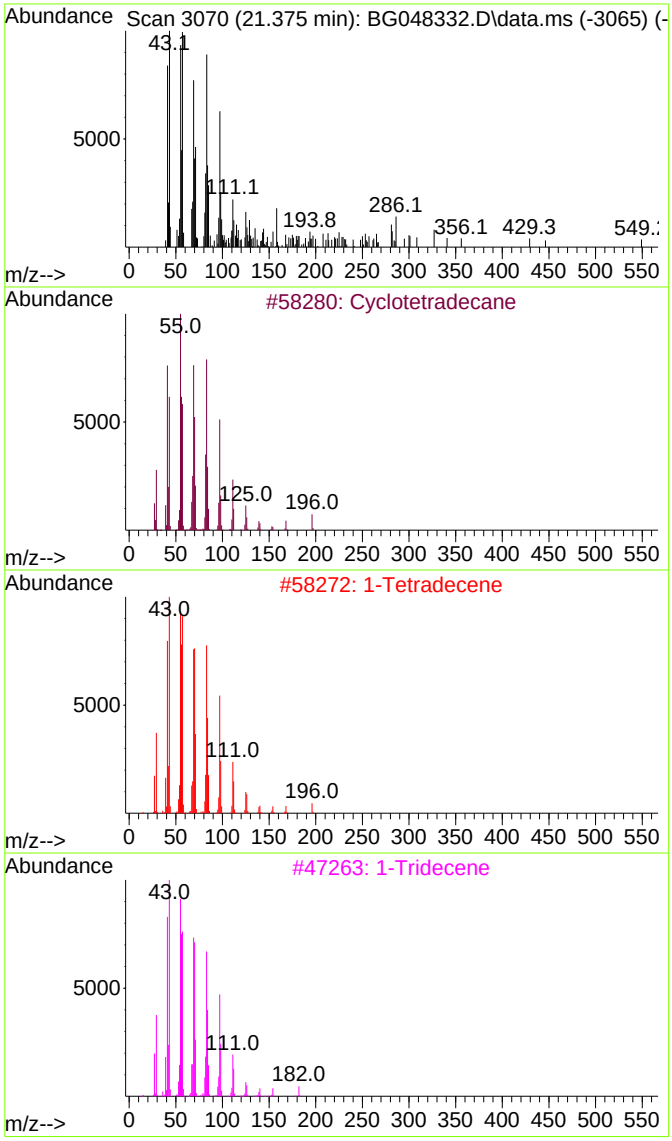
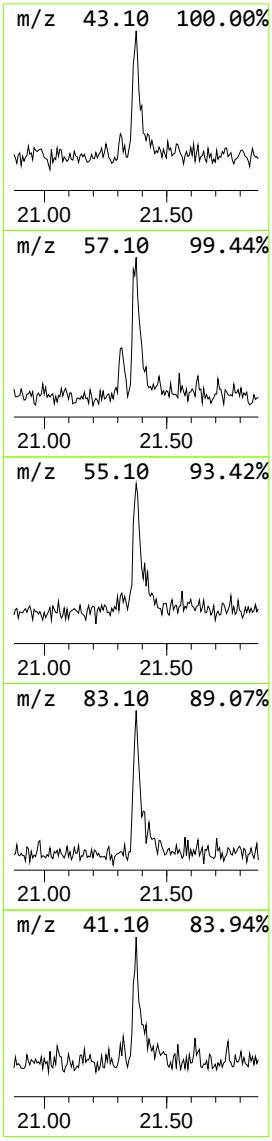
Peak Number 13 Cyclotetradecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.375	3.57 ng	128285	Chrysene-d12	21.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotetradecane	196	C14H28	000295-17-0	95
2	1-Tetradecene	196	C14H28	001120-36-1	91
3	1-Tridecene	182	C13H26	002437-56-1	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	89
5	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	89





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030421\
Data File : BG048332.D
Acq On : 4 Mar 2021 17:25
Operator : CG/JU
Sample : M1545-21
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RIM-7.55

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG021021.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
2-Propanol, 1-(...	7.632	5.2	ng	59928	1	8.102	229406	20.0
2-(2-(2-(2-(2-(...	7.679	4.5	ng	51772	1	8.102	229406	20.0
2-Propanol, 1-(...	7.873	11.9	ng	136134	1	8.102	229406	20.0
Pentanedioic ac...	9.824	125.3	ng	2000620	2	10.922	319317	20.0
unknown10.552	10.552	5.1	ng	81458	2	10.922	319317	20.0
1-Methoxy-3-(2-...	10.693	2.9	ng	45925	2	10.922	319317	20.0
Hexanedioic aci...	11.445	56.9	ng	908770	2	10.922	319317	20.0
1-Phenoxypropan...	11.669	3.8	ng	59846	2	10.922	319317	20.0
Butanoic acid, ...	12.074	4.8	ng	77041	2	10.922	319317	20.0
5,8-Methano-5H-...	12.315	4.1	ng	65260	2	10.922	319317	20.0
2-Methyl-1,5-he...	12.961	4.0	ng	96172	3	14.736	480625	20.0
unknown19.101	19.101	3.6	ng	115311	4	17.485	638919	20.0
Cyclotetradecane	21.375	3.6	ng	128285	5	21.763	718854	20.0