LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(104-108)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.204	13	20	26	rVB2	81373	119274	10.44%	1.315%
2	2.699	99	104	109	rBB3	44048	66648	5.84%	0.735%
3	3.210	186	191	198	rBV4	15382	29038	2.54%	0.320%
4	3.881	301	305	311	rVB2	11799	14467	1.27%	0.160%
5	4.622	428	431	436	rBB2	13166	15236	1.33%	0.168%
6	5.045	499	503	511	rBV	77435	92920	8.14%	1.025%
7	5.416	562	566	567	rBV	36943	37056	3.24%	0.409%
8	5.463	570	574	590	rVB	1131698	1086106	95.10%	11.976%
9	5.669	607	609	613	rBV	17514	16344	1.43%	0.180%
10	5.839	636	638	641	rBV	17598	14417	1.26%	0.159%
11	6.010	664	667	672	rBV2	19420	18170	1.59%	0.200%
12	6.287	713	714	722	rVB	15824	18207	1.59%	0.201%
13	6.475	741	746	749	rBV	1142569	1073043	93.96%	11.832%
14	6.828	802	806	812	rBB	273416	207837	18.20%	2.292%
15	7.392	897	902	905	rBV	728576	700028	61.30%	7.719%
16	8.022	1004	1009	1020	rBV	480492	479819	42.01%	5.291%
17	8.110	1021	1024	1028	rVB	311153	263659	23.09%	2.907%
18	9.192	1203	1208	1211	rBV	1341243	1142028	100.00%	12.592%
19	9.304	1223	1227	1234	rVB2	18546	19417	1.70%	0.214%
20	9.522	1261	1264	1267	rVB	84595	63097	5.52%	0.696%
21	9.869	1320	1323	1327	rBV	389775	308249	26.99%	3.399%
22	10.604	1446	1448	1451	rBV2	58779	49784	4.36%	0.549%
23	10.663	1454	1458	1461	rBV	1060175	891106	78.03%	9.825%
24	11.357	1573	1576	1580	rBV	370490	327252	28.66%	3.608%
25	11.427	1585	1588	1591	rVB	62222	55116	4.83%	0.608%
26	11.751	1638	1643	1646	rVB2	55614	72833	6.38%	0.803%
27	11.886	1662	1666	1671	rBV3	25559	28331	2.48%	0.312%
28	12.057	1692	1695	1698	rBV2	13643	12795	1.12%	0.141%
29	12.457	1756	1763	1766	rBV3	93672	94049	8.24%	1.037%
30	12.545	1774	1778	1782	rVB3	23180	23598	2.07%	0.260%
31	12.951	1842	1847	1850	rBV	1243087	1096639	96.03%	12.092%
32	13.486	1935	1938	1941	rVB3	22228	21765	1.91%	0.240%
33	13.886	2001	2006	2011	rBV7	19553	43933	3.85%	0.484%
34	13.980	2019	2022	2024	rBV	40591	37397	3.27%	0.412%
35	14.010	2024	2027	2030	rVB	306635	261472	22.90%	2.883%
36	14.068	2034	2037	2042	rVB7	9944	13845	1.21%	0.153%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(104-108)

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-BF060321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	14.633	2129	2133	2138	rBV4	33329	38640	3.38%	0.426%
38	15.486	2273	2278	2283	rBV2	161472	215732	18.89%	2.379%

Sum of corrected areas: 9069347

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
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Acq On : 14 Jun 2021 17:46
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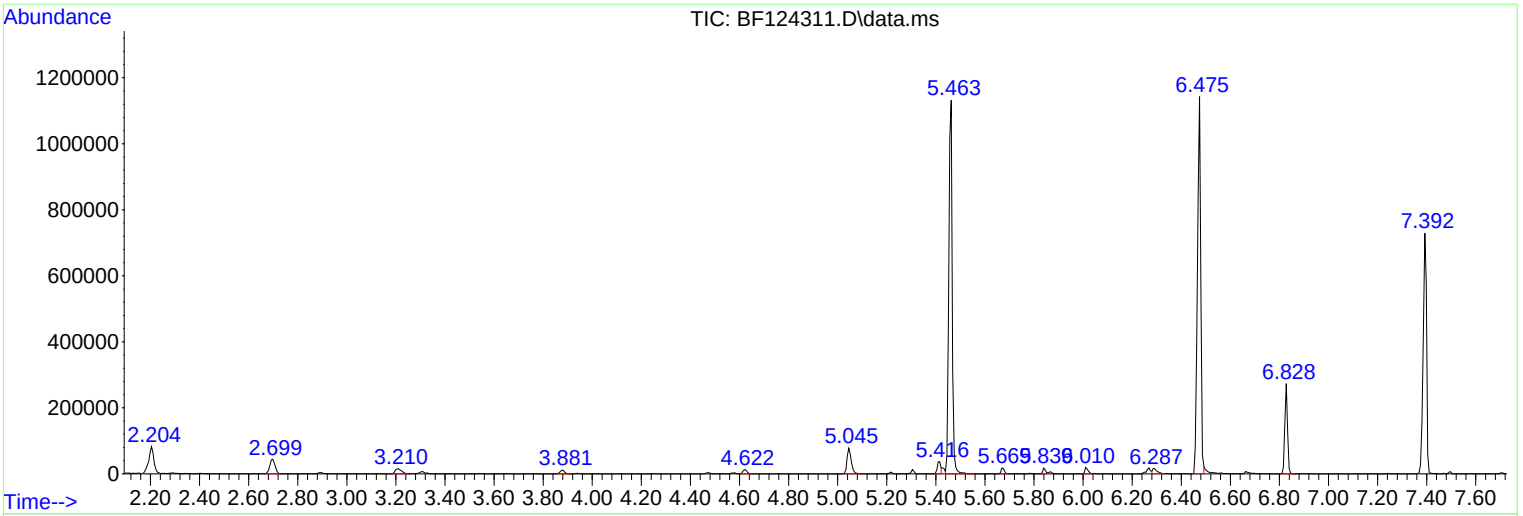
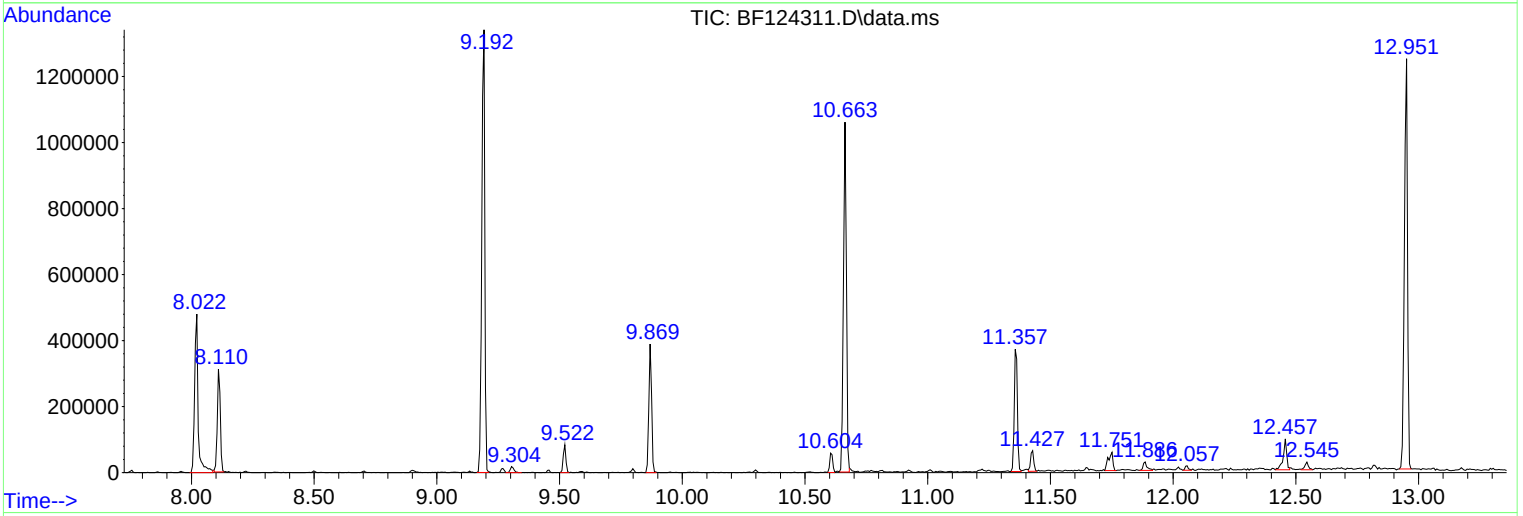
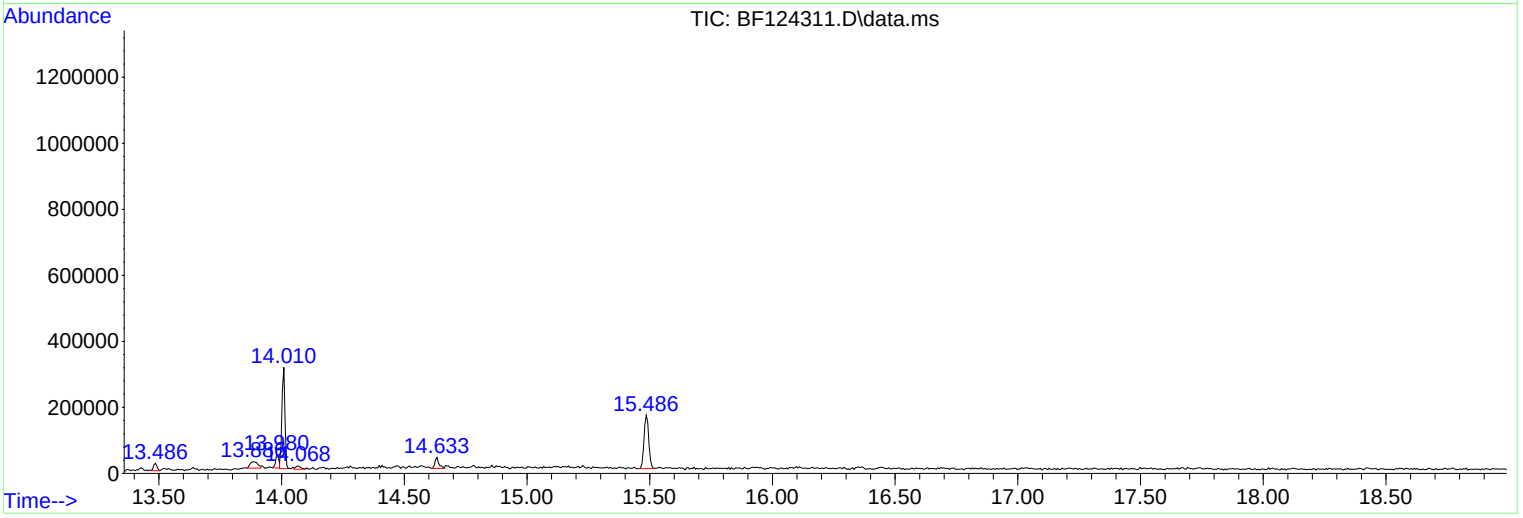
Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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_F\Data\BF061421\
Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

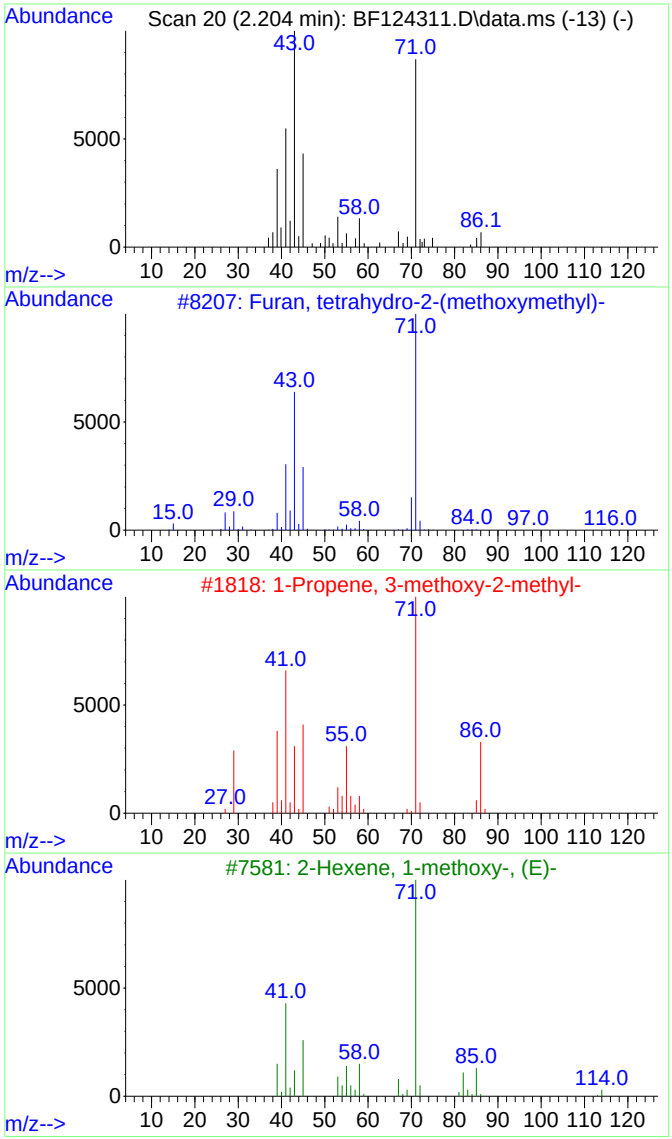
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

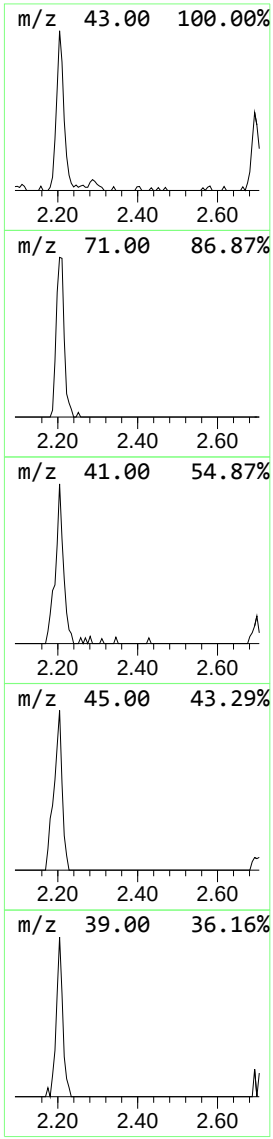
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Furan, tetrahydro-2-(methox... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.204	11.48 ng	119274	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	64
2	1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	64
3	2-Hexene, 1-methoxy-, (E)-	114	C7H14O	056052-83-6	59
4	3-Penten-2-ol	86	C5H10O	001569-50-2	58
5	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	52





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Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(104-108)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

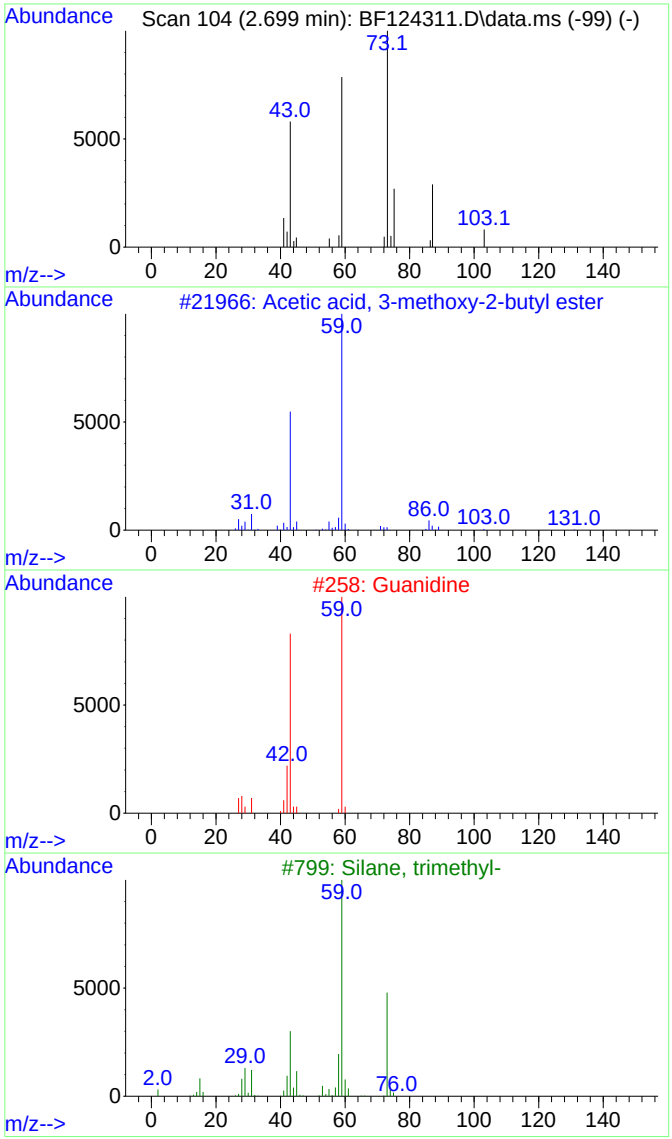
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

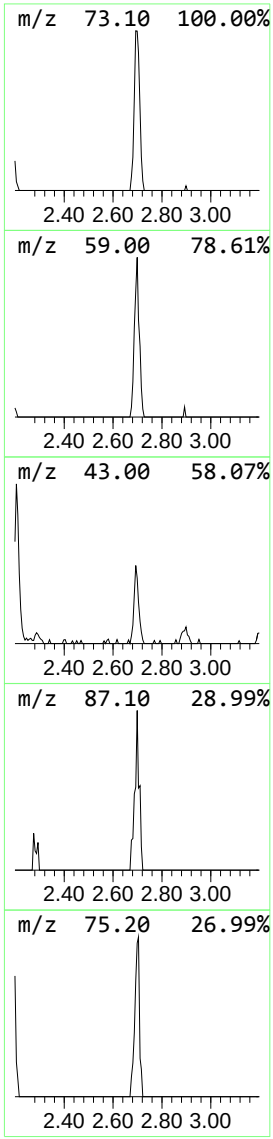
****

Peak Number 2 unknown2.699 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.699	6.41 ng	66648	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 3-methoxy-2-butyl e...	146	C7H14O3	1000151-29-7	25
2	Guanidine	59	CH5N3	000113-00-8	9
3	Silane, trimethyl-	74	C3H10Si	000993-07-7	9
4	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	9
5	(3,3-Dimethyloxiranyl)methanol	102	C5H10O2	1000306-71-7	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

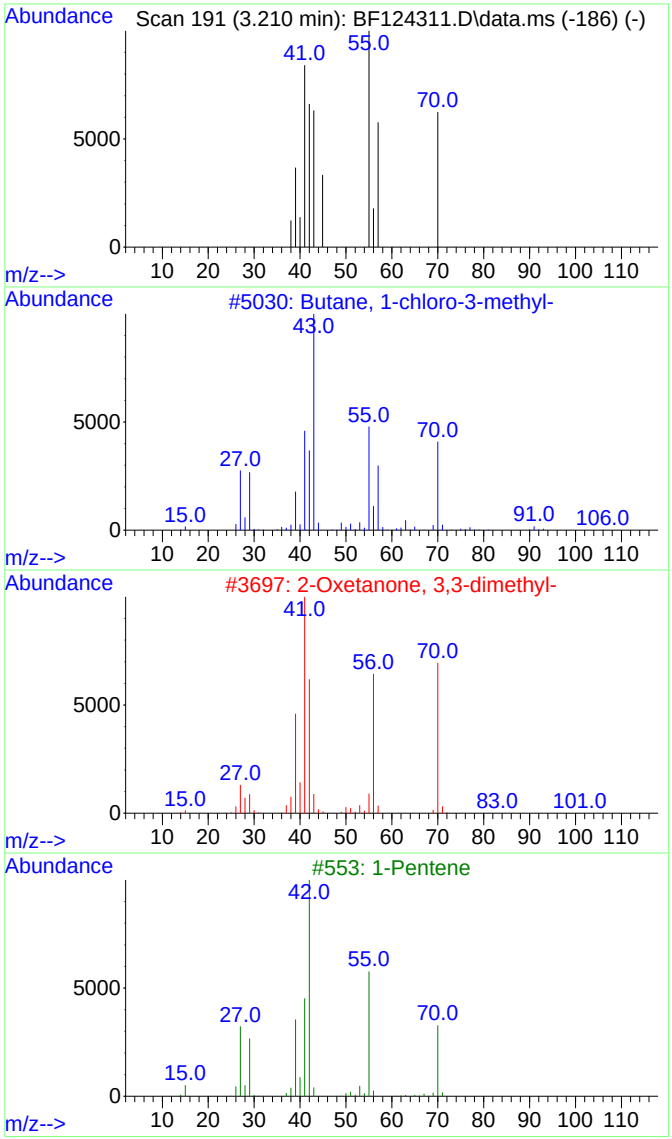
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

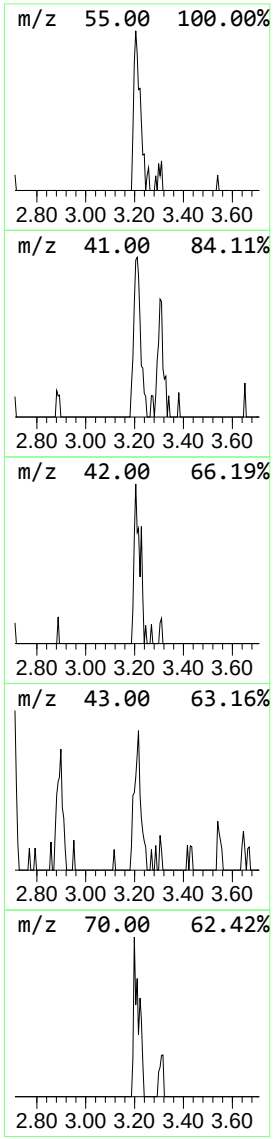
****

Peak Number 3 unknown3.210 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.210	2.79 ng	29038	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-chloro-3-methyl-	106	C5H11Cl	000107-84-6	40
2	2-Oxetanone, 3,3-dimethyl-	100	C5H8O2	001955-45-9	33
3	1-Pentene	70	C5H10	000109-67-1	9
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	9
5	Cyclopropane	42	C3H6	000075-19-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

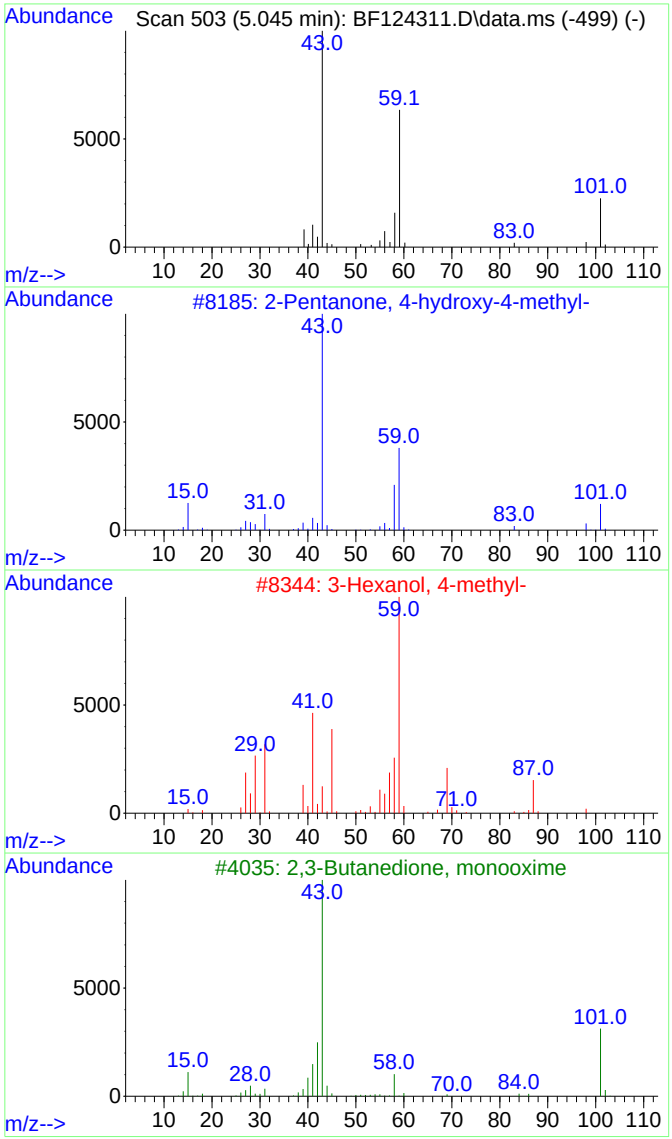
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

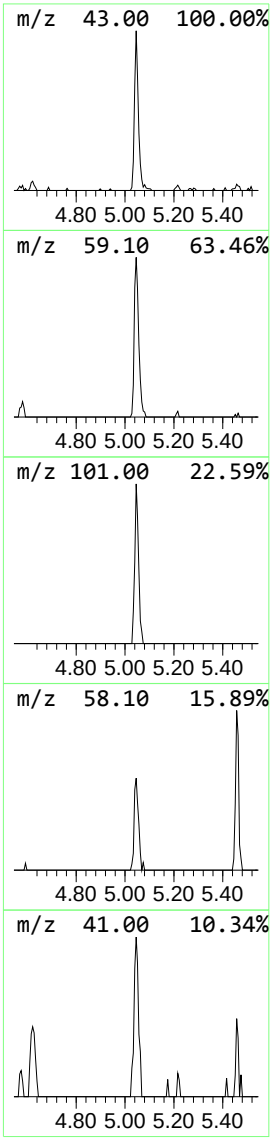
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.045	8.94 ng	92920	1,4-Dichlorobenzene-d4	6.828

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124311.D
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Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

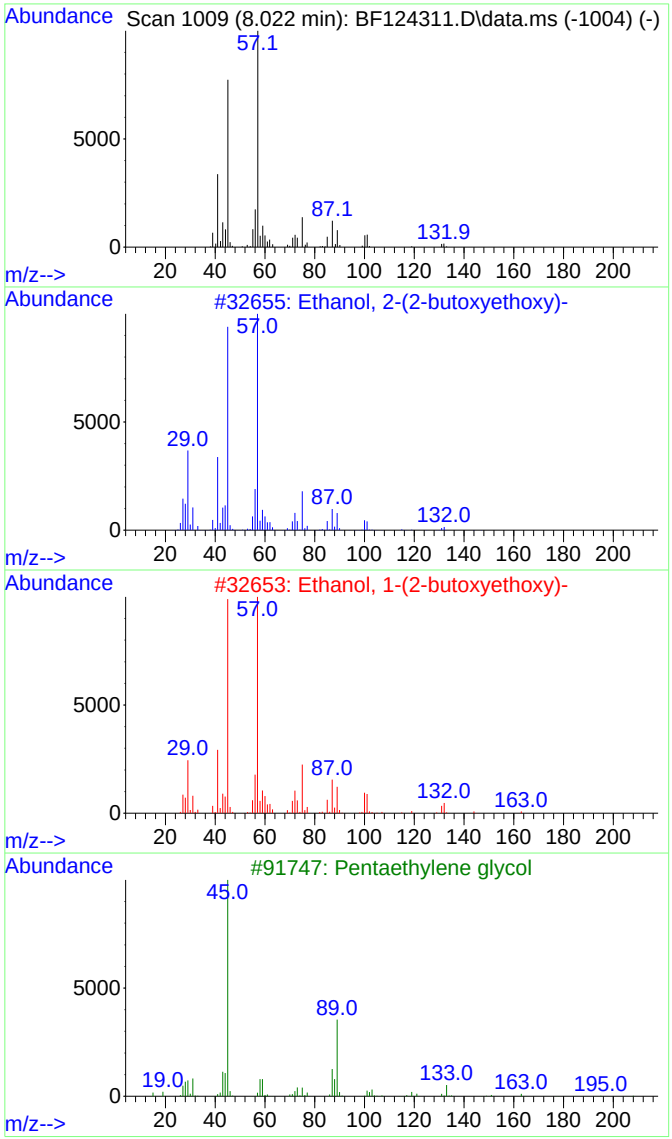
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

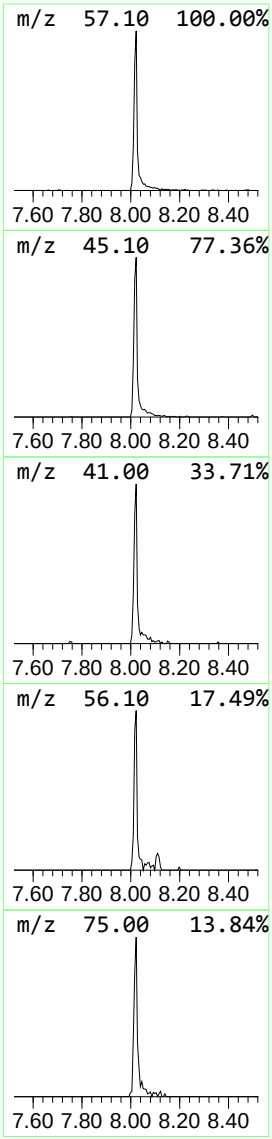
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.022	36.40 ng	479819	Naphthalene-d8	8.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	78
3	Pentaethylene glycol	238	C10H22O6	004792-15-8	53
4	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
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Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(104-108)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

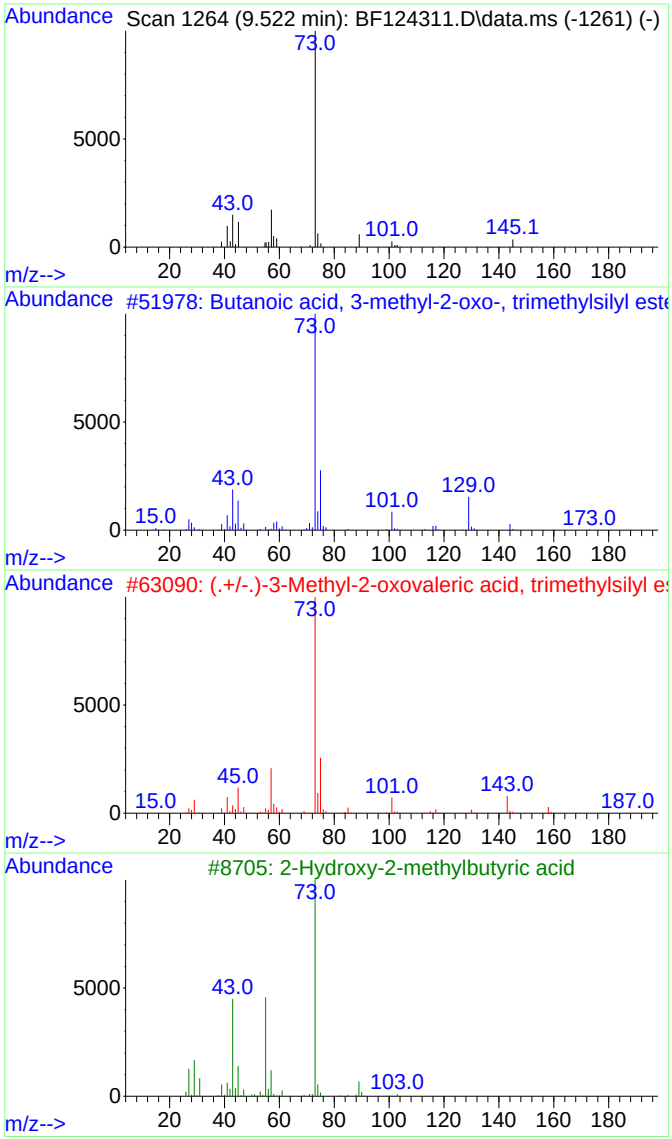
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

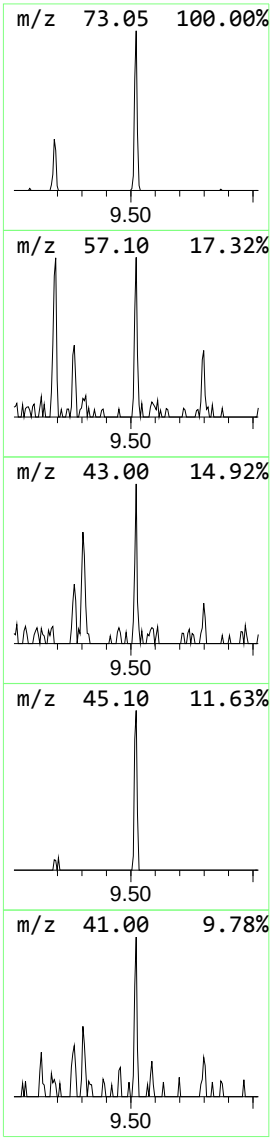
****

Peak Number 6 unknown9.522 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.522	4.09 ng	63097	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 3-methyl-2-oxo-, ...	188	C8H16O3Si	074367-70-7	9
2	(.+/-.)-3-Methyl-2-oxovaleric ac...	202	C9H18O3Si	1000332-85-6	9
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9
5	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	9





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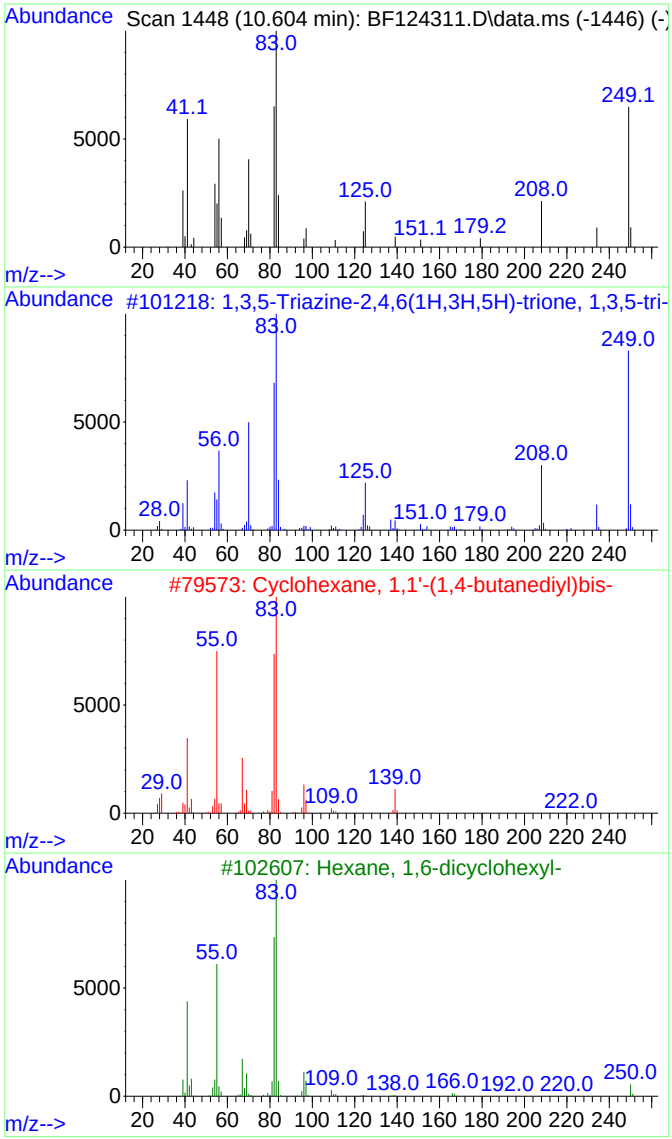
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

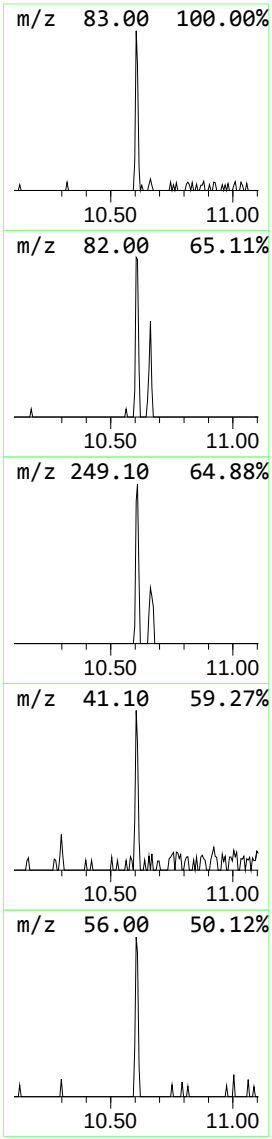
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,3,5-Triazine-2,4,6(1H,3H,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.604	3.23 ng	49784	Acenaphthene-d10	9.869

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4,6(1H,3H,5H)-t...	249	C12H15N3O3	001025-15-6	96
2	Cyclohexane, 1,1'-(1,4-butanediy...	222	C16H30	006165-44-2	27
3	Hexane, 1,6-dicyclohexyl-	250	C18H34	001610-23-7	27
4	Cyclohexane, 1,1'-(1,3-propanedi...	208	C15H28	003178-24-3	25
5	Cyclohexane, octyl-	196	C14H28	001795-15-9	16





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

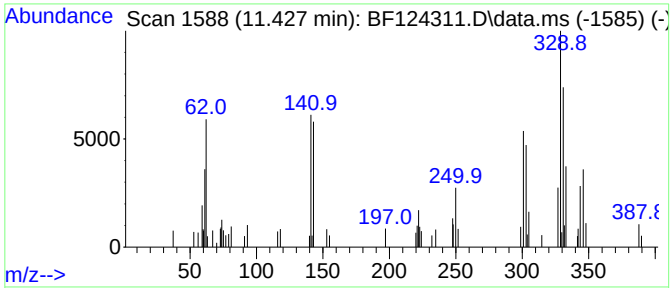
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

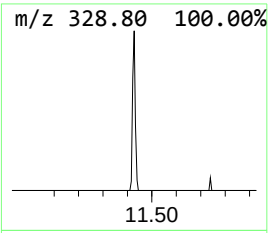
****

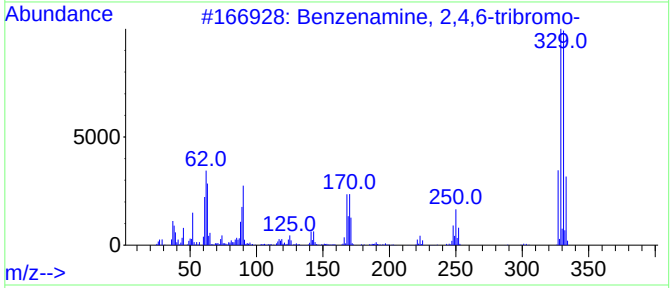
Peak Number 8 Benzenamine, 2,4,6-tribromo- Concentration Rank 8

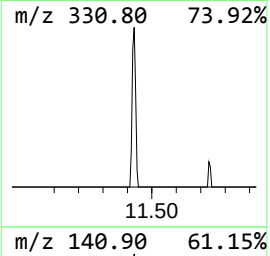
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.427	3.37 ng	55116	Phenanthrene-d10	11.357

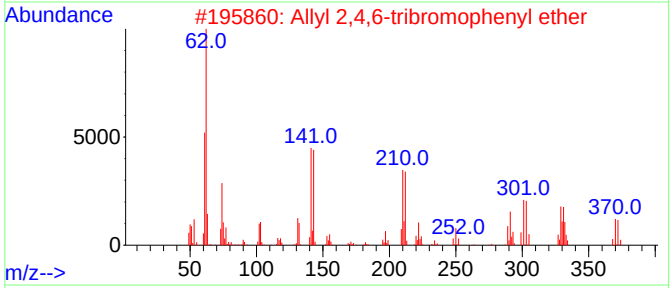
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	55
2	Allyl 2,4,6-tribromophenyl ether	368	C9H7Br3O	003278-89-5	12
3	Tetrachlorvinphos	364	C10H9Cl4O4P	022248-79-9	12
4	2-[3,4-Dichlorophenyl]-4-carboxy...	331	C17H11Cl2NO2	1000253-84-5	10
5	1,2,4-1H-Triazole, 1-(3,5-dichlo...	329	C12H13Cl2N5S	1000266-38-9	10

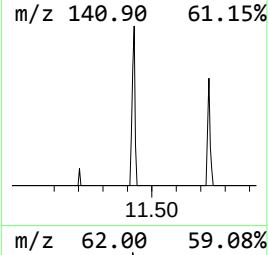


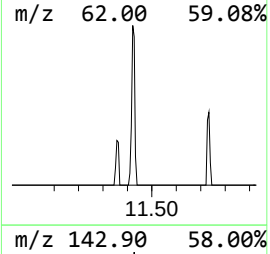


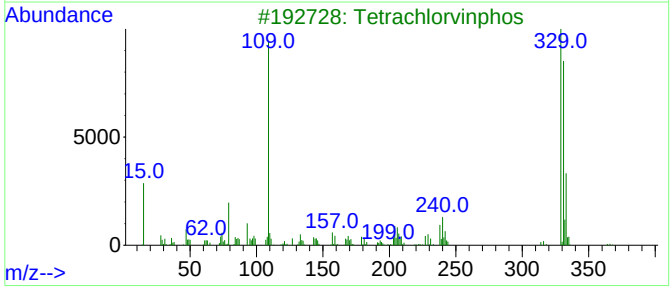


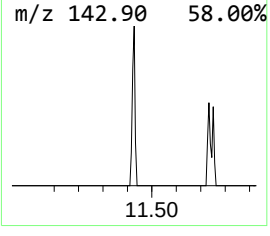












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Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

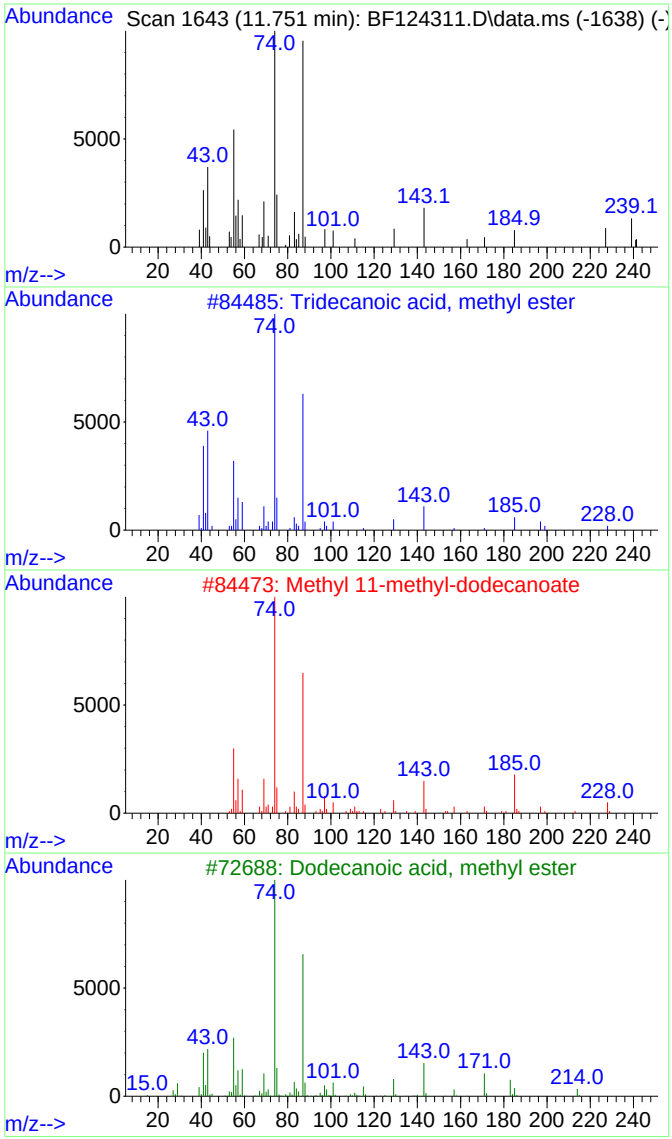
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

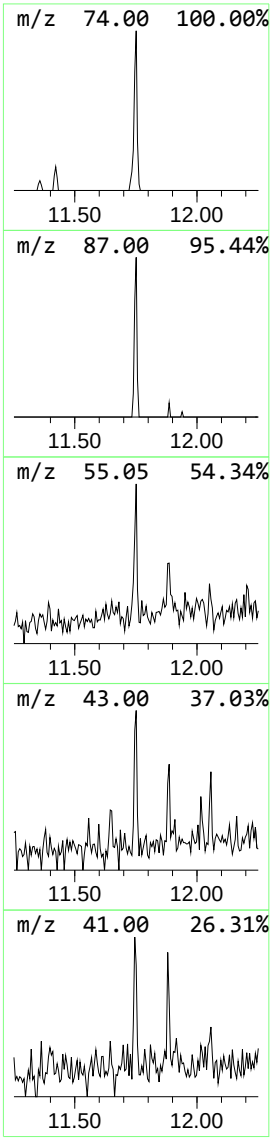
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Tridecanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.751	4.45 ng	72833	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	72
2	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	72
3	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	56
4	Cyclopentaneundecanoic acid, met...	268	C17H32O2	025779-85-5	56
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	53





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Sample : M2687-02
Misc :
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Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

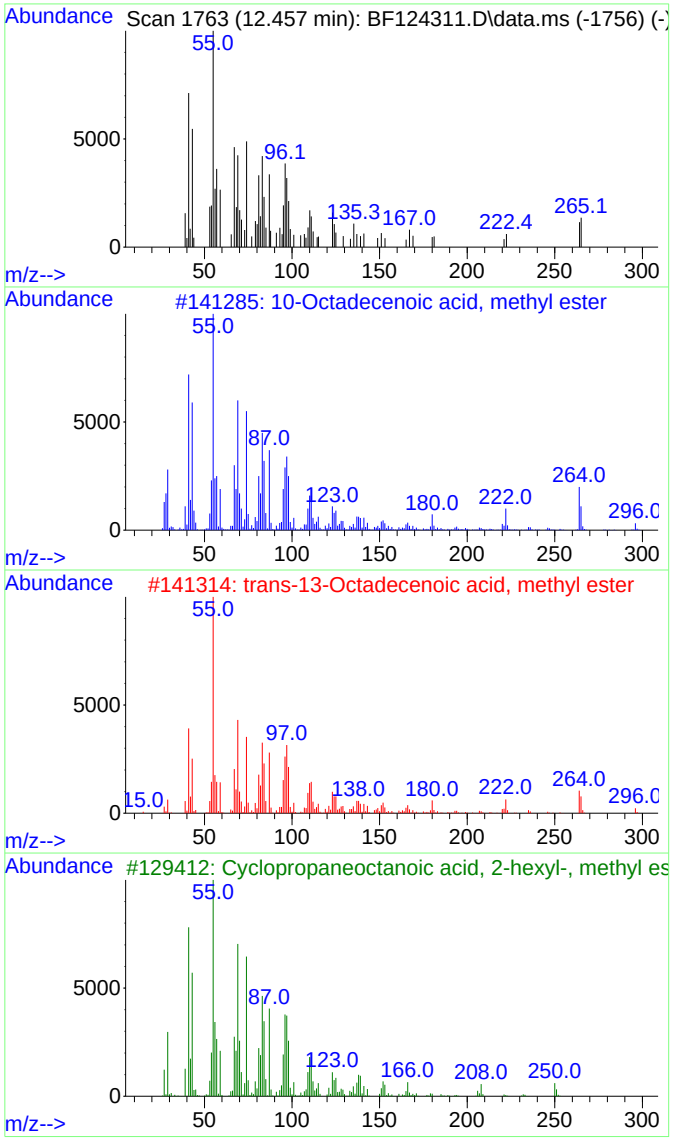
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

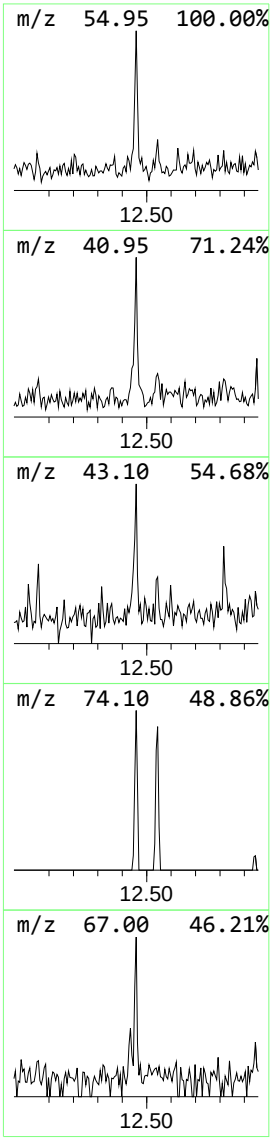
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 10-Octadecenoic acid, methy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.457	5.75 ng	94049	Phenanthrene-d10	11.357

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	90
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	90
3	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	72
4	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	72
5	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	64





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Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

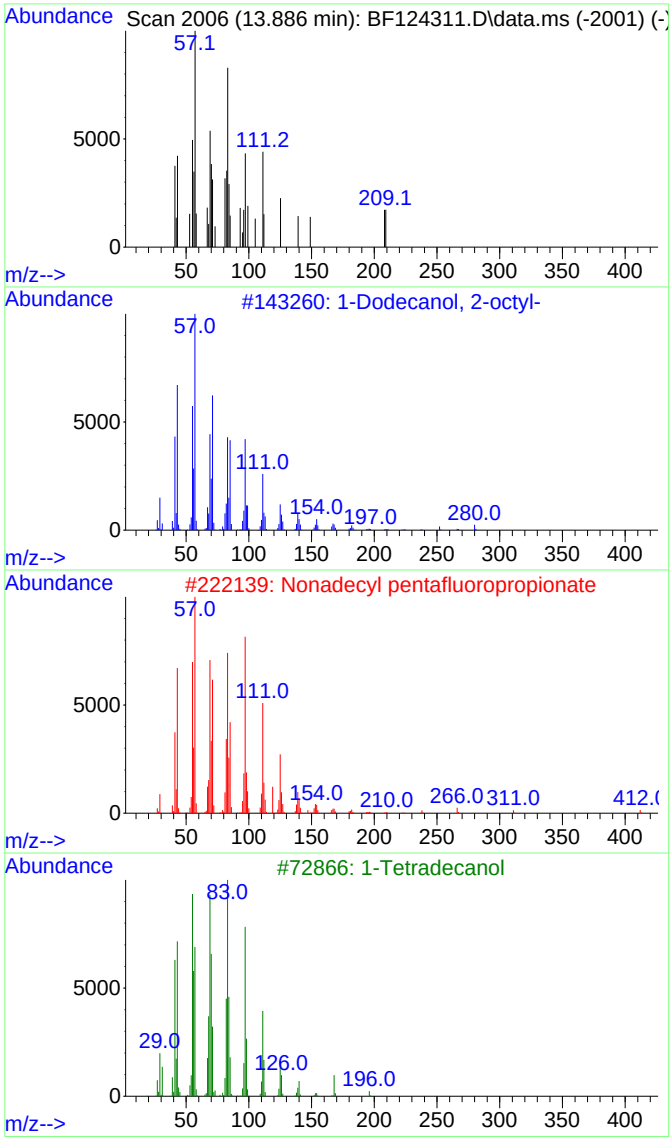
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

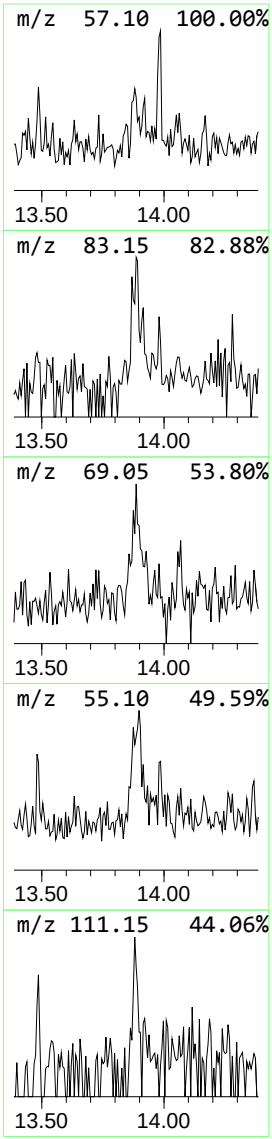
****

Peak Number 11 1-Dodecanol, 2-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.36 ng	43933	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	59
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	58
3	1-Tetradecanol	214	C14H30O	000112-72-1	58
4	n-Pentadecanol	228	C15H32O	000629-76-5	58
5	Formic acid, dodecyl ester	214	C13H26O2	028303-42-6	52





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Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
17-B6(104-108)

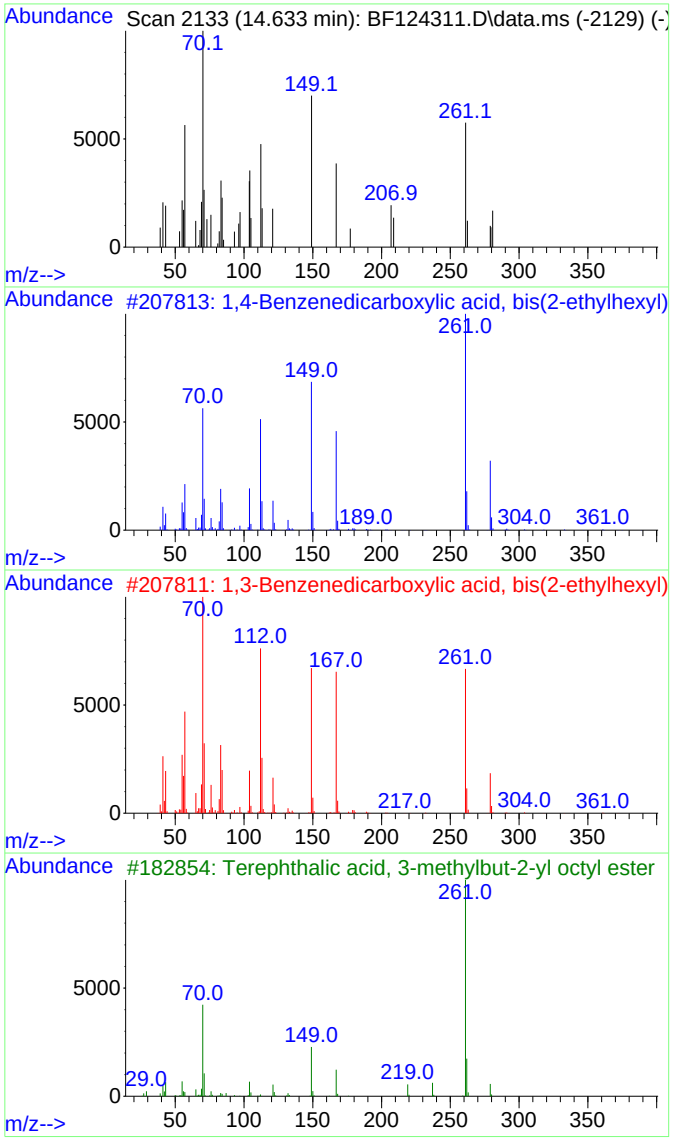
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

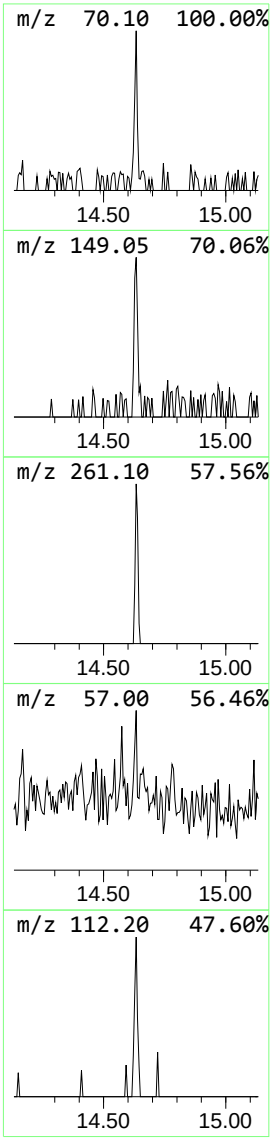
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 1,4-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	2.96 ng	38640	Chrysene-d12	14.009

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	53
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	50
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	50
4	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	32
5	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061421\
Data File : BF124311.D
Acq On : 14 Jun 2021 17:46
Operator : JU/CG
Sample : M2687-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 17-B6(104-108)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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
Furan, tetrahyd...	2.204	11.5	ng	119274	1	6.828	207837	20.0
unknown2.699	2.699	6.4	ng	66648	1	6.828	207837	20.0
unknown3.210	3.210	2.8	ng	29038	1	6.828	207837	20.0
2-Pentanone, 4-...	5.045	8.9	ng	92920	1	6.828	207837	20.0
Ethanol, 2-(2-b...	8.022	36.4	ng	479819	2	8.110	263659	20.0
unknown9.522	9.522	4.1	ng	63097	3	9.869	308249	20.0
1,3,5-Triazine-...	10.604	3.2	ng	49784	3	9.869	308249	20.0
Benzenamine, 2,...	11.427	3.4	ng	55116	4	11.357	327252	20.0
Tridecanoic aci...	11.751	4.5	ng	72833	4	11.357	327252	20.0
10-Octadecenoic...	12.457	5.8	ng	94049	4	11.357	327252	20.0
1-Dodecanol, 2-...	13.886	3.4	ng	43933	5	14.009	261472	20.0
1,4-Benzenedica...	14.633	3.0	ng	38640	5	14.009	261472	20.0