LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-SP1

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-BF012721.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123081.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.216	12	22	28	rBV	703413	944731	11.32%	1.676%
2	5.134	515	518	524	rVB	71745	90800	1.09%	0.161%
3	5.516	577	583	586	rBV	5956182	6272957	75.15%	11.131%
4	6.516	747	753	756	rBV	5549459	6460685	77.40%	11.464%
5	6.716	784	787	793	rBV	82037	98363	1.18%	0.175%
6	6.893	813	817	820	rBV	1710571	1434575	17.19%	2.545%
7	7.451	906	912	915	rBV	3896889	4300603	51.52%	7.631%
8	8.175	1030	1035	1038	rBV	2127606	1926110	23.07%	3.418%
9	9.257	1213	1219	1222	rBV	6978464	7489363	89.72%	13.289%
10	9.334	1228	1232	1235	rBV2	148347	166506	1.99%	0.295%
11	9.369	1235	1238	1246	rVB	237611	261976	3.14%	0.465%
12	9.645	1281	1285	1289	rBV	733317	678018	8.12%	1.203%
13	9.704	1292	1295	1299	rVB2	85731	91635	1.10%	0.163%
14	9.804	1308	1312	1315	rBV4	180859	217133	2.60%	0.385%
15	9.851	1317	1320	1322	rVB	318064	266655	3.19%	0.473%
16	9.933	1328	1334	1337	rBV	2440666	2328049	27.89%	4.131%
17	9.969	1337	1340	1345	rVV4	97594	139748	1.67%	0.248%
18	10.198	1376	1379	1381	rBV3	75880	87137	1.04%	0.155%
19	10.257	1386	1389	1391	rBV4	75700	99267	1.19%	0.176%
20	10.310	1395	1398	1401	rBV2	102643	106099	1.27%	0.188%
21	10.345	1401	1404	1409	rBV2	273177	279933	3.35%	0.497%
22	10.481	1425	1427	1435	rBV2	120632	157609	1.89%	0.280%
23	10.728	1463	1469	1472	rBV	4877902	4941011	59.19%	8.767%
24	11.428	1584	1588	1591	rBV	2501024	2204642	26.41%	3.912%
25	11.957	1675	1678	1681	rBV	796862	703867	8.43%	1.249%
26	12.739	1809	1811	1814	rBV	186465	181389	2.17%	0.322%
27	13.027	1854	1860	1863	rBV	7695179	8347245	100.00%	14.811%
28	13.957	2014	2018	2033	rVB3	375120	1237402	14.82%	2.196%
29	14.074	2034	2038	2042	rBV	2553819	2258610	27.06%	4.008%
30	14.551	2114	2119	2122	rVB2	89741	101609	1.22%	0.180%
31	15.210	2227	2231	2236	rVB	74293	87430	1.05%	0.155%
32	15.345	2251	2254	2263	rVB	46039	90170	1.08%	0.160%
33	15.563	2285	2291	2295	rBV	1593837	1999560	23.95%	3.548%
34	16.215	2391	2402	2419	rBV	52689	307375	3.68%	0.545%

Sum of corrected areas: 56358262

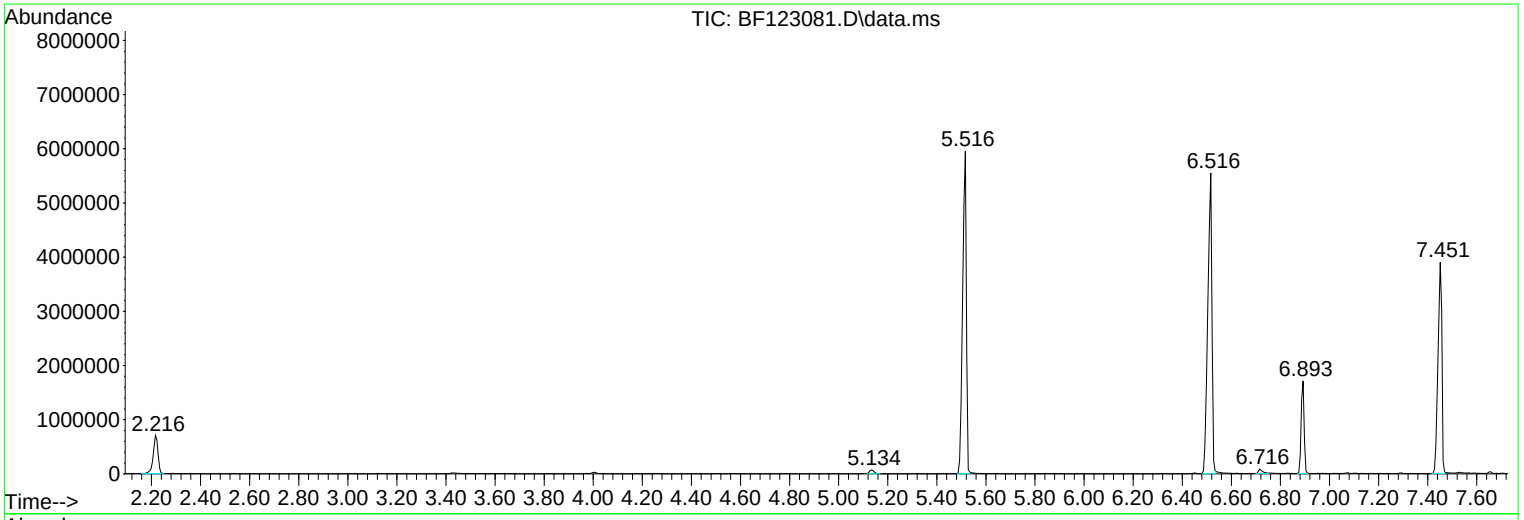
Instrument :
BNA_F
ClientSampleId :
RS-SP1

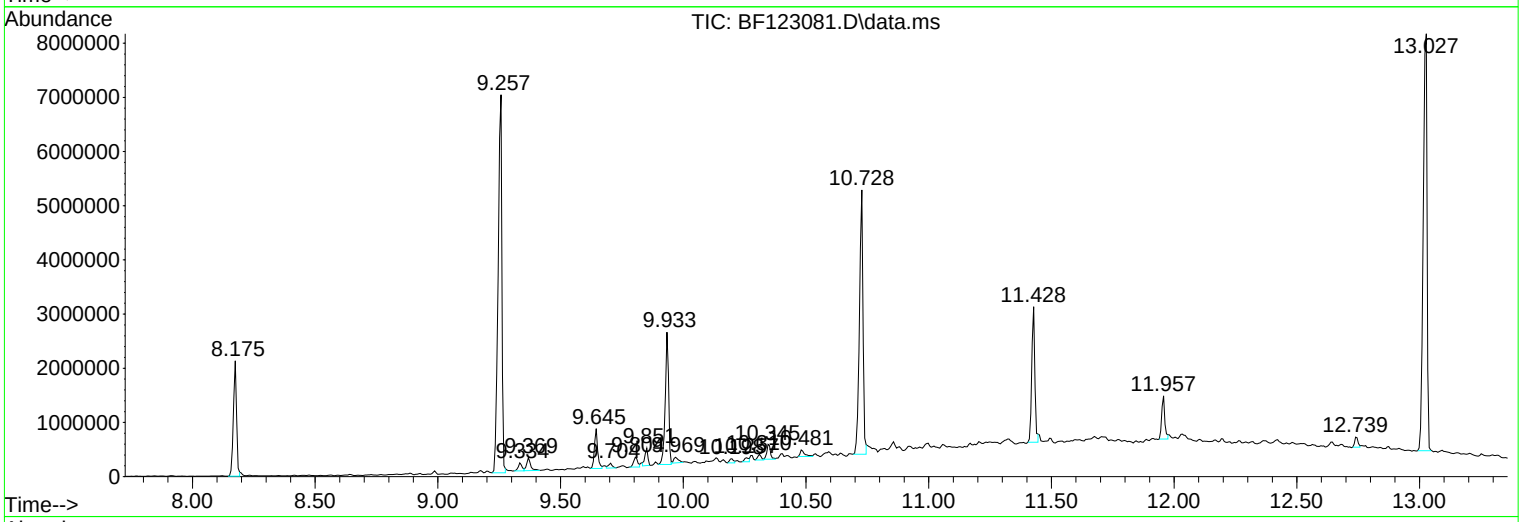
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

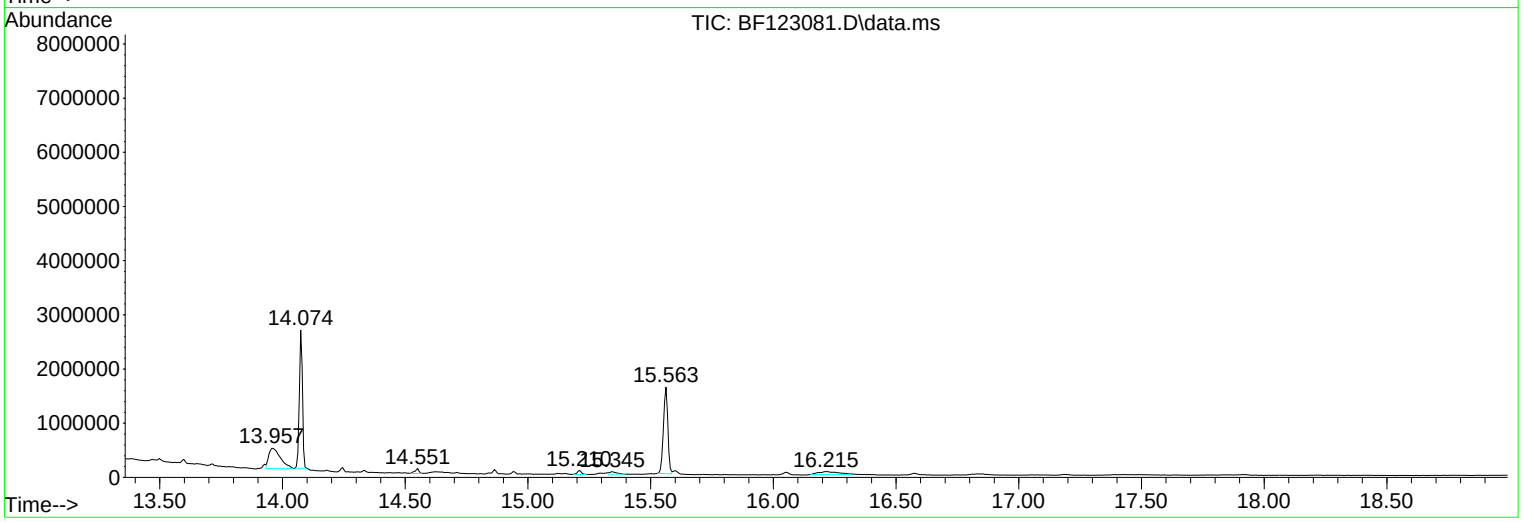
Instrument :
BNA_F
ClientSampleId :
RS-SP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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\BF012921\
Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RS-SP1

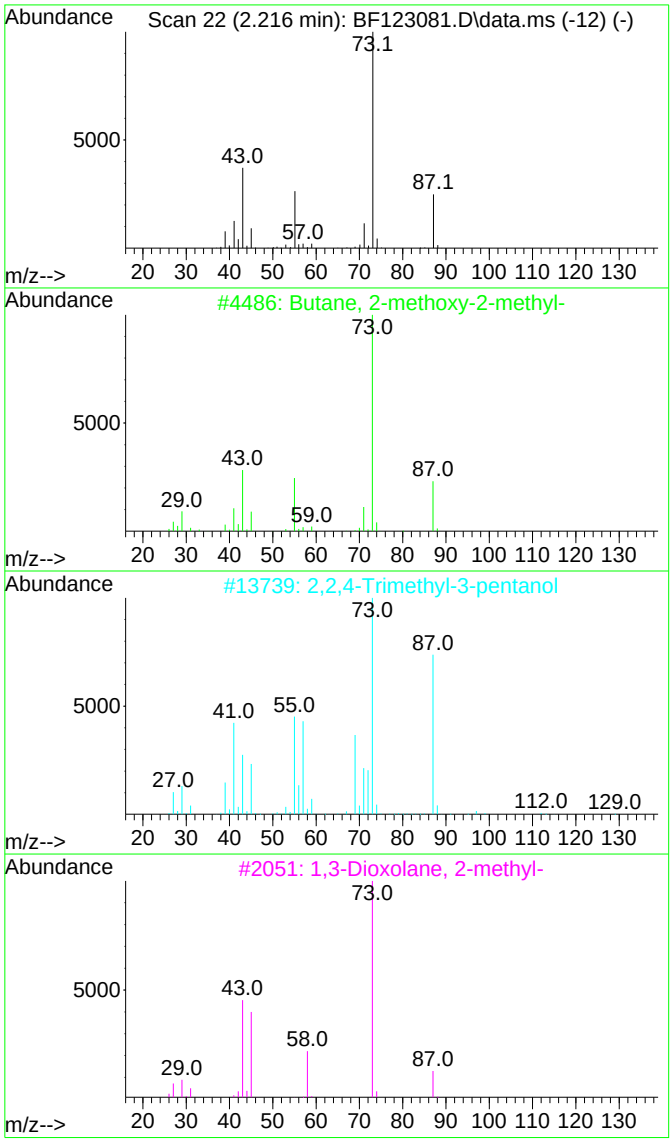
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

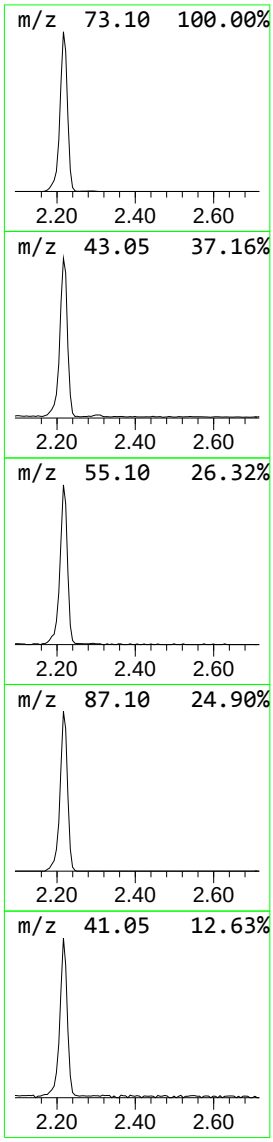
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.216	13.17 ng	944731	1,4-Dichlorobenzene-d4	6.893

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-SP1

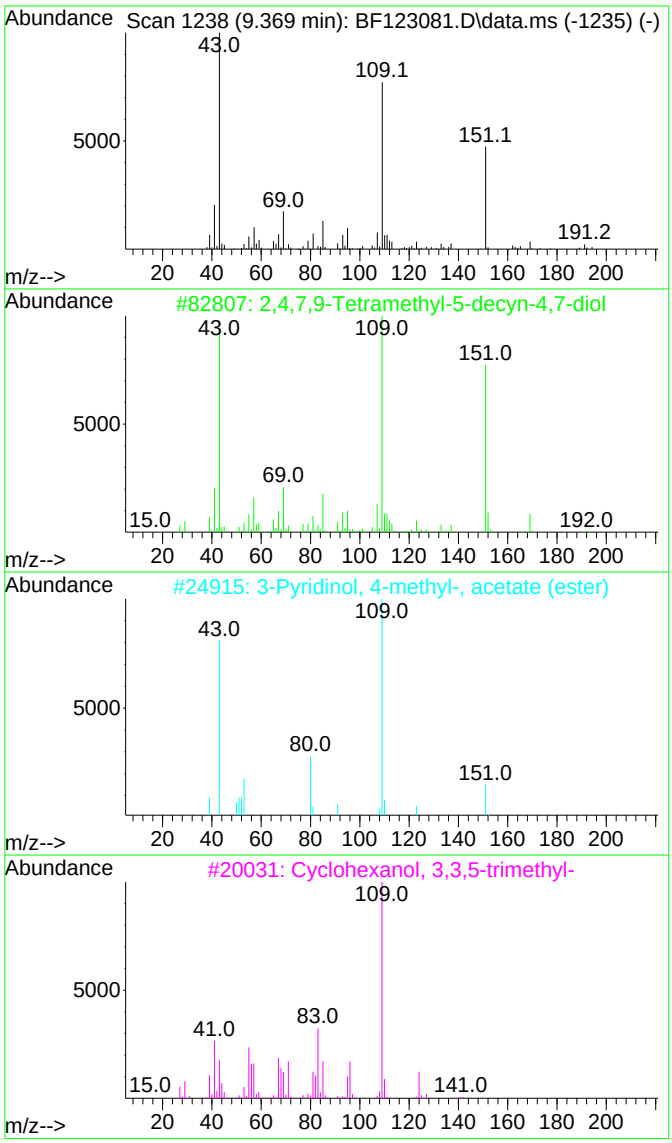
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

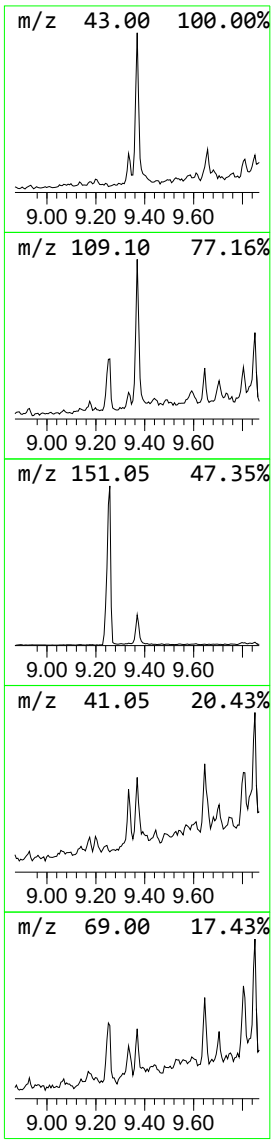
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.369	2.25 ng	261976	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	53
3	Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	47
4	2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	47
5	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RS-SP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

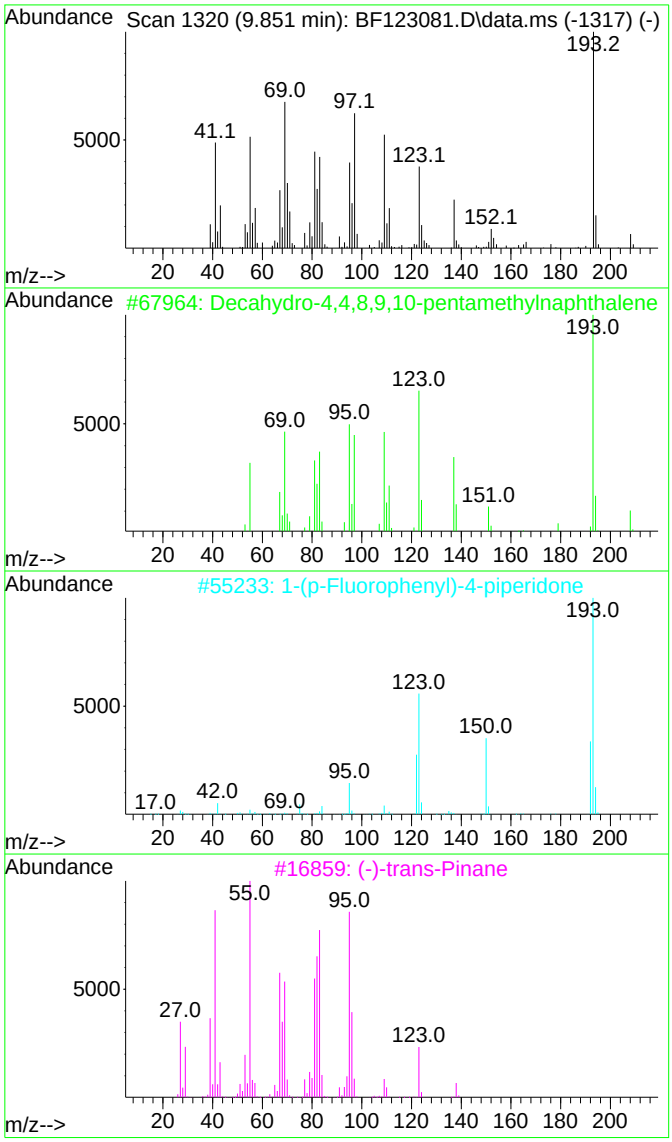
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

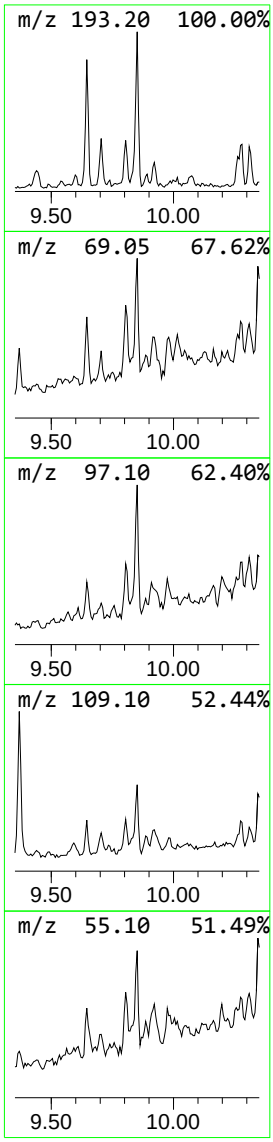
****

Peak Number 3 unknown9.851 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.851	2.29 ng	266655	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	49
2	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
3	(-)-trans-Pinane	138	C10H18	033626-25-4	30
4	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004755-33-3	25
5	[1,1'-Biphenyl]-4-acetonitrile	193	C14H11N	031603-77-7	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-SP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

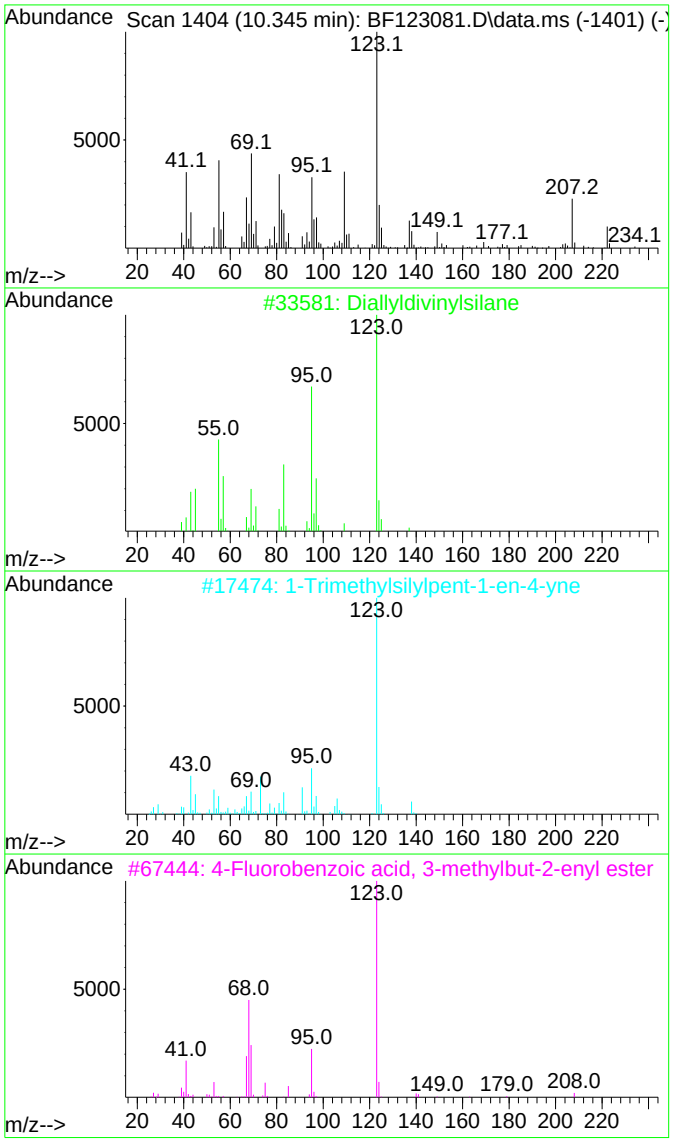
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

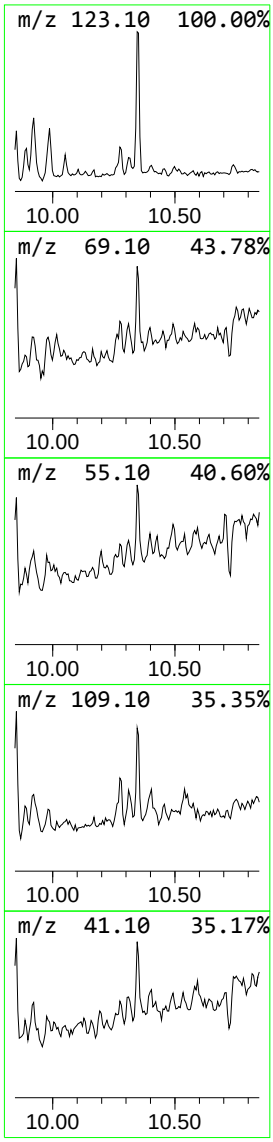
****

Peak Number 4 Diallyldivinylsilane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.345	2.40 ng	279933	Acenaphthene-d10	9.933

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diallyldivinylsilane	164	C10H16Si	119901-88-1	50
2	1-Trimethylsilylpent-1-en-4-yne	138	C8H14Si	079516-25-9	47
3	4-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	1000299-15-1	43
4	N-(4-Nitro-1,8-naphthalimido)-4-...	379	C19H10FN3O5	300690-90-8	43
5	3-Fluorobenzoic acid, 3-methylbu...	208	C12H13FO2	154559-38-3	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-SP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

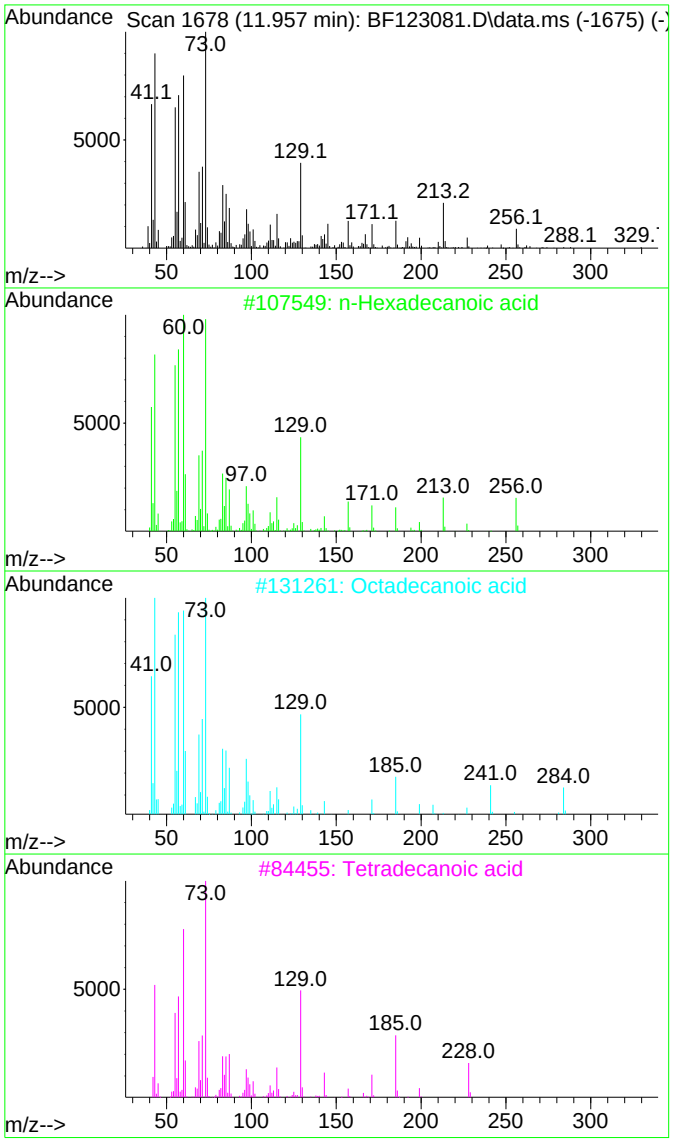
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

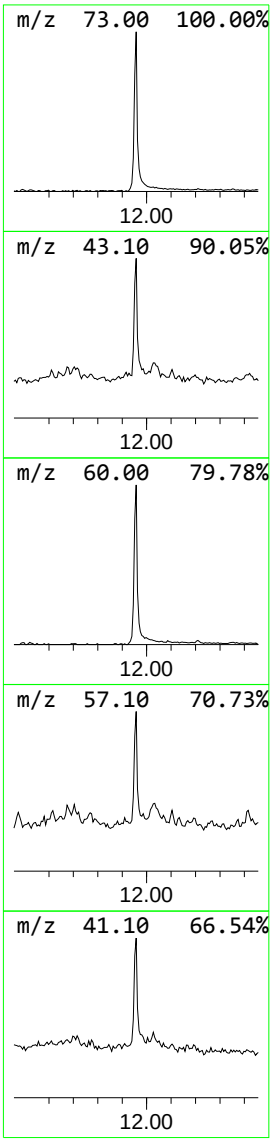
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	6.39 ng	703867	Phenanthrene-d10	11.428

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Tridecanoic acid	214	C13H26O2	000638-53-9	89





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Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-SP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

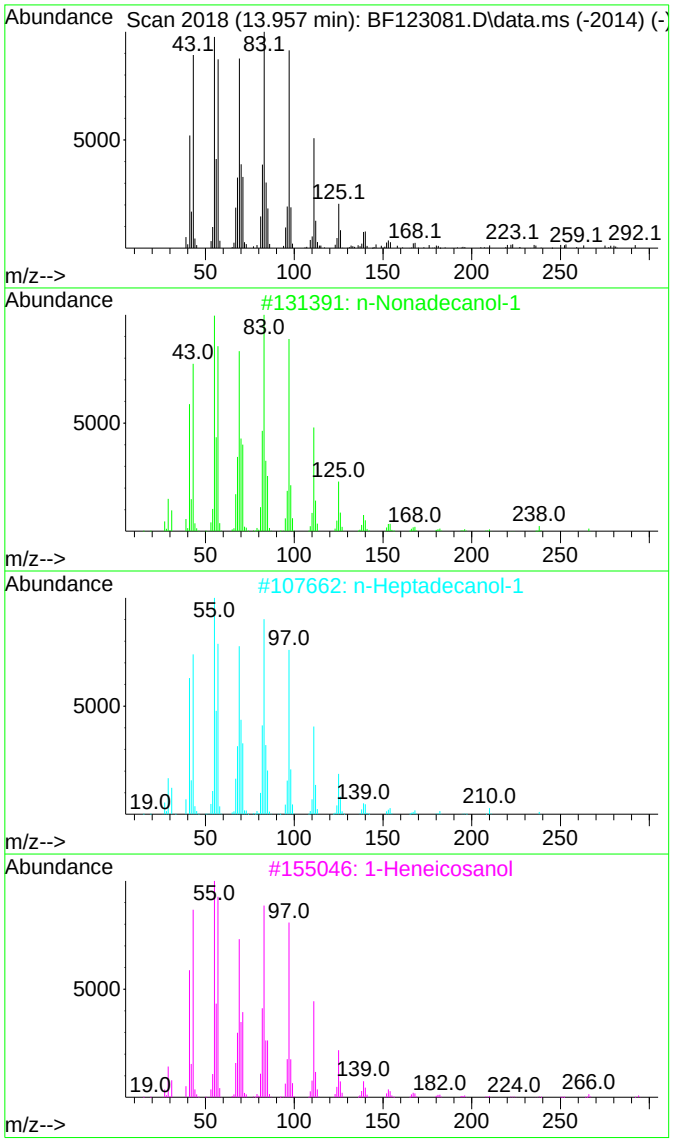
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

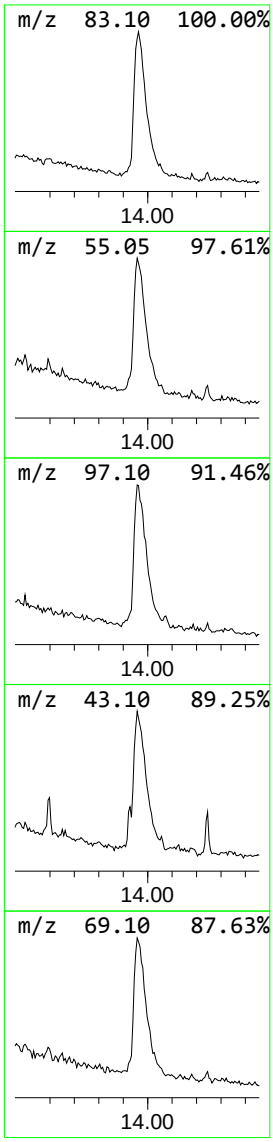
****

Peak Number 6 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.957	10.96 ng	1237400	Chrysene-d12	14.074

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	n-Heptadecanol-1	256	C17H36O	001454-85-9	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Cyclopentadecane	210	C15H30	000295-48-7	93
5	1-Hexadecanol	242	C16H34O	036653-82-4	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RS-SP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

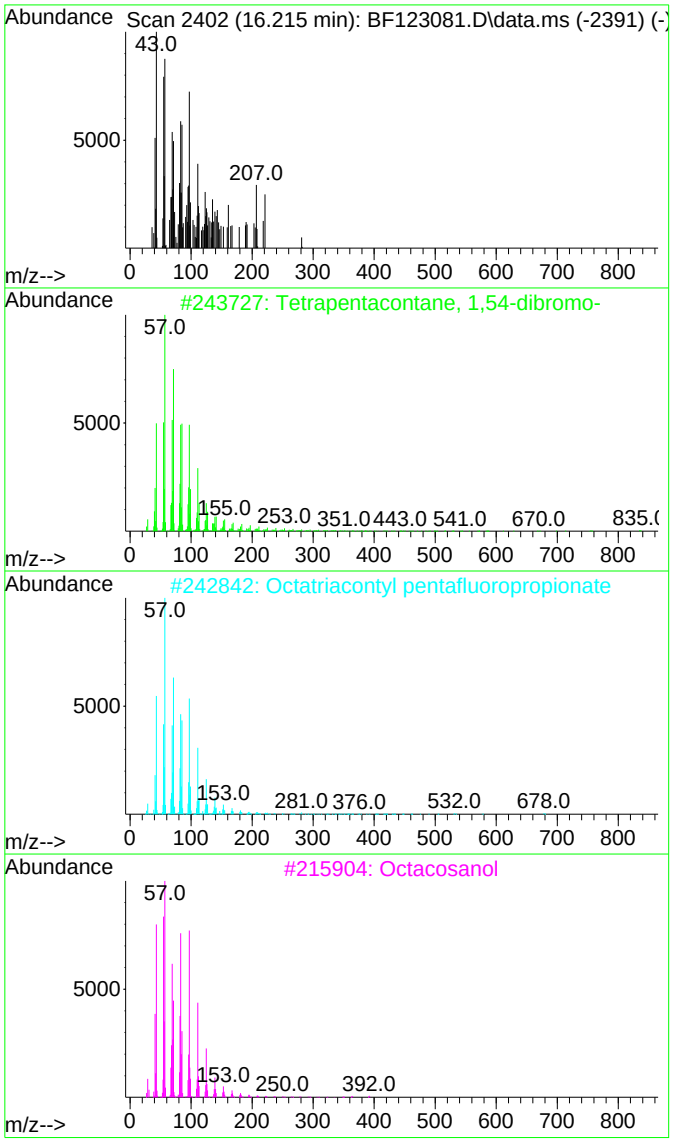
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

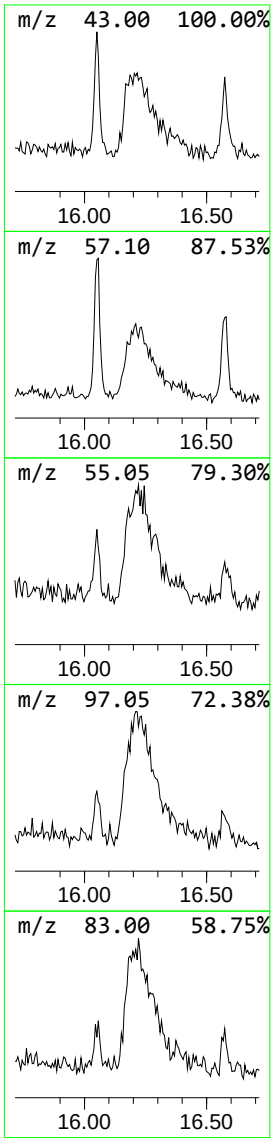
****

Peak Number 7 unknown16.215 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.215	3.07 ng	307375	Perylene-d12	15.563

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	45
2	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	43
3	Octacosanol	410	C28H58O	000557-61-9	38
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	38
5	17-Pentatriacontene	491	C35H70	006971-40-0	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF012921\
Data File : BF123081.D
Acq On : 29 Jan 2021 14:37
Operator : JU/CG
Sample : M1270-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : RS-SP1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012721.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
Butane, 2-metho...	2.216	13.2	ng	944731	1	6.893	1434580	20.0
2,4,7,9-Tetrame...	9.369	2.3	ng	261976	3	9.933	2328050	20.0
unknown9.851	9.851	2.3	ng	266655	3	9.933	2328050	20.0
Diallyldivinyls...	10.345	2.4	ng	279933	3	9.933	2328050	20.0
n-Hexadecanoic ...	11.957	6.4	ng	703867	4	11.428	2204640	20.0
n-Nonadecanol-1	13.957	11.0	ng	1237400	5	14.074	2258610	20.0
unknown16.215	16.215	3.1	ng	307375	6	15.563	1999560	20.0