LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF022818\
Data File : BF103309.D
Acq On : 28 Feb 2018 22:31
Operator : SJ/JU
Sample : J1708-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-222-226

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:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	8	14	21	rVB	335390	437844	9.54%	1.207%
2	5.122	513	516	528	rVB	130206	192516	4.19%	0.530%
3	5.504	576	581	584	rBV	4284448	4484088	97.71%	12.356%
4	6.510	747	752	768	rBV	3568622	4589354	100.00%	12.646%
5	6.645	771	775	779	rBV	3989249	4341339	94.60%	11.963%
6	6.875	810	814	820	rBV	1066631	1001443	21.82%	2.760%
7	7.028	836	840	844	rBV	3323770	3393347	73.94%	9.351%
8	7.439	905	910	913	rBV	2855270	3022545	65.86%	8.329%
9	8.157	1028	1032	1050	rBV	1306593	1303296	28.40%	3.591%
10	9.233	1210	1215	1218	rBV	3873306	4024084	87.68%	11.089%
11	9.298	1224	1226	1229	rVB	66492	52164	1.14%	0.144%
12	9.622	1276	1281	1288	rBV	348147	359288	7.83%	0.990%
13	9.828	1313	1316	1320	rBV	157693	127726	2.78%	0.352%
14	9.910	1327	1330	1338	rVB	1221259	1191812	25.97%	3.284%
15	10.328	1398	1401	1404	rVB	167260	122648	2.67%	0.338%
16	10.704	1461	1465	1478	rBV	1807932	1971507	42.96%	5.433%
17	10.798	1478	1481	1486	rVB	72735	80158	1.75%	0.221%
18	11.404	1580	1584	1598	rBV	917971	909905	19.83%	2.507%
19	11.916	1668	1671	1676	rBV2	58968	65903	1.44%	0.182%
20	12.986	1849	1853	1857	rBV	2449052	2377394	51.80%	6.551%
21	13.868	1999	2003	2014	rBV	458874	548952	11.96%	1.513%
22	14.051	2030	2034	2043	rBV	769786	784935	17.10%	2.163%
23	15.551	2284	2289	2300	rBV	491106	742289	16.17%	2.045%
24	15.980	2359	2362	2367	rVB	58625	74664	1.63%	0.206%
25	16.533	2453	2456	2462	rVB	60754	90734	1.98%	0.250%

Sum of corrected areas: 36289935

LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF022818\
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Operator : SJ/JU
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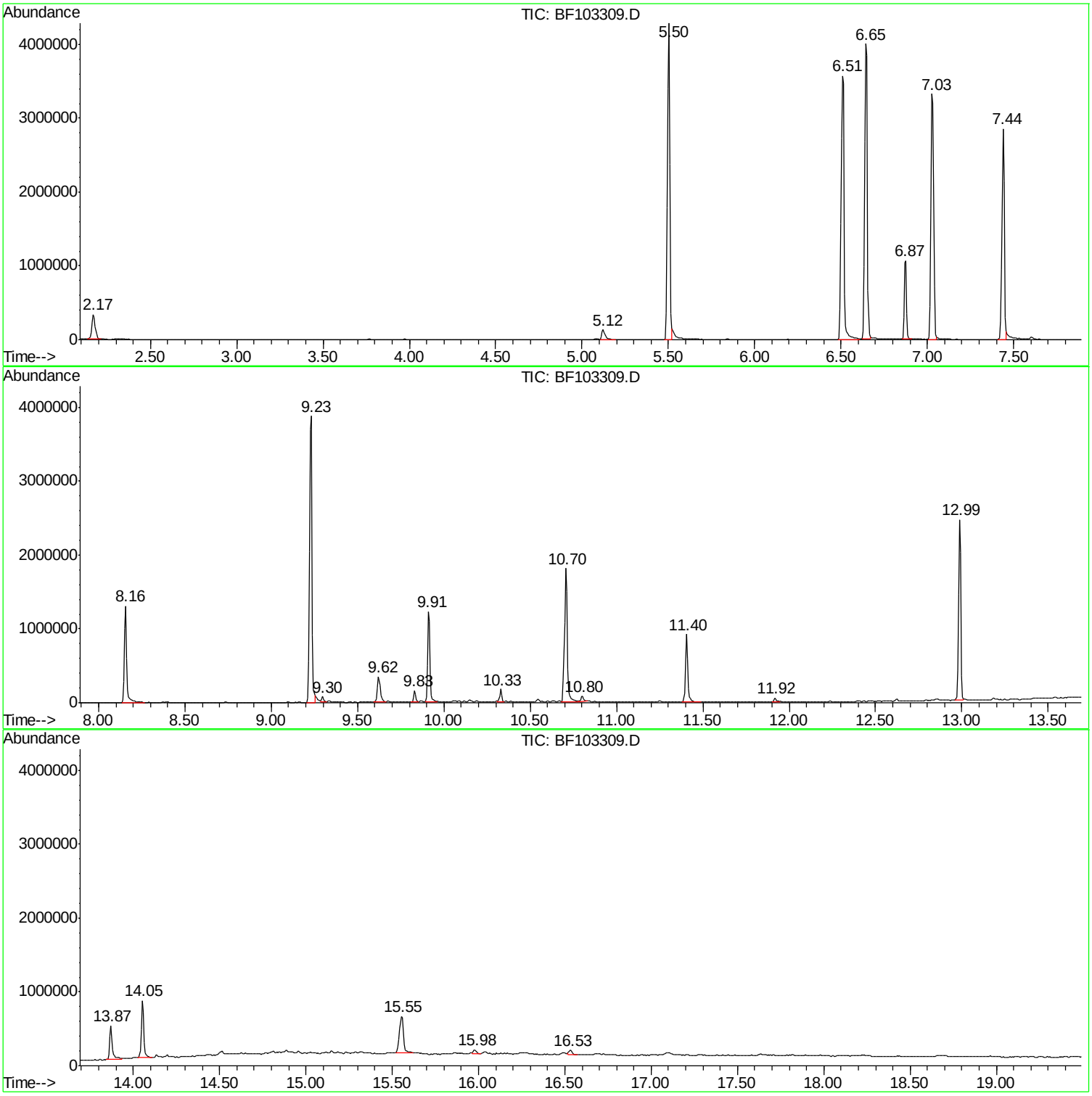
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-222-226

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF103309.D
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
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RO-222-226

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

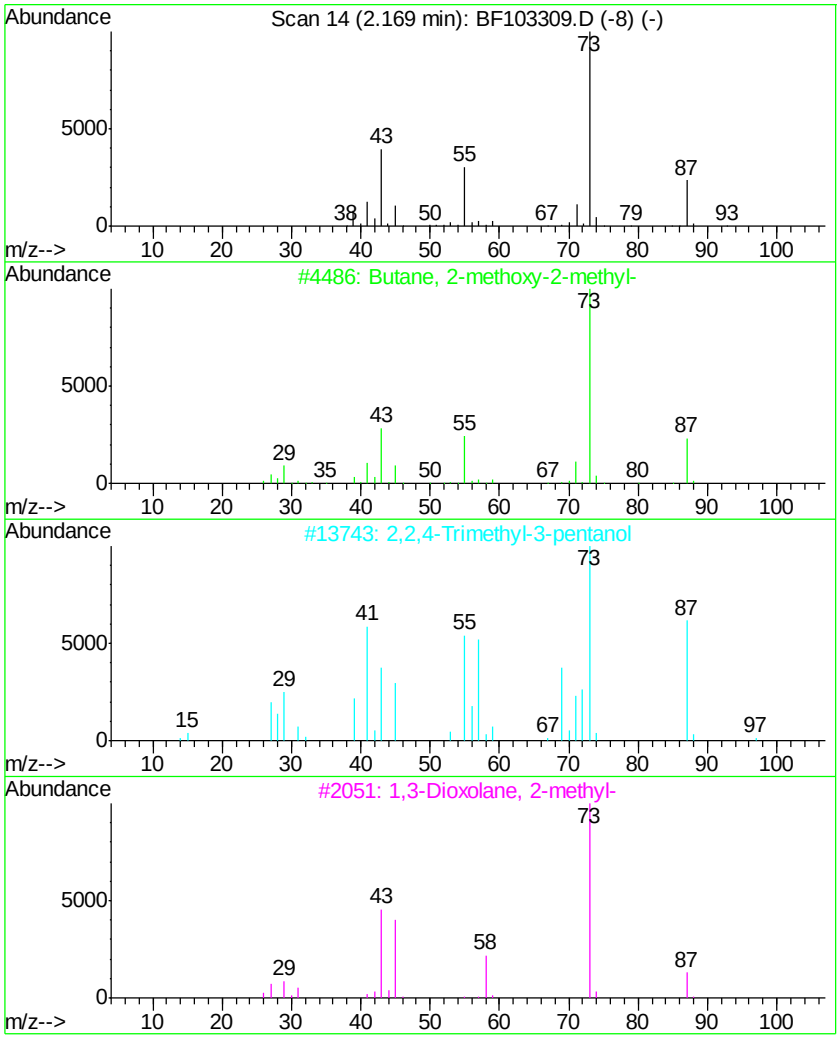
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

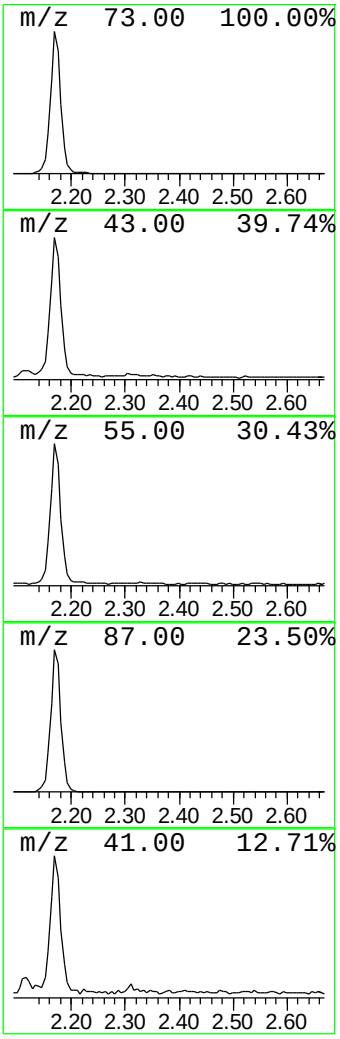
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	8.74 ng	437844	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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ALS Vial : 17 Sample Multiplier: 1

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BNA_F
ClientSampleId :
RO-222-226

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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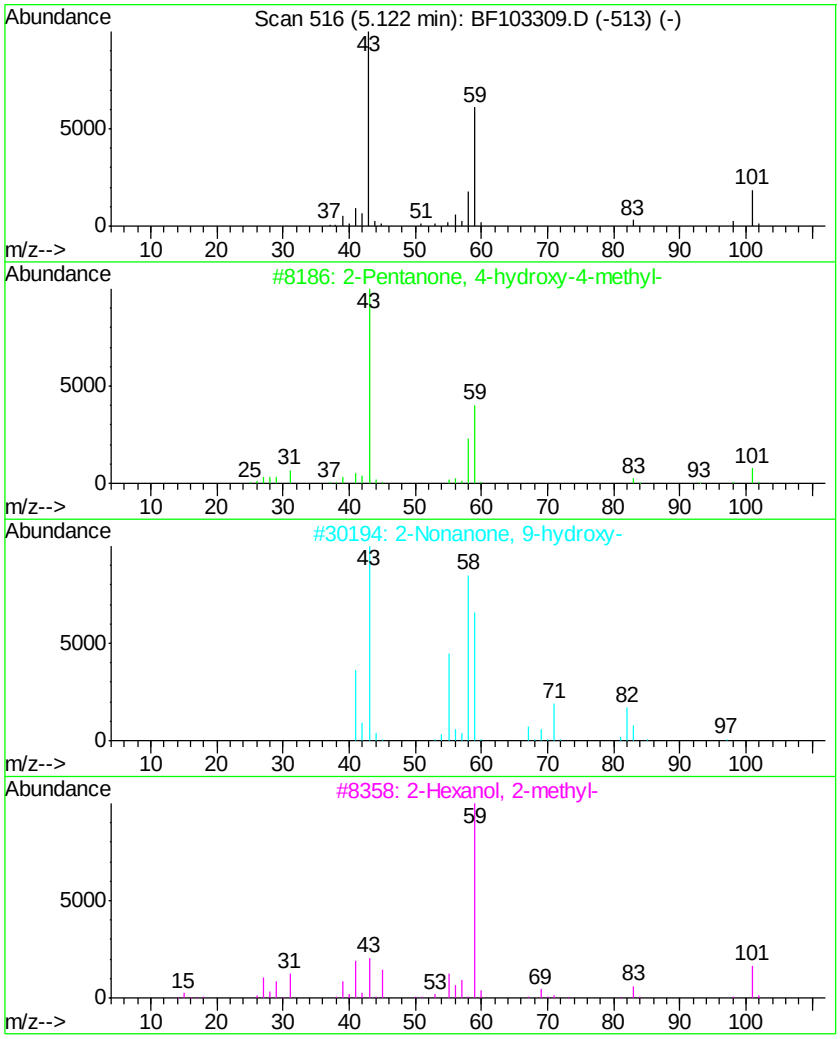
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

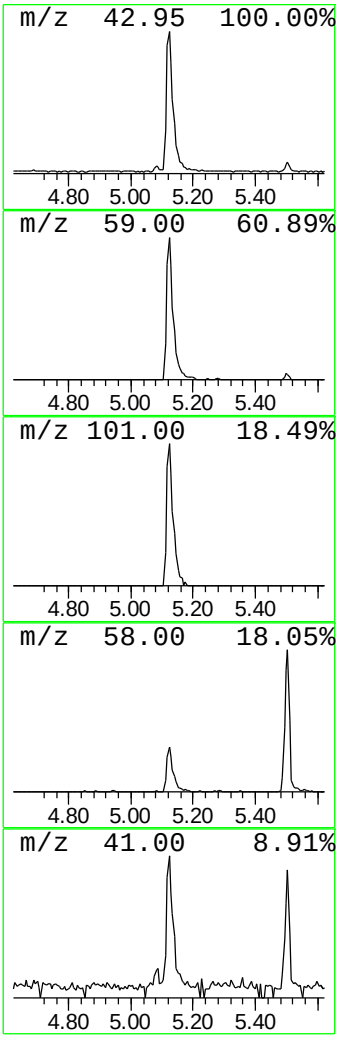
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	3.84 ng	192516	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
5	Acetone	58	C3H6O	000067-64-1	12





Library Search Compound Report

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Data File : BF103309.D
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Sample : J1708-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-222-226

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
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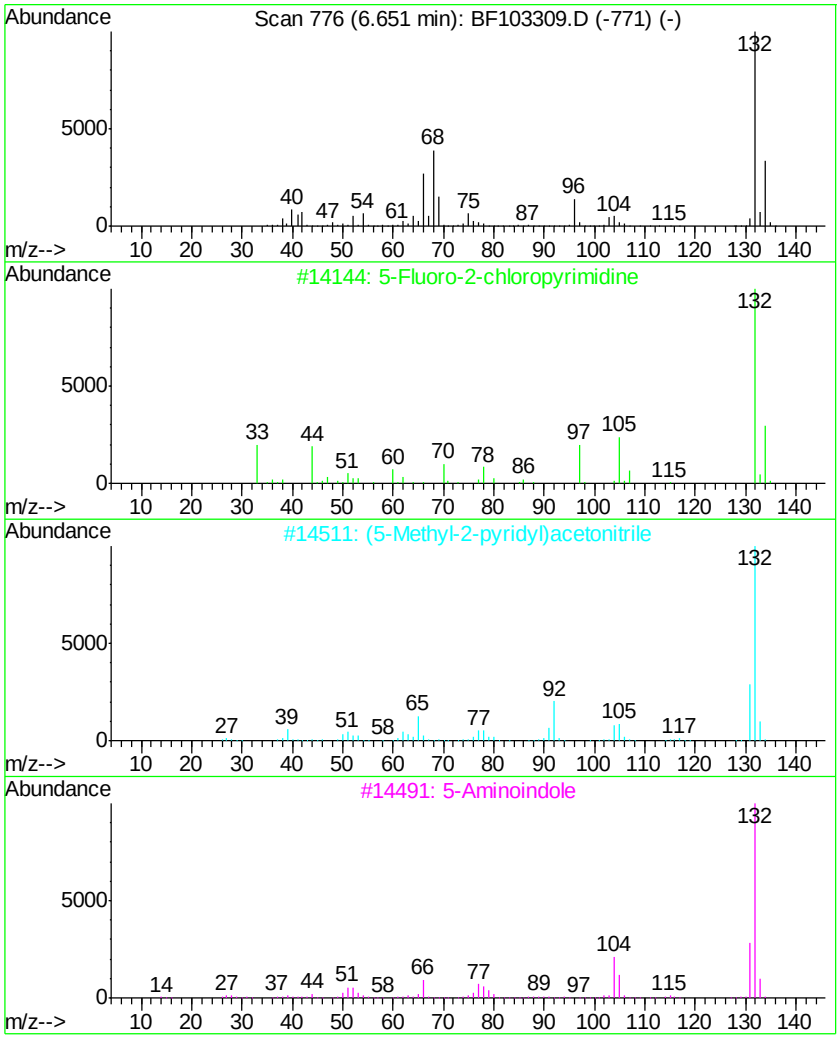
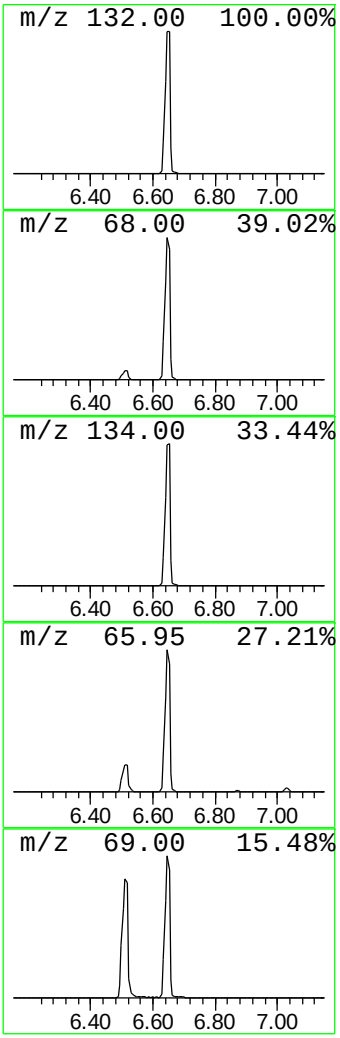
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	86.70 ng	4341340	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RO-222-226

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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TIC Library : C:\DATABASE\NIST11.L
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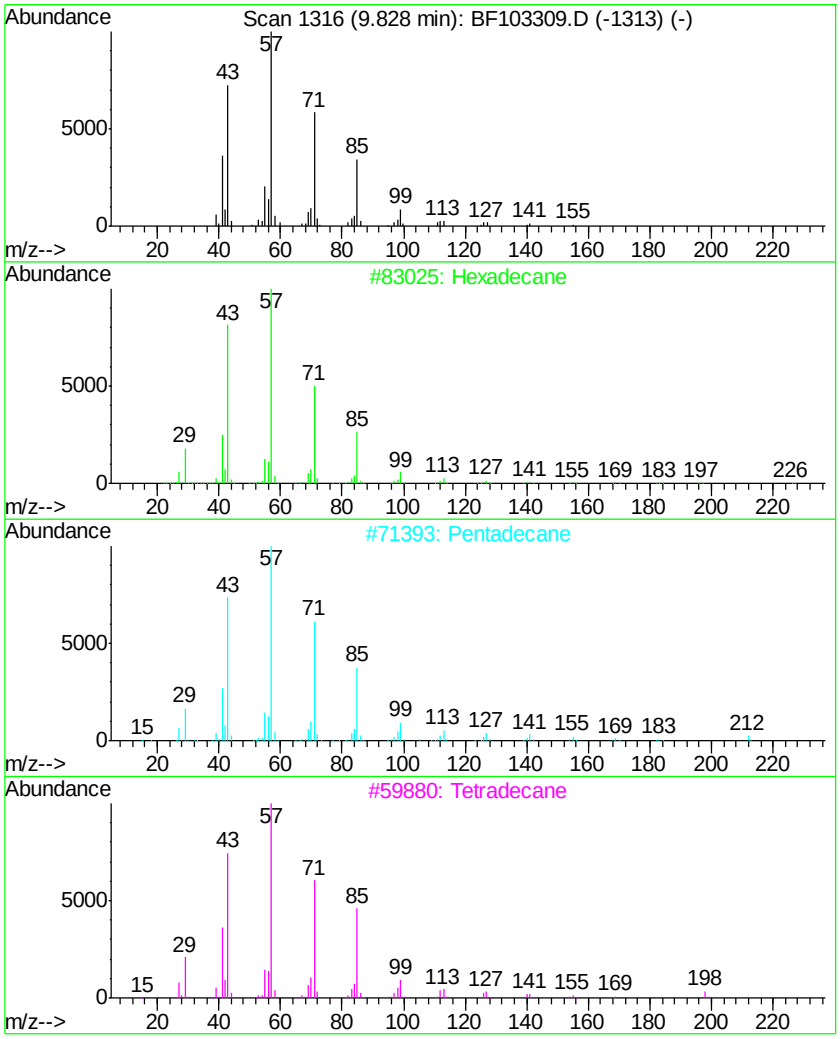
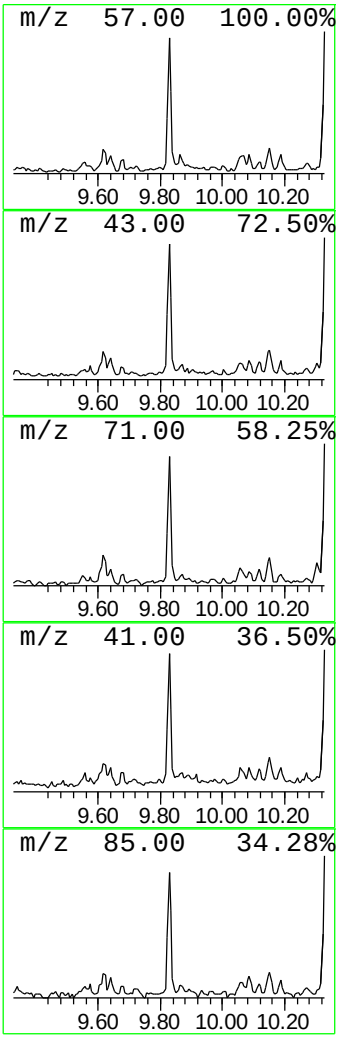
****

Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.83	2.14 ng	127726	Acenaphthene-d10	9.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Pentadecane	212	C15H32	000629-62-9	90
3	Tetradecane	198	C14H30	000629-59-4	90
4	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	78
5	Decane, 3-bromo-	220	C10H21Br	030571-71-2	59





Library Search Compound Report

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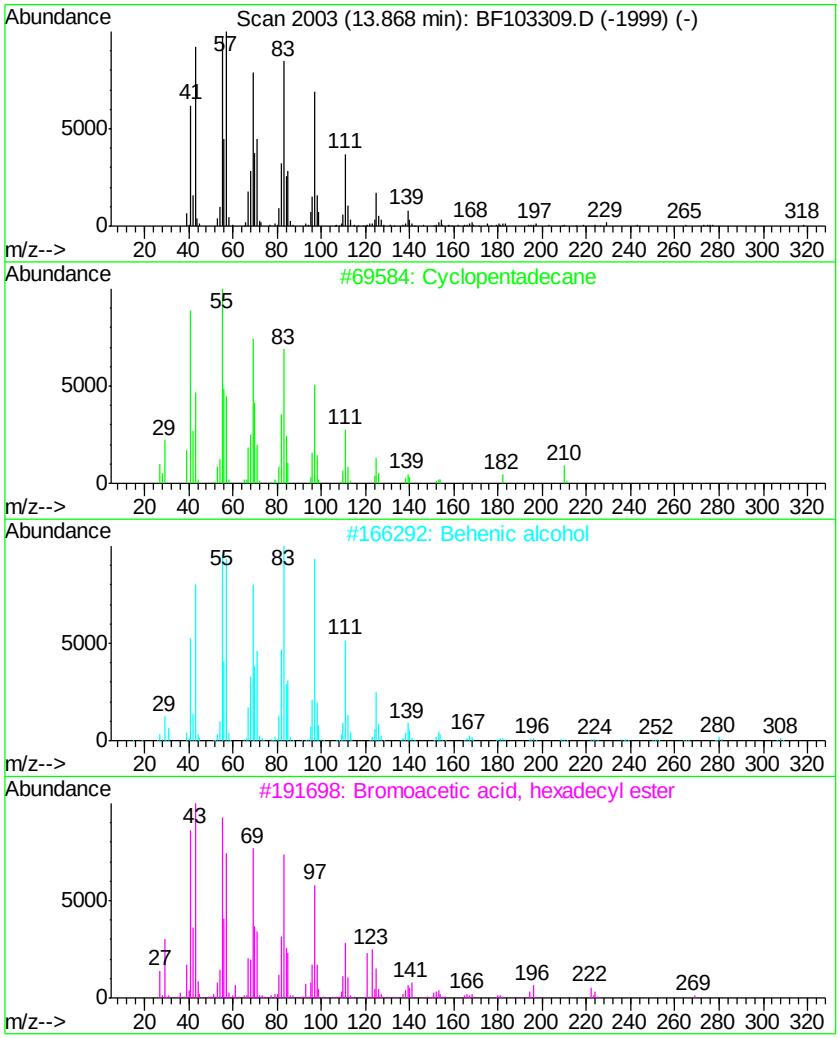
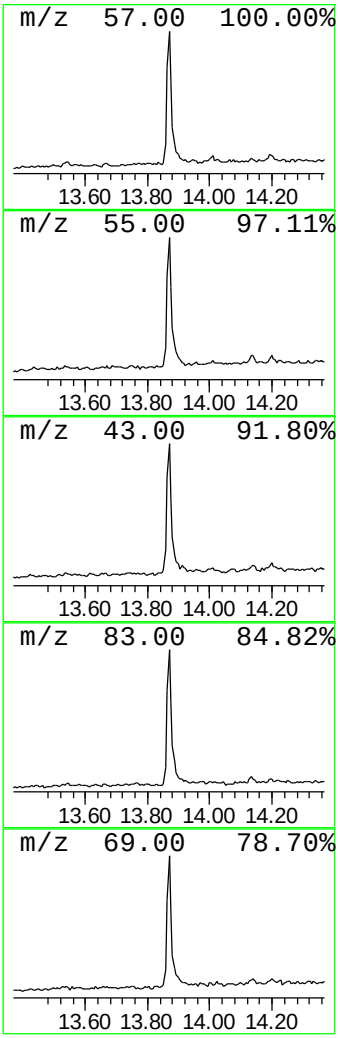
****

Peak Number 7 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	13.99 ng	548952	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





Library Search Compound Report

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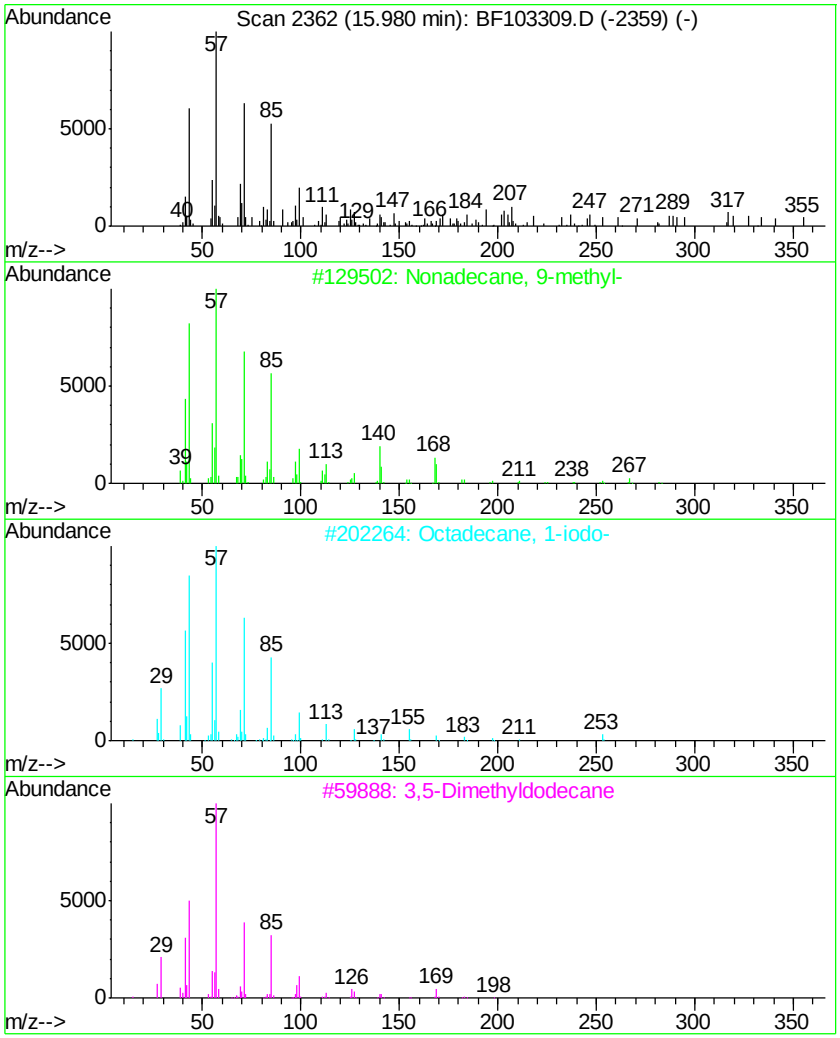
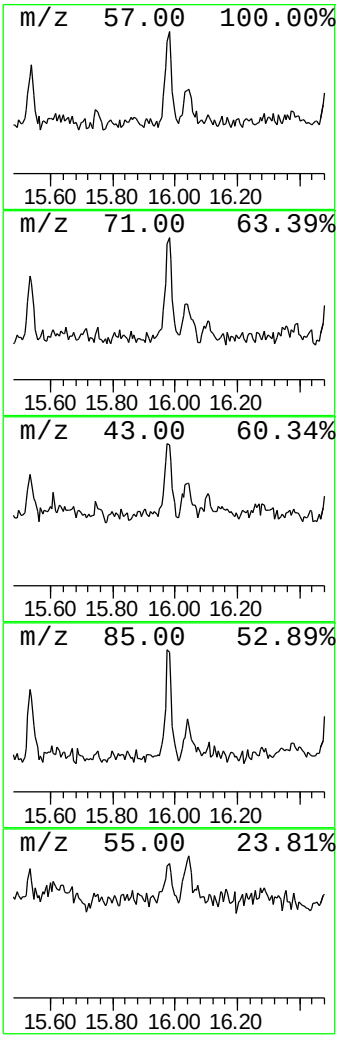
****

Peak Number 8 Nonadecane, 9-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.01 ng	74664	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	76
2	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	64
3	3,5-Dimethyldodecane	198	C14H30	107770-99-0	64
4	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	64
5	Tridecane	184	C13H28	000629-50-5	53





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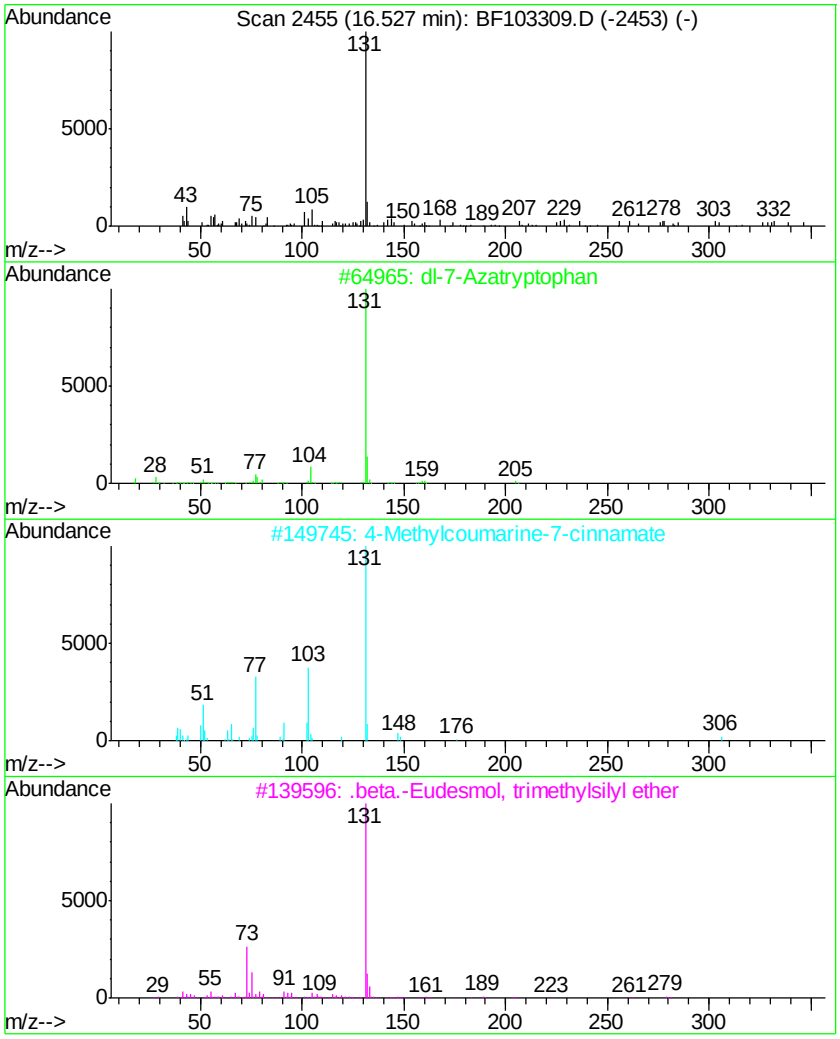
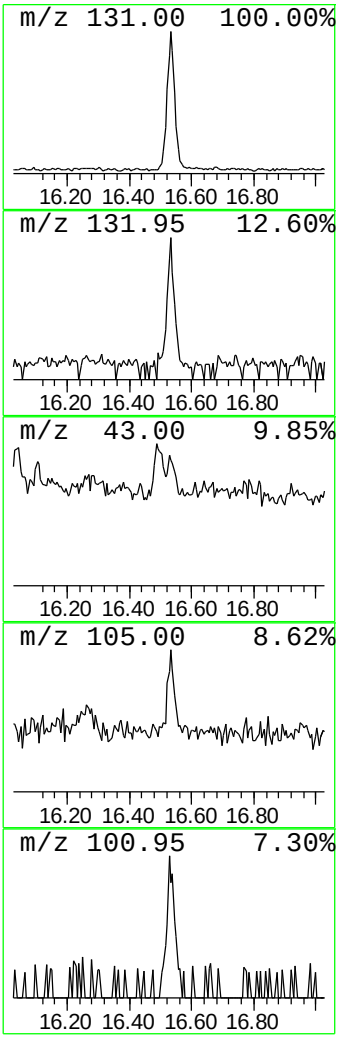
****

Peak Number 9 dl-7-Azatryptophan Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.44 ng	90734	Perylene-d12	15.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-7-Azatryptophan	205	C10H11N3O2	001137-00-4	64
2	4-Methylcoumarine-7-cinnamate	306	C19H14O4	300829-05-4	56
3	.beta.-Eudesmol, trimethylsilyl ...	294	C18H34OSi	1000334-00-1	50
4	3,6-Dioxa-2,7-disilaoctane, 2,2,...	262	C12H30O2Si2	006730-96-7	39
5	Propanedioic acid, nitrile, hydr...	229	C12H11N3O2	294878-35-6	39





Tentatively Identified Compound (LSC) summary

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TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-methoxy...	2.17	8.7	ng	437844	1	6.87	1001440	20.0
2-Pentanone, 4-hy...	5.12	3.8	ng	192516	1	6.87	1001440	20.0
unknown6.65	6.65	86.7	ng	4341340	1	6.87	1001440	20.0
Hexadecane	9.83	2.1	ng	127726	3	9.91	1191810	20.0
Cyclopentadecane	13.87	14.0	ng	548952	5	14.05	784935	20.0
Nonadecane, 9-met...	15.98	2.0	ng	74664	6	15.56	742289	20.0
dl-7-Azatryptophan	16.53	2.4	ng	90734	6	15.56	742289	20.0