LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089523.D
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

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-BF072716.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	1.656	4	6	47	rVB	736354	1737696	100.00%	17.329%
2	4.547	257	259	268	rBV	41034	57246	3.29%	0.571%
3	5.039	300	302	318	rBV7	201253	323095	18.59%	3.222%
4	6.136	397	398	406	rBV2	150065	229469	13.21%	2.288%
5	6.239	406	407	420	rVB	540966	685235	39.43%	6.833%
6	6.479	426	428	439	rBV	179362	214143	12.32%	2.135%
7	6.627	439	441	456	rVV	571718	672173	38.68%	6.703%
8	6.822	456	458	461	rVB	13907	21105	1.21%	0.210%
9	7.027	473	476	477	rBV2	67009	89969	5.18%	0.897%
10	7.050	477	478	487	rVV	501142	566533	32.60%	5.650%
11	7.176	487	489	491	rVV	17131	21220	1.22%	0.212%
12	7.267	493	497	499	rVV2	38285	60460	3.48%	0.603%
13	7.428	507	511	516	rVB2	25593	38773	2.23%	0.387%
14	7.508	516	518	521	rBV	138373	156956	9.03%	1.565%
15	7.702	533	535	537	rBV	20131	21133	1.22%	0.211%
16	7.759	538	540	544	rVV3	231752	355094	20.43%	3.541%
17	7.862	548	549	553	rVV	13333	19076	1.10%	0.190%
18	7.999	556	561	563	rBV2	7686	18893	1.09%	0.188%
19	8.045	563	565	570	rVB4	10669	18167	1.05%	0.181%
20	8.239	579	582	585	rBV	23503	26499	1.52%	0.264%
21	8.422	593	598	600	rVB2	18854	24354	1.40%	0.243%
22	8.536	603	608	610	rBV4	12423	33453	1.93%	0.334%
23	8.673	618	620	622	rVB2	24133	29092	1.67%	0.290%
24	8.845	633	635	637	rBV	1190053	1095041	63.02%	10.920%
25	9.096	655	657	660	rBV2	13982	27437	1.58%	0.274%
26	9.211	663	667	669	rVB3	15214	34580	1.99%	0.345%
27	9.302	674	675	680	rVB3	12123	18216	1.05%	0.182%
28	9.439	684	687	691	rVB3	21134	41456	2.39%	0.413%
29	9.508	691	693	695	rBV	347554	362212	20.84%	3.612%
30	9.656	702	706	710	rBV3	71542	175743	10.11%	1.753%
31	9.713	710	711	714	rVB2	15211	18578	1.07%	0.185%
32	9.839	721	722	724	rBV	54198	86077	4.95%	0.858%
33	10.033	731	739	742	rBV2	213186	428635	24.67%	4.274%
34	10.216	753	755	757	rBV	27099	30857	1.78%	0.308%

LSC Area Percent Report

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Data File : BF089523.D
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

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-BF072716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.262	757	759	760	rBV2	28254	33901	1.95%	0.338%
36	10.296	760	762	764	rBV	409739	555773	31.98%	5.542%
37	10.411	770	772	778	rVV2	24680	43937	2.53%	0.438%
38	10.491	778	779	784	rVB4	13453	27038	1.56%	0.270%
39	10.639	788	792	795	rVB4	10700	23152	1.33%	0.231%
40	10.982	819	822	824	rBV	227598	318623	18.34%	3.177%
41	11.542	869	871	875	rVB	20557	33572	1.93%	0.335%
42	12.319	936	939	942	rBV	12525	21407	1.23%	0.213%
43	12.559	958	960	962	rBV	875195	811836	46.72%	8.096%
44	13.600	1048	1051	1056	rBV	149892	226551	13.04%	2.259%
45	14.925	1164	1167	1173	rBV	150692	193372	11.13%	1.928%

Sum of corrected areas: 10027828

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
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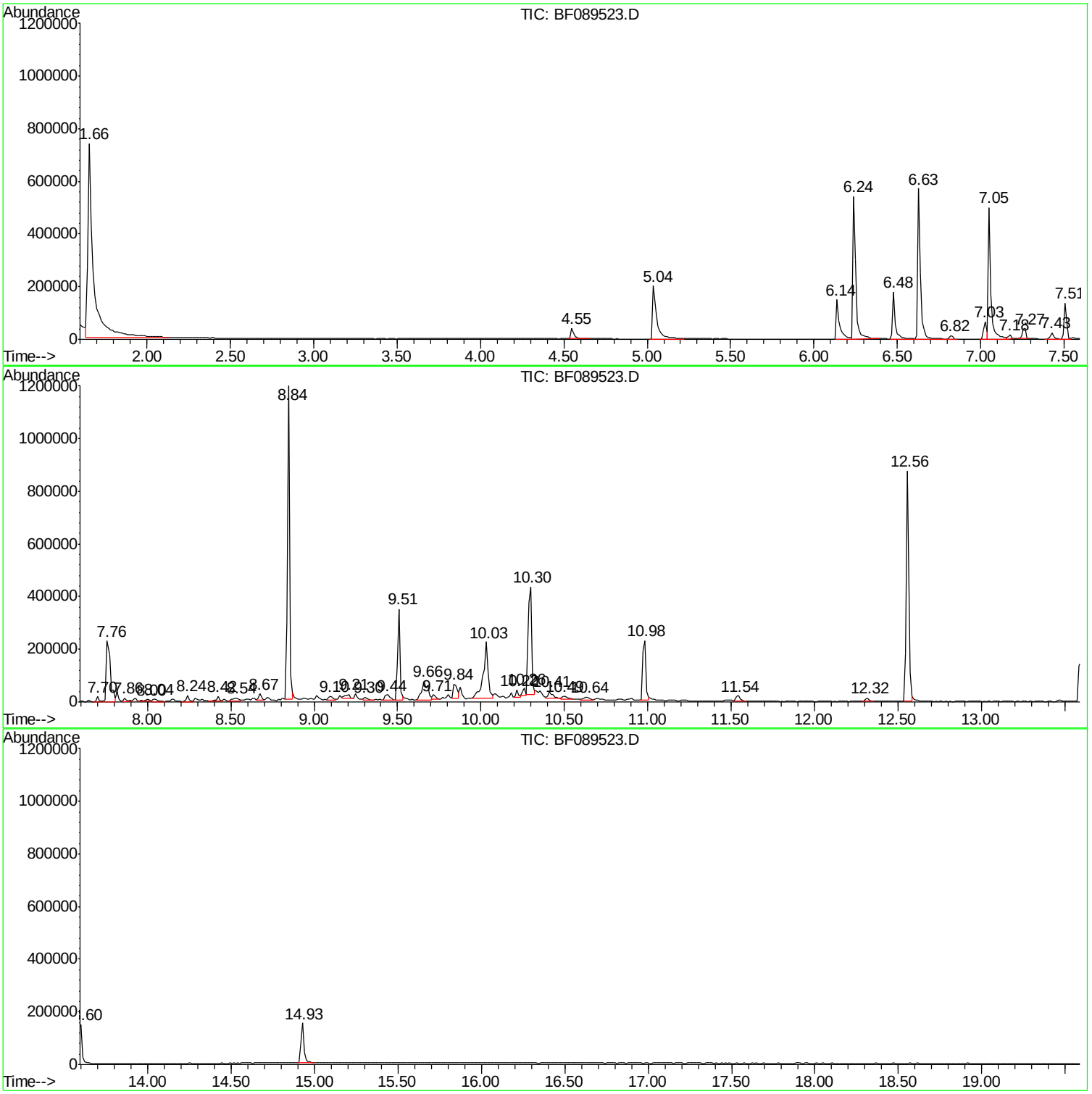
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089523.D
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

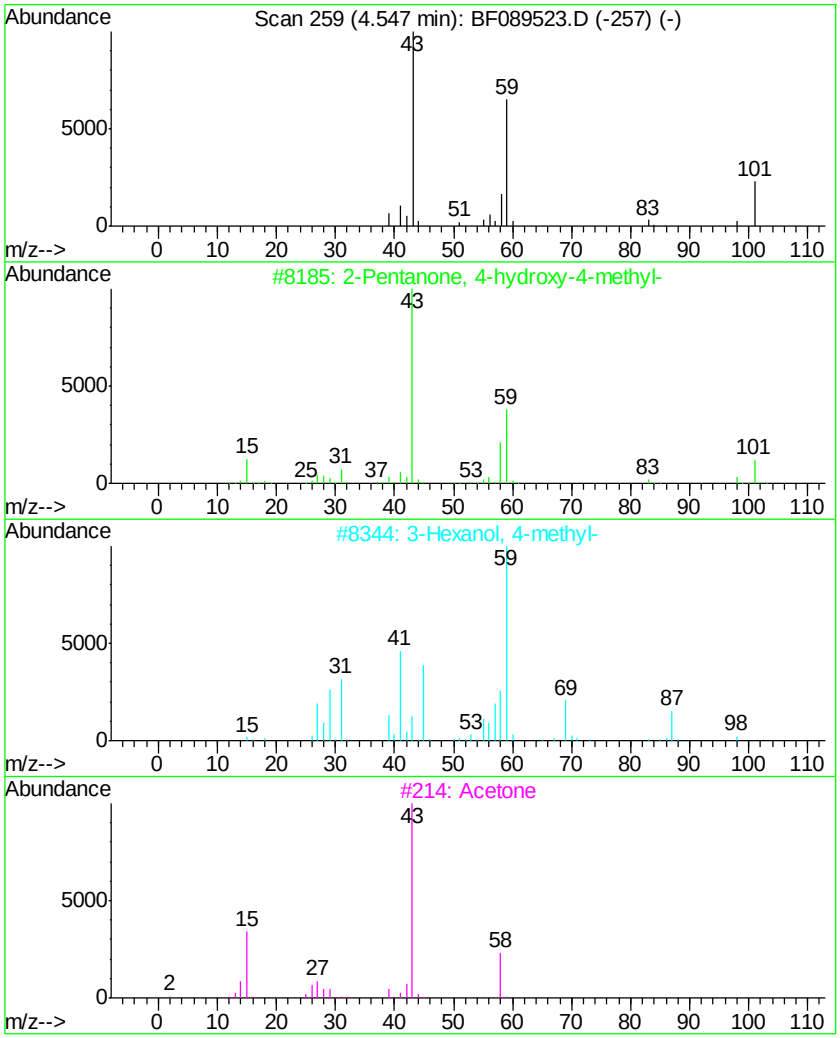
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

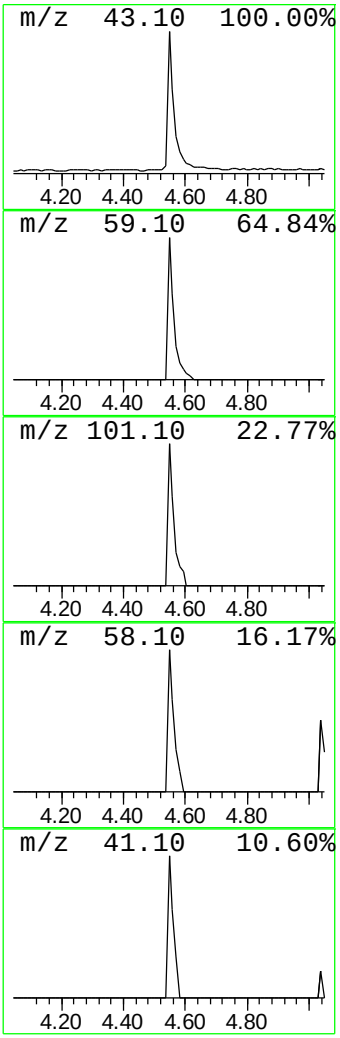
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	5.35 ng	57246	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetone	58	C3H6O	000067-64-1	9
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





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Data File : BF089523.D
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

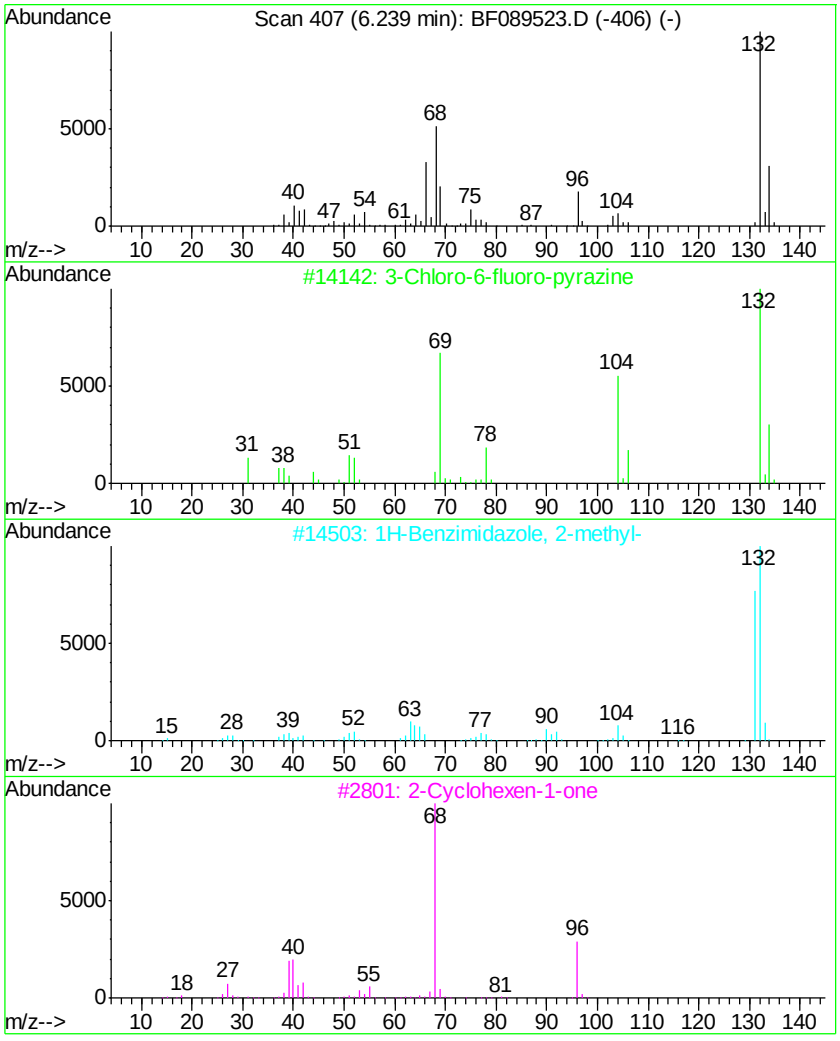
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

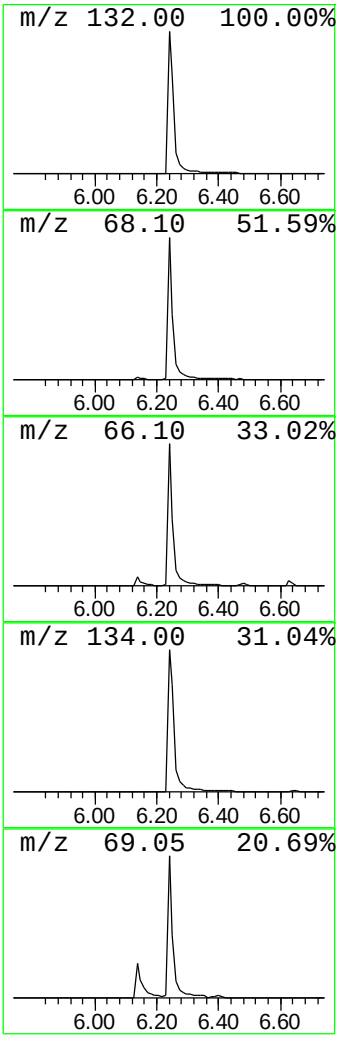
****

Peak Number 3 unknown6.24 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	64.00 ng	685235	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089523.D
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

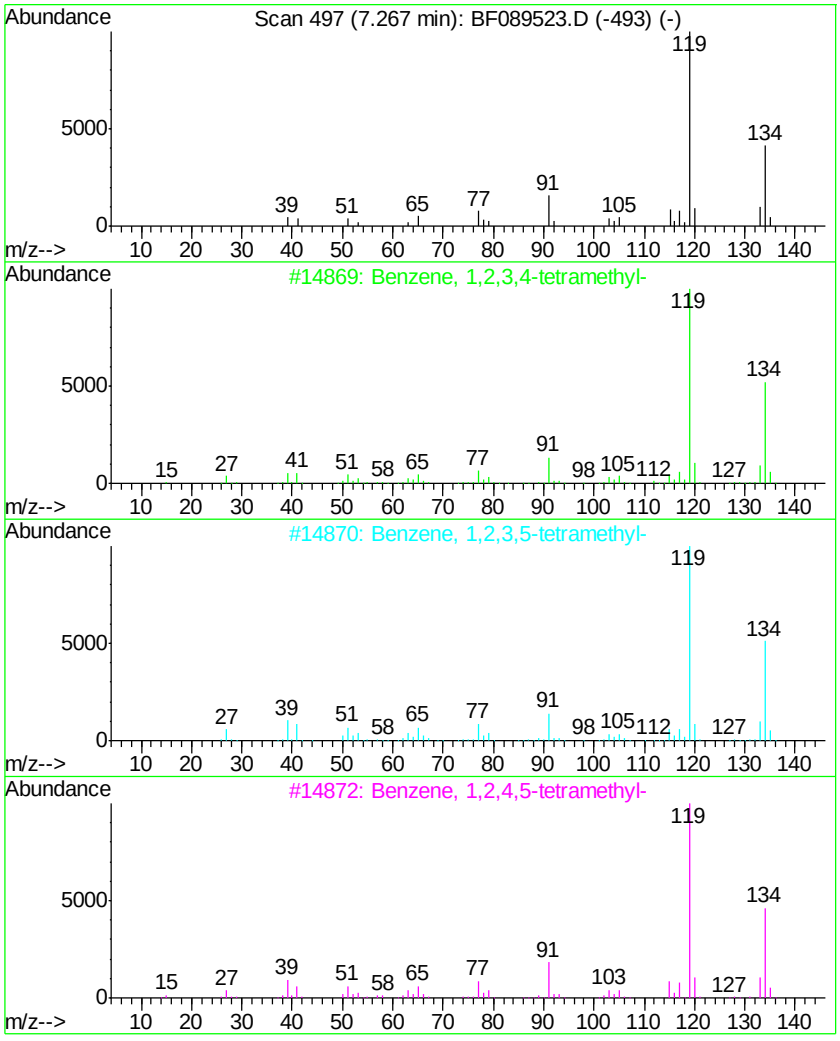
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

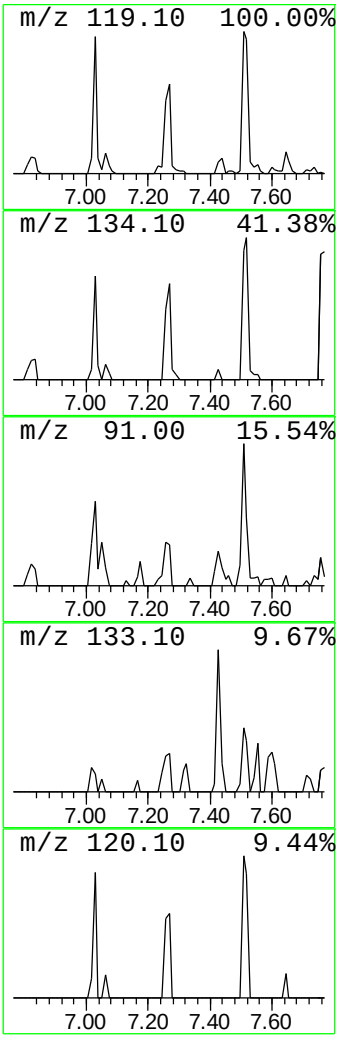
****

Peak Number 5 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.27	3.41 ng	60460	Naphthalene-d8	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
2	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	95
4	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	94
5	o-Cymene	134	C10H14	000527-84-4	94





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089523.D
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

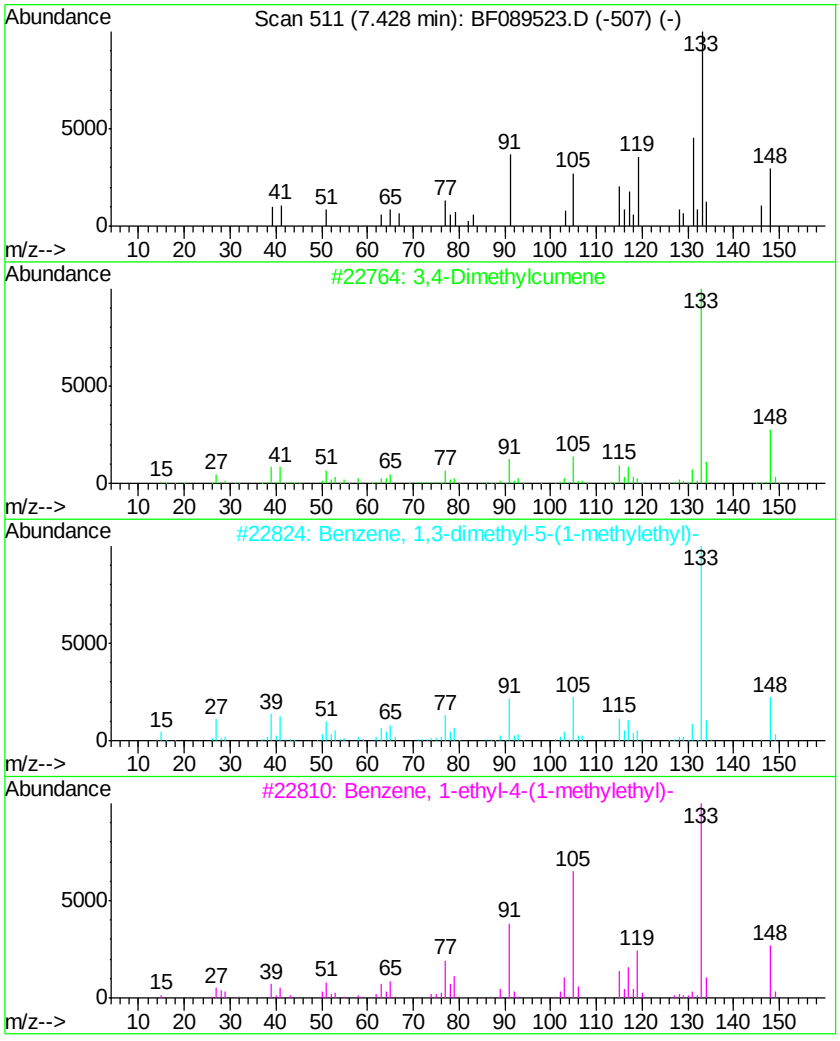
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

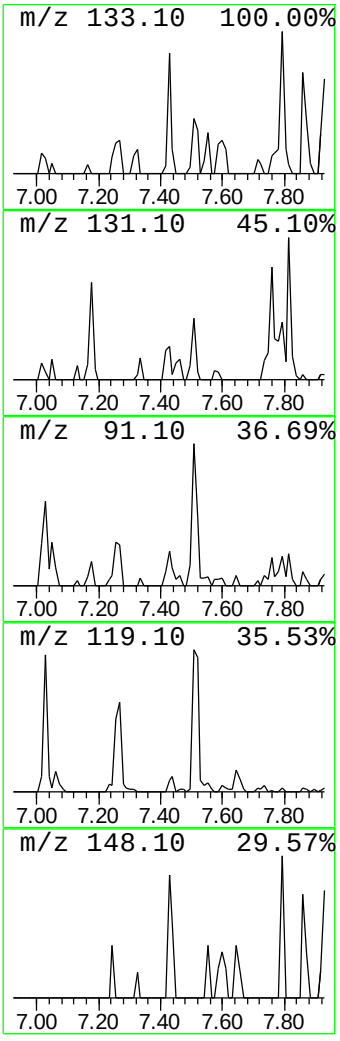
****

Peak Number 6 3,4-Dimethylcumene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.43	2.18 ng	38773	Naphthalene-d8	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dimethylcumene	148	C11H16	1000370-34-1	70
2	Benzene, 1,3-dimethyl-5-(1-methy...	148	C11H16	004706-90-5	50
3	Benzene, 1-ethyl-4-(1-methylethyl)-	148	C11H16	004218-48-8	49
4	1,5,6,7-Tetramethylbicyclo[3.2.0...	148	C11H16	134329-46-7	47
5	Ethanone, 1-(4-ethylphenyl)-	148	C10H12O	000937-30-4	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089523.D
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Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

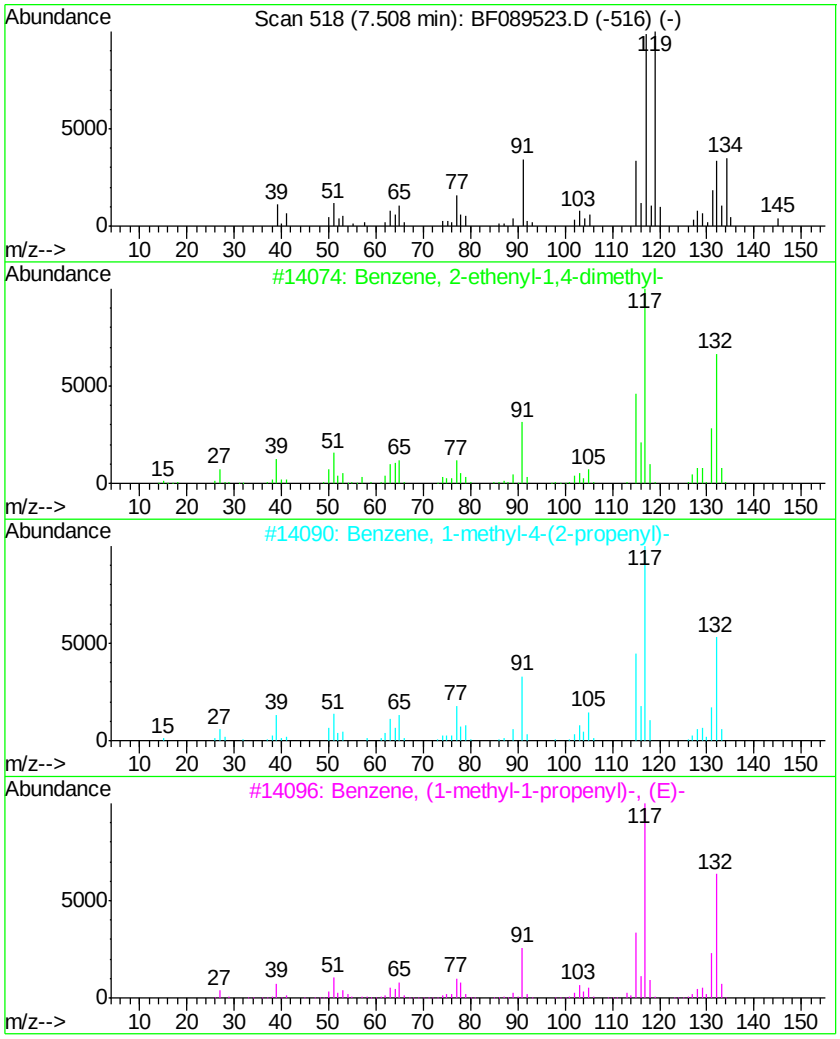
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

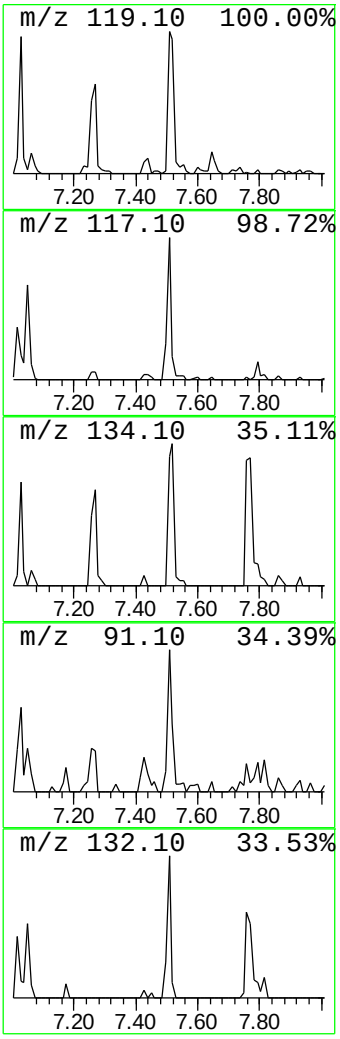
****

Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.51	8.84 ng	156956	Naphthalene-d8	7.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	80
2	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	70
3	Benzene, (1-methyl-1-propenyl)-, ...	132	C10H12	000768-00-3	55
4	Benzene, (1-methyl-1-propenyl)-, ...	132	C10H12	000767-99-7	55
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	55





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Data File : BF089523.D
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Sample : H4251-11
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Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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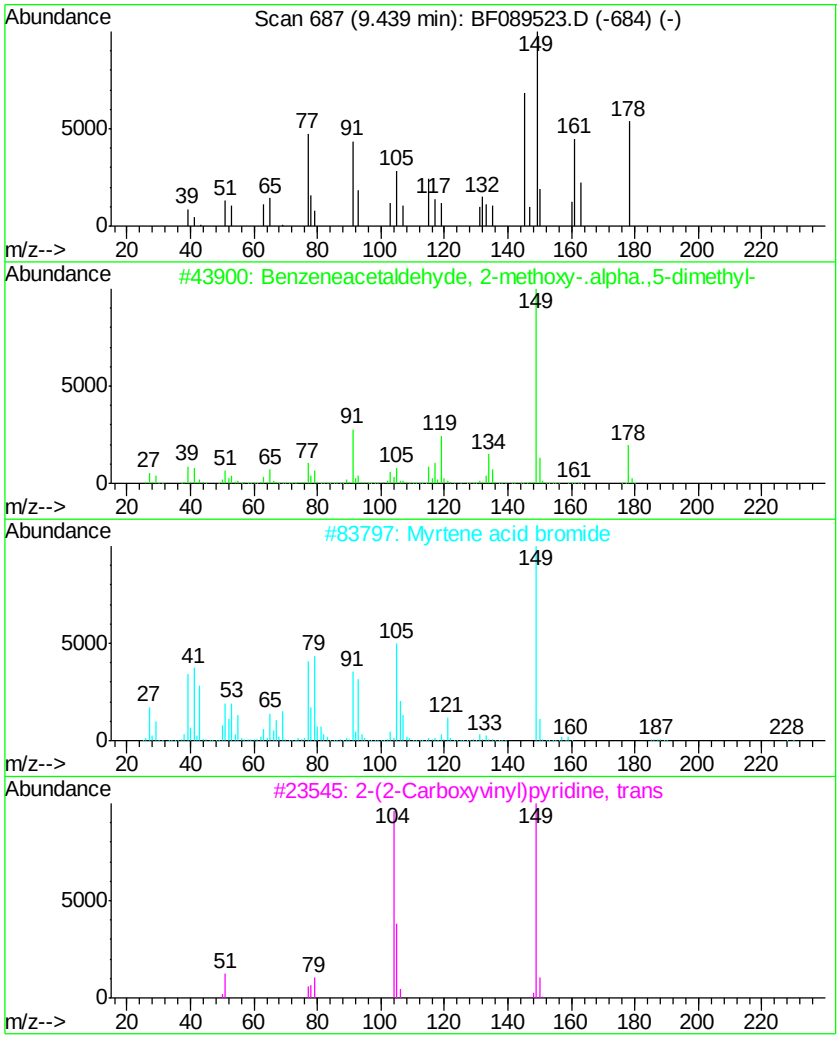
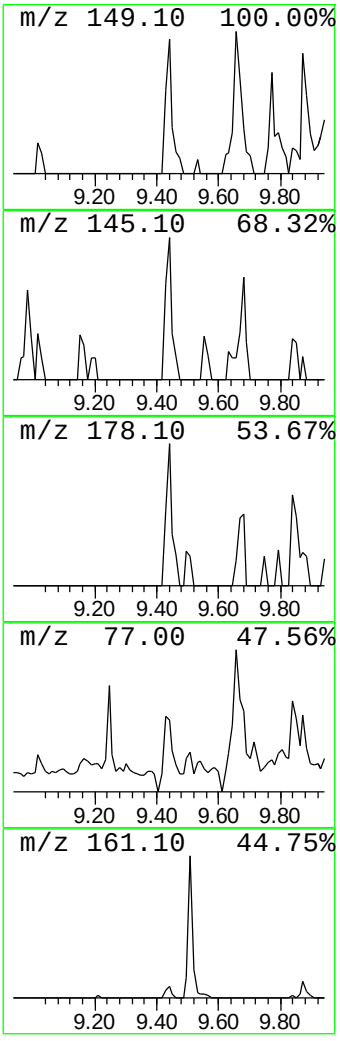
Peak Number 8 unknown9.44 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.44	2.29 ng	41456	Acenaphthene-d10	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneacetaldehyde, 2-methoxy-....	178	C11H14O2	053155-90-1	47
2	Myrtene acid bromide	228	C10H13BrO	1000159-35-0	14
3	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	10
4	Ethanone, 1,1'-(3-amino-2,4-pyri...	178	C9H10N2O2	051460-33-4	9
5	Furo[3,2-b]pyridine, 2-methyl-, ...	149	C8H7NO2	069022-83-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
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Sample : H4251-11
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

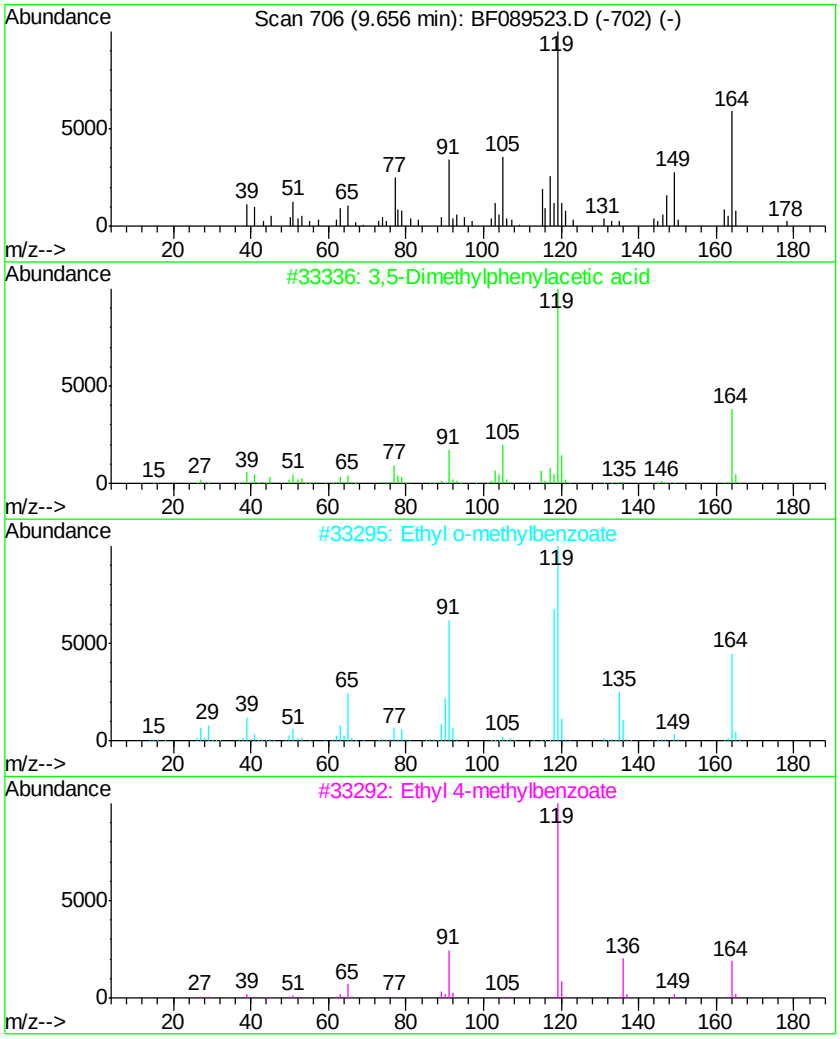
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

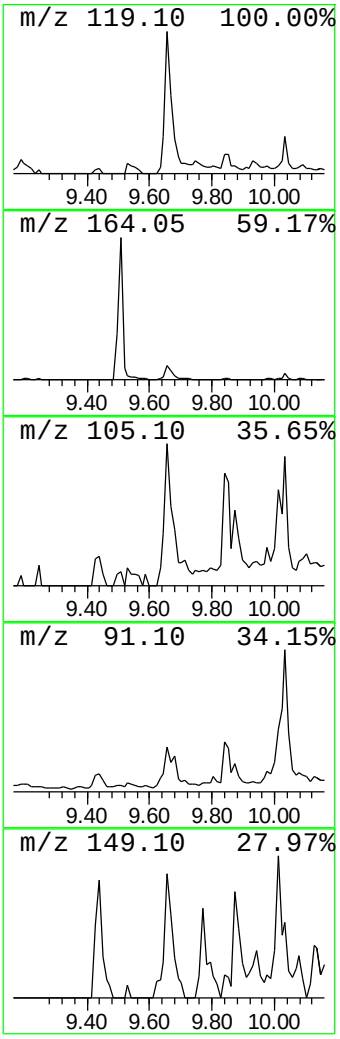
****

Peak Number 9 3,5-Dimethylphenylacetic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.66	9.70 ng	175743	Acenaphthene-d10	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethylphenylacetic acid	164	C10H12O2	042288-46-0	58
2	Ethyl o-methylbenzoate	164	C10H12O2	000087-24-1	46
3	Ethyl 4-methylbenzoate	164	C10H12O2	000094-08-6	46
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	38
5	N-Methyl-o-toluamide	149	C9H11NO	002170-09-4	38





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Data File : BF089523.D
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Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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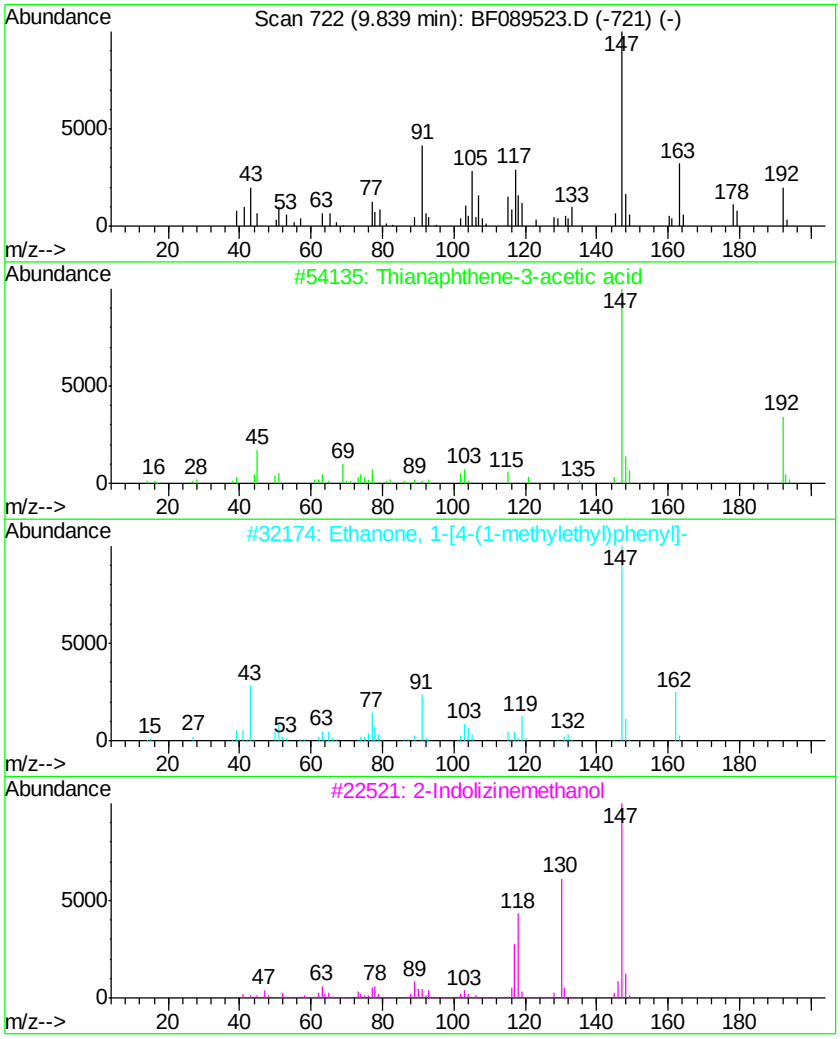
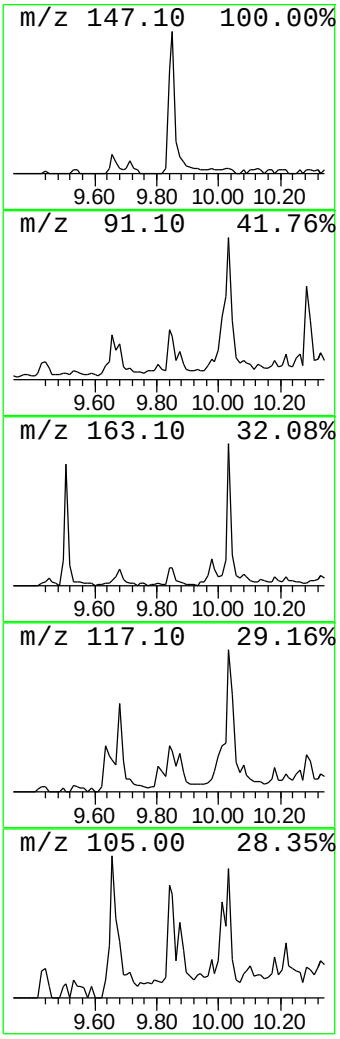
Peak Number 10 unknown9.84 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.84	4.75 ng	86077	Acenaphthene-d10	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thianaphthene-3-acetic acid	192	C10H8O2S	001131-09-5	43
2	Ethanone, 1-[4-(1-methylethyl)ph...	162	C11H14O	000645-13-6	43
3	2-Indolizinemethanol	147	C9H9NO	022320-21-4	43
4	Benzene, 1,2,4-trimethyl-5-(1-me...	162	C12H18	010222-95-4	43
5	Benzene, 1-(1,1-dimethylethyl)-4...	162	C12H18	007364-19-4	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
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Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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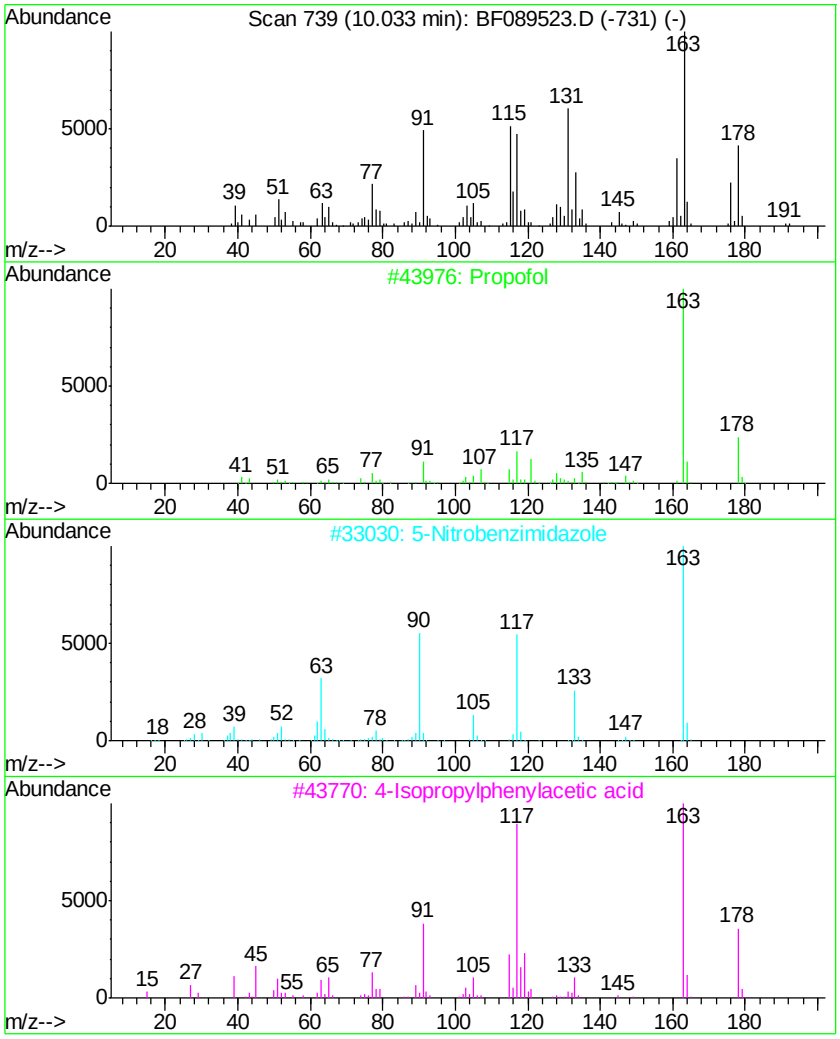
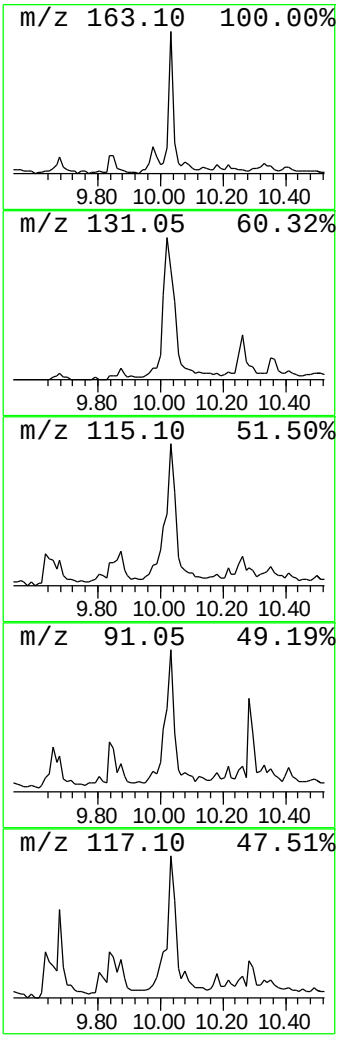
Peak Number 11 unknown10.03 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	23.67 ng	428635	Acenaphthene-d10	9.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propofol	178	C12H18O	002078-54-8	46
2	5-Nitrobenzimidazole	163	C7H5N3O2	1000229-89-5	41
3	4-Isopropylphenylacetic acid	178	C11H14O2	004476-28-2	38
4	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	38
5	2-Methyl-2-phenylthiophane	178	C11H14S	014856-67-8	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089523.D
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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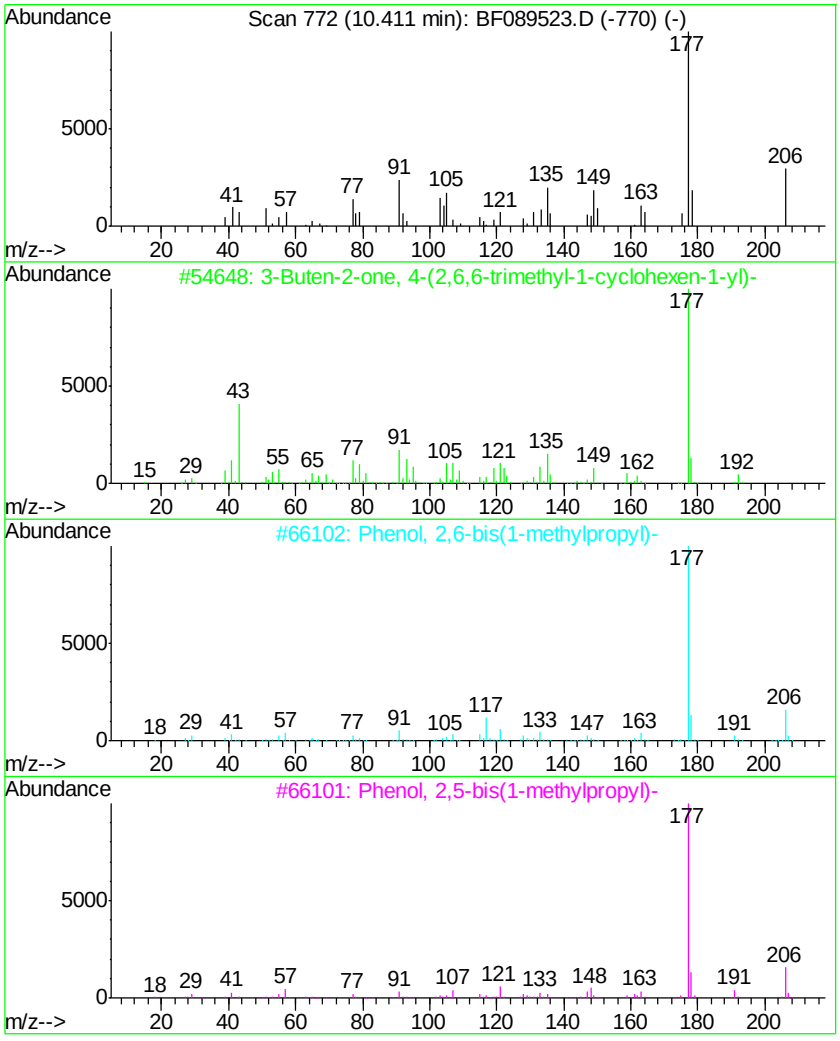
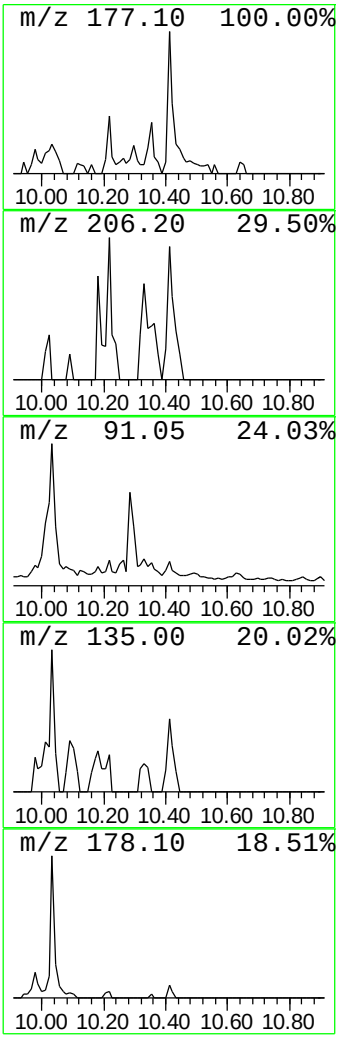
Peak Number 12 3-Buten-2-one, 4-(2,6,6-tri... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	2.76 ng	43937	Phenanthrene-d10	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	50
2	Phenol, 2,6-bis(1-methylpropyl)-	206	C14H22O	005510-99-6	43
3	Phenol, 2,5-bis(1-methylpropyl)-	206	C14H22O	054932-77-3	40
4	2-Thiazolamine, 4-(4-pyridinyl)-	177	C8H7N3S	1000351-69-3	38
5	5-Amino-1,4-dihydro-quinoxaline-...	177	C8H7N3O2	076097-87-5	37





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080116\
Data File : BF089523.D
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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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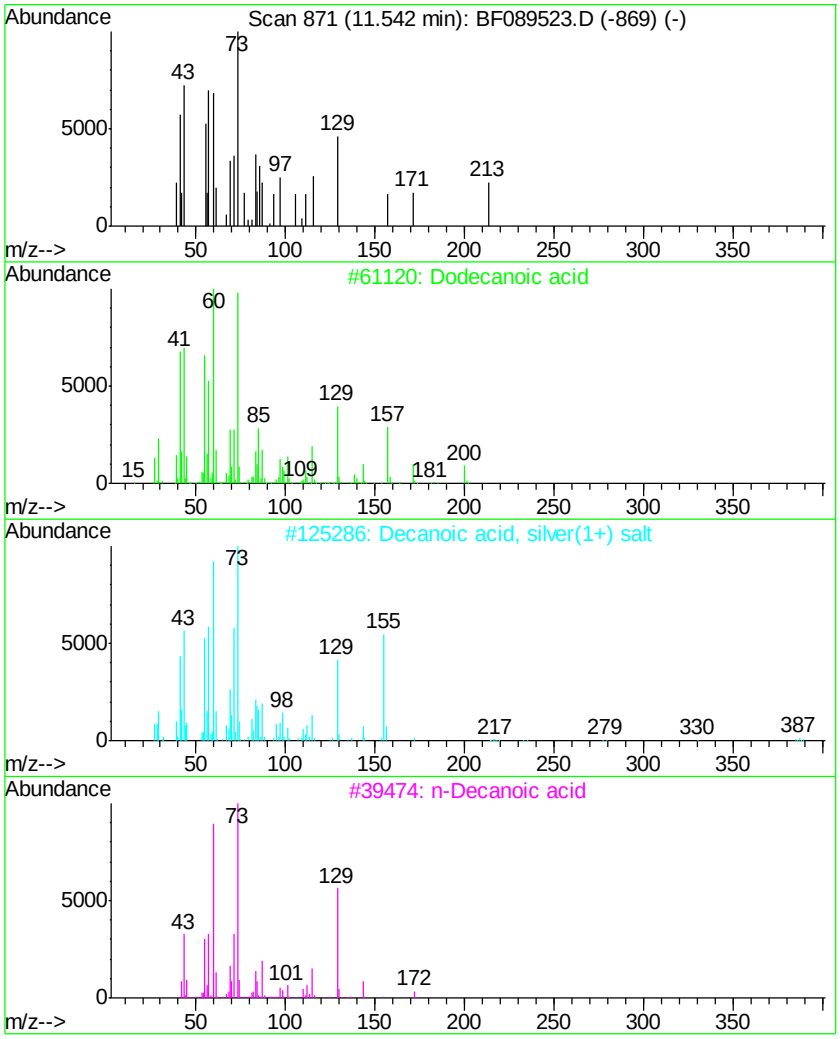
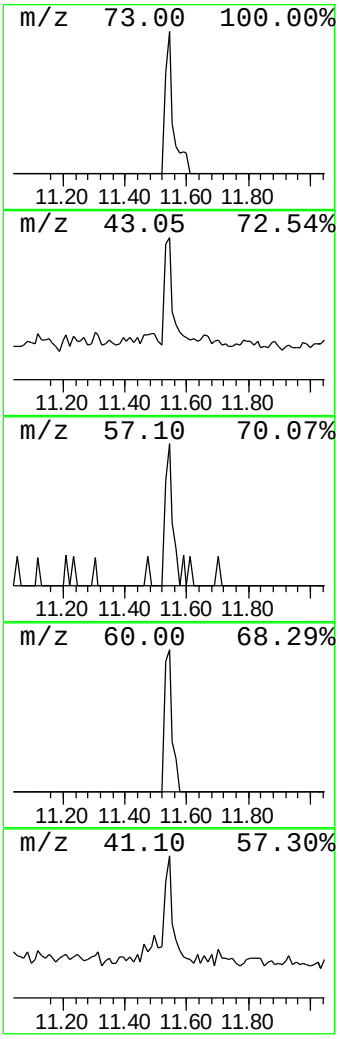
Peak Number 13 Dodecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.54	2.11 ng	33572	Phenanthrene-d10	10.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	53
2	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	47
4	Undecanoic acid	186	C11H22O2	000112-37-8	45
5	.beta.-D-Glucopyranoside, methyl...	292	C14H28O6	1000157-04-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080116\
Data File : BF089523.D
Acq On : 1 Aug 2016 21:26
Operator : UM/SJ
Sample : H4251-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-X

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072716.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-Pentanone, 4-hy...	4.55	5.3	ng	57246	1	6.48	214143	20.0
unknown6.24	6.24	64.0	ng	685235	1	6.48	214143	20.0
Benzene, 1,2,3,4-...	7.27	3.4	ng	60460	2	7.76	355094	20.0
3,4-Dimethylcumene	7.43	2.2	ng	38773	2	7.76	355094	20.0
Benzene, 2-etheny...	7.51	8.8	ng	156956	2	7.76	355094	20.0
unknown9.44	9.44	2.3	ng	41456	3	9.51	362212	20.0
3,5-Dimethylpheny...	9.66	9.7	ng	175743	3	9.51	362212	20.0
unknown9.84	9.84	4.8	ng	86077	3	9.51	362212	20.0
unknown10.03	10.03	23.7	ng	428635	3	9.51	362212	20.0
3-Buten-2-one, 4-...	10.41	2.8	ng	43937	4	10.98	318623	20.0
Dodecanoic acid	11.54	2.1	ng	33572	4	10.98	318623	20.0