LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

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-BF030316.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	4.550	195	198	202	rVB	80554	111878	2.57%	0.280%
2	5.179	250	253	262	rVB	763146	1242761	28.59%	3.112%
3	5.579	285	288	290	rBV	3689741	4315831	99.28%	10.806%
4	6.584	373	376	379	rBV	3046073	3809308	87.63%	9.537%
5	6.733	386	389	391	rBV	3853316	4346997	100.00%	10.884%
6	6.962	407	409	411	rBV	1148920	977471	22.49%	2.447%
7	7.122	420	423	425	rBV	3305082	3457799	79.54%	8.657%
8	7.522	455	458	461	rBV	2376904	2422791	55.73%	6.066%
9	7.602	462	465	467	rVB	59221	67080	1.54%	0.168%
10	8.242	519	521	524	rBV	1353262	1232409	28.35%	3.086%
11	9.328	613	616	618	rBV	3222005	4298062	98.87%	10.761%
12	9.716	648	650	651	rBV	370751	432470	9.95%	1.083%
13	9.933	666	669	671	rVB	88353	97214	2.24%	0.243%
14	10.002	673	675	677	rVB	1317616	1163379	26.76%	2.913%
15	10.425	711	712	714	rVB	138775	124129	2.86%	0.311%
16	10.642	729	731	735	rBV	42139	81627	1.88%	0.204%
17	10.791	741	744	746	rBV	2183540	2232492	51.36%	5.589%
18	10.905	752	754	758	rBV	106645	172907	3.98%	0.433%
19	11.351	790	793	794	rBV	79128	76146	1.75%	0.191%
20	11.488	802	805	806	rBV	976522	1060128	24.39%	2.654%
21	11.511	806	807	808	rVV	94971	70784	1.63%	0.177%
22	11.556	808	811	813	rVB2	37780	53065	1.22%	0.133%
23	12.002	849	850	857	rBV2	254710	388739	8.94%	0.973%
24	12.688	909	910	913	rBV	95875	142117	3.27%	0.356%
25	12.791	917	919	926	rBV	150881	191454	4.40%	0.479%
26	12.916	926	930	933	rVV2	81122	140787	3.24%	0.352%
27	13.065	941	943	946	rVB	2433593	2474873	56.93%	6.196%
28	13.534	982	984	987	rVB	332000	396021	9.11%	0.992%
29	13.957	1019	1021	1027	rVB	313803	382076	8.79%	0.957%
30	14.117	1031	1035	1041	rBV	862759	1044488	24.03%	2.615%
31	14.505	1064	1069	1071	rBV3	25160	70203	1.61%	0.176%
32	14.597	1074	1077	1083	rVB6	45954	149047	3.43%	0.373%
33	14.871	1099	1101	1105	rBV	123753	167347	3.85%	0.419%
34	14.974	1107	1110	1116	rVB4	41180	116700	2.68%	0.292%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

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-BF030316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.157	1123	1126	1130	rBV	68204	149818	3.45%	0.375%
36	15.362	1141	1144	1146	rBV3	367892	795167	18.29%	1.991%
37	15.454	1150	1152	1155	rVB	35128	51626	1.19%	0.129%
38	15.522	1155	1158	1161	rBV	48581	73495	1.69%	0.184%
39	15.580	1161	1163	1166	rBV	522349	823053	18.93%	2.061%
40	16.048	1201	1204	1207	rBV	27803	57418	1.32%	0.144%
41	16.105	1207	1209	1217	rVB6	39119	119941	2.76%	0.300%
42	16.300	1223	1226	1231	rVB5	21128	52260	1.20%	0.131%
43	16.597	1250	1252	1255	rVB	23311	45995	1.06%	0.115%
44	16.734	1262	1264	1268	rVB3	22234	48451	1.11%	0.121%
45	17.043	1287	1291	1296	rBV2	33156	76158	1.75%	0.191%
46	17.477	1326	1329	1335	rBV	21883	62644	1.44%	0.157%
47	17.648	1341	1344	1349	rBV5	30809	74247	1.71%	0.186%

Sum of corrected areas: 39940853

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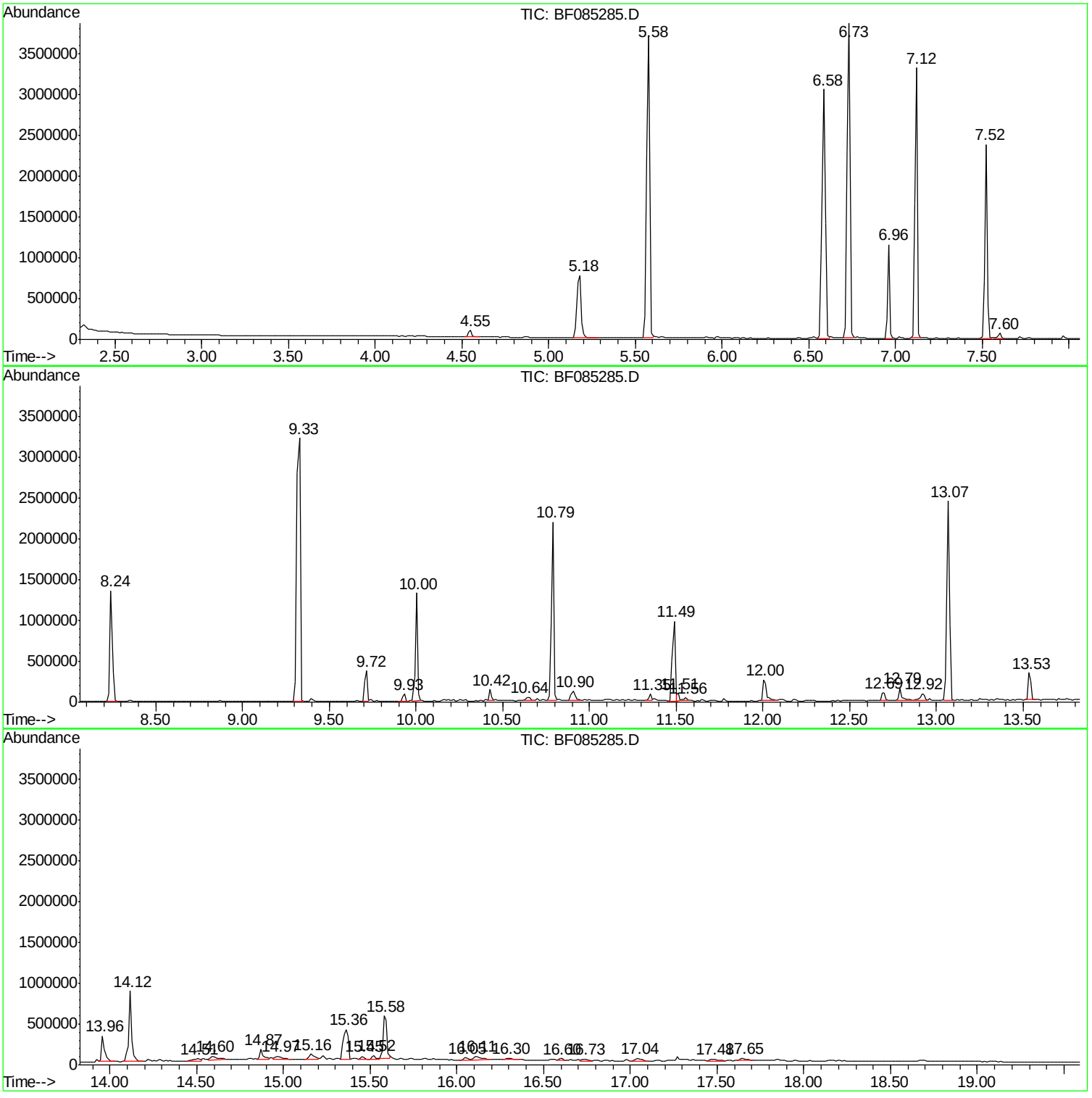
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

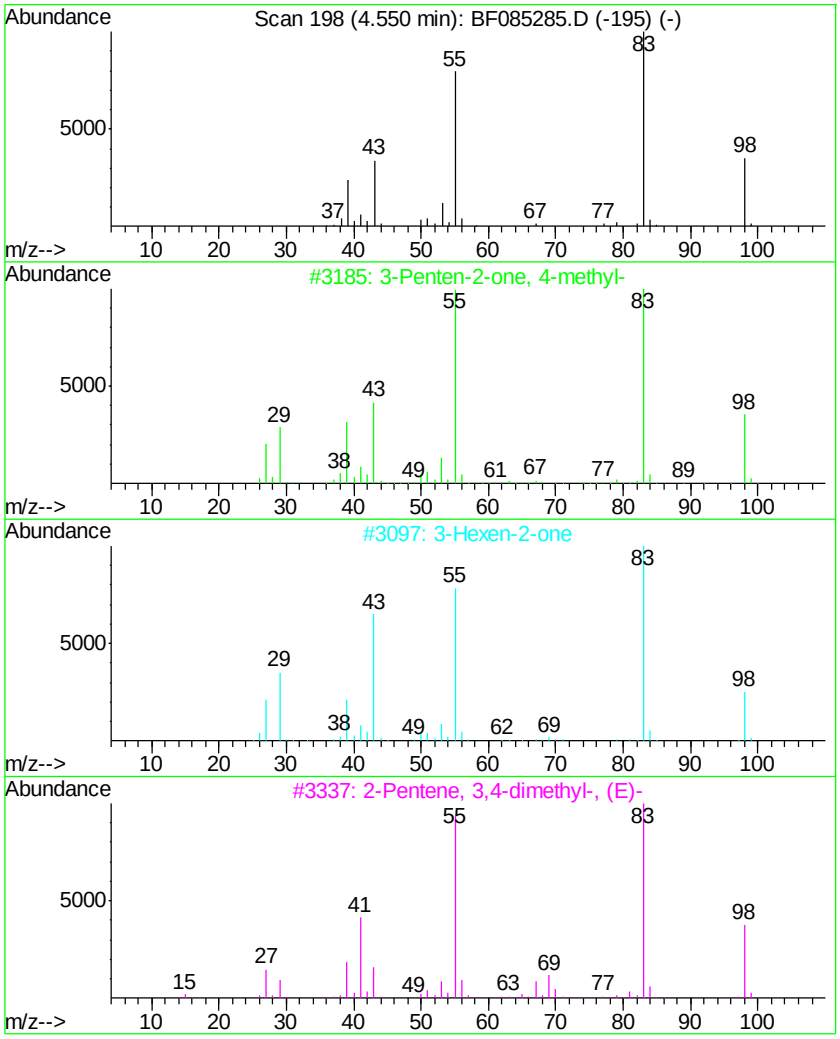
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

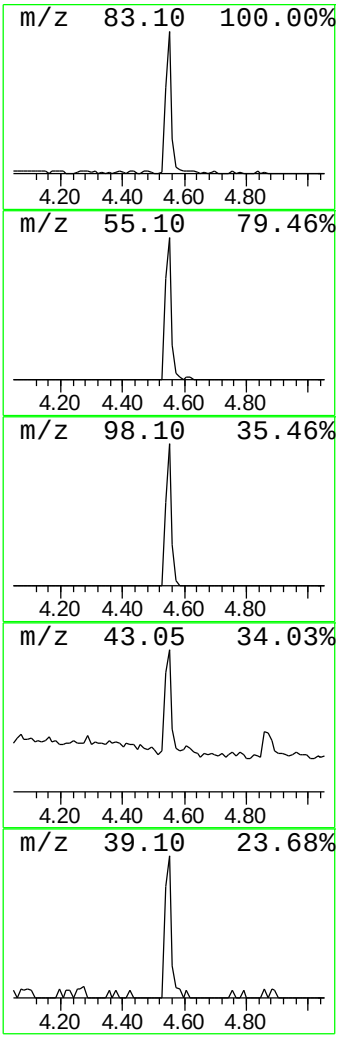
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	2.29 ng	111878	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
5	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

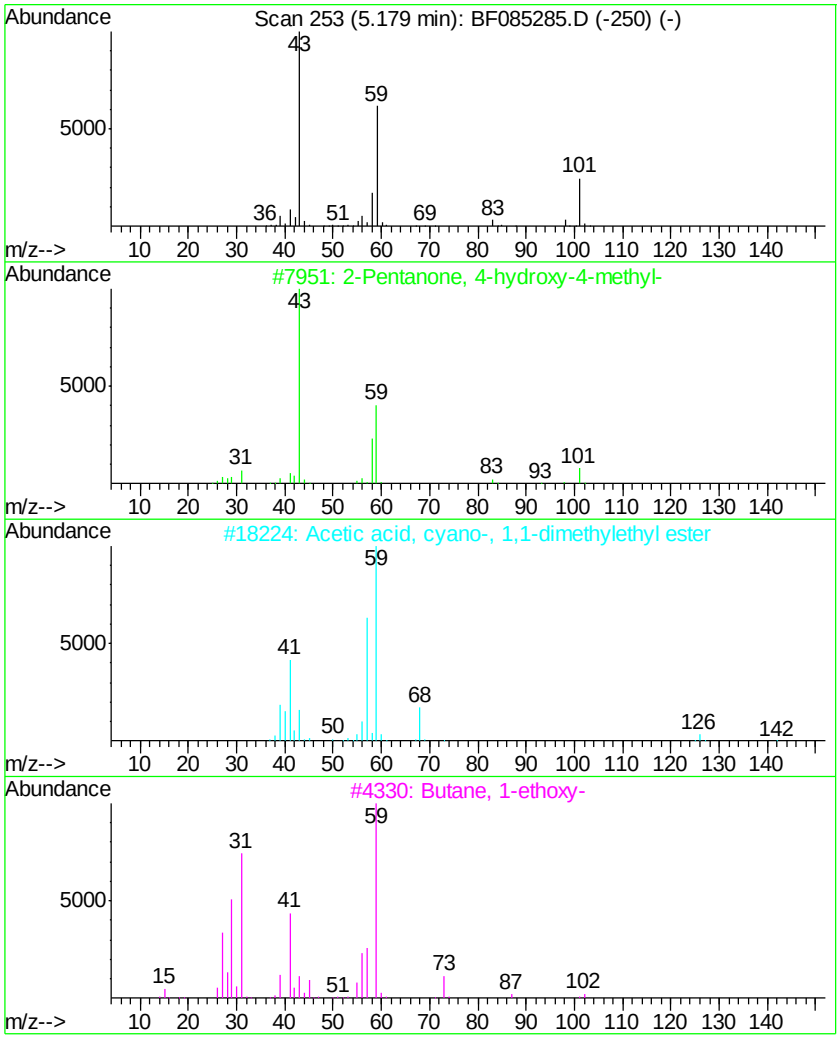
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

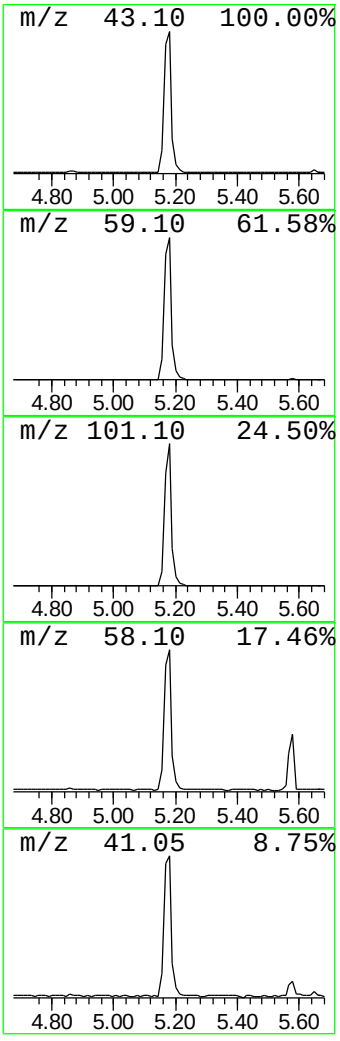
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	25.43 ng	1242760	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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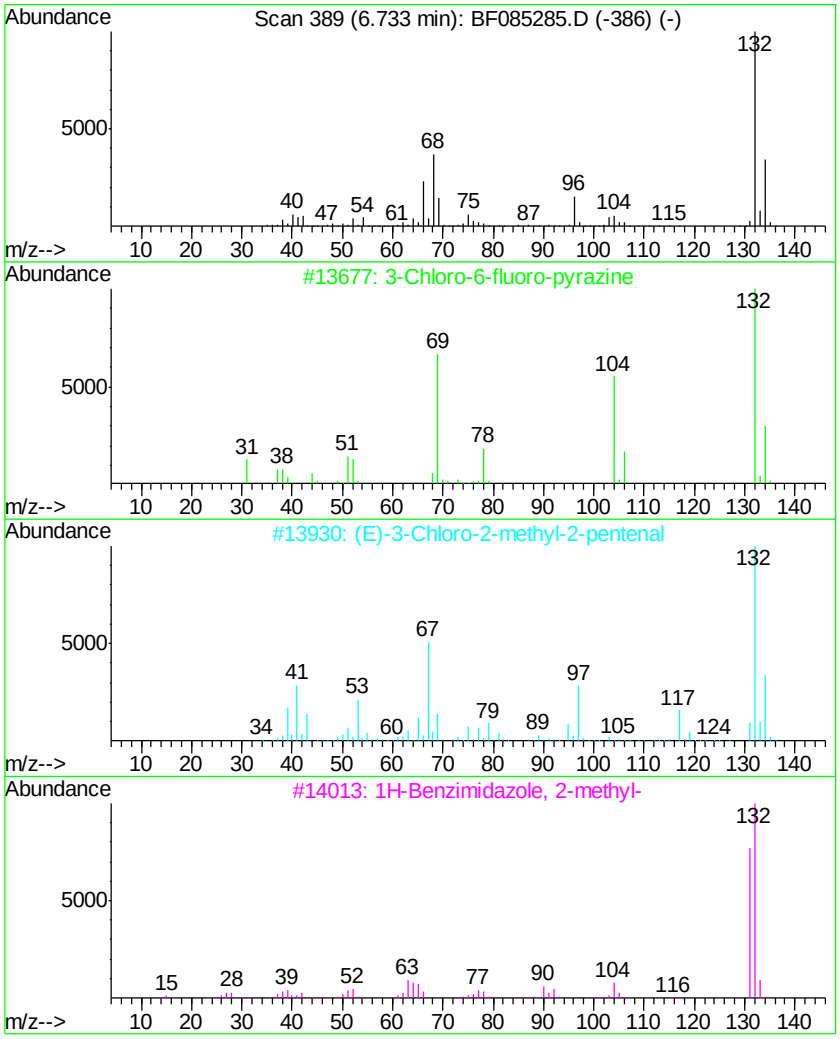
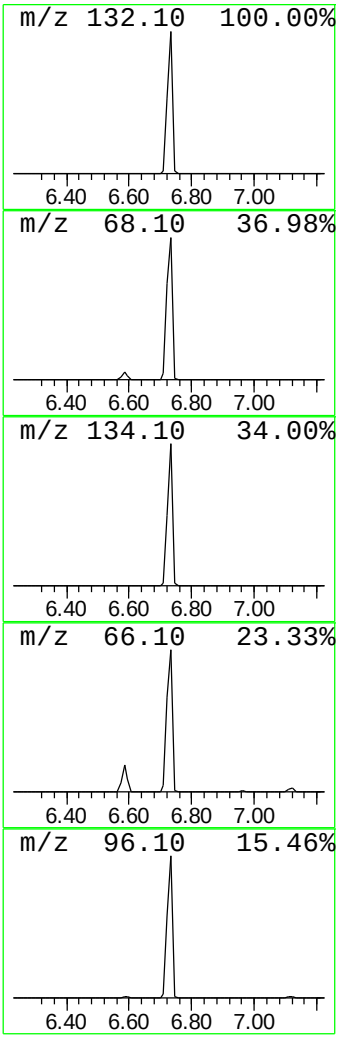
Peak Number 3 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	88.94 ng	4347000	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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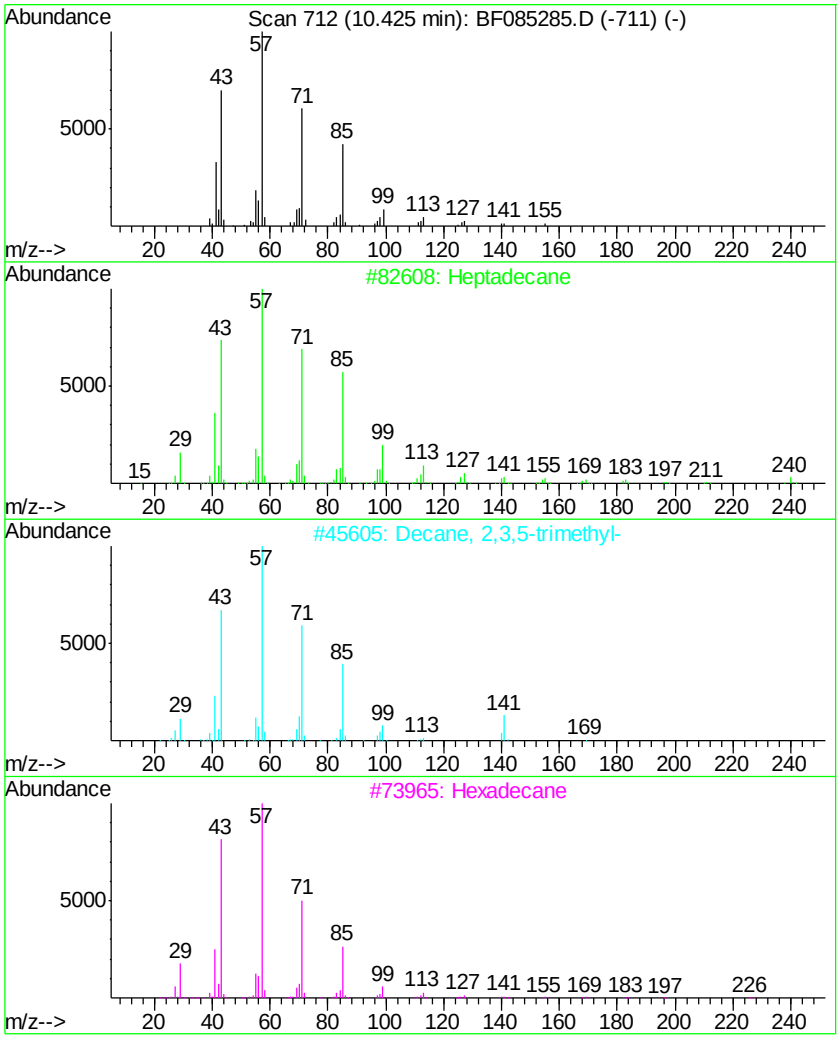
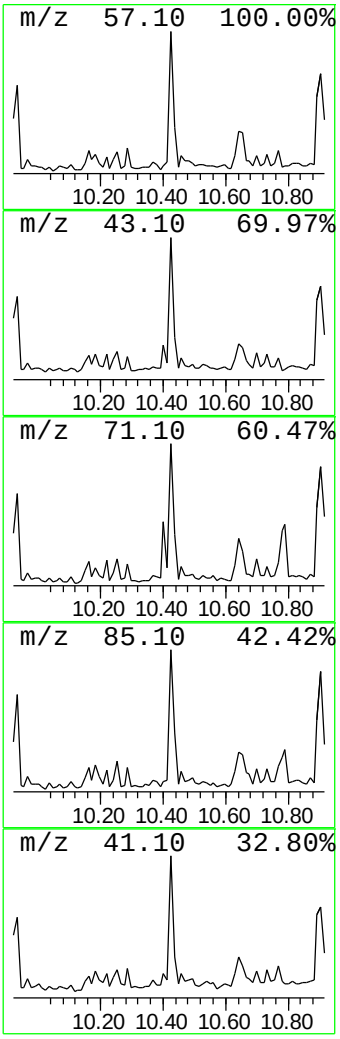
Peak Number 5 Heptadecane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	2.13 ng	124129	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	83
3	Hexadecane	226	C16H34	000544-76-3	80
4	Tridecane	184	C13H28	000629-50-5	72
5	Pentadecane	212	C15H32	000629-62-9	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

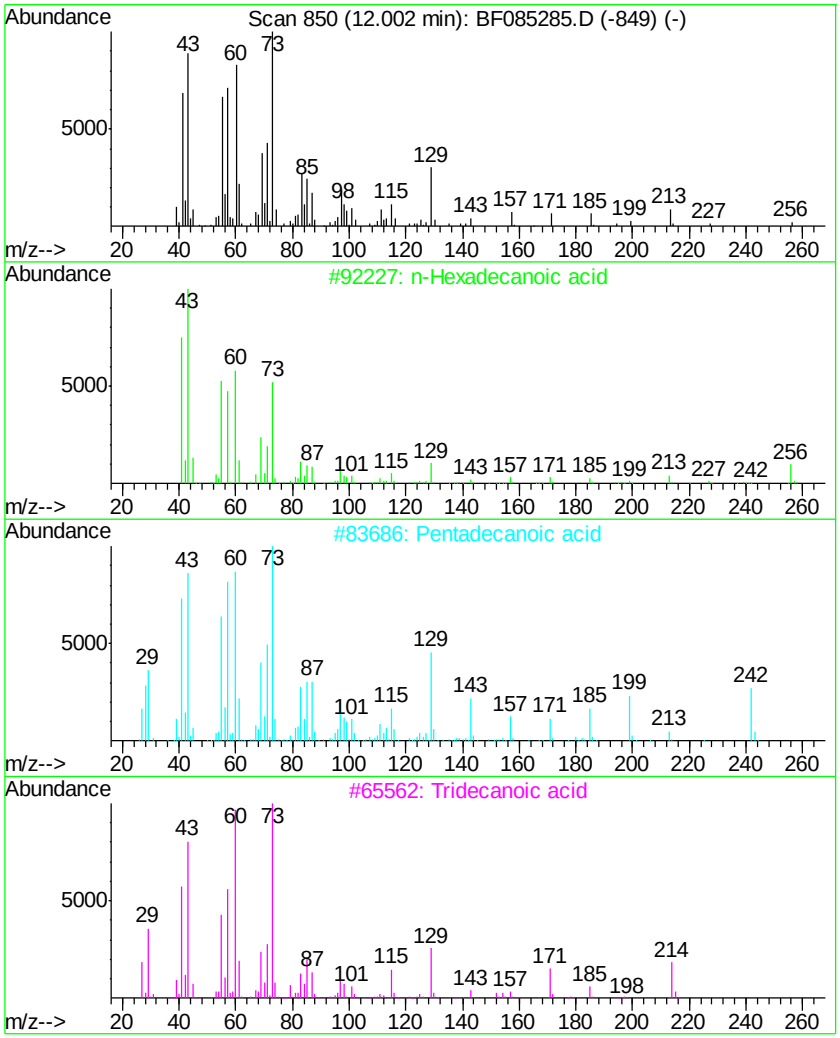
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

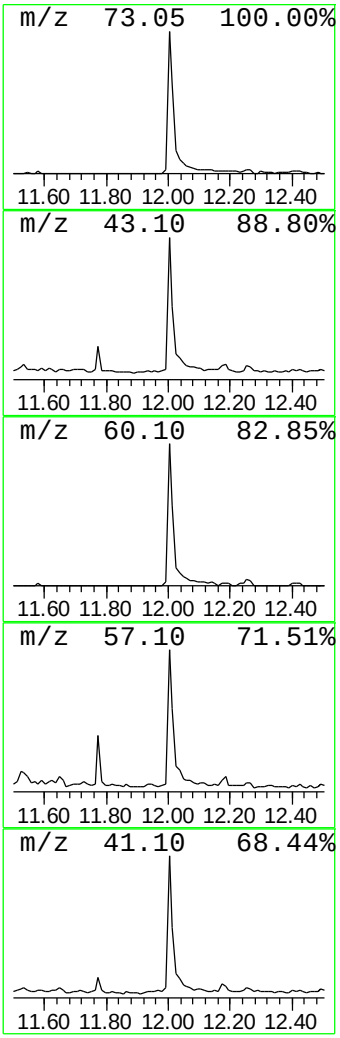
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	7.33 ng	388739	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Undecane	156	C11H24	001120-21-4	18
5	Tetracontane, 3,5,24-trimethyl-	605	C43H88	055162-61-3	18





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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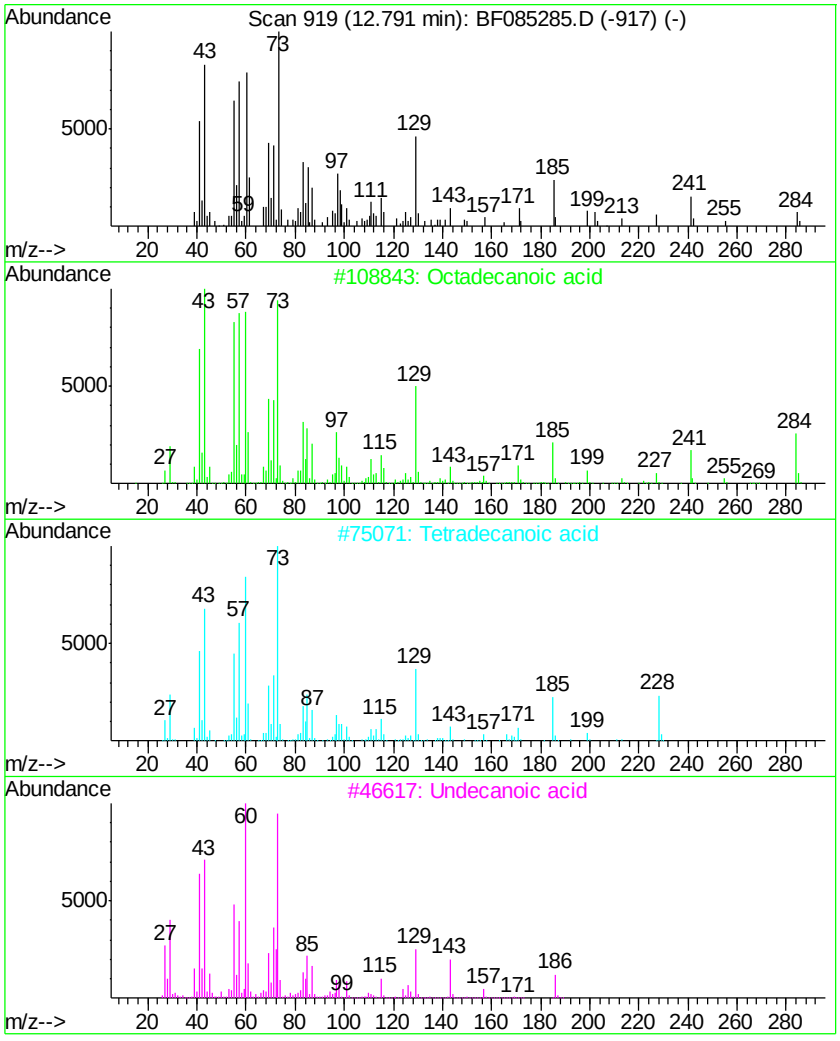
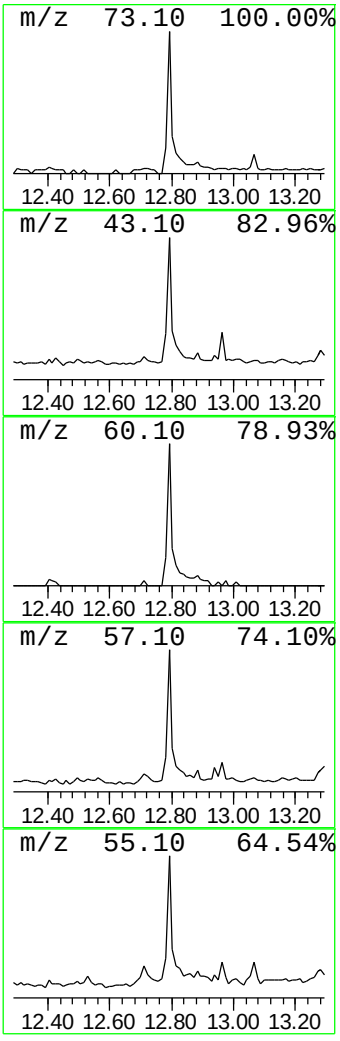
Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	3.61 ng	191454	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Undecanoic acid	186	C11H22O2	000112-37-8	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	74





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Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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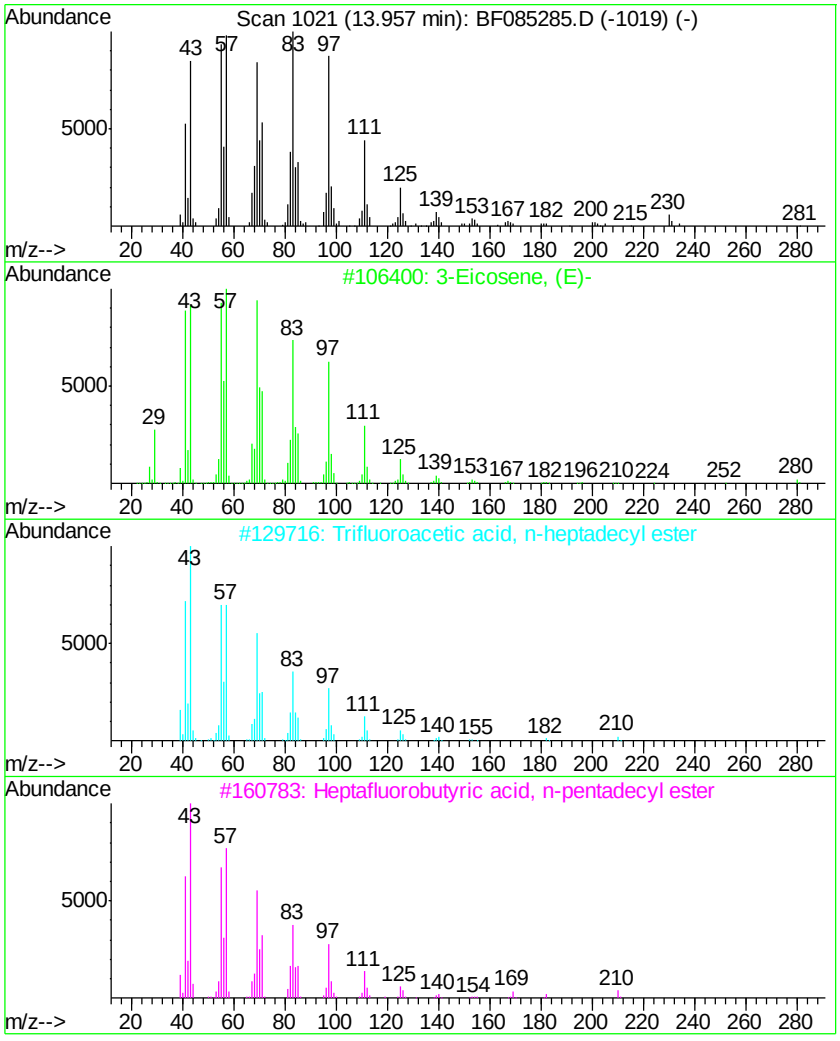
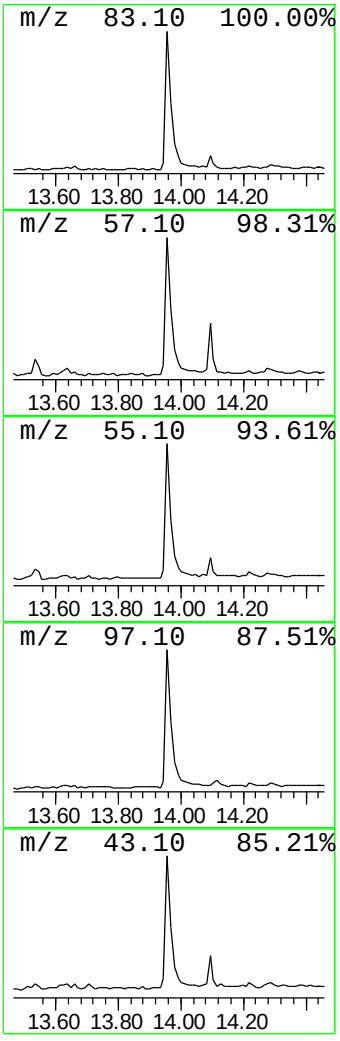
Peak Number 9 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	7.32 ng	382076	Chrysene-d12	14.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
2	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
3	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	90
5	1-Octadecanol	270	C18H38O	000112-92-5	87





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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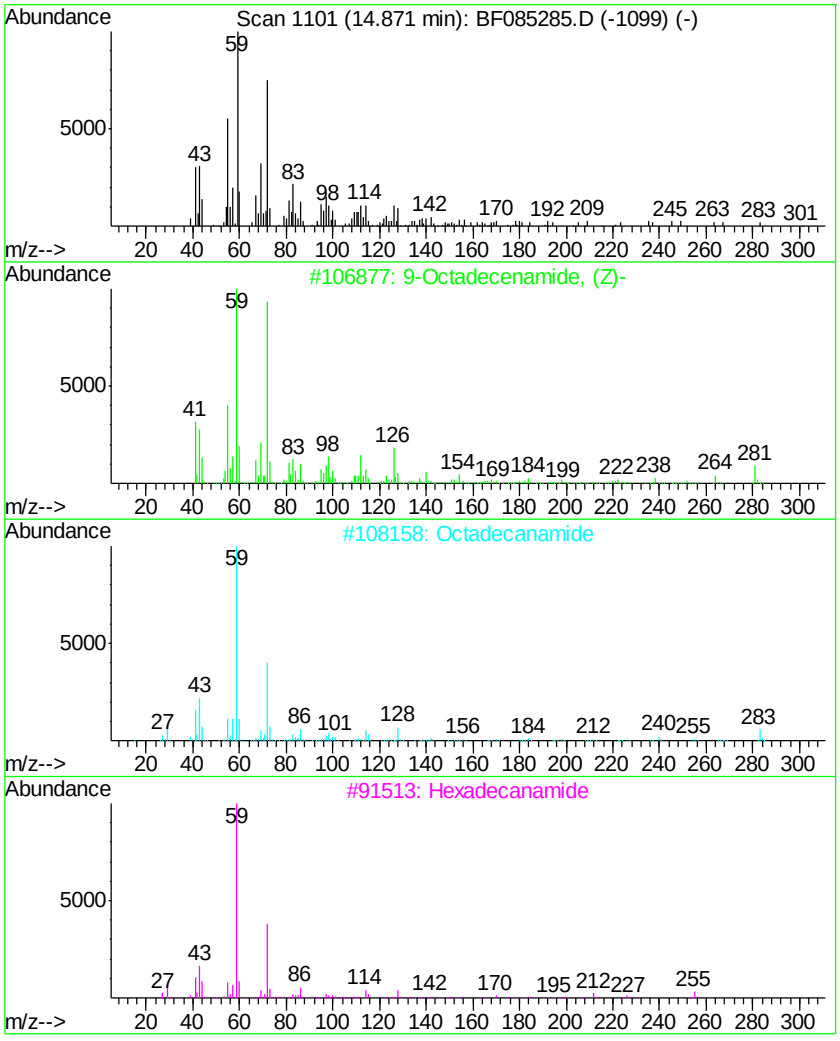
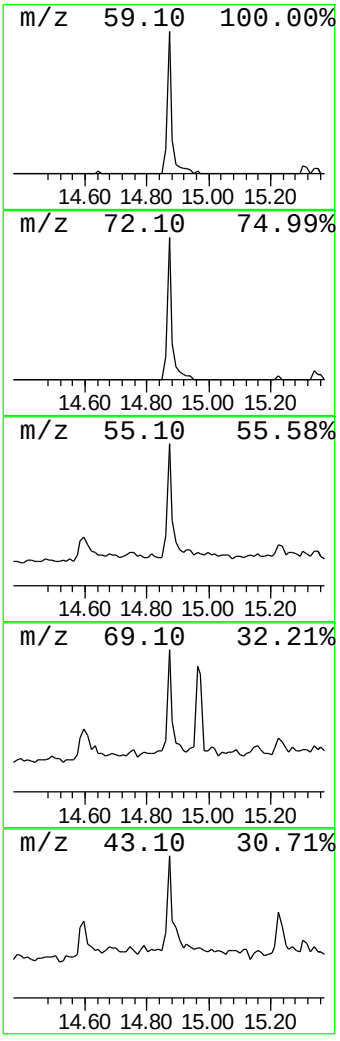
Peak Number 11 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	4.07 ng	167347	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	72
2	Octadecanamide	283	C18H37NO	000124-26-5	50
3	Hexadecanamide	255	C16H33NO	000629-54-9	50
4	Tetradecanamide	227	C14H29NO	000638-58-4	46
5	Dodecanamide	199	C12H25NO	001120-16-7	43





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Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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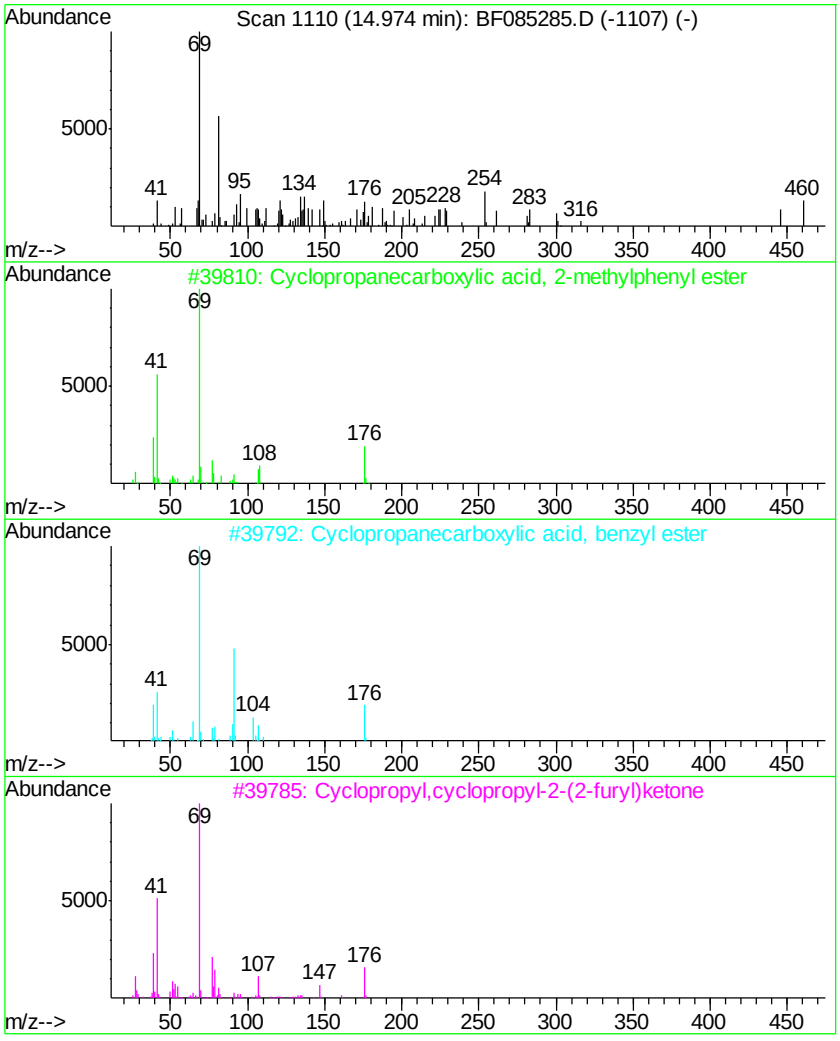
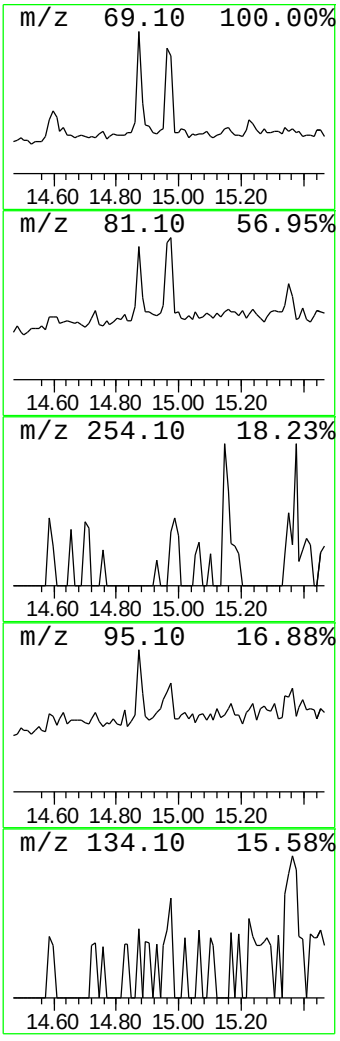
Peak Number 12 unknown14.97 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	2.84 ng	116700	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, 2-m...	176	C11H12O2	026065-44-1	43
2	Cyclopropanecarboxylic acid, ben...	176	C11H12O2	020121-75-9	37
3	Cyclopropyl,cyclopropyl-2-(2-fur...	176	C11H12O2	1000222-13-9	37
4	1-Propyne, 3-(2-bromoethoxy)-	162	C5H7BrO	018668-74-1	25
5	2-Butenoic acid, 4-methylphenyl ...	176	C11H12O2	041873-74-9	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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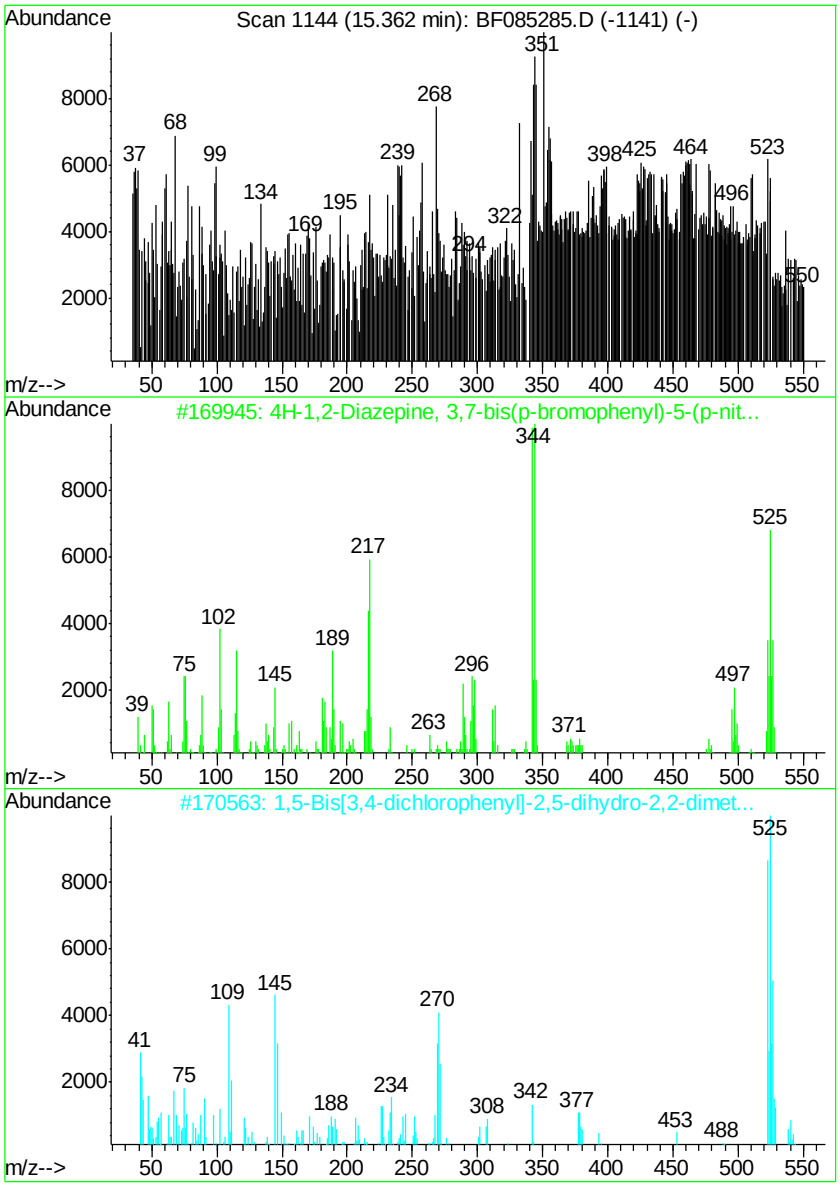
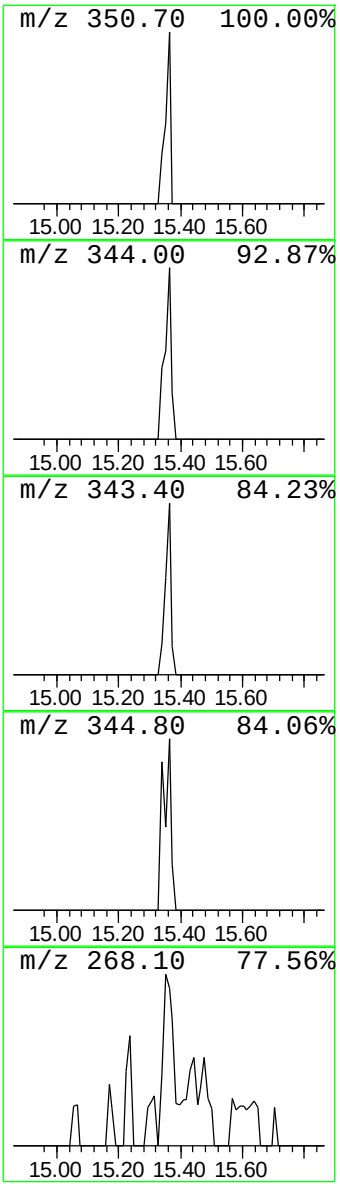
Peak Number 14 unknown15.36 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.36	19.32 ng	795167	Perylene-d12	15.59

Hit# of 2	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,2-Diazepine, 3,7-bis(p-brom...	523	C23H15Br2N3O2	025649-80-3	38
2	1,5-Bis[3,4-dichlorophenyl]-2,5-...	538	C27H18Cl4N4	1000212-73-4	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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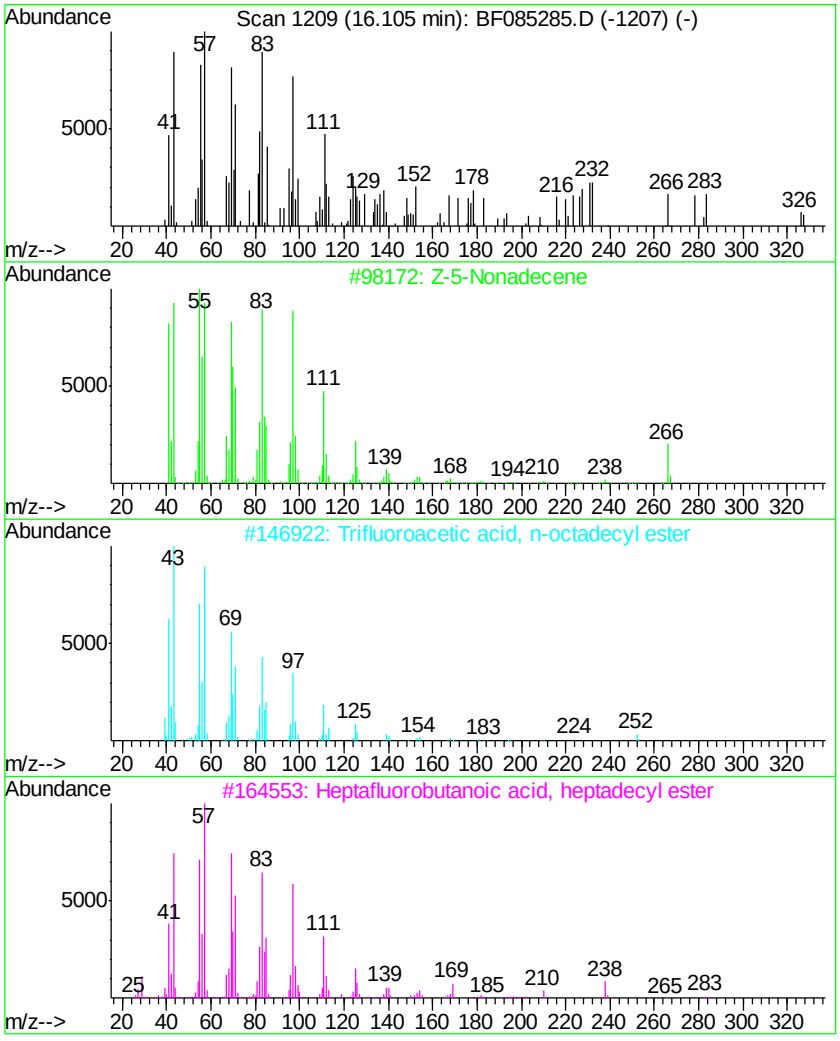
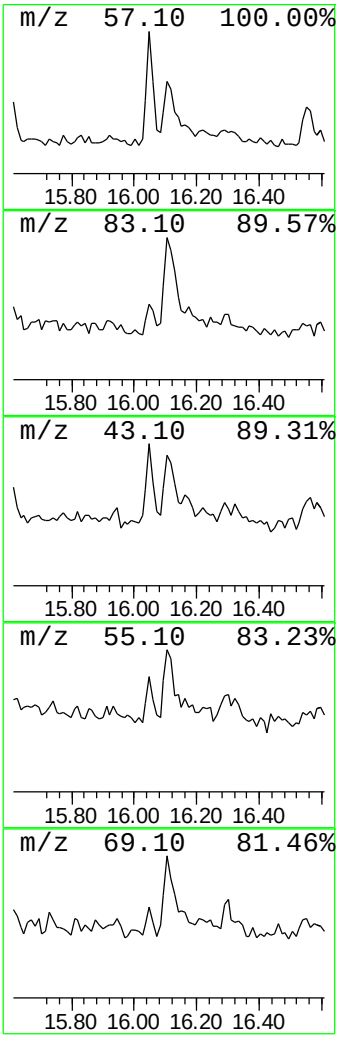
Peak Number 15 Z-5-Nonadecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	2.91 ng	119941	Perylene-d12	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	76
2	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	74
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	74
4	1-Nonadecene	266	C19H38	018435-45-5	68
5	1-Hexacosanol	382	C26H54O	000506-52-5	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085285.D
Acq On : 9 Mar 2016 5:07
Operator : UM/SJ
Sample : H1703-10
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-42COMP(0.5-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.55	2.3	ng	111878	1	6.96	977471	20.0
2-Pentanone, 4-hy...	5.18	25.4	ng	1242760	1	6.96	977471	20.0
unknown6.73	6.73	88.9	ng	4347000	1	6.96	977471	20.0
Heptadecane	10.42	2.1	ng	124129	3	10.00	1163380	20.0
n-Hexadecanoic acid	12.00	7.3	ng	388739	4	11.49	1060130	20.0
Octadecanoic acid	12.79	3.6	ng	191454	4	11.49	1060130	20.0
3-Eicosene, (E)-	13.96	7.3	ng	382076	5	14.12	1044490	20.0
9-Octadecenamide,...	14.87	4.1	ng	167347	6	15.59	823053	20.0
unknown14.97	14.97	2.8	ng	116700	6	15.59	823053	20.0
unknown15.36	15.36	19.3	ng	795167	6	15.59	823053	20.0
Z-5-Nonadecene	16.11	2.9	ng	119941	6	15.59	823053	20.0