LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083176.D
Acq On : 22 Nov 2015 23:37
Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

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-BF112115.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	4.799	243	246	265	rVB	1728635	3281423	52.01%	5.381%
2	5.256	284	286	289	rBV	4912773	5282521	83.73%	8.662%
3	6.319	376	379	381	rBV	5552318	6309086	100.00%	10.346%
4	6.422	386	388	391	rBV	5432383	5331057	84.50%	8.742%
5	6.650	405	408	410	rBV	1276583	1253413	19.87%	2.055%
6	6.810	419	422	424	rBV	3407461	4295288	68.08%	7.043%
7	7.222	455	458	460	rBV	3750692	3905980	61.91%	6.405%
8	7.930	518	520	523	rBV	1162763	1662403	26.35%	2.726%
9	9.016	612	615	618	rBV	6161854	6004122	95.17%	9.846%
10	9.416	648	650	653	rBV	1324356	1136676	18.02%	1.864%
11	9.679	671	673	676	rBV	1525966	1856067	29.42%	3.044%
12	10.136	711	713	714	rVB	98349	94101	1.49%	0.154%
13	10.353	729	732	735	rBV	45928	73541	1.17%	0.121%
14	10.468	740	742	745	rBV	3179030	3632201	57.57%	5.956%
15	10.605	752	754	758	rVB	169686	221920	3.52%	0.364%
16	11.051	789	793	794	rBV	171310	168156	2.67%	0.276%
17	11.165	800	803	805	rBV	1297139	1877185	29.75%	3.078%
18	11.233	806	809	813	rVB2	52574	108695	1.72%	0.178%
19	11.405	822	824	828	rBV2	167426	246952	3.91%	0.405%
20	11.473	828	830	833	rVB	111283	111009	1.76%	0.182%
21	11.713	849	851	855	rVV2	1078594	1074154	17.03%	1.761%
22	11.965	871	873	874	rBV	62757	80427	1.27%	0.132%
23	12.228	892	896	898	rBV2	119191	199372	3.16%	0.327%
24	12.365	906	908	909	rBV	154090	144106	2.28%	0.236%
25	12.411	909	912	916	rVV3	78319	175308	2.78%	0.287%
26	12.491	917	919	922	rVV	364517	417148	6.61%	0.684%
27	12.582	925	927	930	rVV2	289313	347891	5.51%	0.570%
28	12.662	933	934	938	rVB	94510	75278	1.19%	0.123%
29	12.742	938	941	944	rBV	4101925	5367420	85.07%	8.802%
30	12.902	953	955	959	rBV3	37446	100624	1.59%	0.165%
31	12.994	959	963	964	rVV2	60783	92440	1.47%	0.152%
32	13.222	980	983	985	rBV	95299	135500	2.15%	0.222%
33	13.291	985	989	990	rVV2	119081	168828	2.68%	0.277%
34	13.336	990	993	994	rVV2	59142	94403	1.50%	0.155%

LSC Area Percent Report

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Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

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-BF112115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.359	994	995	997	rVB	98800	77061	1.22%	0.126%
36	13.394	997	998	1001	rBV	104290	103469	1.64%	0.170%
37	13.657	1018	1021	1024	rBV	657009	849450	13.46%	1.393%
38	13.702	1024	1025	1028	rVV	75982	104336	1.65%	0.171%
39	13.782	1030	1032	1038	rVB	1657412	1632012	25.87%	2.676%
40	13.977	1047	1049	1051	rBV	103010	115828	1.84%	0.190%
41	14.285	1073	1076	1082	rBV3	91570	233593	3.70%	0.383%
42	14.571	1097	1101	1104	rBV2	96754	205148	3.25%	0.336%
43	14.640	1104	1107	1109	rVV	178549	191424	3.03%	0.314%
44	14.788	1117	1120	1124	rVB	42887	89639	1.42%	0.147%
45	14.868	1125	1127	1129	rBV2	81343	96483	1.53%	0.158%
46	15.040	1140	1142	1145	rBV3	30035	64955	1.03%	0.107%
47	15.142	1149	1151	1154	rVV	848685	1217739	19.30%	1.997%
48	15.200	1154	1156	1159	rVB	42402	63629	1.01%	0.104%
49	15.577	1186	1189	1191	rBV	54529	101328	1.61%	0.166%
50	15.622	1191	1193	1200	rVB3	73429	159281	2.52%	0.261%
51	16.000	1222	1226	1232	rVB4	54101	152849	2.42%	0.251%
52	16.594	1276	1278	1283	rVB5	43978	109071	1.73%	0.179%
53	16.914	1302	1306	1311	rVB7	35154	90636	1.44%	0.149%

Sum of corrected areas: 60982626

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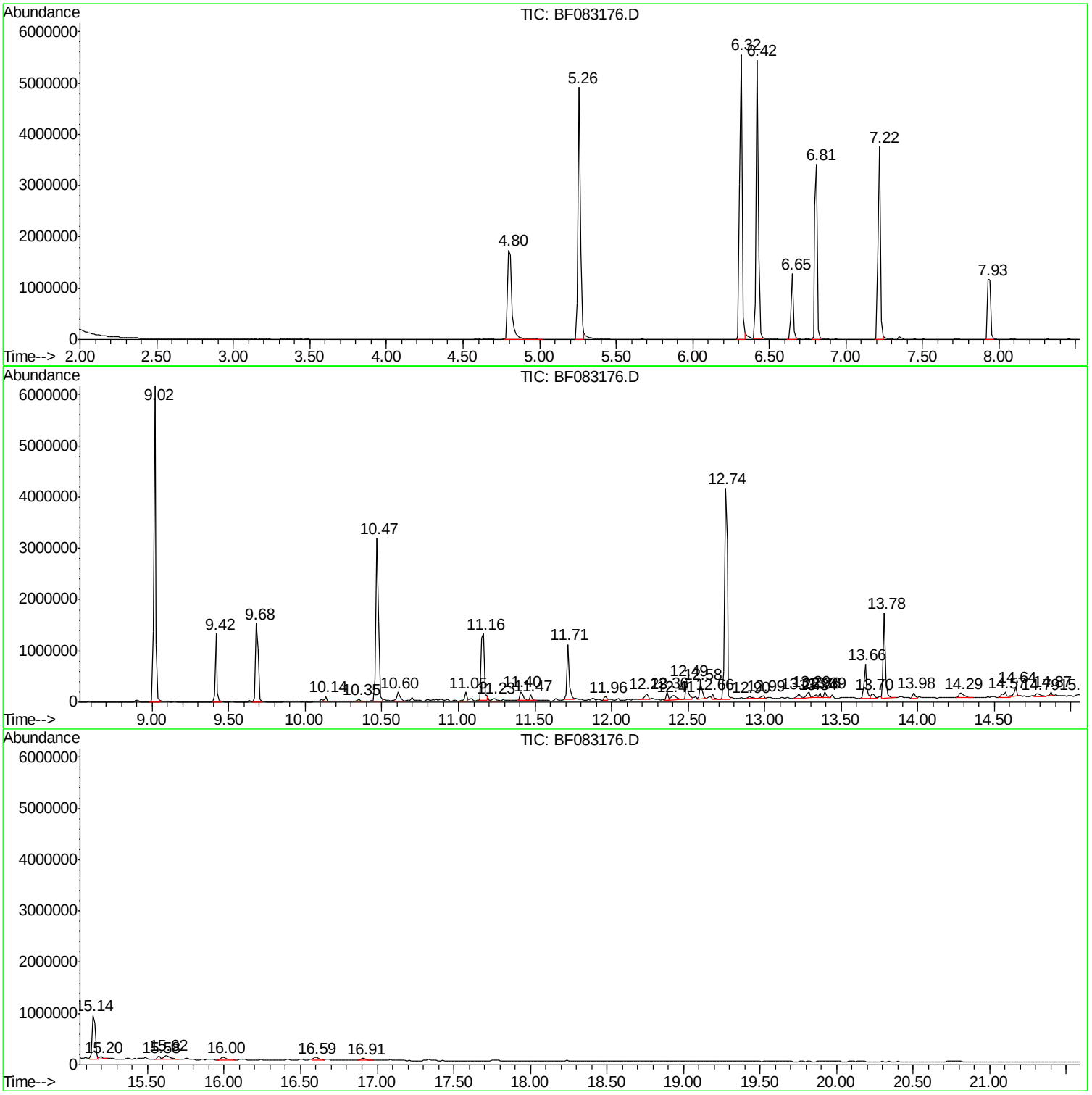
Instrument :
BNA_F
ClientSampleId :
NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

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Data File : BF083176.D
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Operator : UM/IZ
Sample : G4482-01
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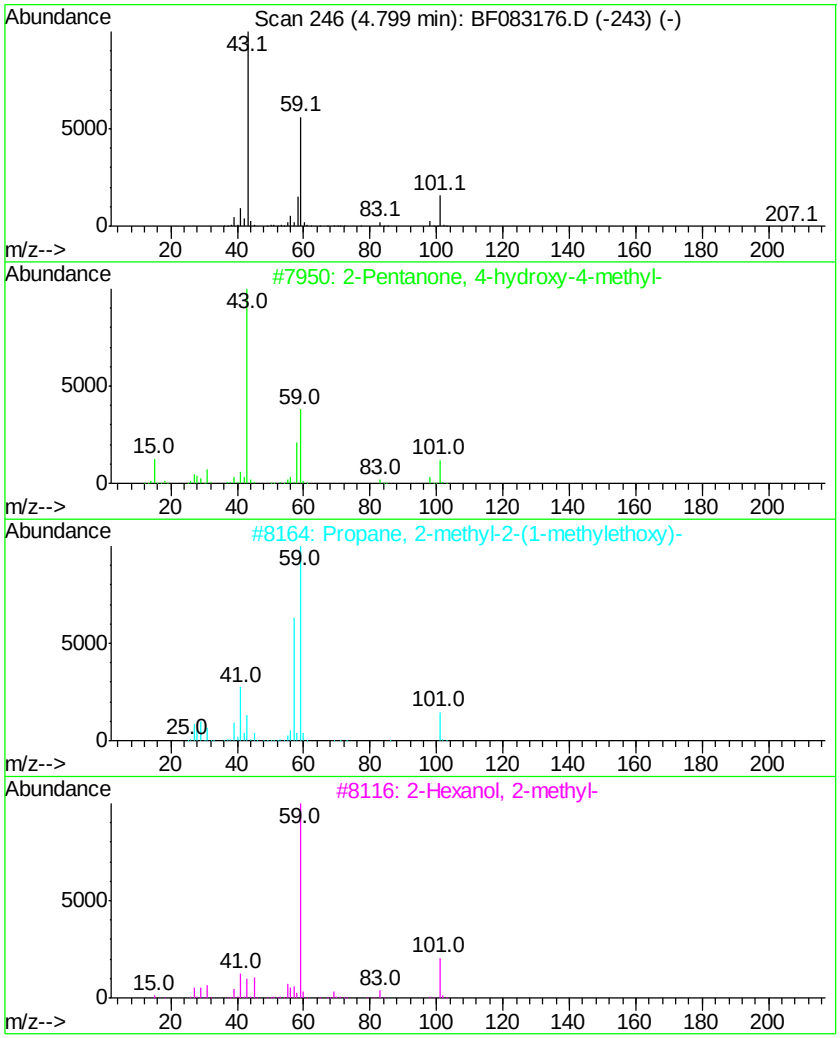
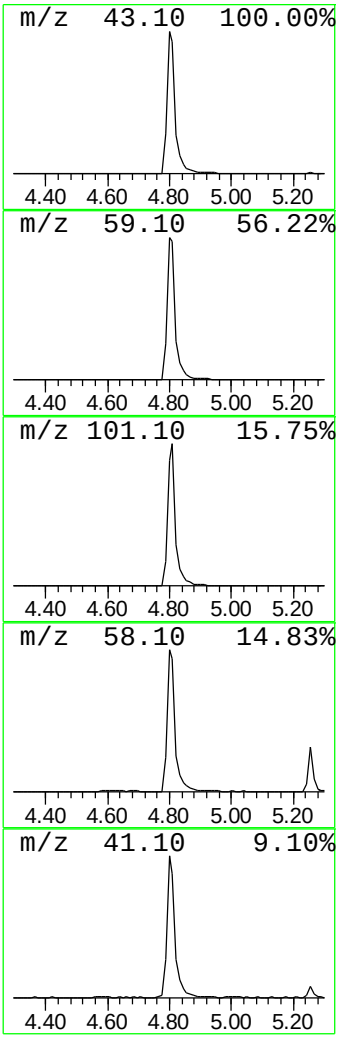
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	52.36 ng	3281420	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





Library Search Compound Report

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Acq On : 22 Nov 2015 23:37
Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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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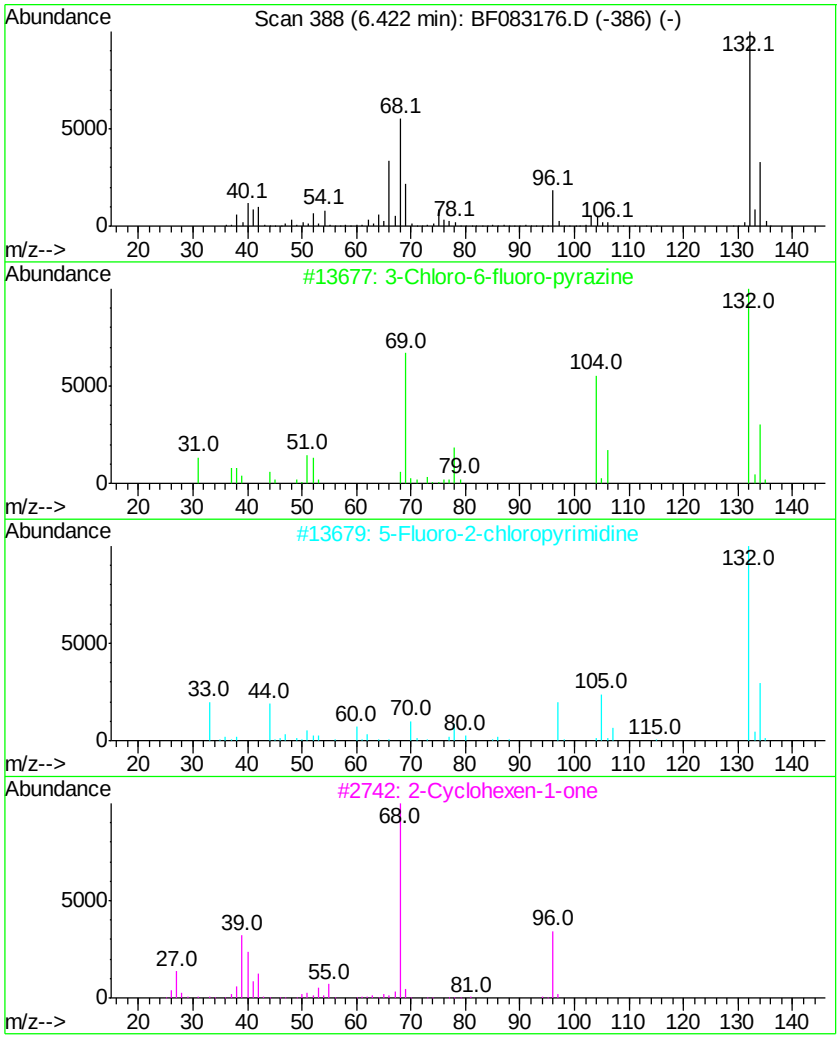
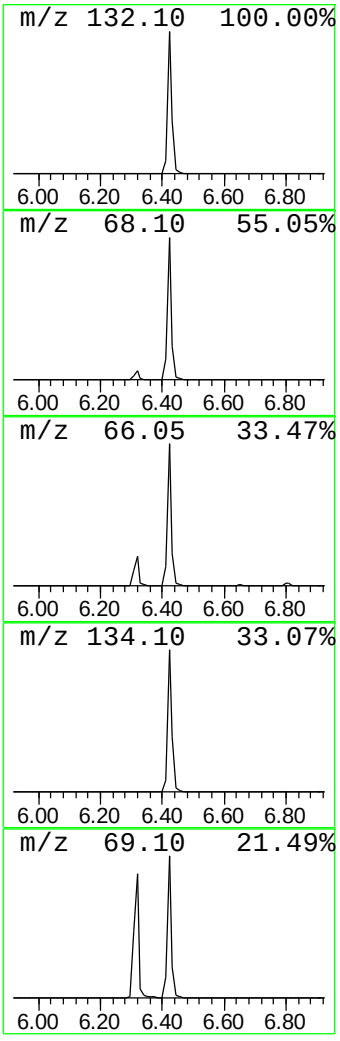
Peak Number 2 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	85.06 ng	5331060	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





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Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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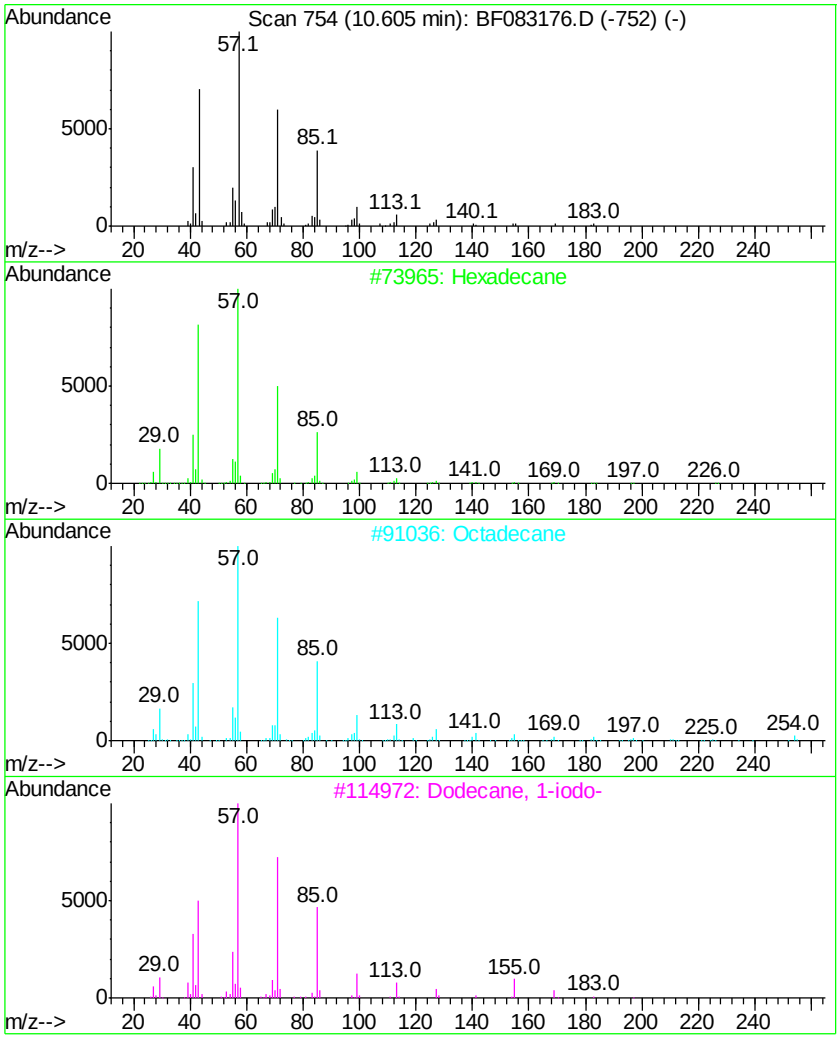
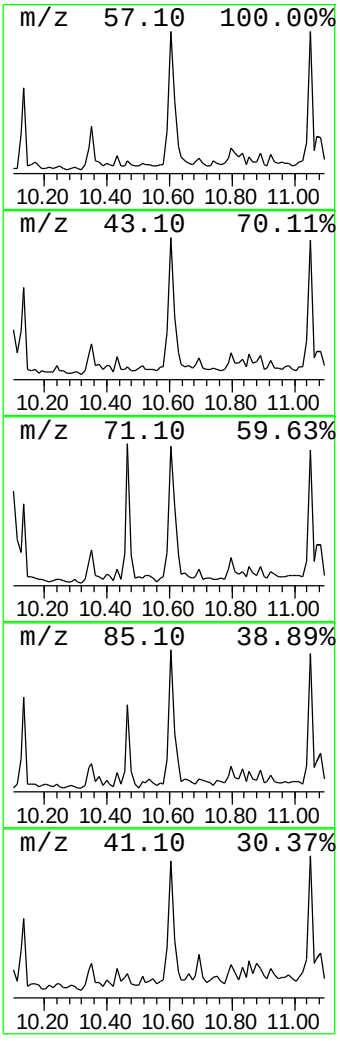
Peak Number 4 Hexadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.36 ng	221920	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Octadecane	254	C18H38	000593-45-3	86
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
4	Heneicosane	296	C21H44	000629-94-7	83
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
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Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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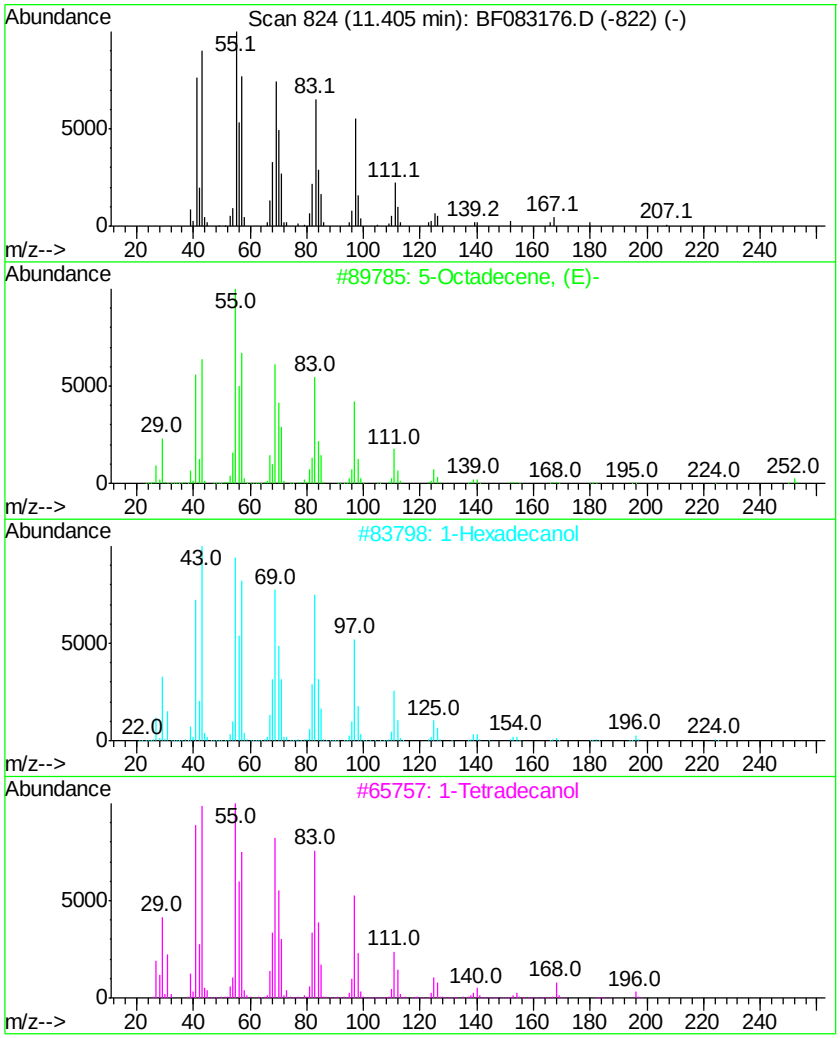
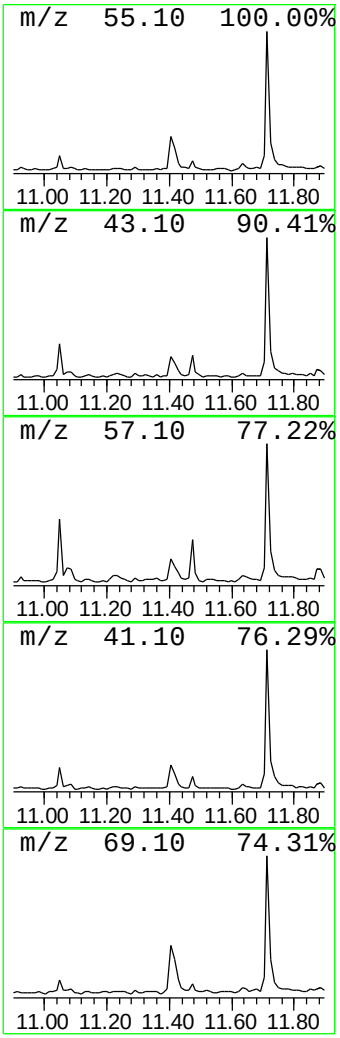
Peak Number 5 5-Octadecene, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.40	2.63 ng	246952	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
2	1-Hexadecanol	242	C16H34O	036653-82-4	91
3	1-Tetradecanol	214	C14H30O	000112-72-1	90
4	2-Tetradecene, (E)-	196	C14H28	035953-53-8	90
5	1-Pentadecanol	228	C15H32O	000629-76-5	87





Library Search Compound Report

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Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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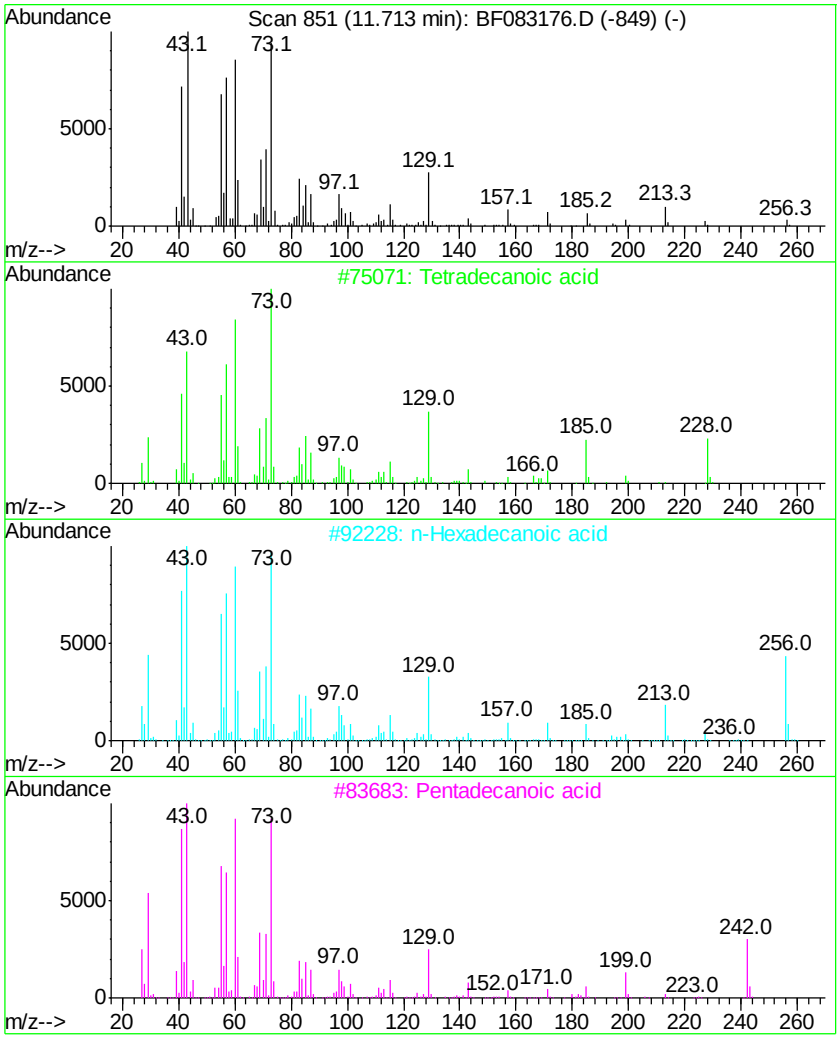
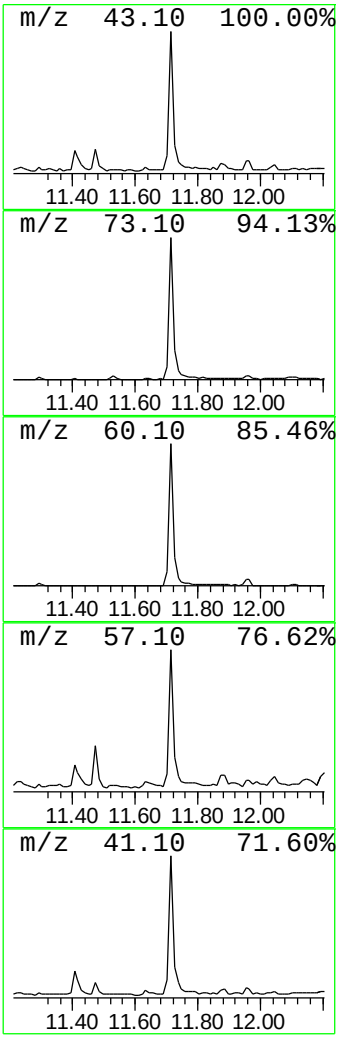
Peak Number 6 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	11.44 ng	1074150	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Butanoic acid	88	C4H8O2	000107-92-6	35





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Instrument : BNA_F
ClientSampleId : NC-HC-004

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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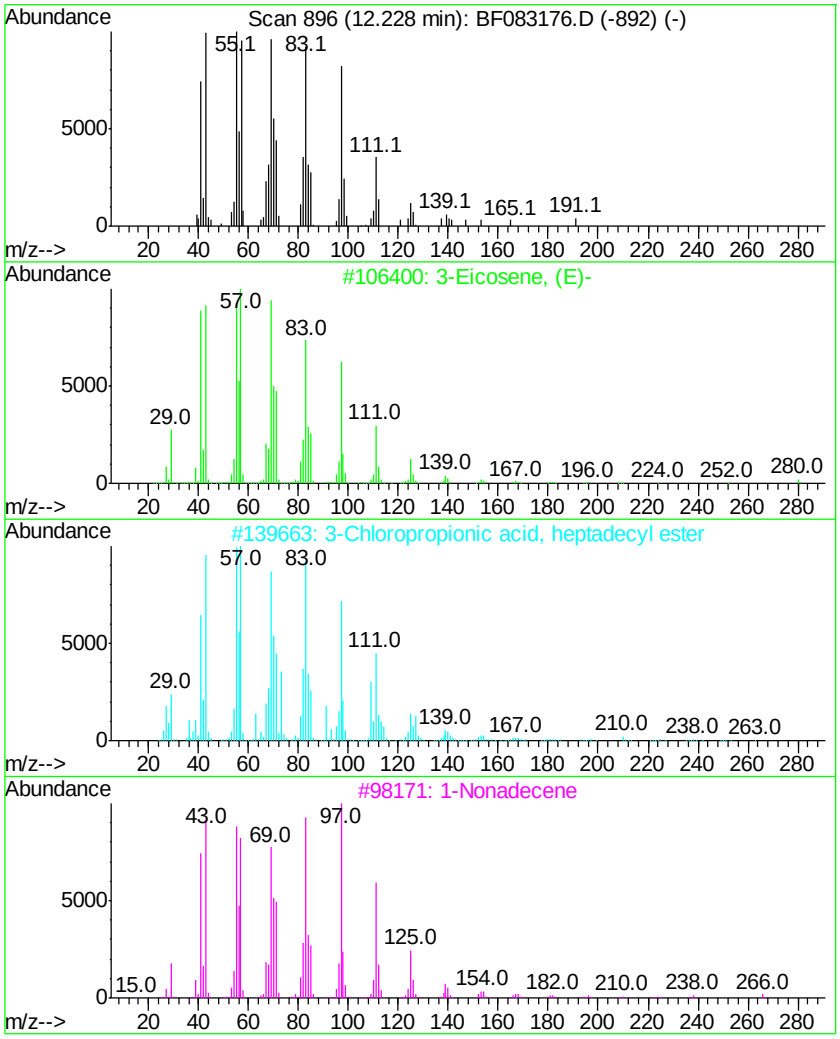
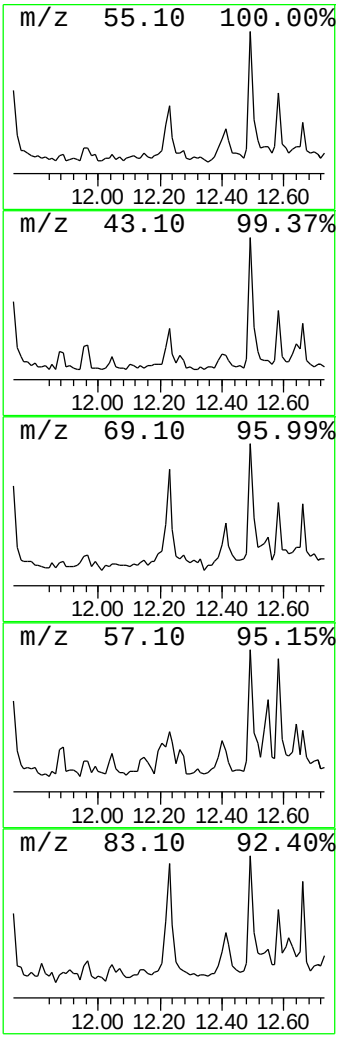
Peak Number 7 3-Eicosene, (E)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	2.12 ng	199372	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	94
2	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
3	1-Nonadecene	266	C19H38	018435-45-5	94
4	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	91
5	4-Heptafluorobutyryloxyhexadecane	438	C20H33F7O2	1000282-97-2	91





Library Search Compound Report

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ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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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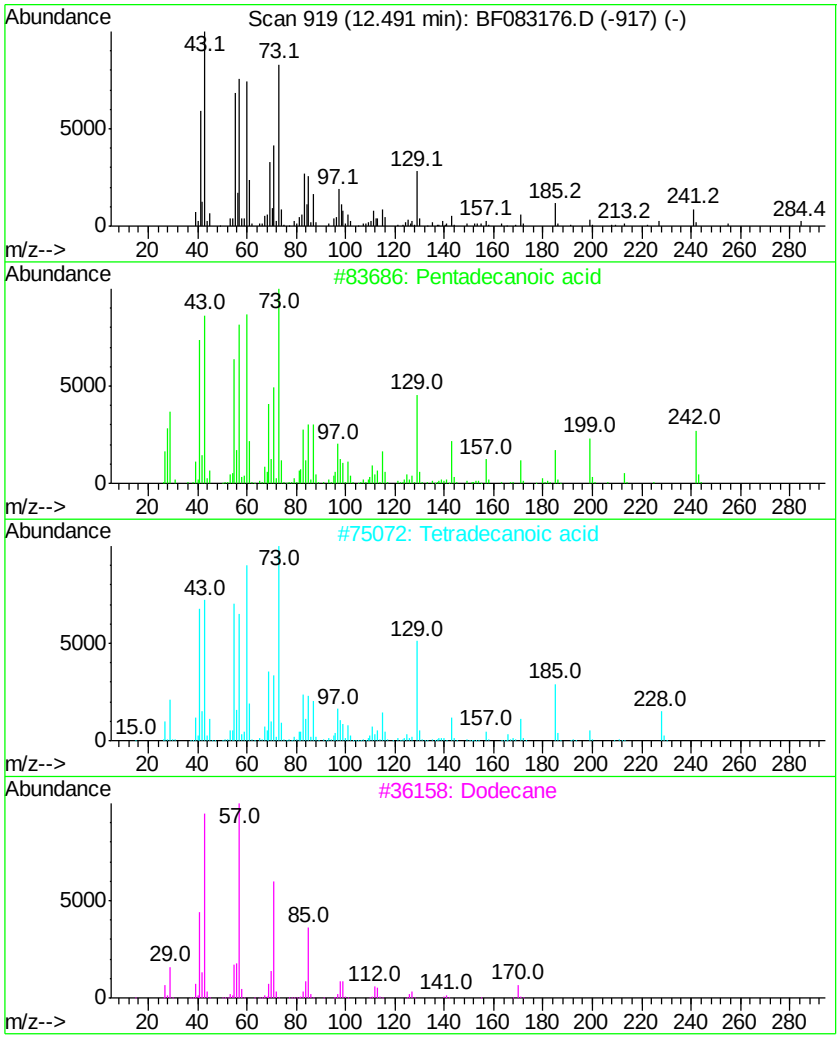
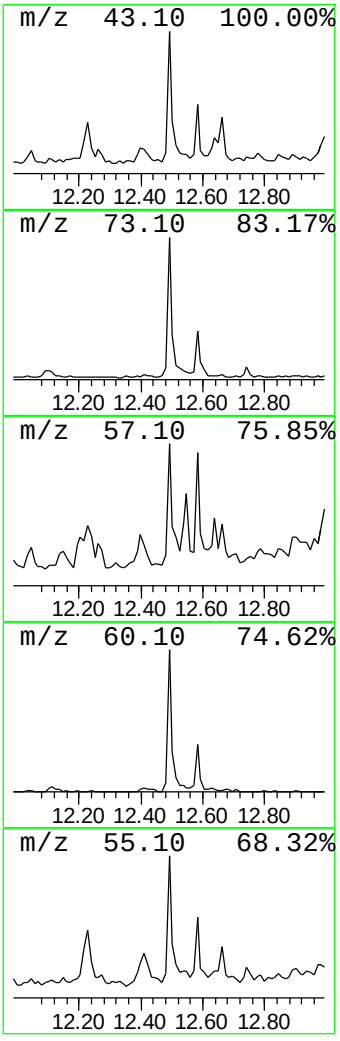
Peak Number 8 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	5.11 ng	417148	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
3	Dodecane	170	C12H26	000112-40-3	18
4	Undecane	156	C11H24	001120-21-4	18
5	Tetradecane	198	C14H30	000629-59-4	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083176.D
Acq On : 22 Nov 2015 23:37
Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.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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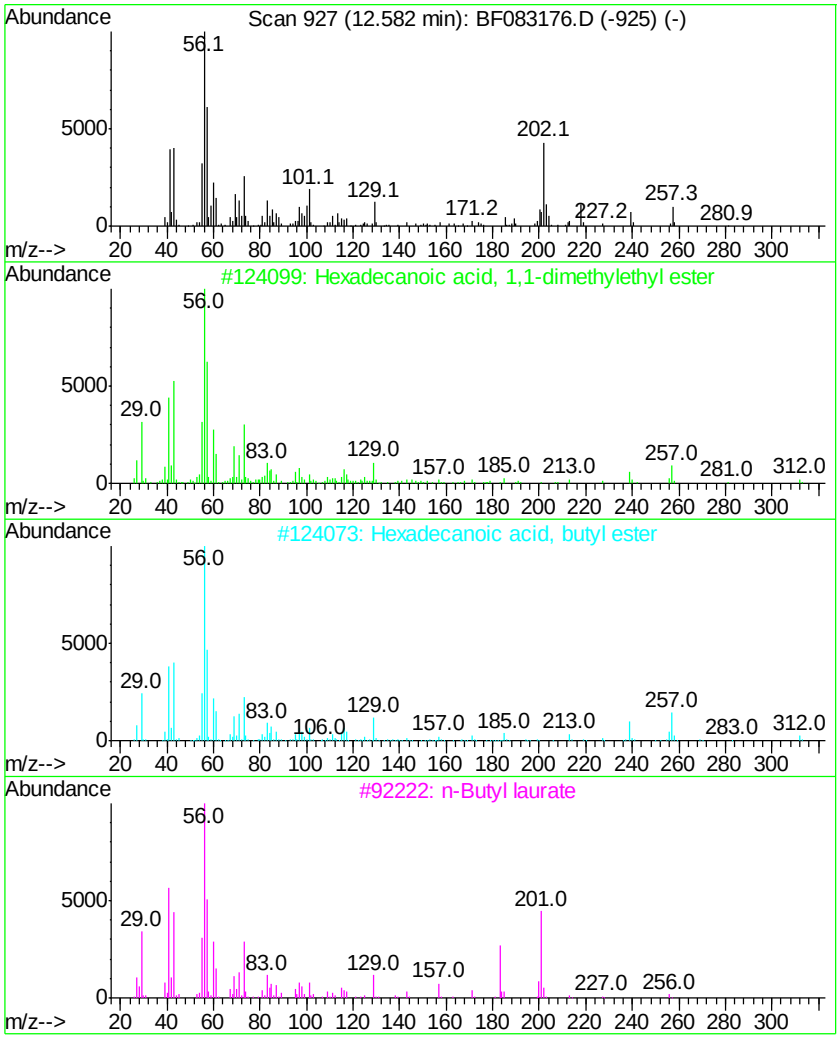
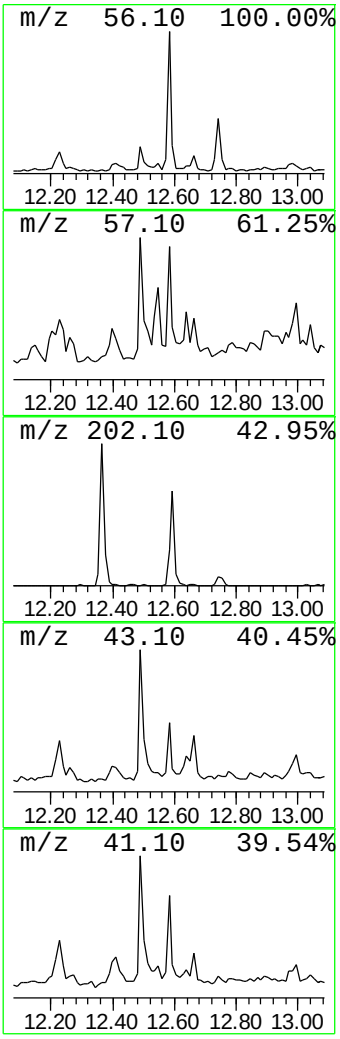
Peak Number 9 Hexadecanoic acid, 1,1-dime... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	4.26 ng	347891	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	53
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	46
3	n-Butyl laurate	256	C16H32O2	000106-18-3	42
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	35
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	35





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Data File : BF083176.D
Acq On : 22 Nov 2015 23:37
Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

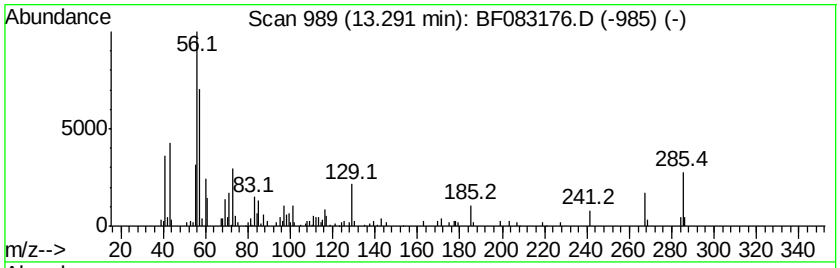
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

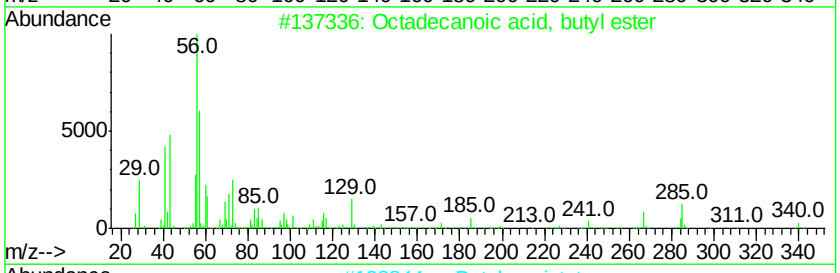
****

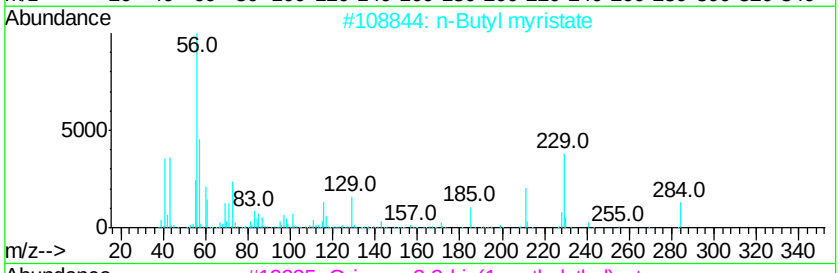
Peak Number 10 Octadecanoic acid, butyl ester Concentration Rank 16

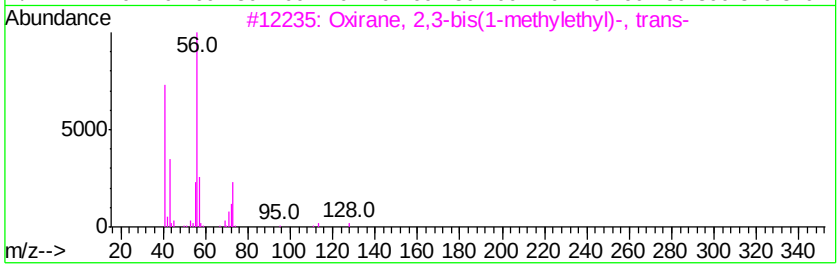
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.29	2.07 ng	168828	Chrysene-d12	13.78

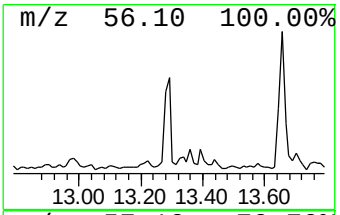
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	74
2	n-Butyl myristate	284	C18H36O2	000110-36-1	64
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	27

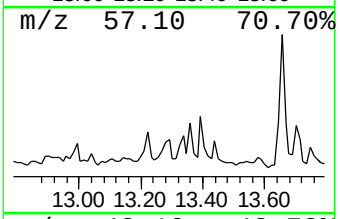


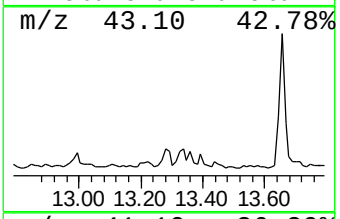


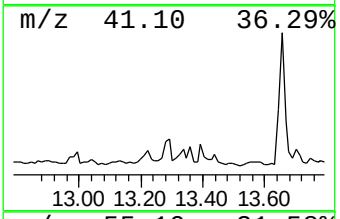


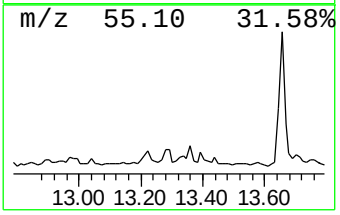












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Data File : BF083176.D
Acq On : 22 Nov 2015 23:37
Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

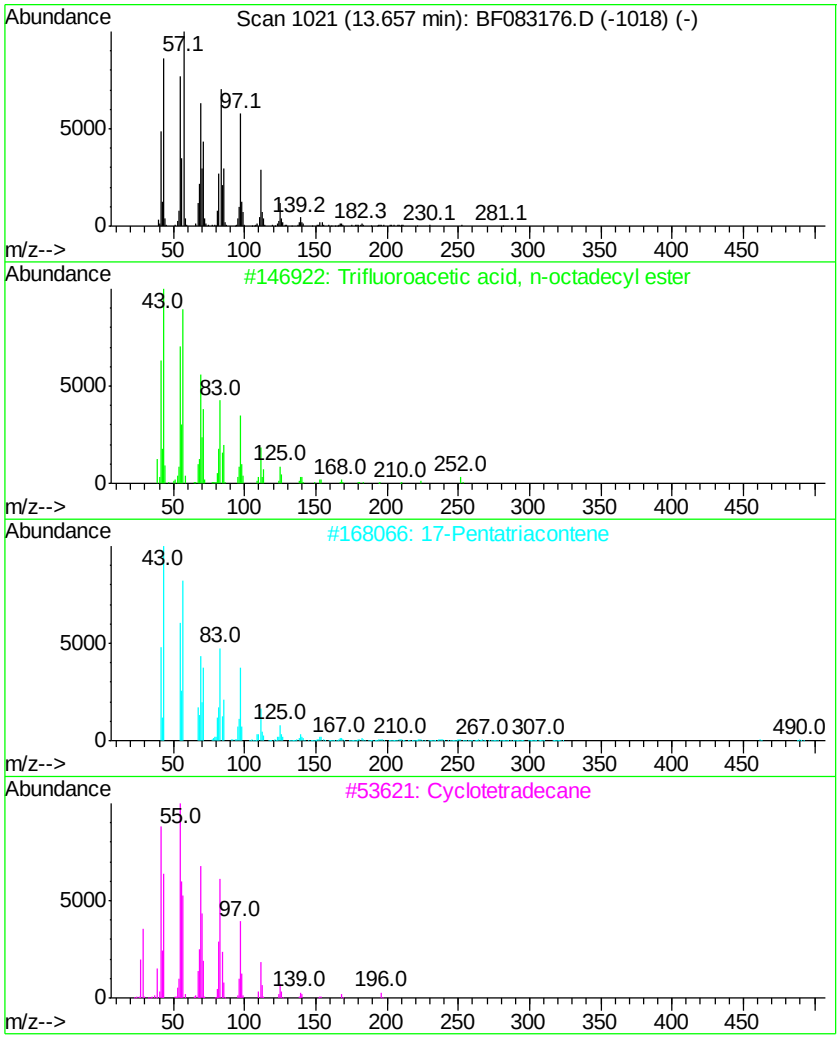
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

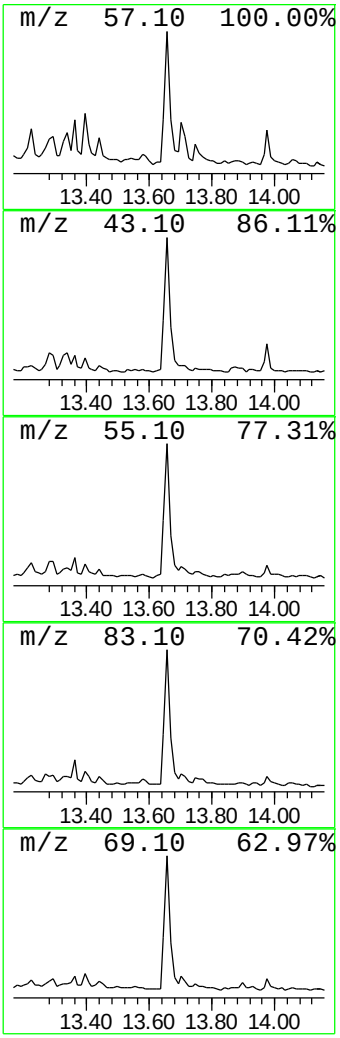
****

Peak Number 11 Trifluoroacetic acid, n-oct... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.66	10.41 ng	849450	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-octadecv...	366	C20H37F3O2	079392-43-1	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Cyclotetradecane	196	C14H28	000295-17-0	91
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





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Sample : G4482-01
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ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

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

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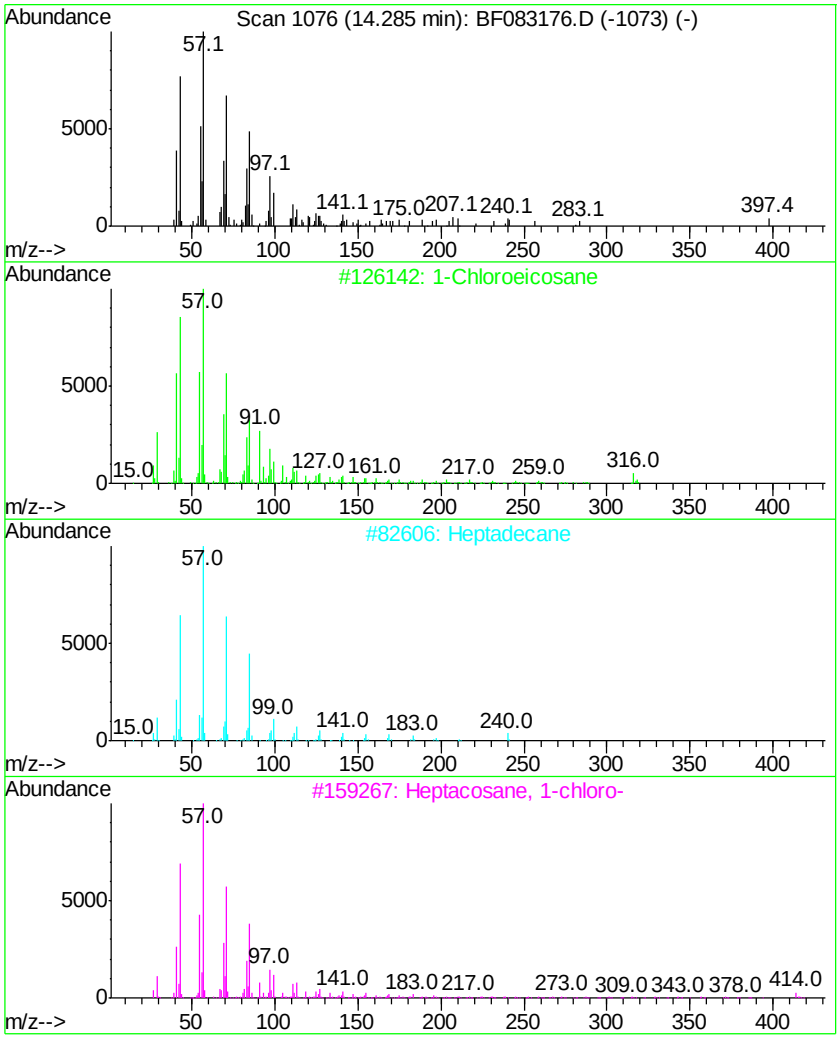
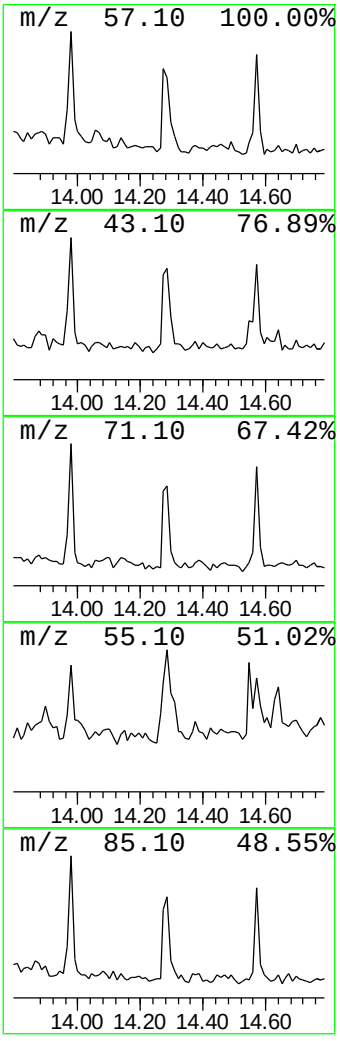
Peak Number 12 1-Chloroeicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.29	2.86 ng	233593	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chloroeicosane	316	C20H41Cl	042217-02-7	86
2	Heptadecane	240	C17H36	000629-78-7	83
3	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
4	10-Methylnonadecane	282	C20H42	056862-62-5	68
5	Tetratetracontane	619	C44H90	007098-22-8	64





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Acq On : 22 Nov 2015 23:37
Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

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TIC Integration Parameters: LSCINT.P

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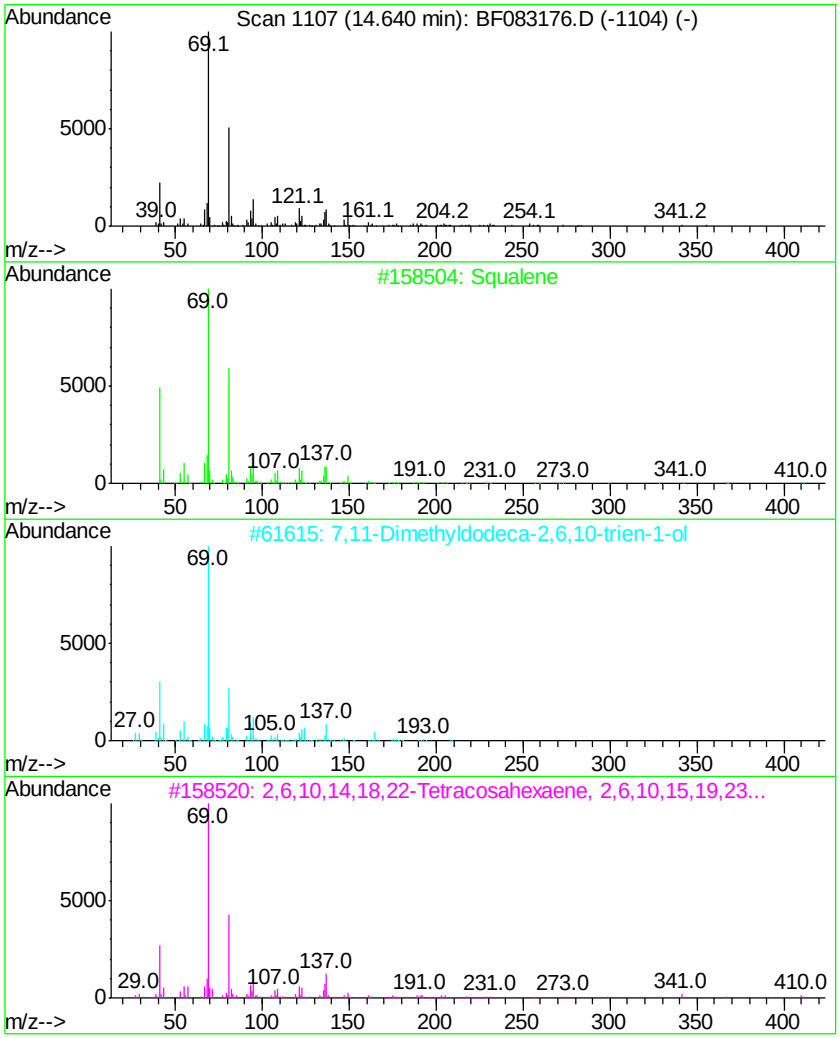
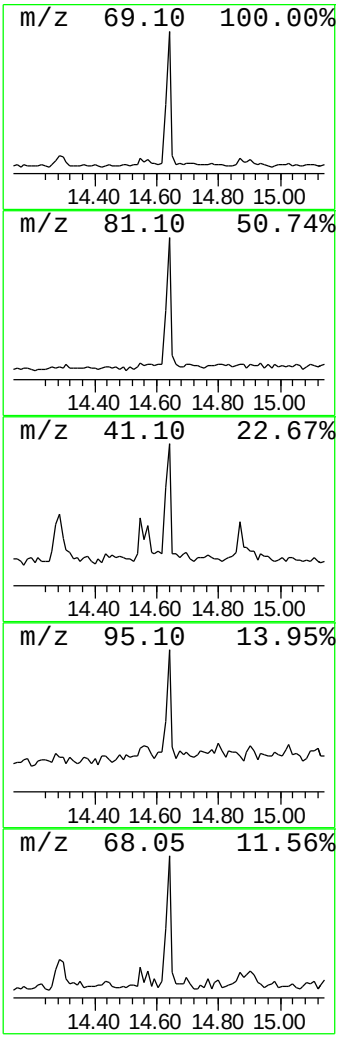
Peak Number 14 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	3.14 ng	191424	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
3	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	78
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	72





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Acq On : 22 Nov 2015 23:37
Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.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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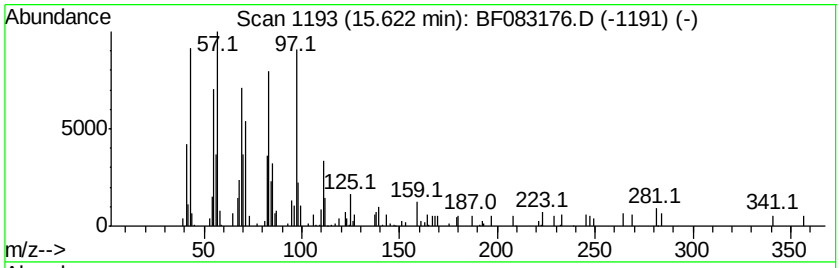
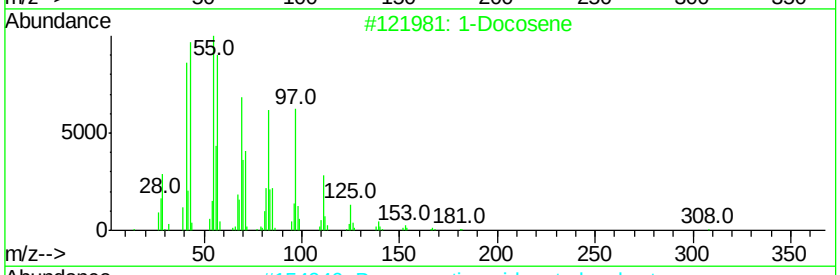
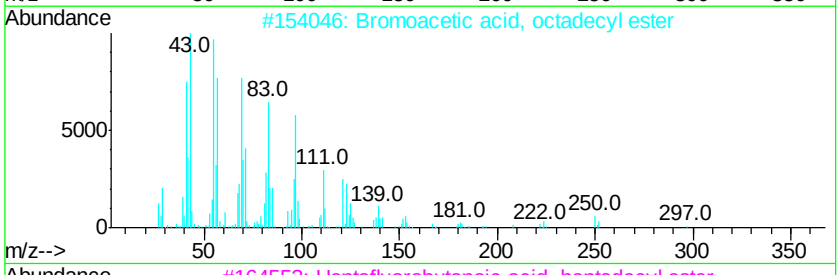
Peak Number 15 1-Docosene Concentration Rank 12

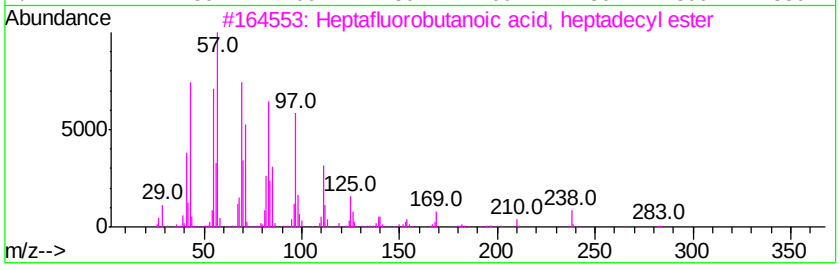
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	2.62 ng	159281	Perylene-d12	15.14

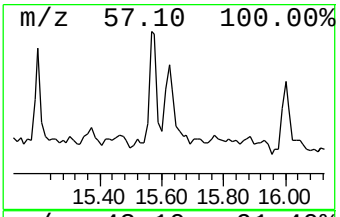
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	87
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	76
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	76
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	76
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	74

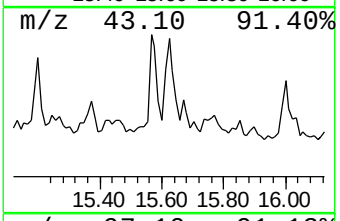


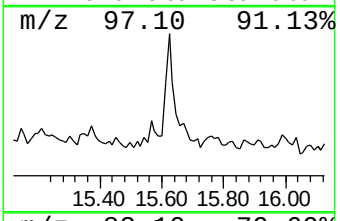


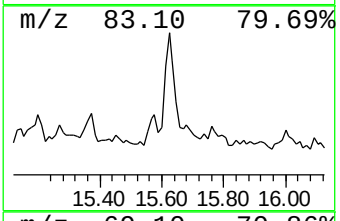


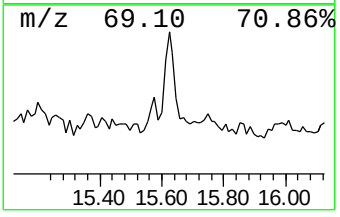












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF112215\
Data File : BF083176.D
Acq On : 22 Nov 2015 23:37
Operator : UM/IZ
Sample : G4482-01
Misc :
ALS Vial : 62 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NC-HC-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.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
2-Pentanone, 4-hy...	4.80	52.4	ng	3281420	1	6.65	1253410	20.0
unknown6.42	6.42	85.1	ng	5331060	1	6.65	1253410	20.0
Hexadecane	10.60	2.4	ng	221920	4	11.16	1877190	20.0
5-Octadecene, (E)-	11.40	2.6	ng	246952	4	11.16	1877190	20.0
Tetradecanoic acid	11.71	11.4	ng	1074150	4	11.16	1877190	20.0
3-Eicosene, (E)-	12.23	2.1	ng	199372	4	11.16	1877190	20.0
Pentadecanoic acid	12.49	5.1	ng	417148	5	13.78	1632010	20.0
Hexadecanoic acid...	12.58	4.3	ng	347891	5	13.78	1632010	20.0
Octadecanoic acid...	13.29	2.1	ng	168828	5	13.78	1632010	20.0
Trifluoroacetic a...	13.66	10.4	ng	849450	5	13.78	1632010	20.0
1-Chloroeicosane	14.29	2.9	ng	233593	5	13.78	1632010	20.0
Squalene	14.64	3.1	ng	191424	6	15.14	1217740	20.0
1-Docosene	15.62	2.6	ng	159281	6	15.14	1217740	20.0