LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

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-BF012417.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	4.270	181	191	193	rBV4	19920	77295	1.66%	0.190%
2	5.139	265	267	270	rBV	539509	791618	17.04%	1.948%
3	5.561	301	304	306	rBV	1629959	2203473	47.42%	5.422%
4	5.881	330	332	338	rVB2	35033	47299	1.02%	0.116%
5	6.579	384	393	397	rBV	1899591	2165286	46.60%	5.328%
6	6.727	403	406	409	rBV	3344243	3174806	68.33%	7.812%
7	6.807	410	413	415	rBV	49353	47302	1.02%	0.116%
8	6.967	424	427	429	rBV	1042126	973269	20.95%	2.395%
9	7.024	431	432	434	rBV	59889	54680	1.18%	0.135%
10	7.127	438	441	443	rBV	2995910	3286411	70.73%	8.087%
11	7.379	453	463	465	rBV	545951	1804845	38.84%	4.441%
12	7.527	473	476	479	rVB	2216642	2960442	63.72%	7.284%
13	7.630	483	485	487	rVV	53060	90062	1.94%	0.222%
14	7.676	487	489	492	rVB3	44890	78460	1.69%	0.193%
15	7.996	511	517	520	rBV3	346498	621503	13.38%	1.529%
16	8.259	537	540	542	rBV	1440815	1316171	28.33%	3.239%
17	8.442	552	556	559	rVB6	27125	50319	1.08%	0.124%
18	8.499	559	561	563	rBV3	33349	60461	1.30%	0.149%
19	8.625	568	572	575	rVV2	400481	684532	14.73%	1.684%
20	8.682	575	577	580	rVV2	35762	48388	1.04%	0.119%
21	8.830	587	590	593	rBV2	74312	106404	2.29%	0.262%
22	8.887	593	595	597	rBV	62414	69154	1.49%	0.170%
23	8.933	597	599	600	rBV2	50304	59067	1.27%	0.145%
24	9.070	609	611	612	rBV	41170	48978	1.05%	0.121%
25	9.173	618	620	623	rBV2	68213	87053	1.87%	0.214%
26	9.345	632	635	637	rBV	4666482	4646274	100.00%	11.433%
27	9.539	649	652	654	rBV	399948	626393	13.48%	1.541%
28	9.688	662	665	667	rBV3	44874	109263	2.35%	0.269%
29	9.733	667	669	671	rVB	149693	143722	3.09%	0.354%
30	9.779	671	673	674	rBV	78341	92984	2.00%	0.229%
31	9.813	674	676	680	rBV2	211060	289126	6.22%	0.711%
32	9.928	683	686	692	rBV4	50845	165918	3.57%	0.408%
33	10.019	692	694	696	rBV	1525532	1390358	29.92%	3.421%
34	10.236	710	713	714	rBV2	160155	190680	4.10%	0.469%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

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-BF012417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.568	741	742	744	rBV	84318	69921	1.50%	0.172%
36	10.808	761	763	766	rBV	2009992	2365009	50.90%	5.819%
37	11.379	811	813	814	rBV	70951	52666	1.13%	0.130%
38	11.505	822	824	827	rBV	1304578	1382139	29.75%	3.401%
39	11.802	848	850	854	rVB	60615	66891	1.44%	0.165%
40	11.939	861	862	869	rVB6	37616	77798	1.67%	0.191%
41	12.042	869	871	876	rBV2	330274	440610	9.48%	1.084%
42	12.831	938	940	943	rBV	166504	190644	4.10%	0.469%
43	12.922	946	948	949	rVV	121407	92706	2.00%	0.228%
44	13.105	961	964	966	rBV	4081613	4527827	97.45%	11.141%
45	13.459	993	995	1004	rBV	79833	226828	4.88%	0.558%
46	13.631	1008	1010	1011	rBV	68396	74297	1.60%	0.183%
47	13.997	1039	1042	1045	rVB	179079	227681	4.90%	0.560%
48	14.145	1053	1055	1058	rBV	1269676	1228613	26.44%	3.023%
49	15.277	1152	1154	1159	rVB2	26938	54718	1.18%	0.135%
50	15.620	1181	1184	1187	rBV	638781	952797	20.51%	2.344%
51	15.665	1187	1188	1192	rVB	34056	47389	1.02%	0.117%

Sum of corrected areas: 40640530

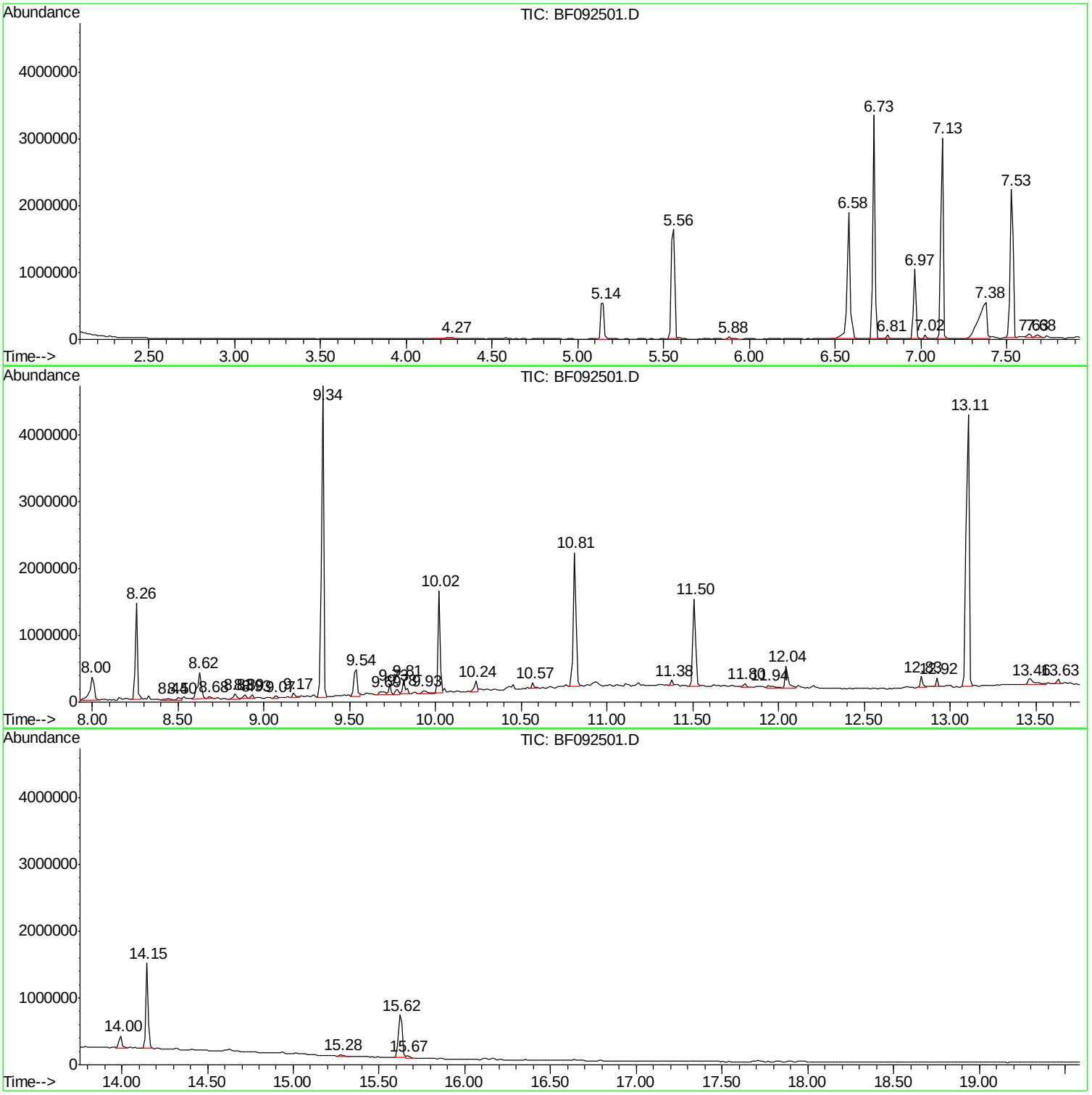
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

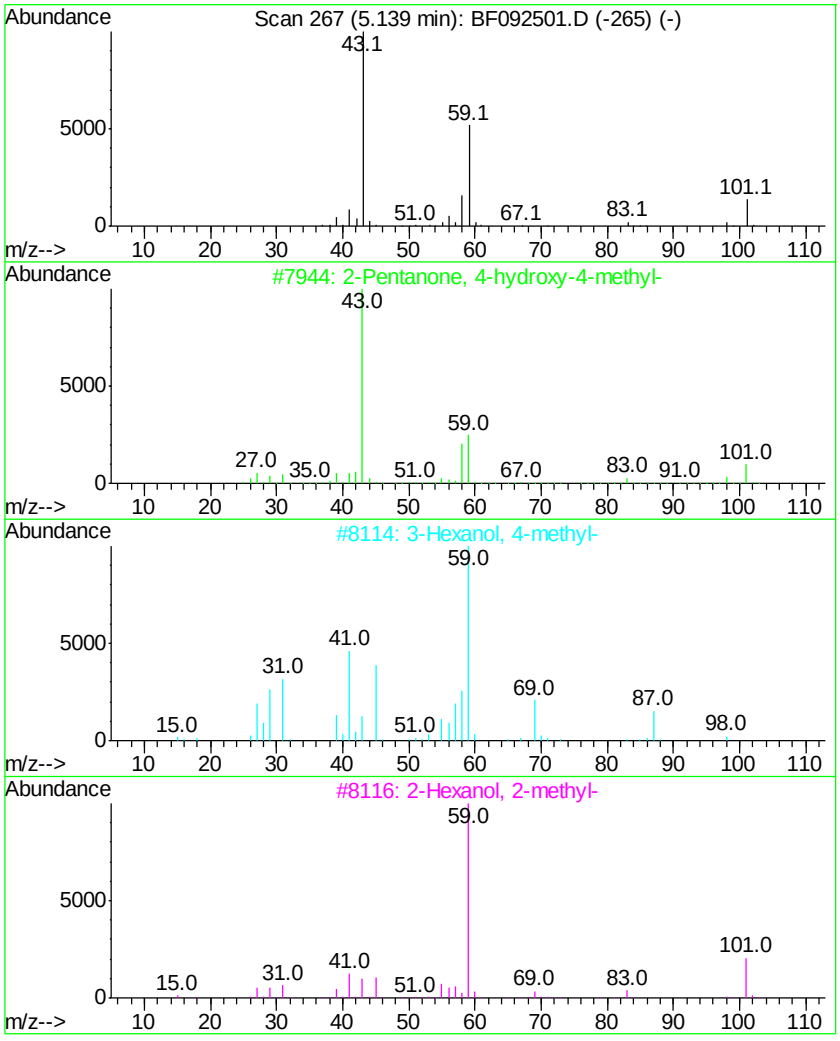
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

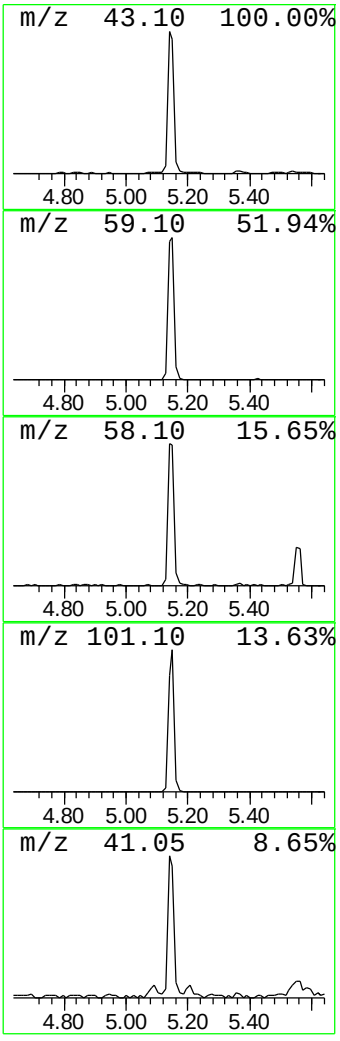
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	16.27 ng	791618	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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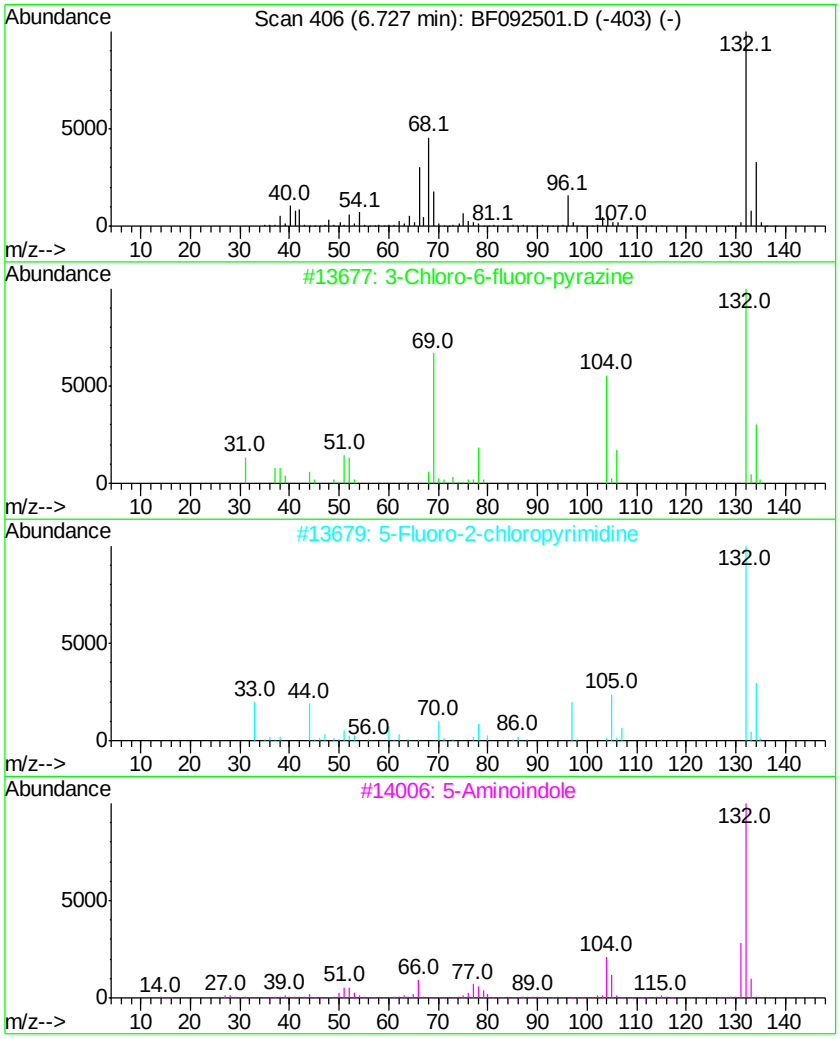
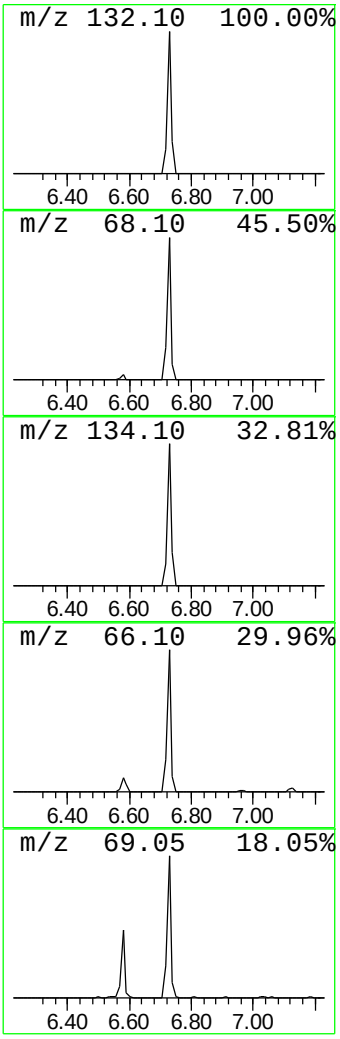
Peak Number 2 unknown6.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	65.24 ng	3174810	1,4-Dichlorobenzene-d4	6.97

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

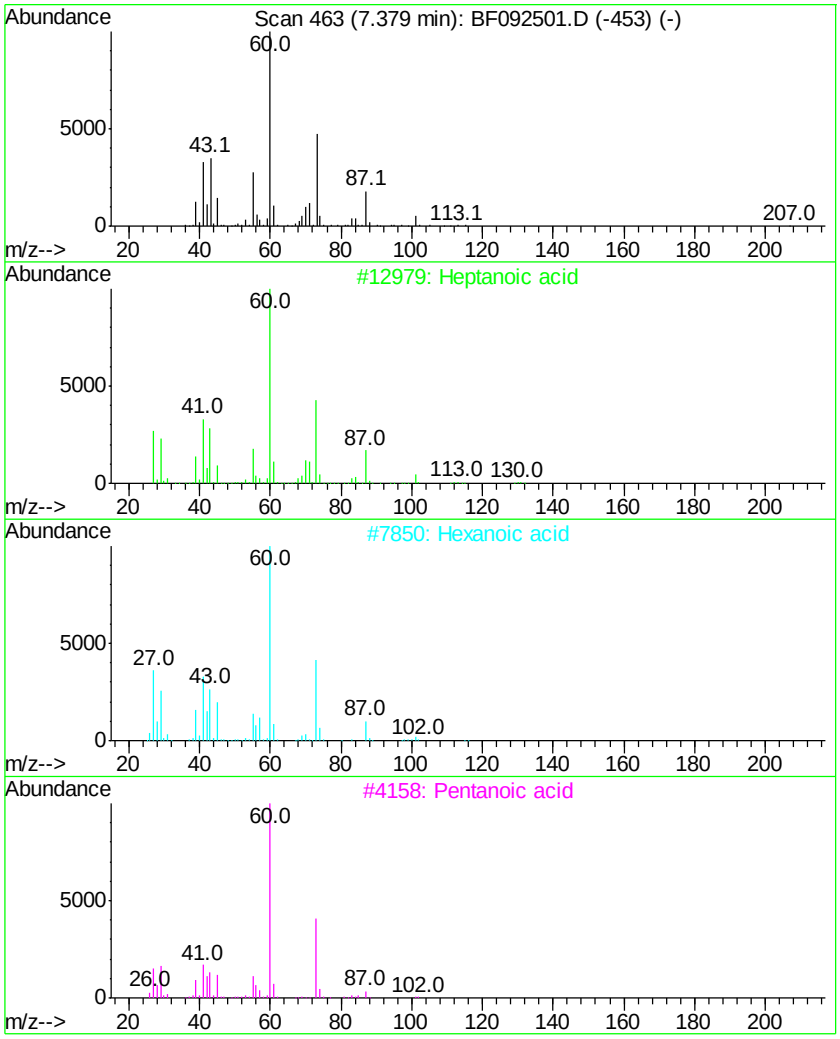
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

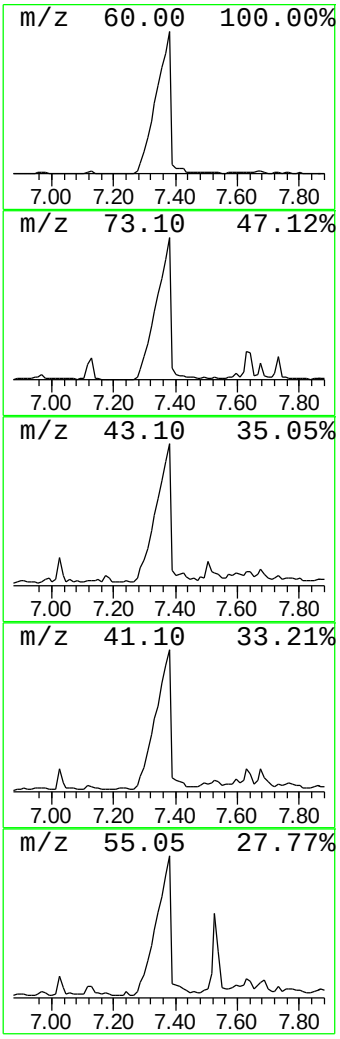
****

Peak Number 4 Heptanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.38	37.09 ng	1804850	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanoic acid	130	C7H14O2	000111-14-8	90
2	Hexanoic acid	116	C6H12O2	000142-62-1	64
3	Pentanoic acid	102	C5H10O2	000109-52-4	64
4	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	62
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	59





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

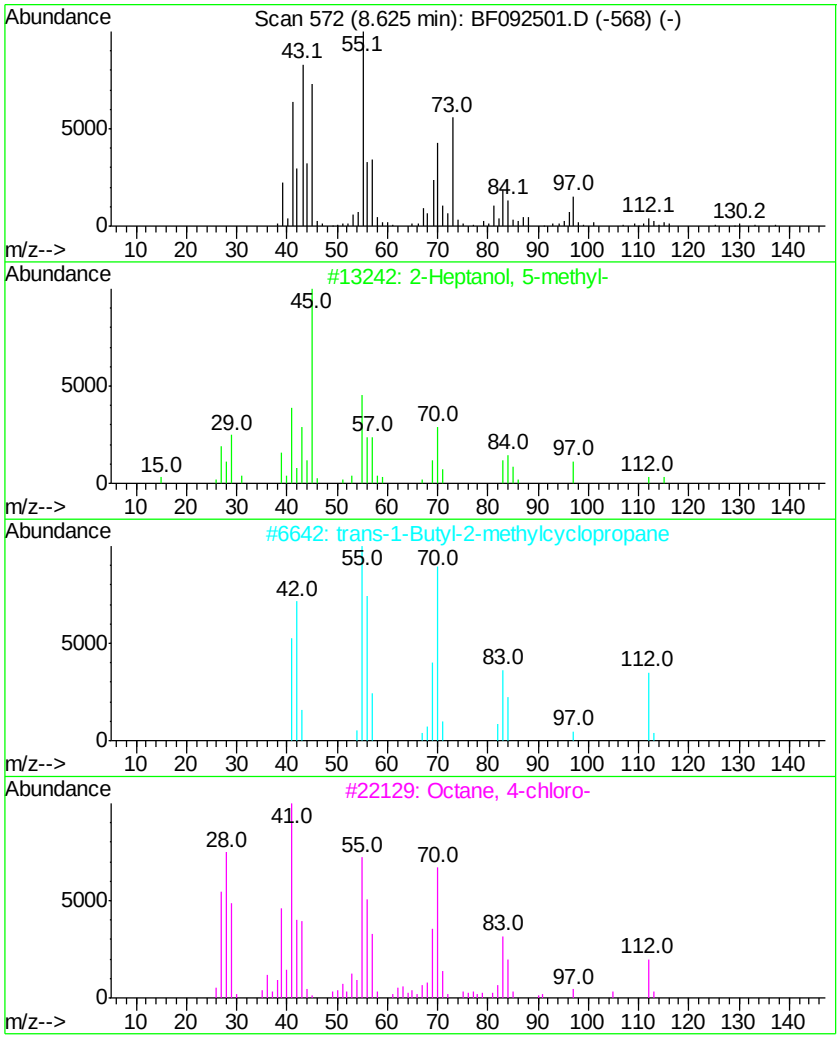
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

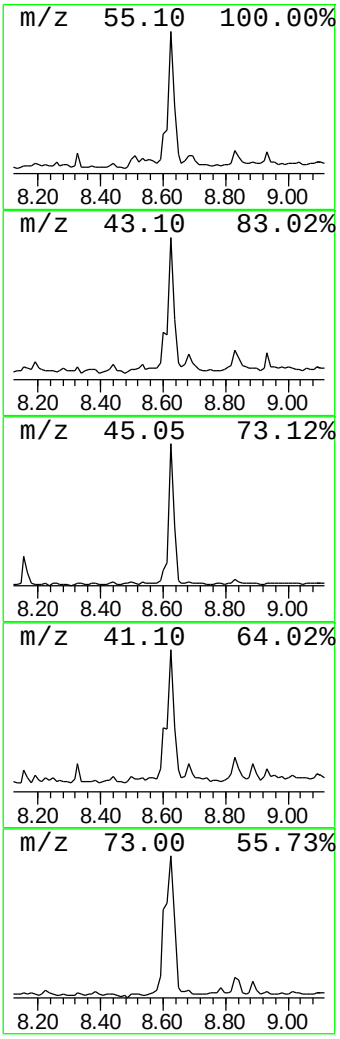
****

Peak Number 5 2-Heptanol, 5-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	10.40 ng	684532	Naphthalene-d8	8.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanol, 5-methyl-	130	C8H18O	054630-50-1	53
2	trans-1-Butyl-2-methylcyclopropane	112	C8H16	038851-70-6	27
3	Octane, 4-chloro-	148	C8H17Cl	000999-07-5	27
4	cis-1-Butyl-2-methylcyclopropane	112	C8H16	038851-69-3	27
5	(2R,4R)-(-)-Pentanediol	104	C5H12O2	042075-32-1	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

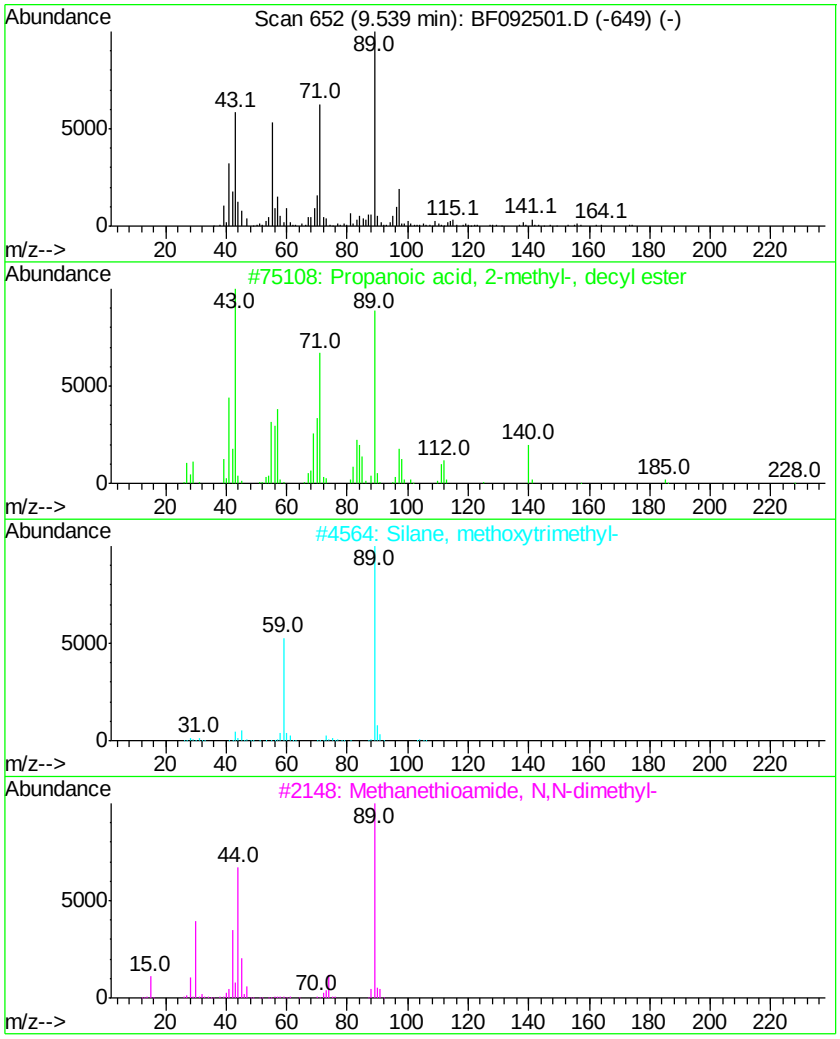
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

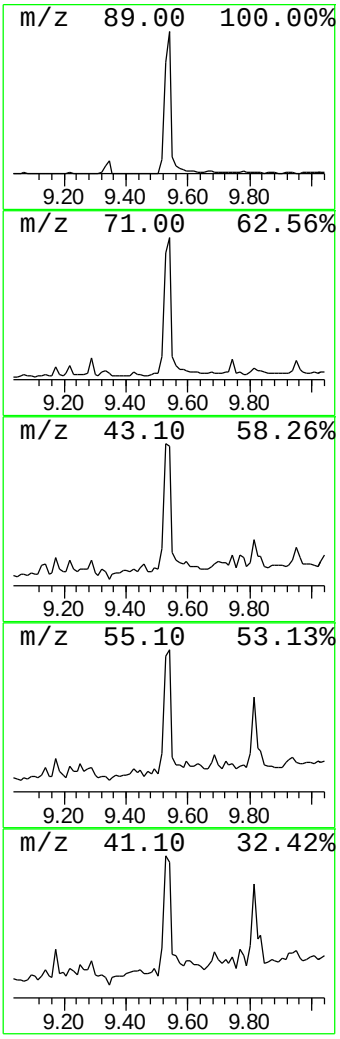
****

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	9.01 ng	626393	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, decyl...	228	C14H28O2	005454-22-8	64
2	Silane, methoxytrimethyl-	104	C4H12OSi	001825-61-2	59
3	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	59
4	3-Hydroxydecanoic acid	188	C10H20O3	033044-91-6	56
5	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	56





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

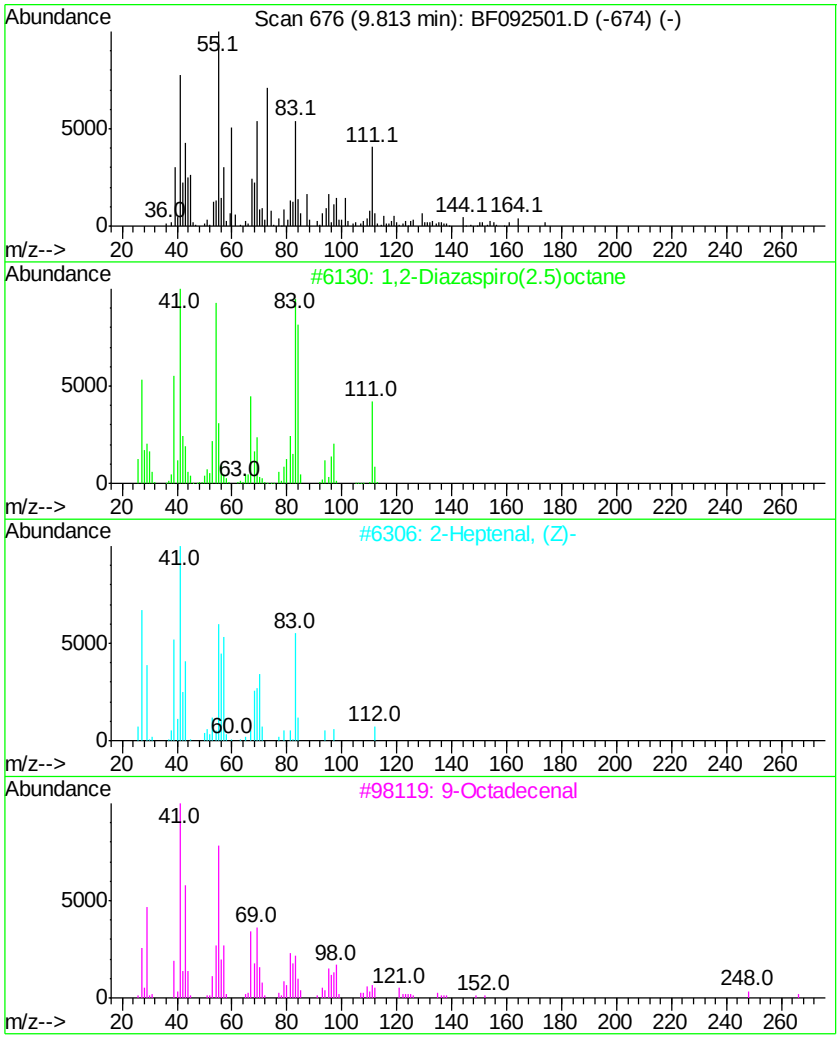
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

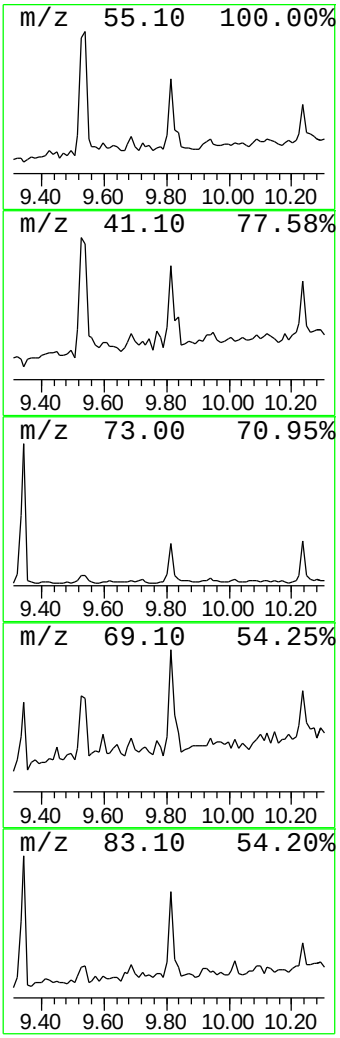
****

Peak Number 7 unknown9.81 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.81	4.16 ng	289126	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Diazaspiro(2.5)octane	112	C6H12N2	000185-79-5	25
2	2-Heptenal, (Z)-	112	C7H12O	057266-86-1	22
3	9-Octadecenal	266	C18H34O	005090-41-5	14
4	4-Octanol, 7-methyl-	144	C9H20O	033933-77-6	14
5	Cyclopentane, 1,1,3-trimethyl-	112	C8H16	004516-69-2	11





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

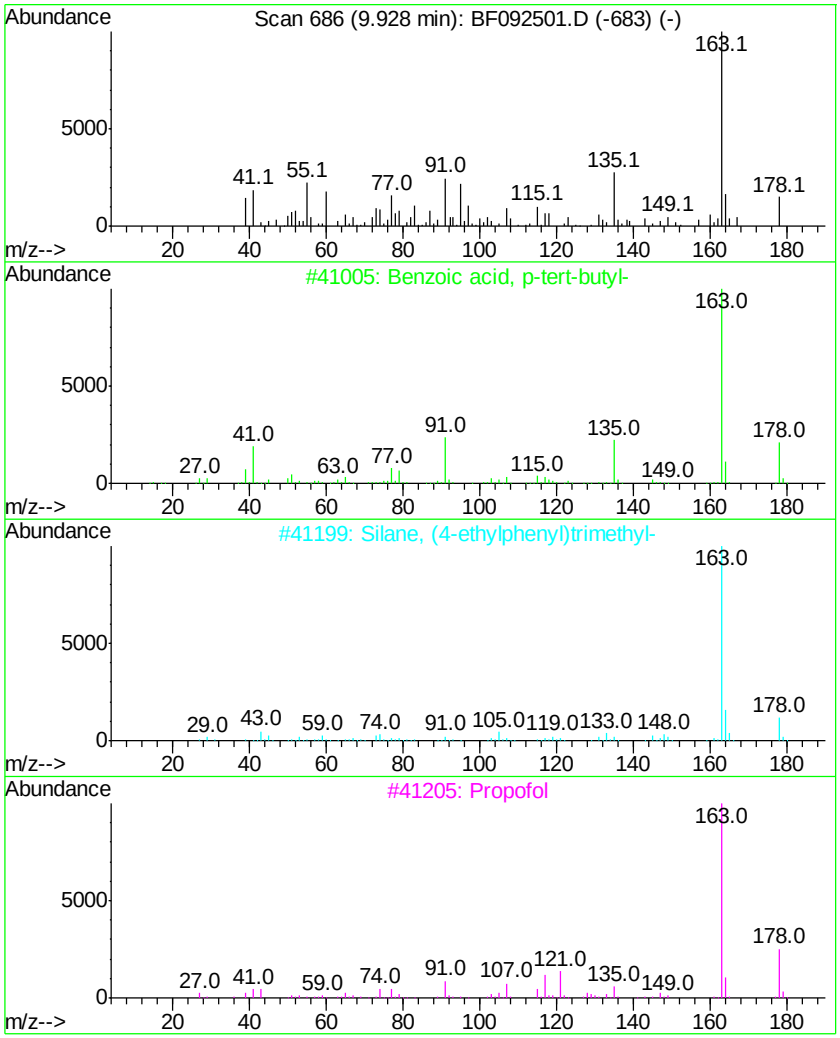
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

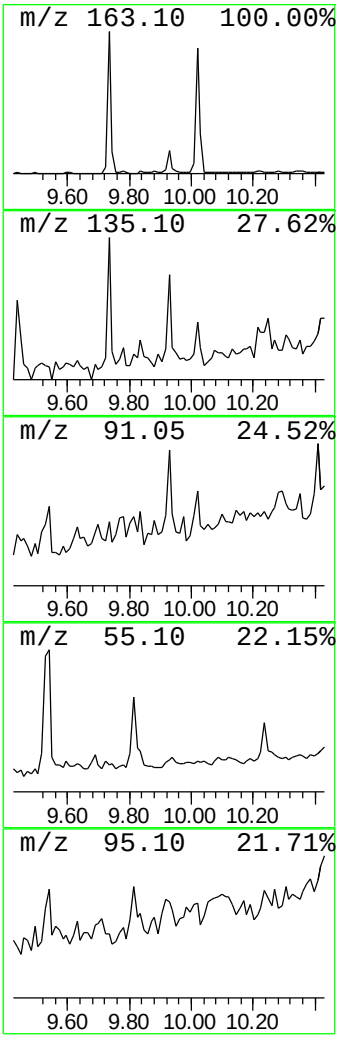
****

Peak Number 8 unknown9.93 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.93	2.39 ng	165918	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	49
2	Silane, (4-ethylphenyl)trimethyl-	178	C11H18Si	017988-50-0	49
3	Propofol	178	C12H18O	002078-54-8	43
4	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	43
5	Hydratropamide, .alpha.-methyl-	163	C10H13NO	000826-54-0	43





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

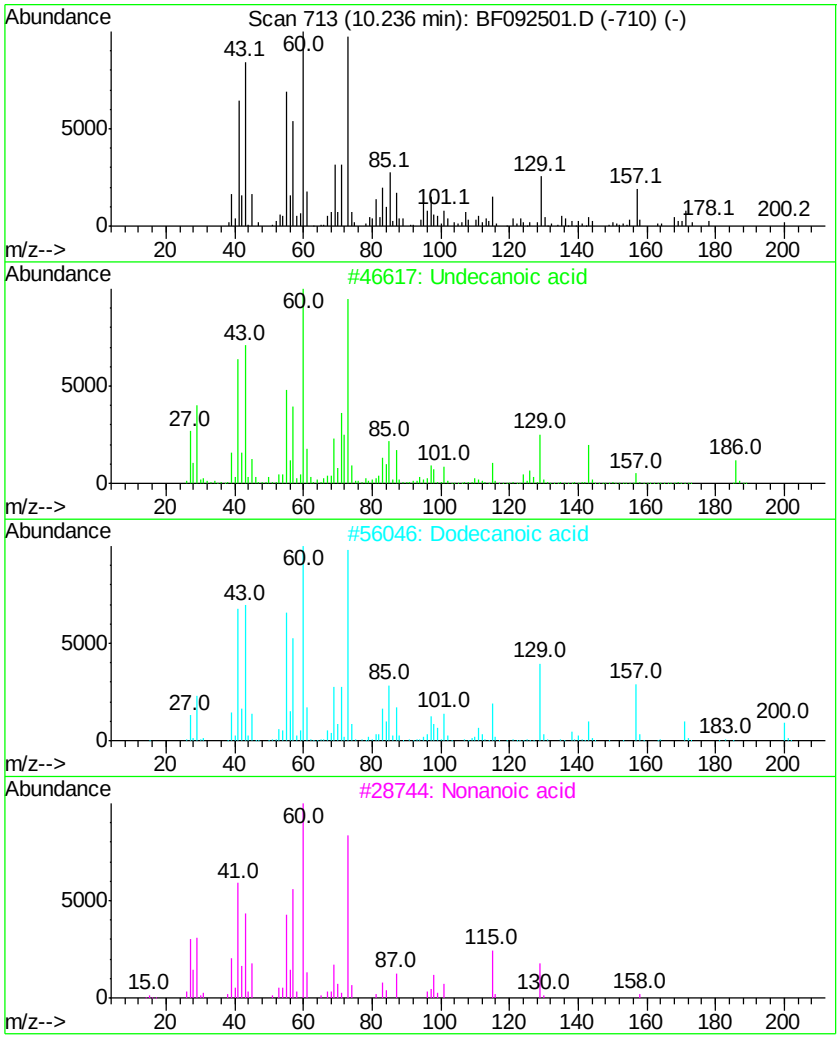
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

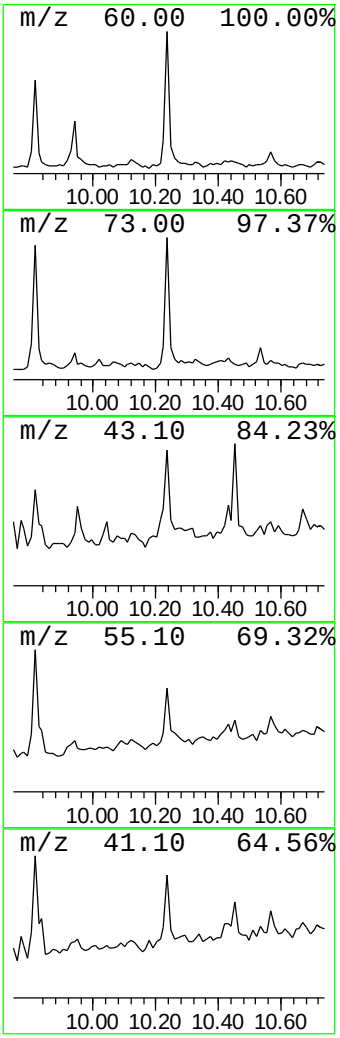
****

Peak Number 9 Undecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.24	2.74 ng	190680	Acenaphthene-d10	10.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	64
2	Dodecanoic acid	200	C12H24O2	000143-07-7	58
3	Nonanoic acid	158	C9H18O2	000112-05-0	53
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	Cyclohexanebutanoic acid	170	C10H18O2	004441-63-8	43





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Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

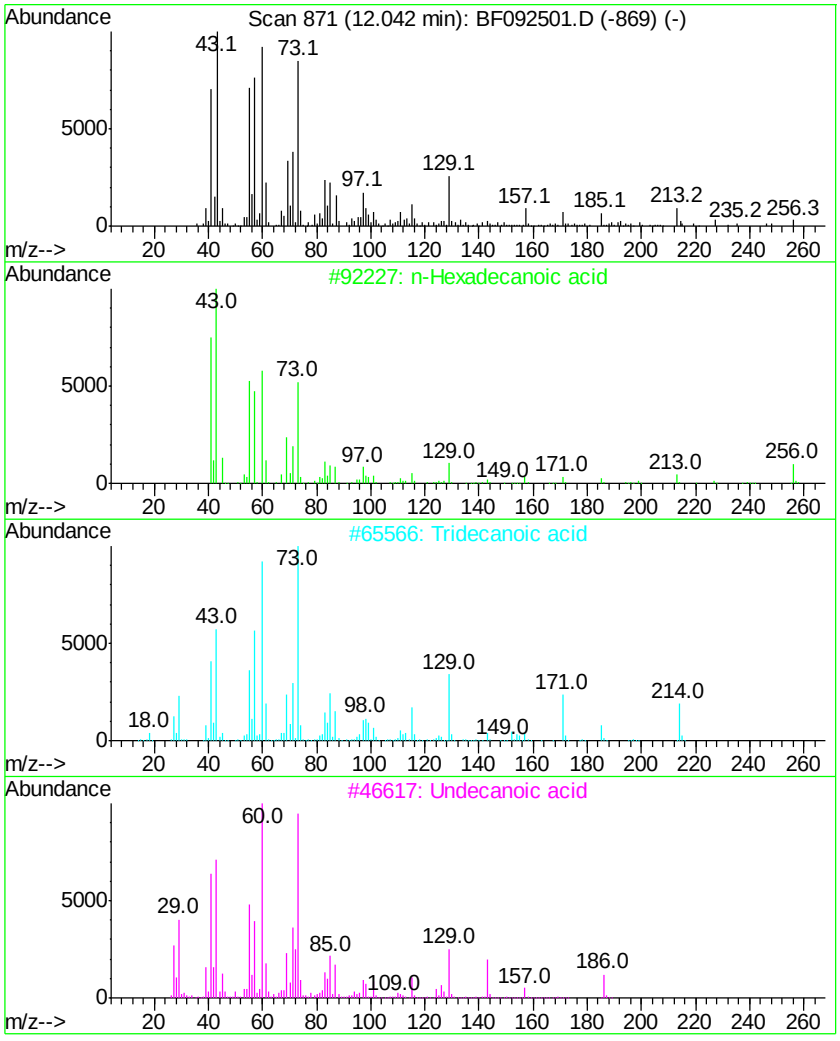
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

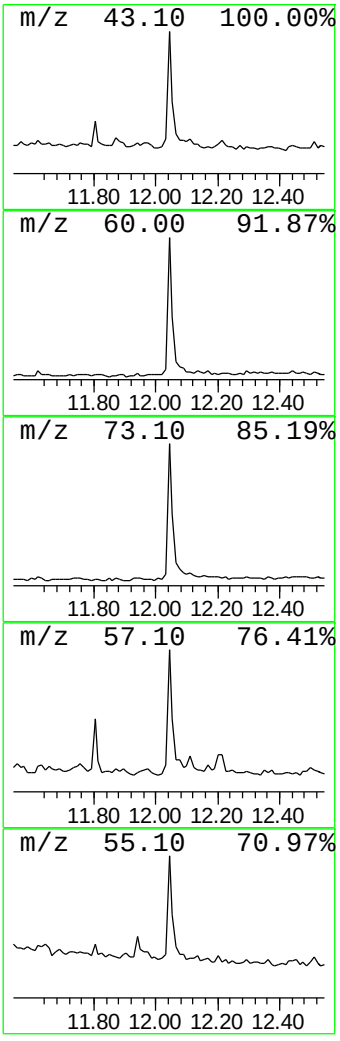
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	6.38 ng	440610	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Undecanoic acid	186	C11H22O2	000112-37-8	86
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	74





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Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.M
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TIC Library : C:\DATABASE\NIST02.L
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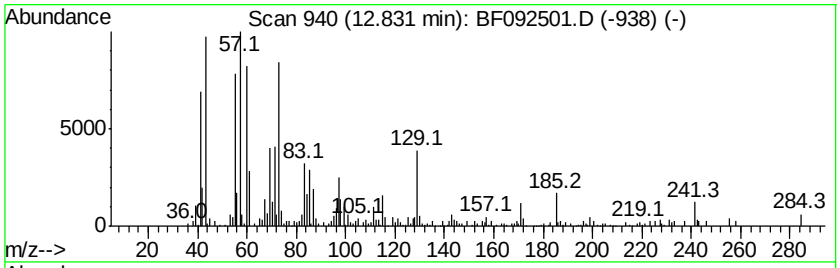
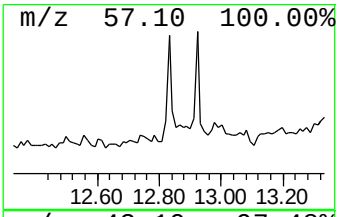
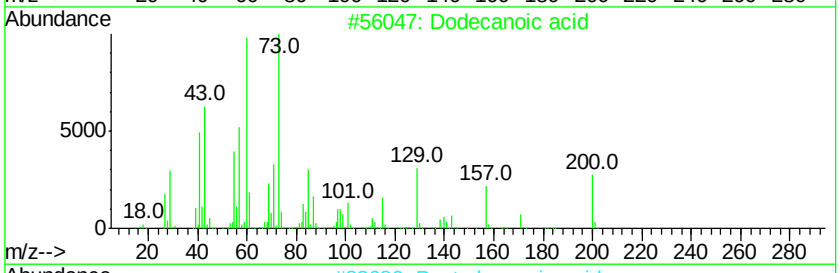
Peak Number 11 Dodecanoic acid Concentration Rank 11

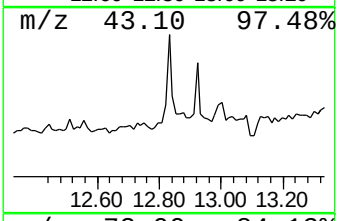
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.83	3.10 ng	190644	Chrysene-d12	14.15

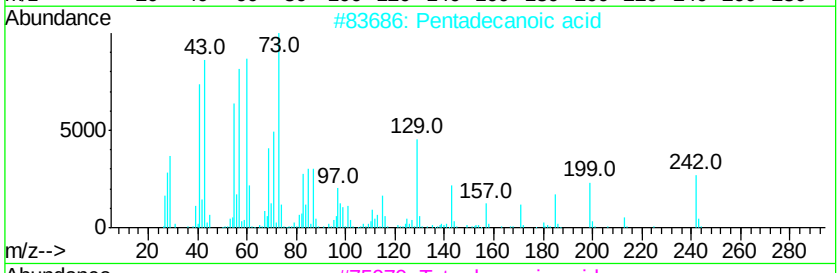
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	83
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	n-Decanoic acid	172	C10H20O2	000334-48-5	68
5	Undecane	156	C11H24	001120-21-4	25

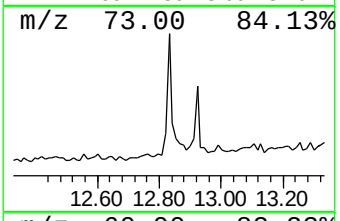


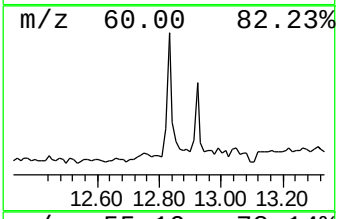


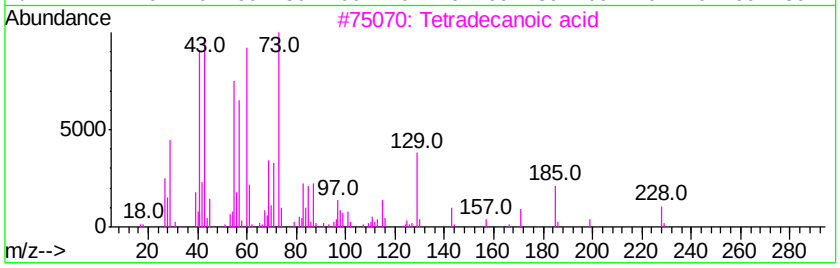


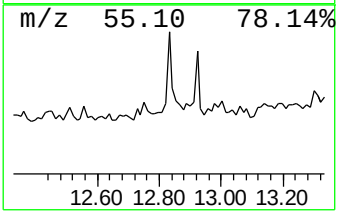












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012417.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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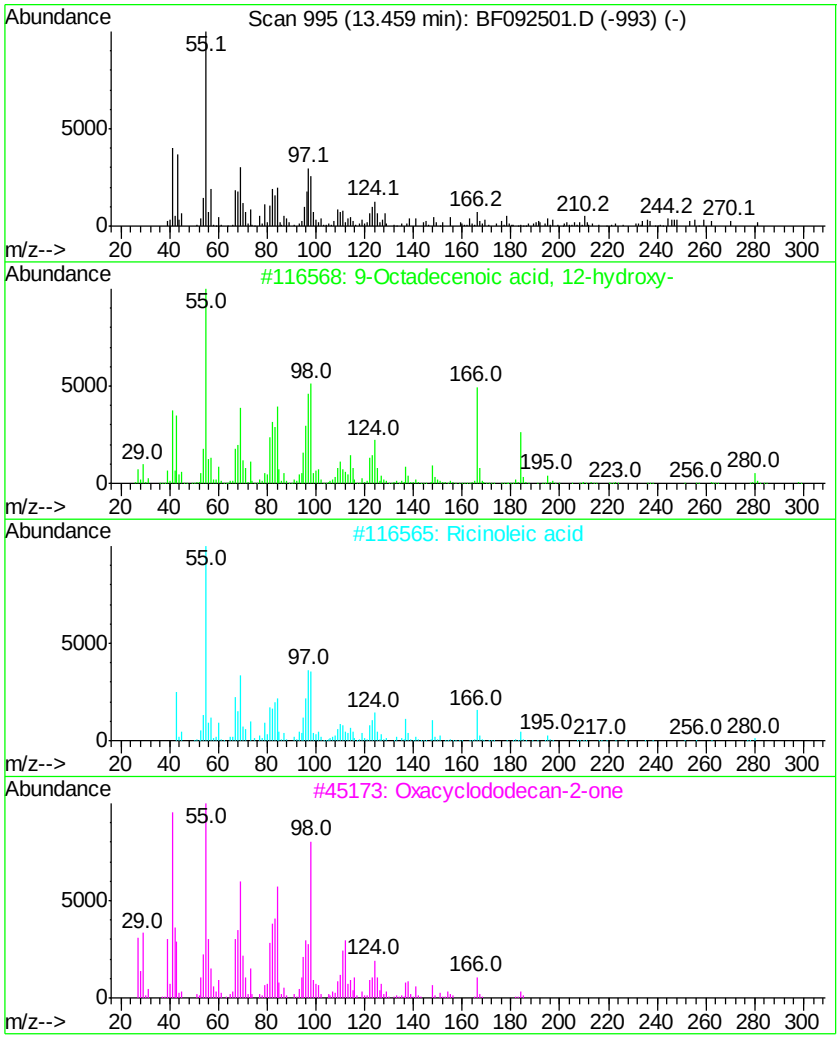
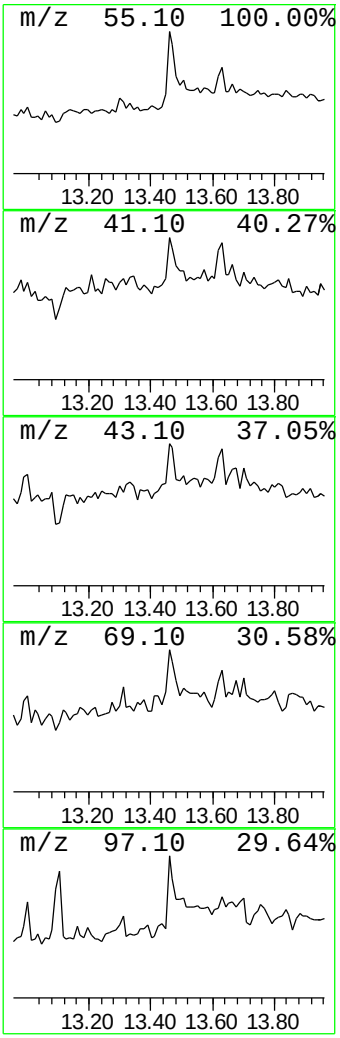
Peak Number 12 9-Octadecenoic acid, 12-hyd... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	3.69 ng	226828	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, 12-hydroxy-	298	C18H34O3	007431-95-0	80
2	Ricinoleic acid	298	C18H34O3	000141-22-0	78
3	Oxacyclododecan-2-one	184	C11H20O2	001725-03-7	64
4	Chloromethyl 8-chloroundecanoate	268	C12H22Cl2O2	080418-94-6	47
5	3-Chloropropionic acid, pentadec...	318	C18H35ClO2	1000281-77-6	27





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Sample : I1312-09
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ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CAS-GW-02

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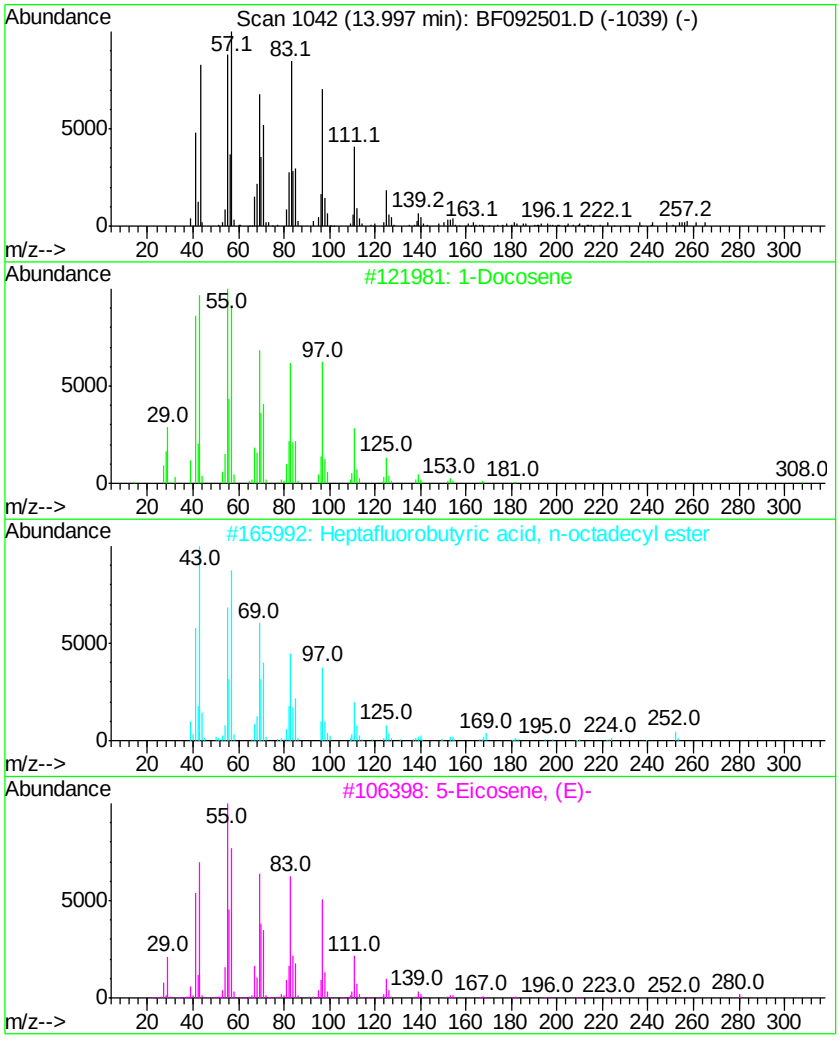
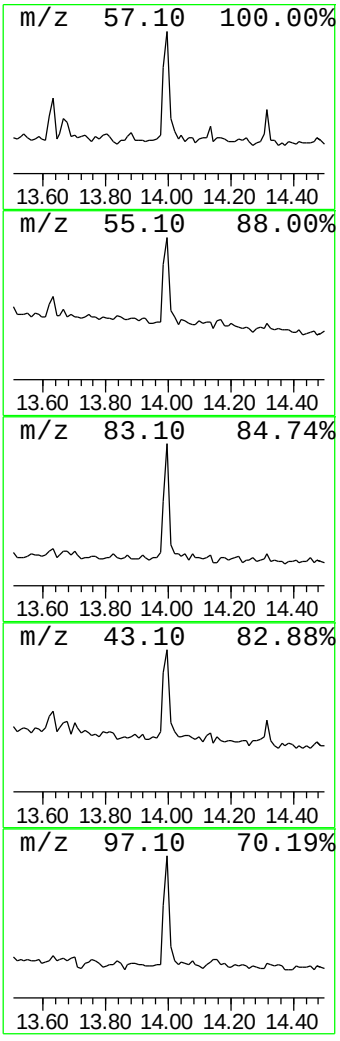
Peak Number 13 1-Docosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.00	3.71 ng	227681	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	91
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
5	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012517\
Data File : BF092501.D
Acq On : 26 Jan 2017 2:32
Operator : SJ/MA
Sample : I1312-09
Misc :
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.14	16.3	ng	791618	1	6.97	973269	20.0
unknown6.73	6.73	65.2	ng	3174810	1	6.97	973269	20.0
Heptanoic acid	7.38	37.1	ng	1804850	1	6.97	973269	20.0
2-Heptanol, 5-met...	8.62	10.4	ng	684532	2	8.26	1316170	20.0
Propanoic acid, 2...	9.54	9.0	ng	626393	3	10.02	1390360	20.0
unknown9.81	9.81	4.2	ng	289126	3	10.02	1390360	20.0
unknown9.93	9.93	2.4	ng	165918	3	10.02	1390360	20.0
Undecanoic acid	10.24	2.7	ng	190680	3	10.02	1390360	20.0
n-Hexadecanoic acid	12.04	6.4	ng	440610	4	11.50	1382140	20.0
Dodecanoic acid	12.83	3.1	ng	190644	5	14.15	1228610	20.0
9-Octadecenoic ac...	13.46	3.7	ng	226828	5	14.15	1228610	20.0
1-Docosene	14.00	3.7	ng	227681	5	14.15	1228610	20.0