LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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	2.250	21	23	32	rVB	46685	111915	1.65%	0.195%
2	4.810	244	247	257	rBV	532228	983723	14.54%	1.712%
3	5.061	266	269	271	rBV	94217	138700	2.05%	0.241%
4	5.256	284	286	291	rBV	3343469	3867272	57.17%	6.730%
5	5.336	291	293	295	rBV	2123021	2312290	34.18%	4.024%
6	5.713	325	326	327	rBV	104237	105036	1.55%	0.183%
7	5.759	327	330	342	rVB2	154823	393346	5.82%	0.685%
8	6.307	376	378	386	rBV2	1910162	2574602	38.06%	4.481%
9	6.421	386	388	391	rBV	4884328	5535359	81.83%	9.633%
10	6.650	406	408	411	rBV	1413802	1270844	18.79%	2.212%
11	6.810	419	422	424	rBV	4878385	4988827	73.75%	8.682%
12	6.947	432	434	440	rBV	309162	468290	6.92%	0.815%
13	7.039	440	442	444	rBV	172809	265452	3.92%	0.462%
14	7.096	446	447	454	rVB	56108	101937	1.51%	0.177%
15	7.222	455	458	461	rBV	3719624	4009349	59.27%	6.978%
16	7.359	468	470	473	rBV2	50691	80824	1.19%	0.141%
17	7.587	487	490	495	rBV3	31541	77569	1.15%	0.135%
18	7.747	503	504	512	rVB	129734	153934	2.28%	0.268%
19	7.942	517	521	523	rVV2	1413719	1850533	27.36%	3.221%
20	8.010	525	527	531	rVB2	99192	152408	2.25%	0.265%
21	8.204	537	544	548	rBV4	41228	140811	2.08%	0.245%
22	8.330	552	555	559	rBV2	55045	107840	1.59%	0.188%
23	8.605	576	579	582	rBV2	58006	80751	1.19%	0.141%
24	8.650	582	583	586	rVV	84062	97204	1.44%	0.169%
25	8.753	589	592	594	rVV2	109677	153293	2.27%	0.267%
26	9.016	612	615	618	rBV	5510622	6764160	100.00%	11.772%
27	9.107	621	623	629	rBV4	49323	109057	1.61%	0.190%
28	9.222	631	633	635	rBV	236844	221038	3.27%	0.385%
29	9.347	642	644	646	rBV	64815	86808	1.28%	0.151%
30	9.416	648	650	653	rVV	237572	281435	4.16%	0.490%
31	9.690	671	674	676	rBV	1430971	1835926	27.14%	3.195%
32	10.479	740	743	745	rBV	3257578	4351372	64.33%	7.573%
33	10.605	752	754	758	rBV	141621	211015	3.12%	0.367%
34	10.696	761	762	767	rVB3	44493	71027	1.05%	0.124%

LSC Area Percent Report

Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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	11.050	791	793	795	rBV2	69556	76991	1.14%	0.134%
36	11.165	800	803	805	rBV	1702955	1803591	26.66%	3.139%
37	11.713	849	851	857	rBV	631341	700084	10.35%	1.218%
38	12.399	909	911	916	rBV3	41417	95696	1.41%	0.167%
39	12.491	917	919	922	rBV2	302277	404485	5.98%	0.704%
40	12.754	939	942	944	rBV	5192964	6369593	94.17%	11.085%
41	13.119	972	974	980	rBV	256327	344179	5.09%	0.599%
42	13.668	1019	1022	1025	rBV	253357	308537	4.56%	0.537%
43	13.782	1030	1032	1035	rBV	1759996	1701510	25.15%	2.961%
44	15.154	1149	1152	1155	rBV	942092	1371412	20.27%	2.387%
45	15.634	1192	1194	1203	rVB10	30390	106597	1.58%	0.186%
46	16.000	1223	1226	1233	rVB4	51891	118187	1.75%	0.206%
47	16.605	1276	1279	1287	rVB3	35893	105323	1.56%	0.183%

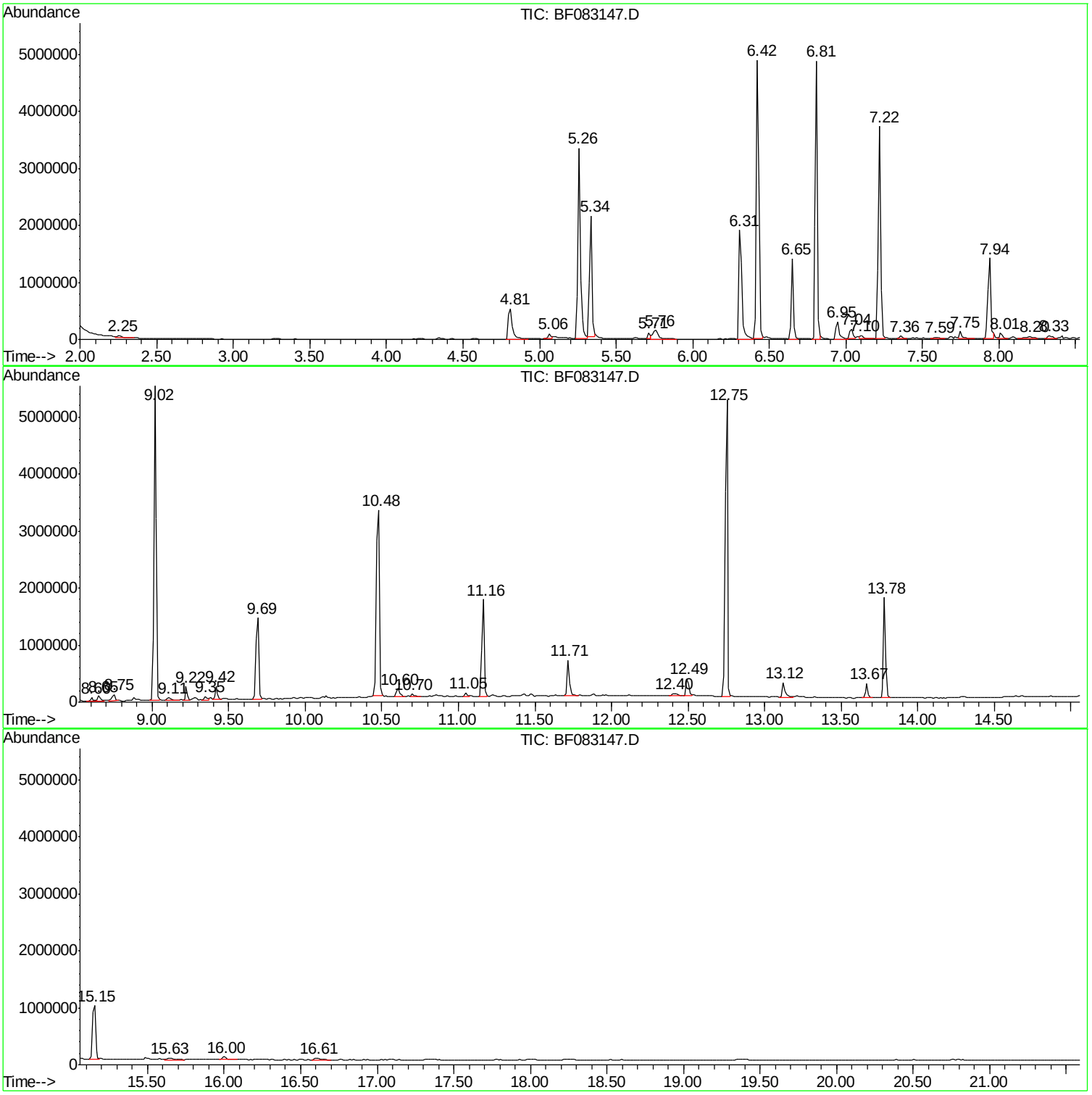
Sum of corrected areas: 57460132

Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-14A-111815

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



Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

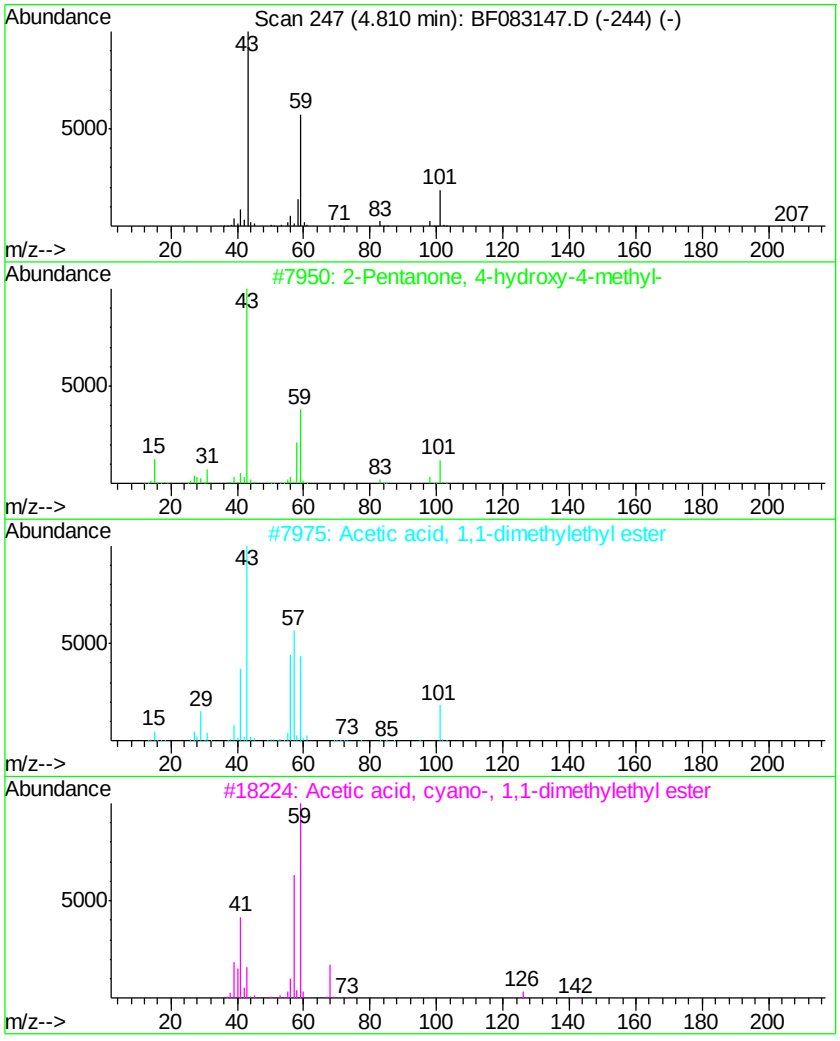
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

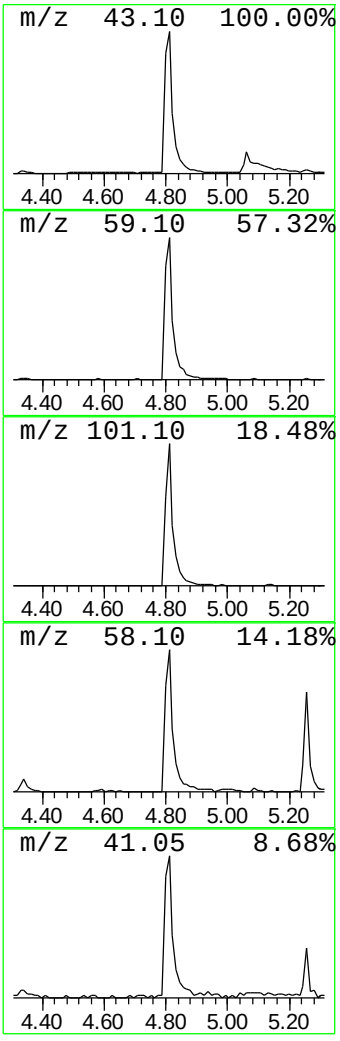
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	15.48 ng	983723	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	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

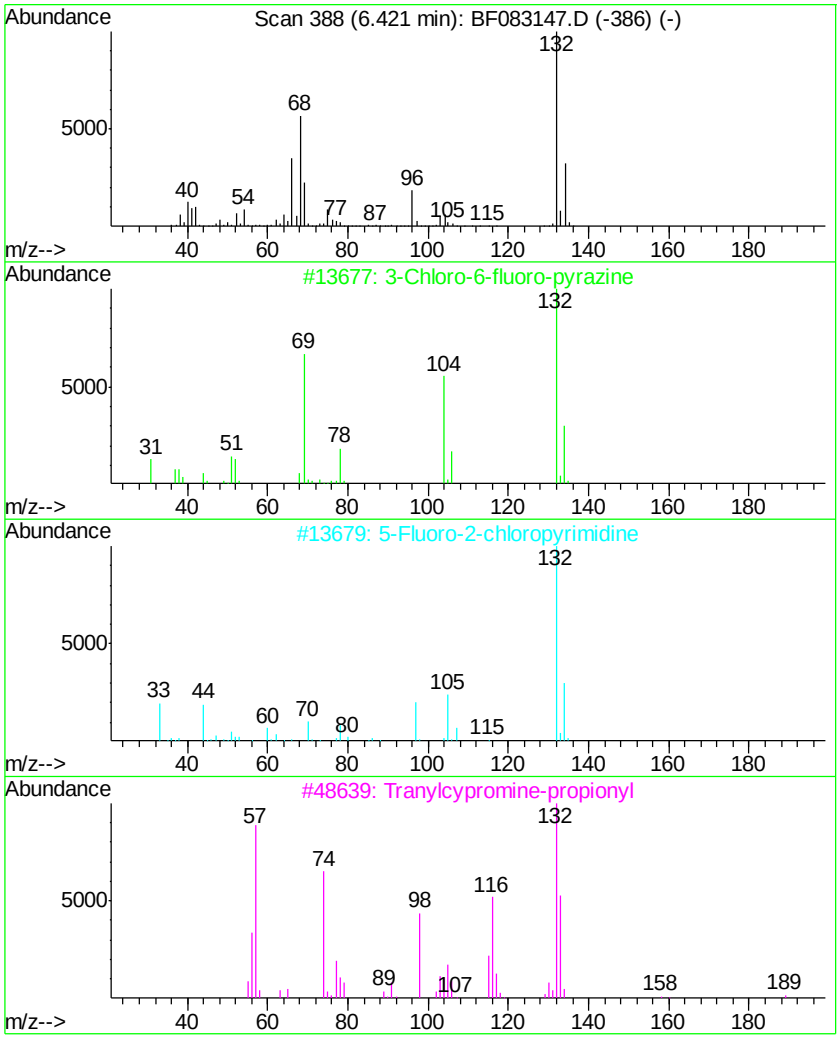
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

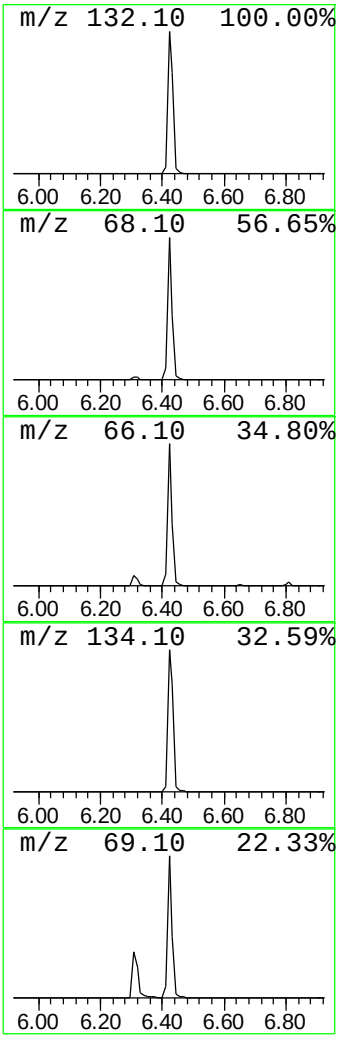
****

Peak Number 5 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	87.11 ng	5535360	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

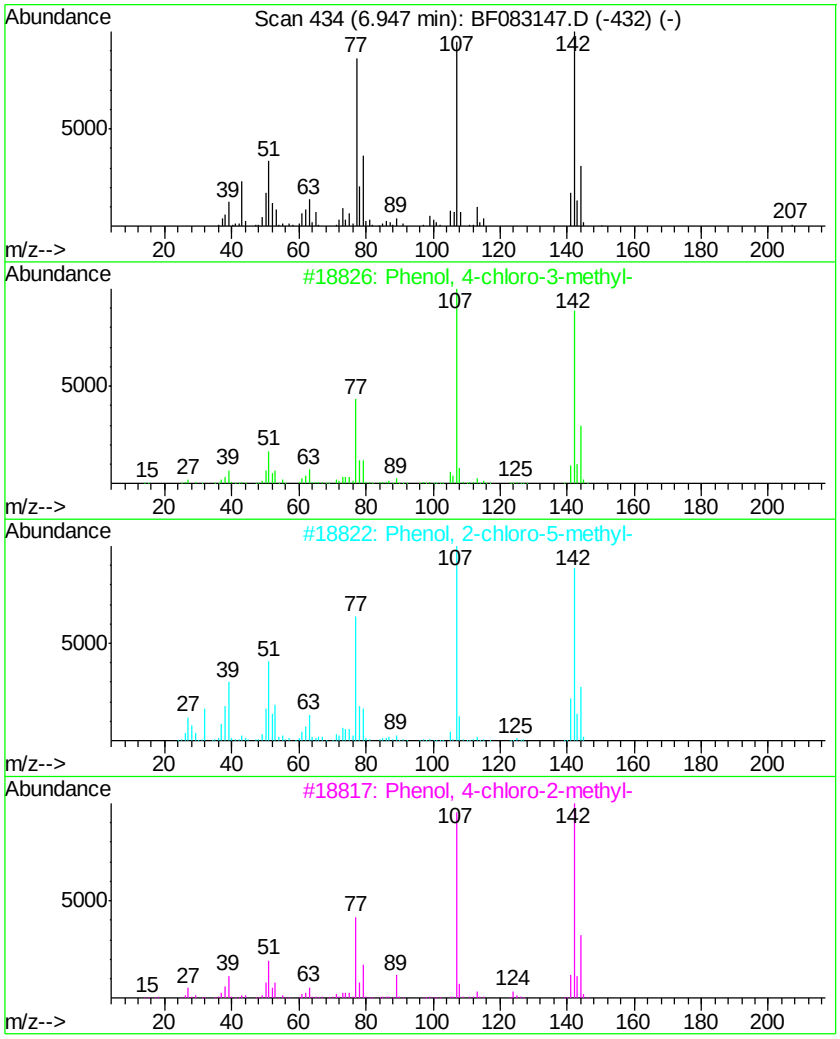
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

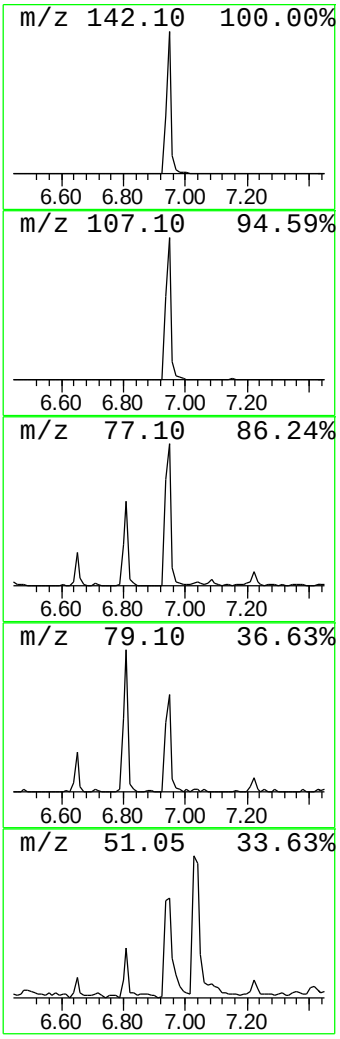
****

Peak Number 7 Phenol, 4-chloro-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.95	7.37 ng	468290	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-chloro-3-methyl-	142	C7H7ClO	000059-50-7	94
2	Phenol, 2-chloro-5-methyl-	142	C7H7ClO	000615-74-7	90
3	Phenol, 4-chloro-2-methyl-	142	C7H7ClO	001570-64-5	83
4	Phenol, 5-chloro-2-methyl-	142	C7H7ClO	005306-98-9	70
5	Phenol, 3-chloro-4-methyl-	142	C7H7ClO	000615-62-3	46





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

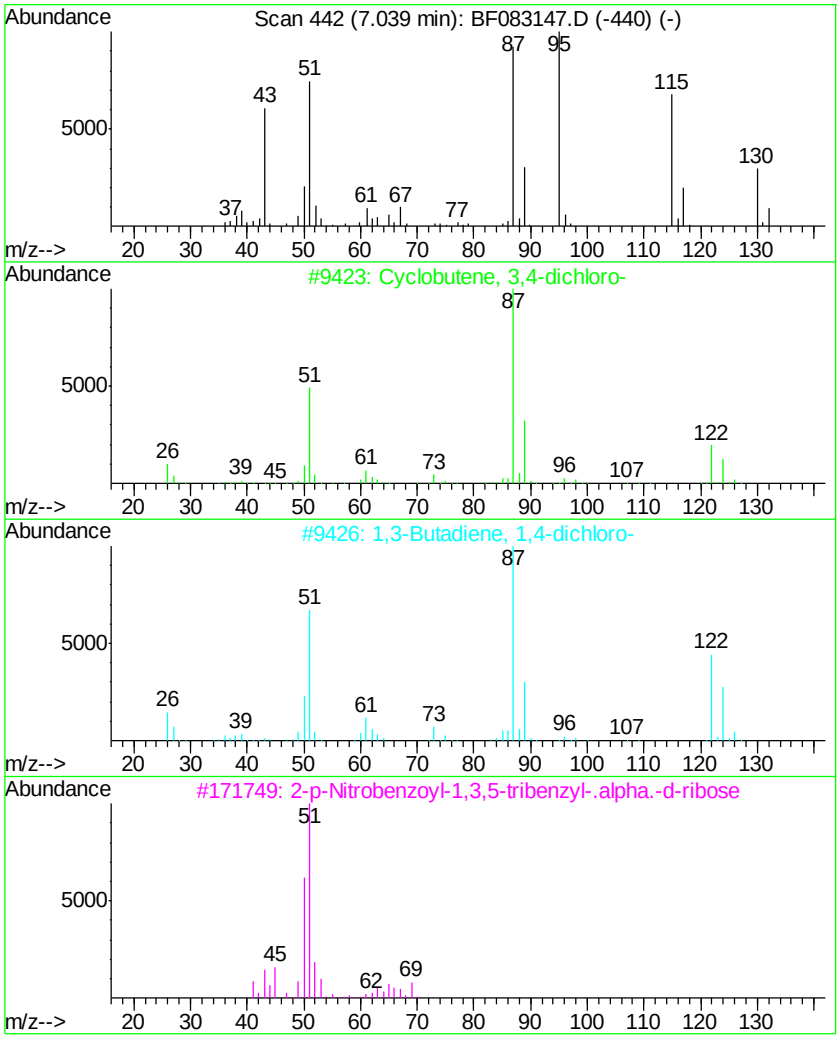
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

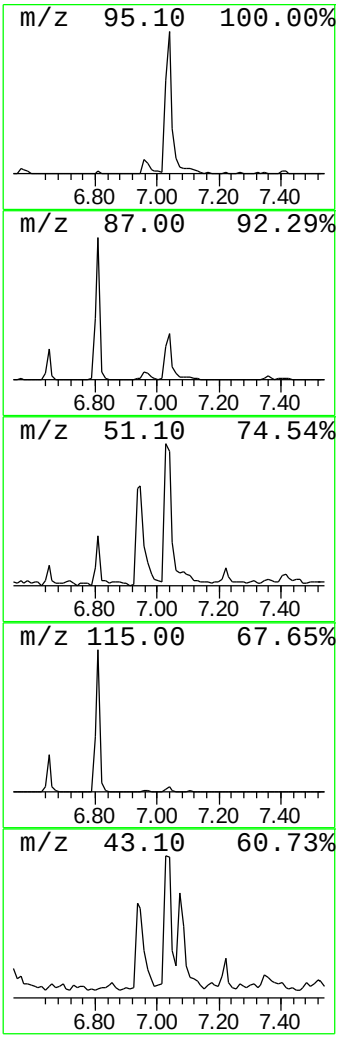
****

Peak Number 8 unknown7.04 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	4.18 ng	265452	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutene, 3,4-dichloro-	122	C4H4Cl2	041326-64-1	42
2	1,3-Butadiene, 1,4-dichloro-	122	C4H4Cl2	002984-42-1	36
3	2-p-Nitrobenzoyl-1,3,5-tribenzyl...	569	C33H31NO8	1000129-85-6	32
4	Difluorochloromethane	86	CHClF2	000075-45-6	32
5	Difluoroacetic acid	96	C2H2F2O2	000381-73-7	23





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

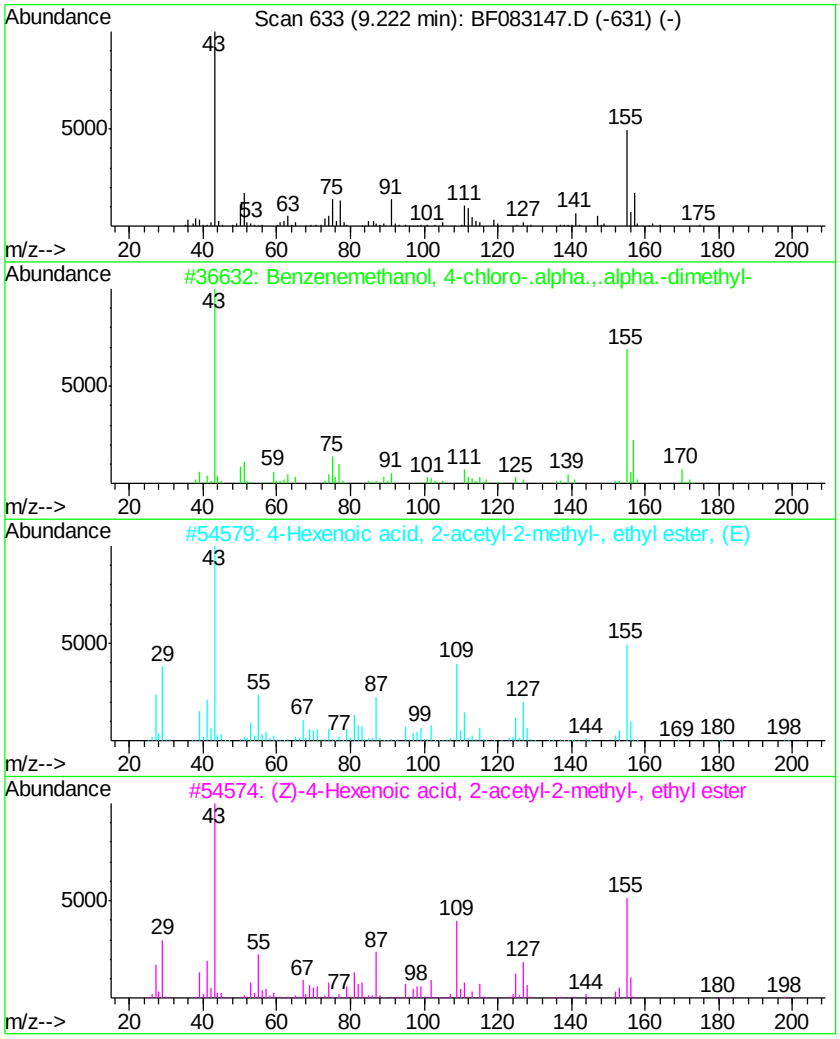
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

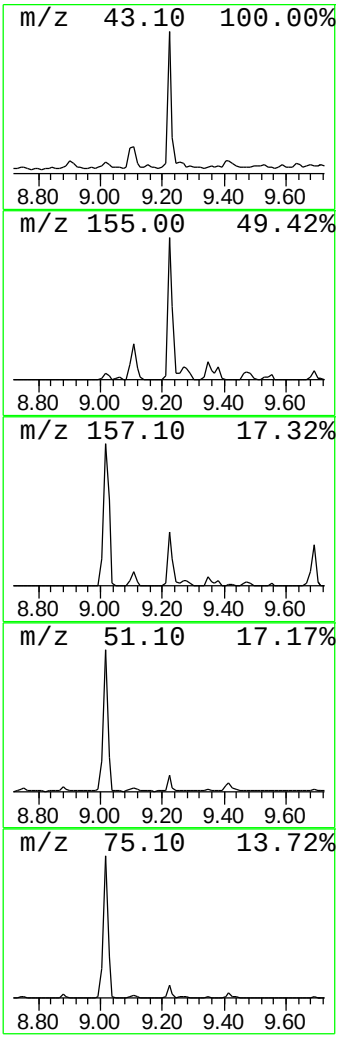
****

Peak Number 9 unknown9.22 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.22	2.41 ng	221038	Acenaphthene-d10	9.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, 4-chloro-.alpha...	170	C9H11ClO	001989-25-9	45
2	4-Hexenoic acid, 2-acetyl-2-meth...	198	C11H18O3	125163-78-2	9
3	(Z)-4-Hexenoic acid, 2-acetyl-2-...	198	C11H18O3	1000159-10-7	9
4	4a-Acetyl-hexahydrobenzo[1,3]dio...	198	C10H14O4	1000192-32-0	9
5	Hexanedioic acid, diethyl ester	202	C10H18O4	000141-28-6	4





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

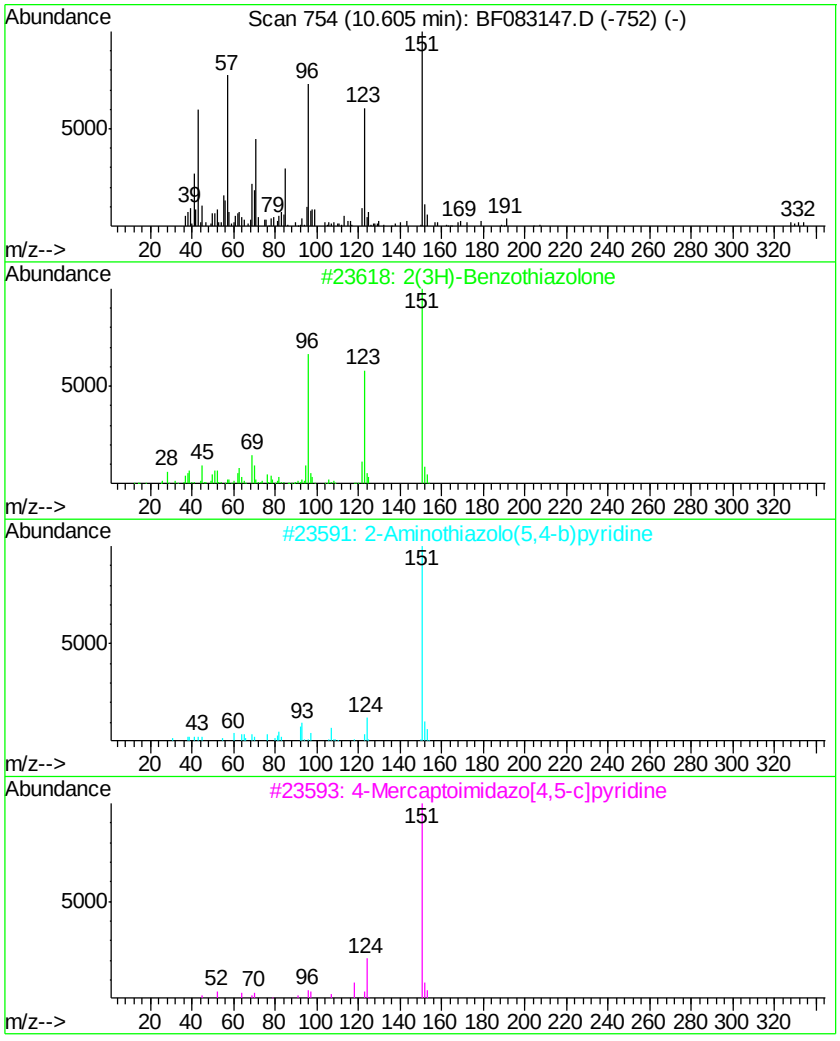
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

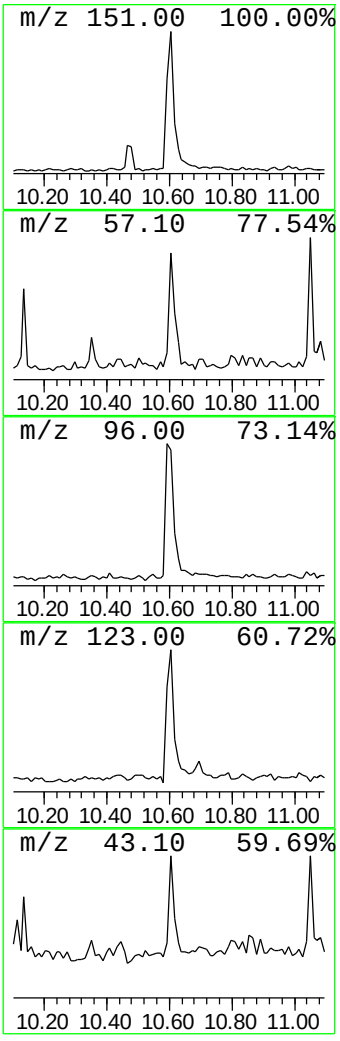
****

Peak Number 10 2(3H)-Benzothiazolone Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.34 ng	211015	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	86
2	2-Aminothiazolo(5,4-b)pyridine	151	C6H5N3S	031784-70-0	18
3	4-Mercaptoimidazo[4,5-c]pyridine	151	C6H5N3S	034550-51-1	14
4	Decane, 1-bromo-2-methyl-	234	C11H23Br	127839-47-8	14
5	Octacosane	394	C28H58	000630-02-4	11





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

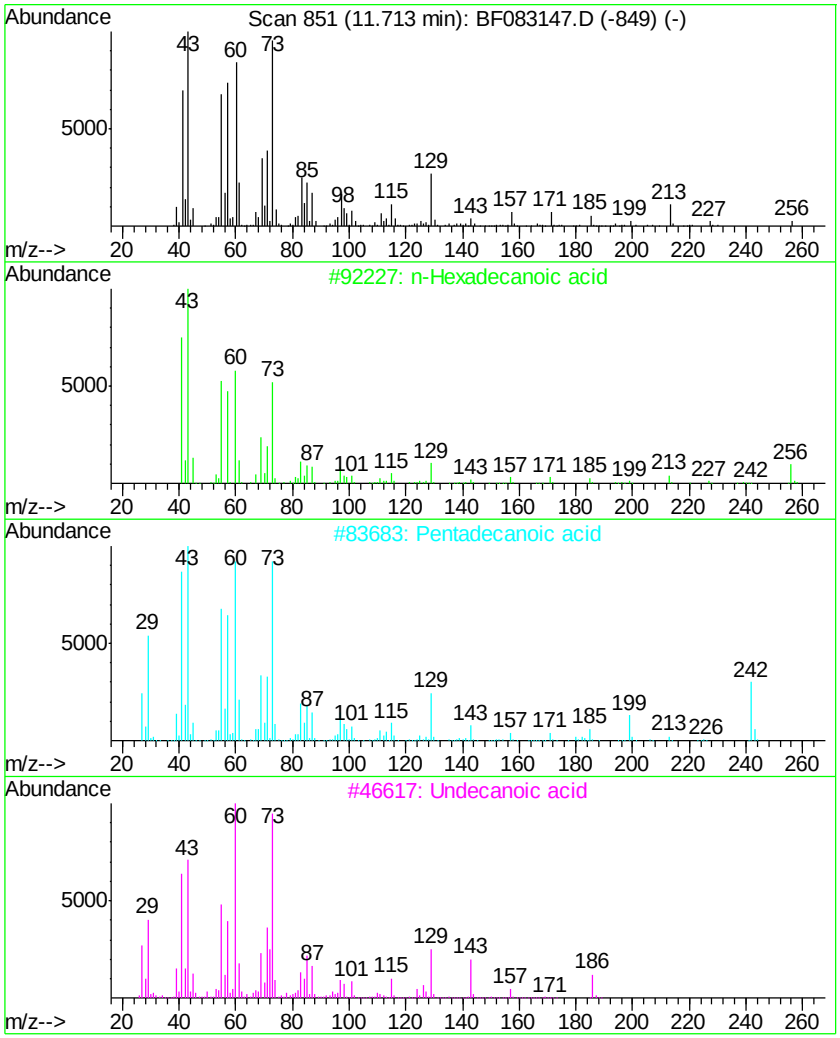
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

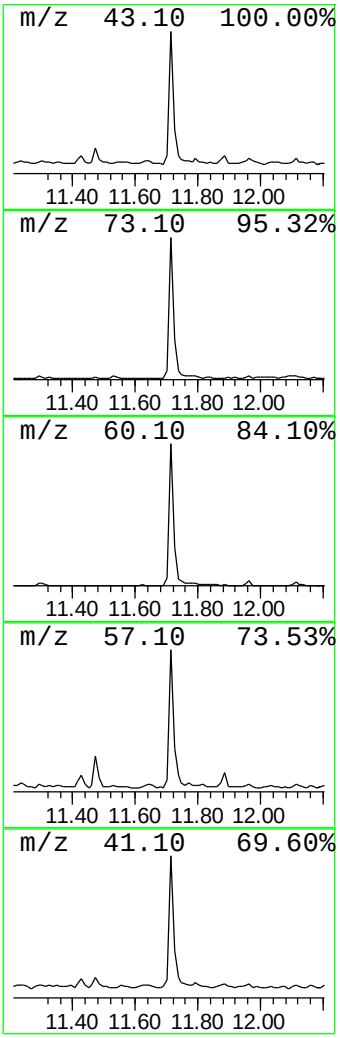
****

Peak Number 11 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	7.76 ng	700084	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Undecanoic acid	186	C11H22O2	000112-37-8	86
4	Undecane	156	C11H24	001120-21-4	43
5	Silane, trichlorodocosyl-	442	C22H45Cl3Si	007325-84-0	18





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

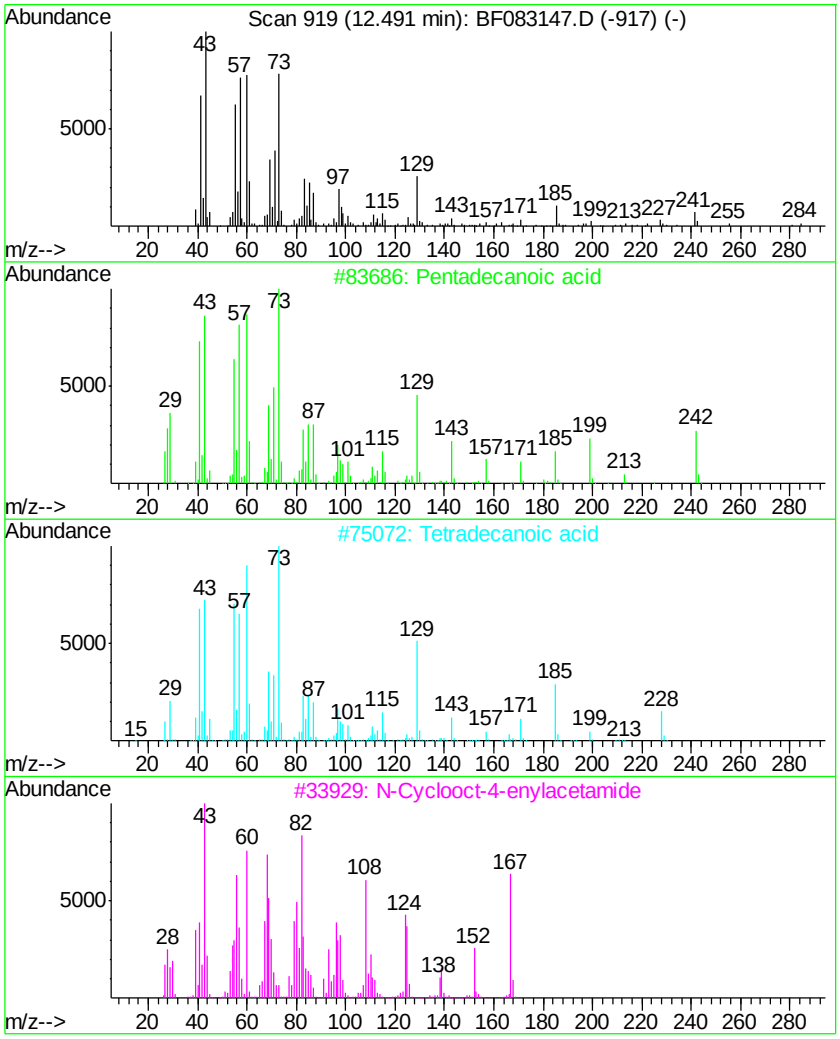
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

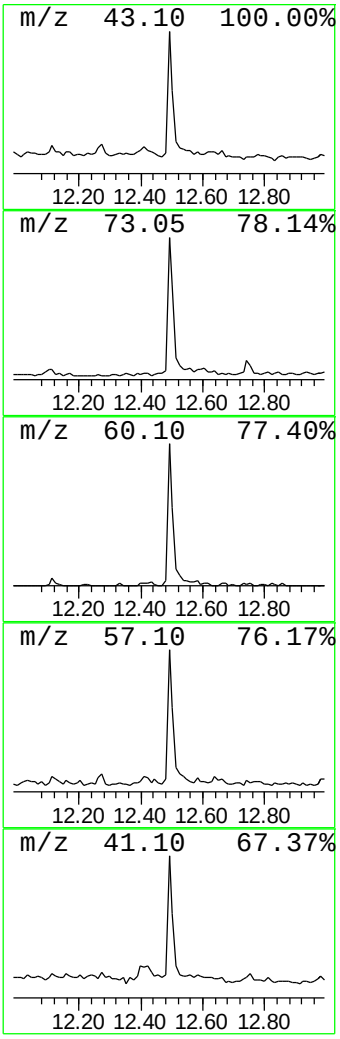
****

Peak Number 12 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	4.75 ng	404485	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	30
4	Amyl Nitrite	117	C5H11NO2	000110-46-3	27
5	Undecane	156	C11H24	001120-21-4	18





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

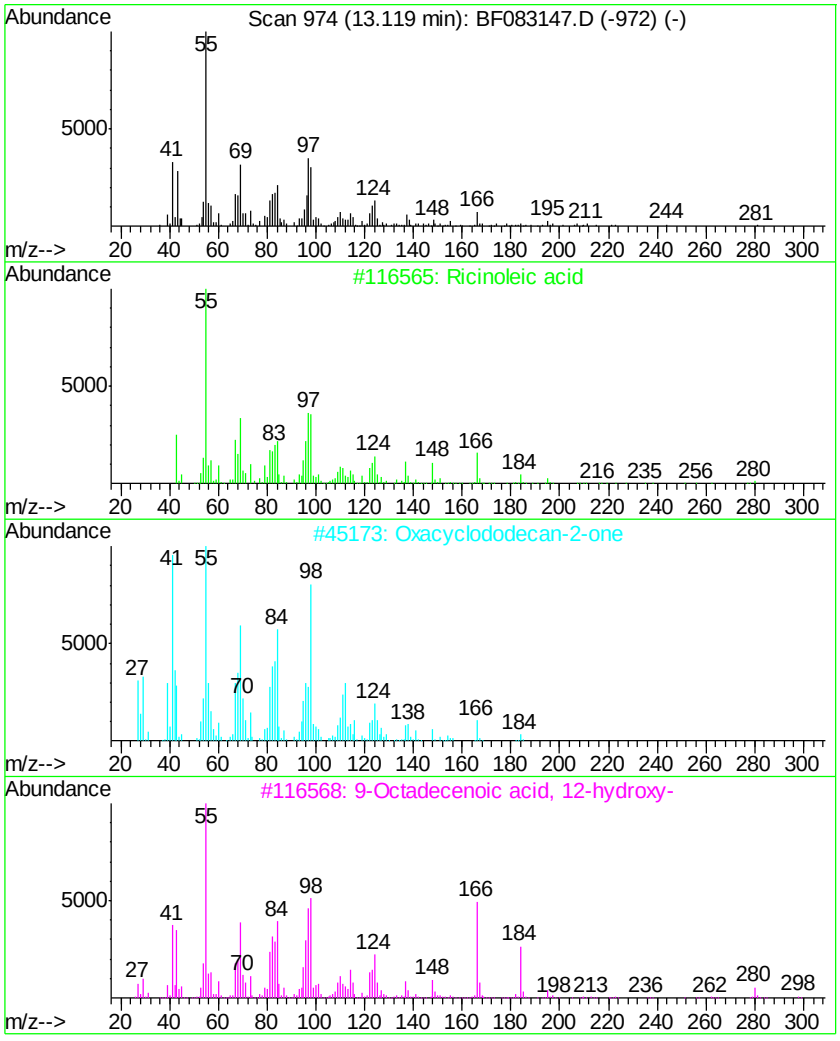
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

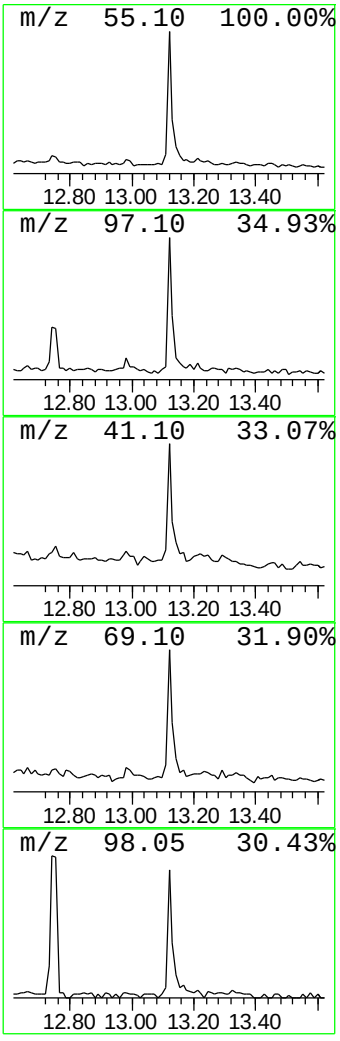
****

Peak Number 13 Ricinoleic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	4.05 ng	344179	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ricinoleic acid	298	C18H34O3	000141-22-0	91
2	Oxacyclododecan-2-one	184	C11H20O2	001725-03-7	89
3	9-Octadecenoic acid, 12-hydroxy-	298	C18H34O3	007431-95-0	72
4	Chloromethyl 5-chloroundecanoate	268	C12H22Cl2O2	080418-91-3	38
5	1,6-Octadiene, 5,7-dimethyl-, (R)-	138	C10H18	085006-04-8	30





Data Path : V:\HPCHEM1\BNA F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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

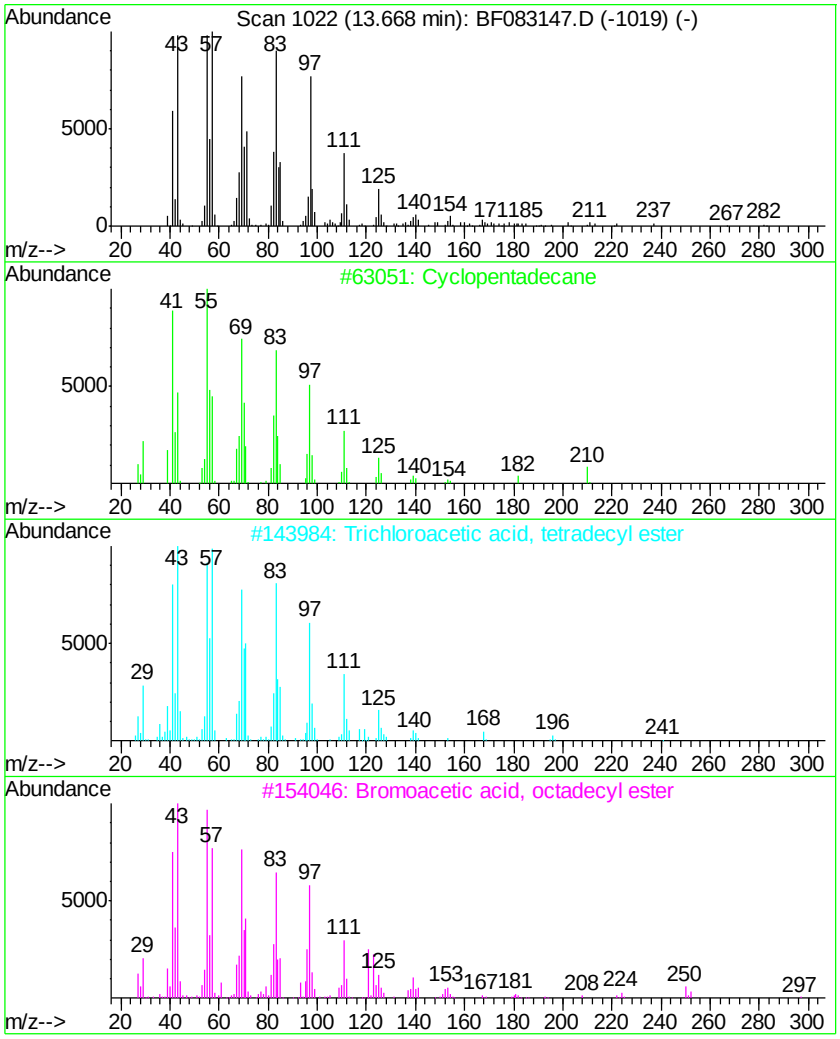
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

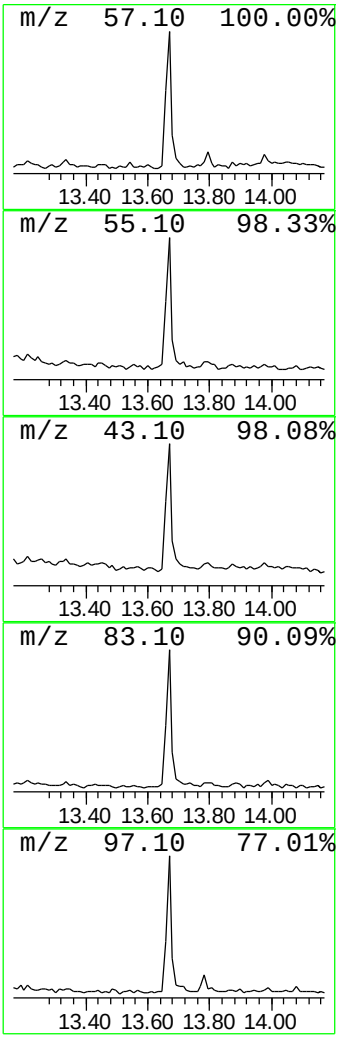
****

Peak Number 14 Cyclopentadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	3.63 ng	308537	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	93
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
4	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
5	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91





Tentatively Identified Compound (LSC) summary

Data Path : V:\HPCHEM1\BNA_F\DATA\BF112115\
Data File : BF083147.D
Acq On : 22 Nov 2015 9:26
Operator : UM/IZ
Sample : G4510-07
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-14A-111815

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...	4.81	15.5	ng	983723	1	6.65	1270840	20.0
unknown6.42	6.42	87.1	ng	5535360	1	6.65	1270840	20.0
Phenol, 4-chloro-...	6.95	7.4	ng	468290	1	6.65	1270840	20.0
unknown7.04	7.04	4.2	ng	265452	1	6.65	1270840	20.0
unknown9.22	9.22	2.4	ng	221038	3	9.69	1835930	20.0
2(3H)-Benzothiazo...	10.60	2.3	ng	211015	4	11.16	1803590	20.0
n-Hexadecanoic acid	11.71	7.8	ng	700084	4	11.16	1803590	20.0
Pentadecanoic acid	12.49	4.8	ng	404485	5	13.78	1701510	20.0
Ricinoleic acid	13.12	4.0	ng	344179	5	13.78	1701510	20.0
Cyclopentadecane	13.67	3.6	ng	308537	5	13.78	1701510	20.0