LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083152.D
Acq On : 22 Nov 2015 11:52
Operator : UM/IZ
Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

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	37	rVB	50908	156886	2.36%	0.260%
2	4.330	203	205	212	rVB2	43558	78790	1.19%	0.131%
3	4.798	244	246	257	rBV	553531	871441	13.11%	1.445%
4	5.061	267	269	274	rBV	56052	102741	1.55%	0.170%
5	5.256	284	286	291	rBV	2800673	3646735	54.87%	6.046%
6	5.336	291	293	295	rBV	1536200	2154472	32.41%	3.572%
7	5.736	325	328	342	rVB2	266173	638838	9.61%	1.059%
8	6.307	376	378	386	rBV	2073939	2471906	37.19%	4.098%
9	6.422	386	388	391	rVV	5268334	5348767	80.47%	8.868%
10	6.479	391	393	399	rVB5	31229	68698	1.03%	0.114%
11	6.650	406	408	410	rBV	1294973	1210467	18.21%	2.007%
12	6.810	419	422	424	rBV	4409509	4834045	72.73%	8.014%
13	6.936	431	433	440	rBV	1005659	1413317	21.26%	2.343%
14	7.027	440	441	444	rBV	535098	567388	8.54%	0.941%
15	7.096	446	447	454	rVB	136079	191899	2.89%	0.318%
16	7.222	455	458	461	rBV	3828742	4013971	60.39%	6.655%
17	7.359	467	470	473	rBV3	61285	100000	1.50%	0.166%
18	7.576	487	489	495	rBV2	120343	170021	2.56%	0.282%
19	7.679	496	498	500	rVV2	49645	69768	1.05%	0.116%
20	7.747	502	504	512	rVB	320248	341100	5.13%	0.566%
21	7.942	517	521	523	rVV2	1401208	1951824	29.37%	3.236%
22	8.010	525	527	531	rVB	106263	149276	2.25%	0.247%
23	8.193	541	543	547	rVB	168949	215703	3.25%	0.358%
24	8.342	552	556	560	rBV	113651	191117	2.88%	0.317%
25	8.410	560	562	563	rVV	139546	160808	2.42%	0.267%
26	8.605	577	579	582	rBV2	64141	137105	2.06%	0.227%
27	8.650	582	583	585	rVV	98911	107731	1.62%	0.179%
28	8.753	589	592	594	rVV2	120519	180839	2.72%	0.300%
29	8.879	601	603	604	rBV	76090	71346	1.07%	0.118%
30	9.016	612	615	618	rBV	5589144	6646672	100.00%	11.019%
31	9.096	620	622	626	rBV	236217	329295	4.95%	0.546%
32	9.222	631	633	635	rVV	1228777	1103992	16.61%	1.830%
33	9.256	635	636	641	rVV2	86108	152265	2.29%	0.252%
34	9.348	642	644	645	rVV	73801	84259	1.27%	0.140%

LSC Area Percent Report

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Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

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	9.416	646	650	653	rVV2	200685	381752	5.74%	0.633%
36	9.462	653	654	658	rVV2	39530	80533	1.21%	0.134%
37	9.690	671	674	676	rBV	1282401	1845348	27.76%	3.059%
38	10.479	740	743	745	rBV	2919814	4325838	65.08%	7.172%
39	10.605	752	754	758	rBV	137301	203721	3.07%	0.338%
40	10.696	761	762	767	rVB4	56889	72215	1.09%	0.120%
41	11.165	800	803	805	rBV	1476421	1737760	26.14%	2.881%
42	11.428	824	826	828	rVB	140673	195013	2.93%	0.323%
43	11.713	849	851	855	rBV	687035	725865	10.92%	1.203%
44	11.965	871	873	876	rVB	63407	72440	1.09%	0.120%
45	12.239	895	897	899	rBV	94080	121749	1.83%	0.202%
46	12.411	909	912	915	rBV3	53917	124101	1.87%	0.206%
47	12.491	917	919	922	rBV	357399	482739	7.26%	0.800%
48	12.754	939	942	944	rBV	5112621	6393977	96.20%	10.600%
49	13.119	972	974	980	rBV	314335	405286	6.10%	0.672%
50	13.668	1020	1022	1030	rVB	224054	282395	4.25%	0.468%
51	13.782	1030	1032	1035	rBV	1683031	1643973	24.73%	2.726%
52	15.142	1149	1151	1155	rBV	790359	1217403	18.32%	2.018%
53	16.605	1276	1279	1286	rVB9	20088	72147	1.09%	0.120%

Sum of corrected areas: 60317737

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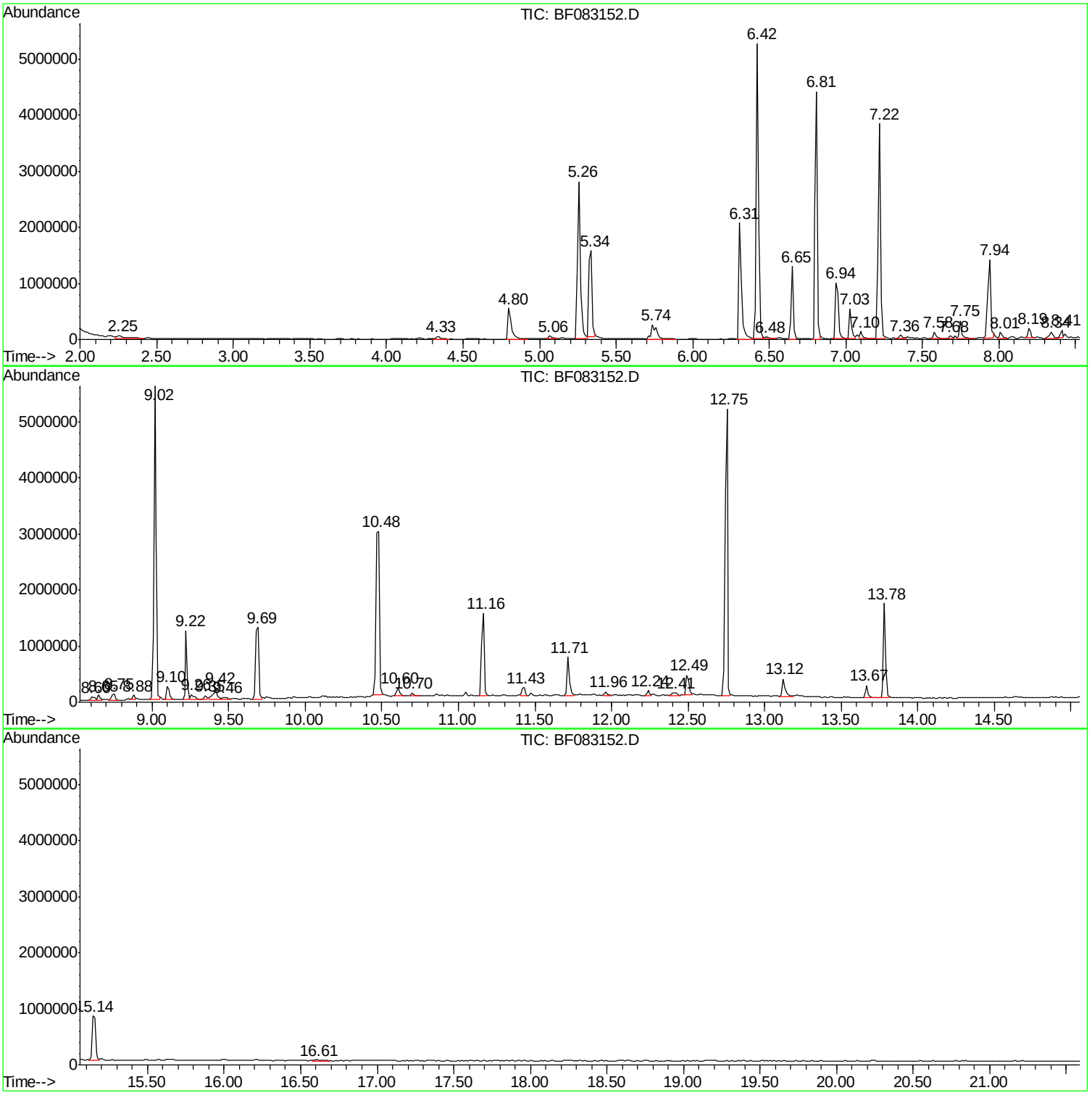
Instrument :
BNA_F
ClientSampleId :
DUP-111815-2

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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Data File : BF083152.D
Acq On : 22 Nov 2015 11:52
Operator : UM/IZ
Sample : G4510-11
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ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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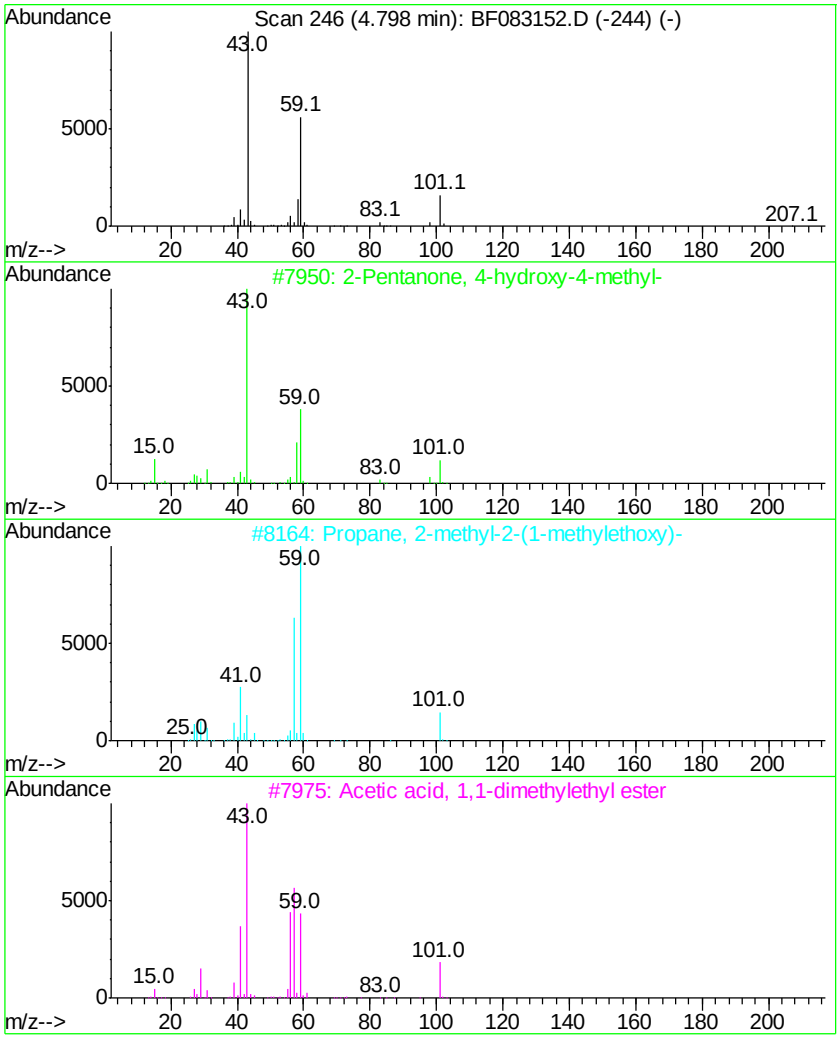
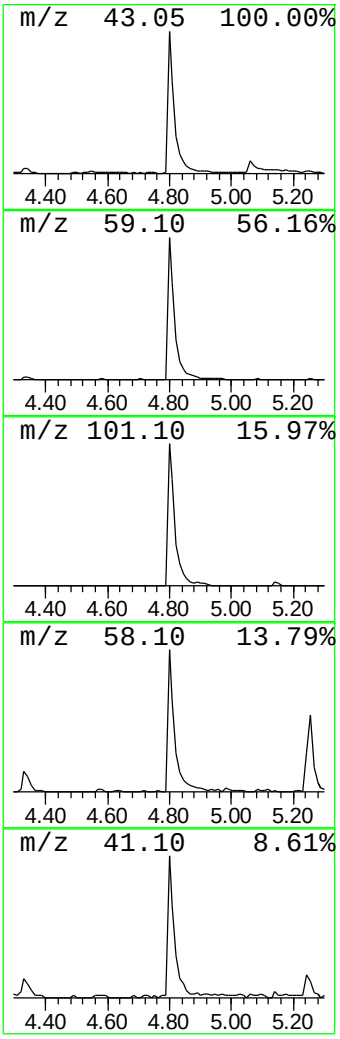
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	14.40 ng	871441	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	42
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083152.D
Acq On : 22 Nov 2015 11:52
Operator : UM/IZ
Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

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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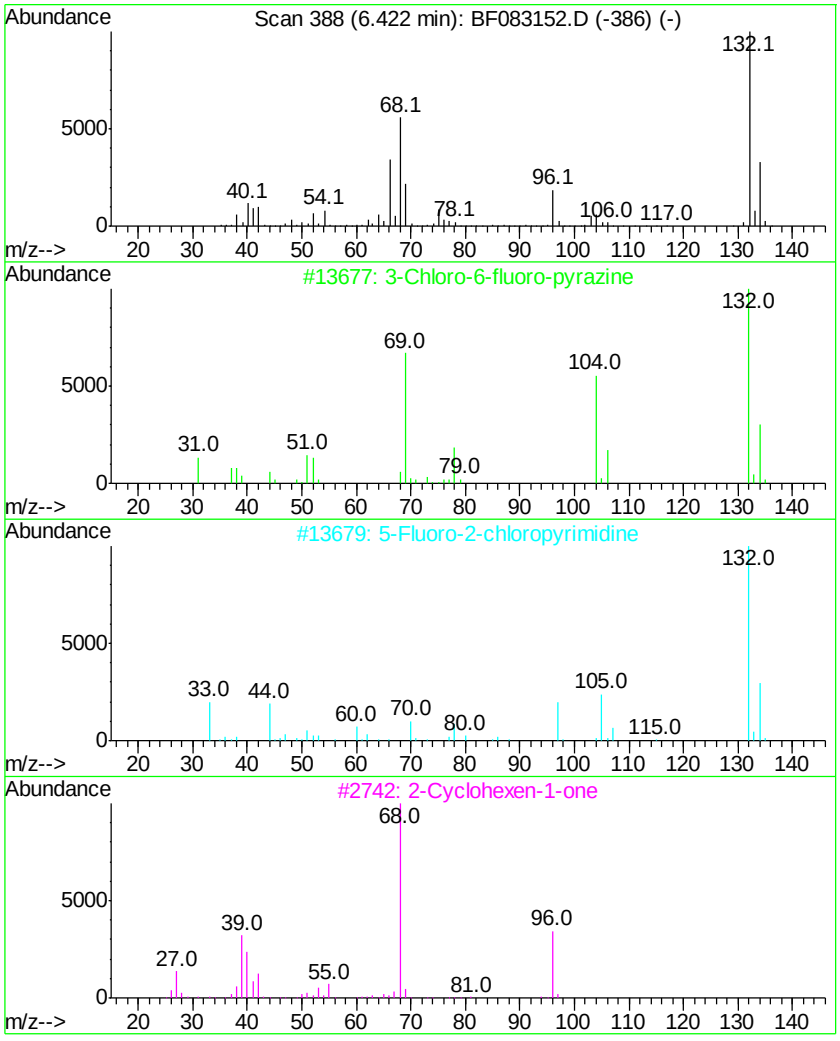
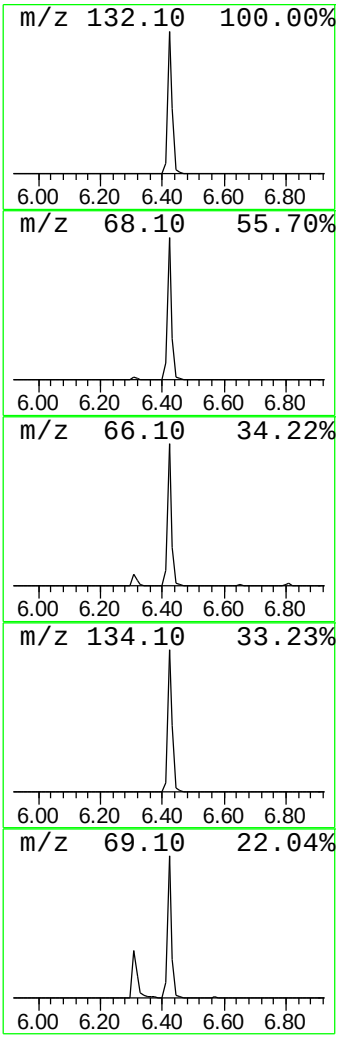
Peak Number 5 unknown6.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	88.38 ng	5348770	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	16
3	2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Aminoindole	132	C8H8N2	005192-03-0	10





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Operator : UM/IZ
Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

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

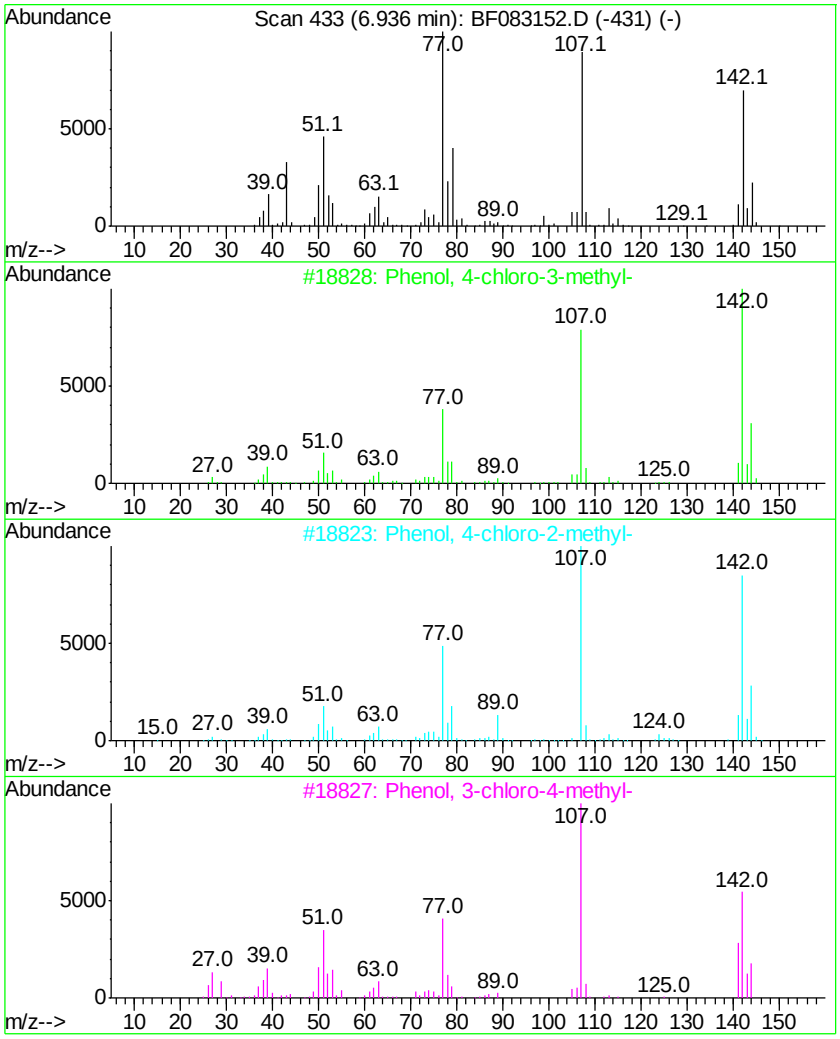
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

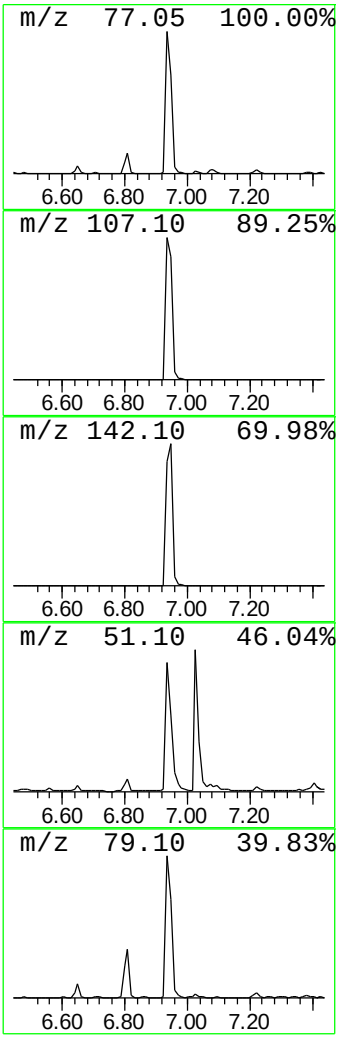
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	23.35 ng	1413320	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, 4-chloro-2-methyl-	142	C7H7ClO	001570-64-5	93
3	Phenol, 3-chloro-4-methyl-	142	C7H7ClO	000615-62-3	58
4	Phenol, 2-chloro-5-methyl-	142	C7H7ClO	000615-74-7	58
5	Phenol, 2-chloro-6-methyl-	142	C7H7ClO	000087-64-9	50





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Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

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

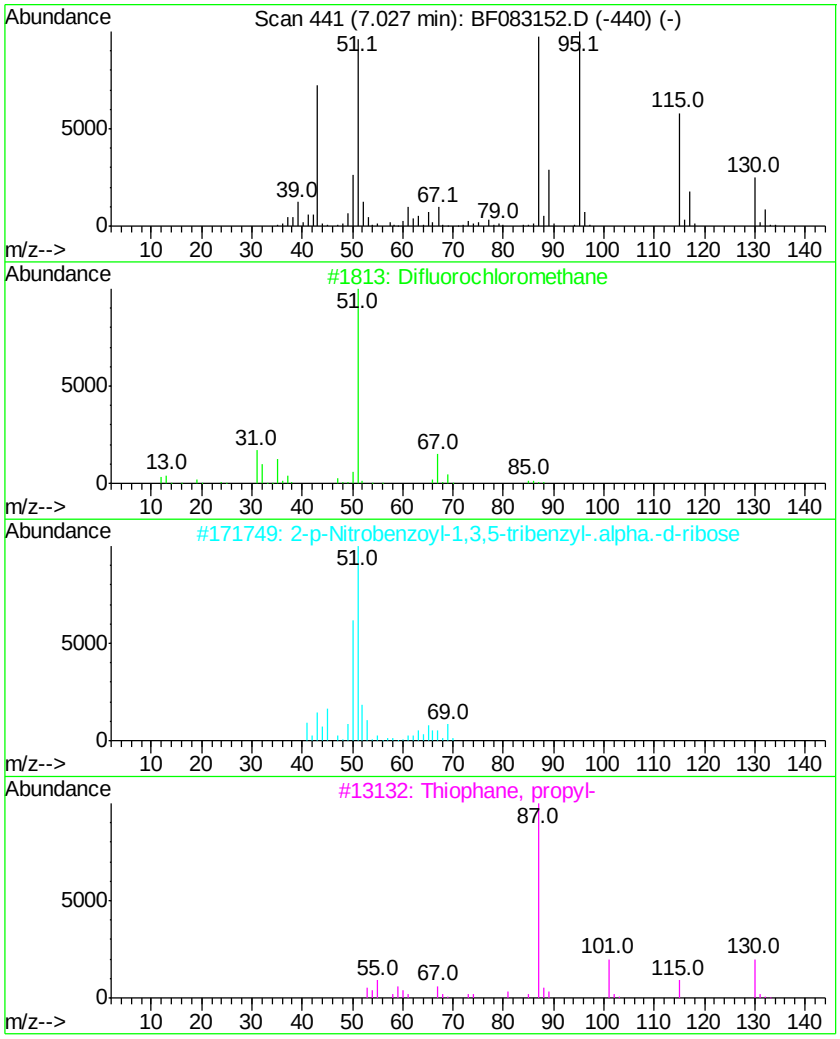
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

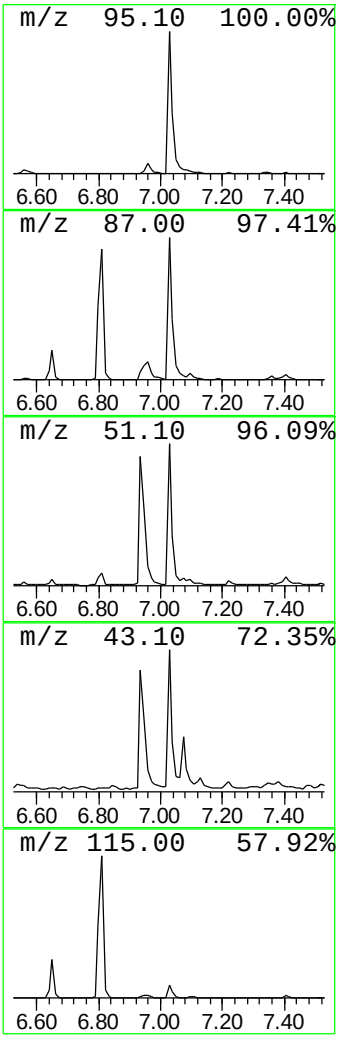
****

Peak Number 8 unknown7.03 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	9.37 ng	567388	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Difluorochloromethane	86	CHClF2	000075-45-6	23
2	2-p-Nitrobenzoyl-1,3,5-tribenzyl...	569	C33H31NO8	1000129-85-6	23
3	Thiophane, propyl-	130	C7H14S	001551-34-4	16
4	2-Butyne, 1,4-dichloro-	122	C4H4Cl2	000821-10-3	9
5	Cyclobutene, 3,4-dichloro-	122	C4H4Cl2	041326-64-1	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : DUP-111815-2

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

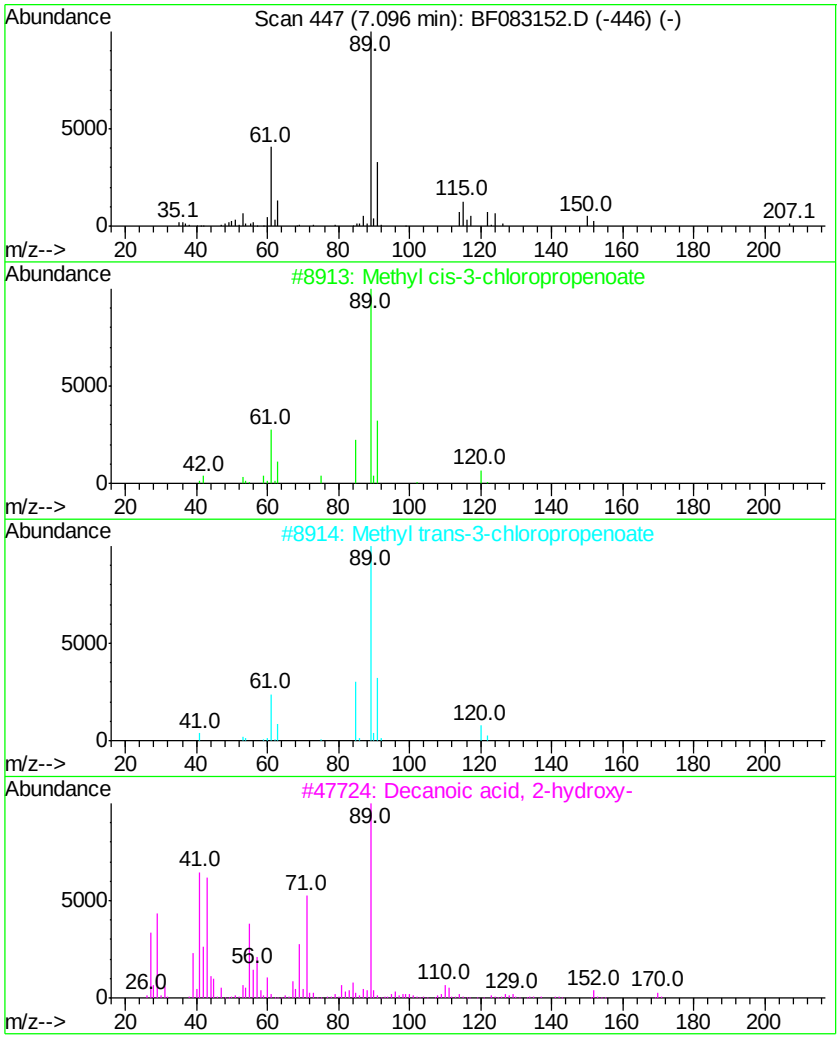
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

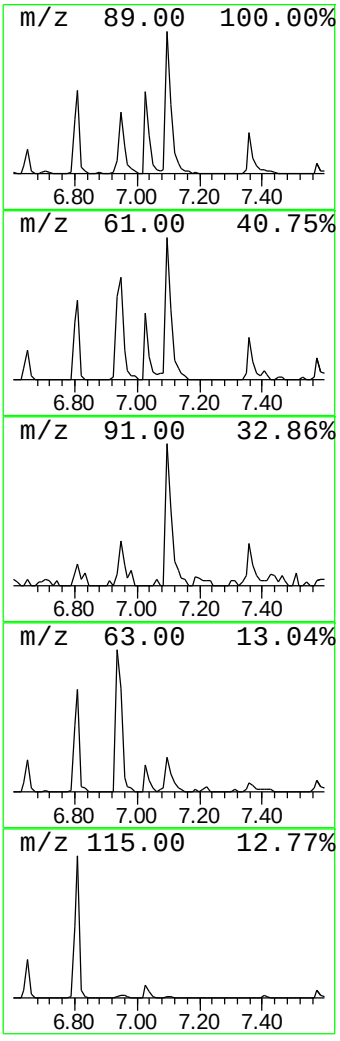
****

Peak Number 9 Methyl cis-3-chloropropenoate Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.10	3.17 ng	191899	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl cis-3-chloropropenoate	120	C4H5ClO2	1000144-78-7	64
2	Methyl trans-3-chloropropenoate	120	C4H5ClO2	1000144-78-8	9
3	Decanoic acid, 2-hydroxy-	188	C10H20O3	005393-81-7	9
4	Propane, 1,2-bis(ethylthio)-	164	C7H16S2	054410-62-7	9
5	Benzenepropanol, .gamma.-[(2-met...	254	C14H22O4	097991-46-3	9





Library Search Compound Report

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

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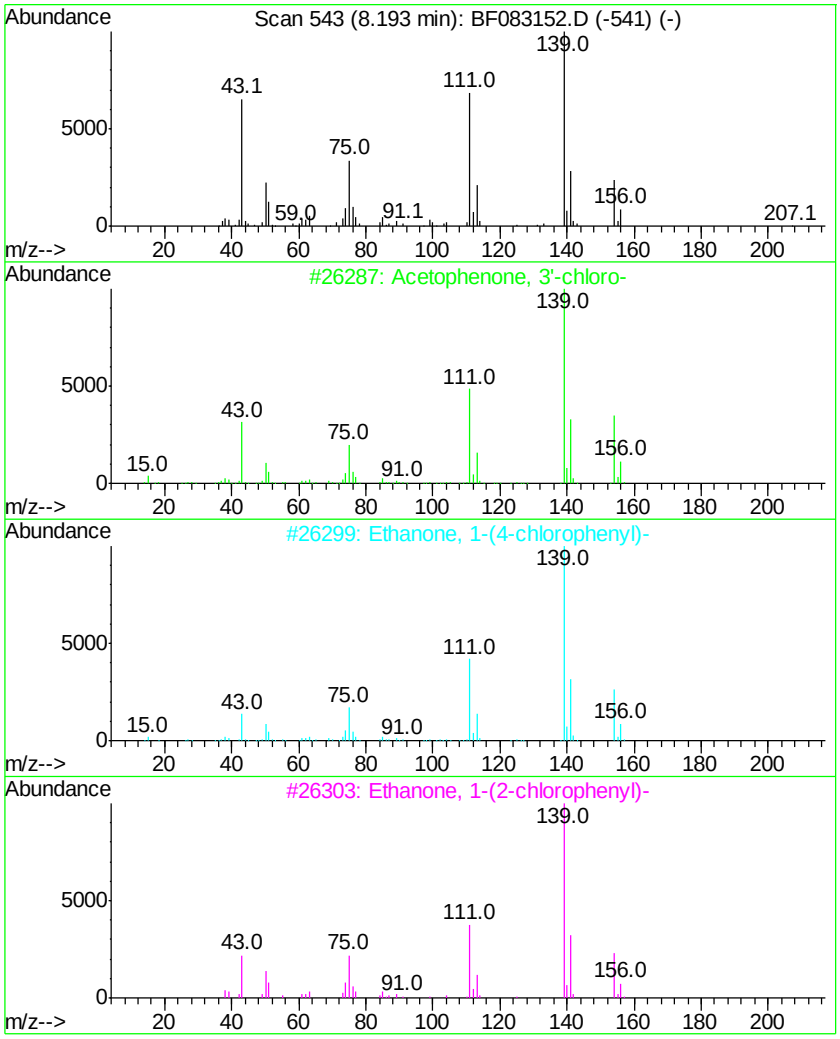
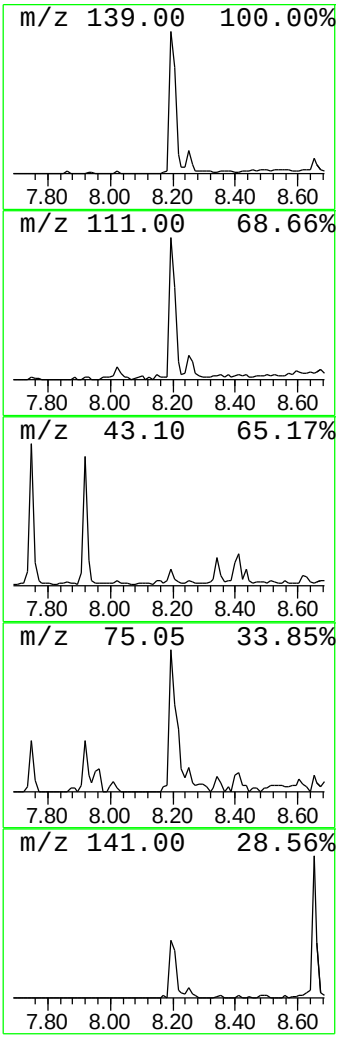
Peak Number 11 Acetophenone, 3'-chloro- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.19	2.21 ng	215703	Naphthalene-d8	7.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetophenone, 3'-chloro-	154	C8H7ClO	000099-02-5	97
2	Ethanone, 1-(4-chlorophenyl)-	154	C8H7ClO	000099-91-2	96
3	Ethanone, 1-(2-chlorophenyl)-	154	C8H7ClO	002142-68-9	81
4	3-Chloroperbenzoic acid	172	C7H5ClO3	000937-14-4	72
5	N-(6-Aminosulfonyl-2-benzothiazo...	367	C14H10ClN3O3S2	313275-69-3	72





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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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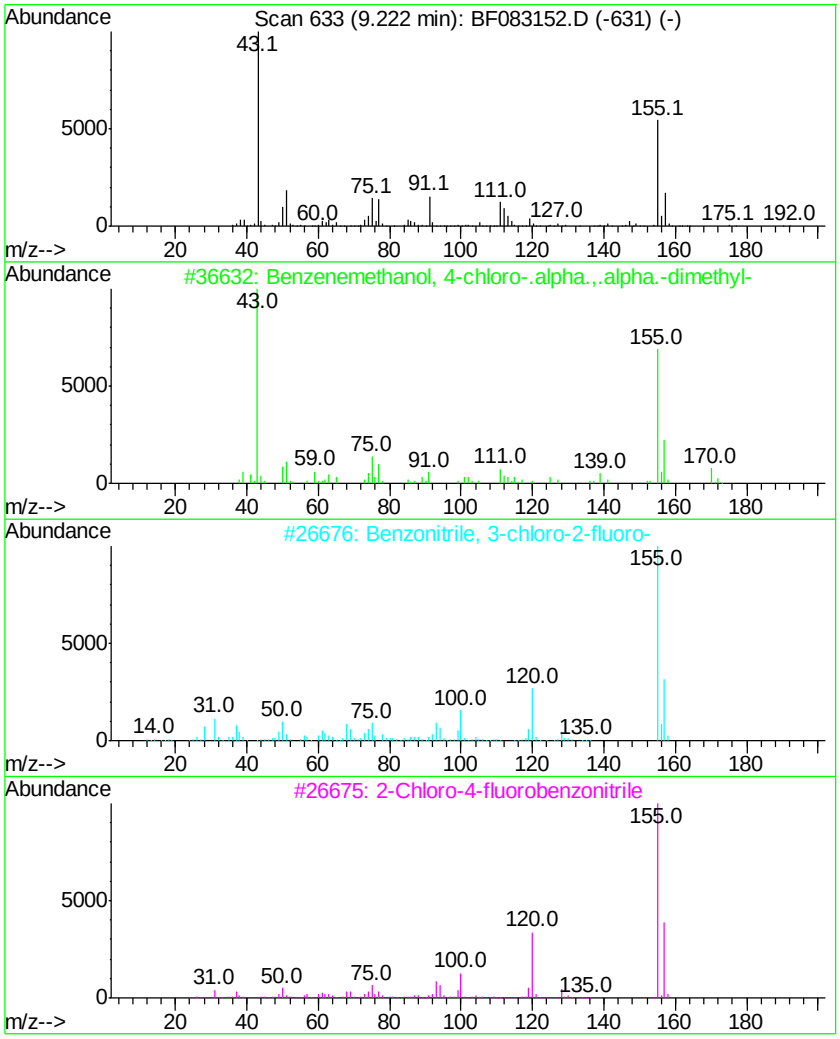
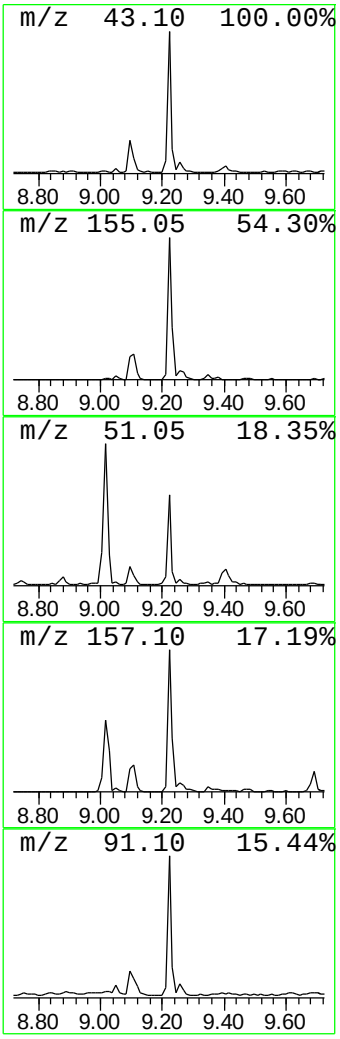
Peak Number 13 Benzenemethanol, 4-chloro-.... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.22	11.97 ng	1103990	Acenaphthene-d10	9.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, 4-chloro-.alpha...	170	C9H11ClO	001989-25-9	50
2	Benzonitrile, 3-chloro-2-fluoro-	155	C7H3ClFN	094087-40-8	43
3	2-Chloro-4-fluorobenzonitrile	155	C7H3ClFN	060702-69-4	38
4	Propane, 1-(3,3,3-trifluoro-1,2-...	256	C5H8ClF3S3	1000226-87-2	38
5	2-Chloro-6-fluorobenzonitrile	155	C7H3ClFN	000668-45-1	38





Library Search Compound Report

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Data File : BF083152.D
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Operator : UM/IZ
Sample : G4510-11
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Instrument : BNA_F
ClientSampleId : DUP-111815-2

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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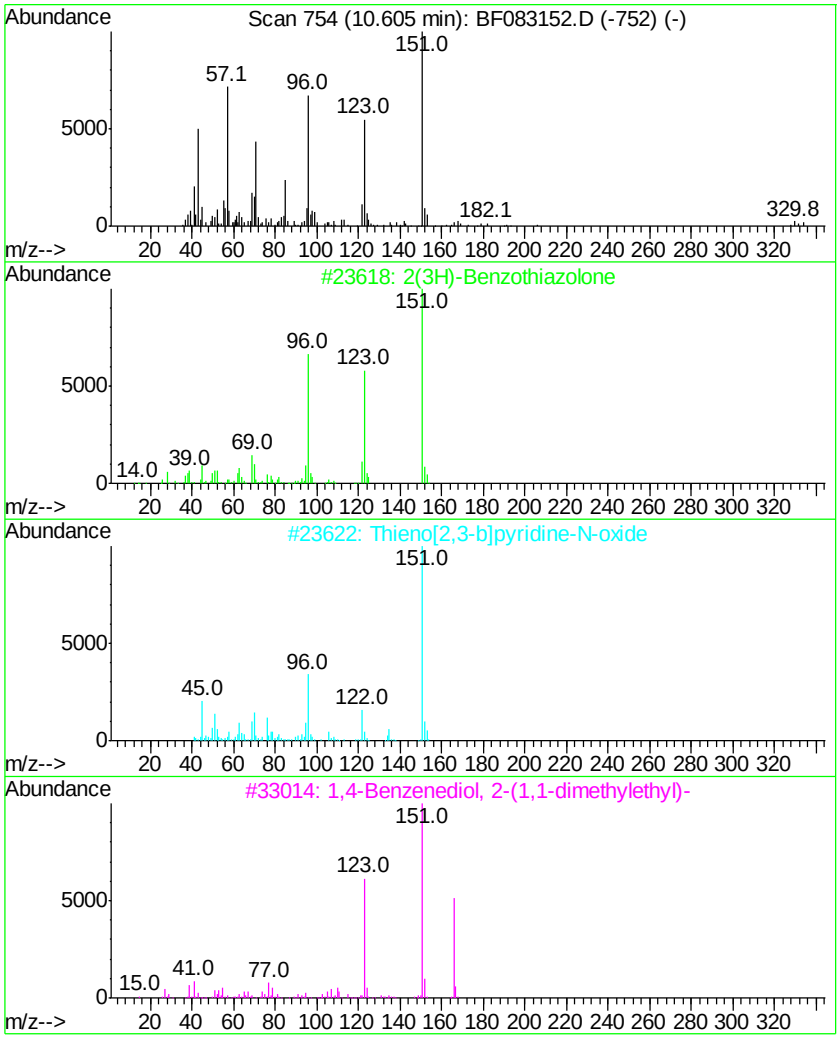
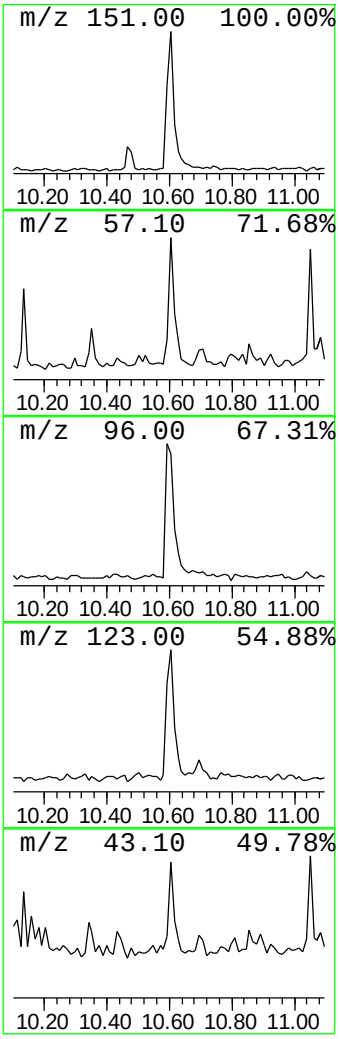
Peak Number 14 2(3H)-Benzothiazolone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.60	2.34 ng	203721	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	89
2	Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	38
3	1,4-Benzenediol, 2-(1,1-dimethyl...	166	C10H14O2	001948-33-0	38
4	Pyridine, 2,3,5,6-tetrafluoro-	151	C5HF4N	002875-18-5	22
5	Benzene, fluoro-	96	C6H5F	000462-06-6	11





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Data File : BF083152.D
Acq On : 22 Nov 2015 11:52
Operator : UM/IZ
Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

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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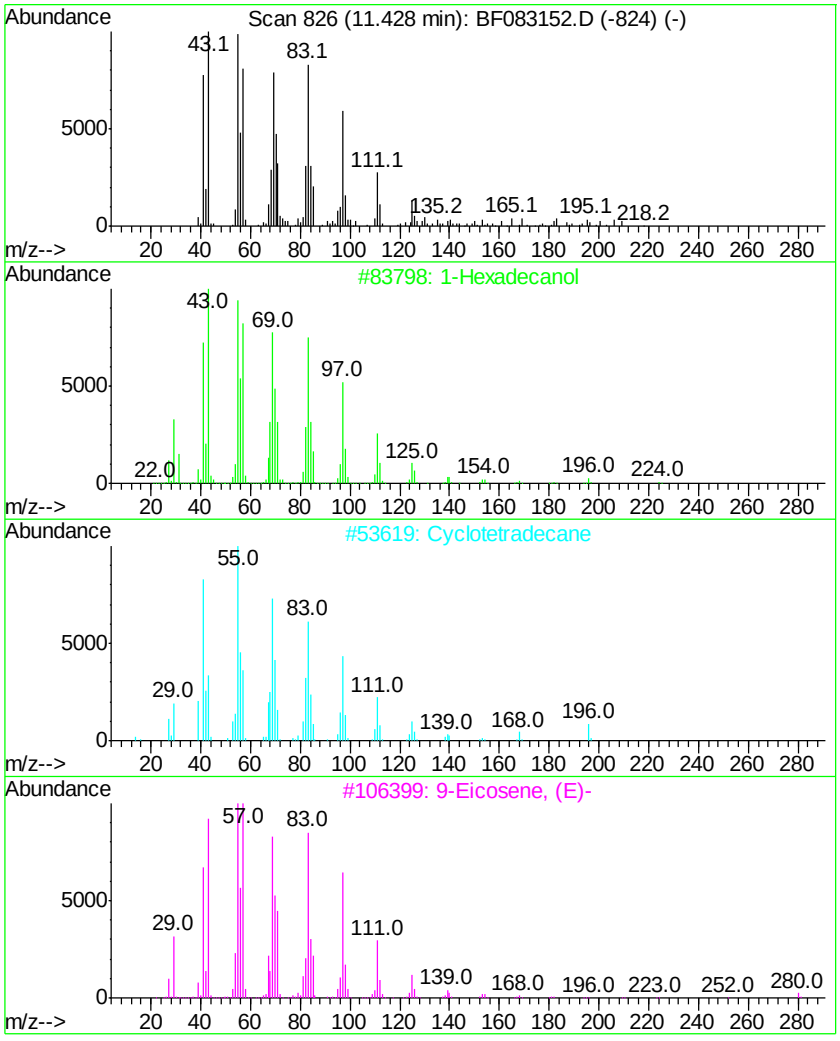
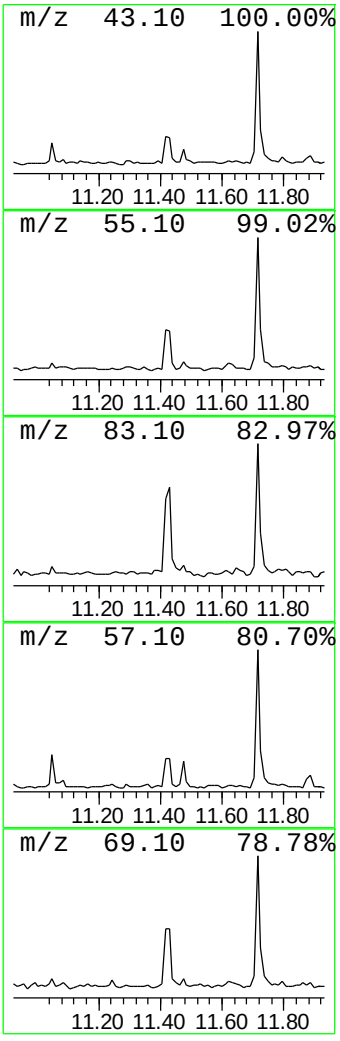
Peak Number 15 1-Hexadecanol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	2.24 ng	195013	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	Cyclotetradecane	196	C14H28	000295-17-0	93
3	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4	1-Pentadecanol	228	C15H32O	000629-76-5	91
5	9-Octadecene, (E)-	252	C18H36	007206-25-9	91





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112215\
Data File : BF083152.D
Acq On : 22 Nov 2015 11:52
Operator : UM/IZ
Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

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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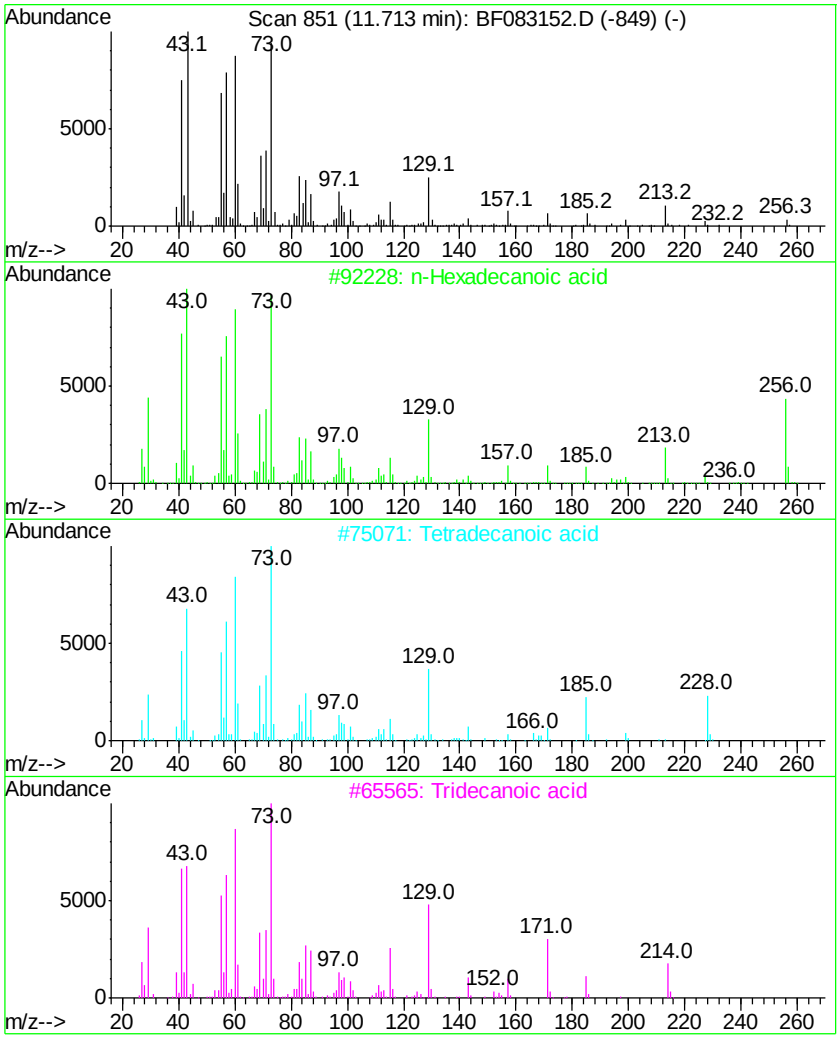
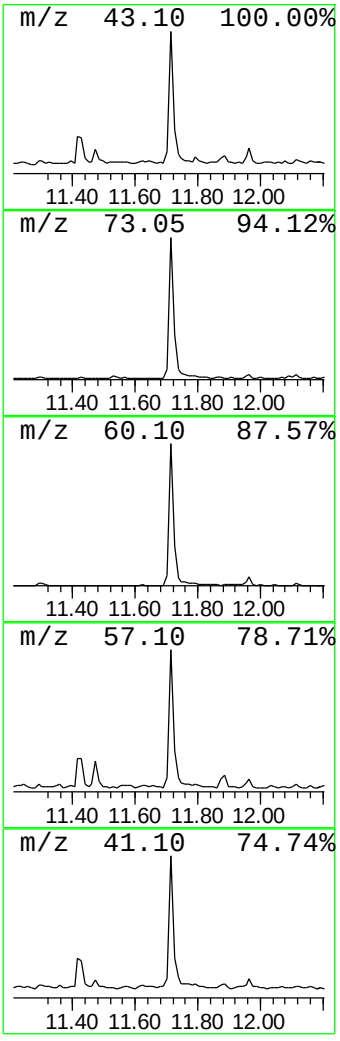
Peak Number 16 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	8.35 ng	725865	Phenanthrene-d10	11.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5	Decane, 2-methyl-	156	C11H24	006975-98-0	25





Library Search Compound Report

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Data File : BF083152.D
Acq On : 22 Nov 2015 11:52
Operator : UM/IZ
Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112115.M
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TIC Integration Parameters: LSCINT.P

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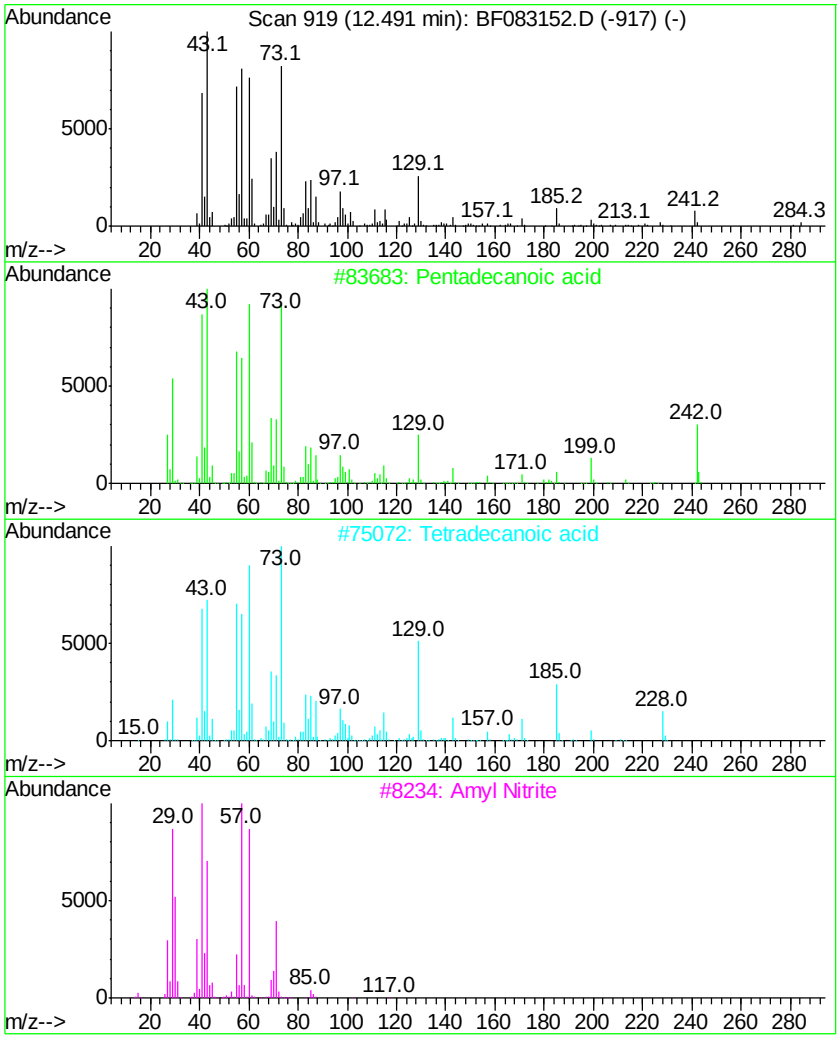
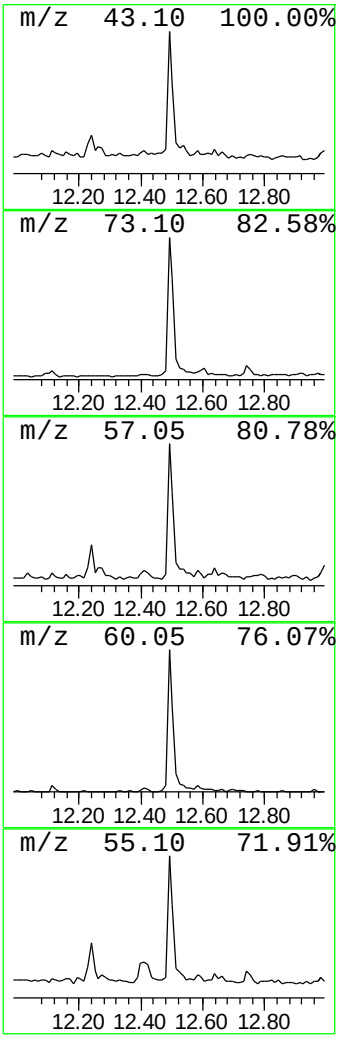
Peak Number 17 Pentadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	5.87 ng	482739	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	81
3	Amyl Nitrite	117	C5H11NO2	000110-46-3	38
4	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	35
5	Undecane	156	C11H24	001120-21-4	18





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Operator : UM/IZ
Sample : G4510-11
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ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF112215.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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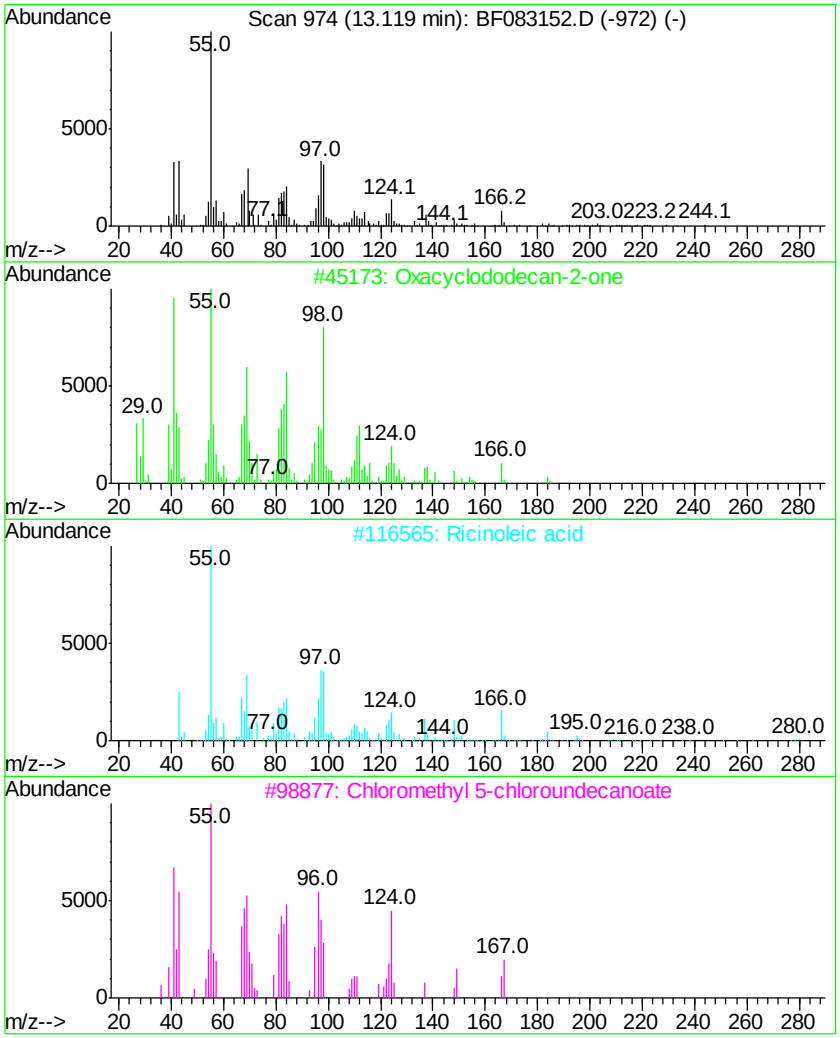
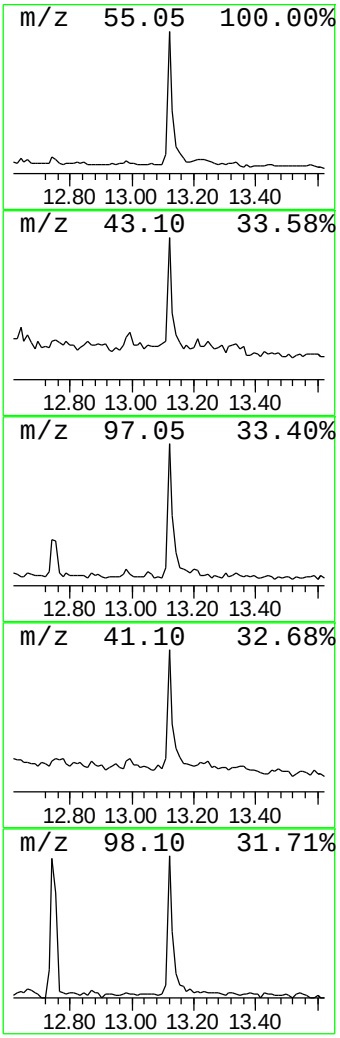
Peak Number 18 Oxacyclododecan-2-one Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.12	4.93 ng	405286	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxacyclododecan-2-one	184	C11H20O2	001725-03-7	89
2	Ricinoleic acid	298	C18H34O3	000141-22-0	47
3	Chloromethyl 5-chloroundecanoate	268	C12H22Cl2O2	080418-91-3	43
4	Oxacyclotridecan-2-one	198	C12H22O2	000947-05-7	38
5	10-Undecenoyl chloride	202	C11H19ClO	038460-95-6	30





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Operator : UM/IZ
Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

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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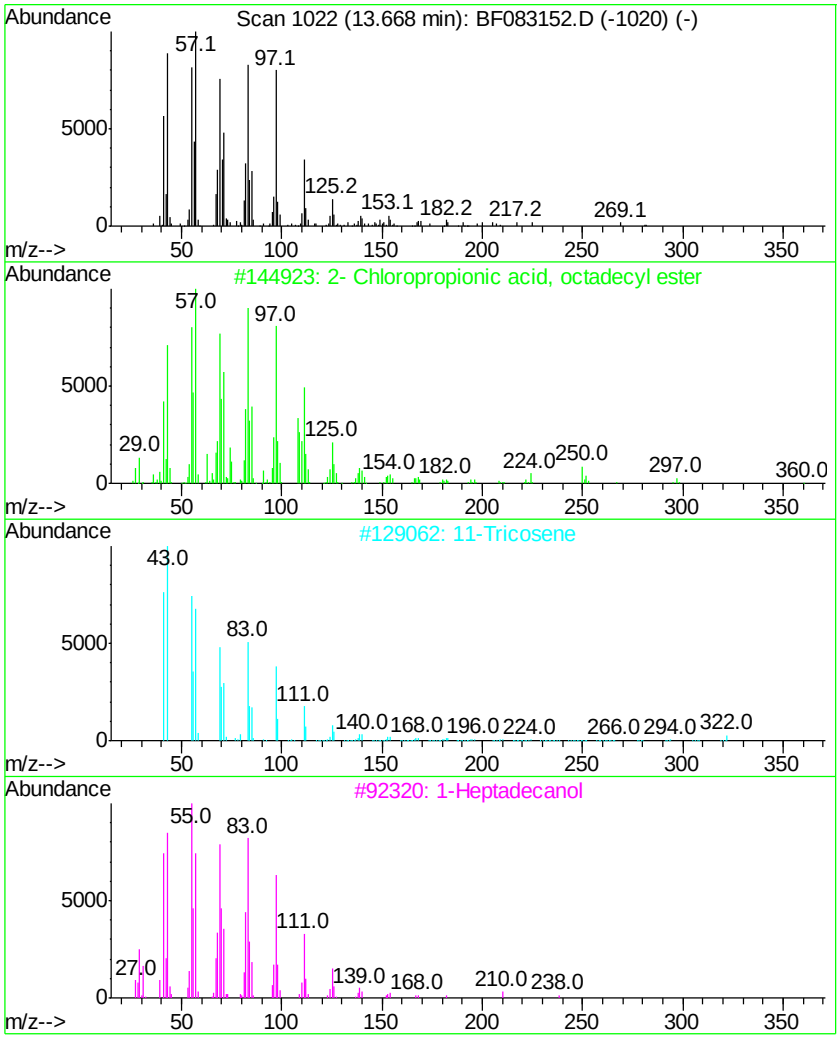
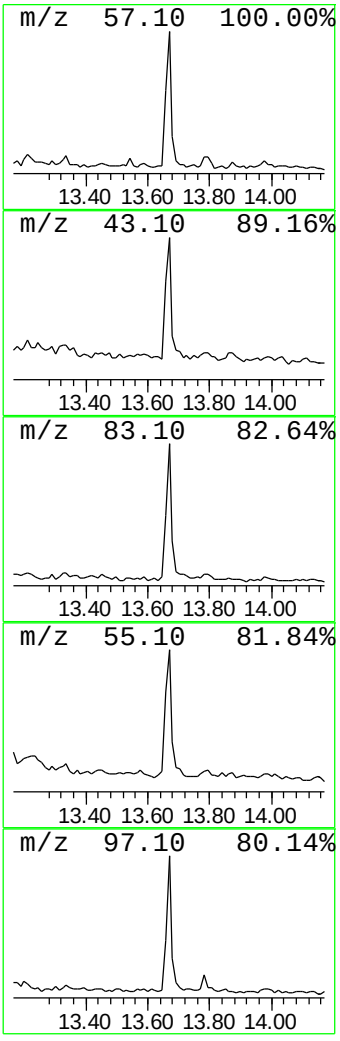
Peak Number 19 2- Chloropropionic acid, oc... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.67	3.44 ng	282395	Chrysene-d12	13.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	90
2	11-Tricosene	322	C23H46	052078-56-5	87
3	1-Heptadecanol	256	C17H36O	001454-85-9	81
4	1-Docosene	308	C22H44	001599-67-3	81
5	1-Hexadecanol	242	C16H34O	036653-82-4	81





Tentatively Identified Compound (LSC) summary

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Data File : BF083152.D
Acq On : 22 Nov 2015 11:52
Operator : UM/IZ
Sample : G4510-11
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DUP-111815-2

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	14.4	ng	871441	1	6.65	1210470	20.0
unknown6.42	6.42	88.4	ng	5348770	1	6.65	1210470	20.0
Phenol, 4-chloro-...	6.94	23.4	ng	1413320	1	6.65	1210470	20.0
unknown7.03	7.03	9.4	ng	567388	1	6.65	1210470	20.0
Methyl cis-3-chlo...	7.10	3.2	ng	191899	1	6.65	1210470	20.0
Acetophenone, 3'-...	8.19	2.2	ng	215703	2	7.94	1951820	20.0
Benzenemethanol, ...	9.22	12.0	ng	1103990	3	9.69	1845350	20.0
2(3H)-Benzothiazo...	10.60	2.3	ng	203721	4	11.16	1737760	20.0
1-Hexadecanol	11.43	2.2	ng	195013	4	11.16	1737760	20.0
n-Hexadecanoic acid	11.71	8.3	ng	725865	4	11.16	1737760	20.0
Pentadecanoic acid	12.49	5.9	ng	482739	5	13.78	1643970	20.0
Oxacyclododecan-2...	13.12	4.9	ng	405286	5	13.78	1643970	20.0
2- Chloropropioni...	13.67	3.4	ng	282395	5	13.78	1643970	20.0