LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

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-BF110715.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	5.001	251	255	267	rVB	2225368	3607933	47.84%	4.848%
2	5.424	289	292	295	rBV	5347091	5921973	78.53%	7.957%
3	6.464	380	383	385	rVB	5306622	7368583	97.71%	9.901%
4	6.590	391	394	396	rBV	6339750	7011218	92.97%	9.420%
5	6.819	411	414	416	rBV	1311951	1410589	18.71%	1.895%
6	6.979	425	428	430	rBV	3947833	5114242	67.82%	6.872%
7	7.379	460	463	465	rBV	3882044	4120628	54.64%	5.537%
8	8.099	524	526	529	rBV	1868370	1832757	24.30%	2.463%
9	9.185	618	621	623	rBV	8029086	7411710	98.28%	9.959%
10	9.573	653	655	658	rBV	1353896	1161342	15.40%	1.560%
11	9.859	677	680	682	rBV	2501571	2275447	30.17%	3.057%
12	10.270	714	716	718	rBV	87950	114851	1.52%	0.154%
13	10.648	746	749	751	rBV	5002541	5024471	66.63%	6.751%
14	10.773	758	760	765	rVB	161352	194813	2.58%	0.262%
15	11.219	798	799	801	rBV2	144296	146681	1.95%	0.197%
16	11.333	807	809	813	rVB	1711117	2499191	33.14%	3.358%
17	11.413	813	816	817	rBV2	123826	154974	2.06%	0.208%
18	11.573	827	830	835	rBV3	152762	276431	3.67%	0.371%
19	11.653	835	837	839	rBV	110781	127354	1.69%	0.171%
20	11.882	854	857	858	rBV2	251616	277330	3.68%	0.373%
21	11.951	861	863	866	rVV2	105101	154122	2.04%	0.207%
22	12.054	870	872	876	rVV	88252	99326	1.32%	0.133%
23	12.134	876	879	883	rVB2	225332	263724	3.50%	0.354%
24	12.385	899	901	905	rBV3	38203	102490	1.36%	0.138%
25	12.545	913	915	917	rBV	577201	494794	6.56%	0.665%
26	12.659	923	925	927	rBV2	63395	94142	1.25%	0.126%
27	12.774	932	935	937	rBV	507661	528340	7.01%	0.710%
28	12.819	938	939	943	rVB2	74648	93051	1.23%	0.125%
29	12.934	946	949	951	rVB	7222310	7541216	100.00%	10.133%
30	13.208	971	973	977	rBV3	68944	110105	1.46%	0.148%
31	13.482	995	997	998	rBV	111215	104476	1.39%	0.140%
32	13.711	1015	1017	1019	rBV2	119168	163653	2.17%	0.220%
33	13.757	1019	1021	1025	rVB	262640	270155	3.58%	0.363%
34	13.837	1025	1028	1032	rBV2	351493	541367	7.18%	0.727%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

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-BF110715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.974	1037	1040	1045	rVV2	2034012	2731680	36.22%	3.670%
36	14.168	1055	1057	1062	rVB3	100339	161294	2.14%	0.217%
37	14.259	1063	1065	1070	rBV2	106570	145671	1.93%	0.196%
38	14.351	1070	1073	1075	rBV	359048	466627	6.19%	0.627%
39	14.385	1075	1076	1080	rVB	222764	260658	3.46%	0.350%
40	14.602	1093	1095	1098	rVB	792840	755182	10.01%	1.015%
41	14.854	1115	1117	1120	rBV2	159865	206924	2.74%	0.278%
42	14.957	1124	1126	1128	rBV	183250	214878	2.85%	0.289%
43	15.002	1128	1130	1135	rVB	132604	299751	3.97%	0.403%
44	15.105	1138	1139	1141	rBV	74894	107842	1.43%	0.145%
45	15.242	1148	1151	1153	rVB	222802	339522	4.50%	0.456%
46	15.288	1153	1155	1158	rVB	73692	106311	1.41%	0.143%
47	15.345	1158	1160	1163	rBV	122057	191381	2.54%	0.257%
48	15.414	1163	1166	1169	rBV	1288634	1544450	20.48%	2.075%
49	15.882	1205	1207	1209	rBV	54101	81184	1.08%	0.109%
50	16.785	1283	1286	1291	rVB2	51989	106296	1.41%	0.143%
51	17.197	1319	1322	1325	rVB2	41273	92444	1.23%	0.124%

Sum of corrected areas: 74425574

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
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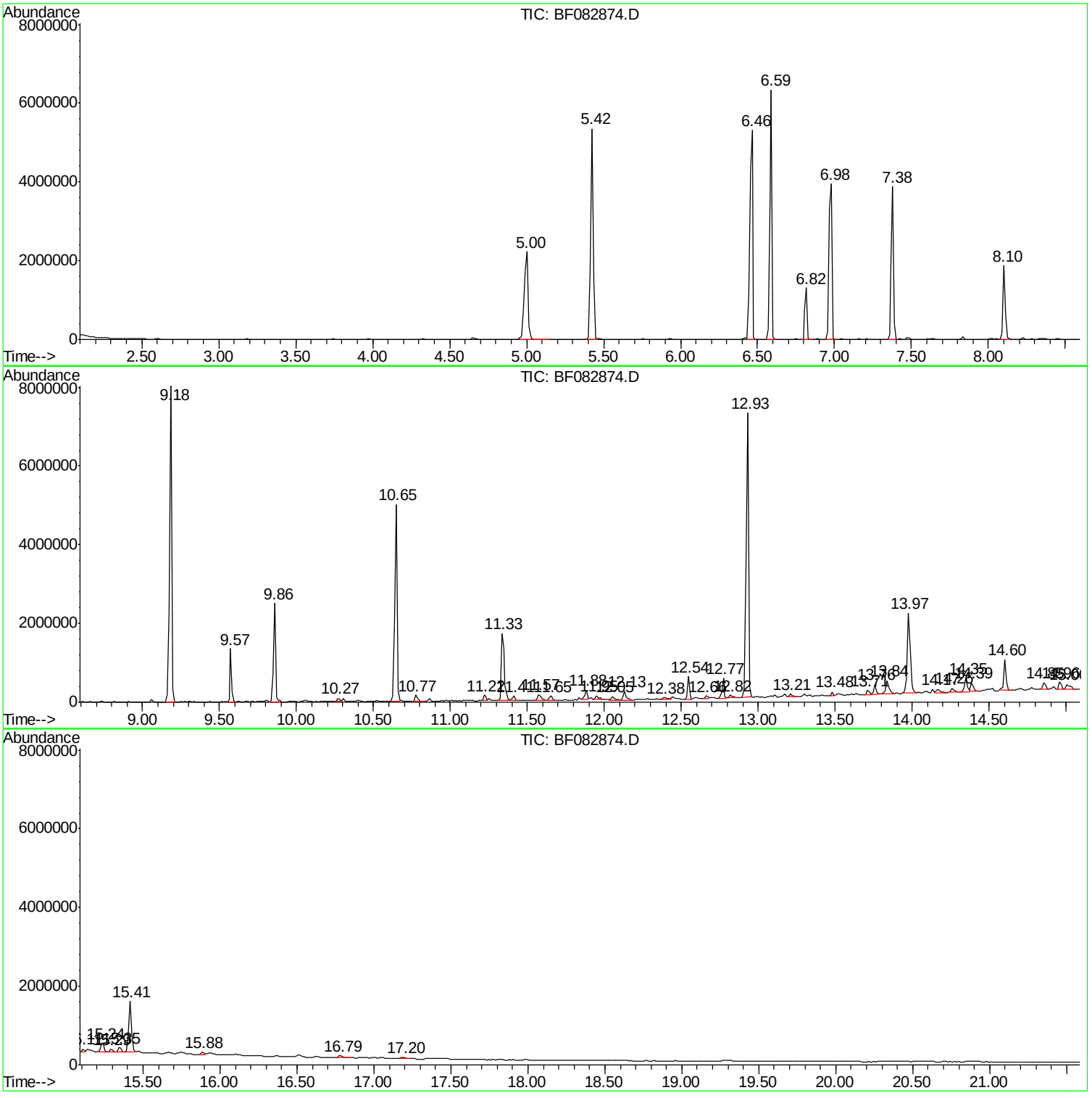
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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 : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

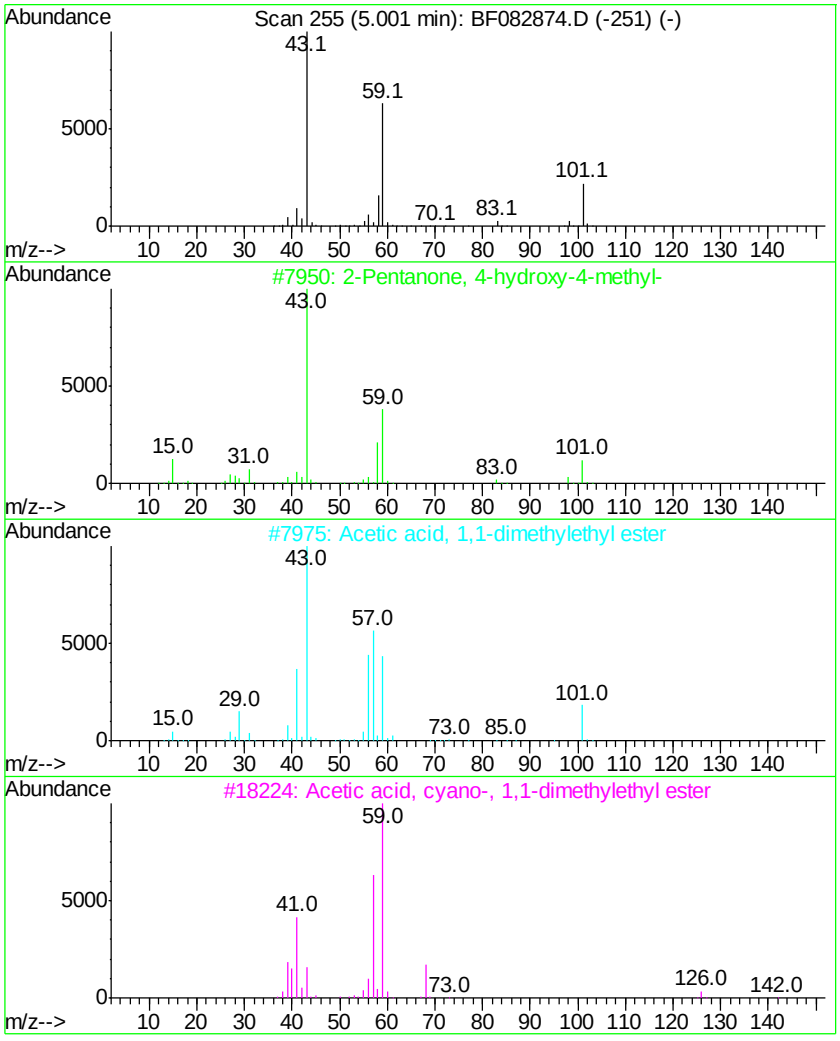
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

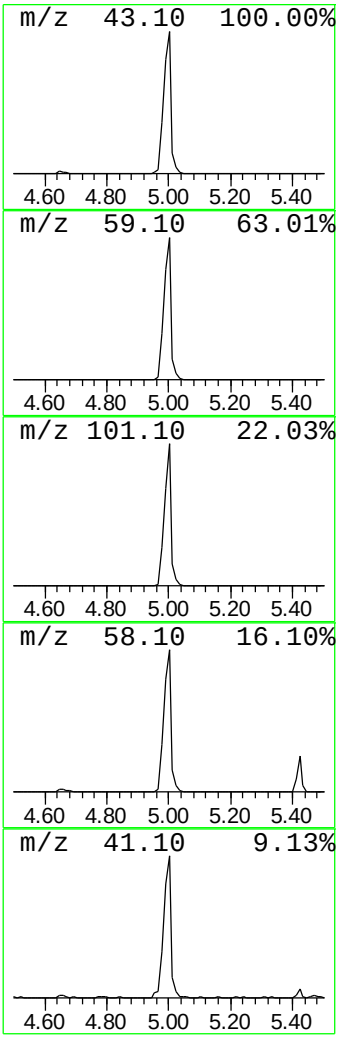
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	51.16 ng	3607930	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

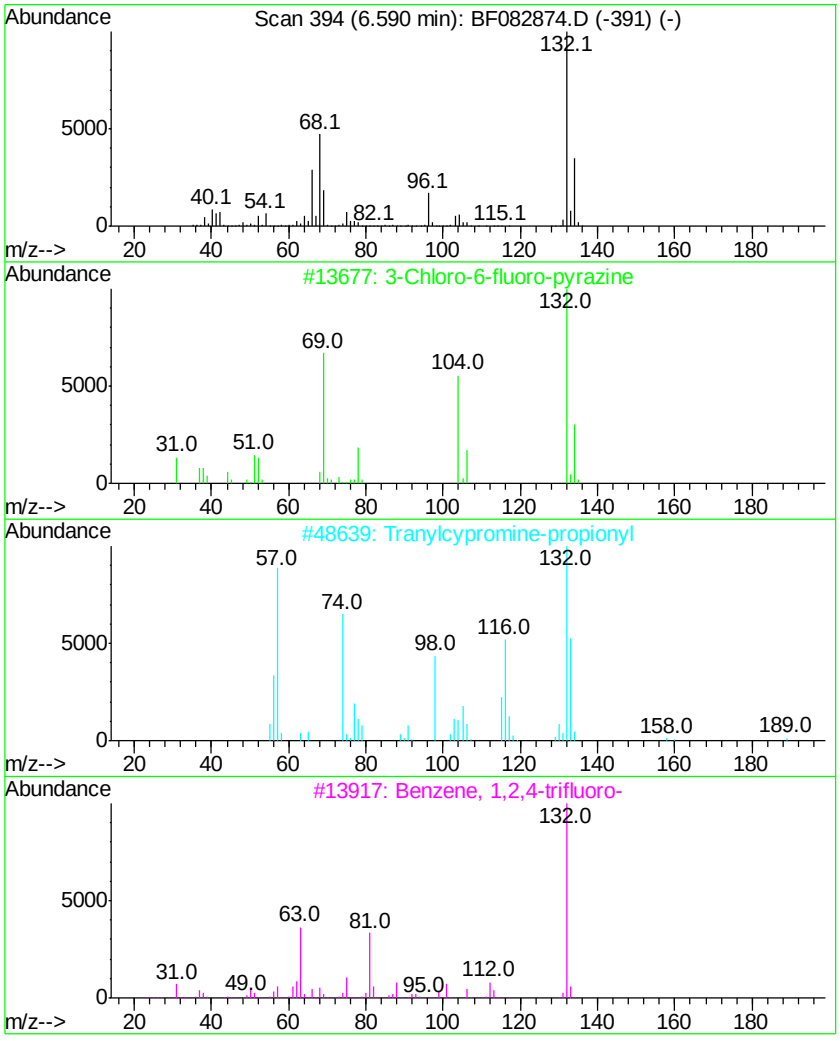
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

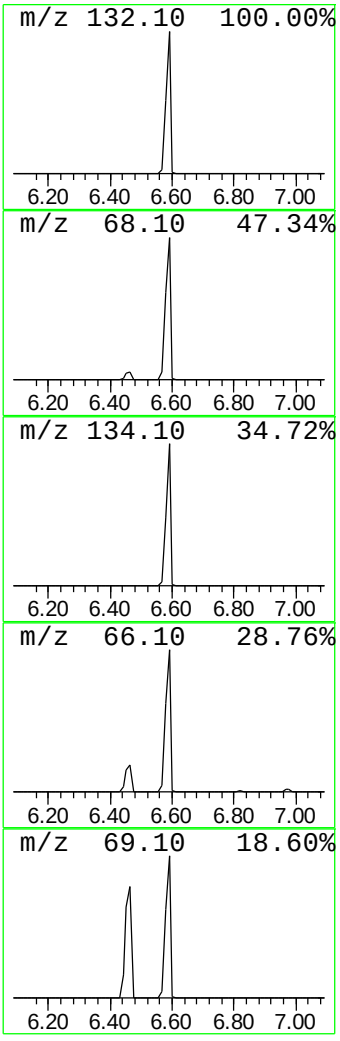
****

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	99.41 ng	7011220	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

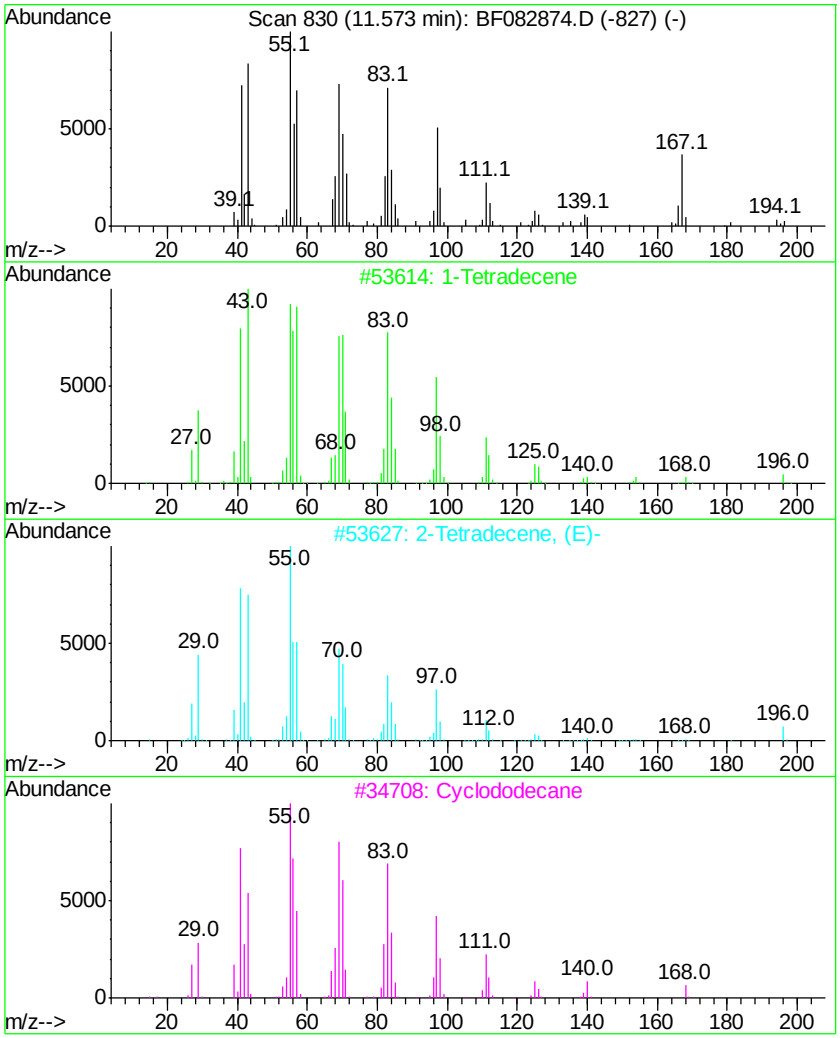
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

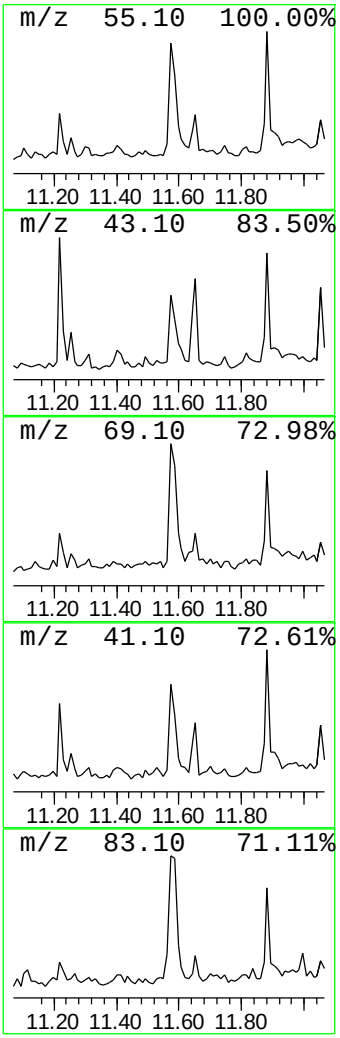
****

Peak Number 4 1-Tetradecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	2.21 ng	276431	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecene	196	C14H28	001120-36-1	97
2	2-Tetradecene, (E)-	196	C14H28	035953-53-8	95
3	Cyclododecane	168	C12H24	000294-62-2	95
4	Cyclotetradecane	196	C14H28	000295-17-0	90
5	1-Pentadecanol	228	C15H32O	000629-76-5	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

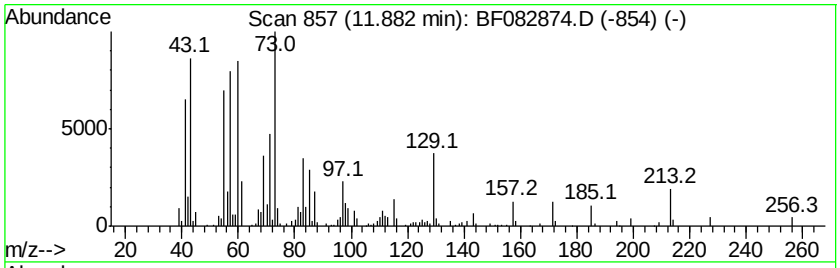
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

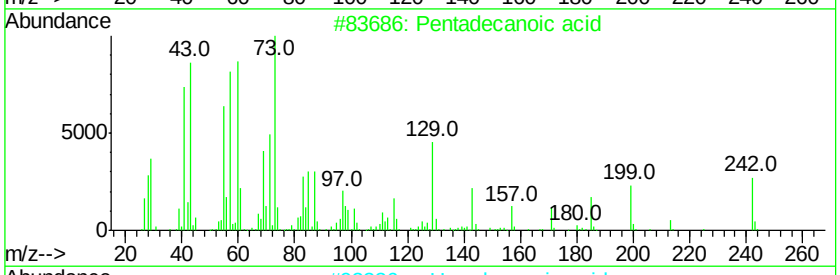
****

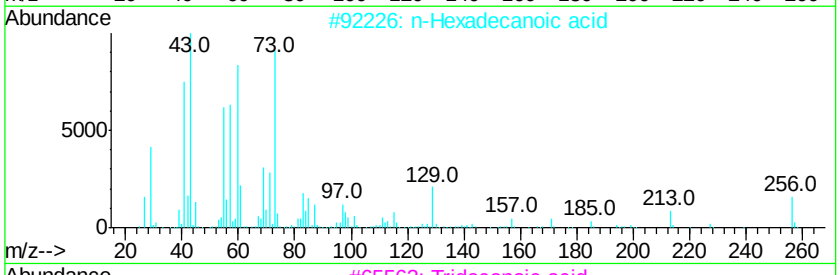
Peak Number 5 Pentadecanoic acid Concentration Rank 10

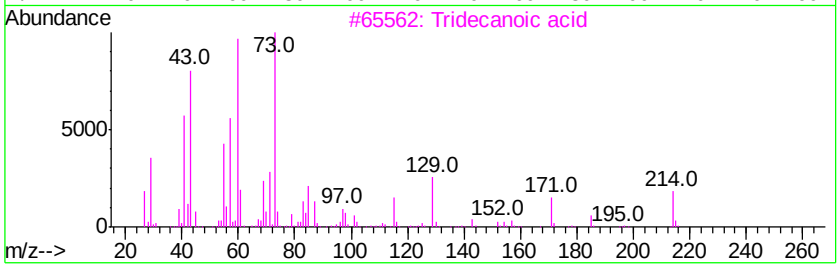
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	2.22 ng	277330	Phenanthrene-d10	11.33

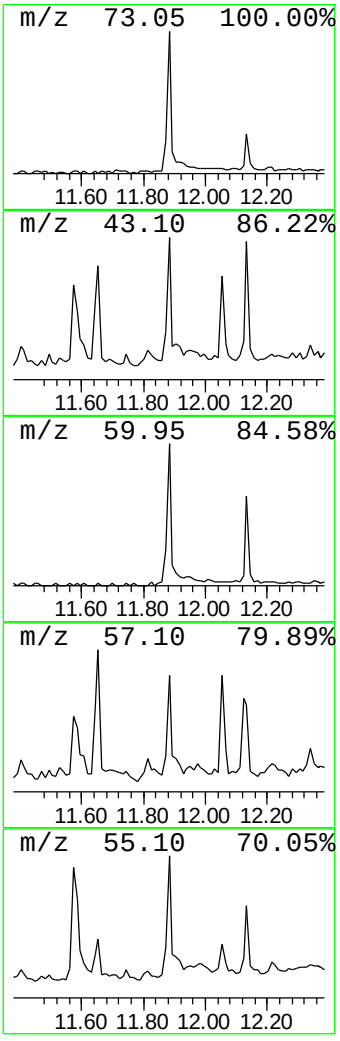
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58











Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

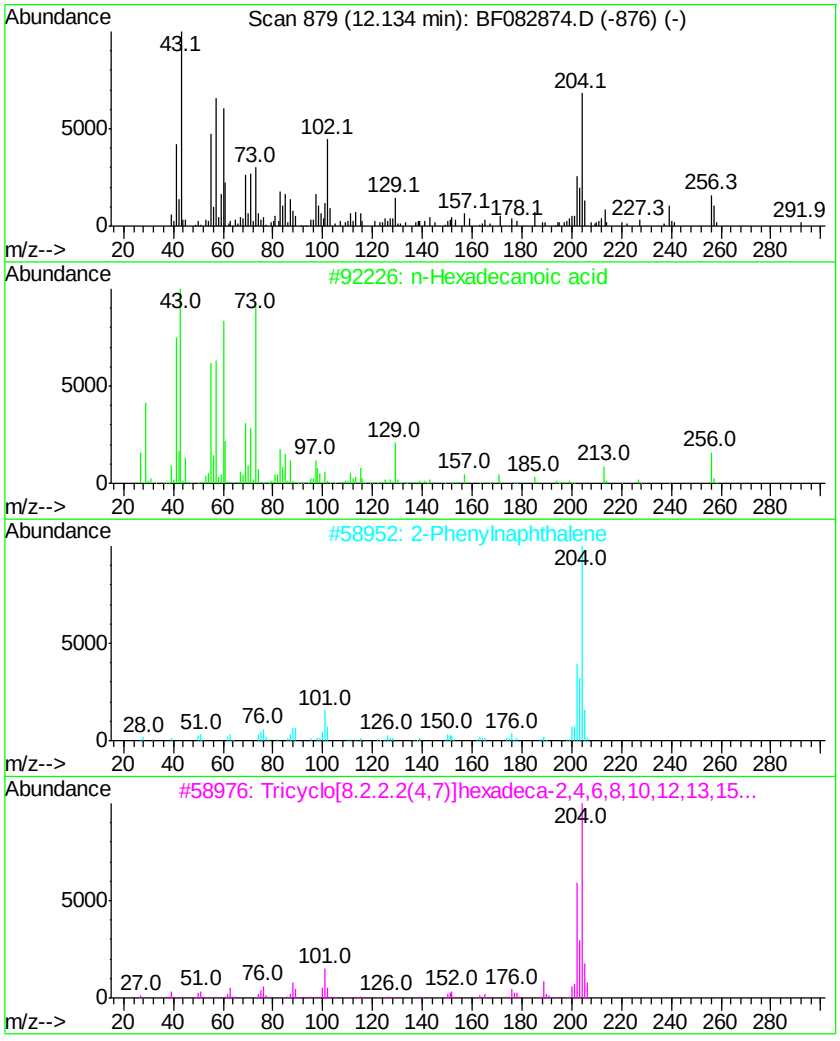
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

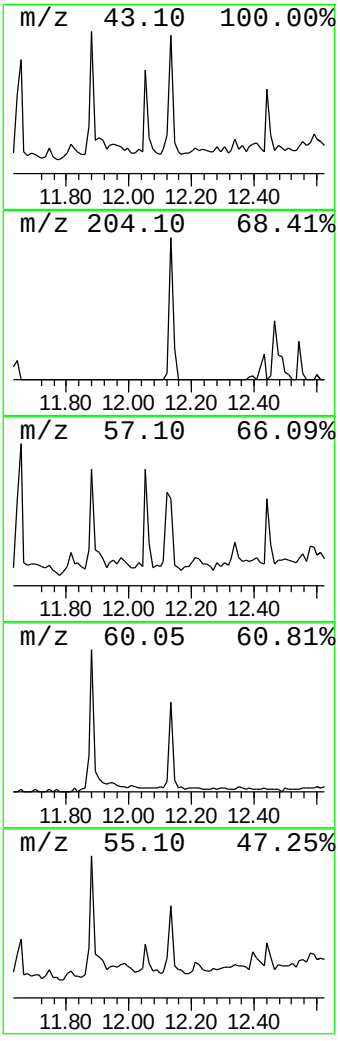
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.13	2.11 ng	263724	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
2	2-Phenylnaphthalene	204	C16H12	035465-71-5	53
3	Tricyclo[8.2.2.2(4,7)]hexadeca-2...	204	C16H12	006572-60-7	45
4	Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	38
5	9,10-di(Chloromethyl)anthracene	274	C16H12Cl2	010387-13-0	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

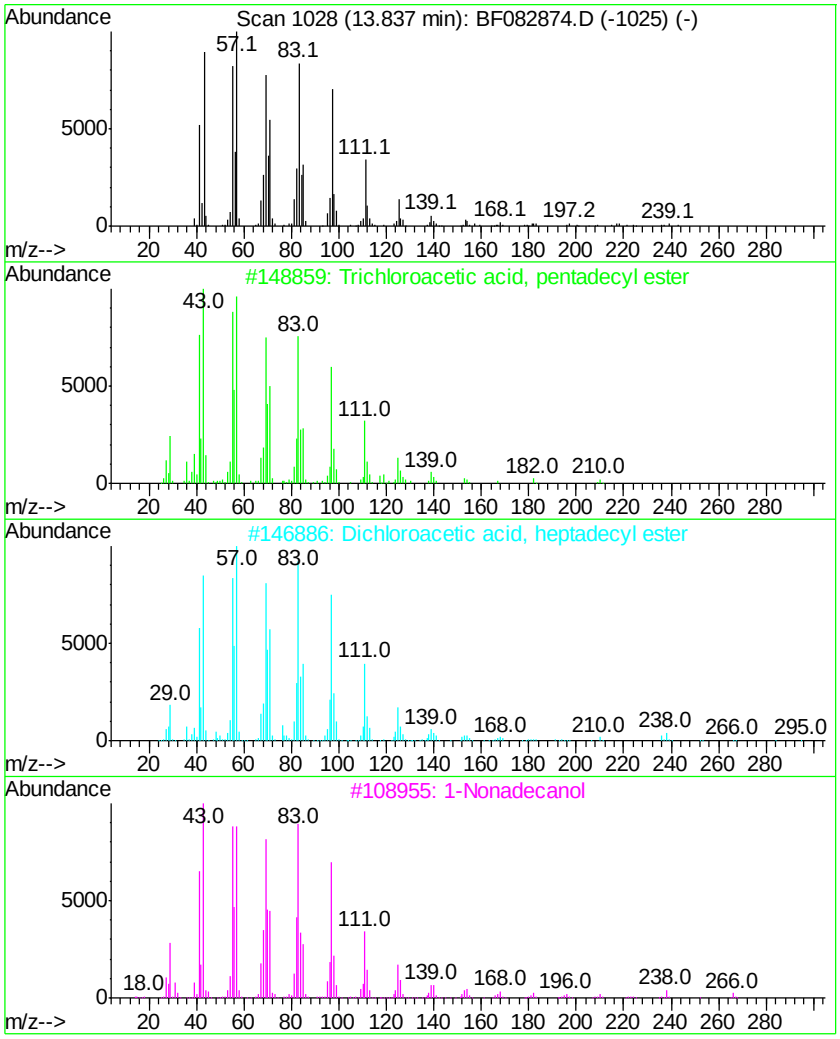
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

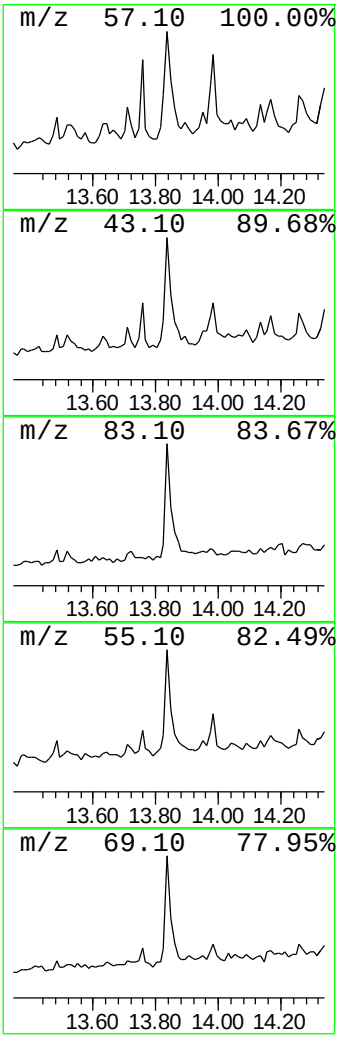
****

Peak Number 7 Trichloroacetic acid, penta... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.84	3.96 ng	541367	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3	1-Nonadecanol	284	C19H40O	001454-84-8	91
4	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
5	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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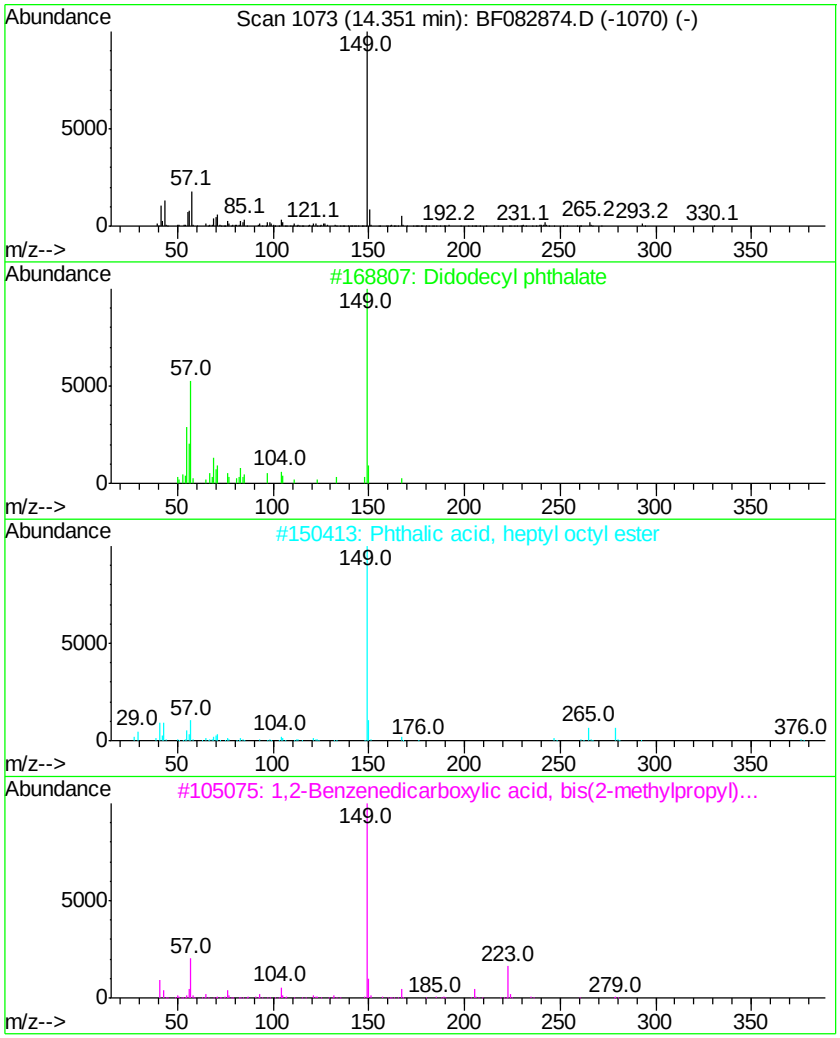
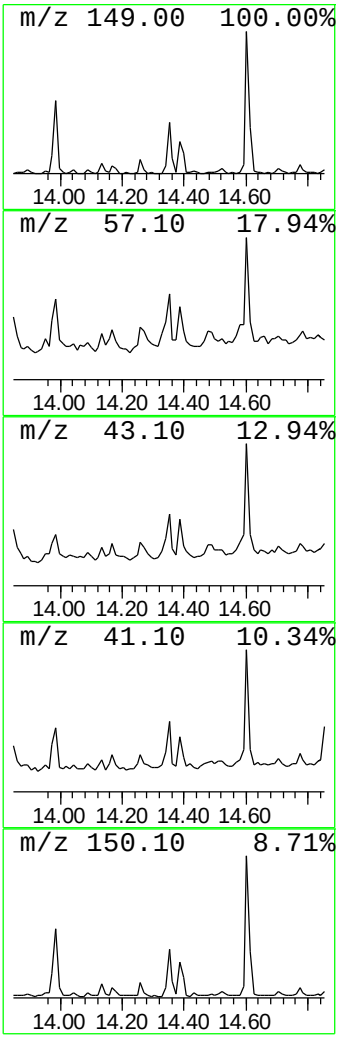
Peak Number 8 Didodecyl phthalate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	3.42 ng	466627	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Didodecyl phthalate	502	C32H54O4	002432-90-8	72
2	Phthalic acid, heptyl octyl ester	376	C23H36O4	088216-58-4	72
3	1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	72
4	1,2-Benzenedicarboxylic acid, di...	362	C22H34O4	003648-21-3	64
5	1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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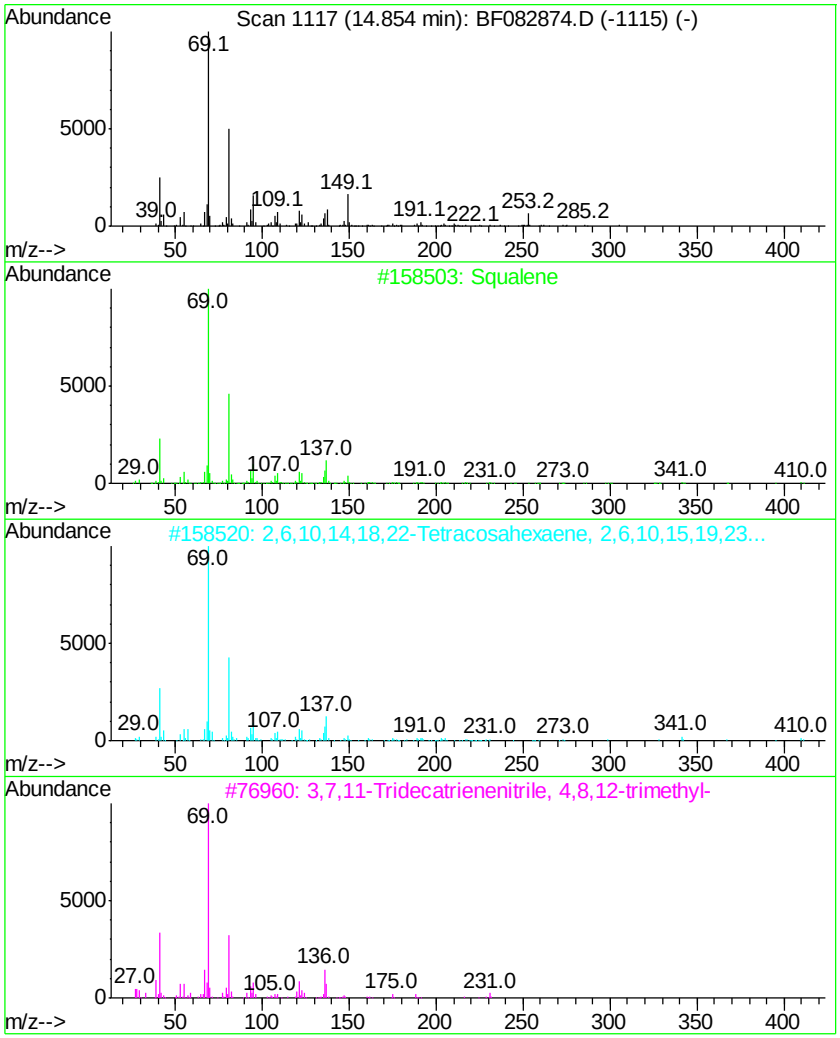
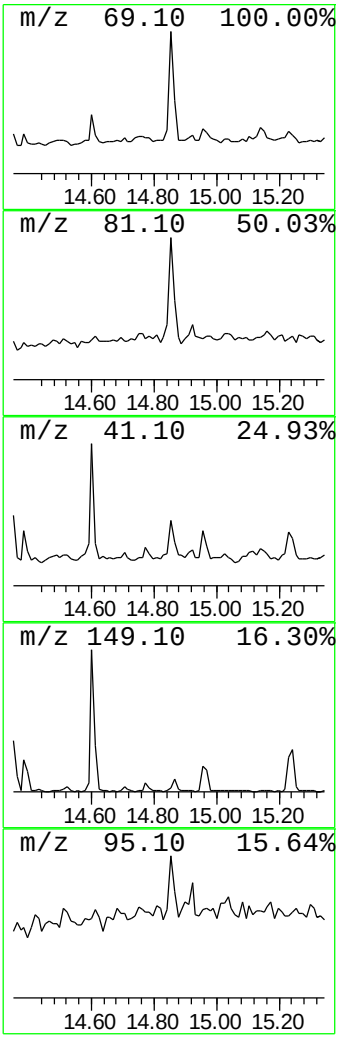
Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.85	2.68 ng	206924	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	80
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
3	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	53





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Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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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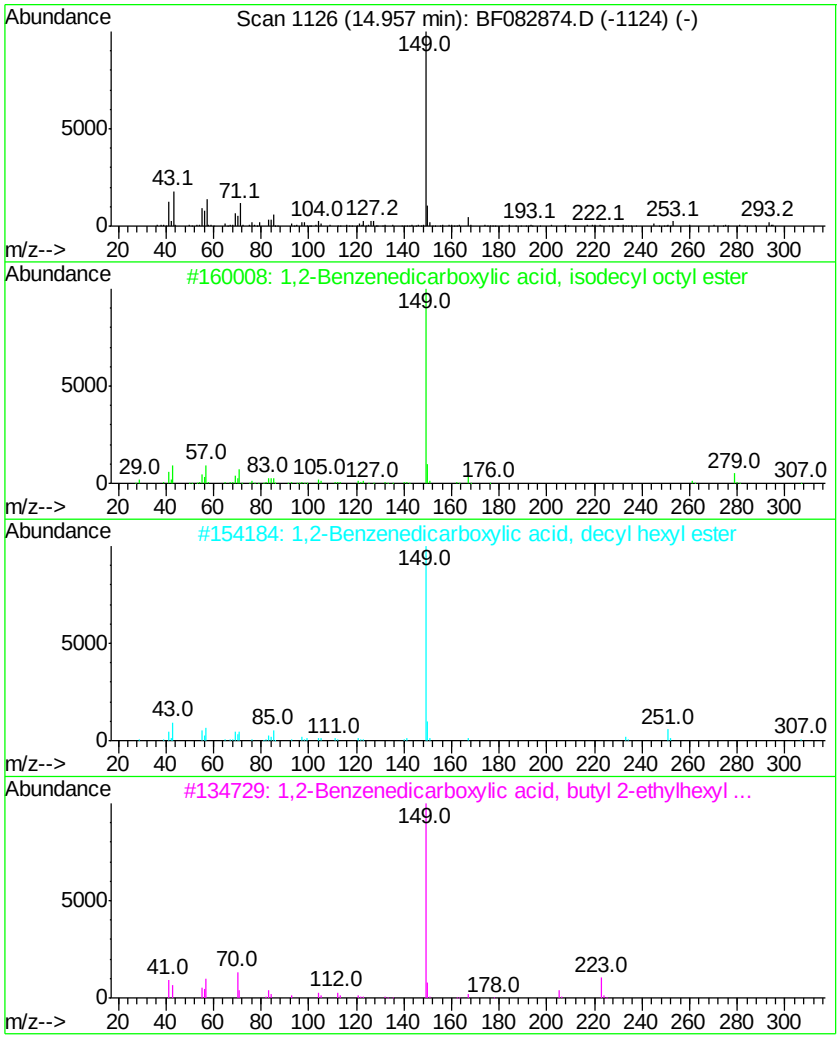
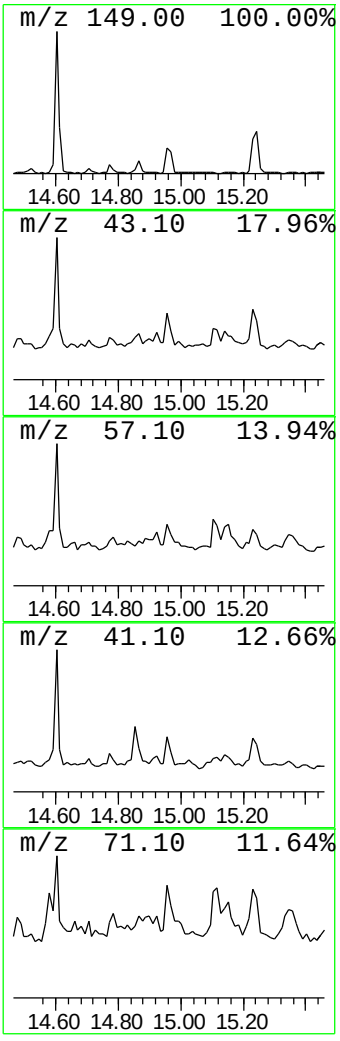
Peak Number 10 1,2-Benzenedicarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.78 ng	214878	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, is...	418	C26H42O4	001330-96-7	86
2	1,2-Benzenedicarboxylic acid, de...	390	C24H38O4	025724-58-7	78
3	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	72
4	1,2-Benzenedicarboxylic acid, bu...	362	C22H34O4	000089-18-9	72
5	Dibutyl phthalate	278	C16H22O4	000084-74-2	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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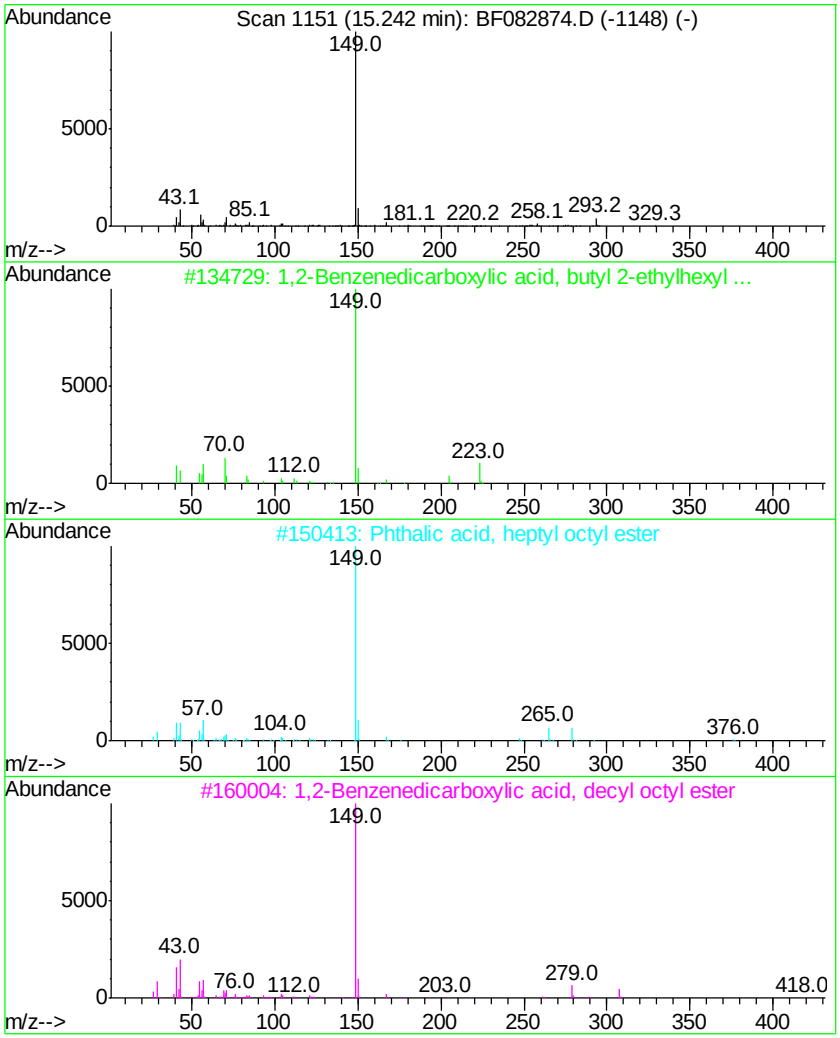
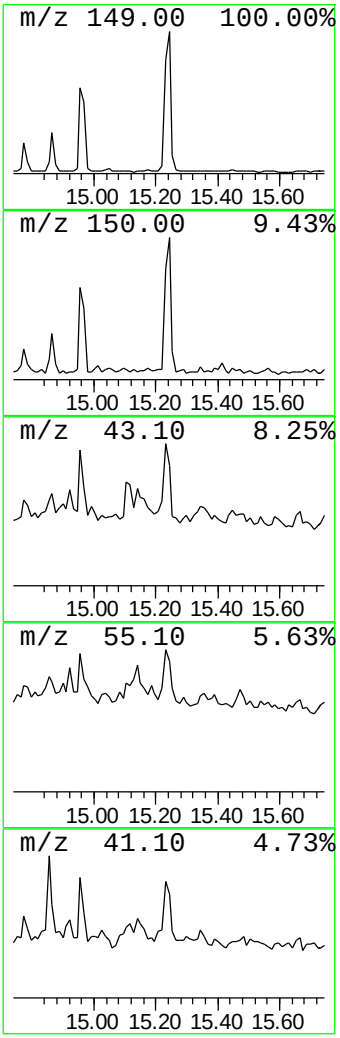
Peak Number 11 1,2-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	4.40 ng	339522	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	50
2	Phthalic acid, heptyl octyl ester	376	C23H36O4	088216-58-4	50
3	1,2-Benzenedicarboxylic acid, de...	418	C26H42O4	000119-07-3	50
4	1,2-Benzenedicarboxylic acid, di...	250	C14H18O4	000131-16-8	39
5	1,2-Benzenedicarboxylic acid, di...	306	C18H26O4	000131-18-0	39





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111015\
Data File : BF082874.D
Acq On : 10 Nov 2015 17:22
Operator : UM/IZ
Sample : G4347-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CWC-7-20151109

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110715.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...	5.00	51.2	ng	3607930	1	6.82	1410590	20.0
unknown6.59	6.59	99.4	ng	7011220	1	6.82	1410590	20.0
1-Tetradecene	11.57	2.2	ng	276431	4	11.33	2499190	20.0
Pentadecanoic acid	11.88	2.2	ng	277330	4	11.33	2499190	20.0
n-Hexadecanoic acid	12.13	2.1	ng	263724	4	11.33	2499190	20.0
Trichloroacetic a...	13.84	4.0	ng	541367	5	13.97	2731680	20.0
Didodecyl phthalate	14.35	3.4	ng	466627	5	13.97	2731680	20.0
Squalene	14.85	2.7	ng	206924	6	15.41	1544450	20.0
1,2-Benzenedicarb...	14.96	2.8	ng	214878	6	15.41	1544450	20.0
1,2-Benzenedicarb...	15.24	4.4	ng	339522	6	15.41	1544450	20.0