LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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	5.195	483	486	504	rBV	158467	249958	4.48%	0.656%
2	5.601	551	555	583	rBV	854443	2017259	36.20%	5.291%
3	6.131	641	645	648	rBV	84381	88300	1.58%	0.232%
4	6.601	722	725	744	rBV	529949	1305457	23.42%	3.424%
5	6.736	744	748	772	rVV	3112200	4135352	74.20%	10.846%
6	6.966	783	787	806	rVB	507612	955215	17.14%	2.505%
7	7.119	808	813	839	rVV	3138949	4281214	76.82%	11.229%
8	7.289	839	842	848	rVB4	51939	79127	1.42%	0.208%
9	7.483	869	875	878	rBV3	74625	112698	2.02%	0.296%
10	7.531	878	883	892	rBV	2088542	2980498	53.48%	7.817%
11	7.595	892	894	899	rVV2	177856	235830	4.23%	0.619%
12	7.636	899	901	906	rVB3	39078	58878	1.06%	0.154%
13	7.719	913	915	920	rBV2	57994	75618	1.36%	0.198%
14	7.760	920	922	926	rVB3	59873	71226	1.28%	0.187%
15	7.813	927	931	939	rVB3	52156	85092	1.53%	0.223%
16	7.972	954	958	966	rBV4	86388	160808	2.89%	0.422%
17	8.148	982	988	990	rBV6	36262	57084	1.02%	0.150%
18	8.242	999	1004	1019	rBV	848091	1183948	21.24%	3.105%
19	8.477	1042	1044	1050	rVB3	56559	61010	1.09%	0.160%
20	8.607	1064	1066	1072	rVB6	43271	73819	1.32%	0.194%
21	8.719	1082	1085	1090	rVB5	59408	82319	1.48%	0.216%
22	8.795	1096	1098	1102	rVB4	42877	57573	1.03%	0.151%
23	8.860	1102	1109	1111	rBV5	41007	71558	1.28%	0.188%
24	9.077	1144	1146	1151	rVB6	58657	91036	1.63%	0.239%
25	9.142	1151	1157	1158	rBV6	65942	109739	1.97%	0.288%
26	9.319	1182	1187	1200	rBV	4573642	5573260	100.00%	14.618%
27	9.666	1243	1246	1250	rVV3	145392	200911	3.60%	0.527%
28	9.707	1250	1253	1259	rVB	398315	410717	7.37%	1.077%
29	9.848	1274	1277	1281	rBV5	56038	98625	1.77%	0.259%
30	9.972	1293	1298	1299	rBV5	54319	88514	1.59%	0.232%
31	10.001	1299	1303	1308	rVV	1219914	1280151	22.97%	3.358%
32	10.360	1362	1364	1366	rVV2	83153	66109	1.19%	0.173%
33	10.383	1366	1368	1374	rVB5	109476	148734	2.67%	0.390%
34	10.671	1415	1417	1422	rVB5	66051	81030	1.45%	0.213%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.742	1425	1429	1434	rVV2	261857	378852	6.80%	0.994%
36	10.795	1434	1438	1447	rVV	2314765	2966841	53.23%	7.782%
37	10.966	1464	1467	1469	rBV	56642	65262	1.17%	0.171%
38	10.995	1469	1472	1475	rVB2	92761	106405	1.91%	0.279%
39	11.030	1475	1478	1480	rBV2	86881	70762	1.27%	0.186%
40	11.495	1554	1557	1570	rBV	893453	1019777	18.30%	2.675%
41	12.007	1640	1644	1656	rVB	327833	384245	6.89%	1.008%
42	12.248	1682	1685	1689	rBV3	54674	56033	1.01%	0.147%
43	12.789	1774	1777	1783	rBV3	83554	94150	1.69%	0.247%
44	13.077	1822	1826	1846	rBV	3459603	3854190	69.16%	10.109%
45	13.954	1972	1975	1982	rVB	229209	219106	3.93%	0.575%
46	14.142	2004	2007	2019	rBV	832008	973818	17.47%	2.554%
47	14.977	2146	2149	2153	rVB	66442	70826	1.27%	0.186%
48	15.248	2193	2195	2200	rVB	53213	60505	1.09%	0.159%
49	15.677	2261	2268	2284	rVB	607863	1107827	19.88%	2.906%
50	16.106	2338	2341	2347	rVB2	45752	69162	1.24%	0.181%

Sum of corrected areas: 38126428

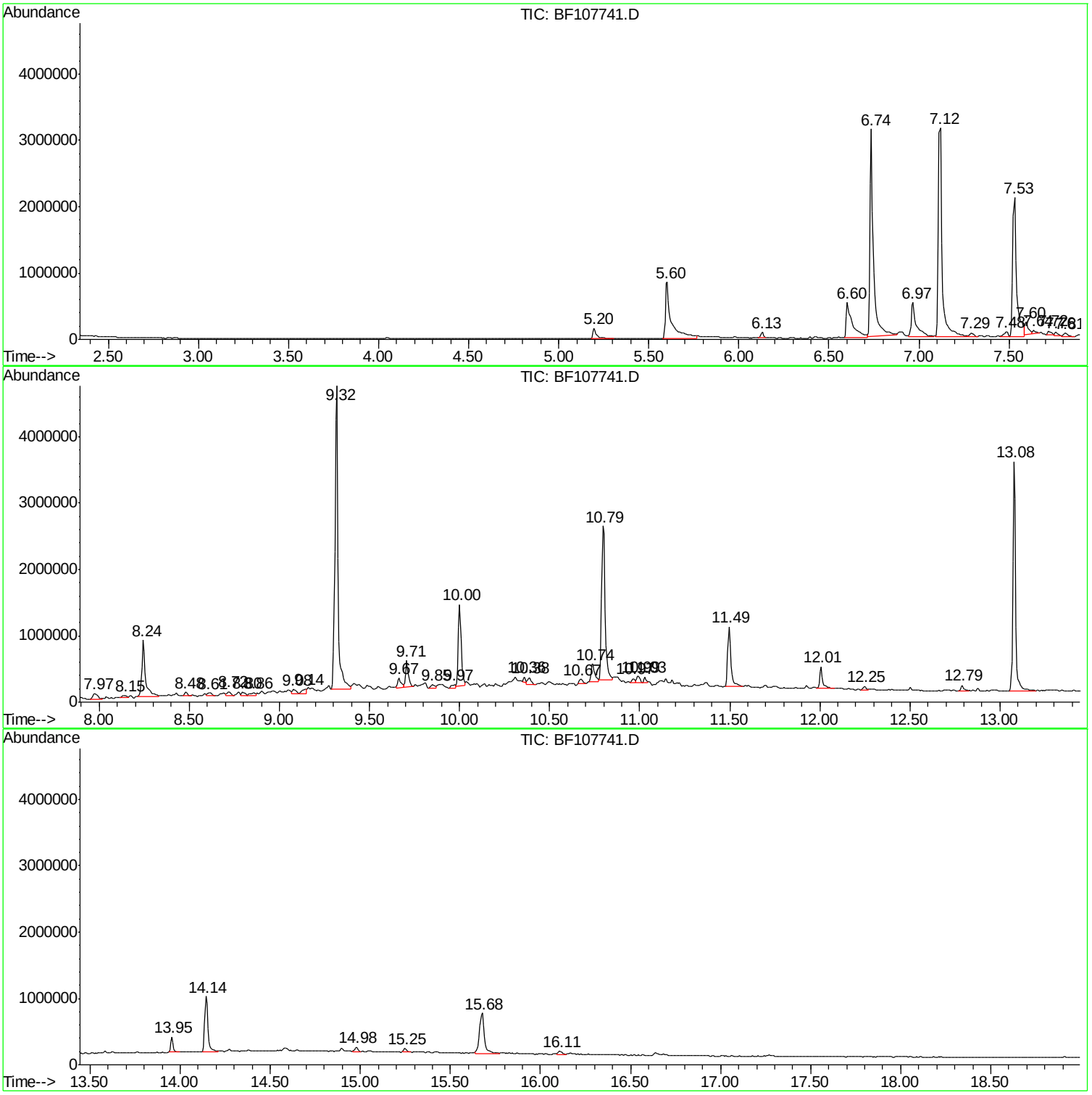
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

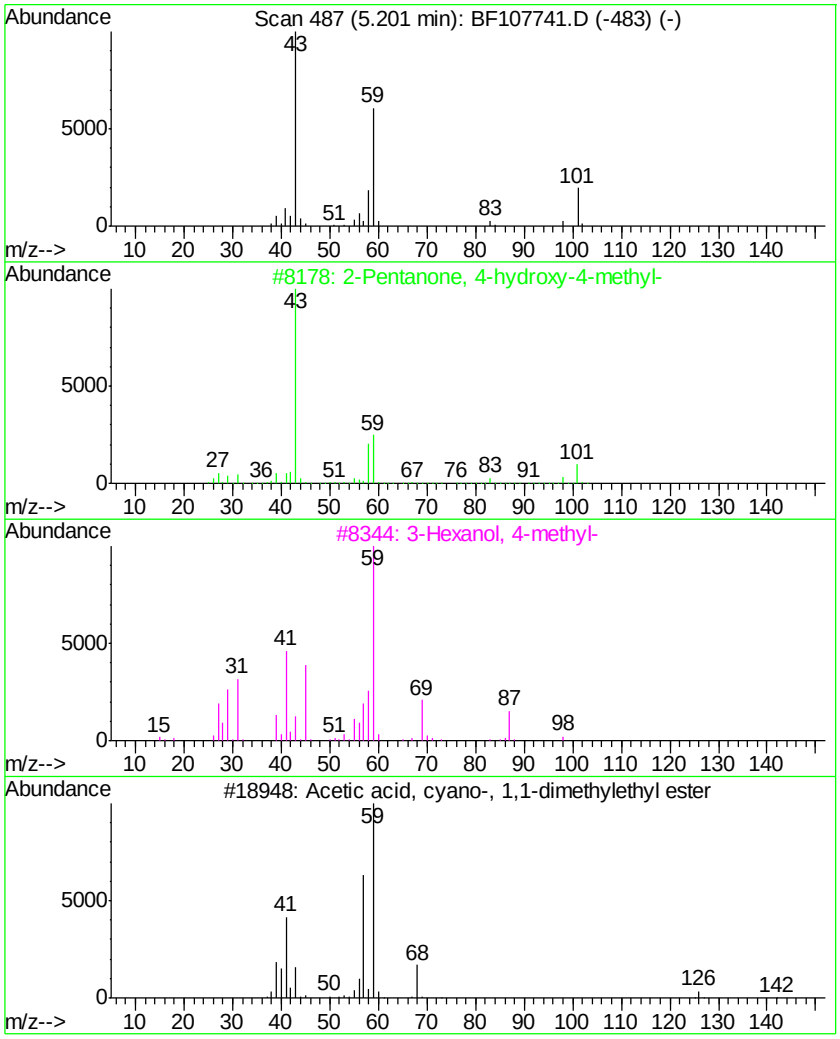
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

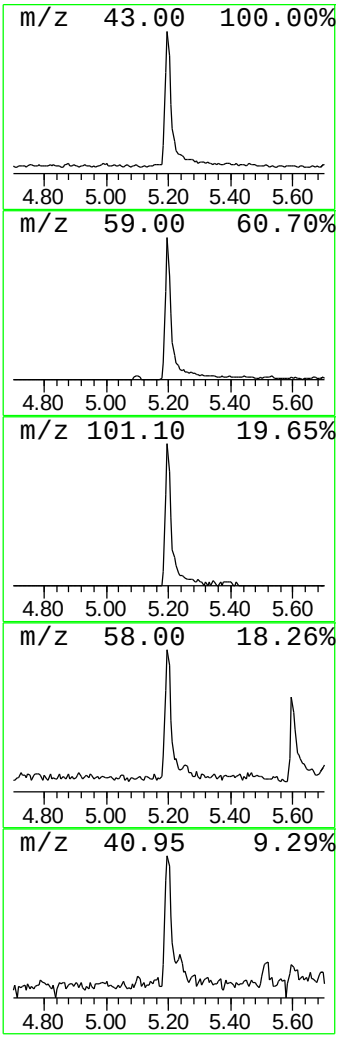
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	5.23 ng	249958	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	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	2-Nonanone	142	C9H18O	000821-55-6	12
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

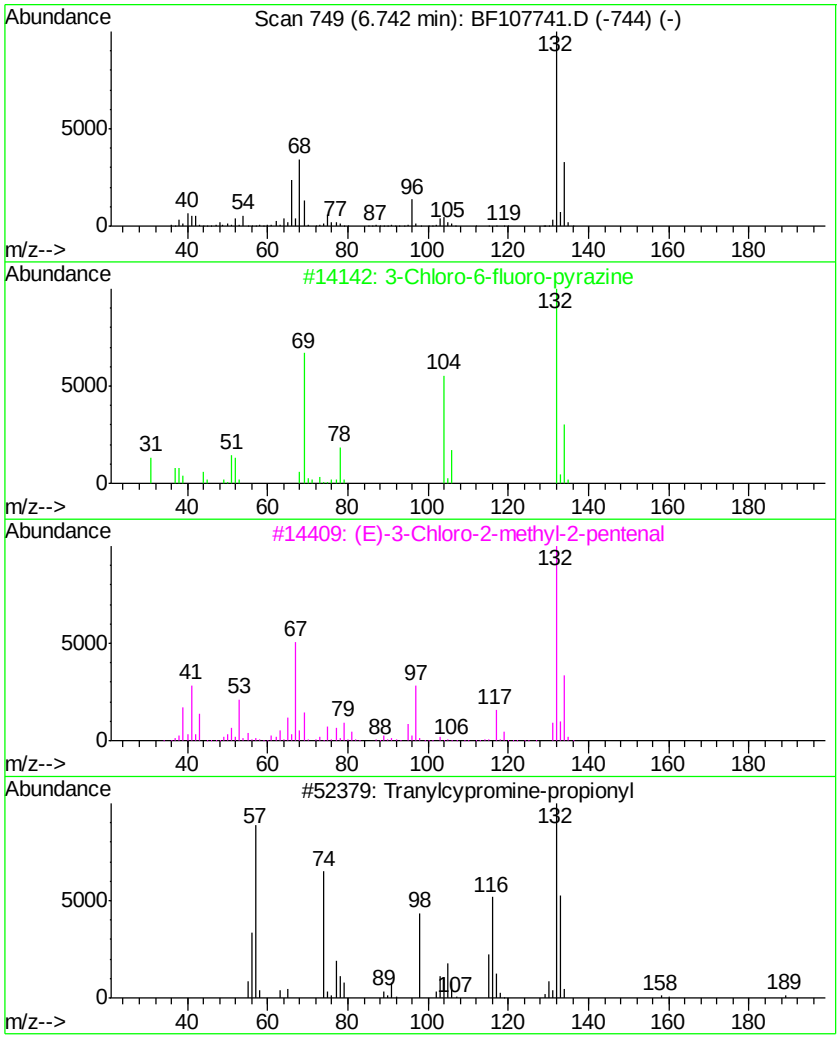
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

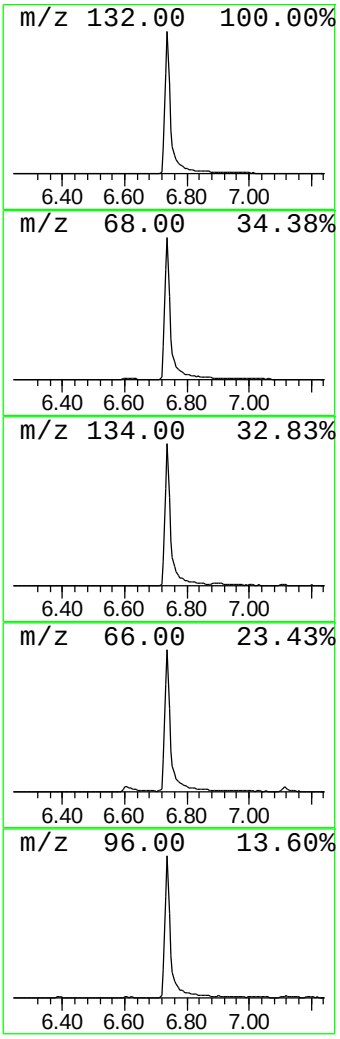
****

Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	86.58 ng	4135350	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	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

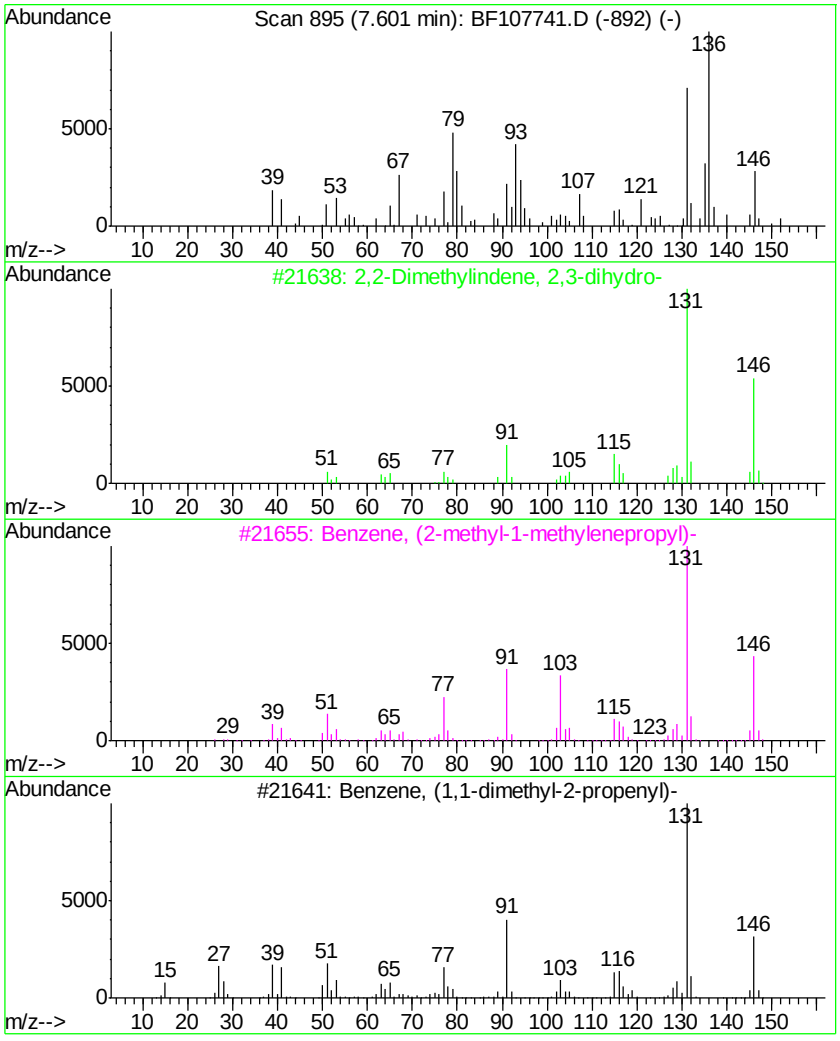
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

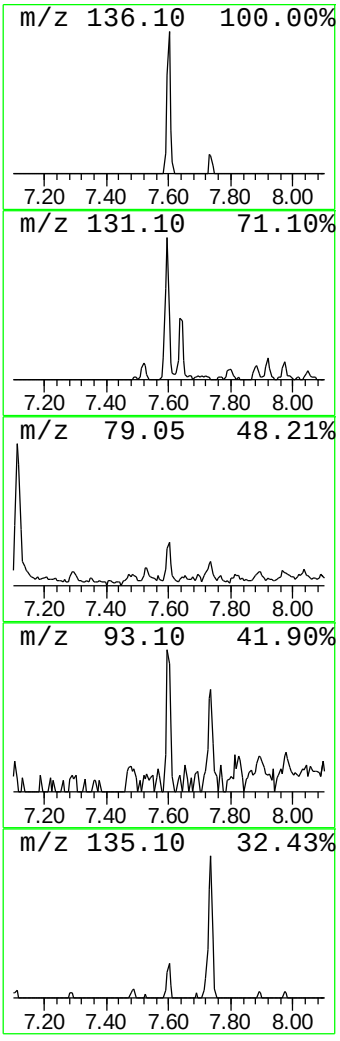
****

Peak Number 4 2,2-Dimethylindene, 2,3-dih... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	4.94 ng	235830	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethylindene, 2,3-dihydro-	146	C11H14	020836-11-7	89
2	Benzene, (2-methyl-1-methylenepr...	146	C11H14	017498-71-4	55
3	Benzene, (1,1-dimethyl-2-propenyl)-	146	C11H14	018321-36-3	55
4	Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	50
5	Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	001559-81-5	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

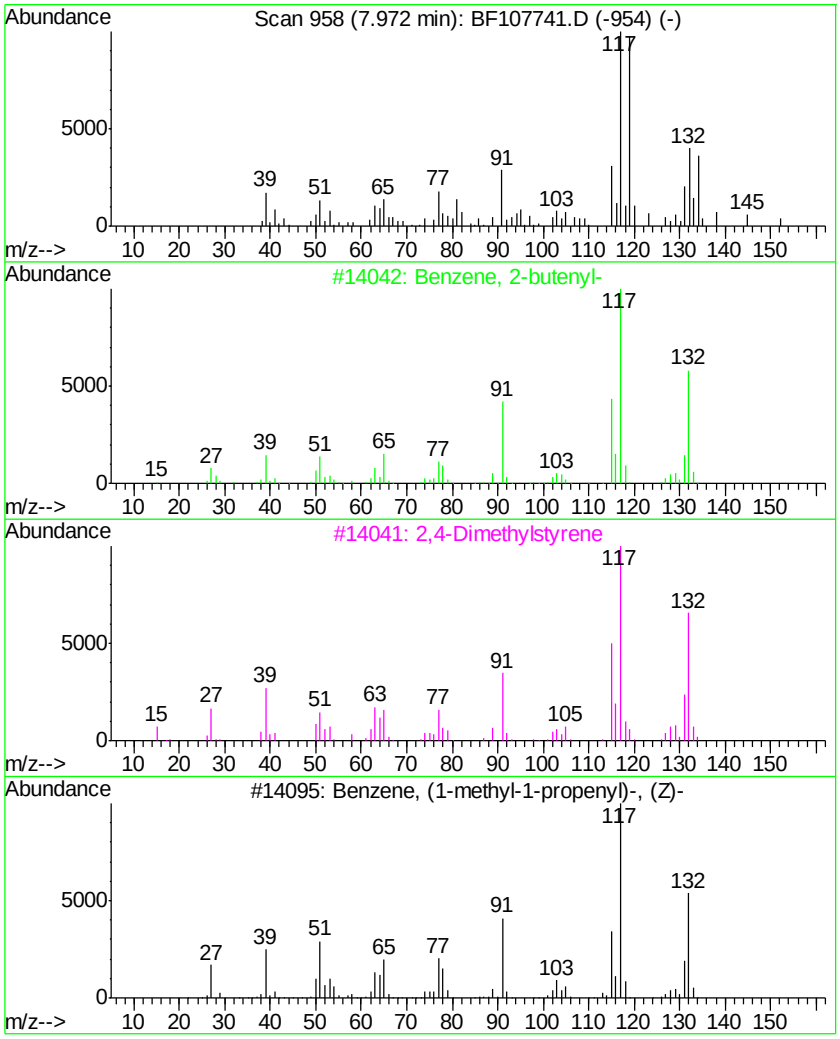
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

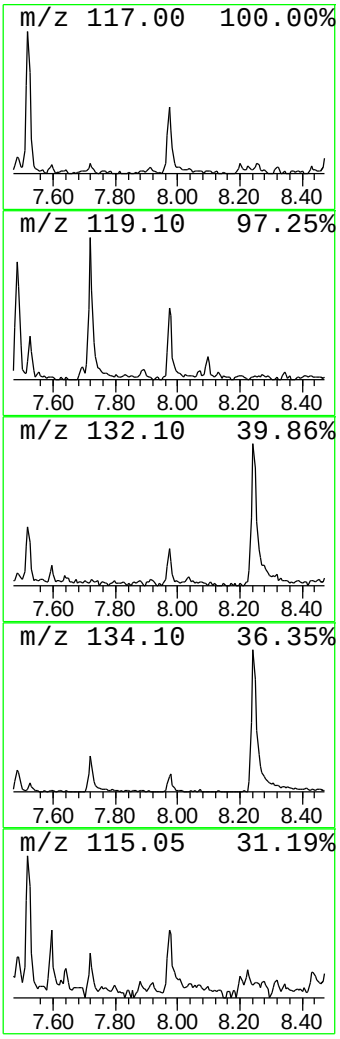
****

Peak Number 5 Benzene, 2-butenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.97	2.72 ng	160808	Naphthalene-d8	8.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-butenyl-	132	C10H12	001560-06-1	87
2	2,4-Dimethylstyrene	132	C10H12	002234-20-0	86
3	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	70
4	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	60
5	3-Phenylbut-1-ene	132	C10H12	000934-10-1	60





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

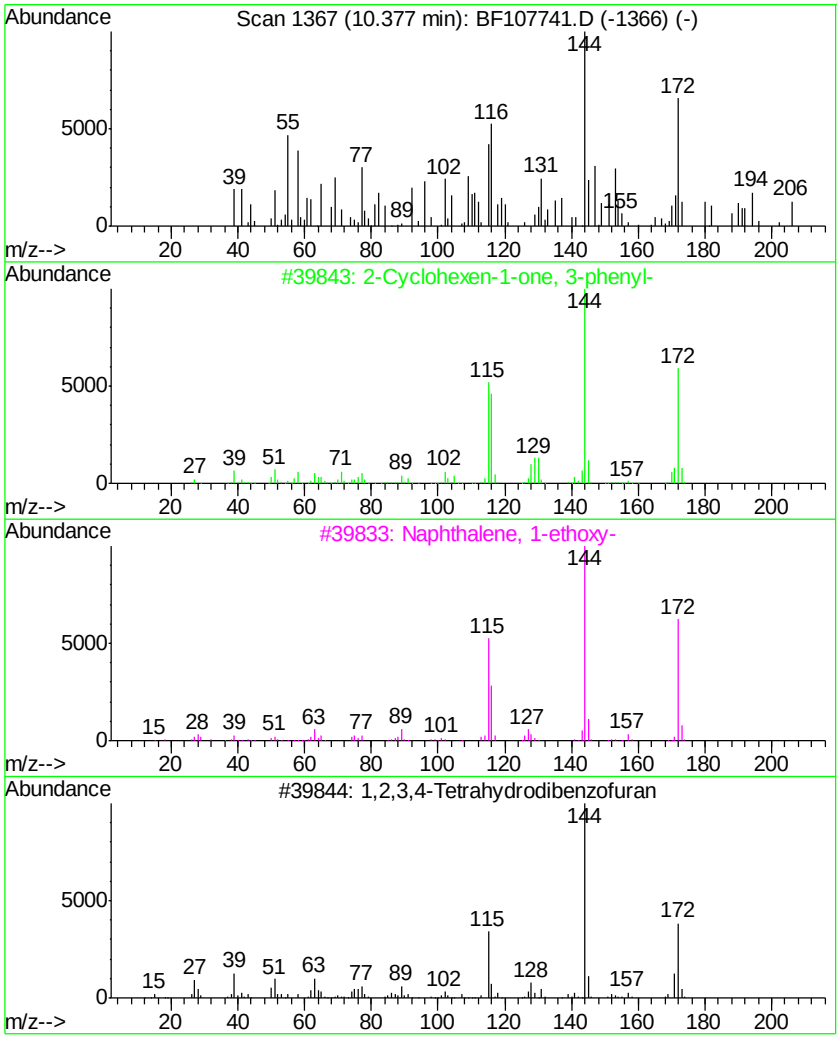
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

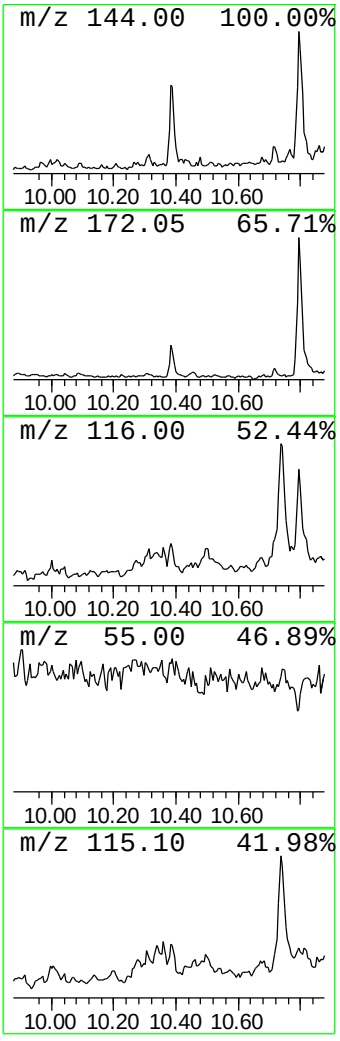
****

Peak Number 6 2-Cyclohexen-1-one, 3-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.32 ng	148734	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-one, 3-phenyl-	172	C12H12O	010345-87-6	58
2	Naphthalene, 1-ethoxy-	172	C12H12O	005328-01-8	52
3	1,2,3,4-Tetrahydrodibenzofuran	172	C12H12O	013130-19-3	43
4	1-Naphthalenecarboxaldehyde, 2-h...	172	C11H8O2	000708-06-5	38
5	2-Naphthalenol	144	C10H8O	000135-19-3	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

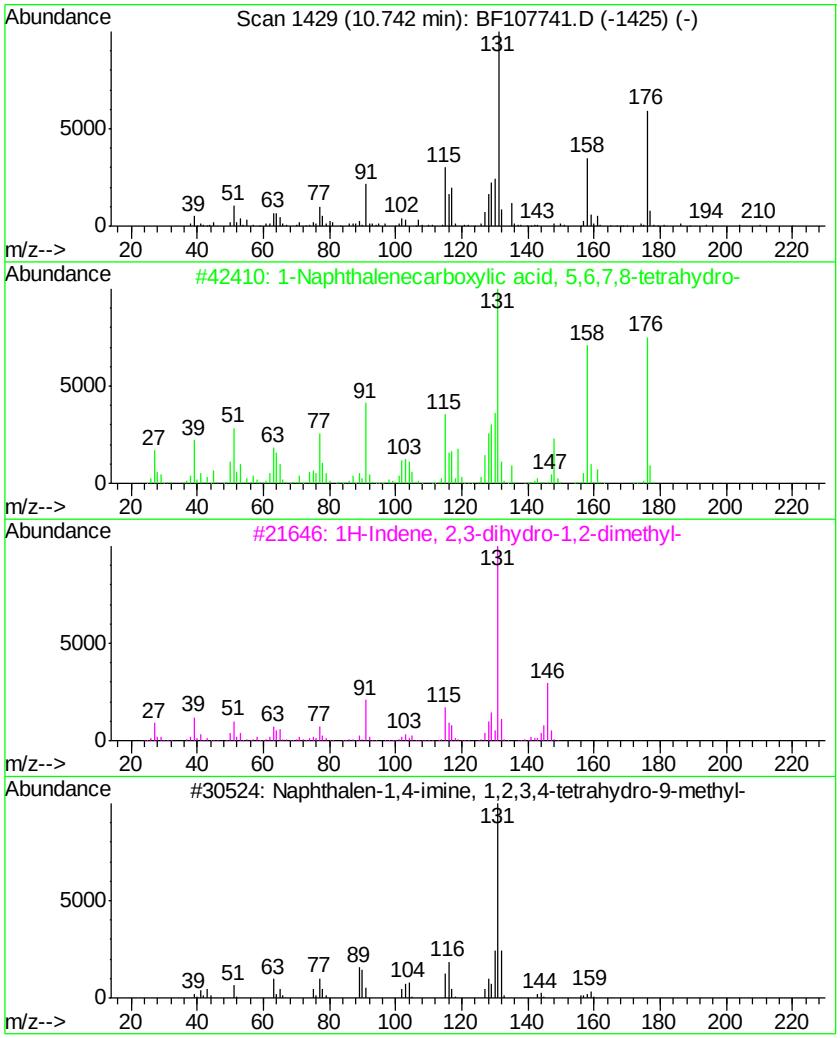
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

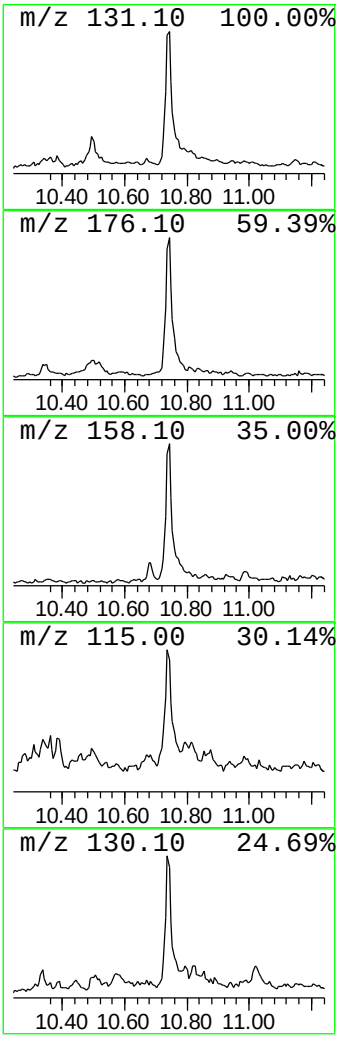
****

Peak Number 7 unknown10.74 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	5.92 ng	378852	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenecarboxylic acid, 5,...	176	C11H12O2	004242-18-6	47
2	1H-Indene, 2,3-dihydro-1,2-dimet...	146	C11H14	017057-82-8	43
3	Naphthalen-1,4-imine, 1,2,3,4-te...	159	C11H13N	055257-99-3	43
4	Benzene, 1-(3-chloro-1-propenyl)...	166	C10H11Cl	1000327-36-5	38
5	Benzene, (2-chloro-2-butenyl)-	166	C10H11Cl	054411-12-0	37





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

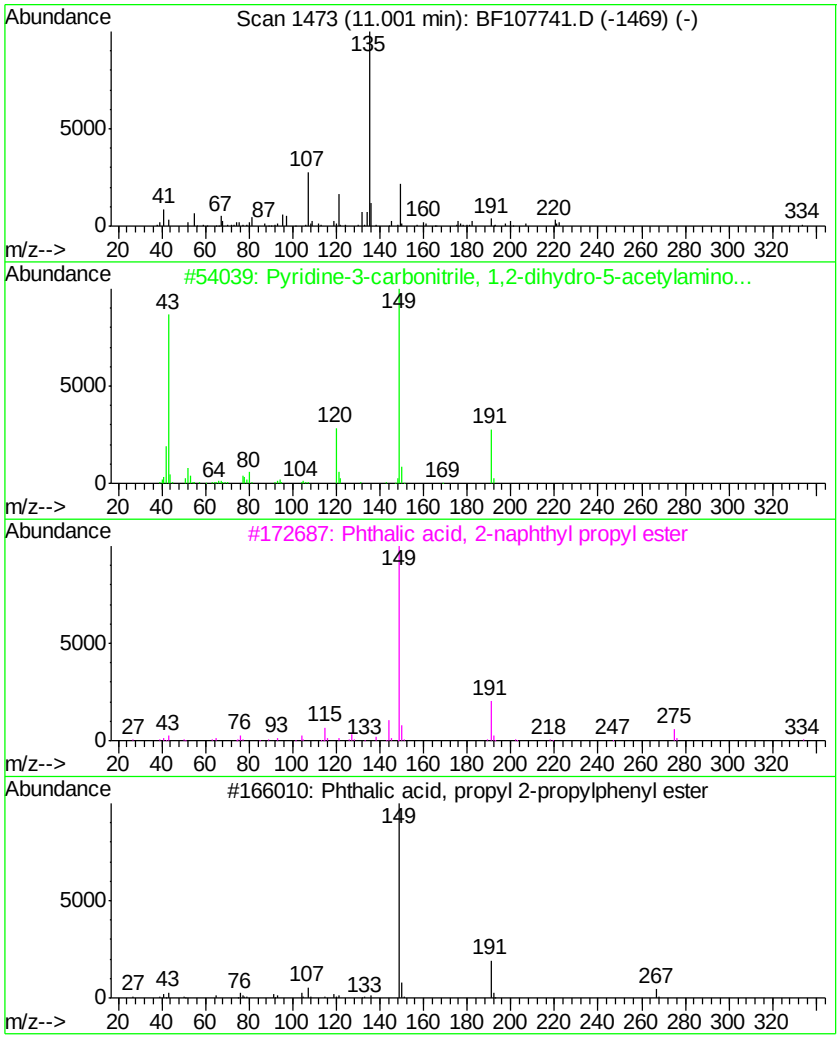
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

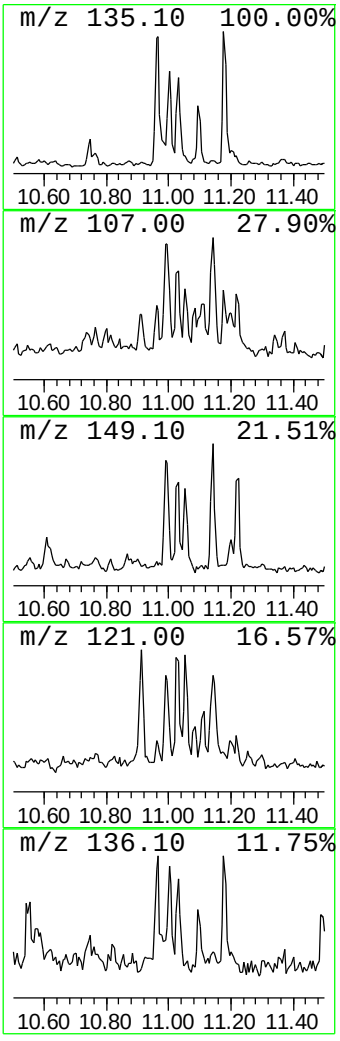
****

Peak Number 8 unknown11.00 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	2.09 ng	106405	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	27
2	Phthalic acid, 2-naphthyl propyl...	334	C21H18O4	1000315-23-9	27
3	Phthalic acid, propyl 2-propylph...	326	C20H22O4	1000357-01-7	27
4	Phthalic acid, 4-methoxyphenyl p...	314	C18H18O5	1000309-77-7	27
5	2-Ethylformanilide	149	C9H11NO	002860-30-2	27





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

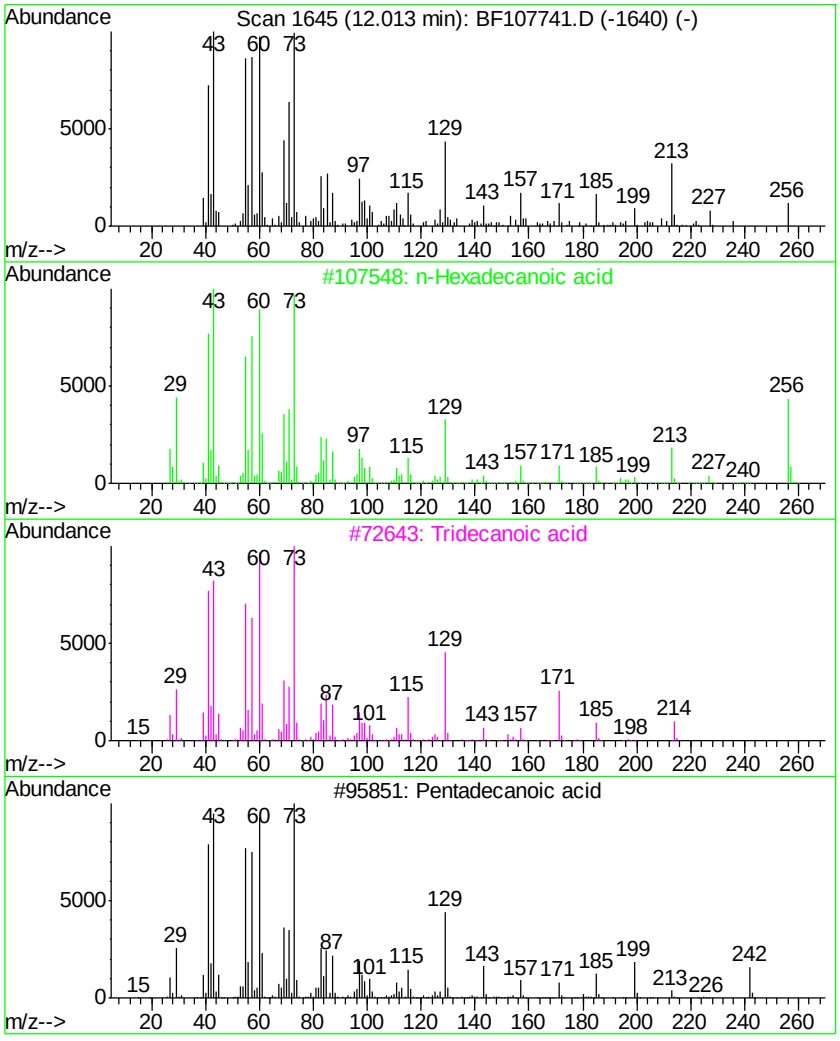
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

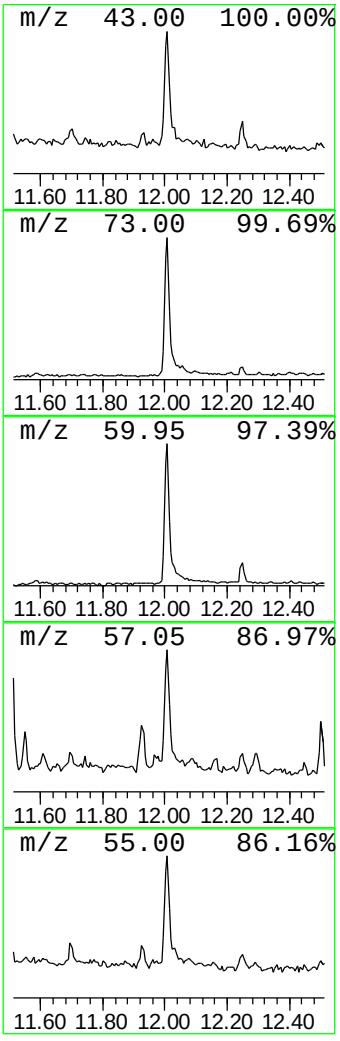
****

Peak Number 9 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	7.54 ng	384245	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

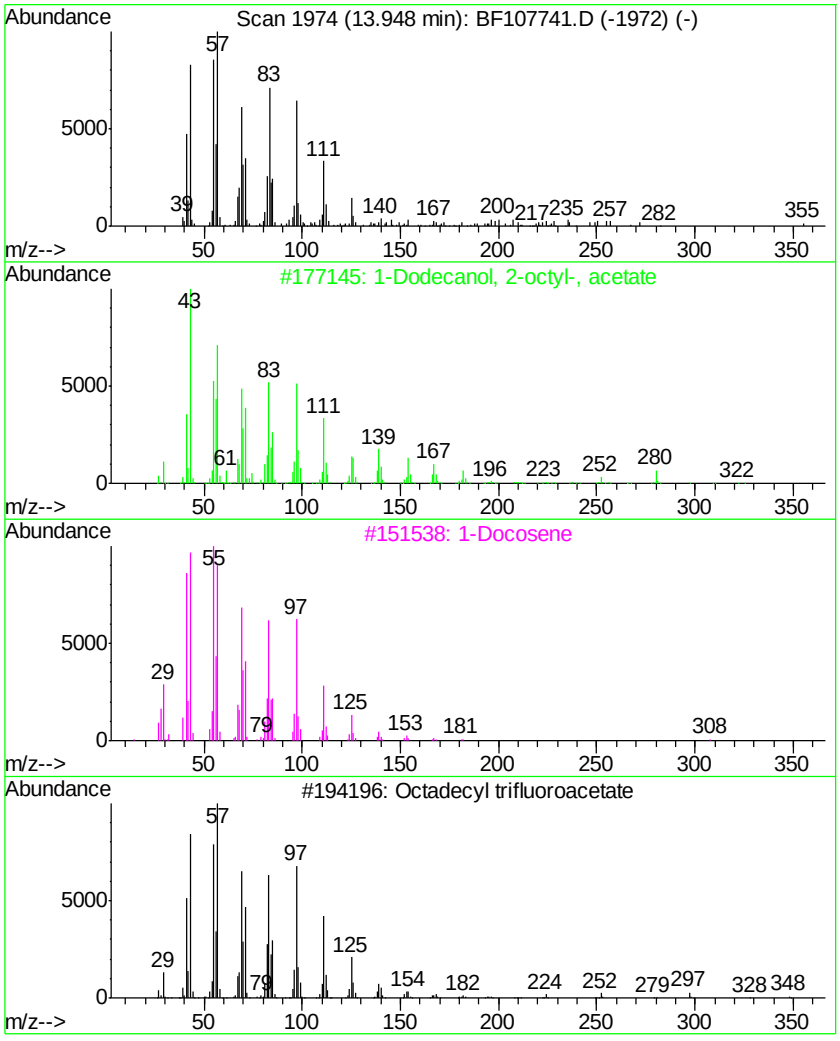
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

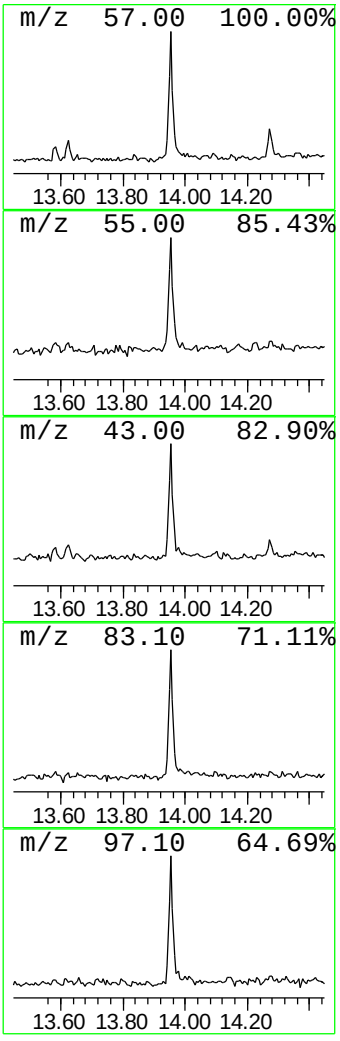
****

Peak Number 10 1-Dodecanol, 2-octyl-, acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	4.50 ng	219106	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-, acetate	340	C22H44O2	074051-84-6	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
5	1-Hexacosanol	382	C26H54O	000506-52-5	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072618\
Data File : BF107741.D
Acq On : 27 Jul 2018 11:16
Operator : JU/SJ
Sample : J4163-02
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-18

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	5.2	ng	249958	1	6.97	955215	20.0
unknown6.74	6.74	86.6	ng	4135350	1	6.97	955215	20.0
2,2-Dimethylinden...	7.60	4.9	ng	235830	1	6.97	955215	20.0
Benzene, 2-butenyl-	7.97	2.7	ng	160808	2	8.24	1183950	20.0
2-Cyclohexen-1-on...	10.38	2.3	ng	148734	3	10.00	1280150	20.0
unknown10.74	10.74	5.9	ng	378852	3	10.00	1280150	20.0
unknown11.00	11.00	2.1	ng	106405	4	11.49	1019780	20.0
n-Hexadecanoic acid	12.01	7.5	ng	384245	4	11.49	1019780	20.0
1-Dodecanol, 2-oc...	13.95	4.5	ng	219106	5	14.14	973818	20.0