LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
Data File : BF102548.D
Acq On : 28 Jan 2018 9:16
Operator : SJ/JU
Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

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-BF012218.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	3.622	257	261	267	rVB	37058	58213	1.28%	0.186%
2	4.904	476	479	487	rBV	51186	66948	1.47%	0.214%
3	5.322	546	550	563	rBV	2256021	2197848	48.15%	7.013%
4	6.351	722	725	743	rBV	1431461	1508233	33.04%	4.813%
5	6.487	743	748	751	rBV	3823044	3632819	79.58%	11.592%
6	6.710	783	786	795	rBV	1133115	966540	21.17%	3.084%
7	6.869	809	813	816	rBV	3681319	3446288	75.50%	10.997%
8	7.281	878	883	893	rBV	2506271	2844773	62.32%	9.077%
9	7.457	910	913	916	rVB	96288	81338	1.78%	0.260%
10	7.992	1001	1004	1018	rBV	1280413	1310877	28.72%	4.183%
11	8.239	1043	1046	1049	rVB	69256	65191	1.43%	0.208%
12	8.551	1096	1099	1103	rBV	75595	72834	1.60%	0.232%
13	8.592	1103	1106	1113	rBV6	48647	81531	1.79%	0.260%
14	8.916	1154	1161	1162	rBV3	35275	59101	1.29%	0.189%
15	9.075	1183	1188	1191	rBV	4620978	4564884	100.00%	14.566%
16	9.169	1202	1204	1209	rBV4	54913	57746	1.27%	0.184%
17	9.339	1228	1233	1235	rBV4	37330	48401	1.06%	0.154%
18	9.416	1244	1246	1249	rBV	55497	47961	1.05%	0.153%
19	9.463	1252	1254	1257	rBV	79659	68358	1.50%	0.218%
20	9.610	1275	1279	1286	rBV7	25750	49419	1.08%	0.158%
21	9.745	1299	1302	1310	rVB2	1326899	1242918	27.23%	3.966%
22	10.175	1371	1375	1378	rBV2	79819	69553	1.52%	0.222%
23	10.357	1403	1406	1416	rBV	230907	269625	5.91%	0.860%
24	10.539	1433	1437	1448	rBV	2095726	2013805	44.12%	6.426%
25	10.645	1452	1455	1456	rVV2	76337	76248	1.67%	0.243%
26	10.663	1456	1458	1464	rVB2	109649	136554	2.99%	0.436%
27	10.869	1491	1493	1496	rBV2	74810	65283	1.43%	0.208%
28	11.092	1524	1531	1533	rBV3	36826	57761	1.27%	0.184%
29	11.233	1549	1555	1562	rBV	1012930	942504	20.65%	3.007%
30	12.633	1789	1793	1797	rVB	274724	218453	4.79%	0.697%
31	12.822	1820	1825	1828	rBV	2993513	3034865	66.48%	9.684%
32	13.339	1909	1913	1917	rBV	167661	140388	3.08%	0.448%
33	13.716	1972	1977	1986	rBV2	46131	90132	1.97%	0.288%
34	13.874	2000	2004	2010	rBV	841770	848178	18.58%	2.706%

LSC Area Percent Report

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Data File : BF102548.D
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Operator : SJ/JU
Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

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-BF012218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.298	2241	2246	2257	rBV2	609320	781547	17.12%	2.494%
36	15.710	2313	2316	2326	rVB4	40612	57282	1.25%	0.183%
37	16.180	2392	2396	2402	rBV3	36470	64374	1.41%	0.205%

Sum of corrected areas: 31338773

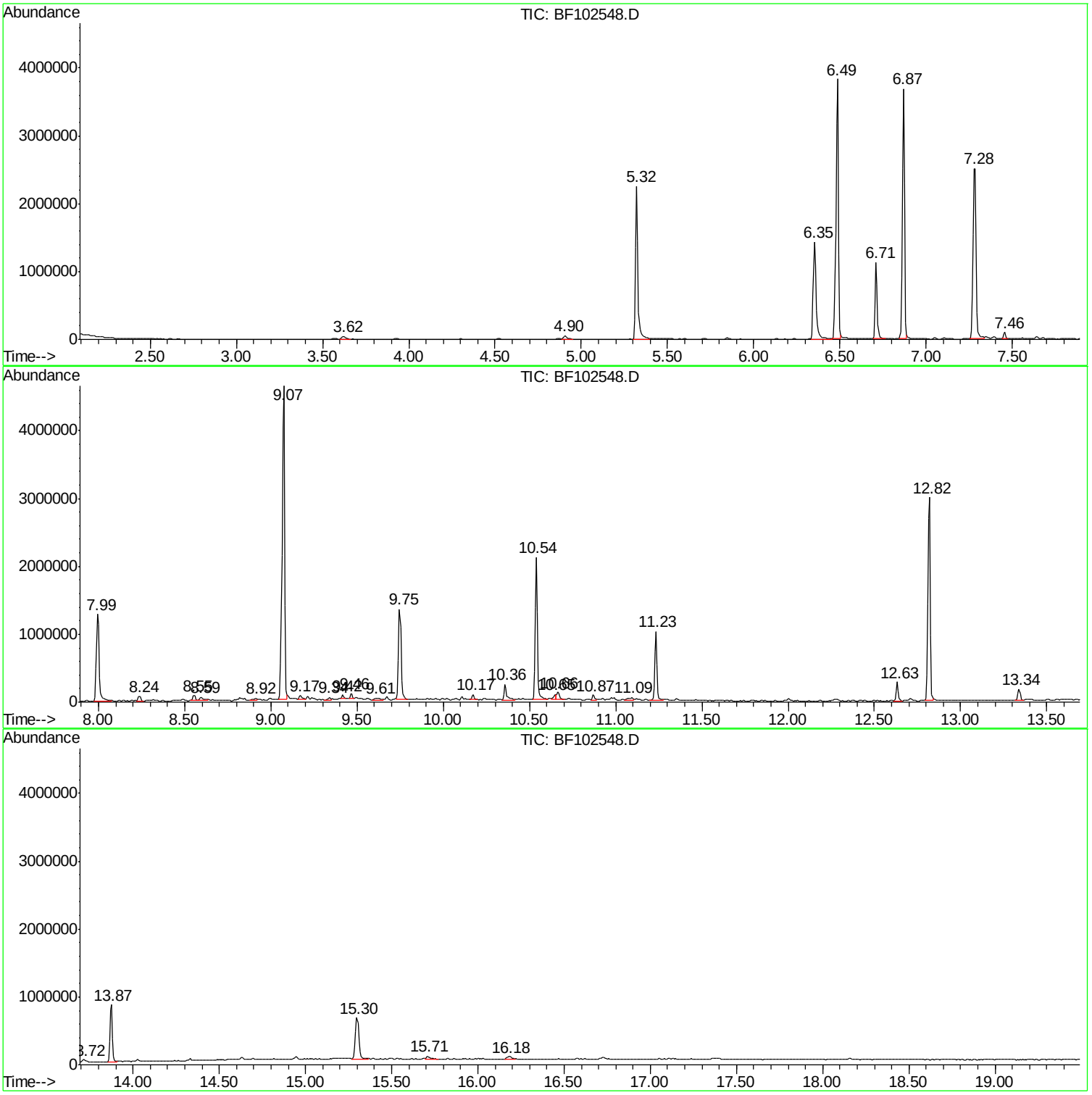
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
Data File : BF102548.D
Acq On : 28 Jan 2018 9:16
Operator : SJ/JU
Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
Data File : BF102548.D
Acq On : 28 Jan 2018 9:16
Operator : SJ/JU
Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

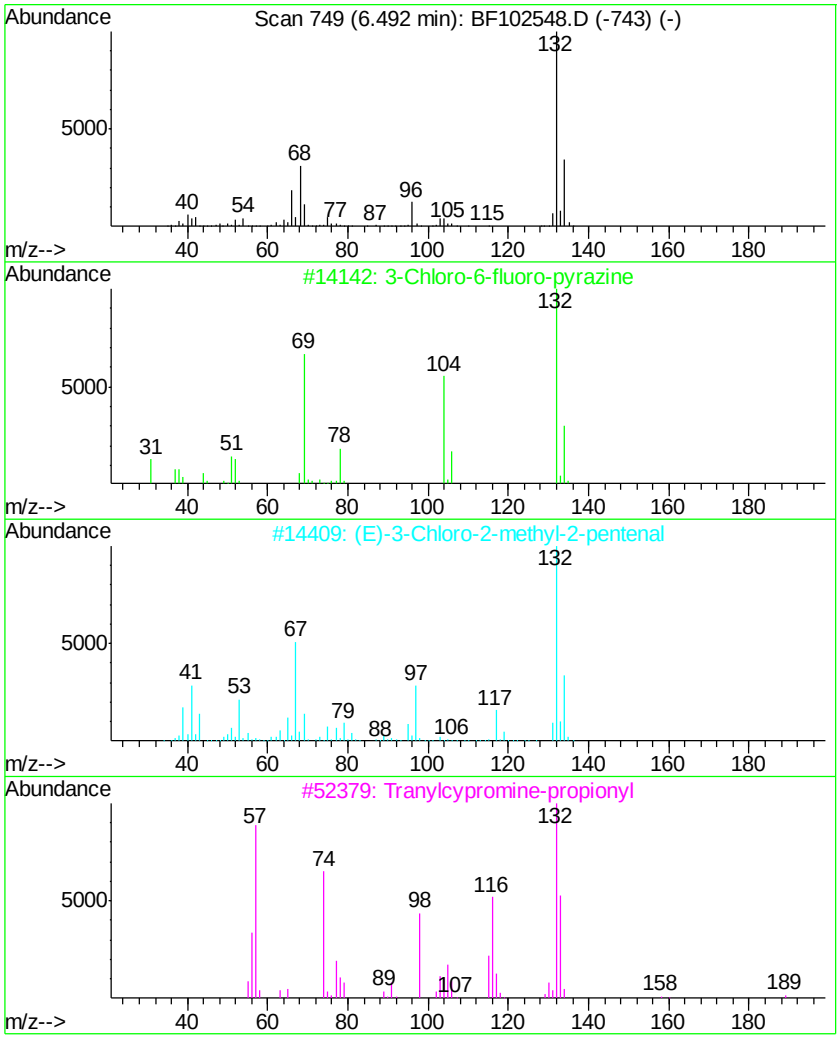
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

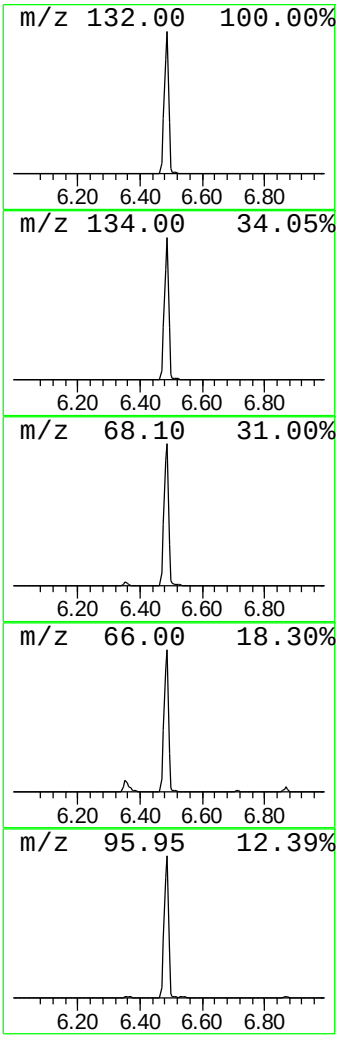
****

Peak Number 1 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	75.17 ng	3632820	1,4-Dichlorobenzene-d4	6.71

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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
Data File : BF102548.D
Acq On : 28 Jan 2018 9:16
Operator : SJ/JU
Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

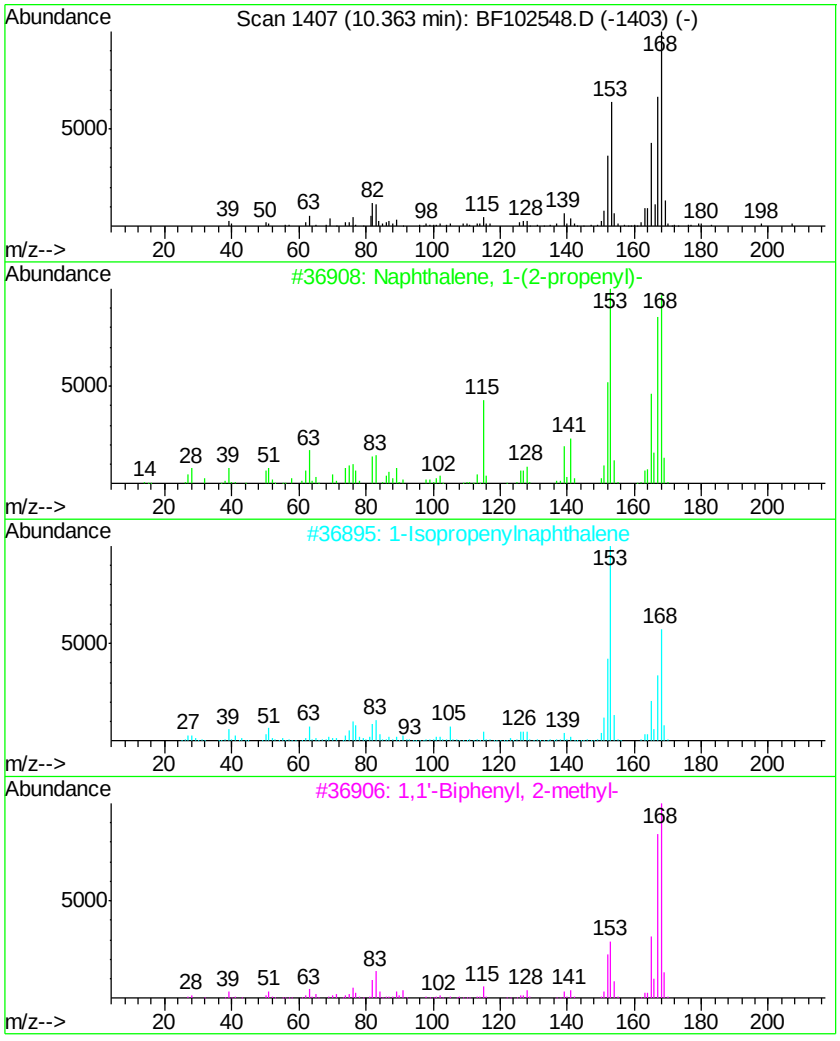
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

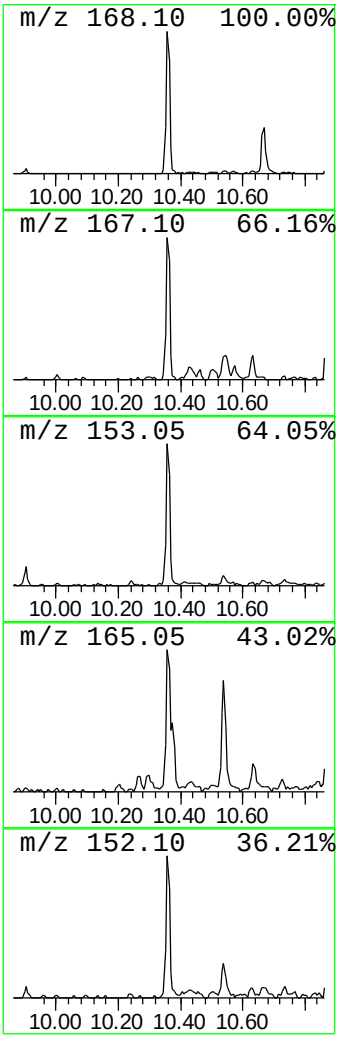
****

Peak Number 3 Naphthalene, 1-(2-propenyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.36	4.34 ng	269625	Acenaphthene-d10	9.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-(2-propenyl)-	168	C13H12	002489-86-3	90
2	1-Isopropenylnaphthalene	168	C13H12	001855-47-6	81
3	1,1'-Biphenyl, 2-methyl-	168	C13H12	000643-58-3	81
4	Nordiphenamid	225	C15H15NO	000954-21-2	72
5	1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	62





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
Data File : BF102548.D
Acq On : 28 Jan 2018 9:16
Operator : SJ/JU
Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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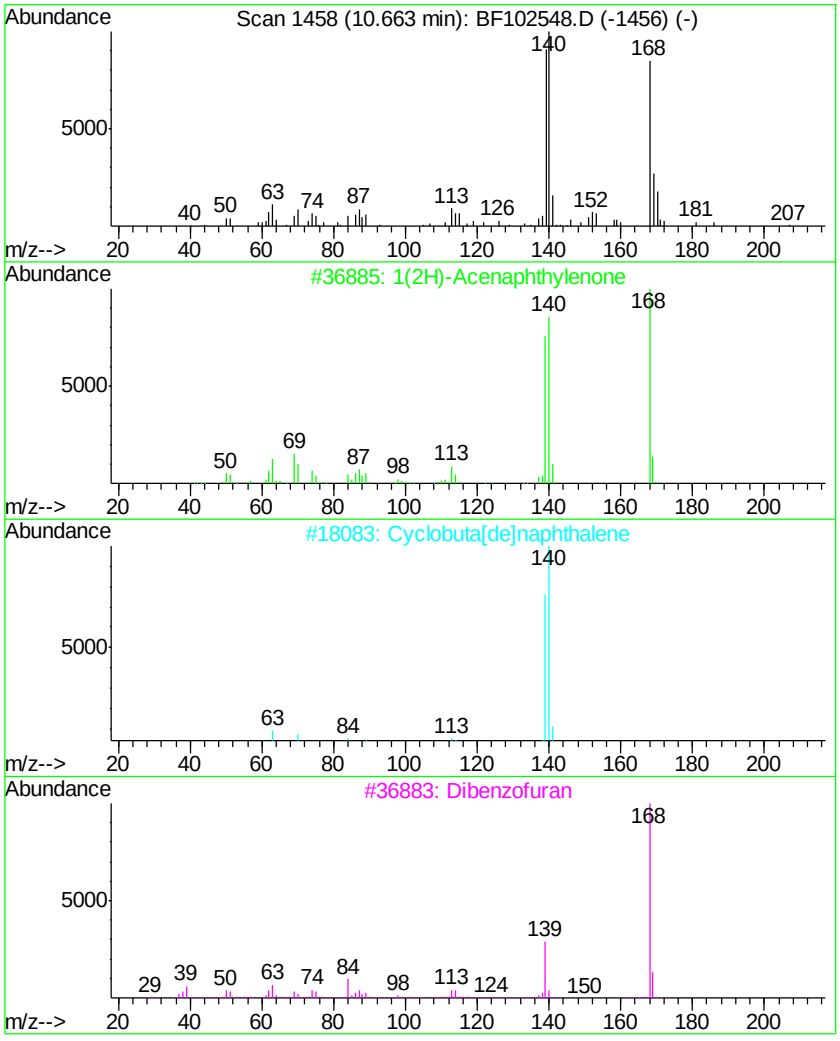
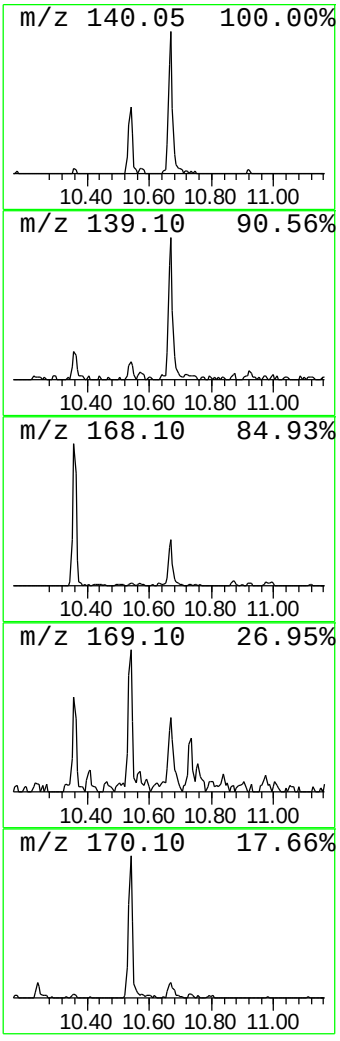
Peak Number 4 1(2H)-Acenaphthylenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.66	2.90 ng	136554	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1(2H)-Acenaphthylenone	168	C12H8O	002235-15-6	95
2	Cyclobuta[de]naphthalene	140	C11H8	024973-91-9	60
3	Dibenzofuran	168	C12H8O	000132-64-9	46
4	Benzaldehyde, 2-fluoro-4-hydroxy-	140	C7H5FO2	000348-27-6	43
5	1-Naphthalenecarbonitrile, 4-amino-	168	C11H8N2	058728-64-6	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
Data File : BF102548.D
Acq On : 28 Jan 2018 9:16
Operator : SJ/JU
Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

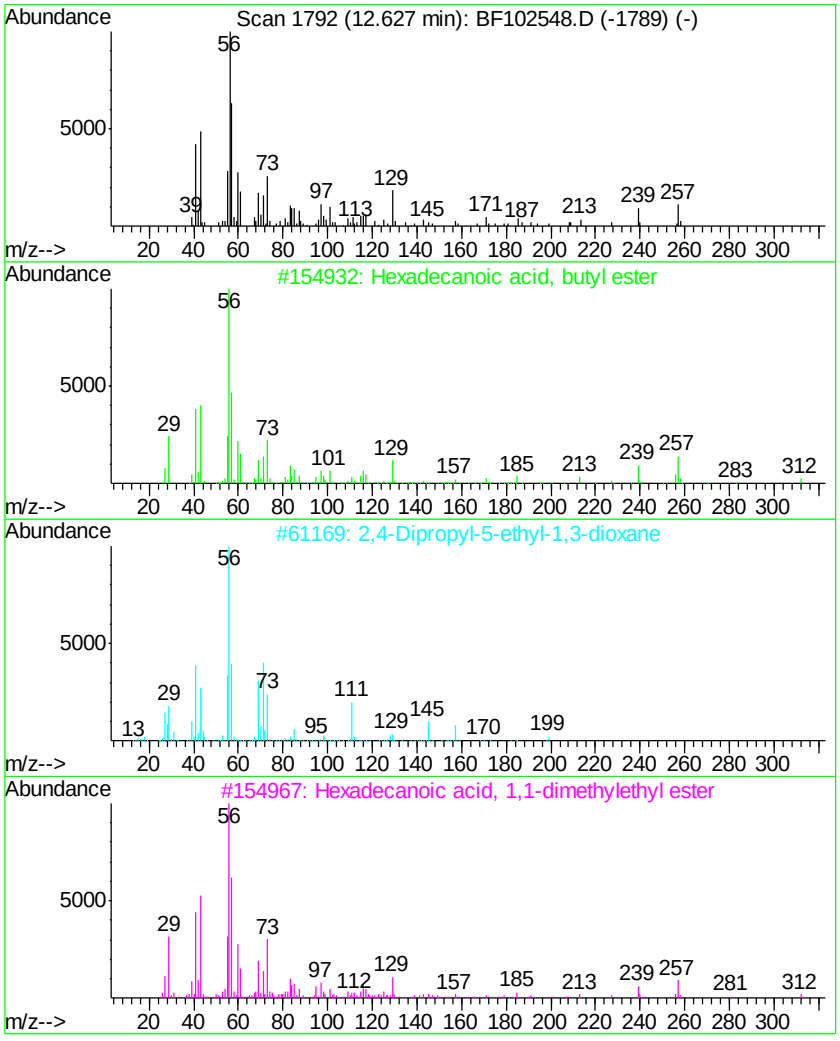
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

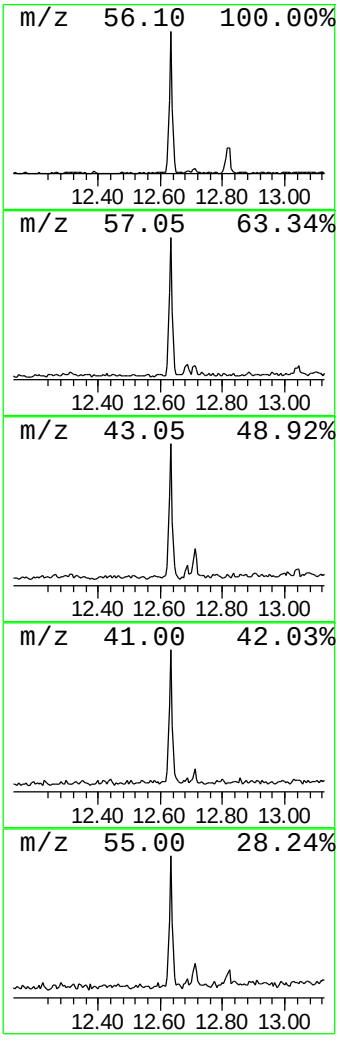
****

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	5.15 ng	218453	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	47
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	47
4	Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	42
5	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	38





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
Data File : BF102548.D
Acq On : 28 Jan 2018 9:16
Operator : SJ/JU
Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

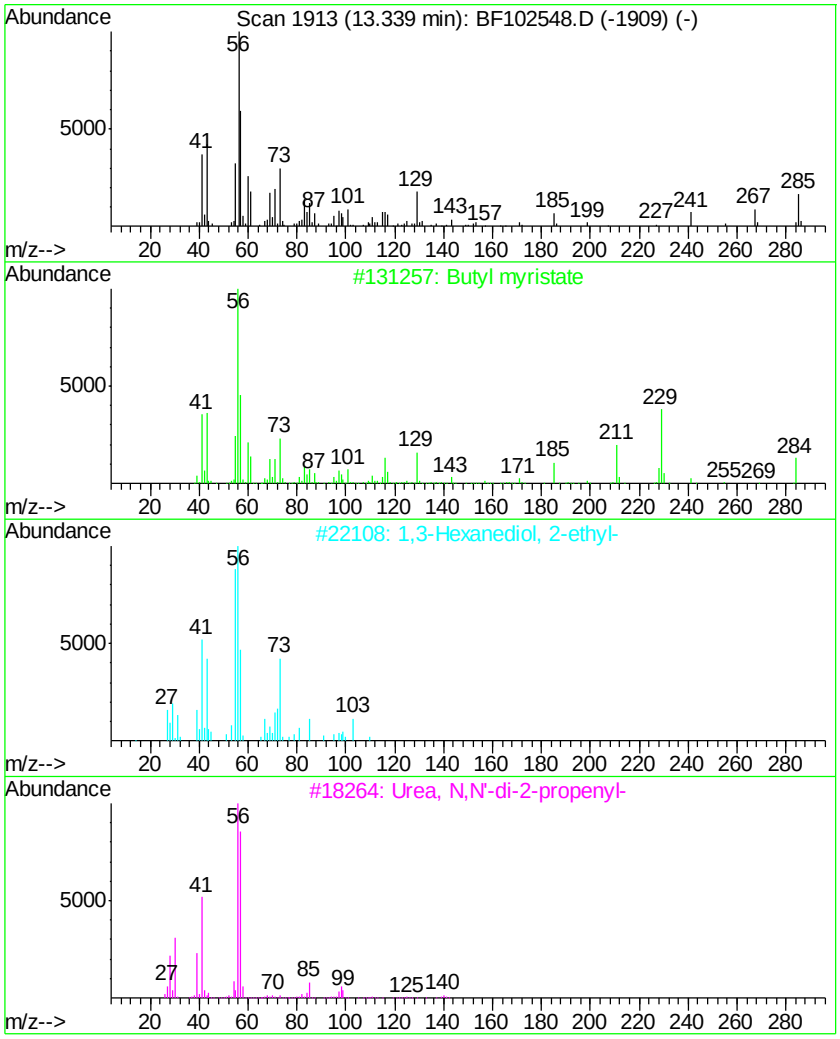
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

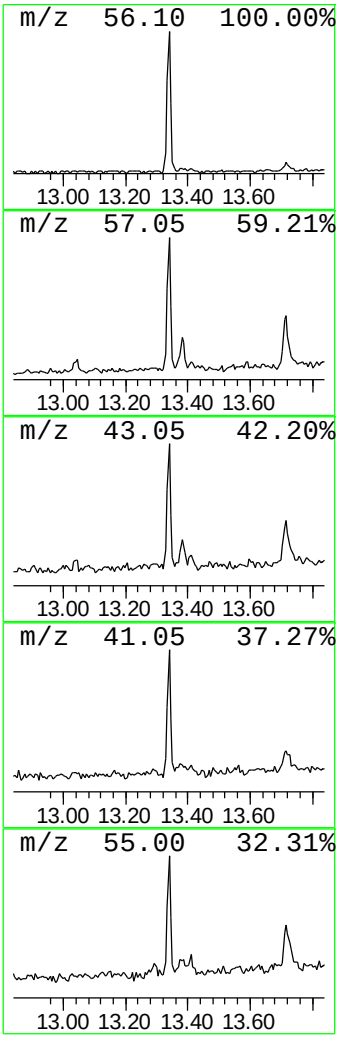
****

Peak Number 6 Butyl myristate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	3.31 ng	140388	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	72
2	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	37
3	Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
4	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	27
5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27





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Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

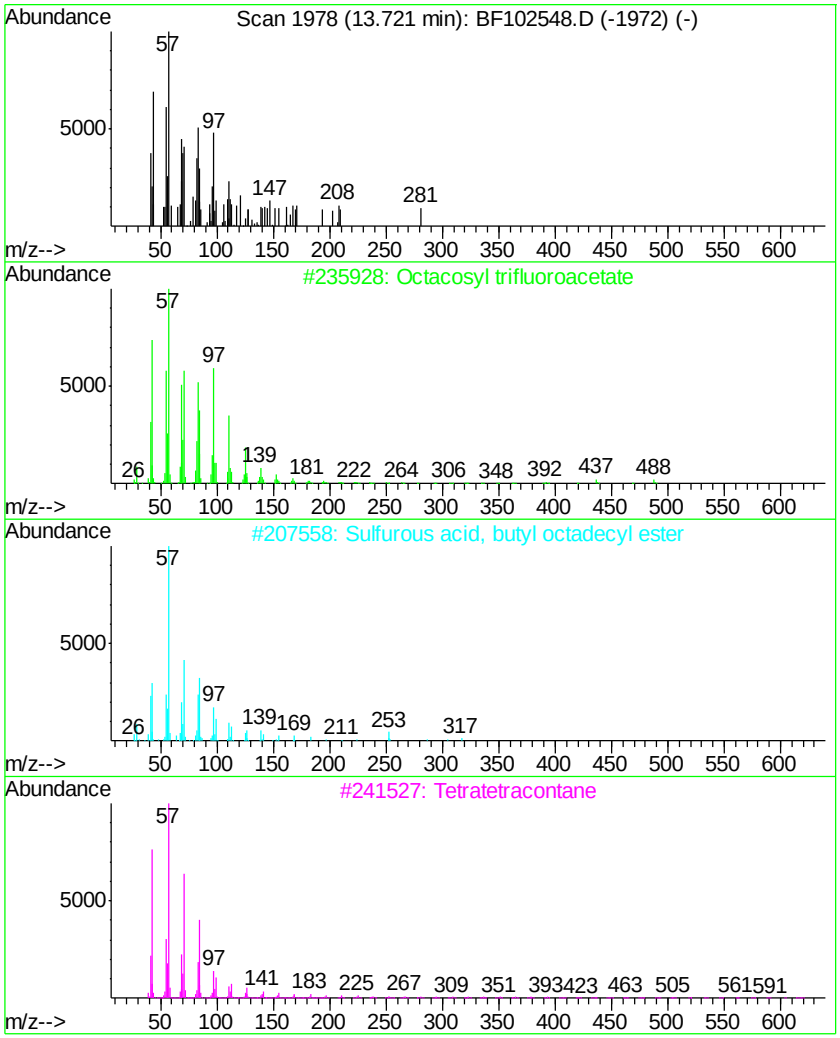
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

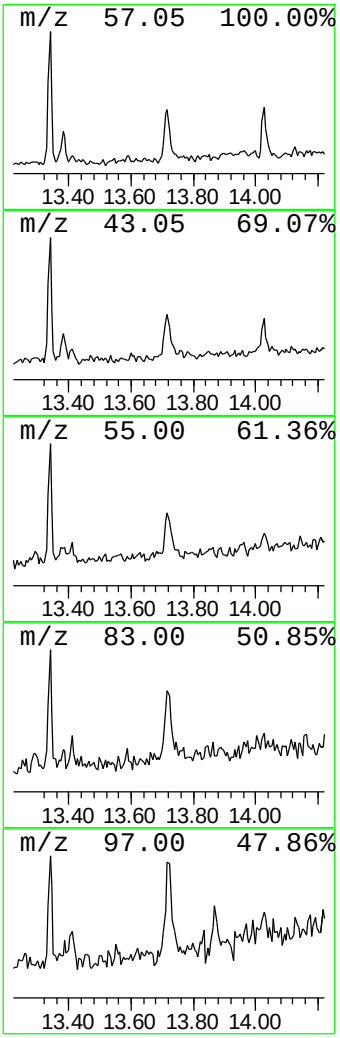
****

Peak Number 7 Octacosyl trifluoroacetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	2.13 ng	90132	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	58
2	Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	52
3	Tetratetracontane	619	C44H90	007098-22-8	50
4	Tritetracontane	605	C43H88	007098-21-7	50
5	Hexacosane	366	C26H54	000630-01-3	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012718\
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Acq On : 28 Jan 2018 9:16
Operator : SJ/JU
Sample : J1321-02
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OWL-C2-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF012218.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
unknown6.49	6.49	75.2	ng	3632820	1	6.71	966540	20.0
Naphthalene, 1-(2...	10.36	4.3	ng	269625	3	9.75	1242920	20.0
1(2H)-Acenaphthyl...	10.66	2.9	ng	136554	4	11.23	942504	20.0
Hexadecanoic acid...	12.63	5.2	ng	218453	5	13.87	848178	20.0
Butyl myristate	13.34	3.3	ng	140388	5	13.87	848178	20.0
Octacosyl trifluo...	13.72	2.1	ng	90132	5	13.87	848178	20.0