LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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	4.922	478	482	493	rVB	168161	231783	7.07%	0.626%
2	5.340	548	553	568	rBV	3077501	3174693	96.81%	8.576%
3	6.369	723	728	745	rBV	2770741	3279251	100.00%	8.858%
4	6.493	745	749	752	rBV	3351105	3150732	96.08%	8.511%
5	6.716	784	787	791	rBV	911778	785242	23.95%	2.121%
6	6.875	810	814	817	rBV	2705167	2363884	72.09%	6.386%
7	7.287	879	884	887	rBV	2005092	1921897	58.61%	5.192%
8	7.998	1001	1005	1021	rVB	1159422	1048324	31.97%	2.832%
9	9.075	1183	1188	1192	rBV	2842899	2787038	84.99%	7.529%
10	9.469	1252	1255	1263	rVB	426419	418972	12.78%	1.132%
11	9.681	1288	1291	1295	rBV	104471	87211	2.66%	0.236%
12	9.751	1299	1303	1308	rVB	1093914	978449	29.84%	2.643%
13	10.181	1369	1376	1379	rBV	135404	118687	3.62%	0.321%
14	10.404	1407	1414	1416	rBV	31548	43129	1.32%	0.117%
15	10.545	1434	1438	1441	rBV	1704811	1492216	45.50%	4.031%
16	10.657	1454	1457	1461	rBV	100513	101788	3.10%	0.275%
17	11.104	1530	1533	1536	rBV2	39101	36433	1.11%	0.098%
18	11.239	1552	1556	1559	rBV	909664	801039	24.43%	2.164%
19	11.769	1642	1646	1649	rBV	98896	87411	2.67%	0.236%
20	12.822	1821	1825	1829	rVB	1920990	1832552	55.88%	4.950%
21	13.027	1857	1860	1863	rBV	273786	255337	7.79%	0.690%
22	13.051	1863	1864	1867	rVB	99373	63496	1.94%	0.172%
23	13.392	1917	1922	1925	rBV2	61833	93209	2.84%	0.252%
24	13.516	1940	1943	1947	rVB2	46484	40809	1.24%	0.110%
25	13.598	1954	1957	1961	rBV	100258	93330	2.85%	0.252%
26	13.716	1973	1977	1985	rBV	1756461	1862296	56.79%	5.031%
27	13.774	1985	1987	1992	rVB4	43228	44846	1.37%	0.121%
28	13.874	2001	2004	2008	rVB	772299	737739	22.50%	1.993%
29	13.974	2017	2021	2023	rBV	64323	66644	2.03%	0.180%
30	14.039	2028	2032	2035	rBV	166501	197199	6.01%	0.533%
31	14.163	2050	2053	2058	rBV	89691	81936	2.50%	0.221%
32	14.351	2081	2085	2092	rBV	1989035	2423069	73.89%	6.546%
33	14.404	2092	2094	2103	rVB2	81434	93771	2.86%	0.253%
34	14.645	2131	2135	2136	rBV	96069	127016	3.87%	0.343%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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	14.780	2155	2158	2166	rVB	144767	153365	4.68%	0.414%
36	14.968	2185	2190	2192	rBV	632223	850918	25.95%	2.299%
37	14.992	2192	2194	2199	rVV	623866	676580	20.63%	1.828%
38	15.045	2200	2203	2207	rVB	138910	153717	4.69%	0.415%
39	15.304	2243	2247	2254	rBV	485430	717801	21.89%	1.939%
40	15.515	2279	2283	2289	rBV2	147401	209498	6.39%	0.566%
41	15.733	2316	2320	2325	rBV	390554	548359	16.72%	1.481%
42	15.786	2325	2329	2335	rVV	193413	321570	9.81%	0.869%
43	15.851	2336	2340	2348	rVB	226388	371134	11.32%	1.003%
44	16.486	2444	2448	2454	rVB2	102617	183530	5.60%	0.496%
45	16.939	2520	2525	2530	rBV2	191023	419562	12.79%	1.133%
46	17.304	2581	2587	2599	rVB4	223869	526351	16.05%	1.422%
47	17.539	2621	2627	2636	rVB4	248319	557781	17.01%	1.507%
48	17.751	2658	2663	2671	rVB5	187710	407251	12.42%	1.100%

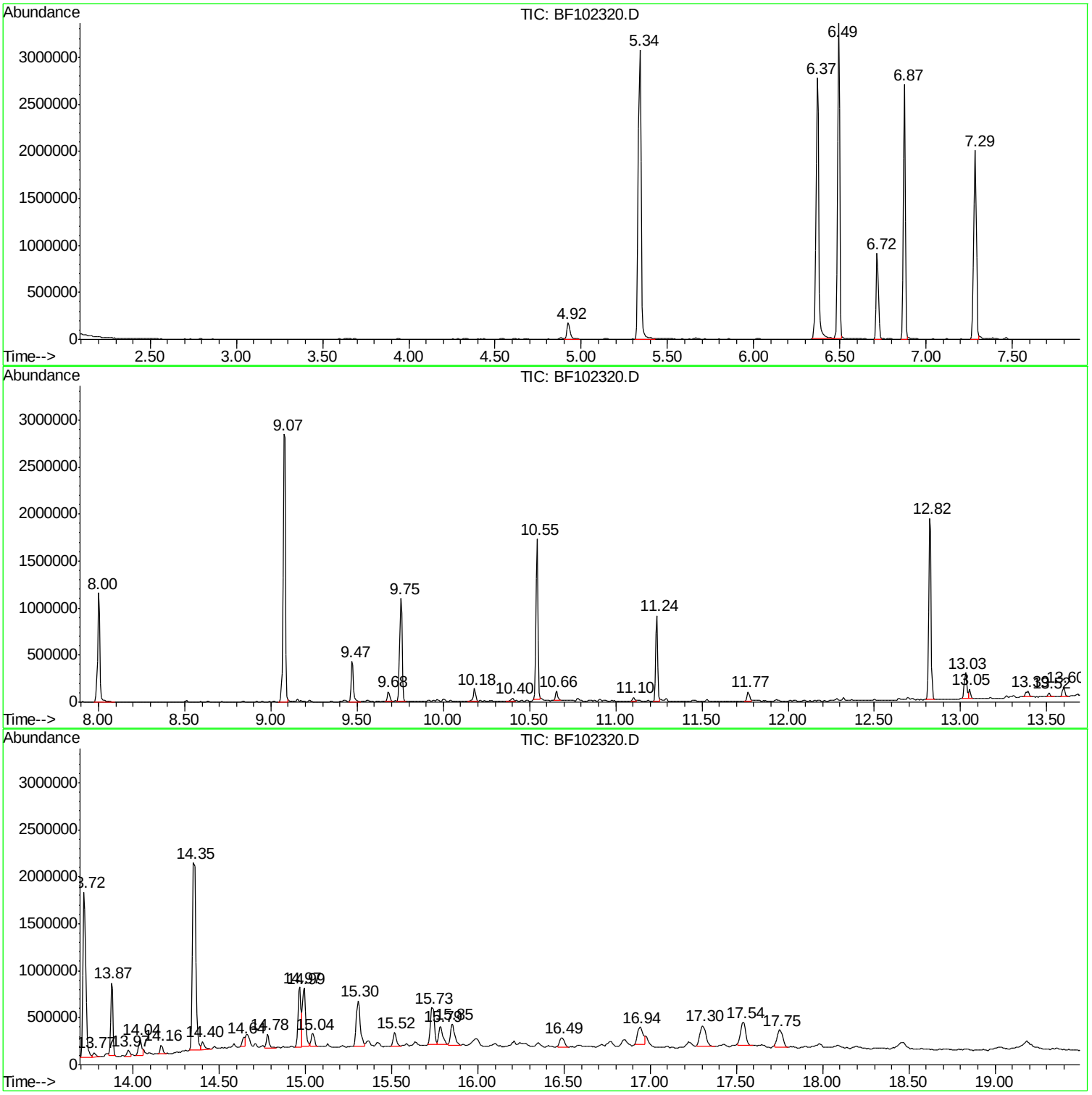
Sum of corrected areas: 37018845

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

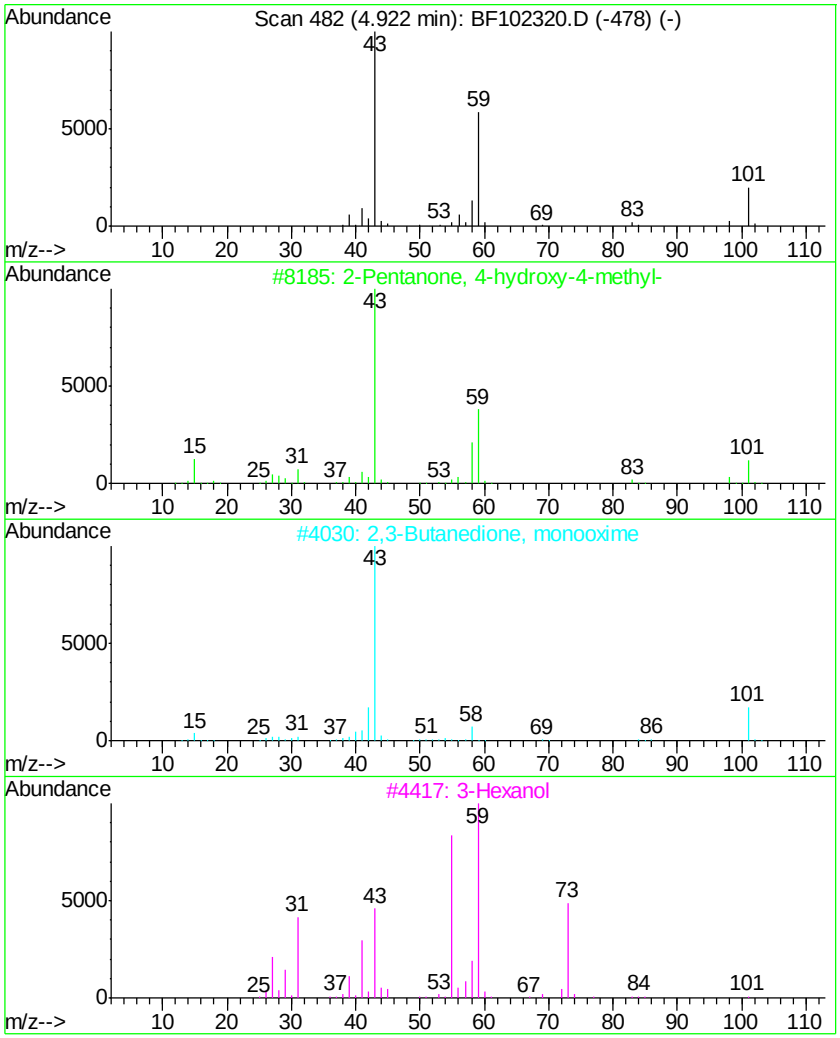
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

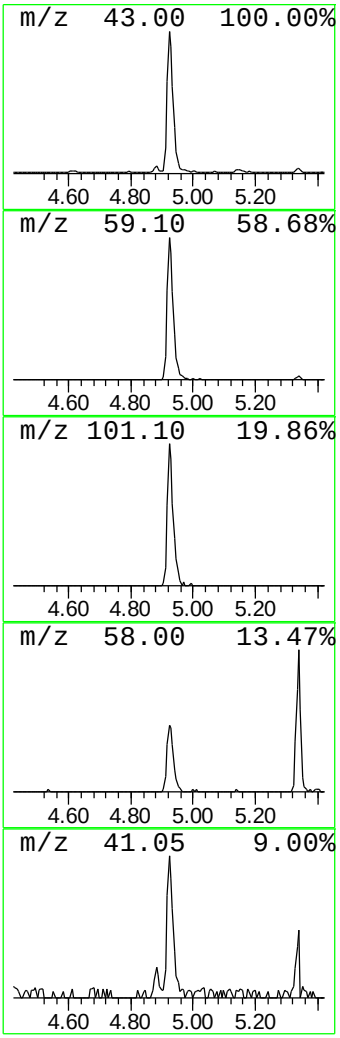
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	5.90 ng	231783	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

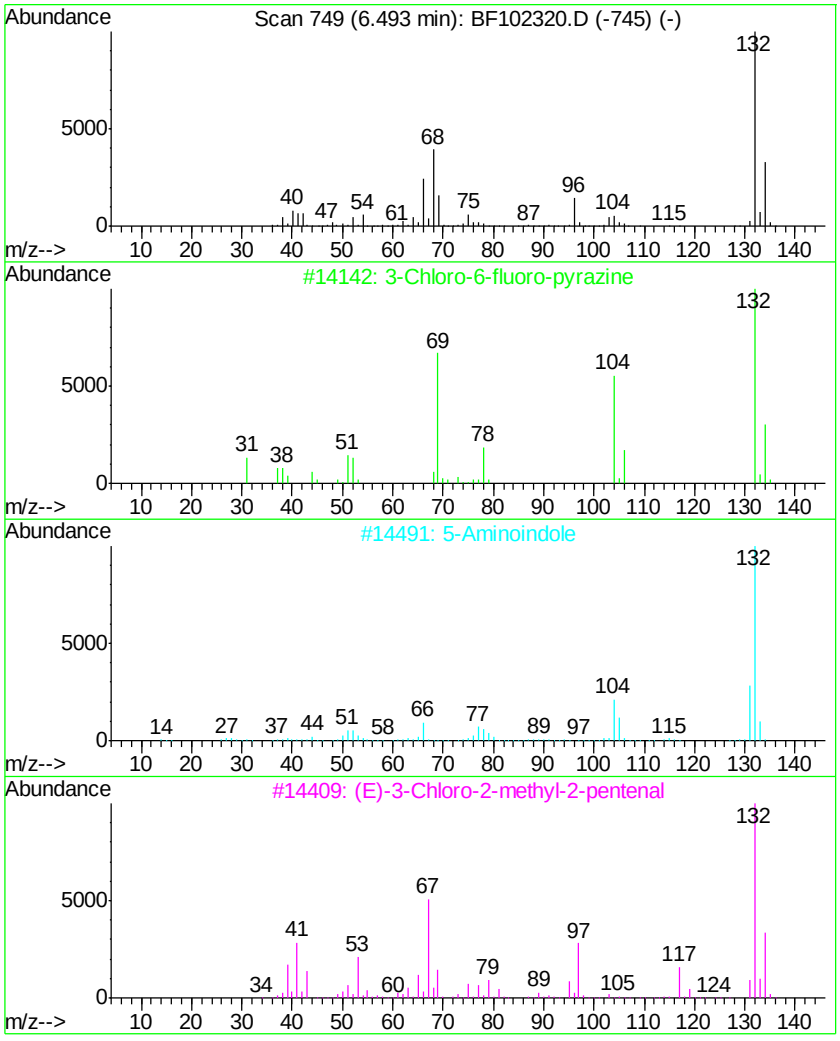
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

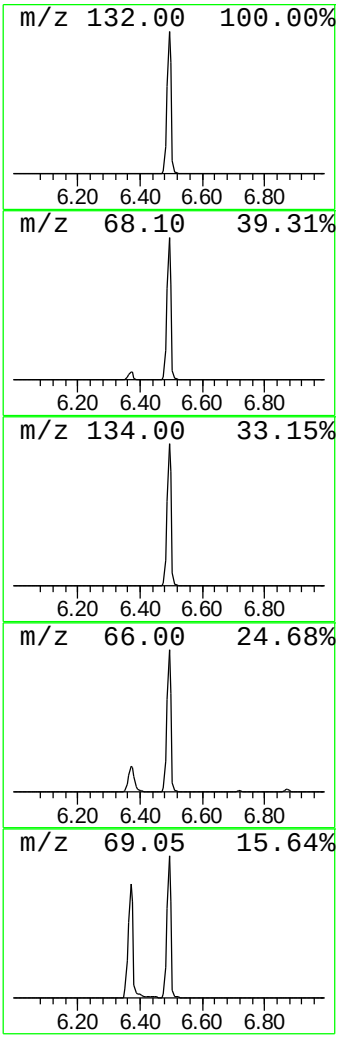
****

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	80.25 ng	3150730	1,4-Dichlorobenzene-d4	6.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

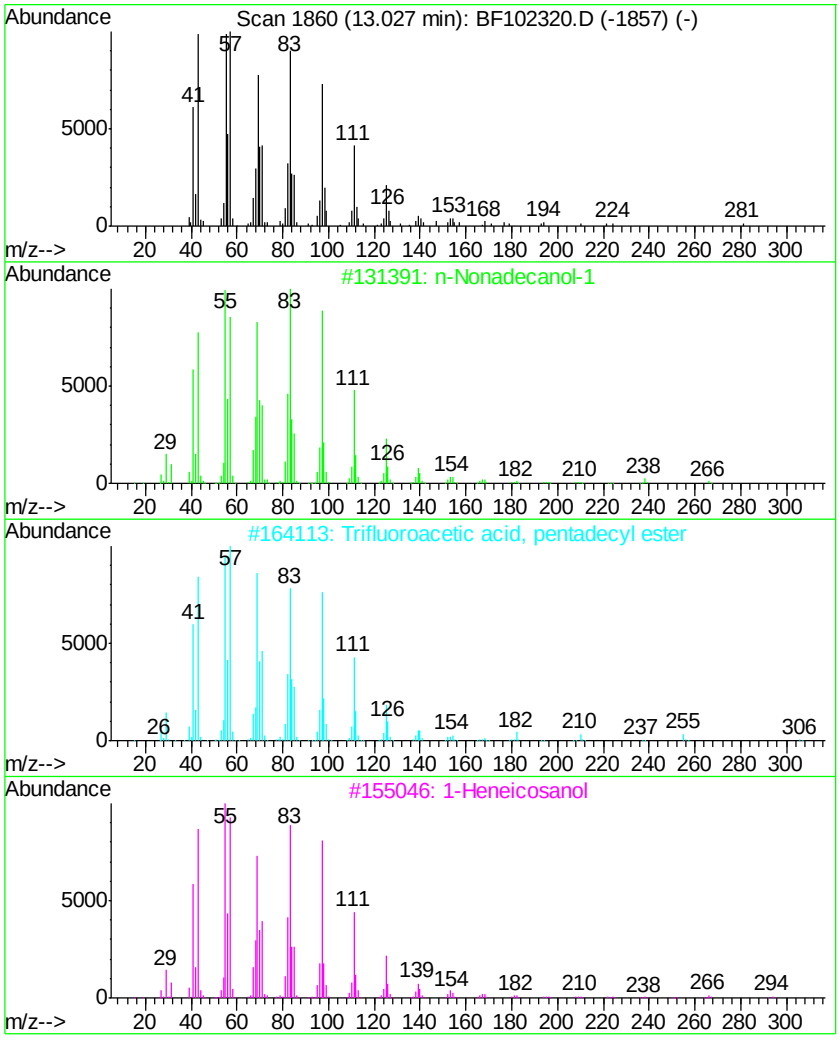
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

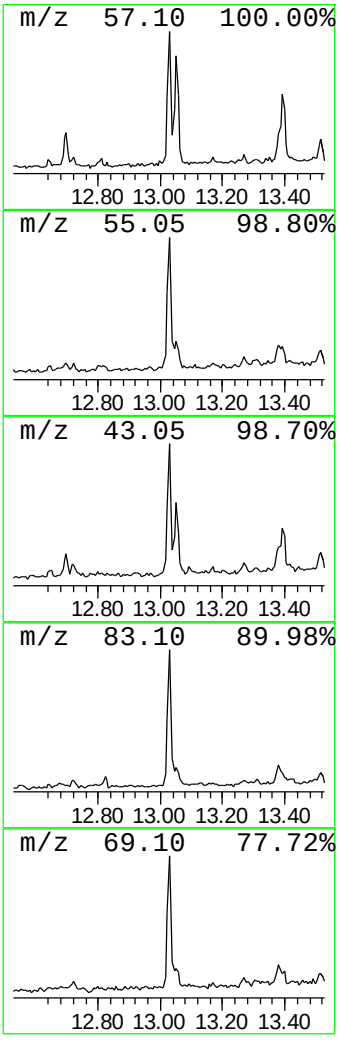
****

Peak Number 4 n-Nonadecanol-1 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.03	6.92 ng	255337	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Behenic alcohol	326	C22H46O	000661-19-8	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

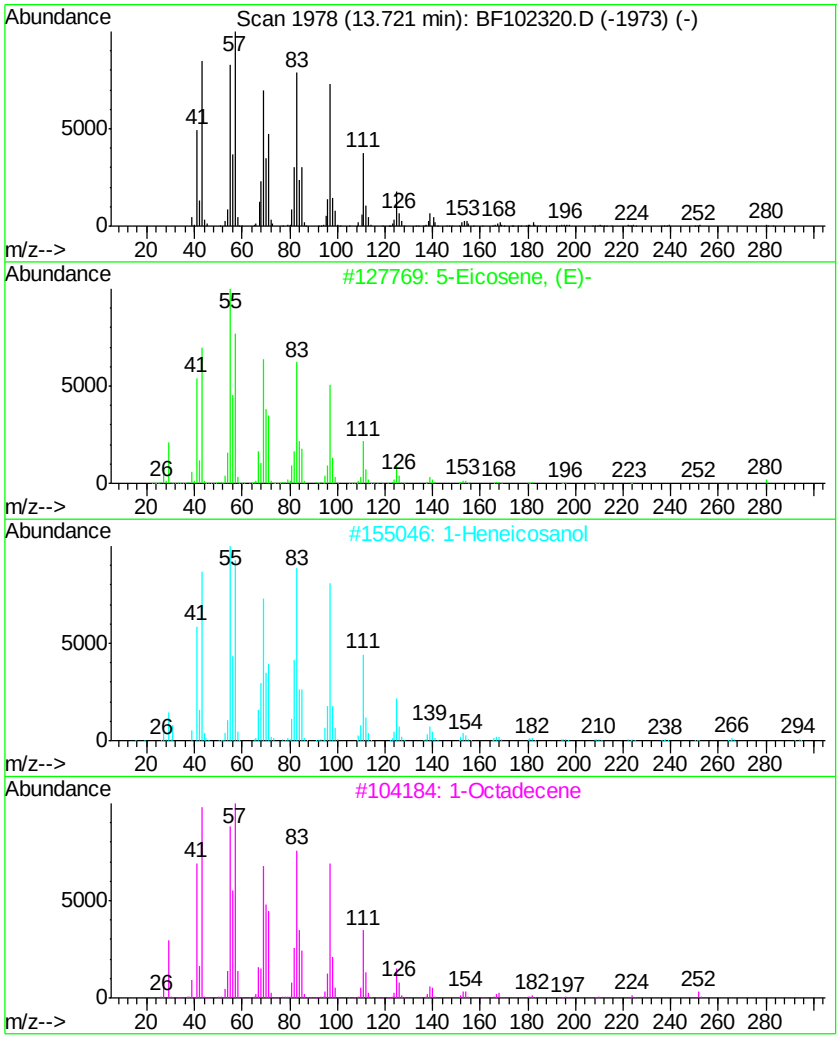
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

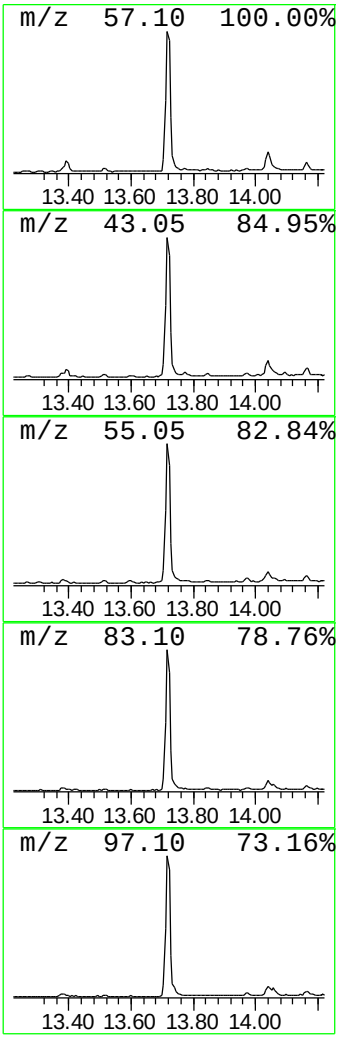
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	50.49 ng	1862300	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Octadecene	252	C18H36	000112-88-9	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

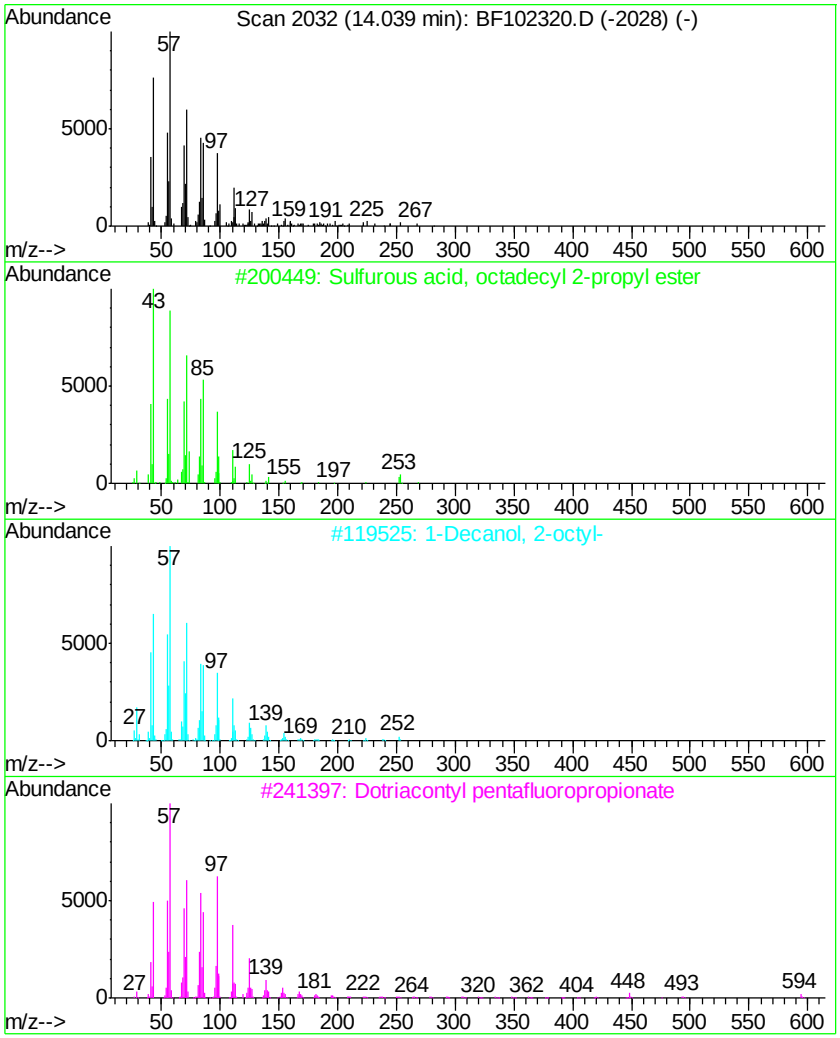
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

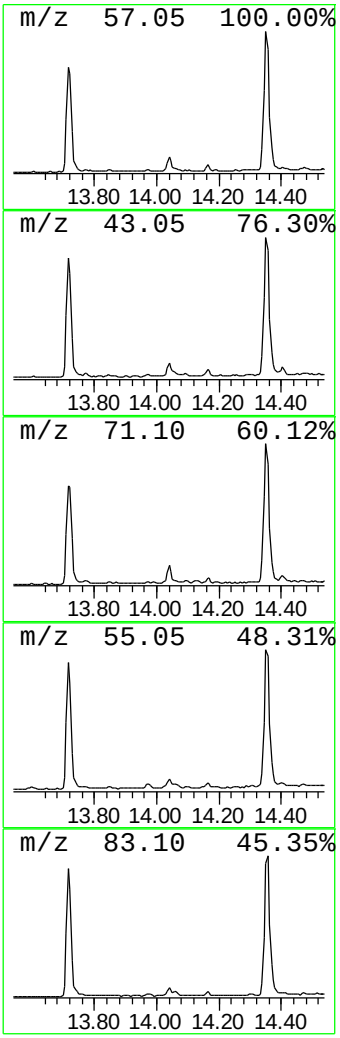
****

Peak Number 6 Sulfurous acid, octadecyl 2... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	5.35 ng	197199	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	90
2	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	90
3	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	90
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87
5	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

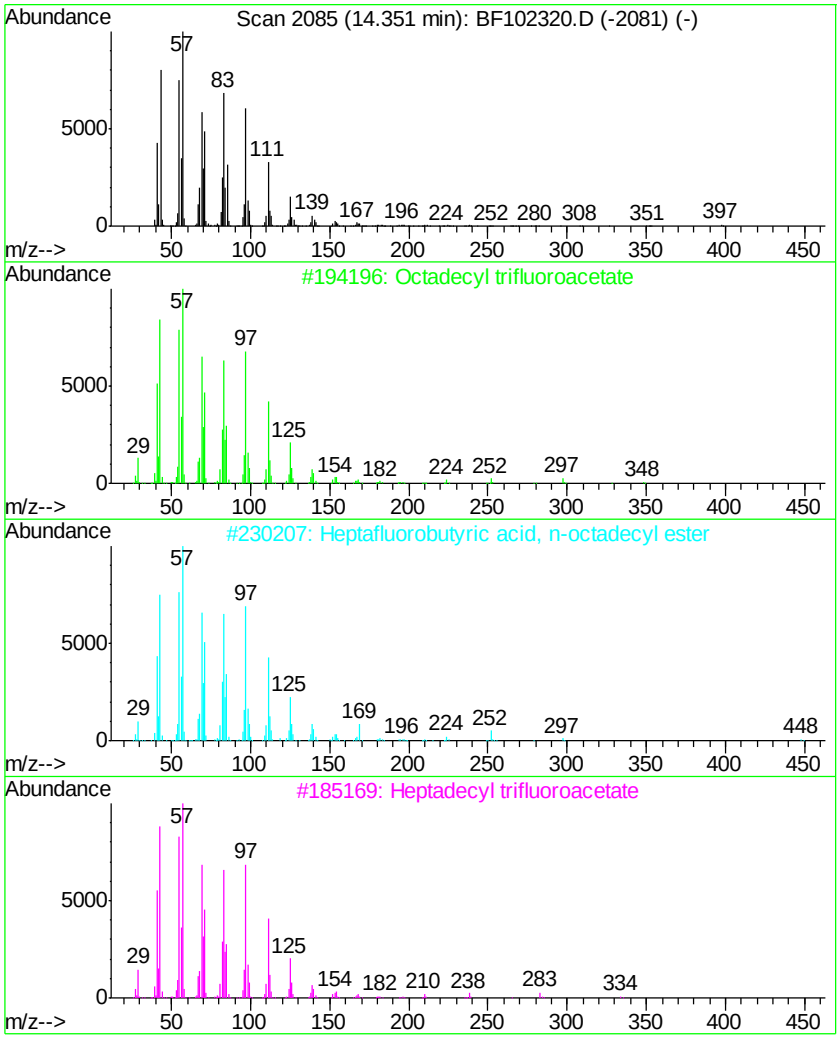
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

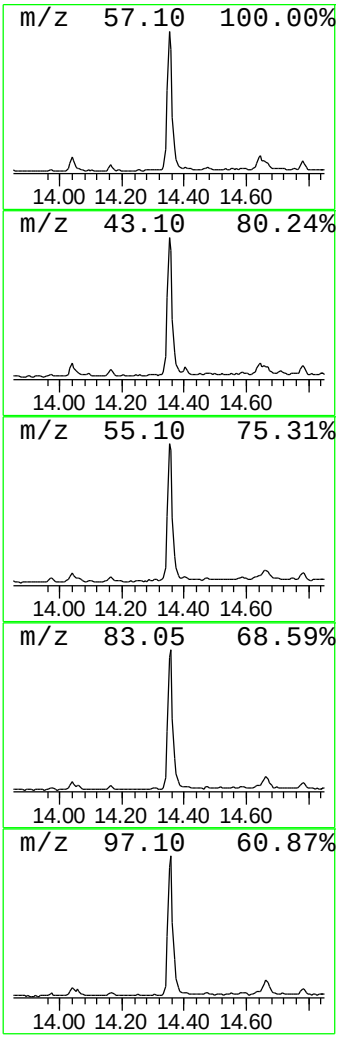
****

Peak Number 7 Octadecyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	65.69 ng	2423070	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

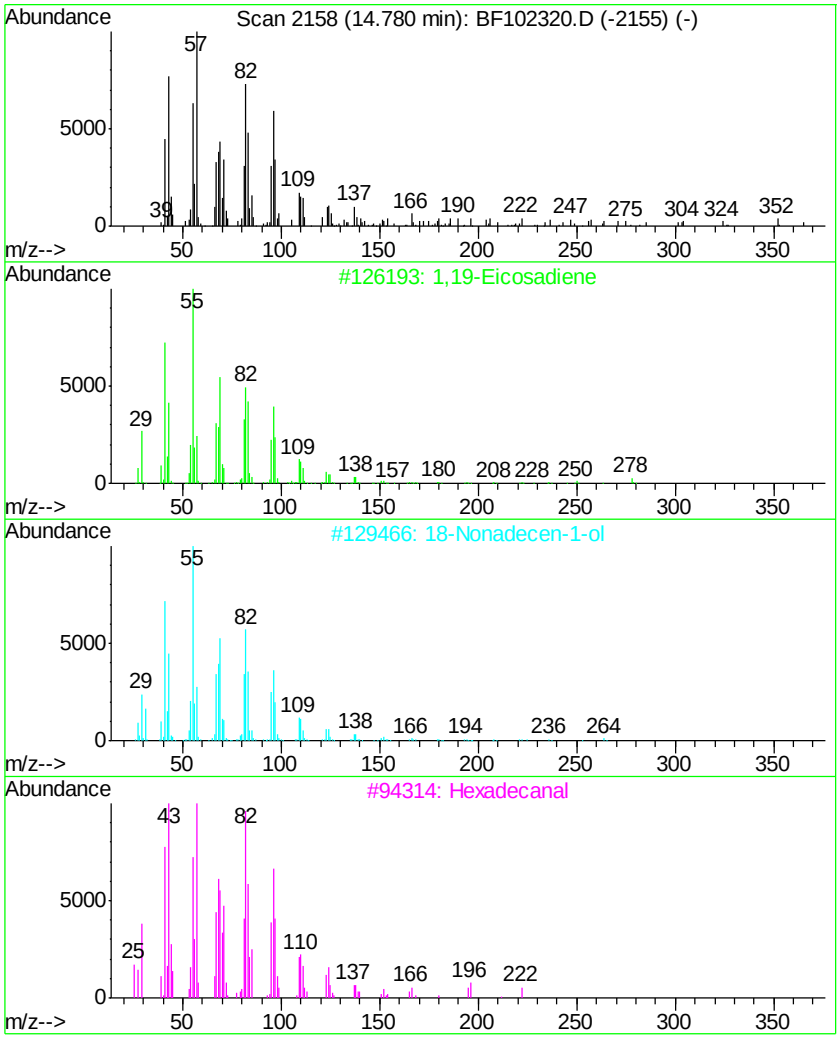
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

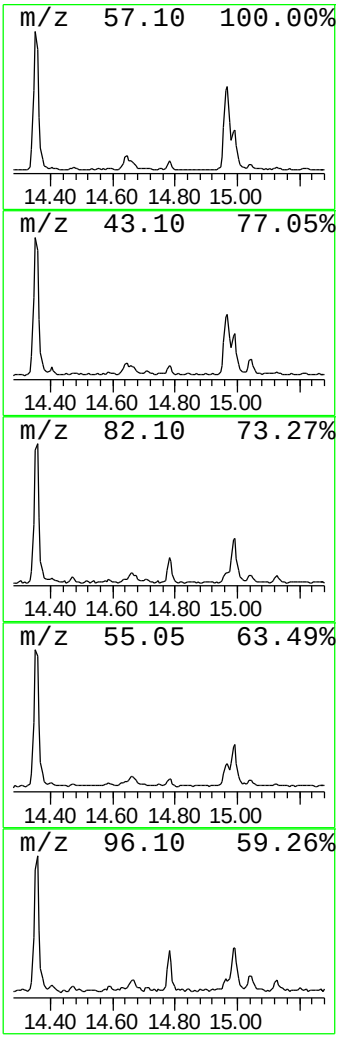
****

Peak Number 8 1,19-Eicosadiene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.78	4.27 ng	153365	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	90
2	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	90
3	Hexadecanal	240	C16H32O	000629-80-1	90
4	Octadecanal	268	C18H36O	000638-66-4	87
5	16-Heptadecenal	252	C17H32O	1000144-57-9	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

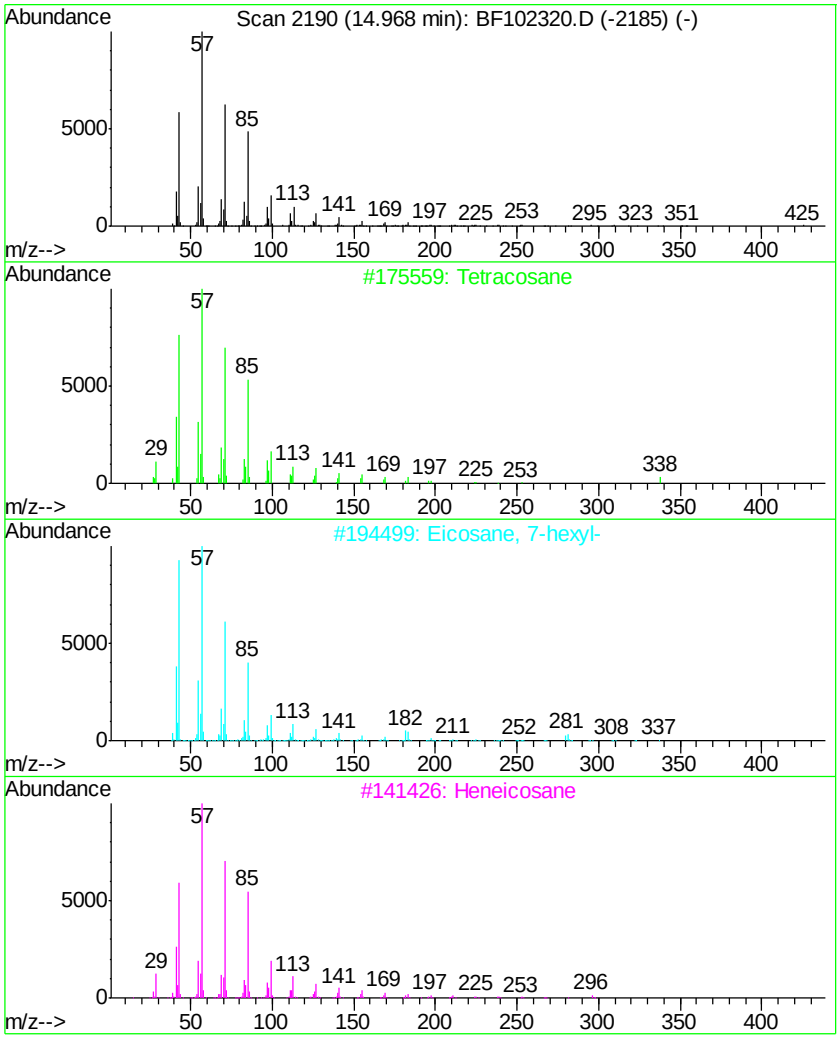
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

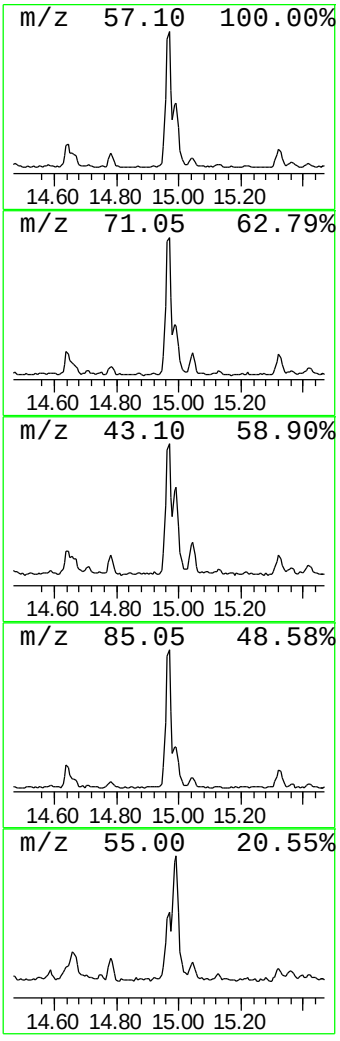
****

Peak Number 9 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	23.71 ng	850918	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3	Heneicosane	296	C21H44	000629-94-7	87
4	Nonadecane	268	C19H40	000629-92-5	86
5	Hexatriacontane	507	C36H74	000630-06-8	83





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

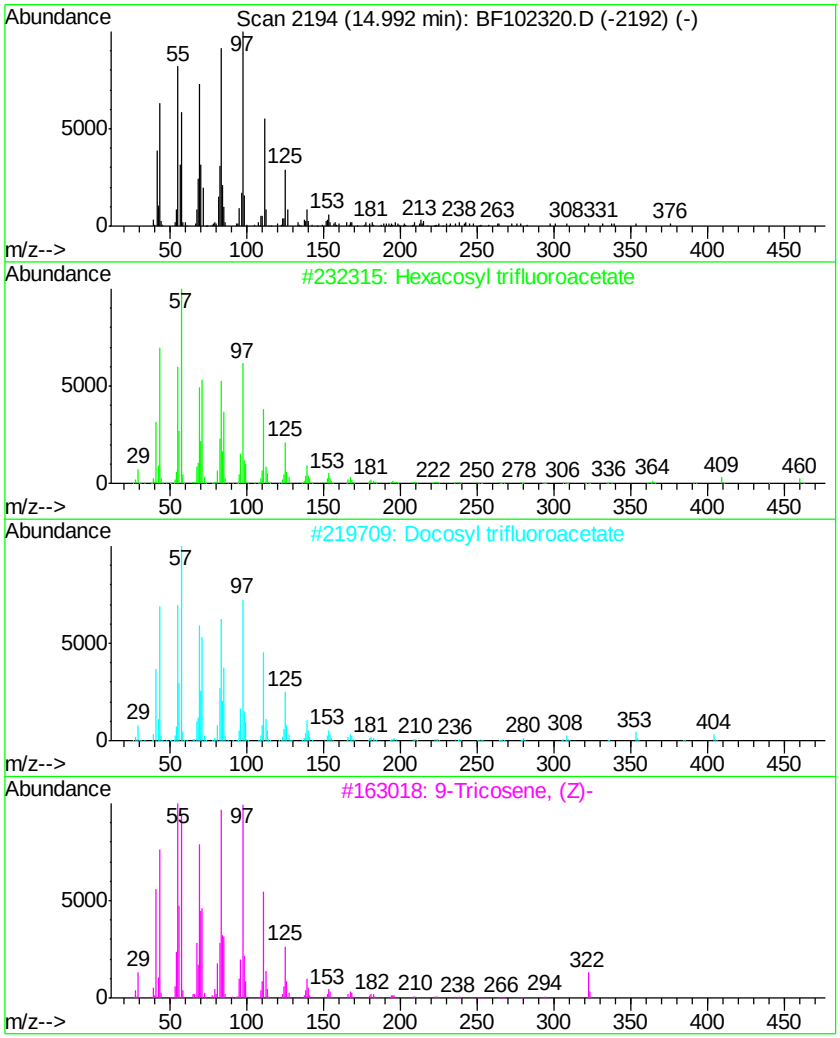
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

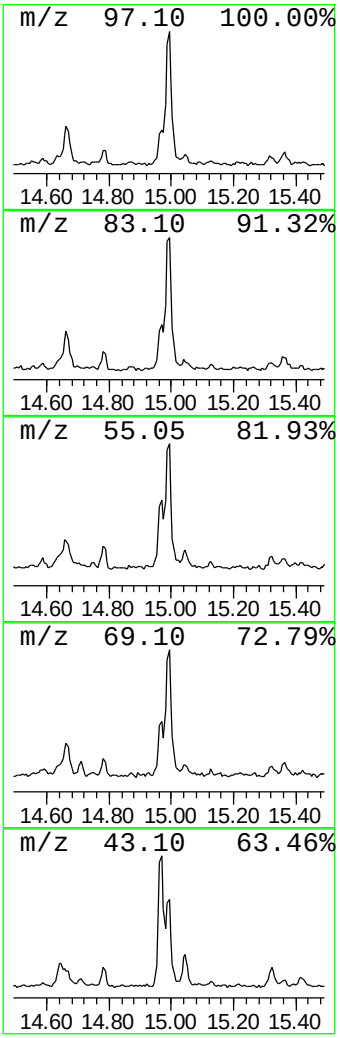
****

Peak Number 10 Hexacosyl trifluoroacetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	18.85 ng	676580	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	87
2	Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	87
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	87
4	Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	86
5	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

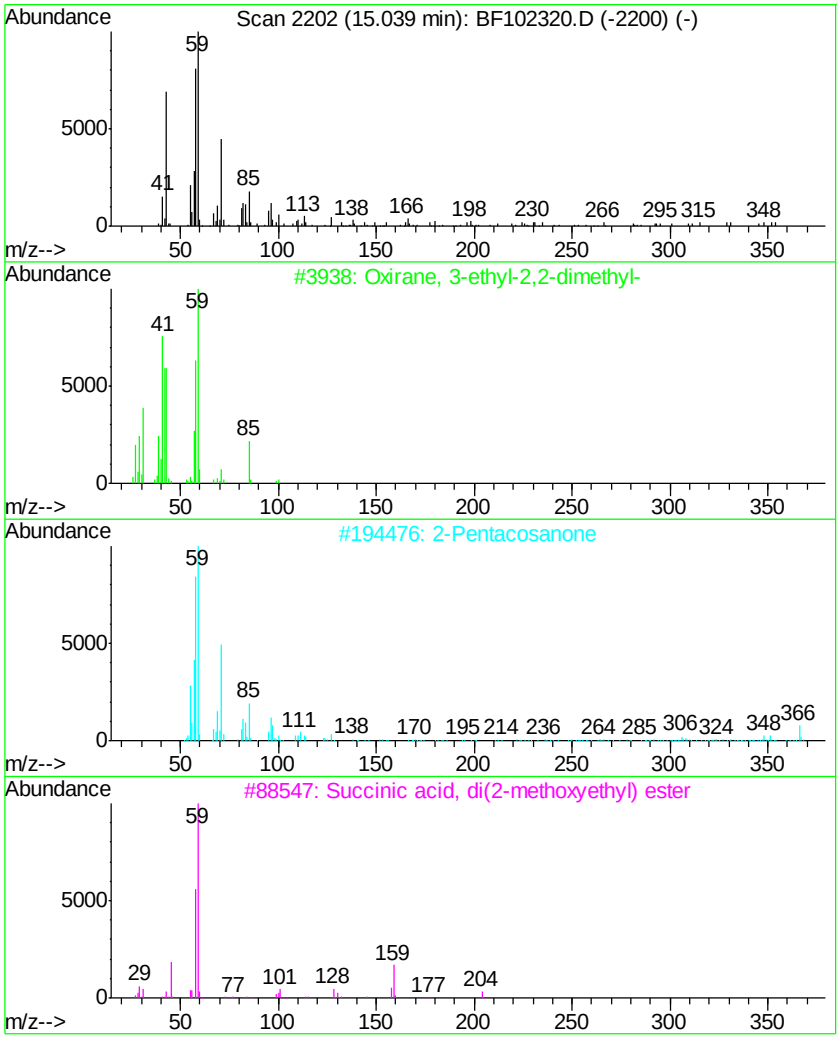
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

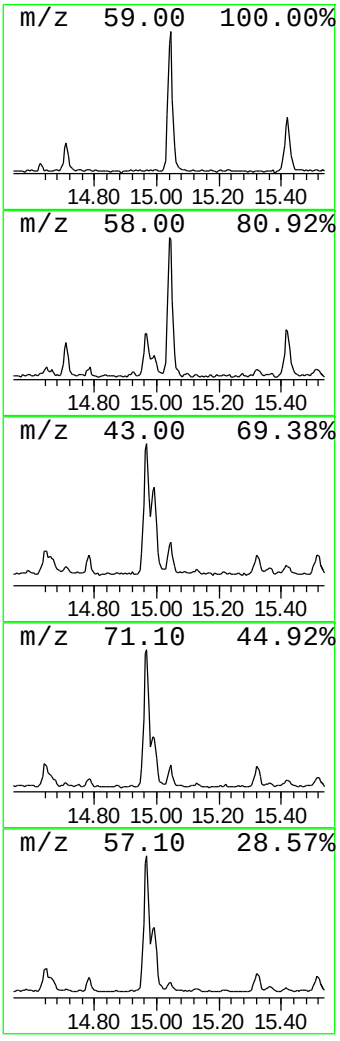
****

Peak Number 11 Oxirane, 3-ethyl-2,2-dimethyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	4.28 ng	153717	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, 3-ethyl-2,2-dimethyl-	100	C6H12O	001192-22-9	52
2	2-Pentacosanone	366	C25H50O	075207-54-4	49
3	Succinic acid, di(2-methoxyethyl...	234	C10H18O6	1000325-81-8	47
4	2-Tridecanone	198	C13H26O	000593-08-8	47
5	2-Tetradecanone	212	C14H28O	002345-27-9	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

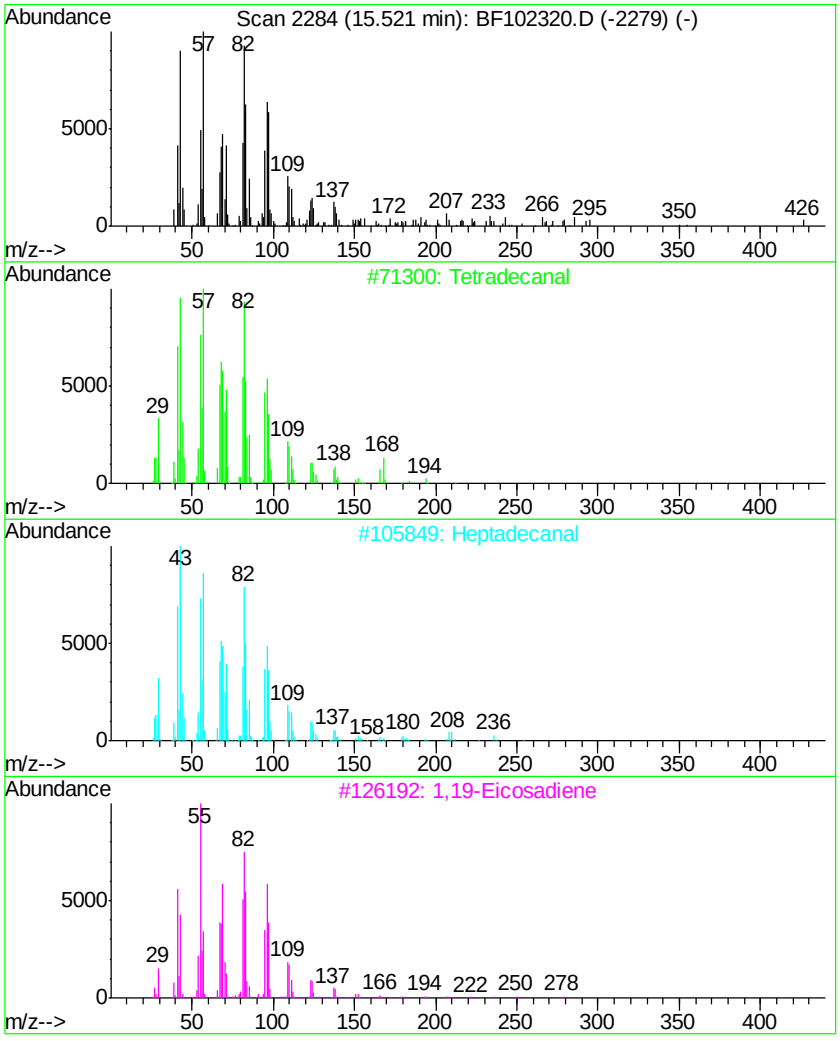
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

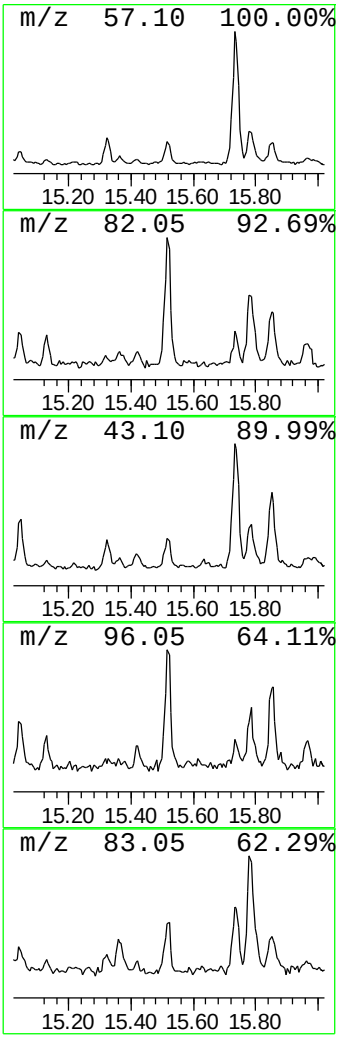
****

Peak Number 12 Tetradecanal Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.52	5.84 ng	209498	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanal	212	C14H28O	000124-25-4	93
2	Heptadecanal	254	C17H34O	1000376-70-0	86
3	1,19-Eicosadiene	278	C20H38	014811-95-1	86
4	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	83
5	Z-2-Dodecenol	184	C12H24O	069064-36-4	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

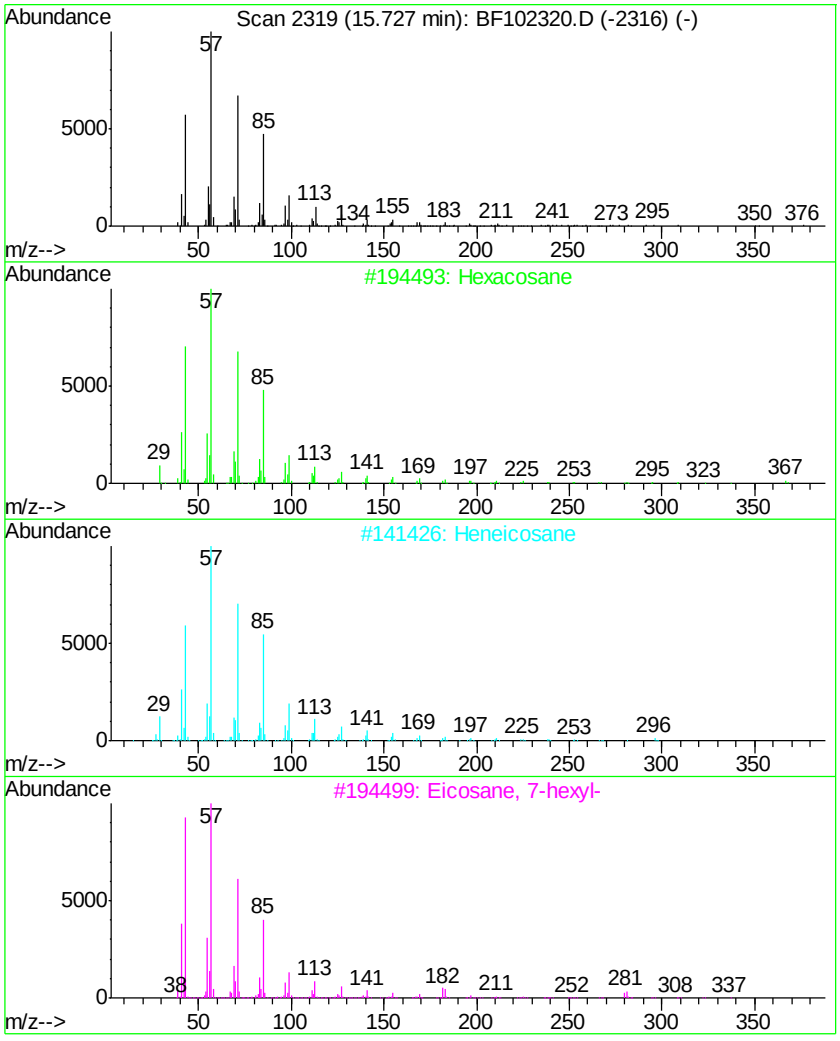
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

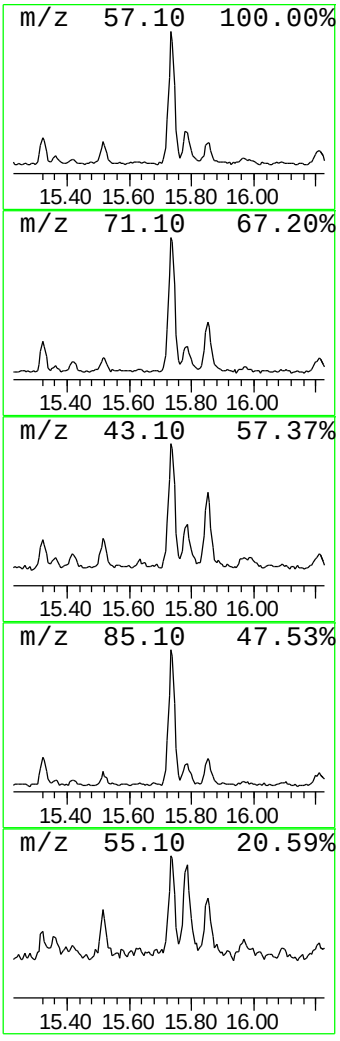
****

Peak Number 13 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	15.28 ng	548359	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
5	Hexadecane	226	C16H34	000544-76-3	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

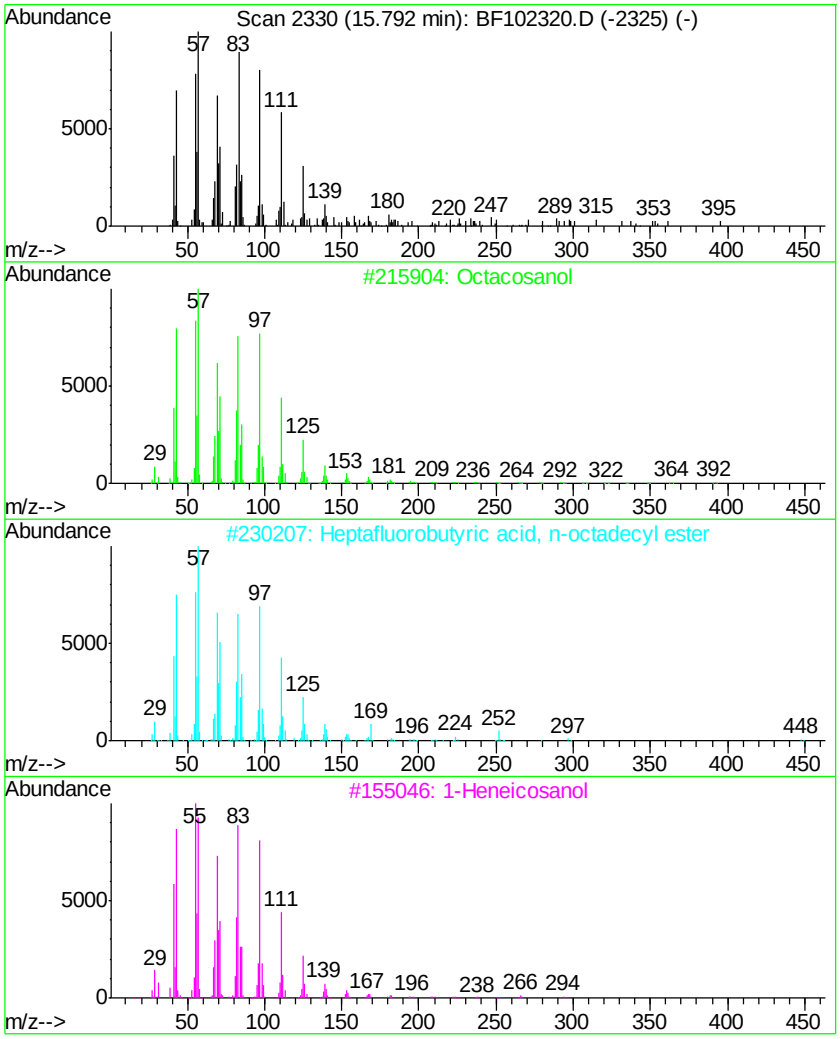
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

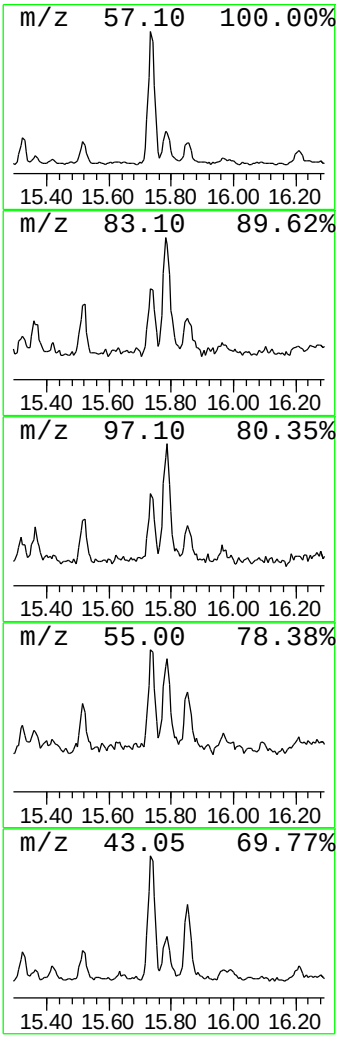
****

Peak Number 14 Octacosanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	8.96 ng	321570	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	94
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	76
3	1-Heneicosanol	312	C21H44O	015594-90-8	76
4	Tricosyl heptafluorobutyrate	536	C27H47F7O2	1000351-83-4	74
5	Cyclotetracosane	336	C24H48	000297-03-0	68





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

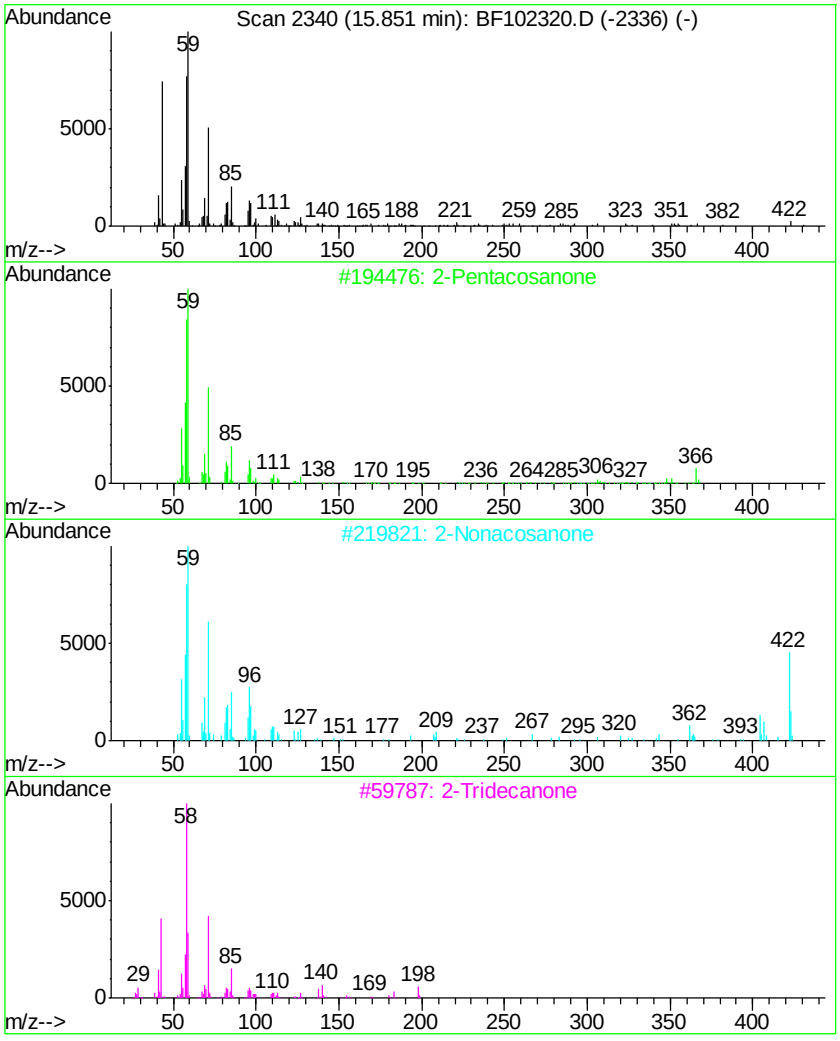
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

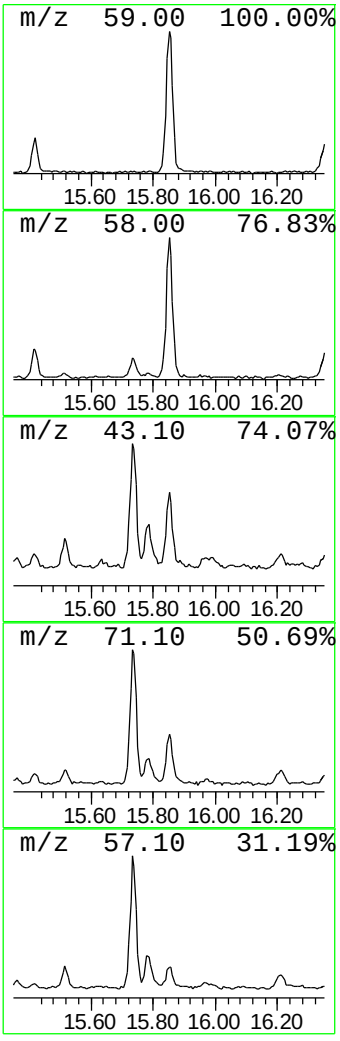
****

Peak Number 15 2-Pentacosanone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	10.34 ng	371134	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentacosanone	366	C25H50O	075207-54-4	91
2	2-Nonacosanone	422	C29H58O	017600-99-6	90
3	2-Tridecanone	198	C13H26O	000593-08-8	53
4	2-Tetradecanone	212	C14H28O	002345-27-9	50
5	2-Pentadecanone	226	C15H30O	002345-28-0	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

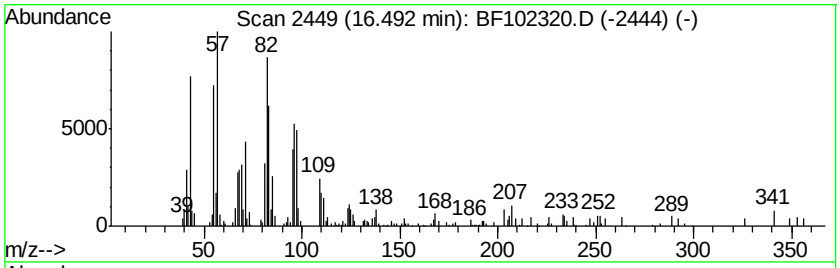
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

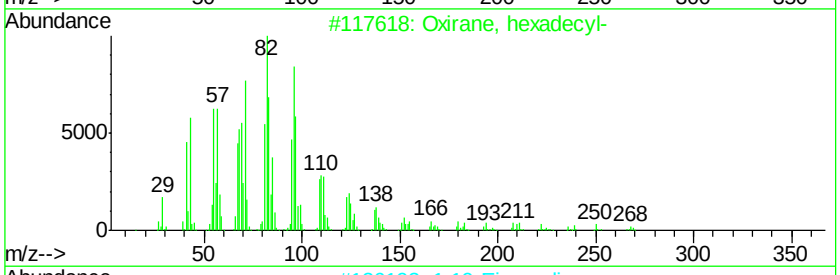
****

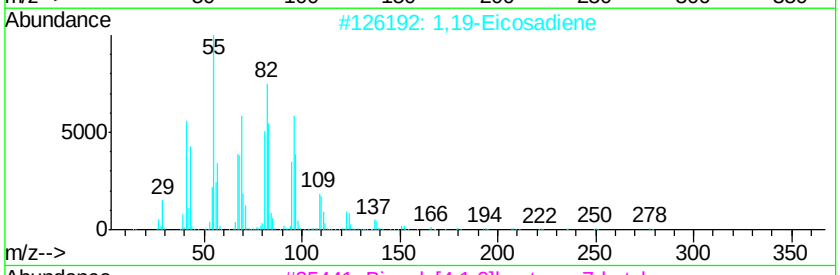
Peak Number 16 Oxirane, hexadecyl- Concentration Rank 18

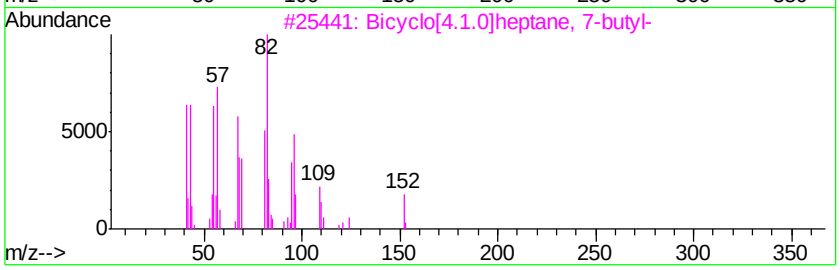
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	5.11 ng	183530	Perylene-d12	15.30

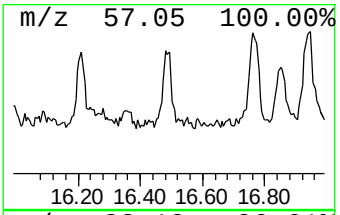
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	80
2	1,19-Eicosadiene	278	C20H38	014811-95-1	64
3	Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	60
4	Benzocyclodecene, tetradecahydro-	194	C14H26	061142-06-1	49
5	Tridecane, 5-cyclohexyl-	266	C19H38	013151-90-1	49

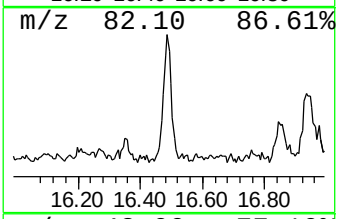


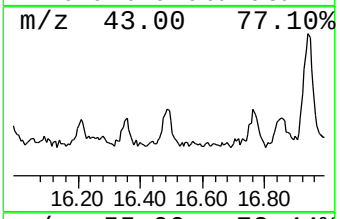


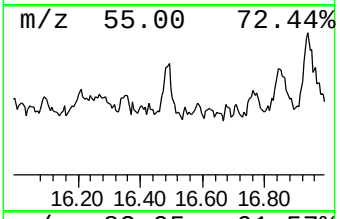


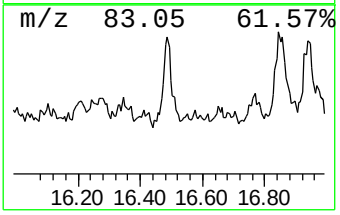












Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

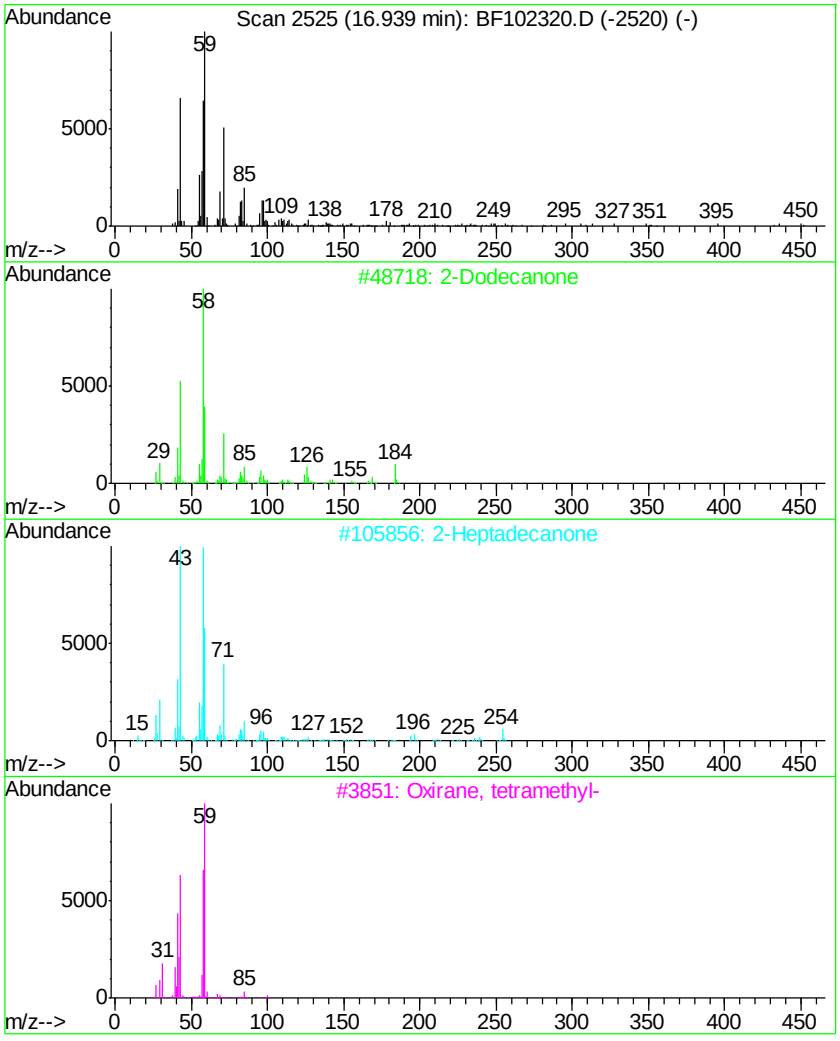
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

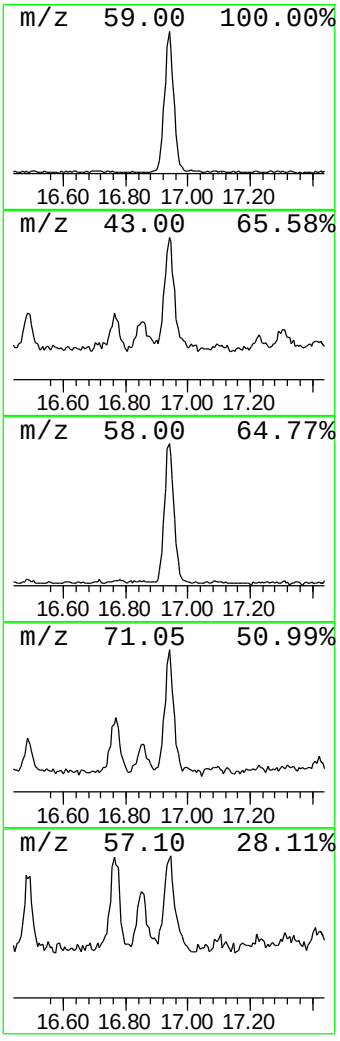
****

Peak Number 17 2-Dodecanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.94	11.69 ng	419562	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dodecanone	184	C12H24O	006175-49-1	59
2	2-Heptadecanone	254	C17H34O	002922-51-2	43
3	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	43
4	trans-2,3-Epoxynonane	142	C9H18O	056820-01-0	35
5	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

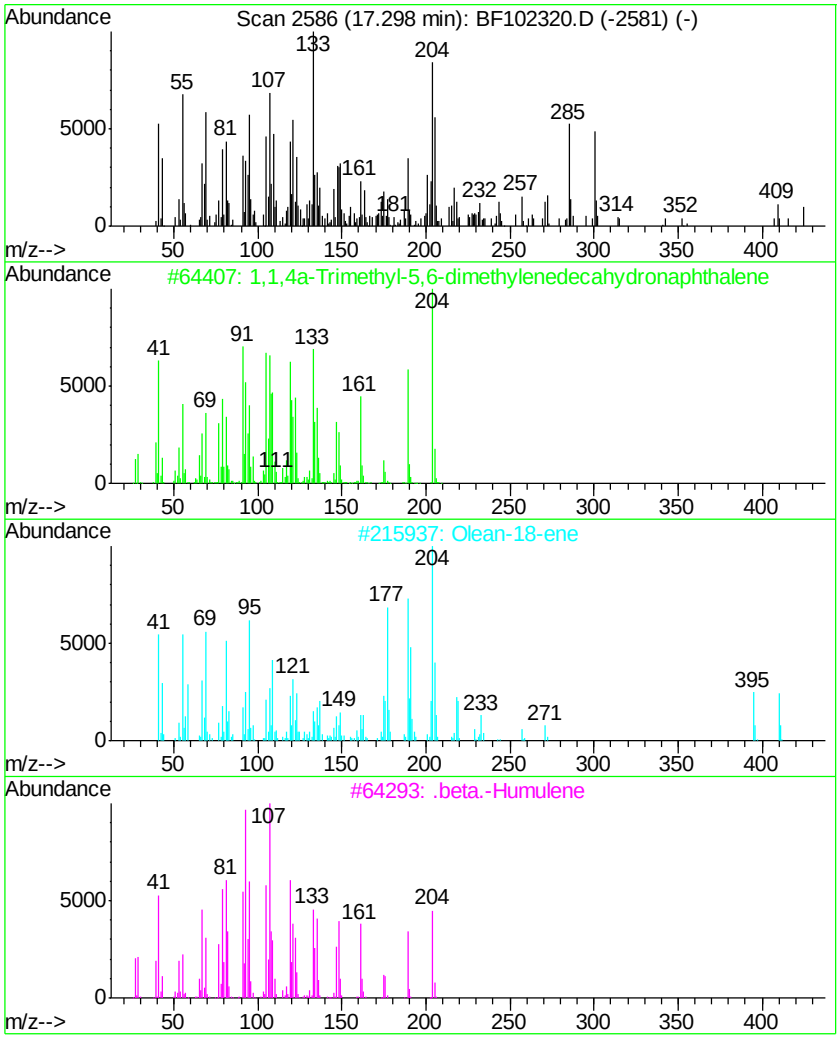
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

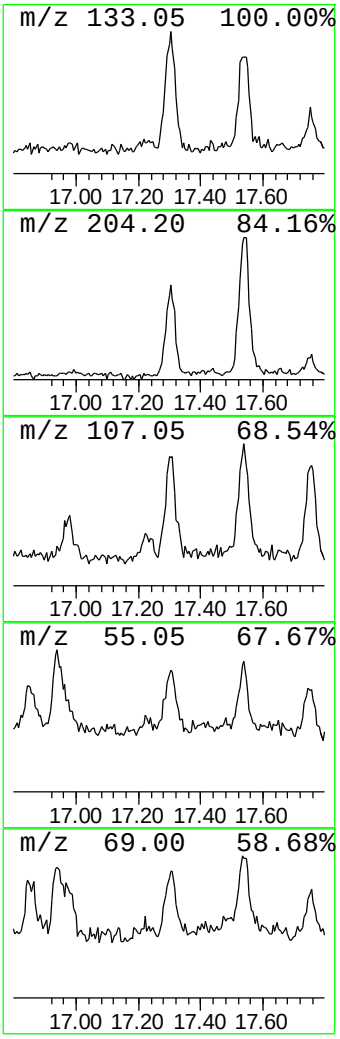
****

Peak Number 18 unknown17.30 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.30	14.67 ng	526351	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	43
2	Olean-18-ene	410	C30H50	000432-11-1	38
3	.beta.-Humulene	204	C15H24	000116-04-1	38
4	Aciphyllene	204	C15H24	087745-31-1	35
5	1,3-Dimethyl-5-(propen-1-yl)adam...	204	C15H24	057040-48-9	30





Data Path : Z:\HPCHEM1\BNA F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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

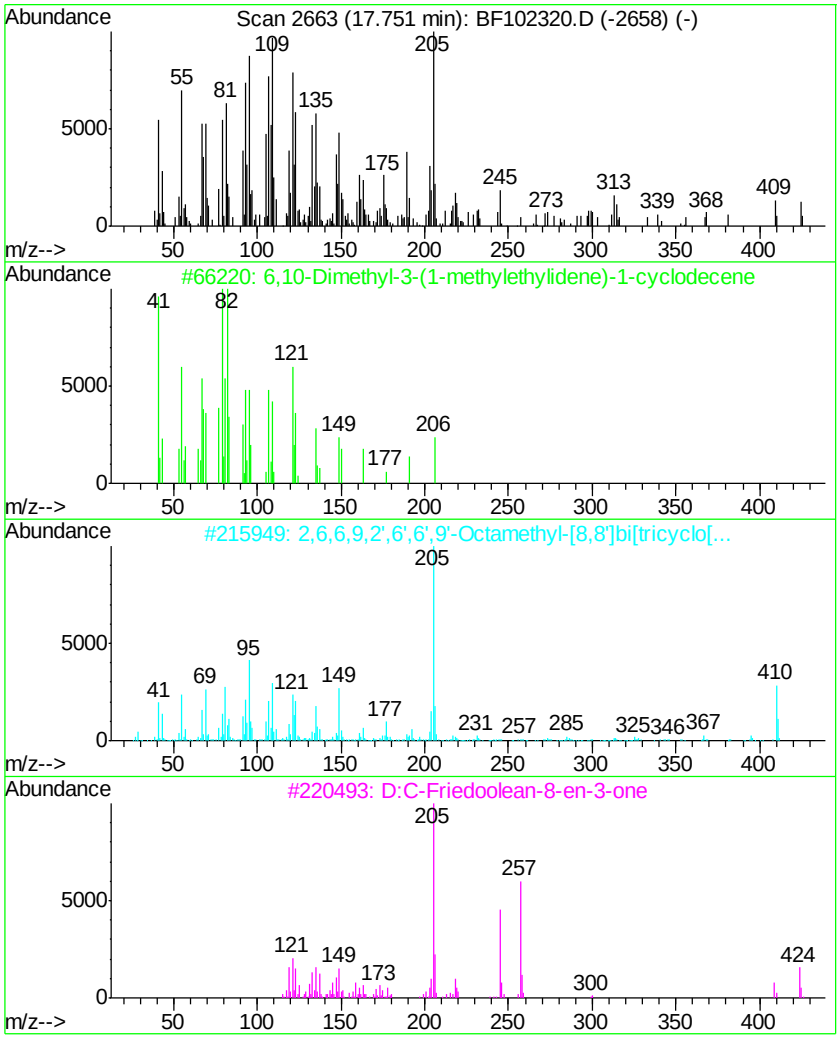
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

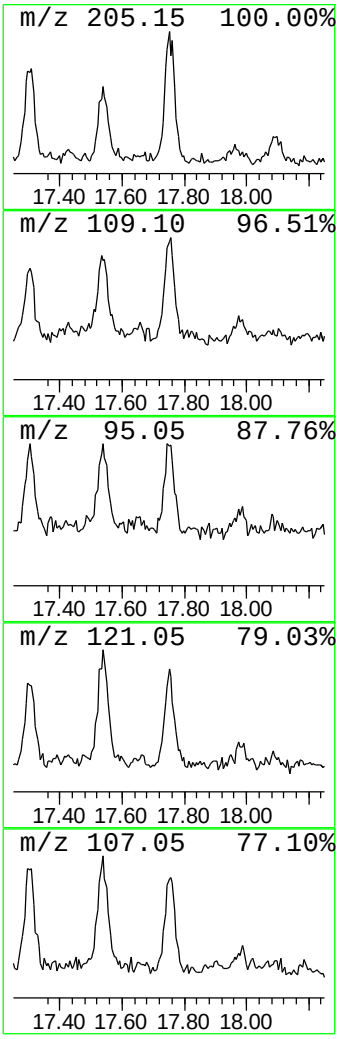
****

Peak Number 20 6,10-Dimethyl-3-(1-methylet... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.75	11.35 ng	407251	Perylene-d12	15.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	52
2	2,6,6,9,2',6',6',9'-Octamethyl-[...	410	C30H50	1000189-48-2	50
3	D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	45
4	1-Isopropenyl-4,5-dimethylbicycl...	330	C21H30OS	1000195-85-4	38
5	1-(2-Pyridyl)piperazine	163	C9H13N3	034803-66-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012218\
Data File : BF102320.D
Acq On : 23 Jan 2018 00:45
Operator : SJ/JU
Sample : J1238-14
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-04-9.5-10.0

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
2-Pentanone, 4-hy...	4.92	5.9	ng	231783	1	6.72	785242	20.0
unknown6.49	6.49	80.3	ng	3150730	1	6.72	785242	20.0
n-Nonadecanol-1	13.03	6.9	ng	255337	5	13.87	737739	20.0
5-Eicosene, (E)-	13.72	50.5	ng	1862300	5	13.87	737739	20.0
Sulfurous acid, o...	14.04	5.3	ng	197199	5	13.87	737739	20.0
Octadecyl trifluo...	14.35	65.7	ng	2423070	5	13.87	737739	20.0
1,19-Eicosadiene	14.78	4.3	ng	153365	6	15.30	717801	20.0
Tetracosane	14.97	23.7	ng	850918	6	15.30	717801	20.0
Hexacosyl trifluo...	14.99	18.9	ng	676580	6	15.30	717801	20.0
Oxirane, 3-ethyl-...	15.04	4.3	ng	153717	6	15.30	717801	20.0
Tetradecanal	15.52	5.8	ng	209498	6	15.30	717801	20.0
Hexacosane	15.73	15.3	ng	548359	6	15.30	717801	20.0
Octacosanol	15.79	9.0	ng	321570	6	15.30	717801	20.0
2-Pentacosanone	15.85	10.3	ng	371134	6	15.30	717801	20.0
Oxirane, hexadecyl-	16.49	5.1	ng	183530	6	15.30	717801	20.0
2-Dodecanone	16.94	11.7	ng	419562	6	15.30	717801	20.0
unknown17.30	17.30	14.7	ng	526351	6	15.30	717801	20.0
6,10-Dimethyl-3-(...	17.75	11.4	ng	407251	6	15.30	717801	20.0