LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102861.D
Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

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-BF020318.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	2.140	4	9	16	rVB	290380	380473	6.46%	0.469%
2	5.110	511	514	524	rVB	129576	160758	2.73%	0.198%
3	5.504	573	581	584	rBV	4573133	4698925	79.82%	5.791%
4	6.516	747	753	762	rBV	4226465	4477225	76.05%	5.517%
5	6.657	772	777	780	rBV	4642671	4390774	74.58%	5.411%
6	6.887	812	816	819	rBV	1546665	1257392	21.36%	1.550%
7	7.045	836	843	846	rBV	3414261	3233670	54.93%	3.985%
8	7.281	880	883	894	rVB2	88725	113421	1.93%	0.140%
9	7.451	906	912	915	rBV	2974844	2940817	49.95%	3.624%
10	7.528	920	925	931	rBV2	79006	99404	1.69%	0.122%
11	7.928	988	993	996	rBV	77906	96871	1.65%	0.119%
12	8.169	1030	1034	1037	rBV	1978910	1532218	26.03%	1.888%
13	9.245	1212	1217	1220	rBV	4205969	3831367	65.08%	4.721%
14	9.316	1226	1229	1232	rVB	131112	96288	1.64%	0.119%
15	9.633	1280	1283	1286	rBV	445865	374864	6.37%	0.462%
16	9.845	1315	1319	1324	rVB	285792	260124	4.42%	0.321%
17	9.922	1329	1332	1336	rBV	1450627	1373666	23.33%	1.693%
18	10.169	1371	1374	1378	rBV3	67219	68611	1.17%	0.085%
19	10.322	1397	1400	1402	rBV	77207	67879	1.15%	0.084%
20	10.345	1402	1404	1407	rVB	269266	216480	3.68%	0.267%
21	10.569	1437	1442	1444	rBV	73162	98986	1.68%	0.122%
22	10.669	1457	1459	1463	rBV3	57724	67903	1.15%	0.084%
23	10.716	1463	1467	1470	rBV	1852511	1764564	29.97%	2.175%
24	10.792	1475	1480	1482	rVV6	34482	60394	1.03%	0.074%
25	10.822	1482	1485	1486	rVV	246890	232743	3.95%	0.287%
26	10.839	1486	1488	1490	rVV	242531	199508	3.39%	0.246%
27	10.886	1493	1496	1499	rVV	467596	423116	7.19%	0.521%
28	10.922	1499	1502	1505	rVV2	510673	622713	10.58%	0.767%
29	10.957	1505	1508	1510	rVV	521075	465260	7.90%	0.573%
30	10.980	1510	1512	1514	rVV	296551	228663	3.88%	0.282%
31	11.022	1514	1519	1520	rVV2	158604	242040	4.11%	0.298%
32	11.069	1524	1527	1530	rVV2	366874	432038	7.34%	0.532%
33	11.104	1530	1533	1535	rVV	504244	417552	7.09%	0.515%
34	11.145	1538	1540	1545	rVB2	251522	221036	3.75%	0.272%

LSC Area Percent Report

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Misc :
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Instrument : BNA_F
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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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.269	1558	1561	1563	rBV	153343	136644	2.32%	0.168%
36	11.416	1582	1586	1589	rBV	1066485	1034354	17.57%	1.275%
37	11.457	1590	1593	1596	rVV	343030	293554	4.99%	0.362%
38	11.698	1631	1634	1636	rBV	157998	128864	2.19%	0.159%
39	11.904	1665	1669	1672	rBV	532739	632658	10.75%	0.780%
40	11.945	1672	1676	1682	rVV2	1090188	1184750	20.12%	1.460%
41	12.498	1767	1770	1776	rVB	385281	423141	7.19%	0.521%
42	12.874	1832	1834	1839	rVB2	336681	426722	7.25%	0.526%
43	12.998	1851	1855	1859	rVB	2318383	2147196	36.47%	2.646%
44	13.469	1932	1935	1938	rBV	262670	208411	3.54%	0.257%
45	13.680	1968	1971	1977	rVB3	195618	180330	3.06%	0.222%
46	13.880	2002	2005	2012	rBV2	555596	700981	11.91%	0.864%
47	13.951	2015	2017	2022	rVB	284755	268982	4.57%	0.331%
48	14.010	2025	2027	2031	rBV3	86521	77377	1.31%	0.095%
49	14.057	2031	2035	2038	rBV	1004759	965949	16.41%	1.190%
50	14.204	2058	2060	2065	rVB	106708	90266	1.53%	0.111%
51	14.327	2079	2081	2084	rBV	236979	211977	3.60%	0.261%
52	14.510	2109	2112	2118	rBV	787877	873797	14.84%	1.077%
53	14.821	2162	2165	2170	rBV	251113	263148	4.47%	0.324%
54	14.968	2187	2190	2196	rVB	829869	857923	14.57%	1.057%
55	15.168	2219	2224	2226	rBV	1778784	2090056	35.50%	2.576%
56	15.192	2226	2228	2235	rVB	1056566	1134290	19.27%	1.398%
57	15.545	2284	2288	2294	rVB2	691802	959257	16.29%	1.182%
58	15.762	2321	2325	2332	rBV	793565	1124821	19.11%	1.386%
59	16.004	2361	2366	2371	rBV	1322753	2092870	35.55%	2.579%
60	16.051	2371	2374	2383	rVB	629355	1055920	17.94%	1.301%
61	16.833	2502	2507	2513	rVB3	288605	533658	9.06%	0.658%
62	17.139	2554	2559	2566	rVB	298929	595232	10.11%	0.734%
63	17.221	2568	2573	2582	rVB5	323491	810526	13.77%	0.999%
64	17.651	2639	2646	2655	rVB2	649885	1529504	25.98%	1.885%
65	17.886	2678	2686	2693	rBV2	1021153	2501548	42.49%	3.083%
66	18.133	2721	2728	2739	rBV2	745948	2137671	36.31%	2.634%
67	18.256	2740	2749	2765	rVB6	1717875	5887235	100.00%	7.255%
68	18.498	2781	2790	2796	rBV2	1012541	3308668	56.20%	4.077%
69	18.721	2821	2828	2832	rBV5	379444	1027208	17.45%	1.266%
70	19.021	2869	2879	2889	rBV5	818203	2556323	43.42%	3.150%
71	19.145	2891	2900	2906	rBV4	696179	2388088	40.56%	2.943%

LSC Area Percent Report

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

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-BF020318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	19.309	2921	2928	2939	rVB3	512831	1518428	25.79%	1.871%
73	19.433	2941	2949	2955	rBV3	607674	1641313	27.88%	2.023%

Sum of corrected areas: 81147383

LSC Report - Integrated Chromatogram

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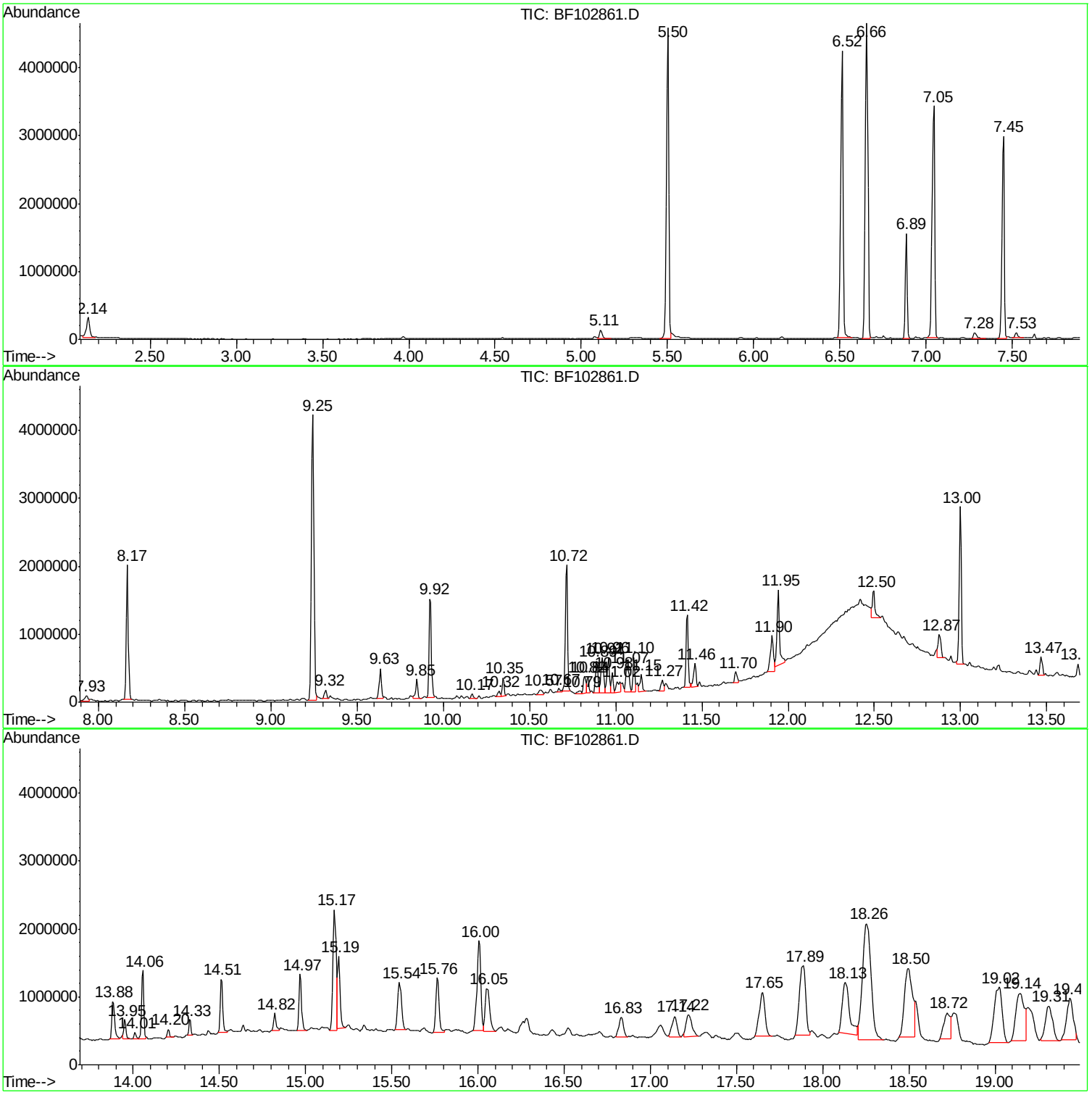
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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\BF020818\
Data File : BF102861.D
Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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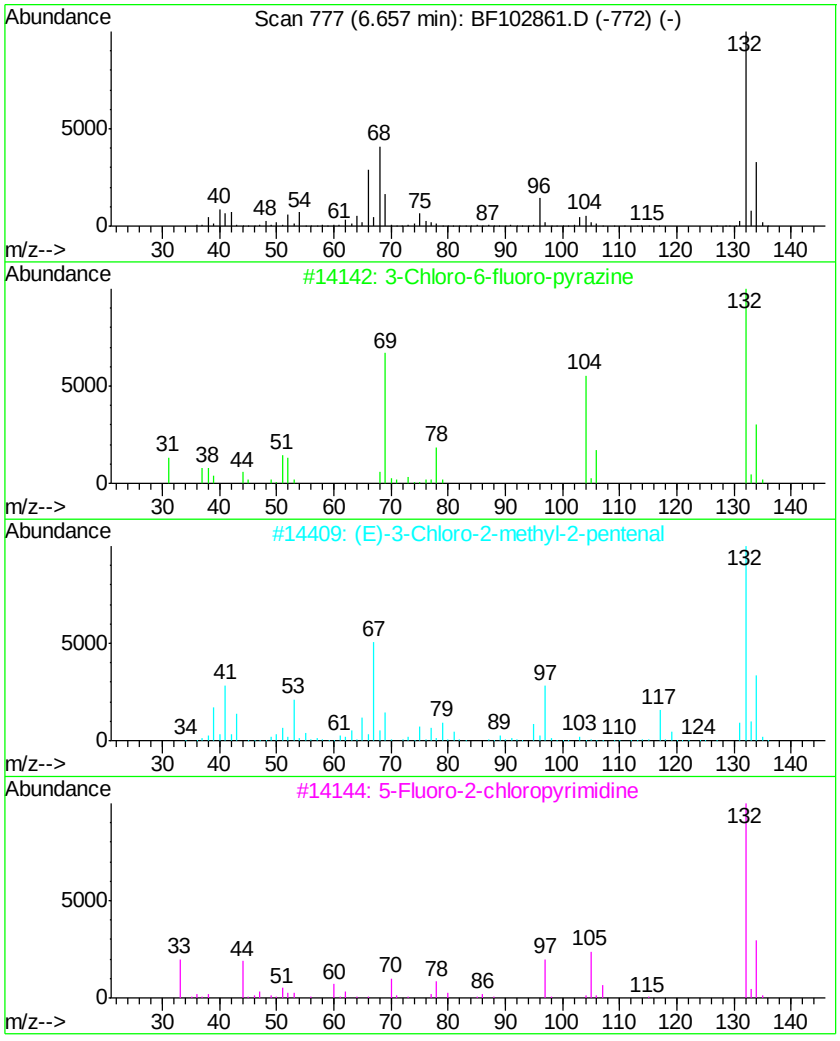
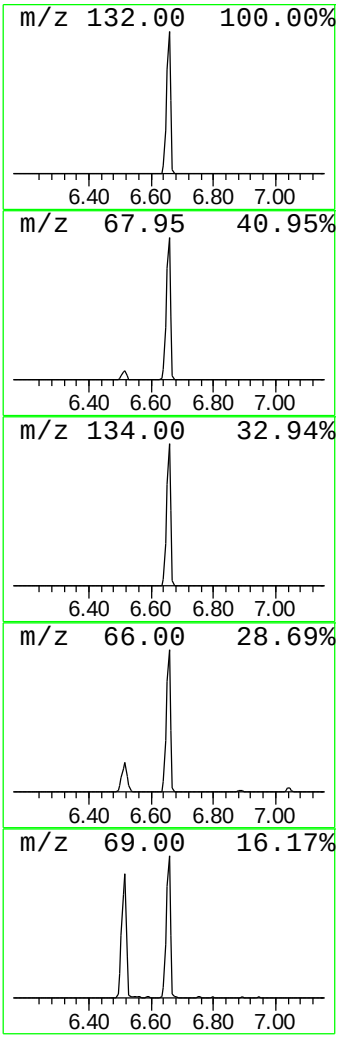
Peak Number 1 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	69.84 ng	4390770	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
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Acq On : 8 Feb 2018 17:34
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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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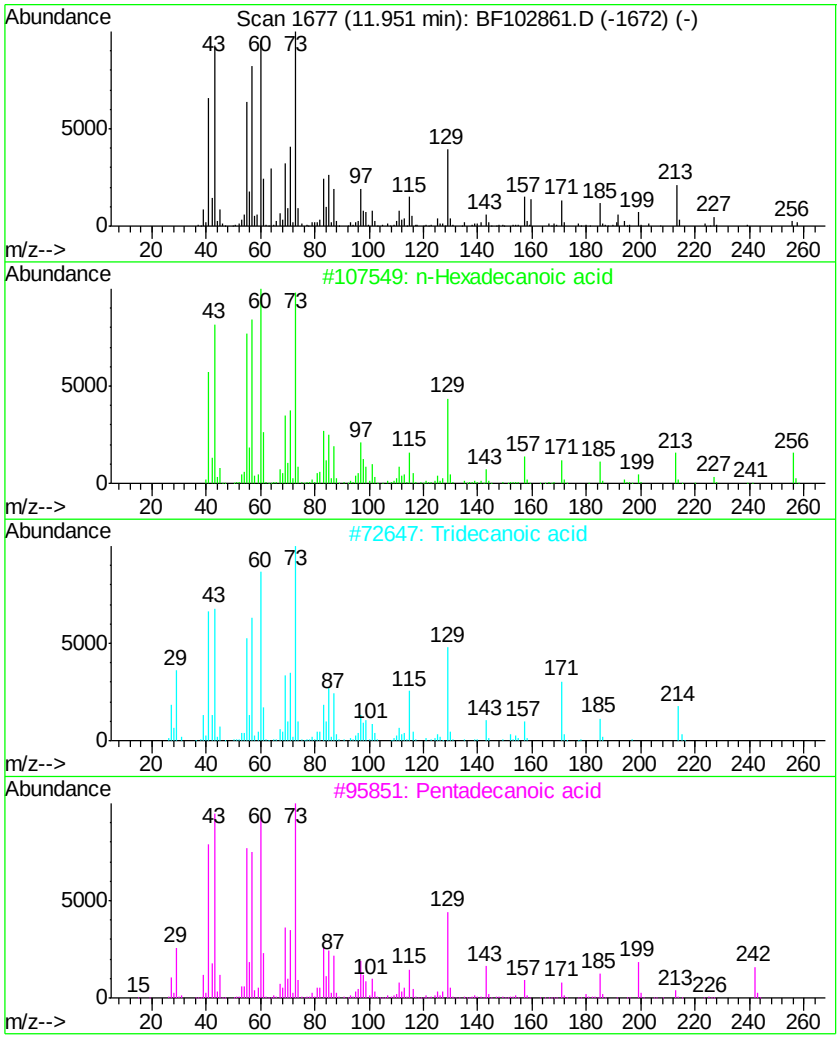
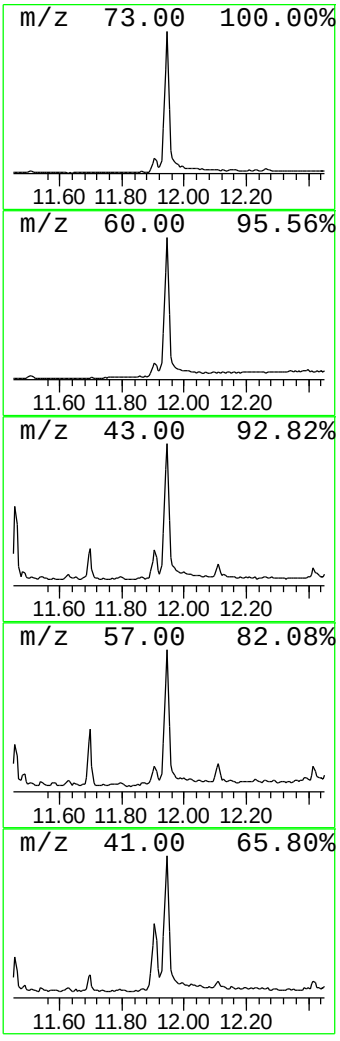
Peak Number 3 n-Hexadecanoic acid Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	22.91 ng	1184750	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Undecanoic acid	186	C11H22O2	000112-37-8	87
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102861.D
Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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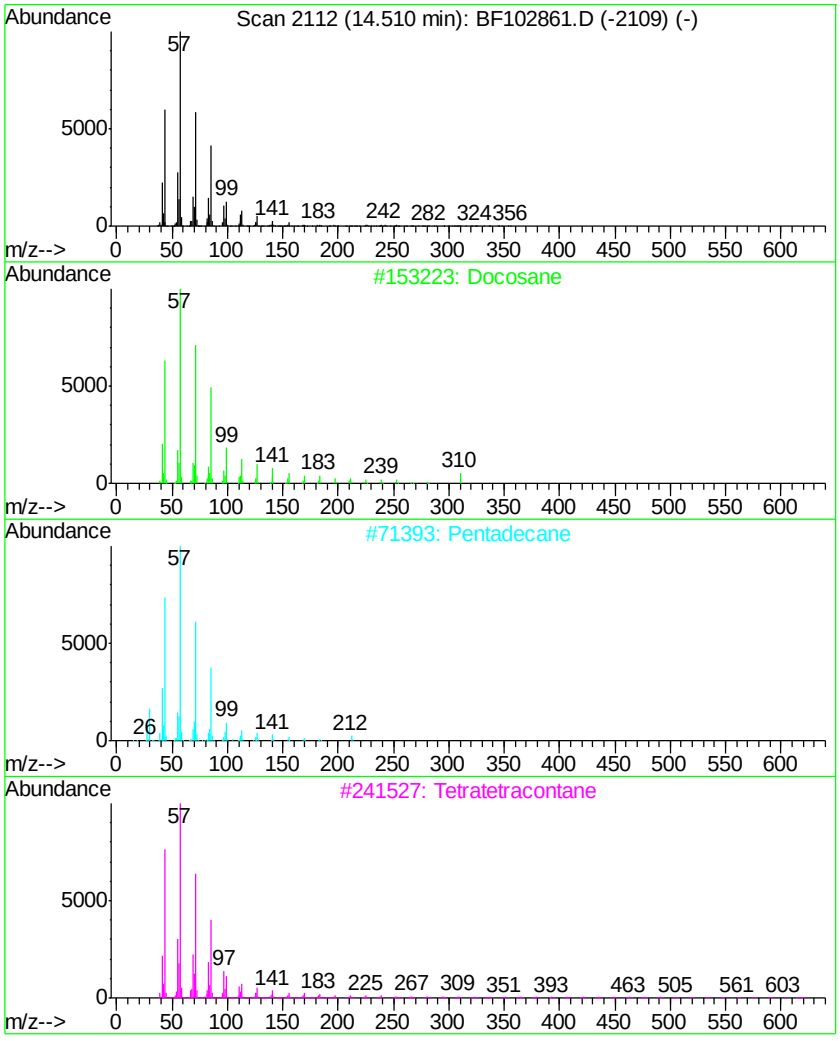
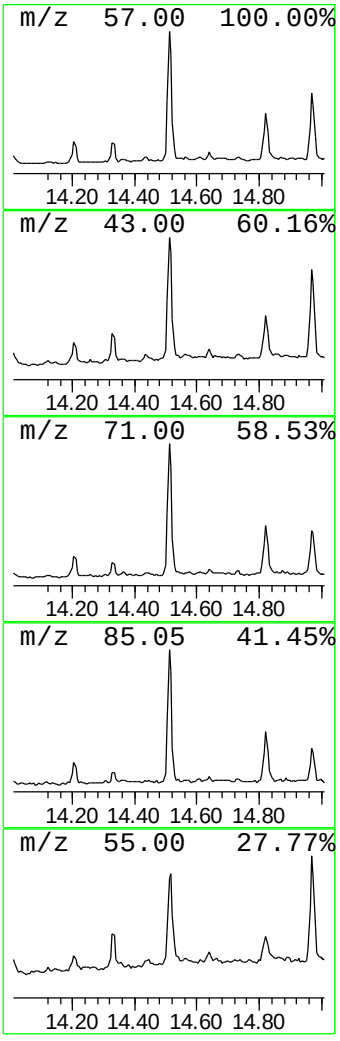
Peak Number 4 Docosane Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.51	18.09 ng	873797	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane	310	C22H46	000629-97-0	95
2	Pentadecane	212	C15H32	000629-62-9	94
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptacosane	380	C27H56	000593-49-7	91





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Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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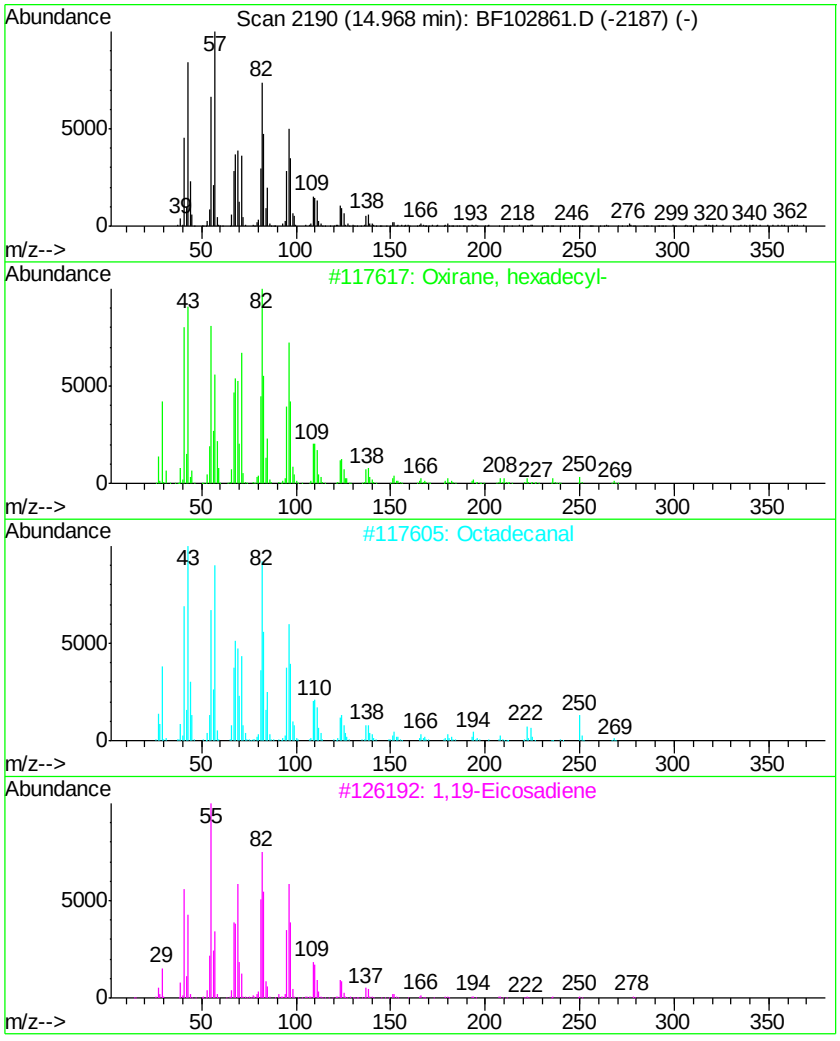
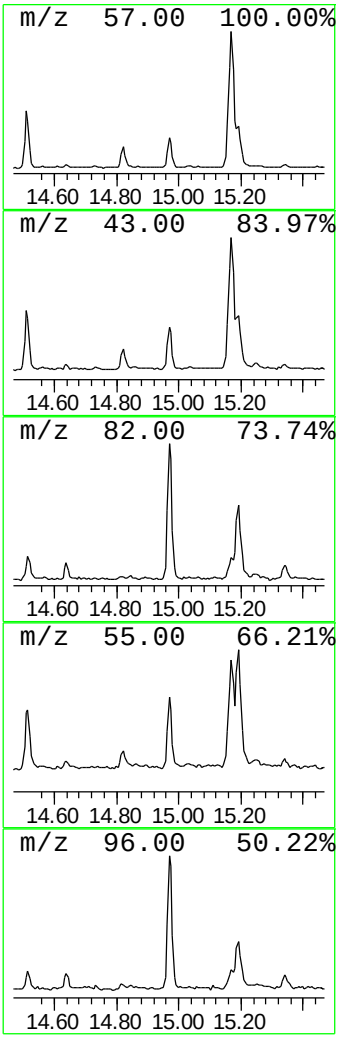
Peak Number 5 Oxirane, hexadecyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.97	17.89 ng	857923	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2	Octadecanal	268	C18H36O	000638-66-4	91
3	1,19-Eicosadiene	278	C20H38	014811-95-1	91
4	17-Octadecenal	266	C18H34O	056554-86-0	91
5	1,16-Hexadecanediol	258	C16H34O2	007735-42-4	90





Library Search Compound Report

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Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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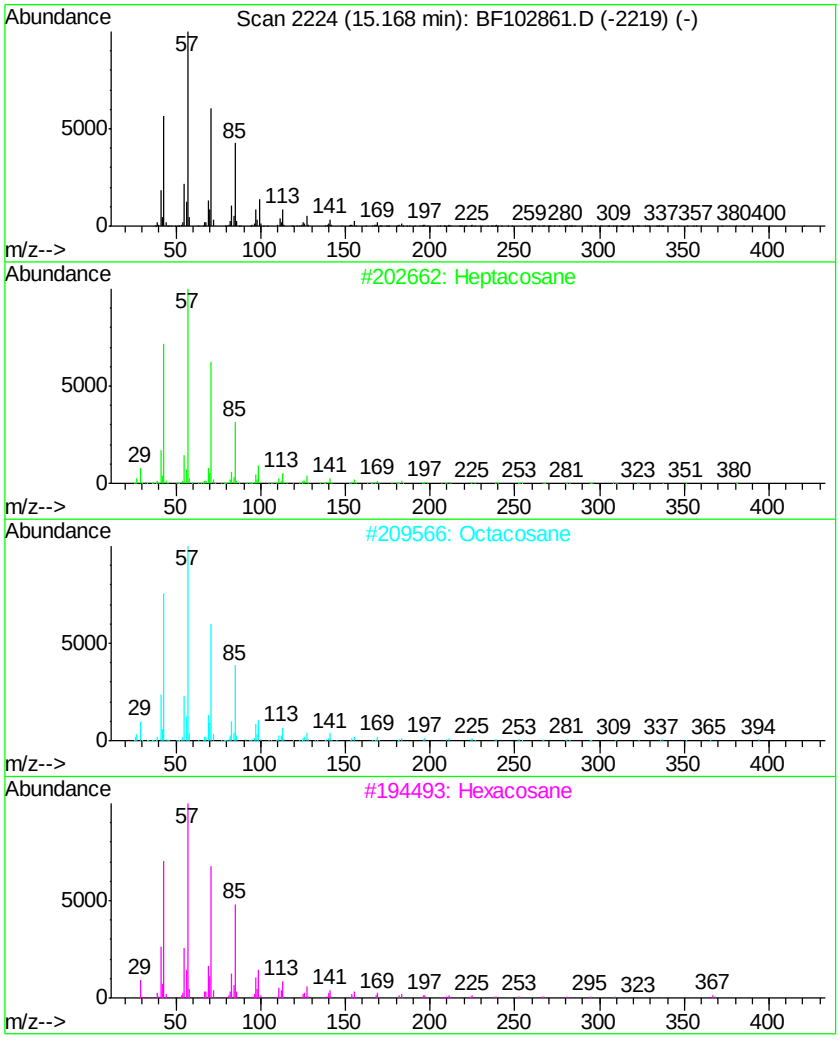
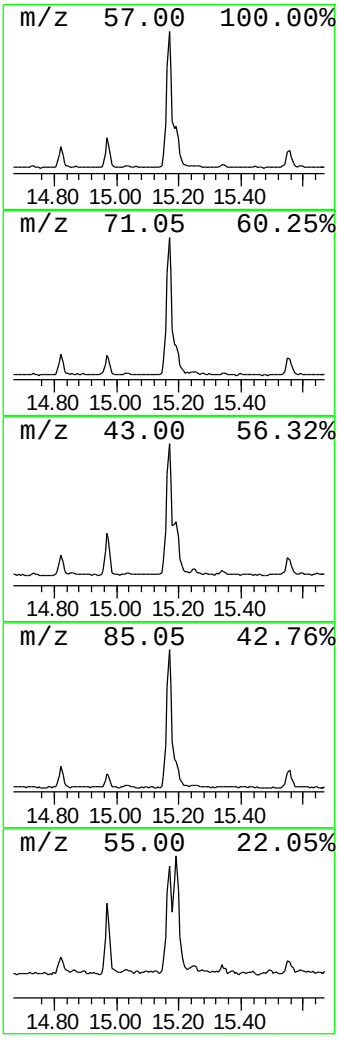
Peak Number 6 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	43.58 ng	2090060	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	90





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Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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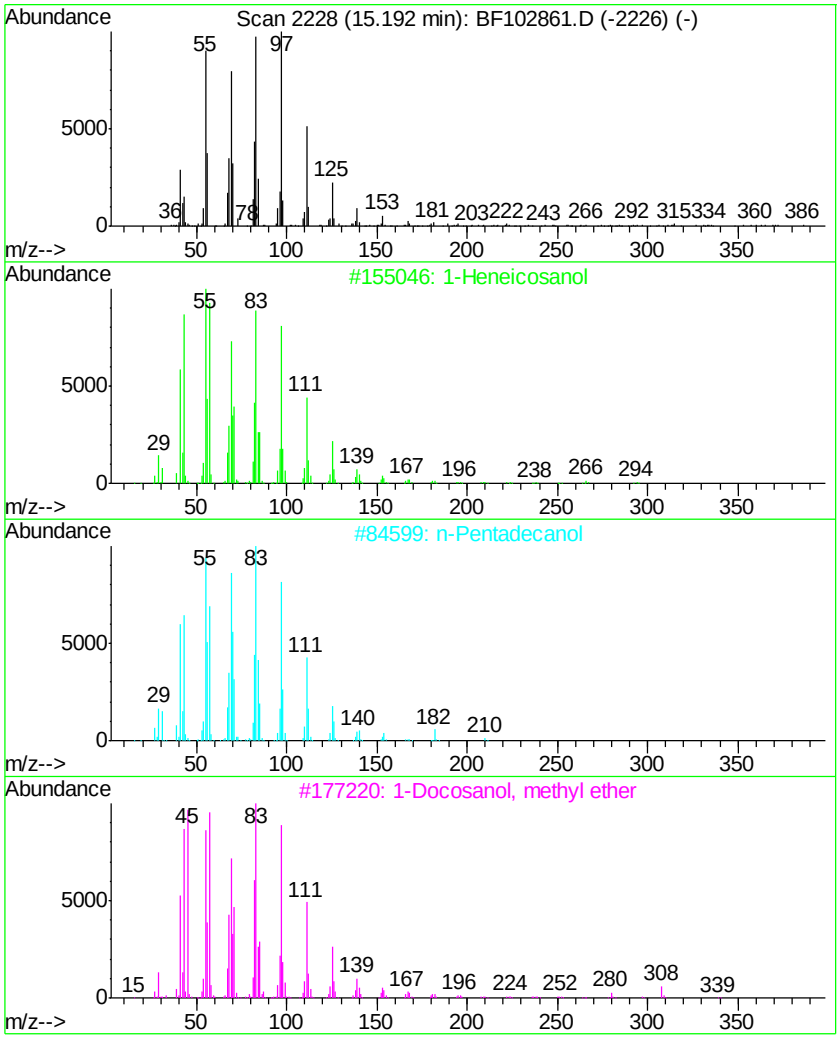
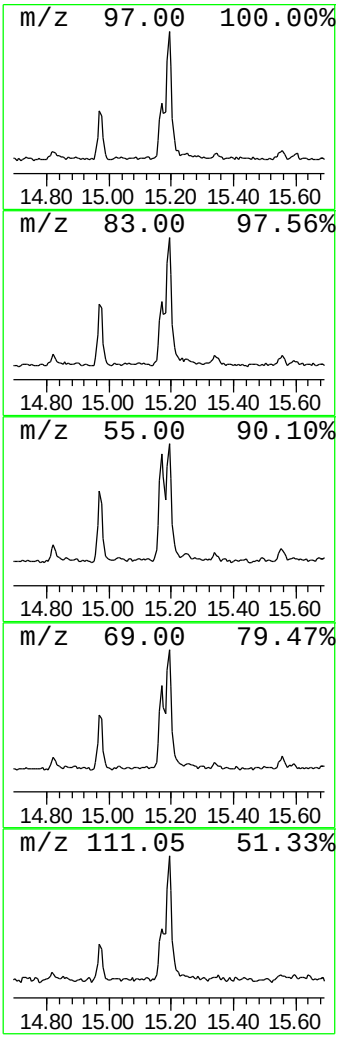
Peak Number 7 1-Heneicosanol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	23.65 ng	1134290	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	83
2	n-Pentadecanol	228	C15H32O	000629-76-5	80
3	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	70
4	Fumaric acid, 2-methylallyl tetr...	366	C22H38O4	1000330-55-3	64
5	Fumaric acid, octadecyl 2,2,3,3,...	582	C27H42F8O4	1000348-79-4	62





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102861.D
Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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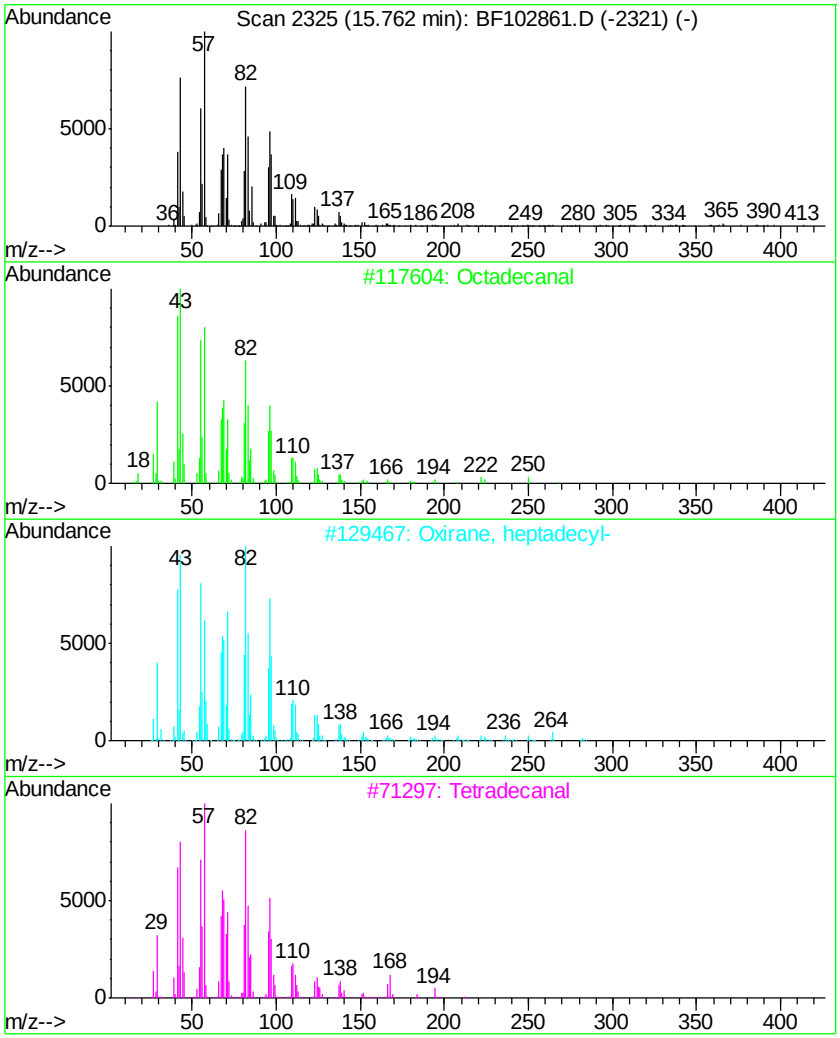
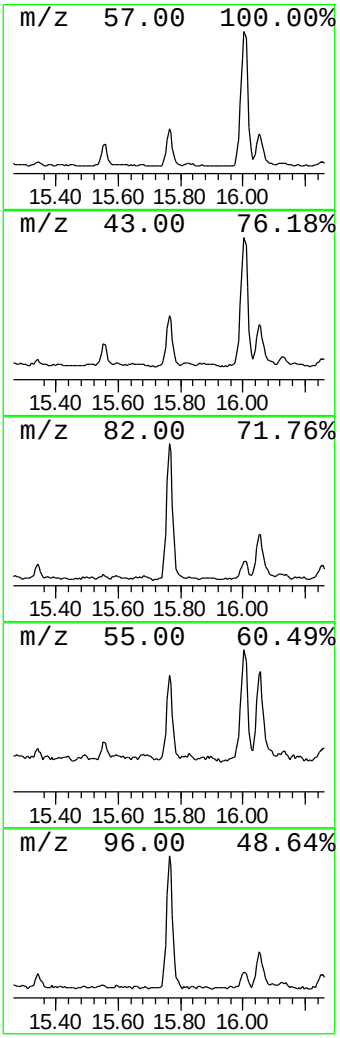
Peak Number 8 Octadecanal Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	23.45 ng	1124820	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3	Tetradecanal	212	C14H28O	000124-25-4	91
4	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
5	17-Octadecenal	266	C18H34O	056554-86-0	91





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Data File : BF102861.D
Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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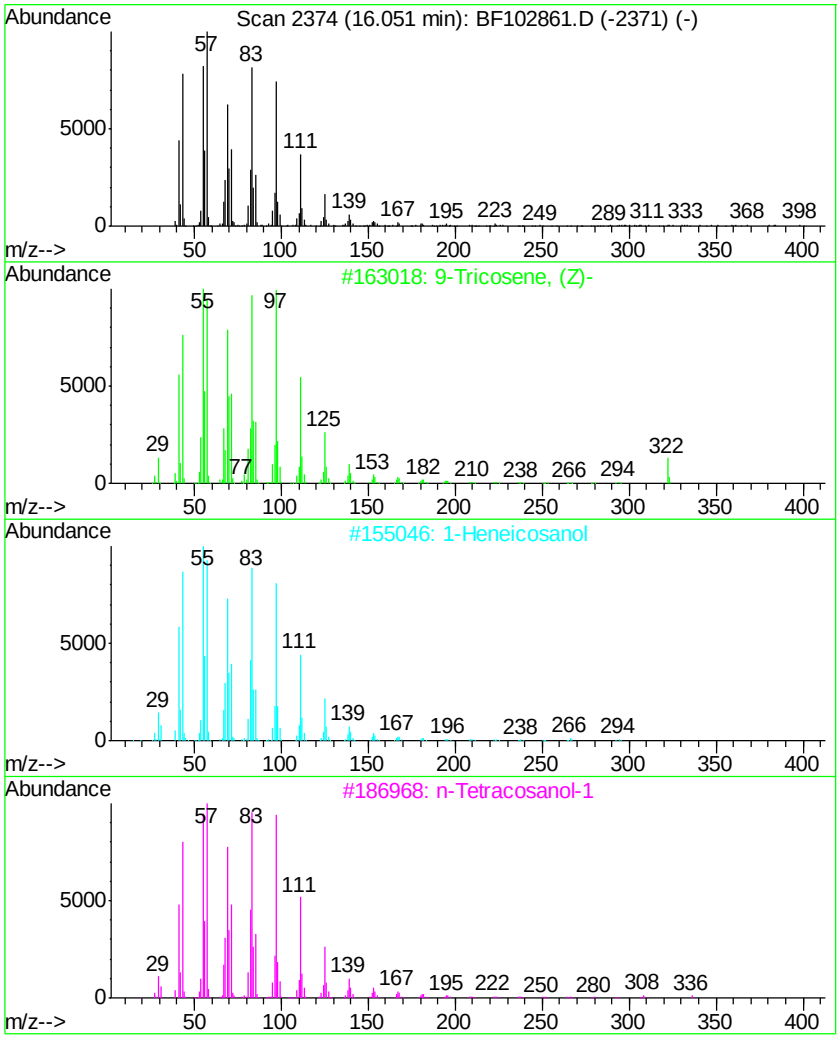
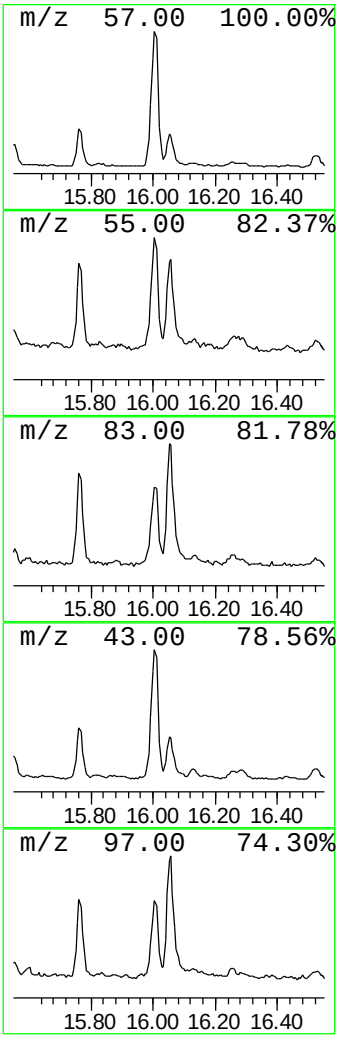
Peak Number 10 9-Tricosene, (Z)- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.05	22.02 ng	1055920	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Behenic alcohol	326	C22H46O	000661-19-8	94
5	Cyclotetracosane	336	C24H48	000297-03-0	91





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Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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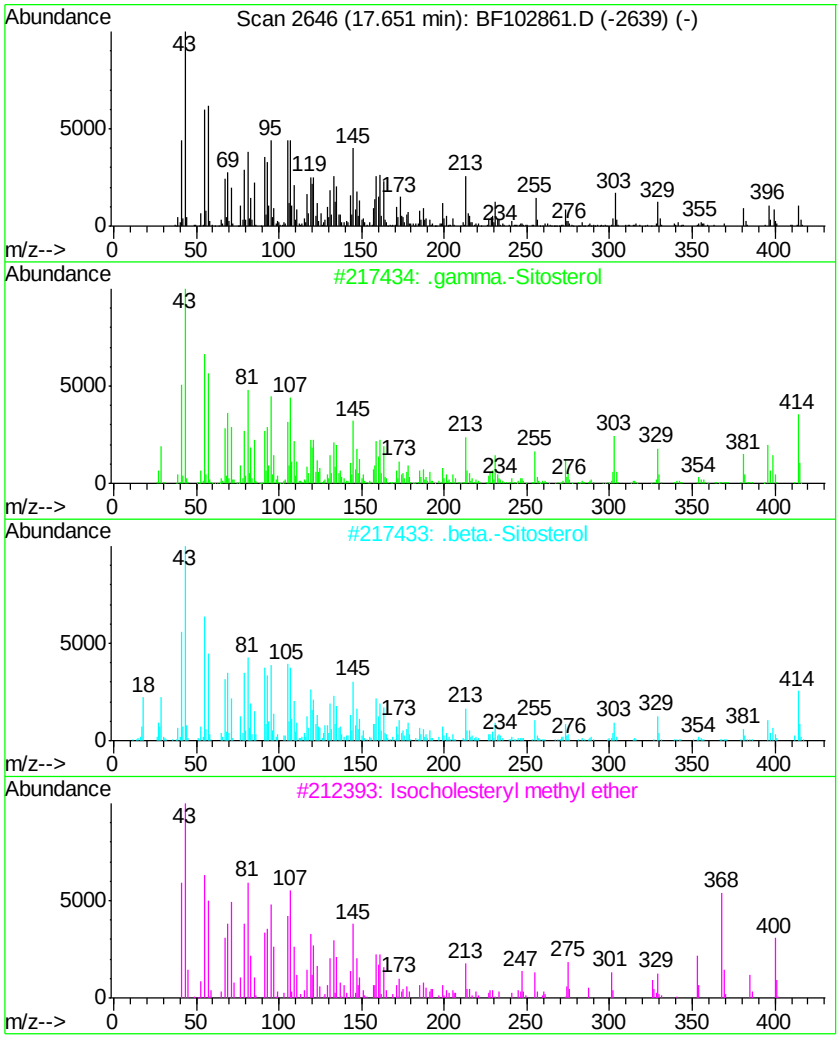
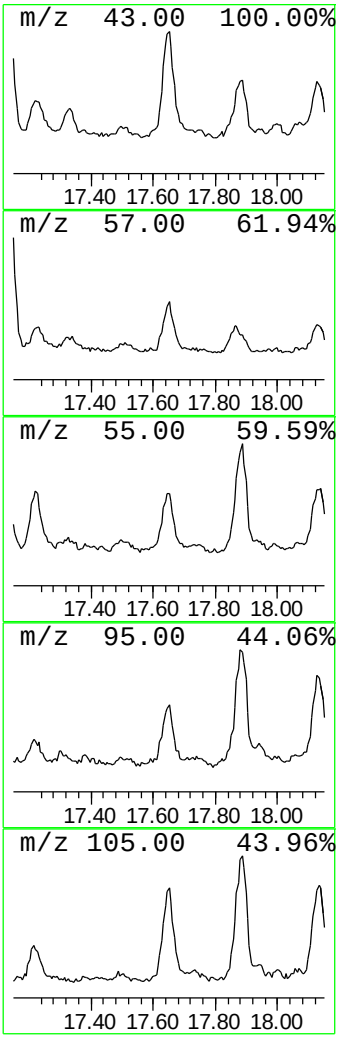
Peak Number 11 .gamma.-Sitosterol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.65	31.89 ng	1529500	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	99
3	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	50
4	Campesterol	400	C28H48O	000474-62-4	47
5	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	46





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Data File : BF102861.D
Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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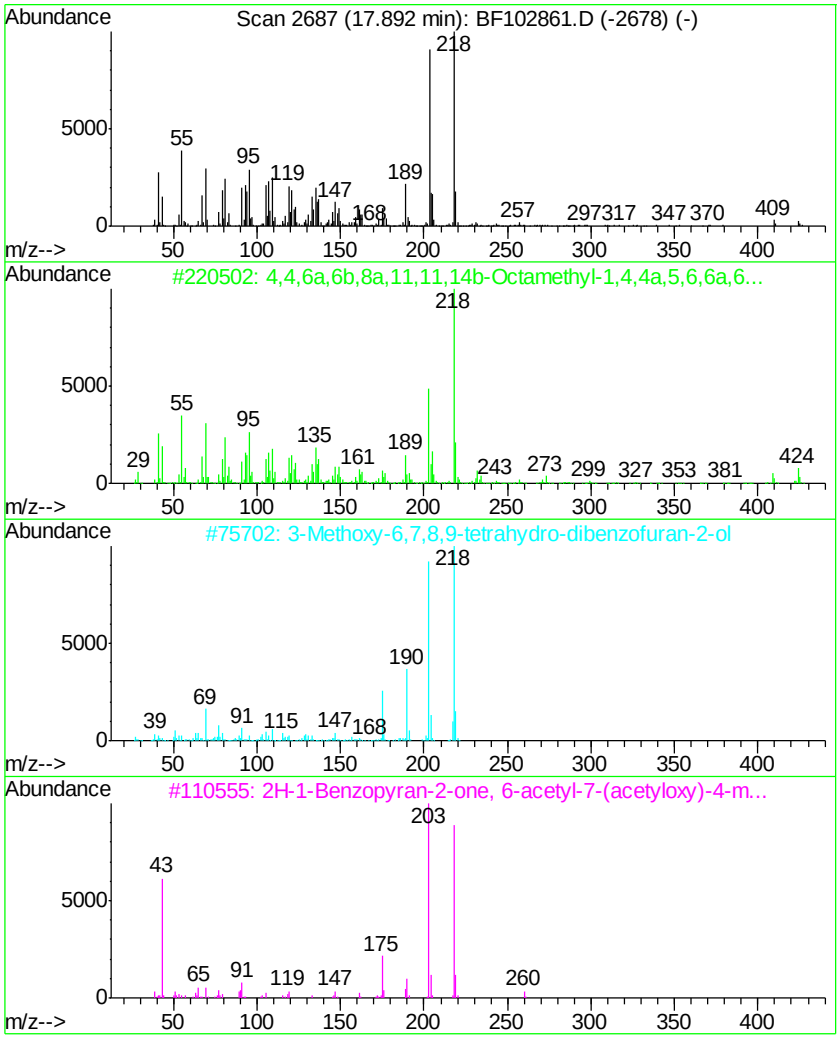
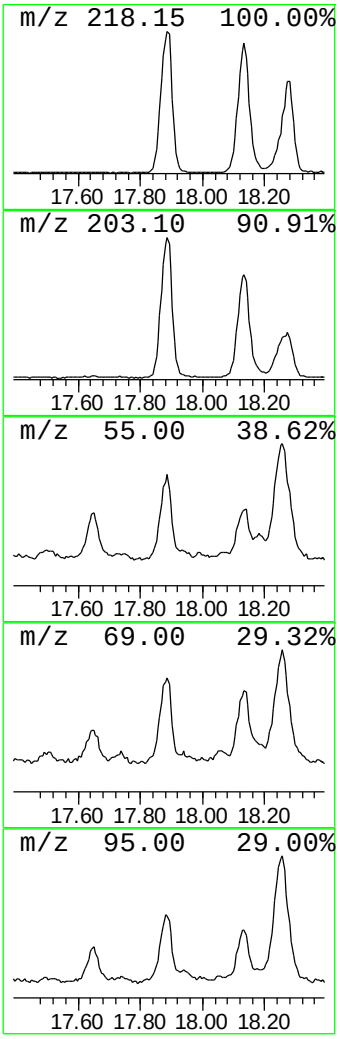
Peak Number 12 unknown17.89 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.89	52.16 ng	2501550	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4,6a,6b,8a,11,11,14b-Octamethy...	424	C30H48O	1000194-62-4	47
2	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	43
3	2H-1-Benzopyran-2-one, 6-acetyl-...	260	C14H12O5	129812-31-3	43
4	5H-Oxazolo[3,2-a]pyridine-8-carb...	218	C12H14N2O2	1000337-58-3	43
5	8-Amino-6,7-dimethoxy-4-methylqu...	218	C12H14N2O2	1000213-07-2	43





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Data File : BF102861.D
Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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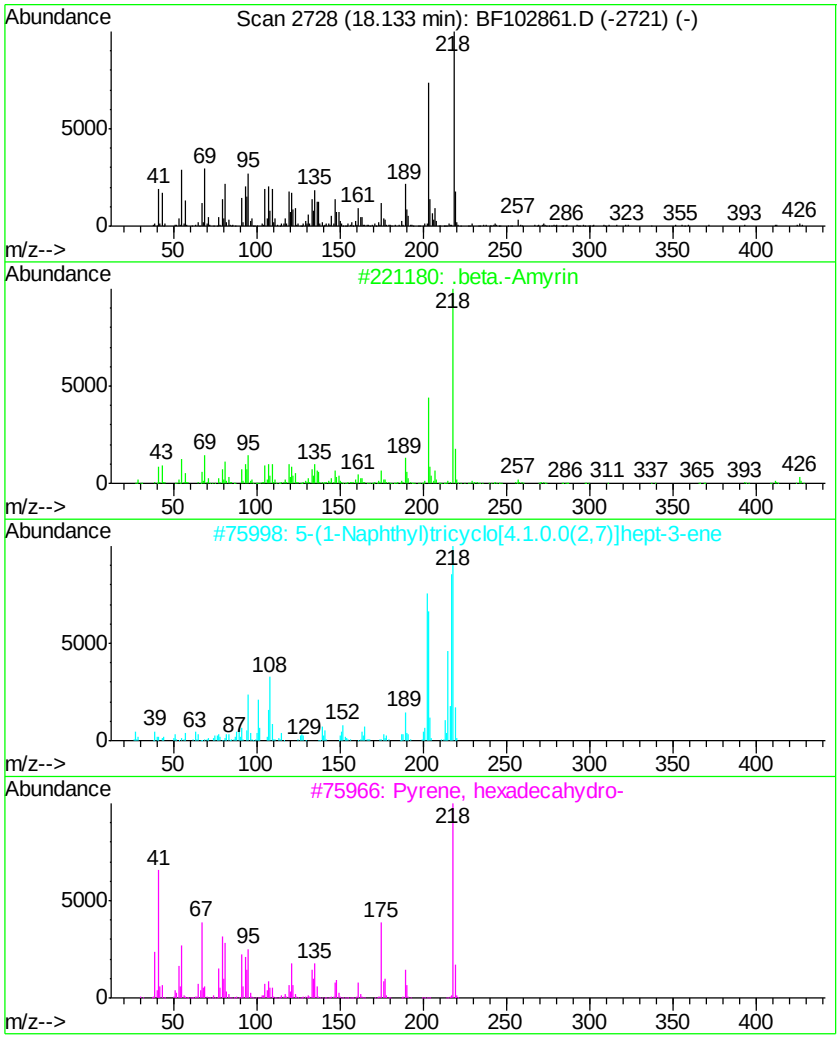
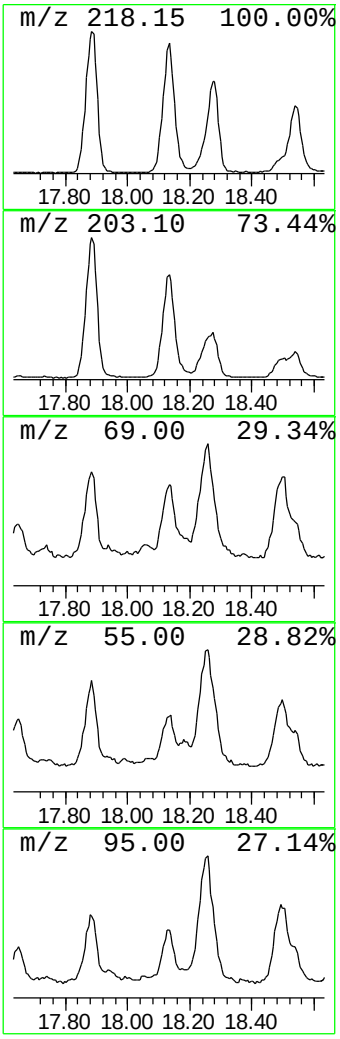
Peak Number 13 .beta.-Amyrin Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.13	44.57 ng	2137670	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Amyrin	426	C30H50O	000559-70-6	87
2	5-(1-Naphthyl)tricyclo[4.1.0.0(2...	218	C17H14	107729-05-5	83
3	Pyrene, hexadecahydro-	218	C16H26	002435-85-0	62
4	3a-Methyl-3,3a-dihydropyrrolo[3,...	218	C11H10N2OS	017163-68-7	58
5	3-Methoxy-6,7,8,9-tetrahydro-dib...	218	C13H14O3	1000186-57-9	52





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102861.D
Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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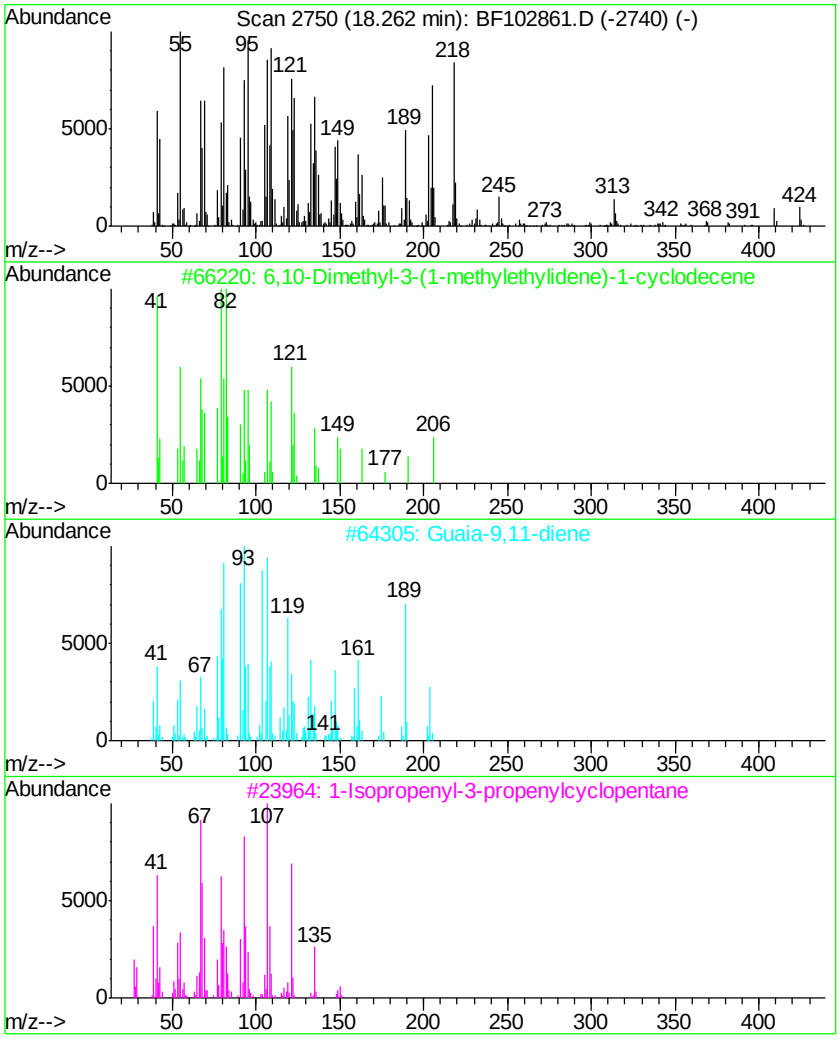
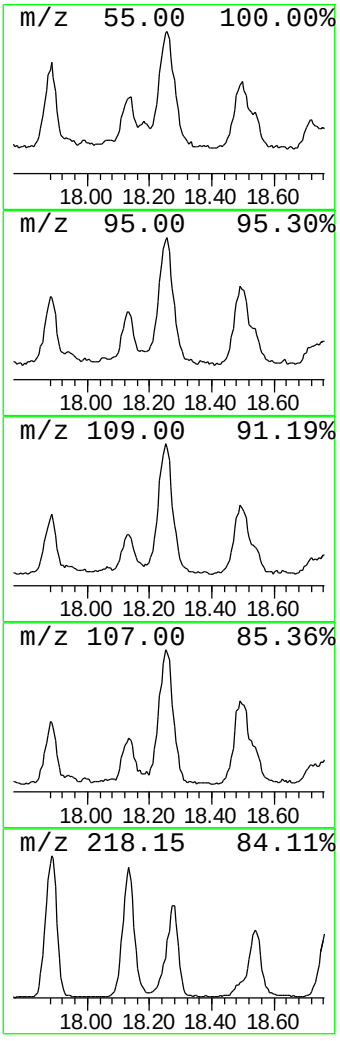
Peak Number 14 unknown18.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	122.75 ng	5887240	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,10-Dimethyl-3-(1-methylethylid...	206	C15H26	069239-71-0	46
2	Guaia-9,11-diene	204	C15H24	1000374-19-8	45
3	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	43
4	2,4,4-Trimethyl-3-(3-methylbuta-...	206	C14H22O	097452-05-6	25
5	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	25





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Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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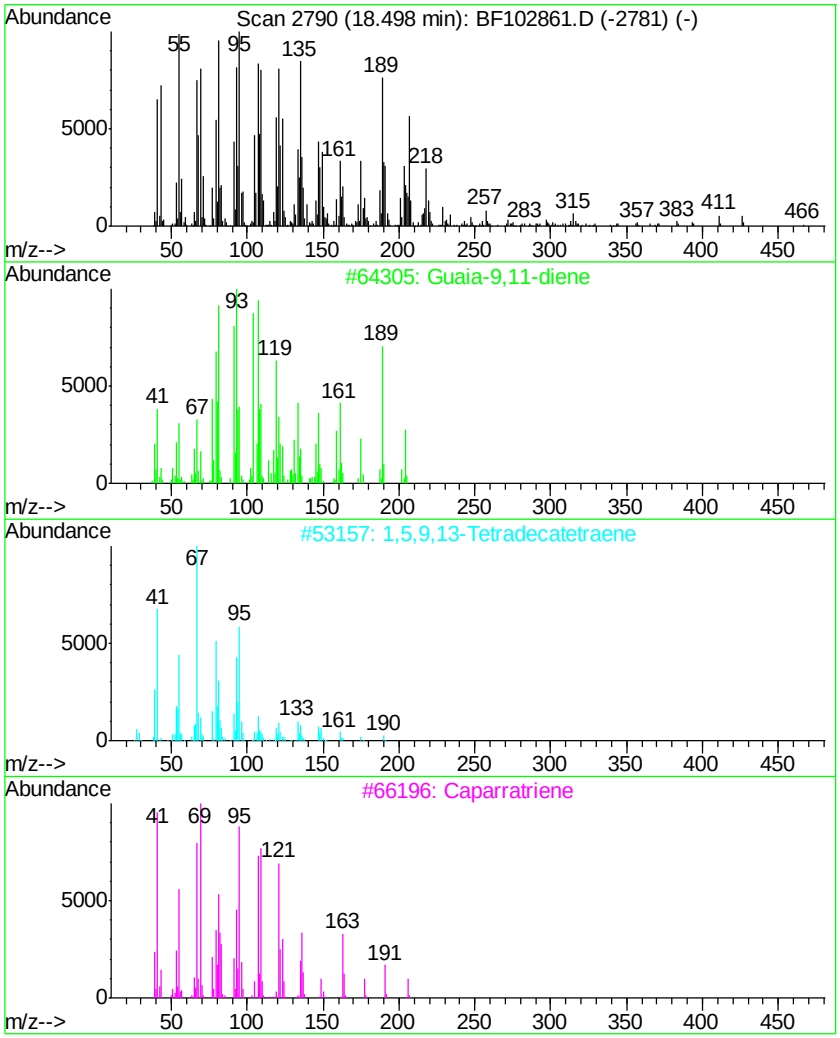
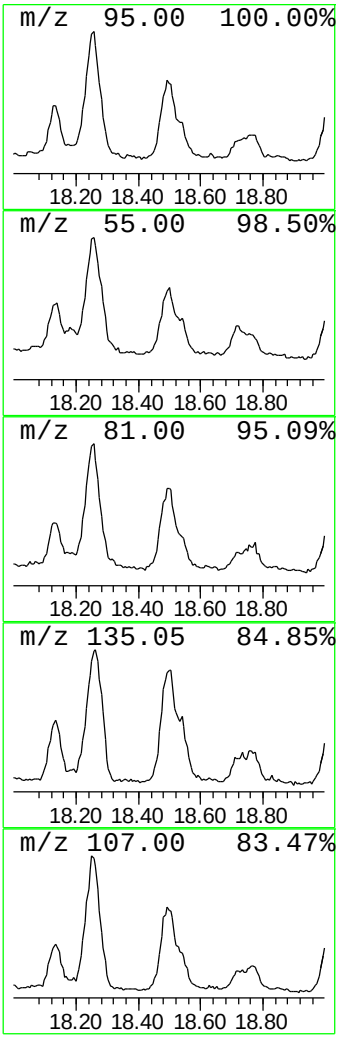
Peak Number 15 Guaia-9,11-diene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	68.98 ng	3308670	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guaia-9,11-diene	204	C15H24	1000374-19-8	80
2	1,5,9,13-Tetradecatetraene	190	C14H22	051487-38-8	62
3	Caparratriene	206	C15H26	1000374-08-7	55
4	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	010219-75-7	48
5	.gamma.-Elemene	204	C15H24	029873-99-2	46





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Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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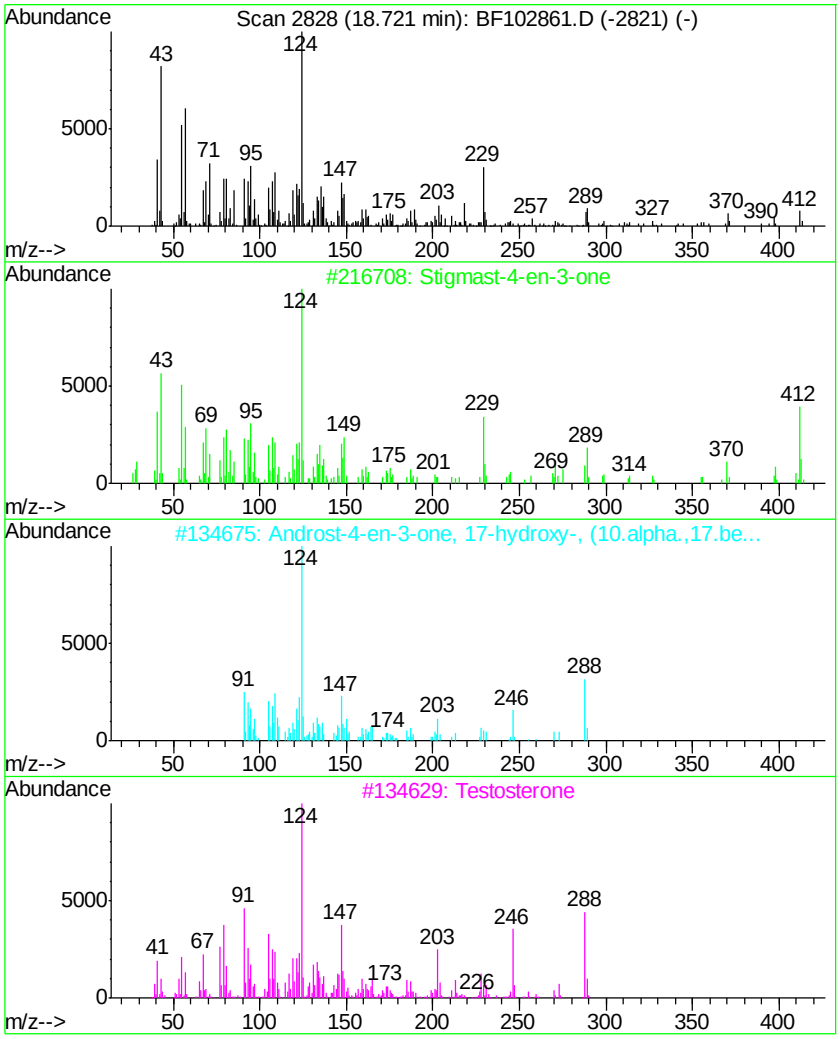
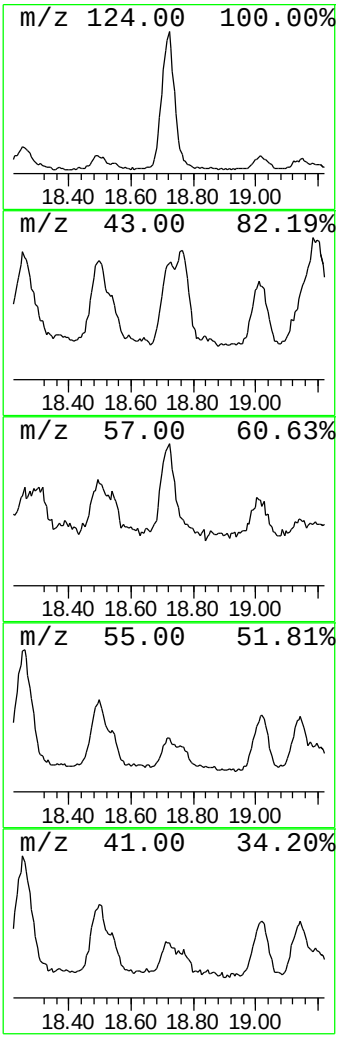
Peak Number 16 Stigmast-4-en-3-one Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.72	21.42 ng	1027210	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmast-4-en-3-one	412	C29H48O	001058-61-3	93
2	Androst-4-en-3-one, 17-hydroxy-,...	288	C19H28O2	000604-39-7	64
3	Testosterone	288	C19H28O2	000058-22-0	55
4	(2,3-Dichlorophenyl)carbamic aci...	311	C14H11Cl2NO3	1000305-08-9	45
5	Species: cyclopent-3-ene-1,1,2-t...	308	C16H12N4O3	1000277-65-8	38





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Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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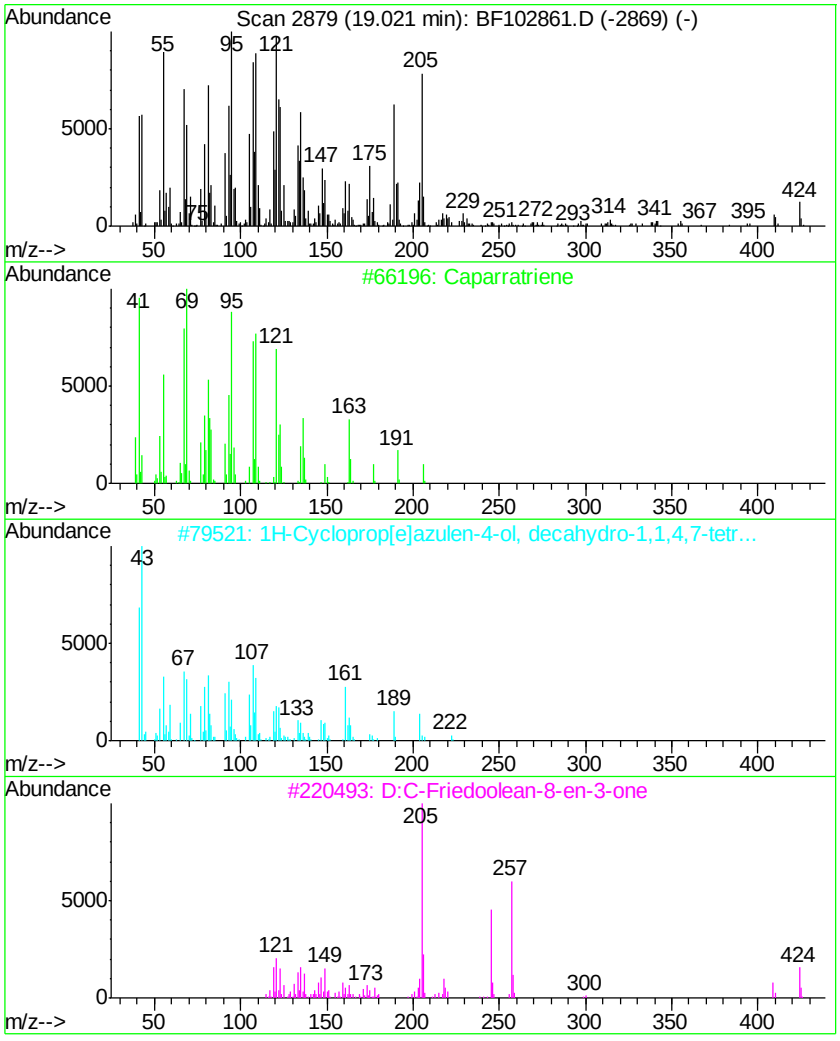
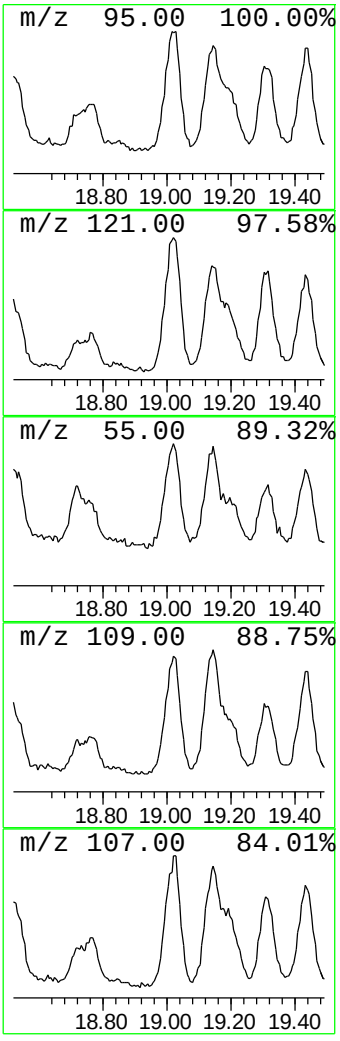
Peak Number 17 Caparratriene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.02	53.30 ng	2556320	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caparratriene	206	C15H26	1000374-08-7	78
2	1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	55
3	D:C-Friedoolean-8-en-3-one	424	C30H48O	022611-26-3	53
4	Lup-20(29)-en-3-one	424	C30H48O	001617-70-5	53
5	Cyclopropa[d]naphthalen-2(4aH)-o...	204	C14H20O	004677-90-1	51





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Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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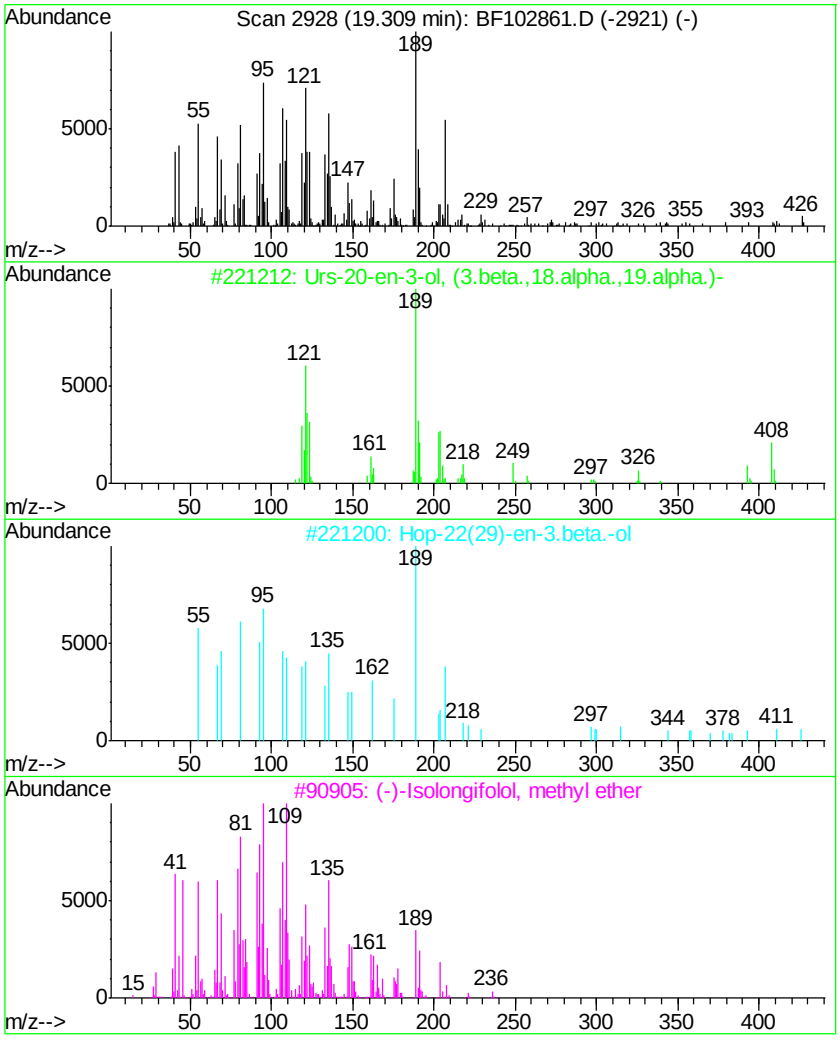
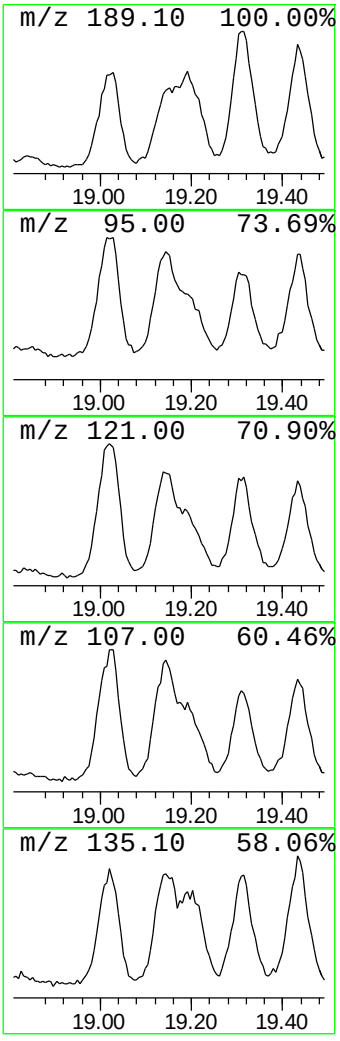
Peak Number 19 Urs-20-en-3-ol, (3.beta.,18... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.31	31.66 ng	1518430	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Urs-20-en-3-ol, (3.beta.,18.alph...	426	C30H50O	000464-98-2	58
2	Hop-22(29)-en-3.beta.-ol	426	C30H50O	058801-23-3	43
3	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	35
4	Isobornyl propionate	210	C13H22O2	002756-56-1	25
5	1,3-Cyclopentadiene, 2,3,4,5-tet...	190	C14H22	1000161-28-7	25





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Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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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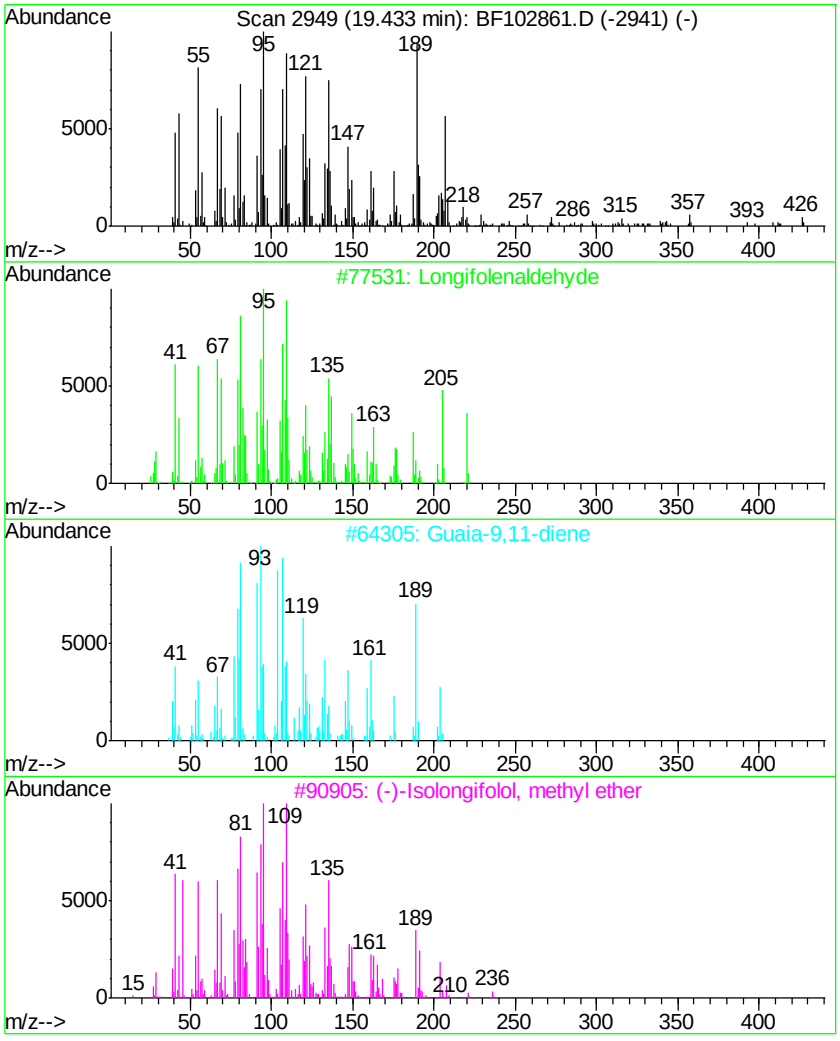
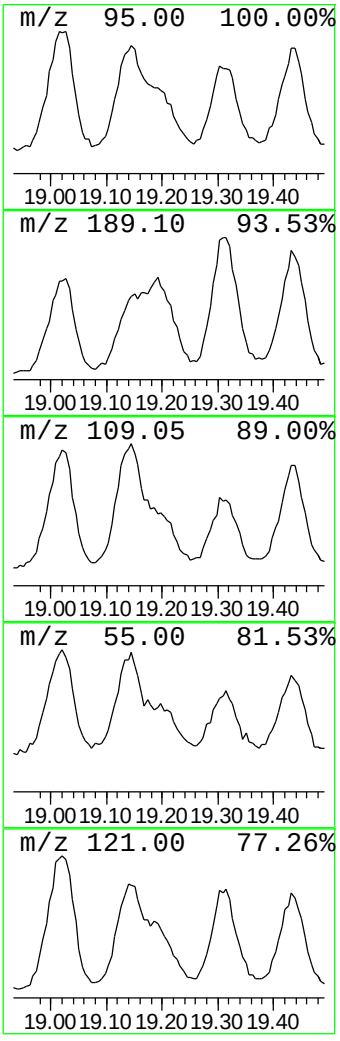
Peak Number 20 Longifolenaldehyde Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.43	34.22 ng	1641310	Perylene-d12	15.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Longifolenaldehyde	220	C15H24O	019890-84-7	66
2	Guaia-9,11-diene	204	C15H24	1000374-19-8	45
3	(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	45
4	6.beta.Bicyclo[4.3.0]nonane, 5.b...	332	C15H25I	1000195-85-9	42
5	Tricyclo[4.3.0.0(7,9)]nonane, 2,...	206	C15H26	054832-82-5	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF020818\
Data File : BF102861.D
Acq On : 8 Feb 2018 17:34
Operator : SJ/JU
Sample : J1470-07
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF020318.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
unknown6.66	6.66	69.8	ng	4390770	1	6.89	1257390	20.0
n-Hexadecanoic acid	11.95	22.9	ng	1184750	4	11.42	1034350	20.0
Docosane	14.51	18.1	ng	873797	5	14.06	965949	20.0
Oxirane, hexadecyl-	14.97	17.9	ng	857923	6	15.54	959257	20.0
Heptacosane	15.17	43.6	ng	2090060	6	15.54	959257	20.0
1-Heneicosanol	15.19	23.6	ng	1134290	6	15.54	959257	20.0
Octadecanal	15.76	23.4	ng	1124820	6	15.54	959257	20.0
9-Tricosene, (Z)-	16.05	22.0	ng	1055920	6	15.54	959257	20.0
.gamma.-Sitosterol	17.65	31.9	ng	1529500	6	15.54	959257	20.0
unknown17.89	17.89	52.2	ng	2501550	6	15.54	959257	20.0
.beta.-Amyrin	18.13	44.6	ng	2137670	6	15.54	959257	20.0
unknown18.26	18.26	122.8	ng	5887240	6	15.54	959257	20.0
Guaia-9,11-diene	18.50	69.0	ng	3308670	6	15.54	959257	20.0
Stigmast-4-en-3-one	18.72	21.4	ng	1027210	6	15.54	959257	20.0
Caparratriene	19.02	53.3	ng	2556320	6	15.54	959257	20.0
Urs-20-en-3-ol, (...	19.31	31.7	ng	1518430	6	15.54	959257	20.0
Longifolenaldehyde	19.43	34.2	ng	1641310	6	15.54	959257	20.0