LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

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-BF040618.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	5.016	488	498	505	rBV	114993	149658	4.96%	0.488%
2	5.410	559	565	568	rBV	2778736	2960945	98.07%	9.664%
3	6.428	732	738	741	rBV	2653749	3010954	99.73%	9.827%
4	6.569	757	762	765	rBV	3052926	3019102	100.00%	9.853%
5	6.628	769	772	775	rBV	156392	123028	4.07%	0.402%
6	6.804	798	802	805	rVB	977305	814273	26.97%	2.658%
7	6.957	824	828	831	rBV	2543638	2183986	72.34%	7.128%
8	7.369	892	898	901	rBV	1862935	1824912	60.45%	5.956%
9	7.439	904	910	914	rVB	30385	37041	1.23%	0.121%
10	8.086	1016	1020	1023	rBV	1288308	1122167	37.17%	3.662%
11	9.163	1198	1203	1206	rBV	3446026	2936061	97.25%	9.582%
12	9.557	1266	1270	1273	rBV	342249	298821	9.90%	0.975%
13	9.698	1291	1294	1298	rBV	43875	36973	1.22%	0.121%
14	9.769	1304	1306	1309	rVB	78588	66460	2.20%	0.217%
15	9.839	1314	1318	1322	rVB2	1481690	1223083	40.51%	3.992%
16	10.245	1384	1387	1389	rBV	33949	33367	1.11%	0.109%
17	10.274	1389	1392	1394	rVB	96341	82641	2.74%	0.270%
18	10.492	1424	1429	1432	rBV2	38731	49585	1.64%	0.162%
19	10.627	1447	1452	1455	rBV	2023255	1934718	64.08%	6.314%
20	10.745	1469	1472	1481	rVB	105826	117494	3.89%	0.383%
21	11.192	1546	1548	1551	rBV2	52817	49541	1.64%	0.162%
22	11.221	1551	1553	1558	rVB	38748	41547	1.38%	0.136%
23	11.327	1567	1571	1573	rBV	1361477	1104291	36.58%	3.604%
24	11.351	1573	1575	1577	rVB	157806	115785	3.84%	0.378%
25	11.827	1653	1656	1658	rBV	69385	59383	1.97%	0.194%
26	11.857	1658	1661	1666	rVV	366855	344418	11.41%	1.124%
27	11.939	1672	1675	1677	rBV2	66585	73716	2.44%	0.241%
28	11.963	1677	1679	1683	rVB	54001	46617	1.54%	0.152%
29	12.304	1734	1737	1739	rBV	42005	35186	1.17%	0.115%
30	12.374	1747	1749	1752	rBV	66787	62534	2.07%	0.204%
31	12.463	1761	1764	1768	rBV4	35758	43608	1.44%	0.142%
32	12.539	1773	1777	1780	rBV	206334	186671	6.18%	0.609%
33	12.639	1791	1794	1801	rBV3	79475	100614	3.33%	0.328%
34	12.768	1813	1816	1818	rVV	232567	176815	5.86%	0.577%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

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-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.815	1822	1824	1829	rVB2	47520	56309	1.87%	0.184%
36	12.915	1837	1841	1845	rBV	2318462	2338392	77.45%	7.632%
37	12.986	1850	1853	1856	rBV	27140	42024	1.39%	0.137%
38	13.098	1870	1872	1874	rVB2	58577	46095	1.53%	0.150%
39	13.198	1886	1889	1892	rBV	44509	45994	1.52%	0.150%
40	13.292	1902	1905	1908	rVV	75873	58986	1.95%	0.193%
41	13.321	1908	1910	1913	rVB	44852	35101	1.16%	0.115%
42	13.398	1919	1923	1928	rVB6	33859	45482	1.51%	0.148%
43	13.504	1937	1941	1947	rVB8	30941	66739	2.21%	0.218%
44	13.604	1955	1958	1962	rVB3	46051	48218	1.60%	0.157%
45	13.715	1972	1977	1980	rBV4	24313	45858	1.52%	0.150%
46	13.809	1990	1993	2002	rVB	564779	514356	17.04%	1.679%
47	13.968	2015	2020	2023	rBV	990475	972350	32.21%	3.173%
48	13.992	2023	2024	2030	rVB	113534	101796	3.37%	0.332%
49	14.357	2082	2086	2090	rVB	35419	40495	1.34%	0.132%
50	14.451	2099	2102	2105	rBV3	94068	88242	2.92%	0.288%
51	14.827	2164	2166	2173	rVB2	30576	33563	1.11%	0.110%
52	15.004	2192	2196	2199	rBV2	70082	100458	3.33%	0.328%
53	15.298	2243	2246	2251	rVB	54335	64684	2.14%	0.211%
54	15.362	2253	2257	2263	rVB	63094	76481	2.53%	0.250%
55	15.427	2263	2268	2272	rBV	673209	816274	27.04%	2.664%
56	15.898	2344	2348	2351	rBV2	41973	69416	2.30%	0.227%
57	15.945	2352	2356	2366	rVB5	89037	175372	5.81%	0.572%
58	16.845	2507	2509	2516	rVB2	22066	38403	1.27%	0.125%
59	16.980	2528	2532	2537	rBV3	26957	54844	1.82%	0.179%
60	17.286	2580	2584	2592	rVB	27644	56594	1.87%	0.185%
61	17.439	2605	2610	2620	rVB9	62916	141450	4.69%	0.462%

Sum of corrected areas: 30639971

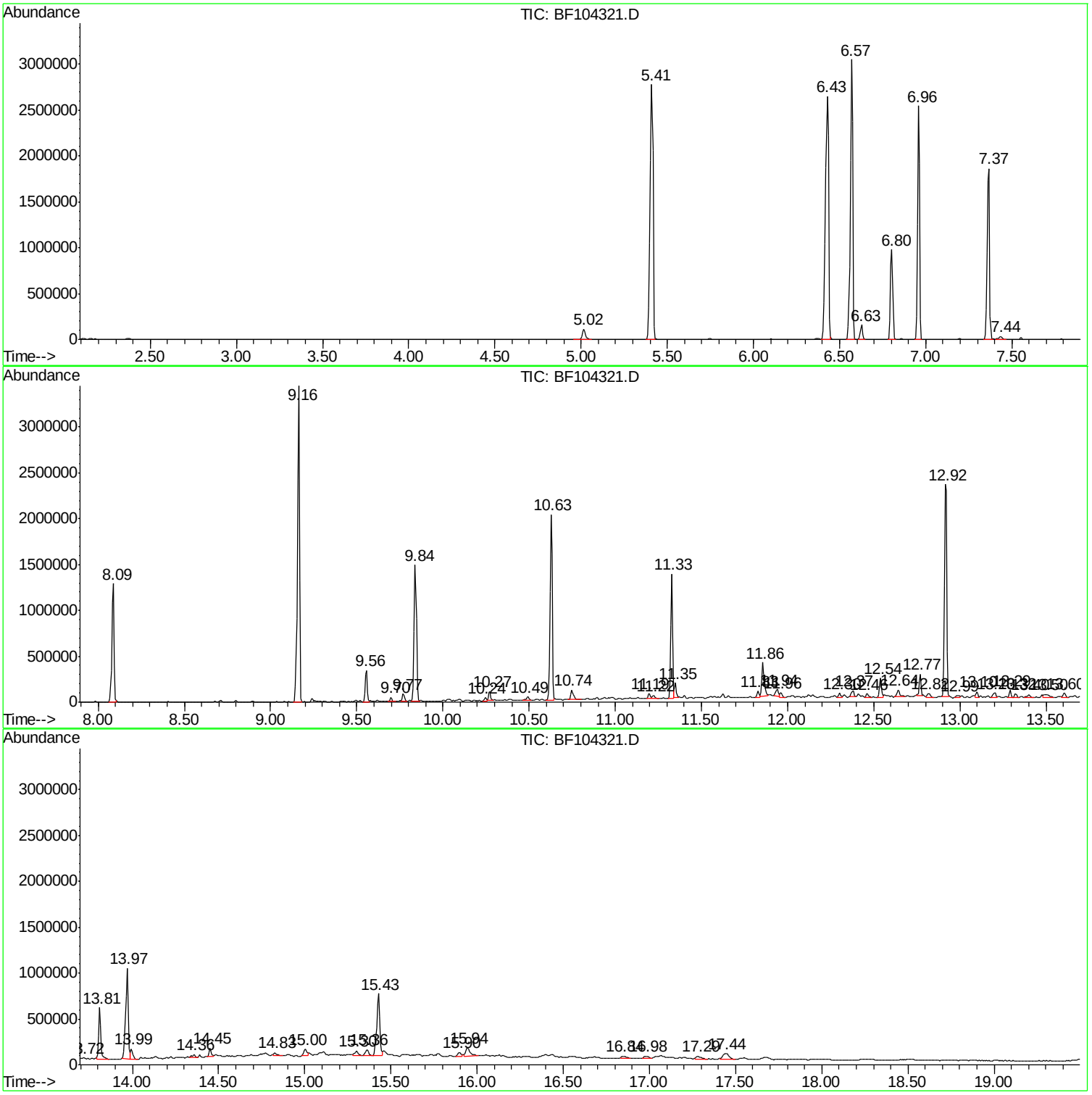
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

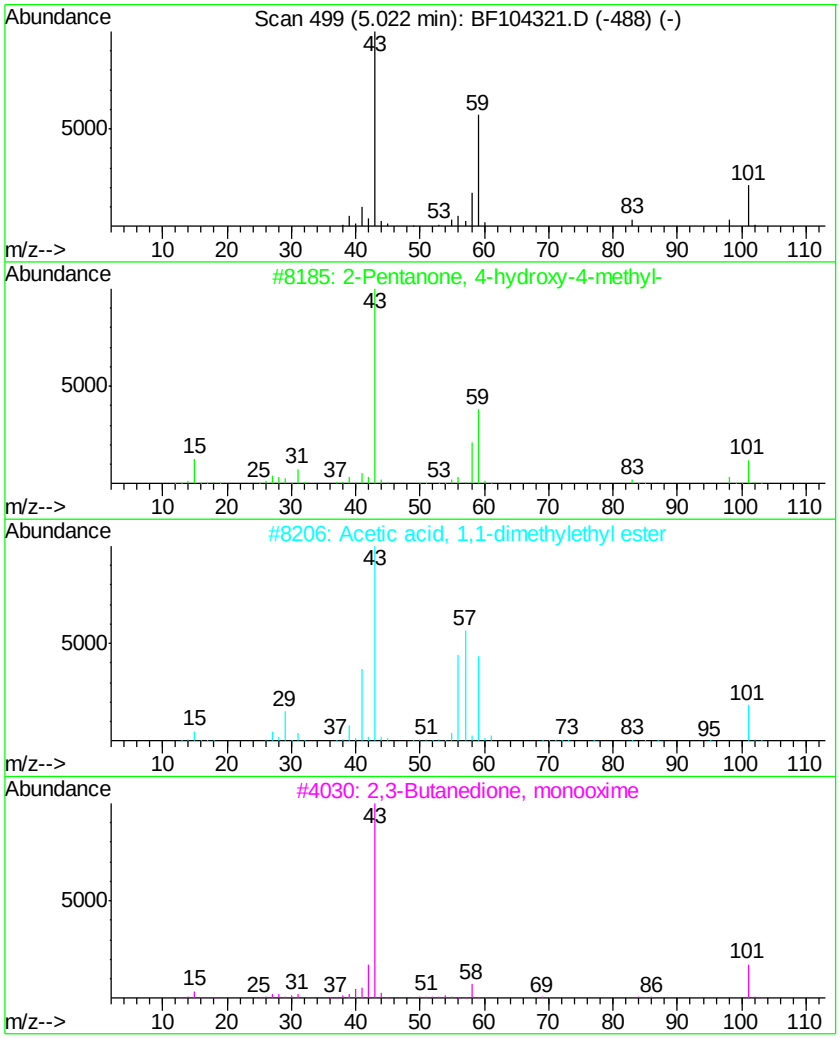
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

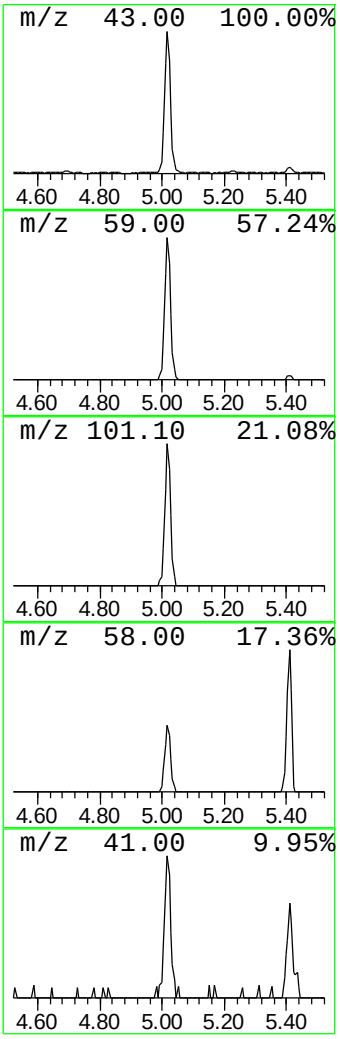
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	3.68 ng	149658	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17





Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

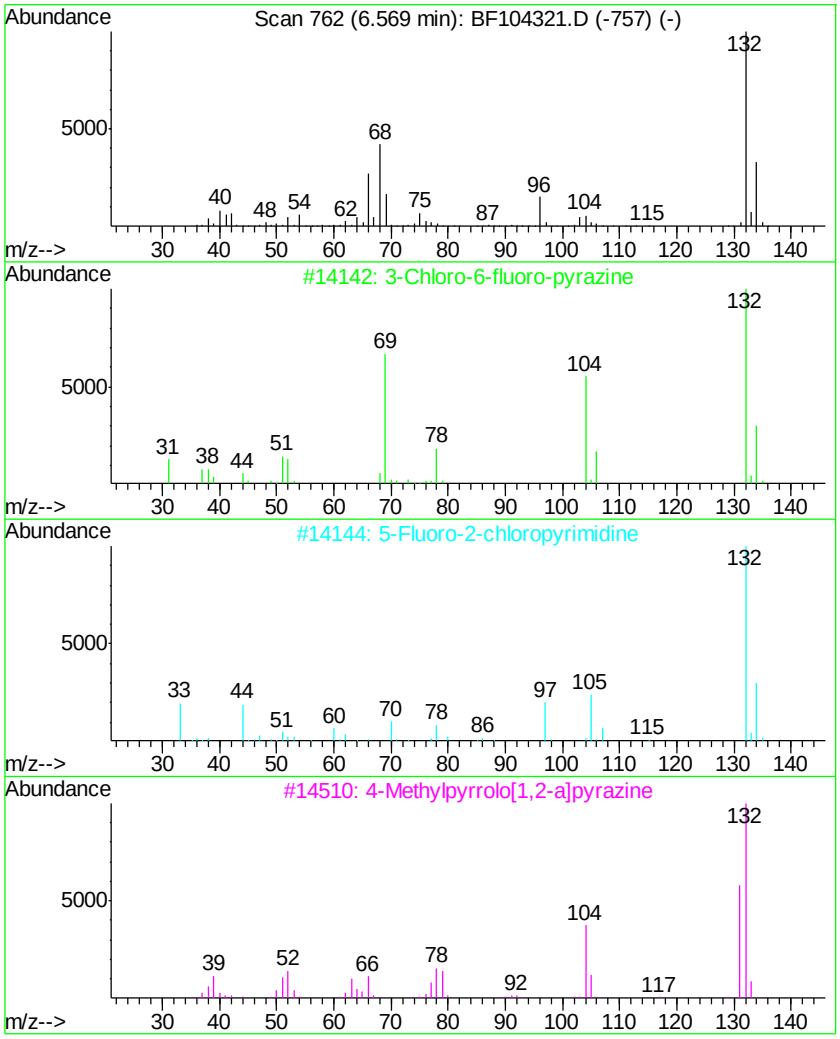
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

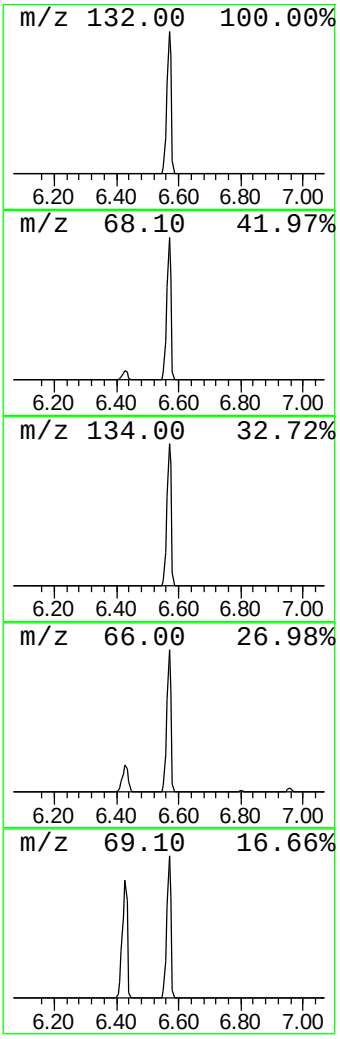
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	74.15 ng	3019100	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
3	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

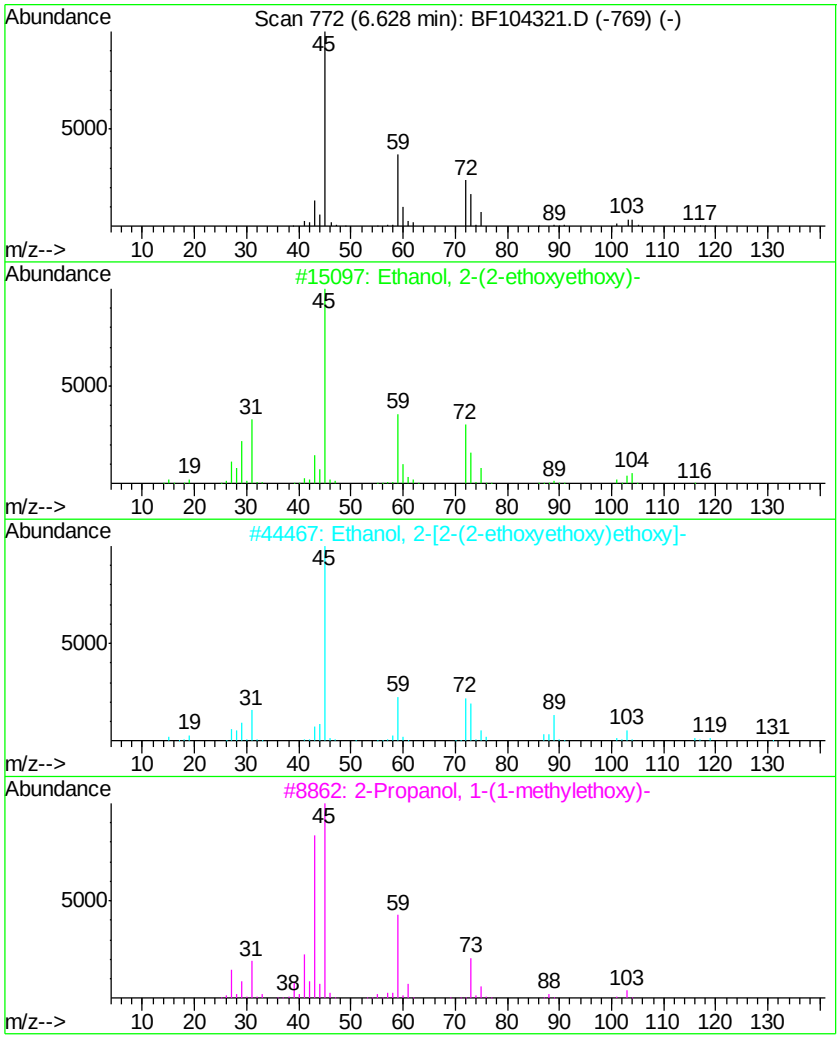
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

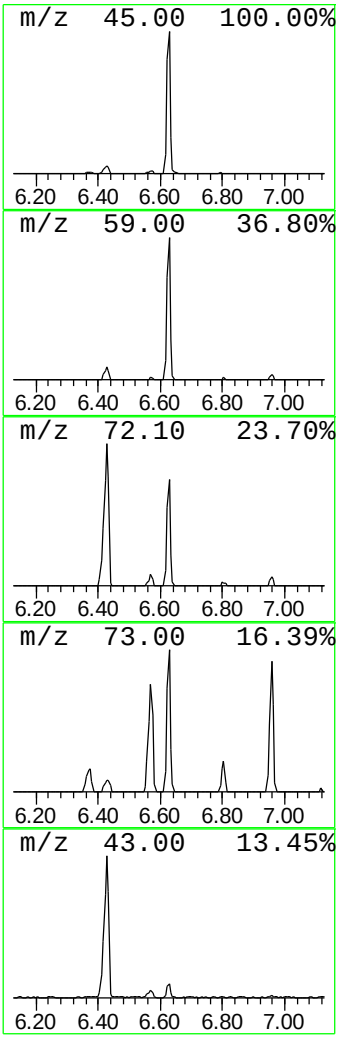
****

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	3.02 ng	123028	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42
5	L-Lactic acid	90	C3H6O3	000079-33-4	38





Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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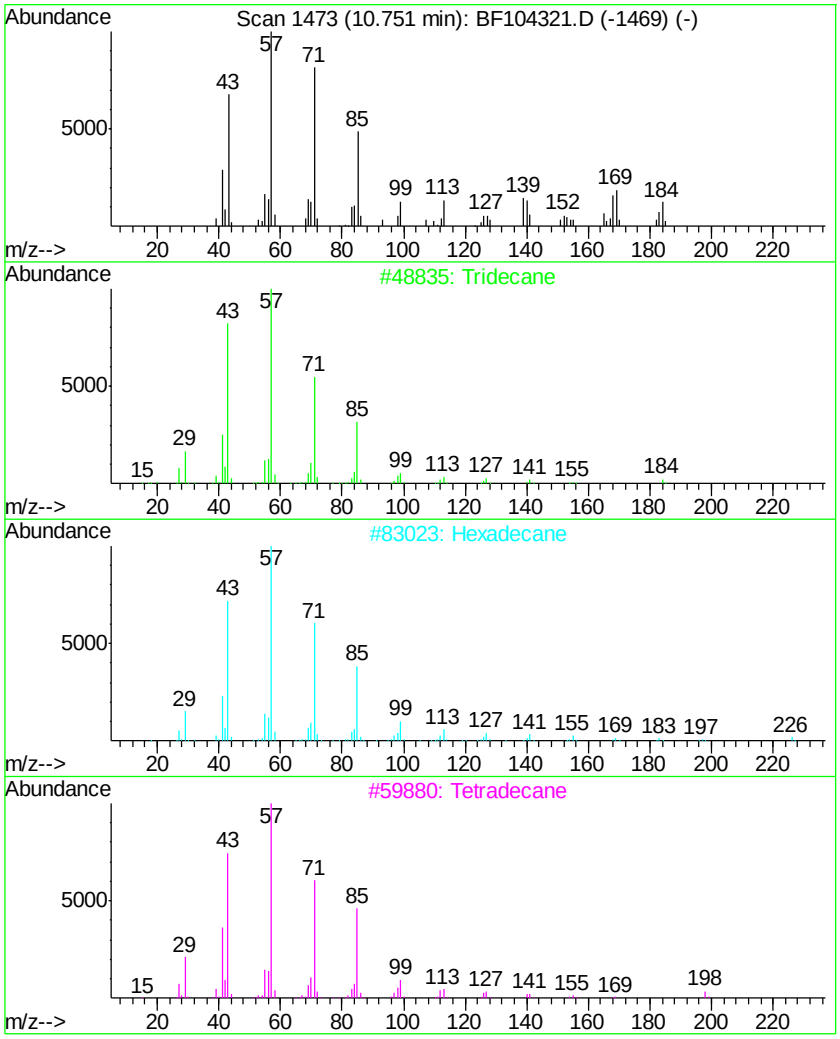
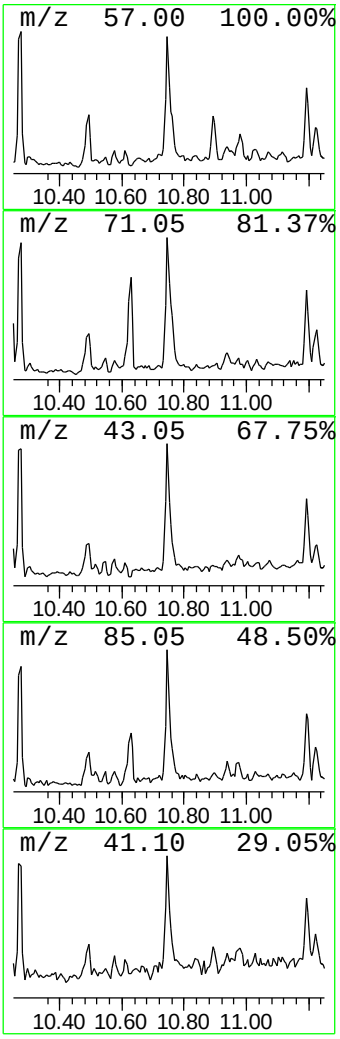
Peak Number 5 Tridecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	2.13 ng	117494	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	92
2	Hexadecane	226	C16H34	000544-76-3	80
3	Tetradecane	198	C14H30	000629-59-4	80
4	Pentadecane	212	C15H32	000629-62-9	80
5	Tetracosane	338	C24H50	000646-31-1	72





Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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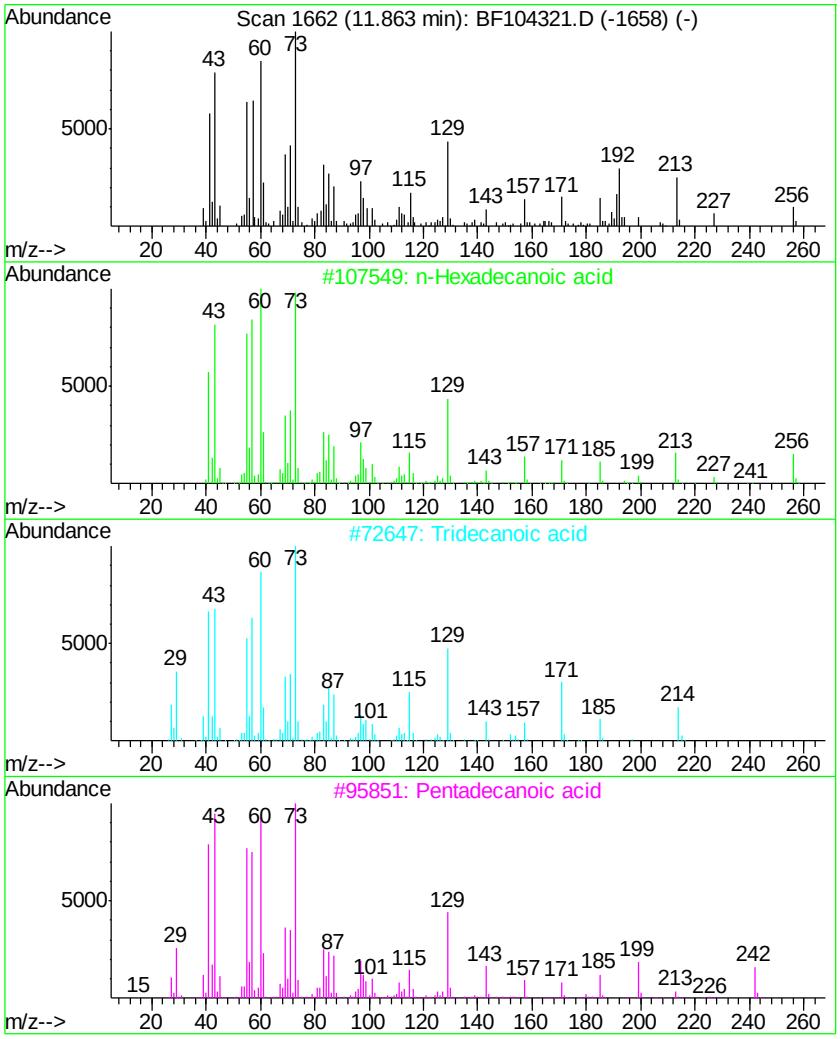
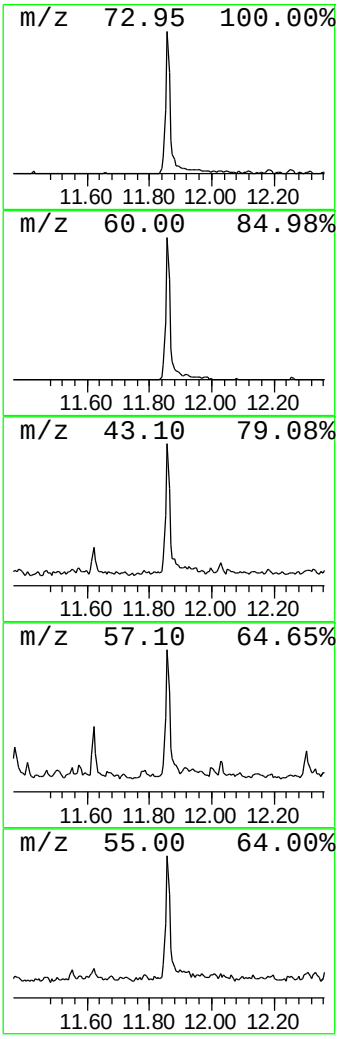
Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	6.24 ng	344418	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Anthracene, 1-methyl-	192	C15H12	000610-48-0	45
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	45





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Acq On : 6 Apr 2018 22:23
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Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

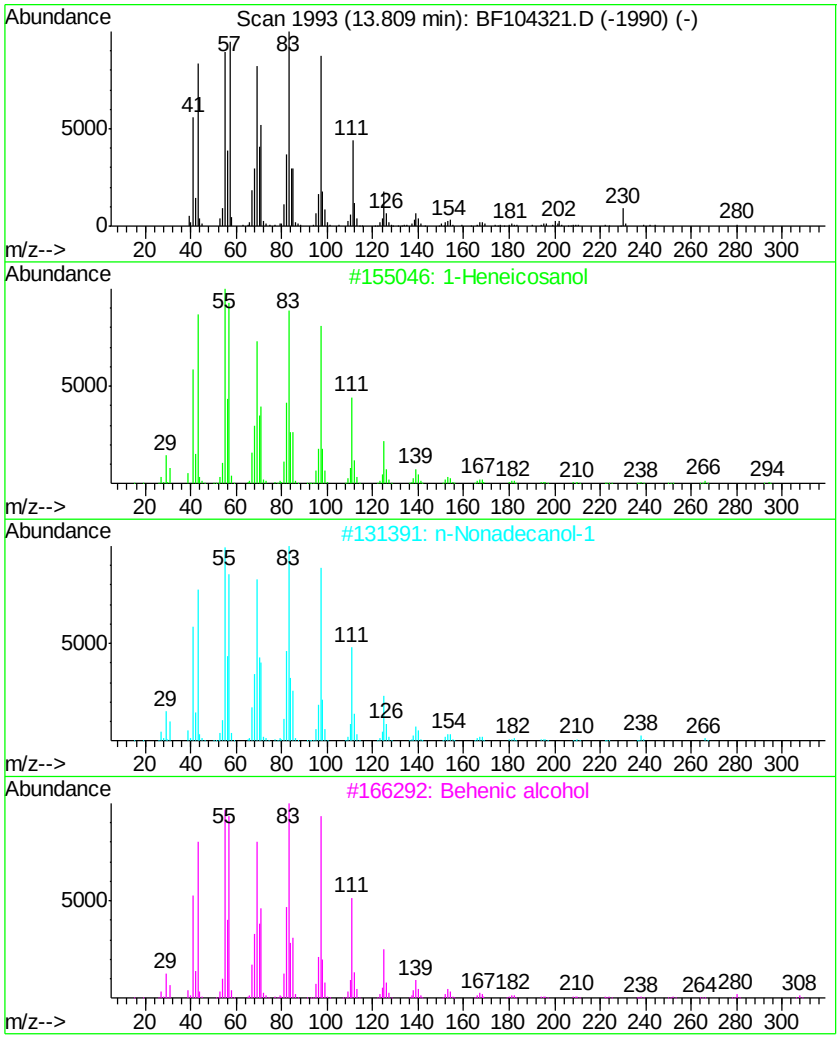
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

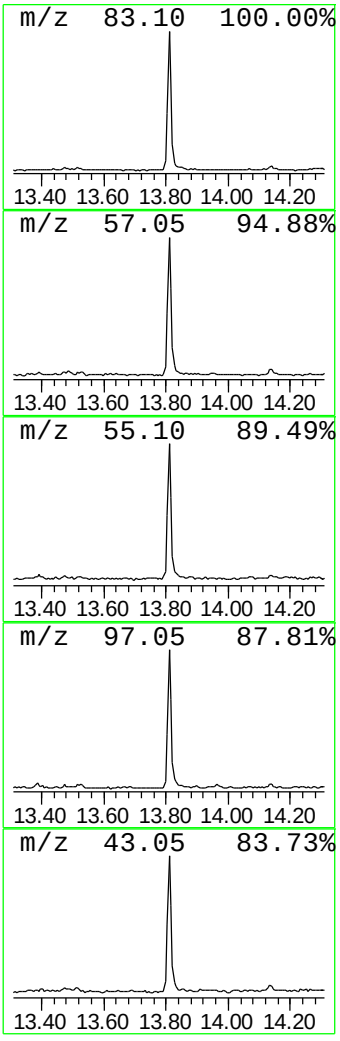
****

Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	10.58 ng	514356	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
3	Behenic alcohol	326	C22H46O	000661-19-8	91
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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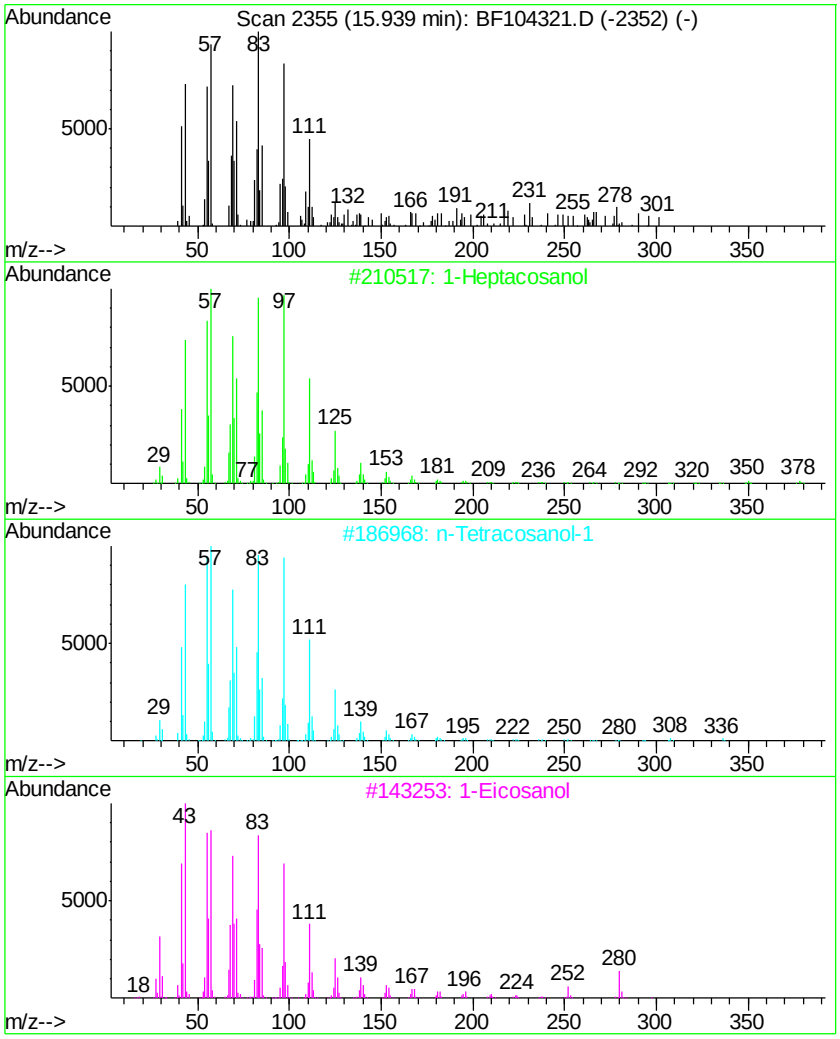
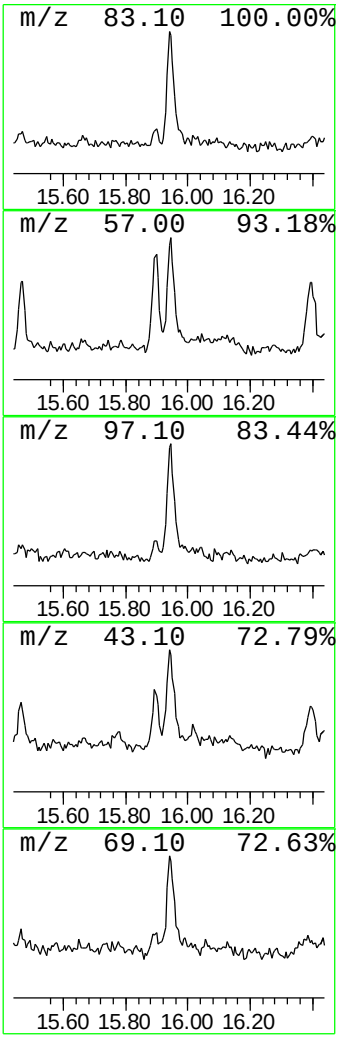
Peak Number 9 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	4.30 ng	175372	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	93
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
3	1-Eicosanol	298	C20H42O	000629-96-9	81
4	Carbonic acid, pentadecyl 2,2,2-...	402	C18H33Cl3O3	1000314-56-1	80
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	74





Data Path : Z:\HPCHEM1\BNA F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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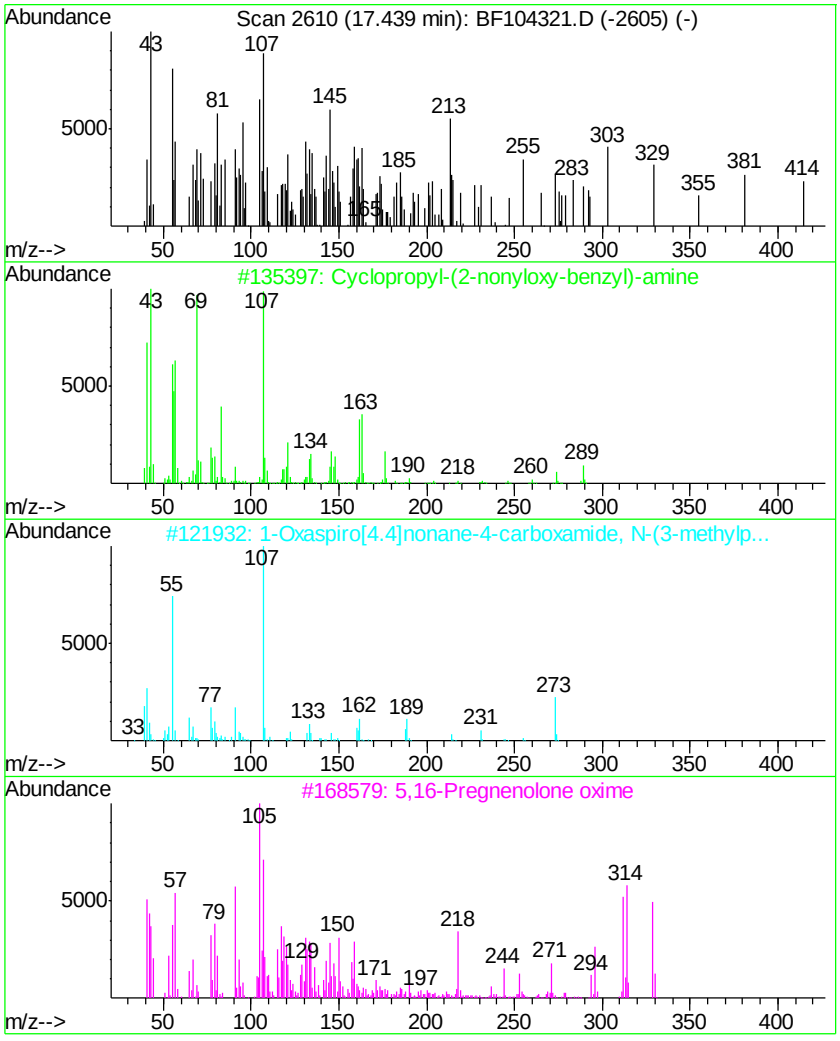
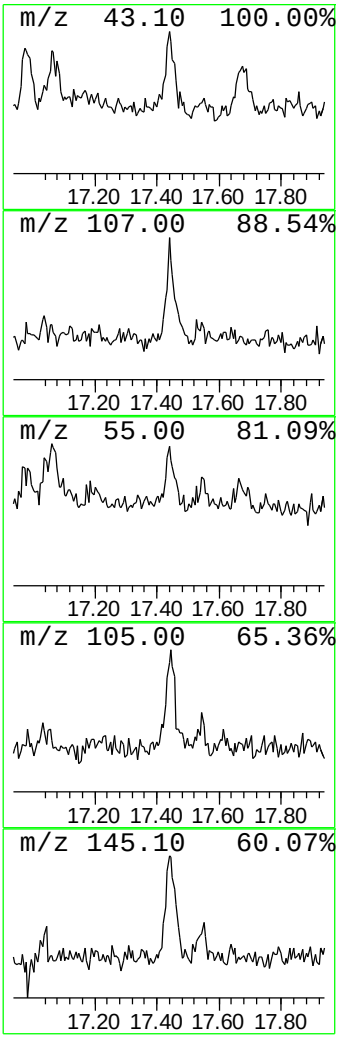
Peak Number 10 unknown17.44 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.44	3.47 ng	141450	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropyl-(2-nonyloxy-benzyl)-...	289	C19H31NO	1000297-00-6	14
2	1-Oxaspiro[4.4]nonane-4-carboxam...	273	C16H19NO3	1000319-97-0	12
3	5,16-Pregnenolone oxime	329	C21H31NO2	001045-71-2	11
4	1-Pyrazineacetamide, N-(2-cyano-...	381	C20H23N5O3	1000319-00-2	10
5	Propionic acid 1-methyl-4-phenyl...	287	C18H25NO2	1000297-46-2	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\Data\BF040618\
Data File : BF104321.D
Acq On : 6 Apr 2018 22:23
Operator : JU/SJ
Sample : J2212-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SP-1-A

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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...	5.02	3.7	ng	149658	1	6.80	814273	20.0
unknown6.57	6.57	74.2	ng	3019100	1	6.80	814273	20.0
Ethanol, 2-(2-eth...	6.63	3.0	ng	123028	1	6.80	814273	20.0
Tridecane	10.75	2.1	ng	117494	4	11.33	1104290	20.0
n-Hexadecanoic acid	11.86	6.2	ng	344418	4	11.33	1104290	20.0
1-Heneicosanol	13.81	10.6	ng	514356	5	13.97	972350	20.0
1-Heptacosanol	15.94	4.3	ng	175372	6	15.43	816274	20.0
unknown17.44	17.44	3.5	ng	141450	6	15.43	816274	20.0