LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF031618\
Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

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-BF031518.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	2.316	34	39	45	rVB	141639	185208	5.09%	0.499%
2	5.216	524	532	539	rBV	96582	119708	3.29%	0.322%
3	5.593	591	596	600	rBV	3264604	3598745	98.86%	9.687%
4	5.916	648	651	660	rVB	267246	225921	6.21%	0.608%
5	6.592	760	766	769	rBV	3362710	3640417	100.00%	9.799%
6	6.616	769	770	779	rVB	32745	40483	1.11%	0.109%
7	6.739	786	791	794	rBV	3741327	3637474	99.92%	9.791%
8	6.969	827	830	834	rVB	1327613	1076085	29.56%	2.897%
9	7.128	853	857	860	rBV	3263421	2742906	75.35%	7.383%
10	7.534	920	926	929	rBV	2478527	2268246	62.31%	6.106%
11	8.251	1044	1048	1051	rBV	1757259	1416011	38.90%	3.812%
12	9.328	1226	1231	1234	rBV	4100106	3540504	97.26%	9.530%
13	9.398	1239	1243	1245	rBV	52772	45374	1.25%	0.122%
14	9.716	1293	1297	1300	rBV	471689	354992	9.75%	0.956%
15	9.869	1320	1323	1326	rBV	85828	72142	1.98%	0.194%
16	9.928	1329	1333	1336	rVV	156558	116793	3.21%	0.314%
17	10.010	1343	1347	1351	rBV2	1656063	1426956	39.20%	3.841%
18	10.404	1410	1414	1416	rBV	41442	43192	1.19%	0.116%
19	10.427	1416	1418	1421	rVB	174944	124322	3.42%	0.335%
20	10.645	1449	1455	1458	rBV	47398	62653	1.72%	0.169%
21	10.804	1477	1482	1485	rBV	1957256	1918240	52.69%	5.163%
22	10.904	1496	1499	1508	rVB	117188	158306	4.35%	0.426%
23	11.351	1571	1575	1578	rBV	78173	64569	1.77%	0.174%
24	11.504	1597	1601	1603	rBV	1405616	1199343	32.95%	3.228%
25	11.527	1603	1605	1610	rVB	223963	178433	4.90%	0.480%
26	11.574	1610	1613	1616	rBV	83256	71436	1.96%	0.192%
27	12.010	1681	1687	1690	rBV2	273774	306969	8.43%	0.826%
28	12.033	1690	1691	1696	rVB2	78837	53127	1.46%	0.143%
29	12.116	1702	1705	1708	rBV3	81656	97504	2.68%	0.262%
30	12.557	1777	1780	1782	rBV	46851	50468	1.39%	0.136%
31	12.639	1791	1794	1799	rVB2	39101	42891	1.18%	0.115%
32	12.721	1804	1808	1811	rBV	525487	510071	14.01%	1.373%
33	12.798	1816	1821	1826	rBV3	106543	148859	4.09%	0.401%
34	12.898	1835	1838	1840	rVB2	53246	50161	1.38%	0.135%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF031618\
Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

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-BF031518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.951	1844	1847	1852	rVB	561437	491863	13.51%	1.324%
36	13.092	1863	1871	1874	rBV	2603652	2497341	68.60%	6.722%
37	13.163	1879	1883	1888	rBV3	53988	84637	2.32%	0.228%
38	13.280	1895	1903	1905	rBV2	87314	151366	4.16%	0.407%
39	13.345	1911	1914	1916	rBV	56667	41923	1.15%	0.113%
40	13.380	1916	1920	1923	rBV2	64121	76085	2.09%	0.205%
41	13.510	1939	1942	1944	rBV2	41067	42149	1.16%	0.113%
42	13.786	1986	1989	1994	rVB	44128	54274	1.49%	0.146%
43	13.974	2015	2021	2030	rVB5	304453	397194	10.91%	1.069%
44	14.115	2043	2045	2047	rBV	57389	59119	1.62%	0.159%
45	14.151	2047	2051	2054	rVV2	1049039	1299382	35.69%	3.498%
46	14.180	2054	2056	2061	rVB	301877	275280	7.56%	0.741%
47	14.545	2116	2118	2120	rVB	65484	48008	1.32%	0.129%
48	15.233	2231	2235	2238	rBV	276875	423802	11.64%	1.141%
49	15.345	2252	2254	2258	rVB	64785	58082	1.60%	0.156%
50	15.557	2286	2290	2296	rVB	158183	219082	6.02%	0.590%
51	15.621	2297	2301	2306	rVB	243745	315881	8.68%	0.850%
52	15.692	2308	2313	2316	rBV	611181	822559	22.60%	2.214%
53	17.251	2574	2578	2587	rVB2	95287	203790	5.60%	0.549%

Sum of corrected areas: 37150326

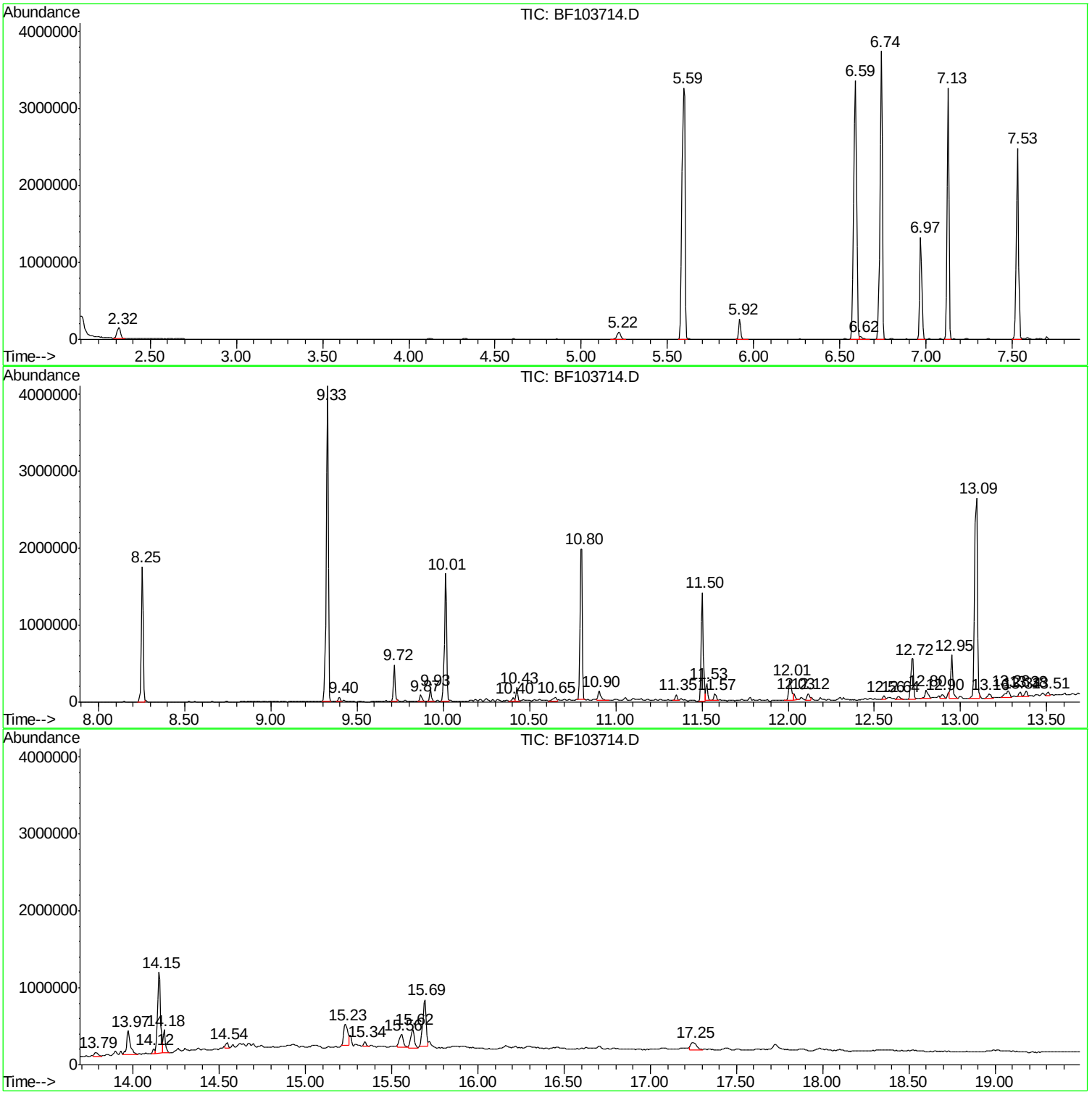
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF031618\
Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF031618\
Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

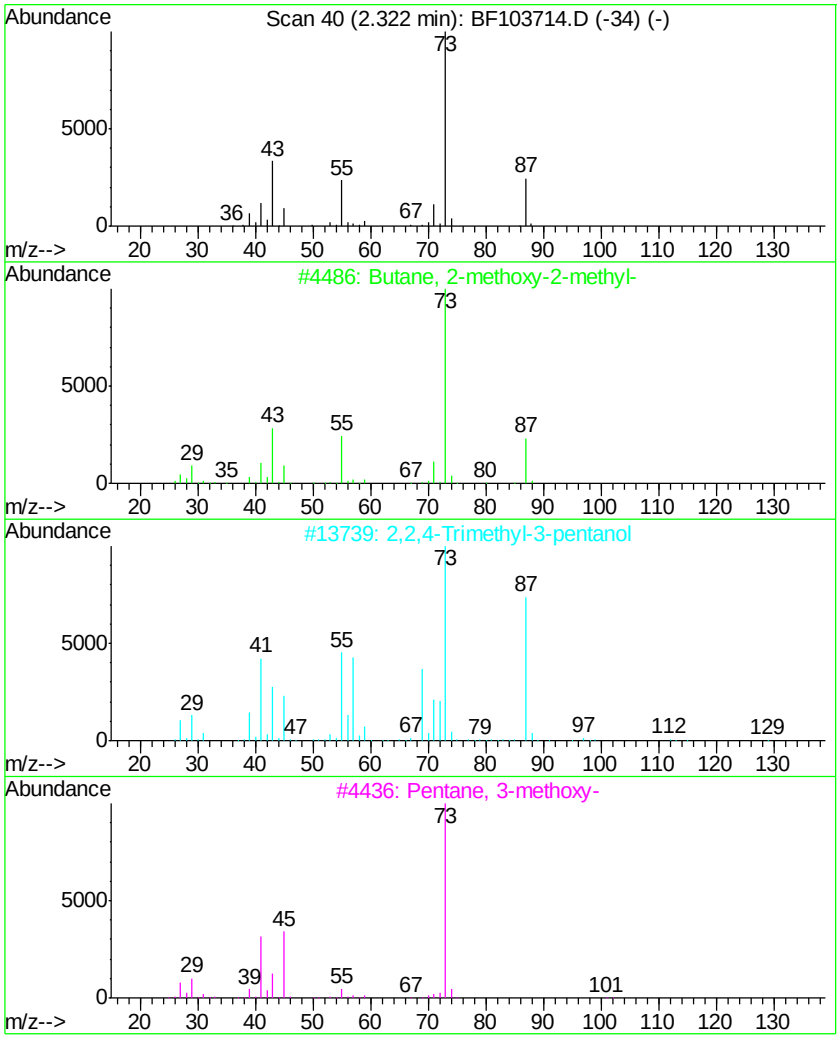
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

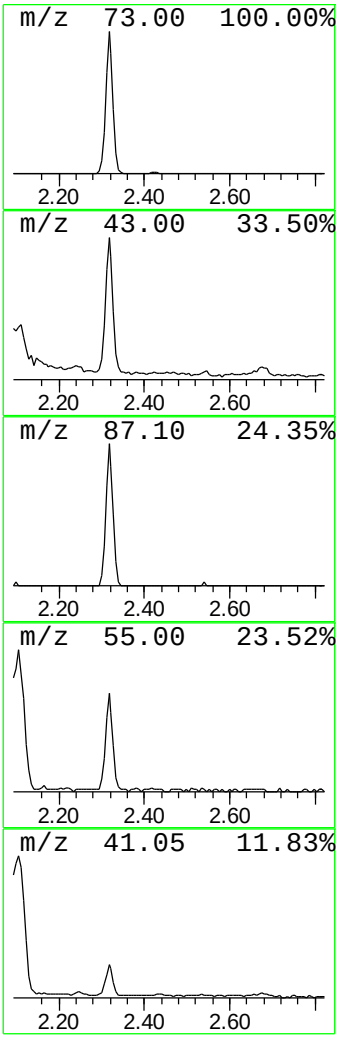
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.32	3.44 ng	185208	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

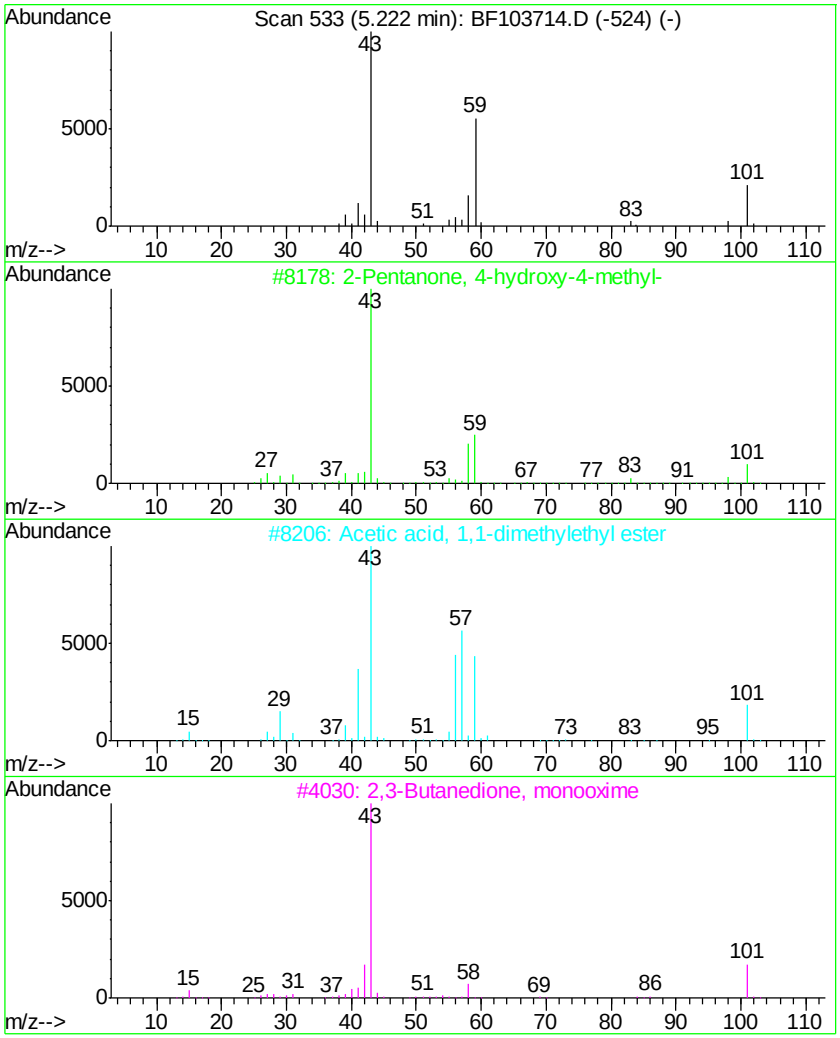
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

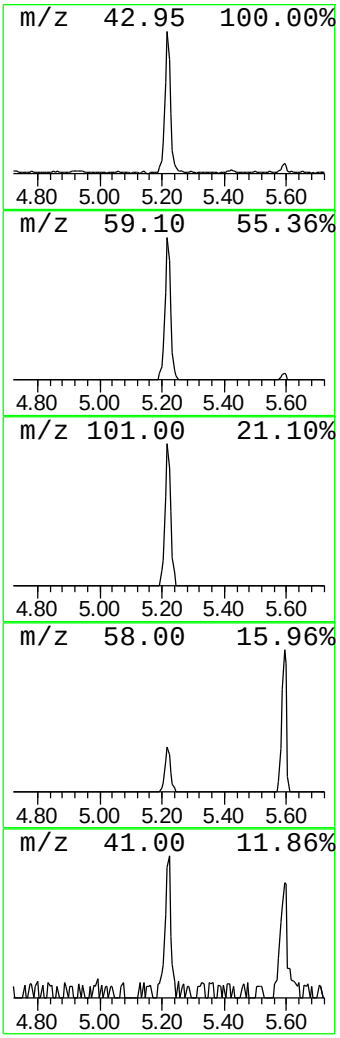
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	2.22 ng	119708	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17





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Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

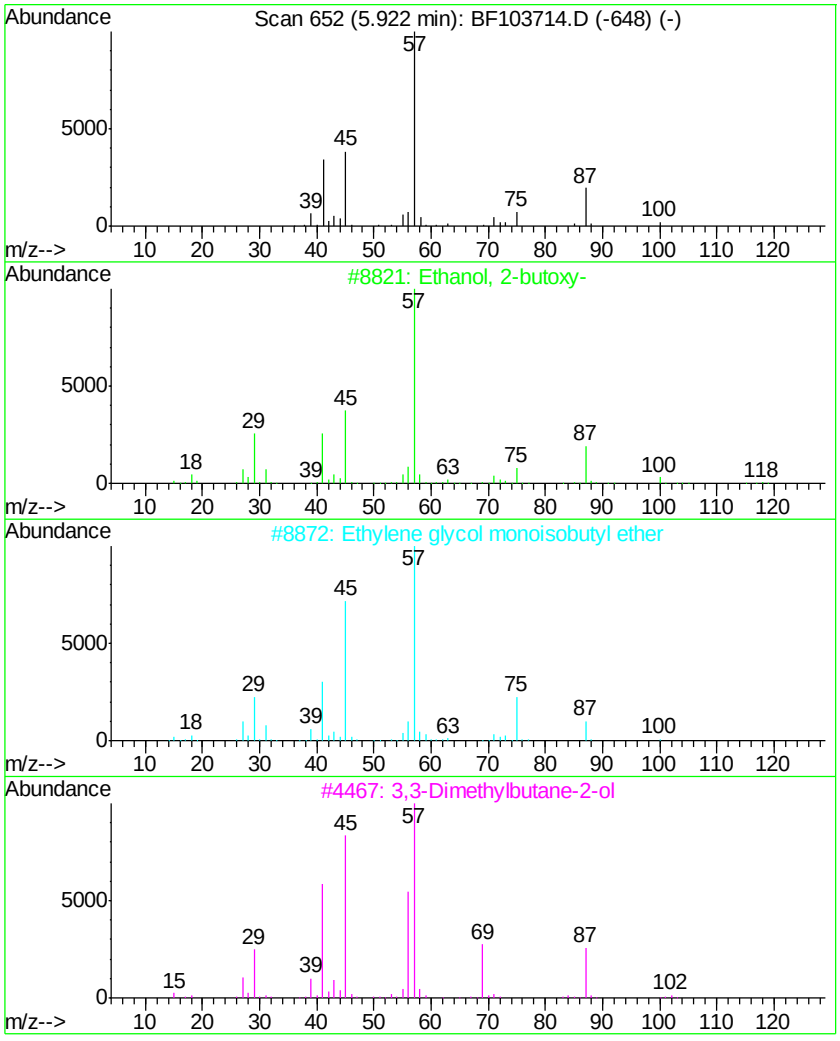
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

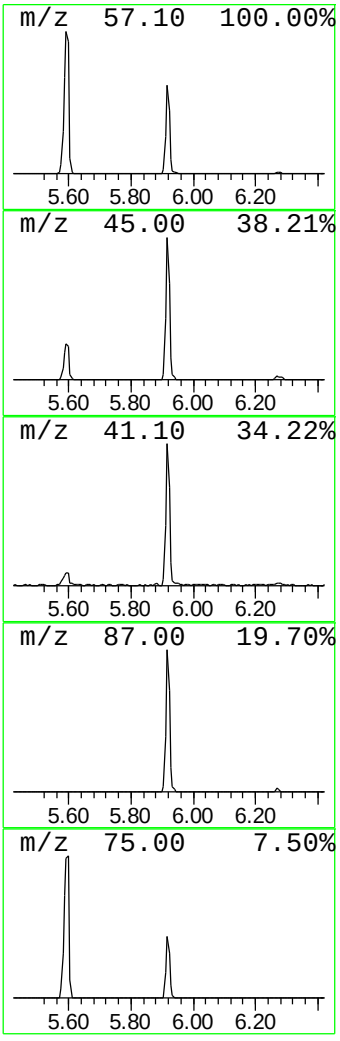
****

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.92	4.20 ng	225921	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
3	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	33
4	Formic acid, 3,3-dimethylbut-2-y...	130	C7H14O2	1000368-20-5	25
5	1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	17





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF031618\
Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

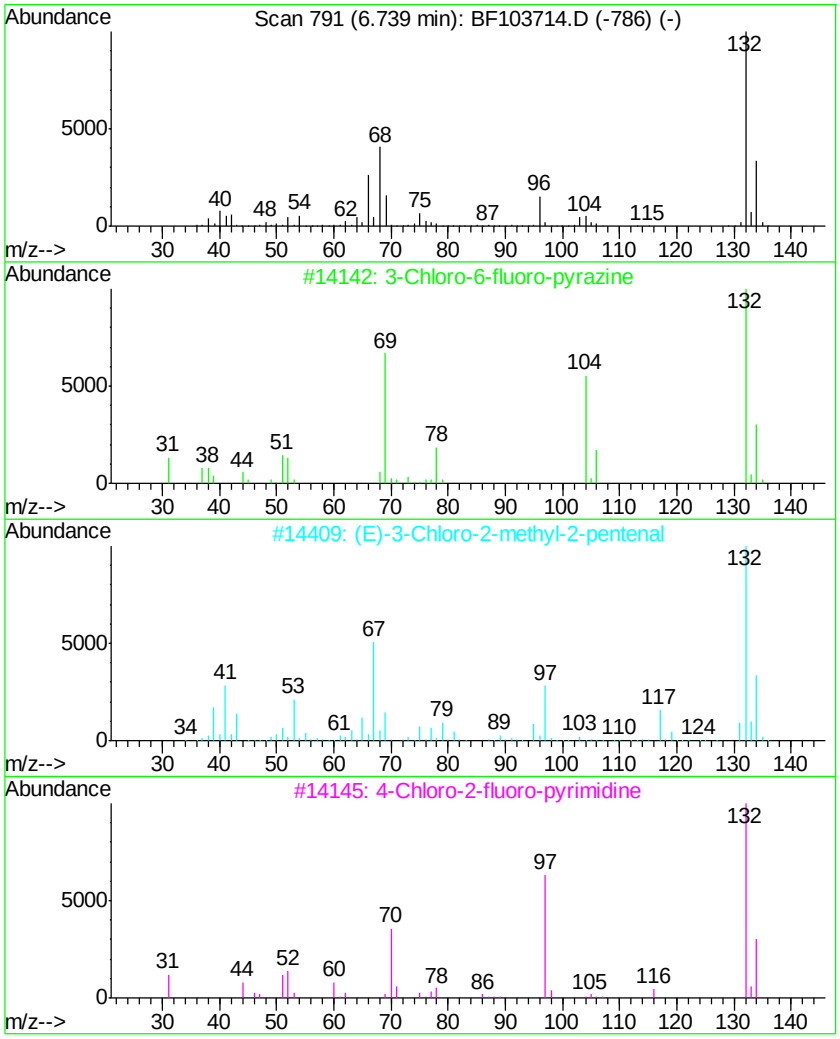
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

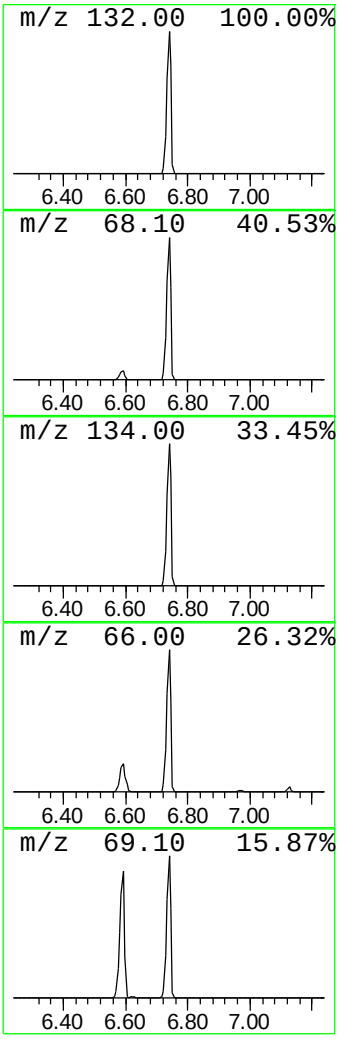
****

Peak Number 4 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	67.61 ng	3637470	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : J1938-05
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Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

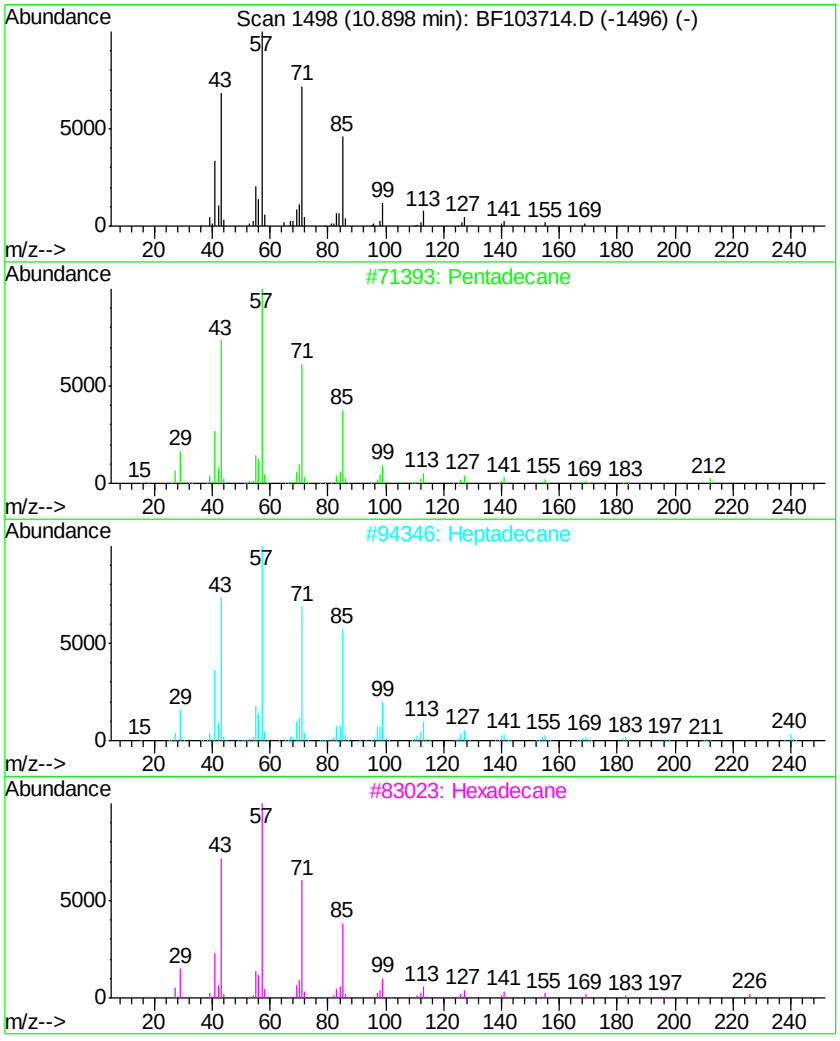
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

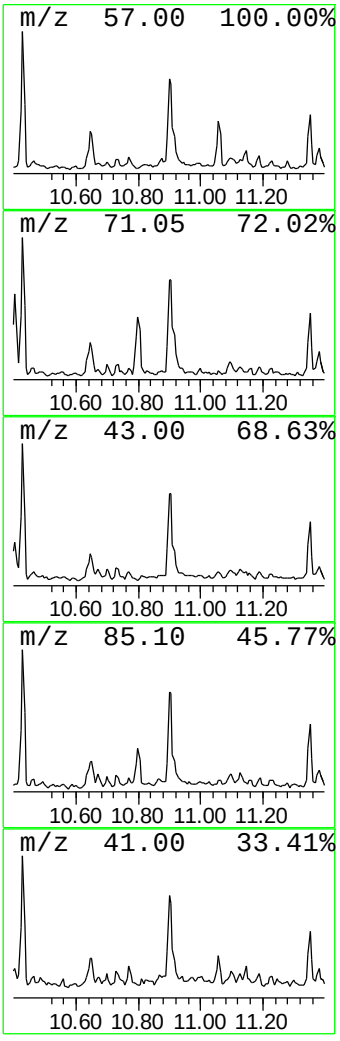
****

Peak Number 6 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.64 ng	158306	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Heptadecane	240	C17H36	000629-78-7	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	90
5	Tetradecane	198	C14H30	000629-59-4	90





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Misc :
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Instrument : BNA_F
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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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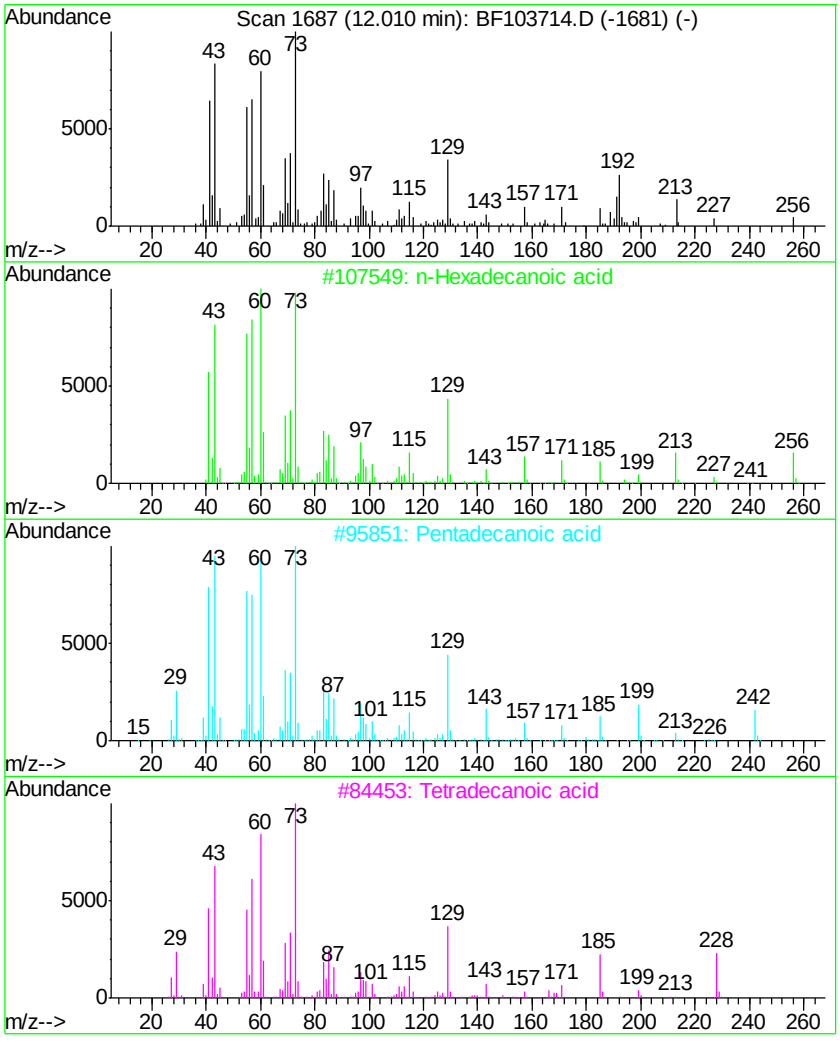
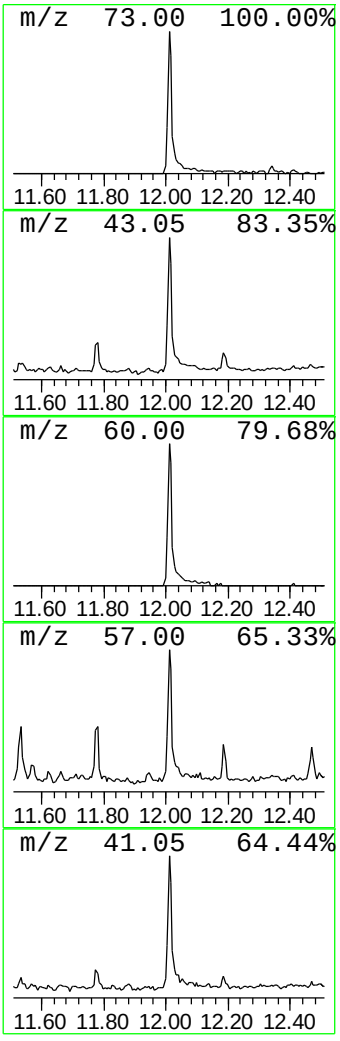
Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	5.12 ng	306969	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4	Tridecanoic acid	214	C13H26O2	000638-53-9	58
5	Methyl-.alpha.-d-ribofuranoside	164	C6H12O5	1000129-83-1	38





Library Search Compound Report

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Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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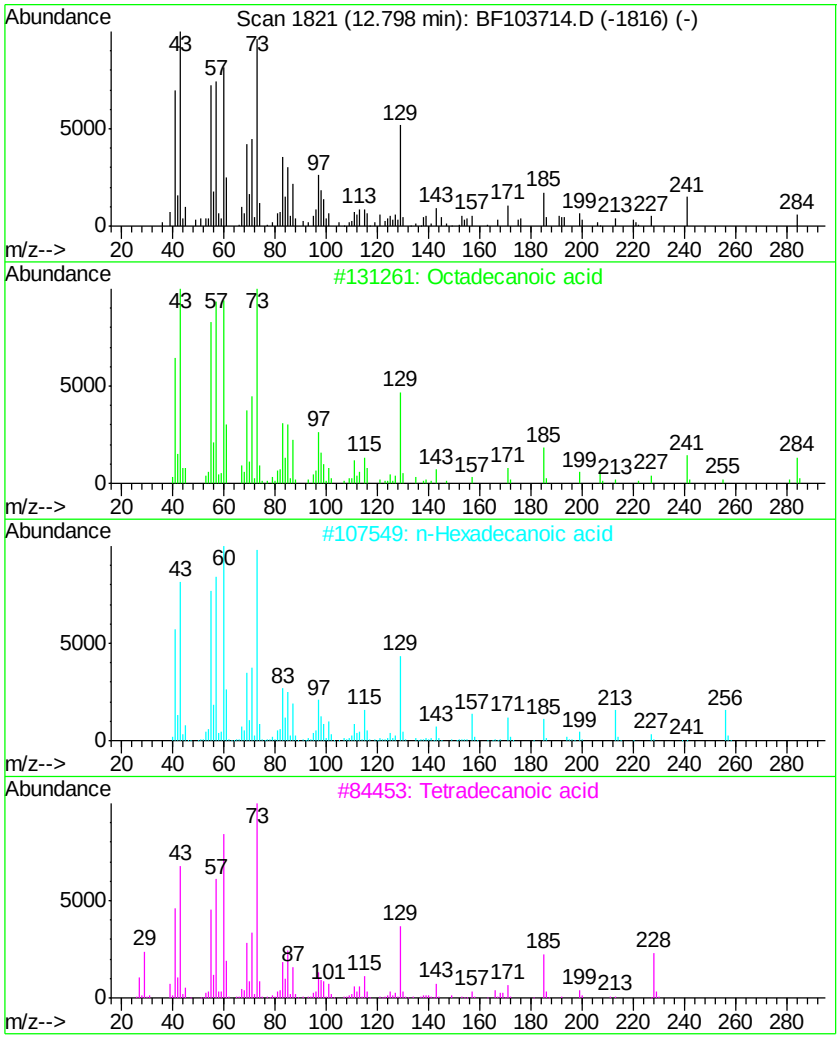
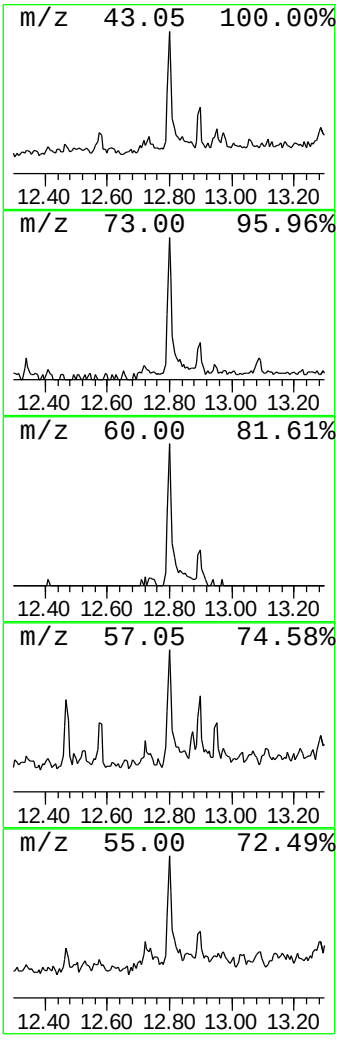
Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.48 ng	148859	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	N-Cyclooct-4-enylacetamide	167	C10H17NO	170952-69-9	25





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Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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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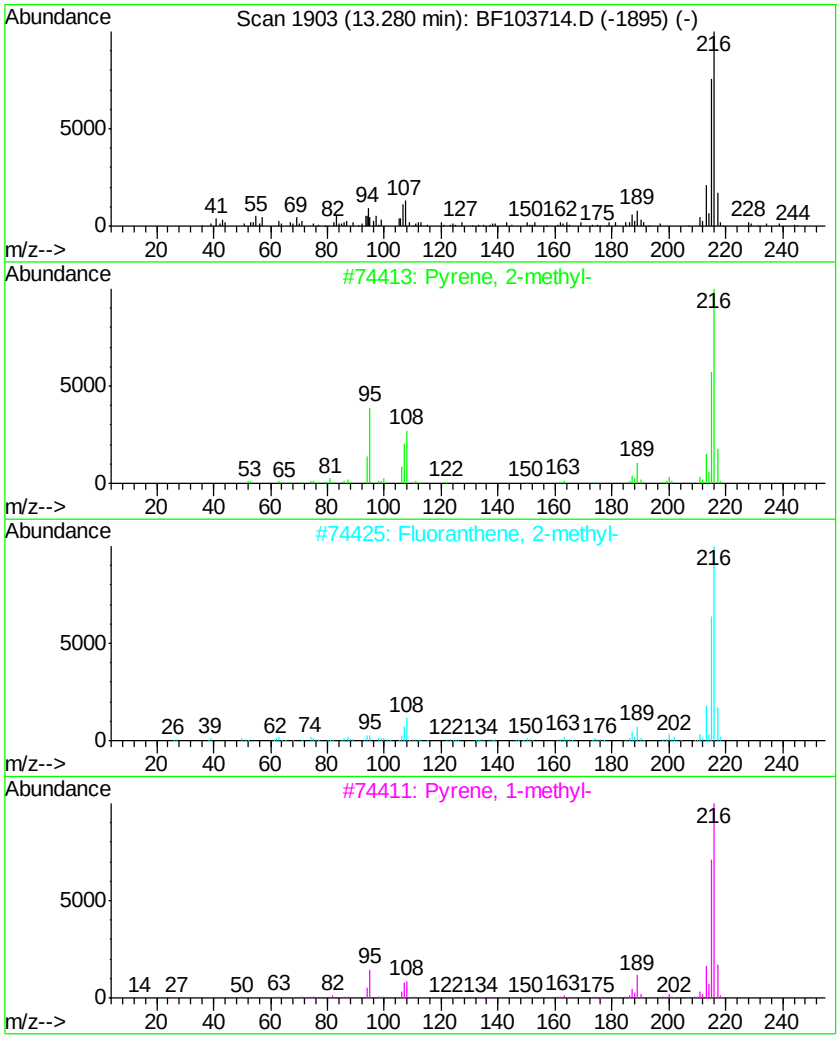
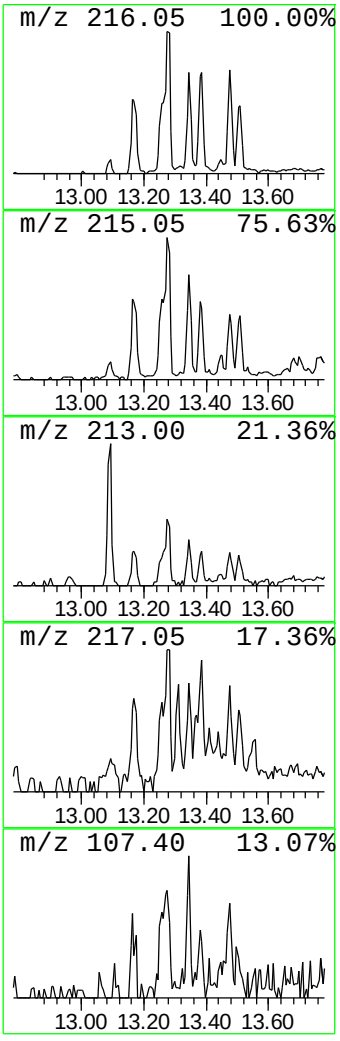
Peak Number 9 Pyrene, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.28	2.33 ng	151366	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene, 2-methyl-	216	C17H12	003442-78-2	94
2	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	93
3	Pyrene, 1-methyl-	216	C17H12	002381-21-7	93
4	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	91
5	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	90





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF031618\
Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

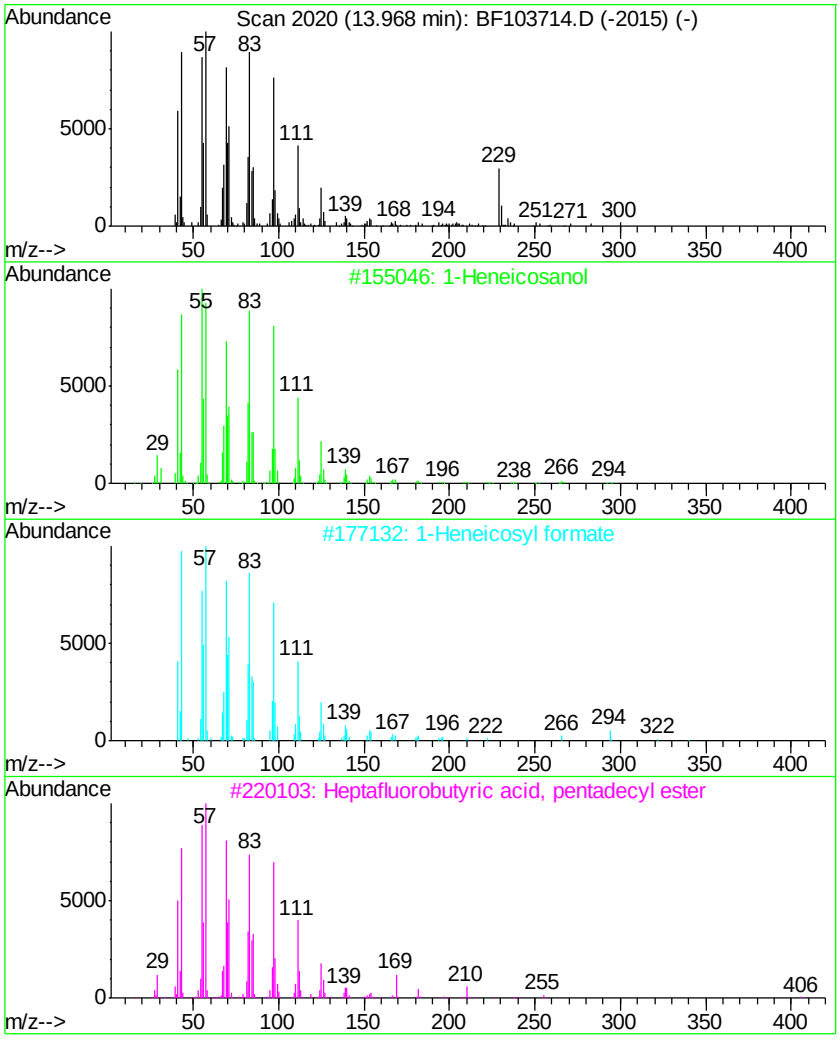
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

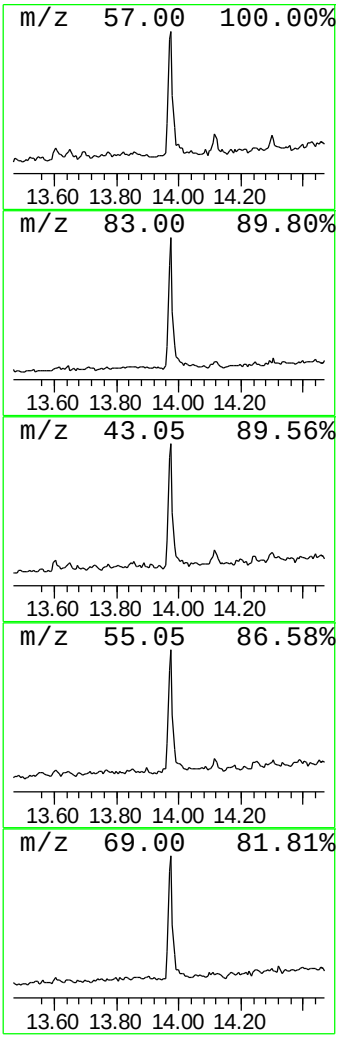
****

Peak Number 10 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	6.11 ng	397194	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF031618\
Data File : BF103714.D
Acq On : 16 Mar 2018 23:20
Operator : JU/SJ
Sample : J1938-05
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.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
Butane, 2-methoxy...	2.32	3.4	ng	185208	1	6.97	1076090	20.0
2-Pentanone, 4-hy...	5.22	2.2	ng	119708	1	6.97	1076090	20.0
Ethanol, 2-butoxy-	5.92	4.2	ng	225921	1	6.97	1076090	20.0
unknown6.74	6.74	67.6	ng	3637470	1	6.97	1076090	20.0
Pentadecane	10.90	2.6	ng	158306	4	11.50	1199340	20.0
n-Hexadecanoic acid	12.01	5.1	ng	306969	4	11.50	1199340	20.0
Octadecanoic acid	12.80	2.5	ng	148859	4	11.50	1199340	20.0
Pyrene, 2-methyl-	13.28	2.3	ng	151366	5	14.16	1299380	20.0
1-Heneicosanol	13.97	6.1	ng	397194	5	14.16	1299380	20.0