LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011019\
Data File : BF111996.D
Acq On : 10 Jan 2019 19:16
Operator : JU/SJ
Sample : K1071-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CPSB-3(10-15)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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	2.169	9	14	19	rVB	34279	45947	1.73%	0.210%
2	5.093	505	511	517	rBV	60121	69181	2.61%	0.316%
3	5.510	577	582	585	rBV	1321206	1229428	46.39%	5.611%
4	6.516	748	753	765	rBV	1404268	1332870	50.29%	6.083%
5	6.651	771	776	779	rBV	1558271	1332415	50.27%	6.081%
6	6.875	810	814	817	rBV	444215	342166	12.91%	1.562%
7	7.034	837	841	844	rBV	1276480	1041382	39.29%	4.752%
8	7.434	904	909	912	rBV	924619	815196	30.76%	3.720%
9	8.157	1028	1032	1035	rBV	500668	416583	15.72%	1.901%
10	9.233	1210	1215	1218	rBV	2477900	2313165	87.28%	10.556%
11	9.616	1277	1280	1285	rVB	188033	156868	5.92%	0.716%
12	9.910	1326	1330	1334	rBV2	1000563	843447	31.82%	3.849%
13	10.698	1460	1464	1475	rVB	1311362	1211686	45.72%	5.530%
14	11.398	1579	1583	1585	rBV	942699	775792	29.27%	3.540%
15	11.422	1585	1587	1590	rVB	70799	53076	2.00%	0.242%
16	11.786	1645	1649	1652	rBV	800543	586822	22.14%	2.678%
17	11.922	1669	1672	1676	rBV2	92736	85888	3.24%	0.392%
18	12.110	1699	1704	1706	rBV4	32359	38629	1.46%	0.176%
19	12.474	1762	1766	1768	rBV	2060877	2091145	78.90%	9.543%
20	12.498	1768	1770	1776	rVB	3317069	2650268	100.00%	12.095%
21	12.580	1780	1784	1787	rBV	319697	266698	10.06%	1.217%
22	12.610	1787	1789	1791	rBV	67703	53441	2.02%	0.244%
23	12.839	1823	1828	1830	rBV	50645	63456	2.39%	0.290%
24	12.857	1830	1831	1836	rVB5	38623	36393	1.37%	0.166%
25	12.980	1848	1852	1856	rBV	2613789	2519729	95.07%	11.499%
26	13.227	1888	1894	1899	rBV4	59461	108684	4.10%	0.496%
27	13.410	1922	1925	1927	rBV3	42722	40659	1.53%	0.186%
28	13.551	1947	1949	1953	rVB	51529	42116	1.59%	0.192%
29	13.874	2001	2004	2017	rVB2	177043	339850	12.82%	1.551%
30	14.039	2028	2032	2035	rVB	471311	452448	17.07%	2.065%
31	14.198	2056	2059	2061	rBV	45589	37055	1.40%	0.169%
32	14.498	2108	2110	2113	rVB2	43796	42953	1.62%	0.196%
33	14.810	2161	2163	2167	rVB2	43529	34587	1.31%	0.158%
34	15.151	2219	2221	2225	rVB	42660	37395	1.41%	0.171%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011019\
Data File : BF111996.D
Acq On : 10 Jan 2019 19:16
Operator : JU/SJ
Sample : K1071-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CPSB-3(10-15)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.515	2279	2283	2294	rVB	274448	405210	15.29%	1.849%

Sum of corrected areas: 21912628

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011019\
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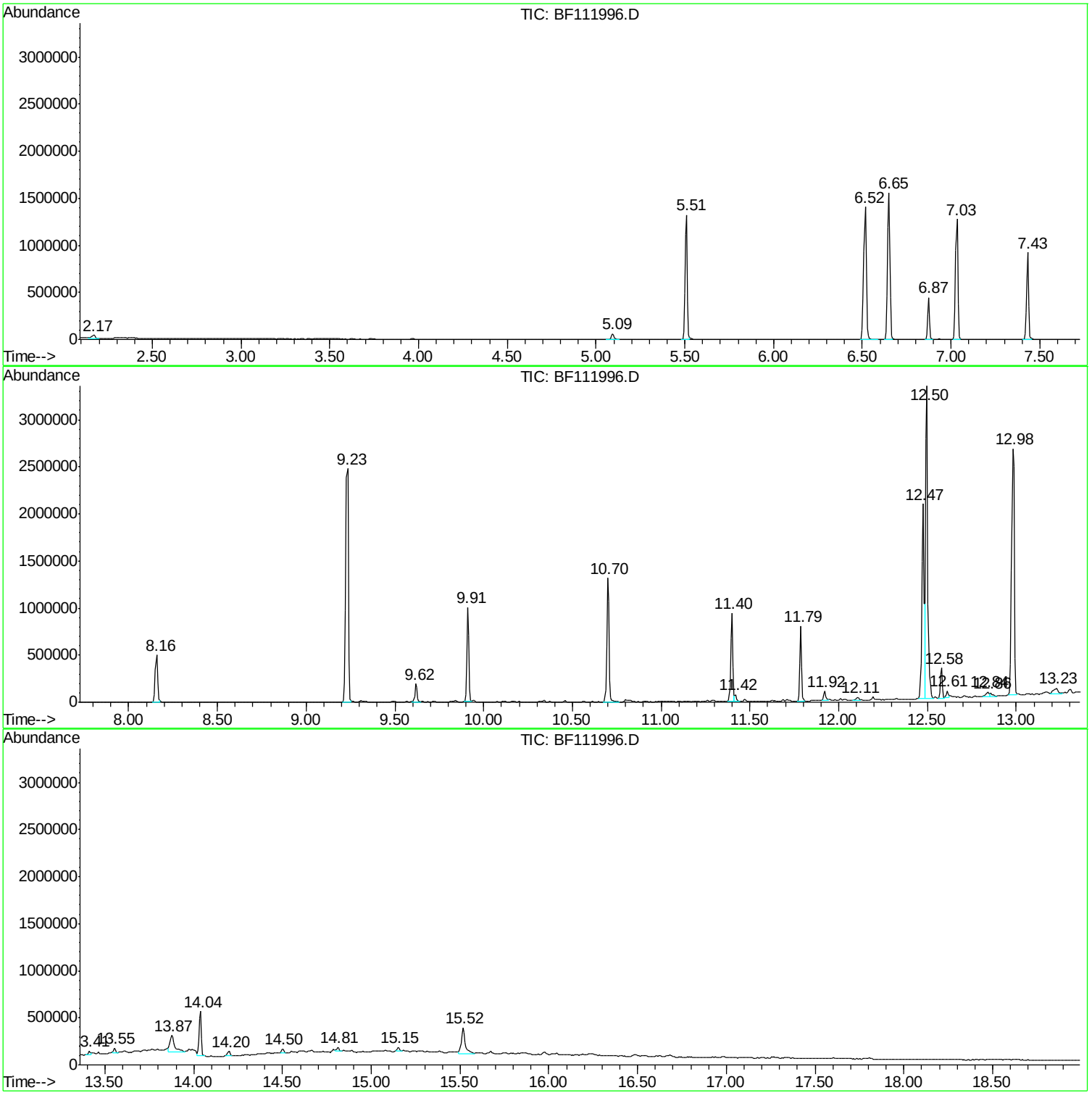
Instrument :
BNA_F
ClientSampleId :
CPSB-3(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
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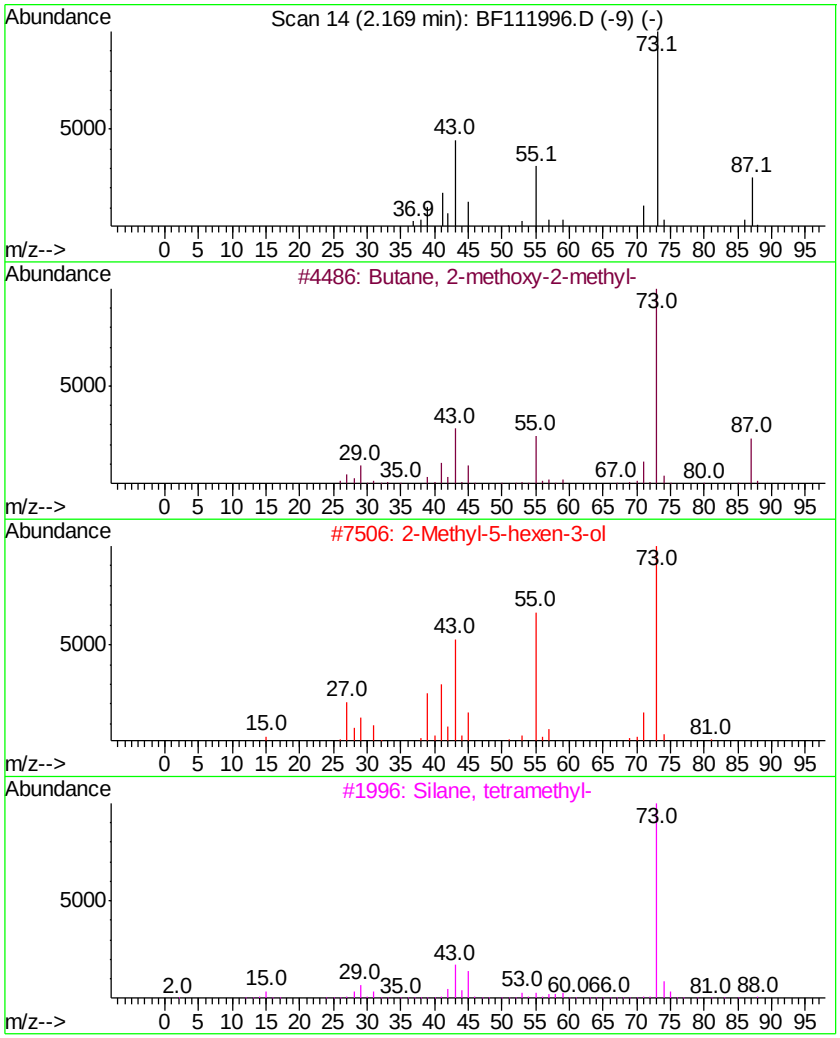
TIC Integration Parameters: LSCINT.P

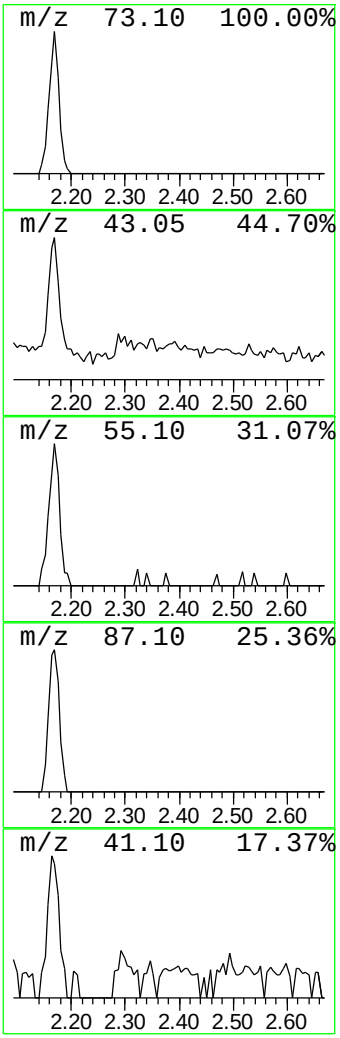
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	2.69 ng	45947	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011019\
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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : CPSB-3(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

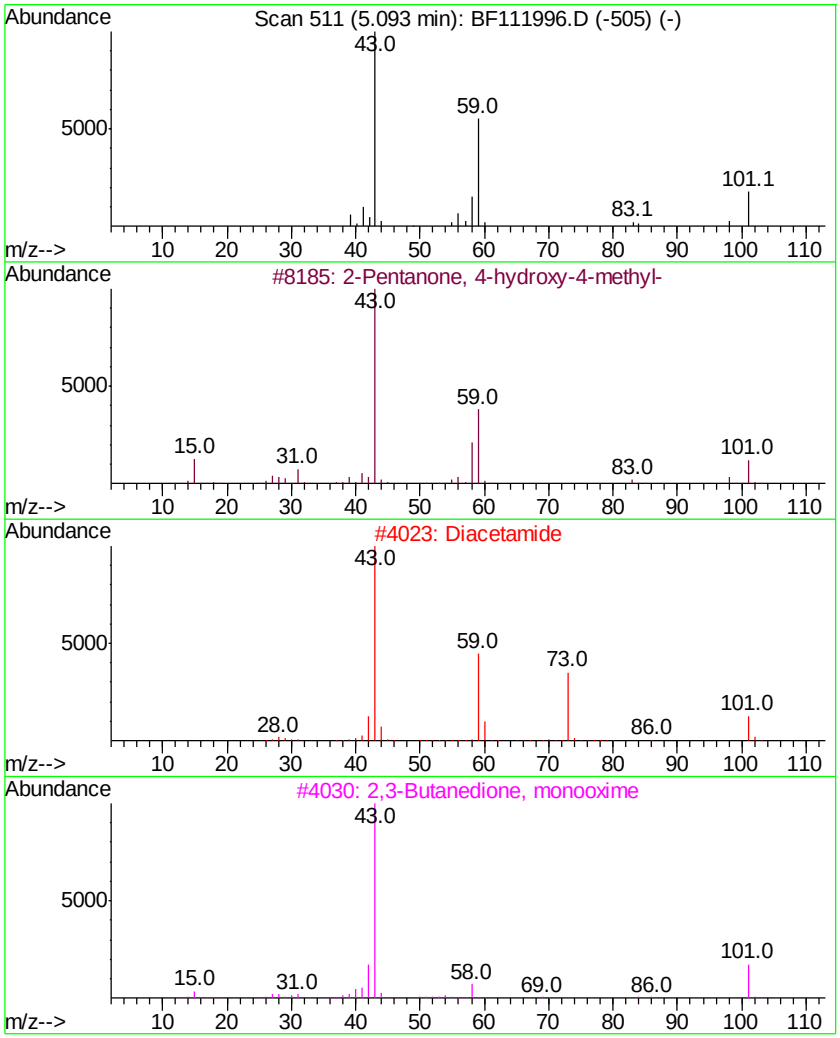
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

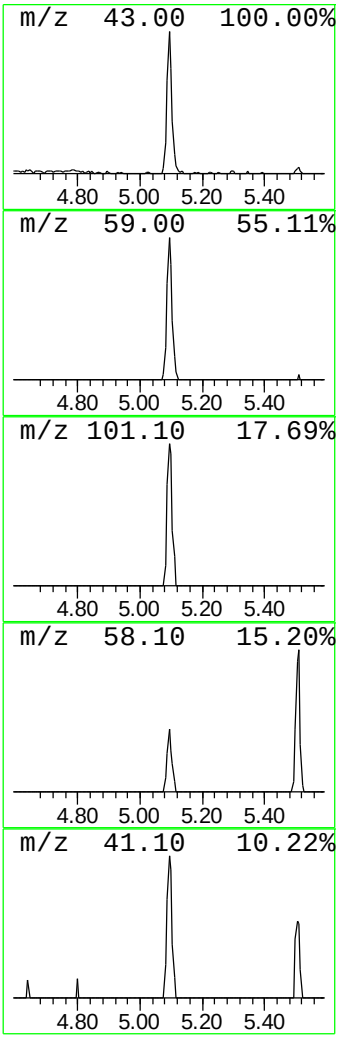
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	4.04 ng	69181	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Diacetamide	101	C4H7NO2	000625-77-4	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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Data File : BF111996.D
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Operator : JU/SJ
Sample : K1071-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CPSB-3(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

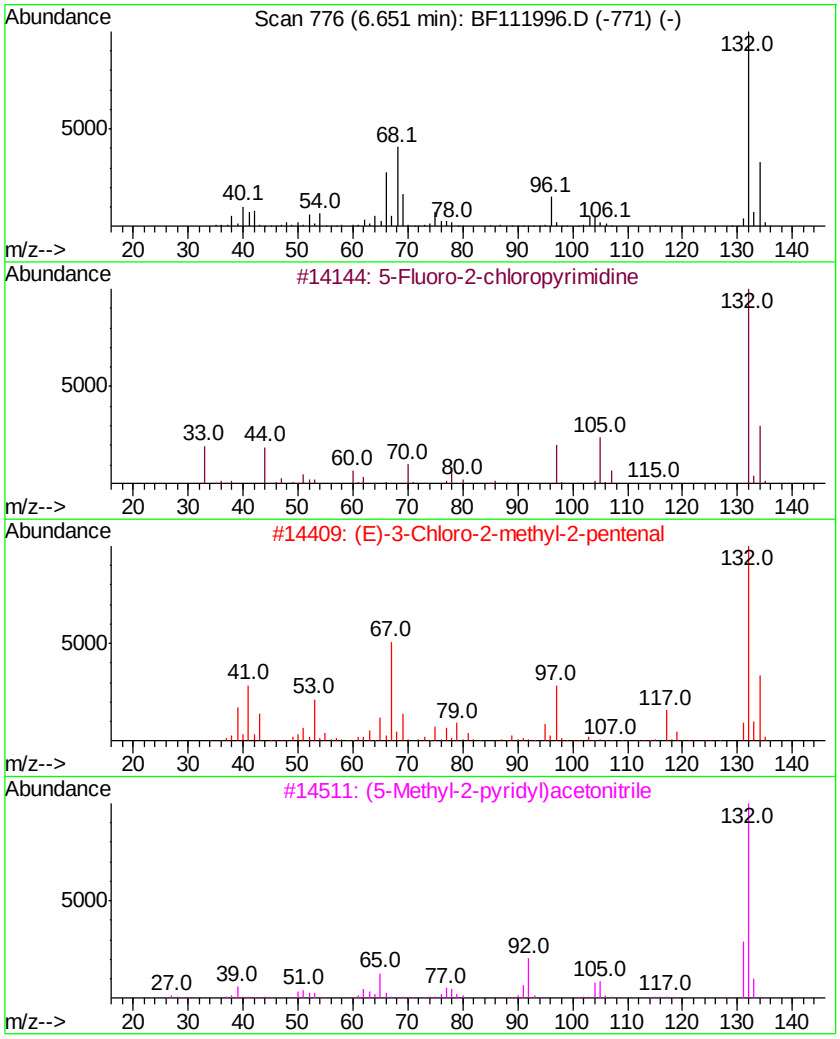
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

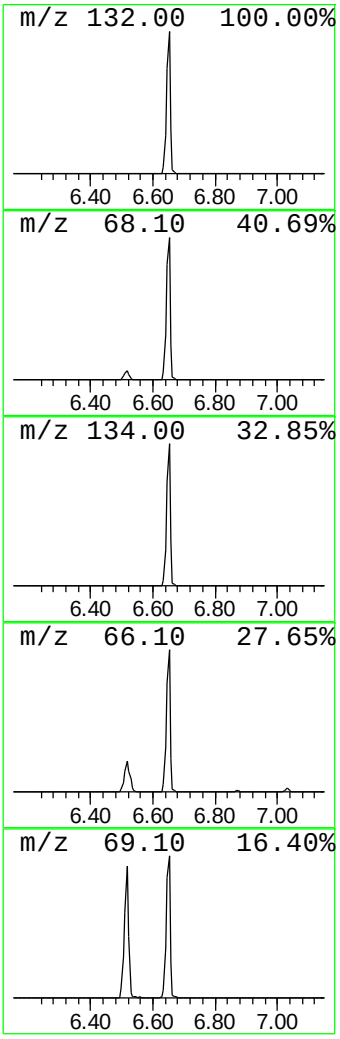
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	77.88 ng	1332420	1,4-Dichlorobenzene-d4	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
5	Xenon	132	Xe	007440-63-3	9





Library Search Compound Report

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Acq On : 10 Jan 2019 19:16
Operator : JU/SJ
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CPSB-3(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
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TIC Library : C:\DATABASE\NIST11.L
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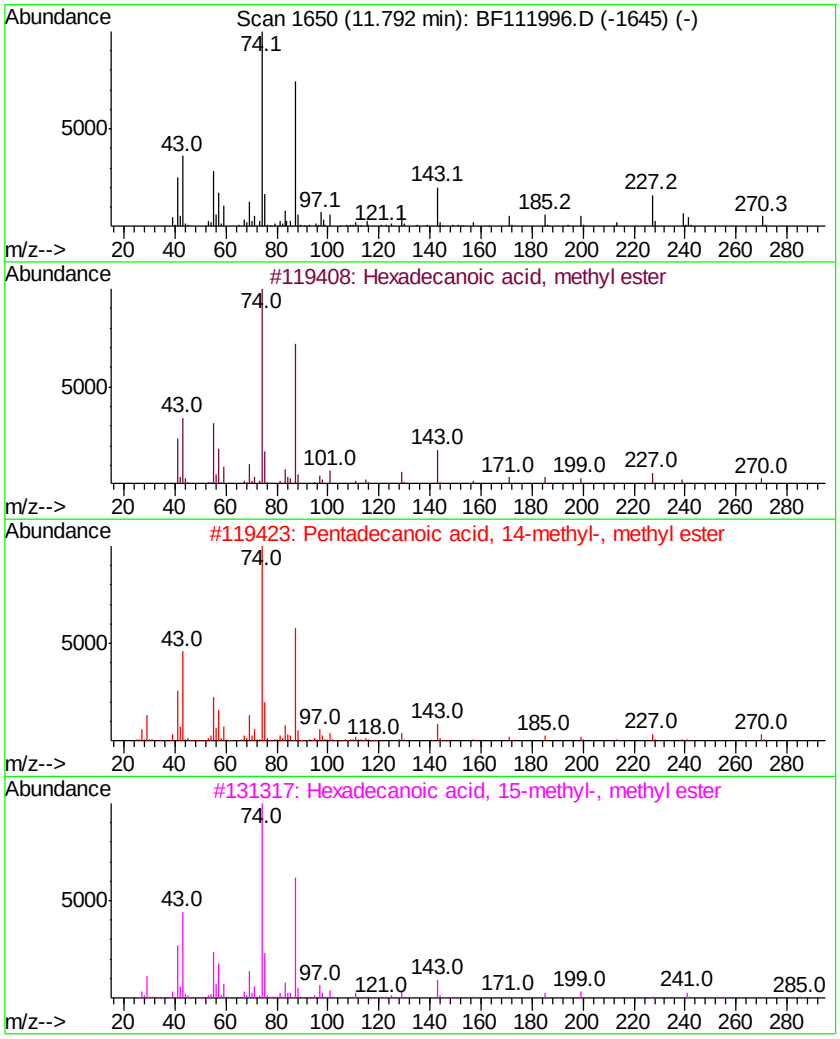
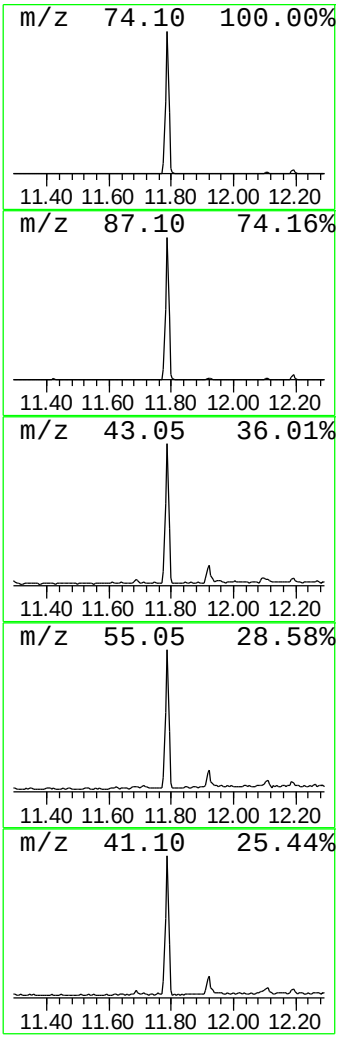
****

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	15.13 ng	586822	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	80





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Data File : BF111996.D
Acq On : 10 Jan 2019 19:16
Operator : JU/SJ
Sample : K1071-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CPSB-3(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

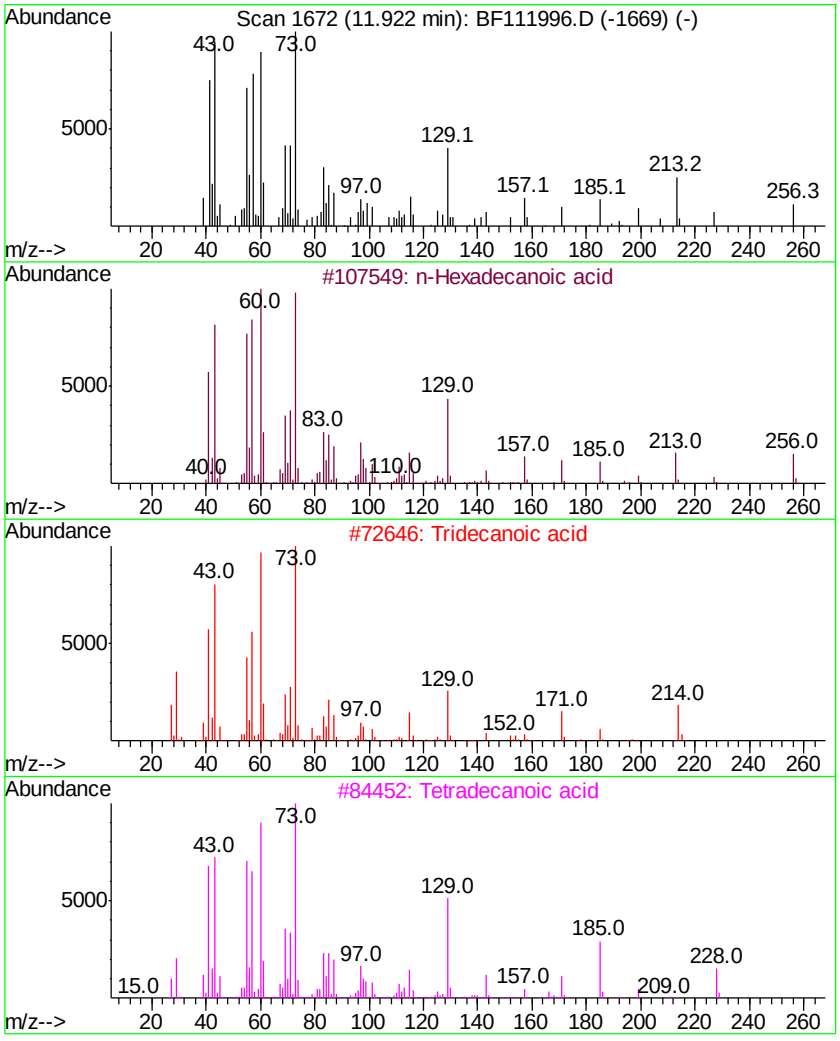
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

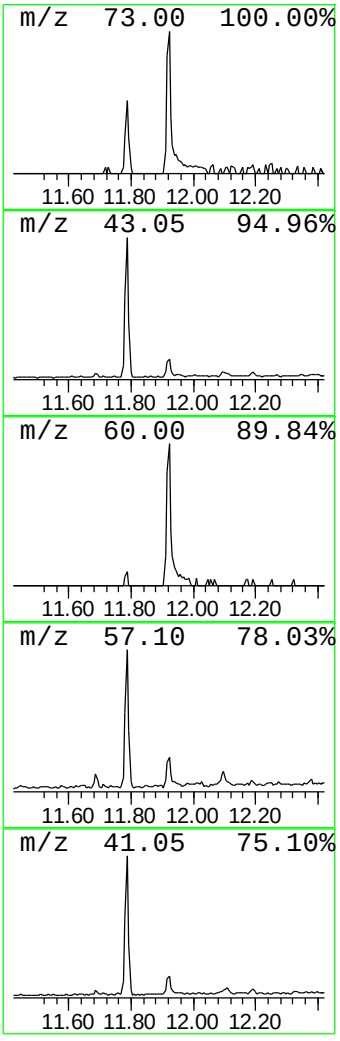
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	2.21 ng	85888	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	76
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Instrument : BNA_F
ClientSampleId : CPSB-3(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

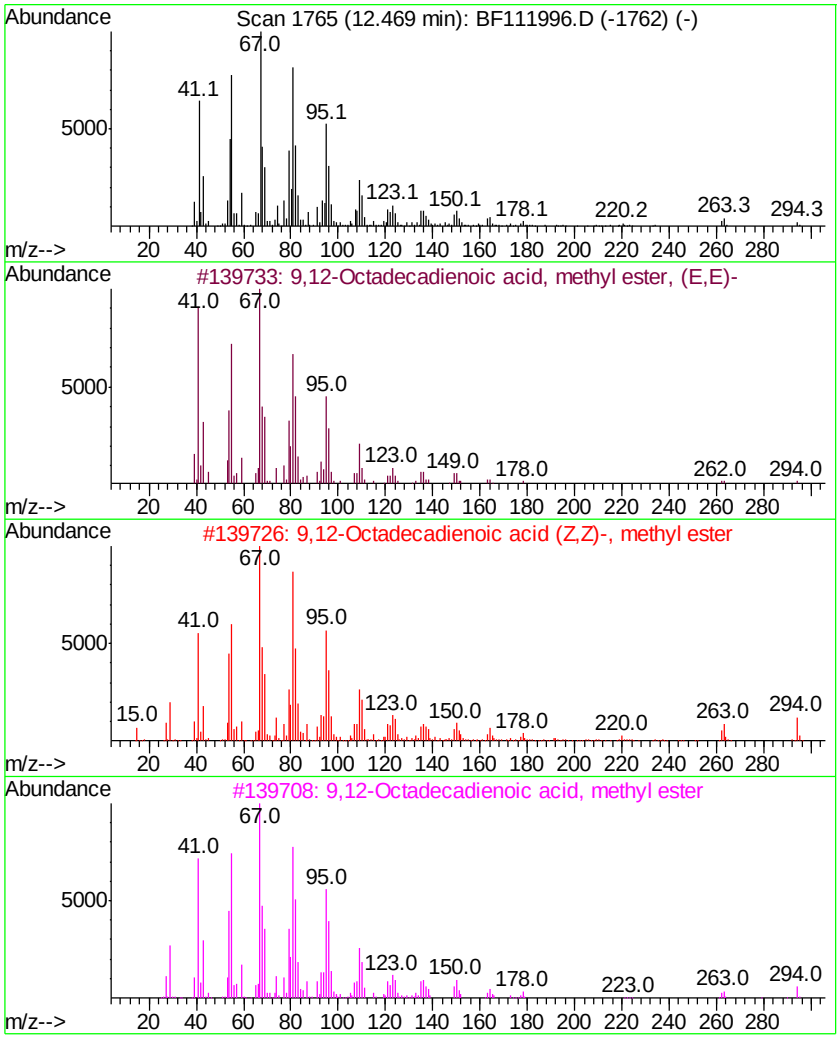
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

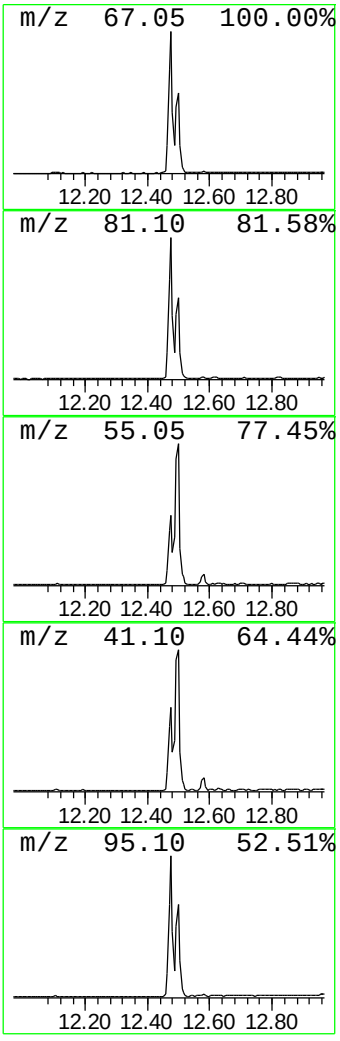
****

Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	53.91 ng	2091150	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99





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Misc :
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Instrument : BNA_F
ClientSampleId : CPSB-3(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

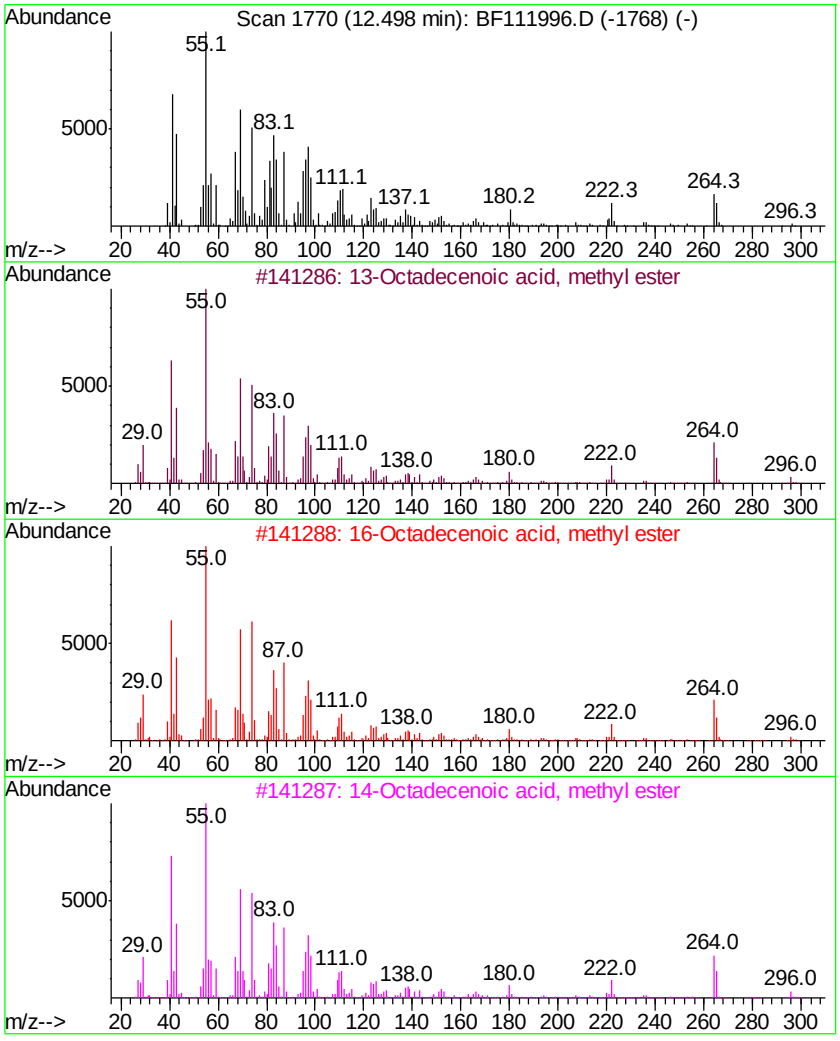
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

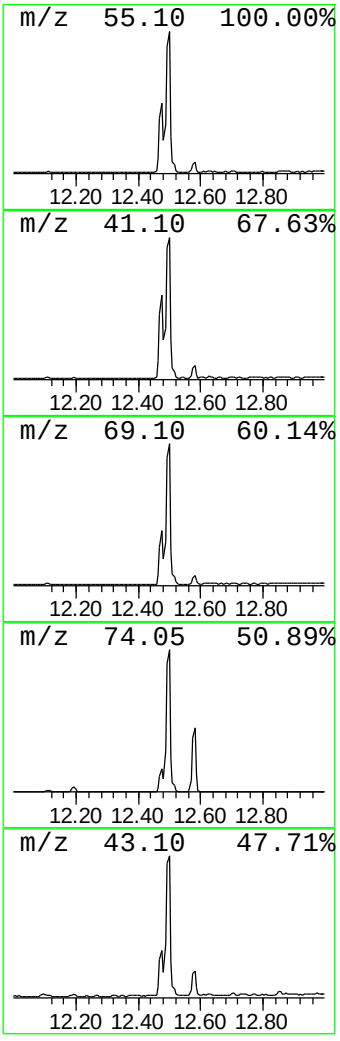
****

Peak Number 8 13-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.50	68.32 ng	2650270	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98
3	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	97
4	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	94
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

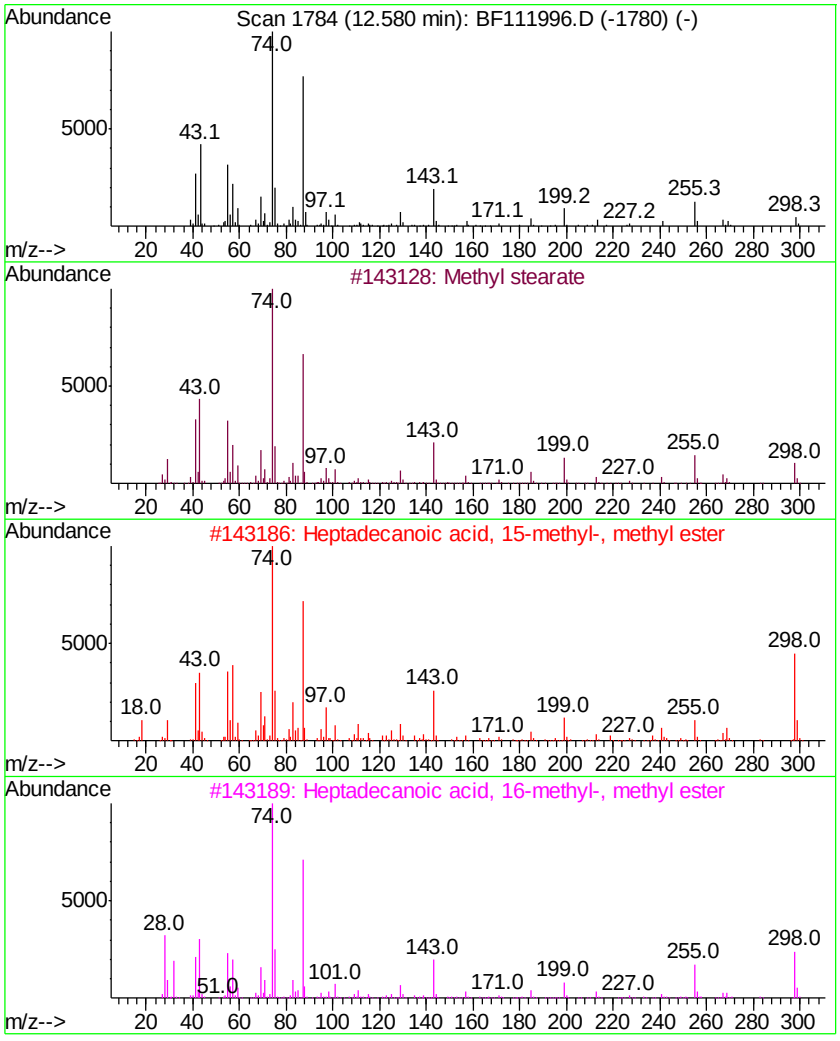
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

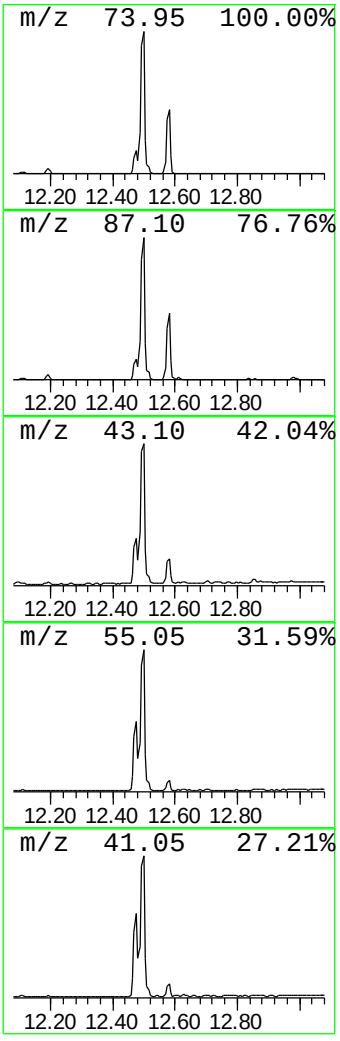
****

Peak Number 9 Methyl stearate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.58	6.88 ng	266698	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	91
3	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	90
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87





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Instrument : BNA_F
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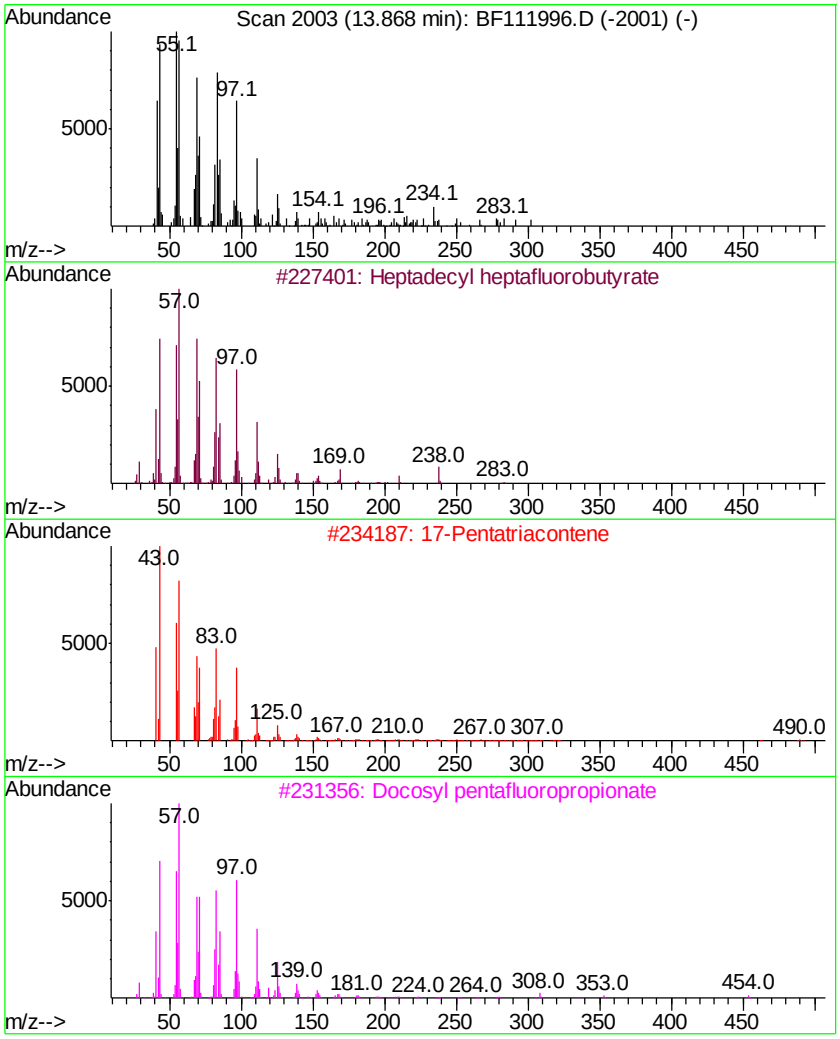
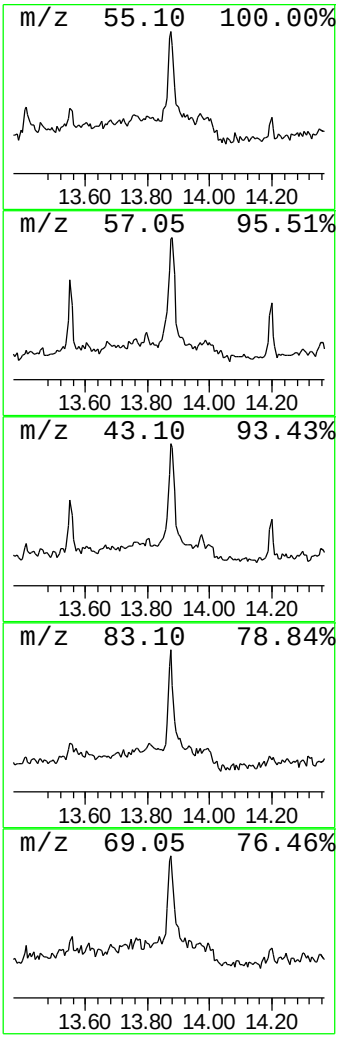
Peak Number 12 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	15.02 ng	339850	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
4	Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011019\
Data File : BF111996.D
Acq On : 10 Jan 2019 19:16
Operator : JU/SJ
Sample : K1071-09
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CPSB-3(10-15)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF010719.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...	2.17	2.7	ng	45947	1	6.87	342166	20.0
2-Pentanone, 4-hy...	5.09	4.0	ng	69181	1	6.87	342166	20.0
unknown6.65	6.65	77.9	ng	1332420	1	6.87	342166	20.0
Hexadecanoic acid...	11.79	15.1	ng	586822	4	11.40	775792	20.0
n-Hexadecanoic acid	11.92	2.2	ng	85888	4	11.40	775792	20.0
9,12-Octadecadien...	12.47	53.9	ng	2091150	4	11.40	775792	20.0
13-Octadecenoic a...	12.50	68.3	ng	2650270	4	11.40	775792	20.0
Methyl stearate	12.58	6.9	ng	266698	4	11.40	775792	20.0
Heptadecyl heptaf...	13.87	15.0	ng	339850	5	14.04	452448	20.0