LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110422.D
Acq On : 2 Nov 2018 20:01
Operator : JU/SJ
Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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	2.257	24	29	36	rVB	74713	104766	6.63%	1.011%
2	5.569	589	592	607	rVB	367620	369095	23.36%	3.563%
3	6.569	758	762	775	rBV	398858	410944	26.01%	3.967%
4	6.722	784	788	795	rBV	449824	425157	26.91%	4.105%
5	6.951	824	827	838	rVB	574674	531085	33.61%	5.127%
6	7.110	850	854	864	rBV	345310	326802	20.68%	3.155%
7	7.516	919	923	935	rBV	224092	250173	15.83%	2.415%
8	8.239	1041	1046	1068	rVB	634179	718170	45.45%	6.933%
9	9.310	1224	1228	1237	rBV	461202	470069	29.75%	4.538%
10	9.704	1289	1295	1302	rVB	50888	60061	3.80%	0.580%
11	9.904	1325	1329	1334	rBV	19300	22213	1.41%	0.214%
12	9.992	1341	1344	1357	rVB	696624	728081	46.08%	7.029%
13	10.404	1411	1414	1417	rBV	39183	34207	2.16%	0.330%
14	10.786	1475	1479	1486	rBV	165966	171576	10.86%	1.656%
15	10.880	1491	1495	1503	rBV2	32982	48045	3.04%	0.464%
16	11.327	1568	1571	1574	rBV	30662	25694	1.63%	0.248%
17	11.486	1594	1598	1607	rBV	653210	630624	39.91%	6.088%
18	11.751	1640	1643	1646	rBV	22617	18213	1.15%	0.176%
19	11.857	1657	1661	1667	rVB	479331	382886	24.23%	3.697%
20	11.992	1681	1684	1686	rBV	18638	18456	1.17%	0.178%
21	12.163	1710	1713	1718	rBV	18027	18526	1.17%	0.179%
22	12.545	1774	1778	1780	rBV	1809112	1580140	100.00%	15.255%
23	12.563	1780	1781	1788	rVV2	1013097	822233	52.04%	7.938%
24	12.645	1792	1795	1800	rVB	162117	149474	9.46%	1.443%
25	12.704	1801	1805	1809	rBV	82041	69451	4.40%	0.671%
26	12.933	1838	1844	1849	rVB	72891	88162	5.58%	0.851%
27	13.063	1863	1866	1870	rBV	350080	314136	19.88%	3.033%
28	13.374	1914	1919	1924	rBV3	20491	29788	1.89%	0.288%
29	13.621	1956	1961	1965	rBV2	17345	22109	1.40%	0.213%
30	13.951	2013	2017	2020	rBV4	26819	32833	2.08%	0.317%
31	14.045	2030	2033	2035	rBV3	13394	18772	1.19%	0.181%
32	14.133	2042	2048	2051	rBV	543127	592867	37.52%	5.724%
33	14.263	2068	2070	2073	rVB	22147	17351	1.10%	0.168%
34	14.568	2119	2122	2129	rVB4	50252	67941	4.30%	0.656%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110422.D
Acq On : 2 Nov 2018 20:01
Operator : JU/SJ
Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.886	2173	2176	2180	rVB	35048	35124	2.22%	0.339%
36	15.021	2194	2199	2205	rBV	32296	58962	3.73%	0.569%
37	15.204	2227	2230	2233	rBV2	25310	38960	2.47%	0.376%
38	15.233	2233	2235	2240	rVB2	71107	74566	4.72%	0.720%
39	15.657	2300	2307	2312	rVB	301875	455723	28.84%	4.400%
40	16.086	2377	2380	2386	rVB3	51667	79863	5.05%	0.771%
41	16.615	2468	2470	2476	rVB2	34827	44758	2.83%	0.432%

Sum of corrected areas: 10358056

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Misc :
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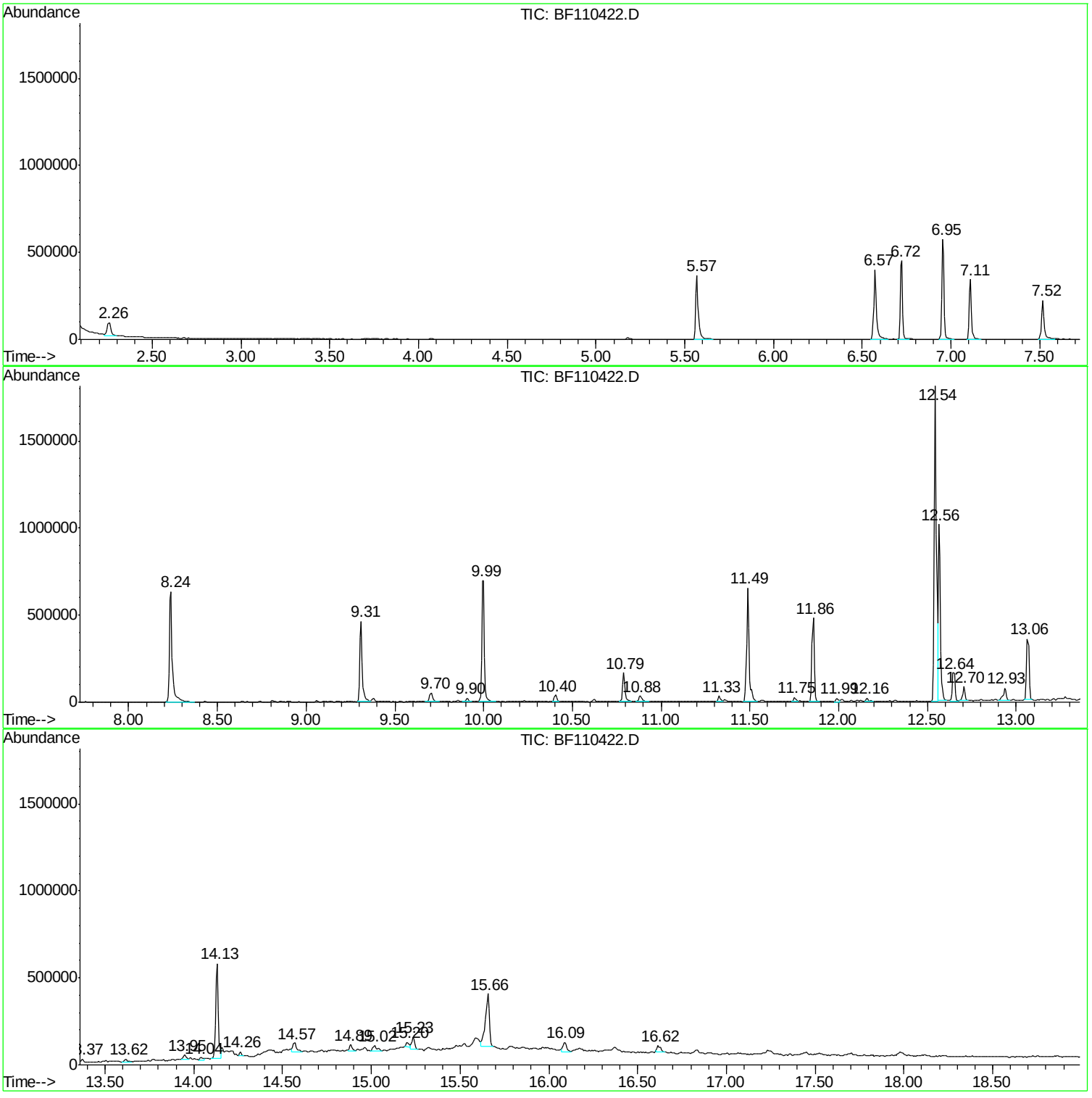
Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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

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Acq On : 2 Nov 2018 20:01
Operator : JU/SJ
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

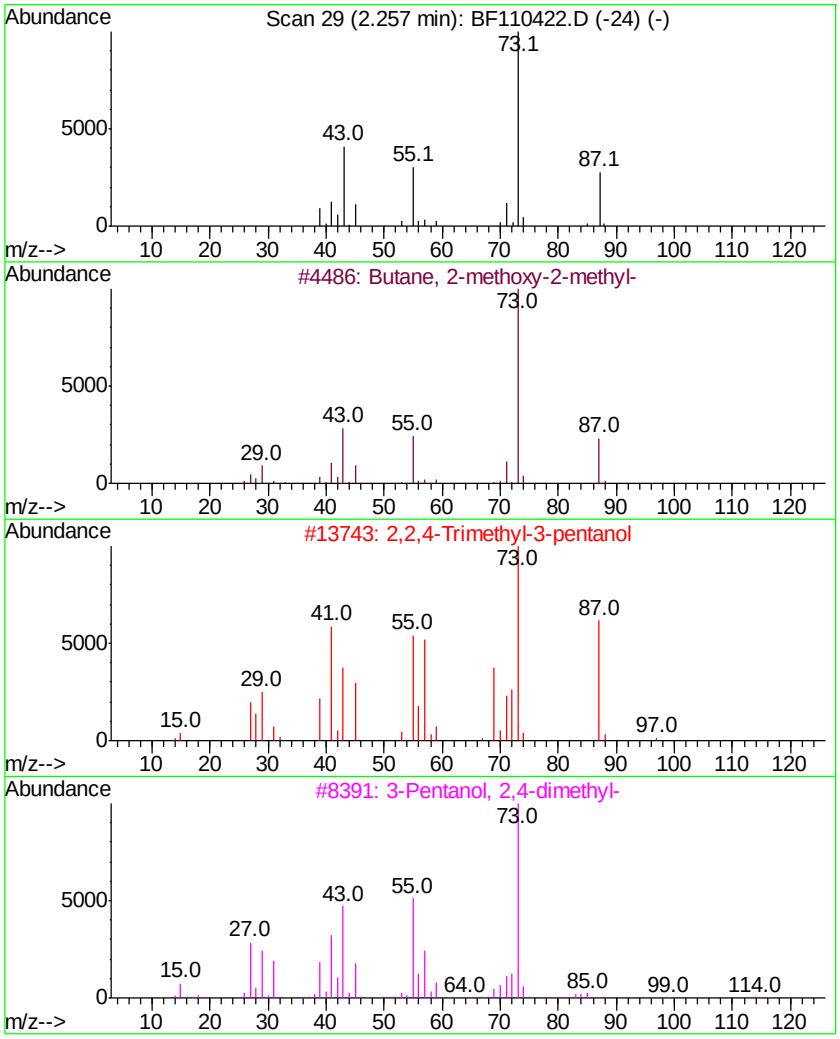
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

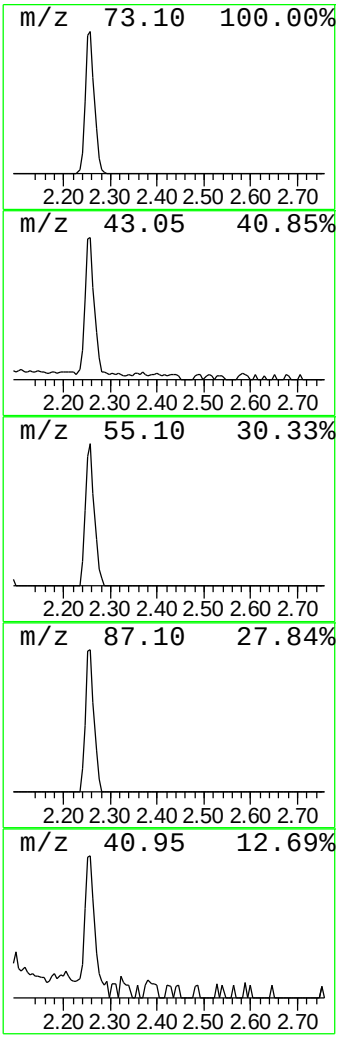
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	3.95 ng	104766	1,4-Dichlorobenzene-d4	6.95

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	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110422.D
Acq On : 2 Nov 2018 20:01
Operator : JU/SJ
Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

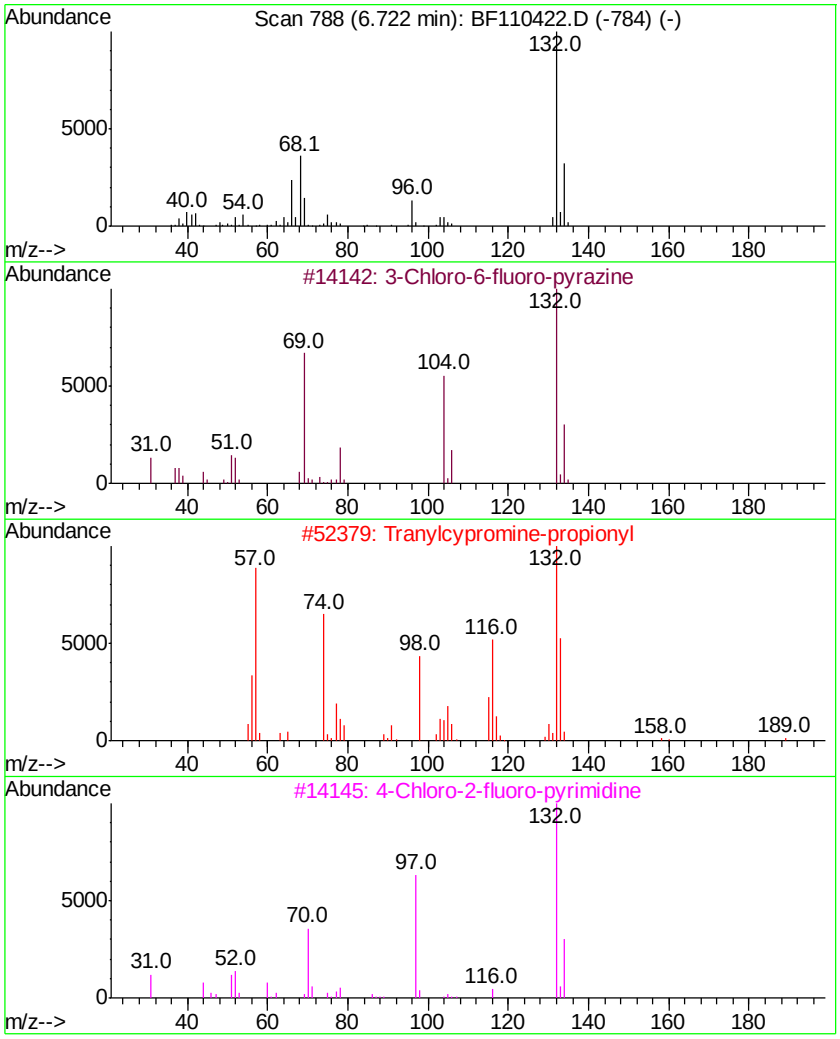
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

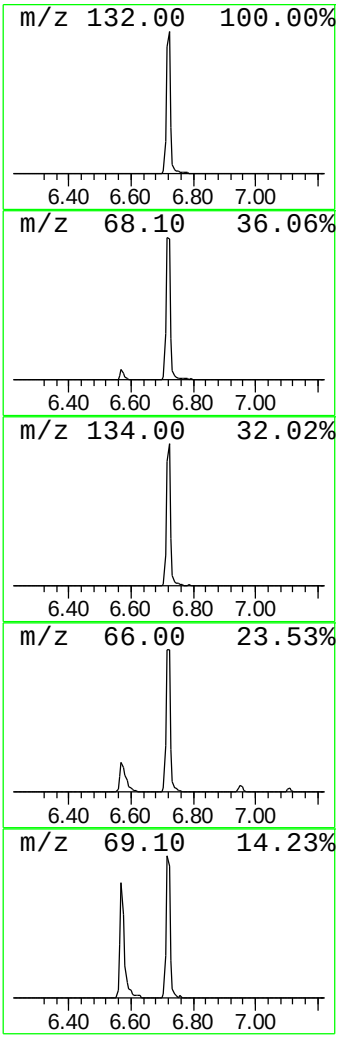
****

Peak Number 2 unknown6.72 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	16.01 ng	425157	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110422.D
Acq On : 2 Nov 2018 20:01
Operator : JU/SJ
Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

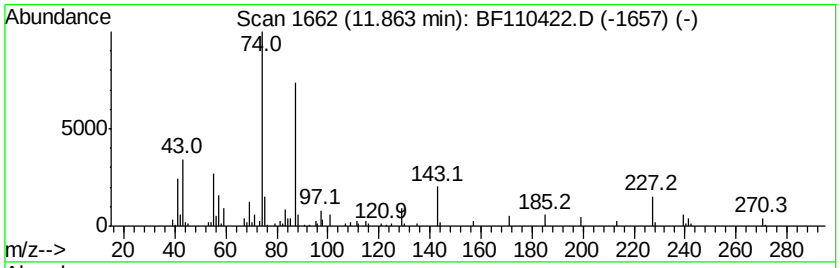
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

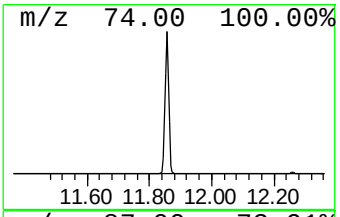
****

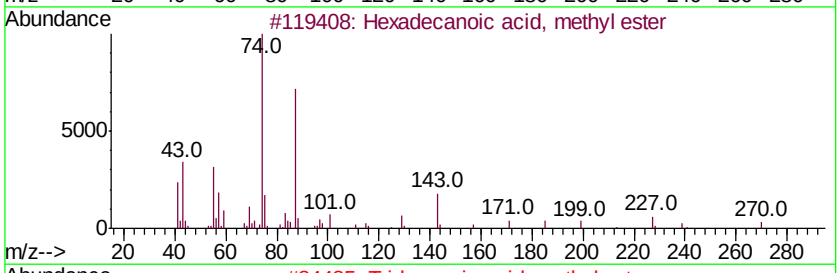
Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

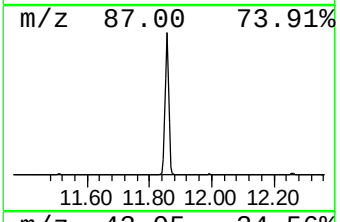
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	12.14 ng	382886	Phenanthrene-d10	11.49

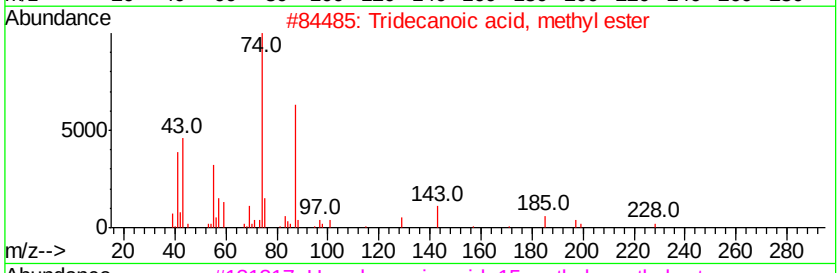
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
4	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86

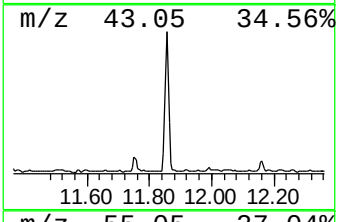


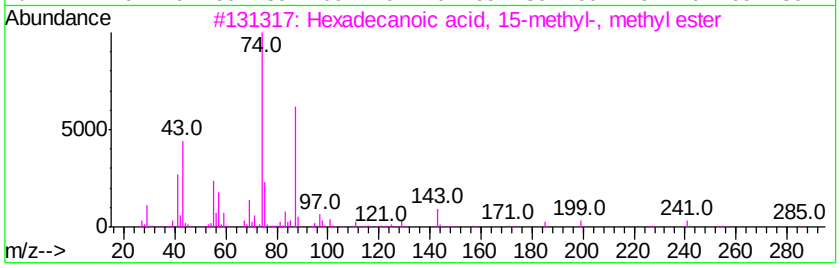


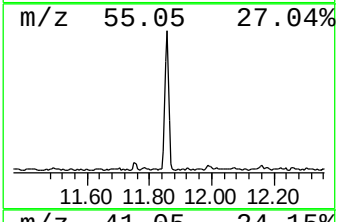


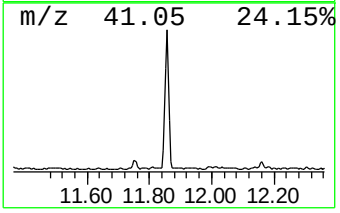












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110422.D
Acq On : 2 Nov 2018 20:01
Operator : JU/SJ
Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

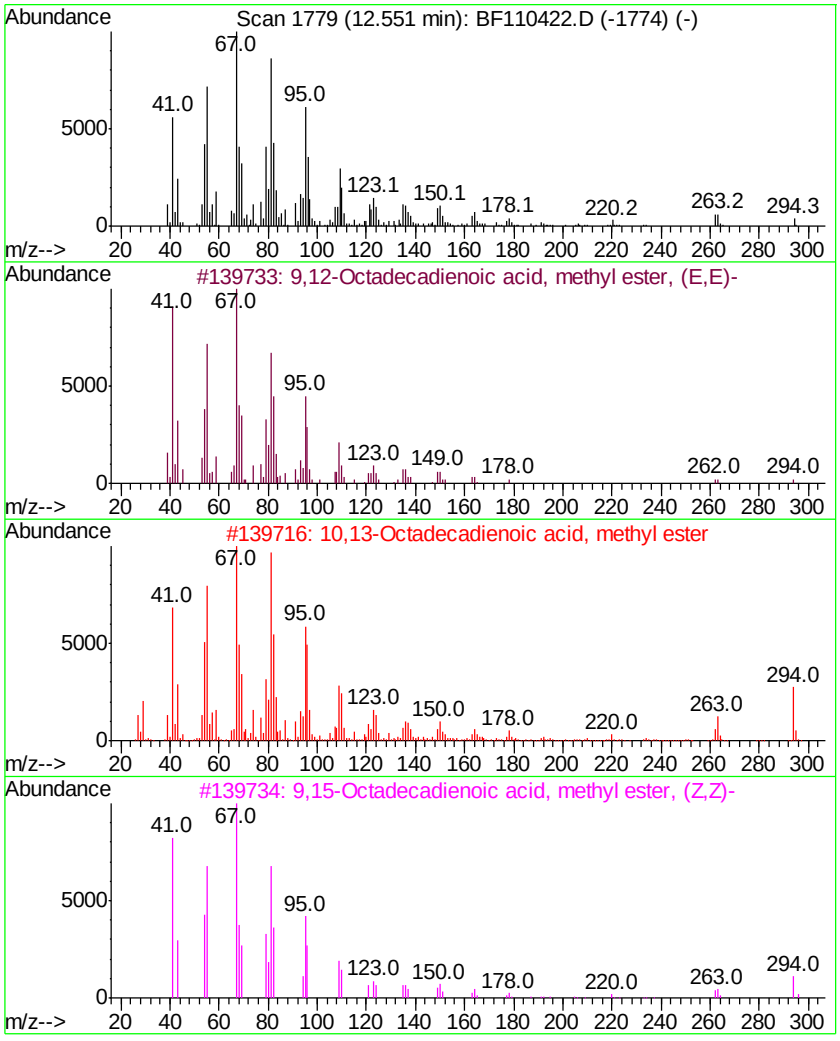
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

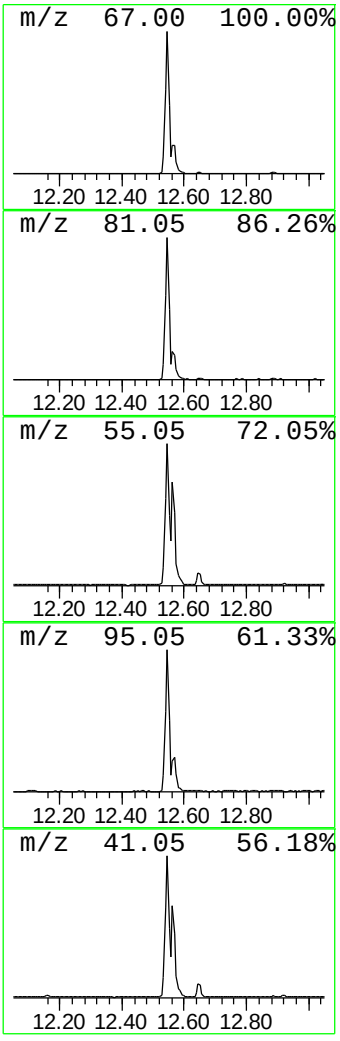
****

Peak Number 5 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	50.11 ng	1580140	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	8,11-Octadecadienoic acid, methy...	294	C19H34O2	056599-58-7	99





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110422.D
Acq On : 2 Nov 2018 20:01
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

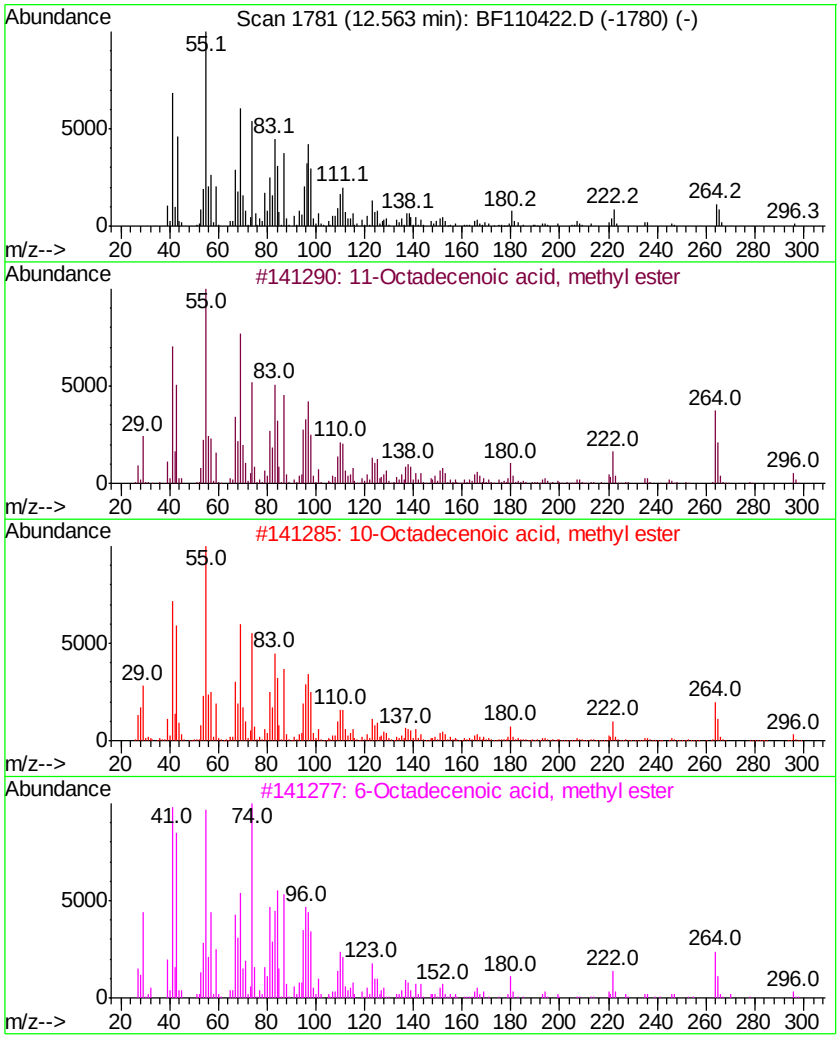
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

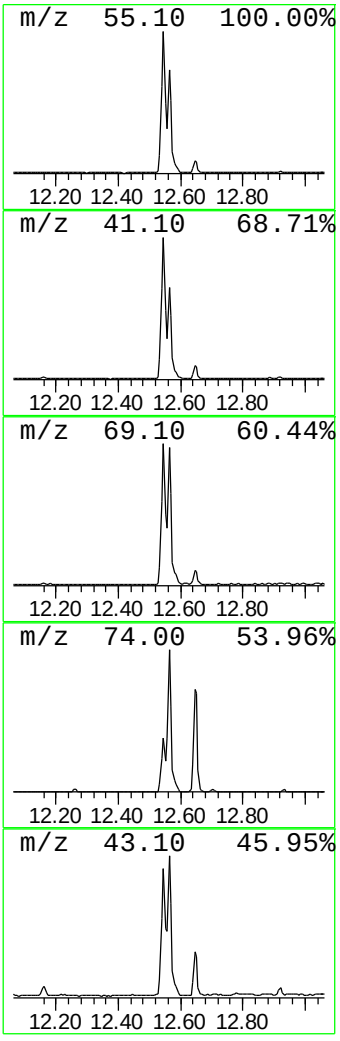
****

Peak Number 6 11-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	26.08 ng	822233	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
3	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	99
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
5	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99





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Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

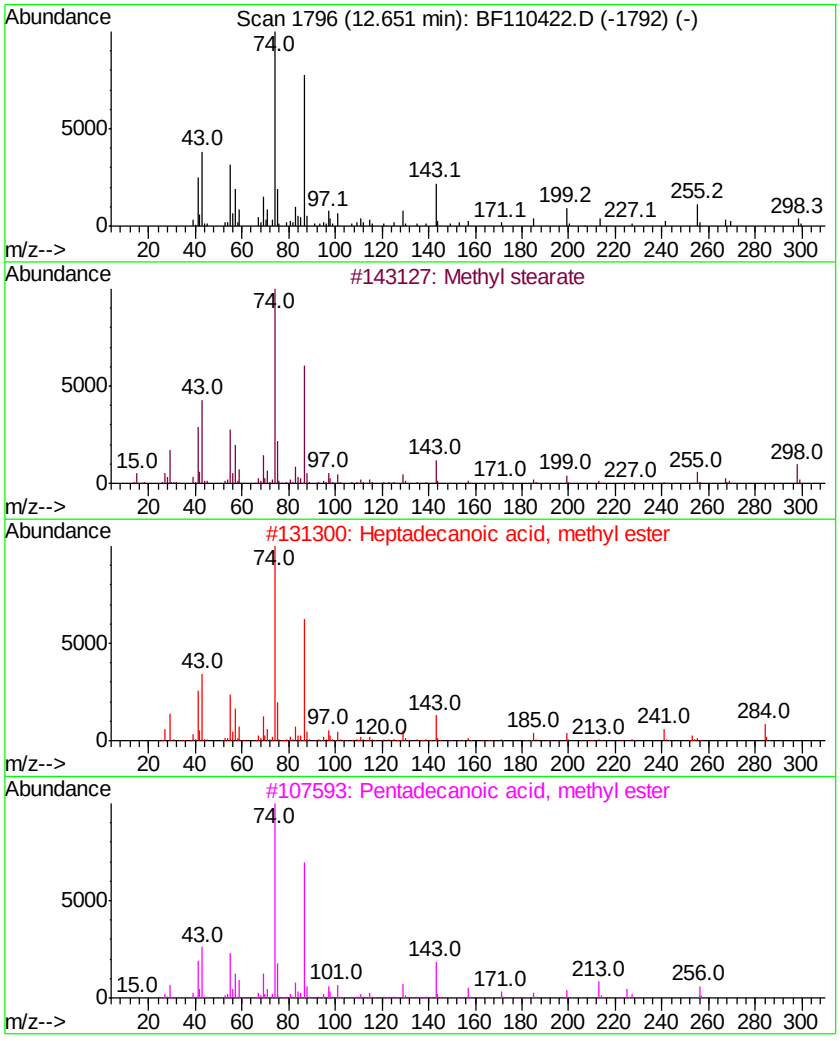
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

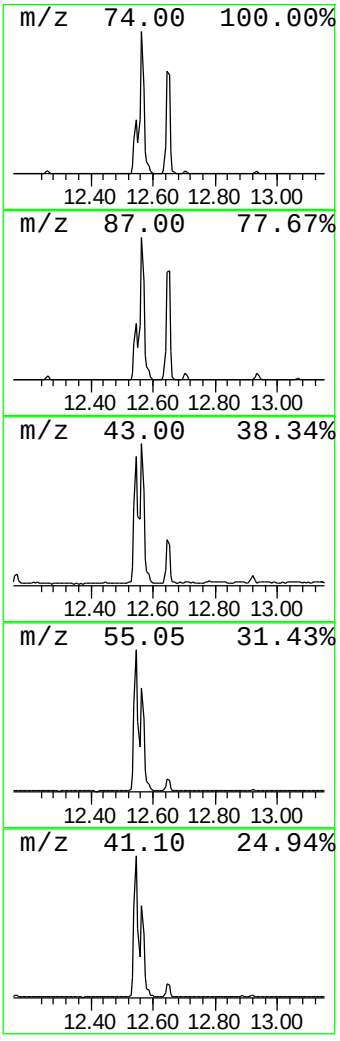
****

Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	4.74 ng	149474	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	95
2	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90
4	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	86
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110422.D
Acq On : 2 Nov 2018 20:01
Operator : JU/SJ
Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

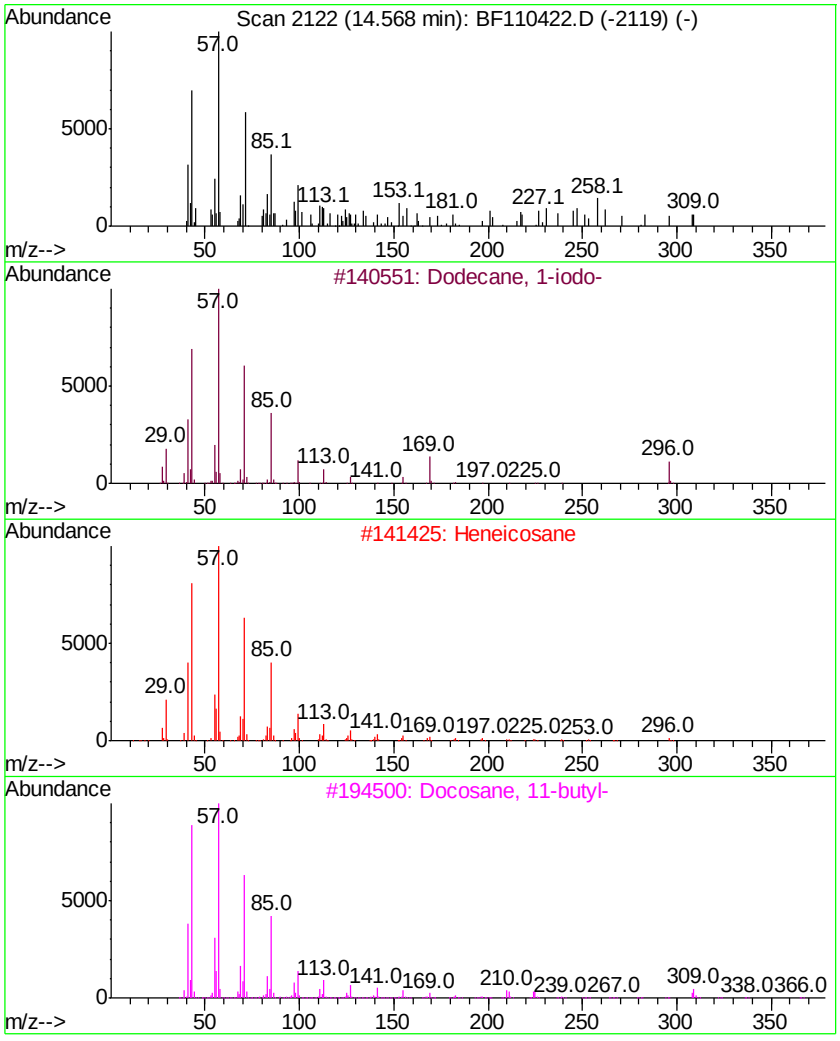
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

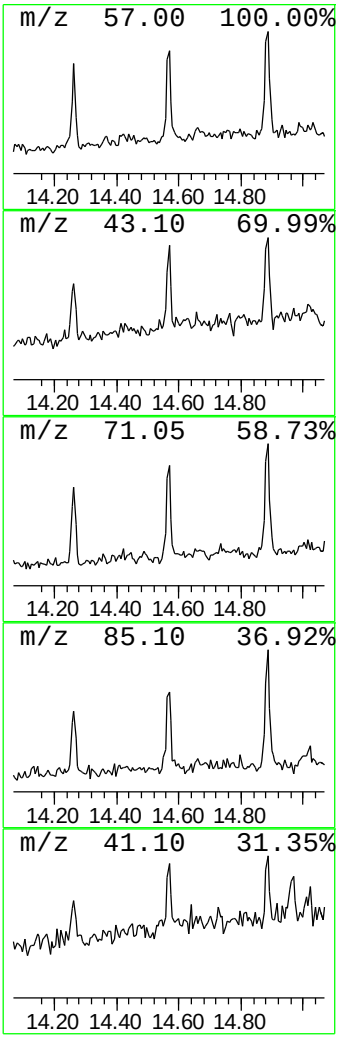
****

Peak Number 8 Dodecane, 1-iodo- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.57	2.29 ng	67941	Chrysene-d12	14.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	60
2	Heneicosane	296	C21H44	000629-94-7	60
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	58
4	Docosane, 11-decyl-	451	C32H66	055401-55-3	52
5	Tetratetracontane	619	C44H90	007098-22-8	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110422.D
Acq On : 2 Nov 2018 20:01
Operator : JU/SJ
Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

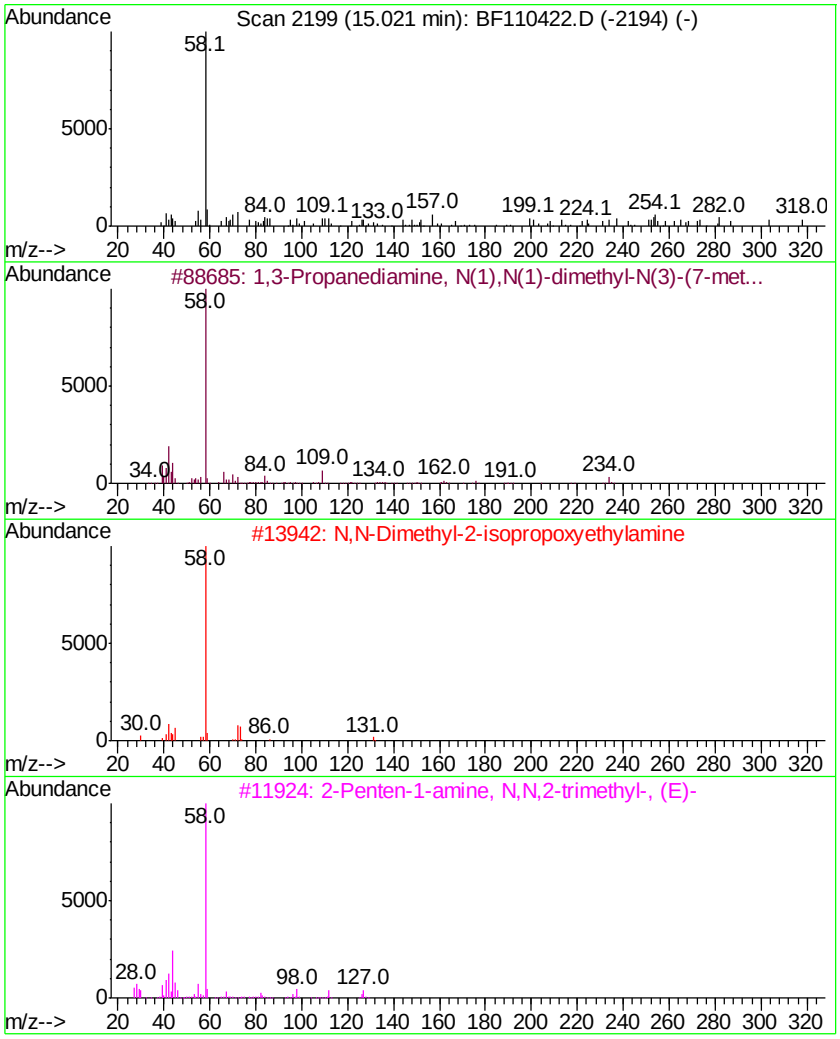
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

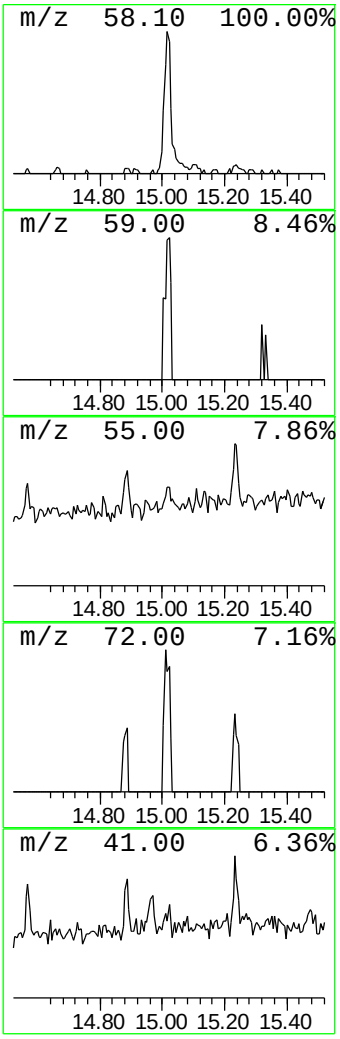
****

Peak Number 9 1,3-Propanediamine, N(1),N(... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	2.59 ng	58962	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Propanediamine, N(1),N(1)-di...	234	C11H18N6	1000338-05-2	53
2	N,N-Dimethyl-2-isopropoxyethylamine	131	C7H17NO	071126-59-5	50
3	2-Penten-1-amine, N,N,2-trimethy...	127	C8H17N	055630-70-1	50
4	1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	50
5	1-Hexanamine, 2-ethyl-N,N-dimethyl-	157	C10H23N	028056-87-3	50





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Operator : JU/SJ
Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
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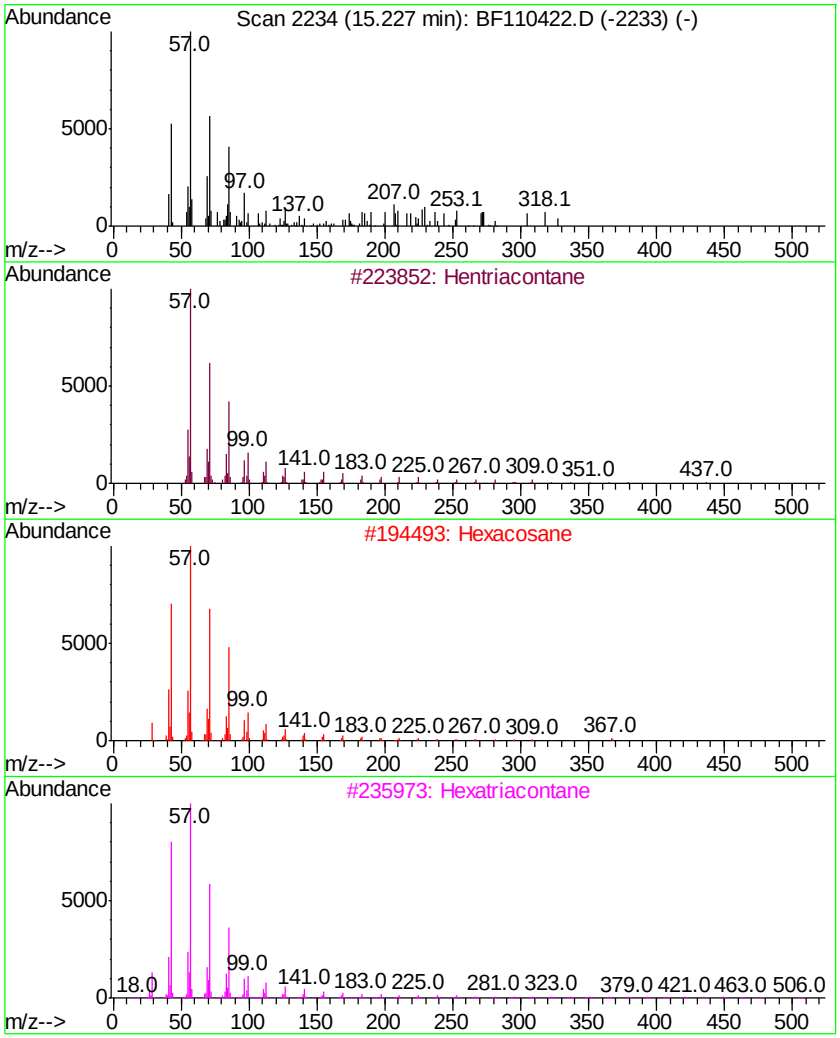
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

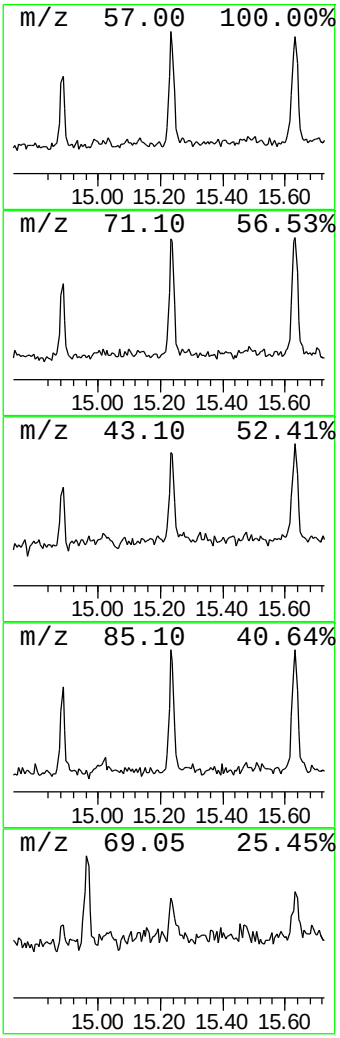
****

Peak Number 10 Hentriacontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	3.27 ng	74566	Perylene-d12	15.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	87
2	Hexacosane	366	C26H54	000630-01-3	87
3	Hexatriacontane	507	C36H74	000630-06-8	83
4	Tetratetracontane	619	C44H90	007098-22-8	83
5	2-methyloctacosane	408	C29H60	1000376-72-8	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110218\
Data File : BF110422.D
Acq On : 2 Nov 2018 20:01
Operator : JU/SJ
Sample : J5767-01 5X
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-110118-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.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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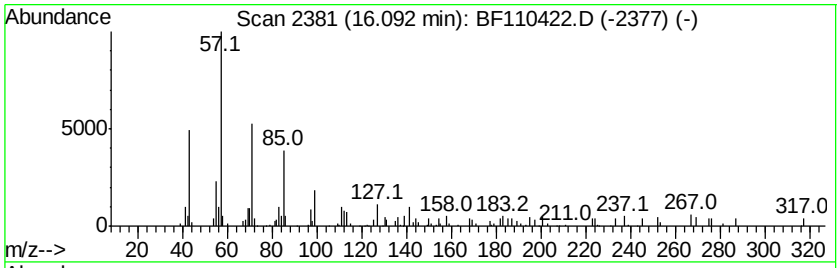
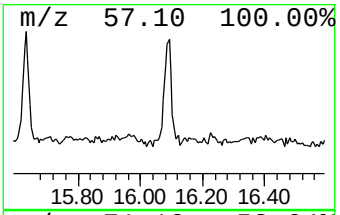
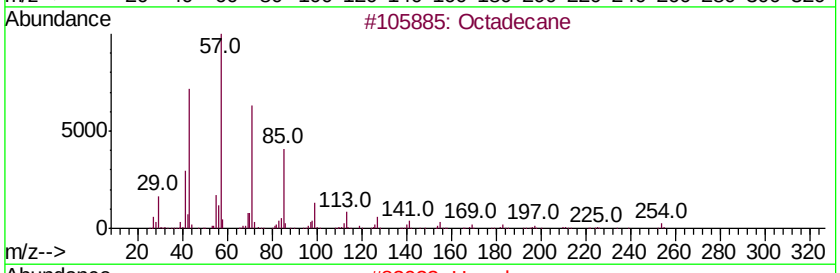
Peak Number 11 Octadecane Concentration Rank 8

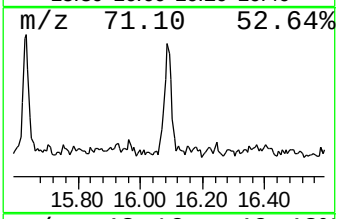
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.09	3.50 ng	79863	Perylene-d12	15.66

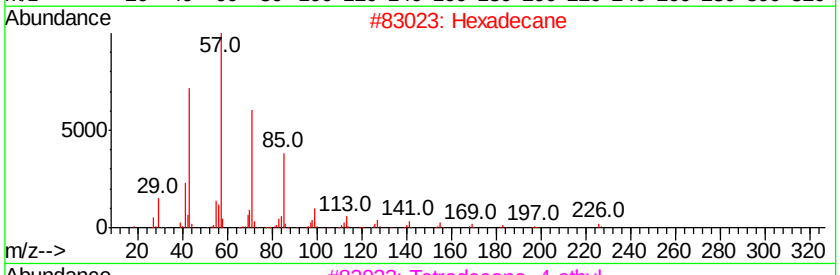
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	50
2	Hexadecane	226	C16H34	000544-76-3	50
3	Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	50
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	50
5	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	50

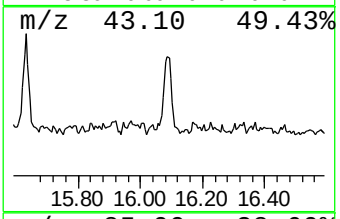


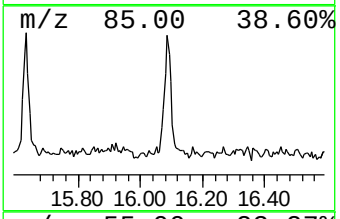


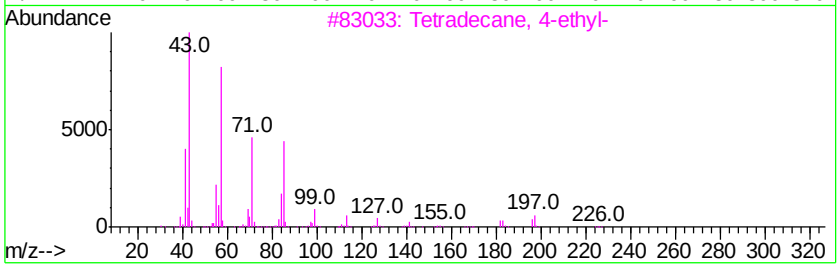


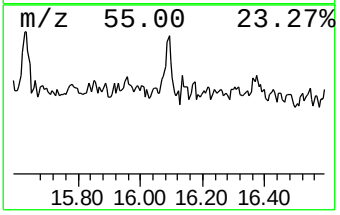












Tentatively Identified Compound (LSC) summary

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Sample : J5767-01 5X
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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...	2.26	4.0	ng	104766	1	6.95	531085	20.0
unknown6.72	6.72	16.0	ng	425157	1	6.95	531085	20.0
Hexadecanoic acid...	11.86	12.1	ng	382886	4	11.49	630624	20.0
9,12-Octadecadien...	12.55	50.1	ng	1580140	4	11.49	630624	20.0
11-Octadecenoic a...	12.56	26.1	ng	822233	4	11.49	630624	20.0
Methyl stearate	12.65	4.7	ng	149474	4	11.49	630624	20.0
Dodecane, 1-iodo-	14.57	2.3	ng	67941	5	14.13	592867	20.0
1,3-Propanediamin...	15.02	2.6	ng	58962	6	15.66	455723	20.0
Hentriacontane	15.23	3.3	ng	74566	6	15.66	455723	20.0
Octadecane	16.09	3.5	ng	79863	6	15.66	455723	20.0