LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113971.D
Acq On : 24 Apr 2019 19:33
Operator : JU/SJ
Sample : K2539-03 10X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-006-B

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-BF042219.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	5.098	508	512	522	rBV	153661	162305	16.17%	1.691%
2	5.516	579	583	591	rVB	16958	22630	2.25%	0.236%
3	6.510	746	752	764	rBV	132791	160915	16.03%	1.676%
4	6.663	773	778	783	rBV	74138	67922	6.77%	0.708%
5	6.740	786	791	794	rBV2	19381	19688	1.96%	0.205%
6	6.898	814	818	826	rBV	705862	669133	66.66%	6.971%
7	7.051	840	844	848	rBV	237424	195865	19.51%	2.040%
8	7.445	905	911	917	rBV	129018	134355	13.38%	1.400%
9	7.498	917	920	924	rVB	17227	17527	1.75%	0.183%
10	8.175	1030	1035	1042	rBV	892018	839448	83.62%	8.745%
11	8.769	1134	1136	1141	rVB	24127	19839	1.98%	0.207%
12	9.251	1214	1218	1228	rBV	291706	280243	27.92%	2.920%
13	9.333	1229	1232	1237	rBV	31918	29738	2.96%	0.310%
14	9.639	1282	1284	1289	rBV2	26637	35902	3.58%	0.374%
15	9.863	1318	1322	1327	rVB	31510	31356	3.12%	0.327%
16	9.933	1330	1334	1344	rVB	924421	892028	88.86%	9.293%
17	10.133	1364	1368	1373	rBV3	9482	14038	1.40%	0.146%
18	10.186	1373	1377	1381	rVB5	8135	13718	1.37%	0.143%
19	10.363	1404	1407	1410	rVB	34822	27995	2.79%	0.292%
20	10.586	1440	1445	1449	rBV2	18186	21955	2.19%	0.229%
21	10.833	1485	1487	1496	rBV2	39376	58197	5.80%	0.606%
22	11.280	1559	1563	1566	rBV	36856	38989	3.88%	0.406%
23	11.316	1566	1569	1574	rVB	29515	31048	3.09%	0.323%
24	11.416	1582	1586	1589	rBV	1004470	877115	87.37%	9.138%
25	11.439	1589	1590	1594	rVV	110182	71682	7.14%	0.747%
26	11.492	1597	1599	1602	rVB	20563	17440	1.74%	0.182%
27	11.645	1619	1625	1627	rBV3	11346	16990	1.69%	0.177%
28	11.710	1633	1636	1638	rBV	38406	27344	2.72%	0.285%
29	11.745	1638	1642	1649	rVB6	10454	17522	1.75%	0.183%
30	11.804	1649	1652	1656	rBV	299251	255191	25.42%	2.659%
31	11.916	1668	1671	1673	rBV	20176	23924	2.38%	0.249%
32	11.945	1673	1676	1679	rVB2	32657	35783	3.56%	0.373%
33	12.027	1687	1690	1692	rBV2	26270	26038	2.59%	0.271%
34	12.116	1703	1705	1708	rVV	40668	33177	3.30%	0.346%

LSC Area Percent Report

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Acq On : 24 Apr 2019 19:33
Operator : JU/SJ
Sample : K2539-03 10X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-006-B

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-BF042219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.151	1708	1711	1714	rVB3	16461	14127	1.41%	0.147%
36	12.210	1719	1721	1723	rBV2	17099	16167	1.61%	0.168%
37	12.233	1723	1725	1730	rVB5	12652	18186	1.81%	0.189%
38	12.392	1750	1752	1758	rBV6	19676	31806	3.17%	0.331%
39	12.469	1761	1765	1766	rBV	33602	37348	3.72%	0.389%
40	12.492	1766	1769	1771	rVV	1022201	890923	88.75%	9.281%
41	12.516	1771	1773	1778	rVB	779016	666505	66.39%	6.944%
42	12.598	1783	1787	1789	rBV	151905	129802	12.93%	1.352%
43	12.627	1789	1792	1795	rVB	121428	101813	10.14%	1.061%
44	12.857	1827	1831	1833	rBV	100488	108317	10.79%	1.128%
45	12.992	1851	1854	1862	rVB	342500	334403	33.31%	3.484%
46	13.233	1892	1895	1901	rBV3	54751	80375	8.01%	0.837%
47	13.574	1950	1953	1956	rBV2	69059	69716	6.94%	0.726%
48	14.057	2031	2035	2038	rBV	1047069	1003858	100.00%	10.458%
49	14.221	2061	2063	2067	rVB	84523	70074	6.98%	0.730%
50	14.539	2114	2117	2120	rBV	85535	79828	7.95%	0.832%
51	15.551	2285	2289	2292	rBV	648434	758647	75.57%	7.903%

Sum of corrected areas: 9598935

LSC Report - Integrated Chromatogram

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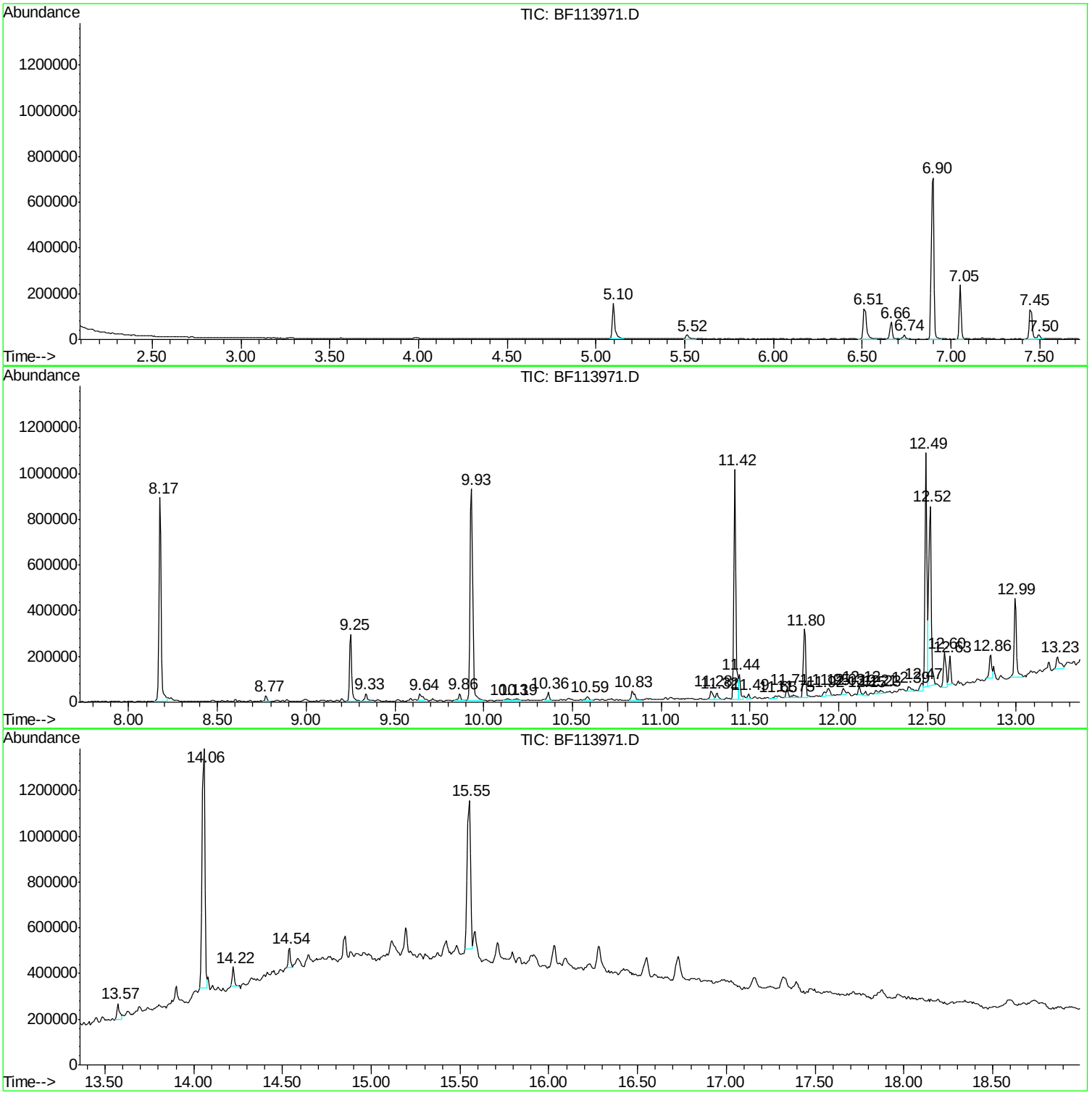
Data File : BF113971.D
Acq On : 24 Apr 2019 19:33
Operator : JU/SJ
Sample : K2539-03 10X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-006-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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 : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113971.D
Acq On : 24 Apr 2019 19:33
Operator : JU/SJ
Sample : K2539-03 10X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-006-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

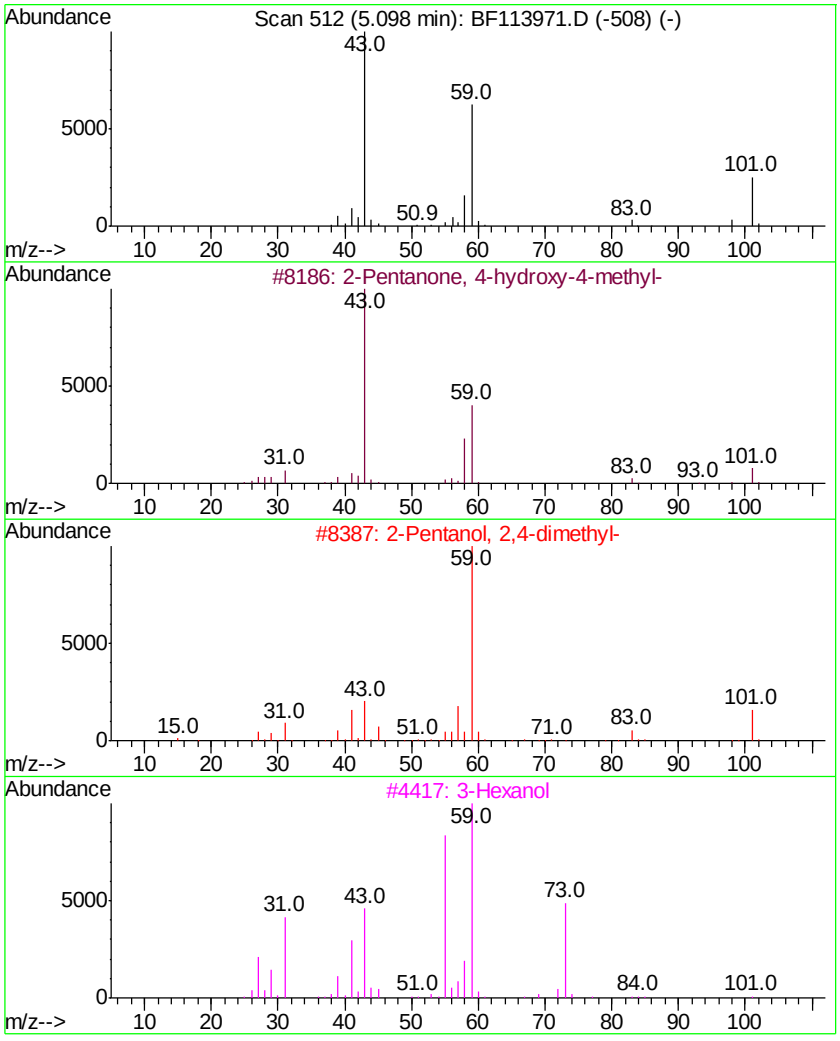
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

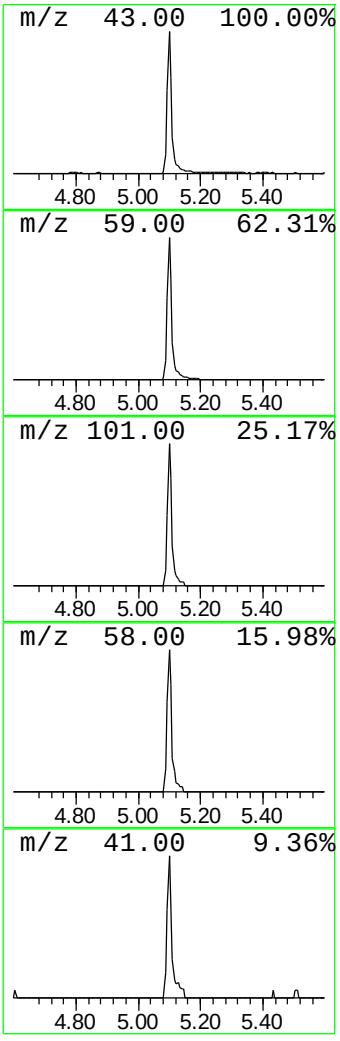
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	4.85 ng	162305	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
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Acq On : 24 Apr 2019 19:33
Operator : JU/SJ
Sample : K2539-03 10X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-006-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

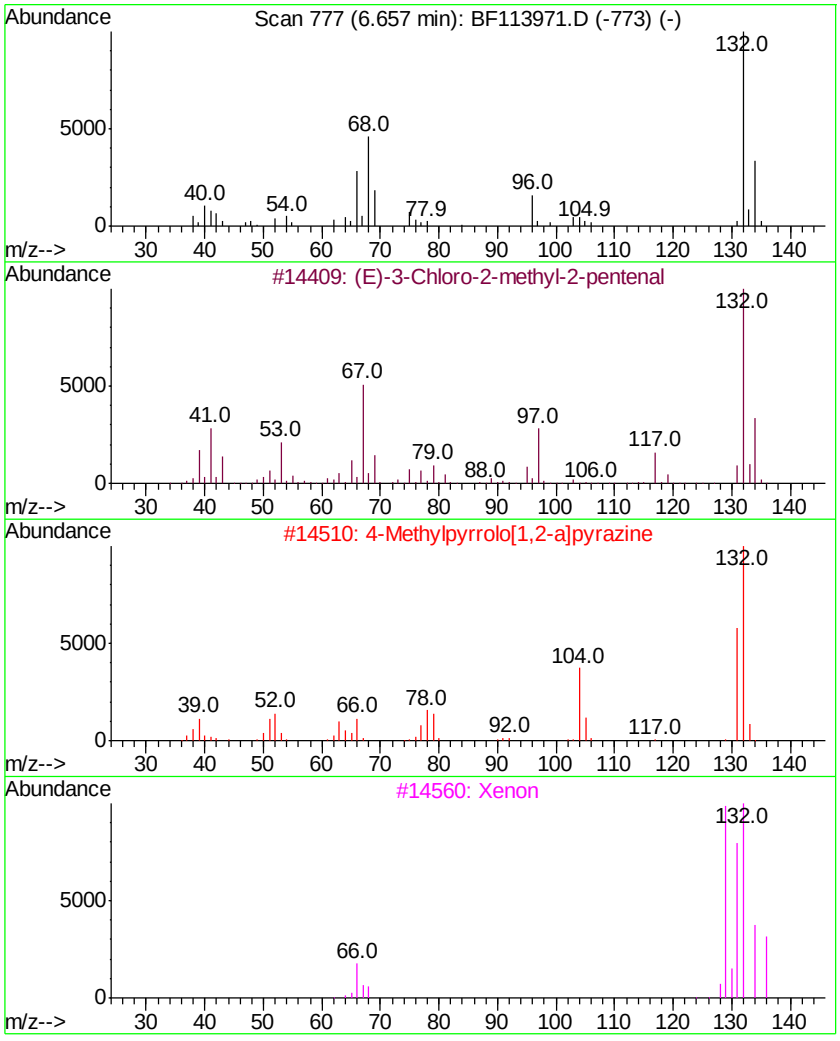
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

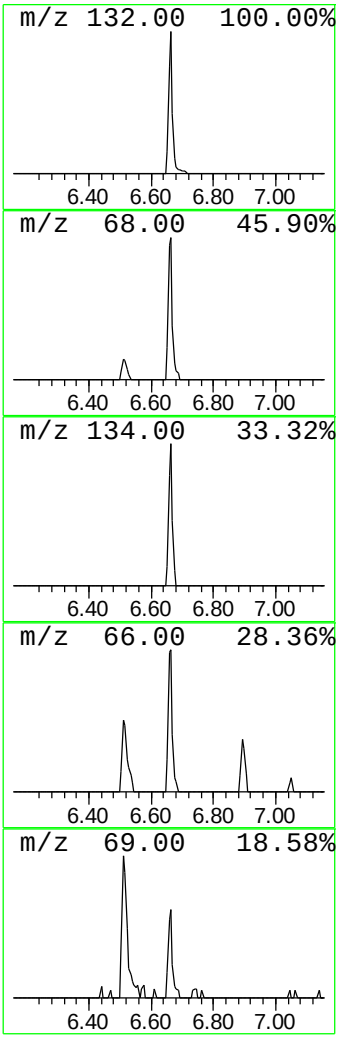
****

Peak Number 2 unknown6.66 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	2.03 ng	67922	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
3	Xenon	132	Xe	007440-63-3	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
Data File : BF113971.D
Acq On : 24 Apr 2019 19:33
Operator : JU/SJ
Sample : K2539-03 10X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-SF-03-006-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

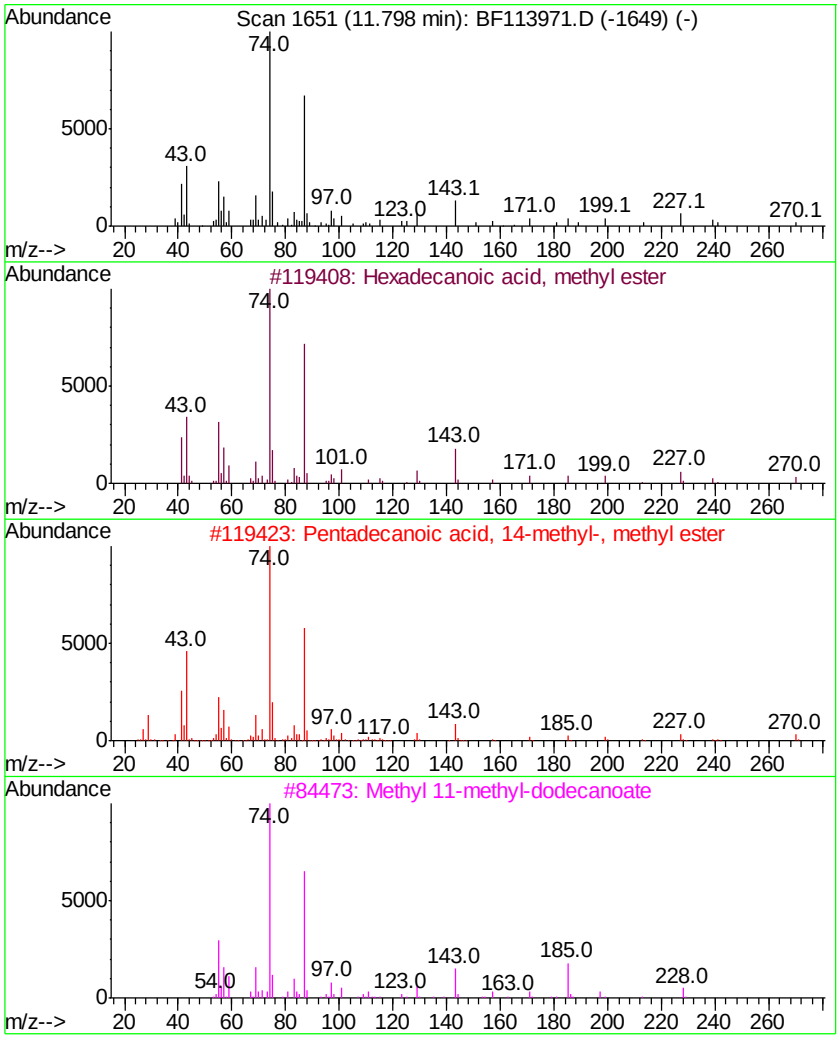
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

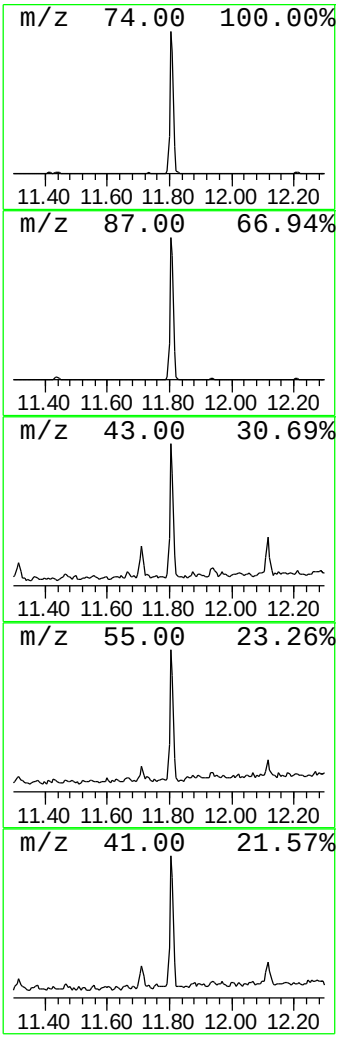
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	5.82 ng	255191	Phenanthrene-d10	11.42

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	97
3	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF042419\
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Acq On : 24 Apr 2019 19:33
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Misc :
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Instrument : BNA_F
ClientSampleId : FK-SF-03-006-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

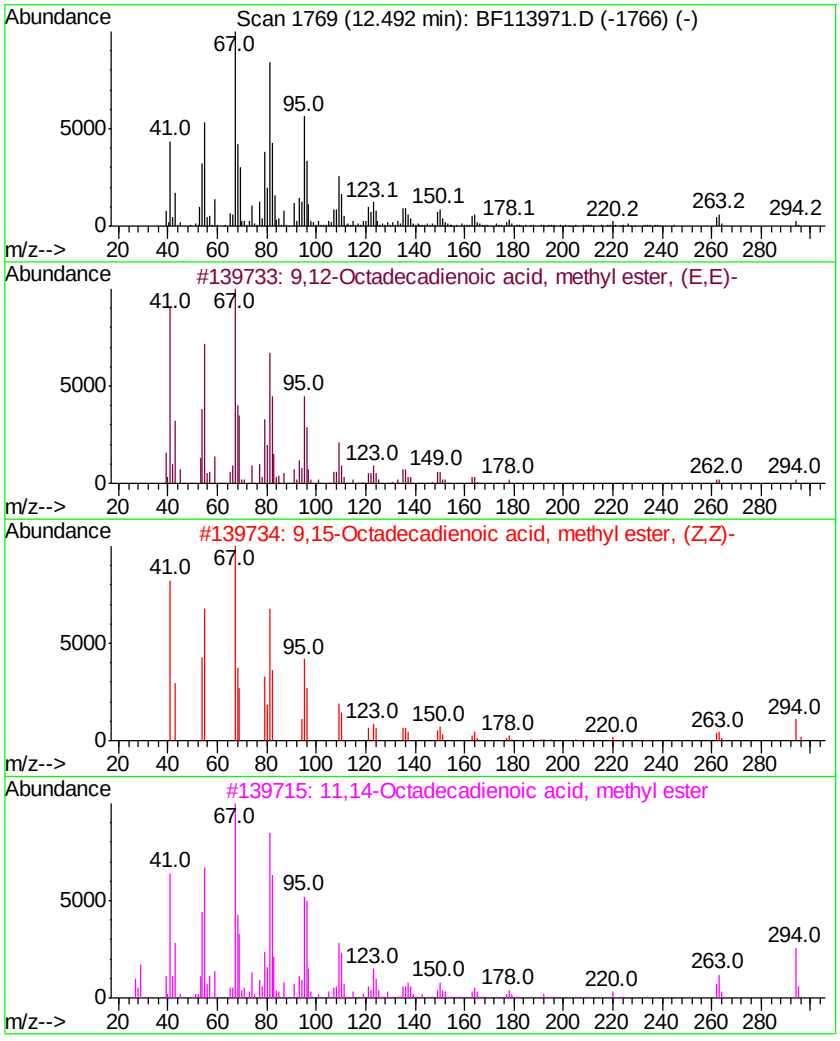
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

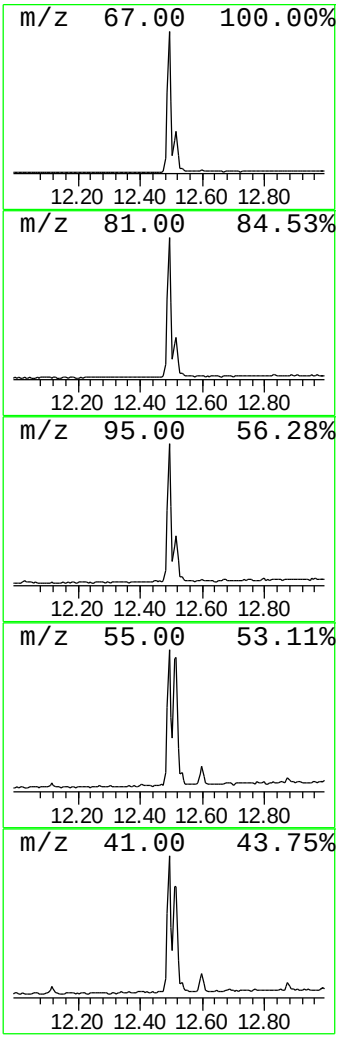
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	20.31 ng	890923	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
3	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

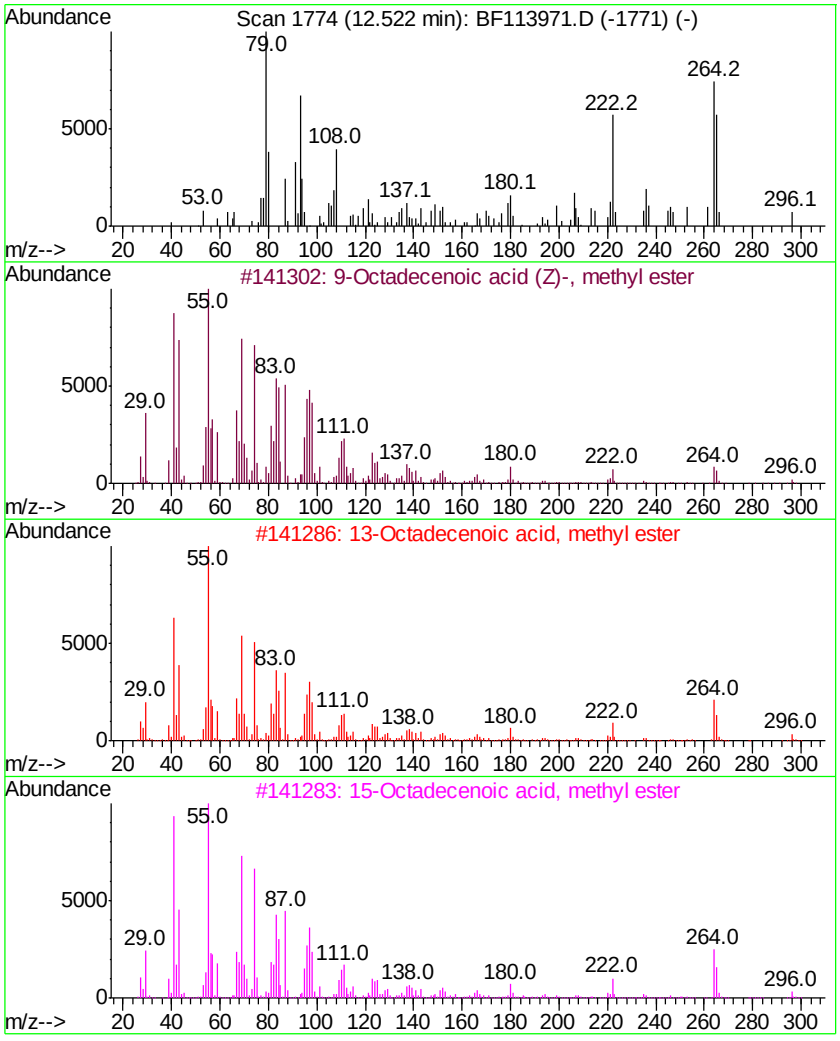
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

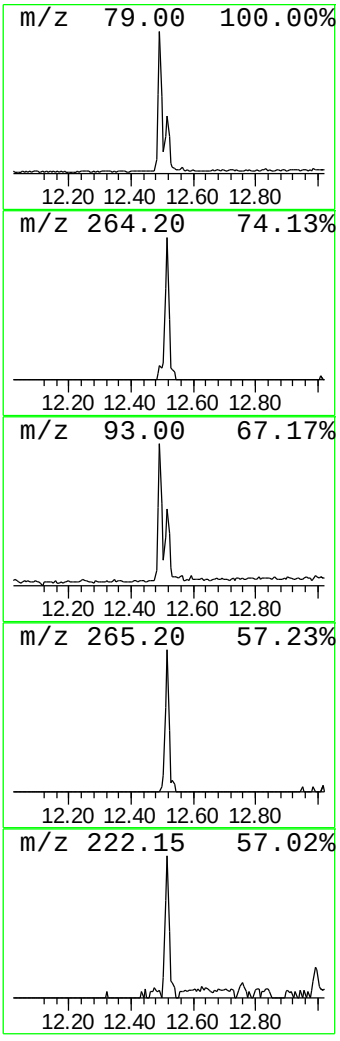
****

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	15.20 ng	666505	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
5	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042419\
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Misc :
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Instrument : BNA_F
ClientSampleId : FK-SF-03-006-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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...	5.10	4.8	ng	162305	1	6.90	669133	20.0
unknown6.66	6.66	2.0	ng	67922	1	6.90	669133	20.0
Hexadecanoic acid...	11.80	5.8	ng	255191	4	11.42	877115	20.0
9,12-Octadecadien...	12.49	20.3	ng	890923	4	11.42	877115	20.0
9-Octadecenoic ac...	12.52	15.2	ng	666505	4	11.42	877115	20.0