LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
Data File : BF110111.D
Acq On : 24 Oct 2018 13:31
Operator : JU/SJ
Sample : J5610-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(6-8)

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	2.310	33	38	45	rVB	463065	614446	14.82%	1.642%
2	3.593	254	256	264	rBV	21753	49783	1.20%	0.133%
3	5.210	527	531	540	rVB	149373	190097	4.58%	0.508%
4	5.593	590	596	599	rBV	3761616	3648762	87.98%	9.749%
5	6.593	760	766	779	rVB2	3501415	4147117	100.00%	11.081%
6	6.740	786	791	794	rBV	3704773	3804424	91.74%	10.165%
7	6.963	826	829	833	rBV	1215998	1101258	26.55%	2.943%
8	7.122	852	856	860	rBV	3235225	2931579	70.69%	7.833%
9	7.528	920	925	928	rBV	2284715	2324459	56.05%	6.211%
10	8.251	1044	1048	1051	rBV	1491299	1328304	32.03%	3.549%
11	9.322	1225	1230	1234	rBV	3944792	3734104	90.04%	9.977%
12	9.716	1293	1297	1301	rVB	638454	530483	12.79%	1.417%
13	9.869	1319	1323	1326	rBV	84773	77383	1.87%	0.207%
14	10.010	1343	1347	1350	rBV	1555286	1262307	30.44%	3.373%
15	10.798	1477	1481	1485	rBV	1988925	1763105	42.51%	4.711%
16	11.504	1597	1601	1603	rBV	1112511	1087433	26.22%	2.906%
17	11.522	1603	1604	1609	rVB	426647	346401	8.35%	0.926%
18	11.575	1609	1613	1617	rBV	109228	104895	2.53%	0.280%
19	12.010	1683	1687	1689	rBV2	157708	174927	4.22%	0.467%
20	12.033	1689	1691	1694	rVB	76118	67622	1.63%	0.181%
21	12.116	1702	1705	1707	rBV2	64514	71538	1.73%	0.191%
22	12.327	1738	1741	1747	rVB3	40859	45803	1.10%	0.122%
23	12.639	1791	1794	1798	rBV	49120	50667	1.22%	0.135%
24	12.716	1804	1807	1811	rBV	712362	578130	13.94%	1.545%
25	12.951	1840	1847	1852	rBV	551436	650879	15.69%	1.739%
26	13.086	1866	1870	1873	rBV	2966963	2547909	61.44%	6.808%
27	13.645	1962	1965	1967	rBV2	65976	70908	1.71%	0.189%
28	13.780	1986	1988	1993	rVB	73025	59785	1.44%	0.160%
29	13.969	2018	2020	2032	rVB4	255994	374164	9.02%	1.000%
30	14.110	2042	2044	2046	rBV2	87627	65252	1.57%	0.174%
31	14.151	2046	2051	2053	rVV2	1049282	1248578	30.11%	3.336%
32	14.174	2053	2055	2059	rVB	282183	237222	5.72%	0.634%
33	14.286	2072	2074	2077	rVB2	112816	99603	2.40%	0.266%
34	14.598	2124	2127	2129	rVB	127588	113850	2.75%	0.304%

LSC Area Percent Report

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(6-8)

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	15.216	2230	2232	2239	rVV	183241	299678	7.23%	0.801%
36	15.268	2239	2241	2249	rVB	186673	236197	5.70%	0.631%
37	15.604	2295	2298	2305	rBV	182456	291919	7.04%	0.780%
38	15.674	2306	2310	2314	rBV2	652729	844700	20.37%	2.257%
39	16.139	2386	2389	2393	rVB	180910	250226	6.03%	0.669%

Sum of corrected areas: 37425897

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
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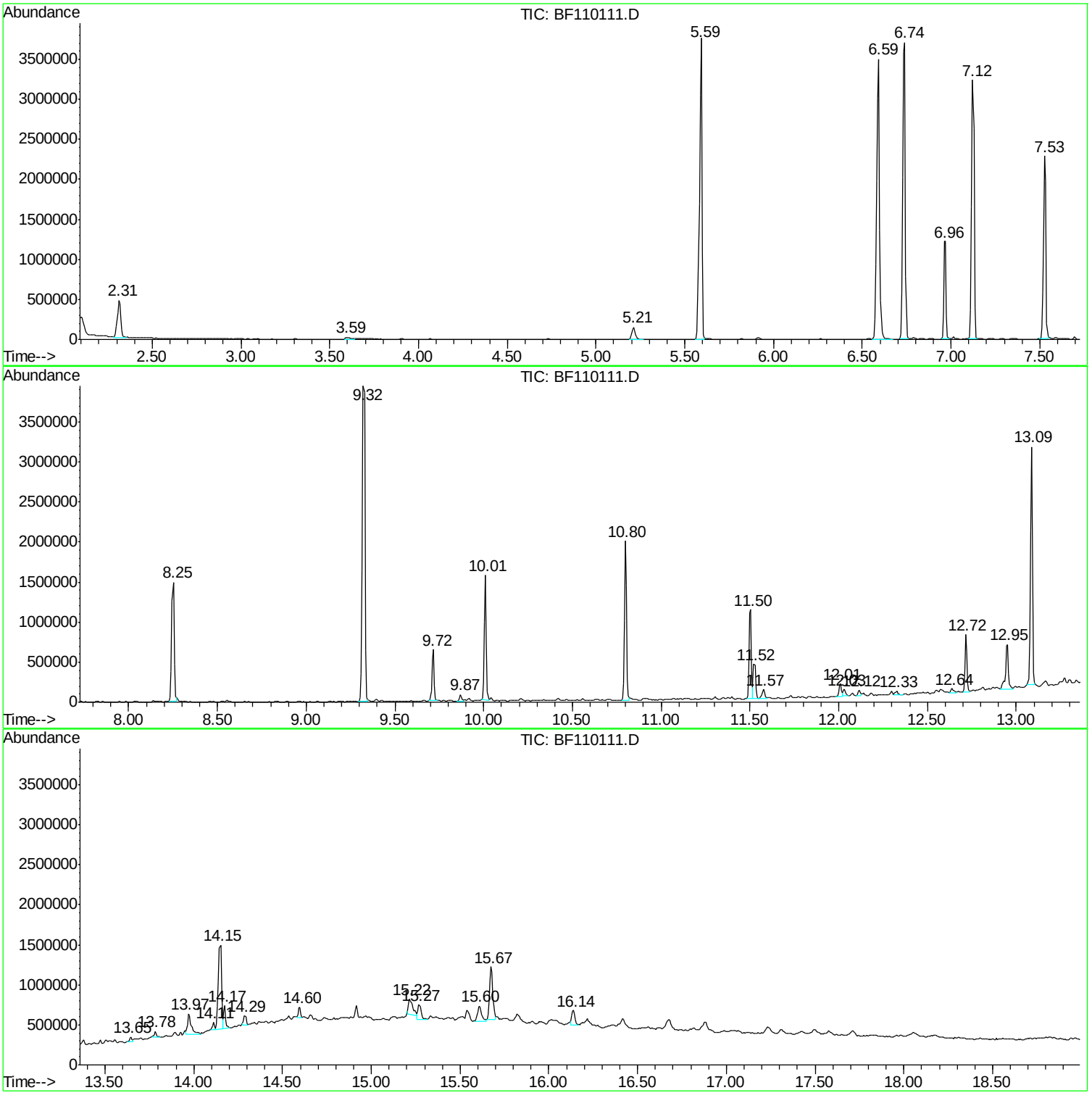
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-3(6-8)

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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
Data File : BF110111.D
Acq On : 24 Oct 2018 13:31
Operator : JU/SJ
Sample : J5610-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(6-8)

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

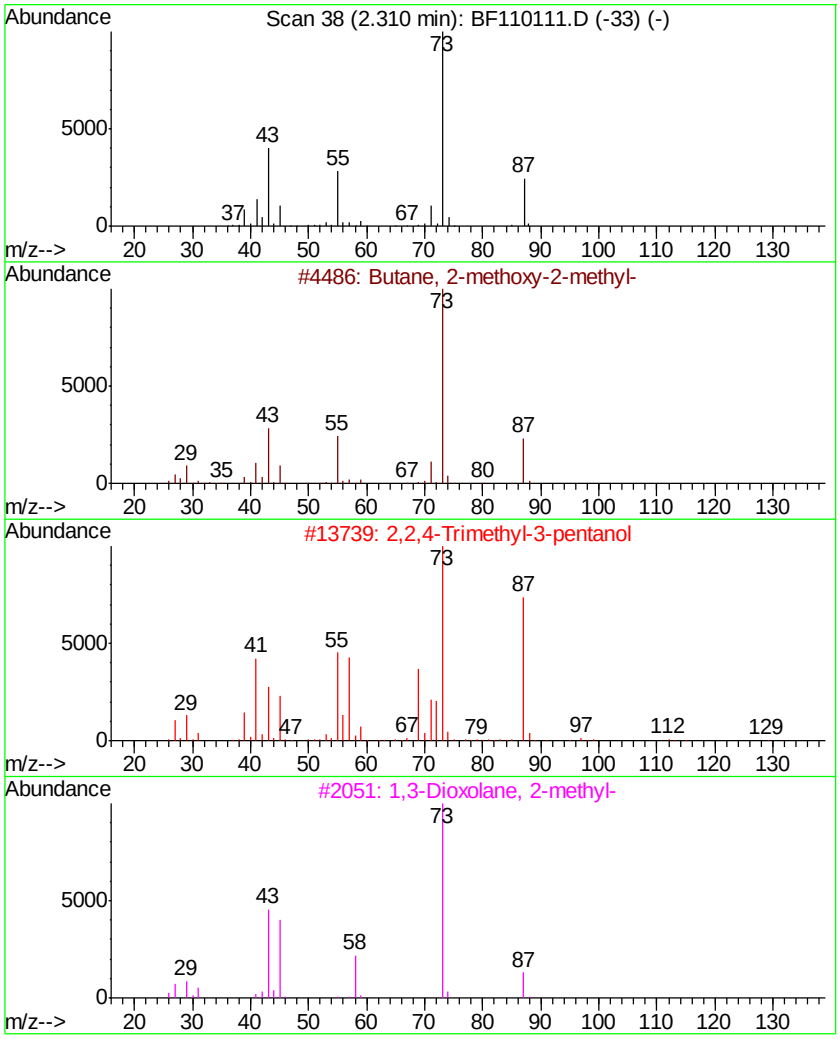
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

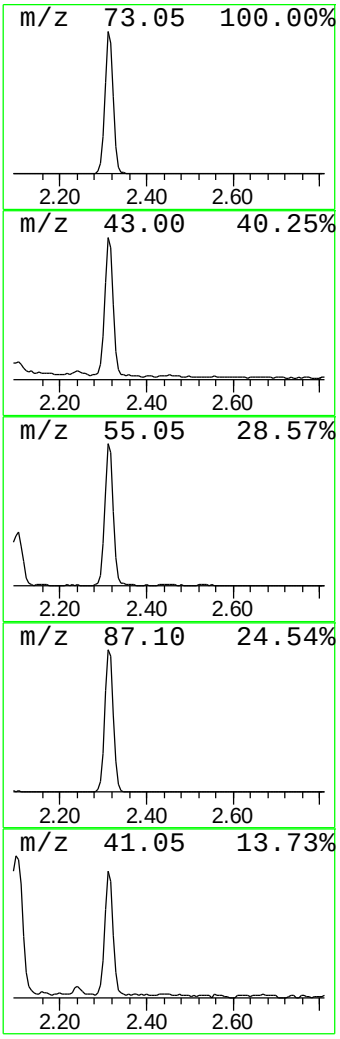
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	11.16 ng	614446	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	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
Data File : BF110111.D
Acq On : 24 Oct 2018 13:31
Operator : JU/SJ
Sample : J5610-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(6-8)

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

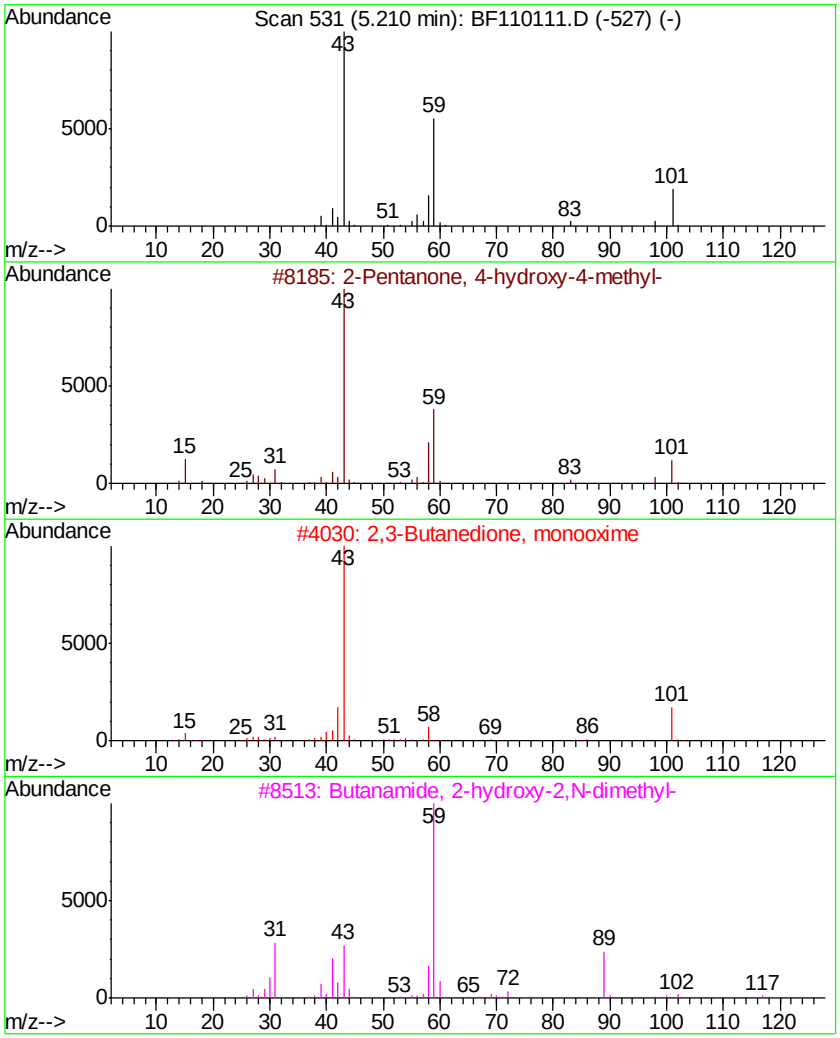
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

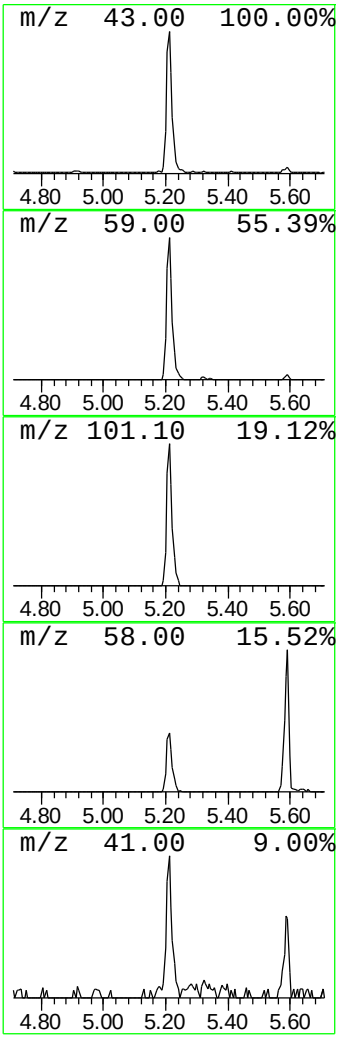
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	3.45 ng	190097	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	59
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	9
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
Data File : BF110111.D
Acq On : 24 Oct 2018 13:31
Operator : JU/SJ
Sample : J5610-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(6-8)

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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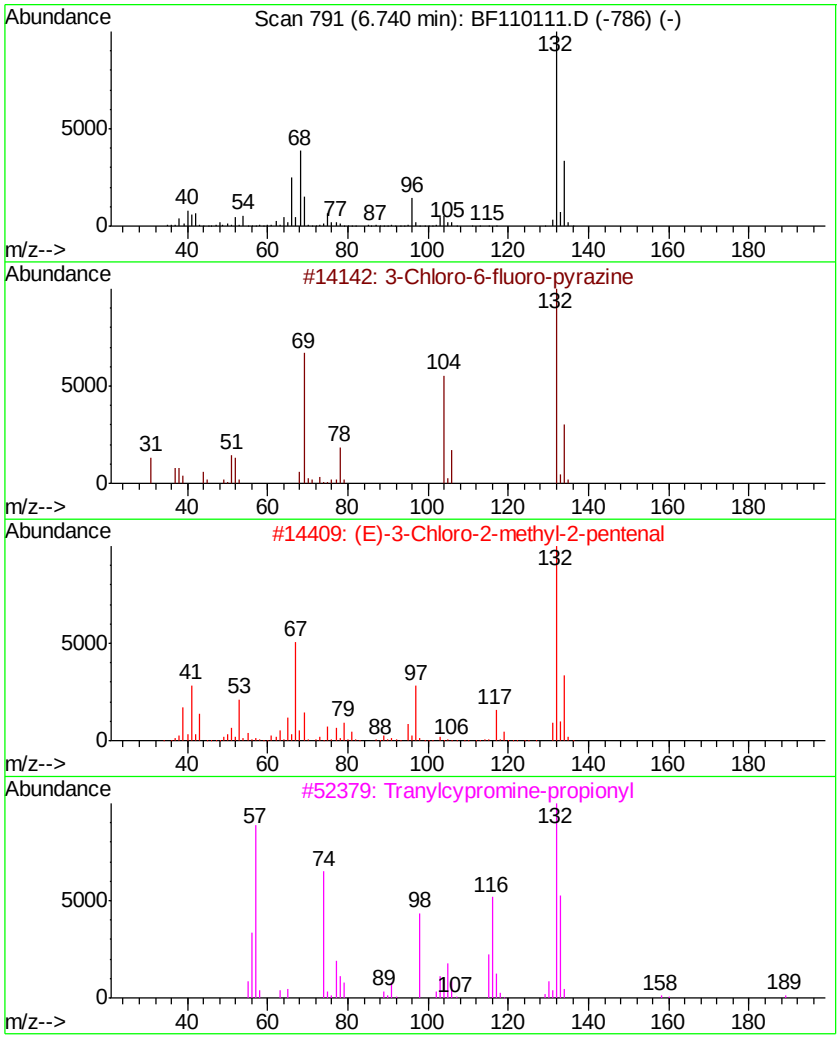
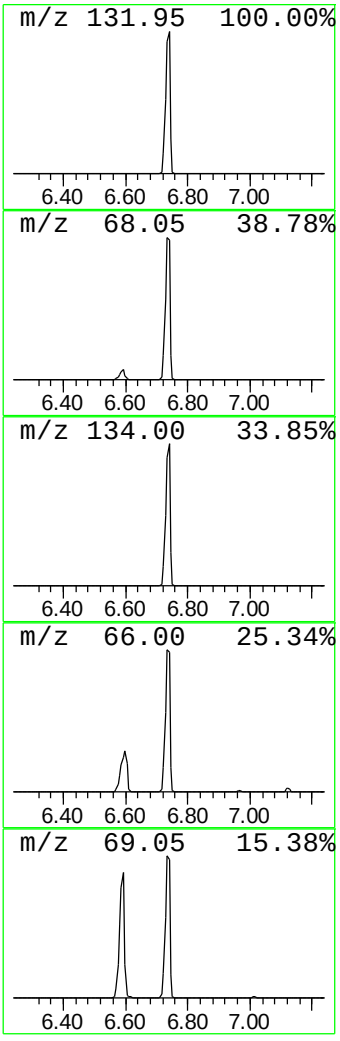
Peak Number 3 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	69.09 ng	3804420	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	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
Data File : BF110111.D
Acq On : 24 Oct 2018 13:31
Operator : JU/SJ
Sample : J5610-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(6-8)

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

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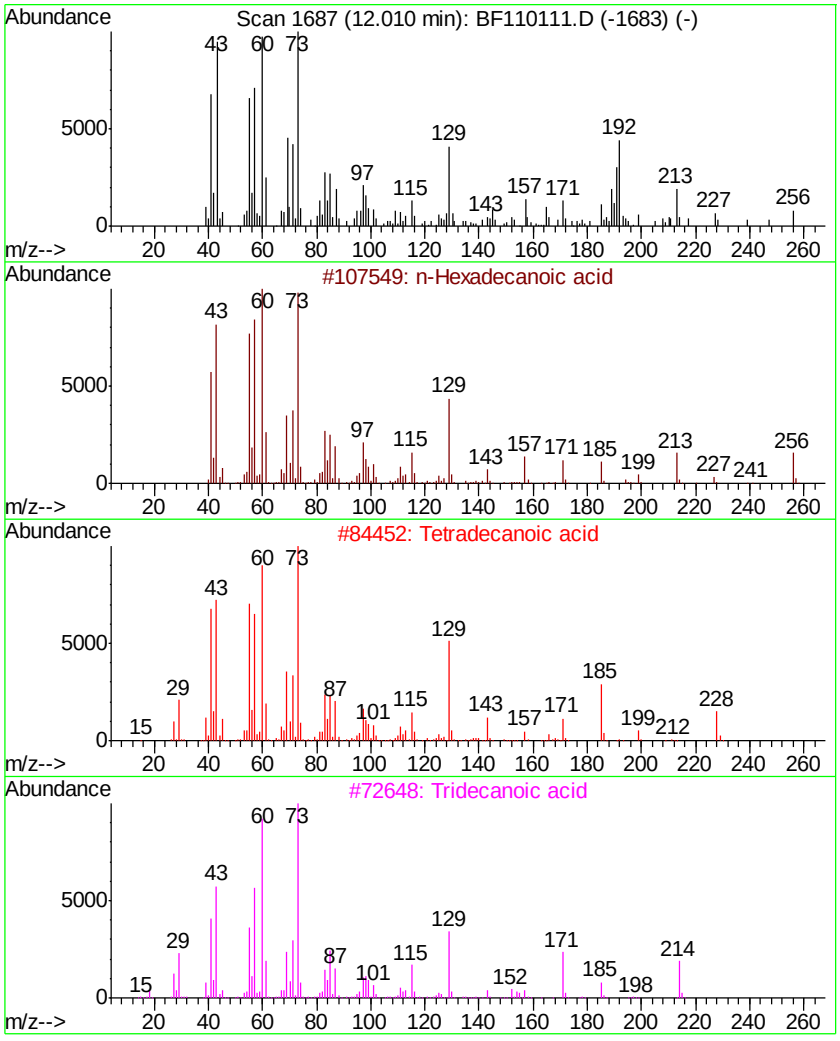
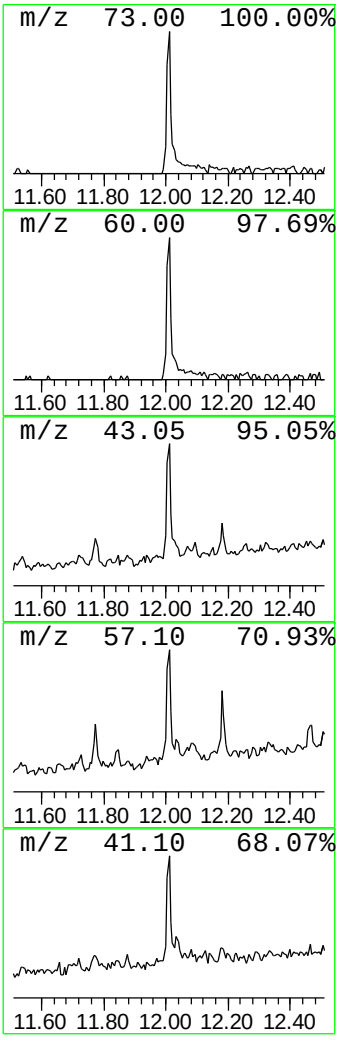
Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.01	3.22 ng	174927	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	78
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF102418\
Data File : BF110111.D
Acq On : 24 Oct 2018 13:31
Operator : JU/SJ
Sample : J5610-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-3(6-8)

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

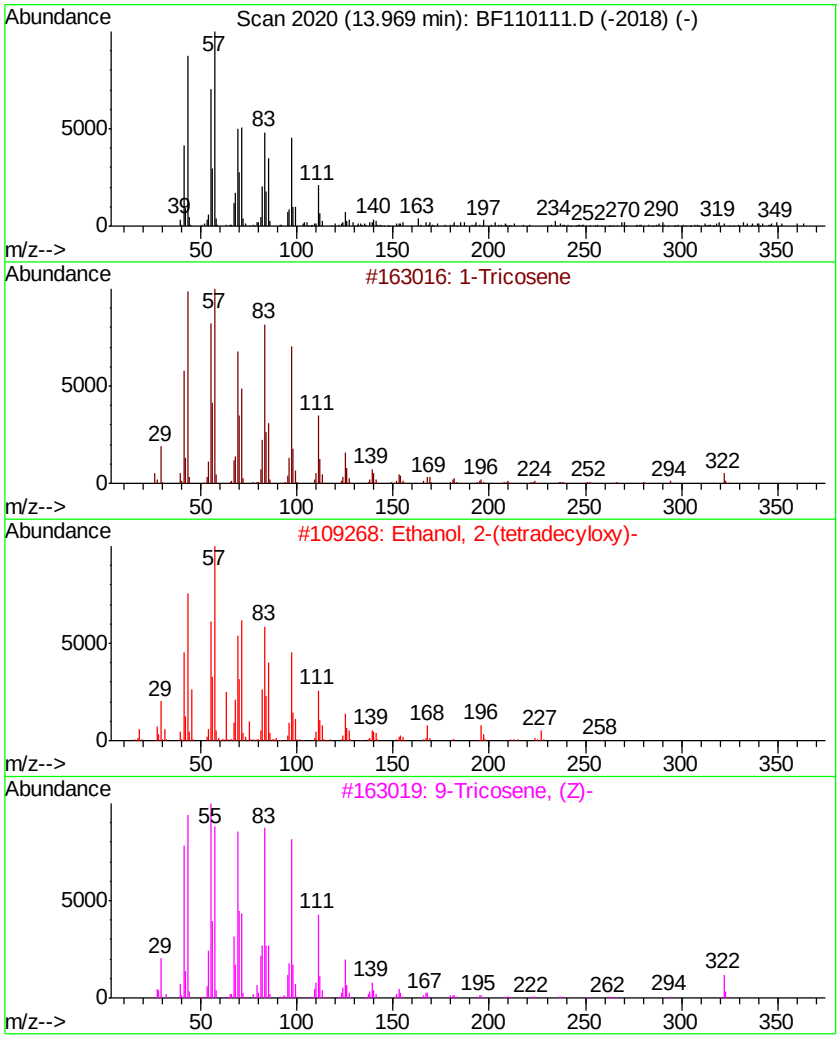
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

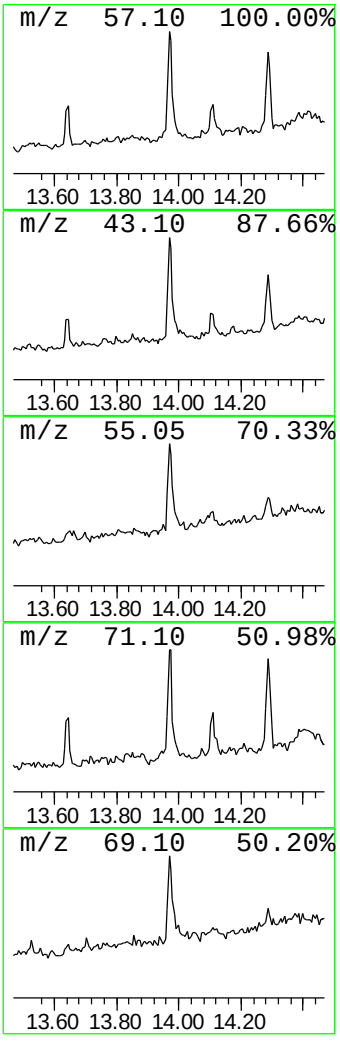
****

Peak Number 6 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	5.99 ng	374164	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	95
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	94
3	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
4	1-Docosene	308	C22H44	001599-67-3	93
5	Octadecane, 1-(ethenyloxy)-	296	C20H40O	000930-02-9	90





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Instrument : BNA_F
ClientSampleId : SB-3(6-8)

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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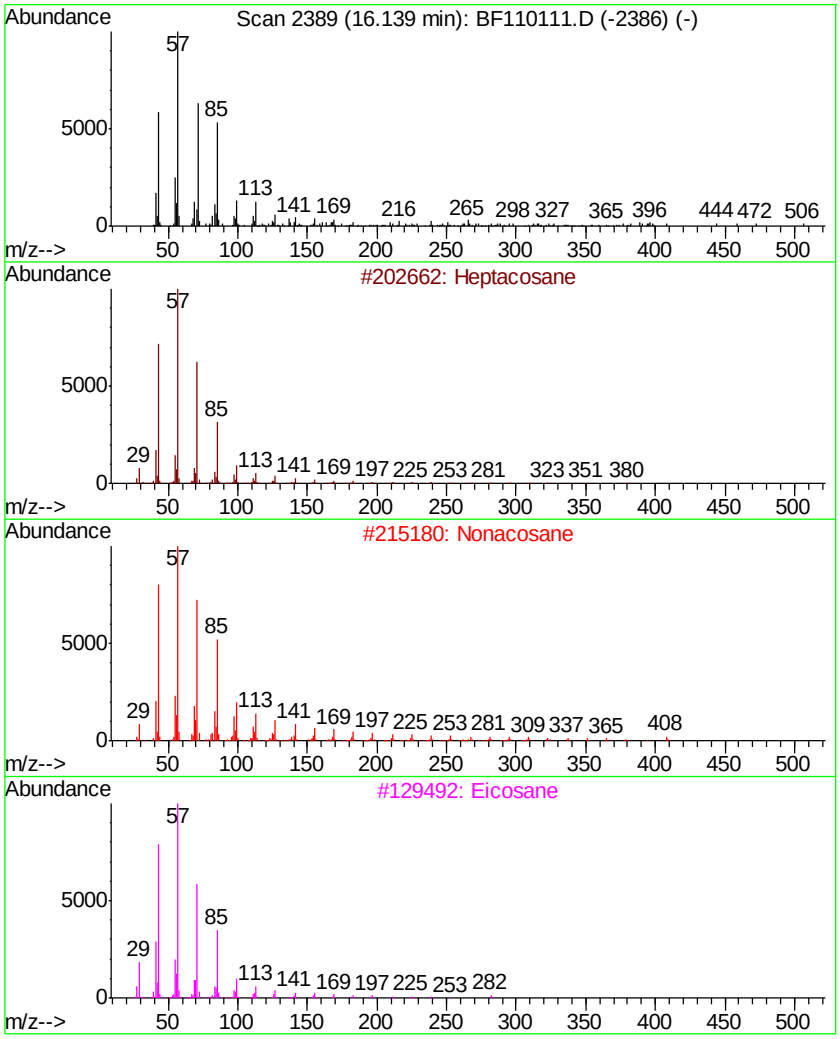
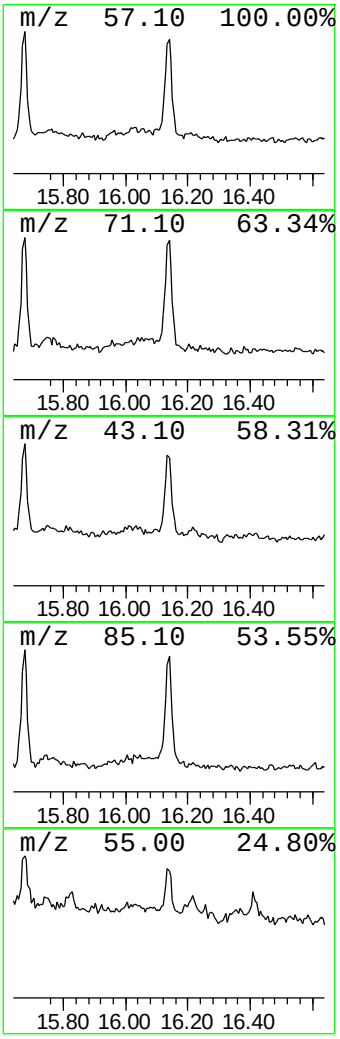
Peak Number 7 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.14	5.92 ng	250226	Perylene-d12	15.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	95
2	Nonacosane	408	C29H60	000630-03-5	93
3	Eicosane	282	C20H42	000112-95-8	91
4	Octadecane, 5,14-dibutyl-	366	C26H54	055282-13-8	83
5	Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	83





Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.31	11.2	ng	614446	1	6.97	1101260	20.0
2-Pentanone, 4-hy...	5.21	3.5	ng	190097	1	6.97	1101260	20.0
unknown6.74	6.74	69.1	ng	3804420	1	6.97	1101260	20.0
n-Hexadecanoic acid	12.01	3.2	ng	174927	4	11.50	1087430	20.0
1-Tricosene	13.97	6.0	ng	374164	5	14.15	1248580	20.0
Heptacosane	16.14	5.9	ng	250226	6	15.67	844700	20.0