LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110618\
Data File : BF110539.D
Acq On : 7 Nov 2018 2:10
Operator : JU/SJ
Sample : J5826-11 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-S

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	2.240	22	26	41	rVB	124623	196262	22.29%	1.921%
2	5.181	523	526	534	rBV	24395	30815	3.50%	0.302%
3	5.575	589	593	609	rBV	724421	760369	86.36%	7.444%
4	6.575	760	763	781	rBV	726427	880440	100.00%	8.619%
5	6.722	785	788	796	rBV	879708	822709	93.44%	8.054%
6	6.957	825	828	835	rBV	528190	450876	51.21%	4.414%
7	7.110	851	854	867	rVB	695833	630567	71.62%	6.173%
8	7.516	920	923	937	rBV	356332	445621	50.61%	4.362%
9	8.239	1042	1046	1068	rVB	469799	533076	60.55%	5.219%
10	9.310	1224	1228	1238	rBV	846850	812274	92.26%	7.952%
11	9.375	1238	1239	1245	rVB2	16012	16599	1.89%	0.162%
12	9.704	1289	1295	1302	rVB	75314	81907	9.30%	0.802%
13	9.857	1318	1321	1326	rBV2	7182	9534	1.08%	0.093%
14	9.904	1326	1329	1334	rVB3	13698	13422	1.52%	0.131%
15	9.998	1341	1345	1358	rVB	534781	519553	59.01%	5.086%
16	10.404	1411	1414	1417	rVB	18996	15571	1.77%	0.152%
17	10.551	1435	1439	1446	rVB3	7812	10547	1.20%	0.103%
18	10.621	1446	1451	1455	rBV3	12391	16026	1.82%	0.157%
19	10.792	1476	1480	1489	rBV	380911	420931	47.81%	4.121%
20	10.880	1491	1495	1500	rBV2	22935	32597	3.70%	0.319%
21	11.098	1529	1532	1535	rVB2	8533	11011	1.25%	0.108%
22	11.127	1535	1537	1541	rBV4	7226	9606	1.09%	0.094%
23	11.327	1568	1571	1573	rBV	28024	21240	2.41%	0.208%
24	11.357	1573	1576	1578	rVB	17469	15177	1.72%	0.149%
25	11.492	1595	1599	1601	rBV	533902	483727	54.94%	4.735%
26	11.516	1601	1603	1607	rVV	125817	115743	13.15%	1.133%
27	11.574	1610	1613	1616	rBV	34658	37748	4.29%	0.370%
28	11.710	1631	1636	1637	rBV5	7891	10559	1.20%	0.103%
29	11.751	1641	1643	1646	rVB	37288	31900	3.62%	0.312%
30	11.916	1667	1671	1674	rBV4	8425	16383	1.86%	0.160%
31	11.992	1681	1684	1687	rBV	44014	50233	5.71%	0.492%
32	12.021	1687	1689	1692	rVV	30816	34045	3.87%	0.333%
33	12.068	1695	1697	1700	rVV2	16658	20940	2.38%	0.205%
34	12.110	1700	1704	1706	rVV	55684	62833	7.14%	0.615%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110618\
Data File : BF110539.D
Acq On : 7 Nov 2018 2:10
Operator : JU/SJ
Sample : J5826-11 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-S

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	12.163	1710	1713	1718	rVB	41408	38472	4.37%	0.377%
36	12.286	1731	1734	1737	rBV	18316	23395	2.66%	0.229%
37	12.439	1758	1760	1763	rVB2	16683	13653	1.55%	0.134%
38	12.468	1763	1765	1768	rBV4	10303	11415	1.30%	0.112%
39	12.545	1774	1778	1782	rBV2	58239	76044	8.64%	0.744%
40	12.710	1802	1806	1809	rBV	256414	223756	25.41%	2.190%
41	12.863	1829	1832	1834	rBV3	16054	16549	1.88%	0.162%
42	12.921	1839	1842	1843	rVV	84335	73075	8.30%	0.715%
43	12.939	1843	1845	1851	rVB	212981	208945	23.73%	2.045%
44	13.068	1863	1867	1871	rBV	806972	701177	79.64%	6.864%
45	13.274	1898	1902	1905	rVB2	53733	71243	8.09%	0.697%
46	13.615	1958	1960	1963	rBV	29542	29884	3.39%	0.293%
47	13.945	2014	2016	2022	rVB3	54193	66753	7.58%	0.653%
48	14.086	2037	2040	2043	rVB	64474	53781	6.11%	0.526%
49	14.139	2044	2049	2052	rBV2	423362	480802	54.61%	4.707%
50	14.739	2148	2151	2155	rVB	243881	222127	25.23%	2.175%
51	15.209	2229	2231	2233	rBV	50934	55926	6.35%	0.547%
52	15.668	2306	2309	2313	rVB	194616	227071	25.79%	2.223%

Sum of corrected areas: 10214909

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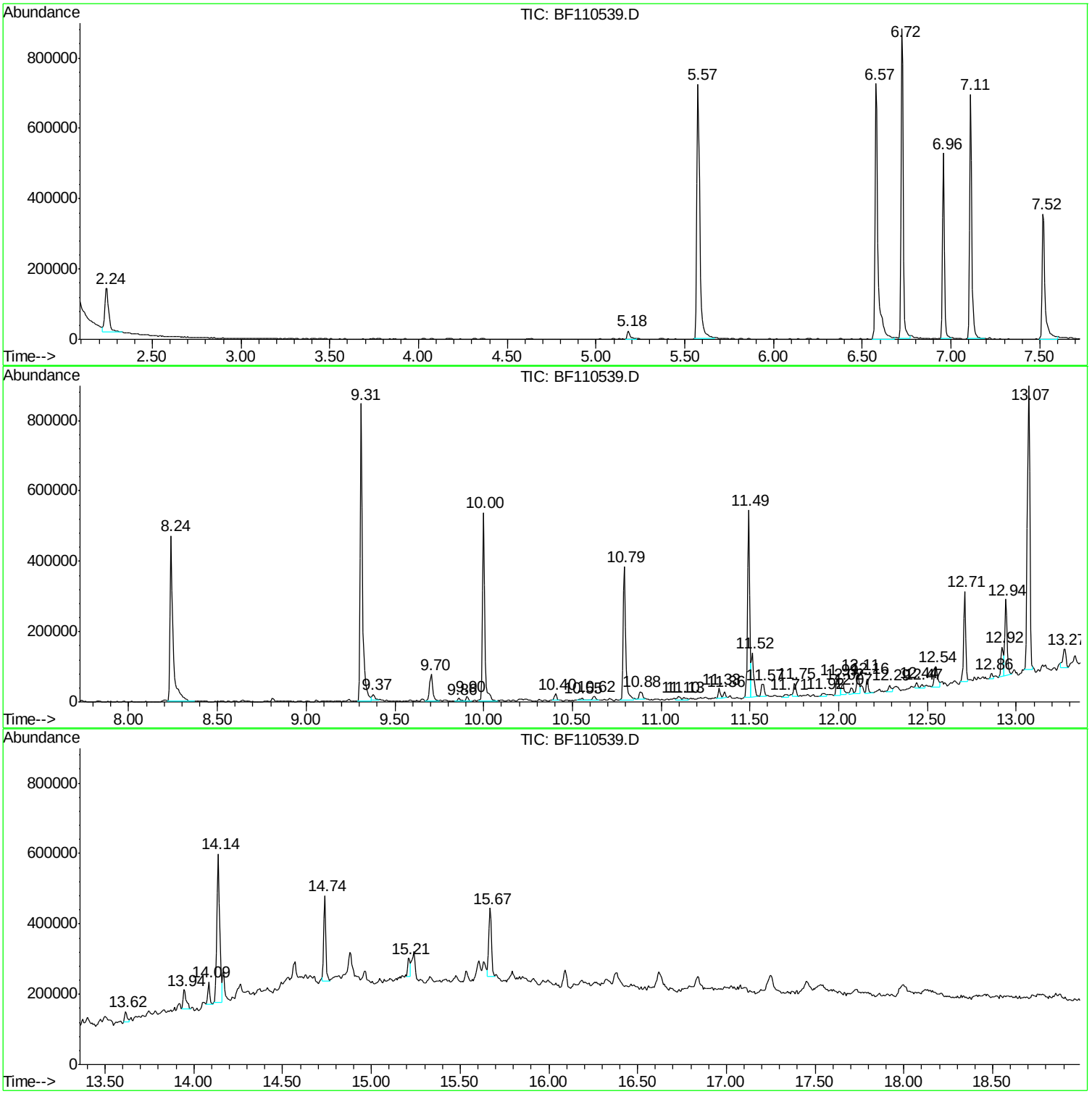
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-S

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\BF110618\
Data File : BF110539.D
Acq On : 7 Nov 2018 2:10
Operator : JU/SJ
Sample : J5826-11 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-S

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

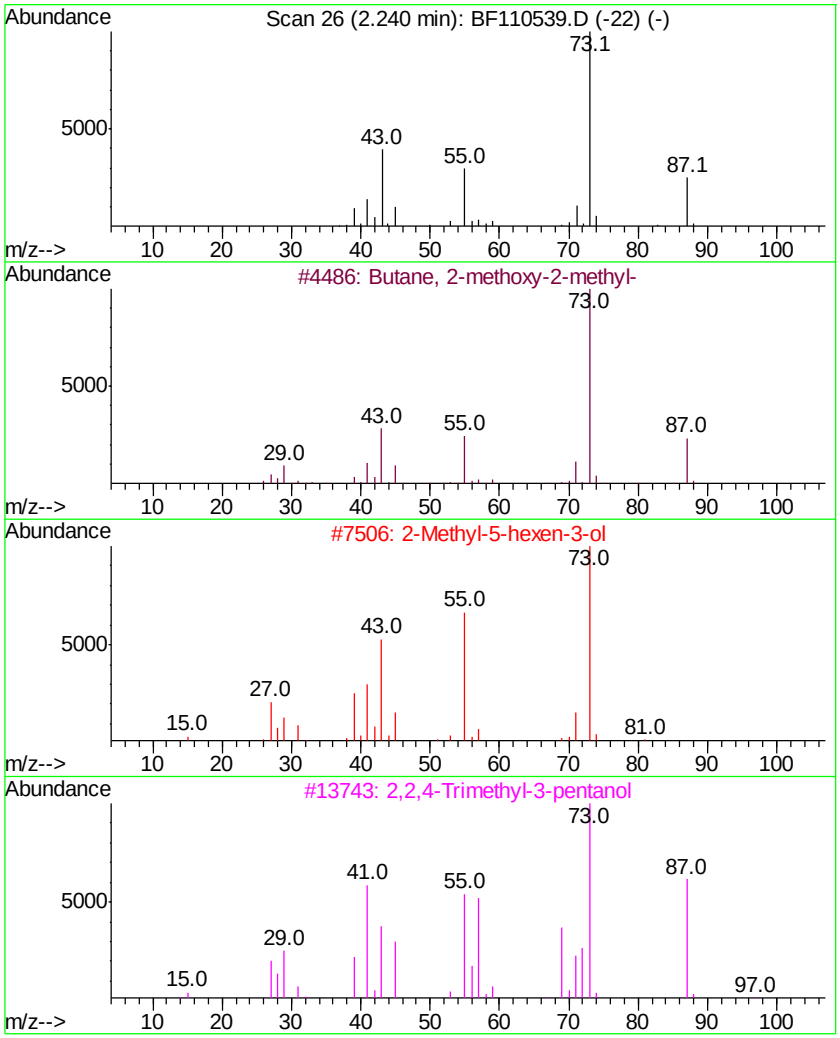
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

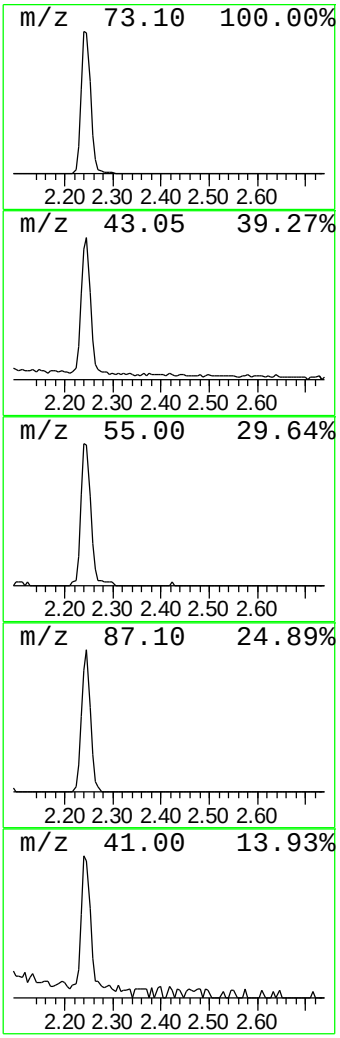
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.24	8.71 ng	196262	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	47
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110618\
Data File : BF110539.D
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Operator : JU/SJ
Sample : J5826-11 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-S

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

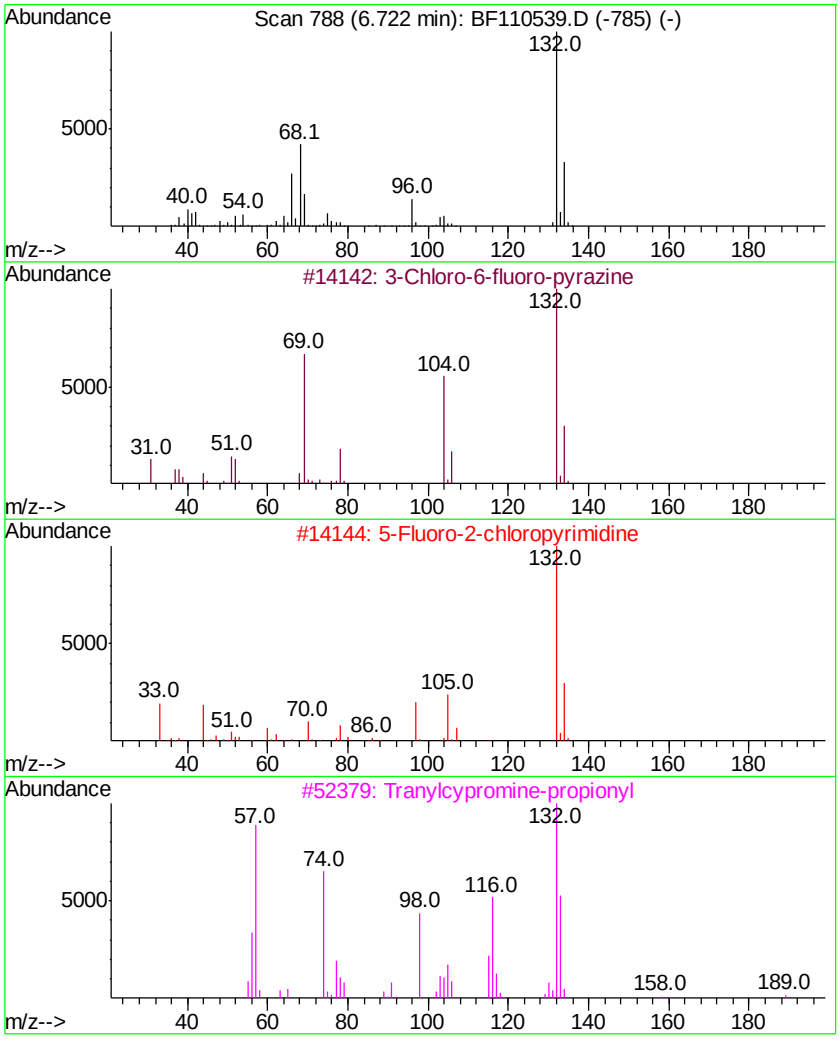
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

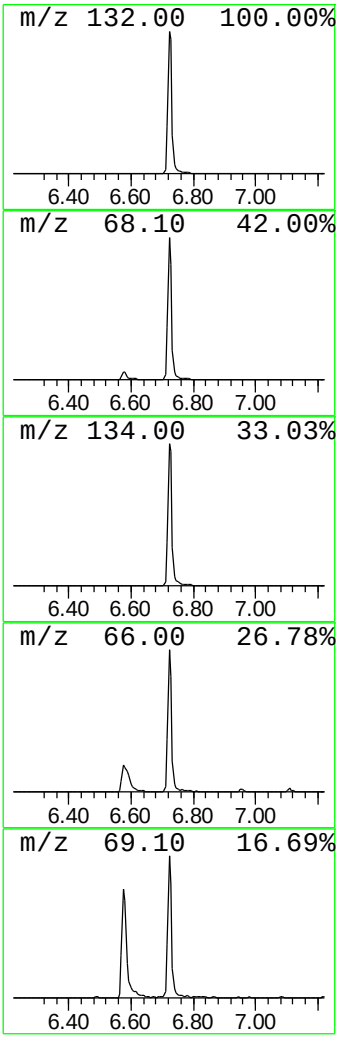
****

Peak Number 2 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	36.49 ng	822709	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110618\
Data File : BF110539.D
Acq On : 7 Nov 2018 2:10
Operator : JU/SJ
Sample : J5826-11 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-S

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

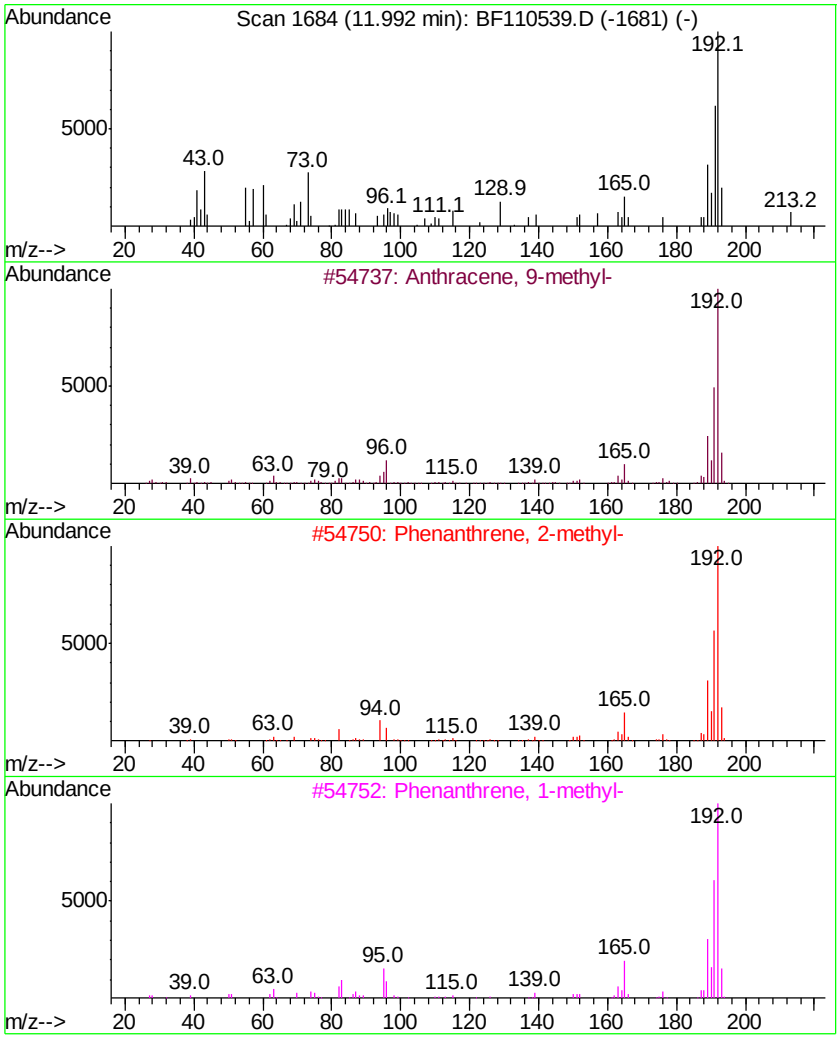
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

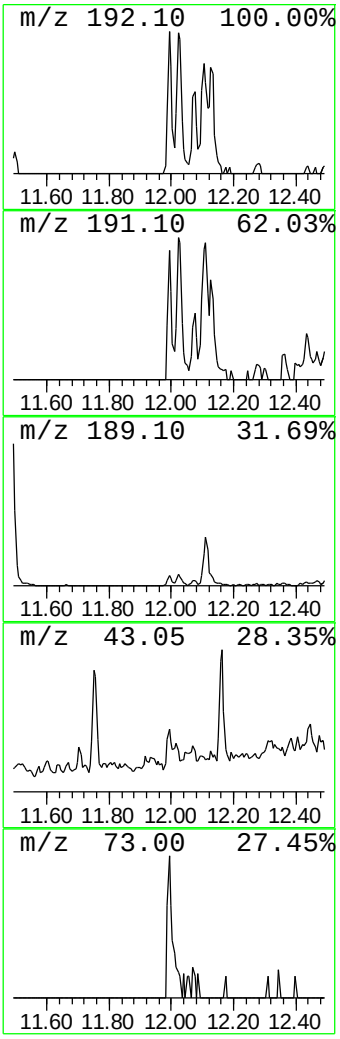
****

Peak Number 4 Anthracene, 9-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.99	2.08 ng	50233	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene, 9-methyl-	192	C15H12	000779-02-2	93
2	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
3	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	78
4	Anthracene, 2-methyl-	192	C15H12	000613-12-7	76
5	Anthracene, 1-methyl-	192	C15H12	000610-48-0	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF110618\
Data File : BF110539.D
Acq On : 7 Nov 2018 2:10
Operator : JU/SJ
Sample : J5826-11 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-S

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

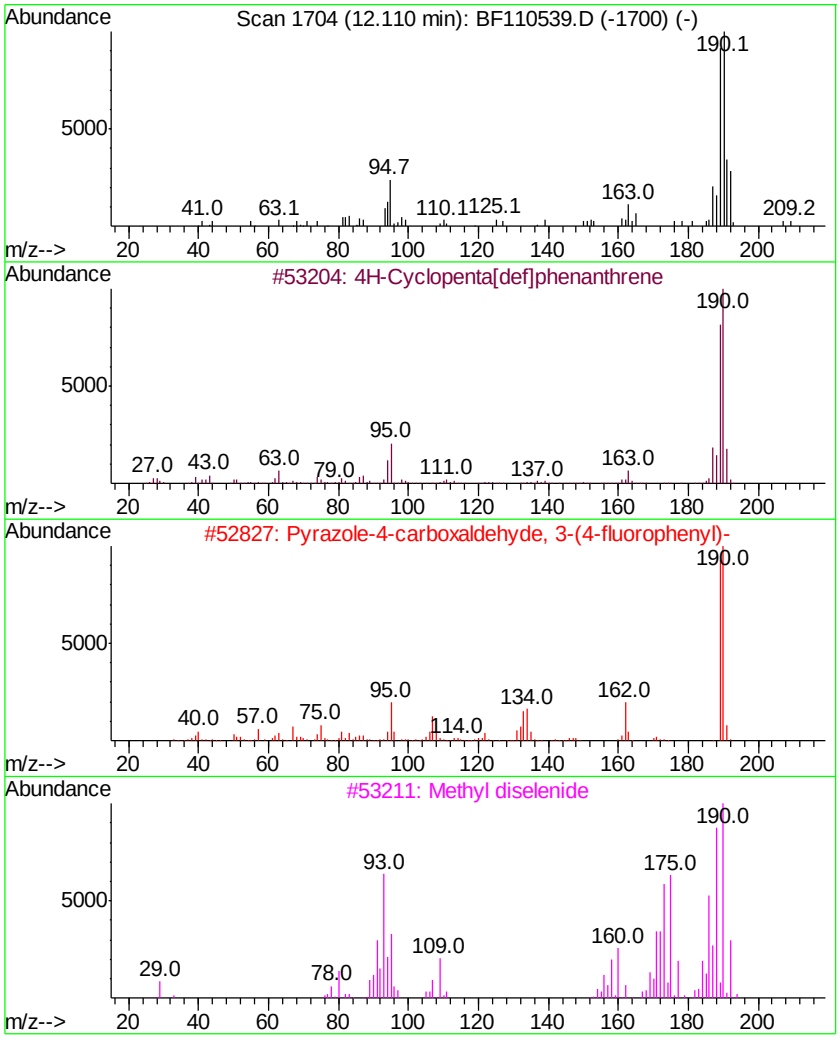
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

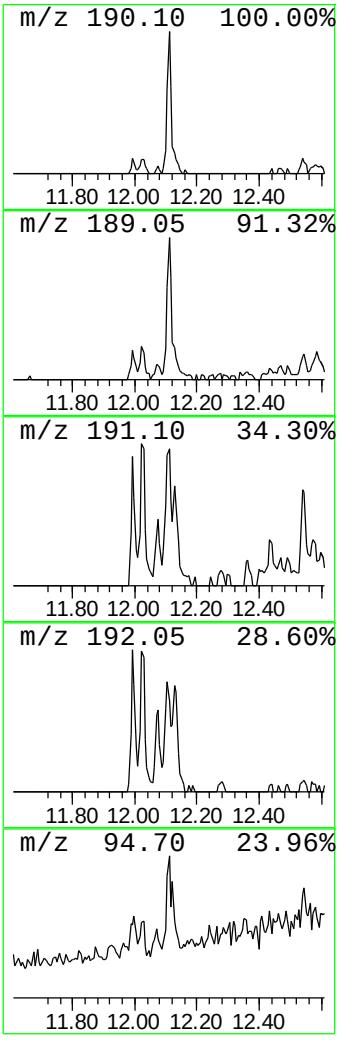
****

Peak Number 5 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.11	2.60 ng	62833	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	81
2	Pyrazole-4-carboxaldehyde, 3-(4-...	190	C10H7FN2O	306936-57-2	52
3	Methyl diselenide	190	C2H6Se2	007101-31-7	46
4	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	23
5	4-Oxo-2-(4-fluorophenyl)-3,4-dih...	190	C10H7FN2O	076128-79-5	17





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Data File : BF110539.D
Acq On : 7 Nov 2018 2:10
Operator : JU/SJ
Sample : J5826-11 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-S

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

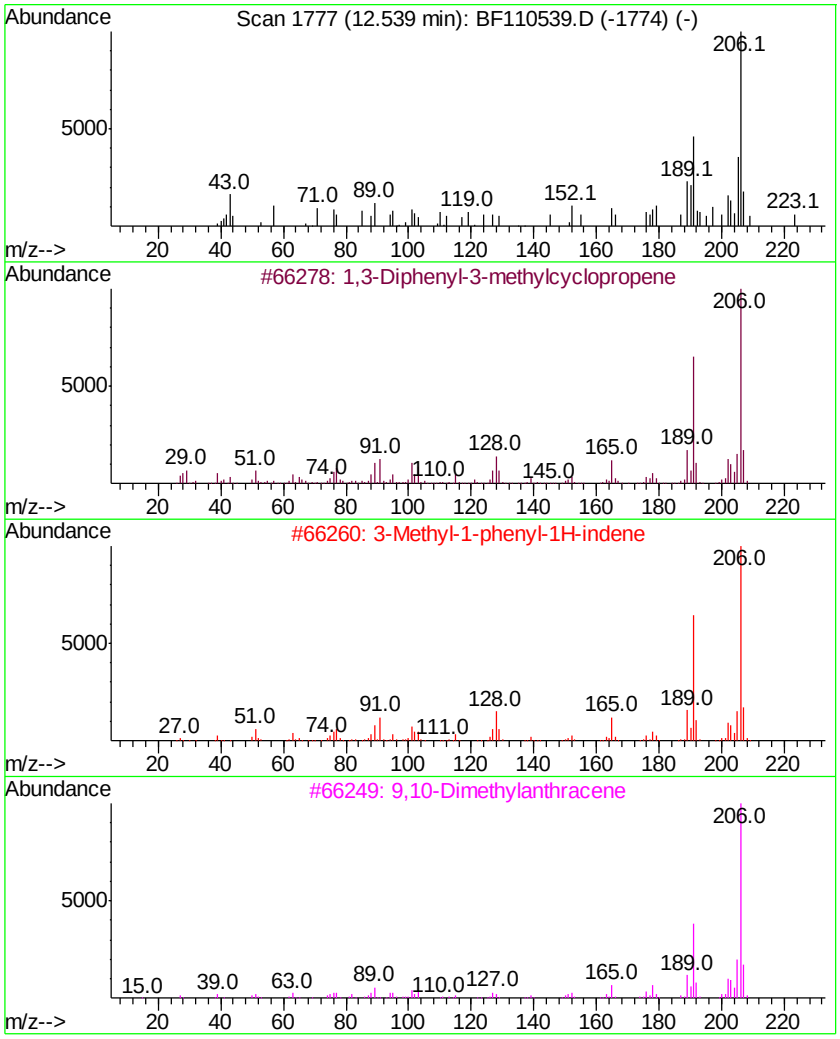
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

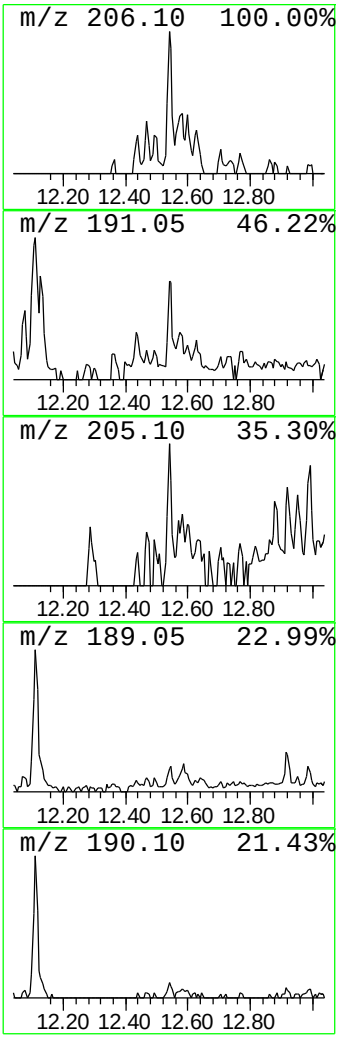
****

Peak Number 6 1,3-Diphenyl-3-methylcyclop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	3.14 ng	76044	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	90
2	3-Methyl-1-phenyl-1H-indene	206	C16H14	022360-63-0	87
3	9,10-Dimethylanthracene	206	C16H14	000781-43-1	78
4	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	64
5	1-Methyl-3-phenyl-1H-indene	206	C16H14	022360-62-9	60





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Acq On : 7 Nov 2018 2:10
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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-S

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

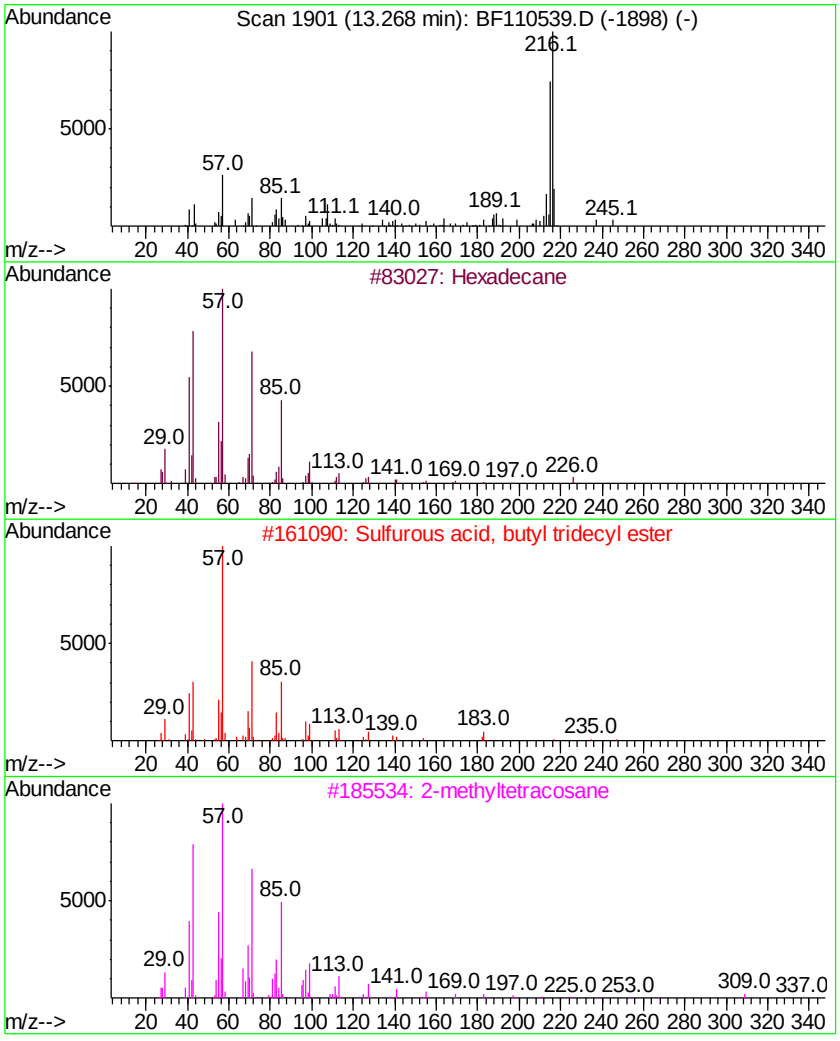
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

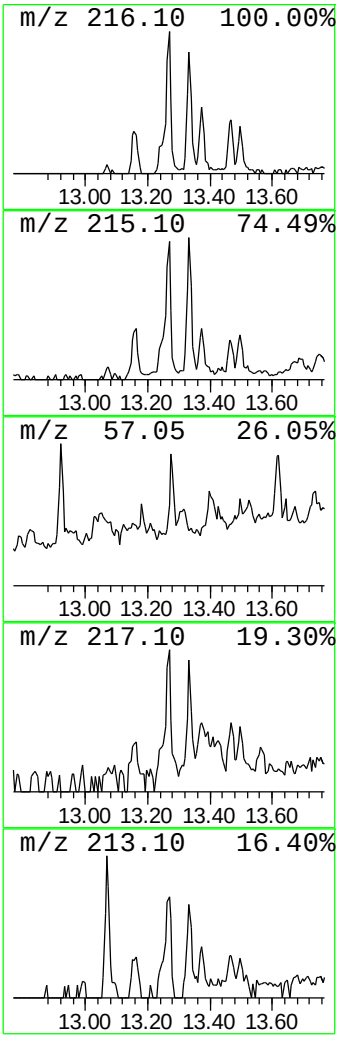
****

Peak Number 7 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	2.96 ng	71243	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	66
2	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	38
3	2-methyltetracosane	352	C25H52	1000376-72-6	38
4	Tetradecane	198	C14H30	000629-59-4	38
5	Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	38





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Sample : J5826-11 2X
Misc :
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Instrument : BNA_F
ClientSampleId : SB-S

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

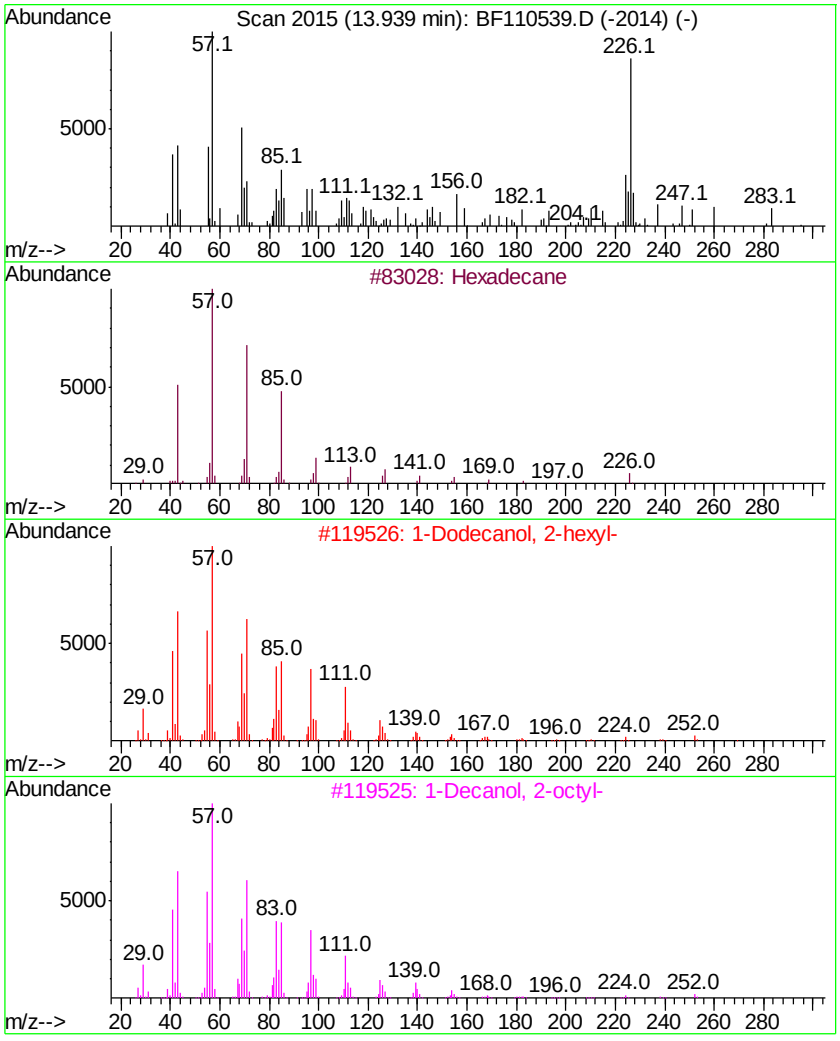
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

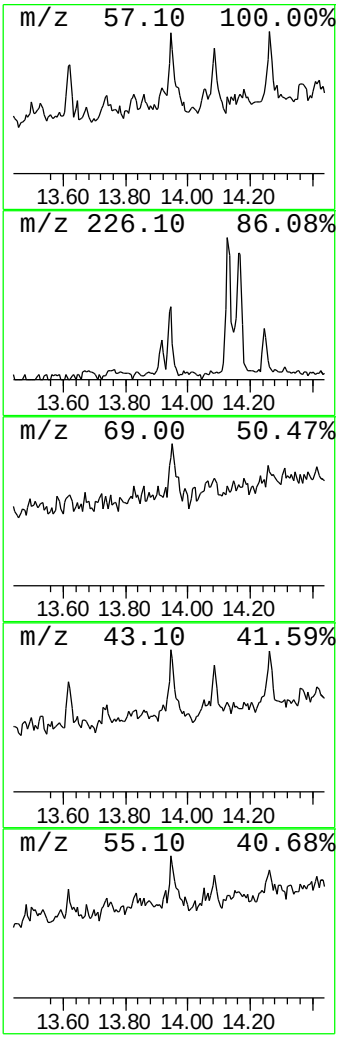
****

Peak Number 8 unknown13.94 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	2.78 ng	66753	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	50
2	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	43
3	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	43
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	38
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF110618\
Data File : BF110539.D
Acq On : 7 Nov 2018 2:10
Operator : JU/SJ
Sample : J5826-11 2X
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-S

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...	2.24	8.7	ng	196262	1	6.96	450876	20.0
unknown6.72	6.72	36.5	ng	822709	1	6.96	450876	20.0
Anthracene, 9-met...	11.99	2.1	ng	50233	4	11.49	483727	20.0
4H-Cyclopenta[def...	12.11	2.6	ng	62833	4	11.49	483727	20.0
1,3-Diphenyl-3-me...	12.54	3.1	ng	76044	4	11.49	483727	20.0
Hexadecane	13.27	3.0	ng	71243	5	14.14	480802	20.0
unknown13.94	13.94	2.8	ng	66753	5	14.14	480802	20.0