LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	4.928	481	483	503	rBV2	28066	75438	5.42%	0.596%
2	5.369	555	558	585	rBV2	88690	284234	20.41%	2.246%
3	6.387	729	731	746	rBV2	105240	236565	16.98%	1.869%
4	6.492	746	749	769	rVB	464604	705544	50.65%	5.575%
5	6.710	783	786	798	rBV	490842	510159	36.63%	4.031%
6	6.863	809	812	827	rBV	850534	869989	62.46%	6.875%
7	7.287	881	884	908	rBV	474457	667403	47.92%	5.274%
8	7.992	1001	1004	1018	rBV	753170	795340	57.10%	6.285%
9	8.204	1037	1040	1046	rBV3	11371	22887	1.64%	0.181%
10	8.563	1098	1101	1110	rVB	35955	34937	2.51%	0.276%
11	8.633	1110	1113	1118	rBV3	14646	24957	1.79%	0.197%
12	8.716	1125	1127	1135	rBV	36704	41695	2.99%	0.329%
13	8.810	1140	1143	1153	rVB	67805	73468	5.27%	0.581%
14	9.063	1182	1186	1195	rVB	1622668	1392881	100.00%	11.007%
15	9.181	1202	1206	1215	rVB	36849	43192	3.10%	0.341%
16	9.469	1252	1255	1261	rVB	201588	176811	12.69%	1.397%
17	9.739	1298	1301	1305	rBV	872549	843214	60.54%	6.663%
18	9.775	1305	1307	1315	rVB	216315	239280	17.18%	1.891%
19	9.863	1318	1322	1328	rBV	16287	25009	1.80%	0.198%
20	9.963	1336	1339	1351	rVB	121239	147357	10.58%	1.164%
21	10.057	1351	1355	1363	rBV4	9085	16740	1.20%	0.132%
22	10.298	1394	1396	1404	rBV	148252	155687	11.18%	1.230%
23	10.457	1421	1423	1428	rBV	146420	132202	9.49%	1.045%
24	10.539	1434	1437	1451	rBV	514477	571209	41.01%	4.514%
25	10.680	1458	1461	1463	rBV	22613	23449	1.68%	0.185%
26	11.039	1519	1522	1524	rBV	48504	43307	3.11%	0.342%
27	11.063	1524	1526	1536	rVB	113214	137757	9.89%	1.089%
28	11.233	1552	1555	1559	rBV	959144	898035	64.47%	7.097%
29	11.263	1559	1560	1568	rVV	102976	113311	8.14%	0.895%
30	11.333	1568	1572	1579	rVB2	21301	32387	2.33%	0.256%
31	11.445	1587	1591	1598	rVB2	44382	47905	3.44%	0.379%
32	11.498	1598	1600	1607	rBV	38715	50328	3.61%	0.398%
33	11.751	1640	1643	1647	rBV	167443	165482	11.88%	1.308%
34	11.780	1647	1648	1655	rVB3	16879	26570	1.91%	0.210%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.992	1681	1684	1687	rVB	52784	41158	2.95%	0.325%
36	12.439	1757	1760	1763	rBV4	16701	20866	1.50%	0.165%
37	12.469	1763	1765	1771	rVB	45681	45825	3.29%	0.362%
38	12.533	1773	1776	1785	rVV	76270	80416	5.77%	0.635%
39	12.621	1788	1791	1793	rBV	46799	39793	2.86%	0.314%
40	12.698	1801	1804	1811	rVB2	32890	39738	2.85%	0.314%
41	12.816	1820	1824	1832	rVB	1291782	1262634	90.65%	9.978%
42	13.321	1907	1910	1914	rVB2	38979	30183	2.17%	0.239%
43	13.692	1969	1973	1981	rBV	198003	216431	15.54%	1.710%
44	13.886	2003	2006	2020	rBV	583822	646174	46.39%	5.106%
45	14.315	2075	2079	2088	rBV2	16507	25906	1.86%	0.205%
46	14.674	2137	2140	2144	rVB	108051	106370	7.64%	0.841%
47	14.921	2178	2182	2185	rBV	20427	19409	1.39%	0.153%
48	15.333	2248	2252	2269	rBV	246456	415660	29.84%	3.285%
49	15.668	2303	2309	2314	rBV5	11764	20580	1.48%	0.163%
50	15.721	2314	2318	2325	rBV5	9337	18529	1.33%	0.146%

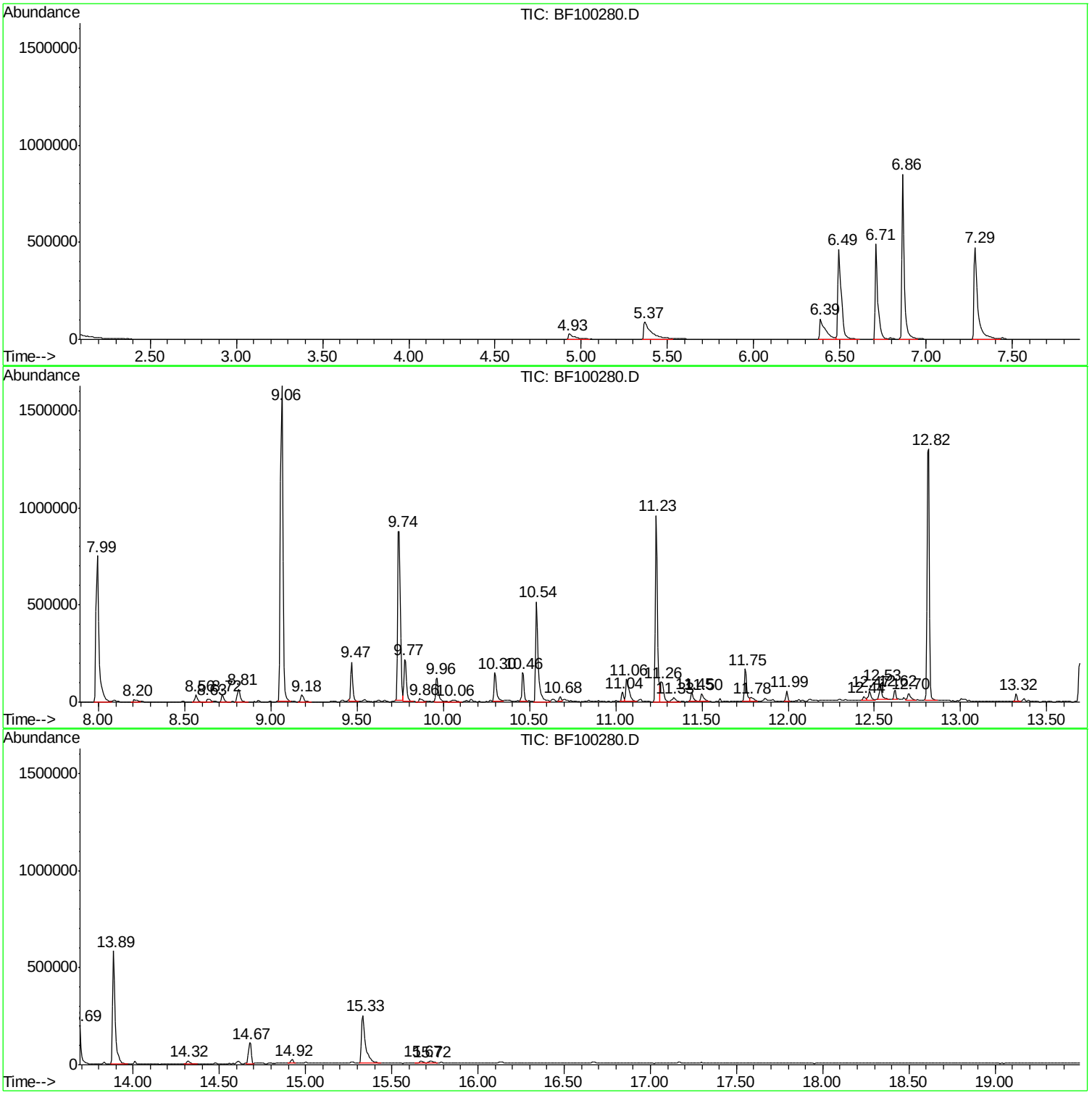
Sum of corrected areas: 12654401

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

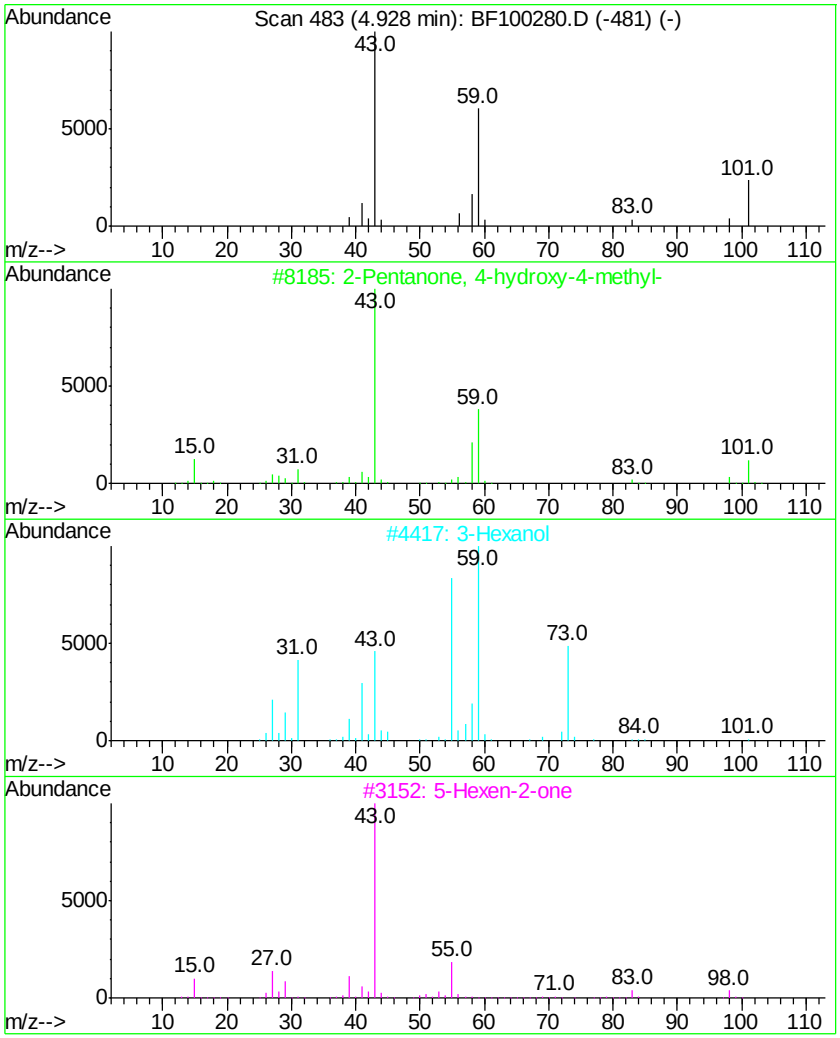
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

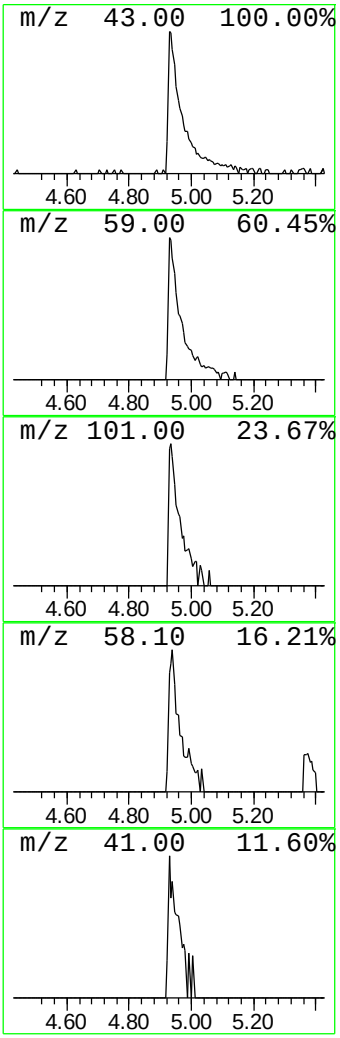
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	2.96 ng	75438	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	3-Hexanol	102	C6H14O	000623-37-0	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

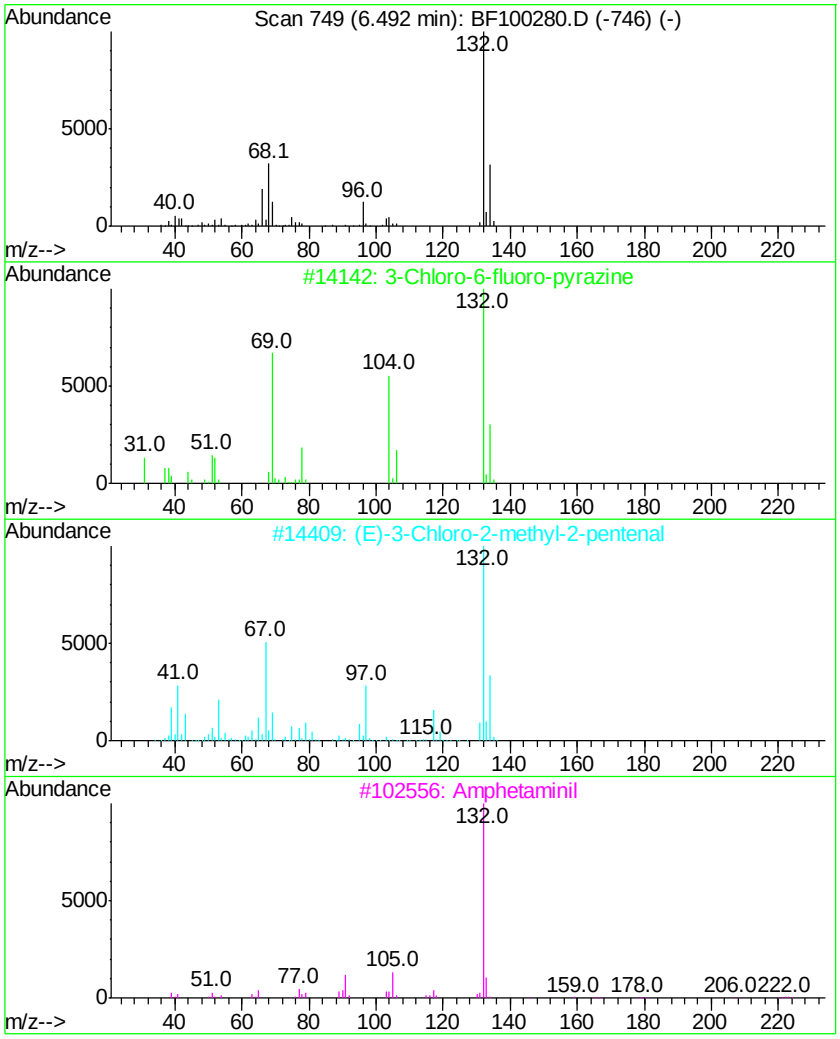
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

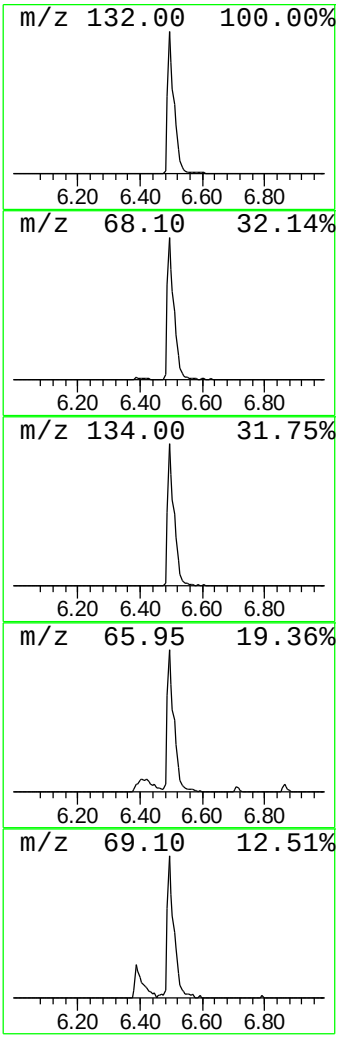
****

Peak Number 2 unknown6.49 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	27.66 ng	705544	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

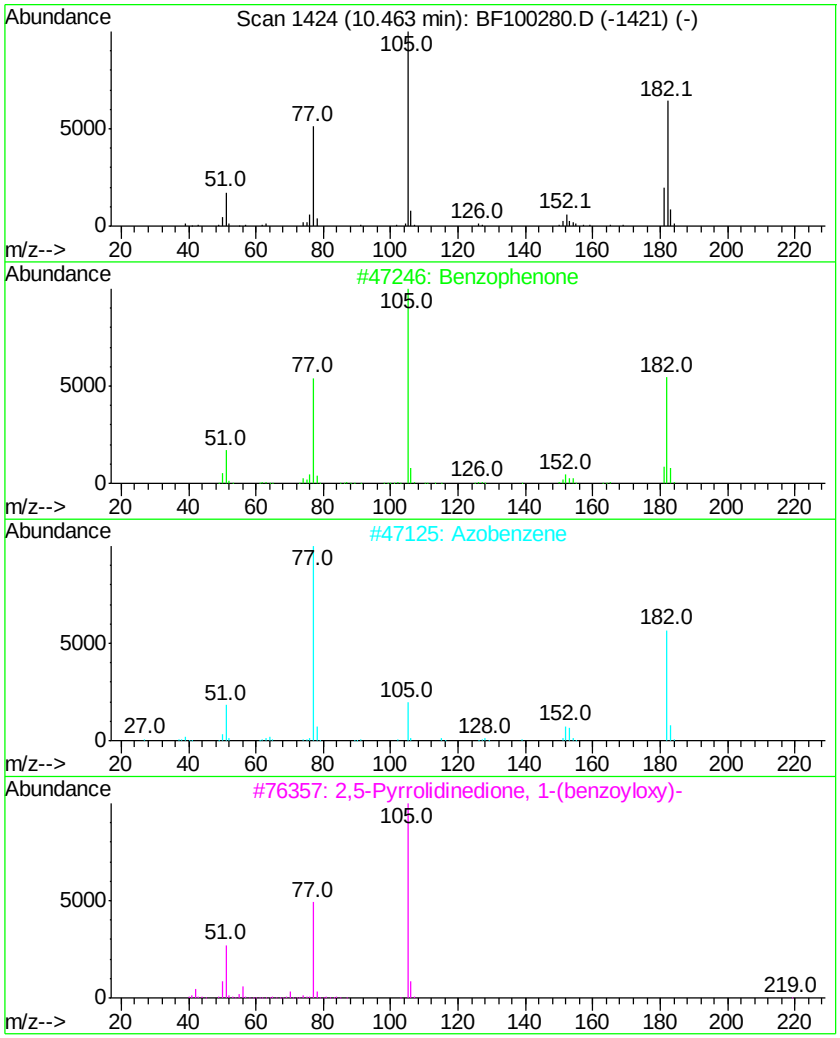
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

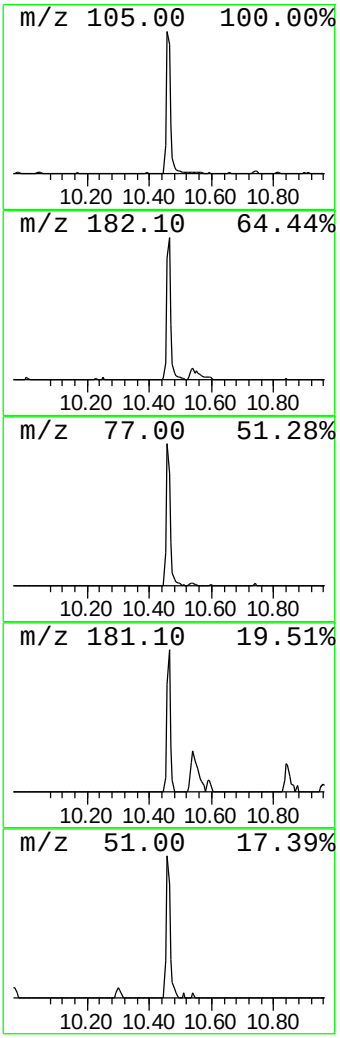
****

Peak Number 4 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.46	3.14 ng	132202	Acenaphthene-d10	9.74

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	2,5-Pyrrolidinedione, 1-(benzoyl...	219	C11H9NO4	023405-15-4	43
4	Butanenitrile, 2,3-bis(benzoylox...	335	C18H13N3O4	1000269-66-6	43
5	Benzoylformic acid	150	C8H6O3	000611-73-4	43





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

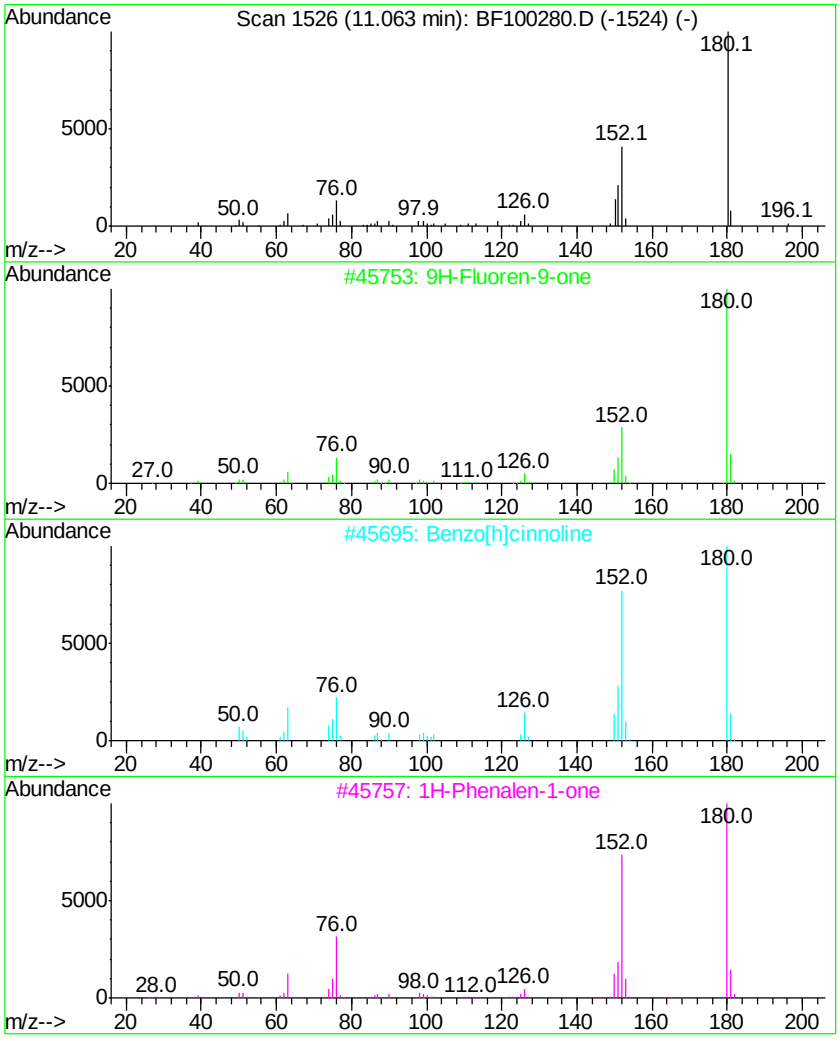
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

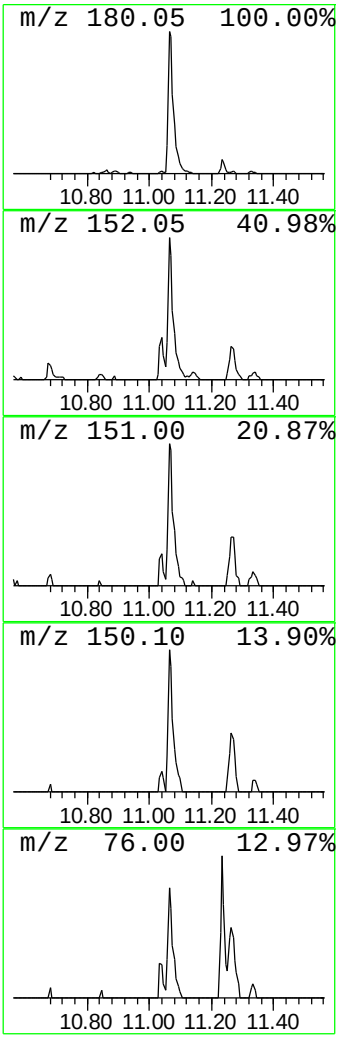
****

Peak Number 5 9H-Fluoren-9-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.06	3.07 ng	137757	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluoren-9-one	180	C13H8O	000486-25-9	91
2	Benzo[h]cinnoline	180	C12H8N2	000230-31-9	86
3	1H-Phenalen-1-one	180	C13H8O	000548-39-0	49
4	5-Methoxy-4-methyl-2,1,3-benzoth...	180	C8H8N2OS	089976-68-1	47
5	7-Nitro-3H-imidazo[4,5-b]pyridin...	180	C6H4N4O3	014432-11-2	25





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

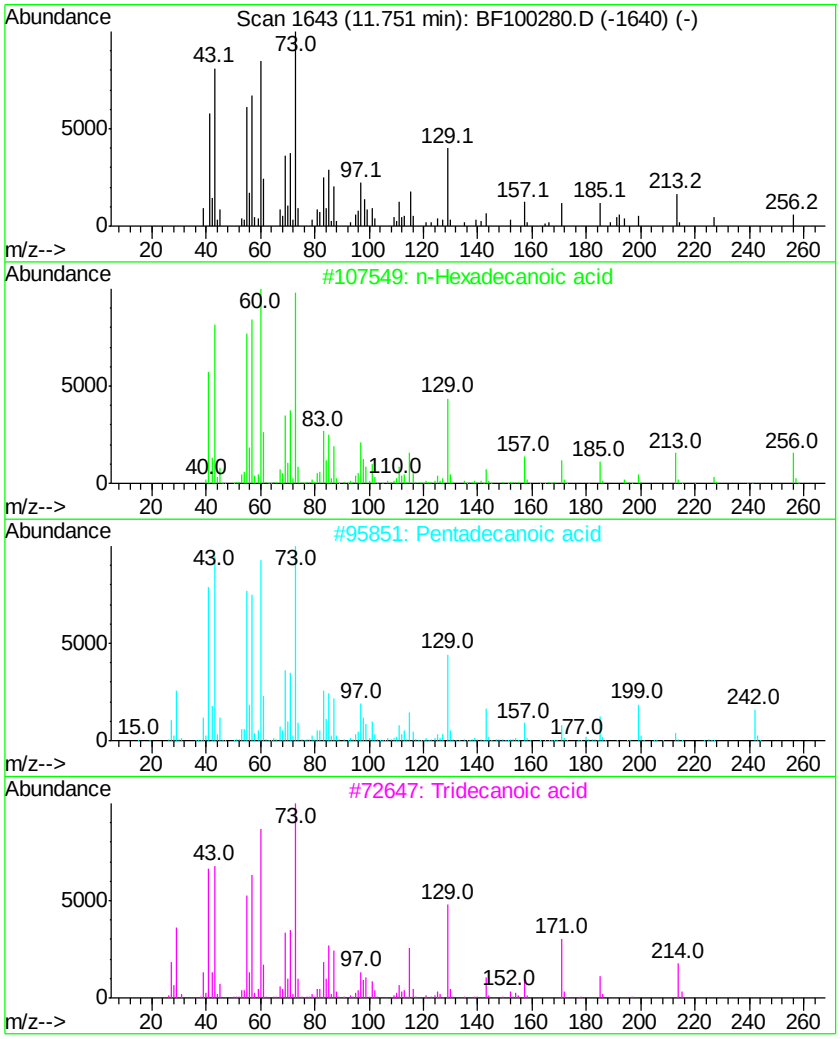
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

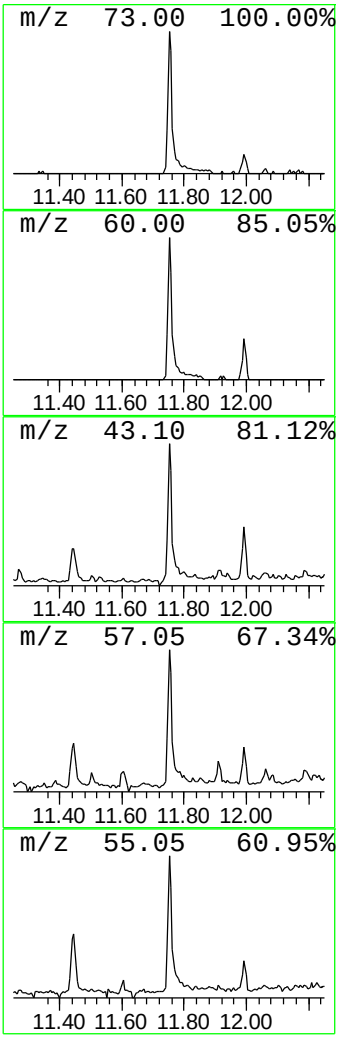
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	3.69 ng	165482	Phenanthrene-d10	11.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Tridecanoic acid	214	C13H26O2	000638-53-9	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Trehalose	342	C12H22O11	000099-20-7	47





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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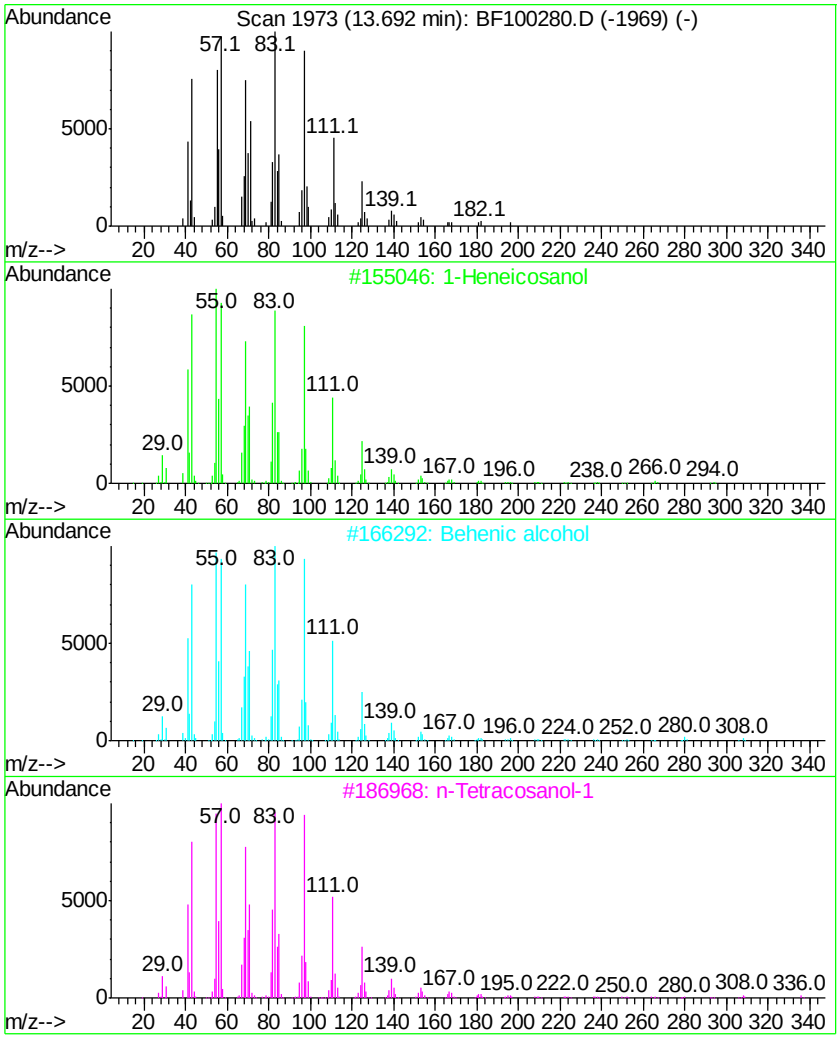
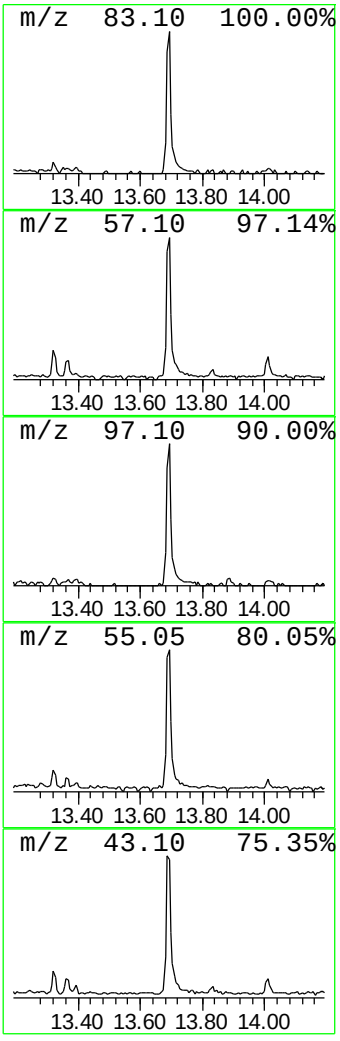
Peak Number 7 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	6.70 ng	216431	Chrysene-d12	13.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4	1-Heptacosanol	396	C27H56O	002004-39-9	93
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

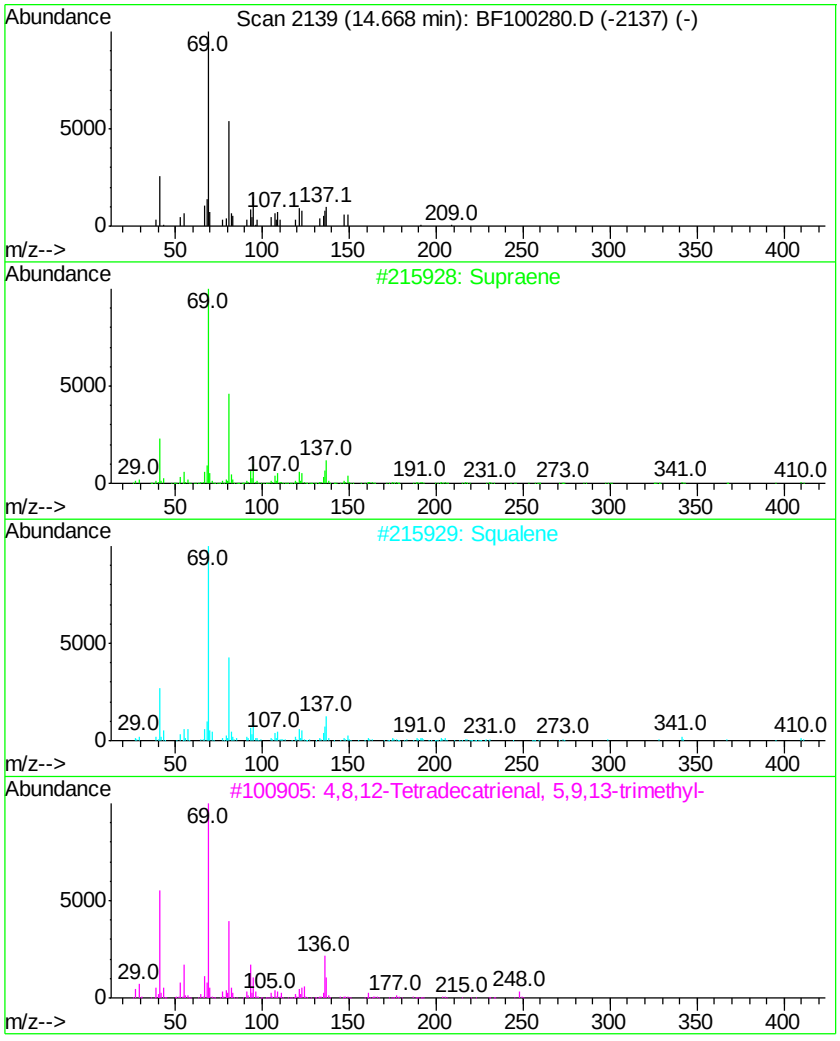
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

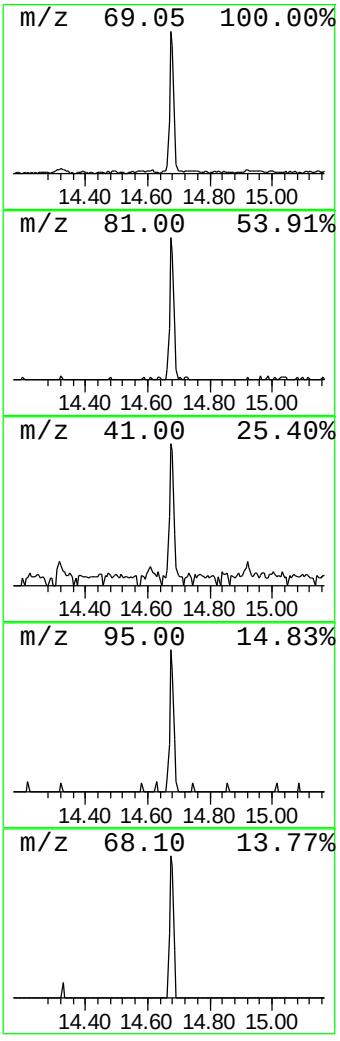
****

Peak Number 8 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	5.12 ng	106370	Perylene-d12	15.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Squalene	410	C30H50	000111-02-4	91
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	47
5	Nerolidol 1	222	C15H26O	1000285-43-5	45





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF110717\
Data File : BF100280.D
Acq On : 7 Nov 2017 13:22
Operator : SJ/JU
Sample : I6336-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CF-1B(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	4.93	3.0	ng	75438	1	6.71	510159	20.0
unknown6.49	6.49	27.7	ng	705544	1	6.71	510159	20.0
Benzophenone	10.46	3.1	ng	132202	3	9.74	843214	20.0
9H-Fluoren-9-one	11.06	3.1	ng	137757	4	11.23	898035	20.0
n-Hexadecanoic acid	11.75	3.7	ng	165482	4	11.23	898035	20.0
1-Heneicosanol	13.69	6.7	ng	216431	5	13.89	646174	20.0
Supraene	14.67	5.1	ng	106370	6	15.33	415660	20.0