LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF122118\
Data File : BF111701.D
Acq On : 21 Dec 2018 21:36
Operator : JU/SJ
Sample : J6192-03 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-01-122018

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-BF121918.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	2.181	11	16	21	rVB	55567	73873	4.01%	0.362%
2	5.116	511	515	521	rVB	95015	101539	5.51%	0.498%
3	5.528	581	585	589	rBV	1785333	1687213	91.55%	8.273%
4	6.192	694	698	705	rVB	117289	103569	5.62%	0.508%
5	6.533	752	756	761	rBV	1937352	1842881	100.00%	9.037%
6	6.610	766	769	772	rVB	34219	29274	1.59%	0.144%
7	6.675	776	780	783	rBV	2127239	1751919	95.06%	8.591%
8	6.904	815	819	822	rBV	1046382	888955	48.24%	4.359%
9	7.057	841	845	849	rBV	1648199	1318498	71.55%	6.465%
10	7.457	909	913	916	rBV	1311460	1041814	56.53%	5.109%
11	8.180	1033	1036	1040	rBV	1178645	1049885	56.97%	5.148%
12	9.257	1215	1219	1222	rBV	2219848	1622442	88.04%	7.956%
13	9.645	1282	1285	1291	rVB	232232	193990	10.53%	0.951%
14	9.939	1331	1335	1339	rVB	1294894	1052845	57.13%	5.163%
15	10.139	1362	1369	1374	rVB7	12621	26647	1.45%	0.131%
16	10.727	1465	1469	1472	rBV	1272441	1155067	62.68%	5.664%
17	10.845	1486	1489	1495	rVB4	22555	37326	2.03%	0.183%
18	10.969	1507	1510	1513	rVB2	22694	23598	1.28%	0.116%
19	11.292	1559	1565	1567	rBV4	20336	26241	1.42%	0.129%
20	11.321	1567	1570	1573	rVB2	21958	23231	1.26%	0.114%
21	11.421	1584	1587	1590	rBV	1160573	1112283	60.36%	5.454%
22	11.445	1590	1591	1595	rVV	231799	165703	8.99%	0.813%
23	11.498	1598	1600	1603	rVB	63163	52008	2.82%	0.255%
24	11.645	1621	1625	1628	rBV2	34348	43235	2.35%	0.212%
25	11.721	1634	1638	1640	rBV2	23823	23910	1.30%	0.117%
26	11.816	1652	1654	1662	rBV7	19800	24676	1.34%	0.121%
27	11.927	1670	1673	1674	rBV	36865	33079	1.79%	0.162%
28	11.951	1674	1677	1681	rVB2	94161	103738	5.63%	0.509%
29	12.004	1683	1686	1689	rBV2	23773	27224	1.48%	0.133%
30	12.039	1689	1692	1694	rBV2	54926	53662	2.91%	0.263%
31	12.221	1720	1723	1724	rBV	32263	29824	1.62%	0.146%
32	12.468	1762	1765	1768	rBV3	44225	59128	3.21%	0.290%
33	12.504	1768	1771	1772	rBV2	47664	47029	2.55%	0.231%
34	12.633	1790	1793	1797	rBV	386011	360182	19.54%	1.766%

LSC Area Percent Report

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HD-01-122018

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
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Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.862	1827	1832	1835	rBV	340720	384260	20.85%	1.884%
36	13.004	1853	1856	1860	rVB	1717688	1546745	83.93%	7.585%
37	13.898	2005	2008	2015	rBV3	190633	252581	13.71%	1.239%
38	14.062	2031	2036	2039	rBV2	1141411	1158205	62.85%	5.679%
39	14.086	2039	2040	2043	rVB	121683	68496	3.72%	0.336%
40	14.533	2114	2116	2121	rVB	201528	197407	10.71%	0.968%
41	15.545	2285	2288	2292	rVB	519874	599177	32.51%	2.938%

Sum of corrected areas: 20393359

LSC Report - Integrated Chromatogram

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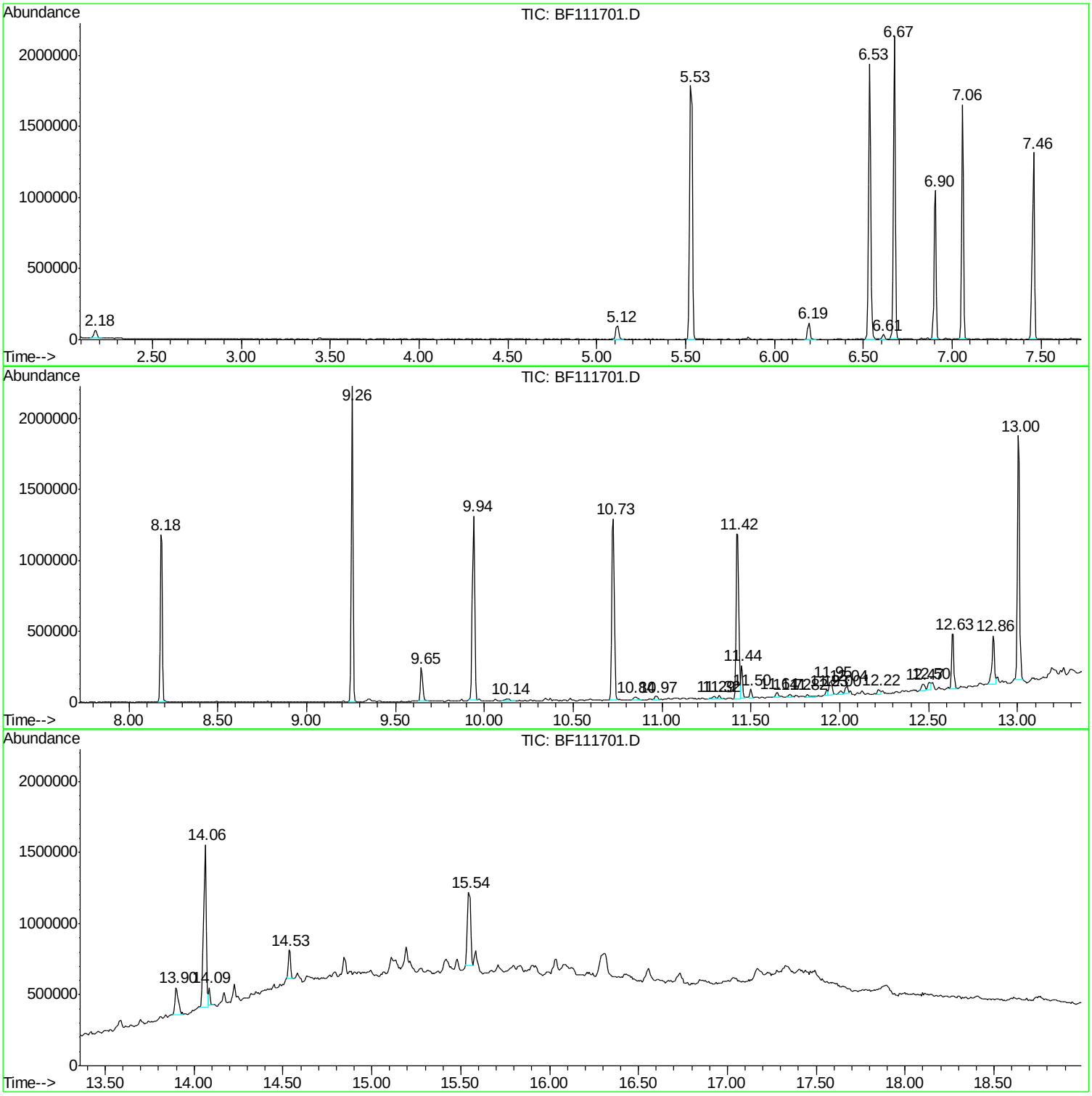
Sample : J6192-03 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-01-122018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.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\BF122118\
Data File : BF111701.D
Acq On : 21 Dec 2018 21:36
Operator : JU/SJ
Sample : J6192-03 2X
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HD-01-122018

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

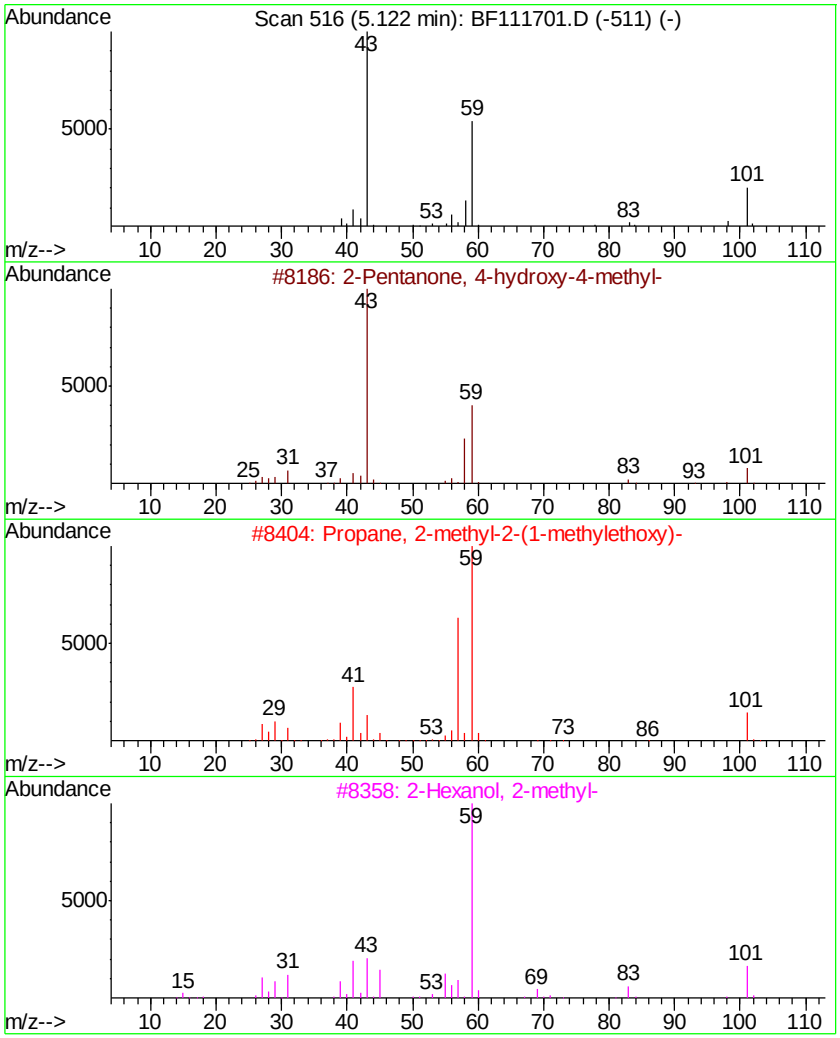
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

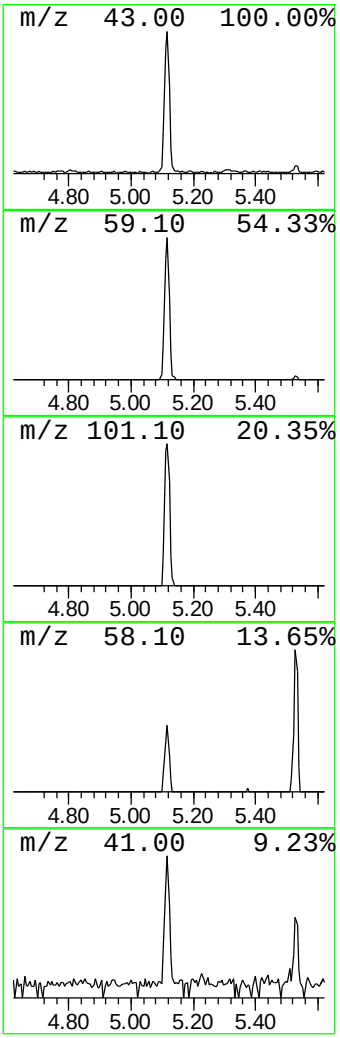
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	2.28 ng	101539	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	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	1,2-Butanediol	90	C4H10O2	000584-03-2	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

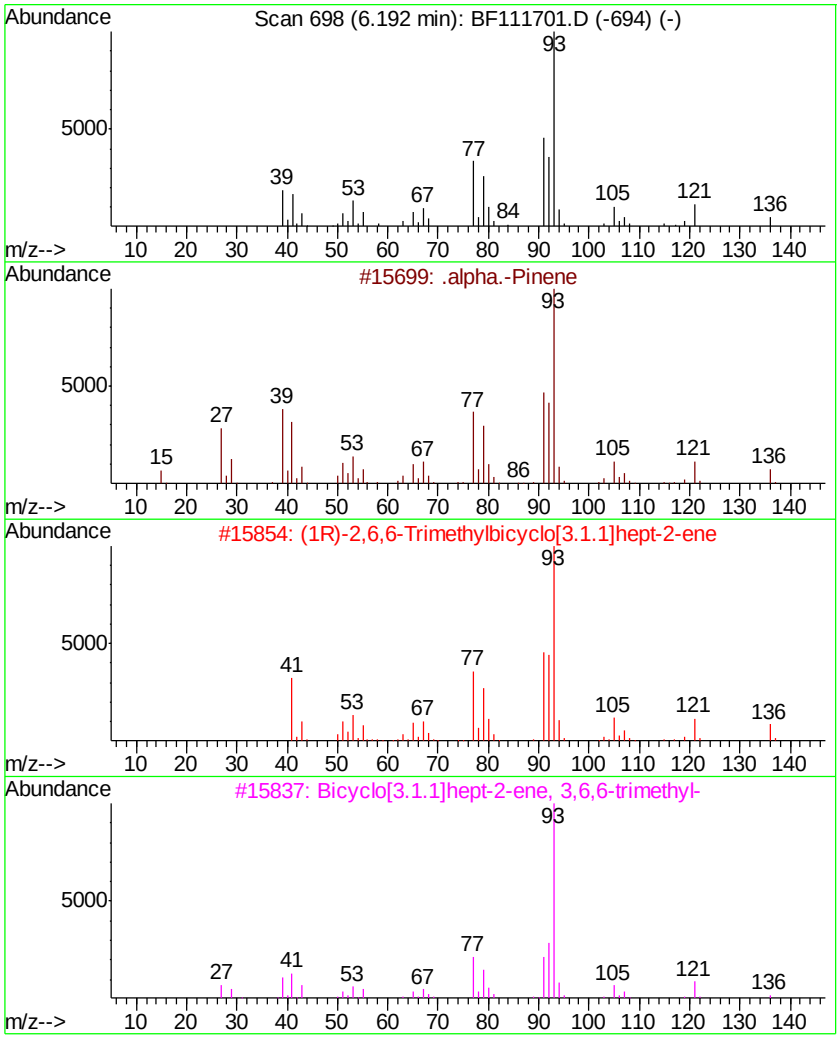
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

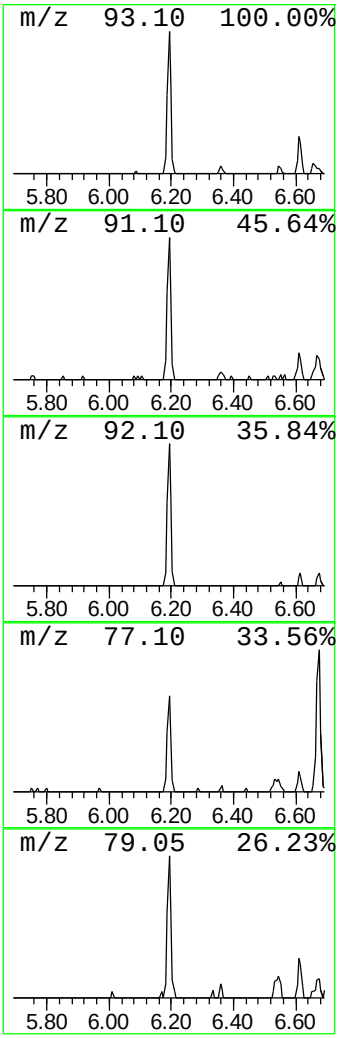
****

Peak Number 2 .alpha.-Pinene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.19	2.33 ng	103569	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	95
2	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	95
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	94
4	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	91
5	(+)-3-Carene	136	C10H16	000498-15-7	91





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

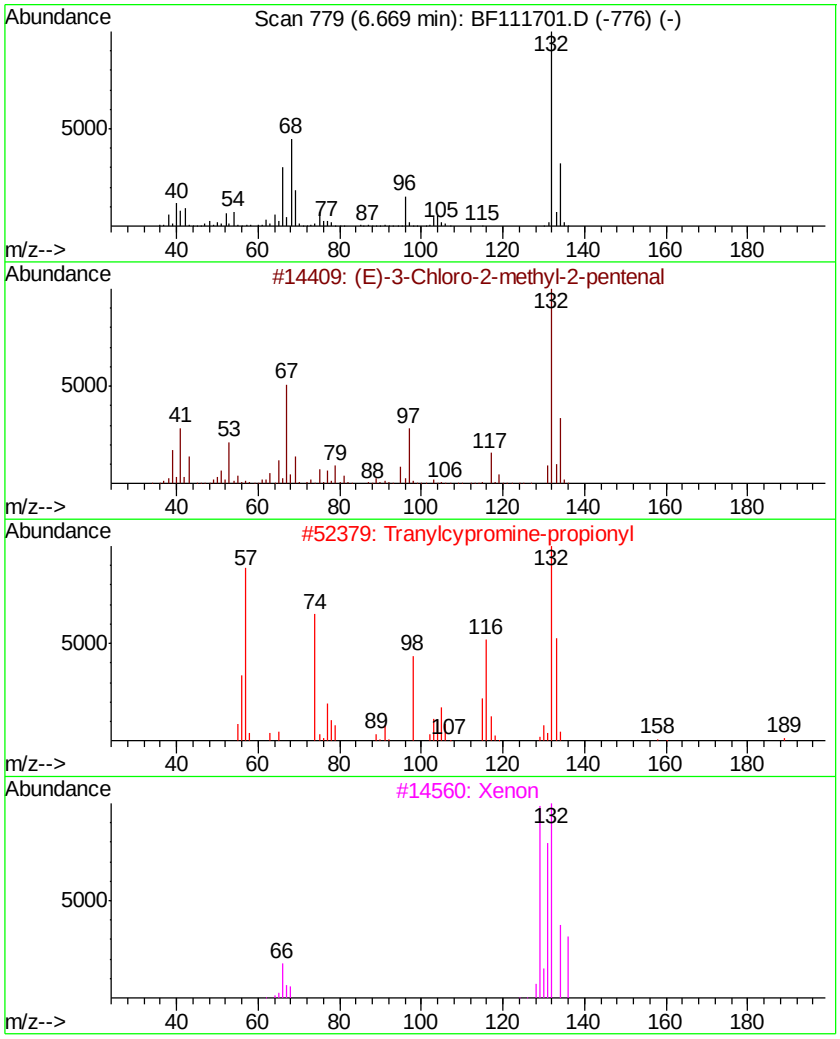
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

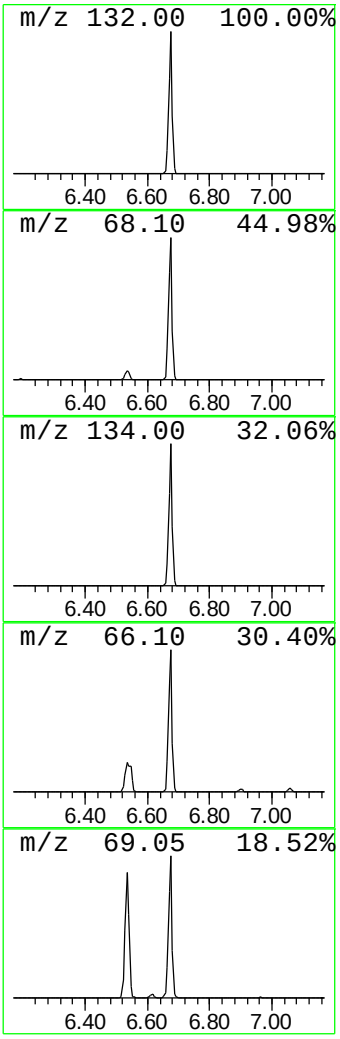
****

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	39.42 ng	1751920	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	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	Xenon	132	Xe	007440-63-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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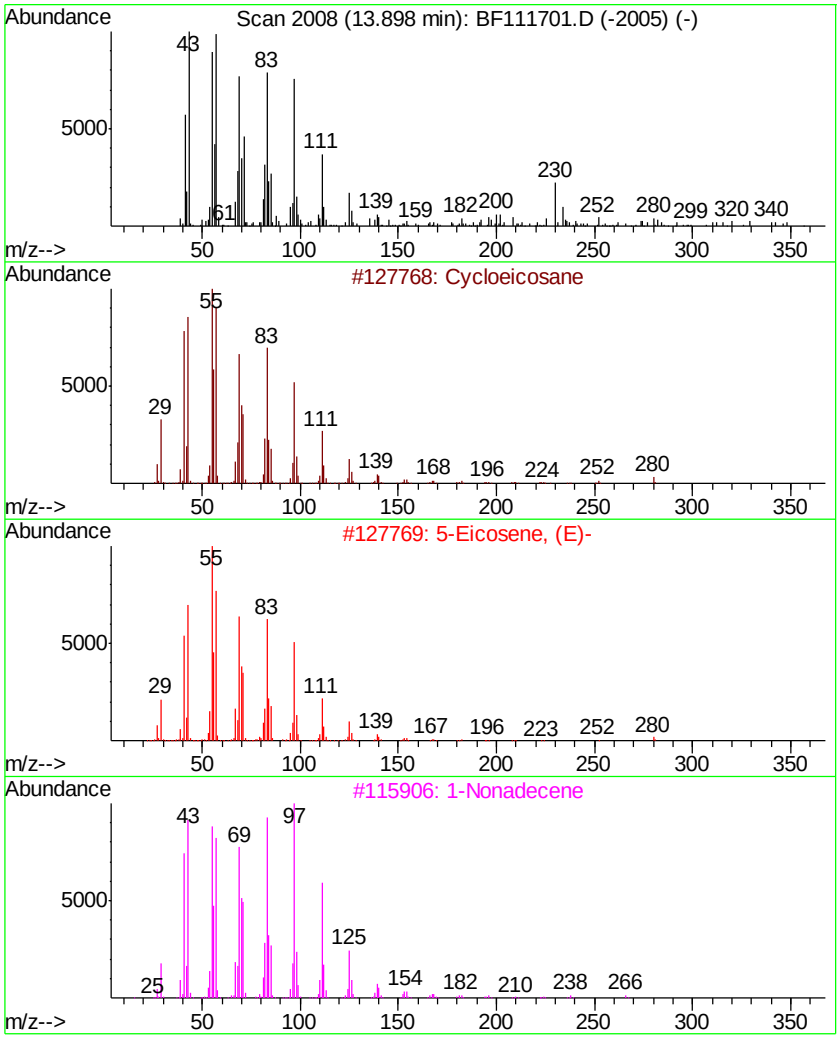
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

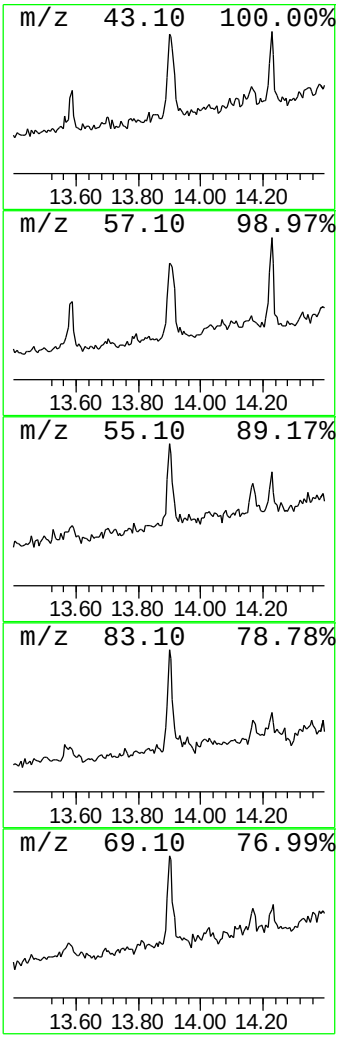
****

Peak Number 5 Cycloeicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.90	4.36 ng	252581	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	97
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
3	1-Nonadecene	266	C19H38	018435-45-5	96
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91





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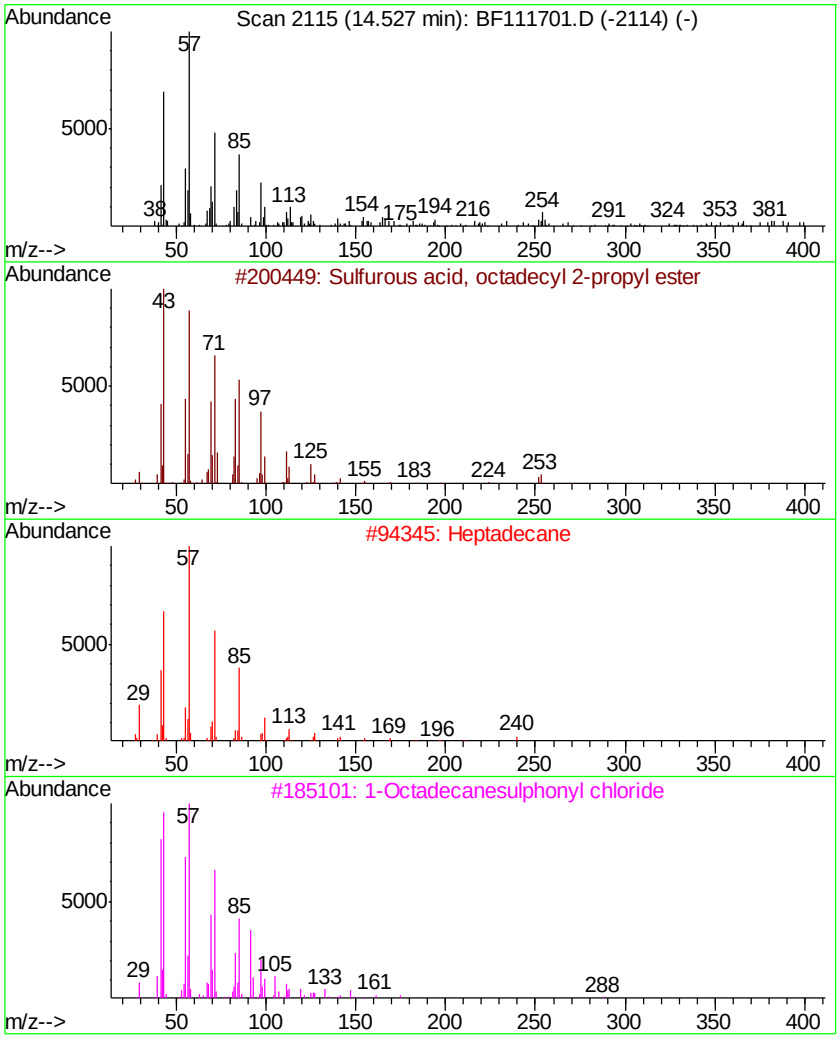
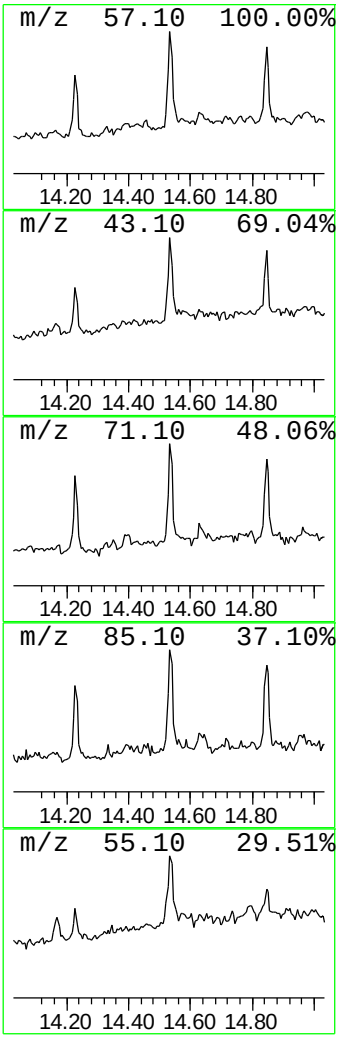
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Sulfurous acid, octadecyl 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.53	3.41 ng	197407	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	87
2	Heptadecane	240	C17H36	000629-78-7	86
3	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	72
4	Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	72
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	72





Tentatively Identified Compound (LSC) summary

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	2.3	ng	101539	1	6.90	888955	20.0
.alpha.-Pinene	6.19	2.3	ng	103569	1	6.90	888955	20.0
unknown6.67	6.67	39.4	ng	1751920	1	6.90	888955	20.0
Cycloeicosane	13.90	4.4	ng	252581	5	14.06	1158210	20.0
Sulfurous acid, o...	14.53	3.4	ng	197407	5	14.06	1158210	20.0