LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092618\
Data File : BF109343.D
Acq On : 26 Sep 2018 18:11
Operator : JU/SJ
Sample : J5070-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200028

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-BF092218.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	4.898	474	478	485	rBV	62182	78406	3.60%	0.335%
2	5.316	544	549	552	rBV	2010857	1915856	87.98%	8.181%
3	6.345	719	724	727	rBV	2125213	2063733	94.78%	8.813%
4	6.475	742	746	749	rBV	2281397	2035912	93.50%	8.694%
5	6.704	782	785	789	rBV	751553	598995	27.51%	2.558%
6	6.863	808	812	815	rBV	1921039	1553882	71.36%	6.636%
7	7.269	876	881	884	rBV	1349662	1293829	59.42%	5.525%
8	7.986	999	1003	1009	rBV	974225	763947	35.08%	3.262%
9	9.063	1182	1186	1189	rBV	2664419	2177484	100.00%	9.299%
10	9.457	1249	1253	1256	rBV	800857	595010	27.33%	2.541%
11	9.733	1297	1300	1304	rBV	947635	864355	39.70%	3.691%
12	10.521	1430	1434	1437	rBV	1637689	1449370	66.56%	6.189%
13	11.016	1515	1518	1523	rVB2	29730	28412	1.30%	0.121%
14	11.216	1548	1552	1554	rBV	930682	885949	40.69%	3.783%
15	11.233	1554	1555	1559	rVV	299312	219162	10.06%	0.936%
16	11.286	1559	1564	1567	rVB	52531	47861	2.20%	0.204%
17	11.439	1586	1590	1593	rBV2	35356	32648	1.50%	0.139%
18	11.716	1633	1637	1639	rBV	31829	25878	1.19%	0.111%
19	11.751	1639	1643	1647	rBV2	156794	180056	8.27%	0.769%
20	11.821	1652	1655	1658	rBV	50842	52768	2.42%	0.225%
21	12.027	1688	1690	1695	rVB	61722	50973	2.34%	0.218%
22	12.339	1741	1743	1749	rVB2	29737	31719	1.46%	0.135%
23	12.421	1753	1757	1760	rBV	414377	380653	17.48%	1.626%
24	12.645	1789	1795	1798	rBV	369803	365729	16.80%	1.562%
25	12.792	1817	1820	1824	rVB	1821456	1700165	78.08%	7.260%
26	12.868	1828	1833	1836	rBV3	27015	38464	1.77%	0.164%
27	12.951	1843	1847	1848	rBV4	26634	25356	1.16%	0.108%
28	12.974	1848	1851	1854	rVB2	46105	45925	2.11%	0.196%
29	13.039	1854	1862	1865	rBV2	34948	43898	2.02%	0.187%
30	13.074	1865	1868	1871	rBV2	41427	43041	1.98%	0.184%
31	13.474	1933	1936	1943	rVB	51982	53437	2.45%	0.228%
32	13.586	1951	1955	1958	rBV2	46243	58613	2.69%	0.250%
33	13.704	1969	1975	1982	rBV3	171315	306095	14.06%	1.307%
34	13.780	1985	1988	1991	rVB2	48799	51222	2.35%	0.219%

LSC Area Percent Report

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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200028

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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.839	1993	1998	2001	rVV2	864434	951658	43.70%	4.064%
36	13.862	2001	2002	2005	rVB	203033	120672	5.54%	0.515%
37	13.945	2011	2016	2018	rBV2	32279	39600	1.82%	0.169%
38	14.057	2032	2035	2039	rVB2	21252	27671	1.27%	0.118%
39	14.221	2059	2063	2066	rVB	40982	42953	1.97%	0.183%
40	14.257	2066	2069	2072	rBV2	31997	39957	1.84%	0.171%
41	14.321	2076	2080	2082	rBV3	24369	28175	1.29%	0.120%
42	14.474	2102	2106	2111	rVB	51988	59380	2.73%	0.254%
43	14.521	2111	2114	2118	rBV2	28291	36244	1.66%	0.155%
44	14.621	2129	2131	2136	rVB4	21627	25933	1.19%	0.111%
45	14.686	2136	2142	2148	rBV3	113573	163443	7.51%	0.698%
46	14.757	2151	2154	2157	rBV2	26318	30203	1.39%	0.129%
47	14.845	2165	2169	2172	rBV	247654	334974	15.38%	1.430%
48	14.939	2182	2185	2189	rVB2	37693	46448	2.13%	0.198%
49	15.121	2212	2216	2222	rVB	158956	193737	8.90%	0.827%
50	15.180	2222	2226	2232	rBV	169125	217543	9.99%	0.929%
51	15.239	2232	2236	2240	rBV	613121	741580	34.06%	3.167%
52	15.686	2308	2312	2316	rBV2	29014	42921	1.97%	0.183%
53	16.580	2459	2464	2474	rVB2	68195	129219	5.93%	0.552%
54	16.986	2528	2533	2539	rVB	46976	86233	3.96%	0.368%

Sum of corrected areas: 23417347

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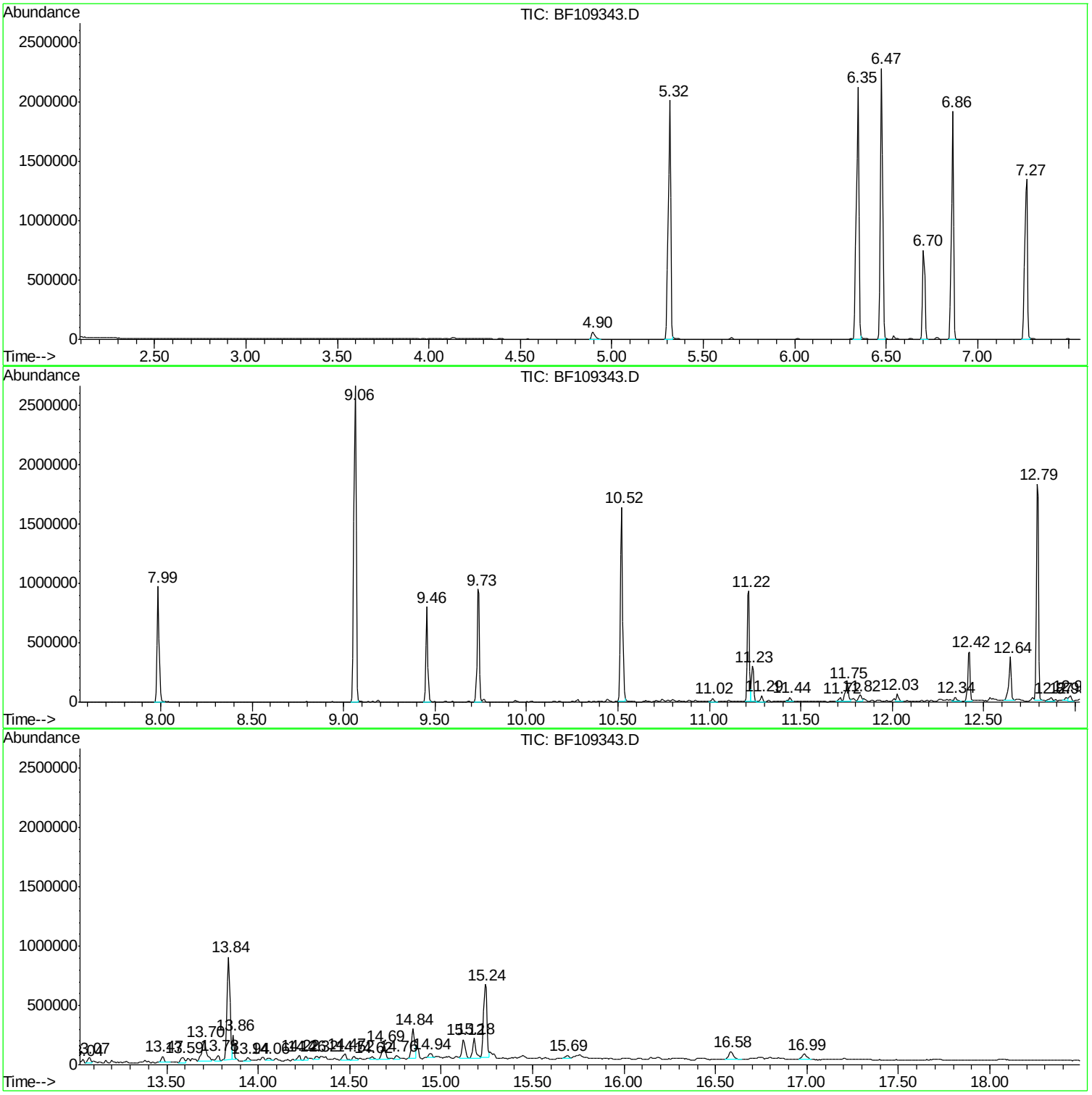
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CS-RBR-200028

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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

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TIC Integration Parameters: LSCINT.P

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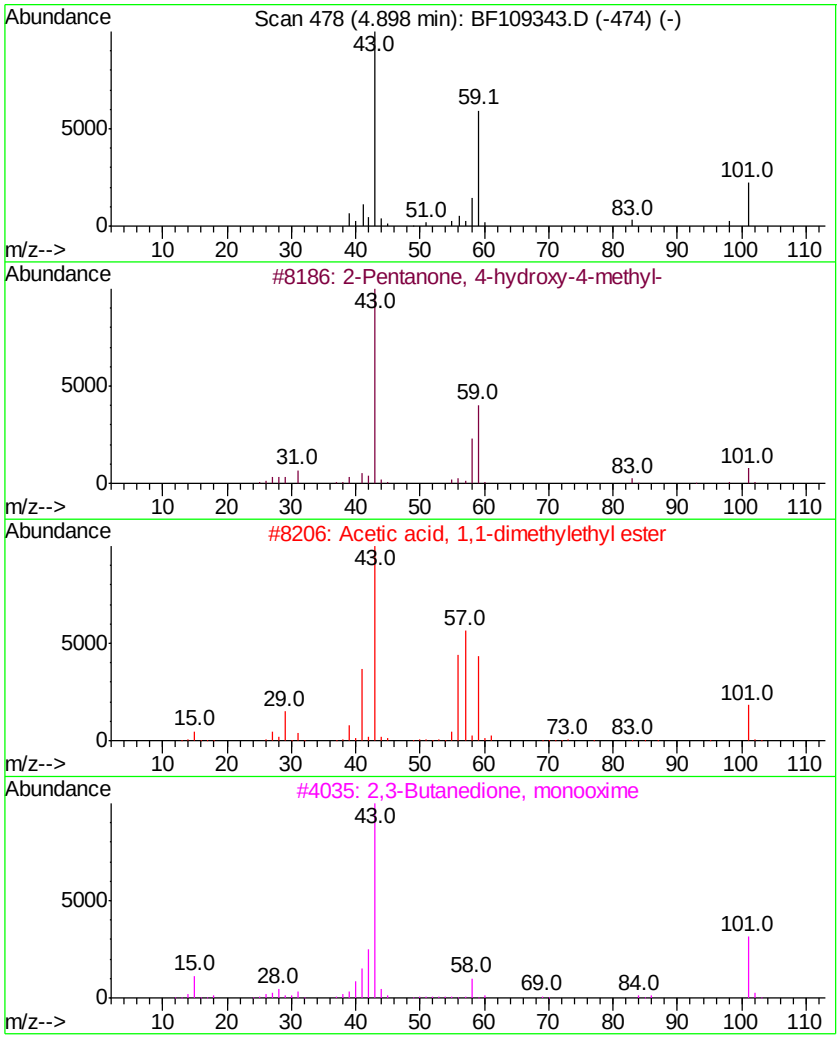
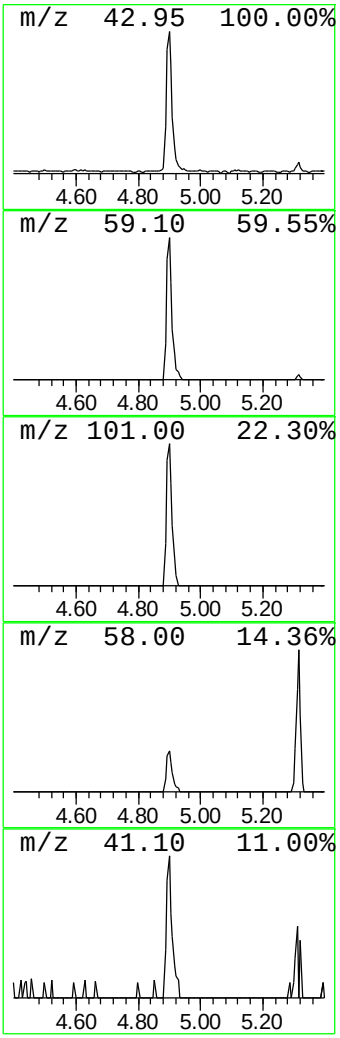
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	2.62 ng	78406	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17





Library Search Compound Report

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Operator : JU/SJ
Sample : J5070-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CS-RBR-200028

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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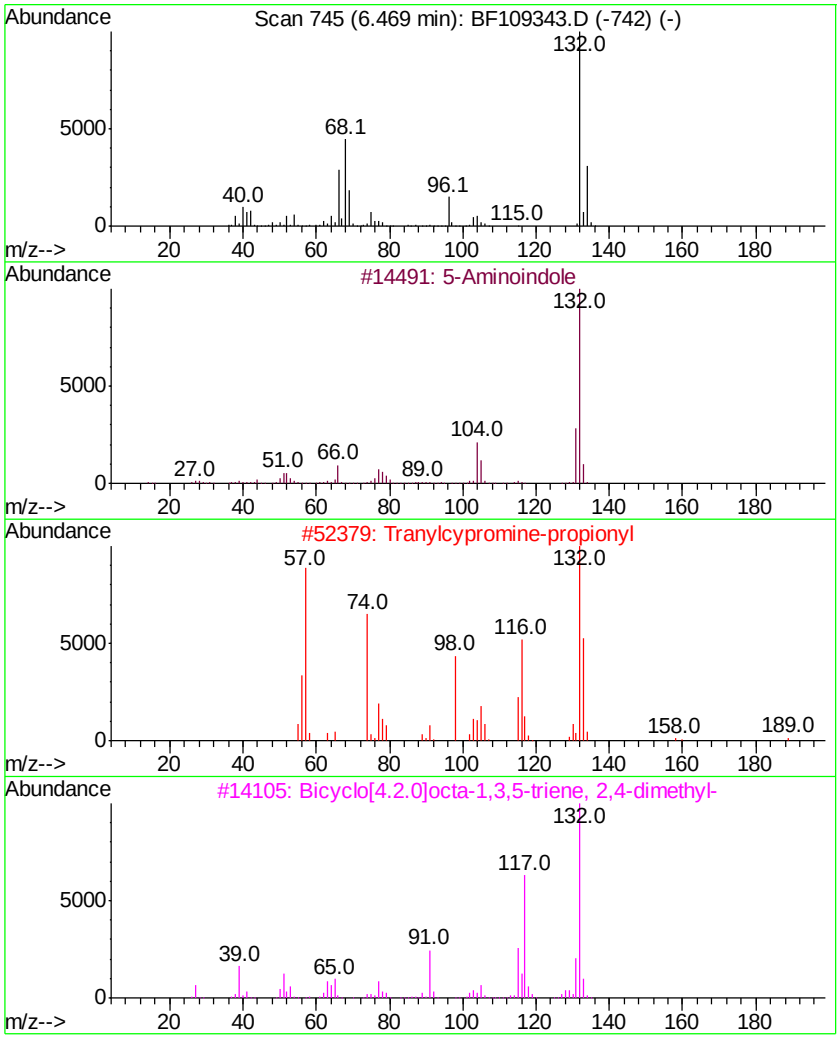
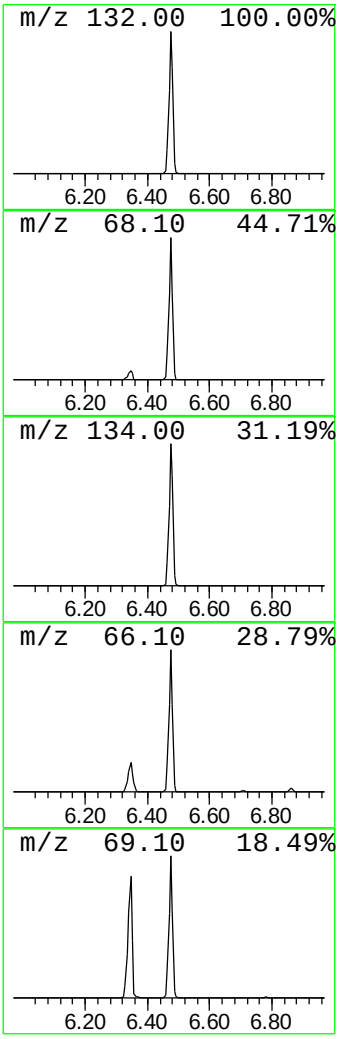
Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	67.98 ng	2035910	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Aminoindole	132	C8H8N2	005192-03-0	12
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





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ClientSampleId : CS-RBR-200028

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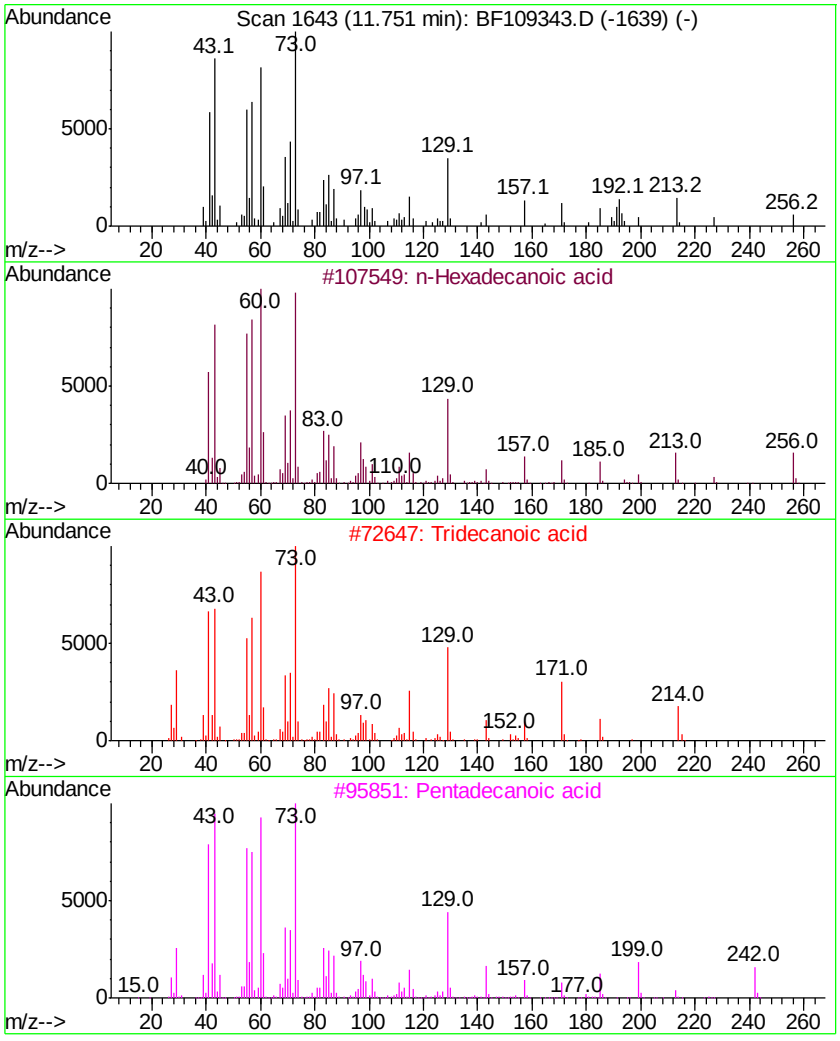
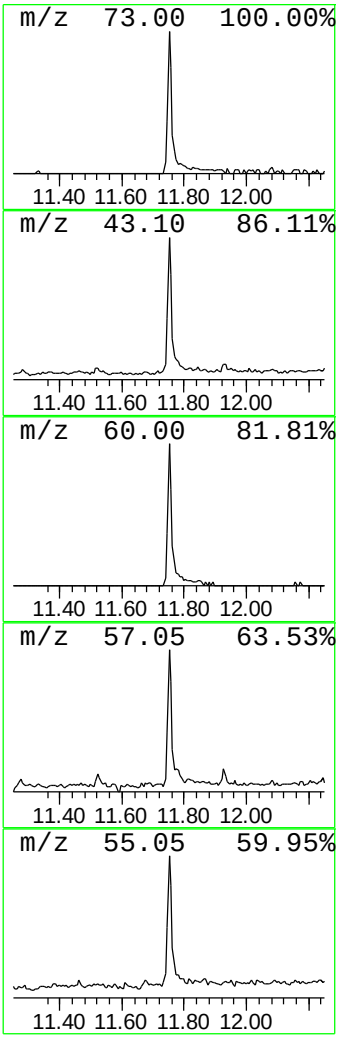
Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	4.06 ng	180056	Phenanthrene-d10	11.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	96
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	25





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
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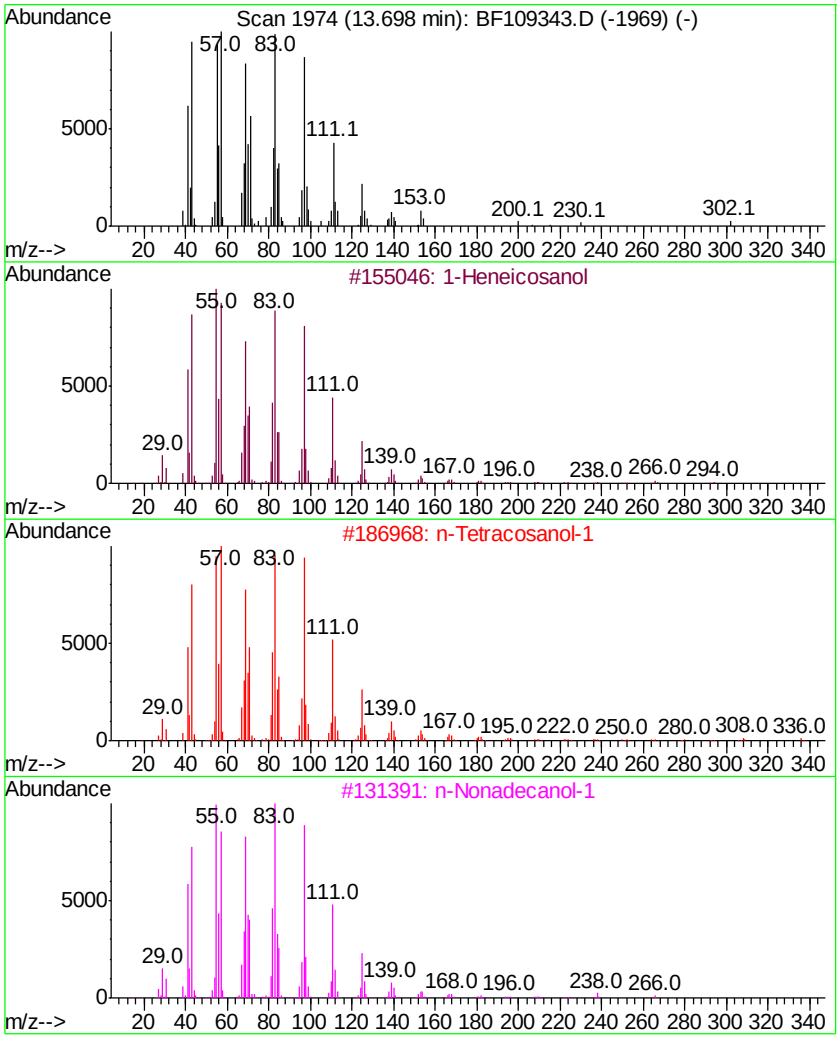
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

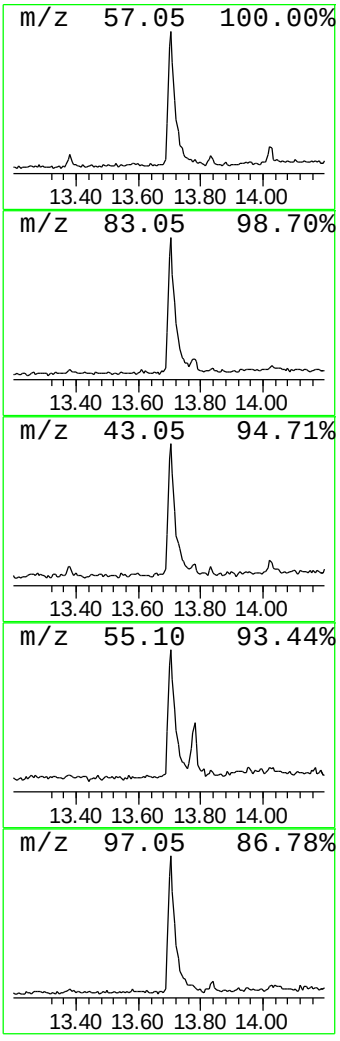
****

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	6.43 ng	306095	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94





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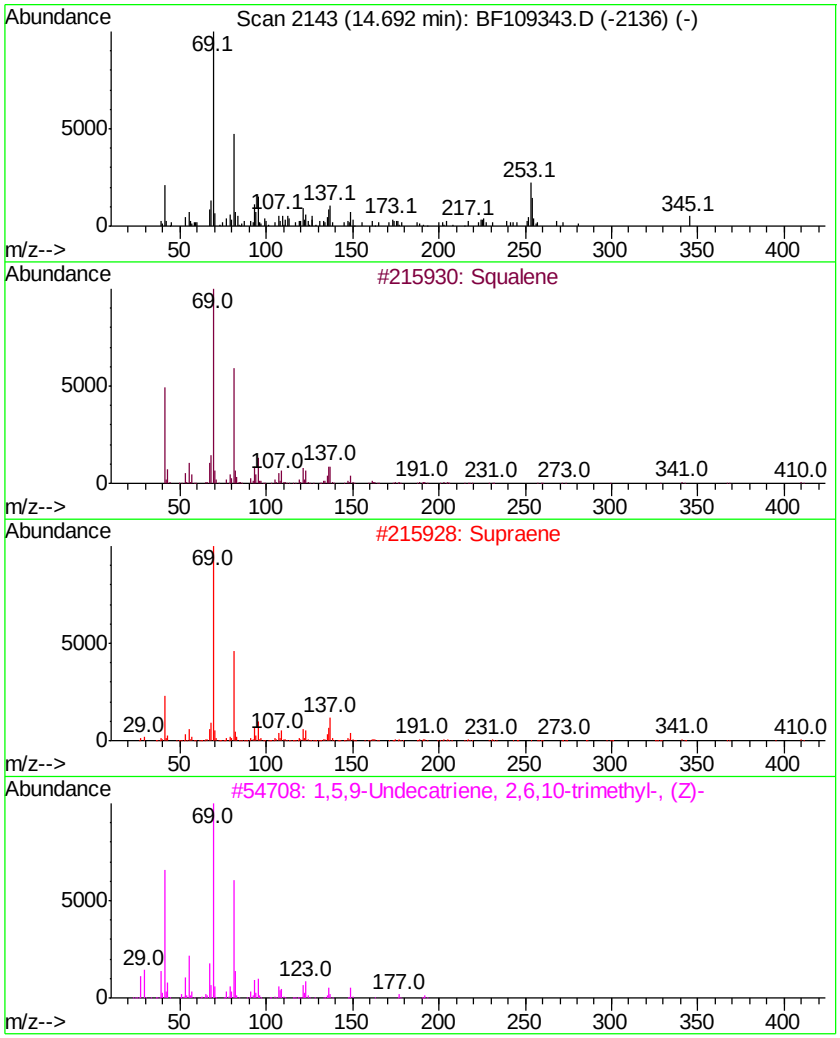
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

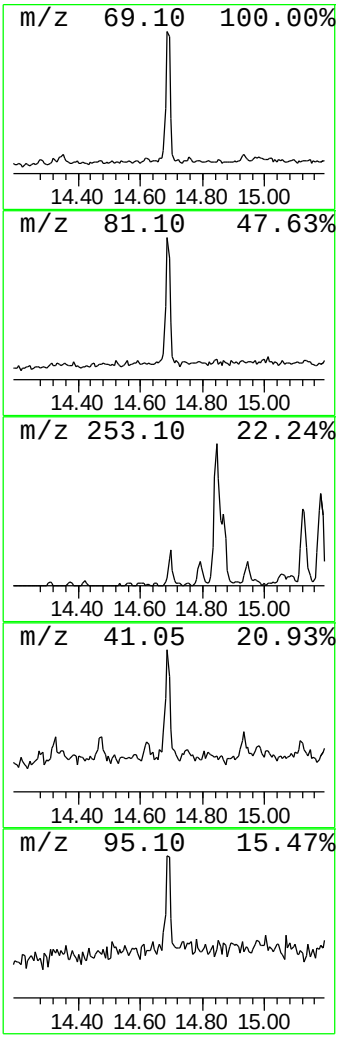
****

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	4.41 ng	163443	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	64
2	Supraene	410	C30H50	007683-64-9	52
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	49
4	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	43
5	Crotonoyl bromide	148	C4H5BrO	055600-70-9	43





Tentatively Identified Compound (LSC) summary

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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...	4.90	2.6	ng	78406	1	6.70	598995	20.0
unknown6.47	6.47	68.0	ng	2035910	1	6.70	598995	20.0
n-Hexadecanoic acid	11.75	4.1	ng	180056	4	11.22	885949	20.0
1-Heneicosanol	13.70	6.4	ng	306095	5	13.84	951658	20.0
Squalene	14.69	4.4	ng	163443	6	15.24	741580	20.0