LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080318\
Data File : BF107950.D
Acq On : 3 Aug 2018 20:54
Operator : JU/SJ
Sample : J4318-07 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BEEBEE-SITE-DEMO-3

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-BF073018.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	5.172	479	482	496	rBV	48224	85508	6.98%	0.671%
2	5.631	553	560	567	rBV5	51395	199323	16.27%	1.563%
3	6.619	724	728	743	rBV	107356	487096	39.75%	3.821%
4	6.731	744	747	764	rVV	274663	682765	55.72%	5.356%
5	6.954	782	785	807	rBV	255895	659793	53.85%	5.175%
6	7.107	807	811	825	rBV	322265	571582	46.65%	4.483%
7	7.542	879	885	887	rBV3	70257	138233	11.28%	1.084%
8	8.236	999	1003	1033	rBV	483600	1053647	85.99%	8.265%
9	8.801	1095	1099	1104	rVB2	10330	14608	1.19%	0.115%
10	9.301	1181	1184	1194	rBV	562945	884434	72.18%	6.937%
11	9.701	1245	1252	1262	rBV2	35171	64465	5.26%	0.506%
12	9.895	1282	1285	1290	rVV	20188	19329	1.58%	0.152%
13	9.989	1297	1301	1320	rBV	859705	1056928	86.26%	8.290%
14	10.395	1367	1370	1374	rBV	21513	18663	1.52%	0.146%
15	10.501	1384	1388	1390	rBV	16083	18292	1.49%	0.143%
16	10.613	1401	1407	1411	rVB3	11190	16038	1.31%	0.126%
17	10.789	1433	1437	1448	rBV	247438	481239	39.28%	3.775%
18	10.877	1448	1452	1460	rVB4	33252	70760	5.78%	0.555%
19	11.072	1481	1485	1488	rBV	100598	85583	6.98%	0.671%
20	11.136	1493	1496	1501	rVB	43914	46224	3.77%	0.363%
21	11.260	1512	1517	1520	rVB6	11259	17038	1.39%	0.134%
22	11.319	1524	1527	1530	rBV2	21555	23012	1.88%	0.181%
23	11.489	1552	1556	1568	rBV2	574337	1090193	88.98%	8.551%
24	11.589	1571	1573	1577	rVV	67049	84752	6.92%	0.665%
25	11.636	1579	1581	1585	rVV	39953	47131	3.85%	0.370%
26	11.677	1586	1588	1595	rVB6	17468	22814	1.86%	0.179%
27	11.748	1597	1600	1602	rBV	23476	20218	1.65%	0.159%
28	11.995	1638	1642	1646	rBV	399516	452992	36.97%	3.553%
29	12.154	1667	1669	1672	rVB	37939	30553	2.49%	0.240%
30	12.295	1689	1693	1697	rBV4	23476	44075	3.60%	0.346%
31	12.542	1731	1735	1738	rBV	43524	55216	4.51%	0.433%
32	12.642	1746	1752	1753	rBV6	37986	63986	5.22%	0.502%
33	12.707	1759	1763	1772	rBV	247302	356166	29.07%	2.794%
34	12.777	1772	1775	1784	rVV2	116992	171271	13.98%	1.343%

LSC Area Percent Report

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Integrator: RTE
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Sampling : 1 Min Area: 3 % of largest Peak
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.918	1796	1799	1800	rBV2	42169	41677	3.40%	0.327%
36	12.942	1800	1803	1811	rVB	164624	228489	18.65%	1.792%
37	13.071	1821	1825	1835	rBV	607520	819626	66.89%	6.429%
38	13.271	1857	1859	1863	rVB3	38085	36688	2.99%	0.288%
39	13.613	1915	1917	1921	rBV2	33785	41445	3.38%	0.325%
40	13.948	1972	1974	1979	rVB3	56720	61876	5.05%	0.485%
41	14.083	1995	1997	2001	rBV	76405	62783	5.12%	0.492%
42	14.142	2003	2007	2022	rVV2	691900	1225267	100.00%	9.611%
43	14.365	2043	2045	2048	rVB	58279	49297	4.02%	0.387%
44	15.230	2187	2192	2199	rBV2	112958	273913	22.36%	2.149%
45	15.671	2263	2267	2280	rVB2	402061	773808	63.15%	6.070%

Sum of corrected areas: 12748796

LSC Report - Integrated Chromatogram

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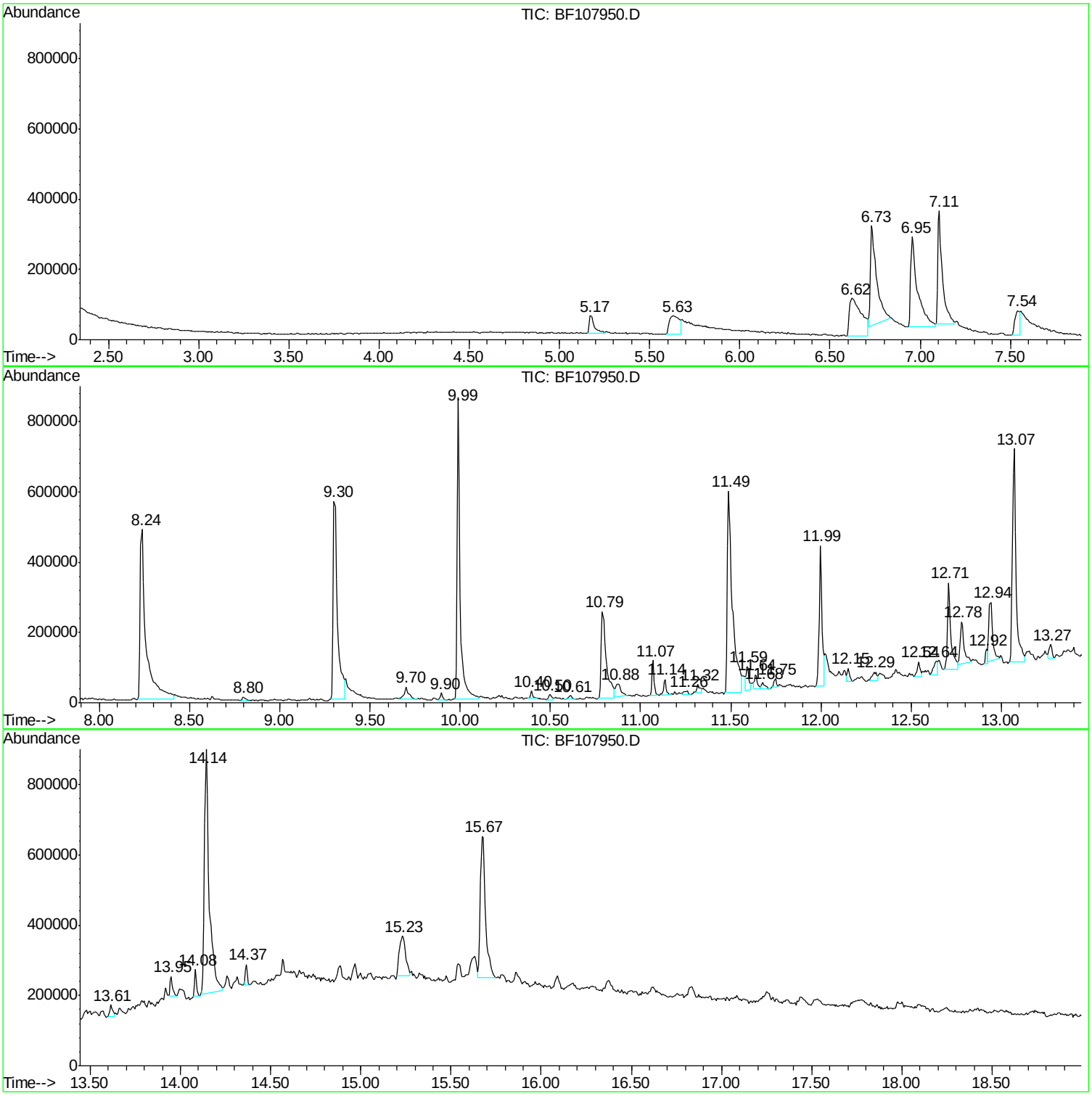
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BEEBEE-SITE-DEMO-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.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\BF080318\
Data File : BF107950.D
Acq On : 3 Aug 2018 20:54
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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BEEBEE-SITE-DEMO-3

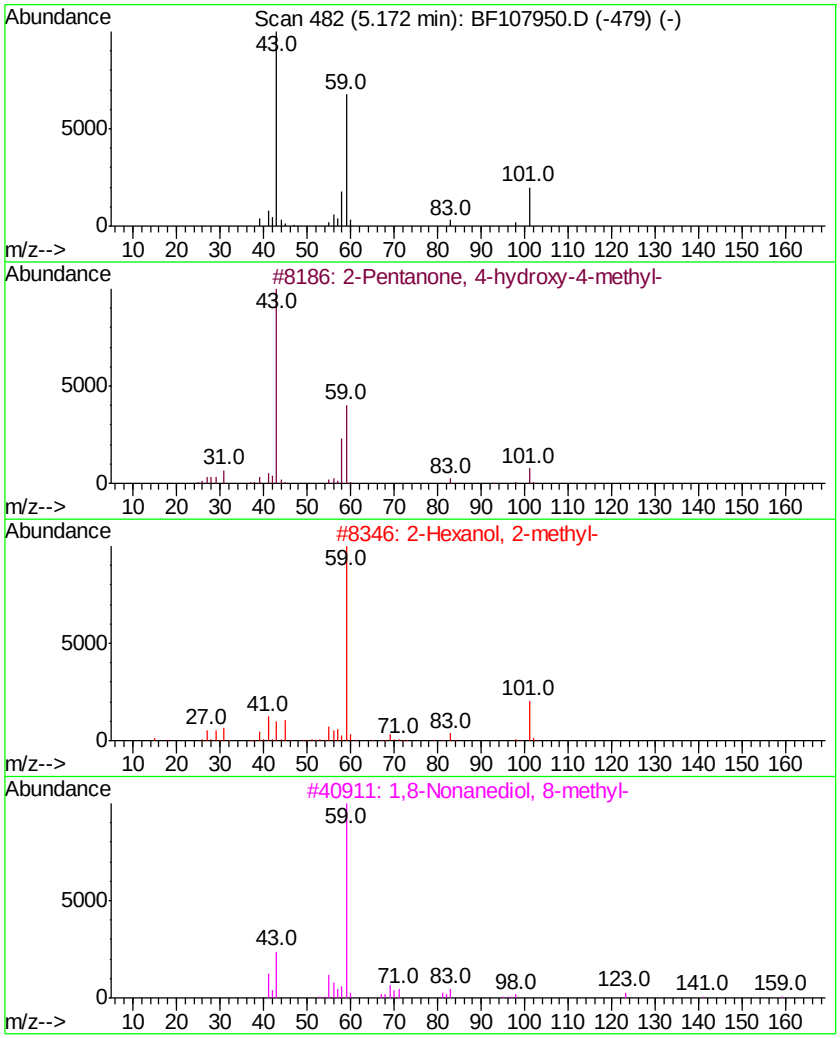
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

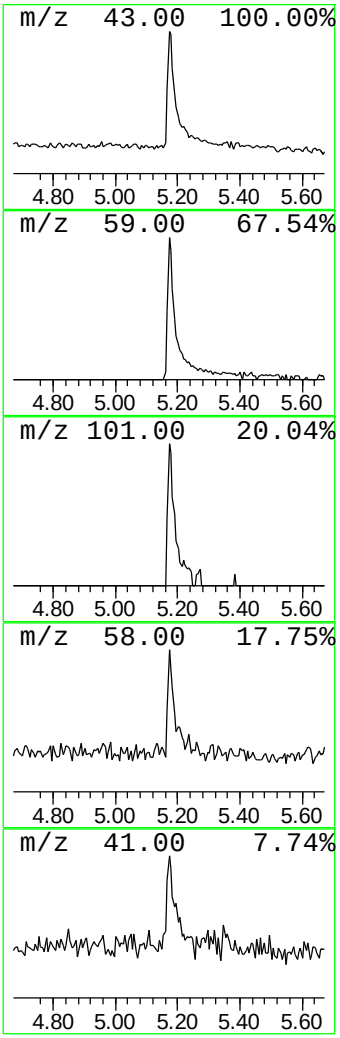
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	2.59 ng	85508	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	37
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5	1,2-Butanediol	90	C4H10O2	000584-03-2	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

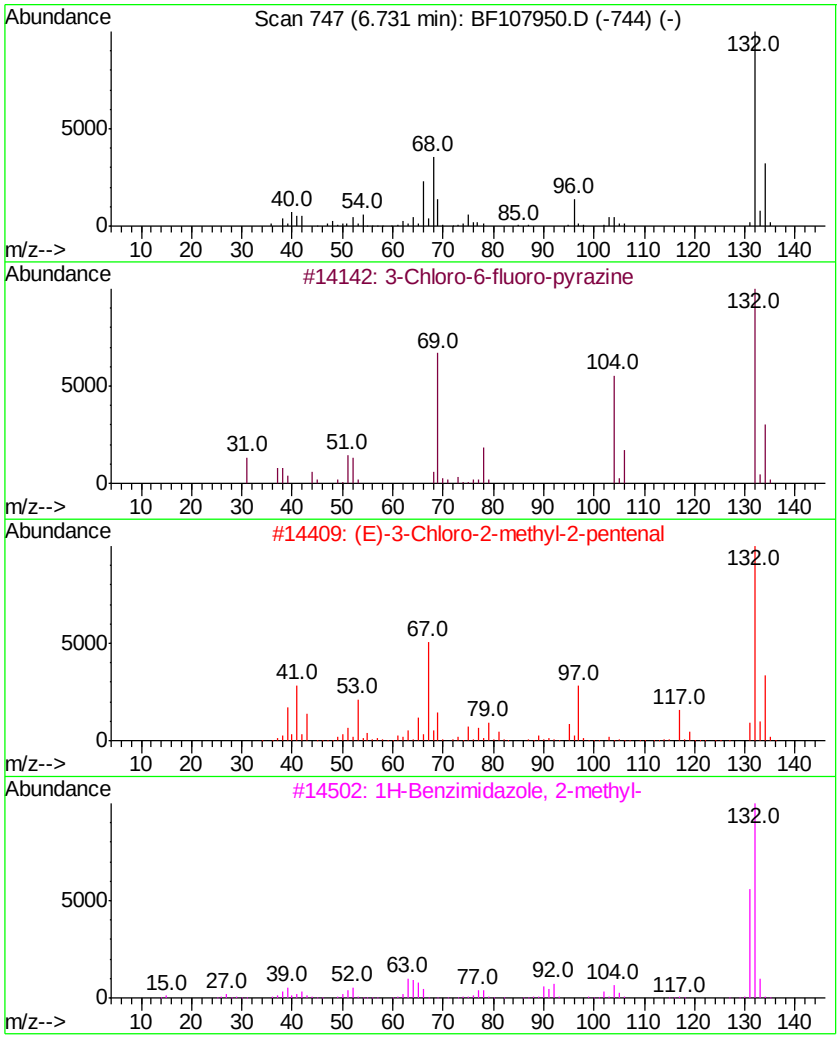
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

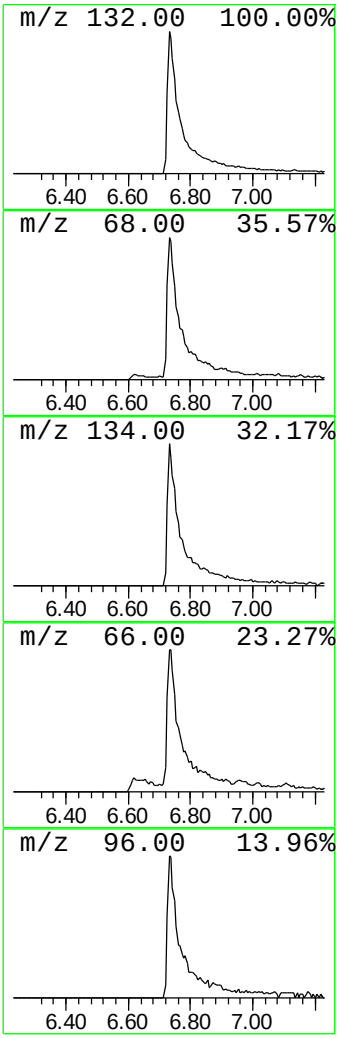
****

Peak Number 2 unknown6.7.3 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	20.70 ng	682765	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Instrument :
BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
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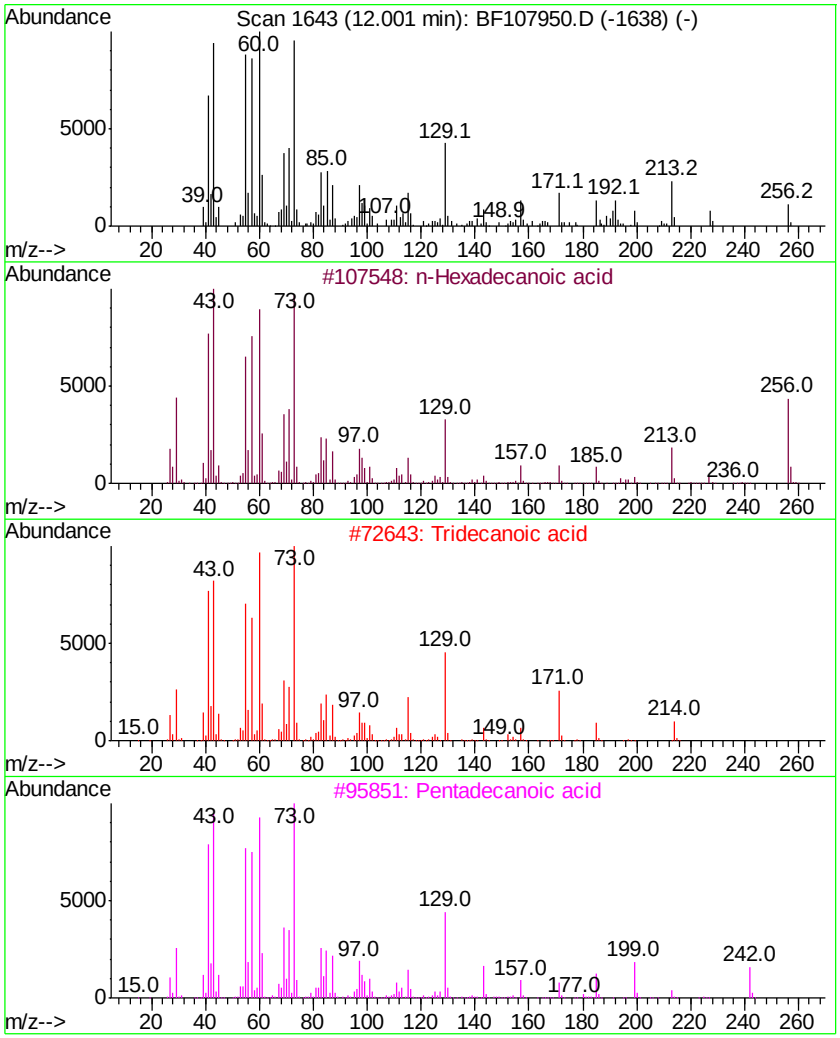
TIC Integration Parameters: LSCINT.P

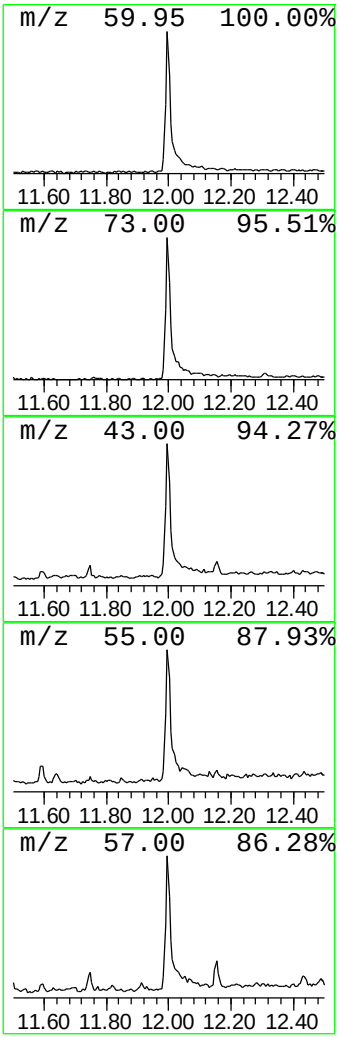
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	8.31 ng	452992	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073018.M
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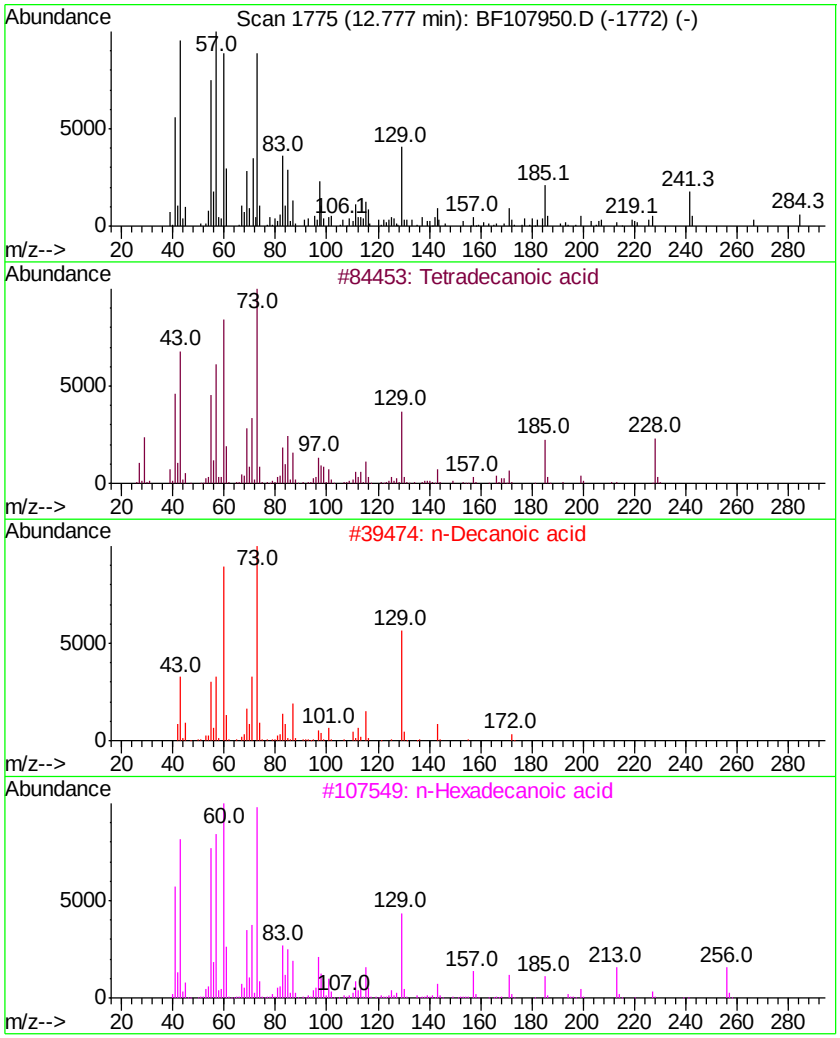
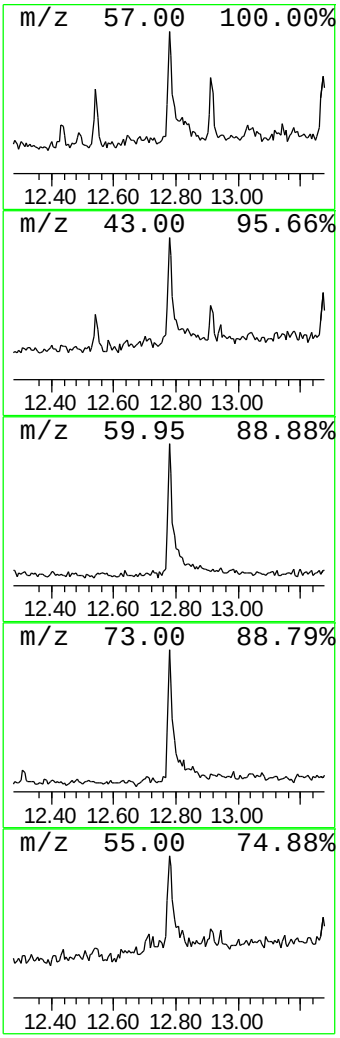
****

Peak Number 5 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	3.14 ng	171271	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
2	n-Decanoic acid	172	C10H20O2	000334-48-5	60
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	53
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	Dodecanoic acid	200	C12H24O2	000143-07-7	47





Tentatively Identified Compound (LSC) summary

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TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	2.6	ng	85508	1	6.95	659793	20.0
unknown6.7.3	6.73	20.7	ng	682765	1	6.95	659793	20.0
n-Hexadecanoic acid	12.00	8.3	ng	452992	4	11.49	1090190	20.0
Tetradecanoic acid	12.78	3.1	ng	171271	4	11.49	1090190	20.0