LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101518\
Data File : BF109893.D
Acq On : 15 Oct 2018 21:41
Operator : JU/SJ
Sample : J5198-17
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-101218-D

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-BF101518.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	2.298	32	36	44	rVB	520054	675785	19.21%	1.753%
2	5.210	526	531	536	rBV	121624	152592	4.34%	0.396%
3	5.592	591	596	599	rBV	3978479	3515221	99.91%	9.120%
4	6.592	760	766	770	rBV	3566821	3518440	100.00%	9.128%
5	6.745	787	792	795	rBV	3949808	3516461	99.94%	9.123%
6	6.975	828	831	835	rBV	1390390	1262634	35.89%	3.276%
7	7.133	854	858	861	rBV	3317541	2707563	76.95%	7.025%
8	7.533	922	926	930	rBV	2271452	2065800	58.71%	5.360%
9	8.263	1046	1050	1053	rBV	1594777	1446462	41.11%	3.753%
10	9.333	1228	1232	1235	rBV	3720005	2992478	85.05%	7.764%
11	9.722	1295	1298	1302	rVB	290925	226849	6.45%	0.589%
12	10.016	1345	1348	1352	rBV	1410816	1283121	36.47%	3.329%
13	10.051	1352	1354	1357	rVB	51892	38719	1.10%	0.100%
14	10.427	1411	1418	1422	rVB4	22699	41330	1.17%	0.107%
15	10.563	1439	1441	1446	rVB	48707	43177	1.23%	0.112%
16	10.804	1478	1482	1486	rBV	1950434	1687252	47.95%	4.377%
17	11.510	1598	1602	1604	rBV	1580691	1317711	37.45%	3.419%
18	11.533	1604	1606	1609	rVV	392156	312989	8.90%	0.812%
19	11.580	1611	1614	1617	rVB	129387	108439	3.08%	0.281%
20	12.015	1684	1688	1690	rBV2	226560	253783	7.21%	0.658%
21	12.033	1690	1691	1695	rVB	105942	87047	2.47%	0.226%
22	12.086	1697	1700	1703	rVB	43276	41292	1.17%	0.107%
23	12.121	1703	1706	1709	rBV2	126291	143223	4.07%	0.372%
24	12.304	1734	1737	1739	rBV	63364	52050	1.48%	0.135%
25	12.557	1774	1780	1782	rBV	65943	88460	2.51%	0.230%
26	12.598	1783	1787	1789	rVV4	42093	63885	1.82%	0.166%
27	12.645	1792	1795	1799	rBV2	44070	52218	1.48%	0.135%
28	12.721	1805	1808	1812	rBV	1073620	877140	24.93%	2.276%
29	12.804	1820	1822	1826	rVB3	62589	73140	2.08%	0.190%
30	12.951	1841	1847	1853	rVV	853746	978758	27.82%	2.539%
31	13.004	1853	1856	1860	rVB2	39190	44709	1.27%	0.116%
32	13.092	1867	1871	1874	rVB	3417638	2852610	81.08%	7.401%
33	13.174	1880	1885	1888	rBV3	65091	128580	3.65%	0.334%
34	13.280	1900	1903	1906	rVB	164175	144791	4.12%	0.376%

LSC Area Percent Report

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Instrument : BNA_F
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Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.310	1906	1908	1911	rBV	38561	41656	1.18%	0.108%
36	13.345	1911	1914	1917	rBV	133579	118174	3.36%	0.307%
37	13.380	1917	1920	1923	rBV2	95132	99663	2.83%	0.259%
38	13.509	1939	1942	1944	rBV2	49727	55036	1.56%	0.143%
39	13.927	2011	2013	2015	rVB	64032	43606	1.24%	0.113%
40	13.974	2018	2021	2029	rVB4	331866	402825	11.45%	1.045%
41	14.151	2046	2051	2054	rBV2	1830199	2090184	59.41%	5.423%
42	14.174	2054	2055	2061	rVB	427407	326730	9.29%	0.848%
43	14.257	2067	2069	2072	rBV	99868	82782	2.35%	0.215%
44	14.604	2126	2128	2131	rVB2	138290	116755	3.32%	0.303%
45	15.215	2229	2232	2236	rBV	288747	440329	12.51%	1.142%
46	15.280	2241	2243	2249	rVB2	176372	203108	5.77%	0.527%
47	15.603	2295	2298	2305	rVB	239770	302457	8.60%	0.785%
48	15.674	2305	2310	2321	rVB	930701	1425770	40.52%	3.699%

Sum of corrected areas: 38543784

LSC Report - Integrated Chromatogram

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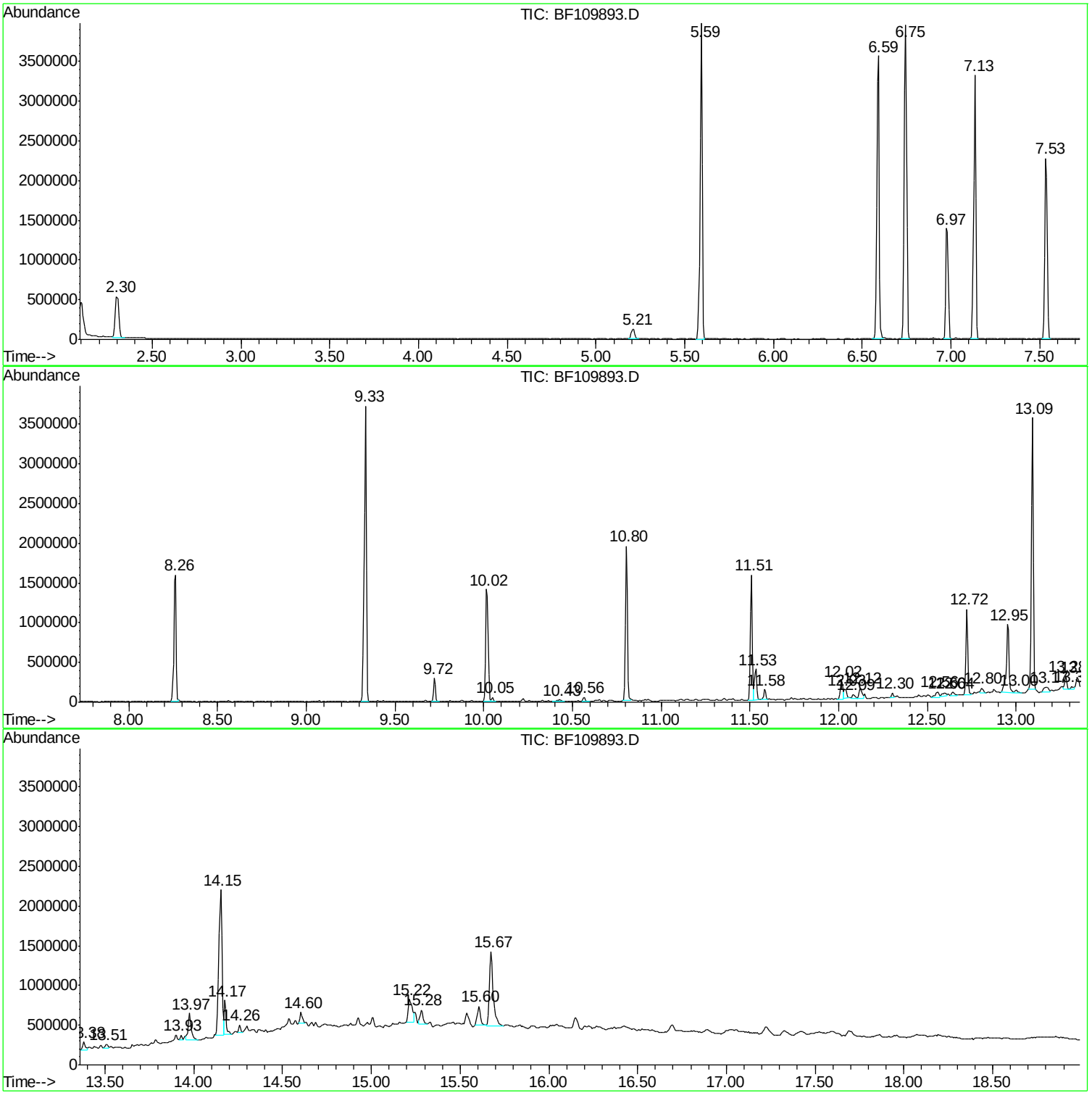
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-101218-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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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Instrument : BNA_F
ClientSampleId : CL-02-101218-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

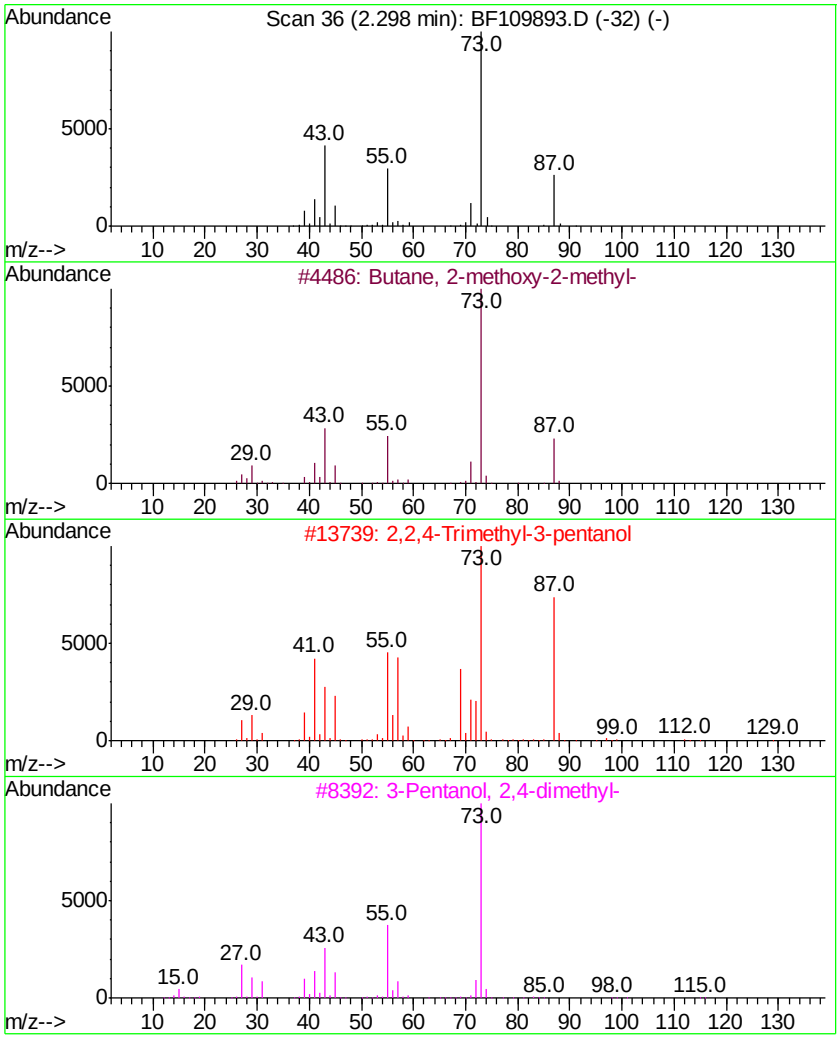
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

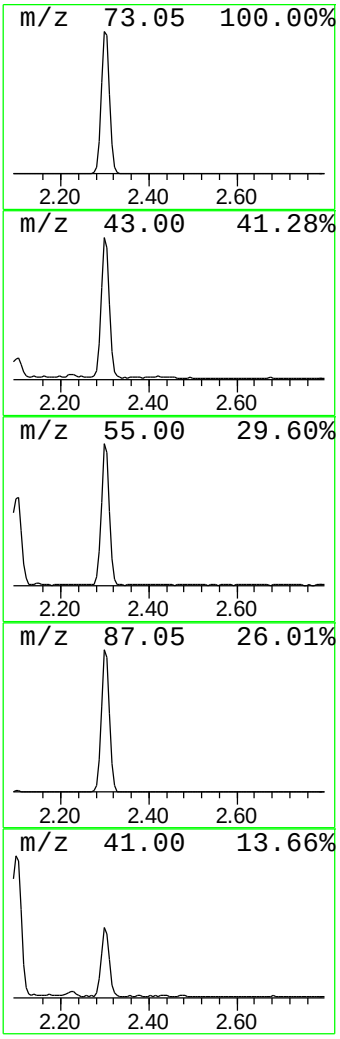
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.30	10.70 ng	675785	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





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Misc :
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Instrument : BNA_F
ClientSampleId : CL-02-101218-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

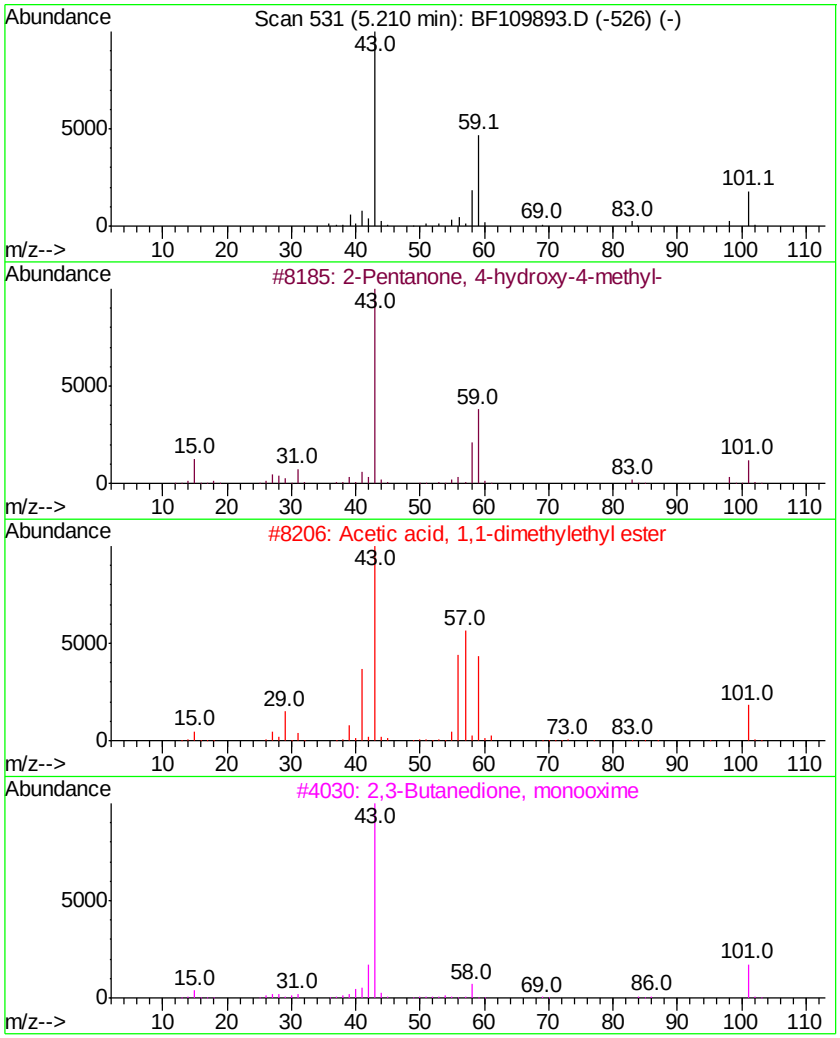
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

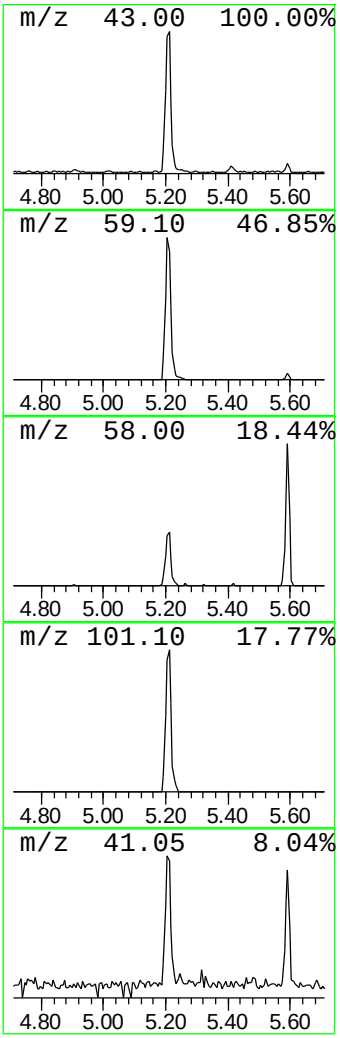
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	2.42 ng	152592	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Acetone	58	C3H6O	000067-64-1	9





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : CL-02-101218-D

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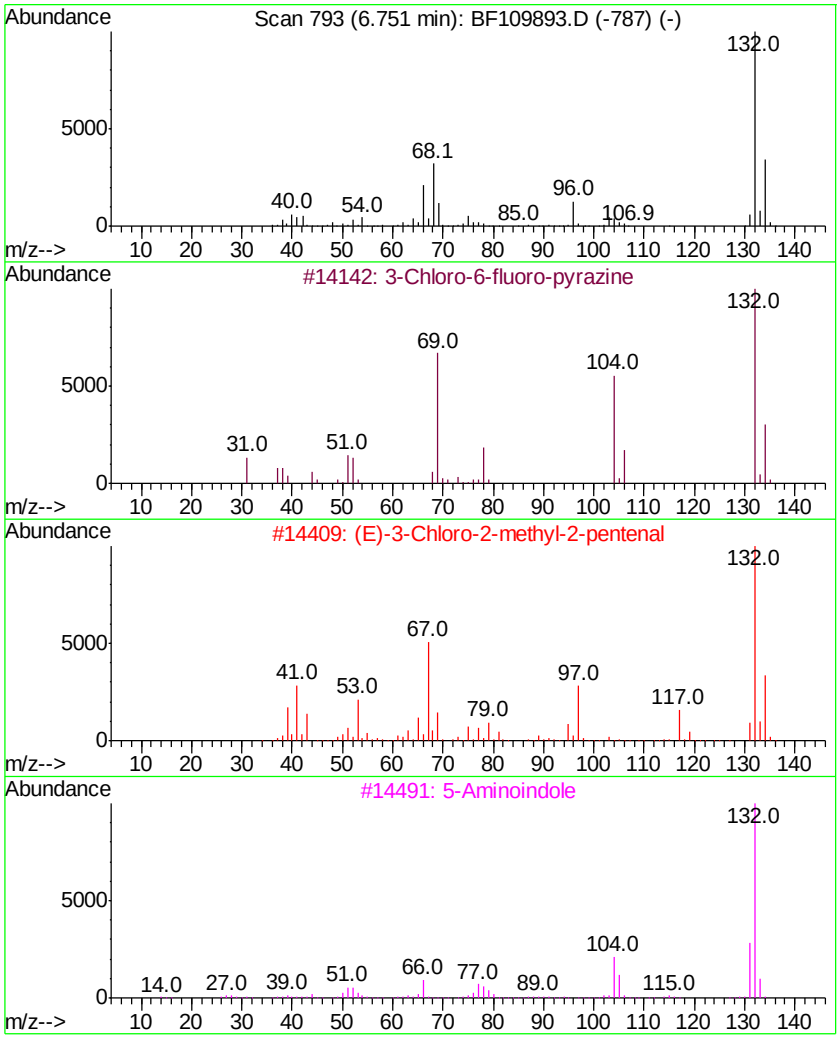
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

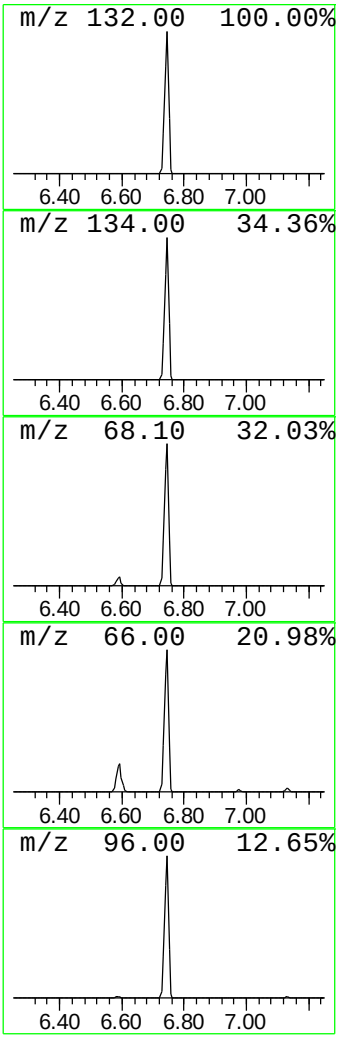
****

Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	55.70 ng	3516460	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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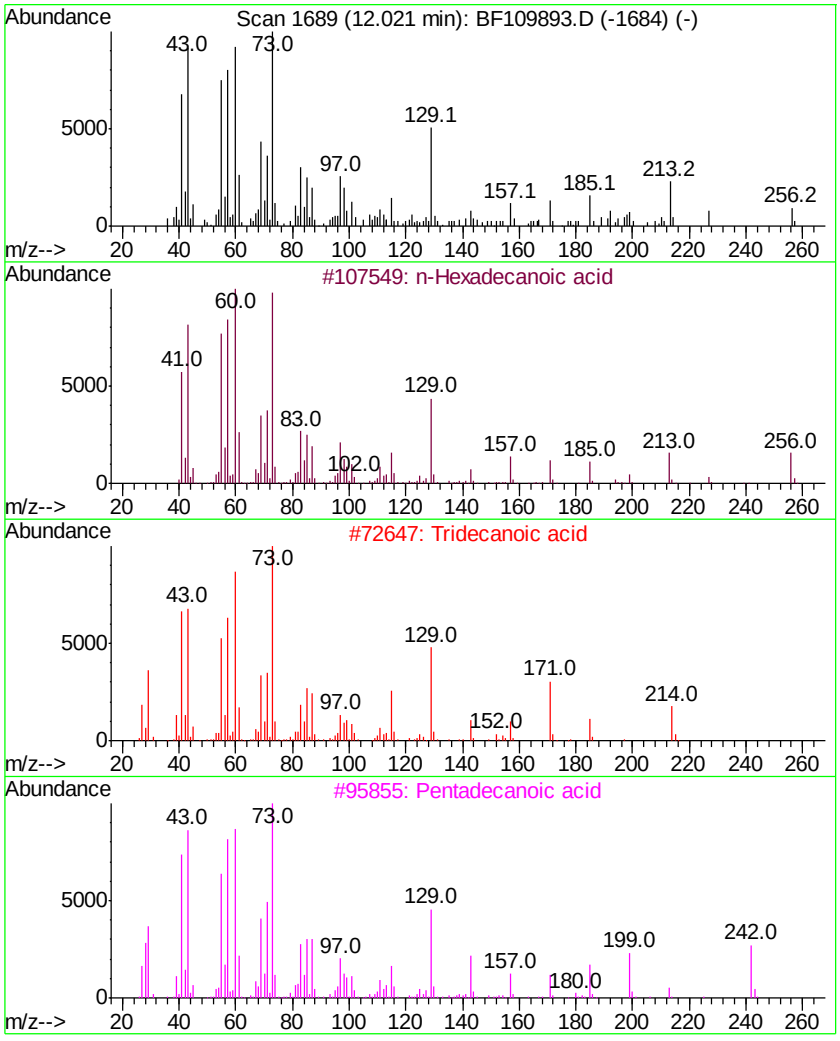
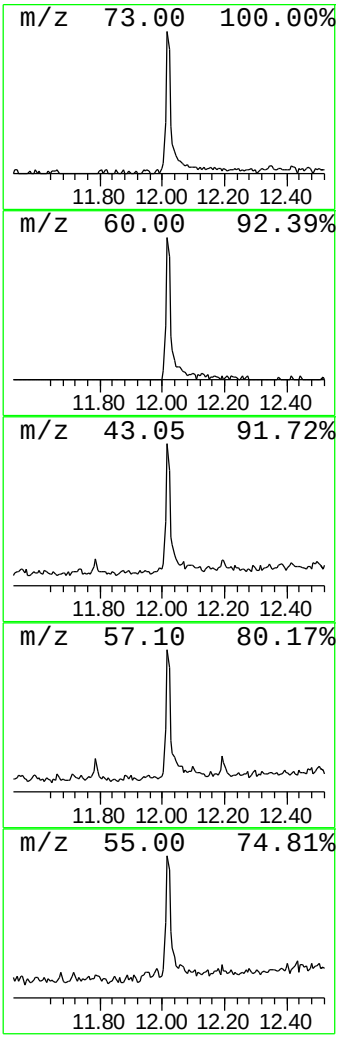
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	3.85 ng	253783	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	18





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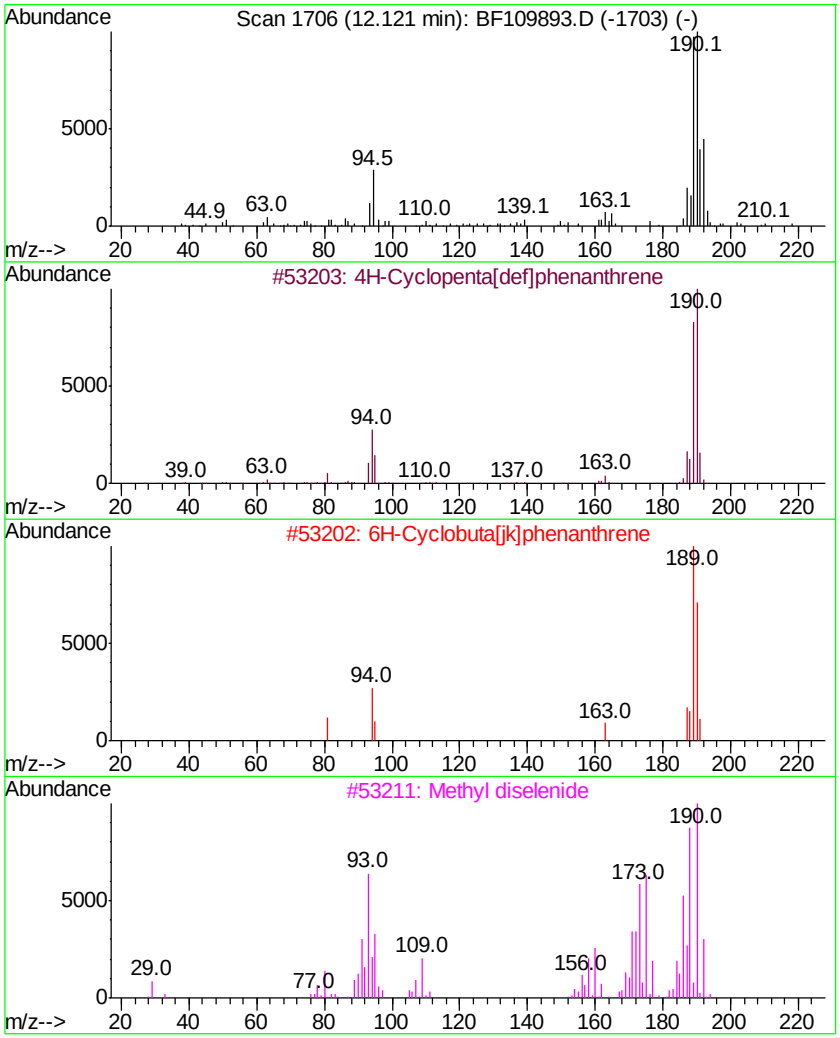
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

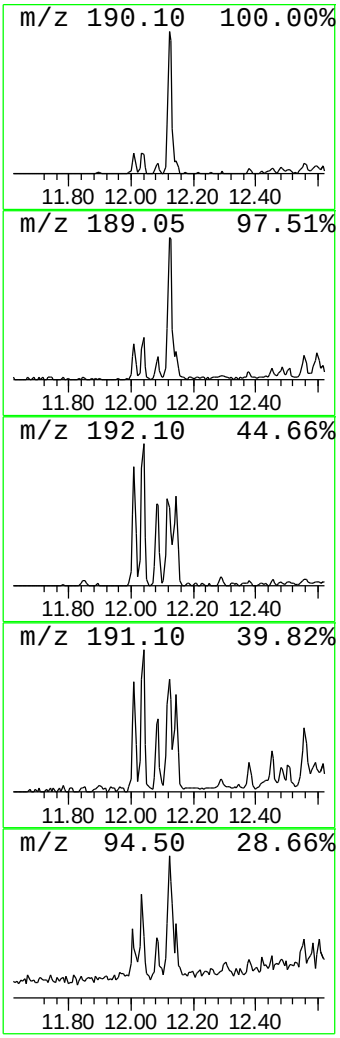
****

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	2.17 ng	143223	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	76
2	6H-Cyclobuta[jk]phenanthrene	190	C15H10	083469-43-6	53
3	Methyl diselenide	190	C2H6Se2	007101-31-7	43
4	2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	37
5	Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	27





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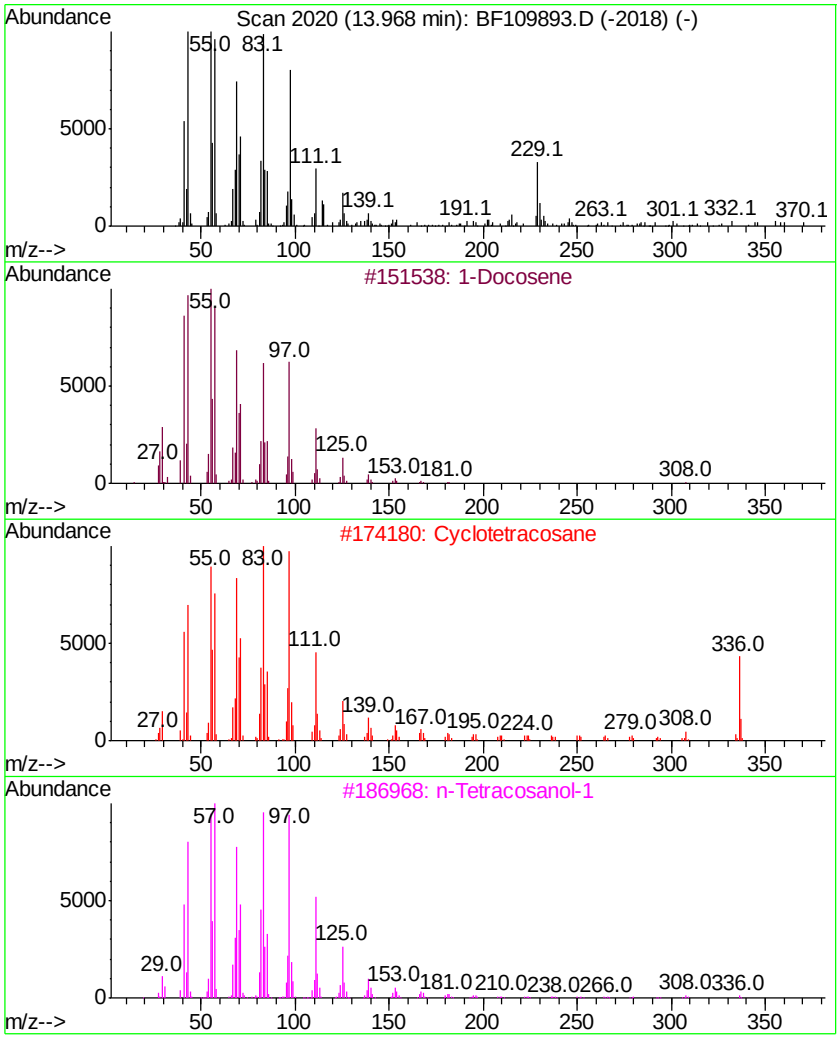
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

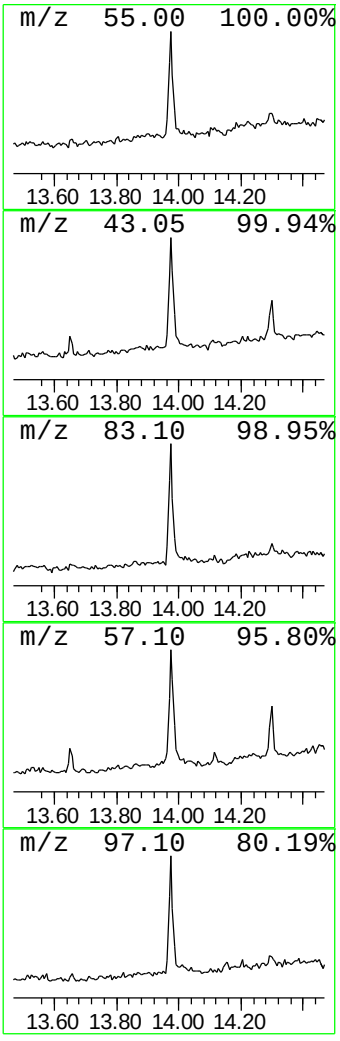
****

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	3.85 ng	402825	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	Cyclotetracosane	336	C24H48	000297-03-0	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	91
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91





Tentatively Identified Compound (LSC) summary

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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...	2.30	10.7	ng	675785	1	6.98	1262630	20.0
2-Pentanone, 4-hy...	5.21	2.4	ng	152592	1	6.98	1262630	20.0
unknown6.75	6.75	55.7	ng	3516460	1	6.98	1262630	20.0
n-Hexadecanoic acid	12.02	3.9	ng	253783	4	11.51	1317710	20.0
4H-Cyclopenta[def...	12.12	2.2	ng	143223	4	11.51	1317710	20.0
1-Docosene	13.97	3.9	ng	402825	5	14.15	2090180	20.0