LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099195.D
Acq On : 7 Oct 2017 15:38
Operator : SJ/JU
Sample : I5586-17 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G56A-0-3

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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	2.128	3	7	14	rVB	75206	92073	5.07%	0.503%
2	4.457	400	403	412	rBV	94943	114434	6.30%	0.625%
3	5.081	504	509	518	rBV	965138	1063806	58.55%	5.810%
4	5.481	574	577	590	rVB	1136710	1021090	56.20%	5.577%
5	6.492	745	749	757	rBV	1555377	1498464	82.47%	8.184%
6	6.634	769	773	776	rBV	1634046	1331970	73.31%	7.275%
7	6.863	808	812	816	rBV	1043175	831296	45.75%	4.540%
8	7.022	833	839	842	rBV	1472810	1342263	73.88%	7.331%
9	7.428	903	908	911	rBV	1107534	957483	52.70%	5.229%
10	8.145	1026	1030	1033	rBV	1326046	1053344	57.97%	5.753%
11	9.216	1208	1212	1216	rBV	2033838	1816933	100.00%	9.923%
12	9.486	1252	1258	1263	rBV4	16757	23610	1.30%	0.129%
13	9.610	1276	1279	1282	rBV	262072	195331	10.75%	1.067%
14	9.822	1310	1315	1318	rBV	23309	23215	1.28%	0.127%
15	9.898	1323	1328	1332	rVV	1143263	1039454	57.21%	5.677%
16	9.933	1332	1334	1337	rVB	22533	19680	1.08%	0.107%
17	10.104	1357	1363	1366	rBV2	22931	27176	1.50%	0.148%
18	10.322	1398	1400	1403	rVB	47372	33535	1.85%	0.183%
19	10.445	1418	1421	1424	rBV2	23376	21202	1.17%	0.116%
20	10.686	1459	1462	1465	rBV	28981	28594	1.57%	0.156%
21	10.792	1477	1480	1485	rBV	56453	78479	4.32%	0.429%
22	10.992	1508	1514	1517	rBV7	12891	21949	1.21%	0.120%
23	11.239	1553	1556	1559	rBV3	46856	41269	2.27%	0.225%
24	11.269	1559	1561	1568	rVB3	22335	38305	2.11%	0.209%
25	11.386	1577	1581	1583	rBV	1014343	862155	47.45%	4.709%
26	11.410	1583	1585	1588	rVV	282114	218200	12.01%	1.192%
27	11.463	1591	1594	1597	rVB	58894	48378	2.66%	0.264%
28	11.598	1613	1617	1619	rBV2	32420	40549	2.23%	0.221%
29	11.616	1619	1620	1625	rVV	30013	25779	1.42%	0.141%
30	11.663	1626	1628	1635	rVB2	22463	22681	1.25%	0.124%
31	11.769	1643	1646	1649	rBV3	22703	20038	1.10%	0.109%
32	11.886	1663	1666	1668	rBV	32693	28163	1.55%	0.154%
33	11.916	1668	1671	1675	rVB	51468	44123	2.43%	0.241%
34	11.998	1682	1685	1687	rBV2	44237	47953	2.64%	0.262%

LSC Area Percent Report

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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G56A-0-3

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:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.021	1687	1689	1692	rVB	27715	22630	1.25%	0.124%
36	12.074	1694	1698	1703	rBV4	22740	29641	1.63%	0.162%
37	12.180	1713	1716	1719	rBV	29879	25529	1.41%	0.139%
38	12.433	1756	1759	1762	rBV	27720	27036	1.49%	0.148%
39	12.463	1762	1764	1768	rBV3	24699	34466	1.90%	0.188%
40	12.598	1784	1787	1790	rBV	307741	249069	13.71%	1.360%
41	12.827	1820	1826	1828	rBV	347985	457430	25.18%	2.498%
42	12.851	1828	1830	1841	rVB	516239	545494	30.02%	2.979%
43	12.968	1846	1850	1853	rBV	1404516	1182253	65.07%	6.457%
44	13.151	1879	1881	1885	rVB	38155	40538	2.23%	0.221%
45	13.221	1891	1893	1896	rVB	27910	19893	1.09%	0.109%
46	13.439	1928	1930	1935	rBV	66952	60117	3.31%	0.328%
47	13.851	1997	2000	2008	rVB4	72015	95430	5.25%	0.521%
48	14.027	2026	2030	2033	rBV	806135	794008	43.70%	4.336%
49	14.051	2033	2034	2037	rVB	102702	52525	2.89%	0.287%
50	15.504	2277	2281	2285	rBV	501649	600881	33.07%	3.282%

Sum of corrected areas: 18309914

LSC Report - Integrated Chromatogram

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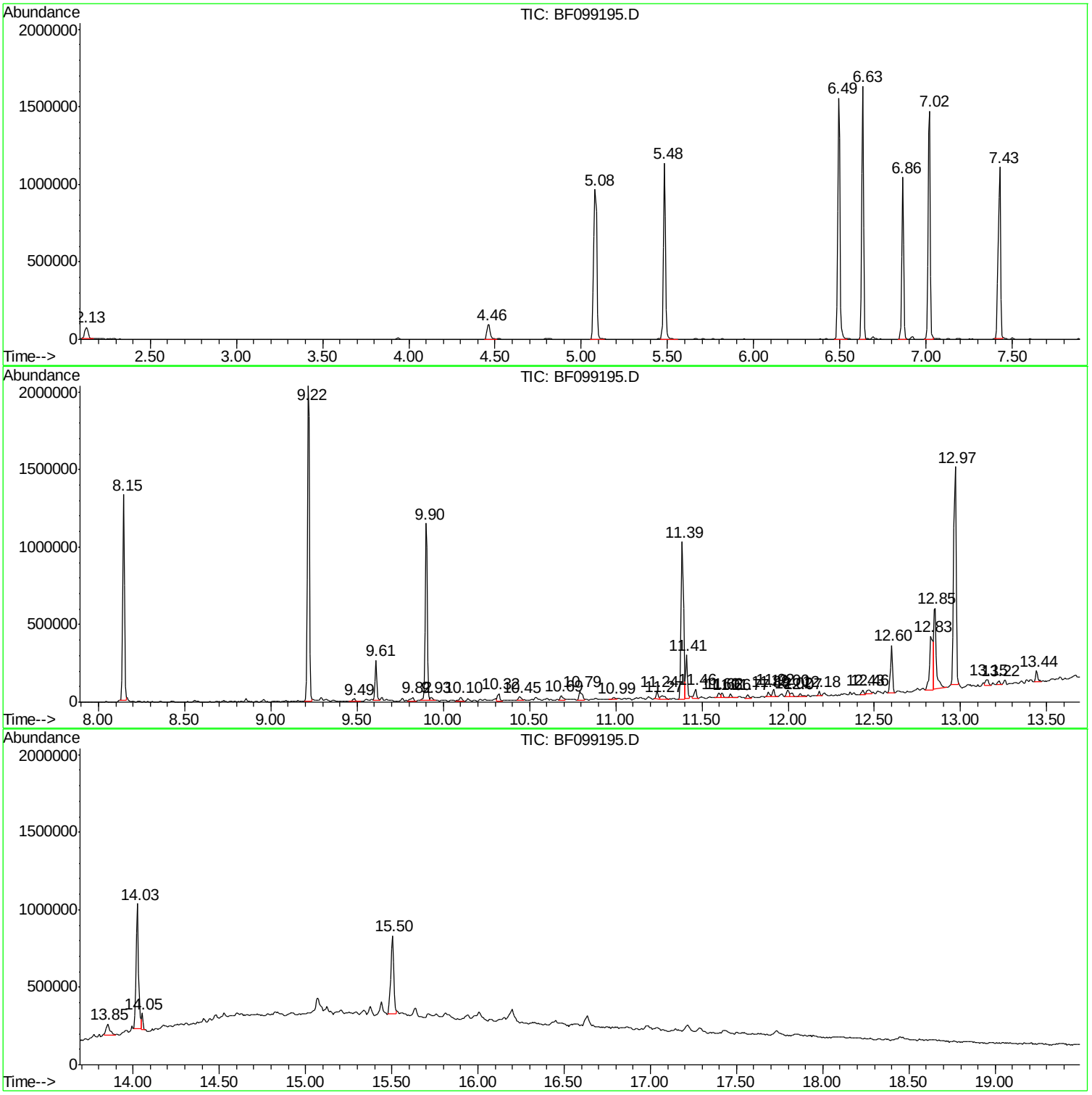
Sample : I5586-17 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G56A-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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:\HPCHEM1\BNA F\DATA\BF100717\
Data File : BF099195.D
Acq On : 7 Oct 2017 15:38
Operator : SJ/JU
Sample : I5586-17 2X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : G56A-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

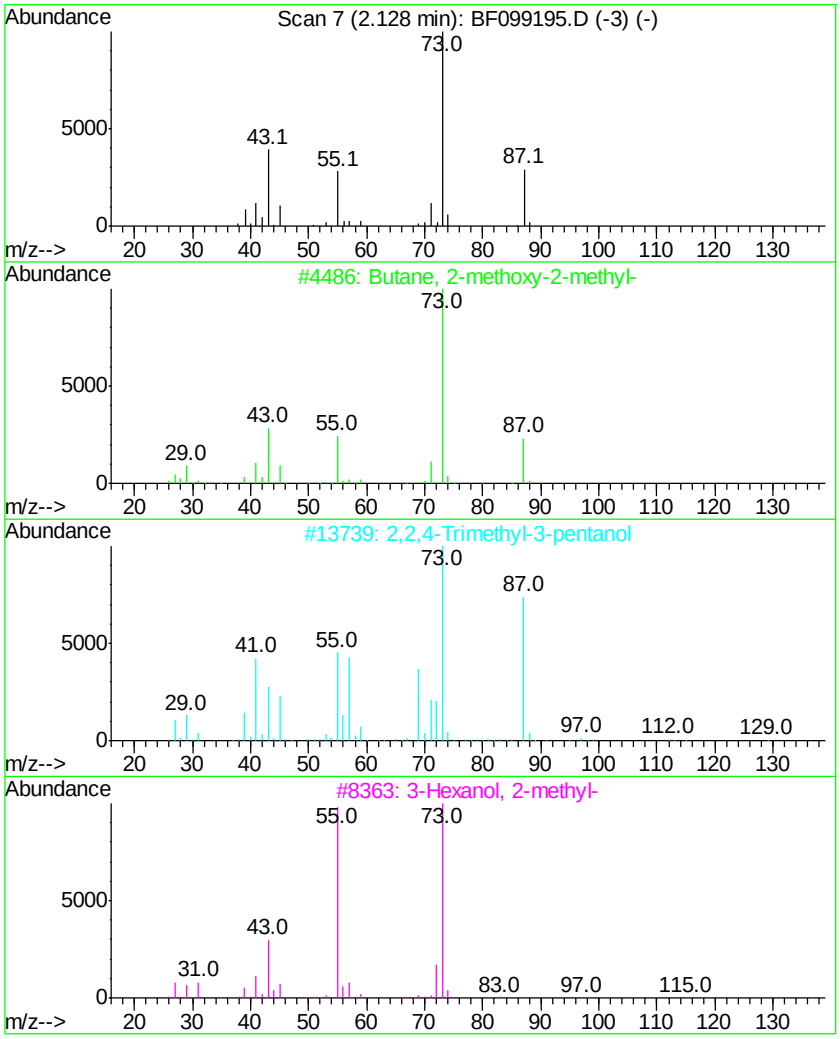
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

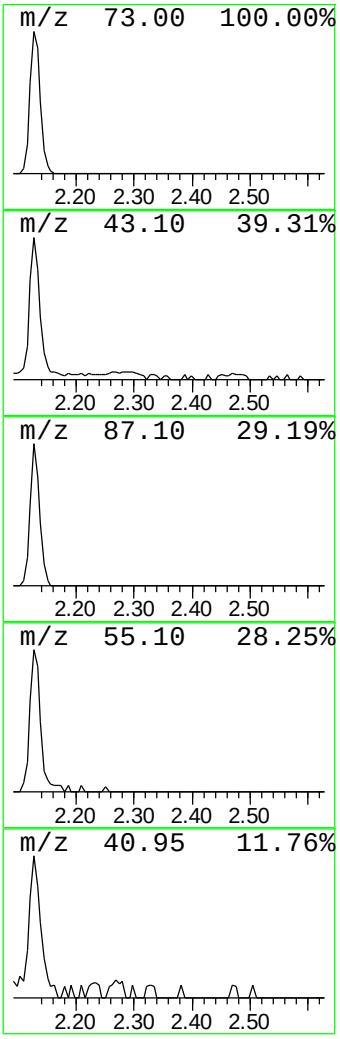
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	2.22 ng	92073	1,4-Dichlorobenzene-d4	6.86

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	39
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Acq On : 7 Oct 2017 15:38
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Instrument : BNA_F
ClientSampleId : G56A-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

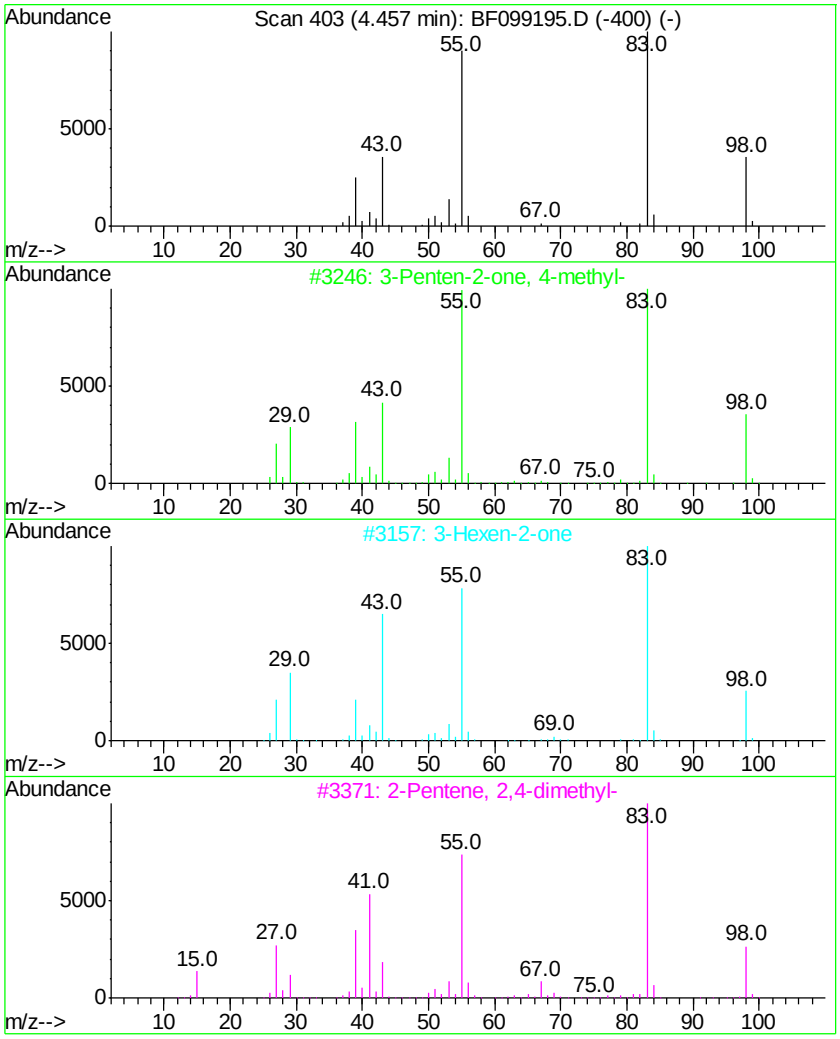
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

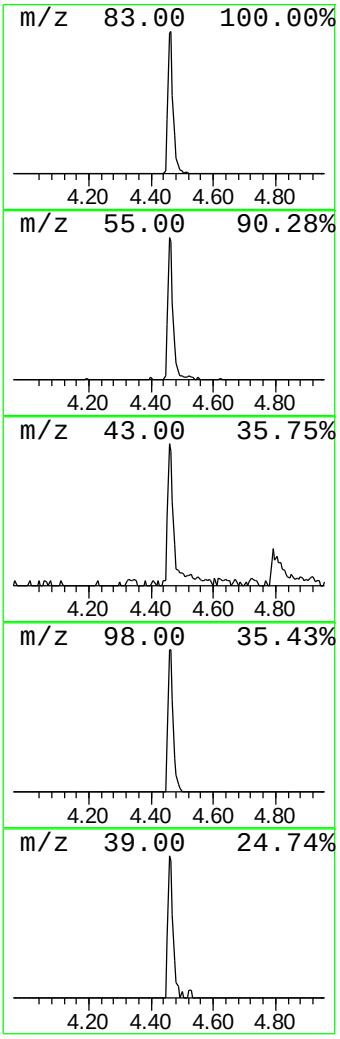
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	2.75 ng	114434	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF100717\
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Acq On : 7 Oct 2017 15:38
Operator : SJ/JU
Sample : I5586-17 2X
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Instrument : BNA_F
ClientSampleId : G56A-0-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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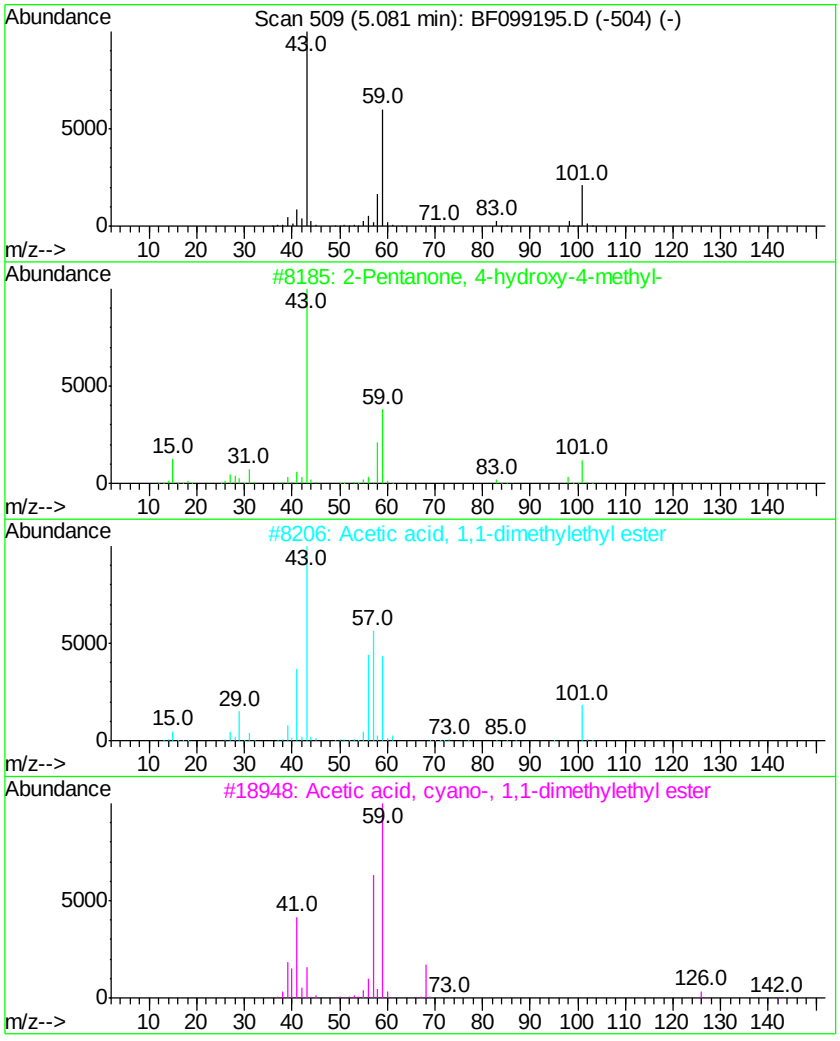
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

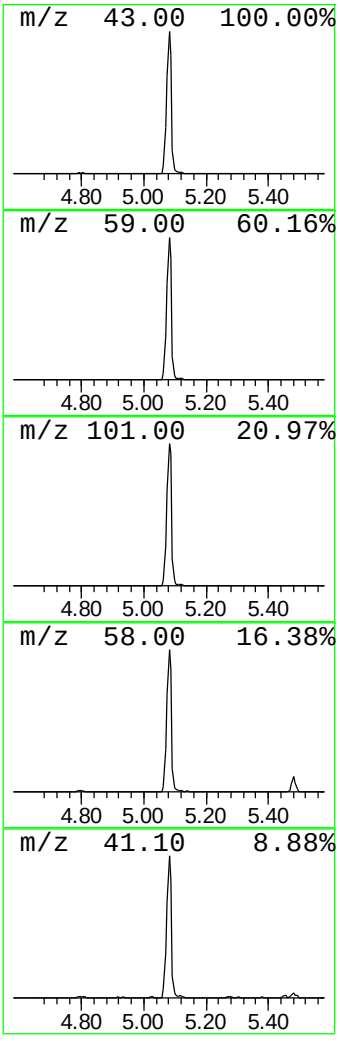
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	25.59 ng	1063810	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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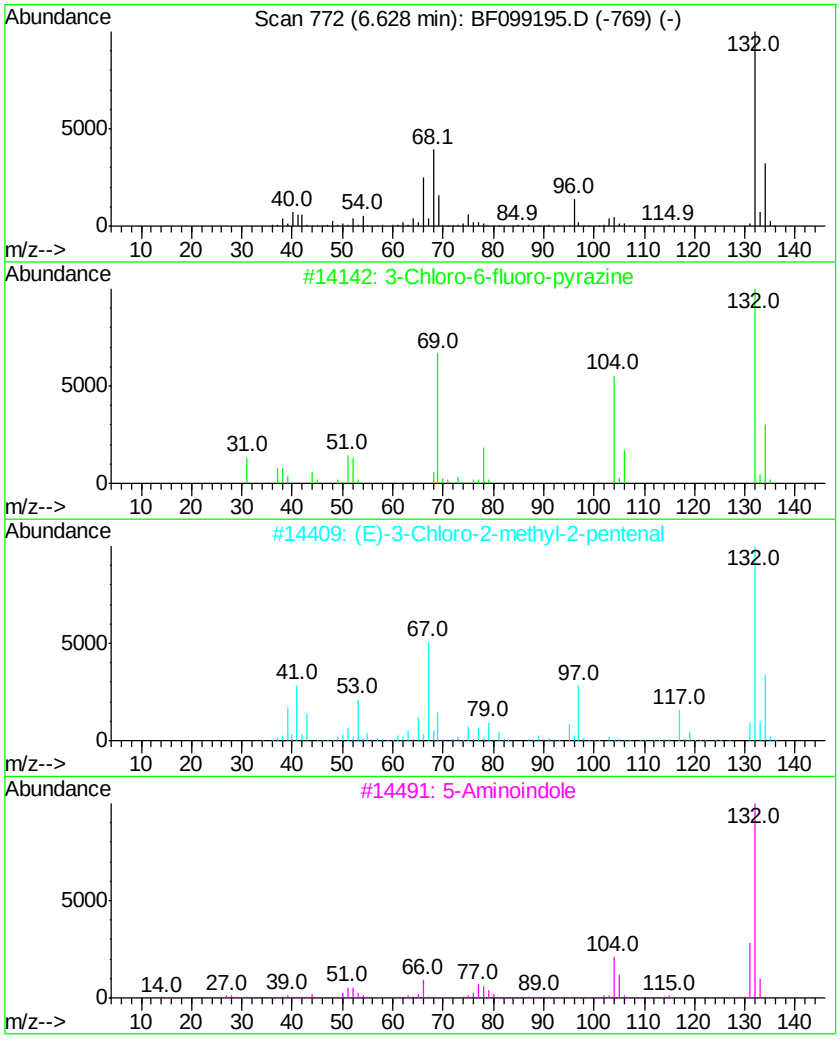
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

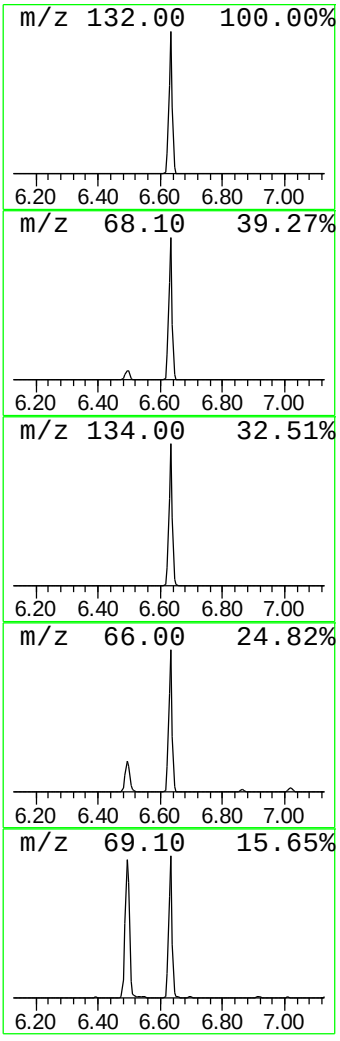
****

Peak Number 4 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	32.05 ng	1331970	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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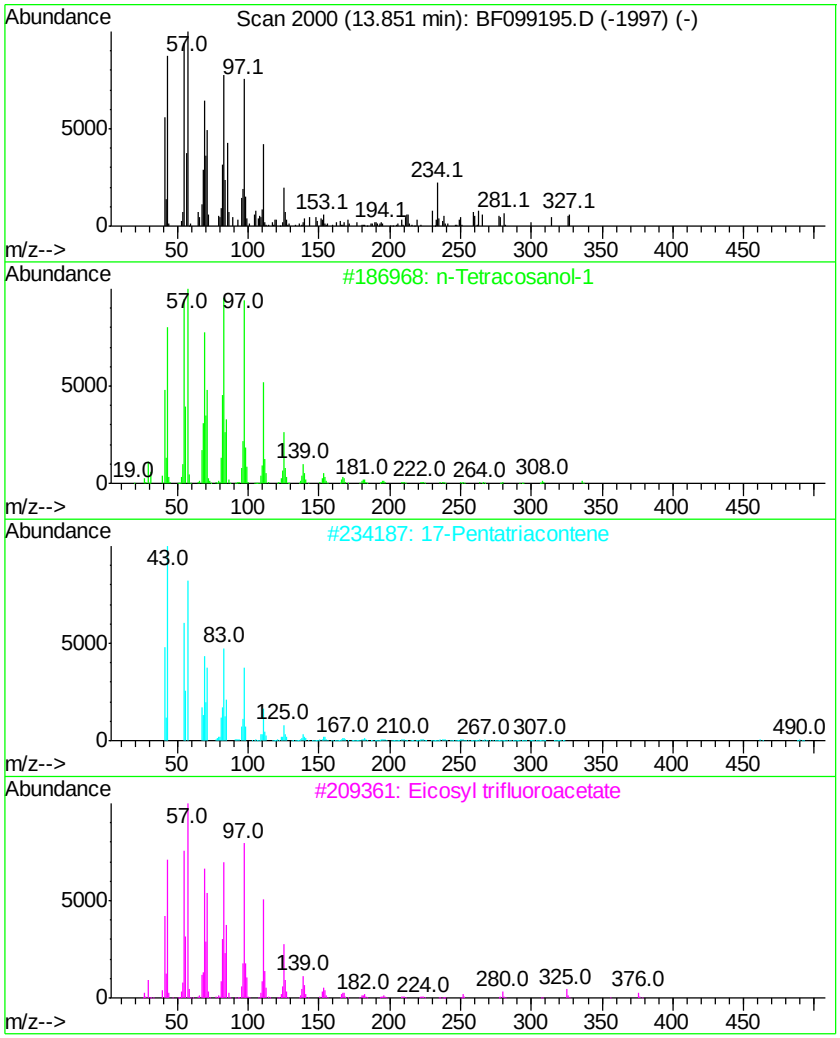
TIC Integration Parameters: LSCINT.P

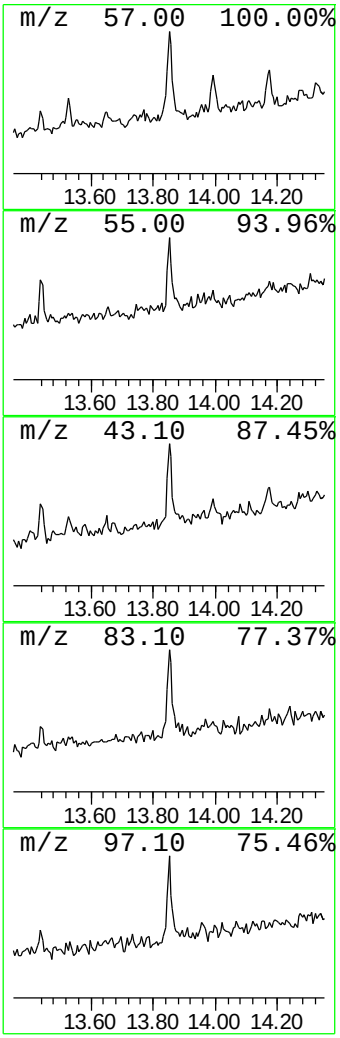
****

Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.40 ng	95430	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	90
3	Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	90
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
5	Octacosanol	410	C28H58O	000557-61-9	87





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...	2.13	2.2	ng	92073	1	6.86	831296	20.0
3-Penten-2-one, 4...	4.46	2.8	ng	114434	1	6.86	831296	20.0
2-Pentanone, 4-hy...	5.08	25.6	ng	1063810	1	6.86	831296	20.0
unknown6.63	6.63	32.0	ng	1331970	1	6.86	831296	20.0
n-Tetracosanol-1	13.85	2.4	ng	95430	5	14.03	794008	20.0