LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
Data File : BF101818.D
Acq On : 29 Dec 2017 10:19
Operator : SJ/JU
Sample : I7000-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15-2(0-2.5)

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-BF121417.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	5.004	493	496	507	rBV	113848	203792	7.38%	0.732%
2	5.404	561	564	598	rBV	1744168	2718978	98.47%	9.772%
3	6.428	735	738	756	rBV	1898602	2761156	100.00%	9.923%
4	6.557	756	760	775	rVB	2524259	2624064	95.03%	9.430%
5	6.781	795	798	808	rBV	981927	931522	33.74%	3.348%
6	6.934	821	824	840	rBV	1833150	1941352	70.31%	6.977%
7	7.351	892	895	914	rBV	1435927	1712156	62.01%	6.153%
8	8.063	1013	1016	1038	rVB	1251479	1272630	46.09%	4.574%
9	9.139	1195	1199	1207	rBV	2420853	2392440	86.65%	8.598%
10	9.204	1207	1210	1214	rVB	65493	53324	1.93%	0.192%
11	9.533	1260	1266	1272	rBV	223240	260784	9.44%	0.937%
12	9.733	1297	1300	1303	rVB	144289	105055	3.80%	0.378%
13	9.822	1311	1315	1318	rBV	1363275	1258342	45.57%	4.522%
14	9.851	1318	1320	1326	rVB	77563	82028	2.97%	0.295%
15	10.033	1347	1351	1353	rBV2	36709	50181	1.82%	0.180%
16	10.233	1382	1385	1388	rVB	146254	110341	4.00%	0.397%
17	10.374	1405	1409	1415	rVB	40230	50103	1.81%	0.180%
18	10.451	1415	1422	1425	rBV3	41478	64859	2.35%	0.233%
19	10.616	1446	1450	1462	rBV	1479950	1565736	56.71%	5.627%
20	10.704	1462	1465	1470	rBV	109735	110586	4.01%	0.397%
21	11.151	1536	1541	1547	rBV4	57328	81445	2.95%	0.293%
22	11.316	1565	1569	1571	rBV	1278657	1249217	45.24%	4.489%
23	11.339	1571	1573	1577	rVV	318299	290952	10.54%	1.046%
24	11.392	1580	1582	1586	rVB	62752	61167	2.22%	0.220%
25	11.563	1608	1611	1616	rBV3	40623	58132	2.11%	0.209%
26	11.821	1651	1655	1658	rBV2	238242	266884	9.67%	0.959%
27	11.927	1670	1673	1676	rBV	49114	55584	2.01%	0.200%
28	12.168	1712	1714	1719	rVB2	23822	28002	1.01%	0.101%
29	12.368	1745	1748	1752	rBV3	29570	38806	1.41%	0.139%
30	12.474	1764	1766	1771	rVB3	22605	30675	1.11%	0.110%
31	12.533	1771	1776	1782	rBV	391765	388578	14.07%	1.396%
32	12.610	1786	1789	1795	rVV	80999	102254	3.70%	0.367%
33	12.692	1800	1803	1809	rVV4	52449	87292	3.16%	0.314%
34	12.745	1809	1812	1813	rVV	85247	89219	3.23%	0.321%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I7000-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15-2(0-2.5)

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.763	1813	1815	1821	rVB	299432	279339	10.12%	1.004%
36	12.892	1833	1837	1842	rBV	2000449	1748474	63.32%	6.284%
37	12.980	1848	1852	1858	rVB3	23407	42765	1.55%	0.154%
38	13.092	1869	1871	1876	rVB2	47468	55407	2.01%	0.199%
39	13.774	1983	1987	1992	rBV2	114483	153285	5.55%	0.551%
40	13.962	2015	2019	2022	rBV2	929940	983362	35.61%	3.534%
41	13.992	2022	2024	2030	rVB	134688	130233	4.72%	0.468%
42	14.686	2139	2142	2149	rVB3	119086	161781	5.86%	0.581%
43	15.015	2194	2198	2200	rBV	125859	168235	6.09%	0.605%
44	15.315	2246	2249	2253	rVB	63715	78509	2.84%	0.282%
45	15.380	2257	2260	2264	rVB	113091	122711	4.44%	0.441%
46	15.433	2265	2269	2275	rBV	632812	803659	29.11%	2.888%

Sum of corrected areas: 27825396

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122917\
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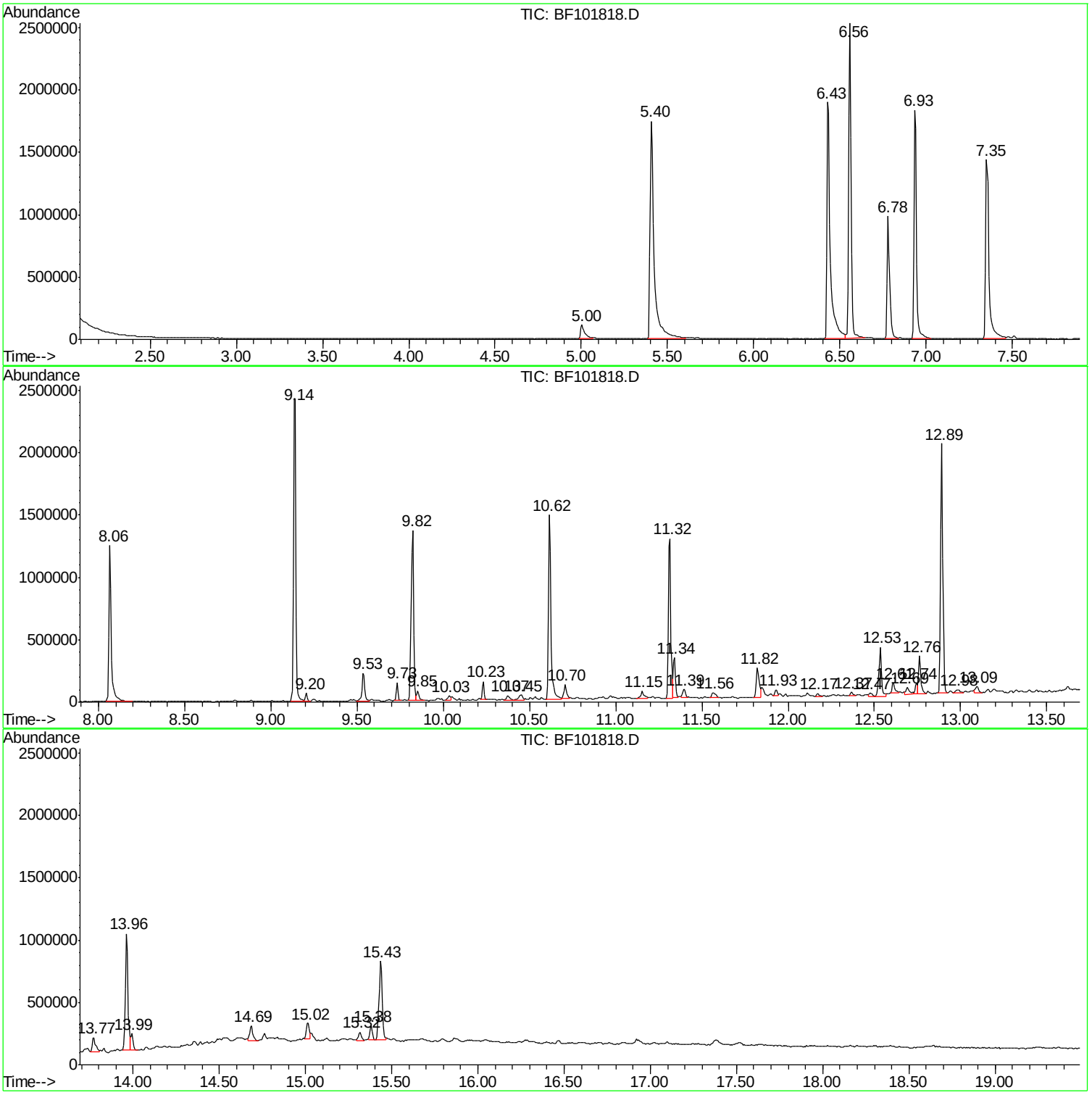
Operator : SJ/JU
Sample : I7000-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15-2(0-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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\BF122917\
Data File : BF101818.D
Acq On : 29 Dec 2017 10:19
Operator : SJ/JU
Sample : I7000-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15-2(0-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

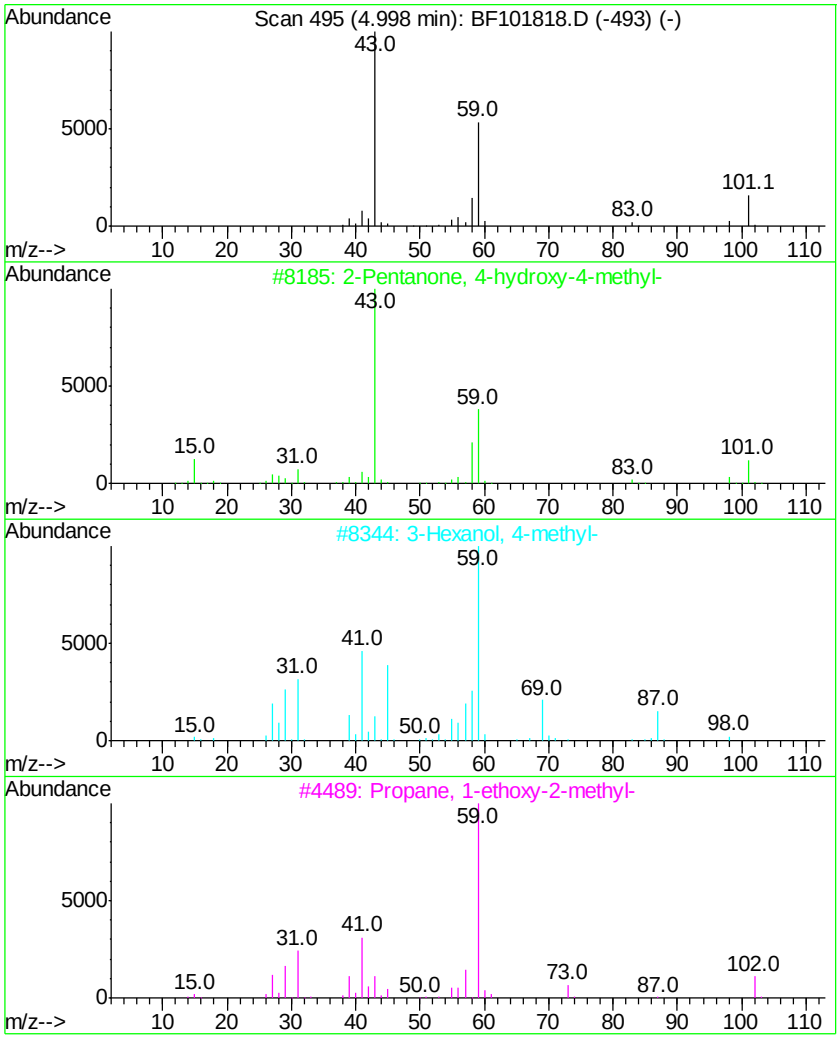
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

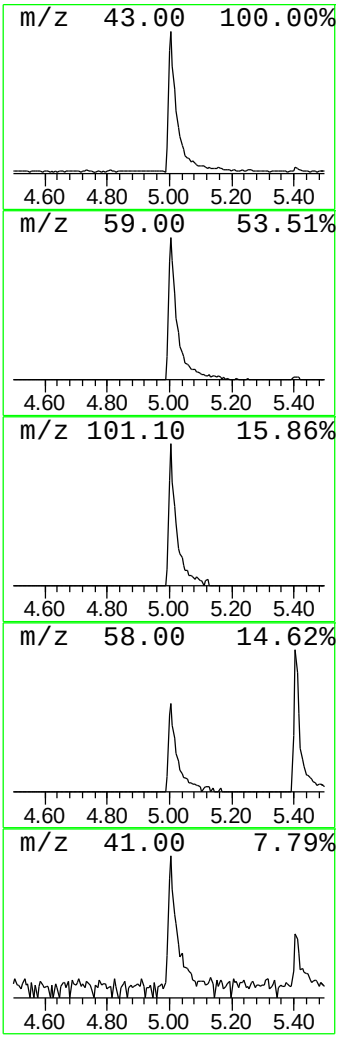
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.38 ng	203792	1,4-Dichlorobenzene-d4	6.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	32
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	23





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Operator : SJ/JU
Sample : I7000-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15-2(0-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

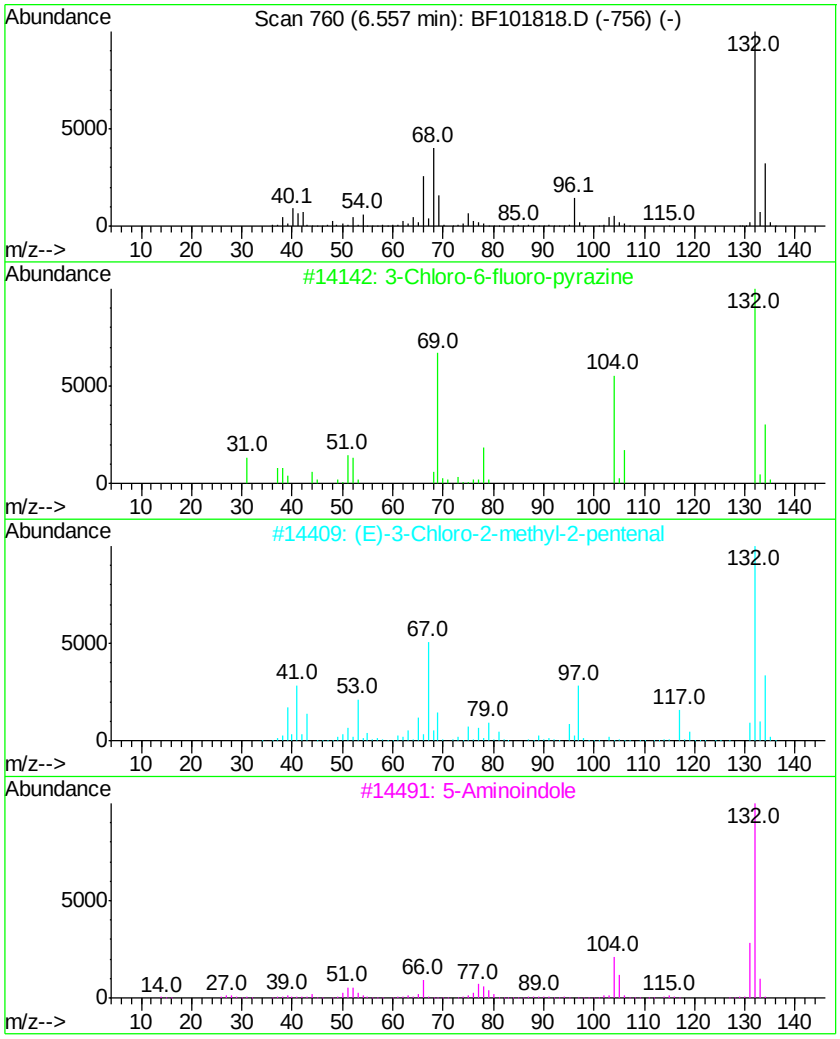
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

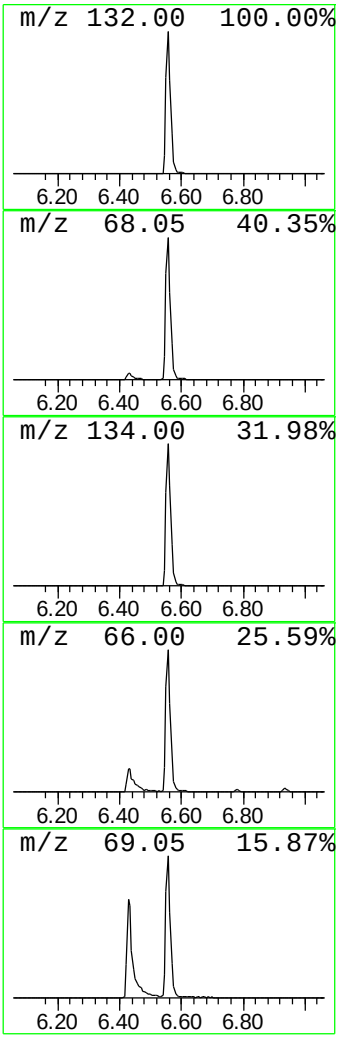
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	56.34 ng	2624060	1,4-Dichlorobenzene-d4	6.78

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Operator : SJ/JU
Sample : I7000-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15-2(0-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

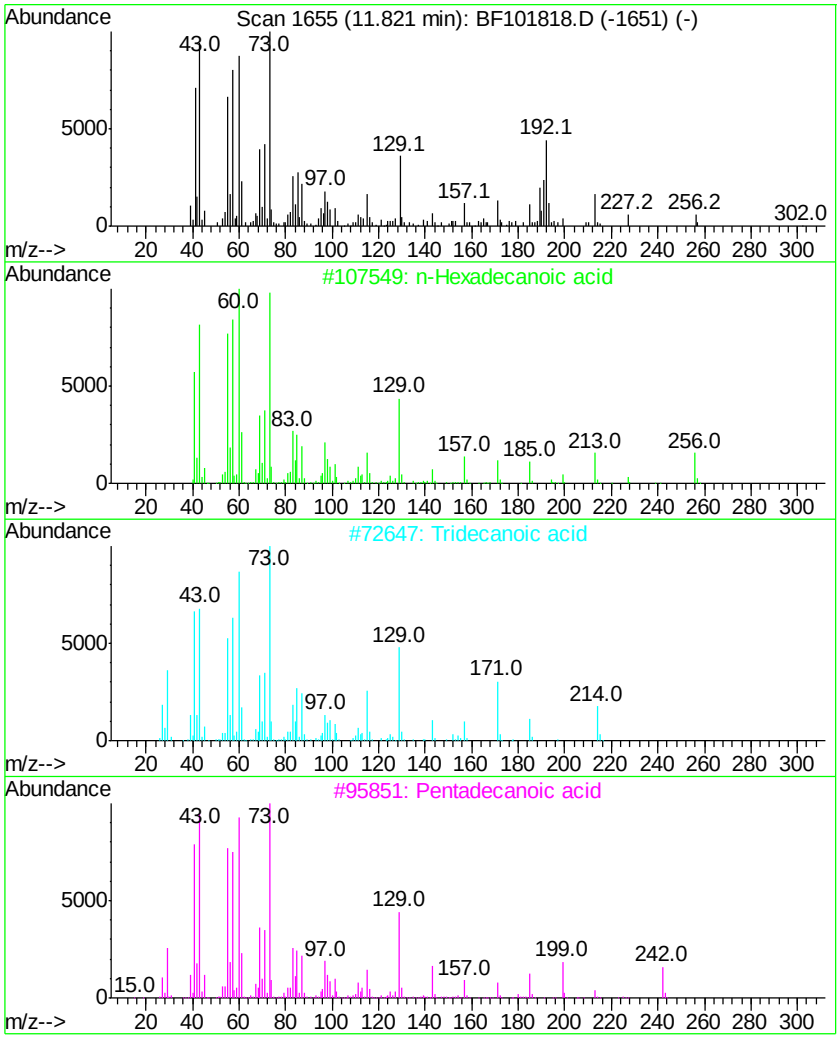
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

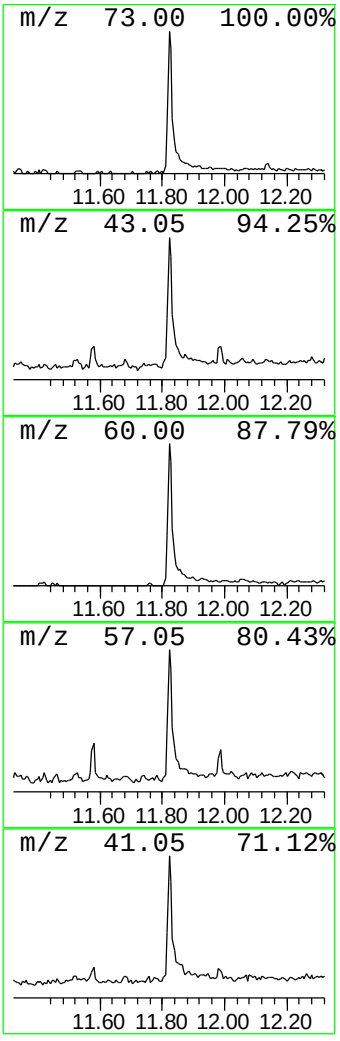
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	4.27 ng	266884	Phenanthrene-d10	11.32

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	n-Decanoic acid	172	C10H20O2	000334-48-5	49





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Operator : SJ/JU
Sample : I7000-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15-2(0-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

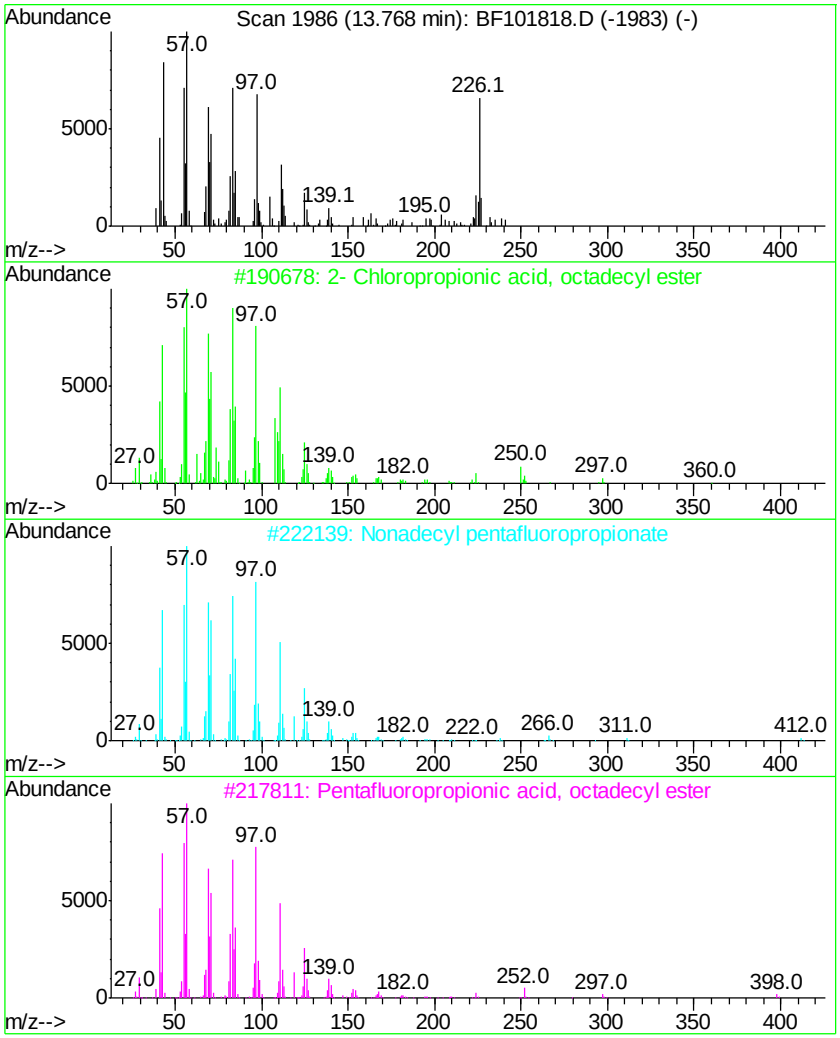
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

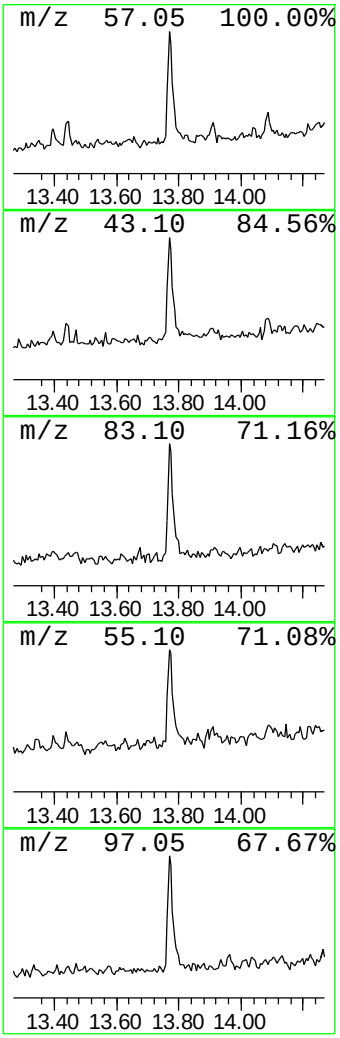
****

Peak Number 5 2- Chloropropionic acid, oc... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	3.12 ng	153285	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	81
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	81
3	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	81
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	81
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81





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Operator : SJ/JU
Sample : I7000-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15-2(0-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

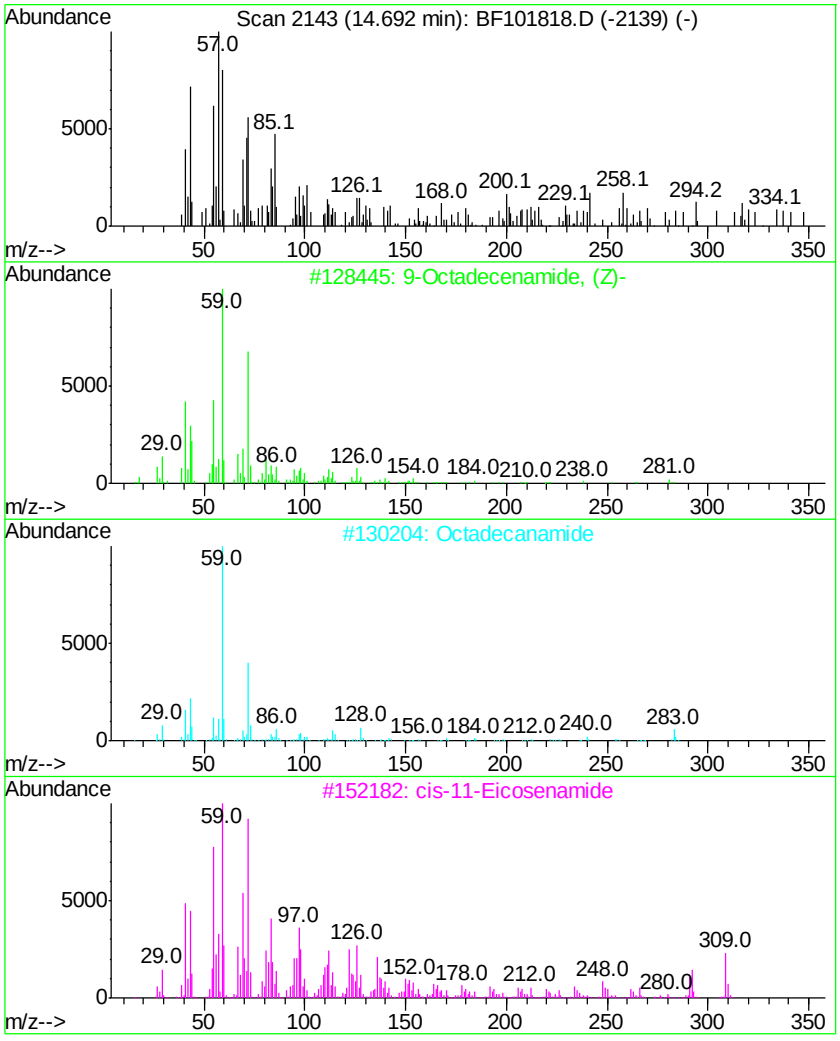
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

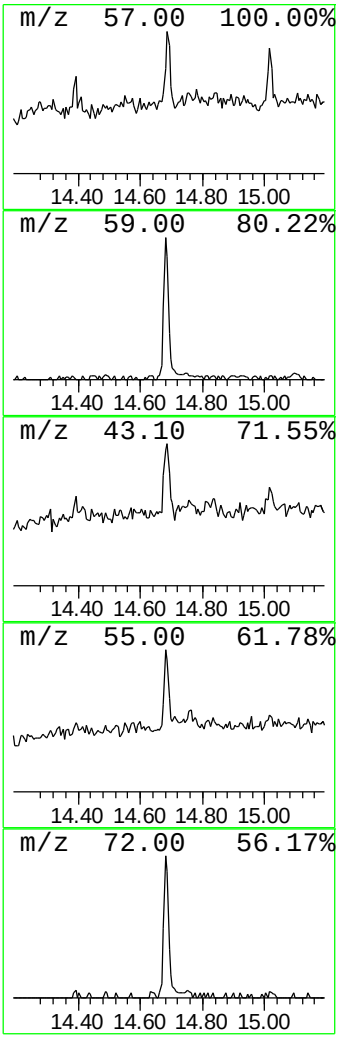
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	3.29 ng	161781	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2	Octadecanamide	283	C18H37NO	000124-26-5	47
3	cis-11-Eicosenamide	309	C20H39NO	010436-08-5	46
4	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	35
5	trans-11-Icosenamide	309	C20H39NO	010586-57-9	35





Tentatively Identified Compound (LSC) summary

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ClientSampleId : TP-15-2(0-2.5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
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
2-Pentanone, 4-hy...	5.00	4.4	ng	203792	1	6.78	931522	20.0
unknown6.56	6.56	56.3	ng	2624060	1	6.78	931522	20.0
n-Hexadecanoic acid	11.82	4.3	ng	266884	4	11.32	1249220	20.0
2- Chloropropioni...	13.77	3.1	ng	153285	5	13.96	983362	20.0
9-Octadecenamide,...	14.69	3.3	ng	161781	5	13.96	983362	20.0