LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096477.D
Acq On : 5 Jul 2017 12:08
Operator : SJ/MA
Sample : I4007-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-MH2094-COMP

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-BF070117.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	3.057	163	165	176	rBV	79529	147922	4.27%	0.496%
2	4.904	474	479	487	rBV	411405	551350	15.91%	1.849%
3	5.328	546	551	554	rBV	2909764	2937824	84.76%	9.853%
4	6.351	716	725	730	rBV	2898338	3466076	100.00%	11.624%
5	6.481	742	747	751	rBV	2956528	3097033	89.35%	10.387%
6	6.710	782	786	790	rBV	888991	758383	21.88%	2.543%
7	6.869	809	813	817	rVB	2508550	2257846	65.14%	7.572%
8	7.275	876	882	885	rBV	2078849	2030003	58.57%	6.808%
9	7.375	894	899	906	rVB	40319	49174	1.42%	0.165%
10	7.992	1000	1004	1007	rBV	1203055	1032959	29.80%	3.464%
11	9.074	1182	1188	1191	rBV	2973049	2607757	75.24%	8.746%
12	9.463	1250	1254	1258	rBV	641646	553454	15.97%	1.856%
13	9.692	1290	1293	1297	rBV	42807	37591	1.08%	0.126%
14	9.745	1297	1302	1306	rVV	1093393	1041742	30.06%	3.494%
15	9.780	1306	1308	1311	rVB	67516	51722	1.49%	0.173%
16	9.951	1334	1337	1341	rVB	55408	45487	1.31%	0.153%
17	10.192	1376	1378	1381	rVB	65785	50711	1.46%	0.170%
18	10.292	1392	1395	1398	rVB	51426	39078	1.13%	0.131%
19	10.533	1431	1436	1440	rBV	1570077	1480846	42.72%	4.966%
20	10.669	1455	1459	1460	rBV	74342	72415	2.09%	0.243%
21	11.033	1517	1521	1525	rVB	41629	41237	1.19%	0.138%
22	11.116	1532	1535	1538	rBV2	80135	87093	2.51%	0.292%
23	11.227	1550	1554	1556	rBV	1079145	938275	27.07%	3.147%
24	11.251	1556	1558	1561	rVV	666356	501316	14.46%	1.681%
25	11.298	1562	1566	1569	rVB	106560	104089	3.00%	0.349%
26	11.451	1586	1592	1596	rBV	66730	67786	1.96%	0.227%
27	11.539	1602	1607	1609	rBV2	47843	44517	1.28%	0.149%
28	11.727	1636	1639	1641	rBV	42469	35500	1.02%	0.119%
29	11.757	1641	1644	1648	rVB2	69249	71596	2.07%	0.240%
30	11.839	1655	1658	1660	rBV	56185	56404	1.63%	0.189%
31	12.039	1691	1692	1696	rVB	46513	36403	1.05%	0.122%
32	12.433	1756	1759	1763	rBV	558860	512963	14.80%	1.720%
33	12.662	1792	1798	1802	rBV	424350	426824	12.31%	1.431%
34	12.815	1820	1824	1827	rVB	1930116	1710794	49.36%	5.738%

LSC Area Percent Report

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Sample : I4007-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-MH2094-COMP

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.092	1868	1871	1874	rBV	34344	35865	1.03%	0.120%
36	13.492	1936	1939	1945	rBV	45335	55140	1.59%	0.185%
37	13.609	1954	1959	1961	rBV2	38986	53252	1.54%	0.179%
38	13.657	1965	1967	1972	rVV2	34221	54527	1.57%	0.183%
39	13.715	1972	1977	1983	rVV2	179452	223964	6.46%	0.751%
40	13.857	1997	2001	2004	rBV2	800004	900268	25.97%	3.019%
41	13.886	2004	2006	2011	rVB	169315	152352	4.40%	0.511%
42	14.715	2143	2147	2152	rBV8	24069	47224	1.36%	0.158%
43	14.868	2169	2173	2176	rBV	160358	239558	6.91%	0.803%
44	14.962	2187	2189	2197	rVB4	59128	104213	3.01%	0.350%
45	15.151	2217	2221	2225	rBV2	89726	111285	3.21%	0.373%
46	15.209	2227	2231	2236	rVV	105773	126780	3.66%	0.425%
47	15.268	2236	2241	2245	rBV	499058	580934	16.76%	1.948%
48	16.203	2396	2400	2405	rBV4	26594	45719	1.32%	0.153%
49	16.621	2467	2471	2481	rVB2	40983	81712	2.36%	0.274%
50	17.027	2536	2540	2550	rVB2	28400	60659	1.75%	0.203%

Sum of corrected areas: 29817622

LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096477.D
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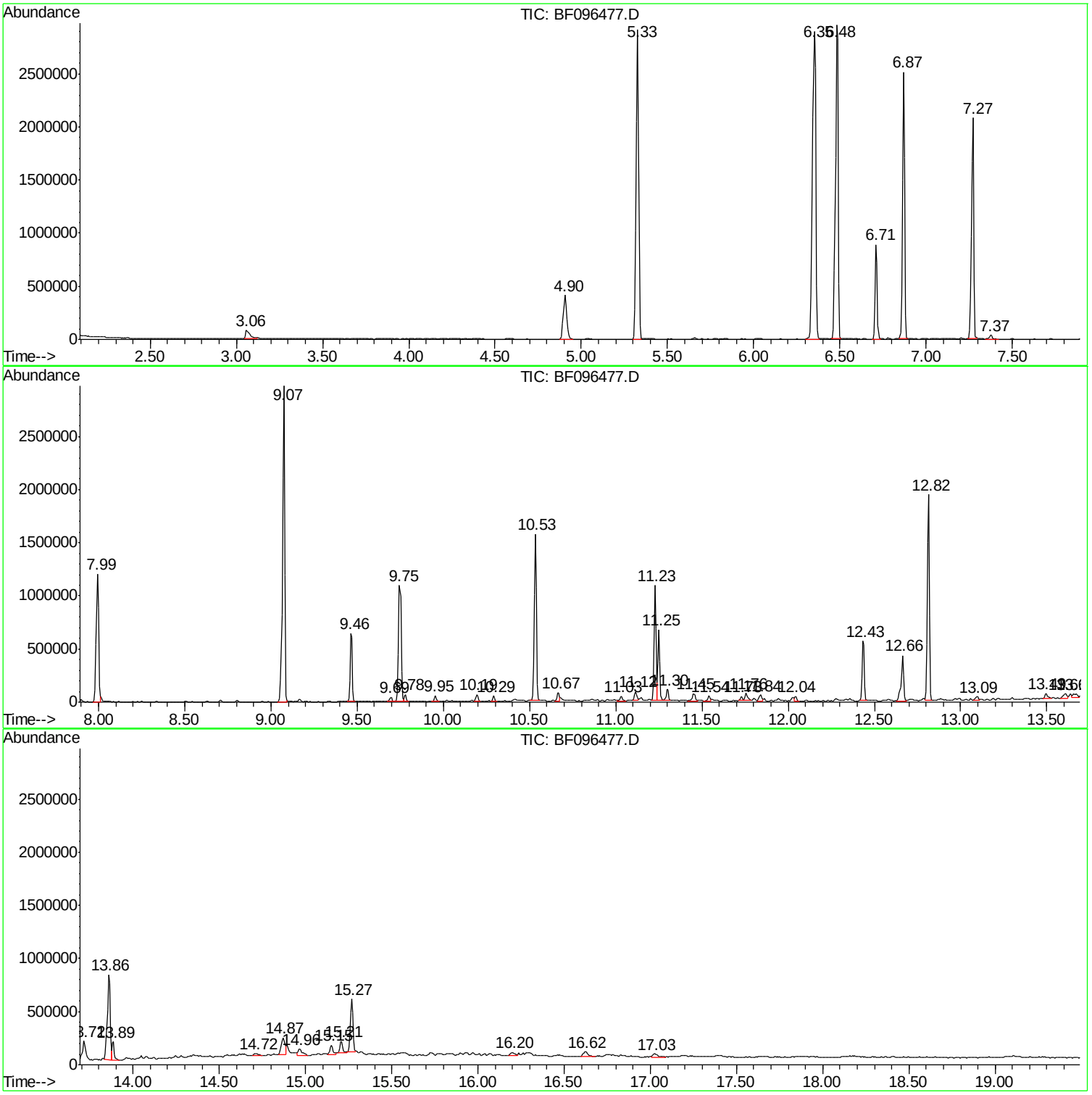
Operator : SJ/MA
Sample : I4007-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-MH2094-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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\BF070517\
Data File : BF096477.D
Acq On : 5 Jul 2017 12:08
Operator : SJ/MA
Sample : I4007-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-MH2094-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

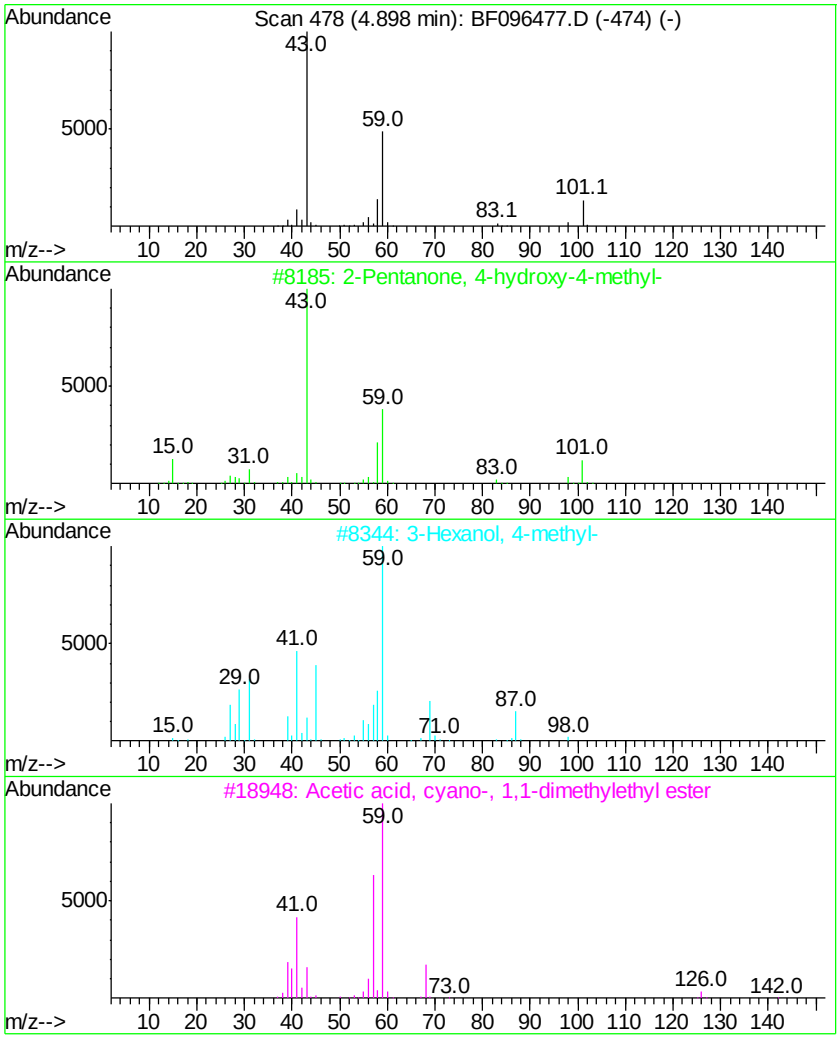
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

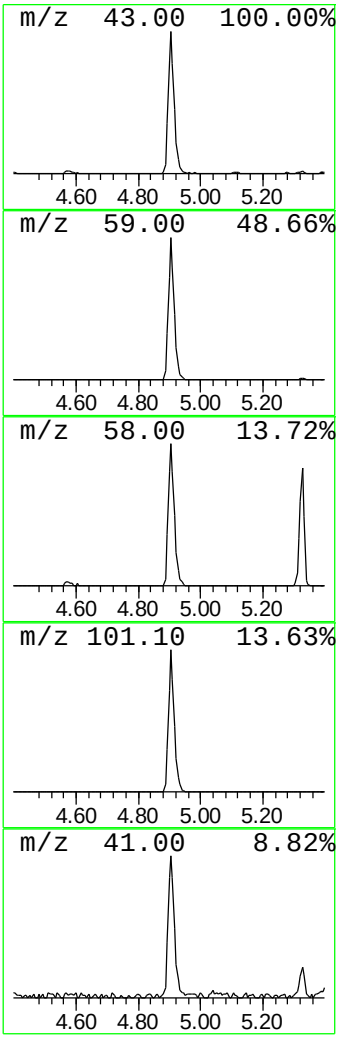
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	14.54 ng	551350	1,4-Dichlorobenzene-d4	6.71

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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
Data File : BF096477.D
Acq On : 5 Jul 2017 12:08
Operator : SJ/MA
Sample : I4007-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-MH2094-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

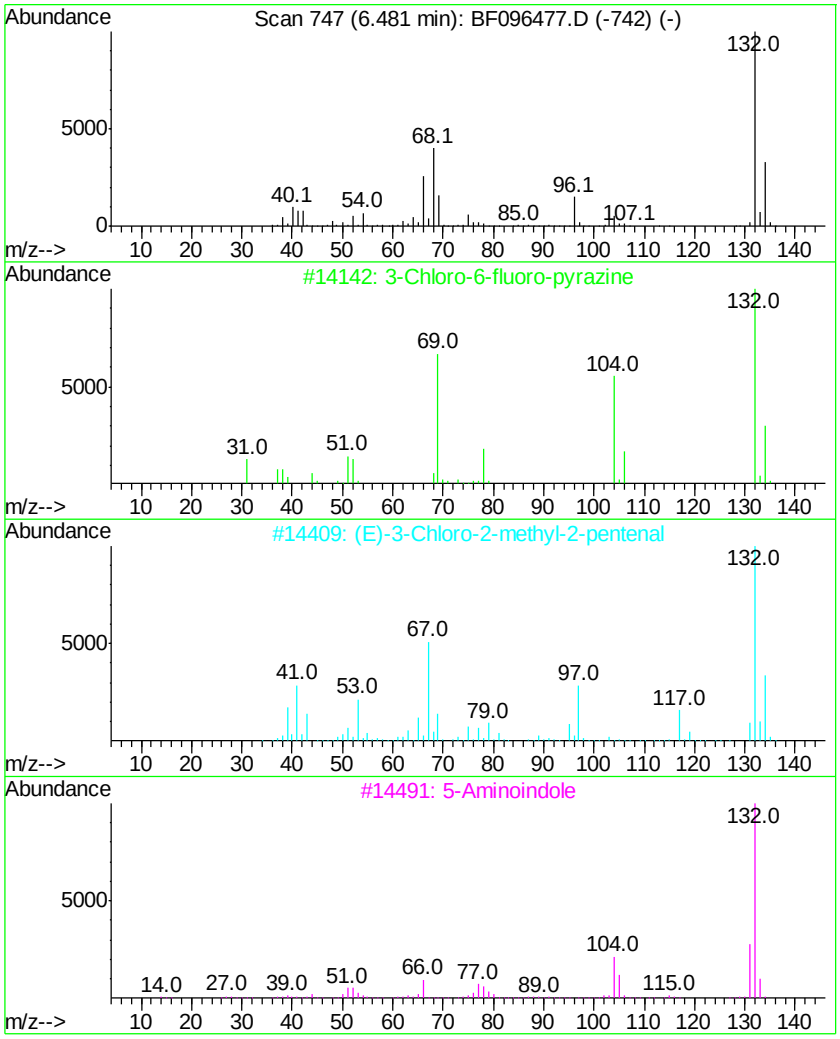
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

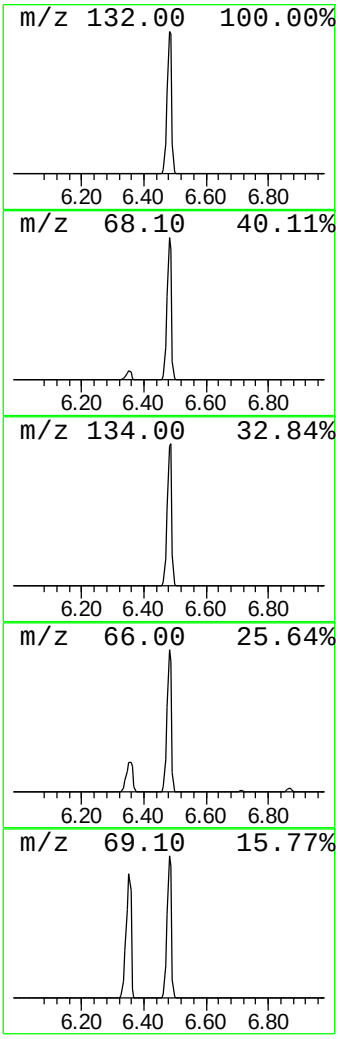
****

Peak Number 3 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	81.67 ng	3097030	1,4-Dichlorobenzene-d4	6.71

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	17
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





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Operator : SJ/MA
Sample : I4007-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP2-MH2094-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

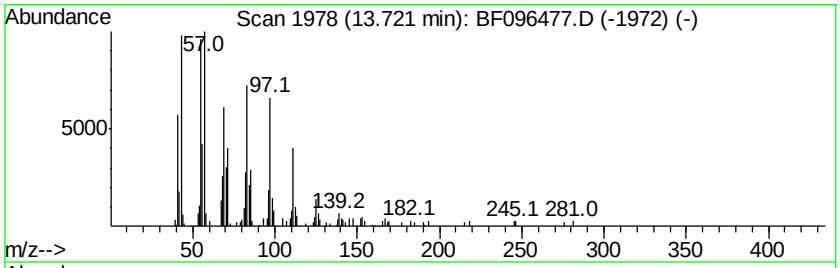
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

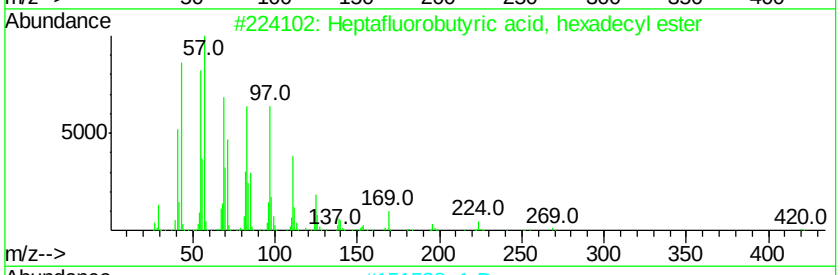
****

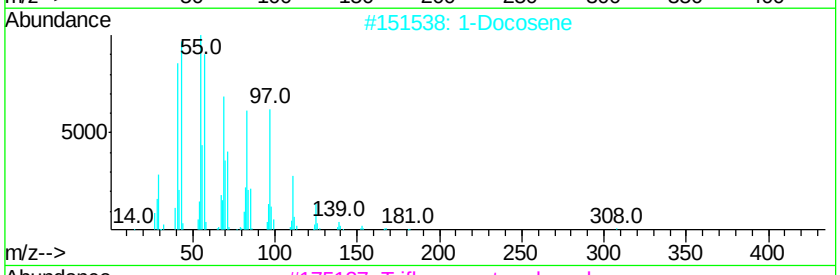
Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 4

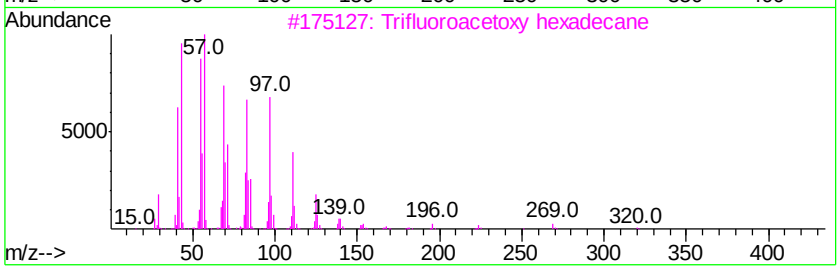
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.98 ng	223964	Chrysene-d12	13.86

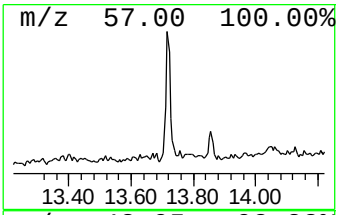
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91

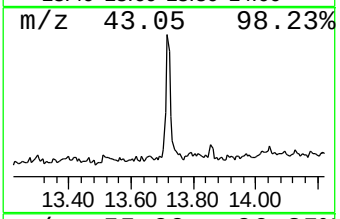


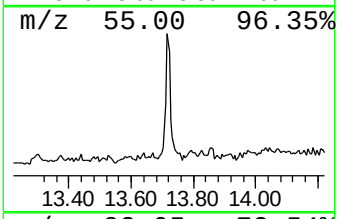


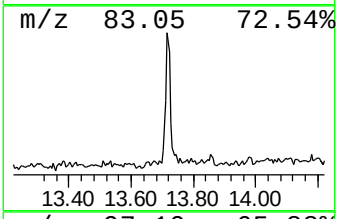


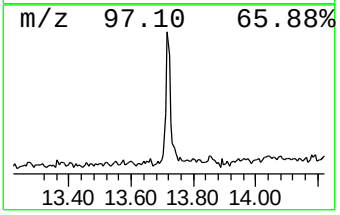












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Misc :
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Instrument : BNA_F
ClientSampleId : TP2-MH2094-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

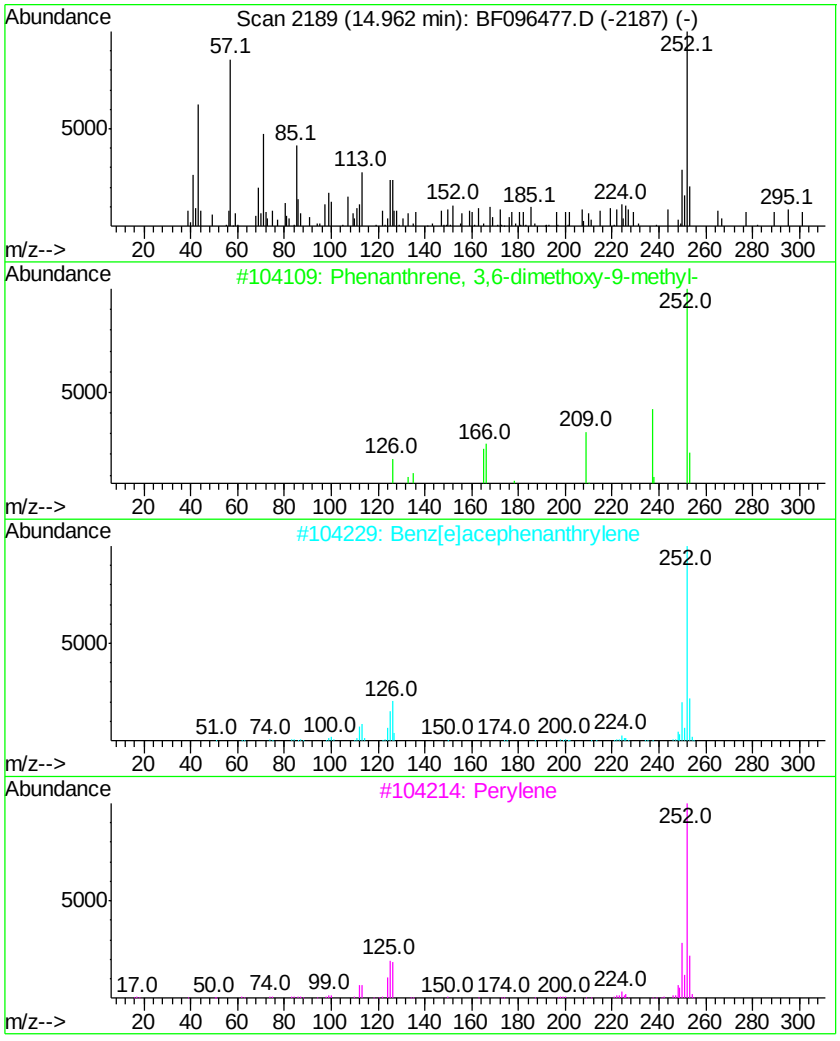
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

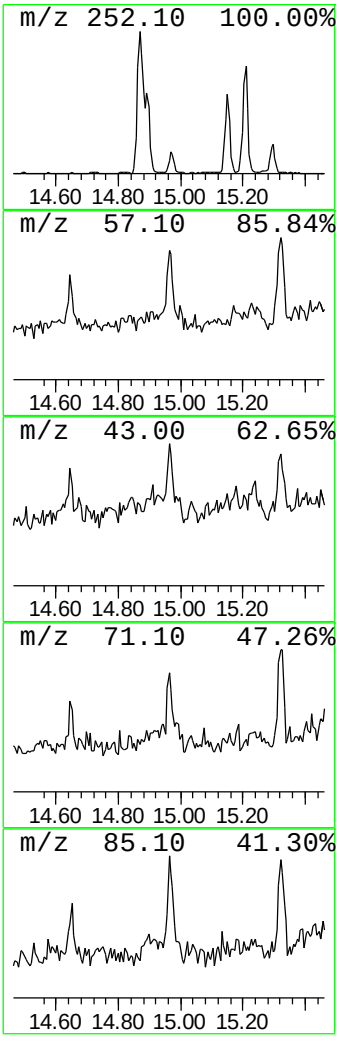
****

Peak Number 6 Phenanthrene, 3,6-dimethoxy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.59 ng	104213	Perylene-d12	15.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 3,6-dimethoxy-9-me...	252	C17H16O2	015638-09-2	59
2	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	50
3	Perylene	252	C20H12	000198-55-0	46
4	Benzo[e]pyrene	252	C20H12	000192-97-2	46
5	Benzo[a]pyrene	252	C20H12	000050-32-8	46





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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...	4.90	14.5	ng	551350	1	6.71	758383	20.0
unknown6.48	6.48	81.7	ng	3097030	1	6.71	758383	20.0
Heptafluorobutyri...	13.72	5.0	ng	223964	5	13.86	900268	20.0
Phenanthrene, 3,6...	14.96	3.6	ng	104213	6	15.27	580934	20.0