LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100852.D
Acq On : 23 Nov 2017 4:21
Operator : SJ/JU
Sample : I6548-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-2-E(4-5)

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-BF110817.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	5.081	505	509	518	rVB	103943	120773	7.56%	0.779%
2	5.475	572	576	580	rBV	1324405	1300785	81.47%	8.393%
3	6.492	743	749	755	rBV	1297742	1362451	85.33%	8.791%
4	6.628	768	772	775	rBV	1493068	1367144	85.63%	8.821%
5	6.857	808	811	815	rVB	595742	498979	31.25%	3.219%
6	7.016	834	838	841	rBV	1348988	1097939	68.77%	7.084%
7	7.422	902	907	910	rBV	946214	836230	52.38%	5.395%
8	8.139	1025	1029	1033	rBV	782775	640049	40.09%	4.130%
9	9.216	1207	1212	1215	rBV	1967216	1596601	100.00%	10.301%
10	9.604	1275	1278	1281	rBV	113318	95283	5.97%	0.615%
11	9.822	1307	1315	1318	rBV	61839	60518	3.79%	0.390%
12	9.898	1324	1328	1331	rBV	796206	665051	41.65%	4.291%
13	10.322	1397	1400	1403	rVB	72580	61420	3.85%	0.396%
14	10.439	1416	1420	1425	rVB2	19991	21227	1.33%	0.137%
15	10.539	1433	1437	1439	rBV2	21750	25348	1.59%	0.164%
16	10.686	1458	1462	1465	rVB	923998	766424	48.00%	4.945%
17	10.792	1477	1480	1486	rBV	76870	82038	5.14%	0.529%
18	11.239	1552	1556	1559	rBV2	62954	50998	3.19%	0.329%
19	11.269	1559	1561	1567	rVB2	23404	27903	1.75%	0.180%
20	11.386	1577	1581	1583	rBV	666750	610062	38.21%	3.936%
21	11.404	1583	1584	1588	rVV	206517	153670	9.62%	0.991%
22	11.457	1590	1593	1596	rVB	48342	40680	2.55%	0.262%
23	11.610	1613	1619	1625	rBV3	17155	37781	2.37%	0.244%
24	11.669	1625	1629	1634	rVB2	37231	37236	2.33%	0.240%
25	11.898	1662	1668	1674	rBV2	53946	109868	6.88%	0.709%
26	11.998	1681	1685	1687	rBV2	37213	38194	2.39%	0.246%
27	12.074	1695	1698	1703	rBV	33183	31734	1.99%	0.205%
28	12.463	1761	1764	1767	rVB2	28114	23142	1.45%	0.149%
29	12.516	1771	1773	1779	rVB4	14616	20783	1.30%	0.134%
30	12.598	1783	1787	1790	rBV	226858	203200	12.73%	1.311%
31	12.827	1820	1826	1831	rBV	209567	231452	14.50%	1.493%
32	12.968	1846	1850	1853	rBV	1151846	1017225	63.71%	6.563%
33	13.039	1858	1862	1867	rBV6	17478	26722	1.67%	0.172%
34	13.127	1874	1877	1879	rBV5	14815	18988	1.19%	0.123%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
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Acq On : 23 Nov 2017 4:21
Operator : SJ/JU
Sample : I6548-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-2-E(4-5)

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-BF110817.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.151	1879	1881	1885	rVB2	27347	27981	1.75%	0.181%
36	13.257	1895	1899	1901	rBV2	23175	23401	1.47%	0.151%
37	13.533	1942	1946	1948	rBV5	13871	18746	1.17%	0.121%
38	13.657	1964	1967	1973	rBV	17886	20536	1.29%	0.132%
39	13.768	1983	1986	1989	rBV3	14677	19678	1.23%	0.127%
40	13.851	1997	2000	2005	rBV4	58548	68191	4.27%	0.440%
41	14.021	2021	2029	2032	rBV2	547647	618823	38.76%	3.993%
42	14.045	2032	2033	2040	rVB	98517	87762	5.50%	0.566%
43	14.404	2092	2094	2098	rVB2	23217	23485	1.47%	0.152%
44	15.062	2202	2206	2213	rBV	95912	187750	11.76%	1.211%
45	15.121	2213	2216	2221	rVV3	25186	38313	2.40%	0.247%
46	15.168	2221	2224	2228	rVB	21257	23294	1.46%	0.150%
47	15.368	2255	2258	2264	rVB	57919	73207	4.59%	0.472%
48	15.427	2265	2268	2275	rVB	85343	105552	6.61%	0.681%
49	15.498	2275	2280	2284	rBV	428413	562280	35.22%	3.628%
50	15.939	2351	2355	2359	rBV2	39266	54701	3.43%	0.353%
51	16.445	2436	2441	2447	rVB3	38692	69081	4.33%	0.446%
52	16.962	2525	2529	2536	rVV3	33195	59826	3.75%	0.386%
53	17.039	2538	2542	2548	rVB6	26464	56181	3.52%	0.362%
54	17.409	2600	2605	2613	rBV2	25754	47161	2.95%	0.304%
55	17.739	2657	2661	2668	rVB6	17910	35167	2.20%	0.227%

Sum of corrected areas: 15499014

LSC Report - Integrated Chromatogram

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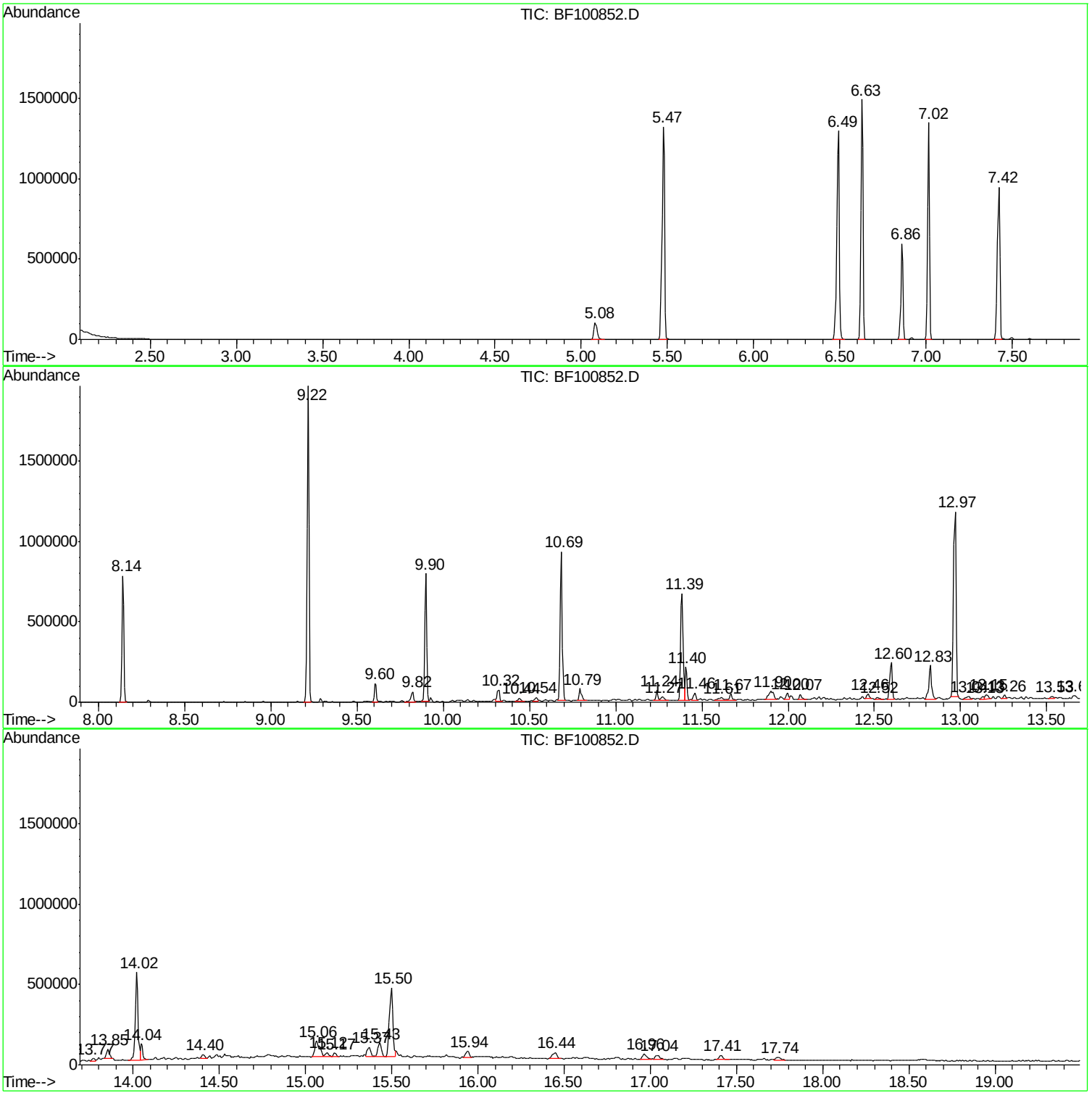
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SAU-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100852.D
Acq On : 23 Nov 2017 4:21
Operator : SJ/JU
Sample : I6548-06
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ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

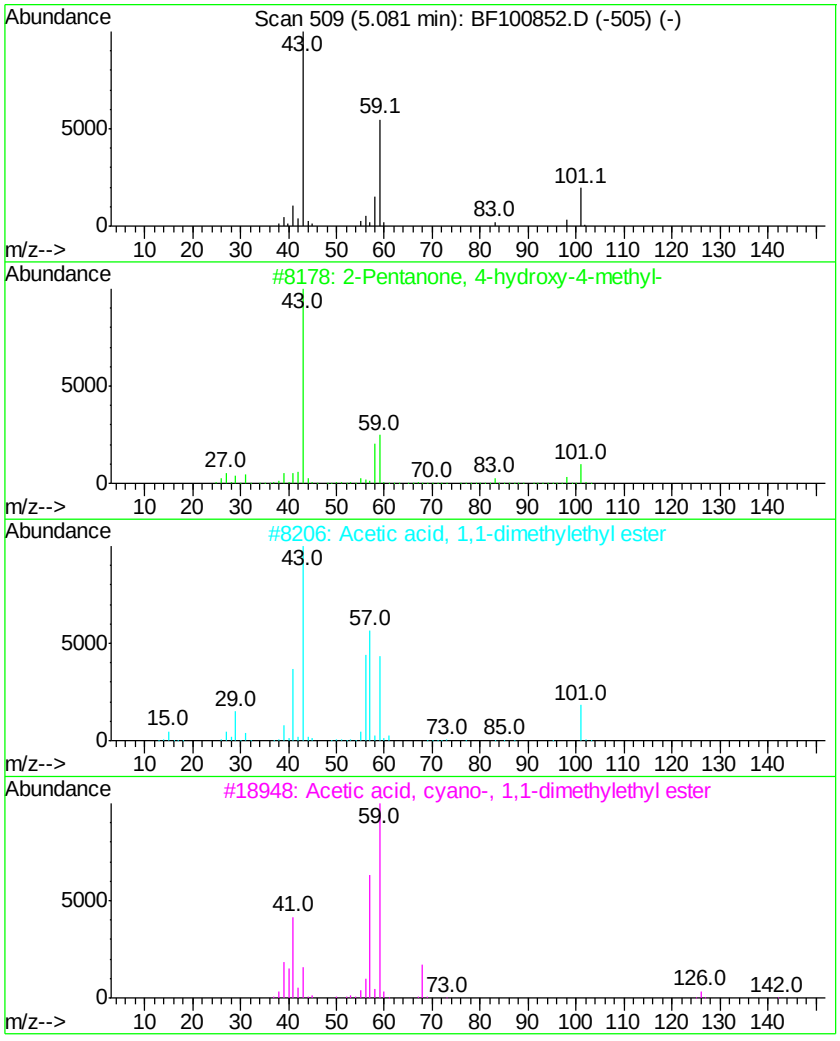
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

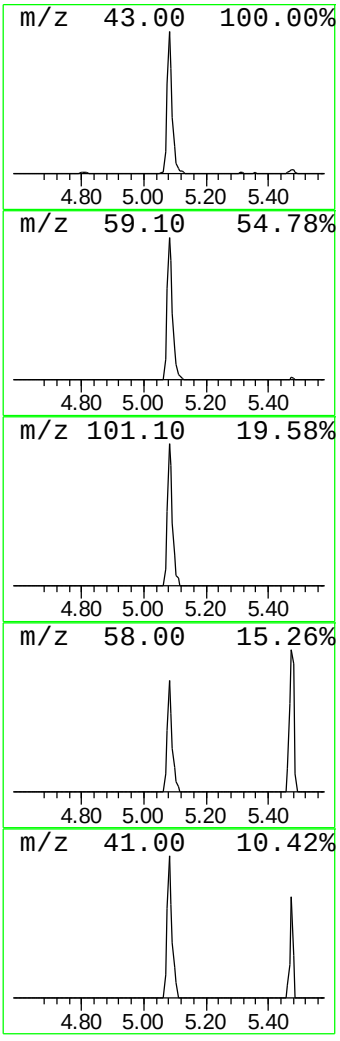
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	4.84 ng	120773	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	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
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Acq On : 23 Nov 2017 4:21
Operator : SJ/JU
Sample : I6548-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

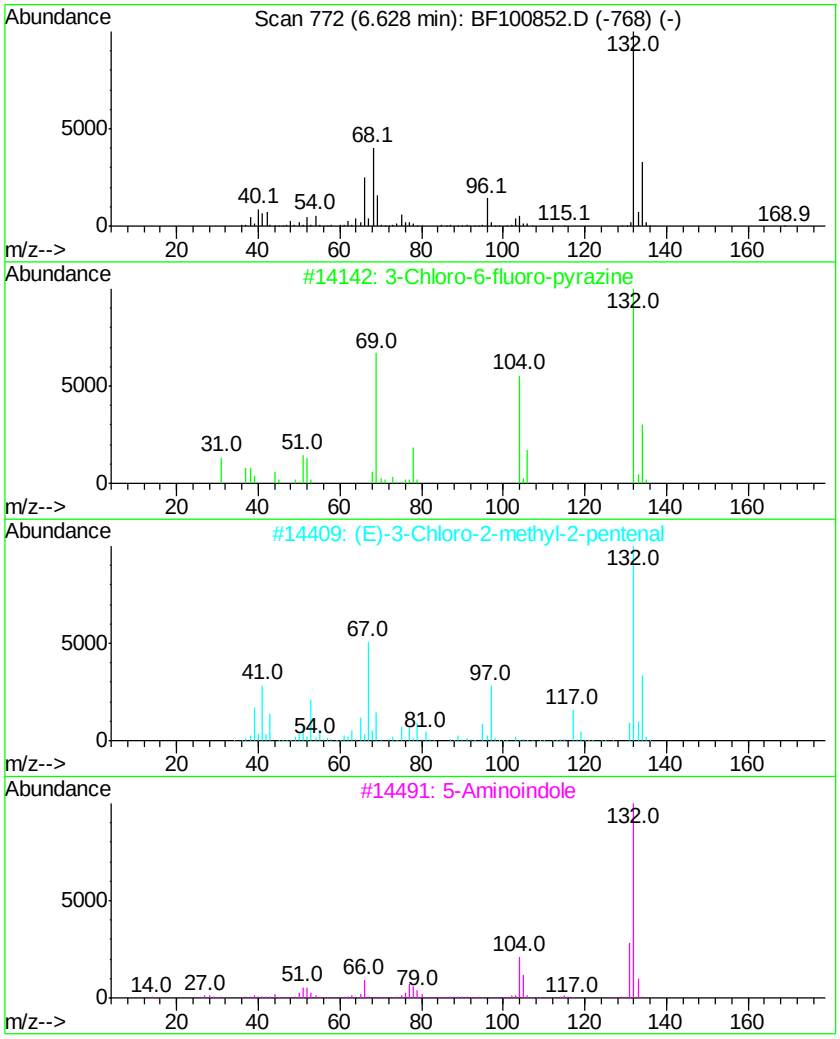
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

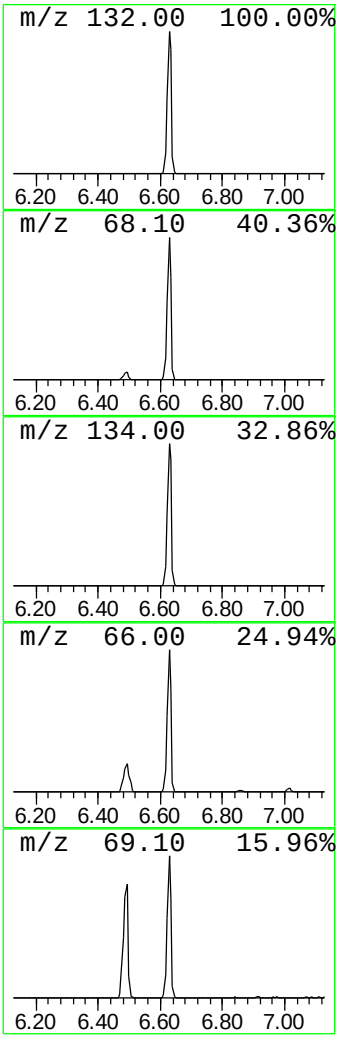
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	54.80 ng	1367140	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	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	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112217\
Data File : BF100852.D
Acq On : 23 Nov 2017 4:21
Operator : SJ/JU
Sample : I6548-06
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

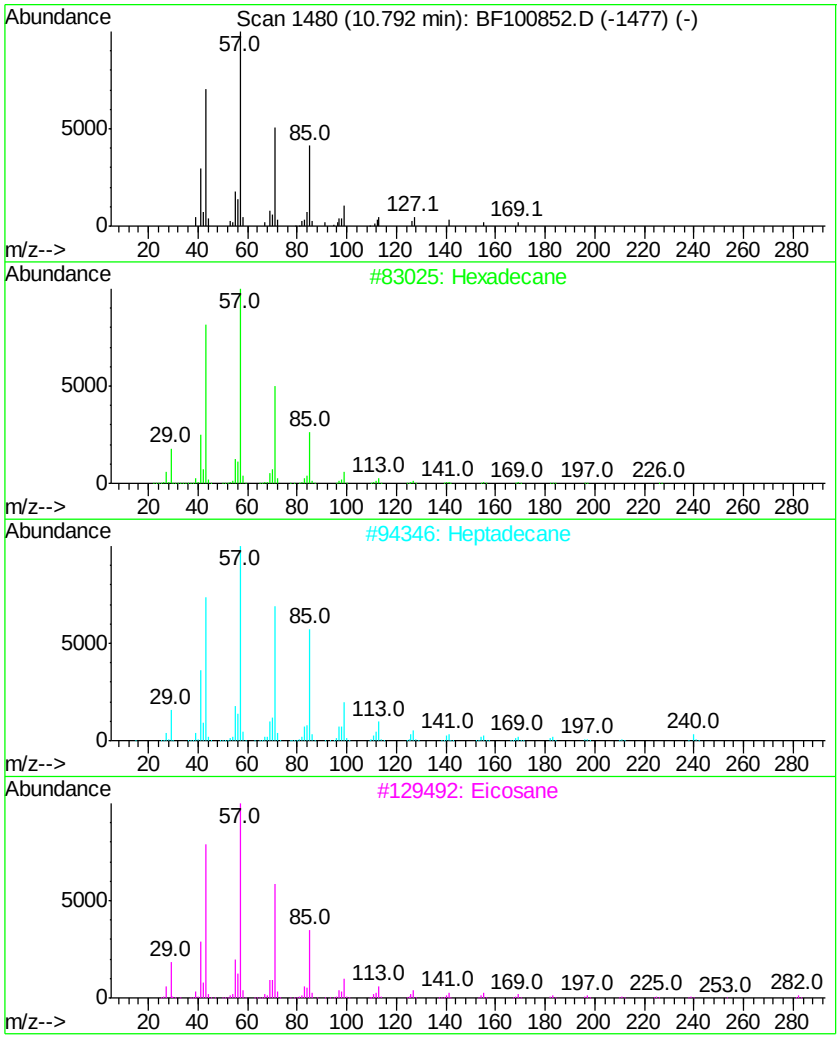
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

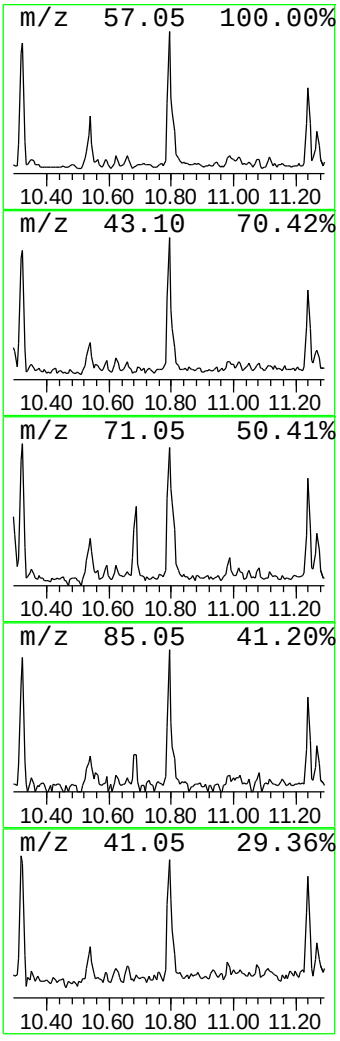
****

Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	2.69 ng	82038	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptadecane	240	C17H36	000629-78-7	86
3	Eicosane	282	C20H42	000112-95-8	64
4	Heptacosane	380	C27H56	000593-49-7	64
5	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	64





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Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SAU-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

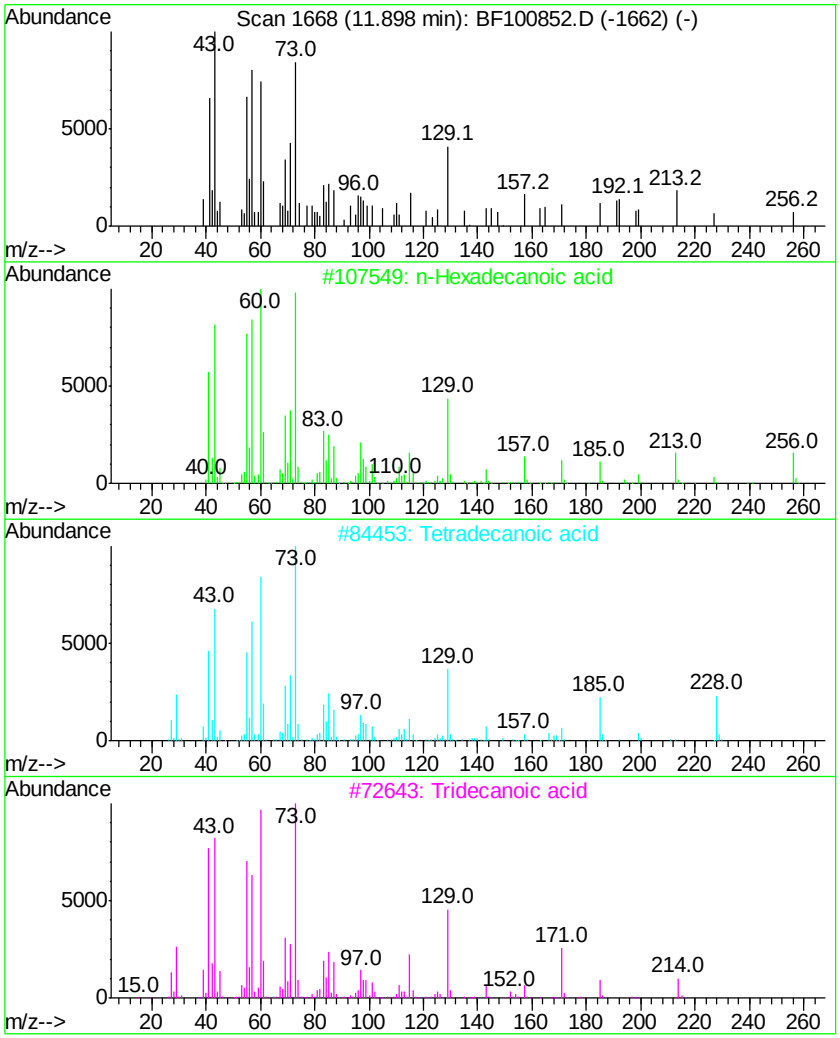
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

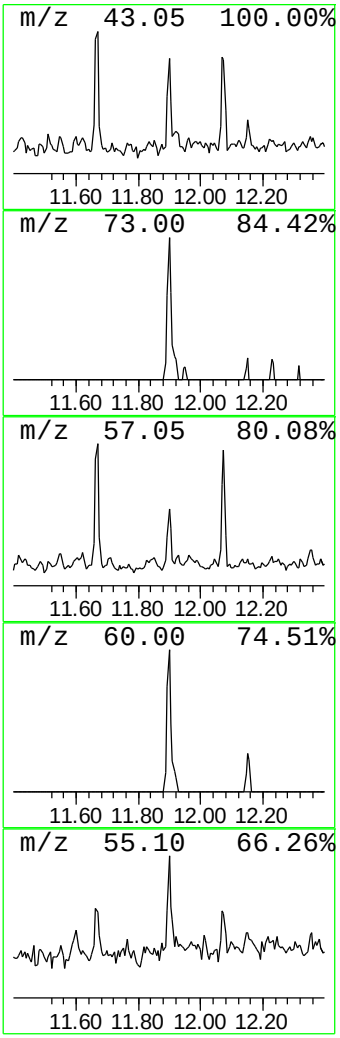
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	3.60 ng	109868	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64





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BNA_F
ClientSampleId :
SAU-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

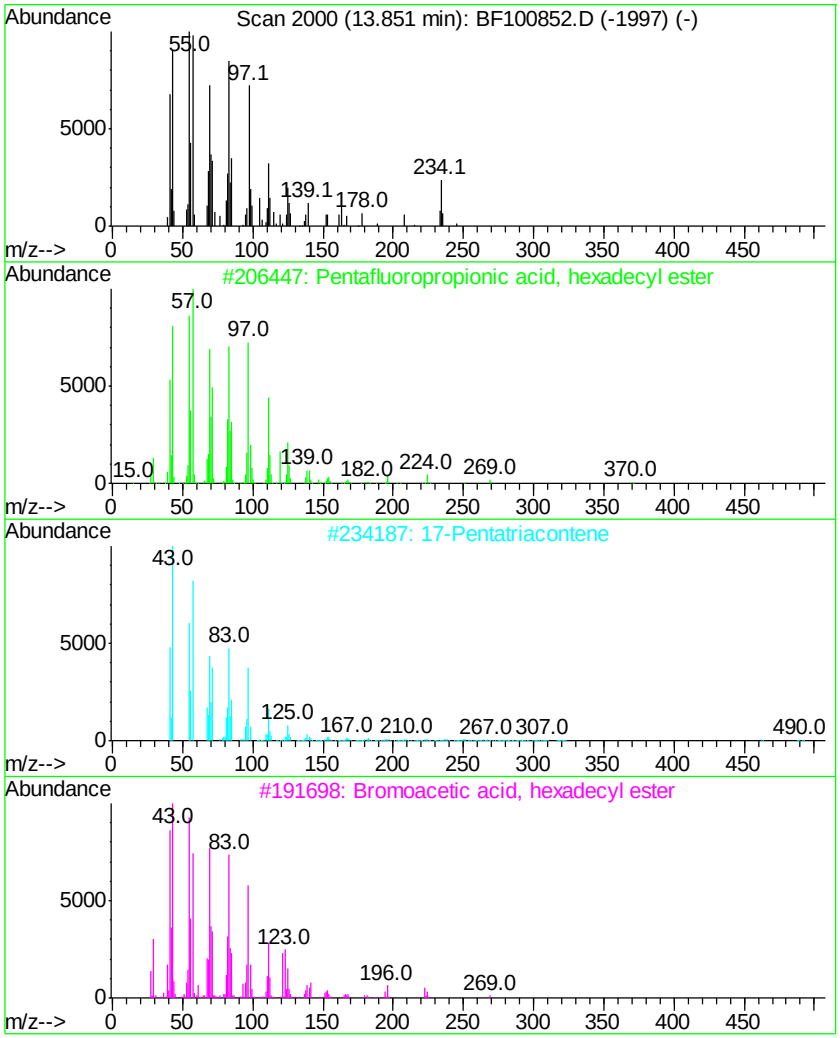
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

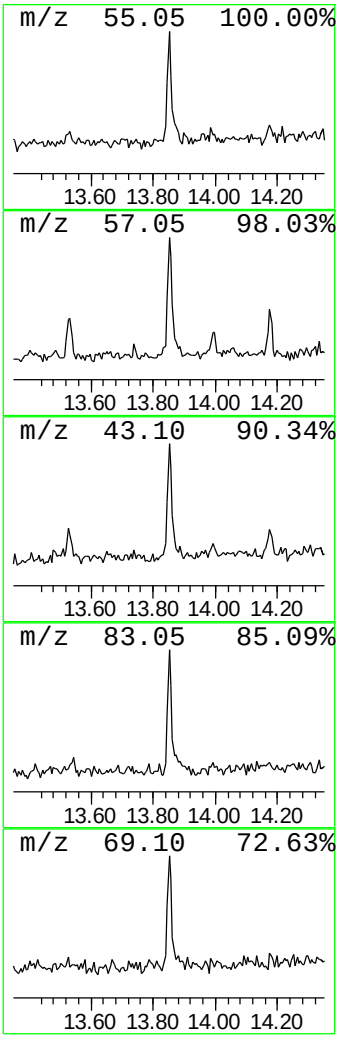
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	2.20 ng	68191	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87
2	17-Pentatriacontene	491	C35H70	006971-40-0	87
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	83
4	1-Eicosanol	298	C20H42O	000629-96-9	83
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	83





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Misc :
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Instrument : BNA_F
ClientSampleId : SAU-2-E(4-5)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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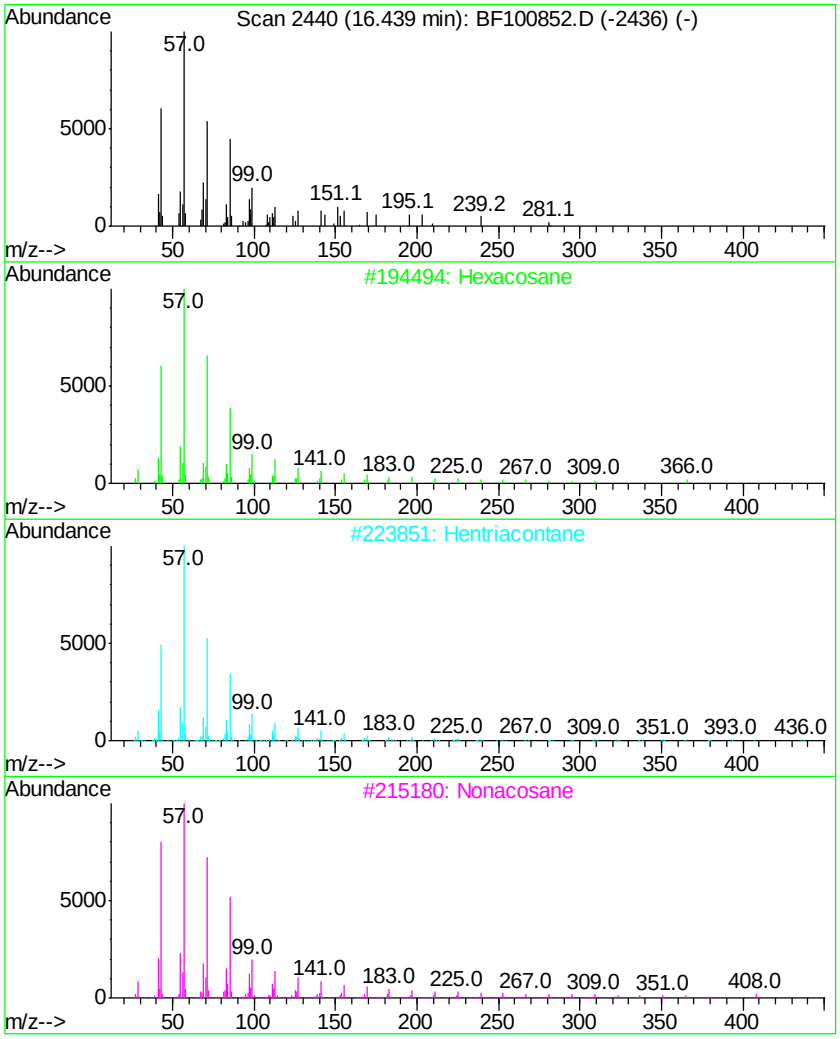
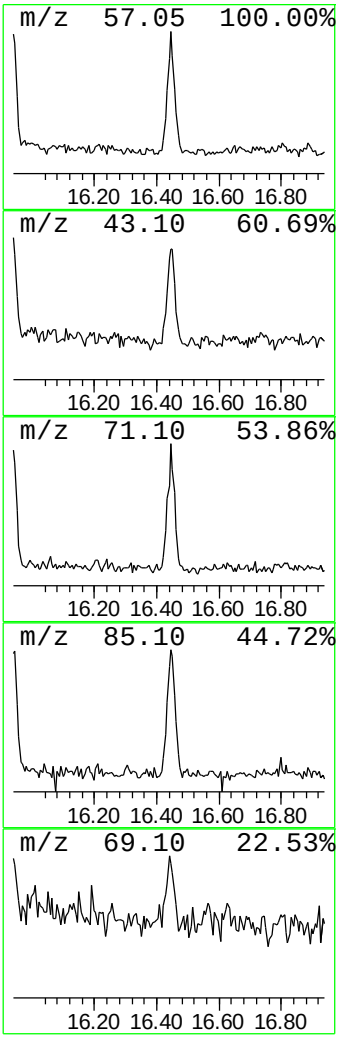
Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.44	2.46 ng	69081	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Nonacosane	408	C29H60	000630-03-5	90
4	Docosane	310	C22H46	000629-97-0	90
5	Heptacosane	380	C27H56	000593-49-7	90





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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...	5.08	4.8	ng	120773	1	6.86	498979	20.0
unknown6.63	6.63	54.8	ng	1367140	1	6.86	498979	20.0
Hexadecane	10.79	2.7	ng	82038	4	11.39	610062	20.0
n-Hexadecanoic acid	11.90	3.6	ng	109868	4	11.39	610062	20.0
Pentafluoropropio...	13.85	2.2	ng	68191	5	14.02	618823	20.0
Hexacosane	16.44	2.5	ng	69081	6	15.50	562280	20.0