LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

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-BF072517.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	3.110	218	225	236	rBV	166311	317099	12.30%	1.320%
2	4.575	470	474	491	rVB	275440	464204	18.01%	1.933%
3	5.046	550	554	572	rBV	2051917	2434866	94.48%	10.138%
4	6.116	731	736	749	rBV	2269886	2577079	100.00%	10.730%
5	6.216	749	753	759	rVB	2419226	2280205	88.48%	9.494%
6	6.440	787	791	796	rBV	644264	609588	23.65%	2.538%
7	6.592	813	817	827	rBV	1742951	1665095	64.61%	6.933%
8	7.010	884	888	899	rBV	1676786	1590237	61.71%	6.621%
9	7.134	906	909	912	rBV	47521	42743	1.66%	0.178%
10	7.304	935	938	945	rBV	103570	117342	4.55%	0.489%
11	7.722	1005	1009	1018	rBV	980774	932446	36.18%	3.882%
12	7.898	1036	1039	1048	rBV	429650	388936	15.09%	1.619%
13	8.798	1187	1192	1195	rBV	2158090	2046907	79.43%	8.522%
14	9.192	1256	1259	1265	rBV	391342	357773	13.88%	1.490%
15	9.457	1300	1304	1313	rVB	830423	831800	32.28%	3.463%
16	9.916	1379	1382	1385	rBV	60293	48504	1.88%	0.202%
17	10.133	1415	1419	1421	rBV2	22477	30056	1.17%	0.125%
18	10.251	1435	1439	1449	rBV	1297662	1304506	50.62%	5.431%
19	10.386	1458	1462	1470	rBV	82797	112720	4.37%	0.469%
20	10.828	1533	1537	1540	rBV2	47906	41621	1.62%	0.173%
21	10.933	1549	1555	1557	rBV	920937	809922	31.43%	3.372%
22	10.957	1557	1559	1563	rVV	69038	62757	2.44%	0.261%
23	11.010	1563	1568	1572	rVB3	25619	31387	1.22%	0.131%
24	11.086	1578	1581	1584	rBV	45415	42768	1.66%	0.178%
25	11.251	1607	1609	1614	rVB2	29173	27255	1.06%	0.113%
26	11.486	1647	1649	1655	rBV2	135738	168544	6.54%	0.702%
27	11.539	1655	1658	1670	rVB3	34875	74695	2.90%	0.311%
28	11.874	1710	1715	1718	rBV3	24654	29040	1.13%	0.121%
29	12.133	1756	1759	1763	rBV	114803	110193	4.28%	0.459%
30	12.180	1763	1767	1770	rBV	291696	250326	9.71%	1.042%
31	12.269	1779	1782	1788	rBV2	53560	70713	2.74%	0.294%
32	12.357	1793	1797	1800	rBV	149334	136540	5.30%	0.568%
33	12.516	1819	1824	1827	rBV	1657809	1638996	63.60%	6.824%
34	12.645	1843	1846	1848	rVB	49847	43885	1.70%	0.183%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

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-BF072517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.692	1848	1854	1859	rVB2	23381	48860	1.90%	0.203%
36	13.304	1956	1958	1963	rVB4	17444	26699	1.04%	0.111%
37	13.439	1977	1981	1989	rVB4	52342	79927	3.10%	0.333%
38	13.551	1996	2000	2003	rBV	751865	717295	27.83%	2.987%
39	13.574	2003	2004	2008	rVB	61175	52561	2.04%	0.219%
40	13.939	2064	2066	2070	rBV4	36268	45546	1.77%	0.190%
41	14.139	2096	2100	2106	rBV9	26802	74643	2.90%	0.311%
42	14.398	2142	2144	2148	rBV	53176	51568	2.00%	0.215%
43	14.545	2166	2169	2177	rVB	67050	120438	4.67%	0.501%
44	14.663	2187	2189	2194	rVB5	24119	29661	1.15%	0.123%
45	14.798	2208	2212	2213	rBV	42508	48868	1.90%	0.203%
46	14.845	2216	2220	2223	rVV	66358	92625	3.59%	0.386%
47	14.892	2224	2228	2232	rVB	482546	495409	19.22%	2.063%
48	15.068	2255	2258	2259	rBV3	32618	31621	1.23%	0.132%
49	15.351	2301	2306	2307	rBV4	33681	51108	1.98%	0.213%
50	15.674	2356	2361	2367	rBV8	41379	108270	4.20%	0.451%
51	16.451	2490	2493	2498	rVB4	20840	28013	1.09%	0.117%
52	16.633	2520	2524	2527	rBV6	24941	34919	1.35%	0.145%
53	16.927	2570	2574	2577	rBV6	15854	27202	1.06%	0.113%
54	16.998	2584	2586	2589	rBV4	22254	34299	1.33%	0.143%
55	18.068	2765	2768	2772	rBV6	23433	48717	1.89%	0.203%
56	18.827	2894	2897	2900	rBV5	20069	30729	1.19%	0.128%
57	19.233	2961	2966	2967	rBV5	24844	48075	1.87%	0.200%

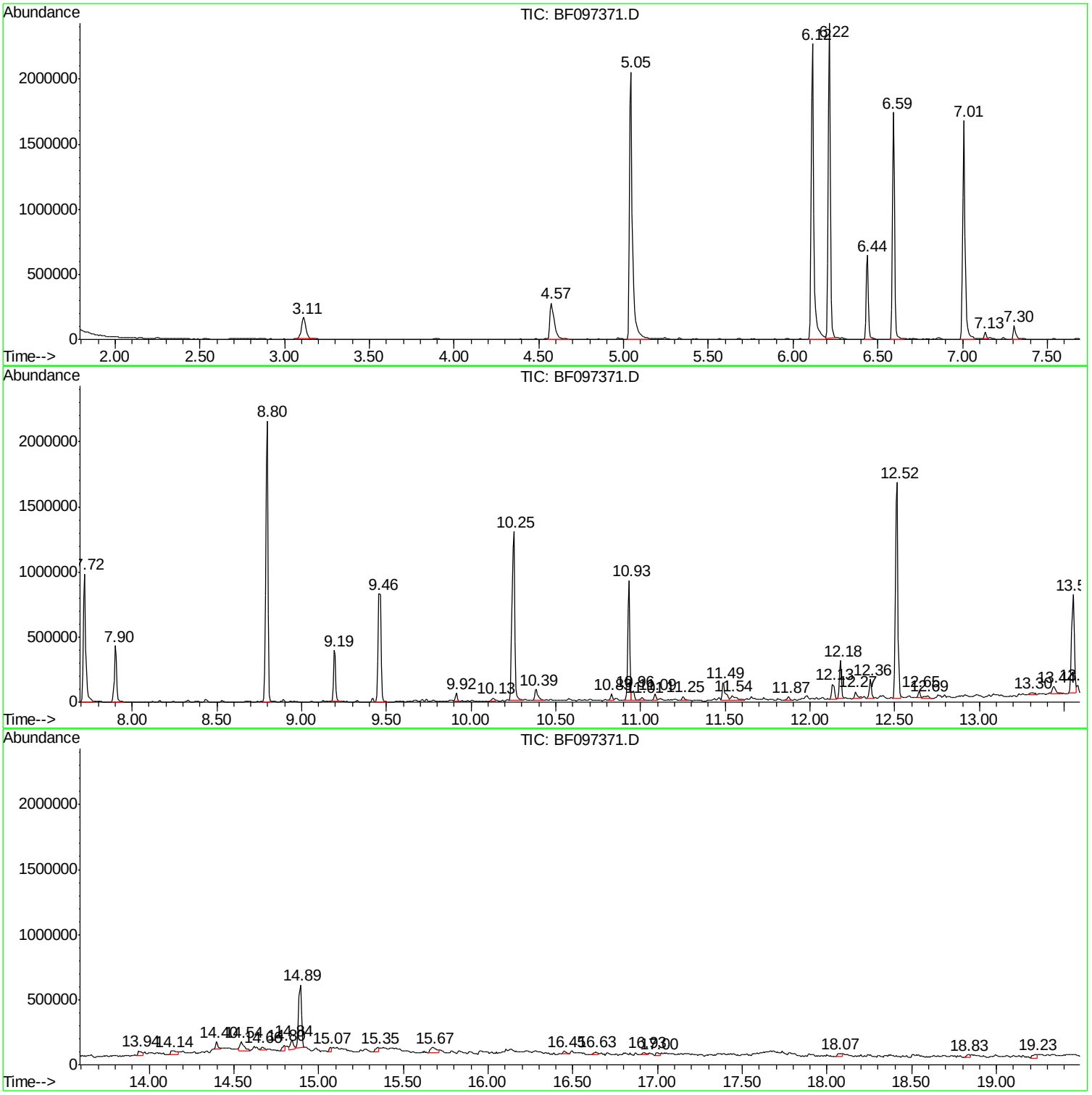
Sum of corrected areas: 24017801

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

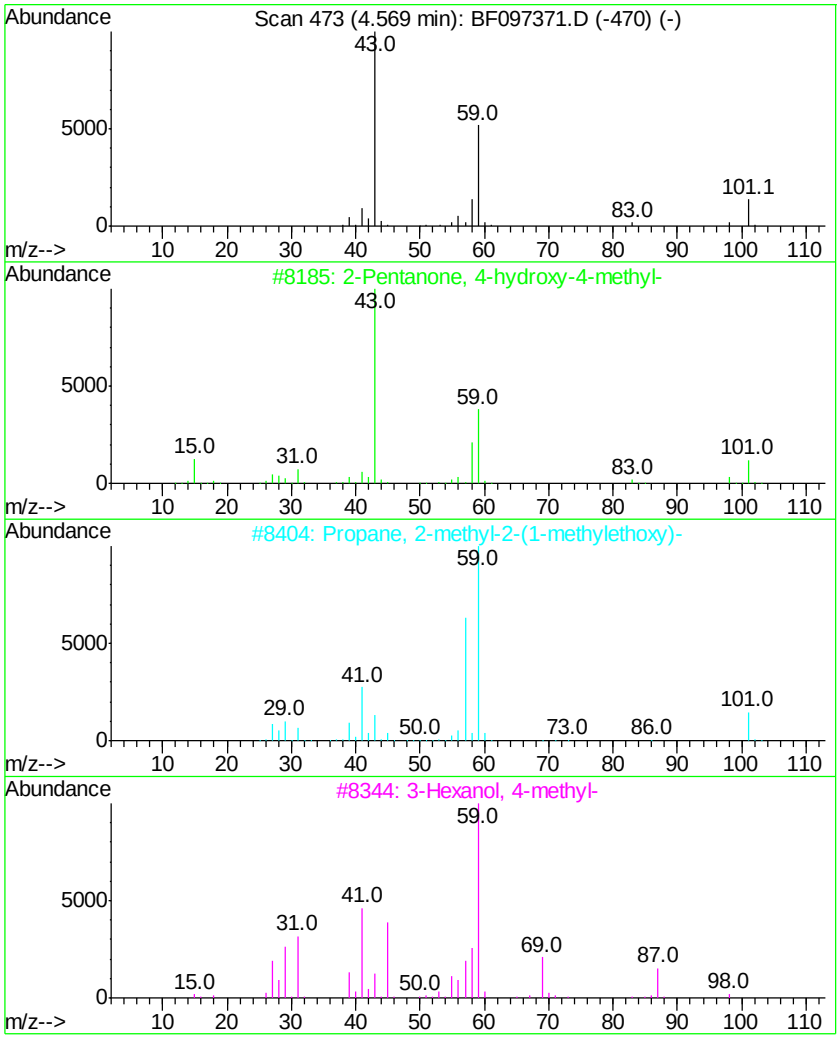
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

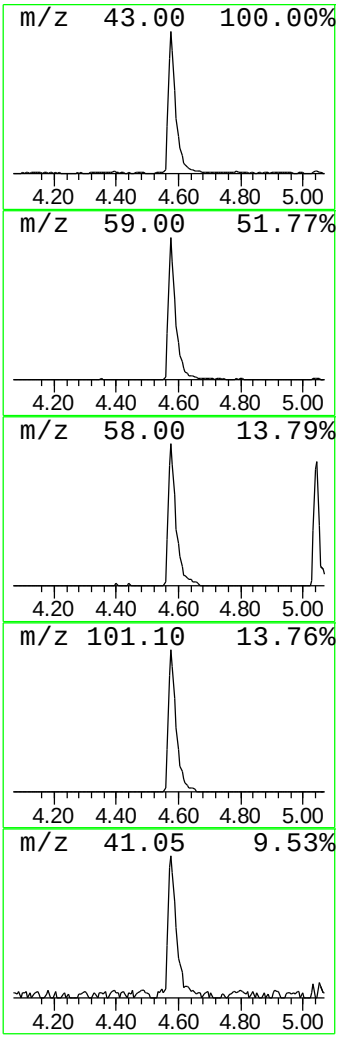
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	15.23 ng	464204	1,4-Dichlorobenzene-d4	6.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

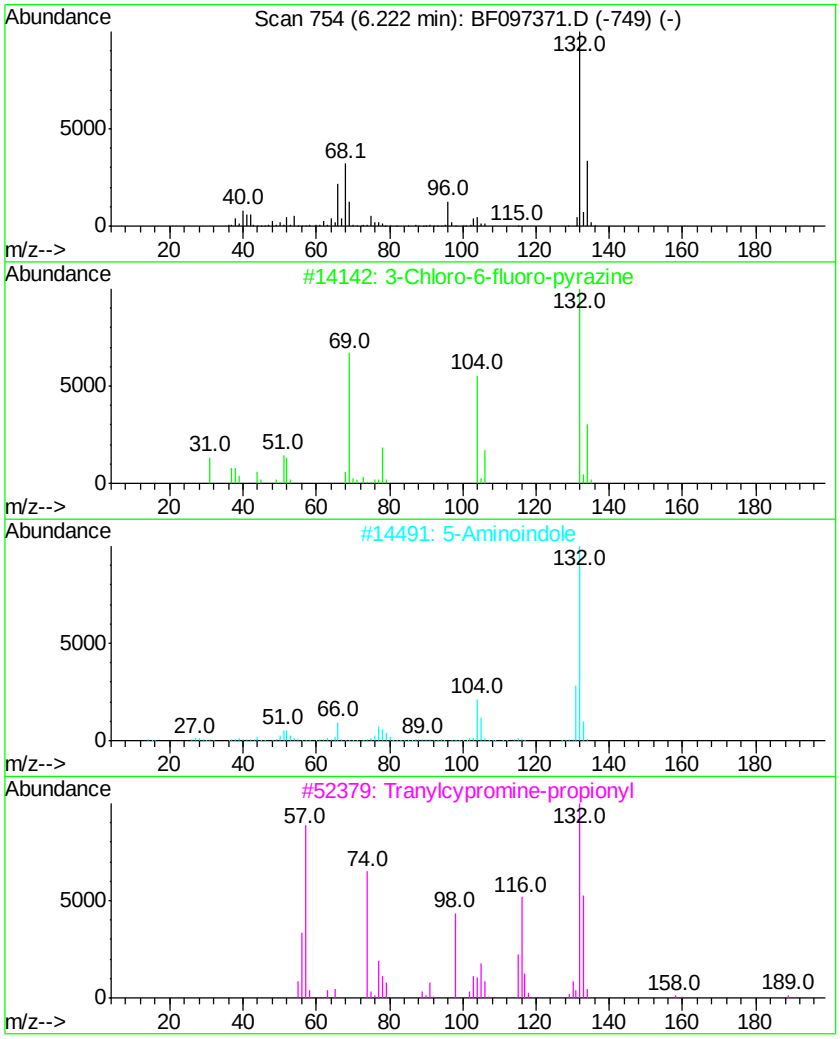
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

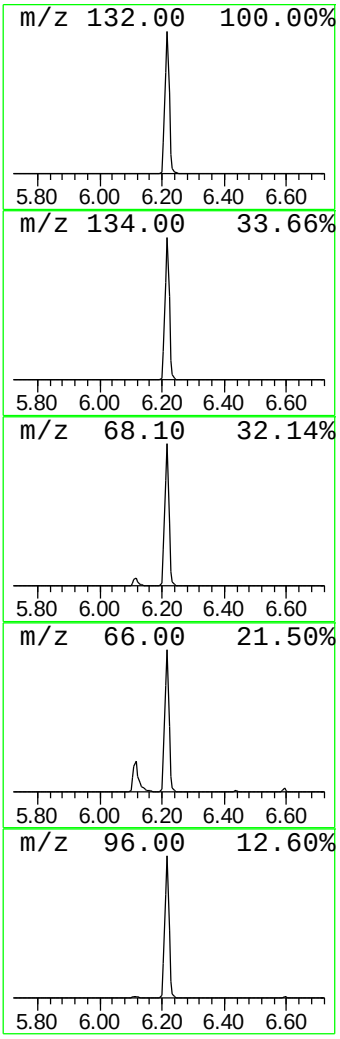
****

Peak Number 3 unknown6.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.22	74.81 ng	2280210	1,4-Dichlorobenzene-d4	6.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

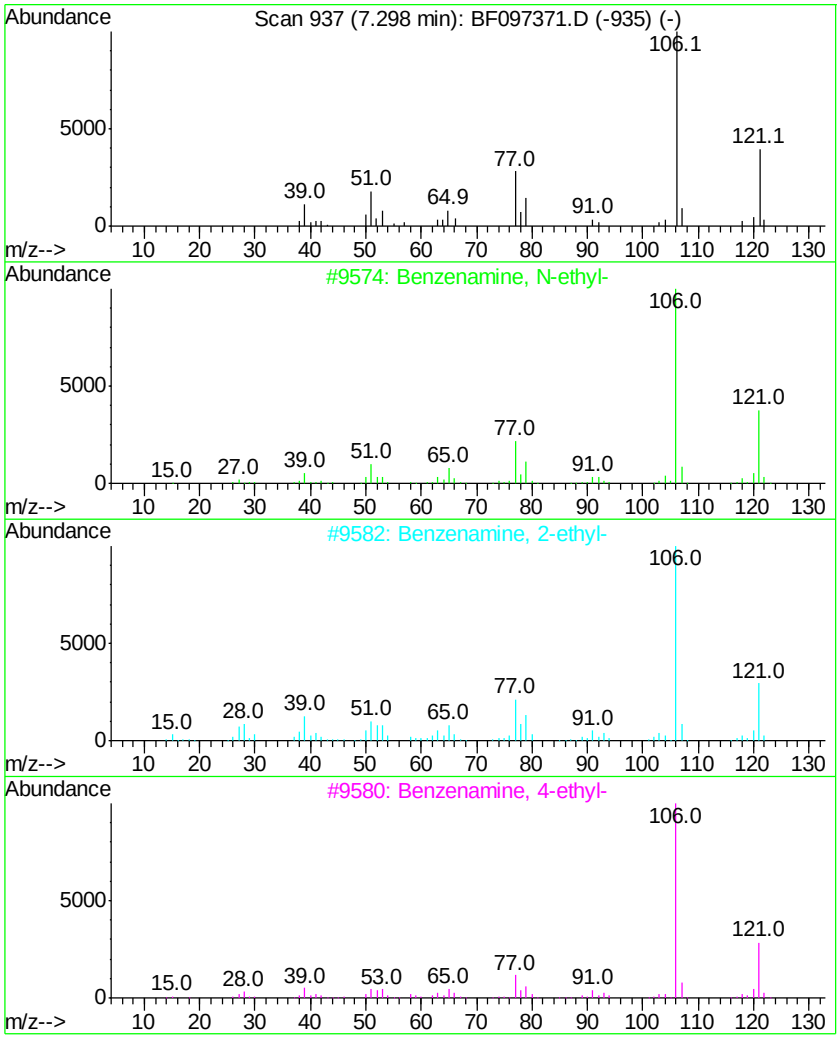
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

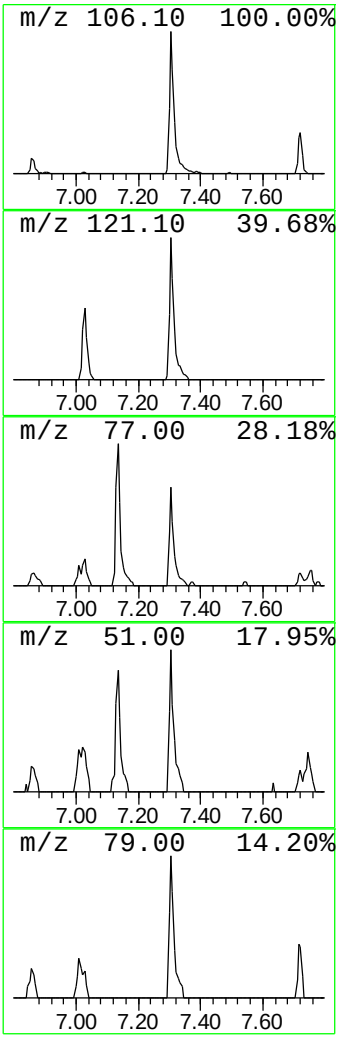
****

Peak Number 5 Benzenamine, N-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.30	2.52 ng	117342	Naphthalene-d8	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, N-ethyl-	121	C8H11N	000103-69-5	95
2	Benzenamine, 2-ethyl-	121	C8H11N	000578-54-1	90
3	Benzenamine, 4-ethyl-	121	C8H11N	000589-16-2	80
4	Pyridine, 2-ethyl-5-methyl-	121	C8H11N	018113-81-0	74
5	4-Isopropylpyridine	121	C8H11N	000696-30-0	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

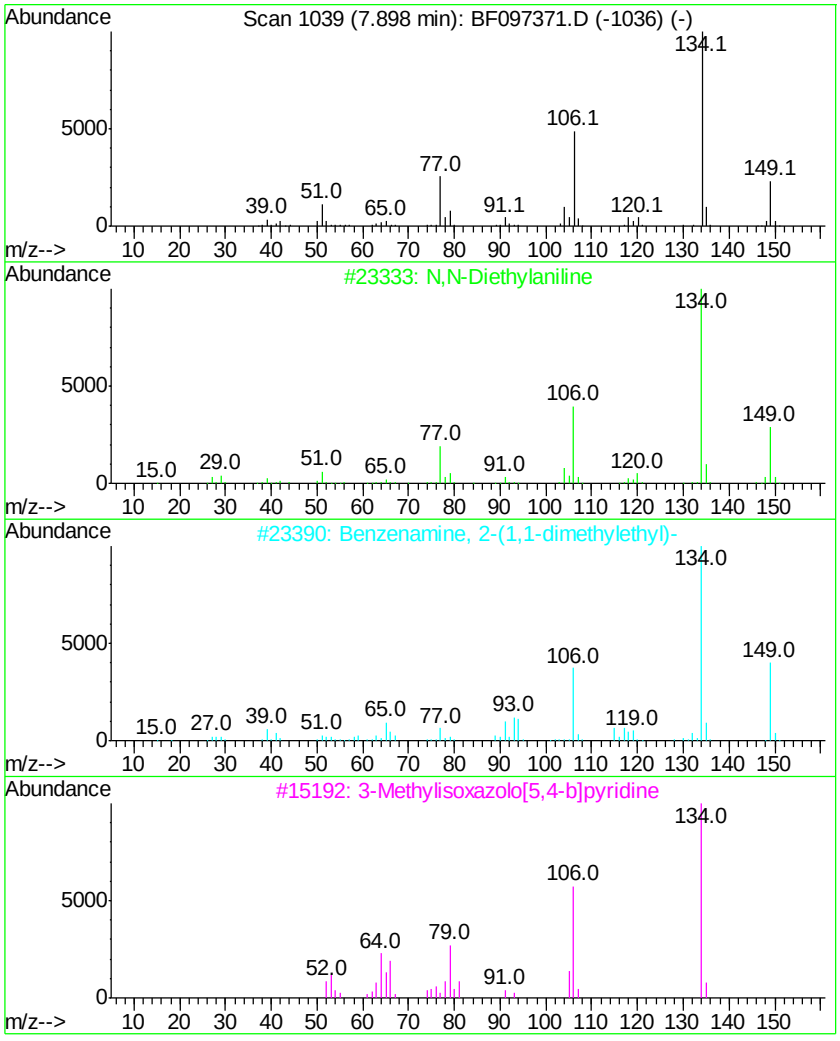
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

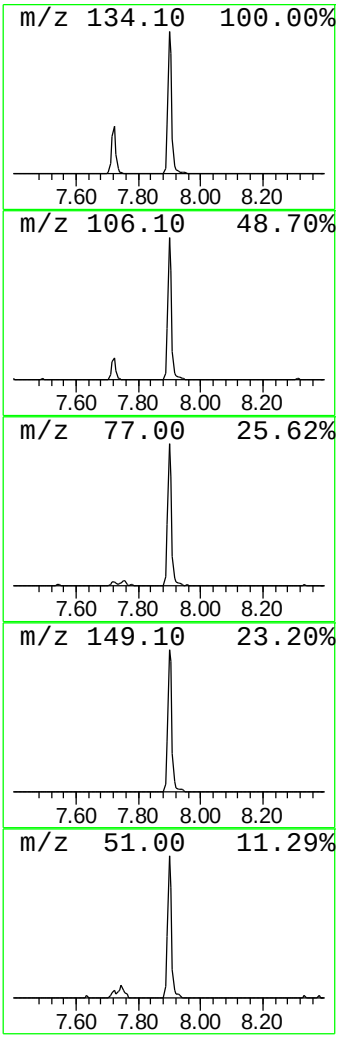
****

Peak Number 6 N,N-Diethylaniline Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.90	8.34 ng	388936	Naphthalene-d8	7.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N-Diethylaniline	149	C10H15N	000091-66-7	96
2	Benzenamine, 2-(1,1-dimethylethyl)-	149	C10H15N	006310-21-0	59
3	3-Methylisoxazolo[5,4-b]pyridine	134	C7H6N2O	058035-50-0	53
4	3,4-Dihydro-1-methylpyrrolo[1,2-...	134	C8H10N2	064608-66-8	53
5	4-t-Butylbenzeneamine	149	C10H15N	000769-92-6	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

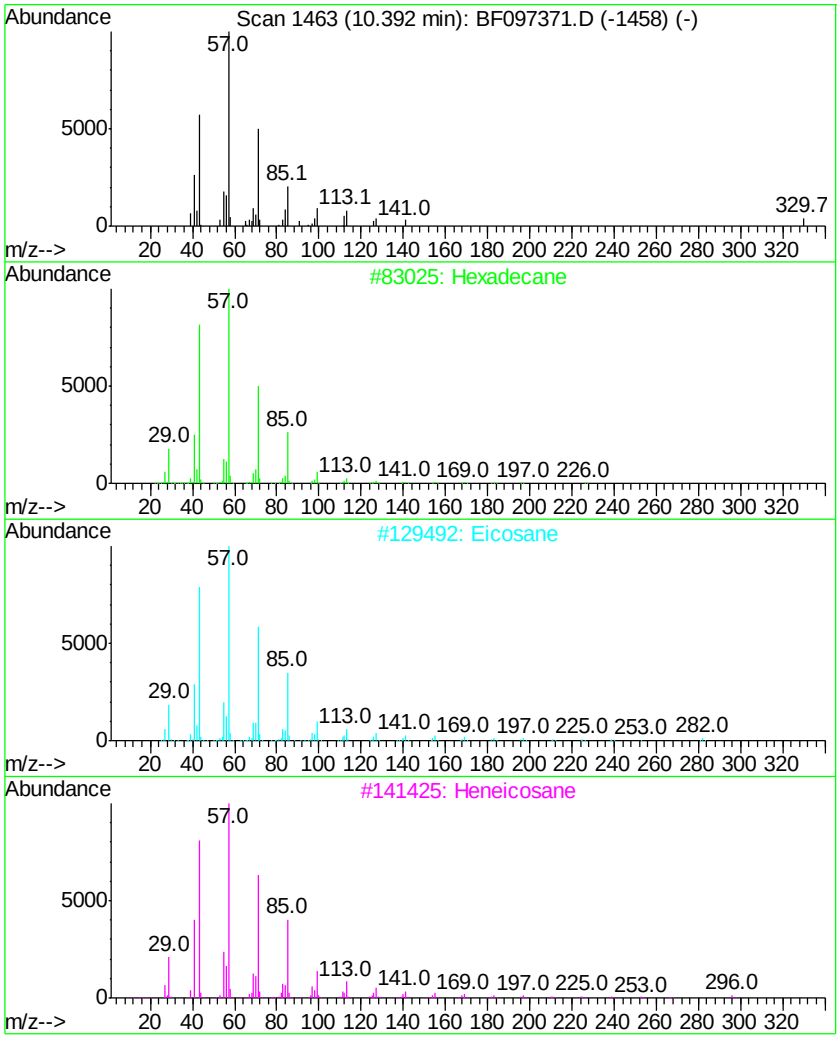
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

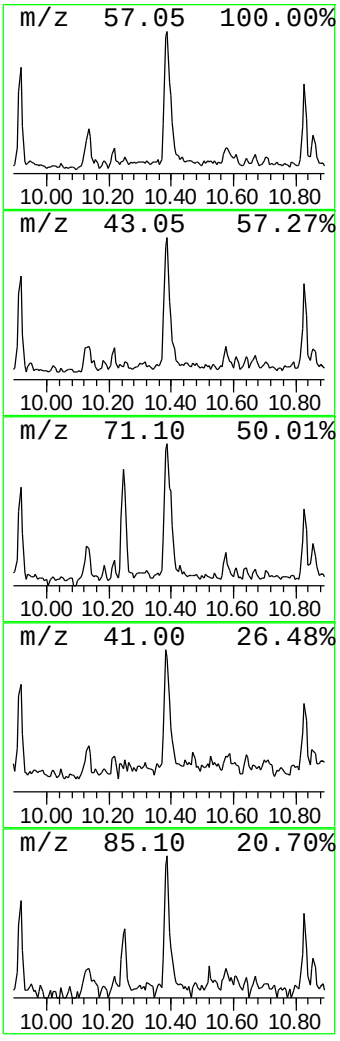
****

Peak Number 7 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.39	2.78 ng	112720	Phenanthrene-d10	10.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Eicosane	282	C20H42	000112-95-8	86
3	Heneicosane	296	C21H44	000629-94-7	86
4	Tetracosane	338	C24H50	000646-31-1	80
5	Pentadecane	212	C15H32	000629-62-9	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

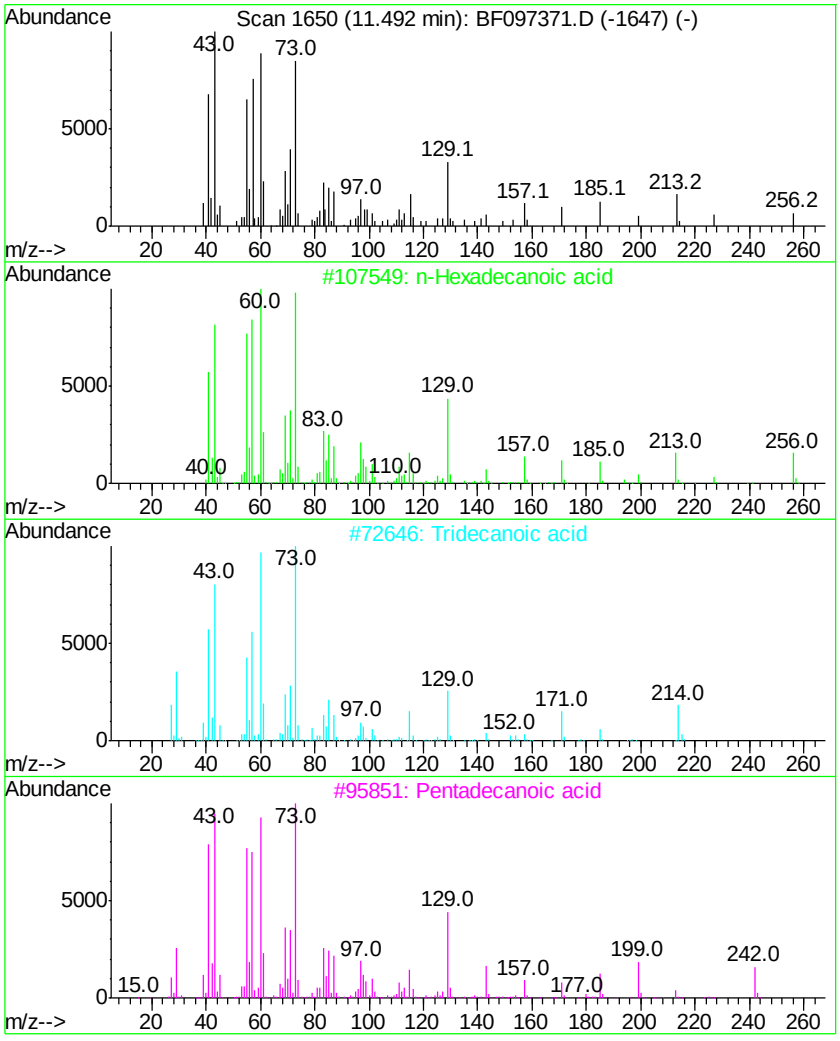
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

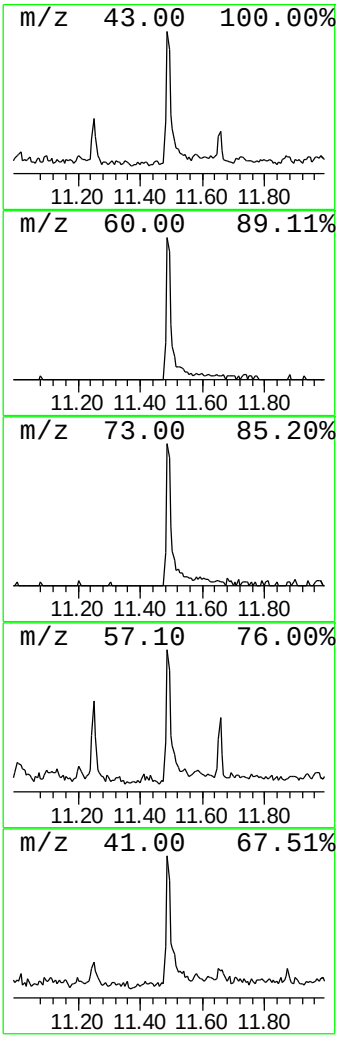
****

Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	4.16 ng	168544	Phenanthrene-d10	10.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

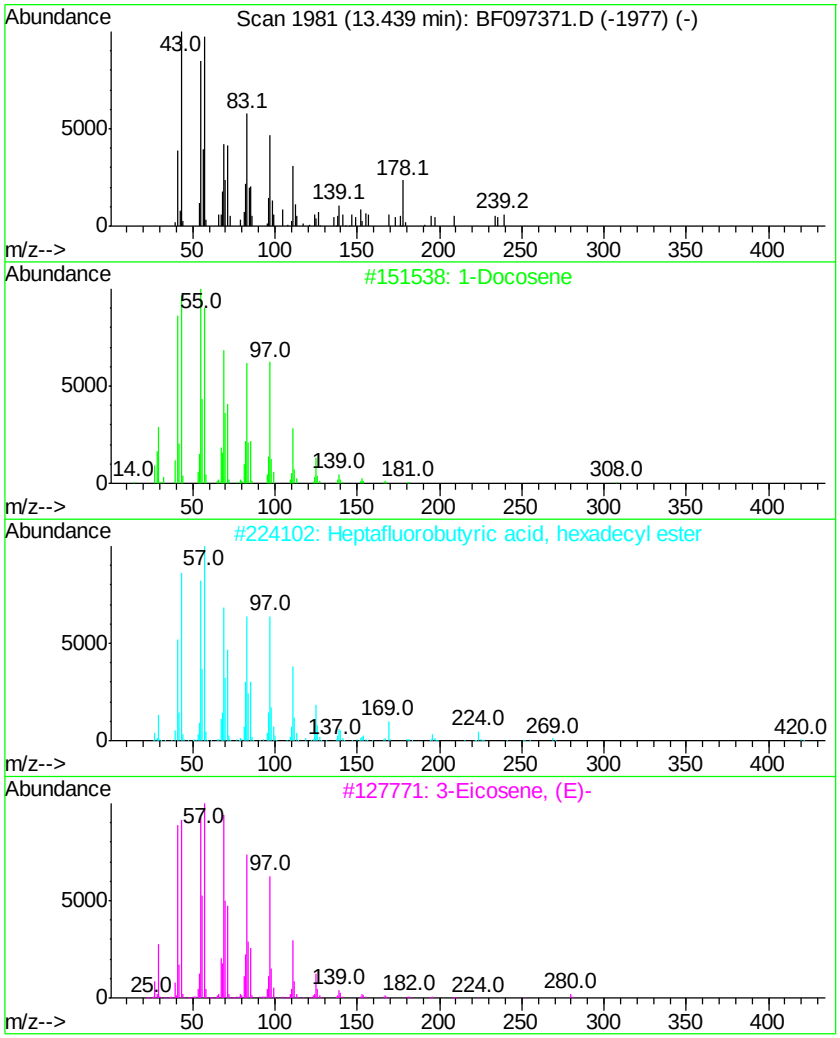
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

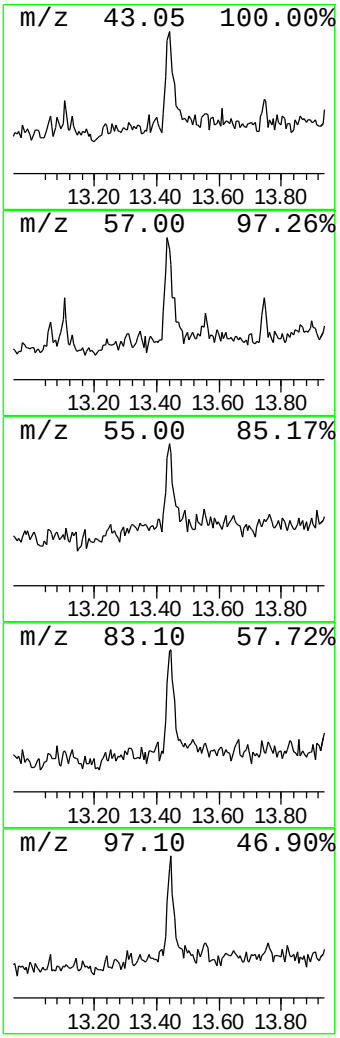
****

Peak Number 9 1-Docosene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	2.23 ng	79927	Chrysene-d12	13.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	83
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	83
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	83
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	81
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	81





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

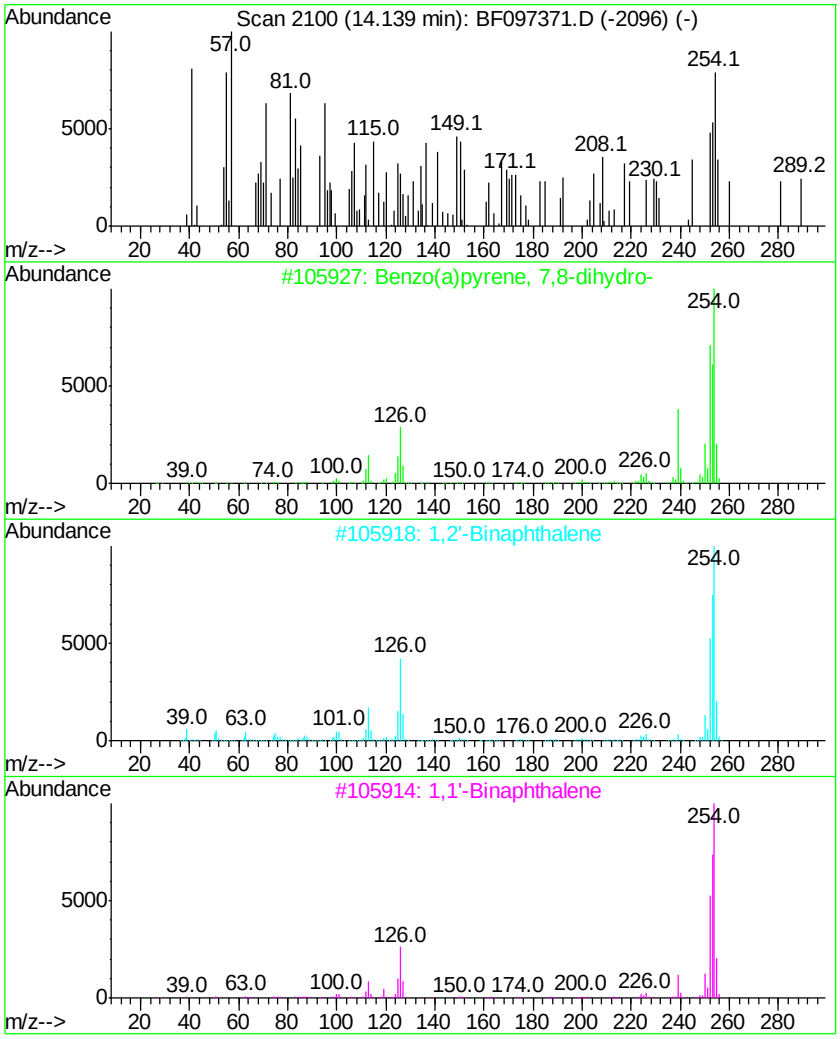
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

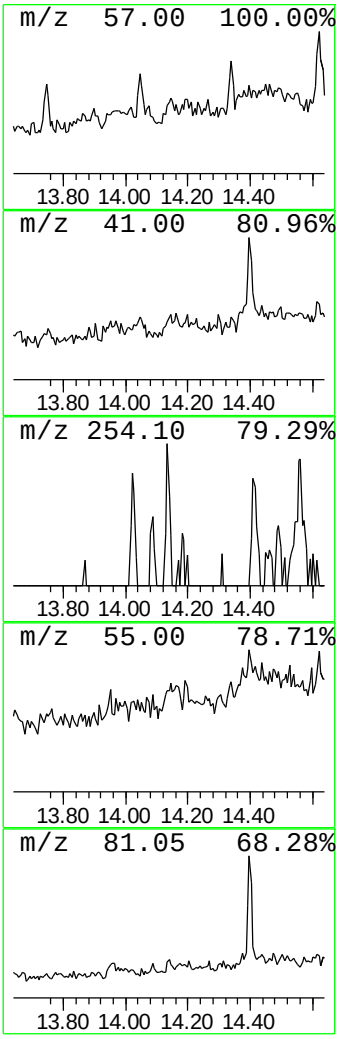
****

Peak Number 10 unknown14.14 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.14	2.08 ng	74643	Chrysene-d12	13.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo(a)pyrene, 7,8-dihydro-	254	C20H14	017573-23-8	30
2	1,2'-Binaphthalene	254	C20H14	004325-74-0	27
3	1,1'-Binaphthalene	254	C20H14	000604-53-5	27
4	Benzenamine, 4-(2-benzothiazolyl...	254	C15H14N2S	010205-56-8	27
5	9,10[1',2']-Benzenoanthracene, 9...	254	C20H14	000477-75-8	27





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

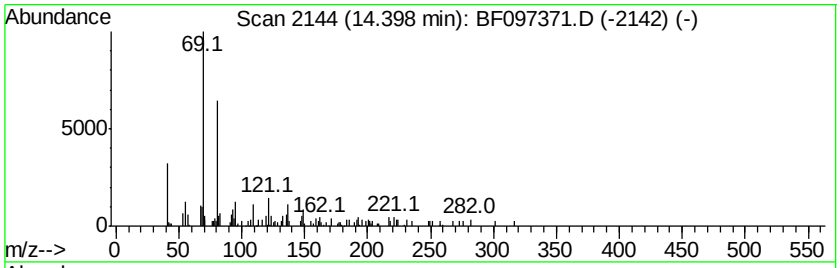
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

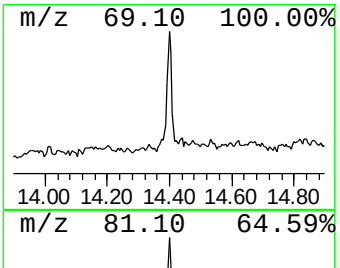
****

Peak Number 11 .psi.,.psi.-Carotene, 7,7',... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.40	2.08 ng	51568	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	68
3	Supraene	410	C30H50	007683-64-9	64
4	3,7,11-Tridecatrienenitrile, 4,8...	231	C16H25N	006006-01-5	64
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

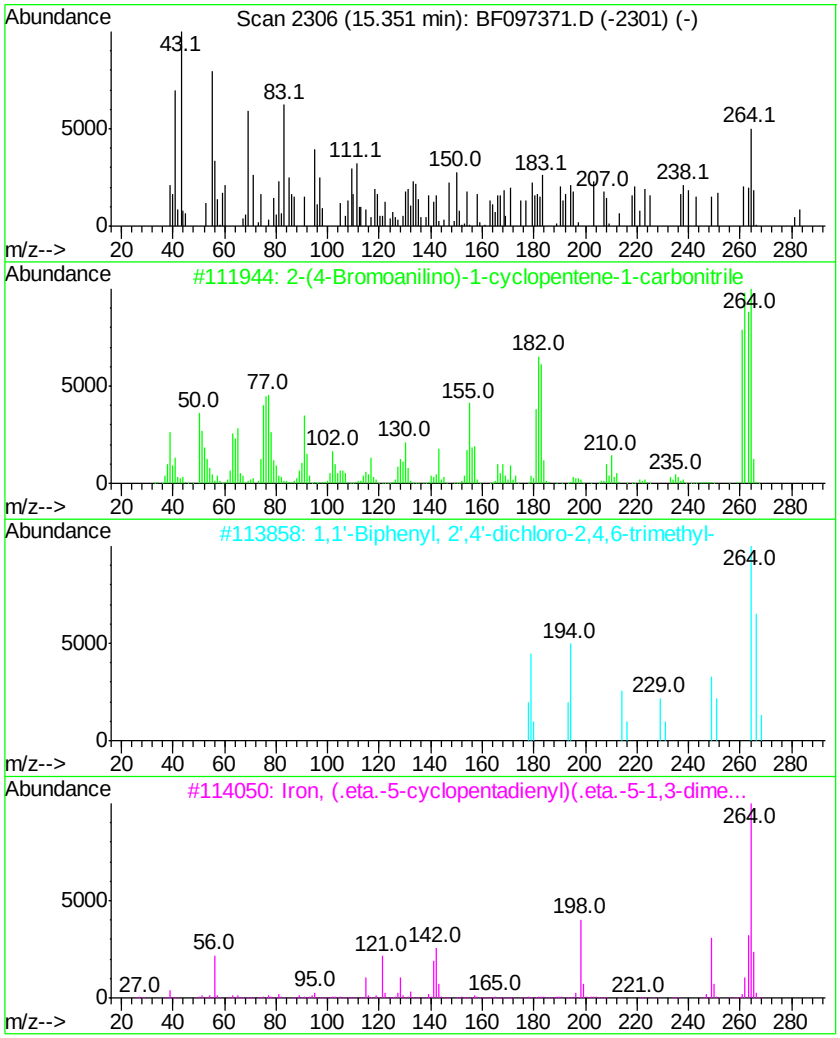
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

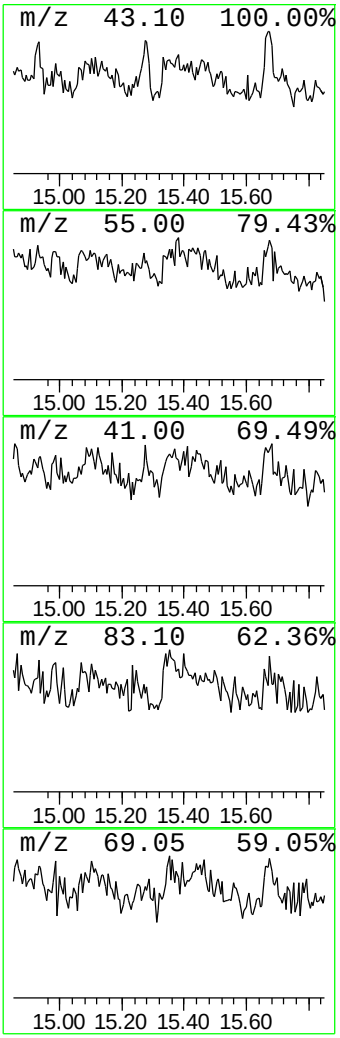
****

Peak Number 12 2-(4-Bromoanilino)-1-cyclop... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.35	2.06 ng	51108	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(4-Bromoanilino)-1-cyclopenten...	262	C12H11BrN2	191980-05-9	92
2	1,1'-Biphenyl, 2',4'-dichloro-2,...	264	C15H14Cl2	075601-31-9	38
3	Iron, (.eta.-5-cyclopentadienyl)...	264	C16H16Fe	1000155-06-6	38
4	Allyl(2,3-dihydro-1H-benzo[4,5]i...	264	C16H16N4	1000322-09-2	25
5	1,2-Dimethyl-5,5-diphenyl-2-imid...	264	C17H16N2O	037927-94-9	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

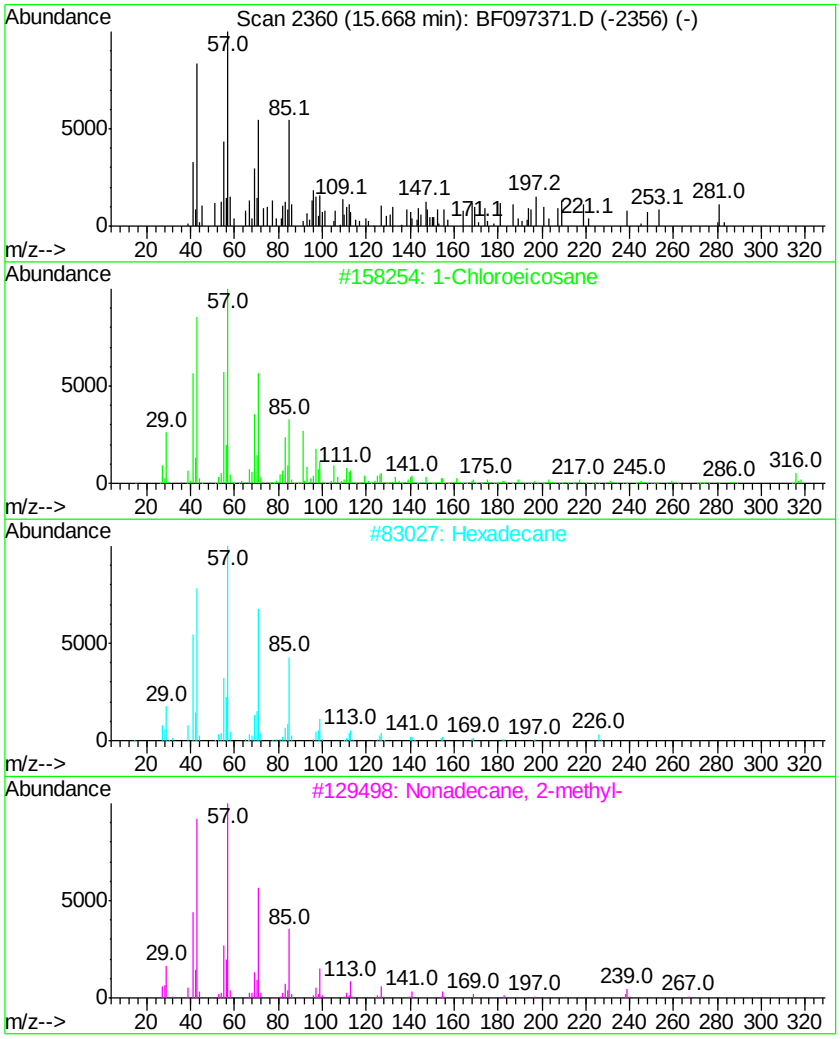
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

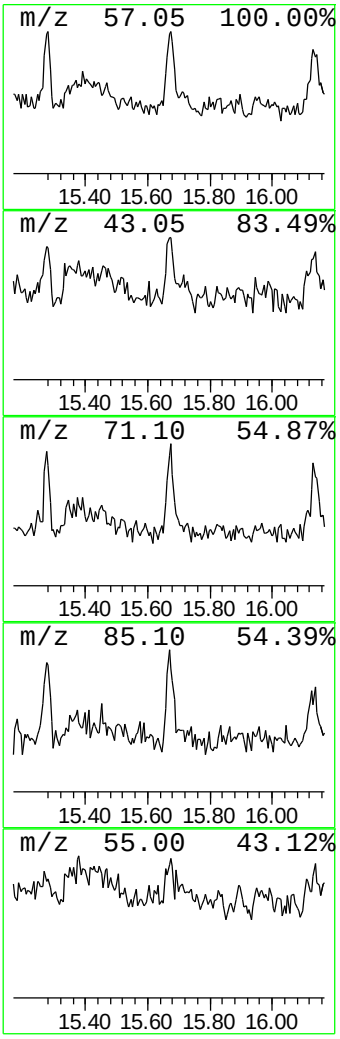
****

Peak Number 13 1-Chloroeicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.67	4.37 ng	108270	Perylene-d12	14.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Chloroeicosane	316	C20H41Cl	042217-02-7	83
2	Hexadecane	226	C16H34	000544-76-3	60
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	52
4	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	49
5	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF080417\
Data File : BF097371.D
Acq On : 4 Aug 2017 22:27
Operator : SJ/JU
Sample : I4555-09
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 2043

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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...	4.57	15.2	ng	464204	1	6.44	609588	20.0
unknown6.22	6.22	74.8	ng	2280210	1	6.44	609588	20.0
Benzenamine, N-et...	7.30	2.5	ng	117342	2	7.72	932446	20.0
N,N-Diethylaniline	7.90	8.3	ng	388936	2	7.72	932446	20.0
Hexadecane	10.39	2.8	ng	112720	4	10.93	809922	20.0
n-Hexadecanoic acid	11.49	4.2	ng	168544	4	10.93	809922	20.0
1-Docosene	13.44	2.2	ng	79927	5	13.55	717295	20.0
unknown14.14	14.14	2.1	ng	74643	5	13.55	717295	20.0
.psi.,.psi.-Carot...	14.40	2.1	ng	51568	6	14.89	495409	20.0
2-(4-Bromoanilino...	15.35	2.1	ng	51108	6	14.89	495409	20.0
1-Chloroeicosane	15.67	4.4	ng	108270	6	14.89	495409	20.0