LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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	4.622	460	465	478	rBV	189490	301761	9.90%	1.133%
2	5.093	541	545	562	rBV	2741465	3047587	100.00%	11.439%
3	6.157	722	726	739	rBV	2335548	2727816	89.51%	10.238%
4	6.257	739	743	750	rVB	2710225	2539987	83.34%	9.533%
5	6.481	777	781	786	rBV	659022	633486	20.79%	2.378%
6	6.634	803	807	811	rBV	2156893	1997971	65.56%	7.499%
7	7.051	873	878	881	rBV	1691762	1713452	56.22%	6.431%
8	7.763	995	999	1002	rBV	1151927	1034938	33.96%	3.884%
9	7.816	1005	1008	1011	rVB	41533	33358	1.09%	0.125%
10	8.839	1177	1182	1186	rBV	2413999	2407722	79.00%	9.037%
11	9.239	1246	1250	1255	rVB	559507	462458	15.17%	1.736%
12	9.369	1265	1272	1275	rBV	46595	45342	1.49%	0.170%
13	9.510	1291	1296	1299	rBV	963216	889570	29.19%	3.339%
14	9.963	1370	1373	1376	rVB	59654	47523	1.56%	0.178%
15	10.181	1405	1410	1413	rBV3	24953	37814	1.24%	0.142%
16	10.298	1426	1430	1436	rBV	1399150	1283404	42.11%	4.817%
17	10.433	1450	1453	1460	rBV	86298	106535	3.50%	0.400%
18	10.880	1524	1529	1532	rBV2	64991	65448	2.15%	0.246%
19	10.986	1543	1547	1549	rBV	804309	748288	24.55%	2.809%
20	11.010	1549	1551	1555	rVV	128659	110487	3.63%	0.415%
21	11.063	1556	1560	1564	rVB	66191	66920	2.20%	0.251%
22	11.486	1622	1632	1634	rBV2	45059	72878	2.39%	0.274%
23	11.516	1634	1637	1639	rVB	37151	32468	1.07%	0.122%
24	11.545	1639	1642	1648	rBV2	162756	184261	6.05%	0.692%
25	11.592	1648	1650	1653	rBV	60993	51258	1.68%	0.192%
26	12.033	1721	1725	1728	rBV	54842	60499	1.99%	0.227%
27	12.069	1728	1731	1733	rVV2	33543	45747	1.50%	0.172%
28	12.122	1737	1740	1745	rVB4	33219	44706	1.47%	0.168%
29	12.192	1748	1752	1755	rBV	316738	310146	10.18%	1.164%
30	12.245	1755	1761	1765	rBV8	21235	48694	1.60%	0.183%
31	12.322	1772	1774	1779	rBV2	66448	106278	3.49%	0.399%
32	12.416	1785	1790	1793	rBV	325141	348741	11.44%	1.309%
33	12.569	1812	1816	1823	rVB	1764902	1757638	57.67%	6.597%
34	12.639	1824	1828	1832	rBV2	41677	64015	2.10%	0.240%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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	12.727	1840	1843	1844	rBV2	29097	35478	1.16%	0.133%
36	12.745	1844	1846	1849	rVB	64730	66253	2.17%	0.249%
37	12.816	1855	1858	1861	rBV3	45688	53598	1.76%	0.201%
38	12.851	1861	1864	1868	rVV	50321	56280	1.85%	0.211%
39	12.939	1876	1879	1882	rBV2	42135	38521	1.26%	0.145%
40	13.316	1940	1943	1945	rBV2	30640	36175	1.19%	0.136%
41	13.410	1957	1959	1961	rBV	33523	33228	1.09%	0.125%
42	13.469	1966	1969	1970	rBV2	40815	40421	1.33%	0.152%
43	13.492	1970	1973	1978	rVB2	141199	161797	5.31%	0.607%
44	13.610	1988	1993	1996	rBV2	720055	838376	27.51%	3.147%
45	13.633	1996	1997	2002	rVB	168113	128070	4.20%	0.481%
46	13.716	2009	2011	2014	rBV	59977	78862	2.59%	0.296%
47	14.092	2070	2075	2077	rBV6	67323	111667	3.66%	0.419%
48	14.463	2136	2138	2142	rVB3	69463	69505	2.28%	0.261%
49	14.604	2158	2162	2165	rBV	227625	346712	11.38%	1.301%
50	14.692	2174	2177	2181	rBV2	119783	175753	5.77%	0.660%
51	14.857	2203	2205	2210	rVB	130006	130681	4.29%	0.490%
52	14.910	2211	2214	2219	rBV2	192646	245589	8.06%	0.922%
53	14.963	2219	2223	2226	rBV	503200	566888	18.60%	2.128%

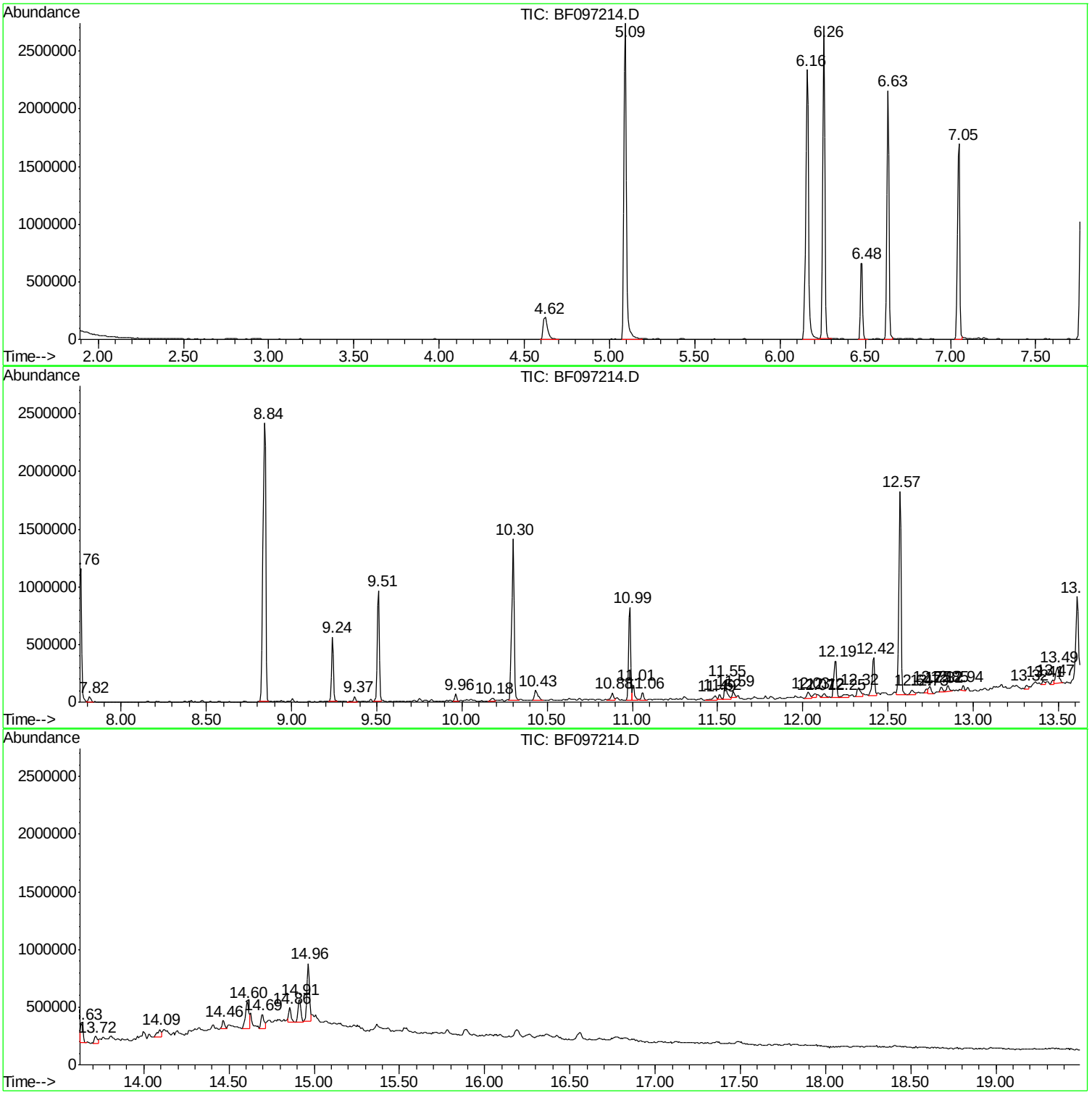
Sum of corrected areas: 26643050

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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

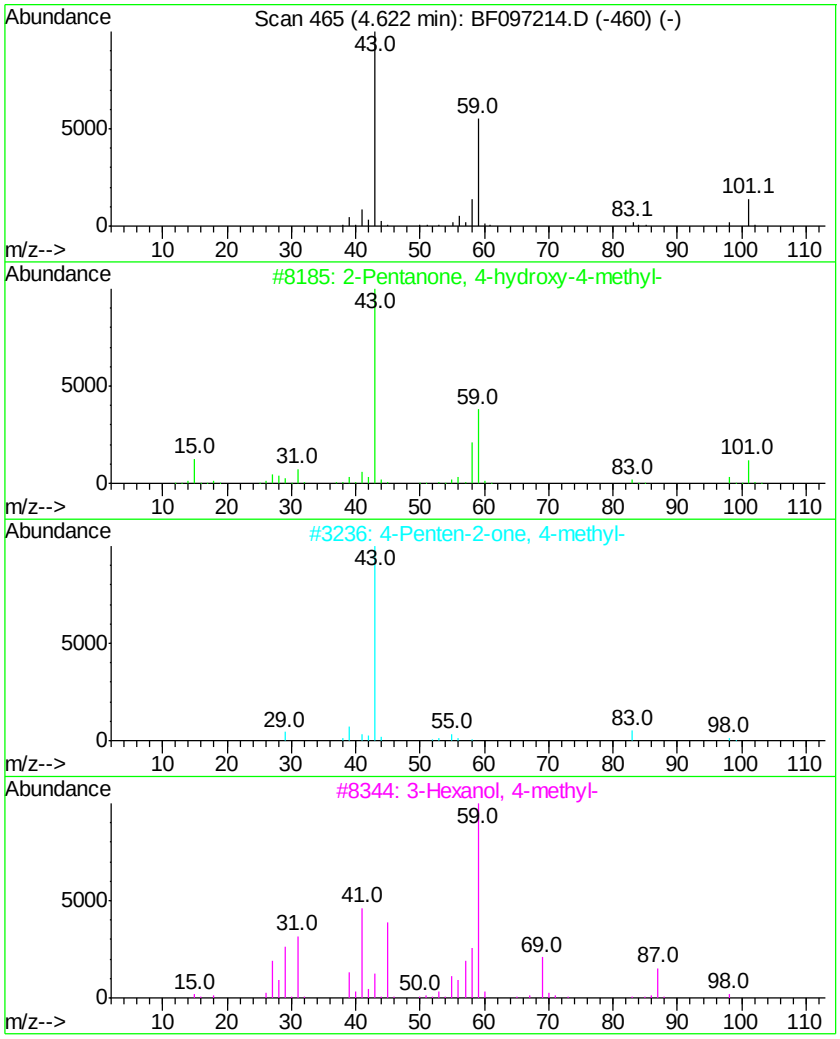
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

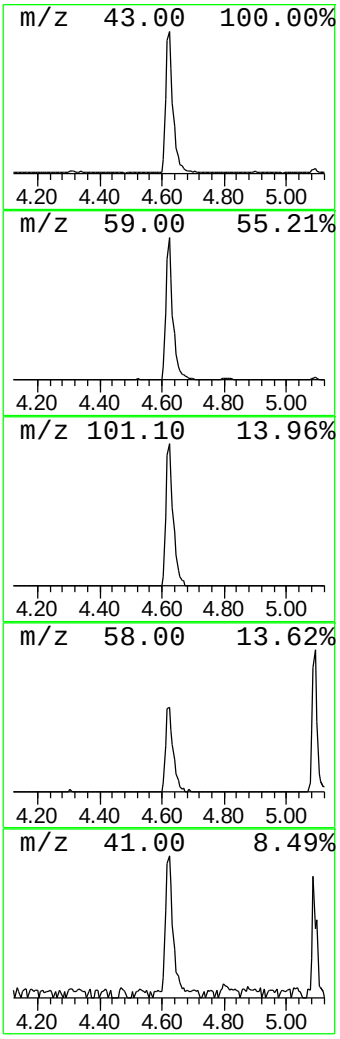
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	9.53 ng	301761	1,4-Dichlorobenzene-d4	6.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
4	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
5	2-Butanone, 3-ethoxy-3-methyl-	130	C7H14O2	036687-99-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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

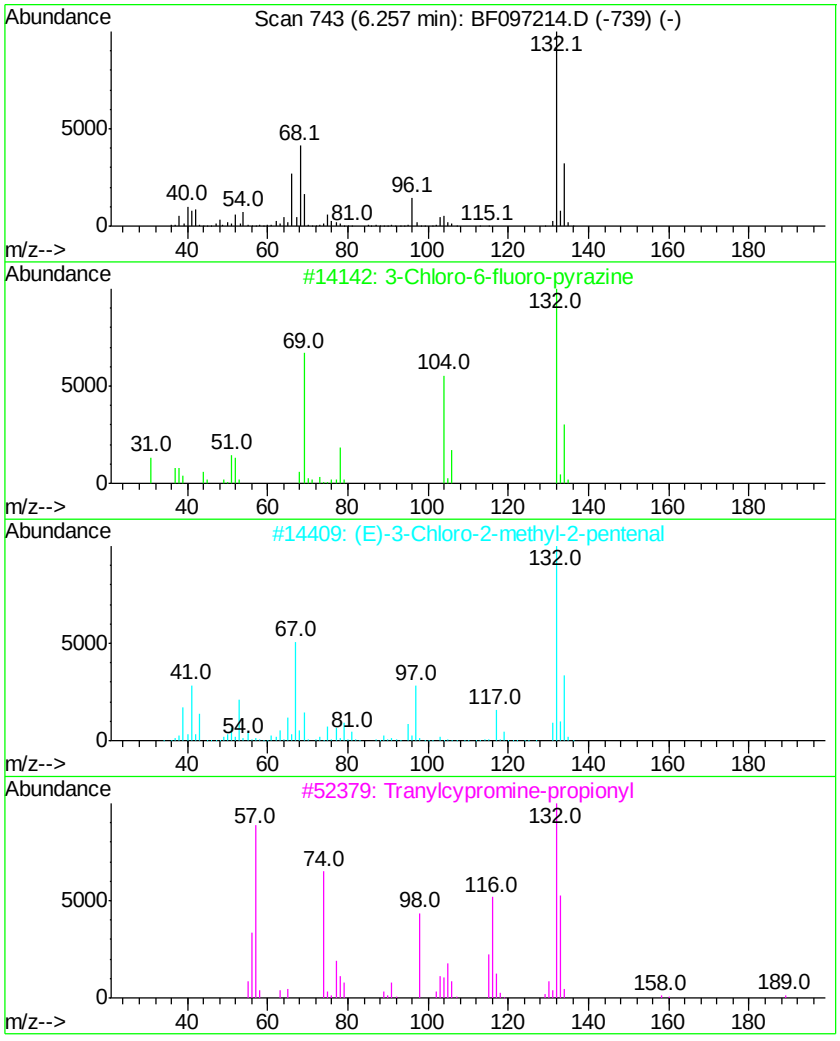
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

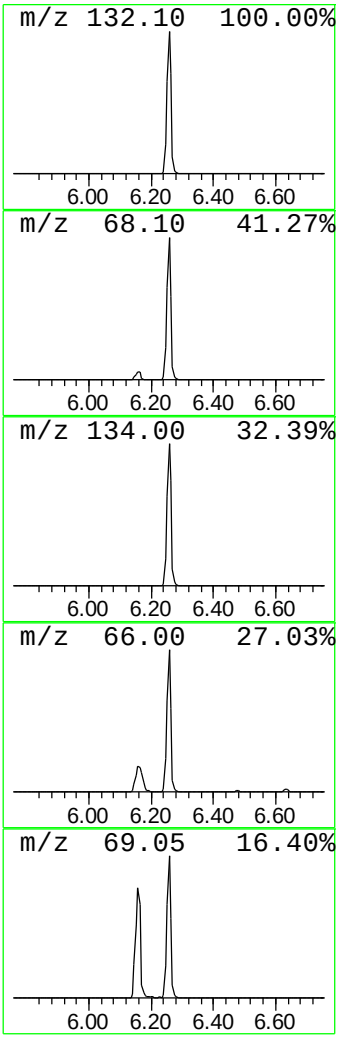
****

Peak Number 2 unknown6.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.26	80.19 ng	2539990	1,4-Dichlorobenzene-d4	6.48

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	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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

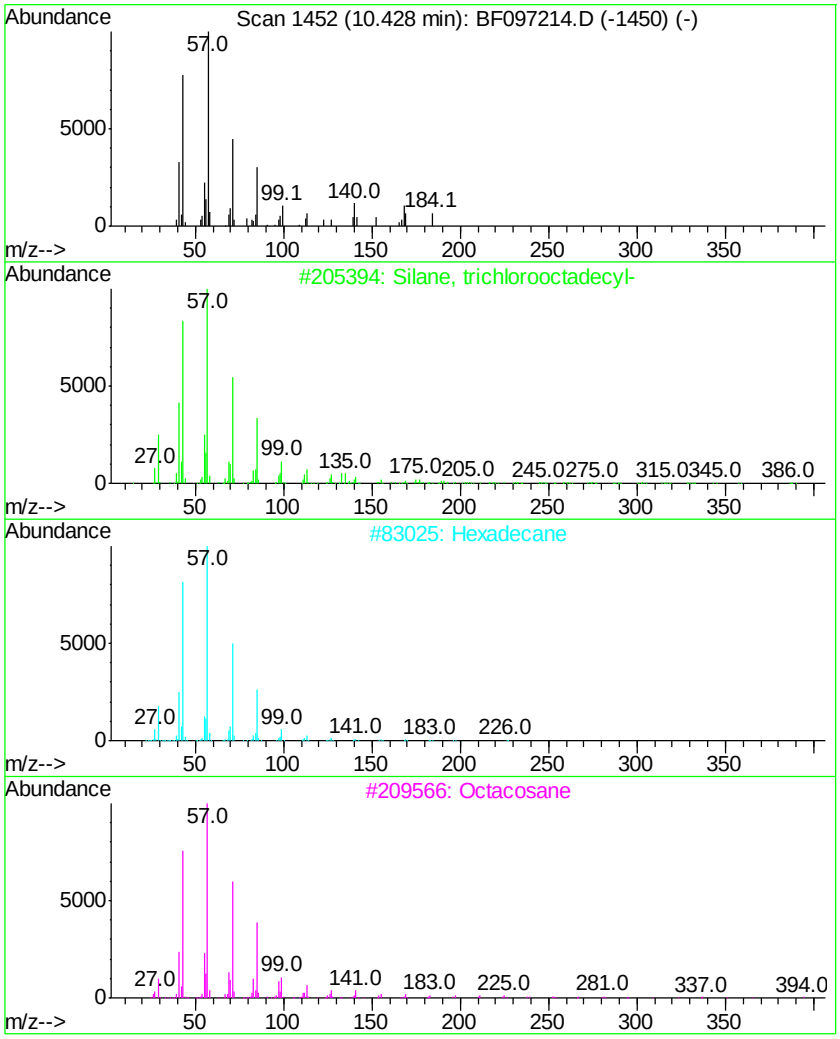
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

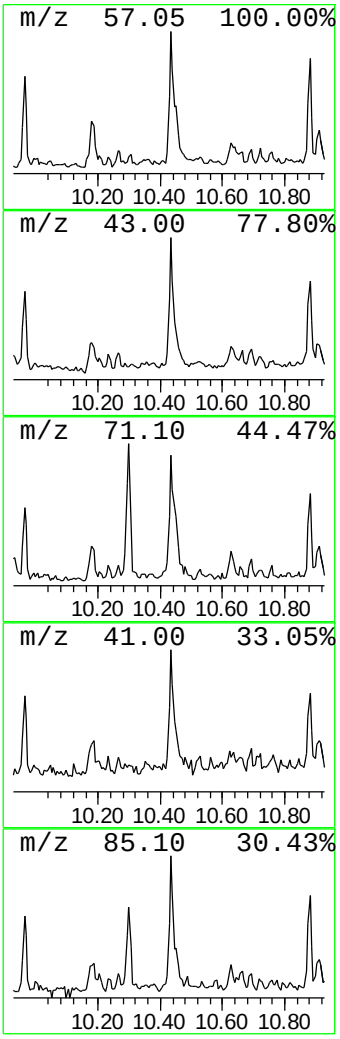
****

Peak Number 4 Silane, trichlorooctadecyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.43	2.85 ng	106535	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
2	Hexadecane	226	C16H34	000544-76-3	86
3	Octacosane	394	C28H58	000630-02-4	86
4	Heptacosane	380	C27H56	000593-49-7	86
5	Eicosane	282	C20H42	000112-95-8	86





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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

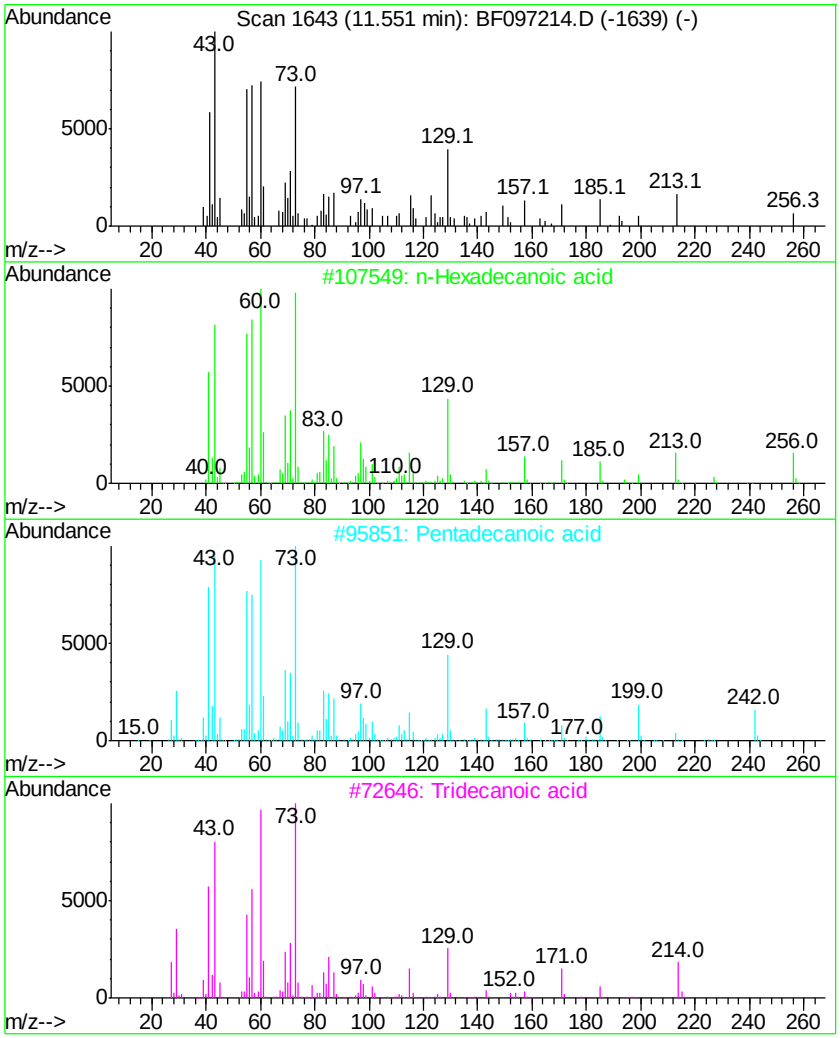
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

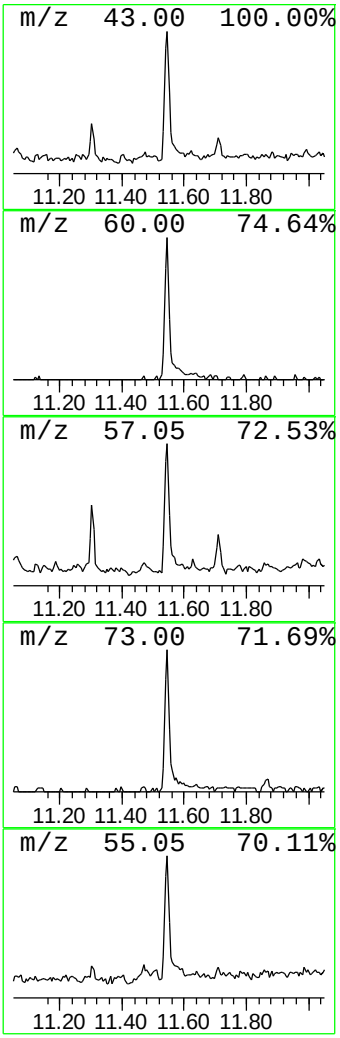
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	4.92 ng	184261	Phenanthrene-d10	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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

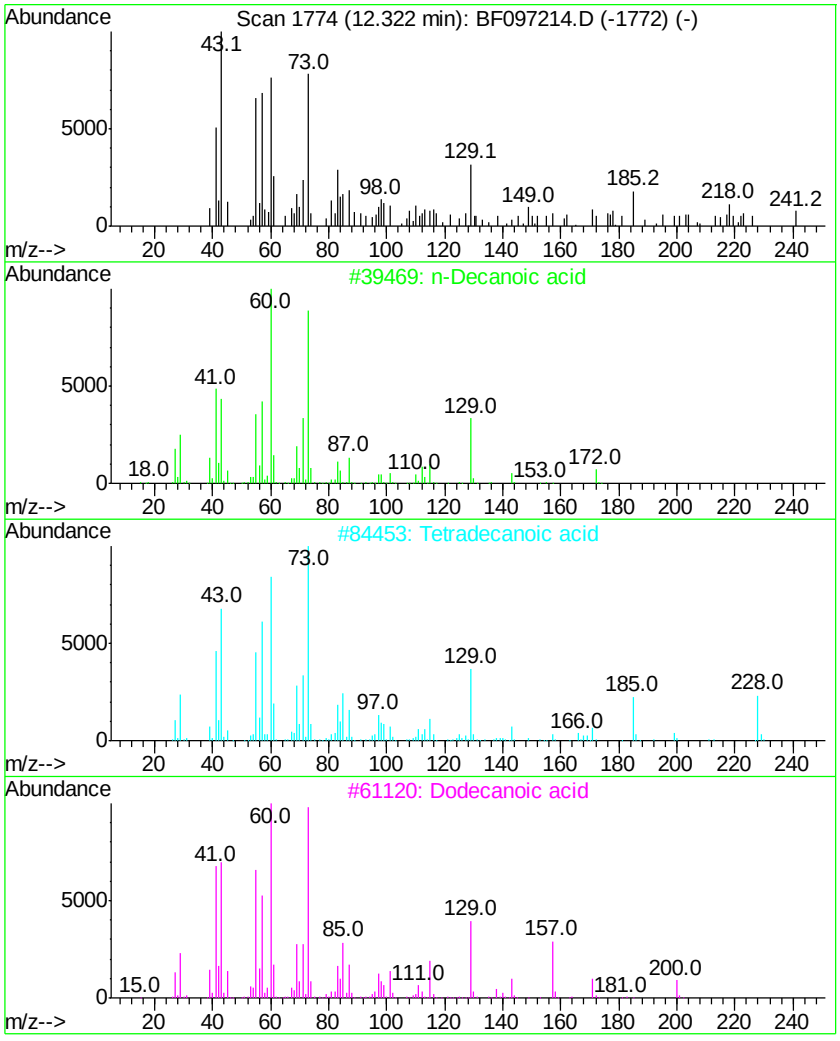
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

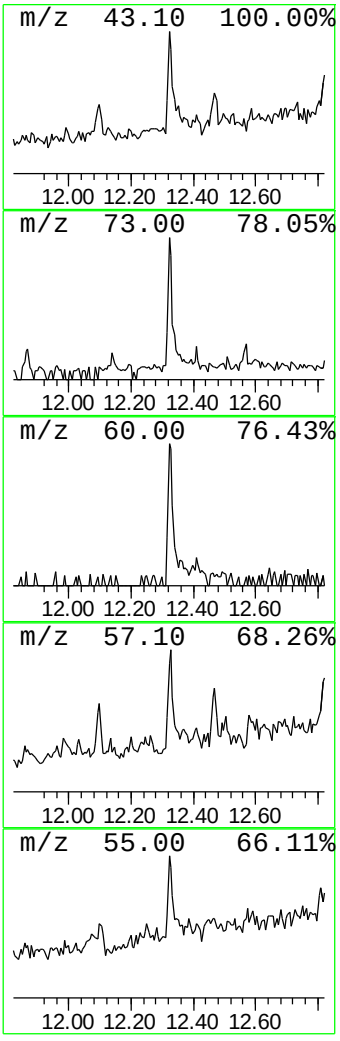
****

Peak Number 6 n-Decanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	2.54 ng	106278	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	58
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Dodecanoic acid	200	C12H24O2	000143-07-7	52
4	Lactose	342	C12H22O11	000063-42-3	47
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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

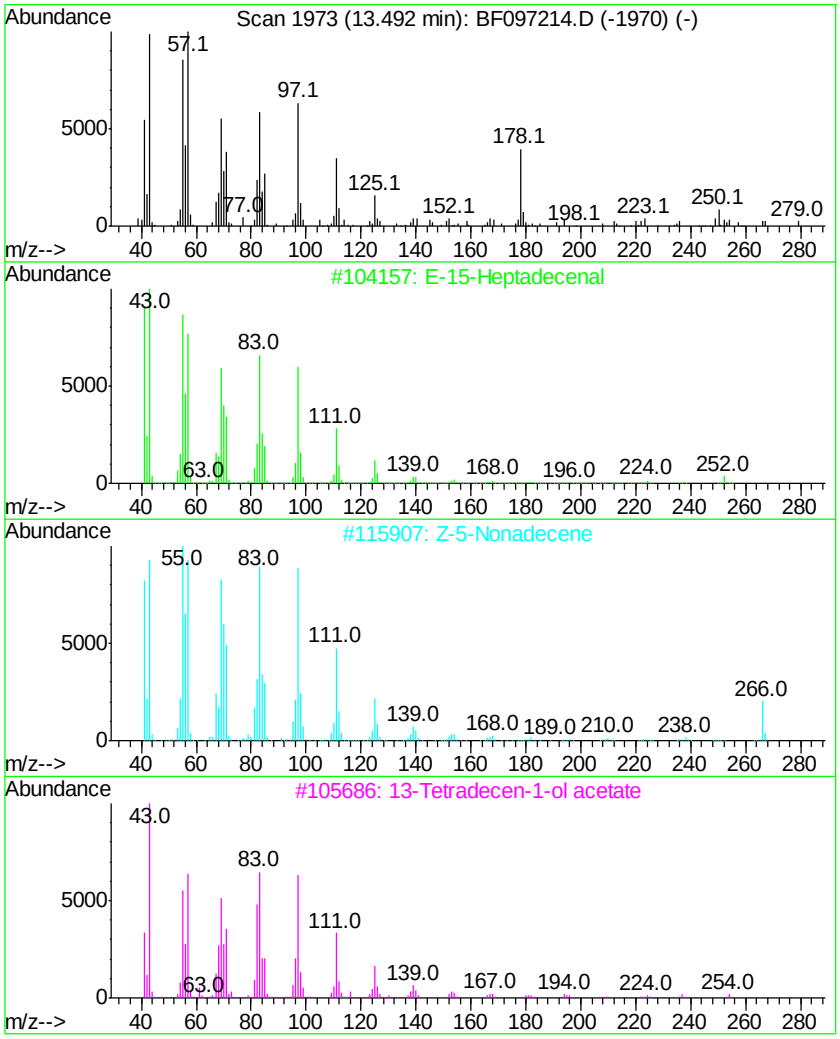
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

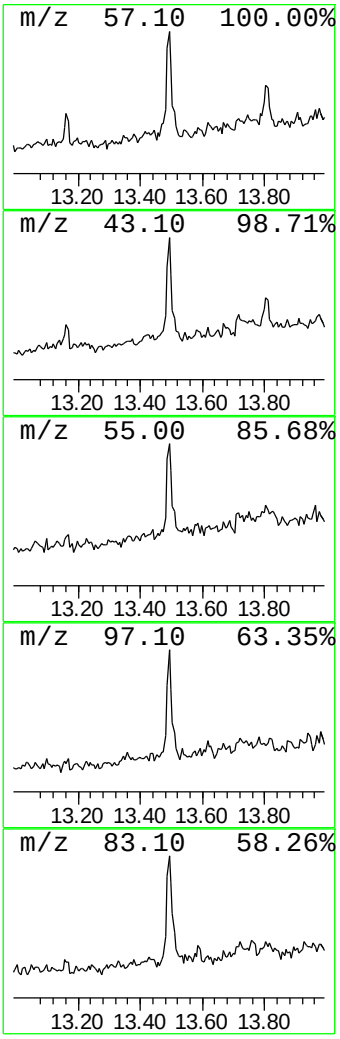
****

Peak Number 7 E-15-Heptadecenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.86 ng	161797	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
2	Z-5-Nonadecene	266	C19H38	1000131-11-8	86
3	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	83
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76
5	1-Docosene	308	C22H44	001599-67-3	70





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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

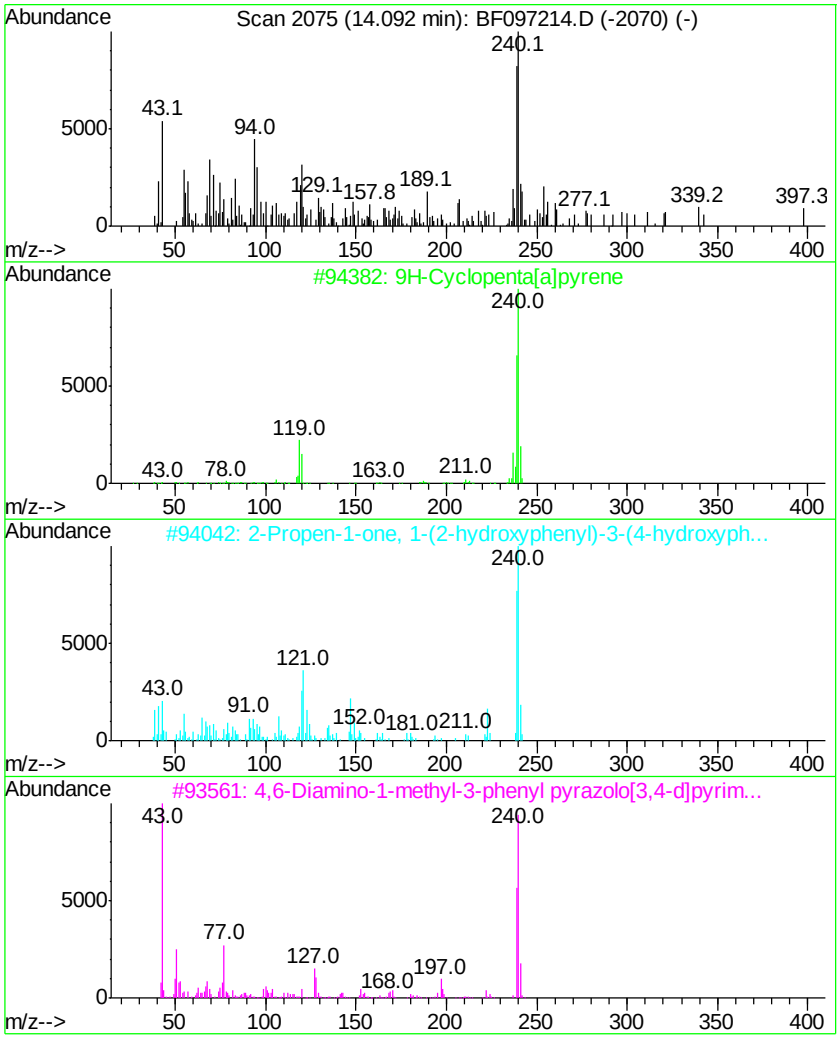
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

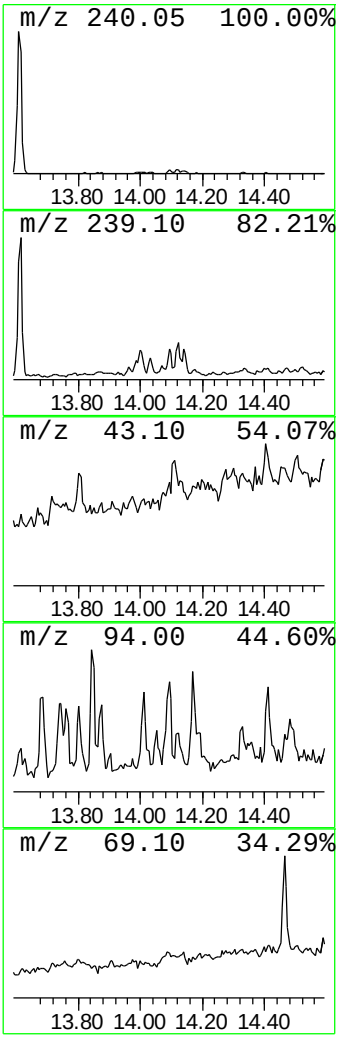
****

Peak Number 8 9H-Cyclopenta[a]pyrene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	2.66 ng	111667	Chrysene-d12	13.61

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Cyclopenta[a]pyrene	240	C19H12	050861-05-7	70
2	2-Propen-1-one, 1-(2-hydroxyphen...	240	C15H12O3	013323-66-5	49
3	4,6-Diamino-1-methyl-3-phenyl py...	240	C12H12N6	058791-67-6	49
4	9H-Pyrrolo[3,2-f]quinolin-9-one,...	240	C15H16N2O	1000319-84-1	49
5	5,6-Dimethyl-4-phenyl-3-cyanopyr...	240	C14H12N2S	094639-18-6	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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

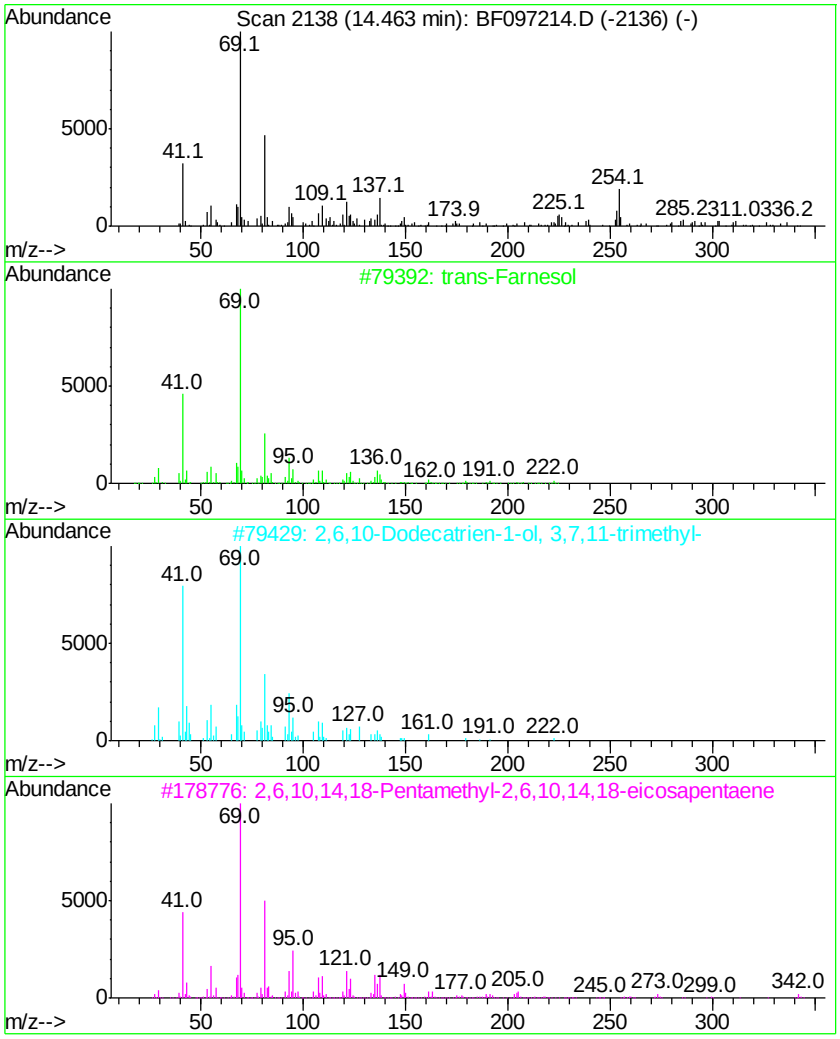
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

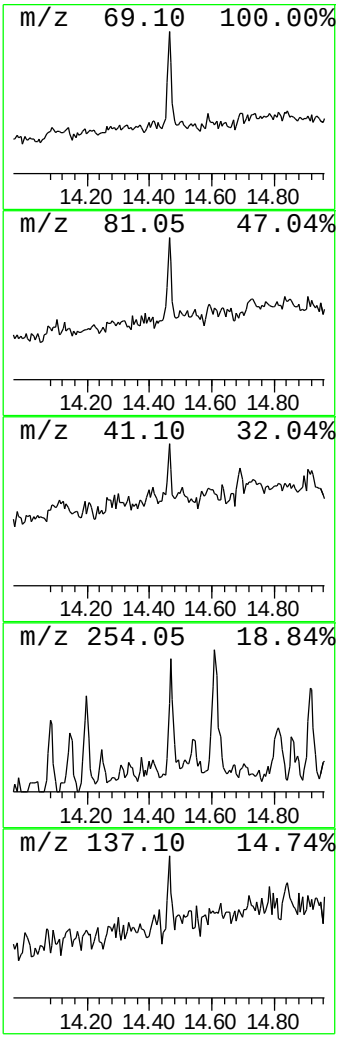
****

Peak Number 9 trans-Farnesol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.45 ng	69505	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Farnesol	222	C15H26O	000106-28-5	64
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
3	2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	59
4	Squalene	410	C30H50	000111-02-4	59
5	trans-Geranylgeraniol	290	C20H34O	024034-73-9	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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

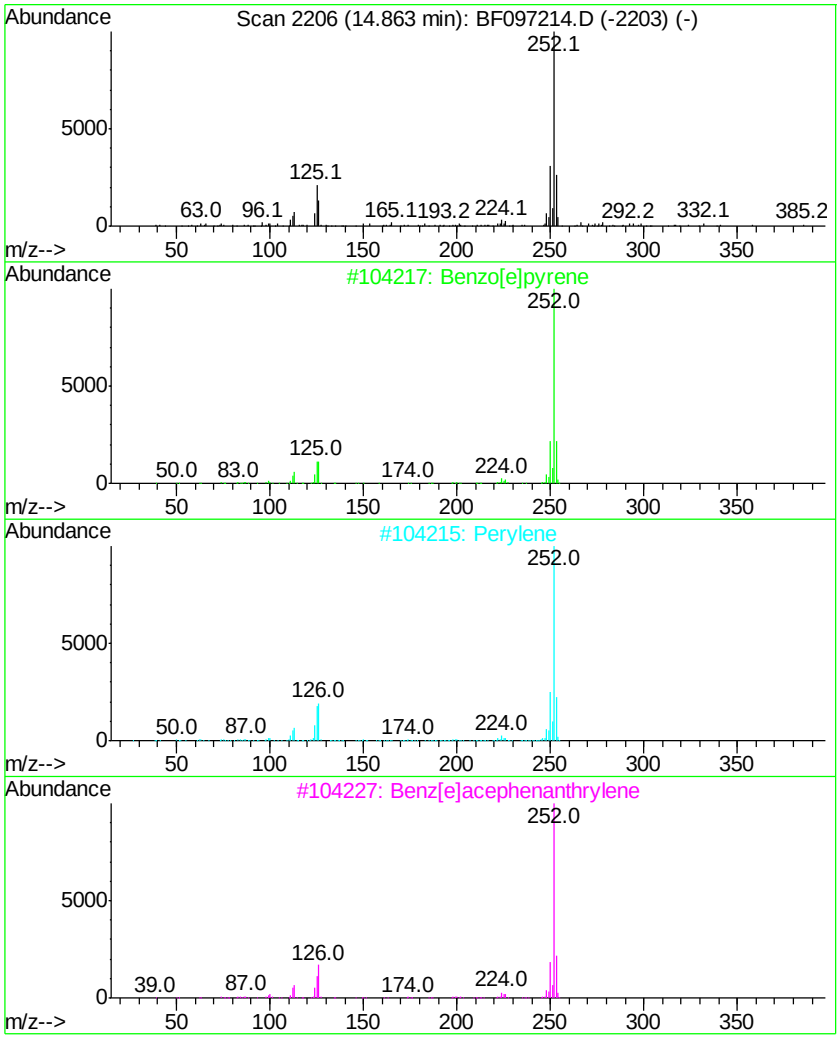
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

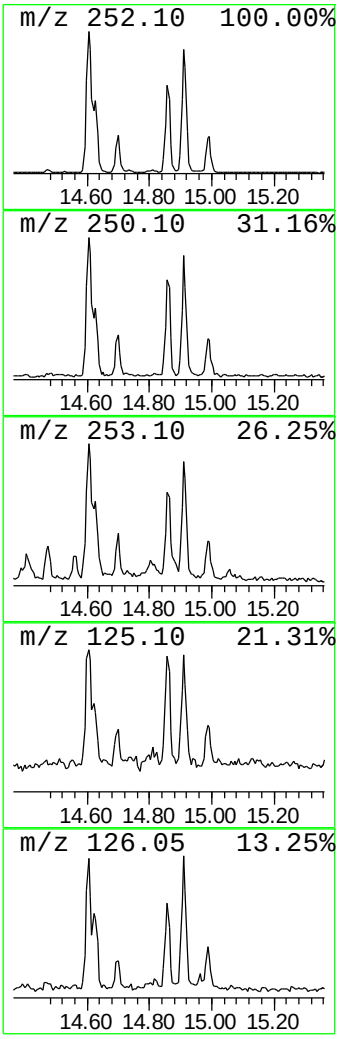
****

Peak Number 11 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	4.61 ng	130681	Perylene-d12	14.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	95
2	Perylene	252	C20H12	000198-55-0	93
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
4	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90
5	Benzo[a]pyrene	252	C20H12	000050-32-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF073117\
Data File : BF097214.D
Acq On : 31 Jul 2017 18:09
Operator : SJ/JU
Sample : I4488-04
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CL-02-072717-B

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...	4.62	9.5	ng	301761	1	6.48	633486	20.0
unknown6.26	6.26	80.2	ng	2539990	1	6.48	633486	20.0
Silane, trichloro...	10.43	2.9	ng	106535	4	10.99	748288	20.0
n-Hexadecanoic acid	11.55	4.9	ng	184261	4	10.99	748288	20.0
n-Decanoic acid	12.32	2.5	ng	106278	5	13.61	838376	20.0
E-15-Heptadecenal	13.49	3.9	ng	161797	5	13.61	838376	20.0
9H-Cyclopenta[a]p...	14.09	2.7	ng	111667	5	13.61	838376	20.0
trans-Farnesol	14.46	2.5	ng	69505	6	14.96	566888	20.0
Benzo[e]pyrene	14.86	4.6	ng	130681	6	14.96	566888	20.0