LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

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-BF050217.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	4.801	501	504	528	rBV	58605	155879	7.01%	0.852%
2	5.472	614	618	651	rBV	897385	1844185	82.90%	10.083%
3	7.107	892	896	910	rBV	1106987	1793124	80.60%	9.804%
4	7.213	910	914	935	rVB	1501056	2224689	100.00%	12.164%
5	7.554	968	972	984	rVB	386910	488918	21.98%	2.673%
6	7.789	1007	1012	1031	rBV	1070969	1365372	61.37%	7.465%
7	8.466	1122	1127	1143	rBV	756179	1127788	50.69%	6.166%
8	9.583	1313	1317	1336	rBV	534607	728321	32.74%	3.982%
9	11.360	1614	1619	1635	rBV	1355831	1639637	73.70%	8.965%
10	12.048	1732	1736	1748	rBV	151464	202638	9.11%	1.108%
11	12.407	1793	1797	1806	rBV2	497457	650185	29.23%	3.555%
12	13.254	1936	1941	1945	rBV2	28857	32029	1.44%	0.175%
13	13.707	2013	2018	2032	rBV	576294	824762	37.07%	4.510%
14	14.024	2068	2072	2076	rBV	28341	34327	1.54%	0.188%
15	14.812	2201	2206	2210	rVV2	407341	514540	23.13%	2.813%
16	14.848	2210	2212	2220	rVV	104405	139055	6.25%	0.760%
17	14.948	2223	2229	2238	rVB	25336	39825	1.79%	0.218%
18	15.653	2345	2349	2352	rBV	19677	22941	1.03%	0.125%
19	15.736	2359	2363	2365	rBV2	37576	46032	2.07%	0.252%
20	15.801	2370	2374	2386	rVB2	120925	164487	7.39%	0.899%
21	16.612	2508	2512	2518	rBV	230850	244755	11.00%	1.338%
22	16.912	2557	2563	2570	rBV	234511	300358	13.50%	1.642%
23	17.153	2600	2604	2609	rBV	1003349	1082654	48.67%	5.920%
24	17.383	2640	2643	2648	rVB	29769	37709	1.70%	0.206%
25	17.471	2653	2658	2662	rBV	22873	23508	1.06%	0.129%
26	17.518	2662	2666	2674	rBV4	27870	49641	2.23%	0.271%
27	17.853	2714	2723	2728	rBV	101145	118591	5.33%	0.648%
28	18.400	2812	2816	2825	rBV2	79203	125247	5.63%	0.685%
29	18.506	2827	2834	2838	rVV2	484150	670775	30.15%	3.668%
30	18.541	2838	2840	2851	rVB2	99980	145630	6.55%	0.796%
31	18.636	2853	2856	2860	rBV2	21475	27638	1.24%	0.151%
32	19.018	2914	2921	2925	rBV2	26483	37586	1.69%	0.206%
33	19.200	2949	2952	2961	rVB4	33297	54833	2.46%	0.300%
34	19.636	3021	3026	3030	rVB2	69244	85006	3.82%	0.465%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

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-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.777	3046	3050	3053	rBV	110441	148524	6.68%	0.812%
36	19.806	3053	3055	3062	rVB3	50521	59546	2.68%	0.326%
37	19.888	3067	3069	3072	rBV	18971	22470	1.01%	0.123%
38	20.071	3096	3100	3104	rBV	66411	75955	3.41%	0.415%
39	20.130	3106	3110	3114	rVV	93497	103635	4.66%	0.567%
40	20.177	3114	3118	3128	rVV	324652	419840	18.87%	2.296%
41	21.435	3328	3332	3334	rBV	36773	47631	2.14%	0.260%
42	21.477	3335	3339	3347	rVB4	140437	240470	10.81%	1.315%
43	21.612	3358	3362	3369	rVB10	35931	71035	3.19%	0.388%
44	21.800	3390	3394	3397	rBV2	31158	57635	2.59%	0.315%

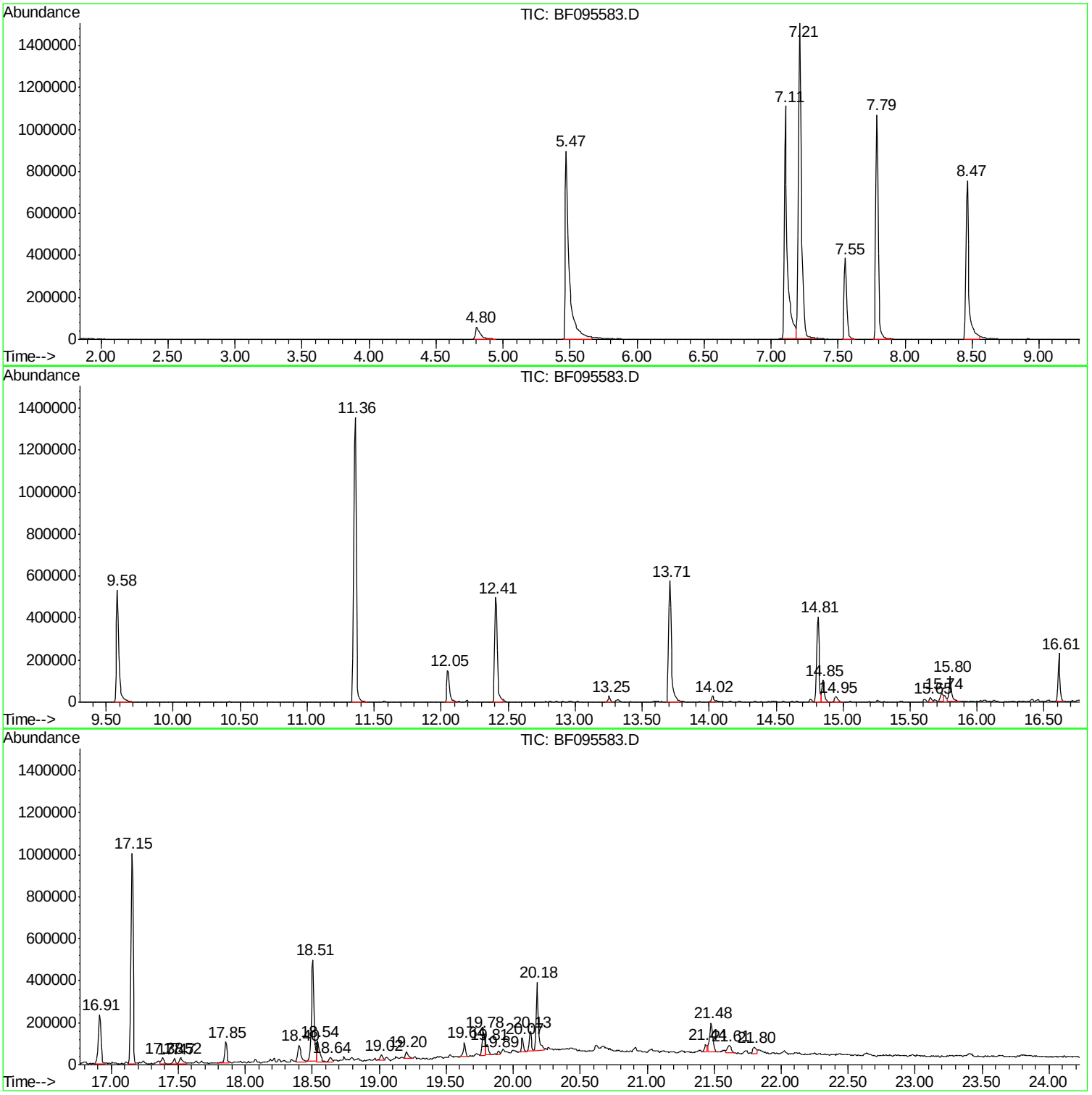
Sum of corrected areas: 18289406

Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

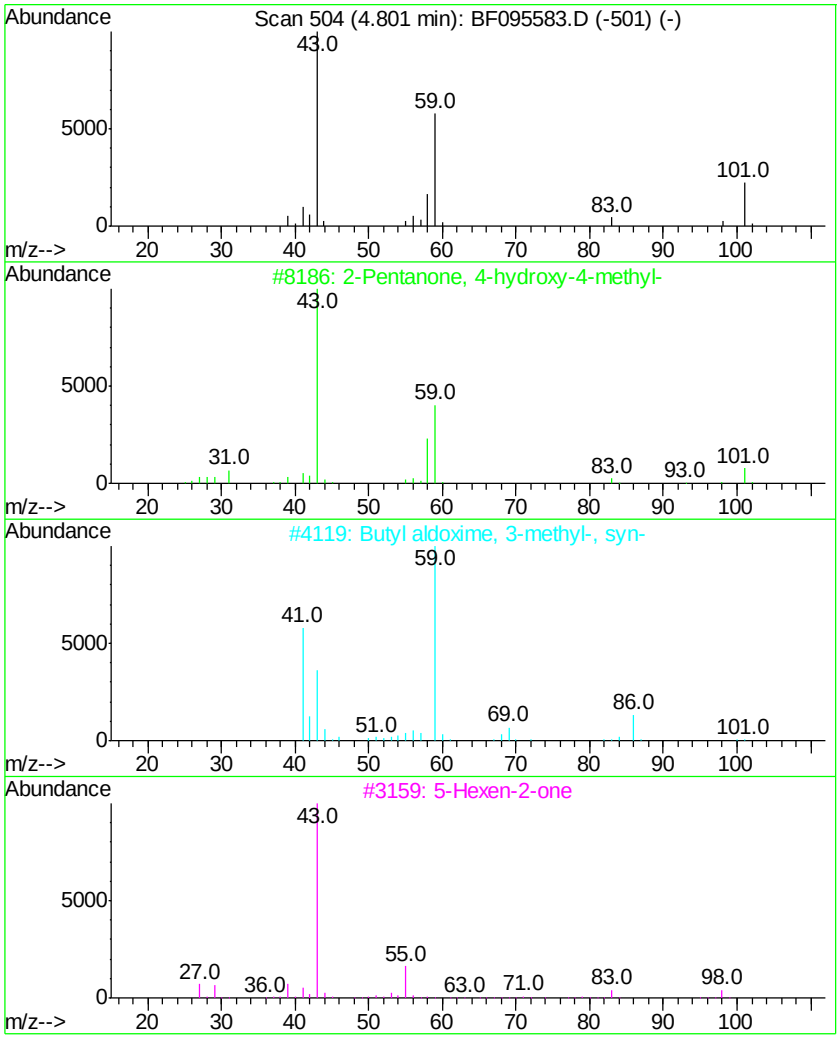
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

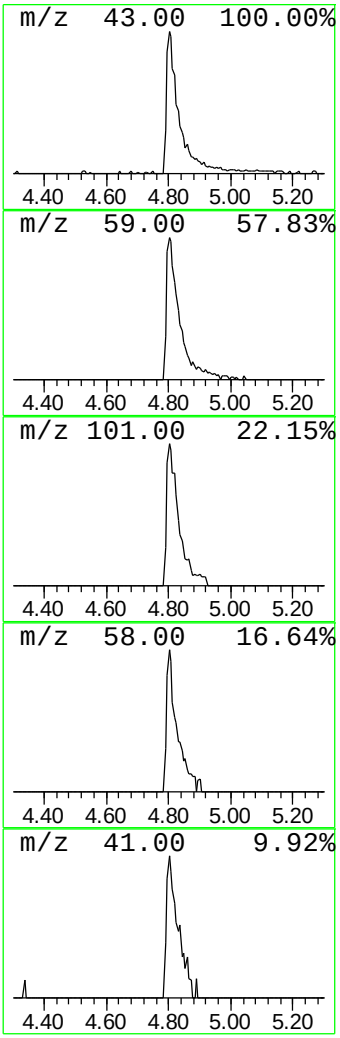
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	6.38 ng	155879	1,4-Dichlorobenzene-d4	7.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

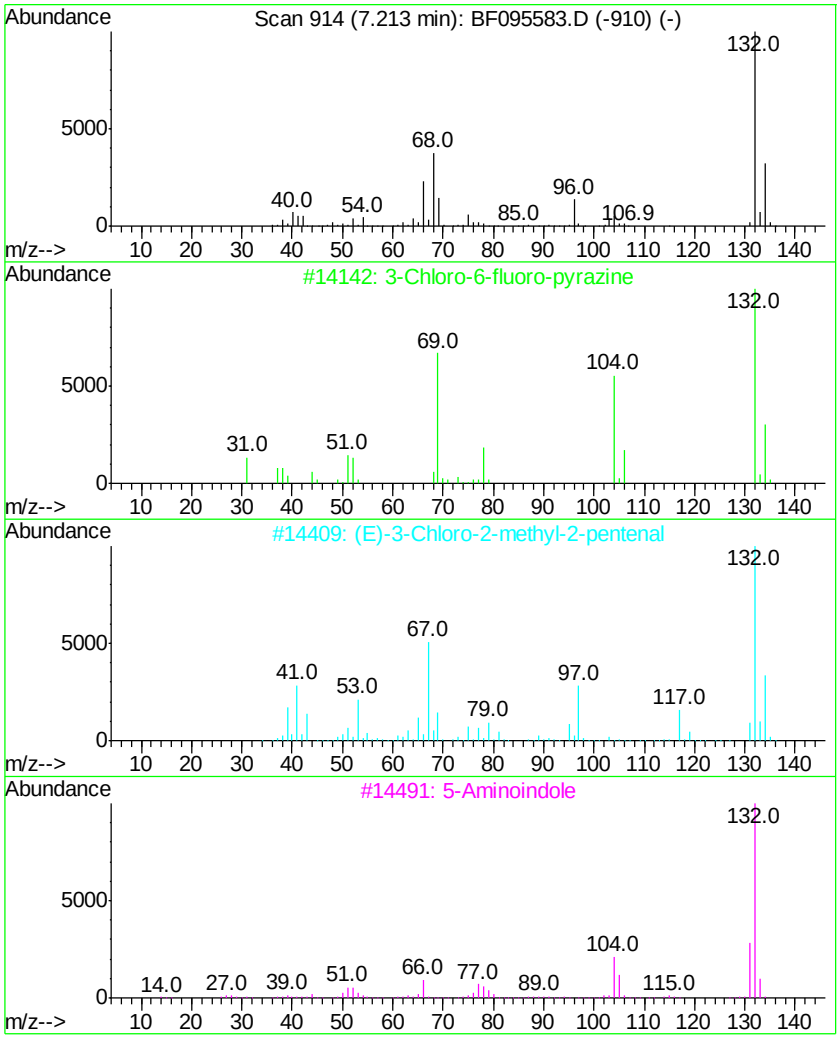
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

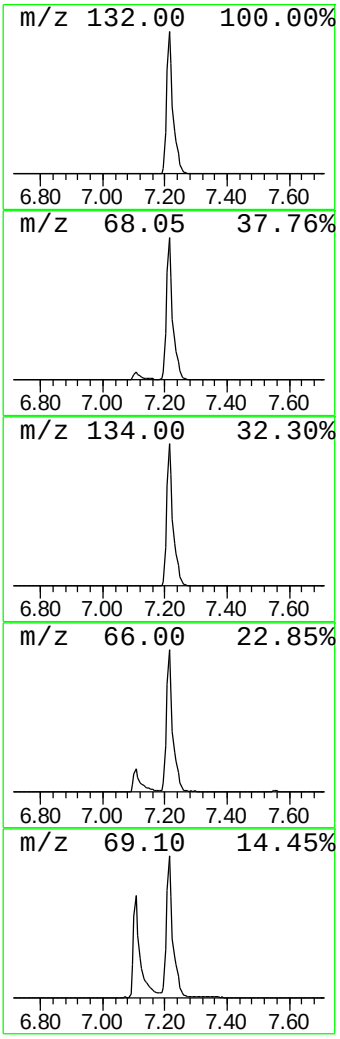
****

Peak Number 2 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	91.00 ng	2224690	1,4-Dichlorobenzene-d4	7.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

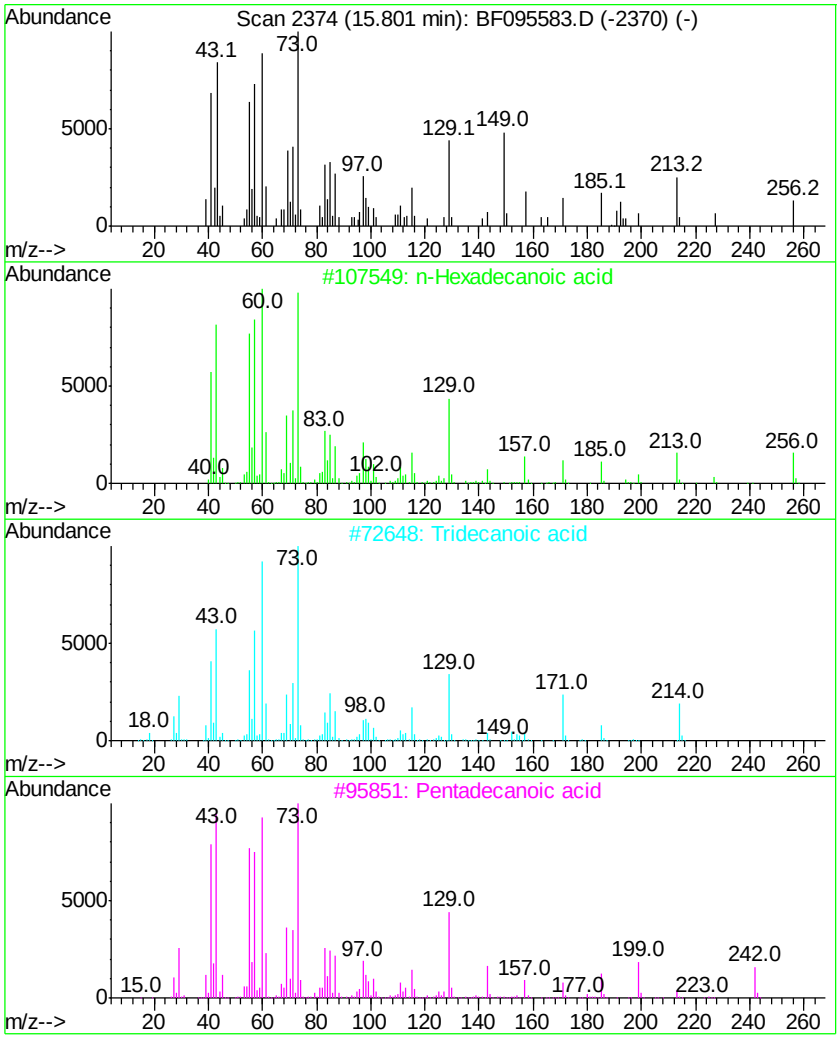
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

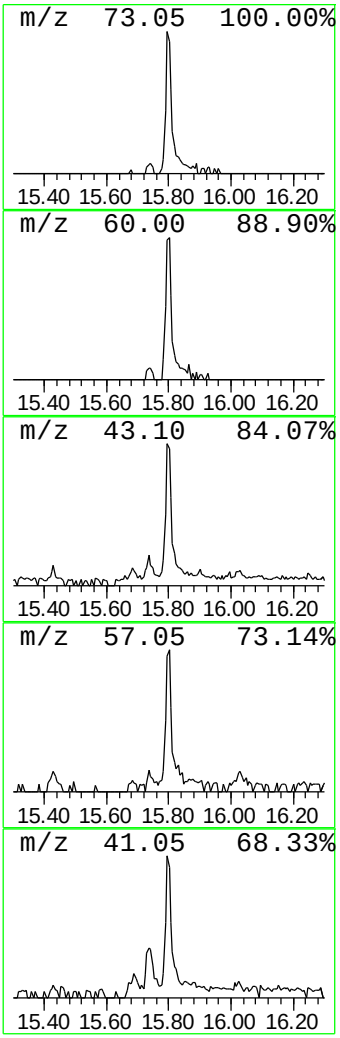
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	6.39 ng	164487	Phenanthrene-d10	14.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

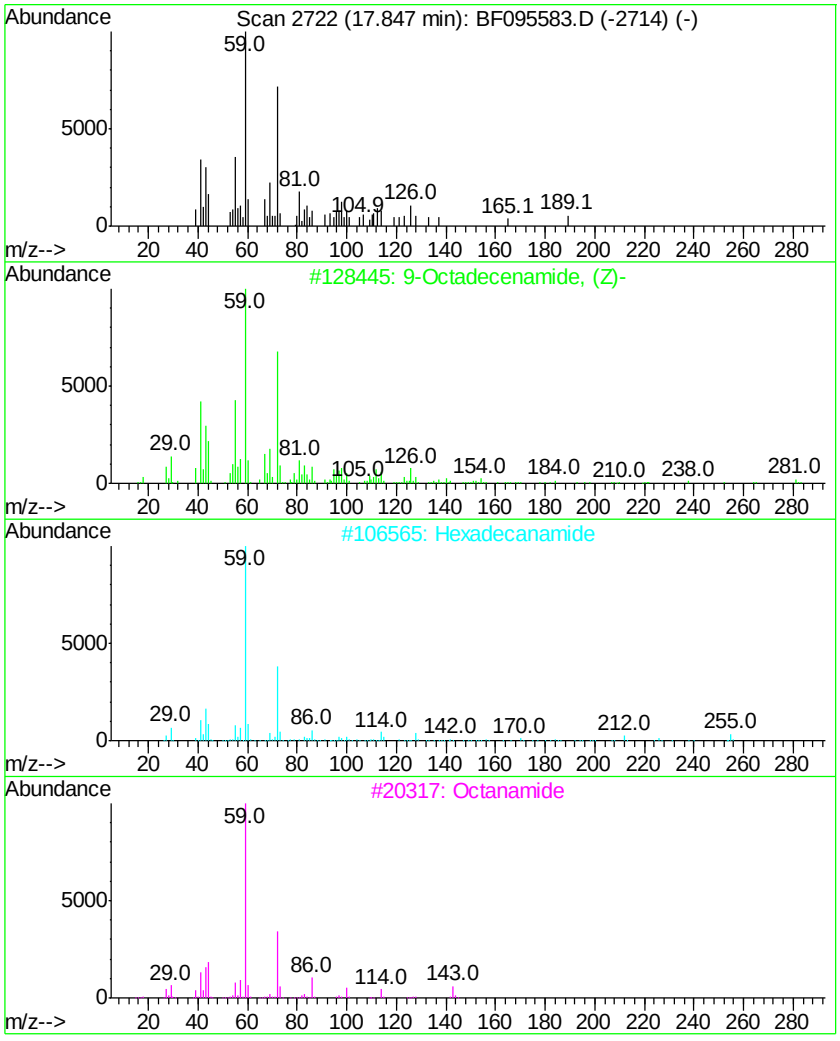
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

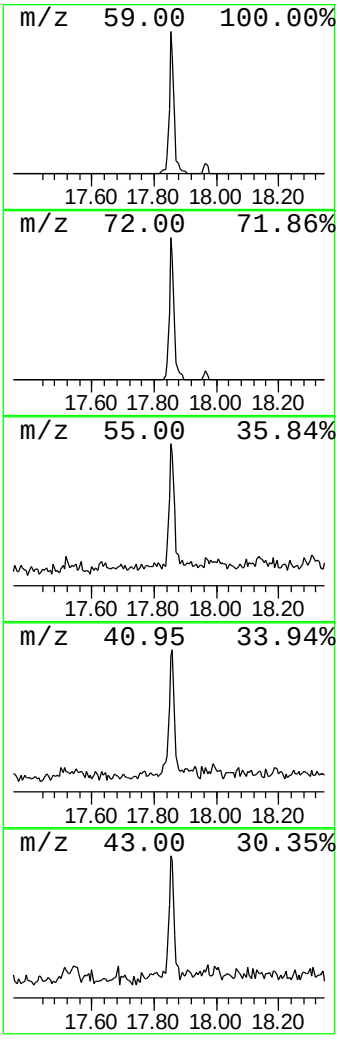
****

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	3.54 ng	118591	Chrysene-d12	18.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Hexadecanamide	255	C16H33NO	000629-54-9	64
3	Octanamide	143	C8H17NO	000629-01-6	53
4	Dodecanamide	199	C12H25NO	001120-16-7	53
5	Decanamide-	171	C10H21NO	002319-29-1	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

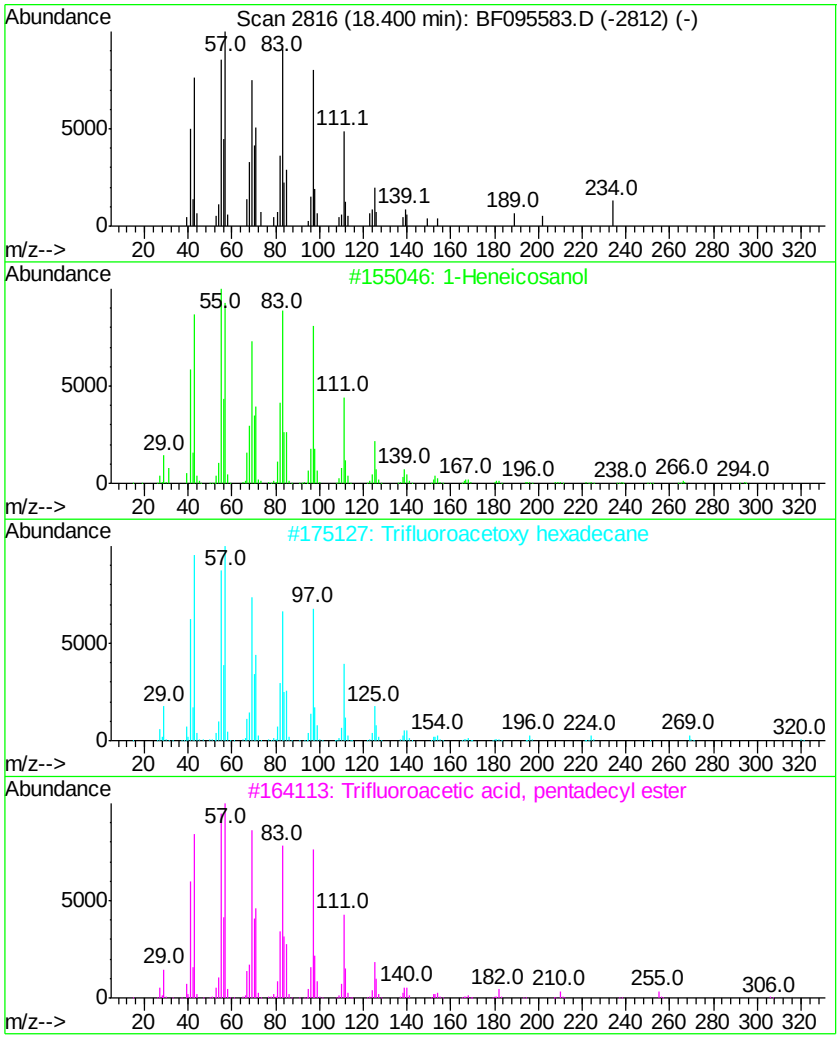
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

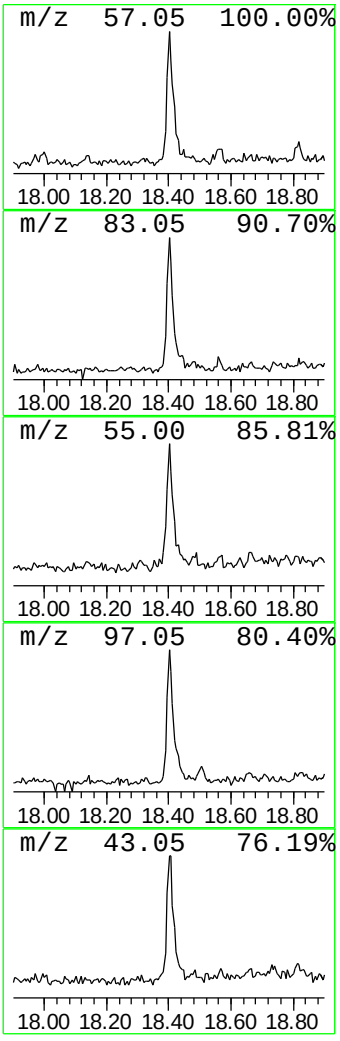
****

Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	3.73 ng	125247	Chrysene-d12	18.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

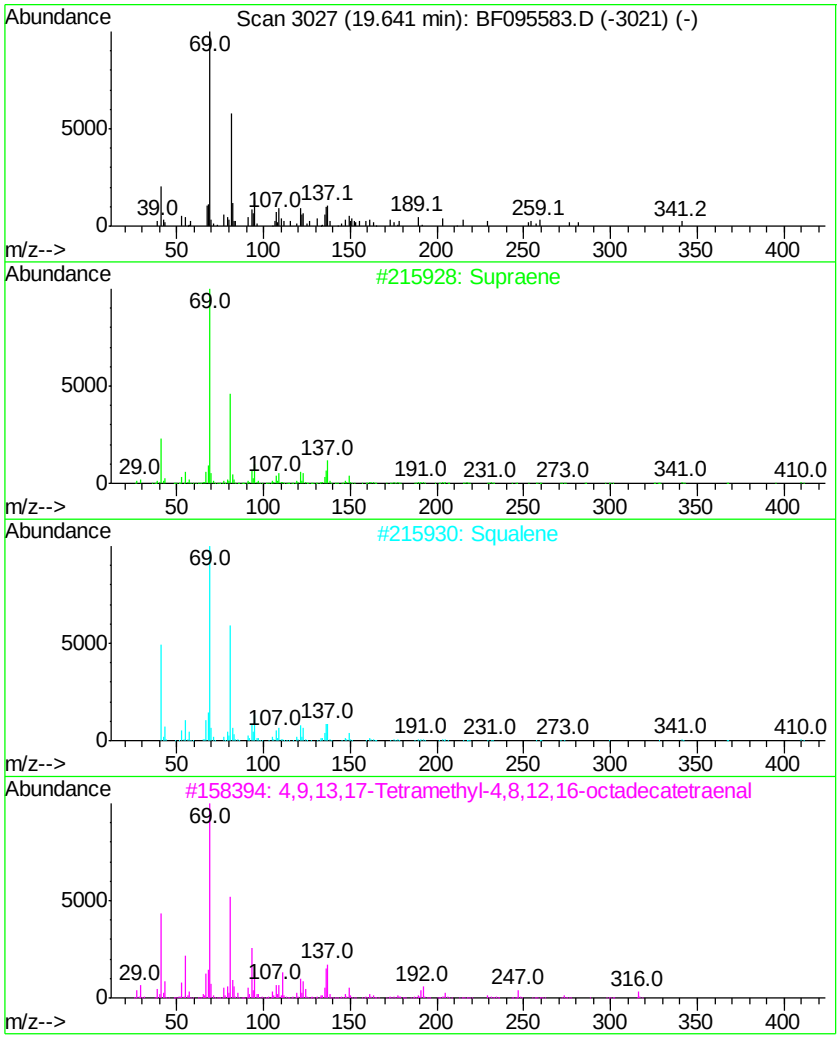
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

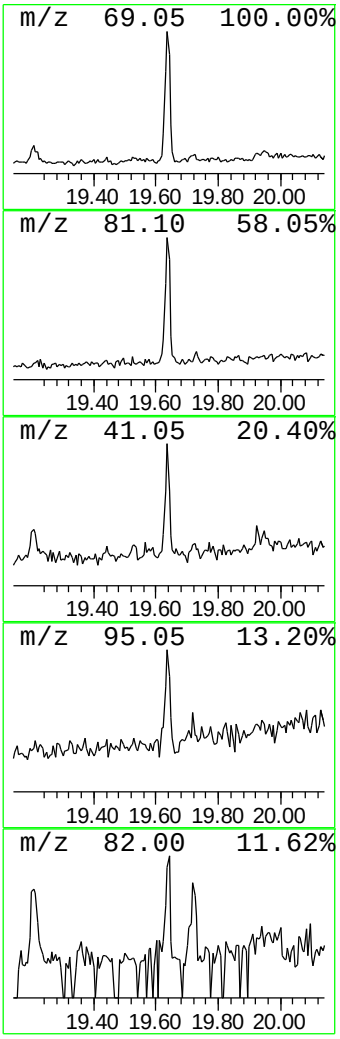
****

Peak Number 7 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.64	4.05 ng	85006	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	87
2	Squalene	410	C30H50	000111-02-4	80
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64
5	4,8,12-Tetradecatrienenitrile, 5...	245	C17H27N	005981-31-7	59





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

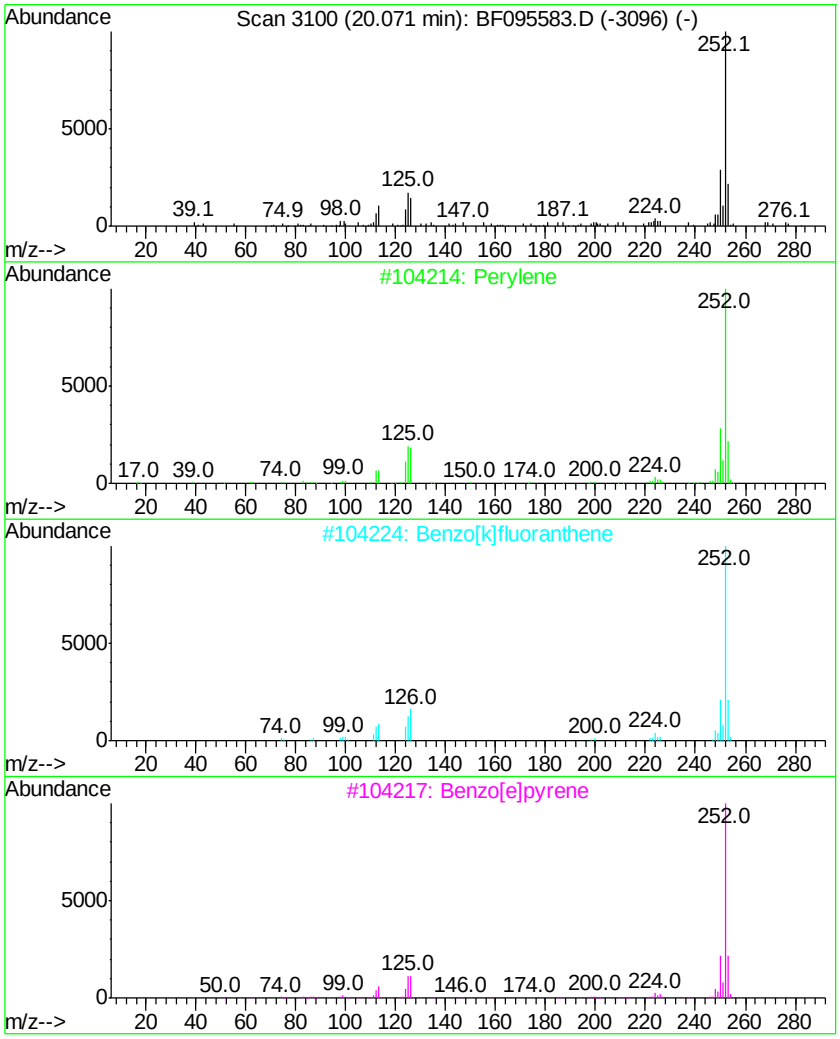
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

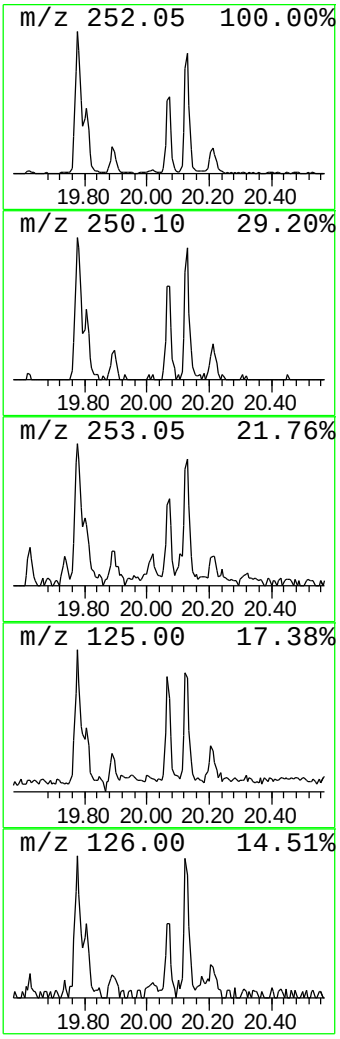
****

Peak Number 8 Perylene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.07	3.62 ng	75955	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	94
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
3	Benzo[e]pyrene	252	C20H12	000192-97-2	93
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	93
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

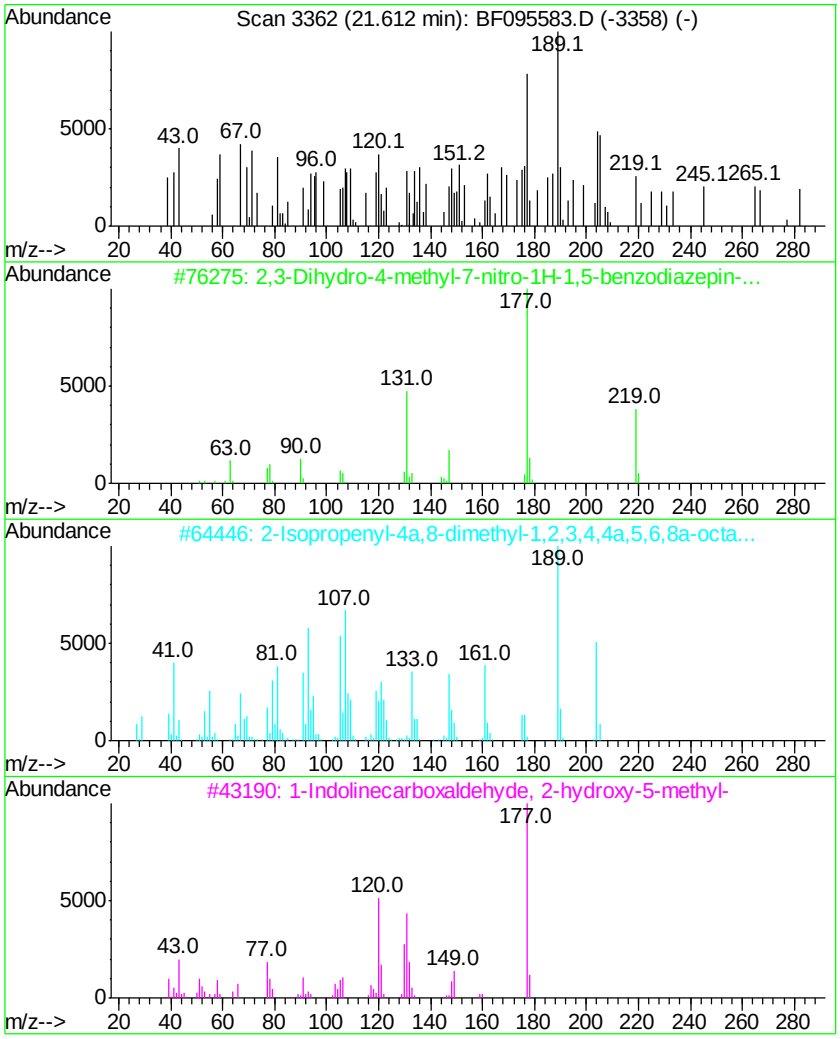
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

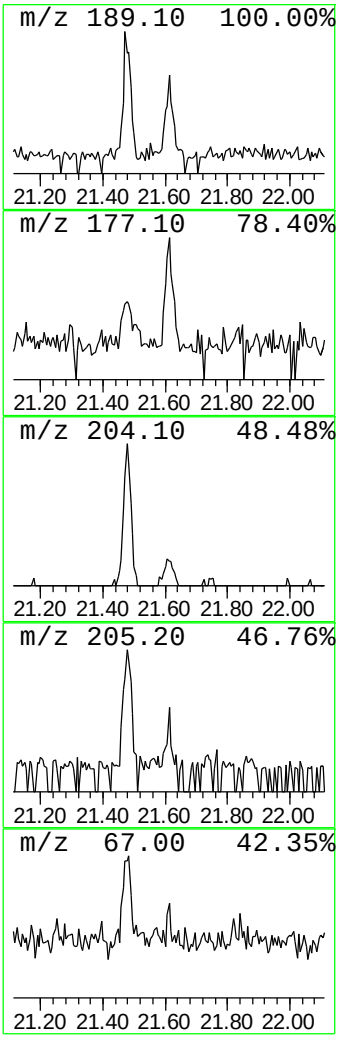
****

Peak Number 9 unknown21.61 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.61	3.38 ng	71035	Perylene-d12	20.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Dihydro-4-methyl-7-nitro-1H-...	219	C10H9N3O3	037546-86-4	22
2	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	1000193-57-0	20
3	1-Indolinecarboxaldehyde, 2-hydr...	177	C10H11NO2	013303-69-0	18
4	Naphthalene, decahydro-4a-methyl...	204	C15H24	000515-17-3	14
5	3,4-Dihydrocoumarin, 4,4,7,8-tet...	204	C13H16O2	040614-36-6	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF053117\
Data File : BF095583.D
Acq On : 1 Jun 2017 1:29
Operator : SJ/MA
Sample : I3302-10
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : NM15-COMP-6-18

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	4.80	6.4	ng	155879	1	7.55	488918	20.0
unknown7.21	7.21	91.0	ng	2224690	1	7.55	488918	20.0
n-Hexadecanoic acid	15.80	6.4	ng	164487	4	14.81	514540	20.0
9-Octadecenamide,...	17.85	3.5	ng	118591	5	18.51	670775	20.0
1-Heneicosanol	18.40	3.7	ng	125247	5	18.51	670775	20.0
Supraene	19.64	4.0	ng	85006	6	20.18	419840	20.0
Perylene	20.07	3.6	ng	75955	6	20.18	419840	20.0
unknown21.61	21.61	3.4	ng	71035	6	20.18	419840	20.0