LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097603.D
Acq On : 11 Aug 2017 19:41
Operator : SJ/JU
Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

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-BF081117.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	1.857	27	29	56	rVB	218428	463849	28.08%	2.678%
2	4.740	515	519	536	rBV2	60199	169862	10.28%	0.981%
3	5.410	629	633	658	rBV	683454	1514187	91.66%	8.741%
4	7.045	907	911	926	rBV	895394	1499759	90.79%	8.657%
5	7.157	926	930	945	rVB	1053635	1651948	100.00%	9.536%
6	7.510	986	990	1011	rVB	443436	648961	39.28%	3.746%
7	7.745	1025	1030	1046	rBV	834875	1192448	72.18%	6.883%
8	8.416	1140	1144	1164	rBV	622083	1019744	61.73%	5.886%
9	9.533	1330	1334	1356	rBV	608468	890795	53.92%	5.142%
10	11.316	1632	1637	1649	rBV	1290152	1632944	98.85%	9.426%
11	12.004	1750	1754	1767	rBV	142629	193076	11.69%	1.115%
12	12.363	1810	1815	1820	rBV2	658923	824135	49.89%	4.757%
13	12.398	1820	1821	1830	rVB	30129	34814	2.11%	0.201%
14	13.216	1956	1960	1967	rBV	35420	42484	2.57%	0.245%
15	13.651	2030	2034	2052	rBV	571258	856992	51.88%	4.947%
16	13.986	2087	2091	2101	rBV	34005	50226	3.04%	0.290%
17	14.721	2210	2216	2218	rBV	19992	23334	1.41%	0.135%
18	14.757	2218	2222	2237	rVB	561401	802205	48.56%	4.631%
19	15.757	2388	2392	2400	rBV2	66244	91314	5.53%	0.527%
20	17.115	2618	2623	2632	rVB	921672	1076924	65.19%	6.216%
21	18.374	2832	2837	2847	rBV2	67354	135832	8.22%	0.784%
22	18.462	2847	2852	2861	rVV	424844	559955	33.90%	3.232%
23	19.892	3091	3095	3097	rBV	17631	22660	1.37%	0.131%
24	20.127	3131	3135	3146	rBV	417190	545974	33.05%	3.152%
25	20.580	3209	3212	3217	rVB4	16131	23505	1.42%	0.136%
26	20.639	3217	3222	3226	rBV6	25882	58849	3.56%	0.340%
27	20.674	3226	3228	3236	rVB9	24694	32024	1.94%	0.185%
28	20.986	3276	3281	3283	rBV5	14090	19630	1.19%	0.113%
29	21.786	3410	3417	3425	rBV8	41469	114161	6.91%	0.659%
30	21.991	3441	3452	3471	rBV2	321717	1010482	61.17%	5.833%
31	22.556	3544	3548	3553	rBV7	15922	31896	1.93%	0.184%
32	23.315	3671	3677	3684	rVB7	36488	88728	5.37%	0.512%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097603.D
Acq On : 11 Aug 2017 19:41
Operator : SJ/JU
Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

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-BF081117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

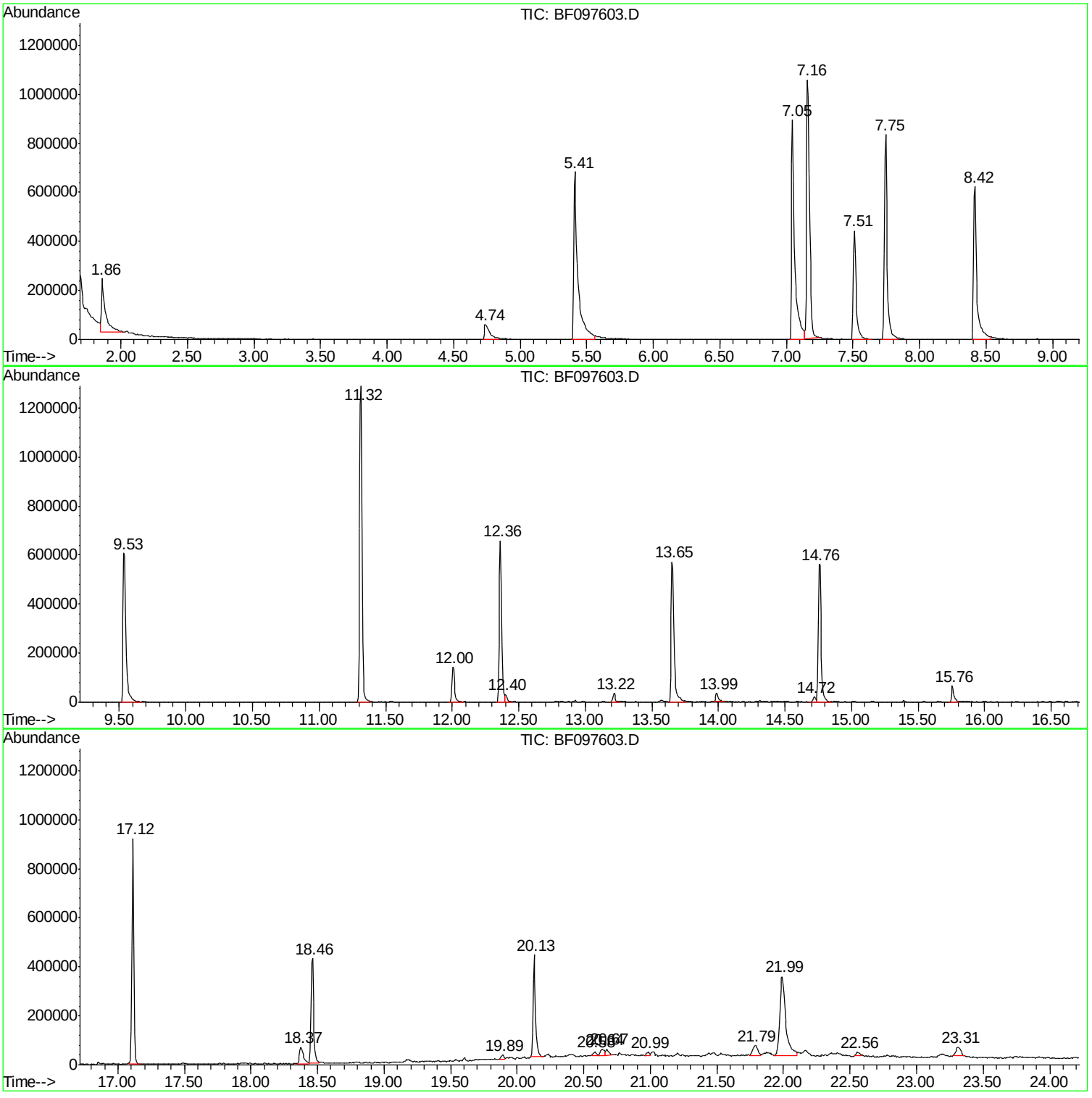
Sum of corrected areas: 17323697

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097603.D
Acq On : 11 Aug 2017 19:41
Operator : SJ/JU
Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

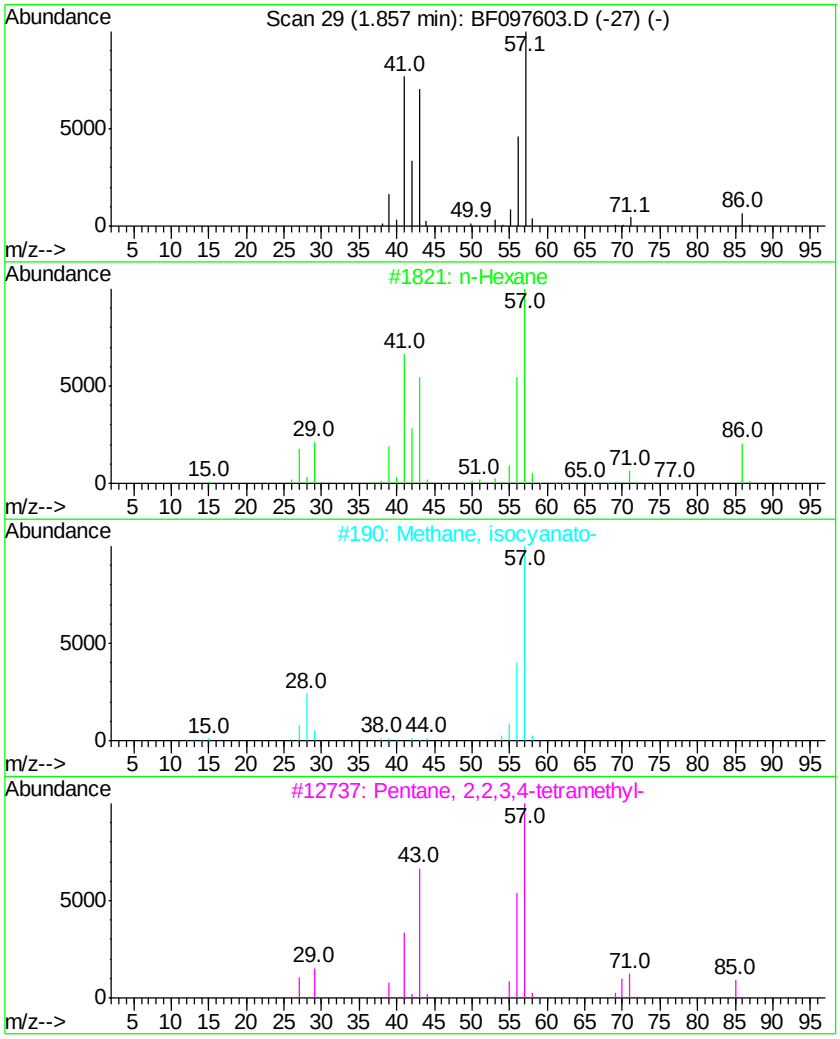
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

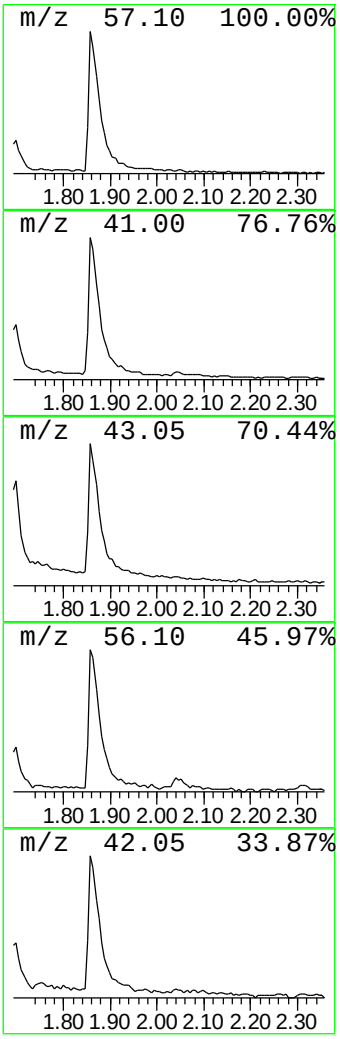
****

Peak Number 1 n-Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.86	14.30 ng	463849	1,4-Dichlorobenzene-d4	7.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	83
2	Methane, isocyanato-	57	C2H3NO	000624-83-9	37
3	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	33
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	33
5	Butane, 2-methyl-	72	C5H12	000078-78-4	17





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097603.D
Acq On : 11 Aug 2017 19:41
Operator : SJ/JU
Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

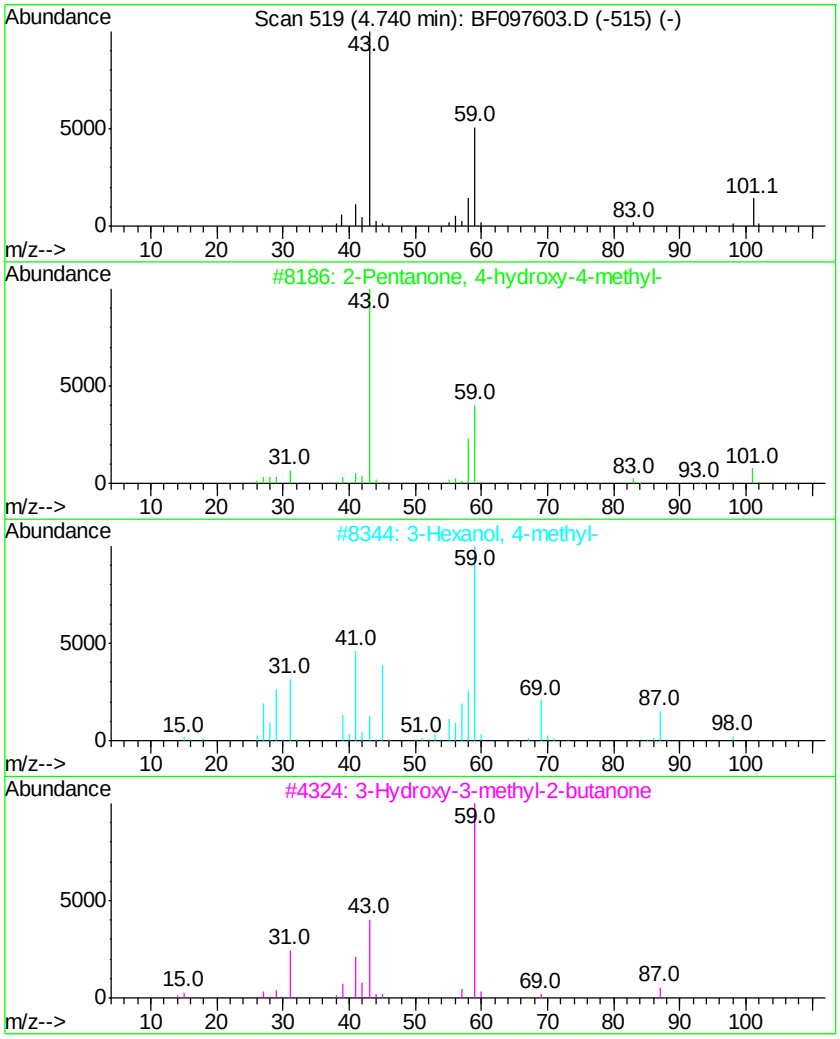
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

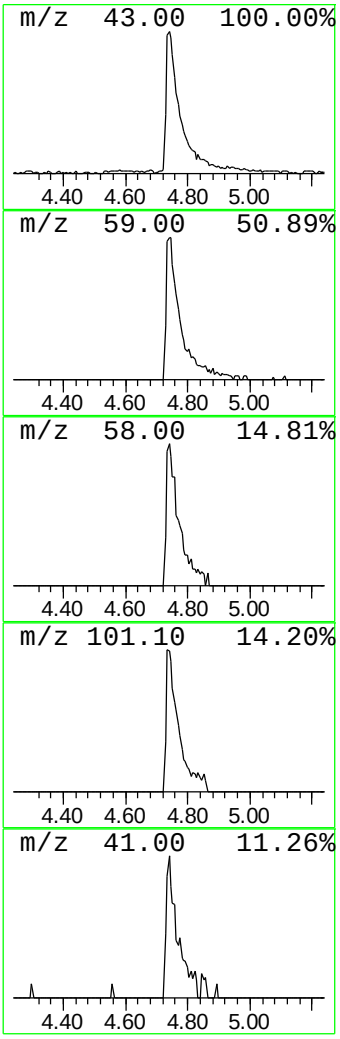
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	5.23 ng	169862	1,4-Dichlorobenzene-d4	7.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
4	Butane	58	C4H10	000106-97-8	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097603.D
Acq On : 11 Aug 2017 19:41
Operator : SJ/JU
Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

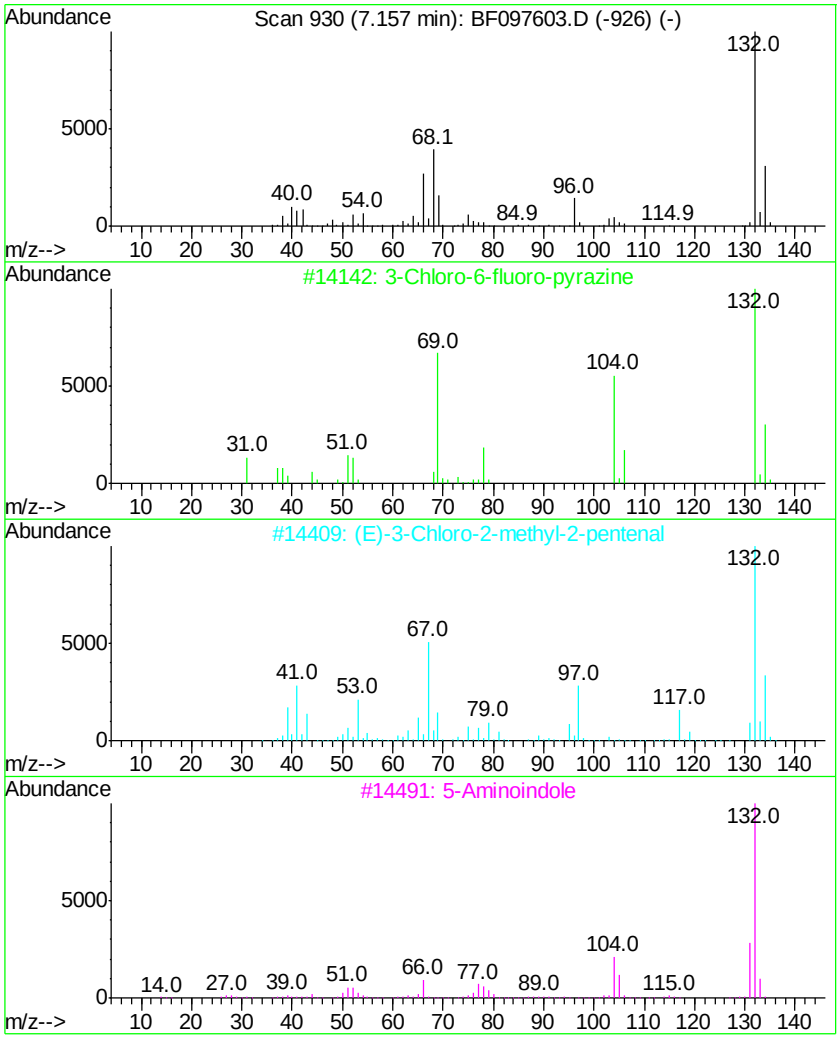
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

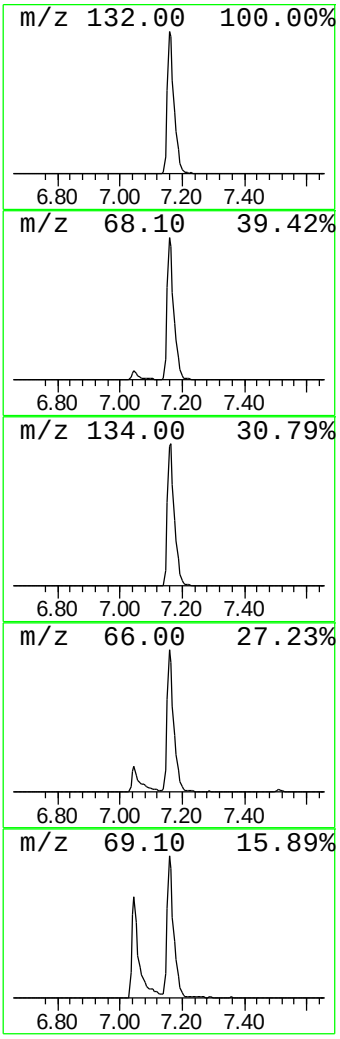
****

Peak Number 3 unknown7.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	50.91 ng	1651950	1,4-Dichlorobenzene-d4	7.51

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





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097603.D
Acq On : 11 Aug 2017 19:41
Operator : SJ/JU
Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

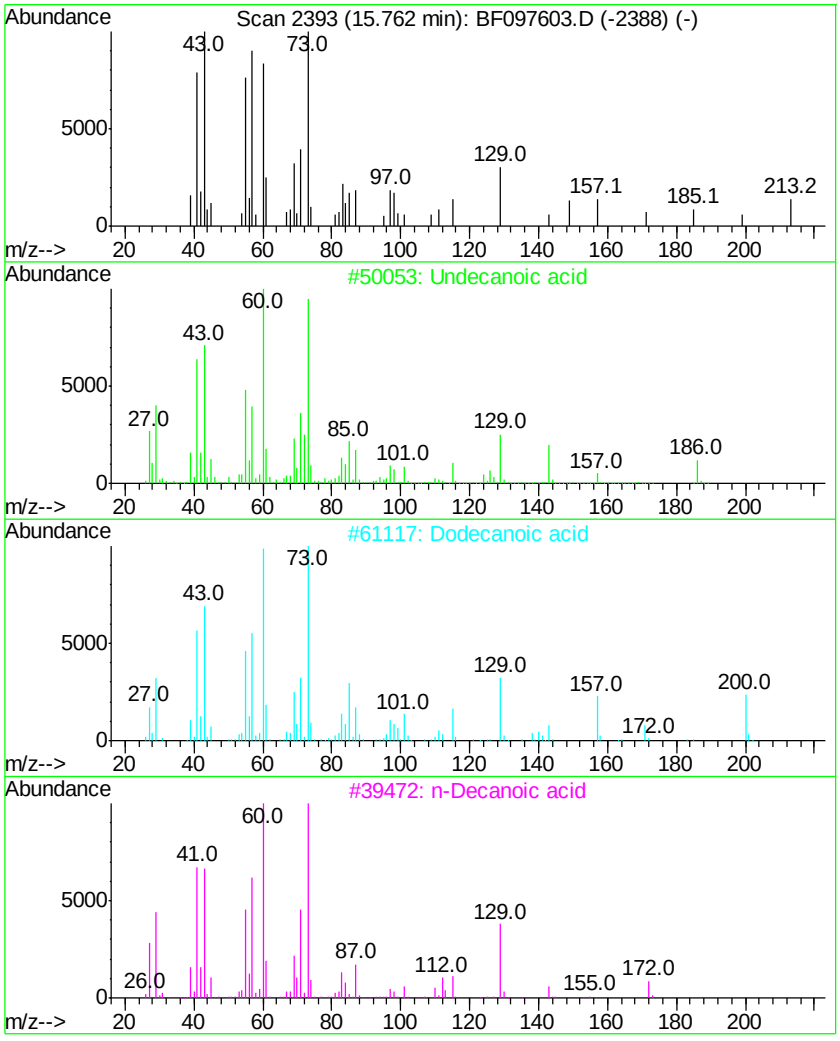
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

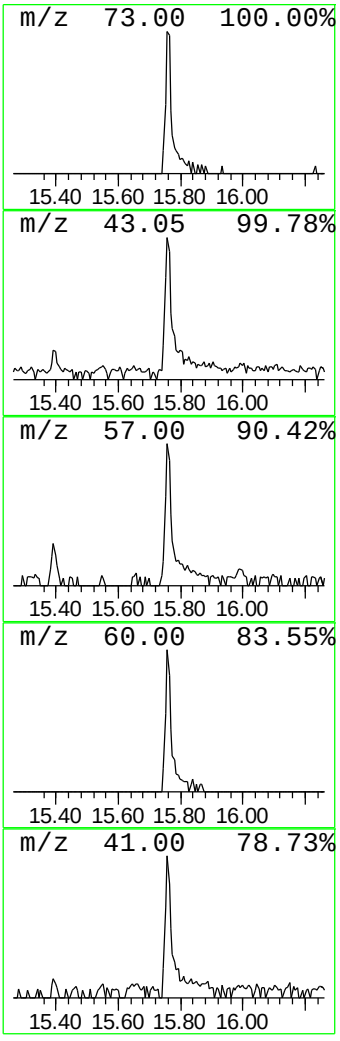
****

Peak Number 5 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.76	2.28 ng	91314	Phenanthrene-d10	14.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	72
2	Dodecanoic acid	200	C12H24O2	000143-07-7	53
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Octanoic acid	144	C8H16O2	000124-07-2	47
5	Undecanoic acid, 10-bromo-	264	C11H21BrO2	018294-93-4	47





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Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

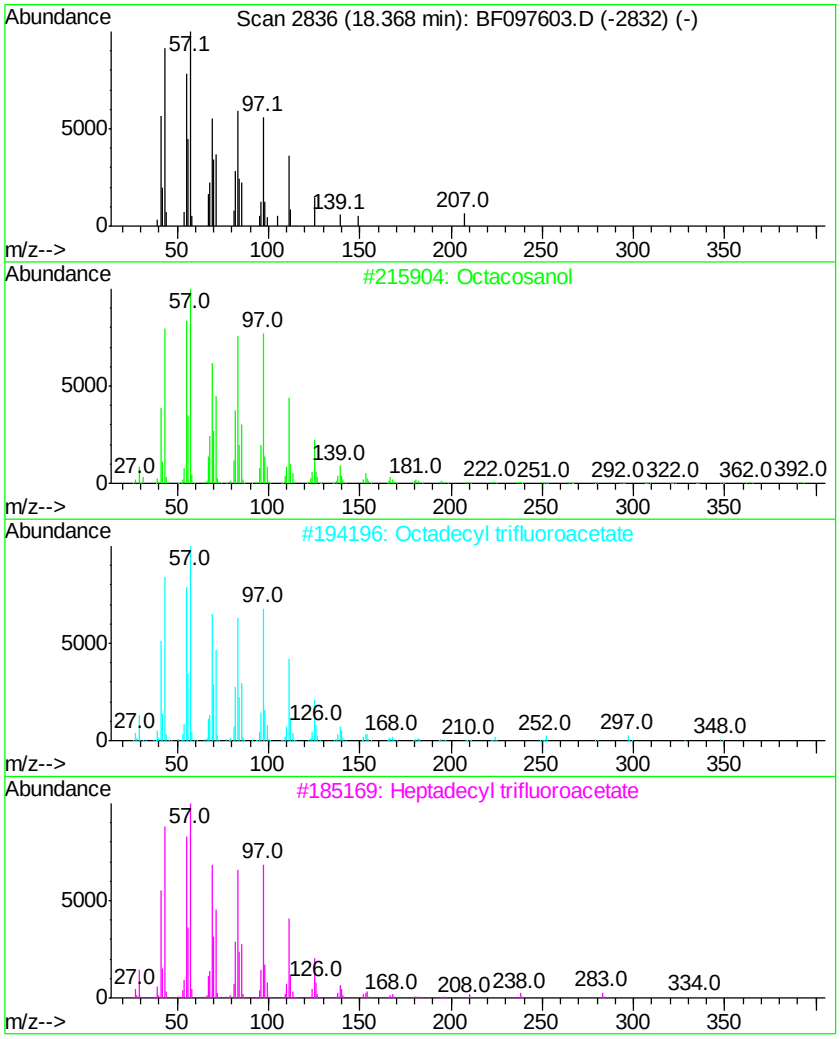
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

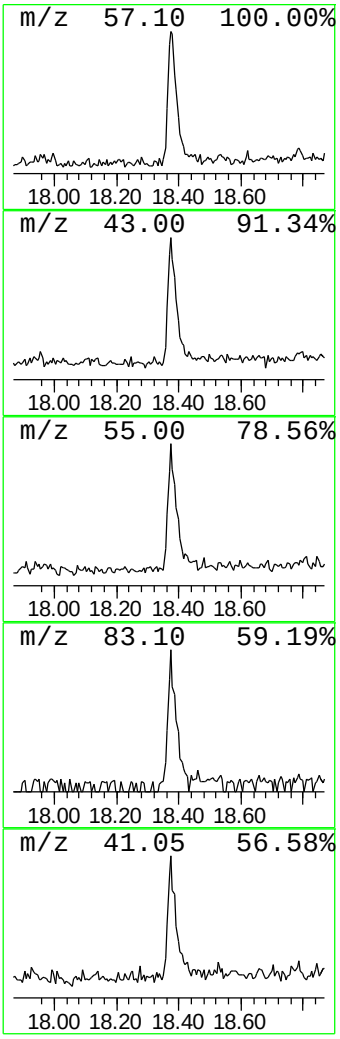
****

Peak Number 6 Octacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.37	4.85 ng	135832	Chrysene-d12	18.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	91
2	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	90





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Data File : BF097603.D
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Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

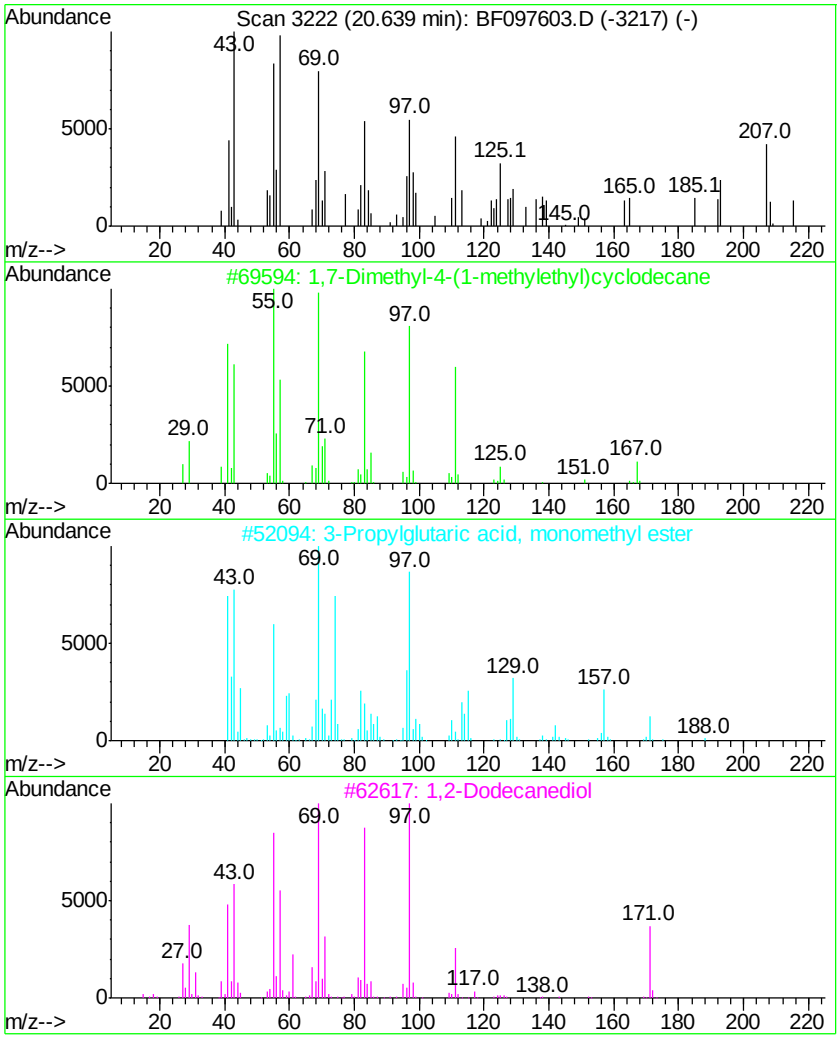
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

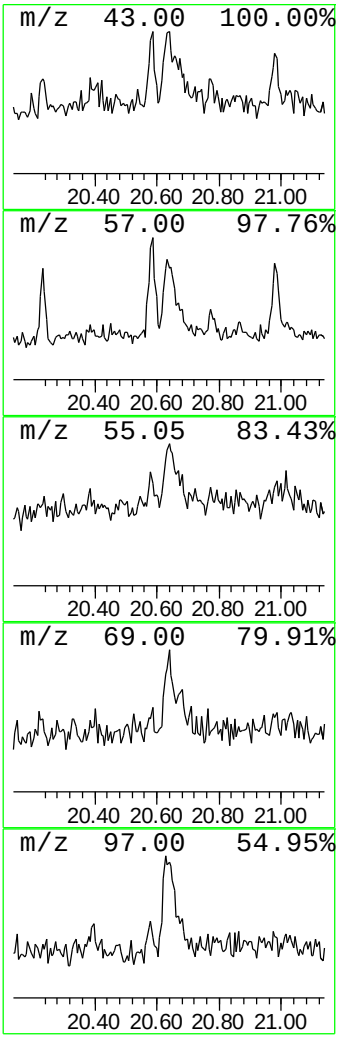
****

Peak Number 7 unknown20.64 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.64	2.16 ng	58849	Perylene-d12	20.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,7-Dimethyl-4-(1-methylethyl)cy...	210	C15H30	000645-10-3	43
2	3-Propylglutaric acid, monomethy...	188	C9H16O4	1000254-25-9	35
3	1,2-Dodecanediol	202	C12H26O2	001119-87-5	35
4	6-Methyl-1,5-diazabicyclo[3.1.0]...	98	C5H10N2	100463-00-1	35
5	Cyclopentanecarboxylic acid, 3-t...	296	C19H36O2	1000280-58-5	27





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ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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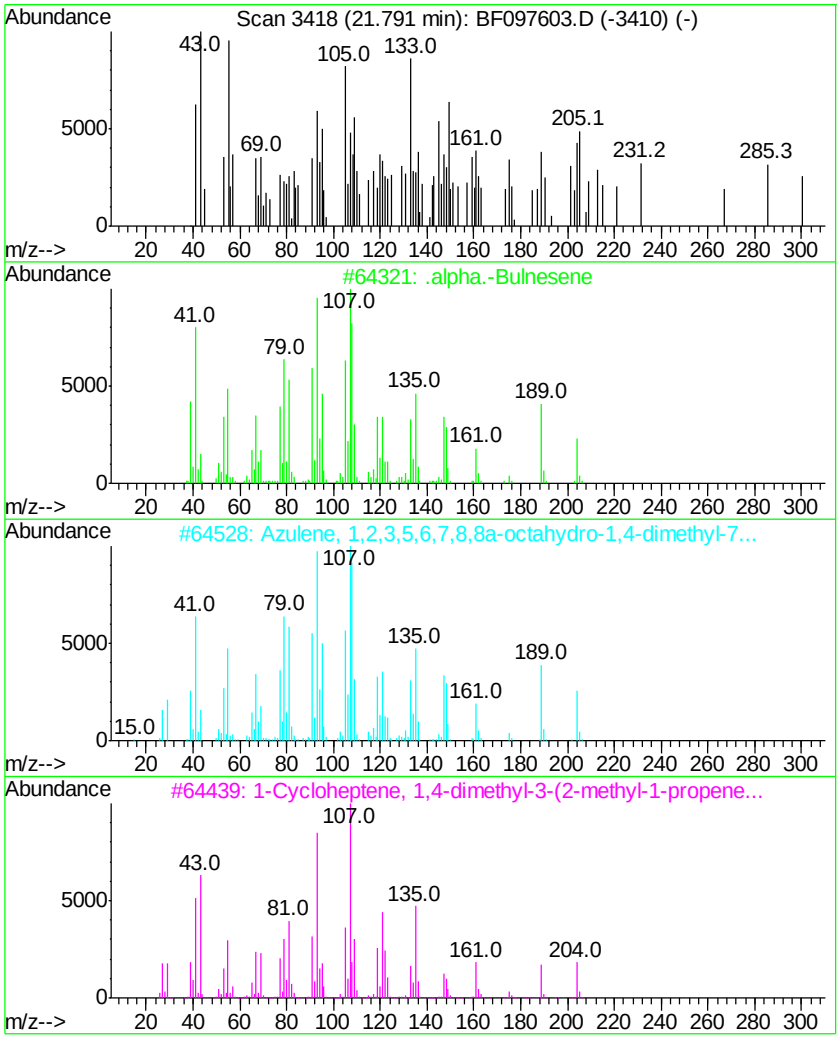
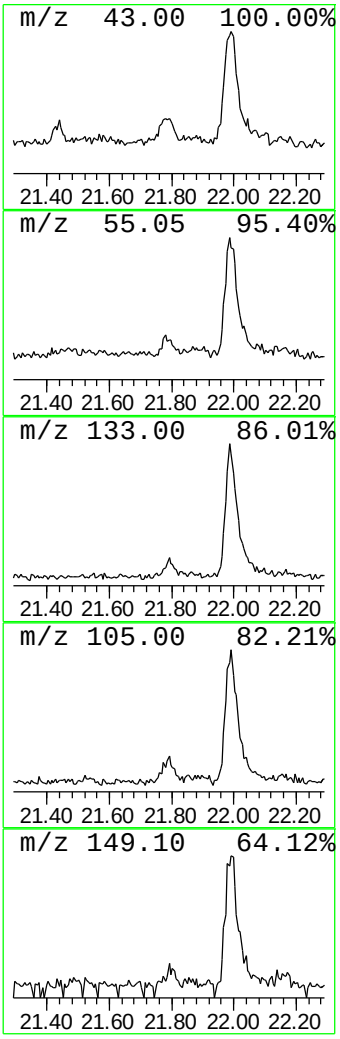
Peak Number 8 unknown21.79 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.79	4.18 ng	114161	Perylene-d12	20.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Bulnesene	204	C15H24	1000374-19-9	35
2	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	35
3	1-Cycloheptene, 1,4-dimethyl-3-(...	204	C15H24	1000159-38-6	25
4	.alpha.-Guaiene	204	C15H24	003691-12-1	22
5	1H-Cycloprop[e]azulene, 1a,2,3,5...	204	C15H24	021747-46-6	20





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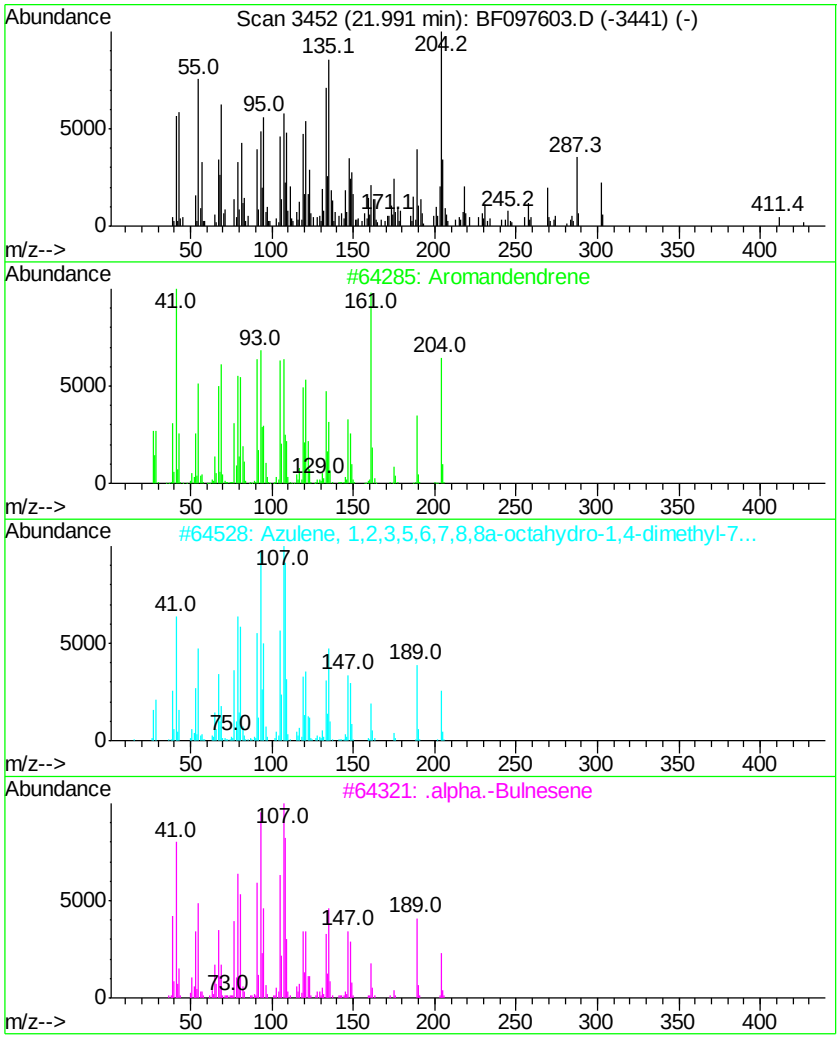
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

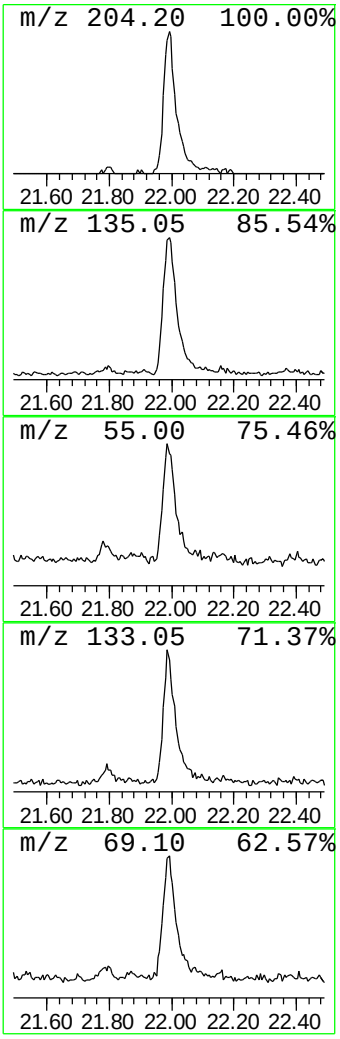
****

Peak Number 9 Aromandendrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.99	37.02 ng	1010480	Perylene-d12	20.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aromandendrene	204	C15H24	000489-39-4	90
2	Azulene, 1,2,3,5,6,7,8,8a-octahy...	204	C15H24	003691-11-0	62
3	.alpha.-Bulnesene	204	C15H24	1000374-19-9	62
4	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	58
5	Naphthalene, decahydro-4a-methyl...	204	C15H24	017066-67-0	53





Data Path : Z:\HPCHEM1\BNA F\DATA\BF081117\
Data File : BF097603.D
Acq On : 11 Aug 2017 19:41
Operator : SJ/JU
Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

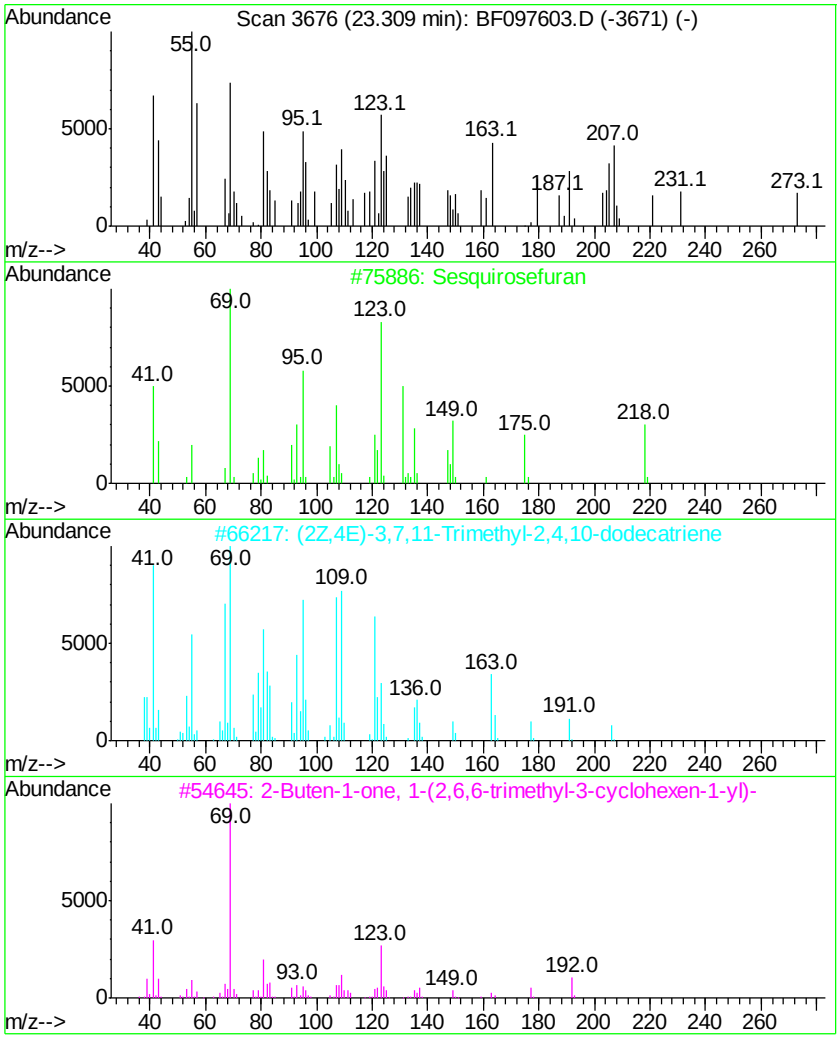
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

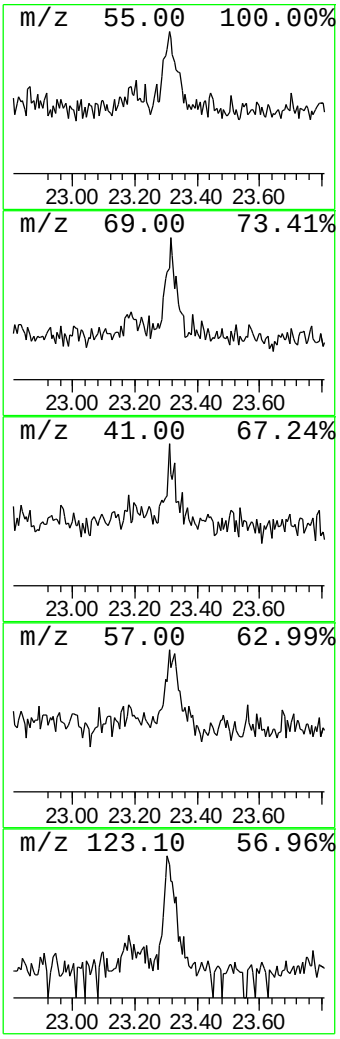
****

Peak Number 10 Sesquirosefuran Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.31	3.25 ng	88728	Perylene-d12	20.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sesquirosefuran	218	C15H22O	039007-93-7	53
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	53
3	2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	041436-42-4	38
4	Tricyclo[4.3.0.0(7,9)]nonane, 2,...	206	C15H26	054832-82-5	38
5	Geraniol	154	C10H18O	000106-24-1	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081117\
Data File : BF097603.D
Acq On : 11 Aug 2017 19:41
Operator : SJ/JU
Sample : I4706-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : OR-02-081017

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081117.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
n-Hexane	1.86	14.3	ng	463849	1	7.51	648961	20.0
2-Pentanone, 4-hy...	4.74	5.2	ng	169862	1	7.51	648961	20.0
unknown7.16	7.16	50.9	ng	1651950	1	7.51	648961	20.0
Undecanoic acid	15.76	2.3	ng	91314	4	14.76	802205	20.0
Octacosanol	18.37	4.8	ng	135832	5	18.46	559955	20.0
unknown20.64	20.64	2.2	ng	58849	6	20.13	545974	20.0
unknown21.79	21.79	4.2	ng	114161	6	20.13	545974	20.0
Aromandendrene	21.99	37.0	ng	1010480	6	20.13	545974	20.0
Sesquirosefuran	23.31	3.3	ng	88728	6	20.13	545974	20.0