LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082020\
Data File : BF121347.D
Acq On : 20 Aug 2020 15:12
Operator : JU/CG
Sample : L3645-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-3

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.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	4.934	469	484	487	rBV	3485120	11750328	100.00%	43.415%
2	6.692	779	783	786	rBV	1259484	996860	8.48%	3.683%
3	7.257	875	879	890	rVV	1384230	1209398	10.29%	4.468%
4	7.975	997	1001	1004	rBV	1596964	1306820	11.12%	4.828%
5	9.051	1179	1184	1187	rBV	2487946	2143796	18.24%	7.921%
6	9.727	1295	1299	1302	rVB	1578993	1437666	12.24%	5.312%
7	10.339	1399	1403	1406	rBV3	170174	195305	1.66%	0.722%
8	10.369	1406	1408	1416	rVB2	149302	230730	1.96%	0.852%
9	11.210	1547	1551	1554	rBV	1585591	1393830	11.86%	5.150%
10	12.792	1816	1820	1823	rBV	1880177	1617987	13.77%	5.978%
11	13.486	1934	1938	1943	rBV2	269293	297883	2.54%	1.101%
12	13.692	1969	1973	1985	rBV	870380	1070092	9.11%	3.954%
13	13.845	1993	1999	2002	rBV	1210617	1194616	10.17%	4.414%
14	14.592	2123	2126	2128	rBV	137193	137721	1.17%	0.509%
15	14.686	2139	2142	2156	rVB2	233571	319931	2.72%	1.182%
16	15.251	2233	2238	2242	rBV	1031952	1322018	11.25%	4.885%
17	15.680	2307	2311	2315	rBV	95397	129592	1.10%	0.479%
18	15.733	2316	2320	2327	rBV4	81767	190053	1.62%	0.702%
19	16.145	2385	2390	2393	rBV3	73227	120509	1.03%	0.445%

Sum of corrected areas: 27065135

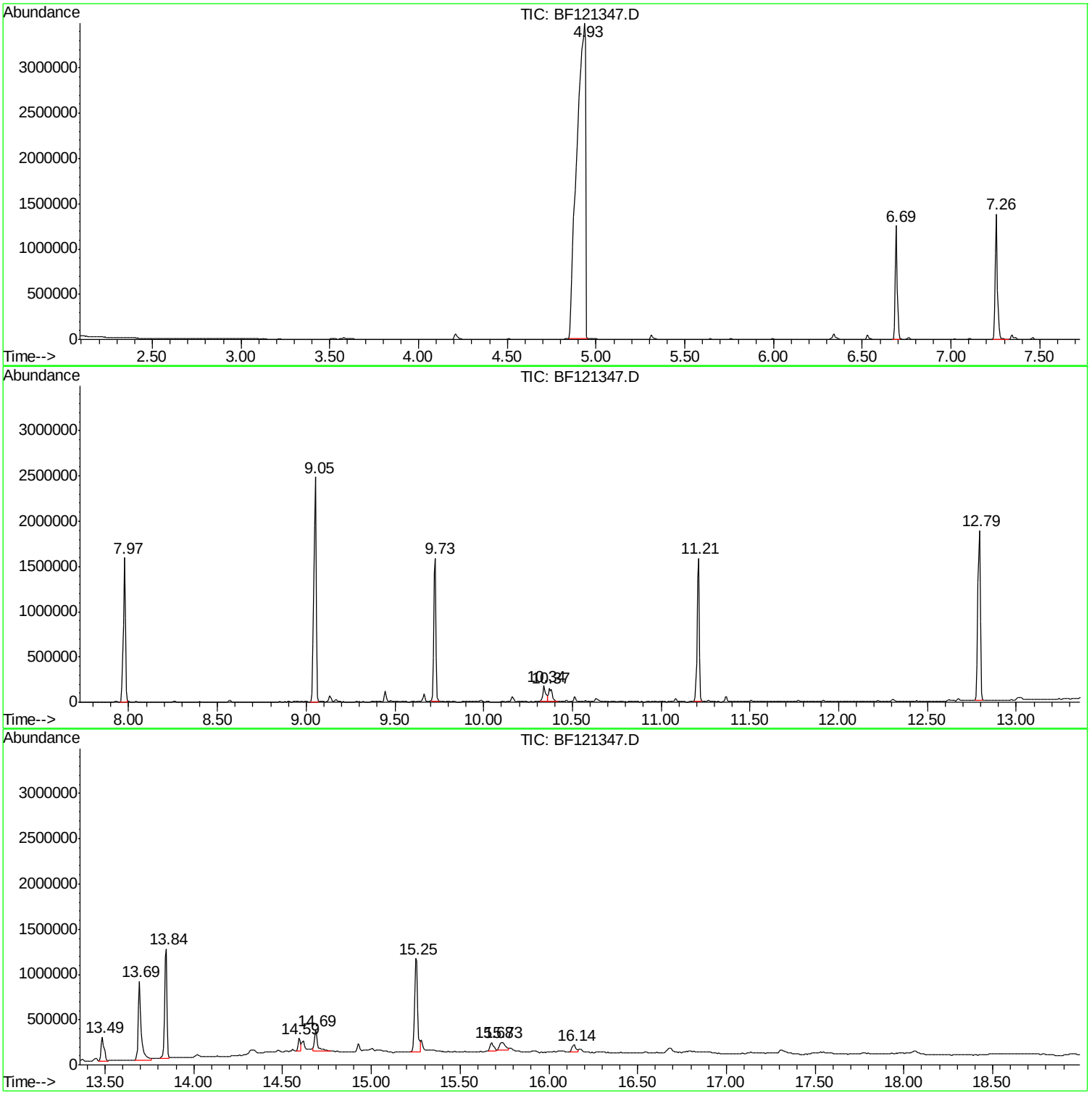
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082020\
Data File : BF121347.D
Acq On : 20 Aug 2020 15:12
Operator : JU/CG
Sample : L3645-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.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:\SVOASRV\HPCHEM1\BNA F\DATA\BF082020\
Data File : BF121347.D
Acq On : 20 Aug 2020 15:12
Operator : JU/CG
Sample : L3645-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

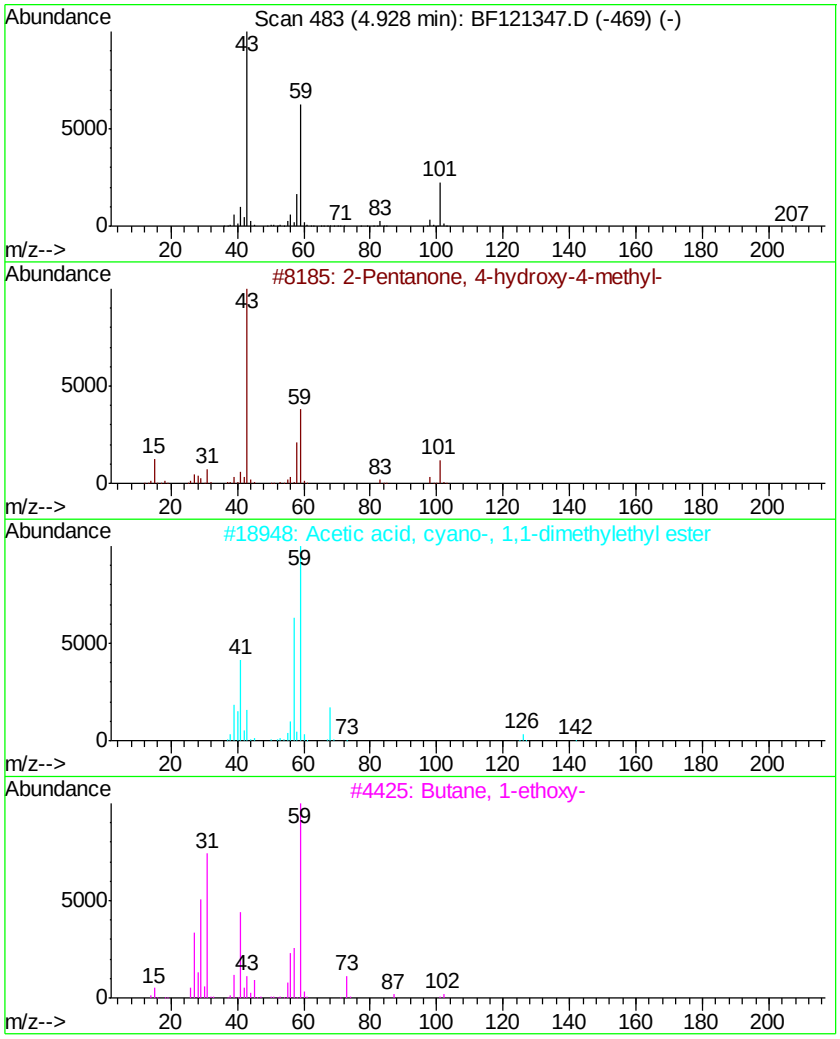
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

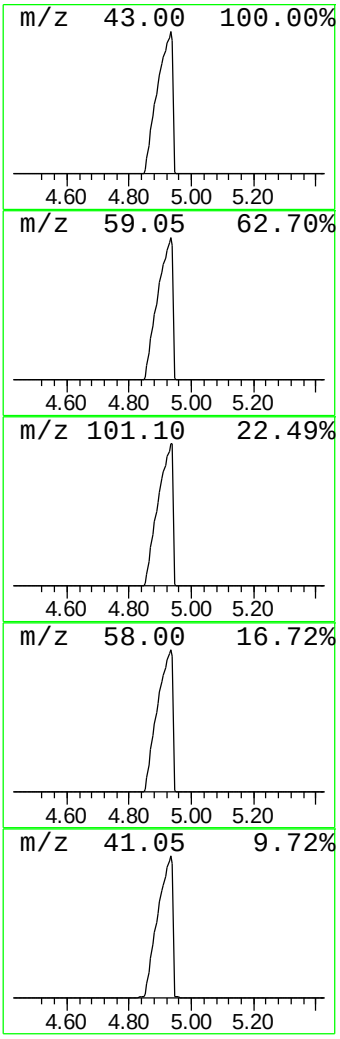
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	235.75 ng	11750300	1,4-Dichlorobenzene-d4	6.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Data File : BF121347.D
Acq On : 20 Aug 2020 15:12
Operator : JU/CG
Sample : L3645-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

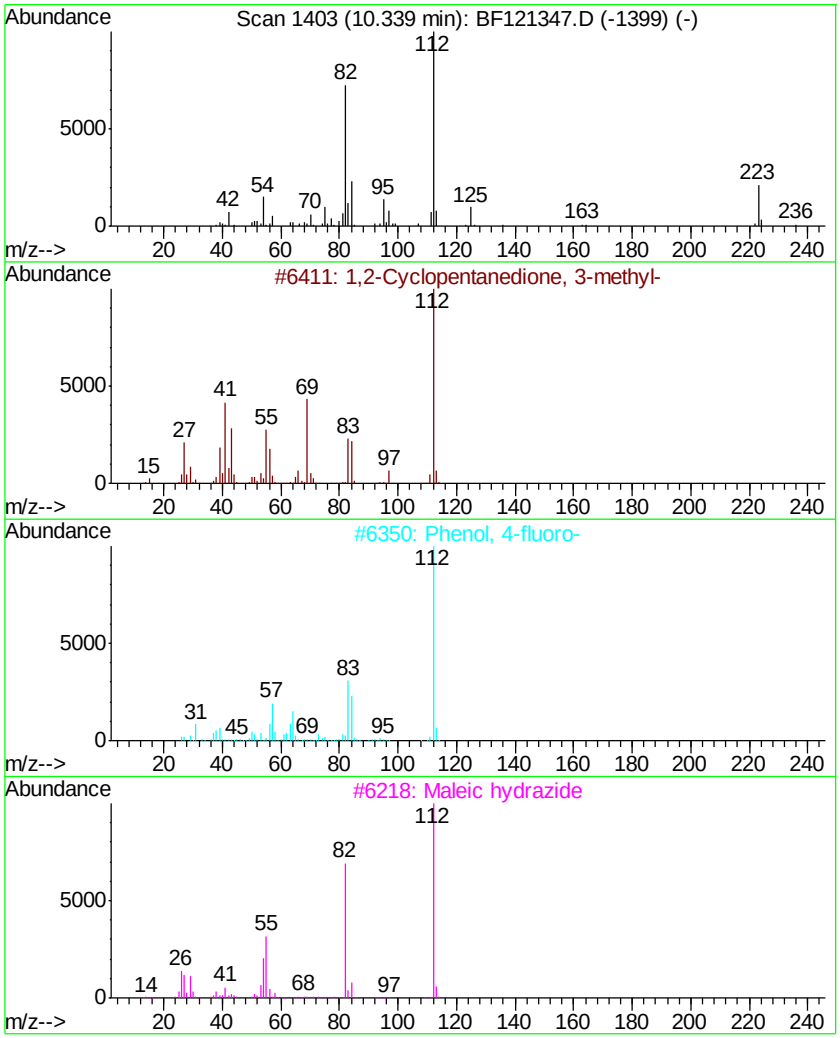
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

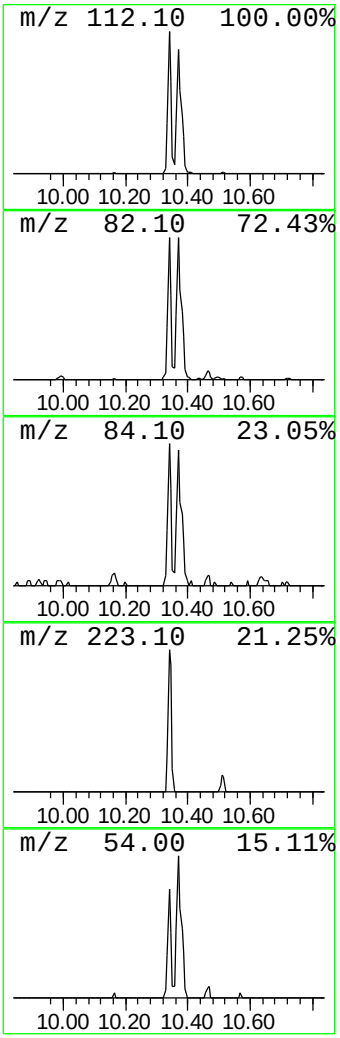
****

Peak Number 2 unknown10.34 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.34	2.72 ng	195305	Acenaphthene-d10	9.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclopentanedione, 3-methyl-	112	C6H8O2	000765-70-8	46
2	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	43
3	Maleic hydrazide	112	C4H4N2O2	000123-33-1	40
4	Phenol, 3-fluoro-	112	C6H5FO	000372-20-3	37
5	4H-1,2,4-Triazol-3-amine, 4-ethyl-	112	C4H8N4	042786-06-1	37





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082020\
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Operator : JU/CG
Sample : L3645-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

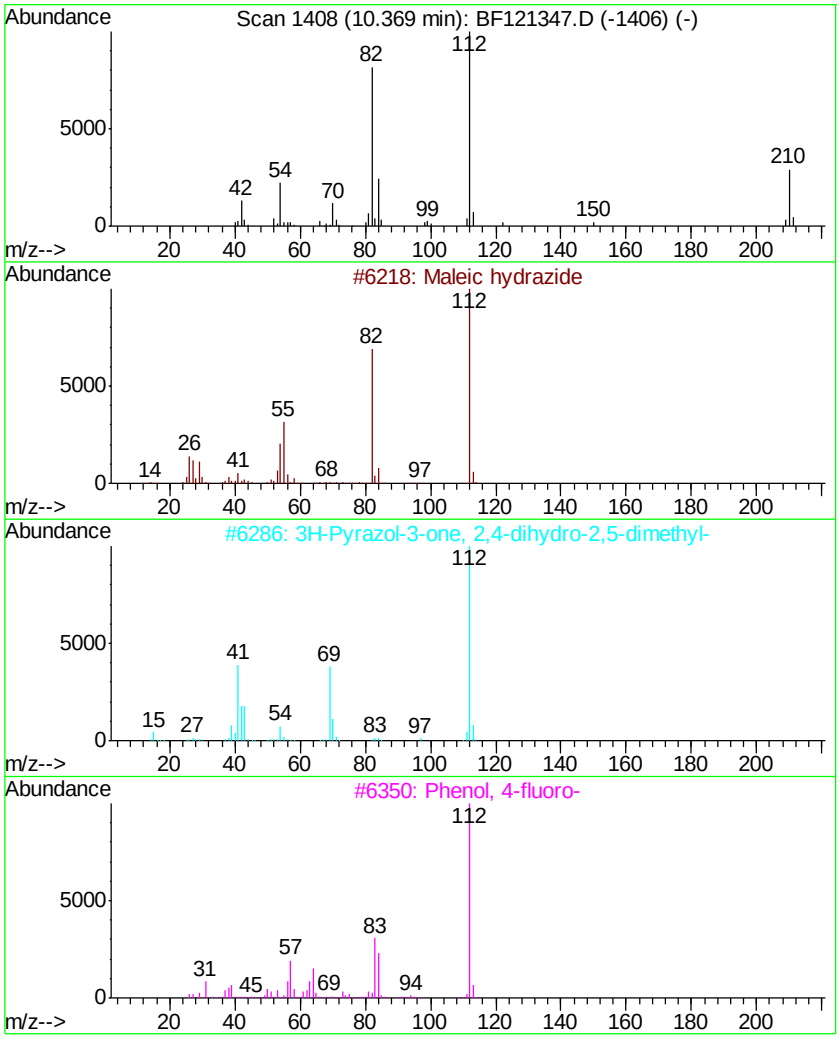
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

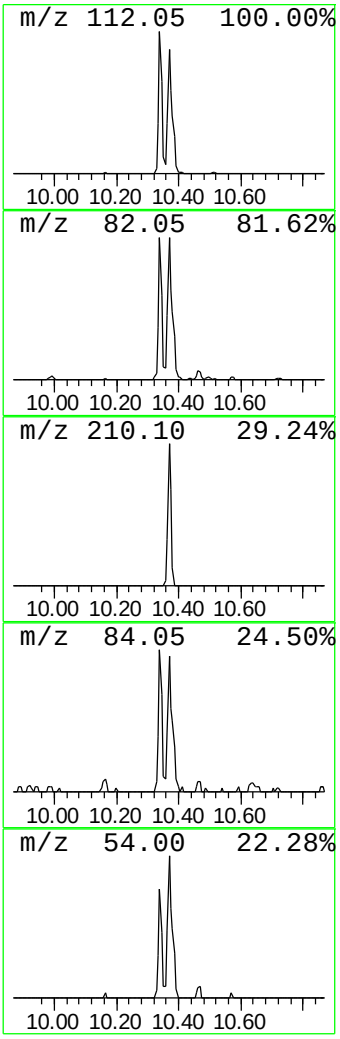
****

Peak Number 3 Maleic hydrazide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.37	3.21 ng	230730	Acenaphthene-d10	9.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Maleic hydrazide	112	C4H4N2O2	000123-33-1	59
2	3H-Pyrazol-3-one, 2,4-dihydro-2,...	112	C5H8N2O	002749-59-9	35
3	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	27
4	2-Cyclopenten-1-one, 2-hydroxy-3...	112	C6H8O2	000080-71-7	25
5	1,3,7-Trimethyluric acid	210	C8H10N4O3	005415-44-1	25





Library Search Compound Report

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Data File : BF121347.D
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Operator : JU/CG
Sample : L3645-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

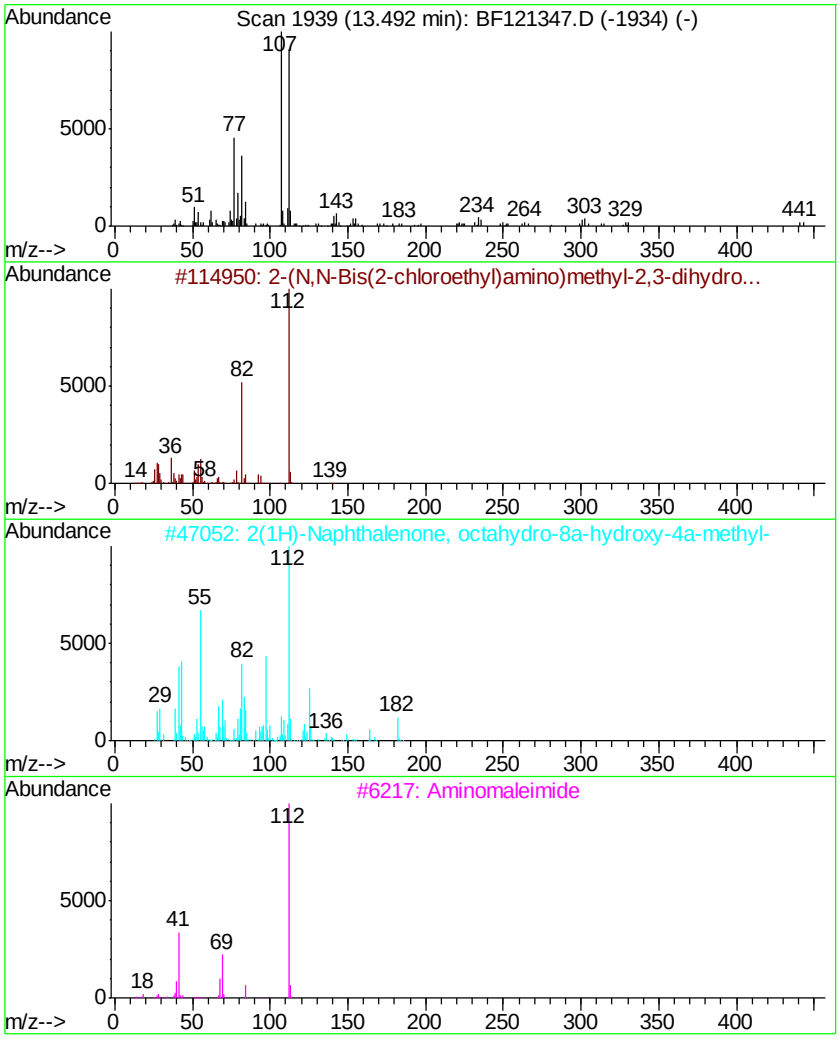
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

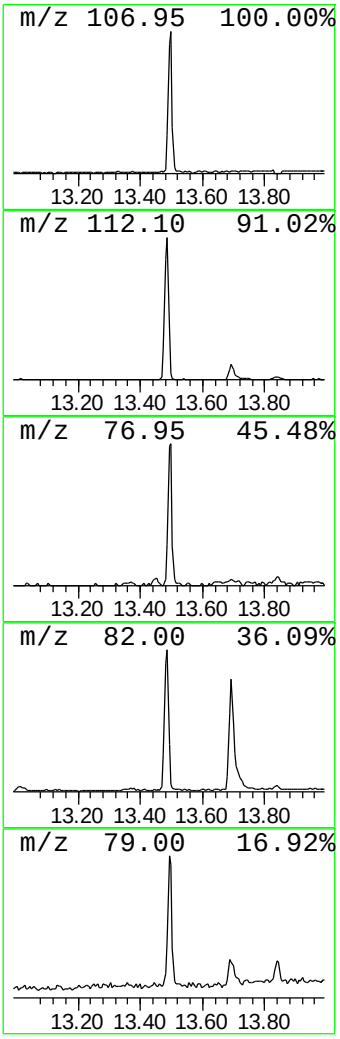
****

Peak Number 4 2-(N,N-Bis(2-chloroethyl)am... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	4.99 ng	297883	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(N,N-Bis(2-chloroethyl)amino)m...	265	C9H13Cl2N3O2	014628-36-5	50
2	2(1H)-Naphthalenone, octahydro-8...	182	C11H18O2	040573-27-1	43
3	Aminomaleimide	112	C4H4N2O2	037770-94-8	43
4	Sulfide,1- propenyl 1-propynyl	112	C6H8S	089533-93-7	43
5	2-Cyclopenten-1-one, 2-hydroxy-3...	112	C6H8O2	000080-71-7	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082020\
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Operator : JU/CG
Sample : L3645-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

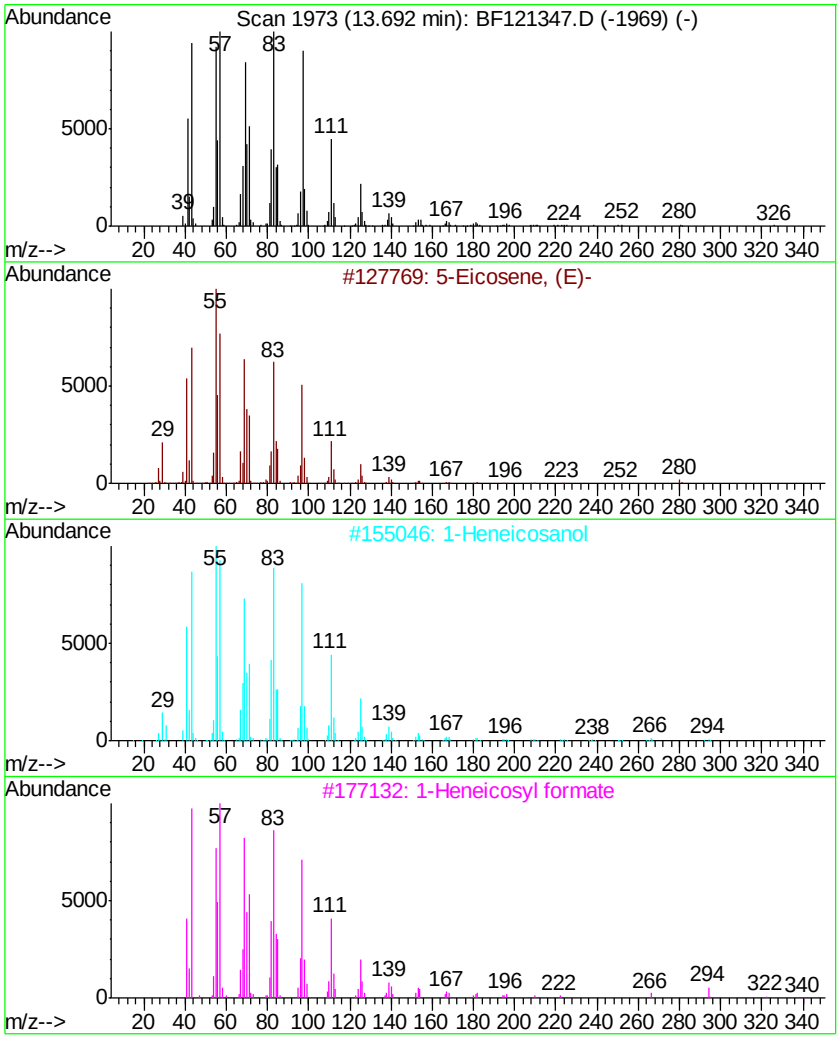
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

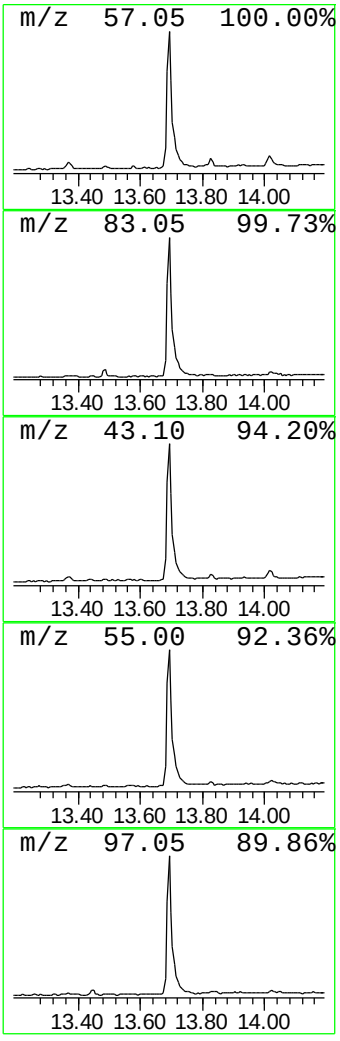
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.69	17.92 ng	1070090	Chrysene-d12	13.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082020\
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Sample : L3645-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

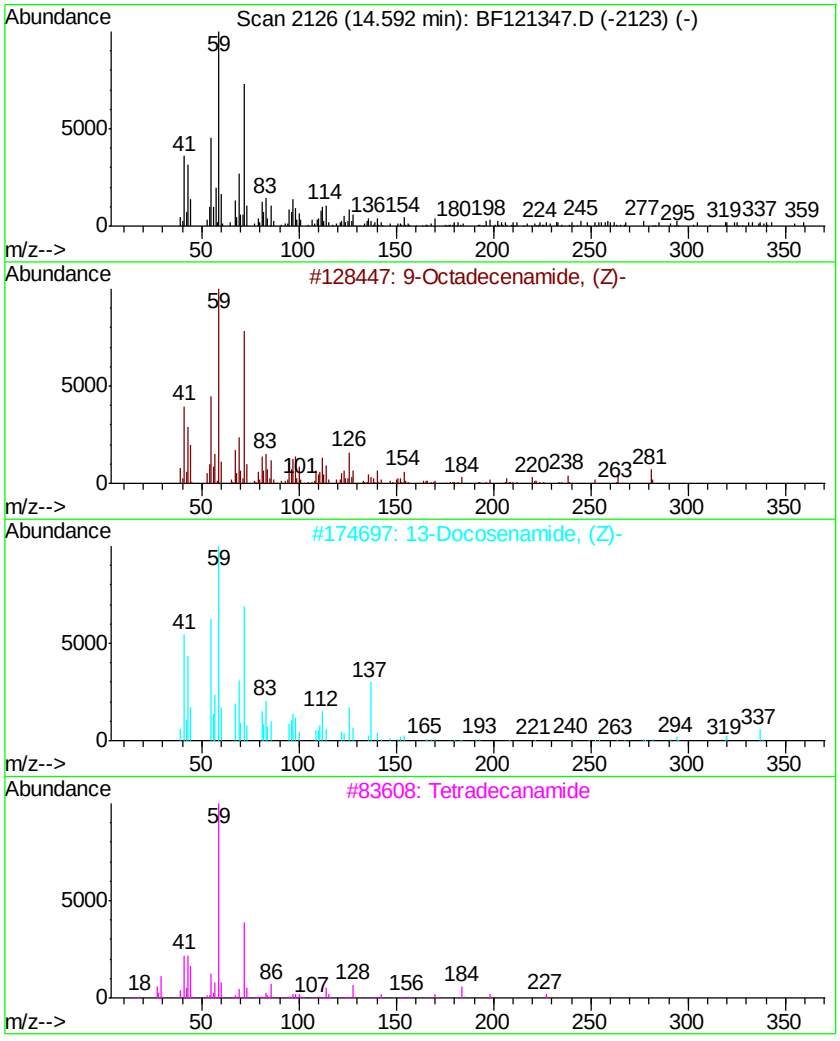
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

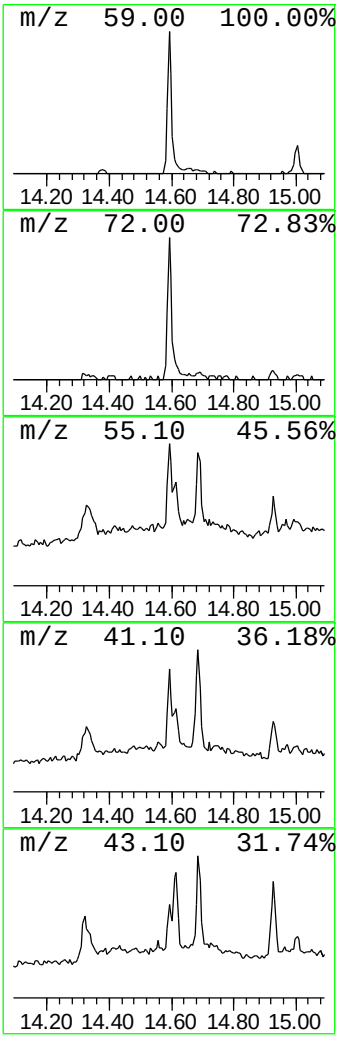
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	2.08 ng	137721	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	87
3	Tetradecanamide	227	C14H29NO	000638-58-4	80
4	2-Hydroxy-2,4-dimethyl-hept-6-en...	156	C9H16O2	1000192-56-0	38
5	Acetic acid, cyanohydroxyimino-,...	128	C4H4N2O3	061295-92-9	35





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Sample : L3645-03
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GW-3

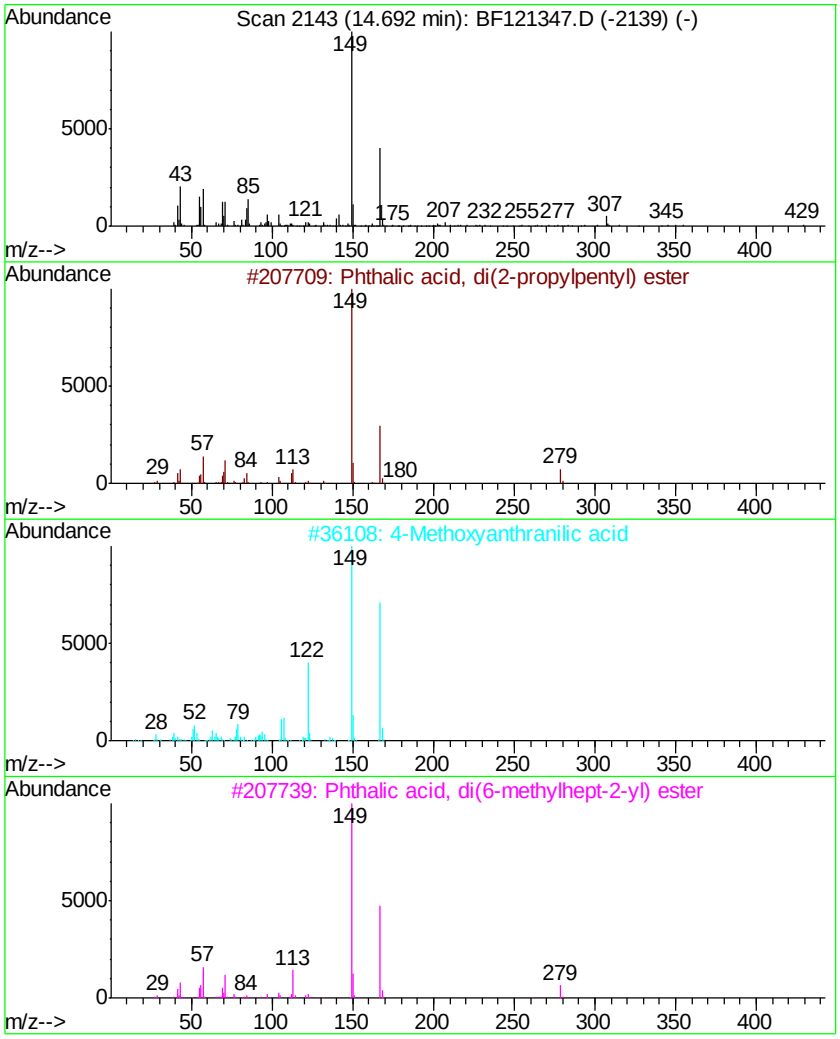
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

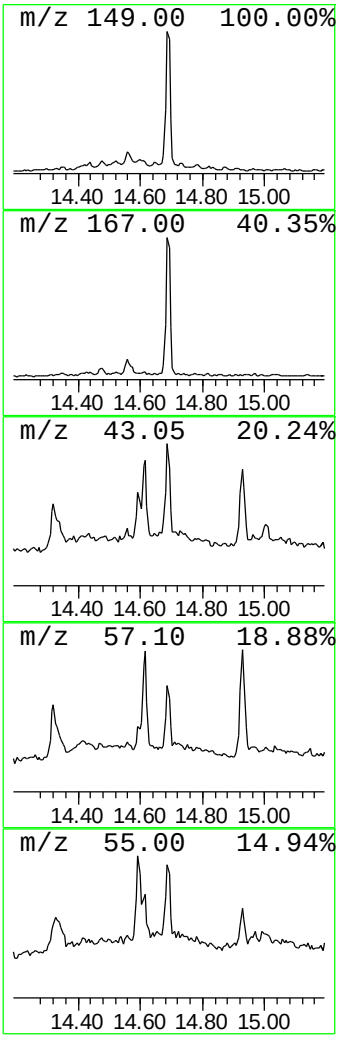
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Phthalic acid, di(2-propylp... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	4.84 ng	319931	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, di(2-propylpentyl...	390	C24H38O4	1000377-93-5	72
2	4-Methoxyanthranilic acid	167	C8H9NO3	004294-95-5	64
3	Phthalic acid, di(6-methylhept-2...	390	C24H38O4	1000377-97-3	64
4	Bis(3-methylbutan-2-yl) phthalate	306	C18H26O4	1000373-65-6	59
5	Dicyclohexyl phthalate	330	C20H26O4	000084-61-7	59





Library Search Compound Report

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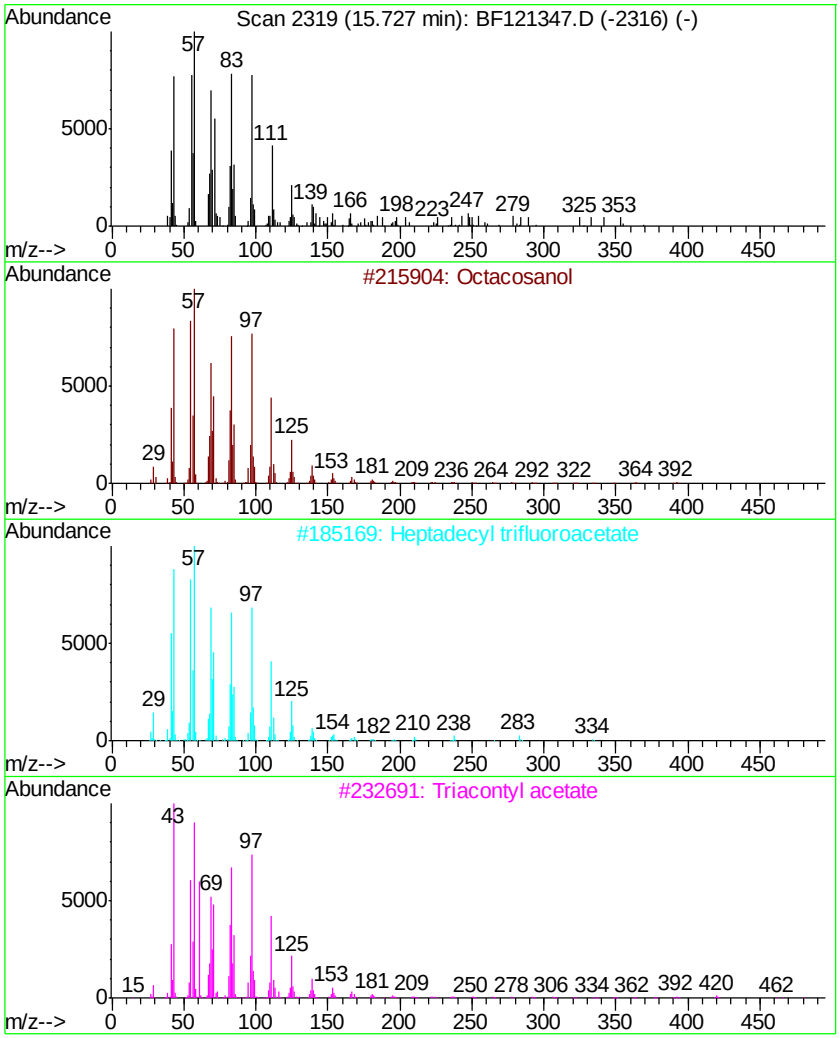
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

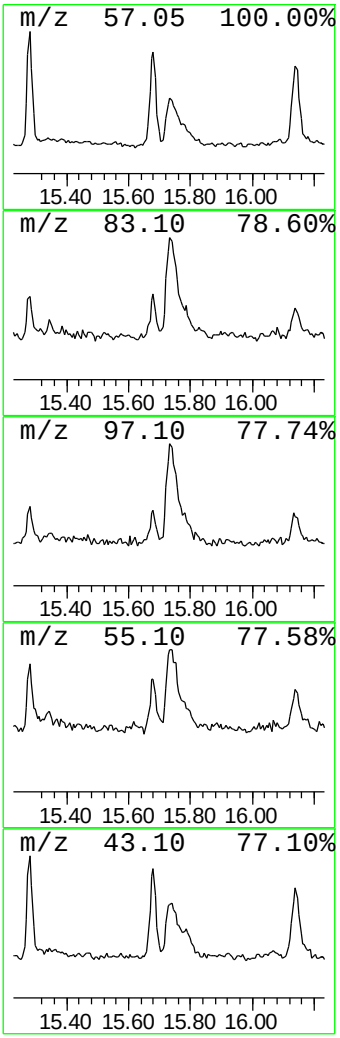
****

Peak Number 8 Octacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.73	2.88 ng	190053	Perylene-d12	15.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	94
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
3	Triacontyl acetate	480	C32H64O2	041755-58-2	94
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082020\
Data File : BF121347.D
Acq On : 20 Aug 2020 15:12
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081920.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...	4.93	235.8	ng	11750300	1	6.69	996860	20.0
unknown10.34	10.34	2.7	ng	195305	3	9.73	1437670	20.0
Maleic hydrazide	10.37	3.2	ng	230730	3	9.73	1437670	20.0
2-(N,N-Bis(2-chlo...	13.49	5.0	ng	297883	5	13.84	1194620	20.0
5-Eicosene, (E)-	13.69	17.9	ng	1070090	5	13.84	1194620	20.0
9-Octadecenamide,...	14.59	2.1	ng	137721	6	15.25	1322020	20.0
Phthalic acid, di...	14.69	4.8	ng	319931	6	15.25	1322020	20.0
Octacosanol	15.73	2.9	ng	190053	6	15.25	1322020	20.0