LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111334.D
Acq On : 12 Dec 2018 21:06
Operator : JU/SJ
Sample : J6331-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

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-BF121218.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	3.246	194	197	206	rBV	82968	184756	2.16%	0.288%
2	5.010	490	497	505	rBV	331939	485700	5.68%	0.757%
3	5.093	507	511	517	rBV	177231	171691	2.01%	0.268%
4	5.416	561	566	570	rBV	6940782	7819204	91.49%	12.187%
5	6.434	733	739	757	rBV	7262910	8546861	100.00%	13.321%
6	6.569	757	762	765	rBV	7828014	7835426	91.68%	12.212%
7	6.792	796	800	804	rBV	1935000	1552097	18.16%	2.419%
8	6.951	823	827	830	rBV	6624208	5959127	69.72%	9.288%
9	7.192	865	868	872	rBV	209471	187930	2.20%	0.293%
10	7.357	889	896	899	rBV2	4767789	5596927	65.49%	8.723%
11	8.075	1014	1018	1021	rBV	2151481	1784802	20.88%	2.782%
12	9.157	1196	1202	1205	rBV	7262773	6938826	81.19%	10.815%
13	9.545	1264	1268	1271	rBV	672818	600330	7.02%	0.936%
14	9.827	1311	1316	1320	rBV2	1888140	1585379	18.55%	2.471%
15	10.616	1445	1450	1453	rBV	3833619	3426495	40.09%	5.340%
16	11.310	1564	1568	1571	rBV	1645921	1434700	16.79%	2.236%
17	11.333	1571	1572	1576	rVV	324319	199640	2.34%	0.311%
18	11.380	1576	1580	1583	rVB2	74024	88939	1.04%	0.139%
19	11.845	1655	1659	1663	rBV2	844189	744201	8.71%	1.160%
20	12.521	1771	1774	1777	rBV	482797	414551	4.85%	0.646%
21	12.627	1789	1792	1798	rBV	369963	421463	4.93%	0.657%
22	12.751	1807	1813	1816	rBV	350226	377089	4.41%	0.588%
23	12.898	1834	1838	1842	rBV	5315478	4959016	58.02%	7.729%
24	12.951	1844	1847	1854	rVV7	50419	86927	1.02%	0.135%
25	13.751	1980	1983	1987	rBV2	228131	313213	3.66%	0.488%
26	13.786	1987	1989	1991	rBV	221733	231798	2.71%	0.361%
27	13.945	2012	2016	2019	rBV	1307551	1381571	16.16%	2.153%
28	15.386	2257	2261	2265	rBV	665566	832180	9.74%	1.297%

Sum of corrected areas: 64160839

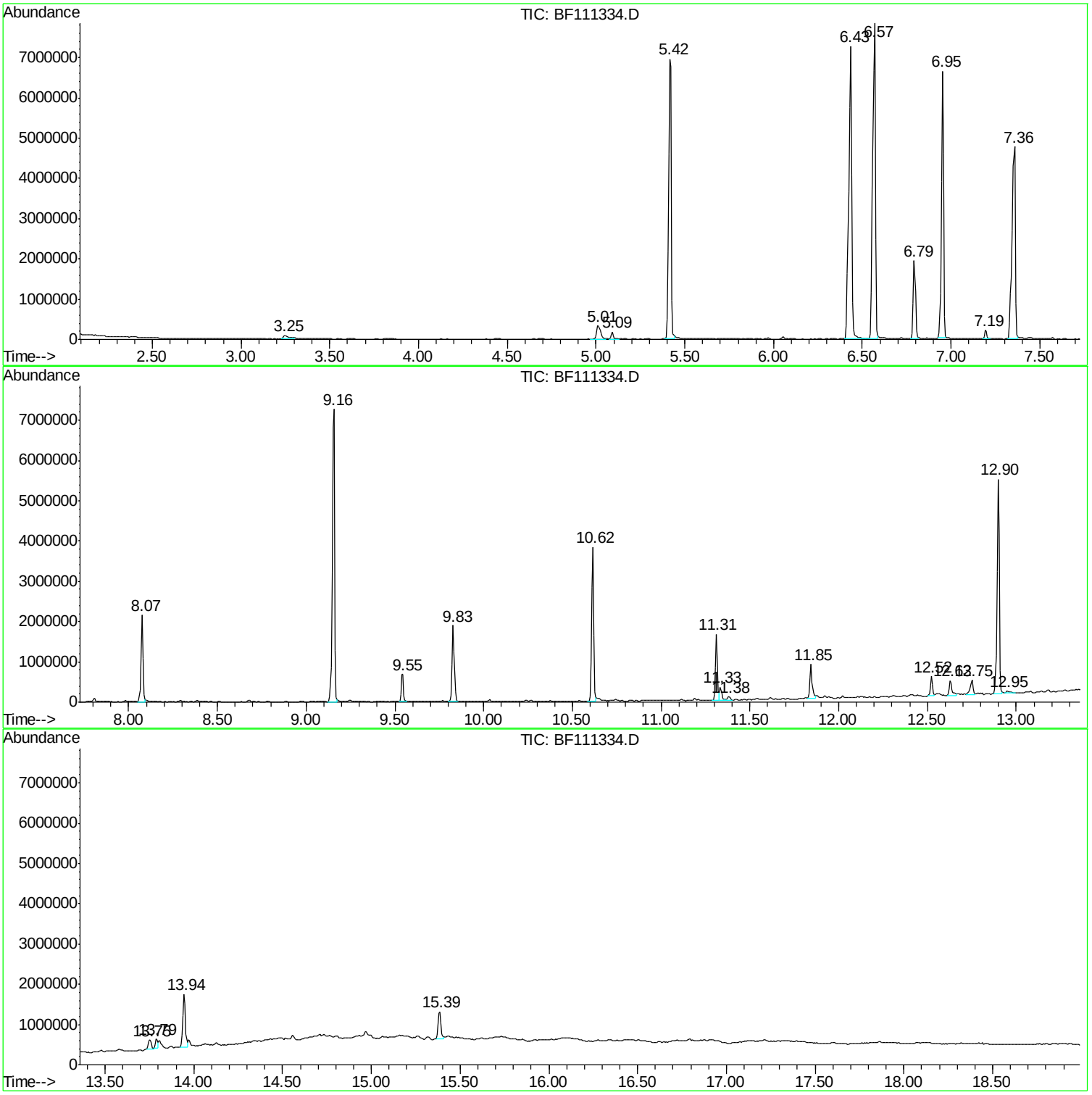
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111334.D
Acq On : 12 Dec 2018 21:06
Operator : JU/SJ
Sample : J6331-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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\BF121218\
Data File : BF111334.D
Acq On : 12 Dec 2018 21:06
Operator : JU/SJ
Sample : J6331-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

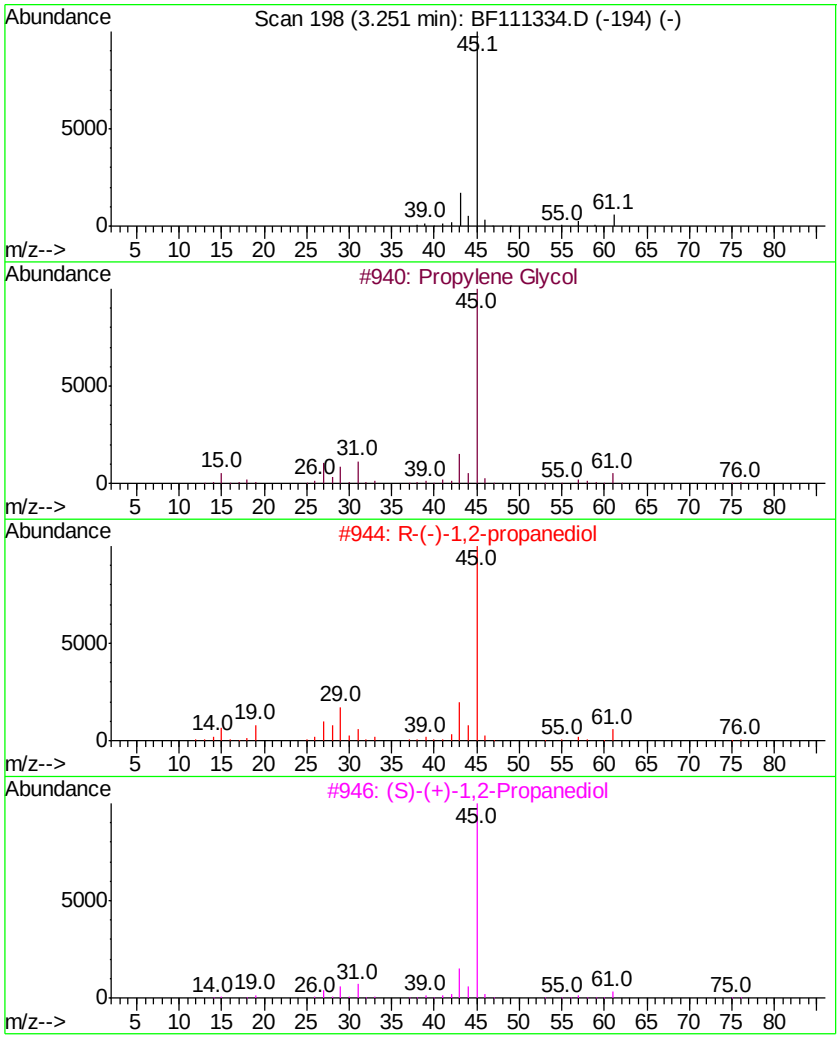
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

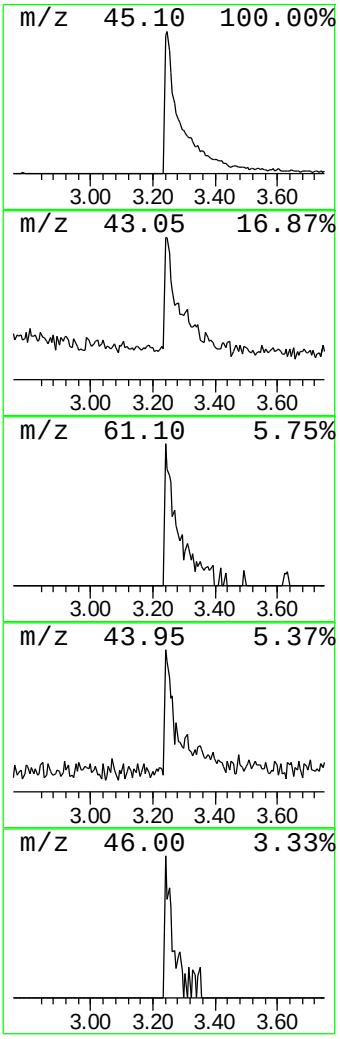
****

Peak Number 1 Propylene Glycol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.25	2.38 ng	184756	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	78
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
4	Butanenitrile, 2-(methoxymethoxy)	129	C6H11NO2	1000196-86-5	9
5	Formamide	45	CH3NO	000075-12-7	7





Library Search Compound Report

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Data File : BF111334.D
Acq On : 12 Dec 2018 21:06
Operator : JU/SJ
Sample : J6331-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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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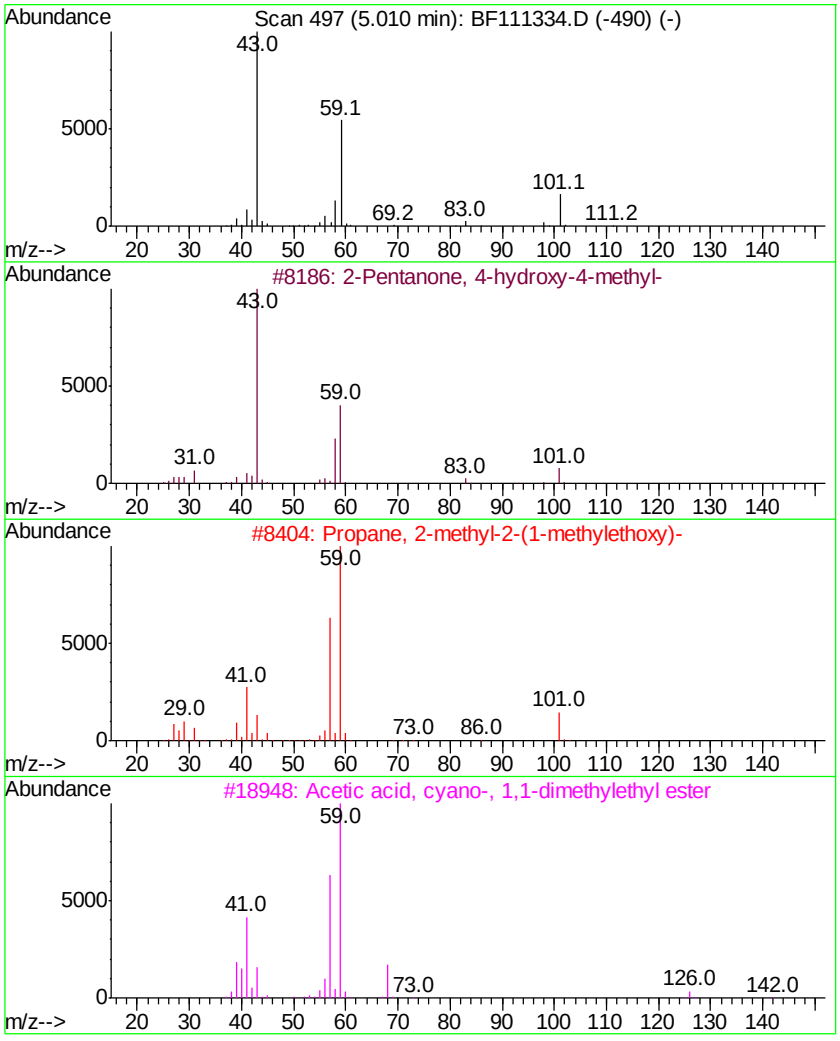
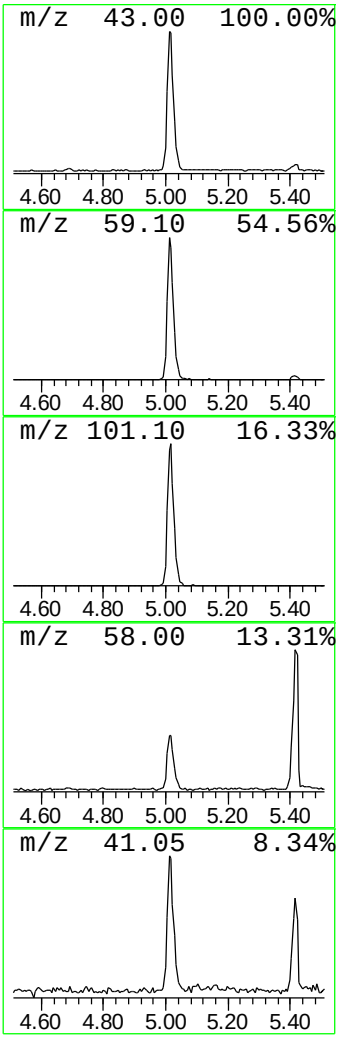
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	6.26 ng	485700	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111334.D
Acq On : 12 Dec 2018 21:06
Operator : JU/SJ
Sample : J6331-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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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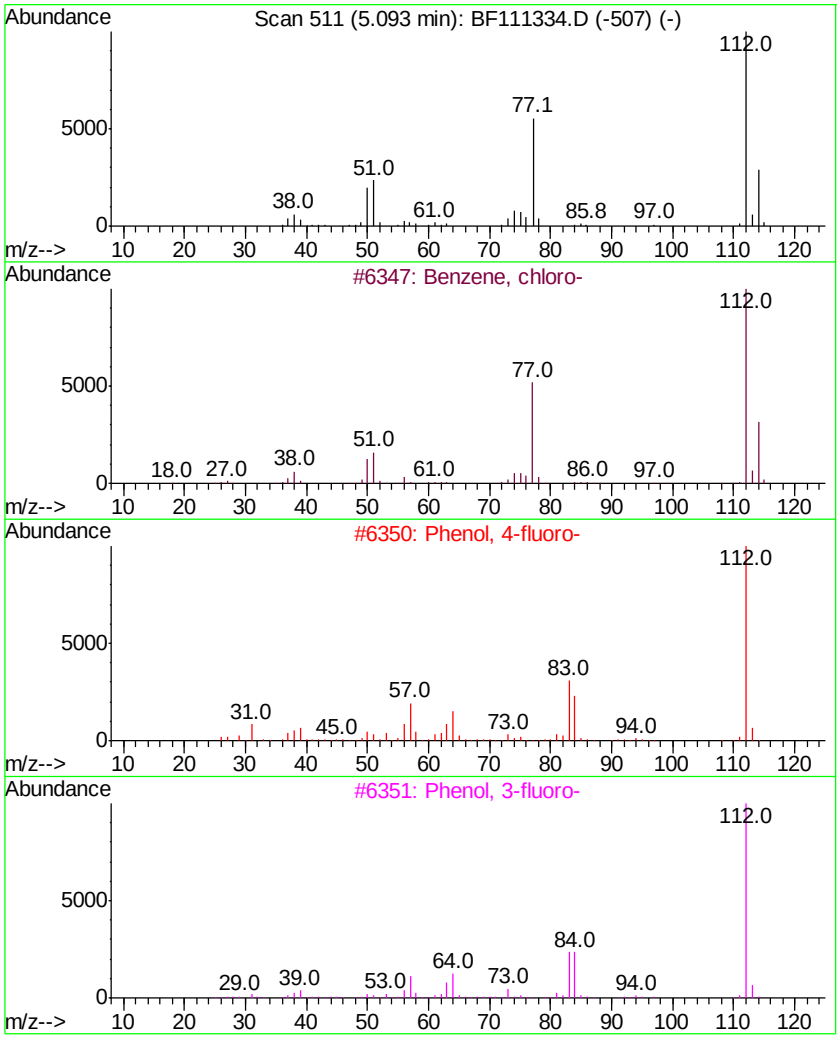
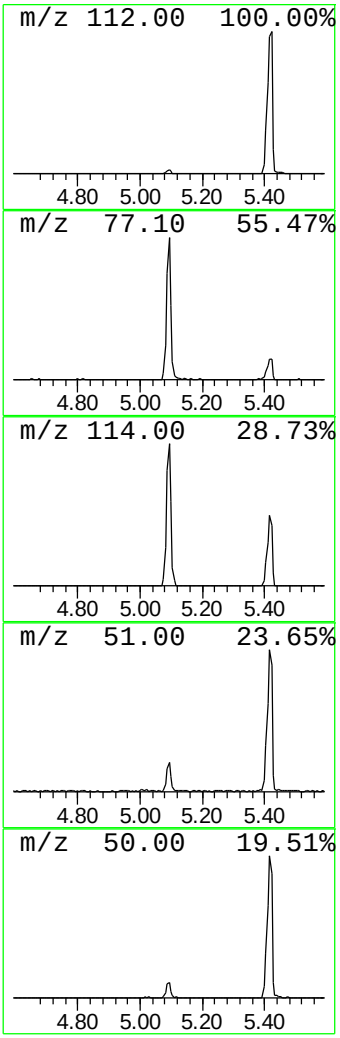
Peak Number 3 Benzene, chloro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	2.21 ng	171691	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, chloro-	112	C6H5Cl	000108-90-7	93
2	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	35
3	Phenol, 3-fluoro-	112	C6H5FO	000372-20-3	35
4	3-Nitropyrrole	112	C4H4N2O2	005930-94-9	16
5	s-Hydroxymethylthiobenzoate	168	C8H8O2S	023853-33-0	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111334.D
Acq On : 12 Dec 2018 21:06
Operator : JU/SJ
Sample : J6331-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

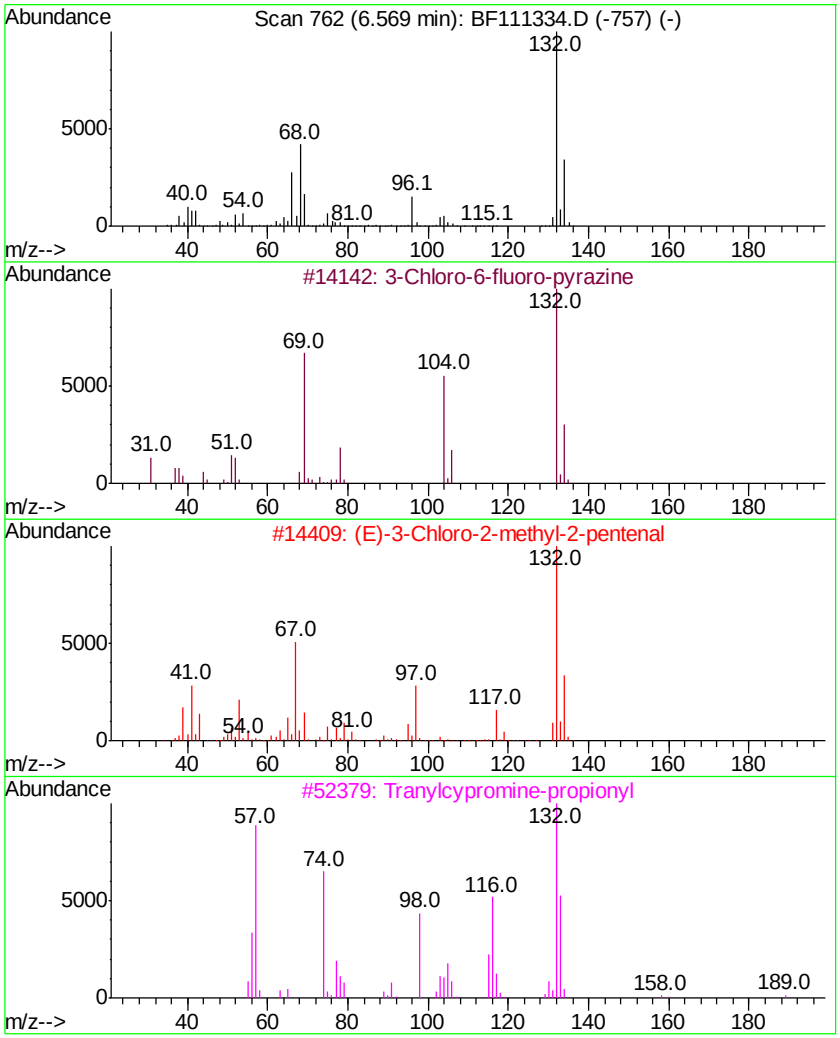
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

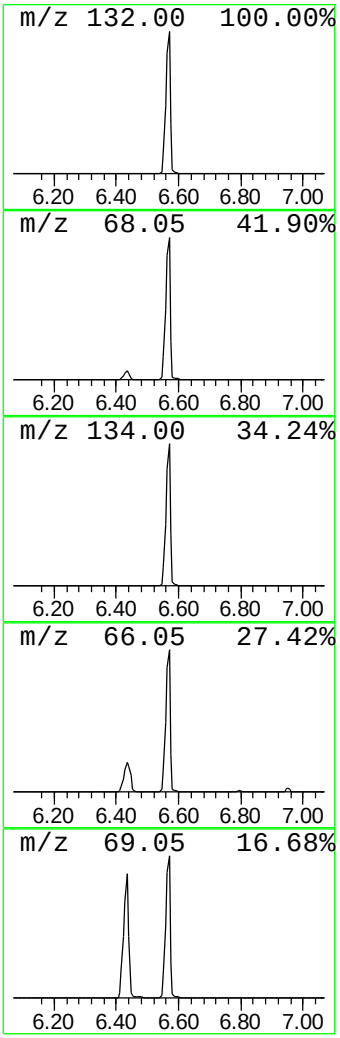
****

Peak Number 4 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	100.97 ng	7835430	1,4-Dichlorobenzene-d4	6.79

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111334.D
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Operator : JU/SJ
Sample : J6331-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

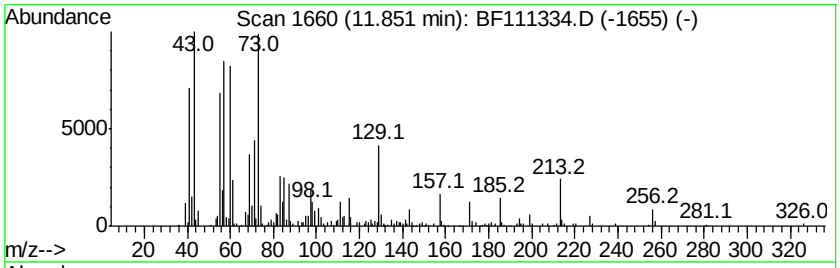
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

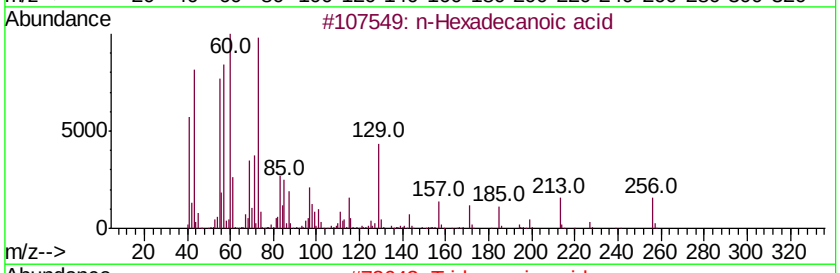
****

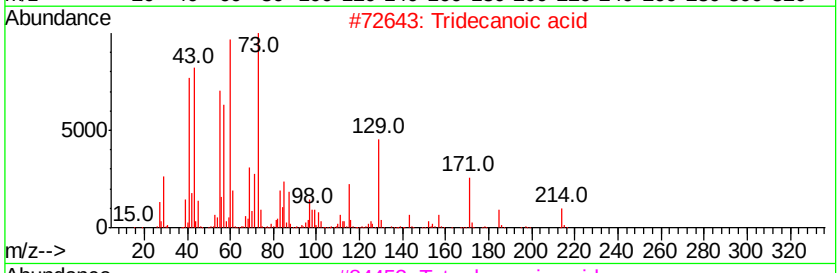
Peak Number 6 n-Hexadecanoic acid Concentration Rank 3

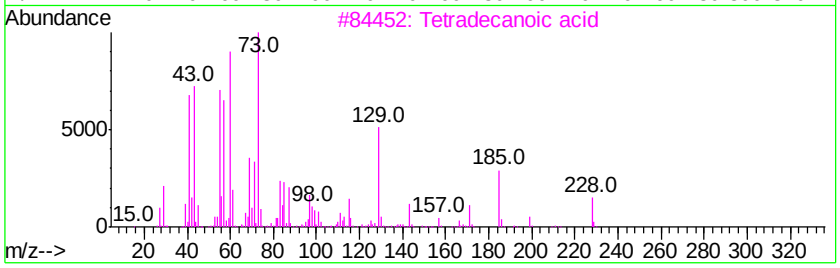
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	10.37 ng	744201	Phenanthrene-d10	11.31

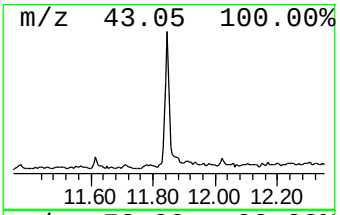
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70

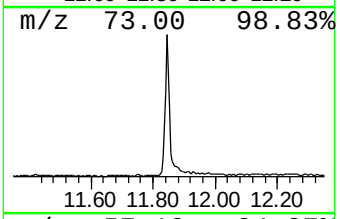


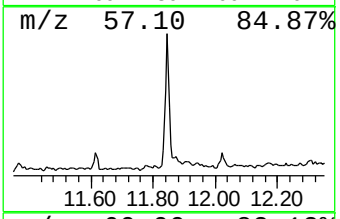


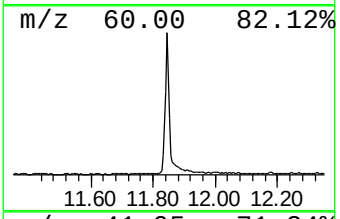


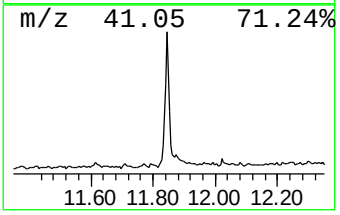












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111334.D
Acq On : 12 Dec 2018 21:06
Operator : JU/SJ
Sample : J6331-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

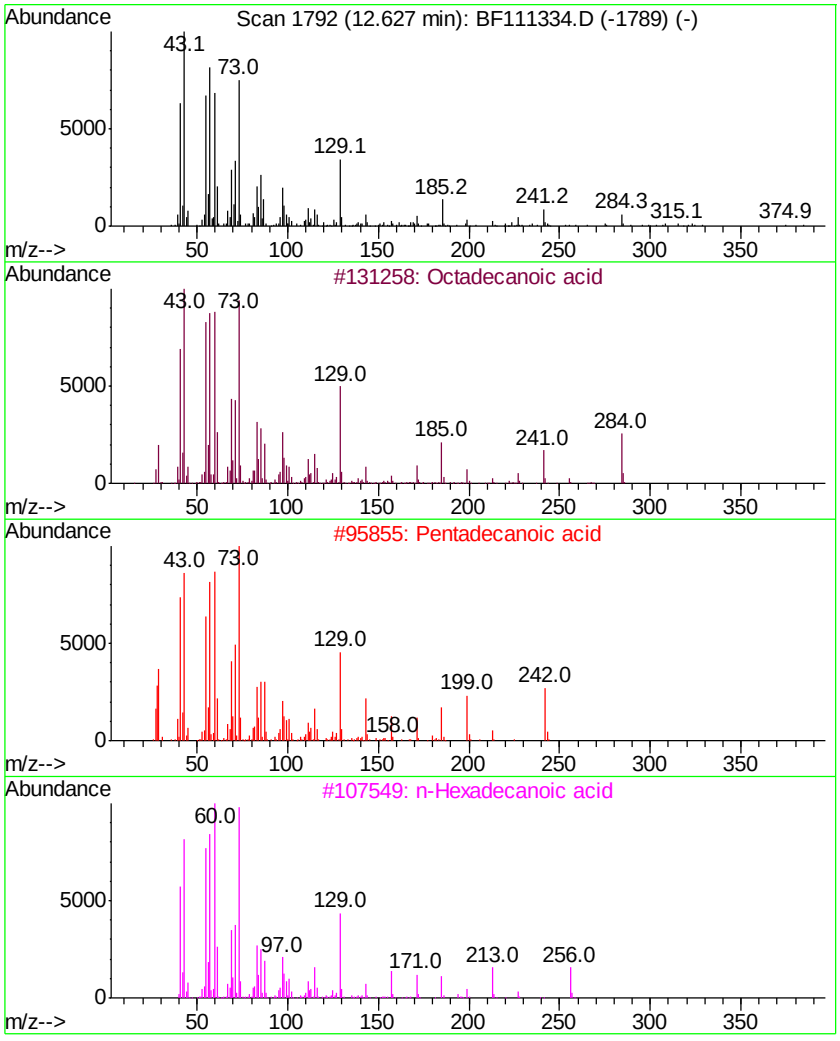
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

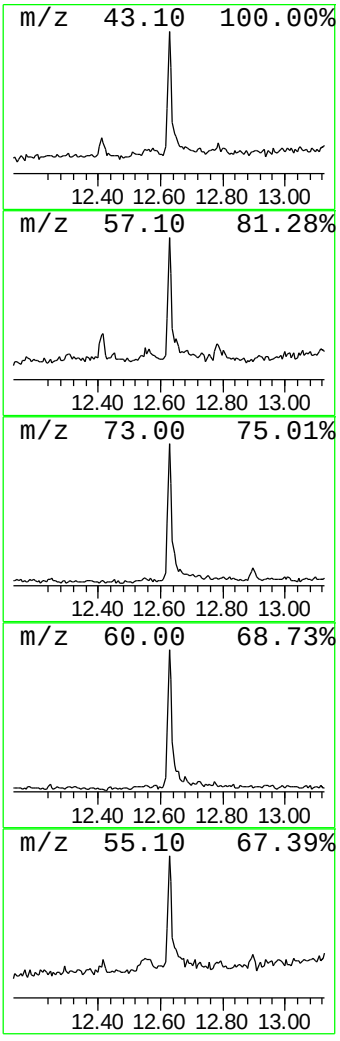
****

Peak Number 7 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	5.88 ng	421463	Phenanthrene-d10	11.31

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	52





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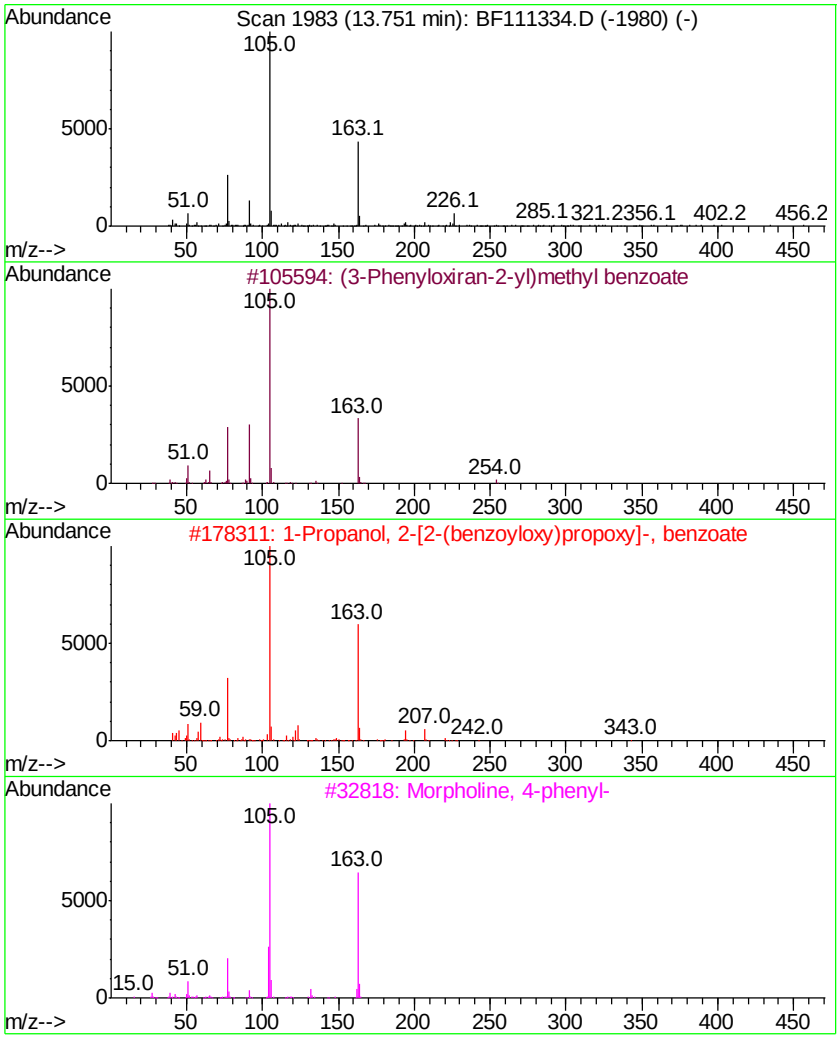
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

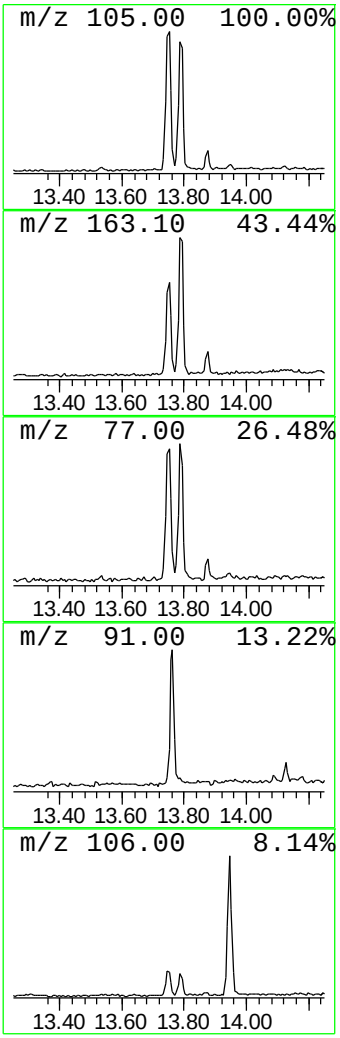
****

Peak Number 8 (3-Phenyloxiran-2-yl)methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	4.53 ng	313213	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3-Phenyloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	64
2	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	50
3	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	47
4	Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	36
5	Benzoic acid, 2,3-dimethylphenyl...	226	C15H14O2	1000360-68-4	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121218\
Data File : BF111334.D
Acq On : 12 Dec 2018 21:06
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Sample : J6331-19
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

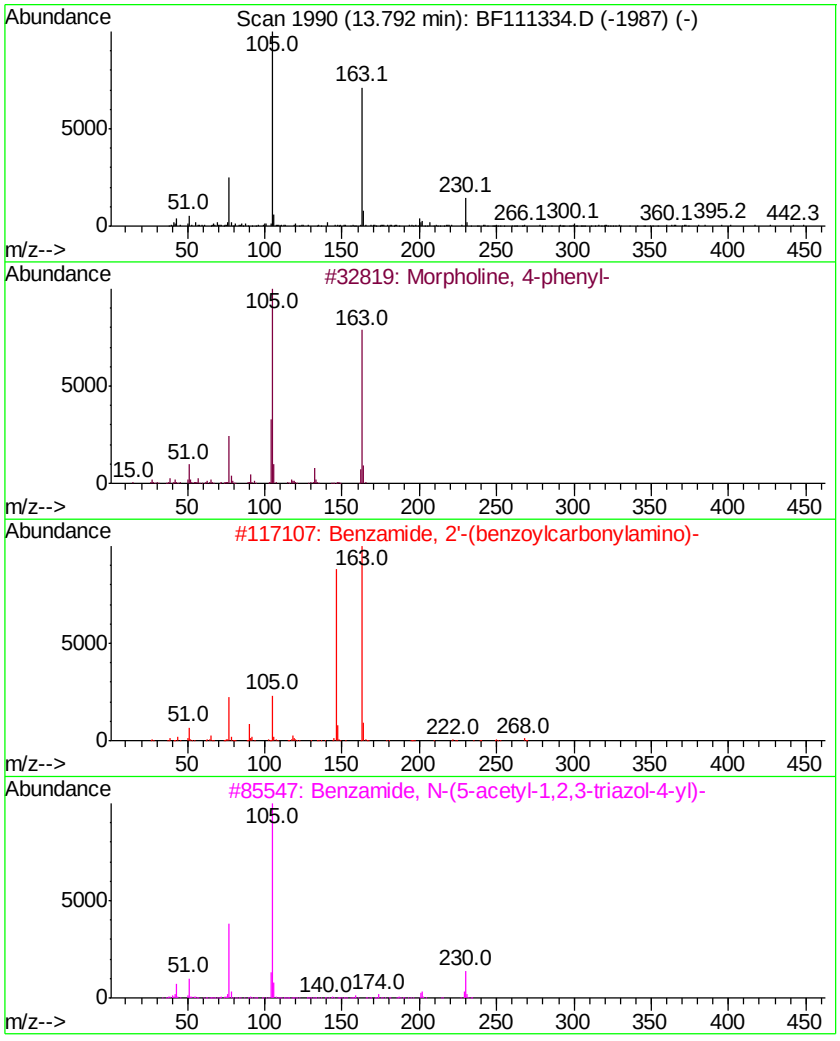
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

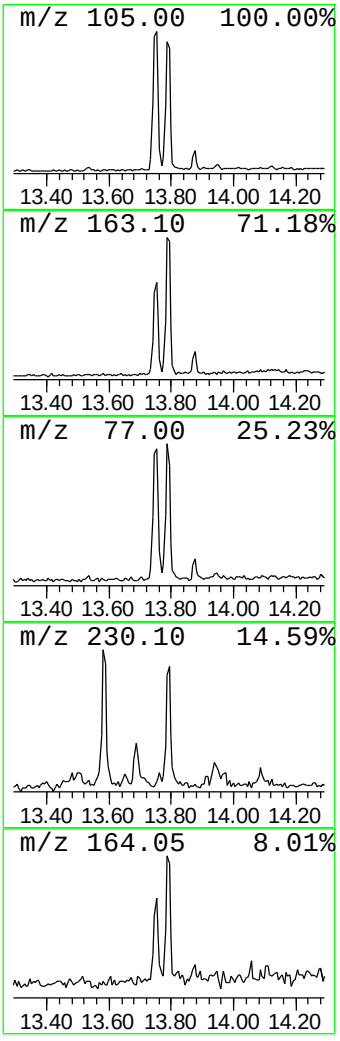
****

Peak Number 9 Morpholine, 4-phenyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	3.36 ng	231798	Chrysene-d12	13.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
2	Benzamide, 2'-(benzoylcarbonylam...	268	C15H12N2O3	129768-51-0	47
3	Benzamide, N-(5-acetyl-1,2,3-tri...	230	C11H10N4O2	129959-33-7	43
4	Ethanone, 1-[2-(dimethylamino)ph...	163	C10H13NO	010336-55-7	42
5	N-(4-Formyl-phenyl)-N-methyl-for...	163	C9H9NO2	079213-80-2	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121218\
Data File : BF111334.D
Acq On : 12 Dec 2018 21:06
Operator : JU/SJ
Sample : J6331-19
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF121218.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
Propylene Glycol	3.25	2.4	ng	184756	1	6.79	1552100	20.0
2-Pentanone, 4-hy...	5.01	6.3	ng	485700	1	6.79	1552100	20.0
Benzene, chloro-	5.09	2.2	ng	171691	1	6.79	1552100	20.0
unknown6.57	6.57	101.0	ng	7835430	1	6.79	1552100	20.0
n-Hexadecanoic acid	11.85	10.4	ng	744201	4	11.31	1434700	20.0
Octadecanoic acid	12.63	5.9	ng	421463	4	11.31	1434700	20.0
(3-Phenyloxiran-2...	13.75	4.5	ng	313213	5	13.94	1381570	20.0
Morpholine, 4-phe...	13.79	3.4	ng	231798	5	13.94	1381570	20.0