LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190854-AMENDED-COMP-A

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_P\METHODS\8270-BP100119.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	4.317	375	379	387	rBV	179724	219055	2.82%	0.486%
2	4.975	481	491	494	rBV	4004118	7770379	100.00%	17.222%
3	5.369	555	558	573	rVB	204441	216939	2.79%	0.481%
4	6.381	727	730	742	rBV3	1138893	1285409	16.54%	2.849%
5	6.516	750	753	761	rVB	521293	413127	5.32%	0.916%
6	6.746	789	792	796	rBV	1692610	1368718	17.61%	3.034%
7	6.905	815	819	822	rBV	4511446	3625482	46.66%	8.036%
8	7.311	883	888	891	rBV	2688025	2532294	32.59%	5.613%
9	7.458	909	913	916	rBV	764564	588221	7.57%	1.304%
10	8.028	1007	1010	1014	rBV	2052931	1777611	22.88%	3.940%
11	9.116	1191	1195	1198	rBV	6073744	5131964	66.05%	11.374%
12	9.510	1258	1262	1265	rBV	1057695	808976	10.41%	1.793%
13	9.746	1298	1302	1307	rBV	164421	277099	3.57%	0.614%
14	9.793	1307	1310	1314	rVB	2671295	2287118	29.43%	5.069%
15	10.704	1461	1465	1468	rBV	688906	622172	8.01%	1.379%
16	11.152	1537	1541	1548	rBV3	203667	314170	4.04%	0.696%
17	11.293	1561	1565	1568	rBV	3038293	2503476	32.22%	5.549%
18	11.363	1574	1577	1581	rVB2	178531	158282	2.04%	0.351%
19	12.516	1770	1773	1777	rVB	152398	124402	1.60%	0.276%
20	12.746	1809	1812	1815	rVB	143112	132810	1.71%	0.294%
21	12.898	1834	1838	1841	rBV	6913114	5982679	76.99%	13.260%
22	13.822	1991	1995	2008	rBV2	257128	560389	7.21%	1.242%
23	13.963	2014	2019	2022	rBV	2824041	2570334	33.08%	5.697%
24	14.451	2099	2102	2105	rBV	113925	98943	1.27%	0.219%
25	14.763	2152	2155	2162	rVB	129142	146863	1.89%	0.326%
26	15.010	2194	2197	2206	rVB	72866	142106	1.83%	0.315%
27	15.104	2209	2213	2218	rVB2	153705	205776	2.65%	0.456%
28	15.369	2255	2258	2264	rVV	73290	116143	1.49%	0.257%
29	15.434	2264	2269	2274	rVV	1908904	2422618	31.18%	5.369%
30	15.487	2275	2278	2291	rVB	117976	198109	2.55%	0.439%
31	15.922	2348	2352	2361	rBV	99740	167398	2.15%	0.371%
32	16.163	2387	2393	2412	rVB10	52746	237696	3.06%	0.527%
33	16.345	2420	2424	2431	rBV5	70474	111521	1.44%	0.247%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20190854-AMENDED-COMP-A

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_P\METHODS\8270-BP100119.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 45118279

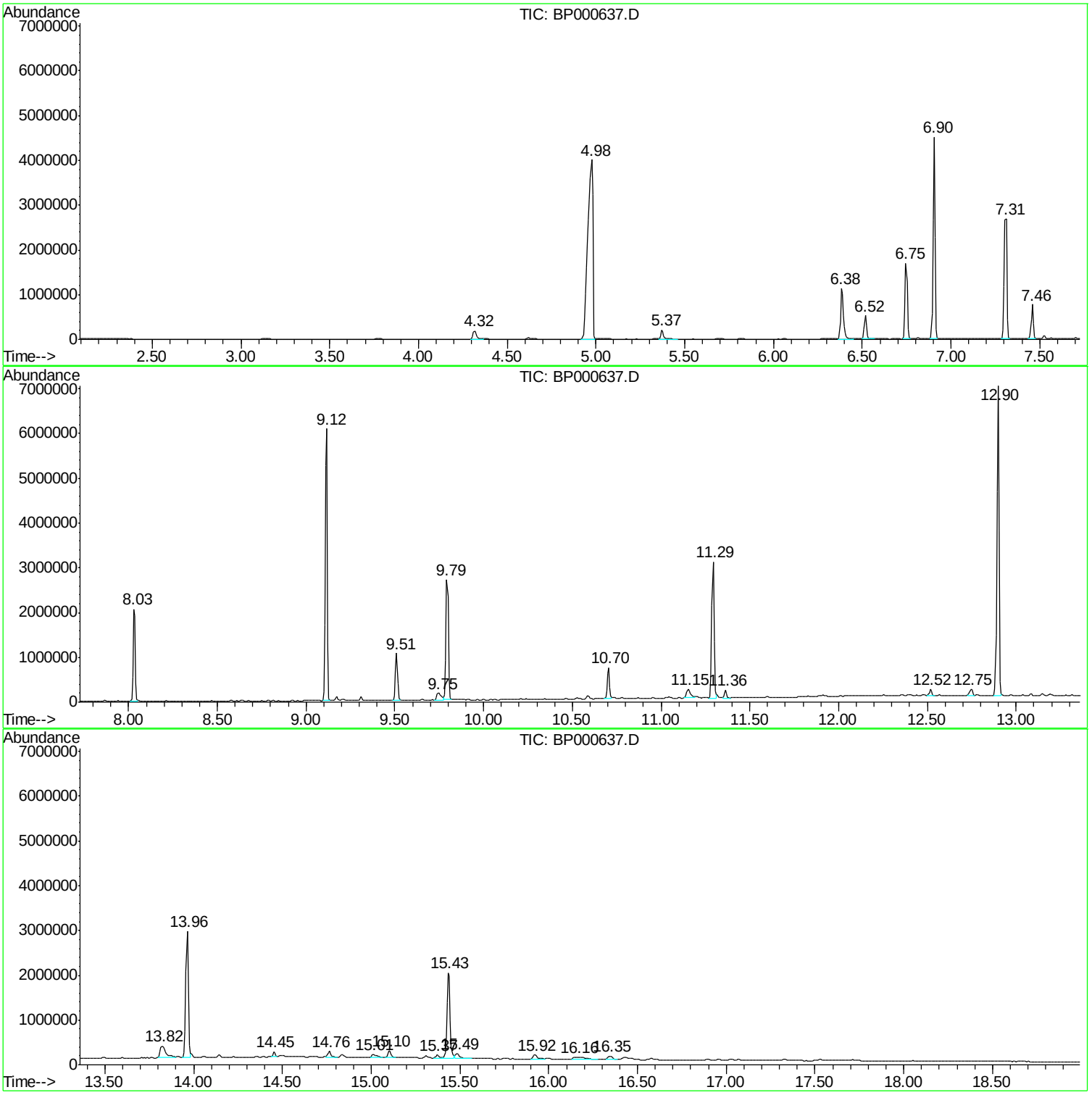
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20190854-AMENDED-COMP-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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 P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190854-AMENDED-COMP-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

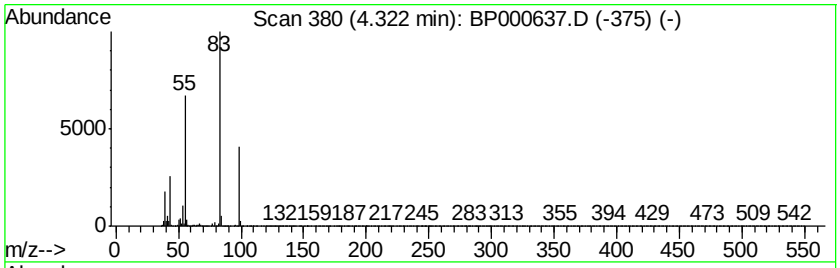
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

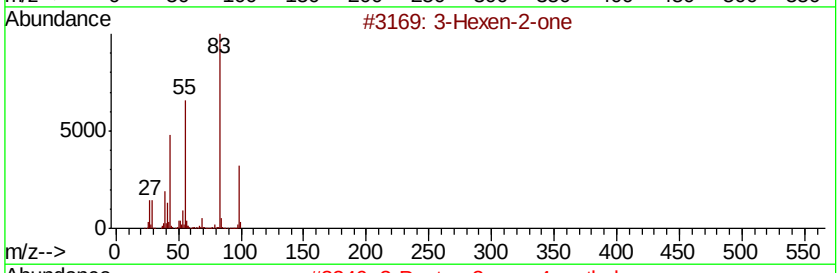
****

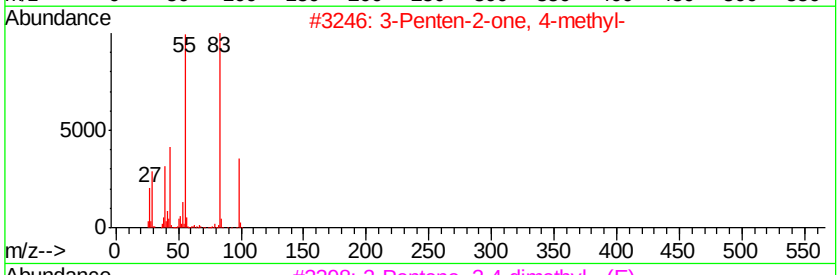
Peak Number 1 3-Hexen-2-one Concentration Rank 7

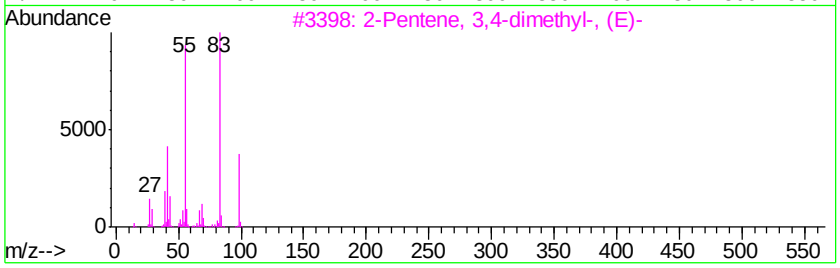
R.T.	EstConc	Area	Relative to ISTD	R.T.
4.32	3.20 ng	219055	1,4-Dichlorobenzene-d4	6.75

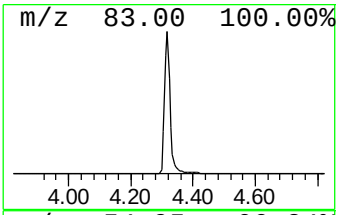
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78
5	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78

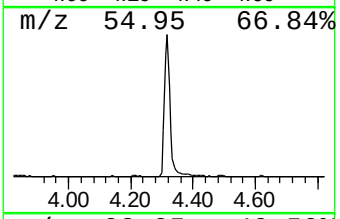


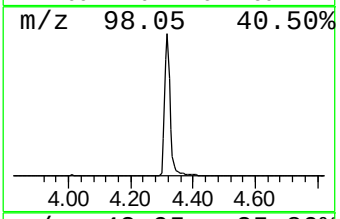


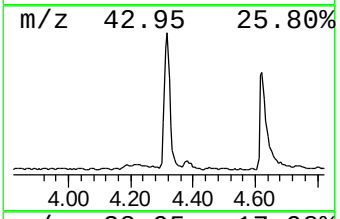


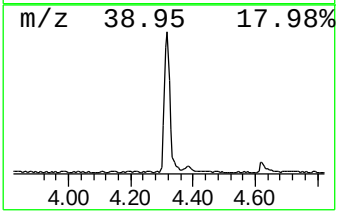












Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190854-AMENDED-COMP-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

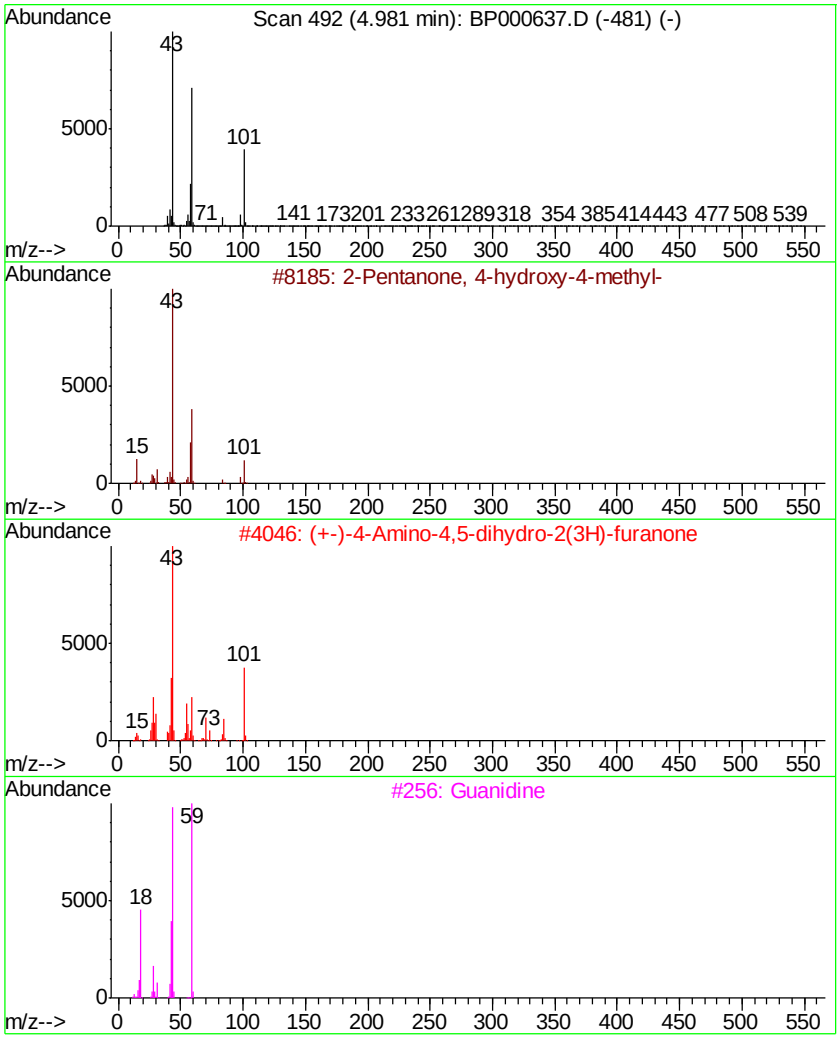
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

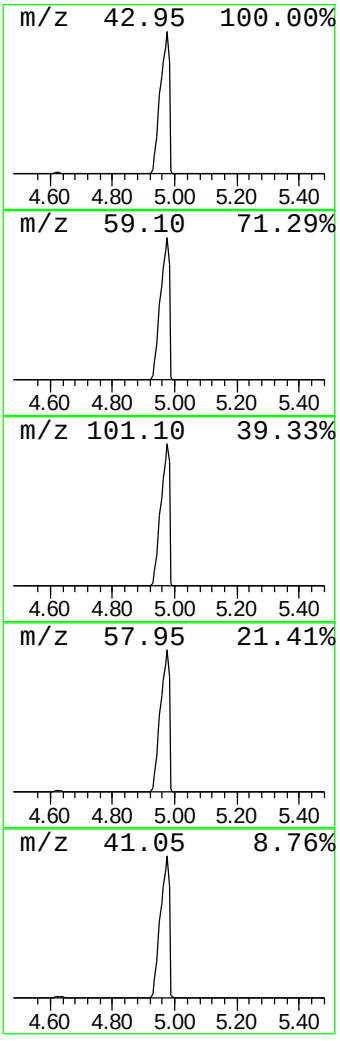
****

Peak Number 2 unknown4.98 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	113.54 ng	7770380	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3	Guanidine	59	CH5N3	000113-00-8	38
4	Acetone	58	C3H6O	000067-64-1	12
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190854-AMENDED-COMP-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

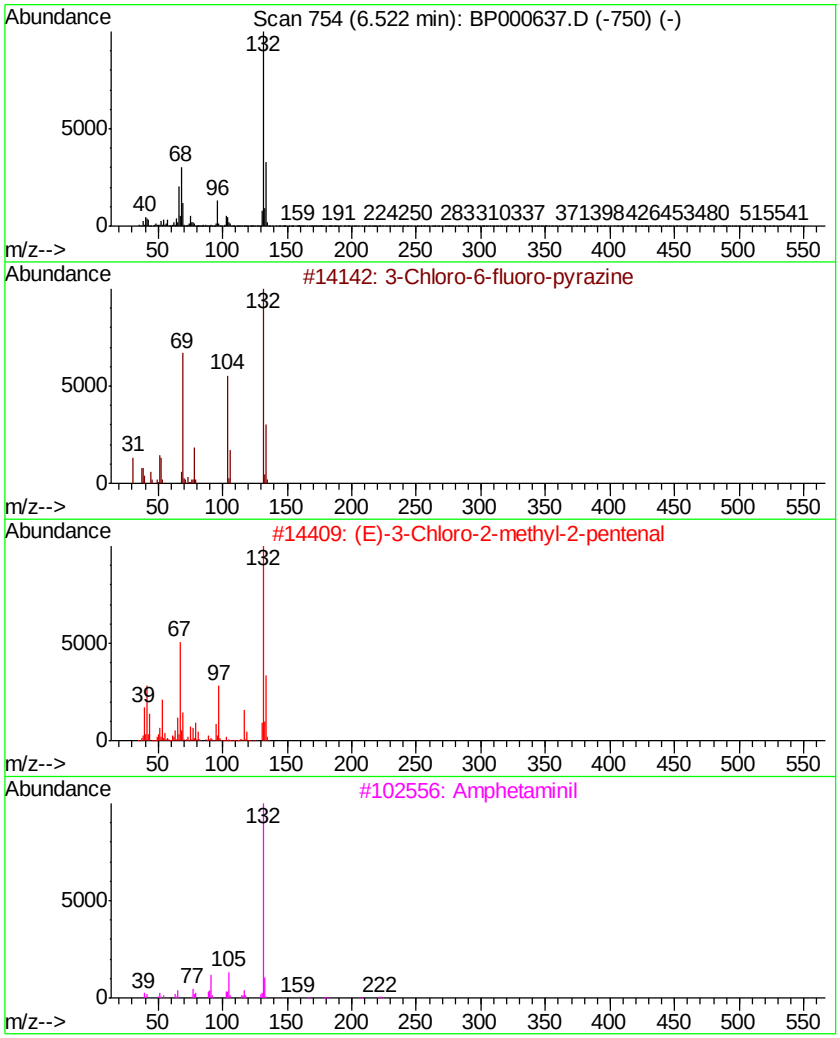
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

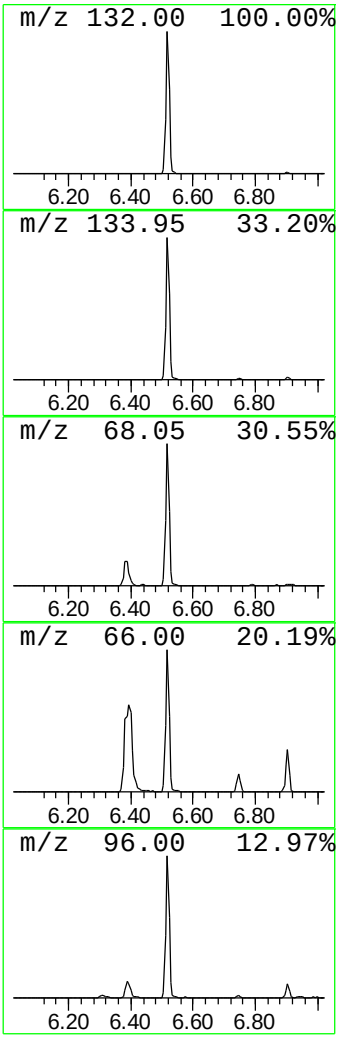
****

Peak Number 3 unknown6.52 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	6.04 ng	413127	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Amphetaminil	250	C17H18N2	017590-01-1	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190854-AMENDED-COMP-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

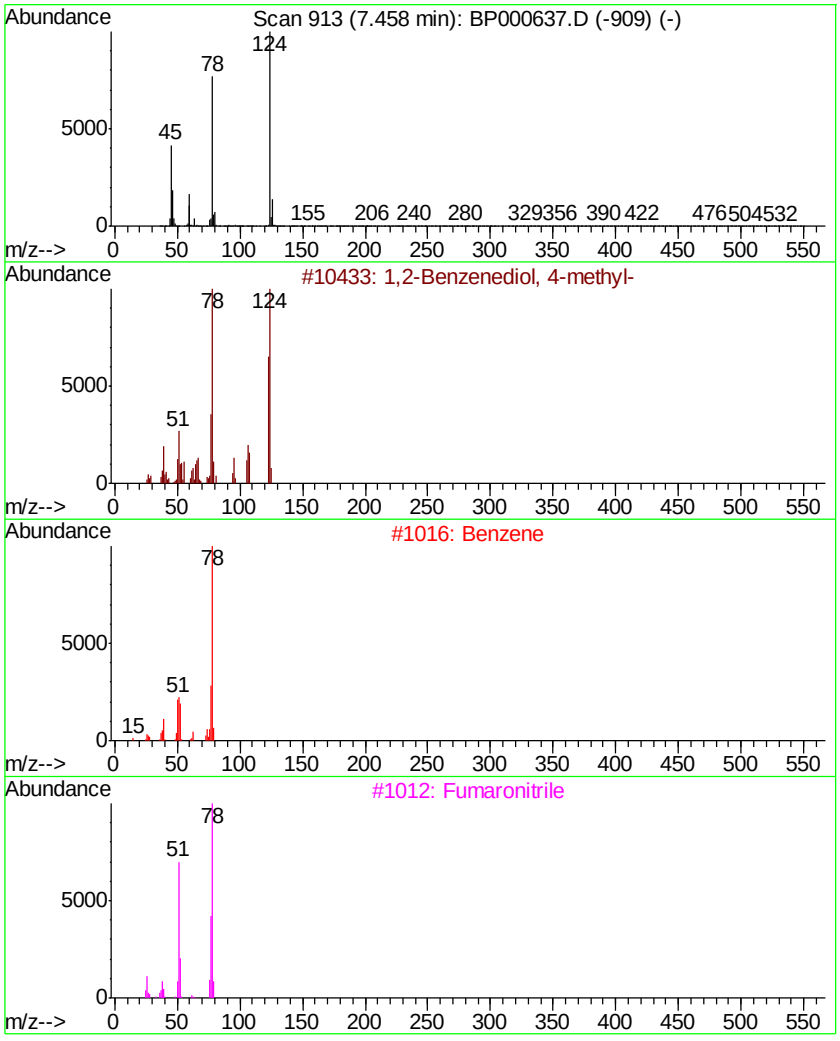
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

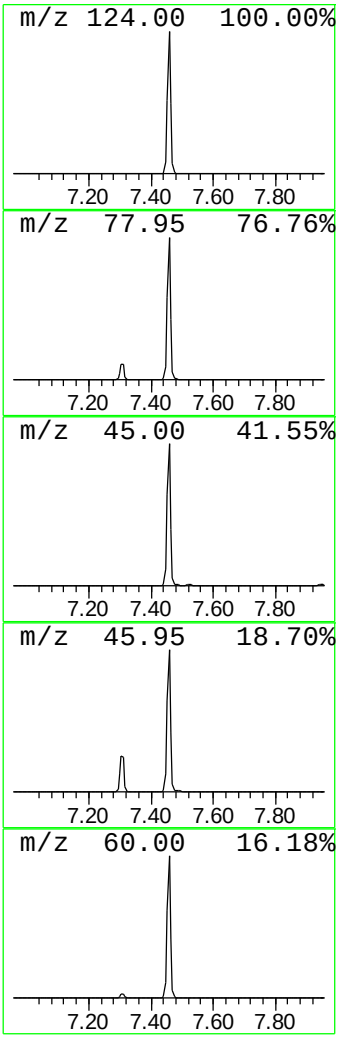
****

Peak Number 5 1,2-Benzenediol, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	6.62 ng	588221	Naphthalene-d8	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	50
2	Benzene	78	C6H6	000071-43-2	9
3	Fumaronitrile	78	C4H2N2	000764-42-1	9
4	2,4-Hexadiyne	78	C6H6	002809-69-0	7
5	Propanedinitrile, methylene-	78	C4H2N2	000922-64-5	7





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190854-AMENDED-COMP-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

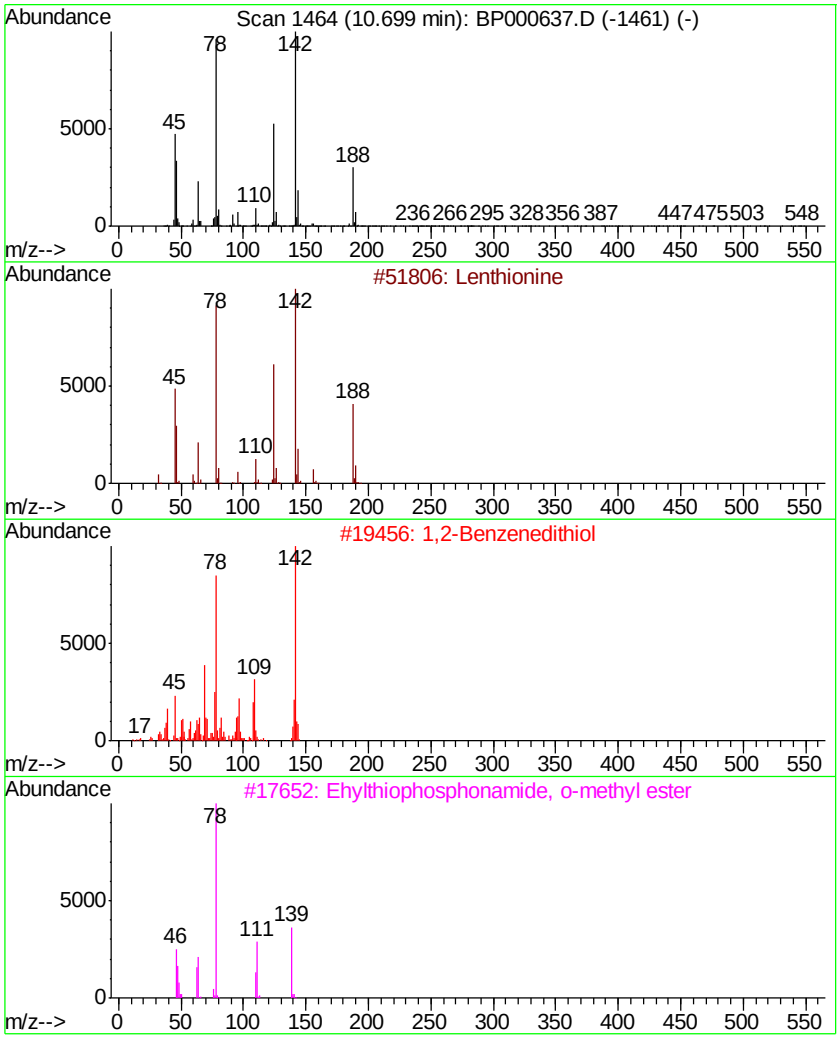
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

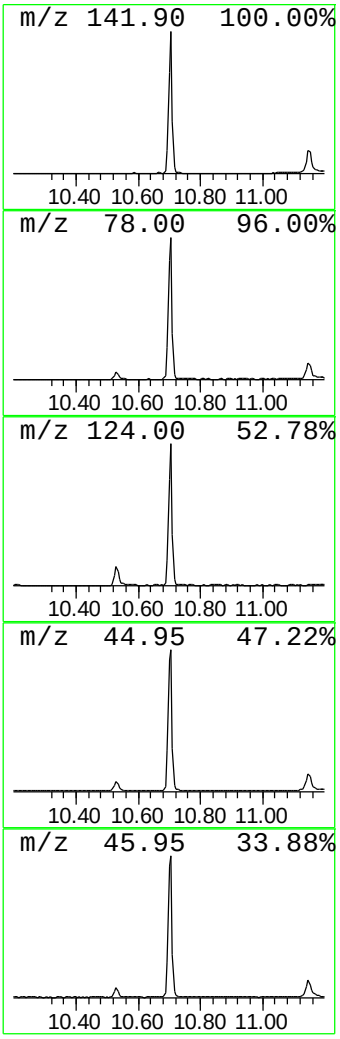
****

Peak Number 6 Lenthionine Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.70	4.97 ng	622172	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	94
2	1,2-Benzenedithiol	142	C6H6S2	017534-15-5	9
3	Ehylthiophosphonamide, o-methyl ...	139	C3H10NOPS	1000306-03-7	9
4	Boronic acid, phenyl-	122	C6H7BO2	000098-80-6	9
5	2,4-Hexadiyne	78	C6H6	002809-69-0	7





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190854-AMENDED-COMP-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

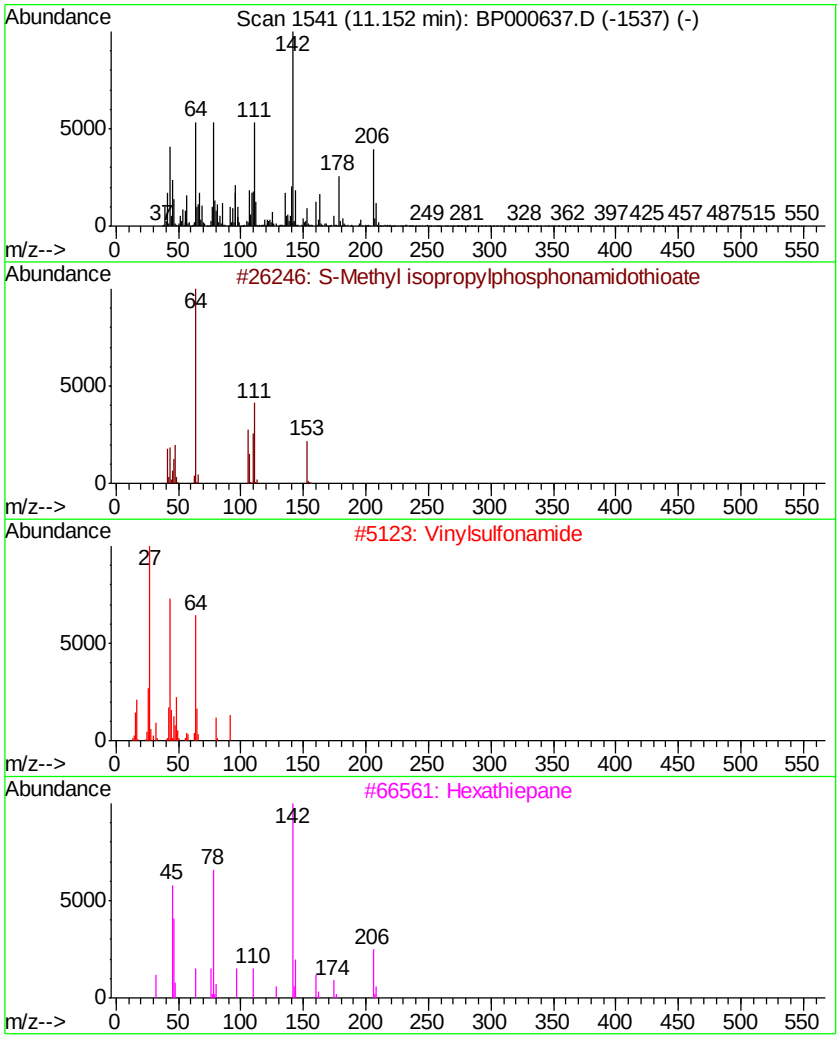
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

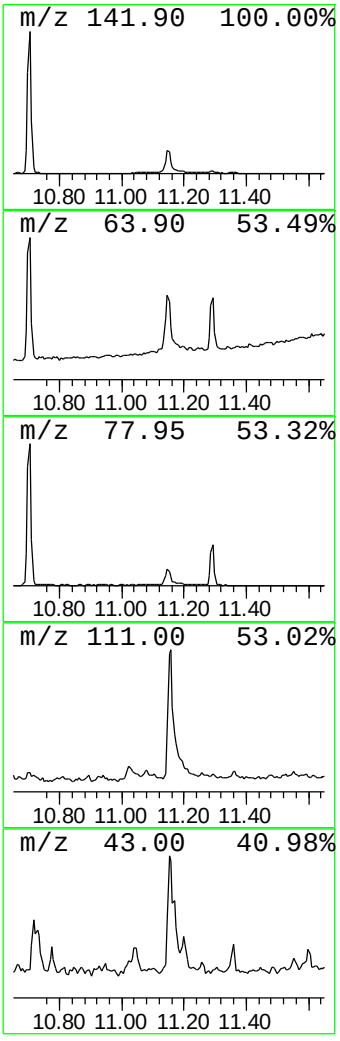
****

Peak Number 7 unknown11.15 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	2.51 ng	314170	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	S-Methyl isopropylphosphonamidot...	153	C4H12NOPS	1000306-04-4	27
2	Vinylsulfonamide	107	C2H5NO2S	002386-58-5	12
3	Hexathiepane	206	CH2S6	017233-71-5	12
4	1,3-Dioxepane, 5,5,6,6-tetrafluoro-	174	C5H6F4O2	001547-52-0	10
5	S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190854-AMENDED-COMP-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

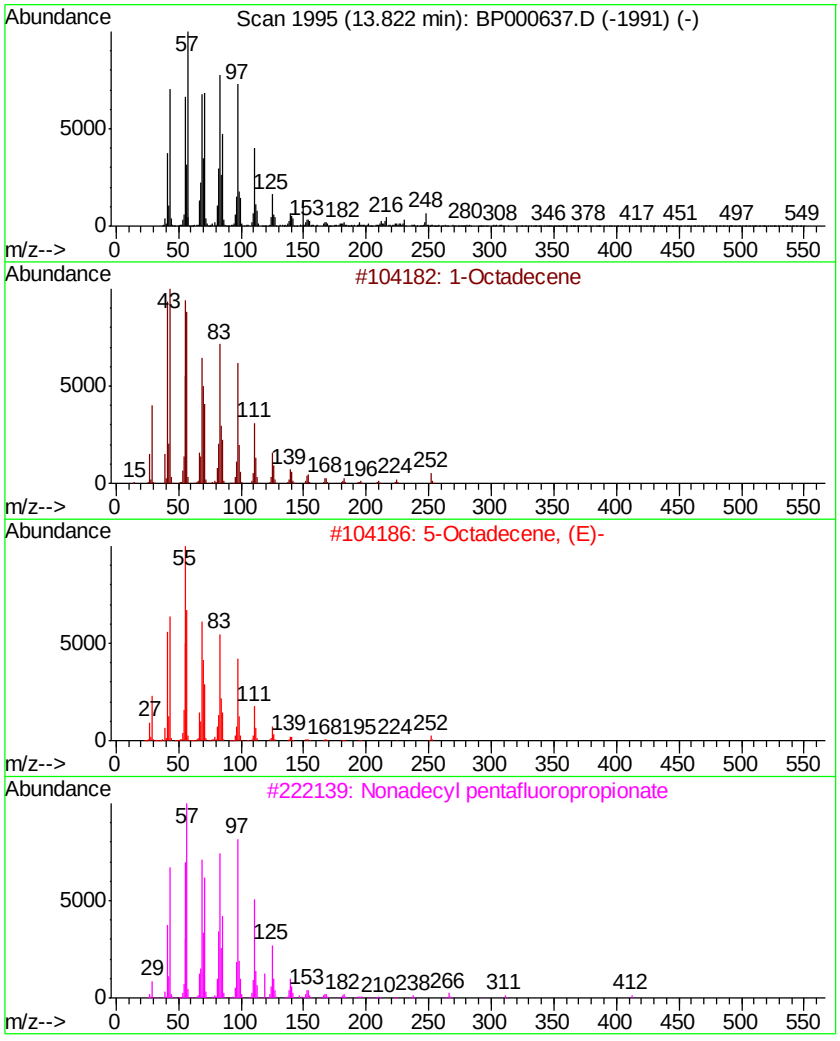
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

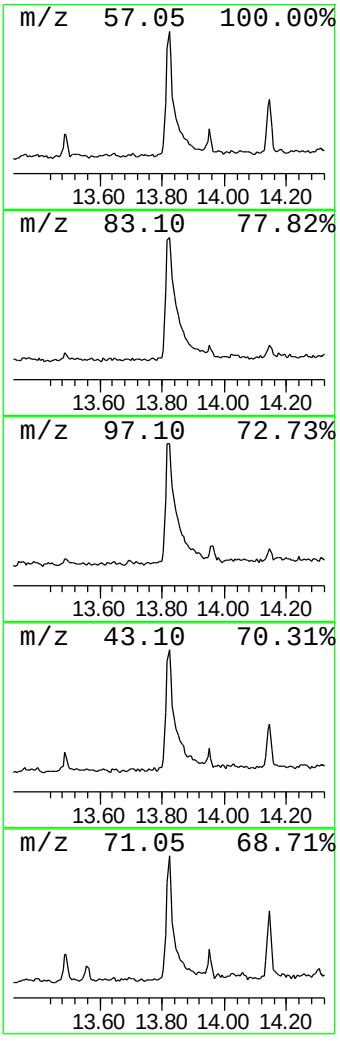
****

Peak Number 8 1-Octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.36 ng	560389	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	93
2	5-Octadecene, (E)-	252	C18H36	007206-21-5	92
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
4	Behenic alcohol	326	C22H46O	000661-19-8	90
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP101119\
Data File : BP000637.D
Acq On : 11 Oct 2019 17:34
Operator : JU
Sample : K5266-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190854-AMENDED-COMP-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP100119.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
3-Hexen-2-one	4.32	3.2	ng	219055	1	6.75	1368720	20.0
unknown4.98	4.98	113.5	ng	7770380	1	6.75	1368720	20.0
unknown6.52	6.52	6.0	ng	413127	1	6.75	1368720	20.0
1,2-Benzenediol, ...	7.46	6.6	ng	588221	2	8.03	1777610	20.0
Lenthionine	10.70	5.0	ng	622172	4	11.29	2503480	20.0
unknown11.15	11.15	2.5	ng	314170	4	11.29	2503480	20.0
1-Octadecene	13.82	4.4	ng	560389	5	13.96	2570330	20.0