LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101319\
Data File : BP000691.D
Acq On : 13 Oct 2019 00:49
Operator : JU
Sample : K5348-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190882-COMPOSITE-N

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	4.964	481	489	492	rBV	2300688	3187809	62.08%	8.623%
2	5.375	556	559	572	rVB	167805	166779	3.25%	0.451%
3	6.387	727	731	741	rBV	1648748	1576483	30.70%	4.264%
4	6.516	750	753	761	rVB	505527	463614	9.03%	1.254%
5	6.746	789	792	796	rBV	1375911	1211062	23.58%	3.276%
6	6.816	801	804	812	rBV	90331	75004	1.46%	0.203%
7	6.905	815	819	822	rBV	4062531	3242605	63.15%	8.771%
8	7.311	884	888	891	rBV	2686992	2255155	43.92%	6.100%
9	7.528	921	925	928	rBV	90613	78551	1.53%	0.212%
10	8.034	1007	1011	1014	rBV	1772880	1533109	29.86%	4.147%
11	9.116	1191	1195	1198	rBV	5774913	4787470	93.23%	12.950%
12	9.452	1247	1252	1256	rBV2	30677	60251	1.17%	0.163%
13	9.510	1259	1262	1267	rVV	836564	630501	12.28%	1.706%
14	9.657	1283	1287	1293	rBV	51164	68840	1.34%	0.186%
15	9.799	1307	1311	1314	rVB	2063547	1832948	35.69%	4.958%
16	10.316	1396	1399	1402	rVB2	103547	93780	1.83%	0.254%
17	10.587	1442	1445	1452	rBV2	153240	188020	3.66%	0.509%
18	10.716	1464	1467	1475	rVB3	52777	90981	1.77%	0.246%
19	11.022	1516	1519	1521	rBV	76038	70693	1.38%	0.191%
20	11.157	1538	1542	1548	rBV	437009	416516	8.11%	1.127%
21	11.293	1561	1565	1568	rBV	2399052	2001682	38.98%	5.415%
22	11.316	1568	1569	1572	rVV	150568	87953	1.71%	0.238%
23	11.363	1574	1577	1581	rVB2	150827	147436	2.87%	0.399%
24	11.916	1669	1671	1680	rVB	86310	117436	2.29%	0.318%
25	12.516	1770	1773	1777	rVB	351866	311809	6.07%	0.843%
26	12.563	1779	1781	1787	rBV4	53255	63371	1.23%	0.171%
27	12.616	1788	1790	1793	rVB2	64192	59651	1.16%	0.161%
28	12.751	1808	1813	1816	rBV	351136	341835	6.66%	0.925%
29	12.898	1834	1838	1841	rBV	5772801	5135087	100.00%	13.891%
30	13.087	1867	1870	1873	rVB	115401	108455	2.11%	0.293%
31	13.122	1873	1876	1878	rBV3	60406	63375	1.23%	0.171%
32	13.151	1878	1881	1884	rVV	89369	89508	1.74%	0.242%
33	13.193	1885	1888	1896	rVB3	55085	81530	1.59%	0.221%
34	13.316	1906	1909	1911	rBV	54642	61519	1.20%	0.166%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101319\
Data File : BP000691.D
Acq On : 13 Oct 2019 00:49
Operator : JU
Sample : K5348-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190882-COMPOSITE-N

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

35	13.816	1990	1994	2001	rBV2	416267	583659	11.37%	1.579%
36	13.963	2014	2019	2022	rBV	2213157	2401715	46.77%	6.497%
37	13.993	2022	2024	2027	rVB	181720	147041	2.86%	0.398%
38	14.451	2100	2102	2105	rBV3	97316	94175	1.83%	0.255%
39	15.010	2194	2197	2201	rBV	196685	296105	5.77%	0.801%
40	15.098	2210	2212	2219	rVB2	106043	174697	3.40%	0.473%
41	15.310	2246	2248	2255	rVB	137421	186215	3.63%	0.504%
42	15.375	2256	2259	2265	rBV	188433	221224	4.31%	0.598%
43	15.440	2265	2270	2274	rBV	1665656	1975862	38.48%	5.345%
44	15.922	2350	2352	2356	rVB	56081	62181	1.21%	0.168%
45	16.904	2515	2519	2525	rVB2	73533	124158	2.42%	0.336%

Sum of corrected areas: 36967850

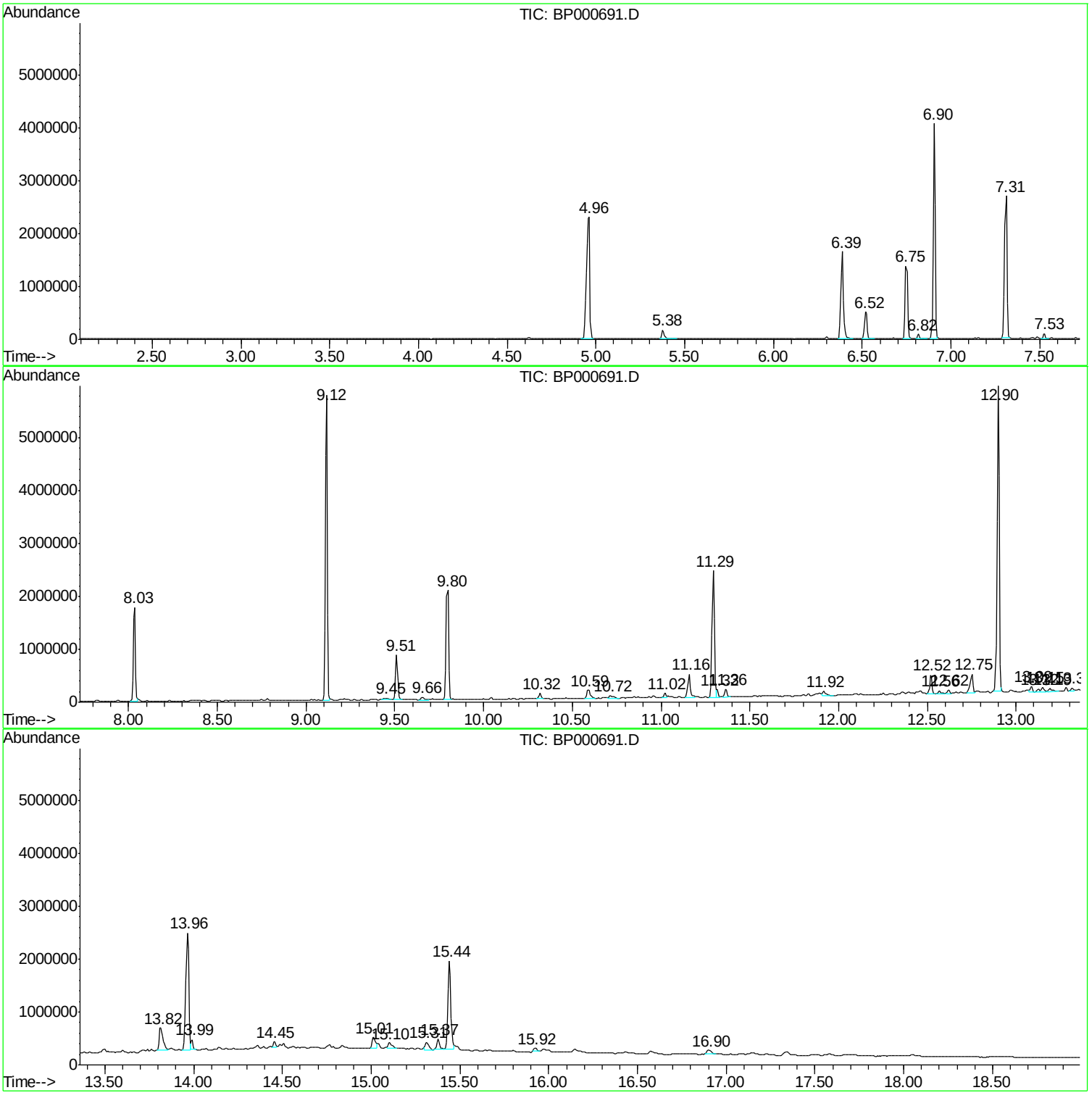
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101319\
Data File : BP000691.D
Acq On : 13 Oct 2019 00:49
Operator : JU
Sample : K5348-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190882-COMPOSITE-N

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\BP101319\
Data File : BP000691.D
Acq On : 13 Oct 2019 00:49
Operator : JU
Sample : K5348-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190882-COMPOSITE-N

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

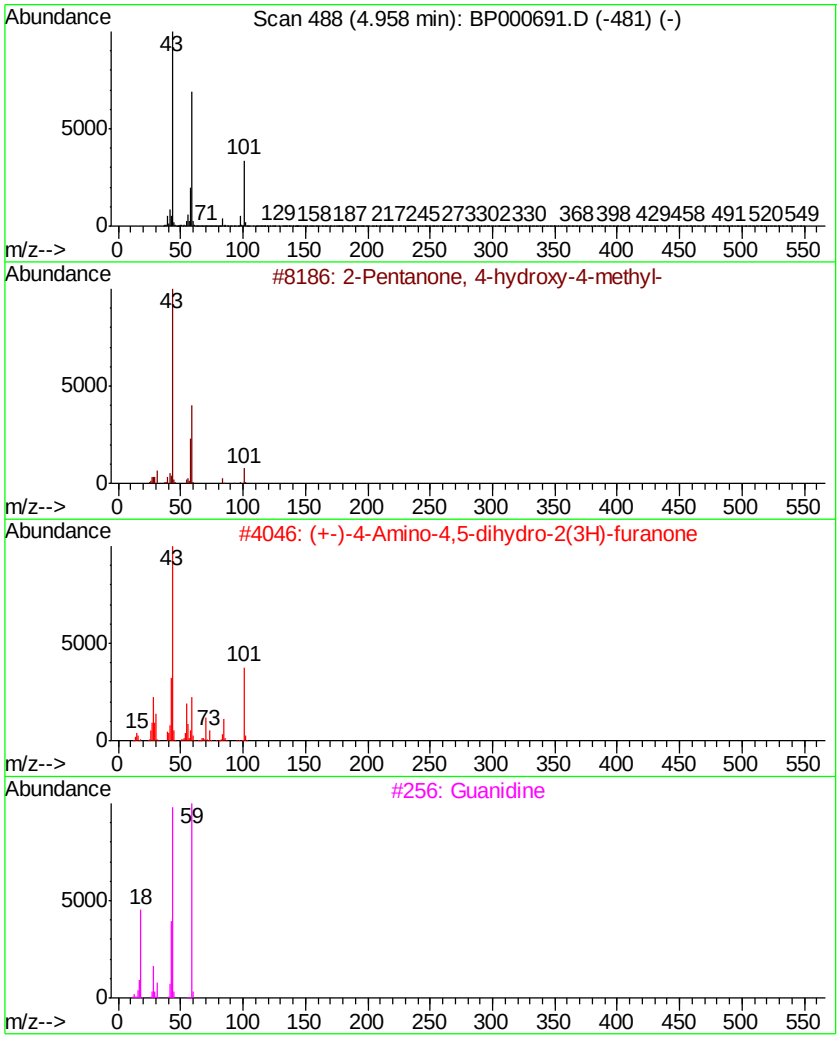
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

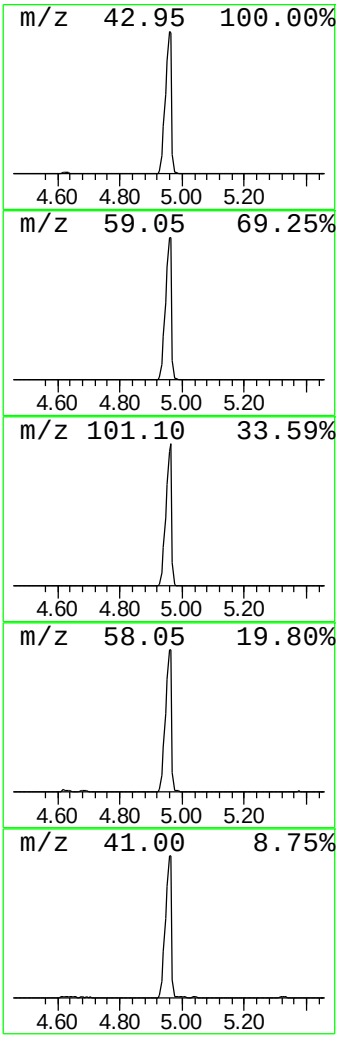
****

Peak Number 1 unknown4.96 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	52.64 ng	3187810	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101319\
Data File : BP000691.D
Acq On : 13 Oct 2019 00:49
Operator : JU
Sample : K5348-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190882-COMPOSITE-N

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

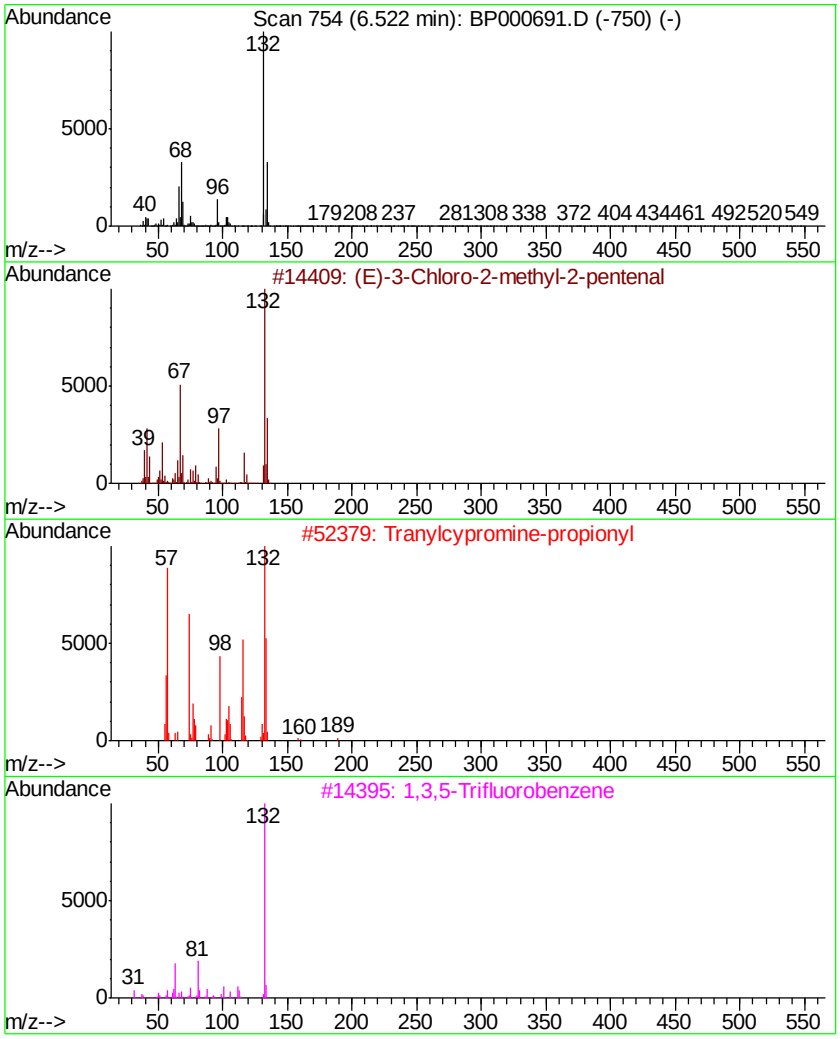
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

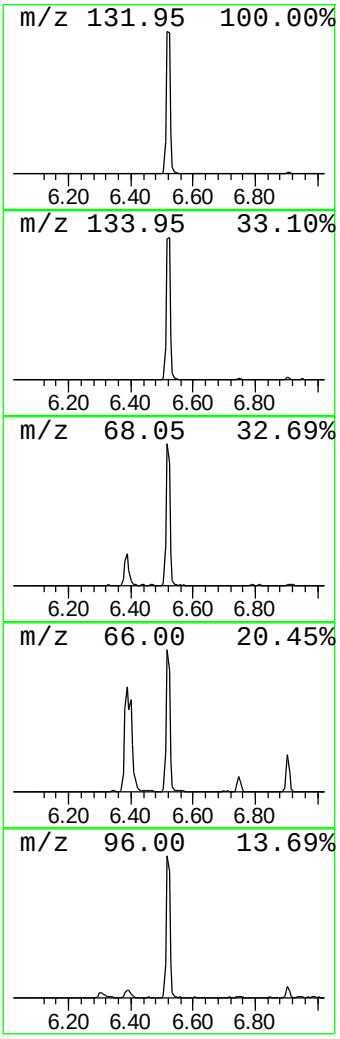
****

Peak Number 2 unknown6.52 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	7.66 ng	463614	1,4-Dichlorobenzene-d4	6.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101319\
Data File : BP000691.D
Acq On : 13 Oct 2019 00:49
Operator : JU
Sample : K5348-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190882-COMPOSITE-N

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

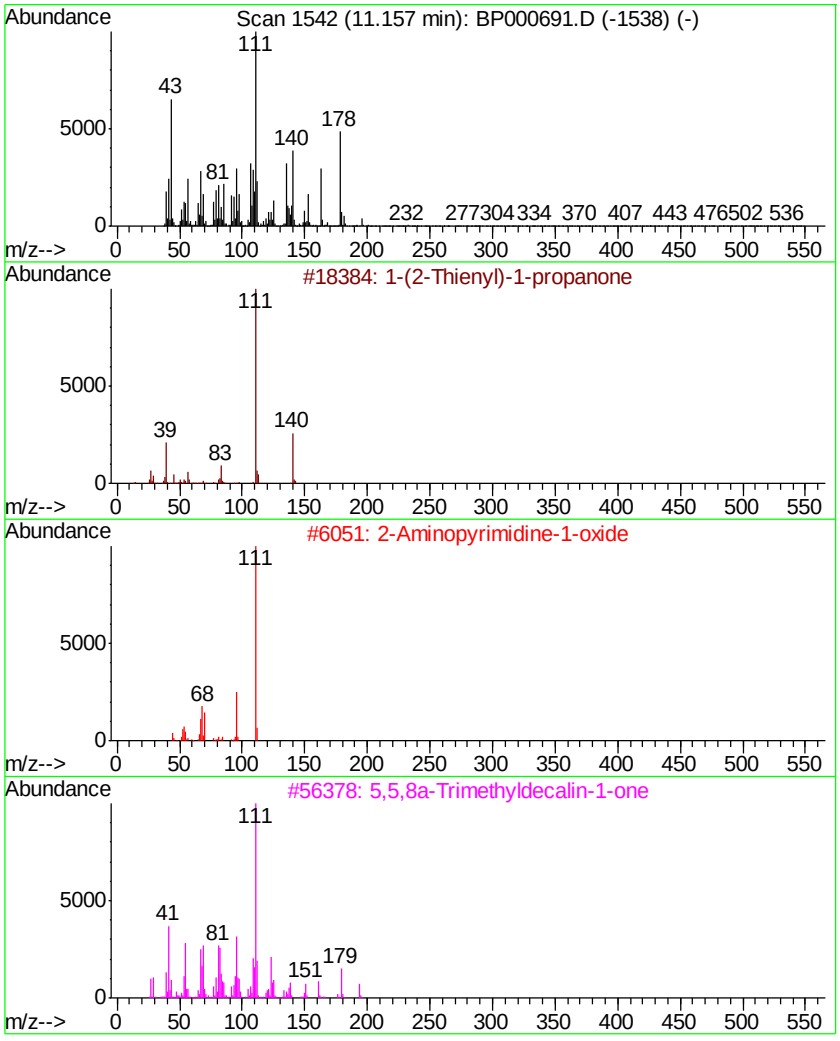
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

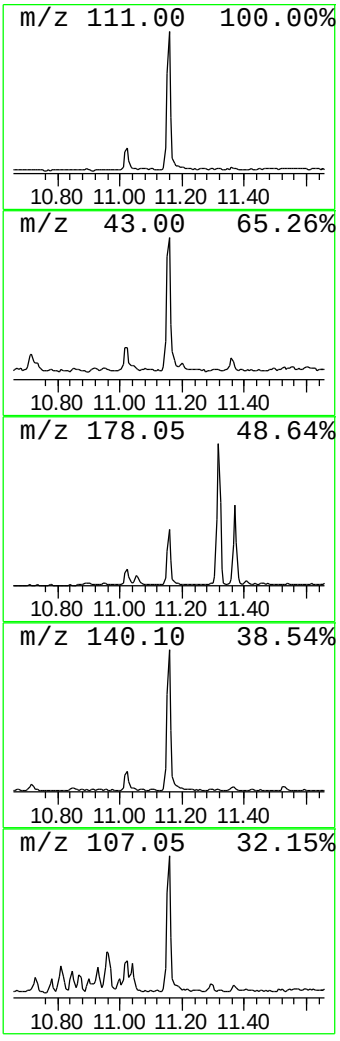
****

Peak Number 4 unknown11.16 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.16	4.16 ng	416516	Phenanthrene-d10	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	27
2	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	25
3	5,5,8a-Trimethyldecalin-1-one	194	C13H22O	1000195-96-1	25
4	Spiro[4.5]decan-6-one	152	C10H16O	013388-94-8	22
5	4-Pyridinol-1-oxide	111	C5H5NO2	006890-62-6	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP101319\
Data File : BP000691.D
Acq On : 13 Oct 2019 00:49
Operator : JU
Sample : K5348-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190882-COMPOSITE-N

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

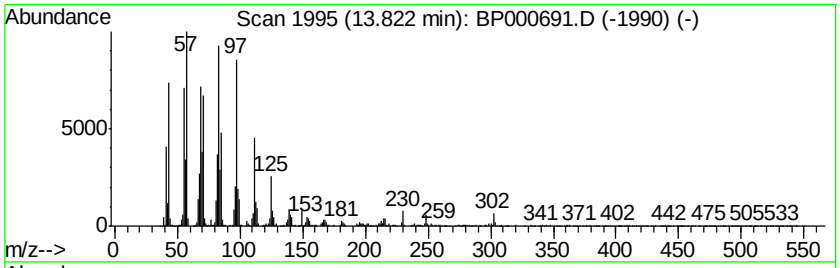
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

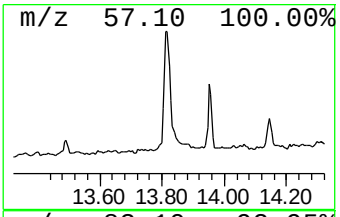
****

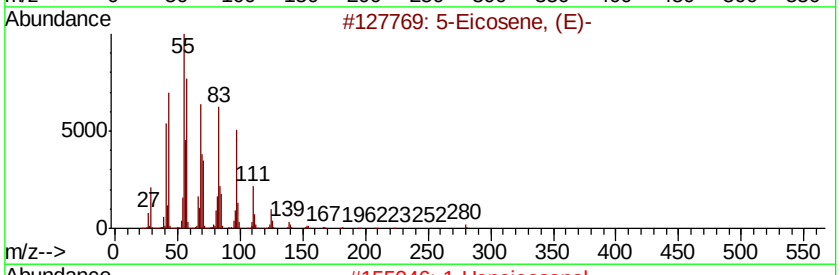
Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

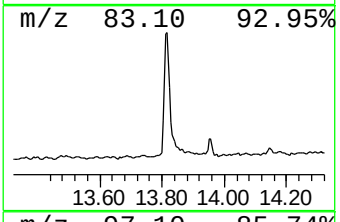
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	4.86 ng	583659	Chrysene-d12	13.96

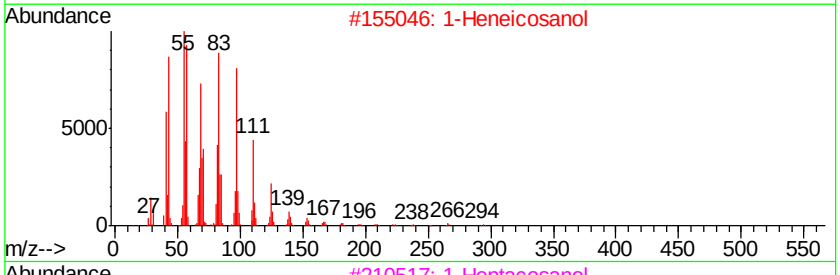
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94

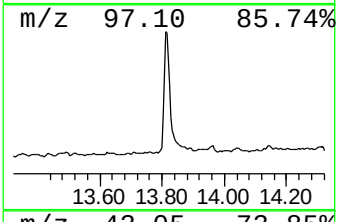


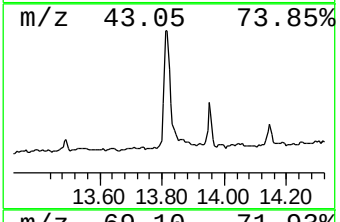


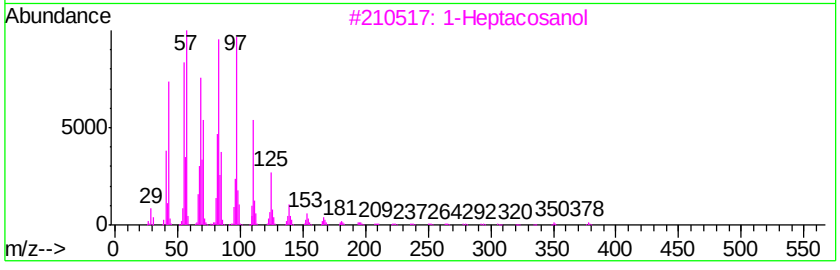


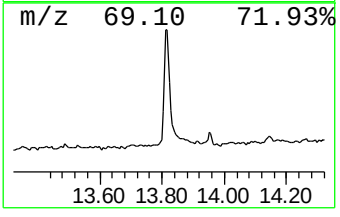












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP101319\
Data File : BP000691.D
Acq On : 13 Oct 2019 00:49
Operator : JU
Sample : K5348-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 20190882-COMPOSITE-N

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
unknown4.96	4.96	52.6	ng	3187810	1	6.75	1211060	20.0
unknown6.52	6.52	7.7	ng	463614	1	6.75	1211060	20.0
unknown11.16	11.16	4.2	ng	416516	4	11.29	2001680	20.0
5-Eicosene, (E)-	13.82	4.9	ng	583659	5	13.96	2401720	20.0