LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041718\
Data File : BM014719.D
Acq On : 17 Apr 2018 12:35
Operator : SJ/JU
Sample : J2313-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A45

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_M\METHODS\SOM-EPA-BM032818MA.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.687	13	17	28	rVB	143801	232013	1.88%	0.185%
2	7.687	690	697	707	rVB2	686984	1160800	9.42%	0.923%
3	7.869	721	728	740	rVB	1774937	2846073	23.09%	2.264%
4	8.087	757	765	773	rBV	1933547	3125063	25.35%	2.486%
5	8.569	839	847	852	rBV	1817119	3017129	24.47%	2.400%
6	8.610	852	854	861	rVB	114141	142693	1.16%	0.114%
7	8.798	879	886	892	rBV	93236	171926	1.39%	0.137%
8	9.263	958	965	976	rBV	1517338	2578015	20.91%	2.051%
9	9.675	1028	1035	1041	rBV	362870	617214	5.01%	0.491%
10	9.751	1041	1048	1065	rVV	2323652	4115076	33.38%	3.273%
11	10.481	1164	1172	1185	rBV	1938458	3272093	26.54%	2.603%
12	11.022	1256	1264	1274	rBV	2781670	4682909	37.99%	3.725%
13	11.298	1304	1311	1323	rVB	302806	530314	4.30%	0.422%
14	11.416	1323	1331	1344	rVB	2619859	4630491	37.56%	3.683%
15	12.639	1533	1539	1545	rVB	140437	219880	1.78%	0.175%
16	13.539	1686	1692	1698	rBV	112162	172200	1.40%	0.137%
17	13.775	1726	1732	1741	rBV2	162355	252562	2.05%	0.201%
18	14.080	1778	1784	1792	rBV	845699	1223076	9.92%	0.973%
19	14.557	1858	1865	1872	rVB	5458030	7393050	59.97%	5.881%
20	14.869	1911	1918	1925	rBV	6239280	9094803	73.77%	7.235%
21	15.169	1963	1969	1975	rVB2	3830753	5965908	48.39%	4.746%
22	15.222	1975	1978	1985	rVB	114600	152106	1.23%	0.121%
23	15.322	1989	1995	2004	rBV	499228	734126	5.95%	0.584%
24	15.810	2071	2078	2084	rBV	230646	331905	2.69%	0.264%
25	15.916	2091	2096	2105	rVB2	111546	185010	1.50%	0.147%
26	16.145	2127	2135	2142	rBV	7229840	10988262	89.13%	8.741%
27	16.239	2144	2151	2162	rBV	2517242	3401360	27.59%	2.706%
28	16.380	2169	2175	2183	rVB	93741	144506	1.17%	0.115%
29	17.880	2423	2430	2437	rBV	4713185	6892891	55.91%	5.483%
30	17.974	2439	2446	2457	rBV2	8072264	11581603	93.95%	9.213%
31	18.504	2530	2536	2543	rBV	1532200	1924182	15.61%	1.531%
32	18.698	2566	2569	2577	rVB	130512	163419	1.33%	0.130%
33	19.851	2761	2765	2770	rVB	98476	138373	1.12%	0.110%
34	19.939	2776	2780	2787	rBV2	114783	170429	1.38%	0.136%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041718\
Data File : BM014719.D
Acq On : 17 Apr 2018 12:35
Operator : SJ/JU
Sample : J2313-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A45

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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_M\METHODS\SOM-EPA-BM032818MA.M
Title : SVOA CALIBRATION

35	20.098	2803	2807	2812	rBV	83986	124319	1.01%	0.099%
36	20.209	2820	2826	2834	rBV2	9017845	12328052	100.00%	9.806%
37	21.962	3119	3124	3131	rBV	4952135	6466695	52.46%	5.144%
38	24.315	3516	3524	3536	rVB2	4272001	9366157	75.97%	7.450%
39	24.474	3544	3551	3562	rVB	2533284	5176686	41.99%	4.118%

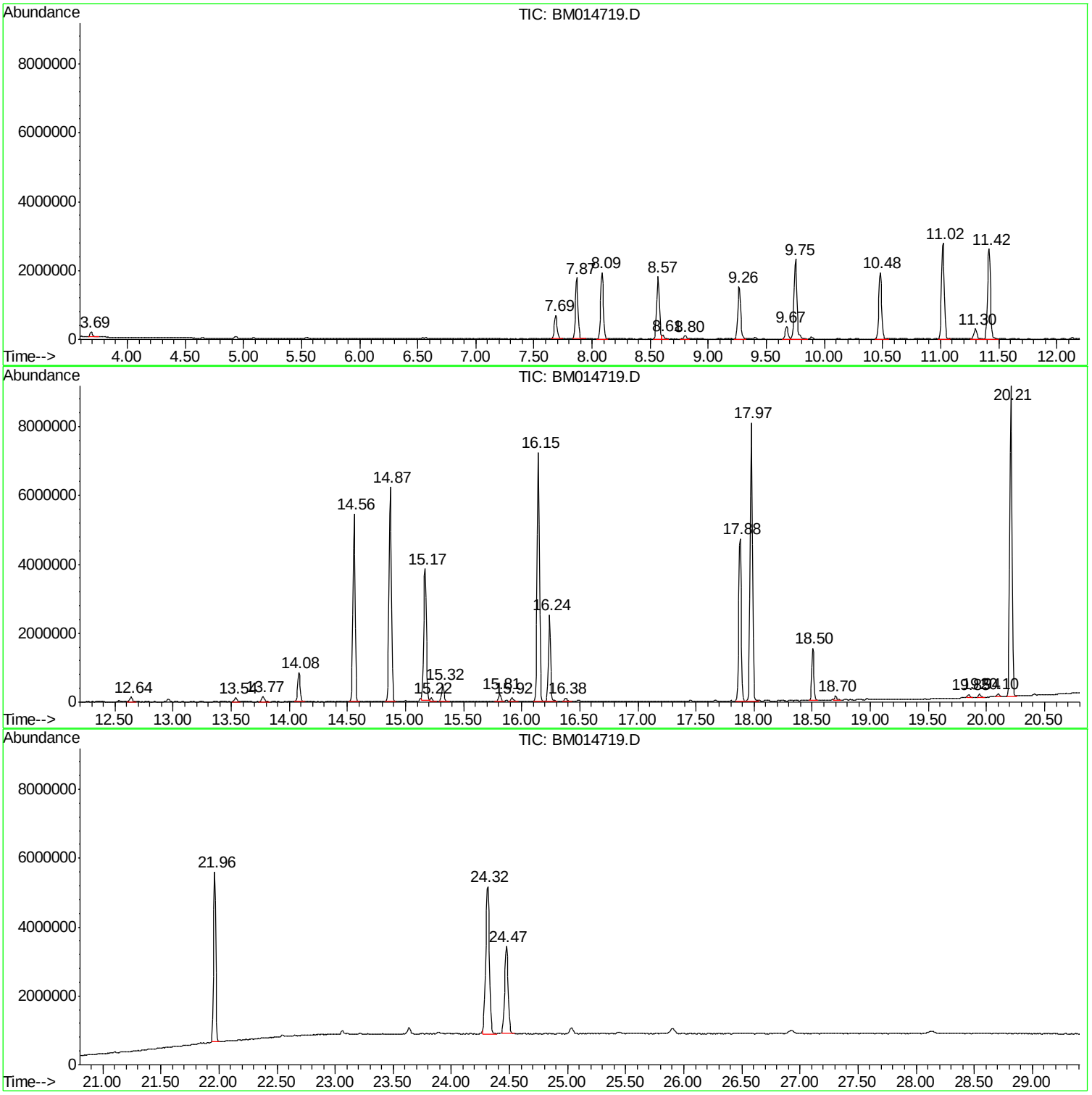
Sum of corrected areas: 125713369

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041718\
Data File : BM014719.D
Acq On : 17 Apr 2018 12:35
Operator : SJ/JU
Sample : J2313-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
F1A45

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041718\
Data File : BM014719.D
Acq On : 17 Apr 2018 12:35
Operator : SJ/JU
Sample : J2313-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A45

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

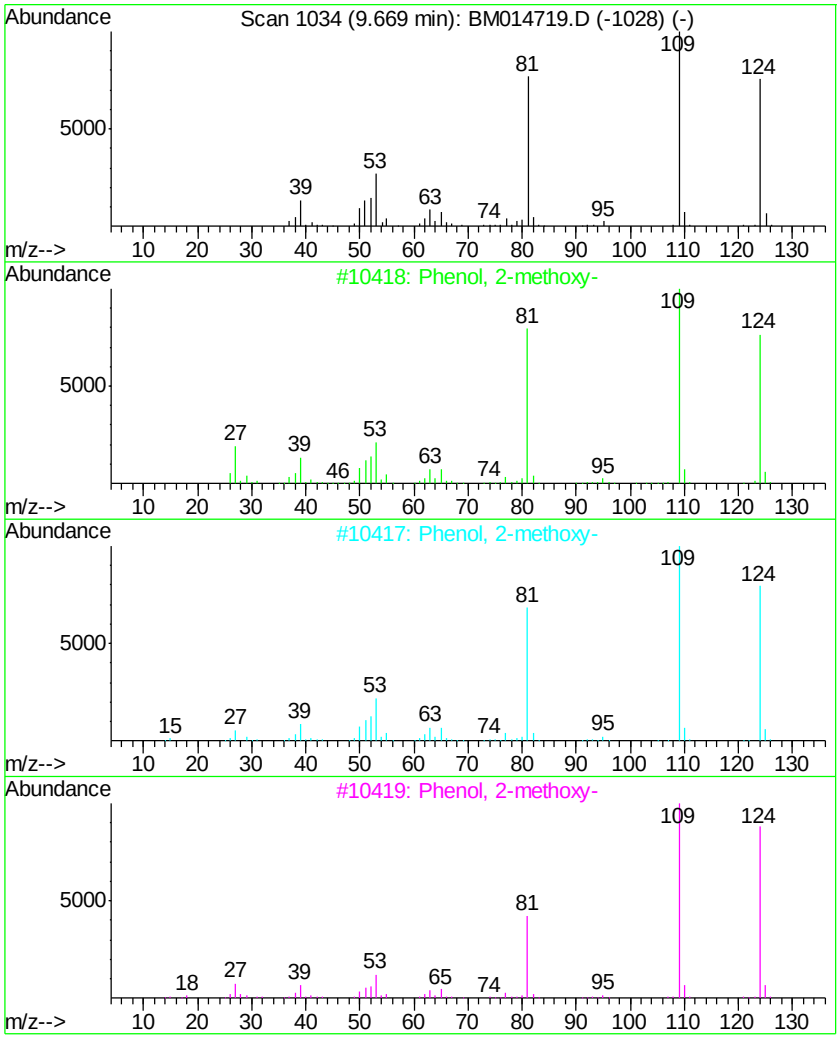
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

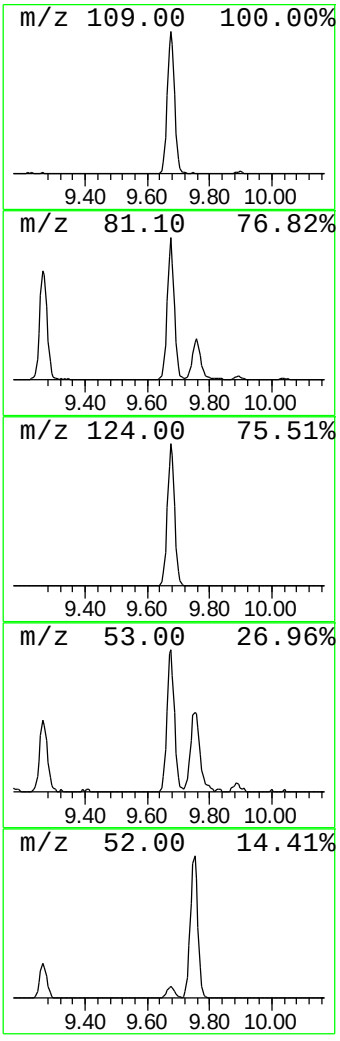
****

Peak Number 1 Phenol, 2-methoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.67	4.09 ng/ul	617214	1,4-Dichlorobenzene-d4	8.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	97
2	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	96
3	Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	95
4	Mequinol	124	C7H8O2	000150-76-5	91
5	Mequinol	124	C7H8O2	000150-76-5	90





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041718\
Data File : BM014719.D
Acq On : 17 Apr 2018 12:35
Operator : SJ/JU
Sample : J2313-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A45

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

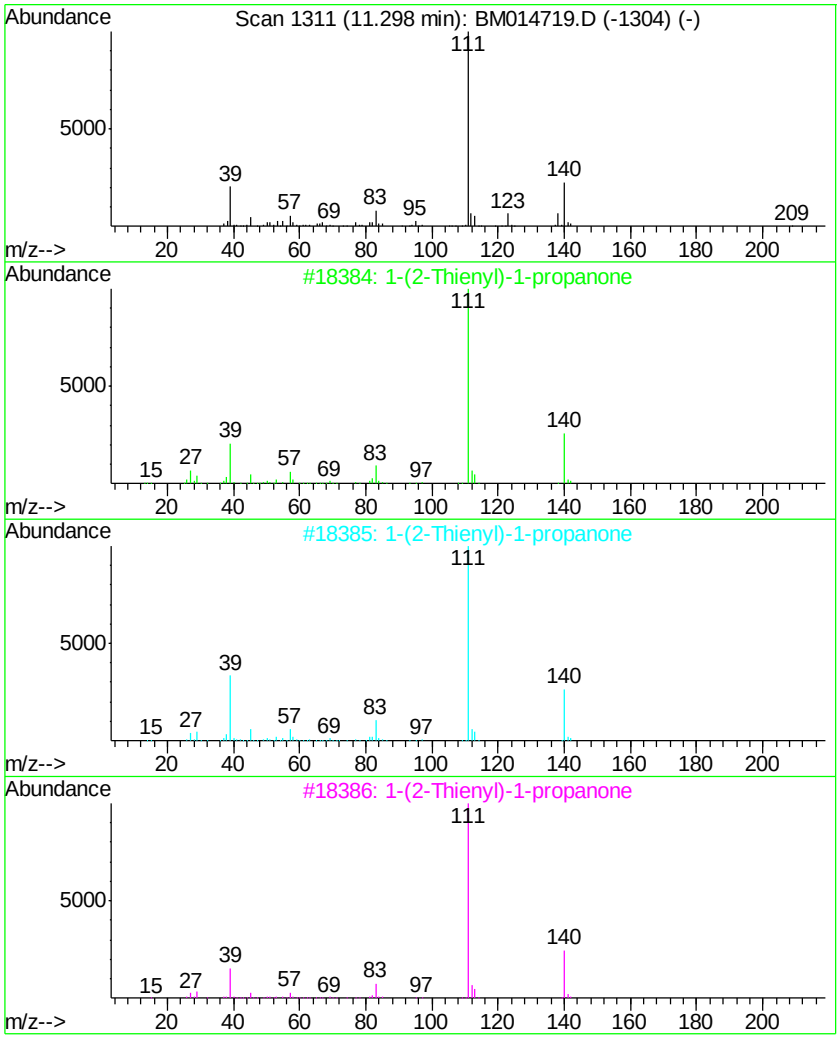
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

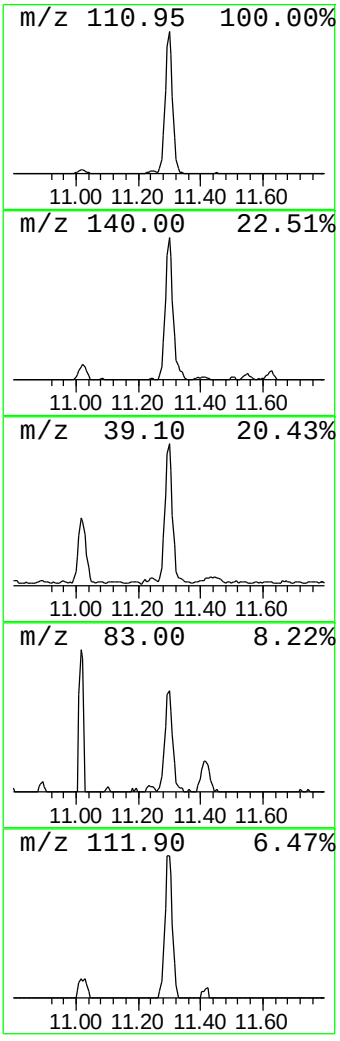
****

Peak Number 2 1-(2-Thienyl)-1-propanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.30	2.29 ng/ul	530314	Naphthalene-d8	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	93
2	1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	93
3	1-(2-Thienyl)-1-propanone	140	C7H8OS	013679-75-9	80
4	Thiophene, 2-methyl-5-propyl-	140	C8H12S	033933-73-2	78
5	Glycine, N-(2-thienylcarbonyl)-,...	199	C8H9NO3S	1000299-60-2	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041718\
Data File : BM014719.D
Acq On : 17 Apr 2018 12:35
Operator : SJ/JU
Sample : J2313-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A45

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

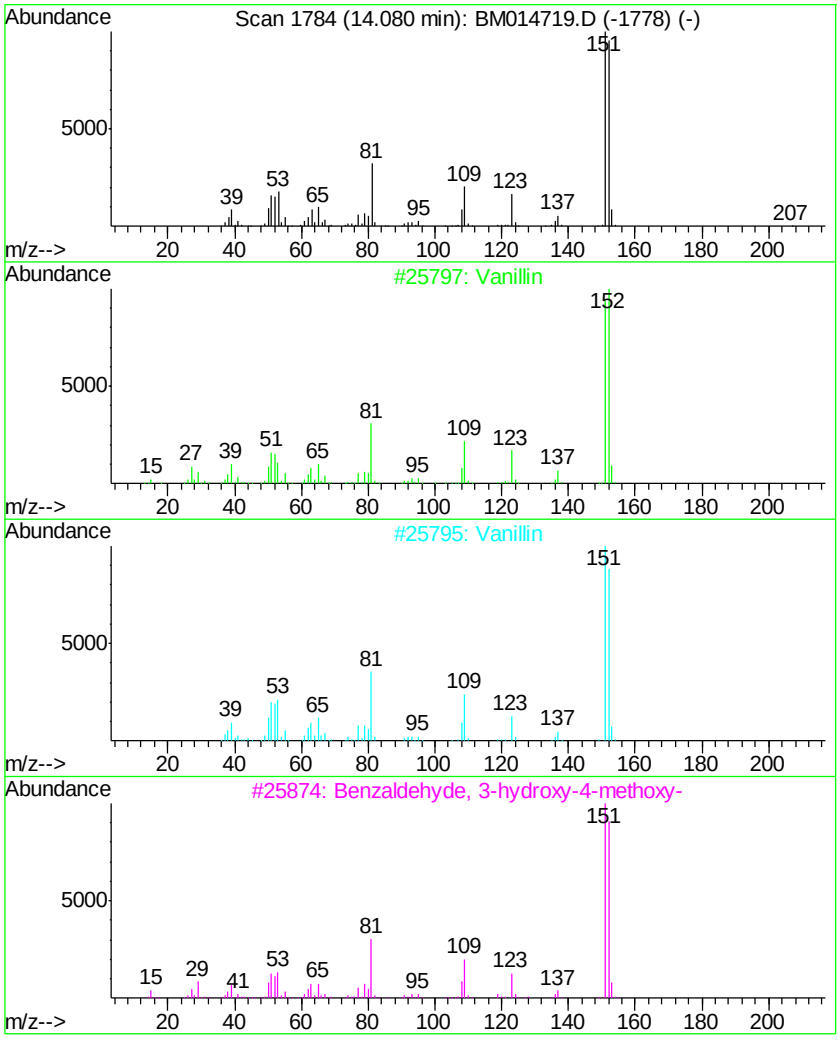
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

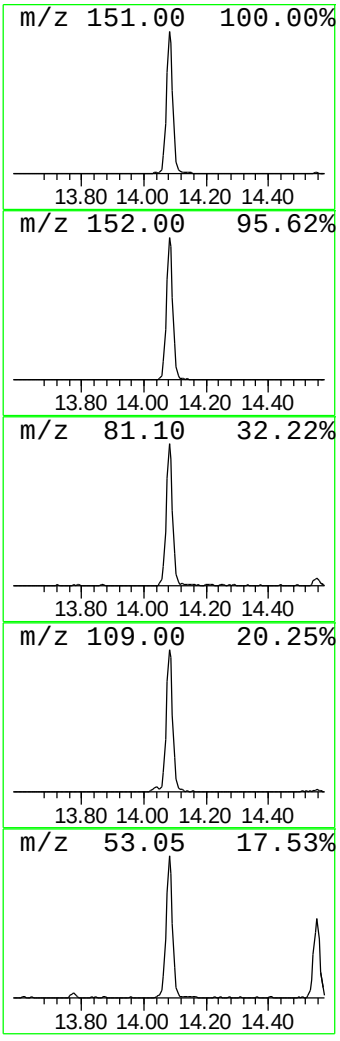
****

Peak Number 3 Vanillin Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	4.10 ng/ul	1223080	Acenaphthene-d10	15.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Vanillin	152	C8H8O3	000121-33-5	97
2	Vanillin	152	C8H8O3	000121-33-5	97
3	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	000621-59-0	97
4	Vanillin	152	C8H8O3	000121-33-5	97
5	Vanillin	152	C8H8O3	000121-33-5	95





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM041718\
Data File : BM014719.D
Acq On : 17 Apr 2018 12:35
Operator : SJ/JU
Sample : J2313-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A45

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA CALIBRATION

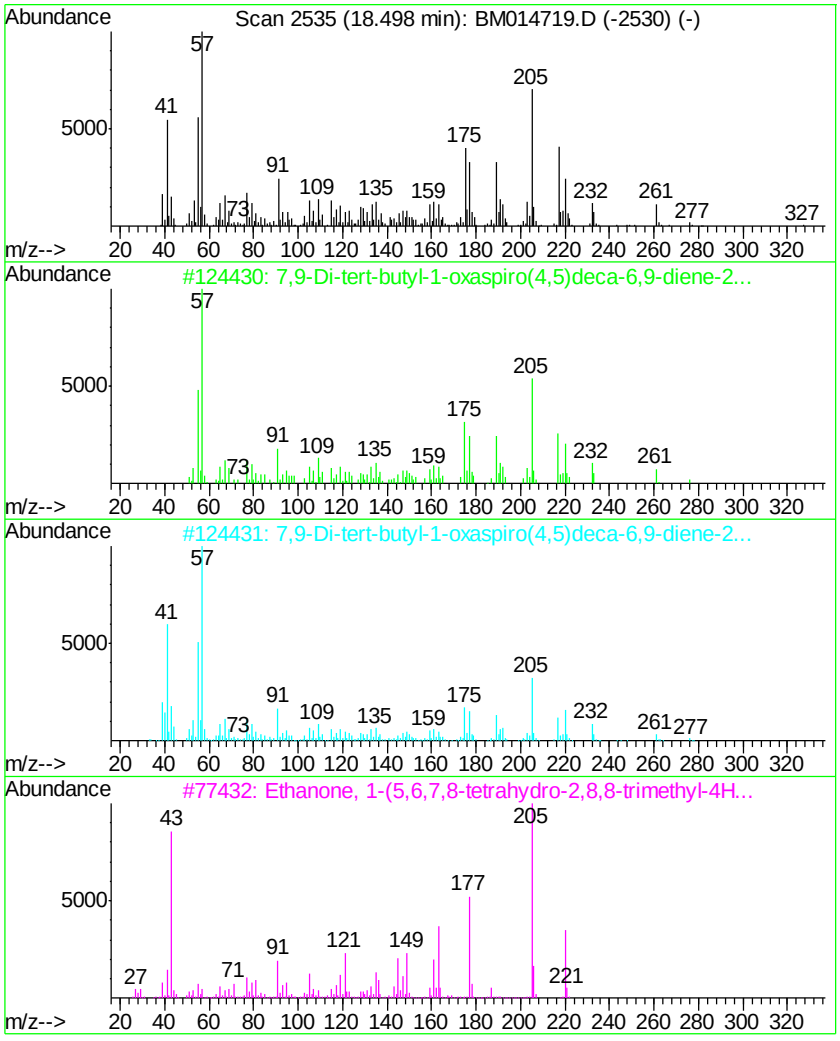
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

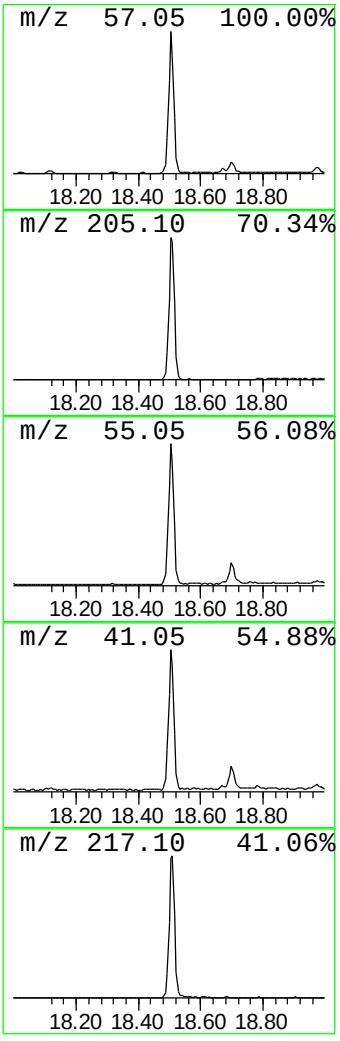
****

Peak Number 4 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	5.58 ng/ul	1924180	Phenanthrene-d10	17.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	99
2	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	97
3	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	46
4	Tricyclo[5.2.2.0(1,6)]undecan-3-...	220	C15H24O	1000159-37-6	43
5	3H-Cyclopenta[1,3]cyclopropa[1,2...	220	C14H20O2	066708-18-7	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM041718\
Data File : BM014719.D
Acq On : 17 Apr 2018 12:35
Operator : SJ/JU
Sample : J2313-19
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : F1A45

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM-EPA-BM032818MA.M
Quant Title : SVOA 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
Phenol, 2-methoxy-	9.67	4.1	ng/ul	617214	1	8.57	3017130	20.0
1-(2-Thienyl)-1-p...	11.30	2.3	ng/ul	530314	2	11.42	4630490	20.0
Vanillin	14.08	4.1	ng/ul	1223080	3	15.17	5965910	20.0
7,9-Di-tert-butyl...	18.50	5.6	ng/ul	1924180	4	17.88	6892890	20.0