LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF36DL

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Title : SVOA CALIBRATION

Signal : TIC: BM043732.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.822	105	108	119	rVV	53002	105220	1.48%	0.224%
2	3.904	119	122	127	rVB	34798	43595	0.61%	0.093%
3	5.051	313	317	321	rBV	15808	19729	0.28%	0.042%
4	6.457	545	556	560	rBV3	20463	35697	0.50%	0.076%
5	6.622	579	584	589	rVB3	20053	33426	0.47%	0.071%
6	6.987	642	646	650	rBV7	5404	7653	0.11%	0.016%
7	7.151	667	674	685	rVV	112748	211102	2.97%	0.450%
8	7.245	685	690	695	rVV	34631	49723	0.70%	0.106%
9	7.304	695	700	709	rVB	100539	163857	2.31%	0.349%
10	7.498	727	733	741	rVB	133491	217881	3.07%	0.464%
11	7.716	767	770	774	rBV6	5489	7133	0.10%	0.015%
12	7.839	786	791	796	rVB8	11888	21691	0.31%	0.046%
13	7.963	805	812	822	rBV	1109907	1804657	25.42%	3.844%
14	8.169	842	847	853	rVB9	13578	20874	0.29%	0.044%
15	8.622	923	924	929	rVB5	12535	11915	0.17%	0.025%
16	8.698	929	937	946	rBV	108233	208994	2.94%	0.445%
17	9.145	1006	1013	1021	rBV	107354	195079	2.75%	0.416%
18	9.751	1110	1116	1123	rBV	13555	32925	0.46%	0.070%
19	9.863	1129	1135	1144	rBV	84293	156192	2.20%	0.333%
20	10.292	1202	1208	1210	rBV7	4489	7442	0.10%	0.016%
21	10.416	1220	1229	1238	rBV	99455	231769	3.26%	0.494%
22	10.639	1265	1267	1273	rVB7	6806	10930	0.15%	0.023%
23	10.775	1282	1290	1304	rBV	1395916	2420551	34.10%	5.156%
24	10.945	1314	1319	1327	rVB2	20019	42336	0.60%	0.090%
25	11.486	1409	1411	1415	rVB5	6199	7280	0.10%	0.016%
26	11.586	1423	1428	1432	rBV7	9993	22458	0.32%	0.048%
27	11.863	1472	1475	1480	rVB6	6854	12157	0.17%	0.026%
28	12.557	1589	1593	1596	rBV6	5725	9430	0.13%	0.020%
29	12.957	1656	1661	1662	rBV5	9739	11544	0.16%	0.025%
30	13.098	1680	1685	1692	rBV3	42902	70839	1.00%	0.151%
31	13.280	1711	1716	1719	rBV6	19387	29135	0.41%	0.062%
32	13.327	1721	1724	1726	rVV4	13495	16842	0.24%	0.036%
33	13.374	1727	1732	1740	rVB	100721	158579	2.23%	0.338%
34	13.439	1741	1743	1746	rVV4	12904	18640	0.26%	0.040%
35	13.498	1749	1753	1758	rVB2	53820	83924	1.18%	0.179%
36	13.598	1765	1770	1776	rBV	172685	271765	3.83%	0.579%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : GCF36DL

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Title : SVOA CALIBRATION

37	13.733	1787	1793	1797	rBV4	116691	212217	2.99%	0.452%
38	13.780	1797	1801	1807	rVB3	64732	115336	1.62%	0.246%
39	13.863	1808	1815	1819	rBV	1658893	2504866	35.28%	5.336%
40	13.904	1819	1822	1832	rVB2	302336	507276	7.15%	1.081%
41	14.021	1837	1842	1849	rVV	274095	514568	7.25%	1.096%
42	14.110	1853	1857	1866	rVB2	140480	229565	3.23%	0.489%
43	14.304	1884	1890	1898	rBV	277761	487580	6.87%	1.039%
44	14.410	1904	1908	1916	rVV2	283788	451374	6.36%	0.961%
45	14.486	1916	1921	1926	rVB	523610	723036	10.18%	1.540%
46	14.604	1935	1941	1947	rBV	2077545	3222891	45.40%	6.865%
47	14.657	1947	1950	1956	rVB2	130637	194610	2.74%	0.415%
48	14.745	1961	1965	1969	rVB2	113922	143355	2.02%	0.305%
49	14.851	1978	1983	1990	rBV3	159473	348049	4.90%	0.741%
50	14.963	1998	2002	2005	rBV2	44910	66066	0.93%	0.141%
51	15.051	2014	2017	2025	rVB2	165492	273410	3.85%	0.582%
52	15.151	2030	2034	2039	rVB3	94757	140861	1.98%	0.300%
53	15.210	2041	2044	2045	rBV3	38816	43191	0.61%	0.092%
54	15.239	2046	2049	2053	rVB	88752	124066	1.75%	0.264%
55	15.598	2105	2110	2116	rBV	374299	568413	8.01%	1.211%
56	15.880	2153	2158	2165	rVB	869188	1240734	17.48%	2.643%
57	16.086	2190	2193	2198	rVB2	119571	140622	1.98%	0.300%
58	17.004	2344	2349	2359	rBV	4608821	7099418	100.00%	15.122%
59	17.092	2361	2364	2368	rVB3	127450	189567	2.67%	0.404%
60	17.356	2403	2409	2420	rBV	2626541	3976544	56.01%	8.470%
61	17.451	2422	2425	2429	rBV	367350	505819	7.12%	1.077%
62	19.209	2721	2724	2728	rVB2	306312	336336	4.74%	0.716%
63	19.745	2812	2815	2820	rVB	509386	622049	8.76%	1.325%
64	20.621	2959	2964	2968	rBV	4288558	5419964	76.34%	11.545%
65	20.662	2968	2971	2980	rVB3	820051	1311808	18.48%	2.794%
66	21.539	3116	3120	3128	rVB	3033266	4036222	56.85%	8.597%
67	23.968	3528	3533	3542	rVB	2221573	4424214	62.32%	9.424%

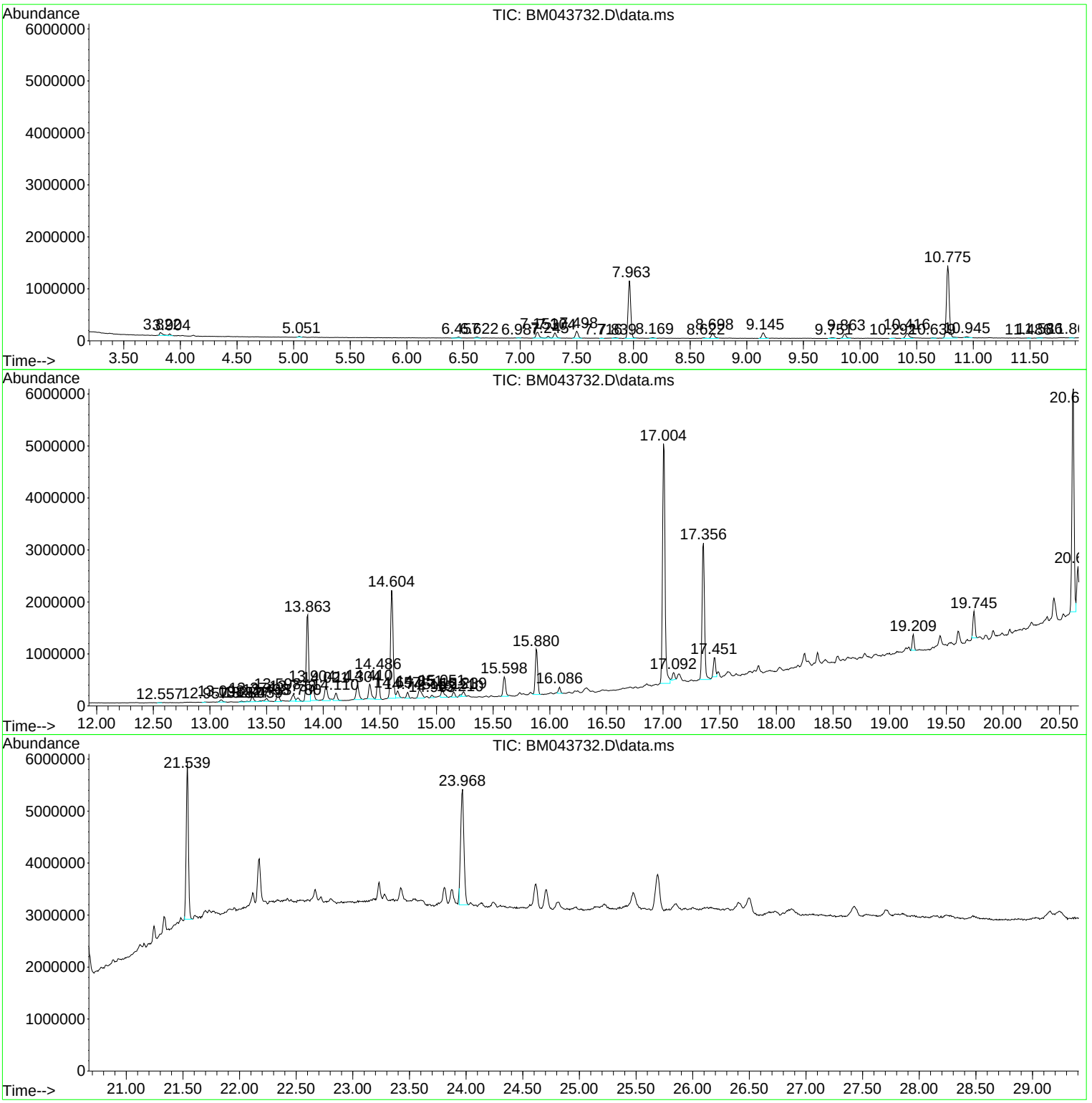
Sum of corrected areas: 46946991

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF36DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
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Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

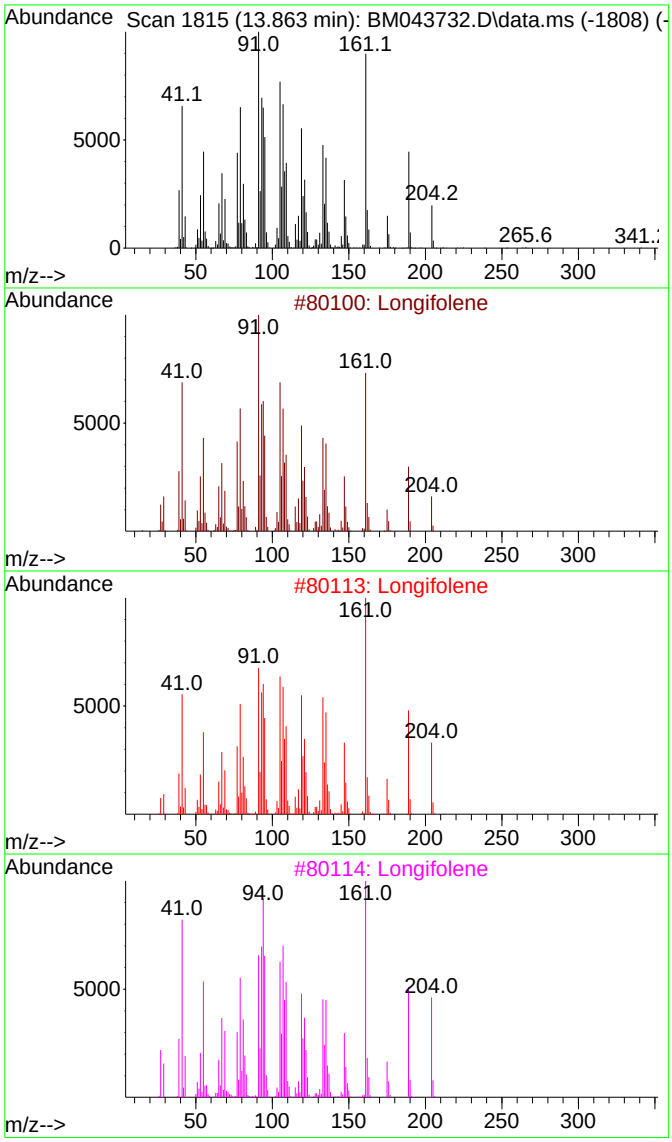
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

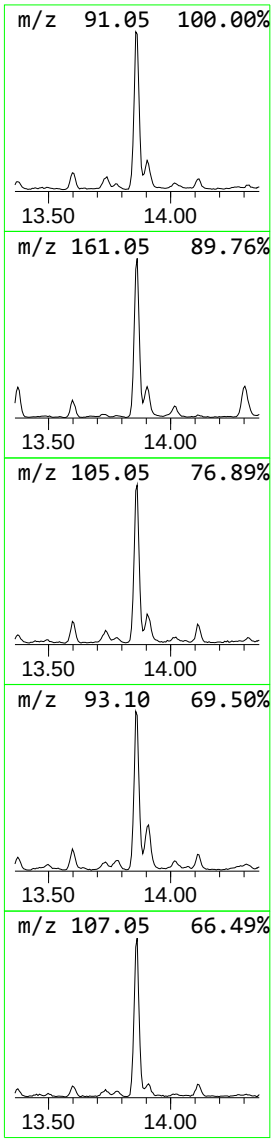
****

Peak Number 1 Longifolene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.863	15.54 ng/ul	2504870	Acenaphthene-d10	14.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Longifolene	204	C15H24	000475-20-7	99
2	Longifolene	204	C15H24	000475-20-7	99
3	Longifolene	204	C15H24	000475-20-7	99
4	Longifolene	204	C15H24	000475-20-7	96
5	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF36DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

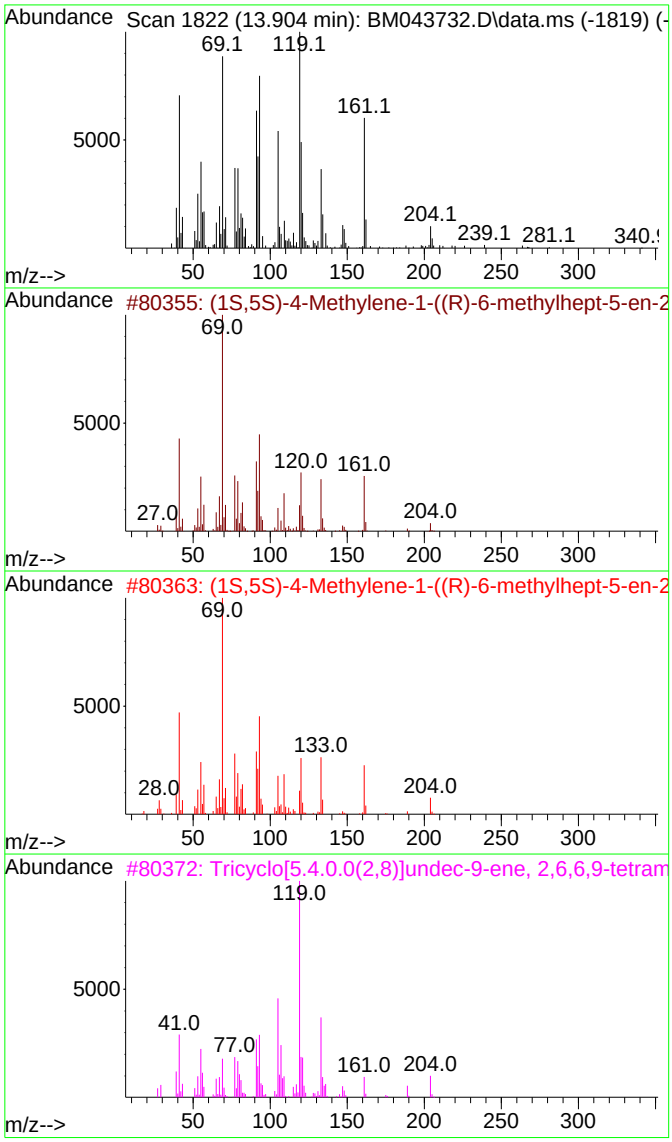
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

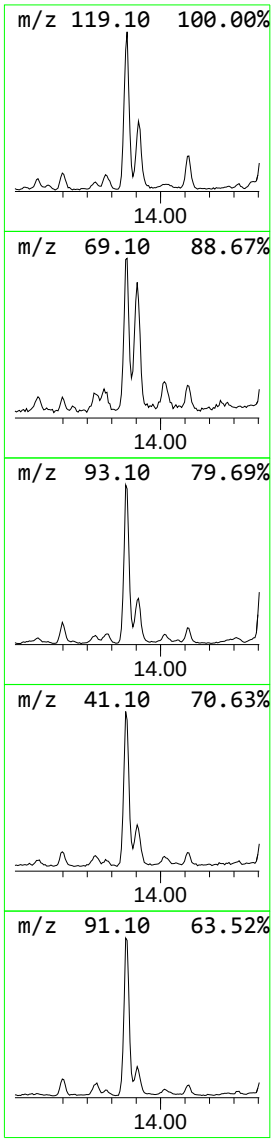
****

Peak Number 2 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	3.15 ng/ul	507276	Acenaphthene-d10	14.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1S,5S)-4-Methylene-1-((R)-6-met...	204	C15H24	058319-04-3	45
2	(1S,5S)-4-Methylene-1-((R)-6-met...	204	C15H24	058319-04-3	43
3	Tricyclo[5.4.0.0(2,8)]undec-9-en...	204	C15H24	005989-08-2	42
4	(1S,5S)-2-Methyl-5-((R)-6-methyl...	204	C15H24	159407-35-9	38
5	1,3-Cyclohexadiene, 5-(1,5-dimet...	204	C15H24	000495-60-3	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF36DL

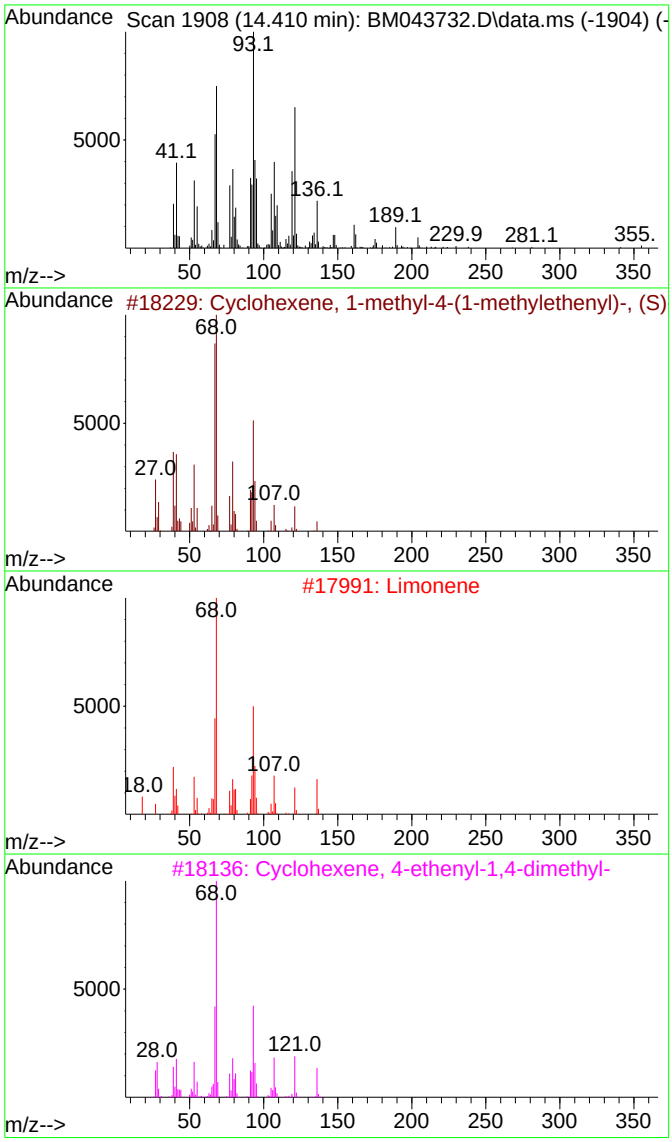
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

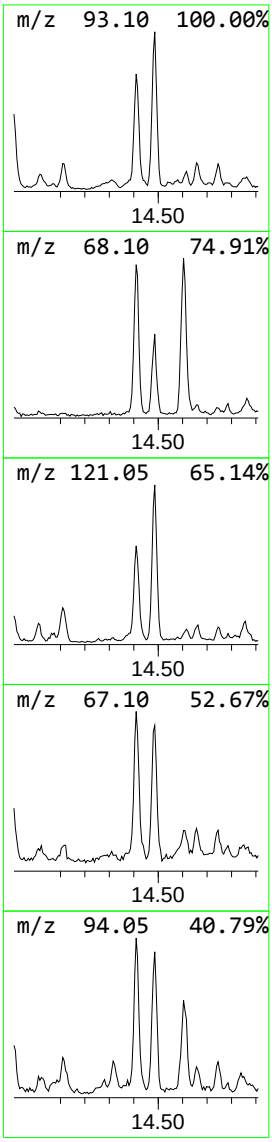
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.410	2.80 ng/ul	451374	Acenaphthene-d10	14.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	87
2	Limonene	136	C10H16	000138-86-3	81
3	Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	81
4	8-Isopropenyl-1,5-dimethyl-cyclo...	204	C15H24	1000193-62-7	60
5	Camphene	136	C10H16	000079-92-5	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF36DL

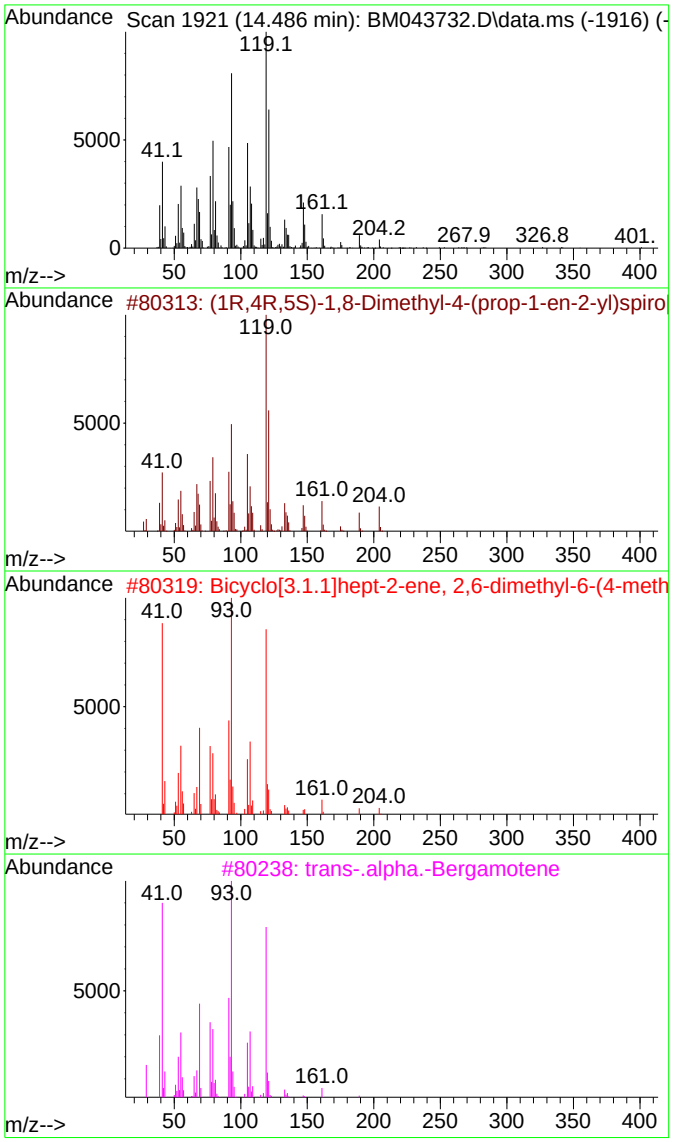
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

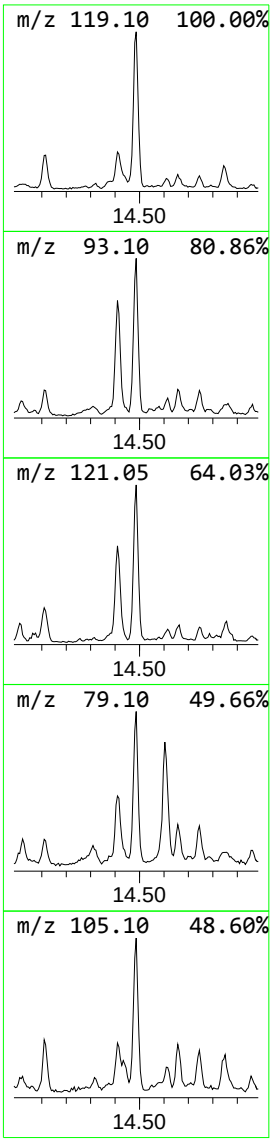
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (1R,4R,5S)-1,8-Dimethyl-4-(... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	4.49 ng/ul	723036	Acenaphthene-d10	14.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R,4R,5S)-1,8-Dimethyl-4-(prop-...	204	C15H24	729602-94-2	95
2	Bicyclo[3.1.1]hept-2-ene, 2,6-di...	204	C15H24	017699-05-7	76
3	trans-.alpha.-Bergamotene	204	C15H24	013474-59-4	64
4	cis-.alpha.-Bergamotene	204	C15H24	018252-46-5	64
5	(1R,4S,5S)-1,8-Dimethyl-4-(prop-...	204	C15H24	043219-80-3	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF36DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

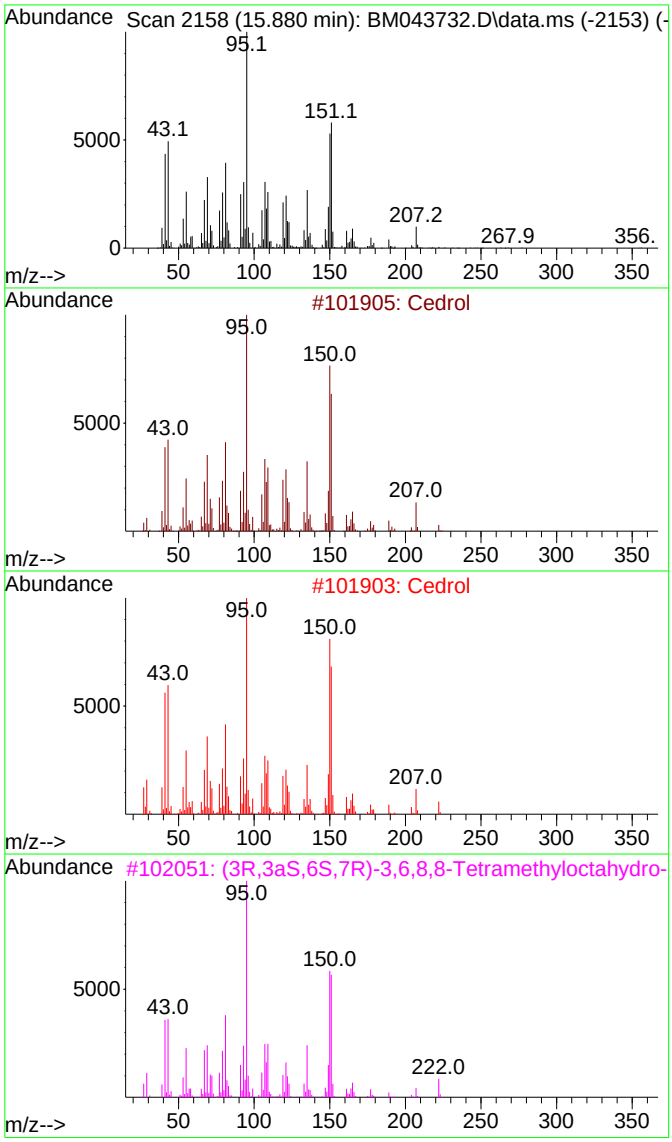
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

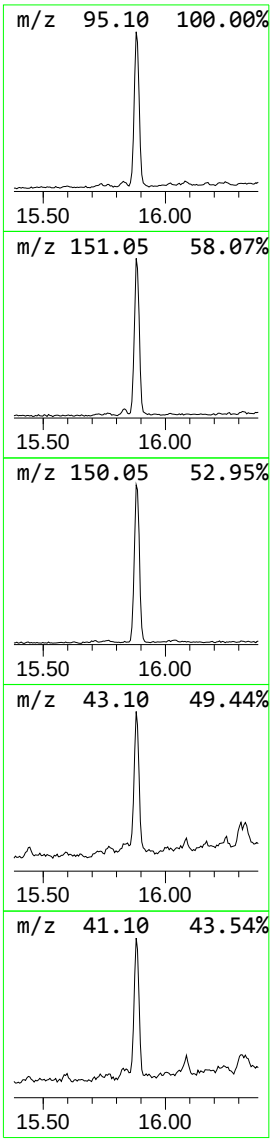
****

Peak Number 5 Cedrol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.880	7.70 ng/ul	1240730	Acenaphthene-d10	14.604

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cedrol	222	C15H26O	000077-53-2	91
2	Cedrol	222	C15H26O	000077-53-2	83
3	(3R,3aS,6S,7R)-3,6,8,8-Tetrameth...	222	C15H26O	019903-73-2	80
4	Cedrol	222	C15H26O	000077-53-2	78
5	(3R,3aS,6S,7R)-3,6,8,8-Tetrameth...	222	C15H26O	019903-73-2	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF36DL

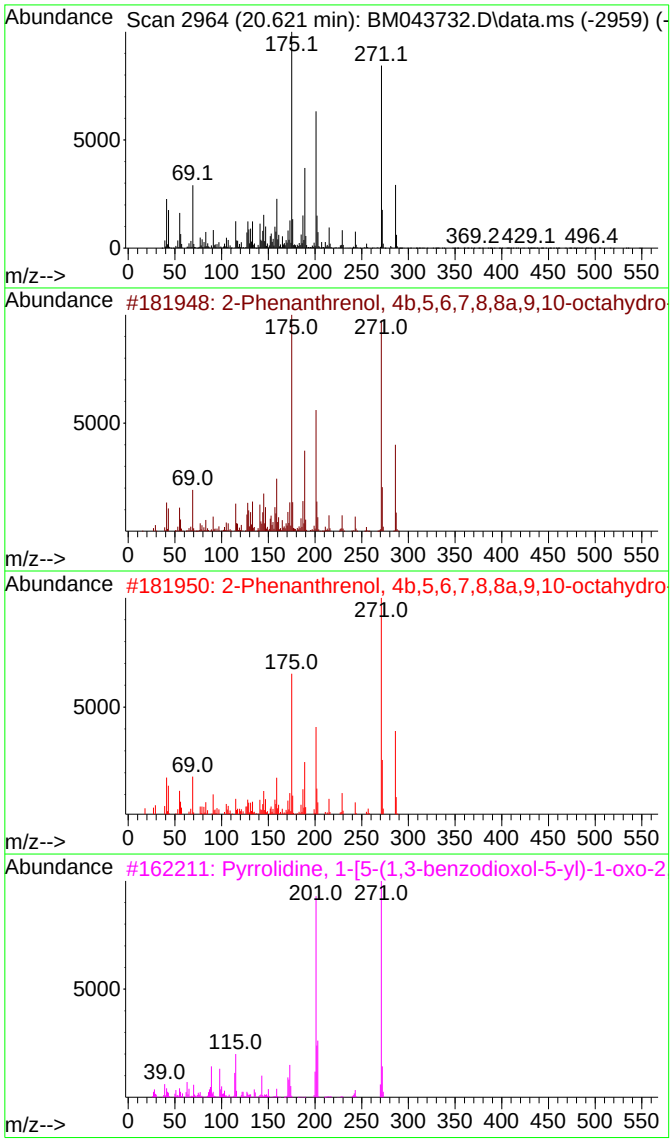
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

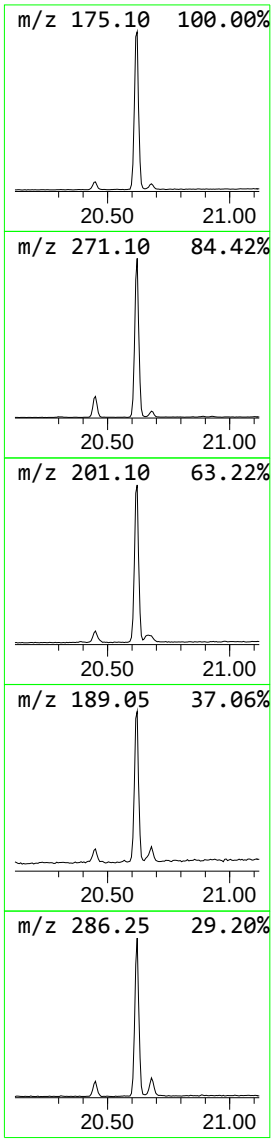
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Phenanthrenol, 4b,5,6,7,8... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.621	26.86 ng/ul	5419960	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	99
2	2-Phenanthrenol, 4b,5,6,7,8,8a,9...	286	C20H30O	000511-15-9	95
3	Pyrrolidine, 1-[5-(1,3-benzodiox...	271	C16H17NO3	025924-78-1	41
4	1-Methyl-3-phenyl-4-azafluorenone	271	C19H13NO	069751-55-9	22
5	Desomorphine	271	C17H21NO2	000427-00-9	20





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF36DL

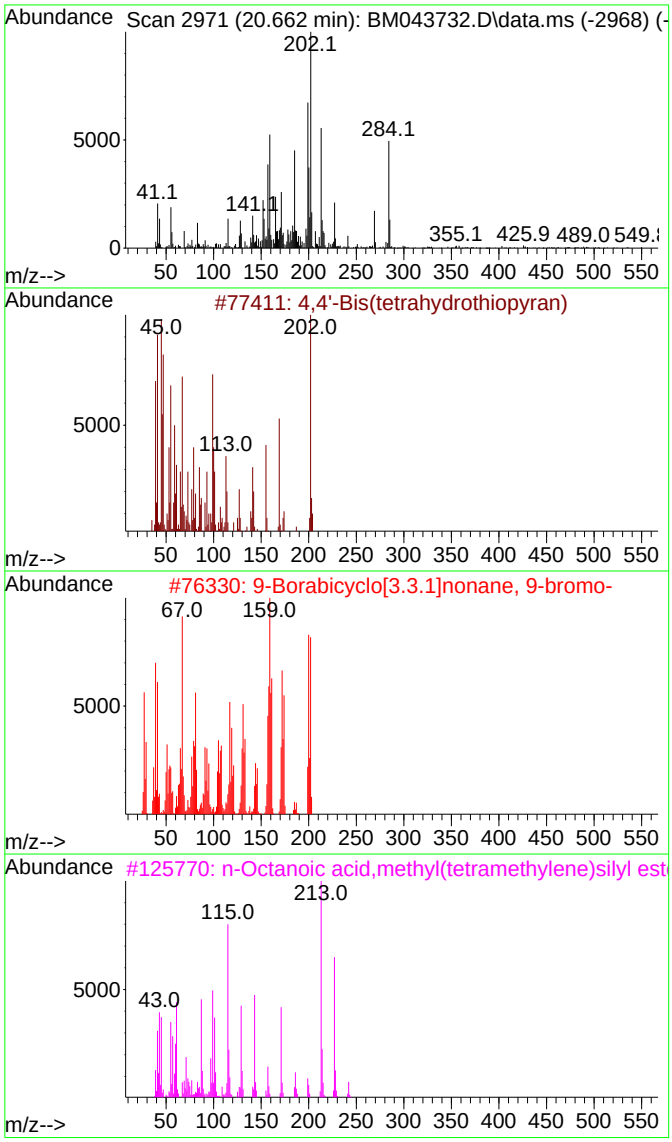
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

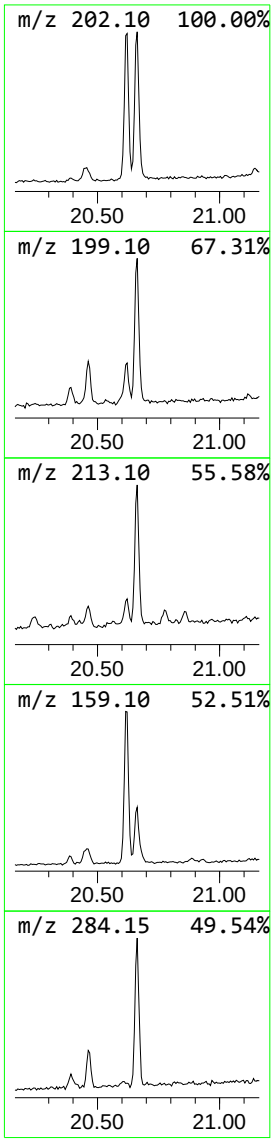
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.662	6.50 ng/ul	1311810	Chrysene-d12	21.539

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	90
2	9-Borabicyclo[3.3.1]nonane, 9-br...	200	C8H14BBr	022086-45-9	70
3	n-Octanoic acid,methyl(tetrameth...	242	C13H26O2Si	1010217-03-7	53
4	3-Methoxy-5-naphthoic acid	202	C12H10O3	007498-58-0	41
5	4-Carbamoyl-3-methoxyquinoline	202	C11H10N2O2	020844-05-7	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM010224\
Data File : BM043732.D
Acq On : 03 Jan 2024 14:31
Operator : MA/JU
Sample : 05919-02DL 5X
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
GCF36DL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\SFAM-EPA-BM121523.MA.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Longifolene	13.863	15.5	ng/ul	2504870	3	14.604	3222890	20.0
unknown-01	13.904	3.1	ng/ul	507276	3	14.604	3222890	20.0
Cyclohexene, 1-...	14.410	2.8	ng/ul	451374	3	14.604	3222890	20.0
(1R,4R,5S)-1,8-...	14.486	4.5	ng/ul	723036	3	14.604	3222890	20.0
Cedrol	15.880	7.7	ng/ul	1240730	3	14.604	3222890	20.0
2-Phenanthrenol...	20.621	26.9	ng/ul	5419960	5	21.539	4036220	20.0
4,4'-Bis(tetrah...	20.662	6.5	ng/ul	1311810	5	21.539	4036220	20.0